



wwPDB EM Validation Summary Report ⓘ

Mar 6, 2026 – 09:12 PM UTC

PDB ID : 9Y9Z / pdb_00009y9z
EMDB ID : EMD-72715
Title : Cryo-EM structure of conoid fiber from Toxoplasma gondii (24-nm repeat)
Authors : Zeng, J.; Zhang, R.
Deposited on : 2025-09-15
Resolution : 3.14 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

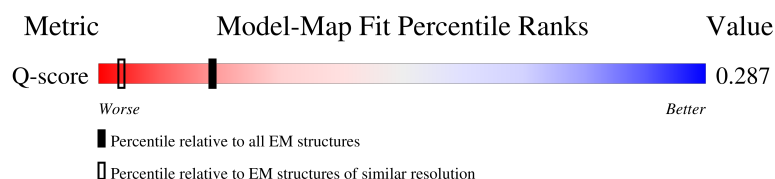
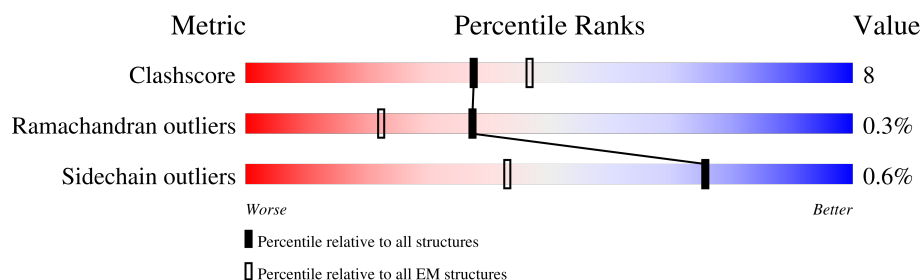
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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

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

The reported resolution of this entry is 3.14 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.



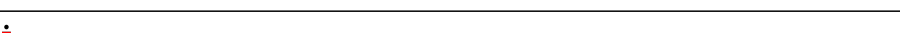
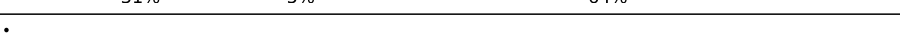
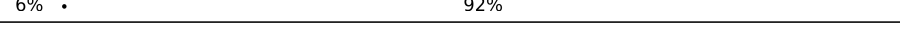
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14483 (2.64 - 3.64)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	954	10% • 88%
1	2	954	8% • 88%
1	A	954	26% 5% 69%
1	B	954	21% • 75%

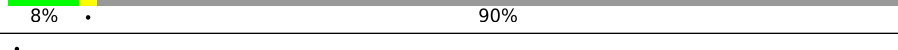
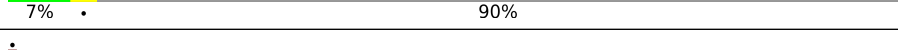
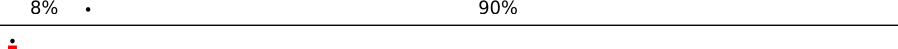
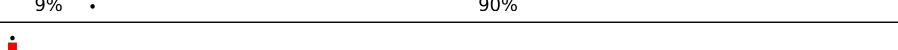
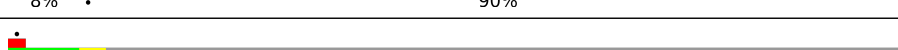
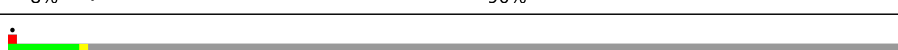
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Mol	Chain	Length	Quality of chain
1	C	954	 12% . 84%
1	D	954	 9% . 88%
1	E	954	 25% . 72%
1	F	954	 28% . 69%
1	G	954	 14% . 82%
1	H	954	 9% . 88%
1	I	954	 10% 28% 7% . . 62%
1	J	954	 9% 26% 7% . . 63%
1	K	954	 17% . 79%
1	L	954	 18% . 79%
1	M	954	 8% 15% 6% . . 77%
1	N	954	 7% 12% 8% . . 78%
1	O	954	 . . . 94%
1	P	954	 . . . 94%
1	Q	954	 31% 5% 64%
1	R	954	 23% . 73%
1	S	954	 16% . 81%
1	T	954	 6% . 92%
1	U	954	 33% 6% 61%
1	V	954	 23% . 73%
1	W	954	 18% . 79%
1	X	954	 8% . 91%
1	Y	954	 28% 8% . . 63%
1	Z	954	 21% . 75%
1	a	954	 11% 6% . 80%

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Mol	Chain	Length	Quality of chain
1	b	954	 8% . 91%
1	c	954	 25% 8% . . 62%
1	d	954	 22% . 74%
1	e	954	 7% . 91%
1	f	954	 7% 8% . . 80%
1	g	954	 9% . 90%
1	h	954	 8% . 90%
1	i	954	 7% . 90%
1	j	954	 8% . 90%
1	k	954	 9% . 90%
1	l	954	 8% . 90%
1	m	954	 8% . 90%
1	n	954	 8% . 91%
1	o	954	 7% . 91%
1	p	954	 7% . 91%
1	q	954	 7% . 91%
1	r	954	 7% . 91%
1	s	954	 5% 8% . 91%
1	t	954	 6% 7% . 91%
1	u	954	 9% . 88%
1	v	954	 10% . 88%
1	w	954	 10% . 88%
1	x	954	 9% . 88%
1	y	954	 9% . 88%
1	z	954	 10% . 88%

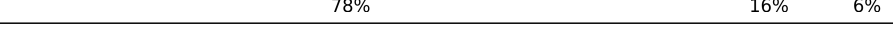
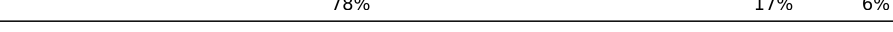
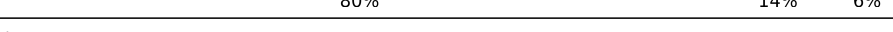
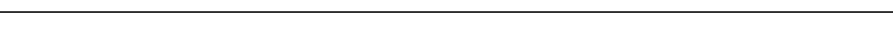
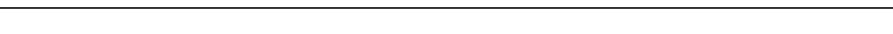
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Mol	Chain	Length	Quality of chain
2	10	410	
2	11	410	
2	12	410	
2	13	410	
2	14	410	
2	15	410	
2	16	410	
2	3	410	
2	4	410	
2	5	410	
2	6	410	
2	7	410	
2	8	410	
2	9	410	
3	1A	453	
3	1C	453	
3	1E	453	
3	1G	453	
3	1I	453	
3	1K	453	
3	1M	453	
3	2A	453	
3	2C	453	
3	2E	453	
3	2G	453	

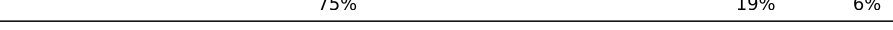
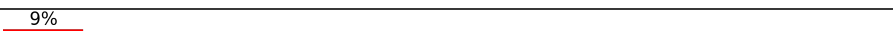
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Mol	Chain	Length	Quality of chain
3	2I	453	
3	2K	453	
3	2M	453	
3	3A	453	
3	3C	453	
3	3E	453	
3	3G	453	
3	3I	453	
3	3K	453	
3	3M	453	
3	4A	453	
3	4C	453	
3	4E	453	
3	4G	453	
3	4I	453	
3	4K	453	
3	4M	453	
3	5A	453	
3	5C	453	
3	5E	453	
3	5G	453	
3	5I	453	
3	5K	453	
3	5M	453	
3	6A	453	

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Mol	Chain	Length	Quality of chain
3	6C	453	 77%17%6%
3	6E	453	 78%16%6%
3	6G	453	 83%12%6%
3	6I	453	 79%16%6%
3	6K	453	 80%15%6%
3	6M	453	 66%29%6%
3	7A	453	 80%15%6%
3	7C	453	 74%20%6%
3	7E	453	 75%19%6%
3	7G	453	 78%17%6%
3	7I	453	 77%17%6%
3	7K	453	 73%22%6%
3	7M	453	 71%23%6%
3	8A	453	 6%75%19%6%
3	8C	453	 76%17%6%
3	8E	453	 74%21%6%
3	8G	453	 79%16%6%
3	8I	453	 76%19%6%
3	8K	453	 69%25%6%
3	8M	453	 5%76%18%6%
3	9A	453	 28%75%20%6%
3	9C	453	 18%76%18%6%
3	9E	453	 9%75%20%6%
3	9G	453	 75%19%6%
3	9I	453	 9%72%22%6%

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Mol	Chain	Length	Quality of chain
3	9K	453	
3	9M	453	
4	1B	449	
4	1D	449	
4	1F	449	
4	1H	449	
4	1J	449	
4	1L	449	
4	1N	449	
4	2B	449	
4	2D	449	
4	2F	449	
4	2H	449	
4	2J	449	
4	2L	449	
4	3B	449	
4	3D	449	
4	3F	449	
4	3H	449	
4	3J	449	
4	3L	449	
4	4B	449	
4	4D	449	
4	4F	449	
4	4H	449	

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Mol	Chain	Length	Quality of chain
4	4J	449	
4	4L	449	
4	5B	449	
4	5D	449	
4	5F	449	
4	5H	449	
4	5J	449	
4	5L	449	
4	5N	449	
4	6B	449	
4	6D	449	
4	6F	449	
4	6H	449	
4	6J	449	
4	6L	449	
4	6N	449	
4	7B	449	
4	7D	449	
4	7F	449	
4	7H	449	
4	7J	449	
4	7L	449	
4	8B	449	
4	8D	449	
4	8F	449	

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Mol	Chain	Length	Quality of chain
4	8H	449	
4	8J	449	
4	8L	449	
4	9B	449	
4	9D	449	
4	9F	449	
4	9H	449	
4	9J	449	
4	9L	449	
5	20	263	
5	21	263	
5	22	263	
5	23	263	
5	24	263	
5	25	263	
5	26	263	
5	27	263	
5	28	263	
5	29	263	
5	30	263	
5	31	263	
5	32	263	
5	33	263	
5	35	263	
5	36	263	

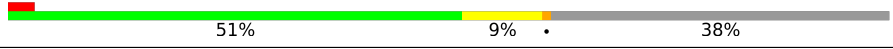
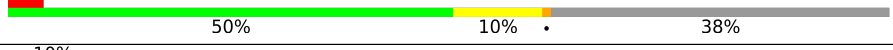
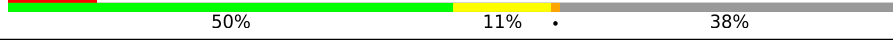
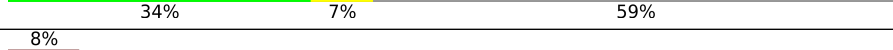
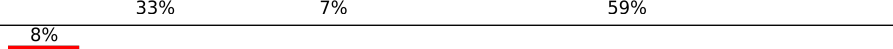
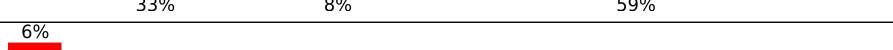
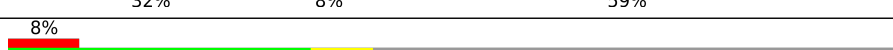
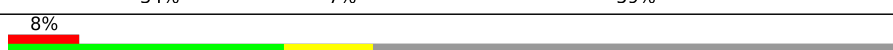
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Mol	Chain	Length	Quality of chain
5	37	263	29% 71% 11% 17%
5	38	263	32% 68% 13% 19%
5	39	263	37% 66% 16% 17%
5	40	263	36% 66% 15% 19%
5	42	263	67% 71% 10% 19%
5	43	263	33% 68% 14% 17%
5	44	263	32% 68% 13% 19%
5	45	263	32% 73% 10% 17%
5	46	263	45% 70% 11% 19%
5	47	263	48% 68% 14% 17%
5	48	263	77% 72% 9% 19%
5	49	263	7% 67% 21% 13%
5	50	263	8% 68% 21% 11%
5	51	263	8% 65% 22% 13%
5	52	263	10% 67% 22% 11%
5	53	263	11% 64% 24% 13%
5	54	263	13% 72% 17% 11%
5	55	263	10% 68% 19% 13%
5	56	263	10% 71% 18% 11%
5	57	263	10% 68% 19% 13%
5	58	263	14% 72% 16% 11%
5	59	263	40% 70% 17% 13%
5	60	263	15% 69% 19% 11%
5	61	263	16% 63% 24% 13%
5	62	263	36% 67% 22% 11%

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Mol	Chain	Length	Quality of chain
6	63	1010	
6	64	1010	
6	65	1010	
6	66	1010	
6	67	1010	
6	68	1010	
6	69	1010	
7	71	416	
7	72	416	
7	73	416	
7	75	416	
7	76	416	
7	77	416	
7	78	416	
7	79	416	
7	80	416	
7	82	416	
7	83	416	
7	84	416	
7	85	416	
7	86	416	
7	87	416	
7	89	416	
7	90	416	
7	91	416	

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Mol	Chain	Length	Quality of chain
7	92	416	
7	93	416	
7	94	416	
7	95	416	
7	96	416	
7	97	416	
8	A1	502	
8	A2	502	
8	A3	502	
8	A4	502	
8	A5	502	
8	A6	502	
8	A7	502	
8	A8	502	
8	A9	502	
9	B1	556	
9	B2	556	
9	B3	556	
9	B4	556	
9	B5	556	
9	B6	556	
9	B7	556	
10	C0	582	
10	C6	582	
10	C7	582	

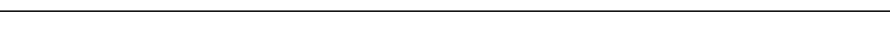
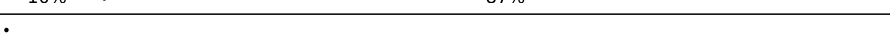
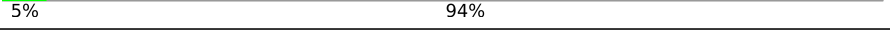
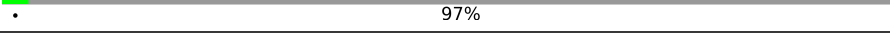
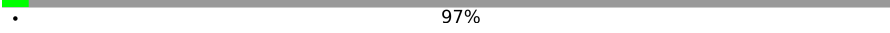
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Mol	Chain	Length	Quality of chain
10	C8	582	
10	C9	582	
10	D0	582	
10	D1	582	
10	D2	582	
10	D3	582	
10	D4	582	
10	D5	582	
10	D6	582	
10	D7	582	
10	D8	582	
10	D9	582	
10	E0	582	
10	E1	582	
10	E2	582	
10	E3	582	
10	E4	582	
10	E5	582	
10	E6	582	
10	E7	582	
10	E8	582	
10	E9	582	
10	F1	582	
10	F2	582	
10	F3	582	

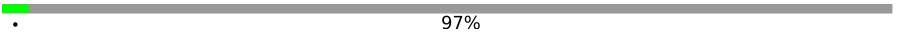
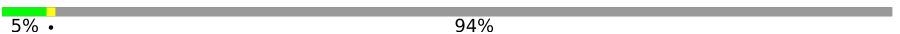
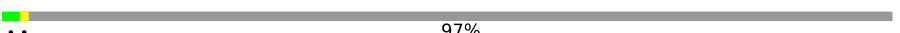
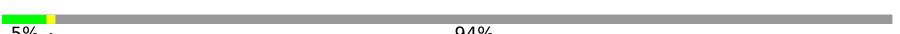
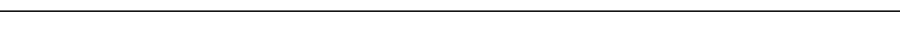
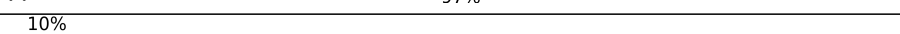
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Mol	Chain	Length	Quality of chain	
11	C1	351		
11	C2	351		
11	C3	351		
11	C4	351		
11	C5	351		
12	F0	783		
12	F5	783		
12	F6	783		
12	F7	783		
12	F8	783		
12	F9	783		
12	G0	783		
12	G1	783		
12	G2	783		
12	G3	783		
12	G4	783		
12	G5	783		
12	G6	783		
12	G7	783		
12	G8	783		
12	G9	783		
12	H0	783		
12	H1	783		
12	H2	783		
12	H3	783		

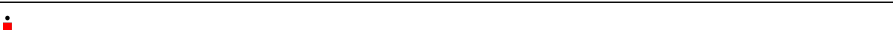
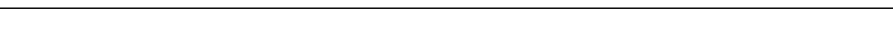
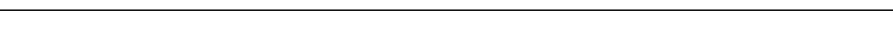
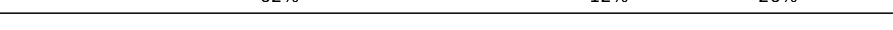
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Mol	Chain	Length	Quality of chain
12	H4	783	 97%
12	H5	783	 94%
12	H6	783	 94%
12	H7	783	 97%
12	H8	783	 94%
12	H9	783	 94%
12	I1	783	 94%
12	I2	783	 94%
12	I3	783	 97%
12	I4	783	 94%
12	I5	783	 94%
12	I6	783	 97%
12	I7	783	 94%
12	I8	783	 94%
12	I9	783	 97%
13	J1	871	 65%
13	J2	871	 65%
13	J3	871	 65%
13	J4	871	 65%
13	J5	871	 65%
13	J6	871	 65%
13	J7	871	 65%
14	K0	256	 63% 11% 26%
14	K1	256	 64% 10% 26%
14	K2	256	 66% 7% 26%

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Mol	Chain	Length	Quality of chain
14	K3	256	
14	K4	256	
14	K5	256	
14	K6	256	
14	K7	256	
14	K8	256	
14	K9	256	
14	L0	256	
14	L1	256	
14	L2	256	
14	L3	256	
14	L4	256	
14	L5	256	
14	L6	256	
14	L7	256	
14	L8	256	
14	L9	256	
14	M1	256	
14	M2	256	
14	M3	256	
14	M4	256	
14	M5	256	
14	M6	256	
14	M7	256	

2 Entry composition [i](#)

There are 17 unique types of molecules in this entry. The entry contains 806376 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 CF2, TGME49_258090.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	294	Total	C	N	O	S	0	0
			2425	1459	480	479	7		
1	B	241	Total	C	N	O	S	0	0
			1998	1212	394	385	7		
1	C	148	Total	C	N	O	S	0	0
			1232	751	239	237	5		
1	D	118	Total	C	N	O	S	0	0
			993	597	197	195	4		
1	E	269	Total	C	N	O	S	0	0
			2215	1345	439	424	7		
1	F	299	Total	C	N	O	S	0	0
			2469	1484	491	487	7		
1	G	170	Total	C	N	O	S	0	0
			1403	857	272	269	5		
1	H	114	Total	C	N	O	S	0	0
			959	578	192	185	4		
1	I	362	Total	C	N	O	S	0	0
			3014	1819	603	582	10		
1	J	356	Total	C	N	O	S	0	0
			2963	1787	593	572	11		
1	K	197	Total	C	N	O	S	0	0
			1637	990	325	317	5		
1	L	202	Total	C	N	O	S	0	0
			1678	1015	330	327	6		
1	M	215	Total	C	N	O	S	0	0
			1786	1077	356	347	6		
1	N	208	Total	C	N	O	S	0	0
			1723	1038	345	334	6		
1	O	57	Total	C	N	O	S	0	0
			465	280	92	90	3		
1	P	54	Total	C	N	O	S	0	0
			444	265	89	87	3		
1	Q	346	Total	C	N	O	S	0	0
			2876	1740	572	554	10		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	254	Total	C	N	O	S	0	0
			2096	1265	420	405	6		
1	S	177	Total	C	N	O	S	0	0
			1468	889	289	285	5		
1	T	77	Total	C	N	O	S	0	0
			647	394	126	123	4		
1	U	372	Total	C	N	O	S	0	0
			3096	1864	617	604	11		
1	V	258	Total	C	N	O	S	0	0
			2121	1278	424	413	6		
1	W	198	Total	C	N	O	S	0	0
			1649	996	326	321	6		
1	X	90	Total	C	N	O	S	0	0
			749	456	149	140	4		
1	Y	356	Total	C	N	O	S	0	0
			2959	1788	593	569	9		
1	Z	243	Total	C	N	O	S	0	0
			2017	1217	406	388	6		
1	1	112	Total	C	N	O	S	0	0
			881	542	170	167	2		
1	2	112	Total	C	N	O	S	0	0
			881	542	170	167	2		
1	a	187	Total	C	N	O	S	0	0
			1559	941	315	298	5		
1	b	85	Total	C	N	O	S	0	0
			731	440	146	141	4		
1	c	359	Total	C	N	O	S	0	0
			2988	1800	600	579	9		
1	d	248	Total	C	N	O	S	0	0
			2057	1241	411	398	7		
1	e	85	Total	C	N	O	S	0	0
			725	436	142	142	5		
1	f	190	Total	C	N	O	S	0	0
			1586	949	322	310	5		
1	g	100	Total	C	N	O	S	0	0
			729	438	143	140	8		
1	h	100	Total	C	N	O	S	0	0
			729	438	143	140	8		
1	i	100	Total	C	N	O	S	0	0
			729	438	143	140	8		
1	j	100	Total	C	N	O	S	0	0
			729	438	143	140	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	k	100	Total	C	N	O	S	0	0
			729	438	143	140	8		
1	l	100	Total	C	N	O	S	0	0
			729	438	143	140	8		
1	m	100	Total	C	N	O	S	0	0
			729	438	143	140	8		
1	n	88	Total	C	N	O	S	0	0
			699	428	140	130	1		
1	o	88	Total	C	N	O	S	0	0
			699	428	140	130	1		
1	p	88	Total	C	N	O	S	0	0
			699	428	140	130	1		
1	q	88	Total	C	N	O	S	0	0
			699	428	140	130	1		
1	r	88	Total	C	N	O	S	0	0
			699	428	140	130	1		
1	s	88	Total	C	N	O	S	0	0
			699	428	140	130	1		
1	t	88	Total	C	N	O	S	0	0
			699	428	140	130	1		
1	u	112	Total	C	N	O	S	0	0
			881	542	170	167	2		
1	v	112	Total	C	N	O	S	0	0
			881	542	170	167	2		
1	w	112	Total	C	N	O	S	0	0
			881	542	170	167	2		
1	x	112	Total	C	N	O	S	0	0
			881	542	170	167	2		
1	y	112	Total	C	N	O	S	0	0
			881	542	170	167	2		
1	z	112	Total	C	N	O	S	0	0
			881	542	170	167	2		

