Full wwPDB EM Validation Report (i)

Aug 30, 2023 – 12:47 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 (i) 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 (i)) were used in the production of this report:

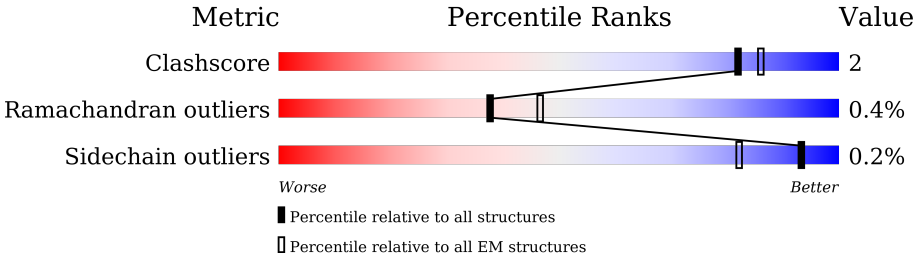
EMDB validation analysis	:	0.0.1.dev50
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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

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

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

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

- Molecule 2 is a protein called MCPv1.

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

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

- Molecule 3 is a protein called MCPv2.

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

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

- Molecule 5 is a protein called MCPv4.

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

- Molecule 6 is a protein called P1v1.

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

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
			Total	C	N	O	S		
7	bH	424	3258	2015	591	642	10	0	0

- Molecule 8 is a protein called P3.

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

- Molecule 9 is a protein called P4.

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

- Molecule 10 is a protein called P5.

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

- Molecule 11 is a protein called P6.

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

- Molecule 12 is a protein called P8.

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

- Molecule 13 is a protein called P9.

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

- Molecule 14 is a protein called P11.

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

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

- Molecule 15 is a protein called P12.

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

- Molecule 16 is a protein called P13.

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

- Molecule 17 is a protein called P15.

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

- Molecule 18 is a protein called P16.

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

- Molecule 19 is a protein called P17.

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

- Molecule 20 is a protein called P18.

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

- Molecule 21 is a protein called P19.

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

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

- Molecule 22 is a protein called P20.

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

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

- Molecule 23 is a protein called P21.

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

- Molecule 24 is a protein called MCPv5.

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

- Molecule 25 is a protein called P22.

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

- Molecule 26 is a protein called P23.

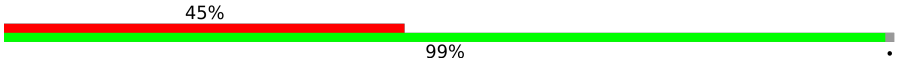
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
26	dm	25	174	111	28	35	0	0
			Total	C	N	O		
26	dn	25	181	116	29	36	0	0
			Total	C	N	O		
26	do	25	182	121	28	33	0	0

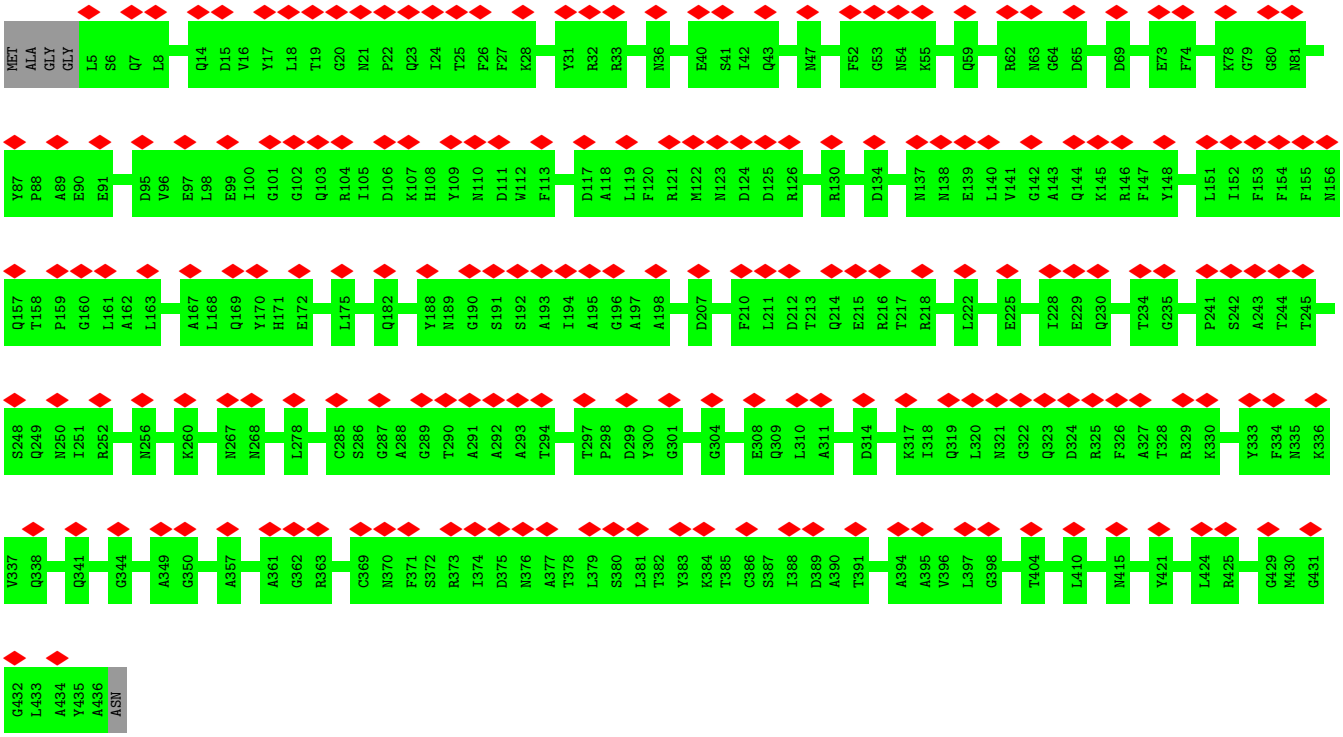
3 Residue-property plots (i)

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

• Molecule 1: Major capsid protein (MCP)

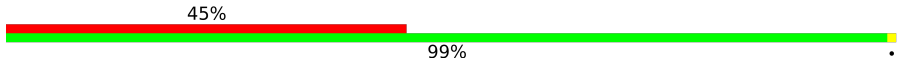
Chain aa:

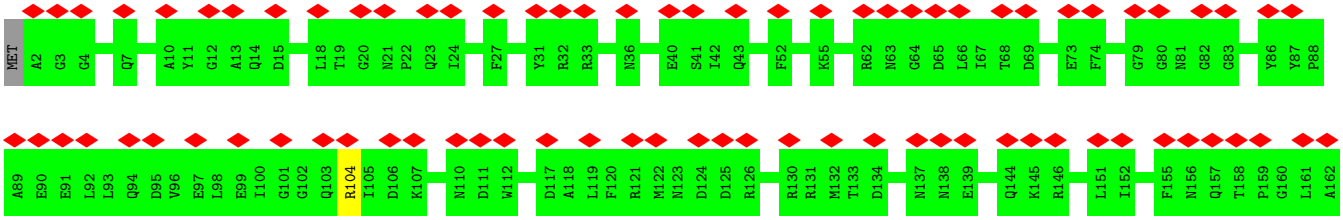


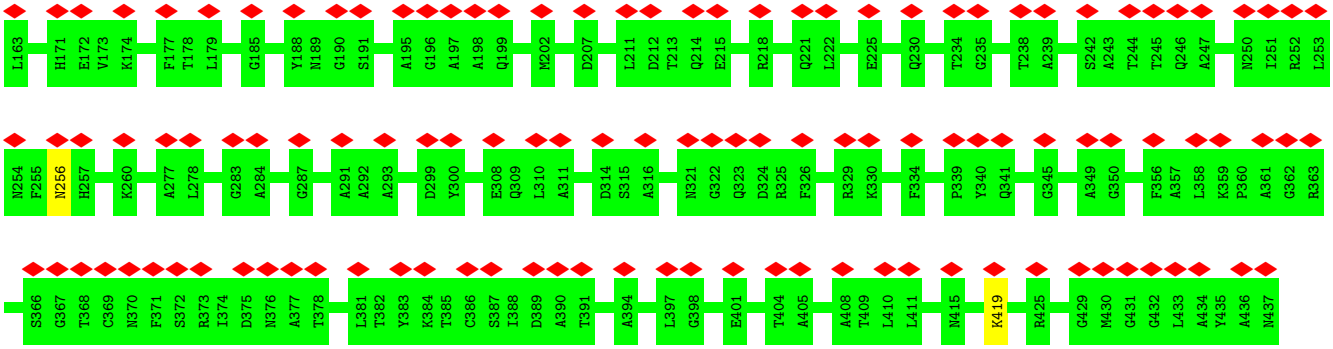


• Molecule 1: Major capsid protein (MCP)

Chain ab:

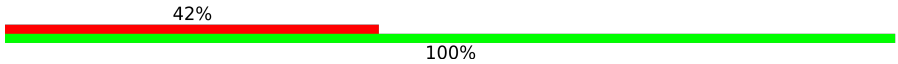


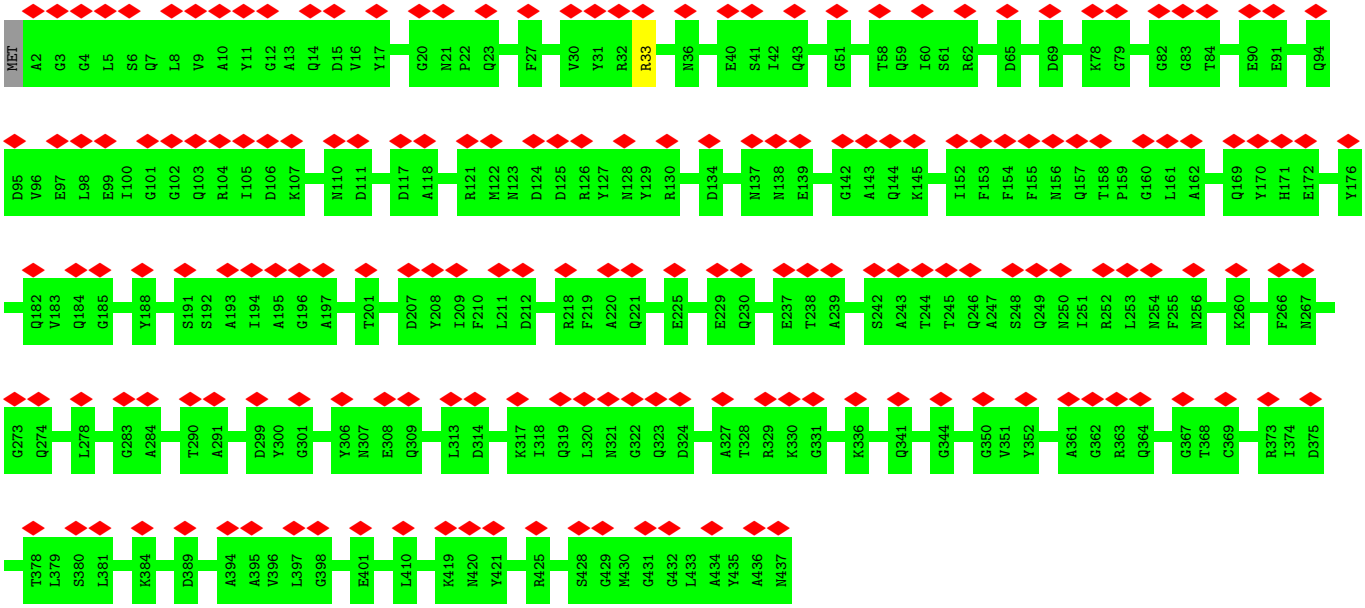




- Molecule 1: Major capsid protein (MCP)

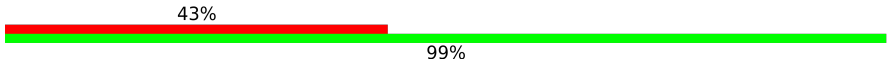
Chain ac:

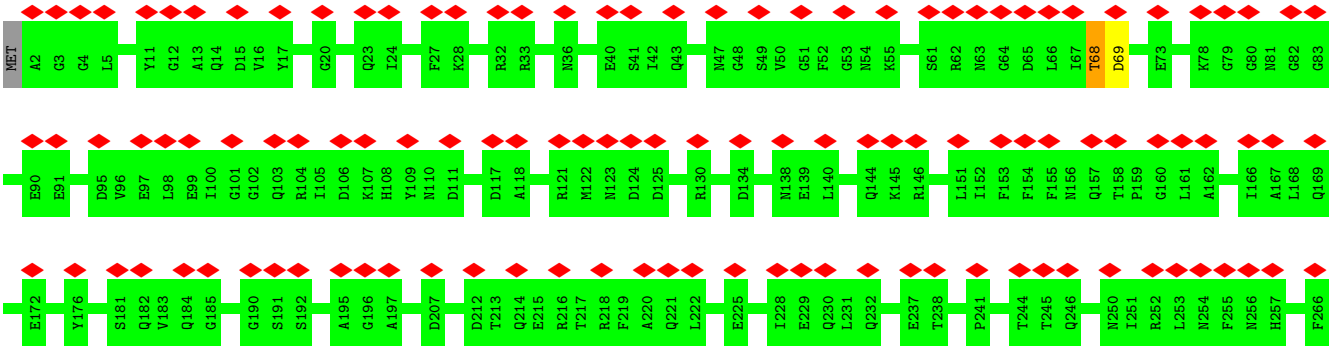


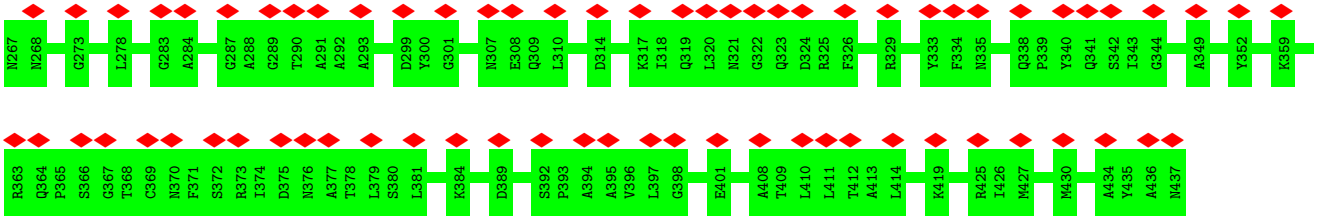


- Molecule 1: Major capsid protein (MCP)

Chain ad:

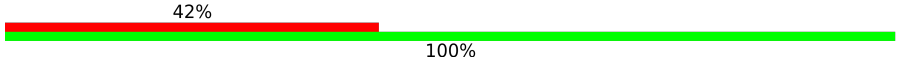


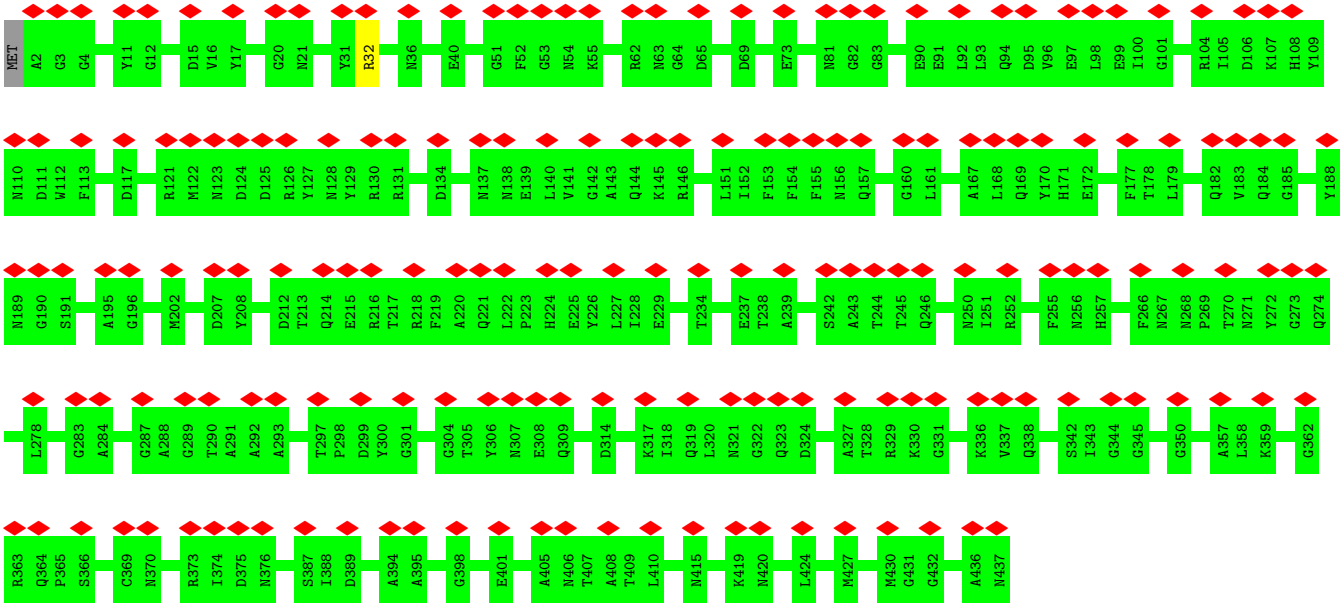




• Molecule 1: Major capsid protein (MCP)

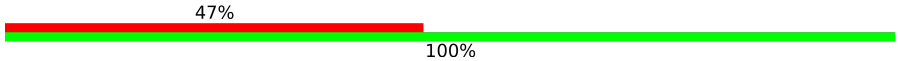
Chain ae:

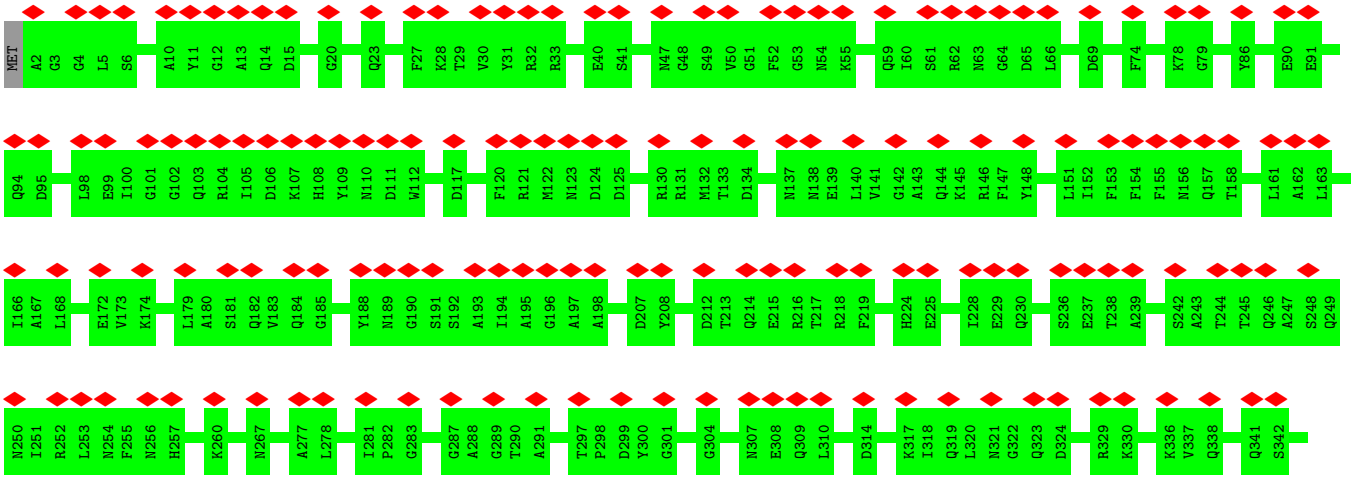


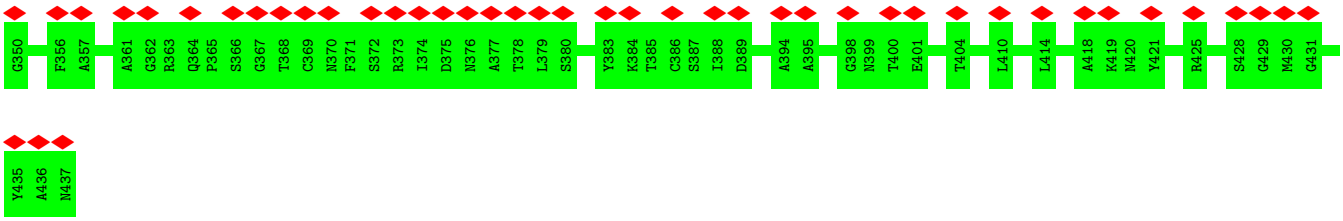


• Molecule 1: Major capsid protein (MCP)

Chain af:

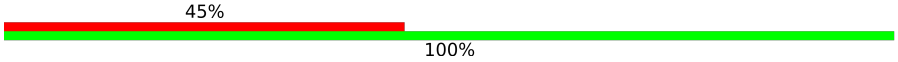






• Molecule 1: Major capsid protein (MCP)

Chain ag:



• Molecule 1: Major capsid protein (MCP)

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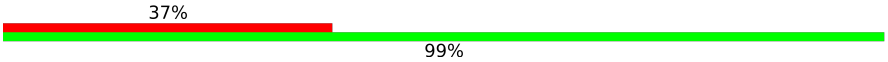
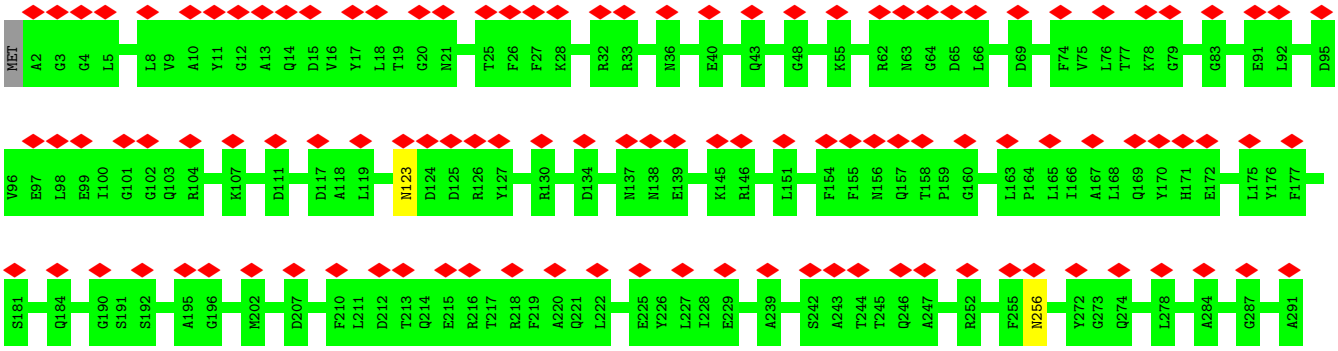
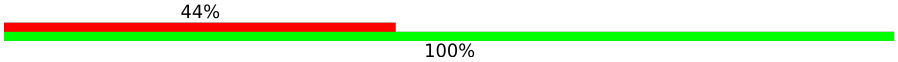
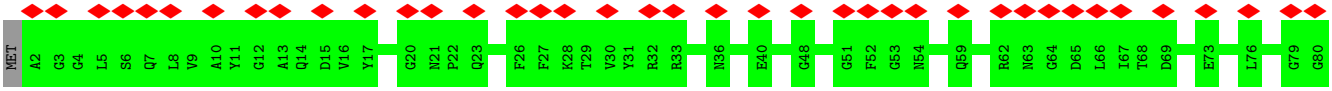


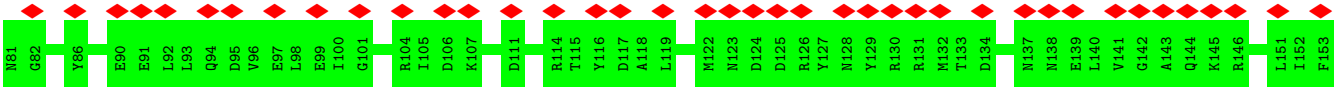


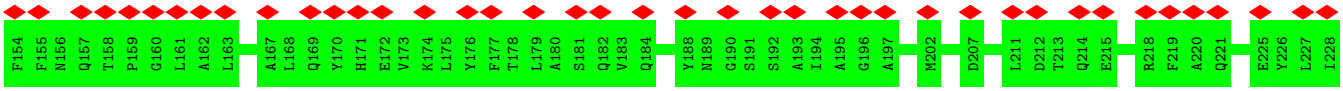
• Molecule 1: Major capsid protein (MCP)

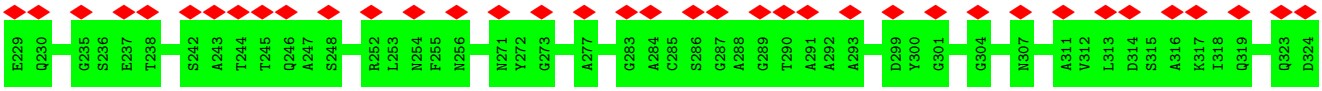
Chain ai:

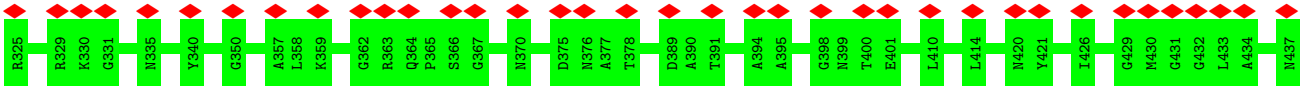






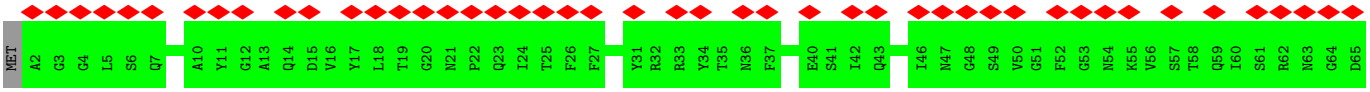


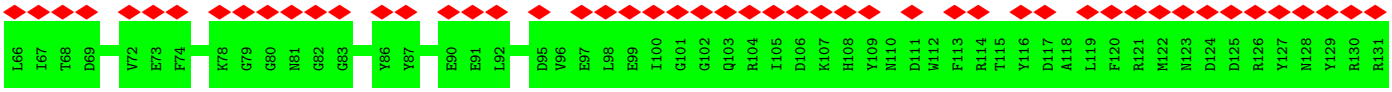


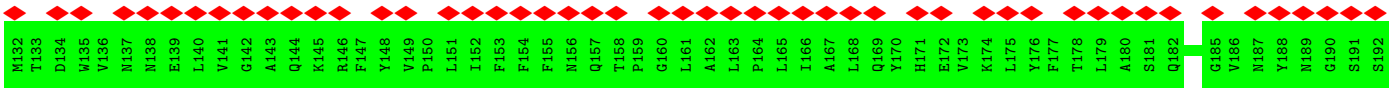


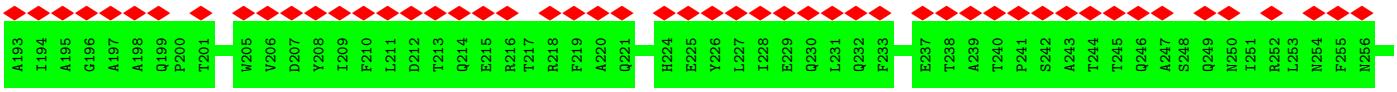
• Molecule 1: Major capsid protein (MCP)

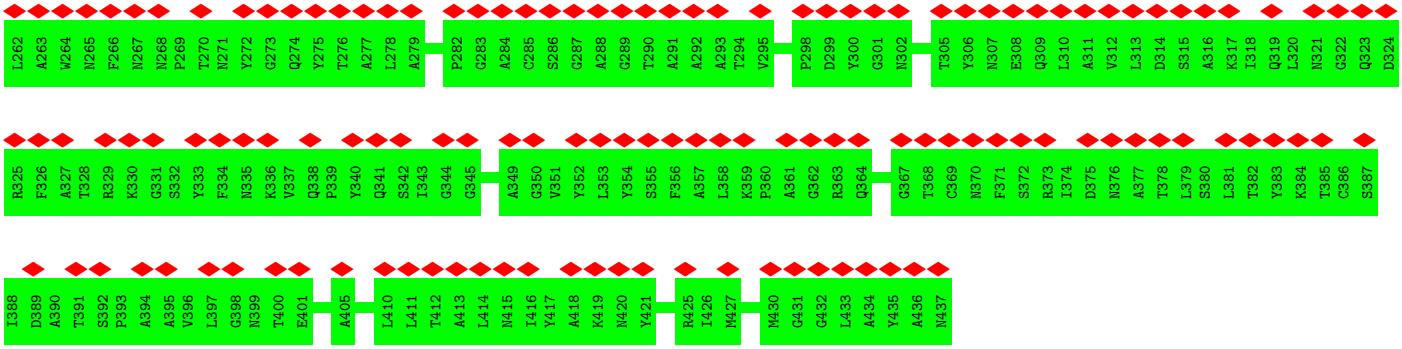
Chain aj:





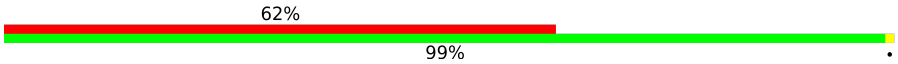


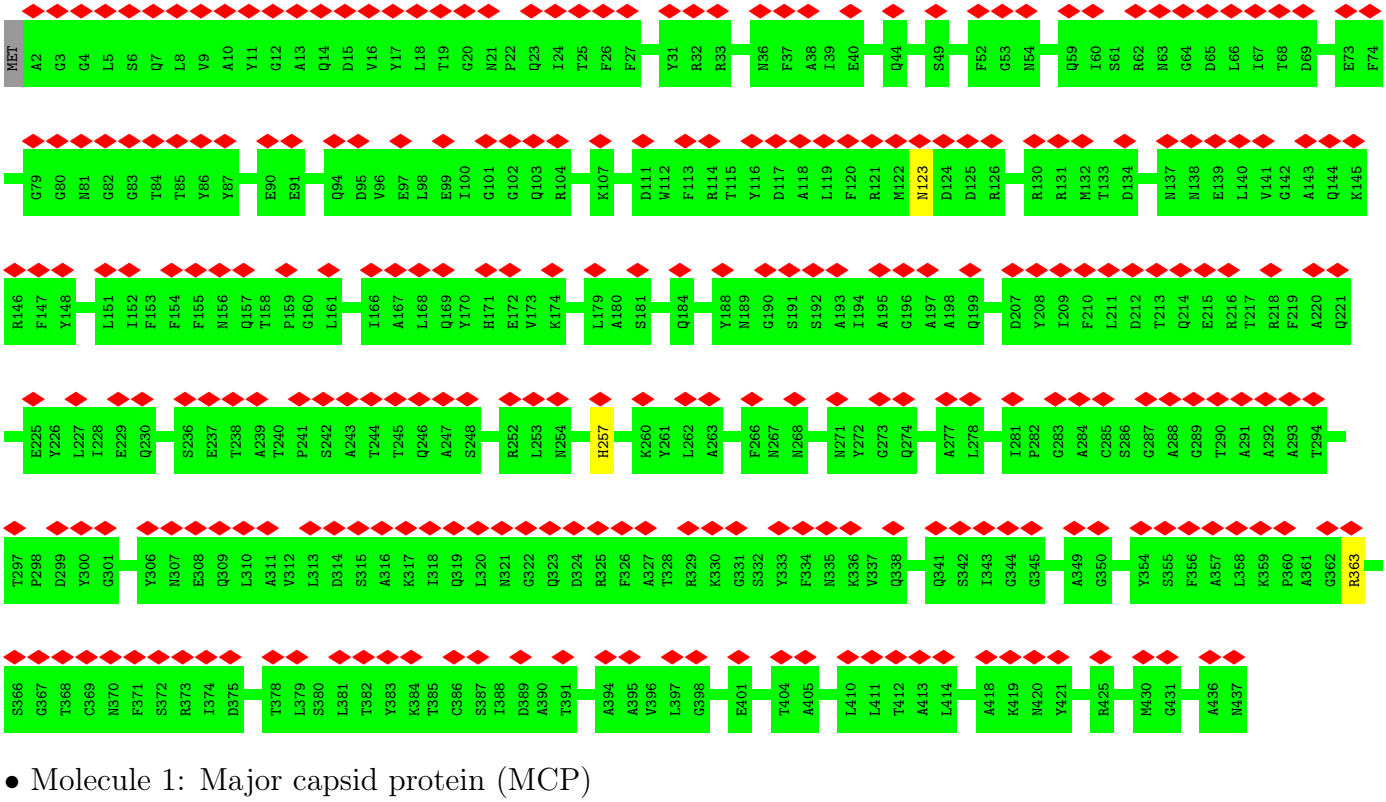




- Molecule 1: Major capsid protein (MCP)

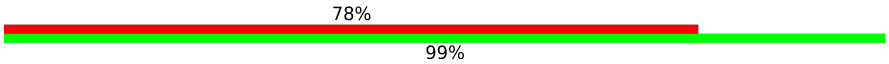
Chain ak:

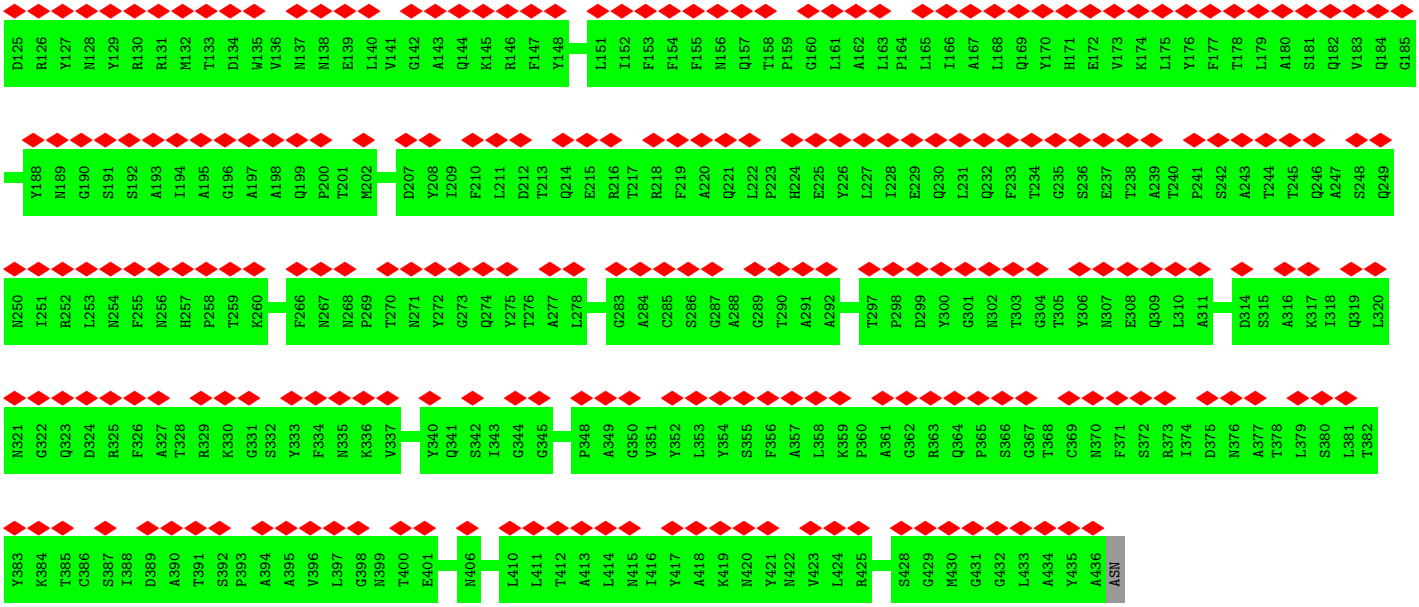




- Molecule 1: Major capsid protein (MCP)

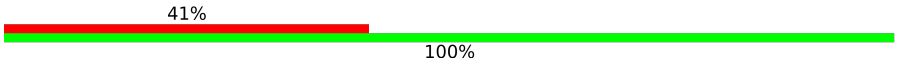
Chain al:

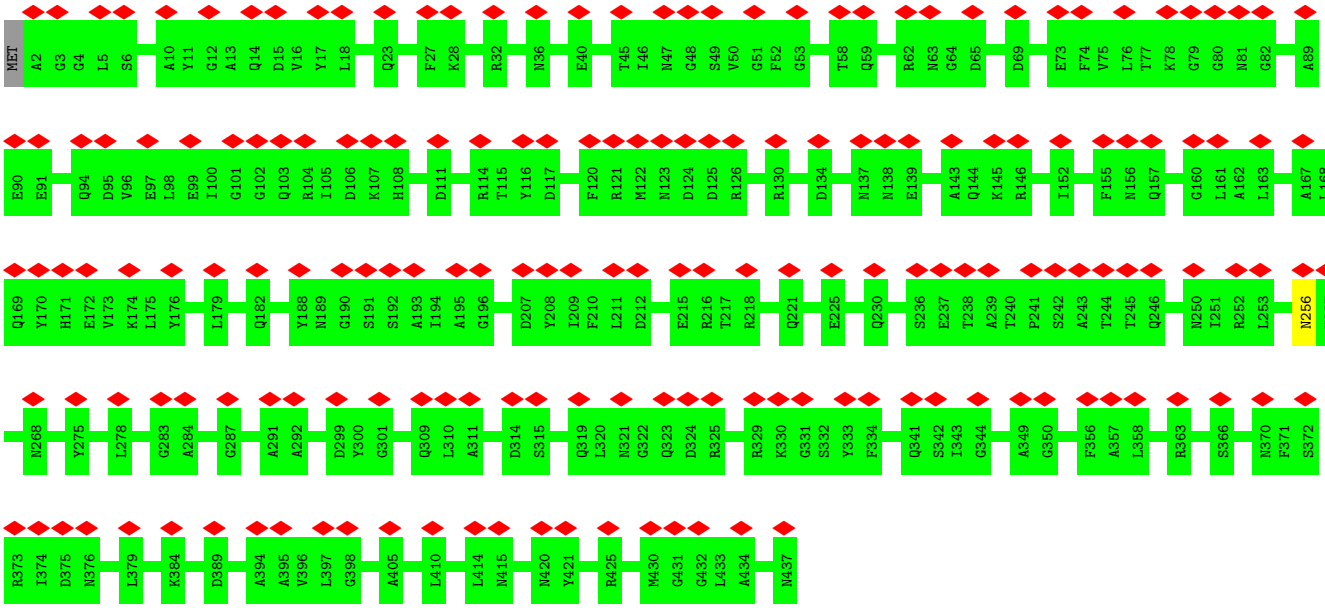




- Molecule 1: Major capsid protein (MCP)

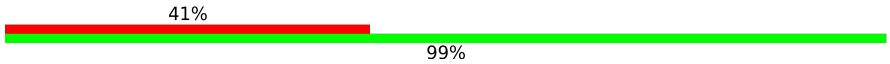
Chain am:

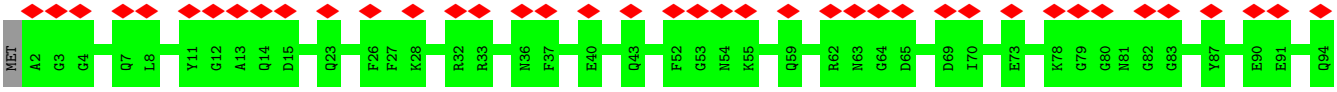


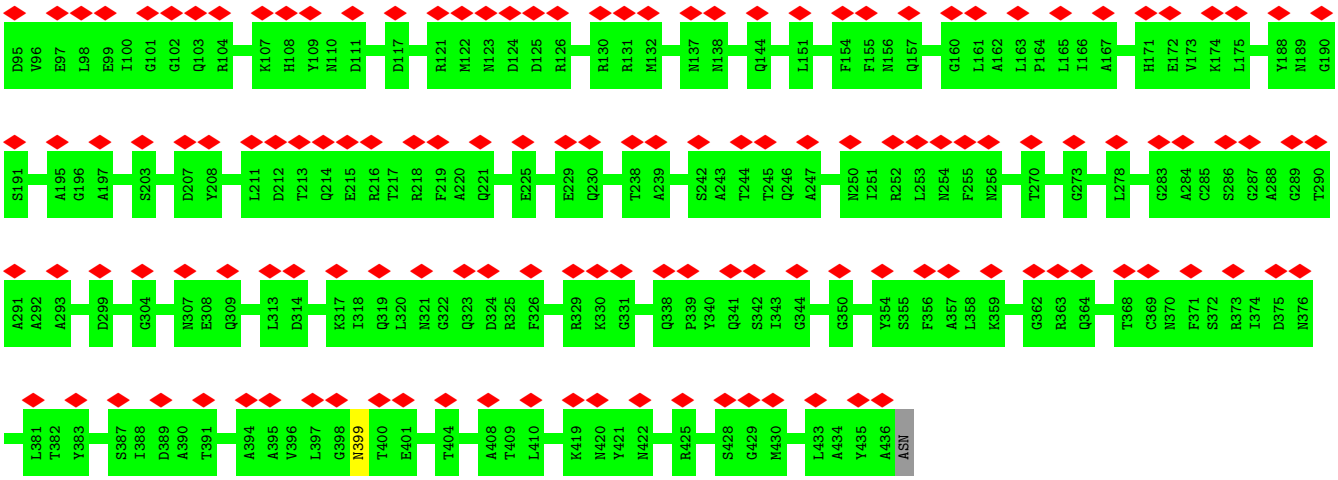


- Molecule 1: Major capsid protein (MCP)

Chain an:

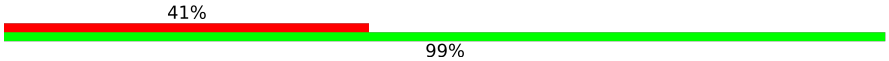


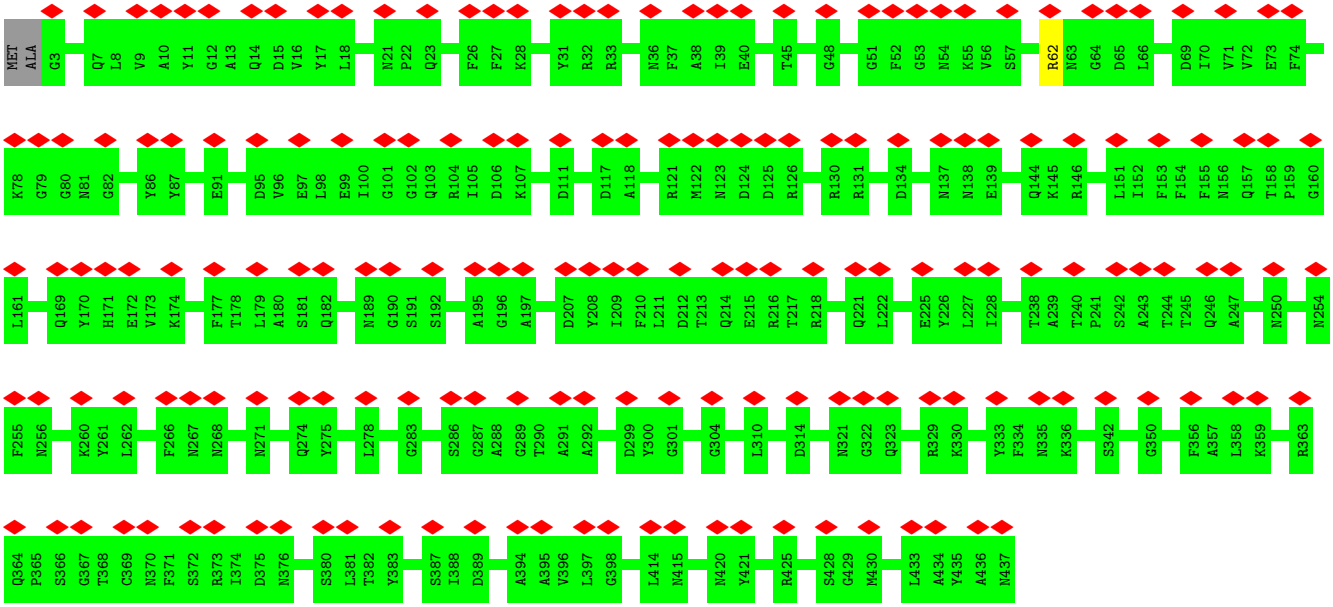




- Molecule 1: Major capsid protein (MCP)

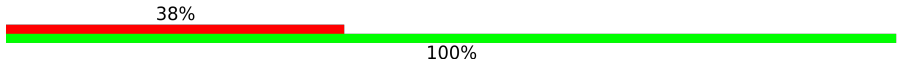
Chain ao:

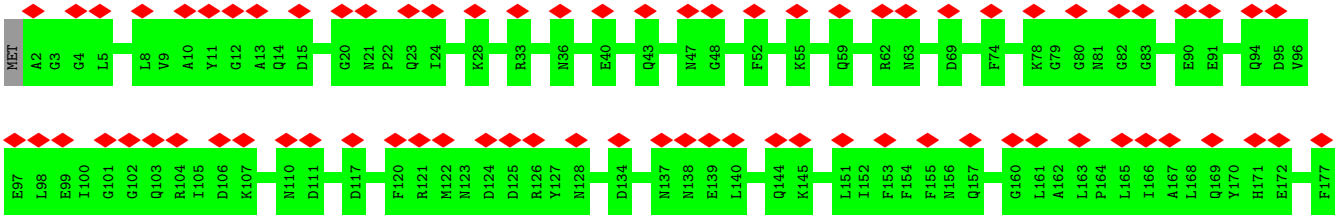


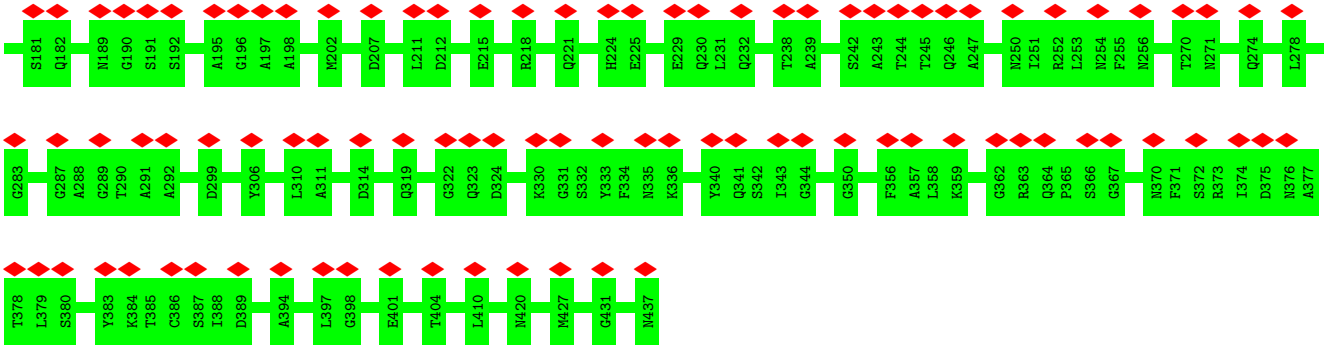


- Molecule 1: Major capsid protein (MCP)

Chain ap:

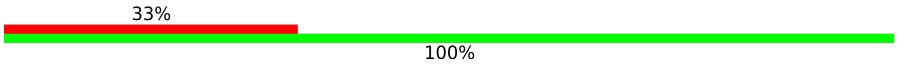


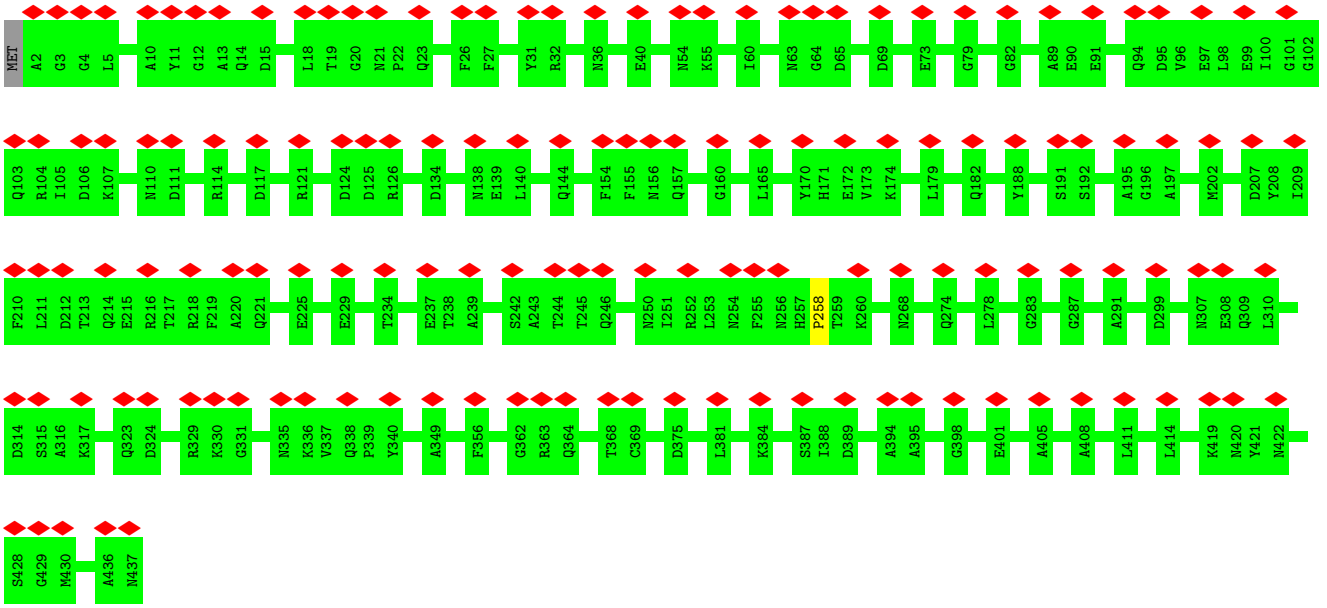




- Molecule 1: Major capsid protein (MCP)

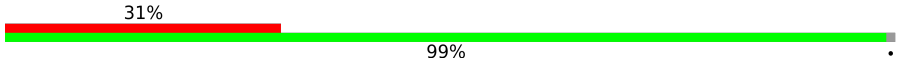
Chain aq:

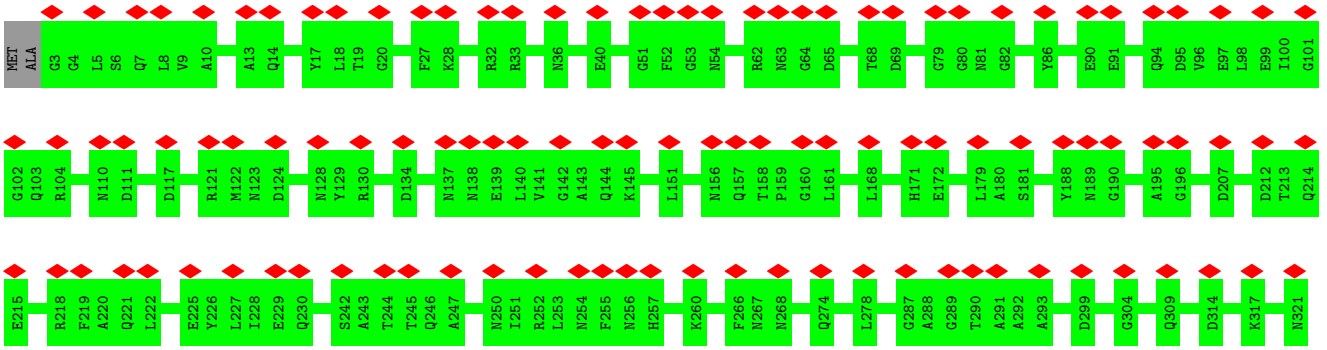


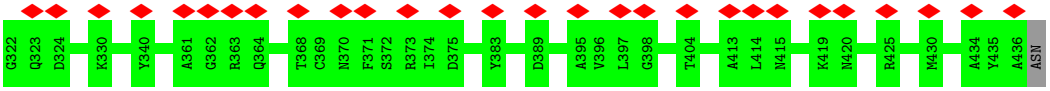


- Molecule 1: Major capsid protein (MCP)

Chain ar:







- Molecule 1: Major capsid protein (MCP)

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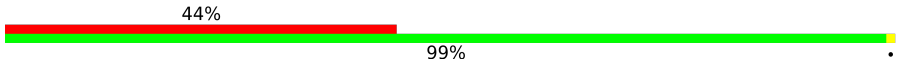
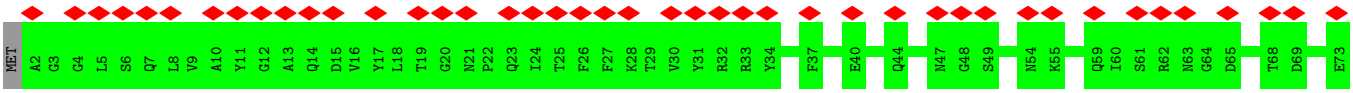
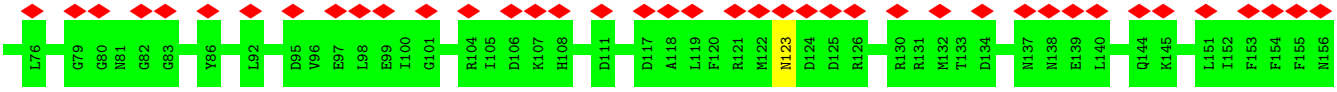
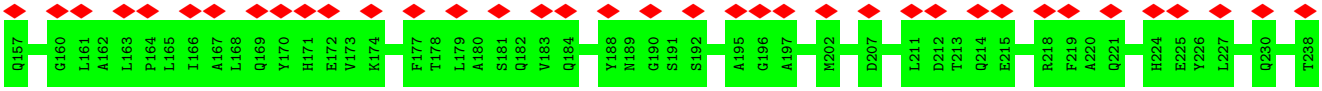
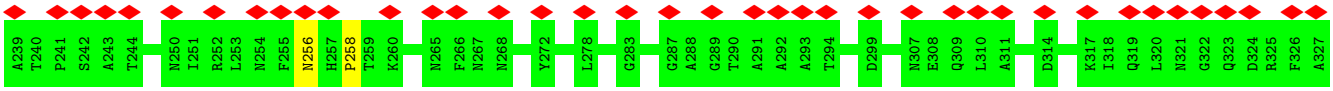
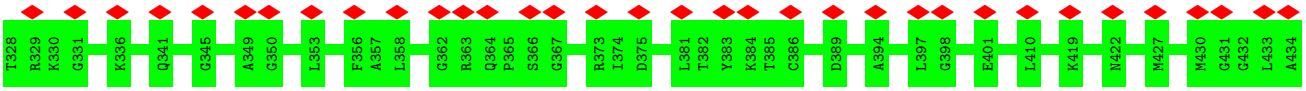






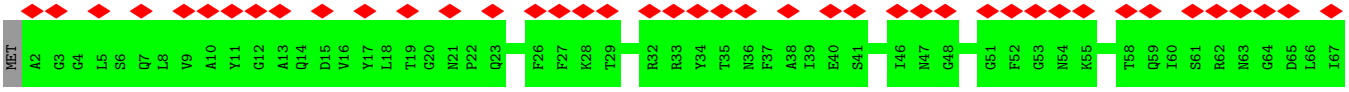


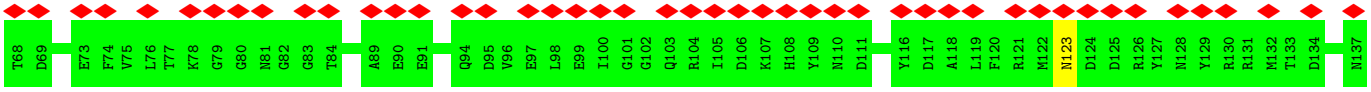


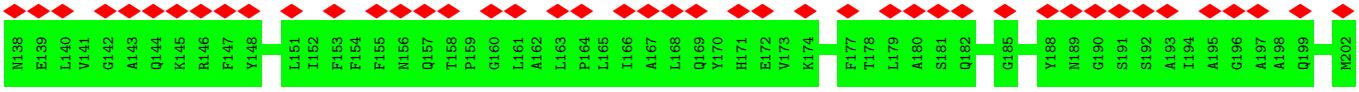


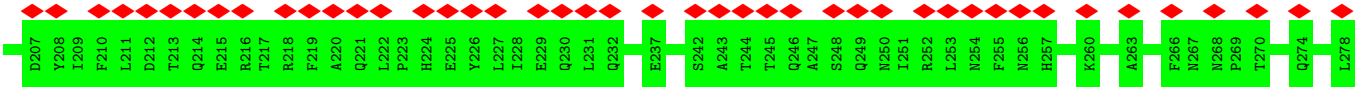
- Molecule 1: Major capsid protein (MCP)

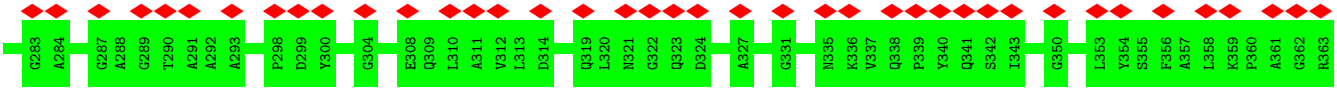
Chain at:

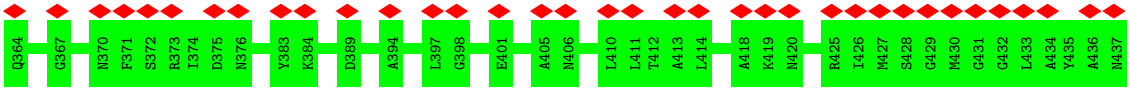






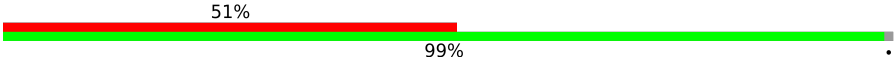


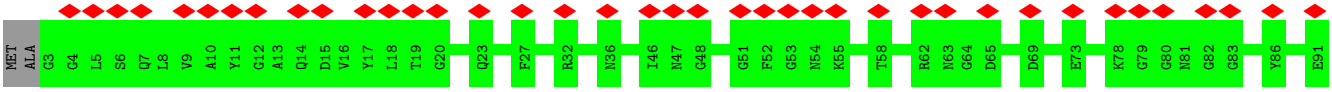


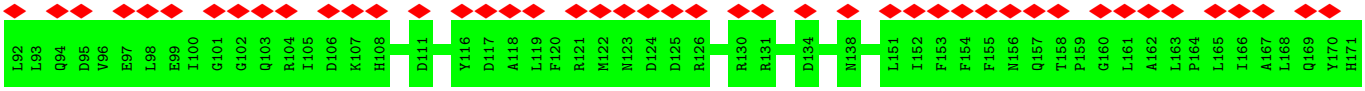


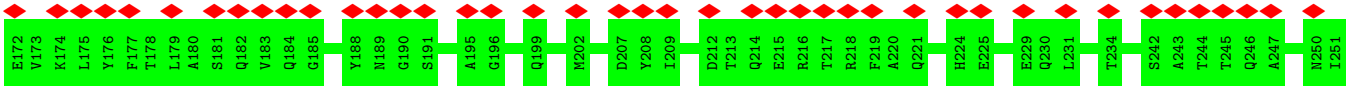
- Molecule 1: Major capsid protein (MCP)

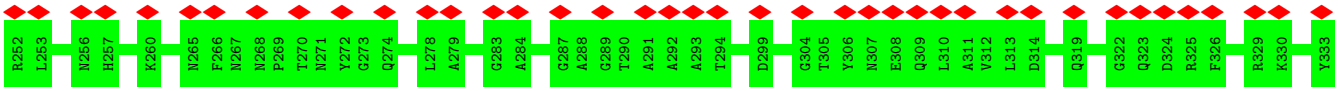
Chain au:

