wwPDB EM Validation Summary Report

Mar 20, 2026 – 05:05 AM UTC

PDB ID	:	7N6G / pdb_00007n6g
EMDB ID	:	EMD-24207
Title	:	C1 of central pair
Authors	:	Han, L.; Zhang, K.
Deposited on	:	2021-06-08
Resolution	:	3.60 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (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 (1)) were used in the production of this report:

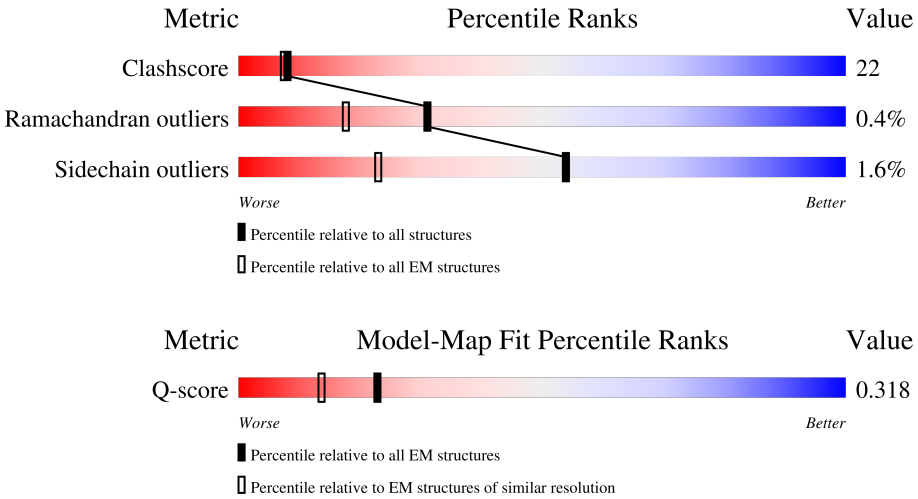
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 3.60 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12797 (3.10 - 4.10)

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	0A	512	11% 56% 41% ·
1	0B	512	44% 51% 46% ·
1	0C	512	15% 62% 35% ·
1	0D	512	22% 60% 38% ·

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Mol	Chain	Length	Quality of chain
1	0E	512	15% 57% 40%
1	0F	512	9% 60% 38%
1	0G	512	24% 61% 36%
1	0H	512	6% 62% 35%
1	0I	512	21% 60% 37%
1	0J	512	20% 61% 37%
1	0K	512	11% 60% 37%
1	0L	512	63% 34%
1	0M	512	6% 64% 33%
1	0N	512	61% 36%
1	0O	512	5% 61% 36%
1	0P	512	62% 59% 38%
1	0Q	512	45% 55% 42%
1	0R	512	7% 58% 39%
1	0S	512	6% 61% 36%
1	0T	512	5% 63% 35%
1	0U	512	62% 35%
1	0V	512	6% 61% 37%
1	0W	512	10% 64% 33%
1	0X	512	8% 58% 39%
1	0Y	512	32% 54% 43%
1	0Z	512	35% 58% 39%
1	1A	512	13% 59% 38%
1	1B	512	85% 53% 45%
1	1C	512	70% 55% 43%

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Mol	Chain	Length	Quality of chain
2	1D	571	62% 24% 12%
2	1E	571	43% 65% 22% 12%
2	1F	571	64% 25% 10%
2	1G	571	31% 67% 22% 10%
3	1H	1102	50% 22% 27%
3	1I	1102	21% 55% 18% 27%
3	6D	1102	49% 23% 27%
4	1J	3965	6% 90%
4	1K	3965	6% 90%
5	1L	2939	13% 5% 81%
5	1M	2939	13% 5% 81%
6	1N	2784	5% 61% 17% 22%
7	1O	3225	68% 14% 18%
8	1P	1023	21% 8% 71%
9	1Q	945	39% 6% 54%
10	1R	446	47% 32% 19%
10	1S	446	5% 31% 27% 41%
11	1T	1638	59% 41%
12	1a	443	19% 60% 36%
12	1c	443	6% 67% 30%
12	1e	443	65% 31%
12	1g	443	66% 31%
12	2a	443	21% 63% 34%
12	2c	443	5% 66% 31%
12	2e	443	6% 67% 30%

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Mol	Chain	Length	Quality of chain
12	2g	443	5% 66% 31%
12	3a	443	19% 64% 33%
12	3c	443	67% 30%
12	3e	443	6% 70% 27%
12	3g	443	65% 33%
12	4a	443	17% 67% 29%
12	4c	443	5% 68% 30%
12	4e	443	67% 29%
12	4g	443	69% 29%
12	5a	443	27% 61% 35%
12	5c	443	6% 66% 31%
12	5e	443	63% 33%
12	5g	443	6% 67% 30%
12	6a	443	30% 63% 33%
12	6c	443	6% 67% 30%
12	6e	443	66% 30%
12	6g	443	69% 28%
12	7a	443	23% 61% 35%
12	7c	443	8% 65% 32%
12	7e	443	5% 62% 35%
12	7g	443	66% 31%
12	8a	443	31% 60% 36%
12	8c	443	5% 66% 31%
12	8e	443	6% 65% 31%
12	8g	443	5% 63% 35%

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Mol	Chain	Length	Quality of chain
12	9a	443	18% 57% 40%
12	9c	443	66% 32%
12	9e	443	5% 65% 32%
12	9g	443	5% 67% 30%
12	Aa	443	17% 59% 37%
12	Ac	443	64% 34%
12	Ae	443	62% 34%
12	Ag	443	64% 33%
12	Ba	443	12% 64% 33%
12	Bc	443	7% 66% 31%
12	Be	443	60% 36%
12	Bg	443	5% 64% 34%
12	Ca	443	12% 63% 34%
12	Cc	443	62% 35%
12	Ce	443	62% 34%
12	Cg	443	65% 32%
12	Da	443	5% 63% 33%
12	Dc	443	70% 28%
12	De	443	62% 35%
12	Dg	443	66% 31%
13	1b	451	8% 56% 38% 5%
13	1d	451	5% 61% 34% 5%
13	1f	451	5% 53% 41% 5%
13	1h	451	9% 61% 34% 5%
13	2b	451	8% 57% 37% 5%

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Mol	Chain	Length	Quality of chain
13	2d	451	7% 59% 36% • 5%
13	2f	451	6% 58% 36% • 5%
13	2h	451	9% 59% 35% • 5%
13	3b	451	8% 58% 36% • 5%
13	3d	451	9% 59% 36% • 5%
13	3f	451	7% 59% 35% • 5%
13	3h	451	13% 58% 36% • 5%
13	4b	451	5% 59% 35% • 5%
13	4d	451	6% 60% 34% • 5%
13	4f	451	7% 62% 33% • 5%
13	4h	451	15% 60% 35% • 5%
13	5b	451	8% 57% 37% • 5%
13	5d	451	9% 58% 36% • 5%
13	5f	451	6% 59% 35% • 5%
13	5h	451	17% 61% 34% • 5%
13	6b	451	8% 58% 36% • 5%
13	6d	451	5% 57% 37% • 5%
13	6f	451	5% 57% 37% • 5%
13	6h	451	11% 59% 36% • 5%
13	7b	451	8% 60% 34% • 5%
13	7d	451	6% 55% 39% • 5%
13	7f	451	5% 58% 37% • 5%
13	7h	451	9% 59% 35% • 5%
13	8b	451	7% 60% 35% • 5%
13	8d	451	8% 60% 35% • 5%

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Mol	Chain	Length	Quality of chain
13	8f	451	6% 55% 40% • 5%
13	8h	451	13% 59% 36% • 5%
13	9b	451	5% 58% 36% • 5%
13	9d	451	5% 59% 35% • 5%
13	9f	451	• 59% 35% • 5%
13	9h	451	11% 60% 35% • 5%
13	Ab	451	5% 57% 37% • 5%
13	Ad	451	7% 59% 36% • 5%
13	Af	451	• 56% 38% • 5%
13	Ah	451	11% 60% 34% • 5%
13	Bb	451	• 55% 39% • 5%
13	Bd	451	• 59% 36% • 5%
13	Bf	451	• 54% 41% • 5%
13	Bh	451	10% 61% 33% • 5%
13	Cb	451	6% 55% 38% • 5%
13	Cd	451	• 57% 37% • 5%
13	Cf	451	• 54% 40% • 5%
13	Ch	451	10% 58% 36% • 5%
13	Db	451	• 56% 38% • 5%
13	Dd	451	• 59% 35% • 5%
13	Df	451	• 55% 39% • 5%
13	Dh	451	10% 59% 35% • 5%
14	2F	168	9% 55% 39% • •
14	2G	168	24% 58% 36% • •
15	2H	196	16% 83% 17% •

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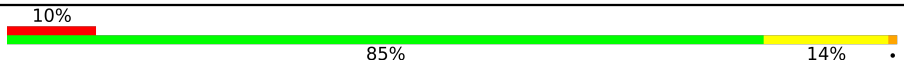
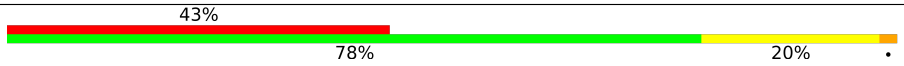
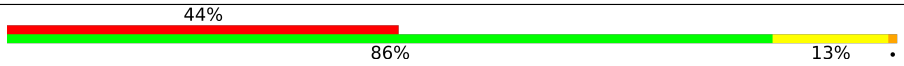
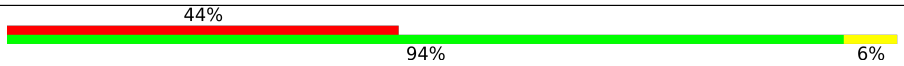
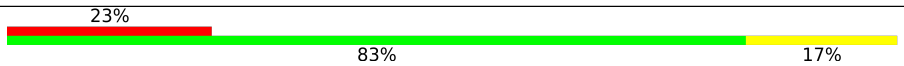
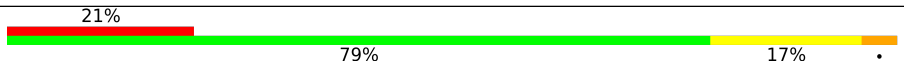
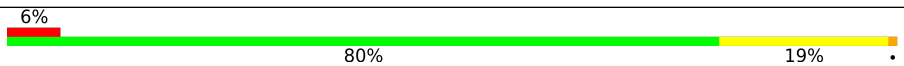
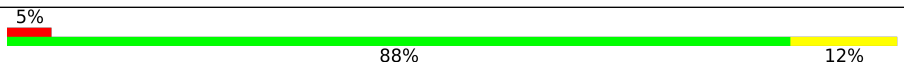
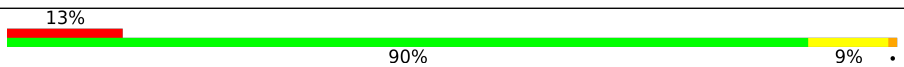
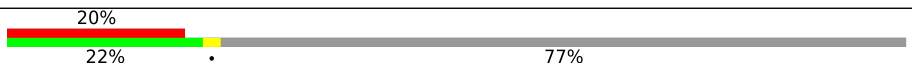
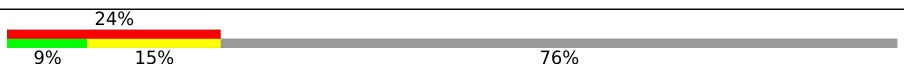
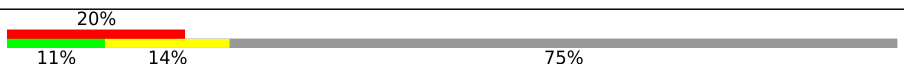
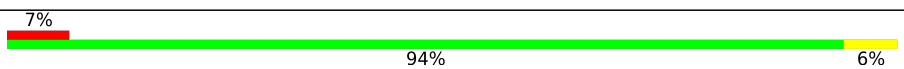
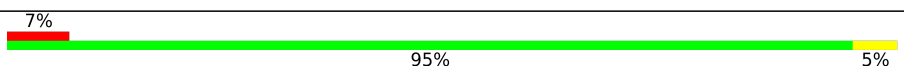
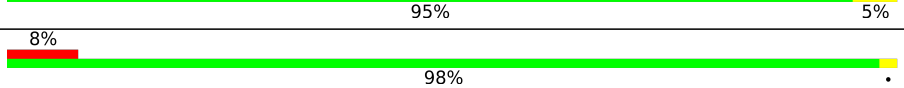
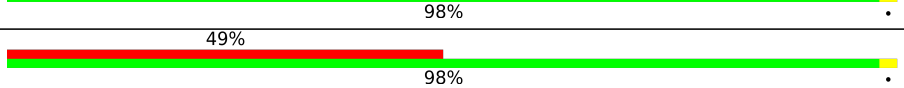
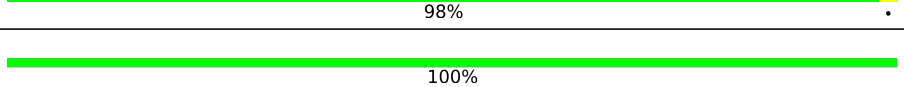
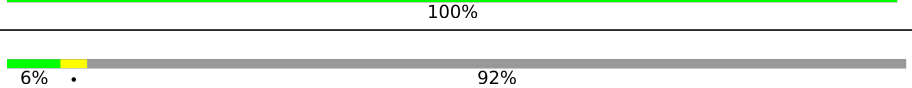
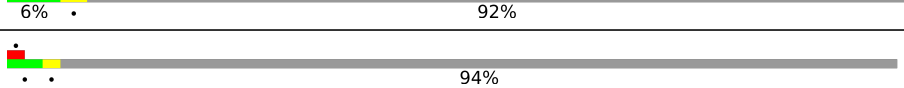
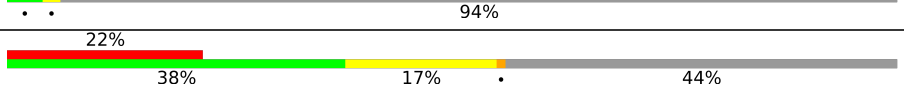
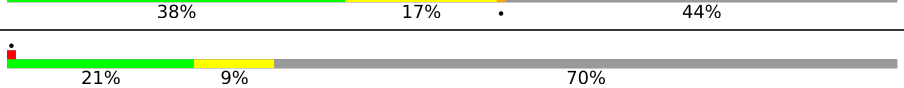
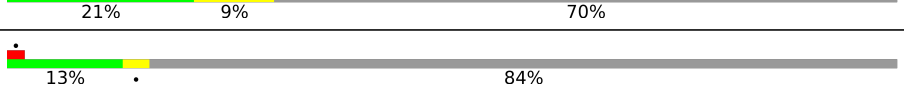
Mol	Chain	Length	Quality of chain
16	2I	108	
17	2J	100	
17	2K	100	
18	2L	54	
19	2M	18	
20	2N	52	
21	2O	47	
22	2P	106	
23	2Q	110	
23	2R	110	
24	2S	447	
24	2T	447	
24	2U	447	
24	2V	447	
25	2W	167	
25	2X	167	
26	2Y	65	
26	2Z	65	
27	3A	36	
27	3B	36	
28	3C	739	
29	3E	1471	
30	3F	795	
30	3G	795	
31	3H	1940	

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Mol	Chain	Length	Quality of chain
31	3I	1940	14% 7% 79%
32	3J	749	30% 19% 50%
32	3K	749	16% 32% 17% 51%
33	3L	401	31% 17% 51%
34	3M	507	37% 40% 36% 24%
34	3N	507	23% 48% 29% 23%
34	3O	507	24% 31% 38% 30%
34	3P	507	21% 35% 35% 30%
34	3Q	507	7% 37% 33% 30%
34	3R	507	14% 45% 26% 29%
34	3S	507	23% 45% 31% 24%
34	3T	507	37% 40% 37% 23%
34	3U	507	6% 38% 32% 30%
34	3V	507	15% 54% 26% 19%
34	3W	507	54% 27% 19%
34	3X	507	47% 24% 29%
34	3Y	507	50% 20% 29%
34	3Z	507	9% 47% 23% 29%
34	4A	507	5% 56% 25% 19%
34	4B	507	15% 52% 29% 19%
35	4C	2215	16% 12% 71%
36	4D	304	5% 50% 45%
37	4E	2301	25% 17% 57%
37	4F	2301	24% 15% 58%
37	4G	2301	24% 15% 58%

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Mol	Chain	Length	Quality of chain
37	4H	2301	25% 15% 58%
38	4I	110	26% 34% 16% 7% 42%
38	4J	110	33% 15% 7% 42%
38	4K	110	5% 33% 15% 7% 42%
38	4L	110	33% 35% 15% 7% 42%
38	4M	110	33% 34% 15% 7% 42%
38	4N	110	35% 33% 16% 7% 42%
38	4O	110	11% 27% 44% 5% 24%
38	4P	110	8% 28% 21% 50%
39	4Q	427	31% 19% 49%
39	4R	427	20% 32% 18% 49%
39	4S	427	9% 30% 20% 49%
40	4T	835	44% 26% 28%
40	4U	835	43% 26% 28%
40	4V	835	43% 26% 28%
41	4W	173	6% 65% 7% 28%
41	4X	173	57% 14% 28%
41	4Y	173	55% 16% 28%
41	4Z	173	54% 17% 28%
41	5A	173	40% 20% 6% 5% 29%
41	5B	173	56% 15% 29%
41	5C	173	56% 15% 29%
41	5D	173	56% 15% 29%
42	5E	286	60% 15% 24%
42	5F	286	11% 63% 13% 24%

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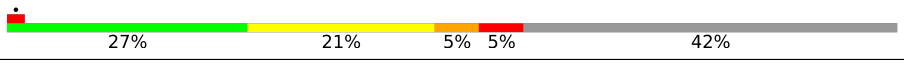
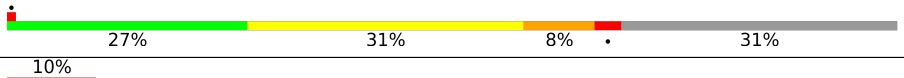
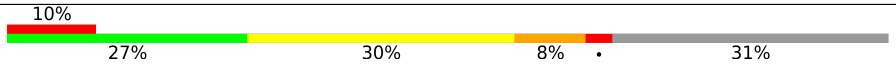
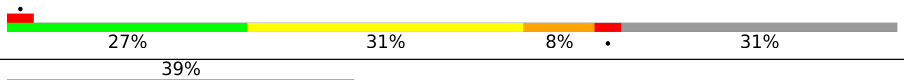
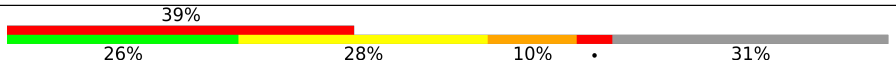
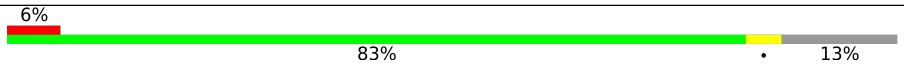
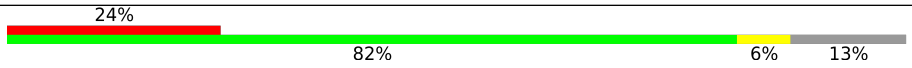
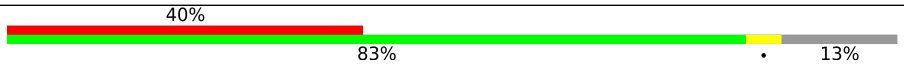
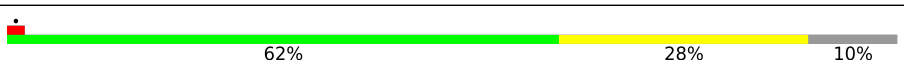
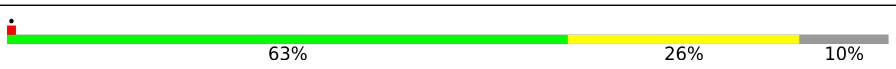
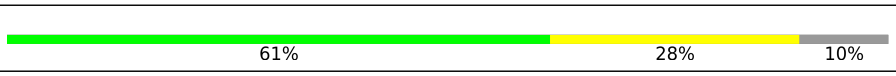
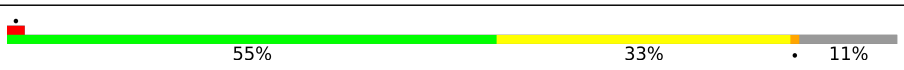
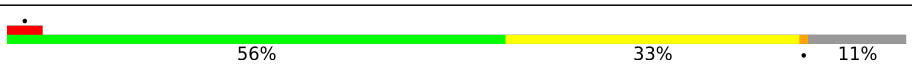
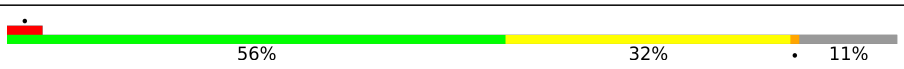
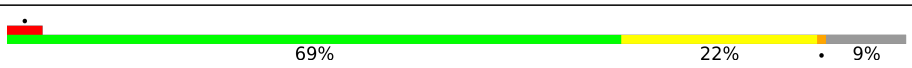
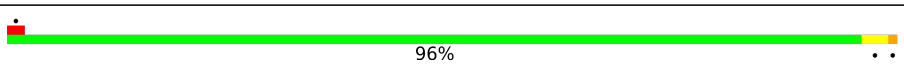
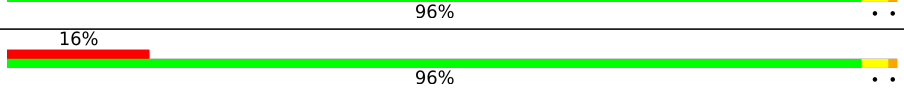
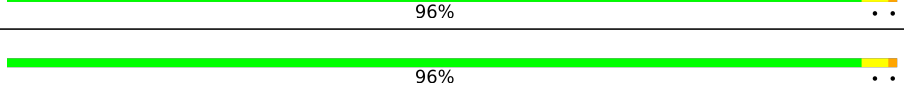
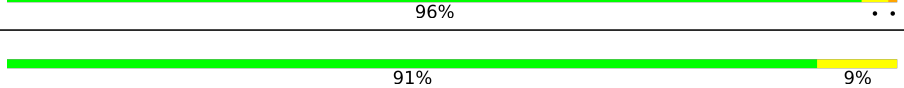
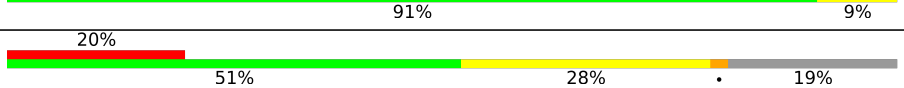
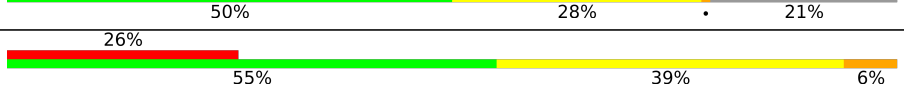
Mol	Chain	Length	Quality of chain
42	5G	286	
42	5H	286	
43	5I	306	
43	5J	306	
43	5K	306	
43	5L	306	
44	5M	163	
44	5N	163	
44	5O	163	
44	5P	163	
44	5Q	163	
44	5R	163	
44	5S	163	
44	5T	163	
44	5U	163	
44	5V	163	
45	5W	137	
45	5X	137	
45	5Y	137	
46	5Z	181	
47	6A	1929	
47	6B	1929	
48	6E	1138	
48	6F	1138	
49	6G	477	

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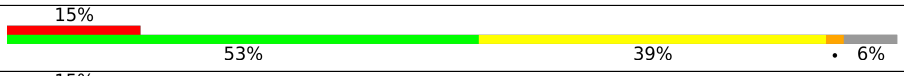
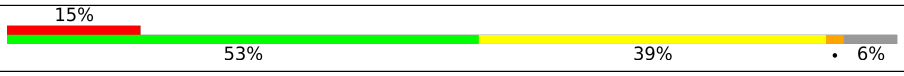
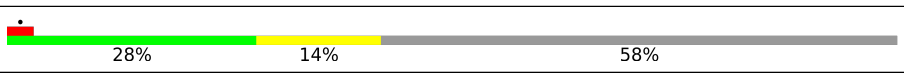
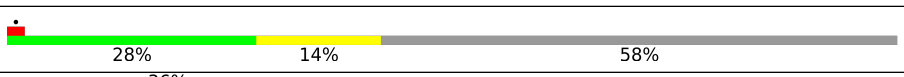
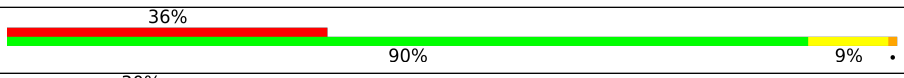
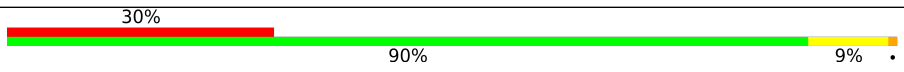
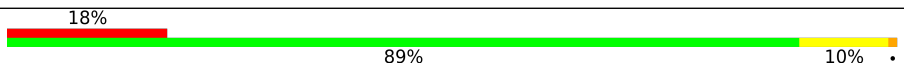
Mol	Chain	Length	Quality of chain
49	6H	477	
49	6I	477	
49	6J	477	
50	6K	651	
50	6L	651	
51	6M	2540	
51	6N	2540	
52	6O	89	
52	6P	89	
52	6Q	89	

2 Entry composition (i)

There are 54 unique types of molecules in this entry. The entry contains 793756 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 PF16.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0A	499	Total	C	N	O	S	0	0
			3528	2217	625	675	11		
1	0B	499	Total	C	N	O	S	0	0
			3528	2217	625	675	11		
1	0C	499	Total	C	N	O	S	0	0
			3528	2217	625	675	11		
1	0D	499	Total	C	N	O	S	0	0
			3528	2217	625	675	11		
1	0E	499	Total	C	N	O	S	0	0
			3528	2217	625	675	11		
1	0F	499	Total	C	N	O	S	0	0
			3528	2217	625	675	11		
1	0G	499	Total	C	N	O	S	0	0
			3528	2217	625	675	11		
1	0L	499	Total	C	N	O	S	0	0
			3528	2217	625	675	11		
1	0M	499	Total	C	N	O	S	0	0
			3528	2217	625	675	11		
1	0N	499	Total	C	N	O	S	0	0
			3528	2217	625	675	11		
1	0O	499	Total	C	N	O	S	0	0
			3528	2217	625	675	11		
1	0P	499	Total	C	N	O	S	0	0
			3528	2217	625	675	11		
1	0Q	499	Total	C	N	O	S	0	0
			3528	2217	625	675	11		
1	0R	499	Total	C	N	O	S	0	0
			3526	2215	625	675	11		
1	0S	499	Total	C	N	O	S	0	0
			3528	2217	625	675	11		
1	0T	499	Total	C	N	O	S	0	0
			3528	2217	625	675	11		
1	0U	499	Total	C	N	O	S	0	0
			3528	2217	625	675	11		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	0V	499	Total	C	N	O	S	0	0
			3528	2217	625	675	11		
1	0X	499	Total	C	N	O	S	0	0
			3528	2217	625	675	11		
1	0Y	499	Total	C	N	O	S	0	0
			3528	2217	625	675	11		
1	0Z	499	Total	C	N	O	S	0	0
			3528	2217	625	675	11		
1	1A	499	Total	C	N	O	S	0	0
			3528	2217	625	675	11		
1	1B	499	Total	C	N	O	S	0	0
			3528	2217	625	675	11		
1	1C	499	Total	C	N	O	S	0	0
			3524	2214	624	675	11		
1	0H	499	Total	C	N	O	S	0	0
			3528	2217	625	675	11		
1	0J	499	Total	C	N	O	S	0	0
			3528	2217	625	675	11		
1	0W	499	Total	C	N	O	S	0	0
			3528	2217	625	675	11		
1	0I	499	Total	C	N	O	S	0	0
			3528	2217	625	675	11		
1	0K	499	Total	C	N	O	S	0	0
			3524	2214	624	675	11		

- Molecule 2 is a protein called FAP194.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1D	504	Total	C	N	O	S	0	0
			3213	1978	593	625	17		
2	1E	504	Total	C	N	O	S	0	0
			3213	1978	593	625	17		
2	1F	516	Total	C	N	O	S	0	0
			3292	2028	606	641	17		
2	1G	516	Total	C	N	O	S	0	0
			3292	2028	606	641	17		

- Molecule 3 is a protein called FAP69.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	1H	803	Total	C	N	O	S	0	0
			5778	3640	1042	1072	24		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	1I	803	Total	C	N	O	S	0	0
			5778	3640	1042	1072	24		
3	6D	801	Total	C	N	O	S	0	0
			6016	3811	1073	1105	27		

- Molecule 4 is a protein called HYDIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	1J	396	Total	C	N	O	S	0	0
			2856	1798	498	552	8		
4	1K	396	Total	C	N	O	S	0	0
			2856	1798	498	552	8		

- Molecule 5 is a protein called FAP47.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	1L	546	Total	C	N	O	S	0	0
			3368	2055	639	663	11		
5	1M	546	Total	C	N	O	S	0	0
			3368	2055	639	663	11		

- Molecule 6 is a protein called FAP46.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	1N	2179	Total	C	N	O	S	1	0
			16109	10108	2968	2963	70		

- Molecule 7 is a protein called FAP54.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	1O	2632	Total	C	N	O	S	0	0
			19593	12378	3583	3552	80		

- Molecule 8 is a protein called HTH_9 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	1P	295	Total	C	N	O	S	0	0
			2266	1435	393	431	7		

- Molecule 9 is a protein called FAP297.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	1Q	437	Total	C	N	O	S	0	0
			2335	1409	460	464	2		

- Molecule 10 is a protein called FAP108.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	1R	361	Total	C	N	O	S	0	0
			2753	1724	494	524	11		
10	1S	264	Total	C	N	O	S	0	0
			1984	1255	355	368	6		

- Molecule 11 is a protein called FAP76.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	1T	972	Total	C	N	O	0	0
			4804	2857	975	972		

- Molecule 12 is a protein called Tubulin beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	1a	428	Total	C	N	O	S	0	0
			3359	2110	576	643	30		
12	1c	431	Total	C	N	O	S	0	0
			3379	2121	579	649	30		
12	1e	428	Total	C	N	O	S	0	0
			3359	2110	576	643	30		
12	1g	431	Total	C	N	O	S	0	0
			3379	2121	579	649	30		
12	2a	428	Total	C	N	O	S	0	0
			3359	2110	576	643	30		
12	2c	431	Total	C	N	O	S	0	0
			3379	2121	579	649	30		
12	2e	428	Total	C	N	O	S	0	0
			3359	2110	576	643	30		
12	2g	431	Total	C	N	O	S	0	0
			3379	2121	579	649	30		
12	3a	428	Total	C	N	O	S	0	0
			3359	2110	576	643	30		
12	3c	431	Total	C	N	O	S	0	0
			3379	2121	579	649	30		
12	3e	428	Total	C	N	O	S	0	0
			3359	2110	576	643	30		

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Mol	Chain	Residues	Atoms					AltConf	Trace
12	3g	431	Total	C	N	O	S	0	0
			3379	2121	579	649	30		
12	4a	428	Total	C	N	O	S	0	0
			3359	2110	576	643	30		
12	4c	431	Total	C	N	O	S	0	0
			3379	2121	579	649	30		
12	4e	428	Total	C	N	O	S	0	0
			3359	2110	576	643	30		
12	4g	431	Total	C	N	O	S	0	0
			3379	2121	579	649	30		
12	5a	428	Total	C	N	O	S	0	0
			3359	2110	576	643	30		
12	5c	431	Total	C	N	O	S	0	0
			3379	2121	579	649	30		
12	5e	428	Total	C	N	O	S	0	0
			3359	2110	576	643	30		
12	5g	431	Total	C	N	O	S	0	0
			3379	2121	579	649	30		
12	6a	428	Total	C	N	O	S	0	0
			3359	2110	576	643	30		
12	6c	431	Total	C	N	O	S	0	0
			3379	2121	579	649	30		
12	6e	428	Total	C	N	O	S	0	0
			3359	2110	576	643	30		
12	6g	431	Total	C	N	O	S	0	0
			3379	2121	579	649	30		
12	7a	428	Total	C	N	O	S	0	0
			3359	2110	576	643	30		
12	7c	431	Total	C	N	O	S	0	0
			3379	2121	579	649	30		
12	7e	428	Total	C	N	O	S	0	0
			3359	2110	576	643	30		
12	7g	431	Total	C	N	O	S	0	0
			3379	2121	579	649	30		
12	8a	428	Total	C	N	O	S	0	0
			3359	2110	576	643	30		
12	8c	431	Total	C	N	O	S	0	0
			3379	2121	579	649	30		
12	8e	428	Total	C	N	O	S	0	0
			3359	2110	576	643	30		
12	8g	431	Total	C	N	O	S	0	0
			3379	2121	579	649	30		

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Mol	Chain	Residues	Atoms					AltConf	Trace
12	9a	428	Total	C	N	O	S	0	0
			3359	2110	576	643	30		
12	9c	431	Total	C	N	O	S	0	0
			3379	2121	579	649	30		
12	9e	428	Total	C	N	O	S	0	0
			3359	2110	576	643	30		
12	9g	431	Total	C	N	O	S	0	0
			3379	2121	579	649	30		
12	Aa	428	Total	C	N	O	S	0	0
			3359	2110	576	643	30		
12	Ac	431	Total	C	N	O	S	0	0
			3379	2121	579	649	30		
12	Ae	428	Total	C	N	O	S	0	0
			3359	2110	576	643	30		
12	Ag	431	Total	C	N	O	S	0	0
			3379	2121	579	649	30		
12	Ba	428	Total	C	N	O	S	0	0
			3359	2110	576	643	30		
12	Bc	431	Total	C	N	O	S	0	0
			3379	2121	579	649	30		
12	Be	428	Total	C	N	O	S	0	0
			3359	2110	576	643	30		
12	Bg	431	Total	C	N	O	S	0	0
			3379	2121	579	649	30		
12	Ca	428	Total	C	N	O	S	0	0
			3359	2110	576	643	30		
12	Cc	431	Total	C	N	O	S	0	0
			3379	2121	579	649	30		
12	Ce	428	Total	C	N	O	S	0	0
			3359	2110	576	643	30		
12	Cg	431	Total	C	N	O	S	0	0
			3379	2121	579	649	30		
12	Da	428	Total	C	N	O	S	0	0
			3359	2110	576	643	30		
12	Dc	431	Total	C	N	O	S	0	0
			3379	2121	579	649	30		
12	De	428	Total	C	N	O	S	0	0
			3359	2110	576	643	30		
12	Dg	431	Total	C	N	O	S	0	0
			3379	2121	579	649	30		

- Molecule 13 is a protein called Tubulin alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	1b	430	Total	C	N	O	S	0	0
			3339	2115	568	634	22		
13	1d	430	Total	C	N	O	S	0	0
			3339	2115	568	634	22		
13	1f	430	Total	C	N	O	S	0	0
			3339	2115	568	634	22		
13	1h	430	Total	C	N	O	S	0	0
			3339	2115	568	634	22		
13	2b	430	Total	C	N	O	S	0	0
			3339	2115	568	634	22		
13	2d	430	Total	C	N	O	S	0	0
			3339	2115	568	634	22		
13	2f	430	Total	C	N	O	S	0	0
			3339	2115	568	634	22		
13	2h	430	Total	C	N	O	S	0	0
			3339	2115	568	634	22		
13	3b	430	Total	C	N	O	S	0	0
			3339	2115	568	634	22		
13	3d	430	Total	C	N	O	S	0	0
			3339	2115	568	634	22		
13	3f	430	Total	C	N	O	S	0	0
			3339	2115	568	634	22		
13	3h	430	Total	C	N	O	S	0	0
			3339	2115	568	634	22		
13	4b	430	Total	C	N	O	S	0	0
			3339	2115	568	634	22		
13	4d	430	Total	C	N	O	S	0	0
			3339	2115	568	634	22		
13	4f	430	Total	C	N	O	S	0	0
			3339	2115	568	634	22		
13	4h	430	Total	C	N	O	S	0	0
			3339	2115	568	634	22		
13	5b	430	Total	C	N	O	S	0	0
			3339	2115	568	634	22		
13	5d	430	Total	C	N	O	S	0	0
			3339	2115	568	634	22		
13	5f	430	Total	C	N	O	S	0	0
			3339	2115	568	634	22		
13	5h	430	Total	C	N	O	S	0	0
			3339	2115	568	634	22		
13	6b	430	Total	C	N	O	S	0	0
			3339	2115	568	634	22		
13	6d	430	Total	C	N	O	S	0	0
			3339	2115	568	634	22		

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Mol	Chain	Residues	Atoms					AltConf	Trace
13	6f	430	Total	C	N	O	S	0	0
			3339	2115	568	634	22		
13	6h	430	Total	C	N	O	S	0	0
			3339	2115	568	634	22		
13	7b	430	Total	C	N	O	S	0	0
			3339	2115	568	634	22		
13	7d	430	Total	C	N	O	S	0	0
			3339	2115	568	634	22		
13	7f	430	Total	C	N	O	S	0	0
			3339	2115	568	634	22		
13	7h	430	Total	C	N	O	S	0	0
			3339	2115	568	634	22		
13	8b	430	Total	C	N	O	S	0	0
			3339	2115	568	634	22		
13	8d	430	Total	C	N	O	S	0	0
			3339	2115	568	634	22		
13	8f	430	Total	C	N	O	S	0	0
			3339	2115	568	634	22		
13	8h	430	Total	C	N	O	S	0	0
			3339	2115	568	634	22		
13	9b	430	Total	C	N	O	S	0	0
			3339	2115	568	634	22		
13	9d	430	Total	C	N	O	S	0	0
			3339	2115	568	634	22		
13	9f	430	Total	C	N	O	S	0	0
			3339	2115	568	634	22		
13	9h	430	Total	C	N	O	S	0	0
			3339	2115	568	634	22		
13	Ab	430	Total	C	N	O	S	0	0
			3339	2115	568	634	22		
13	Ad	430	Total	C	N	O	S	0	0
			3339	2115	568	634	22		
13	Af	430	Total	C	N	O	S	0	0
			3339	2115	568	634	22		
13	Ah	430	Total	C	N	O	S	0	0
			3339	2115	568	634	22		
13	Bb	430	Total	C	N	O	S	0	0
			3339	2115	568	634	22		
13	Bd	430	Total	C	N	O	S	0	0
			3339	2115	568	634	22		
13	Bf	430	Total	C	N	O	S	0	0
			3339	2115	568	634	22		

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Mol	Chain	Residues	Atoms					AltConf	Trace
13	Bh	430	Total	C	N	O	S	0	0
			3339	2115	568	634	22		
13	Cb	430	Total	C	N	O	S	0	0
			3339	2115	568	634	22		
13	Cd	430	Total	C	N	O	S	0	0
			3339	2115	568	634	22		
13	Cf	430	Total	C	N	O	S	0	0
			3339	2115	568	634	22		
13	Ch	430	Total	C	N	O	S	0	0
			3339	2115	568	634	22		
13	Db	430	Total	C	N	O	S	0	0
			3339	2115	568	634	22		
13	Dd	430	Total	C	N	O	S	0	0
			3339	2115	568	634	22		
13	Df	430	Total	C	N	O	S	0	0
			3339	2115	568	634	22		
13	Dh	430	Total	C	N	O	S	0	0
			3339	2115	568	634	22		

- Molecule 14 is a protein called FAP275.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	2F	161	Total	C	N	O	S	0	0
			1228	758	238	228	4		
14	2G	161	Total	C	N	O	S	0	0
			1228	758	238	228	4		

- Molecule 15 is a protein called Unknown protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	2H	196	Total	C	N	O	0	0
			980	588	196	196		

- Molecule 16 is a protein called Unknown protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	2I	108	Total	C	N	O	0	0
			540	324	108	108		

- Molecule 17 is a protein called Unknown protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	2J	100	Total 500	C 300	N 100	O 100	0	0
17	2K	100	Total 500	C 300	N 100	O 100	0	0

- Molecule 18 is a protein called Unknown protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	2L	54	Total 270	C 162	N 54	O 54	0	0

- Molecule 19 is a protein called Unknown protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	2M	18	Total 90	C 54	N 18	O 18	0	0

- Molecule 20 is a protein called Unknown protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	2N	52	Total 260	C 156	N 52	O 52	0	0

- Molecule 21 is a protein called Unknown protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	2O	47	Total 235	C 141	N 47	O 47	0	0

- Molecule 22 is a protein called Unknown protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	2P	106	Total 530	C 318	N 106	O 106	0	0

- Molecule 23 is a protein called Unknown protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	2Q	110	Total 550	C 330	N 110	O 110	0	0
23	2R	110	Total 550	C 330	N 110	O 110	0	0

- Molecule 24 is a protein called FAP289.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	2S	105	Total	C	N	O		0	0
			522	312	105	105			
24	2T	109	Total	C	N	O	S	0	0
			868	530	176	159	3		
24	2U	111	Total	C	N	O	S	0	0
			882	539	178	162	3		
24	2V	109	Total	C	N	O	S	0	0
			868	530	176	159	3		

- Molecule 25 is a protein called Unknown protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	2W	167	Total	C	N	O	0	0
			835	501	167	167		
25	2X	167	Total	C	N	O	0	0
			835	501	167	167		

- Molecule 26 is a protein called Unknown protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	2Y	65	Total	C	N	O	0	0
			325	195	65	65		
26	2Z	65	Total	C	N	O	0	0
			325	195	65	65		

- Molecule 27 is a protein called Unknown protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	3A	36	Total	C	N	O	0	0
			180	108	36	36		
27	3B	36	Total	C	N	O	0	0
			180	108	36	36		

- Molecule 28 is a protein called FAP216.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	3C	61	Total	C	N	O	S	0	0
			480	291	96	92	1		

- Molecule 29 is a protein called FAP92.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	3E	87	Total	C	N	O	0	0
			671	406	142	123		

- Molecule 30 is a protein called FAP99.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	3F	444	Total	C	N	O	S	0	0
			3386	2041	688	650	7		
30	3G	240	Total	C	N	O	S	0	0
			1904	1142	391	367	4		

- Molecule 31 is a protein called FAP74.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	3H	308	Total	C	N	O	S	0	0
			1958	1190	379	387	2		
31	3I	401	Total	C	N	O	S	0	0
			3118	1904	606	601	7		

- Molecule 32 is a protein called FAP360.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	3J	372	Total	C	N	O	S	0	0
			2792	1758	501	519	14		
32	3K	367	Total	C	N	O	S	0	0
			2767	1745	495	513	14		

- Molecule 33 is a protein called FAP279.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	3L	197	Total	C	N	O	S	0	0
			1572	1001	278	287	6		

- Molecule 34 is a protein called FAP7.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	3M	387	Total	C	N	O	S	0	0
			2989	1825	572	580	12		
34	3N	392	Total	C	N	O	S	0	0
			3040	1861	578	589	12		
34	3O	353	Total	C	N	O	S	0	0
			2775	1696	535	532	12		

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Mol	Chain	Residues	Atoms					AltConf	Trace
34	3P	355	Total	C	N	O	S	0	0
			2795	1712	537	534	12		
34	3Q	353	Total	C	N	O	S	0	0
			2775	1696	535	532	12		
34	3R	358	Total	C	N	O	S	0	0
			2814	1723	540	539	12		
34	3S	387	Total	C	N	O	S	0	0
			2989	1825	572	580	12		
34	3T	392	Total	C	N	O	S	0	0
			3040	1861	578	589	12		
34	3U	355	Total	C	N	O	S	0	0
			2795	1712	537	534	12		
34	3V	410	Total	C	N	O	S	0	0
			3192	1954	611	614	13		
34	3W	411	Total	C	N	O	S	0	0
			3198	1956	612	617	13		
34	3X	358	Total	C	N	O	S	0	0
			2814	1723	540	539	12		
34	3Y	358	Total	C	N	O	S	0	0
			2814	1723	540	539	12		
34	3Z	358	Total	C	N	O	S	0	0
			2814	1723	540	539	12		
34	4A	410	Total	C	N	O	S	0	0
			3192	1954	611	614	13		
34	4B	411	Total	C	N	O	S	0	0
			3198	1956	612	617	13		

- Molecule 35 is a protein called FAP81.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	4C	634	Total	C	N	O	S	0	0
			4846	3052	870	902	22		

- Molecule 36 is a protein called FAP15.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	4D	295	Total	C	N	O	S	0	0
			2372	1515	397	442	18		

- Molecule 37 is a protein called PF6.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	4E	983	Total	C	N	O	S	0	0
			7227	4588	1245	1365	29		
37	4F	965	Total	C	N	O	S	0	0
			7056	4482	1212	1335	27		
37	4G	965	Total	C	N	O	S	0	0
			7056	4482	1212	1335	27		
37	4H	965	Total	C	N	O	S	0	0
			7056	4482	1212	1335	27		

- Molecule 38 is a protein called DPY30.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	4I	64	Total	C	N	O	S	0	0
			491	317	84	87	3		
38	4J	64	Total	C	N	O	S	0	0
			491	317	84	87	3		
38	4K	64	Total	C	N	O	S	0	0
			491	317	84	87	3		
38	4L	64	Total	C	N	O	S	0	0
			491	317	84	87	3		
38	4M	64	Total	C	N	O	S	0	0
			491	317	84	87	3		
38	4N	64	Total	C	N	O	S	0	0
			491	317	84	87	3		
38	4O	84	Total	C	N	O	S	0	0
			626	400	106	117	3		
38	4P	55	Total	C	N	O	S	0	0
			424	275	73	73	3		

- Molecule 39 is a protein called FAP305.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	4Q	216	Total	C	N	O	S	0	0
			1778	1127	344	302	5		
39	4R	216	Total	C	N	O	S	0	0
			1778	1127	344	302	5		
39	4S	216	Total	C	N	O	S	0	0
			1778	1127	344	302	5		

- Molecule 40 is a protein called FAP101.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	4T	602	Total 4494	C 2824	N 814	O 839	S 17	0	0
40	4U	602	Total 4494	C 2824	N 814	O 839	S 17	0	0
40	4V	602	Total 4494	C 2824	N 814	O 839	S 17	0	0

- Molecule 41 is a protein called FAP227.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	4W	124	Total 597	C 349	N 124	O 124	0	0
41	4X	124	Total 597	C 349	N 124	O 124	0	0
41	4Y	124	Total 597	C 349	N 124	O 124	0	0
41	4Z	124	Total 597	C 349	N 124	O 124	0	0
41	5A	123	Total 592	C 346	N 123	O 123	0	0
41	5B	123	Total 592	C 346	N 123	O 123	0	0
41	5C	123	Total 592	C 346	N 123	O 123	0	0
41	5D	123	Total 592	C 346	N 123	O 123	0	0

- Molecule 42 is a protein called FAP114.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	5E	216	Total 1562	C 993	N 272	O 292	S 5	0	0
42	5F	216	Total 1562	C 993	N 272	O 292	S 5	0	0
42	5G	216	Total 1562	C 993	N 272	O 292	S 5	0	0
42	5H	165	Total 1307	C 840	N 221	O 241	S 5	0	0

- Molecule 43 is a protein called FAP119.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	5I	211	Total	C	N	O	S	0	0
			1594	1020	276	292	6		
43	5J	211	Total	C	N	O	S	0	0
			1594	1020	276	292	6		
43	5K	211	Total	C	N	O	S	0	0
			1594	1020	276	292	6		
43	5L	211	Total	C	N	O	S	0	0
			1594	1020	276	292	6		

- Molecule 44 is a protein called Calmodulin.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	5M	142	Total	C	N	O		0	0
			699	415	142	142			
44	5N	142	Total	C	N	O		0	0
			699	415	142	142			
44	5O	142	Total	C	N	O		0	0
			699	415	142	142			
44	5Q	146	Total	C	N	O	S	0	0
			1153	710	186	248	9		
44	5R	146	Total	C	N	O	S	0	0
			1153	710	186	248	9		
44	5S	145	Total	C	N	O	S	0	0
			1144	705	185	245	9		
44	5T	145	Total	C	N	O	S	0	0
			1144	705	185	245	9		
44	5U	145	Total	C	N	O	S	0	0
			1144	705	185	245	9		
44	5V	149	Total	C	N	O	S	0	0
			1166	714	190	253	9		
44	5P	146	Total	C	N	O	S	0	0
			1153	710	186	248	9		

- Molecule 45 is a protein called Unknown protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
45	5W	137	Total	C	N	O	0	0
			685	411	137	137		
45	5X	137	Total	C	N	O	0	0
			685	411	137	137		
45	5Y	137	Total	C	N	O	0	0
			685	411	137	137		

- Molecule 46 is a protein called Unknown protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	5Z	181	Total	C	N	O	S	0	0
			978	603	191	181	3		

- Molecule 47 is a protein called CPC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	6A	1558	Total	C	N	O	S	0	0
			11821	7347	2181	2246	47		
47	6B	1558	Total	C	N	O	S	0	0
			11821	7347	2181	2246	47		

- Molecule 48 is a protein called FAP246.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	6E	904	Total	C	N	O	S	0	0
			6892	4372	1255	1236	29		
48	6F	904	Total	C	N	O	S	0	0
			6892	4372	1255	1236	29		

- Molecule 49 is a protein called Phosphopyruvate hydratase.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	6G	476	Total	C	N	O	S	0	0
			3606	2262	615	707	22		
49	6H	476	Total	C	N	O	S	0	0
			3606	2262	615	707	22		
49	6I	476	Total	C	N	O	S	0	0
			3606	2262	615	707	22		
49	6J	476	Total	C	N	O	S	0	0
			3606	2262	615	707	22		

- Molecule 50 is a protein called Heat shock protein 70A.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	6K	609	Total	C	N	O	S	0	0
			4731	2963	821	927	20		
50	6L	609	Total	C	N	O	S	0	0
			4731	2963	821	927	20		

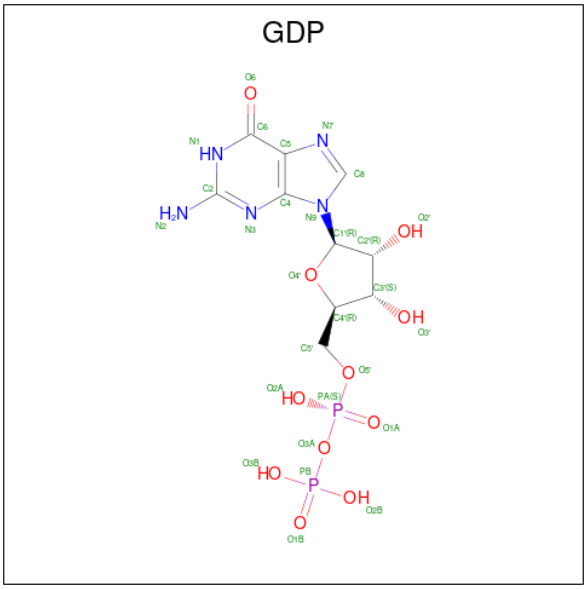
- Molecule 51 is a protein called FAP42.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	6M	1075	Total	C	N	O	S	0	0
			8050	5038	1459	1512	41		
51	6N	1075	Total	C	N	O	S	0	0
			8050	5038	1459	1512	41		

- Molecule 52 is a protein called Unknown protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
52	6O	89	Total	C	N	O	0	0
			444	266	89	89		
52	6P	89	Total	C	N	O	0	0
			444	266	89	89		
52	6Q	89	Total	C	N	O	0	0
			444	266	89	89		

- Molecule 53 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					AltConf
53	1a	1	Total	C	N	O	P	0
			28	10	5	11	2	
53	1c	1	Total	C	N	O	P	0
			28	10	5	11	2	
53	1e	1	Total	C	N	O	P	0
			28	10	5	11	2	
53	1g	1	Total	C	N	O	P	0
			28	10	5	11	2	
53	2a	1	Total	C	N	O	P	0
			28	10	5	11	2	

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Mol	Chain	Residues	Atoms					AltConf
53	2c	1	Total	C	N	O	P	0
			28	10	5	11	2	
53	2e	1	Total	C	N	O	P	0
			28	10	5	11	2	
53	2g	1	Total	C	N	O	P	0
			28	10	5	11	2	
53	3a	1	Total	C	N	O	P	0
			28	10	5	11	2	
53	3c	1	Total	C	N	O	P	0
			28	10	5	11	2	
53	3e	1	Total	C	N	O	P	0
			28	10	5	11	2	
53	3g	1	Total	C	N	O	P	0
			28	10	5	11	2	
53	4a	1	Total	C	N	O	P	0
			28	10	5	11	2	
53	4c	1	Total	C	N	O	P	0
			28	10	5	11	2	
53	4e	1	Total	C	N	O	P	0
			28	10	5	11	2	
53	4g	1	Total	C	N	O	P	0
			28	10	5	11	2	
53	5a	1	Total	C	N	O	P	0
			28	10	5	11	2	
53	5c	1	Total	C	N	O	P	0
			28	10	5	11	2	
53	5e	1	Total	C	N	O	P	0
			28	10	5	11	2	
53	5g	1	Total	C	N	O	P	0
			28	10	5	11	2	
53	6a	1	Total	C	N	O	P	0
			28	10	5	11	2	
53	6c	1	Total	C	N	O	P	0
			28	10	5	11	2	
53	6e	1	Total	C	N	O	P	0
			28	10	5	11	2	
53	6g	1	Total	C	N	O	P	0
			28	10	5	11	2	
53	7a	1	Total	C	N	O	P	0
			28	10	5	11	2	
53	7c	1	Total	C	N	O	P	0
			28	10	5	11	2	

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Mol	Chain	Residues	Atoms					AltConf
53	7e	1	Total	C	N	O	P	0
			28	10	5	11	2	
53	7g	1	Total	C	N	O	P	0
			28	10	5	11	2	
53	8a	1	Total	C	N	O	P	0
			28	10	5	11	2	
53	8c	1	Total	C	N	O	P	0
			28	10	5	11	2	
53	8e	1	Total	C	N	O	P	0
			28	10	5	11	2	
53	8g	1	Total	C	N	O	P	0
			28	10	5	11	2	
53	9a	1	Total	C	N	O	P	0
			28	10	5	11	2	
53	9c	1	Total	C	N	O	P	0
			28	10	5	11	2	
53	9e	1	Total	C	N	O	P	0
			28	10	5	11	2	
53	9g	1	Total	C	N	O	P	0
			28	10	5	11	2	
53	Aa	1	Total	C	N	O	P	0
			28	10	5	11	2	
53	Ac	1	Total	C	N	O	P	0
			28	10	5	11	2	
53	Ae	1	Total	C	N	O	P	0
			28	10	5	11	2	
53	Ag	1	Total	C	N	O	P	0
			28	10	5	11	2	
53	Ba	1	Total	C	N	O	P	0
			28	10	5	11	2	
53	Bc	1	Total	C	N	O	P	0
			28	10	5	11	2	
53	Be	1	Total	C	N	O	P	0
			28	10	5	11	2	
53	Bg	1	Total	C	N	O	P	0
			28	10	5	11	2	
53	Ca	1	Total	C	N	O	P	0
			28	10	5	11	2	
53	Cc	1	Total	C	N	O	P	0
			28	10	5	11	2	
53	Ce	1	Total	C	N	O	P	0
			28	10	5	11	2	

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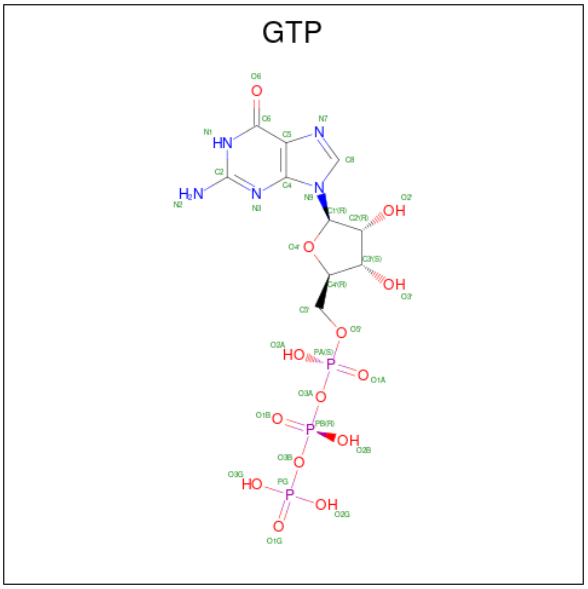
Mol	Chain	Residues	Atoms					AltConf
53	Cg	1	Total	C	N	O	P	0
			28	10	5	11	2	
53	Da	1	Total	C	N	O	P	0
			28	10	5	11	2	
53	Dc	1	Total	C	N	O	P	0
			28	10	5	11	2	
53	De	1	Total	C	N	O	P	0
			28	10	5	11	2	
53	Dg	1	Total	C	N	O	P	0
			28	10	5	11	2	

- Molecule 54 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					AltConf
54	1b	1	Total	C	N	O	P	0
			32	10	5	14	3	
54	1d	1	Total	C	N	O	P	0
			32	10	5	14	3	
54	1f	1	Total	C	N	O	P	0
			32	10	5	14	3	
54	1h	1	Total	C	N	O	P	0
			32	10	5	14	3	
54	2b	1	Total	C	N	O	P	0
			32	10	5	14	3	
54	2d	1	Total	C	N	O	P	0
			32	10	5	14	3	

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Mol	Chain	Residues	Atoms					AltConf
54	2f	1	Total	C	N	O	P	0
			32	10	5	14	3	
54	2h	1	Total	C	N	O	P	0
			32	10	5	14	3	
54	3c	1	Total	C	N	O	P	0
			32	10	5	14	3	
54	3d	1	Total	C	N	O	P	0
			32	10	5	14	3	
54	3f	1	Total	C	N	O	P	0
			32	10	5	14	3	
54	3h	1	Total	C	N	O	P	0
			32	10	5	14	3	
54	4b	1	Total	C	N	O	P	0
			32	10	5	14	3	
54	4d	1	Total	C	N	O	P	0
			32	10	5	14	3	
54	4f	1	Total	C	N	O	P	0
			32	10	5	14	3	
54	4h	1	Total	C	N	O	P	0
			32	10	5	14	3	
54	5c	1	Total	C	N	O	P	0
			32	10	5	14	3	
54	5d	1	Total	C	N	O	P	0
			32	10	5	14	3	
54	5f	1	Total	C	N	O	P	0
			32	10	5	14	3	
54	5h	1	Total	C	N	O	P	0
			32	10	5	14	3	
54	6c	1	Total	C	N	O	P	0
			32	10	5	14	3	
54	6e	1	Total	C	N	O	P	0
			32	10	5	14	3	
54	6g	1	Total	C	N	O	P	0
			32	10	5	14	3	
54	6h	1	Total	C	N	O	P	0
			32	10	5	14	3	
54	7b	1	Total	C	N	O	P	0
			32	10	5	14	3	
54	7e	1	Total	C	N	O	P	0
			32	10	5	14	3	
54	7f	1	Total	C	N	O	P	0
			32	10	5	14	3	

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Mol	Chain	Residues	Atoms					AltConf
54	7h	1	Total	C	N	O	P	0
			32	10	5	14	3	
54	8b	1	Total	C	N	O	P	0
			32	10	5	14	3	
54	8d	1	Total	C	N	O	P	0
			32	10	5	14	3	
54	8f	1	Total	C	N	O	P	0
			32	10	5	14	3	
54	8h	1	Total	C	N	O	P	0
			32	10	5	14	3	
54	9b	1	Total	C	N	O	P	0
			32	10	5	14	3	
54	9e	1	Total	C	N	O	P	0
			32	10	5	14	3	
54	9f	1	Total	C	N	O	P	0
			32	10	5	14	3	
54	9h	1	Total	C	N	O	P	0
			32	10	5	14	3	
54	Ab	1	Total	C	N	O	P	0
			32	10	5	14	3	
54	Ae	1	Total	C	N	O	P	0
			32	10	5	14	3	
54	Af	1	Total	C	N	O	P	0
			32	10	5	14	3	
54	Ah	1	Total	C	N	O	P	0
			32	10	5	14	3	
54	Bb	1	Total	C	N	O	P	0
			32	10	5	14	3	
54	Bd	1	Total	C	N	O	P	0
			32	10	5	14	3	
54	Bf	1	Total	C	N	O	P	0
			32	10	5	14	3	
54	Bh	1	Total	C	N	O	P	0
			32	10	5	14	3	
54	Cc	1	Total	C	N	O	P	0
			32	10	5	14	3	
54	Cd	1	Total	C	N	O	P	0
			32	10	5	14	3	
54	Cf	1	Total	C	N	O	P	0
			32	10	5	14	3	
54	Ch	1	Total	C	N	O	P	0
			32	10	5	14	3	

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Mol	Chain	Residues	Atoms					AltConf
54	Db	1	Total	C	N	O	P	0
			32	10	5	14	3	
54	Dd	1	Total	C	N	O	P	0
			32	10	5	14	3	
54	Df	1	Total	C	N	O	P	0
			32	10	5	14	3	
54	Dh	1	Total	C	N	O	P	0
			32	10	5	14	3	

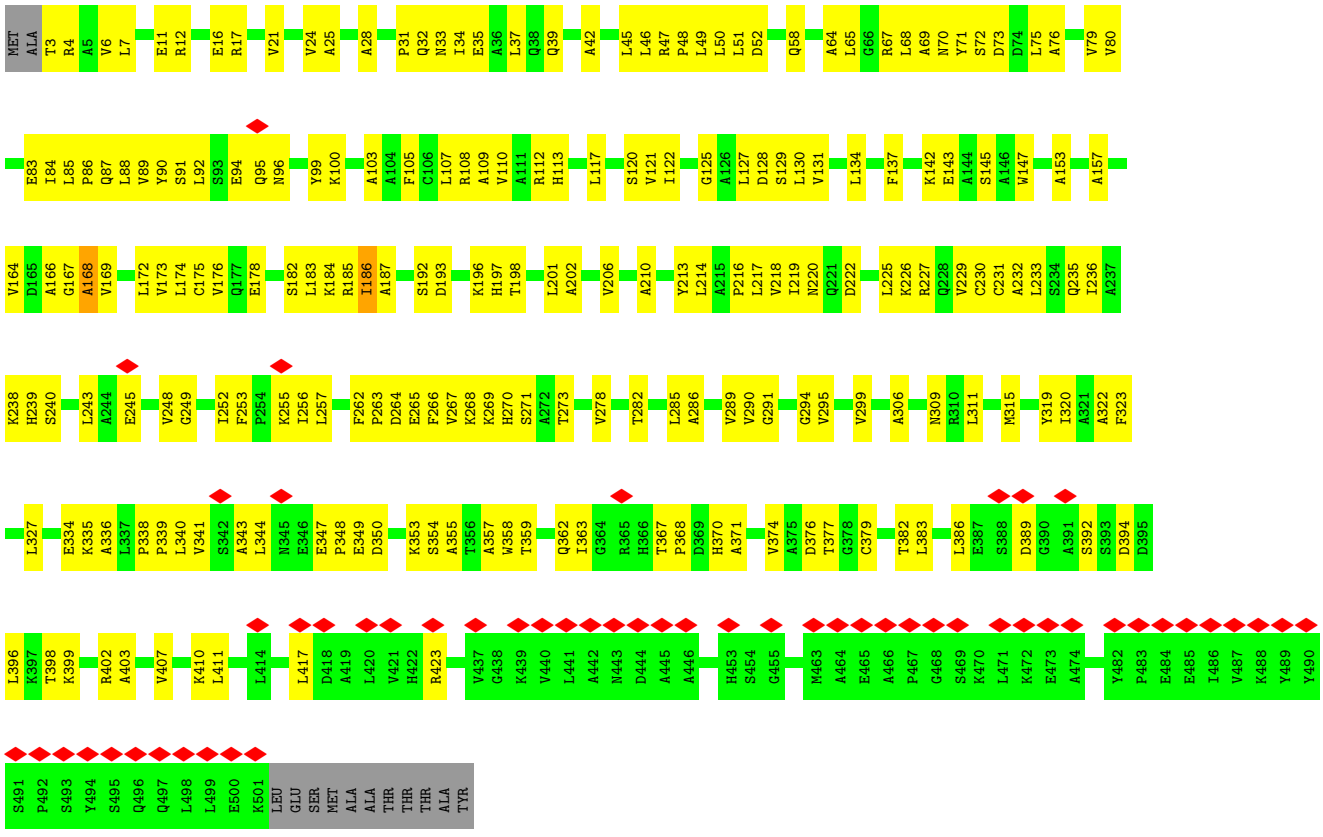
3 Residue-property plots (i)

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: PF16

Chain 0A:

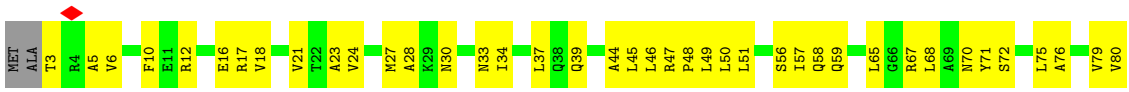


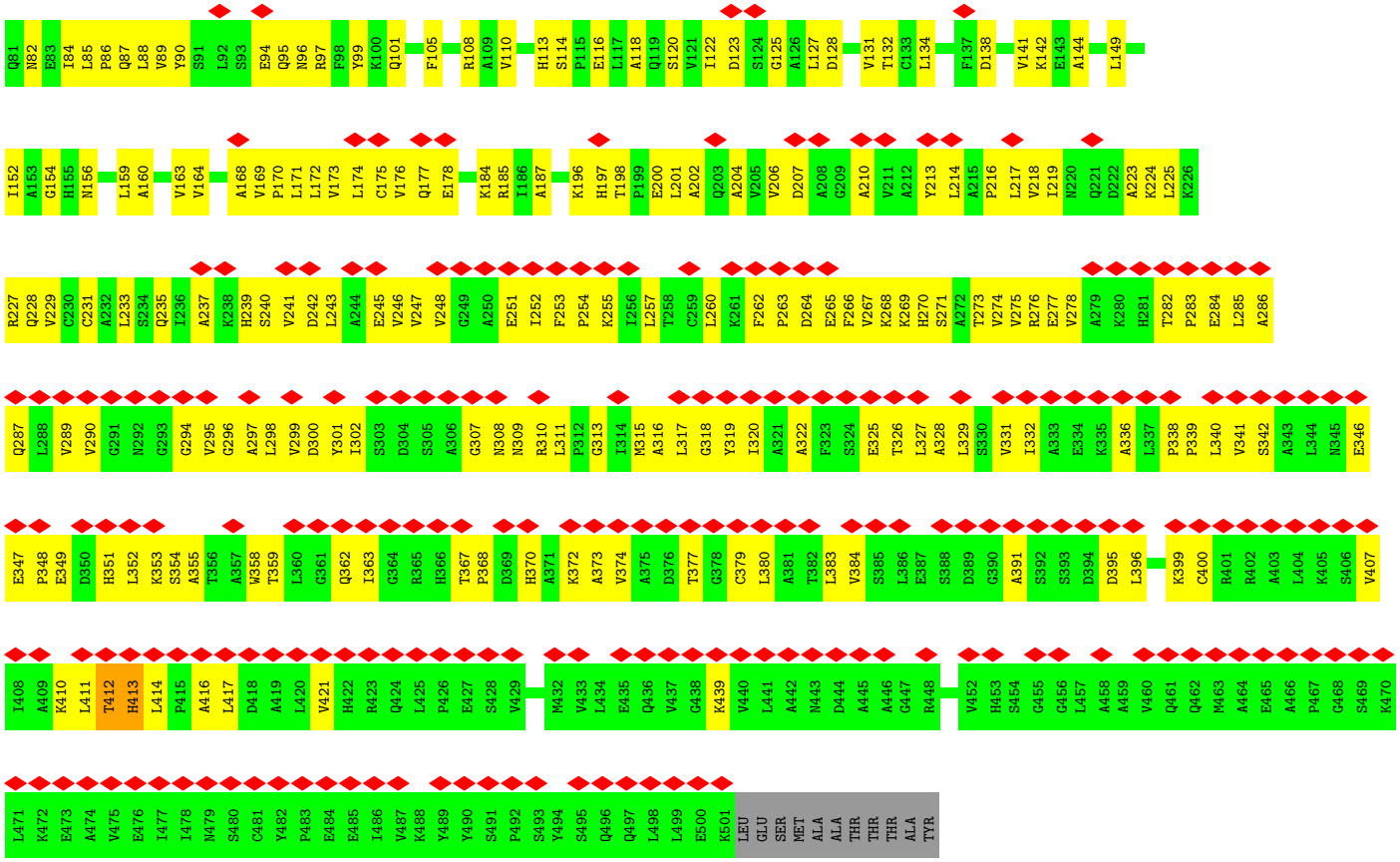


• Molecule 1: PF16

Chain 0B:



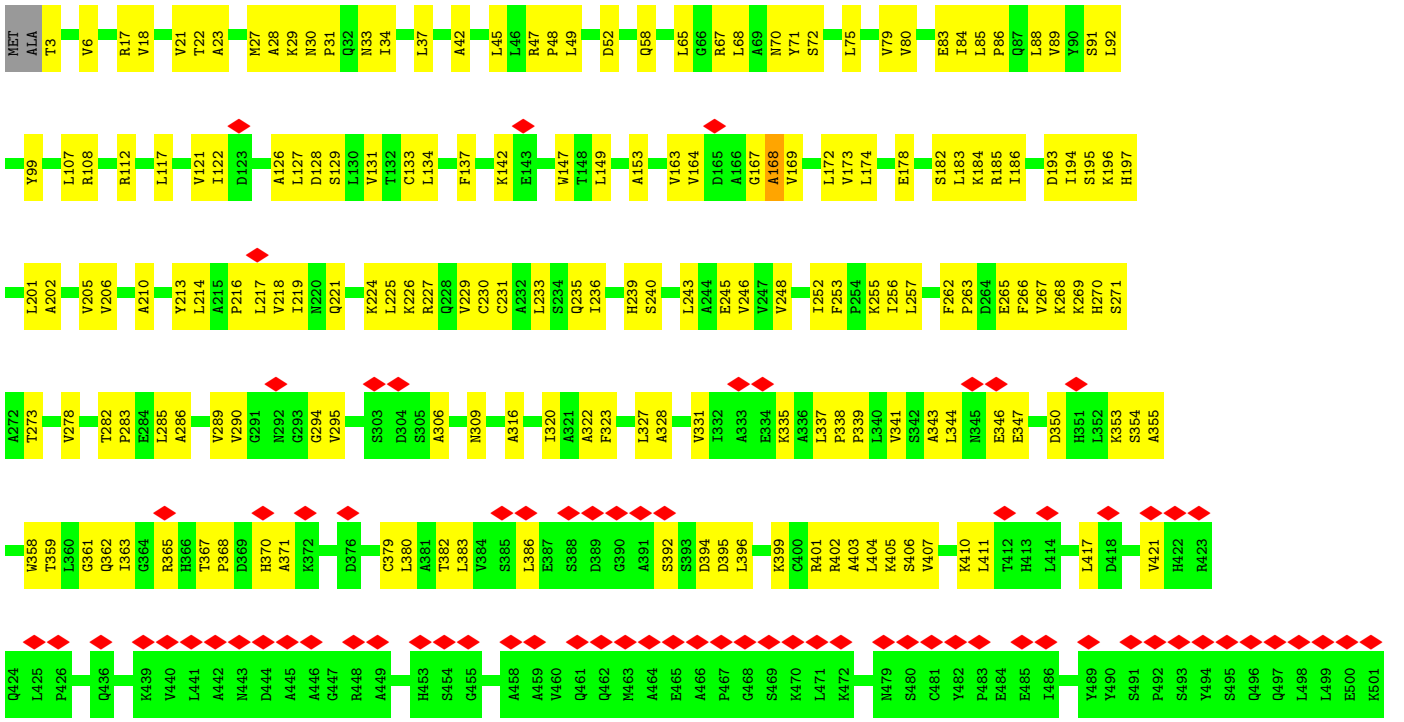




• Molecule 1: PF16

Chain 0C:



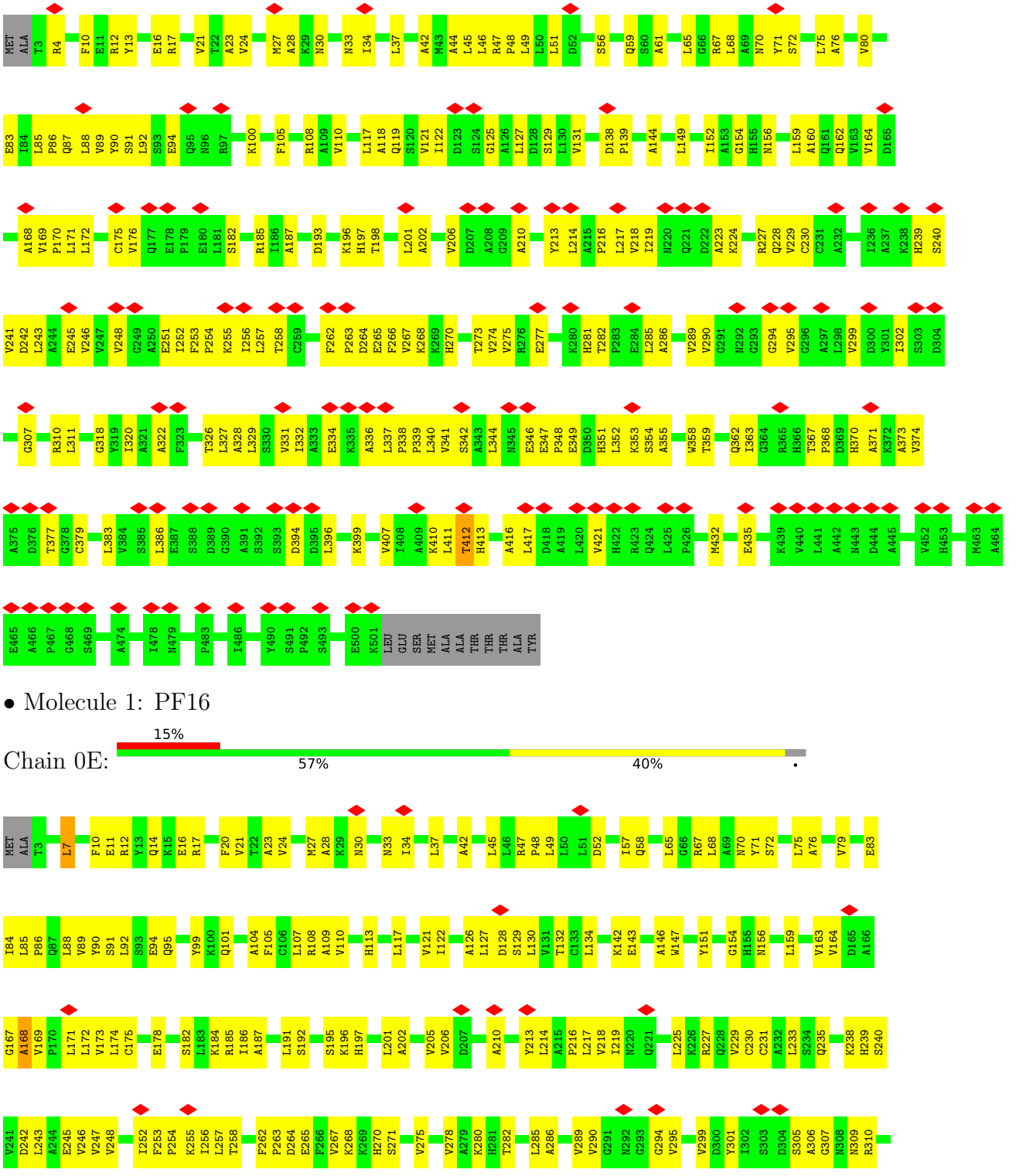




• Molecule 1: PF16

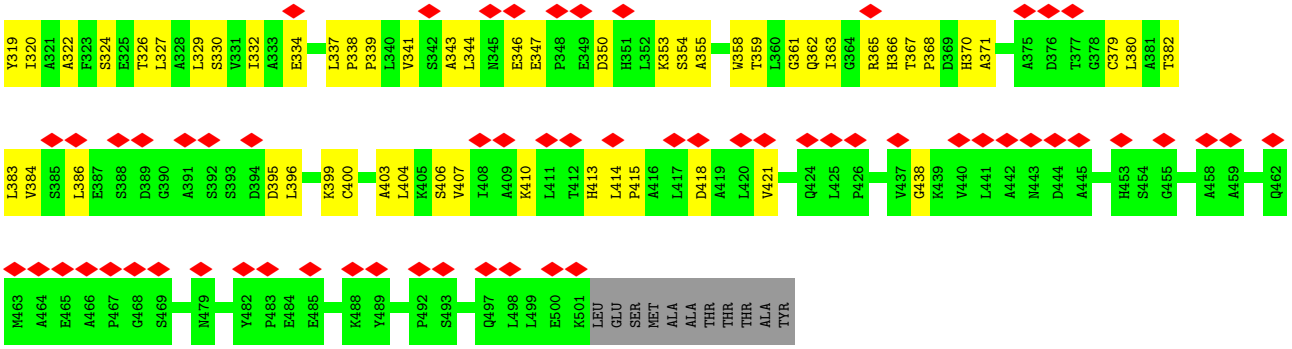
Chain 0D:





• Molecule 1: PF16

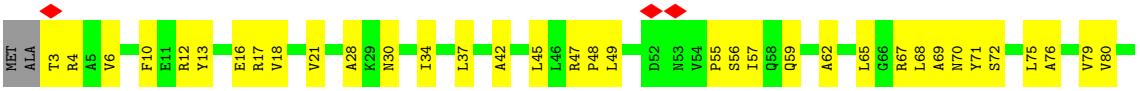
Chain 0E:

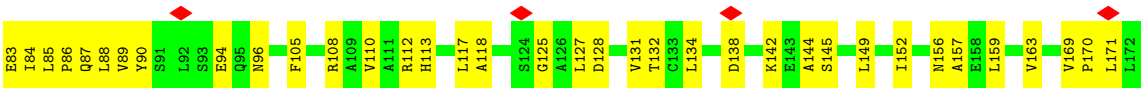


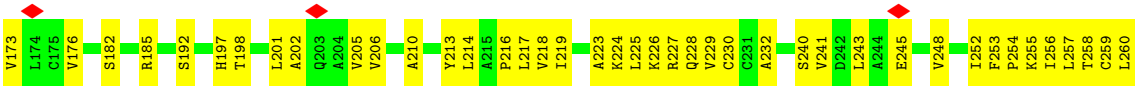
• Molecule 1: PF16

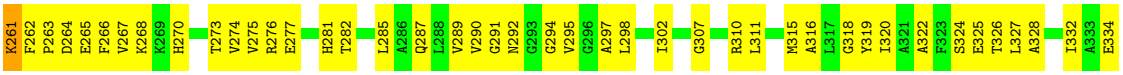
Chain 0F:

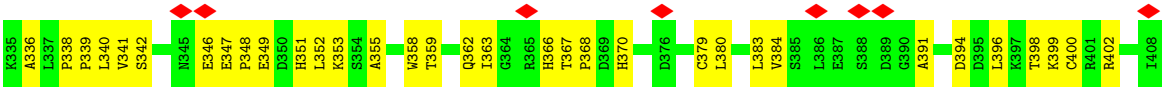


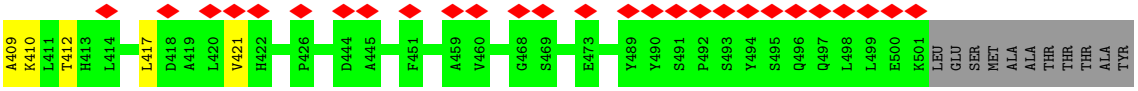








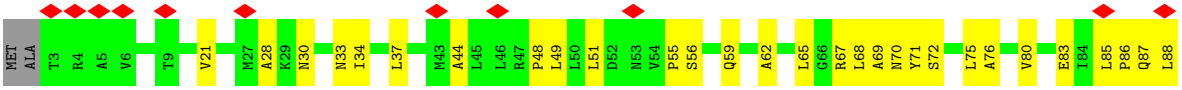


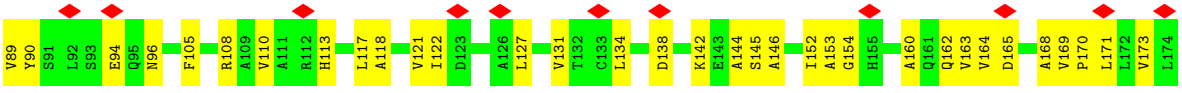


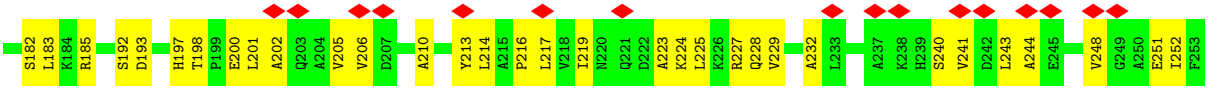
• Molecule 1: PF16

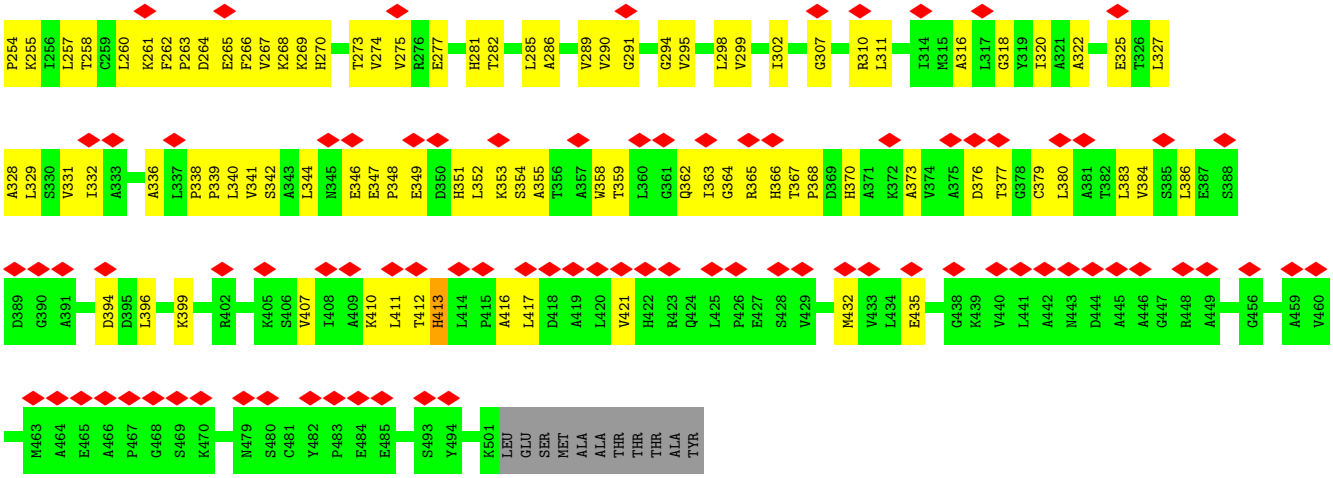
Chain 0G:







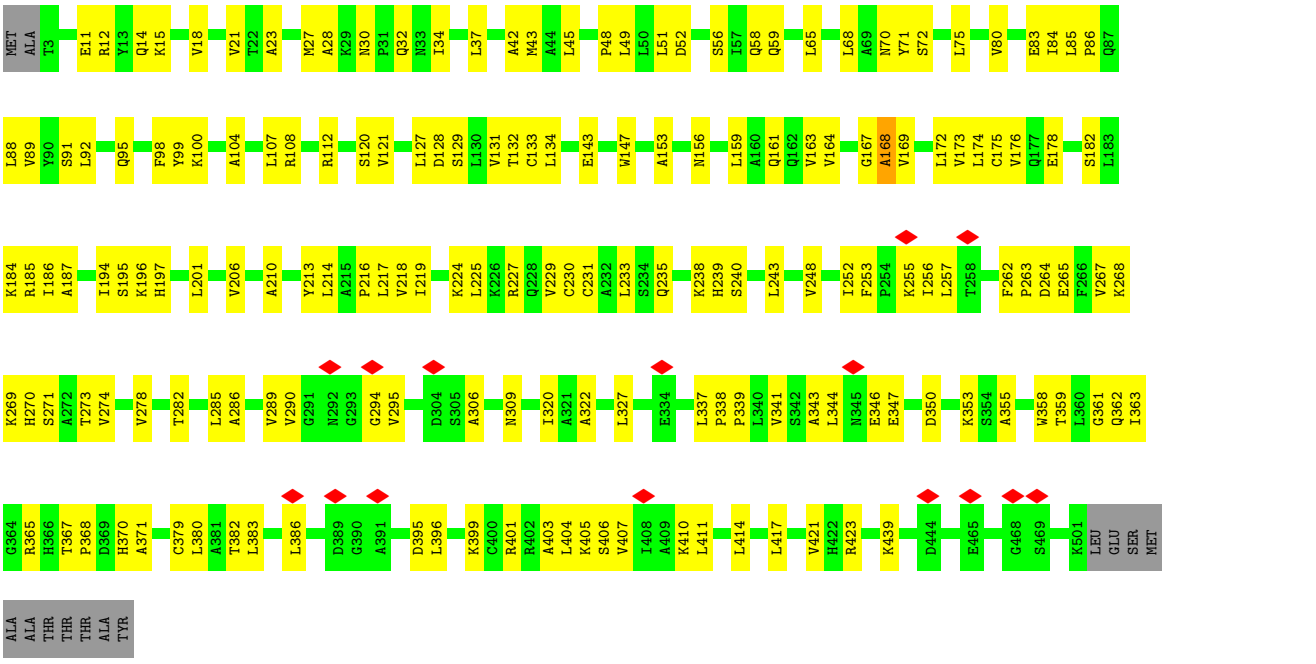




• Molecule 1: PF16

Chain 0L:

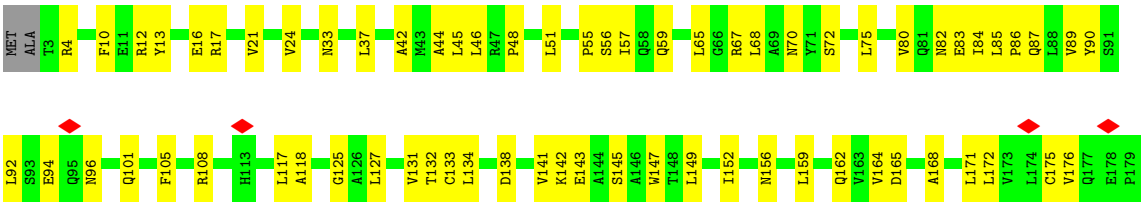


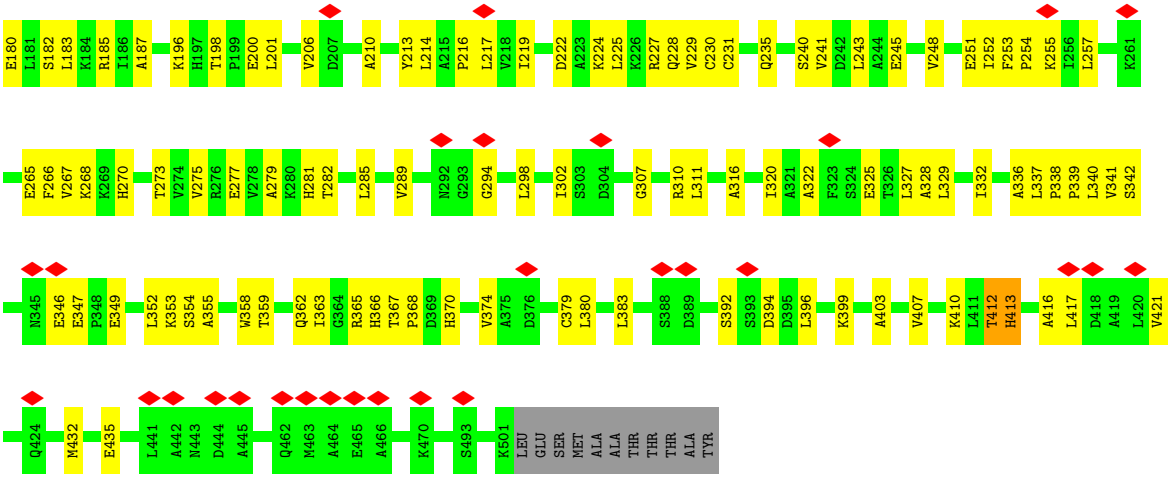


• Molecule 1: PF16

Chain 0M:



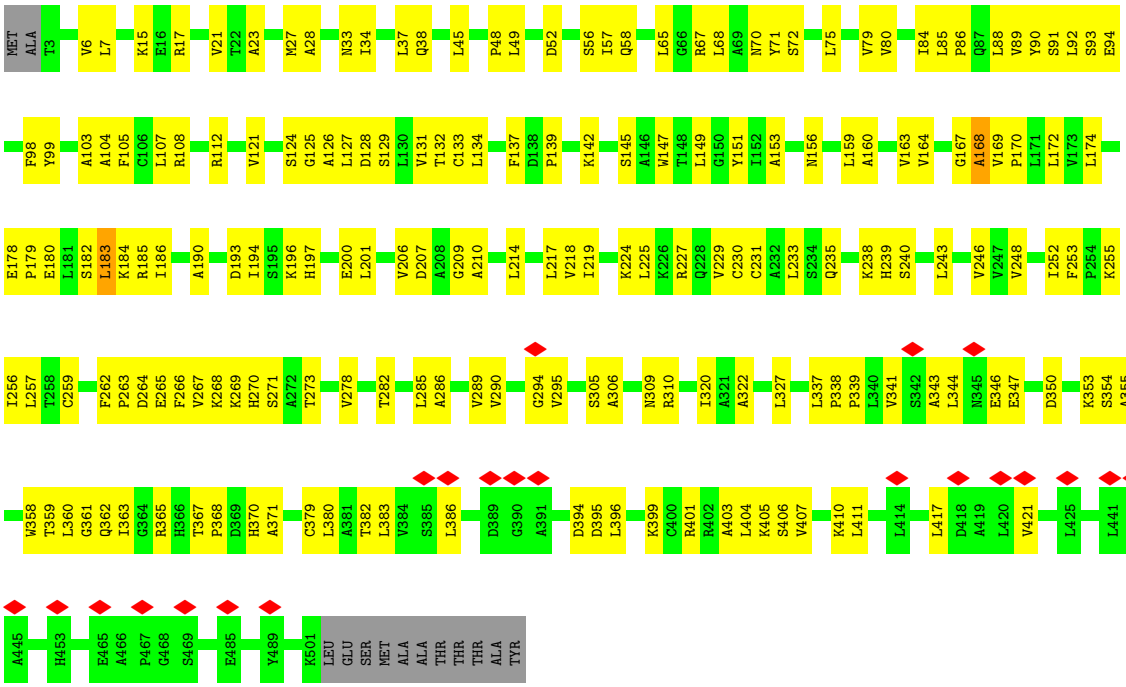




- Molecule 1: PF16

Chain 0N:

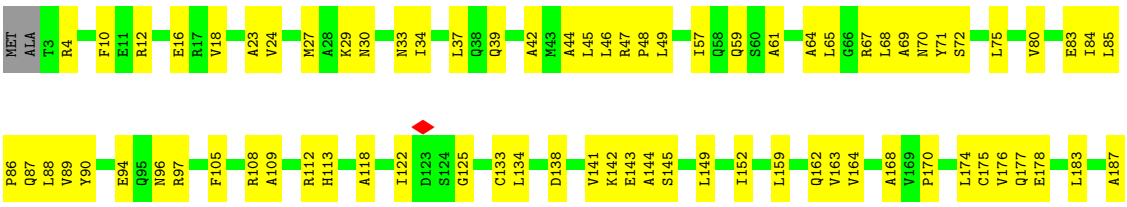


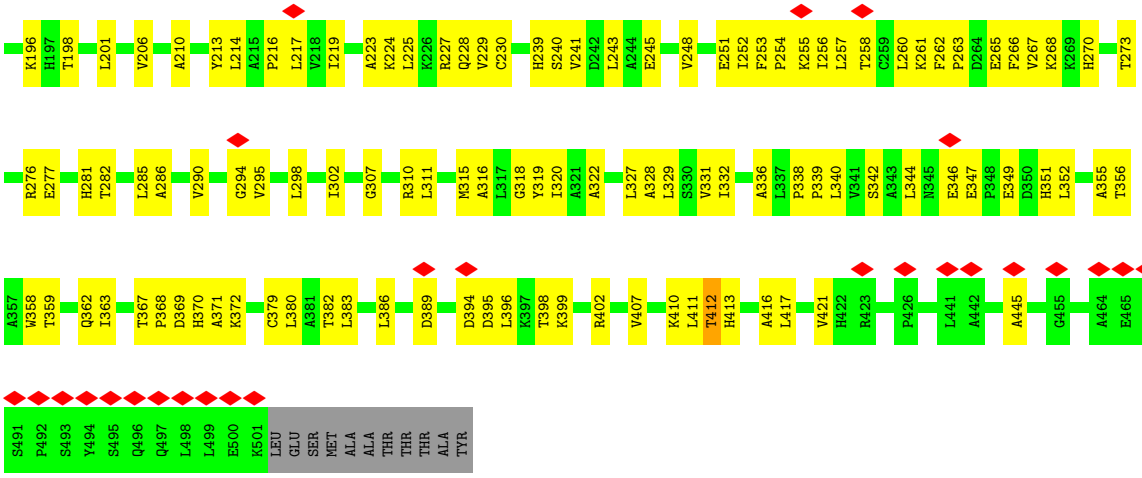


- Molecule 1: PF16

Chain 0O:



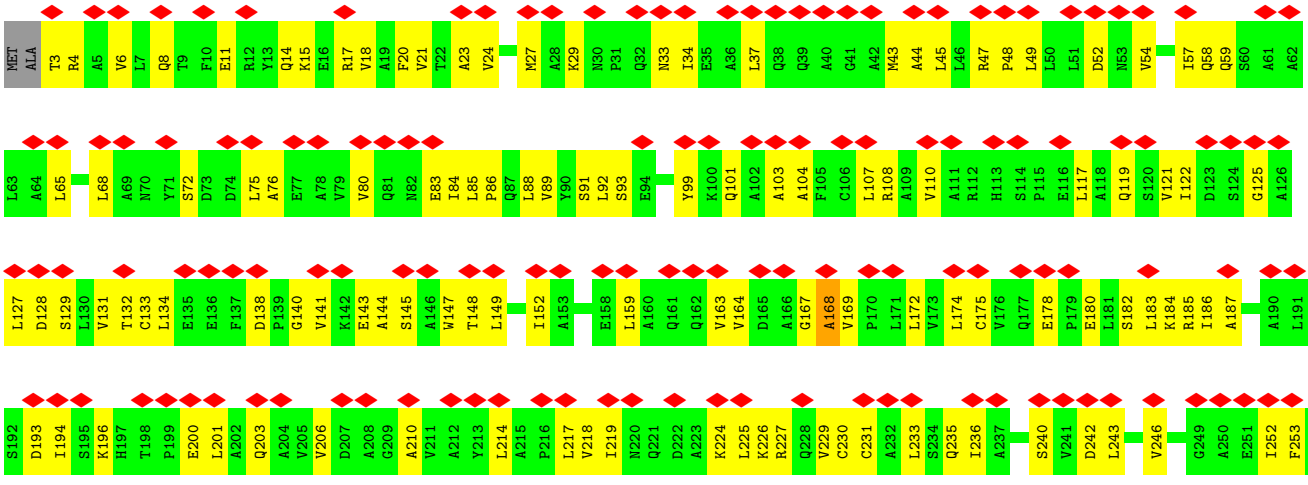




- Molecule 1: PF16

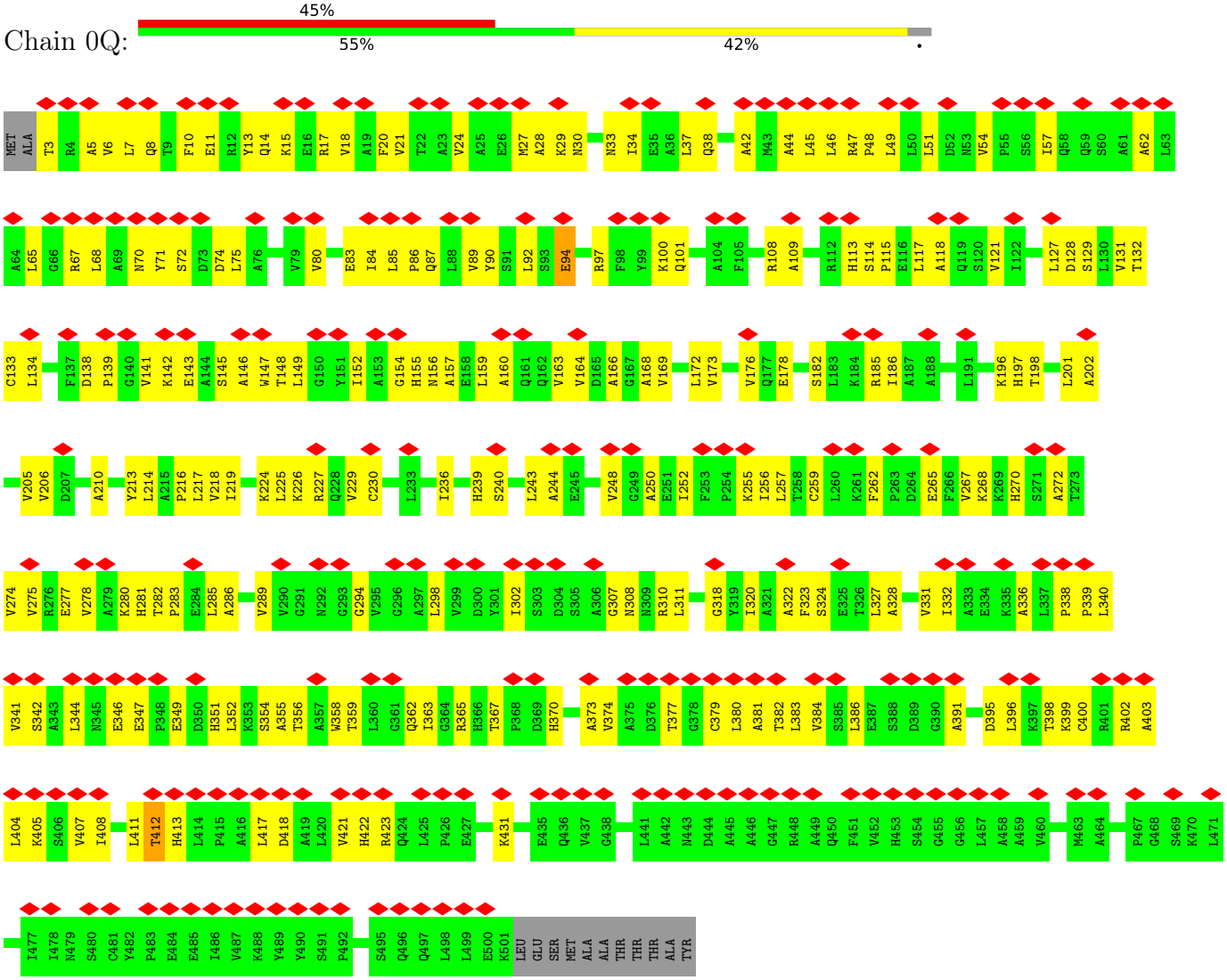
Chain 0P:





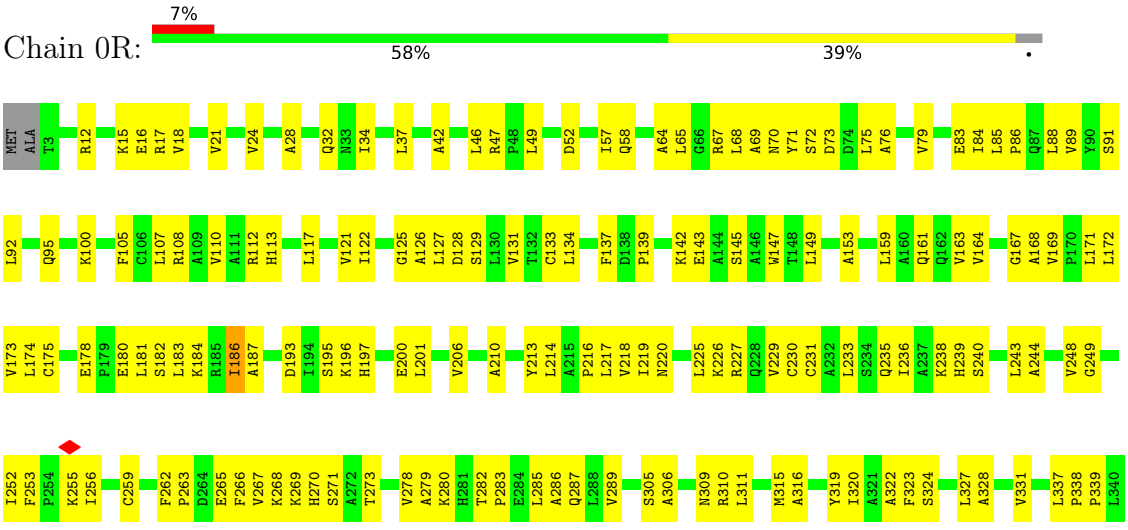
• Molecule 1: PF16

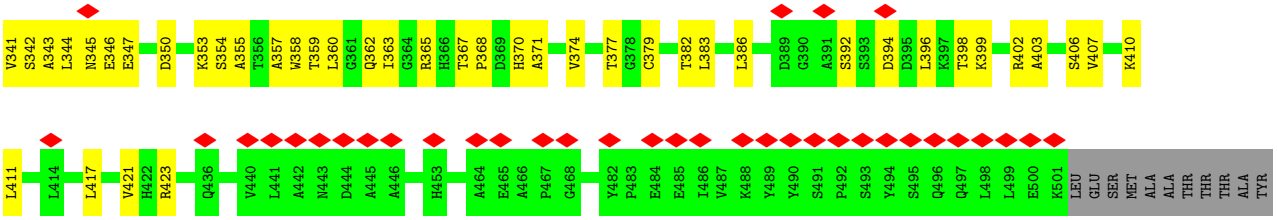
Chain 0Q:



• Molecule 1: PF16

Chain 0R:

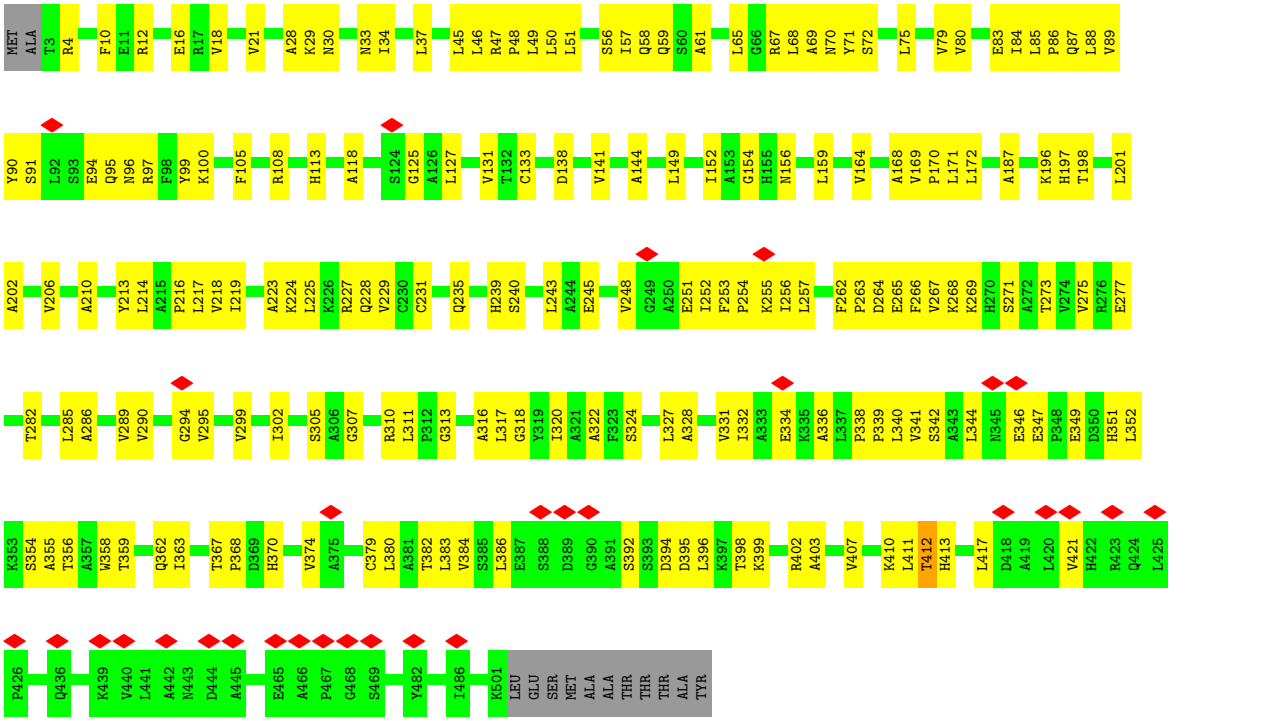




• Molecule 1: PF16

Chain 0S:

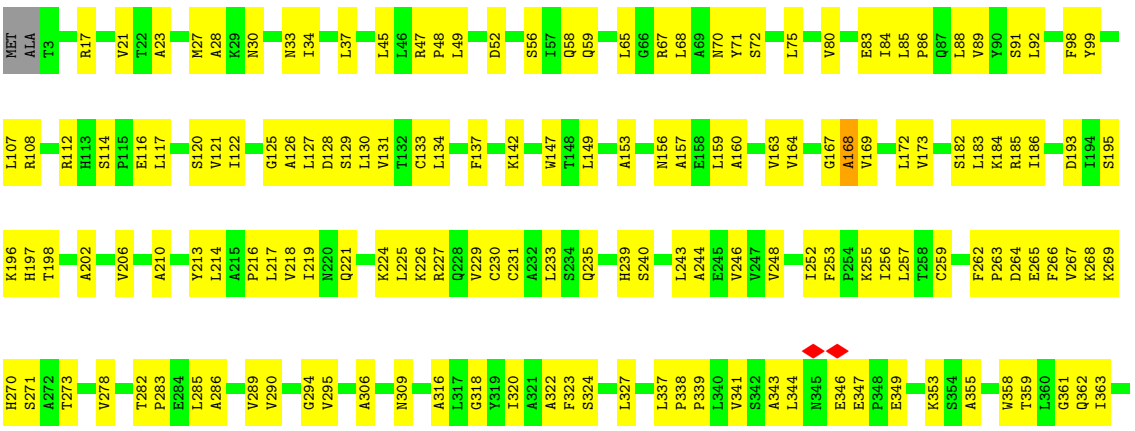


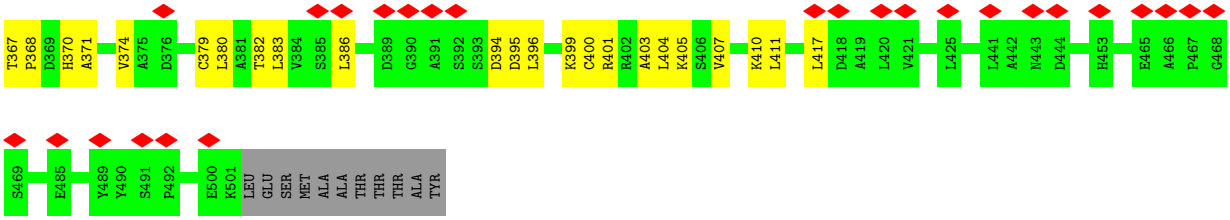


• Molecule 1: PF16

Chain 0T:



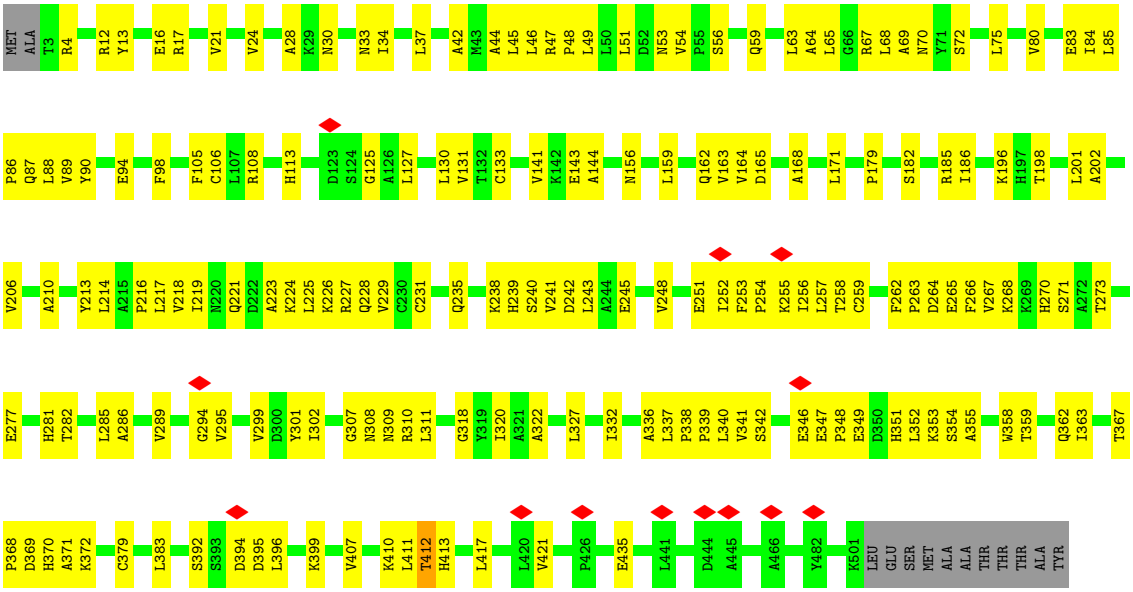




• Molecule 1: PF16

Chain 0U:

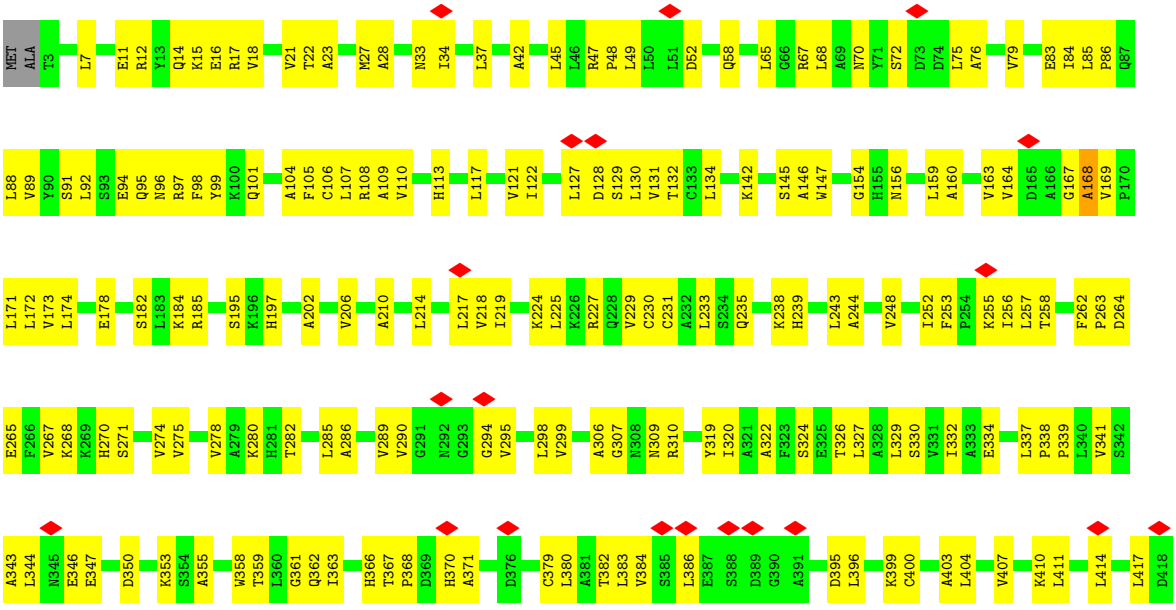


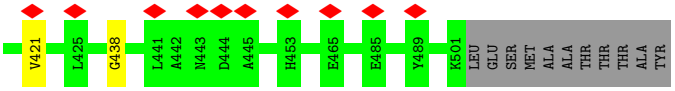


• Molecule 1: PF16

Chain 0V:

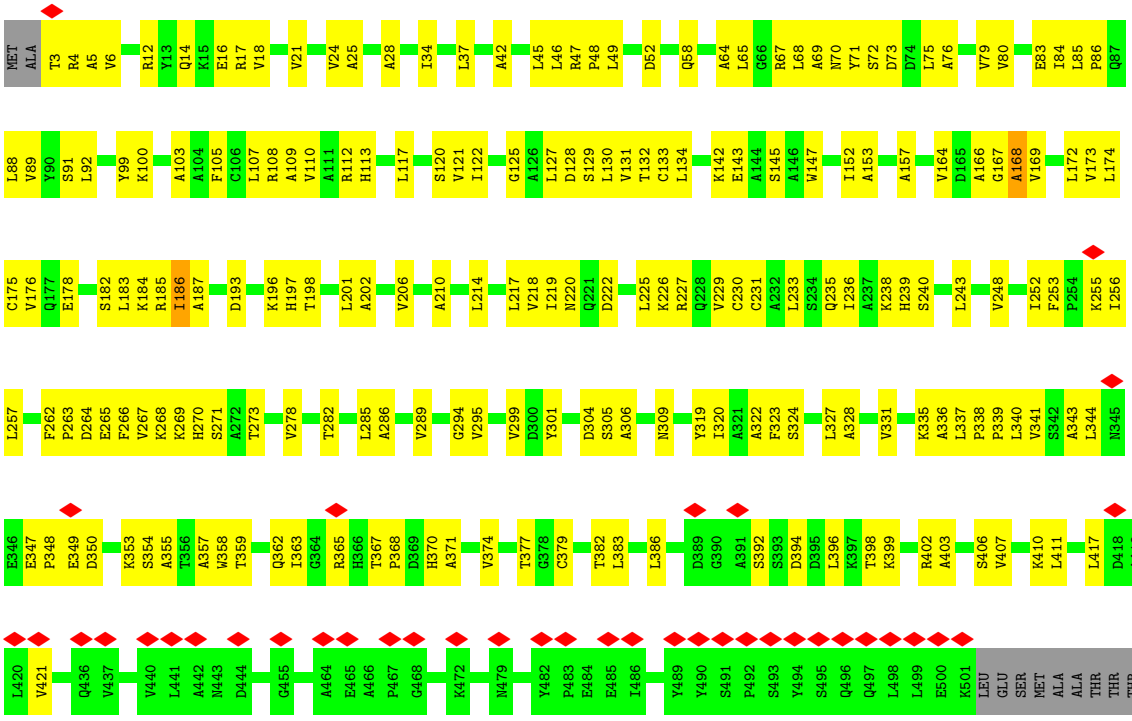






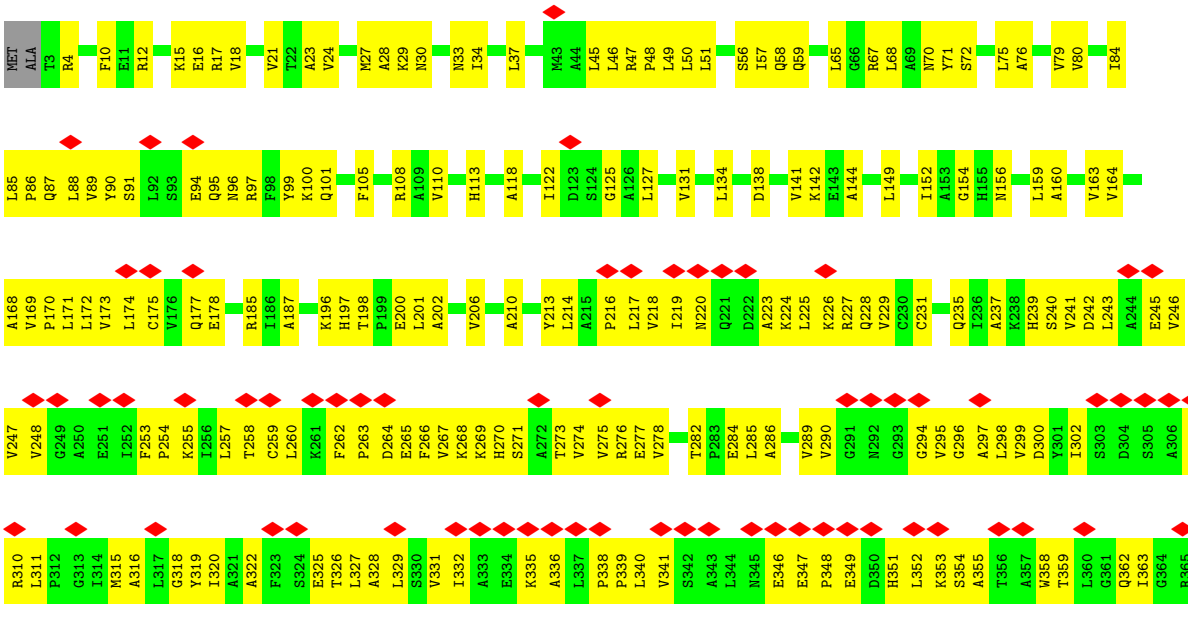
• Molecule 1: PF16

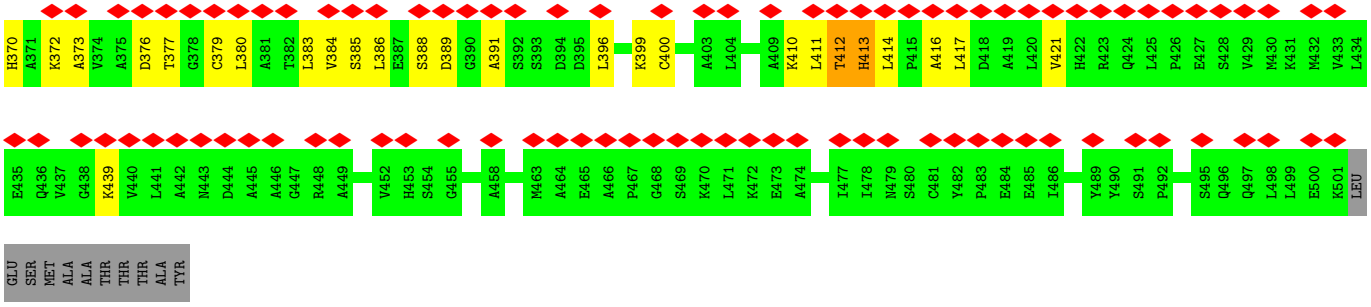




• Molecule 1: PF16



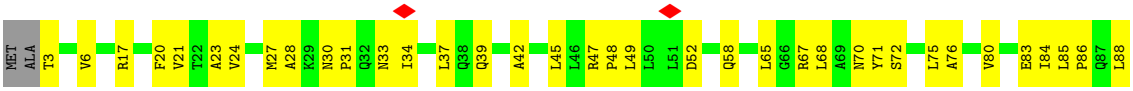


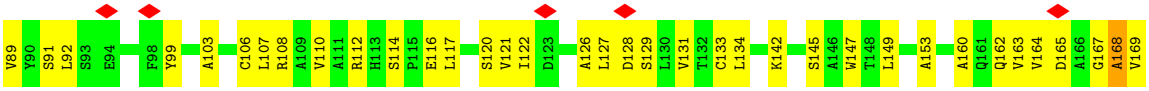


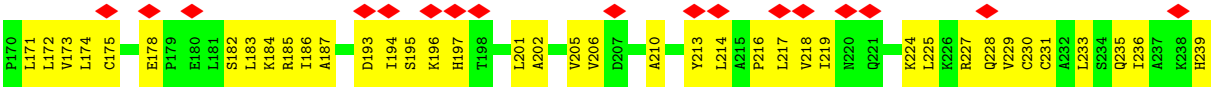
• Molecule 1: PF16

Chain 0Z:



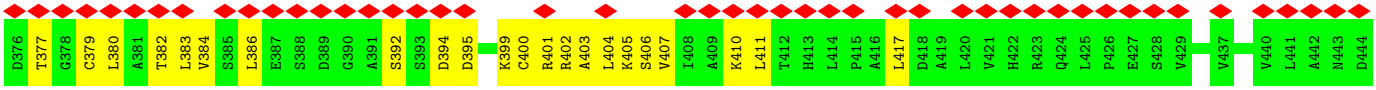


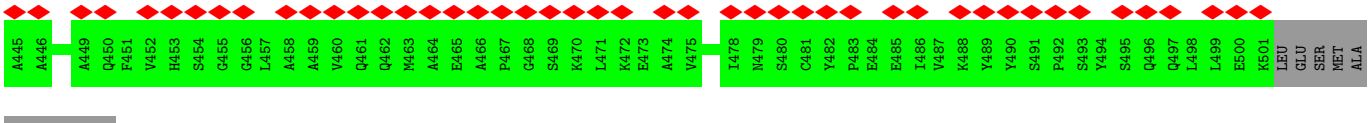








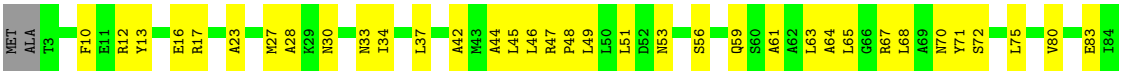


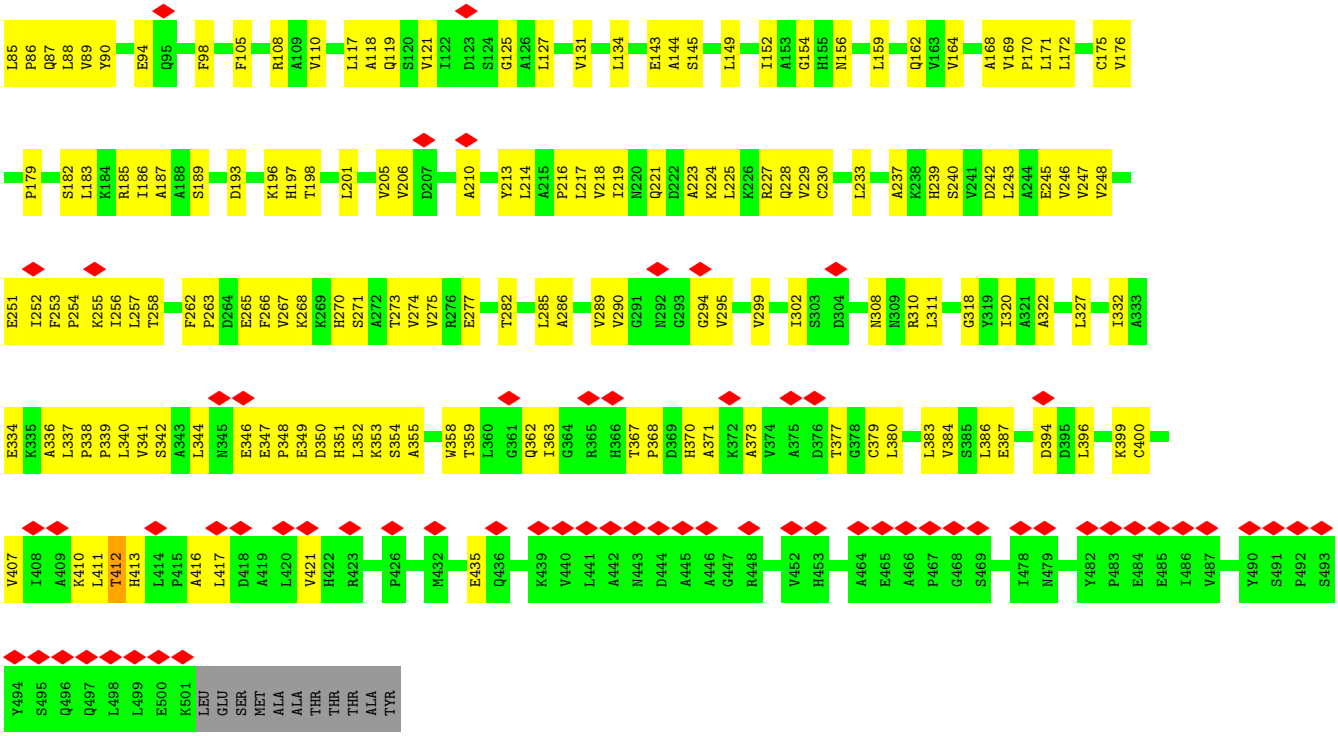


• Molecule 1: PF16

Chain 1A:



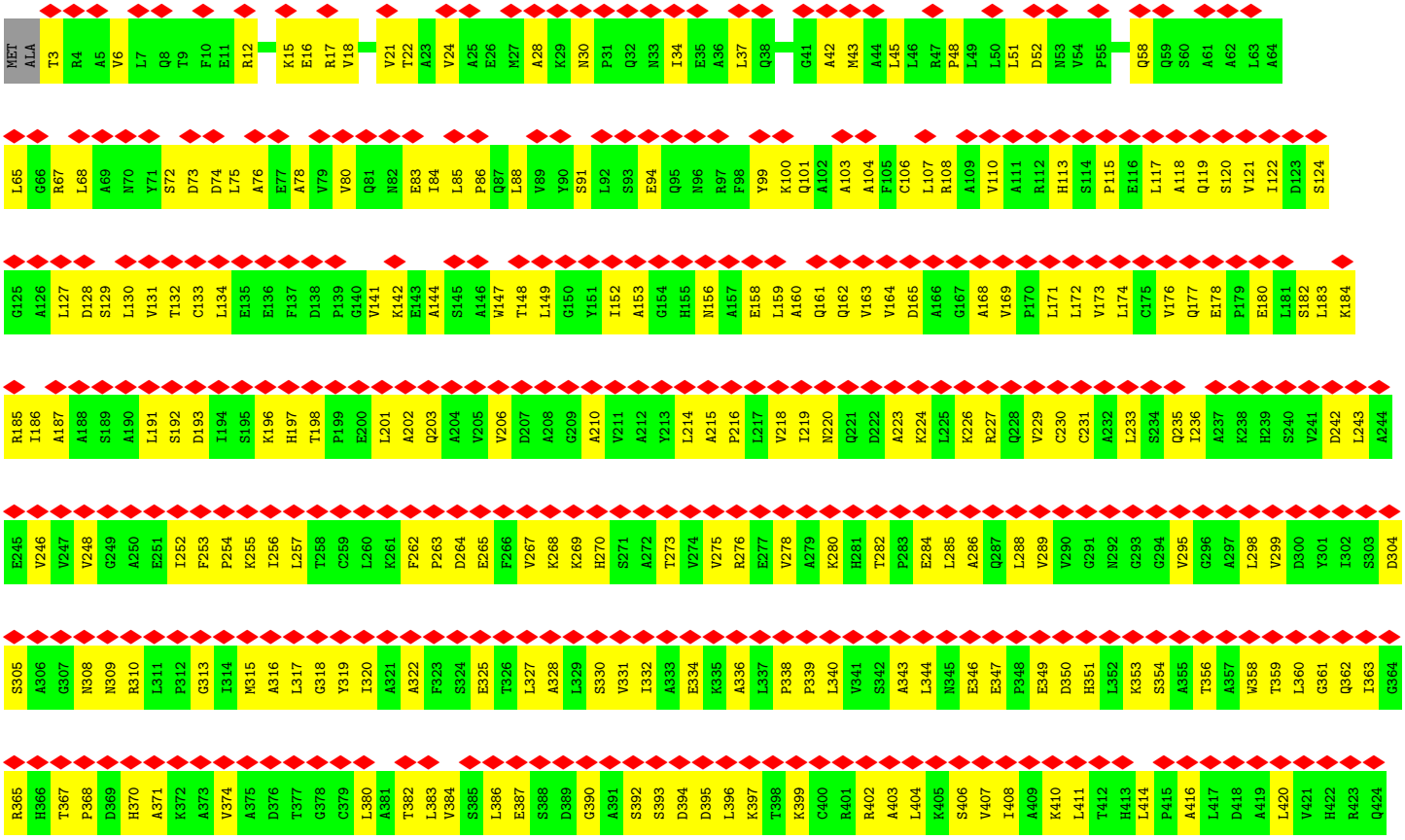




• Molecule 1: PF16

Chain 1B:



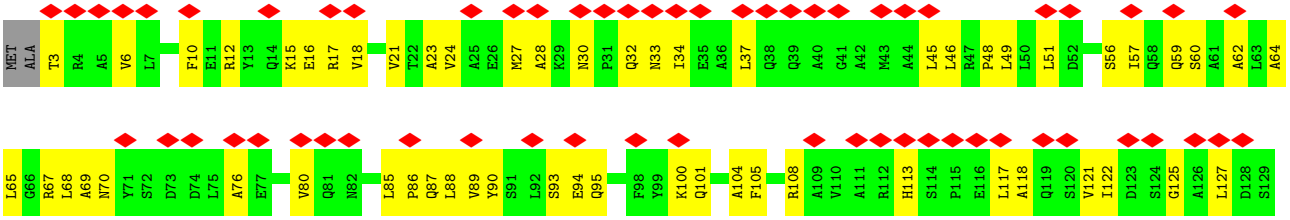




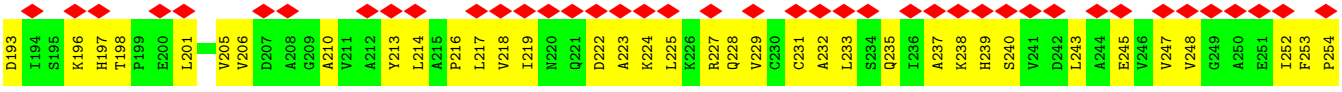
• Molecule 1: PF16

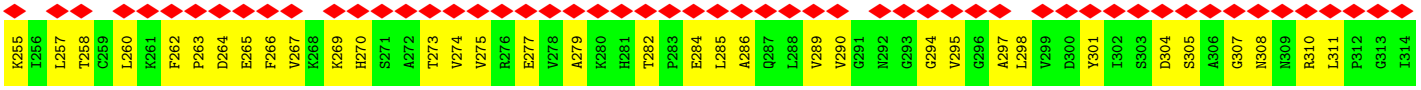
Chain 1C:

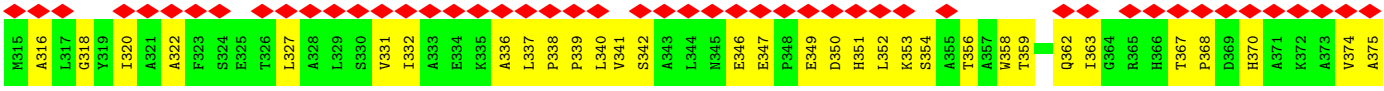


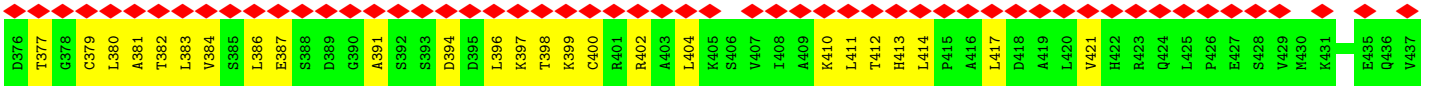


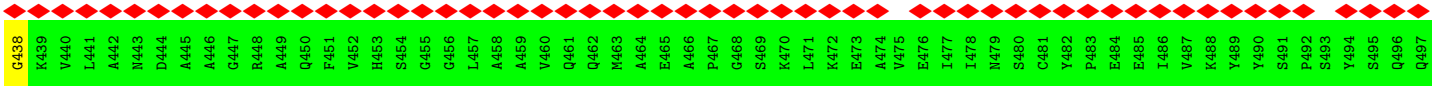


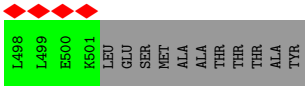








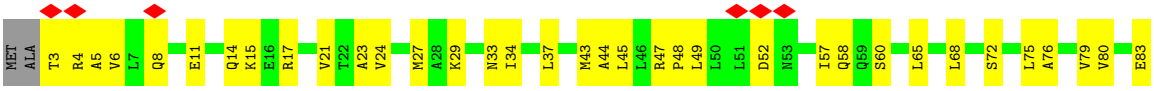


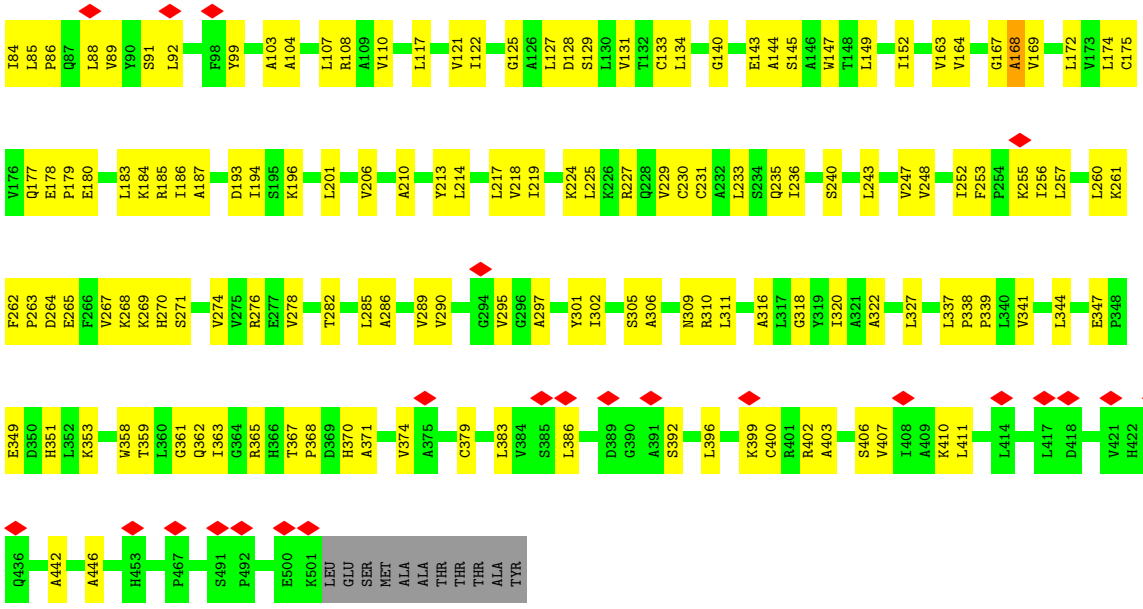


• Molecule 1: PF16

Chain 0H:



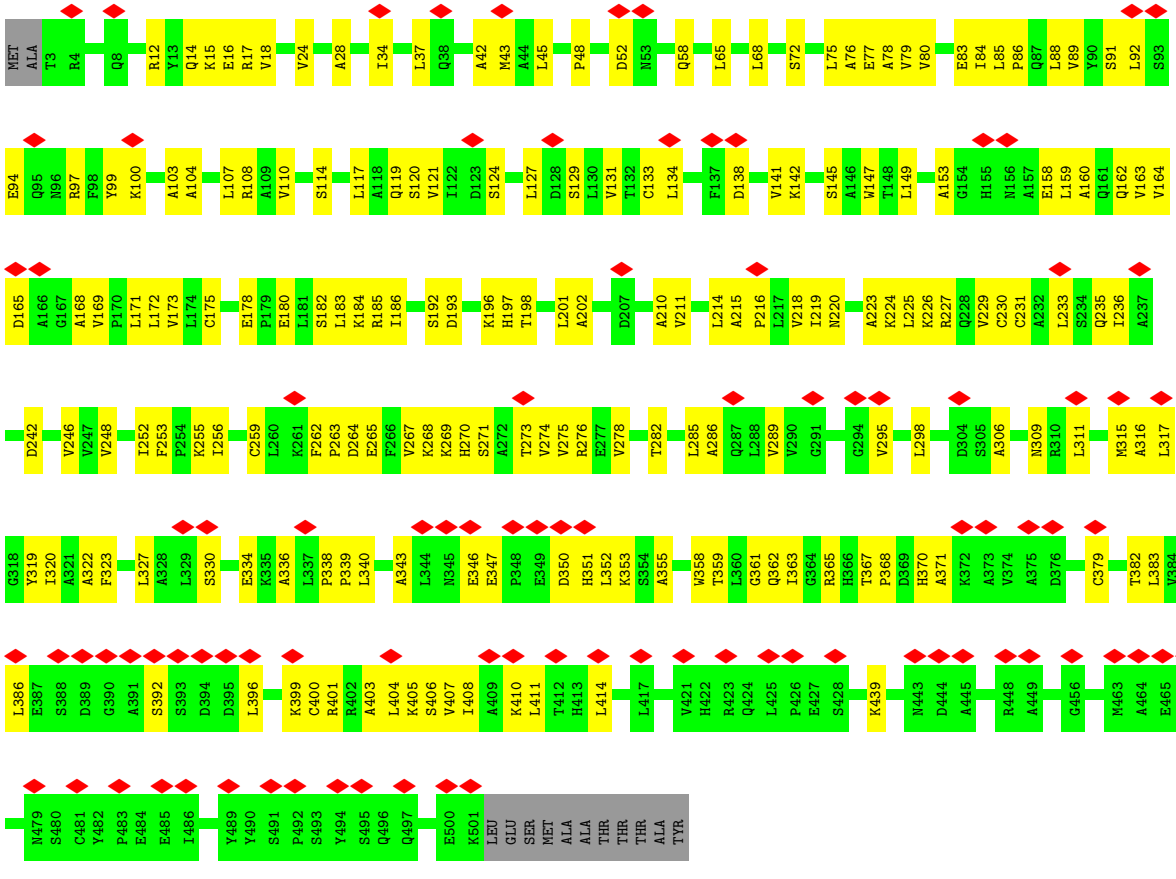




• Molecule 1: PF16

Chain 0J:

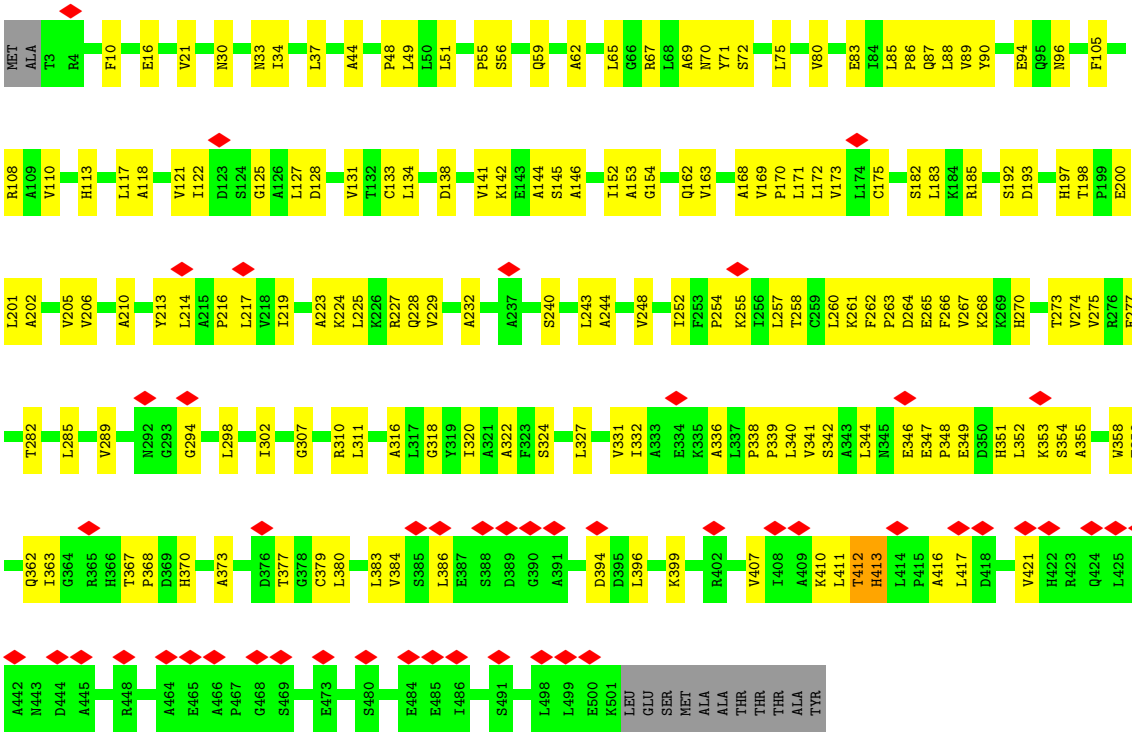




• Molecule 1: PF16

Chain 0W:

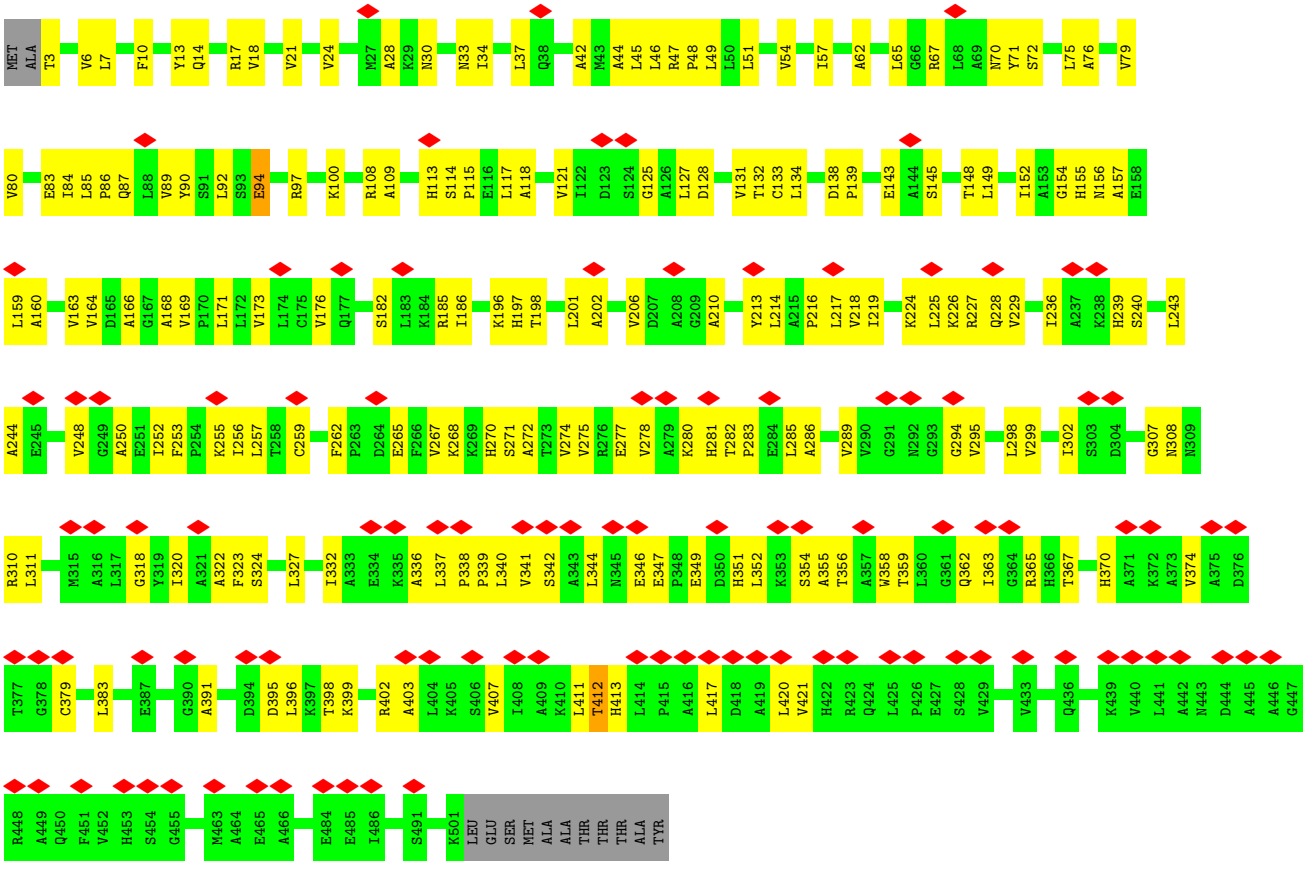




• Molecule 1: PF16

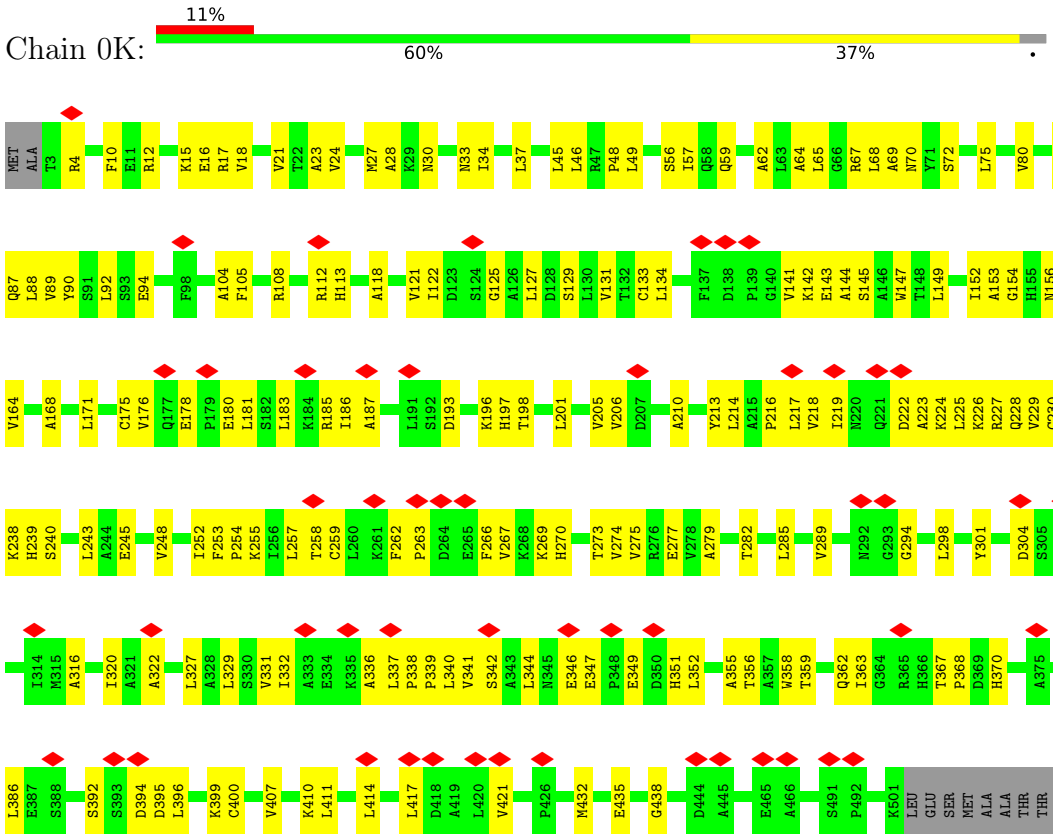
Chain 0I:





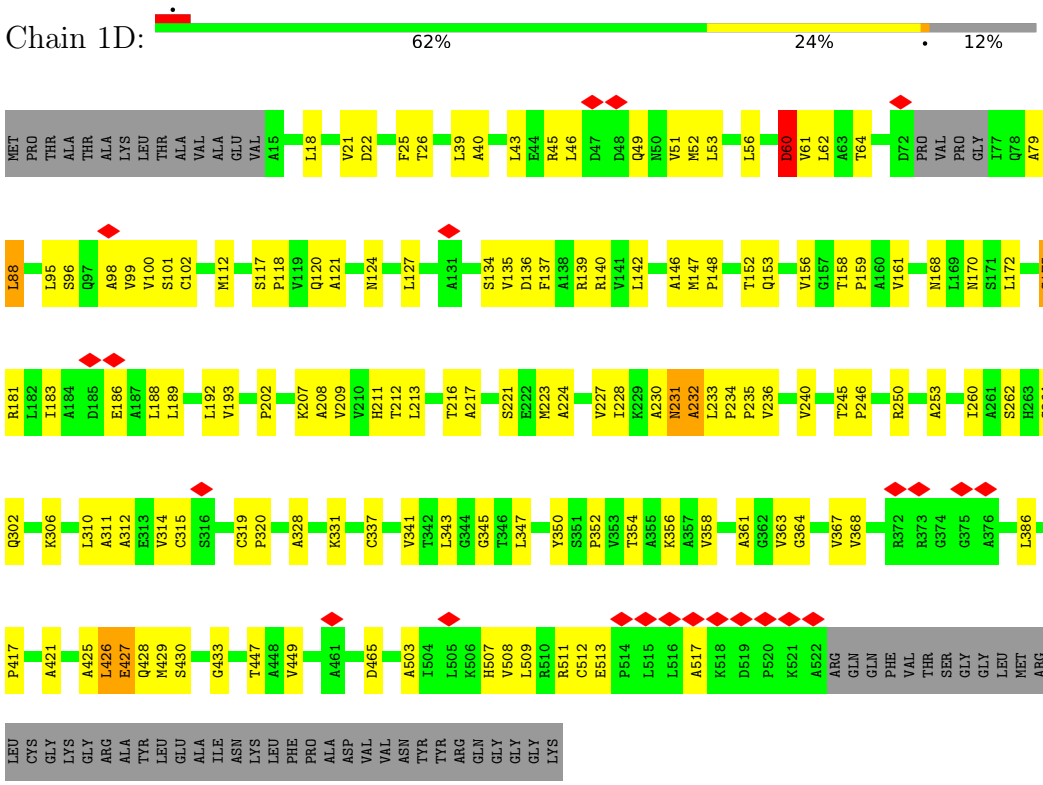
• Molecule 1: PF16

Chain 0K:



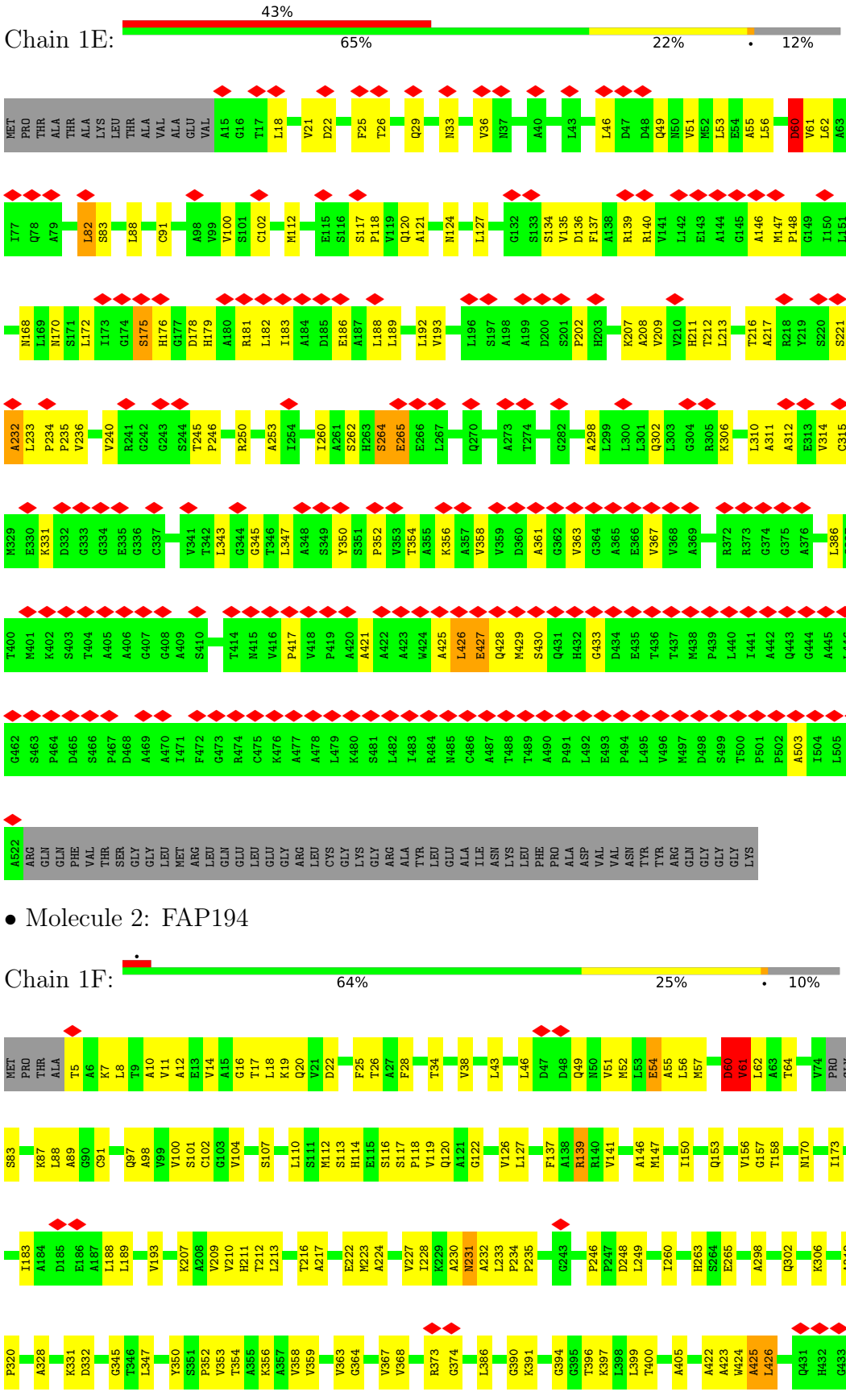
• Molecule 2: FAP194

Chain 1D:



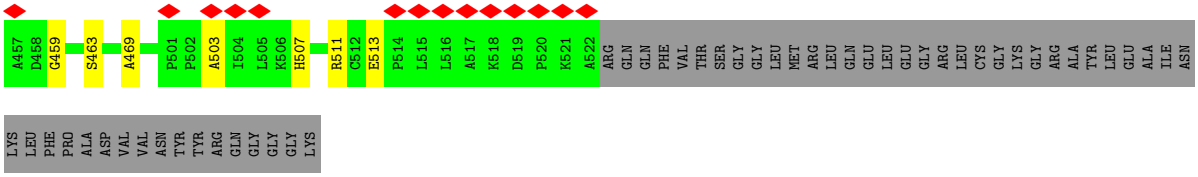
• Molecule 2: FAP194

Chain 1E:



• Molecule 2: FAP194

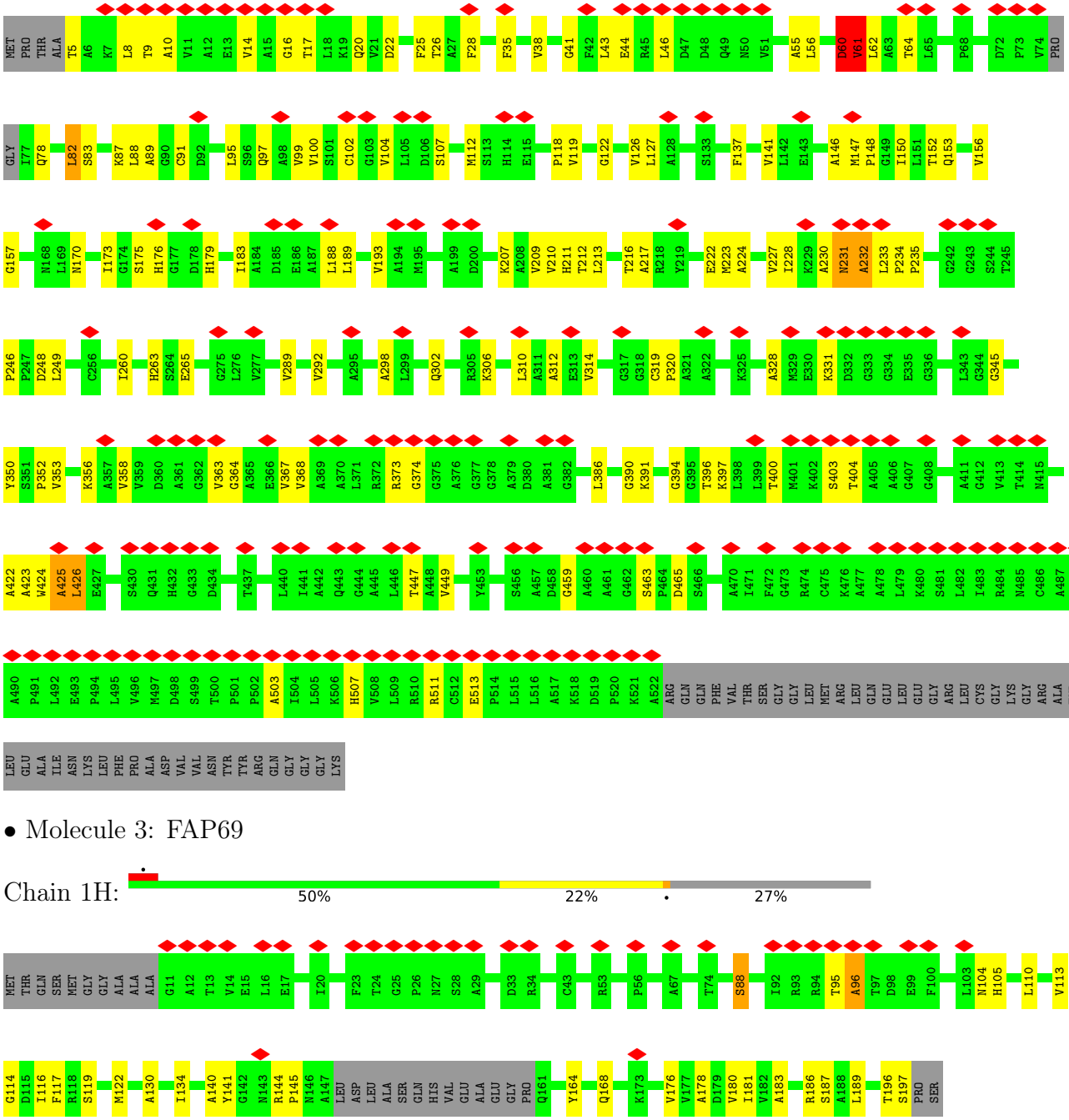
Chain 1F:



• Molecule 2: FAP194

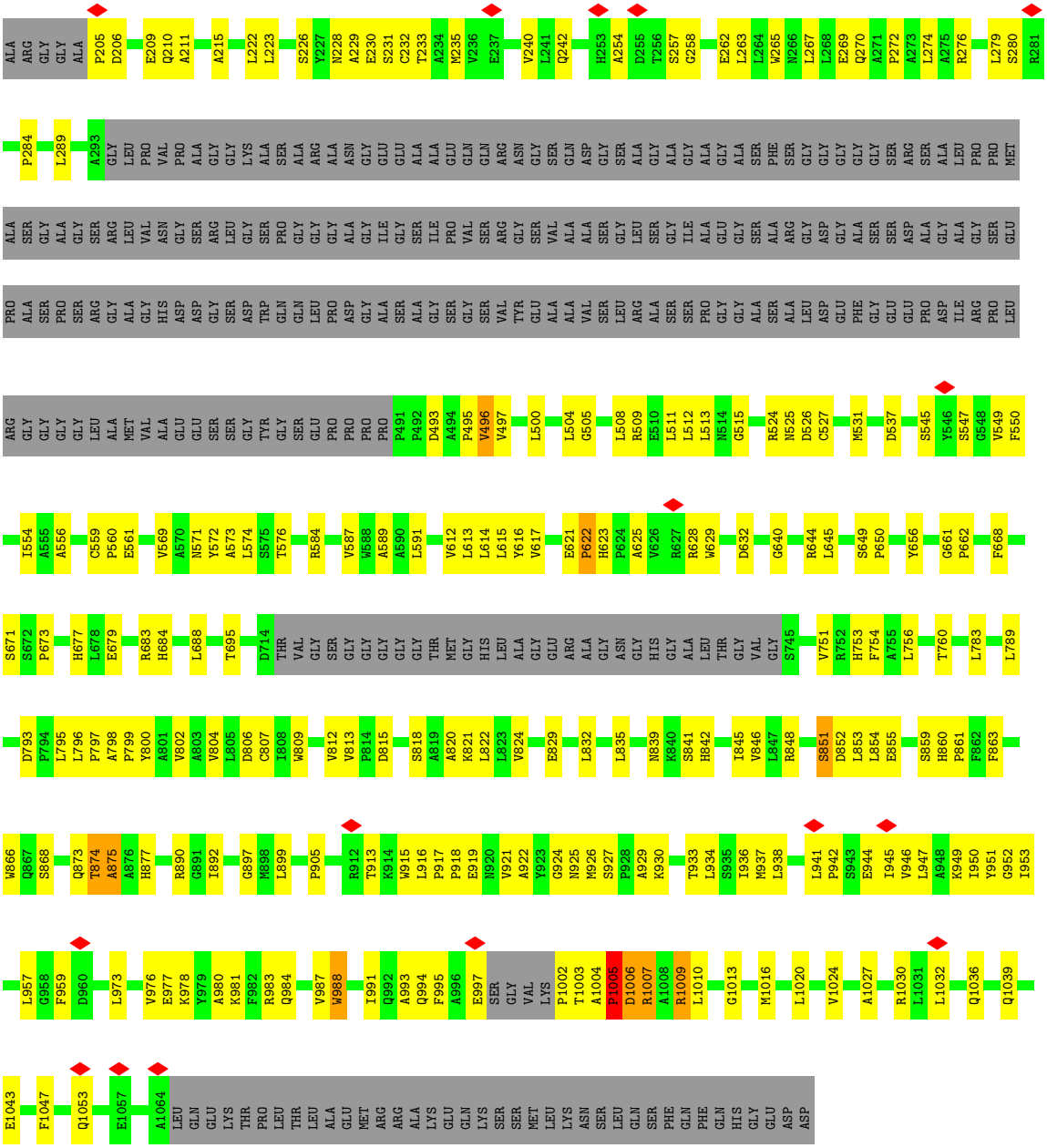
Chain 1G:





• Molecule 3: FAP69

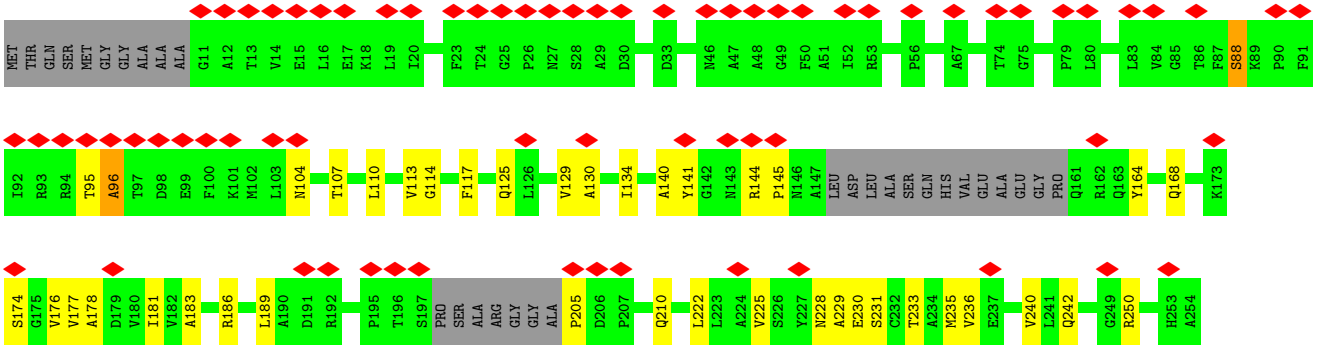
Chain 1H:

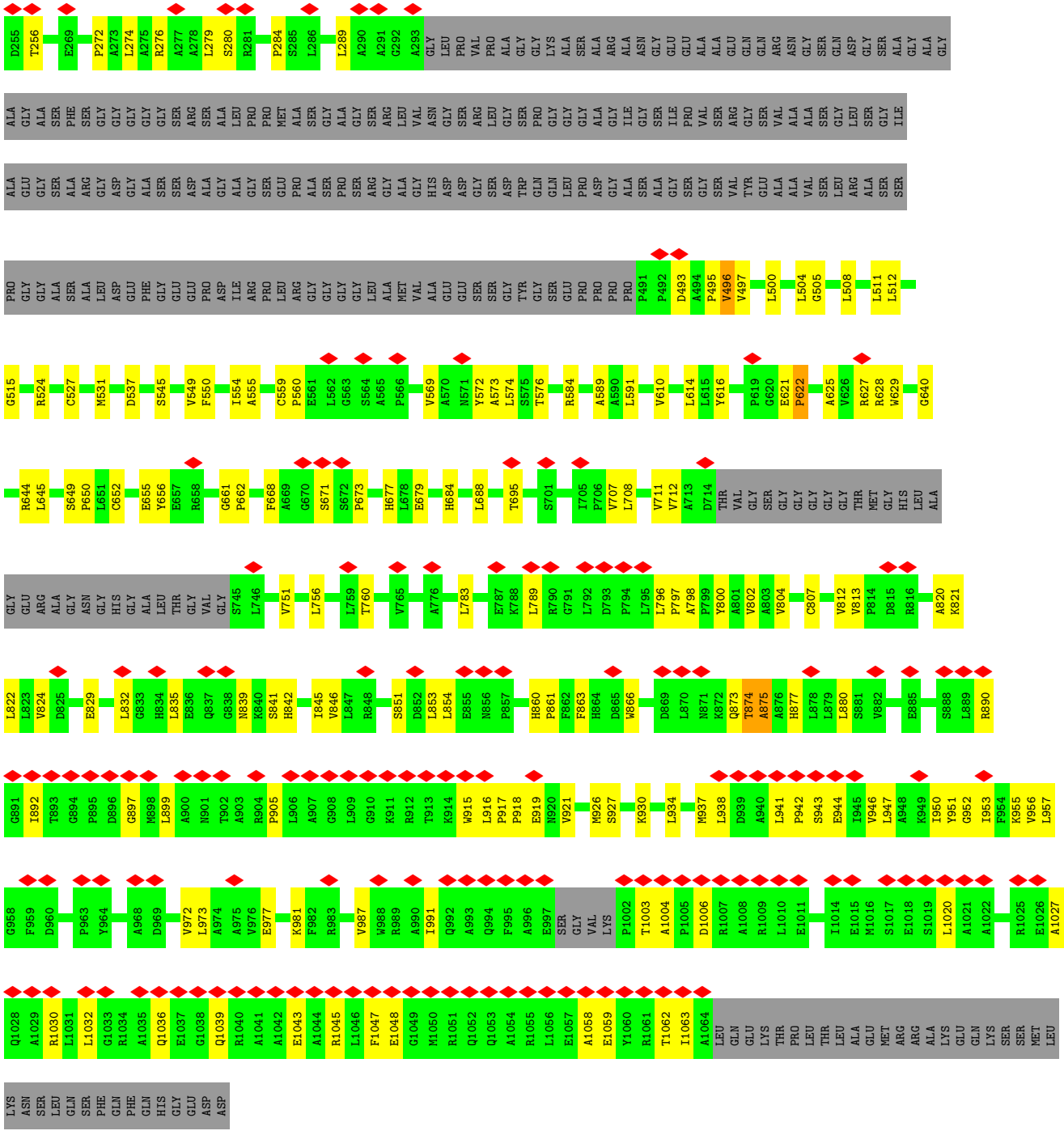


• Molecule 3: FAP69

Chain 1I:



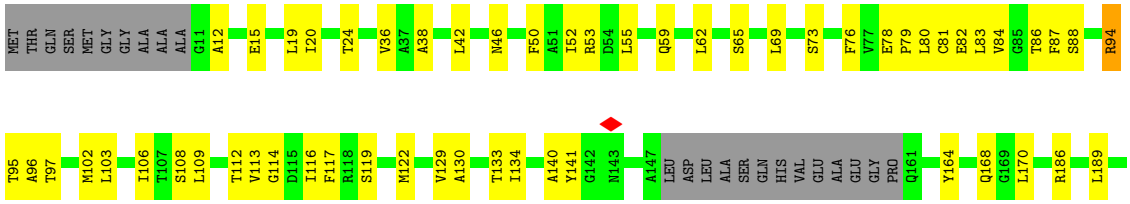


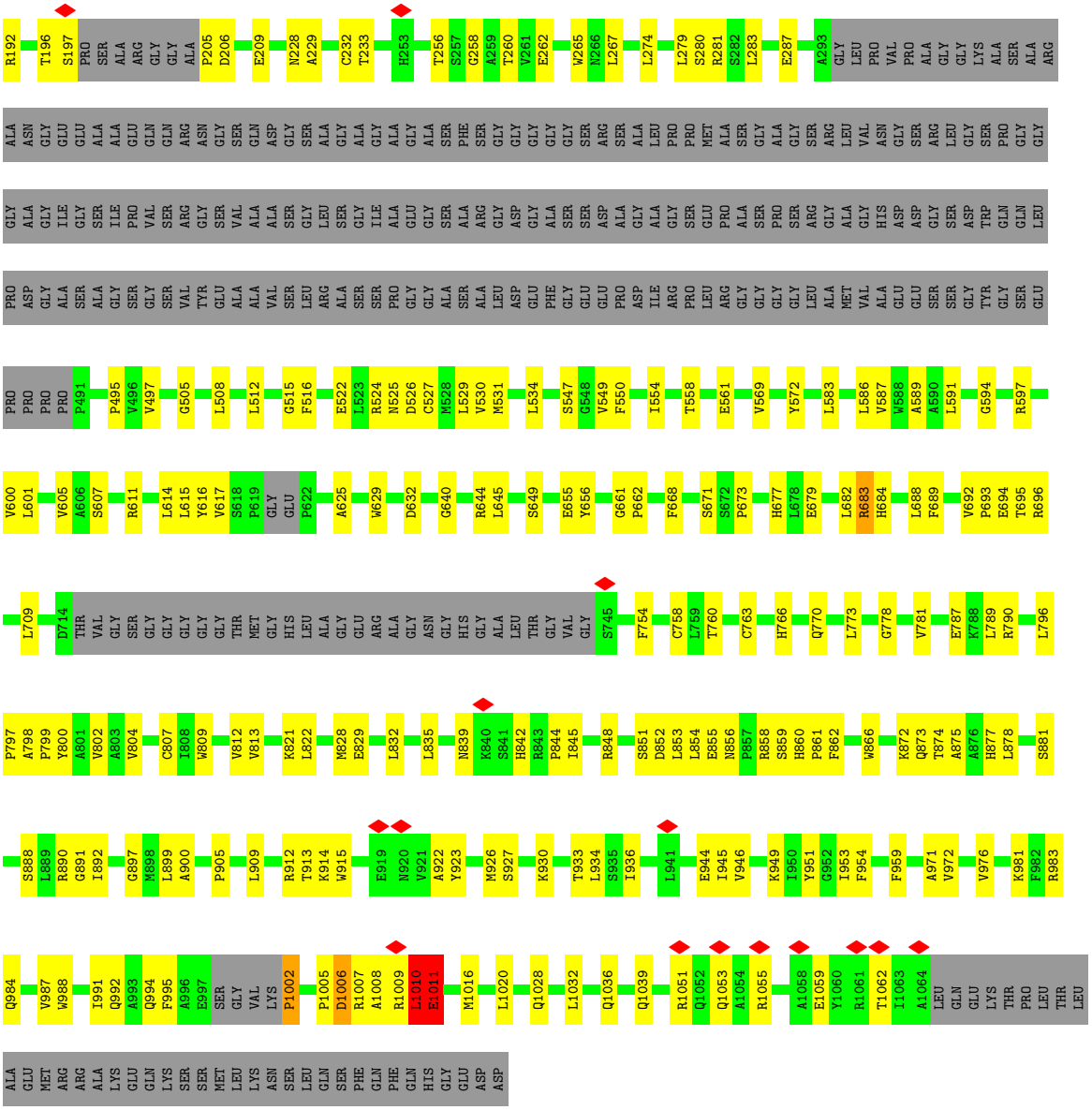


• Molecule 3: FAP69

Chain 6D:



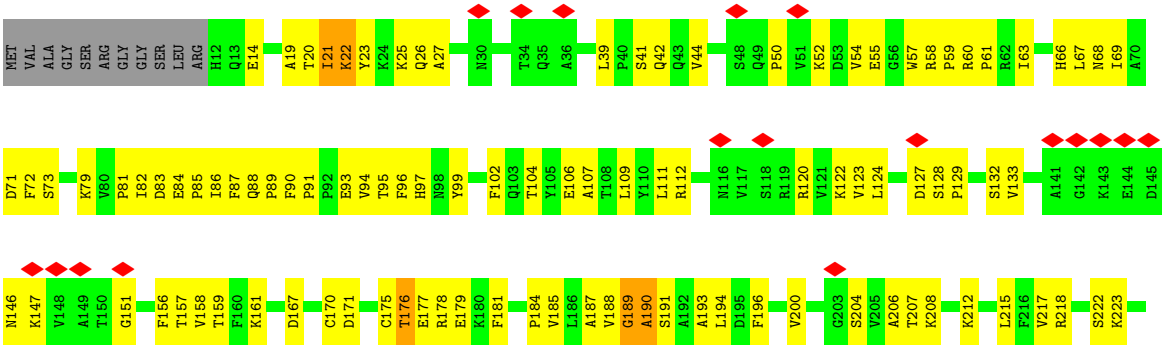


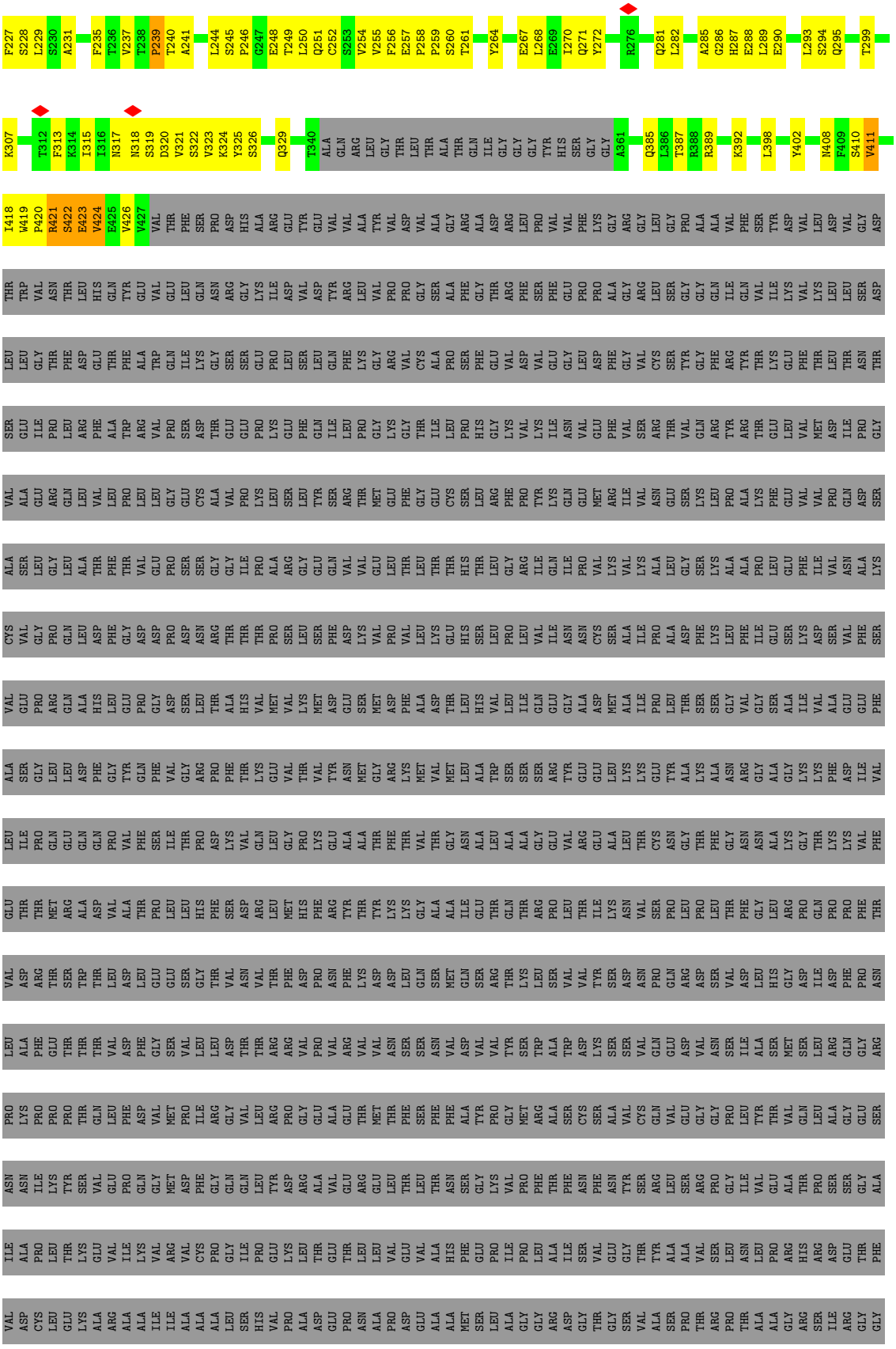


• Molecule 4: HYDIN

Chain 1J:



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K307 T312 F313 K314 I315 T316 N317 N318 S319 D320 V321 S322 V323 K324 Y325 S326 Q329 T340 A361 Q385 L386 T387 R388 R389 K392 L398 Y402 N408 F409 S410 V411
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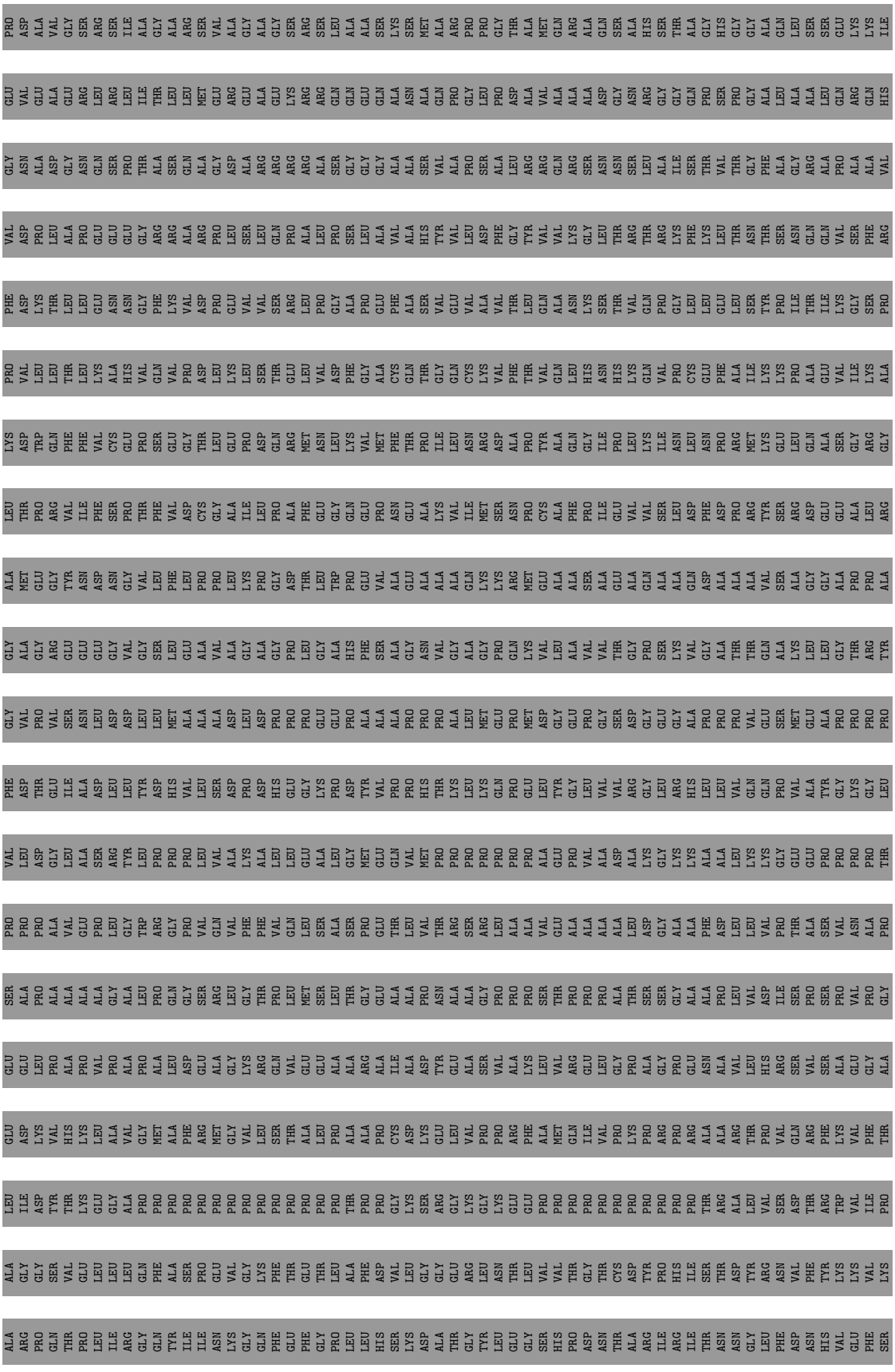
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GLU VAL GLU ALA GLU ARG LEU ARG LEU ILE THR LEU LEU MET GLU ARG GLU ALA GLU LYS ARG ARG GLN GLN GLU GLU GLN ALA ASN ALA GLN PRO GLY LEU PRO ASP ALA VAL ALA ALA ASP GLY ASN ARG GLY GLY GLN PRO SER PRO GLY ALA LEU ALA ALA LEU GLN LEU GLN HIS
GLY ASN ALA ASP GLY ASN GLN SER PRO THR ALA SER GLN ALA GLY ASP ALA ARG ARG ARG ARG ALA SER GLY GLY GLY ALA ALA SER VAL ALA PRO LEU ALA SER ASN ASN SER LEU ALA ILE SER THR VAL THR GLY PHE ALA GLY ARG ALA PRO ALA ALA
VAL ASP PRO LEU ALA PRO GLU GLU GLU GLY ARG ARG ALA ARG PRO LEU SER LEU GLN PRO ALA LEU PRO SER LEU ALA LEU ARG ARG GLN ARG SER ASN ASN SER LEU ALA THR ARG LYS PHE LYS LEU THR ASN THR SER ASN GLN GLN VAL ILE LYS PRO LYS LYS LYS PHE ARG
PHE ASP LYS THR LEU LEU GLU ASN ASN GLY PHE LYS VAL ASP PRO GLU VAL VAL SER ARG LEU PRO GLY ALA PRO GLU ASN ASN LEU PRO GLY LEU GLU VAL ALA VAL THR LEU GLN ALA ASN LYS SER THR VAL GLN PRO GLY LEU GLU LEU SER TYR PRO ILE THR ILE LYS GLY SER ARG
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LYS ASP TRP GLN PHE PHE VAL CYS GLU PRO SER GLU GLY THR LEU GLU PRO ASP GLN ARG MET ASN LEU LYS VAL MET PHE THR PRO ILE LEU GLU PRO ALA GLN GLY ILE PRO LEU LYS ILE ASN LEU ASN PRO ARG MET LYS GLU LEU ASN GLN ALA SER GLY ARG GLY
LEU THR PRO ARG VAL ILE PHE SER PRO THR PHE VAL ASP CYS GLY ALA ILE LEU PRO ALA PHE GLU GLY GLN GLU PRO ASN GLU ALA LYS VAL ILE MET SER ASN PRO CYS ALA PHE PRO ILE GLU VAL VAL SER LEU ASP PHE ASP PRO ARG TYR SER ARG ASP GLU GLU ALA PRO ALA
ALA MET GLU GLY TYR ASN ASP ASN GLY VAL LEU LEU PHE LEU PRO PRO LEU LYS PRO GLY ASP THR LEU TRP PRO GLU VAL ALA GLU ALA GLN LYS LYS ARG MET GLU ALA ALA ALA SER ALA GLU ALA GLN ASP ALA ALA ALA GLN GLY GLY GLY ALA PRO PRO ALA
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GLY VAL PRO VAL SER ASN LEU ASP ASP LEU LEU MET ALA ALA ALA ASP LEU ASP PRO PRO PRO PRO ALA ALA LEU MET GLU PRO PRO MET ASP GLY GLU PRO GLY SER ASP GLY GLU PRO ALA GLU ALA PRO PRO PRO PRO
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SER ALA PRO ALA ALA LEU PRO GLN GLY SER ARG LEU ALA LEU THR GLY GLU ALA THR SER SER GLY ALA ALA PRO LEU VAL ASP ILE SER PRO SER PRO VAL PRO GLY
GLU GLU LEU PRO ALA PRO VAL PRO ALA ALA LEU ARG ALA ILE ALA ASP TYR GLU ALA ALA SER VAL ALA LYS LEU VAL ARG GLU LEU GLY PRO ALA GLY PRO GLU ASN ALA VAL LEU HIS ARG SER VAL SER ALA GLU GLY ALA
GLU ASP LYS VAL HIS LYS LEU ALA VAL GLY PRO MET ALA PHE ARG MET GLY VAL LEU SER THR ALA LEU PRO ALA ALA PRO CYS ASP LYS GLU LEU VAL PRO PRO ARG MET GLN ILE VAL PRO LYS PRO ARG PRO ARG ALA ALA ARG THR PRO VAL GLN ARG PHE LYS VAL PHE THR
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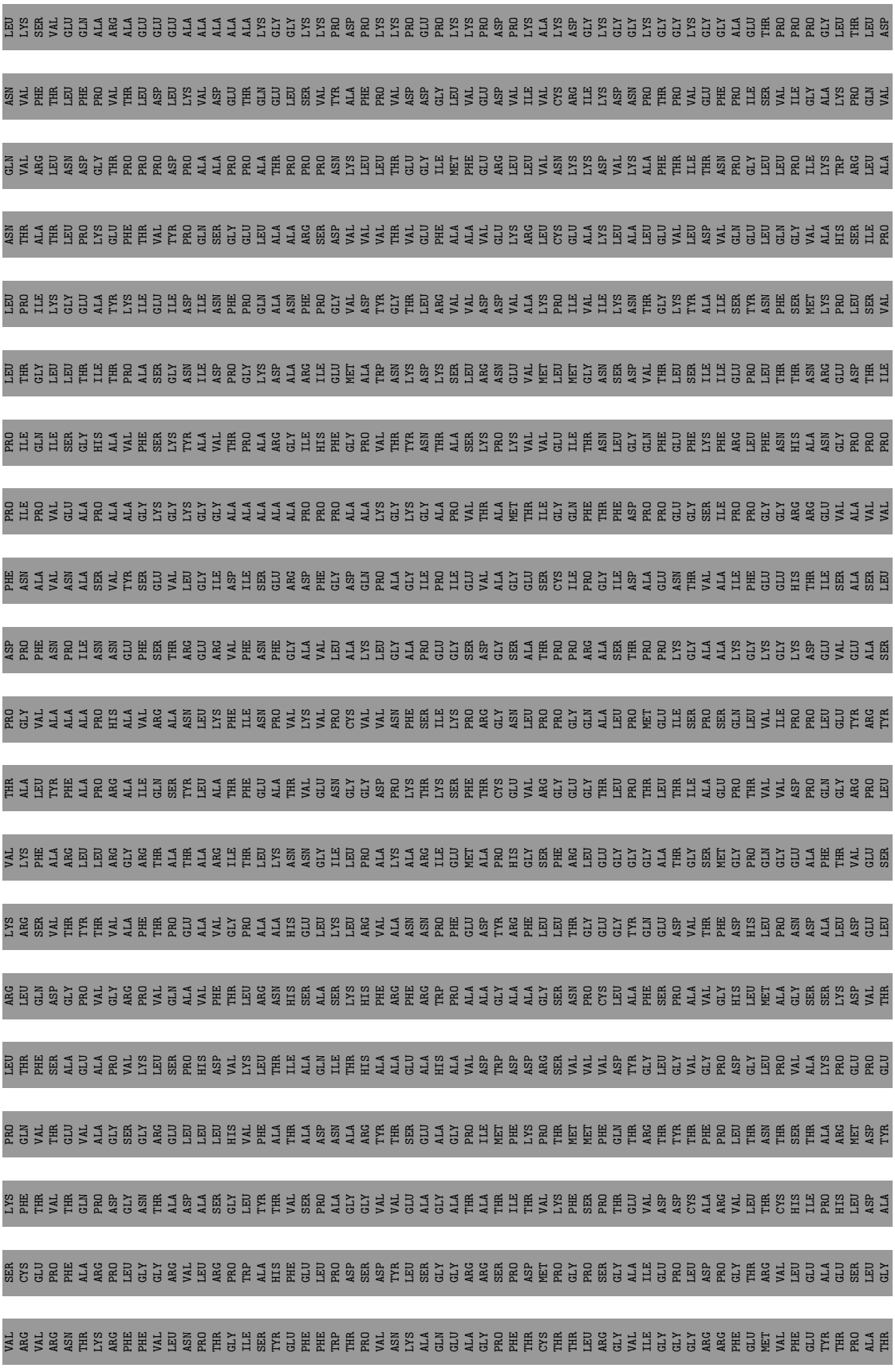
ALA GLY GLY SER VAL GLU GLN PHE ALA LEU LEU LEU GLU ALA PHE ASP VAL LEU GLY GLY GLU ARG LEU ASN THR GLY TYR LEU GLU GLU GLY CYS ASP TYR PRO HIS ILE SER THR ASP TYR ARG ASN VAL PHE TYR LYS LYS VAL LYS
ALA ARG PRO GLN THR PRO LEU ILE ARG GLY GLN TYR ILE ILE ASN LYS GLY GLN PHE GLU PHE GLY PRO LEU LEU HIS SER LYS ASP ALA THR GLY TYR LEU GLU GLY SER HIS PRO ASP ASN THR ALA ARG ILE ARG ILE THR ASN ASN GLY LEU PHE ASP ASN HIS VAL GLU PHE SER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ASN VAL PHE THR LEU PHE PRO VAL THR LEU ASP LEU LYS VAL ASP GLU THR GLN GLU LEU SER VAL TYR ALA PHE PRO VAL ASP ASP GLY LEU VAL GLU ASP VAL ILE VAL CYS ARG ILE LYS ASP ASN PRO THR PRO VAL GLU PHE PRO ILE GLY ALA LYS PRO GLN VAL
GLN VAL ARG LEU ASN ASP GLY THR PRO PRO PRO ASP PRO ALA ALA ALA PRO PRO ALA THR PRO PRO GLU GLY ILE MET PHE GLU ARG LEU LEU VAL ASN LYS LYS ASP VAL LYS TRP ARG LEU ALA
ASN THR ALA THR LEU PRO LYS GLU PHE THR VAL TYR PRO GLN SER GLY GLU LEU ALA ALA ARG SER ASP VAL VAL VAL THR VAL GLU GLU PHE ALA ALA GLU VAL GLU LYS ARG LEU CYS GLU ALA LYS LEU VAL LEU GLY ALA HIS SER LEU PRO
LEU PRO ILE LYS GLY GLU ALA TYR LYS ILE GLU ILE ASP ILE ASN PHE PRO GLN ALA ASN PHE PRO GLY VAL ASP TYR GLY THR LEU ARG VAL VAL ASP ASP VAL ALA LYS PRO ILE VAL ILE LYS ASN THR GLY LYS SER TYR ASN PHE SER MET LYS PRO LEU SER VAL
LEU THR GLY LEU LEU THR ILE THR PRO ALA ALA ASP PRO GLY LYS ASP ALA ARG ILE GLU MET ALA TRP ASN LYS ASP LYS SER LEU ARG LEU GLU LEU THR THR GLY LEU ASN SER ASP VAL THR LEU SER ILE ILE GLU PRO ASP VAL GLN GLU ASP ASN GLU ILE THR ILE
PRO ILE GLN ILE SER GLY HIS ALA VAL PHE SER LYS TYR ALA VAL THR PRO ALA ARG GLY ILE HIS PHE GLY PRO VAL THR TYR ASN THR ALA SER LYS PRO LYS VAL VAL GLU ILE THR ASN LEU GLY GLN PHE GLU PHE LYS PHE ARG LEU PHE ASN HIS ALA ASN GLY PRO PRO
PRO ILE PRO VAL GLU ALA PRO ALA ALA GLY LYS GLY GLY LYS GLY ALA ALA ALA ALA ALA PRO PRO PRO ALA ALA LYS GLY LYS GLY ALA PRO VAL THR MET THR ILE GLY GLN PHE THR PHE ASP PRO GLU GLY GLY SER ILE PRO PRO GLY GLY ARG ARG GLU VAL ALA VAL VAL
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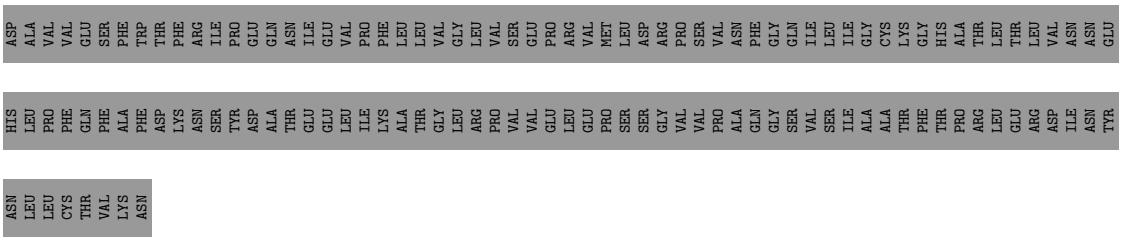
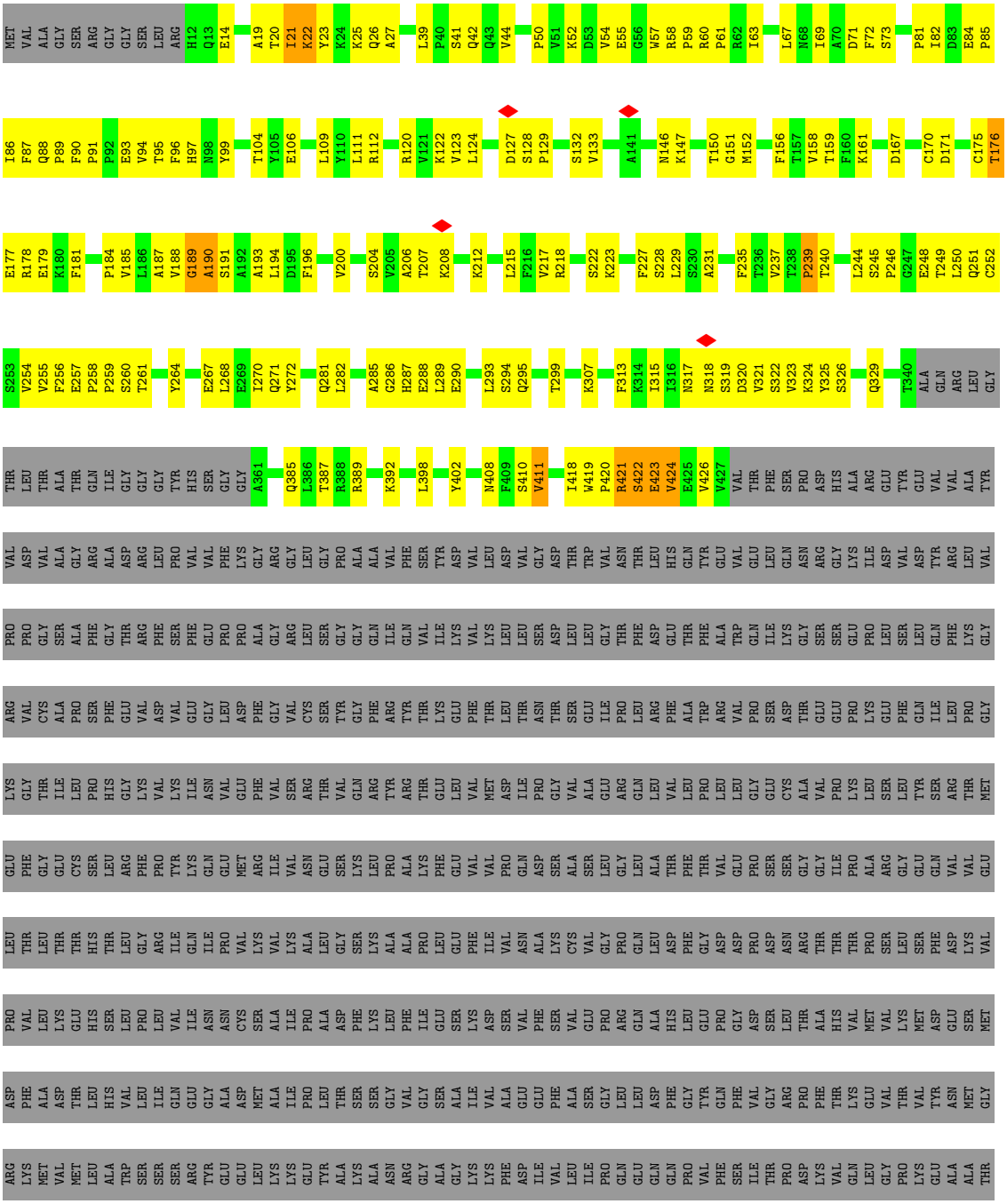
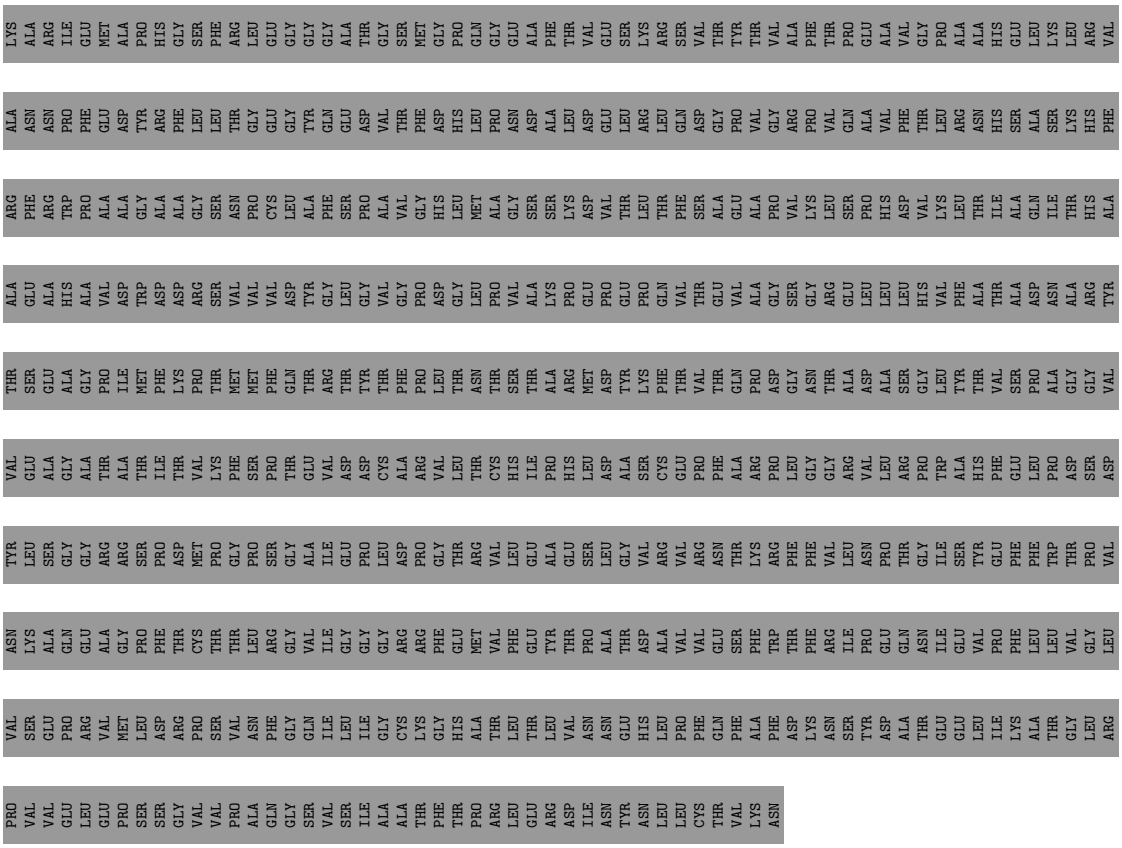
LYS ARG SER VAL THR TYR THR LEU LYS LEU ARG VAL ALA ASN ASN PRO PHE GLU ASP TYR ARG PHE LEU LEU THR GLY GLU GLY TYR GLN GLU ASP VAL THR PHE ASP HIS LEU PRO ASN ASP ALA LEU ASP GLU LEU
ARG LEU GLN ASP GLY PRO VAL GLY ARG PRO VAL GLN ALA VAL PHE ARG PHE ARG TRP PRO ALA ALA ALA GLY SER ASN PRO CYS LEU ALA PHE SER PRO ALA VAL GLY HIS LEU MET ALA PRO LEU PRO ASN ASP ALA LEU ASP GLU VAL
LEU THR PHE SER ALA GLU LYS LEU GLU ALA ALA HIS ALA VAL ALA ALA THR ILE ALA GLN ILE THR HIS ALA ALA VAL ASP TYR GLY LEU GLY VAL GLY PRO ASP LEU THR ASN THR SER THR ALA ARG LYS PRO GLU PRO GLU
PRO GLN VAL THR GLU VAL GLY ARG GLU LEU LEU LEU HIS VAL LYS LEU THR ILE ALA ASP ASN ALA ARG TYR THR ALA ASP ALA GLY ILE THR ARG THR ALA PHE PHE LYS PRO THR MET MET PHE GLN THR ARG THR TYR THR PHE PRO LEU THR ALA ARG MET ASP TYR
LYS PHE THR VAL THR GLN PRO ASP GLY ASN THR ALA ALA ASP ALA GLY GLY VAL VAL SER ALA GLY ALA THR ILE THR VAL LYS PHE SER PRO THR GLU VAL ASP ASP CYS ALA ARG VAL LEU THR CYS HIS ILE PRO HIS LEU ASP ALA
SER CYS GLU PRO PHE ALA ARG PRO LEU GLY GLY ARG ARG SER PRO ASP MET PRO GLY PRO SER GLY ALA ILE GLU ASP PRO GLY THR ARG VAL LEU GLU ALA GLU SER LEU GLY
VAL ARG VAL ARG ASN THR LYS ARG PHE VAL ASN LYS ALA GLN GLU ALA GLY PRO PHE THR CYS THR THR LEU ARG GLY VAL ILE GLY GLY ARG ARG PHE GLU MET VAL PHE GLU TYR THR GLU ILE



• Molecule 4: HYDIN

Chain 1K: 6% 90%

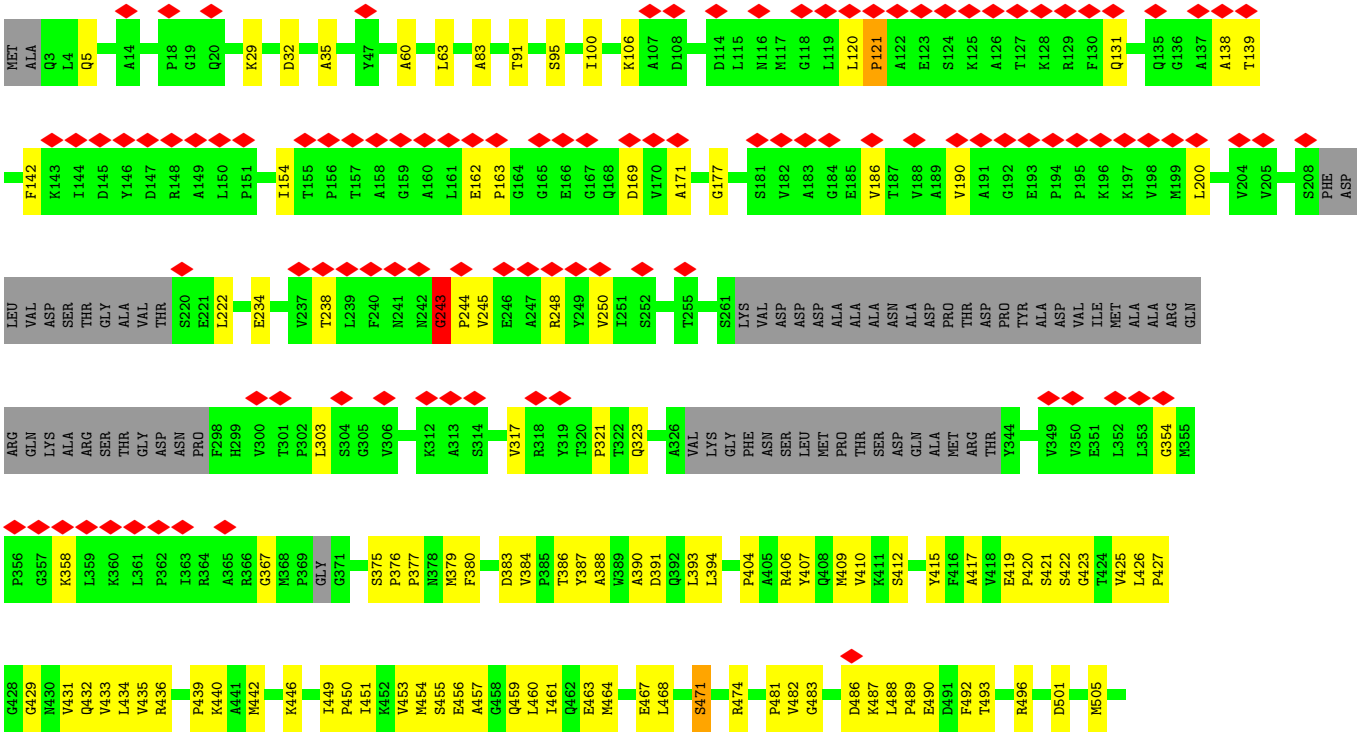


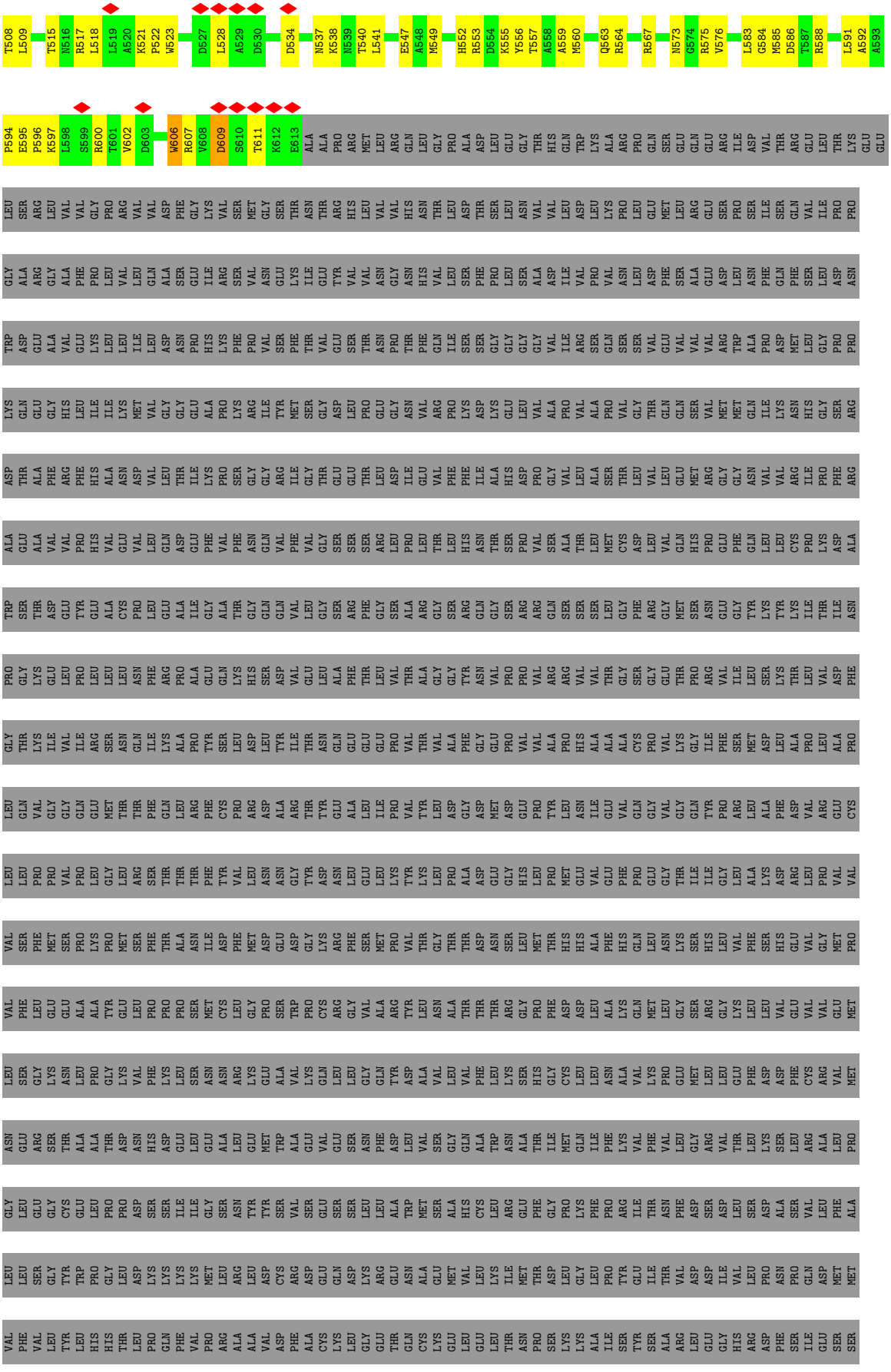


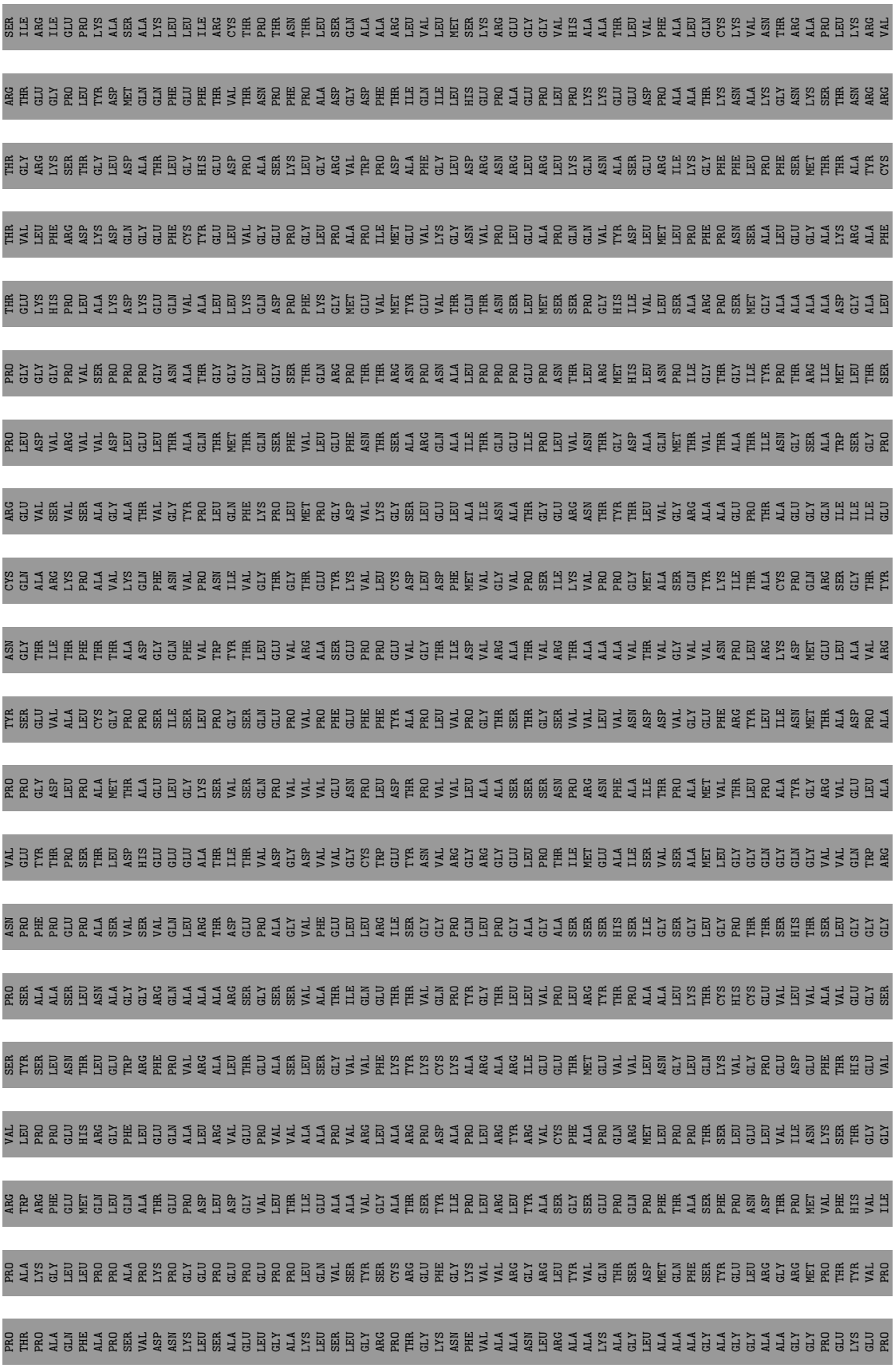
- Molecule 5: FAP47

Chain 1L:






T508 L509 T515 N516 R517 L518 L519 A520 K521 P522 W523 D527 L528 A529 D530 D534 N537 K538 N539 T540 L541 E547 A548 M549 H552 R553 D554 K555 Y556 T557 A558 A559 M560 Q563 R564 R567 N573 G574 R575 V576 L583 G584 M585 D586 T587 R588 L591 A592 A593
P594 E595 P596 K597 L598 S599 R600 T601 V602 D603 W606 R607 V608 D609 S610 T611 K612 E613 ALA ALA PRO ARG MET LEU ARG GLN LEU GLY PRO ALA ASP LEU GLU GLY THR HIS GLN TRP LYS ALA ARG PRO GLN SER GLU GLN GLU ARG ILE PRO LEU THR LYS GLU GLU
LEU SER ARG LEU VAL VAL GLY PRO ARG VAL VAL ASP PHE GLY LYS VAL SER MET GLY SER THR ASN THR ARG HIS LEU VAL VAL HIS ASN THR LEU ASP THR SER LEU ASN VAL VAL LEU ASP PHE SER ALA GLU ASP LEU LYS PRO LEU GLU MET LEU ARG GLU GLN SER PRO SER ILE SER GLN VAL ILE PRO PRO
GLY ALA ARG GLY ALA PHE PRO LEU VAL LEU GLN ALA SER GLU ILE ARG SER VAL ASN GLU LYS ILE GLU TYR VAL VAL ASN GLY ASN HIS VAL LEU SER PHE PRO LEU SER ALA ASP ILE VAL PRO VAL ASN LEU ASP PHE SER ALA GLU ASP ASN
TRP ASP GLU ALA VAL GLU LYS LEU LEU ILE LEU ASP ASN PRO HIS LYS PHE PRO VAL SER PHE THR VAL GLU SER THR ASN PRO THR PHE GLN ILE SER SER GLY GLY GLY VAL ILE ARG SER GLN SER SER VAL GLU VAL GLU GLN VAL VAL ARG TRP ALA PRO ASP MET LEU GLY PRO PRO
LYS GLN GLU GLY HIS LEU ILE ILE LYS MET VAL GLY GLY GLU ALA PRO LYS ARG ILE TYR MET SER GLY ASP LEU PRO GLU GLY ASN VAL ARG PRO LYS ASP LYS GLU LEU VAL ALA PRO VAL ALA PRO VAL GLY THR GLN GLN GLN SER VAL MET MET GLN ILE LYS ASN HIS GLY SER ARG
ASP THR ALA PHE ARG PHE HIS ALA ASN ASP VAL LEU THR ILE LYS PRO SER GLY GLY ARG ILE GLY THR GLU GLU THR LEU ASP ILE GLU VAL PHE PHE ILE ALA HIS ASP PRO GLY VAL LEU ALA SER THR LEU VAL LEU GLU MET ARG GLY GLY ASN VAL VAL ARG ILE PRO PHE ARG
ALA GLU ALA VAL VAL PRO HIS VAL LEU GLU VAL LEU GLN ASP GLU PHE VAL PHE ASN GLN VAL PHE VAL GLY SER SER SER ARG LEU PRO LEU THR LEU HIS ASN THR SER PRO VAL SER ALA THR LEU MET CYS ASP LEU VAL LEU GLN HIS PRO GLU PHE GLN LEU LEU CYS PRO LYS ASP ALA
TRP SER THR ASP GLU TYR GLU ALA CYS PRO LEU GLU LEU GLY GLN LEU ALA GLY SER ARG PHE GLY SER ALA ARG GLY SER ARG GLN GLY GLY SER SER SER LEU GLY PHE ARG GLY MET SER ASN GLU GLY TYR LYS TYR LYS ILE THR ILE ASN
PRO GLY LYS GLU LEU PRO LEU LEU LEU ASN PHE ARG PRO ALA GLU GLN LYS HIS SER ASP VAL GLU LEU ALA PHE THR LEU VAL THR ALA GLY GLY TYR ASN VAL PRO PRO VAL ARG ARG VAL THR GLY SER GLY GLU THR PRO ARG VAL ILE LEU SER LYS THR LEU VAL ASP PHE
GLY THR LYS ILE VAL ILE ARG SER ASN GLN GLU GLU GLU PRO VAL THR VAL ALA PHE GLY GLU PRO VAL THR ALA PRO HIS ALA ALA ALA CYS PRO VAL LYS GLY ILE PHE SER MET ASP LEU ALA PRO LEU ALA PRO
LEU GLN VAL GLY GLY GLN GLU MET THR THR PHE GLN LEU ARG PHE CYS PRO ARG ASP ALA ARG THR TYR GLU ALA LEU GLU ILE PRO VAL TYR LEU ASP GLY ASP MET ASP GLU PRO VAL ALA GLN GLY VAL VAL GLY GLN TYR PRO ARG LEU LEU ALA PHE ASP VAL ARG GLU CYS
LEU LEU PRO PRO VAL PRO LEU GLY GLU LEU ARG SER THR THR PHE TYR VAL LEU ASN ASN GLY TYR ASP ASN LEU GLU GLU LEU LYS TYR LYS LEU PRO ALA ASP GLU GLY HIS LEU PRO MET GLU VAL GLU PHE PRO GLU GLY THR ILE ILE GLY LEU ALA LYS ASP ARG LEU PRO VAL VAL
VAL SER PHE MET SER PRO LYS PRO MET SER PHE THR ALA ASN ILE ASP PHE ASP GLY LYS ARG PHE SER MET PRO VAL THR GLY THR THR ASP ASN SER LEU MET THR HIS ALA PHE HIS GLN LEU ASN LYS SER HIS LEU VAL PHE SER HIS GLU VAL ALA LYS ASP VAL PRO
VAL PHE LEU GLU GLU ALA TYR GLU LEU PRO PRO SER ARG CYS LEU GLY PRO SER TRP PRO CYS ARG GLY VAL ALA ARG TYR LEU ASN ALA THR THR THR ARG GLY PRO PHE ASP ASP LEU ALA LYS GLN LEU GLY SER ARG GLY VAL GLU VAL PRO LEU LEU LEU VAL GLU VAL GLU MET
LEU SER GLY LYS ASN LEU PRO GLY GLN LYS VAL PHE LYS LEU SER ASN ARG LYS GLU ALA VAL LYS GLN LEU LEU GLY LYS GLN TYR ASP ALA VAL LEU LEU PHE LEU LEU VAL ASN ALA THR ILE MET GLN ILE PHE LYS VAL PHE PRO VAL LEU GLU MET LEU LEU ASP PHE CYS ARG VAL
ASN GLU ARG SER THR ALA ALA THR ASP ASN HIS ASP GLU LEU GLU LEU MET TRP ALA GLU VAL GLU SER ASN PHE ASP LEU VAL ALA GLU VAL ALA LEU GLN ILE PHE LYS VAL PHE VAL LEU GLY ARG VAL THR LEU GLU PHE ASP ASP SER LEU ARG ALA LEU PRO
GLY LEU GLU GLY PRO PRO ASP SER SER ILE ILE GLY SER ALA LEU GLU SER LEU LEU ARG GLU PHE GLY PRO LYS PHE PRO ARG ILE THR ASN PHE ASP SER ALA SER VAL LEU ASP SER ALA SER PHE PRO ARG ILE PHE ALA
LEU LEU SER GLY TYR TRP LYS LYS LEU LEU GLY SER ASP LYS ARG GLU MET LYS LEU ASP ILE GLU ASP LYS ILE GLY LEU ASP LYS ILE GLU ASP LYS ILE GLY LEU PRO LYS ILE GLU ASP LYS ILE GLY LEU PRO LYS ILE GLU ASP LYS ILE GLY LEU PRO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ARG THR GLU GLY PRO LEU TYR ASP MET GLN GLN PHE GLU PHE THR VAL THR ASN PRO PHE PRO ALA ASP GLY ASP PHE THR ILE GLN ILE LEU HIS GLU PRO ALA GLU PRO LEU PRO LYS LYS GLU GLU ASP PRO ALA ALA THR LYS ASN ASN LYS SER THR ASN ARG ARG
THR GLY ARG LYS SER THR GLY LEU ASP ALA THR LEU GLY ASP PRO ALA SER LYS LEU GLY ARG VAL TRP PRO ASP ALA PHE GLY PHE GLY LEU ASP ARG VAL LEU ARG ASN ARG LEU ARG LYS GLN ASN ALA SER GLU ARG ILE LYS GLY PHE PHE LEU ASN ALA LYS GLY ASN SER MET THR THR ALA ARG CYS
THR VAL LEU PHE ARG ASP LYS ASP GLN GLY GLU PHE CYS TYR GLU LEU VAL GLY GLU PRO GLY LEU PRO ALA PRO ILE MET GLU VAL LYS GLY ASN VAL PRO LEU GLU GLU VAL TYR ASP LEU MET LEU PRO PHE PRO ASN SER ALA GLU GLY PHE ALA PHE
THR GLU LYS HIS PRO LEU ALA LYS ASP LYS GLU GLN VAL ALA ALA LEU LEU LYS GLN ASP PRO PHE LYS GLY MET GLU VAL MET TYR GLU VAL THR GLN THR ASN ASN ARG LEU GLU GLU ILE MET SER SER PRO GLY HIS ILE VAL LEU SER ALA ARG PRO SER MET SER GLY ALA ALA ASP GLY ALA LEU
PRO GLY GLY GLY PRO VAL SER PRO PRO PRO GLY GLY ASN ALA THR GLY GLY GLU GLN ARG PRO THR THR ARG ASN PRO ASN PRO ASN ALA LEU PRO PRO ASN THR GLY ILE TYR PRO THR GLY ILE GLY THR PHE PRO ASN SER MET GLY GLY ALA ALA ARG MET HIS LEU ASN PRO ILE GLY THR GLY ILE TYR PRO THR ARG GLU ILE PRO GLY SER GLY
PRO LEU ASP VAL ARG VAL ASP LEU GLU LEU THR ALA GLN THR MET THR GLN SER PHE VAL LEU GLU PHE ASN THR SER ALA ARG GLN ALA ILE THR GLN GLU ILE PRO LEU VAL ASN THR GLY ASP ALA ALA GLN MET THR VAL THR ALA ALA THR ILE ASN GLY SER ALA TRP SER GLY PRO
ARG GLU VAL SER VAL ALA GLY ALA THR VAL GLY TYR PRO LEU GLN PHE LYS PRO LEU MET PRO GLY ASP VAL LYS GLY SER LEU GLU ARG ASN THR TYR THR LEU GLY ARG ALA GLU PRO THR ALA GLU GLY ILE ILE GLU
CYS GLN ALA ARG LYS PRO GLN PHE ASN VAL PRO ASN ILE VAL GLY THR GLY THR GLU TYR LYS VAL LEU CYS ASP LEU ASP PHE MET VAL GLY VAL PRO SER ILE LYS VAL PRO PRO GLY MET ALA SER GLN TYR LYS ILE THR ALA ALA CYS PRO GLN ARG SER GLY THR TYR
ASN GLY THR ILE THR PHE VAL TRP TYR THR LEU GLU VAL ARG ALA SER GLU PRO PRO GLU VAL GLY THR ILE ASP VAL ARG ALA THR VAL ARG THR ALA ALA ALA VAL THR VAL GLY VAL VAL ASN PRO LEU ARG LYS ASP MET GLU LEU ALA VAL ARG
TYR SER GLU VAL ALA LEU CYS GLY PRO PRO SER ILE SER LEU PRO GLY SER GLN GLU PRO VAL PRO PHE GLU PHE PHE TYR ALA PRO LEU VAL PRO GLY THR SER THR GLY SER VAL VAL LEU VAL ASN ASP ASP VAL GLY GLU PHE ARG TYR LEU ILE ALA PRO THR
PRO PRO GLY ASP LEU PRO ALA MET THR ALA GLU GLU LEU GLY LYS SER VAL SER GLN PRO VAL VAL VAL GLU ASN PRO LEU ASP THR PRO VAL VAL LEU LEU ALA ALA SER SER SER PRO ARG ASN PHE ALA ILE THR PRO ALA MET VAL THR LEU GLY PRO ALA TYR GLY ARG VAL VAL ALA
VAL GLU TYR THR PRO SER THR LEU ASP HIS GLU GLU GLU ALA THR ILE THR VAL ASP GLY VAL CYS TRP GLU TYR ASN VAL ARG GLY ARG GLY LEU PRO THR ILE MET GLU ALA ILE SER VAL SER ALA MET LEU GLU GLY GLY GLN GLN GLY GLN GLY VAL VAL GLN LEU GLY
ASN PRO PHE PRO GLU PRO ALA SER VAL GLN LEU ARG THR ASP GLU PRO ALA GLY VAL PHE GLU LEU LEU ARG ILE SER GLY GLY PRO GLN LEU PRO GLY ALA SER SER HIS SER ILE GLY SER GLY LEU GLY PRO THR THR SER HIS THR SER LEU GLY PRO THR
PRO SER ALA ALA SER ALA GLY ASN ALA GLY PRO GLN GLU THR THR VAL GLN PRO TYR GLY THR LEU GLU LEU VAL PRO LEU ARG TYR THR PRO ALA ALA LEU LYS THR CYS HIS CYS GLU VAL LEU GLY VAL SER
SER TYR SER LEU ASN THR LEU GLU TRP ARG PHE PRO VAL ARG GLN ALA ALA ARG ALA LEU GLU ILE GLU GLU THR MET GLU VAL VAL LEU ASN GLY LEU GLN LYS VAL GLY PRO GLU ASP GLU PHE THR HIS GLU VAL
VAL LEU PRO PRO GLU HIS ARG GLY PHE LEU GLU GLN ALA LEU ARG VAL GLU PRO VAL VAL ARG LEU ALA ARG PRO PRO ASP ALA PRO LEU ARG TYR ARG VAL CYS PHE ALA PRO GLN ARG MET LEU PRO PRO THR SER LEU GLU VAL ILE ASN LYS SER THR GLY GLY
ARG TRP ARG PHE GLU MET GLN LEU GLN ALA ALA THR GLU PRO ASP LEU ASP GLY VAL LEU THR ILE GLU ALA ALA VAL GLY ALA THR SER TYR ILE PRO LEU ARG LEU TYR ARG ALA SER GLY SER GLU PRO GLN PRO PHE THR ALA SER PHE PRO GLU ASN ASP THR PRO MET VAL PHE HIS VAL ILE
PRO ALA LYS GLY LEU LEU PRO PRO LYS PRO GLY GLU LEU GLU VAL PRO GLU GLU PRO VAL PRO LEU GLN VAL SER TYR SER CYS ARG GLU PHE GLY LYS VAL VAL ARG GLY ARG LEU TYR VAL GLN THR SER ASP MET GLN PHE SER TYR GLU LEU ARG GLY PRO THR TYR VAL PRO
PRO THR PRO ALA GLN PHE ALA PRO SER LEU GLY ARG PRO THR GLY LYS ASN PHE VAL ALA ASN LEU ARG ALA ALA LYS ALA GLY LEU ALA ALA ALA GLY GLY GLY PRO GLU LYS GLU PRO



• Molecule 5: FAP47

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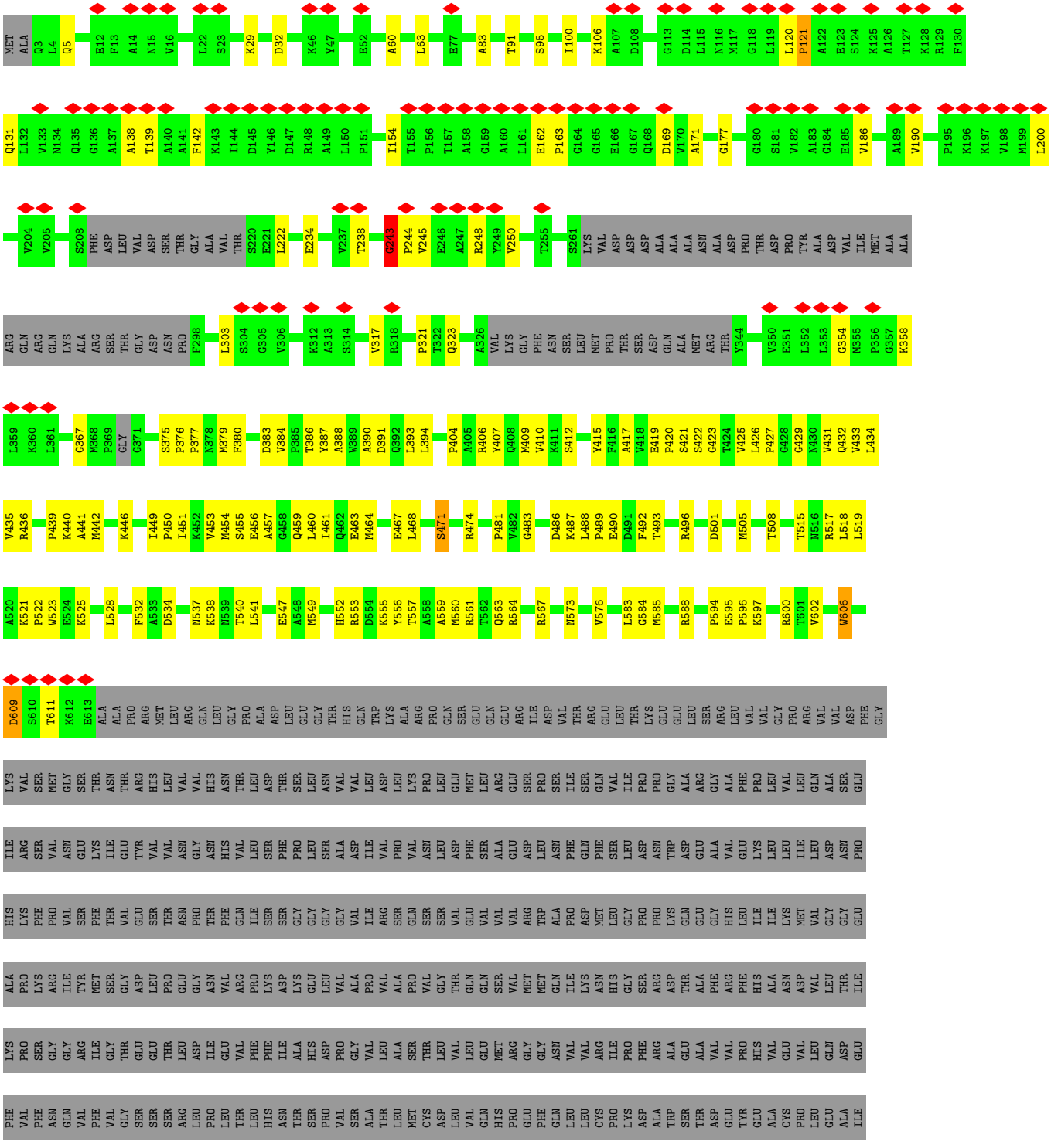

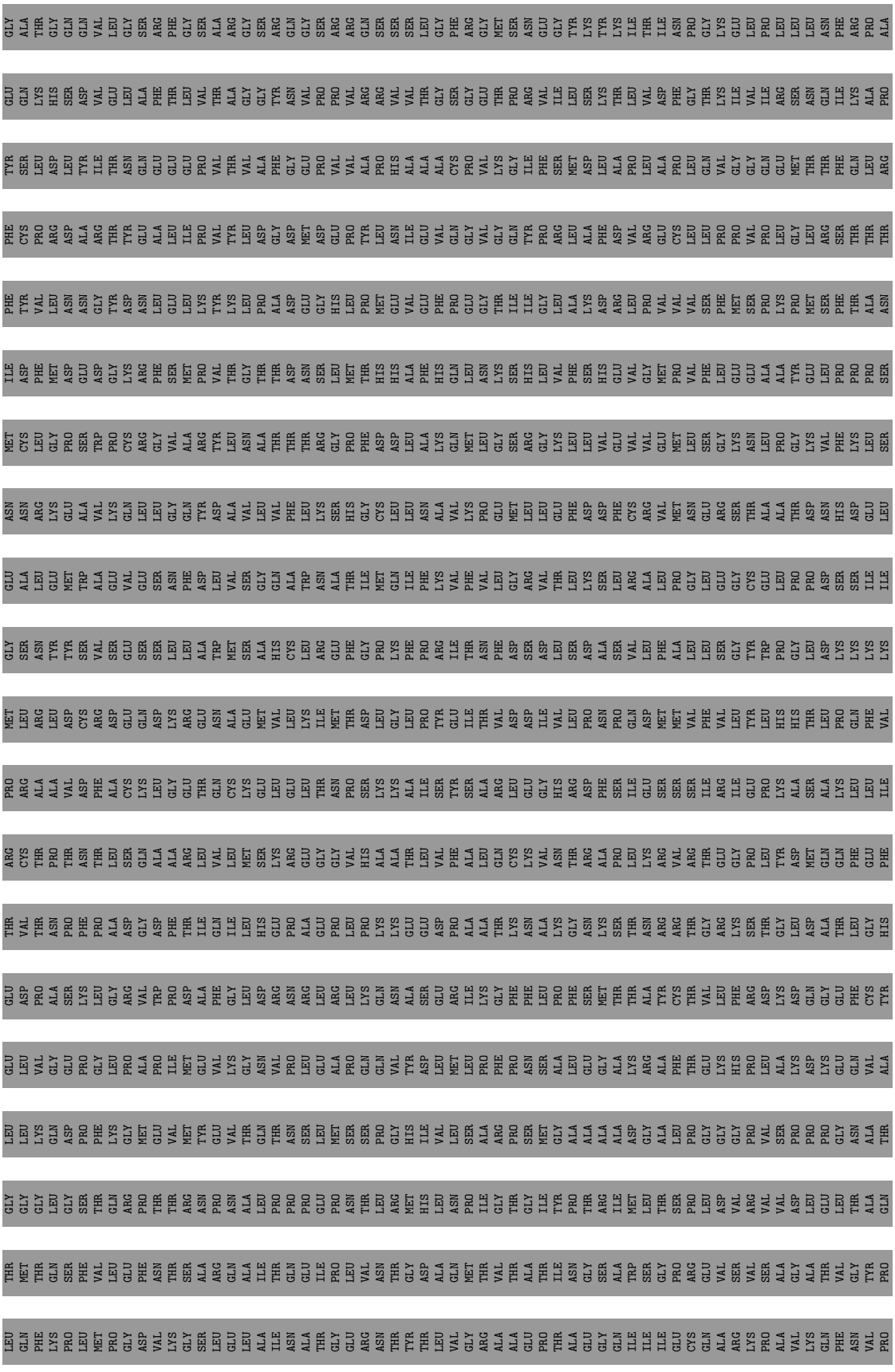
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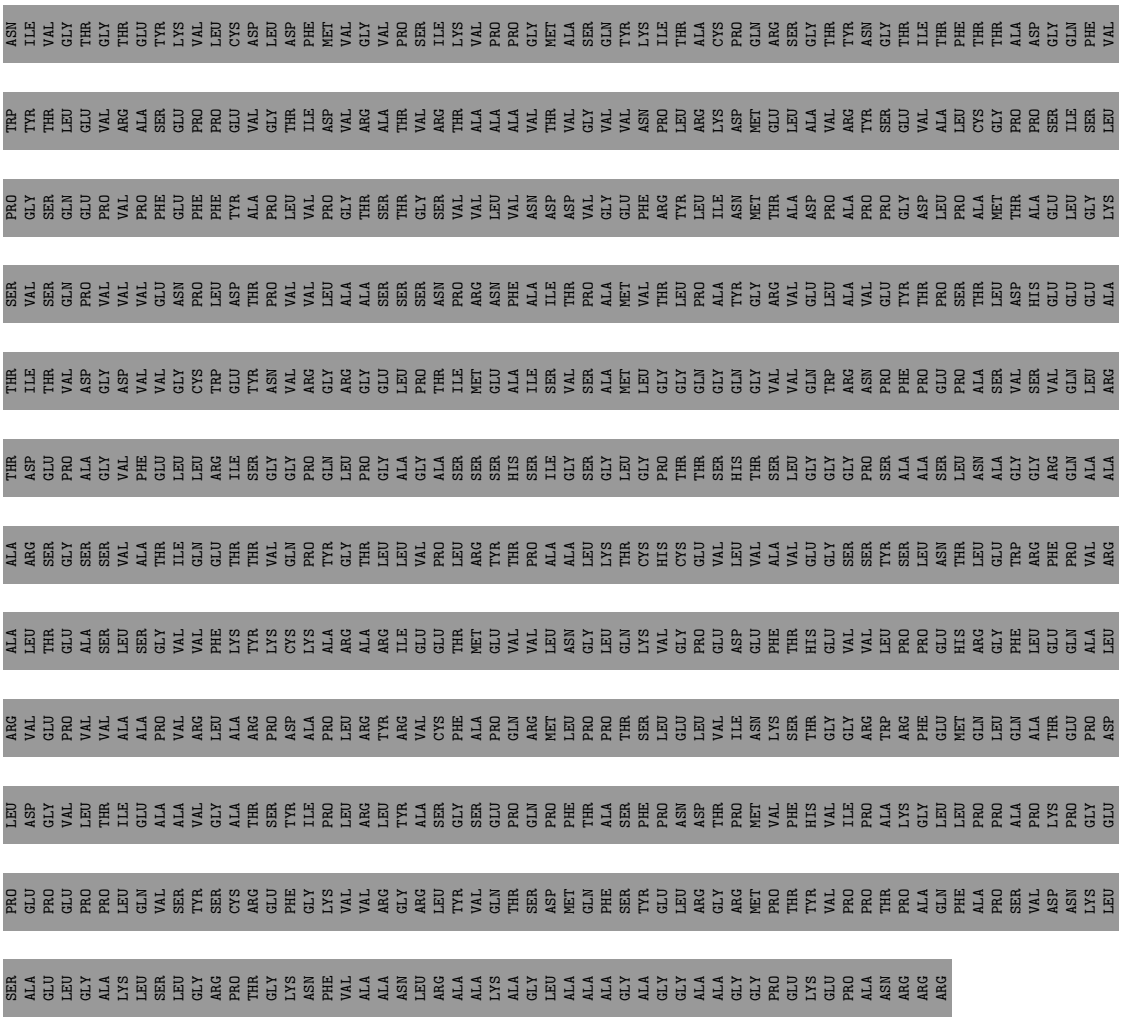
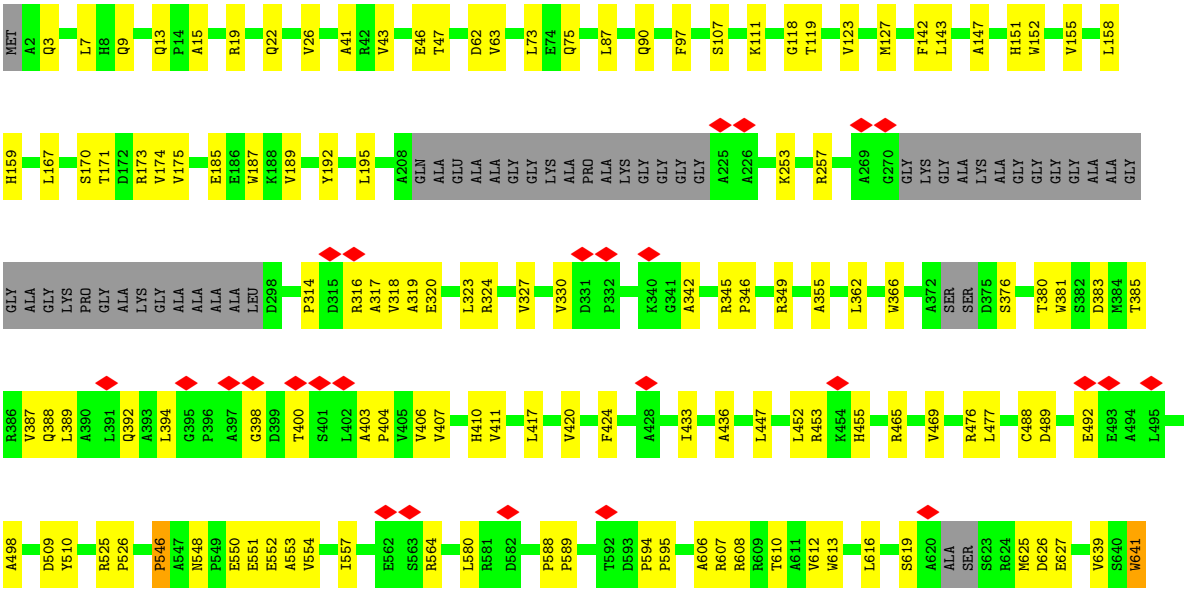
GLU GLN LYS HIS SER ASP VAL GLU LEU ALA PHE THR LEU VAL THR ALA GLY GLY TYR ASN VAL PRO PRO VAL ARG ARG VAL VAL THR GLY SER GLY GLU THR PRO ARG VAL ILE LEU SER LYS THR LEU GLY PHE GLY THR LYS ILE VAL ILE ARG SER ASN GLN ILE LYS ALA PRO
TYR SER LEU ASP LEU TYR ILE THR ASN GLN GLU GLU GLU PRO VAL THR VAL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

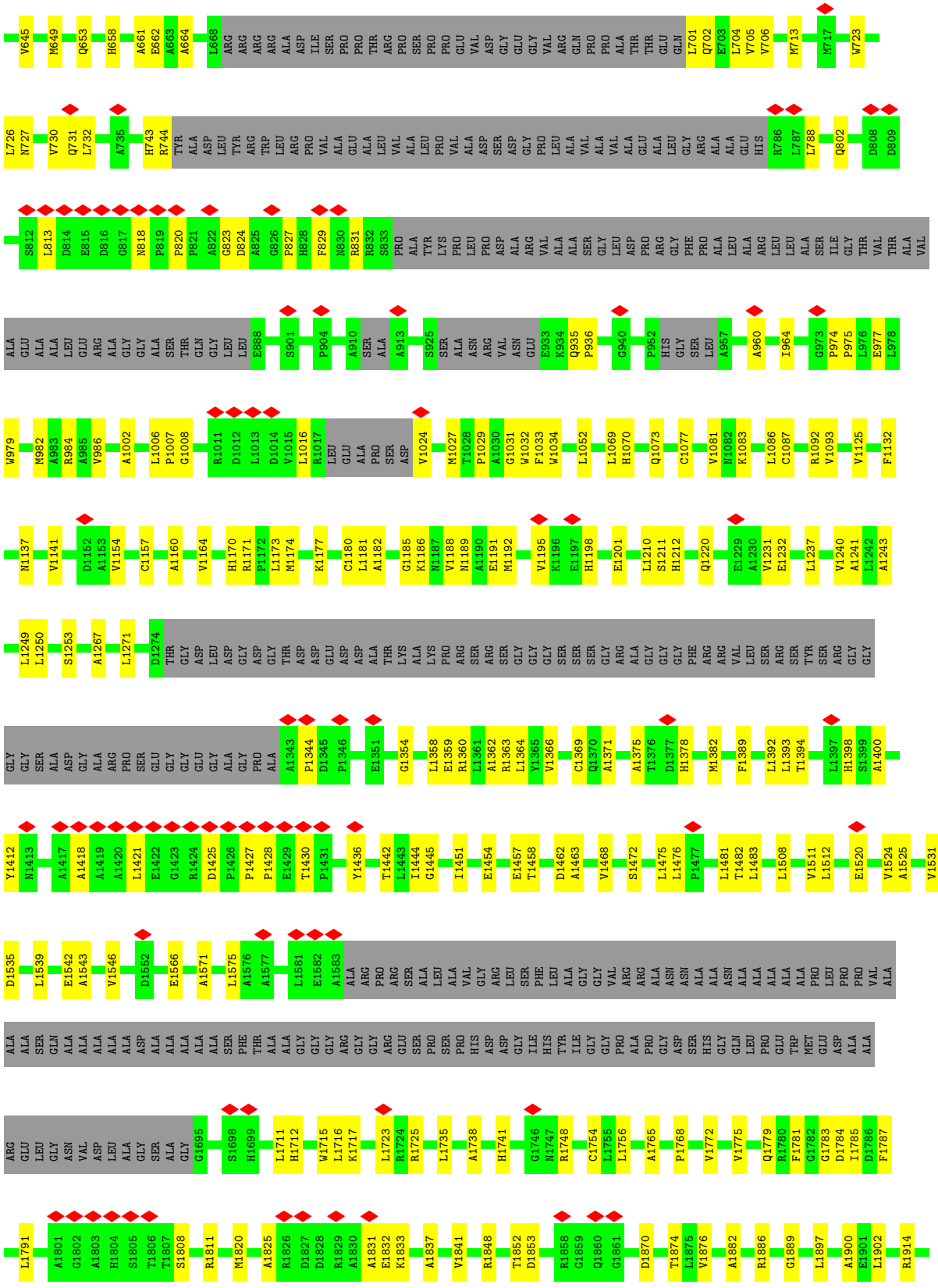


• Molecule 6: FAP46

Chain 1N:



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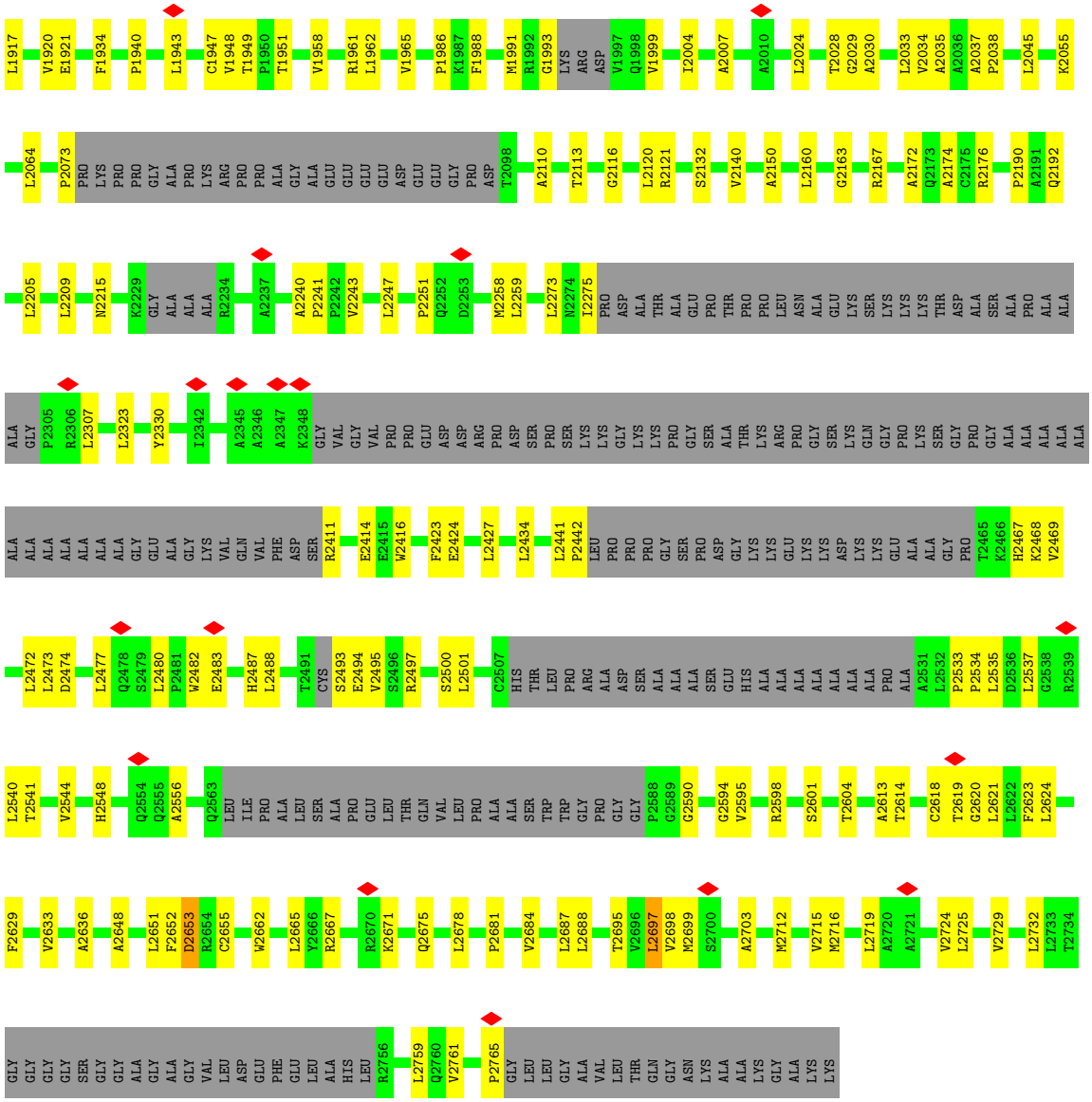
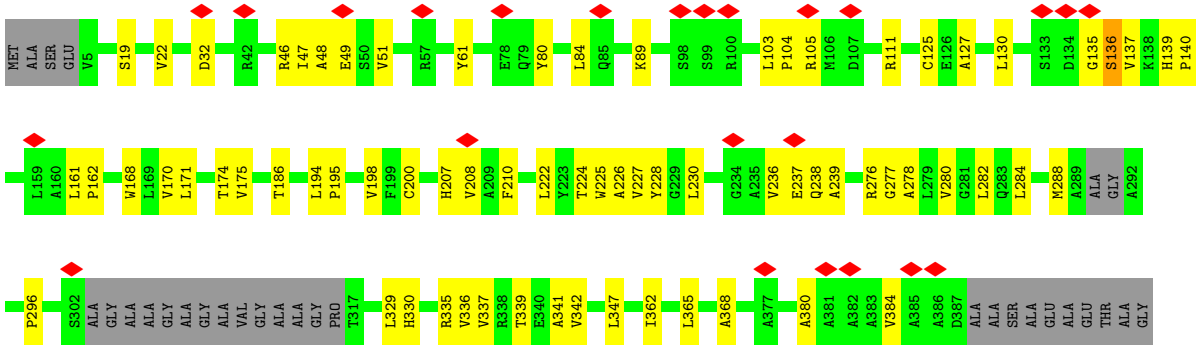
L726 N727 V730 Q731 L732 A735 H743 R744 R786 L787 L788 Q802 D808 D809
S812 L813 D814 E815 D816 G817 N818 P819 P820 P821 A822 G823 D824 A825 G826 P827 H828 F829 N830 A831 R832 S833
E888 S901 P904 A910 A913 S925 E933 K934 Q935 P936 G940 P952 A957 A960 I964 G973 P974 P975 L976 E977 L978
W979 M982 A983 R984 A985 V986 A1002 L1006 P1007 G1008 R1011 D1012 L1013 D1014 V1015 L1016 R1017 V1024 M1027 T1028 P1029 A1030 G1031 W1032 F1033 W1034 L1052 L1069 H1070 Q1073 C1077 V1081 N1082 K1083 L1086 C1087 R1092 V1093 V1125 F1132
N1137 V1141 D1152 A1153 V1154 C1157 A1160 V1164 H1170 R1171 P1172 L1173 M1174 K1177 C1180 L1181 A1182 G1185 K1186 N1187 V1188 N1189 A1190 E1191 M1192 V1195 K1196 E1197 H1198 E1201 L1210 S1211 H1212 Q1220 E1229 A1230 V1231 E1232 L1237 V1240 A1241 L1242 A1243
L1249 L1250 S1253 A1267 L1271 D1274
A1343 P1344 D1345 P1346 E1351 G1354 L1358 E1359 R1360 L1361 A1362 R1363 L1364 Y1365 V1366 C1369 Q1370 A1371 A1375 T1376 D1377 H1378 M1382 F1389 L1392 L1393 T1394 L1397 H1398 S1399 A1400
Y1412 N1413 A1417 A1418 A1419 A1420 L1421 E1422 G1423 R1424 D1425 P1426 P1427 P1428 E1429 T1430 P1431 Y1436 T1442 L1443 I1444 G1445 I1451 E1454 E1457 T1458 D1462 A1463 V1468 S1472 L1475 L1476 P1477 L1481 T1482 L1483 L1508 V1511 L1512 E1520 V1524 A1525 V1531
D1535 L1539 E1542 A1543 V1546 D1552 E1566 A1571 L1575 A1576 A1577 L1581 E1582 A1583
A1738 H1741 G1746 N1747 R1748 C1754 K1755 L1756 A1765 P1768 V1772 V1775 Q1779 R1780 F1781 G1782 G1783 D1784 I1785 D1786 F1787
L1791 A1801 G1802 A1803 H1804 S1805 T1806 T1807 S1808 R1811 M1820 A1825 R1826 D1827 D1828 R1829 A1830 A1831 E1832 K1833 A1837 V1841 R1848 T1852 D1853 R1858 G1859 Q1860 G1861 D1870 T1874 L1875 V1876 A1882 R1886 G1889 L1897 A1900 E1901 L1902 R1914

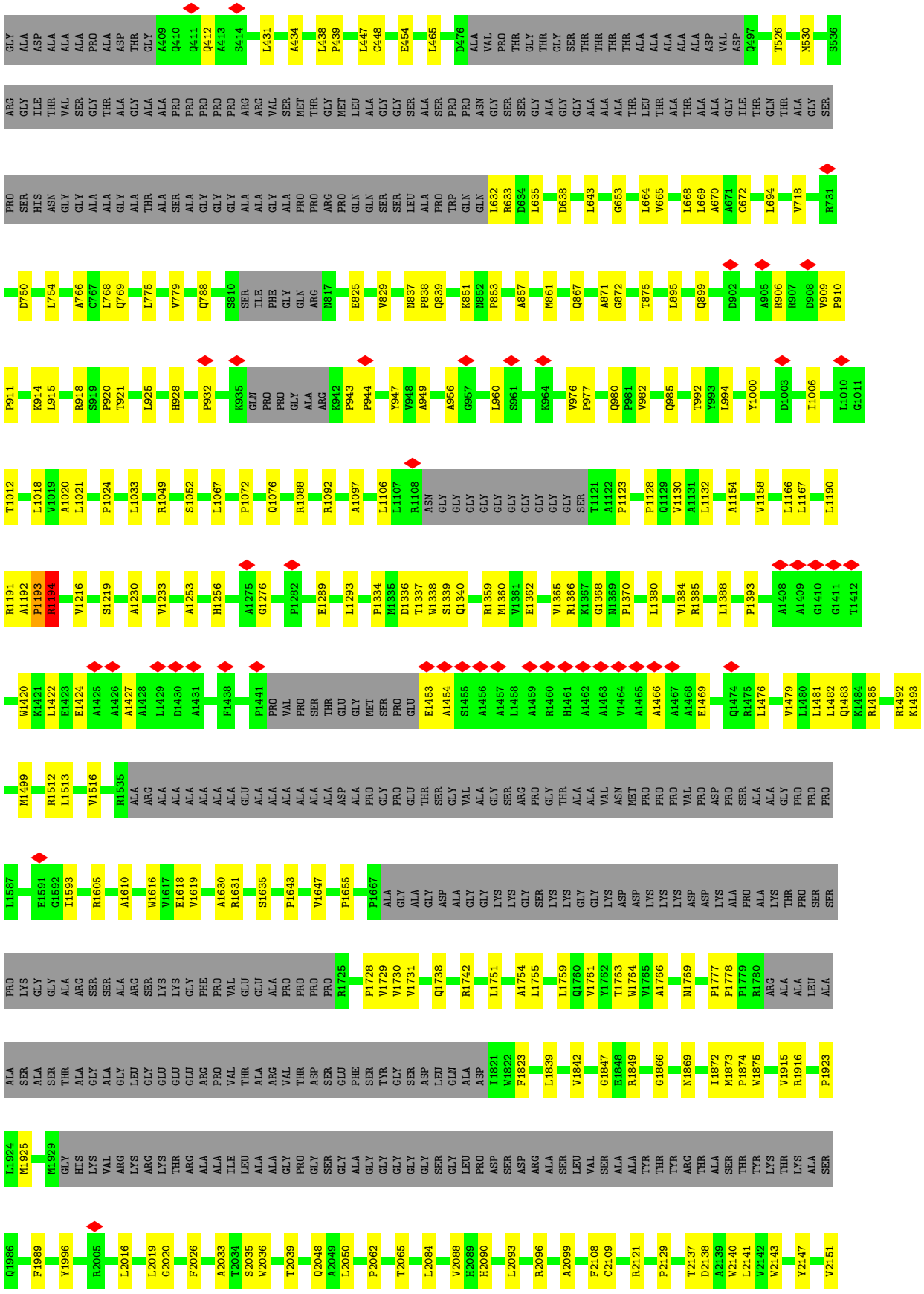


• Molecule 7: FAP54

Chain 1O:



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ARG GLY ILE THR VAL SER GLY THR ALA GLY ALA ALA PRO PRO PRO PRO PRO ARG ARG VAL SER MET THR GLY MET LEU ALA GLY GLY SER ALA SER PRO PRO ASN GLY SER SER GLY ALA GLY GLY ALA ALA ALA THR LEU THR ALA THR ALA ALA ALA GLY ILE THR GLN THR ALA GLY SER
PRO SER HIS ASN GLY GLY ALA ALA GLY ALA THR ALA SER ALA GLY GLY GLY ALA ALA GLY ALA PRO PRO ARG PRO GLN GLN GLN SER SER SER LEU ALA PRO TRP GLN GLN L632 R633 D634 L635 D638 L643 G653 L664 V665 L668 L669 A670 A671 C672 L694 V718 R731
D750 L754 A766 C767 L768 Q769 L775 V779 Q788 S810 SER ILE PHE GLY GLN ARG N817 E825 V829 N837 P838 Q839 K851 N852 P853 A857 M861 Q867 A871 G872 T875 L895 Q899 D902 A905 R906 D908 V909 P910
P911 K914 L915 R918 S919 P920 T921 L925 H928 P932 K935 GLN PRO PRO GLY ALA ARG K942 P943 P944 Y947 V948 A949 A956 G957 L960 S961 K964 V976 P977 Q980 P981 V982 Q985 T992 Y993 L994 Y1000 D1003 I1006 L1010 G1011
T1012 L1018 V1019 A1020 L1021 P1024 L1033 R1049 S1052 L1067 P1072 Q1076 R1088 R1092 A1097 L1106 L1107 R1108 ASN GLY GLY GLY GLY GLY GLY GLY GLY SER T1121 A1122 P1123 P1128 Q1129 V1130 A1131 L1132 A1154 V1158 L1166 L1167 L1190
R1191 A1192 P1193 R1194 V1216 S1219 A1230 V1233 A1253 H1256 A1275 G1276 P1282 E1289 L1293 P1334 M1335 D1336 T1337 W1338 S1339 Q1340 R1359 M1360 V1361 E1362 V1365 R1366 K1367 G1368 N1369 P1370 L1380 V1384 R1385 L1388 P1393 A1408 A1409 G1410 G1411 T1412
W1420 K1421 L1422 E1423 E1424 A1425 A1426 A1427 A1428 L1429 D1430 A1431 F1438 P1441 PRO VAL PRO SER THR GLU GLY MET SER PRO GLU E1453 A1454 S1455 A1456 A1457 L1458 A1459 R1460 H1461 A1462 A1463 V1464 A1465 A1466 A1467 A1468 E1469 Q1474 R1475 L1476 V1479 L1480 L1481 L1482 Q1483 K1484 R1485 R1492 K1493
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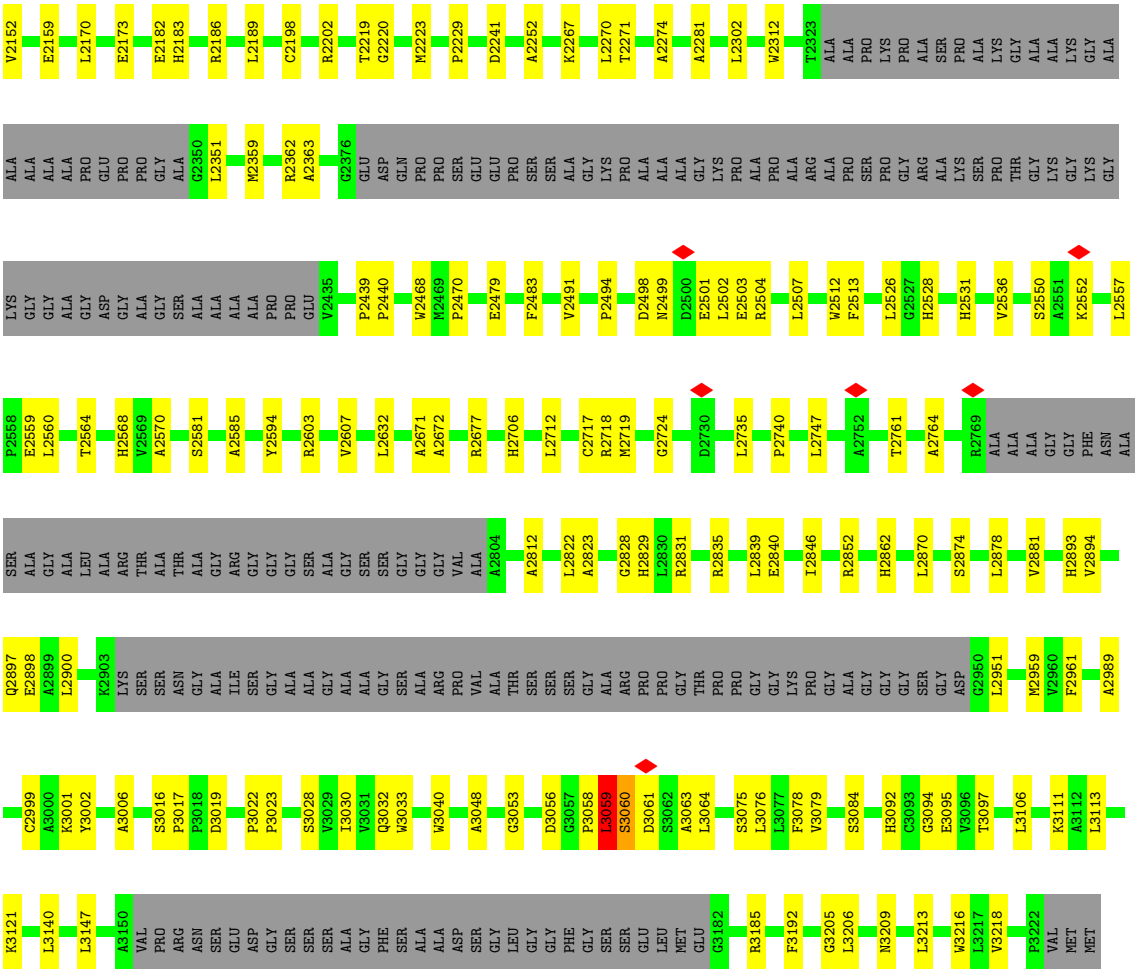
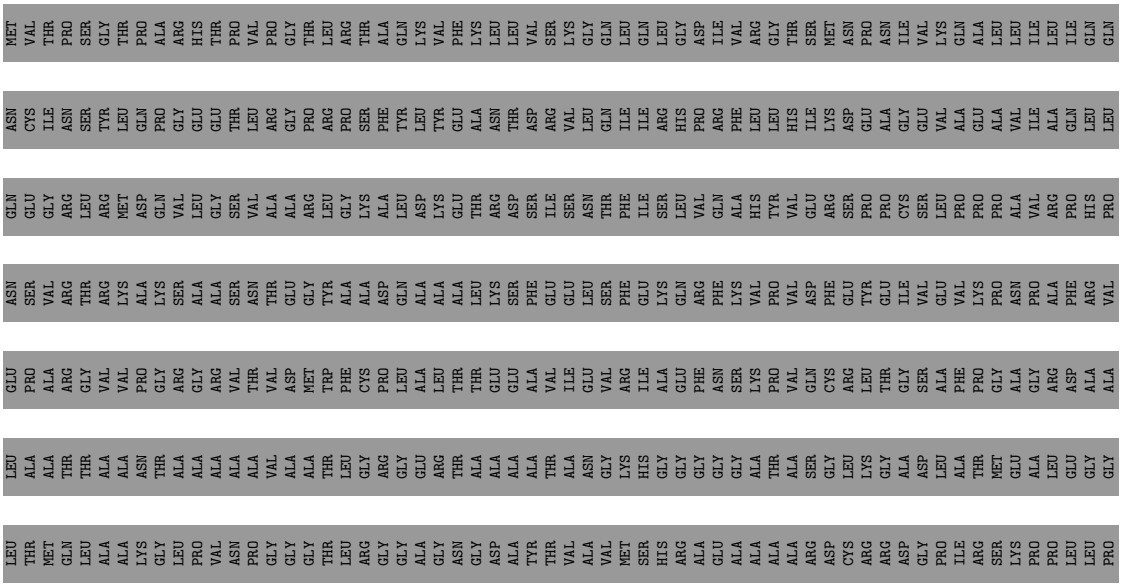
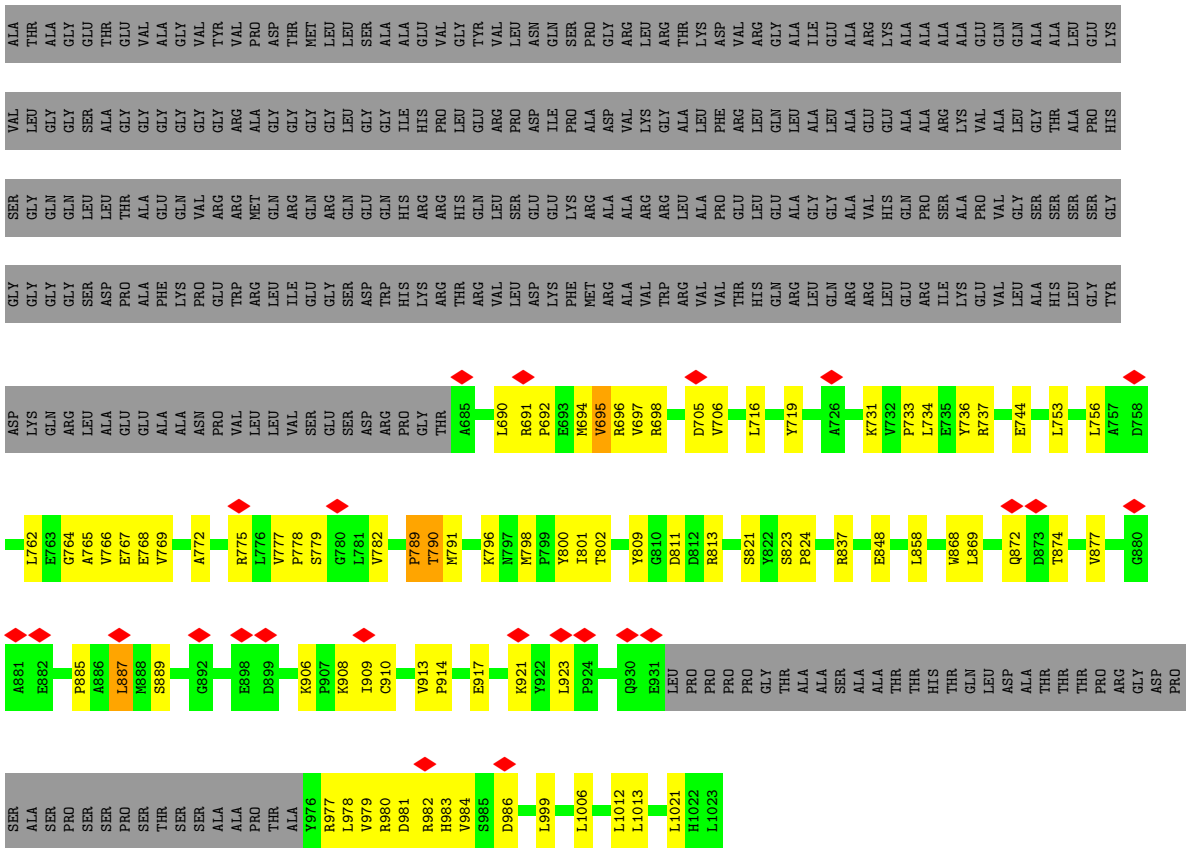


• Molecule 8: HTH_9 domain-containing protein

Chain 1P:



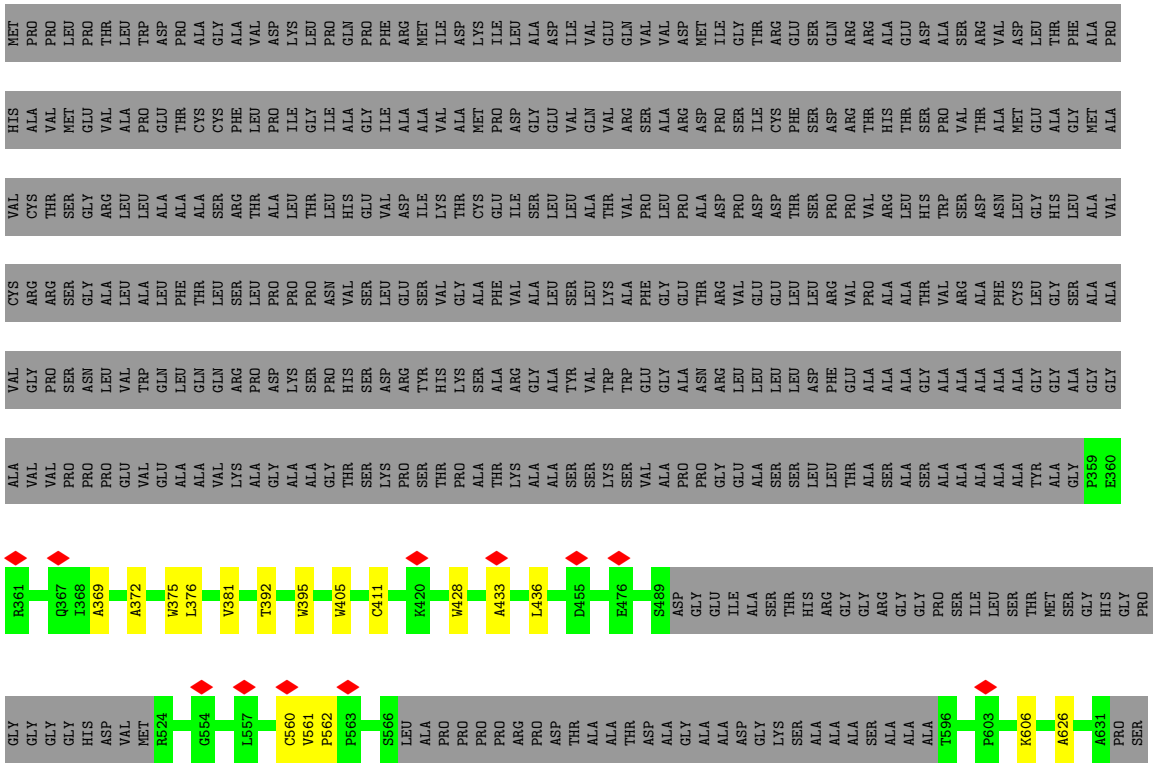


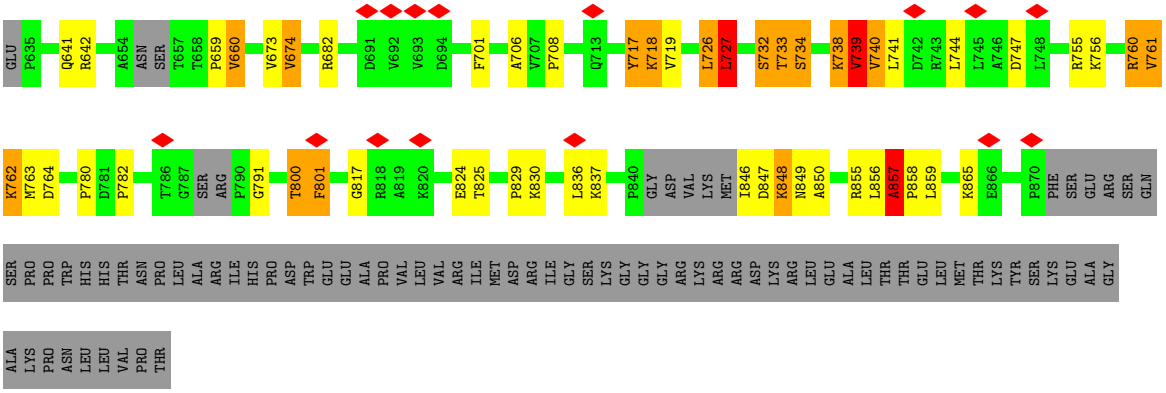


• Molecule 9: FAP297

Chain 1Q:



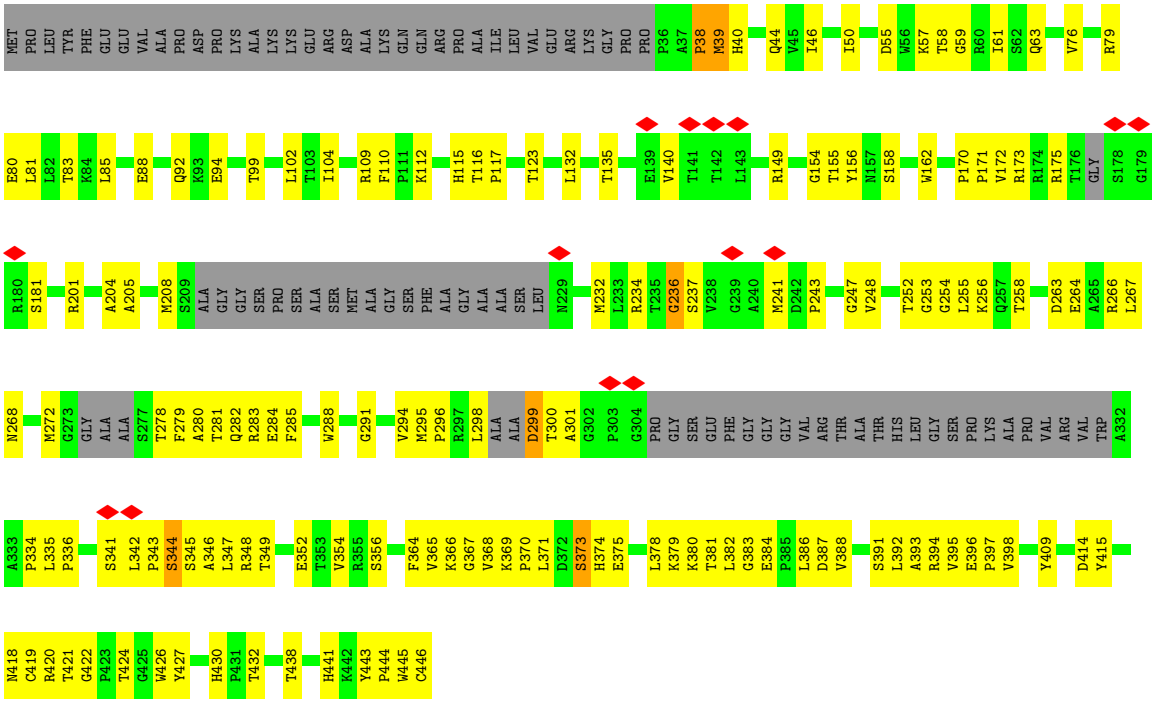




• Molecule 10: FAP108

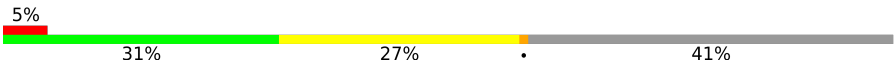
Chain 1R:

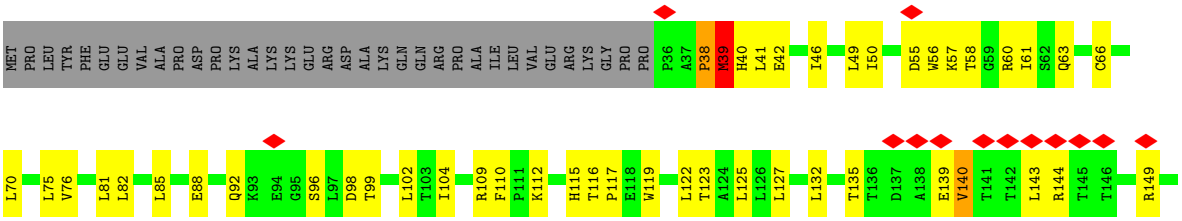


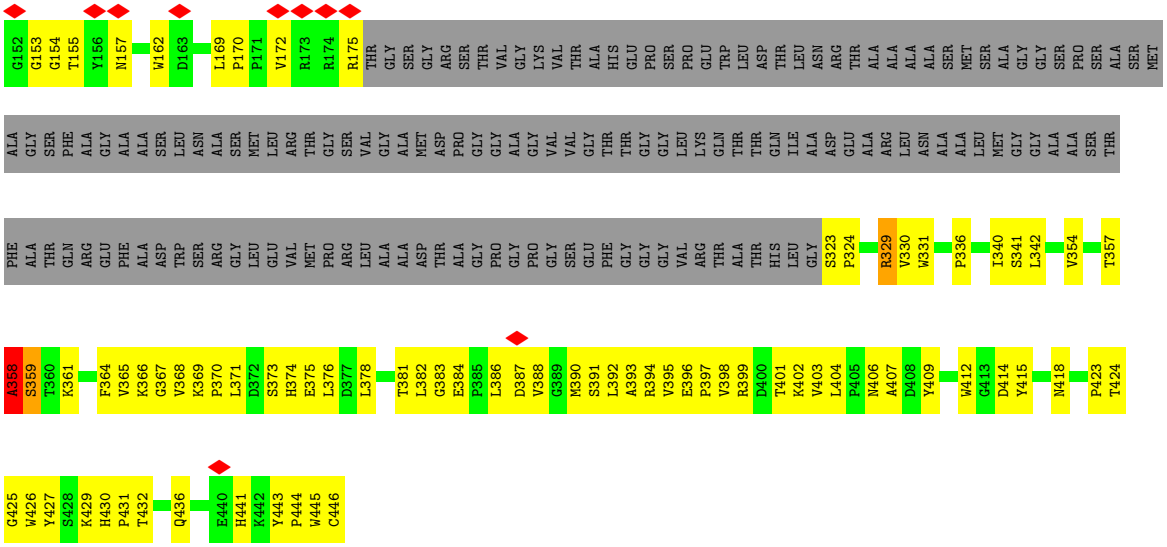


• Molecule 10: FAP108

Chain 1S:



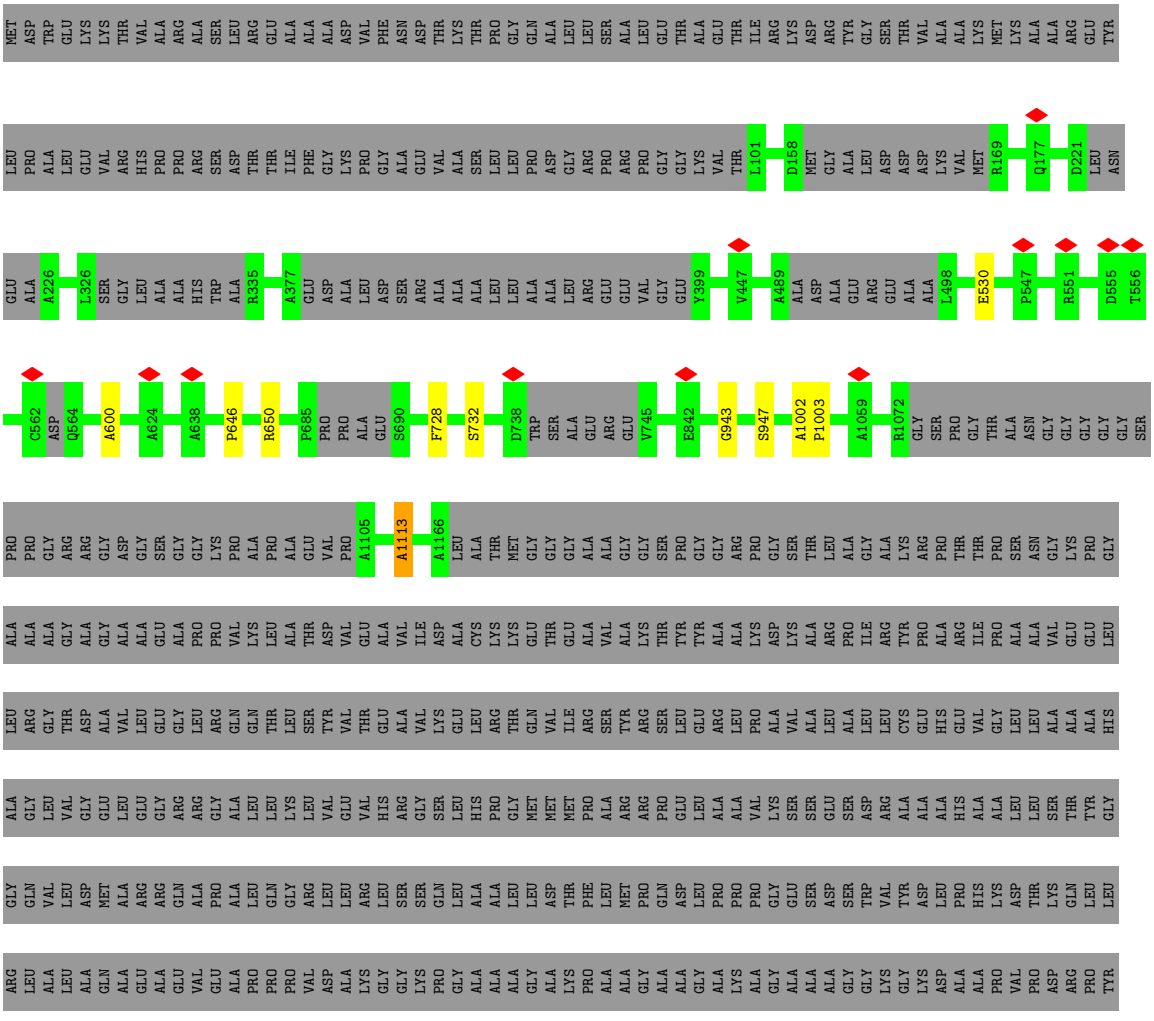


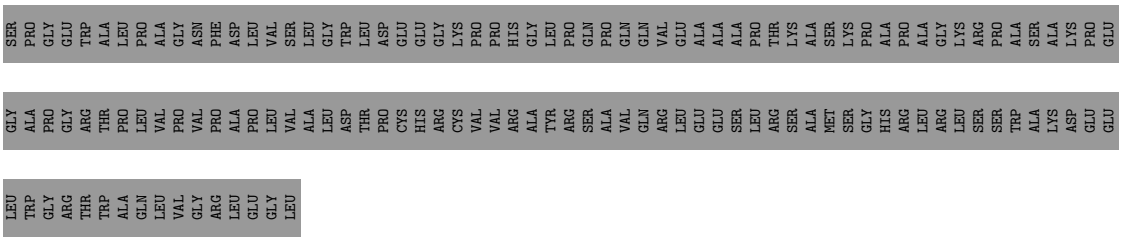


• Molecule 11: FAP76

Chain 1T:



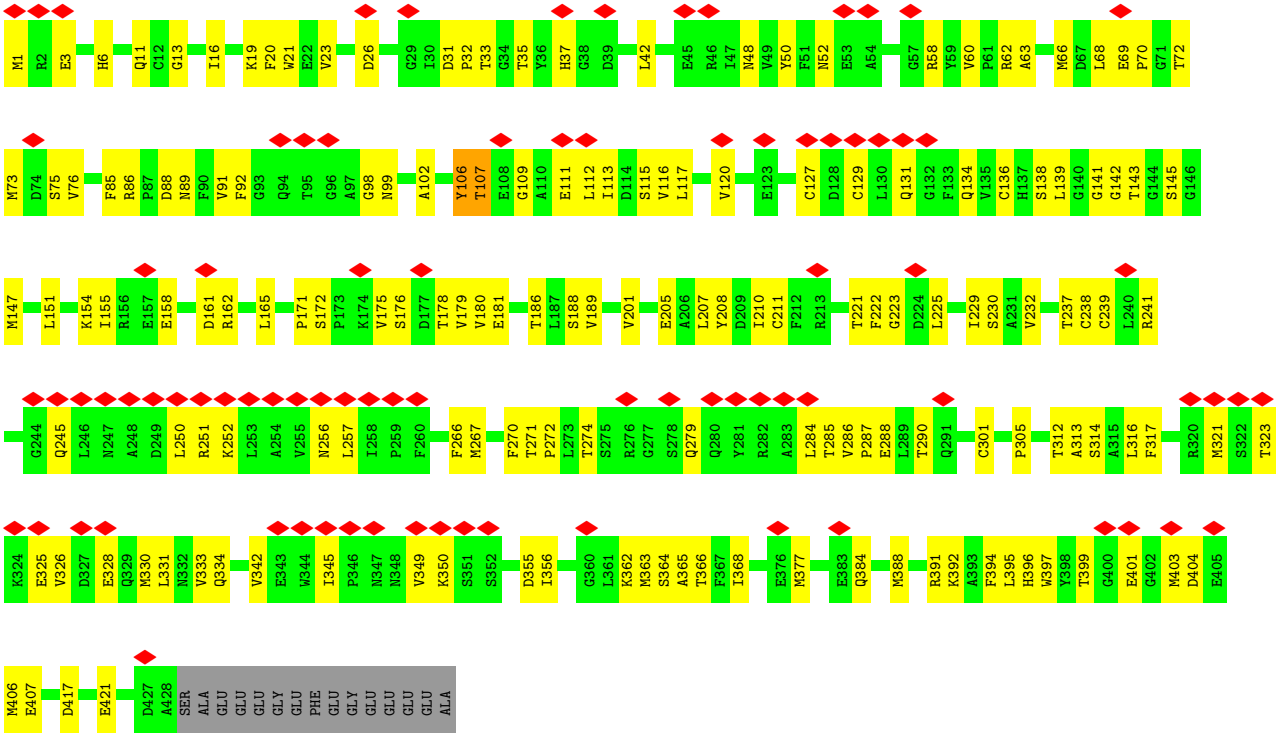




• Molecule 12: Tubulin beta

Chain 1a:

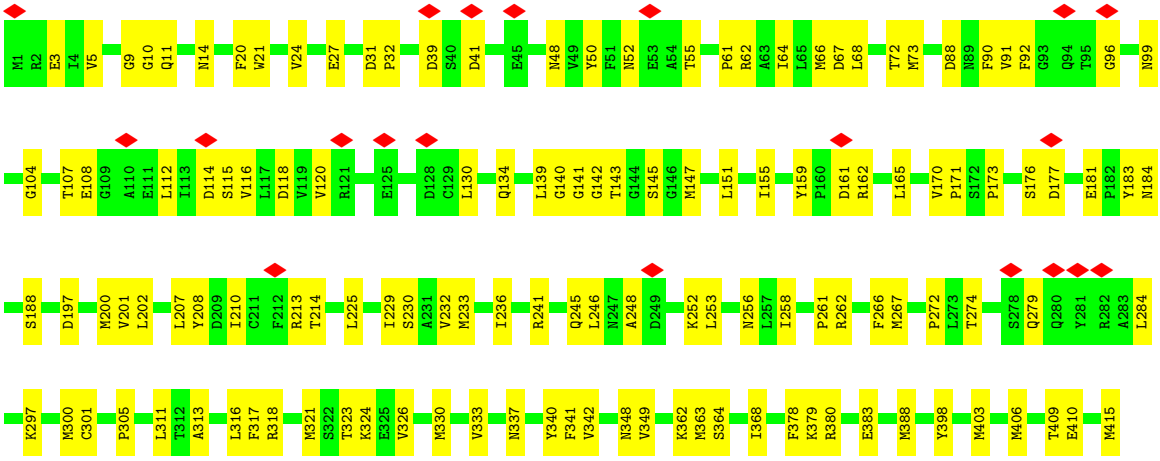


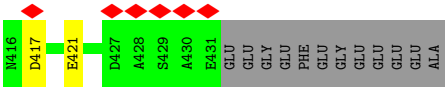


• Molecule 12: Tubulin beta

Chain 1c:



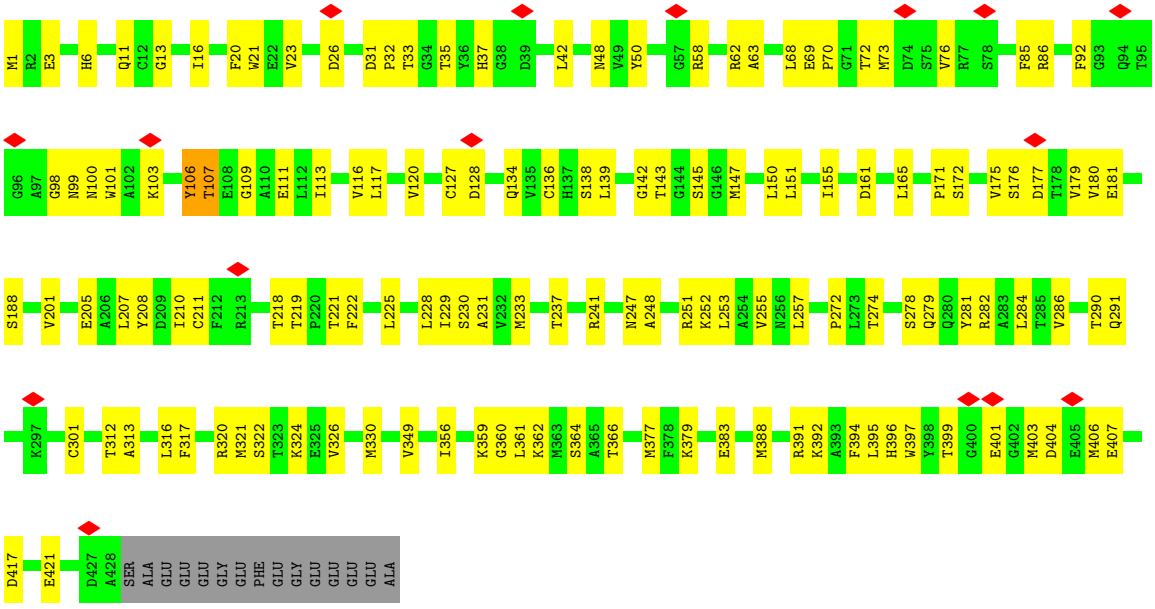




• Molecule 12: Tubulin beta

Chain 1e:

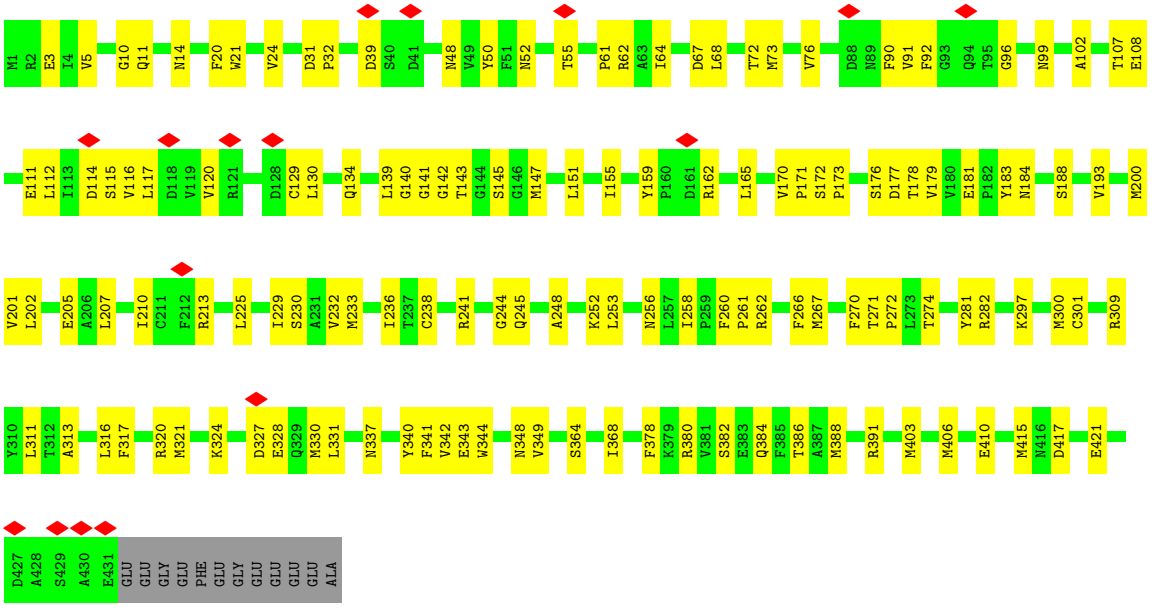




• Molecule 12: Tubulin beta

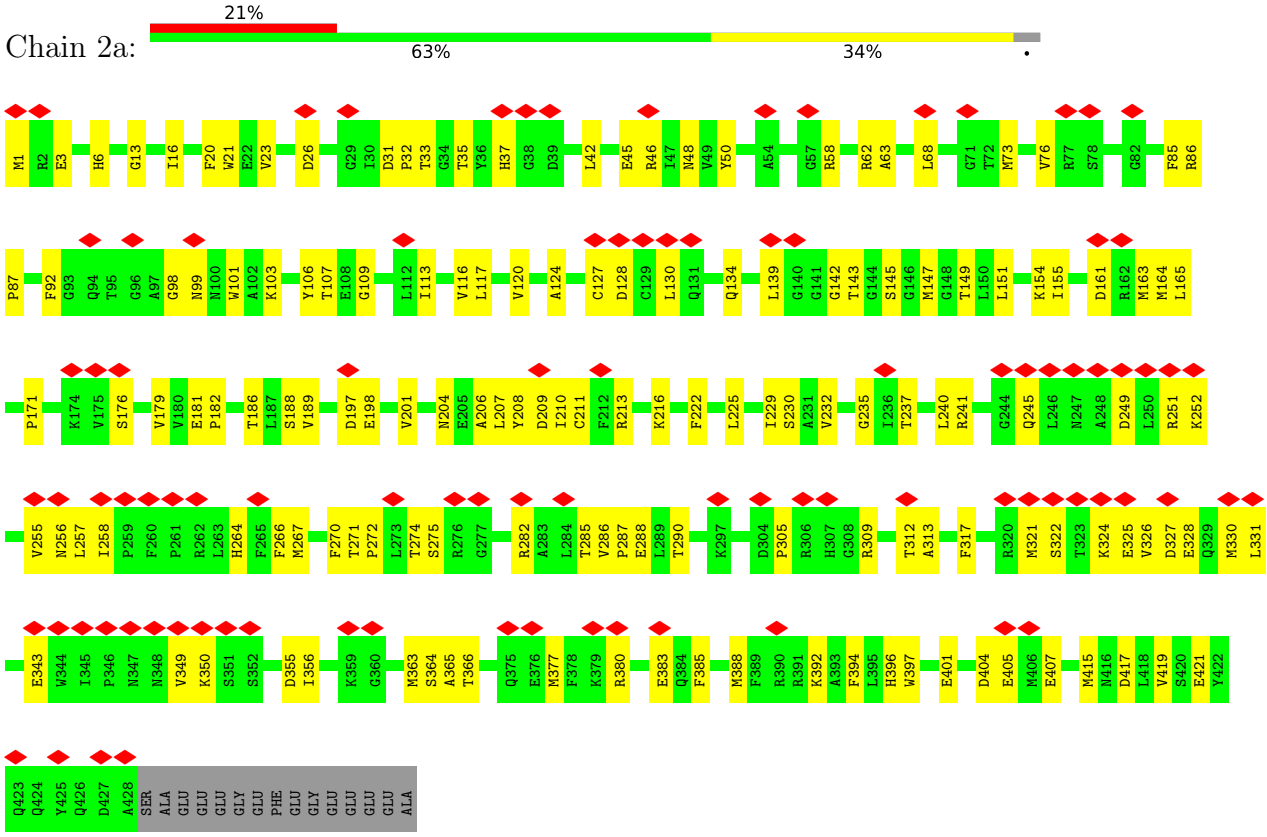
Chain 1g:





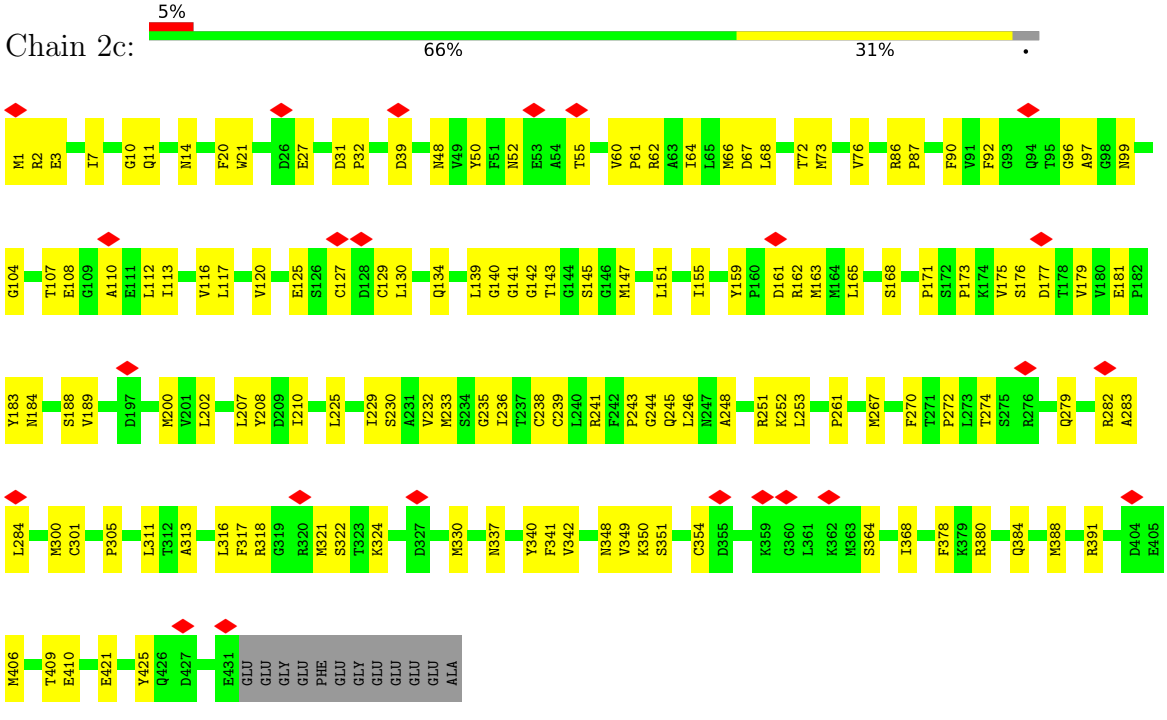
• Molecule 12: Tubulin beta

Chain 2a:



• Molecule 12: Tubulin beta

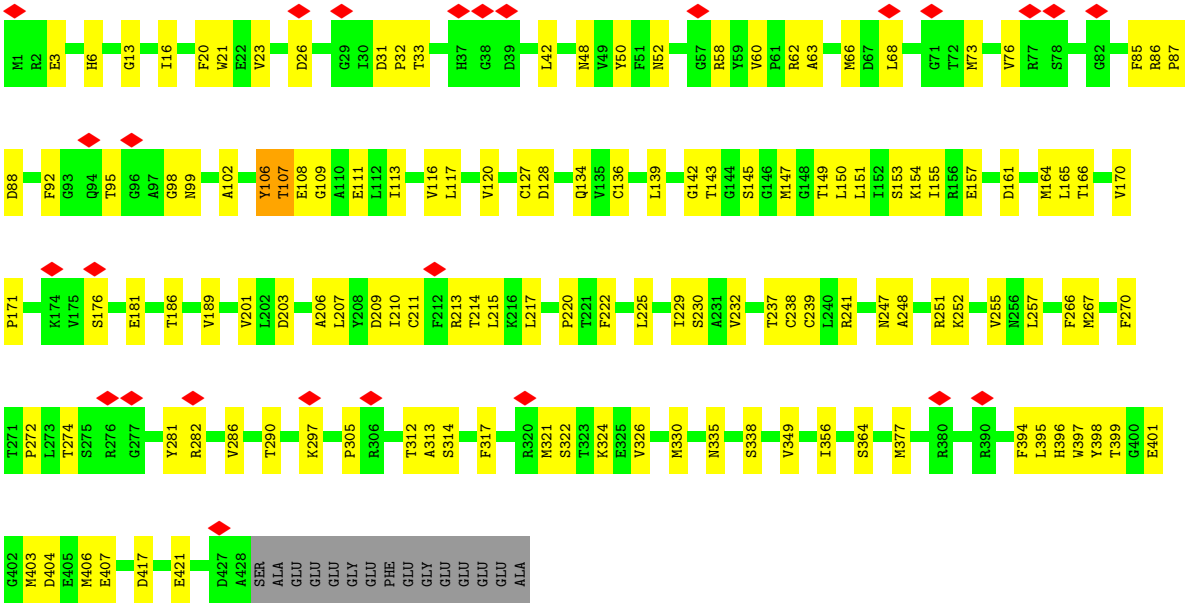
Chain 2c:



• Molecule 12: Tubulin beta

Chain 2e:

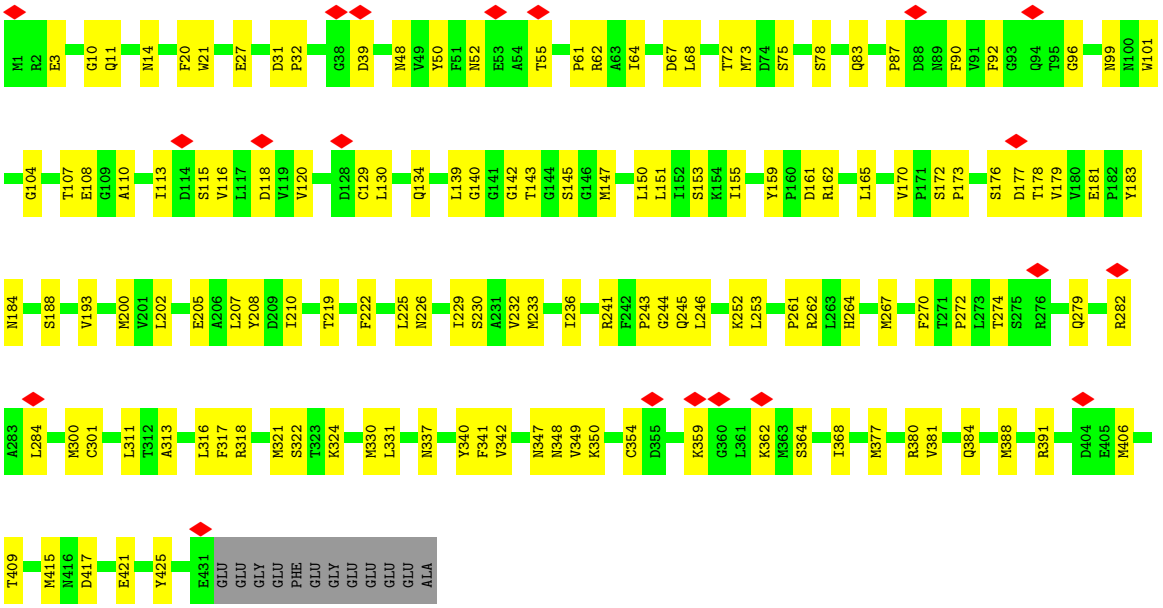




• Molecule 12: Tubulin beta

Chain 2g:

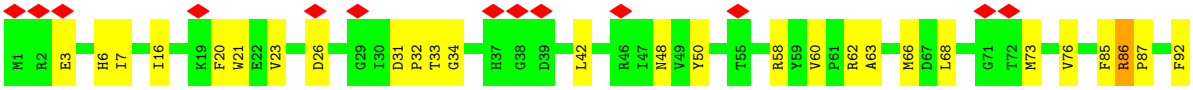


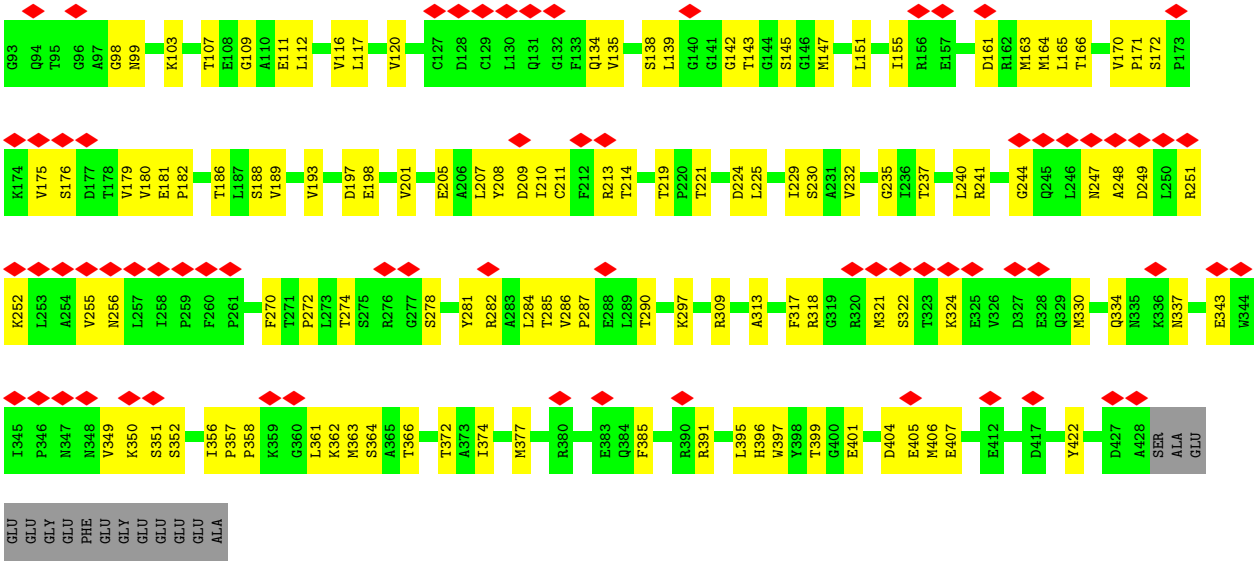


• Molecule 12: Tubulin beta

Chain 3a:



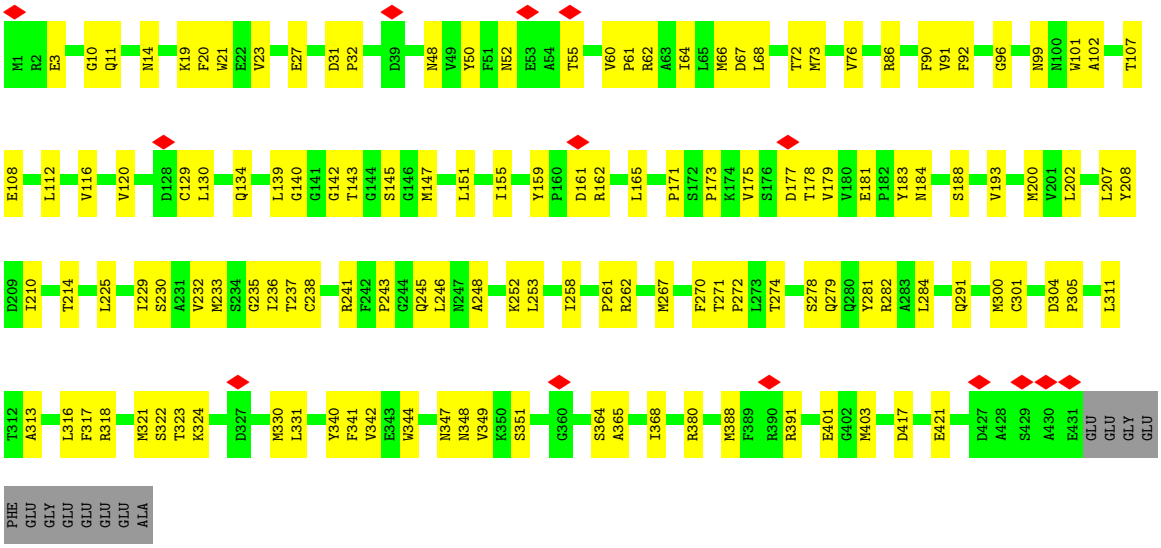




• Molecule 12: Tubulin beta

Chain 3c:

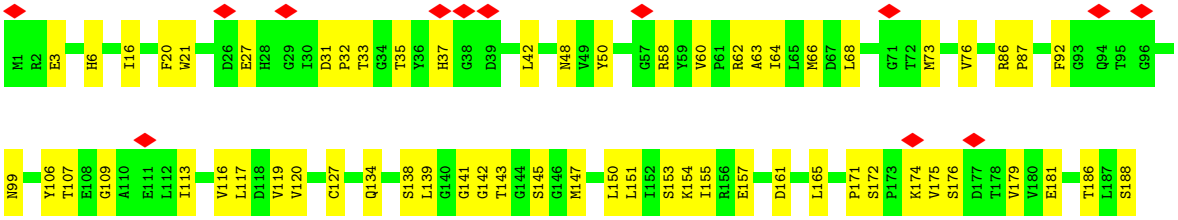


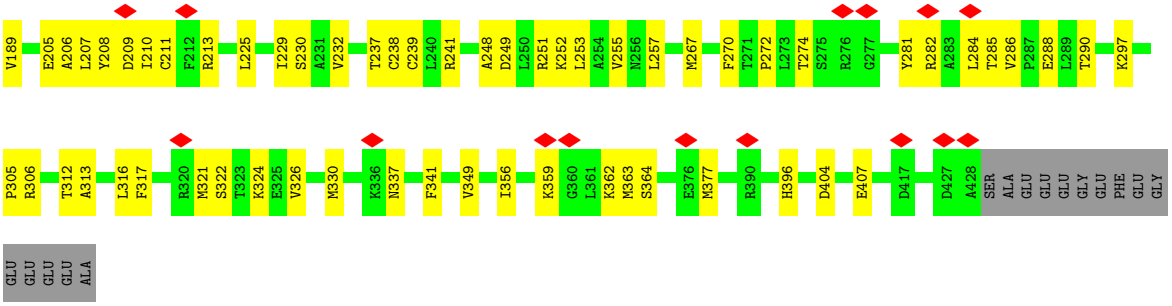


• Molecule 12: Tubulin beta

Chain 3e:



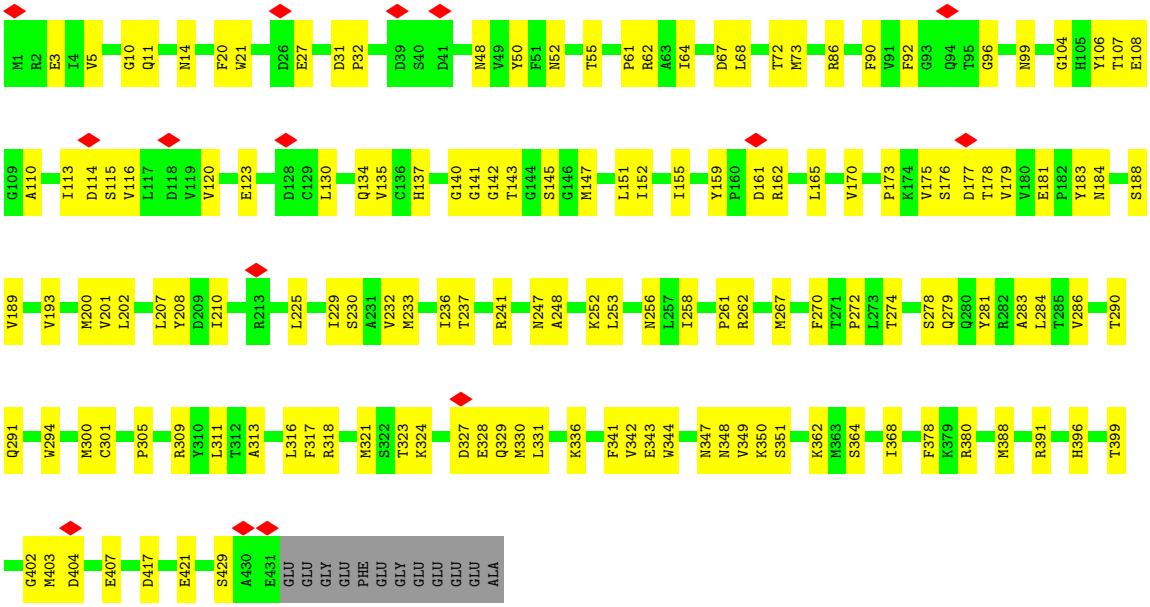




• Molecule 12: Tubulin beta

Chain 3g:

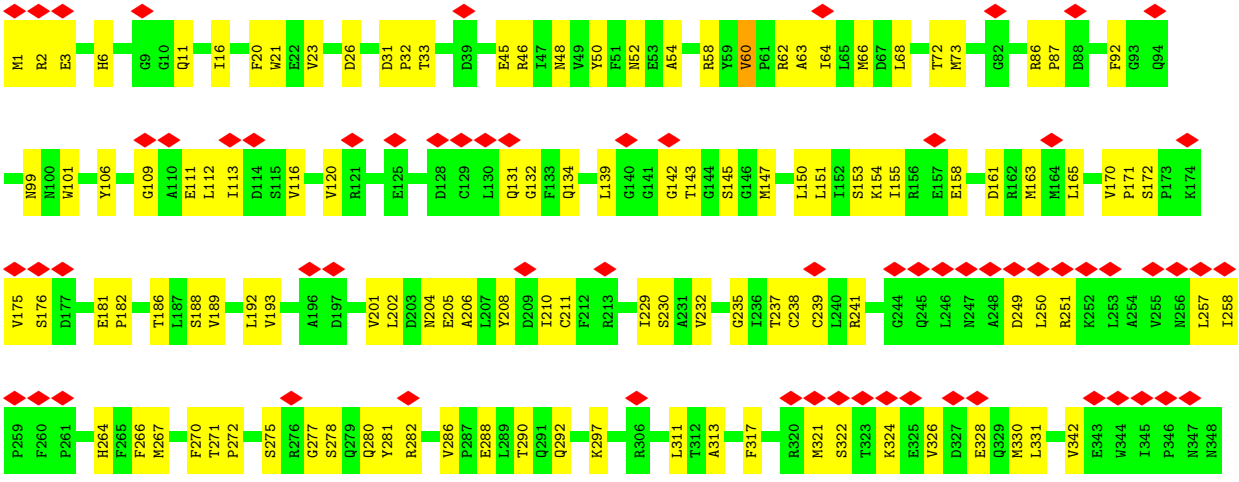


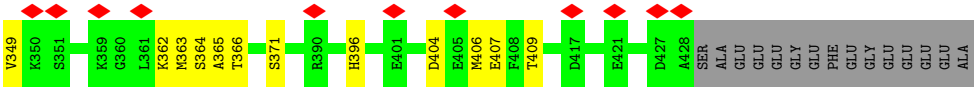


• Molecule 12: Tubulin beta

Chain 4a:



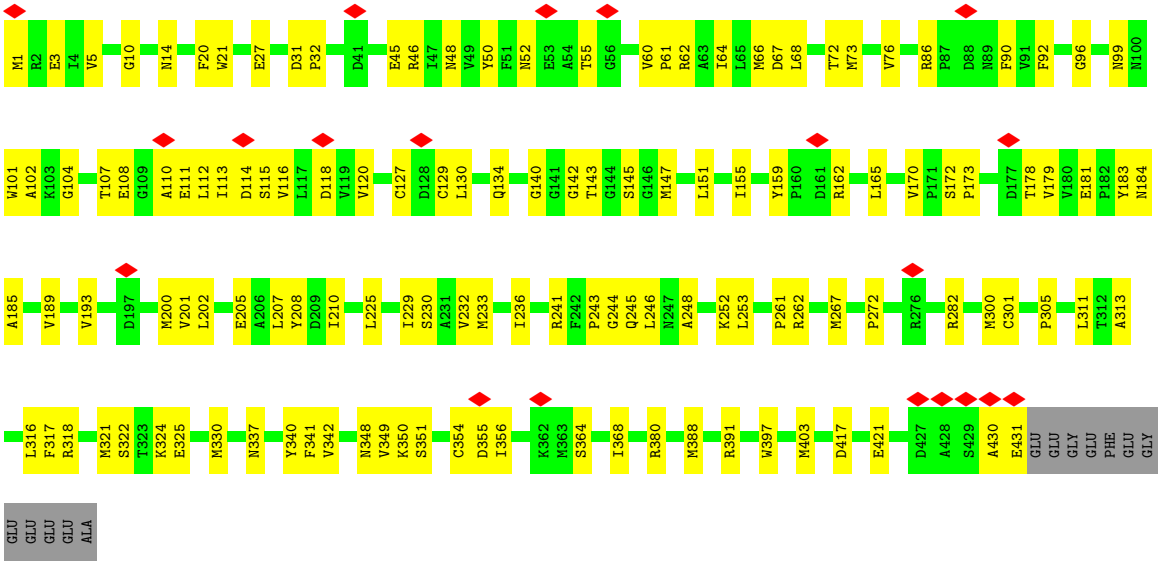




• Molecule 12: Tubulin beta

Chain 4c:

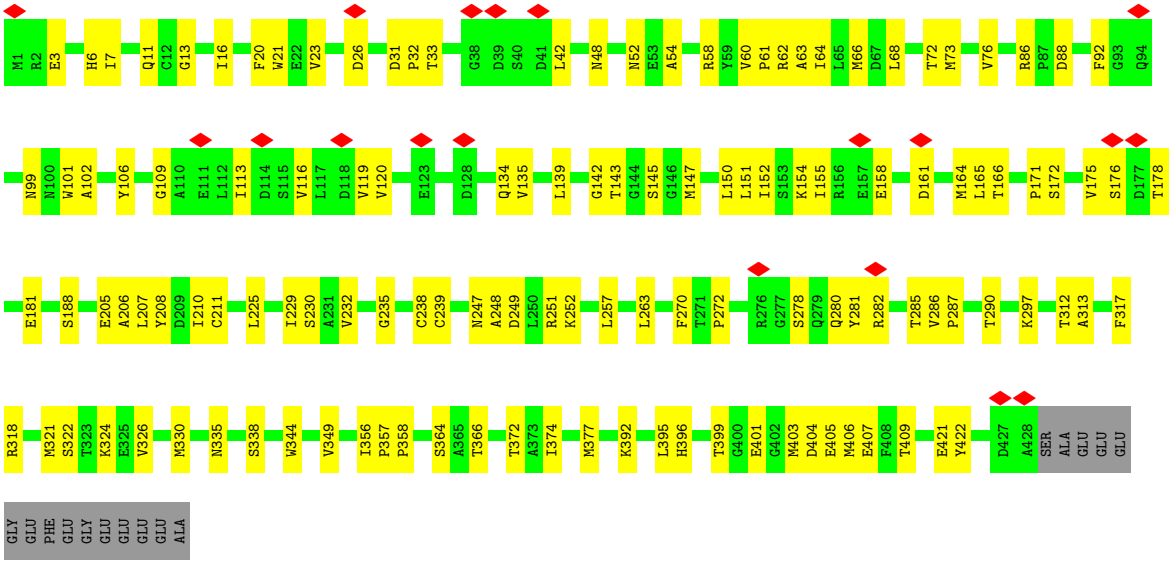




• Molecule 12: Tubulin beta

Chain 4e:

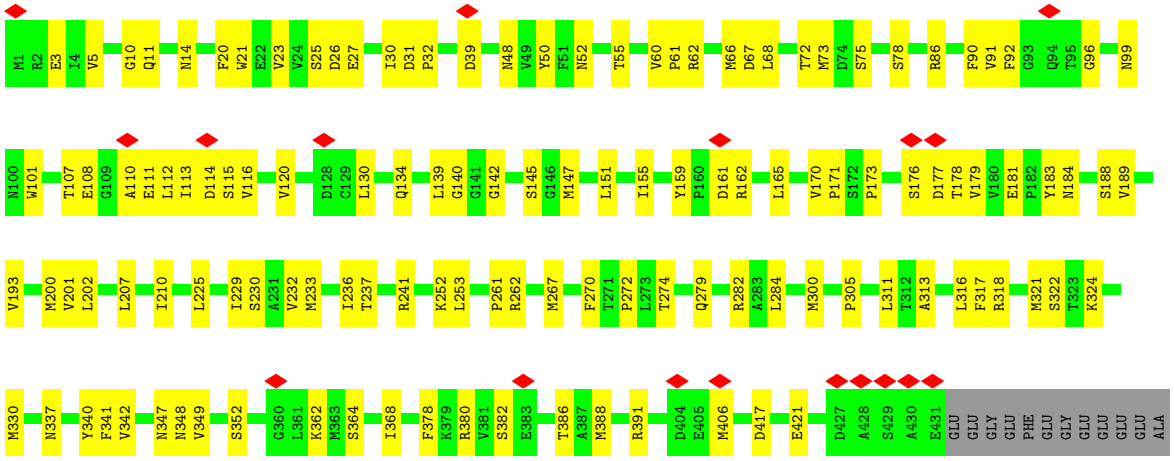




• Molecule 12: Tubulin beta

Chain 4g:

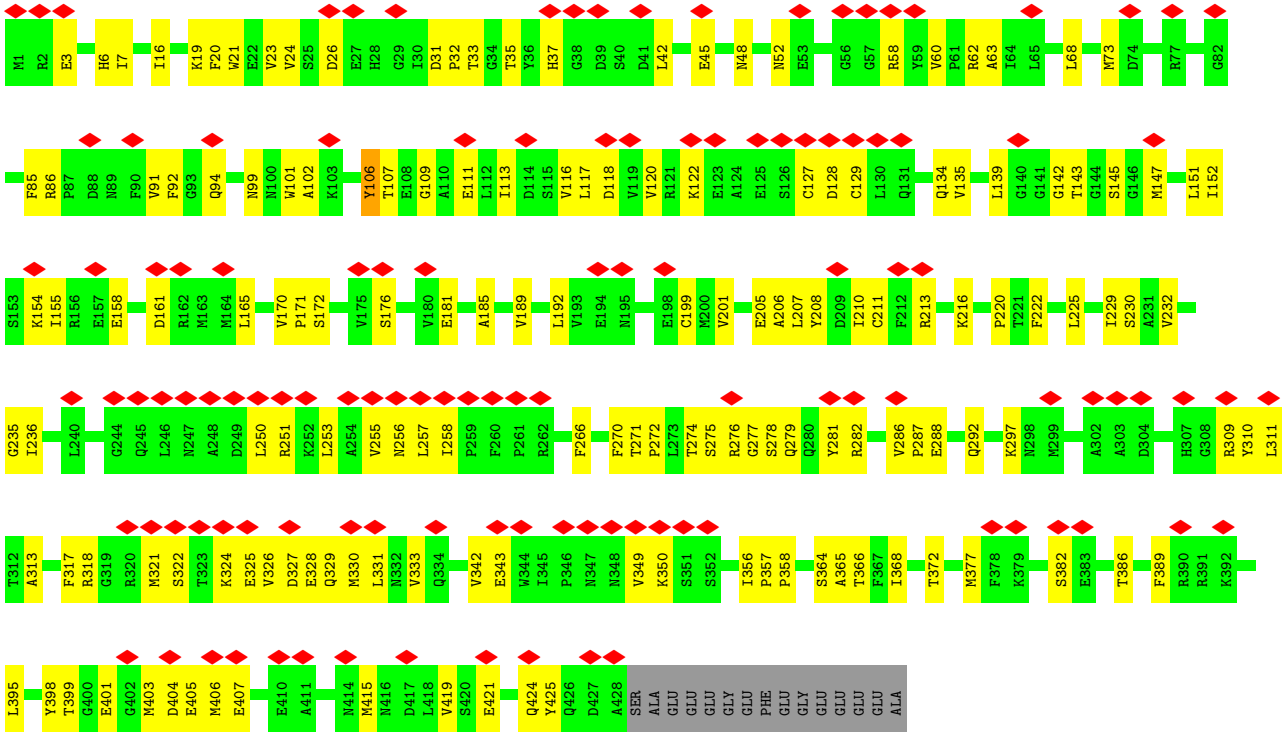




• Molecule 12: Tubulin beta

Chain 5a:

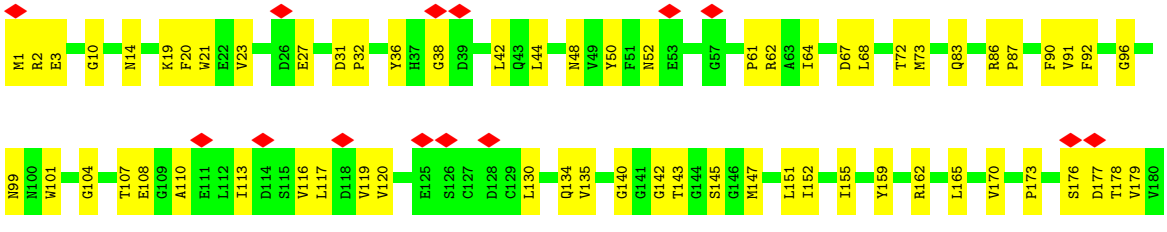


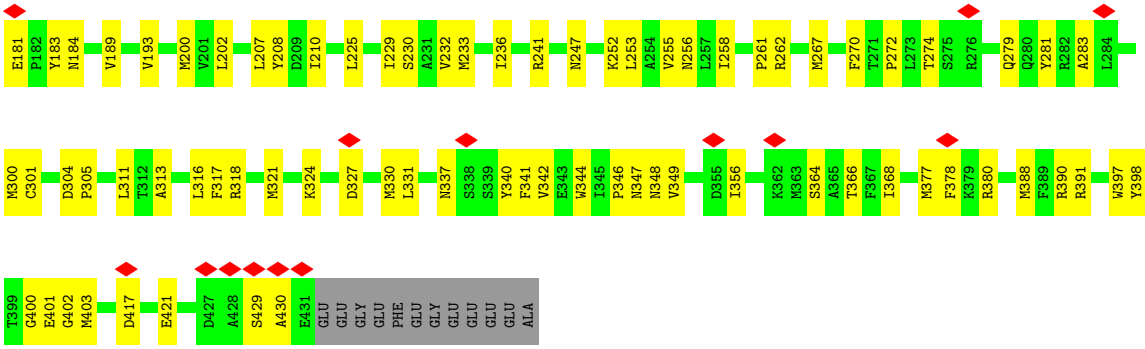


• Molecule 12: Tubulin beta

Chain 5c:



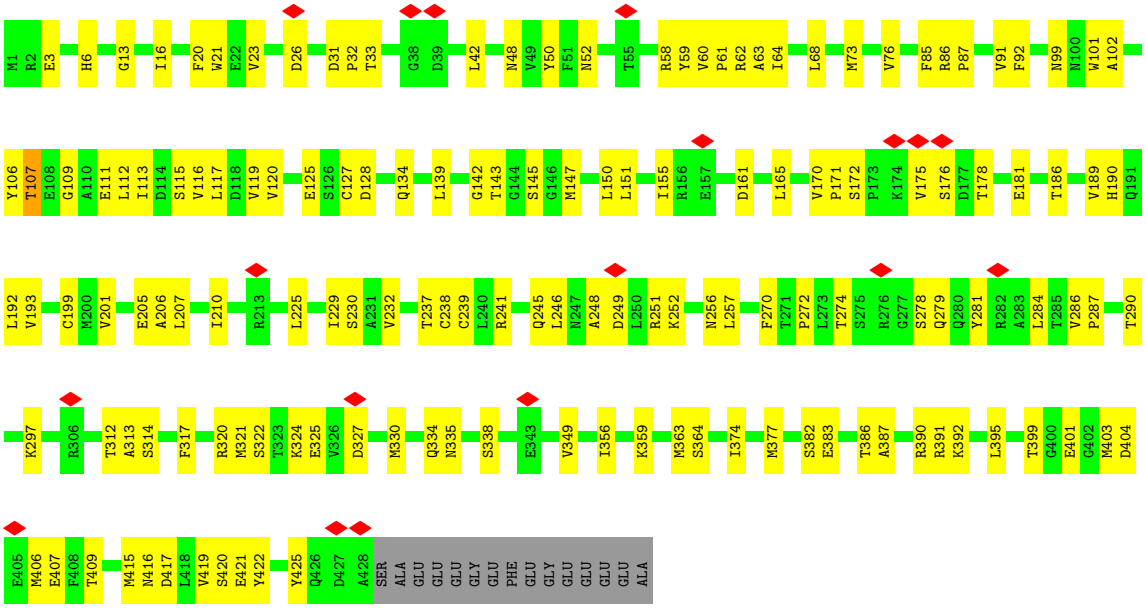




• Molecule 12: Tubulin beta

Chain 5e:

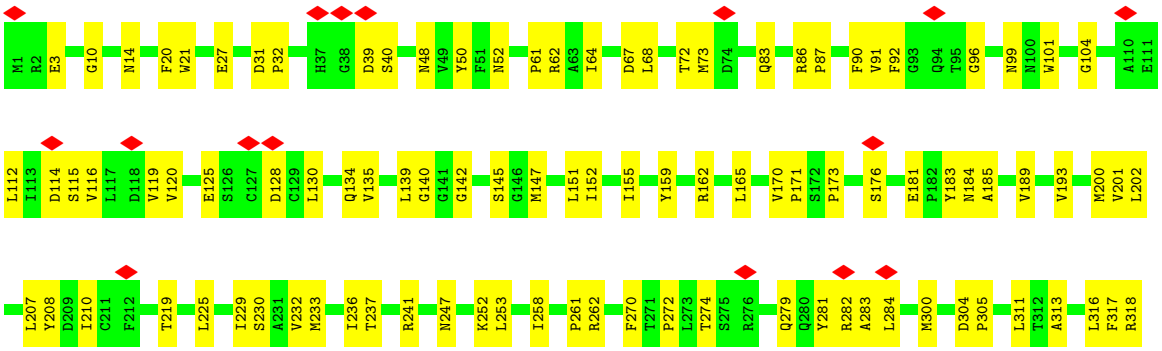


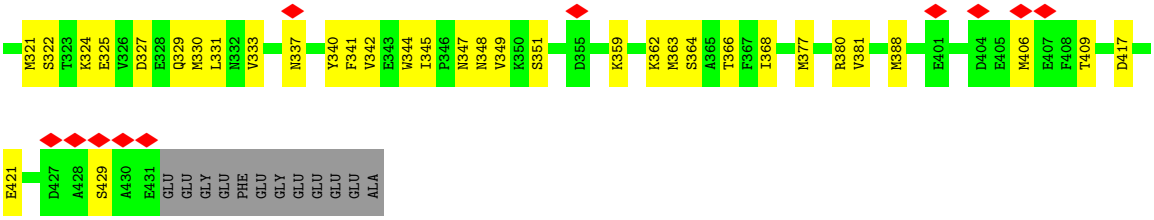


• Molecule 12: Tubulin beta

Chain 5g:



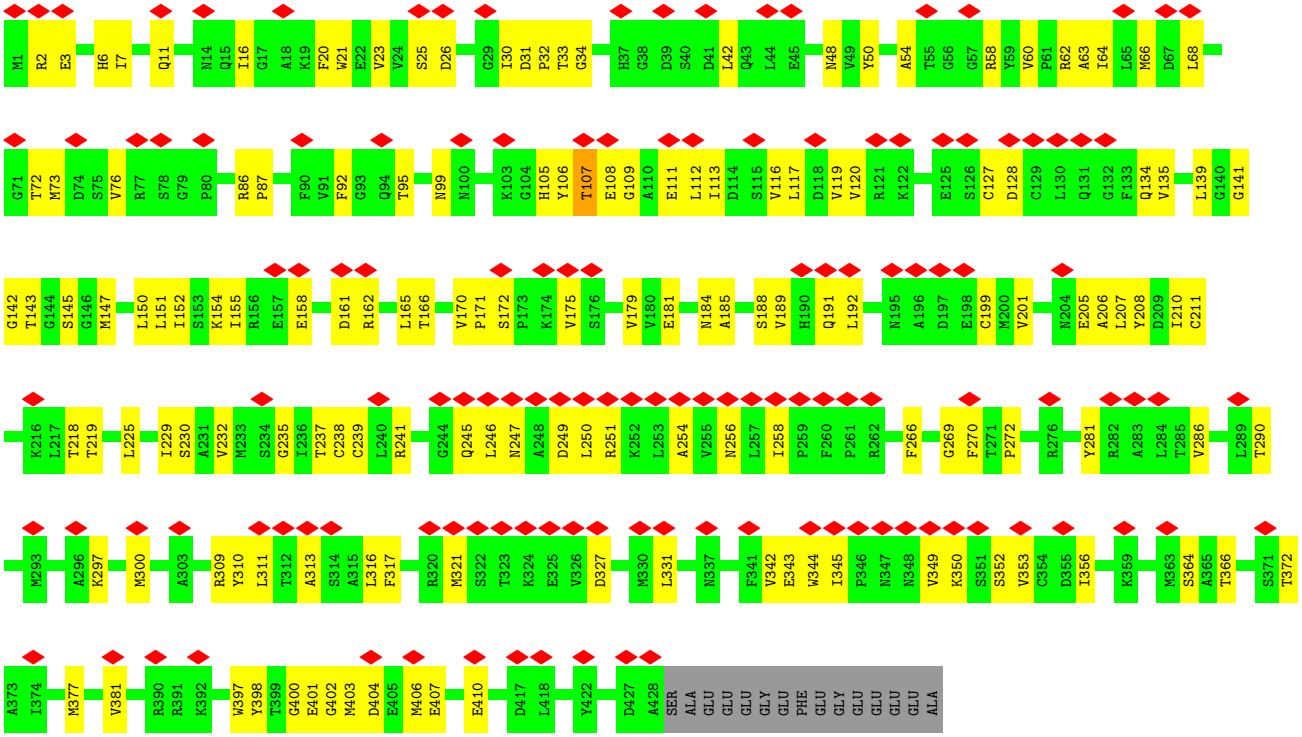




• Molecule 12: Tubulin beta

Chain 6a:

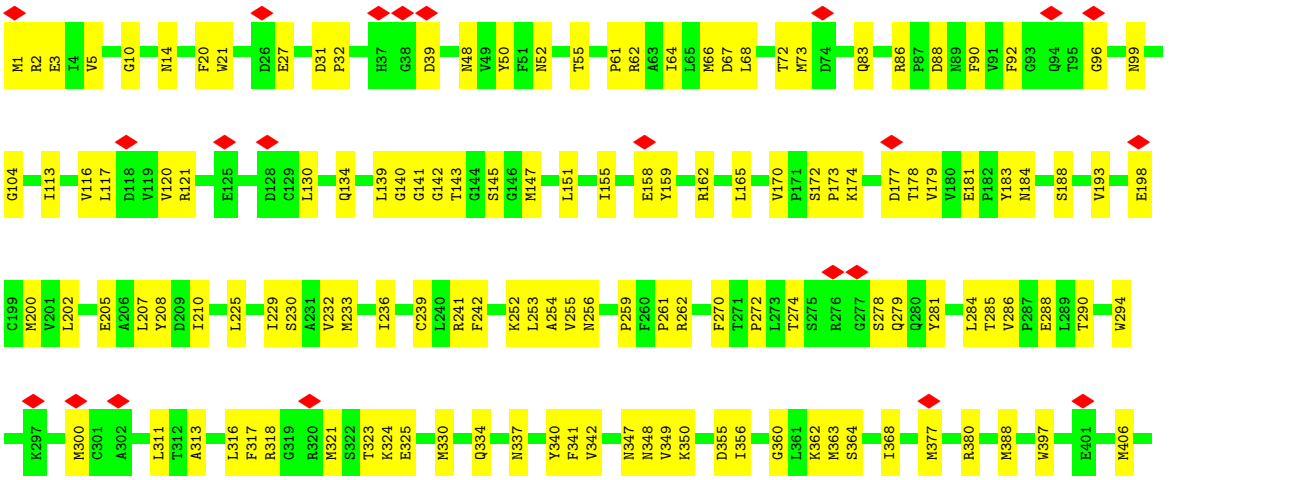


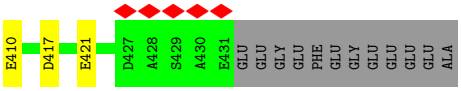


• Molecule 12: Tubulin beta

Chain 6c:



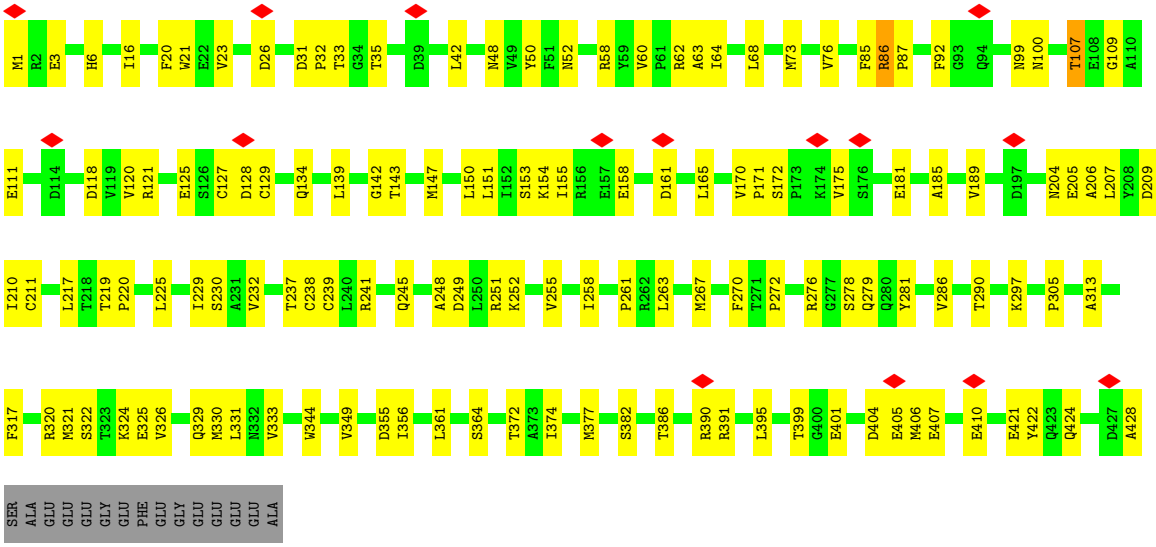




• Molecule 12: Tubulin beta

Chain 6e:

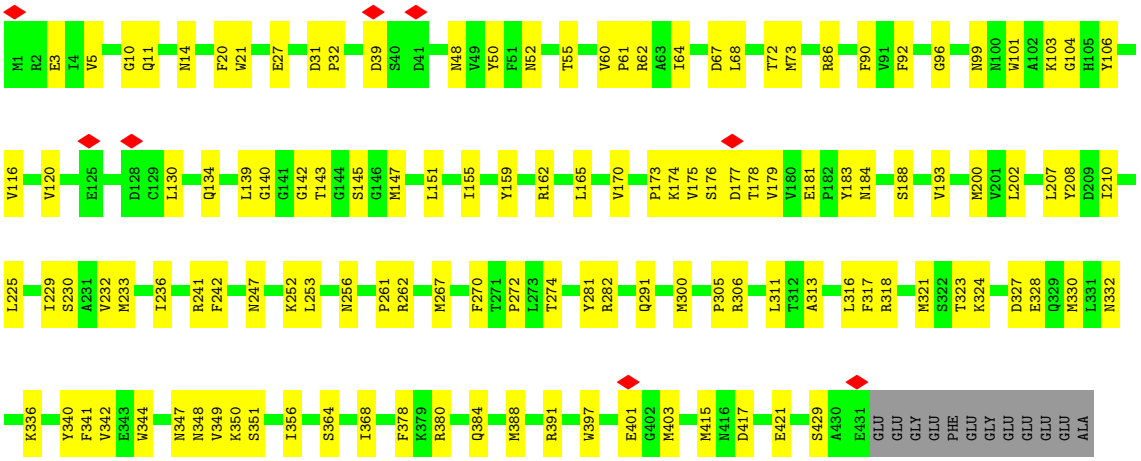




• Molecule 12: Tubulin beta

Chain 6g:

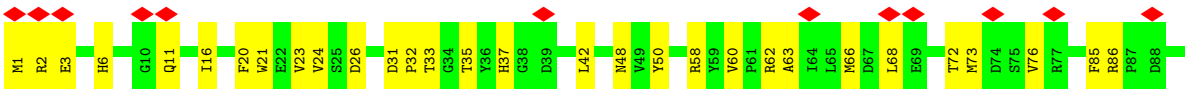


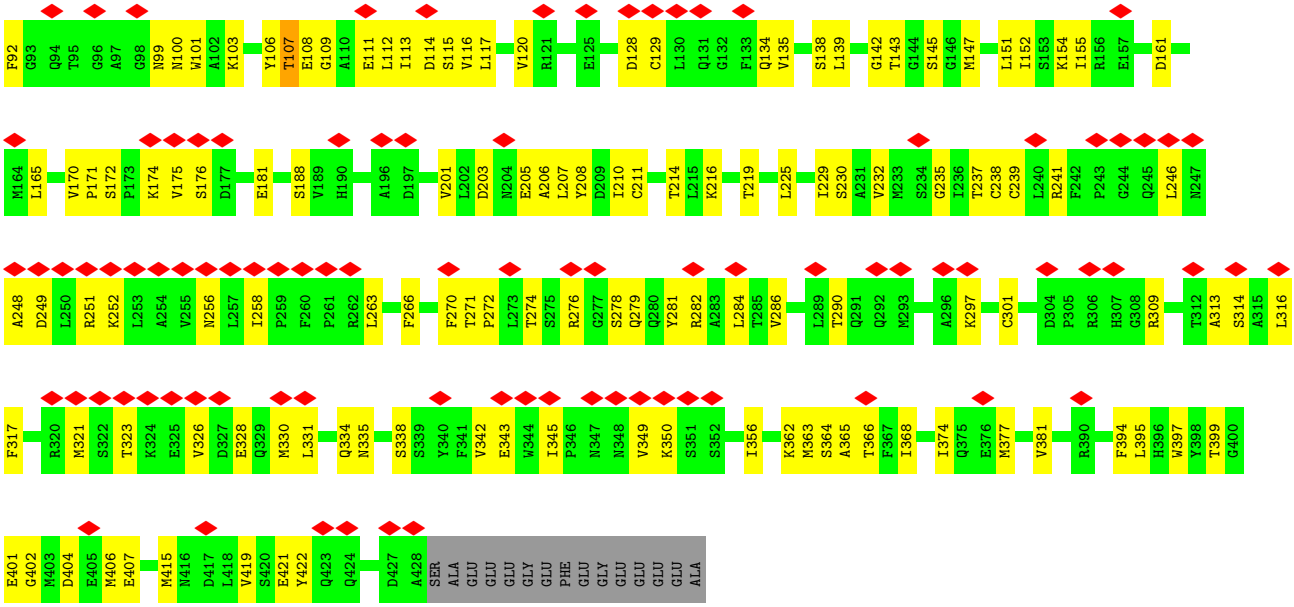


• Molecule 12: Tubulin beta

Chain 7a:



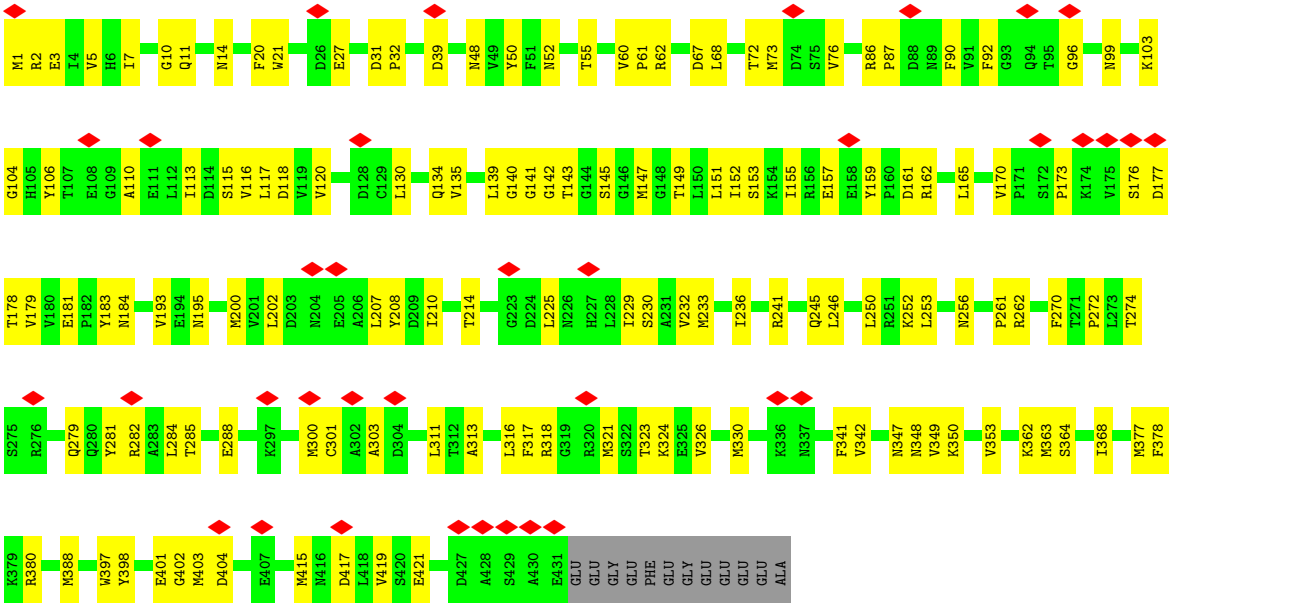




• Molecule 12: Tubulin beta

Chain 7c:

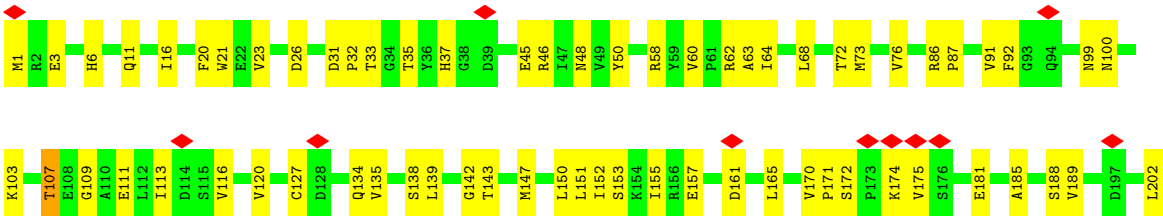


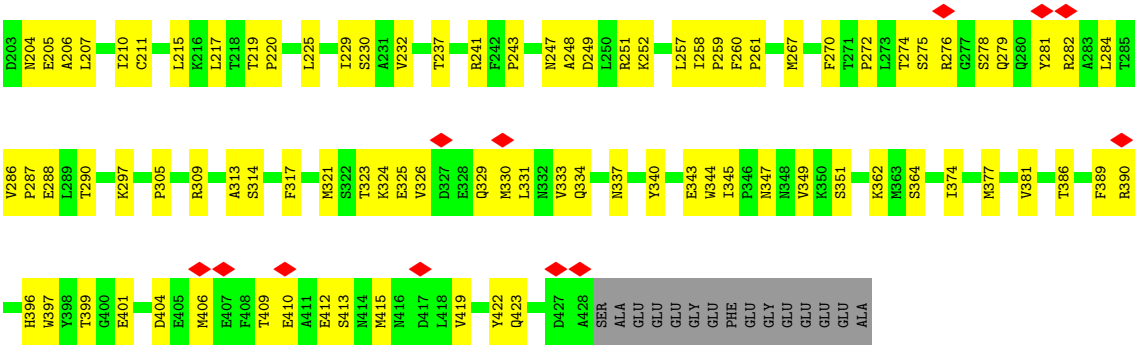


• Molecule 12: Tubulin beta

Chain 7e:



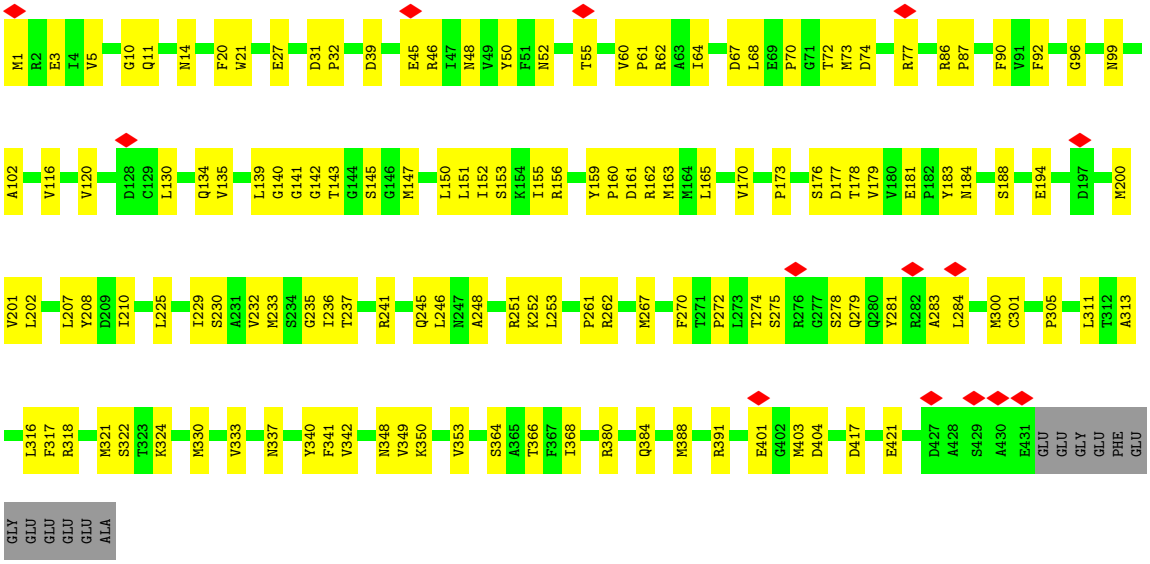




• Molecule 12: Tubulin beta

Chain 7g:

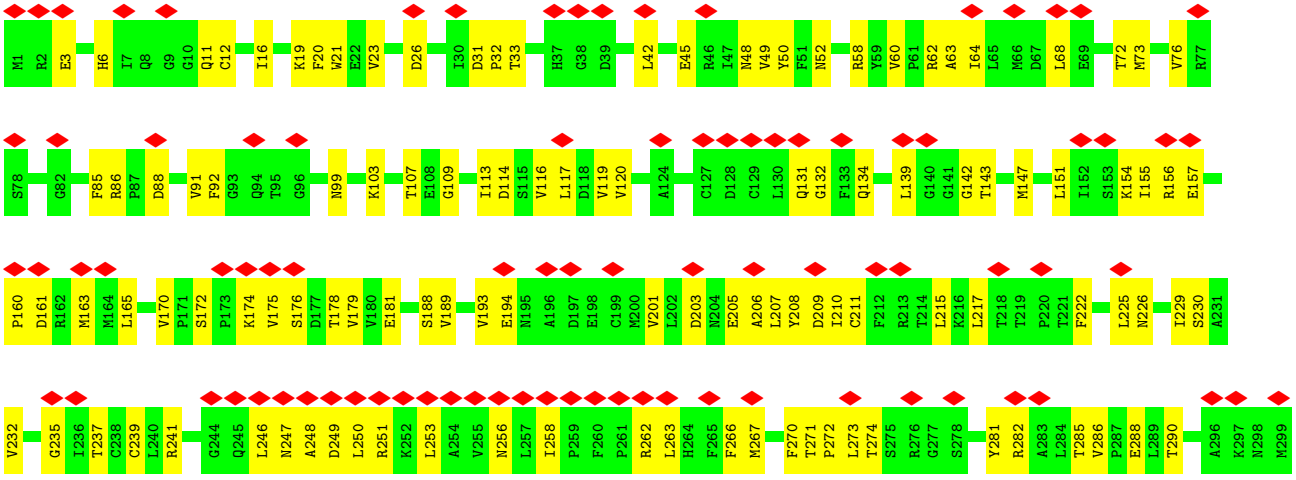


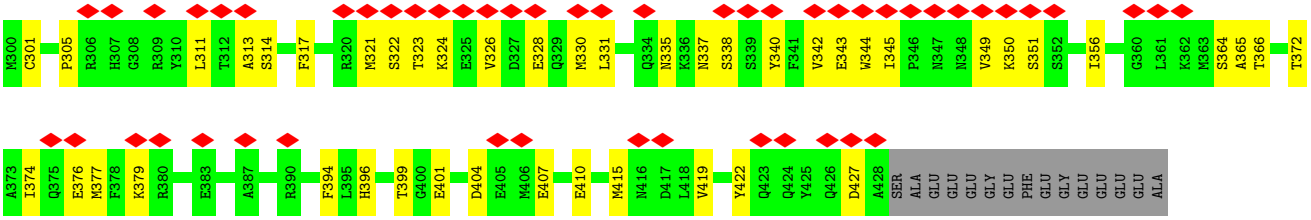


• Molecule 12: Tubulin beta

Chain 8a:



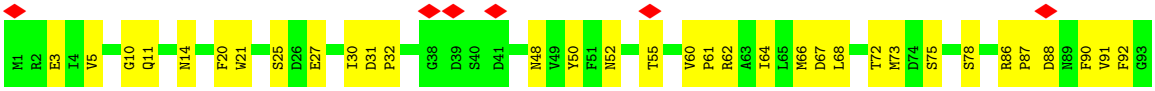




• Molecule 12: Tubulin beta

Chain 8c:

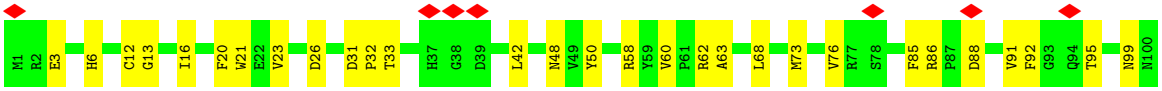




• Molecule 12: Tubulin beta

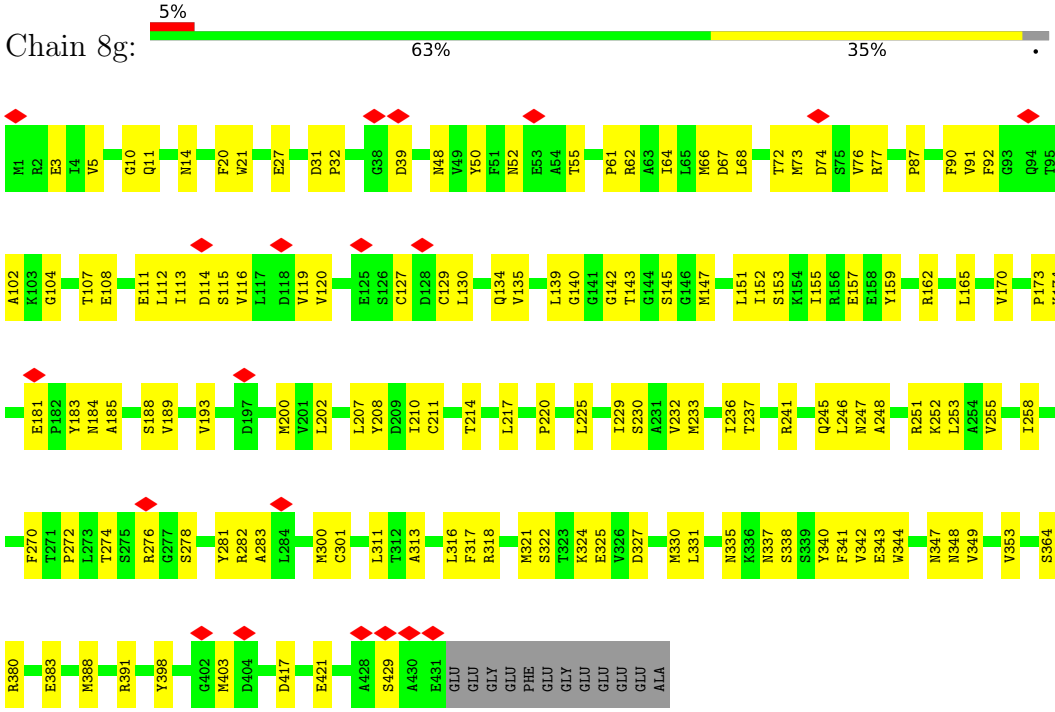
Chain 8e:





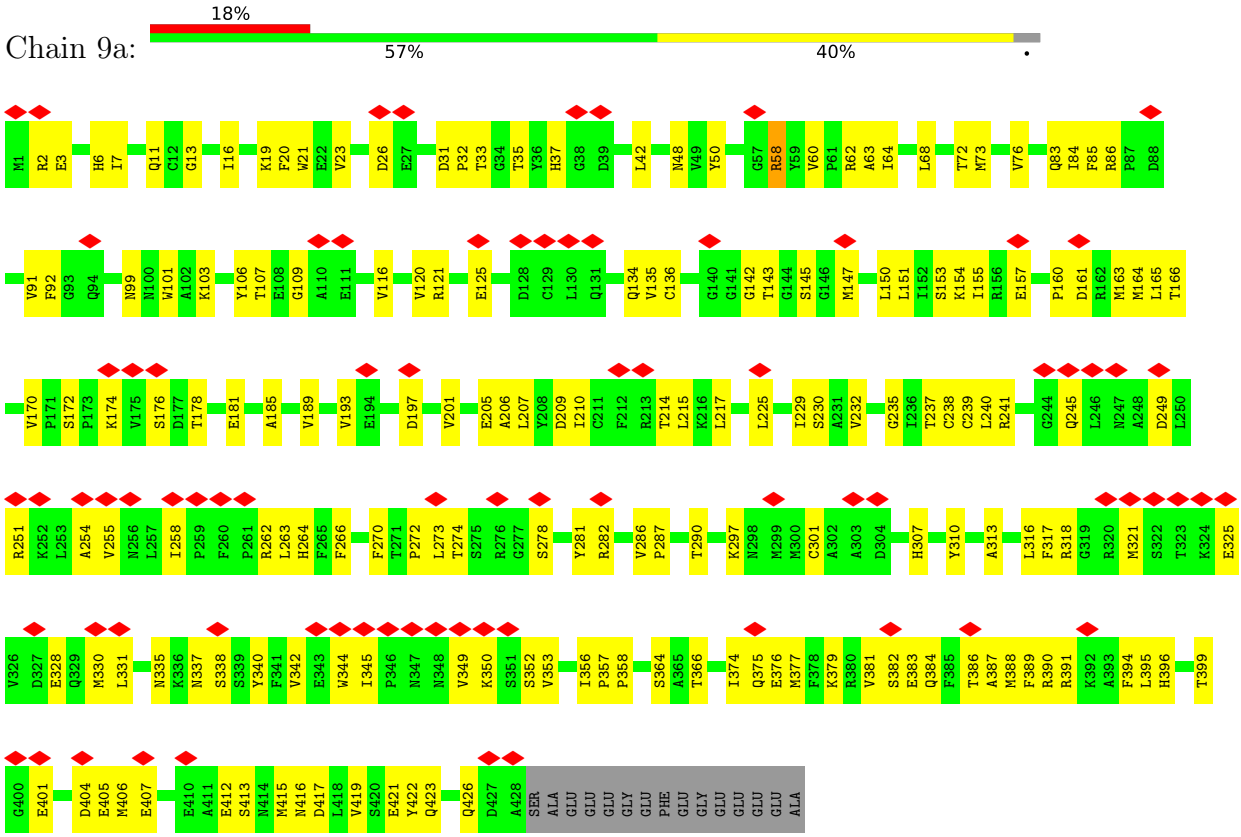
• Molecule 12: Tubulin beta

Chain 8g:



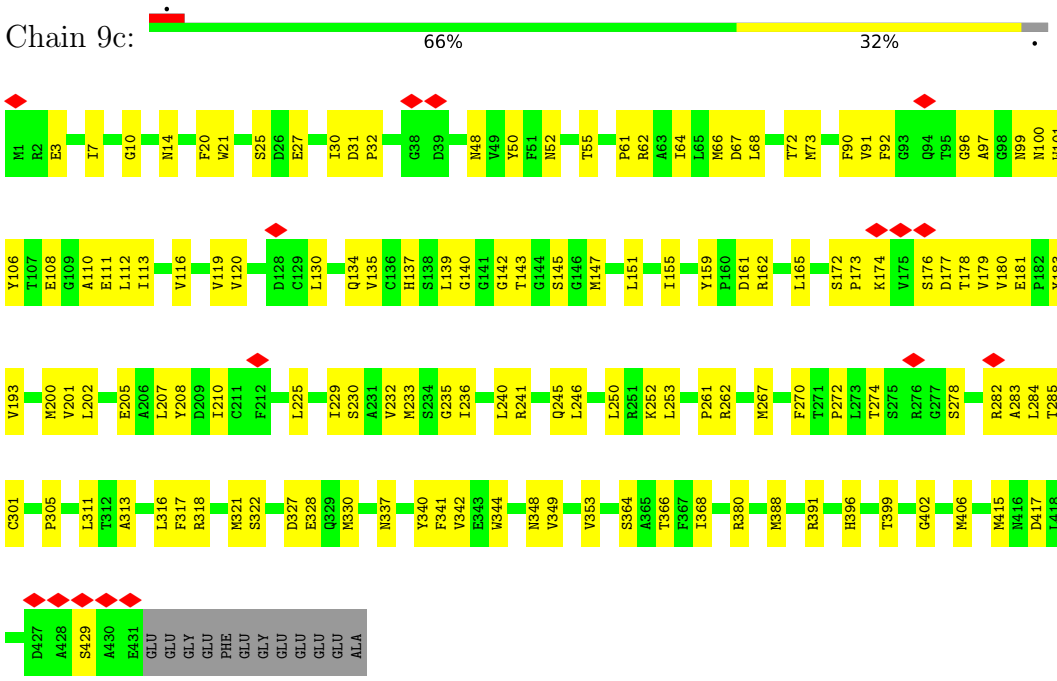
• Molecule 12: Tubulin beta

Chain 9a:



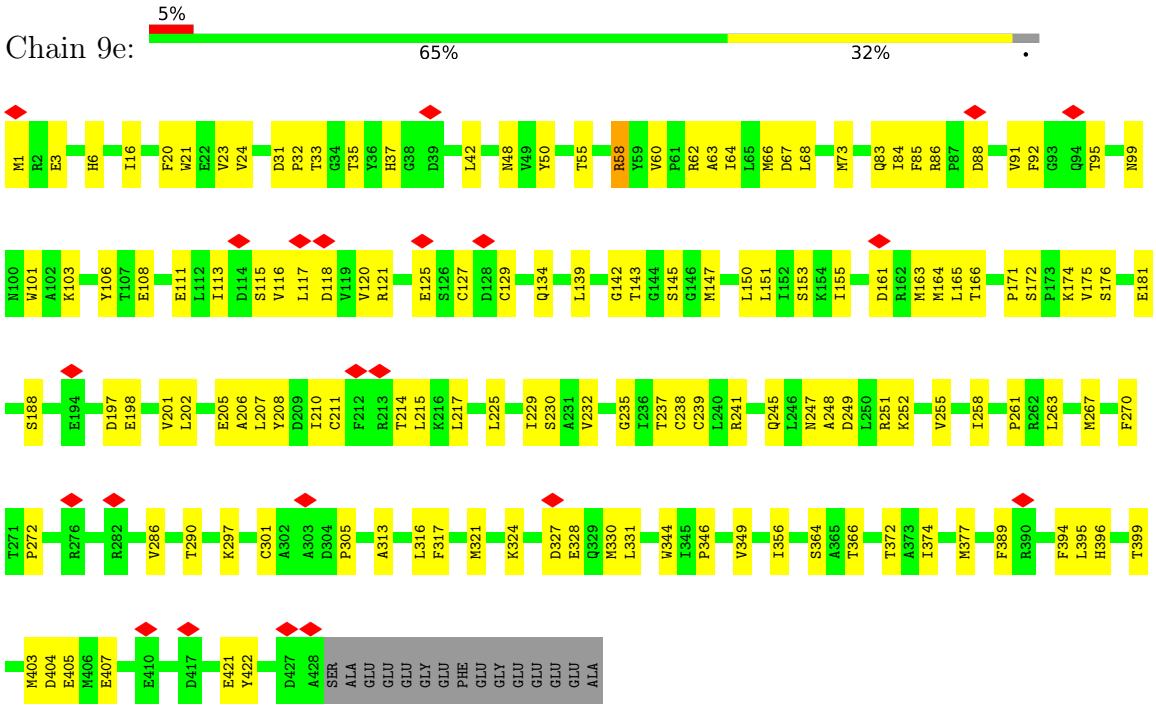
• Molecule 12: Tubulin beta

Chain 9c:



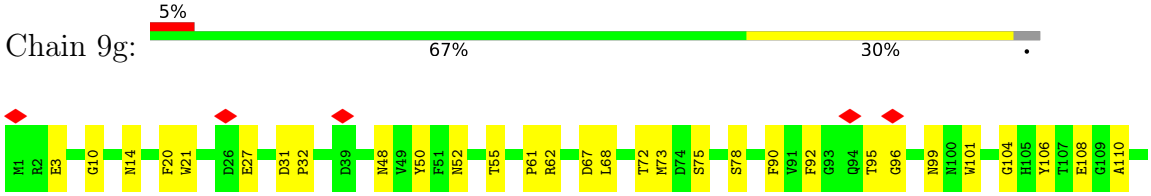
• Molecule 12: Tubulin beta

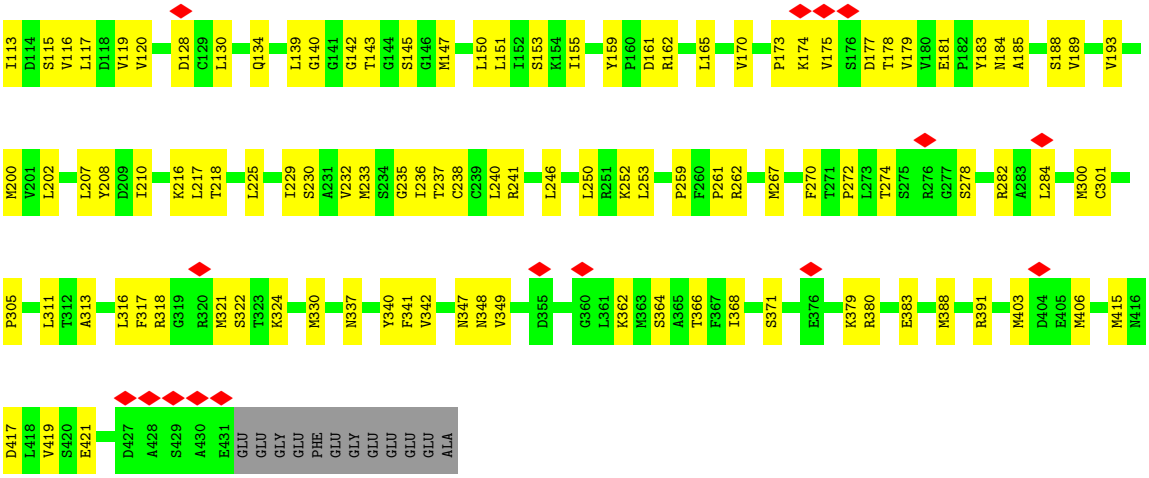
Chain 9e:



• Molecule 12: Tubulin beta

Chain 9g:

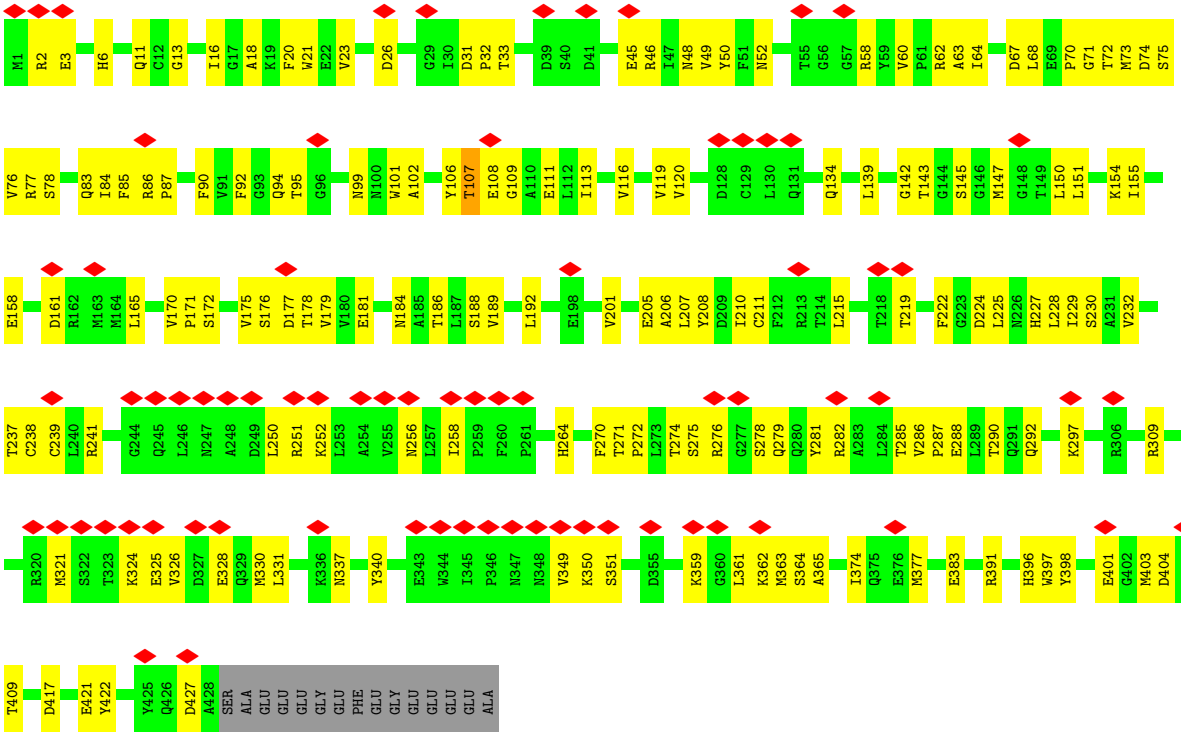




• Molecule 12: Tubulin beta

Chain Aa:

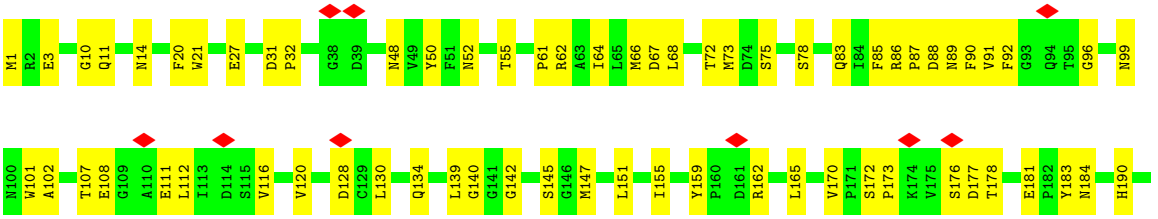


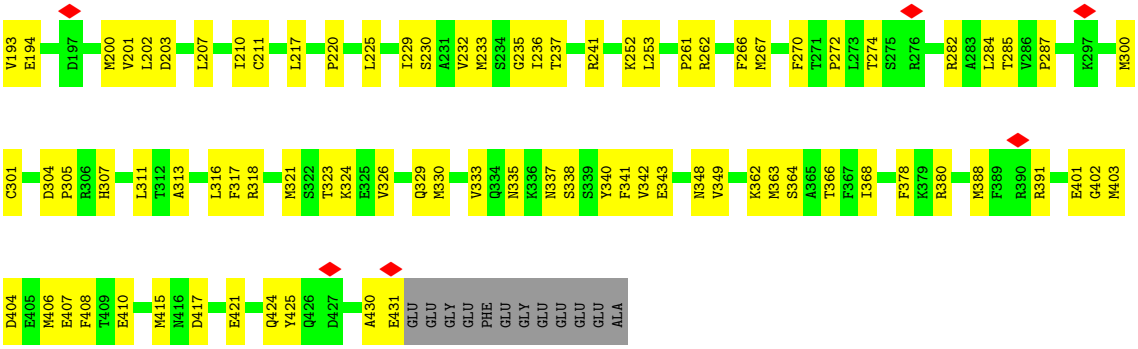


• Molecule 12: Tubulin beta

Chain Ac:



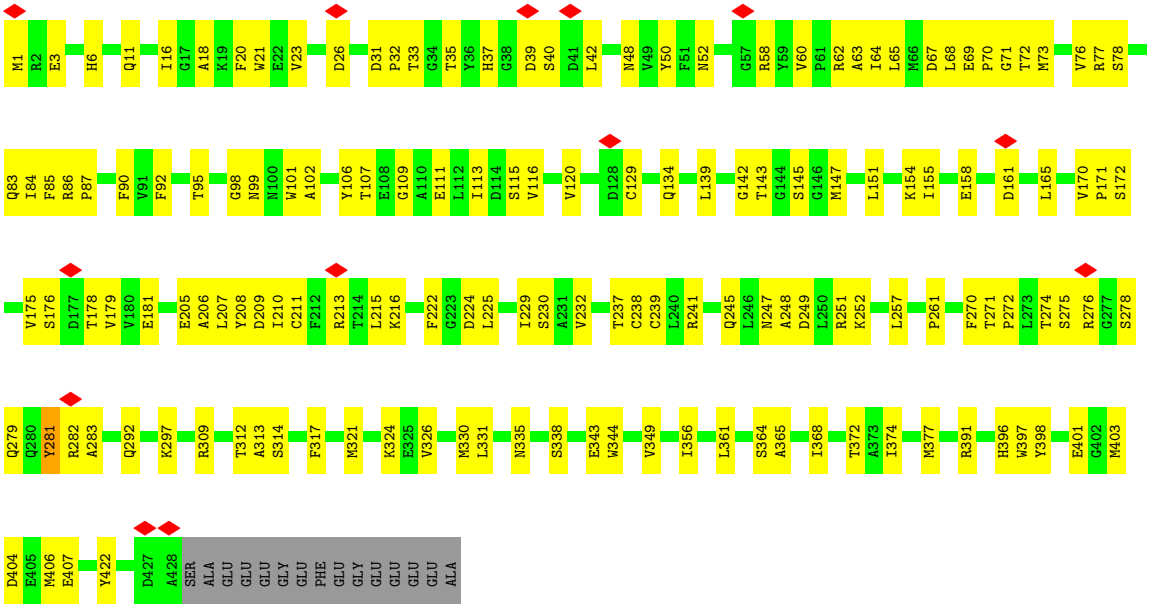




• Molecule 12: Tubulin beta

Chain Ae:

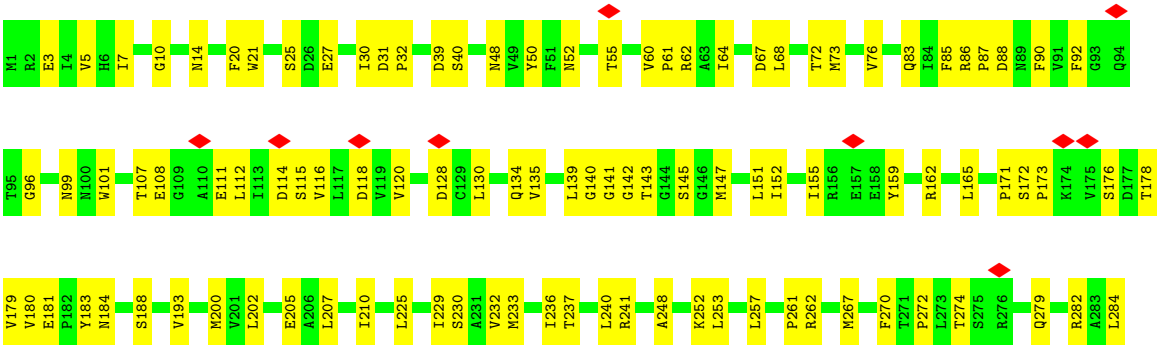


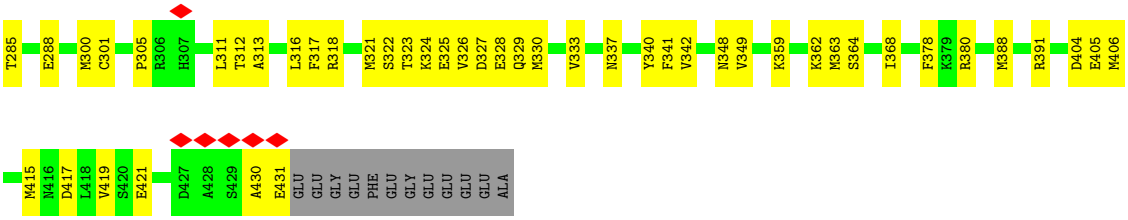


• Molecule 12: Tubulin beta

Chain Ag:



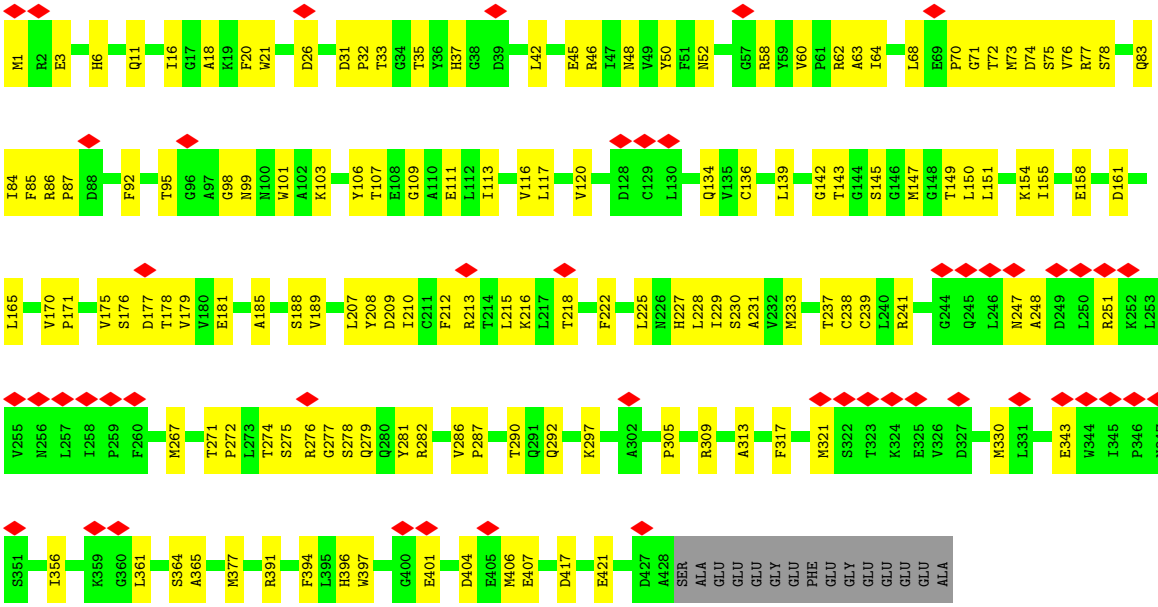




• Molecule 12: Tubulin beta

Chain Ba:

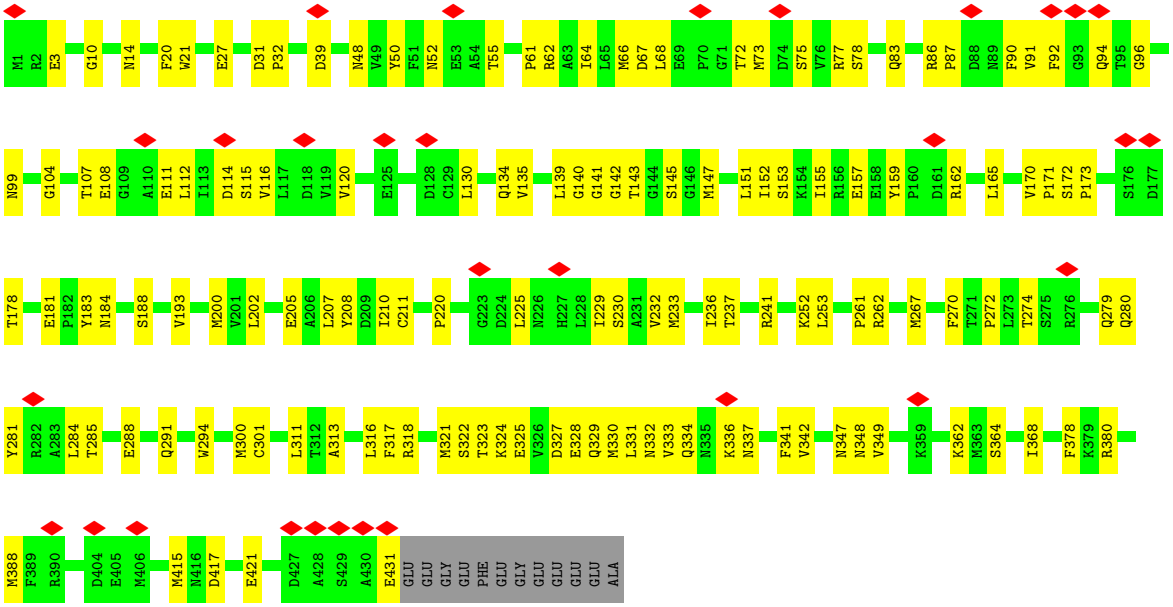




• Molecule 12: Tubulin beta

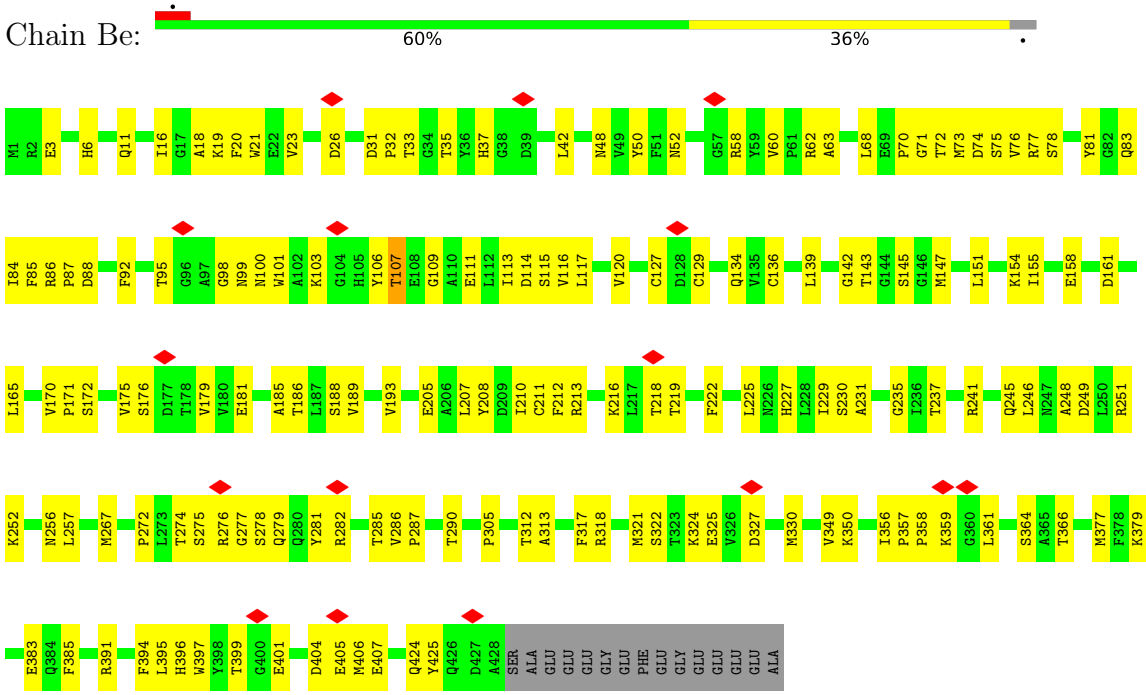
Chain Bc:





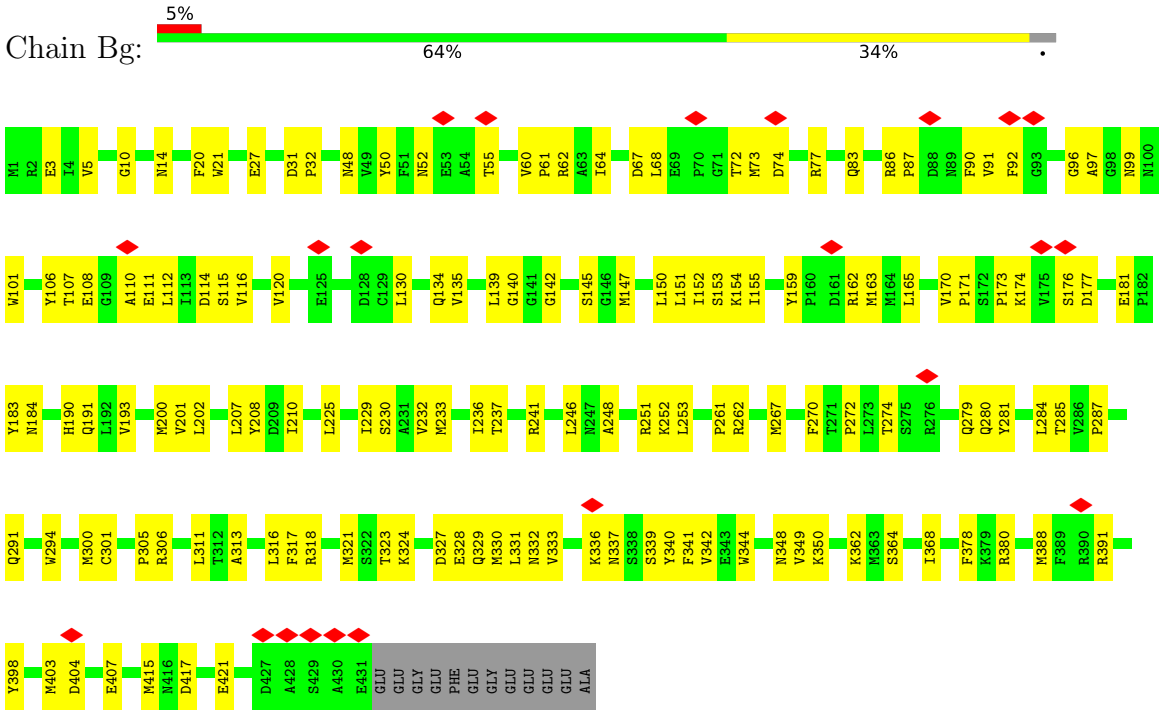
• Molecule 12: Tubulin beta

Chain Be:



• Molecule 12: Tubulin beta

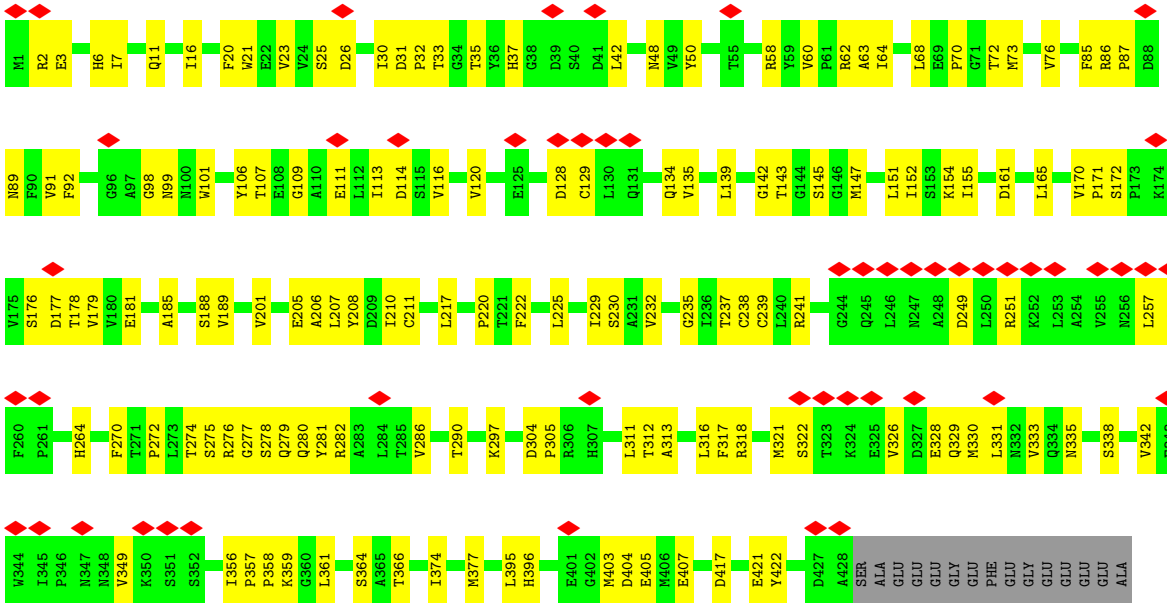
Chain Bg:



• Molecule 12: Tubulin beta

Chain Ca:

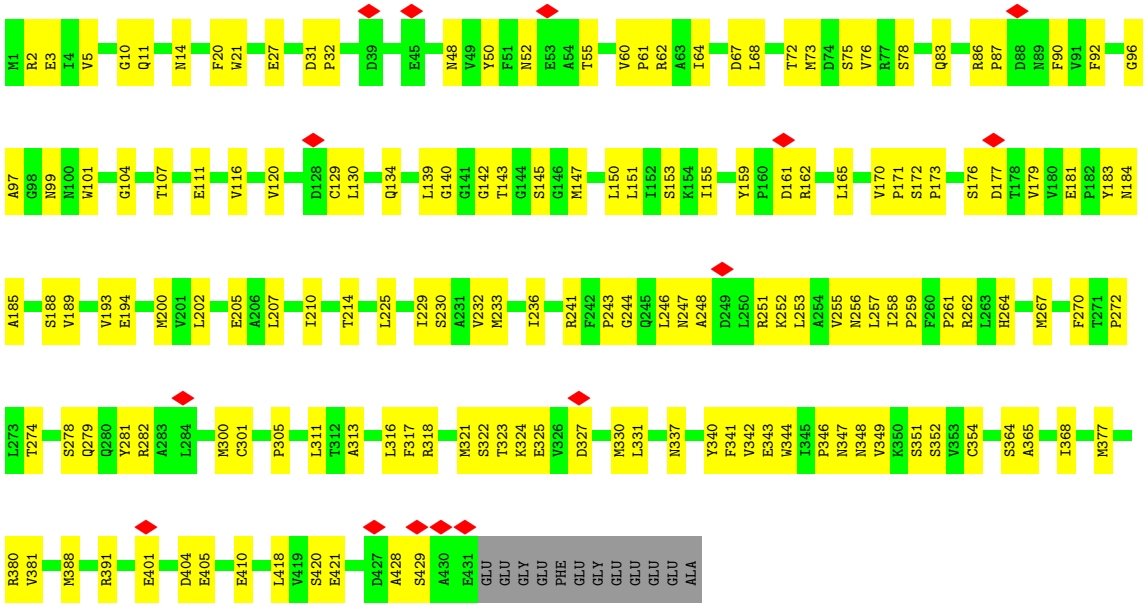




• Molecule 12: Tubulin beta

Chain Cc:

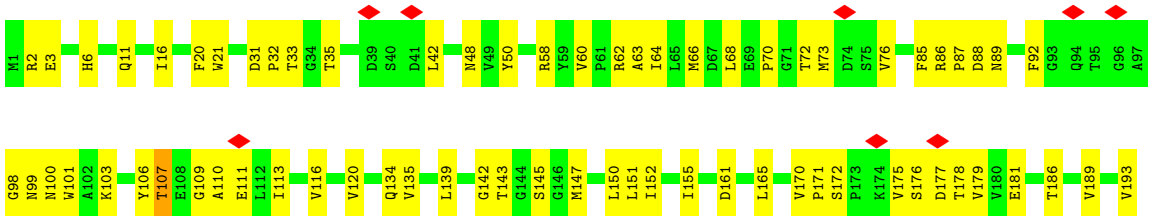


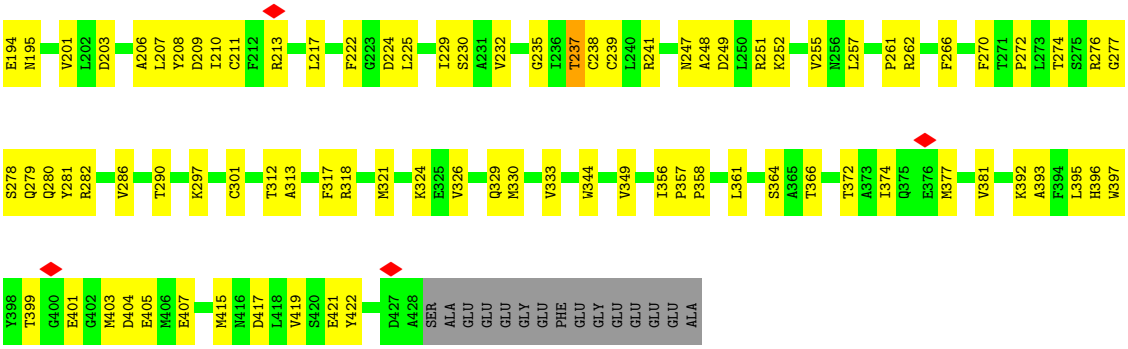


• Molecule 12: Tubulin beta

Chain Ce:



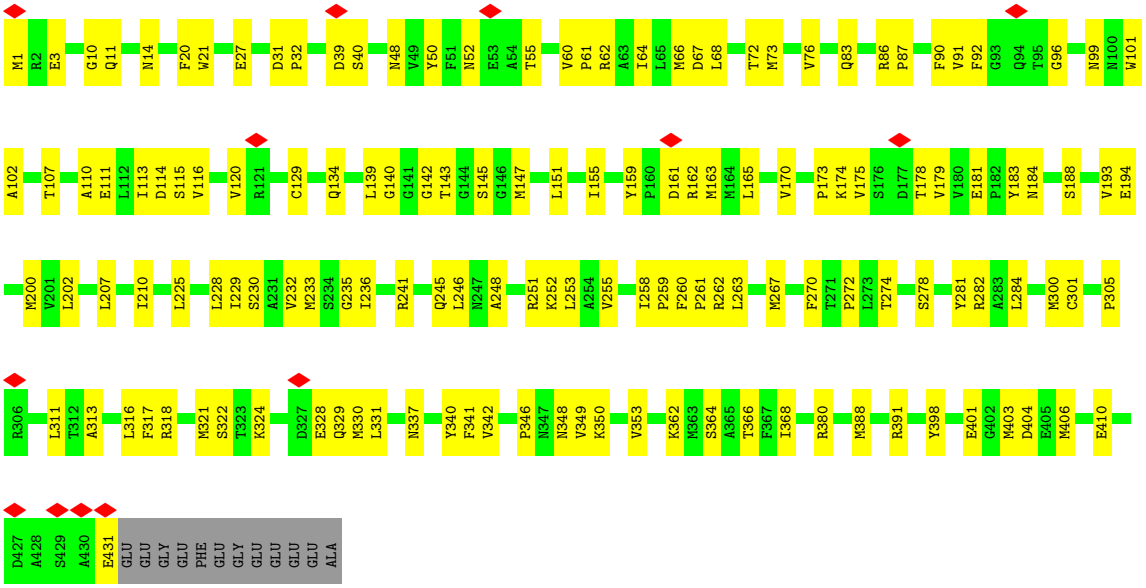




• Molecule 12: Tubulin beta

Chain Cg:

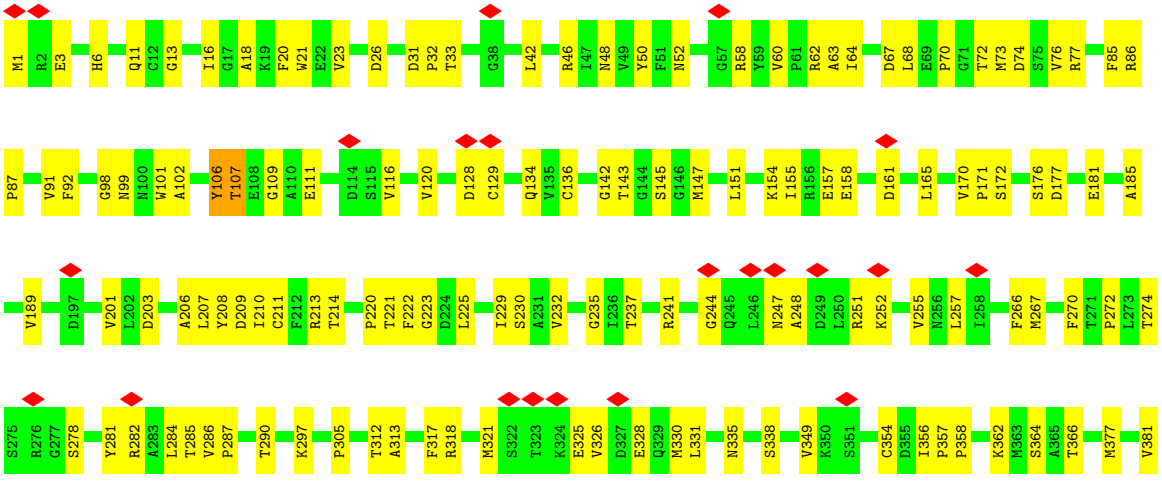




• Molecule 12: Tubulin beta

Chain Da:



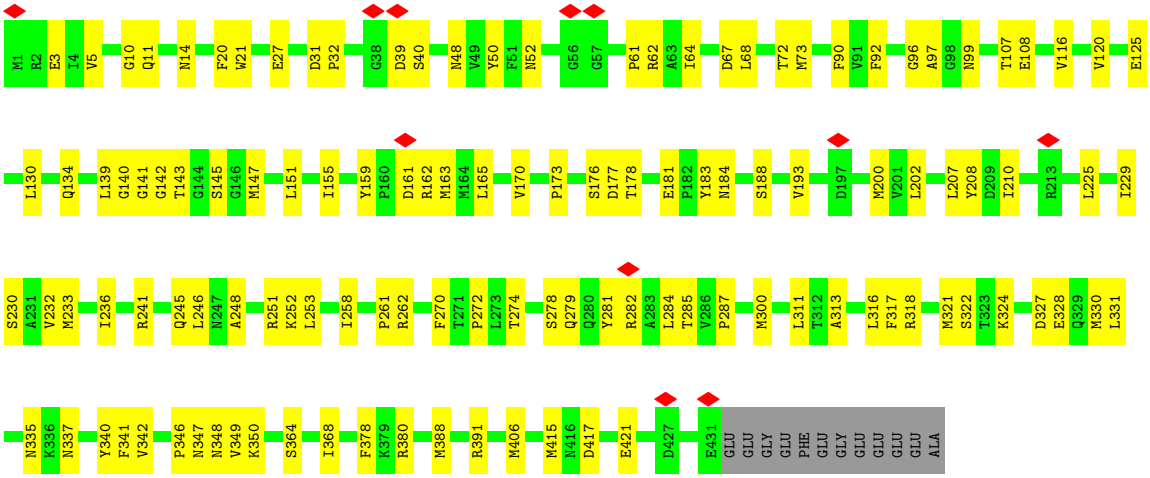




• Molecule 12: Tubulin beta

Chain Dc:

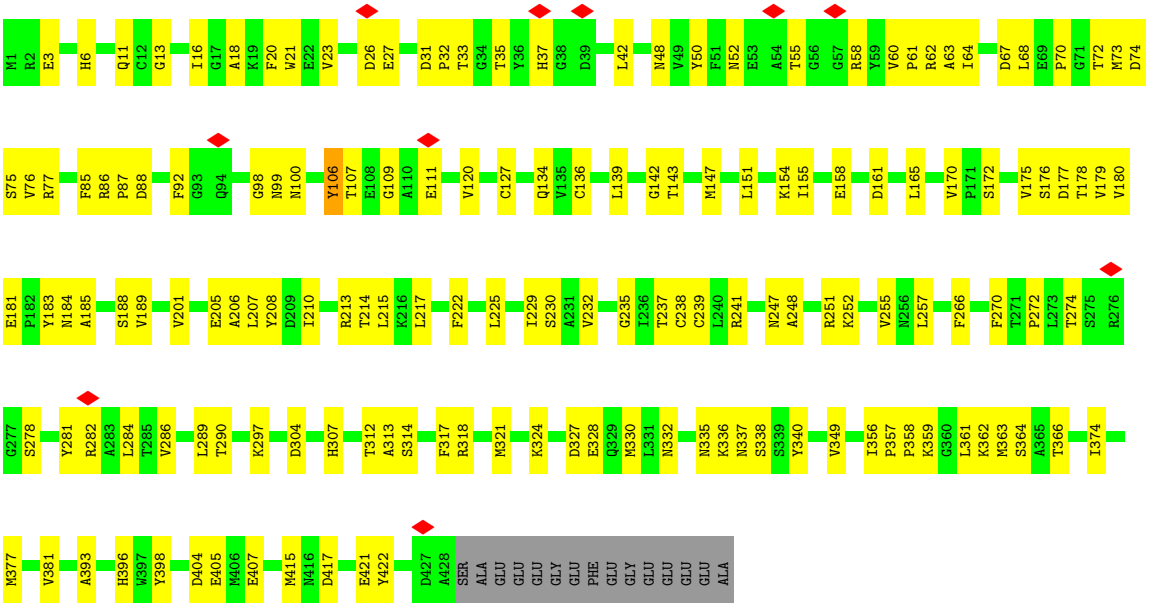




• Molecule 12: Tubulin beta

Chain De:

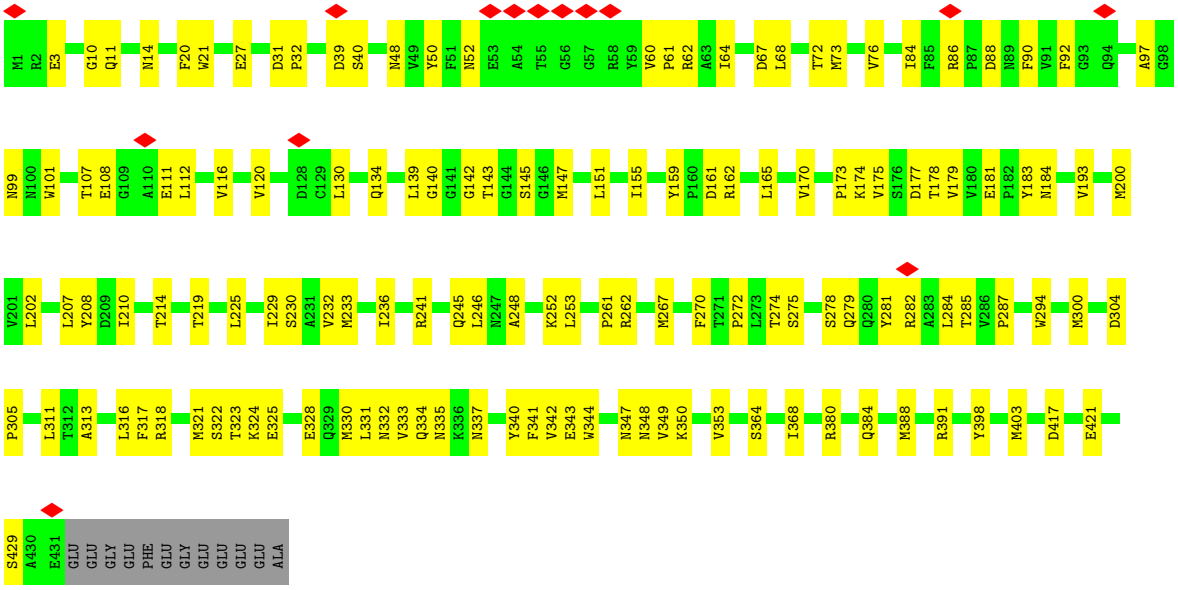




• Molecule 12: Tubulin beta

Chain Dg:

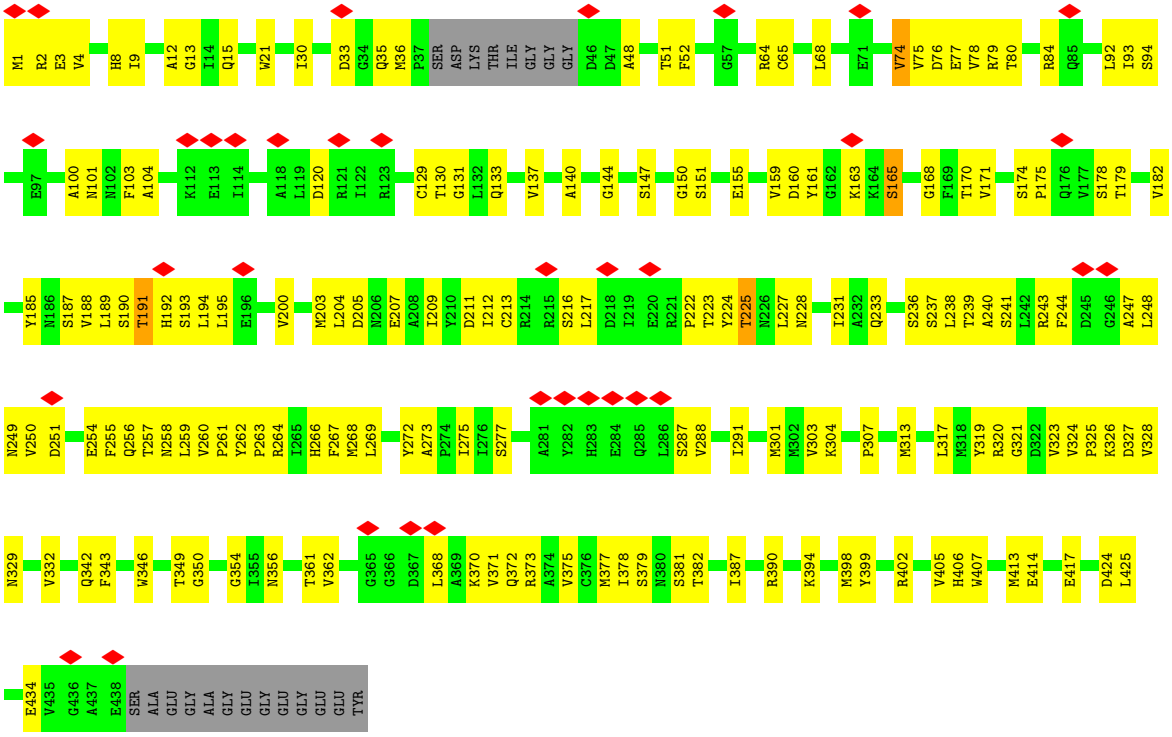




• Molecule 13: Tubulin alpha

Chain 1b:

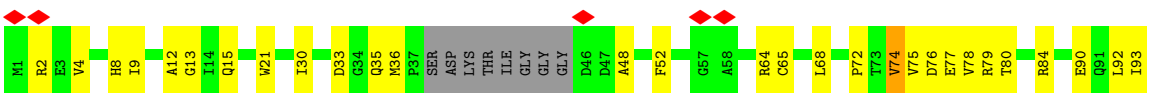


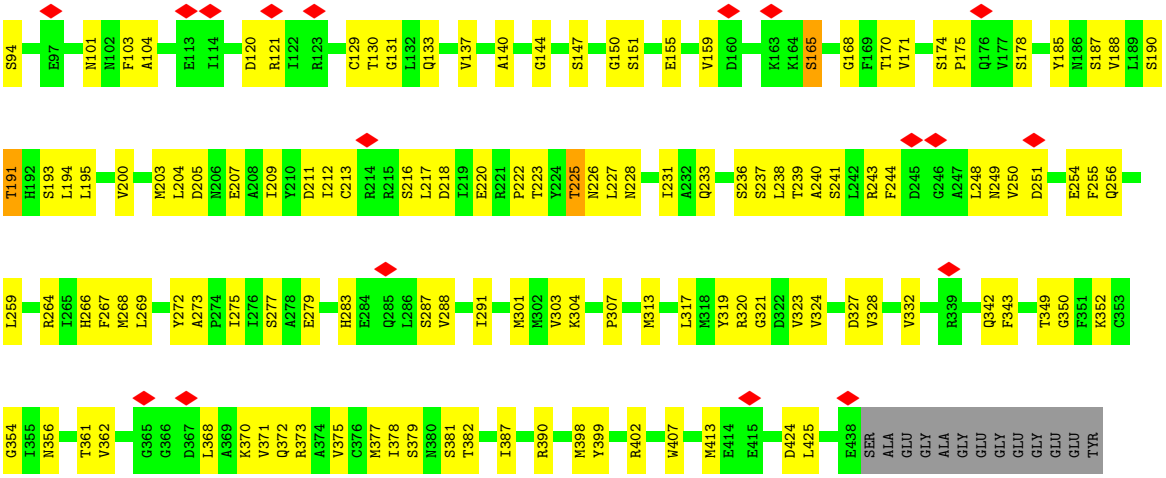


• Molecule 13: Tubulin alpha

Chain 1d:



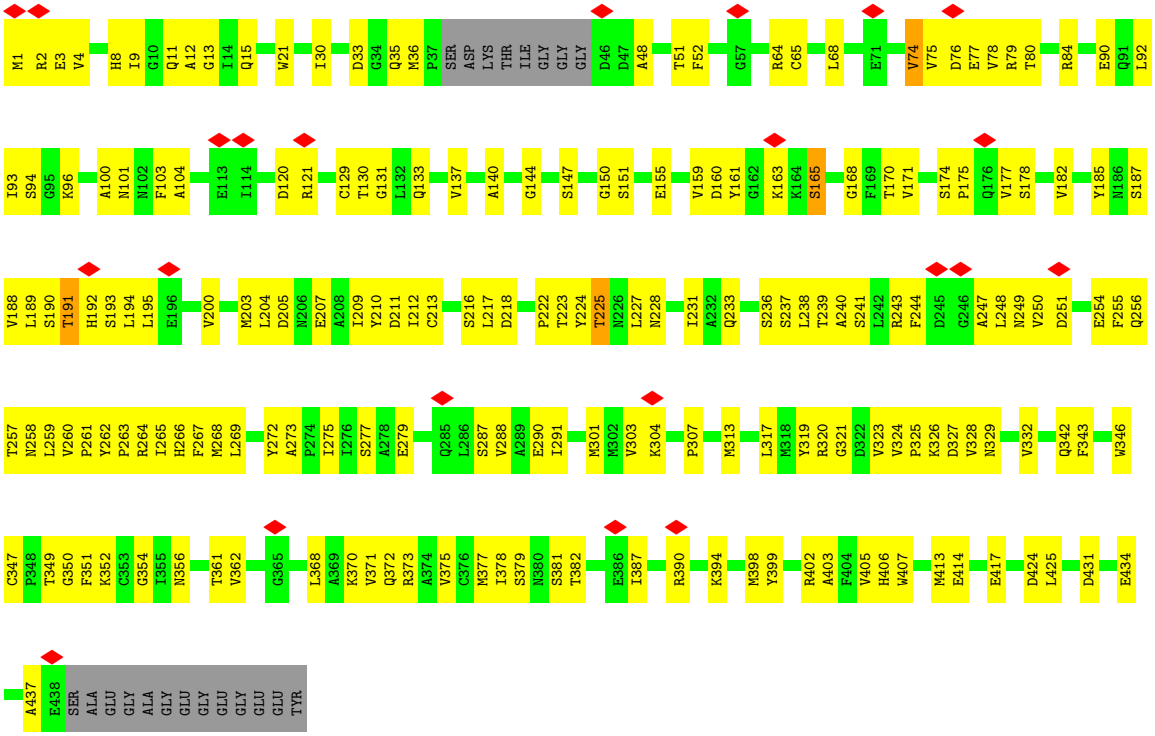




• Molecule 13: Tubulin alpha

Chain 1f:

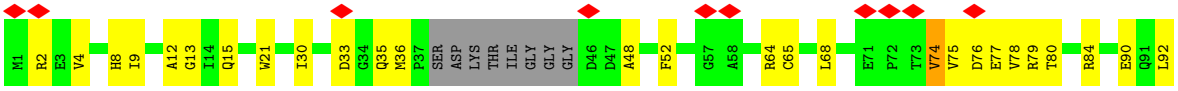


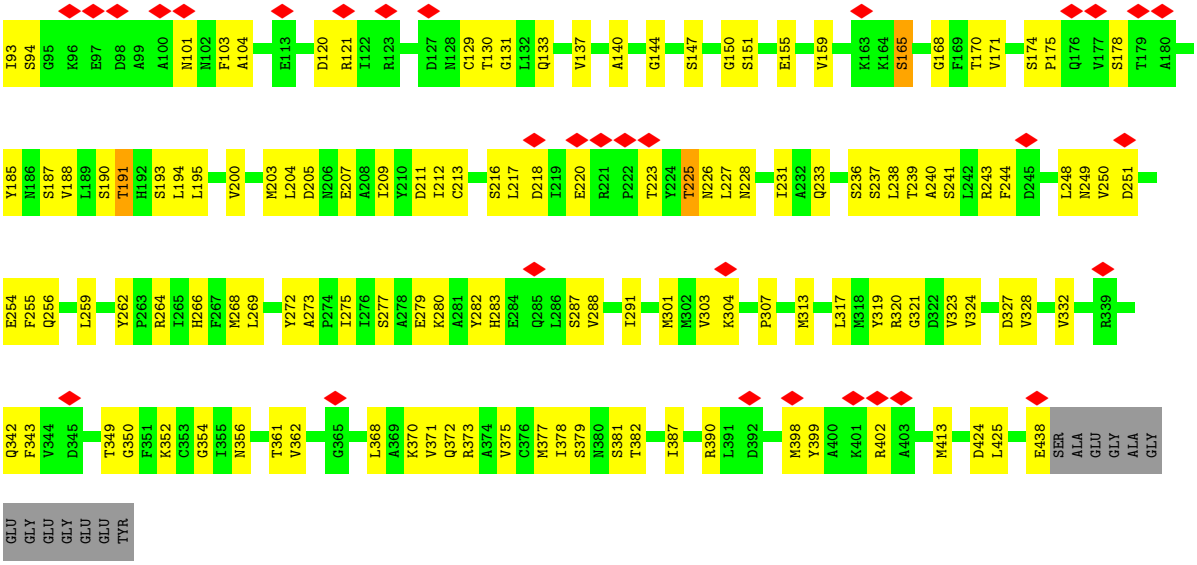


• Molecule 13: Tubulin alpha

Chain 1h:



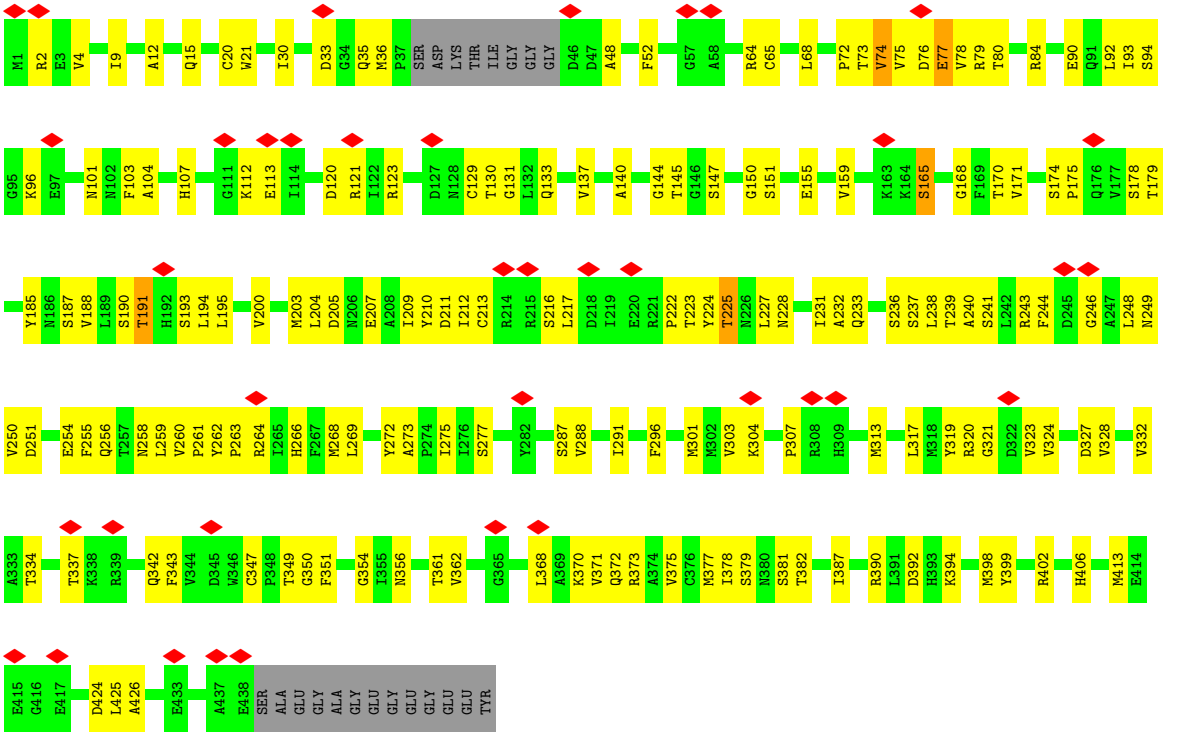




• Molecule 13: Tubulin alpha

Chain 2b:

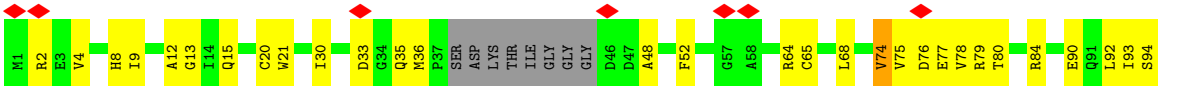


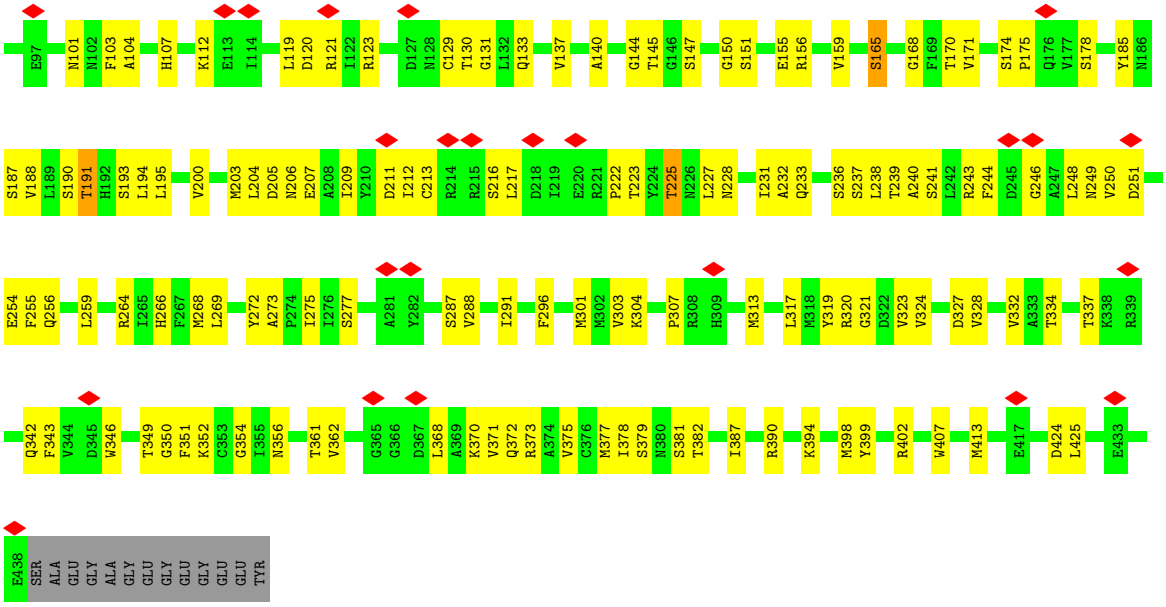


• Molecule 13: Tubulin alpha

Chain 2d:



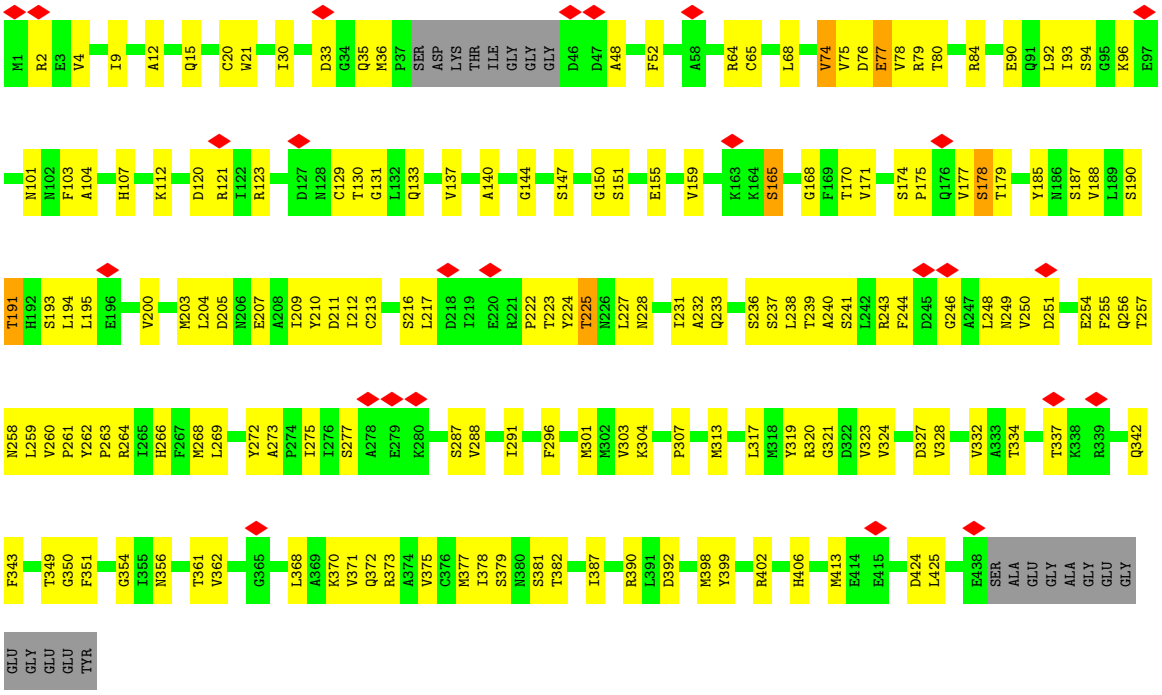




• Molecule 13: Tubulin alpha

Chain 2f:

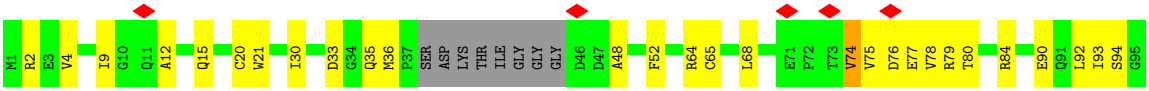


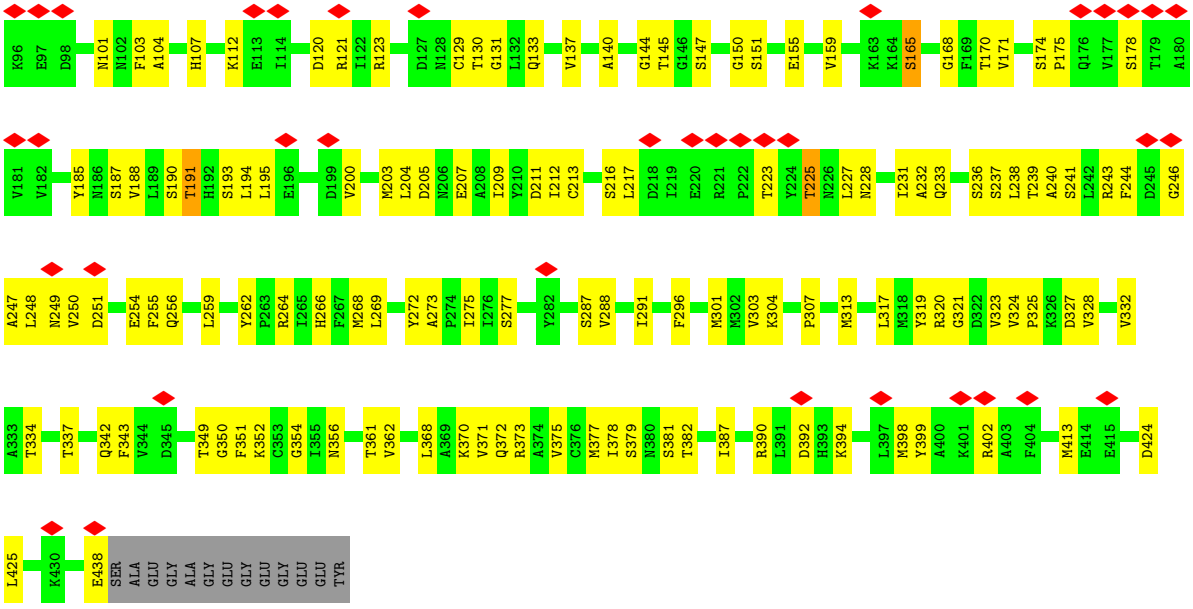


• Molecule 13: Tubulin alpha

Chain 2h:



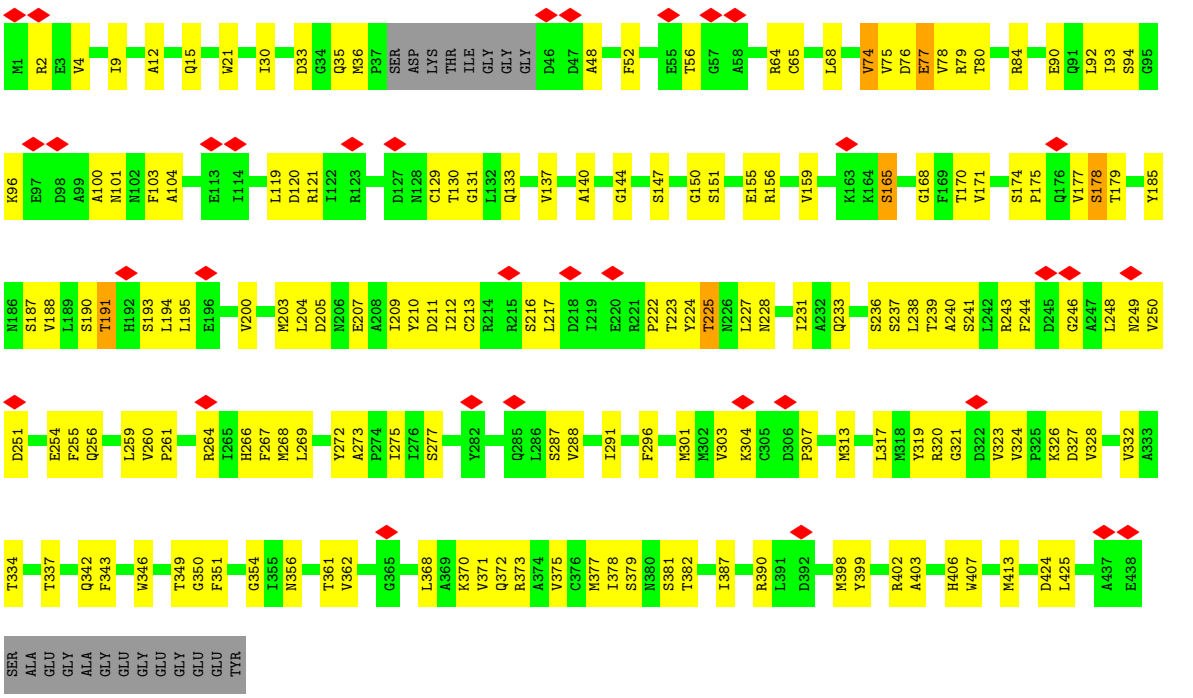




• Molecule 13: Tubulin alpha

Chain 3b:

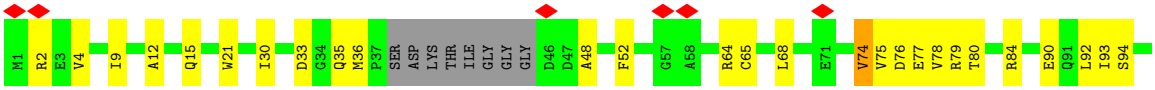


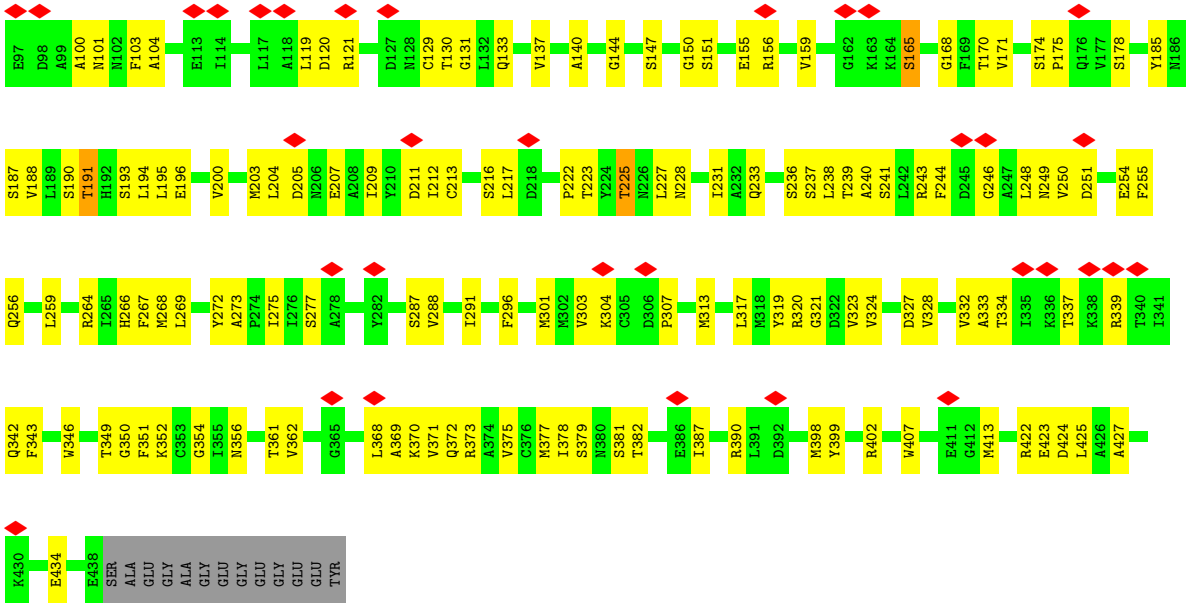


• Molecule 13: Tubulin alpha

Chain 3d:



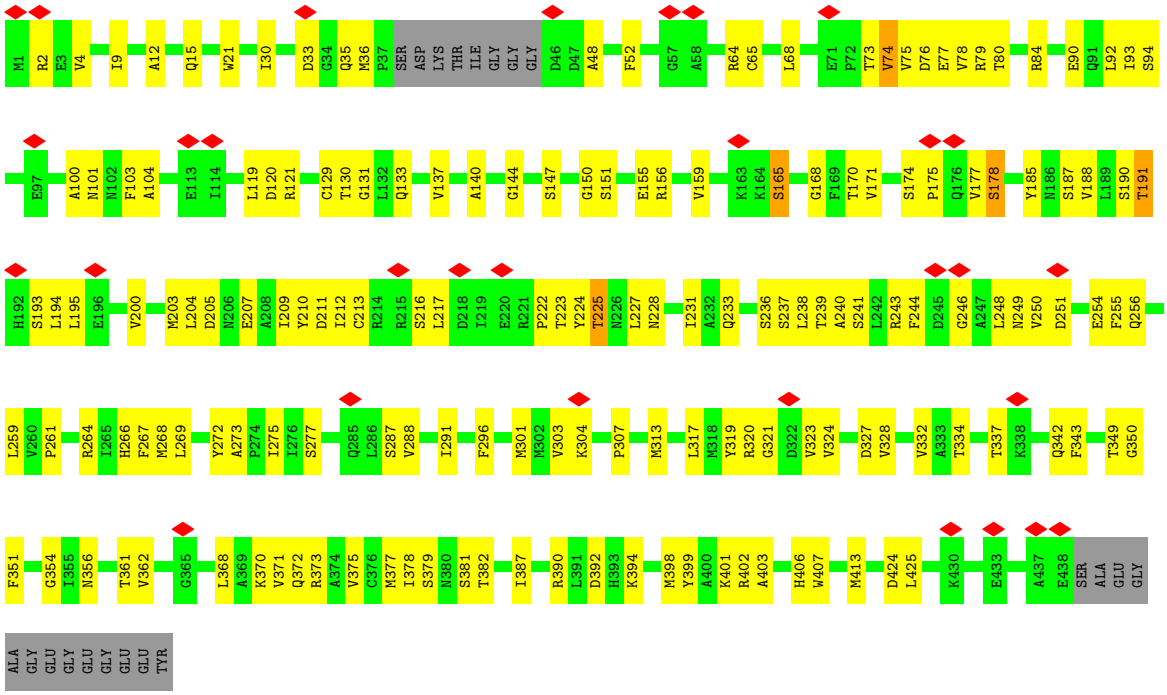




• Molecule 13: Tubulin alpha

Chain 3f:

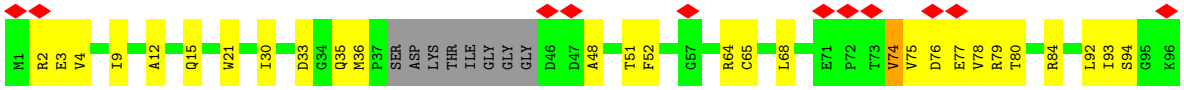


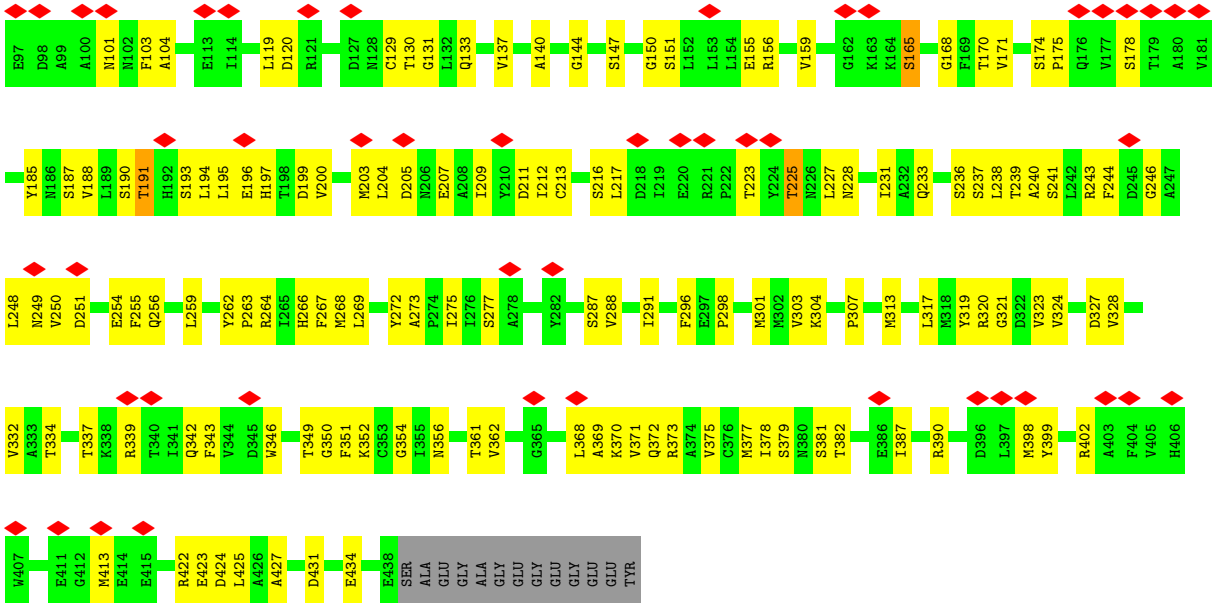


• Molecule 13: Tubulin alpha

Chain 3h:



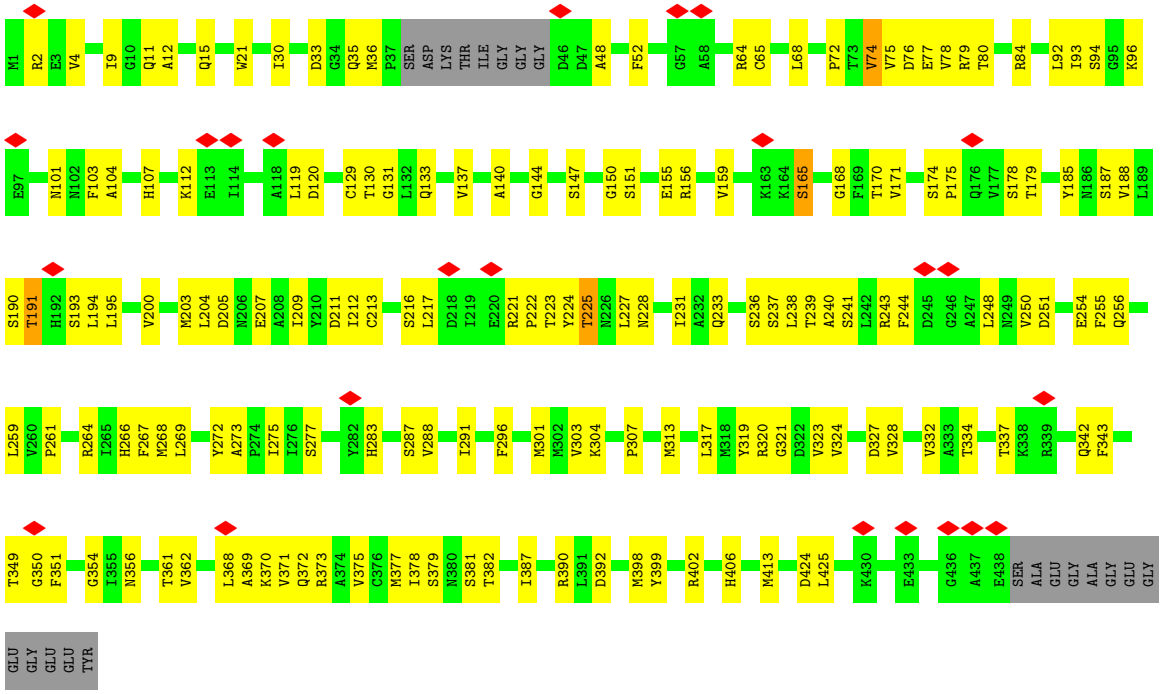




• Molecule 13: Tubulin alpha

Chain 4b:

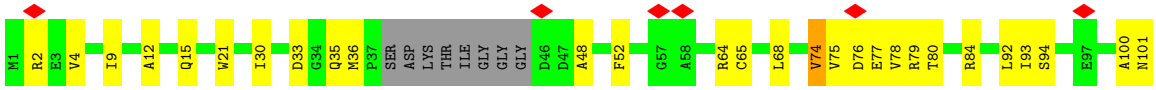


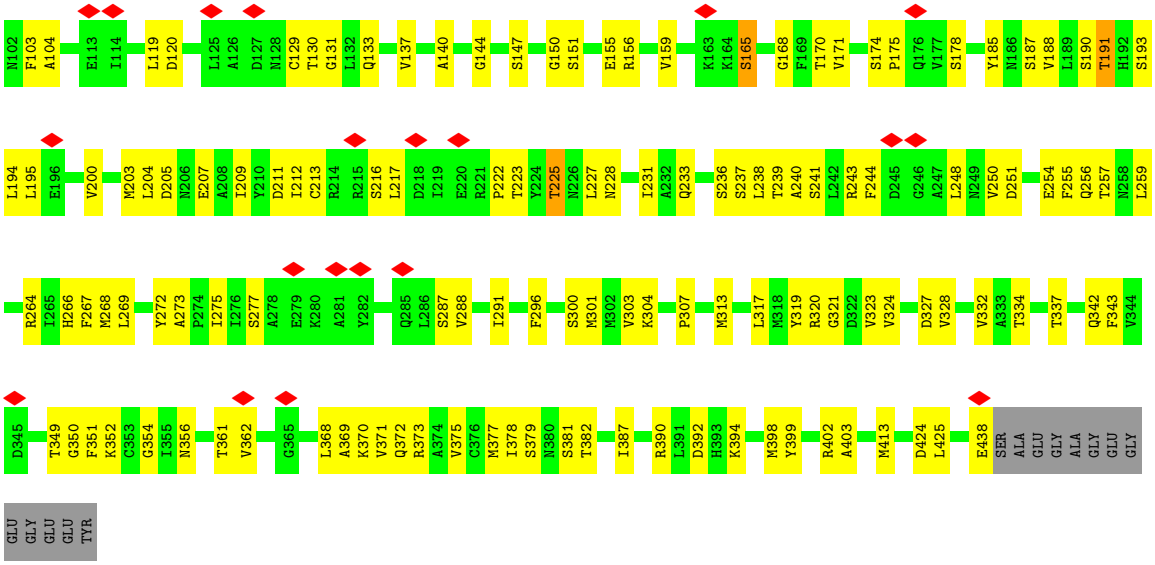


• Molecule 13: Tubulin alpha

Chain 4d:



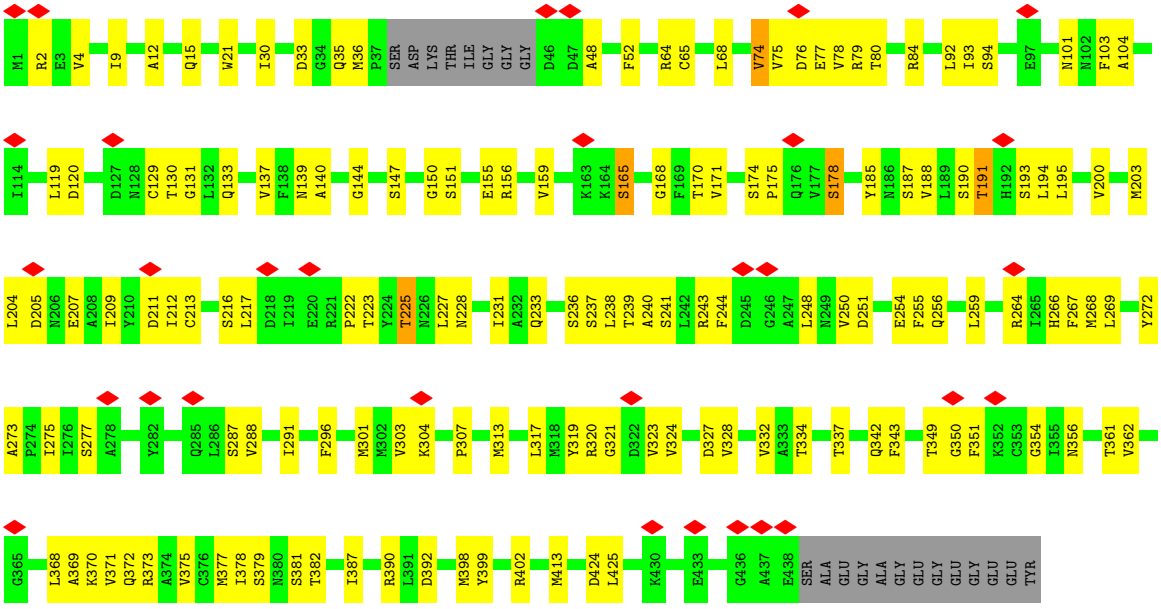




• Molecule 13: Tubulin alpha

Chain 4f:

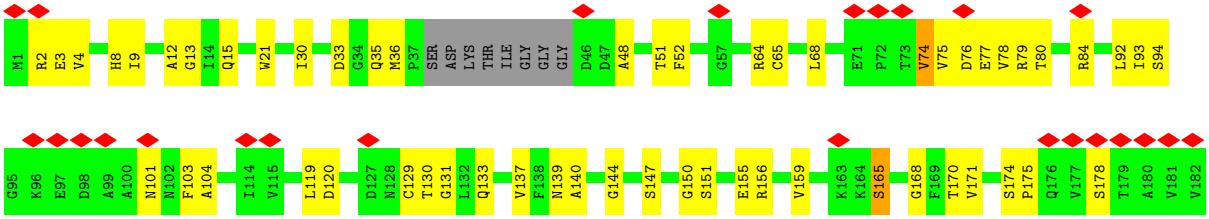


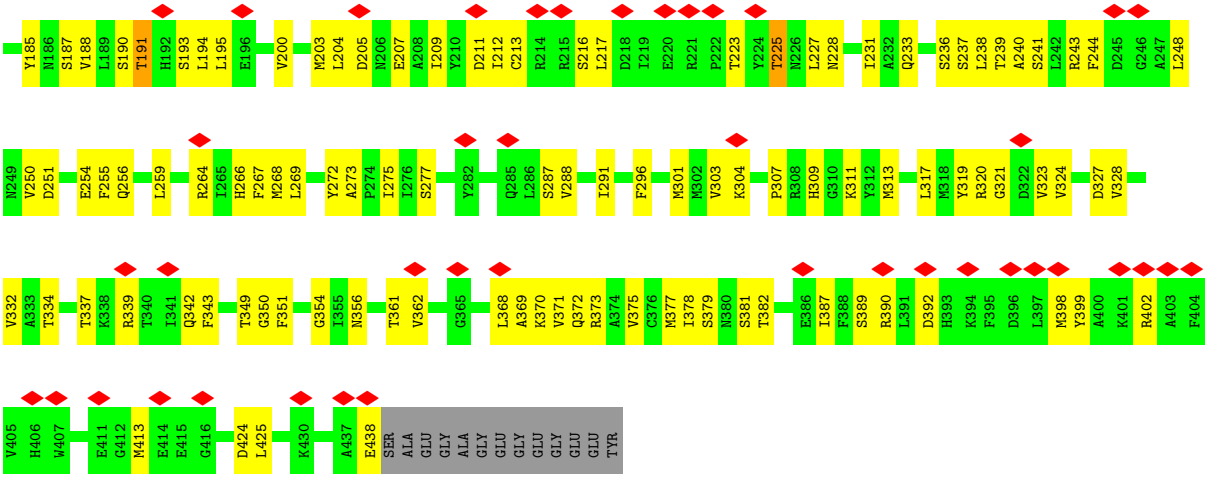


• Molecule 13: Tubulin alpha

Chain 4h:



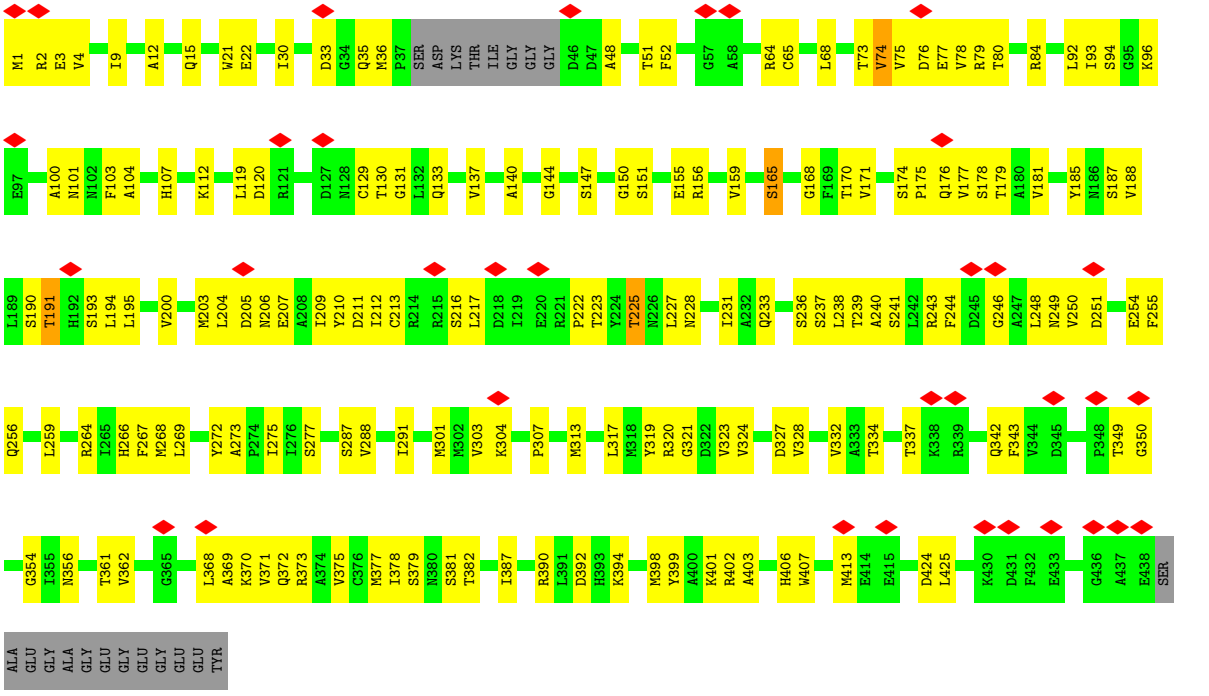




• Molecule 13: Tubulin alpha

Chain 5b:

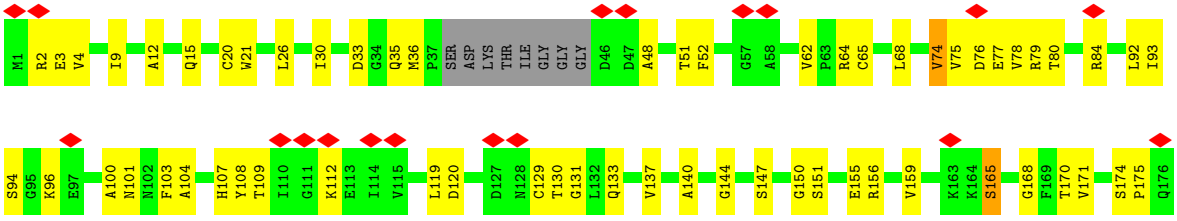


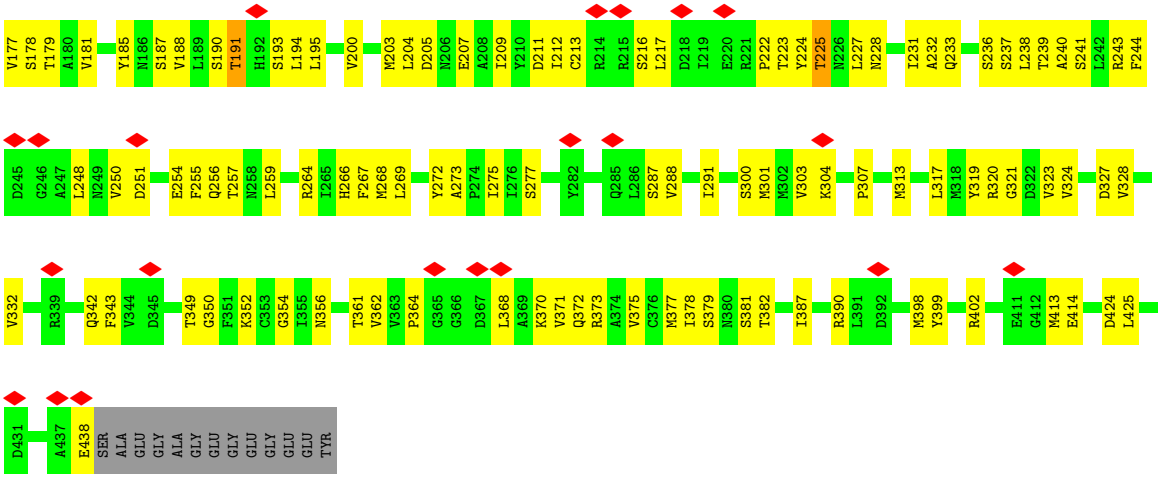


• Molecule 13: Tubulin alpha

Chain 5d:



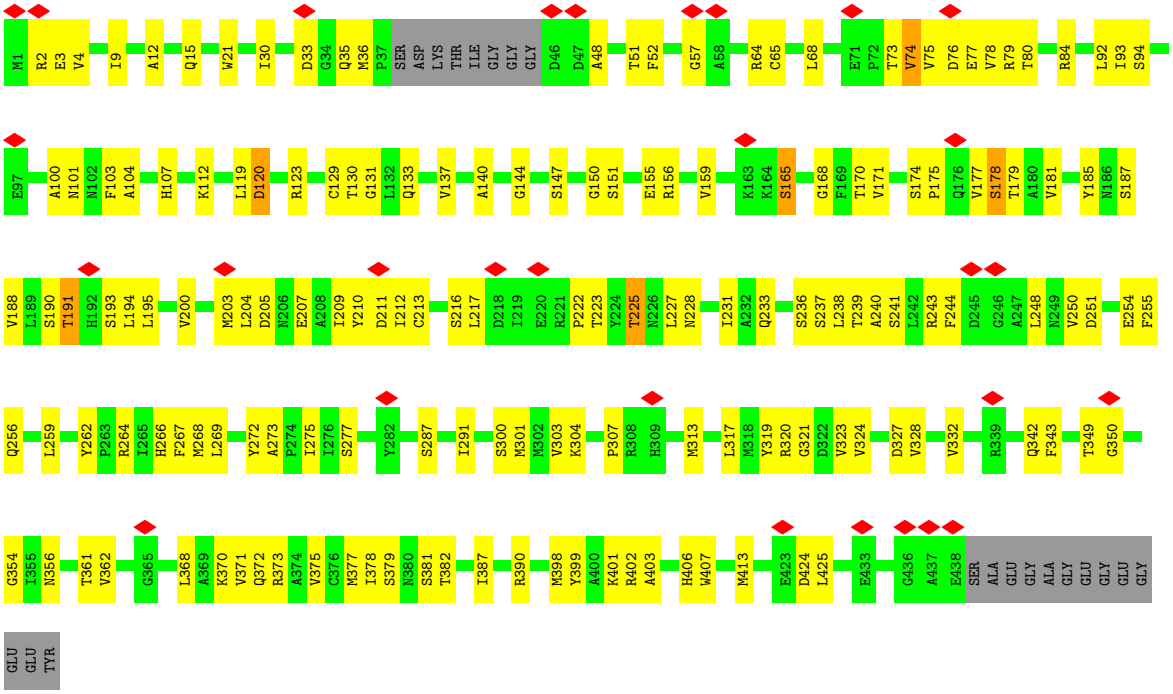




• Molecule 13: Tubulin alpha

Chain 5f:

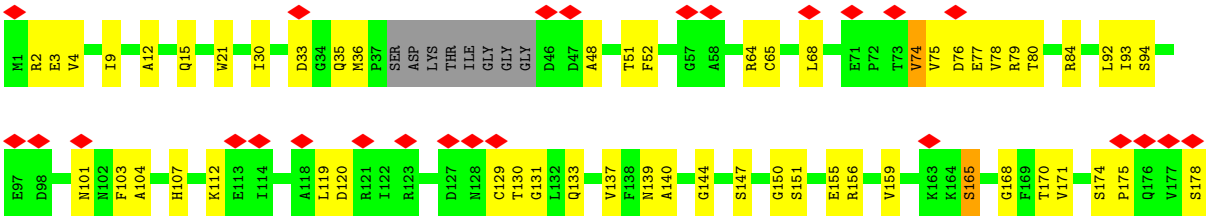


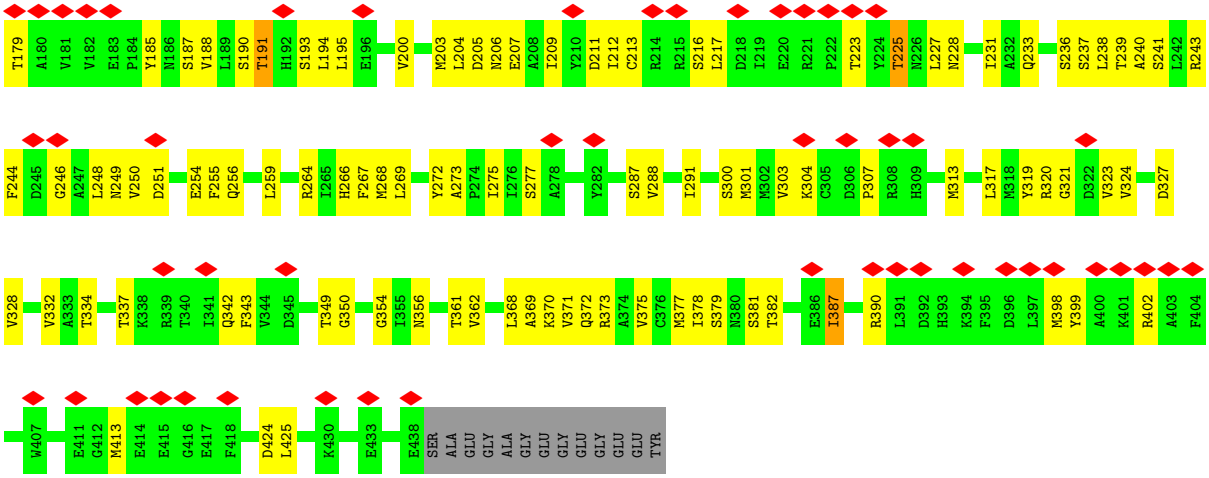


• Molecule 13: Tubulin alpha

Chain 5h:

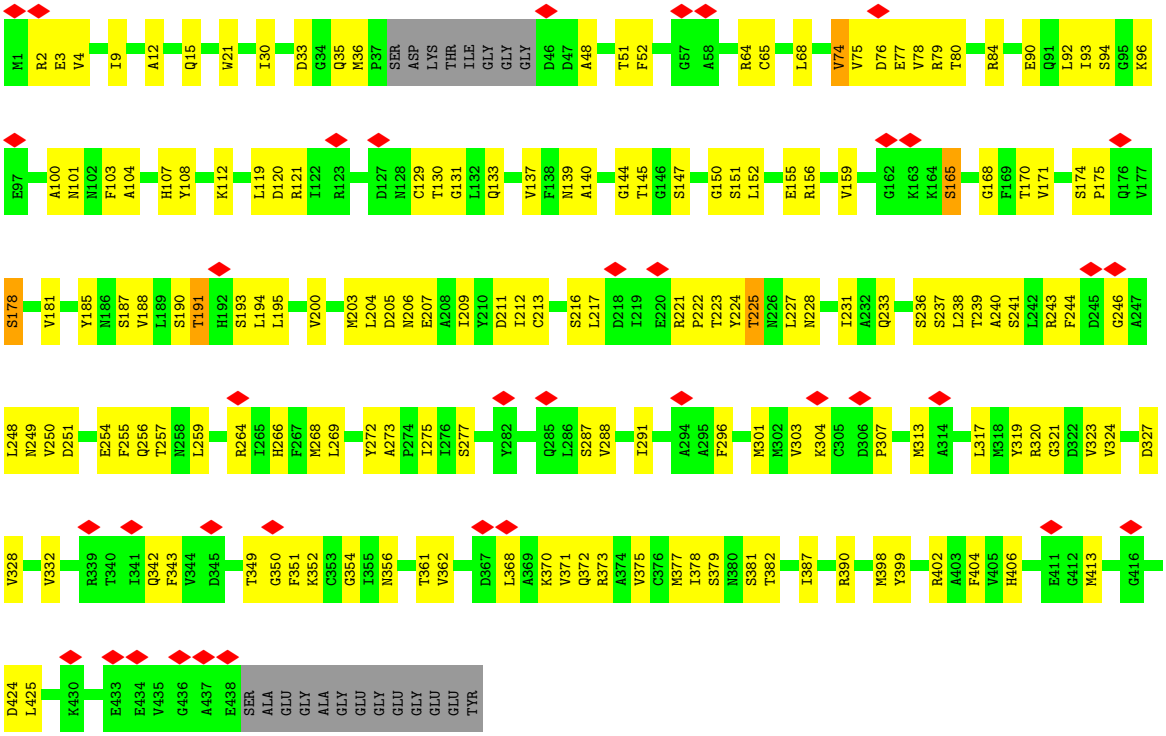






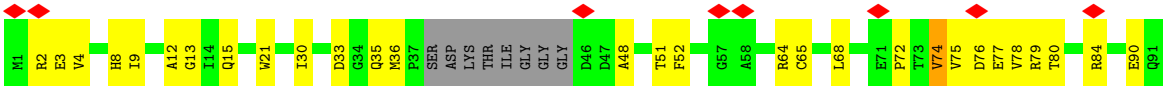
• Molecule 13: Tubulin alpha

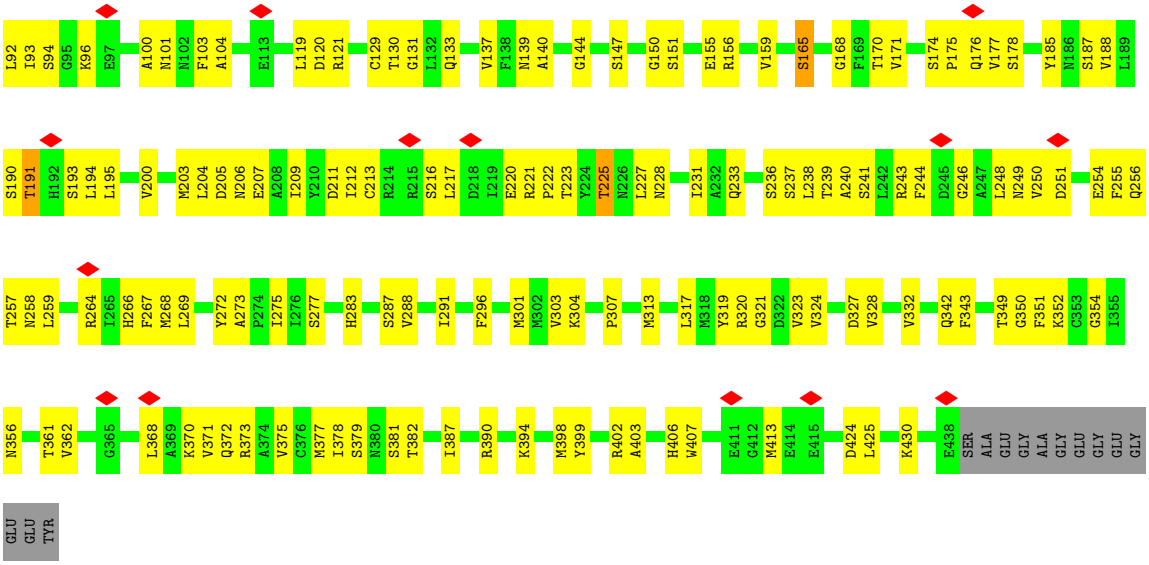




• Molecule 13: Tubulin alpha



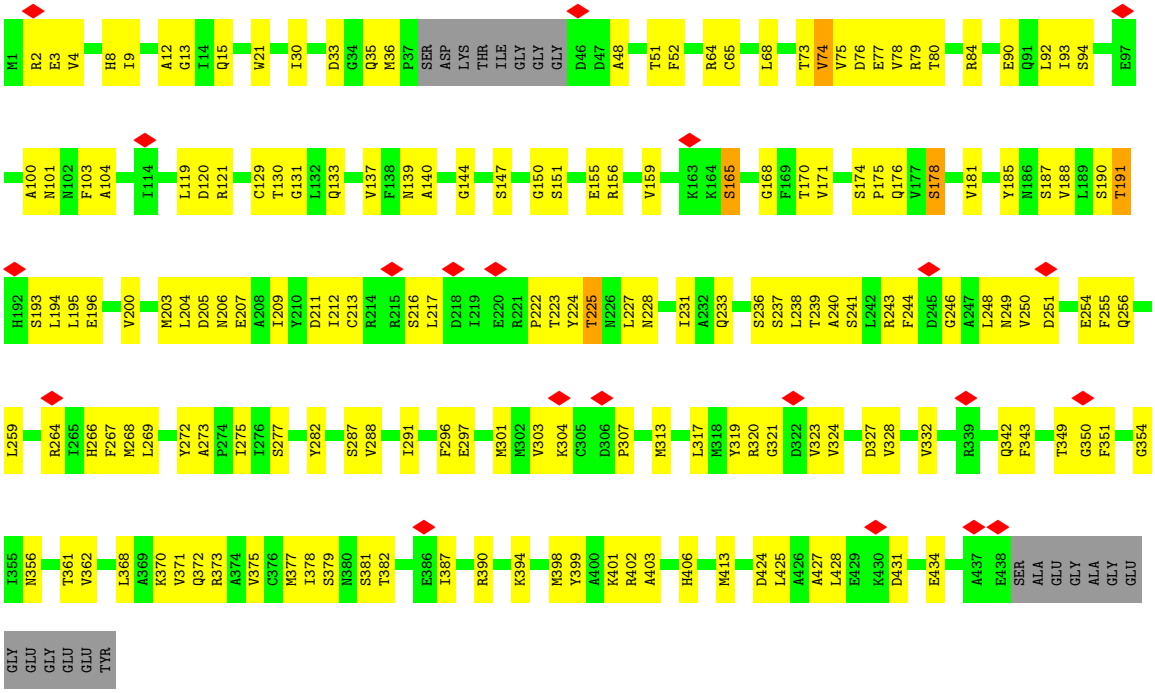




• Molecule 13: Tubulin alpha

Chain 6f:

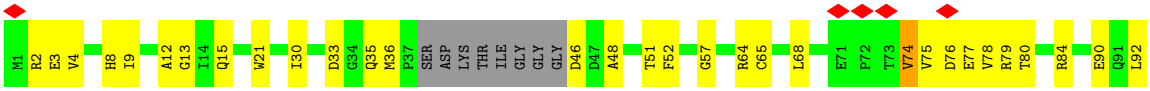


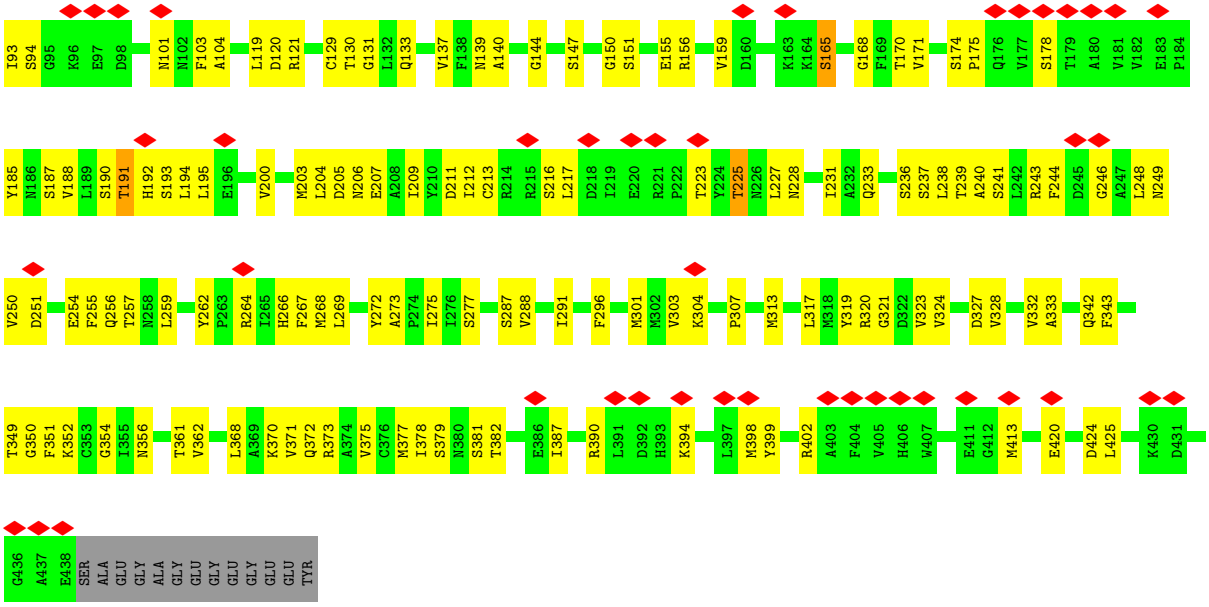


• Molecule 13: Tubulin alpha

Chain 6h:



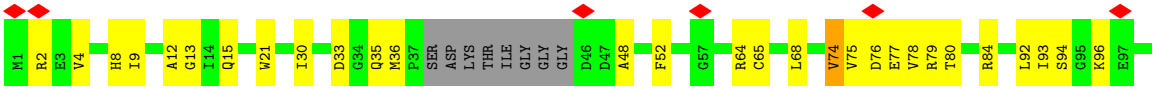




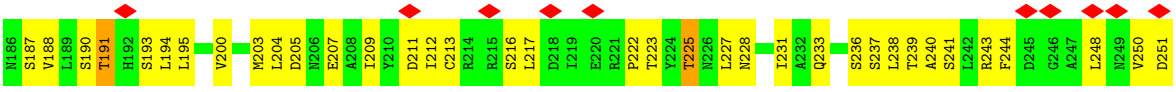
• Molecule 13: Tubulin alpha

Chain 7b:

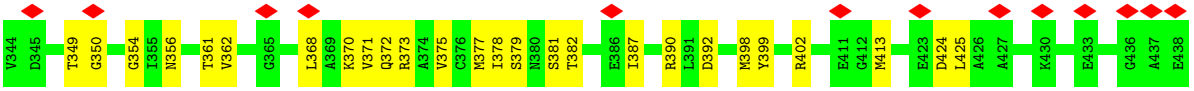


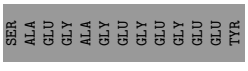








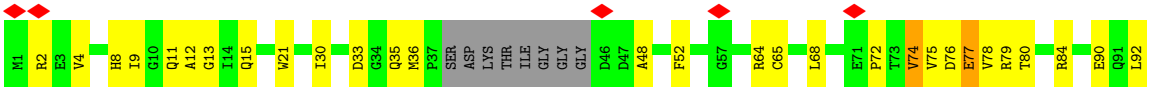


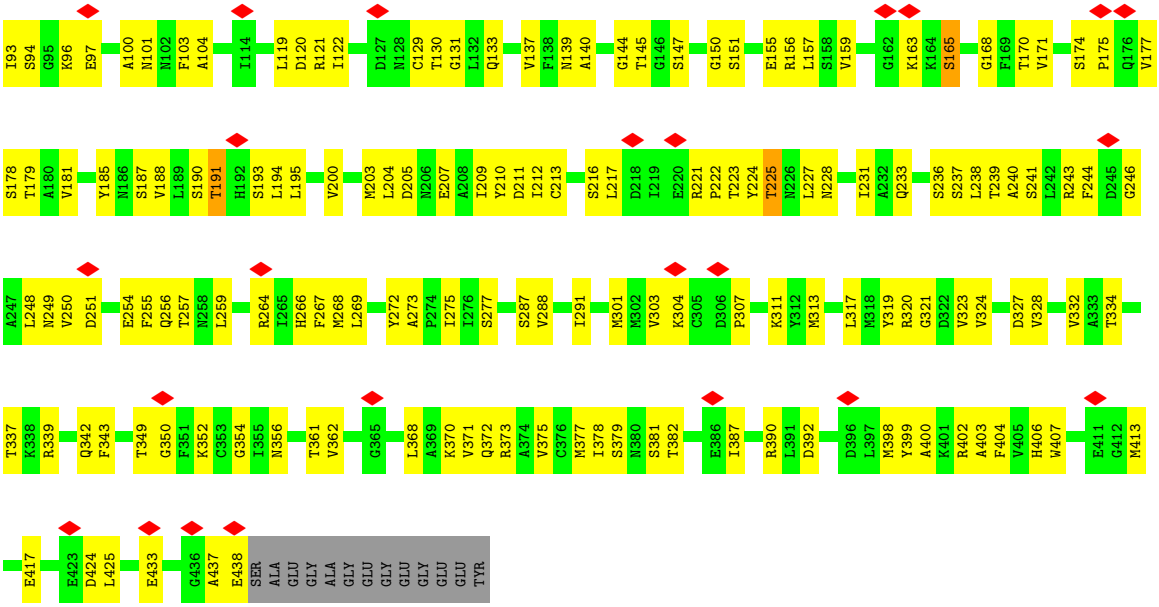


• Molecule 13: Tubulin alpha

Chain 7d:



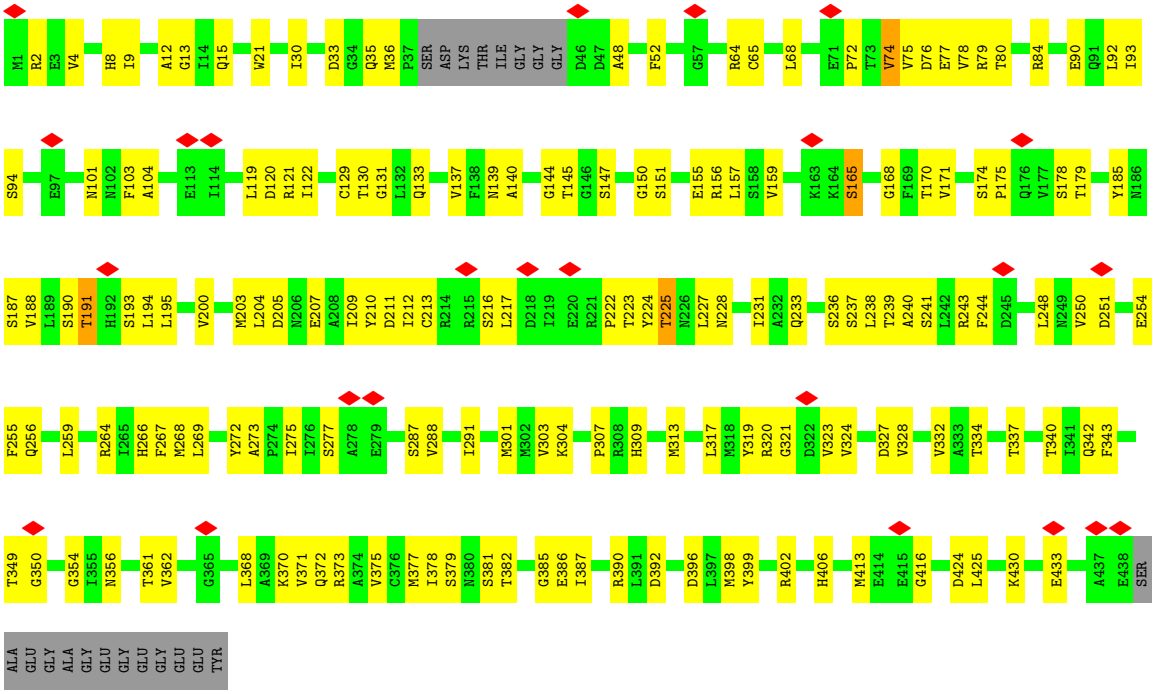




• Molecule 13: Tubulin alpha

Chain 7f:

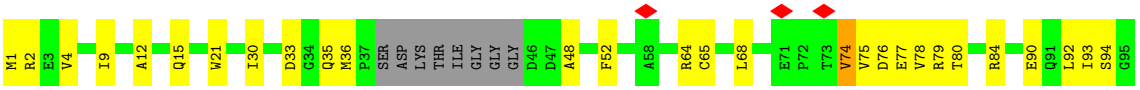


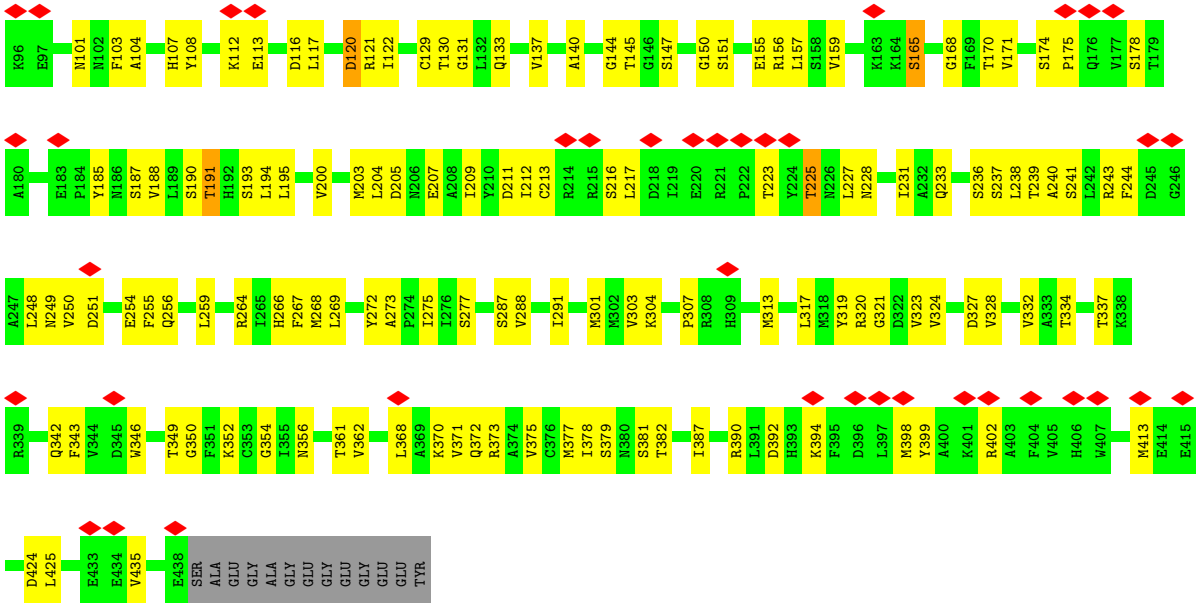


• Molecule 13: Tubulin alpha

Chain 7h:



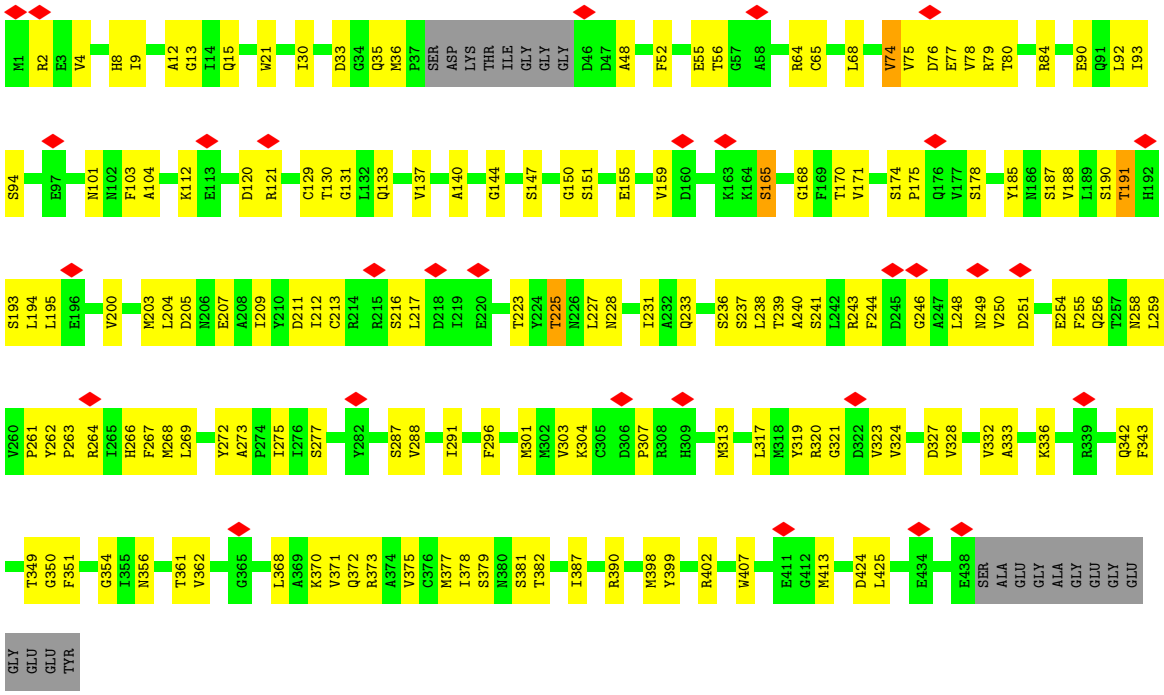




• Molecule 13: Tubulin alpha

Chain 8b:

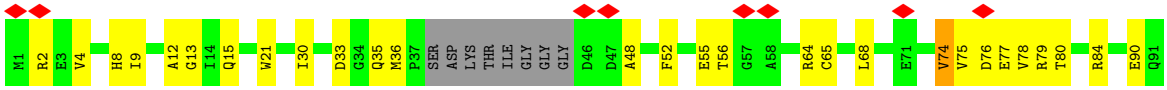


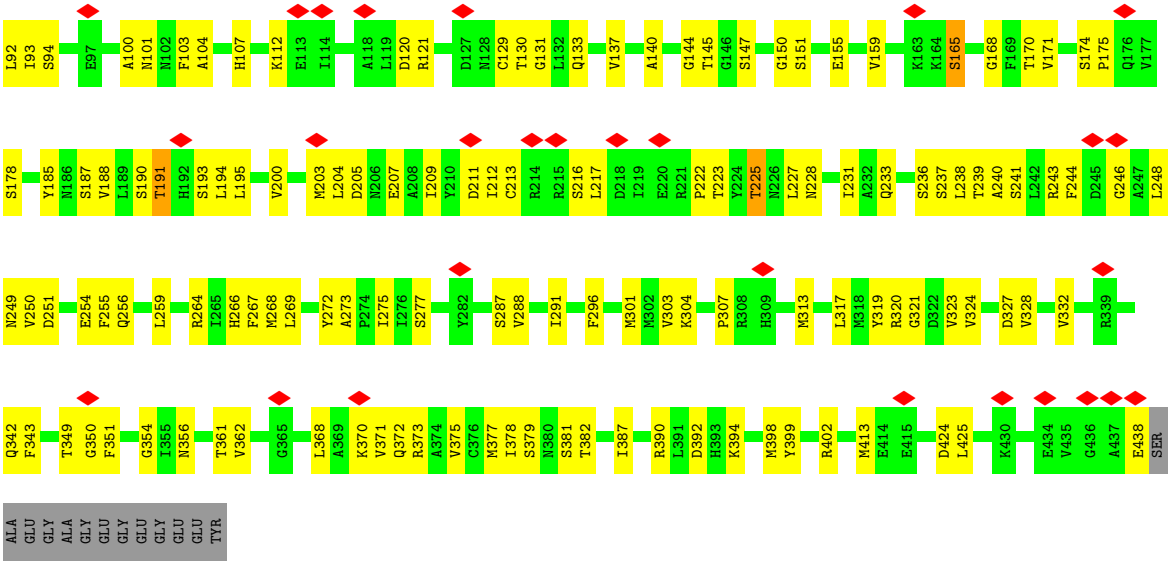


• Molecule 13: Tubulin alpha

Chain 8d:



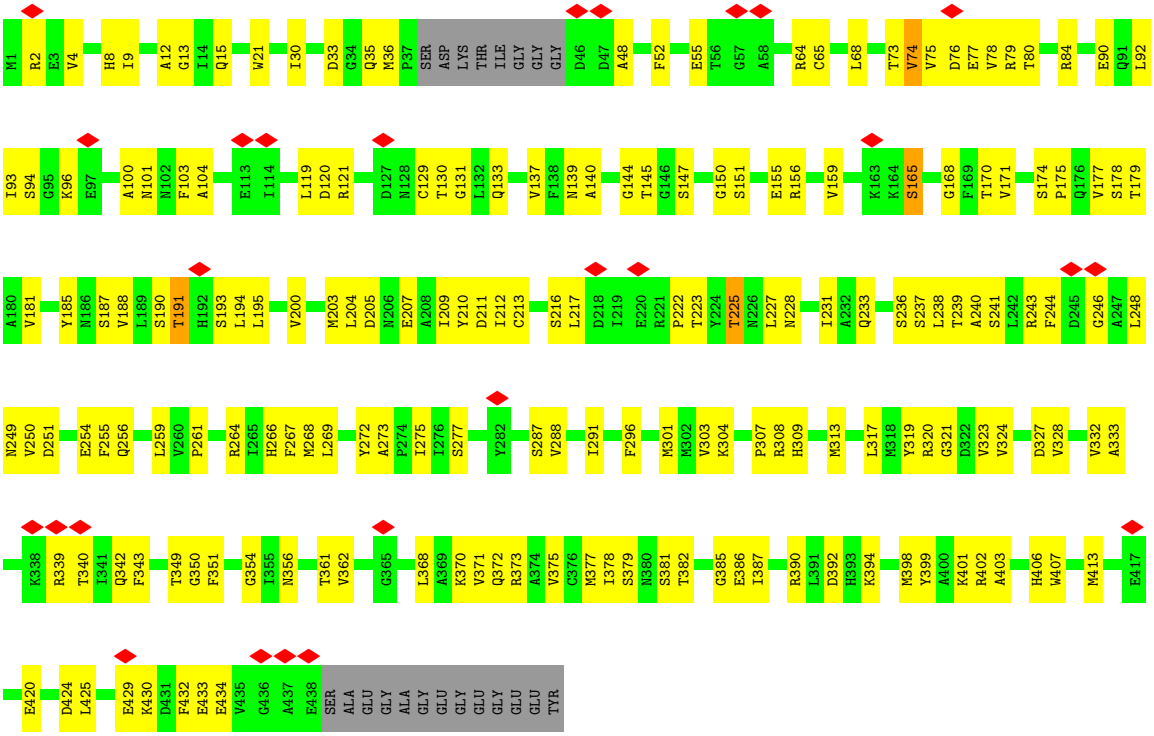




• Molecule 13: Tubulin alpha

Chain 8f:

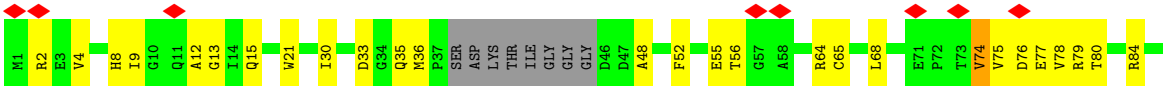


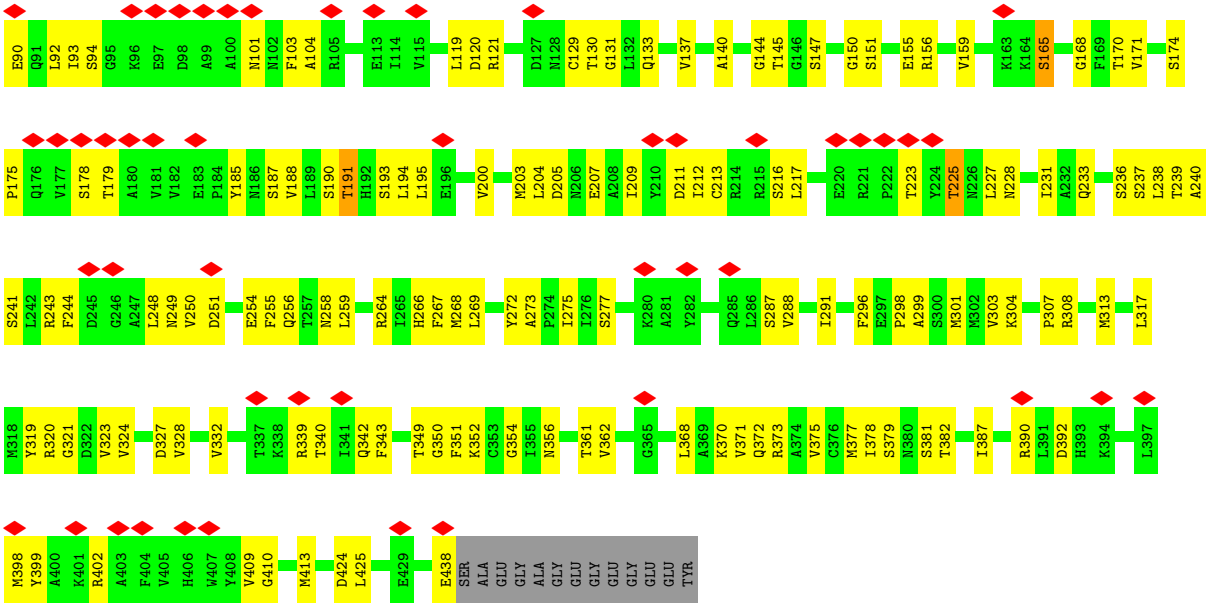


• Molecule 13: Tubulin alpha

Chain 8h:



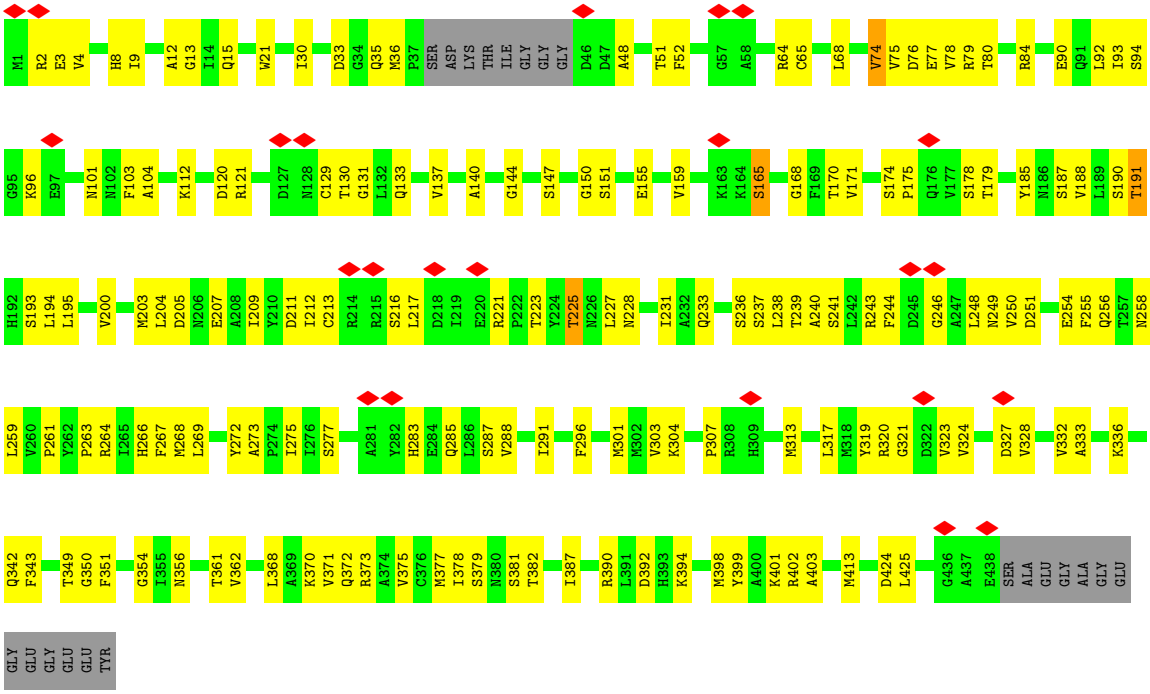




• Molecule 13: Tubulin alpha

Chain 9b:

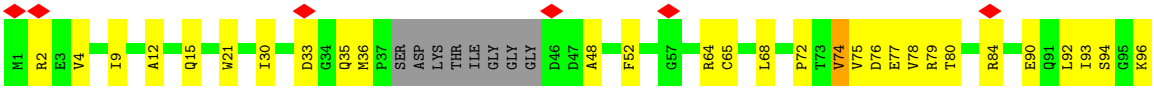


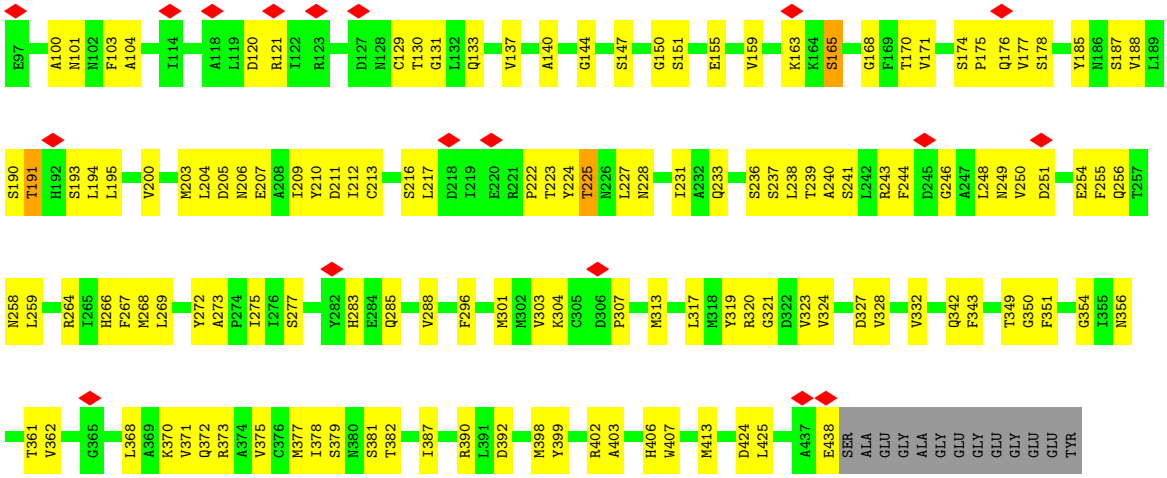


• Molecule 13: Tubulin alpha

Chain 9d:



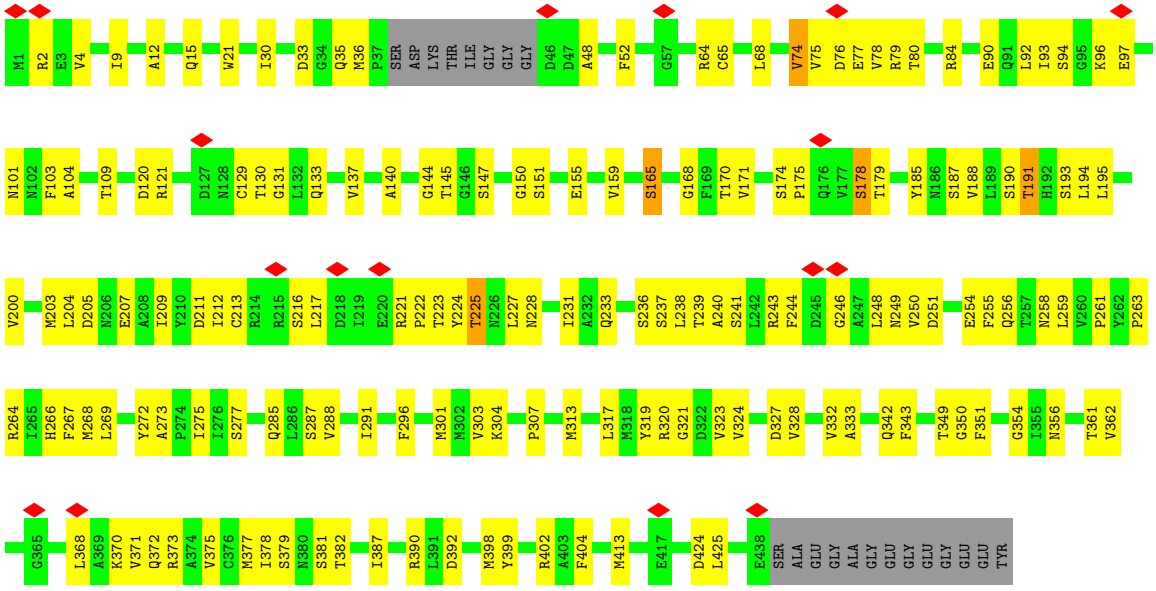




• Molecule 13: Tubulin alpha

Chain 9f:

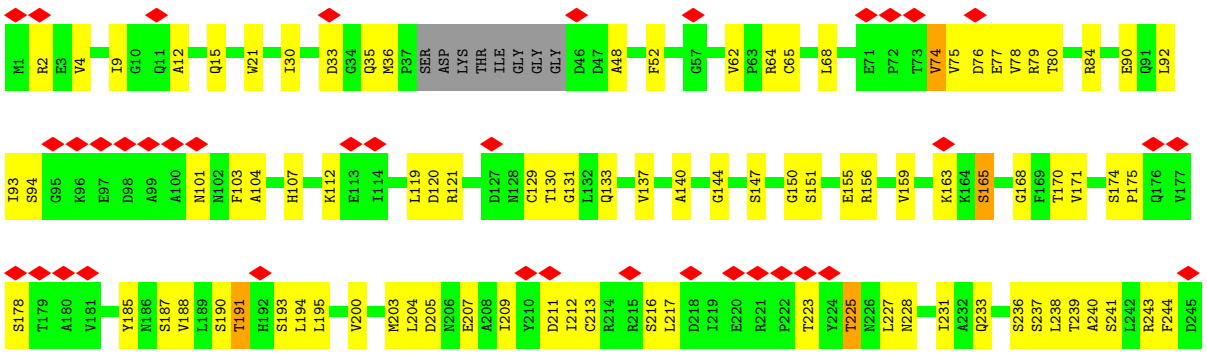


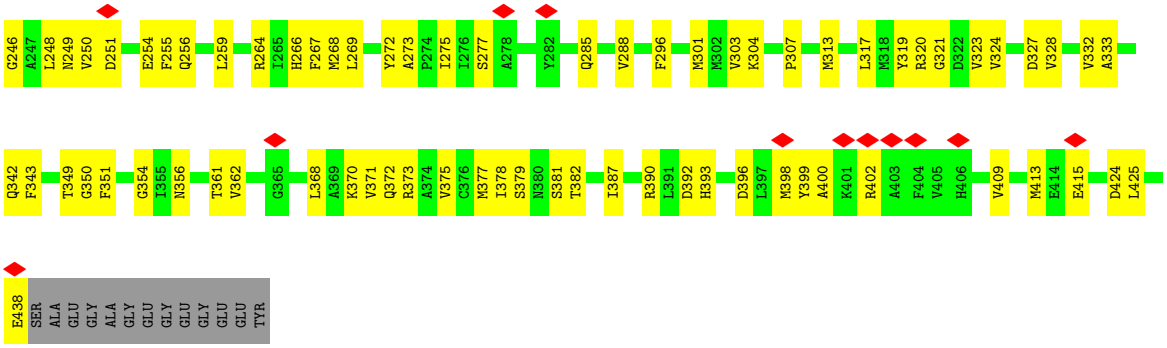


• Molecule 13: Tubulin alpha

Chain 9h:



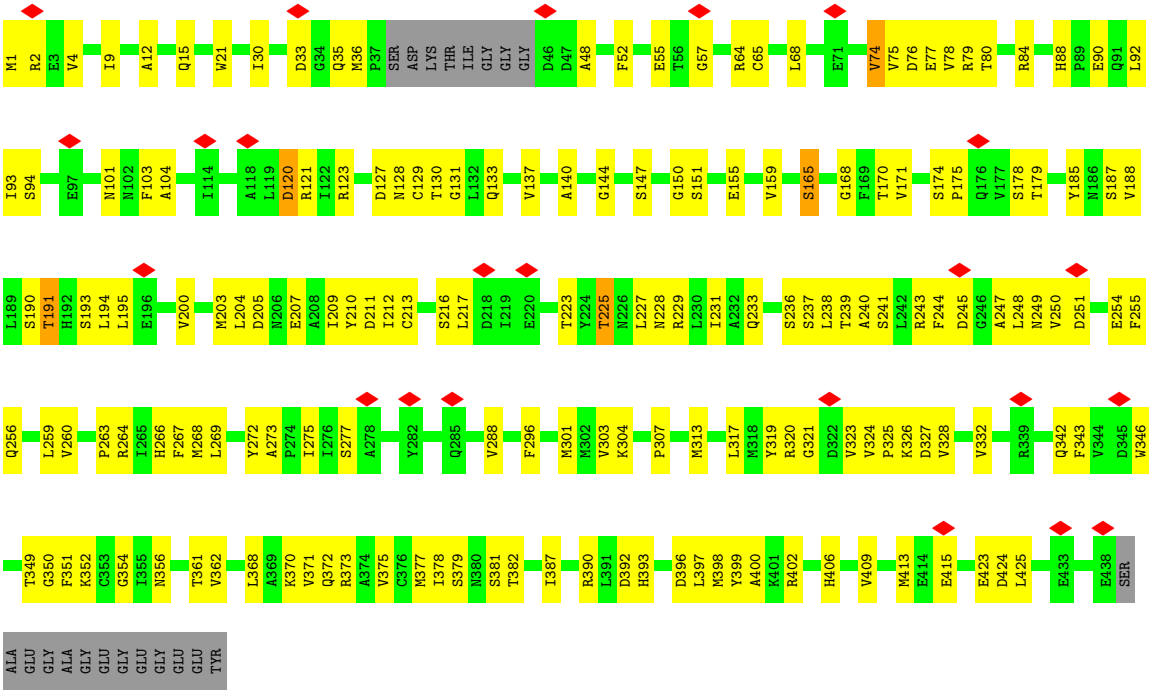




• Molecule 13: Tubulin alpha

Chain Ab:

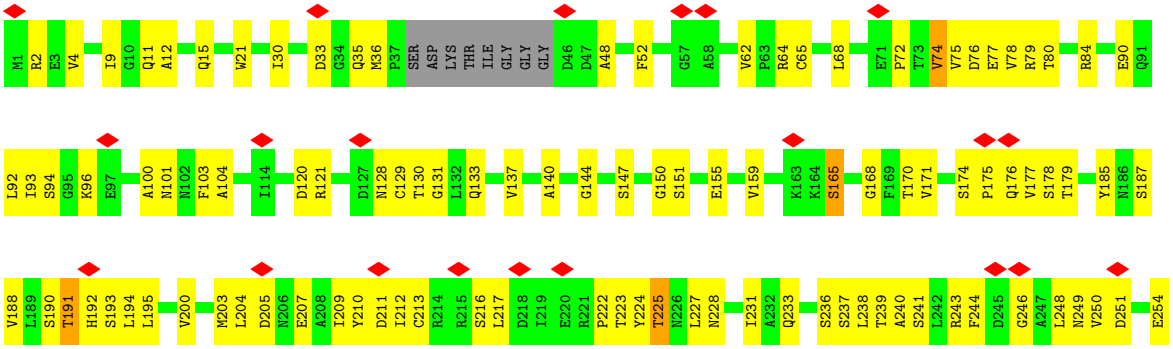


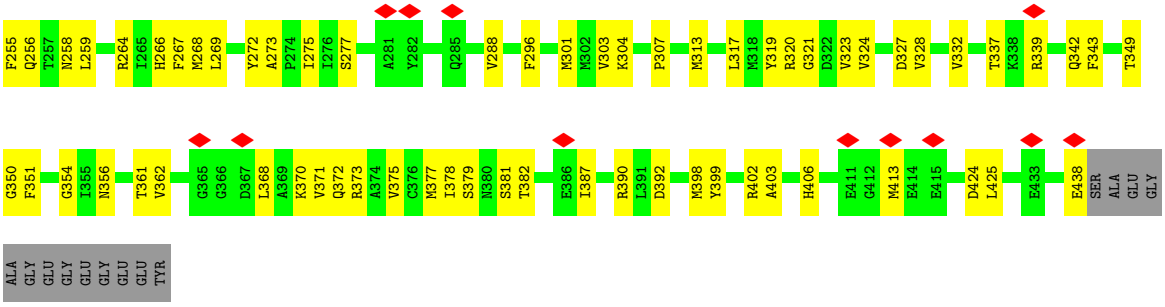


• Molecule 13: Tubulin alpha

Chain Ad:



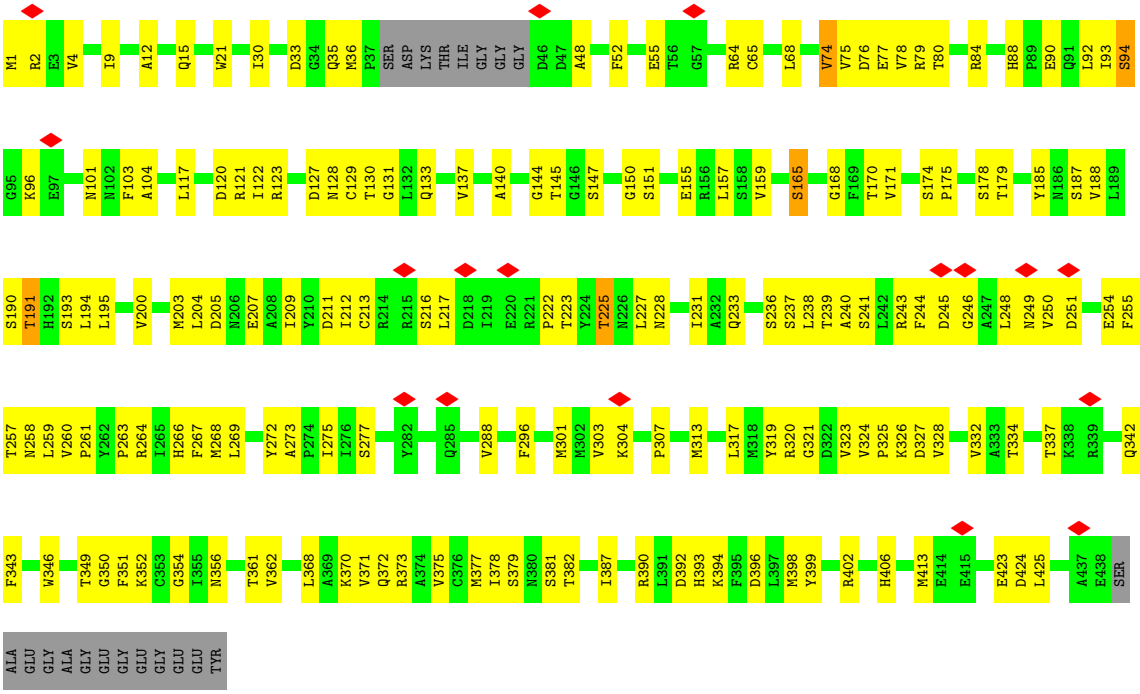




• Molecule 13: Tubulin alpha

Chain Af:

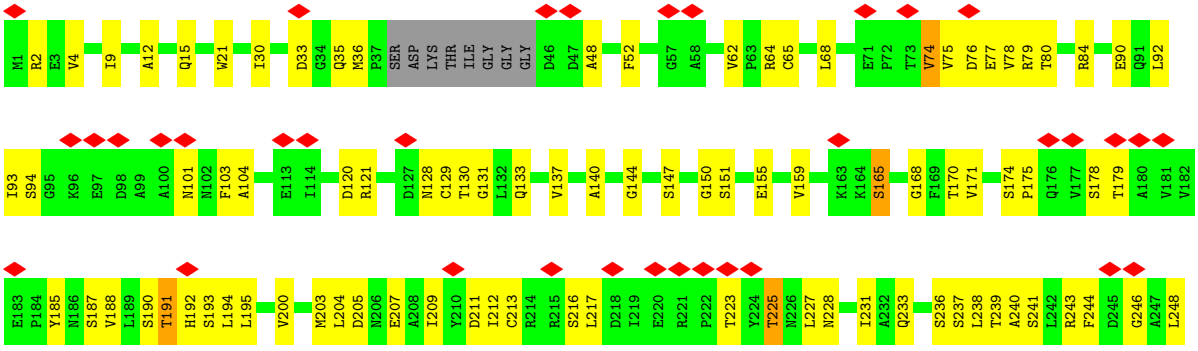


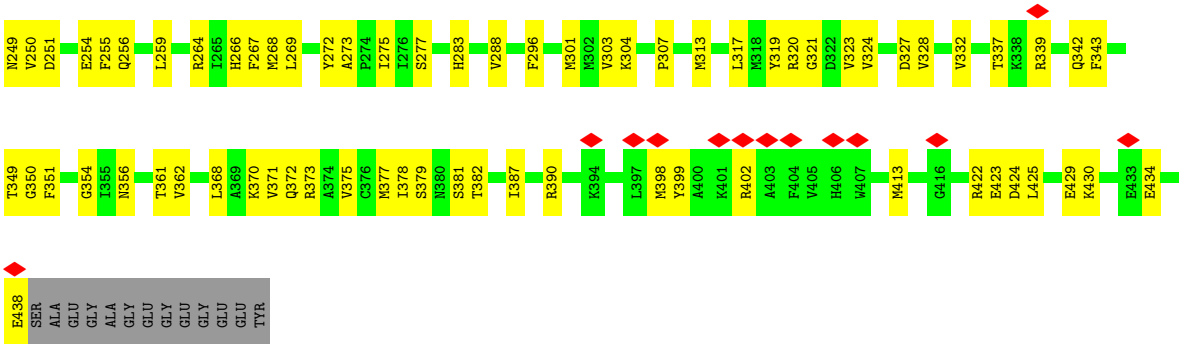


• Molecule 13: Tubulin alpha

Chain Ah:



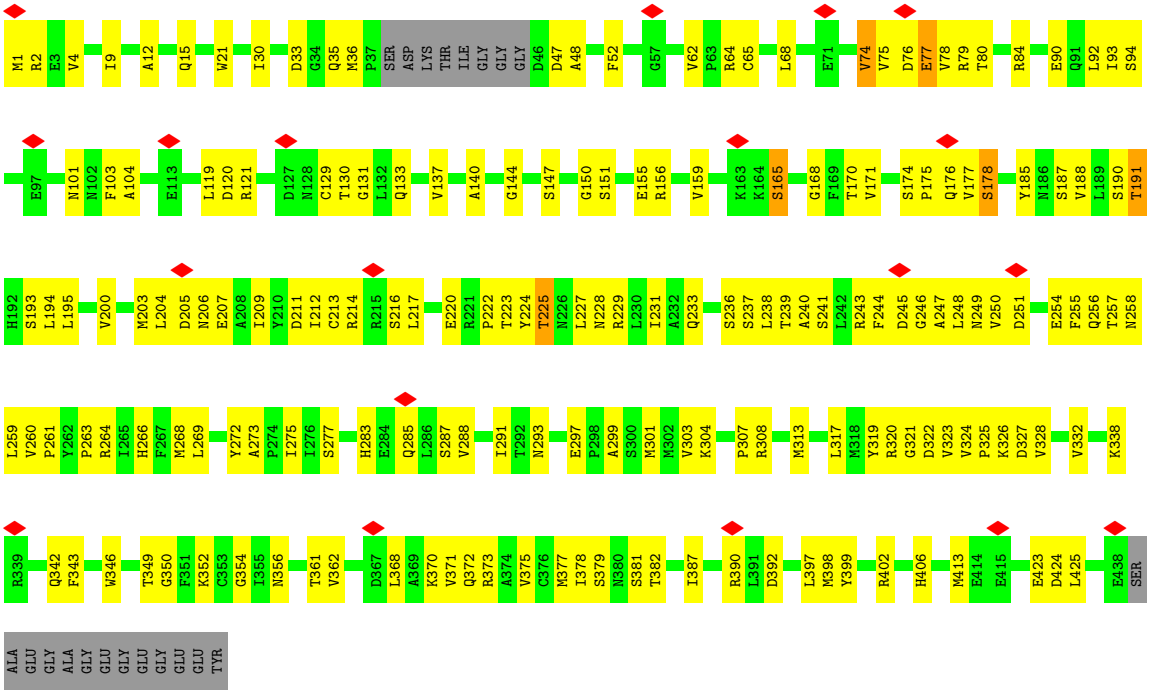




• Molecule 13: Tubulin alpha

Chain Bb:

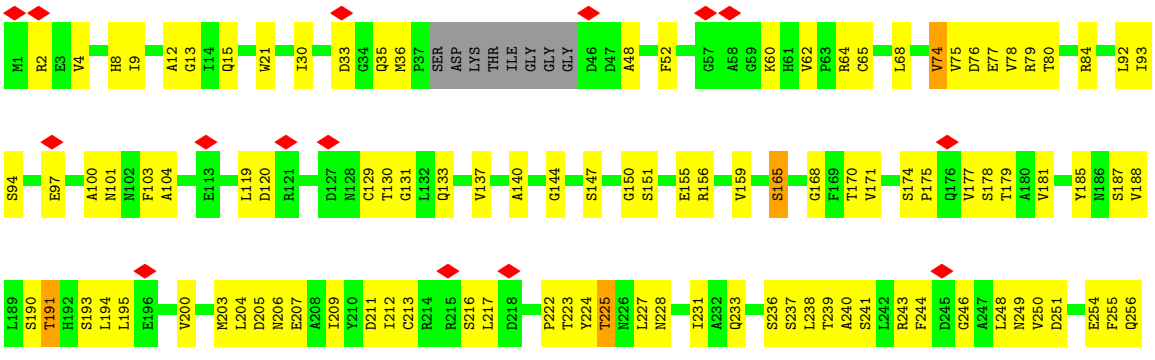


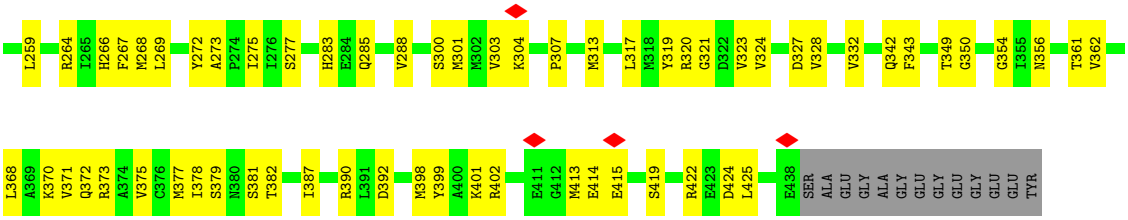


• Molecule 13: Tubulin alpha

Chain Bd:



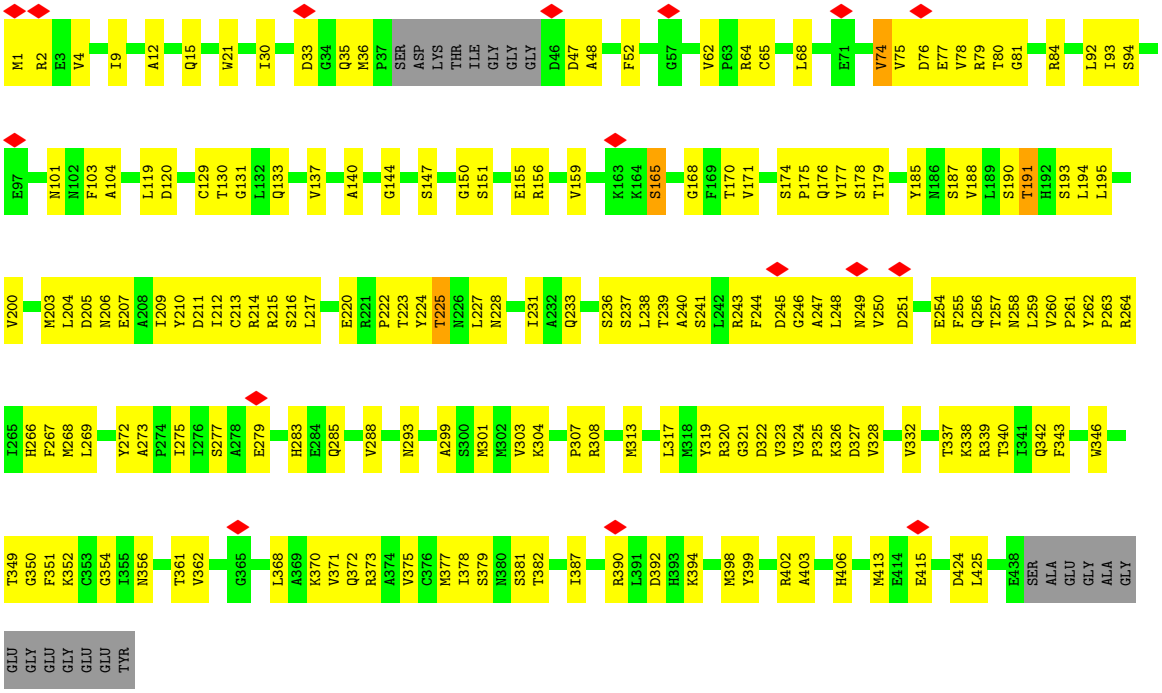




• Molecule 13: Tubulin alpha

Chain Bf:

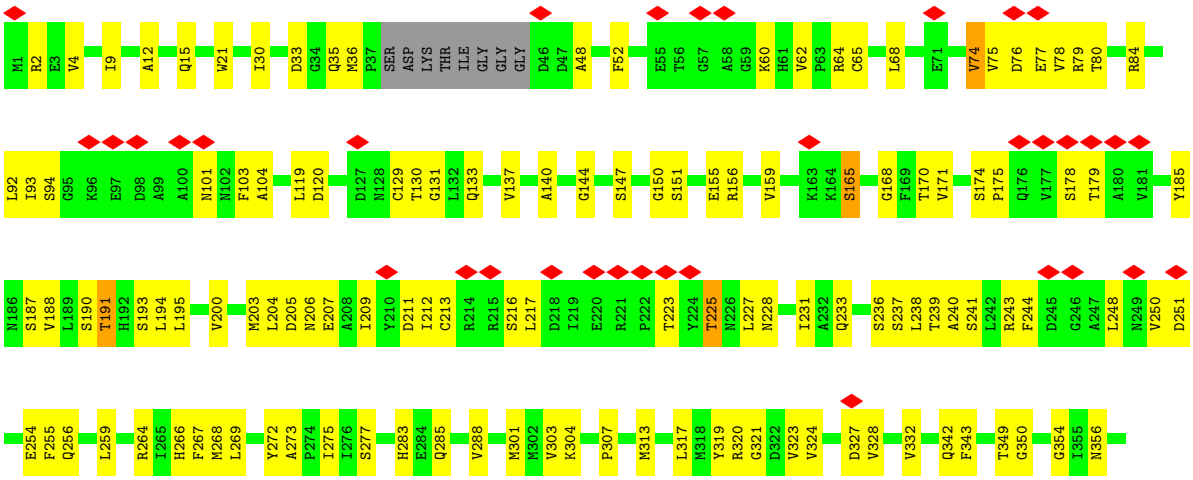


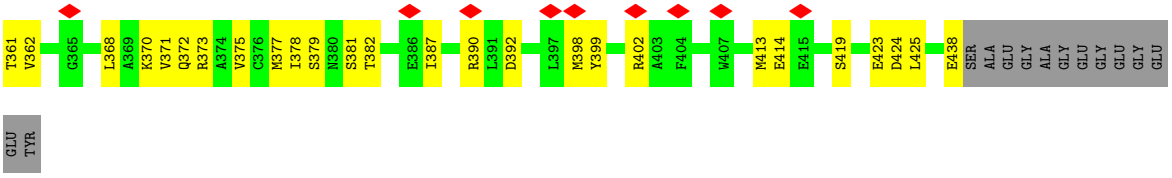


• Molecule 13: Tubulin alpha

Chain Bh:



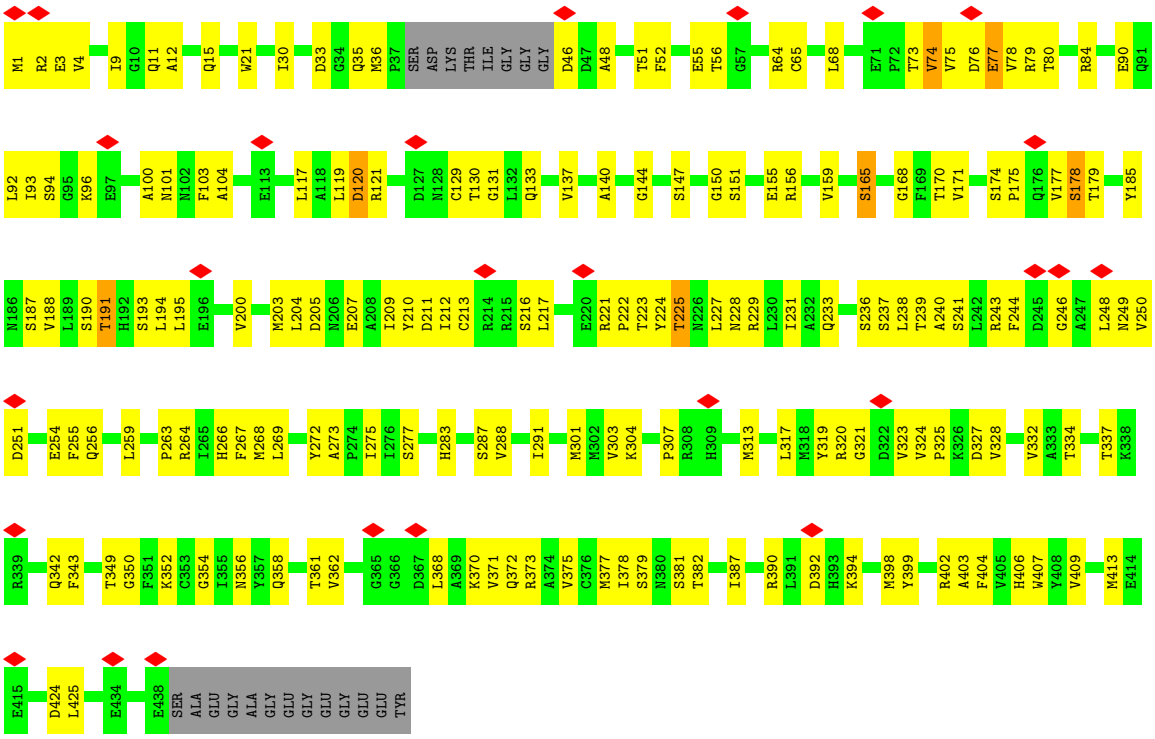




• Molecule 13: Tubulin alpha

Chain Cb:

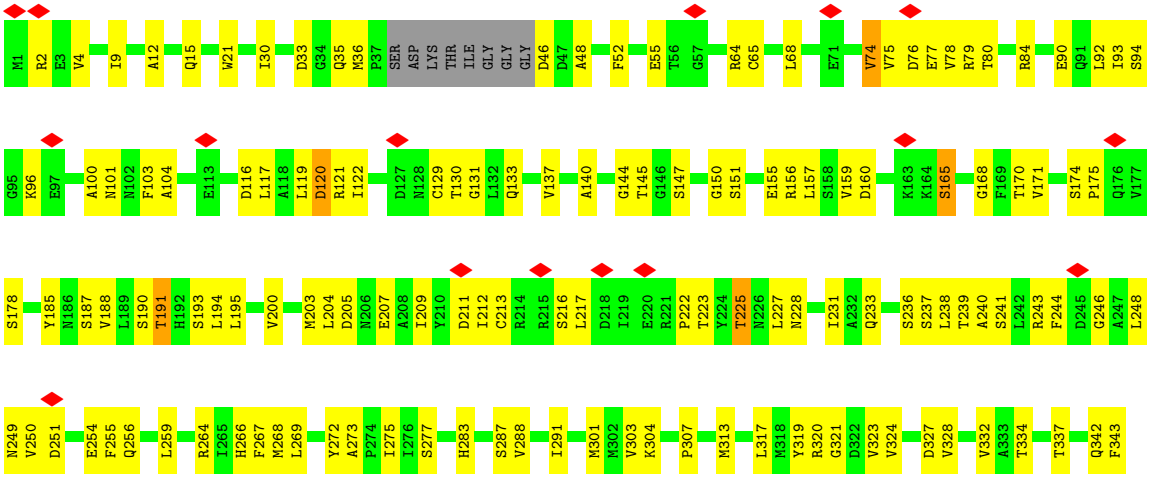




• Molecule 13: Tubulin alpha

Chain Cd:



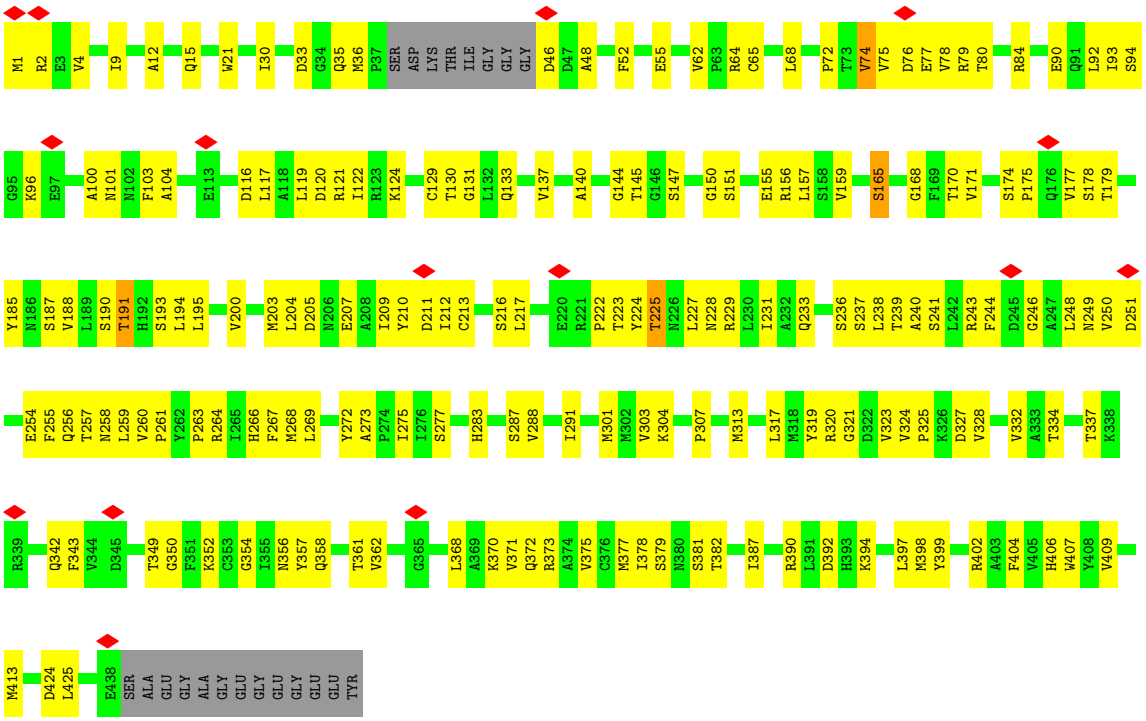




• Molecule 13: Tubulin alpha

Chain Cf:

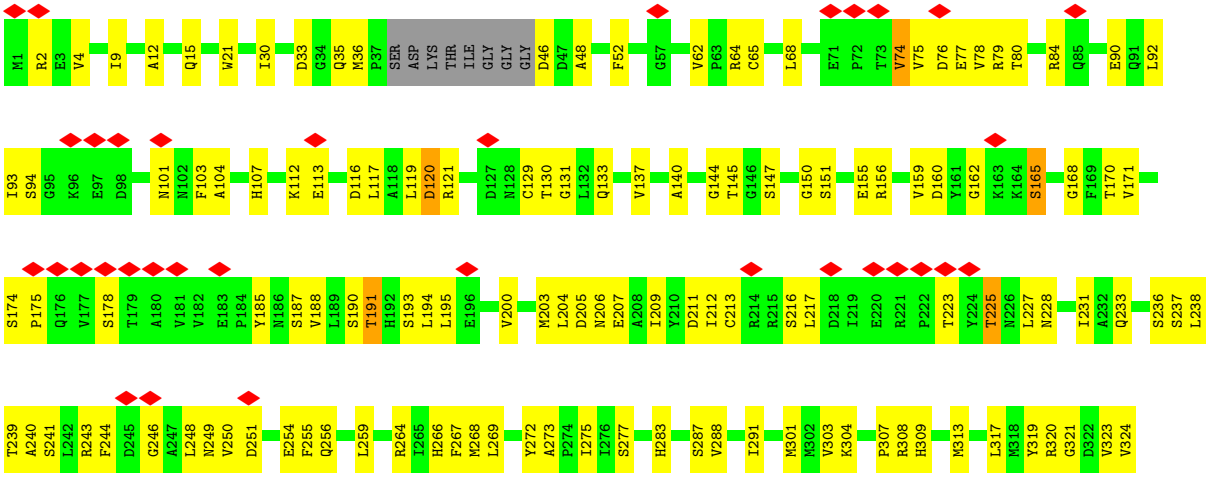


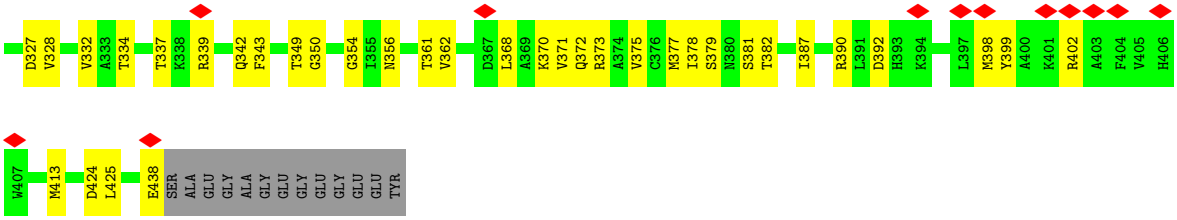


• Molecule 13: Tubulin alpha

Chain Ch:



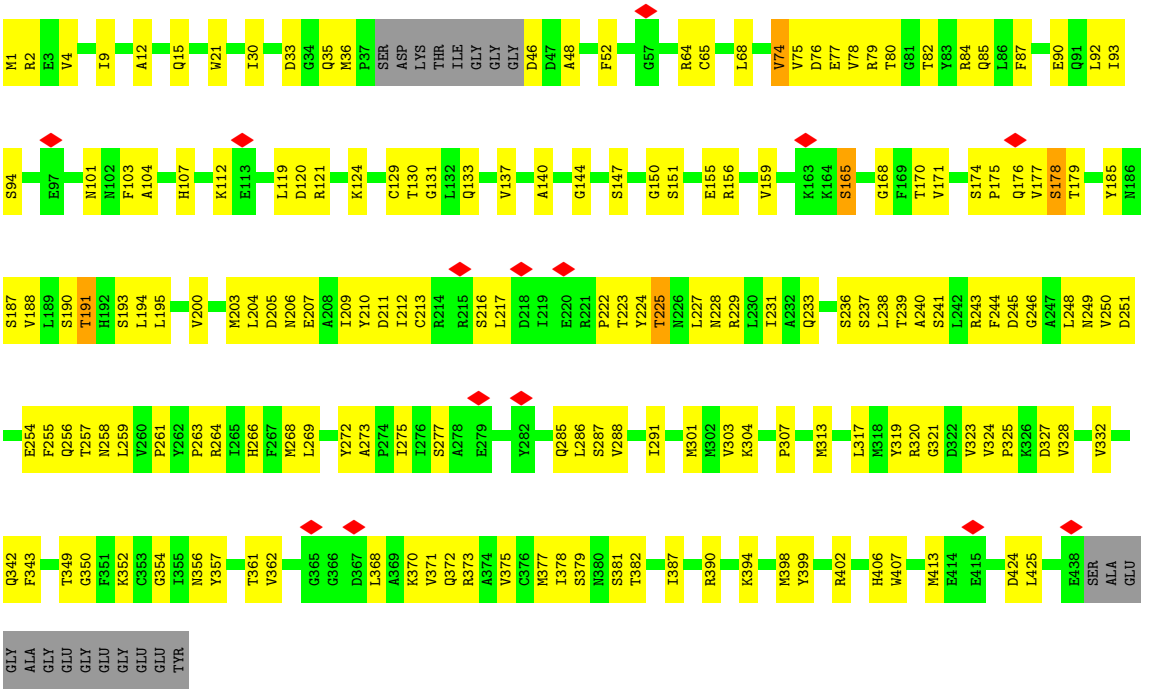




• Molecule 13: Tubulin alpha

Chain Db:

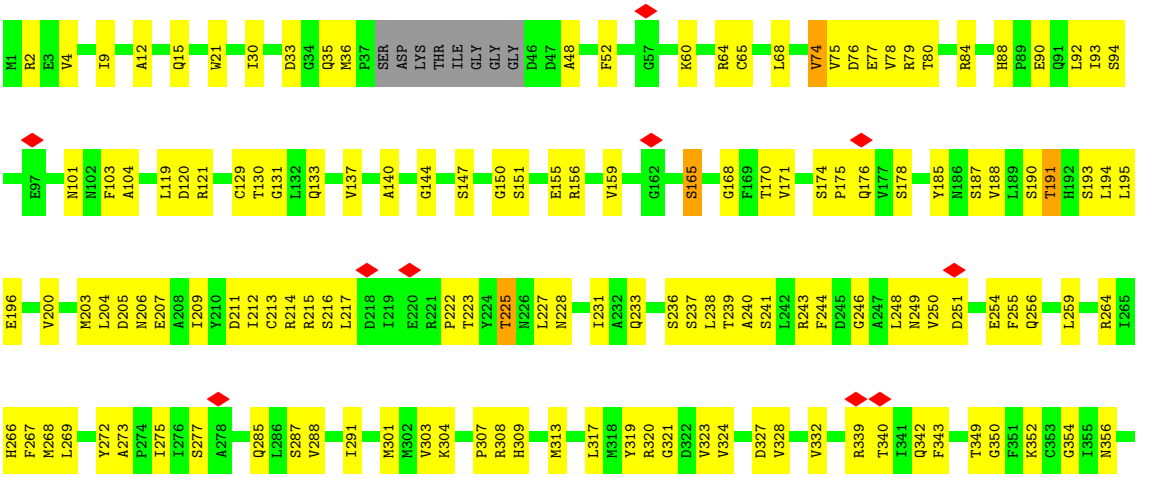


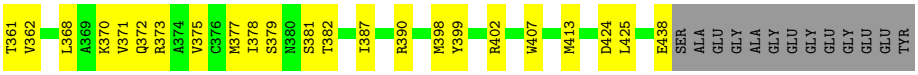


• Molecule 13: Tubulin alpha

Chain Dd:



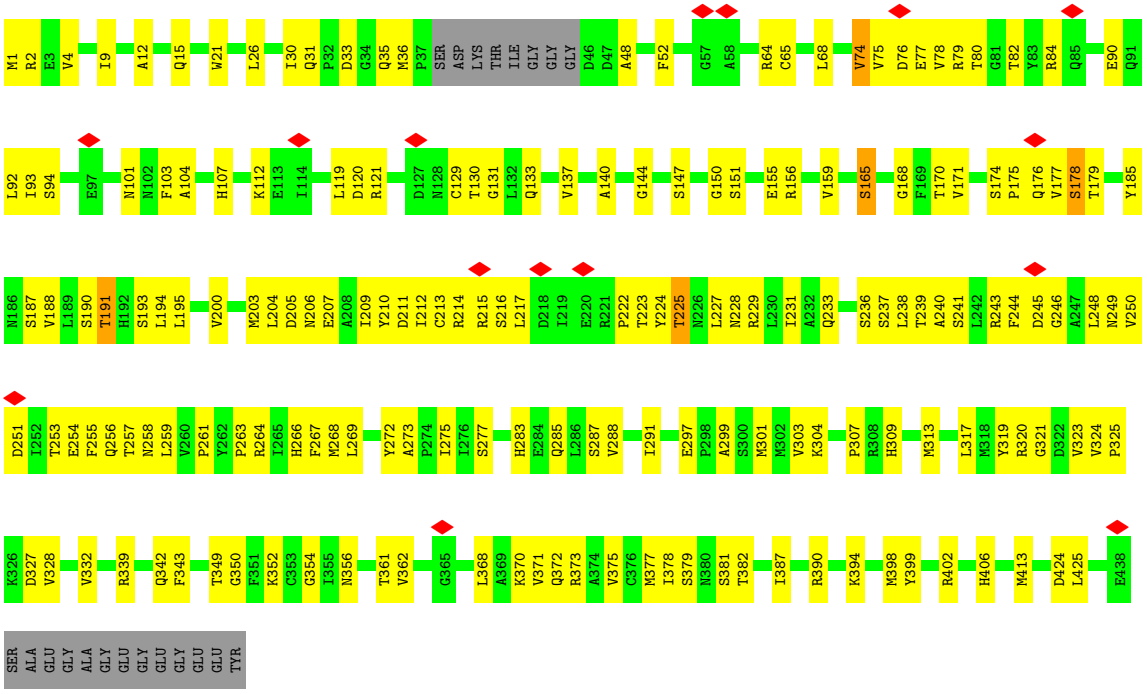




• Molecule 13: Tubulin alpha

Chain Df:

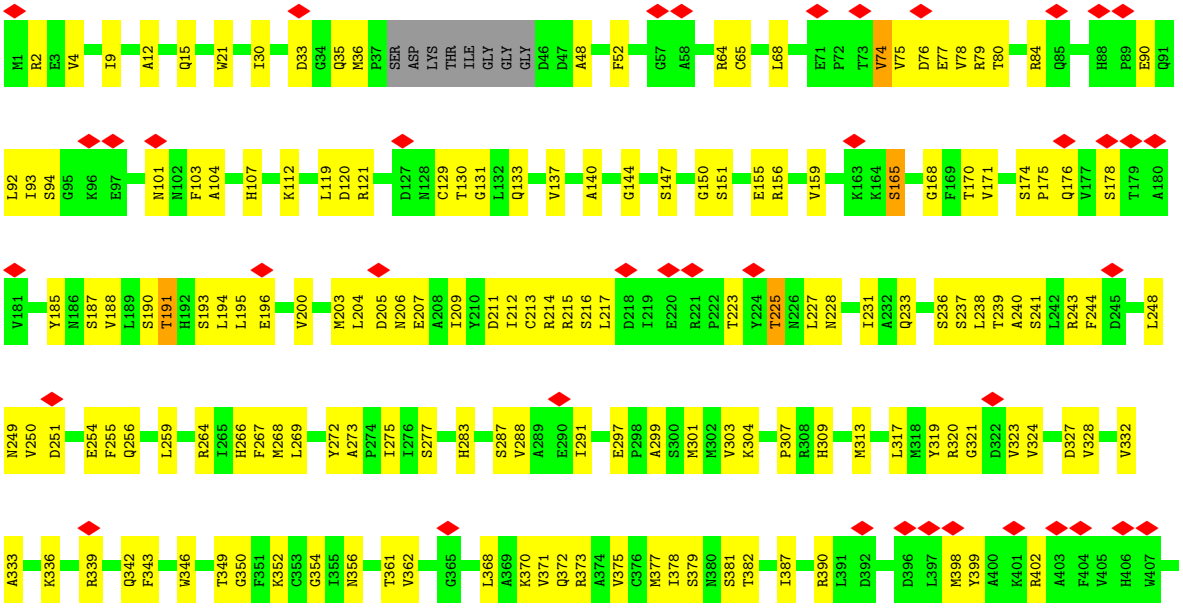


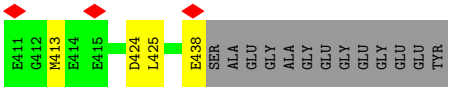


• Molecule 13: Tubulin alpha

Chain Dh:

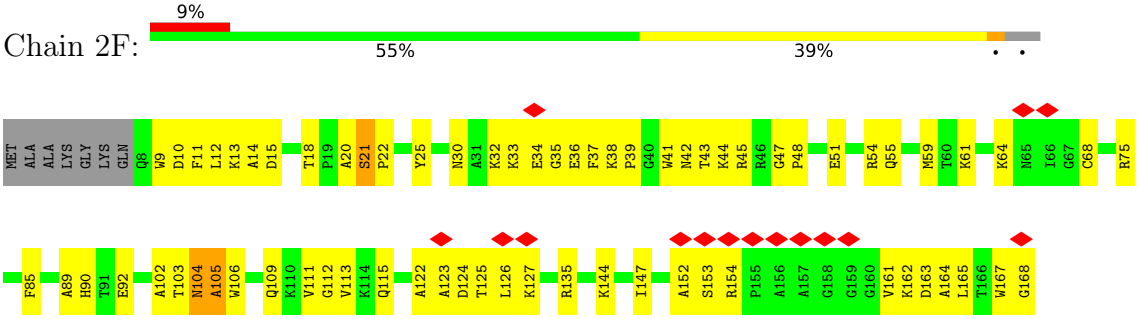






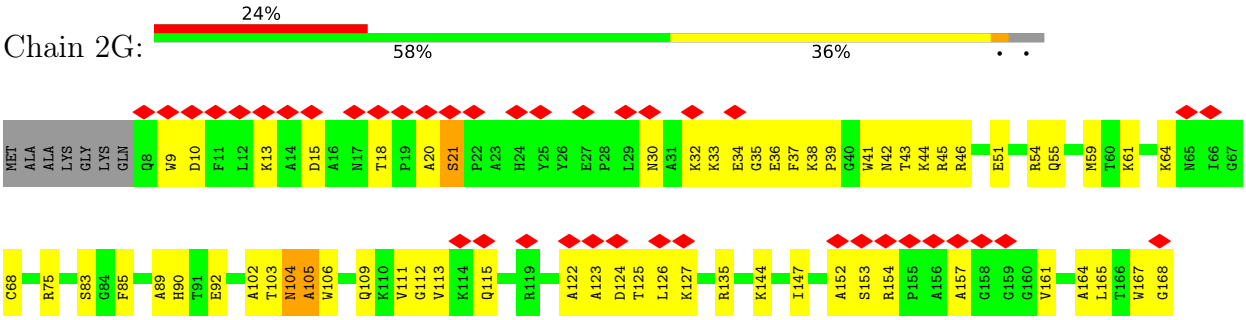
• Molecule 14: FAP275

Chain 2F:



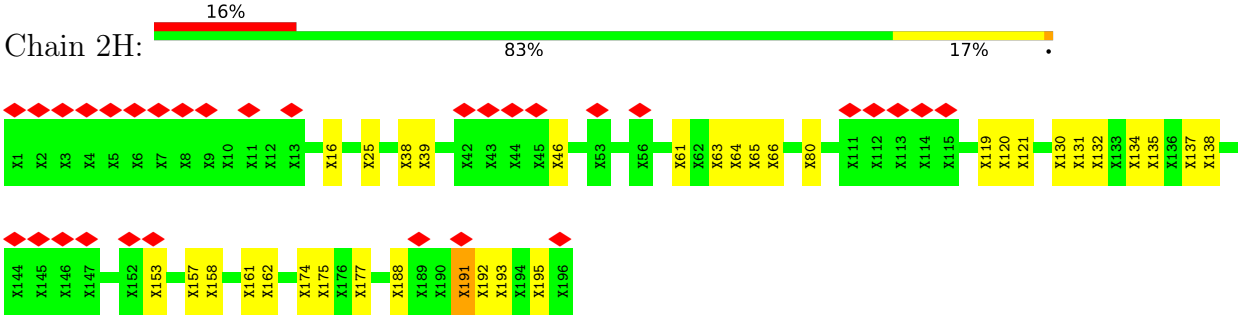
• Molecule 14: FAP275

Chain 2G:



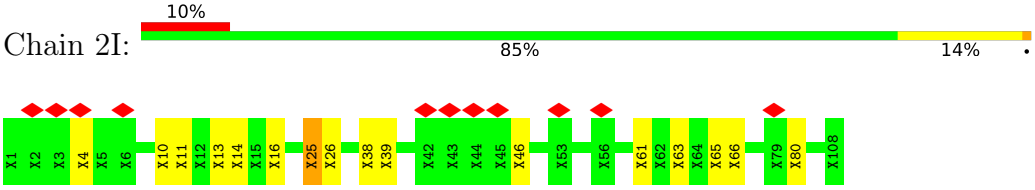
• Molecule 15: Unknown protein

Chain 2H:



• Molecule 16: Unknown protein

Chain 2I:



• Molecule 17: Unknown protein

Chain 2J:

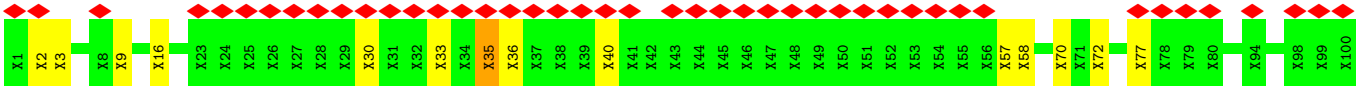




• Molecule 17: Unknown protein

Chain 2K:

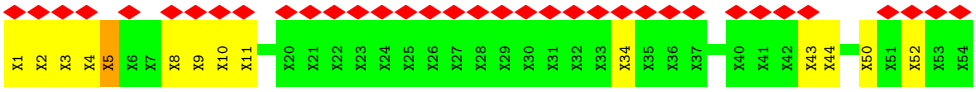




• Molecule 18: Unknown protein

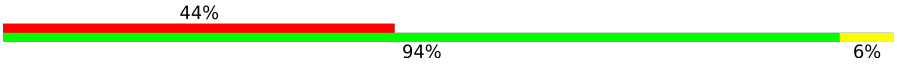
Chain 2L:

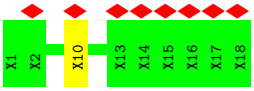




• Molecule 19: Unknown protein

Chain 2M:

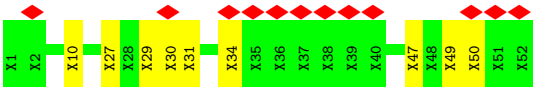




• Molecule 20: Unknown protein

Chain 2N:

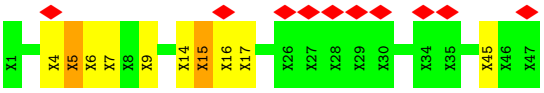




• Molecule 21: Unknown protein

Chain 2O:

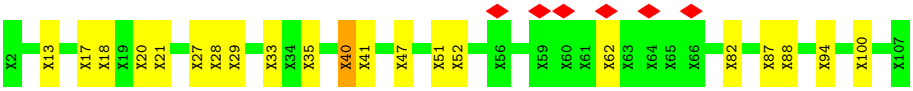




• Molecule 22: Unknown protein

Chain 2P:

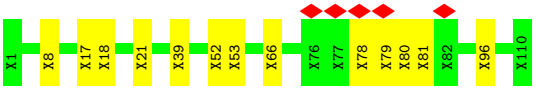




• Molecule 23: Unknown protein

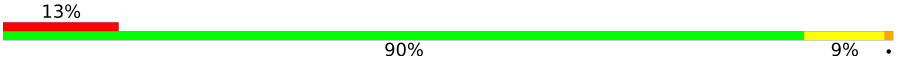
Chain 2Q:

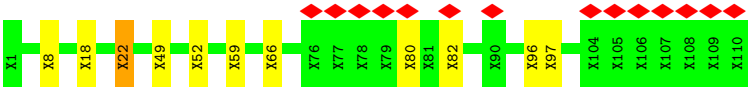




• Molecule 23: Unknown protein

Chain 2R:

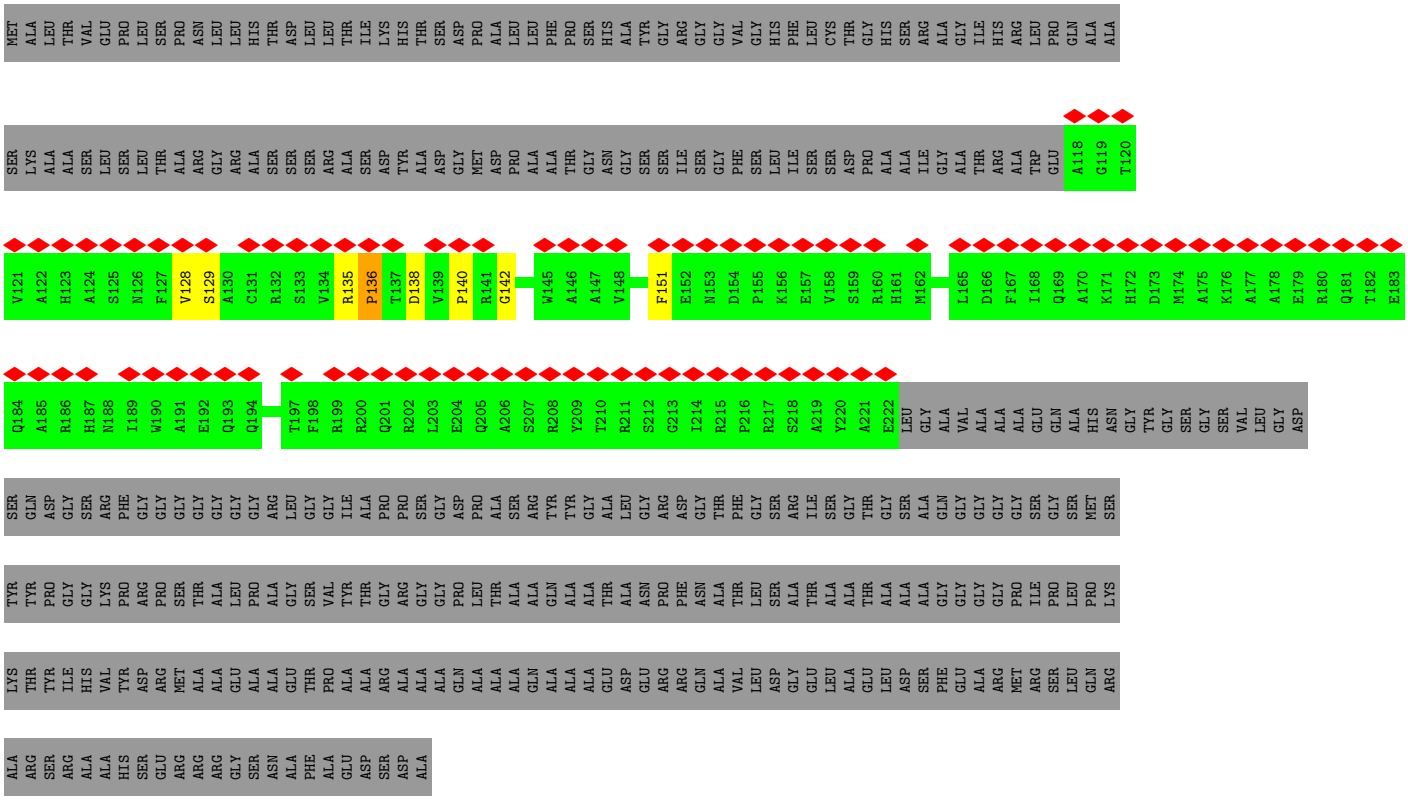




• Molecule 24: FAP289

Chain 2S:

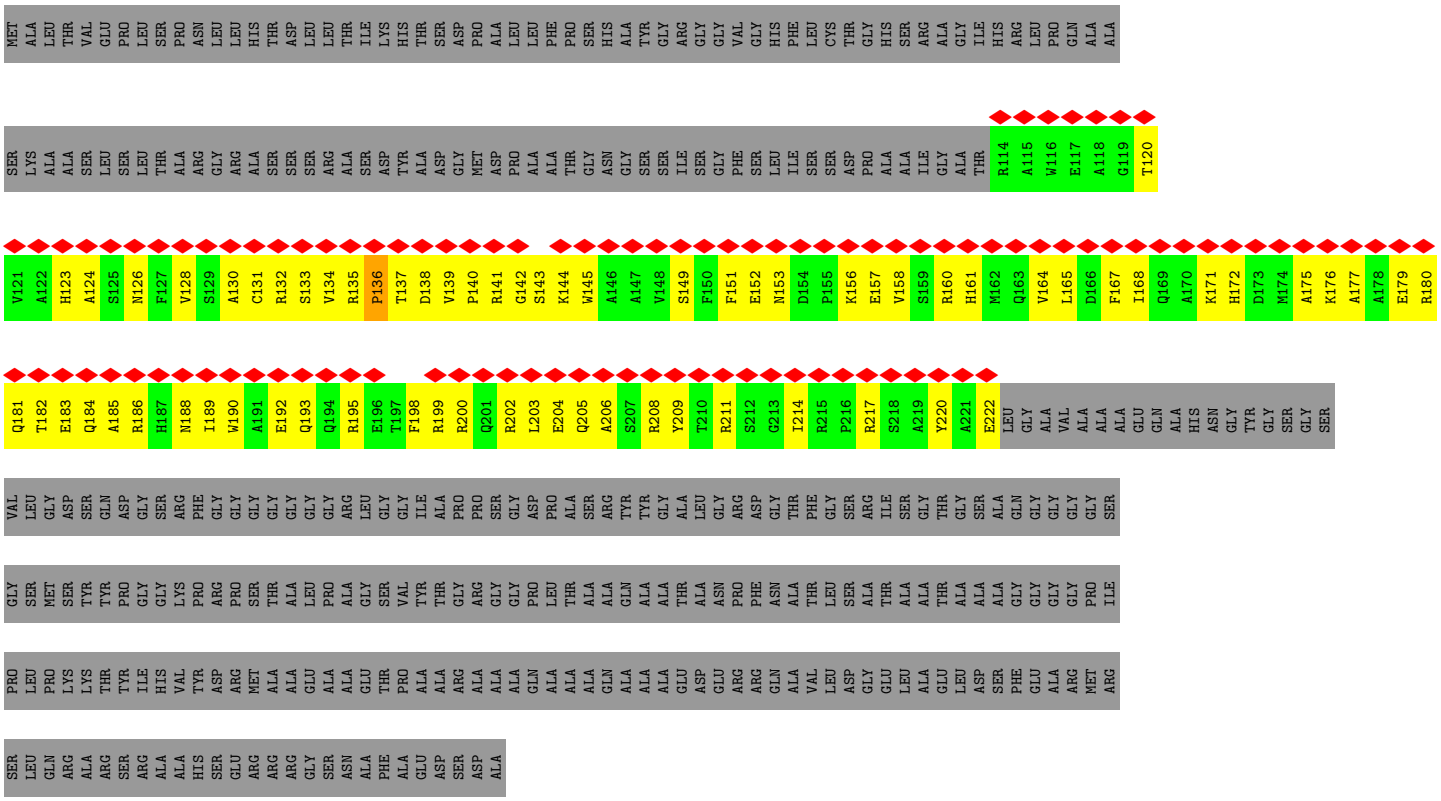




• Molecule 24: FAP289

Chain 2T:

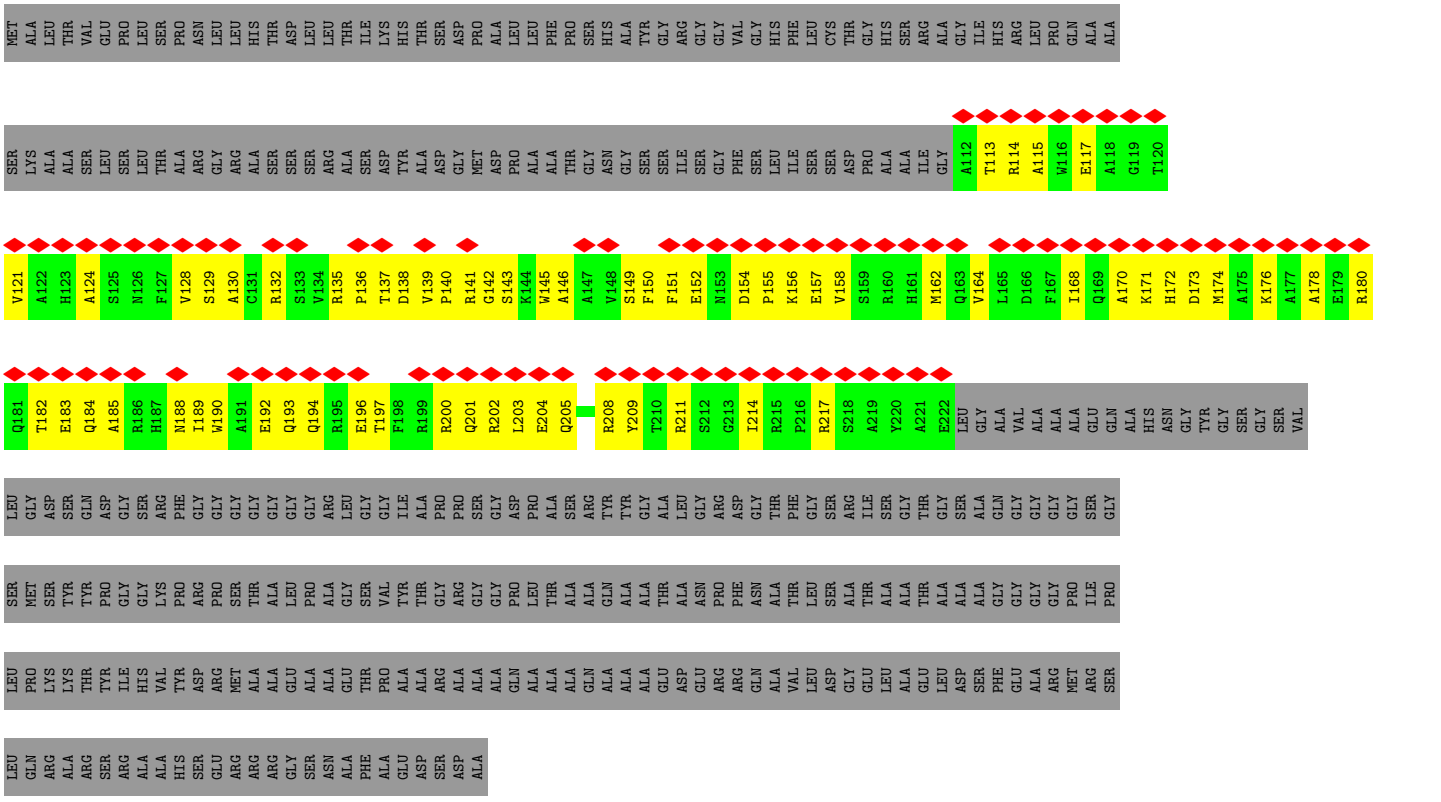




• Molecule 24: FAP289

Chain 2U:

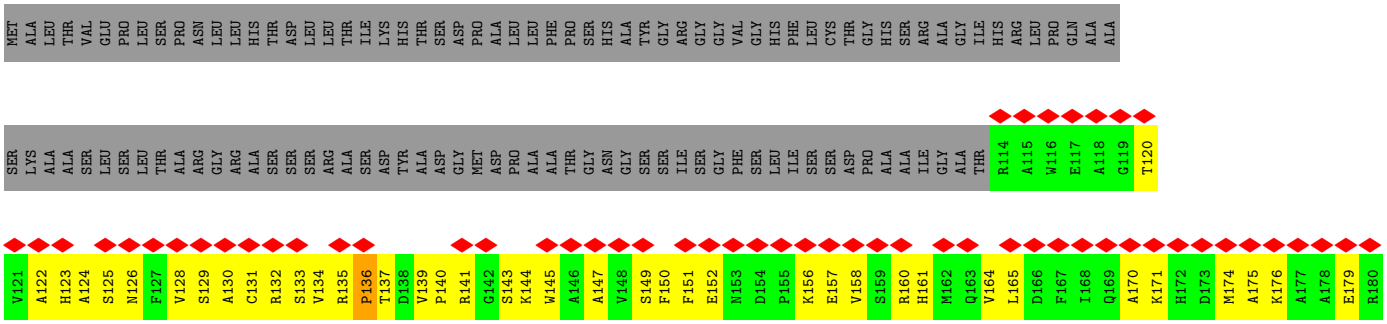




• Molecule 24: FAP289

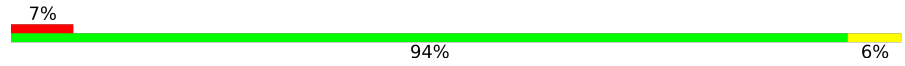
Chain 2V:

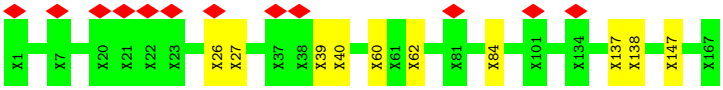




• Molecule 25: Unknown protein

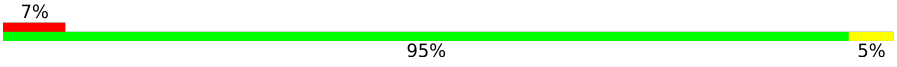
Chain 2W:

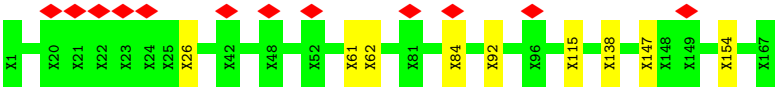




• Molecule 25: Unknown protein

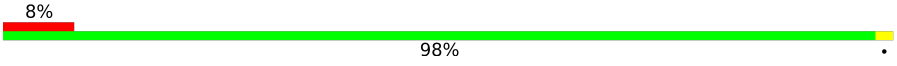
Chain 2X:

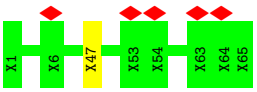




• Molecule 26: Unknown protein

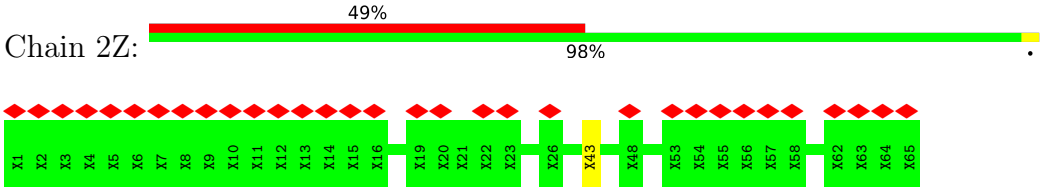
Chain 2Y:





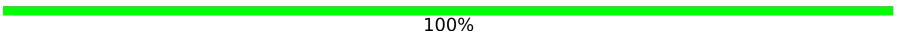
• Molecule 26: Unknown protein

Chain 2Z:



• Molecule 27: Unknown protein

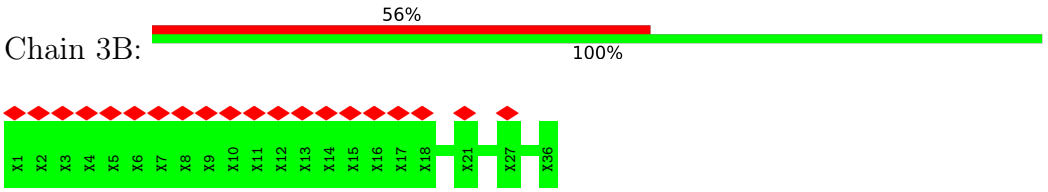
Chain 3A:



There are no outlier residues recorded for this chain.

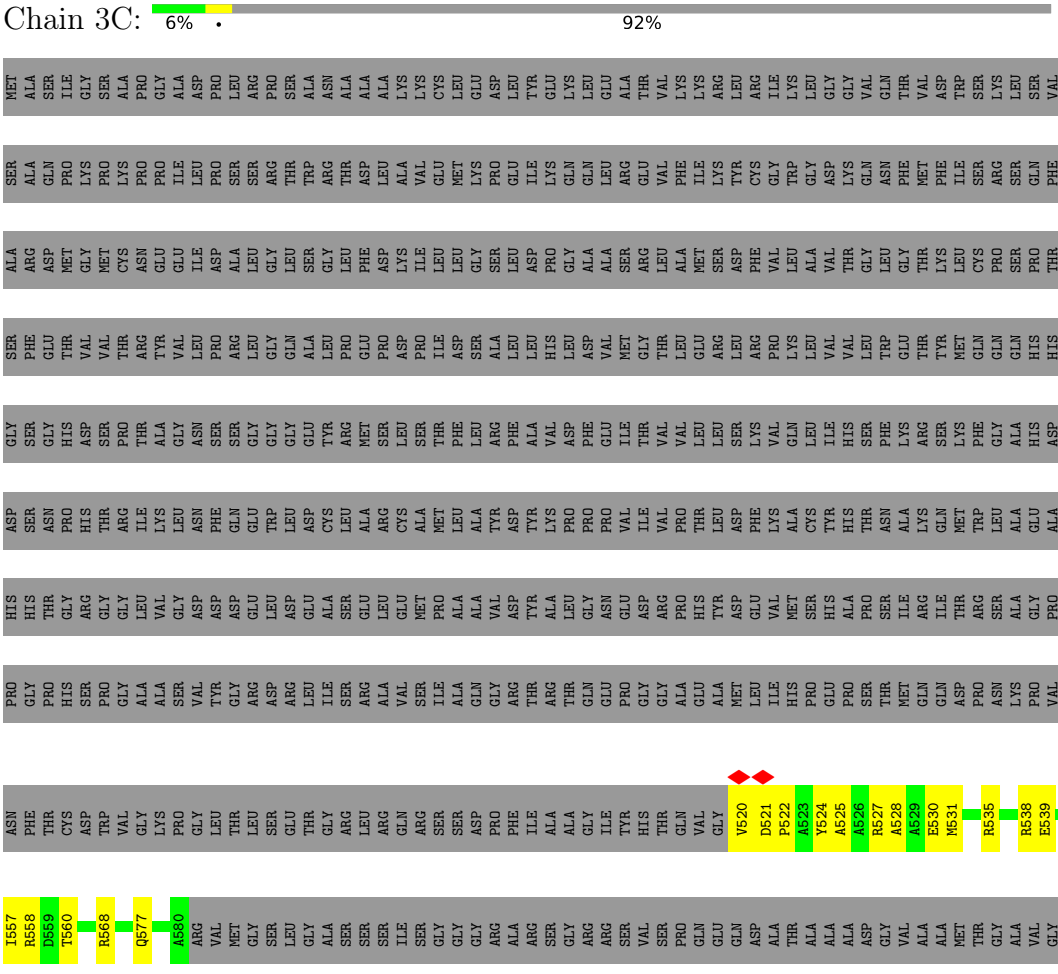
• Molecule 27: Unknown protein

Chain 3B:



• Molecule 28: FAP216

Chain 3C:



GLY SER GLY GLY GLY ARG ARG SER VAL PRO PRO GLN SER MET ARG SER GLY SER ALA PRO ARG LEU SER GLY ALA LEU GLY SER GLY GLY GLY ALA GLY THR VAL ASP GLY GLY GLY ALA GLY GLY GLY THR ILE VAL PRO GLY LEU GLU ALA VAL MET ALA ARG THR GLY GLY ARG SER

ALA LEU HIS ALA ALA THR THR GLY SER VAL SER PRO ALA LYS HIS SER ARG THR LEU LEU GLN GLU LEU GLN GLN ALA LEU ASP VAL GLU SER LYS LEU PRO GLN HIS ALA THR THR ILE ALA GLY HIS GLY GLN ILE ARG PHE GLY

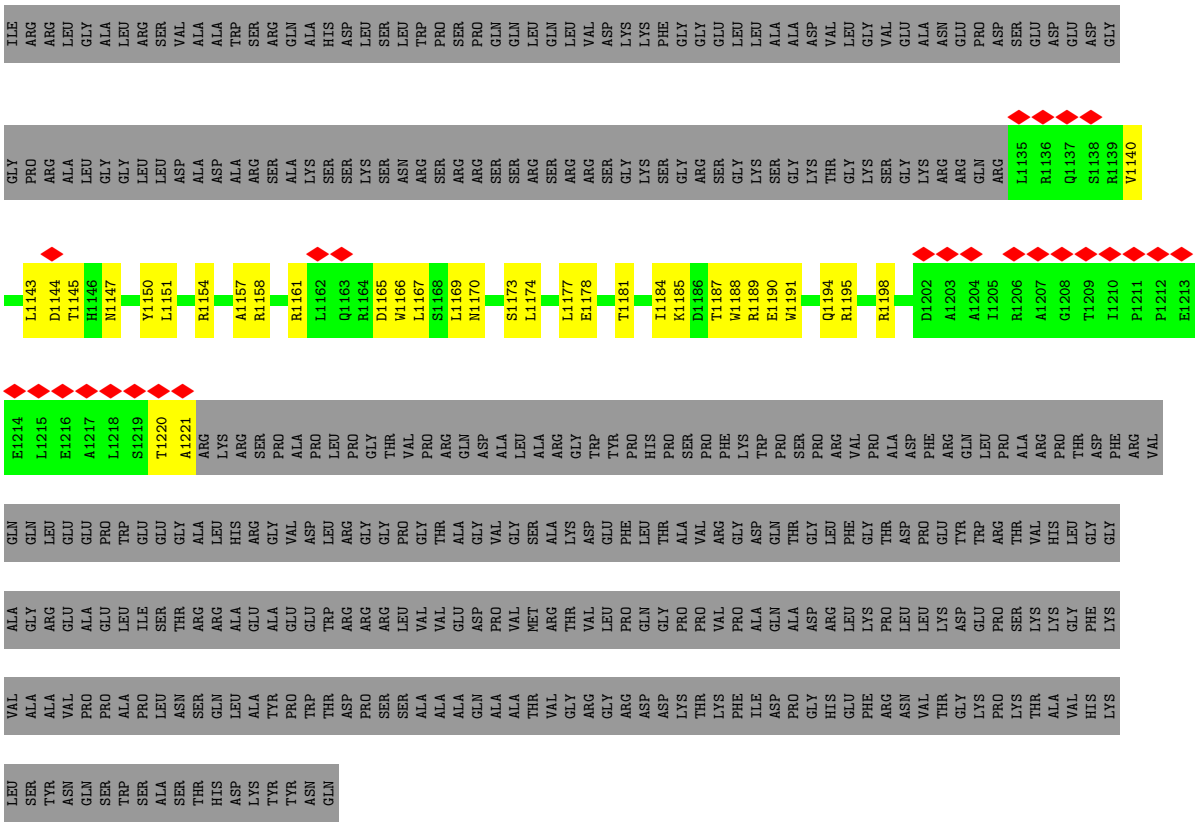
- Molecule 29: FAP92

Chain 3E: 94%

MET ALA PRO LYS ALA LYS GLY PRO ASP PRO ALA GLU ALA ALA ALA PRO VAL GLY PRO SER GLN GLU LEU HIS LEU VAL LEU LYS VAL ARG MET ARG LEU LYS PRO PRO ALA PRO GLU ARG PRO PRO GLN GLU PRO PRO ALA GLN PRO SER THR PRO PRO SER ALA GLU GLU PRO SER GLN

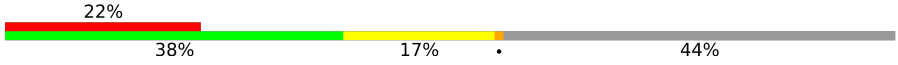
THR GLY ALA ASP THR ALA SER ALA ALA LYS ASP ALA LYS GLY ARG ALA LYS SER PRO PRO LYS LYS PRO VAL THR PRO GLY SER ALA ARG LYS ALA ALA ALA ALA GLU ALA ALA ALA ALA ALA ALA ALA ALA ALA ALA ALA LEU ALA LYS PRO VAL ASP PRO ALA

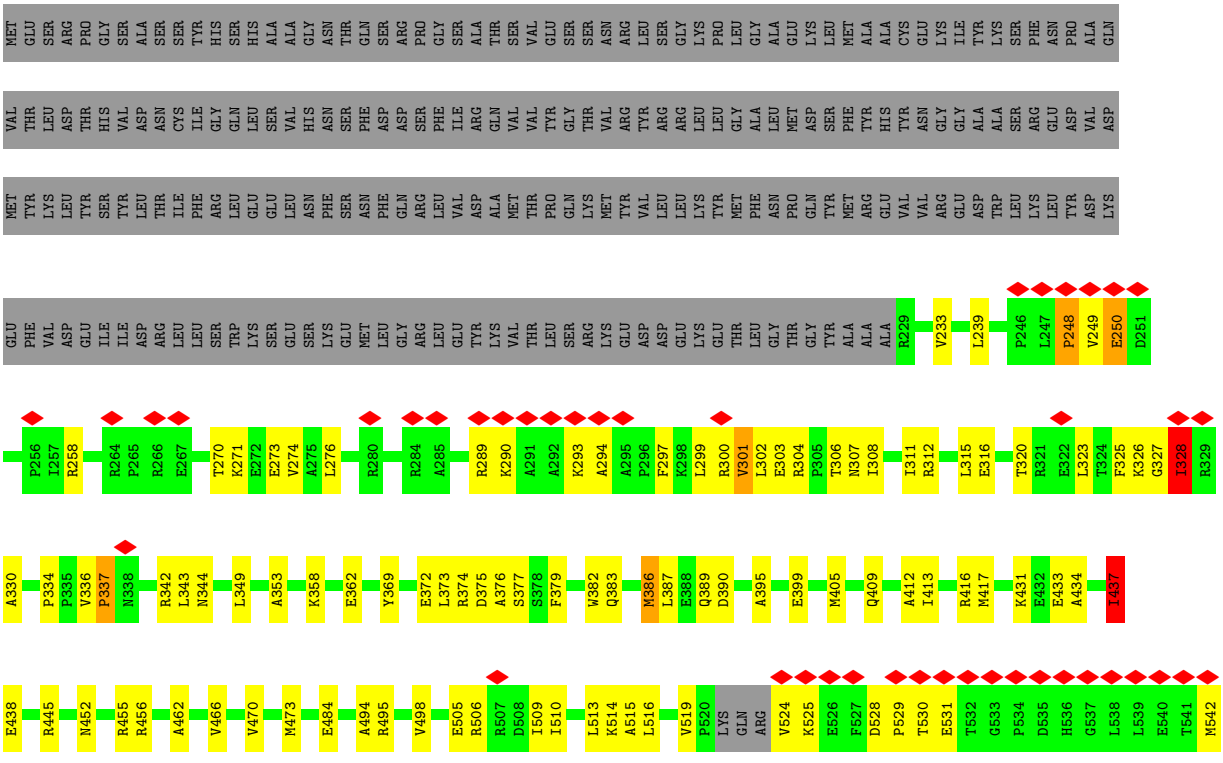
ALA LEU VAL LEU THR VAL LYS TYR THR PRO LEU GLY GLY ALA GLU ALA VAL VAL GLY PRO VAL LYS PRO LEU LYS PRO ALA VAL ALA ALA ALA ALA ALA ALA ALA ALA ALA ALA ALA

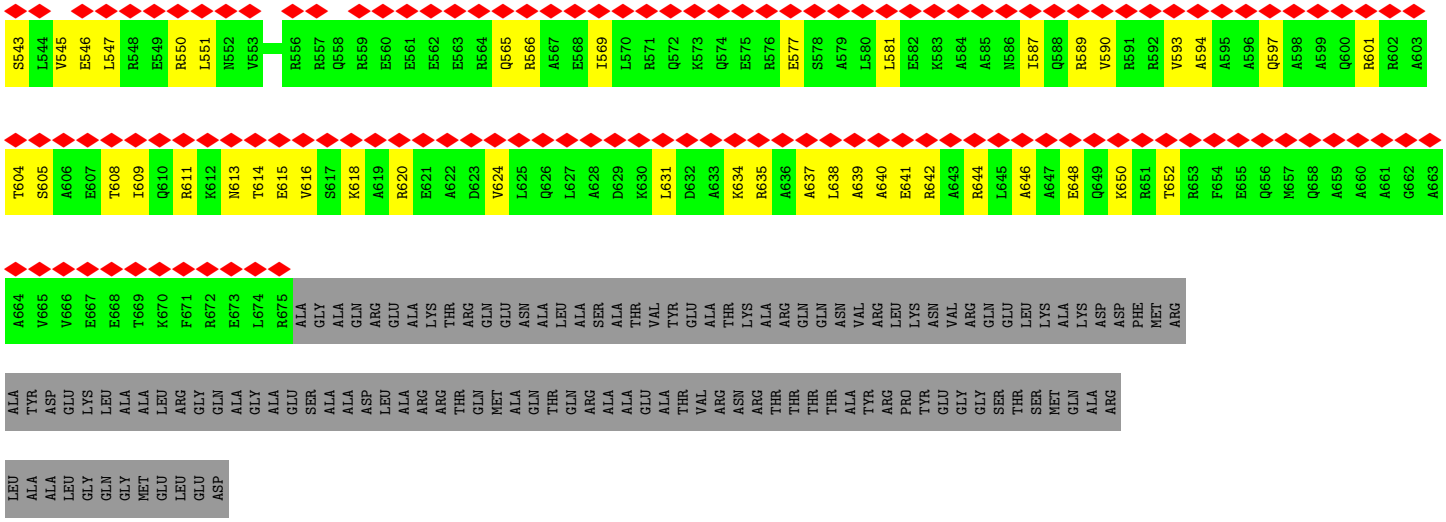


• Molecule 30: FAP99

Chain 3F:

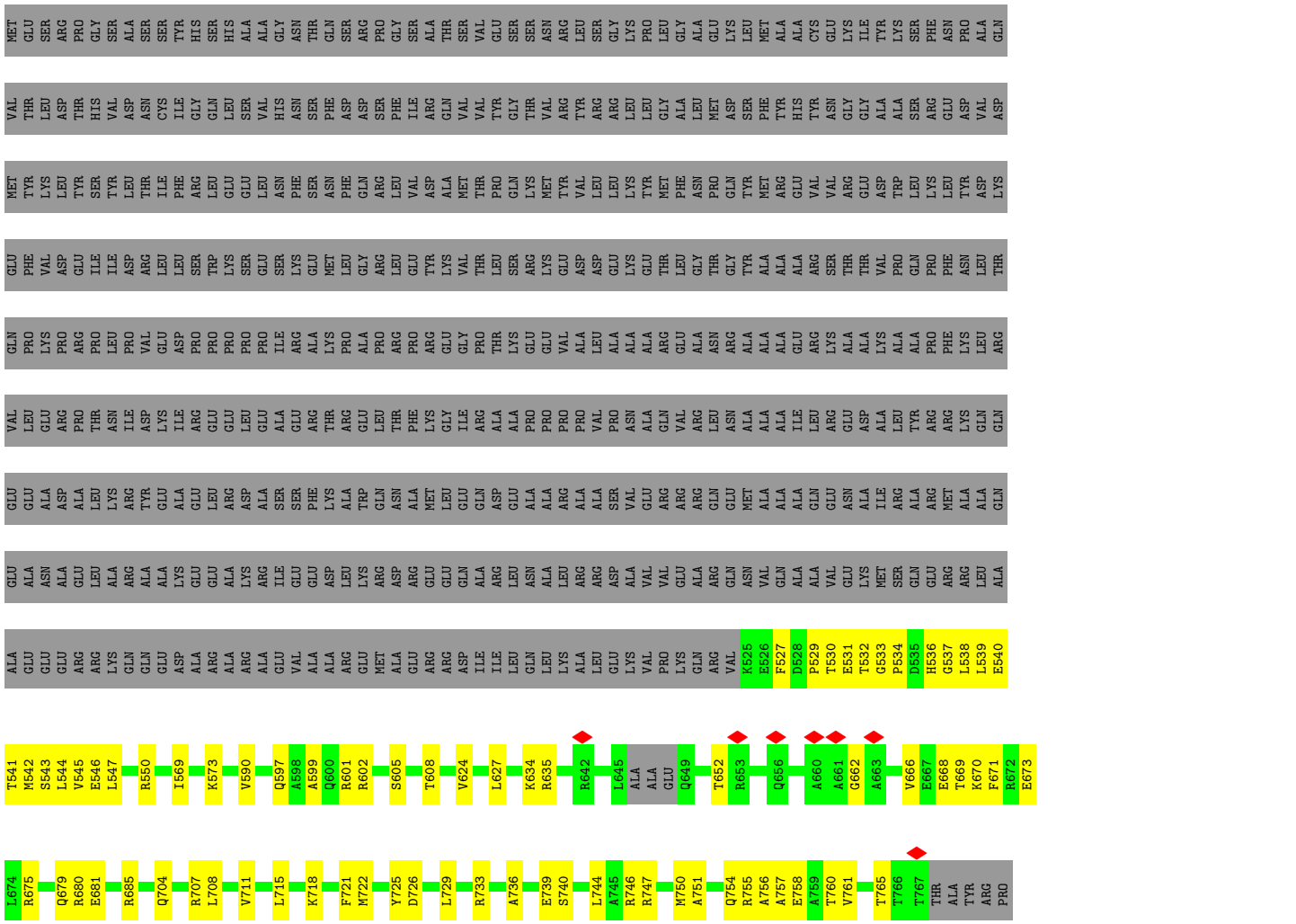






- Molecule 30: FAP99

Chain 3G:

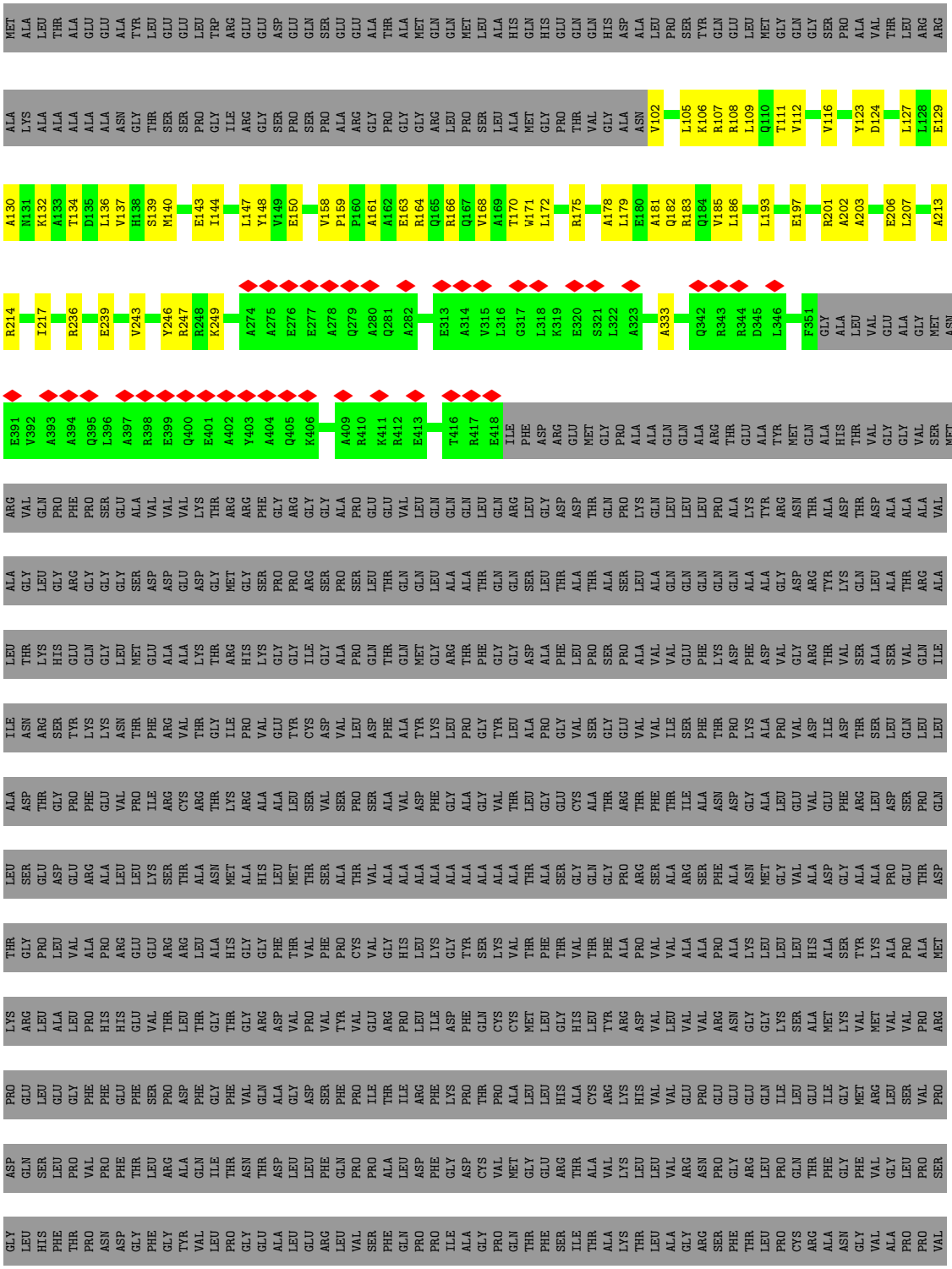


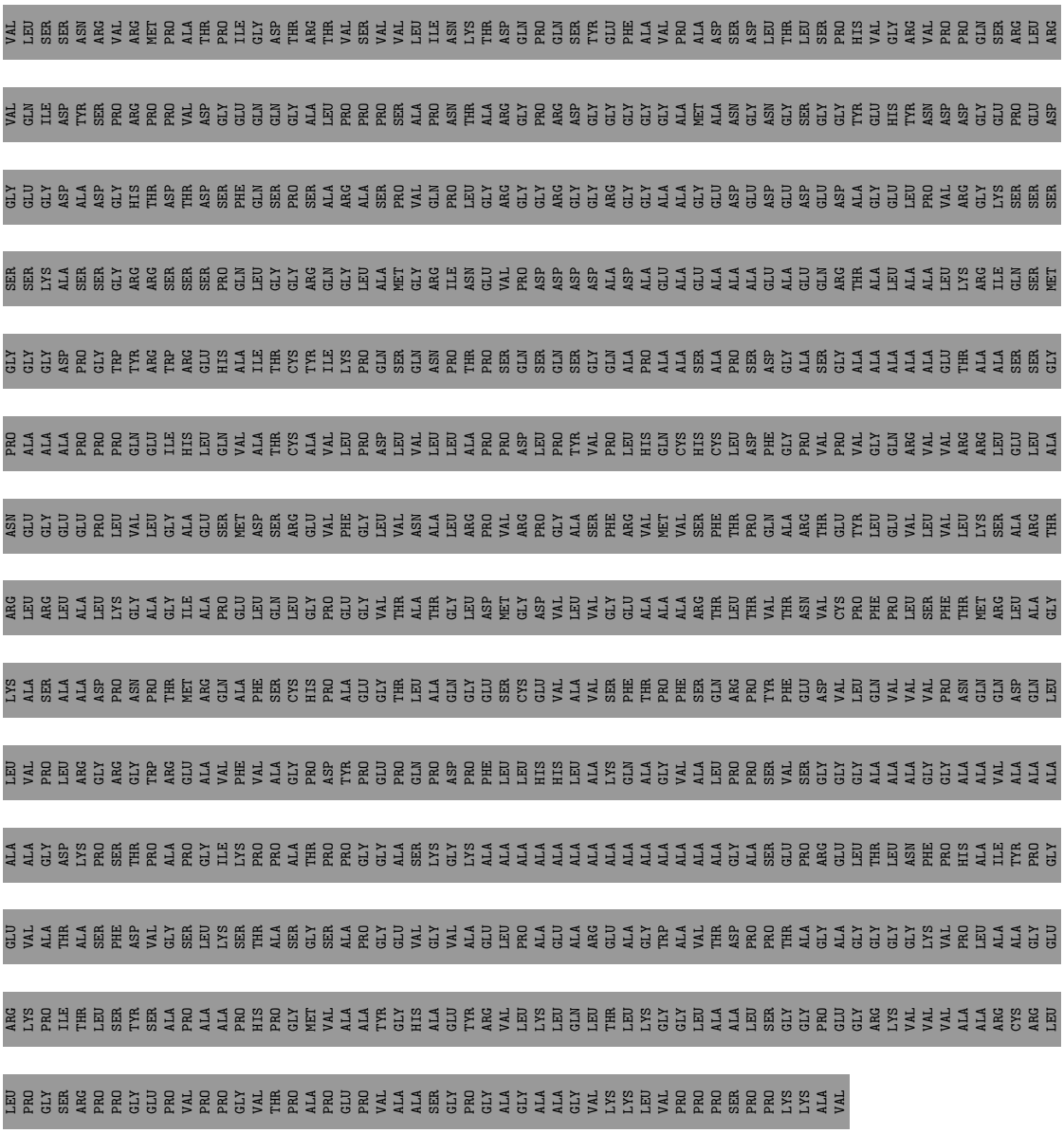


• Molecule 31: FAP74

Chain 3H:



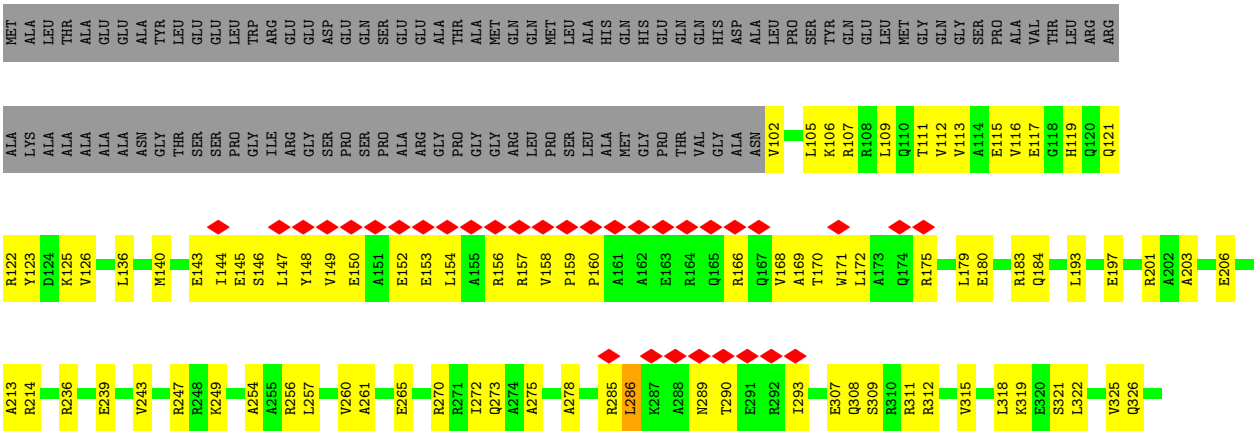


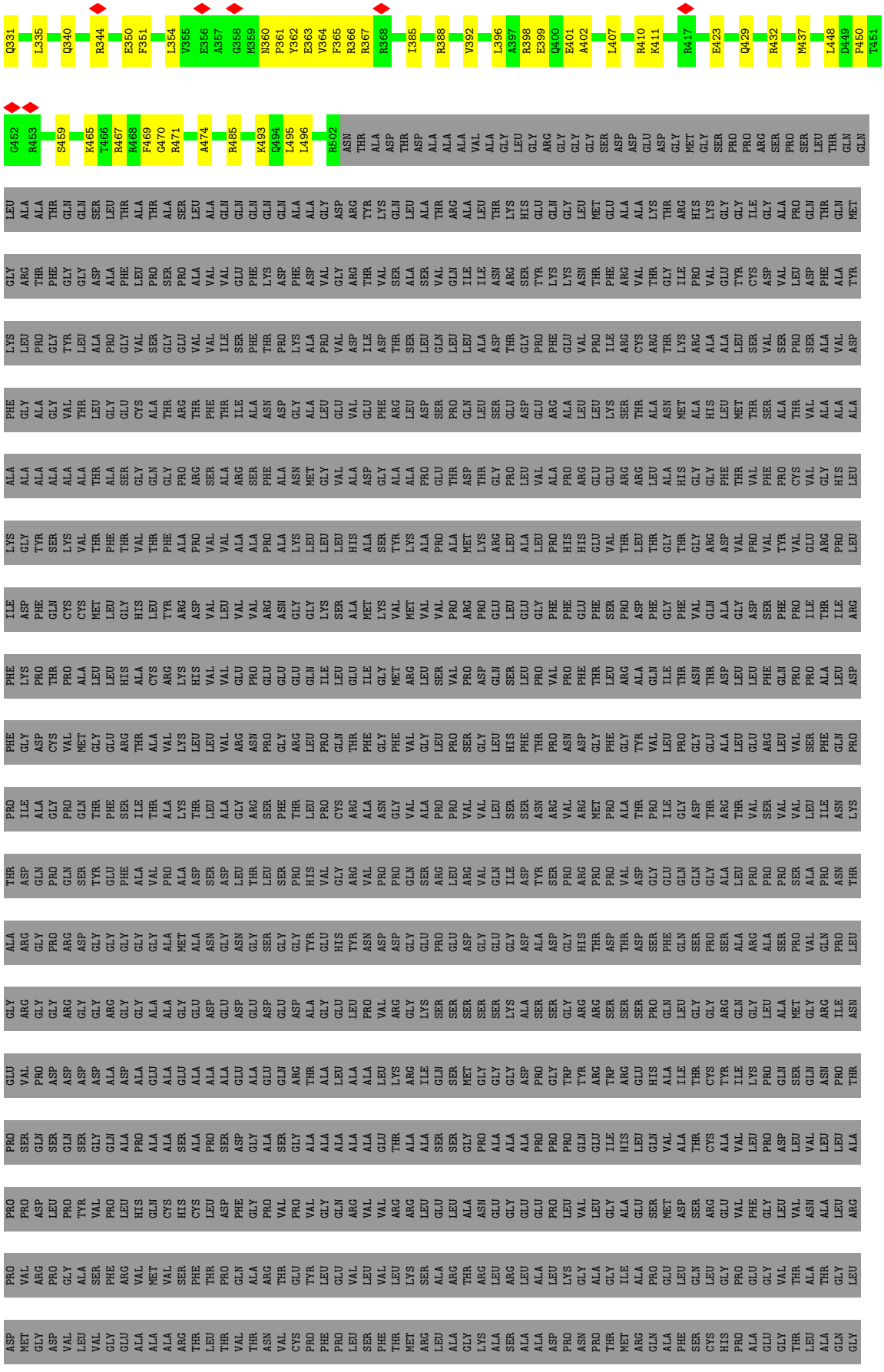


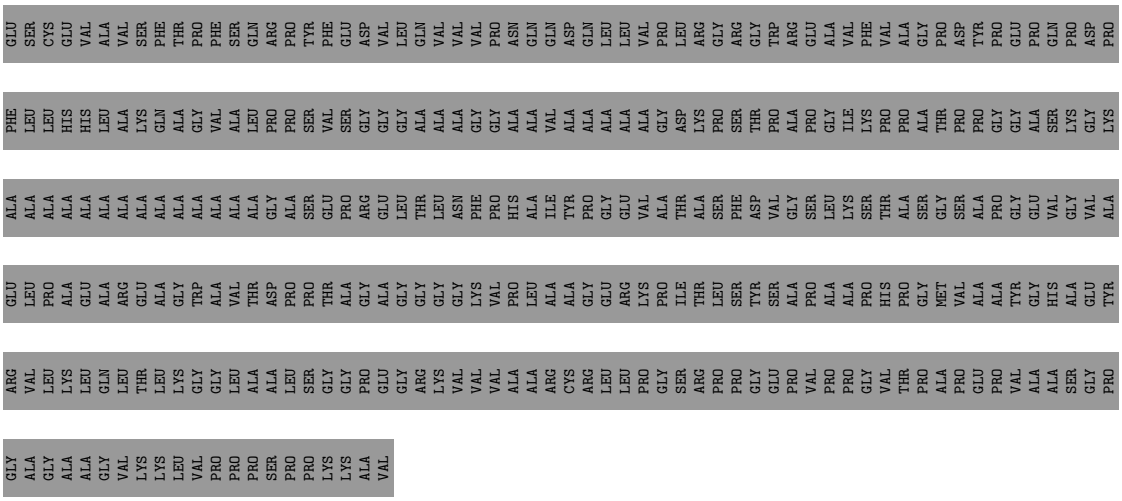
• Molecule 31: FAP74

Chain 3I:





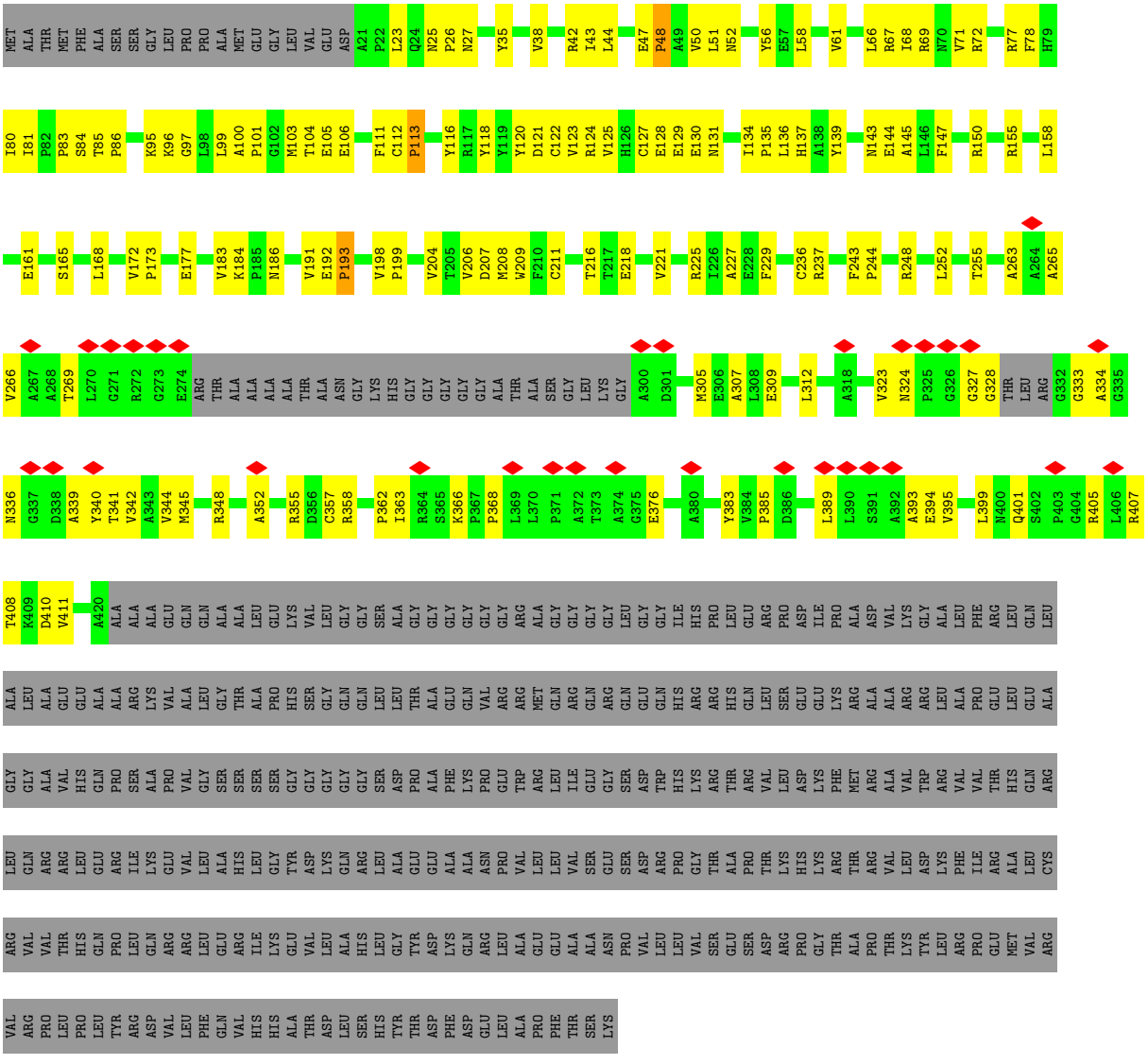

Q331 L335 Q340 R344 E350 F351 L354 V355 E356 A357 G358 M359 N360 P361 Y362 E363 V364 F365 R366 R367 R368 I385 R388 V392 L396 A397 R398 E399 Q400 E401 A402 L407 R410 K411 R417 E423 Q429 R432 M437 L448 D449 P450 T451
G452 R453 S459 K465 T466 R467 R468 F469 G470 R471 A474 R485 K493 Q494 L495 L496 R502 N503 T504 A505 D506 T507 D508 L509 D510 G511 S512 D513 P514 G515 M516 G517 S518 P519 R520 S521 P522 P523 G524 Q525 R526 S527 A528 P529 G530 Q531 L532 T533 N534 Q535 M536



• Molecule 32: FAP360

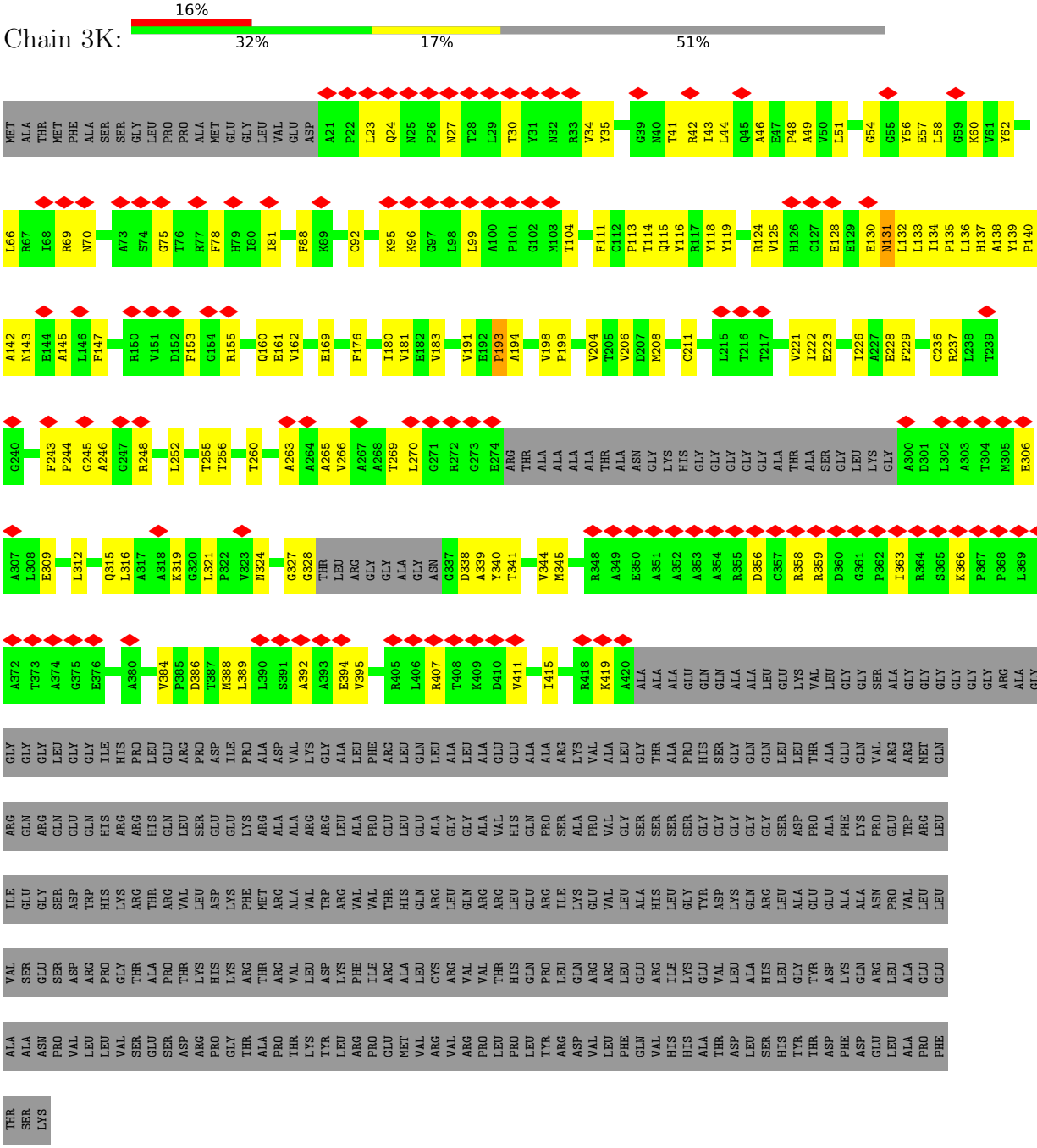
Chain 3J:





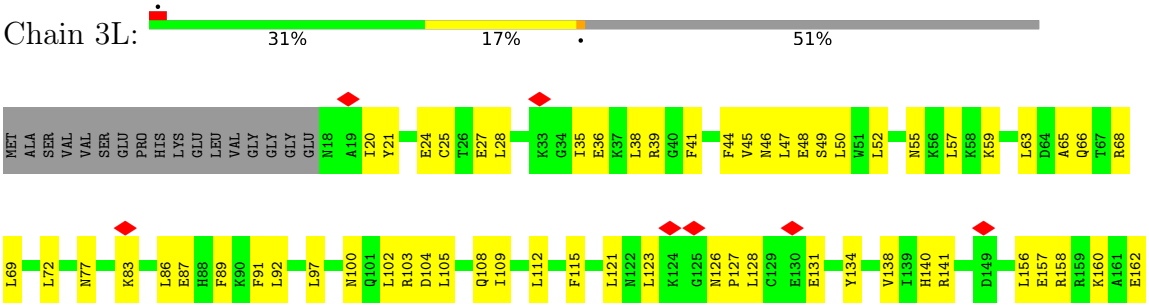
• Molecule 32: FAP360

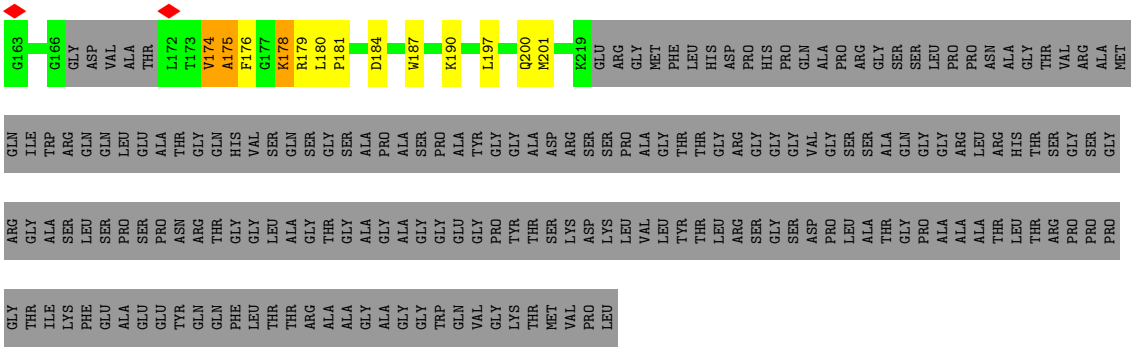
Chain 3K:



• Molecule 33: FAP279

Chain 3L:

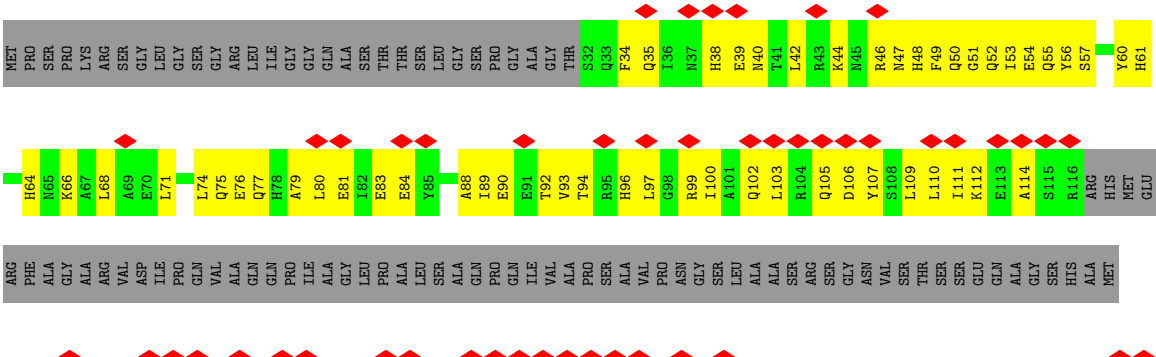




• Molecule 34: FAP7

Chain 3M:



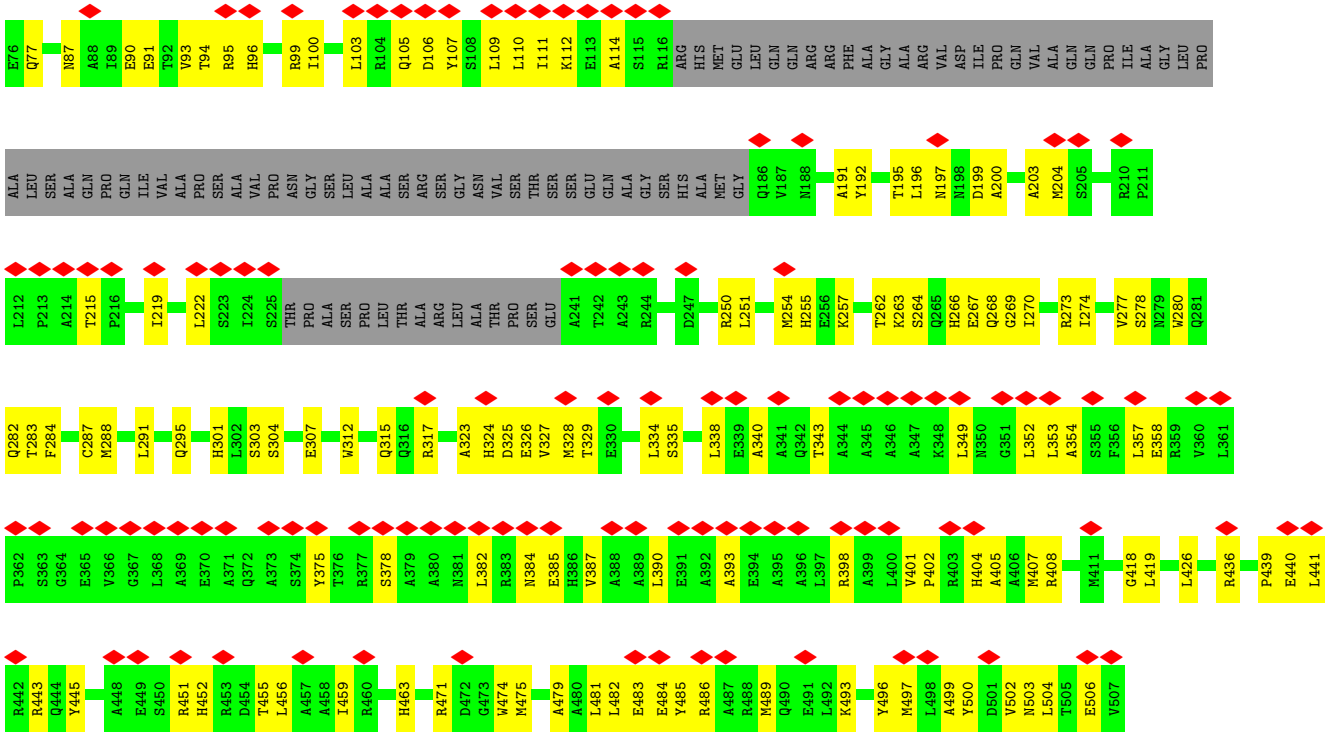


• Molecule 34: FAP7

Chain 3N:

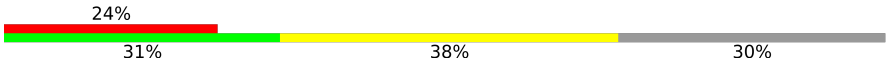


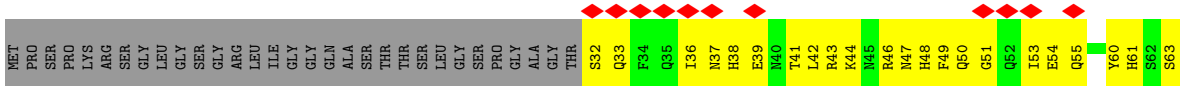




- Molecule 34: FAP7

Chain 3O:

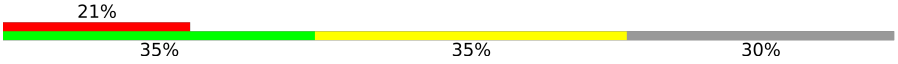


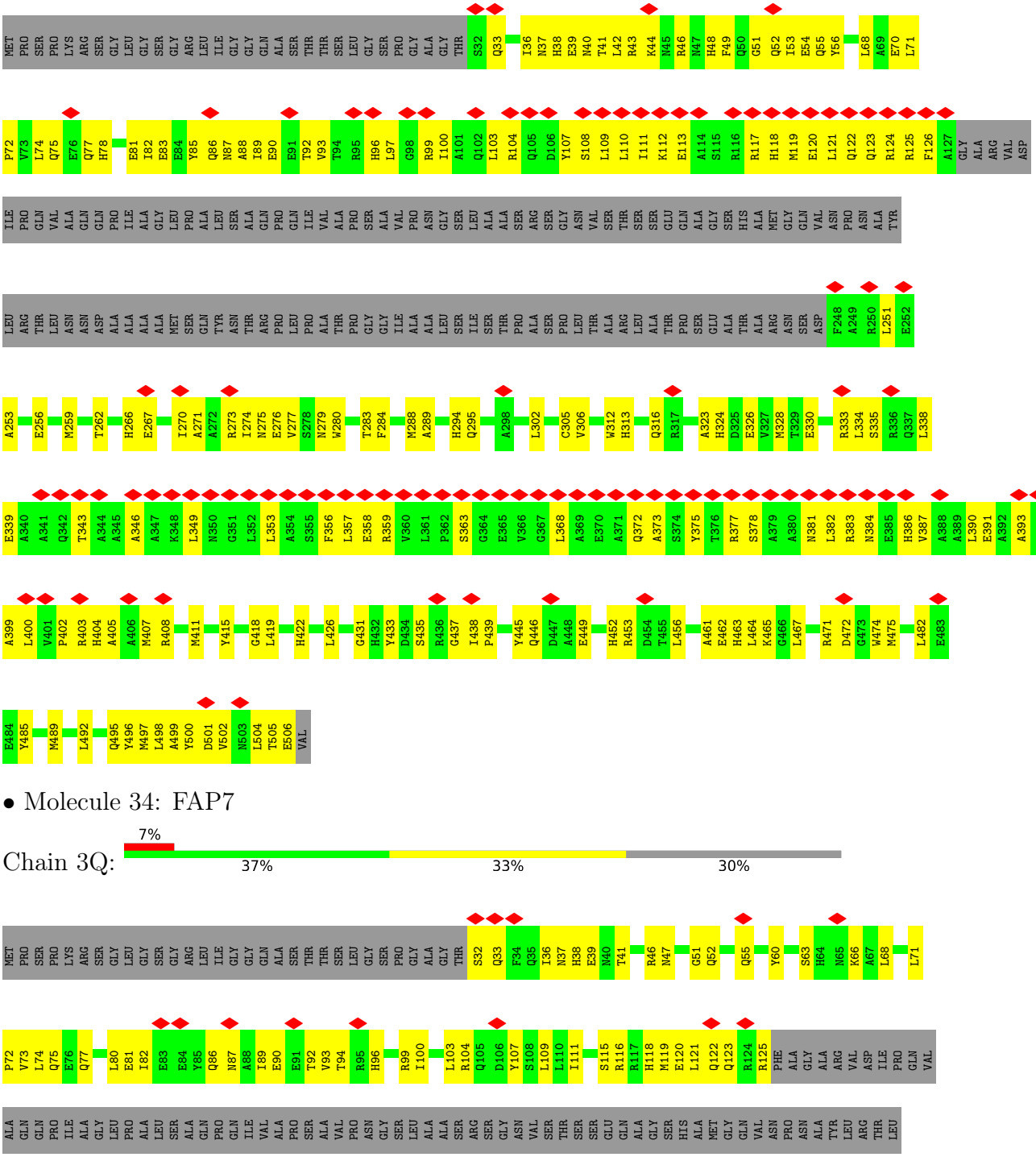




• Molecule 34: FAP7

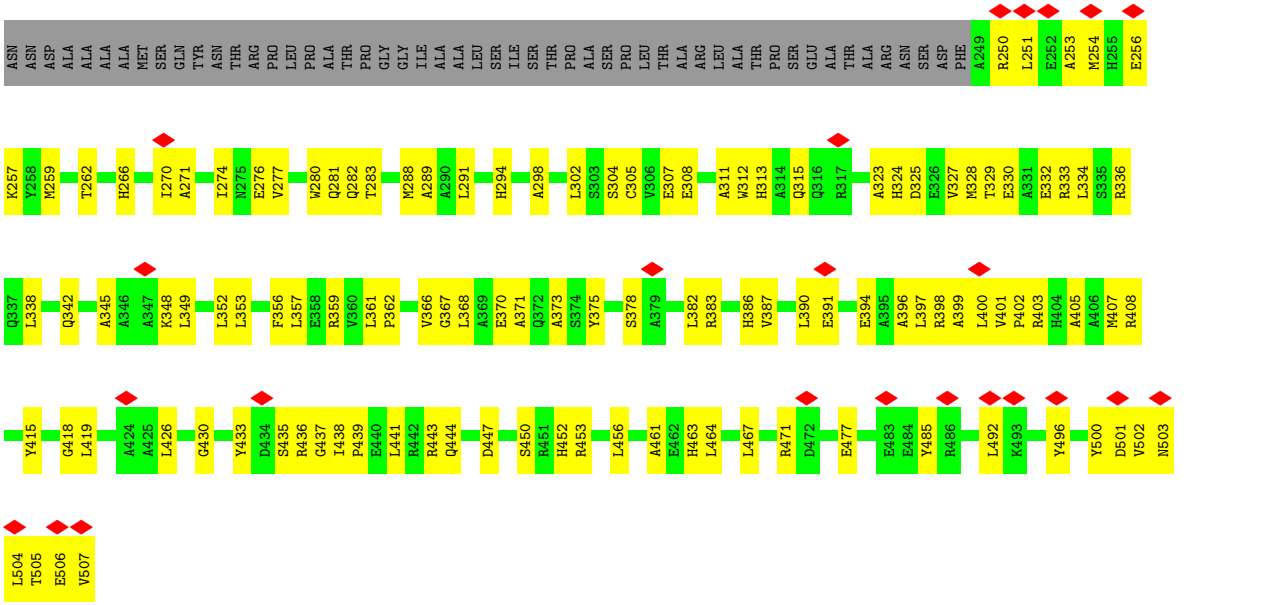
Chain 3P:





• Molecule 34: FAP7

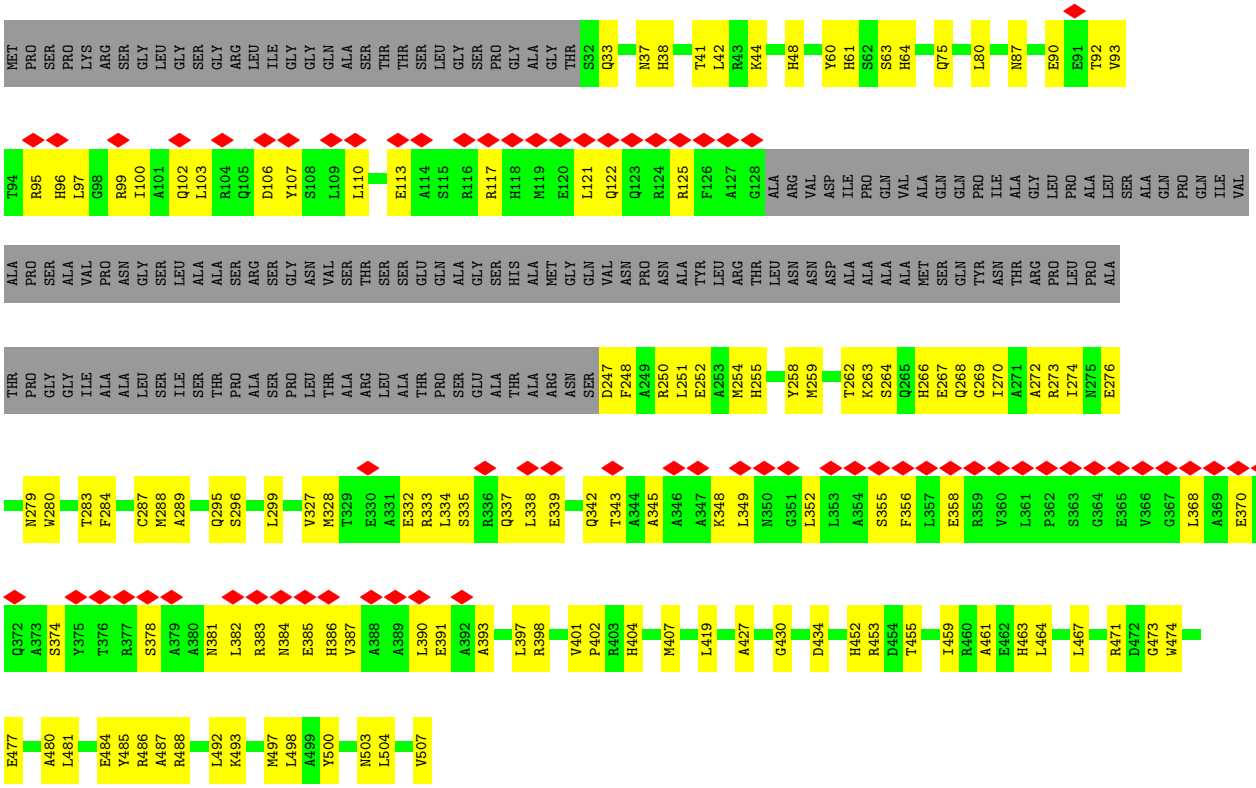
Chain 3Q:



• Molecule 34: FAP7

Chain 3R:

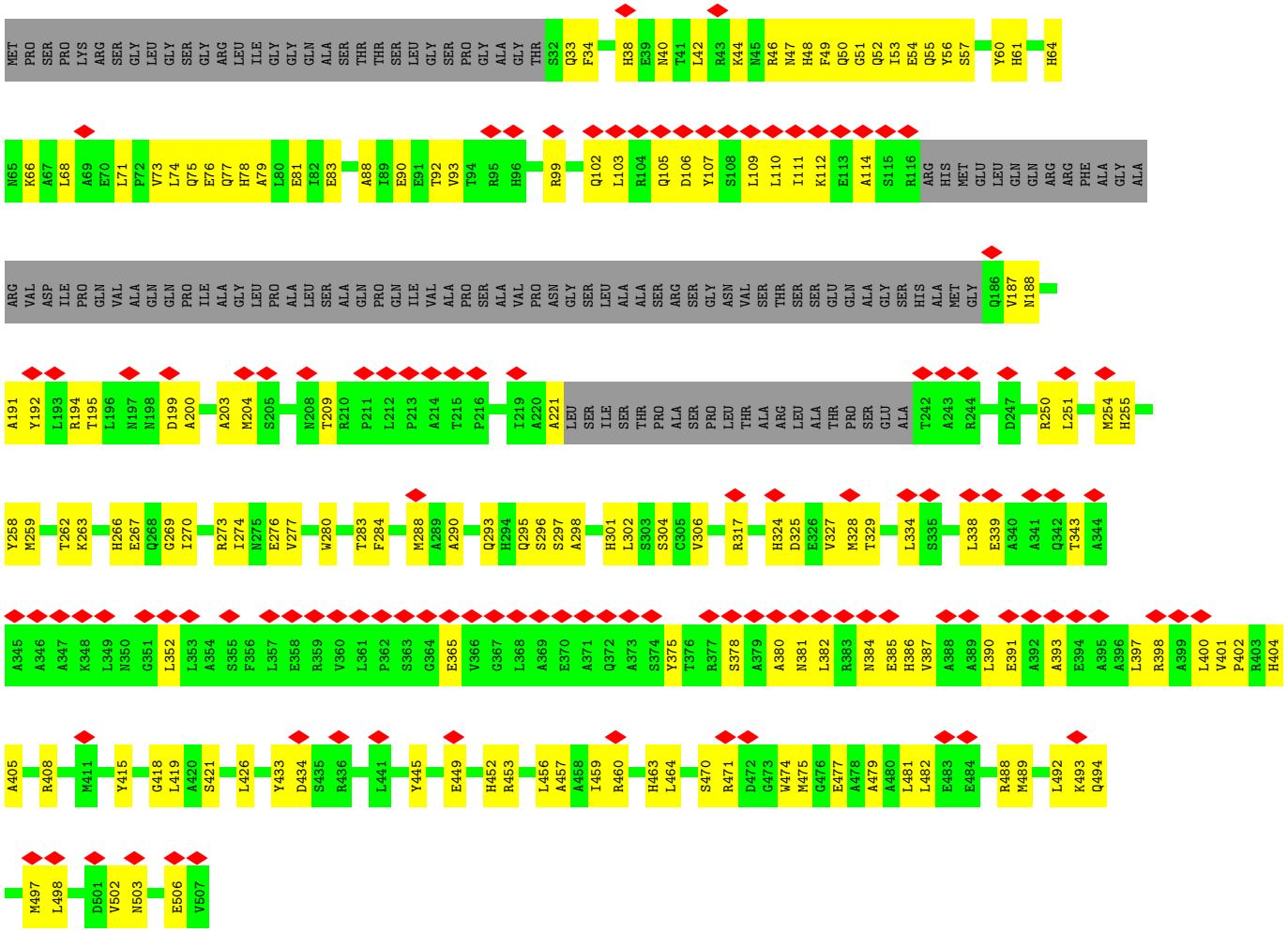




• Molecule 34: FAP7

Chain 3S:

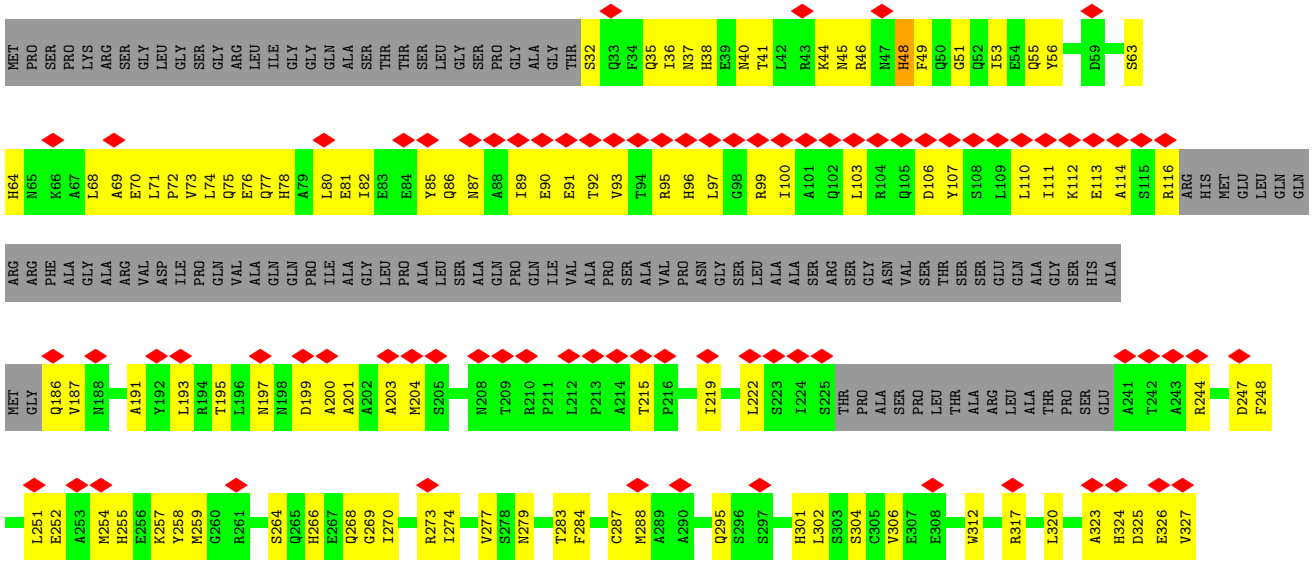


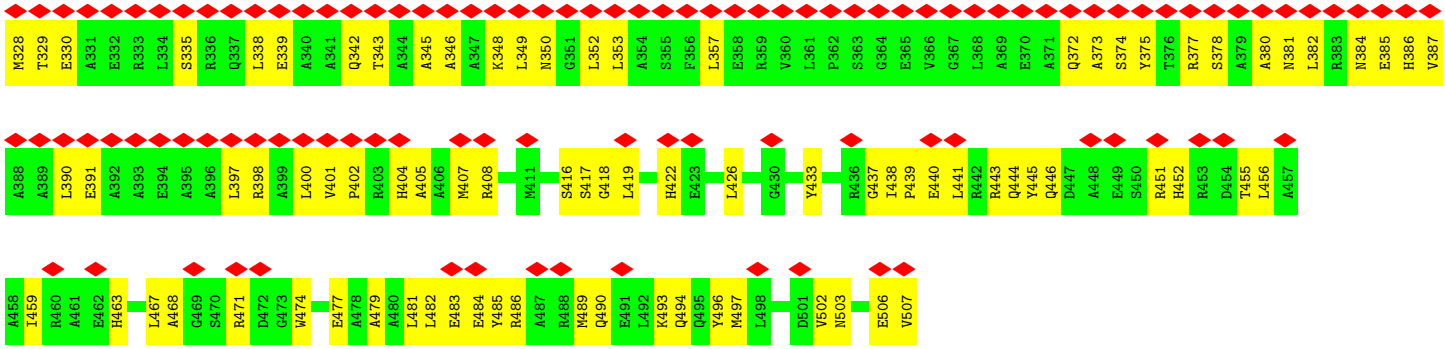


• Molecule 34: FAP7

Chain 3T:

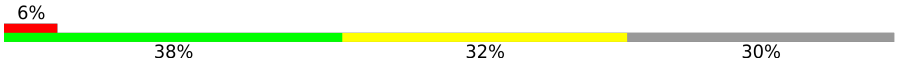


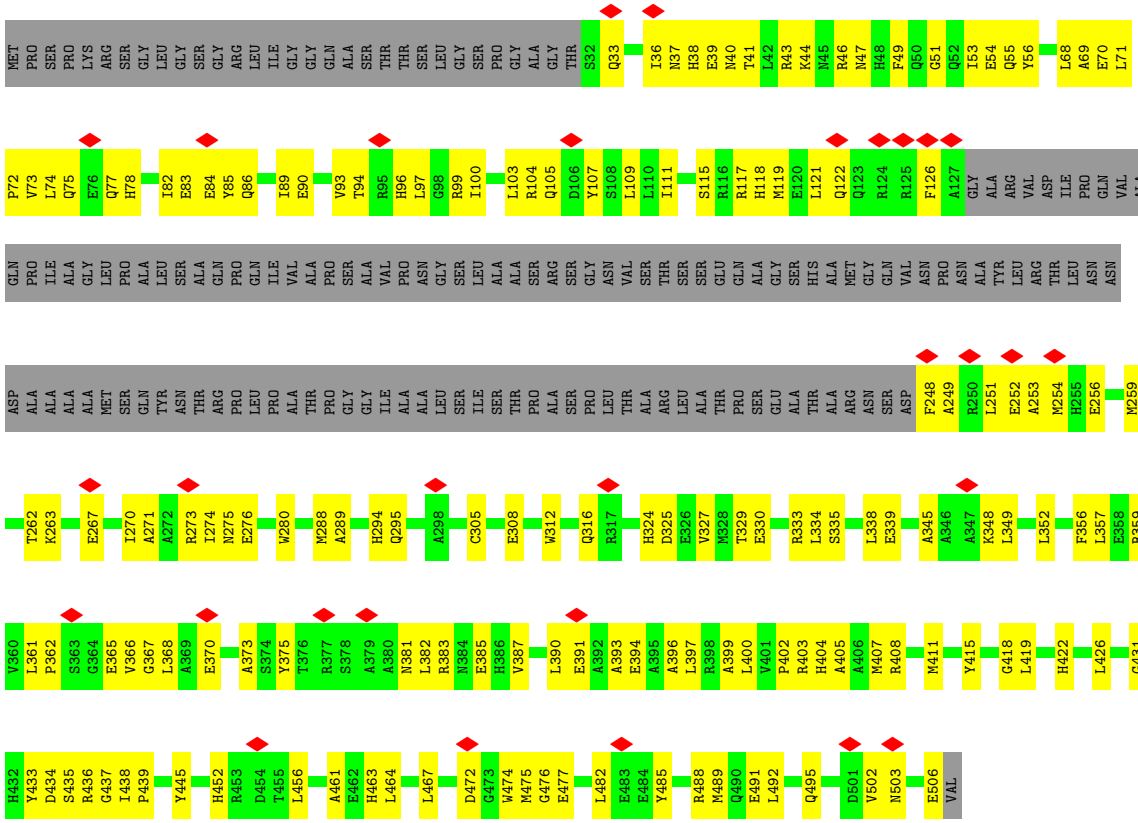




• Molecule 34: FAP7

Chain 3U:

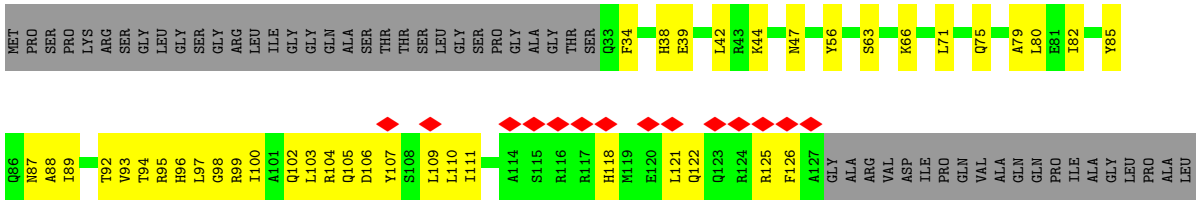


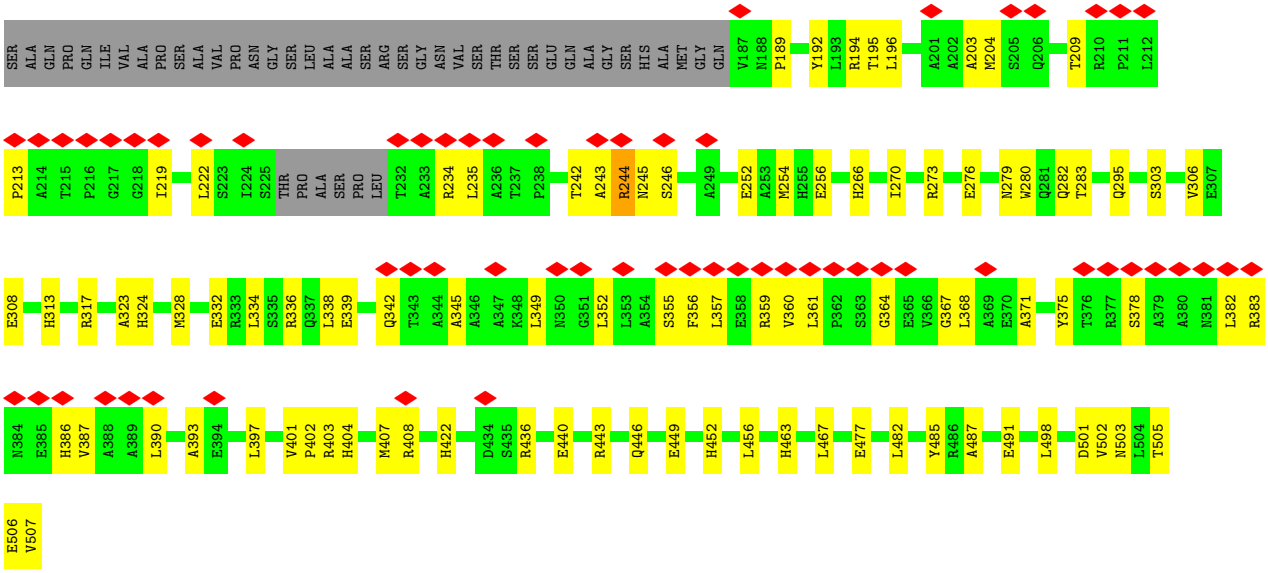


• Molecule 34: FAP7

Chain 3V:



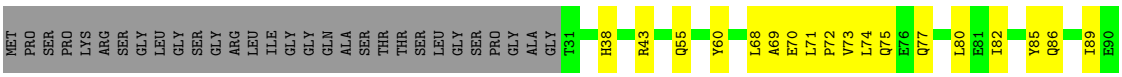




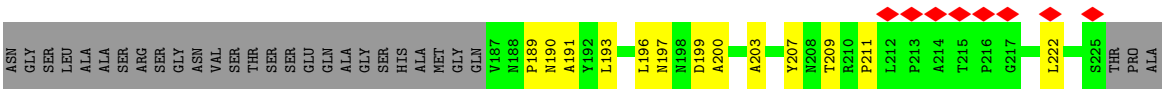
• Molecule 34: FAP7

Chain 3W:

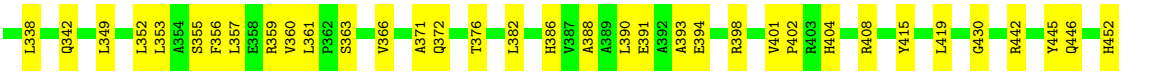


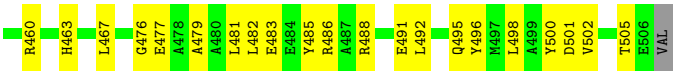






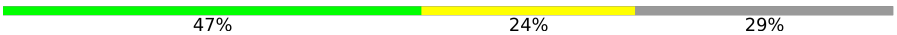


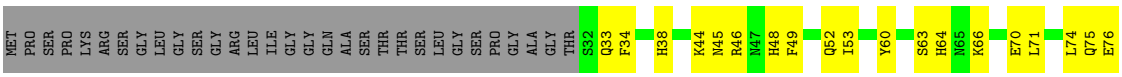




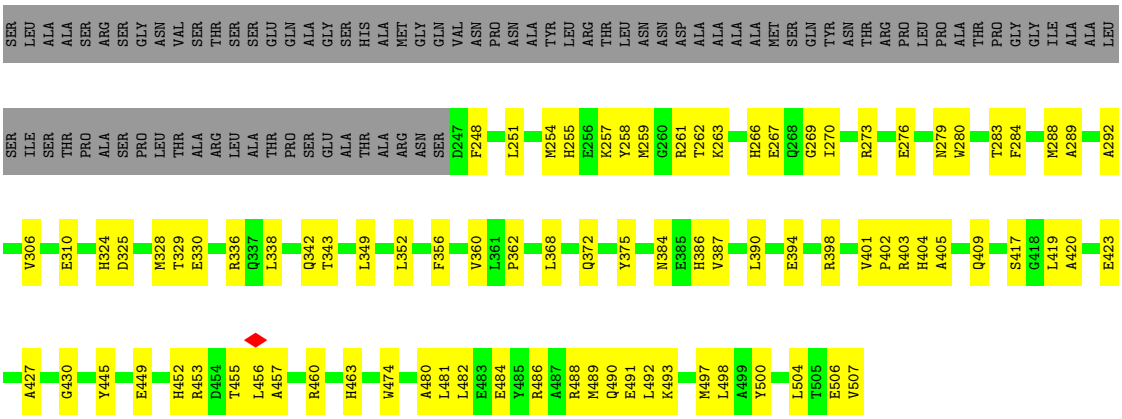
• Molecule 34: FAP7

Chain 3X:





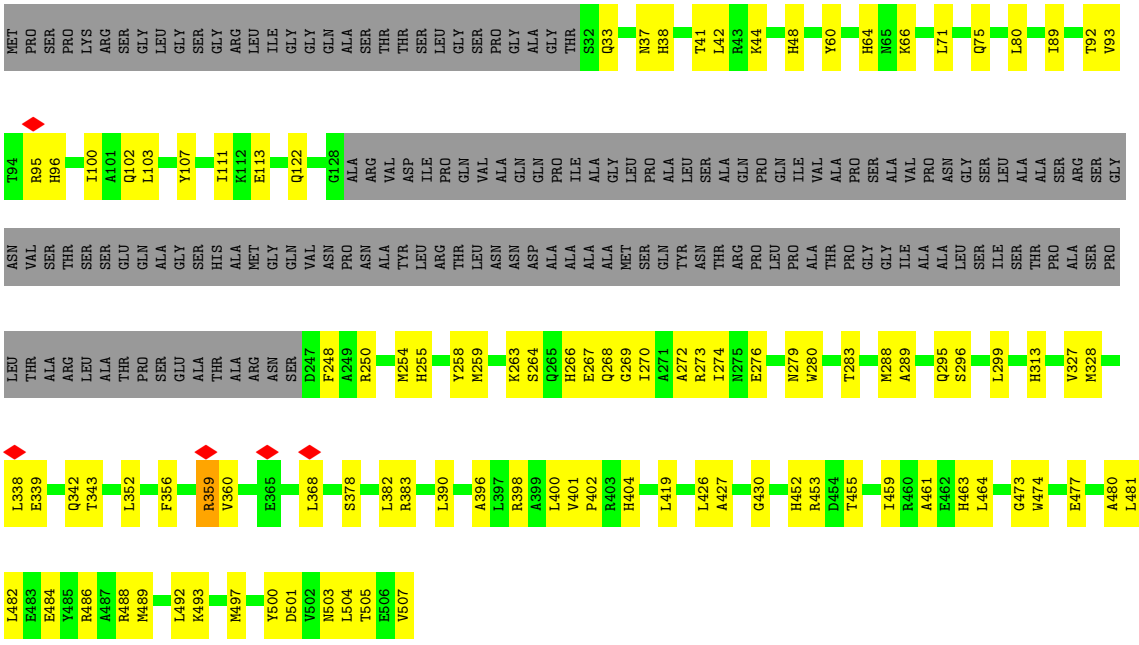




• Molecule 34: FAP7

Chain 3Y:

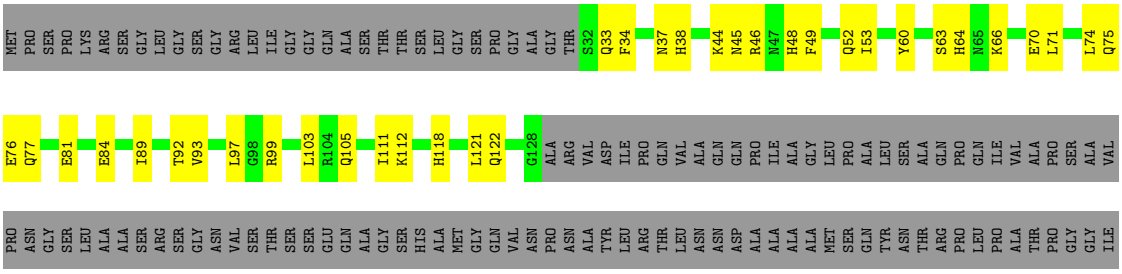


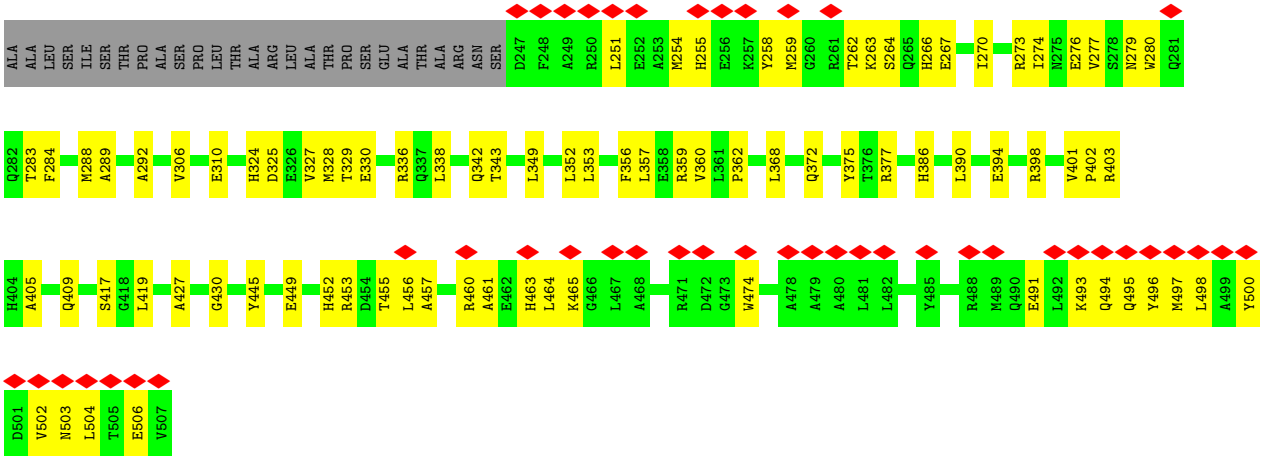


• Molecule 34: FAP7

Chain 3Z:



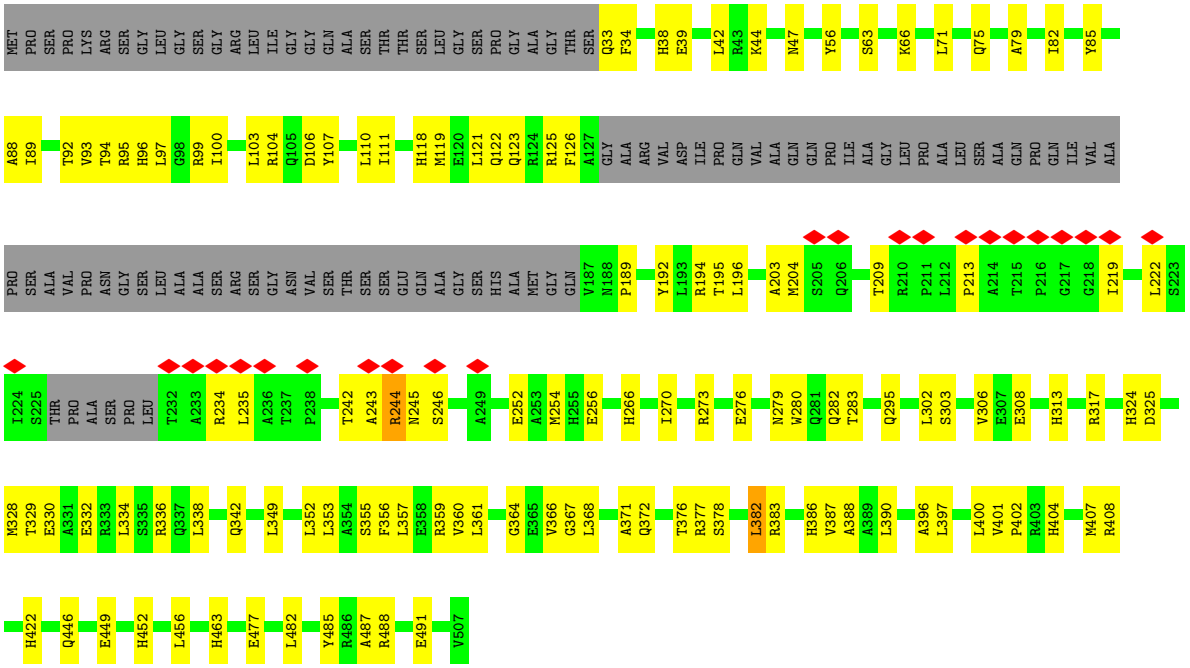




• Molecule 34: FAP7

Chain 4A:

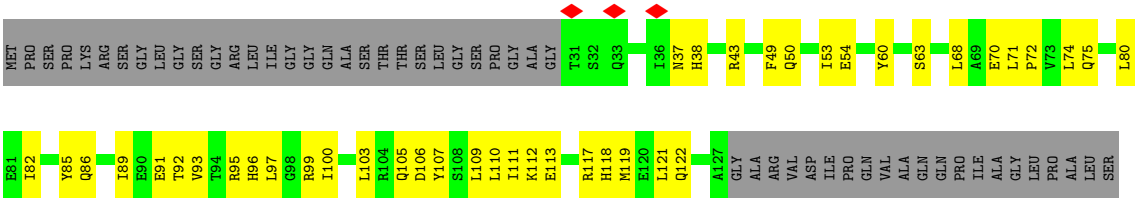


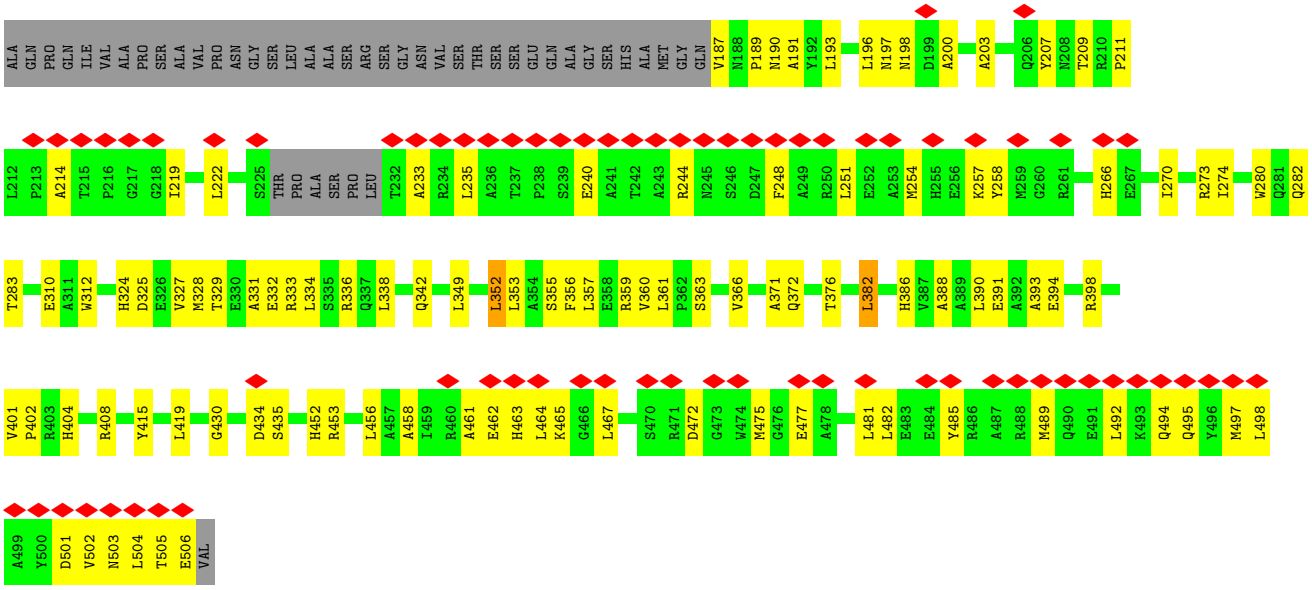


• Molecule 34: FAP7

Chain 4B:



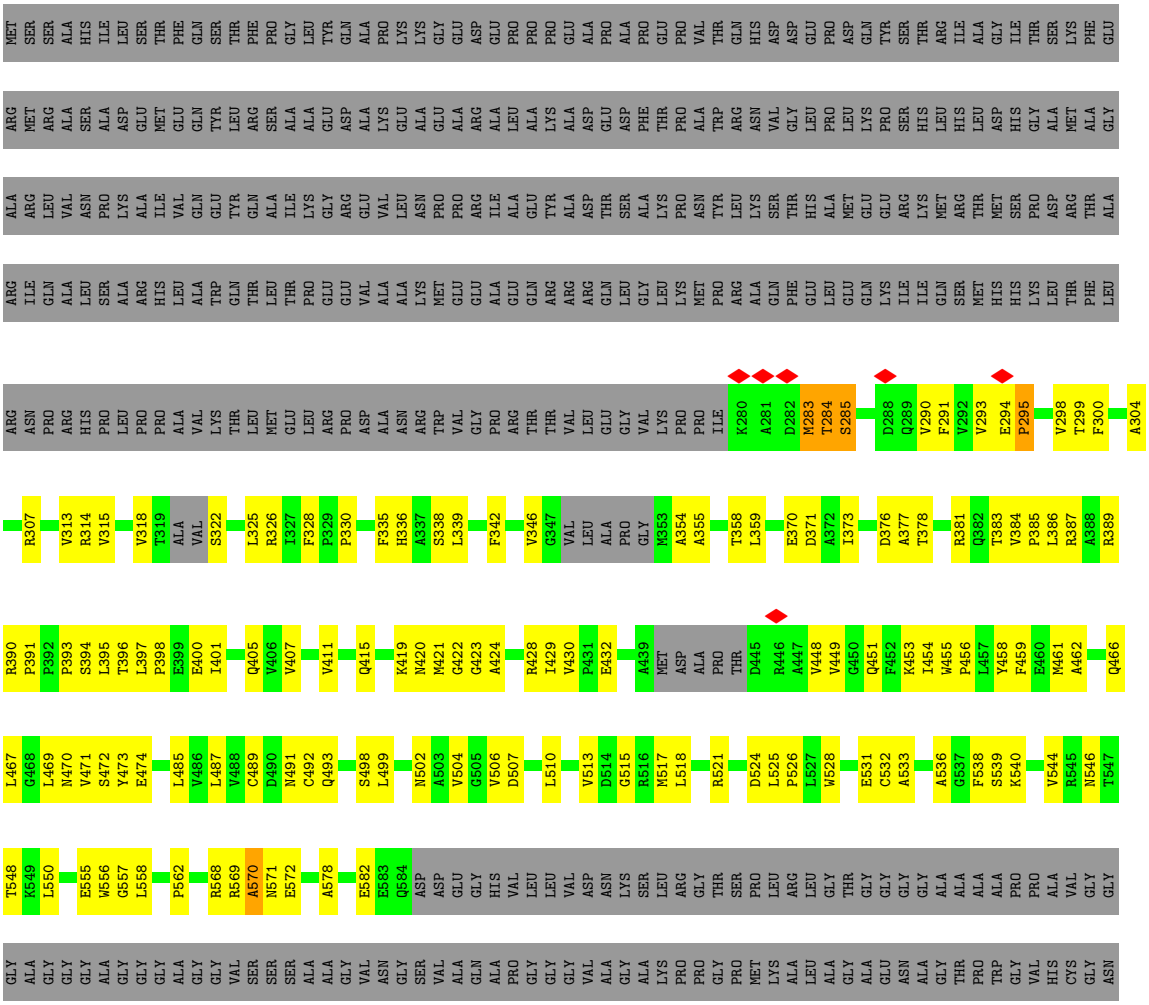


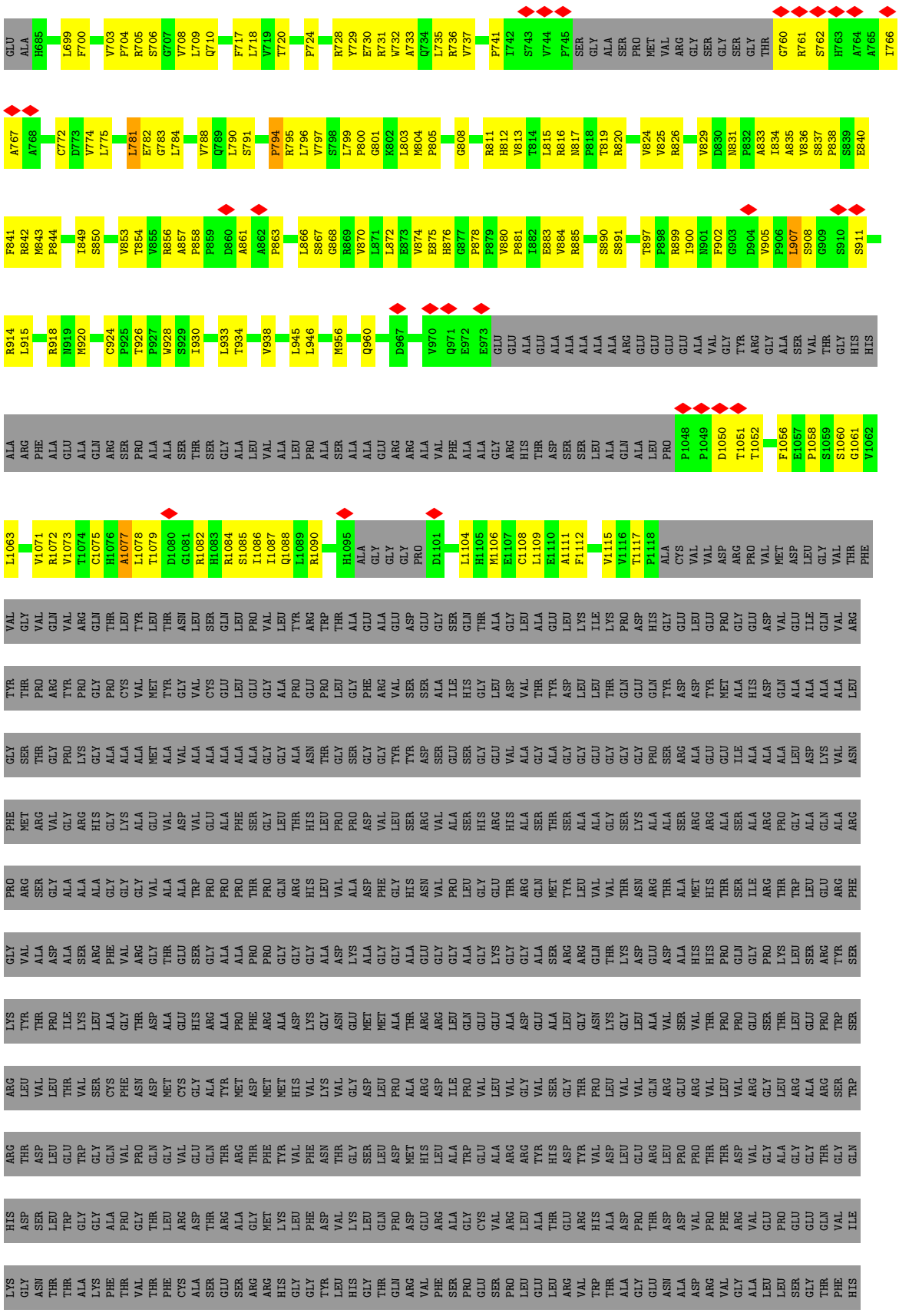


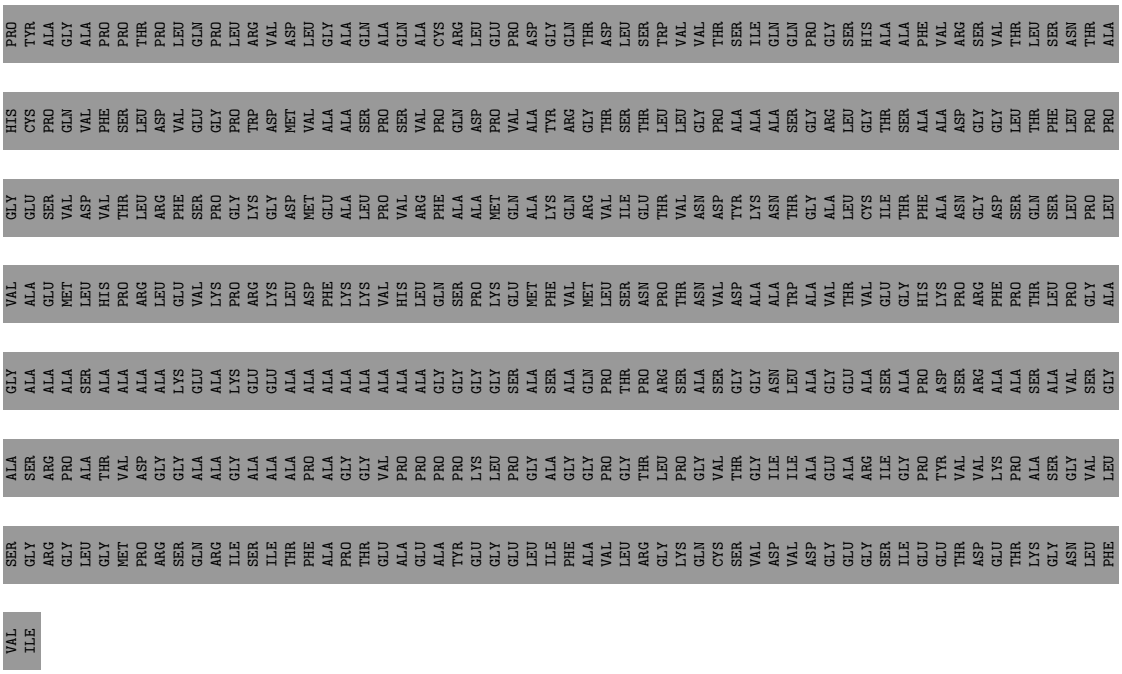
• Molecule 35: FAP81

Chain 4C:





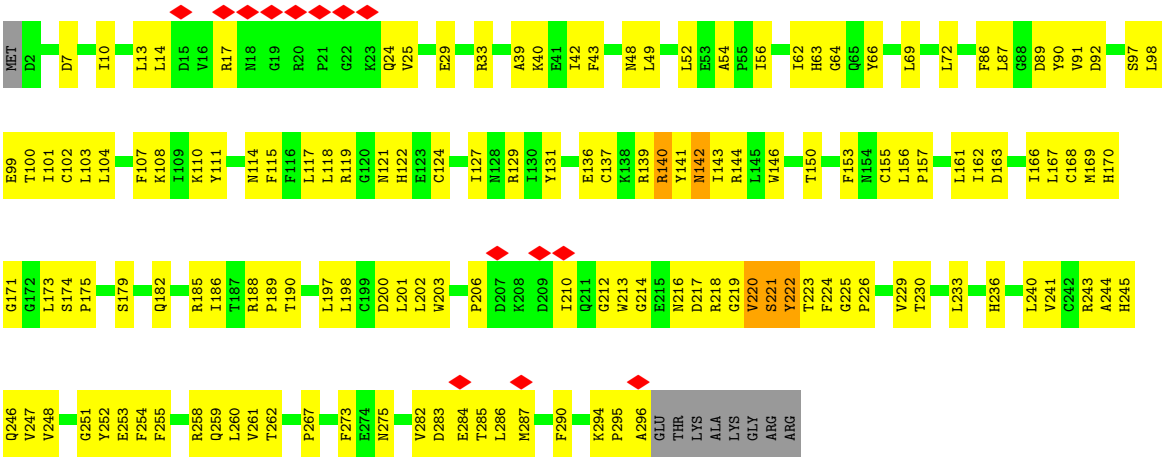

GLU ALA H685 L699 F700 V703 P704 R705 S706 G707 V708 L709 Q710 F717 L718 V719 T720 P724 R728 Y729 E730 R731 W732 A733 Q734 L735 R736 V737 P741 I742 S743 V744 P745 SER GLY ALA SER PRO MET VAL ARG GLY SER GLY SER GLY THR G760 R761 S762 H763 A764 A765 I766
A767 A768 C772 D773 V774 L775 L781 E782 G783 L784 V788 Q789 L790 S791 P794 R795 L796 V797 S798 L799 P800 G801 K802 L803 M804 P805 G808 R811 H812 V813 T814 L815 R816 N817 P818 T819 R820 V824 V825 R826 V829 D830 N831 P832 A833 I834 A835 V836 S837 P838 S839 E840
F841 R842 M843 P844 I849 S850 V853 T854 V855 R856 A857 P858 P859 D860 A861 A862 P863 L866 S867 G868 R869 V870 L871 L872 E873 V874 E875 H876 G877 P878 P879 V880 P881 I882 E883 V884 R885 S890 S891 T897 P898 R899 I900 N901 F902 G903 D904 V905 P906 L907 S908 G909 S910 S911
R914 L915 R918 N919 M920 C924 P925 T926 P927 W928 S929 I930 L933 T934 V938 L945 L946 M956 Q960 D967 V970 Q971 E972 E973 GLU GLU ALA GLU ALA ALA ALA ALA ALA ARG GLU GLU GLU GLU ALA VAL GLY TYR ARG GLY ALA SER VAL THR GLY HIS HIS
ALA ARG PHE ALA GLU ALA GLN ARG SER PRO ALA ALA SER THR SER GLY ALA LEU VAL ALA LEU PRO ALA SER ALA ALA GLU ARG ARG ALA VAL PHE ALA ALA GLY ARG HIS THR ASP SER SER LEU ALA GLN ALA LEU PRO P1048 P1049 D1050 T1051 T1052 F1056 E1057 P1058 S1059 S1060 G1061 V1062
L1063 V1071 R1072 V1073 T1074 C1075 H1076 A1077 L1078 T1079 D1080 G1081 R1082 H1083 R1084 S1085 I1086 I1087 Q1088 L1089 R1090 H1095 ALA GLY GLY GLY PRO D1101 L1104 H1105 M1106 E1107 C1108 L1109 E1110 A1111 F1112 V1115 V1116 T1117 P1118 ALA CYS VAL VAL ASP ARG PRO VAL MET ASP LEU GLY VAL THR PHE
VAL GLY VAL GLN VAL ARG GLN THR LEU TYR LEU THR ASN LEU SER GLN THR ALA GLY LEU ALA GLU LEU LYS ILE LYS PRO ASP HIS GLY GLU LEU GLU PRO GLY GLU ASP VAL GLU ILE GLN VAL ARG
TYR THR PRO ARG TYR PRO GLY PRO CYS VAL MET TYR GLY VAL CYS GLU LEU LEU GLU GLY ALA PRO GLU PRO LEU GLY PHE ARG VAL SER SER ALA ILE HIS GLY LEU ASP VAL THR TYR ASP LEU LEU THR GLN GLU GLN TYR ASP ASP TYR MET ALA HIS ASP GLN ALA ALA ALA LEU
GLY SER THR GLY PRO LYS GLY ALA ALA MET MET ALA VAL ALA ALA ALA ALA GLY GLY ALA ASN THR GLY SER GLY GLY TYR TYR ASP SER GLU SER GLY GLU VAL ALA GLY GLU GLY GLY GLY PRO SER ARG ALA GLU GLU ILE ALA ALA ALA LEU ASP LYS VAL ASN
PHE MET ARG VAL GLY ARG HIS GLY LYS ALA GLU VAL ASP VAL GLU ALA PHE SER GLY LEU THR HIS LEU PRO PRO ASP VAL LEU SER ARG VAL ALA SER HIS ARG HIS ALA SER THR SER ALA ALA GLY SER LYS ALA ALA SER ARG ALA ALA SER ARG ALA ALA ARG PRO GLY ALA GLN ALA ARG
PRO ARG SER GLY ALA ALA ALA GLY GLY GLY VAL ALA TRP PRO PRO PRO THR PRO GLN ARG HIS LEU VAL ALA ASP PHE GLY HIS ASN VAL PRO LEU GLY GLU THR ARG GLN MET TYR LEU VAL VAL THR ASN ARG THR ALA MET HIS THR SER ILE ARG THR TRP LEU SER GLU ARG PHE
GLY VAL ALA ASP ALA SER ARG GLY GLY THR GLU SER GLY ALA ALA PRO PRO GLY GLY ALA GLU GLY GLY ALA GLY LYS GLY GLY ALA SER ARG GLN GLN THR LYS ASP GLU ASP ALA HIS HIS PRO GLN GLY PRO LYS LEU SER ARG TYR SER
LYS TYR THR PRO ILE LYS LEU ALA GLY THR ASP ALA GLU HIS ARG ALA PRO PHE ARG ALA ASP LYS GLY ASN GLU MET MET ALA THR ARG ARG LEU GLN GLU GLU GLU ALA ASP GLU ALA LEU GLY ASN LYS GLY LEU ALA VAL SER ALA VAL THR PRO GLU GLU SER THR LEU GLU PRO TRP SER
ARG LEU VAL LEU THR VAL SER CYS PHE ASN ASP MET CYS GLY ALA TYR MET ASP MET MET HIS VAL LYS VAL GLY ASP LEU PRO ALA ARG ASP ILE PRO VAL LEU VAL VAL GLY VAL SER GLY THR PRO LEU VAL VAL LEU VAL ARG GLY LEU ARG ALA ARG SER TRP
ARG THR ASP LEU GLU TRP GLY GLN VAL PRO GLN GLY VAL GLU GLN THR ARG ARG THR PHE THR VAL PHE ASP ASN THR GLY SER LEU ASP MET HIS LEU ALA TRP GLU ALA ARG ARG TYR HIS ASP TYR VAL ASP LEU GLU LEU ARG PRO PRO THR THR ASP VAL GLY GLY ALA GLY GLY THR GLY GLN
HIS ASP SER LEU TRP GLY GLY ALA PRO GLY THR LEU ARG ASP SER LEU GLN PRO ASP GLU ARG VAL LYS LEU GLN THR GLN ARG VAL PHE SER PRO GLU SER PRO LEU GLU LEU ARG GLY TRP THR ALA GLY GLU ASN ALA ASP VAL PRO THR THR ASP VAL GLU PRO GLU GLU SER GLY THR VAL ILE
LYS GLY ASN THR THR ALA LYS PHE THR VAL THR PHE CYS ALA SER GLU SER ARG ARG HIS GLY GLY TYR LEU HIS LEU GLY THR GLN ARG VAL PHE SER PRO GLU SER PRO LEU GLU LEU ARG VAL TRP THR ALA GLY GLU ASN ALA ASP ARG VAL PRO THR THR ASP VAL GLY ALA LEU LEU SER GLY THR ALA HIS



• Molecule 36: FAP15

Chain 4D:

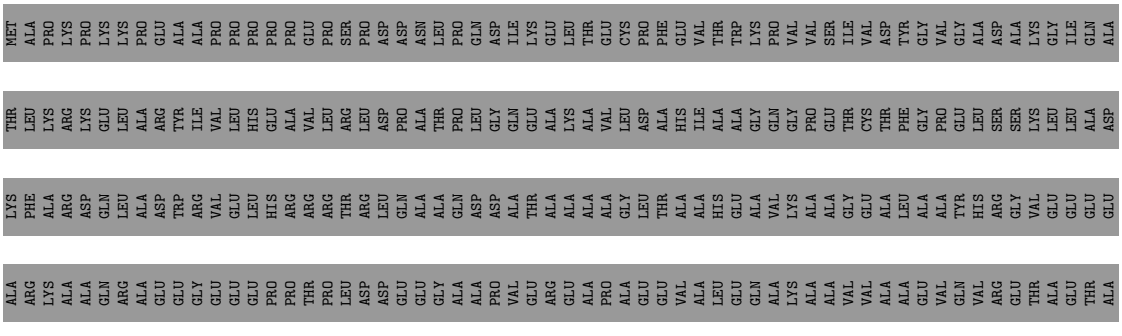


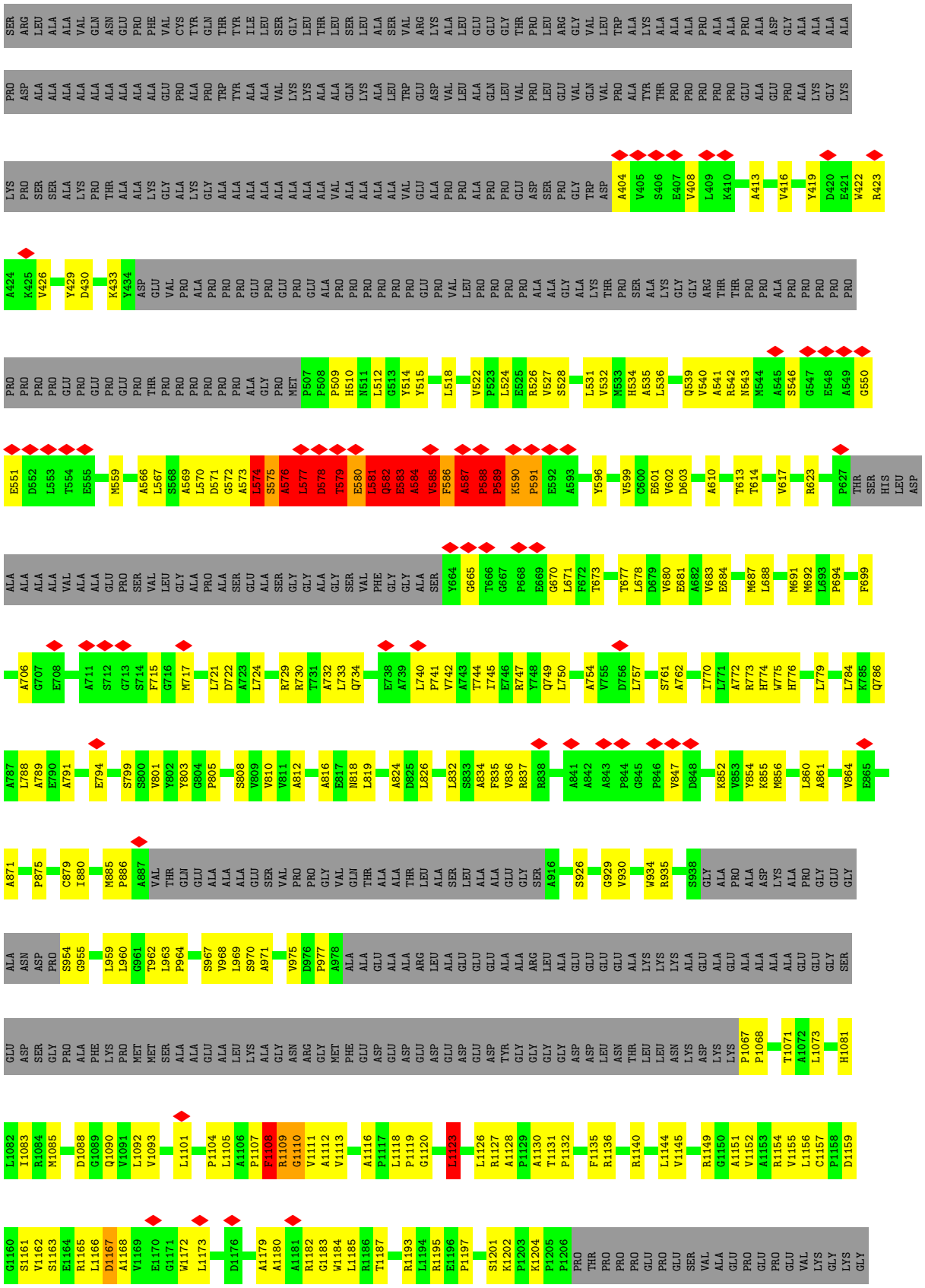


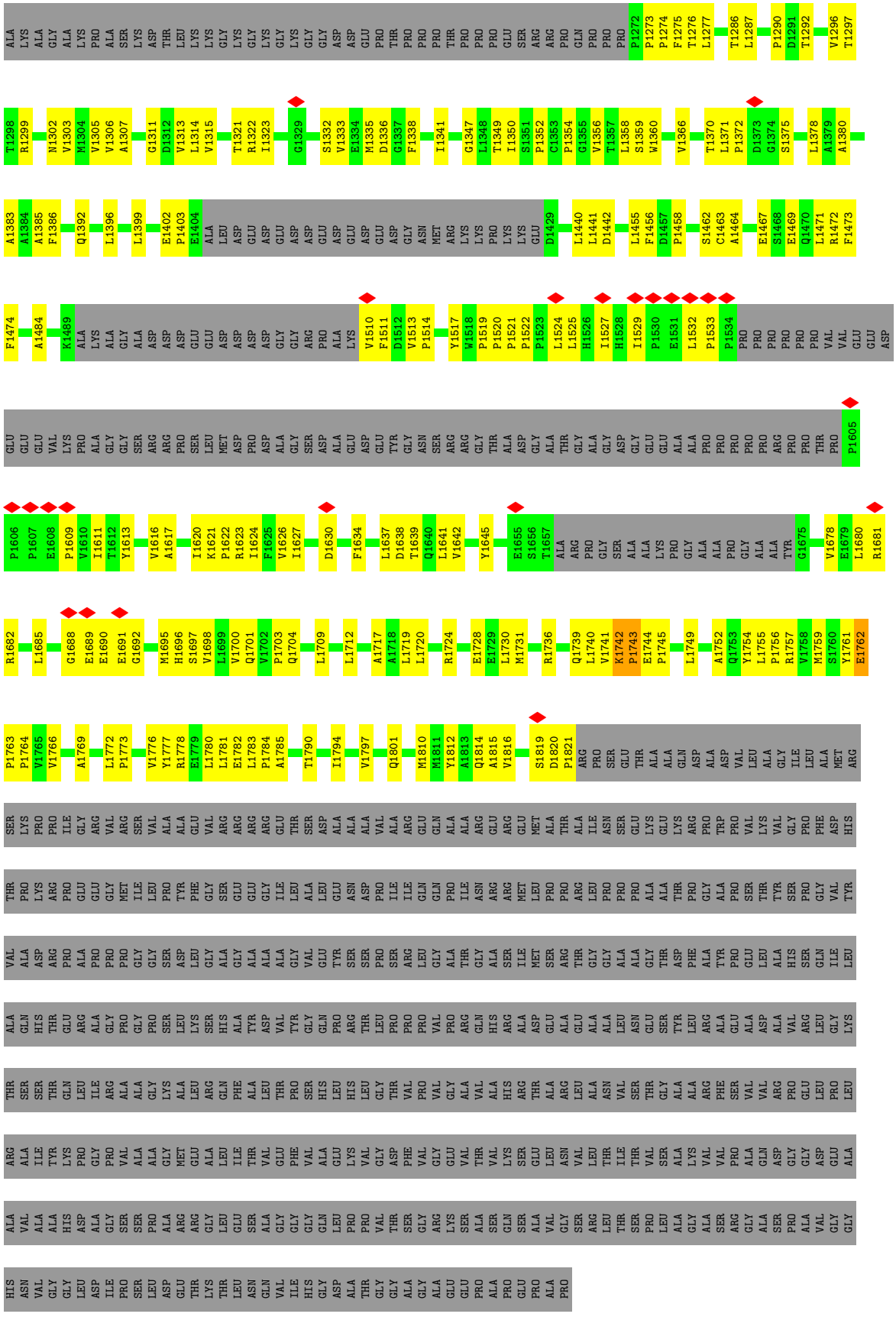
• Molecule 37: PF6

Chain 4E:





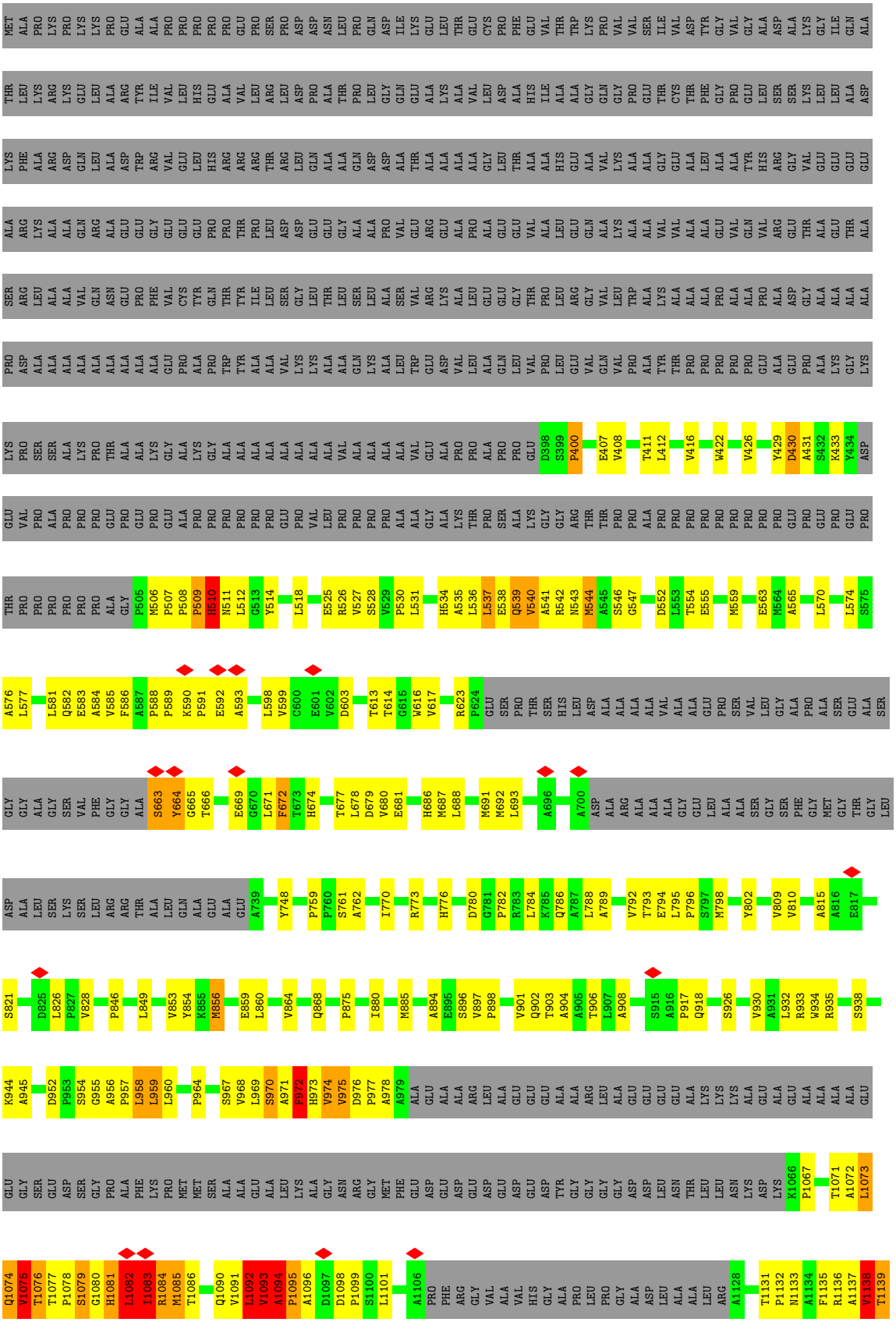


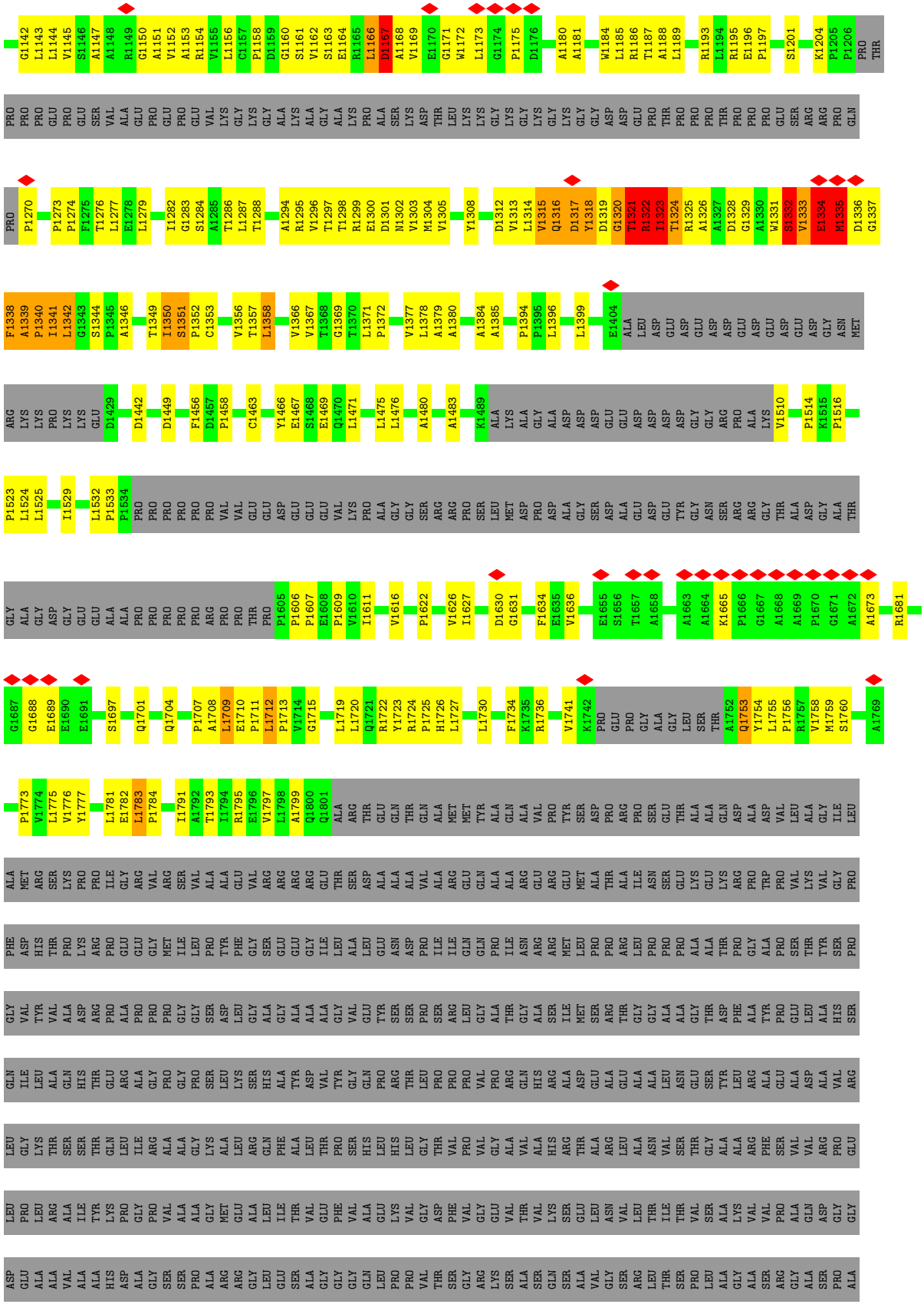


• Molecule 37: PF6

Chain 4F:





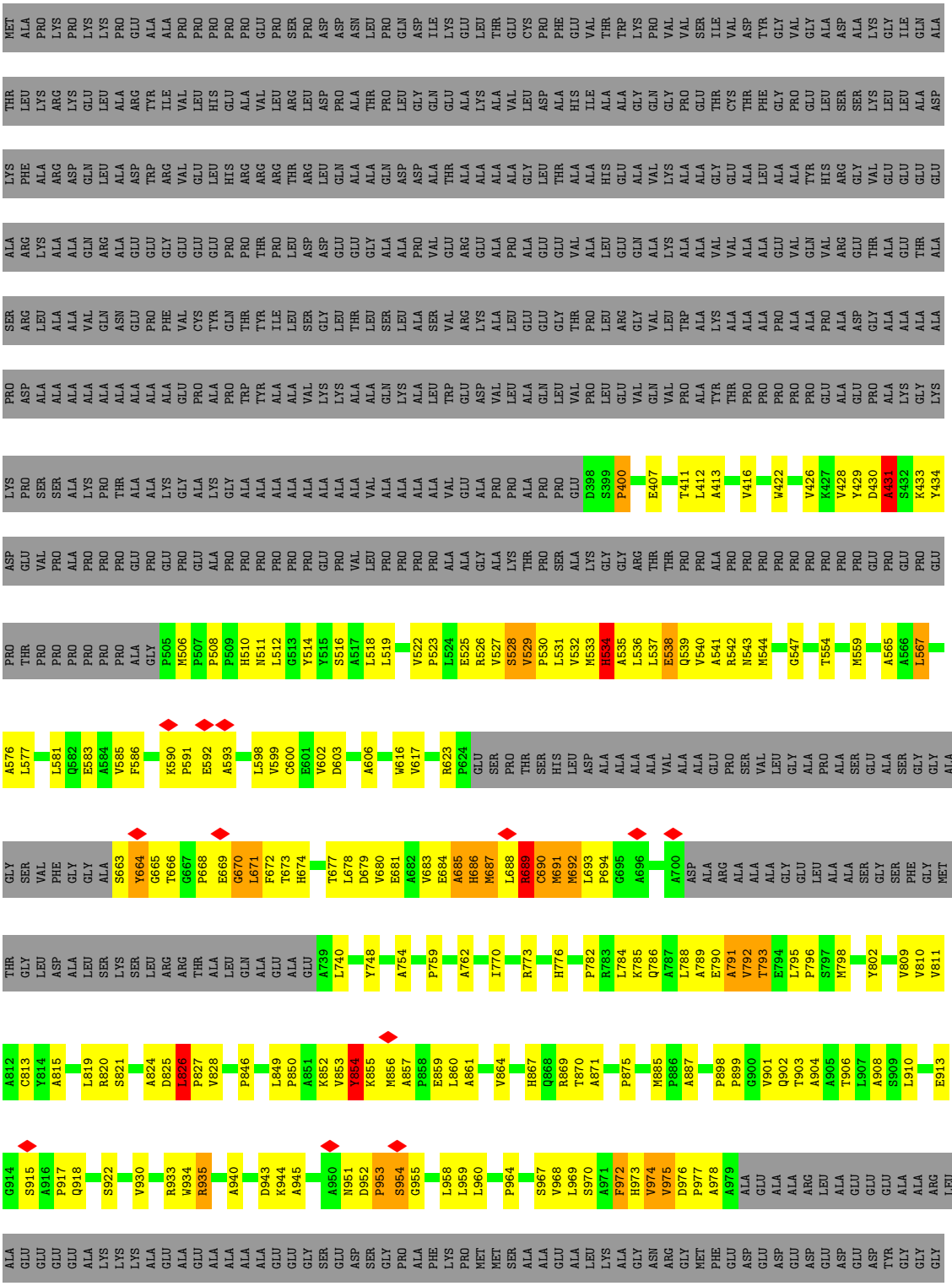


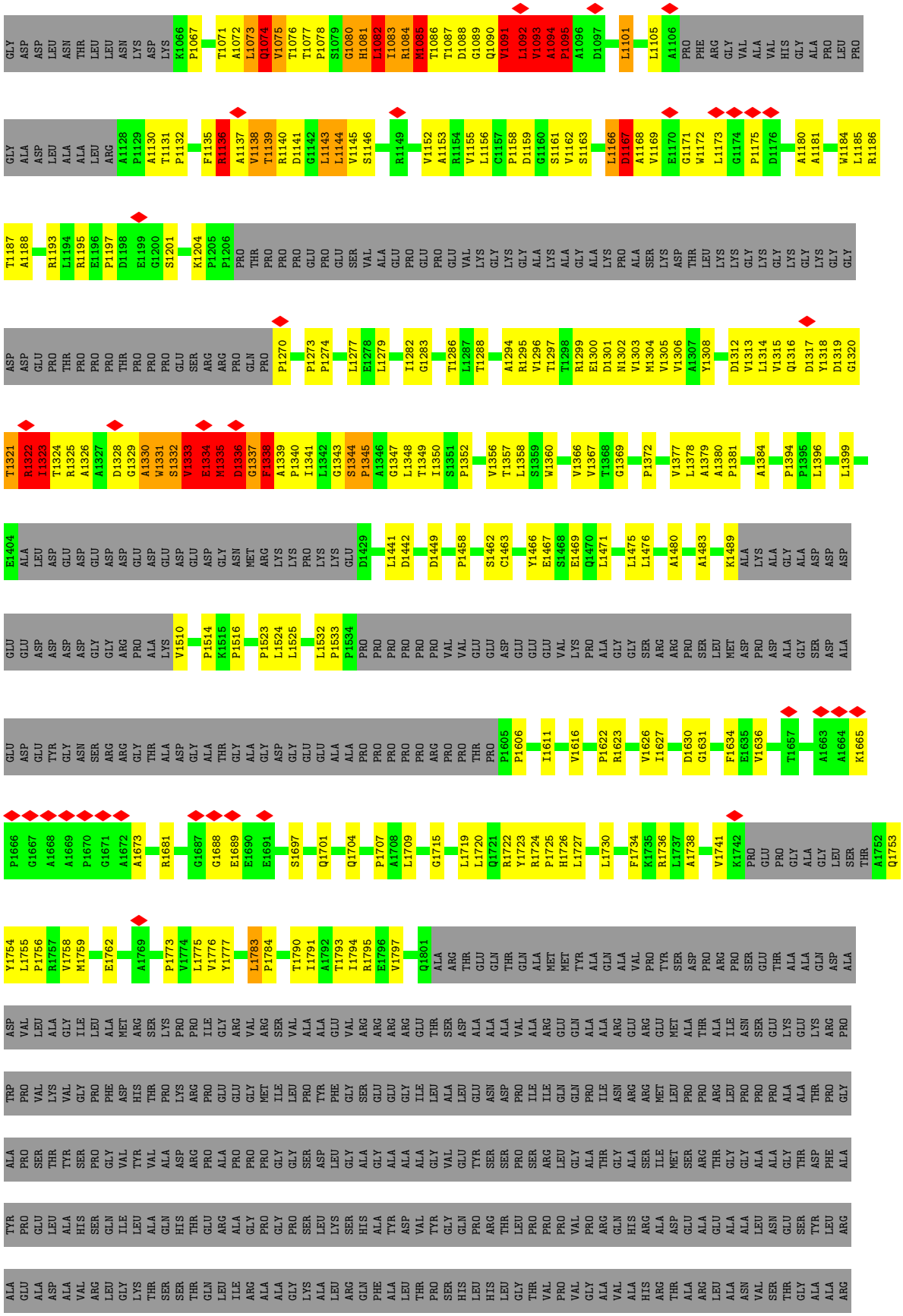


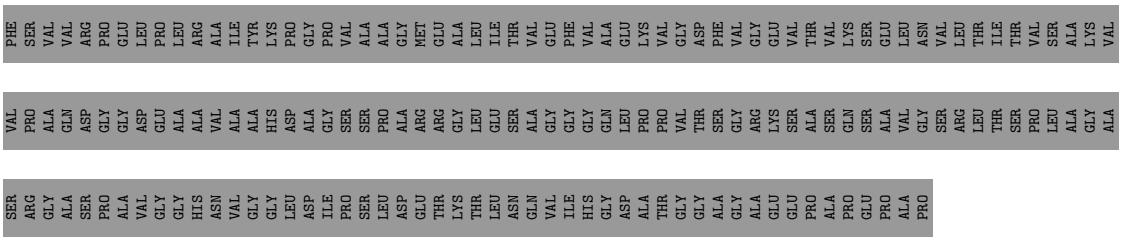
• Molecule 37: PF6

Chain 4G:









• Molecule 37: PF6

Chain 4H:











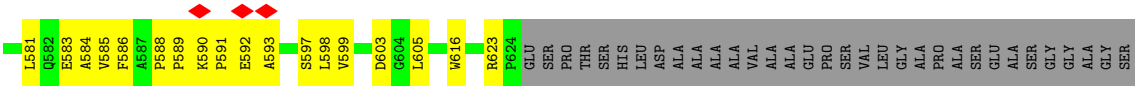


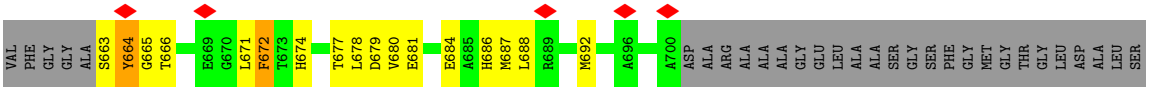






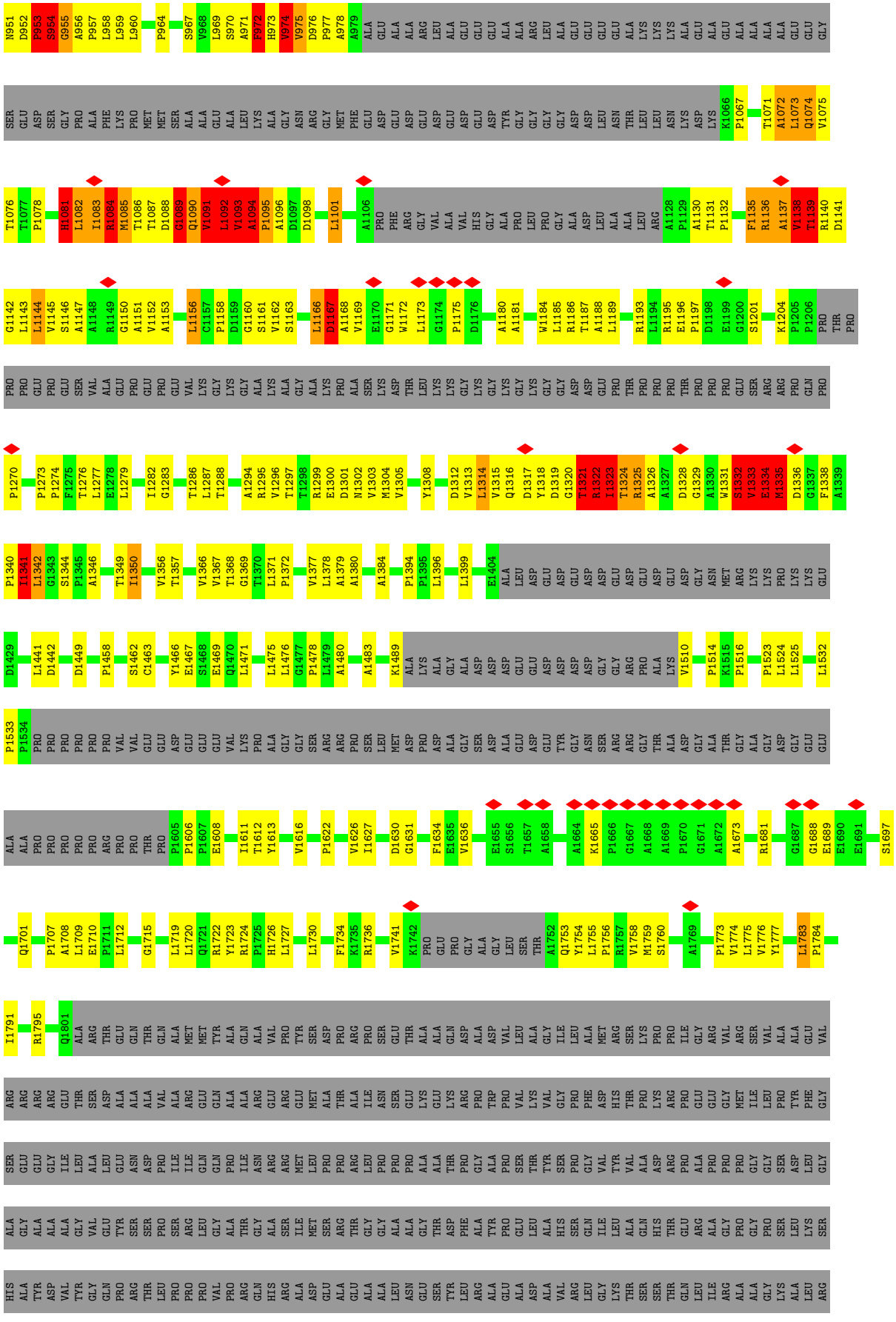


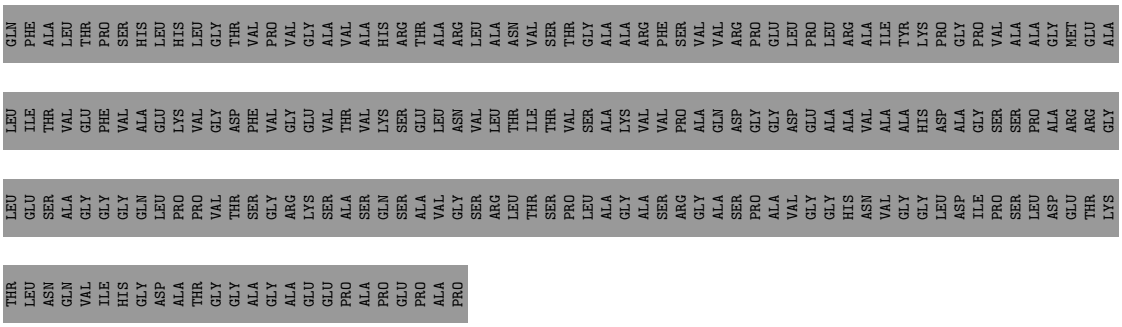






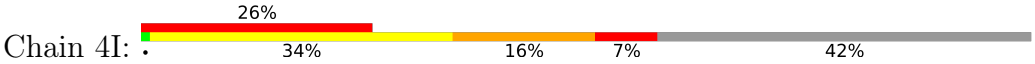


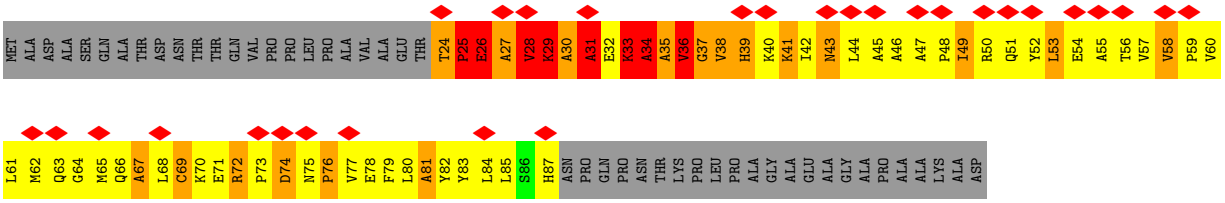




• Molecule 38: DPY30

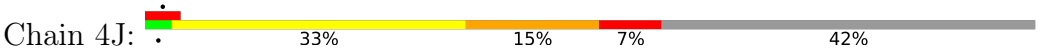
Chain 4I:

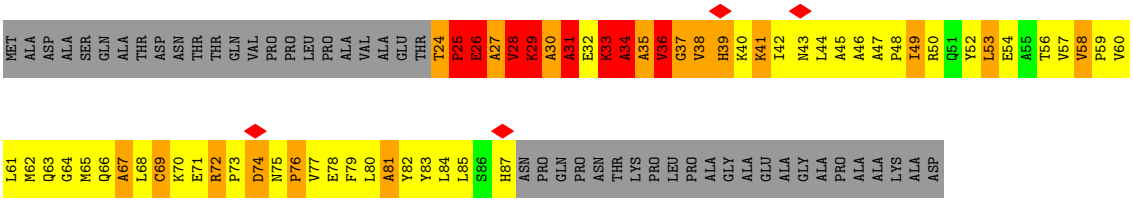




• Molecule 38: DPY30

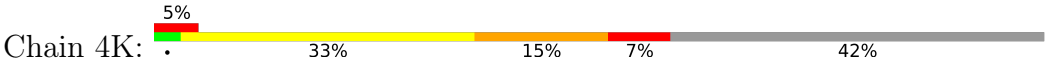
Chain 4J:

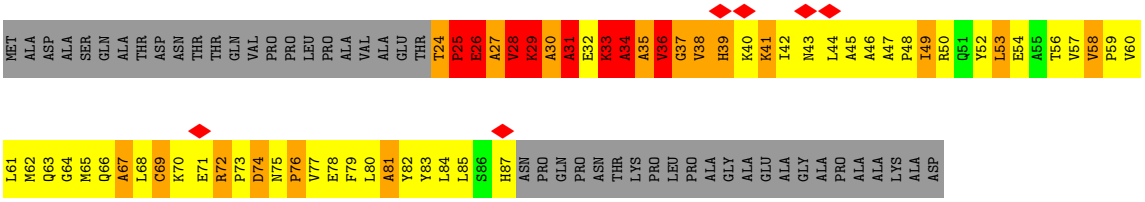




• Molecule 38: DPY30

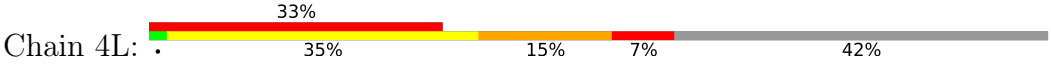
Chain 4K:



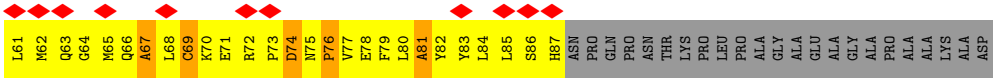


• Molecule 38: DPY30

Chain 4L:

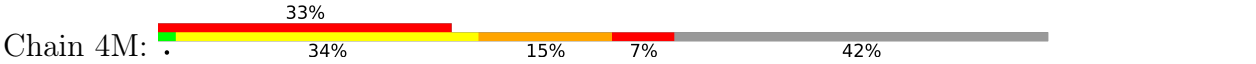


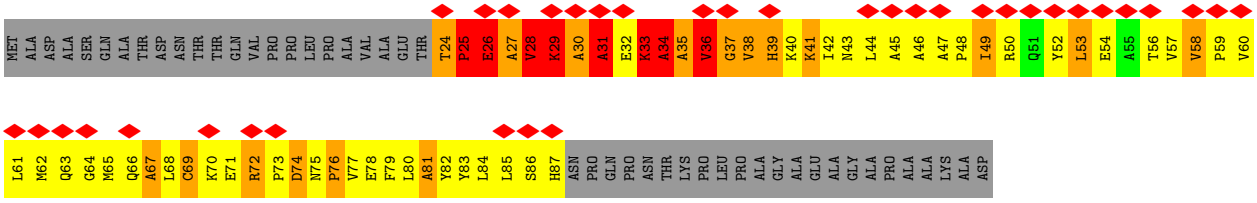




• Molecule 38: DPY30

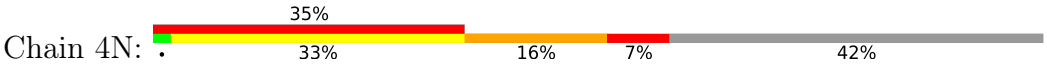
Chain 4M:

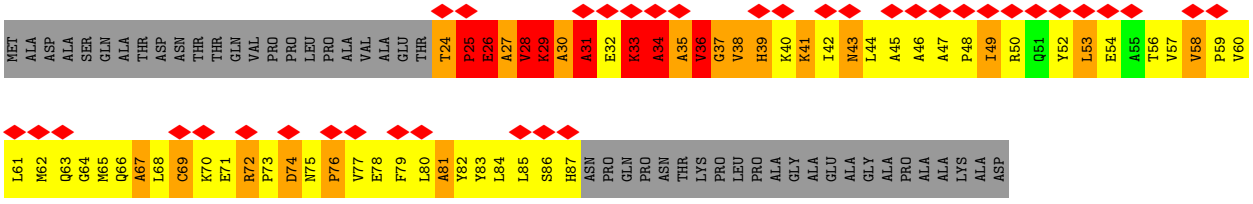




• Molecule 38: DPY30

Chain 4N:

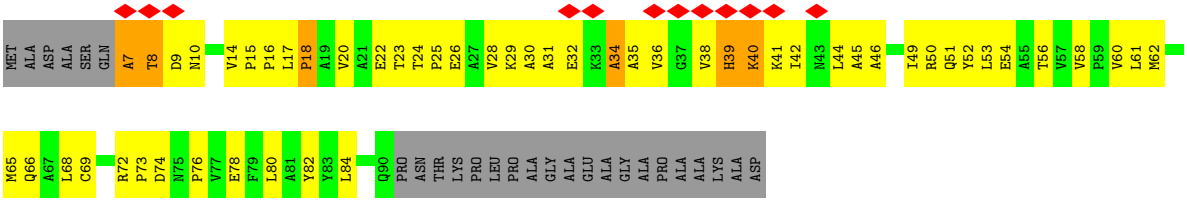




• Molecule 38: DPY30

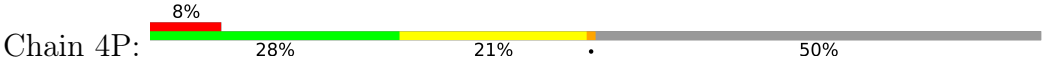
Chain 4O:

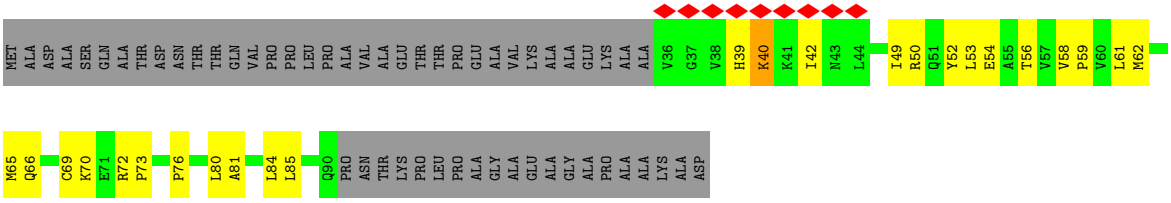




• Molecule 38: DPY30

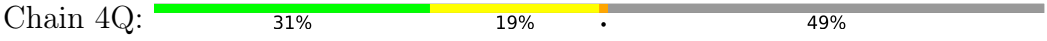
Chain 4P:

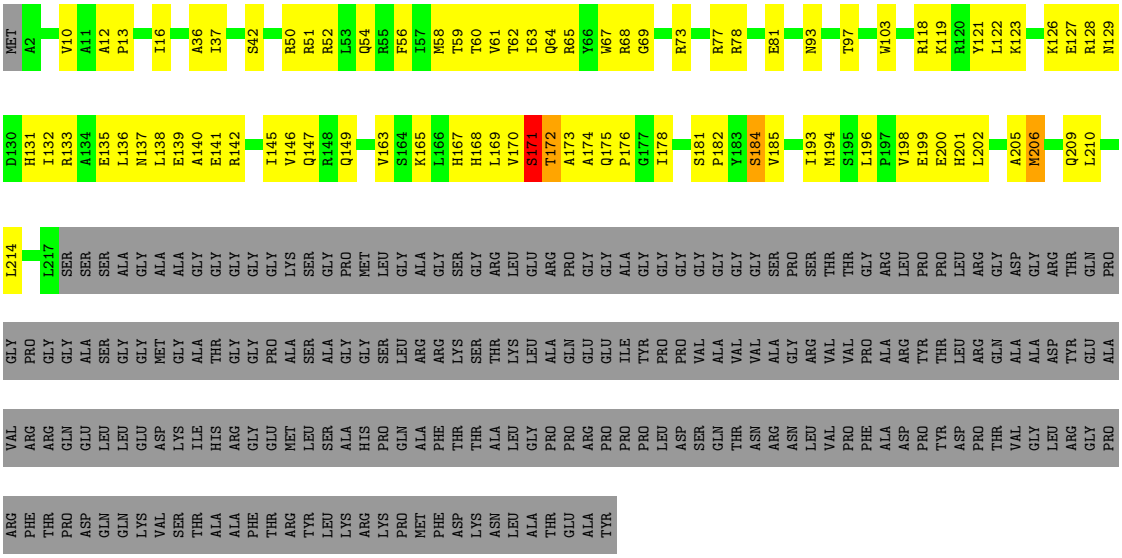




• Molecule 39: FAP305

Chain 4Q:

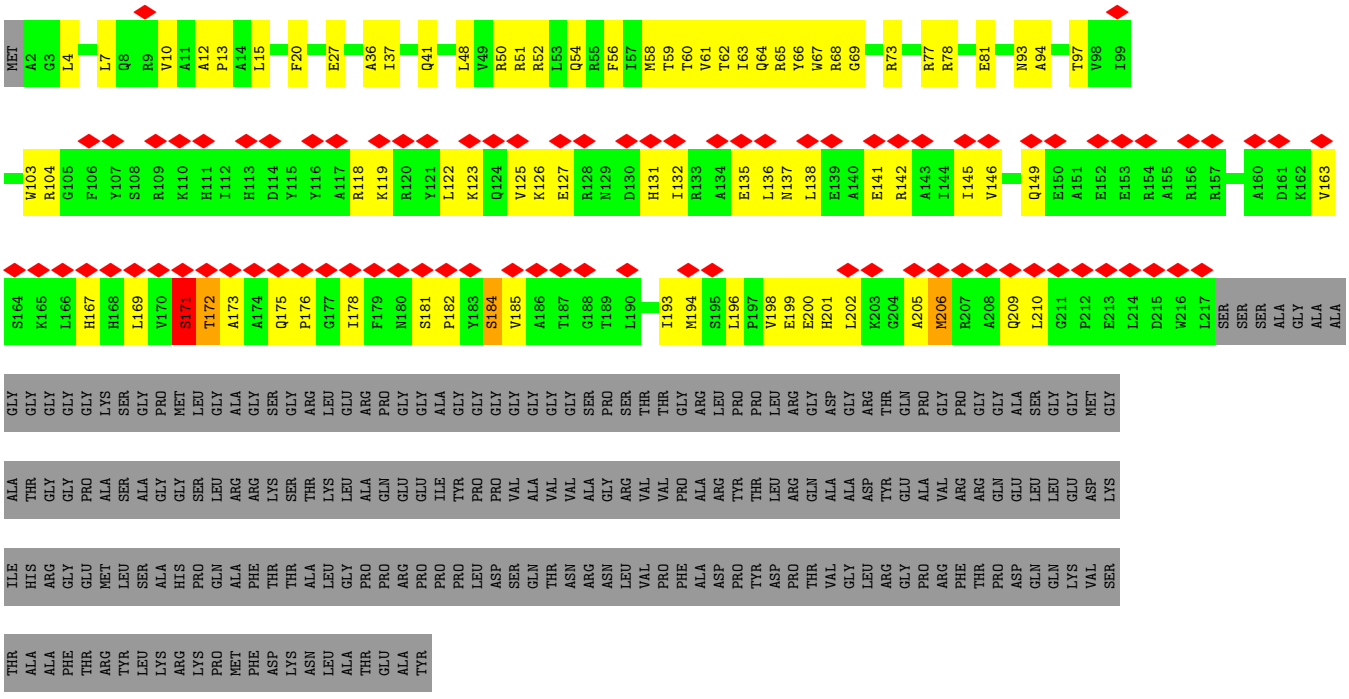




• Molecule 39: FAP305

Chain 4R:

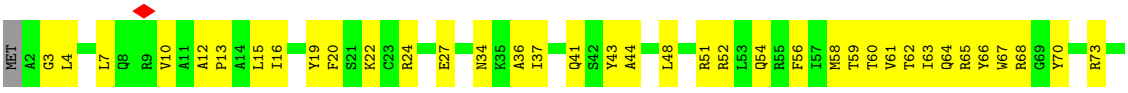


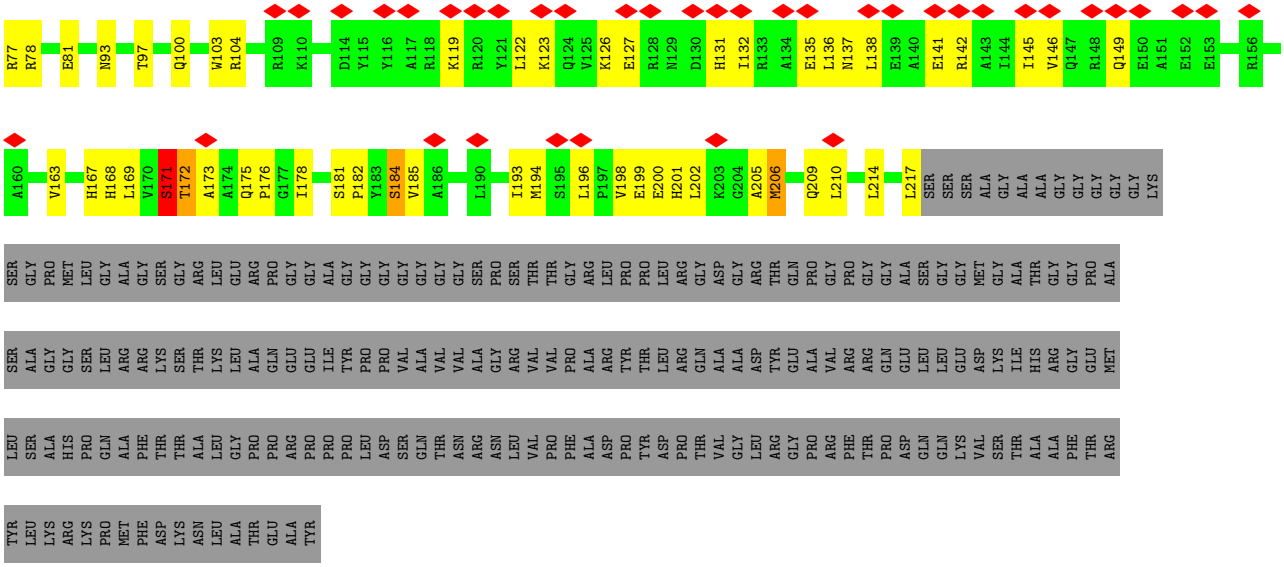


• Molecule 39: FAP305

Chain 4S:



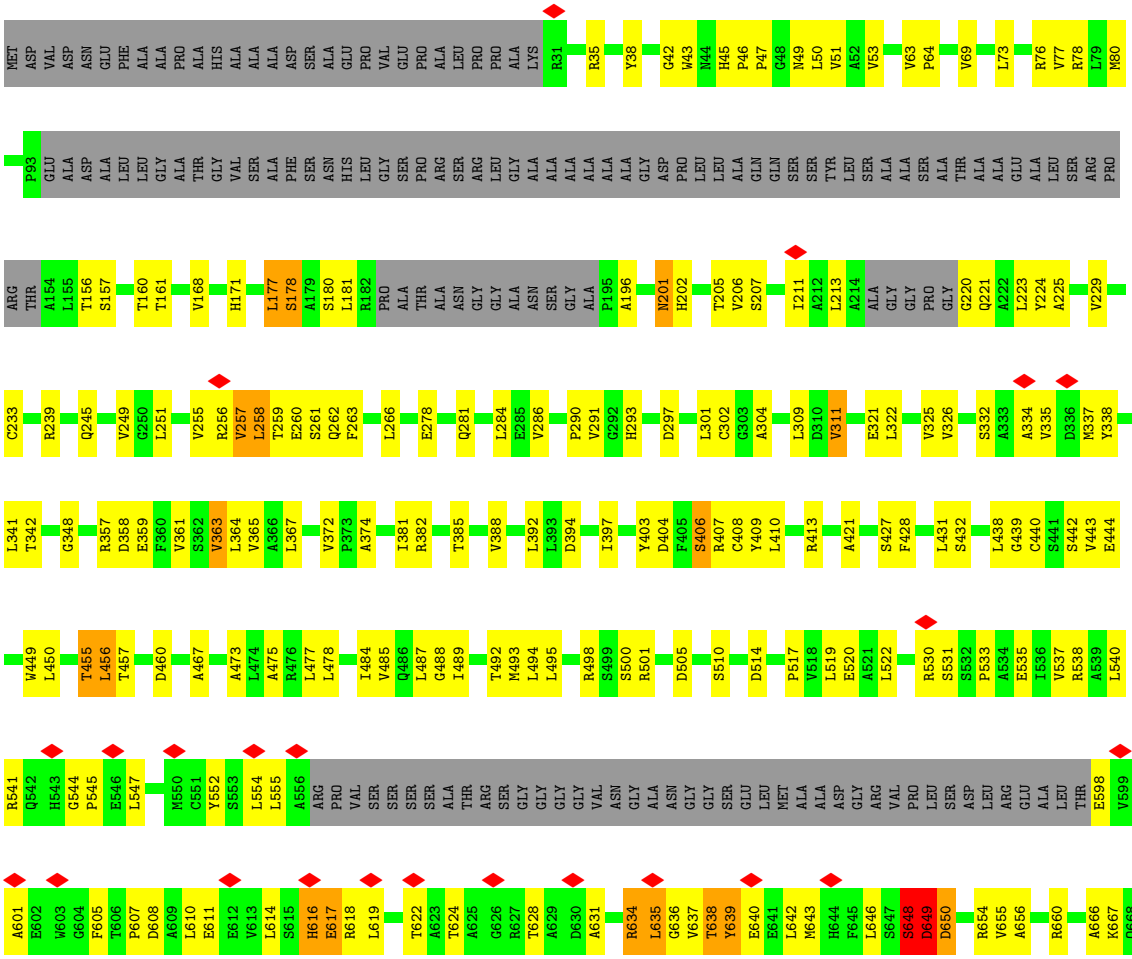


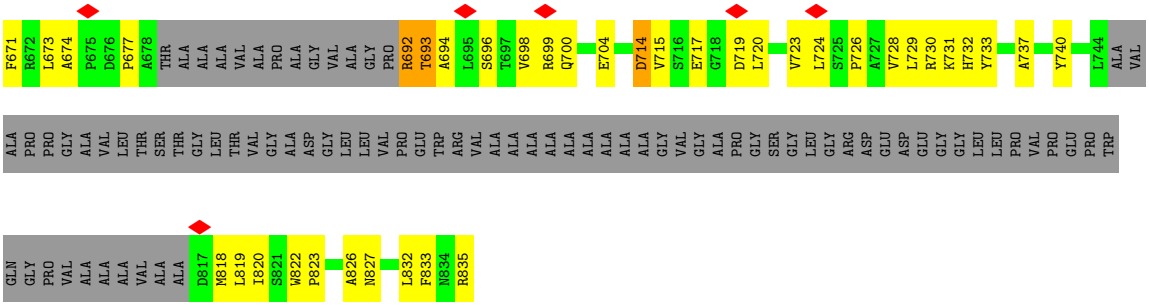


• Molecule 40: FAP101

Chain 4T:



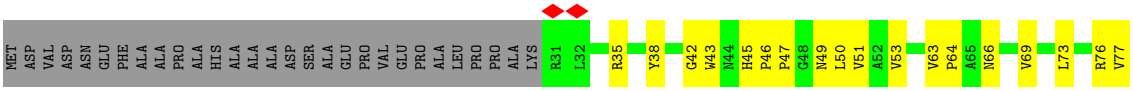


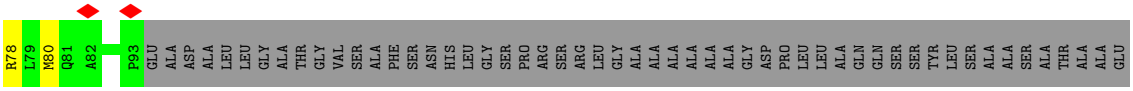


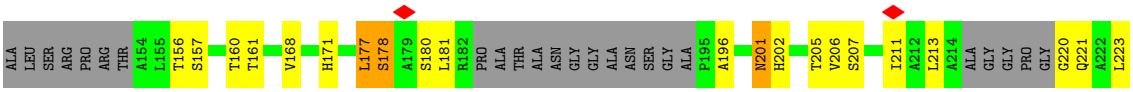
• Molecule 40: FAP101

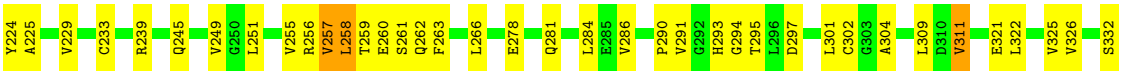
Chain 4U:

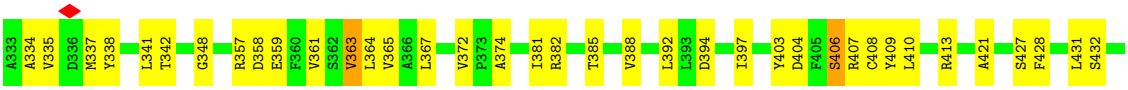


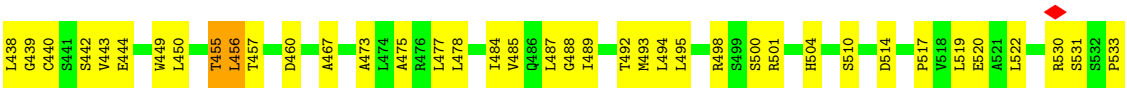


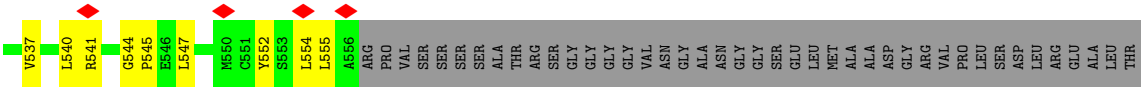




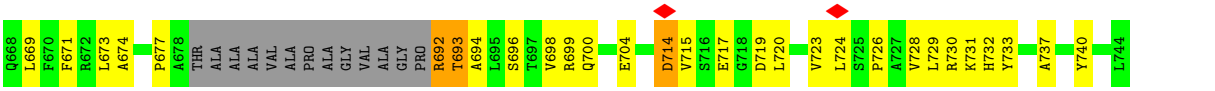


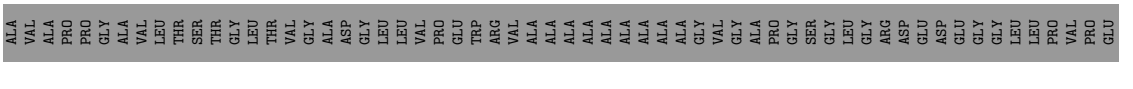


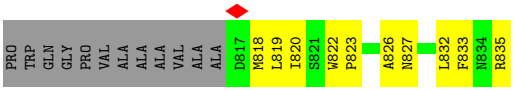








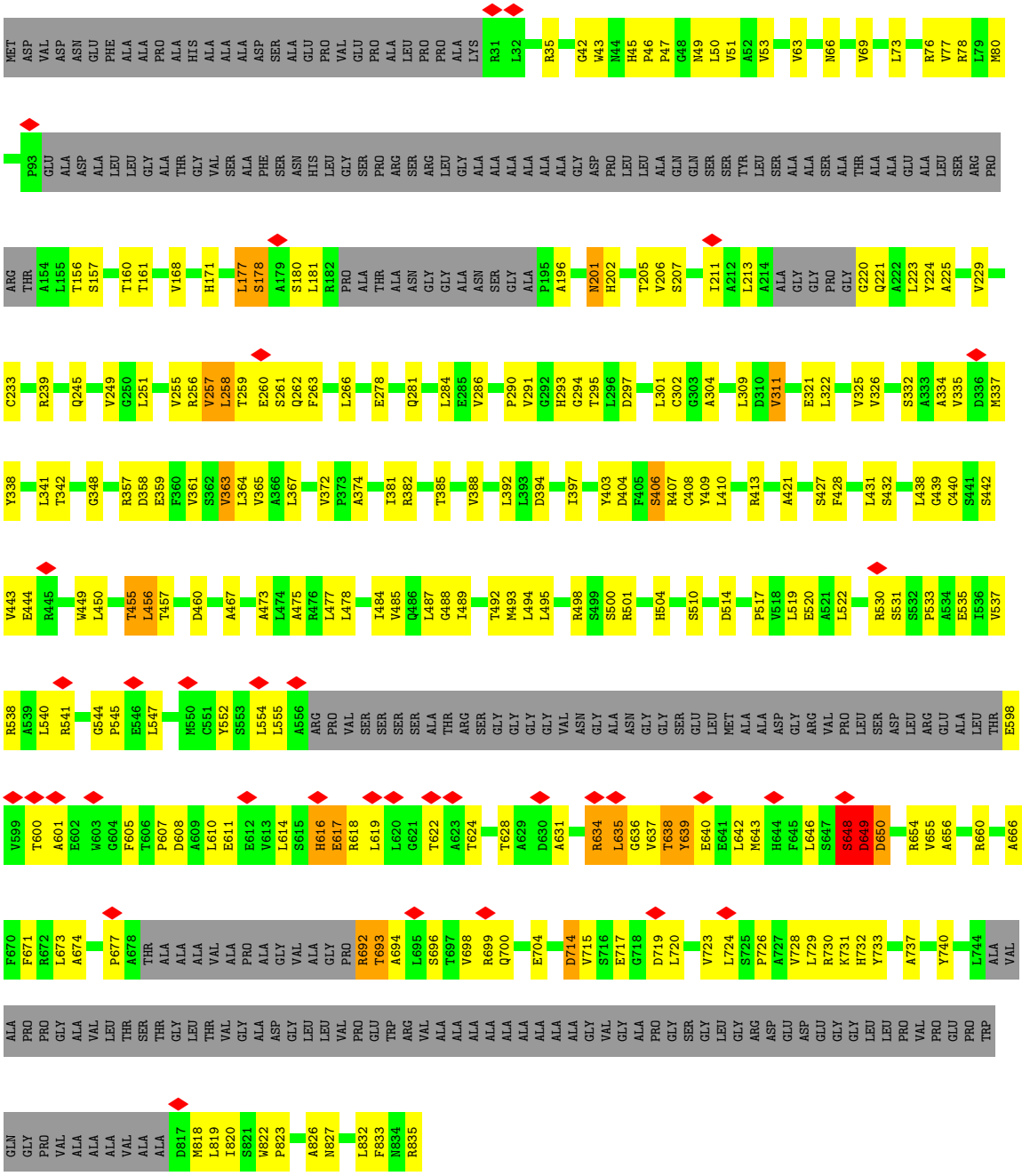




• Molecule 40: FAP101

Chain 4V:

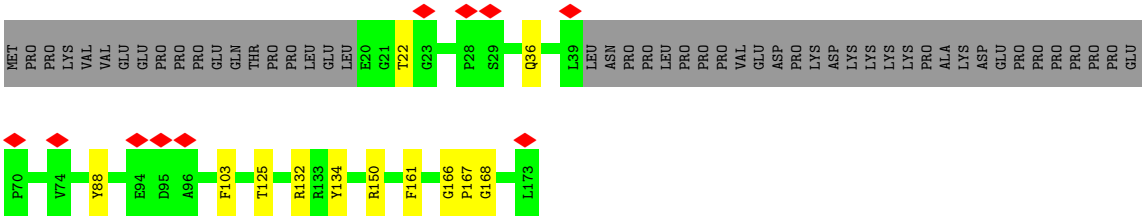




• Molecule 41: FAP227

Chain 4W:

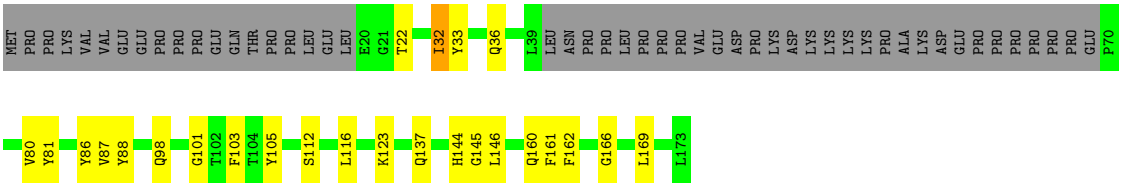




• Molecule 41: FAP227

Chain 4X:

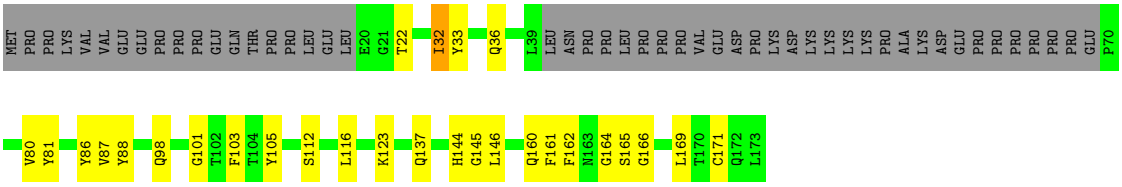




• Molecule 41: FAP227

Chain 4Y:

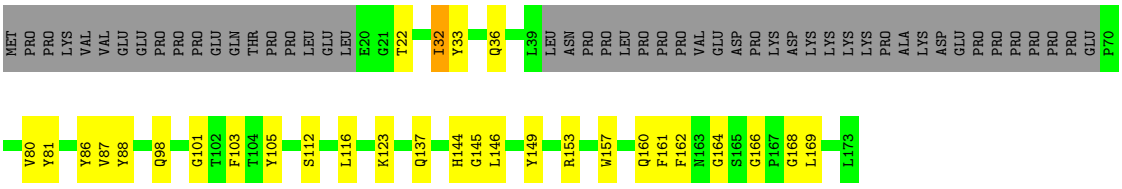




• Molecule 41: FAP227

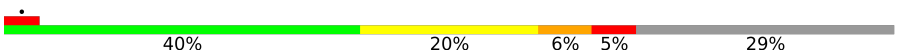
Chain 4Z:

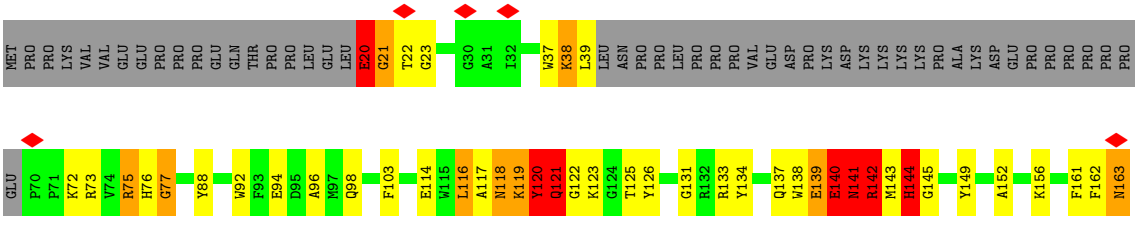


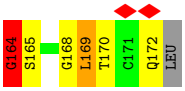


• Molecule 41: FAP227

Chain 5A:







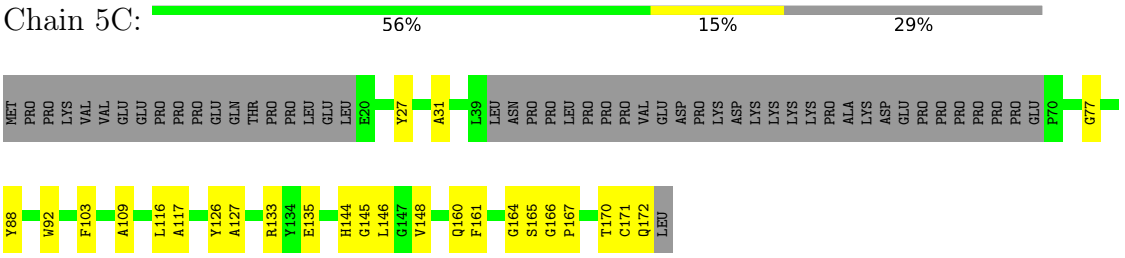
• Molecule 41: FAP227

Chain 5B:



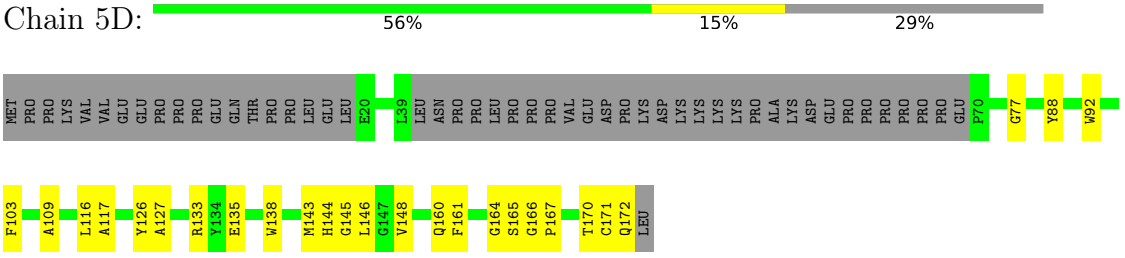
• Molecule 41: FAP227

Chain 5C:



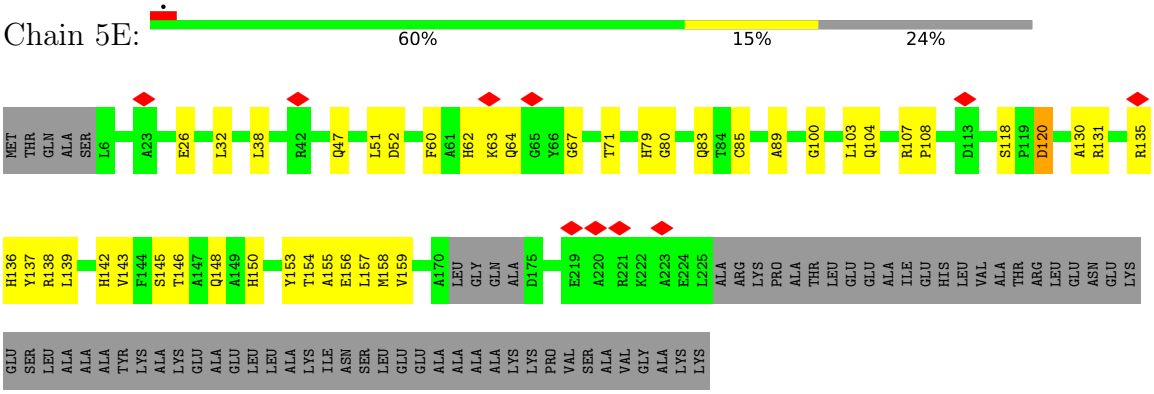
• Molecule 41: FAP227

Chain 5D:



• Molecule 42: FAP114

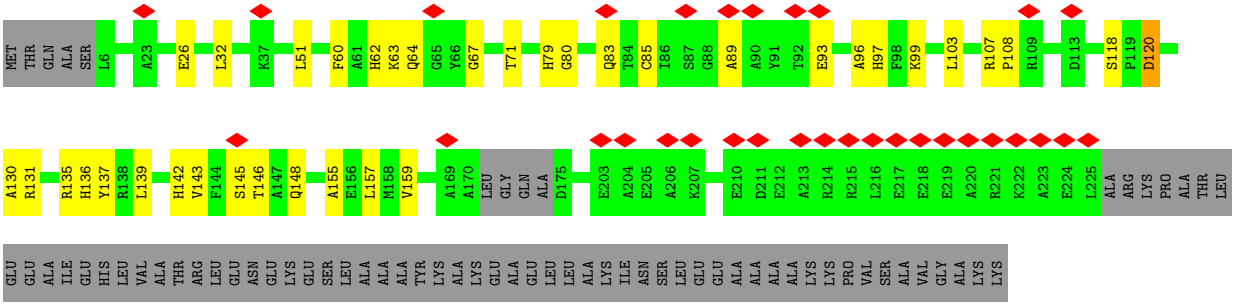
Chain 5E:



• Molecule 42: FAP114

Chain 5F:

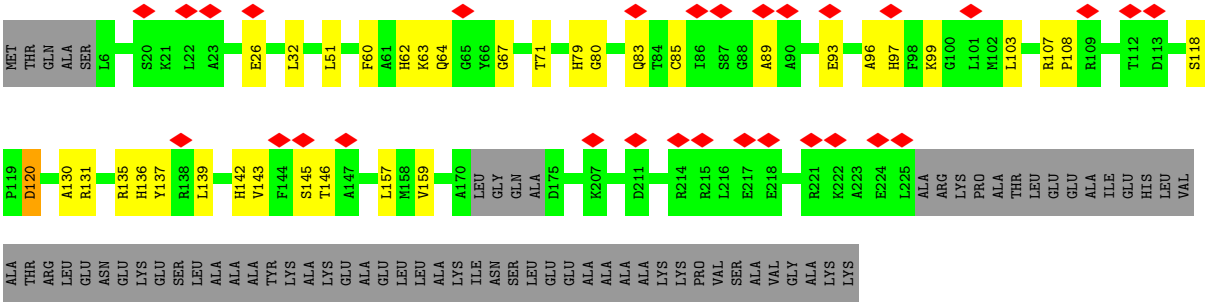




• Molecule 42: FAP114

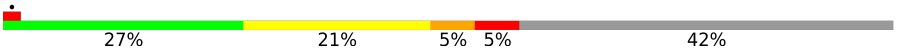
Chain 5G:

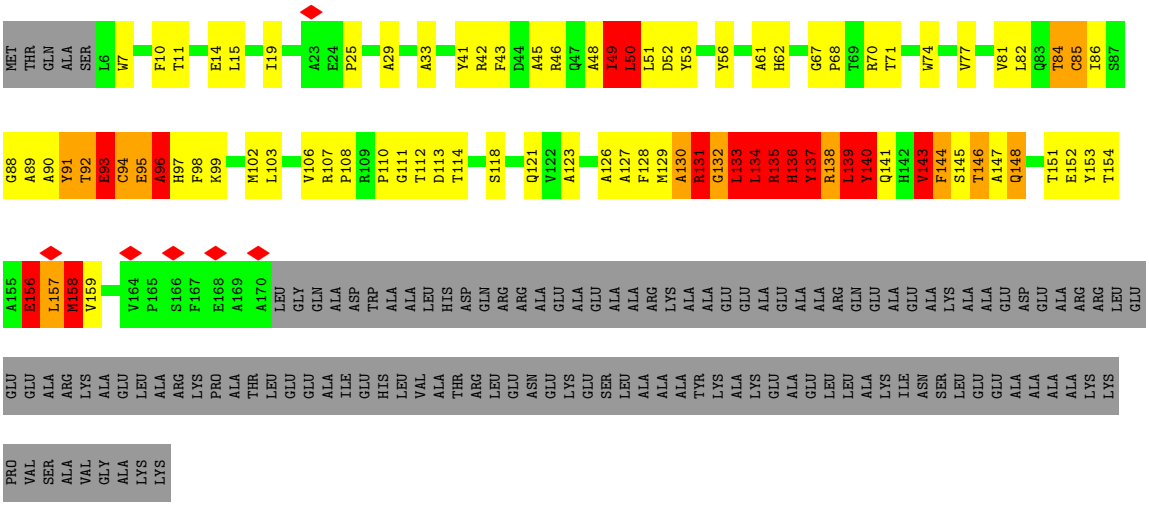




• Molecule 42: FAP114

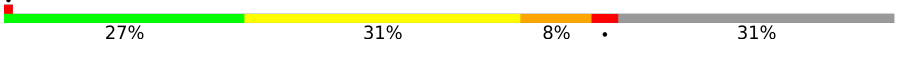
Chain 5H:

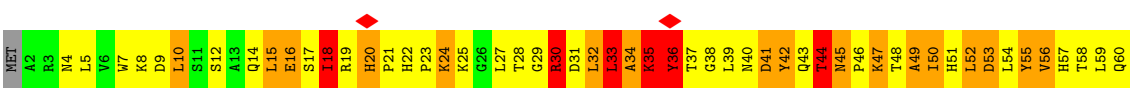


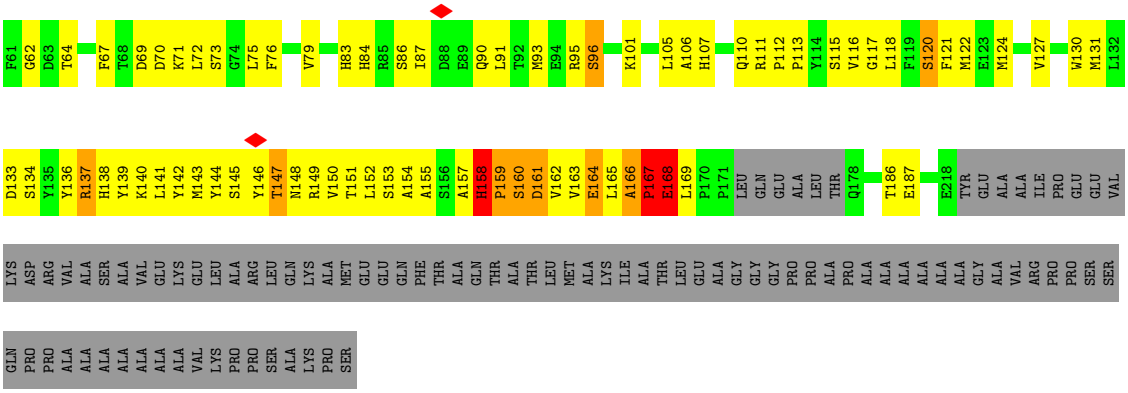


• Molecule 43: FAP119

Chain 5I:



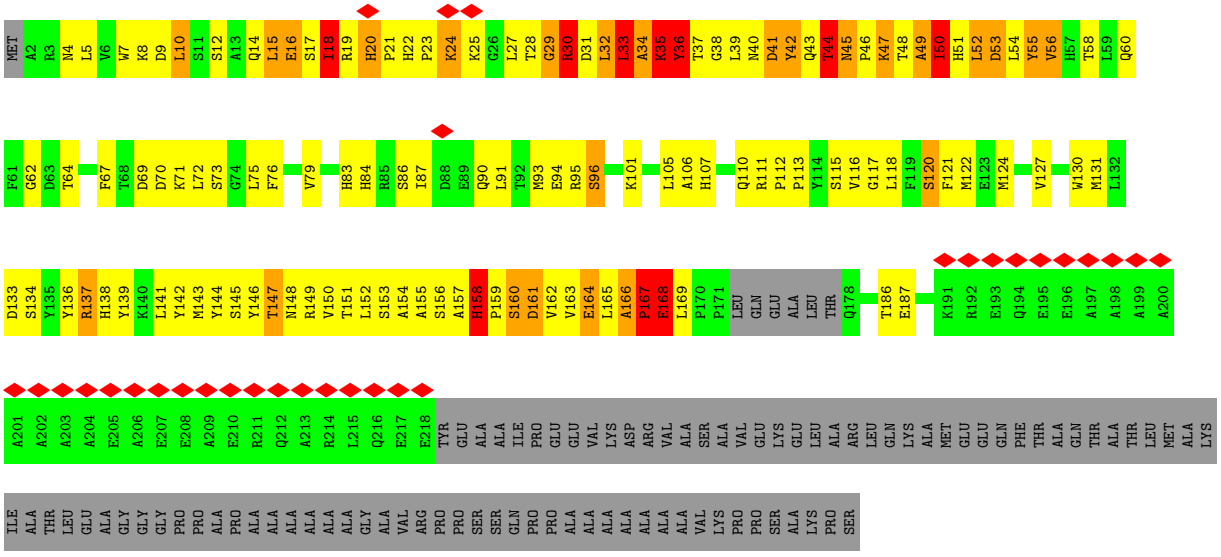




• Molecule 43: FAP119

Chain 5J:

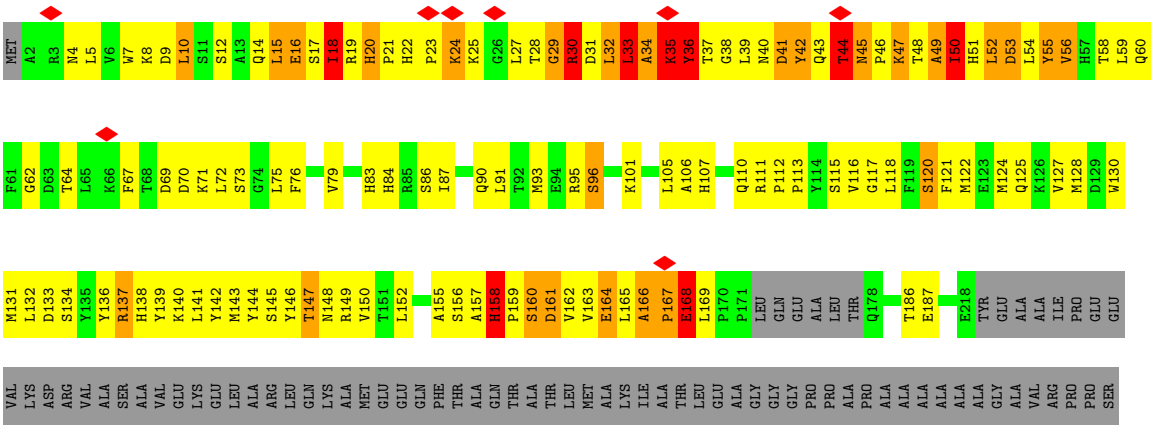


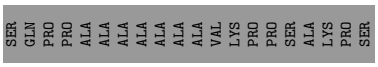


• Molecule 43: FAP119

Chain 5K:



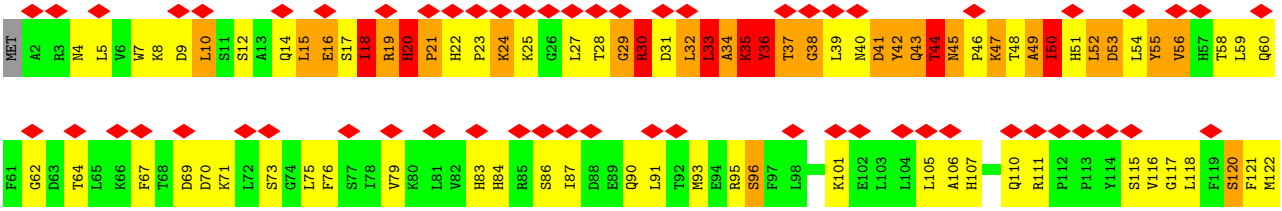




• Molecule 43: FAP119

Chain 5L:

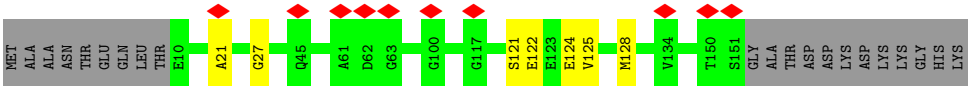




• Molecule 44: Calmodulin

Chain 5M:

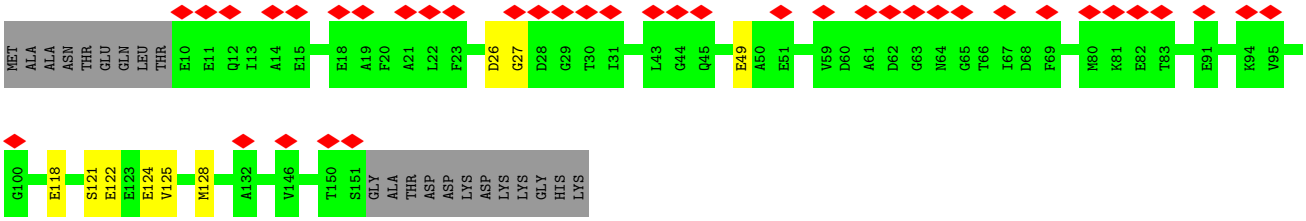




• Molecule 44: Calmodulin

Chain 5N:

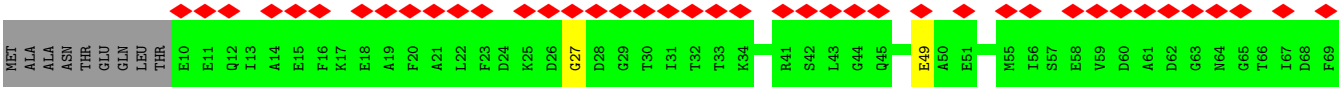


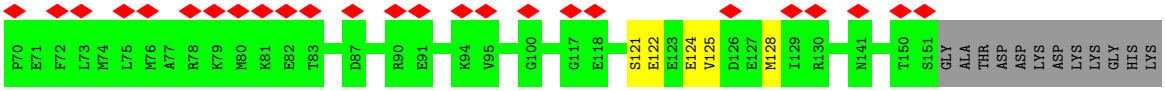


• Molecule 44: Calmodulin

Chain 5O:



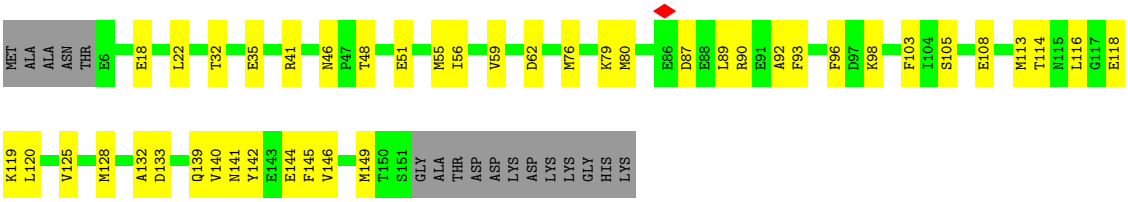




• Molecule 44: Calmodulin

Chain 5Q:

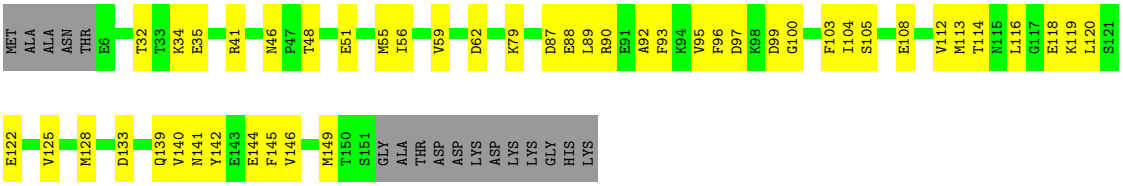




• Molecule 44: Calmodulin

Chain 5R:

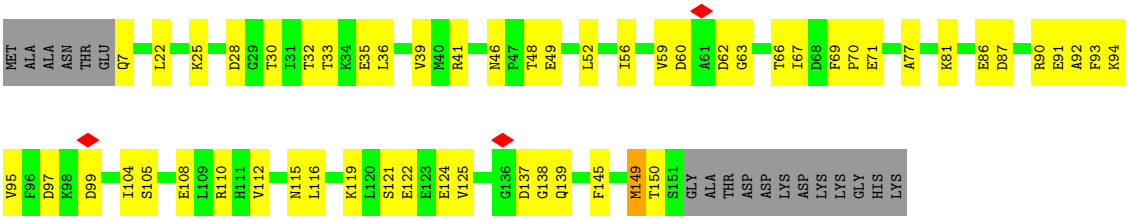




• Molecule 44: Calmodulin

Chain 5S:

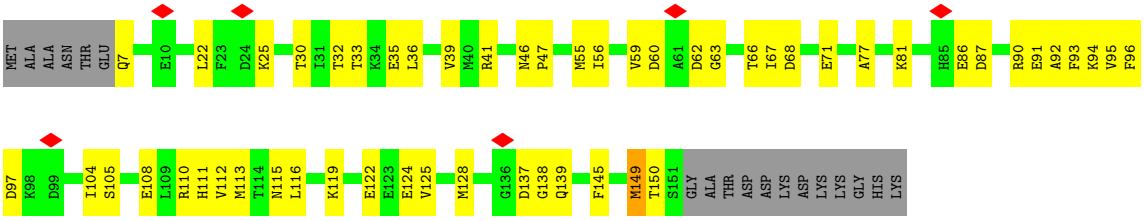




• Molecule 44: Calmodulin

Chain 5T:

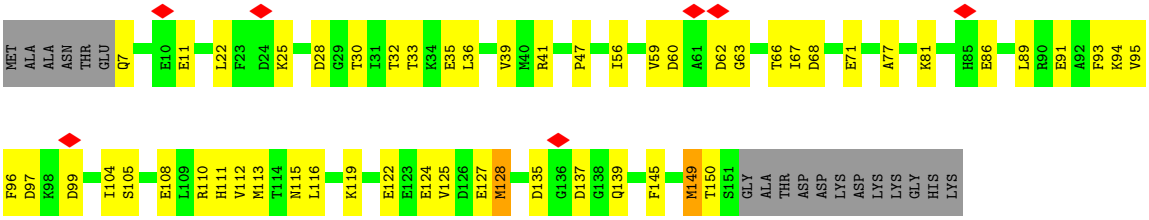




• Molecule 44: Calmodulin

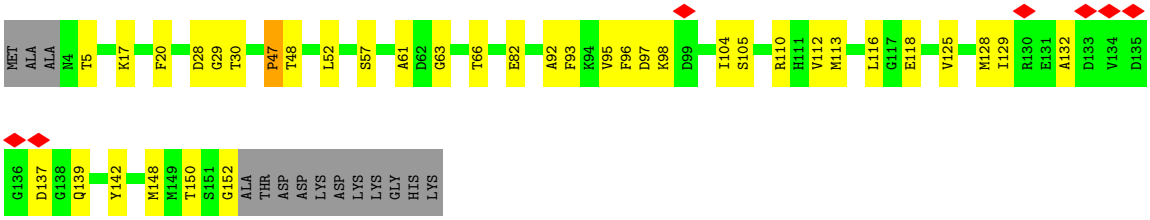
Chain 5U:





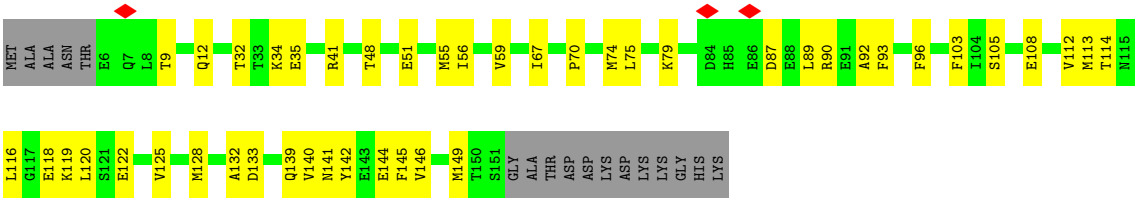
• Molecule 44: Calmodulin



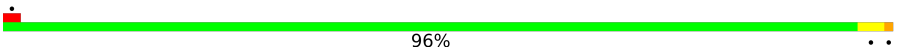


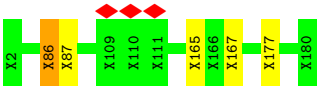
• Molecule 44: Calmodulin



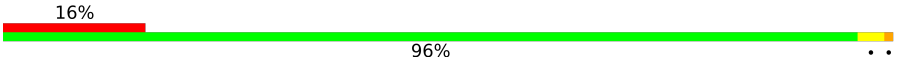


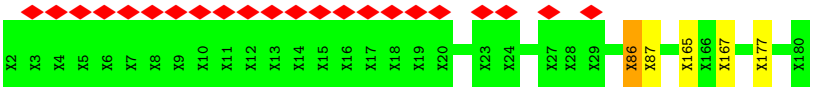
• Molecule 45: Unknown protein



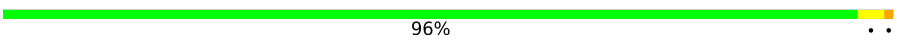


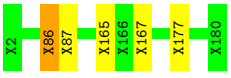
• Molecule 45: Unknown protein





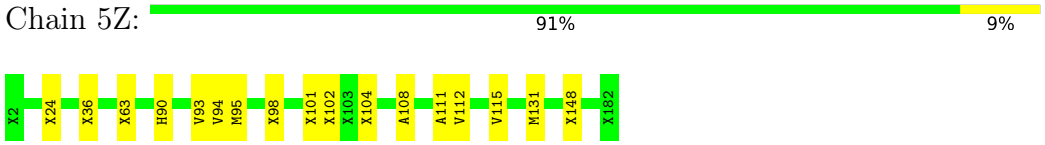
• Molecule 45: Unknown protein





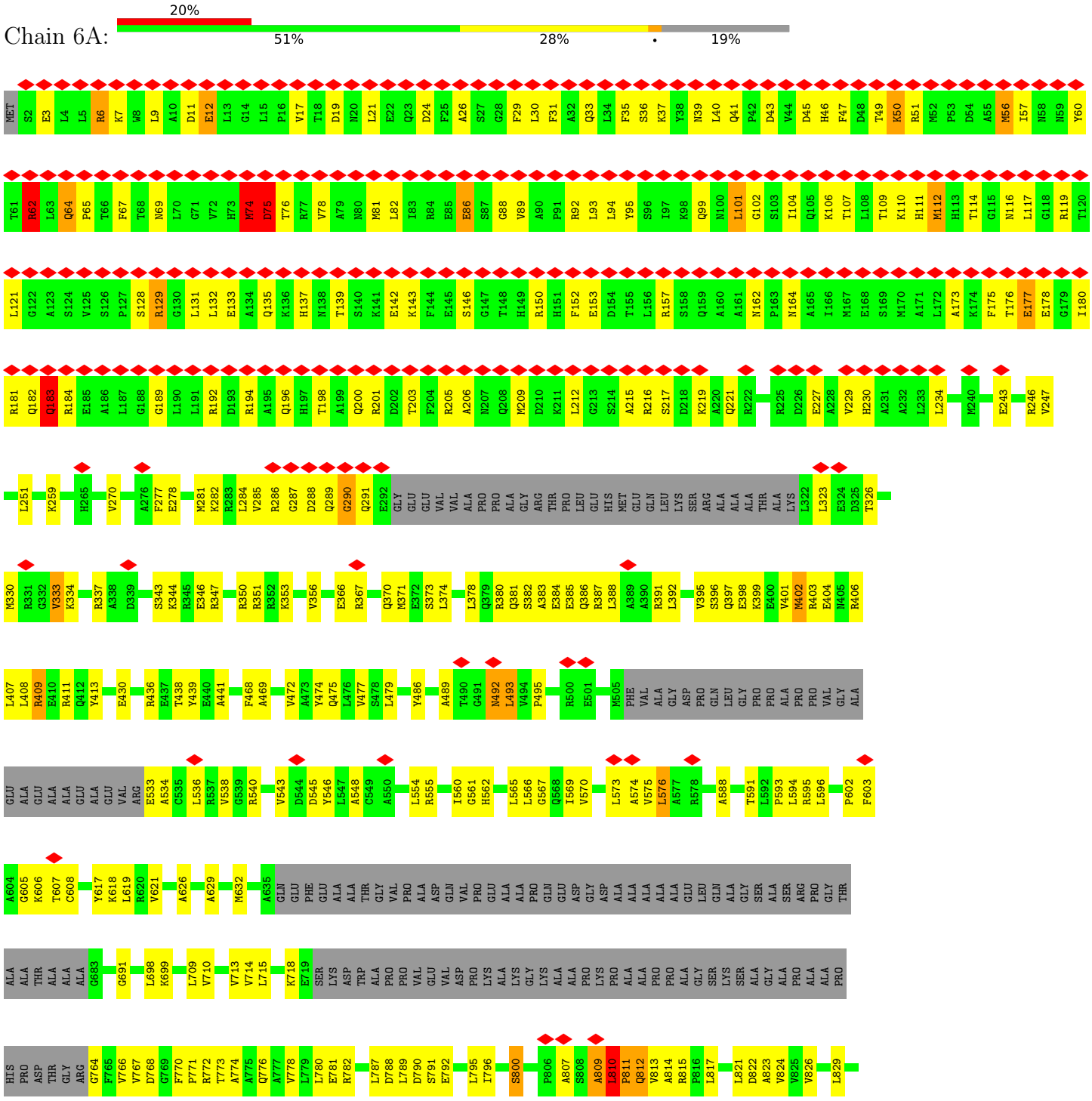
• Molecule 46: Unknown protein

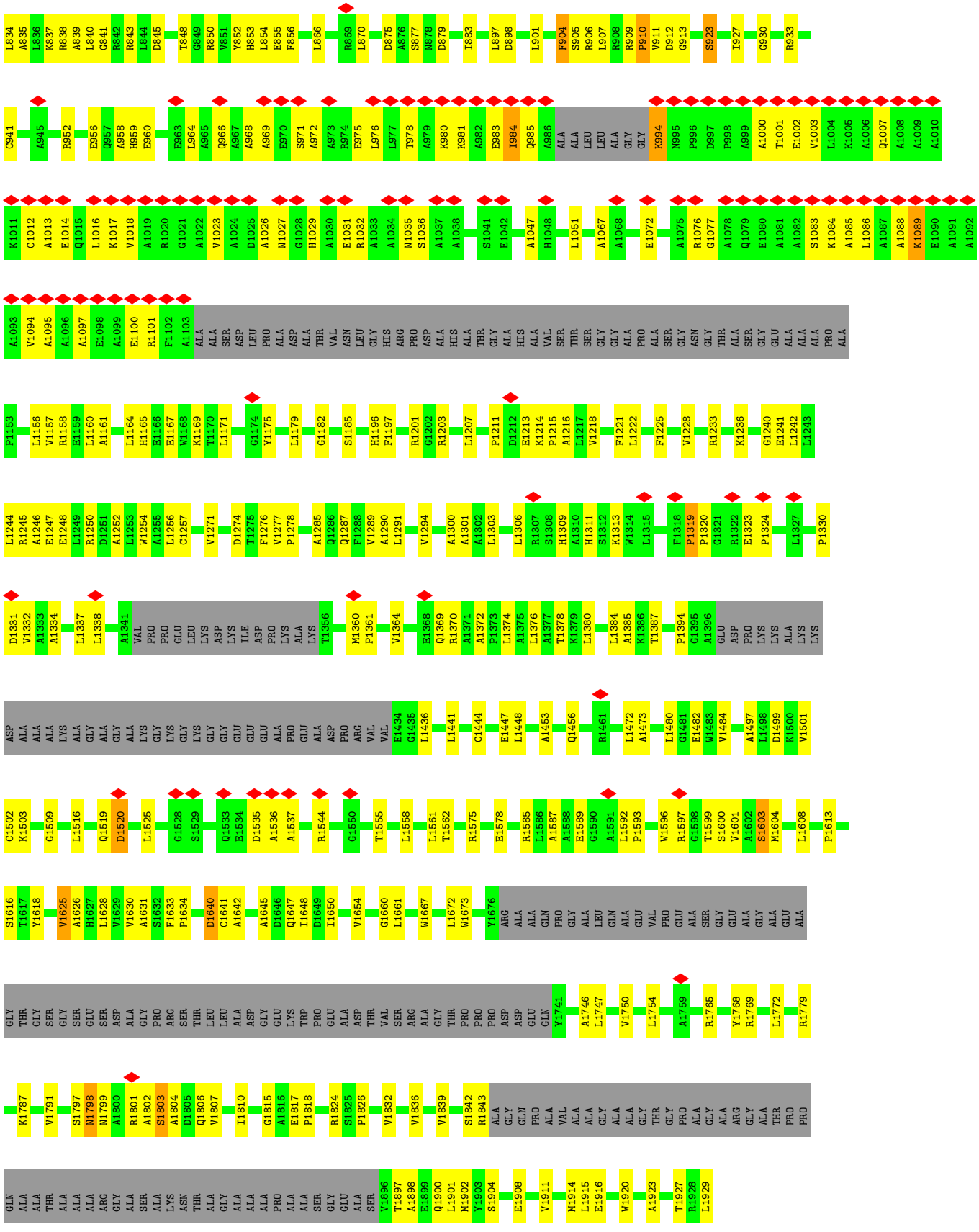
Chain 5Z:



• Molecule 47: CPC1

Chain 6A:

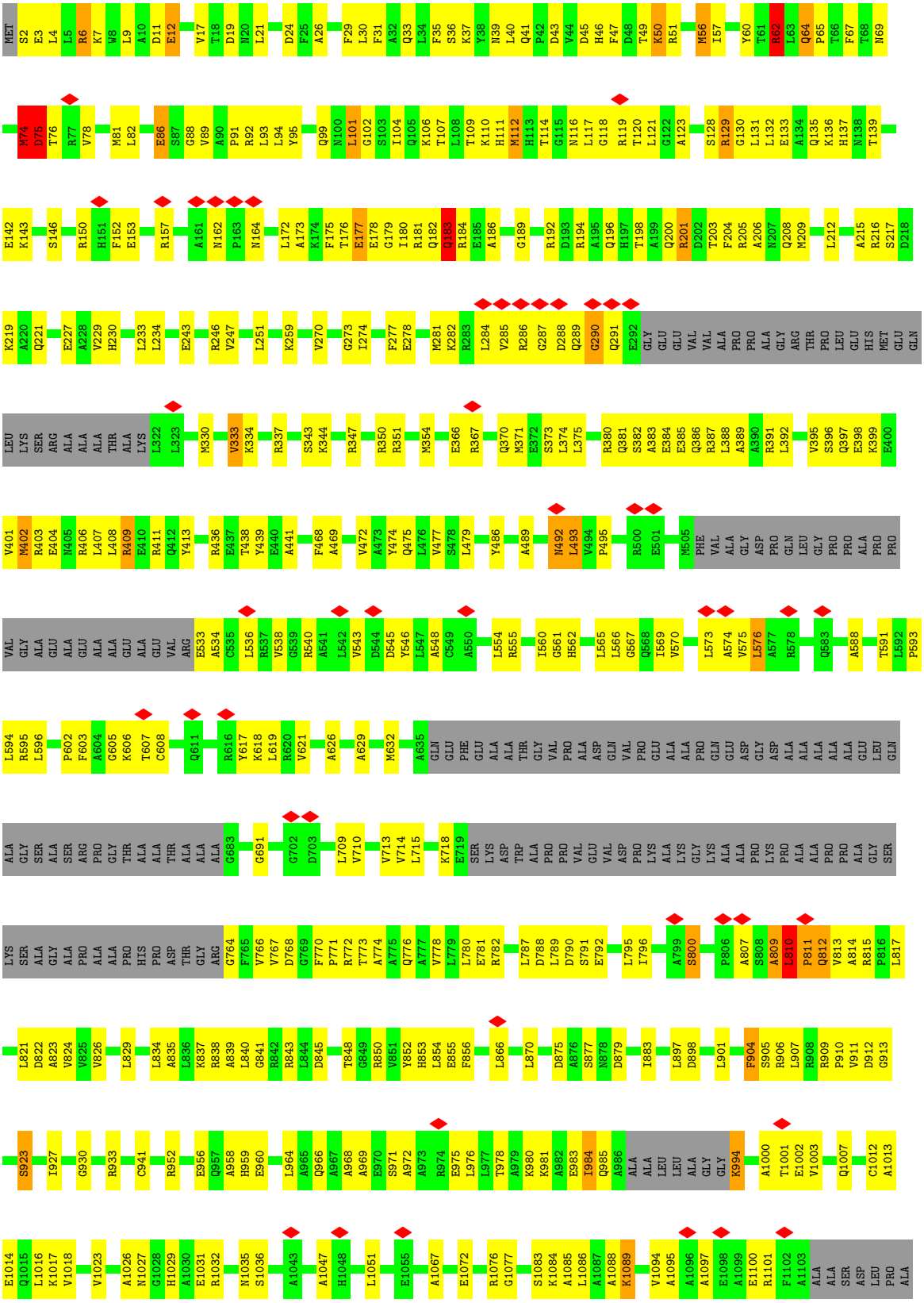


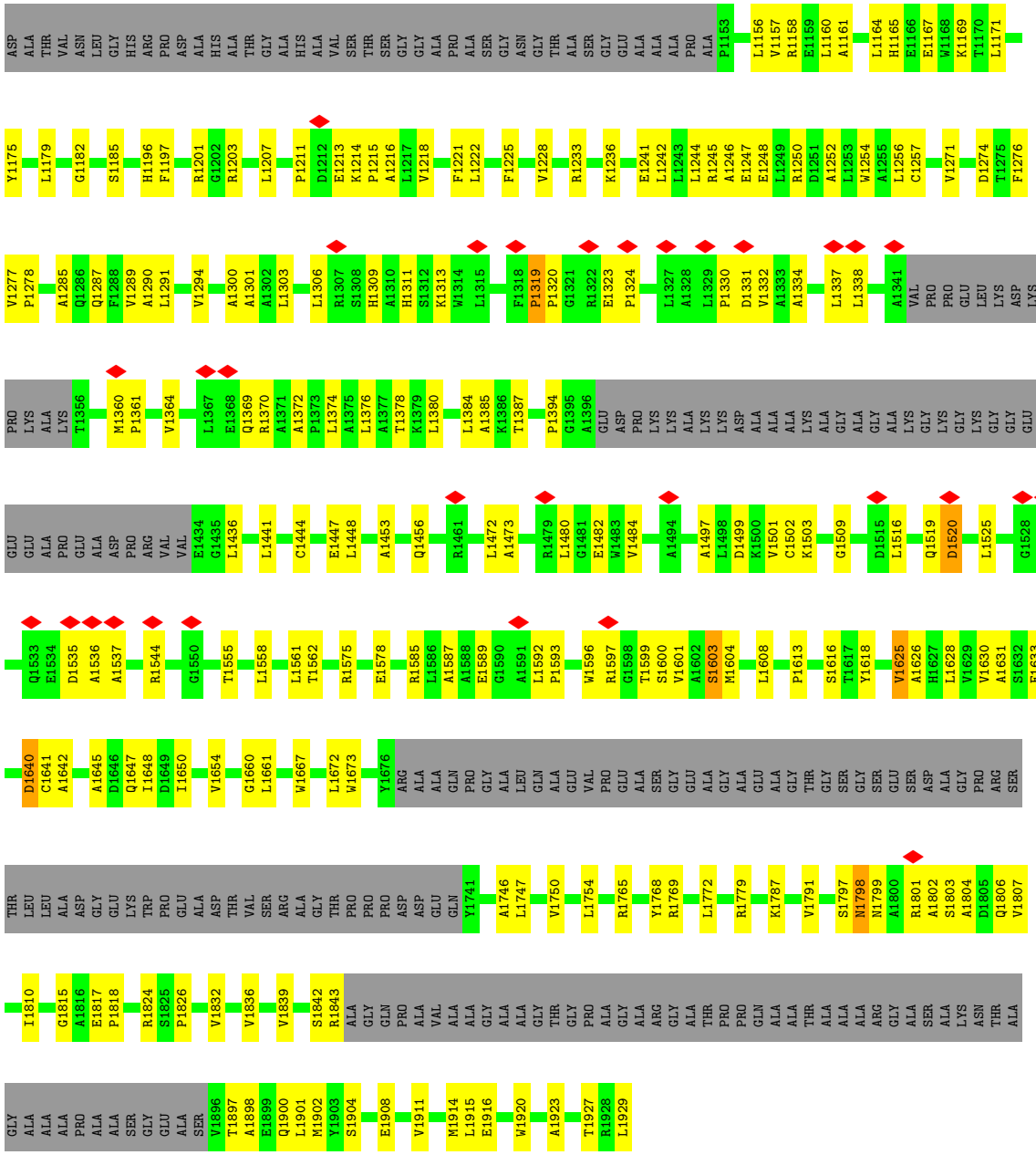


• Molecule 47: CPC1

Chain 6B:


50%
28%
19%

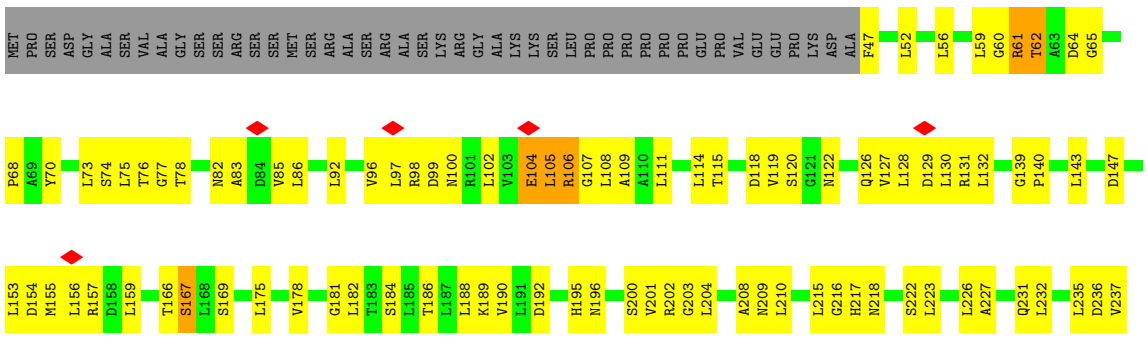

MET S2 E3 L4 L5 R6 K7 W8 L9 A10 D11 E12 V17 T18 D19 N20 L21 D24 F25 A26 F29 L30 F31 A32 Q33 L34 F35 S36 K37 Y38 N39 L40 Q41 F42 D43 V44 D45 H46 F47 D48 T49 K50 R51 M56 I57 Y60 T61 R62 L63 Q64 P65 T66 F67 T68 N69
M74 D75 T76 R77 V78 M81 L82 E86 S87 G88 V89 A90 P91 R92 L93 L94 Y95 Q99 N100 L101 G102 S103 I104 Q105 K106 T107 L108 T109 K110 H111 M112 H113 T114 G115 N116 L117 G118 R119 T120 L121 G122 A123 S128 R129 G130 L131 L132 E133 A134 Q135 K136 H137 N138 T139
E142 K143 S146 R150 H151 F152 E153 R157 A161 N162 P163 N164 L172 A173 K174 F175 T176 E177 E178 G179 I180 R181 Q182 Q183 R184 E185 A186 G189 R192 D193 R194 A195 Q196 H197 T198 A199 Q200 R201 D202 T203 F204 R205 A206 N207 Q208 M209 L212 A215 R216 S217 D218
K219 A220 Q221 E227 A228 V229 H230 L233 L234 E243 R246 V247 L251 K259 V270 G273 I274 F277 E278 M281 K282 R283 L284 V285 R286 G287 D288 Q289 G290 Q291 E292 GLY GLU GLU VAL VAL ALA PRO PRO ALA GLY ARG THR PRO LEU GLU HIS MET GLU GLN
LEU LYS SER ARG ALA ALA ALA THR ALA LYS L322 L323 M330 V333 K334 R337 S343 K344 R347 R350 R351 M354 E366 R367 Q370 M371 E372 S373 L374 L375 R380 Q381 S382 A383 E384 E385 Q386 R387 L388 A389 A390 R391 L392 V395 S396 Q397 E398 K399 E400
V401 M402 R403 E404 N405 R406 L407 L408 R409 E410 R411 Q412 Y413 R436 E437 T438 Y439 E440 A441 F468 A469 V472 A473 Y474 Q475 L476 V477 S478 L479 Y486 A489 N492 L493 V494 P495 R500 E501 M505 PHE VAL ALA GLY ASP PRO GLN LEU GLY PRO PRO ALA PRO PRO
VAL GLY ALA GLU ALA ALA GLU ALA ALA GLU ALA GLU VAL ARG E533 A534 C535 L536 R537 V538 G539 R540 A541 L542 V543 D544 D545 Y546 L547 A548 C549 A550 L554 R555 I560 G561 H562 L565 L566 G567 Q568 I569 V570 L573 A574 V575 L576 A577 R578 Q583 A588 T591 L592 P593
L594 R595 L596 P602 F603 A604 G605 K606 T607 C608 Q611 R616 Y617 K618 L619 R620 V621 A626 A629 M632 A635 GLN GLU PHE GLU ALA ALA ALA THR GLY VAL PRO ALA ASP GLN VAL PRO GLU ALA ALA ALA PRO GLN GLU ASP GLY ASP ALA ALA ALA ALA ALA GLU LEU GLN
ALA GLY SER ALA SER ARG PRO GLY THR ALA ALA THR ALA ALA ALA G683 G691 G702 D703 L709 V710 V713 V714 L715 K718 E719 SER LYS ASP TRP ALA PRO PRO VAL GLU VAL ASP PRO LYS ALA ALA LYS GLY LYS ALA ALA PRO LYS PRO ALA ALA ALA PRO PRO ALA GLY SER
LYS SER ALA GLY ALA PRO ALA PRO HIS PRO ASP THR GLY ARG G764 F765 V766 V767 D768 G769 F770 P771 R772 T773 A774 A775 Q776 A777 V778 L779 L780 E781 R782 L787 D788 L789 D790 S791 E792 L795 I796 A799 S800 P806 A807 S808 A809 L810 P811 Q812 V813 A814 R815 P816 L817
L821 D822 A823 V824 V825 V826 L829 L834 A835 L836 K837 R838 A839 L840 C841 R842 R843 L844 D845 T848 G849 R850 V851 Y852 H853 L854 E855 F856 L866 L870 D875 A876 S877 N878 D879 I883 L897 D898 L901 F904 S905 R906 L907 R908 R909 P910 V911 D912 G913
S923 I927 G930 R933 C941 R952 E956 Q957 A958 H959 E960 L964 A965 Q966 A967 A968 A969 E970 S971 A972 A973 R974 E975 L976 L977 T978 A979 K980 K981 A982 E983 I984 Q985 A986 ALA ALA LEU LEU ALA GLY GLY K994 A1000 T1001 E1002 V1003 Q1007 C1012 A1013
E1014 Q1015 L1016 K1017 V1018 V1023 A1026 N1027 G1028 H1029 A1030 E1031 R1032 N1035 S1036 A1043 A1047 H1048 L1051 E1055 A1067 E1072 R1076 G1077 S1083 K1084 A1085 L1086 A1087 A1088 K1089 V1094 A1095 A1096 A1097 E1098 A1099 E1100 R1101 F1102 A1103 ALA ALA SER ASP LEU PRO ALA

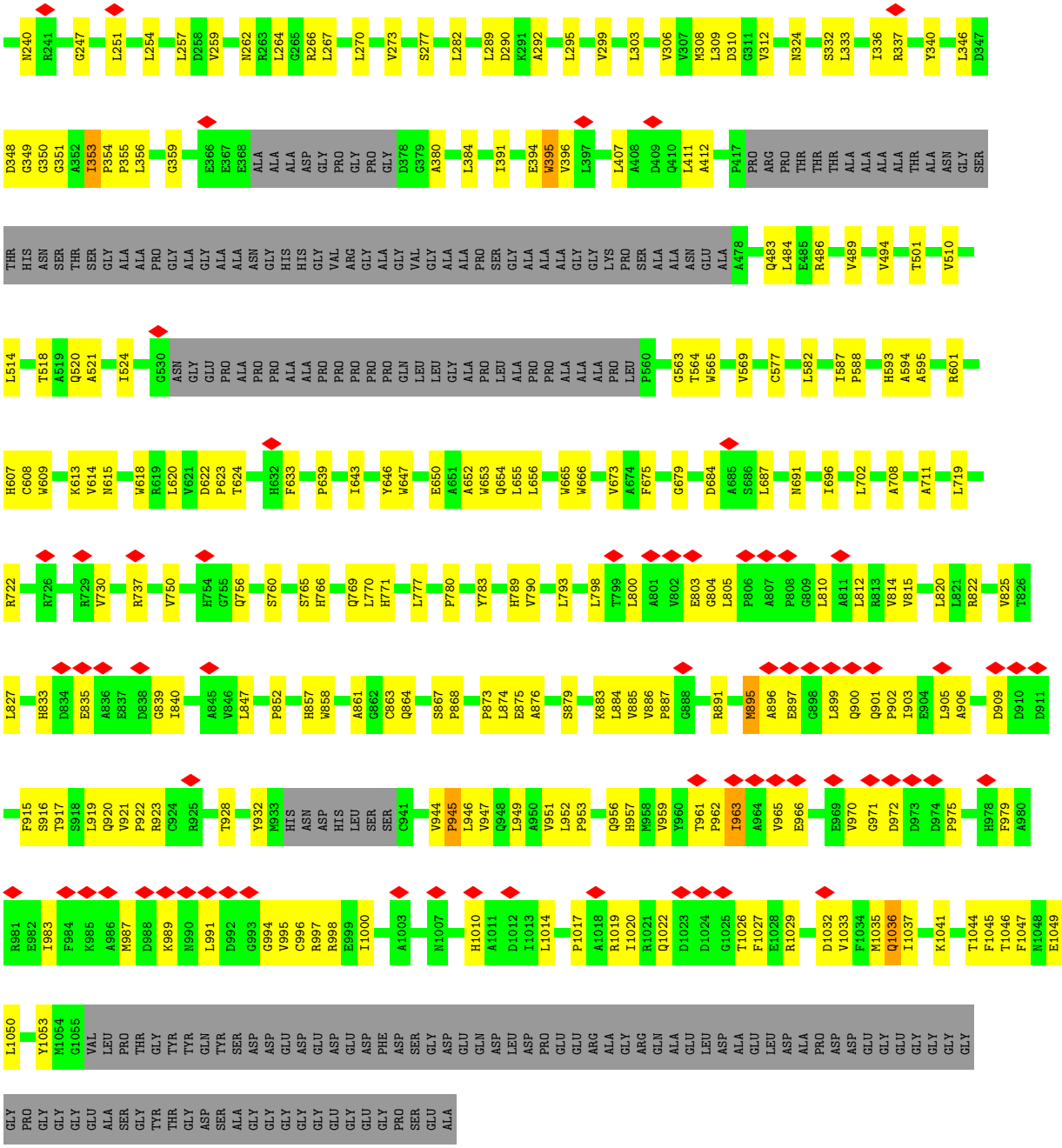


• Molecule 48: FAP246

Chain 6E:

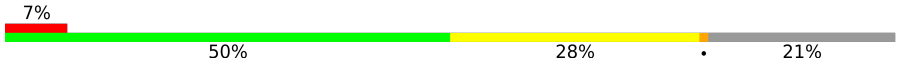


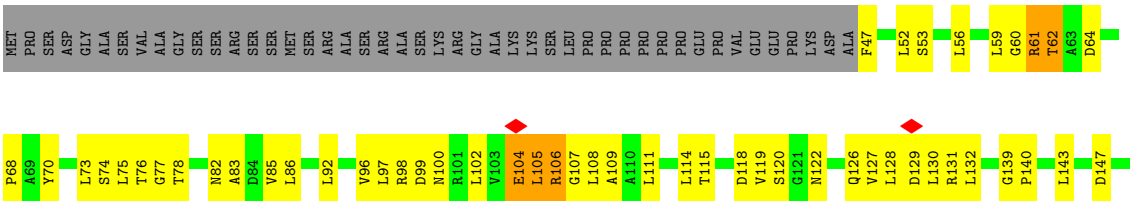


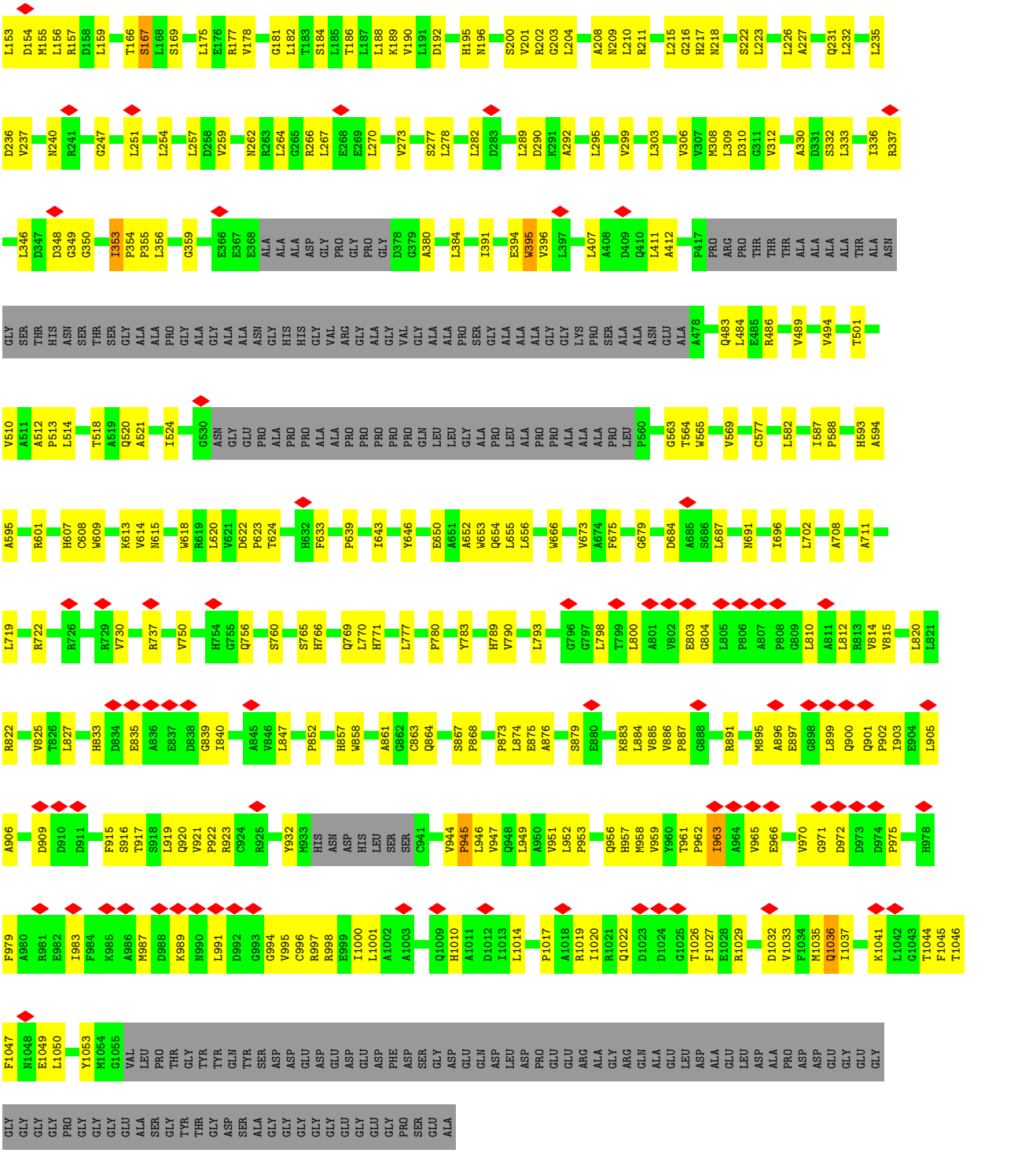


• Molecule 48: FAP246

Chain 6F:



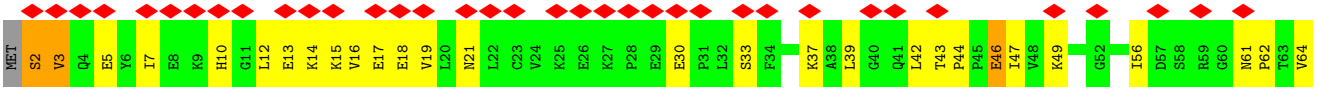


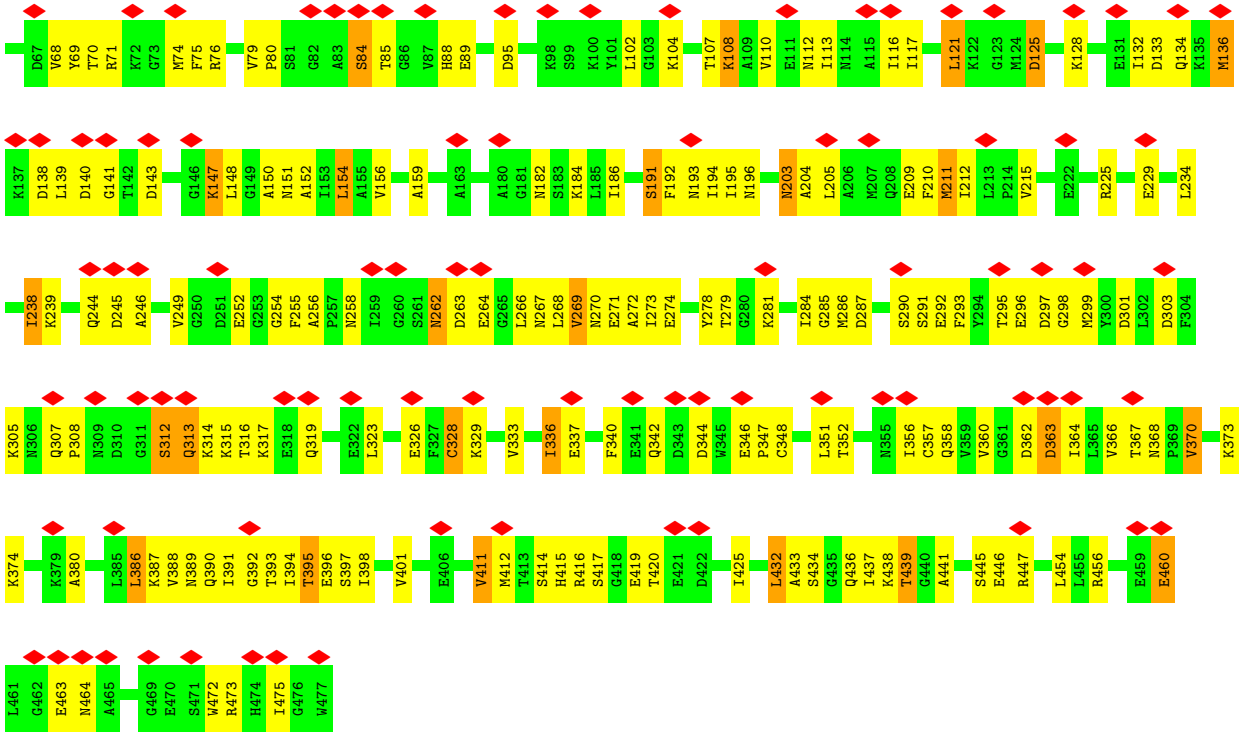


• Molecule 49: Phosphopyruvate hydratase

Chain 6G:



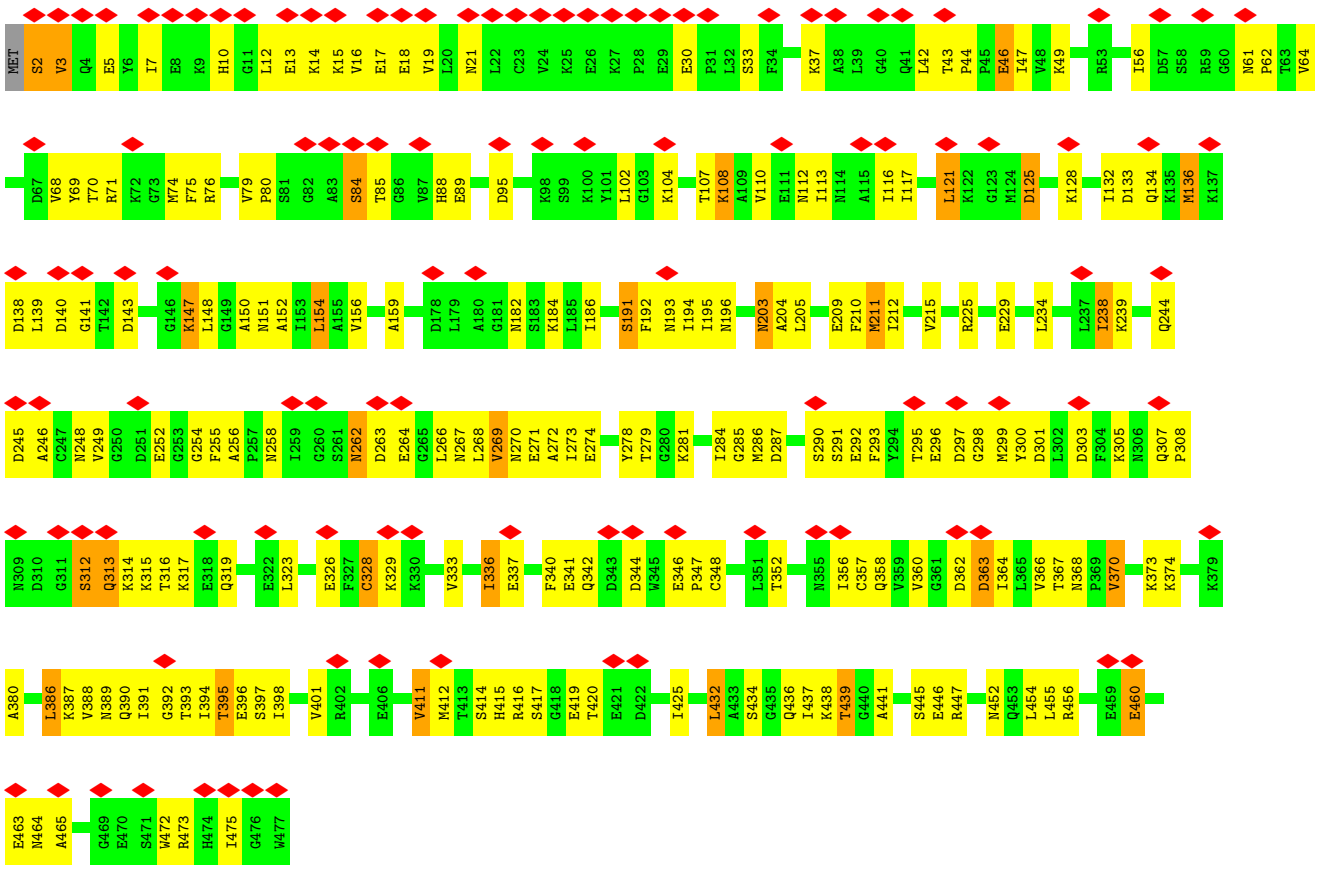




• Molecule 49: Phosphopyruvate hydratase

Chain 6H:





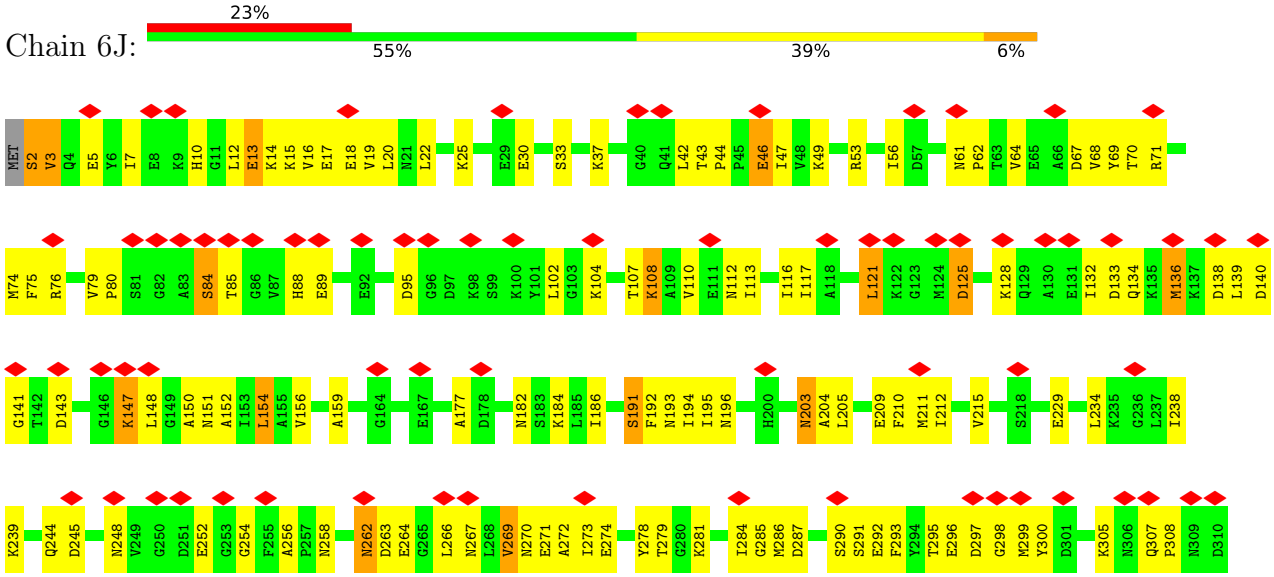
• Molecule 49: Phosphopyruvate hydratase

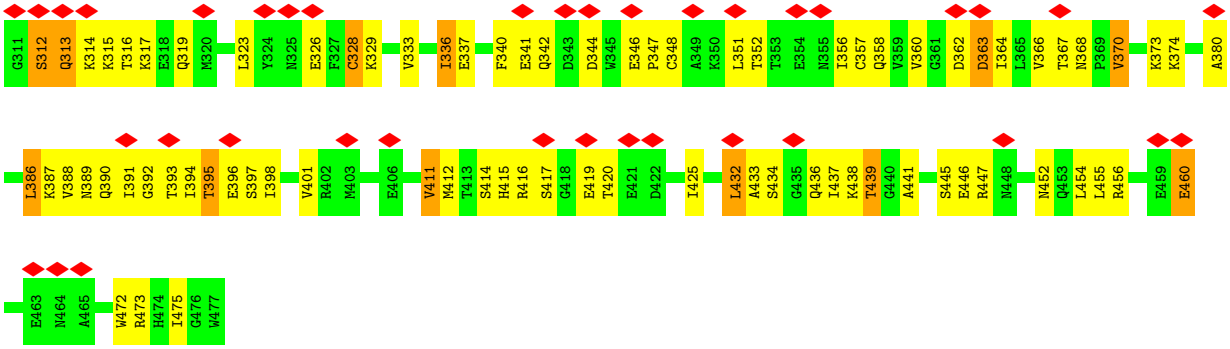
Chain 6I:



• Molecule 49: Phosphopyruvate hydratase

Chain 6J:

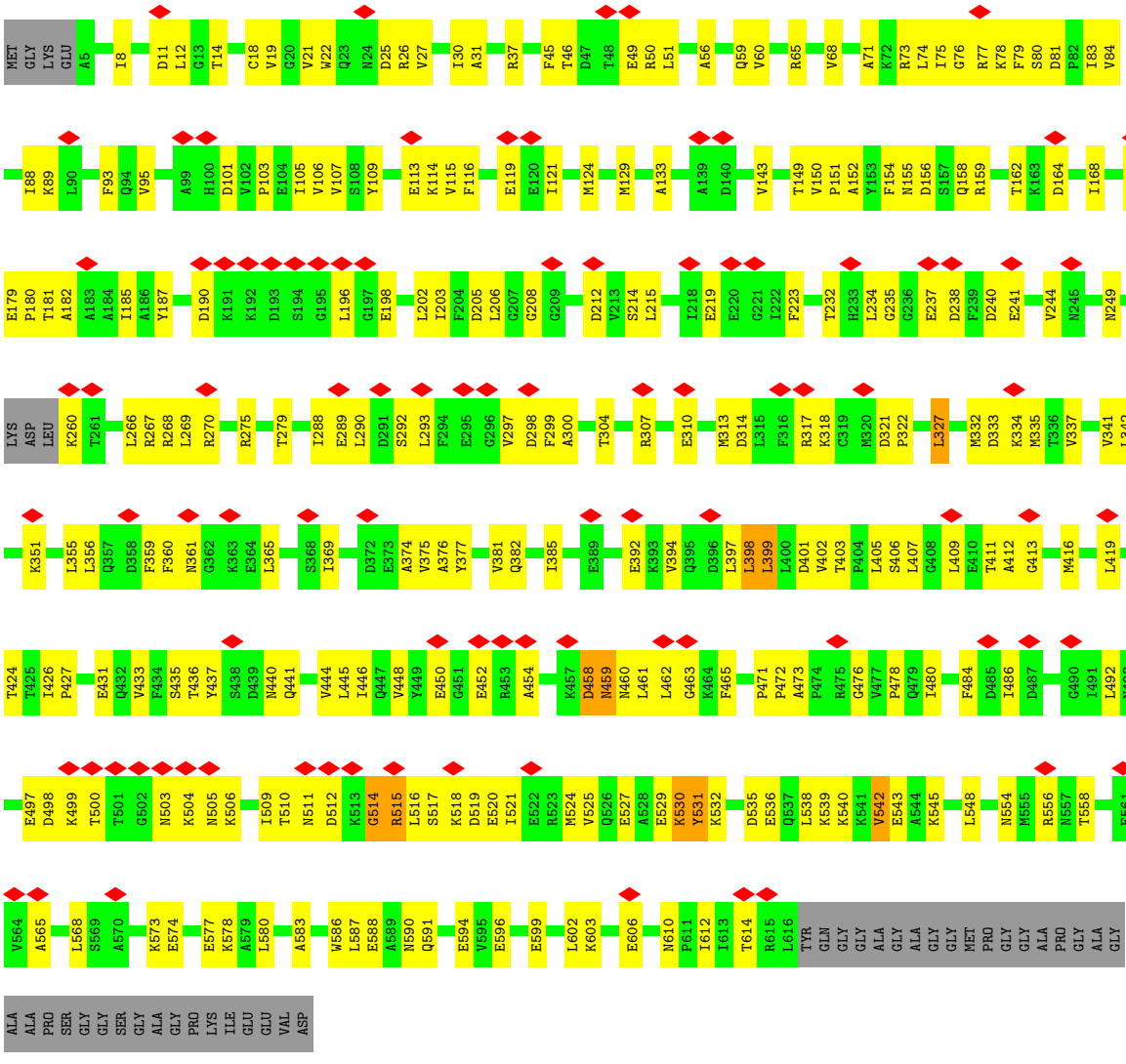




• Molecule 50: Heat shock protein 70A

Chain 6K:

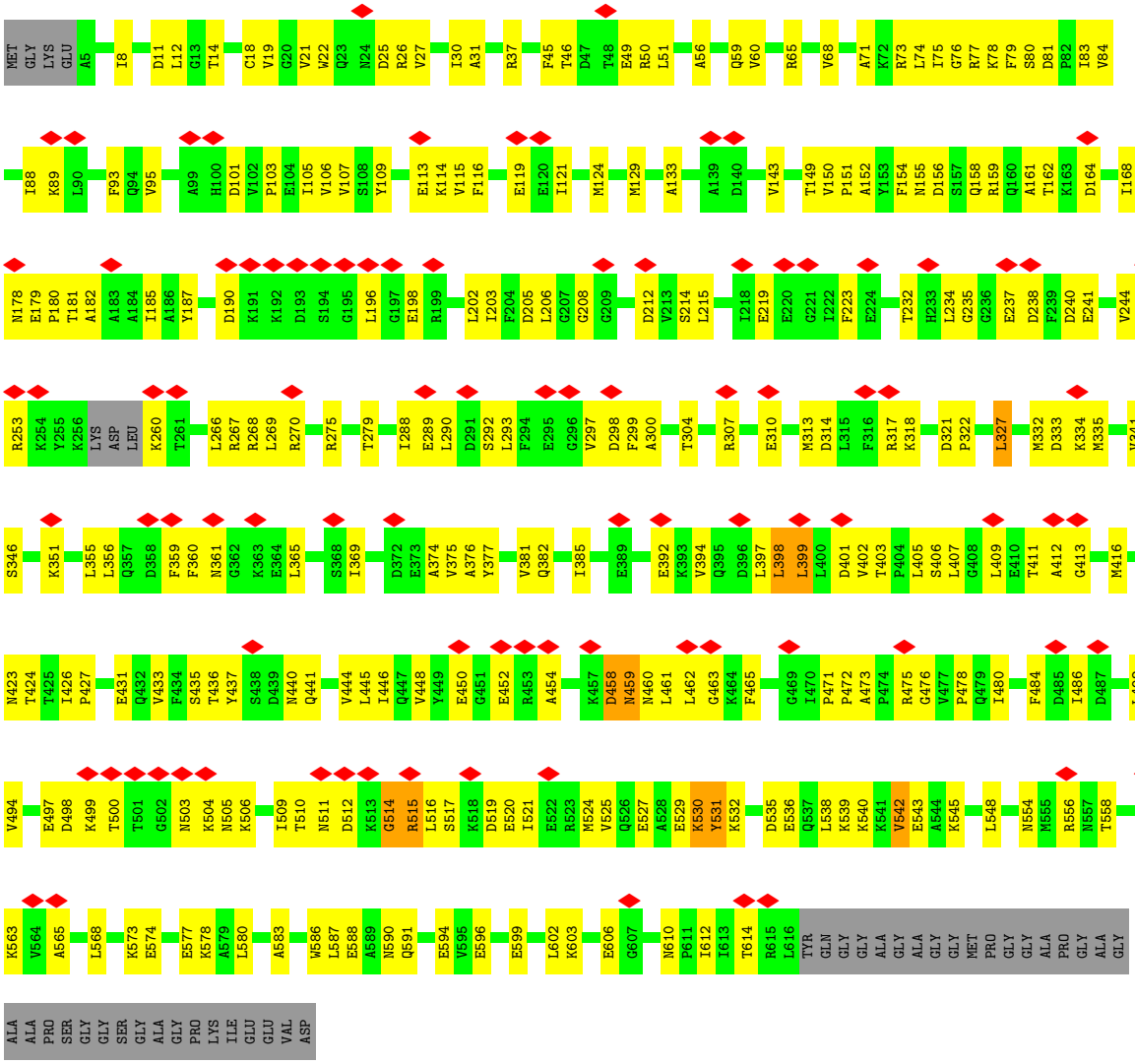




• Molecule 50: Heat shock protein 70A

Chain 6L:

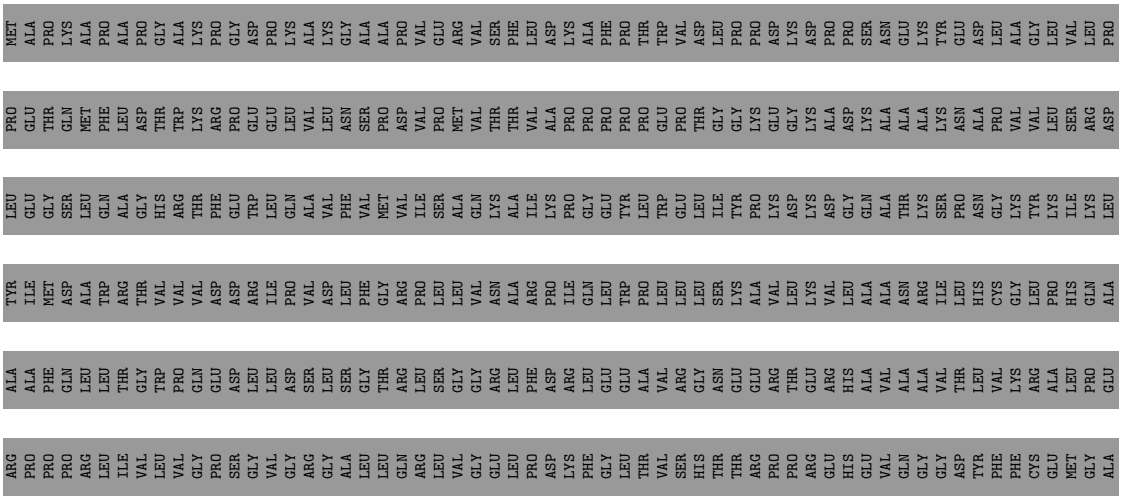


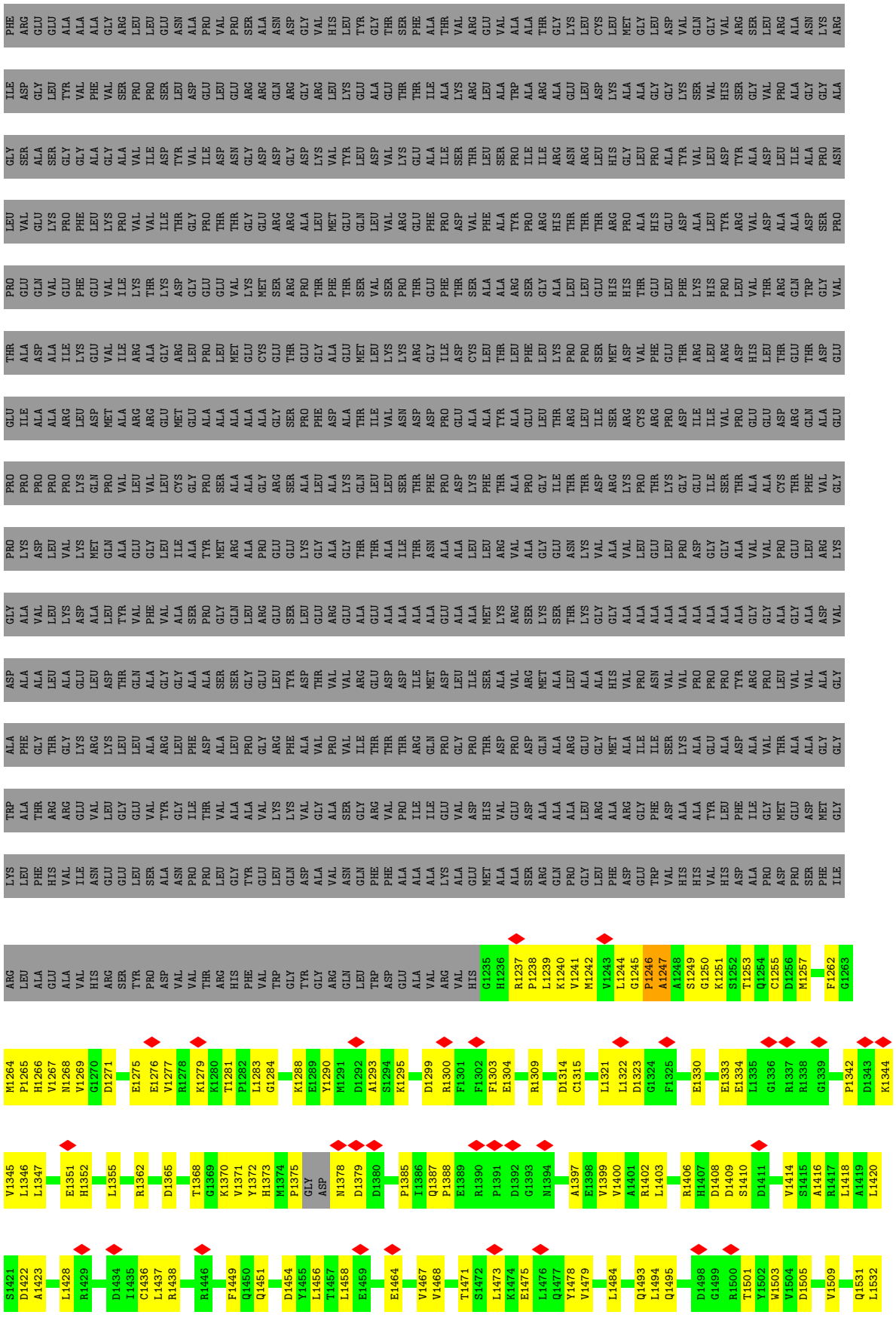


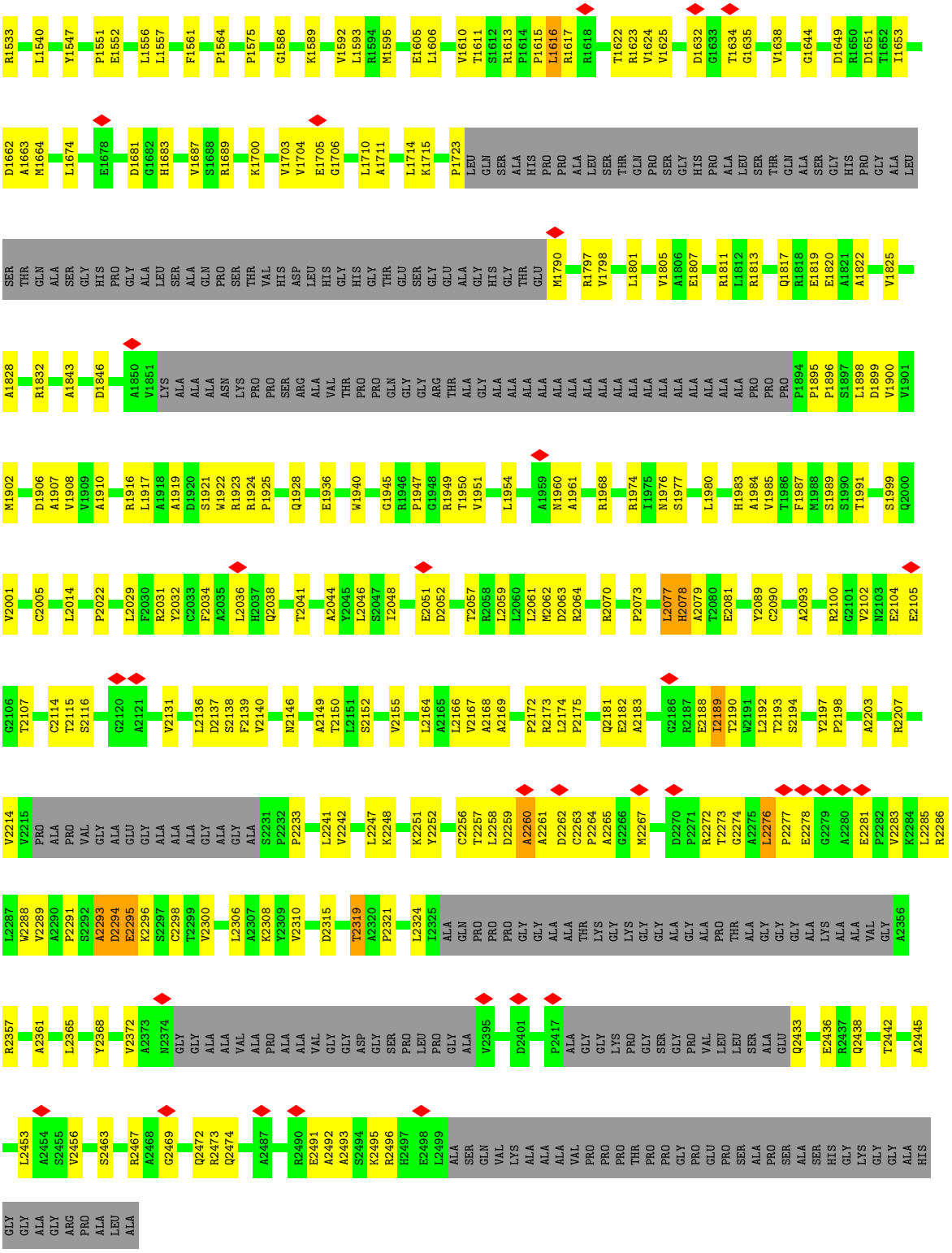
• Molecule 51: FAP42

Chain 6M:







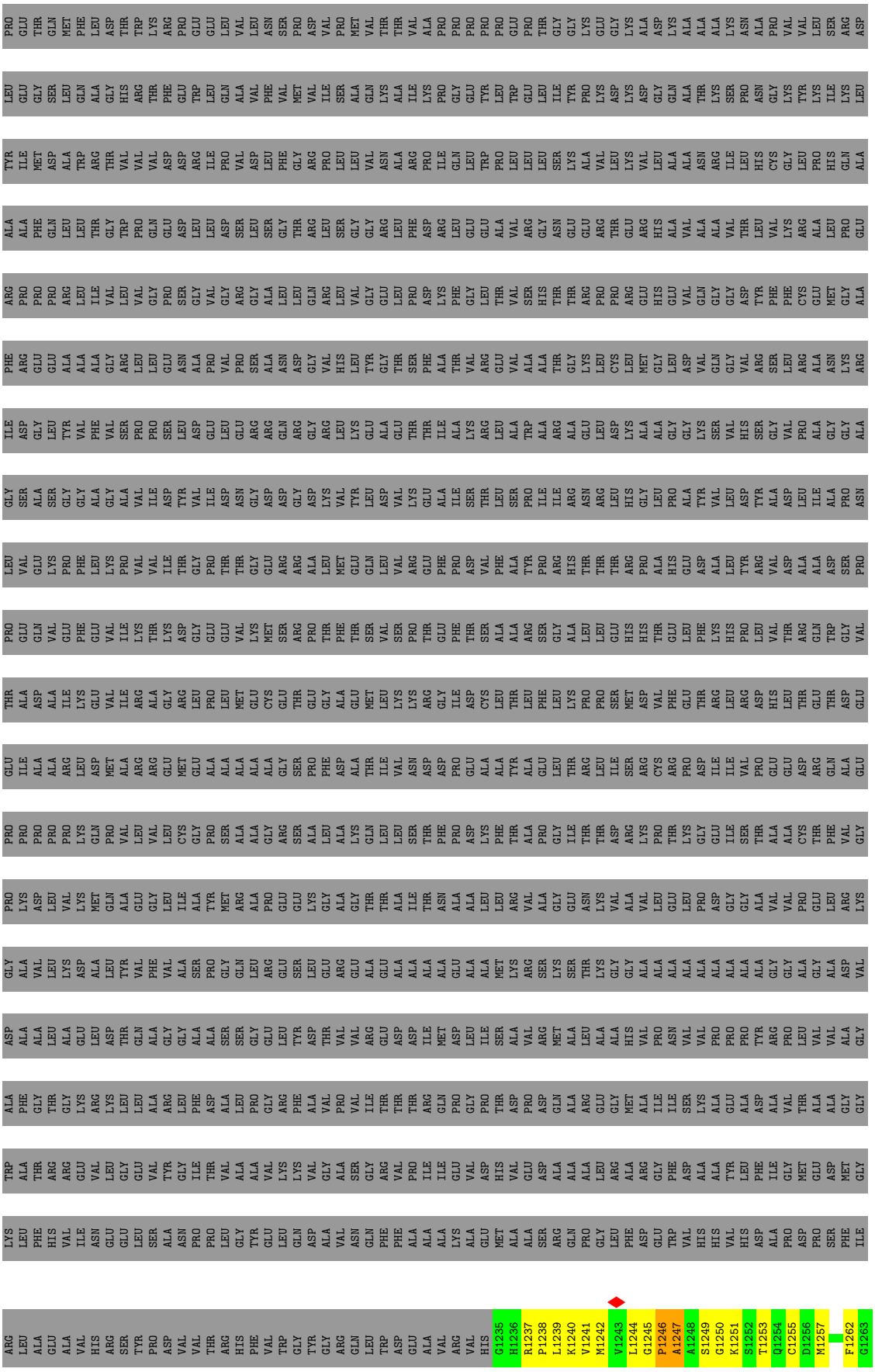


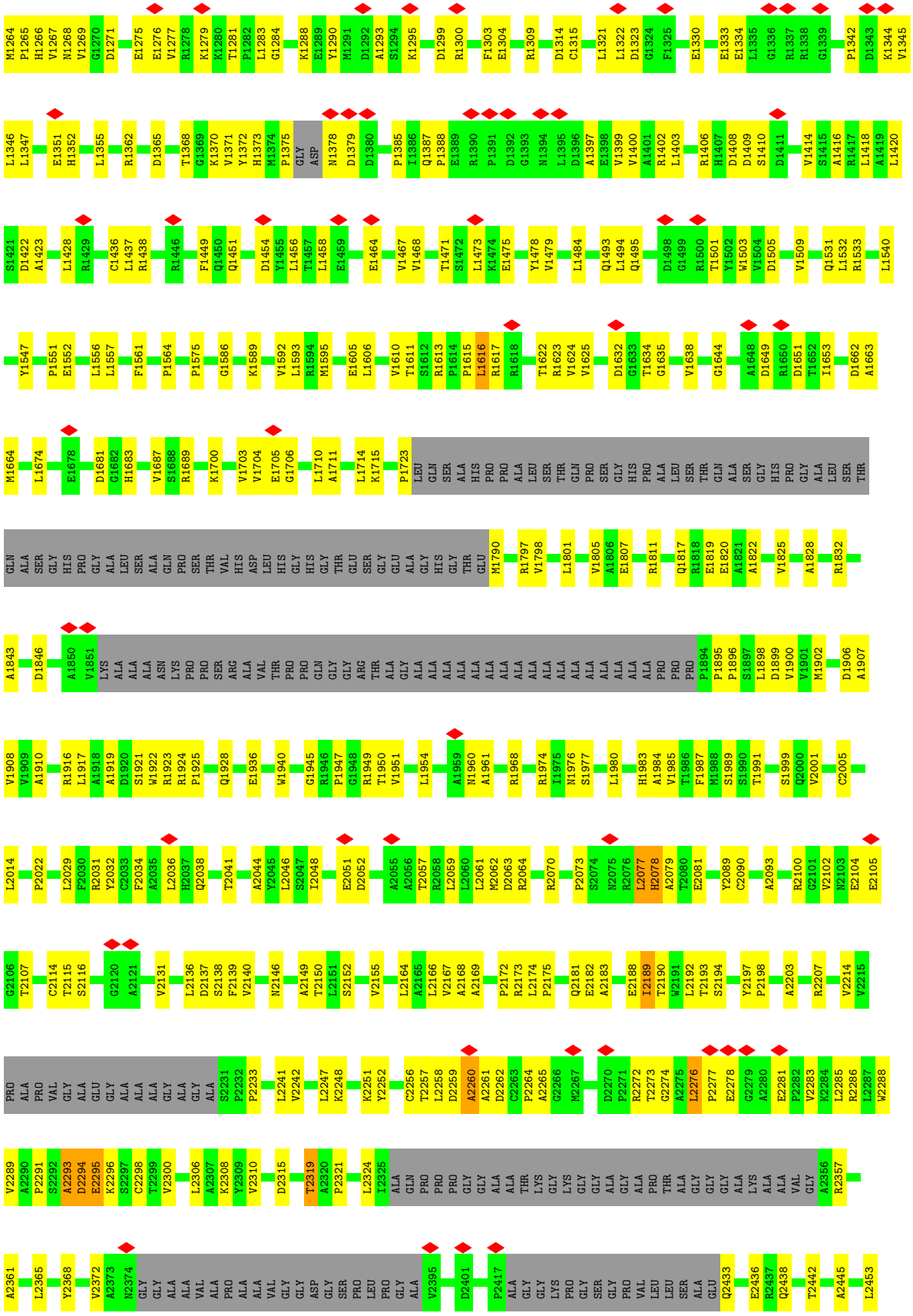
• Molecule 51: FAP42

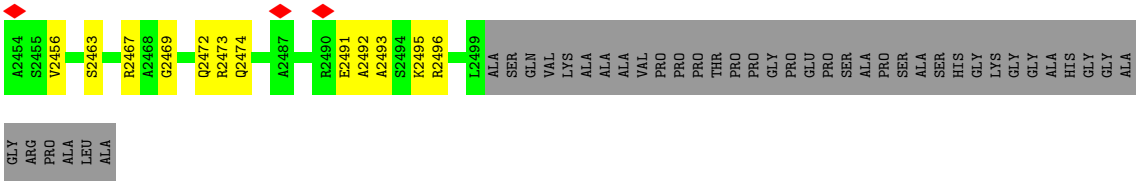
Chain 6N:





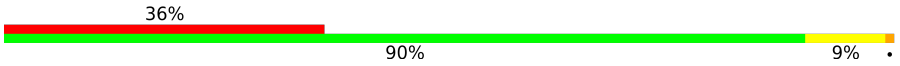

G1235
H1236
R1237
P1238
L1239
K1240
V1241
M1242
V1243
L1244
G1245
P1246
A1247
A1248
S1249
G1250
K1251
S1252
T1253
Q1254
C1255
D1256
M1257
F1262
G1263

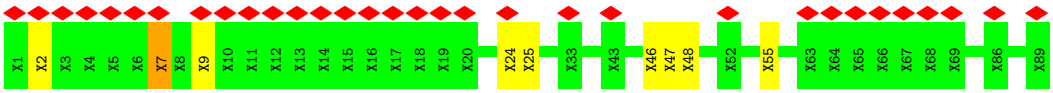




• Molecule 52: Unknown protein

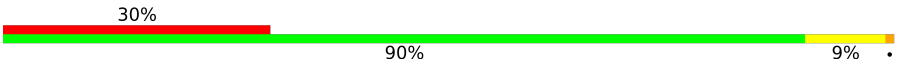
Chain 6O:

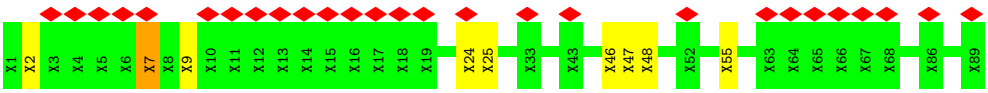




• Molecule 52: Unknown protein

Chain 6P:

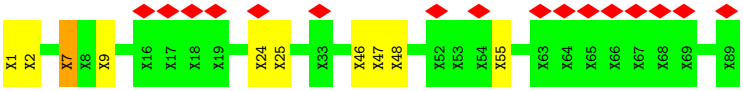




• Molecule 52: Unknown protein

Chain 6Q:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	190727	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	38.6	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	9.598	Depositor
Minimum map value	0.000	Depositor
Average map value	0.037	Depositor
Map value standard deviation	0.103	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	1169.0691, 795.33936, 764.7494	wwPDB
Map dimensions	879, 598, 575	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.329999, 1.329999, 1.329999	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, GTP

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	0A	0.31	0/3578	0.49	1/4885 (0.0%)
1	0B	0.23	0/3578	0.47	0/4885
1	0C	0.20	0/3578	0.42	0/4885
1	0D	0.21	0/3578	0.45	0/4885
1	0E	0.26	0/3578	0.46	1/4885 (0.0%)
1	0F	0.26	0/3578	0.47	1/4885 (0.0%)
1	0G	0.22	0/3578	0.43	0/4885
1	0H	0.21	0/3578	0.45	0/4885
1	0I	0.21	0/3578	0.42	0/4885
1	0J	0.21	0/3578	0.42	0/4885
1	0K	0.21	0/3574	0.41	0/4881
1	0L	0.22	0/3578	0.44	0/4885
1	0M	0.20	0/3578	0.42	0/4885
1	0N	0.25	0/3578	0.47	1/4885 (0.0%)
1	0O	0.21	0/3578	0.43	0/4885
1	0P	0.21	0/3578	0.44	0/4885
1	0Q	0.23	0/3578	0.45	0/4885
1	0R	0.28	0/3575	0.47	1/4880 (0.0%)
1	0S	0.21	0/3578	0.43	0/4885
1	0T	0.20	0/3578	0.41	0/4885
1	0U	0.20	0/3578	0.42	0/4885
1	0V	0.22	0/3578	0.43	0/4885
1	0W	0.22	0/3578	0.43	0/4885
1	0X	0.23	0/3578	0.44	1/4885 (0.0%)
1	0Y	0.22	0/3578	0.47	0/4885
1	0Z	0.21	0/3578	0.43	0/4885
1	1A	0.22	0/3578	0.45	0/4885
1	1B	0.28	0/3578	0.48	0/4885
1	1C	0.22	0/3574	0.43	0/4881
2	1D	0.25	0/3240	0.60	4/4420 (0.1%)
2	1E	0.25	0/3240	0.58	3/4420 (0.1%)
2	1F	0.28	1/3319 (0.0%)	0.65	5/4529 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
2	1G	0.24	0/3319	0.60	4/4529 (0.1%)
3	1H	0.33	1/5878 (0.0%)	0.56	10/8010 (0.1%)
3	1I	0.21	0/5878	0.43	0/8010
3	6D	0.31	1/6127 (0.0%)	0.50	8/8328 (0.1%)
4	1J	0.23	0/2918	0.59	6/3984 (0.2%)
4	1K	0.23	0/2918	0.59	6/3984 (0.2%)
5	1L	0.22	0/3404	0.56	1/4660 (0.0%)
5	1M	0.22	0/3404	0.56	1/4660 (0.0%)
6	1N	0.23	1/16403 (0.0%)	0.46	5/22333 (0.0%)
7	1O	0.21	0/19999	0.44	1/27280 (0.0%)
8	1P	0.22	0/2329	0.49	1/3190 (0.0%)
9	1Q	0.30	0/2347	0.86	13/3241 (0.4%)
10	1R	0.28	0/2816	0.56	0/3832
10	1S	0.37	0/2034	0.72	5/2779 (0.2%)
11	1T	0.14	0/4794	0.25	0/6657
12	1a	0.21	0/3433	0.43	2/4646 (0.0%)
12	1c	0.17	0/3453	0.38	0/4673
12	1e	0.21	0/3433	0.42	2/4646 (0.0%)
12	1g	0.17	0/3453	0.38	0/4673
12	2a	0.19	0/3433	0.42	2/4646 (0.0%)
12	2c	0.17	0/3453	0.37	0/4673
12	2e	0.20	0/3433	0.41	2/4646 (0.0%)
12	2g	0.18	0/3453	0.38	0/4673
12	3a	0.29	3/3433 (0.1%)	0.45	2/4646 (0.0%)
12	3c	0.17	0/3453	0.37	0/4673
12	3e	0.20	0/3433	0.40	2/4646 (0.0%)
12	3g	0.17	0/3453	0.37	0/4673
12	4a	0.25	0/3433	0.45	2/4646 (0.0%)
12	4c	0.17	0/3453	0.38	0/4673
12	4e	0.18	0/3433	0.41	0/4646
12	4g	0.16	0/3453	0.36	0/4673
12	5a	0.22	0/3433	0.45	2/4646 (0.0%)
12	5c	0.17	0/3453	0.37	0/4673
12	5e	0.22	0/3433	0.43	0/4646
12	5g	0.16	0/3453	0.37	0/4673
12	6a	0.22	0/3433	0.43	0/4646
12	6c	0.17	0/3453	0.38	0/4673
12	6e	0.24	0/3433	0.47	2/4646 (0.0%)
12	6g	0.17	0/3453	0.37	0/4673
12	7a	0.21	0/3433	0.43	0/4646
12	7c	0.17	0/3453	0.39	0/4673
12	7e	0.23	0/3433	0.46	0/4646
12	7g	0.18	0/3453	0.39	0/4673

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
12	8a	0.22	0/3433	0.42	0/4646
12	8c	0.17	0/3453	0.39	0/4673
12	8e	0.21	0/3433	0.45	2/4646 (0.0%)
12	8g	0.17	0/3453	0.38	0/4673
12	9a	0.23	0/3433	0.46	3/4646 (0.1%)
12	9c	0.16	0/3453	0.37	0/4673
12	9e	0.22	0/3433	0.44	1/4646 (0.0%)
12	9g	0.17	0/3453	0.37	0/4673
12	Aa	0.24	0/3433	0.45	0/4646
12	Ac	0.19	0/3453	0.40	0/4673
12	Ae	0.22	0/3433	0.43	1/4646 (0.0%)
12	Ag	0.16	0/3453	0.37	0/4673
12	Ba	0.23	0/3433	0.45	2/4646 (0.0%)
12	Bc	0.18	0/3453	0.38	0/4673
12	Be	0.23	0/3433	0.45	2/4646 (0.0%)
12	Bg	0.20	0/3453	0.41	0/4673
12	Ca	0.23	0/3433	0.42	0/4646
12	Cc	0.18	0/3453	0.38	0/4673
12	Ce	0.25	0/3433	0.43	1/4646 (0.0%)
12	Cg	0.18	0/3453	0.38	0/4673
12	Da	0.24	0/3433	0.44	2/4646 (0.0%)
12	Dc	0.17	0/3453	0.37	0/4673
12	De	0.20	0/3433	0.42	2/4646 (0.0%)
12	Dg	0.18	0/3453	0.39	0/4673
13	1b	0.17	0/3410	0.36	0/4623
13	1d	0.17	0/3410	0.36	0/4623
13	1f	0.17	0/3410	0.36	0/4623
13	1h	0.16	0/3410	0.36	0/4623
13	2b	0.17	0/3410	0.36	0/4623
13	2d	0.17	0/3410	0.36	0/4623
13	2f	0.17	0/3410	0.36	0/4623
13	2h	0.17	0/3410	0.36	0/4623
13	3b	0.17	0/3410	0.36	0/4623
13	3d	0.17	0/3410	0.36	0/4623
13	3f	0.17	0/3410	0.36	0/4623
13	3h	0.17	0/3410	0.36	0/4623
13	4b	0.17	0/3410	0.36	0/4623
13	4d	0.17	0/3410	0.36	0/4623
13	4f	0.17	0/3410	0.36	0/4623
13	4h	0.17	0/3410	0.36	0/4623
13	5b	0.17	0/3410	0.36	0/4623
13	5d	0.17	0/3410	0.36	0/4623
13	5f	0.17	0/3410	0.36	0/4623

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
13	5h	0.17	0/3410	0.36	0/4623
13	6b	0.17	0/3410	0.36	0/4623
13	6d	0.17	0/3410	0.36	0/4623
13	6f	0.17	0/3410	0.36	0/4623
13	6h	0.17	0/3410	0.36	0/4623
13	7b	0.17	0/3410	0.36	0/4623
13	7d	0.17	0/3410	0.36	0/4623
13	7f	0.17	0/3410	0.36	0/4623
13	7h	0.17	0/3410	0.36	0/4623
13	8b	0.17	0/3410	0.36	0/4623
13	8d	0.17	0/3410	0.36	0/4623
13	8f	0.17	0/3410	0.36	0/4623
13	8h	0.17	0/3410	0.36	0/4623
13	9b	0.16	0/3410	0.36	0/4623
13	9d	0.17	0/3410	0.36	0/4623
13	9f	0.17	0/3410	0.36	0/4623
13	9h	0.17	0/3410	0.36	0/4623
13	Ab	0.17	0/3410	0.36	0/4623
13	Ad	0.17	0/3410	0.36	0/4623
13	Af	0.17	0/3410	0.36	0/4623
13	Ah	0.17	0/3410	0.36	0/4623
13	Bb	0.16	0/3410	0.36	0/4623
13	Bd	0.16	0/3410	0.36	0/4623
13	Bf	0.17	0/3410	0.36	0/4623
13	Bh	0.17	0/3410	0.36	0/4623
13	Cb	0.17	0/3410	0.36	0/4623
13	Cd	0.17	0/3410	0.36	0/4623
13	Cf	0.17	0/3410	0.36	0/4623
13	Ch	0.17	0/3410	0.36	0/4623
13	Db	0.17	0/3410	0.36	0/4623
13	Dd	0.17	0/3410	0.36	0/4623
13	Df	0.17	0/3410	0.36	0/4623
13	Dh	0.17	0/3410	0.36	0/4623
14	2F	0.27	0/1257	0.60	0/1700
14	2G	0.27	0/1257	0.60	0/1700
24	2S	0.18	0/521	0.34	0/726
24	2T	0.30	0/886	0.54	0/1193
24	2U	0.32	0/900	0.54	0/1213
24	2V	0.25	0/886	0.51	0/1193
28	3C	0.23	0/484	0.43	0/651
29	3E	0.37	0/682	0.58	0/926
30	3F	0.33	3/3405 (0.1%)	0.56	6/4572 (0.1%)
30	3G	0.26	0/1911	0.47	0/2553

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
31	3H	0.20	0/1966	0.32	0/2686
31	3I	0.23	0/3146	0.43	1/4233 (0.0%)
32	3J	0.24	0/2849	0.49	0/3878
32	3K	0.24	0/2824	0.45	0/3845
33	3L	0.26	0/1597	0.45	0/2147
34	3M	0.26	0/3035	0.52	0/4097
34	3N	0.25	0/3089	0.51	1/4173 (0.0%)
34	3O	0.26	0/2819	0.50	0/3798
34	3P	0.26	0/2841	0.49	0/3827
34	3Q	0.25	0/2819	0.48	0/3798
34	3R	0.26	0/2860	0.45	0/3853
34	3S	0.24	0/3035	0.50	0/4097
34	3T	0.27	0/3089	0.54	1/4173 (0.0%)
34	3U	0.27	0/2841	0.47	0/3827
34	3V	0.24	0/3244	0.48	2/4381 (0.0%)
34	3W	0.23	0/3250	0.44	0/4389
34	3X	0.24	0/2860	0.48	0/3853
34	3Y	0.25	0/2860	0.44	1/3853 (0.0%)
34	3Z	0.25	0/2860	0.50	0/3853
34	4A	0.23	0/3244	0.46	3/4381 (0.1%)
34	4B	0.23	0/3250	0.46	2/4389 (0.0%)
35	4C	0.30	0/4954	0.61	1/6754 (0.0%)
36	4D	0.31	0/2424	0.60	4/3278 (0.1%)
37	4E	1.20	61/7406 (0.8%)	1.12	79/10145 (0.8%)
37	4F	1.57	81/7235 (1.1%)	1.36	147/9923 (1.5%)
37	4G	1.34	74/7235 (1.0%)	1.31	137/9923 (1.4%)
37	4H	1.24	71/7235 (1.0%)	1.25	125/9923 (1.3%)
38	4I	1.87	17/501 (3.4%)	2.27	31/681 (4.6%)
38	4J	1.87	18/501 (3.6%)	2.27	31/681 (4.6%)
38	4K	1.87	18/501 (3.6%)	2.27	31/681 (4.6%)
38	4L	1.87	18/501 (3.6%)	2.27	31/681 (4.6%)
38	4M	1.87	17/501 (3.4%)	2.27	31/681 (4.6%)
38	4N	1.87	18/501 (3.6%)	2.27	31/681 (4.6%)
38	4O	0.40	0/639	0.86	3/876 (0.3%)
38	4P	0.32	0/433	0.60	0/589
39	4Q	0.25	0/1813	0.56	0/2442
39	4R	0.25	0/1813	0.56	0/2442
39	4S	0.24	0/1813	0.56	0/2442
40	4T	0.24	0/4582	0.58	0/6245
40	4U	0.24	0/4582	0.58	0/6245
40	4V	0.24	0/4582	0.58	0/6245
41	4W	0.20	0/595	0.49	0/816
41	4X	0.21	0/595	0.58	0/816

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
41	4Y	0.20	0/595	0.59	0/816
41	4Z	0.22	0/595	0.62	0/816
41	5A	2.66	21/590 (3.6%)	2.45	45/809 (5.6%)
41	5B	0.19	0/590	0.63	0/809
41	5C	0.19	0/590	0.63	0/809
41	5D	0.19	0/590	0.64	0/809
42	5E	0.26	0/1599	0.52	0/2187
42	5F	0.26	0/1599	0.52	0/2187
42	5G	0.26	0/1599	0.52	0/2187
42	5H	3.22	63/1345 (4.7%)	2.24	75/1833 (4.1%)
43	5I	1.56	30/1631 (1.8%)	1.54	37/2219 (1.7%)
43	5J	1.56	30/1631 (1.8%)	1.54	35/2219 (1.6%)
43	5K	1.56	30/1631 (1.8%)	1.54	37/2219 (1.7%)
43	5L	1.56	30/1631 (1.8%)	1.54	37/2219 (1.7%)
44	5M	0.20	0/698	0.43	0/969
44	5N	0.20	0/698	0.43	0/969
44	5O	0.20	0/698	0.43	0/969
44	5P	0.24	0/1166	0.46	0/1563
44	5Q	0.25	0/1166	0.46	0/1563
44	5R	0.25	0/1166	0.47	0/1563
44	5S	0.23	0/1157	0.49	1/1551 (0.1%)
44	5T	0.24	0/1157	0.49	1/1551 (0.1%)
44	5U	0.26	0/1157	0.53	2/1551 (0.1%)
44	5V	0.26	0/1178	0.47	0/1580
46	5Z	0.19	0/270	0.37	0/367
47	6A	0.31	0/12005	0.74	15/16230 (0.1%)
47	6B	0.31	0/12005	0.74	15/16230 (0.1%)
48	6E	0.23	0/7053	0.58	4/9607 (0.0%)
48	6F	0.23	0/7053	0.58	4/9607 (0.0%)
49	6G	0.28	0/3663	0.67	1/4941 (0.0%)
49	6H	0.28	0/3663	0.67	1/4941 (0.0%)
49	6I	0.28	0/3663	0.67	1/4941 (0.0%)
49	6J	0.28	0/3663	0.67	1/4941 (0.0%)
50	6K	0.24	0/4798	0.58	0/6478
50	6L	0.24	0/4798	0.58	0/6478
51	6M	0.23	0/8204	0.54	1/11178 (0.0%)
51	6N	0.23	0/8204	0.54	1/11178 (0.0%)
52	6O	0.21	0/33	0.93	0/44
52	6P	0.22	0/33	0.93	0/44
52	6Q	0.21	0/33	0.93	0/44
All	All	0.41	607/793581 (0.1%)	0.56	1126/1077552 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	0B	0	1
1	0D	0	1
1	0F	0	1
1	0G	0	1
1	0I	0	1
1	0K	0	1
1	0M	0	1
1	0O	0	1
1	0Q	0	1
1	0S	0	1
1	0U	0	1
1	0V	0	1
1	0W	0	1
1	0Y	0	1
1	1A	0	1
1	1C	0	1
2	1D	0	4
2	1E	0	4
2	1F	0	4
2	1G	0	4
3	1H	0	3
3	1I	0	3
3	6D	0	2
4	1J	0	7
4	1K	0	7
5	1L	0	8
5	1M	0	8
6	1N	0	2
7	1O	0	8
8	1P	0	1
9	1Q	0	16
10	1R	0	4
10	1S	0	7
11	1T	0	2
12	1a	0	1
12	1e	0	1
12	2a	0	1
12	2e	0	1
12	3e	0	1
12	5e	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
12	6a	0	1
12	6e	0	1
12	7a	0	1
12	7e	0	1
12	8a	0	1
12	8e	0	1
12	9a	0	1
12	Aa	0	1
12	Be	0	1
12	Ce	0	1
12	Da	0	1
14	2F	0	2
14	2G	0	2
15	2H	0	10
16	2I	0	4
17	2J	0	7
17	2K	0	4
18	2L	0	7
20	2N	0	1
21	2O	0	3
22	2P	0	3
23	2R	0	1
24	2T	0	1
24	2U	0	1
24	2V	0	1
25	2W	0	3
25	2X	0	2
30	3F	0	2
31	3I	0	1
32	3J	0	3
32	3K	0	2
33	3L	0	2
35	4C	0	8
36	4D	0	1
37	4E	0	18
37	4F	0	20
37	4G	1	24
37	4H	0	25
38	4I	0	8
38	4J	0	8
38	4K	0	8
38	4L	0	8

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Mol	Chain	#Chirality outliers	#Planarity outliers
38	4M	0	8
38	4N	0	8
38	4O	0	4
38	4P	0	1
40	4T	0	8
40	4U	0	8
40	4V	0	8
41	4X	0	1
41	4Y	0	1
41	4Z	0	1
41	5A	0	7
41	5B	0	1
41	5C	0	1
41	5D	0	1
42	5H	0	13
43	5I	0	5
43	5J	0	5
43	5K	0	5
43	5L	0	5
44	5V	0	1
45	5W	0	2
45	5X	0	2
45	5Y	0	2
46	5Z	0	2
47	6A	0	12
47	6B	0	12
48	6E	0	6
48	6F	0	6
49	6G	0	1
49	6H	0	1
49	6I	0	1
49	6J	0	1
50	6K	0	5
50	6L	0	5
51	6M	0	6
51	6N	0	6
52	6O	0	4
52	6P	0	4
52	6Q	0	4
All	All	1	491

The worst 5 of 607 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	5H	135	ARG	CB-CG	49.57	3.01	1.52
37	4G	690	CYS	CB-SG	43.99	3.26	1.81
41	5A	120	TYR	CA-C	41.01	2.04	1.52
37	4F	1333	VAL	CA-C	39.93	1.99	1.52
42	5H	137	TYR	CB-CG	39.69	2.38	1.51

The worst 5 of 1126 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	4E	581	LEU	CD1-CG-CD2	-28.75	47.54	110.80
37	4E	581	LEU	CA-C-N	26.39	156.16	120.54
37	4E	581	LEU	C-N-CA	26.39	156.16	120.54
37	4H	1333	VAL	CA-CB-CG1	-24.47	68.80	110.40
37	4H	1082	LEU	CD1-CG-CD2	-23.86	58.31	110.80

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
37	4G	793	THR	CB

5 of 491 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0B	94	GLU	Peptide
1	0D	94	GLU	Peptide
1	0F	94	GLU	Peptide
1	0G	94	GLU	Peptide
1	0M	94	GLU	Peptide

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	0A	3528	0	3398	261	0
1	0B	3528	0	3398	207	0
1	0C	3528	0	3398	160	0
1	0D	3528	0	3398	156	0
1	0E	3528	0	3398	191	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0F	3528	0	3398	181	0
1	0G	3528	0	3398	157	0
1	0H	3528	0	3398	168	0
1	0I	3528	0	3398	166	0
1	0J	3528	0	3398	156	0
1	0K	3524	0	3387	159	0
1	0L	3528	0	3398	152	0
1	0M	3528	0	3398	146	0
1	0N	3528	0	3398	175	0
1	0O	3528	0	3398	149	0
1	0P	3528	0	3398	183	0
1	0Q	3528	0	3398	193	0
1	0R	3526	0	3392	231	0
1	0S	3528	0	3398	150	0
1	0T	3528	0	3398	147	0
1	0U	3528	0	3398	164	0
1	0V	3528	0	3398	168	0
1	0W	3528	0	3398	151	0
1	0X	3528	0	3398	187	0
1	0Y	3528	0	3398	190	0
1	0Z	3528	0	3398	178	0
1	1A	3528	0	3398	177	0
1	1B	3528	0	3398	249	0
1	1C	3524	0	3387	190	0
2	1D	3213	0	2961	142	0
2	1E	3213	0	2961	120	0
2	1F	3292	0	3041	137	0
2	1G	3292	0	3041	105	0
3	1H	5778	0	5643	387	0
3	1I	5778	0	5643	144	0
3	6D	6016	0	6134	304	0
4	1J	2856	0	2628	185	0
4	1K	2856	0	2628	169	0
5	1L	3368	0	2576	140	0
5	1M	3368	0	2576	156	0
6	1N	16109	0	16167	393	0
7	1O	19593	0	19851	345	0
8	1P	2266	0	2195	104	0
9	1Q	2335	0	1383	28	0
10	1R	2753	0	2738	257	0
10	1S	1984	0	1875	209	0
11	1T	4804	0	2553	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	1a	3359	0	3249	141	0
12	1c	3379	0	3265	103	0
12	1e	3359	0	3249	148	0
12	1g	3379	0	3265	108	0
12	2a	3359	0	3249	111	0
12	2c	3379	0	3265	127	0
12	2e	3359	0	3249	115	0
12	2g	3379	0	3265	121	0
12	3a	3359	0	3249	146	0
12	3c	3379	0	3262	117	0
12	3e	3359	0	3249	102	0
12	3g	3379	0	3265	130	0
12	4a	3359	0	3249	133	0
12	4c	3379	0	3265	97	0
12	4e	3359	0	3249	105	0
12	4g	3379	0	3265	89	0
12	5a	3359	0	3249	135	0
12	5c	3379	0	3262	134	0
12	5e	3359	0	3249	143	0
12	5g	3379	0	3265	105	0
12	6a	3359	0	3249	135	0
12	6c	3379	0	3263	114	0
12	6e	3359	0	3247	132	0
12	6g	3379	0	3262	112	0
12	7a	3359	0	3249	147	0
12	7c	3379	0	3265	116	0
12	7e	3359	0	3247	171	0
12	7g	3379	0	3265	120	0
12	8a	3359	0	3249	142	0
12	8c	3379	0	3265	106	0
12	8e	3359	0	3249	127	0
12	8g	3379	0	3265	126	0
12	9a	3359	0	3249	168	0
12	9c	3379	0	3265	113	0
12	9e	3359	0	3247	143	0
12	9g	3379	0	3265	106	0
12	Aa	3359	0	3249	188	0
12	Ac	3379	0	3265	132	0
12	Ae	3359	0	3247	183	0
12	Ag	3379	0	3265	116	0
12	Ba	3359	0	3249	172	0
12	Bc	3379	0	3265	124	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	Be	3359	0	3249	203	0
12	Bg	3379	0	3265	154	0
12	Ca	3359	0	3249	136	0
12	Cc	3379	0	3262	143	0
12	Ce	3359	0	3249	156	0
12	Cg	3379	0	3265	127	0
12	Da	3359	0	3249	134	0
12	Dc	3379	0	3265	95	0
12	De	3359	0	3249	160	0
12	Dg	3379	0	3265	123	0
13	1b	3339	0	3277	142	0
13	1d	3339	0	3277	104	0
13	1f	3339	0	3277	180	0
13	1h	3339	0	3277	101	0
13	2b	3339	0	3277	130	0
13	2d	3339	0	3277	104	0
13	2f	3339	0	3277	121	0
13	2h	3339	0	3277	110	0
13	3b	3339	0	3277	122	0
13	3d	3339	0	3277	115	0
13	3f	3339	0	3277	110	0
13	3h	3339	0	3277	133	0
13	4b	3339	0	3277	107	0
13	4d	3339	0	3277	97	0
13	4f	3339	0	3277	94	0
13	4h	3339	0	3277	108	0
13	5b	3339	0	3277	132	0
13	5d	3339	0	3277	115	0
13	5f	3339	0	3277	113	0
13	5h	3339	0	3277	95	0
13	6b	3339	0	3277	123	0
13	6d	3339	0	3277	124	0
13	6f	3339	0	3277	152	0
13	6h	3339	0	3277	112	0
13	7b	3339	0	3277	104	0
13	7d	3339	0	3277	143	0
13	7f	3339	0	3277	120	0
13	7h	3339	0	3277	124	0
13	8b	3339	0	3277	107	0
13	8d	3339	0	3277	100	0
13	8f	3339	0	3277	152	0
13	8h	3339	0	3277	113	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	9b	3339	0	3277	112	0
13	9d	3339	0	3277	119	0
13	9f	3339	0	3277	107	0
13	9h	3339	0	3277	112	0
13	Ab	3339	0	3277	159	0
13	Ad	3339	0	3277	126	0
13	Af	3339	0	3277	149	0
13	Ah	3339	0	3277	124	0
13	Bb	3339	0	3277	163	0
13	Bd	3339	0	3277	118	0
13	Bf	3339	0	3277	180	0
13	Bh	3339	0	3277	100	0
13	Cb	3339	0	3277	144	0
13	Cd	3339	0	3277	115	0
13	Cf	3339	0	3277	149	0
13	Ch	3339	0	3277	120	0
13	Db	3339	0	3277	140	0
13	Dd	3339	0	3277	116	0
13	Df	3339	0	3277	158	0
13	Dh	3339	0	3277	120	0
14	2F	1228	0	1191	104	0
14	2G	1228	0	1191	84	0
15	2H	980	0	215	34	0
16	2I	540	0	116	14	0
17	2J	500	0	104	19	0
17	2K	500	0	109	12	0
18	2L	270	0	59	8	0
19	2M	90	0	21	1	0
20	2N	260	0	60	10	0
21	2O	235	0	52	8	0
22	2P	530	0	118	21	0
23	2Q	550	0	115	20	0
23	2R	550	0	119	15	0
24	2S	522	0	253	7	0
24	2T	868	0	822	110	0
24	2U	882	0	841	92	0
24	2V	868	0	822	83	0
25	2W	835	0	172	10	0
25	2X	835	0	174	9	0
26	2Y	325	0	67	1	0
26	2Z	325	0	67	1	0
27	3A	180	0	38	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	3B	180	0	38	0	0
28	3C	480	0	479	37	0
29	3E	671	0	603	51	0
30	3F	3386	0	3295	216	0
30	3G	1904	0	1949	130	0
31	3H	1958	0	1625	68	0
31	3I	3118	0	3149	141	0
32	3J	2792	0	2798	179	0
32	3K	2767	0	2778	115	0
33	3L	1572	0	1588	94	0
34	3M	2989	0	2857	199	0
34	3N	3040	0	2941	147	0
34	3O	2775	0	2688	207	0
34	3P	2795	0	2702	204	0
34	3Q	2775	0	2688	159	0
34	3R	2814	0	2718	163	0
34	3S	2989	0	2857	164	0
34	3T	3040	0	2941	204	0
34	3U	2795	0	2702	164	0
34	3V	3192	0	3096	143	0
34	3W	3198	0	3099	150	0
34	3X	2814	0	2718	140	0
34	3Y	2814	0	2718	120	0
34	3Z	2814	0	2718	128	0
34	4A	3192	0	3096	128	0
34	4B	3198	0	3099	142	0
35	4C	4846	0	4828	314	0
36	4D	2372	0	2332	152	0
37	4E	7227	0	7208	1038	0
37	4F	7056	0	7016	1088	0
37	4G	7056	0	7018	1073	0
37	4H	7056	0	7019	993	0
38	4I	491	0	510	263	0
38	4J	491	0	510	192	0
38	4K	491	0	510	232	0
38	4L	491	0	509	552	0
38	4M	491	0	509	587	0
38	4N	491	0	510	646	0
38	4O	626	0	632	79	0
38	4P	424	0	429	38	0
39	4Q	1778	0	1814	115	0
39	4R	1778	0	1814	79	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	4S	1778	0	1814	133	0
40	4T	4494	0	4484	186	0
40	4U	4494	0	4484	186	0
40	4V	4494	0	4484	180	0
41	4W	597	0	286	10	0
41	4X	597	0	286	15	0
41	4Y	597	0	286	20	0
41	4Z	597	0	286	19	0
41	5A	592	0	282	151	0
41	5B	592	0	284	13	0
41	5C	592	0	284	13	0
41	5D	592	0	284	13	0
42	5E	1562	0	1410	64	0
42	5F	1562	0	1410	53	0
42	5G	1562	0	1410	50	0
42	5H	1307	0	1255	803	0
43	5I	1594	0	1501	184	0
43	5J	1594	0	1501	174	0
43	5K	1594	0	1501	211	0
43	5L	1594	0	1498	1336	0
44	5M	699	0	322	5	0
44	5N	699	0	322	7	0
44	5O	699	0	322	7	0
44	5P	1153	0	1085	47	0
44	5Q	1153	0	1085	43	0
44	5R	1153	0	1085	45	0
44	5S	1144	0	1079	48	0
44	5T	1144	0	1079	50	0
44	5U	1144	0	1079	65	0
44	5V	1166	0	1094	37	0
45	5W	685	0	153	2	0
45	5X	685	0	153	2	0
45	5Y	685	0	153	2	0
46	5Z	978	0	442	13	0
47	6A	11821	0	11632	627	0
47	6B	11821	0	11632	672	0
48	6E	6892	0	6896	290	0
48	6F	6892	0	6896	302	0
49	6G	3606	0	3611	194	0
49	6H	3606	0	3611	195	0
49	6I	3606	0	3611	183	0
49	6J	3606	0	3611	188	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
50	6K	4731	0	4753	223	0
50	6L	4731	0	4753	227	0
51	6M	8050	0	8003	291	0
51	6N	8050	0	8003	285	0
52	6O	444	0	103	3	0
52	6P	444	0	103	3	0
52	6Q	444	0	103	7	0
53	1a	28	0	12	2	0
53	1c	28	0	12	0	0
53	1e	28	0	12	3	0
53	1g	28	0	12	0	0
53	2a	28	0	12	1	0
53	2c	28	0	12	1	0
53	2e	28	0	12	0	0
53	2g	28	0	12	0	0
53	3a	28	0	12	1	0
53	3c	28	0	12	0	0
53	3e	28	0	12	1	0
53	3g	28	0	12	0	0
53	4a	28	0	12	1	0
53	4c	28	0	12	0	0
53	4e	28	0	12	0	0
53	4g	28	0	12	0	0
53	5a	28	0	12	0	0
53	5c	28	0	12	0	0
53	5e	28	0	12	0	0
53	5g	28	0	12	0	0
53	6a	28	0	12	0	0
53	6c	28	0	12	0	0
53	6e	28	0	12	1	0
53	6g	28	0	12	0	0
53	7a	28	0	12	1	0
53	7c	28	0	12	0	0
53	7e	28	0	12	2	0
53	7g	28	0	12	0	0
53	8a	28	0	12	0	0
53	8c	28	0	12	1	0
53	8e	28	0	12	0	0
53	8g	28	0	12	0	0
53	9a	28	0	12	0	0
53	9c	28	0	12	0	0
53	9e	28	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
53	9g	28	0	12	0	0
53	Aa	28	0	12	0	0
53	Ac	28	0	12	0	0
53	Ae	28	0	12	0	0
53	Ag	28	0	12	0	0
53	Ba	28	0	12	1	0
53	Bc	28	0	12	0	0
53	Be	28	0	12	1	0
53	Bg	28	0	12	1	0
53	Ca	28	0	12	0	0
53	Cc	28	0	12	1	0
53	Ce	28	0	12	0	0
53	Cg	28	0	12	0	0
53	Da	28	0	12	0	0
53	Dc	28	0	12	0	0
53	De	28	0	12	0	0
53	Dg	28	0	12	1	0
54	1b	32	0	12	5	0
54	1d	32	0	12	4	0
54	1f	32	0	12	4	0
54	1h	32	0	12	3	0
54	2b	32	0	12	7	0
54	2d	32	0	12	6	0
54	2f	32	0	12	5	0
54	2h	32	0	12	4	0
54	3c	32	0	12	5	0
54	3d	32	0	12	3	0
54	3f	32	0	12	4	0
54	3h	32	0	12	3	0
54	4b	32	0	12	4	0
54	4d	32	0	12	3	0
54	4f	32	0	12	5	0
54	4h	32	0	12	3	0
54	5c	32	0	12	4	0
54	5d	32	0	12	3	0
54	5f	32	0	12	5	0
54	5h	32	0	12	5	0
54	6c	32	0	12	6	0
54	6e	32	0	12	4	0
54	6g	32	0	12	5	0
54	6h	32	0	12	4	0
54	7b	32	0	12	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	7e	32	0	12	5	0
54	7f	32	0	12	5	0
54	7h	32	0	12	4	0
54	8b	32	0	12	4	0
54	8d	32	0	12	4	0
54	8f	32	0	12	5	0
54	8h	32	0	12	5	0
54	9b	32	0	12	5	0
54	9e	32	0	12	4	0
54	9f	32	0	12	7	0
54	9h	32	0	12	3	0
54	Ab	32	0	12	6	0
54	Ae	32	0	12	4	0
54	Af	32	0	12	7	0
54	Ah	32	0	12	4	0
54	Bb	32	0	12	6	0
54	Bd	32	0	12	5	0
54	Bf	32	0	12	6	0
54	Bh	32	0	12	5	0
54	Cc	32	0	12	6	0
54	Cd	32	0	12	5	0
54	Cf	32	0	12	6	0
54	Ch	32	0	12	5	0
54	Db	32	0	12	5	0
54	Dd	32	0	12	5	0
54	Df	32	0	12	5	0
54	Dh	32	0	12	4	0
All	All	793756	0	755740	34194	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 22.

The worst 5 of 34194 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:4H:972:PHE:CB	37:4H:972:PHE:CG	1.75	1.65
37:4H:1091:VAL:CG2	37:4H:1091:VAL:CB	1.75	1.63
37:4F:1324:THR:CG2	37:4F:1324:THR:CB	1.77	1.62
37:4G:1323:ILE:CB	37:4G:1323:ILE:CA	1.79	1.60
37:4E:579:THR:CG2	37:4E:579:THR:CB	1.77	1.59

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	0A	497/512 (97%)	486 (98%)	10 (2%)	1 (0%)	43	72
1	0B	497/512 (97%)	485 (98%)	10 (2%)	2 (0%)	30	61
1	0C	497/512 (97%)	488 (98%)	8 (2%)	1 (0%)	43	72
1	0D	497/512 (97%)	486 (98%)	10 (2%)	1 (0%)	43	72
1	0E	497/512 (97%)	486 (98%)	10 (2%)	1 (0%)	43	72
1	0F	497/512 (97%)	484 (97%)	12 (2%)	1 (0%)	43	72
1	0G	497/512 (97%)	484 (97%)	11 (2%)	2 (0%)	30	61
1	0H	497/512 (97%)	484 (97%)	12 (2%)	1 (0%)	43	72
1	0I	497/512 (97%)	486 (98%)	10 (2%)	1 (0%)	43	72
1	0J	497/512 (97%)	489 (98%)	8 (2%)	0	100	100
1	0K	497/512 (97%)	492 (99%)	5 (1%)	0	100	100
1	0L	497/512 (97%)	487 (98%)	9 (2%)	1 (0%)	43	72
1	0M	497/512 (97%)	485 (98%)	10 (2%)	2 (0%)	30	61
1	0N	497/512 (97%)	487 (98%)	9 (2%)	1 (0%)	43	72
1	0O	497/512 (97%)	488 (98%)	8 (2%)	1 (0%)	43	72
1	0P	497/512 (97%)	484 (97%)	12 (2%)	1 (0%)	43	72
1	0Q	497/512 (97%)	486 (98%)	10 (2%)	1 (0%)	43	72
1	0R	497/512 (97%)	486 (98%)	10 (2%)	1 (0%)	43	72
1	0S	497/512 (97%)	485 (98%)	11 (2%)	1 (0%)	43	72
1	0T	497/512 (97%)	488 (98%)	8 (2%)	1 (0%)	43	72
1	0U	497/512 (97%)	487 (98%)	9 (2%)	1 (0%)	43	72
1	0V	497/512 (97%)	487 (98%)	9 (2%)	1 (0%)	43	72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0W	497/512 (97%)	485 (98%)	10 (2%)	2 (0%)	30	61
1	0X	497/512 (97%)	487 (98%)	9 (2%)	1 (0%)	43	72
1	0Y	497/512 (97%)	484 (97%)	11 (2%)	2 (0%)	30	61
1	0Z	497/512 (97%)	488 (98%)	8 (2%)	1 (0%)	43	72
1	1A	497/512 (97%)	487 (98%)	9 (2%)	1 (0%)	43	72
1	1B	497/512 (97%)	488 (98%)	9 (2%)	0	100	100
1	1C	497/512 (97%)	491 (99%)	6 (1%)	0	100	100
2	1D	500/571 (88%)	453 (91%)	39 (8%)	8 (2%)	7	36
2	1E	500/571 (88%)	454 (91%)	37 (7%)	9 (2%)	6	34
2	1F	512/571 (90%)	464 (91%)	43 (8%)	5 (1%)	12	45
2	1G	512/571 (90%)	464 (91%)	41 (8%)	7 (1%)	9	38
3	1H	791/1102 (72%)	764 (97%)	22 (3%)	5 (1%)	21	54
3	1I	791/1102 (72%)	769 (97%)	18 (2%)	4 (0%)	24	57
3	6D	787/1102 (71%)	766 (97%)	18 (2%)	3 (0%)	30	61
4	1J	392/3965 (10%)	344 (88%)	39 (10%)	9 (2%)	5	30
4	1K	392/3965 (10%)	344 (88%)	39 (10%)	9 (2%)	5	30
5	1L	540/2939 (18%)	476 (88%)	61 (11%)	3 (1%)	21	54
5	1M	540/2939 (18%)	476 (88%)	61 (11%)	3 (1%)	21	54
6	1N	2132/2784 (77%)	2080 (98%)	51 (2%)	1 (0%)	100	100
7	1O	2594/3225 (80%)	2506 (97%)	84 (3%)	4 (0%)	43	72
8	1P	291/1023 (28%)	274 (94%)	15 (5%)	2 (1%)	18	51
9	1Q	423/945 (45%)	336 (79%)	59 (14%)	28 (7%)	1	12
10	1R	351/446 (79%)	326 (93%)	21 (6%)	4 (1%)	11	43
10	1S	260/446 (58%)	237 (91%)	17 (6%)	6 (2%)	5	30
11	1T	952/1638 (58%)	942 (99%)	8 (1%)	2 (0%)	43	72
12	1a	426/443 (96%)	410 (96%)	16 (4%)	0	100	100
12	1c	429/443 (97%)	408 (95%)	21 (5%)	0	100	100
12	1e	426/443 (96%)	411 (96%)	15 (4%)	0	100	100
12	1g	429/443 (97%)	406 (95%)	23 (5%)	0	100	100
12	2a	426/443 (96%)	410 (96%)	16 (4%)	0	100	100
12	2c	429/443 (97%)	407 (95%)	22 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	2e	426/443 (96%)	412 (97%)	14 (3%)	0	100	100
12	2g	429/443 (97%)	407 (95%)	22 (5%)	0	100	100
12	3a	426/443 (96%)	411 (96%)	15 (4%)	0	100	100
12	3c	429/443 (97%)	406 (95%)	23 (5%)	0	100	100
12	3e	426/443 (96%)	411 (96%)	15 (4%)	0	100	100
12	3g	429/443 (97%)	406 (95%)	23 (5%)	0	100	100
12	4a	426/443 (96%)	408 (96%)	18 (4%)	0	100	100
12	4c	429/443 (97%)	403 (94%)	26 (6%)	0	100	100
12	4e	426/443 (96%)	410 (96%)	16 (4%)	0	100	100
12	4g	429/443 (97%)	406 (95%)	23 (5%)	0	100	100
12	5a	426/443 (96%)	409 (96%)	17 (4%)	0	100	100
12	5c	429/443 (97%)	404 (94%)	25 (6%)	0	100	100
12	5e	426/443 (96%)	411 (96%)	15 (4%)	0	100	100
12	5g	429/443 (97%)	403 (94%)	26 (6%)	0	100	100
12	6a	426/443 (96%)	408 (96%)	18 (4%)	0	100	100
12	6c	429/443 (97%)	404 (94%)	25 (6%)	0	100	100
12	6e	426/443 (96%)	408 (96%)	18 (4%)	0	100	100
12	6g	429/443 (97%)	405 (94%)	24 (6%)	0	100	100
12	7a	426/443 (96%)	410 (96%)	16 (4%)	0	100	100
12	7c	429/443 (97%)	403 (94%)	26 (6%)	0	100	100
12	7e	426/443 (96%)	405 (95%)	21 (5%)	0	100	100
12	7g	429/443 (97%)	403 (94%)	26 (6%)	0	100	100
12	8a	426/443 (96%)	408 (96%)	18 (4%)	0	100	100
12	8c	429/443 (97%)	405 (94%)	24 (6%)	0	100	100
12	8e	426/443 (96%)	410 (96%)	16 (4%)	0	100	100
12	8g	429/443 (97%)	408 (95%)	21 (5%)	0	100	100
12	9a	426/443 (96%)	407 (96%)	19 (4%)	0	100	100
12	9c	429/443 (97%)	404 (94%)	25 (6%)	0	100	100
12	9e	426/443 (96%)	408 (96%)	18 (4%)	0	100	100
12	9g	429/443 (97%)	407 (95%)	22 (5%)	0	100	100
12	Aa	426/443 (96%)	412 (97%)	14 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	Ac	429/443 (97%)	405 (94%)	24 (6%)	0	100	100
12	Ae	426/443 (96%)	413 (97%)	13 (3%)	0	100	100
12	Ag	429/443 (97%)	408 (95%)	21 (5%)	0	100	100
12	Ba	426/443 (96%)	408 (96%)	18 (4%)	0	100	100
12	Bc	429/443 (97%)	407 (95%)	22 (5%)	0	100	100
12	Be	426/443 (96%)	407 (96%)	19 (4%)	0	100	100
12	Bg	429/443 (97%)	403 (94%)	26 (6%)	0	100	100
12	Ca	426/443 (96%)	414 (97%)	12 (3%)	0	100	100
12	Cc	429/443 (97%)	406 (95%)	23 (5%)	0	100	100
12	Ce	426/443 (96%)	408 (96%)	18 (4%)	0	100	100
12	Cg	429/443 (97%)	410 (96%)	19 (4%)	0	100	100
12	Da	426/443 (96%)	412 (97%)	14 (3%)	0	100	100
12	Dc	429/443 (97%)	407 (95%)	22 (5%)	0	100	100
12	De	426/443 (96%)	409 (96%)	17 (4%)	0	100	100
12	Dg	429/443 (97%)	404 (94%)	25 (6%)	0	100	100
13	1b	426/451 (94%)	409 (96%)	17 (4%)	0	100	100
13	1d	426/451 (94%)	409 (96%)	17 (4%)	0	100	100
13	1f	426/451 (94%)	409 (96%)	17 (4%)	0	100	100
13	1h	426/451 (94%)	409 (96%)	17 (4%)	0	100	100
13	2b	426/451 (94%)	409 (96%)	17 (4%)	0	100	100
13	2d	426/451 (94%)	409 (96%)	17 (4%)	0	100	100
13	2f	426/451 (94%)	409 (96%)	17 (4%)	0	100	100
13	2h	426/451 (94%)	409 (96%)	17 (4%)	0	100	100
13	3b	426/451 (94%)	409 (96%)	17 (4%)	0	100	100
13	3d	426/451 (94%)	410 (96%)	16 (4%)	0	100	100
13	3f	426/451 (94%)	409 (96%)	17 (4%)	0	100	100
13	3h	426/451 (94%)	409 (96%)	17 (4%)	0	100	100
13	4b	426/451 (94%)	409 (96%)	17 (4%)	0	100	100
13	4d	426/451 (94%)	409 (96%)	17 (4%)	0	100	100
13	4f	426/451 (94%)	409 (96%)	17 (4%)	0	100	100
13	4h	426/451 (94%)	409 (96%)	17 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	5b	426/451 (94%)	409 (96%)	17 (4%)	0	100	100
13	5d	426/451 (94%)	409 (96%)	17 (4%)	0	100	100
13	5f	426/451 (94%)	409 (96%)	17 (4%)	0	100	100
13	5h	426/451 (94%)	409 (96%)	17 (4%)	0	100	100
13	6b	426/451 (94%)	409 (96%)	17 (4%)	0	100	100
13	6d	426/451 (94%)	409 (96%)	17 (4%)	0	100	100
13	6f	426/451 (94%)	409 (96%)	17 (4%)	0	100	100
13	6h	426/451 (94%)	409 (96%)	17 (4%)	0	100	100
13	7b	426/451 (94%)	409 (96%)	17 (4%)	0	100	100
13	7d	426/451 (94%)	409 (96%)	17 (4%)	0	100	100
13	7f	426/451 (94%)	409 (96%)	17 (4%)	0	100	100
13	7h	426/451 (94%)	409 (96%)	17 (4%)	0	100	100
13	8b	426/451 (94%)	409 (96%)	17 (4%)	0	100	100
13	8d	426/451 (94%)	409 (96%)	17 (4%)	0	100	100
13	8f	426/451 (94%)	409 (96%)	17 (4%)	0	100	100
13	8h	426/451 (94%)	409 (96%)	17 (4%)	0	100	100
13	9b	426/451 (94%)	409 (96%)	17 (4%)	0	100	100
13	9d	426/451 (94%)	409 (96%)	17 (4%)	0	100	100
13	9f	426/451 (94%)	409 (96%)	17 (4%)	0	100	100
13	9h	426/451 (94%)	409 (96%)	17 (4%)	0	100	100
13	Ab	426/451 (94%)	409 (96%)	17 (4%)	0	100	100
13	Ad	426/451 (94%)	409 (96%)	17 (4%)	0	100	100
13	Af	426/451 (94%)	409 (96%)	17 (4%)	0	100	100
13	Ah	426/451 (94%)	409 (96%)	17 (4%)	0	100	100
13	Bb	426/451 (94%)	409 (96%)	17 (4%)	0	100	100
13	Bd	426/451 (94%)	409 (96%)	17 (4%)	0	100	100
13	Bf	426/451 (94%)	409 (96%)	17 (4%)	0	100	100
13	Bh	426/451 (94%)	409 (96%)	17 (4%)	0	100	100
13	Cb	426/451 (94%)	409 (96%)	17 (4%)	0	100	100
13	Cd	426/451 (94%)	409 (96%)	17 (4%)	0	100	100
13	Cf	426/451 (94%)	409 (96%)	17 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	Ch	426/451 (94%)	409 (96%)	17 (4%)	0	100	100
13	Db	426/451 (94%)	409 (96%)	17 (4%)	0	100	100
13	Dd	426/451 (94%)	409 (96%)	17 (4%)	0	100	100
13	Df	426/451 (94%)	409 (96%)	17 (4%)	0	100	100
13	Dh	426/451 (94%)	409 (96%)	17 (4%)	0	100	100
14	2F	159/168 (95%)	144 (91%)	14 (9%)	1 (1%)	21	54
14	2G	159/168 (95%)	144 (91%)	14 (9%)	1 (1%)	21	54
24	2S	103/447 (23%)	100 (97%)	2 (2%)	1 (1%)	12	45
24	2T	107/447 (24%)	104 (97%)	3 (3%)	0	100	100
24	2U	109/447 (24%)	100 (92%)	9 (8%)	0	100	100
24	2V	107/447 (24%)	103 (96%)	4 (4%)	0	100	100
28	3C	59/739 (8%)	59 (100%)	0	0	100	100
29	3E	85/1471 (6%)	79 (93%)	6 (7%)	0	100	100
30	3F	440/795 (55%)	426 (97%)	11 (2%)	3 (1%)	18	51
30	3G	236/795 (30%)	231 (98%)	5 (2%)	0	100	100
31	3H	304/1940 (16%)	304 (100%)	0	0	100	100
31	3I	399/1940 (21%)	393 (98%)	6 (2%)	0	100	100
32	3J	366/749 (49%)	349 (95%)	17 (5%)	0	100	100
32	3K	361/749 (48%)	345 (96%)	15 (4%)	1 (0%)	36	65
33	3L	193/401 (48%)	184 (95%)	7 (4%)	2 (1%)	12	45
34	3M	381/507 (75%)	369 (97%)	12 (3%)	0	100	100
34	3N	386/507 (76%)	379 (98%)	7 (2%)	0	100	100
34	3O	349/507 (69%)	342 (98%)	7 (2%)	0	100	100
34	3P	351/507 (69%)	347 (99%)	4 (1%)	0	100	100
34	3Q	349/507 (69%)	344 (99%)	5 (1%)	0	100	100
34	3R	354/507 (70%)	351 (99%)	3 (1%)	0	100	100
34	3S	381/507 (75%)	371 (97%)	10 (3%)	0	100	100
34	3T	386/507 (76%)	378 (98%)	8 (2%)	0	100	100
34	3U	351/507 (69%)	348 (99%)	3 (1%)	0	100	100
34	3V	404/507 (80%)	397 (98%)	6 (2%)	1 (0%)	43	72
34	3W	405/507 (80%)	399 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	3X	354/507 (70%)	349 (99%)	5 (1%)	0	100	100
34	3Y	354/507 (70%)	352 (99%)	2 (1%)	0	100	100
34	3Z	354/507 (70%)	349 (99%)	5 (1%)	0	100	100
34	4A	404/507 (80%)	396 (98%)	7 (2%)	1 (0%)	43	72
34	4B	405/507 (80%)	401 (99%)	4 (1%)	0	100	100
35	4C	618/2215 (28%)	585 (95%)	29 (5%)	4 (1%)	21	54
36	4D	293/304 (96%)	285 (97%)	6 (2%)	2 (1%)	18	51
37	4E	961/2301 (42%)	923 (96%)	28 (3%)	10 (1%)	12	45
37	4F	943/2301 (41%)	874 (93%)	49 (5%)	20 (2%)	5	31
37	4G	943/2301 (41%)	872 (92%)	57 (6%)	14 (2%)	8	37
37	4H	943/2301 (41%)	881 (93%)	47 (5%)	15 (2%)	7	36
38	4I	62/110 (56%)	41 (66%)	16 (26%)	5 (8%)	1	8
38	4J	62/110 (56%)	41 (66%)	16 (26%)	5 (8%)	1	8
38	4K	62/110 (56%)	41 (66%)	16 (26%)	5 (8%)	1	8
38	4L	62/110 (56%)	41 (66%)	16 (26%)	5 (8%)	1	8
38	4M	62/110 (56%)	41 (66%)	16 (26%)	5 (8%)	1	8
38	4N	62/110 (56%)	41 (66%)	16 (26%)	5 (8%)	1	8
38	4O	82/110 (74%)	71 (87%)	9 (11%)	2 (2%)	4	29
38	4P	53/110 (48%)	49 (92%)	3 (6%)	1 (2%)	6	33
39	4Q	214/427 (50%)	207 (97%)	5 (2%)	2 (1%)	14	46
39	4R	214/427 (50%)	207 (97%)	5 (2%)	2 (1%)	14	46
39	4S	214/427 (50%)	207 (97%)	5 (2%)	2 (1%)	14	46
40	4T	588/835 (70%)	544 (92%)	31 (5%)	13 (2%)	5	30
40	4U	588/835 (70%)	544 (92%)	31 (5%)	13 (2%)	5	30
40	4V	588/835 (70%)	544 (92%)	31 (5%)	13 (2%)	5	30
41	4W	120/173 (69%)	118 (98%)	2 (2%)	0	100	100
41	4X	120/173 (69%)	108 (90%)	12 (10%)	0	100	100
41	4Y	120/173 (69%)	107 (89%)	13 (11%)	0	100	100
41	4Z	120/173 (69%)	107 (89%)	13 (11%)	0	100	100
41	5A	119/173 (69%)	101 (85%)	12 (10%)	6 (5%)	1	16
41	5B	119/173 (69%)	106 (89%)	12 (10%)	1 (1%)	16	49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
41	5C	119/173 (69%)	106 (89%)	12 (10%)	1 (1%)	16 49
41	5D	119/173 (69%)	106 (89%)	12 (10%)	1 (1%)	16 49
42	5E	212/286 (74%)	210 (99%)	2 (1%)	0	100 100
42	5F	212/286 (74%)	210 (99%)	2 (1%)	0	100 100
42	5G	212/286 (74%)	210 (99%)	2 (1%)	0	100 100
42	5H	163/286 (57%)	139 (85%)	16 (10%)	8 (5%)	1 16
43	5I	207/306 (68%)	179 (86%)	23 (11%)	5 (2%)	4 29
43	5J	207/306 (68%)	179 (86%)	23 (11%)	5 (2%)	4 29
43	5K	207/306 (68%)	179 (86%)	23 (11%)	5 (2%)	4 29
43	5L	207/306 (68%)	179 (86%)	23 (11%)	5 (2%)	4 29
44	5M	140/163 (86%)	137 (98%)	3 (2%)	0	100 100
44	5N	140/163 (86%)	137 (98%)	3 (2%)	0	100 100
44	5O	140/163 (86%)	137 (98%)	3 (2%)	0	100 100
44	5P	144/163 (88%)	139 (96%)	5 (4%)	0	100 100
44	5Q	144/163 (88%)	139 (96%)	5 (4%)	0	100 100
44	5R	144/163 (88%)	140 (97%)	4 (3%)	0	100 100
44	5S	143/163 (88%)	141 (99%)	2 (1%)	0	100 100
44	5T	143/163 (88%)	142 (99%)	1 (1%)	0	100 100
44	5U	143/163 (88%)	141 (99%)	2 (1%)	0	100 100
44	5V	147/163 (90%)	143 (97%)	3 (2%)	1 (1%)	18 51
46	5Z	39/181 (22%)	39 (100%)	0	0	100 100
47	6A	1536/1929 (80%)	1453 (95%)	64 (4%)	19 (1%)	10 41
47	6B	1536/1929 (80%)	1453 (95%)	64 (4%)	19 (1%)	10 41
48	6E	894/1138 (79%)	839 (94%)	52 (6%)	3 (0%)	36 65
48	6F	894/1138 (79%)	839 (94%)	52 (6%)	3 (0%)	36 65
49	6G	474/477 (99%)	456 (96%)	17 (4%)	1 (0%)	43 72
49	6H	474/477 (99%)	456 (96%)	17 (4%)	1 (0%)	43 72
49	6I	474/477 (99%)	456 (96%)	17 (4%)	1 (0%)	43 72
49	6J	474/477 (99%)	456 (96%)	17 (4%)	1 (0%)	43 72
50	6K	605/651 (93%)	580 (96%)	21 (4%)	4 (1%)	18 51
50	6L	605/651 (93%)	580 (96%)	21 (4%)	4 (1%)	18 51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
51	6M	1059/2540 (42%)	1011 (96%)	40 (4%)	8 (1%)	16 49
51	6N	1059/2540 (42%)	1011 (96%)	40 (4%)	8 (1%)	16 49
52	6O	7/89 (8%)	6 (86%)	1 (14%)	0	100 100
52	6P	7/89 (8%)	6 (86%)	1 (14%)	0	100 100
52	6Q	7/89 (8%)	6 (86%)	1 (14%)	0	100 100
All	All	102979/147699 (70%)	98412 (96%)	4161 (4%)	406 (0%)	31 61

5 of 406 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	1D	61	VAL
2	1D	265	GLU
2	1D	427	GLU
2	1E	61	VAL
2	1E	265	GLU

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	0A	333/408 (82%)	333 (100%)	0	100 100
1	0B	333/408 (82%)	333 (100%)	0	100 100
1	0C	333/408 (82%)	333 (100%)	0	100 100
1	0D	333/408 (82%)	333 (100%)	0	100 100
1	0E	333/408 (82%)	333 (100%)	0	100 100
1	0F	333/408 (82%)	333 (100%)	0	100 100
1	0G	333/408 (82%)	333 (100%)	0	100 100
1	0H	333/408 (82%)	333 (100%)	0	100 100
1	0I	333/408 (82%)	333 (100%)	0	100 100
1	0J	333/408 (82%)	333 (100%)	0	100 100
1	0K	332/408 (81%)	332 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0L	333/408 (82%)	333 (100%)	0	100	100
1	0M	333/408 (82%)	333 (100%)	0	100	100
1	0N	333/408 (82%)	333 (100%)	0	100	100
1	0O	333/408 (82%)	333 (100%)	0	100	100
1	0P	333/408 (82%)	333 (100%)	0	100	100
1	0Q	333/408 (82%)	333 (100%)	0	100	100
1	0R	332/408 (81%)	332 (100%)	0	100	100
1	0S	333/408 (82%)	333 (100%)	0	100	100
1	0T	333/408 (82%)	333 (100%)	0	100	100
1	0U	333/408 (82%)	333 (100%)	0	100	100
1	0V	333/408 (82%)	333 (100%)	0	100	100
1	0W	333/408 (82%)	333 (100%)	0	100	100
1	0X	333/408 (82%)	333 (100%)	0	100	100
1	0Y	333/408 (82%)	333 (100%)	0	100	100
1	0Z	333/408 (82%)	333 (100%)	0	100	100
1	1A	333/408 (82%)	333 (100%)	0	100	100
1	1B	333/408 (82%)	333 (100%)	0	100	100
1	1C	332/408 (81%)	332 (100%)	0	100	100
2	1D	256/415 (62%)	256 (100%)	0	100	100
2	1E	256/415 (62%)	256 (100%)	0	100	100
2	1F	263/415 (63%)	263 (100%)	0	100	100
2	1G	263/415 (63%)	263 (100%)	0	100	100
3	1H	547/811 (67%)	546 (100%)	1 (0%)	87	85
3	1I	547/811 (67%)	546 (100%)	1 (0%)	87	85
3	6D	620/811 (76%)	619 (100%)	1 (0%)	87	85
4	1J	278/3239 (9%)	276 (99%)	2 (1%)	76	78
4	1K	278/3239 (9%)	276 (99%)	2 (1%)	76	78
5	1L	201/2456 (8%)	196 (98%)	5 (2%)	42	63
5	1M	201/2456 (8%)	196 (98%)	5 (2%)	42	63
6	1N	1553/1962 (79%)	1553 (100%)	0	100	100
7	1O	1932/2270 (85%)	1932 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	1P	236/790 (30%)	236 (100%)	0	100	100
9	1Q	55/728 (8%)	55 (100%)	0	100	100
10	1R	295/353 (84%)	295 (100%)	0	100	100
10	1S	195/353 (55%)	195 (100%)	0	100	100
11	1T	1/1185 (0%)	1 (100%)	0	100	100
12	1a	368/379 (97%)	368 (100%)	0	100	100
12	1c	370/379 (98%)	370 (100%)	0	100	100
12	1e	368/379 (97%)	368 (100%)	0	100	100
12	1g	370/379 (98%)	370 (100%)	0	100	100
12	2a	368/379 (97%)	368 (100%)	0	100	100
12	2c	370/379 (98%)	370 (100%)	0	100	100
12	2e	368/379 (97%)	368 (100%)	0	100	100
12	2g	370/379 (98%)	370 (100%)	0	100	100
12	3a	368/379 (97%)	368 (100%)	0	100	100
12	3c	370/379 (98%)	370 (100%)	0	100	100
12	3e	368/379 (97%)	368 (100%)	0	100	100
12	3g	370/379 (98%)	370 (100%)	0	100	100
12	4a	368/379 (97%)	367 (100%)	1 (0%)	86	83
12	4c	370/379 (98%)	370 (100%)	0	100	100
12	4e	368/379 (97%)	368 (100%)	0	100	100
12	4g	370/379 (98%)	370 (100%)	0	100	100
12	5a	368/379 (97%)	368 (100%)	0	100	100
12	5c	370/379 (98%)	370 (100%)	0	100	100
12	5e	368/379 (97%)	368 (100%)	0	100	100
12	5g	370/379 (98%)	370 (100%)	0	100	100
12	6a	368/379 (97%)	368 (100%)	0	100	100
12	6c	370/379 (98%)	370 (100%)	0	100	100
12	6e	368/379 (97%)	368 (100%)	0	100	100
12	6g	370/379 (98%)	370 (100%)	0	100	100
12	7a	368/379 (97%)	368 (100%)	0	100	100
12	7c	370/379 (98%)	370 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	7e	368/379 (97%)	368 (100%)	0	100	100
12	7g	370/379 (98%)	370 (100%)	0	100	100
12	8a	368/379 (97%)	368 (100%)	0	100	100
12	8c	370/379 (98%)	370 (100%)	0	100	100
12	8e	368/379 (97%)	368 (100%)	0	100	100
12	8g	370/379 (98%)	370 (100%)	0	100	100
12	9a	368/379 (97%)	368 (100%)	0	100	100
12	9c	370/379 (98%)	370 (100%)	0	100	100
12	9e	368/379 (97%)	368 (100%)	0	100	100
12	9g	370/379 (98%)	370 (100%)	0	100	100
12	Aa	368/379 (97%)	368 (100%)	0	100	100
12	Ac	370/379 (98%)	370 (100%)	0	100	100
12	Ae	368/379 (97%)	368 (100%)	0	100	100
12	Ag	370/379 (98%)	370 (100%)	0	100	100
12	Ba	368/379 (97%)	368 (100%)	0	100	100
12	Bc	370/379 (98%)	370 (100%)	0	100	100
12	Be	368/379 (97%)	368 (100%)	0	100	100
12	Bg	370/379 (98%)	370 (100%)	0	100	100
12	Ca	368/379 (97%)	368 (100%)	0	100	100
12	Cc	370/379 (98%)	370 (100%)	0	100	100
12	Ce	368/379 (97%)	368 (100%)	0	100	100
12	Cg	370/379 (98%)	370 (100%)	0	100	100
12	Da	368/379 (97%)	368 (100%)	0	100	100
12	Dc	370/379 (98%)	370 (100%)	0	100	100
12	De	368/379 (97%)	368 (100%)	0	100	100
12	Dg	370/379 (98%)	370 (100%)	0	100	100
13	1b	361/374 (96%)	347 (96%)	14 (4%)	28	54
13	1d	361/374 (96%)	347 (96%)	14 (4%)	28	54
13	1f	361/374 (96%)	347 (96%)	14 (4%)	28	54
13	1h	361/374 (96%)	347 (96%)	14 (4%)	28	54
13	2b	361/374 (96%)	347 (96%)	14 (4%)	28	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	2d	361/374 (96%)	347 (96%)	14 (4%)	28	54
13	2f	361/374 (96%)	347 (96%)	14 (4%)	28	54
13	2h	361/374 (96%)	347 (96%)	14 (4%)	28	54
13	3b	361/374 (96%)	347 (96%)	14 (4%)	28	54
13	3d	361/374 (96%)	347 (96%)	14 (4%)	28	54
13	3f	361/374 (96%)	347 (96%)	14 (4%)	28	54
13	3h	361/374 (96%)	347 (96%)	14 (4%)	28	54
13	4b	361/374 (96%)	347 (96%)	14 (4%)	28	54
13	4d	361/374 (96%)	347 (96%)	14 (4%)	28	54
13	4f	361/374 (96%)	347 (96%)	14 (4%)	28	54
13	4h	361/374 (96%)	347 (96%)	14 (4%)	28	54
13	5b	361/374 (96%)	347 (96%)	14 (4%)	28	54
13	5d	361/374 (96%)	347 (96%)	14 (4%)	28	54
13	5f	361/374 (96%)	347 (96%)	14 (4%)	28	54
13	5h	361/374 (96%)	347 (96%)	14 (4%)	28	54
13	6b	361/374 (96%)	347 (96%)	14 (4%)	28	54
13	6d	361/374 (96%)	347 (96%)	14 (4%)	28	54
13	6f	361/374 (96%)	347 (96%)	14 (4%)	28	54
13	6h	361/374 (96%)	347 (96%)	14 (4%)	28	54
13	7b	361/374 (96%)	347 (96%)	14 (4%)	28	54
13	7d	361/374 (96%)	347 (96%)	14 (4%)	28	54
13	7f	361/374 (96%)	347 (96%)	14 (4%)	28	54
13	7h	361/374 (96%)	347 (96%)	14 (4%)	28	54
13	8b	361/374 (96%)	347 (96%)	14 (4%)	28	54
13	8d	361/374 (96%)	347 (96%)	14 (4%)	28	54
13	8f	361/374 (96%)	347 (96%)	14 (4%)	28	54
13	8h	361/374 (96%)	347 (96%)	14 (4%)	28	54
13	9b	361/374 (96%)	347 (96%)	14 (4%)	28	54
13	9d	361/374 (96%)	347 (96%)	14 (4%)	28	54
13	9f	361/374 (96%)	347 (96%)	14 (4%)	28	54
13	9h	361/374 (96%)	347 (96%)	14 (4%)	28	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	Ab	361/374 (96%)	347 (96%)	14 (4%)	28	54
13	Ad	361/374 (96%)	347 (96%)	14 (4%)	28	54
13	Af	361/374 (96%)	347 (96%)	14 (4%)	28	54
13	Ah	361/374 (96%)	347 (96%)	14 (4%)	28	54
13	Bb	361/374 (96%)	347 (96%)	14 (4%)	28	54
13	Bd	361/374 (96%)	347 (96%)	14 (4%)	28	54
13	Bf	361/374 (96%)	347 (96%)	14 (4%)	28	54
13	Bh	361/374 (96%)	347 (96%)	14 (4%)	28	54
13	Cb	361/374 (96%)	347 (96%)	14 (4%)	28	54
13	Cd	361/374 (96%)	347 (96%)	14 (4%)	28	54
13	Cf	361/374 (96%)	347 (96%)	14 (4%)	28	54
13	Ch	361/374 (96%)	347 (96%)	14 (4%)	28	54
13	Db	361/374 (96%)	347 (96%)	14 (4%)	28	54
13	Dd	361/374 (96%)	347 (96%)	14 (4%)	28	54
13	Df	361/374 (96%)	347 (96%)	14 (4%)	28	54
13	Dh	361/374 (96%)	347 (96%)	14 (4%)	28	54
14	2F	115/119 (97%)	112 (97%)	3 (3%)	40	62
14	2G	115/119 (97%)	112 (97%)	3 (3%)	40	62
24	2T	85/313 (27%)	85 (100%)	0	100	100
24	2U	87/313 (28%)	87 (100%)	0	100	100
24	2V	85/313 (27%)	85 (100%)	0	100	100
28	3C	45/580 (8%)	45 (100%)	0	100	100
29	3E	59/1095 (5%)	59 (100%)	0	100	100
30	3F	303/642 (47%)	301 (99%)	2 (1%)	76	78
30	3G	187/642 (29%)	187 (100%)	0	100	100
31	3H	114/1457 (8%)	114 (100%)	0	100	100
31	3I	301/1457 (21%)	301 (100%)	0	100	100
32	3J	286/576 (50%)	286 (100%)	0	100	100
32	3K	285/576 (50%)	285 (100%)	0	100	100
33	3L	165/318 (52%)	165 (100%)	0	100	100
34	3M	291/386 (75%)	291 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	3N	302/386 (78%)	302 (100%)	0	100	100
34	3O	275/386 (71%)	275 (100%)	0	100	100
34	3P	276/386 (72%)	276 (100%)	0	100	100
34	3Q	275/386 (71%)	275 (100%)	0	100	100
34	3R	278/386 (72%)	278 (100%)	0	100	100
34	3S	291/386 (75%)	291 (100%)	0	100	100
34	3T	302/386 (78%)	302 (100%)	0	100	100
34	3U	276/386 (72%)	276 (100%)	0	100	100
34	3V	317/386 (82%)	317 (100%)	0	100	100
34	3W	318/386 (82%)	318 (100%)	0	100	100
34	3X	278/386 (72%)	278 (100%)	0	100	100
34	3Y	278/386 (72%)	278 (100%)	0	100	100
34	3Z	278/386 (72%)	278 (100%)	0	100	100
34	4A	317/386 (82%)	317 (100%)	0	100	100
34	4B	318/386 (82%)	318 (100%)	0	100	100
35	4C	525/1698 (31%)	525 (100%)	0	100	100
36	4D	260/267 (97%)	260 (100%)	0	100	100
37	4E	743/1694 (44%)	738 (99%)	5 (1%)	76	78
37	4F	722/1694 (43%)	714 (99%)	8 (1%)	65	74
37	4G	722/1694 (43%)	710 (98%)	12 (2%)	53	69
37	4H	722/1694 (43%)	711 (98%)	11 (2%)	57	70
38	4I	51/83 (61%)	42 (82%)	9 (18%)	2	12
38	4J	51/83 (61%)	42 (82%)	9 (18%)	2	12
38	4K	51/83 (61%)	42 (82%)	9 (18%)	2	12
38	4L	51/83 (61%)	42 (82%)	9 (18%)	2	12
38	4M	51/83 (61%)	42 (82%)	9 (18%)	2	12
38	4N	51/83 (61%)	42 (82%)	9 (18%)	2	12
38	4O	65/83 (78%)	65 (100%)	0	100	100
38	4P	44/83 (53%)	44 (100%)	0	100	100
39	4Q	178/330 (54%)	174 (98%)	4 (2%)	45	65
39	4R	178/330 (54%)	174 (98%)	4 (2%)	45	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
39	4S	178/330 (54%)	174 (98%)	4 (2%)	45 65
40	4T	464/605 (77%)	450 (97%)	14 (3%)	36 59
40	4U	464/605 (77%)	450 (97%)	14 (3%)	36 59
40	4V	464/605 (77%)	450 (97%)	14 (3%)	36 59
42	5E	132/215 (61%)	129 (98%)	3 (2%)	44 64
42	5F	132/215 (61%)	129 (98%)	3 (2%)	44 64
42	5G	132/215 (61%)	129 (98%)	3 (2%)	44 64
42	5H	132/215 (61%)	124 (94%)	8 (6%)	17 45
43	5I	155/247 (63%)	137 (88%)	18 (12%)	5 25
43	5J	155/247 (63%)	137 (88%)	18 (12%)	5 25
43	5K	155/247 (63%)	137 (88%)	18 (12%)	5 25
43	5L	155/247 (63%)	137 (88%)	18 (12%)	5 25
44	5P	125/137 (91%)	125 (100%)	0	100 100
44	5Q	125/137 (91%)	125 (100%)	0	100 100
44	5R	125/137 (91%)	125 (100%)	0	100 100
44	5S	124/137 (90%)	124 (100%)	0	100 100
44	5T	124/137 (90%)	124 (100%)	0	100 100
44	5U	124/137 (90%)	124 (100%)	0	100 100
44	5V	126/137 (92%)	126 (100%)	0	100 100
46	5Z	22/22 (100%)	22 (100%)	0	100 100
47	6A	1147/1408 (82%)	1122 (98%)	25 (2%)	45 65
47	6B	1147/1408 (82%)	1122 (98%)	25 (2%)	45 65
48	6E	710/864 (82%)	701 (99%)	9 (1%)	61 72
48	6F	710/864 (82%)	701 (99%)	9 (1%)	61 72
49	6G	383/384 (100%)	345 (90%)	38 (10%)	7 31
49	6H	383/384 (100%)	345 (90%)	38 (10%)	7 31
49	6I	383/384 (100%)	345 (90%)	38 (10%)	7 31
49	6J	383/384 (100%)	346 (90%)	37 (10%)	8 31
50	6K	511/533 (96%)	505 (99%)	6 (1%)	63 73
50	6L	511/533 (96%)	505 (99%)	6 (1%)	63 73
51	6M	827/1940 (43%)	820 (99%)	7 (1%)	73 77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
51	6N	827/1940 (43%)	820 (99%)	7 (1%)	73 77
All	All	78493/114873 (68%)	77261 (98%)	1232 (2%)	54 69

5 of 1232 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	8f	94	SER
13	Cd	361	THR
13	9b	77	GLU
13	8f	77	GLU
13	Af	165	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 1608 such sidechains are listed below:

Mol	Chain	Res	Type
44	5T	111	HIS
51	6N	1254	GLN
1	0K	162	GLN
12	5c	347	ASN
44	5S	111	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

104 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
53	GDP	1a	501	-	29,30,30	1.17	2 (6%)	45,47,47	1.75	7 (15%)
54	GTP	9h	501	-	33,34,34	0.99	2 (6%)	50,54,54	1.57	8 (16%)
53	GDP	2g	501	-	29,30,30	1.15	2 (6%)	45,47,47	1.75	7 (15%)
54	GTP	1f	501	-	33,34,34	0.99	2 (6%)	50,54,54	1.56	8 (16%)
54	GTP	Db	501	-	33,34,34	0.99	2 (6%)	50,54,54	1.56	8 (16%)
53	GDP	2c	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	7 (15%)
53	GDP	Ba	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.74	7 (15%)
54	GTP	7h	501	-	33,34,34	0.99	2 (6%)	50,54,54	1.56	8 (16%)
53	GDP	3g	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.75	7 (15%)
53	GDP	6e	502	-	29,30,30	1.17	3 (10%)	45,47,47	1.73	7 (15%)
54	GTP	9f	501	-	33,34,34	0.99	2 (6%)	50,54,54	1.56	8 (16%)
54	GTP	5c	501	-	33,34,34	1.00	2 (6%)	50,54,54	1.56	8 (16%)
53	GDP	9a	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.73	7 (15%)
54	GTP	7e	501	-	33,34,34	0.99	2 (6%)	50,54,54	1.56	8 (16%)
54	GTP	Ah	501	-	33,34,34	1.00	3 (9%)	50,54,54	1.56	8 (16%)
54	GTP	8f	501	-	33,34,34	0.99	2 (6%)	50,54,54	1.56	8 (16%)
54	GTP	Bd	501	-	33,34,34	0.98	2 (6%)	50,54,54	1.56	8 (16%)
53	GDP	6a	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.73	7 (15%)
53	GDP	Dg	501	-	29,30,30	1.15	2 (6%)	45,47,47	1.75	7 (15%)
53	GDP	Cc	502	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
53	GDP	8c	501	-	29,30,30	1.15	2 (6%)	45,47,47	1.76	7 (15%)
54	GTP	2d	501	-	33,34,34	0.99	2 (6%)	50,54,54	1.56	8 (16%)
53	GDP	Ae	502	-	29,30,30	1.16	2 (6%)	45,47,47	1.75	7 (15%)
54	GTP	6e	501	-	33,34,34	0.99	3 (9%)	50,54,54	1.56	8 (16%)
53	GDP	1e	501	-	29,30,30	1.15	2 (6%)	45,47,47	1.75	7 (15%)
54	GTP	9e	501	-	33,34,34	0.99	2 (6%)	50,54,54	1.56	8 (16%)
53	GDP	9c	501	-	29,30,30	1.15	2 (6%)	45,47,47	1.77	7 (15%)
54	GTP	Dh	501	-	33,34,34	0.99	2 (6%)	50,54,54	1.56	8 (16%)
53	GDP	4e	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.74	7 (15%)
54	GTP	8d	501	-	33,34,34	0.99	2 (6%)	50,54,54	1.56	8 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
54	GTP	2b	501	-	33,34,34	0.99	2 (6%)	50,54,54	1.56	8 (16%)
53	GDP	8a	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.74	7 (15%)
53	GDP	8e	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.74	7 (15%)
53	GDP	9e	502	-	29,30,30	1.17	3 (10%)	45,47,47	1.74	7 (15%)
54	GTP	8h	501	-	33,34,34	1.00	3 (9%)	50,54,54	1.56	8 (16%)
53	GDP	Be	501	-	29,30,30	1.16	2 (6%)	45,47,47	1.74	7 (15%)
53	GDP	7c	501	-	29,30,30	1.16	2 (6%)	45,47,47	1.74	7 (15%)
53	GDP	Ce	501	-	29,30,30	1.16	2 (6%)	45,47,47	1.74	7 (15%)
53	GDP	3c	502	-	29,30,30	1.16	3 (10%)	45,47,47	1.74	7 (15%)
53	GDP	5a	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.74	7 (15%)
54	GTP	3d	501	-	33,34,34	0.99	2 (6%)	50,54,54	1.56	8 (16%)
53	GDP	Ca	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.74	7 (15%)
53	GDP	4c	501	-	29,30,30	1.16	2 (6%)	45,47,47	1.74	7 (15%)
54	GTP	Af	501	-	33,34,34	0.99	2 (6%)	50,54,54	1.56	8 (16%)
53	GDP	Dc	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.74	7 (15%)
54	GTP	4b	501	-	33,34,34	0.99	2 (6%)	50,54,54	1.56	8 (16%)
54	GTP	Bh	501	-	33,34,34	0.99	2 (6%)	50,54,54	1.57	8 (16%)
54	GTP	Ab	501	-	33,34,34	0.99	2 (6%)	50,54,54	1.56	8 (16%)
54	GTP	5f	501	-	33,34,34	0.99	2 (6%)	50,54,54	1.56	8 (16%)
53	GDP	3a	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.75	7 (15%)
53	GDP	5e	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.73	7 (15%)
54	GTP	3h	501	-	33,34,34	0.98	2 (6%)	50,54,54	1.56	8 (16%)
53	GDP	7e	502	-	29,30,30	1.17	3 (10%)	45,47,47	1.74	7 (15%)
54	GTP	Bb	501	-	33,34,34	0.99	2 (6%)	50,54,54	1.56	8 (16%)
54	GTP	4f	501	-	33,34,34	0.99	2 (6%)	50,54,54	1.56	8 (16%)
54	GTP	6h	501	-	33,34,34	0.99	2 (6%)	50,54,54	1.57	8 (16%)
54	GTP	Ae	501	-	33,34,34	0.98	2 (6%)	50,54,54	1.56	8 (16%)
53	GDP	4g	501	-	29,30,30	1.15	2 (6%)	45,47,47	1.74	7 (15%)
53	GDP	2a	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.74	7 (15%)
53	GDP	9g	501	-	29,30,30	1.14	2 (6%)	45,47,47	1.77	7 (15%)
53	GDP	3e	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.75	7 (15%)
54	GTP	Df	501	-	33,34,34	0.99	2 (6%)	50,54,54	1.56	8 (16%)
54	GTP	8b	501	-	33,34,34	0.98	2 (6%)	50,54,54	1.57	8 (16%)
53	GDP	Cg	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.74	7 (15%)
54	GTP	2f	501	-	33,34,34	0.99	2 (6%)	50,54,54	1.56	8 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
53	GDP	5g	501	-	29,30,30	1.15	2 (6%)	45,47,47	1.75	7 (15%)
53	GDP	6g	502	-	29,30,30	1.16	2 (6%)	45,47,47	1.74	7 (15%)
53	GDP	5c	502	-	29,30,30	1.16	3 (10%)	45,47,47	1.74	7 (15%)
54	GTP	4h	501	-	33,34,34	0.99	2 (6%)	50,54,54	1.56	8 (16%)
54	GTP	6c	501	-	33,34,34	0.99	2 (6%)	50,54,54	1.56	8 (16%)
54	GTP	1b	501	-	33,34,34	0.99	2 (6%)	50,54,54	1.56	8 (16%)
53	GDP	De	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.74	7 (15%)
54	GTP	1d	501	-	33,34,34	0.99	2 (6%)	50,54,54	1.57	8 (16%)
54	GTP	4d	501	-	33,34,34	0.98	2 (6%)	50,54,54	1.56	8 (16%)
53	GDP	1g	501	-	29,30,30	1.16	2 (6%)	45,47,47	1.75	7 (15%)
53	GDP	7a	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.74	7 (15%)
54	GTP	5h	501	-	33,34,34	0.99	2 (6%)	50,54,54	1.56	8 (16%)
53	GDP	Bg	501	-	29,30,30	1.15	2 (6%)	45,47,47	1.75	7 (15%)
54	GTP	7b	501	-	33,34,34	0.99	2 (6%)	50,54,54	1.56	8 (16%)
54	GTP	Cf	501	-	33,34,34	0.99	2 (6%)	50,54,54	1.56	8 (16%)
53	GDP	1c	501	-	29,30,30	1.15	2 (6%)	45,47,47	1.75	7 (15%)
53	GDP	Aa	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.74	7 (15%)
54	GTP	Ch	501	-	33,34,34	1.00	3 (9%)	50,54,54	1.56	8 (16%)
54	GTP	7f	501	-	33,34,34	0.98	1 (3%)	50,54,54	1.56	8 (16%)
54	GTP	6g	501	-	33,34,34	0.99	2 (6%)	50,54,54	1.56	8 (16%)
54	GTP	Cd	501	-	33,34,34	0.99	2 (6%)	50,54,54	1.56	8 (16%)
54	GTP	1h	501	-	33,34,34	0.99	2 (6%)	50,54,54	1.56	8 (16%)
53	GDP	Ac	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.74	7 (15%)
54	GTP	9b	501	-	33,34,34	0.99	2 (6%)	50,54,54	1.56	8 (16%)
53	GDP	Bc	501	-	29,30,30	1.15	2 (6%)	45,47,47	1.77	7 (15%)
54	GTP	Dd	501	-	33,34,34	1.00	2 (6%)	50,54,54	1.56	8 (16%)
53	GDP	7g	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.75	7 (15%)
54	GTP	3c	501	-	33,34,34	0.99	2 (6%)	50,54,54	1.56	8 (16%)
53	GDP	Da	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.74	7 (15%)
53	GDP	6c	502	-	29,30,30	1.15	2 (6%)	45,47,47	1.75	7 (15%)
53	GDP	Ag	501	-	29,30,30	1.15	2 (6%)	45,47,47	1.74	7 (15%)
54	GTP	Bf	501	-	33,34,34	0.99	2 (6%)	50,54,54	1.56	8 (16%)
53	GDP	8g	501	-	29,30,30	1.15	2 (6%)	45,47,47	1.74	7 (15%)
53	GDP	2e	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.74	7 (15%)
54	GTP	2h	501	-	33,34,34	0.98	2 (6%)	50,54,54	1.56	8 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
54	GTP	5d	501	-	33,34,34	0.99	2 (6%)	50,54,54	1.56	8 (16%)
54	GTP	Cc	501	-	33,34,34	0.99	2 (6%)	50,54,54	1.56	8 (16%)
54	GTP	3f	501	-	33,34,34	0.99	2 (6%)	50,54,54	1.56	8 (16%)
53	GDP	4a	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.73	7 (15%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
53	GDP	1a	501	-	-	3/16/32/32	0/3/3/3
54	GTP	9h	501	-	-	2/22/38/38	0/3/3/3
53	GDP	2g	501	-	-	3/16/32/32	0/3/3/3
54	GTP	1f	501	-	-	2/22/38/38	0/3/3/3
54	GTP	Db	501	-	-	2/22/38/38	0/3/3/3
53	GDP	2c	501	-	-	3/16/32/32	0/3/3/3
53	GDP	Ba	501	-	-	3/16/32/32	0/3/3/3
54	GTP	7h	501	-	-	2/22/38/38	0/3/3/3
53	GDP	3g	501	-	-	3/16/32/32	0/3/3/3
53	GDP	6e	502	-	-	3/16/32/32	0/3/3/3
54	GTP	9f	501	-	-	2/22/38/38	0/3/3/3
54	GTP	5c	501	-	-	2/22/38/38	0/3/3/3
53	GDP	9a	501	-	-	3/16/32/32	0/3/3/3
54	GTP	7e	501	-	-	2/22/38/38	0/3/3/3
54	GTP	Ah	501	-	-	2/22/38/38	0/3/3/3
54	GTP	8f	501	-	-	2/22/38/38	0/3/3/3
54	GTP	Bd	501	-	-	2/22/38/38	0/3/3/3
53	GDP	6a	501	-	-	3/16/32/32	0/3/3/3
53	GDP	Dg	501	-	-	3/16/32/32	0/3/3/3
53	GDP	Cc	502	-	-	3/16/32/32	0/3/3/3
53	GDP	8c	501	-	-	3/16/32/32	0/3/3/3
54	GTP	2d	501	-	-	2/22/38/38	0/3/3/3
53	GDP	Ae	502	-	-	3/16/32/32	0/3/3/3
54	GTP	6e	501	-	-	2/22/38/38	0/3/3/3
53	GDP	1e	501	-	-	3/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	GTP	9e	501	-	-	2/22/38/38	0/3/3/3
53	GDP	9c	501	-	-	3/16/32/32	0/3/3/3
54	GTP	Dh	501	-	-	2/22/38/38	0/3/3/3
53	GDP	4e	501	-	-	3/16/32/32	0/3/3/3
54	GTP	8d	501	-	-	2/22/38/38	0/3/3/3
54	GTP	2b	501	-	-	2/22/38/38	0/3/3/3
53	GDP	8a	501	-	-	3/16/32/32	0/3/3/3
53	GDP	8e	501	-	-	3/16/32/32	0/3/3/3
53	GDP	9e	502	-	-	3/16/32/32	0/3/3/3
54	GTP	8h	501	-	-	2/22/38/38	0/3/3/3
53	GDP	Be	501	-	-	3/16/32/32	0/3/3/3
53	GDP	7c	501	-	-	3/16/32/32	0/3/3/3
53	GDP	Ce	501	-	-	3/16/32/32	0/3/3/3
53	GDP	3c	502	-	-	3/16/32/32	0/3/3/3
53	GDP	5a	501	-	-	3/16/32/32	0/3/3/3
54	GTP	3d	501	-	-	2/22/38/38	0/3/3/3
53	GDP	Ca	501	-	-	3/16/32/32	0/3/3/3
53	GDP	4c	501	-	-	3/16/32/32	0/3/3/3
54	GTP	Af	501	-	-	2/22/38/38	0/3/3/3
53	GDP	Dc	501	-	-	3/16/32/32	0/3/3/3
54	GTP	4b	501	-	-	2/22/38/38	0/3/3/3
54	GTP	Bh	501	-	-	2/22/38/38	0/3/3/3
54	GTP	Ab	501	-	-	2/22/38/38	0/3/3/3
54	GTP	5f	501	-	-	2/22/38/38	0/3/3/3
53	GDP	3a	501	-	-	3/16/32/32	0/3/3/3
53	GDP	5e	501	-	-	3/16/32/32	0/3/3/3
54	GTP	3h	501	-	-	2/22/38/38	0/3/3/3
53	GDP	7e	502	-	-	3/16/32/32	0/3/3/3
54	GTP	Bb	501	-	-	2/22/38/38	0/3/3/3
54	GTP	4f	501	-	-	2/22/38/38	0/3/3/3
54	GTP	6h	501	-	-	2/22/38/38	0/3/3/3
54	GTP	Ae	501	-	-	2/22/38/38	0/3/3/3
53	GDP	4g	501	-	-	3/16/32/32	0/3/3/3
53	GDP	2a	501	-	-	3/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
53	GDP	9g	501	-	-	3/16/32/32	0/3/3/3
53	GDP	3e	501	-	-	3/16/32/32	0/3/3/3
54	GTP	Df	501	-	-	2/22/38/38	0/3/3/3
54	GTP	8b	501	-	-	2/22/38/38	0/3/3/3
53	GDP	Cg	501	-	-	3/16/32/32	0/3/3/3
54	GTP	2f	501	-	-	2/22/38/38	0/3/3/3
53	GDP	5g	501	-	-	3/16/32/32	0/3/3/3
53	GDP	6g	502	-	-	3/16/32/32	0/3/3/3
53	GDP	5c	502	-	-	3/16/32/32	0/3/3/3
54	GTP	4h	501	-	-	2/22/38/38	0/3/3/3
54	GTP	6c	501	-	-	2/22/38/38	0/3/3/3
54	GTP	1b	501	-	-	2/22/38/38	0/3/3/3
53	GDP	De	501	-	-	3/16/32/32	0/3/3/3
54	GTP	1d	501	-	-	2/22/38/38	0/3/3/3
54	GTP	4d	501	-	-	2/22/38/38	0/3/3/3
53	GDP	1g	501	-	-	3/16/32/32	0/3/3/3
53	GDP	7a	501	-	-	3/16/32/32	0/3/3/3
54	GTP	5h	501	-	-	2/22/38/38	0/3/3/3
53	GDP	Bg	501	-	-	3/16/32/32	0/3/3/3
54	GTP	7b	501	-	-	2/22/38/38	0/3/3/3
54	GTP	Cf	501	-	-	2/22/38/38	0/3/3/3
53	GDP	1c	501	-	-	3/16/32/32	0/3/3/3
53	GDP	Aa	501	-	-	3/16/32/32	0/3/3/3
54	GTP	Ch	501	-	-	2/22/38/38	0/3/3/3
54	GTP	7f	501	-	-	2/22/38/38	0/3/3/3
54	GTP	6g	501	-	-	2/22/38/38	0/3/3/3
54	GTP	Cd	501	-	-	2/22/38/38	0/3/3/3
54	GTP	1h	501	-	-	2/22/38/38	0/3/3/3
53	GDP	Ac	501	-	-	3/16/32/32	0/3/3/3
54	GTP	9b	501	-	-	2/22/38/38	0/3/3/3
53	GDP	Bc	501	-	-	3/16/32/32	0/3/3/3
54	GTP	Dd	501	-	-	2/22/38/38	0/3/3/3
53	GDP	7g	501	-	-	3/16/32/32	0/3/3/3
54	GTP	3c	501	-	-	2/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
53	GDP	Da	501	-	-	3/16/32/32	0/3/3/3
53	GDP	6c	502	-	-	3/16/32/32	0/3/3/3
53	GDP	Ag	501	-	-	3/16/32/32	0/3/3/3
54	GTP	Bf	501	-	-	2/22/38/38	0/3/3/3
53	GDP	8g	501	-	-	3/16/32/32	0/3/3/3
53	GDP	2e	501	-	-	3/16/32/32	0/3/3/3
54	GTP	2h	501	-	-	2/22/38/38	0/3/3/3
54	GTP	5d	501	-	-	2/22/38/38	0/3/3/3
54	GTP	Cc	501	-	-	2/22/38/38	0/3/3/3
54	GTP	3f	501	-	-	2/22/38/38	0/3/3/3
53	GDP	4a	501	-	-	3/16/32/32	0/3/3/3

The worst 5 of 241 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	8a	501	GDP	C5-C4	3.20	1.47	1.38
53	4e	501	GDP	C5-C4	3.17	1.47	1.38
53	2e	501	GDP	C5-C4	3.16	1.47	1.38
53	5e	501	GDP	C5-C4	3.16	1.47	1.38
53	3a	501	GDP	C5-C4	3.16	1.47	1.38

The worst 5 of 780 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	7e	502	GDP	C5-C4-N3	-6.20	118.53	128.39
53	6e	502	GDP	C5-C4-N3	-6.18	118.55	128.39
53	3e	501	GDP	C5-C4-N3	-6.18	118.56	128.39
53	4a	501	GDP	C5-C4-N3	-6.17	118.57	128.39
53	4e	501	GDP	C5-C4-N3	-6.16	118.59	128.39

There are no chirality outliers.

5 of 260 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
53	1a	501	GDP	C5'-O5'-PA-O3A
53	1a	501	GDP	C5'-O5'-PA-O1A
53	1a	501	GDP	C5'-O5'-PA-O2A
53	1c	501	GDP	C5'-O5'-PA-O3A
53	1c	501	GDP	C5'-O5'-PA-O1A

There are no ring outliers.

68 monomers are involved in 264 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
53	1a	501	GDP	2	0
54	9h	501	GTP	3	0
54	1f	501	GTP	4	0
54	Db	501	GTP	5	0
53	2c	501	GDP	1	0
53	Ba	501	GDP	1	0
54	7h	501	GTP	4	0
53	6e	502	GDP	1	0
54	9f	501	GTP	7	0
54	5c	501	GTP	4	0
54	7e	501	GTP	5	0
54	Ah	501	GTP	4	0
54	8f	501	GTP	5	0
54	Bd	501	GTP	5	0
53	Dg	501	GDP	1	0
53	Cc	502	GDP	1	0
53	8c	501	GDP	1	0
54	2d	501	GTP	6	0
54	6e	501	GTP	4	0
53	1e	501	GDP	3	0
54	9e	501	GTP	4	0
54	Dh	501	GTP	4	0
54	8d	501	GTP	4	0
54	2b	501	GTP	7	0
54	8h	501	GTP	5	0
53	Be	501	GDP	1	0
54	3d	501	GTP	3	0
54	Af	501	GTP	7	0
54	4b	501	GTP	4	0
54	Bh	501	GTP	5	0
54	Ab	501	GTP	6	0
54	5f	501	GTP	5	0
53	3a	501	GDP	1	0
54	3h	501	GTP	3	0
53	7e	502	GDP	2	0
54	Bb	501	GTP	6	0
54	4f	501	GTP	5	0
54	6h	501	GTP	4	0
54	Ae	501	GTP	4	0
53	2a	501	GDP	1	0

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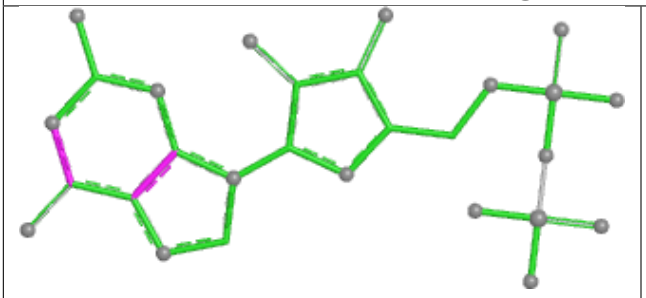
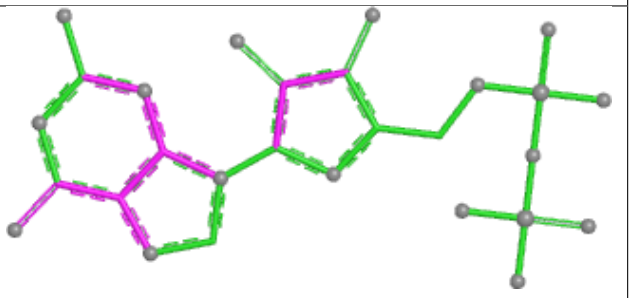
Mol	Chain	Res	Type	Clashes	Symm-Clashes
53	3e	501	GDP	1	0
54	Df	501	GTP	5	0
54	8b	501	GTP	4	0
54	2f	501	GTP	5	0
54	4h	501	GTP	3	0
54	6c	501	GTP	6	0
54	1b	501	GTP	5	0
54	1d	501	GTP	4	0
54	4d	501	GTP	3	0
53	7a	501	GDP	1	0
54	5h	501	GTP	5	0
53	Bg	501	GDP	1	0
54	7b	501	GTP	5	0
54	Cf	501	GTP	6	0
54	Ch	501	GTP	5	0
54	7f	501	GTP	5	0
54	6g	501	GTP	5	0
54	Cd	501	GTP	5	0
54	1h	501	GTP	3	0
54	9b	501	GTP	5	0
54	Dd	501	GTP	5	0
54	3c	501	GTP	5	0
54	Bf	501	GTP	6	0
54	2h	501	GTP	4	0
54	5d	501	GTP	3	0
54	Cc	501	GTP	6	0
54	3f	501	GTP	4	0
53	4a	501	GDP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

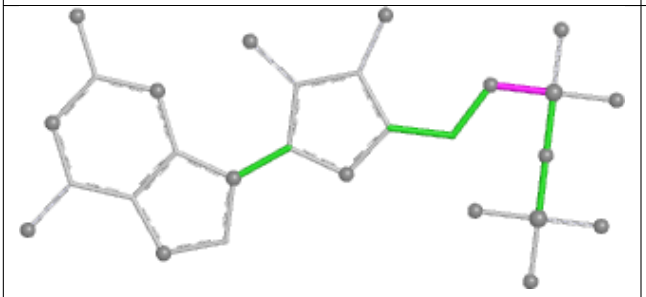
Ligand GDP 1a 501



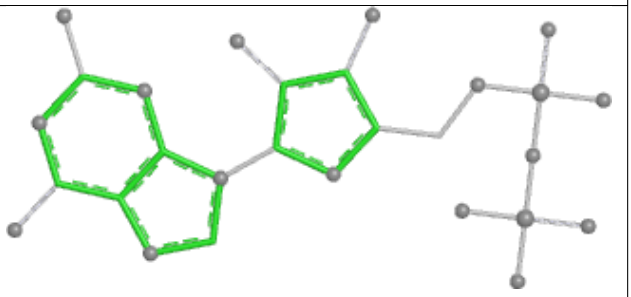
Bond lengths



Bond angles

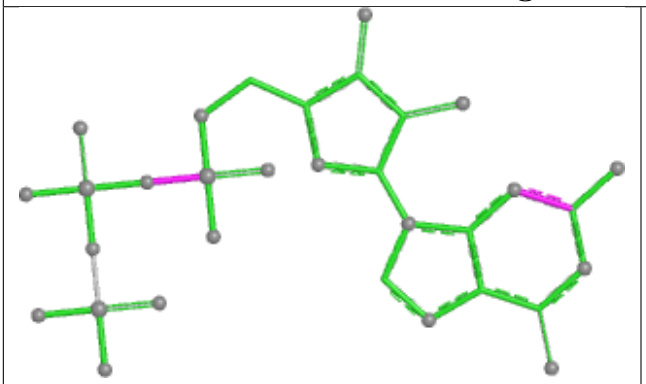


Torsions

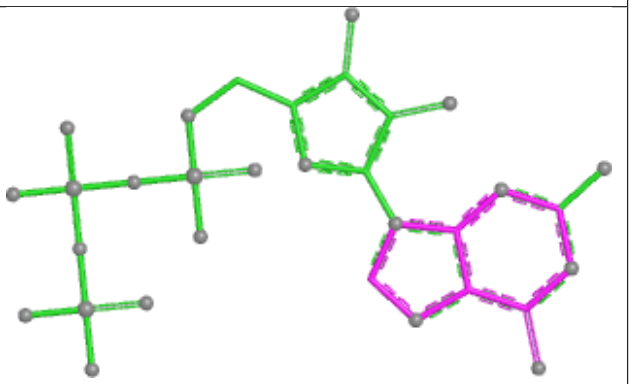


Rings

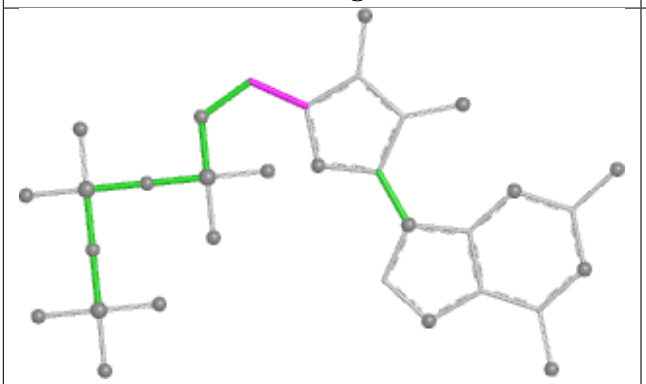
Ligand GTP 9h 501



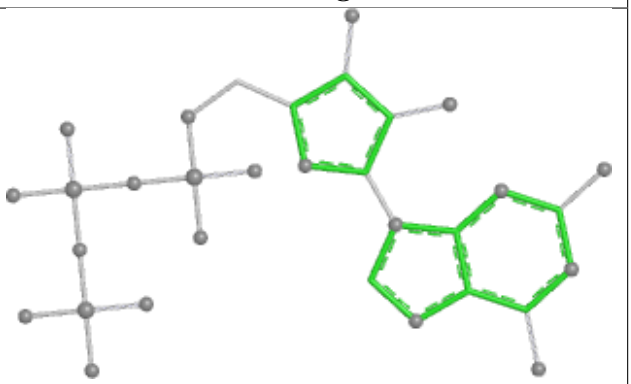
Bond lengths



Bond angles

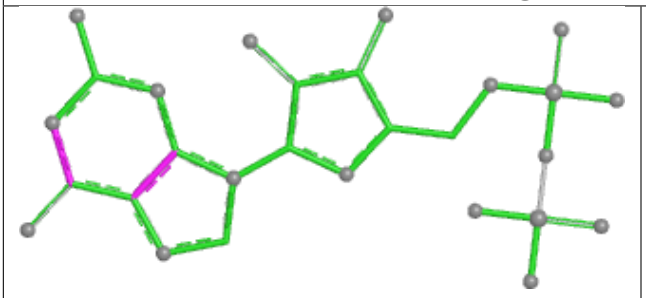


Torsions

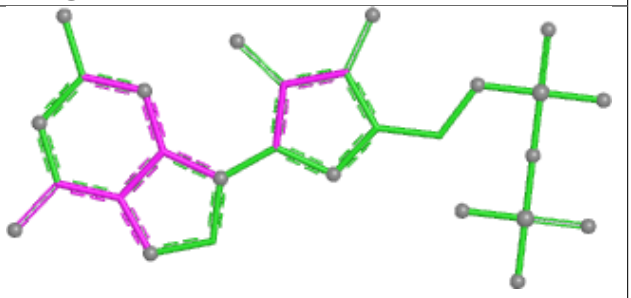


Rings

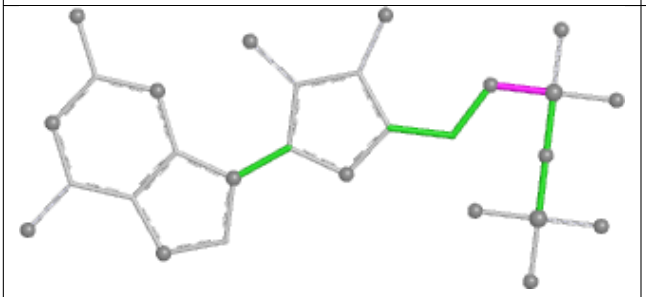
Ligand GDP 2g 501



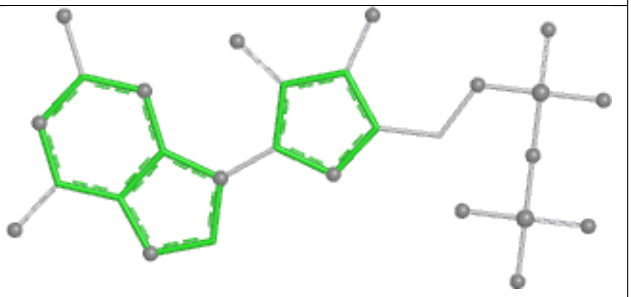
Bond lengths



Bond angles

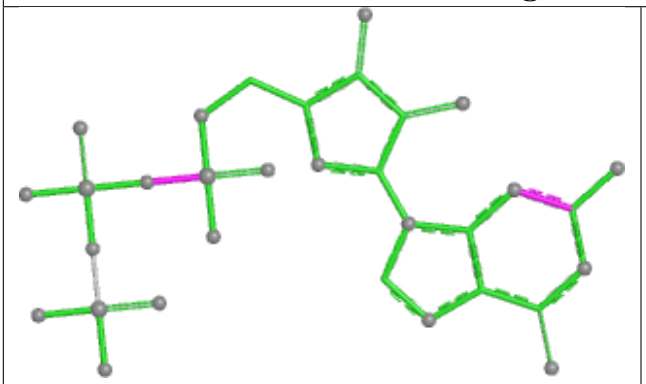


Torsions

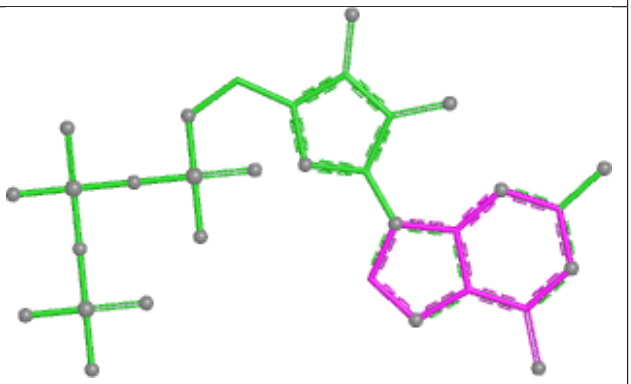


Rings

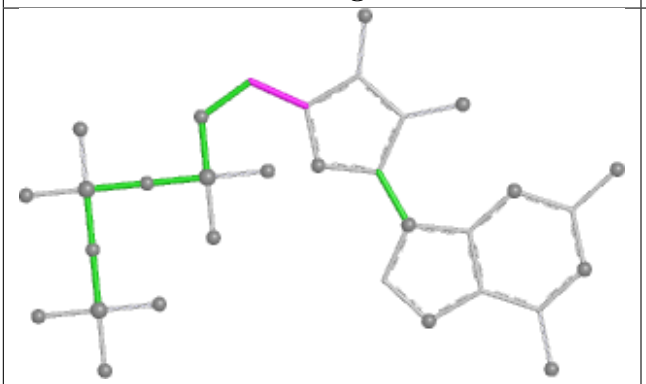
Ligand GTP 1f 501



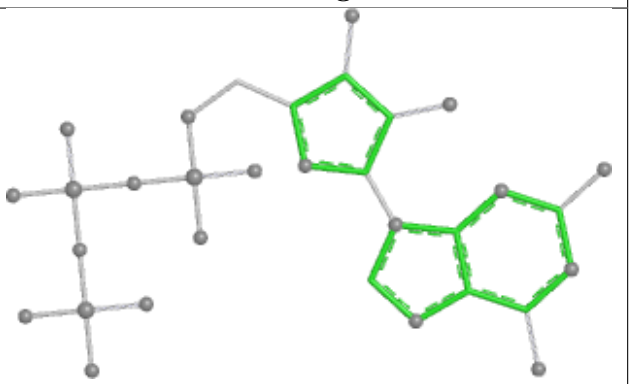
Bond lengths



Bond angles

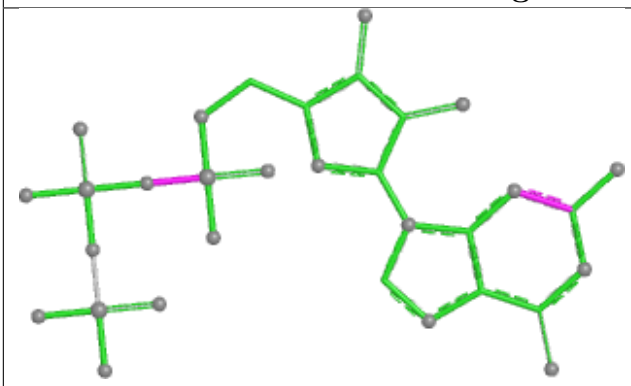


Torsions

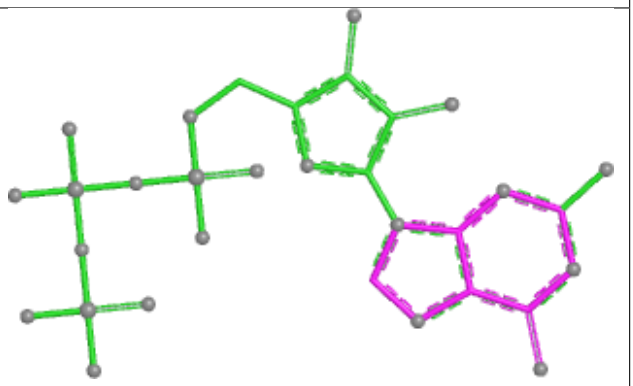


Rings

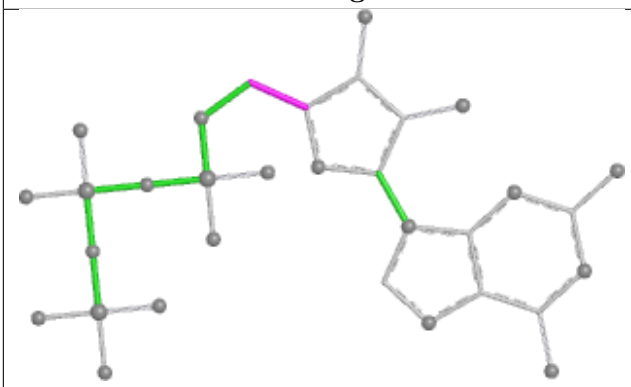
Ligand GTP Db 501



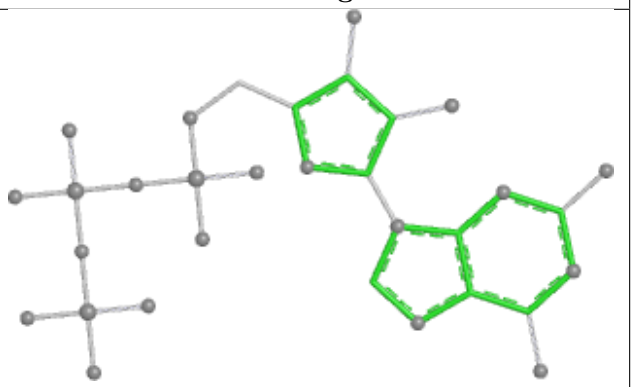
Bond lengths



Bond angles

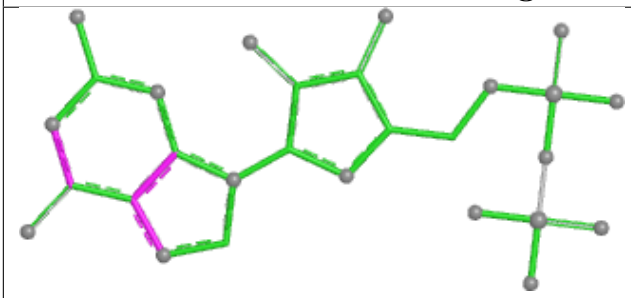


Torsions



Rings

Ligand GDP 2c 501



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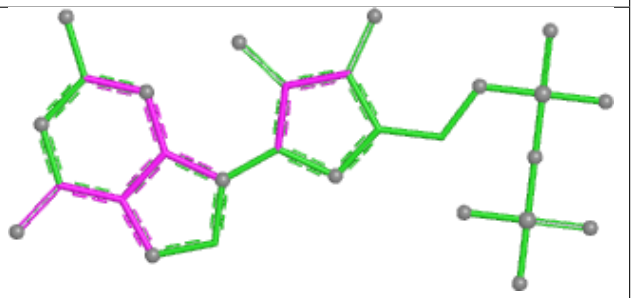

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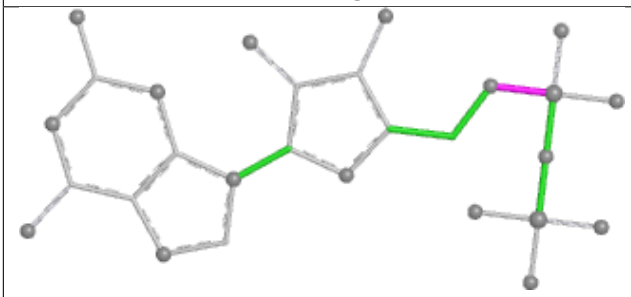

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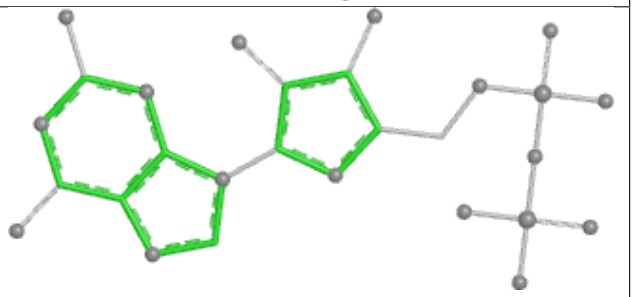
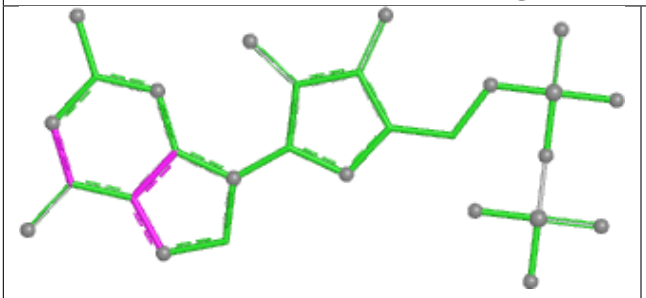


Rings

Ligand GDP Ba 501



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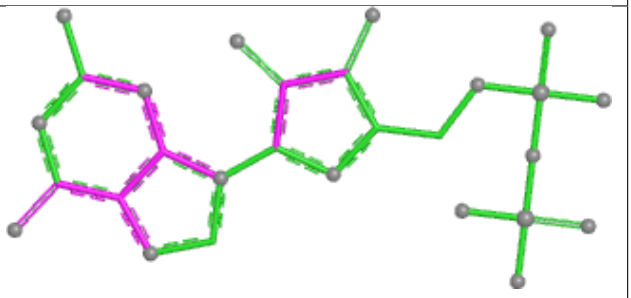

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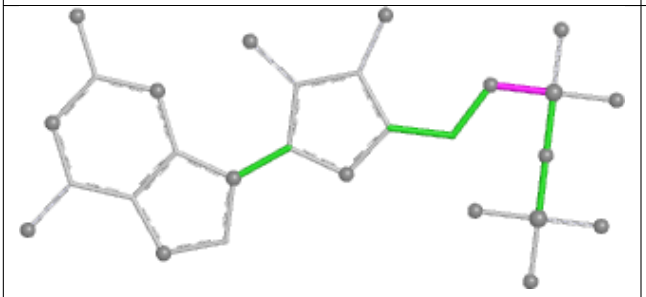

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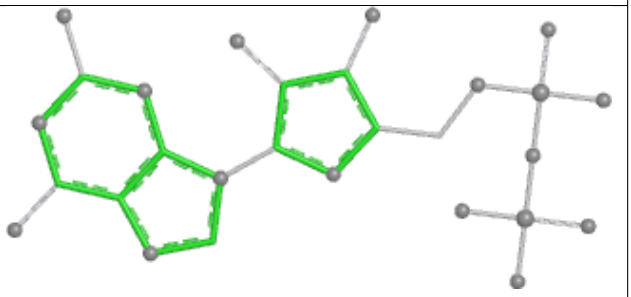

Rings

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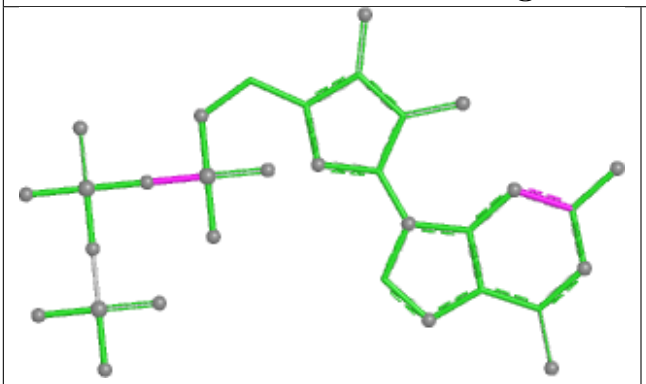

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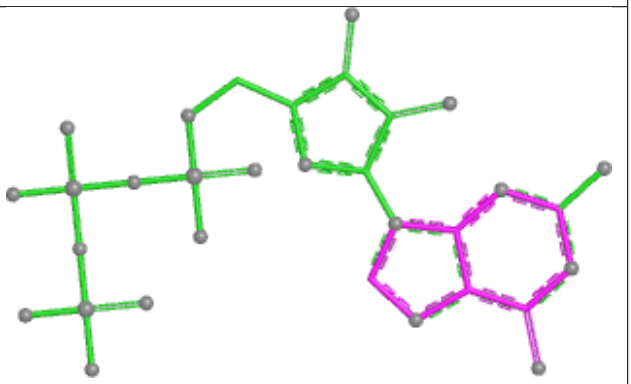

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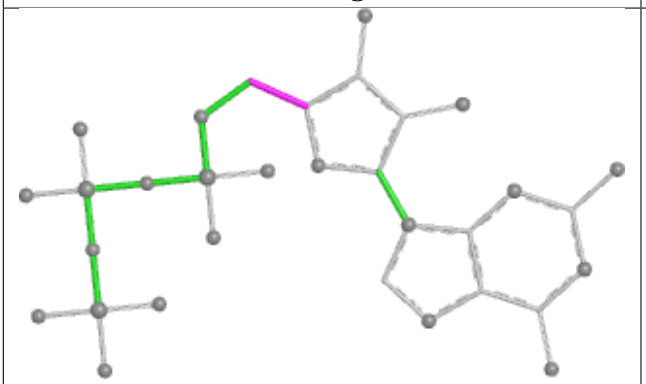

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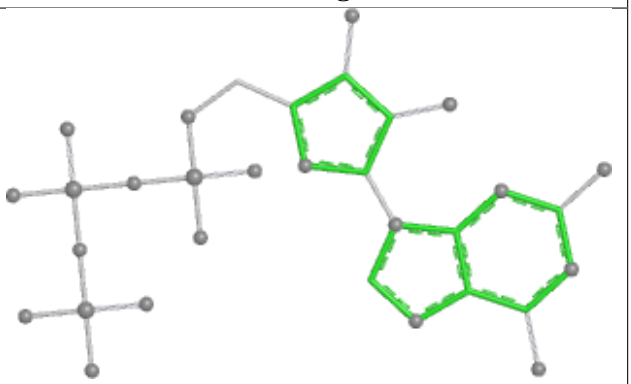