- Molecule 2 is a protein called CF1, TGME49_222350.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	10	175	Total	C	N	O	S	0	0
			1493	913	298	275	7		
2	11	177	Total	C	N	O	S	0	0
			1512	925	303	277	7		
2	12	175	Total	C	N	O	S	0	0
			1493	913	298	275	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	13	177	Total	C	N	O	S	0	0
			1512	925	303	277	7		
2	14	175	Total	C	N	O	S	0	0
			1493	913	298	275	7		
2	15	88	Total	C	N	O	S	0	0
			764	473	155	133	3		
2	16	97	Total	C	N	O	S	0	0
			834	516	167	147	4		
2	3	177	Total	C	N	O	S	0	0
			1512	925	303	277	7		
2	4	175	Total	C	N	O	S	0	0
			1493	913	298	275	7		
2	5	177	Total	C	N	O	S	0	0
			1512	925	303	277	7		
2	6	175	Total	C	N	O	S	0	0
			1493	913	298	275	7		
2	7	177	Total	C	N	O	S	0	0
			1512	925	303	277	7		
2	8	175	Total	C	N	O	S	0	0
			1493	913	298	275	7		
2	9	177	Total	C	N	O	S	0	0
			1512	925	303	277	7		

- Molecule 3 is a protein called Tubulin alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	1A	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
3	1C	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
3	1E	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
3	1G	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
3	1I	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
3	1K	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
3	1M	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
3	2A	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	2C	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
3	2E	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
3	2G	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
3	2I	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
3	2K	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
3	2M	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
3	3A	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
3	3C	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
3	3E	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
3	3G	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
3	3I	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
3	3K	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
3	3M	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
3	4A	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
3	4C	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
3	4E	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
3	4G	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
3	4I	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
3	4K	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
3	4M	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
3	5A	428	Total 3325	C 2105	N 569	O 625	S 26	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	5C	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
3	5E	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
3	5G	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
3	5I	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
3	5K	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
3	5M	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
3	6A	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
3	6C	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
3	6E	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
3	6G	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
3	6I	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
3	6K	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
3	6M	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
3	7A	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
3	7C	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
3	7E	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
3	7G	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
3	7I	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
3	7K	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
3	7M	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
3	8A	428	Total 3325	C 2105	N 569	O 625	S 26	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	8C	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
3	8E	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
3	8G	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
3	8I	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
3	8K	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
3	8M	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
3	9A	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
3	9C	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
3	9E	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
3	9G	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
3	9I	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
3	9K	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
3	9M	428	Total 3325	C 2105	N 569	O 625	S 26	0	0

- Molecule 4 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	1B	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	1D	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	1F	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	1H	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	1J	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	1L	426	Total 3331	C 2094	N 569	O 641	S 27	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	1N	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	2B	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	2D	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	2F	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	2H	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	2J	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	2L	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	3B	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	3D	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	3F	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	3H	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	3J	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	3L	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	4B	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	4D	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	4F	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	4H	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	4J	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	4L	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	5B	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	5D	426	Total 3331	C 2094	N 569	O 641	S 27	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	5F	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	5H	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	5J	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	5L	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	5N	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	6B	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	6D	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	6F	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	6H	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	6J	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	6L	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	6N	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	7B	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	7D	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	7F	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	7H	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	7J	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	7L	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	8B	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	8D	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	8F	426	Total 3331	C 2094	N 569	O 641	S 27	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	8H	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	8J	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	8L	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	9B	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	9D	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	9F	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	9H	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	9J	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	9L	426	Total 3331	C 2094	N 569	O 641	S 27	0	0

- Molecule 5 is a protein called Spindle assembly abnormal protein 6 N-terminal domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	20	225	Total 1814	C 1144	N 318	O 339	S 13	0	0
5	21	225	Total 1815	C 1146	N 318	O 339	S 12	0	0
5	22	225	Total 1814	C 1144	N 318	O 339	S 13	0	0
5	23	225	Total 1815	C 1146	N 318	O 339	S 12	0	0
5	24	225	Total 1814	C 1144	N 318	O 339	S 13	0	0
5	25	225	Total 1815	C 1146	N 318	O 339	S 12	0	0
5	26	225	Total 1814	C 1144	N 318	O 339	S 13	0	0
5	27	225	Total 1815	C 1146	N 318	O 339	S 12	0	0
5	28	225	Total 1814	C 1144	N 318	O 339	S 13	0	0
5	29	225	Total 1815	C 1146	N 318	O 339	S 12	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	30	225	Total	C	N	O	S	0	0
			1814	1144	318	339	13		
5	31	225	Total	C	N	O	S	0	0
			1815	1146	318	339	12		
5	32	225	Total	C	N	O	S	0	0
			1814	1144	318	339	13		
5	33	165	Total	C	N	O	S	0	0
			1321	836	220	255	10		
5	35	217	Total	C	N	O	S	0	0
			1744	1106	301	325	12		
5	36	213	Total	C	N	O	S	0	0
			1723	1090	304	317	12		
5	37	217	Total	C	N	O	S	0	0
			1744	1106	301	325	12		
5	38	213	Total	C	N	O	S	0	0
			1723	1090	304	317	12		
5	39	217	Total	C	N	O	S	0	0
			1744	1106	301	325	12		
5	40	213	Total	C	N	O	S	0	0
			1723	1090	304	317	12		
5	42	213	Total	C	N	O	S	0	0
			1723	1090	304	317	12		
5	43	217	Total	C	N	O	S	0	0
			1744	1106	301	325	12		
5	44	213	Total	C	N	O	S	0	0
			1723	1090	304	317	12		
5	45	217	Total	C	N	O	S	0	0
			1744	1106	301	325	12		
5	46	213	Total	C	N	O	S	0	0
			1723	1090	304	317	12		
5	47	217	Total	C	N	O	S	0	0
			1744	1106	301	325	12		
5	48	213	Total	C	N	O	S	0	0
			1723	1090	304	317	12		
5	49	230	Total	C	N	O	S	0	0
			1841	1161	323	344	13		
5	50	233	Total	C	N	O	S	0	0
			1853	1166	326	348	13		
5	51	230	Total	C	N	O	S	0	0
			1841	1161	323	344	13		
5	52	233	Total	C	N	O	S	0	0
			1853	1166	326	348	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	53	230	Total	C	N	O	S	0	0
			1841	1161	323	344	13		
5	54	233	Total	C	N	O	S	0	0
			1853	1166	326	348	13		
5	55	230	Total	C	N	O	S	0	0
			1841	1161	323	344	13		
5	56	233	Total	C	N	O	S	0	0
			1853	1166	326	348	13		
5	57	230	Total	C	N	O	S	0	0
			1841	1161	323	344	13		
5	58	233	Total	C	N	O	S	0	0
			1853	1166	326	348	13		
5	59	230	Total	C	N	O	S	0	0
			1841	1161	323	344	13		
5	60	233	Total	C	N	O	S	0	0
			1853	1166	326	348	13		
5	61	230	Total	C	N	O	S	0	0
			1841	1161	323	344	13		
5	62	233	Total	C	N	O	S	0	0
			1853	1166	326	348	13		

- Molecule 6 is a protein called CIP3, TGME49_225020.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	63	623	Total	C	N	O	S	0	0
			5055	3170	940	928	17		
6	64	623	Total	C	N	O	S	0	0
			5055	3170	940	928	17		
6	65	623	Total	C	N	O	S	0	0
			5055	3170	940	928	17		
6	66	623	Total	C	N	O	S	0	0
			5055	3170	940	928	17		
6	67	623	Total	C	N	O	S	0	0
			5055	3170	940	928	17		
6	68	623	Total	C	N	O	S	0	0
			5055	3170	940	928	17		
6	69	623	Total	C	N	O	S	0	0
			5055	3170	940	928	17		

- Molecule 7 is a protein called CF6, TGME49_245640.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	71	170	Total	C	N	O	S	0	0
			1382	881	251	243	7		
7	72	170	Total	C	N	O	S	0	0
			1382	881	251	243	7		
7	73	170	Total	C	N	O	S	0	0
			1382	881	251	243	7		
7	75	170	Total	C	N	O	S	0	0
			1382	881	251	243	7		
7	76	170	Total	C	N	O	S	0	0
			1382	881	251	243	7		
7	77	170	Total	C	N	O	S	0	0
			1382	881	251	243	7		
7	78	170	Total	C	N	O	S	0	0
			1382	881	251	243	7		
7	79	170	Total	C	N	O	S	0	0
			1382	881	251	243	7		
7	80	170	Total	C	N	O	S	0	0
			1382	881	251	243	7		
7	82	170	Total	C	N	O	S	0	0
			1382	881	251	243	7		
7	83	170	Total	C	N	O	S	0	0
			1382	881	251	243	7		
7	84	170	Total	C	N	O	S	0	0
			1382	881	251	243	7		
7	85	170	Total	C	N	O	S	0	0
			1382	881	251	243	7		
7	86	170	Total	C	N	O	S	0	0
			1382	881	251	243	7		
7	87	170	Total	C	N	O	S	0	0
			1382	881	251	243	7		
7	89	170	Total	C	N	O	S	0	0
			1382	881	251	243	7		
7	90	170	Total	C	N	O	S	0	0
			1382	881	251	243	7		
7	91	170	Total	C	N	O	S	0	0
			1382	881	251	243	7		
7	92	170	Total	C	N	O	S	0	0
			1382	881	251	243	7		
7	93	170	Total	C	N	O	S	0	0
			1382	881	251	243	7		
7	94	170	Total	C	N	O	S	0	0
			1382	881	251	243	7		
7	95	170	Total	C	N	O	S	0	0
			1382	881	251	243	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
7	96	170	Total	C	N	O	S	0	0
			1382	881	251	243	7		
7	97	170	Total	C	N	O	S	0	0
			1382	881	251	243	7		

- Molecule 8 is a protein called CF4, TGME49_246720.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	A1	325	Total	C	N	O	S	0	0
			2582	1631	455	482	14		
8	A2	325	Total	C	N	O	S	0	0
			2582	1631	455	482	14		
8	A3	232	Total	C	N	O	S	0	0
			1844	1157	327	347	13		
8	A4	142	Total	C	N	O	S	0	0
			1016	628	183	199	6		
8	A5	325	Total	C	N	O	S	0	0
			2582	1631	455	482	14		
8	A6	325	Total	C	N	O	S	0	0
			2582	1631	455	482	14		
8	A7	325	Total	C	N	O	S	0	0
			2582	1631	455	482	14		
8	A8	325	Total	C	N	O	S	0	0
			2582	1631	455	482	14		
8	A9	128	Total	C	N	O	S	0	0
			1020	658	178	183	1		

- Molecule 9 is a protein called CF3, TGME49_255895.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	B1	257	Total	C	N	O	S	0	0
			2055	1287	388	369	11		
9	B2	257	Total	C	N	O	S	0	0
			2055	1287	388	369	11		
9	B3	257	Total	C	N	O	S	0	0
			2055	1287	388	369	11		
9	B4	257	Total	C	N	O	S	0	0
			2055	1287	388	369	11		
9	B5	257	Total	C	N	O	S	0	0
			2055	1287	388	369	11		
9	B6	257	Total	C	N	O	S	0	0
			2055	1287	388	369	11		

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Mol	Chain	Residues	Atoms					AltConf	Trace
9	B7	257	Total	C	N	O	S	0	0
			2055	1287	388	369	11		

- Molecule 10 is a protein called CPH1, TGME49_266630.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	C0	184	Total	C	N	O	S	0	0
			1471	938	257	261	15		
10	C6	184	Total	C	N	O	S	0	0
			1471	938	257	261	15		
10	C7	184	Total	C	N	O	S	0	0
			1471	938	257	261	15		
10	C8	184	Total	C	N	O	S	0	0
			1471	938	257	261	15		
10	C9	184	Total	C	N	O	S	0	0
			1471	938	257	261	15		
10	D0	272	Total	C	N	O	S	0	0
			2197	1400	389	390	18		
10	D1	184	Total	C	N	O	S	0	0
			1471	938	257	261	15		
10	D2	184	Total	C	N	O	S	0	0
			1471	938	257	261	15		
10	D3	272	Total	C	N	O	S	0	0
			2197	1400	389	390	18		
10	D4	272	Total	C	N	O	S	0	0
			2197	1400	389	390	18		
10	D5	272	Total	C	N	O	S	0	0
			2197	1400	389	390	18		
10	D6	272	Total	C	N	O	S	0	0
			2197	1400	389	390	18		
10	D7	272	Total	C	N	O	S	0	0
			2197	1400	389	390	18		
10	D8	272	Total	C	N	O	S	0	0
			2197	1400	389	390	18		
10	D9	272	Total	C	N	O	S	0	0
			2197	1400	389	390	18		
10	E0	272	Total	C	N	O	S	0	0
			2197	1400	389	390	18		
10	E1	272	Total	C	N	O	S	0	0
			2197	1400	389	390	18		
10	E2	272	Total	C	N	O	S	0	0
			2197	1400	389	390	18		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	E3	272	Total	C	N	O	S	0	0
			2197	1400	389	390	18		
10	E4	272	Total	C	N	O	S	0	0
			2197	1400	389	390	18		
10	E5	272	Total	C	N	O	S	0	0
			2197	1400	389	390	18		
10	E6	272	Total	C	N	O	S	0	0
			2197	1400	389	390	18		
10	E7	272	Total	C	N	O	S	0	0
			2197	1400	389	390	18		
10	E8	272	Total	C	N	O	S	0	0
			2197	1400	389	390	18		
10	E9	272	Total	C	N	O	S	0	0
			2197	1400	389	390	18		
10	F1	272	Total	C	N	O	S	0	0
			2197	1400	389	390	18		
10	F2	272	Total	C	N	O	S	0	0
			2197	1400	389	390	18		
10	F3	272	Total	C	N	O	S	0	0
			2197	1400	389	390	18		

- Molecule 11 is a protein called Microtubule associated protein SPM1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	C1	30	Total	C	N	O	S	0	0
			237	155	38	43	1		
11	C2	30	Total	C	N	O		0	0
			238	158	36	44			
11	C3	30	Total	C	N	O		0	0
			242	159	39	44			
11	C4	27	Total	C	N	O		0	0
			214	140	35	39			
11	C5	30	Total	C	N	O		0	0
			239	158	38	43			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C1	93	ARG	PRO	conflict	UNP A0A7J6K285
C2	93	ARG	PRO	conflict	UNP A0A7J6K285
C3	93	ARG	PRO	conflict	UNP A0A7J6K285
C4	93	ARG	PRO	conflict	UNP A0A7J6K285
C5	93	ARG	PRO	conflict	UNP A0A7J6K285

- Molecule 12 is a protein called PRP, TGME49_291880.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	F0	107	Total	C	N	O	S	0	0
			883	576	150	153	4		
12	F5	102	Total	C	N	O	S	0	0
			847	554	142	148	3		
12	F6	107	Total	C	N	O	S	0	0
			883	576	150	153	4		
12	F7	102	Total	C	N	O	S	0	0
			847	554	142	148	3		
12	F8	107	Total	C	N	O	S	0	0
			883	576	150	153	4		
12	F9	102	Total	C	N	O	S	0	0
			847	554	142	148	3		
12	G0	50	Total	C	N	O		0	0
			412	253	82	77			
12	G1	102	Total	C	N	O	S	0	0
			847	554	142	148	3		
12	G2	107	Total	C	N	O	S	0	0
			883	576	150	153	4		
12	G3	102	Total	C	N	O	S	0	0
			847	554	142	148	3		
12	G4	107	Total	C	N	O	S	0	0
			883	576	150	153	4		
12	G5	102	Total	C	N	O	S	0	0
			847	554	142	148	3		
12	G6	107	Total	C	N	O	S	0	0
			883	576	150	153	4		
12	G7	102	Total	C	N	O	S	0	0
			847	554	142	148	3		
12	G8	107	Total	C	N	O	S	0	0
			883	576	150	153	4		
12	G9	44	Total	C	N	O		0	0
			365	222	73	70			
12	H0	24	Total	C	N	O		0	0
			184	114	30	40			
12	H1	24	Total	C	N	O		0	0
			184	114	30	40			
12	H2	44	Total	C	N	O		0	0
			365	222	73	70			
12	H3	50	Total	C	N	O		0	0
			412	253	82	77			
12	H4	24	Total	C	N	O		0	0
			184	114	30	40			

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Mol	Chain	Residues	Atoms				AltConf	Trace
12	H5	44	Total	C	N	O	0	0
			365	222	73	70		
12	H6	50	Total	C	N	O	0	0
			412	253	82	77		
12	H7	24	Total	C	N	O	0	0
			184	114	30	40		
12	H8	44	Total	C	N	O	0	0
			365	222	73	70		
12	H9	50	Total	C	N	O	0	0
			412	253	82	77		
12	I1	44	Total	C	N	O	0	0
			365	222	73	70		
12	I2	50	Total	C	N	O	0	0
			412	253	82	77		
12	I3	24	Total	C	N	O	0	0
			184	114	30	40		
12	I4	44	Total	C	N	O	0	0
			365	222	73	70		
12	I5	50	Total	C	N	O	0	0
			412	253	82	77		
12	I6	24	Total	C	N	O	0	0
			184	114	30	40		
12	I7	44	Total	C	N	O	0	0
			365	222	73	70		
12	I8	50	Total	C	N	O	0	0
			412	253	82	77		
12	I9	24	Total	C	N	O	0	0
			184	114	30	40		

- Molecule 13 is a protein called CF5, TGME49_297180.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	J1	308	Total	C	N	O	S	0	0
			2488	1572	457	452	7		
13	J2	308	Total	C	N	O	S	0	0
			2488	1572	457	452	7		
13	J3	308	Total	C	N	O	S	0	0
			2488	1572	457	452	7		
13	J4	308	Total	C	N	O	S	0	0
			2488	1572	457	452	7		
13	J5	308	Total	C	N	O	S	0	0
			2488	1572	457	452	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
13	J6	308	Total	C	N	O	S	0	0
			2488	1572	457	452	7		
13	J7	308	Total	C	N	O	S	0	0
			2488	1572	457	452	7		

- Molecule 14 is a protein called DCX, TGME49_256030.

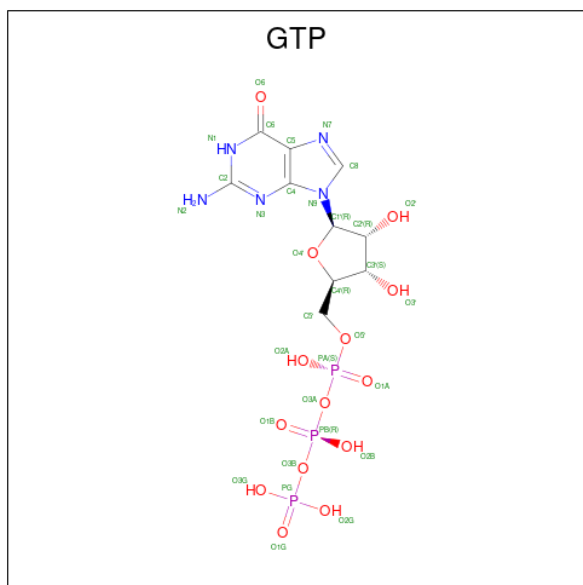
Mol	Chain	Residues	Atoms					AltConf	Trace
14	K0	189	Total	C	N	O	S	0	0
			1537	983	269	281	4		
14	K1	189	Total	C	N	O	S	0	0
			1537	983	269	281	4		
14	K2	189	Total	C	N	O	S	0	0
			1537	983	269	281	4		
14	K3	189	Total	C	N	O	S	0	0
			1537	983	269	281	4		
14	K4	189	Total	C	N	O	S	0	0
			1537	983	269	281	4		
14	K5	189	Total	C	N	O	S	0	0
			1537	983	269	281	4		
14	K6	189	Total	C	N	O	S	0	0
			1537	983	269	281	4		
14	K7	189	Total	C	N	O	S	0	0
			1537	983	269	281	4		
14	K8	189	Total	C	N	O	S	0	0
			1537	983	269	281	4		
14	K9	189	Total	C	N	O	S	0	0
			1537	983	269	281	4		
14	L0	189	Total	C	N	O	S	0	0
			1537	983	269	281	4		
14	L1	189	Total	C	N	O	S	0	0
			1537	983	269	281	4		
14	L2	189	Total	C	N	O	S	0	0
			1537	983	269	281	4		
14	L3	189	Total	C	N	O	S	0	0
			1537	983	269	281	4		
14	L4	132	Total	C	N	O	S	0	0
			1073	696	185	189	3		
14	L5	189	Total	C	N	O	S	0	0
			1537	983	269	281	4		
14	L6	189	Total	C	N	O	S	0	0
			1537	983	269	281	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
14	L7	189	Total	C	N	O	S	0	0
			1537	983	269	281	4		
14	L8	189	Total	C	N	O	S	0	0
			1537	983	269	281	4		
14	L9	189	Total	C	N	O	S	0	0
			1537	983	269	281	4		
14	M1	125	Total	C	N	O	S	0	0
			1011	656	170	182	3		
14	M2	189	Total	C	N	O	S	0	0
			1537	983	269	281	4		
14	M3	189	Total	C	N	O	S	0	0
			1537	983	269	281	4		
14	M4	189	Total	C	N	O	S	0	0
			1537	983	269	281	4		
14	M5	189	Total	C	N	O	S	0	0
			1537	983	269	281	4		
14	M6	189	Total	C	N	O	S	0	0
			1537	983	269	281	4		
14	M7	189	Total	C	N	O	S	0	0
			1537	983	269	281	4		

- Molecule 15 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
15	1A	1	Total	C	N	O	P	0
			32	10	5	14	3	