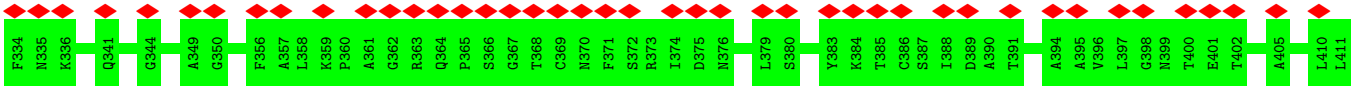


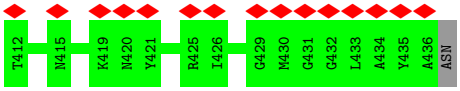






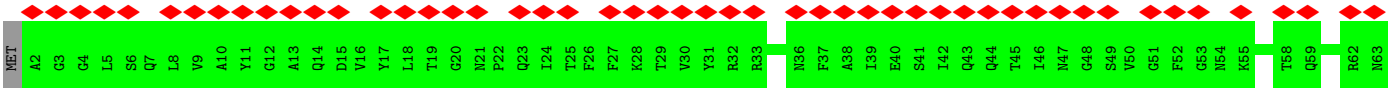


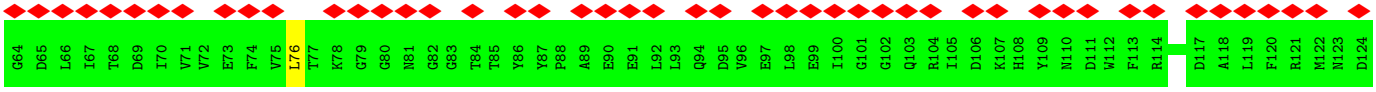


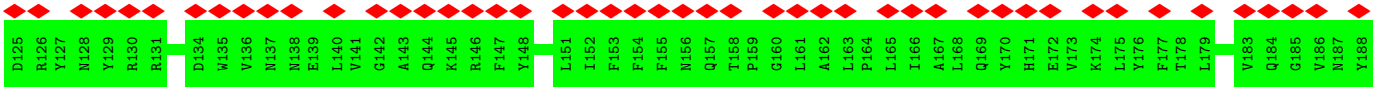


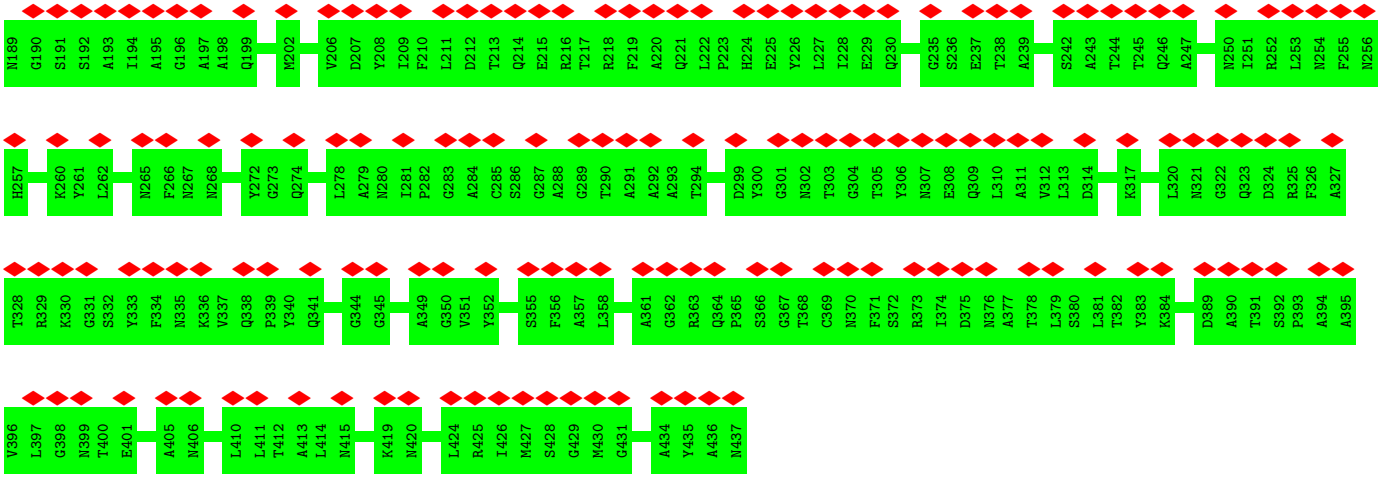
- Molecule 1: Major capsid protein (MCP)

Chain av:



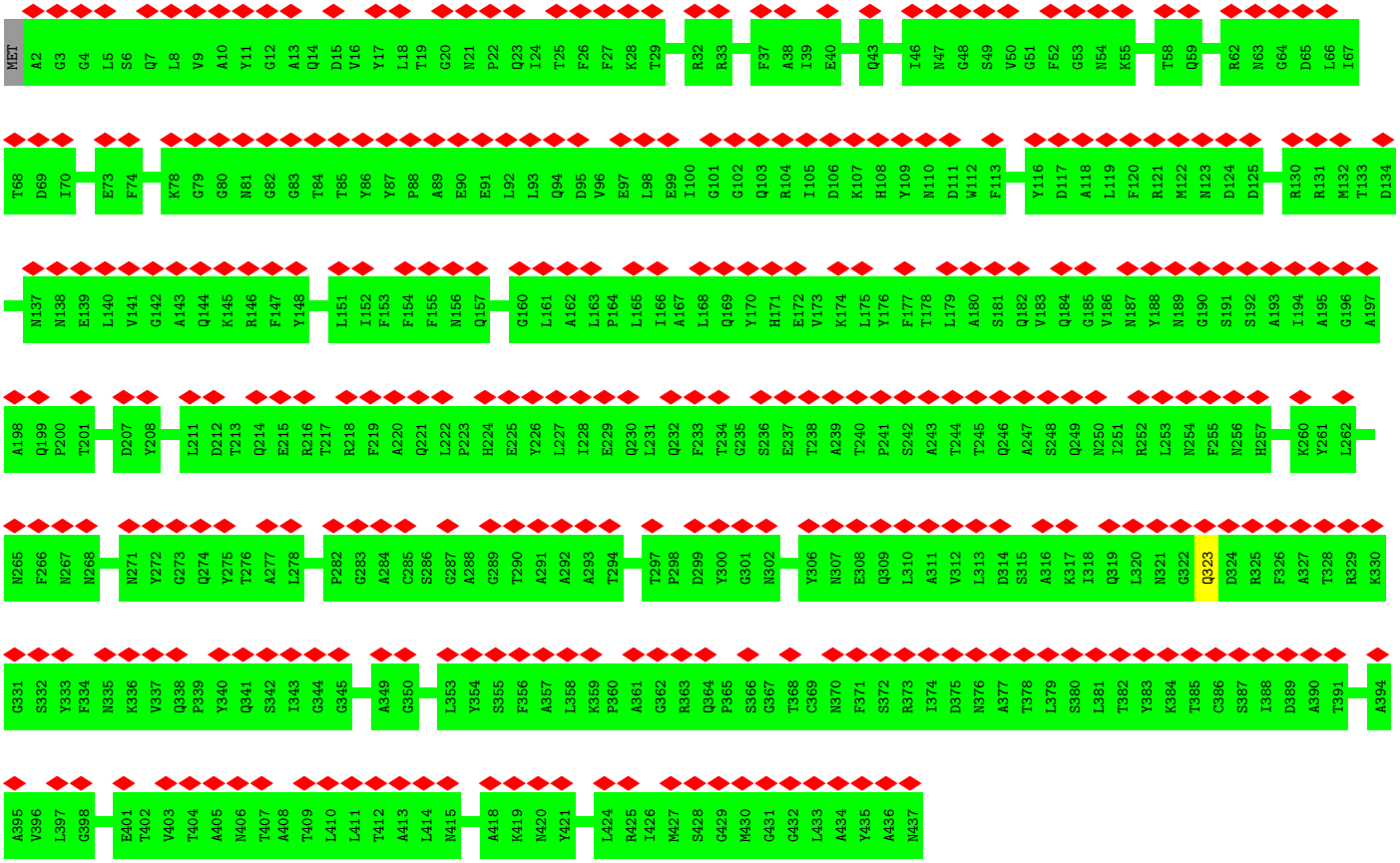






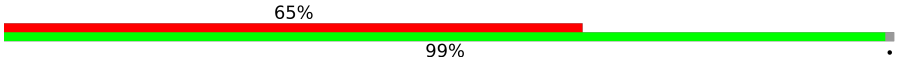
• Molecule 1: Major capsid protein (MCP)

Chain aw:



• Molecule 1: Major capsid protein (MCP)

Chain ax:



MET ALA G3 G4 L5 S6 Q7 L8 V9 A10 Y11 G12 A13 Q14 Y17 L18 T19 G20 N21 P22 Q23 I24 T25 F26 F27 K28 T29 V30 Y31 R32 R33 Y34 T35 N36 F37 A38 I39 E40 Q43 N47 G48 G51 F52 G53 N54 K55 Q59 R62 N63 G64 D65 L66 I67 T68

D69 E73 F74 K78 G79 G80 N81 G82 Y86 A89 E90 E91 L92 L93 Q94 D95 V96 E97 L98 E99 I100 G101 G102 Q103 R104 I105 D106 K107 H108 Y109 N110 D111 W112 F113 Y116 D117 A118 L119 F120 R121 M122 N123 D124 D125 R126 Y127 N128 Y129 R130 R131 M132 T133 D134 W135 V136

N137 N138 E139 L140 V141 G142 A143 Q144 K145 R146 F147 Y148 L151 I152 F153 F154 F155 N156 Q157 T158 P159 G160 L161 A167 L168 Q169 Y170 H171 E172 V173 K174 F177 T178 L179 A180 S181 Q182 V183 Q184 G185 Y188 N189 G190 S191 S192 A193 I194 A195 G196 A197 D207 Y208 L211 D212

T213 Q214 E215 R216 T217 R218 F219 A220 Q221 L222 E225 Y226 L227 I228 E229 Q230 E237 T238 A239 T240 P241 S242 A243 T244 T245 Q246 A247 S248 Q249 N250 I251 R252 L253 N254 F255 N256 H257 Y261 L262 N265 F266 N267 N268 P269 T270 Q274 A277 L278 P282 G283 A284 G287

A288 G289 T290 A291 A292 A293 T294 D299 Y300 G301 N302 T303 G304 T305 Y306 N307 E308 Q309 L310 A311 V312 L313 D314 S315 A316 K317 I318 Q319 L320 N321 G322 G323 D324 R325 F326 A327 T328 R329 K330 G331 S332 Y333 F334 N335 K336 V337 Q338 P339 Y340 Q341 S342 I343 G344 G345 V346 A349 G350 V351

Y352 L353 Y354 S355 F356 A357 L358 K359 P360 A361 G362 R363 Q364 P365 S366 G367 T368 C369 N370 F371 S372 R373 I374 D375 N376 A377 T378 L379 S380 L381 K384 T385 C386 S387 I388 D389 A390 T391 A395 V396 L397 G398 E401 T402 V403 T404 A405 A408 T409 L410 L411 T412 A413 L414 N415

K419 N420 Y421 N422 V423 L424 R425 I426 M427 S428 G429 M430 G431 G432 L433 A434 Y435 A436 ASN

- Molecule 1: Major capsid protein (MCP)

Chain ay:

MET ALA G3 G4 L5 S6 Q7 L8 V9 A10 Y11 G12 A13 Q14 D15 V16 Y17 L18 T19 G20 N21 P22 Q23 I24 T25 F26 F27 K28 T29 V30 Y31 R32 R33 Y34 T35 N36 F37 A38 I39 E40 S41 I42 Q43 Q44 T45 I46 N47 G48 S49 V50 G51 F52 G53 N54 K55 V56 S57 T58 Q59

R62 N63 G64 D65 L66 I67 T68 D69 I70 V71 V72 E73 F74 V75 L76 T77 K78 G79 G80 N81 G82 G83 T84 T85 Y86 Y87 P88 A89 E90 E91 L92 L93 Q94 D95 V96 E97 L98 E99 I100 G101 G102 Q103 R104 I105 D106 K107 H108 Y109 N110 D111 W112 F113 R114 T115 Y116 D117 A118 L119 F120 R121

M122 N123 D124 D125 R126 Y127 N128 Y129 R130 R131 M132 T133 D134 W135 V136 N137 N138 E139 L140 V141 G142 A143 Q144 K145 R146 F147 Y148 L151 I152 F153 F154 F155 N156 Q157 T158 P159 G160 L161 A162 L163 P164 L165 I166 A167 L168 Q169 Y170 H171 E172 V173 K174 L175 Y176 F177 T178 L179 A180 S181 Q182

V183 Q184 G185 V186 N187 Y188 N189 G190 S191 S192 A193 I194 A195 G196 A197 A198 Q199 P200 T201 M202 S203 V204 W205 V206 D207 Y208 I209 F210 L211 D212 T213 Q214 E215 R216 T217 R218 F219 A220 Q221 L222 P223 H224 E225 Y226 L227 I228 E229 Q230 L231 Q232 F233 T234 G235 S236 E237 T238 A239 T240 P241 S242

A243 T244 T245 Q246 A247 S248 Q249 N250 I251 R252 L253 N254 F255 N256 H257 K260 Y261 L262 A263 W264 N265 F266 N267 N268 P269 T270 N271 Y272 G273 Q274 Y275 T276 A277 L278 A279 N280 I281 P282 G283 A284 C285 S286 G287 A288 G289 T290 A291 A292 A293 T294 V295 T296 T297 P298 D299 Y300 G301 N302 T303

G304 T305 Y306 N307 E308 Q309 L310 A311 V312 L313 D314 S315 A316 K317 I318 Q319 L320 N321 G322 Q323 D324 R325 F326 A327 T328 R329 K330 G331 S332 Y333 F334 N335 K336 V337 Q338 P339 Y340 Q341 S342 I343 G344 G345 V346 T347 P348 A349 G350 V351 Y352 L353 Y354 S355 F356 A357 L358 K359 P360 A361 G362 R363

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R425 I426 M427 S428 G429 M430 G431 G432 L433 A434 Y435 A436 N437

- Molecule 1: Major capsid protein (MCP)

Chain az: 89% 99%

MET ALA G3 G4 L5 S6 Q7 L8 V9 A10 Y11 G12 A13 Q14 D15 V16 Y17 L18 T19 G20 N21 P22 Q23 I24 T25 F26 F27 K28 Y31 R32 R33 Y34 T35 N36 F37 A38 I39 E40 S41 I42 Q43 Q44 T45 I46 N47 G48 S49 V50 G51 F52 G53 N54 K55 V56 S57 T58 Q59 I60 S61

R62 N63 G64 D65 L66 I67 T68 D69 V72 E73 F74 V75 L76 T77 K78 G79 G80 N81 G82 G83 T84 T85 Y86 Y87 P88 A89 E90 E91 L92 L93 Q94 D95 V96 E97 L98 E99 I100 G101 G102 Q103 R104 I105 D106 K107 H108 Y109 N110 D111 W112 F113 R114 T115 Y116 D117 A118 L119 F120 R121 M122

N123 D124 D125 R126 Y127 N128 Y129 R130 R131 M132 T133 D134 W135 V136 N137 N138 E139 L140 V141 G142 A143 Q144 K145 R146 F147 Y148 L151 I152 F153 F154 F155 N156 Q157 T158 P159 G160 L161 A162 L163 P164 L165 I166 A167 L168 Q169 Y170 H171 E172 V173 K174 L175 Y176 F177 T178 L179 A180 S181 Q182 V183

Q184 G185 V186 N187 Y188 N189 G190 S191 S192 A193 I194 A195 G196 A197 A198 Q199 P200 T201 M202 S203 V204 W205 V206 D207 Y208 I209 F210 L211 D212 T213 Q214 E215 R216 T217 R218 F219 A220 Q221 L222 P223 H224 E225 Y226 L227 I228 E229 Q230 L231 Q232 F233 T234 G235 S236 E237 T238 A239 T240 P241 S242 A243

T244 T245 Q246 A247 S248 Q249 N250 I251 R252 L253 N254 F255 N256 H257 Y261 L262 A263 W264 N265 F266 N267 N268 M271 Y272 G273 Q274 Y275 T276 A277 L278 A279 N280 I281 P282 G283 A284 C285 S286 G287 A288 G289 T290 A291 A292 A293 T294 V295 T296 T297 P298 D299 Y300 G301 N302 T303 G304 T305 Y306

N307 E308 Q309 L310 A311 V312 L313 D314 S315 A316 K317 I318 Q319 L320 N321 G322 Q323 D324 R325 F326 A327 T328 R329 K330 G331 S332 Y333 F334 N335 K336 V337 Q338 P339 Y340 Q341 S342 I343 G344 G345 V346 T347 P348 A349 G350 V351 Y352 L353 Y354 S355 F356 A357 L358 K359 P360 A361 G362 R363 Q364 P365 S366

G367 T368 C369 N370 F371 S372 R373 I374 D375 N376 A377 T378 L379 S380 L381 T382 Y383 K384 T385 C386 S387 I388 D389 A390 T391 S392 P393 A394 A395 V396 L397 G398 N399 T400 E401 T402 V403 T404 A405 N406 T407 A408 T409 L410 L411 T412 A413 L414 N415 I416 Y417 A418 K419 N420 Y421 L424 R425 I426 M427

S428 G429 M430 G431 G432 L433 A434 Y435 A436 ASN

- Molecule 1: Major capsid protein (MCP)

Chain aA: 85% 99%

MET ALA G3 G4 L5 S6 Q7 L8 V9 A10 Y11 G12 A13 Q14 D15 V16 Y17 L18 T19 G20 N21 P22 Q23 I24 T25 F26 F27 K28 T29 V30 Y31 R32 R33 Y34 T35 N36 F37 A38 I39 E40 S41 I42 Q43 Q44 T45 I46 N47 G48 G51 F52 G53 N54 K55 T58 Q59 I60 S61 R62

N63 G64 D65 L66 I67 T68 D69 I70 V71 V72 E73 F74 V75 L76 T77 K78 G79 G80 N81 G82 G83 T84 T85 Y86 Y87 P88 A89 E90 E91 L92 D95 V96 E97 L98 E99 I100 G101 G102 Q103 R104 I105 D106 K107 H108 Y109 N110 D111 W112 F113 R114 T115 Y116 D117 A118 L119 F120 R121 M122 N123

D124 D125 R126 Y127 N128 Y129 R130 R131 M132 T133 D134 W135 V136 N137 N138 E139 L140 V141 G142 A143 Q144 K145 R146 F147 L151 I152 F153 F154 F155 N156 Q157 T158 P159 G160 L161 A162 L163 P164 L165 I166 A167 L168 Q169 Y170 H171 E172 V173 K174 L175 Y176 F177 T178 L179 A180 S181 Q182 V183 Q184 G185

Y188 N189 G190 S191 S192 A193 I194 A195 G196 A197 A198 Q199 P200 T201 M202 S203 V204 W205 V206 D207 Y208 I209 F210 L211 D212 T213 Q214 E215 R216 T217 R218 F219 A220 Q221 L222 P223 H224 E225 Y226 L227 I228 E229 Q230 F233 T234 G235 S236 E237 T238 A239 T240 P241 S242 A243 T244 T245 Q246 A247

S248 Q249 N250 I251 R252 L253 N254 F255 N256 H257 P258 T259 K260 Y261 L262 A263 W264 N265 F266 N267 N268 P269 T270 N271 Y272 G273 Q274 Y275 T276 A277 L278 A279 N280 I281 P282 G283 A284 C285 S286 G287 A288 G289 T290 A291 A292 A293 T294 V295 T296 T297 P298 D299 Y300 G301 N302 T303 G304 T305 Y306 N307

E308 Q309 L310 A311 V312 L313 D314 S315 A316 K317 I318 Q319 L320 N321 G322 Q323 D324 R325 F326 A327 T328 R329 K330 G331 S332 Y333 F334 N335 K336 V337 Q338 P339 Y340 Q341 S342 I343 G344 G345 V346 T347 P348 A349 G350 V351 Y352 L353 Y354 S355 F356 A357 L358 K359 P360 A361 G362 R363 Q364 P365 S366 G367

T368 C369 N370 F371 S372 R373 I374 D375 N376 A377 T378 L379 S380 L381 T382 Y383 K384 T385 C386 S387 I388 D389 A390 T391 S392 P393 A394 A395 V396 L397 G398 N399 T400 E401 T402 V403 T404 A405 N406 T407 A408 T409 L410 L411 T412 A413 L414 Y417 A418 K419 N420 Y421 N422 V423 L424 R425 I426 M427 S428

G429 M430 G431 G432 L433 A434 Y435 A436 M437

- Molecule 1: Major capsid protein (MCP)

Chain aB: 81% 100%

MET ALA G3 G4 L5 S6 Q7 A10 Y11 G12 A13 Q14 D15 V16 Y17 L18 T19 G20 N21 P22 Q23 I24 T25 F26 F27 K28 T29 V30 Y31 R32 R33 Y34 T35 N36 F37 A38 I39 E40 S41 I42 Q43 Q44 T45 I46 N47 G48 S49 V50 G51 F52 G53 N54 K55 V56 S57 T58 Q59 I60 S61

R62 N63 G64 D65 L66 I67 T68 D69 I70 E73 F74 V75 L76 T77 K78 G79 G80 N81 G82 G83 T84 T85 Y86 Y87 P88 A89 E90 E91 L92 L93 Q94 D95 V96 E97 L98 E99 I100 G101 G102 Q103 R104 I105 D106 K107 H108 Y109 N110 D111 W112 F113 R114 D117 A118 L119 F120 R121 M122 N123

D124 D125 R126 R130 R131 M132 T133 D134 W135 V136 N137 N138 E139 L140 V141 G142 A143 Q144 K145 R146 F147 Y148 L151 I152 F153 F154 F155 N156 Q157 T158 P159 G160 L161 A162 L163 P164 L165 I166 A167 L168 Q169 Y170 H171 E172 V173 K174 L175 Y176 F177 T178 L179 A180 S181 Q184 G185 V186 N187

Y188 N189 G190 S191 S192 A193 I194 A195 G196 A197 A198 Q199 M202 W205 V206 D207 Y208 I209 F210 L211 D212 T213 Q214 E215 R216 T217 R218 F219 A220 Q221 L222 P223 H224 E225 Y226 L227 I228 E229 Q230 L231 Q232 F233 T234 G235 S236 E237 T238 A239 T240 P241 S242 A243 T244 T245 Q246 A247 S248 Q249

N250 I251 R252 L253 N254 F255 N256 H257 K260 Y261 L262 A263 W264 N265 F266 N267 N268 N271 Y272 G273 Q274 Y275 T276 A277 L278 A279 N280 I281 P282 G283 A284 C285 S286 G287 A288 G289 T290 A291 A292 A293 T294 T297 P298 D299 Y300 G301 N302 T303 G304 T305 Y306 N307 E308 Q309 L310 A311 V312

L313 D314 S315 A316 K317 I318 Q319 L320 N321 G322 Q323 D324 R325 F326 A327 T328 R329 K330 G331 S332 Y333 F334 N335 K336 V337 Q338 P339 Y340 Q341 S342 I343 G344 G345 A349 G350 V351 Y352 L353 Y354 S355 F356 A357 L358 K359 P360 A361 G362 R363 Q364 P365 S366 G367 T368 C369 N370 F371 S372 R373 I374

D375 N376 A377 T378 L379 S380 L381 T382 Y383 K384 T385 C386 S387 I388 D389 A390 T391 S392 P393 A394 A395 V396 L397 G398 N399 T400 E401 T402 V403 T404 A405 N406 T409 L410 L411 T412 A413 L414 N415 I416 Y417 A418 K419 N420 Y421 N422 V423 L424 R425 I426 M427 S428 G429 M430 G431 G432 L433 A434 Y435

A436 N437

- Molecule 1: Major capsid protein (MCP)

Chain aC: 78% 100%

MET A2 G3 G4 L5 S6 Q7 L8 V9 A10 Y11 G12 A13 Q14 D15 V16 Y17 L18 T19 G20 N21 P22 Q23 I24 T25 F26 F27 K28 T29 V30 Y31 R32 R33 N36 F37 E40 S41 I42 I46 N47 G48 S49 V50 G51 F52 G53 N54 K55 V56 S57 T58 Q59 I60 S61 R62 N63 G64

D65 L66 I67 T68 D69 E73 F74 V75 L76 T77 K78 G79 G80 N81 G82 G83 T84 T85 Y86 Y87 P88 A89 E90 E91 L92 L93 Q94 D95 V96 E97 L98 E99 I100 G101 G102 Q103 R104 I105 D106 K107 H108 Y109 N110 D111 W112 F113 R114 T115 Y116 D117 A118 L119 F120 R121 M122 N123 D124 D125 R126

Y127 N128 Y129 R130 R131 M132 T133 D134 N137 N138 E139 L140 V141 G142 A143 Q144 K145 R146 F147 Y148 V149 P150 L151 I152 F153 F154 F155 N156 Q157 T158 P159 G160 L161 A162 L163 P164 L165 I166 Q169 Y170 H171 E172 V173 K174 L175 Y176 F177 T178 L179 A180 S181 Q182 V183 Q184 G185 Y188 N189

G190 S191 S192 A193 I194 A195 G196 A197 A198 Q199 P200 T201 M202 D207 Y208 I209 F210 L211 D212 T213 Q214 E215 R216 T217 R218 F219 A220 Q221 L222 P223 H224 E225 Y226 L227 I228 E229 Q230 L231 Q232 F233 T234 G235 S236 E237 T238 A239 T240 P241 S242 A243 T244 T245 Q246 A247 S248 Q249 N250 I251 R252

L253 N254 F255 N256 H257 P258 T259 K260 Y261 L262 A263 F266 N267 N268 P269 T270 N271 Y272 G273 Q274 Y275 T276 A277 L278 A279 N280 I281 P282 G283 A284 C285 S286 G287 A288 G289 T290 A291 A292 A293 T296 D299 Y300 G301 N302 T303 G304 T305 Y306 N307 E308 Q309 L310 A311 V312 L313 D314 S315

A316 K317 I318 Q319 L320 N321 G322 Q323 D324 R325 F326 A327 T328 R329 K330 G331 F334 N335 K336 V337 Q338 P339 Y340 Q341 S342 I343 G344 G345 P348 A349 G350 V351 Y352 L353 Y354 S355 F356 A357 L358 K359 P360 A361 G362 R363 Q364 P365 S366 G367 T368 C369 N370 F371 S372 R373 I374 D375 N376 A377

T378 L379 S380 L381 T382 Y383 K384 T385 C386 S387 I388 D389 A390 T391 S392 P393 A394 A395 V396 L397 G398 N399 T400 E401 T402 V403 T404 A405 N406 T407 A408 L411 T412 A413 L414 N415 I416 Y417 N420 Y421 N422 V423 L424 R425 S428 G429 M430 G431 G432 L433 A434 Y435 A436 N437

- Molecule 1: Major capsid protein (MCP)

Chain aD: 78% 99%

MET ALA G3 G4 L5 S6 Q7 L8 V9 A10 Y11 G12 A13 Q14 D15 V16 Y17 L18 T19 G20 N21 P22 Q23 I24 T25 F26 F27 K28 Y31 R32 R33 Y34 T35 N36 F37 A38 I39 E40 S41 I42 Q43 Q44 N47 G48 S49 V50 G51 F52 G53 N54 K55 V56 S57 T58 Q59 I60 S61 R62

N63 G64 D65 L66 I67 T68 D69 I70 V71 V72 E73 F74 V75 L76 T77 K78 G79 G80 N81 G82 G83 T84 T85 Y86 Y87 P88 A89 E90 E91 L92 L93 Q94 D95 V96 E97 L98 E99 I100 G101 G102 Q103 R104 I105 D106 K107 H108 Y109 N110 D111 W112 F113 R114 T115 Y116 D117 A118 L119 F120 R121 M122

N123 D124 D125 R126 Y127 N128 Y129 R130 R131 M132 T133 D134 N137 N138 E139 L140 V141 G142 A143 Q144 K145 R146 F147 Y148 V149 P150 L151 I152 F153 F154 F155 N156 Q157 T158 P159 G160 L161 A162 L163 P164 L165 I166 A167 L168 Q169 Y170 H171 E172 V173 K174 L175 Y176 F177 T178 L179 A180 S181 Q184

G185 V186 N187 Y188 N189 G190 S191 S192 A193 I194 A195 G196 A197 A198 Q199 P200 T201 M202 V205 V206 D207 Y208 I209 F210 L211 D212 T213 Q214 E215 R216 T217 R218 F219 A220 Q221 L222 E225 E229 Q230 L231 Q232 F233 T234 G235 S236 E237 T238 A239 T240 P241 S242 A243 T244 T245 Q246 A247 S248

Q249 N250 I251 R252 L253 N254 F255 N256 H257 P258 T259 K260 Y261 L262 A263 W264 N265 F266 N267 N268 P269 T270 N271 Y272 G273 Q274 A277 L278 P282 G283 A284 C285 S286 G287 A288 G289 T290 A291 A292 A293 T294 T297 P298 D299 N302 T303 G304 T305 Y306 N307 E308 Q309 L310 A311 V312 L313

D314 S315 A316 K317 I318 Q319 L320 N321 G322 Q323 D324 R325 F326 A327 T328 R329 K330 G331 S332 Y333 F334 N335 K336 V337 Q338 P339 Y340 Q341 S342 I343 G344 G345 V346 T347 P348 A349 G350 V351 Y352 L353 Y354 S355 F356 A357 L358 K359 P360 A361 G362 R363 Q364 P365 S366 G367 T368 C369 N370 F371 S372 R373

I374 D375 N376 L379 S380 L381 T382 Y383 K384 T385 C386 S387 I388 D389 A390 A394 L397 G398 N399 T400 E401 T404 A405 N406 T407 A408 T409 L410 A413 L414 N415 I416 Y417 A418 K419 N420 Y421 N422 V423 L424 R425 I426 M427 S428 G429 M430 G431 G432 L433 A434 Y435 A436 ASN

- Molecule 1: Major capsid protein (MCP)

Chain aE: 52% 100%

MET A2 G3 G4 L5 S6 V9 A10 Y11 G12 A13 Q14 D15 V16 Y17 L18 T19 G20 N21 P22 Q23 I24 T25 F26 F27 N36 E40 N47 G51 F52 G53 R62 N63 G64 D65 L66 I67 T68 D69 E73 G79 G80 N81 G82 Y86 A89 E90 E91 L92 L93

Q94 D95 V96 E97 L98 E99 I100 G101 G102 Q103 R104 I105 D106 K107 H108 Y109 N110 D111 R114 T115 Y116 D117 A118 L119 F120 R121 M122 N123 D124 D125 R126 R130 R131 D134 N137 N138 E139 L140 K145 Y148 L151 I152 F153 F154 F155 N156 Q157 T158 P159 G160 L161 L165

I166 A167 L168 Q169 Y170 H171 E172 V173 K174 L175 Y176 F177 T178 L179 Q182 V183 N187 Y188 N189 G190 S191 S192 A193 I194 A195 G196 A197 A198 Q199 D207 F210 L211 D212 T213 Q214 E215 R216 T217 R218 F219 A220 E225 Y226 L227 I228 E229 Q230 L231 Q232 F233 T234 E237 T238 A239

T240 P241 S242 A243 T244 T245 Q246 A247 S248 Q249 N250 I251 R252 L253 N254 F255 N256 H257 P258 N267 Y272 G273 Q274 L278 I281 P282 G283 G287 A291 A292 A293 T294 D299 G304 N307 E308 Q309 L310 A311 D314 S315 A316 K317 I318 Q319 L320 N321 G322 Q323 D324

R325 F326 A327 T328 R329 K330 G331 S332 Y333 F334 N335 Q338 P339 Y340 Q341 S342 G345 G350 F356 A357 L358 K359 P360 A361 G362 R363 C369 N370 F371 S372 R373 I374 D375 N376 A377 T378 L379 S380 L381 T382 Y383 K384 S387 I388 D389 A390 T391 A394 A395 V396 L397 G398 N399

T400 E401 T402 A405 A408 L411 T412 A413 L414 A418 R425 I426 M427 S428 G429 M430 G431 G432 L433 A436 M437

- Molecule 1: Major capsid protein (MCP)

Chain aF: 44% 99%

MET ALA G3 G4 L5 S6 Q7 L8 V9 A10 Y11 G12 A13 Q14 D15 V16 Y17 L18 T19 G20 N21 P22 Q23 F27 K28 Y31 R32 R33 E40 S41 I42 Q43 N47 F52 G53 N54 T58 Q59 R62 N63 G64 D65 L66 I67 T68 D69 E73 F74 K78 G79 G80

N81 Y86 E90 E91 Q94 D95 V96 E97 L98 E99 I100 G101 G102 Q103 R104 I105 D106 K107 N110 D111 R121 M122 N123 D124 D125 R126 M132 T133 D134 W135 V136 N137 N138 E139 L140 V141 G142 A143 Q144 K145 Y148 L151 I152 F153 F154 F155 N156 Q157 T158 P159 G160 L161

I166 A167 L168 Q169 Y170 H171 E172 V173 K174 L175 Y176 Q182 V183 Y188 N189 G190 S191 S192 A193 I194 A195 G196 A197 I198 Q199 M202 S203 D207 Y208 D212 T213 Q214 E215 R216 T217 R218 F219 A220 Q221 L222 Q230 T234 E237 T238 A239 T240 P241 S242 A243 T244 T245

Q246 A247 N250 I251 R252 L253 N256 Q274 L278 G283 S286 G287 A288 A291 A292 D299 Y300 G301 G304 T305 Y306 N307 L310 A311 D314 K317 I318 Q319 L320 N321 G322 Q323 D324 R329 K330 G331 F334 N335 K336 V337 Q338 Q341 S342 I343 G344

G345 A349 G350 F356 K359 R363 S366 G367 R373 I374 D375 N376 L381 T382 Y383 K384 T385 C386 S387 I388 D389 A394 A395 V396 L397 G398 N399 T400 T404 A405 K419 L424 R425 I426 M427 S428 G429 M430 A434 Y435 A436 ASN

- Molecule 1: Major capsid protein (MCP)

Chain aG: 59% 99%

MET ALA G3 G4 L5 S6 Q7 L8 V9 A10 Y11 G12 A13 V16 Y17 G20 N21 P22 Q23 F27 K28 Y31 R32 R33 M36 E40 Q43 Q44 T45 I46 N47 G48 S49 F52 G53 N54 K55 R62 N63 G64 D65 L66 I67 T68 D69 E73 F74 V75 L76 T77

K78 G79 G80 N81 G82 Y86 Y87 E91 L92 L93 Q94 D95 V96 E97 L98 E99 I100 G101 G102 Q103 R104 I105 D106 K107 H108 Y109 N110 D111 W112 F113 R114 D117 A118 L119 F120 R121 M122 N123 D124 D125 R126 R130 R131 M132 T133 D134 N137 N138 E139 L140 V141 G142 A143 Q144 K145

R146 F147 Y148 L151 I152 F153 F154 F155 N156 Q157 G160 L161 A162 L163 P164 L165 L168 Q169 Y170 H171 E172 V173 K174 L175 Y176 F177 T178 L179 A180 S181 Q182 V183 Q184 Y188 N189 G190 S191 S192 A193 I194 A195 G196 A197 A198 M202 D207 Y208 I209 F210 L211 D212 T213 Q214 E215

R216 T217 R218 F219 A220 Q221 L222 E225 Y226 L227 I228 E229 Q230 F233 T234 G235 S236 E237 T238 A239 S242 A243 T244 T245 Q246 A247 S248 Q249 N250 I251 R252 L253 N254 F255 N256 K260 F266 N267 N268 P269 T270 N271 Y272 G273 Q274 L278 T281 P282 G283 A284 C285 S286 G287

A288 G289 T290 A291 A292 A293 P298 D299 Y300 G301 E308 Q309 L310 A311 V312 L313 D314 K317 I318 Q319 L320 N321 G322 Q323 D324 R325 F326 A327 T328 R329 K330 G331 S332 Y333 F334 N335 K336 Q341 S342 I343 G344 A349 G350 V351 Y352 L353 L358 K359 P360 A361 G362 R363 S366

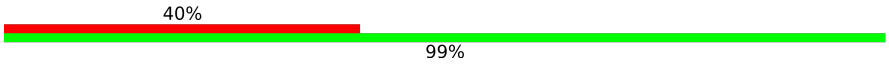
G367 T368 C369 N370 F371 S372 R373 I374 D375 N376 L379 S380 L381 T382 Y383 K384 D389 A390 T391 A394 A395 V396 L397 G398 N399 T400 E401 T402 V403 T407 L410 A413 L414 N415 K419 N420 R425 S428 G429 M430 G431 A434 Y435 A436 N437

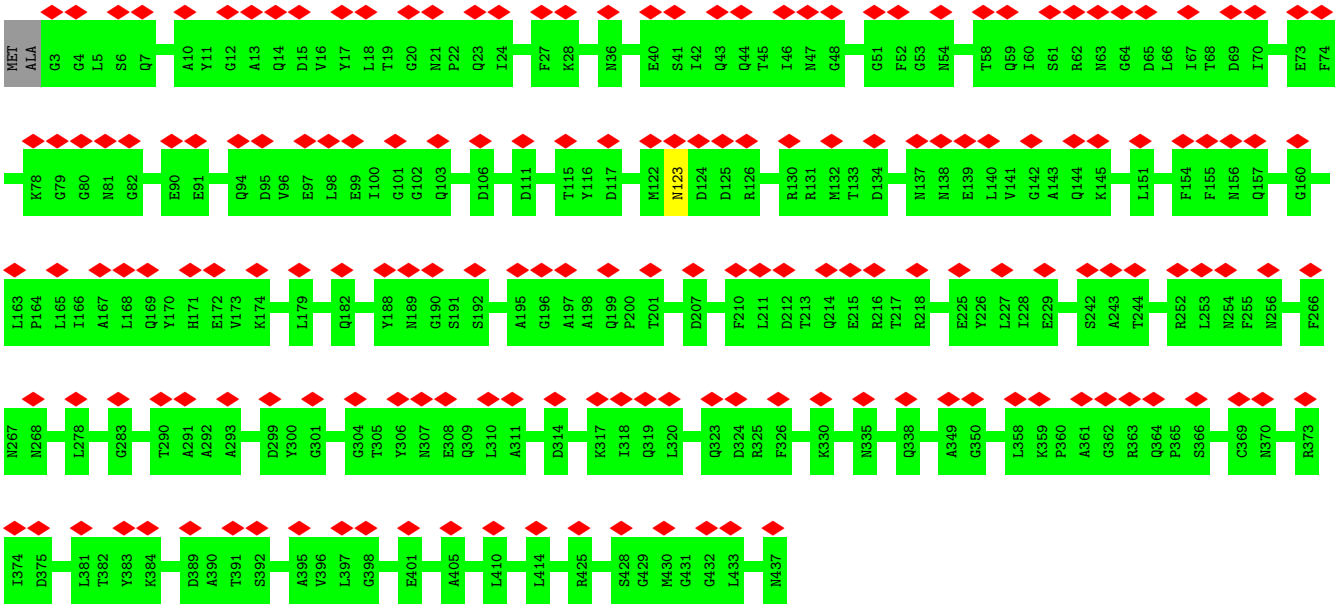
- Molecule 1: Major capsid protein (MCP)

Chain aH: 38% 99%

- Molecule 1: Major capsid protein (MCP)

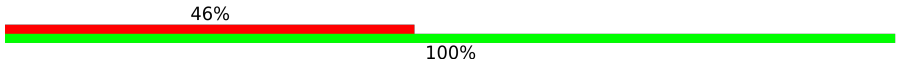
Chain aI:

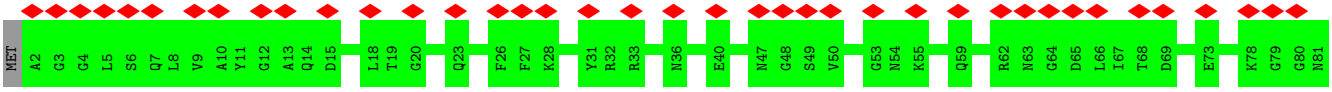


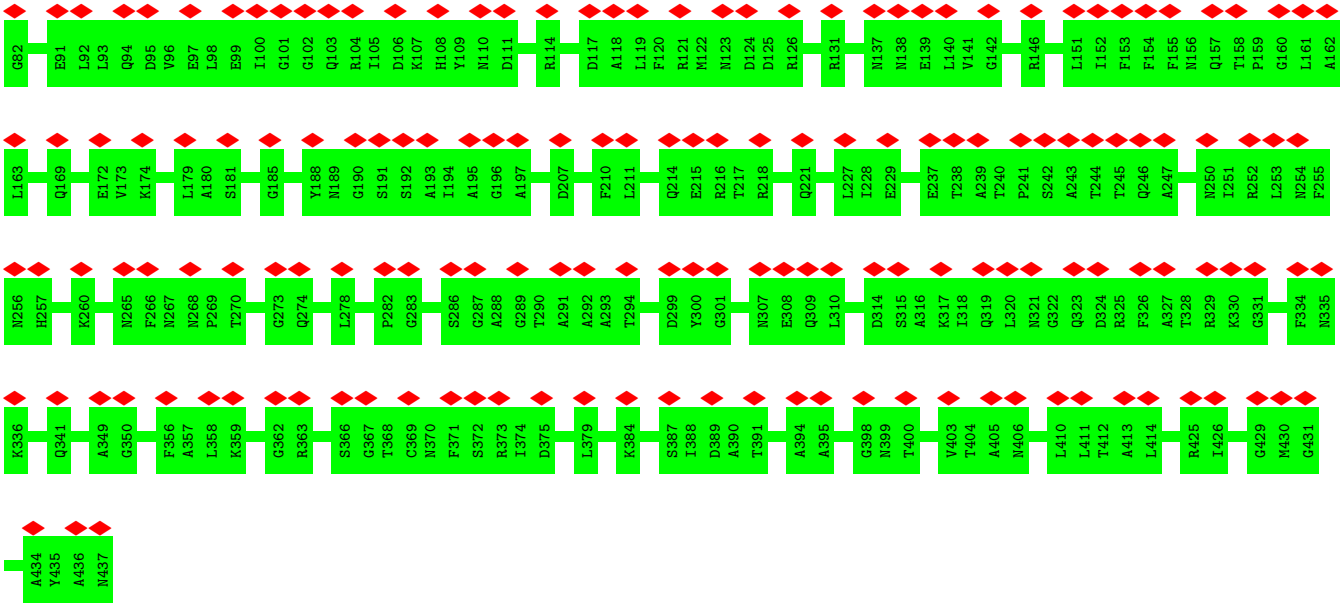


- Molecule 1: Major capsid protein (MCP)

Chain aJ:

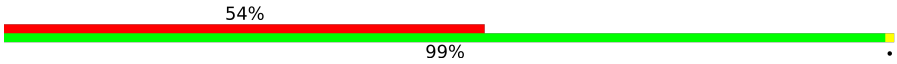


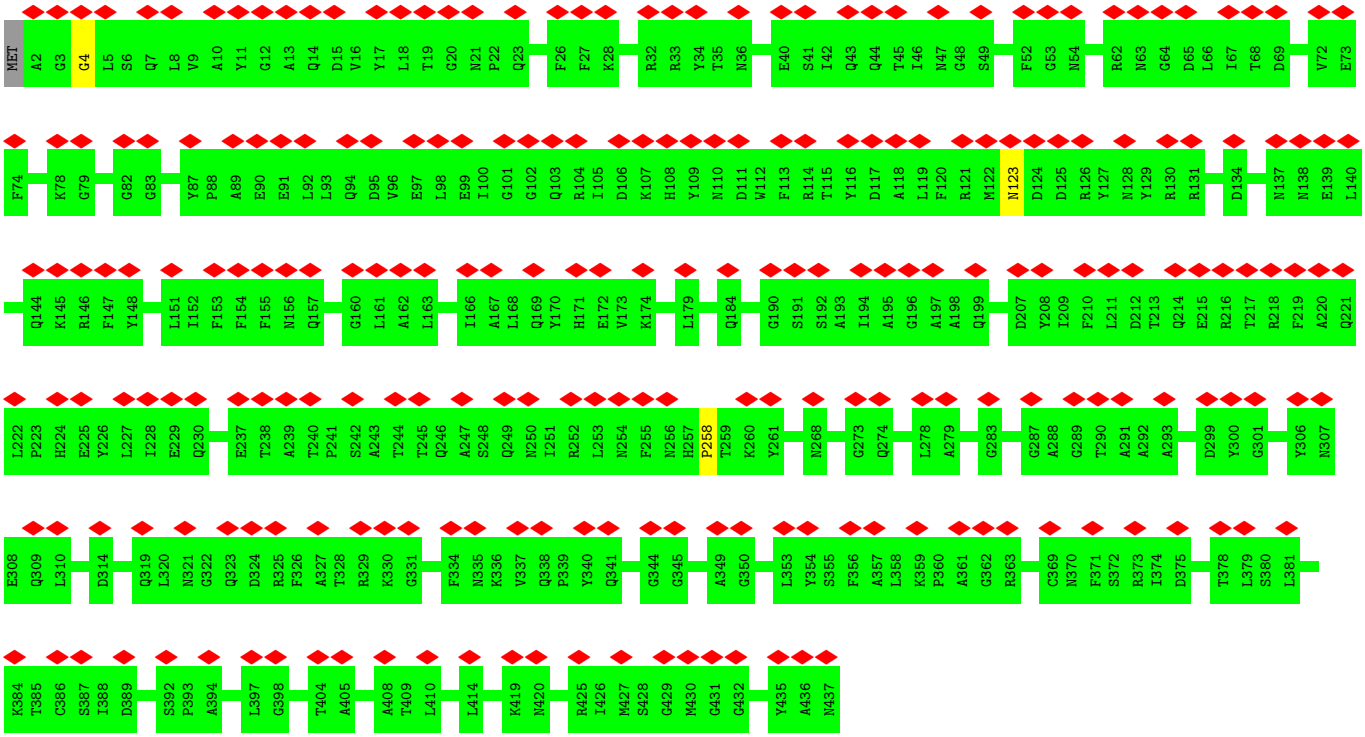




- Molecule 1: Major capsid protein (MCP)

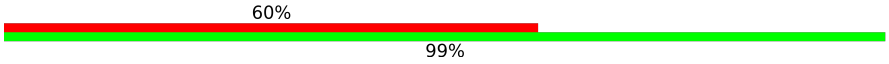
Chain aK:

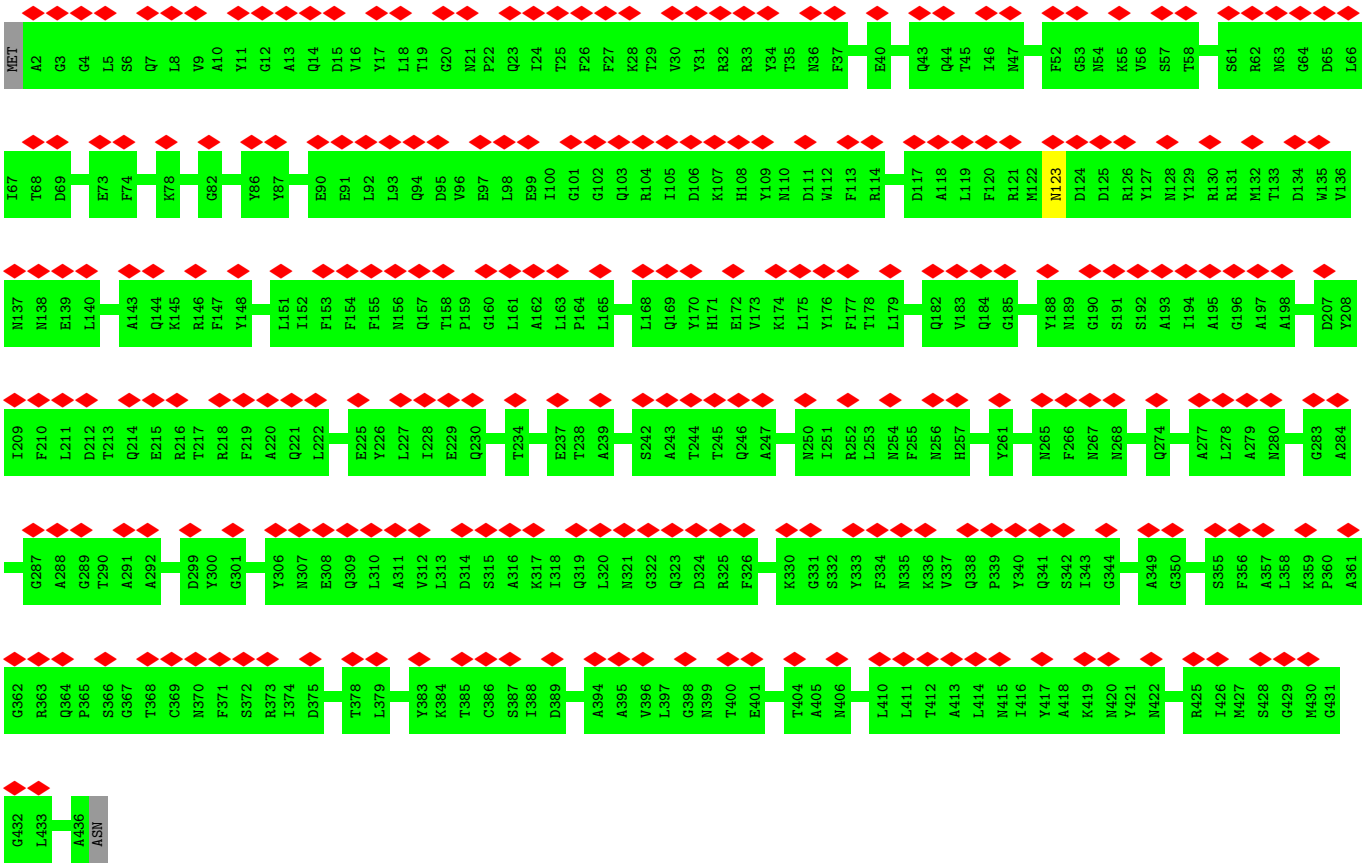




- Molecule 1: Major capsid protein (MCP)

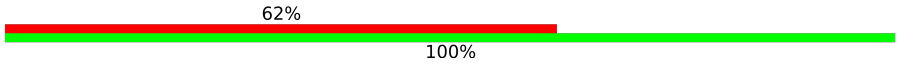
Chain aL:

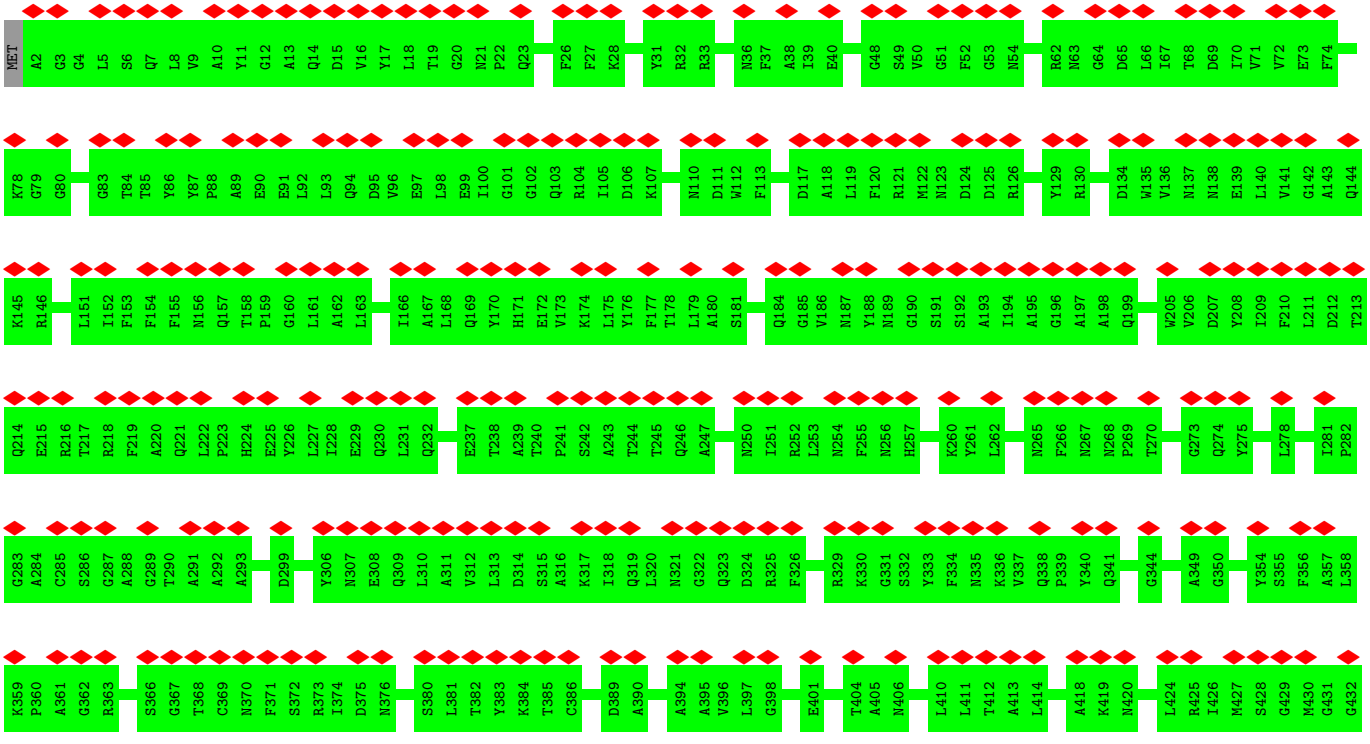


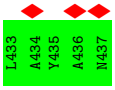


- Molecule 1: Major capsid protein (MCP)

Chain aM:

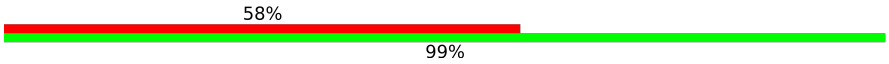


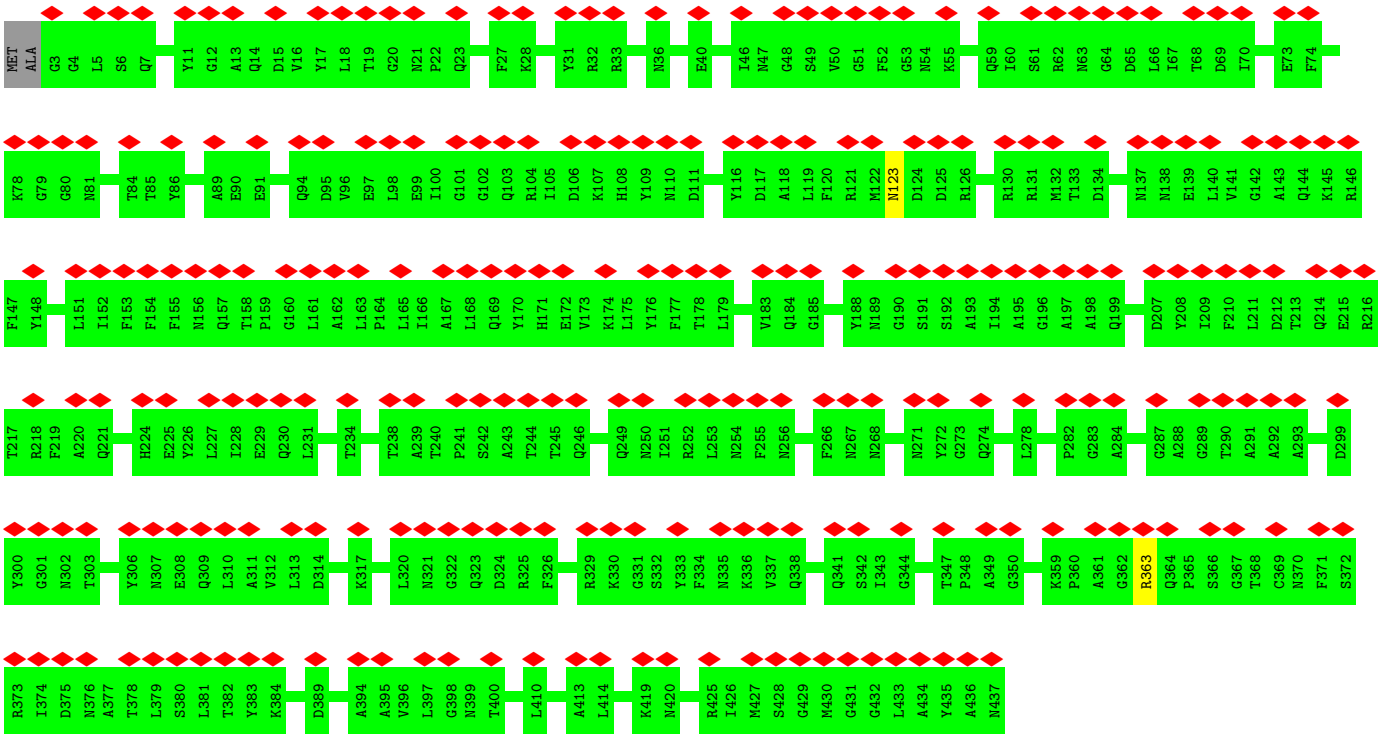




• Molecule 1: Major capsid protein (MCP)

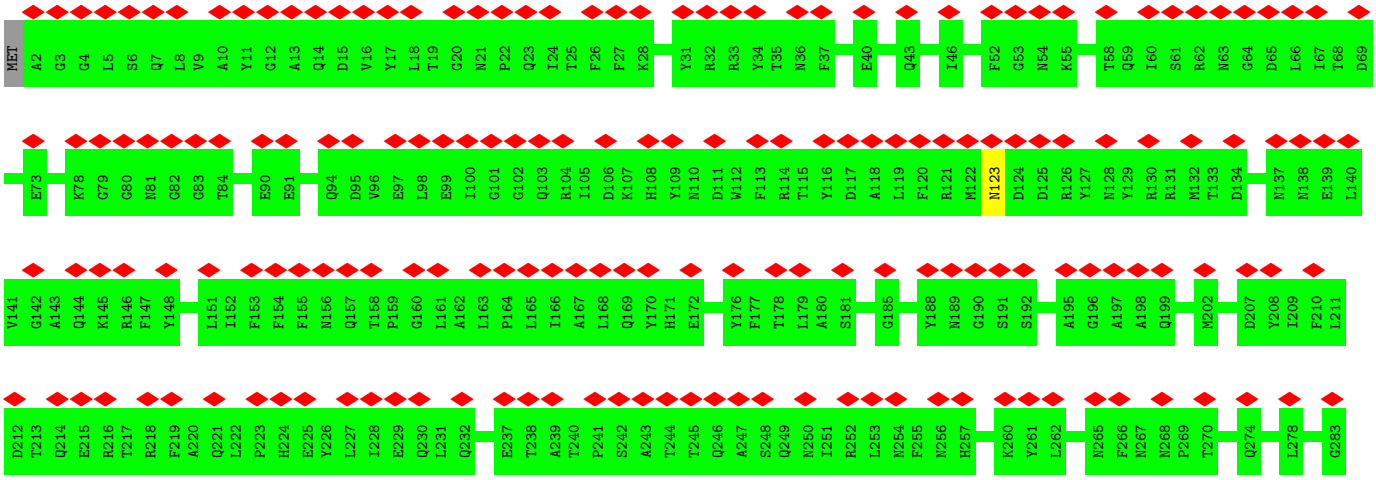
Chain aN:

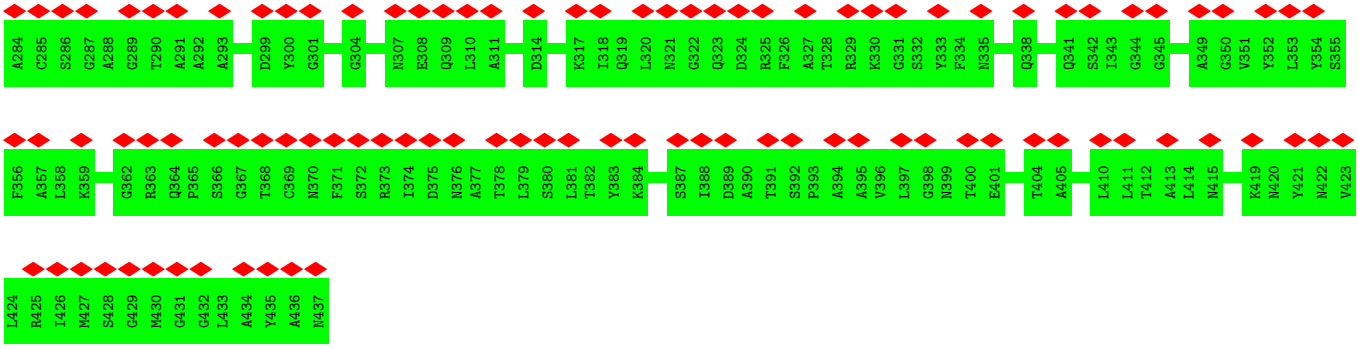




• Molecule 1: Major capsid protein (MCP)

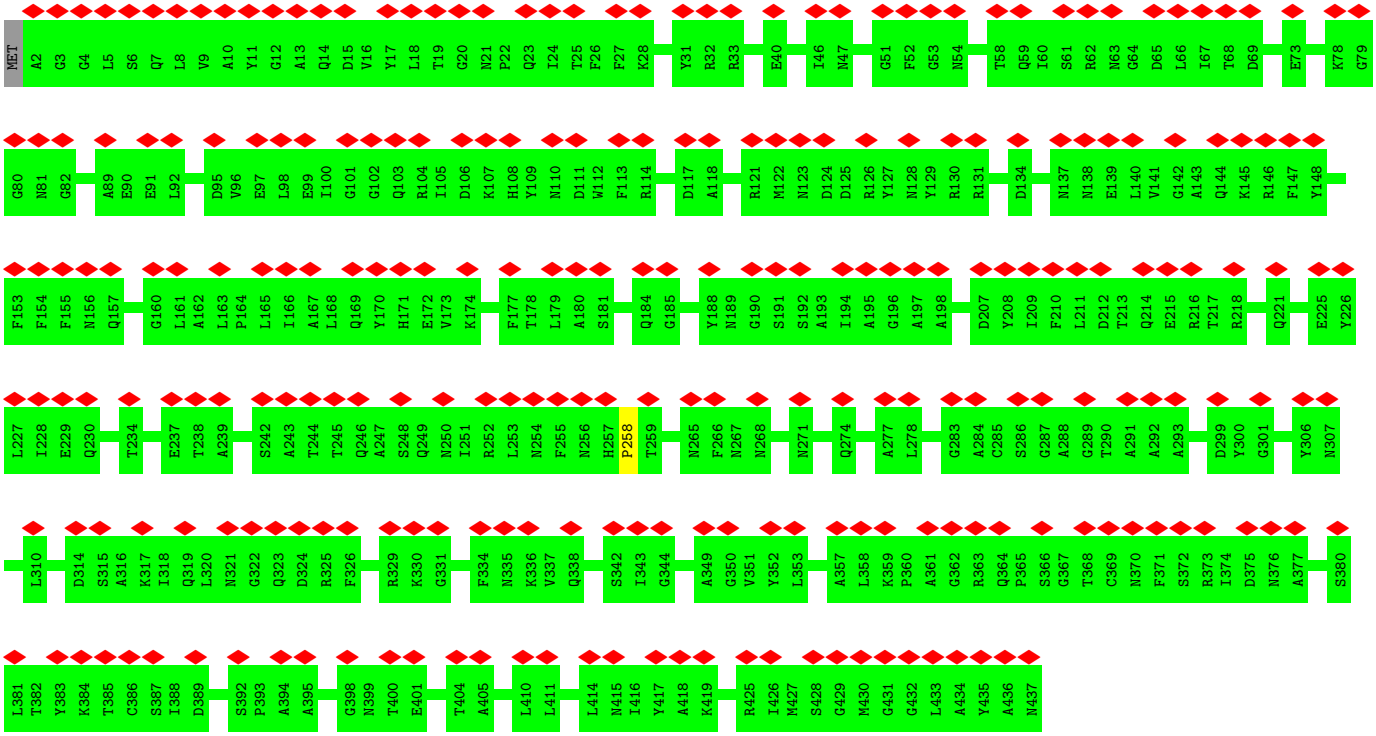
Chain aO:





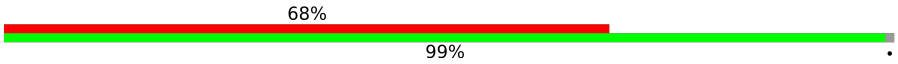
- Molecule 1: Major capsid protein (MCP)

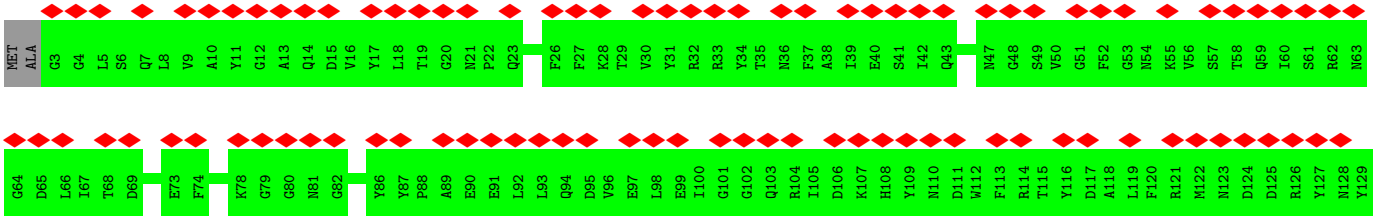
Chain aP:



- Molecule 1: Major capsid protein (MCP)

Chain aQ:





R130 R131 M132 W135 V136 N137 N138 E139 L140 V141 G142 A143 Q144 K145 R146 F147 Y148 L151 I152 F153 F154 F155 N156 Q157 G160 L161 A162 L163 P164 L165 I166 A167 L168 Q169 Y170 H171 E172 V173 K174 L175 Y176 F177 T178 L179 A180 S181 Q182 V183 Q184 G185 Y188 N189 G190 S191 S192 A193

I194 A195 G196 A197 A198 Q199 P200 T201 M202 D207 Y208 I209 F210 L211 D212 T213 Q214 E215 R216 T217 R218 F219 A220 Q221 E225 E229 Q230 L231 Q232 F233 T234 E237 T238 A239 S242 A243 T244 T245 Q246 A247 S248 Q249 N250 I251 R252 L253 N254 F255 N256 H257 P258 T259 K260 N265

F266 N267 N268 P269 T270 N271 Y272 G273 Q274 A277 L278 G283 A284 C285 S286 G287 A288 G289 T290 A291 A292 A293 T294 D299 G304 N307 E308 Q309 L310 A311 V312 L313 D314 K317 I318 Q319 L320 N321 G322 Q323 D324 R325 F326 A327 T328 R329 K330 G331 S332 Y333 F334 N335 K336 V337

Q338 P339 Y340 Q341 S342 I343 G344 G345 A349 G350 V351 Y352 L353 Y354 S355 F356 A357 L358 K359 G362 R363 Q364 P365 S366 G367 T368 C369 N370 F371 S372 R373 I374 D375 N376 A377 T378 L379 S380 L381 T382 Y383 K384 D389 A390 T391 A394 A395 V396 L397 G398 N399 T400 E401 T402 V403 T404

A405 A408 T409 L410 L411 T412 A413 L414 N415 A418 K419 N420 Y421 N422 R425 S428 G429 M430 G431 G432 L433 A434 Y435 A436 ASN

- Molecule 1: Major capsid protein (MCP)

Chain aR: 71% 99%

MET A2 G3 G4 L5 S6 Q7 L8 V9 A10 Y11 G12 A13 Q14 D15 V16 Y17 L18 T19 G20 N21 P22 Q23 I24 T25 F26 F27 K28 T29 V30 Y31 R32 R33 Y34 T35 N36 F37 A38 I39 E40 S41 Q44 T45 I46 N47 G48 S49 V50 G51 F52 G53 N54 Q59 R62 N63 G64 D65

L66 I67 T68 D69 I70 E73 K78 G79 G80 N81 G82 G83 T84 T85 Y86 Y87 P88 A89 E90 E91 L92 L93 Q94 D95 V96 E97 L98 E99 I100 G101 G102 Q103 R104 I105 D106 K107 H108 Y109 N110 D111 W112 F113 R114 T115 Y116 D117 A118 L119 F120 R121 M122 N123 D124 D125 R126 Y127 N128 Y129

R130 R131 M132 T133 D134 W135 V136 N137 N138 E139 L140 V141 G142 A143 Q144 K145 R146 F147 L151 I152 F153 F154 F155 N156 Q157 T158 P159 G160 L161 A162 L163 P164 L165 I166 A167 L168 Q169 Y170 H171 E172 V173 K174 L175 Y176 F177 T178 L179 A180 S181 Q182 V183 Q184 G185 Y188 N189 G190 S191 S192

A193 I194 A195 G196 A197 A198 Q199 W205 V206 D207 Y208 I209 F210 L211 D212 T213 Q214 E215 R216 T217 R218 F219 L222 P223 H224 E225 Y226 L227 I228 E229 Q230 L231 Q232 F233 T234 G235 S236 E237 T238 A239 T240 P241 S242 A243 T244 T245 Q246 A247 S248 Q249 N250 I251 R252 L253 N254 F255 N256 H257

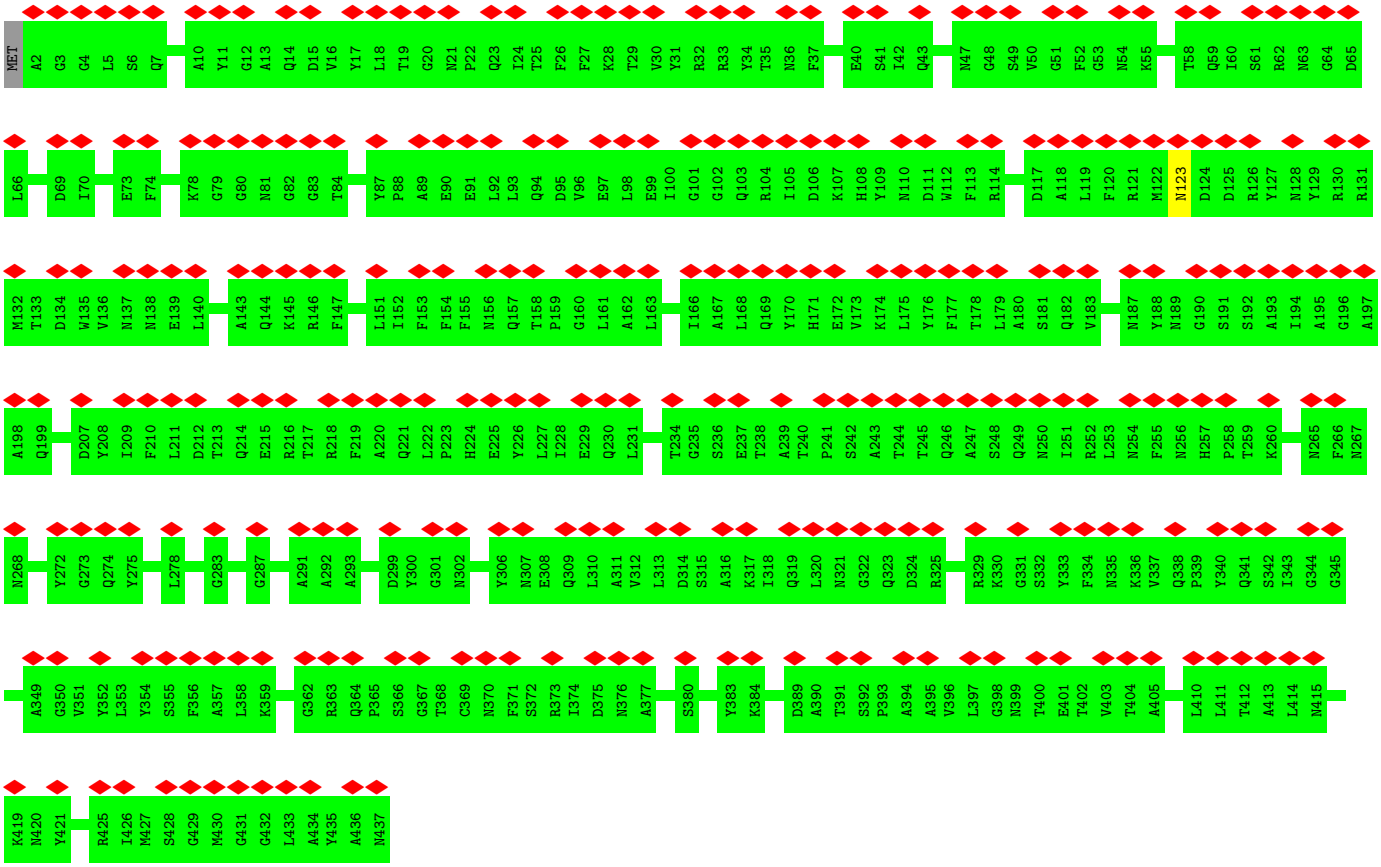
P258 T259 K260 N265 F266 N267 N268 N271 Y272 G273 Q274 Y275 L278 A279 A284 G287 A288 G289 T290 A291 A292 A293 D299 Y300 G301 N302 Y306 N307 E308 Q309 L310 A311 V312 L313 D314 S315 A316 K317 I318 Q319 L320 N321 G322 Q323 D324 R325 F326 A327 T328 R329 K330 Y333

F334 N335 K336 V337 Q338 P339 Y340 Q341 S342 I343 G344 G345 A349 G350 V351 Y352 L353 Y354 S355 F356 A357 L358 K359 P360 A361 G362 R363 Q364 P365 S366 G367 T368 C369 N370 F371 S372 R373 I374 D375 N376 A377 T378 L379 S380 L381 T382 Y383 K384 T385 C386 S387 I388 D389 A390 T391 S392 P393 A394 A395

V396 L397 G398 N399 T400 E401 T402 V403 T404 A405 N406 T407 L410 L414 N415 A418 K419 N420 Y421 N422 V423 L424 R425 I426 M427 S428 G429 M430 G431 G432 L433 A434 Y435 A436 N437

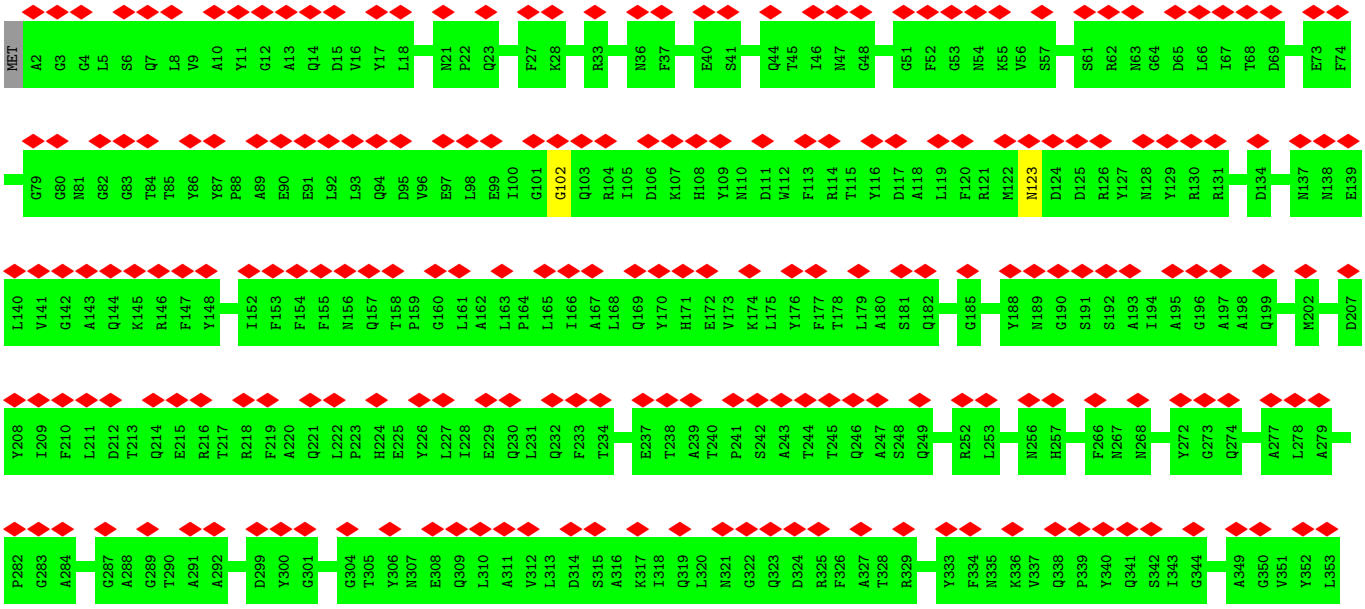
- Molecule 1: Major capsid protein (MCP)

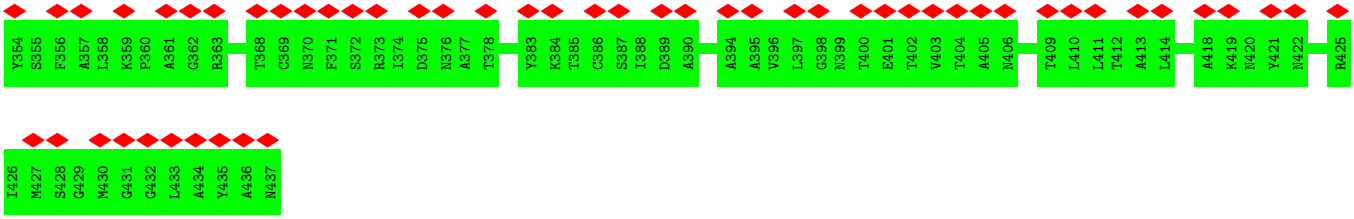
Chain aS: 65% 100%



- Molecule 1: Major capsid protein (MCP)

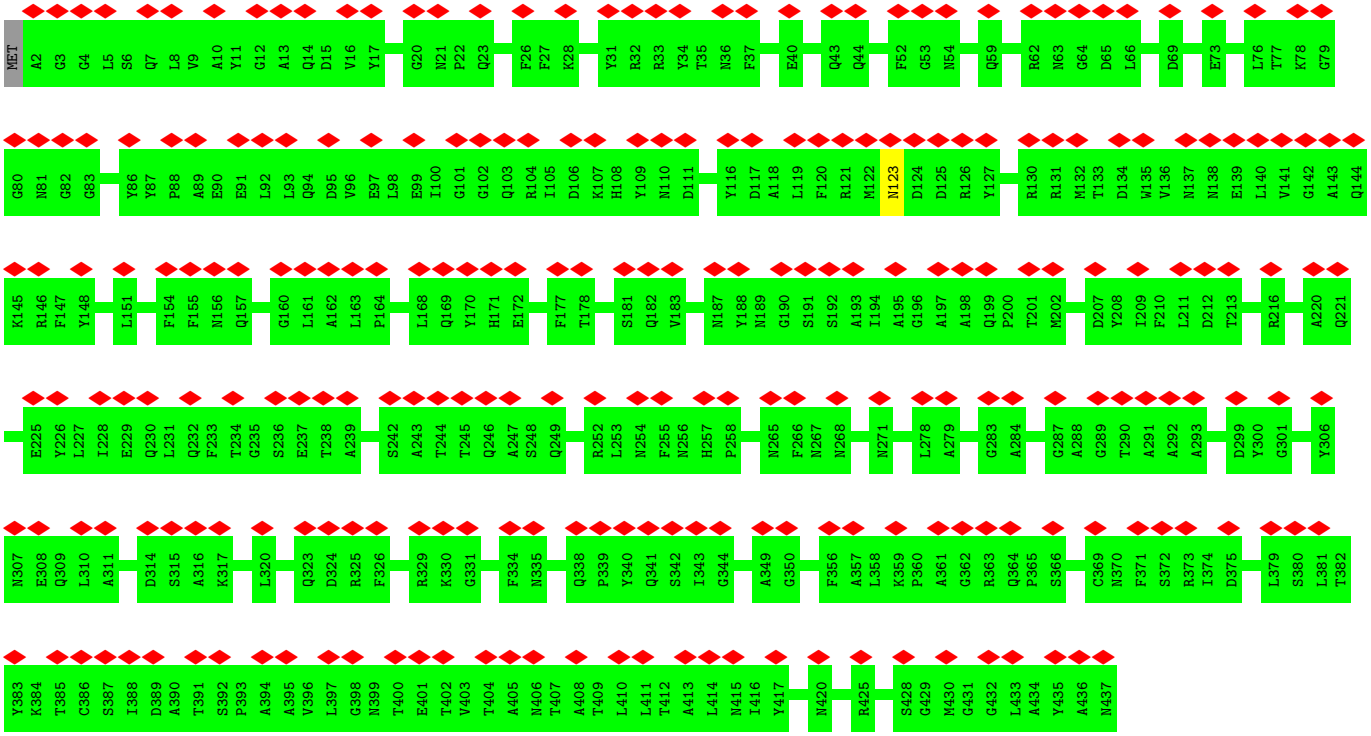
Chain aT: 62% 99%





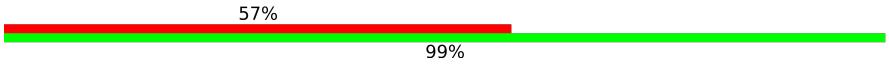
- Molecule 1: Major capsid protein (MCP)

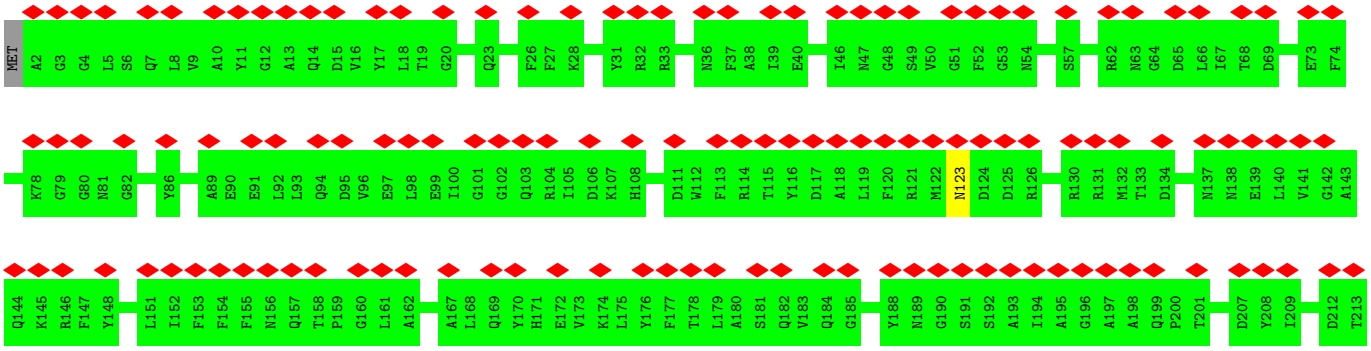
Chain aU:

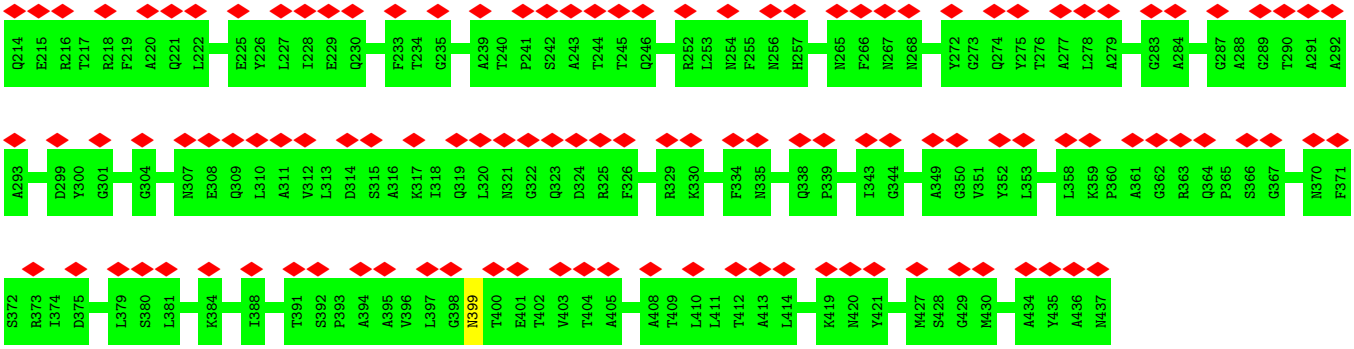


- Molecule 1: Major capsid protein (MCP)

Chain aV:

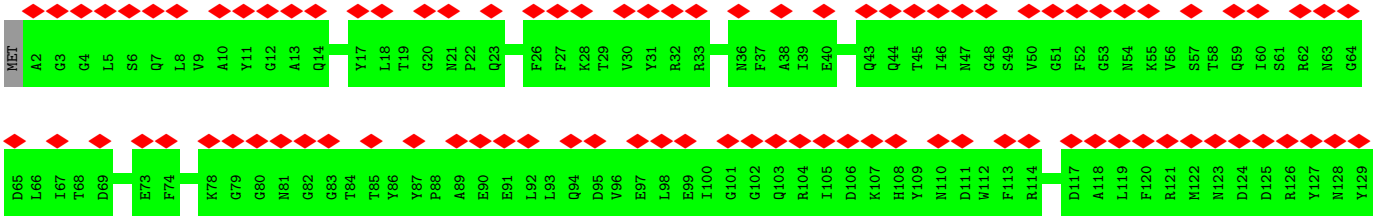






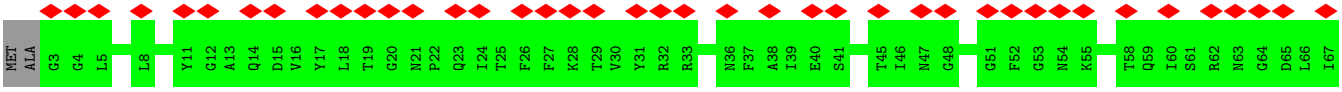
- Molecule 1: Major capsid protein (MCP)

Chain aW:



- Molecule 1: Major capsid protein (MCP)

Chain aX:



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M132 T133 D134 W135 V136 N137 N138 E139 L140 V141 G142 A143 Q144 K145 R146 F147 Y148 L151 I152 F153 F154 F155 N156 Q157 G160 L161 I166 A167 L168 Q169 Y170 H171 E172 V173 K174 L175 Y176 F177 T178 L179 A180 S181 Q182 V183 Q184 G185 V186 N187 Y188 N189 G190 S191 S192 A193 I194 A195 G196

A197 A198 Q199 M202 W205 V206 D207 Y208 I209 F210 L211 D212 T213 Q214 E215 R216 T217 R218 Q221 L222 P223 H224 E225 Y226 L227 I228 E229 Q230 F233 T234 G235 S236 E237 T238 A239 T240 P241 S242 A243 T244 T245 Q246 A247 S248 Q249 N250 I251 R252 L253 N254 F255 N256 H257 K260 Y261

L262 A263 W264 N265 F266 N267 N268 P269 T270 N271 Y272 G273 Q274 Y275 T276 A277 L278 A279 N280 G283 A284 G287 A288 G289 T290 A291 A292 A293 P298 D299 N302 T303 G304 T305 Y306 N307 E308 Q309 L310 A311 V312 L313 D314 S315 A316 K317 I318 Q319 L320 N321 G322 Q323 D324 R325 F326 A327

T328 R329 K330 G331 S332 Y333 F334 N335 K336 V337 Q338 P339 Y340 Q341 S342 I343 G344 G345 A349 G350 Y354 S355 F356 A357 L358 K359 P360 A361 G362 R363 Q364 P365 S366 G367 T368 C369 N370 F371 S372 R373 I374 D375 N376 A377 T378 L379 S380 L381 T382 Y383 K384 T385 C386 S387 I388 D389 S392

P393 A394 A395 V396 L397 G398 N399 T400 E401 T402 V403 T404 A405 N406 T407 L410 L411 T412 A413 L414 N415 I416 Y417 A418 K419 N420 Y421 R425 I426 M427 S428 G429 M430 G431 G432 L433 A434 Y435 A436 N437

- Molecule 1: Major capsid protein (MCP)

Chain aY: 72% 100%

MET A2 G3 G4 L5 S6 Q7 L8 V9 A10 Y11 G12 A13 Q14 D15 V16 Y17 L18 T19 G20 N21 P22 Q23 I24 T25 F26 F27 K28 T29 V30 Y31 R32 R33 Y34 T35 N36 F37 E40 S41 I42 T45 I46 N47 G48 S49 V50 G51 F52 G53 R62 N63 G64 D65 L66 I67 T68 D69

E73 L76 T77 K78 G79 G80 N81 G82 G83 T84 T85 Y86 Y87 E90 E91 L92 L93 Q94 D95 V96 E97 L98 E99 I100 G101 G102 Q103 R104 I105 D106 K107 H108 Y109 N110 D111 W112 F113 R114 T115 Y116 D117 A118 L119 F120 R121 M122 N123 D124 D125 R126 Y127 N128 Y129 R130 R131 D134

W135 V136 N137 N138 E139 L140 V141 G142 A143 Q144 K145 R146 F147 Y148 L151 I152 F153 F154 F155 N156 Q157 T158 P159 G160 L161 A162 L163 I166 A167 L168 Q169 Y170 H171 E172 V173 K174 F177 T178 L179 A180 S181 Q184 G185 Y188 N189 G190 S191 S192 A193 I194 A195 G196 A197 A198 Q199

P200 T201 M202 D207 Y208 I209 F210 L211 D212 T213 Q214 E215 R216 T217 R218 F219 A220 Q221 L222 E225 Y226 L227 I228 E229 Q230 L231 Q232 F233 S236 E237 T238 A239 T240 P241 S242 A243 T244 T245 Q246 A247 S248 Q249 N250 I251 R252 L253 N254 F255 N256 H257 K260 Y261 L262 N265 F266

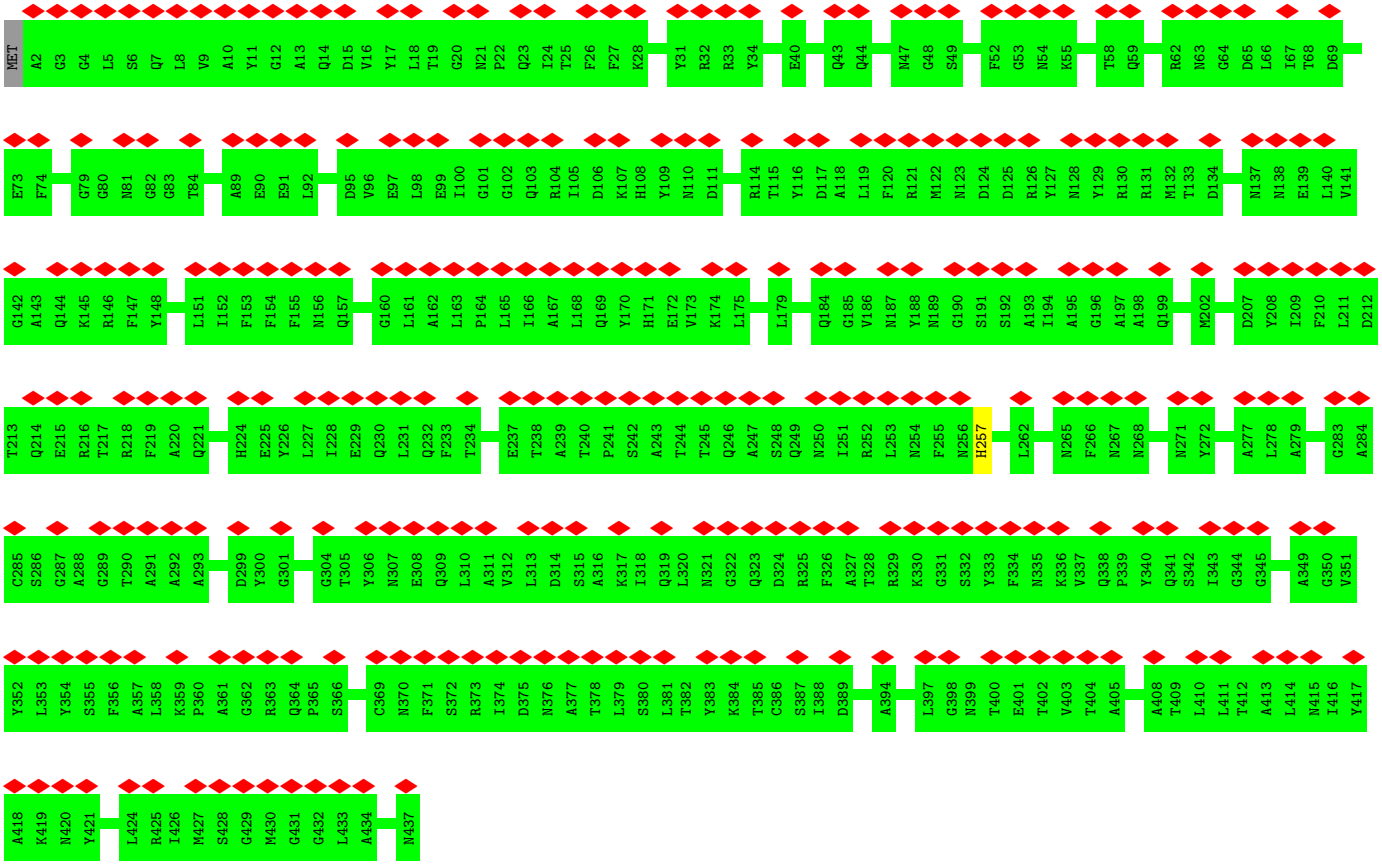
N267 N268 N271 Y272 G273 Q274 Y275 L278 A279 N280 I281 P282 G283 A284 C285 S286 G287 A288 G289 T290 A291 A292 A293 D299 Y300 G301 N302 T303 Y306 N307 E308 Q309 L310 A311 V312 L313 D314 S315 A316 K317 I318 Q319 L320 N321 G322 Q323 D324 R325 F326 A327 T328 B329 K330 G331 S332 Y333

F334 N335 K336 V337 Q338 Q341 S342 I343 G344 G345 A349 G350 V351 Y352 L353 Y354 S355 F356 A357 L358 K359 P360 A361 G362 R363 Q364 P365 S366 G367 T368 C369 N370 F371 S372 R373 I374 D375 N376 A377 T378 L379 S380 L381 T382 Y383 K384 T385 C386 D389 A390 T391 S392 P393 A394 A395 V396 L397

G398 N399 T400 E401 T404 A405 N406 T407 A408 T409 L410 L411 T412 A413 L414 N415 K419 N422 R425 I426 M427 S428 G429 M430 G431 G432 L433 A434 Y435 A436 N437

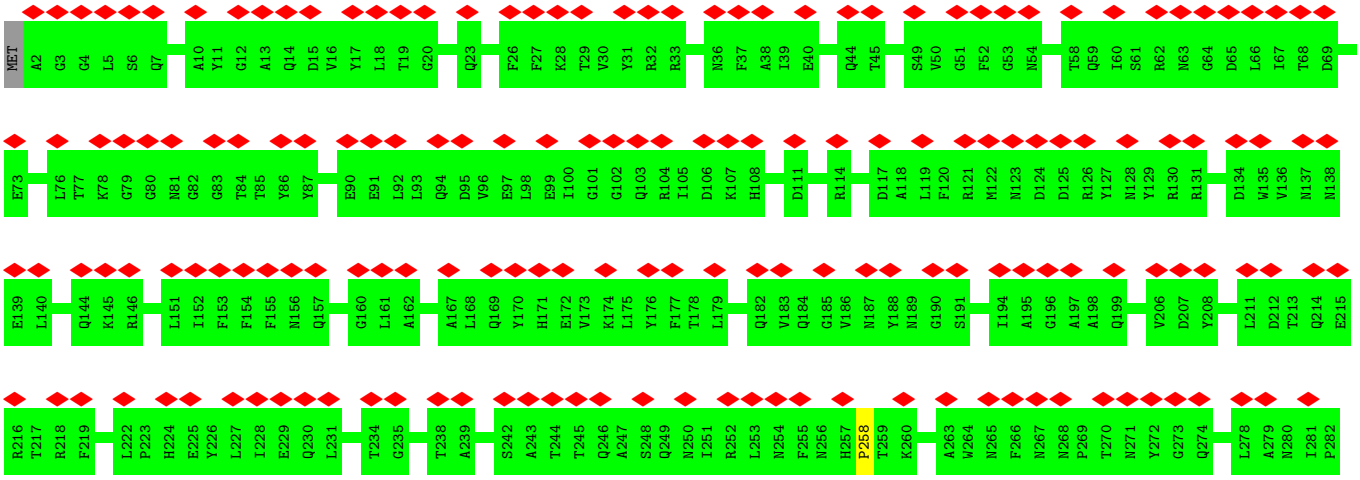
• Molecule 1: Major capsid protein (MCP)

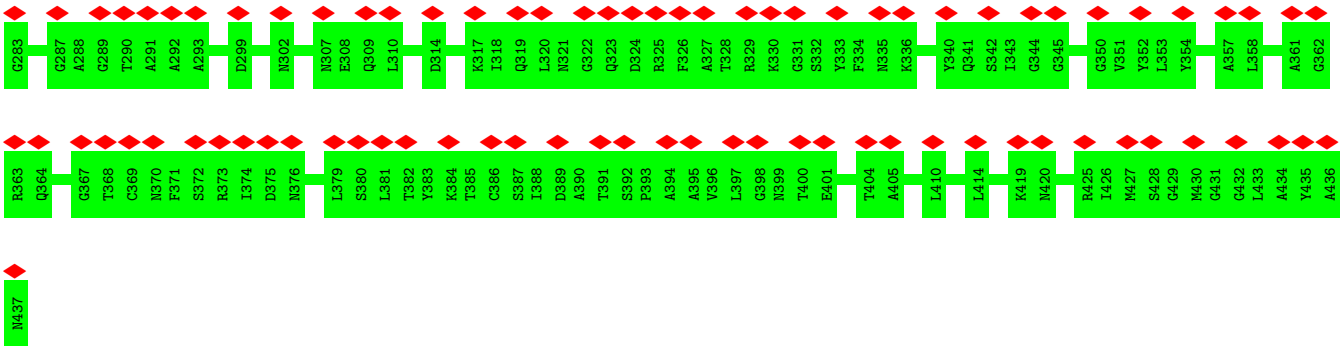
Chain aZ: 66% 100%



• Molecule 1: Major capsid protein (MCP)

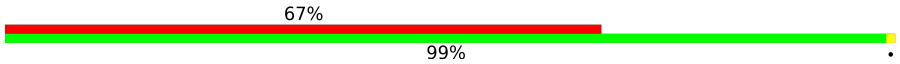
Chain ba: 57% 100%

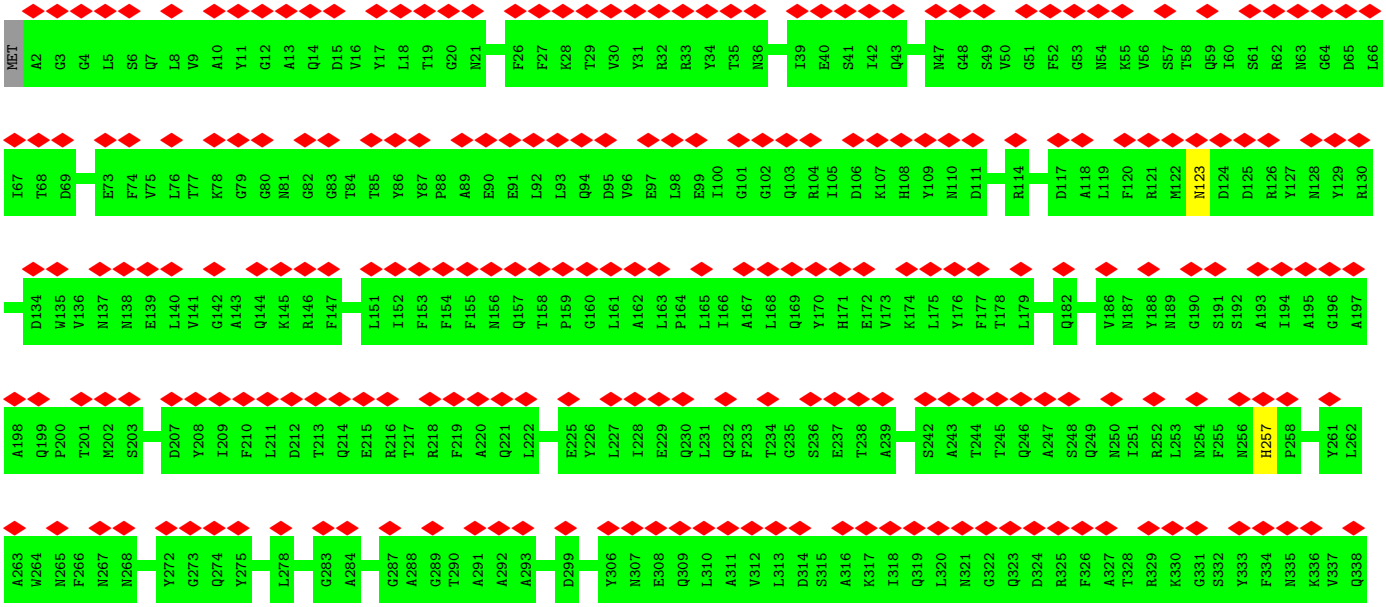




• Molecule 1: Major capsid protein (MCP)

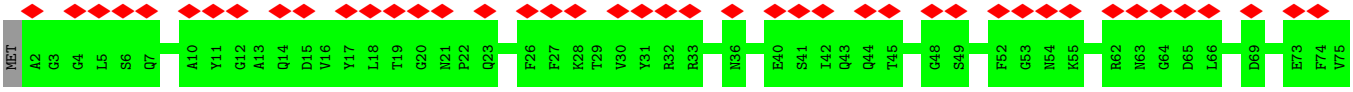
Chain bb:

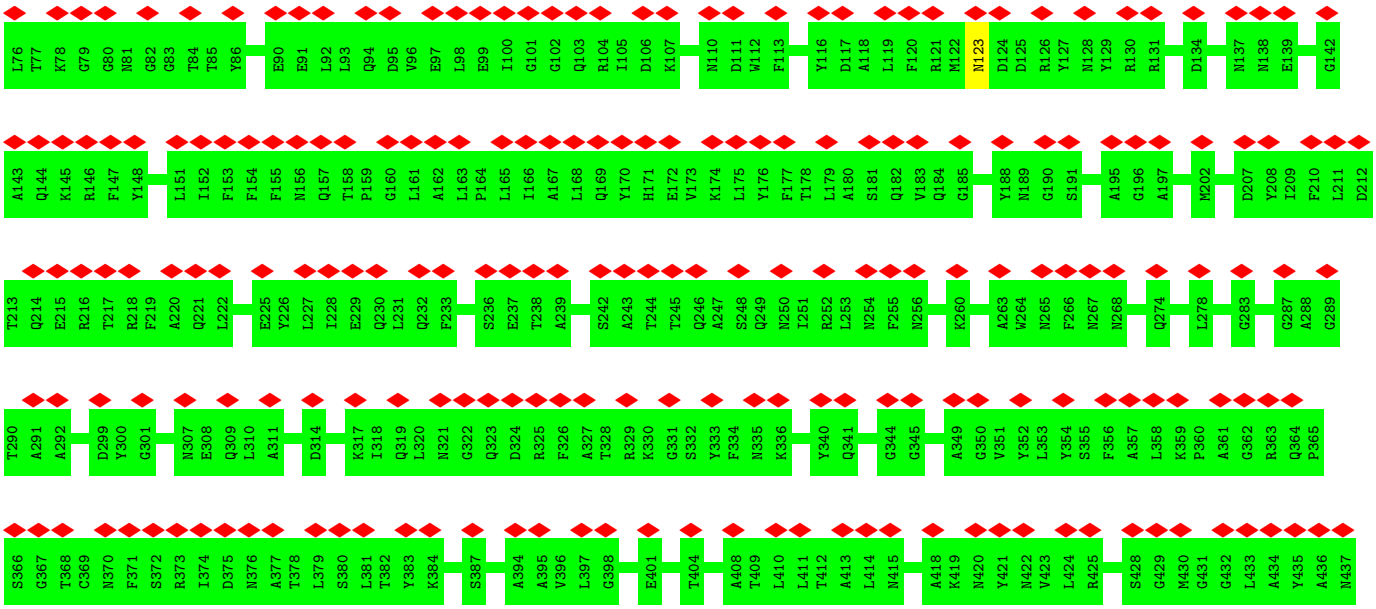




• Molecule 1: Major capsid protein (MCP)

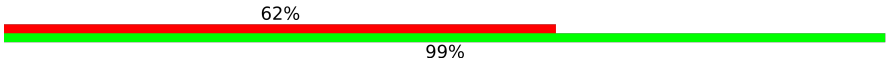
Chain bc:

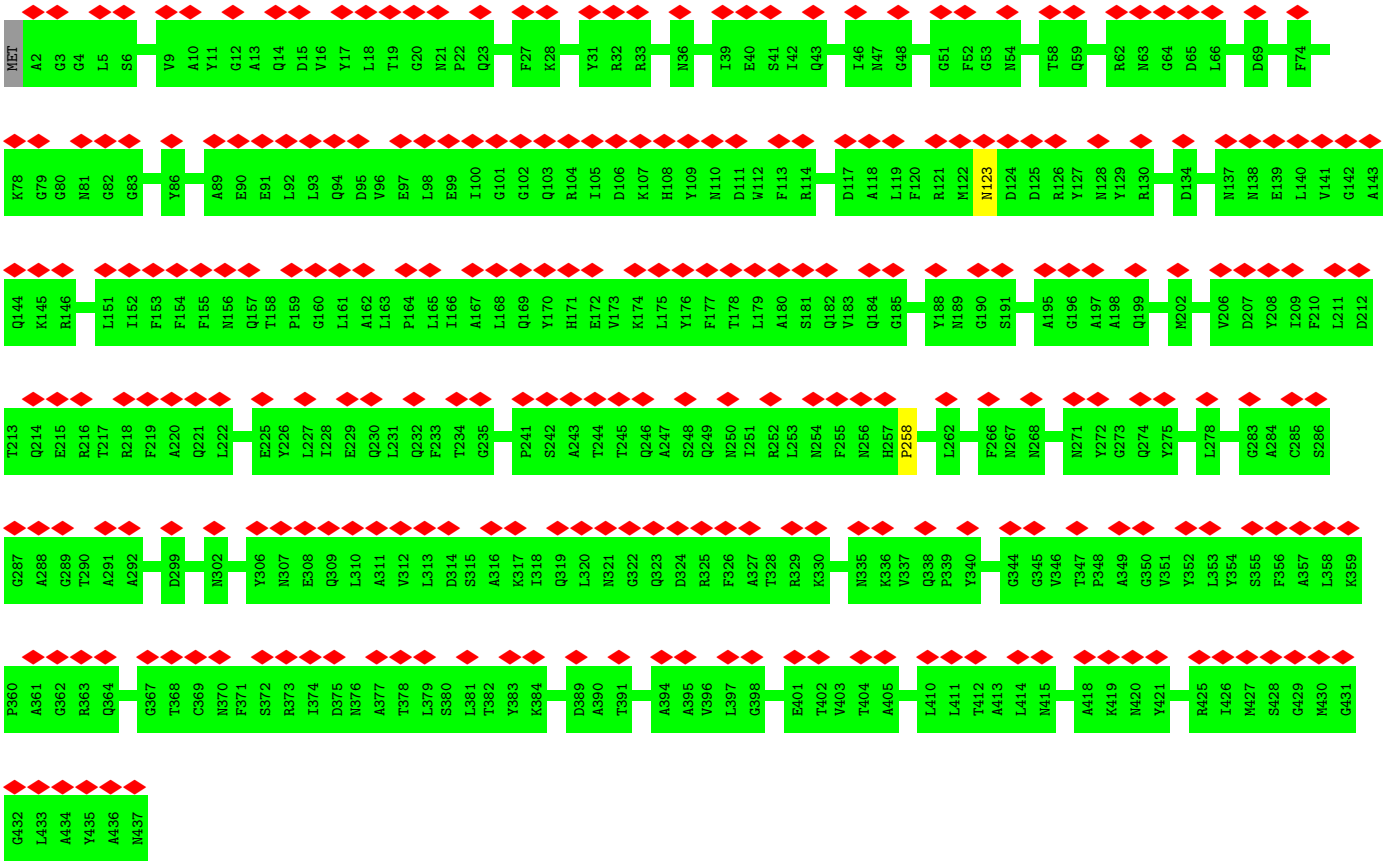




- Molecule 1: Major capsid protein (MCP)

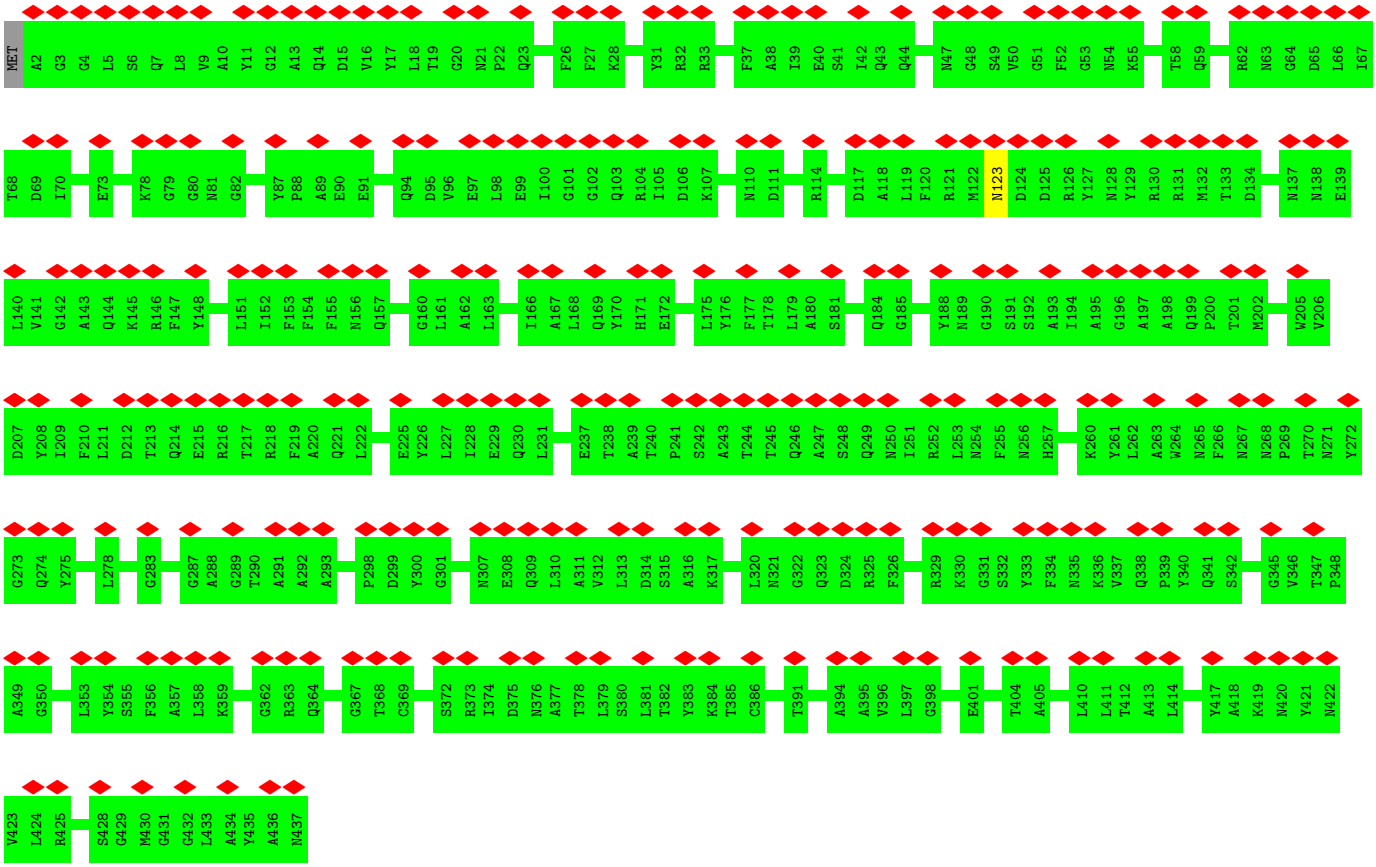
Chain bd:





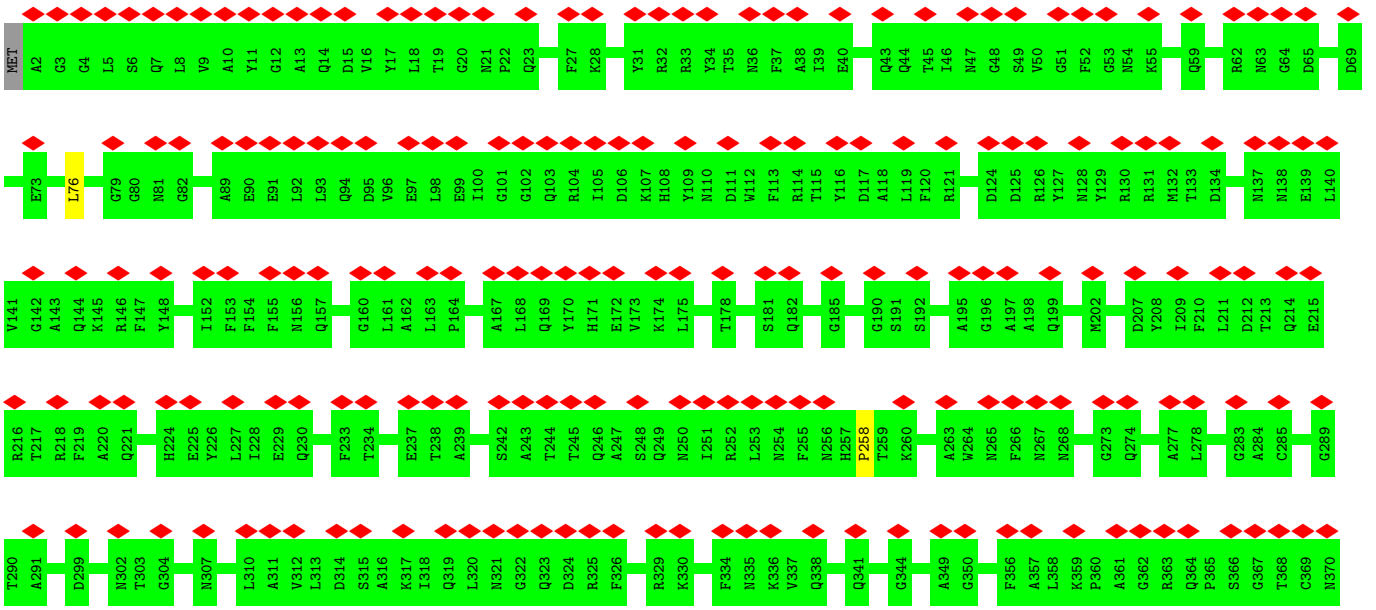
- Molecule 1: Major capsid protein (MCP)

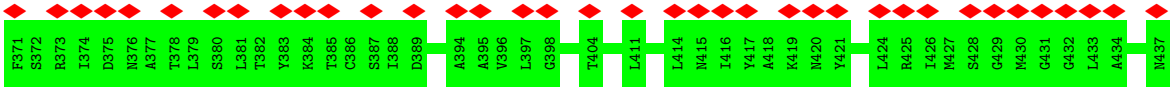
Chain be: 61% 100%



- Molecule 1: Major capsid protein (MCP)

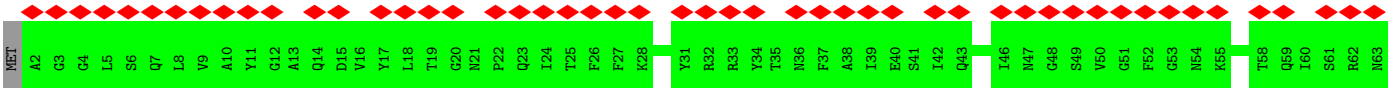
Chain bf: 55% 99%

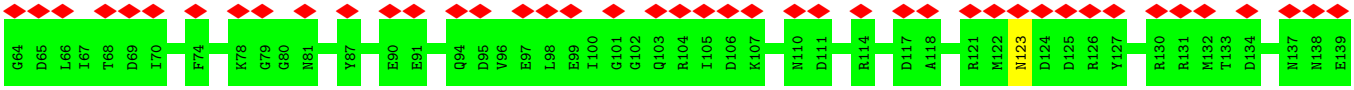


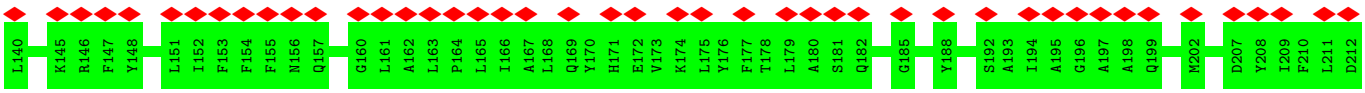


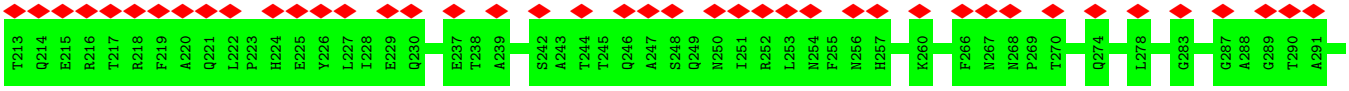
• Molecule 1: Major capsid protein (MCP)

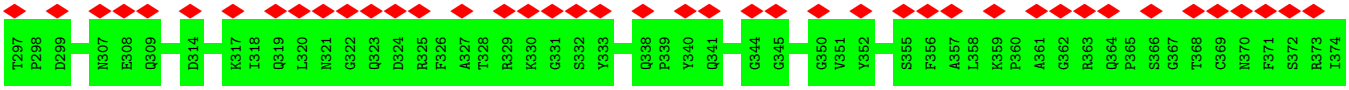
Chain bg:

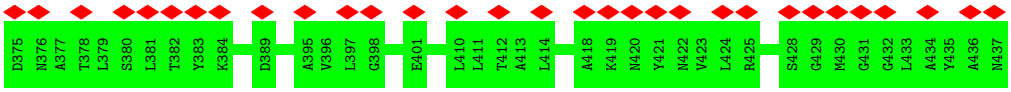






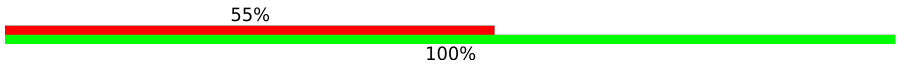


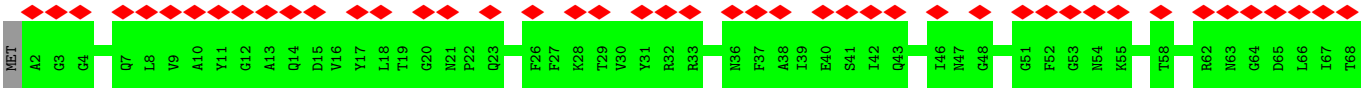


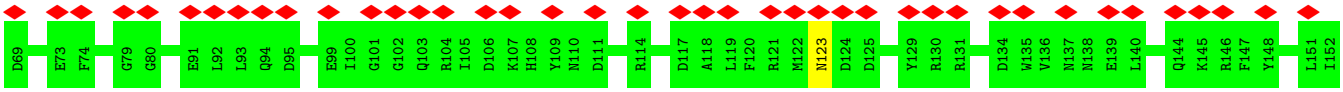


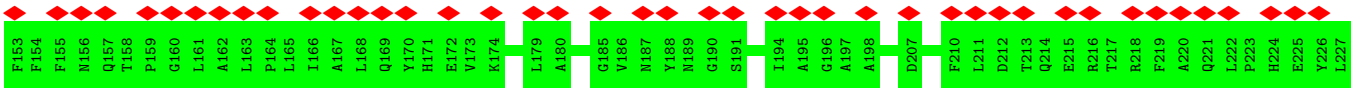
• Molecule 1: Major capsid protein (MCP)

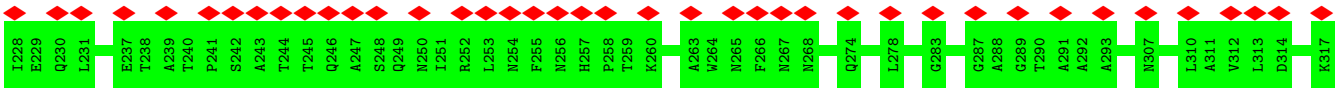
Chain bh:

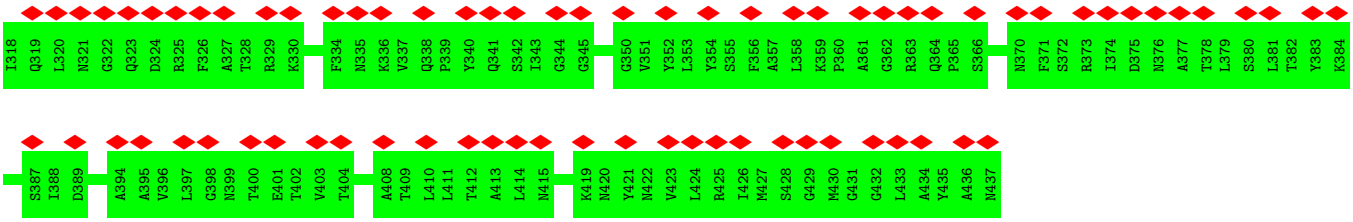






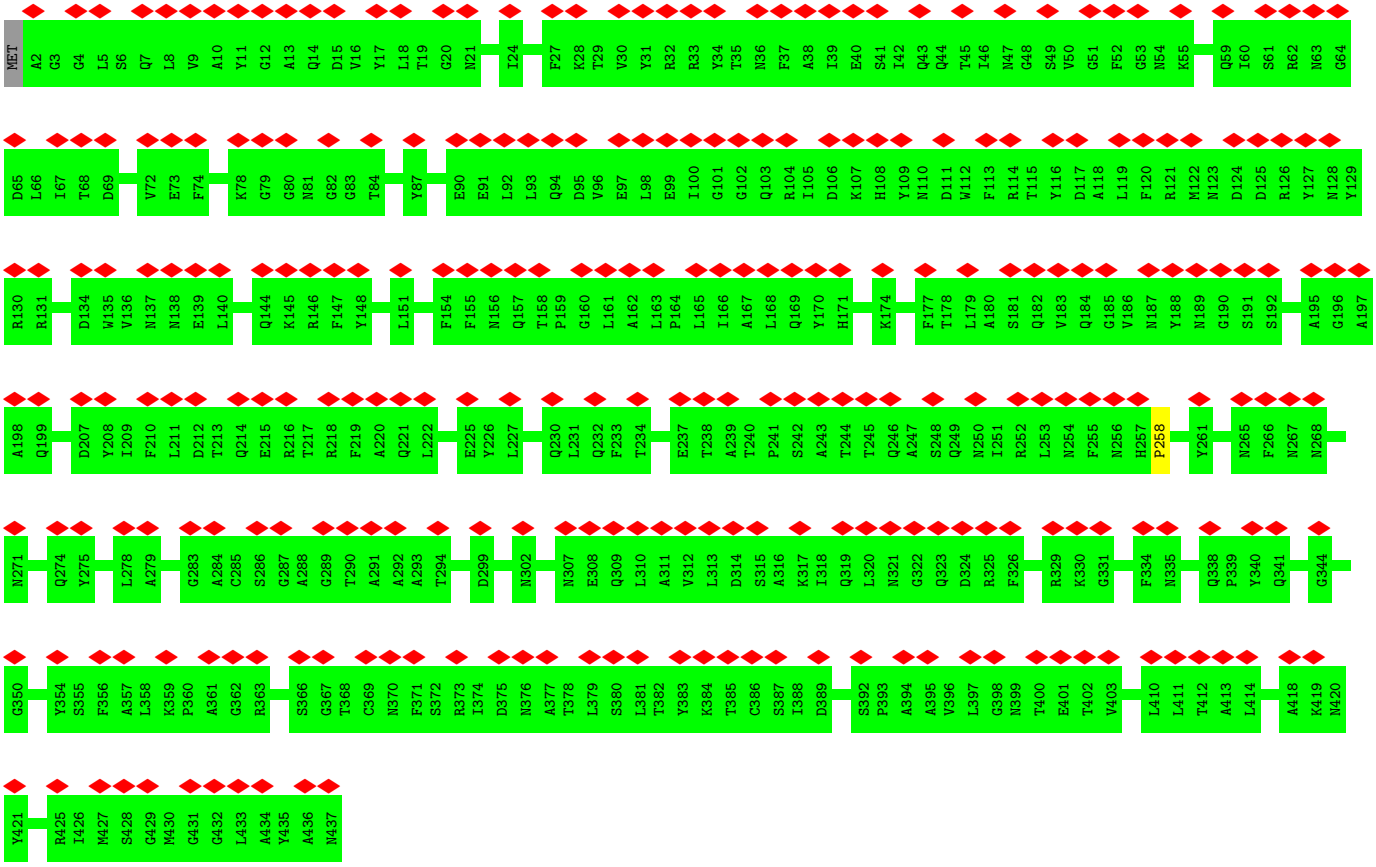






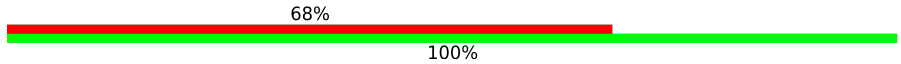
- Molecule 1: Major capsid protein (MCP)

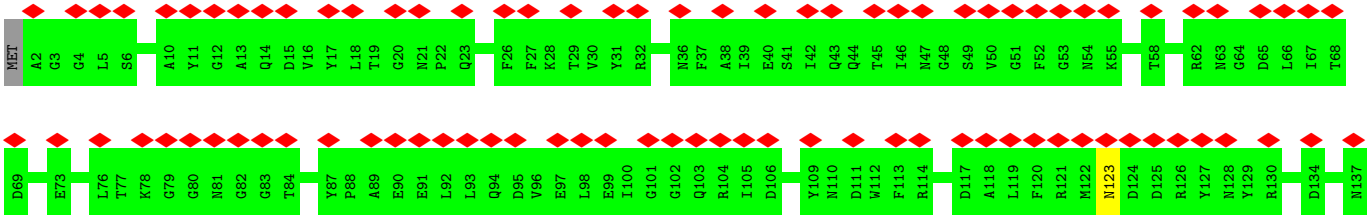
Chain bi:



- Molecule 1: Major capsid protein (MCP)

Chain bj:





N138 E139 L140 V141 G142 A143 Q144 K145 R146 F147 Y148 L151 I152 F153 F154 F155 N156 Q157 T158 P159 G160 L161 A162 L163 P164 L165 I166 A167 L168 Q169 Y170 H171 E172 V173 K174 L175 Y176 F177 T178 L179 A180 S181 Q182 V183 Q184 G185 V186 N187 Y188 N189 G190 S191 S192 A193 I194 A195 G196 A197 A198

Q199 M202 D207 Y208 L211 D212 T213 Q214 E215 R216 T217 R218 F219 A220 Q221 L222 E225 Y226 L227 I228 E229 Q230 L231 T234 G235 S236 E237 T238 S242 A243 T244 T245 Q246 A247 S248 Q249 N250 I251 R252 L253 N254 F255 N256 H257 L262 A263 W264 N265 F266 N267 N268 P269 T270

N271 Y272 G273 Q274 A277 L278 G283 A284 G287 A288 G289 T290 A291 A292 A293 P298 D299 Y300 G301 N302 T303 G304 T305 Q309 L310 A311 V312 L313 D314 S315 A316 K317 I318 Q319 L320 N321 G322 Q323 D324 R325 F326 R329 K330 G331 F334 N335 K336 V337 Q338 P339 Y340 Q341 S342

I343 G344 G345 V346 T347 P348 A349 G350 V351 Y352 L353 Y354 S355 F356 A357 L358 K359 P360 A361 G362 R363 S366 G367 T368 C369 N370 F371 S372 R373 I374 D375 N376 A377 T378 L379 S380 L381 T382 Y383 K384 T385 C386 S387 I388 D389 A390 T391 S392 P393 A394 A395 V396 L397 G398 N399 T400 E401 T404

A405 N406 L410 L411 T412 A413 L414 K419 N420 Y421 L424 R425 I426 M427 S428 G429 M430 G431 G432 L433 A434 Y435 A436 N437

- Molecule 1: Major capsid protein (MCP)

Chain bk: 61% 99%

MET A2 G3 G4 L5 S6 Q7 L8 V9 A10 Y11 G12 A13 Q14 D15 V16 Y17 L18 T19 G20 N21 T25 F26 F27 K28 T29 V30 Y31 R32 N36 F37 E40 Q43 Q44 T45 I46 N47 G48 S49 V50 G51 F52 G53 N54 T58 Q59 R62 N63 G64 D65 D69 E73

F74 V75 L76 T77 K78 G79 G80 N81 G82 G83 Y86 Y87 P88 A89 E90 E91 L92 L93 Q94 D95 V96 E97 L98 E99 I100 G101 G102 Q103 R104 I105 D106 K107 H108 Y109 N110 D111 W112 F113 D117 A118 L119 F120 R121 M122 N123 D124 D125 R126 Y127 N128 Y129 R130 R131 D134 N137 N138

E139 L140 V141 G142 A143 Q144 K145 R146 F147 Y148 L151 I152 F153 F154 F155 N156 Q157 L161 P164 L165 I166 A167 L168 Q169 Y170 H171 E172 V173 K174 F177 Q182 V183 Q184 G185 Y188 N189 G190 S191 S192 A193 I194 A195 G196 A197 A198 Q199 M202 V206 D207 Y208 I209 F210

L211 D212 T213 Q214 E215 R216 T217 R218 F219 A220 Q221 E225 Y226 L227 I228 E229 Q230 L231 Q232 F233 T234 T238 A239 T240 P241 S242 A243 T244 T245 Q246 A247 S248 Q249 N250 I251 R252 L253 N254 H257 K260 Y261 L262 A263 W264 N265 F266 N267 N268 N271 Q274 A277 L278 A279

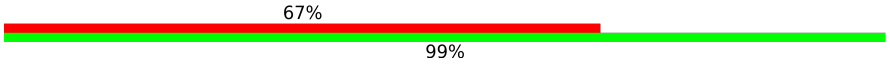
N280 I281 P282 G283 A284 G289 T290 A291 A292 A293 D299 Y300 G301 Y306 N307 L310 A311 V312 L313 D314 S315 A316 K317 I318 Q319 L320 N321 G322 Q323 D324 A327 T328 R329 K330 G331 S332 Y333 F334 N335 K336 V337 Q338 Q341 S342 I343 G344 G345 A349 G350 V351 Y352 L353 Y354

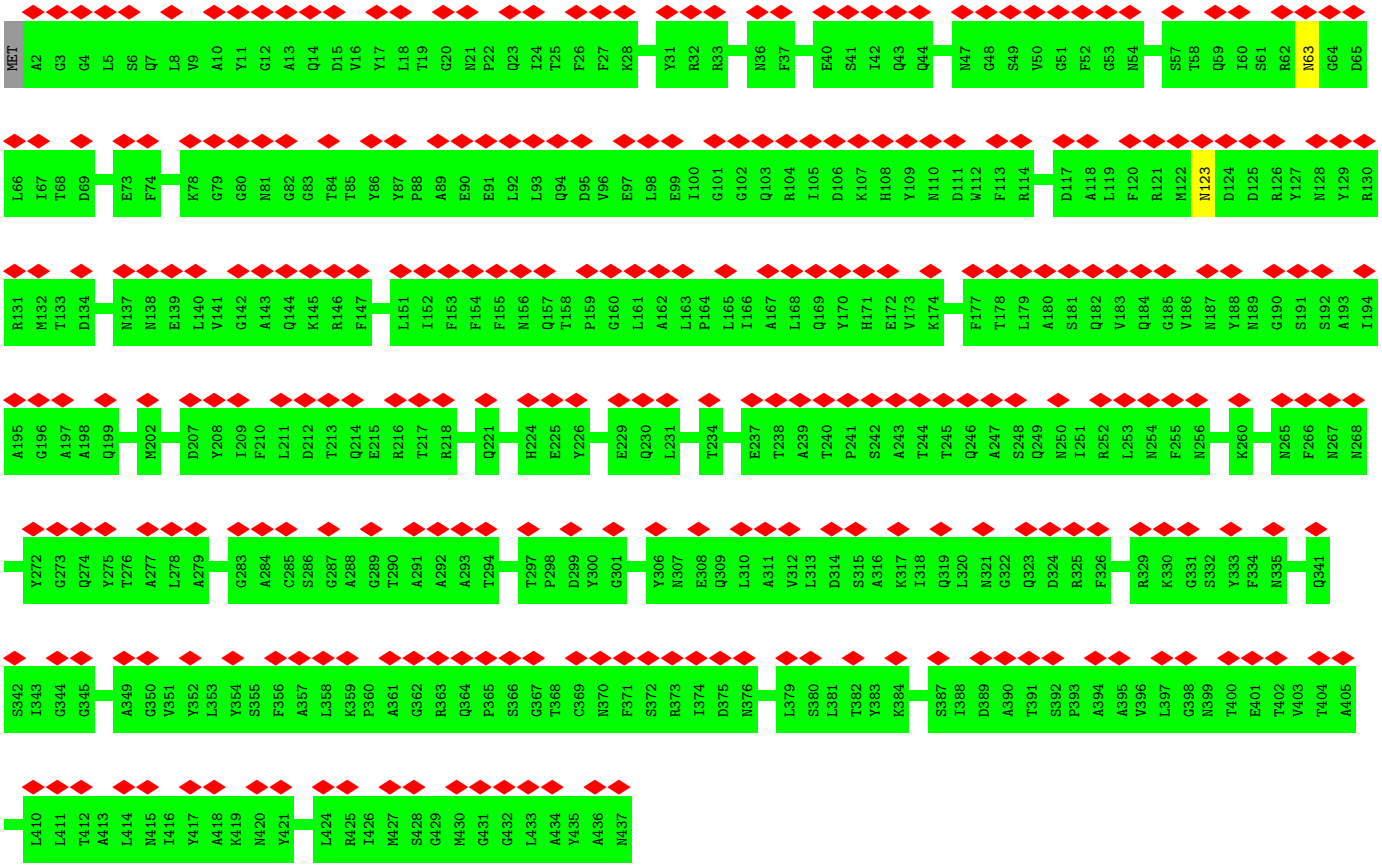
S355 F356 A357 L358 K359 P360 A361 G362 R363 Q364 P365 S366 C369 N370 R373 I374 D375 N376 L379 S380 L381 T382 Y383 K384 T385 C386 S387 I388 D389 A394 A395 V396 L397 G398 N399 T400 E401 T402 V403 T404 A405 L410 L411 T412 A413 L414 A418 K419 N420 Y421 L424 R425 I426

M430 G431 G432 L433 A434 Y435 A436 N437

- Molecule 1: Major capsid protein (MCP)

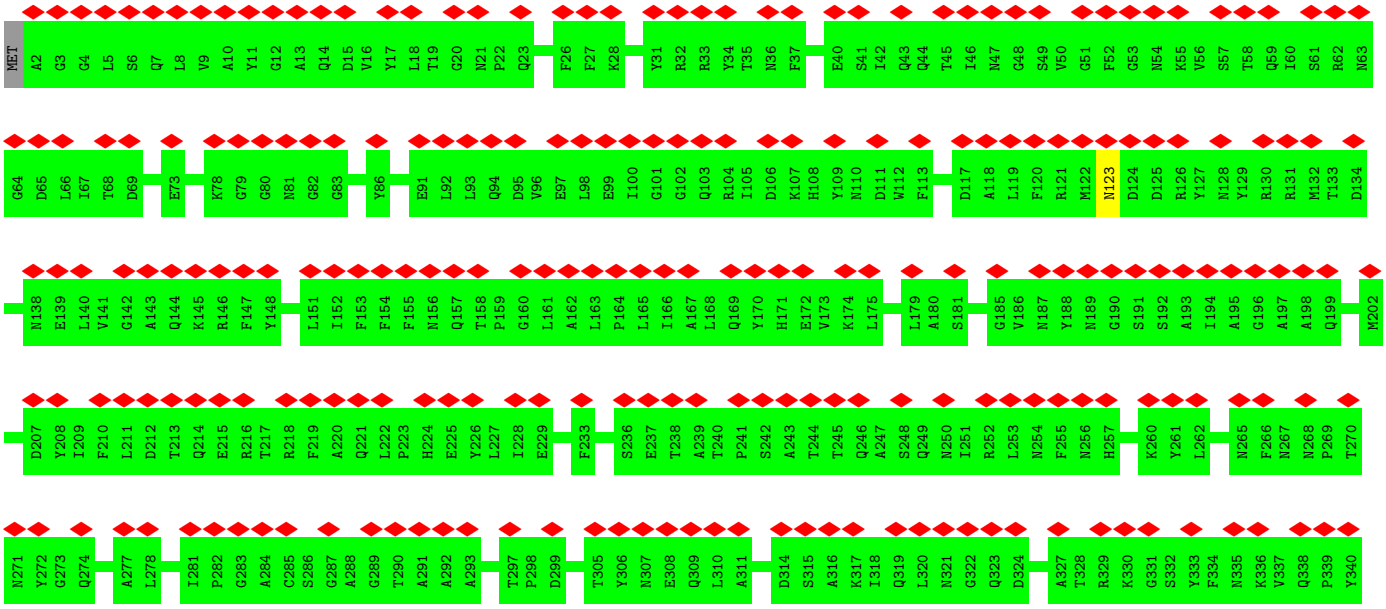
Chain bl:

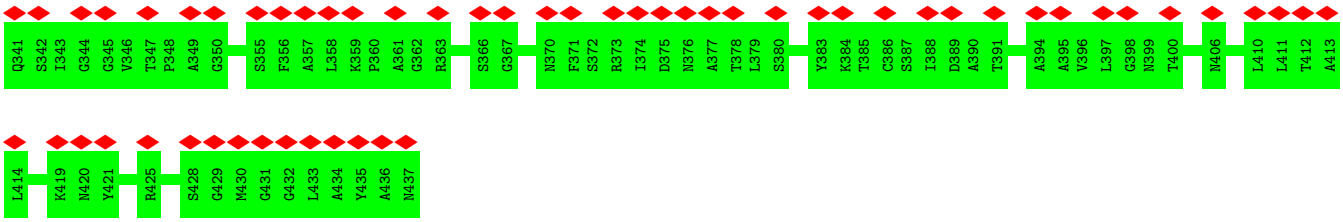




- Molecule 1: Major capsid protein (MCP)

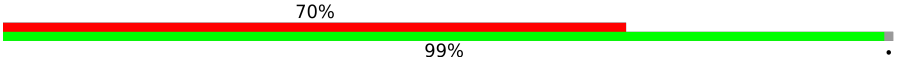
Chain bm:

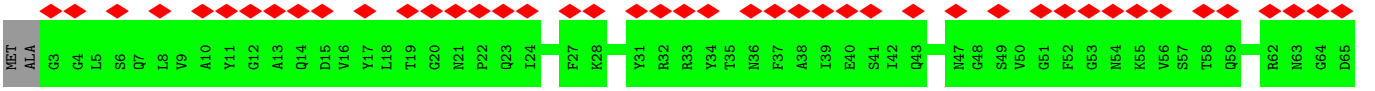


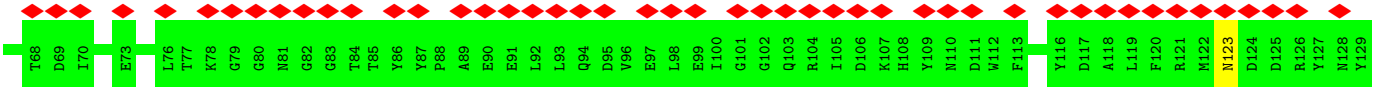


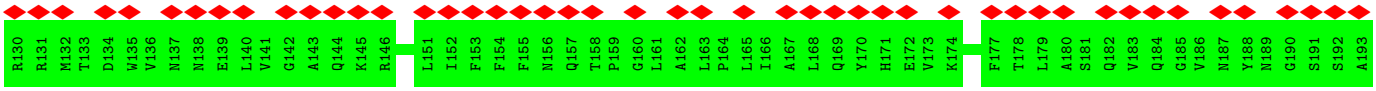
• Molecule 1: Major capsid protein (MCP)

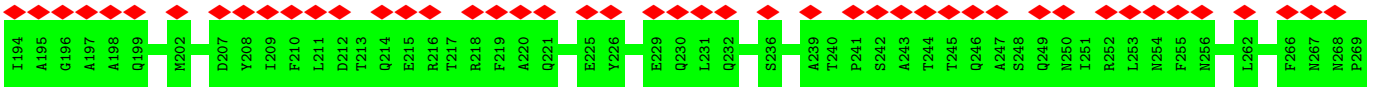
Chain bn:

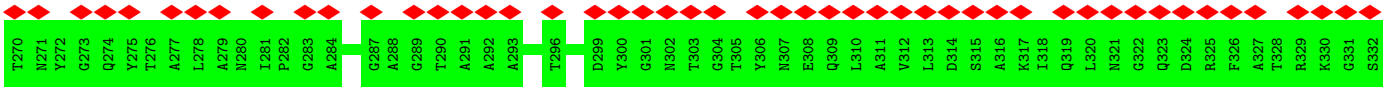


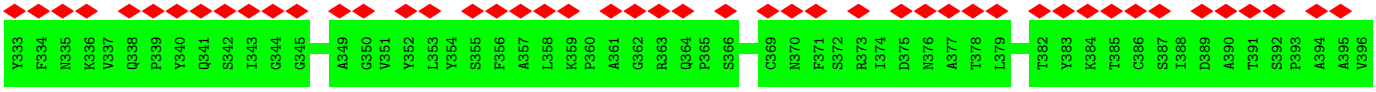


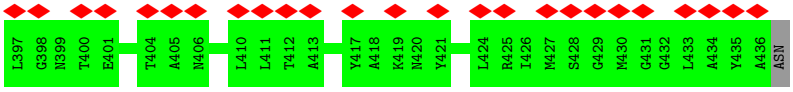






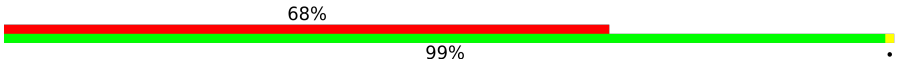


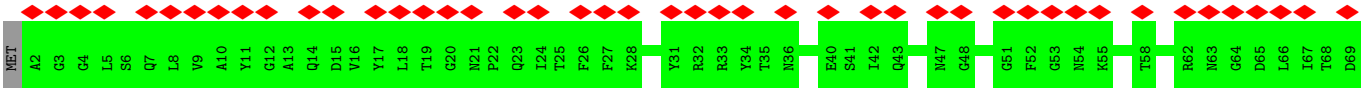


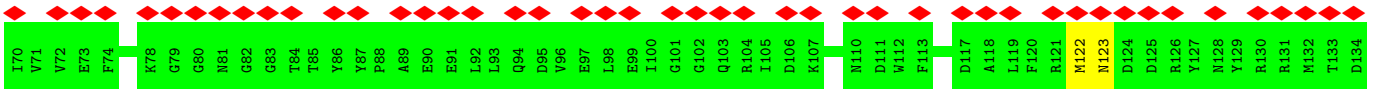


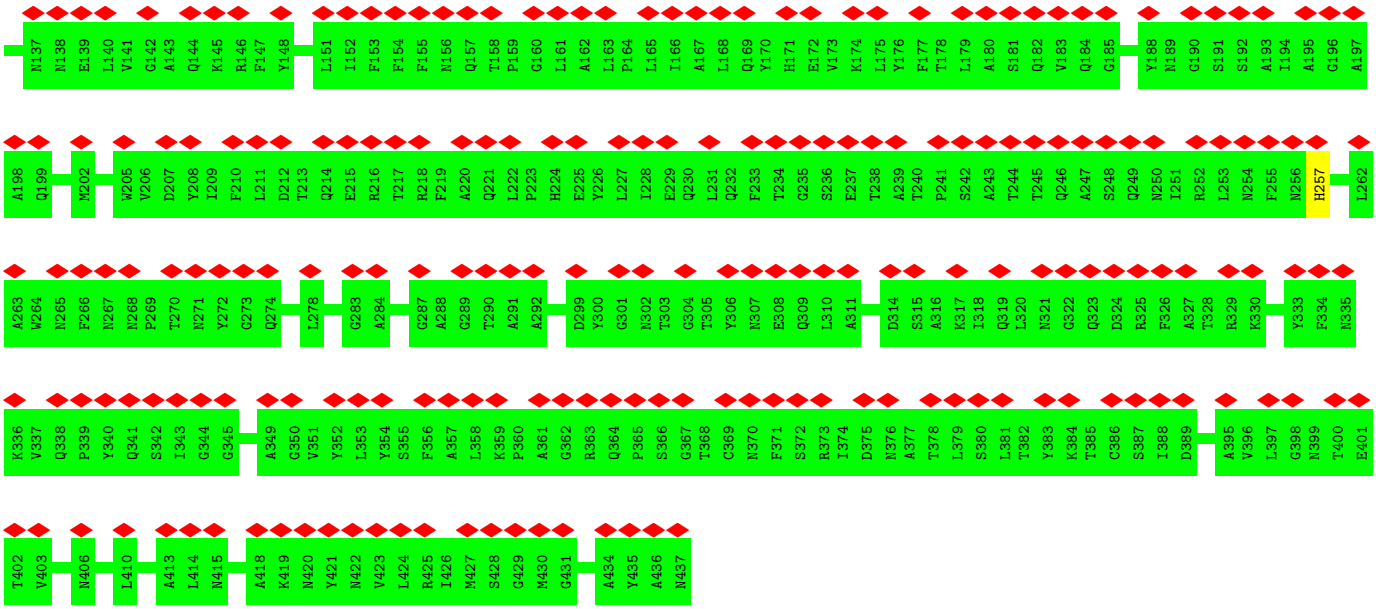
• Molecule 1: Major capsid protein (MCP)

Chain bo:



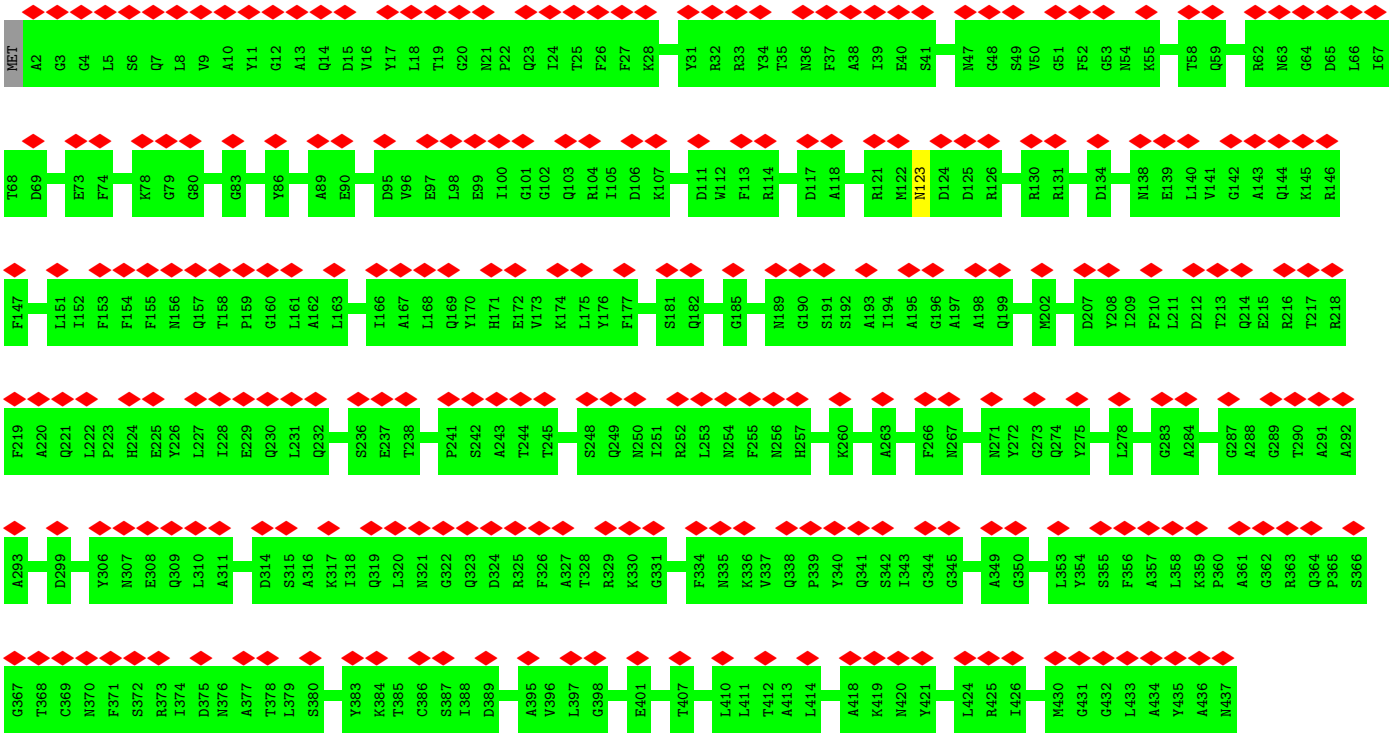






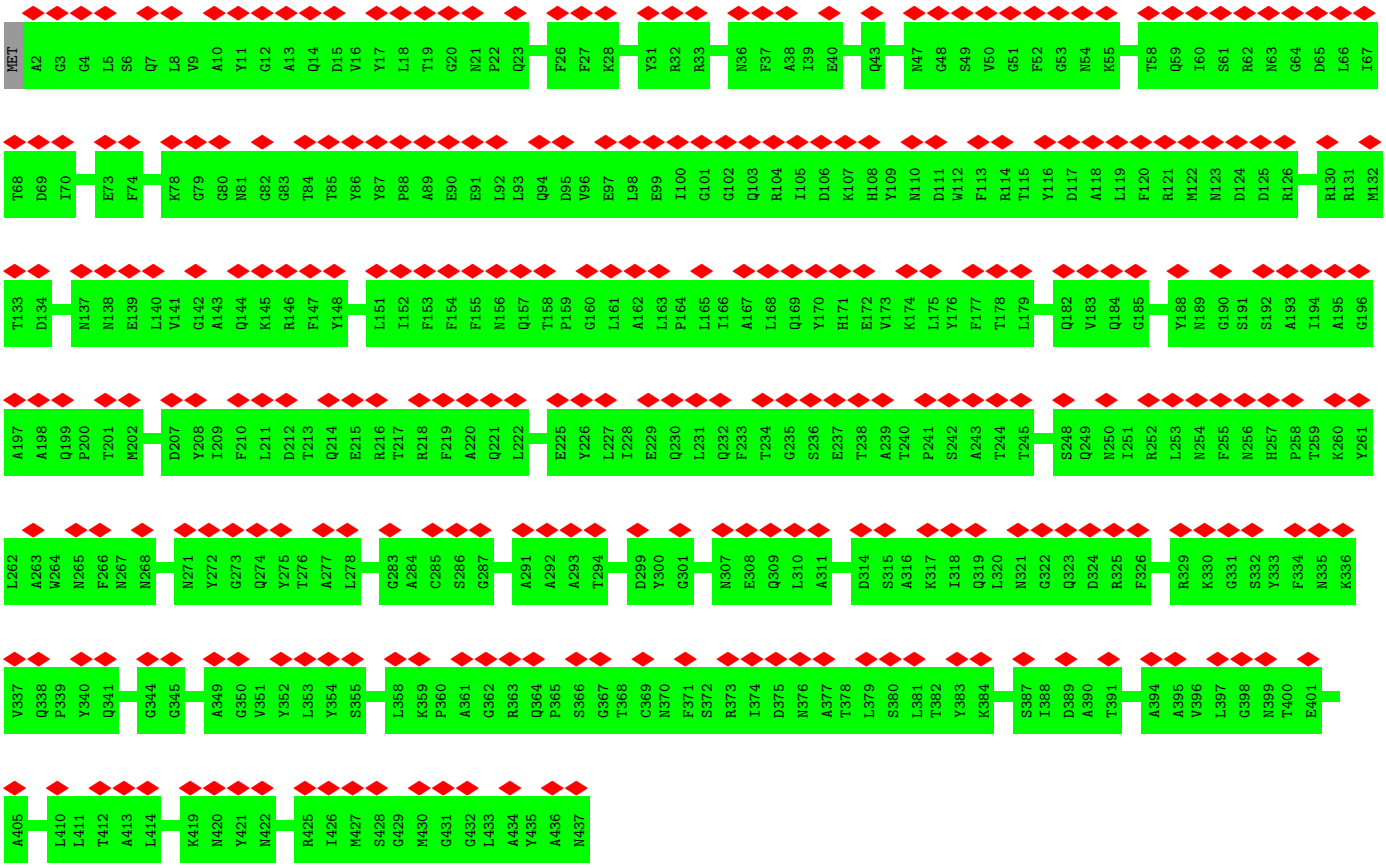
- Molecule 1: Major capsid protein (MCP)

Chain bp:



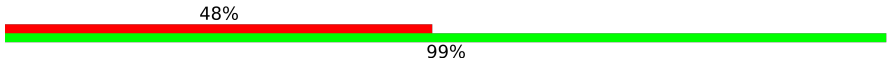
- Molecule 1: Major capsid protein (MCP)

Chain bq:



- Molecule 1: Major capsid protein (MCP)

Chain br:



• Molecule 1: Major capsid protein (MCP)

Chain bs: 58% 100%

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T68 D69 E73 F74 K78 G79 G80 T84 T85 Y86 Y87 P88 A89 E90 E91 L92 L93 Q94 D95 V96 E97 L98 E99 I100 G101 G102 Q103 R104 I105 D106 K107 N110 D111 W112 F113 R114 D117 R121 M122 N123 D124 D125 R126 Y127 N128 Y129 R130 R131 D134 N137 N138 E139

L140 A143 Q144 K145 Y148 L151 I152 F153 F154 F155 N156 Q157 T158 P159 G160 L161 A162 L163 P164 L165 I166 A167 L168 Q169 Y170 H171 E172 V173 K174 S181 Q182 Y188 N189 G190 S191 S192 A193 I194 A195 G196 A197 A198 Q199 M202 D207 Y208 I209 F210 L211 D212 T213 Q214 E215

R216 T217 R218 F219 L222 P223 H224 E225 Y226 L227 I228 E229 Q230 L231 Q232 F233 T234 G235 S236 E237 T238 A239 T240 P241 S242 A243 T244 T245 Q246 A247 N250 I251 R252 L253 N254 F255 N256 K260 W264 N265 F266 N267 N268 N271 Y272 G273 Q274 A279 G287 T290 A291 A292

A293 D299 N307 E308 Q309 L310 A311 V312 L313 D314 S315 A316 K317 I318 Q319 L320 N321 G322 Q323 D324 R325 F326 A327 T328 R329 K330 G331 S332 N335 K336 V337 Q338 P339 Y340 Q341 S342 I343 G344 G345 A349 G350 V351 Y352 F356 A357 A361 G362 R363 Q364 P365 S366 G367 N370

F371 S372 R373 I374 D375 N376 A377 T378 L379 S380 L381 T382 Y383 K384 D389 A394 L397 G398 E401 T404 L410 L411 T412 A413 K419 N420 Y421 R425 I426 M427 S428 G429 M430 G431 G432 L433 A434 Y435 A436 N437

• Molecule 1: Major capsid protein (MCP)

Chain bt: 56% 99%

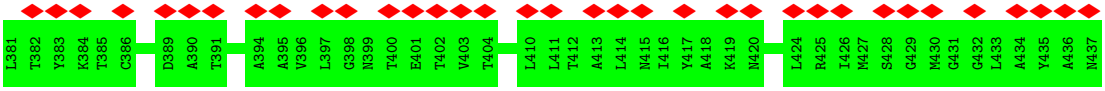
MET ALA G3 G4 L5 S6 Q7 A10 Y11 G12 A13 Q14 D15 L18 T19 G20 N21 P22 Q23 I24 T25 F26 P27 K28 R32 R33 N36 F37 A38 I39 E40 N47 G48 S49 F52 G53 N54 K55 T58 R62 N63 G64 D65 L66 I67 T68 D69 E73 K78

G82 A89 E90 E91 L92 L93 Q94 D95 V96 E97 L98 E99 I100 G101 G102 Q103 R104 I105 D106 K107 H108 Y109 N110 D111 W112 F113 R114 T115 Y116 D117 A118 R121 M122 N123 D124 D125 R126 Y127 R130 D134 N138 E139 L140 V141 G142 K145 L151 I152 F153 F154 F155 N156 Q157

T158 P159 G160 L161 A162 L163 P164 L165 I166 A167 E172 V173 K174 L175 Y176 L179 A180 S181 Y188 N189 G190 S191 S192 A195 G196 A197 A198 Q199 M202 V206 D207 Y208 I209 F210 L211 D212 T213 Q214 E215 R216 T217 R218 F219 A220 Q221 L222 P223 H224 E225 Y226 L227 I228 E229 Q230

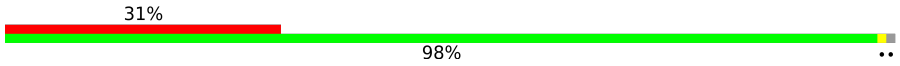
L231 Q232 F233 E237 T238 P241 S242 A243 T244 T245 Q246 A247 S248 Q249 N250 I251 R252 L253 N254 F255 N256 H257 P258 T259 K260 N265 F266 N267 N268 N271 Y272 G273 Q274 L278 A279 G283 A284 G287 A291 D299 Y300 G301 N302 N307 E308 Q309 L310 A311 V312 L313

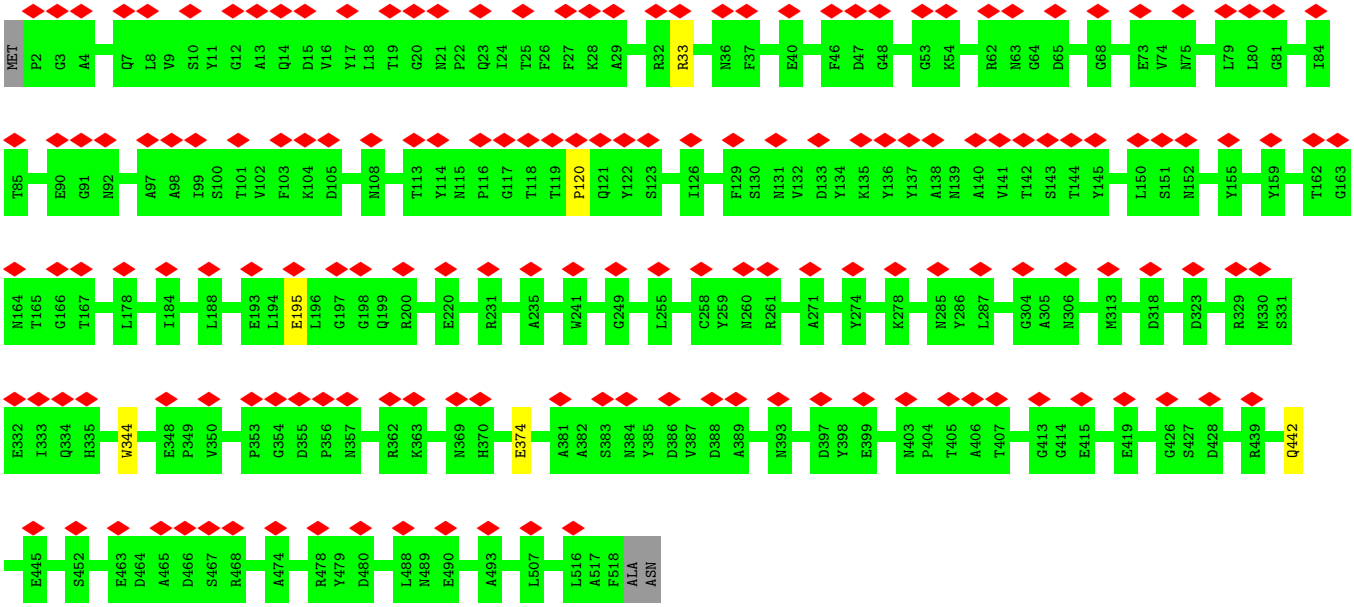
D314 S315 A316 K317 I318 Q319 L320 N321 G322 Q323 D324 R325 F326 A327 K330 G331 S332 Y333 F334 N335 K336 P339 Y340 Q341 S342 I343 G344 G345 A349 G350 L353 Y354 S355 F356 A357 L358 K359 P360 A361 G362 R363 Q364 P365 S366 G367 T368 G369 N370 F371 S372 R373 I374 D375 L379 S380



- Molecule 2: MCPv1

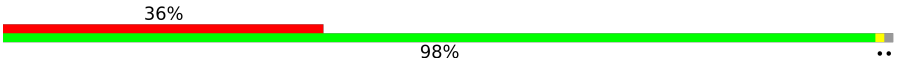
Chain bu:

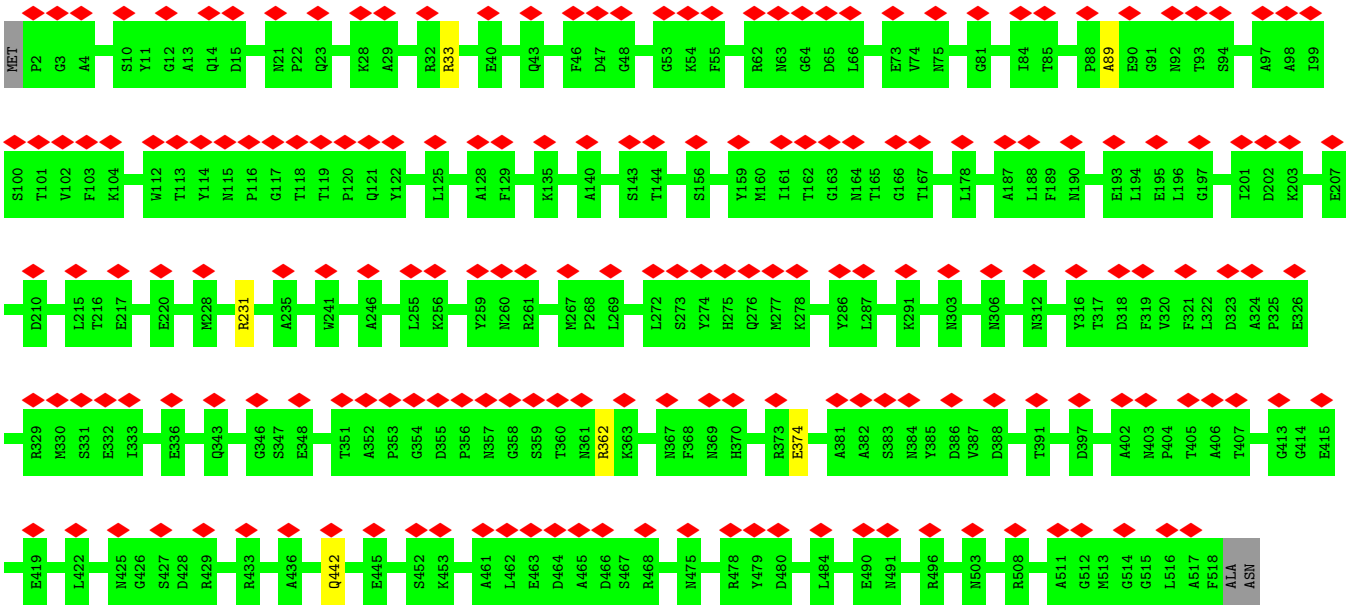




- Molecule 2: MCPv1

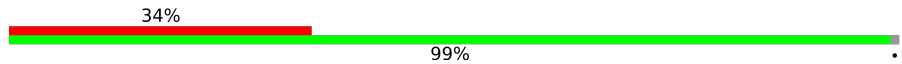
Chain bv:

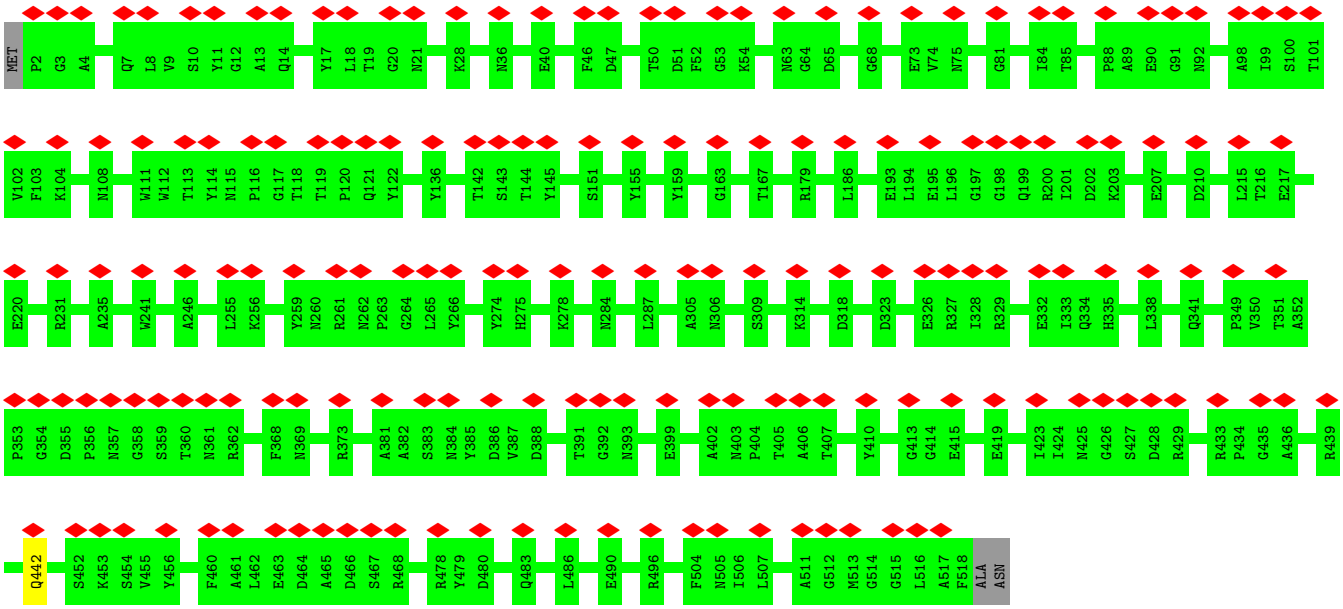




- Molecule 2: MCPv1

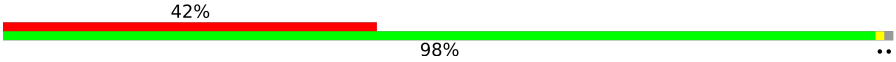
Chain bw:

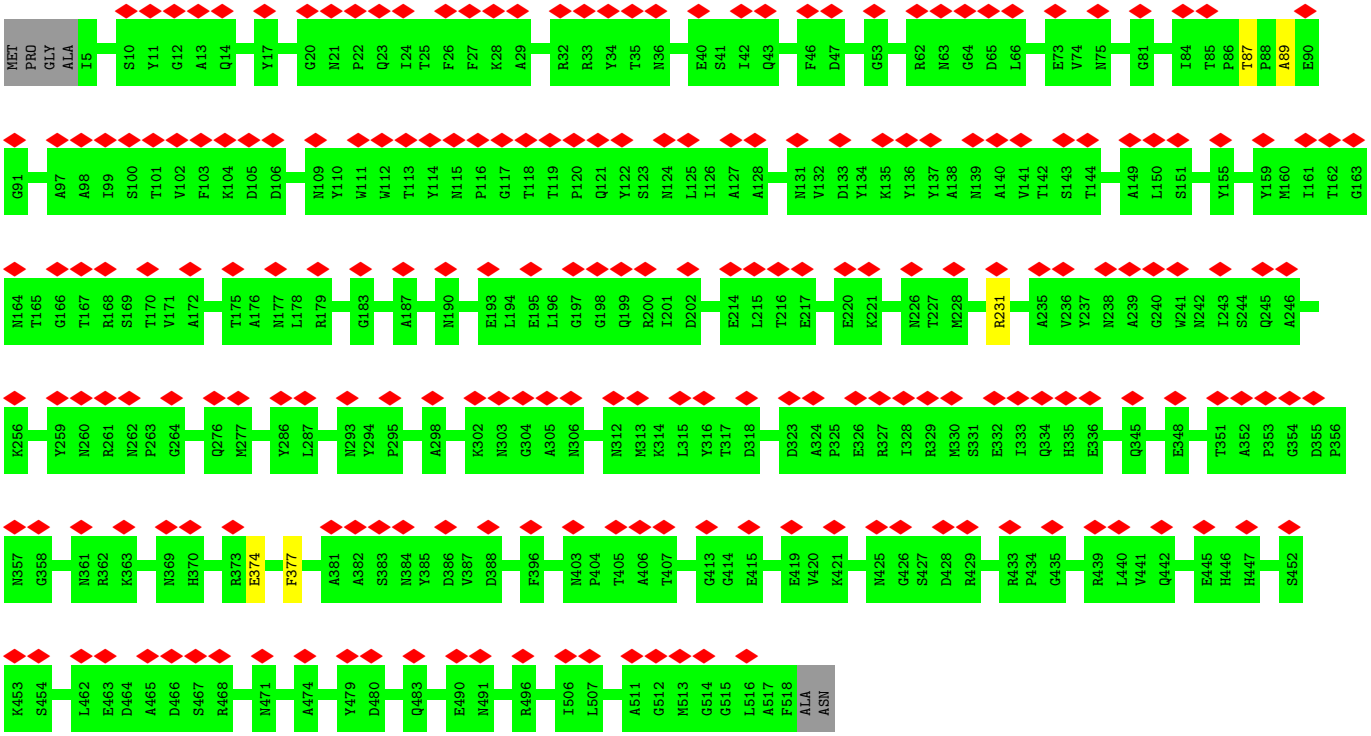




- Molecule 2: MCPv1

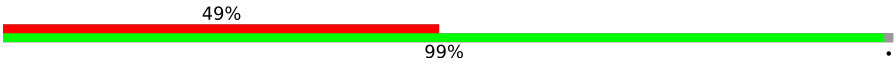
Chain bx:

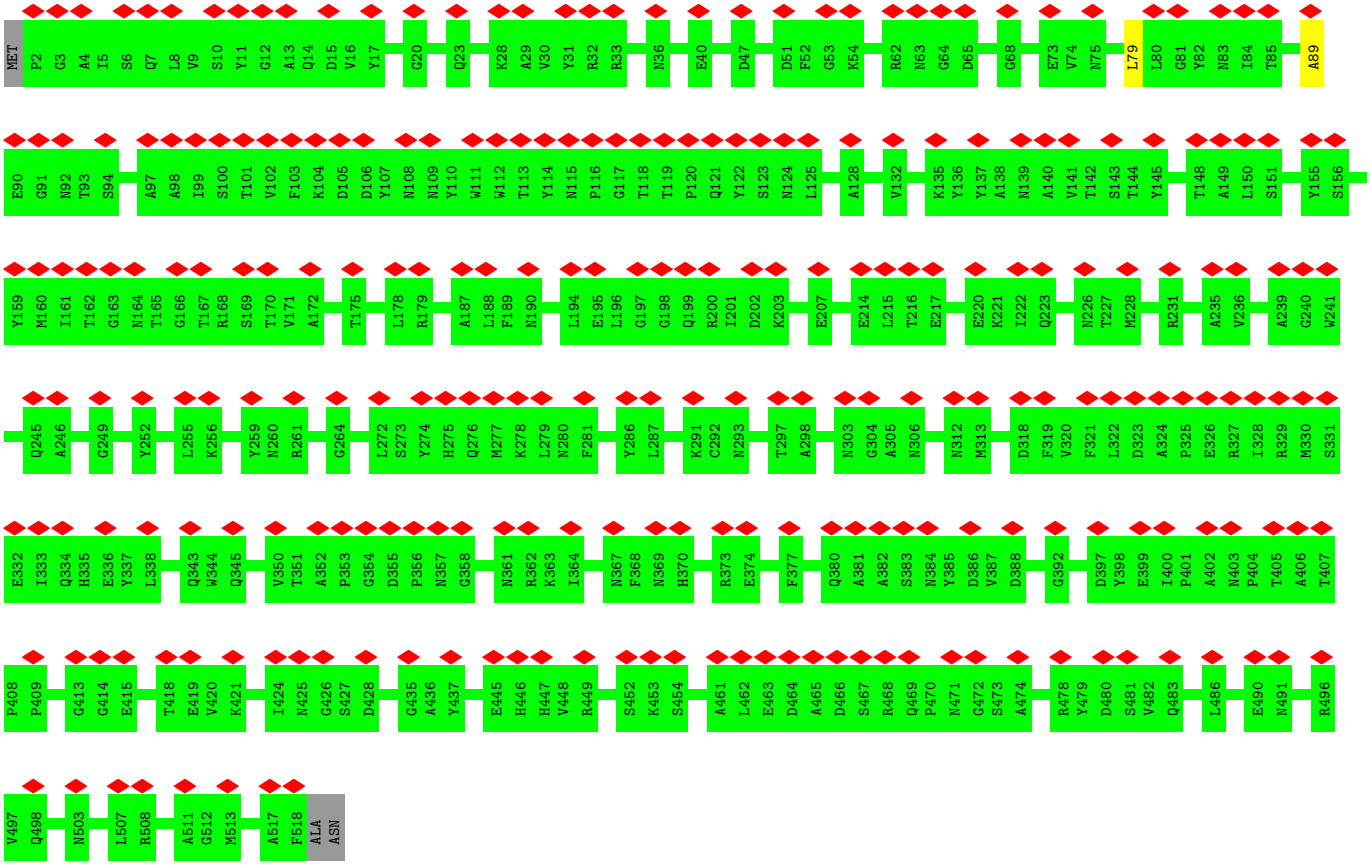




- Molecule 2: MCPv1

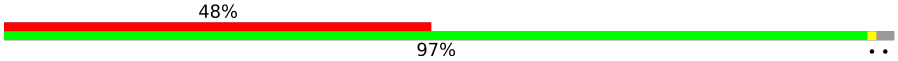
Chain by:

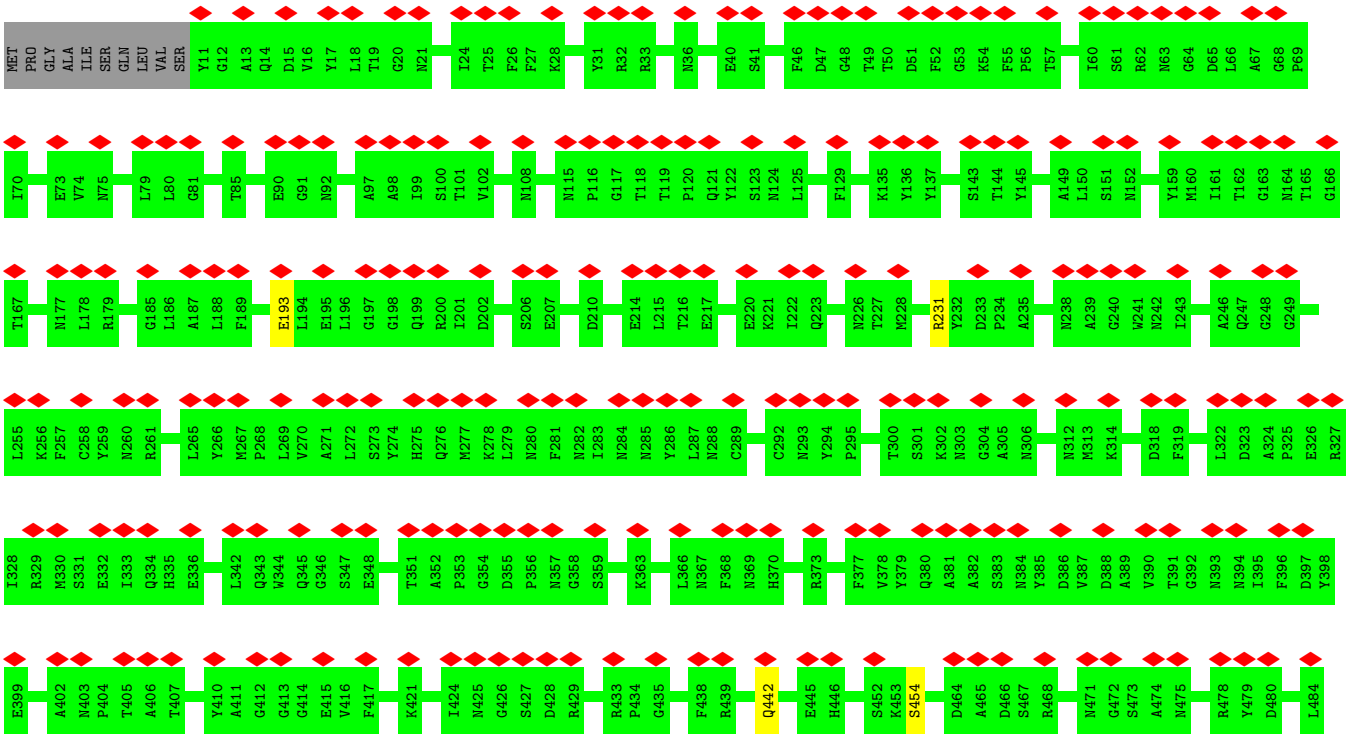


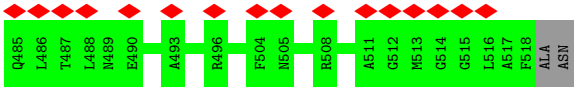


- Molecule 2: MCPv1

Chain bz:

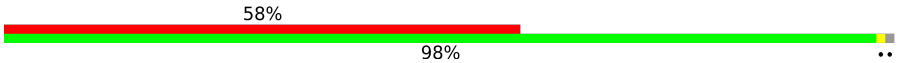


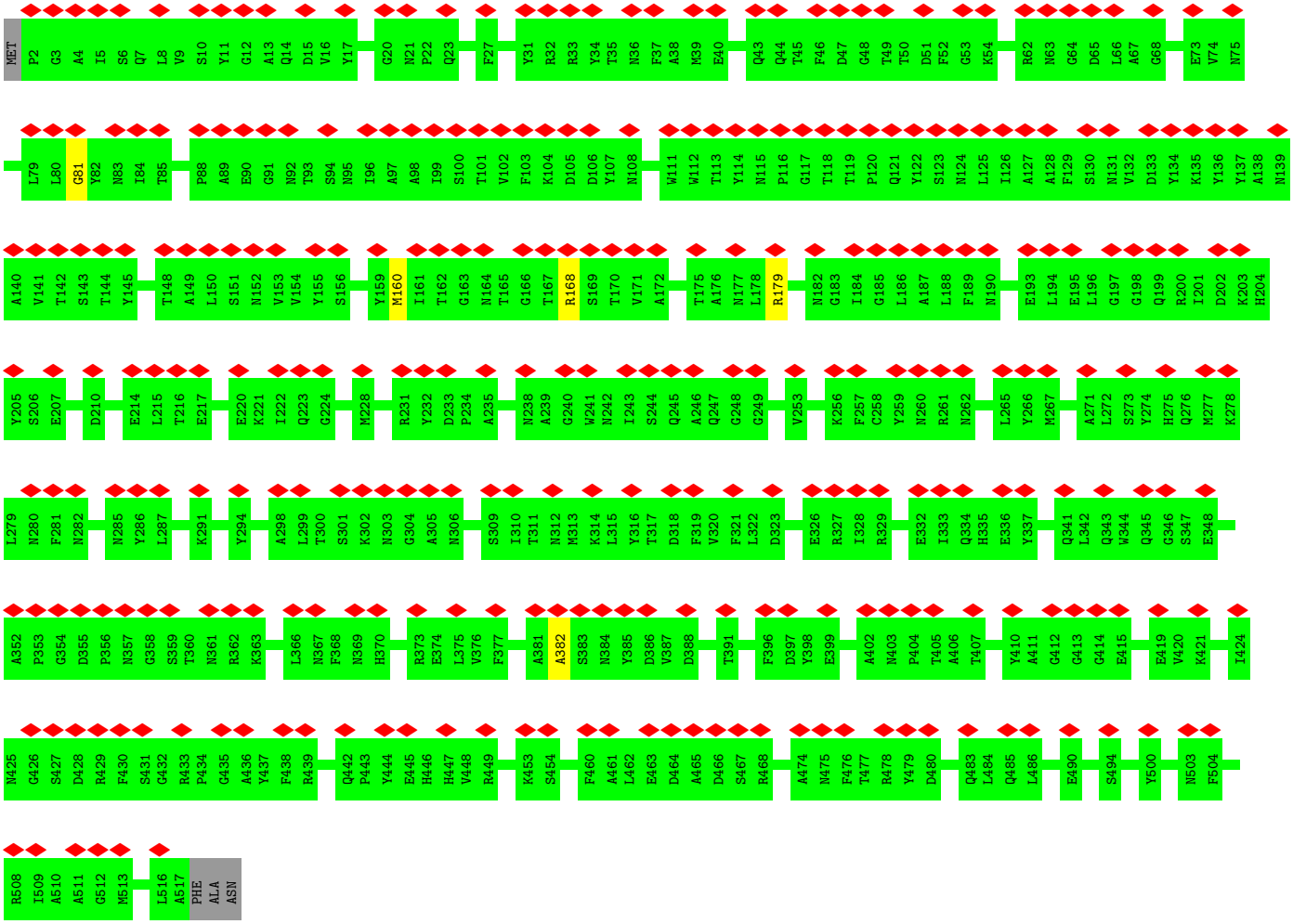




- Molecule 2: MCPv1

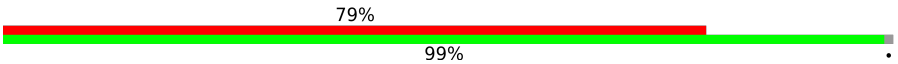
Chain bA:

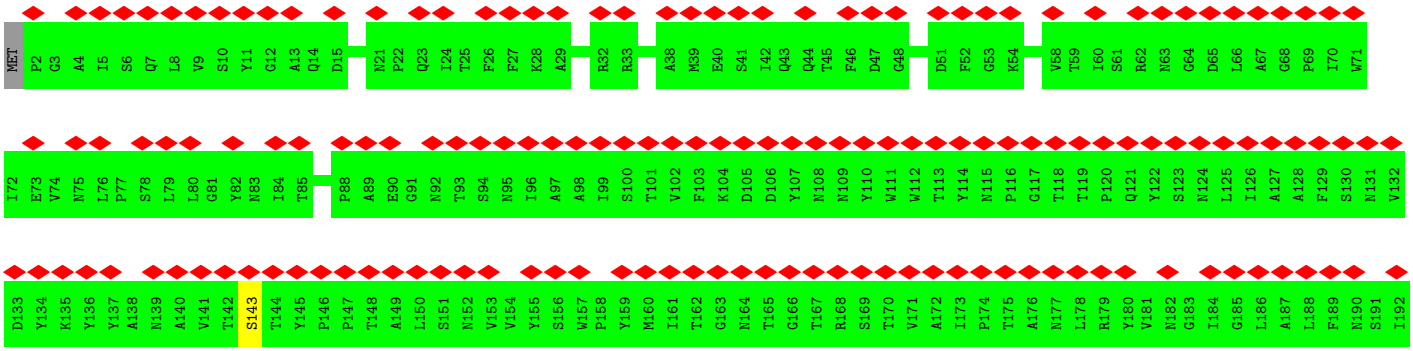




- Molecule 2: MCPv1

Chain bB:





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Y259 N260 R261 N262 P263 G264 L265 Y266 M267 P268 L269 V270 A271 L272 S273 Y274 H275 Q276 M277 K278 L279 N280 F281 N282 I283 N284 N285 Y286 L287 N288 C289 V290 K291 C292 N293 Y294 P295 V296 T297 A298 L299 T300 S301 K302 N303 G304 A305 N306 P307 L308 S309 I310 T311 N312 M313 K314 L315 Y316 T317 D318

F319 V320 F321 L322 D323 A324 P325 E326 R327 I328 R329 M330 S331 E332 I333 Q334 H335 E336 Y337 L338 Q341 L342 Q343 W344 Q345 G346 S347 E348 P349 V350 T351 A352 P353 G354 D355 P356 N357 G358 S359 T360 N361 R362 K363 I364 N367 F368 N369 H370 P371 V372 R373 E374 L375 V376 F377 V378 Y379 Q380

A381 A382 S383 N384 Y385 D386 V387 D388 A389 V390 T391 G392 N393 N394 I395 F396 D397 Y398 E399 I400 P401 A402 N403 P404 T405 A406 T407 P408 P409 Y410 A411 G412 G413 G414 E415 E419 V420 K421 L422 I423 I424 N425 G426 S427 D428 R429 F430 S431 G432 R433 P434 G435 A436 Y437 F438 R439 L440 V441 Q442

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L507 R508 I509 A510 A511 G512 M513 G514 G515 L516 A517 F518 ALA ASN

- Molecule 3: MCPv2

Chain bC: 61% 99%

MET D2 P3 T4 T5 R6 F7 R8 G9 S10 D11 V12 P13 V14 H15 N16 E17 D18 H19 M20 V21 F22 A23 K24 E27 I28 G29 L30 Q31 G32 R33 Q34 G35 F36 Y37 T38 N39 T40 N41 V42 A43 T44 N45 T46 Y47 N48 H49 V50 Y51 T52 G55 G56 H57 T58 G59 G60 K61 F62

T63 Q64 D65 I66 Y67 T68 T69 D70 L71 L72 I73 A74 A75 K76 D77 E78 K79 A80 D81 K82 I83 P84 L85 D86 K87 R88 M89 D90 G91 T92 E95 G96 T97 F98 V99 Q100 L101 L102 S103 R104 G105 P106 Q107 D108 V109 Y110 L111 T112 Y113 N114 P115 Q116 I117 S118 L119 F120 K121 R122 K123

Y124 K125 A131 I132 E133 E137 R138 G146 T147 R148 N149 S154 K155 N156 G157 D158 G161 N162 M163 L169 P170 N171 L172 G173 T174 P175 G176 G177 T178 W179 A180 P181 T182 M183 T187 F188 S189 R192 M193 R194 I195 G196 D197 V200 D209 I210 D211 D212 K213 M214

F215 C216 I221 Q222 D225 E226 L227 I228 K229 R230 N231 T236 D237 Q238 E239 W240 E241 L242 I243 L246 K247 F248 F249 C250 C251 K252 R253 N254 T255 G256 K257 Q258 Q259 F260 L264 N265 M266 D267 T268 N269 E275 F276 L281 N282 L287 P288 T289 G290 S291 I292 L293 P294

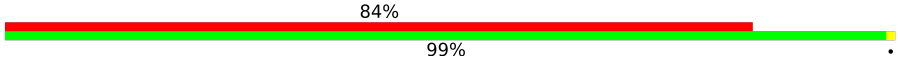
D295 I296 Q297 D300 D306 L310 D311 D312 T313 E314 K315 F316 R317 F318 A319 Q320 D321 Y325 L326 I327 E328 Q329 M333 D334 S335 L336 A339 T342 S343 G344 Q345 T346 Y347 N348 K349 T350 D351 V352 Y353 V354 D355 M356 K357 E358 L359 N360 K361 K364 E367 I368

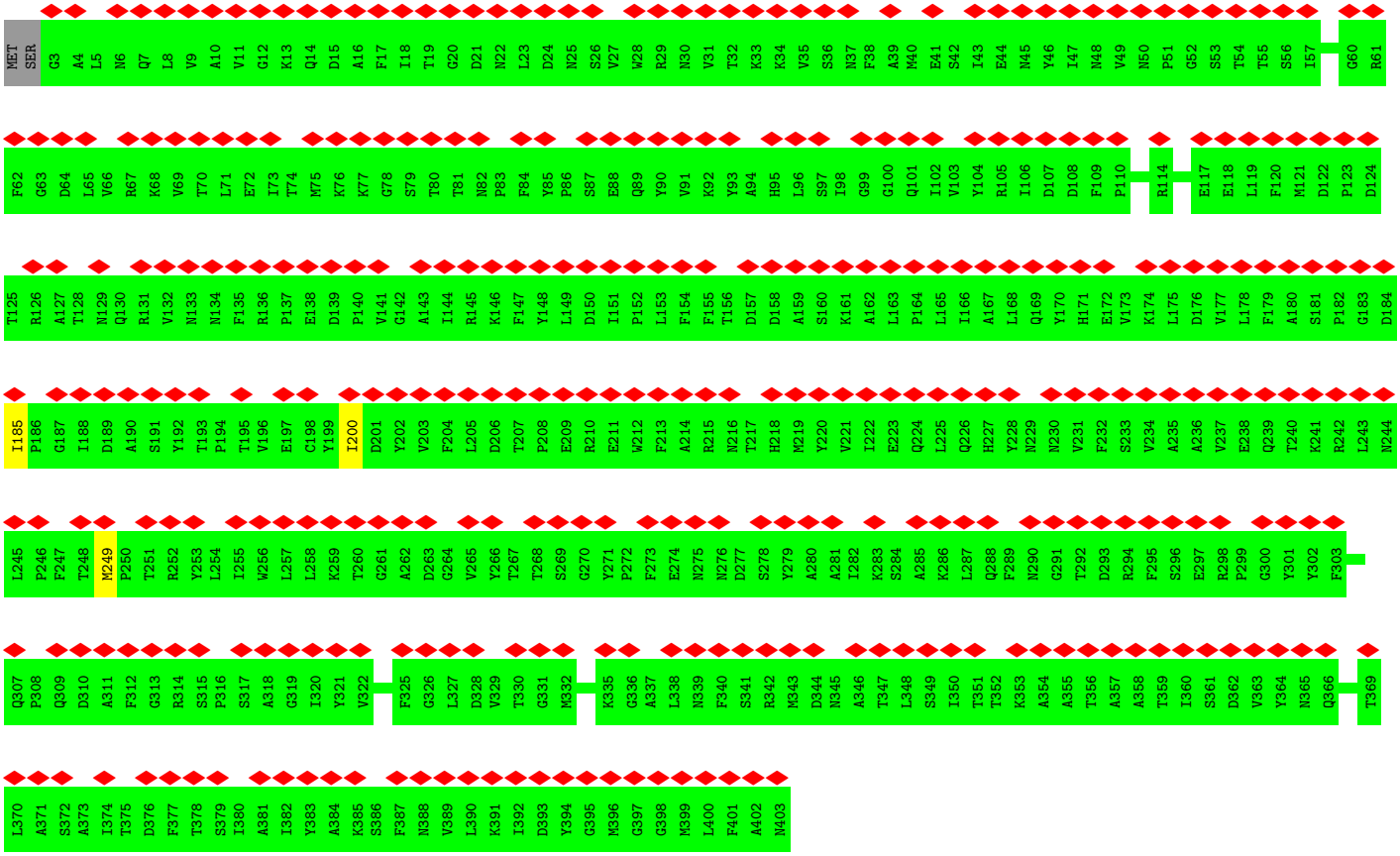
E372 Q373 G374 S375 T376 S377 F378 D379 Y380 V381 D382 I383 I384 E385 S386 A387 T388 F389 Y390 L391 N392 S393 D394 E395 Q396 F397 K398 T399 R400 A401 G402 E403 L407 V408 Q409 P410 Y411 Q412 H413 F414 K415 R416 P419 T420 S421 N422 I423 S424 T425 F426 S427 F428 A429 L430 D431 A432 G433 S434

F435 Q436 G439 N442 F443 A444 P445 R448 T449 R450 F451 A452 F453 K454 I455 Q458 T459 T460 P461 H462 V463 I464 R465 L466 L471 F476 E477 S478 G479 L480 V481 K482 L483 L484 F485 N486

- Molecule 4: MCPv3

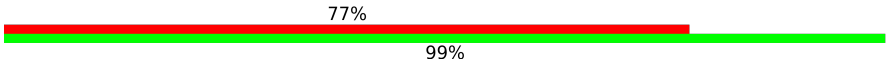
Chain bD:

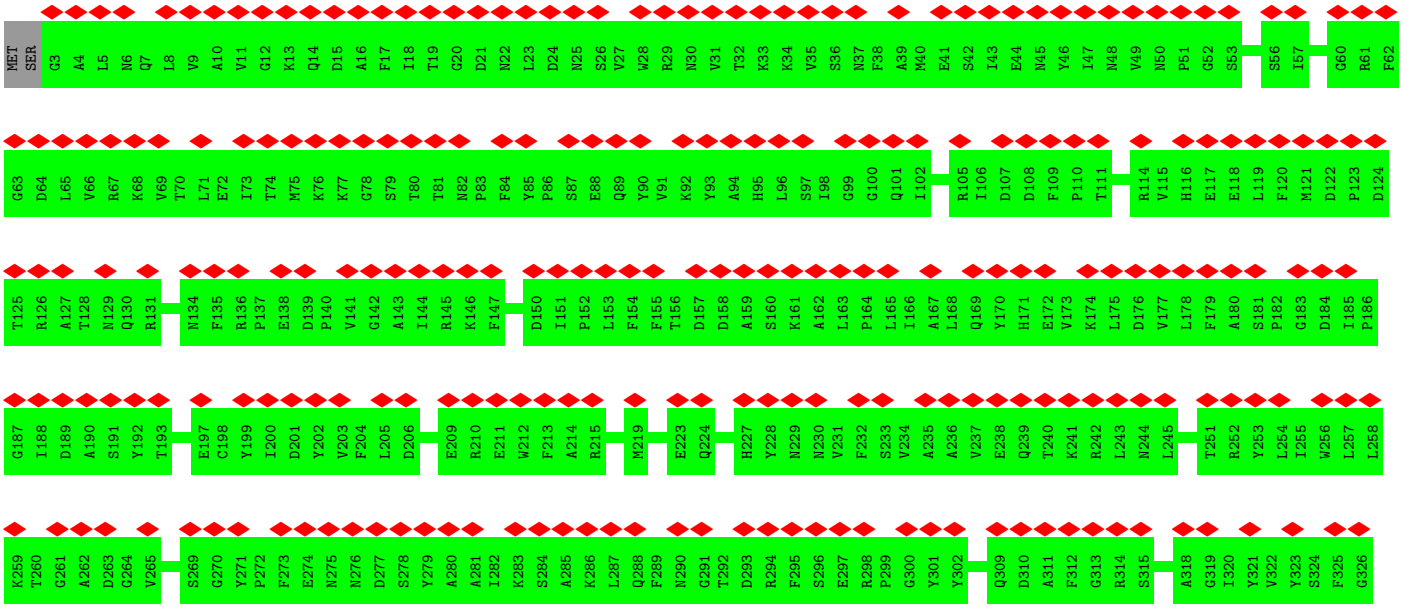


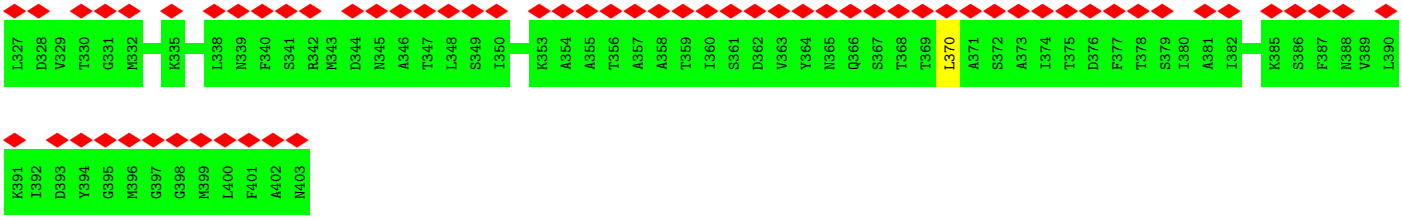


- Molecule 4: MCPv3

Chain bF:

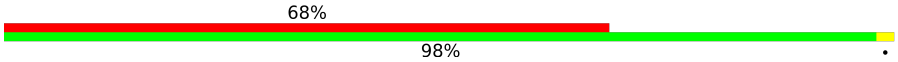


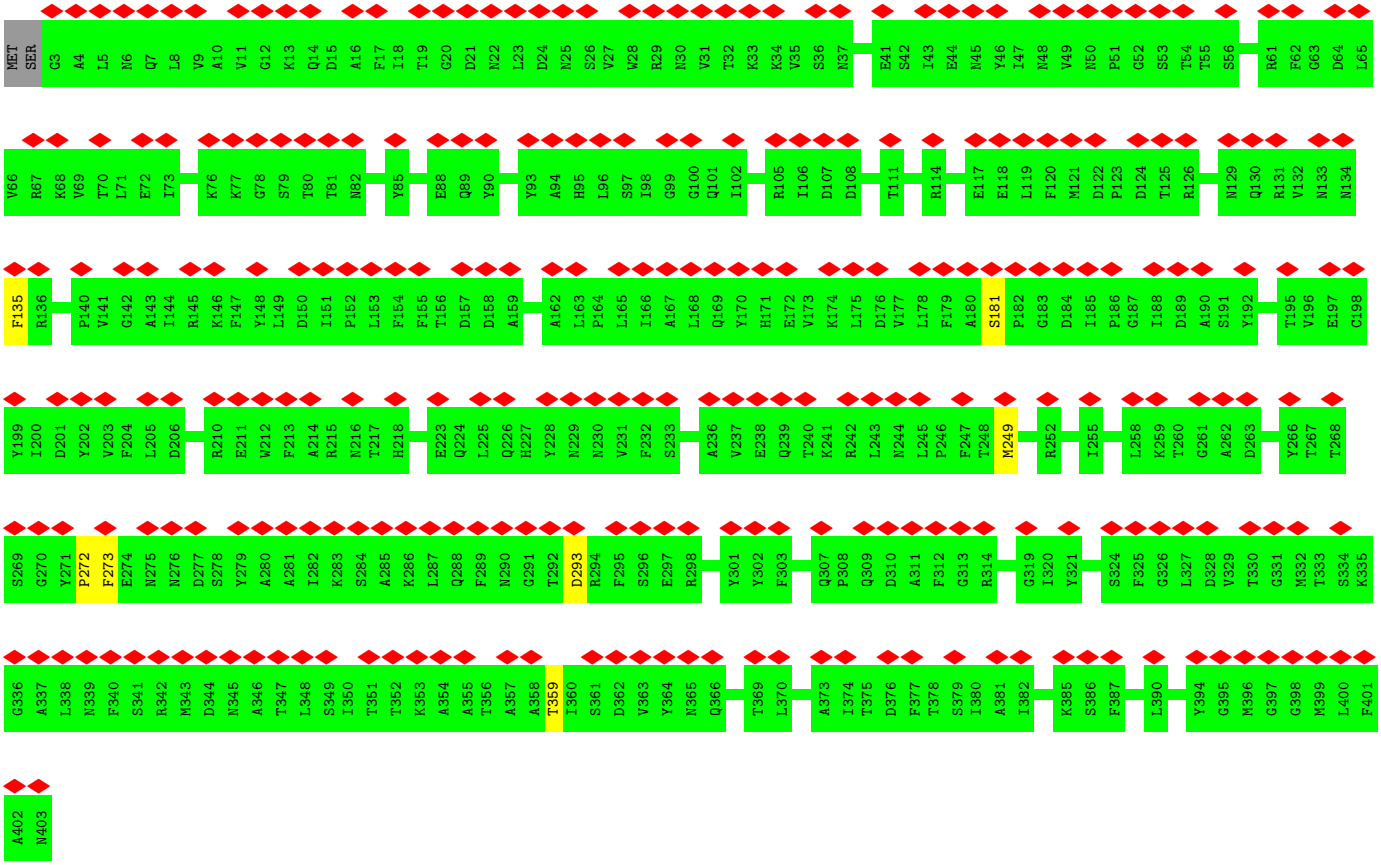




- Molecule 4: MCPv3

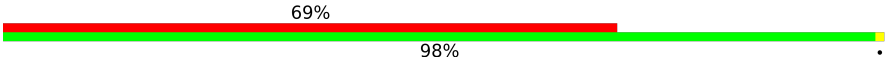
Chain cX:

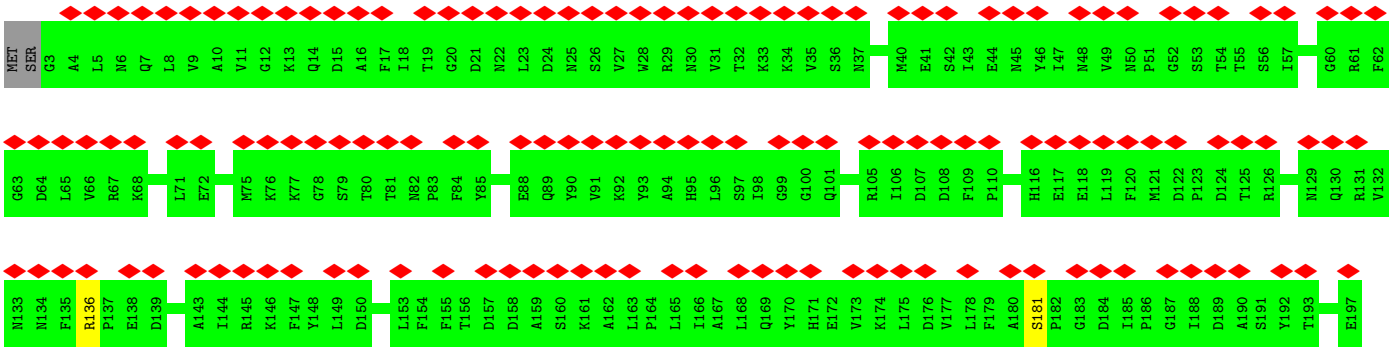


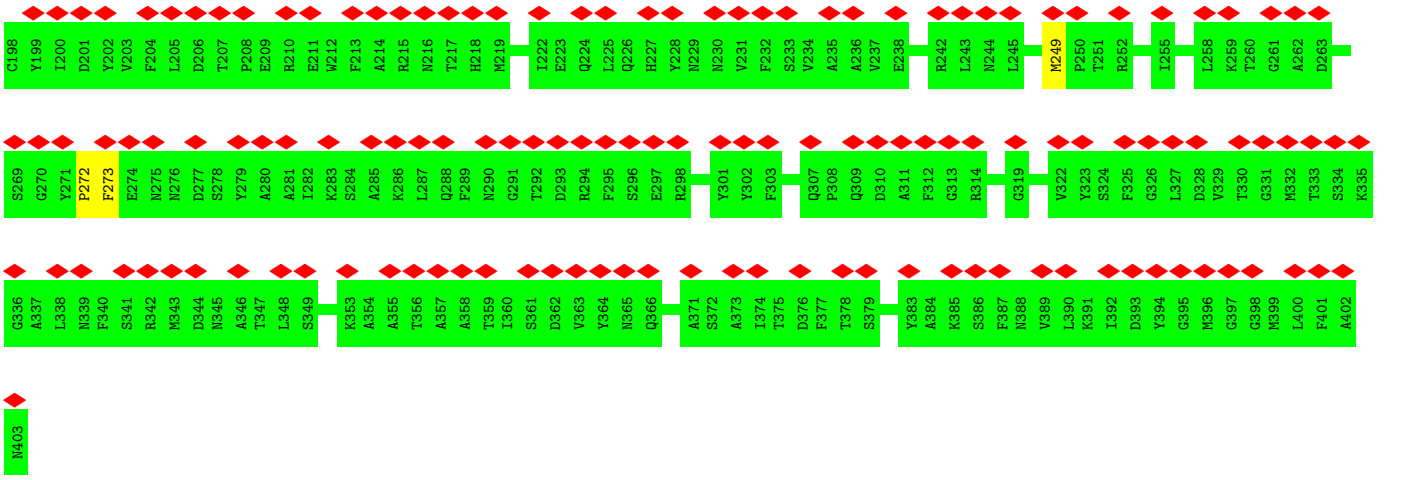


- Molecule 4: MCPv3

Chain cZ:

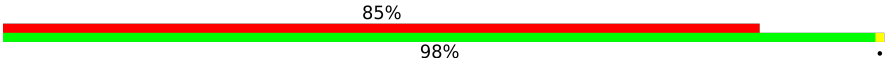


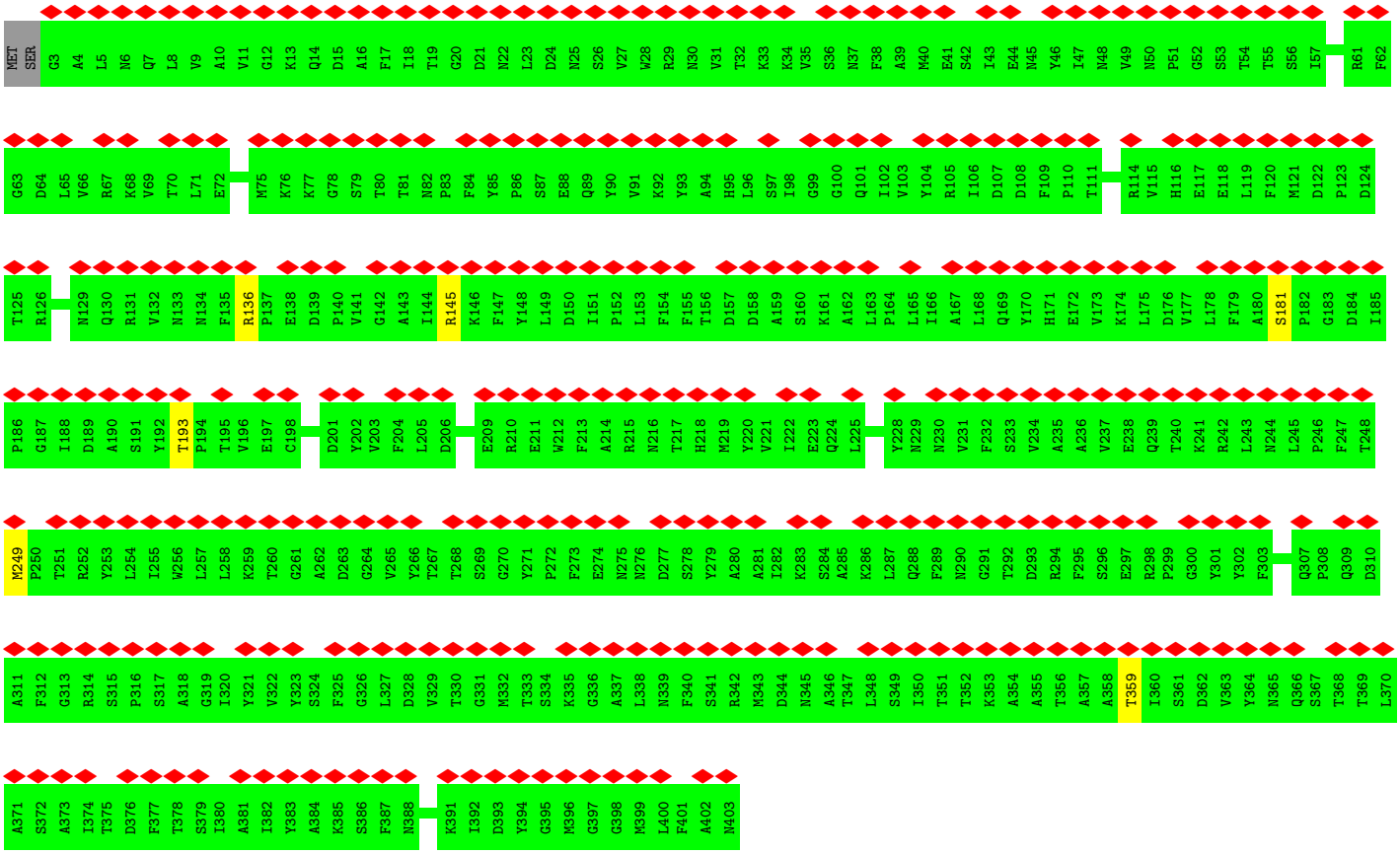




- Molecule 4: MCPv3

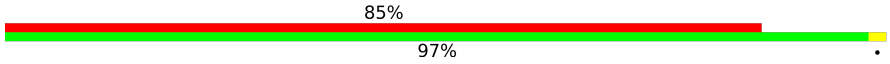
Chain dd:

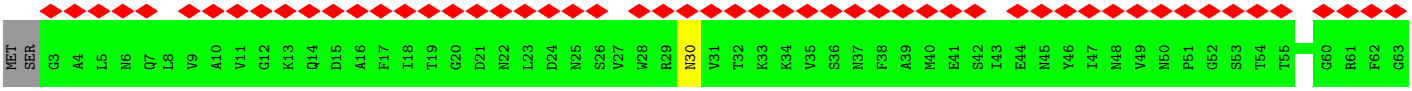




- Molecule 4: MCPv3

Chain df:





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A127 T128 N129 Q130 R131 V132 N133 N134 F135 R136 P137 E138 D139 P140 V141 G142 A143 I144 R145 K146 F147 Y148 L149 D150 I151 P152 L153 F154 F155 T156 D157 D158 A159 S160 K161 A162 L163 P164 L165 I166 A167 L168 Q169 Y170 H171 E172 V173 K174 L175 D176 V177 L178 F179 A180 S181 P182 G183 D184 I185 P186

G187 I188 D189 A190 S191 Y192 T193 P194 T195 V196 E197 C198 Y199 I200 D201 Y202 V203 F204 L205 D206 T207 P208 E209 R210 E211 W212 F213 A214 R215 N216 T217 H218 M219 Y220 V221 I222 E223 Q224 H227 Y228 N229 F232 S233 V234 A235 A236 V237 E238 Q239 T240 K241 R242 L243 N244 L245 P246 F247 T248

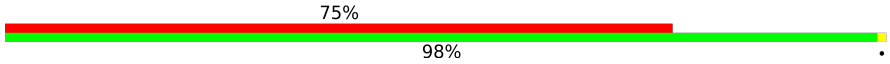
M249 P250 T251 R252 Y253 L254 I255 W256 L257 L258 K259 T260 G261 A262 D263 G264 V265 Y266 S269 G270 Y271 P272 F273 E274 N275 N276 D277 S278 Y279 A280 A281 I282 K283 S284 A285 K286 L287 Q288 F289 N290 G291 T292 D293 R294 F295 S296 E297 R298 P299 G300 Y301 Y302 F303 Q307 P308 Q309 D310 A311

F312 G313 R314 S315 A318 G319 I320 Y321 V322 Y323 S324 F325 G326 L327 D328 V329 T330 G331 M332 T333 S334 K335 G336 A337 L338 N339 F340 S341 R342 M343 D344 N345 A346 T347 L348 S349 I350 T351 T352 K353 A354 A355 T356 A357 A358 T359 I360 S361 D362 V363 Y364 N365 Q366 S367 T368 T369 L370 A371 S372

A373 I374 T375 D376 F377 T378 S379 I380 A381 I382 Y383 A384 K385 S386 F387 N388 V389 L390 K391 I392 D393 Y394 G395 M396 G397 G398 M399 L400 F401 A402 N403

- Molecule 4: MCPv3

Chain dj:



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L65 V66 R67 K68 E72 M75 K76 K77 G78 S79 T80 T81 N82 P83 F84 Y85 P86 S87 E88 Q89 Y90 V91 K92 Y93 A94 H95 G99 G100 Q101 I102 V103 Y104 R105 I106 D107 D108 F109 P110 T111 W112 T113 R114 V115 H116 E117 E118 L119 F120 M121 D122 P123 D124 T125 R126 R131 V132

N133 N134 F135 R136 P137 E138 D139 P140 V141 G142 A143 I144 R145 K146 F147 Y148 L149 D150 I151 P152 L153 F154 F155 T156 D157 D158 A159 S160 K161 A162 L163 P164 L165 I166 A167 L168 Q169 Y170 H171 E172 V173 K174 L175 D176 V177 L178 F179 A180 S181 P182 G183 D184 I185 P186 G187 I188 D189 A190 S191 Y192

T193 E197 D201 Y202 V203 F204 L205 D206 R210 E211 W212 F213 A214 R215 N216 T217 H218 M219 I222 E223 Q224 L225 Q226 H227 Y228 N229 N230 V231 F232 A235 A236 V237 E238 Q239 R242 L243 N244 L245 P246 F247 T248 M249 R252 Y253 L254 I255 W256 L257 L258 K259 T260 G261 A262

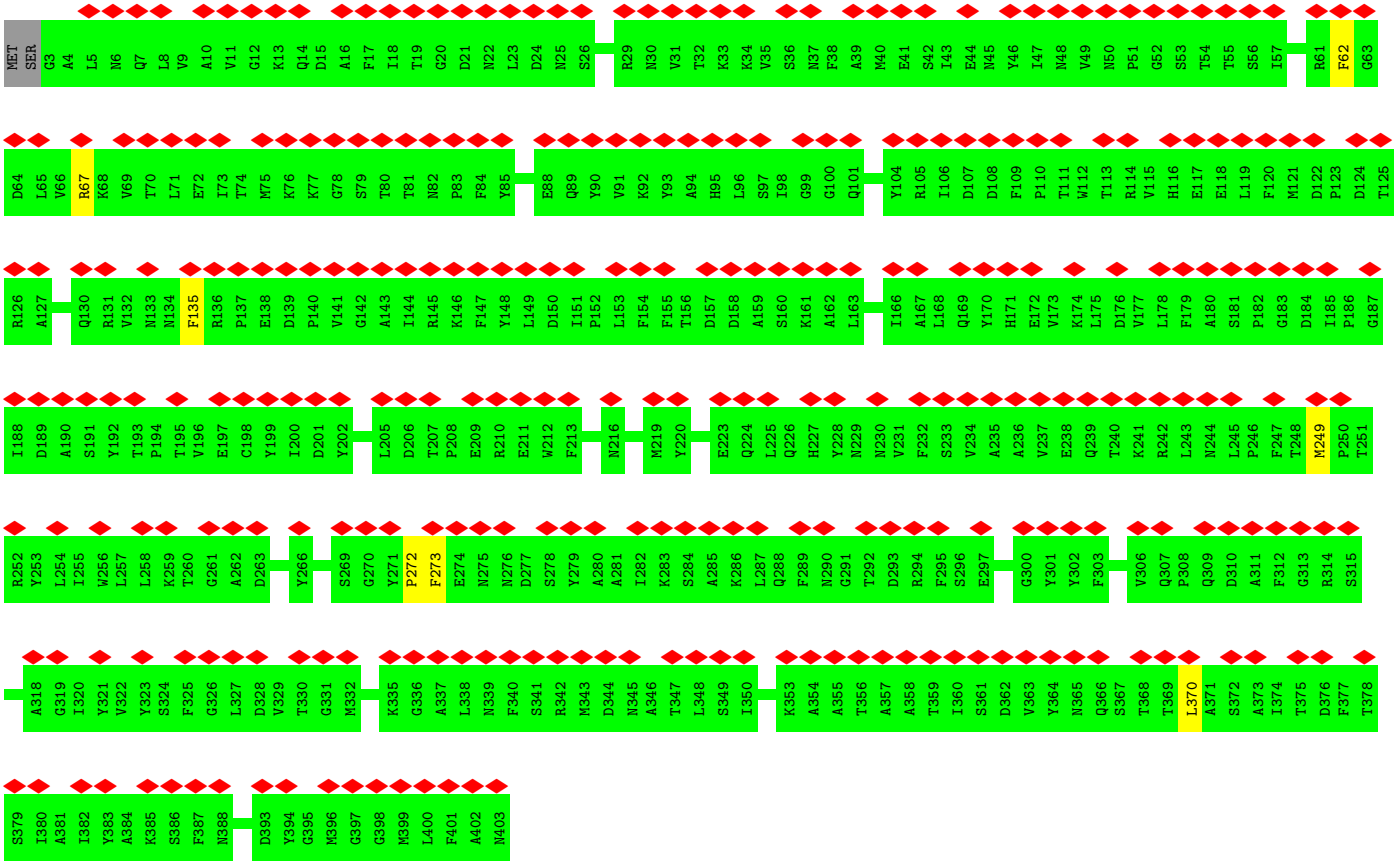
D263 G264 V265 Y266 S269 G270 Y271 P272 F273 E274 N275 N276 D277 S278 Y279 A280 A281 I282 K283 S284 L287 Q288 F289 N290 G291 T292 D293 R294 F295 S296 E297 R298 P299 G300 Y301 Y302 V306 Q307 P308 Q309 D310 A311 F312 G313 R314 S315 A318 G319 I320 Y321 V322 Y323 S324 F325 G326 L327

D328 V329 T330 G331 M332 K335 G336 A337 L338 N339 F340 S341 R342 M343 D344 N345 A346 T347 L348 S349 I350 T351 T352 K353 A354 A355 T356 A357 A358 T359 I360 S361 D362 V363 Y364 N365 Q366 S367 T368 T369 L370 A371 S372 A373 I374 T375 D376 F377 T378 S379 I380 A381 I382 Y383 A384 K385 S386 F387 N388

I392 D393 Y394 G395 M396 G397 G398 M399 L400 F401 A402 N403

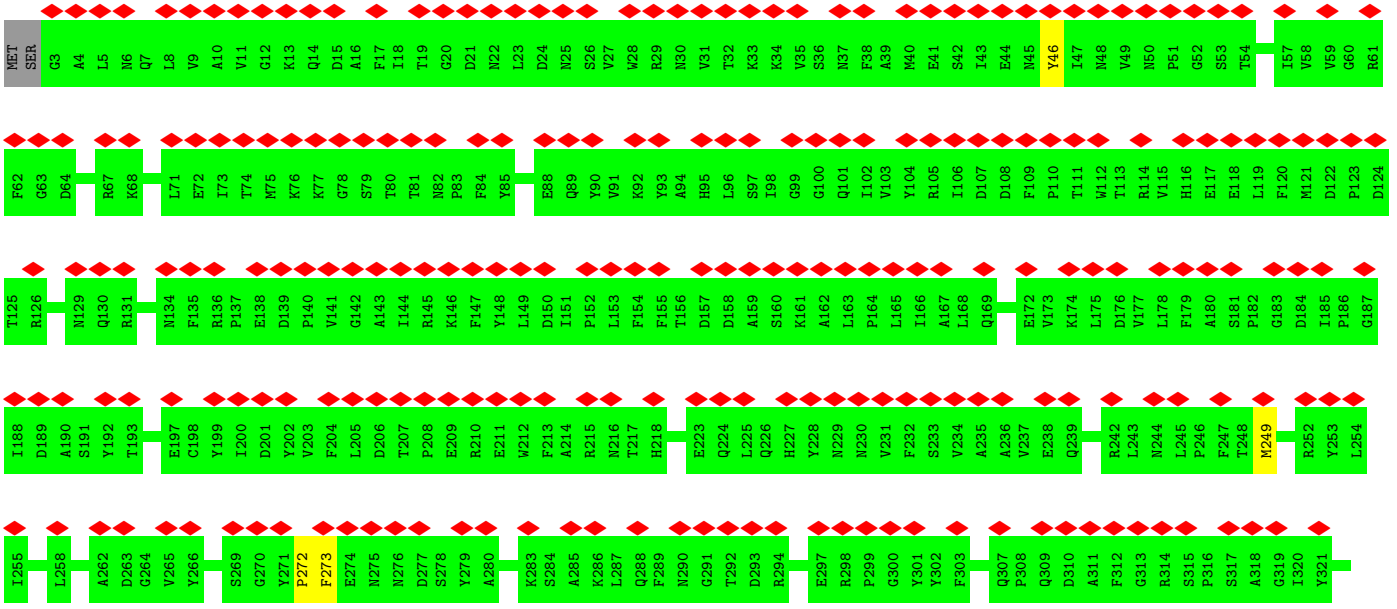
- Molecule 4: MCPv3

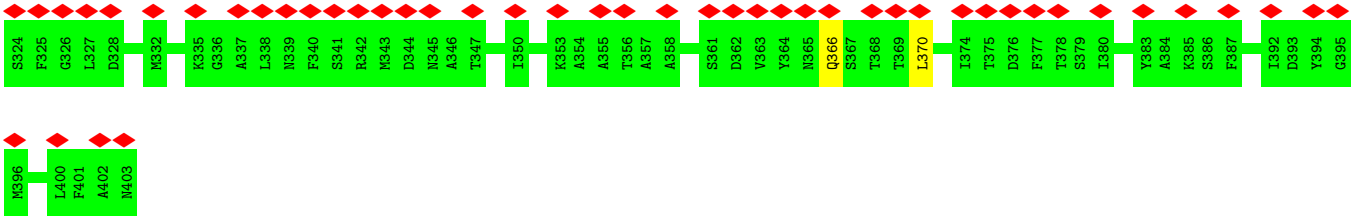
Chain dk: 76% 98%



- Molecule 4: MCPv3

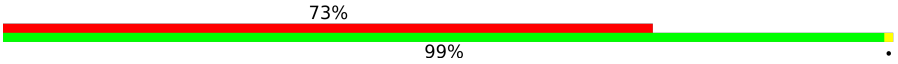
Chain dl: 70% 98%

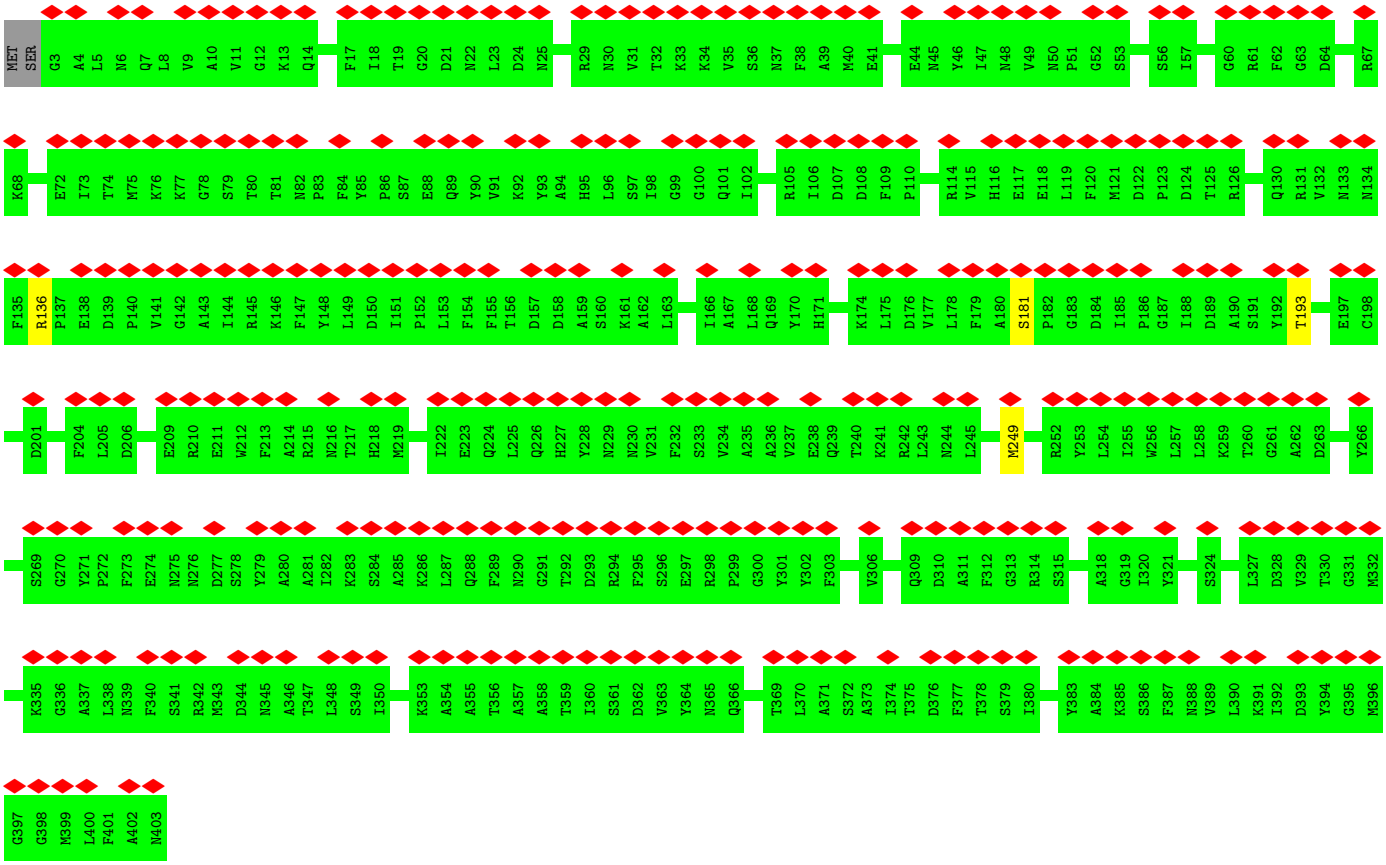




- Molecule 4: MCPv3

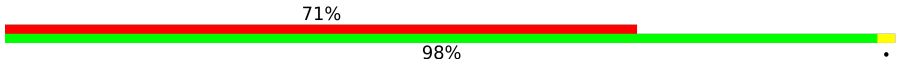
Chain dp:

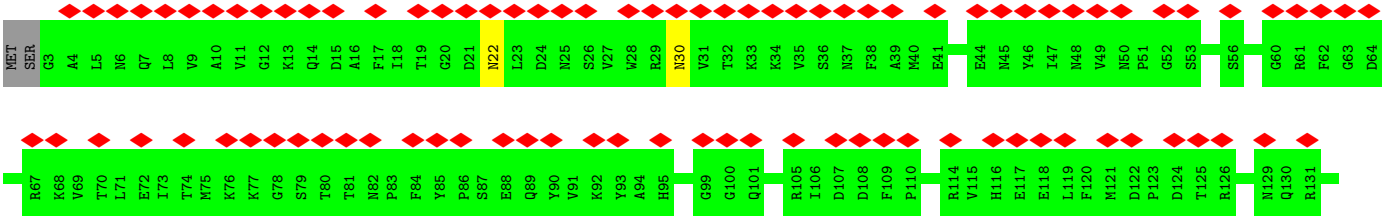




- Molecule 4: MCPv3

Chain dr:





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E197 C198 Y199 I200 D201 Y202 V203 F204 L205 D206 E209 R210 E211 W212 F213 A214 R215 N216 T217 H218 M219 Y220 E223 Q224 L225 Q226 H227 Y228 N229 N230 V231 F232 S233 Y234 A235 A236 V237 E238 Q239 T240 K241 R242 L243 N244 L245 F246 F247 T248 M249 R252 Y253 L254 I255 L258 K259 T260

G261 A262 D263 G264 V265 Y266 S269 G270 Y271 P272 F273 E274 N275 N276 D277 S278 Y279 A280 A281 S284 A285 K286 L287 Q288 F289 N290 G291 T292 D293 R294 F295 S296 E297 R298 Y301 Y302 F303 V306 Q307 P308 Q309 D310 A311 F312 G313 R314 A318 G319 I320 Y321 V322 Y323 S324 F325 G326

L327 D328 V329 T330 G331 M332 K335 G336 A337 L338 N339 F340 S341 R342 M343 D344 T347 L348 S349 I350 K353 A354 A355 T356 A357 A358 T359 I360 S361 D362 V363 Y364 N365 Q366 S367 T368 T369 L370 I374 T375 D376 F377 T378 S379 I382 Y383 A384 K385 S386 F387 N388 V389 L390 K391 I392

D393 Y394 G395 M396 G397 G398 M399 L400 F401 A402 N403

- Molecule 5: MCPv4

Chain bE: 74% 99%

MET VAL S3 G4 G5 V6 V7 Q8 L9 I10 S11 Y12 G13 A14 Q15 D16 I19 S20 G21 G22 P23 K24 T25 I26 F27 K28 S29 Y30 V31 K32 K33 V34 N35 N36 F37 A38 I39 D40 A41 V42 K43 I46 M49 G50 N51 G52 N53 P54 S55 P59 R60 N61 G62 D63 L64 I65

K66 R69 L70 E71 I72 T73 L74 K75 K76 G77 T78 G79 Q80 S81 F82 Y83 P84 A85 E86 Q87 L88 I89 S90 Y91 L92 K95 I96 G97 G98 N99 I100 I101 Q102 K103 I104 D105 D106 F107 S108 N109 F110 C111 R112 I113 R114 N115 E116 L117 F118 M119 D120 P121 D122 E123 R124 H125 T126 D127

Y128 R129 V130 N131 N132 F133 S134 S135 S136 D137 V138 V139 G140 S141 V142 K143 Y144 D148 L149 P150 L151 F152 F153 S154 K155 D156 T157 S158 V159 A160 L161 P162 L163 Q167 Y168 H169 D170 I171 E172 L173 D174 F175 R176 F177 N178 D179 V180 S181 T182 I183 Q184 G185 V186 D187 A188 S189 Y190 T191

E195 M196 Y197 I198 D199 Y200 V201 Y202 L203 E204 Q205 Q206 E207 R208 I209 K210 L211 V212 E213 K214 F217 Y218 N219 I220 E221 Q222 Y226 R227 K228 D229 I230 T231 F232 P233 A234 L235 S236 S237 T238 F239 K240 L241 D242 I243 P244 F245 N246 N247 P248 S249 R250 F251 Y255 F256 N257 T258

D259 S260 F261 G262 I263 Y264 N265 T266 S267 G268 L269 Y270 F271 N272 S273 N274 D275 A276 A277 A278 E281 S282 A283 L286 L287 N288 G289 T290 E291 R292 F293 K294 S295 R296 E297 G298 M299 Y300 F301 N302 C303 V304 Q305 P306 Q307 Q308 A309 L310 G311 R312 S316 G317 I318 Y319 M320 Y321 A322

F323 G324 E325 D326 V327 A328 N329 A330 K333 G334 A335 L336 D337 M338 S339 R340 V341 N342 E343 L344 Q347 L348 K351 N352 A355 A356 N357 V358 Y359 T360 V361 Y362 N363 E366 T367 L368 A369 S370 S371 T372 S373 T374 Y375 K376 G377 I378 T379 L380 N384 L388 Q389 V390 R391

S392 G393 L394 G395 A396 V397 M398 F399 ASP SER

- Molecule 5: MCPv4

Chain cY: 83% 98%

MET VAL S3 G4 G5 V6 V7 Q8 L9 I10 S11 Y12 G13 A14 Q15 Y18 I19 S20 G21 G22 P23 K24 T25 I26 F27 K28 S29 Y30 V31 K32 K33 V34 N35 N36 F37 A38 I39 D40 S41 V42 K43 I46 N47 G48 M49 G50 N51 G52 N53 P54 S55 V56 L57 R60 N61 G62 D63

L64 I65 K66 S67 I68 R69 L70 E71 L74 K75 K76 G77 T78 G79 Q80 S81 F82 Y83 P84 A85 E86 Q87 L88 I89 S90 Y91 L92 A93 L94 K95 I96 G97 G98 N99 I100 I101 Q102 K103 I104 D105 D106 F107 S108 N109 F110 C111 R112 I113 R114 N115 E116 L117 F118 M119 D120 P121 D122 E123 R124

H125 T126 D127 Y128 R129 V130 N131 N132 F133 S134 S135 S136 D137 G140 S141 V142 K143 Y144 F145 F146 L147 D148 L149 P150 L151 F152 F153 S154 K155 D156 T157 S158 V159 A160 L161 P162 L163 I164 A165 L166 Q167 Y168 H169 D170 I171 E172 L173 D174 F175 R176 F177 N178 D179 V180 S181 T182 I183 Q184 G185

V186 D187 A188 S189 Y190 T191 E195 M196 Y197 I198 D199 Y200 V201 Y202 L203 E204 Q205 Q206 E207 R208 I209 K210 L211 V212 E213 K214 P215 L216 F217 Y218 N219 I220 E221 Q222 C223 N224 F225 Y226 R227 K228 D229 I230 T231 F232 P233 A234 L235 S236 S237 T238 F239 K240 L241 D242 I243 P244 F245 N246 N247

P248 S249 R250 F251 Y255 F256 N257 T258 D259 S260 F261 G262 I263 Y264 S267 G268 L269 Y270 F271 N272 S273 N274 D275 A276 A277 A278 P279 L280 E281 S282 A283 V284 M285 L286 L287 N288 G289 T290 E291 R292 F293 K294 S295 R296 E297 G298 M299 Y300 F301 N302 Q305 P306 Q307 Q308 A309 L310 G311

R312 S315 S316 G317 I318 Y319 M320 Y321 A322 F323 G324 E325 D326 V327 A328 N329 A330 T331 S332 K333 G334 A335 L336 D337 M338 S339 R340 V341 N342 E343 L344 S345 L346 Q347 L348 K351 N352 A353 T354 A355 N356 N357 V358 Y359 T360 V361 Y362 M363 P364 Q365 E366 T367 L368 A369 S370 S373 T374

Y375 K376 G377 I378 T379 L380 F381 S382 T383 N384 W385 N386 V387 L388 Q389 V390 R391 S392 G393 L394 G395 A396 V397 M398 F399 ASP SER

- Molecule 5: MCPv4

Chain de: 86% 99%

MET VAL S3 G4 G5 V6 V7 Q8 L9 I10 S11 Y12 G13 A14 Q15 D16 V17 Y18 I19 S20 G21 G22 P23 K24 T25 I26 F27 K28 S29 Y30 V31 K32 K33 V34 N35 N36 F37 A38 I39 D40 S41 V42 K43 I44 P45 I46 N47 G48 M49 G50 N51 G52 N53 P54 S55 V56 L57 I58 P59 R60

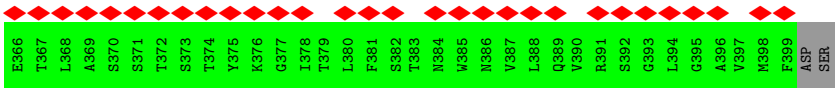
N61 G62 D63 L64 I65 K66 S67 I68 R69 L70 E71 I72 T73 L74 K75 K76 G77 T78 G79 Q80 S81 F82 Y83 P84 A85 E86 Q87 L88 I89 S90 Y91 L92 A93 L94 K95 I96 G97 G98 N99 I100 I101 Q102 K103 I104 D105 D106 F107 S108 N109 F110 C111 R112 I113 R114 N115 E116 L117 F118 M119 D120

P121 D122 E123 R124 H125 T126 D127 Y128 R129 V130 F133 S134 S135 S136 D137 V138 V139 G140 S141 V142 K143 Y144 F145 F146 L147 D148 L149 P150 L151 F152 F153 S154 K155 D156 T157 S158 V159 A160 L161 P162 L163 I164 A165 L166 Q167 Y168 H169 D170 I171 E172 L173 D174 F175 R176 F177 N178 D179 V180 S181

T182 I183 Q184 G185 V186 D187 A188 S189 Y190 T191 P192 T193 I194 E195 M196 Y197 I198 D199 Y200 V201 Y202 L203 E204 Q205 Q206 E207 R208 I209 K210 L211 V212 E213 K214 F217 Y218 N219 I220 E221 Q222 F225 Y226 R227 K228 D229 I230 T231 F232 P233 A234 L235 S236 S237 T238 F239 K240 L241 D242 I243

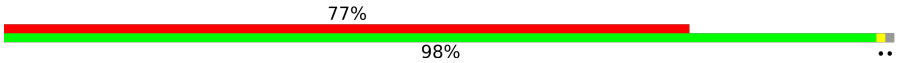
P244 F245 N246 N247 P248 S249 R250 F251 L252 V253 W254 Y255 F256 N257 T258 D259 S260 F261 G262 I263 Y264 N265 T266 S267 G268 L269 Y270 F271 N272 S273 N274 D275 A276 A277 A278 P279 L280 E281 S282 A283 V284 M285 L286 L287 N288 G289 T290 E291 R292 F293 K294 S295 R296 E297 G298 M299 Y300 F301 N302 C303

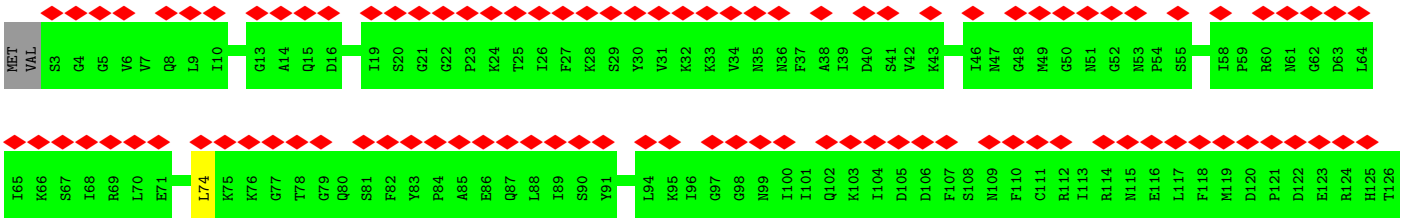
V304 Q305 P306 Q307 Q308 A309 L310 G311 R312 S315 S316 G317 I318 Y319 M320 Y321 A322 F323 G324 E325 D326 V327 A328 N329 A330 T331 S332 K333 G334 A335 L336 D337 M338 S339 R340 V341 N342 E343 L344 S345 L346 Q347 L348 K351 N352 A353 T354 A355 A356 N357 V358 Y359 T360 V361 Y362 M363 P364 Q365



- Molecule 5: MCPv4

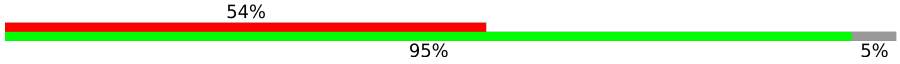
Chain dq:

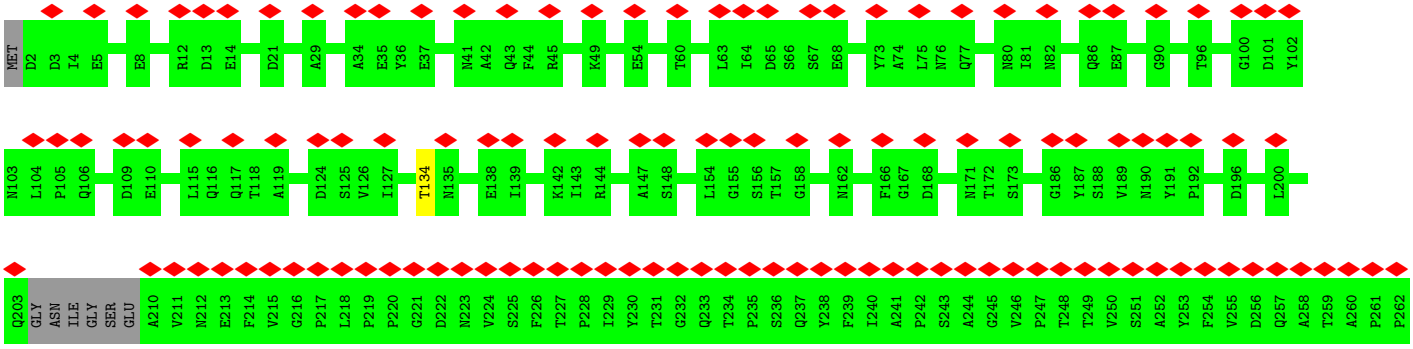


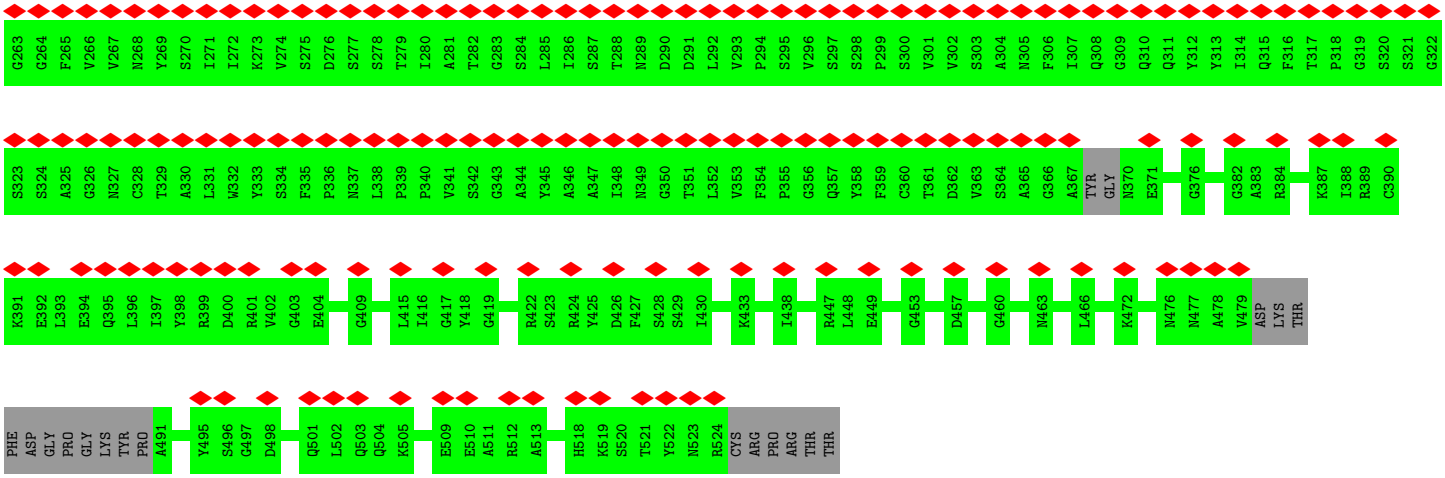


- Molecule 6: P1v1

Chain bG:

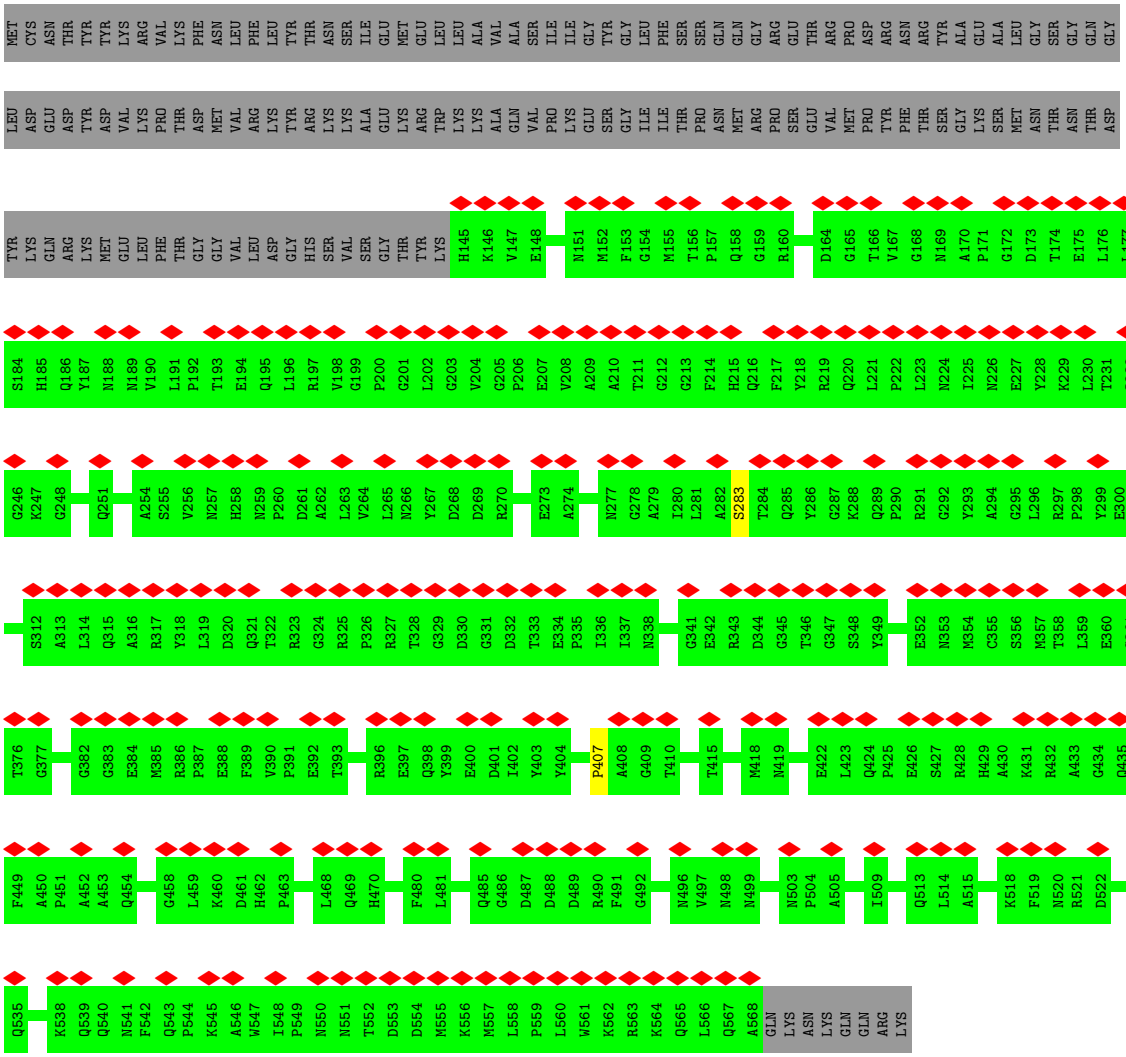






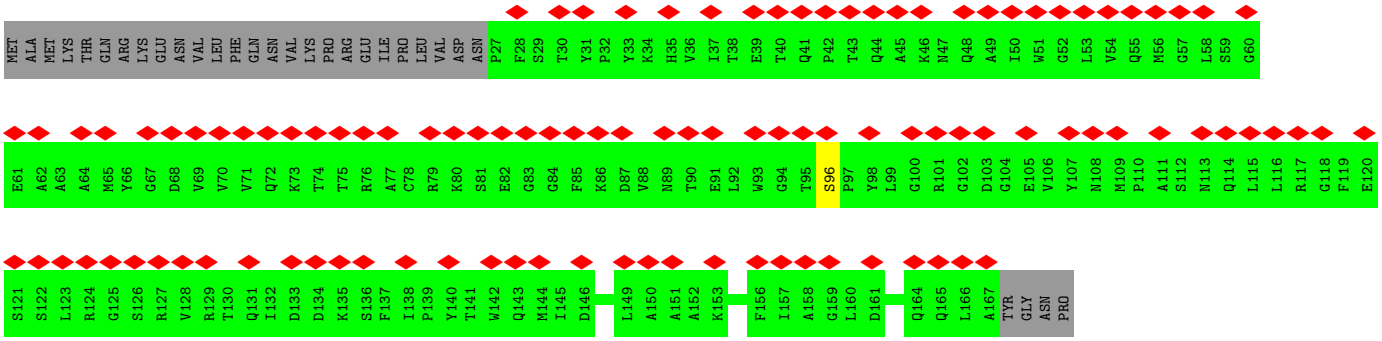
- Molecule 7: P2

Chain bH:



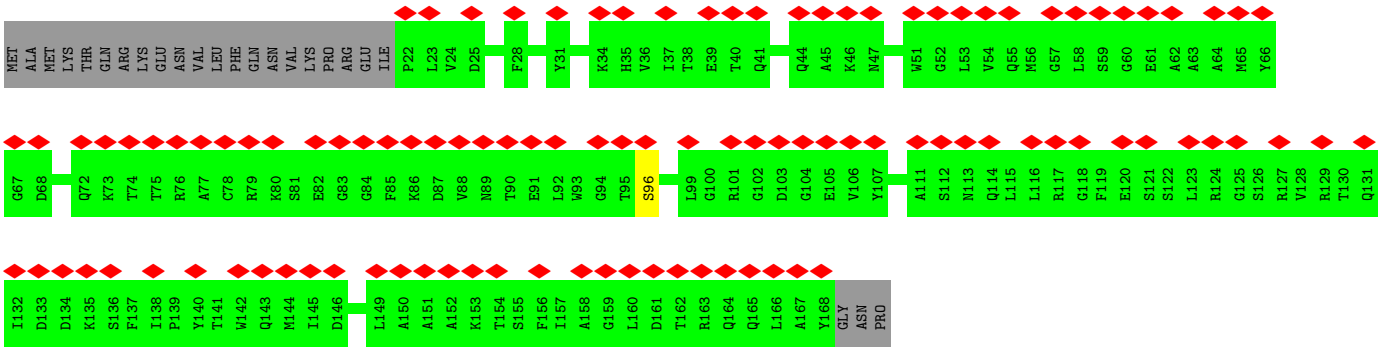
- Molecule 8: P3

Chain bI:



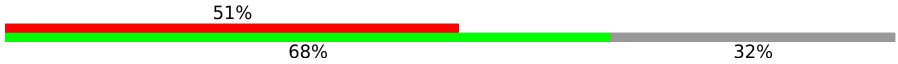
- Molecule 8: P3

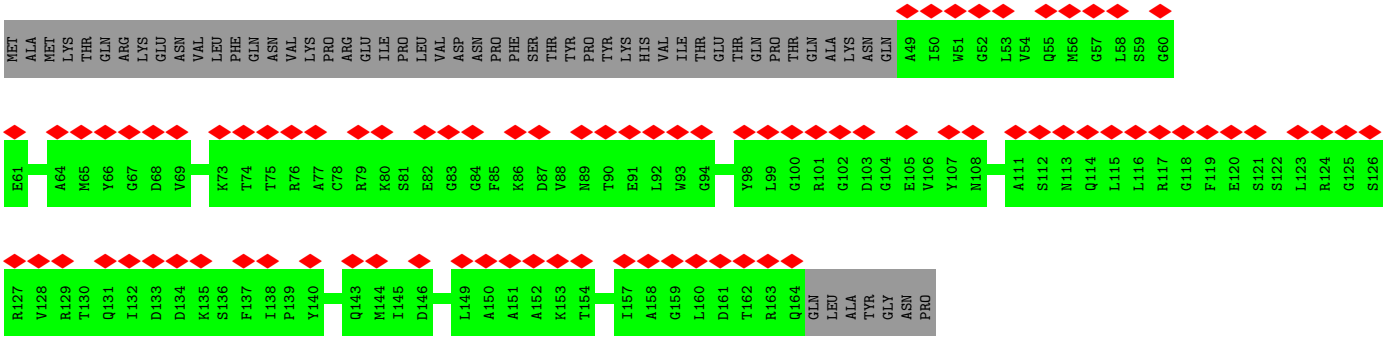
Chain bJ:



- Molecule 8: P3

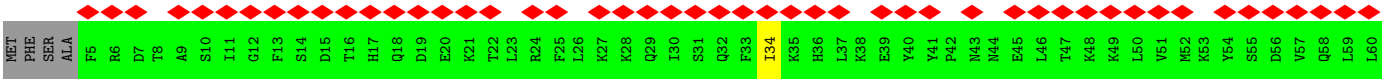
Chain bK:

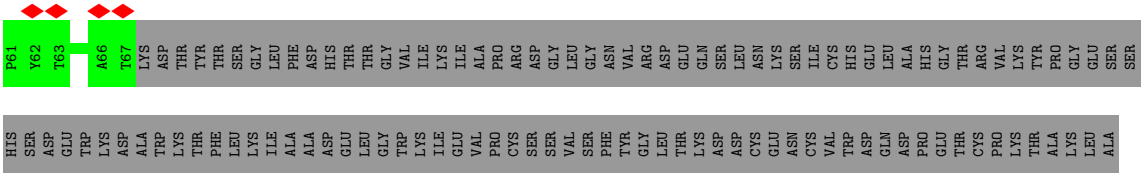




- Molecule 9: P4

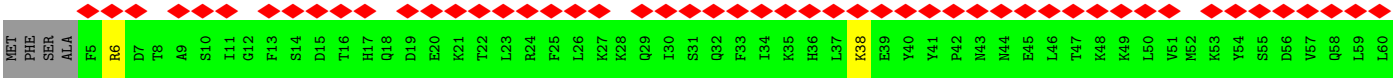
Chain bL:

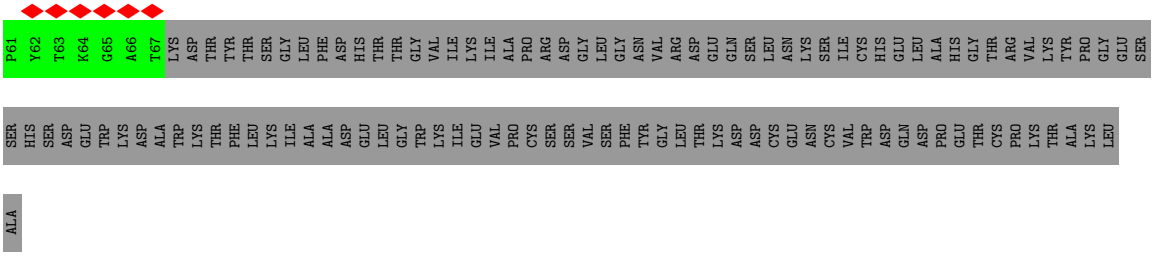




• Molecule 9: P4

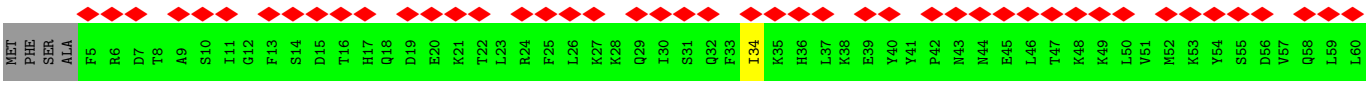
Chain bM:

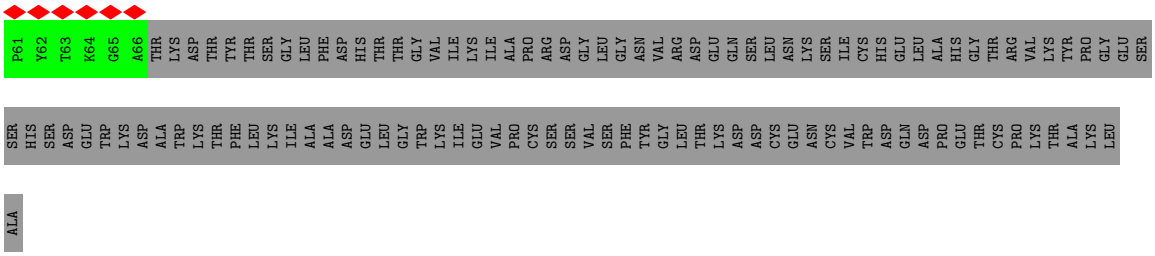




• Molecule 9: P4

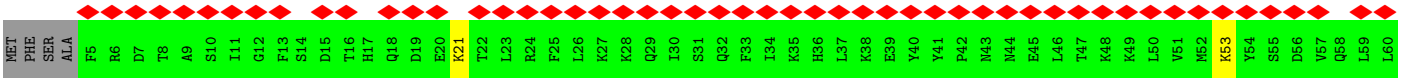
Chain bN:

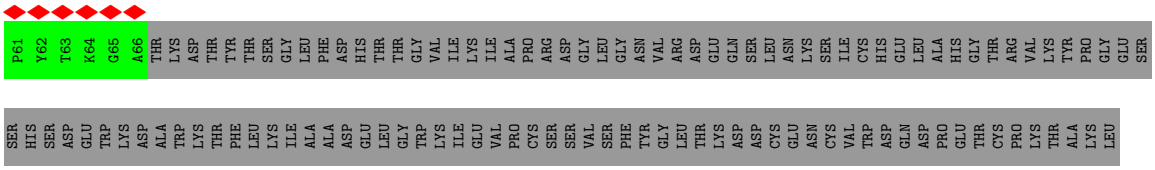




• Molecule 9: P4

Chain bO:





ALA

- Molecule 10: P5

Chain bP: 77% 97%

MET ASP SER R4 L5 S6 A7 A8 I11 R12 A13 A14 R15 I16 S17 M18 I19 P20 G21 G22 V23 D24 G25 L26 V27 I28 N29 Y30 A31 E32 G33 G34 E35 P36 A37 W38 V39 P42 L43 K44 K45 Q46 K47 P48 L49 P50 N51 N52 L53 C54 Y55 T56 L59 E60 D61 I62 A63

R64 K65 R66 E67 A68 V69 I70 A71 K72 Y73 T74 K75 Q76 P77 L78 G81 T82 T83 F84 T85 H86 V87 L88 N89 A90 S91 H92 L93 N94 E95 Q96 Y97 T98 R99 V100 K101 A104 L105 P106 D107 K108 E109 F110 P111 I112 I113 E114 T115 E116 K117 Y118 P119 E120 P121 P122 I123 L124 W125

E126 T127 T128 I129 G130 A131 P132 S133 R134 L135 F136 D137 R138 S139 D140 G141 V142 K143 Y144 V145 ARG

- Molecule 11: P6

Chain bQ: 63% 73% 25%

MET ILE LEU VAL GLY ILE ALA VAL LEU ILE LEU LEU ALA VAL PHE ALA ILE LEU TYR TYR LYS GLN LYS GLU LYS PHE VAL VAL VAL GLY LYS PHE VAL GLU PRO ILE PRO SER ASN PRO GLY GLN ASP PHE THR LEU LEU PRO MET ASP GLN THR Y53 T54 F55 A56 D57 P58 V59 P60

D61 T62 A63 T64 A65 F66 D67 V68 V69 L70 S71 R72 F73 T74 D75 K76 K77 A78 P79 A80 D81 L82 L83 K84 G85 A86 T87 F88 P89 E90 A91 A92 P93 Y94 T95 D96 S97 E98 V99 E100 N101 I102 S103 K104 L105 A106 L107 S108 R109 V110 K111 G112 P113 D114 A115 P116 V117 L118 S119 F120

I121 S122 V123 E124 Y125 A126 A127 K128 G129 V130 D131 N132 K133 K134 N135 T136 H137 Y138 D139 I140 A141 F142 M143 V144 Y145 D146 Q147 V148 K149 N150 F151 S152 L153 K154 L155 V156 L157 V158 A159 V160 L161 D162 A163 K164 N165 K166 L167 W168 I169 K170 K171 F172 S173 S174 F175 N176 S177 F178 T179 P180

K181 D182 K183 G184 P185 K186 G187 V188 E189 N190 I191 D192 E193 T194 P195 L196 A197 E198 F199 I200 P201 D202 F203 V204 Q205 R208 K211 D212 N213 A214 ASN VAL

- Molecule 12: P8

Chain bR: 55% 92% 8%

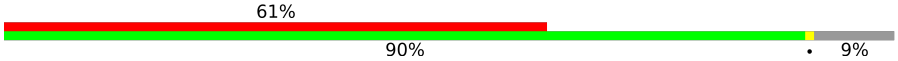
MET GLU THR ILE GLY ASN PHE ILE GLN ASN MET A12 F13 E16 N17 P18 Y19 K20 L21 S22 G23 D24 F25 G26 N27 L30 E31 P32 A36 R39 I40 L41 H42 E43 P47 E51 F52 R55 K56 D59 F60 I61 Q62 K63 K64 L65 I66 S67 E68 T69 K70 R71

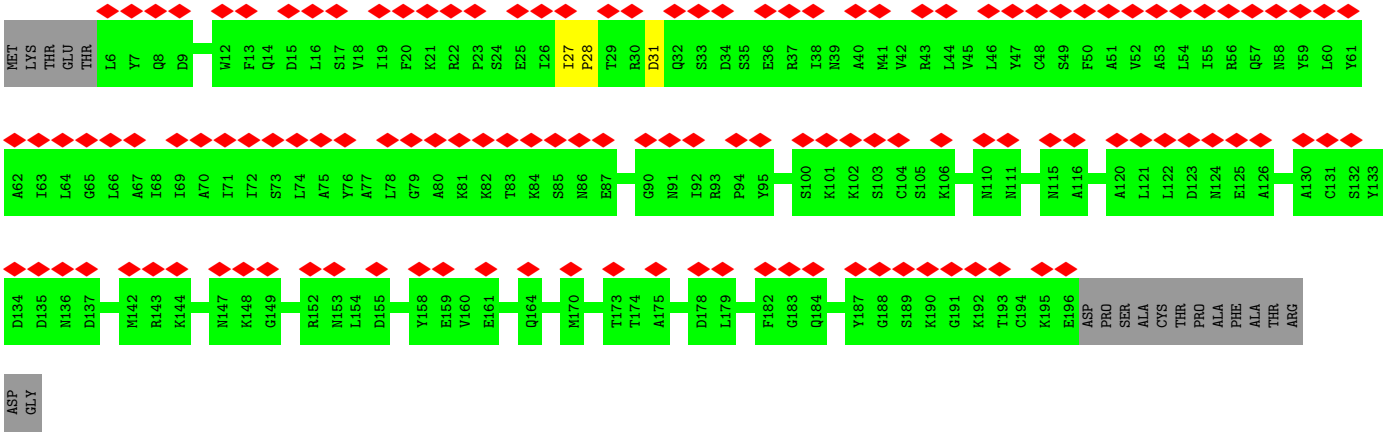
Y72 T73 S74 F75 D76 I77 G78 P79 Q80 N81 E82 D83 E84 M87 M88 M89 Y93 D96 S97 T98 F99 D100 G101 N102 I103 K104 A105 G106 L107 R108 K109 L110 L113 E117 R127 A130 L131 R134 D135 A136 S137 L138 P139 F140 S141 G142 G143 G144 E145 E146 A147 F148

K149 R150 P151 E152 L153 A154 T155 L156 K157 G158 S159 K160 V161 L162 S163 G164 F165 L166 P167 L168 D169 R170 ASN ALA SER

- Molecule 13: P9

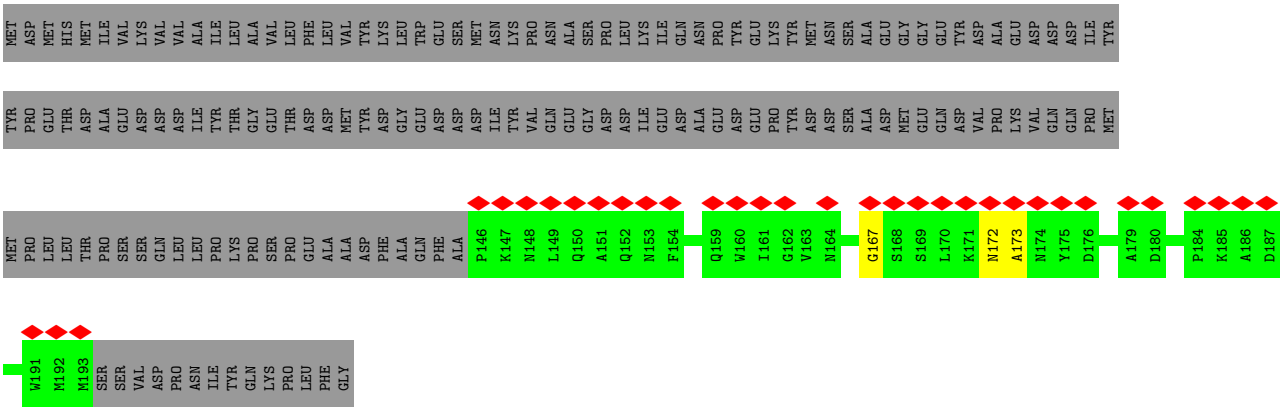
Chain bS:





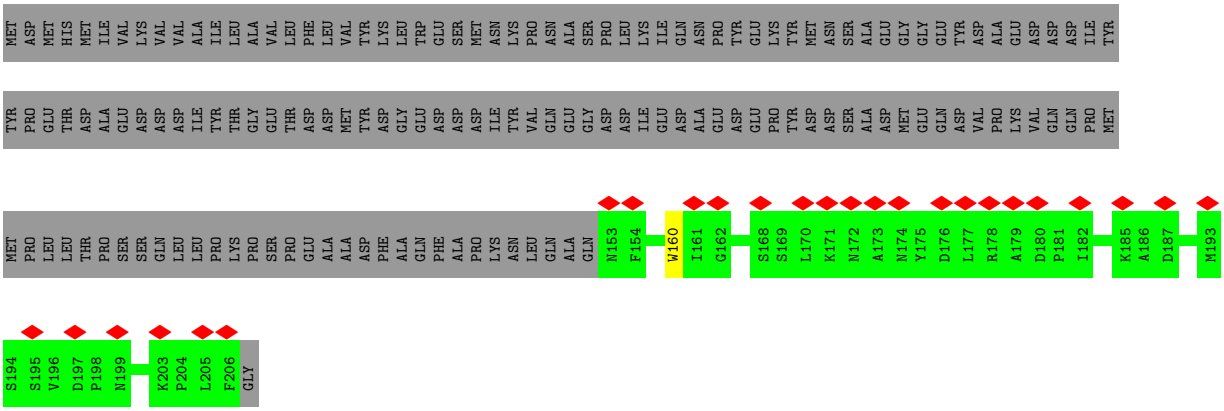
- Molecule 14: P11

Chain bT:



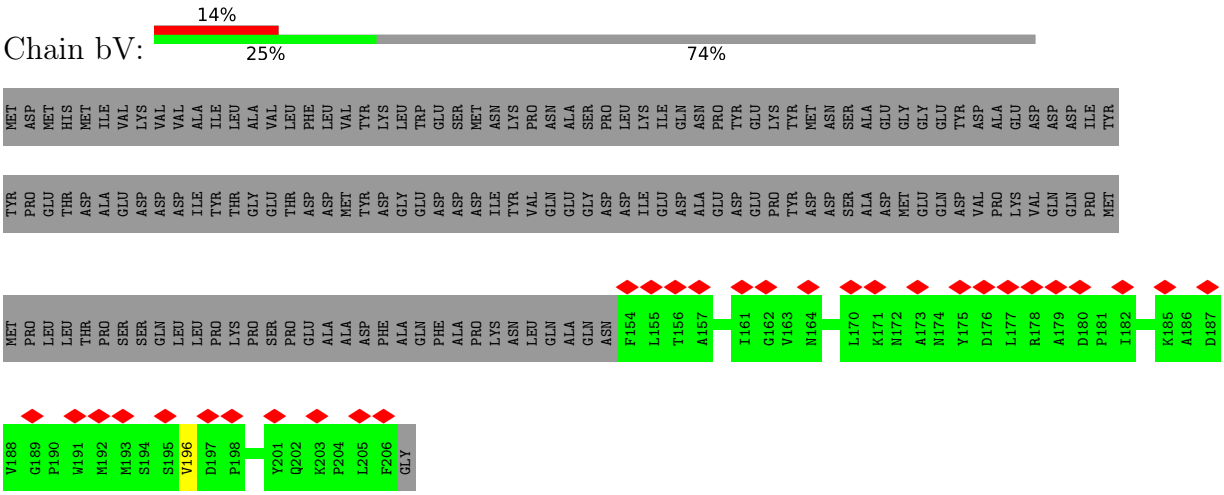
- Molecule 14: P11

Chain bU:



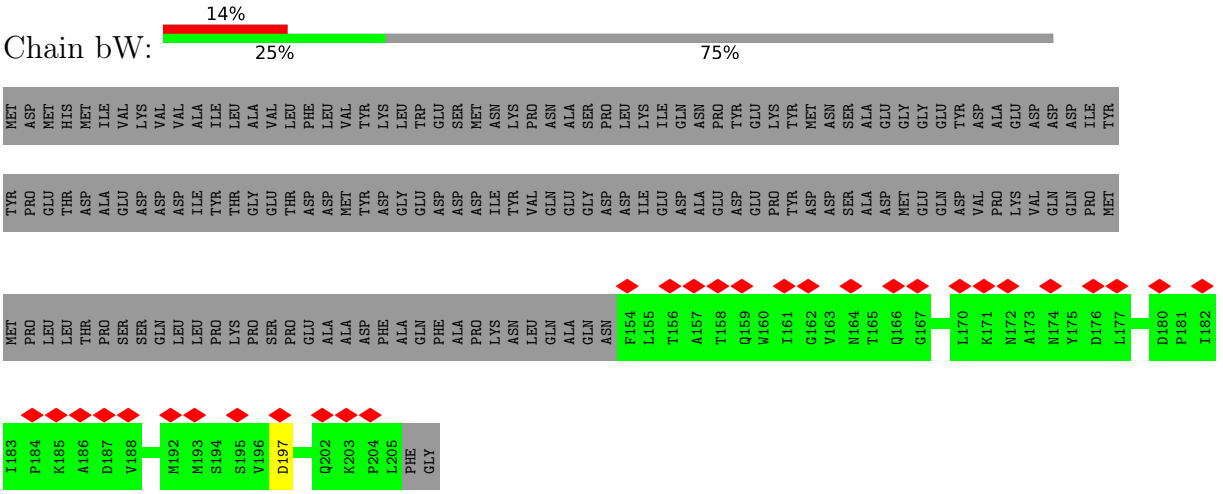
- Molecule 14: P11

Chain bV:



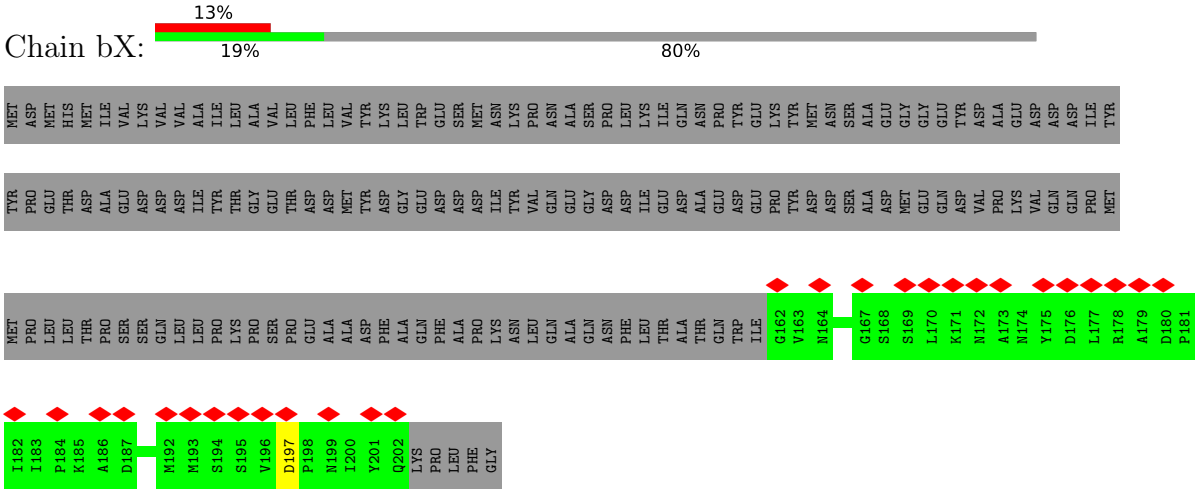
- Molecule 14: P11

Chain bW:



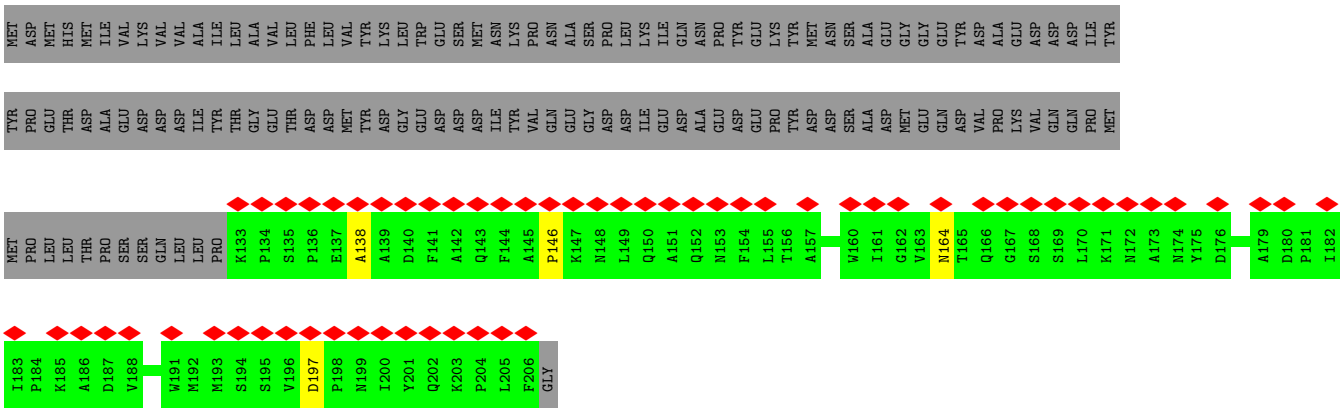
- Molecule 14: P11

Chain bX:



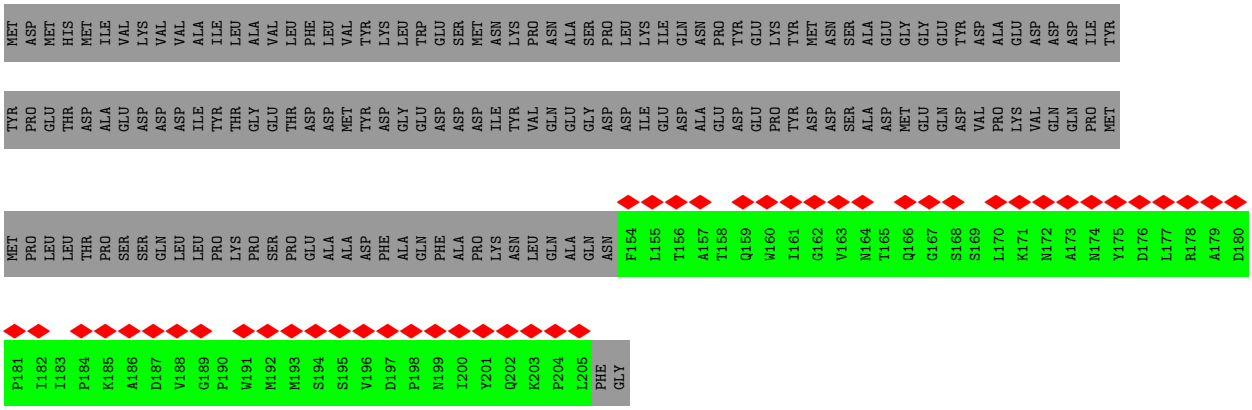
- Molecule 14: P11

Chain bY:



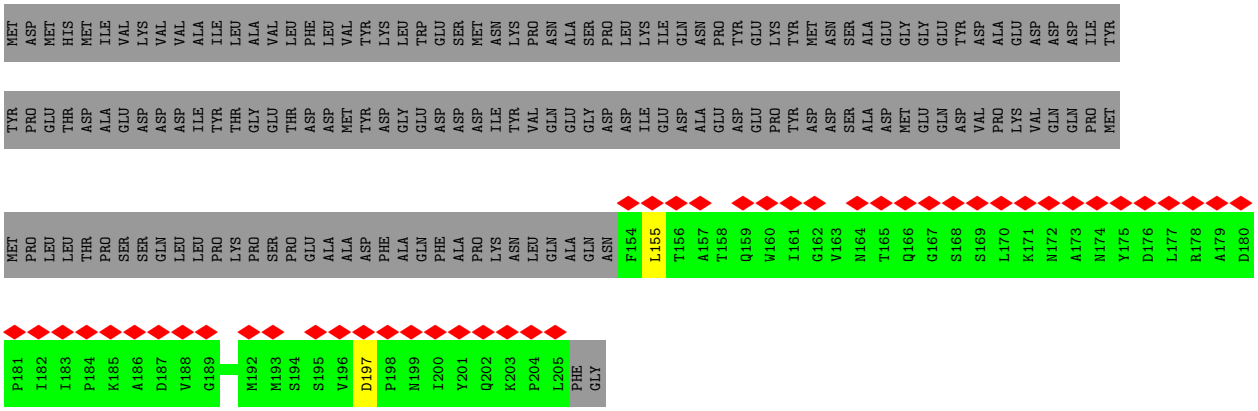
- Molecule 14: P11

Chain bZ:



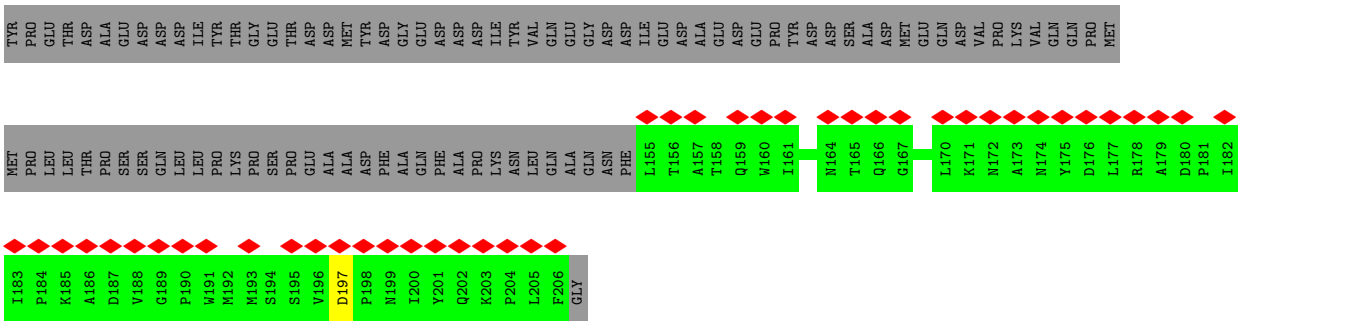
- Molecule 14: P11

Chain ca:



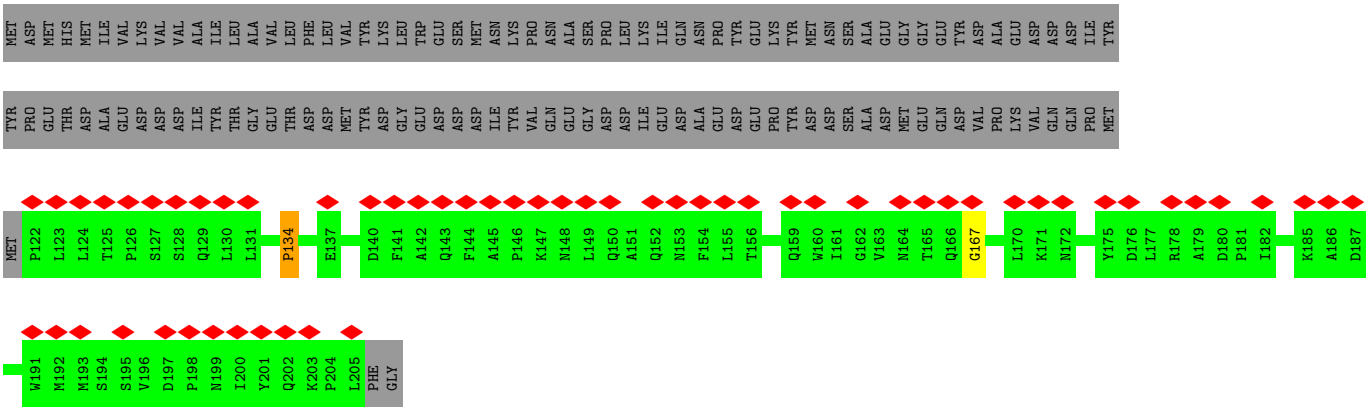
- Molecule 14: P11

Chain cb:



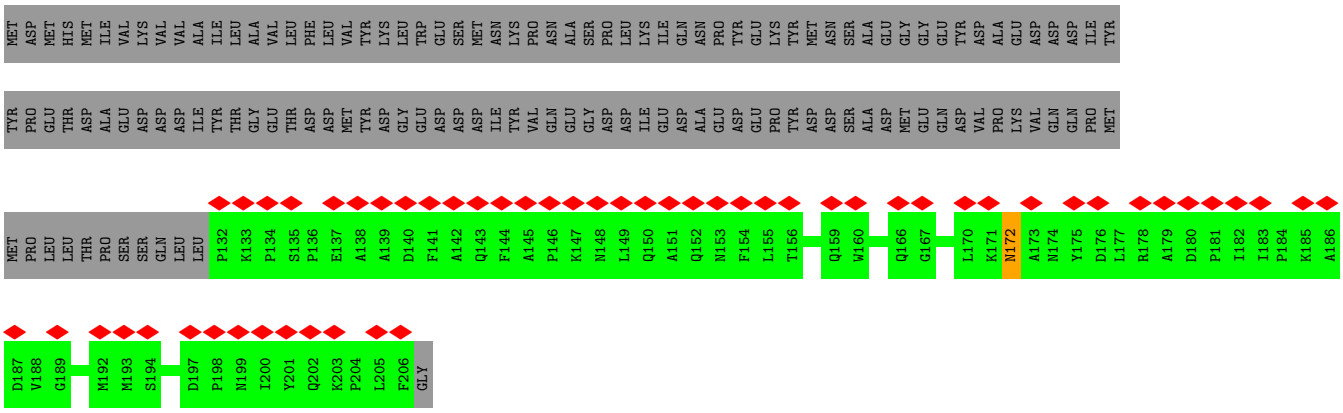
- Molecule 14: P11

Chain cc:



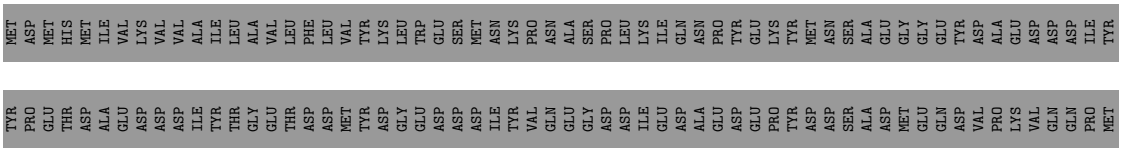
- Molecule 14: P11

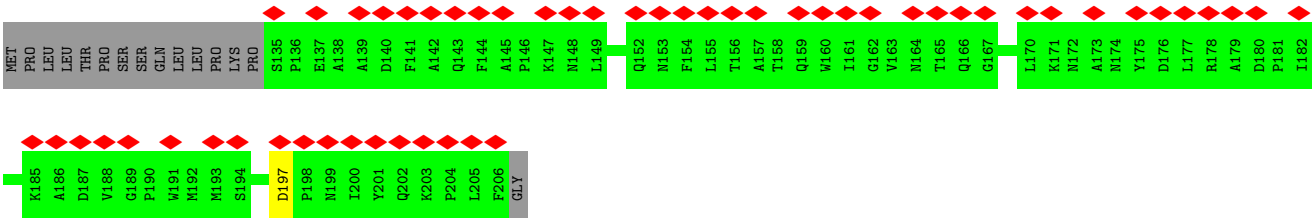
Chain cd:



- Molecule 14: P11

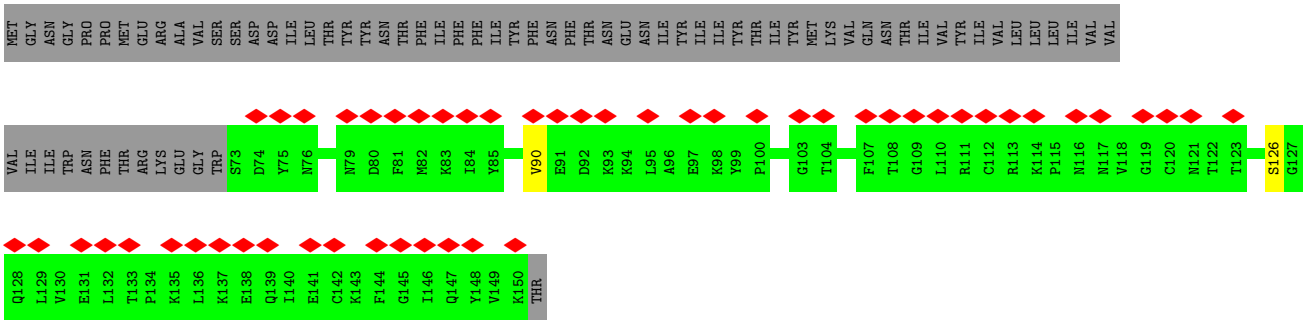
Chain ce:





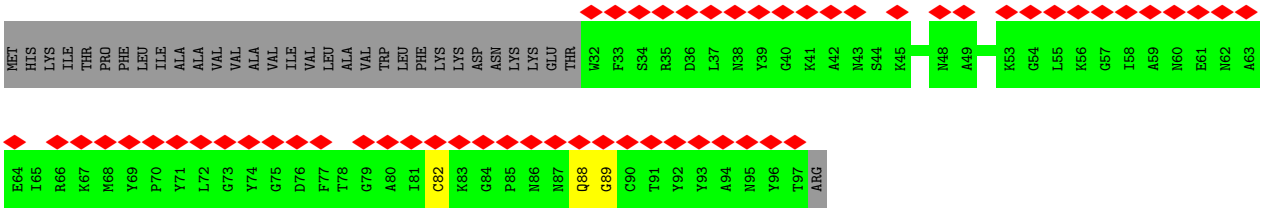
- Molecule 15: P12

Chain cf:



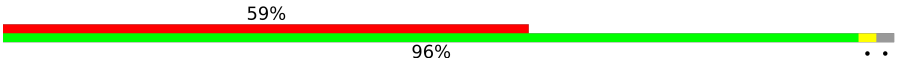
- Molecule 16: P13

Chain cg:



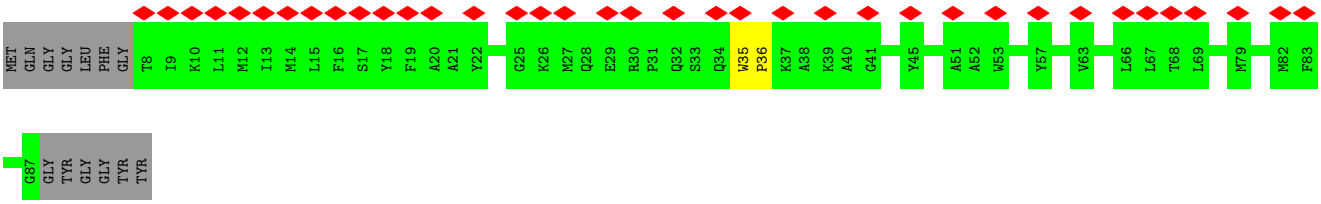
- Molecule 17: P15

Chain ch:



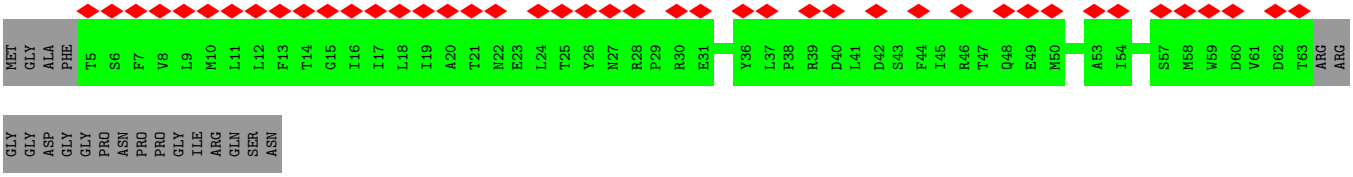
- Molecule 18: P16

Chain ci:



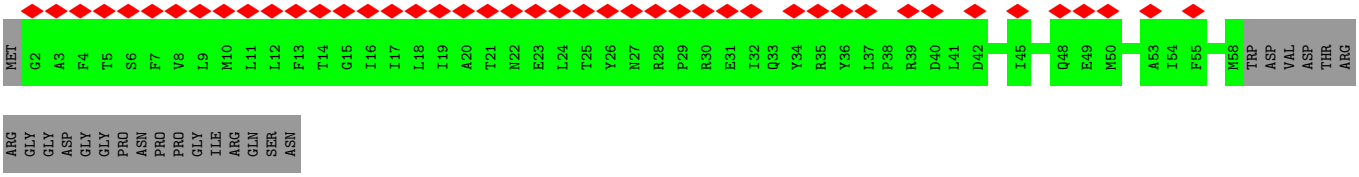
• Molecule 19: P17

Chain cj:



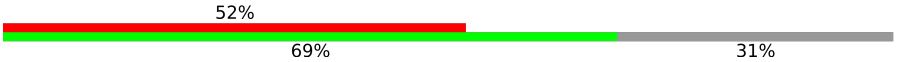
• Molecule 19: P17

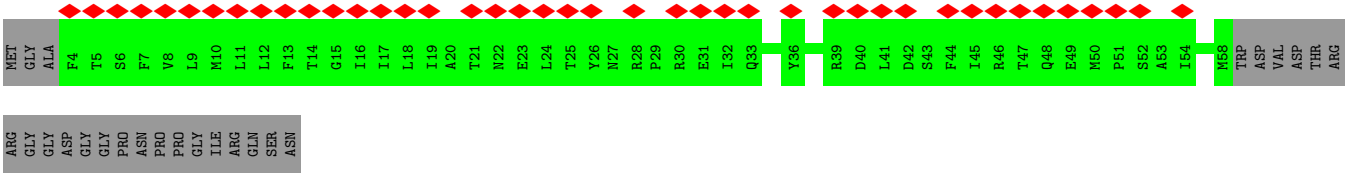
Chain ck:



• Molecule 19: P17

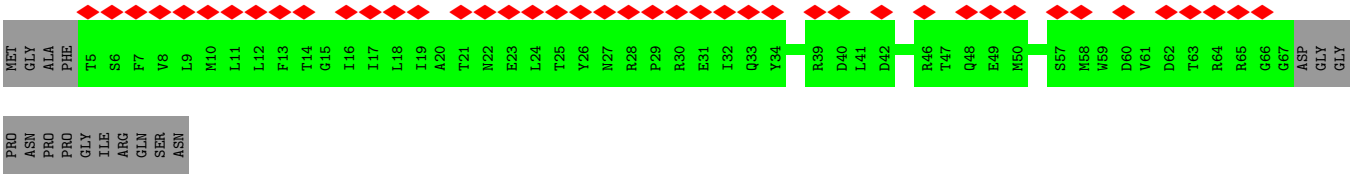
Chain cl:





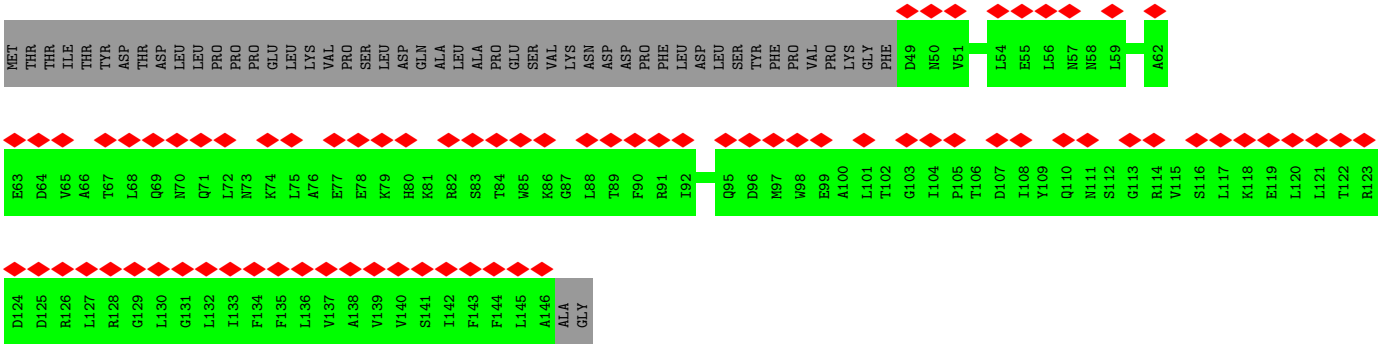
• Molecule 19: P17

Chain cm:



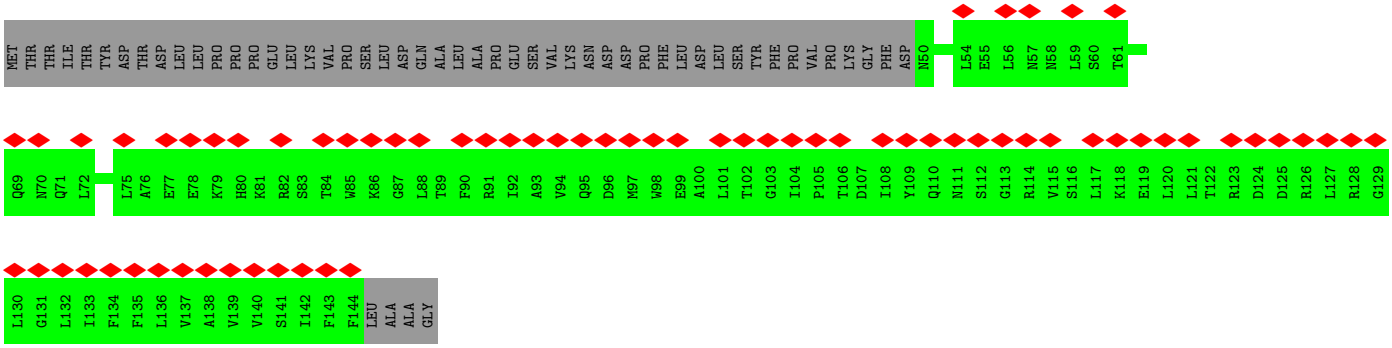
• Molecule 20: P18

Chain cn:



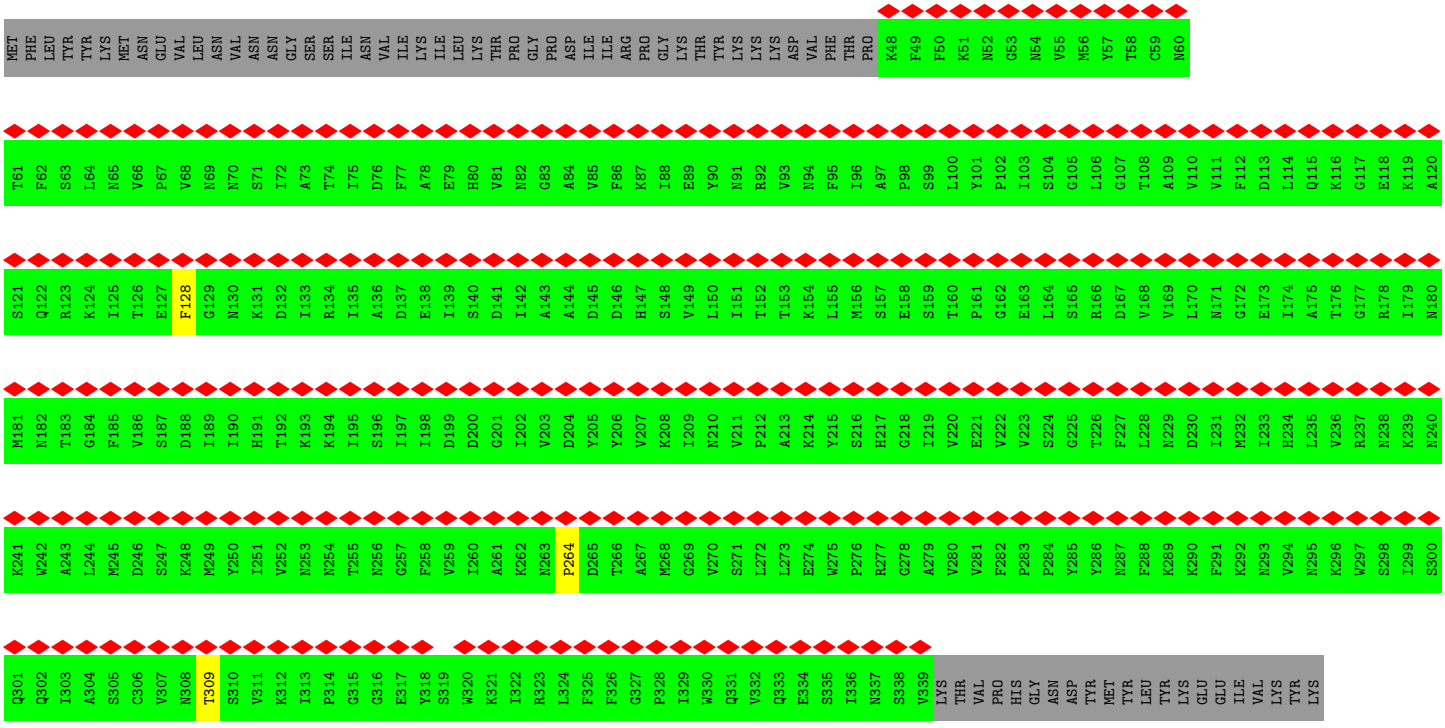
- Molecule 20: P18

Chain co:



- Molecule 21: P19

Chain cp:



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

- Molecule 21: P19

Chain cq: 75% 74% 25%

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 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 Y222 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 cr: 76% 77% 23%

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 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 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 cs: 73% 72% 27%

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

THR PHE SER LEU 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 ct: 76% 77% 23%

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 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 cu: 74% 74% 26%

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 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 cv: 72% 77% • 23%

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 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 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 cw: 71% 73% 26%

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 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 cx: 63% 77% 23%

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 M52 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 E173 I174 A175 T176 G177 R178 I179 N180 M181 N182 T183 G184

F185 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 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 cy:

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 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 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 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 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

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 cB:

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 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 cC:

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 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 cD: 77% 76% 23%

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 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 cE: 73% 73% 26%

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 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 cF: 74% 76% 23%

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 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 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 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 cG: 74% 74% 25%

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 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 cH: 63% 77% 23%

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 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 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 L170 N171 I174 A175 T176 G177 R178 I179 N180 M181 N182 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 S216 H217 V220 E221 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 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 cI: 74% 74% 26%

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 Y223 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 N338 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: 71% 76% • 23%

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

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 cK:

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 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 P285 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 cL:

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 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 cM: 73% 73% 27%