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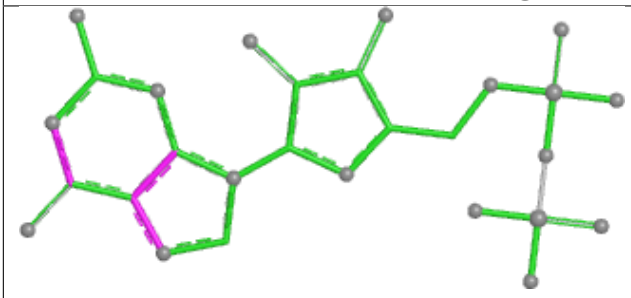
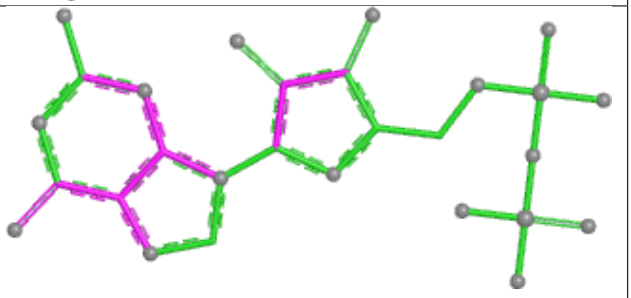
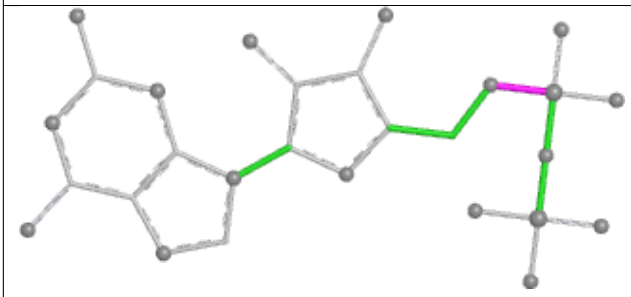
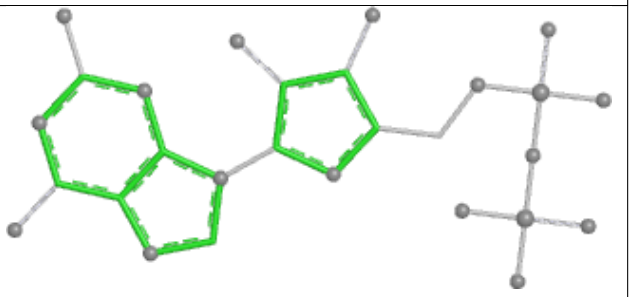
 Bond lengths	 Bond angles
 Torsions	 Rings

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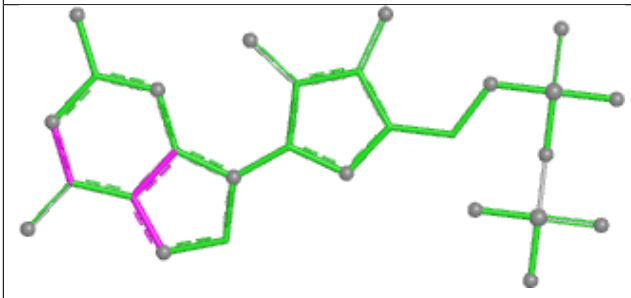
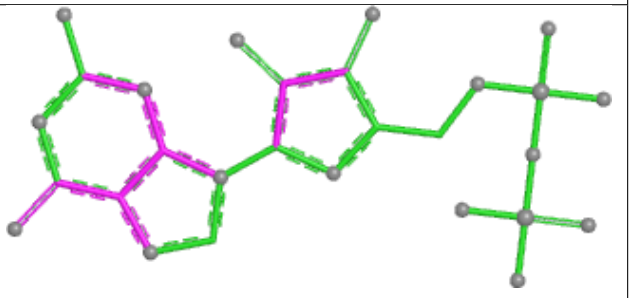
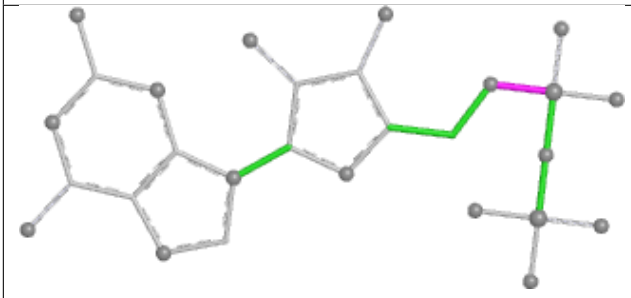
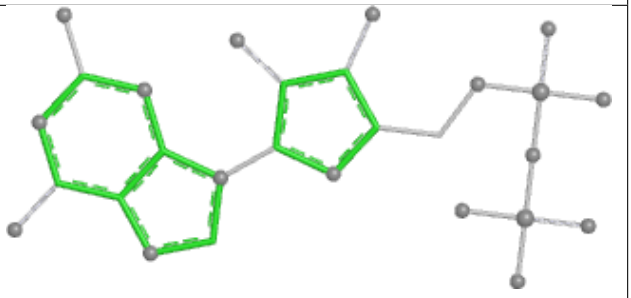
 Bond lengths	 Bond angles
 Torsions	 Rings

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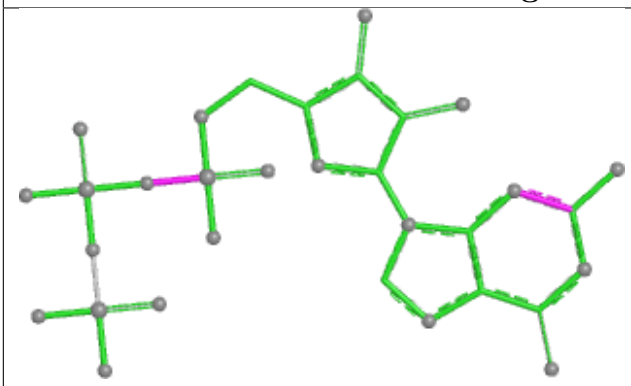

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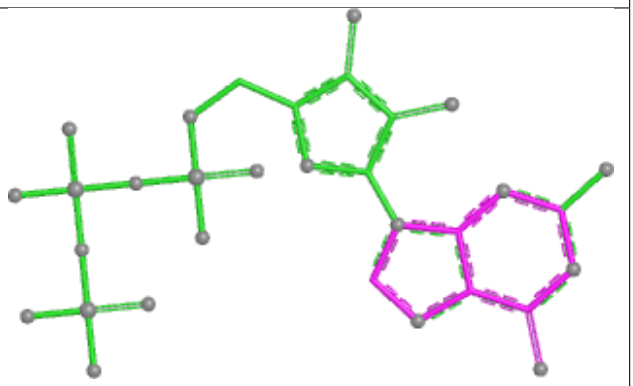

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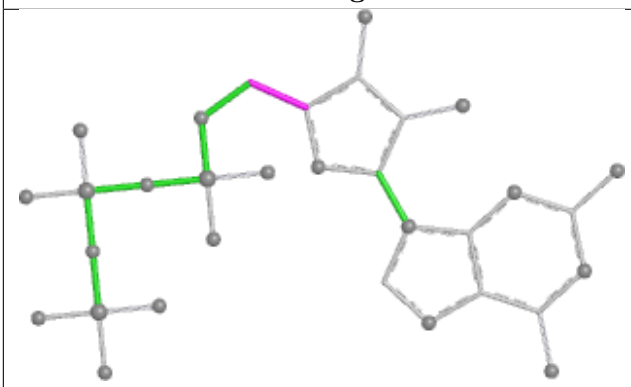

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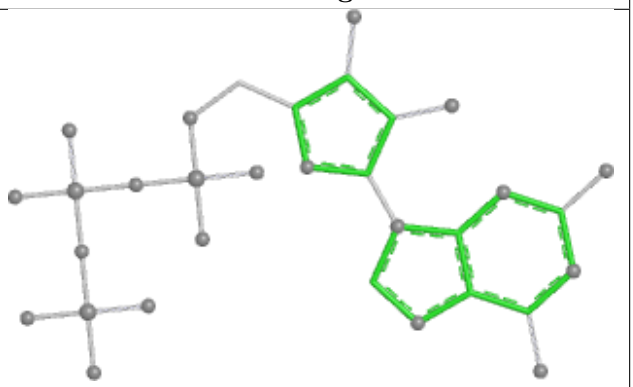

Rings

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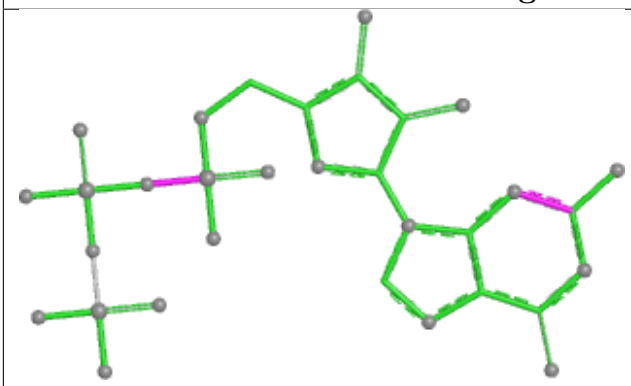

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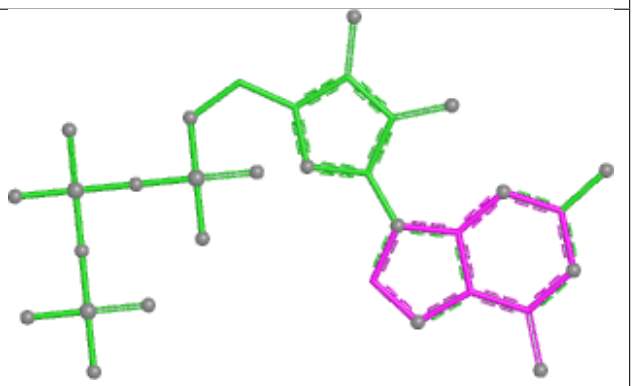

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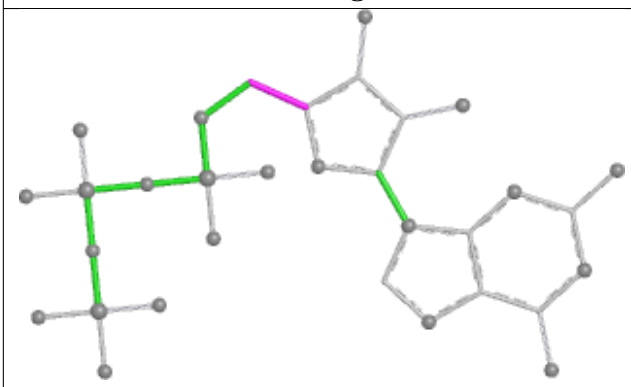

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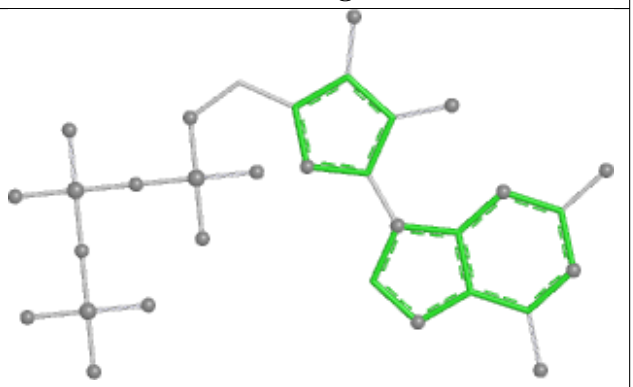

Rings

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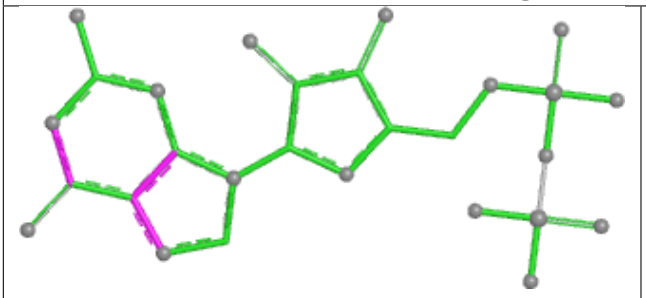

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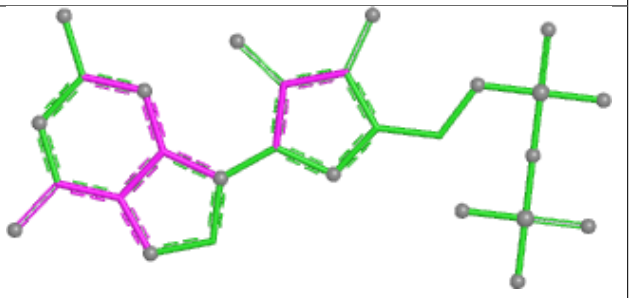

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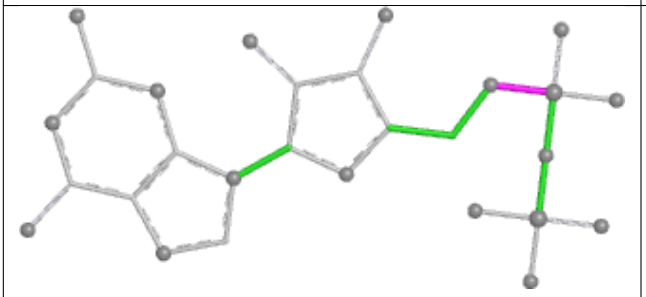

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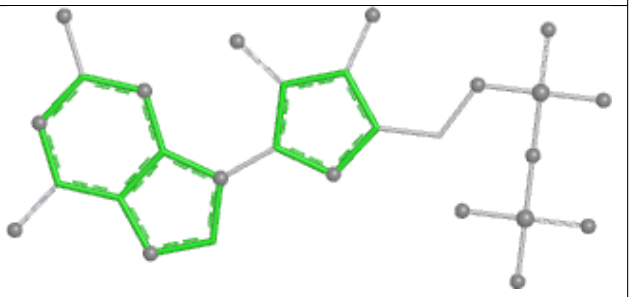

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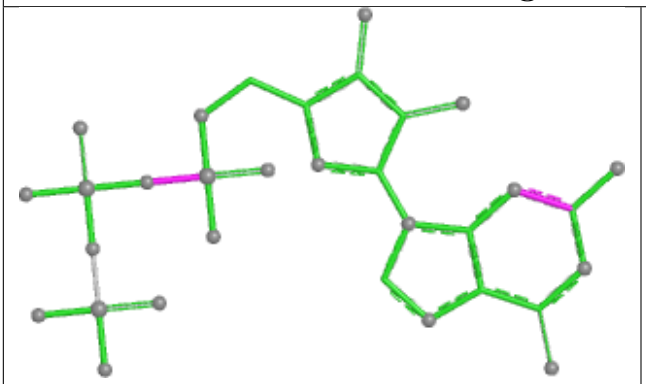

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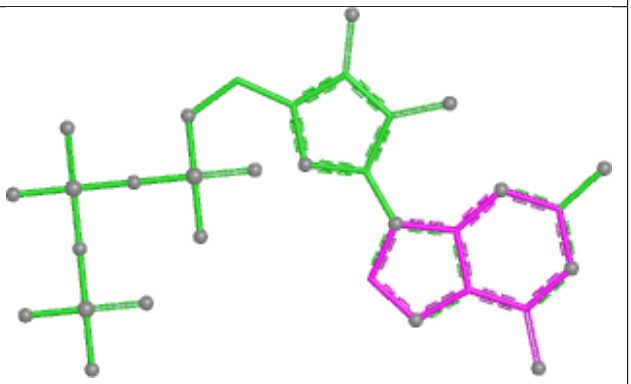

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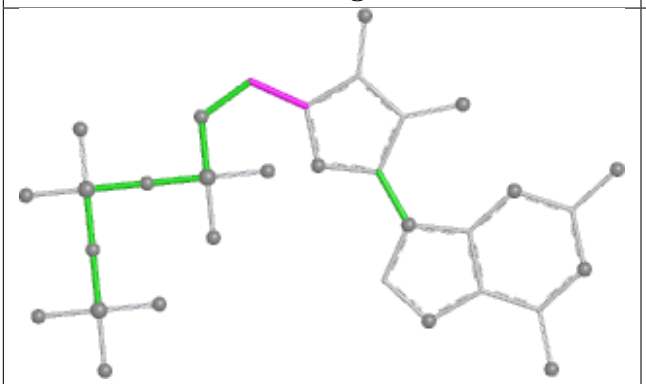

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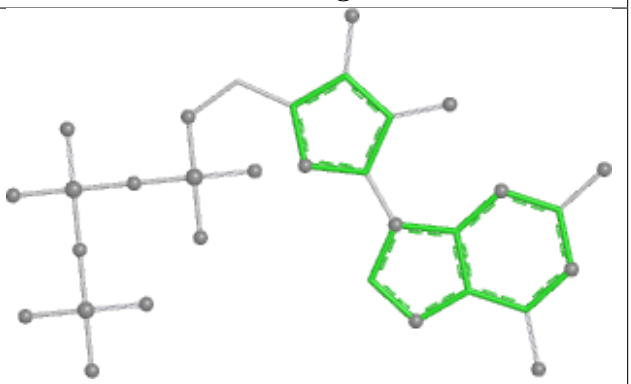

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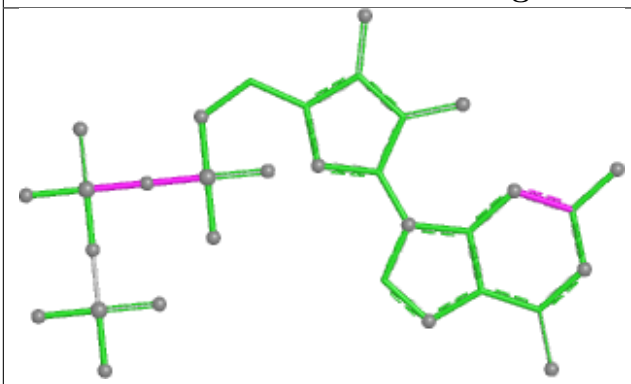

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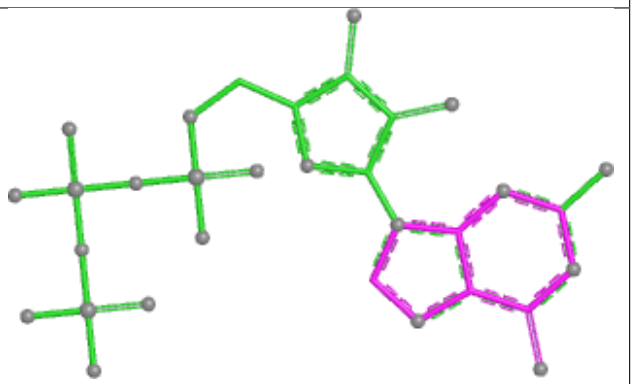

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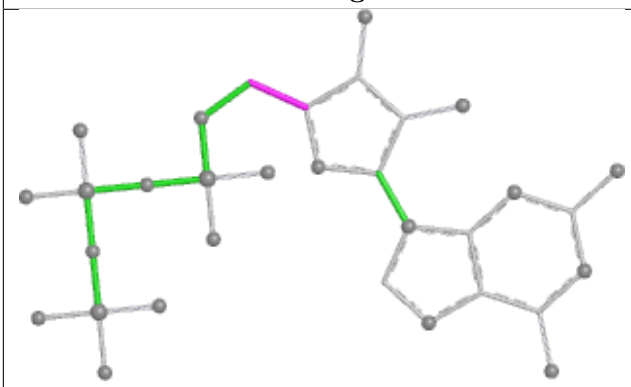

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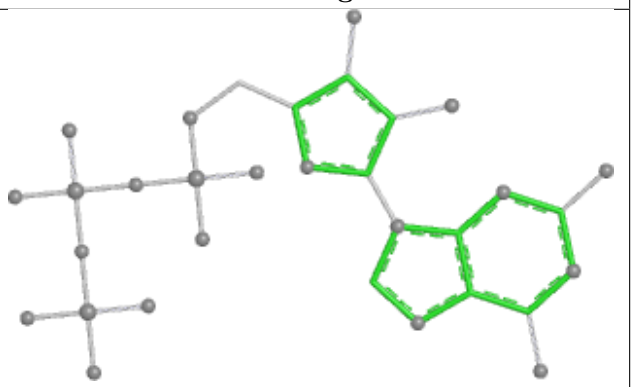

Rings

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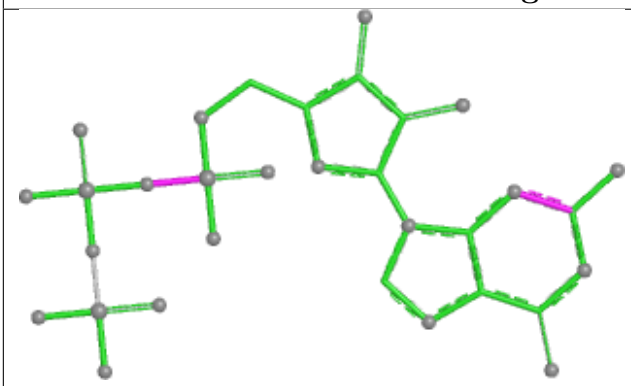

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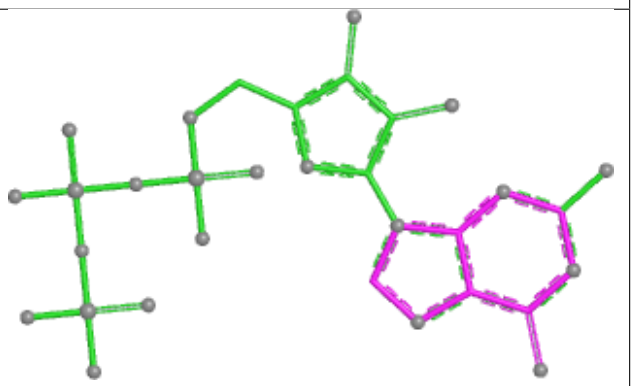

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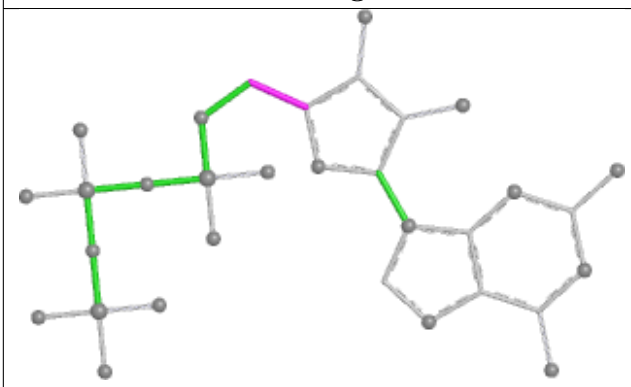

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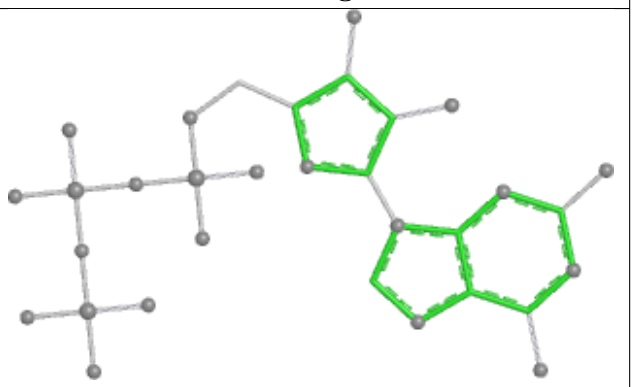

Rings

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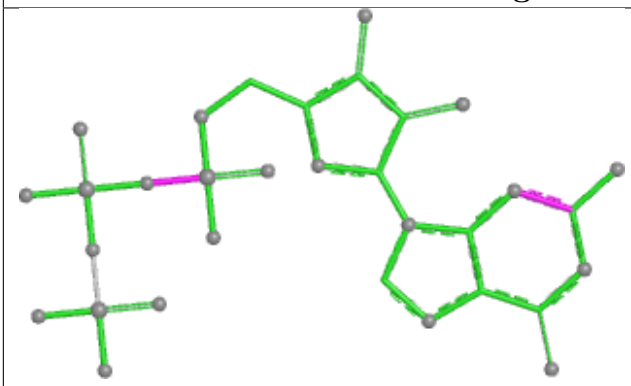

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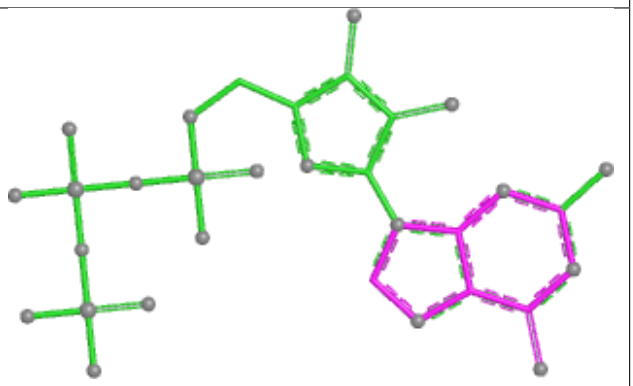

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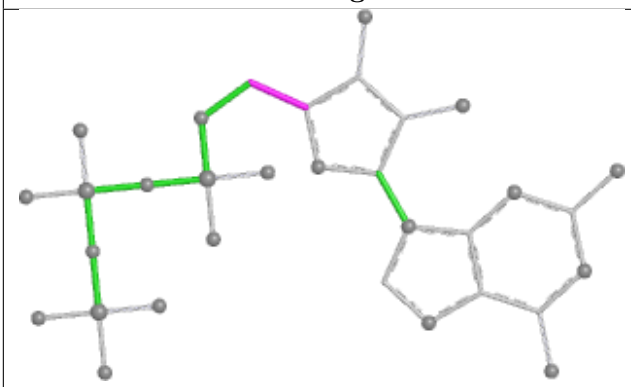

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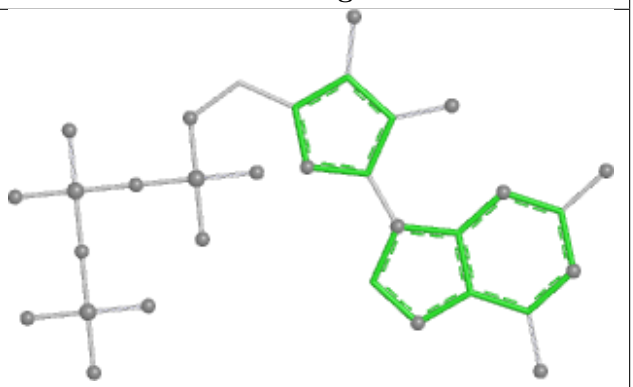

Rings

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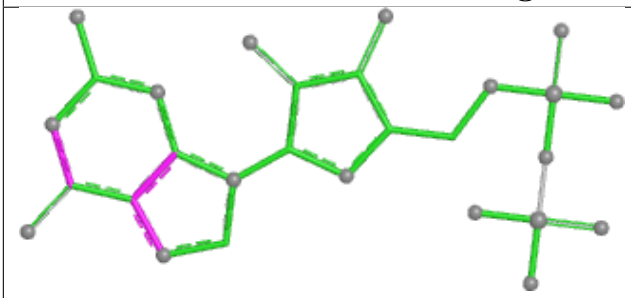

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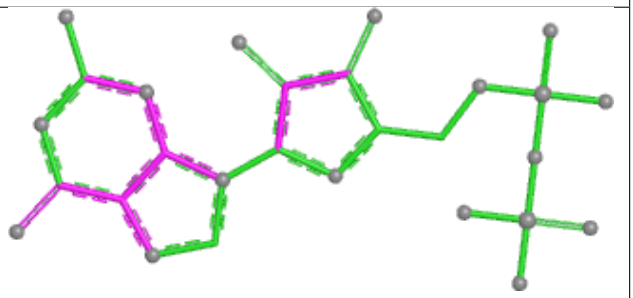

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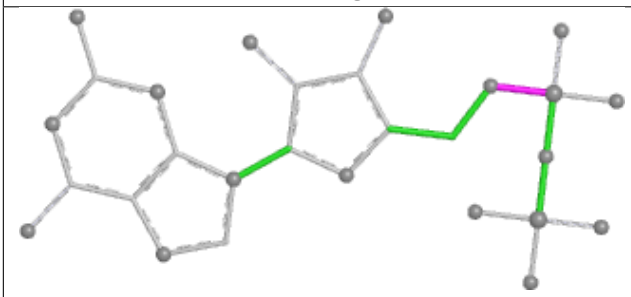

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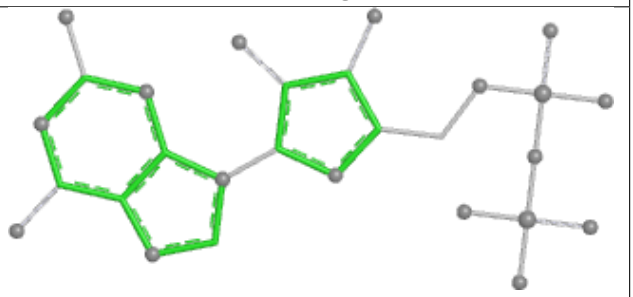
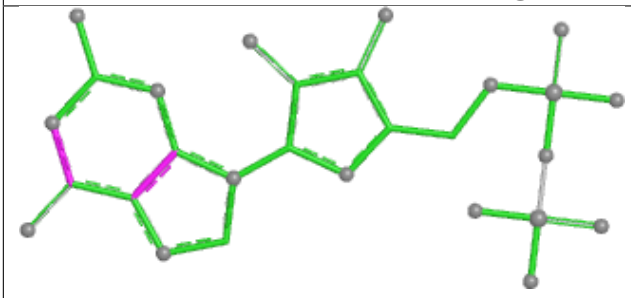


Rings

Ligand GDP Dg 501



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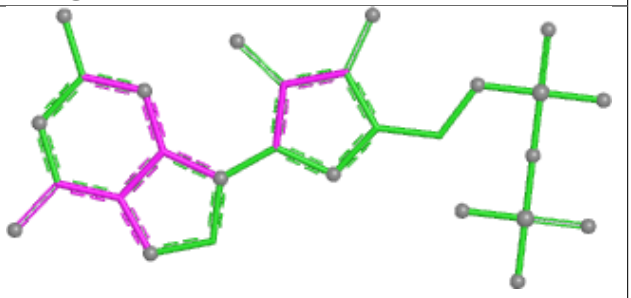

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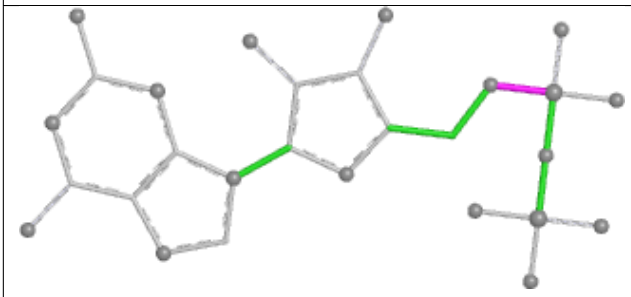

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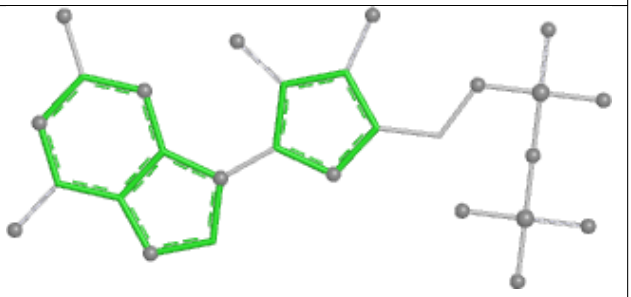
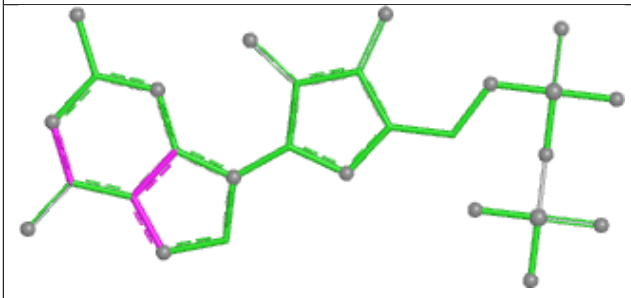


Rings

Ligand GDP Cc 502



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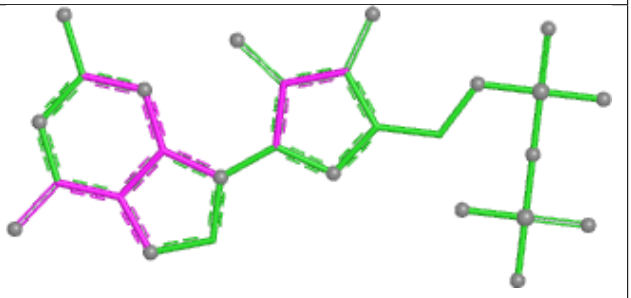

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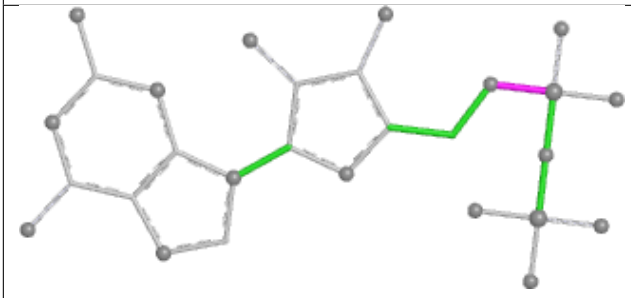

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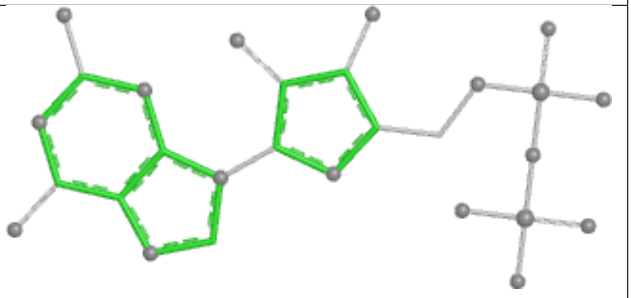
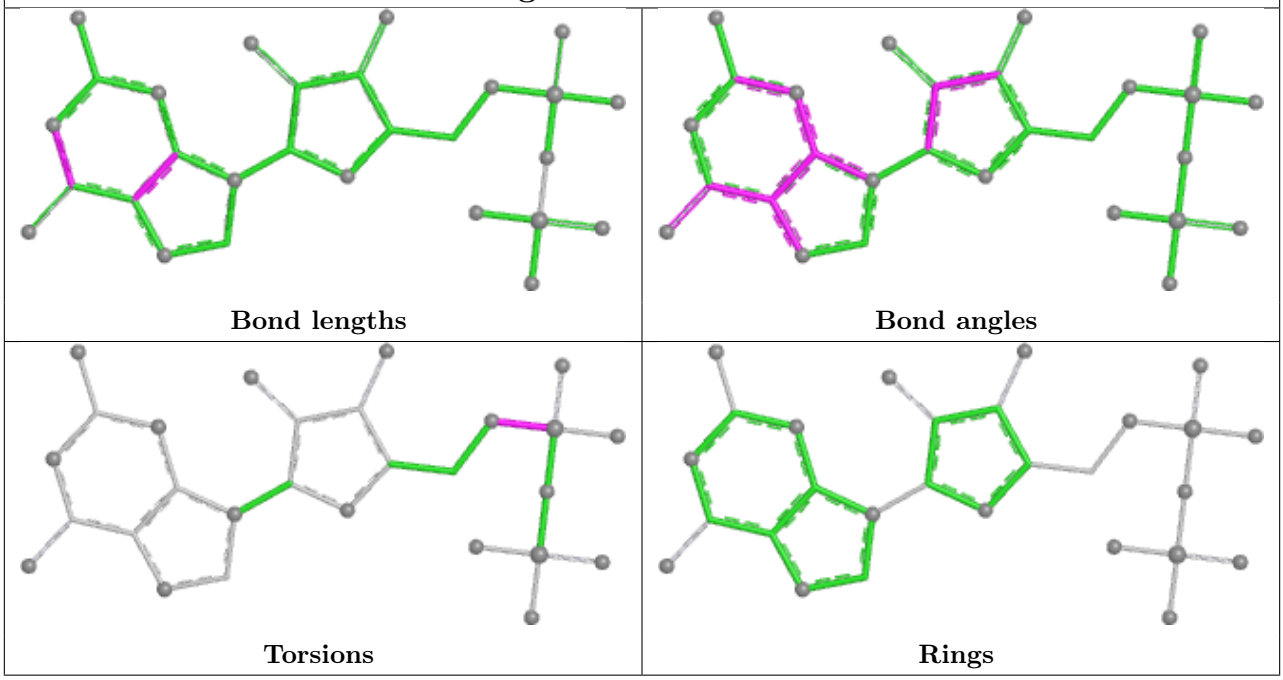


Rings

Ligand GDP 8c 501



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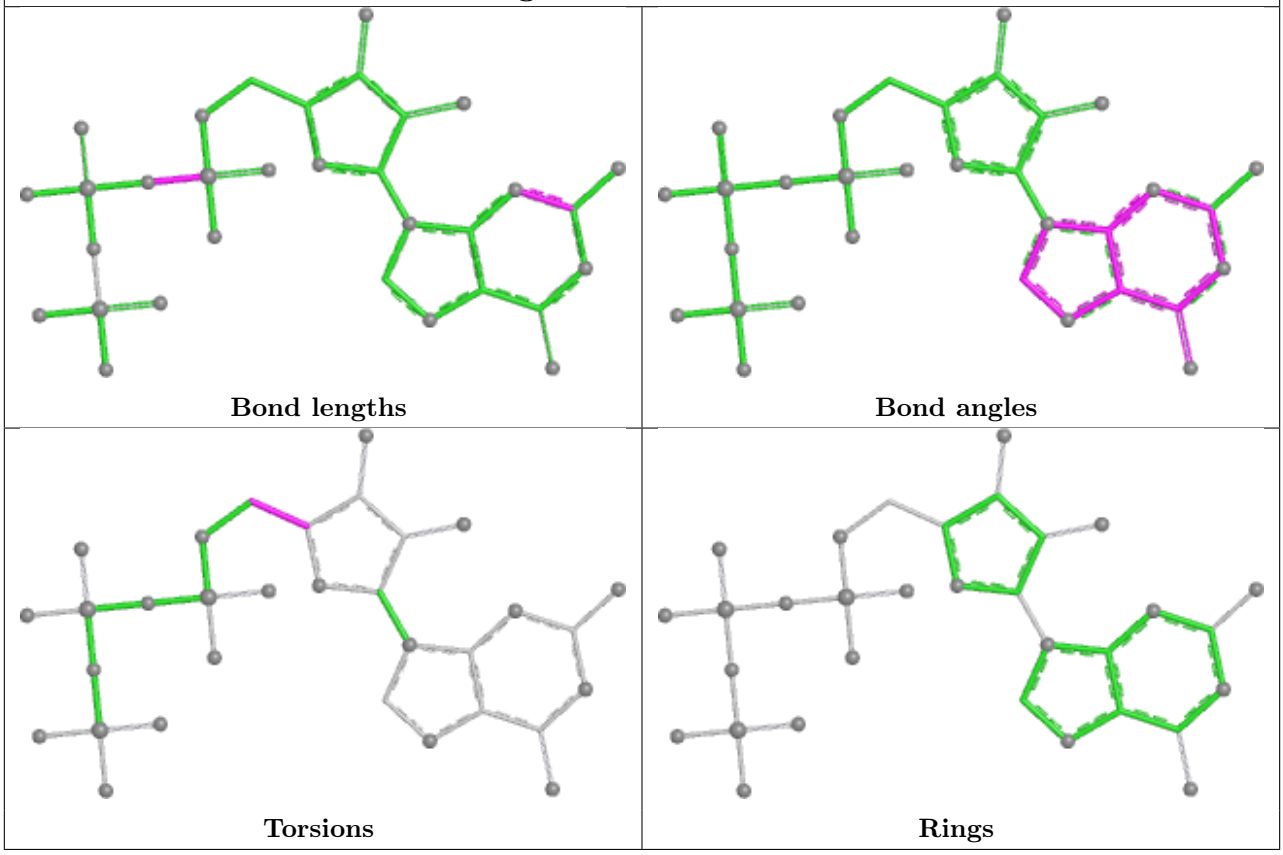

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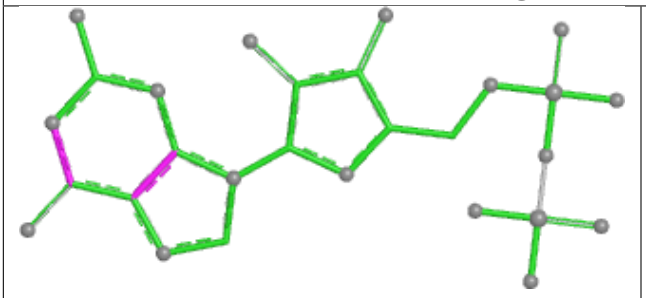

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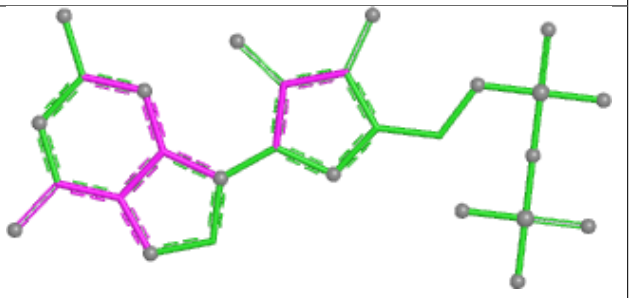

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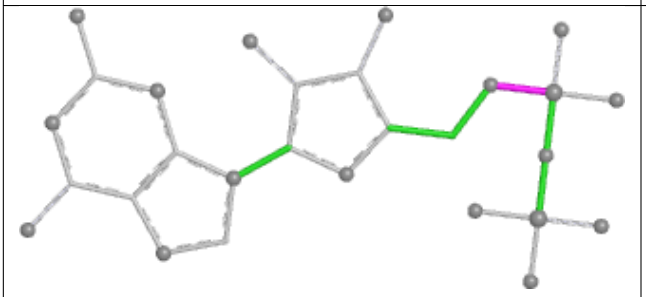

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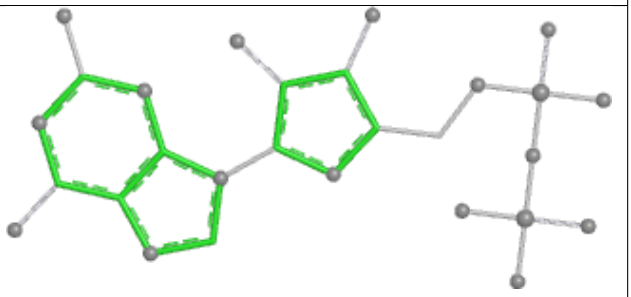

Rings

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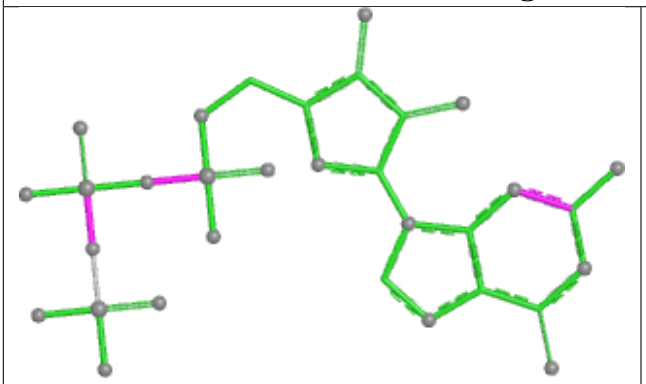

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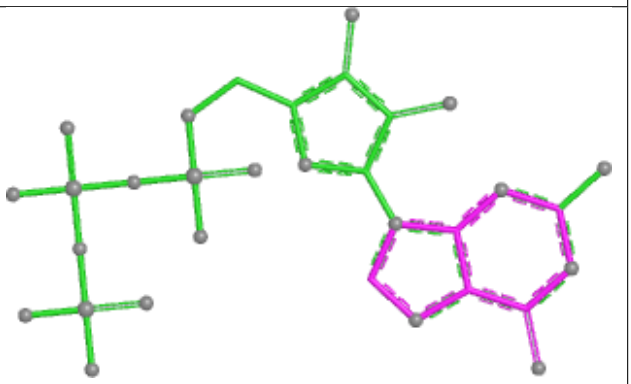

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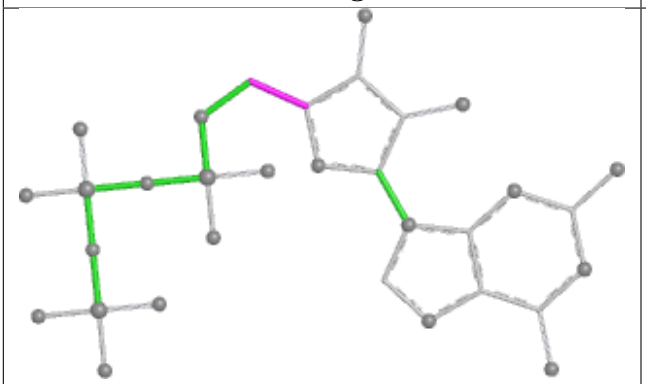

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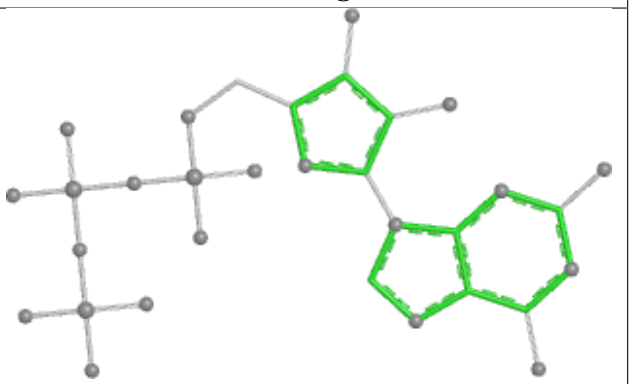

Rings

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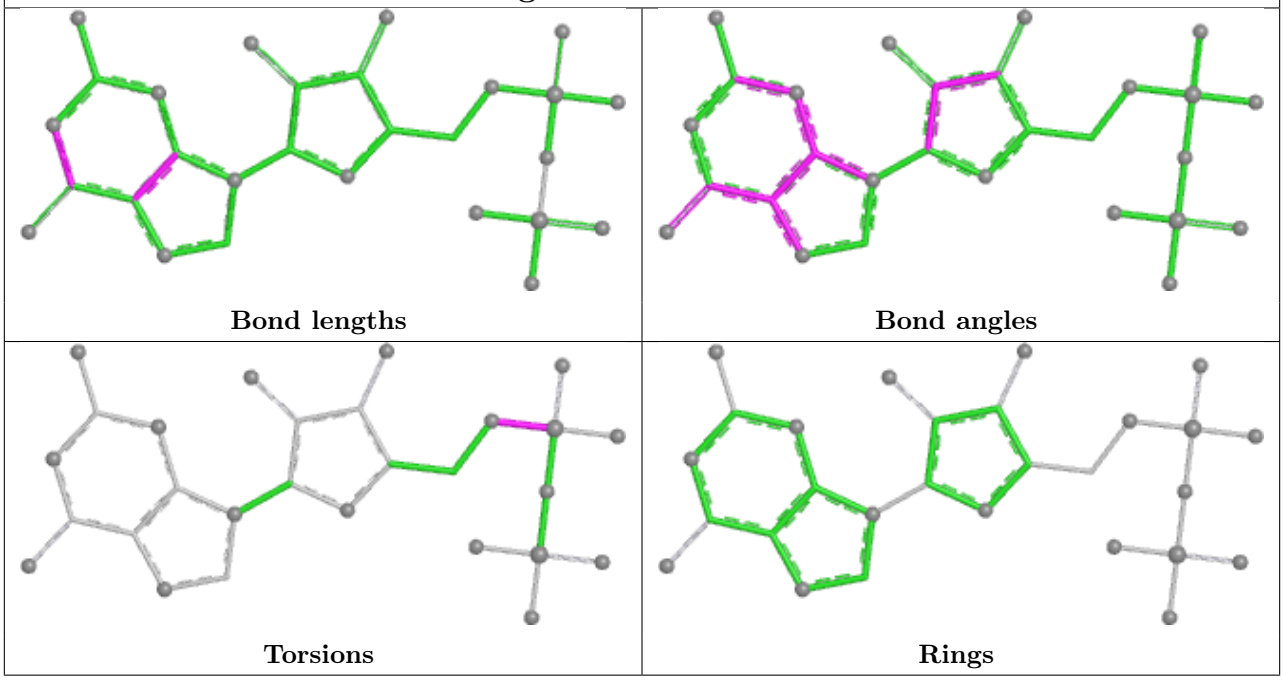

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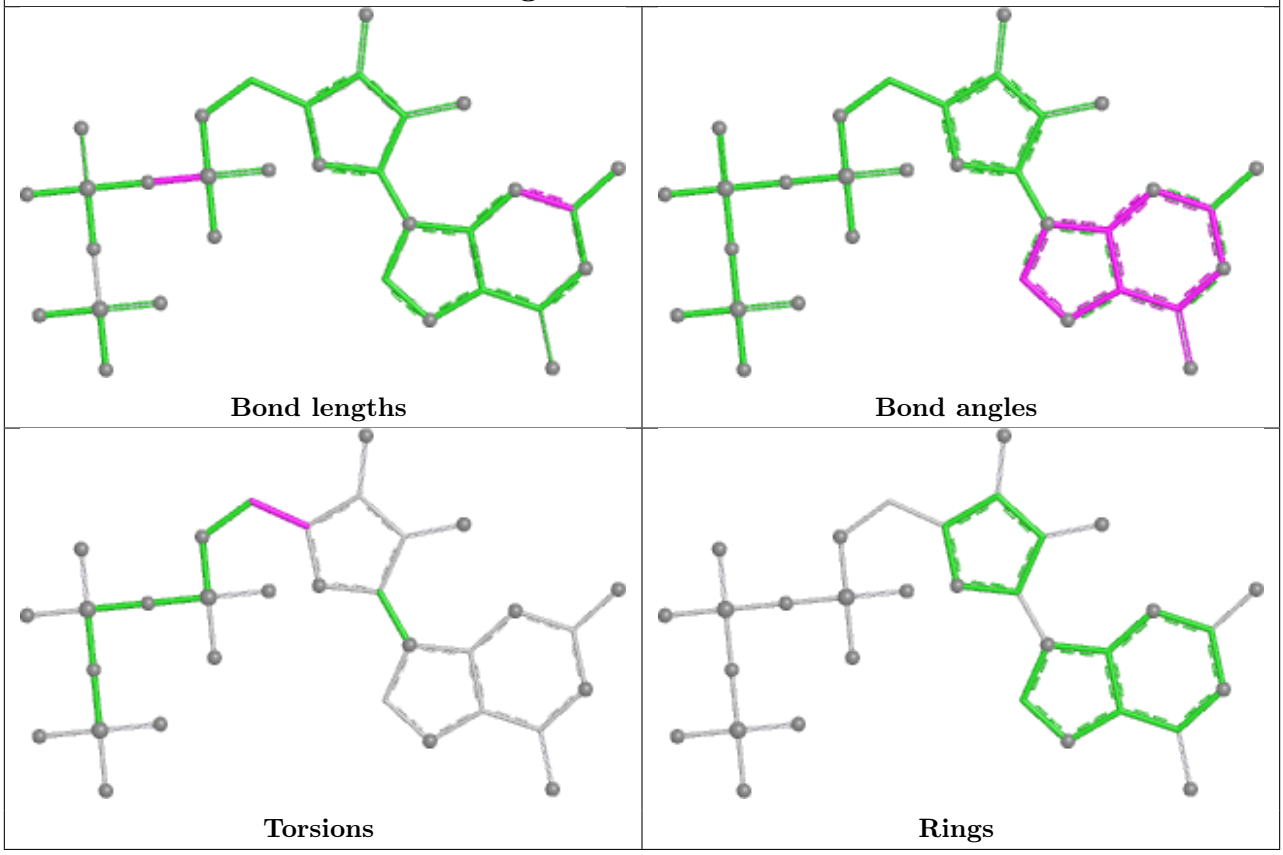

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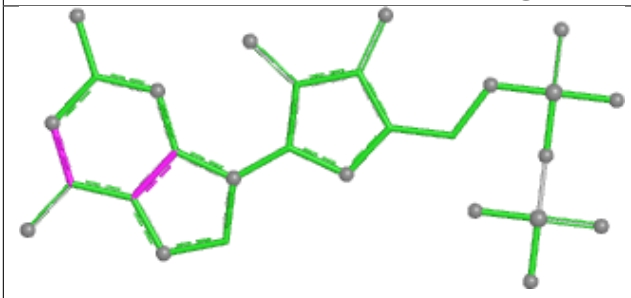

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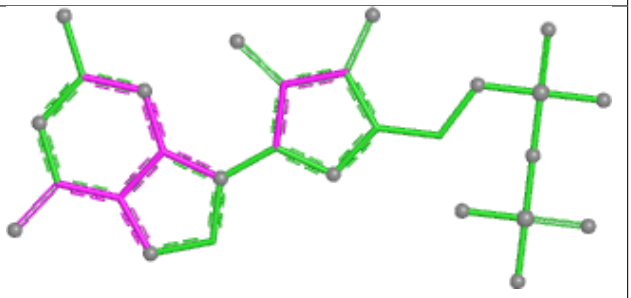

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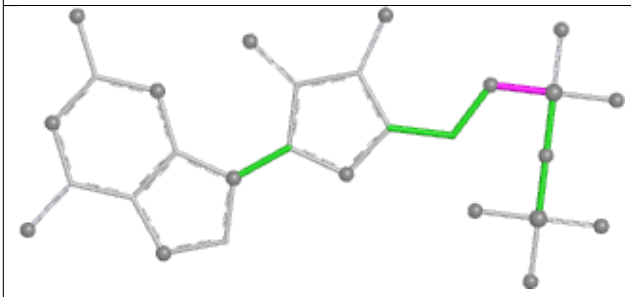

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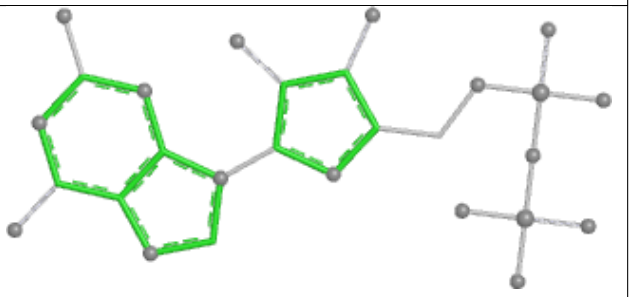

Rings

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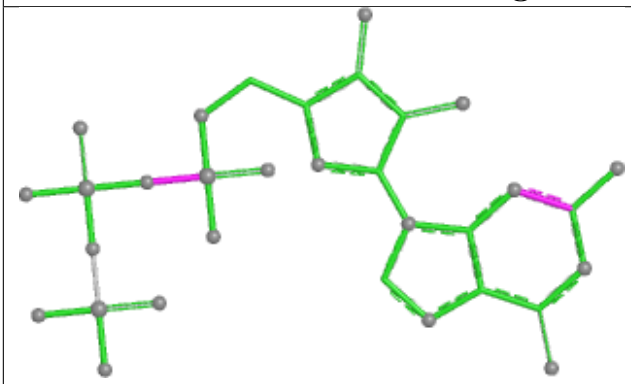

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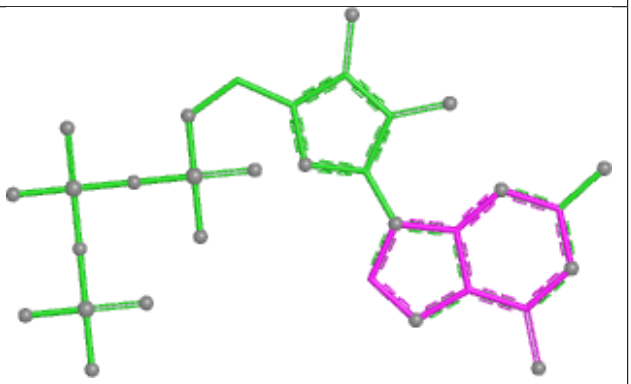

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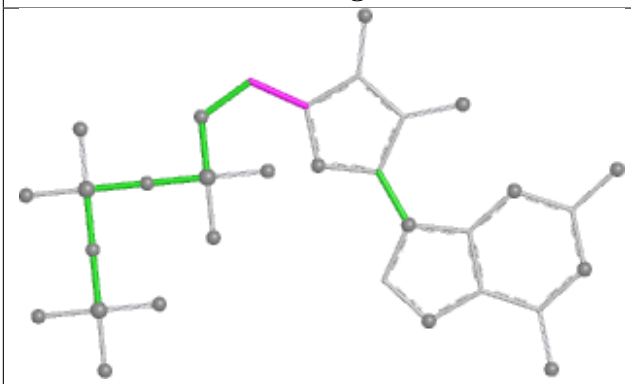

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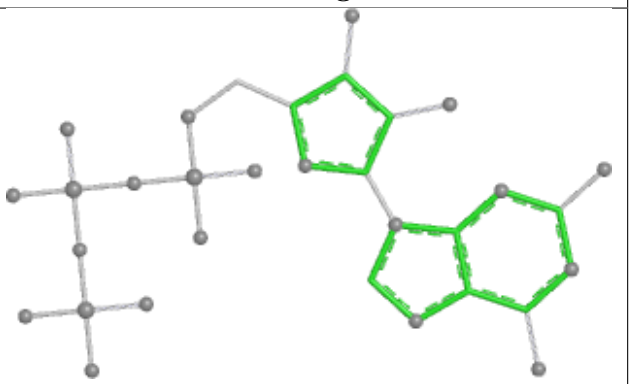
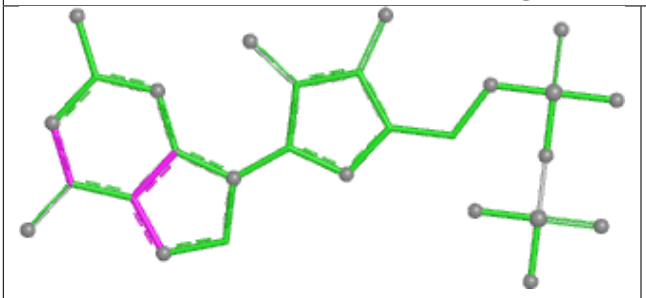


Rings

Ligand GDP 4e 501



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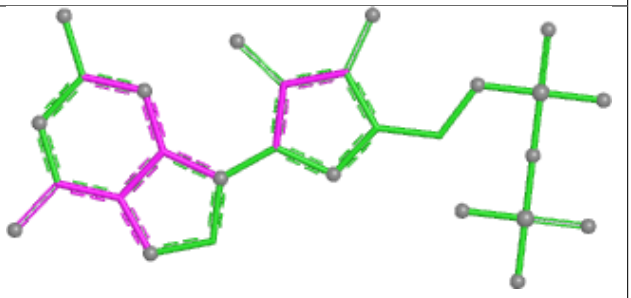

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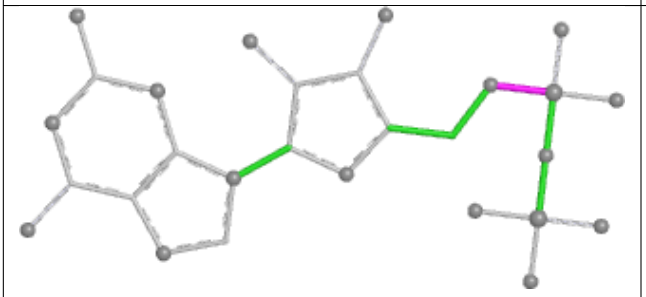

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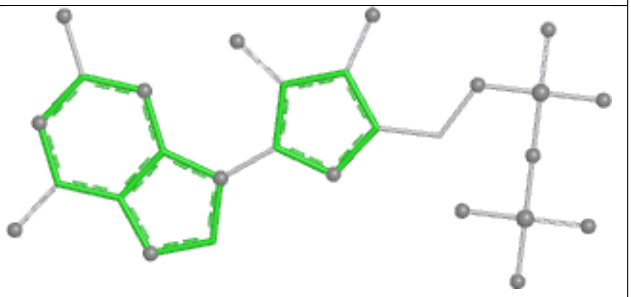

Rings

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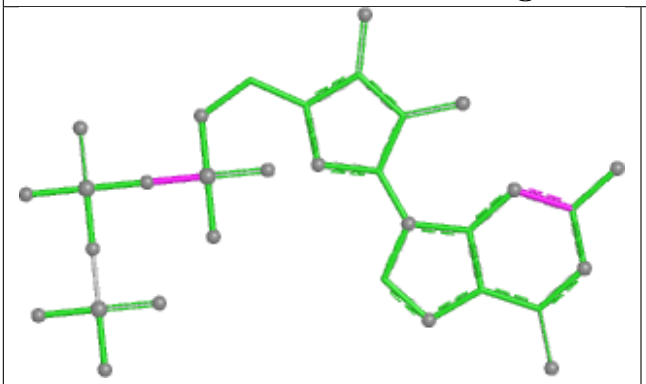

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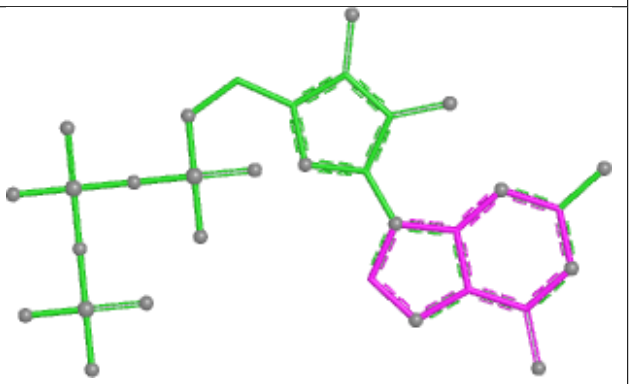

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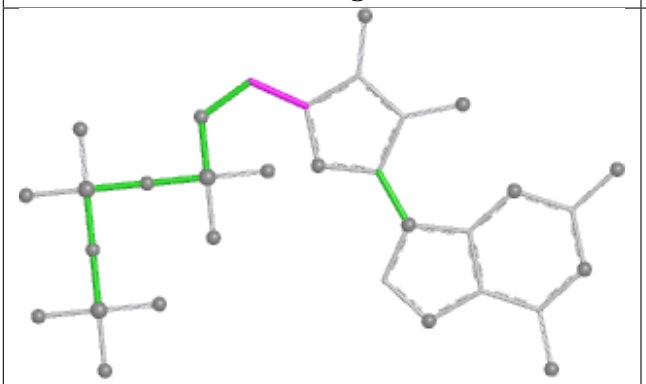

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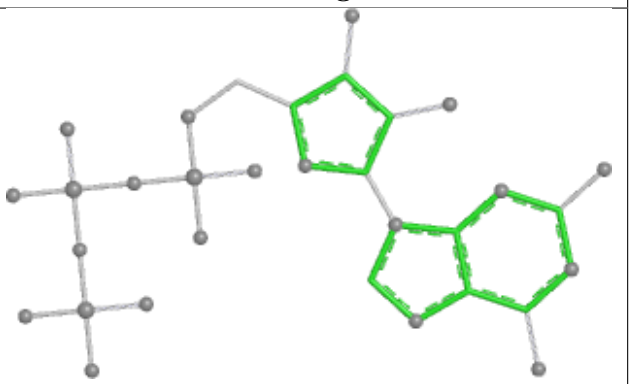

Rings

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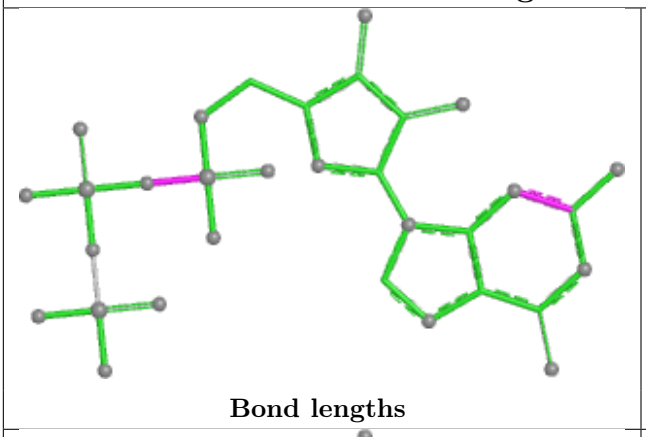

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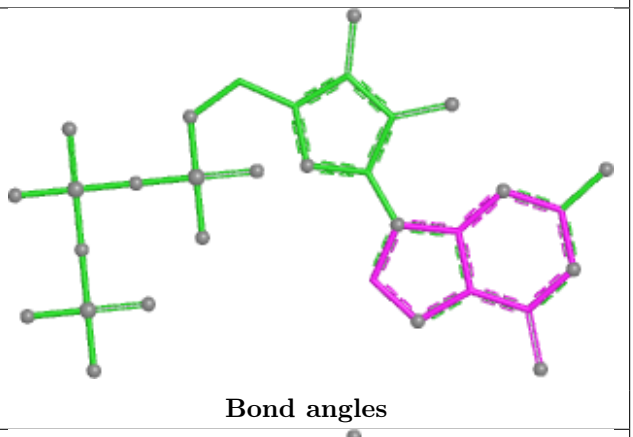

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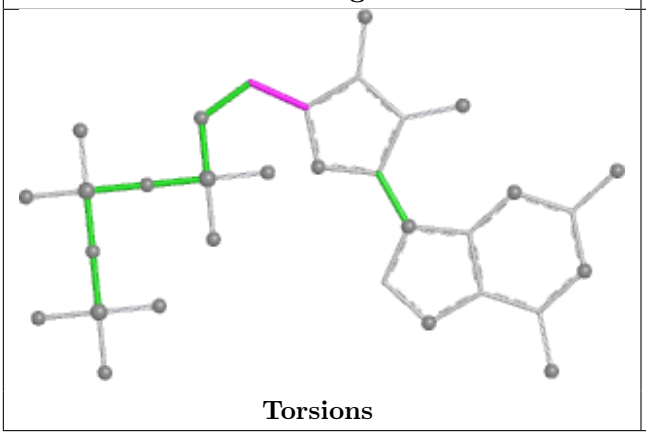

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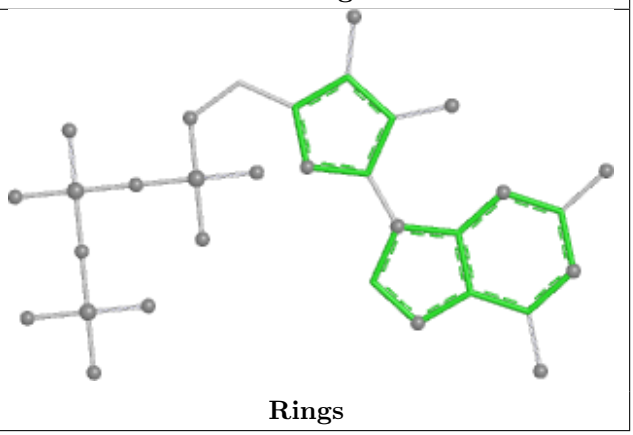

Rings

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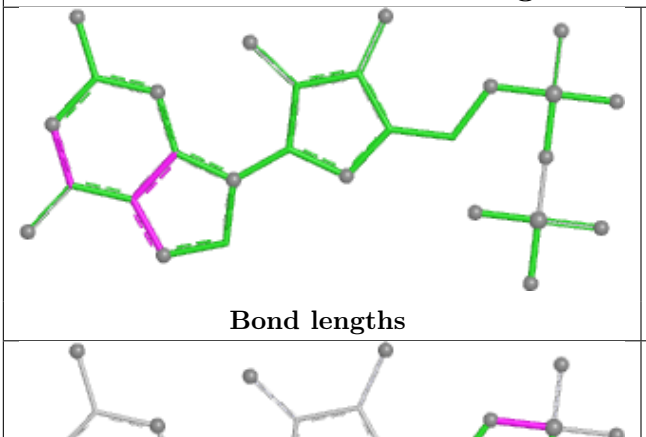

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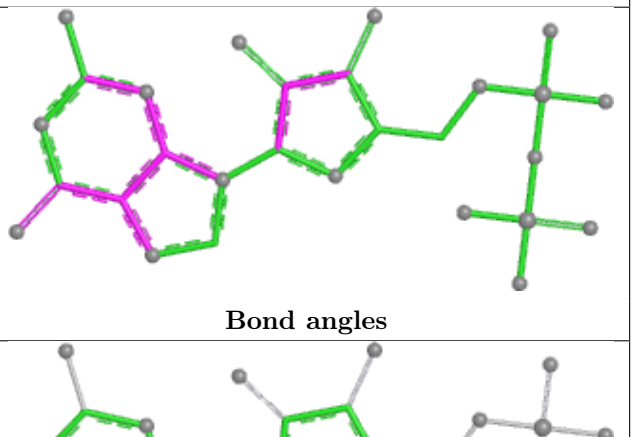

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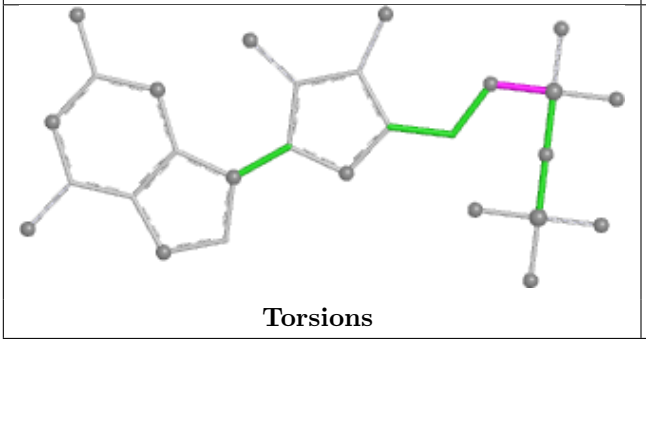

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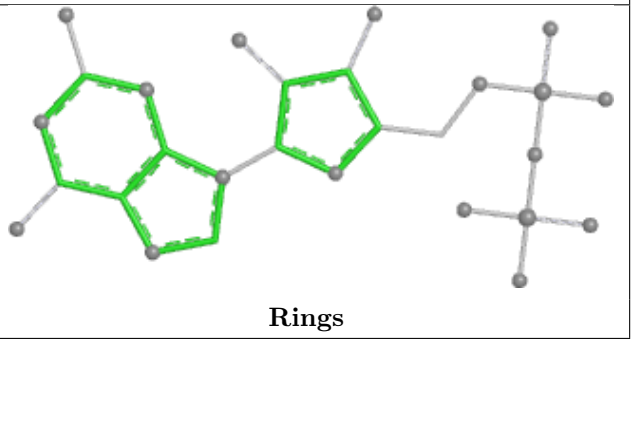

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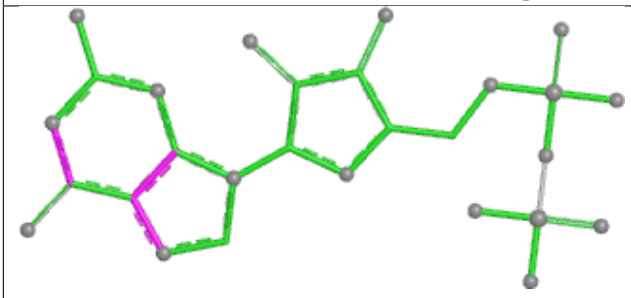

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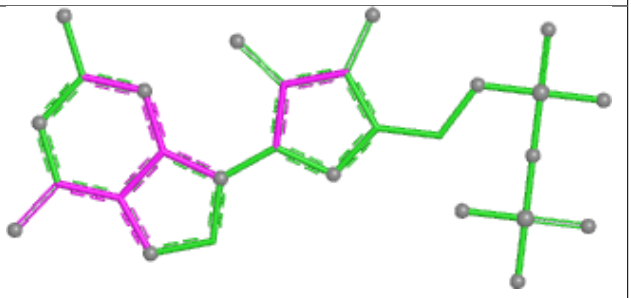

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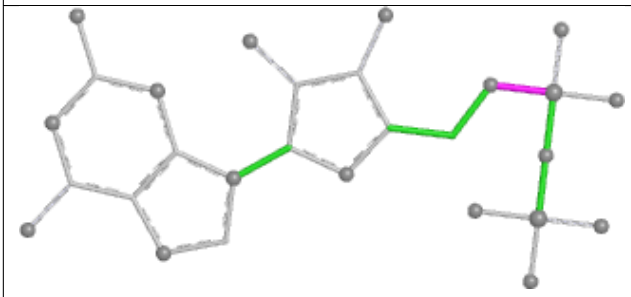

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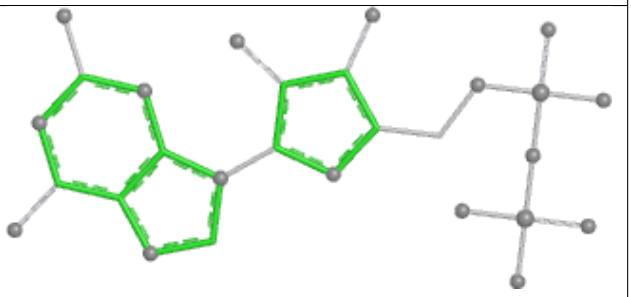

Rings

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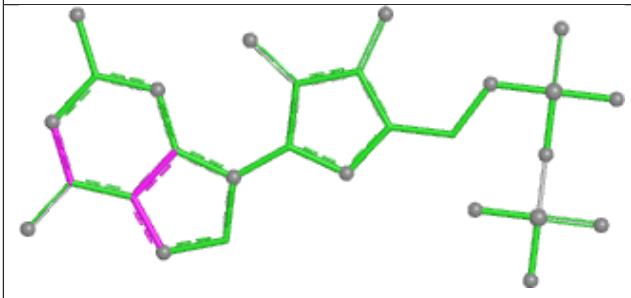

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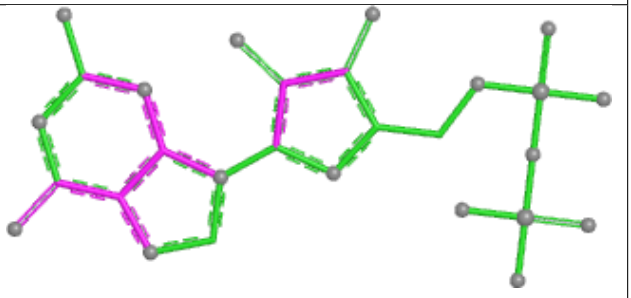

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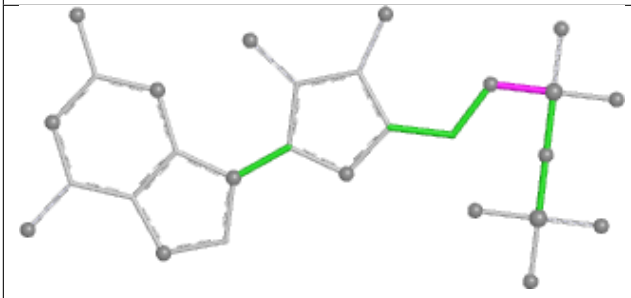

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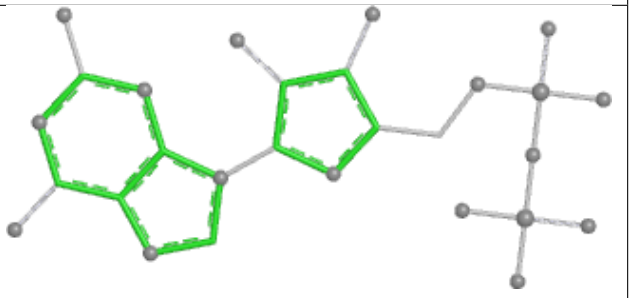

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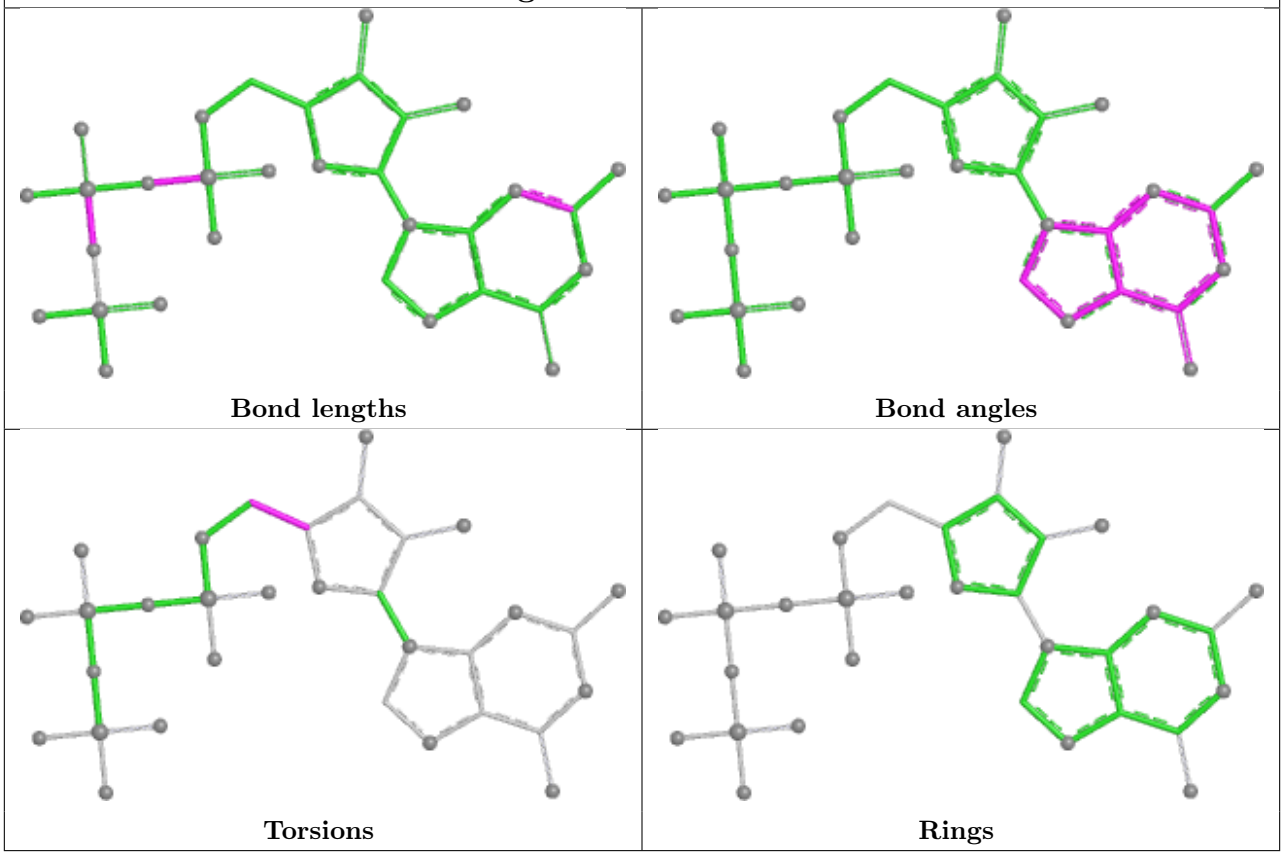

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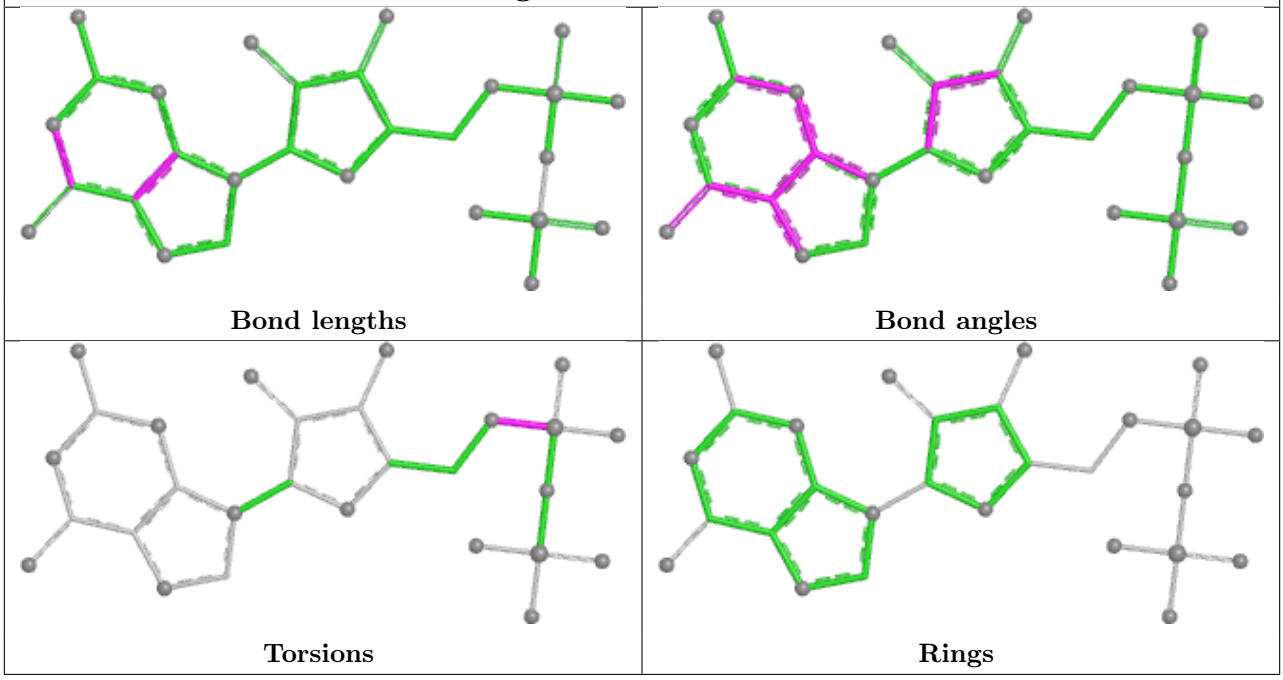

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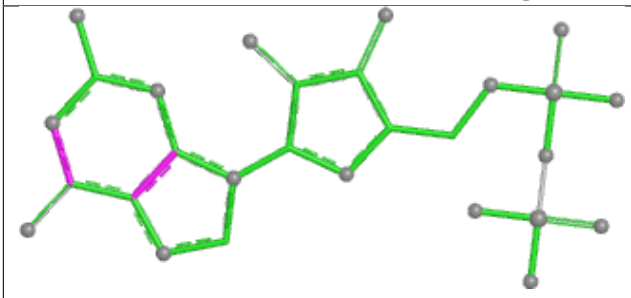

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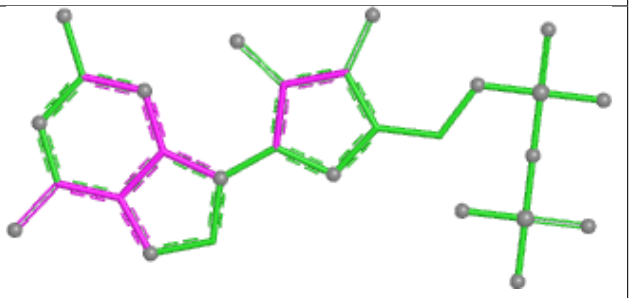

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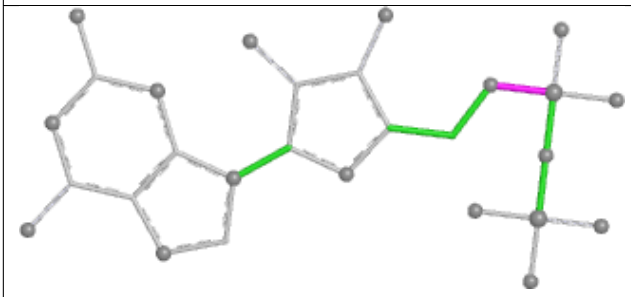

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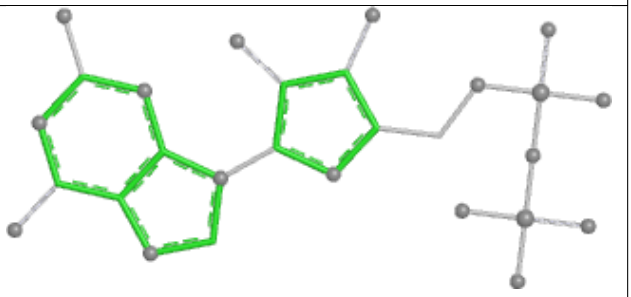

Rings

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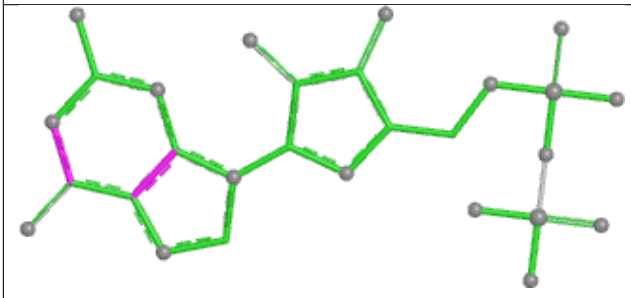

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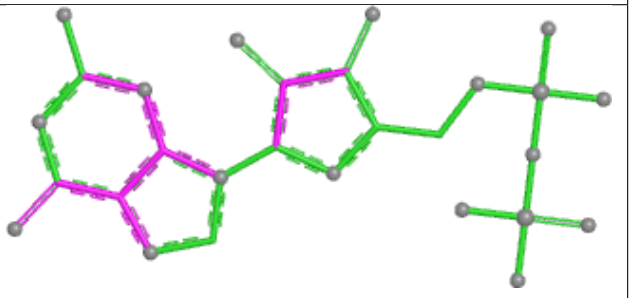

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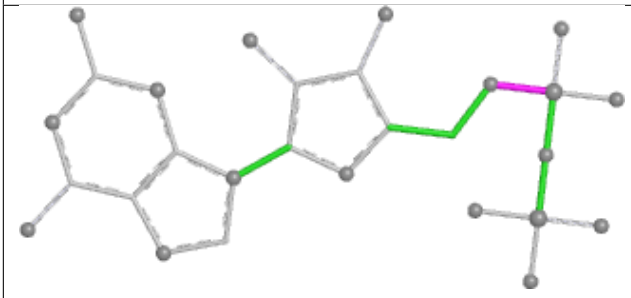

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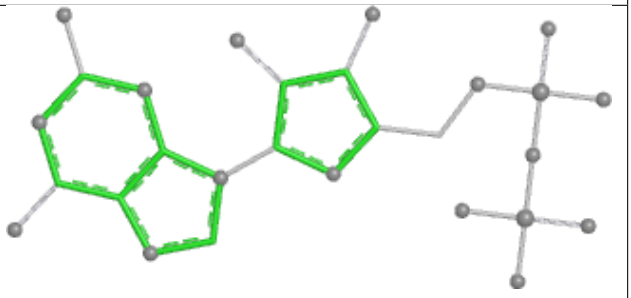

Rings

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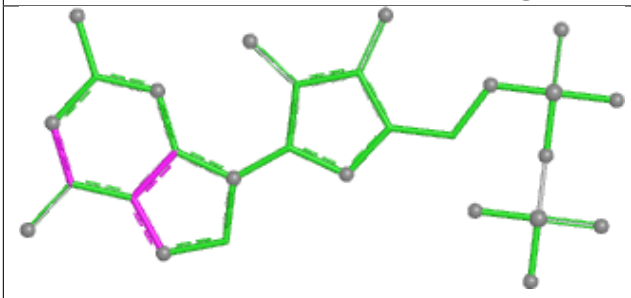

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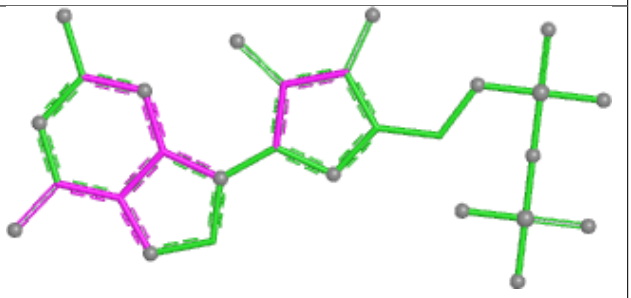

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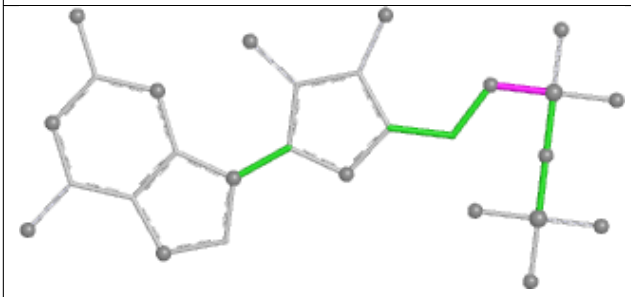

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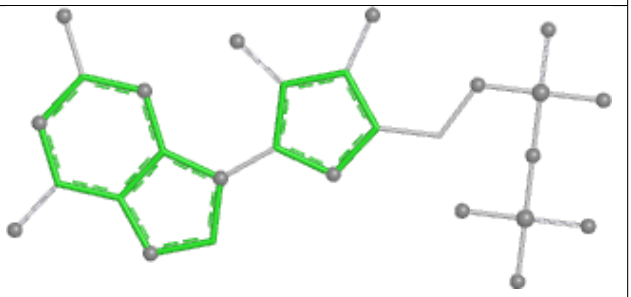

Rings

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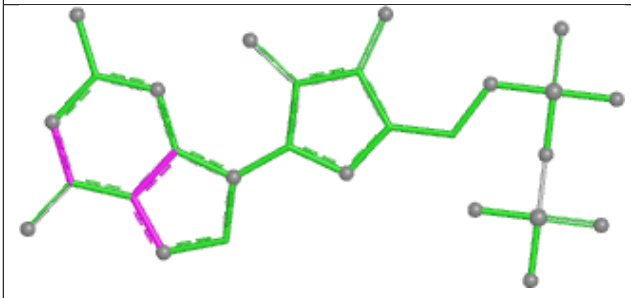

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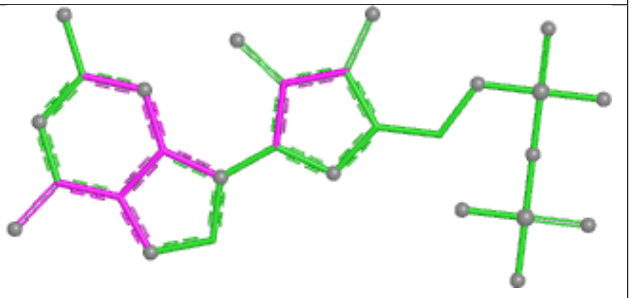

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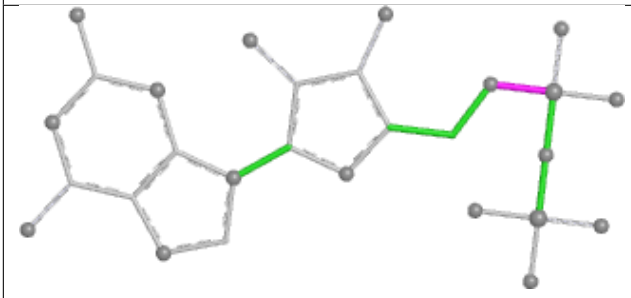

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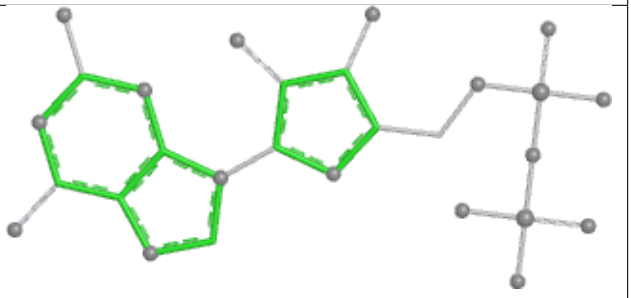

Rings

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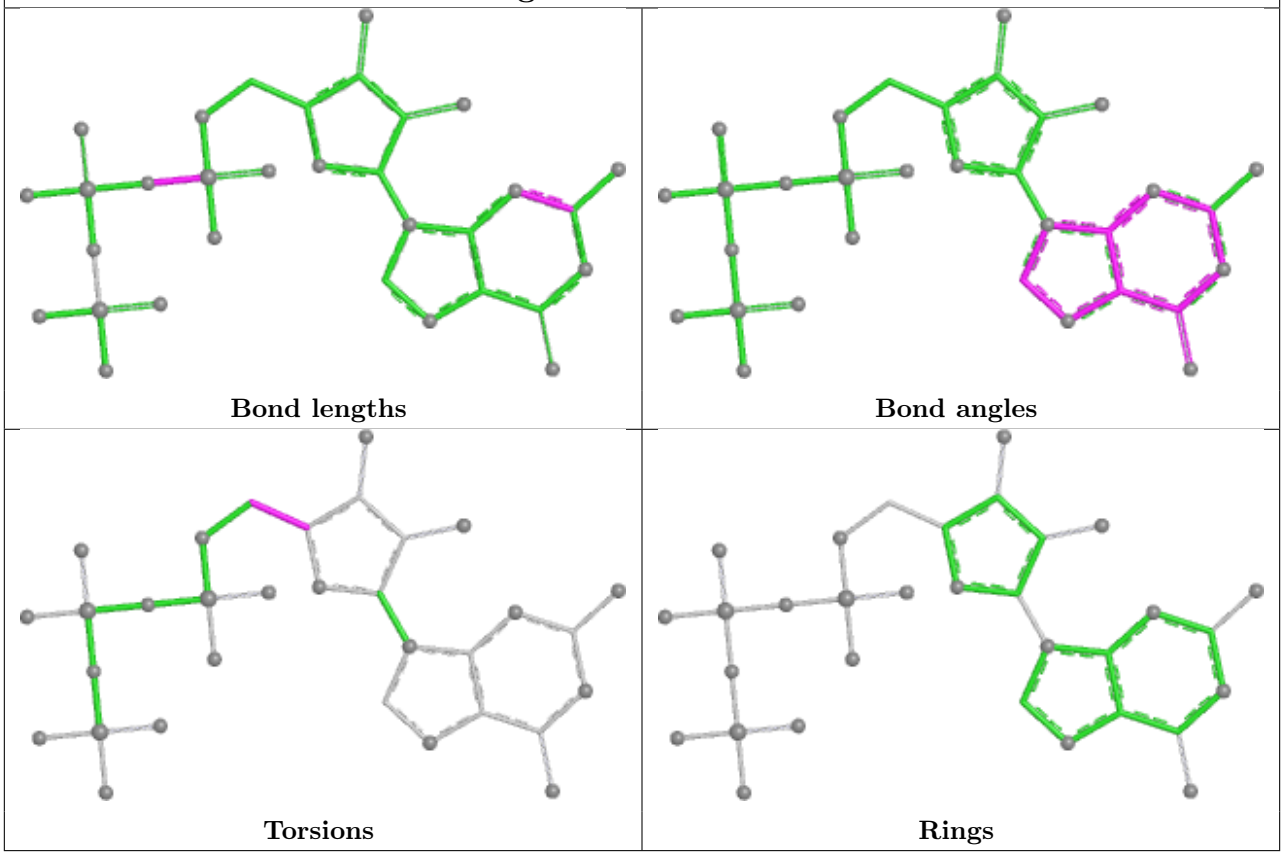

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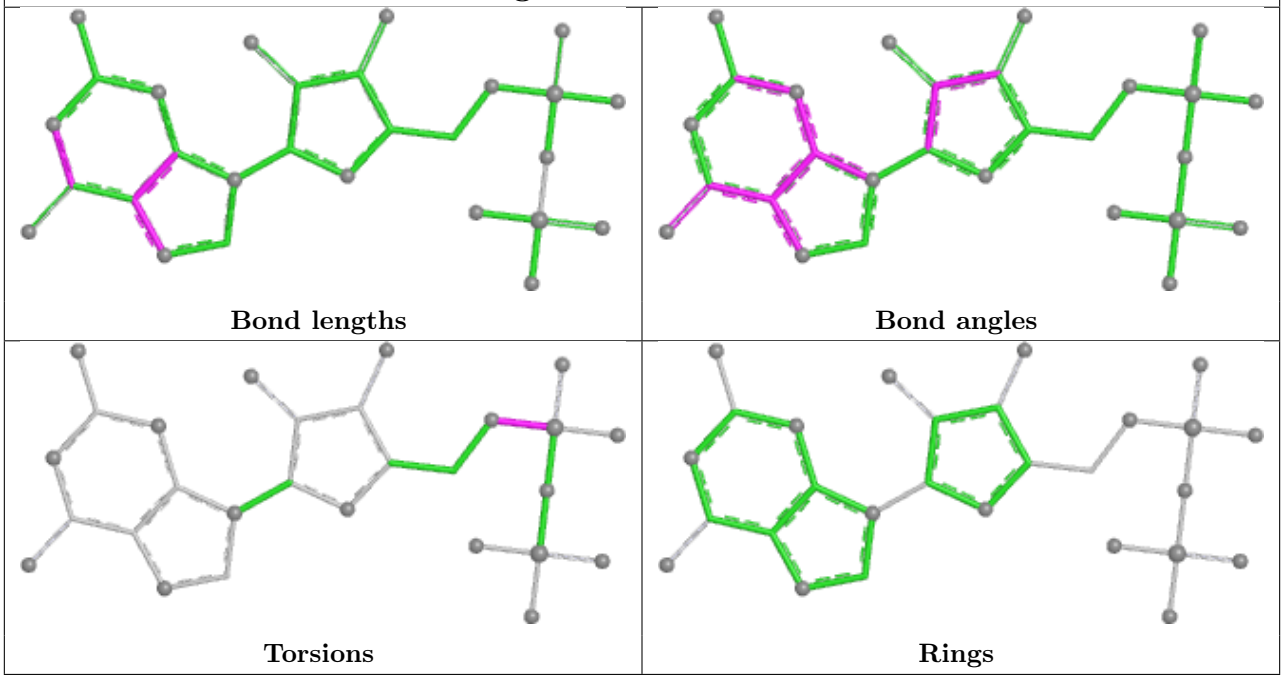

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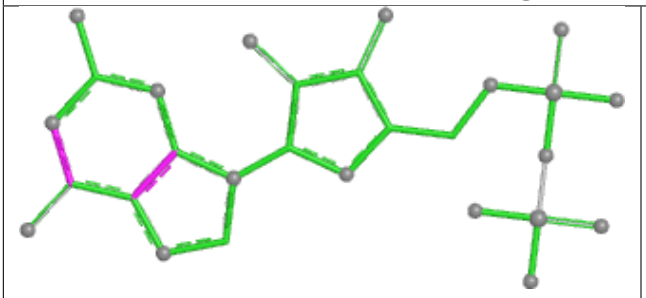

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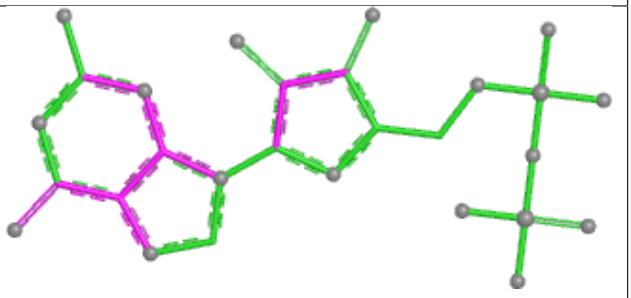

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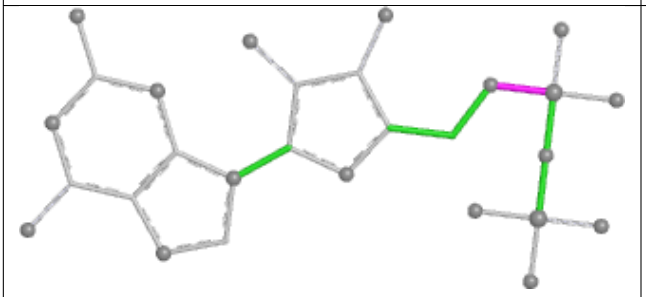

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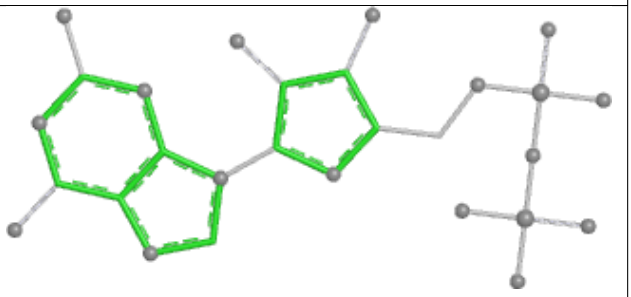

Rings

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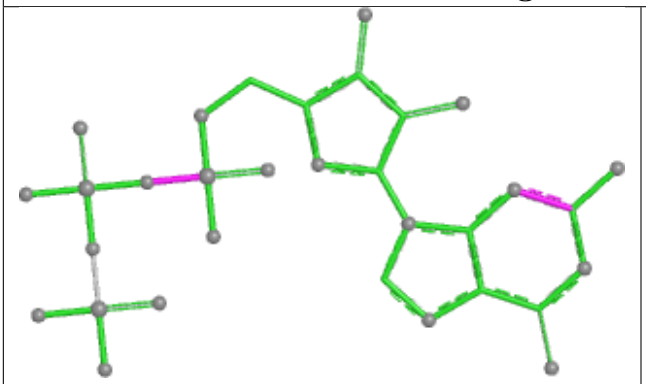

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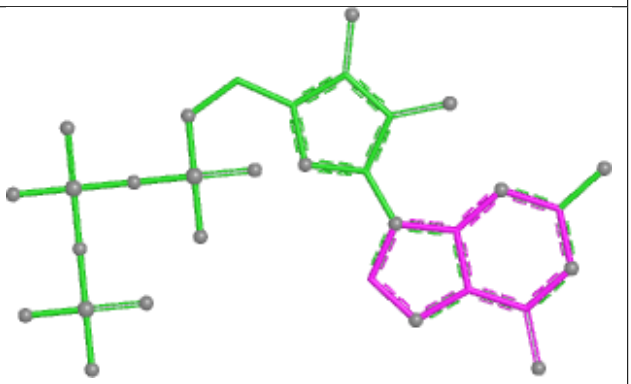

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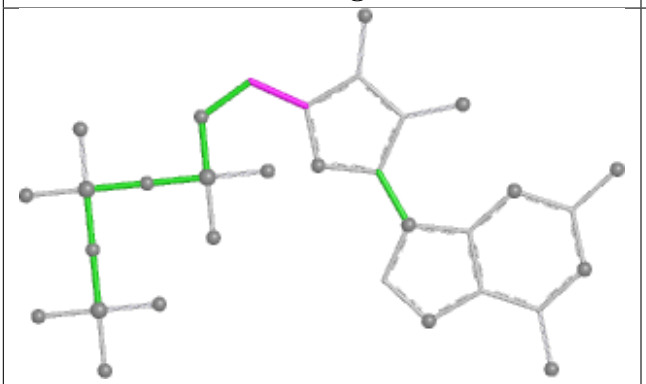

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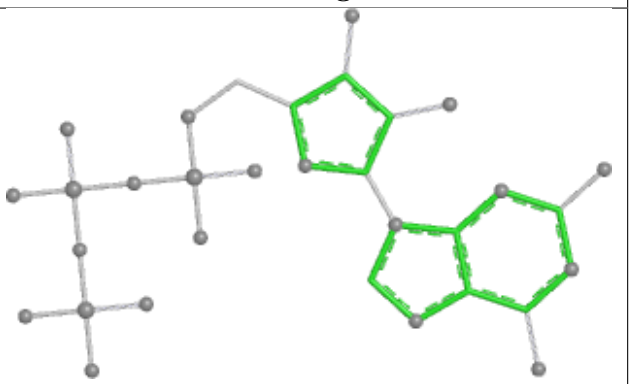

Rings

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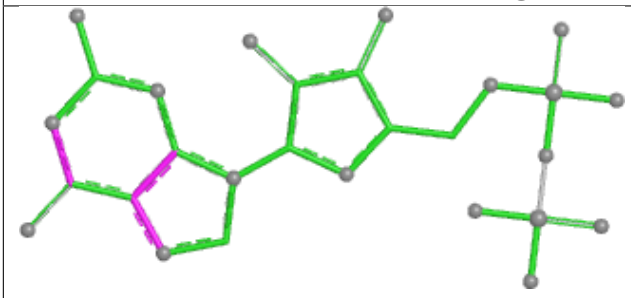

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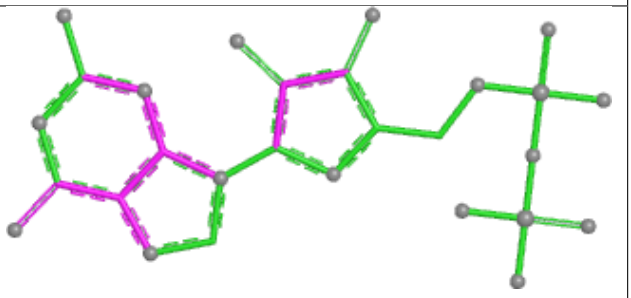

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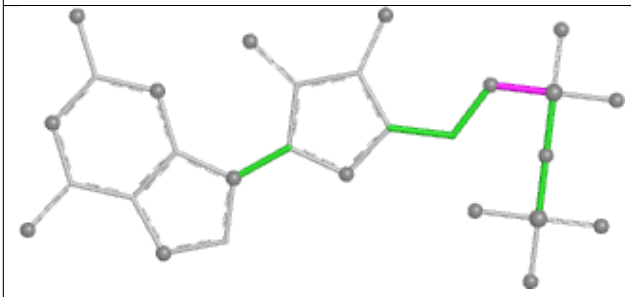

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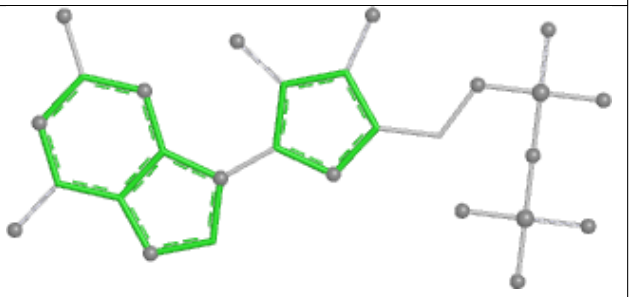

Rings

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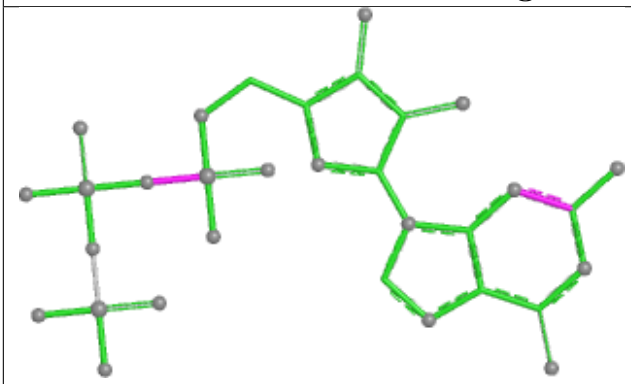

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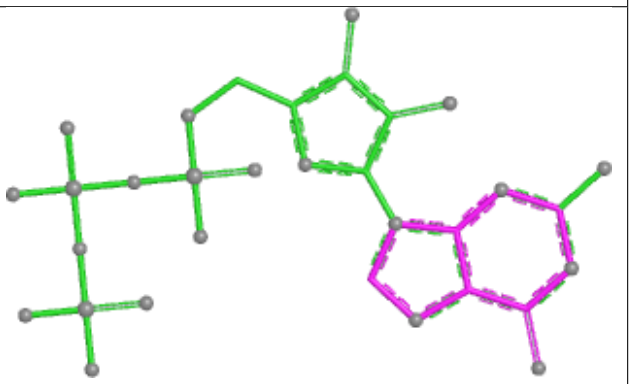

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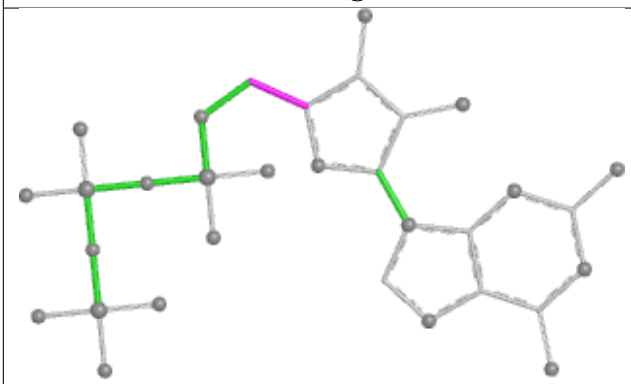

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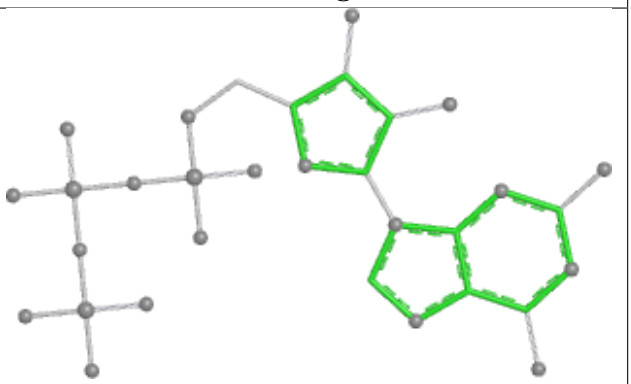

Rings

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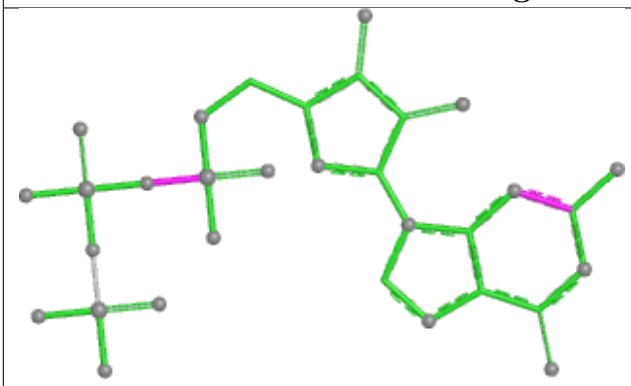

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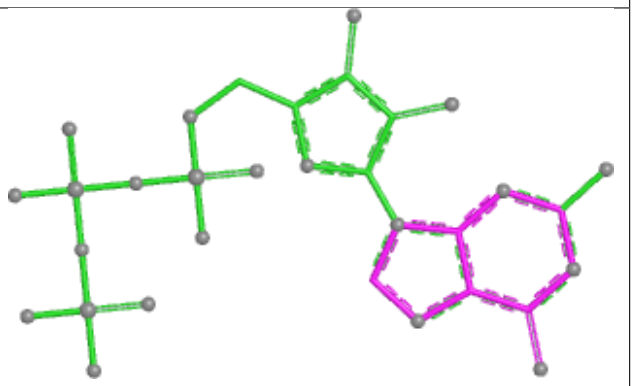

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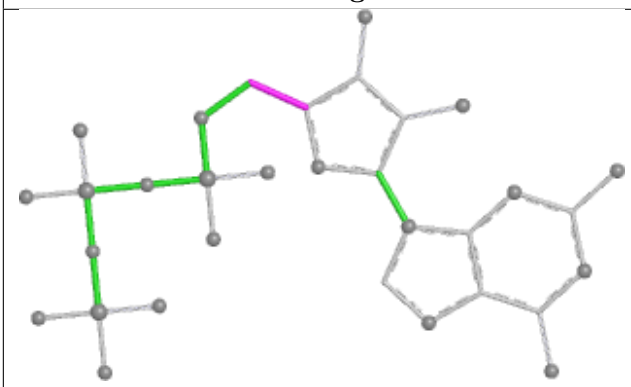

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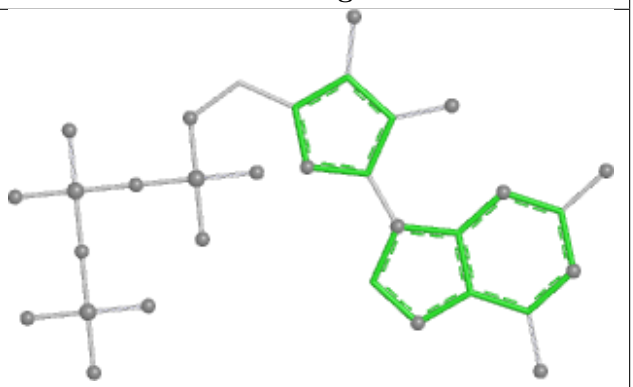

Rings

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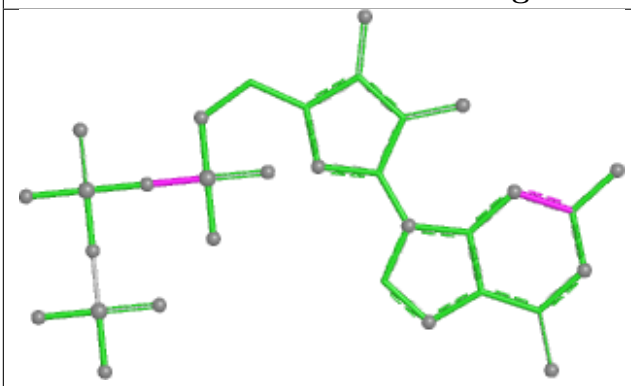

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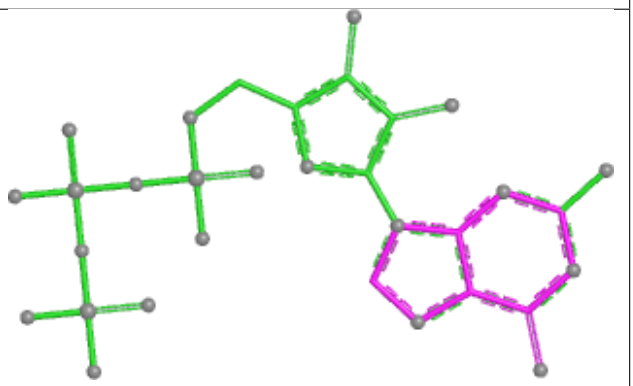

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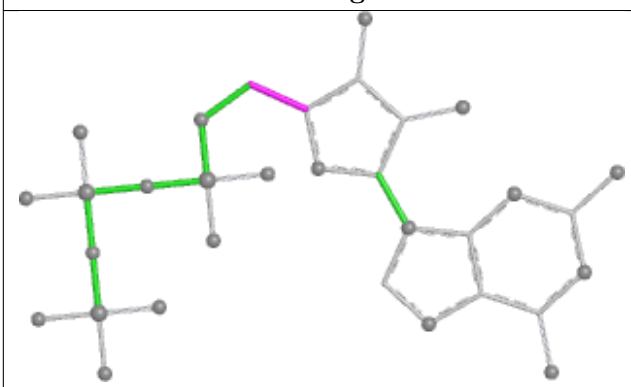

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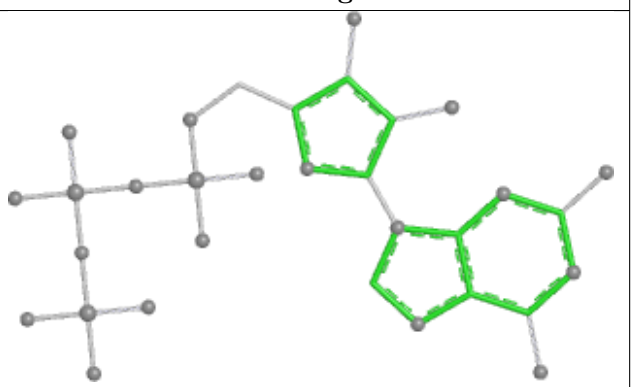

Rings

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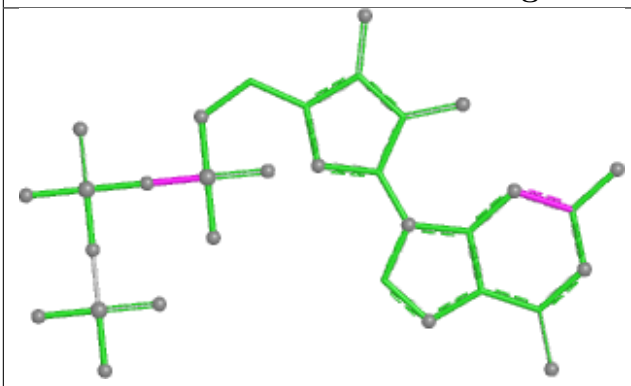

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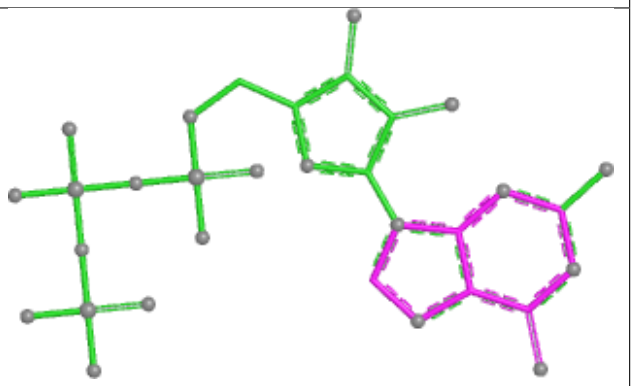

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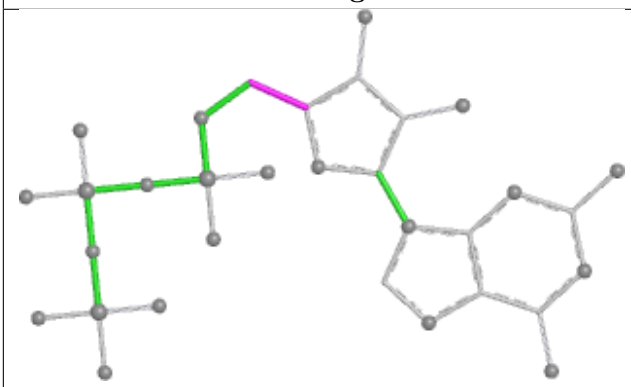

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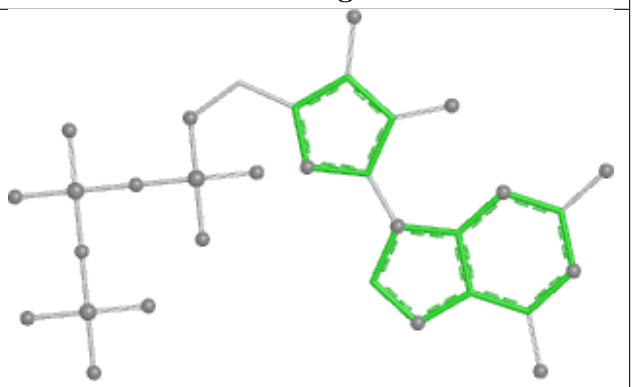

Rings

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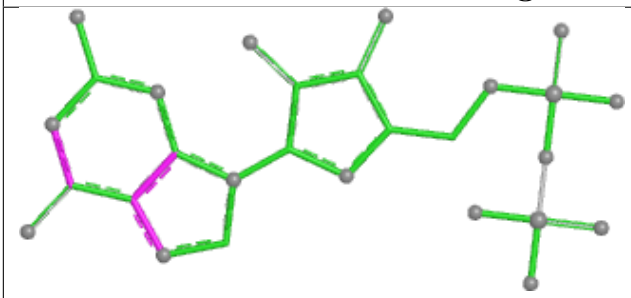

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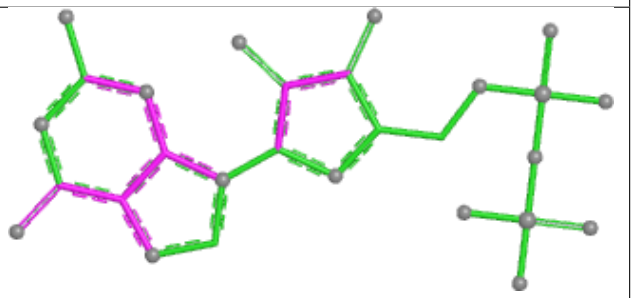

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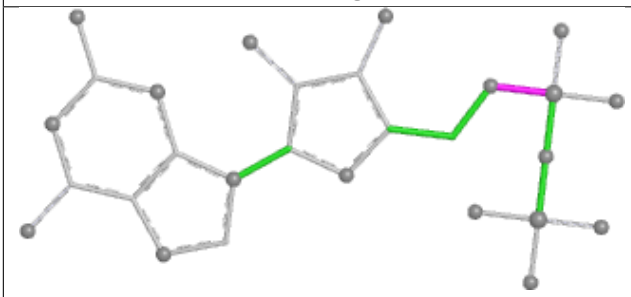

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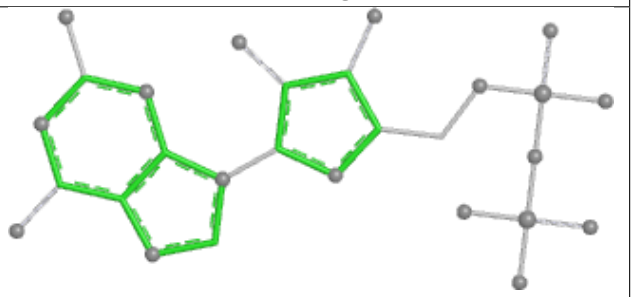

Rings

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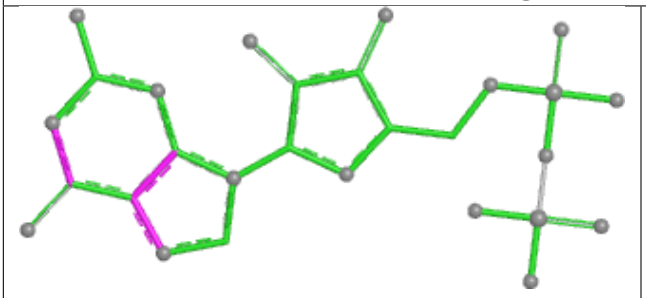

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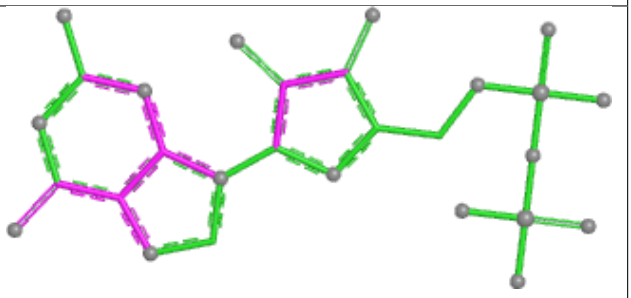

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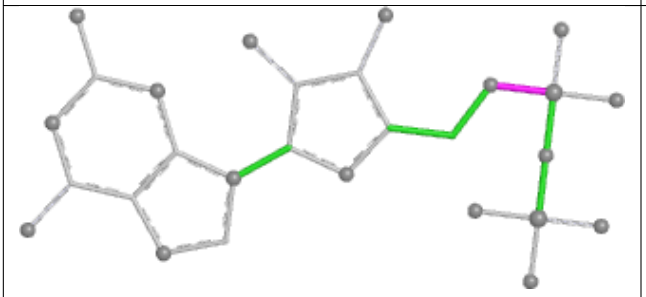

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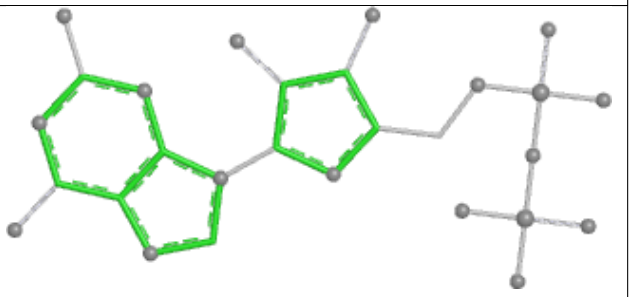

Rings

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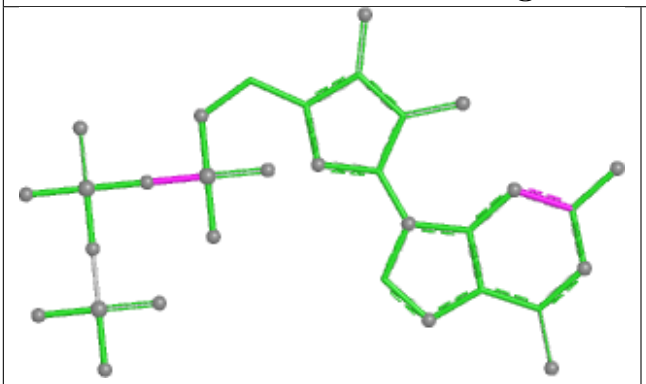

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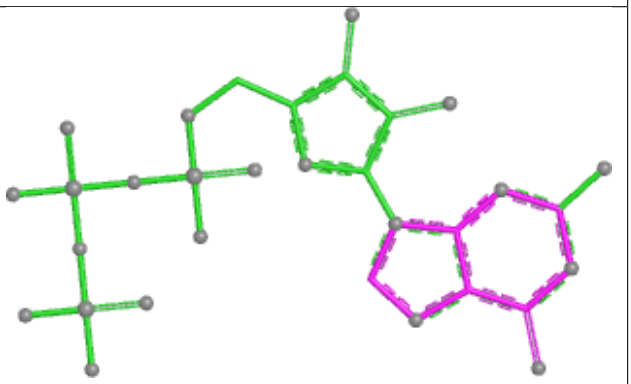

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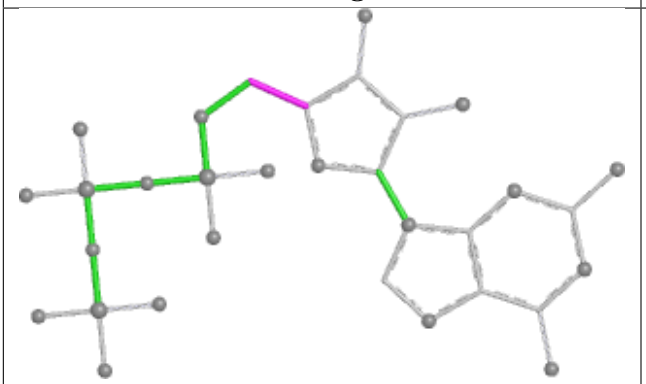

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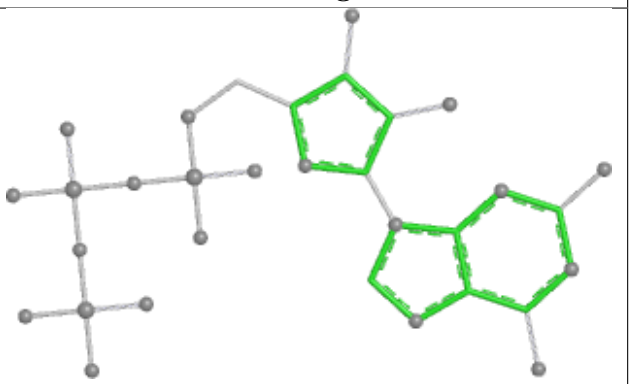

Rings

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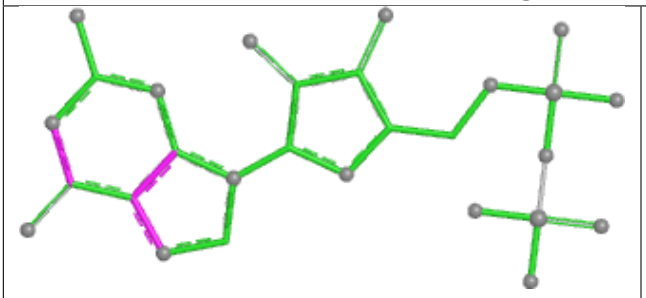

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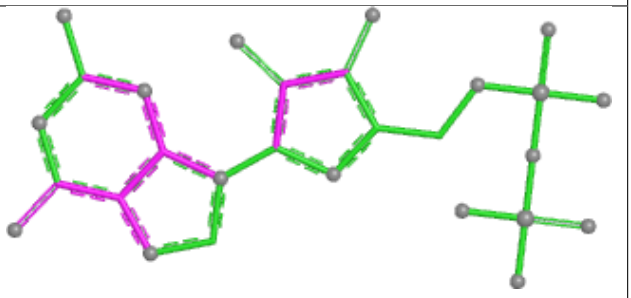

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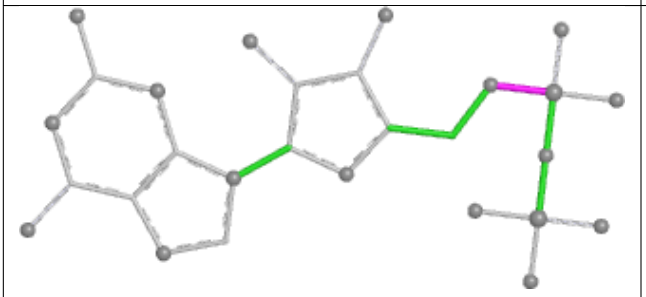

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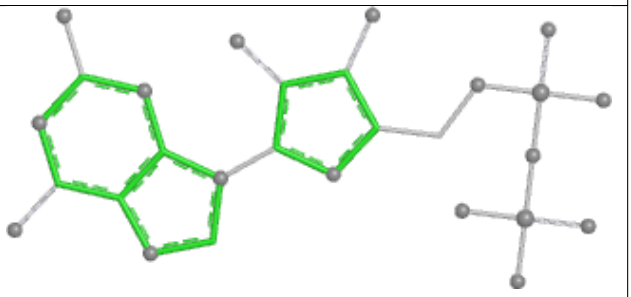

Rings

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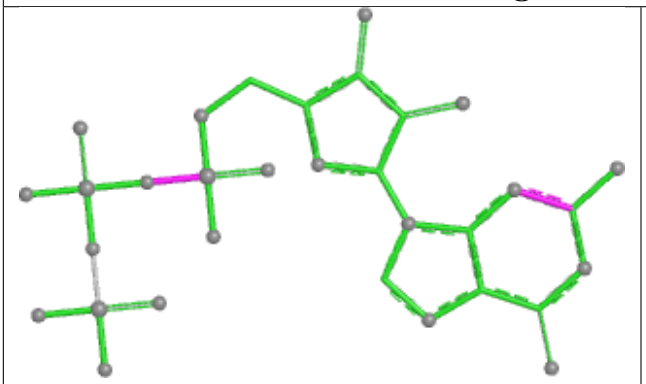

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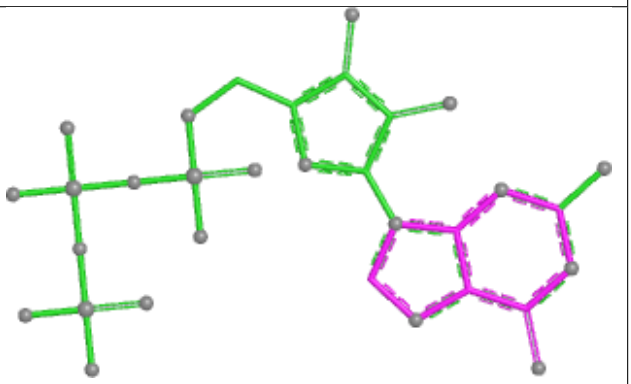

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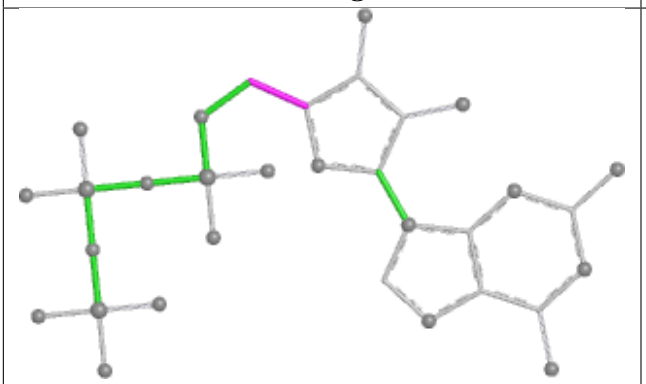

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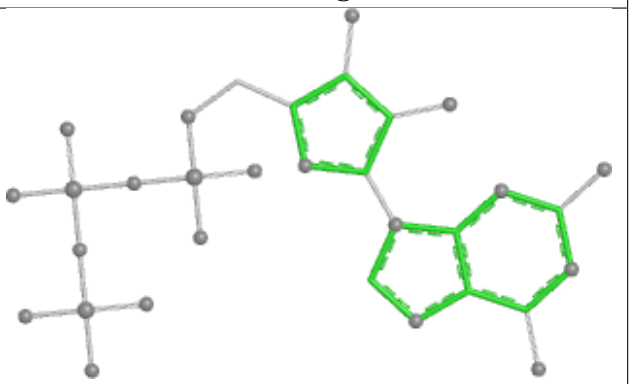

Rings

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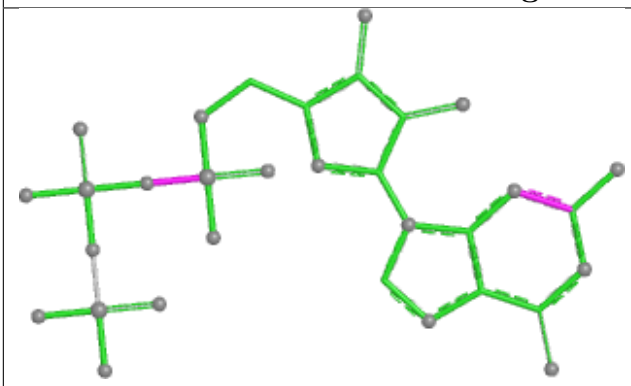

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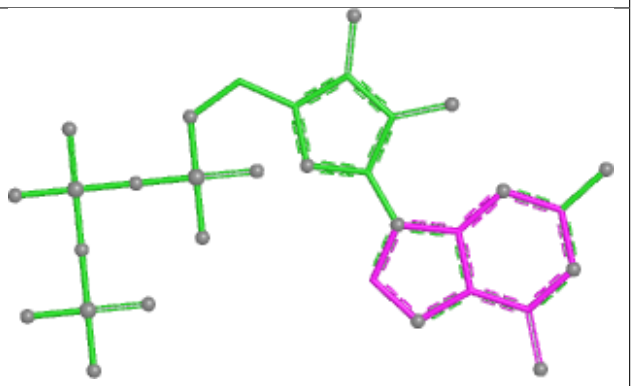

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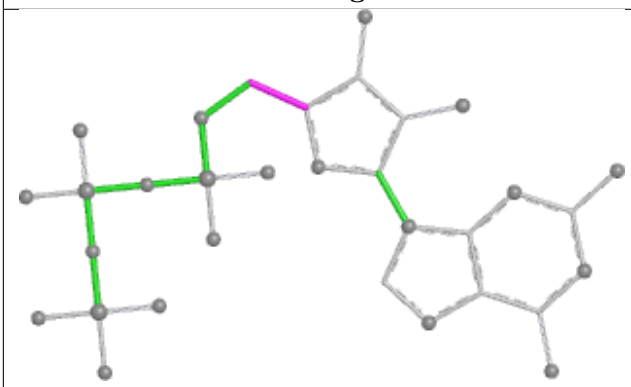

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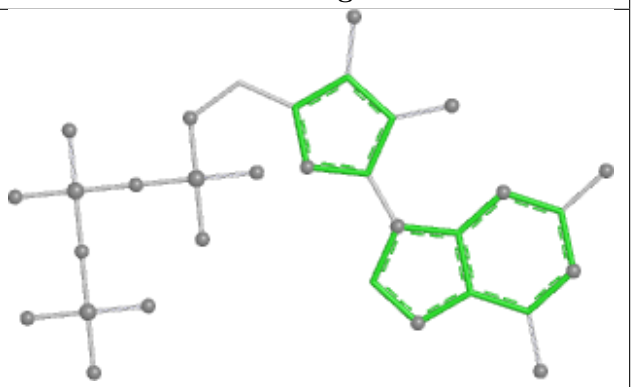
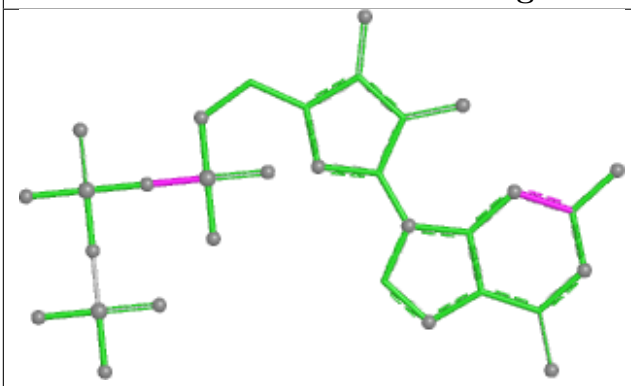


Rings

Ligand GTP 6h 501



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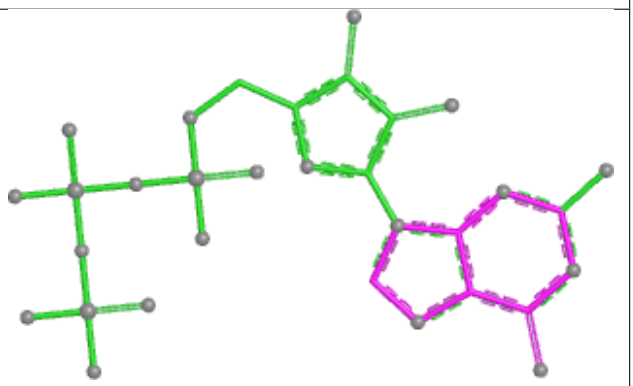
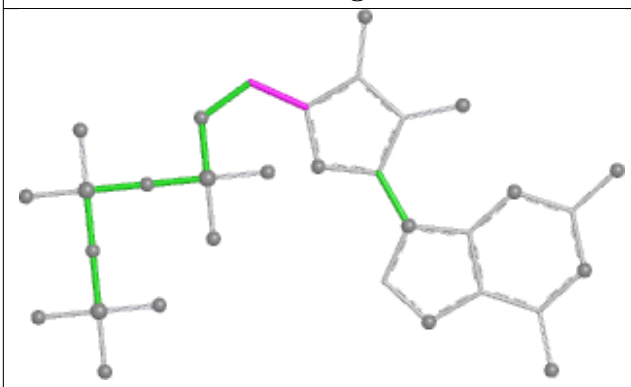
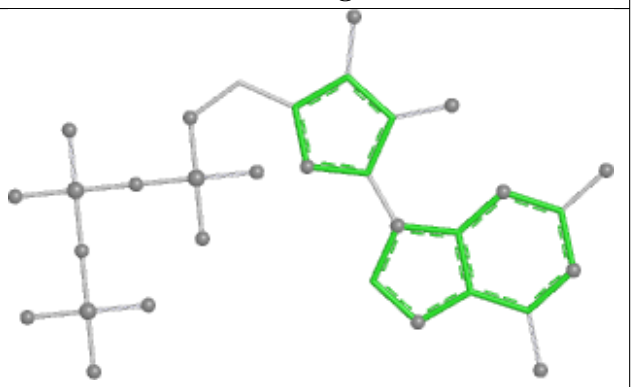


Bond angles

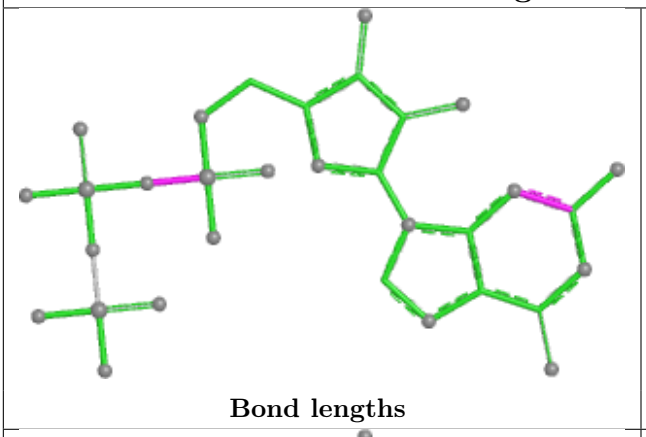


Torsions



Rings

Ligand GTP Ae 501



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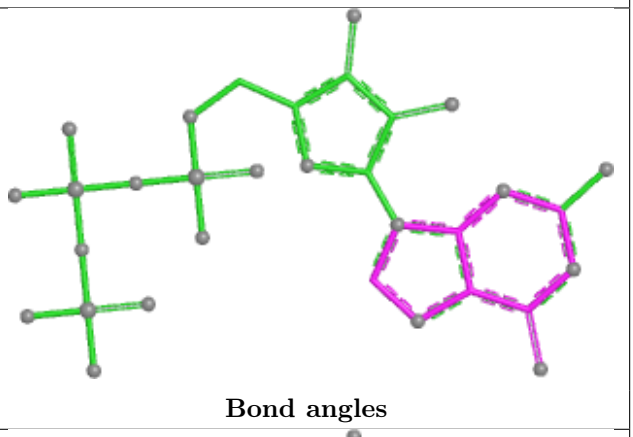

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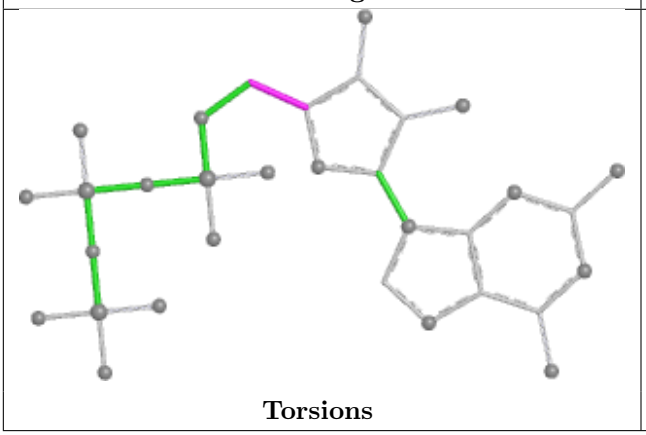

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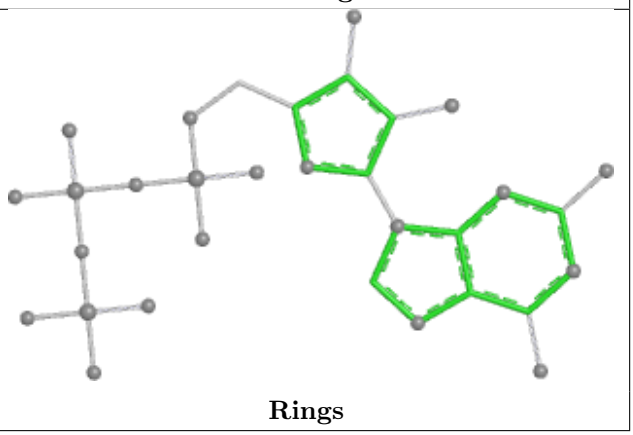
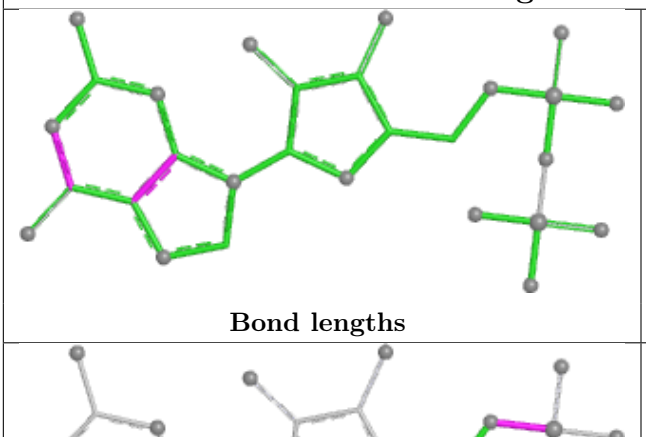


Rings

Ligand GDP 4g 501



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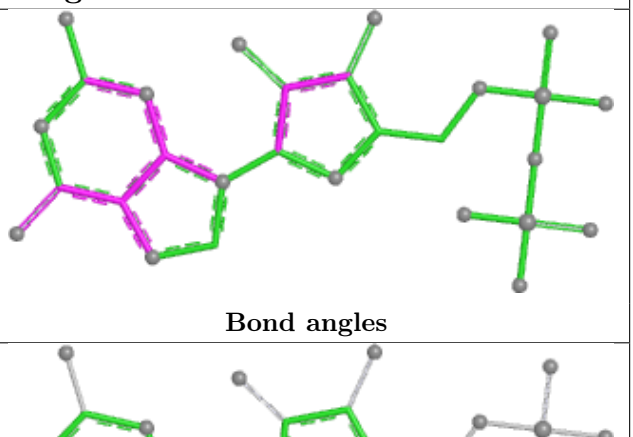

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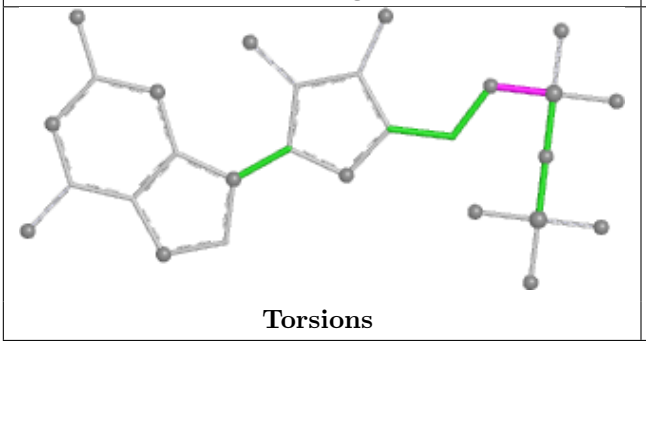

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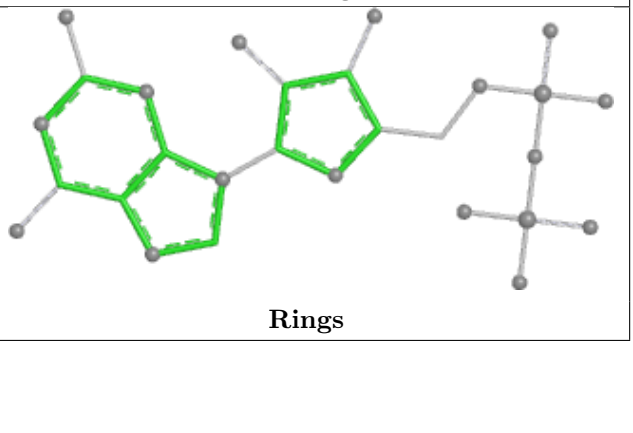
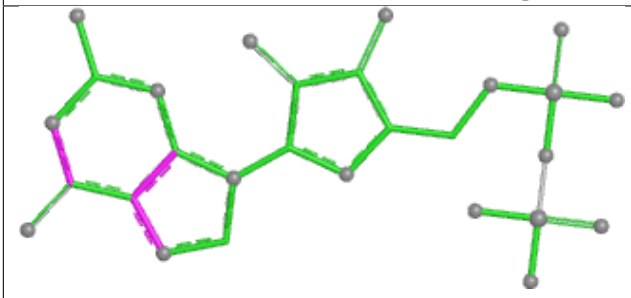


Rings

Ligand GDP 2a 501



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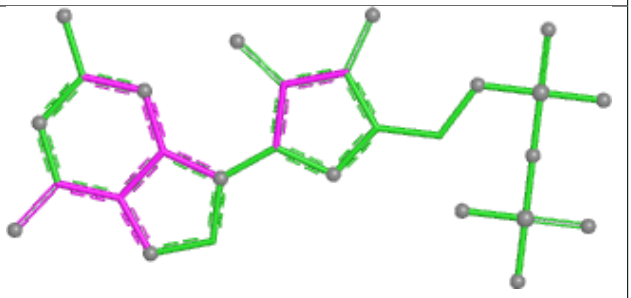

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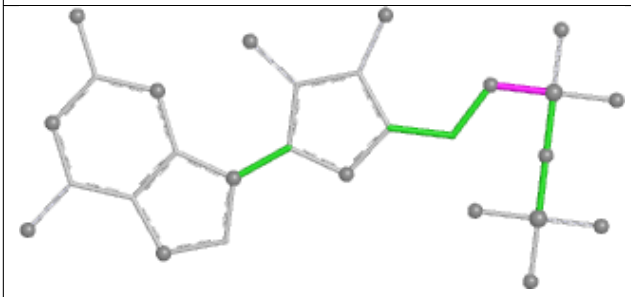

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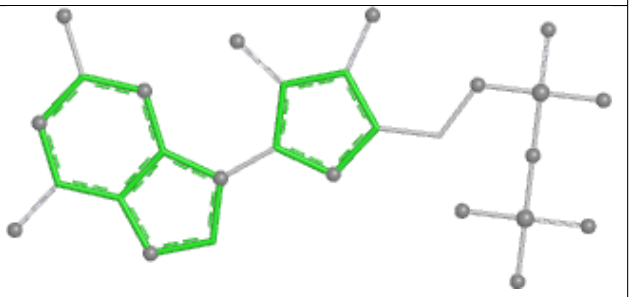
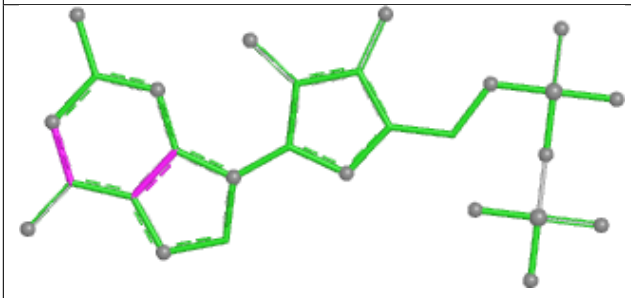


Rings

Ligand GDP 9g 501



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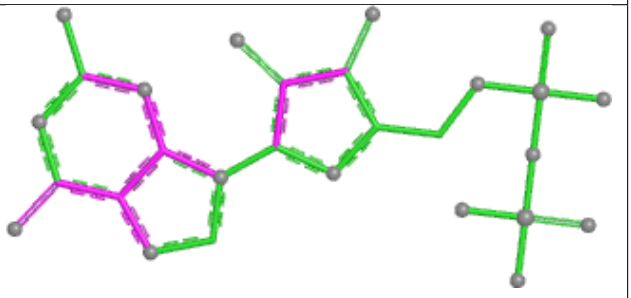

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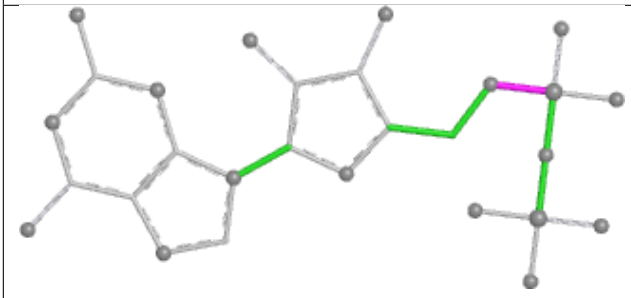

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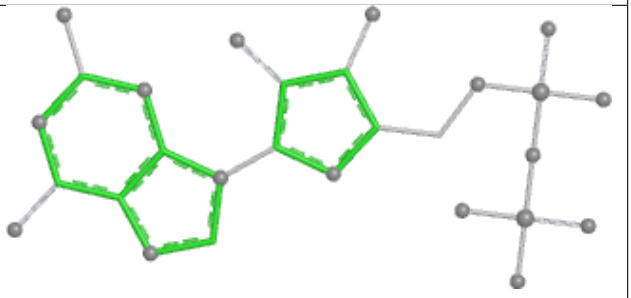
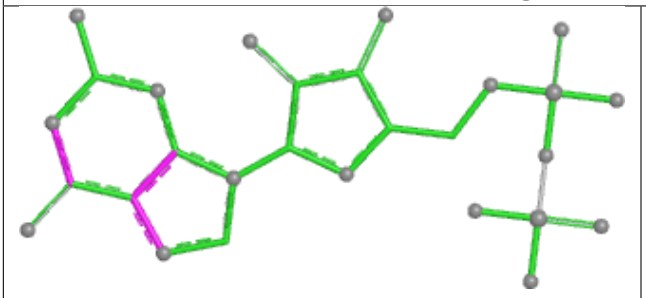


Rings

Ligand GDP 3e 501



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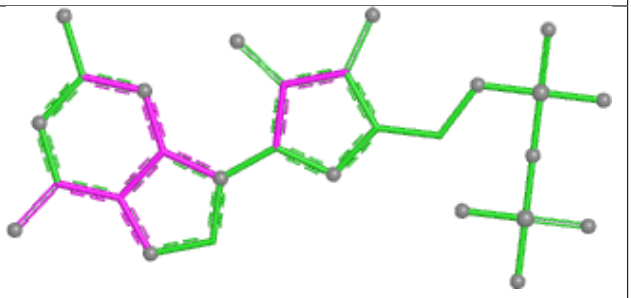

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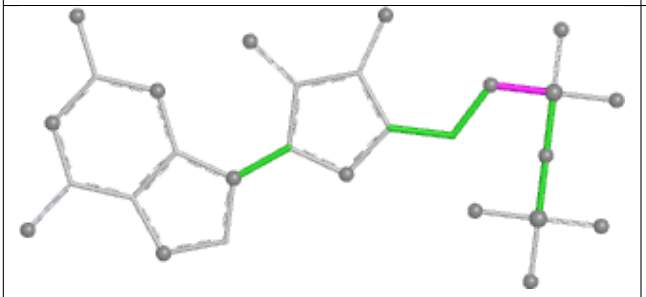

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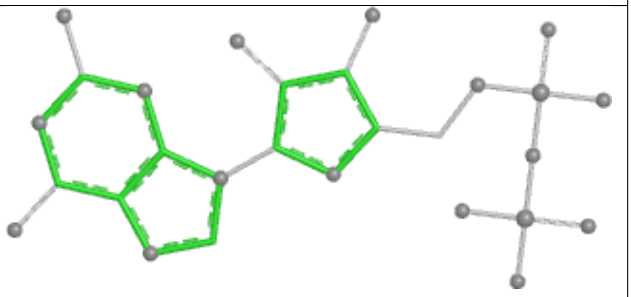

Rings

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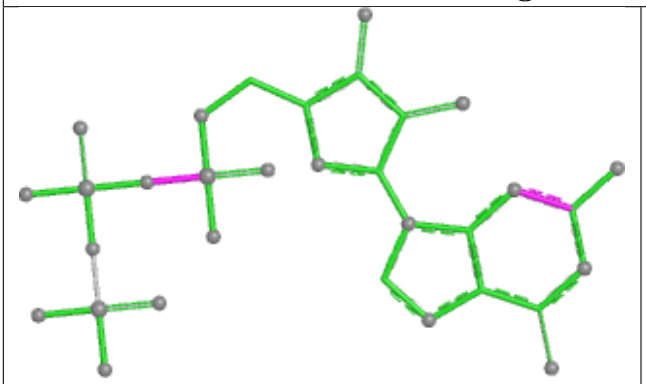

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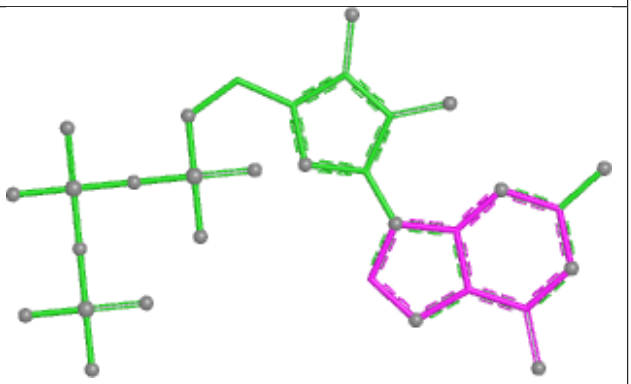

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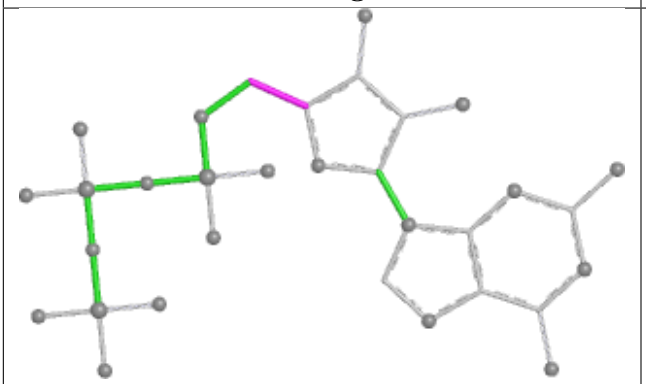