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Mol	Chain	Residues	Atoms					AltConf
15	1C	1	Total 32	C 10	N 5	O 14	P 3	0
15	1E	1	Total 32	C 10	N 5	O 14	P 3	0
15	1G	1	Total 32	C 10	N 5	O 14	P 3	0
15	1I	1	Total 32	C 10	N 5	O 14	P 3	0
15	1K	1	Total 32	C 10	N 5	O 14	P 3	0
15	1M	1	Total 32	C 10	N 5	O 14	P 3	0
15	2A	1	Total 32	C 10	N 5	O 14	P 3	0
15	2C	1	Total 32	C 10	N 5	O 14	P 3	0
15	2E	1	Total 32	C 10	N 5	O 14	P 3	0
15	2G	1	Total 32	C 10	N 5	O 14	P 3	0
15	2I	1	Total 32	C 10	N 5	O 14	P 3	0
15	2K	1	Total 32	C 10	N 5	O 14	P 3	0
15	2M	1	Total 32	C 10	N 5	O 14	P 3	0
15	3A	1	Total 32	C 10	N 5	O 14	P 3	0
15	3C	1	Total 32	C 10	N 5	O 14	P 3	0
15	3E	1	Total 32	C 10	N 5	O 14	P 3	0
15	3G	1	Total 32	C 10	N 5	O 14	P 3	0
15	3I	1	Total 32	C 10	N 5	O 14	P 3	0
15	3K	1	Total 32	C 10	N 5	O 14	P 3	0
15	3M	1	Total 32	C 10	N 5	O 14	P 3	0
15	4A	1	Total 32	C 10	N 5	O 14	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
15	4C	1	Total 32	C 10	N 5	O 14	P 3	0
15	4E	1	Total 32	C 10	N 5	O 14	P 3	0
15	4G	1	Total 32	C 10	N 5	O 14	P 3	0
15	4I	1	Total 32	C 10	N 5	O 14	P 3	0
15	4K	1	Total 32	C 10	N 5	O 14	P 3	0
15	4M	1	Total 32	C 10	N 5	O 14	P 3	0
15	5A	1	Total 32	C 10	N 5	O 14	P 3	0
15	5C	1	Total 32	C 10	N 5	O 14	P 3	0
15	5E	1	Total 32	C 10	N 5	O 14	P 3	0
15	5G	1	Total 32	C 10	N 5	O 14	P 3	0
15	5I	1	Total 32	C 10	N 5	O 14	P 3	0
15	5K	1	Total 32	C 10	N 5	O 14	P 3	0
15	5M	1	Total 32	C 10	N 5	O 14	P 3	0
15	6A	1	Total 32	C 10	N 5	O 14	P 3	0
15	6C	1	Total 32	C 10	N 5	O 14	P 3	0
15	6E	1	Total 32	C 10	N 5	O 14	P 3	0
15	6G	1	Total 32	C 10	N 5	O 14	P 3	0
15	6I	1	Total 32	C 10	N 5	O 14	P 3	0
15	6K	1	Total 32	C 10	N 5	O 14	P 3	0
15	6N	1	Total 32	C 10	N 5	O 14	P 3	0
15	7A	1	Total 32	C 10	N 5	O 14	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
15	7C	1	Total 32	C 10	N 5	O 14	P 3	0
15	7E	1	Total 32	C 10	N 5	O 14	P 3	0
15	7G	1	Total 32	C 10	N 5	O 14	P 3	0
15	7I	1	Total 32	C 10	N 5	O 14	P 3	0
15	7K	1	Total 32	C 10	N 5	O 14	P 3	0
15	7M	1	Total 32	C 10	N 5	O 14	P 3	0
15	8A	1	Total 32	C 10	N 5	O 14	P 3	0
15	8C	1	Total 32	C 10	N 5	O 14	P 3	0
15	8E	1	Total 32	C 10	N 5	O 14	P 3	0
15	8G	1	Total 32	C 10	N 5	O 14	P 3	0
15	8I	1	Total 32	C 10	N 5	O 14	P 3	0
15	8K	1	Total 32	C 10	N 5	O 14	P 3	0
15	8M	1	Total 32	C 10	N 5	O 14	P 3	0
15	9A	1	Total 32	C 10	N 5	O 14	P 3	0
15	9C	1	Total 32	C 10	N 5	O 14	P 3	0
15	9E	1	Total 32	C 10	N 5	O 14	P 3	0
15	9G	1	Total 32	C 10	N 5	O 14	P 3	0
15	9I	1	Total 32	C 10	N 5	O 14	P 3	0
15	9K	1	Total 32	C 10	N 5	O 14	P 3	0
15	9M	1	Total 32	C 10	N 5	O 14	P 3	0

- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
16	1A	1	Total	Mg	0
			1	1	
16	1C	1	Total	Mg	0
			1	1	
16	1E	1	Total	Mg	0
			1	1	
16	1G	1	Total	Mg	0
			1	1	
16	1I	1	Total	Mg	0
			1	1	
16	1K	1	Total	Mg	0
			1	1	
16	2A	1	Total	Mg	0
			1	1	
16	2C	1	Total	Mg	0
			1	1	
16	2E	1	Total	Mg	0
			1	1	
16	2G	1	Total	Mg	0
			1	1	
16	2I	1	Total	Mg	0
			1	1	
16	2K	1	Total	Mg	0
			1	1	
16	3A	1	Total	Mg	0
			1	1	
16	3C	1	Total	Mg	0
			1	1	
16	3E	1	Total	Mg	0
			1	1	
16	3G	1	Total	Mg	0
			1	1	
16	3I	1	Total	Mg	0
			1	1	
16	3K	1	Total	Mg	0
			1	1	
16	4A	1	Total	Mg	0
			1	1	
16	4C	1	Total	Mg	0
			1	1	
16	4E	1	Total	Mg	0
			1	1	
16	4G	1	Total	Mg	0
			1	1	

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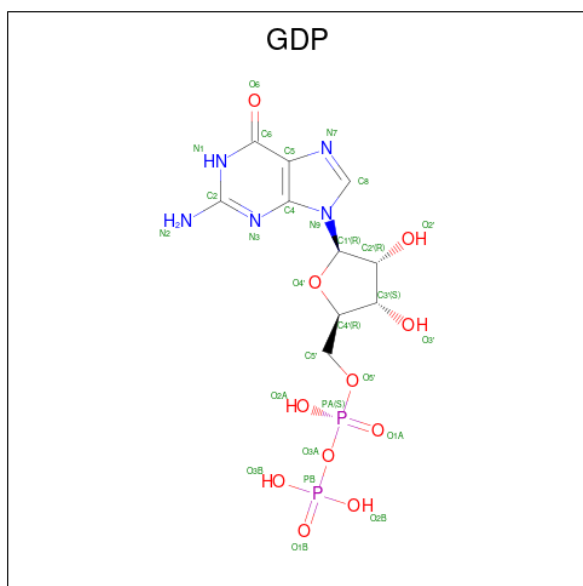
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
16	4I	1	1	1	0
16	4K	1	1	1	0
16	5A	1	1	1	0
16	5C	1	1	1	0
16	5E	1	1	1	0
16	5G	1	1	1	0
16	5I	1	1	1	0
16	5K	1	1	1	0
16	6A	1	1	1	0
16	6C	1	1	1	0
16	6E	1	1	1	0
16	6G	1	1	1	0
16	6I	1	1	1	0
16	6K	1	1	1	0
16	7B	1	1	1	0
16	7C	1	1	1	0
16	7E	1	1	1	0
16	7G	1	1	1	0
16	7I	1	1	1	0
16	7K	1	1	1	0
16	8A	1	1	1	0

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Mol	Chain	Residues	Atoms		AltConf
16	8C	1	Total	Mg	0
			1	1	
16	8E	1	Total	Mg	0
			1	1	
16	8G	1	Total	Mg	0
			1	1	
16	8I	1	Total	Mg	0
			1	1	
16	8K	1	Total	Mg	0
			1	1	
16	9A	1	Total	Mg	0
			1	1	
16	9C	1	Total	Mg	0
			1	1	
16	9E	1	Total	Mg	0
			1	1	
16	9G	1	Total	Mg	0
			1	1	
16	9I	1	Total	Mg	0
			1	1	
16	9K	1	Total	Mg	0
			1	1	

- Molecule 17 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
17	1B	1	Total 28	C 10	N 5	O 11	P 2	0
17	1D	1	Total 28	C 10	N 5	O 11	P 2	0
17	1F	1	Total 28	C 10	N 5	O 11	P 2	0
17	1H	1	Total 28	C 10	N 5	O 11	P 2	0
17	1J	1	Total 28	C 10	N 5	O 11	P 2	0
17	1L	1	Total 28	C 10	N 5	O 11	P 2	0
17	1N	1	Total 28	C 10	N 5	O 11	P 2	0
17	2B	1	Total 28	C 10	N 5	O 11	P 2	0
17	2D	1	Total 28	C 10	N 5	O 11	P 2	0
17	2F	1	Total 28	C 10	N 5	O 11	P 2	0
17	2H	1	Total 28	C 10	N 5	O 11	P 2	0
17	2J	1	Total 28	C 10	N 5	O 11	P 2	0
17	2L	1	Total 28	C 10	N 5	O 11	P 2	0
17	3B	1	Total 28	C 10	N 5	O 11	P 2	0
17	3D	1	Total 28	C 10	N 5	O 11	P 2	0
17	3F	1	Total 28	C 10	N 5	O 11	P 2	0
17	3H	1	Total 28	C 10	N 5	O 11	P 2	0
17	3J	1	Total 28	C 10	N 5	O 11	P 2	0
17	3L	1	Total 28	C 10	N 5	O 11	P 2	0
17	4B	1	Total 28	C 10	N 5	O 11	P 2	0
17	4D	1	Total 28	C 10	N 5	O 11	P 2	0
17	4F	1	Total 28	C 10	N 5	O 11	P 2	0

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Mol	Chain	Residues	Atoms					AltConf
17	4H	1	Total 28	C 10	N 5	O 11	P 2	0
17	4J	1	Total 28	C 10	N 5	O 11	P 2	0
17	4L	1	Total 28	C 10	N 5	O 11	P 2	0
17	5B	1	Total 28	C 10	N 5	O 11	P 2	0
17	5D	1	Total 28	C 10	N 5	O 11	P 2	0
17	5F	1	Total 28	C 10	N 5	O 11	P 2	0
17	5H	1	Total 28	C 10	N 5	O 11	P 2	0
17	5J	1	Total 28	C 10	N 5	O 11	P 2	0
17	5L	1	Total 28	C 10	N 5	O 11	P 2	0
17	5N	1	Total 28	C 10	N 5	O 11	P 2	0
17	6B	1	Total 28	C 10	N 5	O 11	P 2	0
17	6D	1	Total 28	C 10	N 5	O 11	P 2	0
17	6F	1	Total 28	C 10	N 5	O 11	P 2	0
17	6H	1	Total 28	C 10	N 5	O 11	P 2	0
17	6J	1	Total 28	C 10	N 5	O 11	P 2	0
17	6L	1	Total 28	C 10	N 5	O 11	P 2	0
17	6N	1	Total 28	C 10	N 5	O 11	P 2	0
17	7B	1	Total 28	C 10	N 5	O 11	P 2	0
17	7D	1	Total 28	C 10	N 5	O 11	P 2	0
17	7F	1	Total 28	C 10	N 5	O 11	P 2	0
17	7H	1	Total 28	C 10	N 5	O 11	P 2	0

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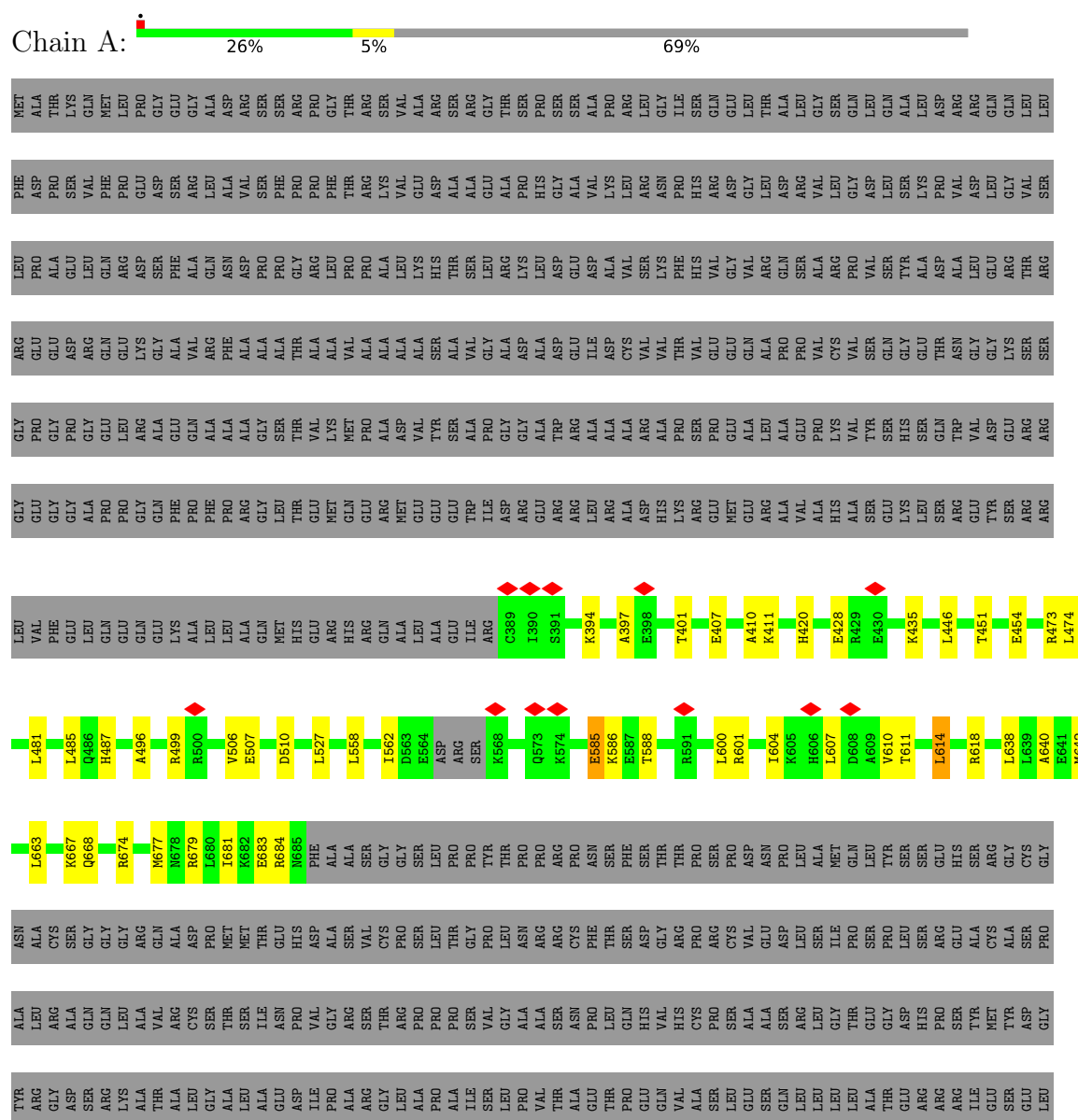
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Mol	Chain	Residues	Atoms					AltConf
17	7J	1	Total	C	N	O	P	0
			28	10	5	11	2	
17	7L	1	Total	C	N	O	P	0
			28	10	5	11	2	
17	8B	1	Total	C	N	O	P	0
			28	10	5	11	2	
17	8D	1	Total	C	N	O	P	0
			28	10	5	11	2	
17	8F	1	Total	C	N	O	P	0
			28	10	5	11	2	
17	8H	1	Total	C	N	O	P	0
			28	10	5	11	2	
17	8J	1	Total	C	N	O	P	0
			28	10	5	11	2	
17	8L	1	Total	C	N	O	P	0
			28	10	5	11	2	
17	9B	1	Total	C	N	O	P	0
			28	10	5	11	2	
17	9D	1	Total	C	N	O	P	0
			28	10	5	11	2	
17	9F	1	Total	C	N	O	P	0
			28	10	5	11	2	
17	9H	1	Total	C	N	O	P	0
			28	10	5	11	2	
17	9J	1	Total	C	N	O	P	0
			28	10	5	11	2	
17	9L	1	Total	C	N	O	P	0
			28	10	5	11	2	

3 Residue-property plots

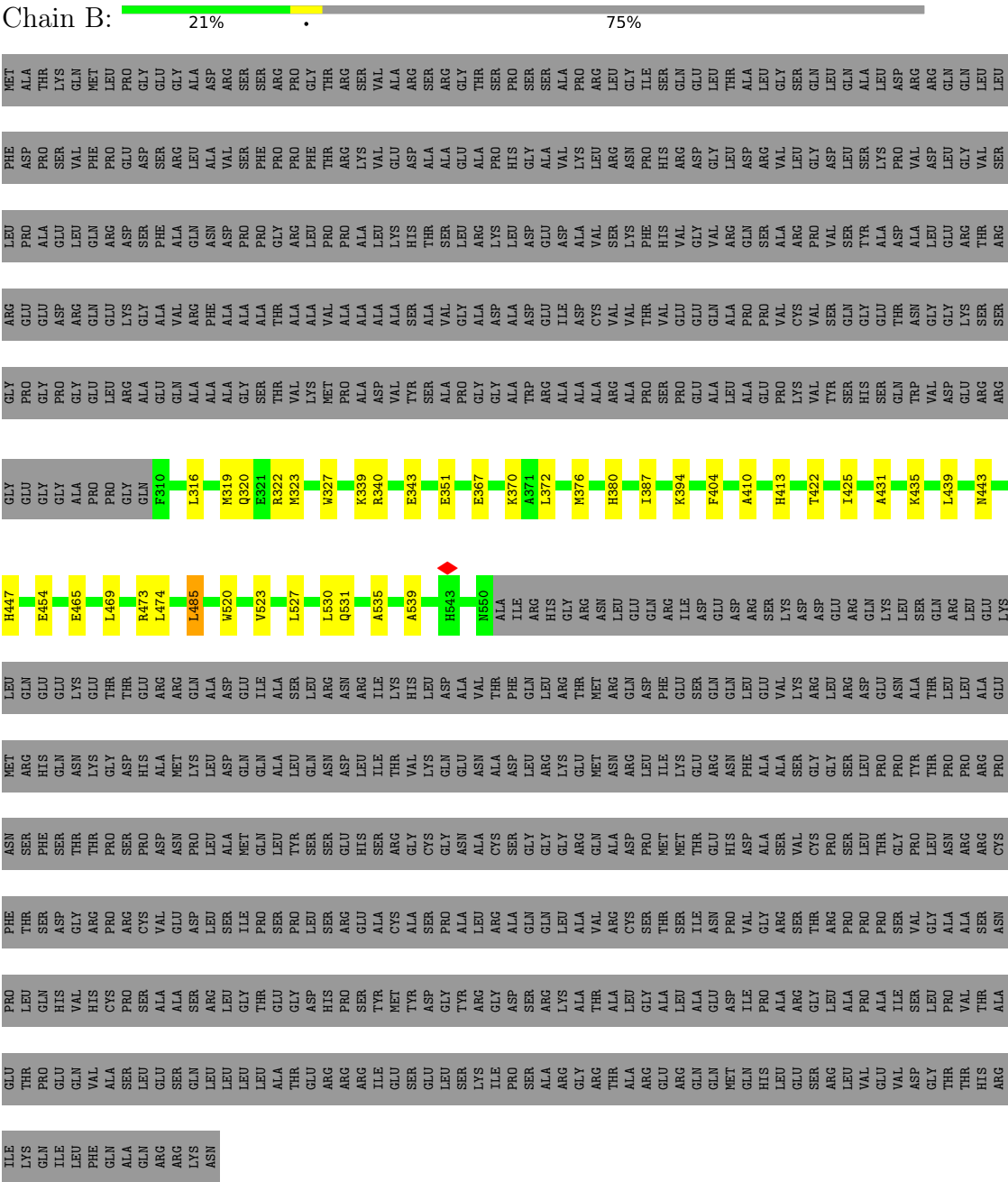
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: CF2, TGME49_258090

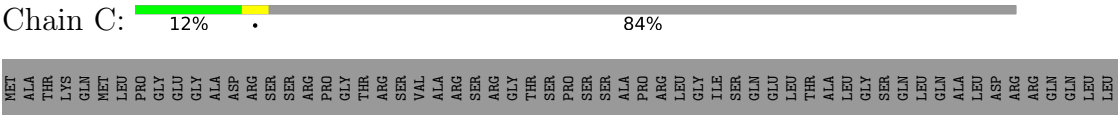


SER	LYS	PHE	ILE	THR	PRO	SER	GLN	ALA	ARG	GLY	ARG	THR	ALA	GLY	ASP	GLN	ARG	GLY	THR	THR	HIS	ARG	ILE	LYS	LYS	GLN	ILE	LEU	PHE	GLN	ALA	GLN	ARG	ARG	LYS	ASN
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● Molecule 1: CF2, TGME49_258090