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

THR PHE 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

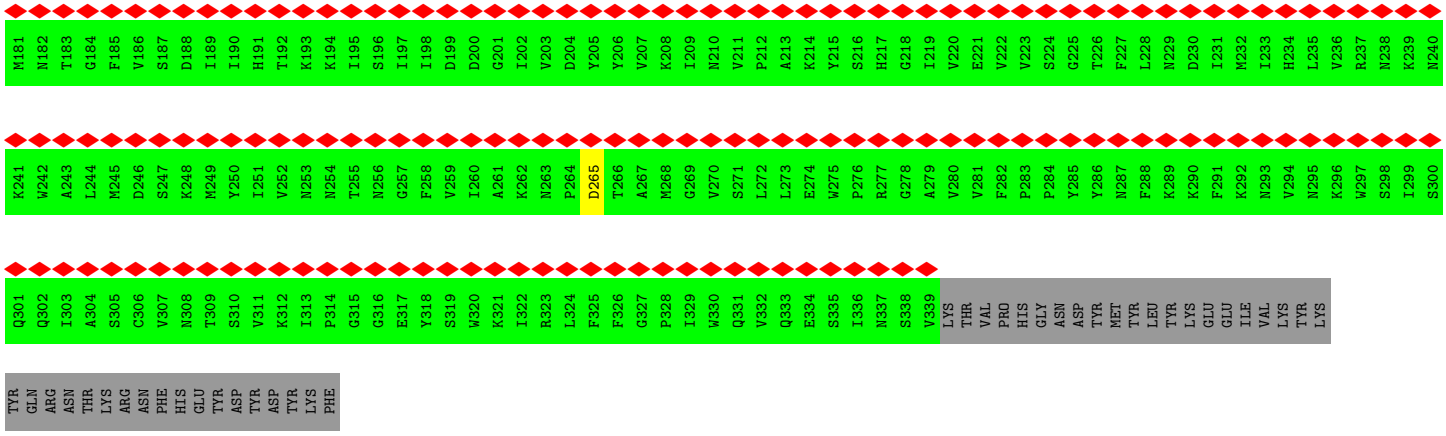
- Molecule 21: P19

Chain cN: 77% 76% 23%

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

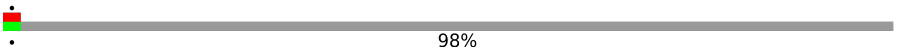
T61 F62 S63 L64 N65 V66 P67 V68 N69 N70 S71 I72 A73 T74 I75 D76 F77 A78 E79 H80 V81 N82 G83 A84 V85 F86 K87 I88 E89 Y90 N91 R92 V93 N94 F95 I96 A97 P98 S99 L100 Y101 P102 I103 S104 G105 L106 G107 T108 A109 V110 V111 F112 D113 L114 Q115 K116 G117 E118 K119 A120

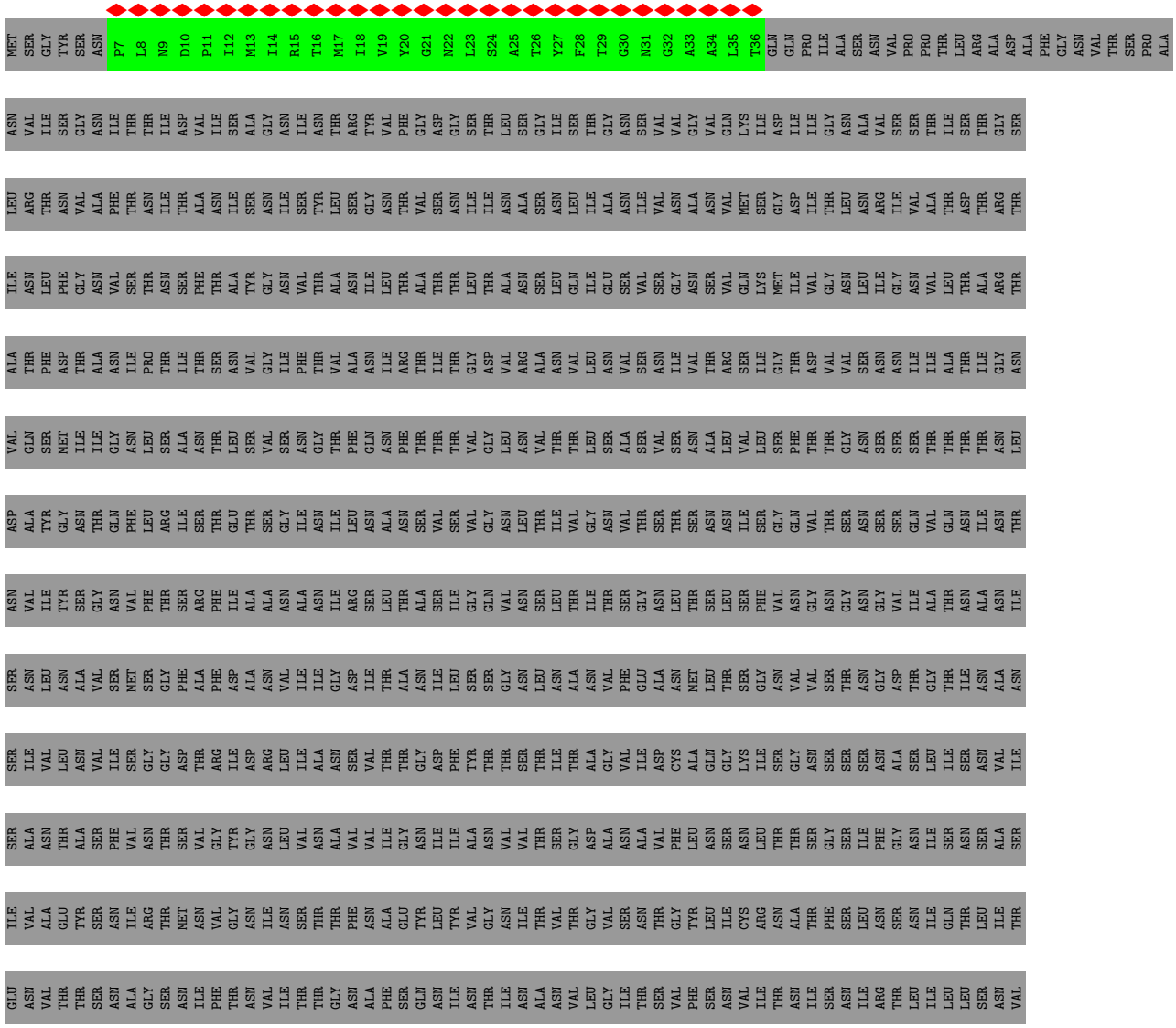
S121 Q122 R123 K124 I125 T126 E127 F128 G129 N130 K131 D132 I133 R134 I135 A136 D137 E138 I139 S140 D141 I142 A143 A144 D145 D146 H147 S148 V149 L150 I151 T152 T153 K154 L155 M156 S157 E158 S159 T160 P161 G162 E163 L164 S165 R166 D167 V168 V169 L170 N171 G172 E173 I174 A175 T176 G177 R178 I179 N180

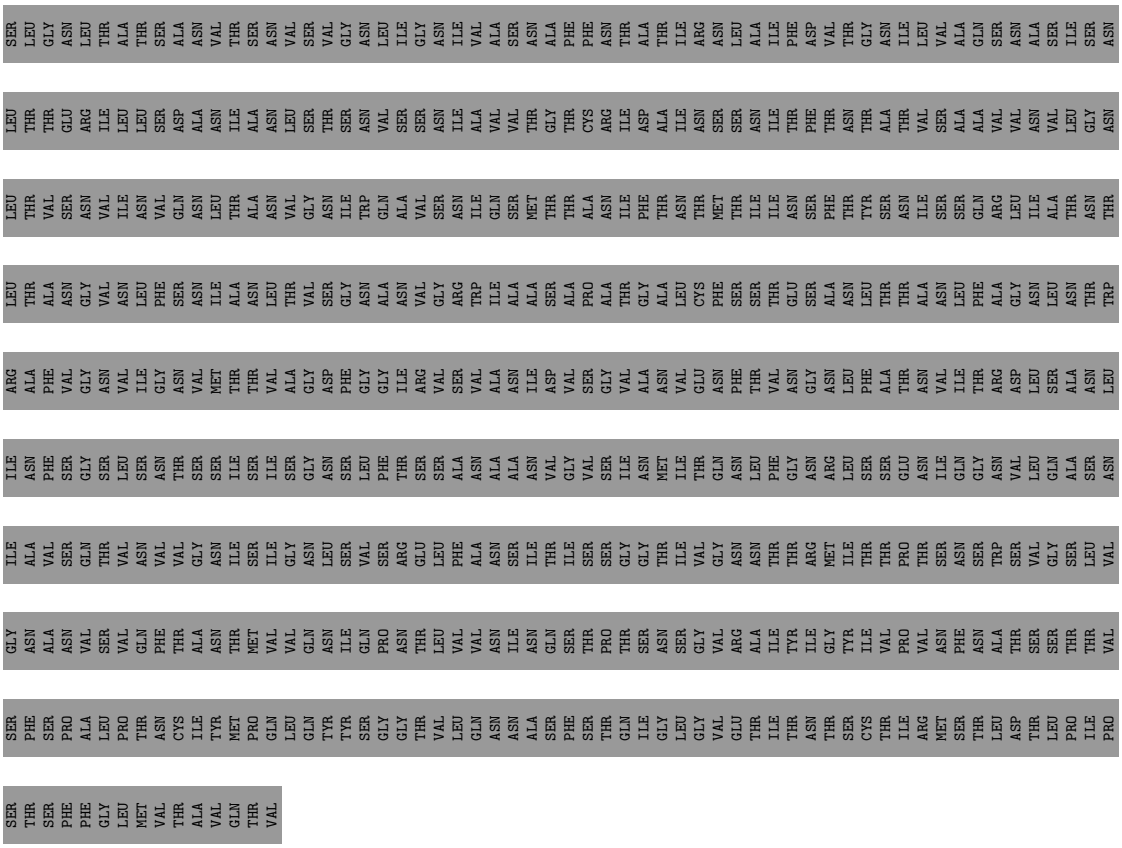


- Molecule 22: P20

Chain cO:

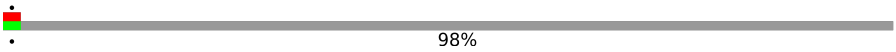


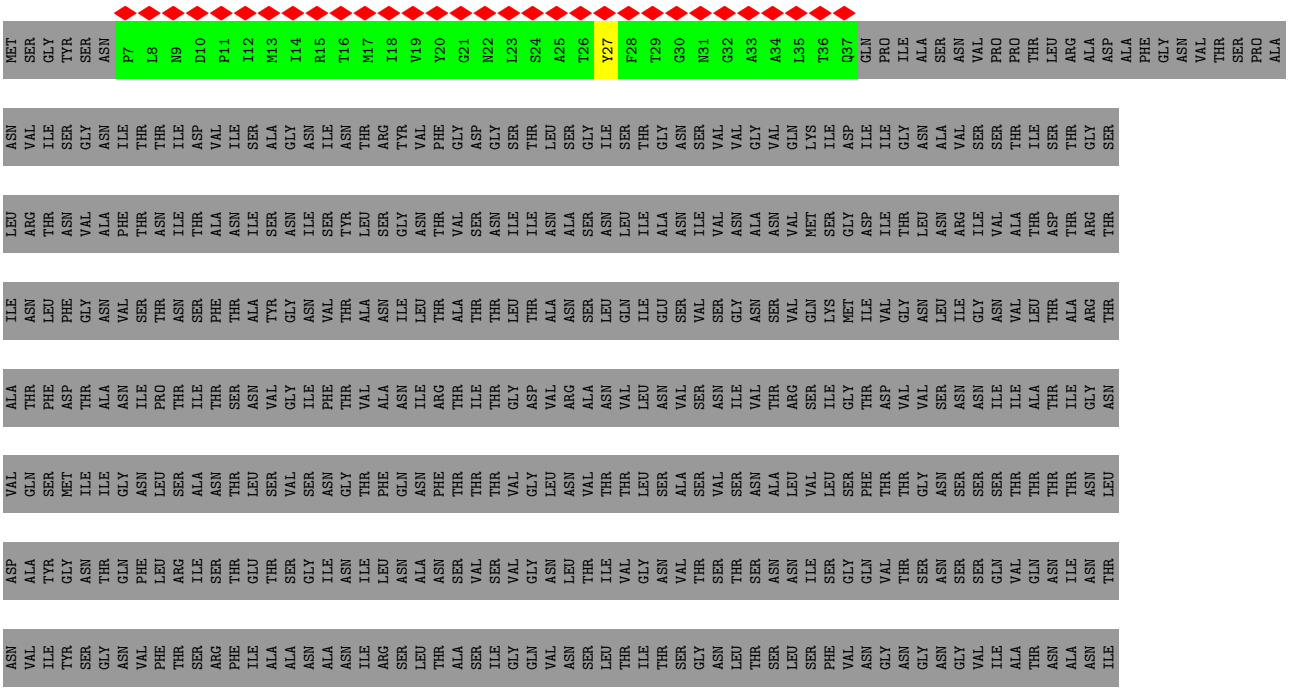




- Molecule 22: P20

Chain cQ:





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SER ILE VAL LEU ASN VAL ILE SER GLY GLY ASP THR ARG ILE ASP ARG LEU ILE ALA ASN SER VAL THR THR GLY ASP PHE TYR THR THR SER THR ILE THR ALA GLY VAL ILE ASP CYS ALA GLN GLY LYS ILE SER GLY ASN SER SER SER ASN ALA SER LEU ILE SER ASN VAL ILE

SER ALA ASN THR ALA SER PHE VAL ASN THR SER VAL GLY TYR GLY ASN LEU VAL ASN ASN VAL ILE GLY ASN ILE ILE ALA ASN VAL VAL THR SER GLY ASP ALA ASN ALA VAL PHE LEU ASN SER ASN LEU THR THR SER GLY SER ILE PHE GLY ASN ILE SER ASN SER ALA

ILE VAL ALA GLU TYR SER ASN ILE ARG THR MET ASN VAL GLY GLY ASN ILE ASN SER THR THR PHE ASN ALA GLU TYR LEU TYR VAL ALA GLY VAL SER ASN ILE THR VAL THR GLY VAL SER ASN THR GLY TYR LEU ILE CYS ARG ASN ALA THR PHE SER LEU ASN SER ILE ARG THR ASN SER ILE GLN THR ILE

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- Molecule 22: P20

Chain da: 98%

MET SER GLY TYR SER N6 P7 L8 N9 D10 P11 I12 M13 I14 R15 T16 M17 I18 V19 Y20 G21 N22 L23 S24 A25 T26 Y27 F28 T29 G30 N31 G32 A33 A34 L35 T36 Q37 GLN PRO ILE ALA SER ASN VAL PRO PRO THR LEU ARG ALA ASP ALA PHE GLY ASN VAL THR SER PRO ALA

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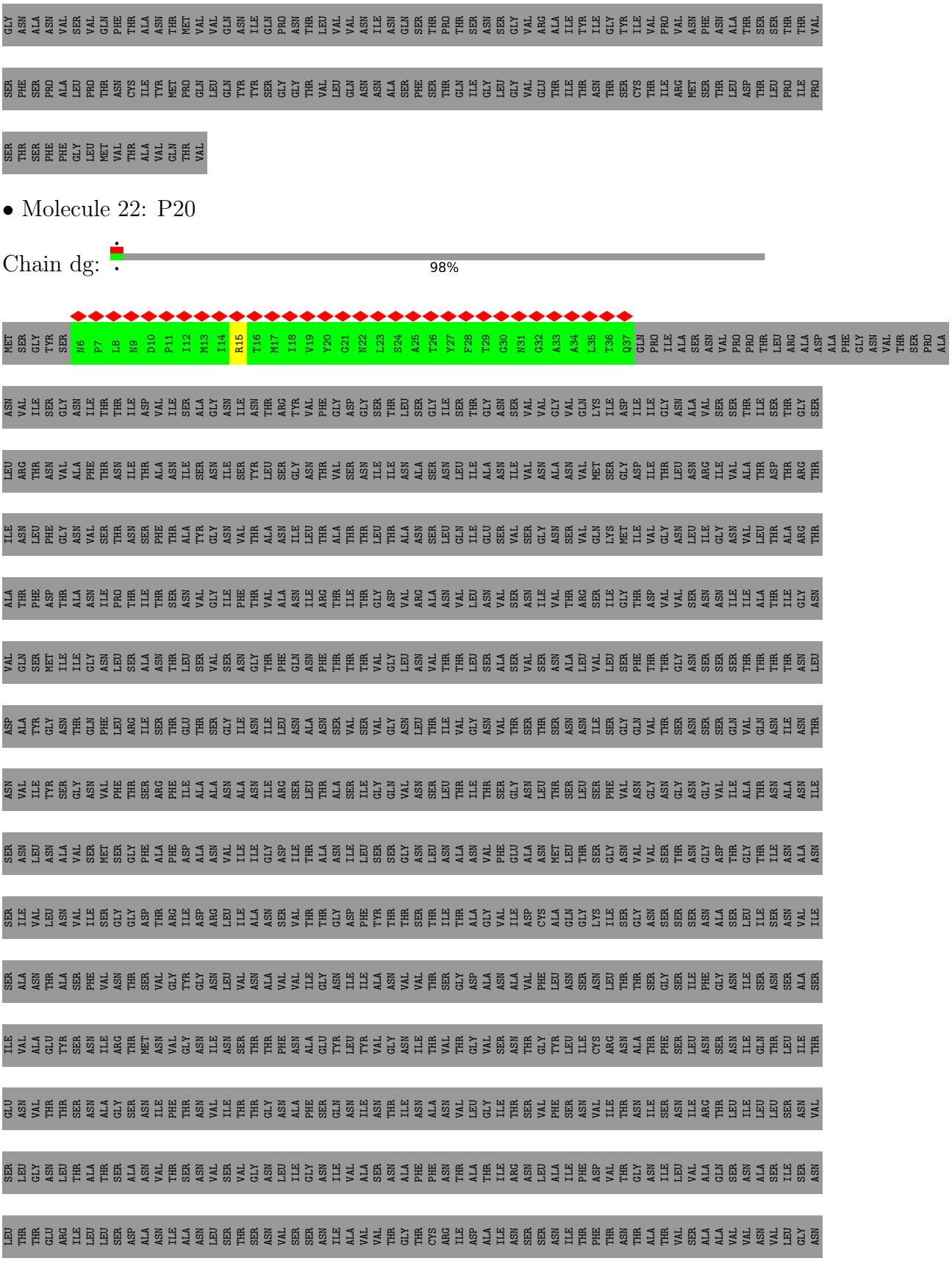
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• Molecule 22: P20
Chain dg:
98%
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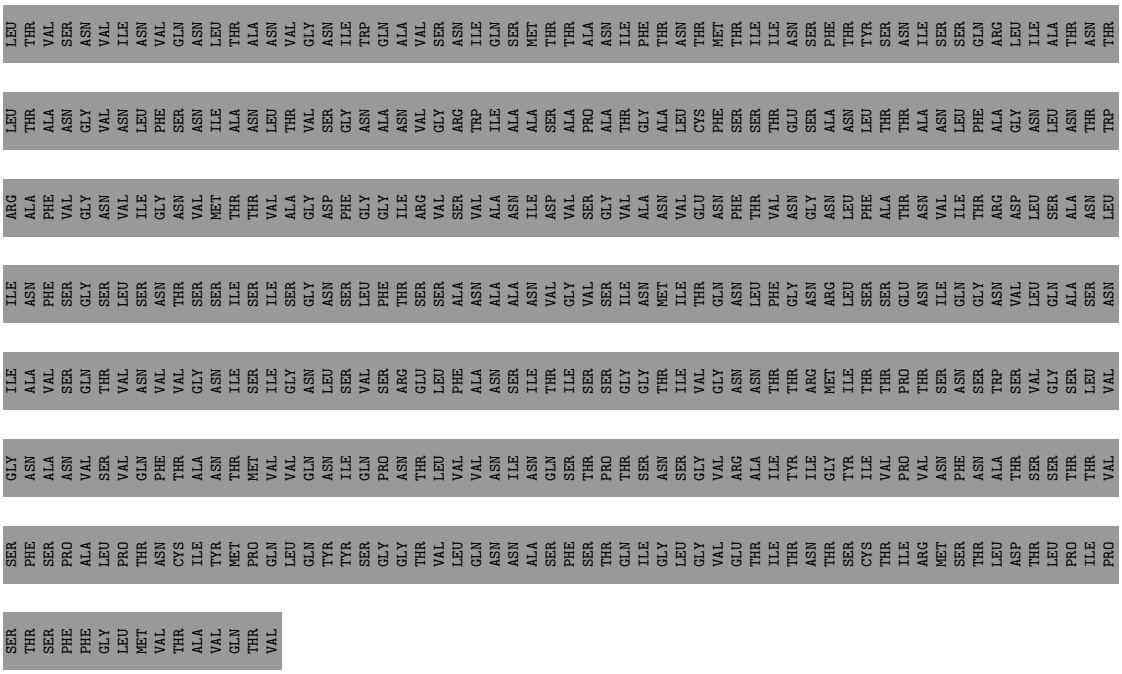
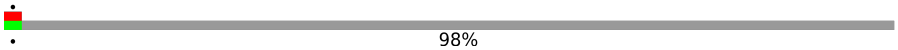
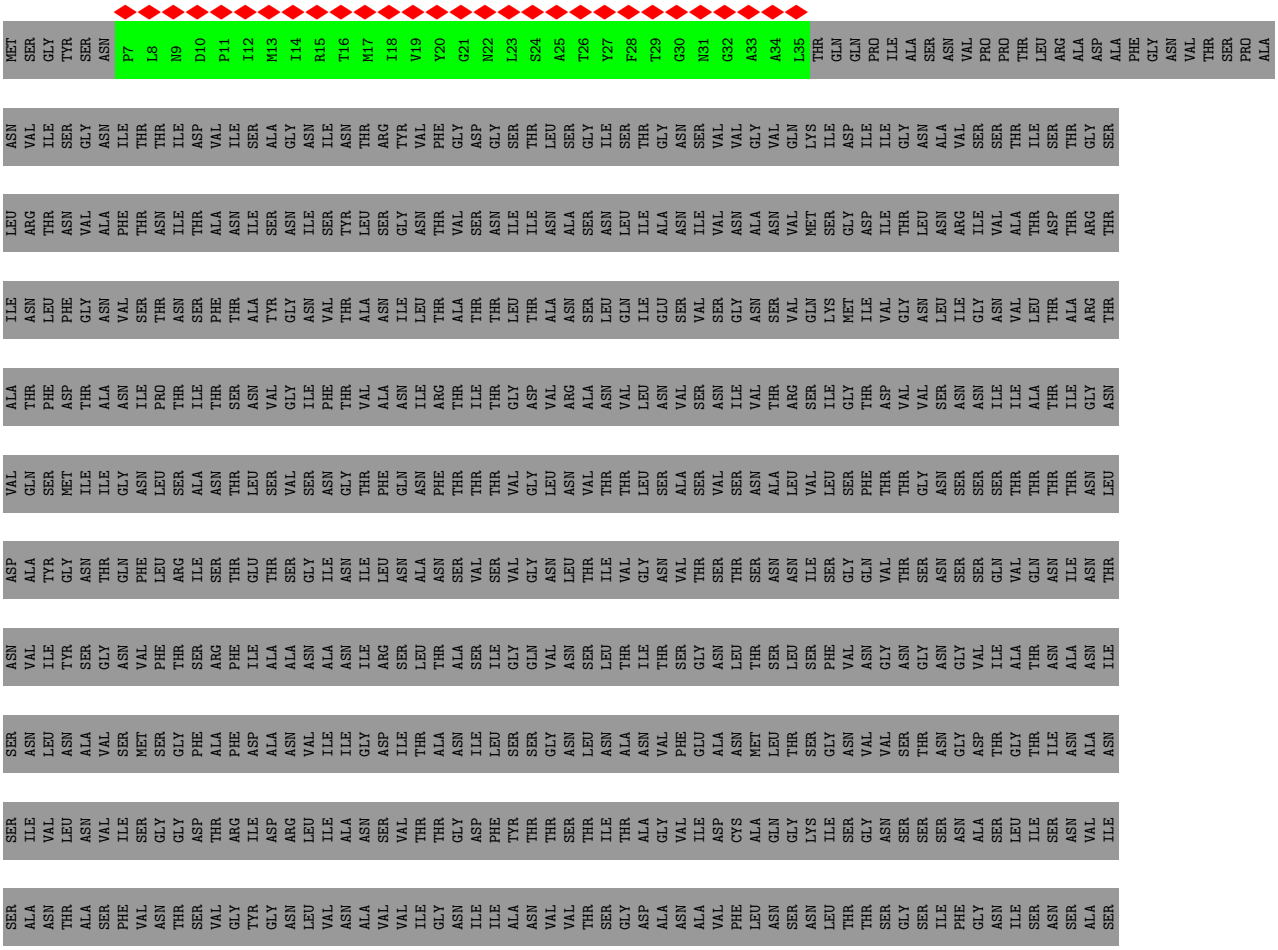


- Molecule 22: P20

Chain di:





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GLU ASN VAL THR THR SER ASN ALA GLY SER ASN ILE PHE THR ASN VAL ILE THR ILE ASN THR ILE ASN ALA ASN VAL LEU GLY ILE THR SER VAL PHE SER ASN VAL ILE THR ASN ILE SER ASN ILE ARG THR LEU ILE LEU LEU SER ASN VAL

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LEU THR THR GLU ARG ILE LEU LEU SER ASP ALA ASN ILE ALA ASN LEU SER THR SER ASN VAL SER SER ASN ILE ILE ALA VAL VAL THR GLY THR CYS ARG ILE ASP ALA ILE ASN SER SER ILE THR PHE THR ASN THR ALA THR VAL SER ALA ALA VAL VAL ASN VAL LEU GLY

LEU THR VAL SER ASN VAL ILE ASN VAL GLN ASN LEU THR ALA ASN VAL GLY ASN ILE TRP GLN ALA VAL SER ASN ILE GLN SER MET THR ASN ILE ILE ASN SER PHE THR TYR SER ASN ILE SER SER ALA ALA GLN ARG LEU ILE ALA THR ASN THR

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- Molecule 22: P20

Chain ds: 98%

MET SER GLY TYR SER N6 P7 L8 N9 D10 P11 I12 M13 I14 R15 T16 M17 I18 V19 Y20 G21 N22 L23 S24 A25 T26 Y27 F28 T29 G30 N31 G32 A33 A34 L35 T36 Q37 GLN PRO ILE ALA SER ASN VAL PRO PRO THR LEU ARG ALA ASP ALA PHE GLY ASN VAL THR SER PRO ALA

ASN VAL ILE SER GLY ASN ILE THR THR ILE 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 SER THR ILE SER THR GLY SER

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

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 VAL SER ASN ILE VAL THR ARG SER ILE GLY THR ASP VAL VAL SER ASN ASN ILE ILE ALA THR ILE GLY ASN

VAL GLN SER MET ILE ILE GLY ASN LEU SER ALA ASN THR THR LEU SER VAL GLY LEU ASN VAL THR THR LEU SER ALA SER VAL SER ASN ALA LEU VAL LEU SER PHE THR THR GLY ASN SER SER SER THR THR THR ASN LEU

ASP ALA TYR GLY ASN THR GLN PHE LEU ARG ILE SER THR GLU THR SER GLY ILE ASN ILE LEU ASN ALA ASN SER VAL SER VAL 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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- Molecule 22: P20

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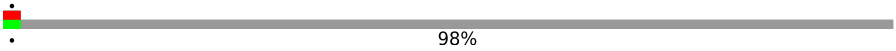

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ASN VAL ILE SER GLY ASN ILE THR THR ILE ASP VAL ILE SER ALA GLY ASN ILE ASN THR ARG TYR VAL PHE GLY ASP GLY SER THR LEU SER GLY ILE SER THR GLY ILE ASN SER VAL VAL GLY VAL GLN LYS ILE ASP ILE ILE GLY ASN ALA VAL SER SER THR ILE SER THR GLY SER

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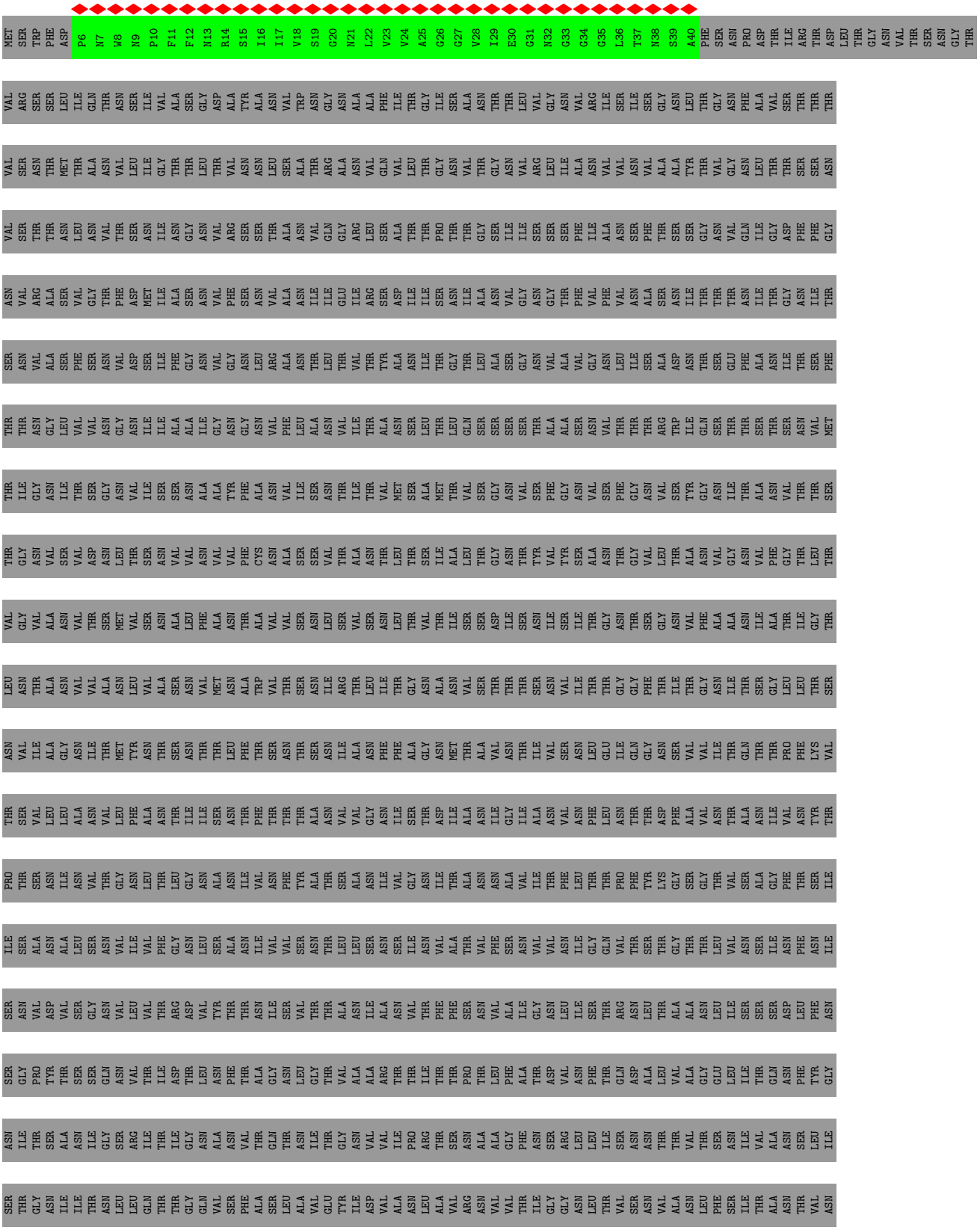
Chain cP: 97%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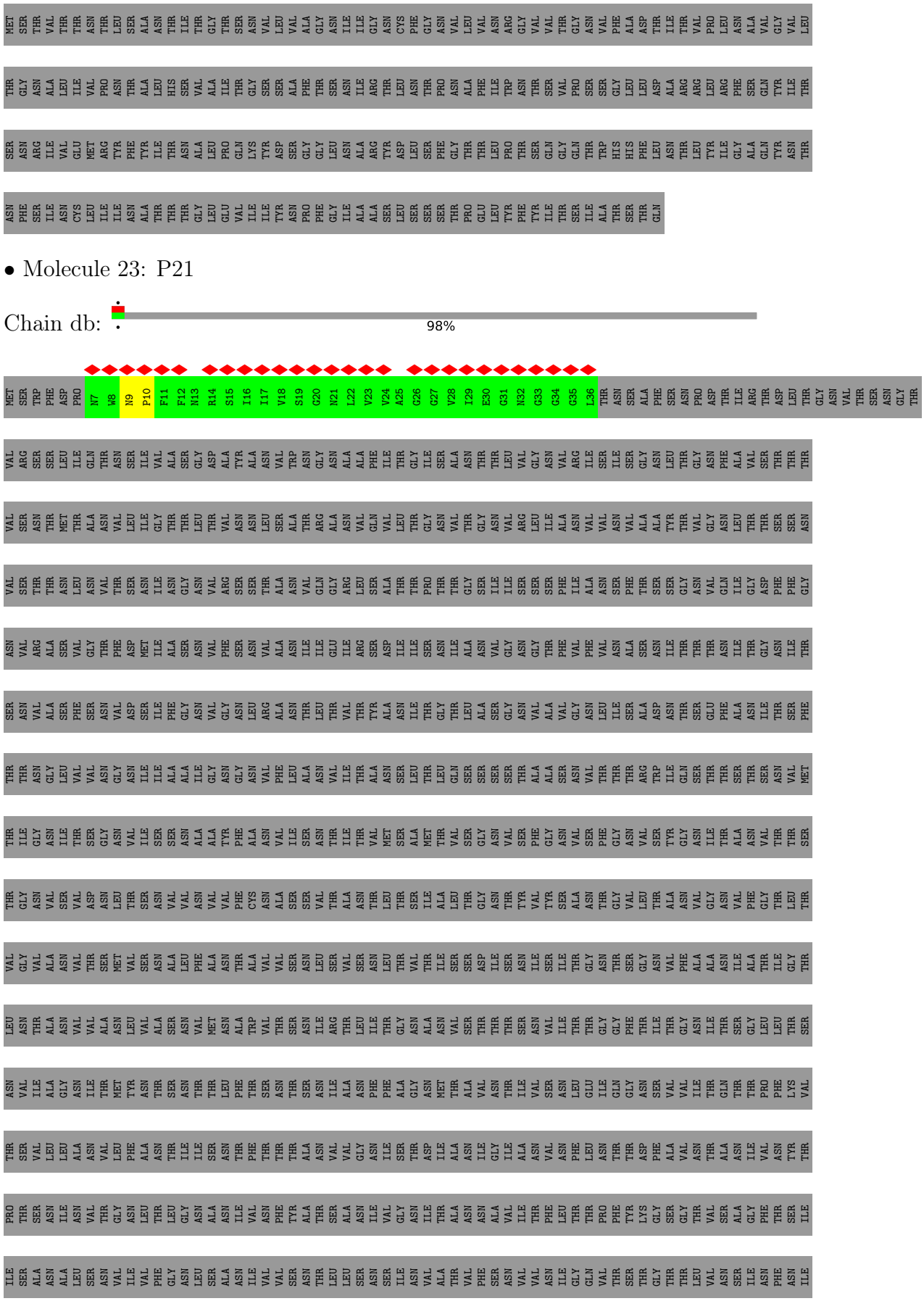
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SER ASN ARG ILE VAL GLU MET ARG TYR PHE ILE THR ASN ALA LEU PRO GLN LYS TYR ASP SER GLY GLY LEU ASN ALA ARG TYR ASP LEU SER PHE GLY THR THR LEU PRO THR SER GLN GLY GLN THR TRP HIS HIS PHE LEU ASN THR LEU TYR ILE GLY ALA GLN TYR ASN THR
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• Molecule 23: P21
Chain db:
98%
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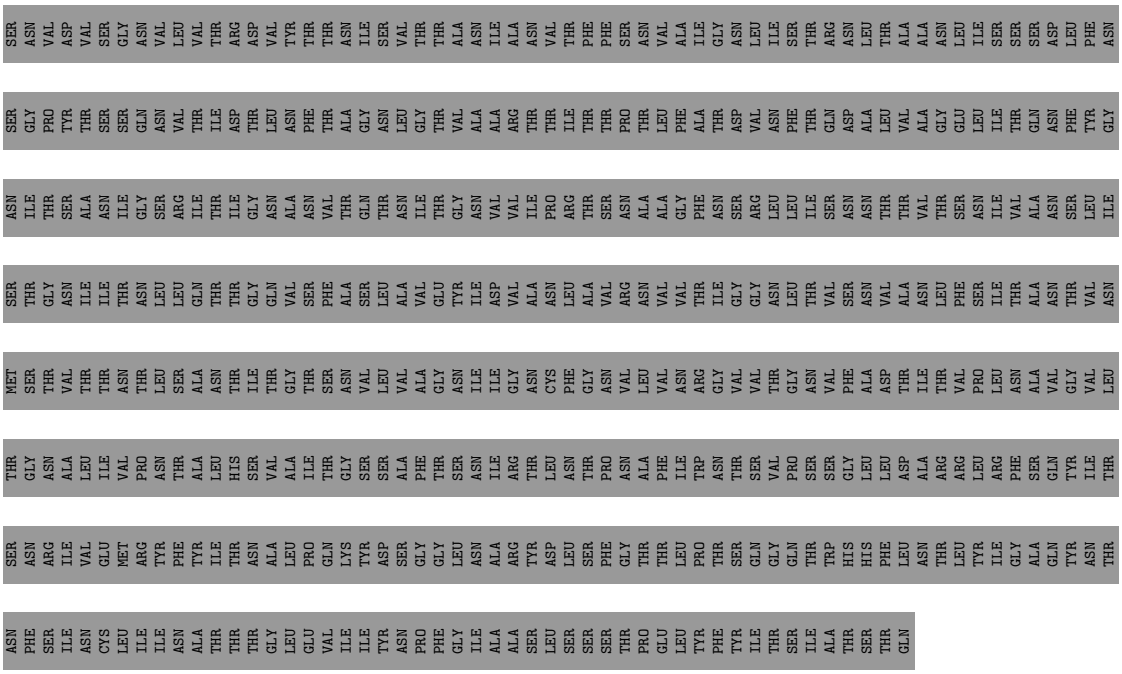

- Molecule 23: P21

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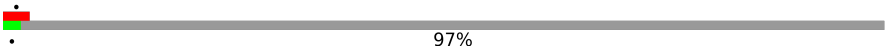

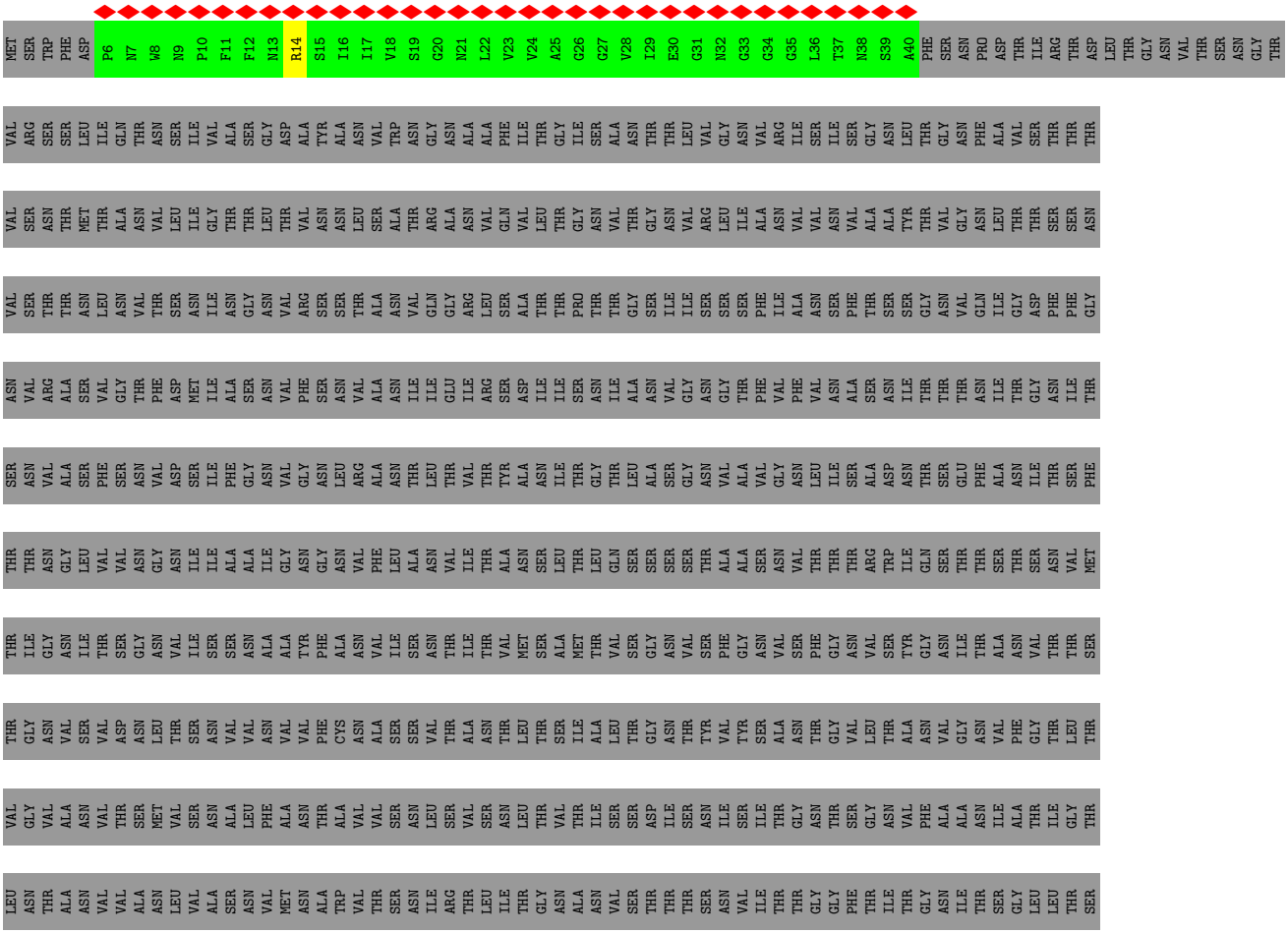

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PRO THR SER ASN ILE ASN VAL THR GLY ASN LEU THR LEU GLY ASN ALA ASN ILE VAL ASN PHE TYR ALA THR SER ALA ASN ILE ILE VAL GLY ASN ILE THR ALA ASN ASN ALA VAL ILE THR PHE LEU THR THR PRO PHE TYR LYS GLY SER GLY THR VAL SER ALA GLY PHE THR SER ILE

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

MET SER THR VAL THR THR ASN THR LEU SER ALA ASN THR ILE THR GLY THR SER ASN VAL LEU VAL ALA ALA GLY ASN ILE ILE GLY ASN CYS PHE GLY ASN VAL LEU VAL ASN ARG GLY VAL VAL THR GLY ASN VAL PHE ALA ASP THR ILE THR VAL PRO LEU ASN ALA VAL GLY VAL LEU

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

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

ASN PHE SER ILE ASN CYS LEU ILE ILE ASN ALA THR THR THR GLY LEU GLU VAL ILE ILE TYR ASN PRO PHE GLY ILE ALA ALA SER LEU SER SER SER THR PRO GLU LEU TYR PHE TYR ILE THR SER ILE ALA THR SER THR GLN

- Molecule 23: P21

Chain dt: 97%

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 GLY ASN VAL ARG ILE SER ILE SER GLY ASN LEU THR GLY ASN PHE ALA VAL SER THR THR THR

VAL SER ASN THR MET THR ALA ASN VAL LEU ILE GLY THR THR LEU THR VAL ASN ASN LEU SER ALA ALA THR ARG ALA ASN VAL GLN VAL LEU THR GLY ASN VAL THR GLY VAL LEU ILE ALA ASN VAL VAL ASN VAL ALA ALA TYR THR VAL GLY ASN LEU THR THR SER SER ASN

VAL SER THR THR ASN LEU ASN VAL THR SER SER ASN ILE ASN GLY ASN VAL THR SER ASN SER ALA ASN VAL ARG SER SER THR ASN ILE ILE ASN GLY ASN VAL ALA ASN SER PHE ILE ALA ASN SER PHE THR SER SER GLY ASN VAL 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 ARG SER ASP ILE ILE SER ASN ILE ALA ASN VAL GLY ASN GLY THR PHE VAL PHE VAL ASN ALA SER ASN ILE THR THR THR ASN ILE THR GLY ASN ILE THR

SER ASN VAL ALA SER PHE SER ASN VAL ASP SER ILE ILE PHE GLY ASN VAL GLY ASN LEU ARG ALA ASN THR LEU THR VAL THR TYR ALA ASN ILE THR GLY THR LEU ALA SER GLY ASN VAL ALA VAL GLY ASN VAL ILE ILE SER ALA ASP ASN 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 PHE LEU ALA ALA ASN VAL ILE THR ALA ASN SER LEU THR LEU GLN SER SER SER SER THR ALA ALA ALA SER ASN VAL THR THR THR ARG TRP ILE GLN SER THR THR THR SER ASN VAL MET

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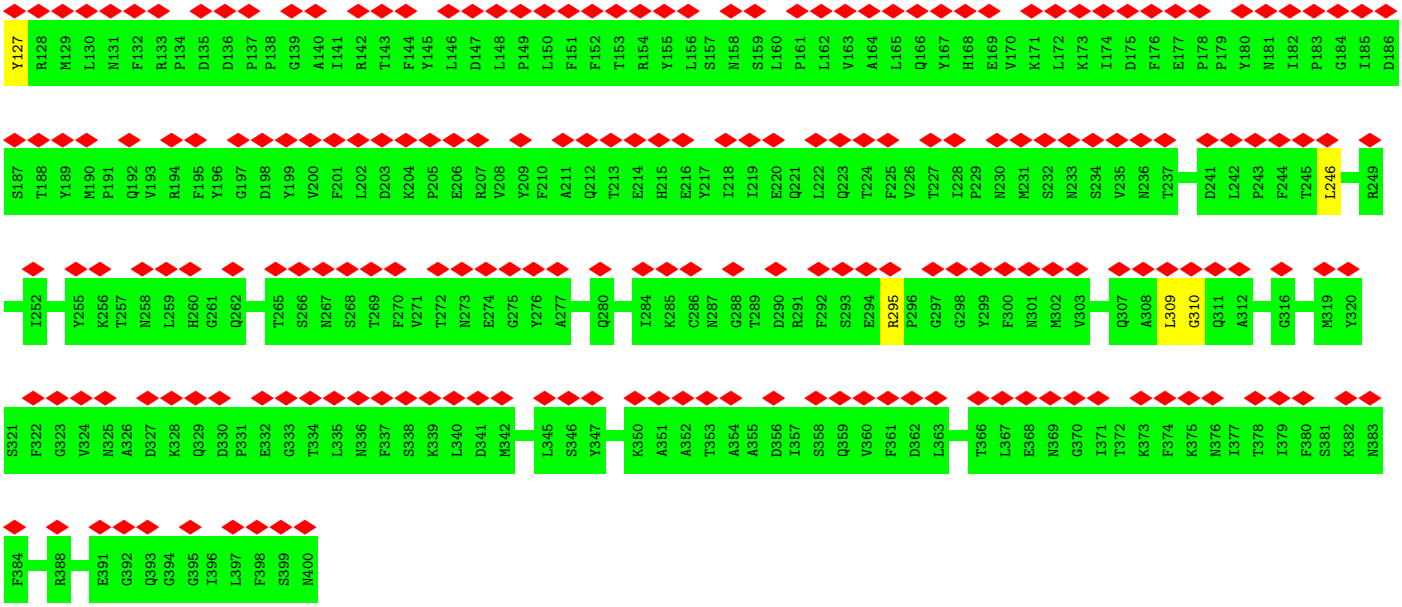
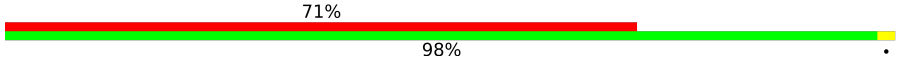
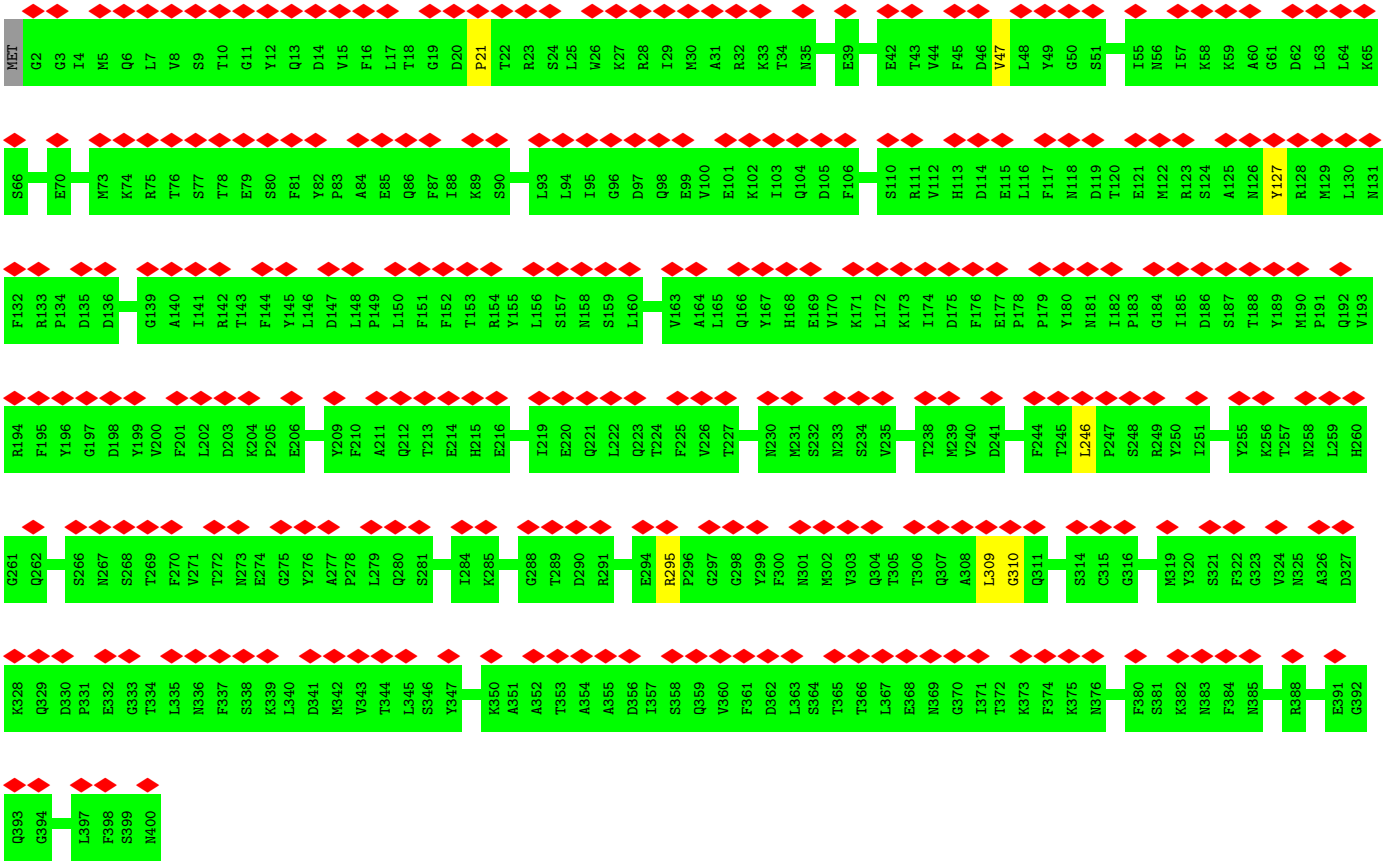


- Molecule 24: MCPv5

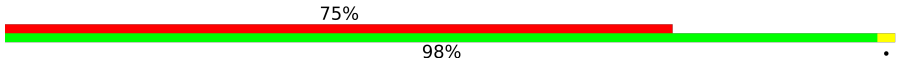
Chain cS:





- Molecule 24: MCPv5

Chain cT:



MET G2 G3 I4 M5 Q6 L7 V8 S9 T10 G11 Y12 Q13 D14 V15 F16 L17 T18 G19 D20 P21 T22 R23 S24 L25 W26 K27 R28 I29 M30 A31 R32 K33 T34 N35 F36 A37 I38 E39 S40 I41 E42 F45 D46 V47 L48 Y49 G50 S51 T52 S53 F54 I55 N56 I57 K58 K59 A60 G61

D62 L63 L64 K65 S66 L69 E70 M73 K74 R75 T76 S77 T78 E79 S80 F81 Y82 E85 Q86 F87 I88 K89 S90 L91 T92 L93 L94 I95 G96 D97 Q98 E99 V100 E101 K102 I103 Q104 D105 F106 P107 S110 R111 V112 H113 D114 E115 L116 F117 N118 D119 T120 E121 M122 R123 S124 A125

N126 Y127 R128 M129 L130 N131 F132 R133 P134 D135 D136 G139 A140 I141 R142 T143 F144 Y145 L146 D147 L148 P149 L150 F151 F152 T153 R154 Y155 L156 S157 N158 S159 L160 P161 L162 V163 A164 L165 Q166 Y167 H168 E169 V170 K171 L172 K173 I174 D175 F176 E177 P178 P179 Y180 N181 I182 P183 G184 I185 D186

S187 T188 Y189 M190 R194 F195 Y196 G197 D198 Y199 V200 F201 L202 D203 K204 Y209 F210 A211 Q212 T213 E214 H215 E216 I219 E220 Q223 T224 F225 V226 T227 I228 P229 N230 M231 S232 N233 S234 V235 N236 T237 T238 M239 V240 D241 L242 P243 F244 T245 L246 R249 Y255 K256 T257 N258

L259 H260 G261 Q262 Y263 S266 N267 S268 T269 F270 V271 T272 N273 E274 G275 Y276 A277 P278 L279 Q280 S281 A282 K285 C286 N287 G288 T289 D290 R291 E294 R295 P296 G297 G298 Y299 F300 N301 M302 V303 Q304 T305 T306 Q307 A308 L309 G310 Q311 A312 P313 S314 C315 G316 I317 Y318 M319 Y320 S321

F322 G323 V324 N325 A326 D327 K328 Q329 D330 P331 E332 G333 T334 L335 N336 F337 S338 K339 L340 D341 M342 L345 T348 N349 K350 A351 A352 T353 A354 A355 D356 I357 S358 Q359 V360 F361 D362 L363 T366 L367 E368 N369 G370 I371 T372 K373 F374 K375 N376 I377 F380 S381 K382 N383 F384

R388 I389 V390 E391 G392 Q393 G394 G395 I396 L397 F398 S399 N400

- Molecule 25: P22

Chain cU: 97%

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

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

ILE PRO SER ILE VAL THR ALA ASP ILE ARG GLY ASN ILE 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 ASN GLY PHE PHE ILE GLY ASN GLY SER 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 TYR PHE PHE GLY ASN GLY 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 ILE 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

GLY ALA LEU LEU THR GLY ILE THR ALA THR ALA ASN ILE PRO SER ILE VAL THR ALA ASN ILE 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

PHE ILE GLY ASN GLY SER LEU LEU SER GLY ILE 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 THR ALA THR PHE GLY ASN ILE ALA ASN VAL LEU PHE ASN ASN GLY ASN VAL THR ALA ALA GLY GLY ASN GLY PHE

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 VAL THR ALA

ALA ASP 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

THR ALA ALA GLY GLY ASN GLY TYR PHE PHE GLY ASN GLY GLU 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 ILE ALA THR PHE GLY ASN ILE ALA ASN VAL LEU PHE ASN

ASN GLY ASN VAL THR ALA ALA ASP GLY ASN GLY TYR PHE PHE GLY ASN GLY GLY SER GLN LEU THR GLY VAL ALA 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 TYR PHE PHE GLY ASN GLY GLY SER GLN LEU 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 ILE ALA THR PHE GLY ASN ILE ALA ASN ILE

ALA ASN VAL LEU PHE ASN ASN GLY ASN VAL THR ALA ALA GLY GLY ASN GLY 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 THR 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 GLY GLU 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 THR

ALA 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 THR PHE LEU ASN PHE SER THR ILE THR ALA ASP ILE ARG GLY ASN ILE ILE GLY ASN TYR ALA ASN VAL GLY ASN VAL ALA GLY GLY

SER 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 THR SER LEU THR PHE SER THR ILE ARG ALA ASP ILE ARG GLY ASN ILE ILE GLY ASN TYR ALA ASN VAL ALA ASN VAL ILE ALA GLY ASN

VAL 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 SER ASP GLY LEU PHE ARG GLY GLY PRO THR ASN GLN SER ASN ASN ALA LEU ILE LEU ARG GLY ILE GLY GLY THR ASN VAL

ASN 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 GLY PHE TYR SER LEU SER TYR ASP SER SER VAL VAL VAL GLY GLN VAL VAL SER ASN SER THR

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

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

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

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

VAL GLU ASP LEU GLU GLN THR ILE ASN VAL LEU LYS THR GLN VAL GLN MET LEU LEU LEU GLY ASN ILE

- Molecule 25: P22

Chain cV: 97%

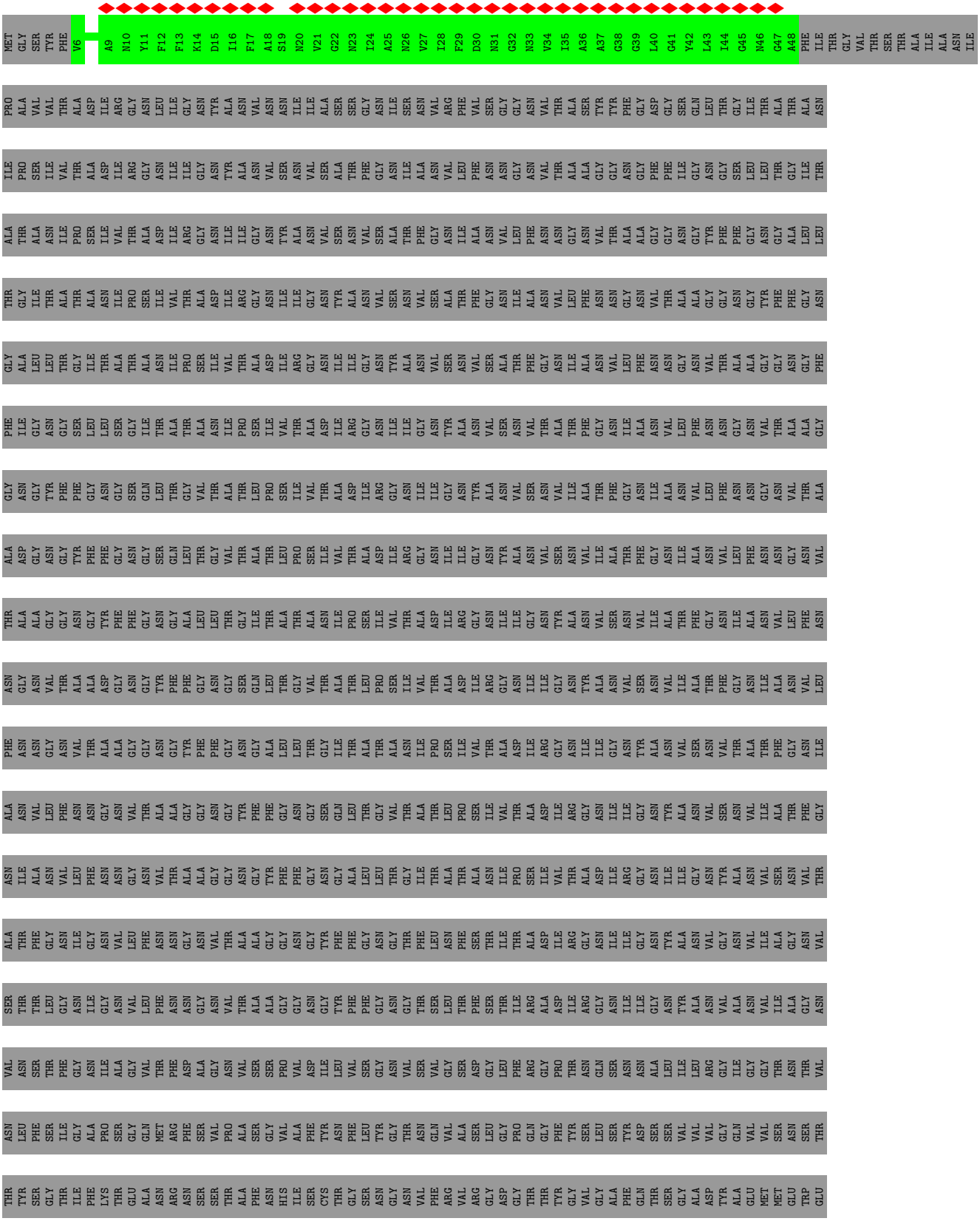
MET GLY SER TYR PHE V6 N10 Y11 F12 F13 K14 D15 I16 F17 A18 S19 N20 V21 G22 N23 I24 A25 N26 V27 I28 F29 D30 N31 G32 N33 V34 I35 A36 A37 G38 G39 L40 G41 Y42 L43 I44 G45 N46 G47 A48 PHE ILE THR GLY VAL THR SER THR ALA ILE ALA ASN ILE PRO