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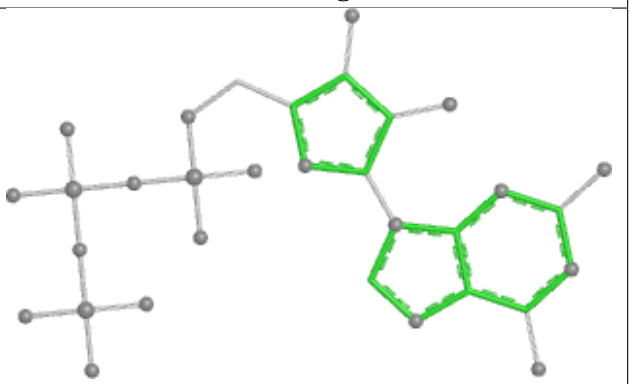

Rings

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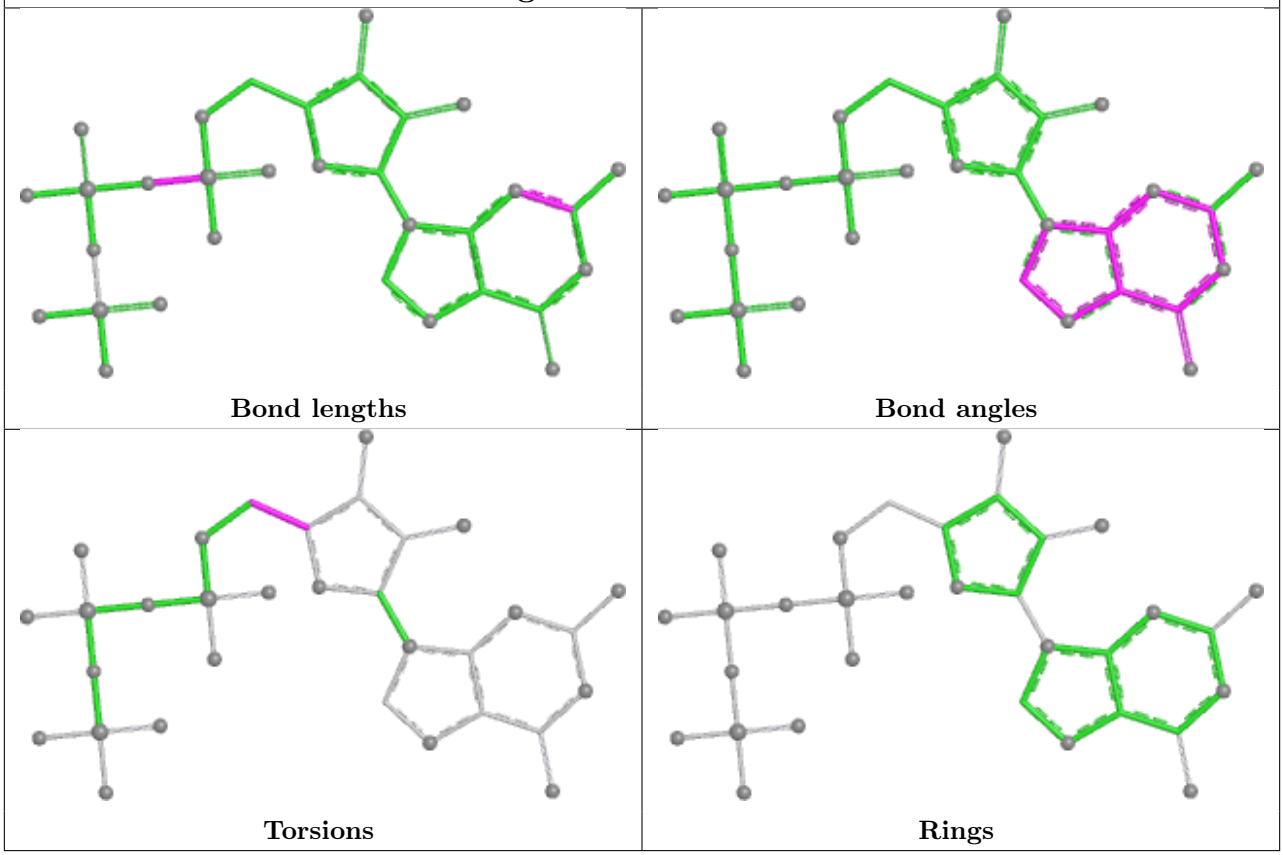

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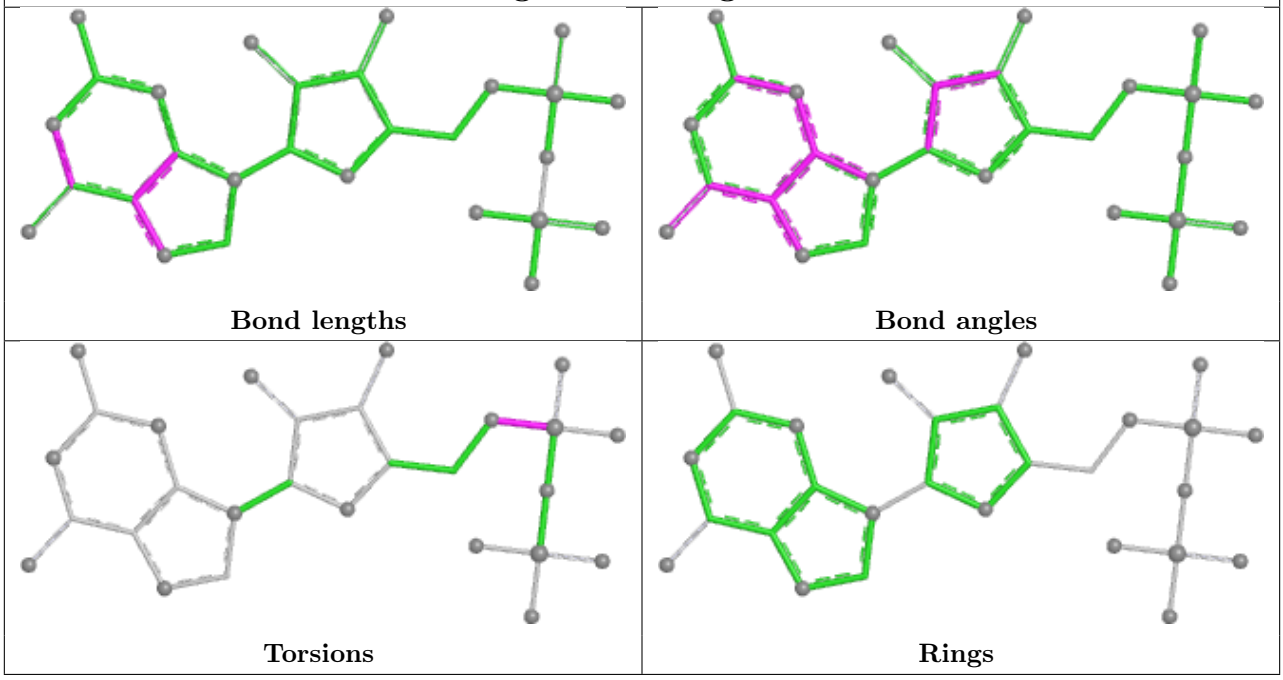

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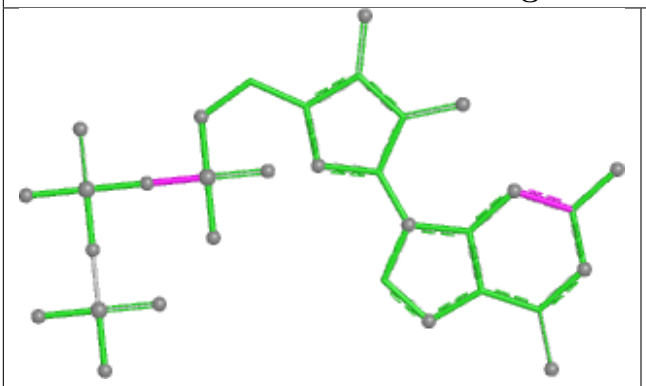

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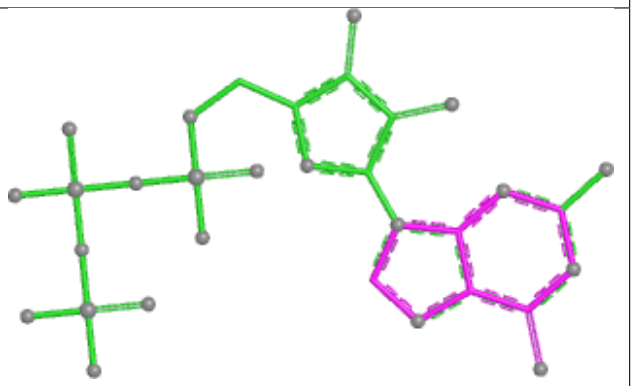

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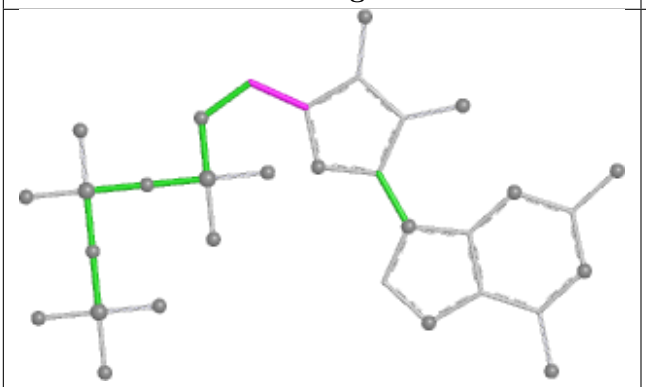

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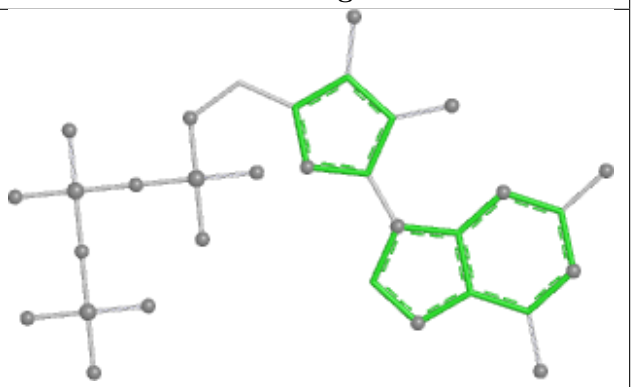

Rings

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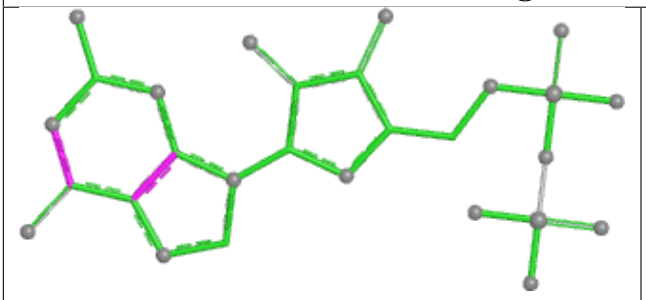

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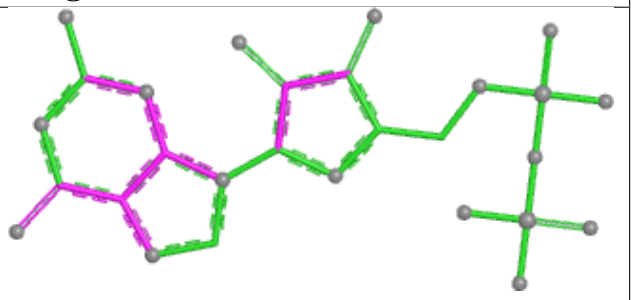

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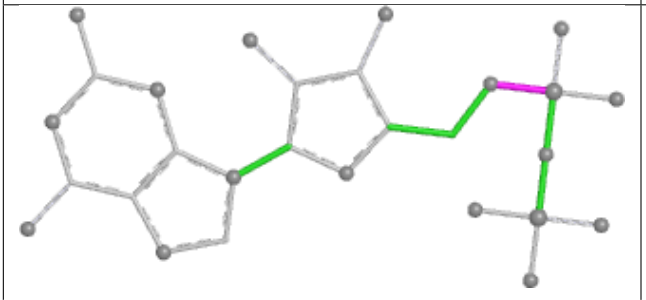

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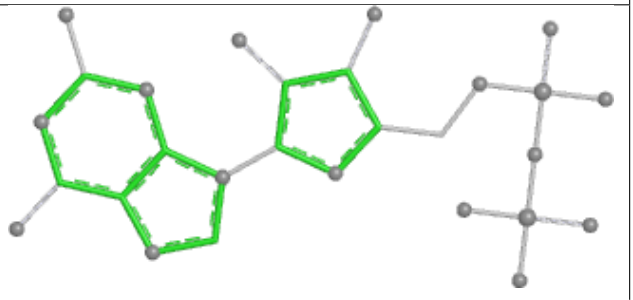

Rings

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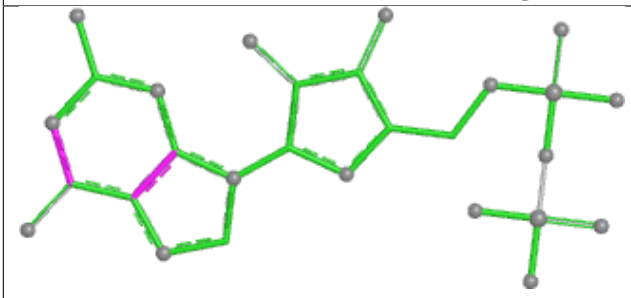	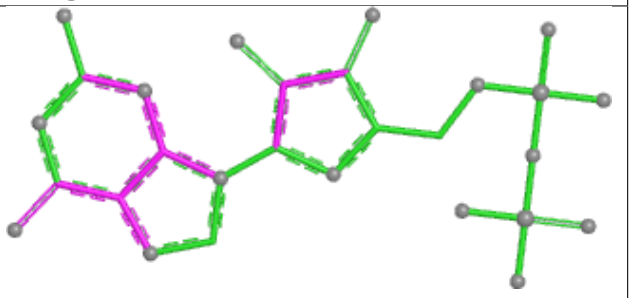
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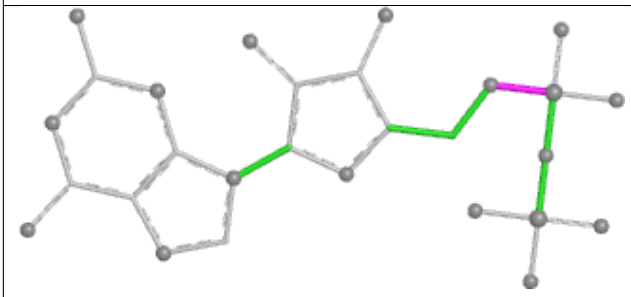	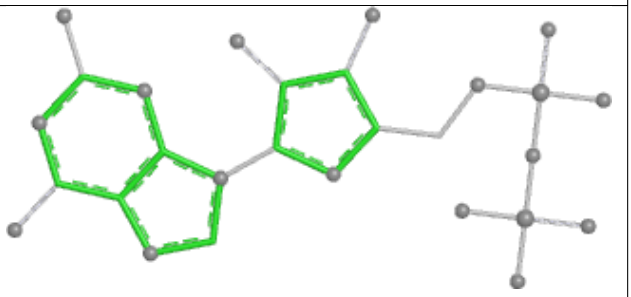
Torsions	Rings

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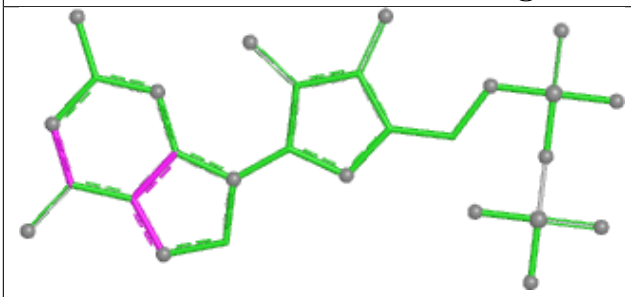	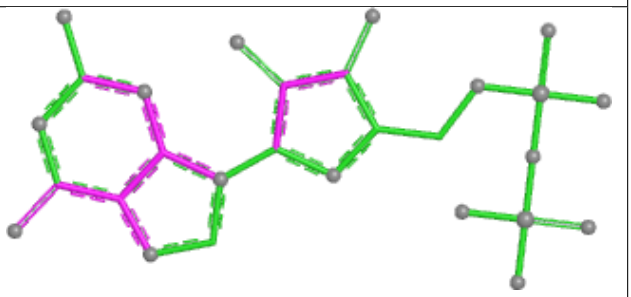
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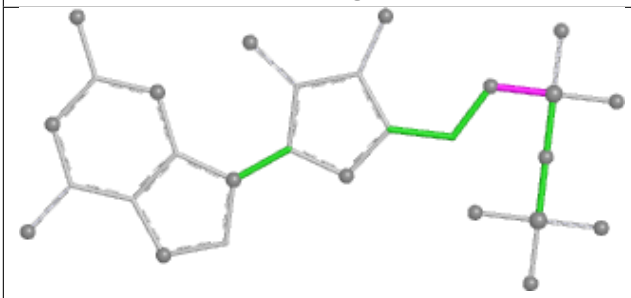
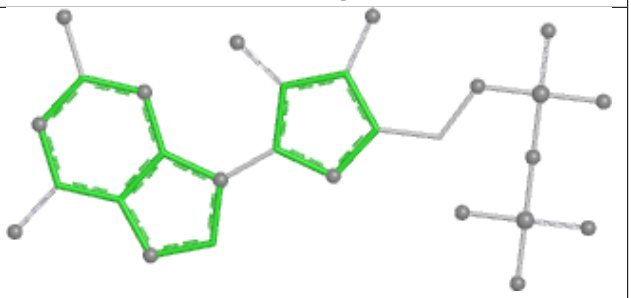
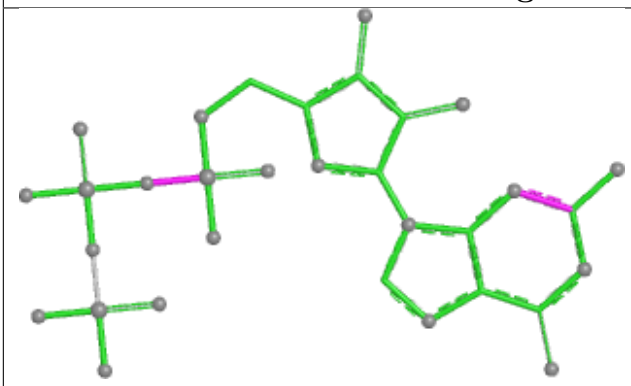
	
Torsions	Rings

Ligand GTP 4h 501



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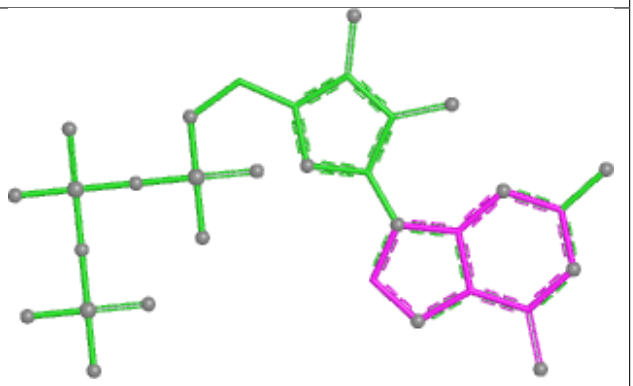

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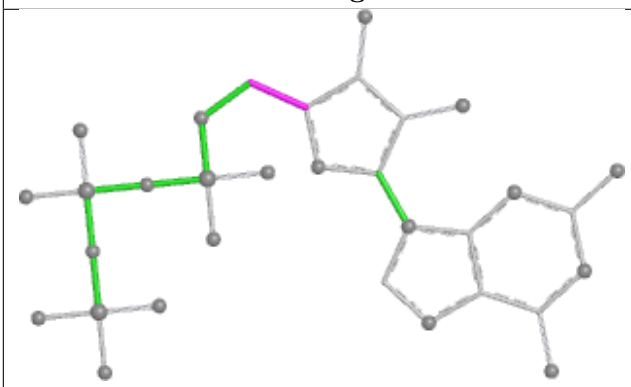

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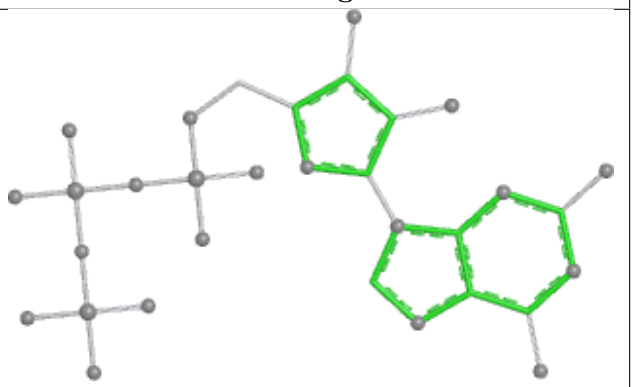
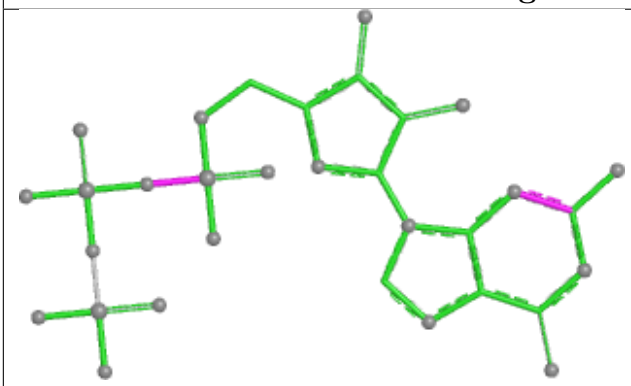


Rings

Ligand GTP 6c 501



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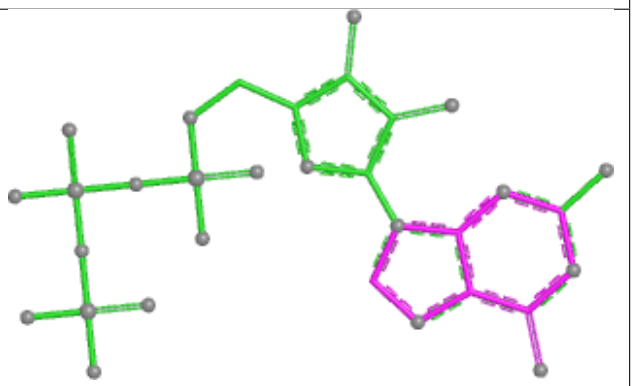

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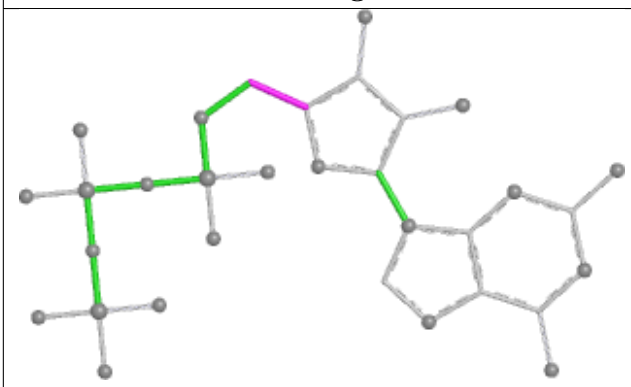

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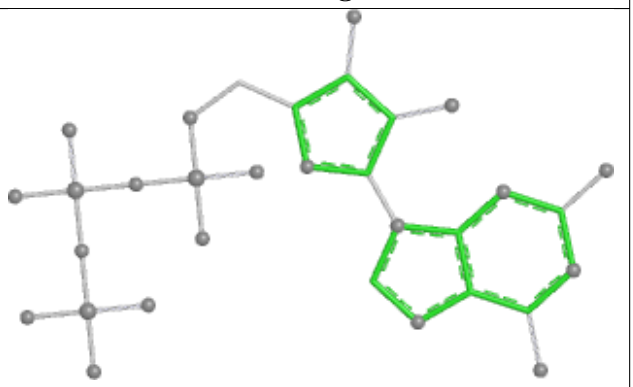
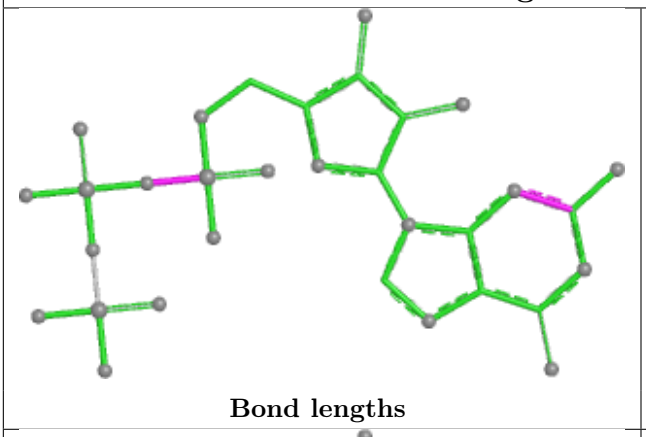


Rings

Ligand GTP 1b 501



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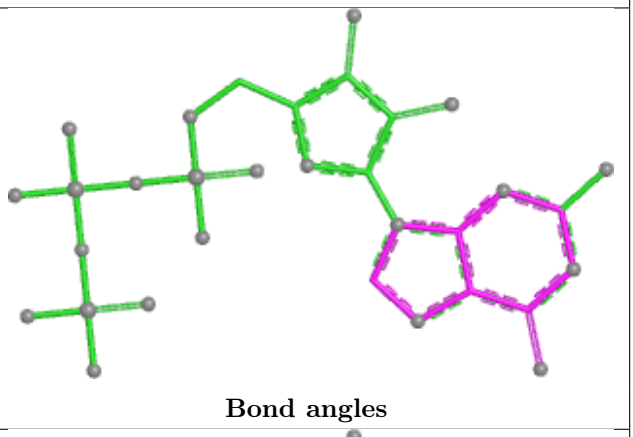

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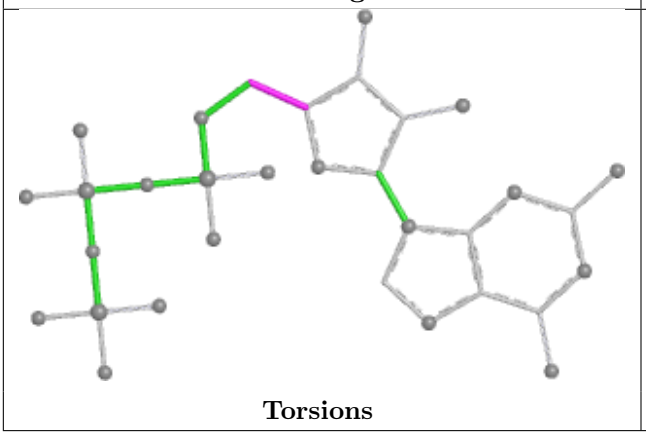

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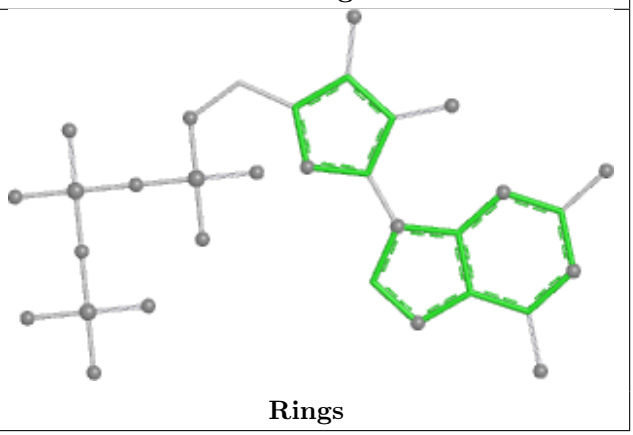
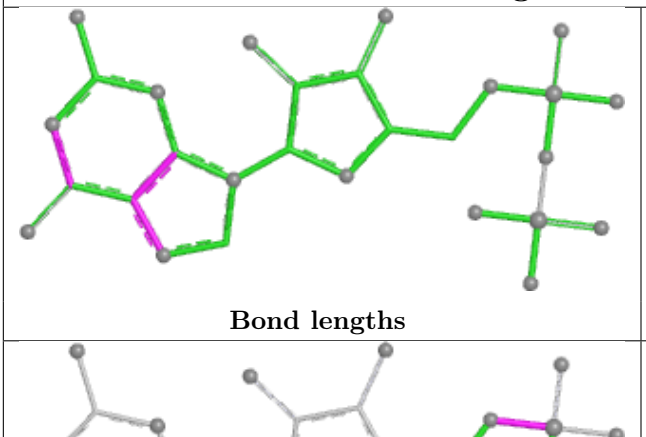


Rings

Ligand GDP De 501



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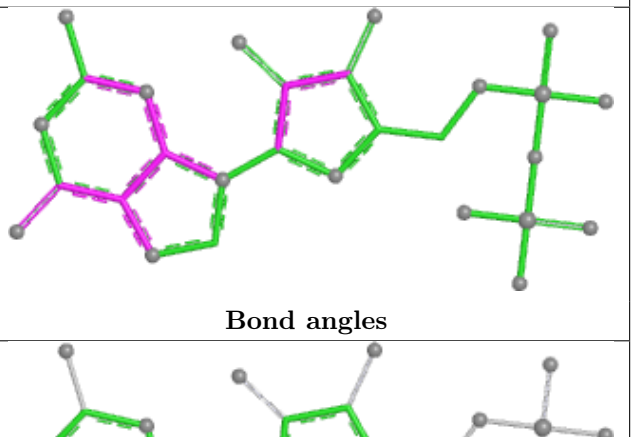
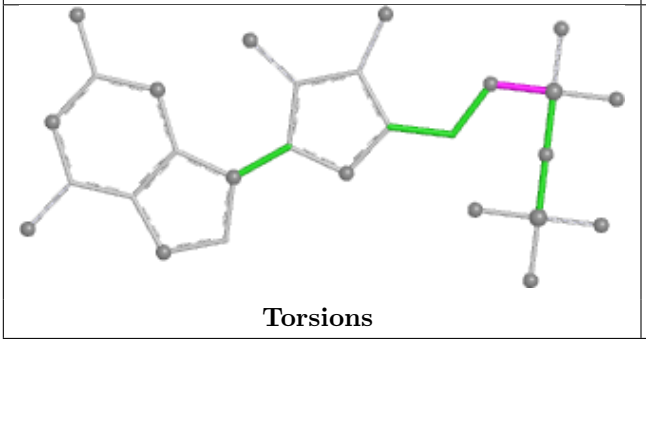


Bond angles



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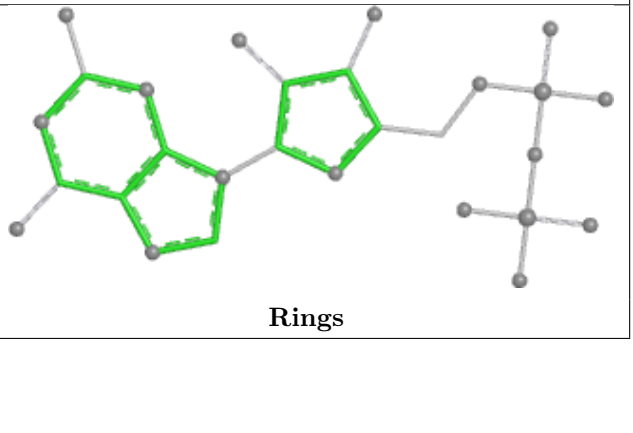
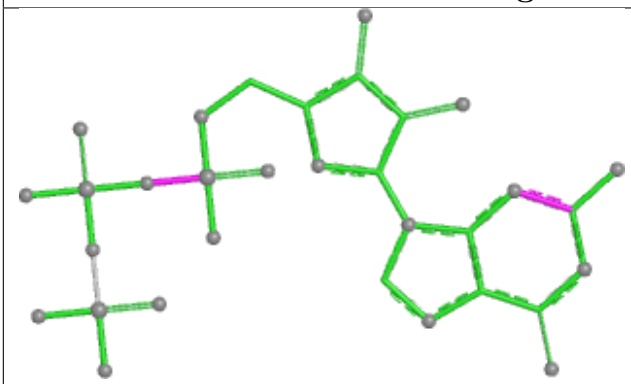


Rings

Ligand GTP 1d 501



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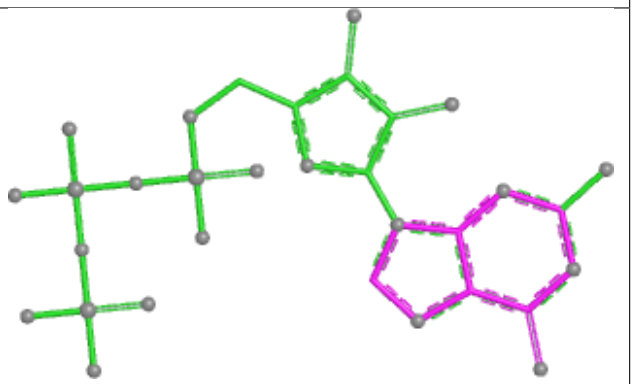

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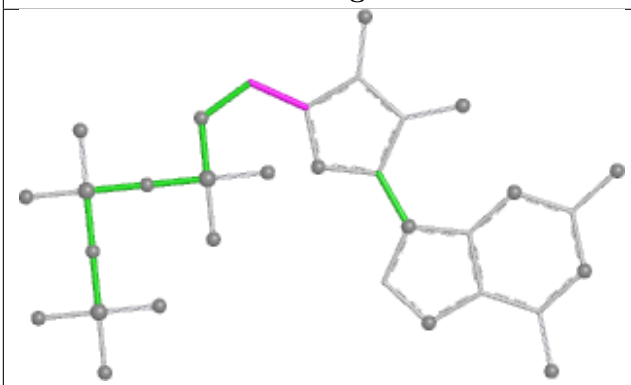

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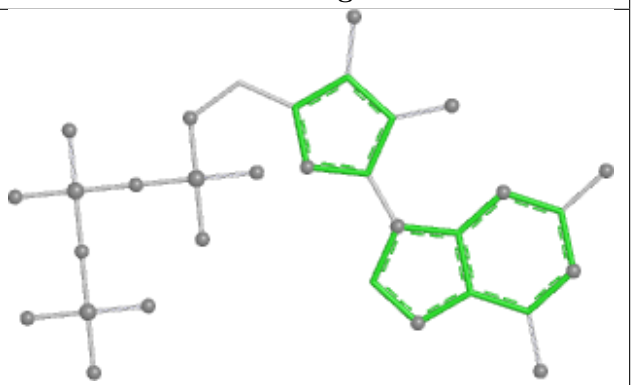

Rings

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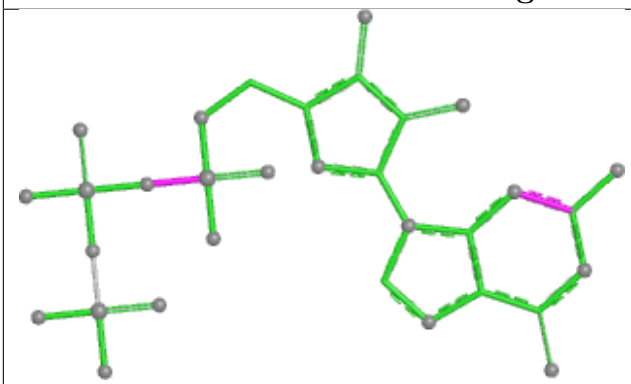

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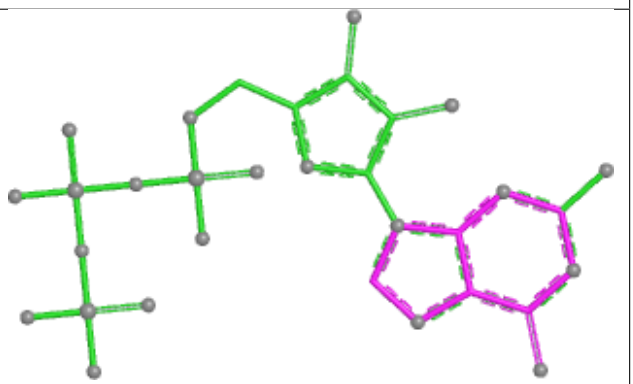

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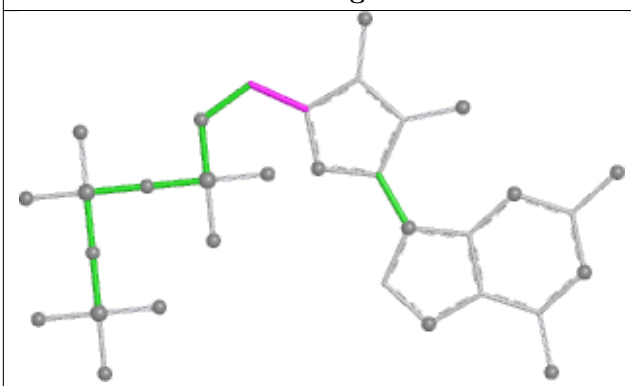

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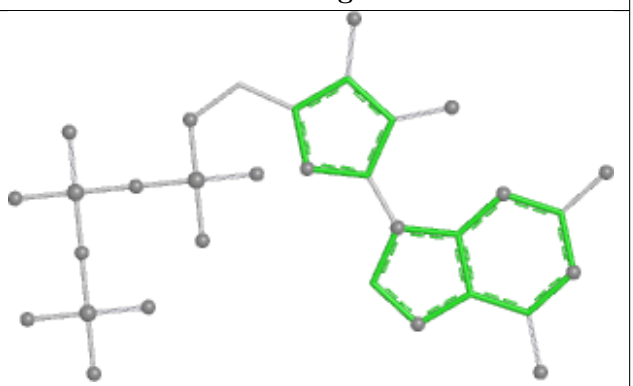
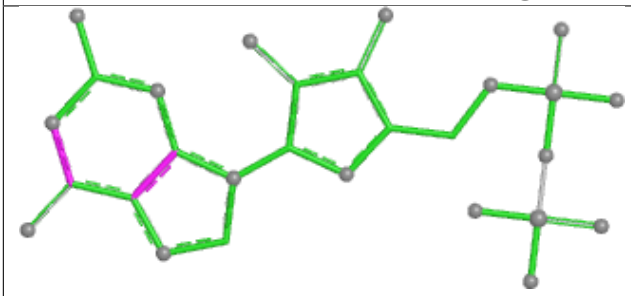


Rings

Ligand GDP 1g 501



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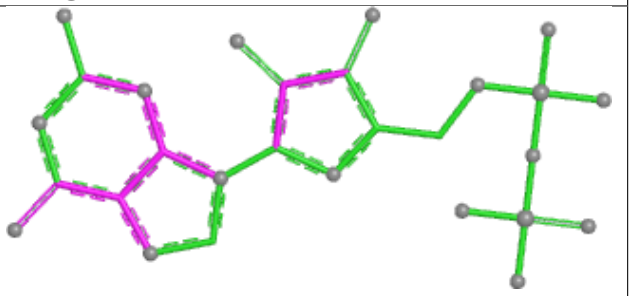

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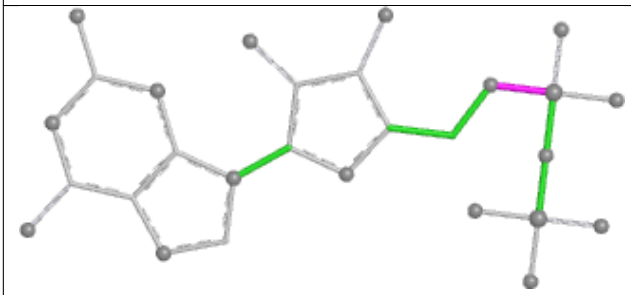

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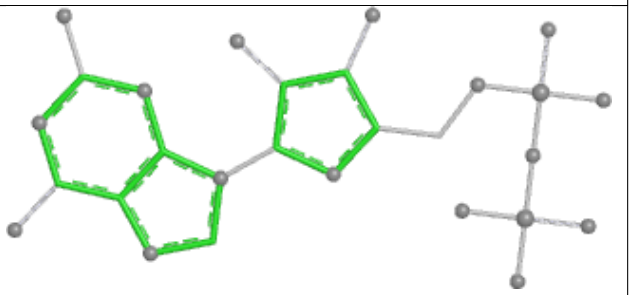
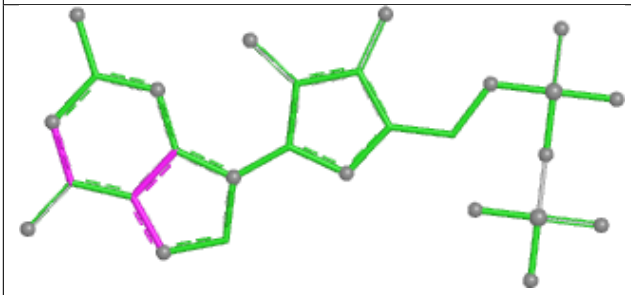


Rings

Ligand GDP 7a 501



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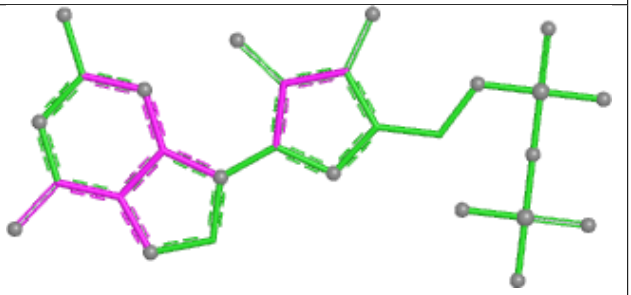

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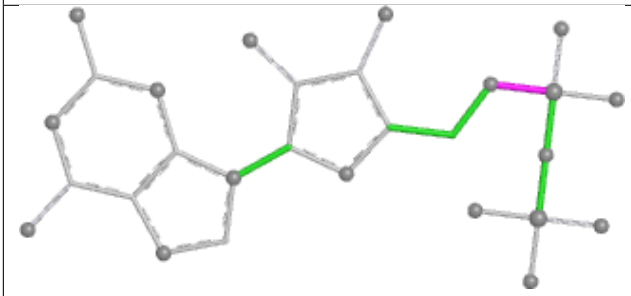

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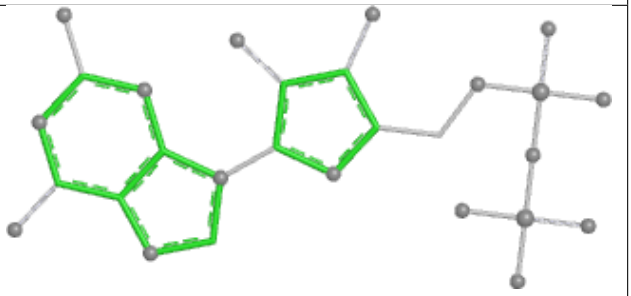

Rings

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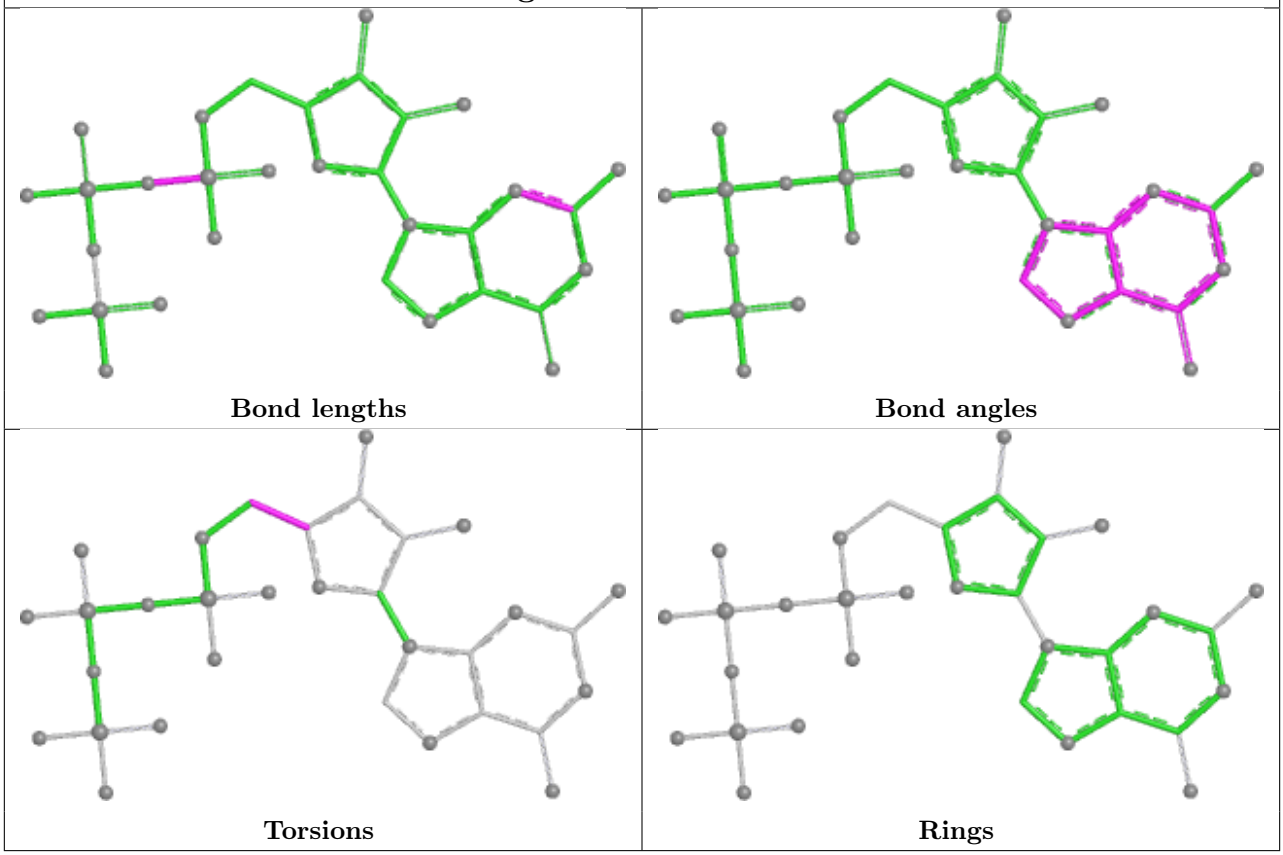

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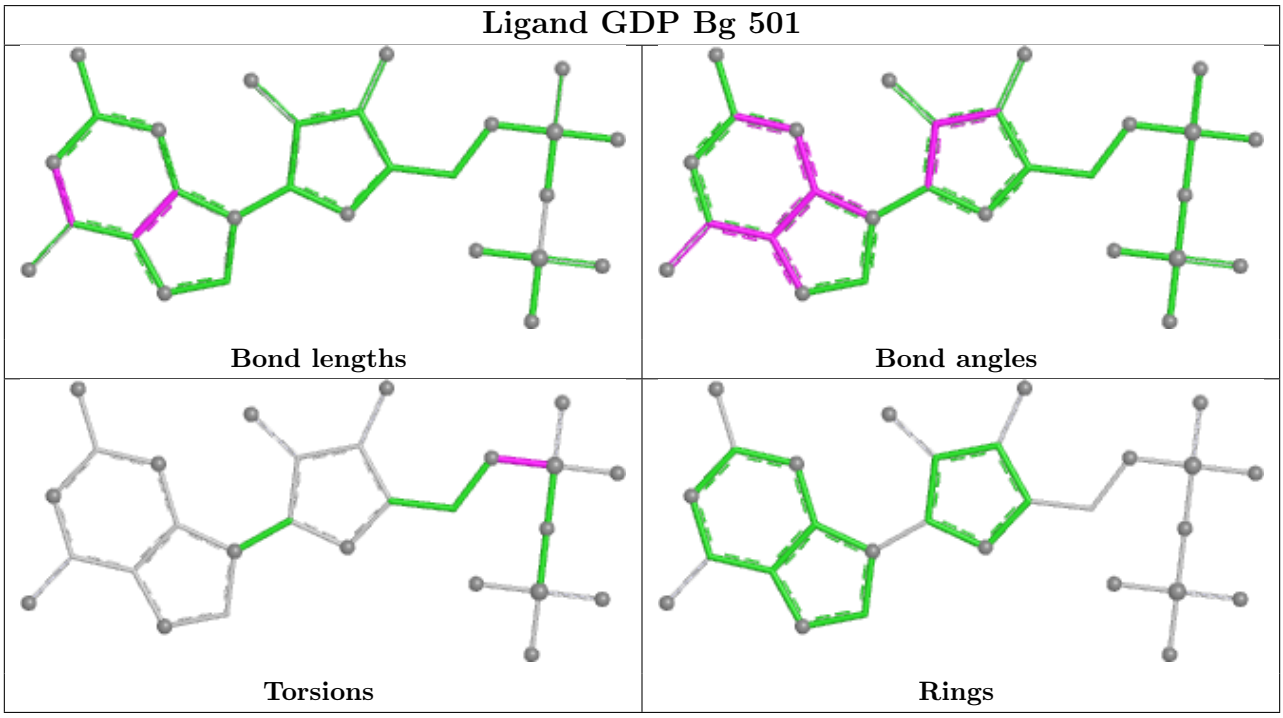

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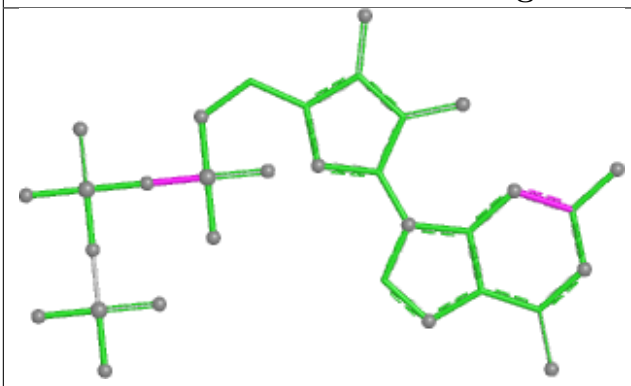

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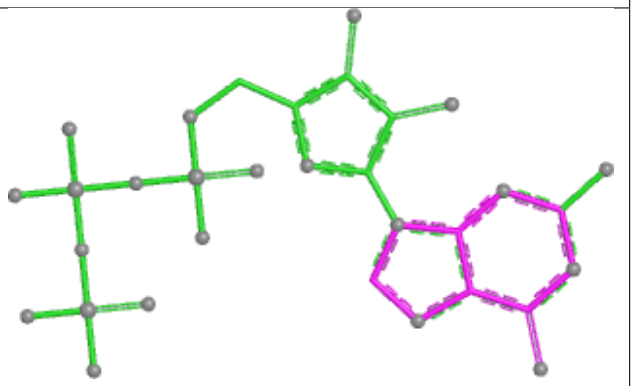

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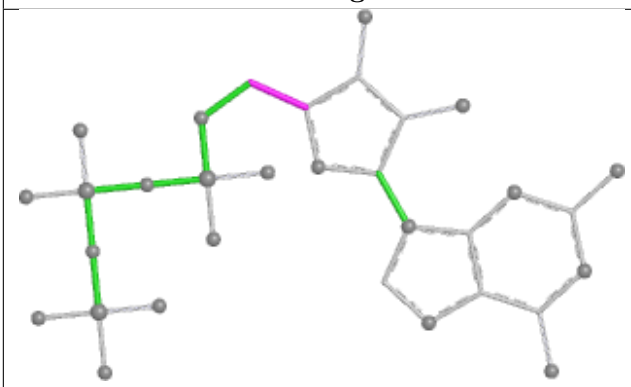

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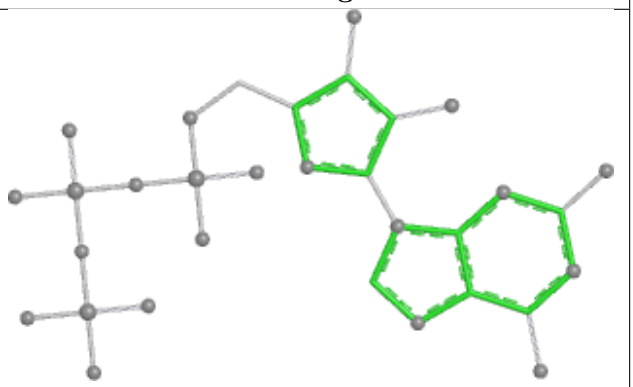

Rings

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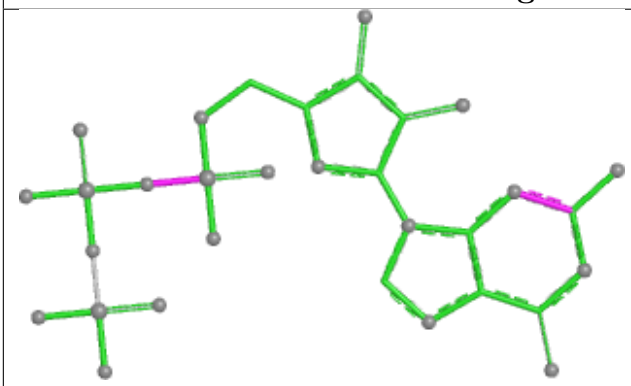

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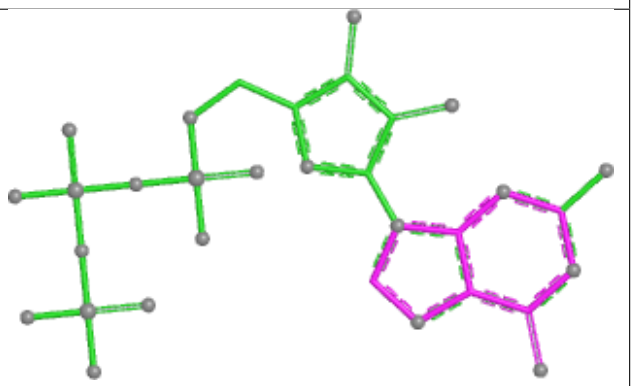

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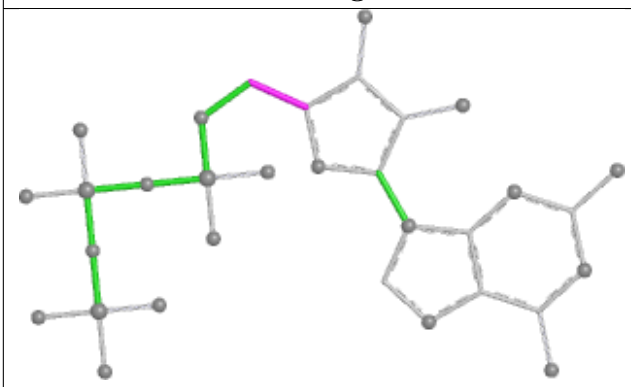

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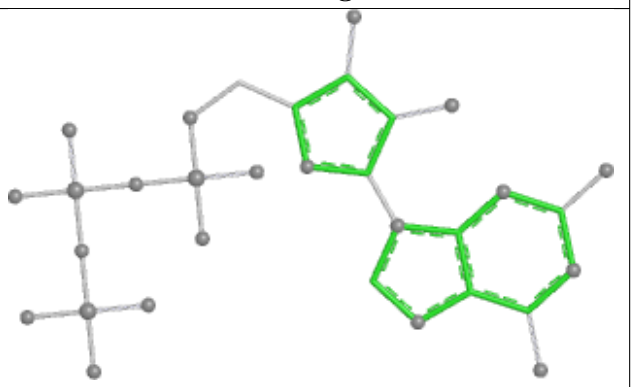
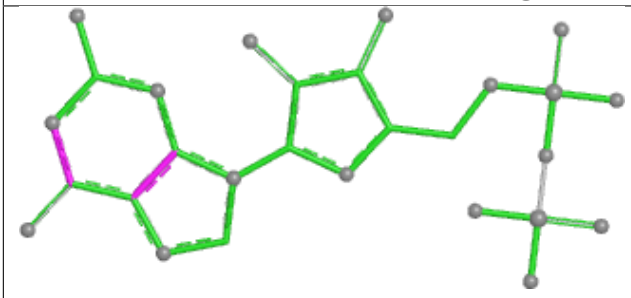
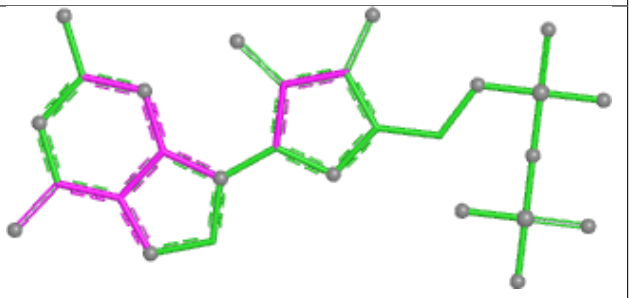
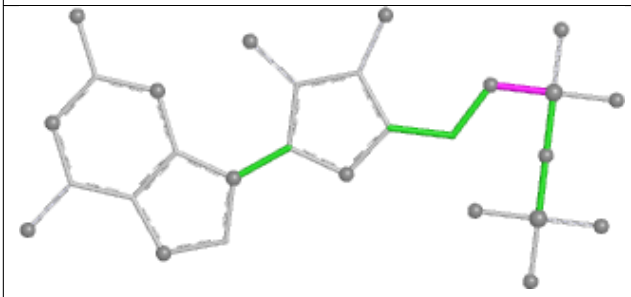
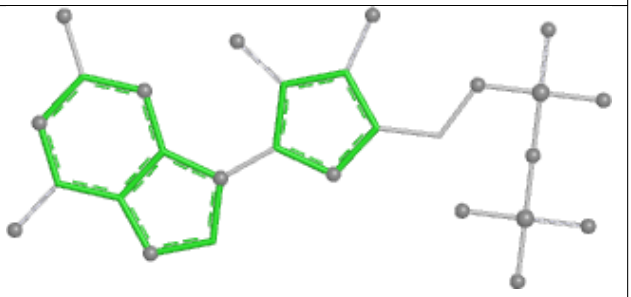


Rings

Ligand GDP 1c 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

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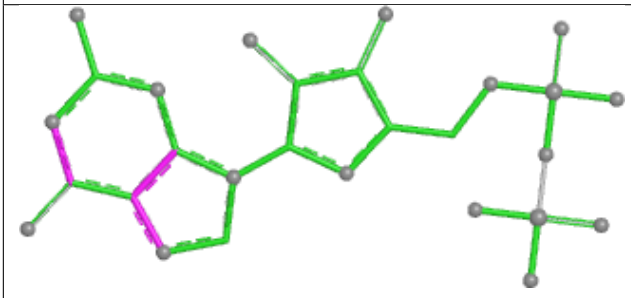
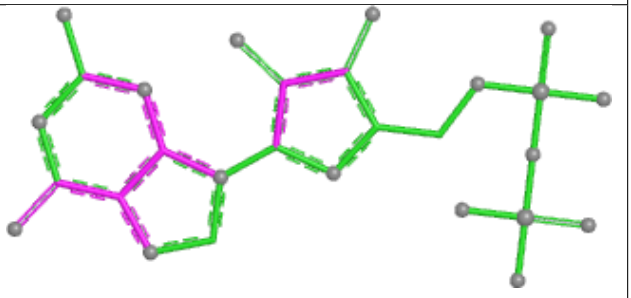
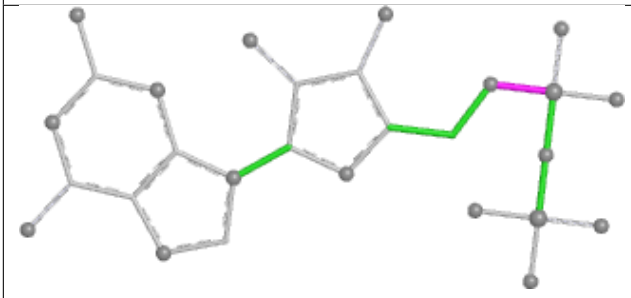
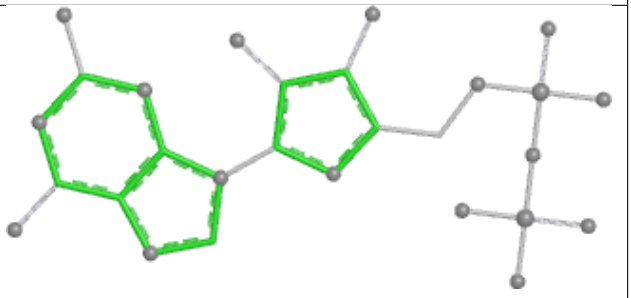
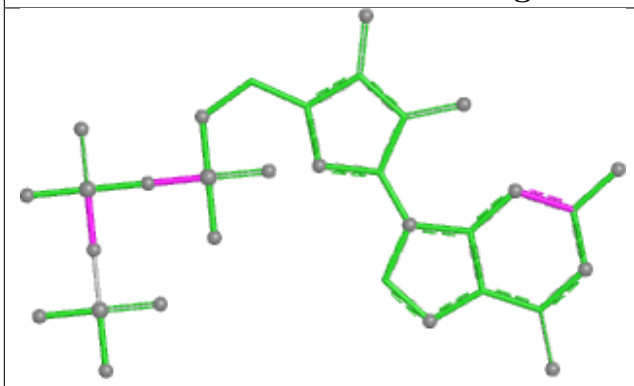
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GTP Ch 501



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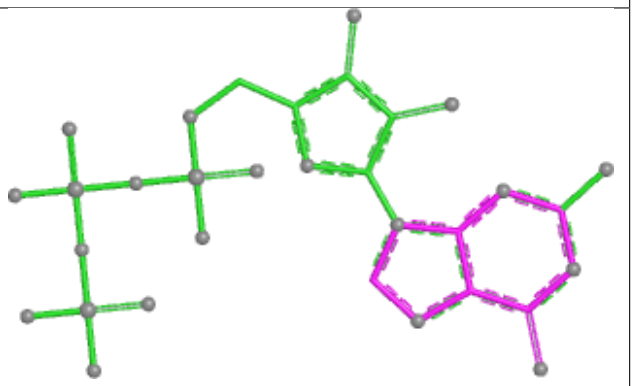

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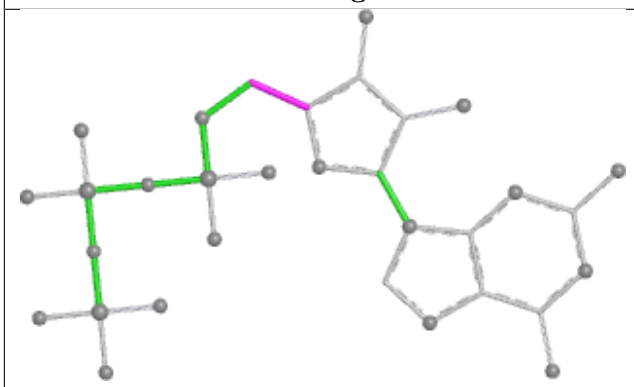

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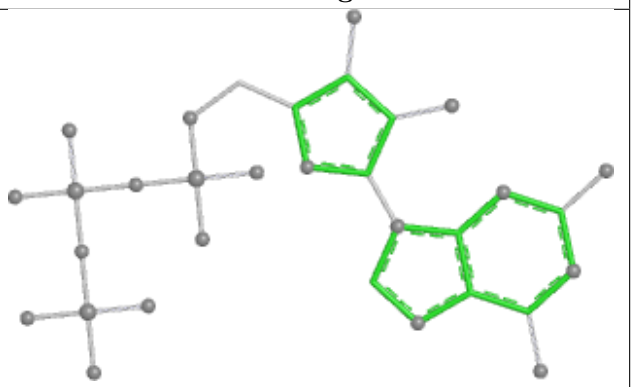
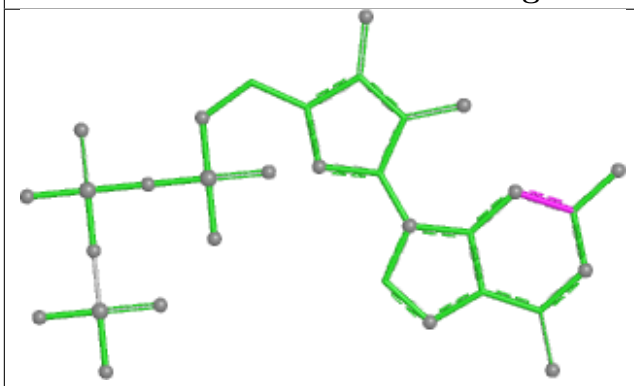


Rings

Ligand GTP 7f 501



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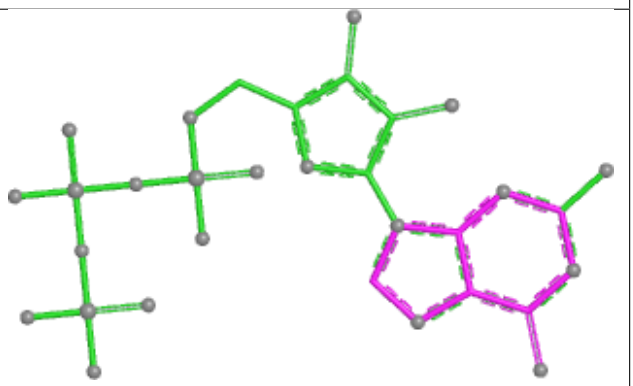

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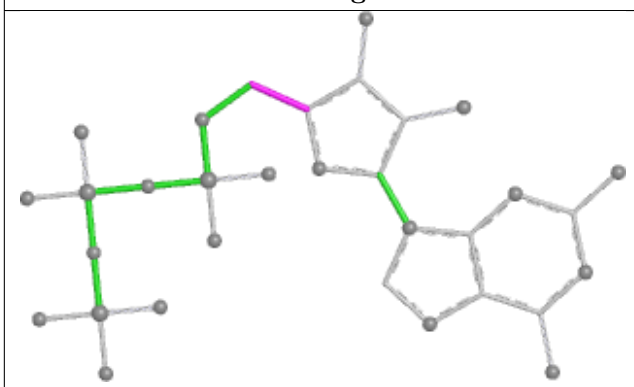

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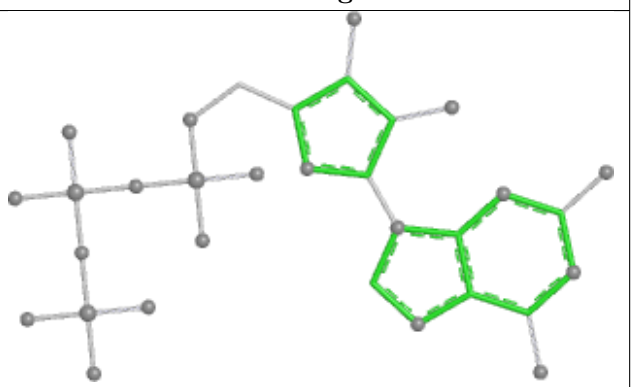

Rings

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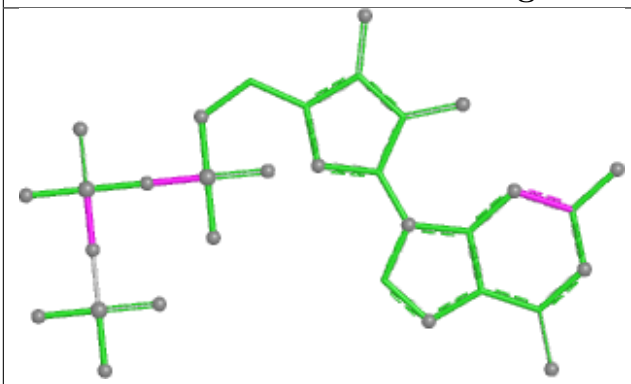

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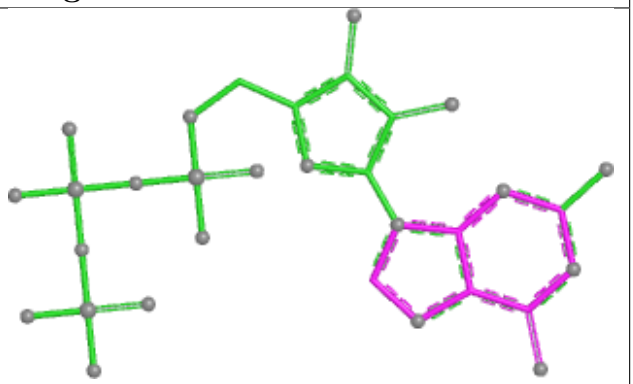
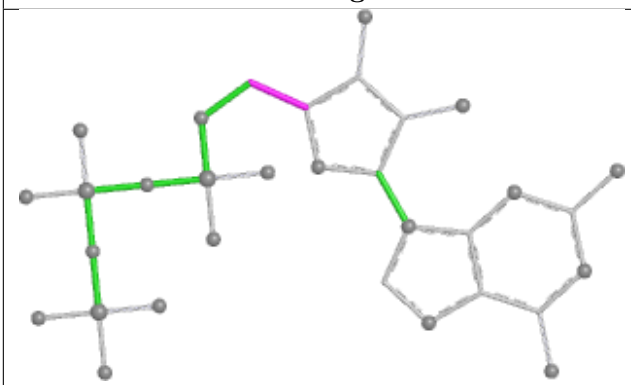


Bond angles



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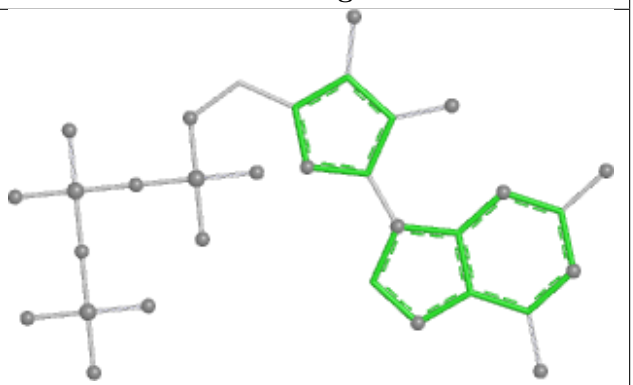
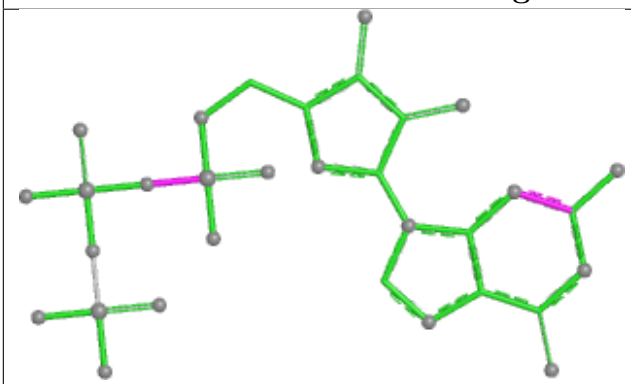


Rings

Ligand GTP Cd 501



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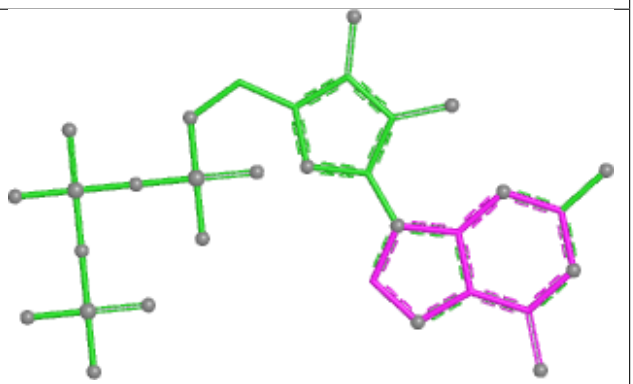

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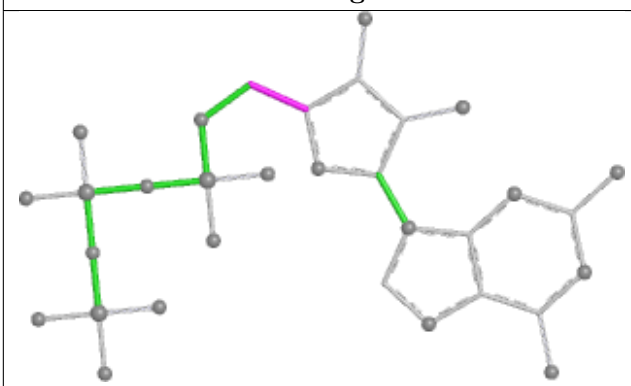

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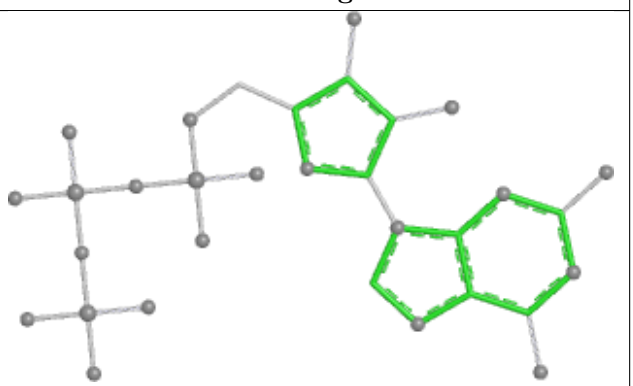
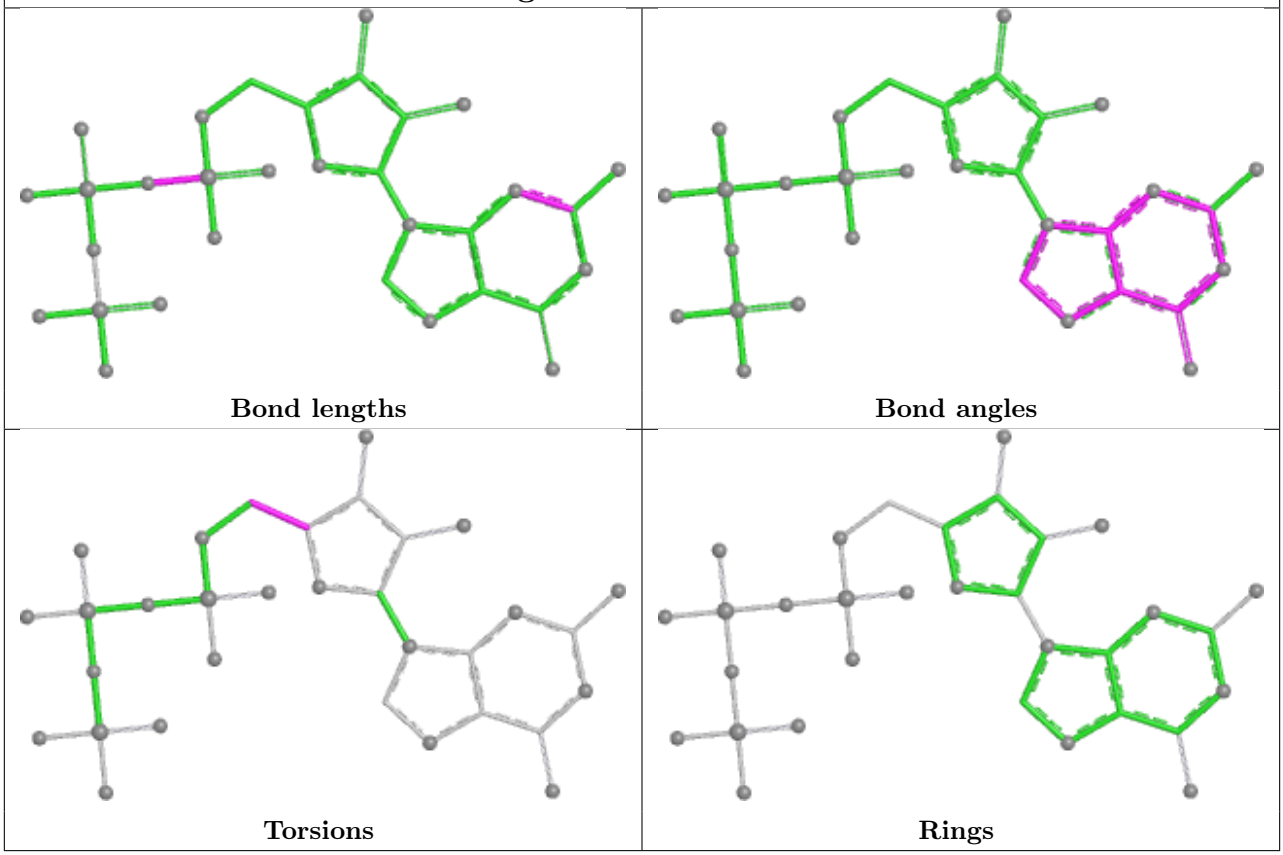
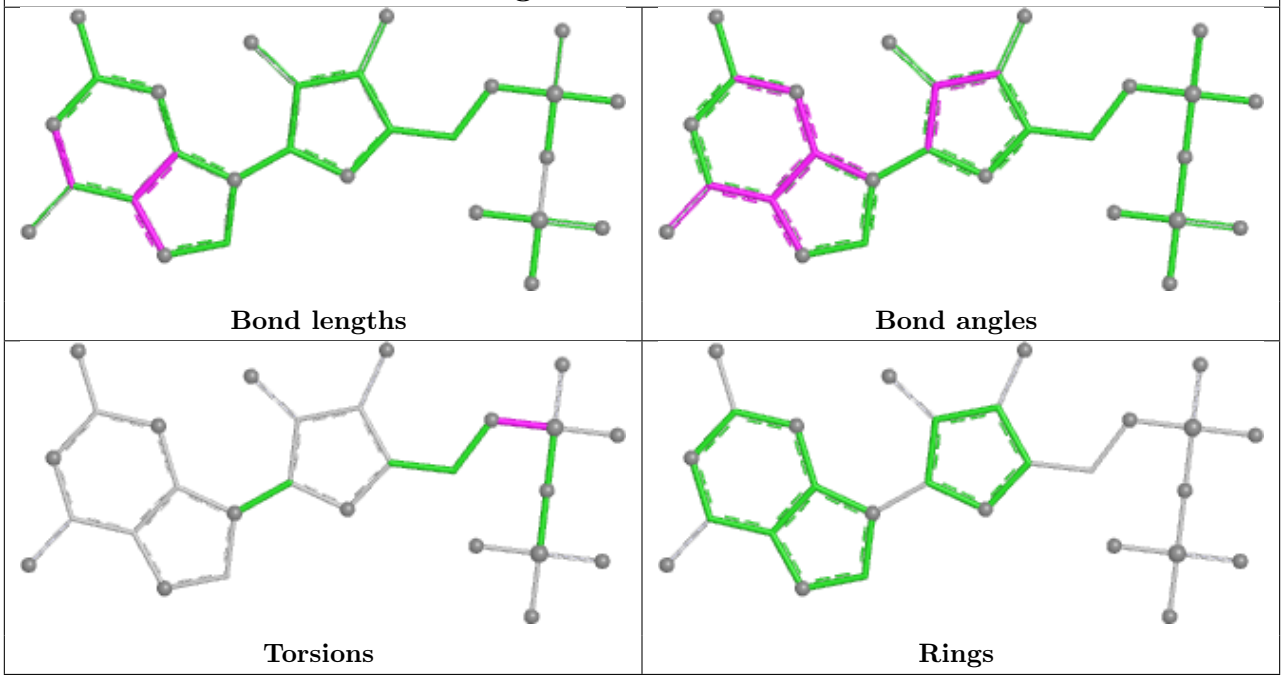


Rings

Ligand GTP 1h 501



Ligand GDP Ac 501



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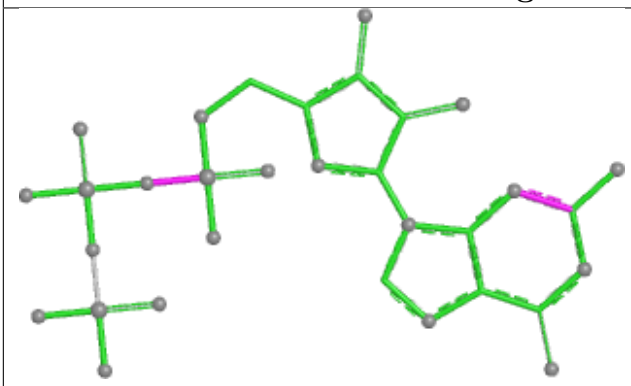
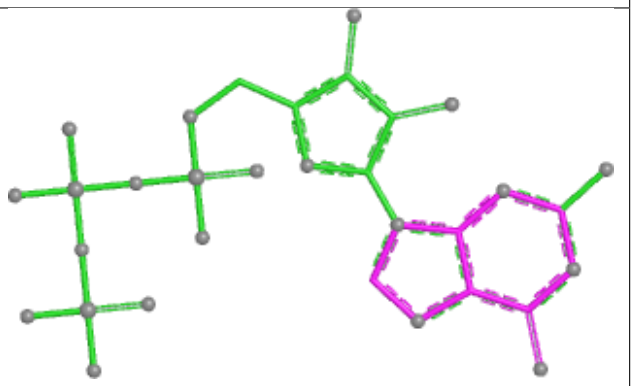
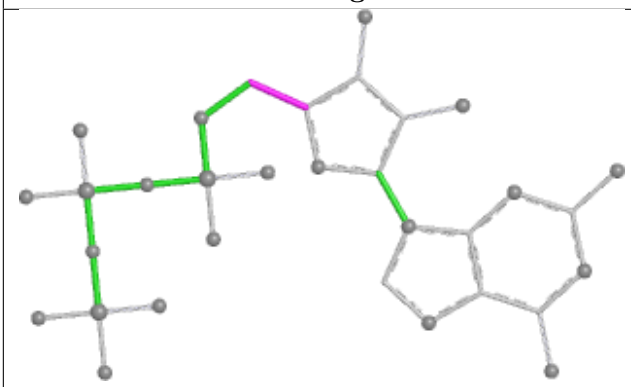


Bond lengths



Bond angles



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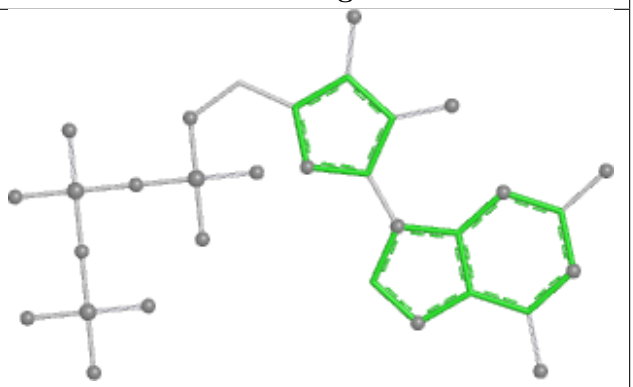
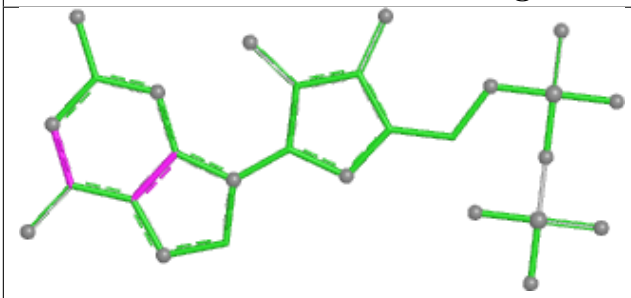
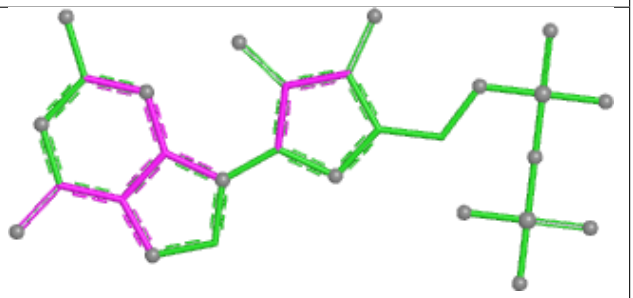


Rings

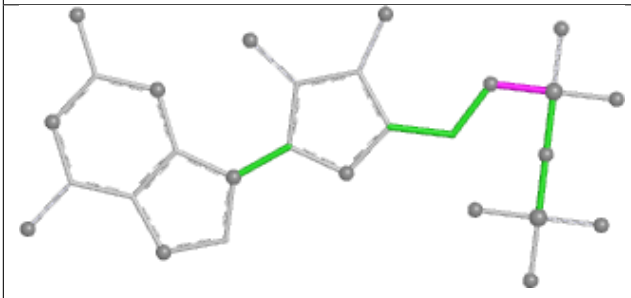
Ligand GDP Bc 501



Bond lengths



Bond angles



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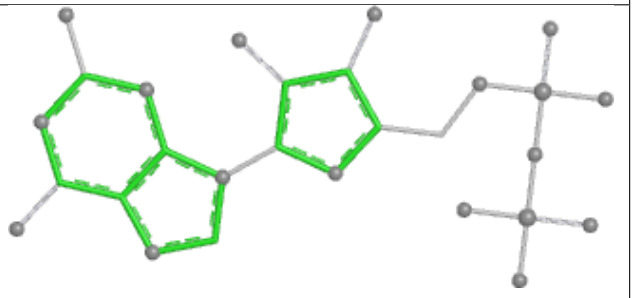
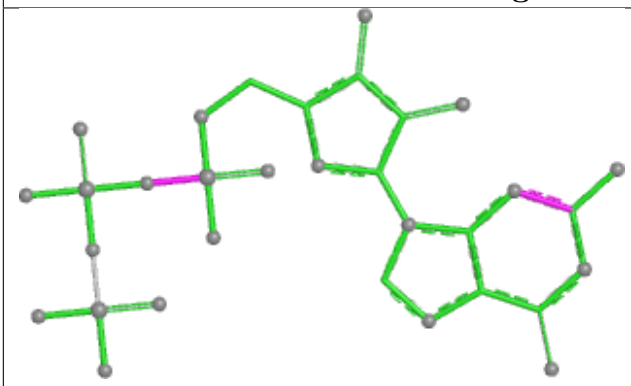


Rings

Ligand GTP Dd 501



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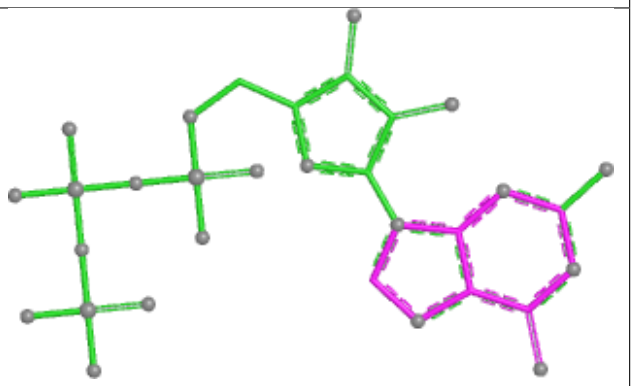

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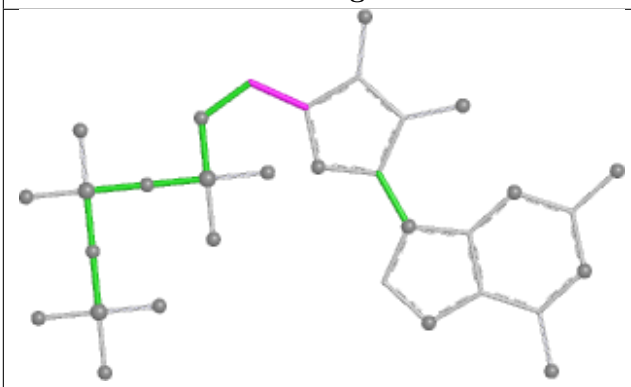

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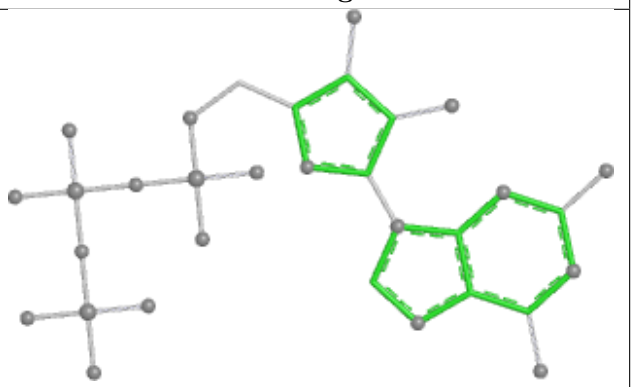

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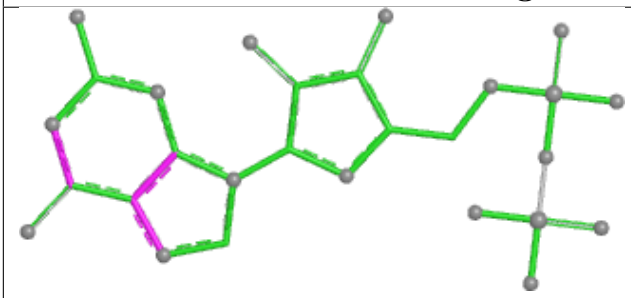

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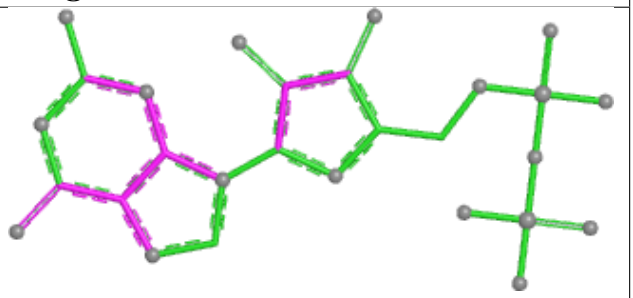

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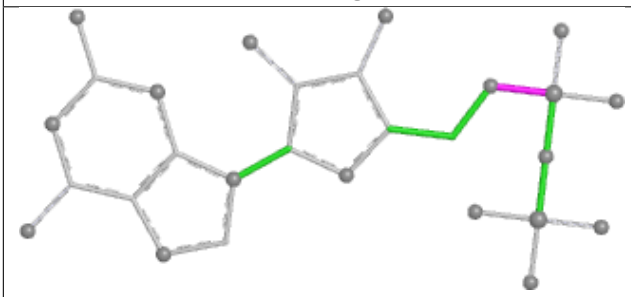

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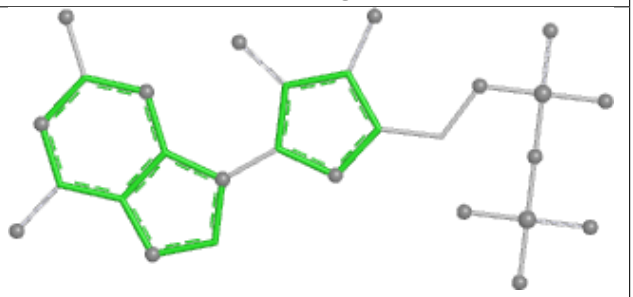

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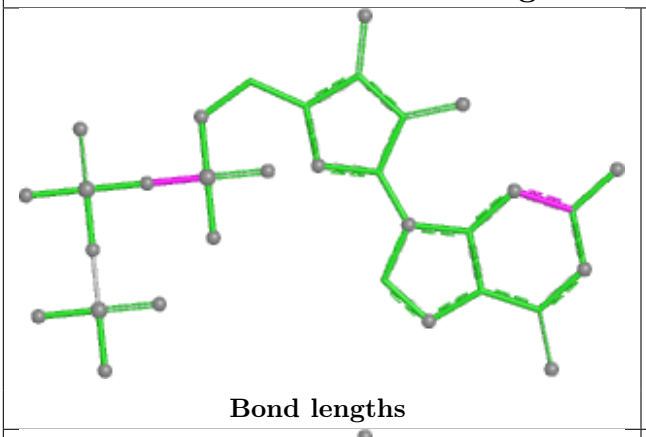

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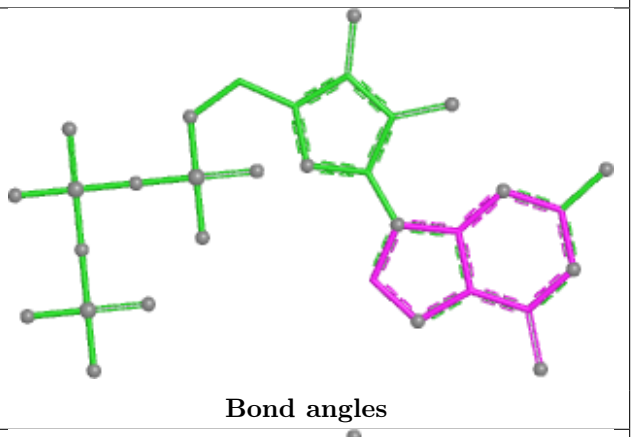

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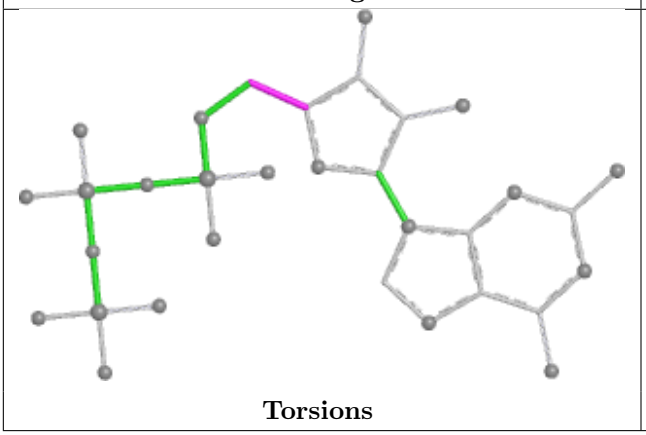

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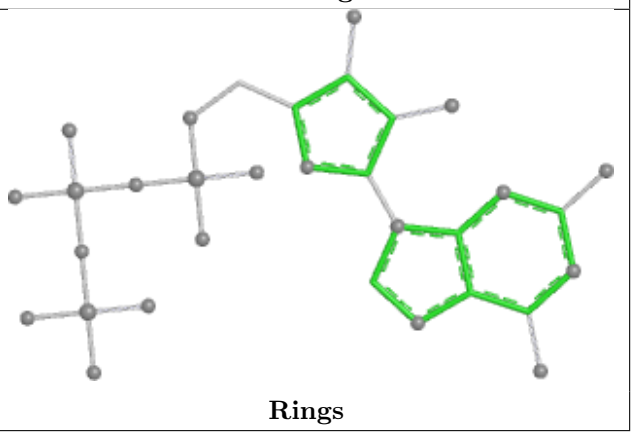
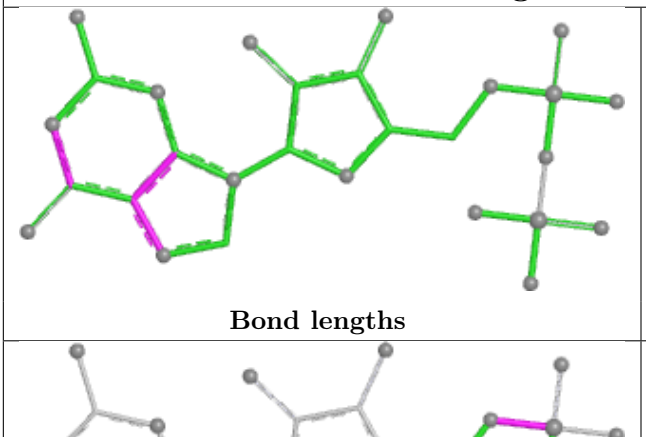


Rings

Ligand GDP Da 501



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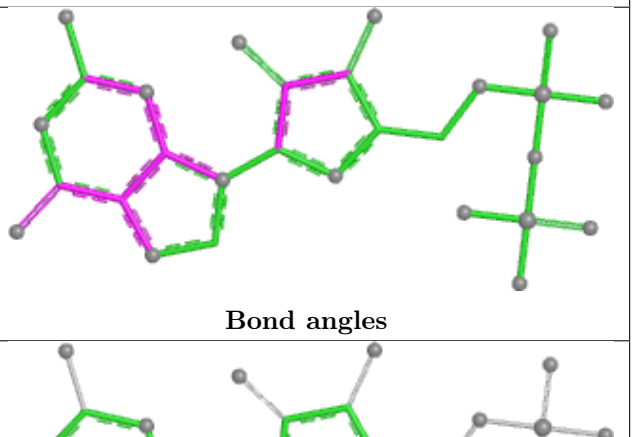

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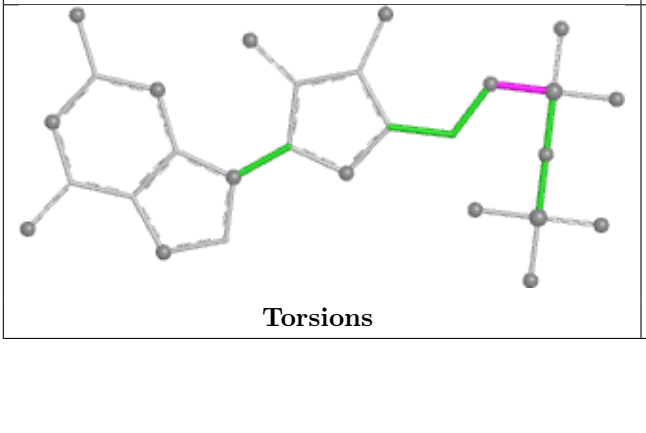

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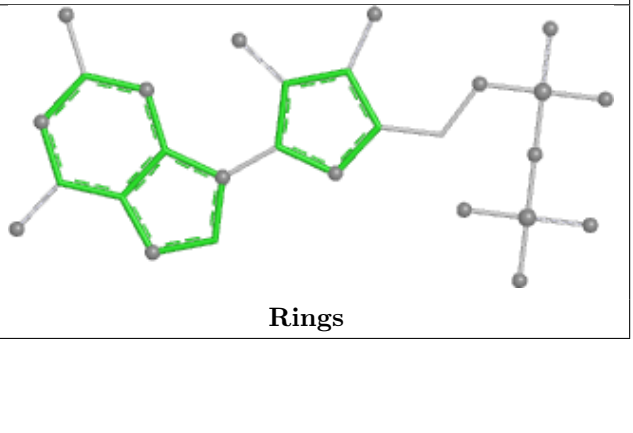
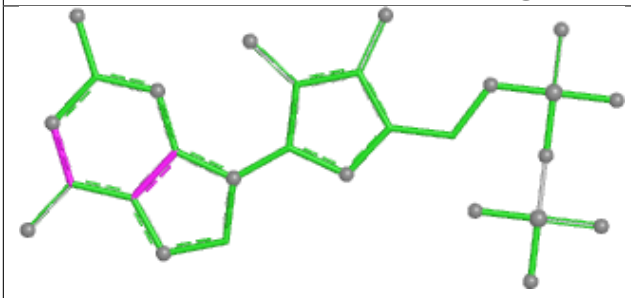


Rings

Ligand GDP 6c 502



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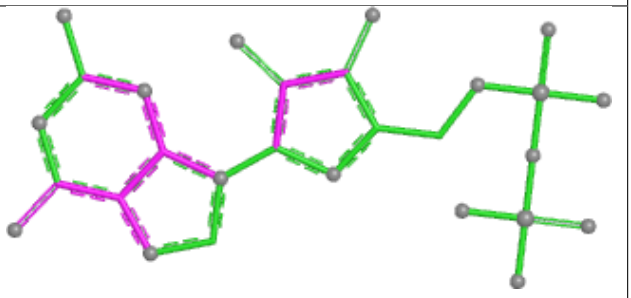

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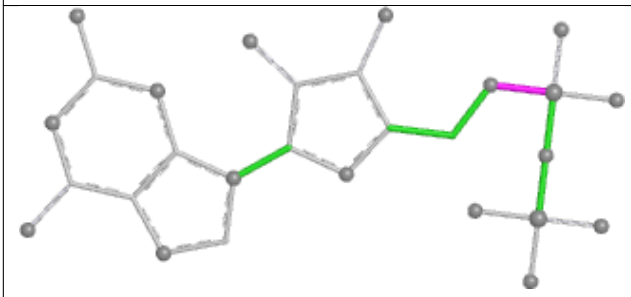

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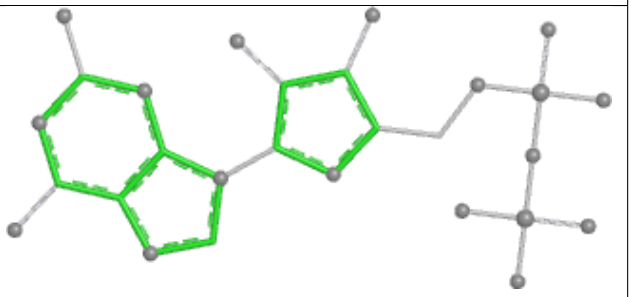
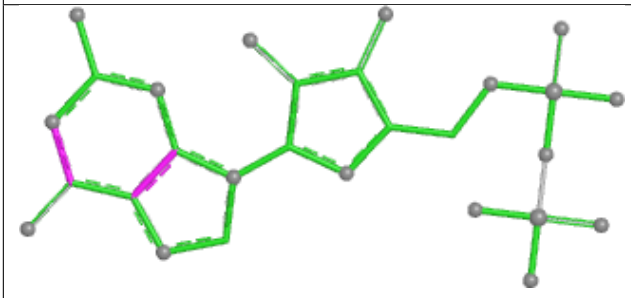


Rings

Ligand GDP Ag 501



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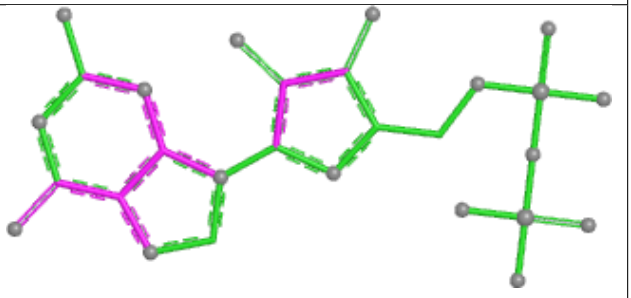

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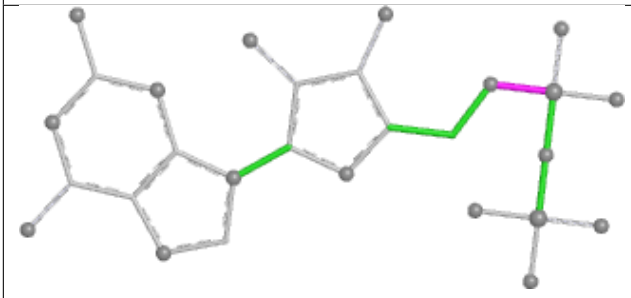

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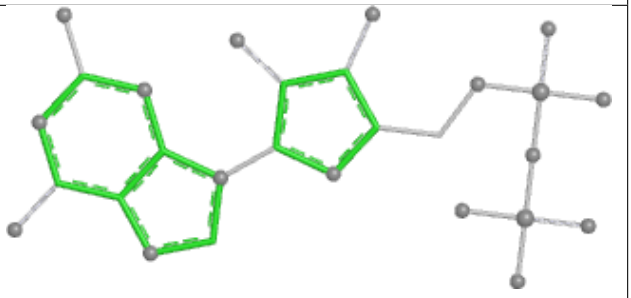
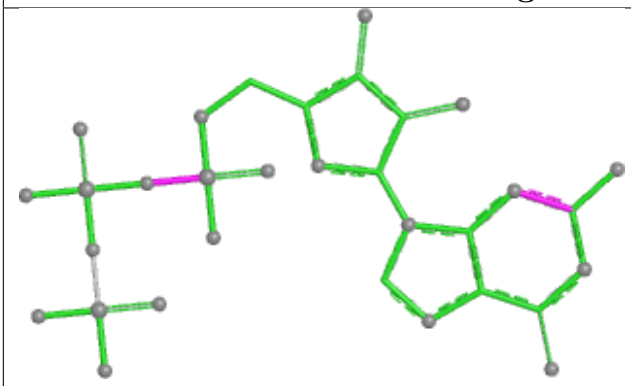


Rings

Ligand GTP Bf 501



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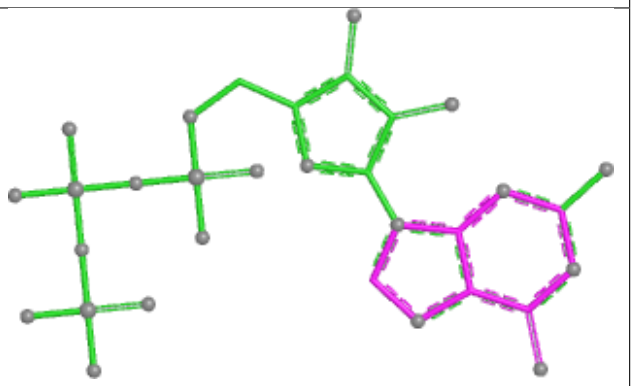

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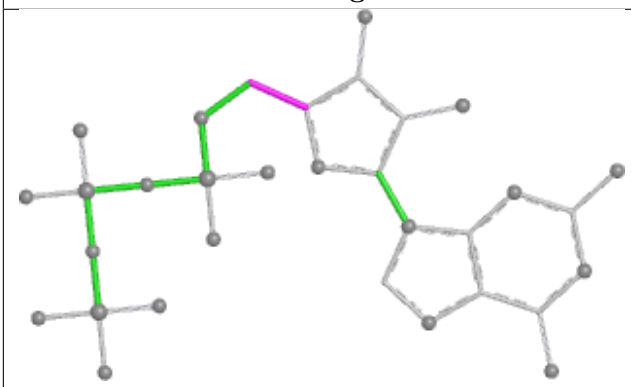

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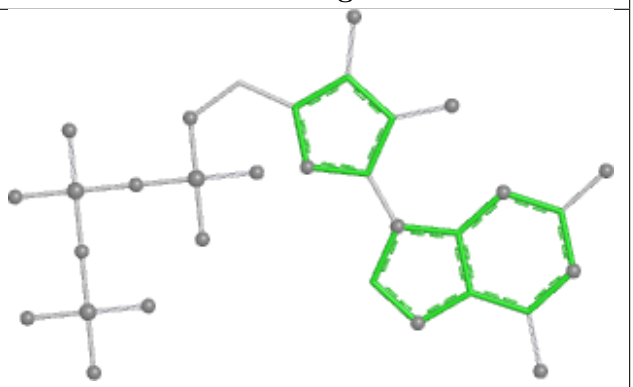
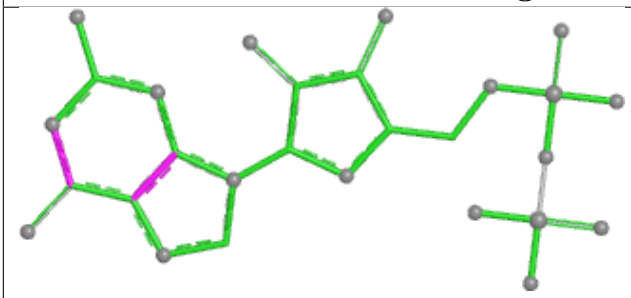


Rings

Ligand GDP 8g 501



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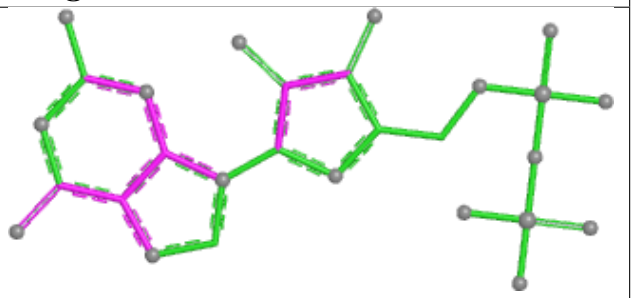

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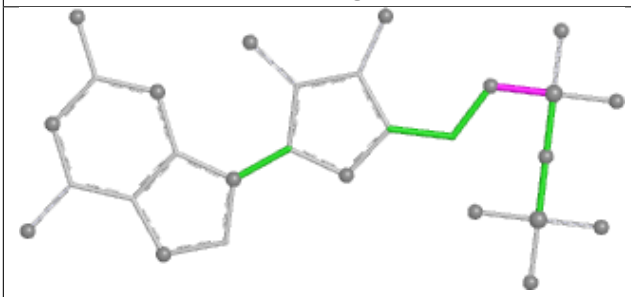

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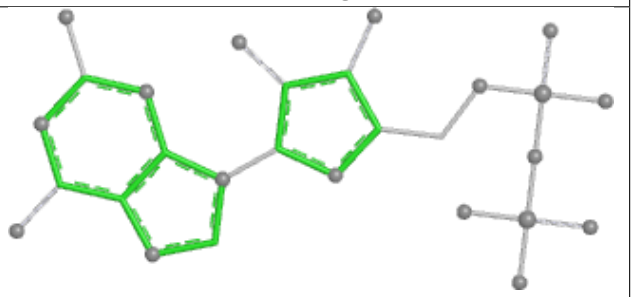

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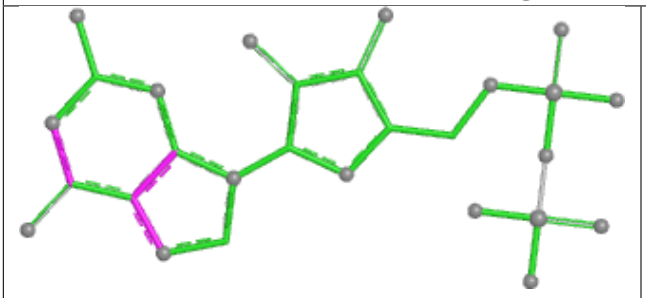

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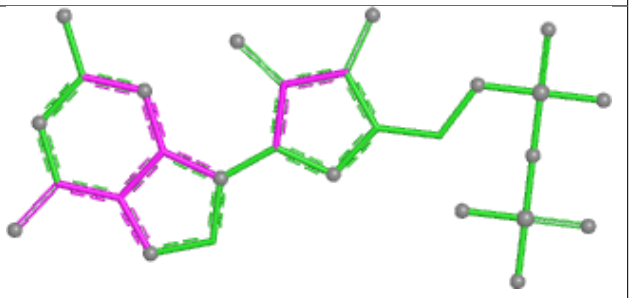

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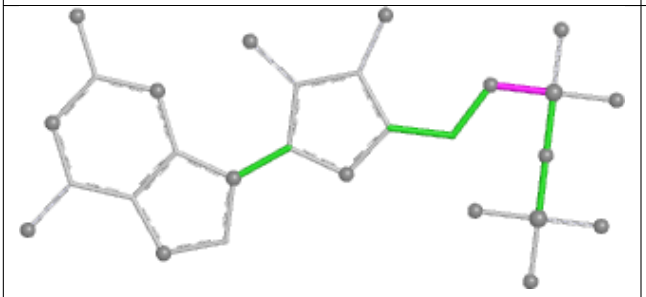

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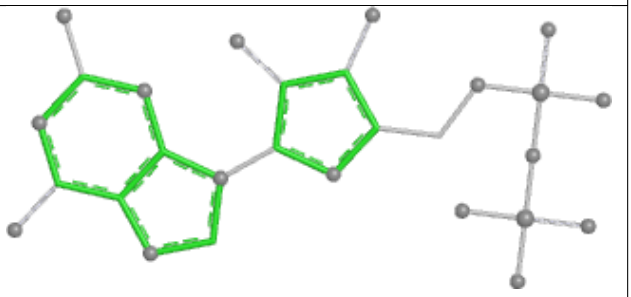
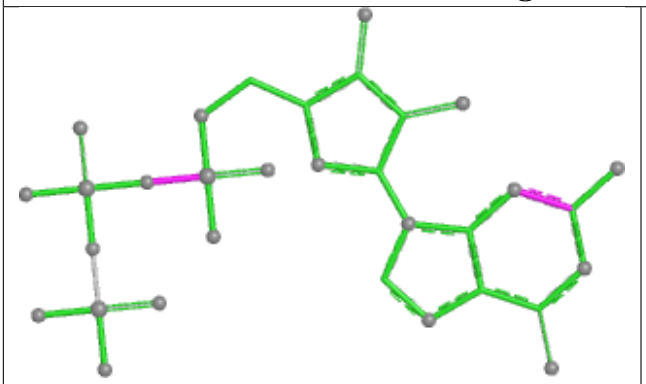


Rings

Ligand GTP 2h 501



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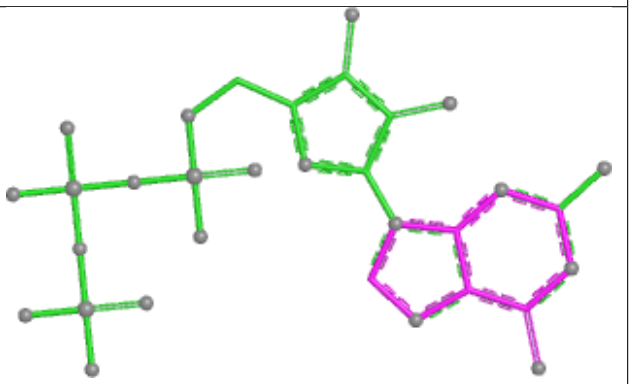

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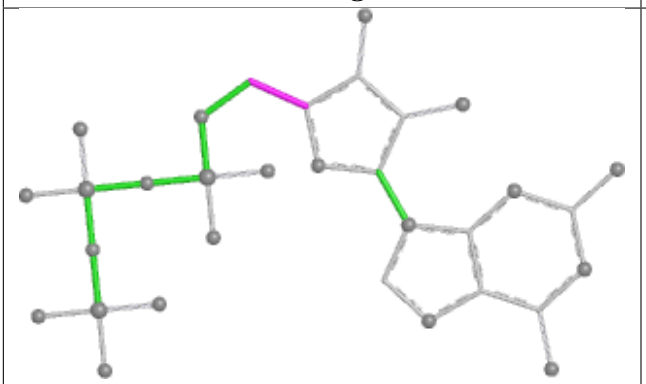

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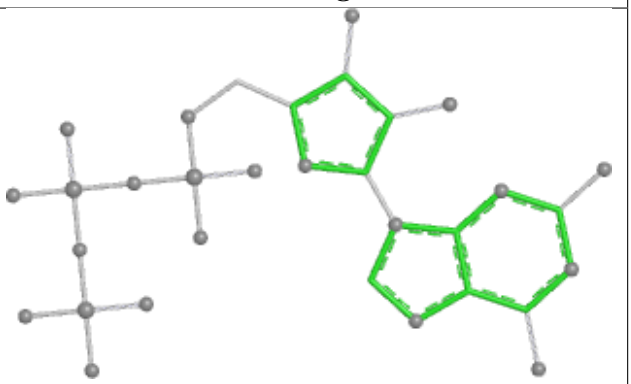
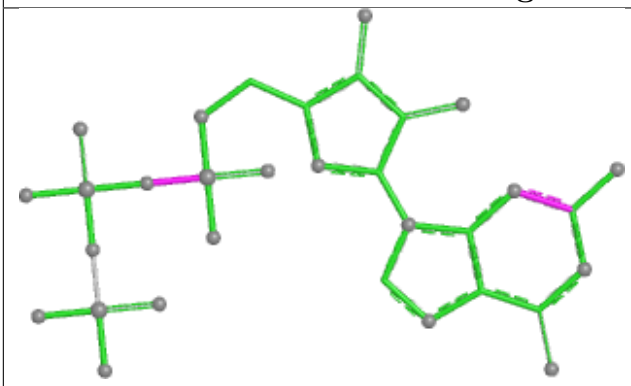


Rings

Ligand GTP 5d 501



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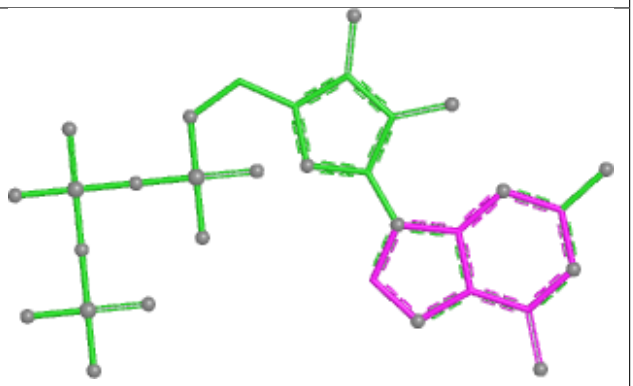
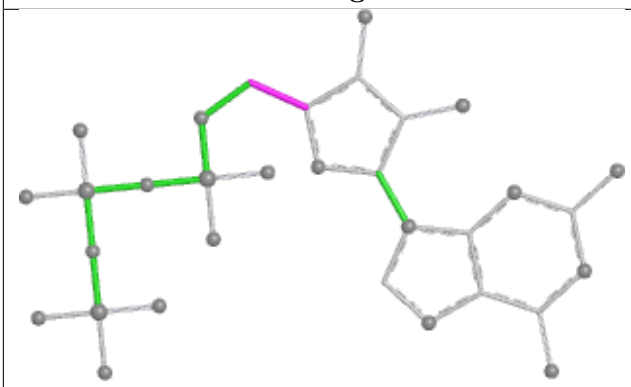


Bond angles



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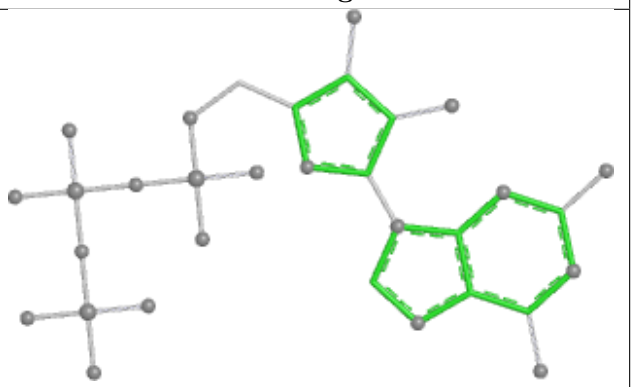
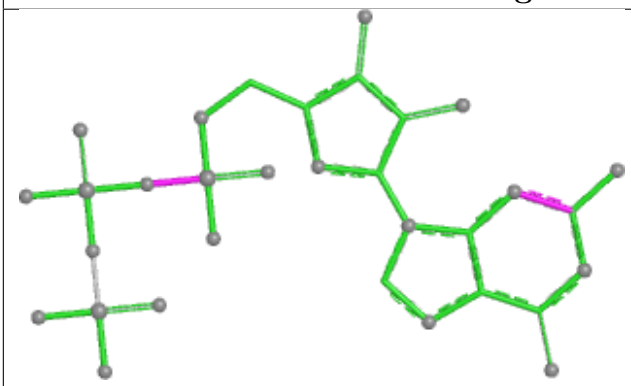


Rings

Ligand GTP Cc 501



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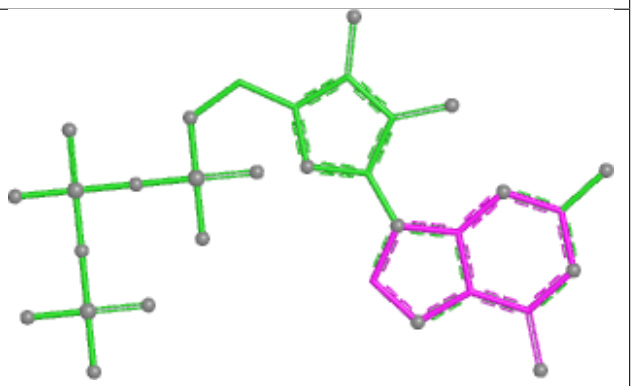
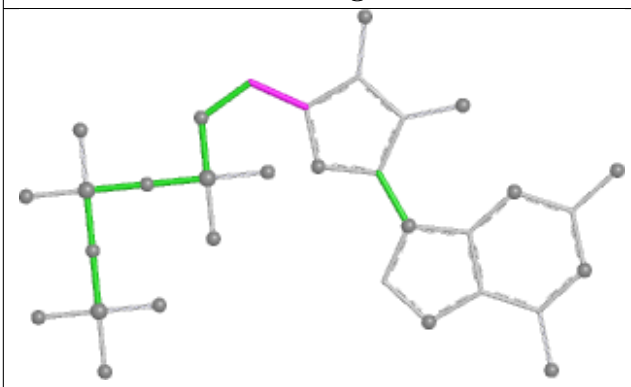


Bond angles



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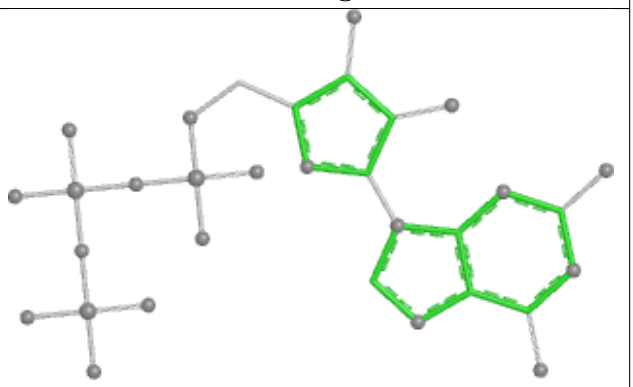
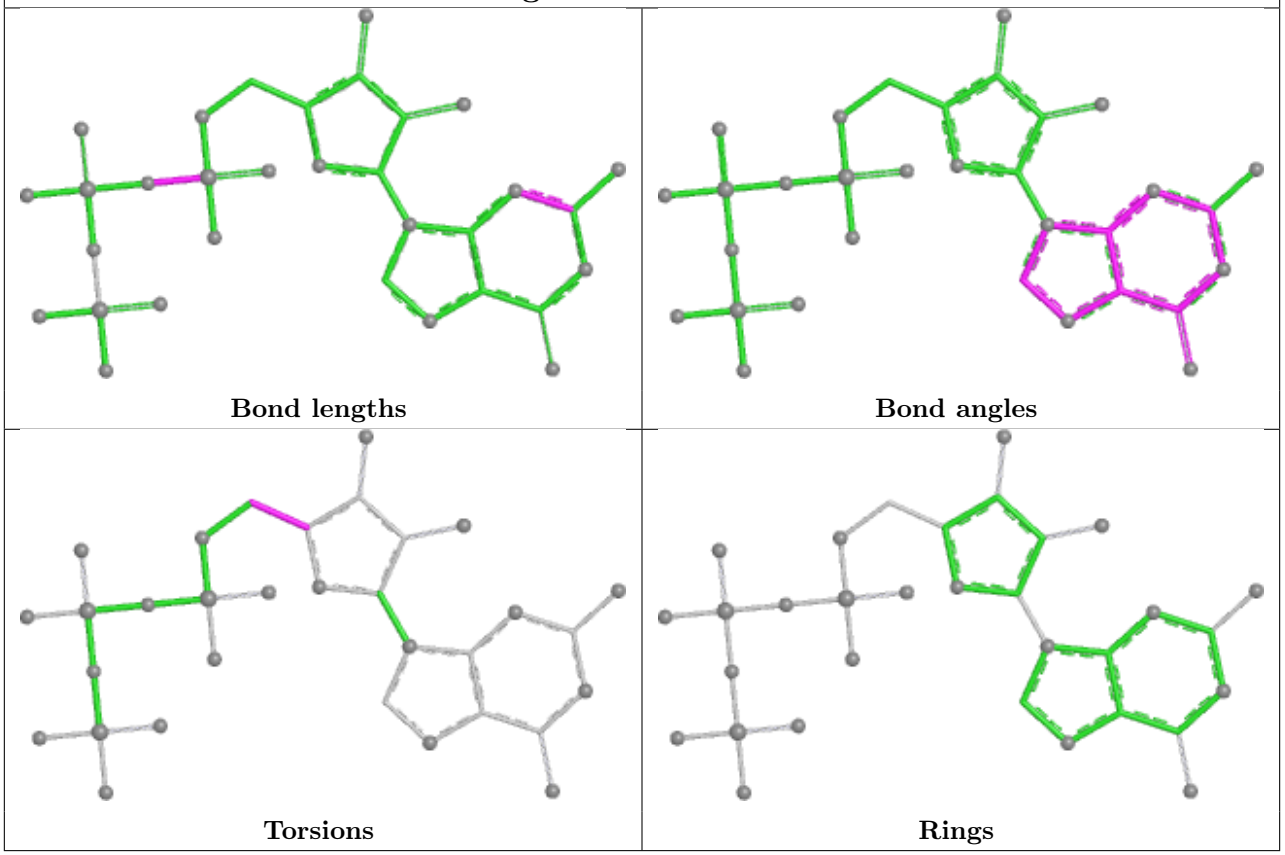
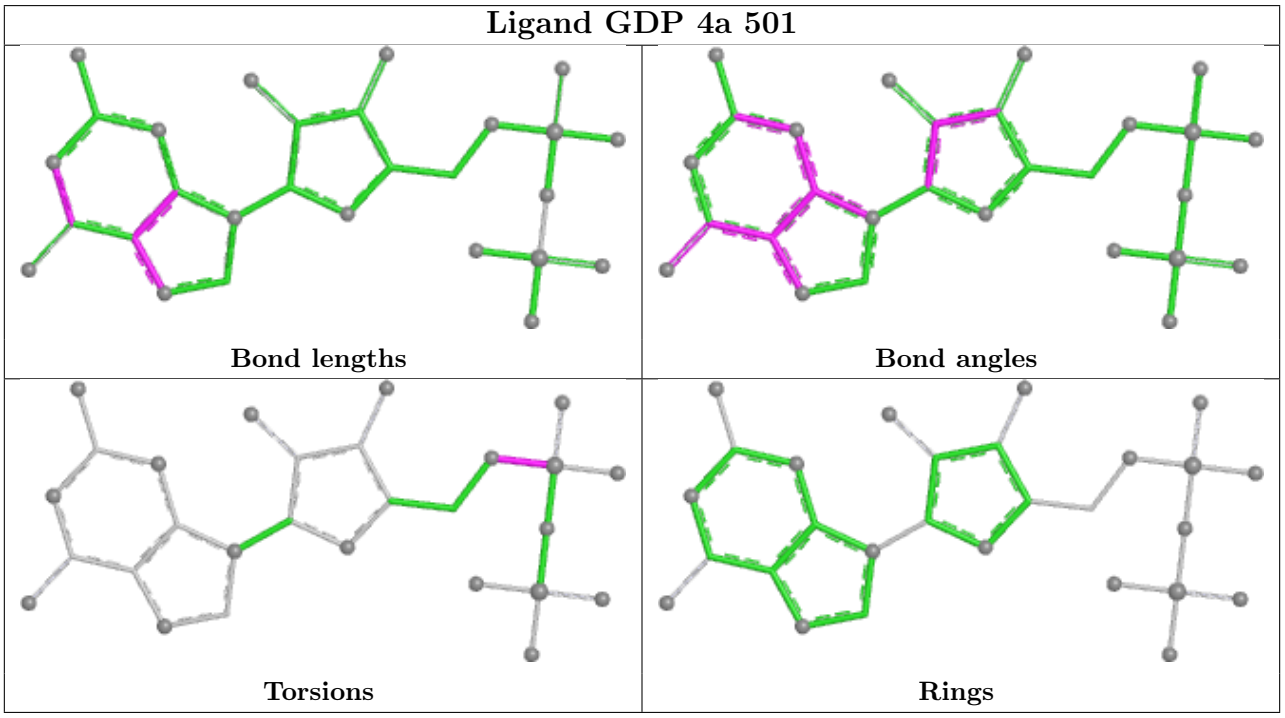


Rings

Ligand GTP 3f 501



Ligand GDP 4a 501



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
37	4F	5
37	4E	3
46	5Z	2
45	5W	1
45	5X	1
45	5Y	1
43	5I	1
43	5J	1
43	5L	1
43	5K	1
37	4G	1
41	5A	1

The worst 5 of 19 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	5W	111:UNK	C	154:UNK	N	23.64
1	5X	111:UNK	C	154:UNK	N	23.64
1	5Y	111:UNK	C	154:UNK	N	23.64
1	5Z	14:UNK	C	15:UNK	N	3.57
1	5Z	44:UNK	C	45:UNK	N	3.20

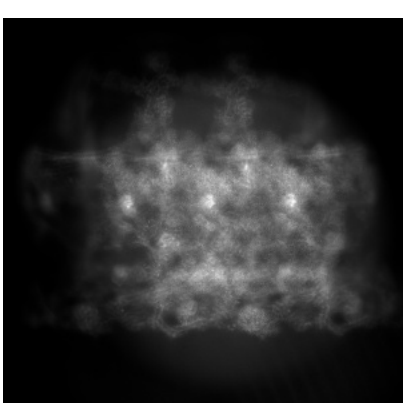
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-24207. These allow visual inspection of the internal detail of the map and identification of artifacts.

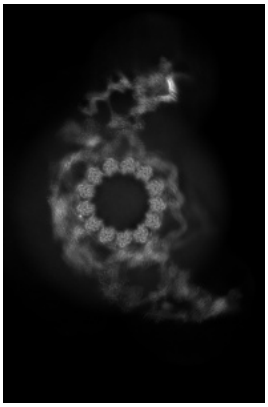
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

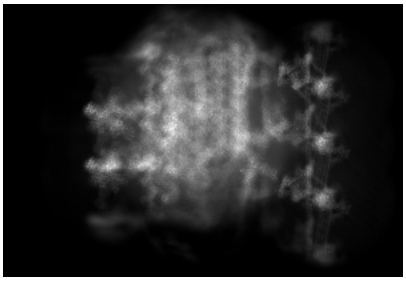
6.1.1 Primary map



X



Y

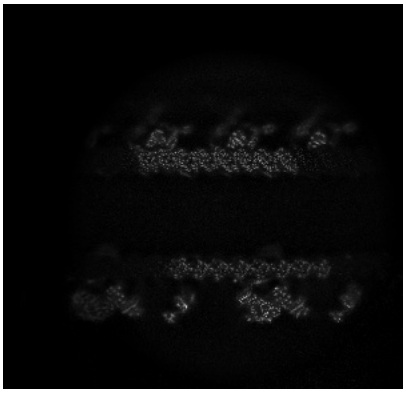


Z

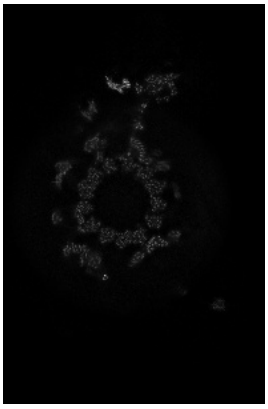
The images above show the map projected in three orthogonal directions.

6.2 Central slices

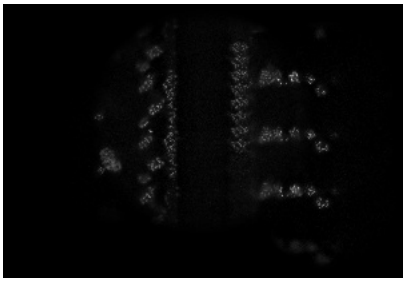
6.2.1 Primary map



X Index: 439



Y Index: 299

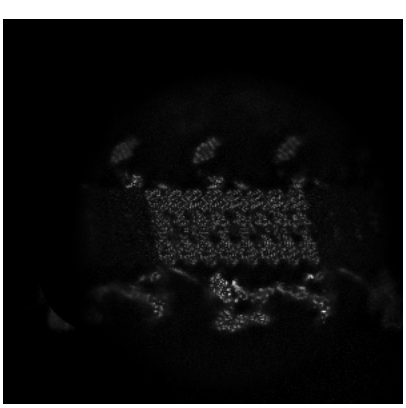


Z Index: 287

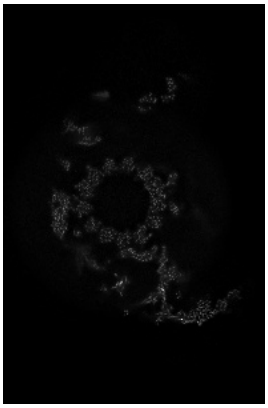
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

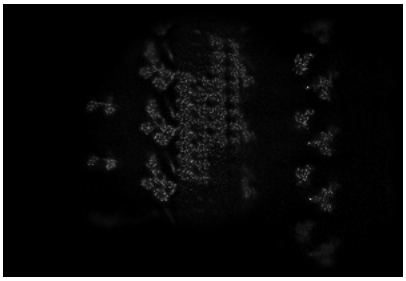
6.3.1 Primary map



X Index: 373



Y Index: 362

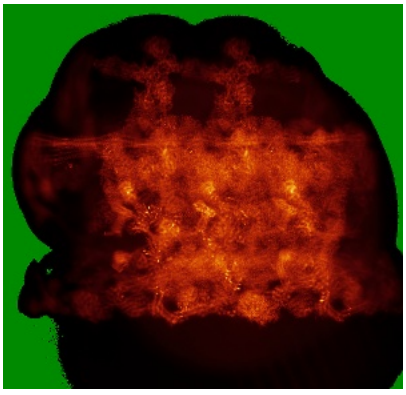


Z Index: 325

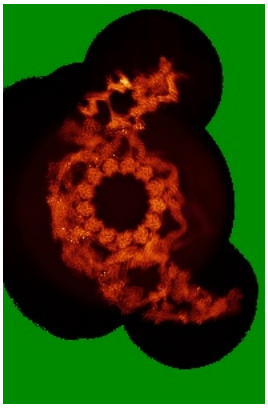
The images above show the largest variance slices of the map in three orthogonal directions.

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

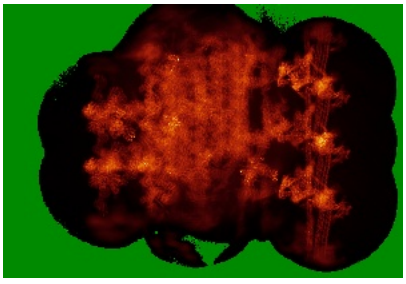
6.4.1 Primary map



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

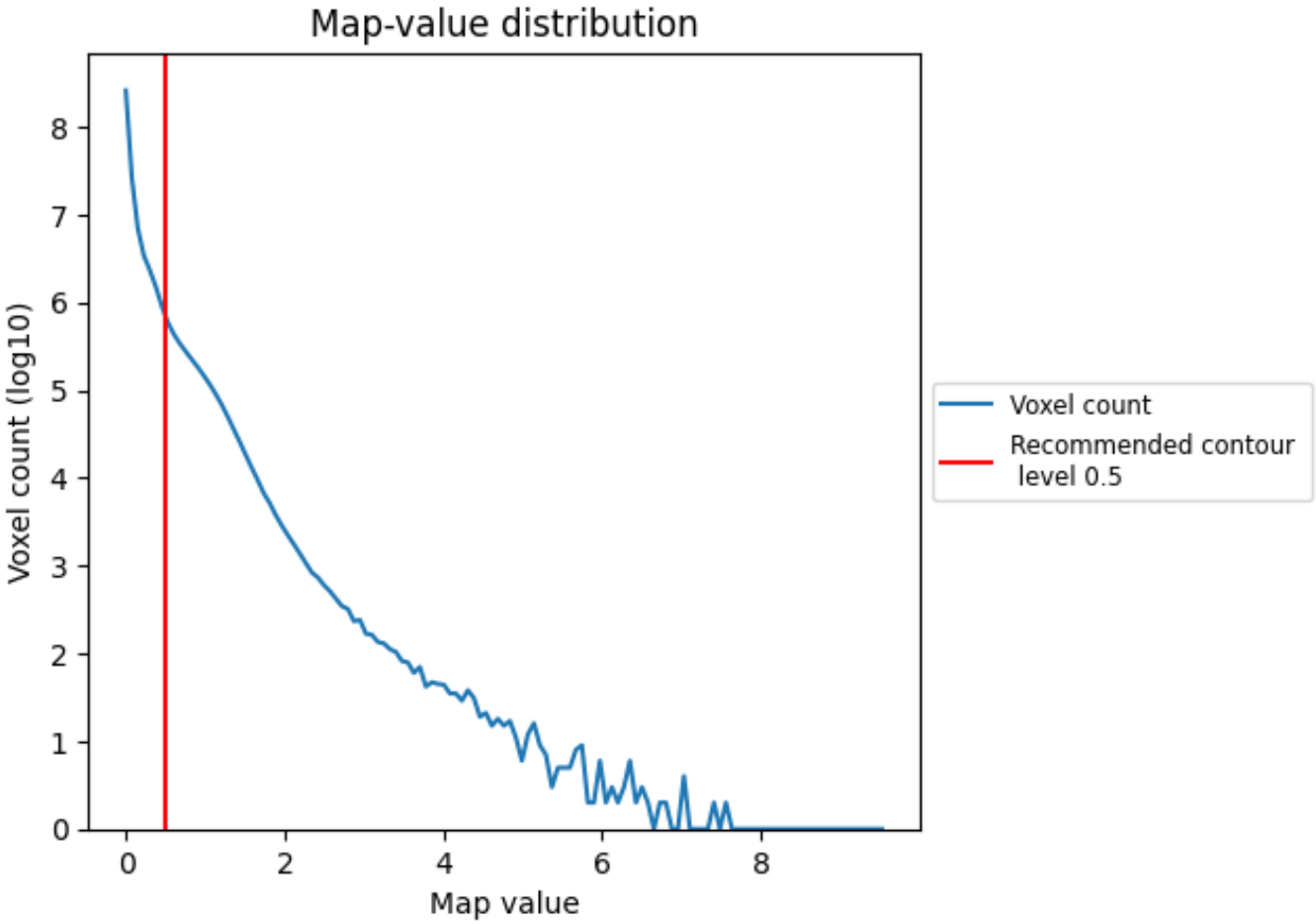
6.6 Mask visualisation (i)

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

7 Map analysis

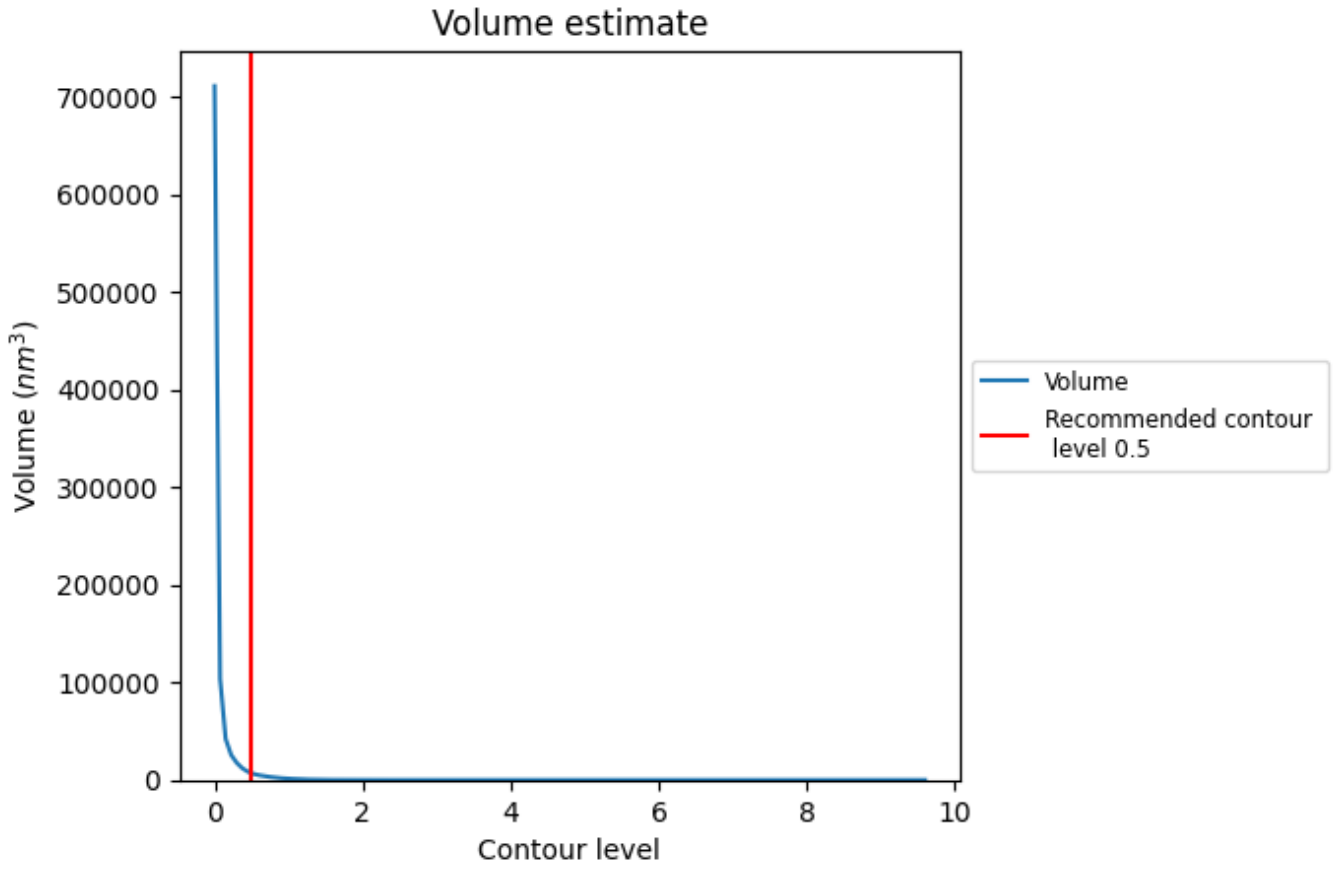
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

7.2 Volume estimate (i)



The volume at the recommended contour level is 7012 nm^3; this corresponds to an approximate mass of 6334 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)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

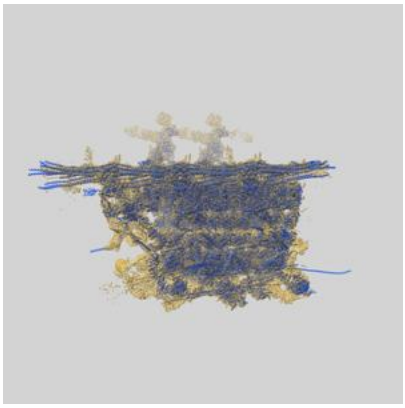
8 Fourier-Shell correlation

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

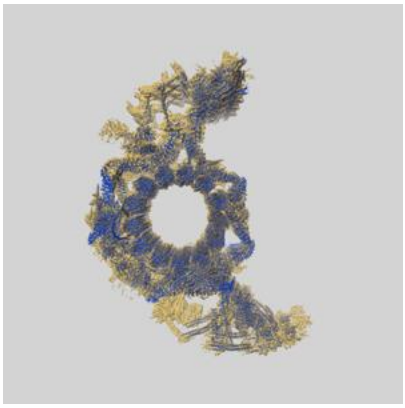
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-24207 and PDB model 7N6G. Per-residue inclusion information can be found in section 3 on page 38.

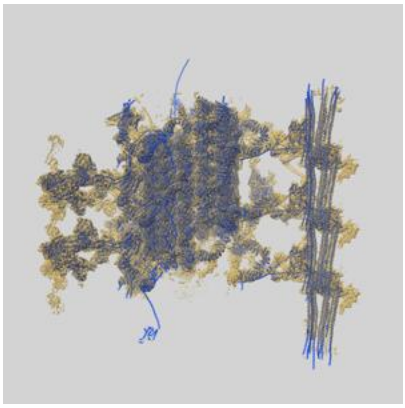
9.1 Map-model overlay



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.5 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.

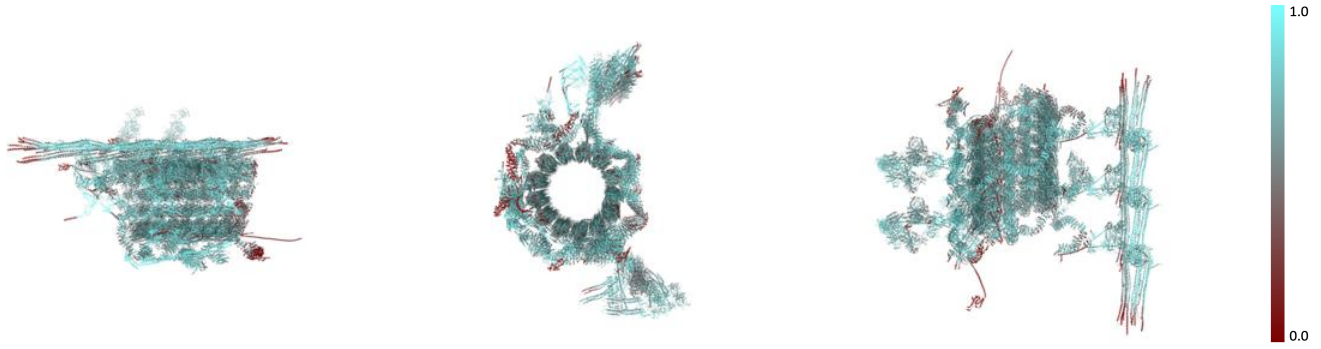
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

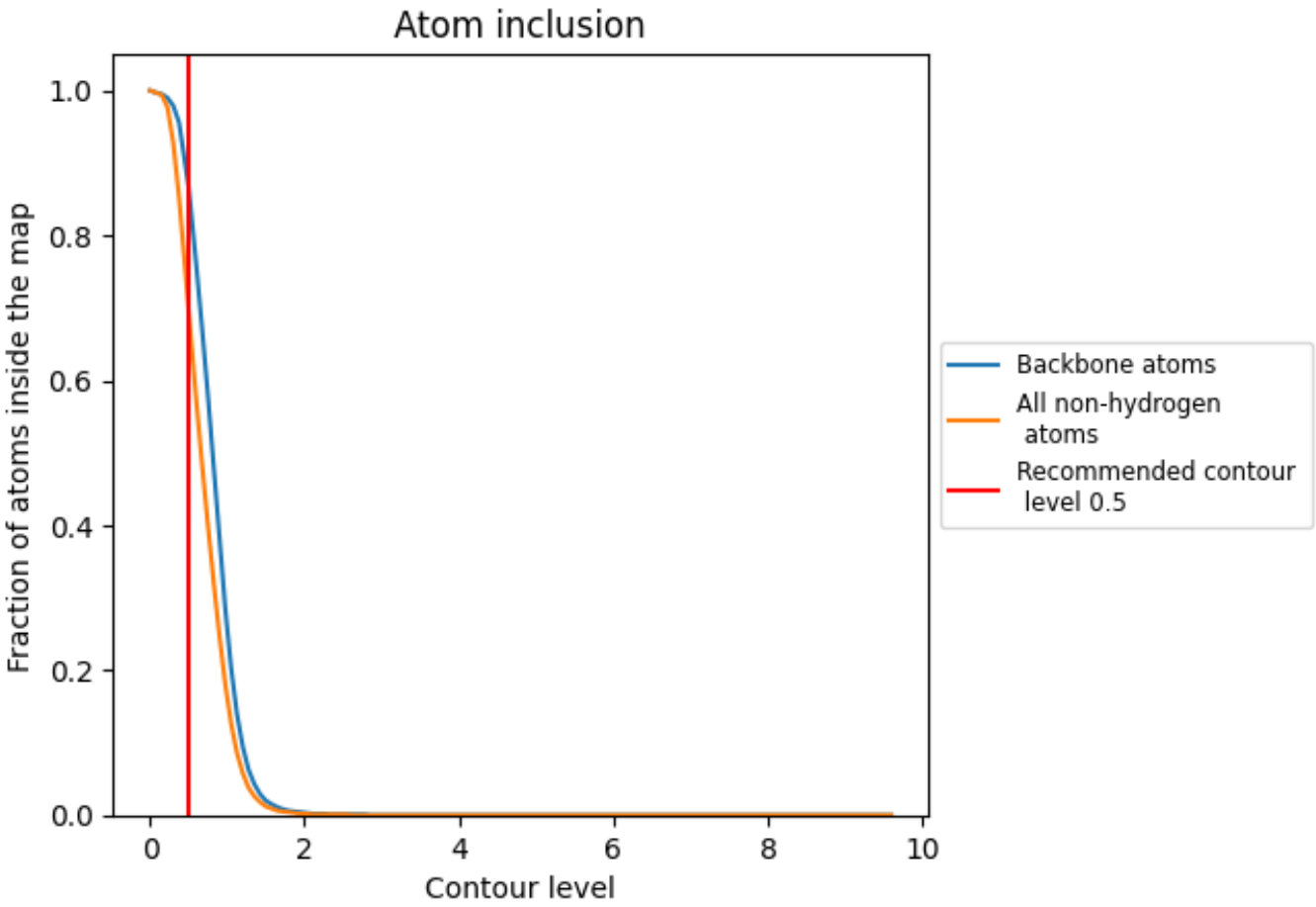
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.5).

9.4 Atom inclusion (i)



At the recommended contour level, 87% of all backbone atoms, 70% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6960	0.3180
0A	0.7500	0.2650
0B	0.4550	0.2100
0C	0.6700	0.2090
0D	0.5900	0.2200
0E	0.6450	0.2060
0F	0.7680	0.1910
0G	0.6020	0.1330
0H	0.7430	0.1760
0I	0.6340	0.1160
0J	0.6820	0.1290
0K	0.7380	0.1500
0L	0.8380	0.2400
0M	0.7780	0.2260
0N	0.8270	0.2890
0O	0.8100	0.2820
0P	0.3490	0.0250
0Q	0.4880	0.0040
0R	0.7990	0.2820
0S	0.7650	0.2540
0T	0.7850	0.2600
0U	0.8390	0.2950
0V	0.7750	0.2540
0W	0.7460	0.2130
0X	0.7530	0.2590
0Y	0.5600	0.2060
0Z	0.5210	0.1890
1A	0.7210	0.2450
1B	0.1150	0.0410
1C	0.2580	0.0910
1D	0.8500	0.2490
1E	0.4590	0.1400
1F	0.8270	0.2670
1G	0.5340	0.1640
1H	0.7510	0.2730



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Chain	Atom inclusion	Q-score
1I	0.5270	0.2020
1J	0.7930	0.3180
1K	0.8360	0.3780
1L	0.6760	0.3030
1M	0.7230	0.2800
1N	0.7710	0.2690
1O	0.8370	0.3480
1P	0.7480	0.2890
1Q	0.8610	0.3240
1R	0.7810	0.3770
1S	0.7220	0.3510
1T	0.9540	0.2390
1a	0.5810	0.3640
1b	0.6930	0.3740
1c	0.7180	0.4100
1d	0.7270	0.4010
1e	0.7370	0.3940
1f	0.7380	0.3980
1g	0.7530	0.4240
1h	0.7000	0.4050
2F	0.6800	0.3690
2G	0.5980	0.3540
2H	0.7460	0.4360
2I	0.8300	0.4640
2J	0.4780	0.3790
2K	0.5120	0.4210
2L	0.2930	0.3280
2M	0.4440	0.3760
2N	0.7190	0.4510
2O	0.7280	0.3910
2P	0.8360	0.4620
2Q	0.8730	0.4280
2R	0.8070	0.4500
2S	0.2160	0.3650
2T	0.0950	0.2800
2U	0.2200	0.3280
2V	0.2560	0.3120
2W	0.8800	0.4280
2X	0.8160	0.4210
2Y	0.8120	0.3760
2Z	0.4890	0.3490
2a	0.5660	0.3220

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Chain	Atom inclusion	Q-score
2b	0.7120	0.3890
2c	0.7380	0.4000
2d	0.7280	0.4040
2e	0.7040	0.3520
2f	0.7400	0.4020
2g	0.7580	0.4150
2h	0.6870	0.4000
3A	0.8110	0.3150
3B	0.4170	0.2640
3C	0.7290	0.3540
3E	0.5680	0.3030
3F	0.4460	0.2260
3G	0.7000	0.2620
3H	0.7530	0.3050
3I	0.6460	0.2630
3J	0.7750	0.3570
3K	0.5320	0.2870
3L	0.7380	0.2520
3M	0.3960	0.2500
3N	0.5050	0.2670
3O	0.4690	0.2650
3P	0.4890	0.2650
3Q	0.6330	0.2930
3R	0.6270	0.2790
3S	0.5110	0.2690
3T	0.3670	0.2580
3U	0.6340	0.2820
3V	0.6330	0.2710
3W	0.7740	0.3370
3X	0.7780	0.3250
3Y	0.7830	0.3240
3Z	0.6600	0.2850
3a	0.5670	0.3380
3b	0.6940	0.3860
3c	0.7580	0.4050
3d	0.7050	0.3890
3e	0.7140	0.3830
3f	0.7160	0.3950
3g	0.7560	0.4240
3h	0.6470	0.3860
4A	0.7600	0.3150
4B	0.6350	0.2930

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Chain	Atom inclusion	Q-score
4C	0.7520	0.3040
4D	0.7410	0.2810
4E	0.7300	0.2730
4F	0.7550	0.3670
4G	0.7590	0.3660
4H	0.7570	0.3710
4I	0.4340	0.0160
4J	0.6900	0.2770
4K	0.6710	0.2600
4L	0.3640	-0.0330
4M	0.3550	-0.0260
4N	0.3590	-0.0290
4O	0.7110	0.2630
4P	0.6930	0.2780
4Q	0.8390	0.3110
4R	0.5310	0.1910
4S	0.6980	0.2050
4T	0.7240	0.3110
4U	0.7230	0.2980
4V	0.7170	0.3050
4W	0.8510	0.3030
4X	0.9970	0.3010
4Y	0.9900	0.2330
4Z	0.9950	0.2190
4a	0.6040	0.3270
4b	0.7130	0.3790
4c	0.7460	0.4040
4d	0.7230	0.3970
4e	0.7260	0.3990
4f	0.7340	0.3820
4g	0.7520	0.4110
4h	0.6350	0.3530
5A	0.8630	0.1960
5B	1.0000	0.2960
5C	0.9870	0.1560
5D	0.9950	0.1740
5E	0.8180	0.3270
5F	0.7170	0.2200
5G	0.7330	0.2050
5H	0.7770	0.2400
5I	0.8210	0.3050
5J	0.7320	0.2860

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Chain	Atom inclusion	Q-score
5K	0.7840	0.2660
5L	0.3860	-0.0190
5M	0.8910	0.2500
5N	0.6780	0.1350
5O	0.5380	0.1390
5P	0.7090	0.2840
5Q	0.8310	0.2110
5R	0.8460	0.2190
5S	0.7590	0.3020
5T	0.7410	0.2960
5U	0.7430	0.2920
5V	0.7660	0.2950
5W	0.9610	0.2070
5X	0.7900	0.3030
5Y	0.9940	0.2860
5Z	0.9180	0.3220
5a	0.5220	0.2690
5b	0.6960	0.3700
5c	0.7250	0.3810
5d	0.7120	0.3840
5e	0.7060	0.3660
5f	0.7290	0.3770
5g	0.7290	0.3600
5h	0.6290	0.3390
6A	0.5910	0.1920
6B	0.7190	0.2660
6D	0.8090	0.3340
6E	0.7320	0.3210
6F	0.7260	0.3150
6G	0.5100	0.2830
6H	0.5140	0.2820
6I	0.5360	0.3380
6J	0.5370	0.3450
6K	0.5900	0.3200
6L	0.5880	0.3230
6M	0.6980	0.3180
6N	0.6940	0.3250
6O	0.6130	0.1910
6P	0.6550	0.1850
6Q	0.7770	0.2210
6a	0.5320	0.2520
6b	0.6940	0.3470

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Chain	Atom inclusion	Q-score
6c	0.7050	0.3350
6d	0.7170	0.3820
6e	0.7360	0.3800
6f	0.7350	0.3740
6g	0.7710	0.3940
6h	0.6550	0.3590
7a	0.5520	0.2620
7b	0.6890	0.3570
7c	0.6930	0.3500
7d	0.6890	0.3600
7e	0.7100	0.3520
7f	0.7500	0.3800
7g	0.7700	0.4040
7h	0.6850	0.3800
8a	0.4880	0.2030
8b	0.6950	0.3660
8c	0.7040	0.3770
8d	0.6830	0.3650
8e	0.6910	0.3670
8f	0.7250	0.3570
8g	0.7400	0.3760
8h	0.6410	0.3520
9a	0.5970	0.3180
9b	0.7240	0.3890
9c	0.7390	0.3950
9d	0.7120	0.3780
9e	0.7110	0.3630
9f	0.7430	0.3920
9g	0.7340	0.3810
9h	0.6700	0.3700
Aa	0.6200	0.3240
Ab	0.7200	0.3880
Ac	0.7560	0.4150
Ad	0.7180	0.3880
Ae	0.7500	0.4060
Af	0.7560	0.4000
Ag	0.7560	0.4130
Ah	0.6720	0.3740
Ba	0.6750	0.4000
Bb	0.7550	0.4110
Bc	0.7460	0.3610
Bd	0.7530	0.4020

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Chain	Atom inclusion	Q-score
Be	0.7620	0.4010
Bf	0.7700	0.4060
Bg	0.7530	0.3840
Bh	0.7010	0.3960
Ca	0.6860	0.4150
Cb	0.7430	0.4180
Cc	0.7710	0.4190
Cd	0.7560	0.4180
Ce	0.7650	0.4000
Cf	0.7660	0.4210
Cg	0.7590	0.4260
Ch	0.6860	0.4070
Da	0.7310	0.4170
Db	0.7830	0.4210
Dc	0.8150	0.4470
Dd	0.7790	0.4220
De	0.7820	0.4110
Df	0.7750	0.4200
Dg	0.7880	0.4240
Dh	0.6840	0.3920