● Molecule 1: CF2, TGME49_258090





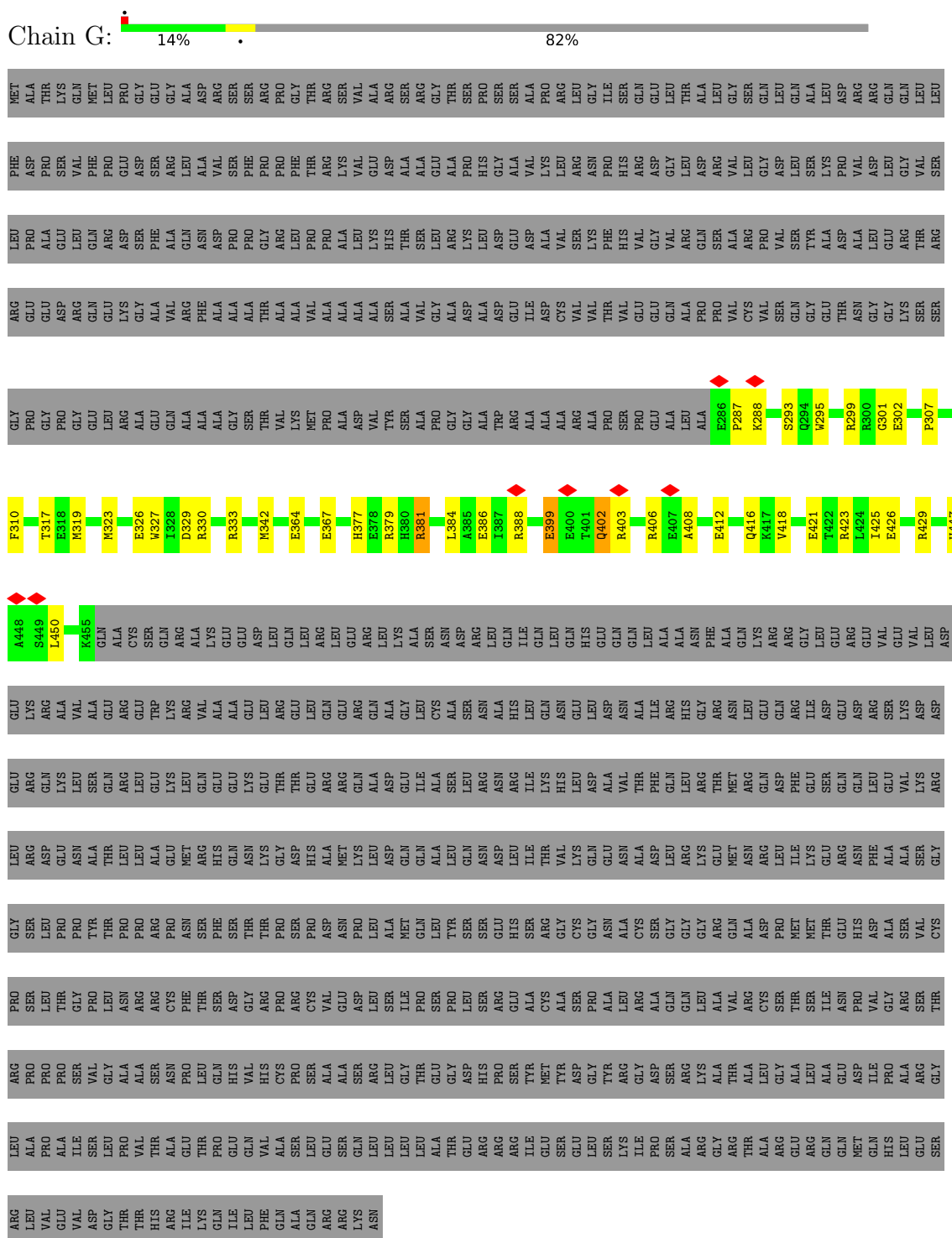
[illegible]

- Molecule 1: CF₂, TGME49_258090

Chain F: 28% 69%

[illegible]

- Molecule 1: CF₂, TGME49 258090



- Molecule 1: CF₂, TGME49 258090

ARG	GLU	ALA	VAL	ASP	ALA	ARG	GLN
ARG	SER	ALA	GLU	ASN	MET	ARG	GLU
LYS	GLN	SER	GLN	PRO	GLP	GLN	ARG
ASN	LEU	ARG	LEU	LEU	LEU	ALA	GLN
	LEU	GLY	TLE	MET	GLN	GLY	GLY
	LEU	THR	PRO	GLN	GLN	TLE	LEU
	ALA	GLU	SER	LEU	ALA	CYS	GLY
	THR	GLY	PRO	TYR	LEU	SER	ALA
	GLU	ASP	LEU	SER	GLN	LEU	SER
	ARG	HIS	SER	SER	ASN	ARG	ASN
	ARG	PRO	ARG	GLU	ASP	ALA	ALA
	ARG	SER	GLU	HIS	LEU	ARG	HIS
	TLE	MET	ALA	SER	TLE	LEU	GLN
	GLU	MET	CYS	ARG	THR	GLN	GLN
	SER	TYR	ALA	GLY	VAL	HIS	GLN
	GLU	ASP	SER	CYS	LYS	LEU	GLU
	LEU	GLY	PRO	GLY	GLN	ASP	LEU
	SER	TYR	ALA	ASN	GLN	ALA	LEU
	LYS	ARG	LEU	ALA	GLU	VAL	ASN
	TLE	GLY	ARG	CYS	ALA	THR	ALA
	PRO	ASP	ALA	SER	ASP	PHE	TLE
	SER	SER	SER	GLY	LEU	GLN	ARG
	ALA	ARG	GLN	GLY	ARG	LEU	HIS
	ARG	LYS	LEU	GLY	LYS	ARG	GLY
	GLY	ALA	ALA	ARG	GLU	THR	ARG
	THR	THR	VAL	GLN	MET	MET	LEU
	ALA	LEU	CYS	ASP	ARG	GLN	GLU
	ARG	GLY	SER	PRO	LEU	ASP	GLN
	GLU	ALA	THR	MET	TLE	PHE	ARG
	ARG	LEU	SER	MET	GLY	GLU	ASP
	GLN	ALA	TLE	THR	ASP	SER	ASN
	GLN	GLU	ASN	GLU	GLU	GLN	GLU
	MET	ASP	PRO	HIS	ASN	GLN	ASP
	GLN	TLE	VAL	ASP	PHE	LEU	ARG
	HIS	PRO	GLY	ALA	ALA	GLU	SER
	LEU	ALA	ARG	SER	ALA	VAL	LYS
	GLU	ARG	SER	VAL	SER	LYS	ASP
	SER	GLY	THR	CYS	GLY	ARG	GLU
	ARG	LEU	ARG	PRO	GLY	LEU	GLU
	LEU	PRO	PRO	SER	SER	ARG	ARG
	VAL	PRO	PRO	LEU	LEU	ASP	GLN
	GLU	ALA	PRO	THR	PRO	GLU	LYS
	VAL	TLE	SER	GLY	ALA	ASN	LEU
	ASP	SER	VAL	PRO	TYR	ALA	SER
	GLY	LEU	GLY	LEU	THR	THR	GLN
	THR	PRO	ALA	ASN	PRO	LEU	LEU
	THR	VAL	ALA	ARG	PRO	LEU	ARG
	HIS	THR	SER	ARG	PRO	ALA	GLU
	ARG	ALA	ASN	CYS	PRO	GLU	LYS
	TLE	GLU	PRO	PHE	ASN	MET	LEU
	LYS	THR	LEU	THR	SER	ARG	GLN
	GLN	PRO	GLN	SER	PHE	HIS	GLU
	TLE	GLU	HIS	ASP	SER	GLN	GLU
	LEU	GLN	VAL	GLY	THR	ASN	LYS
	PHN	VAL	HIS	ARG	THR	GLY	THR
	GLN	ALA	CYS	PRO	PRO	GLY	GLY
	ALA	SER	PRO	ARG	THR	ASP	THR
	GLN	LEU	SER	CYS	PRO	HIS	GLN

- Molecule 1: CF₂, TGME49 258090

[illegible]

GLY
THR
THR
HIS
ARG
ILE
LYS
GLN
ILE
LEU
PHE
GLN
ALA
GLN
ARG
ARG
LYS
ASN

- Molecule 1: CF₂, TGME49 258090



LEU	VAL	PHE	LEU	GLN	GLU	GLN	GLY	ALA	LEU	LEU	ALA	GLN	MET	HIS	GLU	HIS	ARG	GLN	ALA	LEU	ALA	GLU	ILE	CYS	ILE	SER	GLU	LYS	THR	ASP	ALA	ALA	GLU	GLU	GLU	THR	GLN	ARG	PHE	GLN	ARG	GLU	GLA	SER	ALA	LYS	GLU	HIS	GLN	LEU	GLN	GLN	LEU	VAL	HIS
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[illegible]

Category	Number of Genes
H487	1
Q490	1
N494	1
F495	1
A496	1
Q497	1
R498	1
R499	1
R500	1
E503	1
R504	1
E505	1
L509	1
D510	1
F511	1
K512	1
V515	1
A516	1
E517	1
K521	1
R522	1
V523	1
A524	1
A525	1
E526	1
L527	1
R528	1
E529	1
L530	1
Q531	1
E532	1
R533	1
Q534	1
A535	1
G536	1
L537	1
C538	1
A539	1
S540	1
N541	1
A542	1
H543	1
L544	1
Q545	1
N546	1
E547	1
L548	1
D549	1
N550	1
A551	1
TLE	0
ARG	0
HIS	0
TTY	0

[illegible]

T616	M617	R618	E621	F622	S623	Q624	Q625	L626	K629	R630	L631	R632	D633	A636	T637	L638	L639	A640	E641	M642	R643	Q644	Q645	N646	K647	M652	K653	L654	D655	Q656	L659	D662	K667	Q668	L673	R674	K675	E676	M677	N678	R679	E683	R684	PHE	ALA	ALA	SER	GLY
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SER	LEU	THR	GLY	PRO	LEU	ASN	ARG	ARG	CYS	PHI	THR	SER	SER	ASP	GLY	ARG	PRO	ARG	ARG	CYS	VAL	GLU	GLU	ASP	LEU	SER	SER	ILE	PRO	SER	PRO	PRO	LEU	LEU	GLU	ARG	ALA	ALA	CYS	CYS	ALA	ALA	SER	SER	PRO	PRO	ALA	ALA	ALA	LEU	LEU	ALA	VAL	VAL	ARG	CYS	SER	SER	THR	SER	THR	ILE	ASN	PRO	VAL	GLY	ARG	SER	SER	THR	ARG
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PRO	PRO	PRO	SER	VAL	GLY	ALA	ALA	SER	ASN	PRO	LEU	GLN	HIS	VAL	HIS	CYS	PRO	SER	ALA	ALA	ARG	LEU	GLY	THR	GLU	GLY	ASP	HIS	PRO	SER	SER	TYR	MET	TYR	ASP	GLY	TYR	ARG	GLY	ASP	SER	ARG	LYS	ALA	ALA	THR	ALA	LEU	GLY	ALA	ALA	GLU	ASP	ILE	PRO	ALA	ALA	ARG	GLY	LEU
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- Molecule 1: CF₂, TGME49 258090



ILE	GLU	GLU	TYR	ALA	SER	N661	ARG	ASN	LEU	GLU	THR	LEU	VAL	GLY	ARG	LEU	GLN	THR	GLU	THR	VAL	GLY	GLY	ARG	LEU	GLN	GLY	PRO	GLY	ASP	PHE	MET	
SER	SER	GLU	TYR	ALA	GLY	D662	ASN	ALA	GLN	THR	ARG	PHE	GLU	GLY	ASN	GLN	GLN	ARG	GLY	THR	GLU	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	PRO	GLY	ALA	
LEU	LEU	GLU	ASP	SER	CYS	L663	ILE	HIS	GLN	ILE	ILE	LEU	GLN	GLN	ILE	LEU	GLN	GLN	GLY	GLU	GLU	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	
SER	SER	GLU	TYR	ALA	ASN	T665	HIS	ASN	GLN	ASN	HIS	GLN	GLN	GLN	ASN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	
LYS	LYS	GLU	TYR	ALA	ASN	V666	HIS	ASN	GLN	GLU	LEU	HIS	GLN	GLN	GLU	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	
ILE	ILE	GLU	GLY	ARG	ALA	K667	LEU	GLU	GLU	GLU	LEU	GLN	GLN	GLN	GLU	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	
PRO	PRO	ASP	ASP	ALA	SER	Q668	ALA	ASN	GLN	ASN	VAL	GLN	GLN	GLN	ASN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	
ALA	ALA	ARG	ARG	GLN	GLY	E669	THR	THR	THR	THR	THR	ALA	LEU	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	
ARG	ARG	GLY	LYS	LEU	GLY	L673	PHE	ILE	ALA	ILE	PHE	LEU	ALA	ALA	ARG	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	
GLY	GLY	R674	ALA	ALA	ARG	K675	GLN	ARG	ALA	ARG	GLN	LEU	ALA	ALA	GLN	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	
THR	THR	ARG	THR	VAL	GLN	E676	LEU	HIS	ASN	GLY	LEU	GLN	ASN	GLN	GLY	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	
ALA	ALA	THR	ALA	ARG	ALA	M677	ARG	GLY	PHE	ARG	ARG	GLY	PHE	GLY	ARG	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA
ARG	ARG	ALA	LEU	CYS	ASP	M678	THR	ARG	ALA	ARG	THR	ALA	ALA	ALA	GLN	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA
GLY	GLY	PRO	GLY	SER	PRO	N679	MET	ASN	GLN	ASN	MET	HIS	GLN	GLN	THR	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	
LEU	LEU	MET	LEU	THR	MET	L680	ARG	LEU	LYS	LEU	ARG	GLY	LYS	GLY	ARG	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	
GLU	GLU	GLY	ALA	SER	MET	G683	GLN	GLU	ARG	GLU	GLN	ARG	GLY	GLY	GLN	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	
GLN	GLN	ALA	ALA	ILE	THR	R684	ASN	ASP	GLN	ASP	GLN	ARG	GLY	GLY	GLN	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	
GLN	GLN	ASP	ASP	PRO	HIS	N685	PHE	GLY	GLY	ILE	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	
ILE	ILE	GLN	ILE	VAL	ASP	F686																											

Chain P: 94%





[illegible]

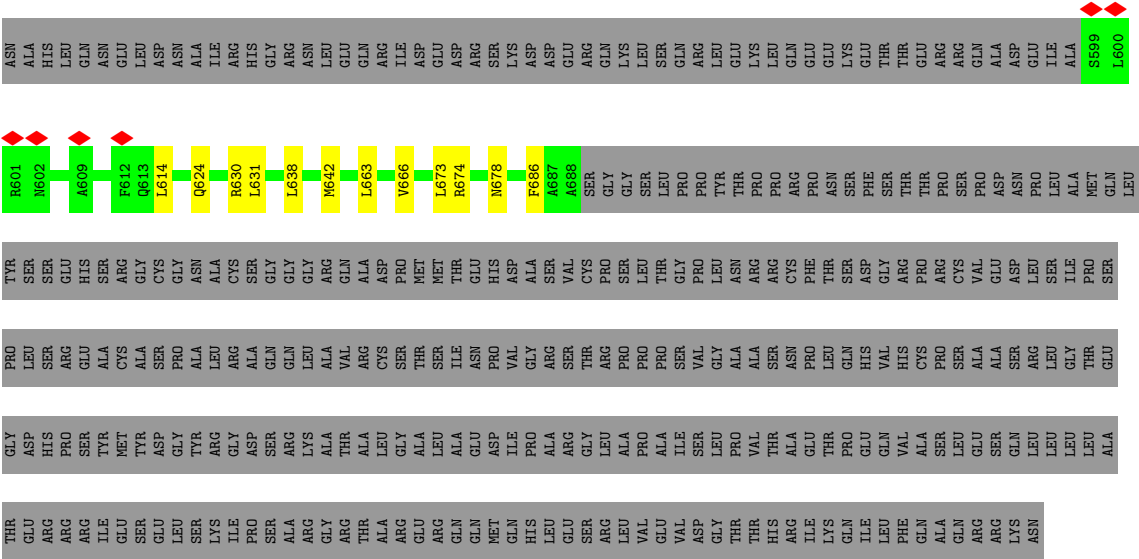
- Molecule 1: CF₂, TGME49 258090



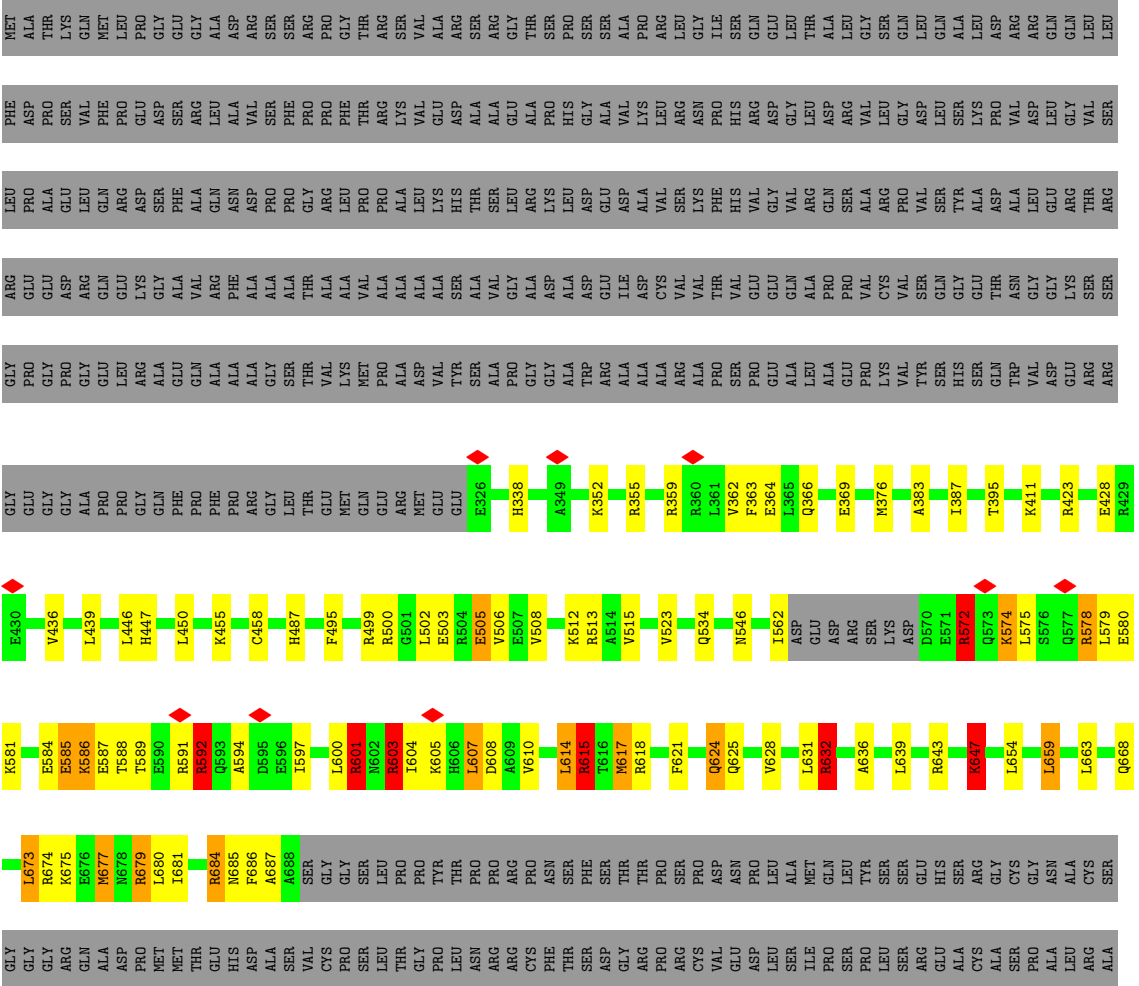
ARG	GLN	ALA	LEU	SER	MET	THR	ILE	GLY	ASP	PHE
GLN	GLU	ASP	ALA	ILE	THR	GLU	PRO	GLY	GLU	GLU
MET	ASP	THR	ASN	PRO	HIS	GLY	GLY	GLY	ASP	PRO
GLN	ILE	VAL	ASP	VAL	ASP	ASP	ALA	ALA	ARG	LEU
HIS	PRO	GLY	GLY	GLY	ALA	F686	PRO	PRO	GLN	PHE
LEU	ALA	ARG	ALA	ARG	SER	A687	VAL	GLY	GLU	PRO
GLU	ARG	SER	GLY	SER	CYS	A688	VAL	GLY	ASP	GLY
SER	ARG	THR	GLY	THR	GLY	GLY	THR	PHE	ASP	SER
LEU	LEU	PRO	ALA	PRO	SER	GLY	PRO	ALA	ARG	GLY
VAL	VAL	PRO	PRO	PRO	GLY	E517	PRO	PRO	GLN	ALA
GLU	GLU	ALA	PRO	THR	THR	R518	SER	PHE	ALA	ASP
VAL	VAL	ILE	ILE	SER	GLY	E519	LEU	PRO	ASN	ALA
ASP	ASP	GLY	VAL	VAL	PRO	W520	PRO	ARG	ARG	VAL
GLY	GLY	LEU	GLY	GLY	LEU	W521	PRO	ALA	PRO	PRO
THR	THR	PRO	ALA	ASN	THR	R522	TYR	ALA	PRO	SER
THR	THR	THR	VAL	ARG	ARG	Q534	PRO	THR	GLY	PRO
HIS	HIS	ARG	THR	SER	ARG	D339	PRO	VAL	ARG	PRO
ARG	ARG	ALA	ASN	PRO	CYS	L548	PRO	VAL	THR	PHE
ILE	ILE	THR	PRO	PHE	THR	ASN	ASN	ALA	ALA	LYS
GLN	GLN	THR	LEU	SER	THR	SER	SER	ALA	LEU	VAL
ILE	ILE	GLU	HIS	GLY	ASP	R661	THR	ALA	GLY	ALA
LEU	LEU	GLN	VAL	GLY	GLY	F562	SER	SER	ASP	ARG
PHE	PHE	VAL	VAL	HIS	ARG	D563	THR	ALA	THR	ALA
GLN	GLN	ALA	CYS	PRO	PRO	R572	PRO	VAL	VAL	ARG
ALA	ALA	LEU	PRO	ARG	THR	GLY	THR	GLY	GLY	THR
GLN	GLN	LEU	SER	CYS	CYS	R340	PRO	PRO	ARG	ALA
ARG	ARG	GLU	THR	ALA	VAL	E341	SER	GLY	ALA	THR
ARG	ARG	SER	ALA	ALA	GLU	M342	PRO	GLY	LYS	SER
LYS	LYS	ASN	SER	ASP	ASP	L579	PRO	ALA	LEU	HIS
ASN	ASN	LEU	ARG	ASN	ASN	E580	ASN	TRP	ASP	GLY
		LEU	LEU	LEU	LEU	R344	PRO	ARG	GLU	GLY
		LEU	LEU	LEU	ILE	E584	LEU	ALA	ASP	ALA
		LEU	GLY	ALA	PRO	R360	PRO	ALA	ILE	ASP
		LEU	THR	THR	PRO	M617	ALA	ALA	ASP	ALA
		ALA	GLN	SER	GLN	L365	MET	ALA	CYS	VAL
		THR	GLY	GLY	PRO	K370	GLN	ARG	VAL	SER
		GLU	LEU	LEU	LEU	Q624	THR	VAL	LYS	THR
		ARG	ASP	SER	TYR	L631	TYR	THR	PHE	ILE
		ARG	HIS	SER	SER	R373	SER	VAL	HIS	SER
		PRO	PRO	ARG	ARG	T637	SER	GLY	VAL	ARG
		ARG	SER	GLU	GLU	L638	GLU	GLY	ASP	GLY
		ILE	TYR	ALA	ALA	L639	ALA	ALA	GLN	VAL
		SER	MET	CYS	SER	A640	SER	ARG	ARG	ASP
		THR	TYR	ALA	ARG	E641	ASP	PRO	GLN	LEU
		GLU	GLY	GLY	GLY	M642	GLY	VAL	ARG	ARG
		LEU	CYS	CYS	PRO	Q645	TYR	ARG	VAL	VAL
		SER	ALA	GLY	ALA	T401	ALA	CYS	ARG	LEU
		THR	ASN	LEU	LEU	R406	ASN	VAL	PRO	GLY
		ARG	GLY	ARG	ARG	D396	GLY	VAL	GLN	THR
		ILE	ALA	ALA	ALA	L654	GLU	ARG	VAL	ASP
		PRO	ASP	CYS	CYS	D655	ALA	TYR	LEU	LEU
		SER	SER	GLN	SER	Q656	GLY	HIS	GLY	SER
		ALA	ARG	GLY	GLY	K411	THR	GLY	ALA	LYS
		ARG	LYS	LEU	LEU	L415	GLN	THR	ASP	PRO
		ARG	ALA	THR	ALA	V418	TRP	ASN	VAL	VAL
		GLY	THR	VAL	VAL	E421	ALA	GLN	GLY	ASP
		ALA	ALA	ARG	ARG	T422	THR	GLY	GLY	ASP
		ALA	LEU	CYS	CYS	E676	ALA	GLY	LYS	ARG
		GLY	GLY	SER	SER	M677	ALA	THR	GLY	GLY
		ALA	ALA	THR	THR		THR	ARG	SER	SER