ALA VAL VAL THR ALA ASP ILE ARG GLY ASN LEU ILE GLY ASN TYR ALA ASN VAL ASN ASN ILE ILE ALA SER SER GLY ASN ILE SER ASN VAL ARG PHE VAL SER GLY GLY ASN VAL THR ALA SER TYR TYR PHE GLY ASP GLY SER GLN 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 GLY ASN VAL THR ALA ALA GLY GLY GLY ASN GLY PHE PHE ILE GLY ASN GLY SER LEU LEU THR GLY ILE THR ALA THR ALA

| | | |

Chain cW: 97%


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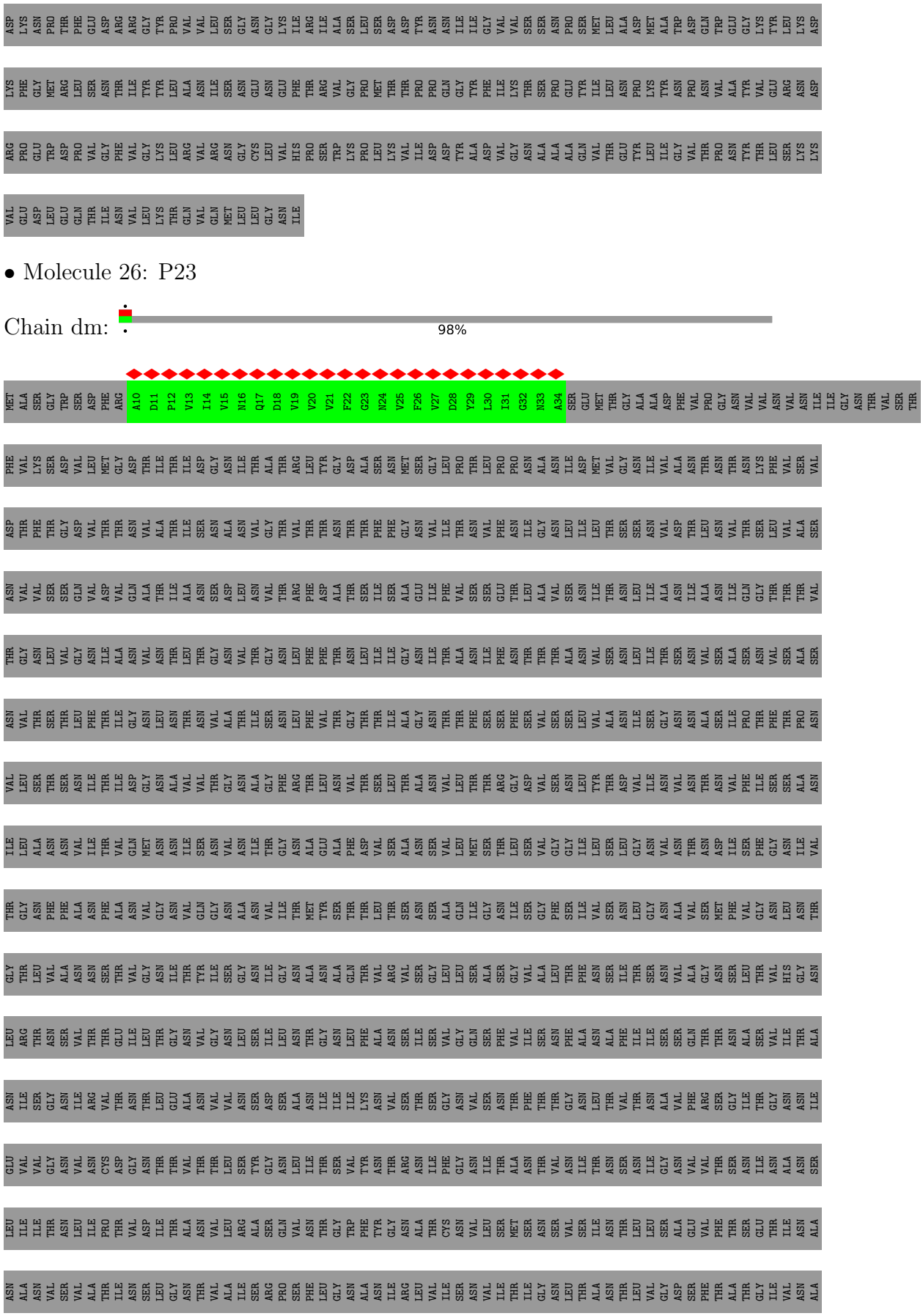
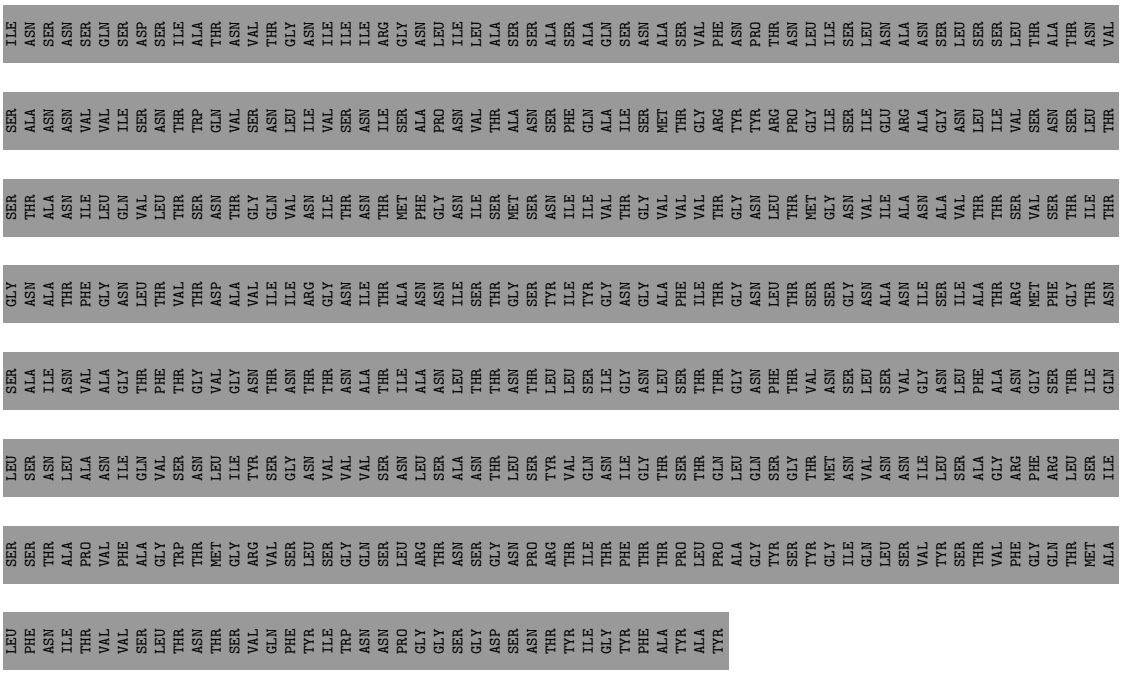
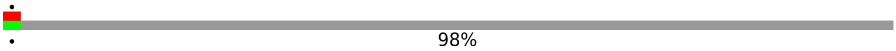
ALA ASP GLY ASN GLY TYR PHE PHE GLY ASN GLY SER GLN LEU THR GLY VAL THR ALA THR LEU PRO SER ILE VAL THR ALA ASP ILE ARG GLY ASN ILE ILE GLY ASN TYR ALA ASN VAL SER ASN VAL ILE ALA THR PHE GLY ASN ILE ALA ASN VAL LEU PHE ASN ASN GLY ASN VAL
THR ALA ALA GLY GLY ASN GLY TYR PHE PHE GLY ASN GLY ALA LEU LEU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

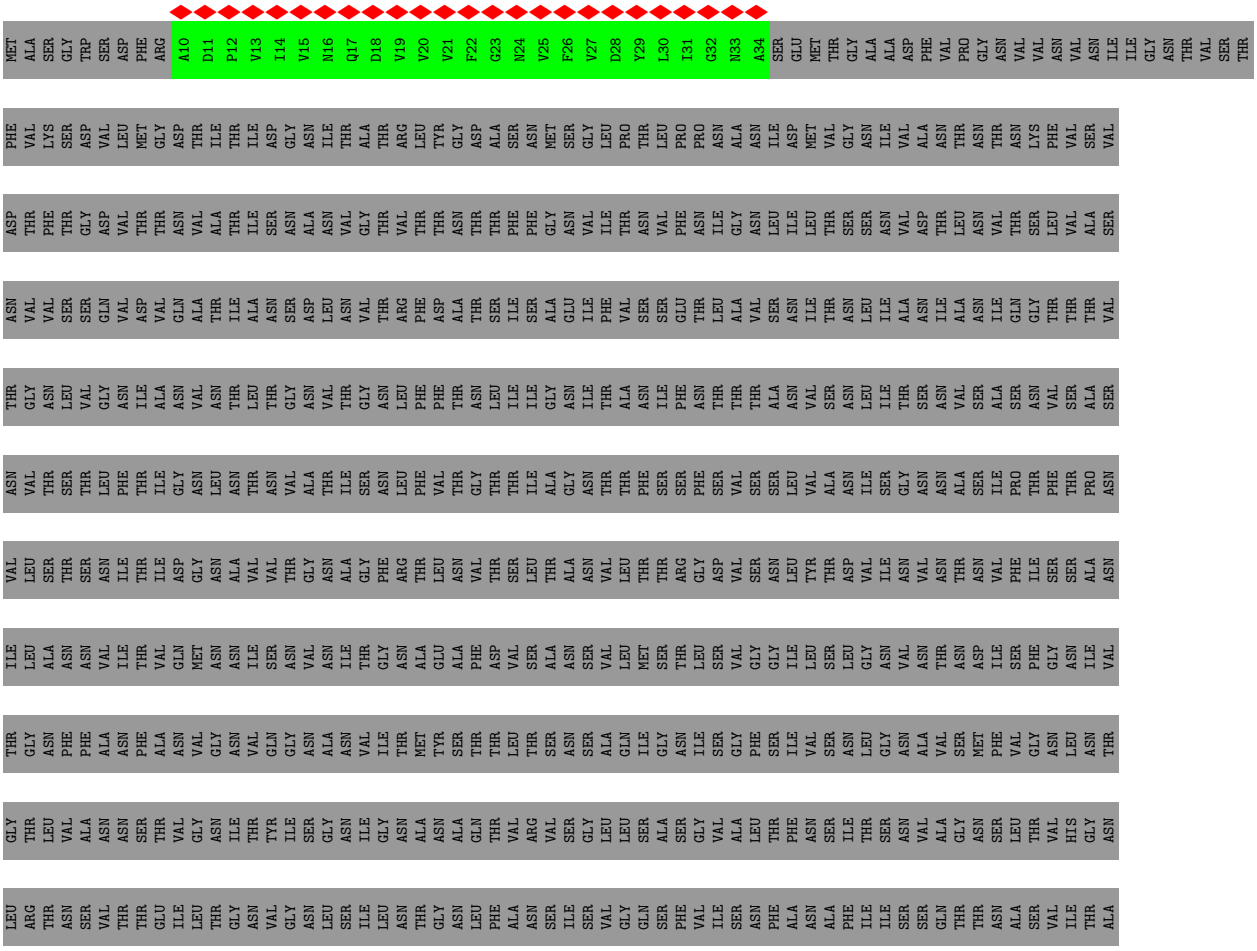

ASP LYS ASN PRO THR PHE GLU ASP ARG ARG GLY TYR PRO VAL VAL LEU SER GLY ASN GLY LYS ILE ARG ILE ALA SER LEU SER ASP ASP TYR ASN ASN ILE ILE GLY VAL VAL SER SER ASN PRO SER MET LEU ALA ASP MET ALA TRP ASP GLN TRP GLU GLY LYS TYR LEU LYS ASP
LYS PHE GLY MET ARG LEU SER ASN THR ILE TYR TYR LEU ALA ASN ILE SER ASN GLU ASN GLU PHE THR ARG VAL GLY PRO MET THR THR PRO PRO GLN GLY TYR PHE ILE LYS THR SER PRO GLU TYR ILE LEU ASN PRO LYS TYR ASN PRO ASN VAL ALA TYR VAL GLU ARG ASN ASP
ARG PRO GLU TRP ASP PRO VAL GLY PHE VAL GLY LYS LEU ARG VAL ARG ASN GLY CYS LEU VAL HIS PRO SER TRP LYS PRO LEU LYS VAL ILE ASP ASP TYR ALA ASP VAL GLY ASN ALA ALA ALA GLN VAL THR GLU TYR LEU ILE GLY VAL THR PRO ASN TYR THR LEU SER LYS LYS
VAL GLU ASP LEU GLU GLN THR ILE ASN VAL LEU LYS THR GLN VAL GLN MET LEU LEU GLY ASN ILE
• Molecule 26: P23
Chain dm:
98%
MET ALA SER GLY TRP SER ASP PHE ARG A10 D11 P12 V13 I14 V15 N16 Q17 D18 V19 V20 V21 P22 G23 N24 V25 F26 V27 D28 Y29 L30 I31 G32 N33 A34 SER GLU MET THR GLY ALA ALA ASP PHE VAL PRO GLY ASN VAL VAL ASN VAL ASN ILE ILE GLY ASN THR VAL SER THR
PHE VAL LYS SER ASP VAL LEU MET GLY ASP THR ILE THR ILE ASP GLY ASN ILE THR ALA THR ARG LEU TYR GLY ASP ALA SER ASN MET SER GLY LEU PRO THR LEU PRO PRO ASN ALA ASN ILE ASP MET VAL GLY ASN ILE VAL ALA ASN THR ASN THR ASN LYS PHE VAL SER VAL
ASP THR PHE THR GLY ASP VAL THR THR ASN VAL ALA THR ILE SER ASN ALA ASN VAL GLY THR VAL THR THR ASN THR THR PHE PHE GLY ASN VAL ILE THR ASN VAL PHE ASN ILE GLY ASN LEU ILE LEU THR SER SER ASN VAL ASP THR LEU ASN VAL THR SER LEU VAL ALA SER
ASN VAL VAL SER SER GLN VAL ASP VAL GLN ALA THR ILE ALA ASN SER ASP LEU ASN VAL THR ARG PHE ASP ALA THR SER ILE SER ALA GLU ILE PHE VAL SER SER GLU THR LEU ALA VAL SER ASN ILE THR ASN LEU ILE ALA ASN ILE ALA ASN ILE GLN GLY THR THR VAL
THR GLY ASN LEU VAL GLY ASN ILE ALA ASN VAL THR ASN THR LEU THR GLY ASN VAL THR GLY ASN LEU PHE PHE THR ASN LEU ILE ILE GLY ASN ILE THR ALA ASN ILE PHE ASN THR THR THR ASN VAL SER ASN LEU ILE THR SER ASN VAL SER ALA SER ASN VAL SER ALA SER
ASN VAL THR SER THR LEU PHE THR ILE GLY ASN LEU ASN THR ASN VAL ALA THR ILE SER ASN LEU PHE VAL THR GLY THR THR ILE ALA GLY ASN THR THR PHE SER SER PHE SER VAL SER SER LEU VAL ALA ASN ILE SER GLY ASN ASN ALA SER ILE PRO THR PHE THR PRO ASN
VAL LEU SER THR SER ASN ILE THR ILE ASP GLY ASN ALA VAL VAL THR GLY ASN ALA GLY PHE ARG THR LEU ASN VAL THR SER LEU THR ALA ASN VAL LEU THR THR ARG GLY ASP VAL SER ASN LEU TYR THR ASP VAL ILE ASN VAL ASN THR ASN VAL PHE ILE SER ALA ASN
ILE LEU ALA ASN ASN VAL ILE ILE THR VAL GLN GLN MET ASN ASN ILE SER ASN VAL ALA 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 ILE VAL
THR GLY ASN PHE PHE ALA ASN PHE ALA ASN VAL GLY ASN VAL GLN GLY ASN ALA ASN VAL ILE THR MET TYR SER THR THR THR LEU THR SER ASN SER ALA GLN ILE GLY ASN ILE SER GLY PHE SER ILE VAL SER ASN LEU GLY ASN ALA VAL SER MET PHE VAL GLY ASN LEU ASN THR
GLY THR LEU VAL ALA ASN ASN SER THR VAL GLY ASN ILE THR TYR ILE SER GLY ASN ILE GLY ASN ALA ALA ASN ALA GLN THR VAL ARG VAL SER GLY LEU LEU SER ALA SER GLY VAL ALA LEU THR PHE ASN SER ILE ILE THR SER ASN VAL ALA GLY ASN THR ASN ILE THR
LEU ARG THR ASN SER VAL THR THR GLU ILE LEU THR GLY ASN VAL LEU SER LEU THR THR GLY ASN LEU PHE ALA ASN SER ILE SER VAL GLN GLN SER ILE LEU ASN THR ALA ILE ILE ILE SER ASN ALA PHE ILE ILE SER SER GLN THR THR ASN ILE THR
ASN ILE SER GLY ASN ILE ARG VAL THR ASN THR LEU GLU ALA ASN ILE ILE ILE LYS ASN VAL VAL SER THR SER GLY ASN VAL THR THR GLY ASN LEU THR VAL THR ASN ALA VAL PHE ARG SER GLY ILE THR ASN ALA
GLU VAL VAL GLY ASN VAL CYS ASP GLY ASN THR THR VAL THR THR LEU SER TYR GLY ASN LEU VAL TYR ASN THR ARG ASN ILE PHE GLY ASN ILE THR ALA ASN THR VAL ASN ILE THR ASN SER ASN ILE GLY ASN VAL VAL THR SER ASN ILE THR ASN ALA
LEU ILE ILE THR ASN LEU ILE PRO THR VAL ASP ILE THR ASN VAL ALA THR ILE ALA ASN VAL LEU ARG ALA SER ILE ILE THR VAL ALA ASN VAL LEU SER MET SER ASN SER VAL SER ILE ILE ASN THR THR LEU SER ALA GLU VAL PHE THR SER GLU THR ILE ASN ASN ALA
ASN ALA ASN VAL SER VAL ALA THR ILE SER ASN VAL 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 VAL GLY ASP SER PHE THR ALA THR GLY ILE VAL ASN ALA

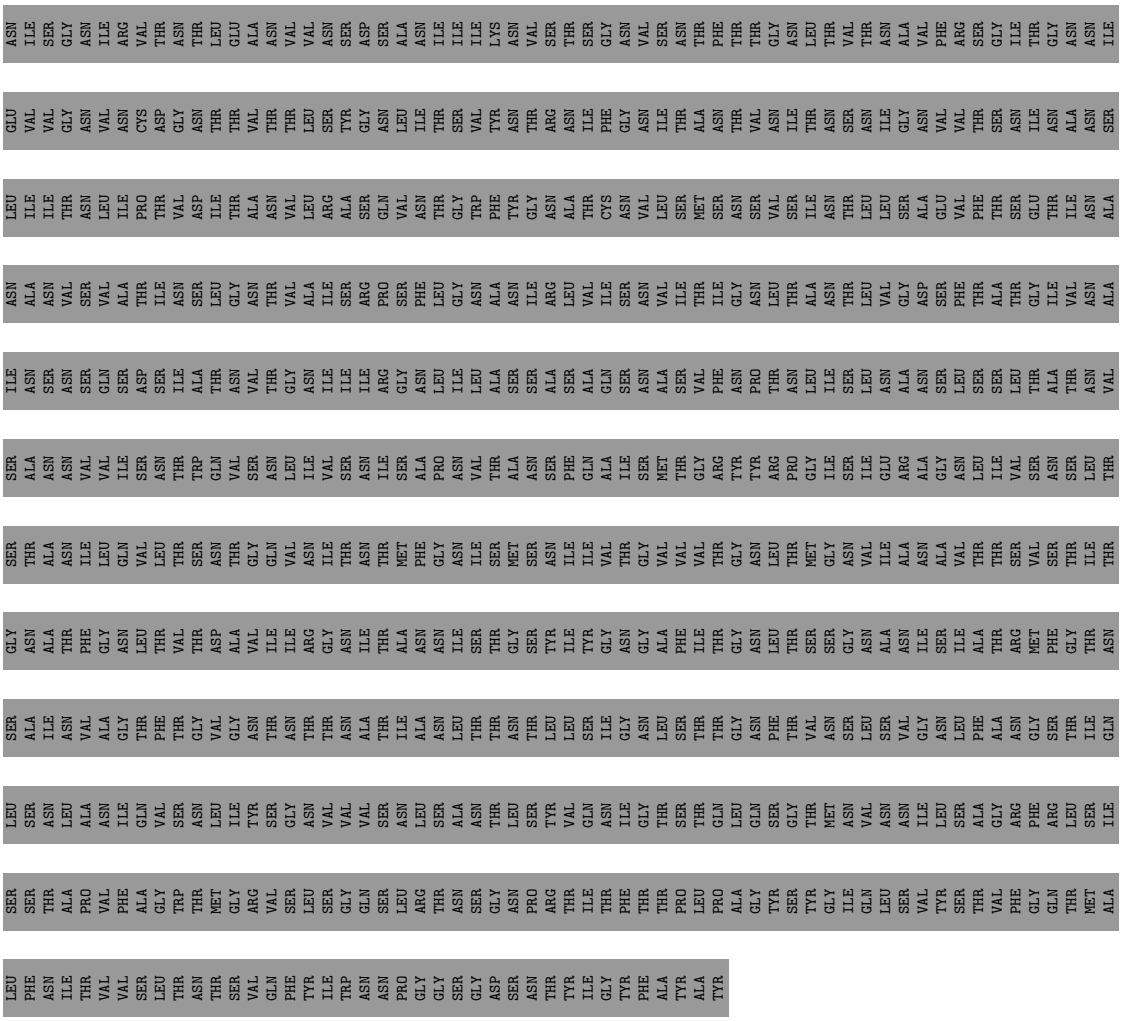


- Molecule 26: P23

Chain dn:

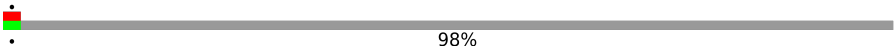


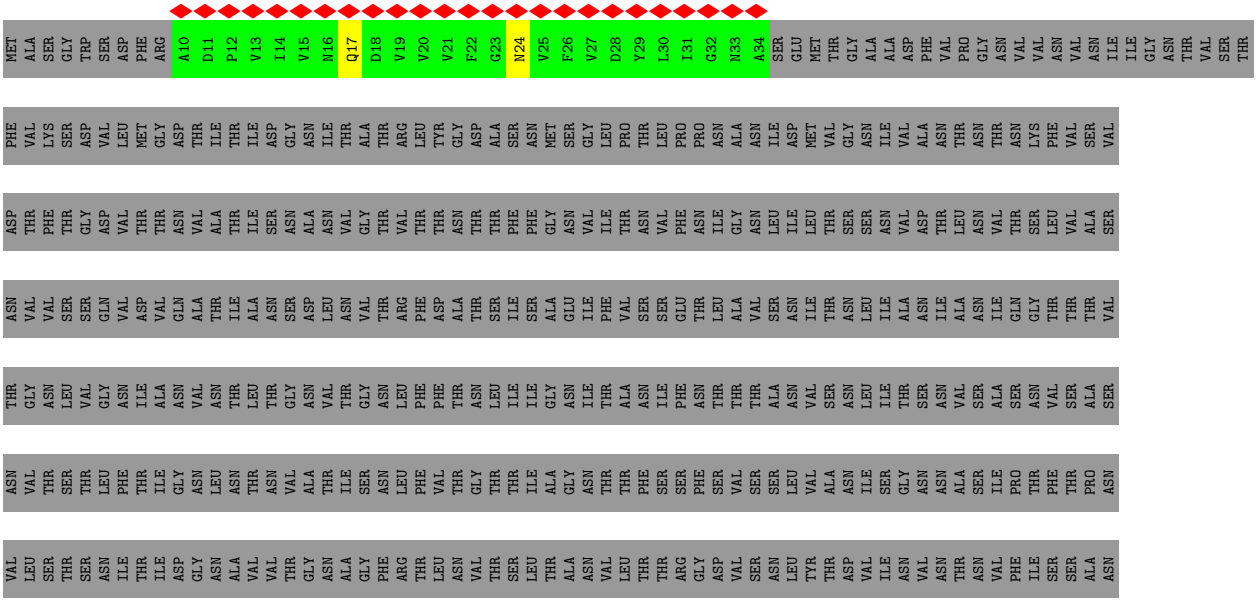




- Molecule 26: P23

Chain do:





| | | |

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 (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	aA	0.55	0/3468	0.69	0/4728
1	aB	0.58	0/3468	0.71	0/4728
1	aC	0.58	0/3473	0.71	0/4735
1	aD	0.60	0/3460	0.76	0/4717
1	aE	0.57	0/3473	0.72	0/4735
1	aF	0.58	0/3460	0.70	0/4717
1	aG	0.56	0/3468	0.70	0/4728
1	aH	0.55	0/3460	0.72	0/4717
1	aI	0.57	0/3468	0.71	0/4728
1	aJ	0.58	0/3473	0.70	0/4735
1	aK	0.55	0/3473	0.74	1/4735 (0.0%)
1	aL	0.58	0/3465	0.73	0/4724
1	aM	0.57	0/3473	0.71	0/4735
1	aN	0.58	0/3468	0.71	0/4728
1	aO	0.57	0/3473	0.72	0/4735
1	aP	0.57	0/3473	0.71	0/4735
1	aQ	0.58	0/3460	0.72	0/4717
1	aR	0.58	0/3473	0.73	0/4735
1	aS	0.57	0/3473	0.71	0/4735
1	aT	0.58	0/3473	0.70	0/4735
1	aU	0.58	0/3473	0.70	0/4735
1	aV	0.56	0/3473	0.69	0/4735
1	aW	0.56	0/3473	0.71	0/4735
1	aX	0.58	0/3468	0.72	0/4728
1	aY	0.57	0/3473	0.71	0/4735
1	aZ	0.57	0/3473	0.71	0/4735
1	aa	0.84	0/3452	0.83	0/4707
1	ab	0.88	0/3473	0.88	0/4735
1	ac	0.83	0/3473	0.82	1/4735 (0.0%)
1	ad	0.57	0/3473	0.71	1/4735 (0.0%)
1	ae	0.56	0/3473	0.69	0/4735
1	af	0.57	0/3473	0.71	0/4735
1	ag	0.57	0/3473	0.70	0/4735
1	ah	0.56	0/3473	0.70	0/4735

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

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

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

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

There are no bond length outliers.

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 (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

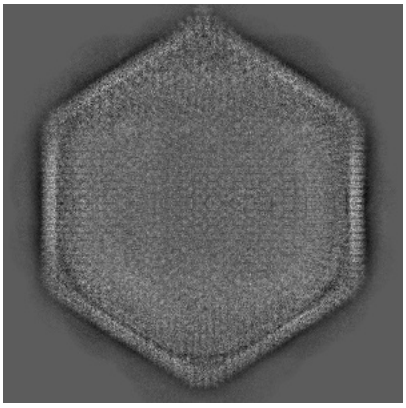
6 Map visualisation (i)

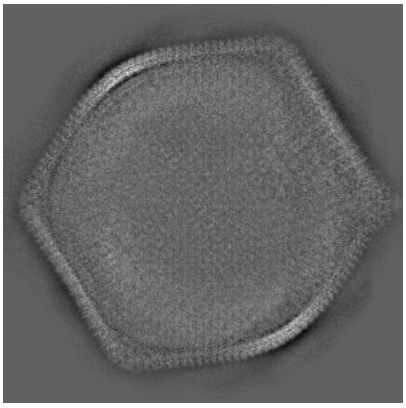
This section contains visualisations of the EMDB entry EMD-34438. These allow visual inspection of the internal detail of the map and identification of artifacts.

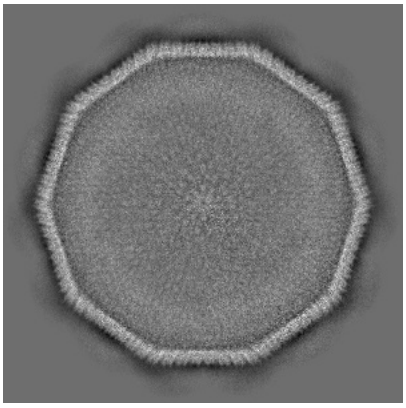
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

6.1.1 Primary map


X

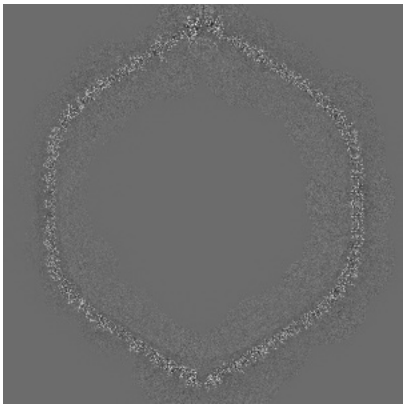

Y

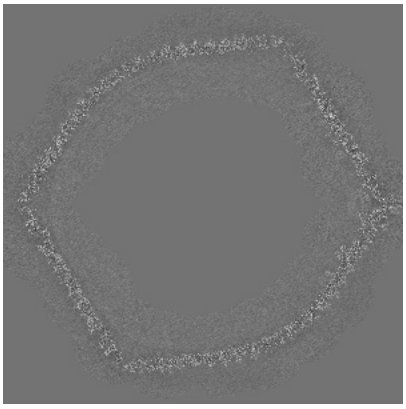

Z

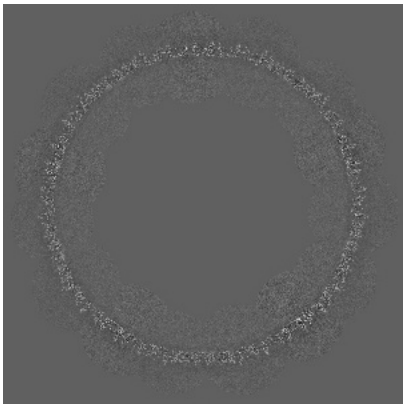
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map


X Index: 600

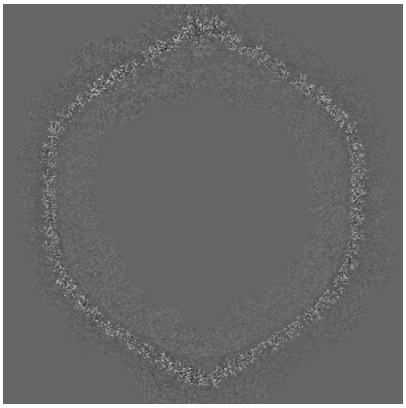

Y Index: 600

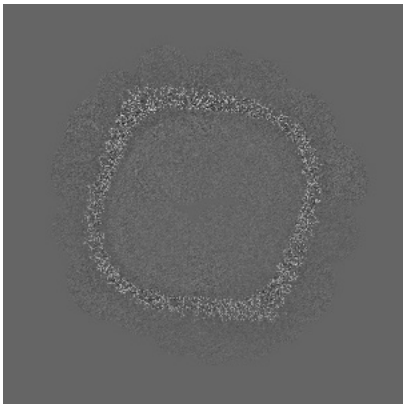

Z Index: 600

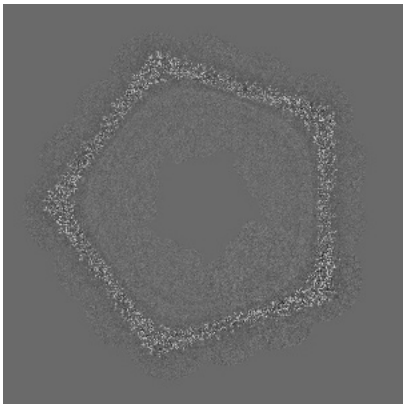
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map


X Index: 628

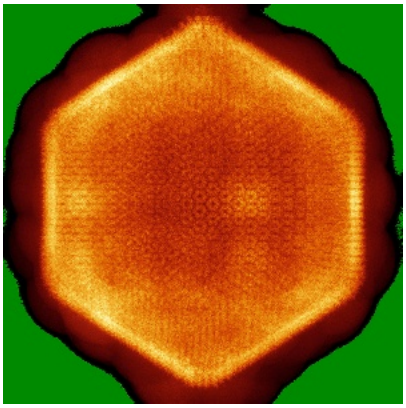

Y Index: 257

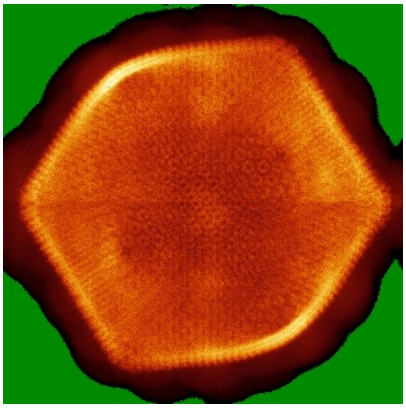

Z Index: 320

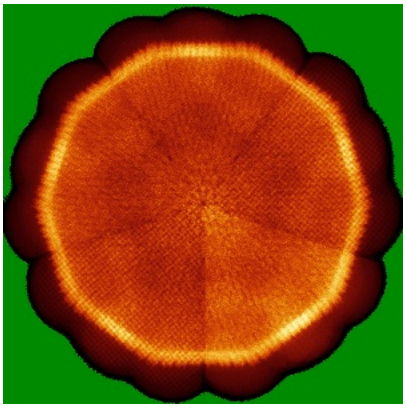
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map


X

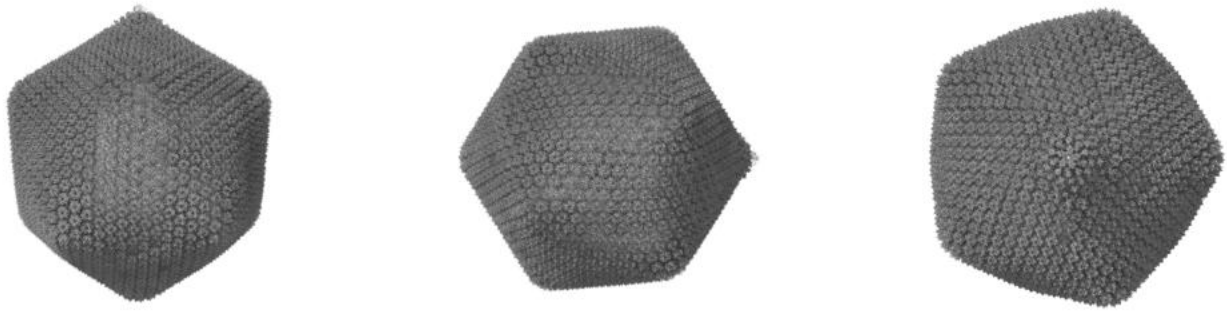

Y


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

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

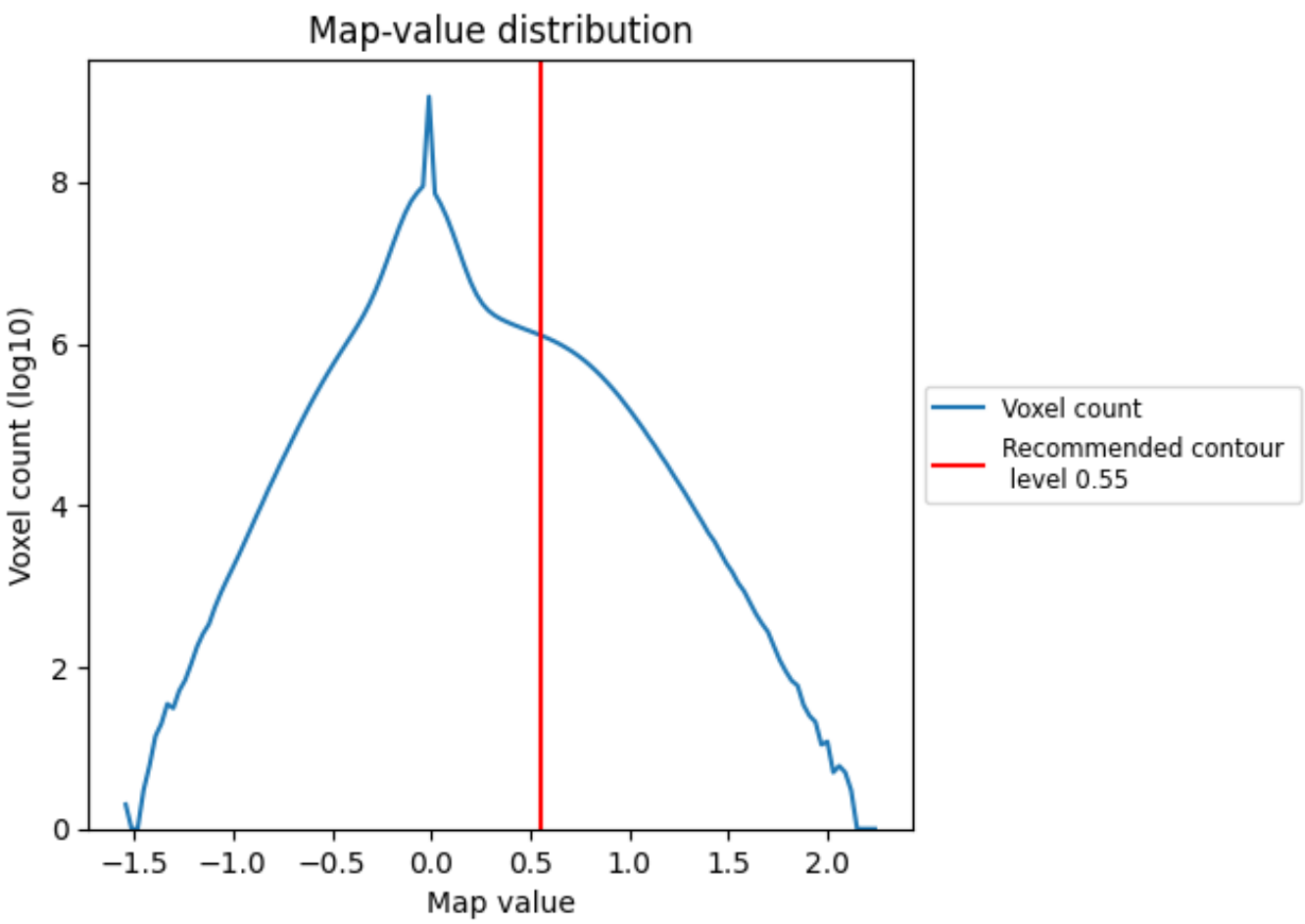
6.6 Mask visualisation (i)

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

7 Map analysis (i)

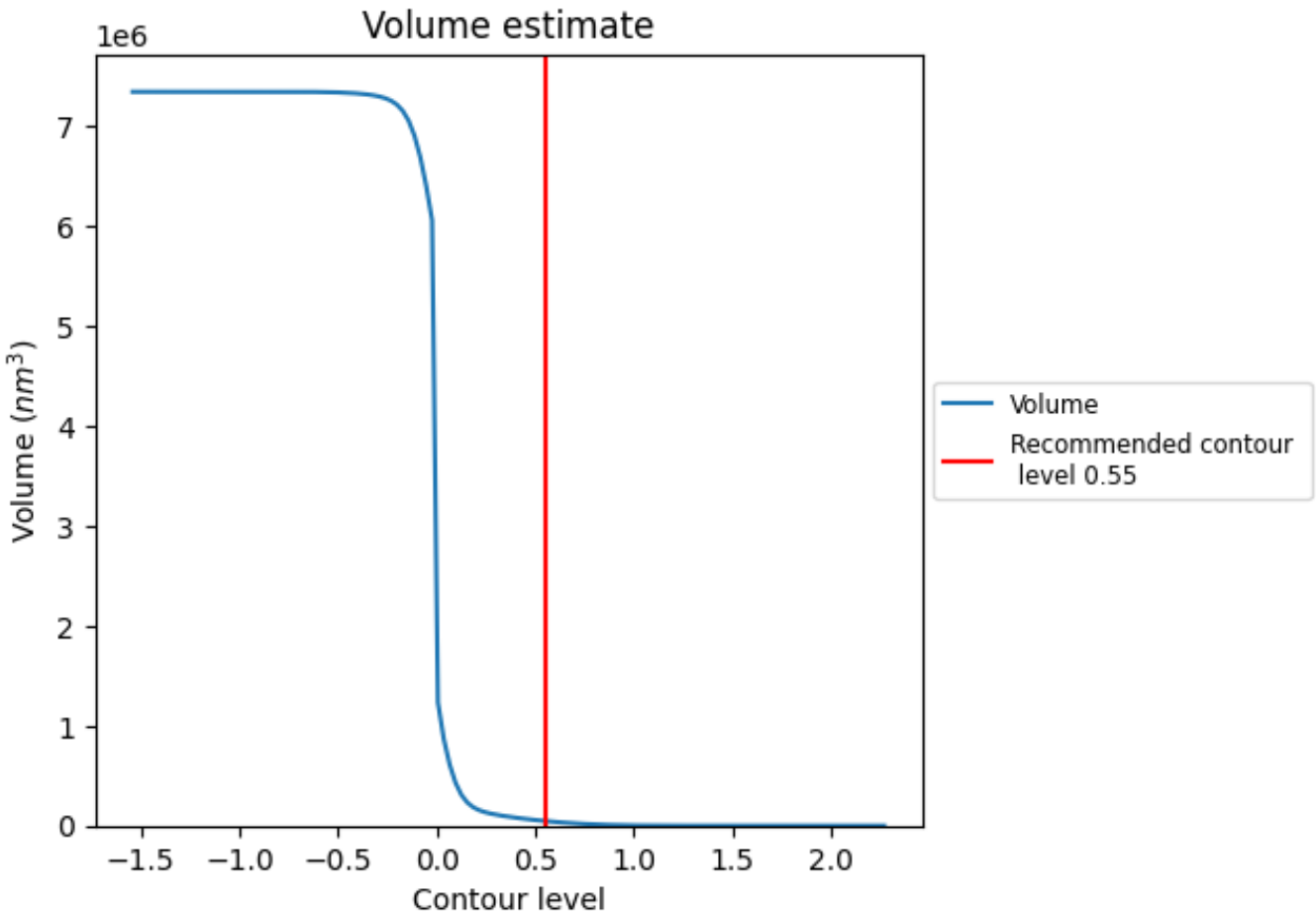
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

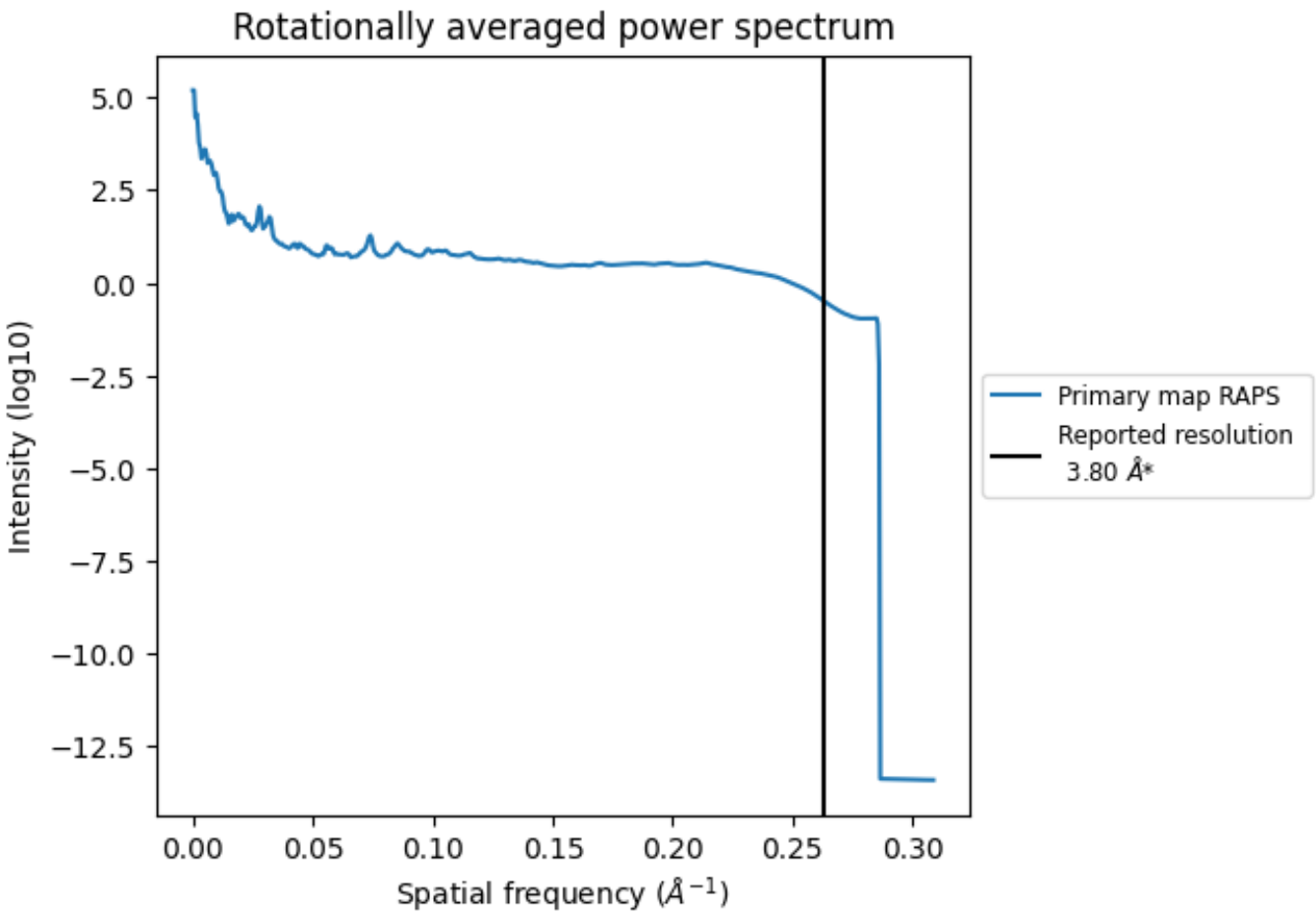
7.2 Volume estimate (i)



The volume at the recommended contour level is 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 (i)

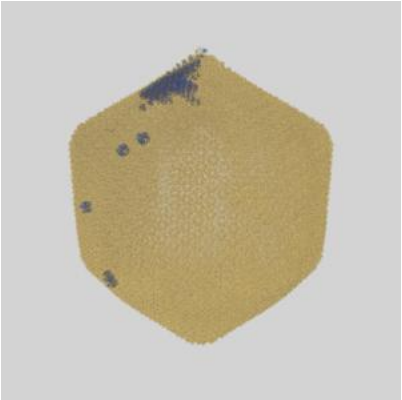
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit (i)

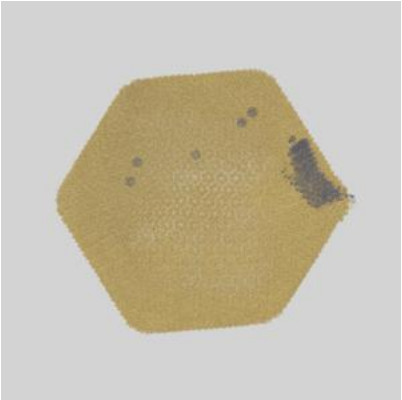
This section contains information regarding the fit between EMDB map EMD-34438 and PDB model 8H2I. Per-residue inclusion information can be found in section 3 on page 22.

9.1 Map-model overlays

9.1.1 Map-model overlay (i)



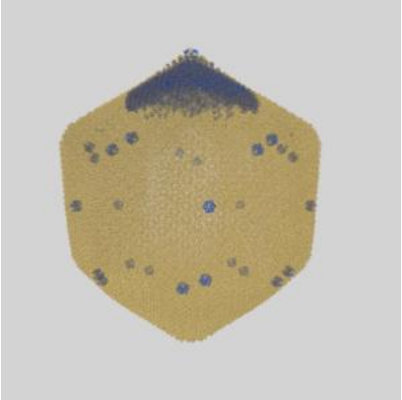
X



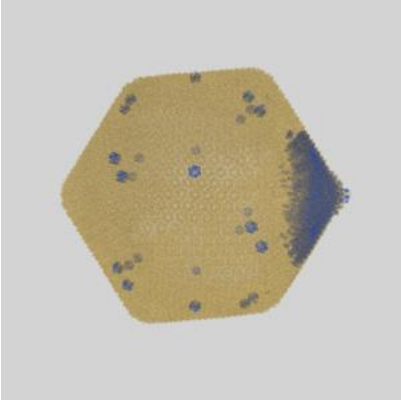
Y

Z

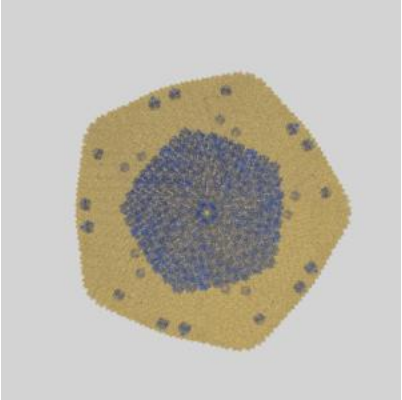
9.1.2 Map-model assembly overlay (i)



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.

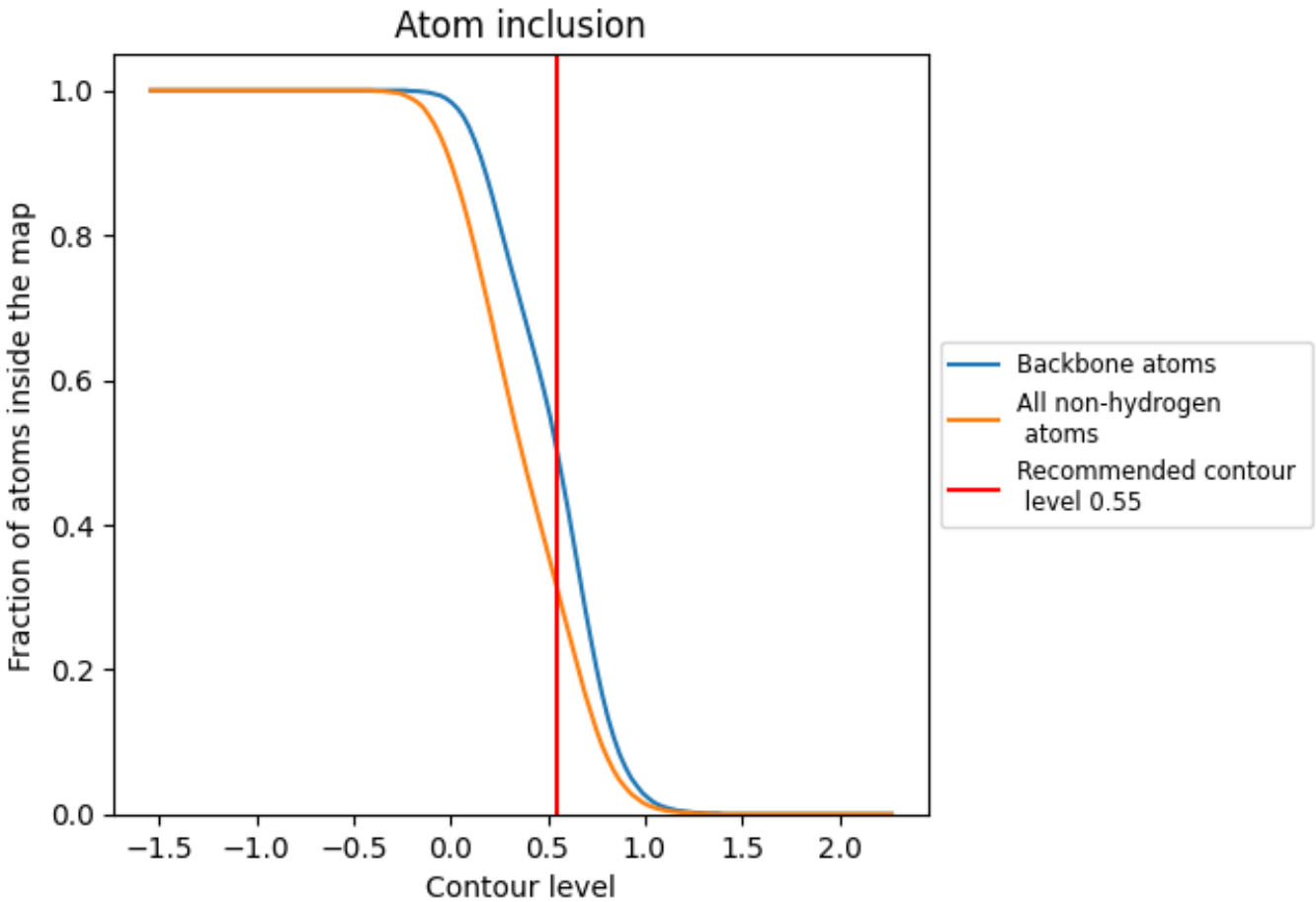
9.2 Q-score mapped to coordinate model (i)

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 (i)

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	0.3110	0.3620
aA	0.2580	0.3860
aB	0.2670	0.3810
aC	0.2860	0.3790
aD	0.2940	0.3800
aE	0.3830	0.4000
aF	0.4160	0.3950
aG	0.3710	0.3900
aH	0.4420	0.4010
aI	0.4390	0.4000
aJ	0.4140	0.3930
aK	0.3900	0.3960
aL	0.3660	0.3930
aM	0.3610	0.3940
aN	0.3690	0.3970
aO	0.3660	0.3900
aP	0.3750	0.3960
aQ	0.3370	0.3910
aR	0.3310	0.3900
aS	0.3510	0.3970
aT	0.3660	0.3910
aU	0.3800	0.3960
aV	0.3800	0.3970
aW	0.3310	0.3900
aX	0.3340	0.3900
aY	0.3320	0.3900
aZ	0.3520	0.3910
aa	0.4210	0.3970
ab	0.4250	0.3940
ac	0.4330	0.4050
ad	0.4340	0.3980
ae	0.4250	0.4010
af	0.4220	0.4010
ag	0.4150	0.3910
ah	0.4500	0.4050

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Chain	Atom inclusion	Q-score
ai	0.4230	0.3990
aj	0.3020	0.3830
ak	0.3610	0.3940
al	0.2940	0.3800
am	0.4340	0.3980
an	0.4370	0.3950
ao	0.4260	0.3960
ap	0.4430	0.3980
aq	0.4620	0.3980
ar	0.4610	0.4010
as	0.4250	0.3900
at	0.3850	0.3990
au	0.3930	0.4020
av	0.3320	0.3890
aw	0.3030	0.3940
ax	0.3480	0.3980
ay	0.2330	0.3780
az	0.2220	0.3830
bA	0.3620	0.3680
bB	0.2710	0.3590
bC	0.3450	0.3730
bD	0.2300	0.3510
bE	0.2900	0.3580
bF	0.2640	0.3460
bG	0.3260	0.3190
bH	0.3210	0.3860
bI	0.3010	0.3470
bJ	0.3120	0.3430
bK	0.3060	0.3660
bL	0.2550	0.2560
bM	0.2370	0.2780
bN	0.2580	0.2770
bO	0.2130	0.2690
bP	0.2440	0.3230
bQ	0.2140	0.3340
bR	0.3370	0.3500
bS	0.3120	0.3890
bT	0.3150	0.3600
bU	0.4400	0.3720
bV	0.3780	0.3510
bW	0.3780	0.3380
bX	0.3420	0.3510

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Chain	Atom inclusion	Q-score
bY	0.2230	0.3100
bZ	0.1960	0.3360
ba	0.3790	0.3920
bb	0.3440	0.3980
bc	0.3710	0.3880
bd	0.3590	0.3920
be	0.3650	0.3910
bf	0.3860	0.3930
bg	0.3700	0.3880
bh	0.3880	0.3900
bi	0.3690	0.3950
bj	0.3390	0.3920
bk	0.3720	0.3900
bl	0.3490	0.3960
bm	0.3400	0.3930
bn	0.3350	0.4010
bo	0.3390	0.3910
bp	0.3670	0.3890
bq	0.3350	0.3870
br	0.3990	0.3920
bs	0.3730	0.3880
bt	0.3840	0.3930
bu	0.4830	0.3820
bv	0.4510	0.3760
bw	0.4610	0.3780
bx	0.4270	0.3790
by	0.4070	0.3760
bz	0.4050	0.3700
cA	0.0000	0.1280
cB	0.0590	0.2680
cC	0.0010	0.2080
cD	0.0220	0.2300
cE	0.0380	0.2070
cF	0.1190	0.2600
cG	0.0270	0.1770
cH	0.2280	0.2810
cI	0.0090	0.2100
cJ	0.1480	0.2890
cK	0.0010	0.1880
cL	0.0800	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	0.0080	0.4540
cQ	0.0130	0.4490
cR	0.2880	0.3690
cS	0.3090	0.3610
cT	0.2750	0.3470
cU	0.1420	0.4210
cV	0.1580	0.4140
cW	0.1700	0.4200
cX	0.3110	0.3360
cY	0.2550	0.3320
cZ	0.3020	0.3400
ca	0.2260	0.3680
cb	0.2460	0.3550
cc	0.2610	0.3240
cd	0.2650	0.3370
ce	0.3120	0.3590
cf	0.3640	0.3430
cg	0.1610	0.3070
ch	0.3600	0.3560
ci	0.4020	0.3530
cj	0.2720	0.3750
ck	0.2080	0.3810
cl	0.2500	0.3610
cm	0.2690	0.3710
cn	0.2410	0.3910
co	0.2670	0.3680
cp	0.0240	0.2540
cq	0.0000	0.1670
cr	0.0610	0.2610
cs	0.0020	0.1780
ct	0.0520	0.2710
cu	0.0010	0.1850
cv	0.1610	0.2950
cw	0.1090	0.2620
cx	0.2120	0.2930
cy	0.0350	0.2420
cz	0.0110	0.2100
da	0.0880	0.4680
db	0.1110	0.4280
dc	0.1120	0.4710
dd	0.2410	0.3720

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Chain	Atom inclusion	Q-score
de	0.2250	0.3630
df	0.2390	0.3680
dg	0.0080	0.4510
dh	0.0080	0.4250
di	0.0000	0.4400
dj	0.2870	0.3620
dk	0.2660	0.3550
dl	0.2990	0.3340
dm	0.0000	0.3540
dn	0.0110	0.3860
do	0.0000	0.3280
dp	0.3010	0.3750
dq	0.2960	0.3750
dr	0.3090	0.3720
ds	0.0300	0.4410
dt	0.0170	0.4570
du	0.0040	0.4400