- Molecule 1: CF₂, TGME49 258090





● Molecule 1: CF2, TGME49_258090



SER	ALA	ARG	GLY	ARG	THR	ALA	ALA	ARG	GLU	GLN	GLN	MET	GLN	HIS	LEU	GLU	SER	ARG	LEU	VAL	GLU	VAL	ASP	GLY	THR	THR	HIS	ARG	ILE	LYS	GLN	ILE	LEU	PHE	GLN	ALA	GLN	ARG	ARG	LYS	ASN
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- Molecule 1: CF₂, TGME49_258090

Chain Z:  21% . 75%

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

GLY	Q320	0.320	1
GLU	E321	0.321	2
GLY	R322	0.322	3
ALA	E323	0.323	4
PRO	R324	0.324	5
PRO	E325	0.325	6
GLY	R326	0.326	7
GLN	E327	0.327	8
PHE	R328	0.328	9
PHE	E329	0.329	10
PRO	R330	0.330	11
ARG	E331	0.331	12
GLY	R332	0.332	13
LEU	E333	0.333	14
THR	R334	0.334	15
GLU	E335	0.335	16
MET	R336	0.336	17
Q320	E337	0.337	18
E321	R338	0.338	19
R322	E339	0.339	20
E323	R340	0.340	21
R330	E341	0.341	22
R340	R342	0.342	23
E341	E343	0.343	24
R342	R344	0.344	25
E343	E345	0.345	26
R344	R346	0.346	27
E345	E347	0.347	28
R346	R348	0.348	29
E347	E349	0.349	30
R348	R350	0.350	31
E349	E351	0.351	32
R350	R352	0.352	33
E351	E353	0.353	34
R352	R354	0.354	35
E353	E355	0.355	36
R354	R356	0.356	37
E355	E357	0.357	38
R356	R358	0.358	39
E357	E359	0.359	40
R358	R360	0.360	41
E359	E361	0.361	42
R360	R362	0.362	43
E361	E363	0.363	44
R362	R364	0.364	45
E363	E365	0.365	46
R364	R366	0.366	47
E365	E367	0.367	48
R366	R368	0.368	49
E367	E369	0.369	50
R368	R370	0.370	51
E369	E371	0.371	52
R370	R372	0.372	53
E371	E373	0.373	54
R372	R374	0.374	55
E373	E375	0.375	56
R374	R376	0.376	57
E375	E377	0.377	58
R376	R378	0.378	59
E377	E379	0.379	60
R378	R380	0.380	61
E379	E381	0.381	62
R380	R382	0.382	63
E381	E383	0.383	64
R382	R384	0.384	65
E383	E385	0.385	66
R384	R386	0.386	67
E385	E387	0.387	68
R386	R388	0.388	69
E387	E389	0.389	70
R388	R390	0.390	71
E389	E391	0.391	72
R390	R392	0.392	73
E391	E393	0.393	74
R392	R394	0.394	75
E393	E395	0.395	76
R394	R396	0.396	77
E395	E397	0.397	78
R396	R398	0.398	79
E397	E399	0.399	80
R398	R400	0.400	81
E399	E401	0.401	82
R400	R402	0.402	83
E401	E403	0.403	84
R402	R404	0.404	85
E403	E405	0.405	86
R404	R406	0.406	87
E405	E407	0.407	88
R406	R408	0.408	89
E407	E409	0.409	90
R408	R410	0.410	91
E409	E411	0.411	92
R410	R412	0.412	93
E411	E413	0.413	94
R412	R414	0.414	95
E413	E415	0.415	96
R414	R416	0.416	97
E415	E417	0.417	98
R416	R418	0.418	99
E417	E419	0.419	100
R418	R420	0.420	101
E419	E421	0.421	102
R420	R422	0.422	103
E421	E423	0.423	104
R422	R424	0.424	105
E423	E425	0.425	106
R424	R426	0.426	107
E425	E427	0.427	108
R426	R428	0.428	109
E427	E429	0.429	110
R428	R430	0.430	111
E429	A431	0.431	112
R430	R432	0.432	113
E431	E433	0.433	114
R432	R434	0.434	115
E433	E435	0.435	116
R434	R436	0.436	117
E435	E437	0.437	118
R436	R438	0.438	119
E437	E439	0.439	120
R438	R440	0.440	121
E439	E441	0.441	122
R440	R442	0.442	123
E441	E443	0.443	124
R442	R444	0.444	125
E443	E445	0.445	126
R444	R446	0.446	127
E445	E447	0.447	128
R446	R448	0.448	129
E447	E449	0.449	130
R448	R450	0.450	131

Category	Value
K463	1.00
L467	0.98
K468	0.97
L469	0.96
R470	0.95
L471	0.94
L485	0.93
K486	0.92
R487	0.91
E488	0.90
K489	0.89
Q490	0.88
L491	0.87
N494	0.86
K498	0.85
L502	0.84
E505	0.83
V506	0.82
E507	0.81
V508	0.80
R513	0.79
L527	0.78
S540	0.77
L544	0.76
L558	0.75
L562	0.74
ASP	0.73
GLU	0.72
ASP	0.71
ASP	0.70
ARG	0.69
SER	0.68
LYS	0.67
ASP	0.66
ASP	0.65
GLU	0.64
ARG	0.63
GLN	0.62
LYS	0.61
LEU	0.60
SER	0.59
GLN	0.58
ARG	0.57
LEU	0.56
GLU	0.55
LYS	0.54
LEU	0.53
GLN	0.52

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

- Molecule 1: CF₂, TGME49_258090

HIS
P842
M845
Y846
D847

R850
L859
G860
A861
T866

R869
L877
P878
V879
T880
A881
T883
P884
E885
Q886
V887

Q893
L896

R917
T918
R941
K953
ASN

[illegible]



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

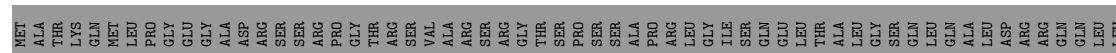
- Molecule 1: CF₂, TGME49_258090



M652	L582	K411	GLY	GLY	ARG	LEU	PHE	MET
K653	Q583	E584	GLU	PRO	GLU	ASP	ASP	THR
L654	E585	H413	GLY	PRO	GLU	ASP	PRO	THR
Q657	K586	R423	ALA	GLY	ARG	GLN	VAL	GLN
K658	E587	R429	PRO	PRO	GLU	GLN	PHE	WET
L659	T588	R429	PRO	PRO	LEU	ARG	PRO	LEU
D662	T589	R429	GLY	ARG	LYS	ASP	GLU	PRO
L663	E590	K435	GLN	ALA	GLY	PHE	ASP	GLY
L664	R591	K435	PHE	GLU	ALA	ALA	SER	GLY
T665	R592	L439	PRO	GLN	VAL	VAL	ARG	ALA
T665	Q593	L439	PHE	ALA	ARG	GLN	LEU	GLY
V666	A594	L446	PRO	ALA	PHE	ASN	ALA	ASP
K667	D595	L446	ARG	ALA	ALA	ASP	VAL	ARG
Q668	E596	L469	GLY	GLY	ALA	ASP	VAL	SER
E669	T597	L469	LEU	SER	ALA	PHE	SER	SER
M670	A598	R473	THR	THR	THR	GLY	PRO	ARG
	S599	R473	GLU	VAL	ARG	ARG	PRO	PRO
L673	L600	Q489	MET	LYS	ALA	LEU	PHE	GLY
R674	R601	Q489	GLN	MET	VAL	LEU	THR	THR
K675	M602	F495	GLU	PRO	ALA	PRO	THR	THR
E676	R603	F495	ARG	ALA	ALA	ALA	LYS	SER
M677	I604	R500	MET	ASP	ALA	LEU	VAL	VAL
M678	K605	R500	GLU	VAL	ALA	LYS	GLU	ALA
R679	R606	K512	GLU	TYR	SER	HIS	ASP	ALA
L680	L607	WU	GLU	SER	THR	ASP	ASP	ARG
I681	V610	V515	R327	ALA	VAL	THR	ALA	SER
K682	T611	R328	PRO	ALA	GLY	ARG	GLU	ALA
E683	T611	R329	GLY	GLY	ALA	LEU	GLU	THR
R684	R612	E519	D329	GLY	ASP	LYS	PRO	SER
M685	Q613	R522	R330	ALA	ALA	LEU	HIS	PRO
PHE	L614	R522	THR	ARG	ASP	ASP	GLY	SER
ALA	R615	R523	ALA	ARG	GLU	ASP	ALA	SER
ALA	T616	E526	L334	ILE	ASP	ASP	VAL	ALA
SER	M617	E526	R337	ALA	ASP	VAL	LYS	PRO
GLY	R618	Q534	R338	ALA	CYS	VAL	LEU	ARG
SER	Q619	L537	R339	ARG	VAL	ARG	LEU	LEU
LEU	S623	L537	R340	VAL	VAL	GLY	ASP	GLY
PRO	Q624	E559	R344	PRO	VAL	VAL	ARG	THR
PRO	Q625	Q560	R344	SER	VAL	VAL	GLY	LEU
TYR	L626	R561	R344	PRO	THR	GLY	LEU	ALA
THR	E627	T562	R360	GLU	GLU	VAL	GLY	GLY
PRO	Q628	E567	L361	ALA	GLN	VAL	LEU	THR
PRO	K629	R566	L373	ALA	PRO	GLN	ASP	ALA
ARG	R630	S567	A374	GLU	PRO	SER	ARG	LEU
PRO	L631	R568	A374	PRO	VAL	ALA	VAL	GLY
ASN	R632	D569	R375	LYS	CYS	ARG	SER	SER
SER	R632	R570	R376	VAL	VAL	PRO	LEU	GLN
PHE	L638	E571	H377	TYR	SER	VAL	GLY	GLN
THR	E641	R572	R388	HIS	GLY	TYR	SER	LEU
THR	Q642	Q573	R388	SER	GLY	ALA	LYS	LEU
PRO	R643	K574	A397	GLN	THR	ASP	PRO	ASP
SER	H644	L575	A397	THR	ASN	ALA	VAL	ARG
PRO	PRO	S576	E400	VAL	GLY	LEU	ASP	ARG
ASP	K647	Q577	E400	ASP	LYS	ARG	GLY	GLN
ASN	G648	R578	R403	GLU	SER	THR	VAL	LEU
PRO	D649	E580	R403	ARG	SER	ARG	SER	THR



Chain e: 7% 91%



[illegible]

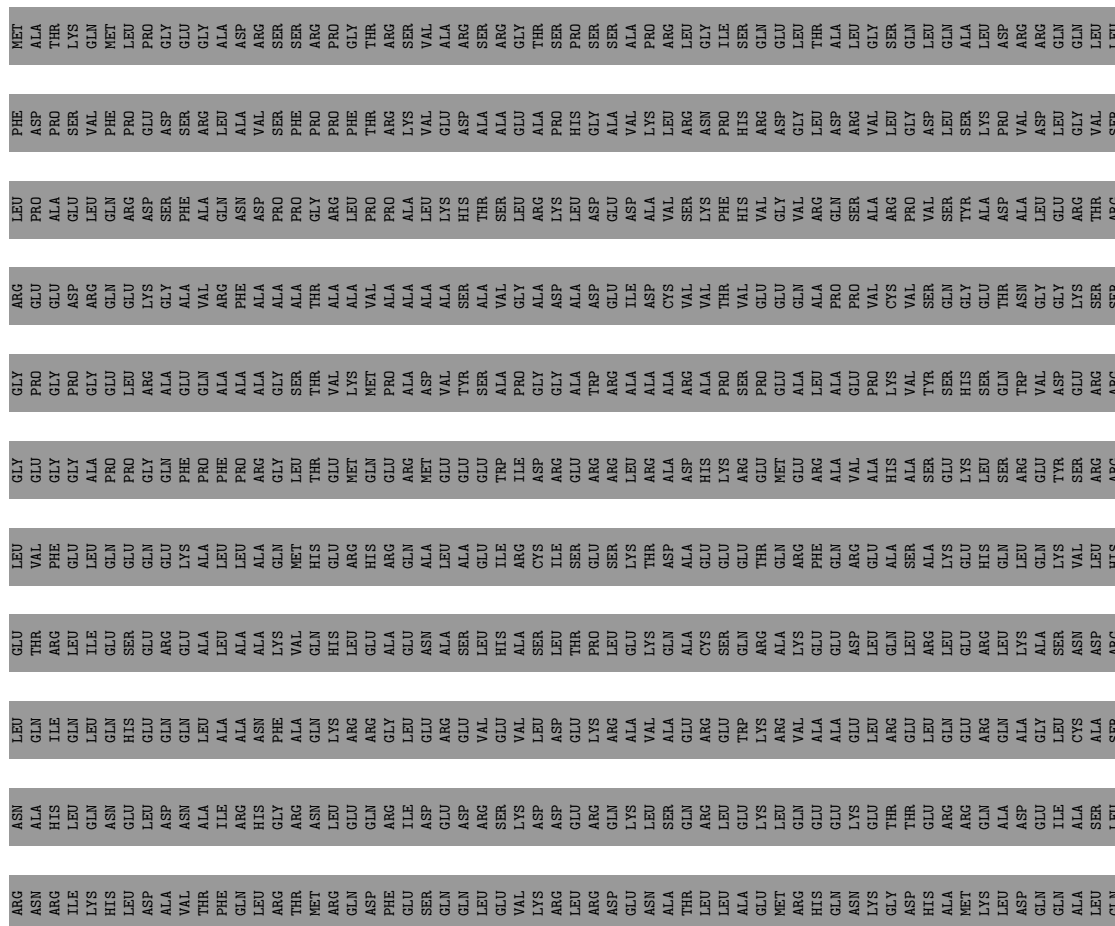
- Molecule 1: CF₂, TGME49_258090



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



- Molecule 1: CF₂, TGME49 258090





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

N954

Chain 0: 7% 91%

[illegible]

A horizontal timeline of the 1950s. It features a central green bar with yellow segments. The years 1940, 1941, 1945, 1949, 1952, 1953, and 1954 are marked. Above the timeline, there are red diamond shapes: one above 1941, and three above 1952, 1953, and 1954.

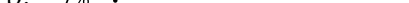
- Chain p:  7% 91%

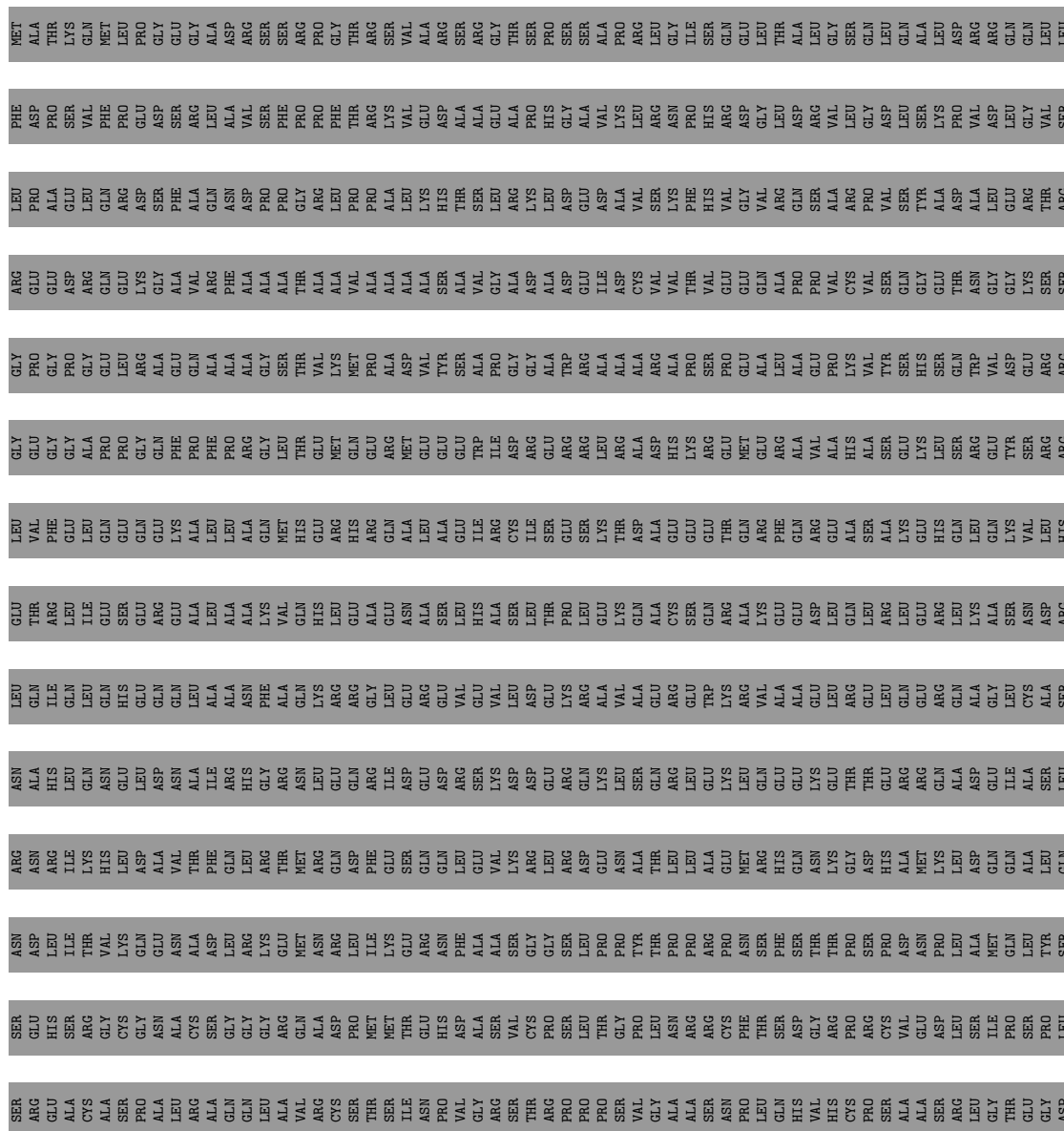


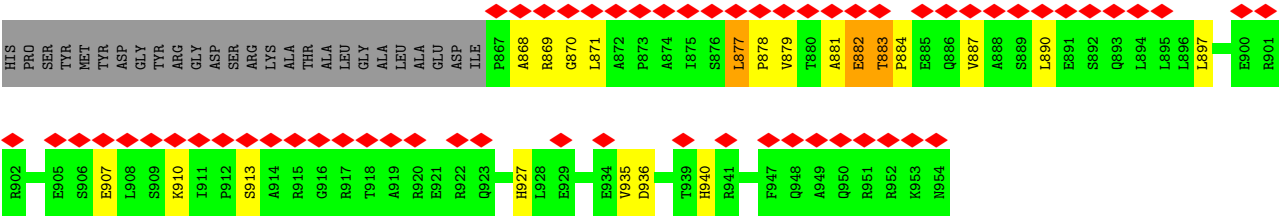
Diagram illustrating a 4x4 grid of colored squares (green, yellow, blue, red) and a corresponding 4x4 grid of colored diamonds (green, yellow, blue, red). The green squares are labeled R941, I942, K943, Q944. The yellow squares are labeled R951, R952, K953, N954. The blue squares are labeled R961, R962, K963, N964. The red squares are labeled R971, R972, K973, N974.

Chain r: 7% 91%

[illegible]

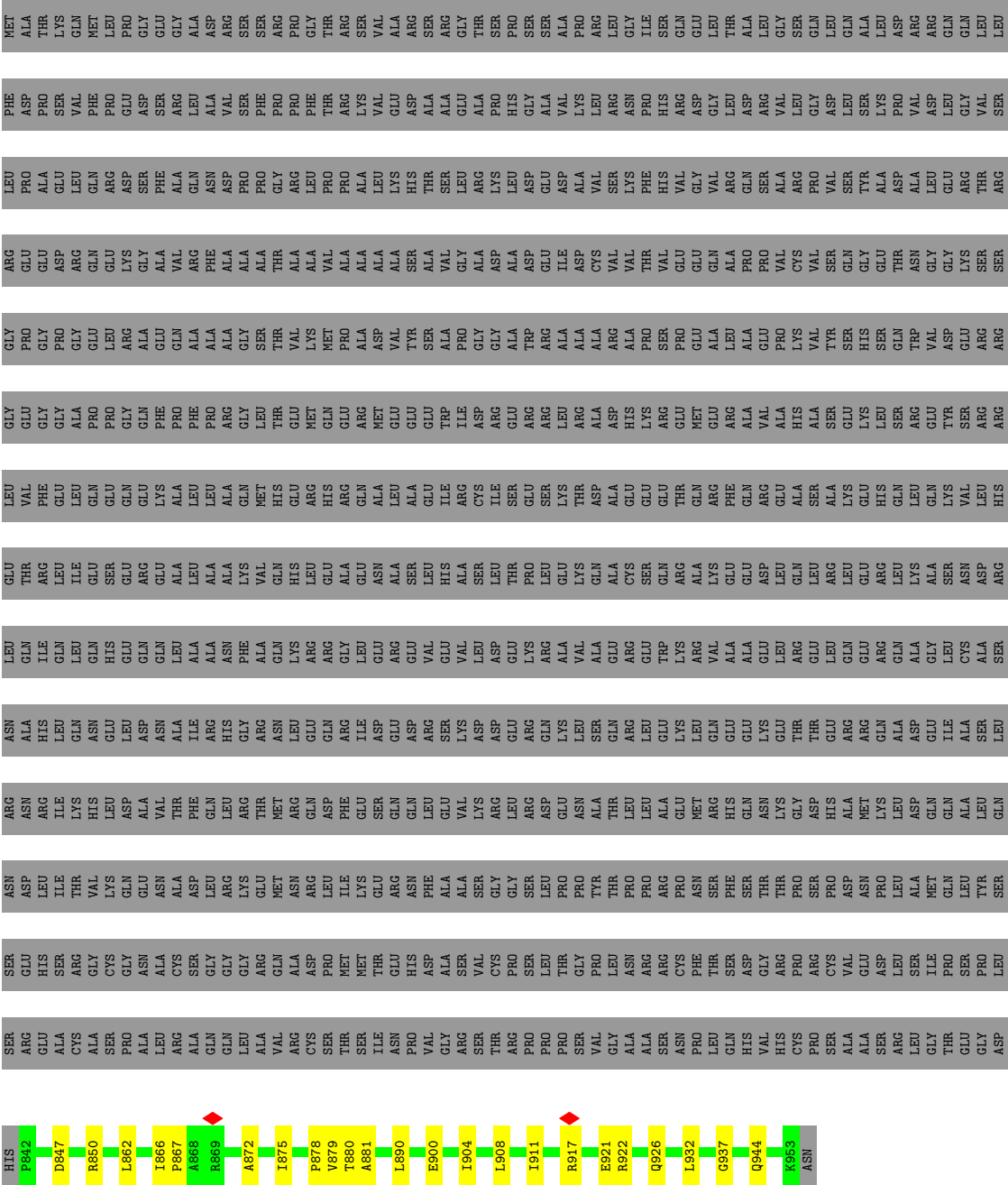
- Molecule 1: CF₂, TGME49_258090



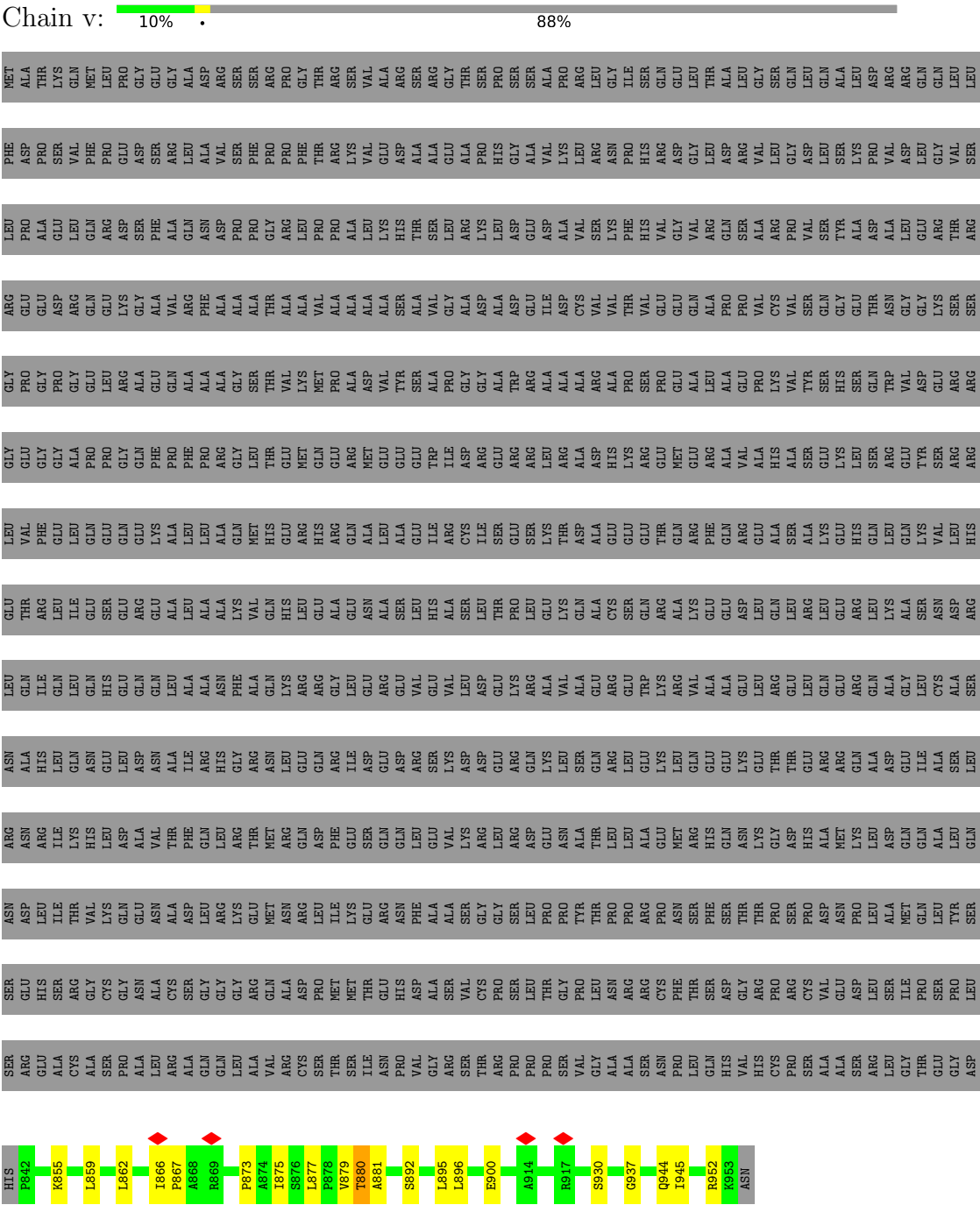


• Molecule 1: CF2, TGME49_258090

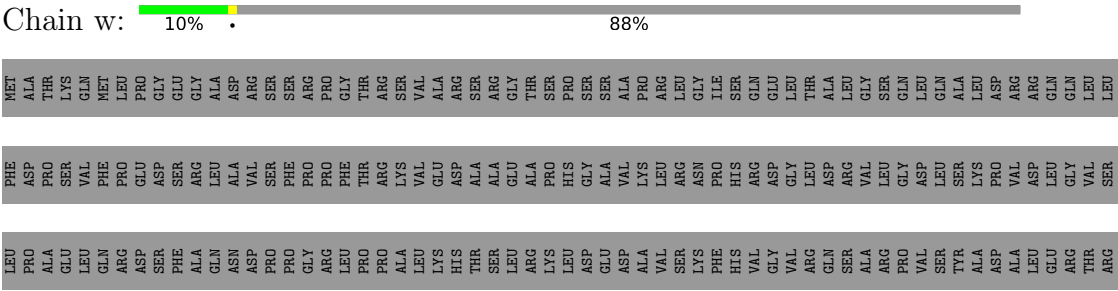
Chain u: 9% . 88%

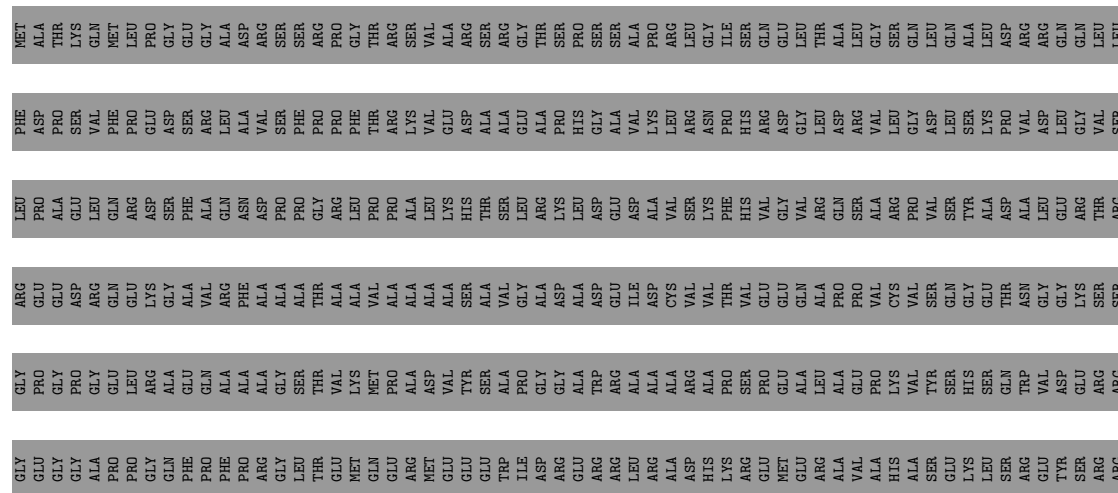


• Molecule 1: CF2, TGME49_258090



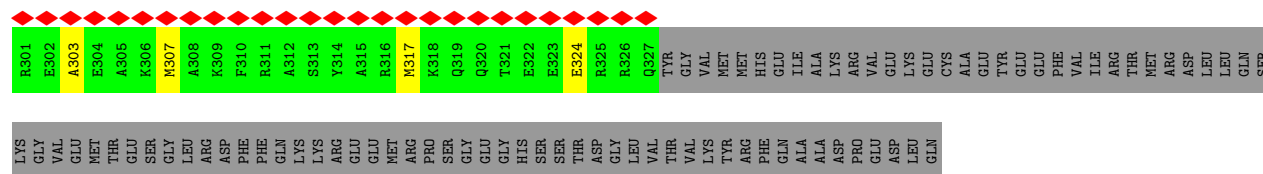
● Molecule 1: CF2, TGME49_258090



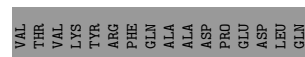
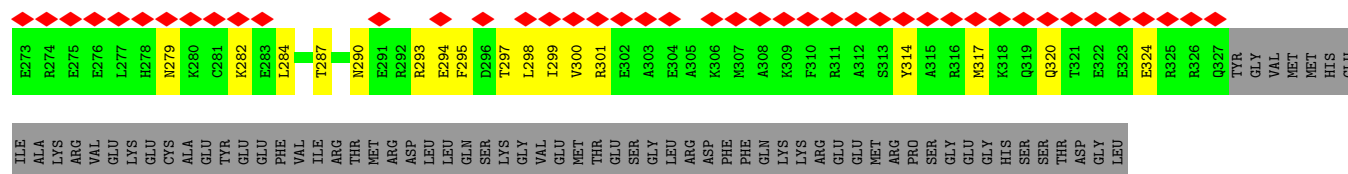
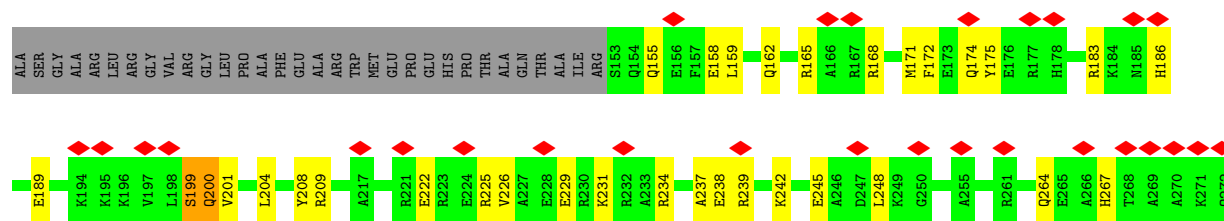
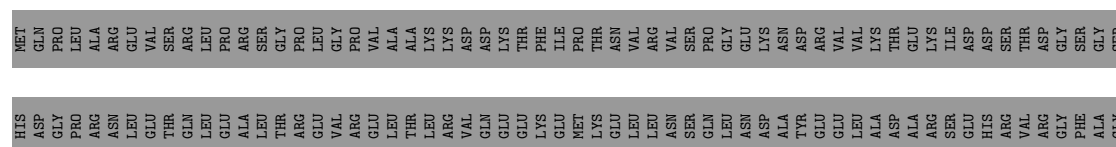
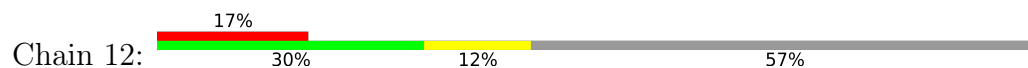


LEU	GLN	THR	GLU	LEU	GLY	GLY	PRO	GLY	ARG	LEU	PHE	MET
GLN	THR	ARG	THR	PHE	GLY	GLY	GLY	GLU	GLU	PRO	ASP	THR
LEU	GLN	LEU	LEU	GLU	GLY	PRO	GLY	GLY	ASP	GLU	SER	ALA
GLN	ILE	GLU	ILE	LEU	ALA	PRO	GLU	GLN	GLN	ARG	VAL	GLN
GLN	GLU	GLU	GLU	PRO	GLY	LEU	ARG	GLU	GLU	ARG	PHE	MET
HIS	SER	GLU	SER	PRO	GLY	LEU	GLY	LYS	GLY	ASP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

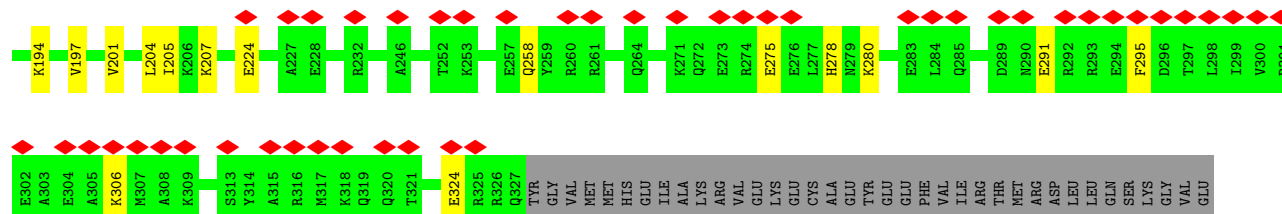
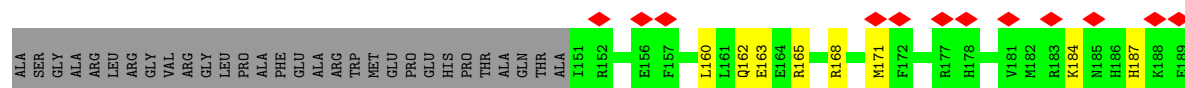
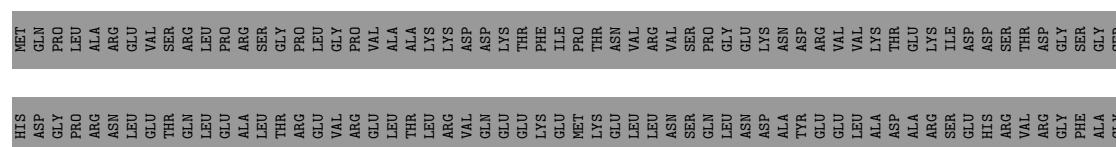
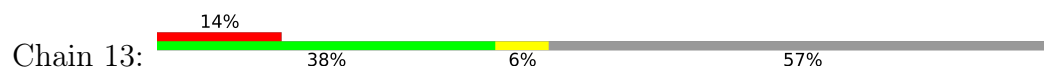




• Molecule 2: CF1, TGME49_222350

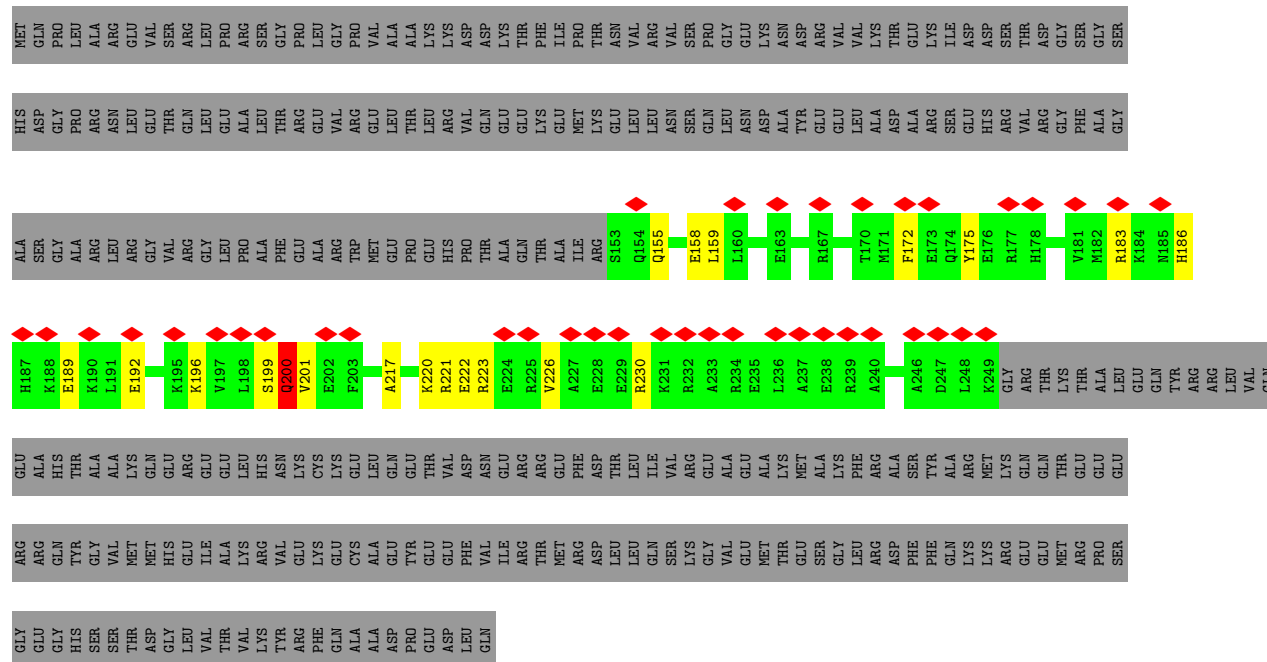


• Molecule 2: CF1, TGME49_222350

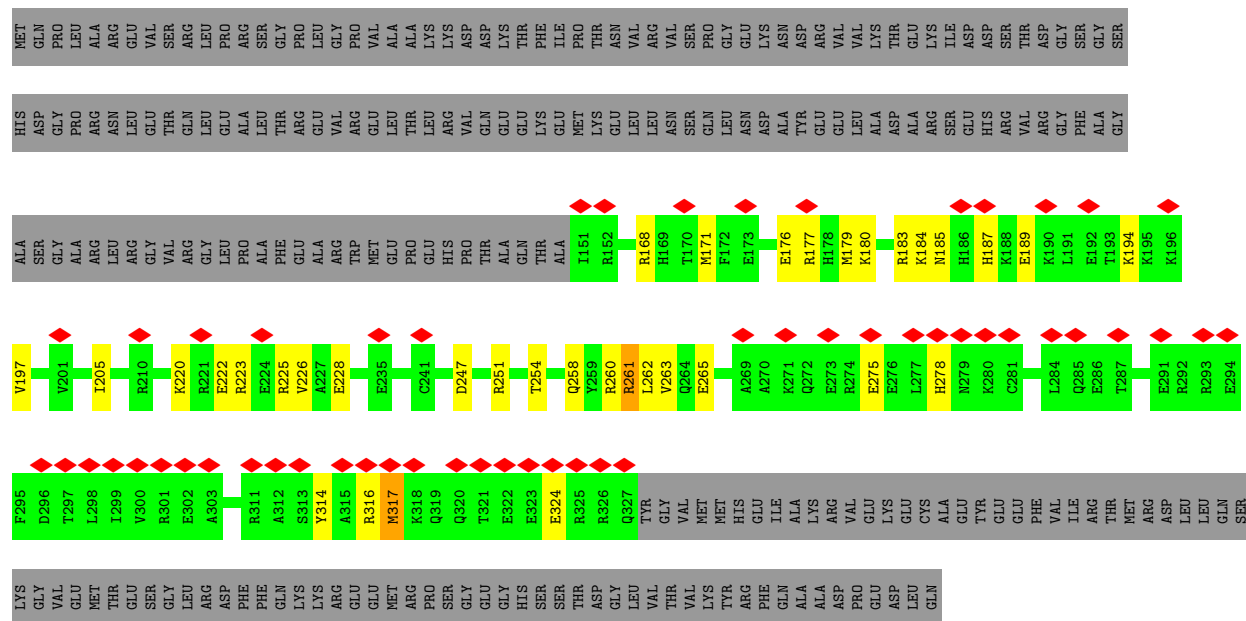
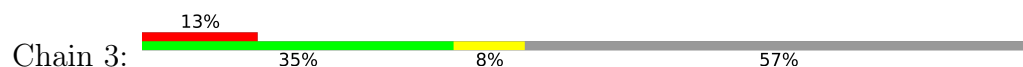




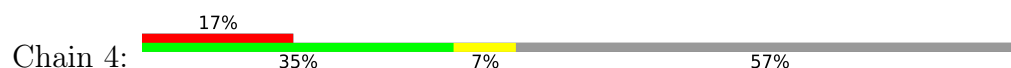
• Molecule 2: CF1, TGME49_222350

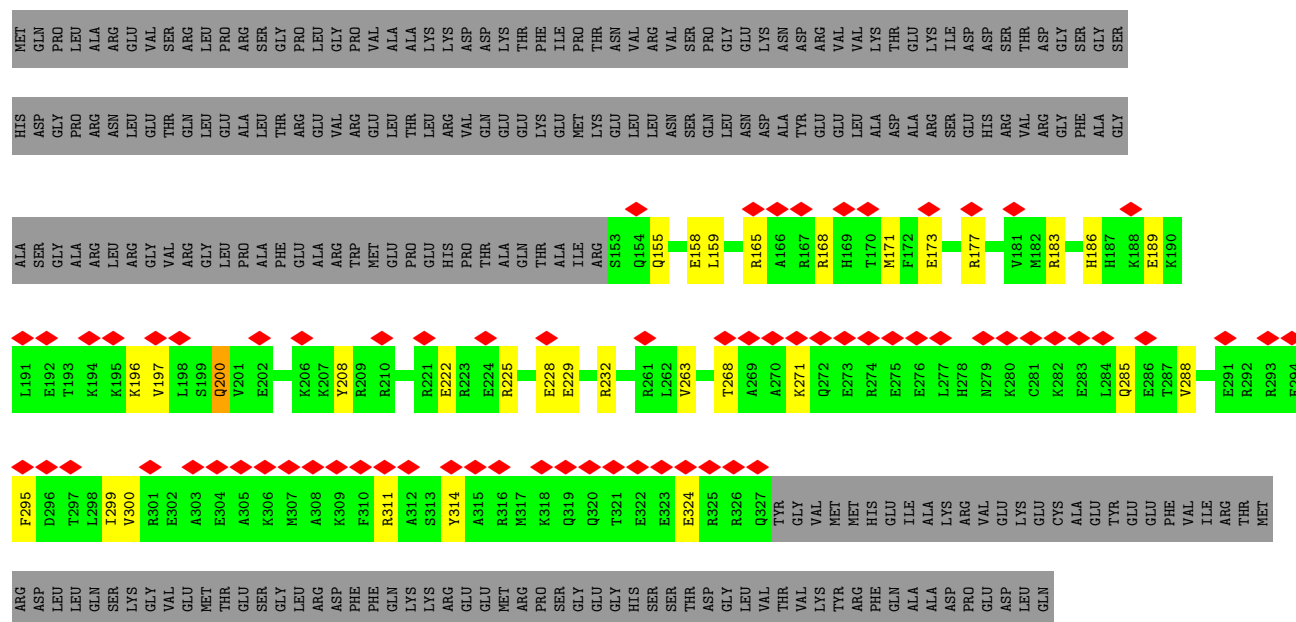


• Molecule 2: CF1, TGME49_222350

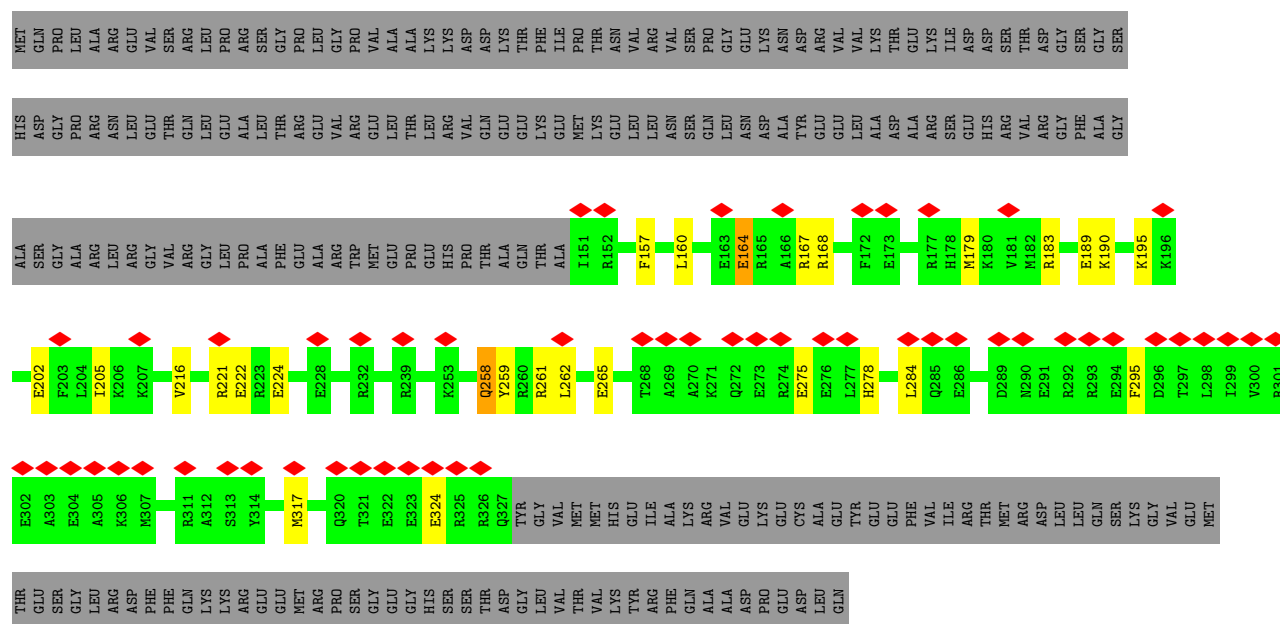
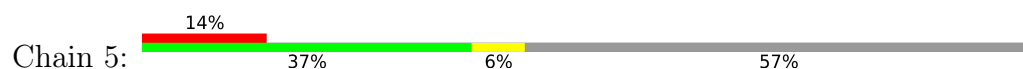


• Molecule 2: CF1, TGME49_222350

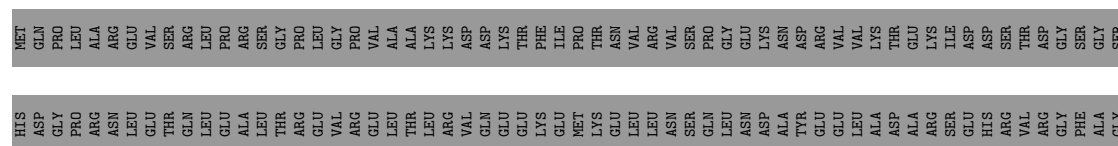
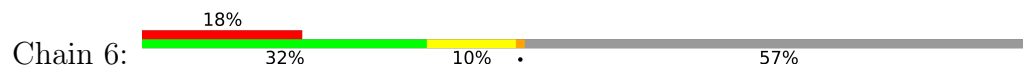


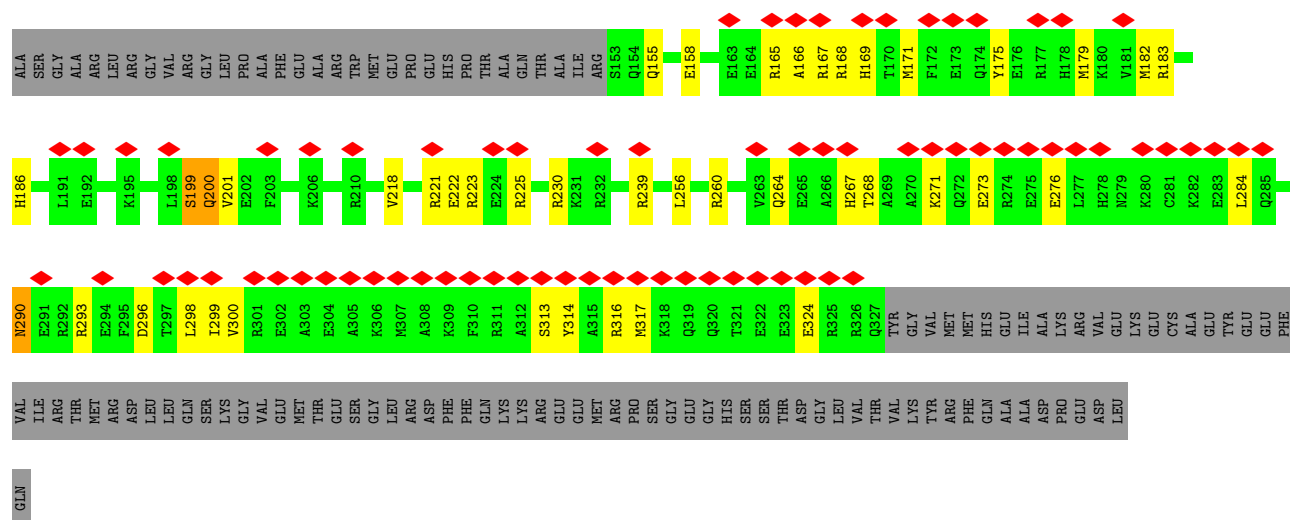


• Molecule 2: CF1, TGME49_222350

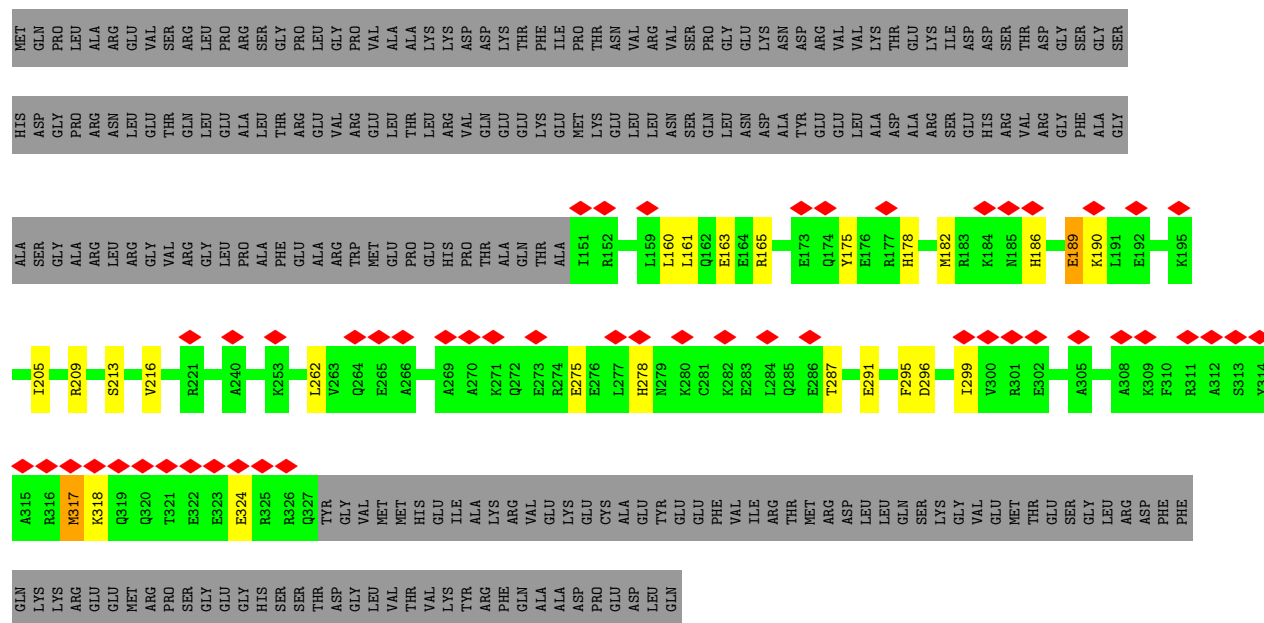
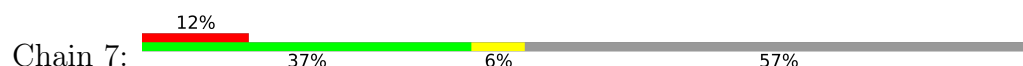


• Molecule 2: CF1, TGME49_222350

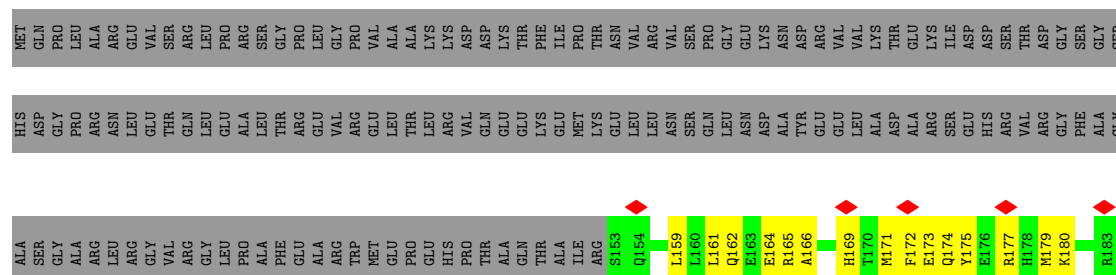
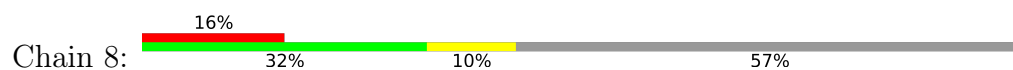


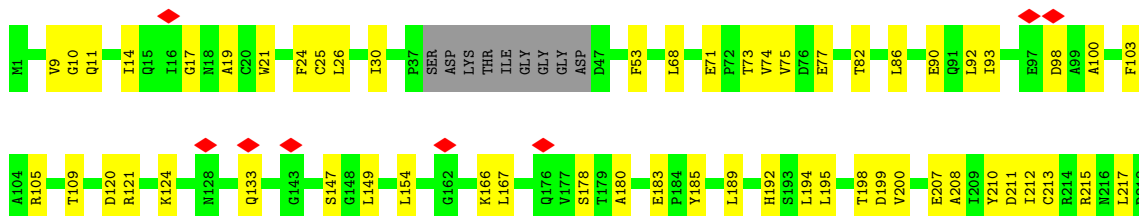


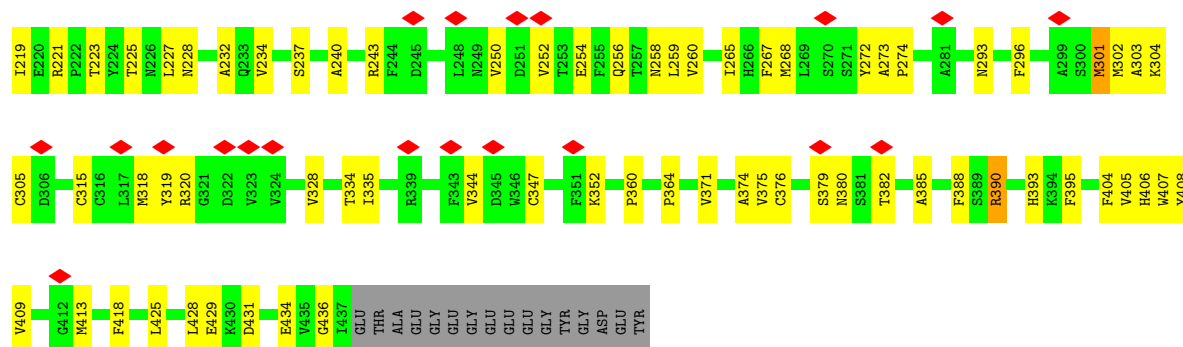
• Molecule 2: CF1, TGME49_222350



• Molecule 2: CF1, TGME49_222350

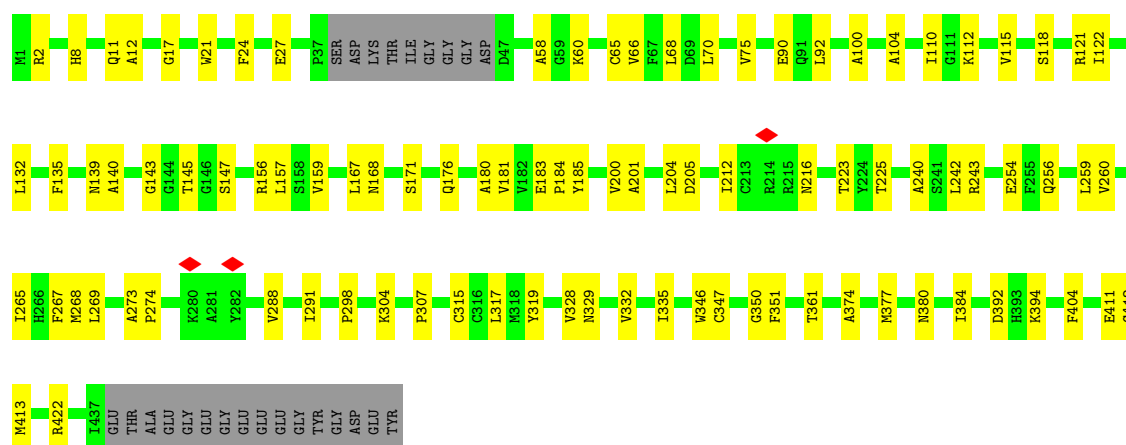






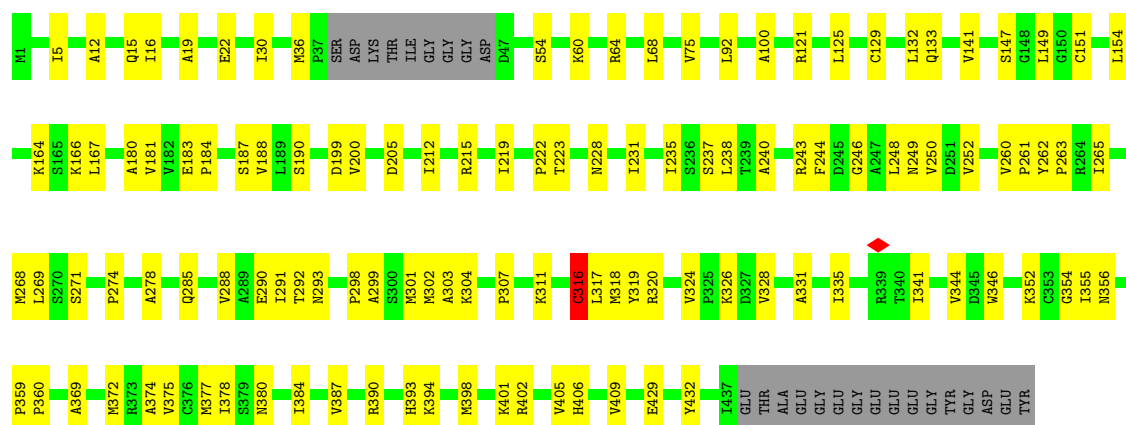
• Molecule 3: Tubulin alpha chain

Chain 1C: 74% 21% 6%



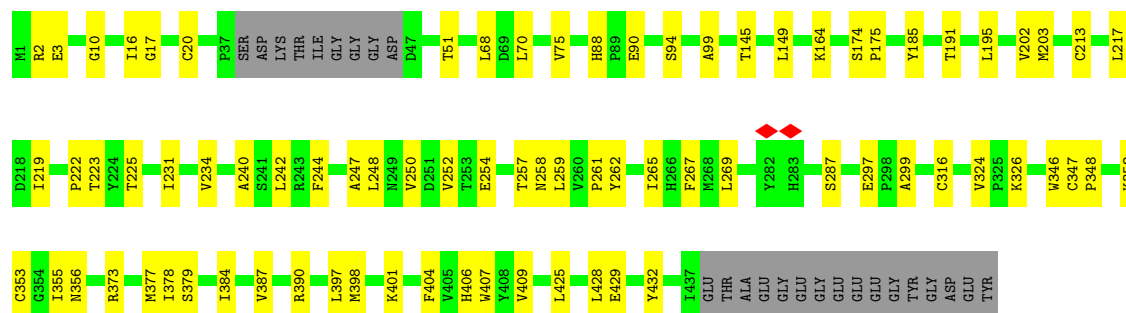
• Molecule 3: Tubulin alpha chain

Chain 1E: 68% 26% 6%



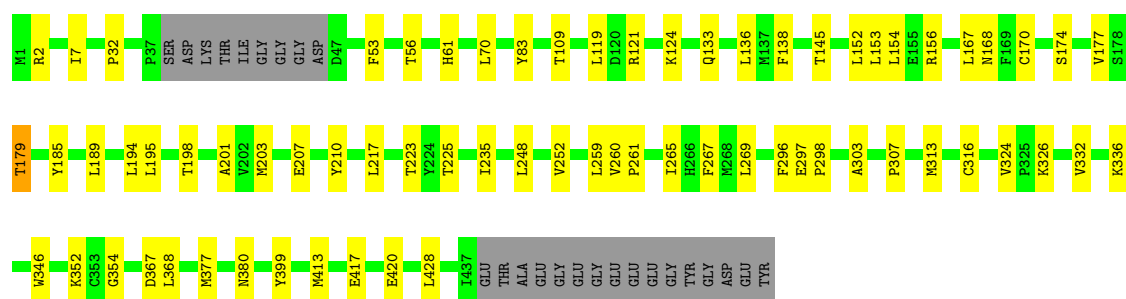
• Molecule 3: Tubulin alpha chain

Chain 1G: 77% 17% 6%



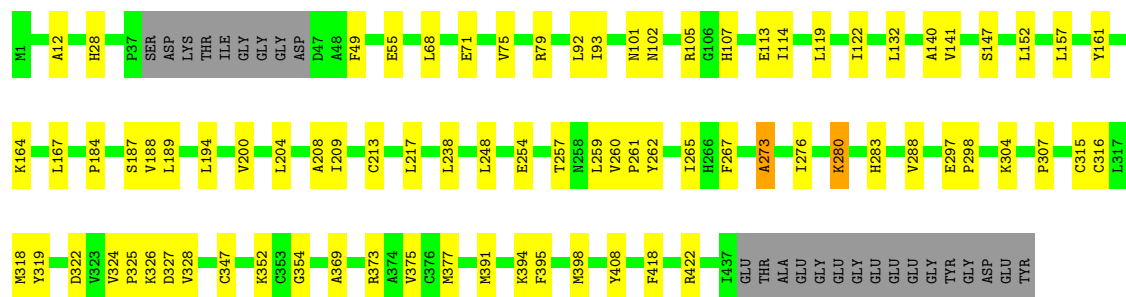
• Molecule 3: Tubulin alpha chain

Chain 1I: 79% 15% 6%



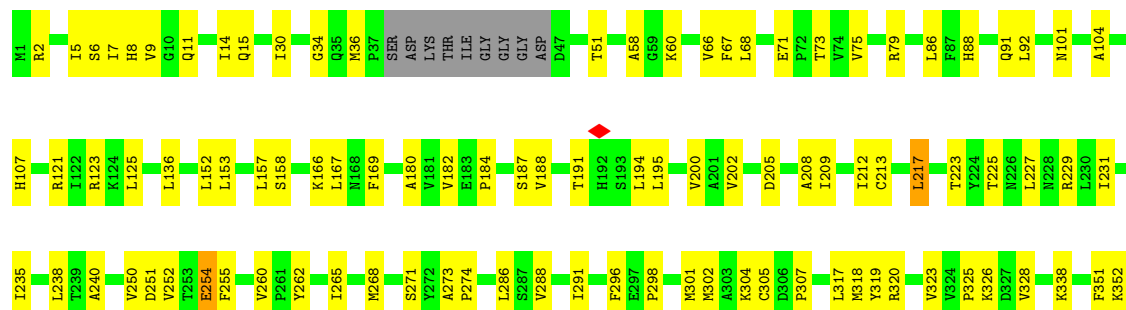
• Molecule 3: Tubulin alpha chain

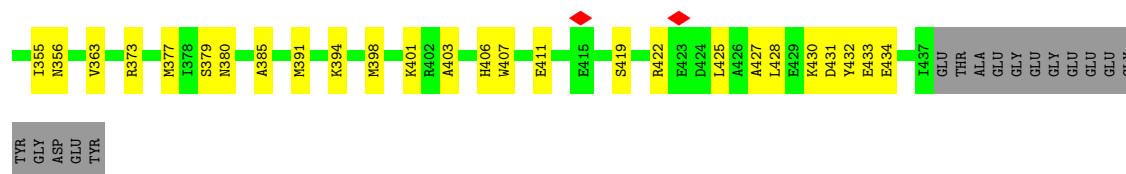
Chain 1K: 77% 17% 6%



• Molecule 3: Tubulin alpha chain

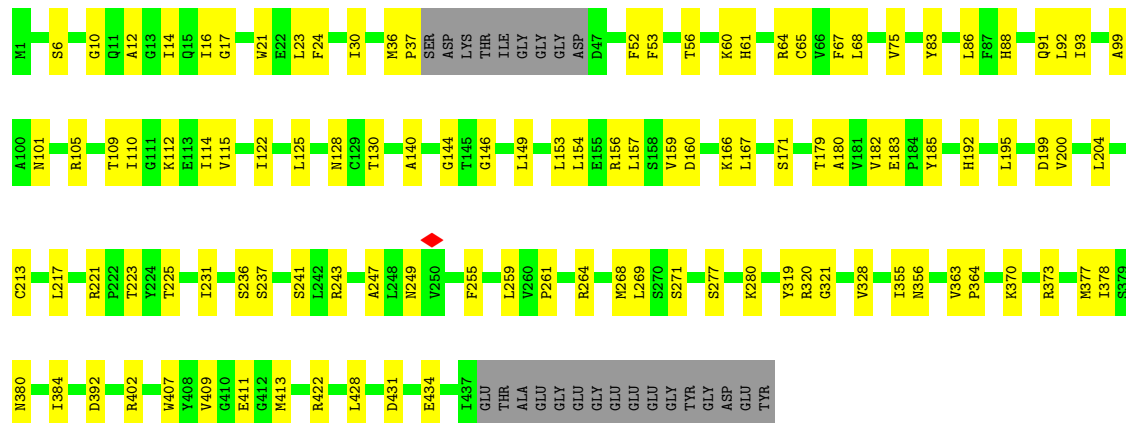
Chain 1M: 67% 27% 6%





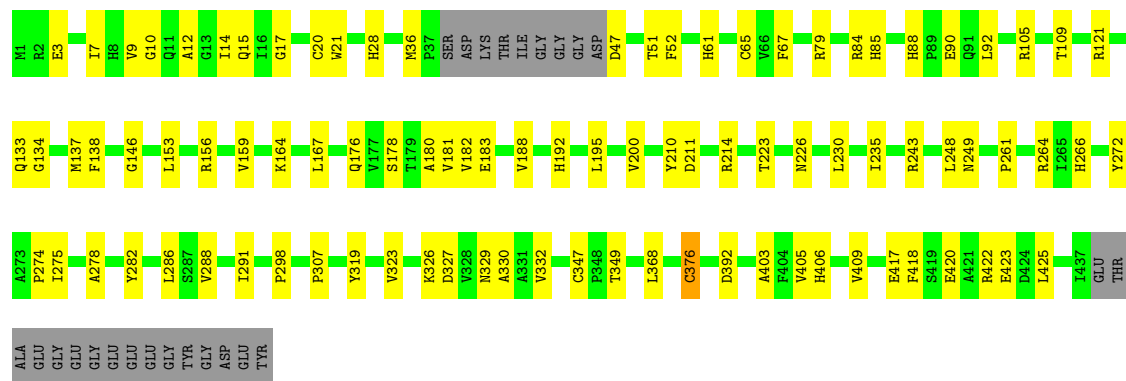
• Molecule 3: Tubulin alpha chain

Chain 2A:



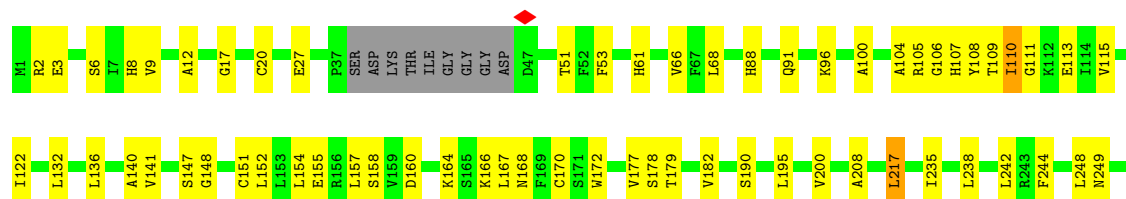
• Molecule 3: Tubulin alpha chain

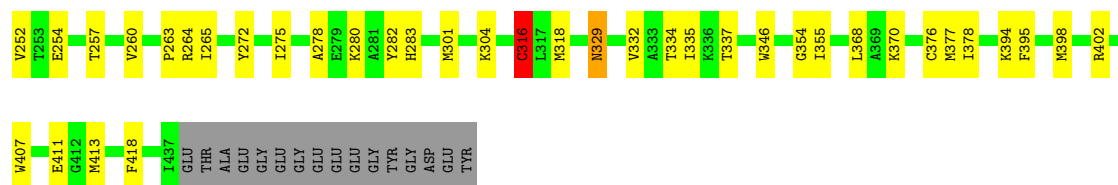
Chain 2C:



• Molecule 3: Tubulin alpha chain

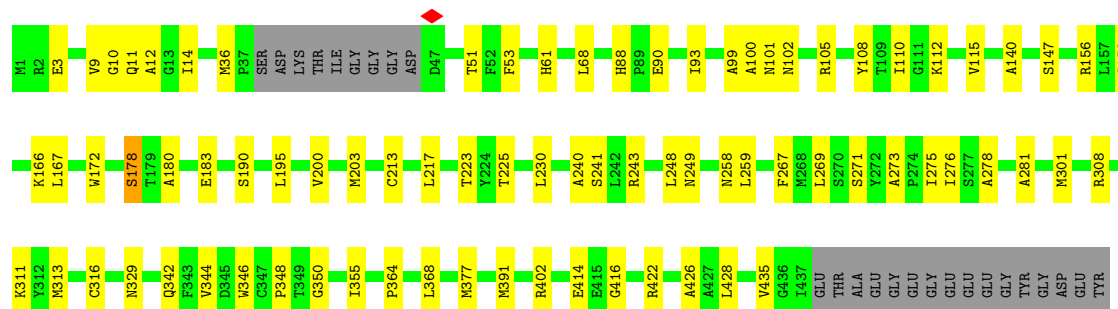
Chain 2E:





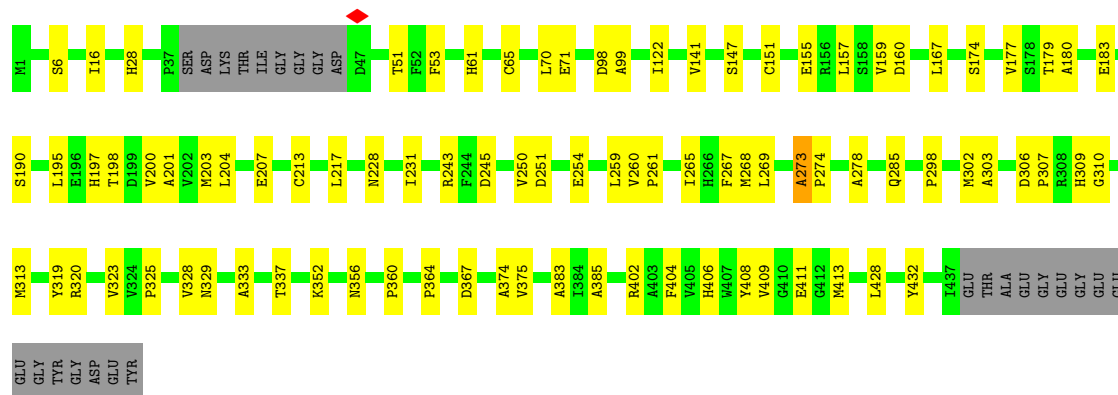
- Molecule 3: Tubulin alpha chain

Chain 2G:



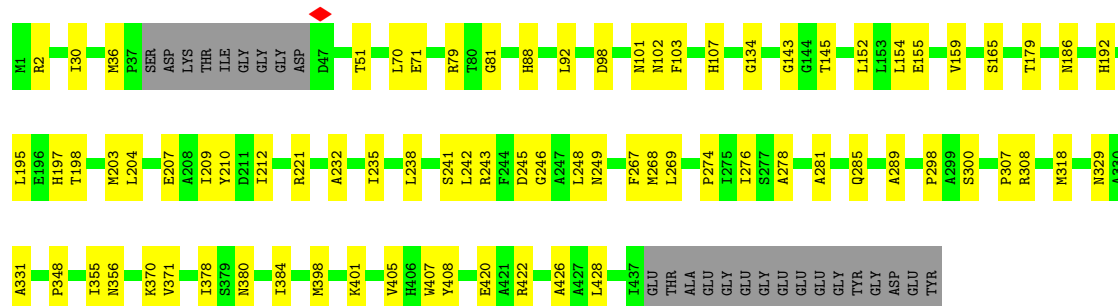
- Molecule 3: Tubulin alpha chain

Chain 2I:

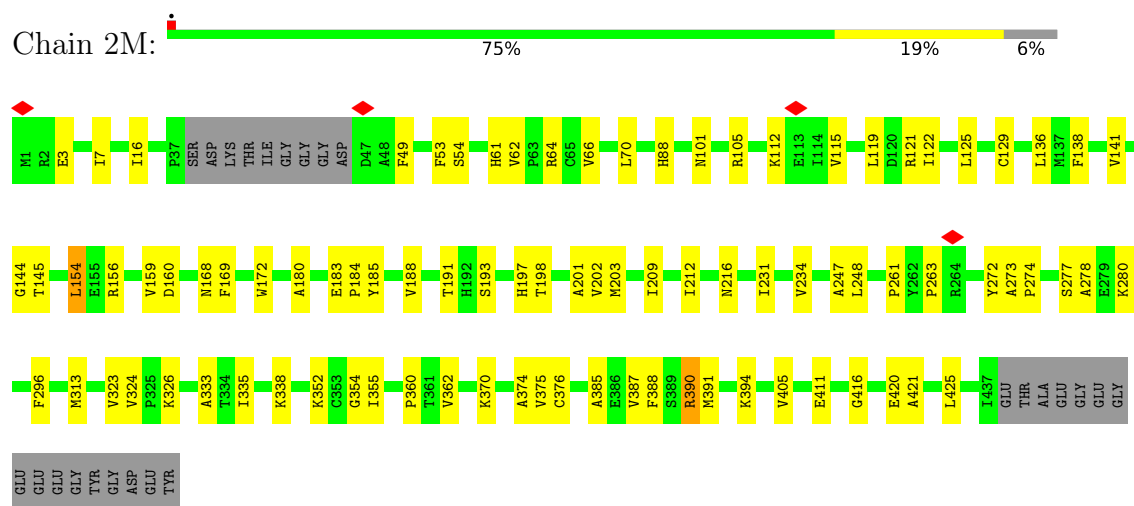


- Molecule 3: Tubulin alpha chain

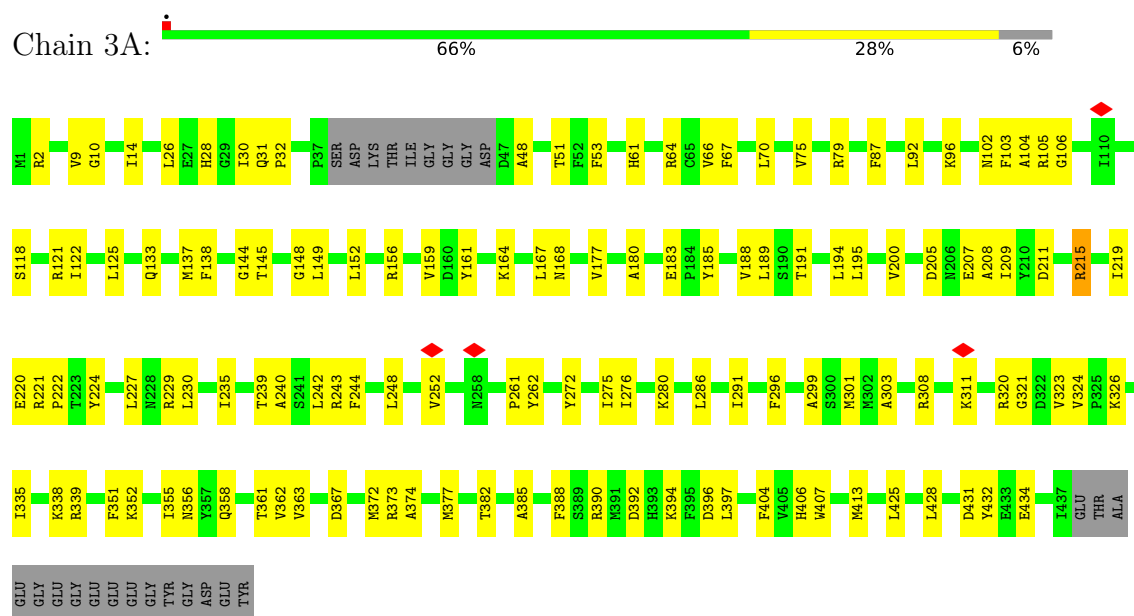
Chain 2K:



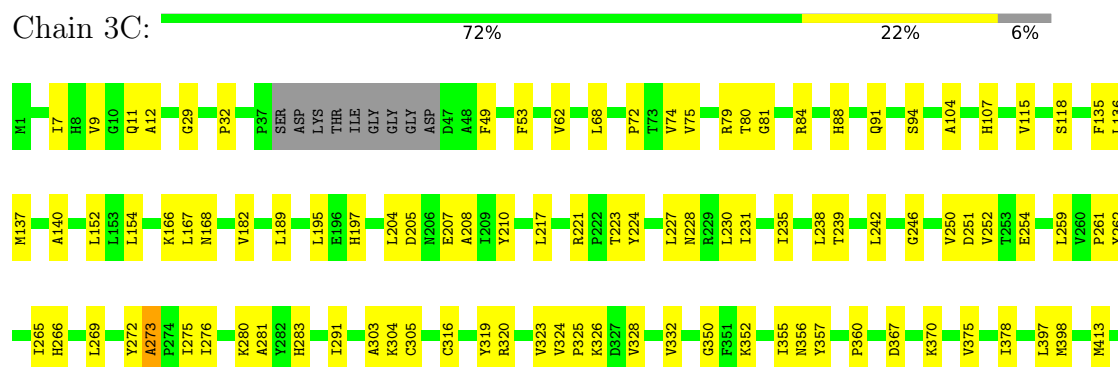
- Molecule 3: Tubulin alpha chain

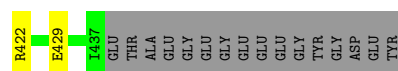


- Molecule 3: Tubulin alpha chain



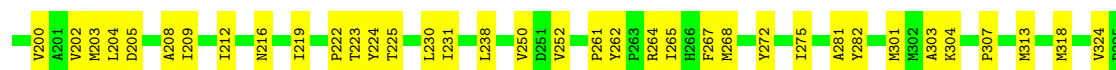
- Molecule 3: Tubulin alpha chain





- Molecule 3: Tubulin alpha chain

Chain 3E: 78% 16% 6%



- Molecule 3: Tubulin alpha chain

Chain 3G: 83% 11% 6%



- Molecule 3: Tubulin alpha chain

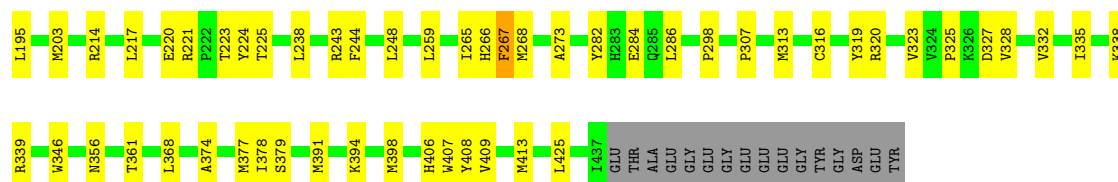
Chain 3I: 79% 15% 6%



- Molecule 3: Tubulin alpha chain

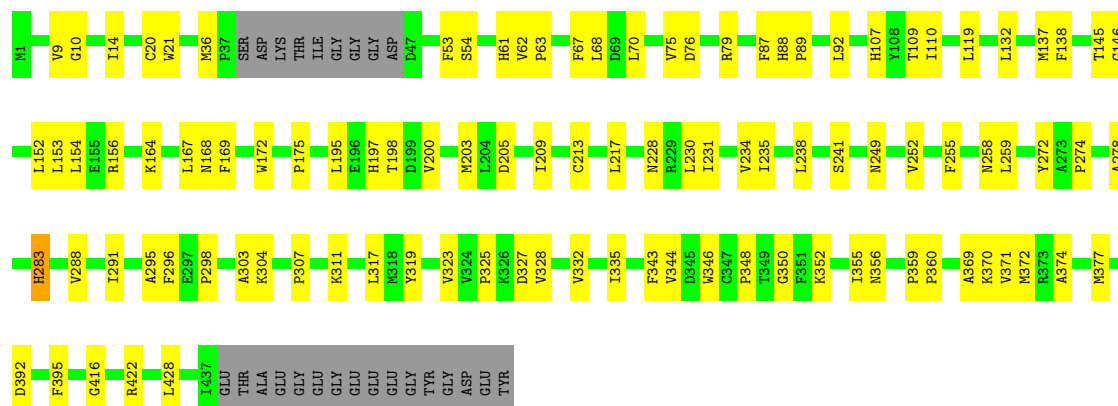
Chain 3K: 77% 17% 6%





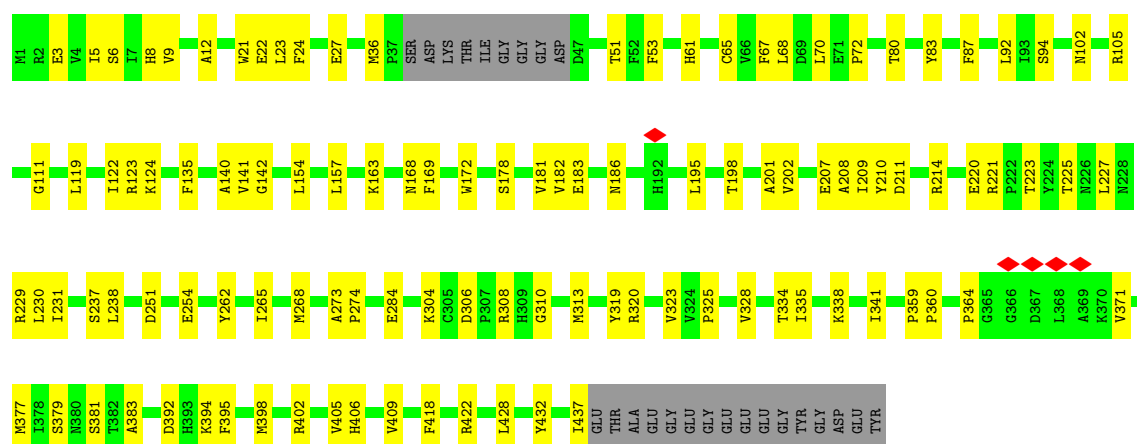
• Molecule 3: Tubulin alpha chain

Chain 3M: 72% 23% 6%



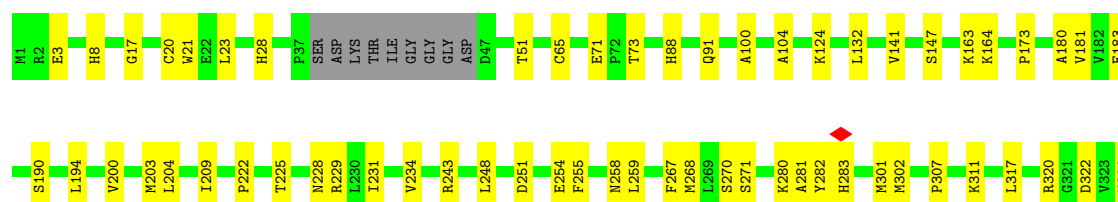
• Molecule 3: Tubulin alpha chain

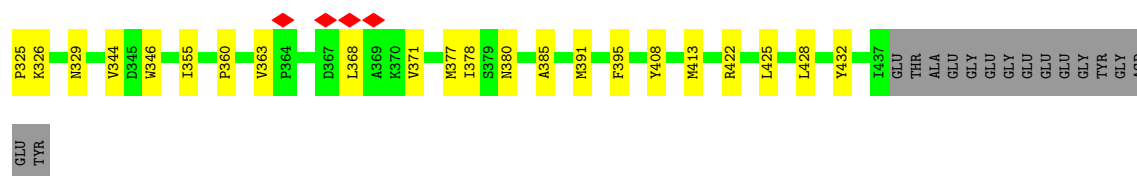
Chain 4A: 70% 24% 6%



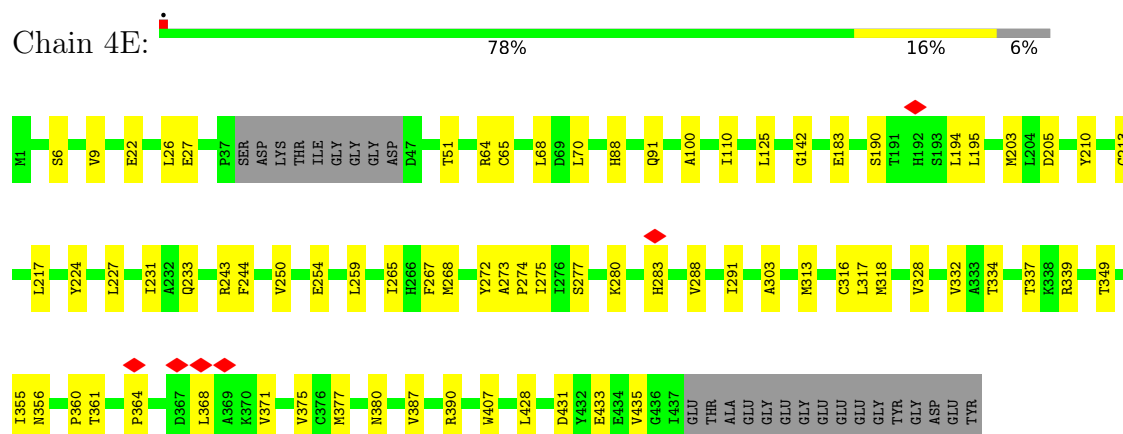
• Molecule 3: Tubulin alpha chain

Chain 4C: 76% 18% 6%

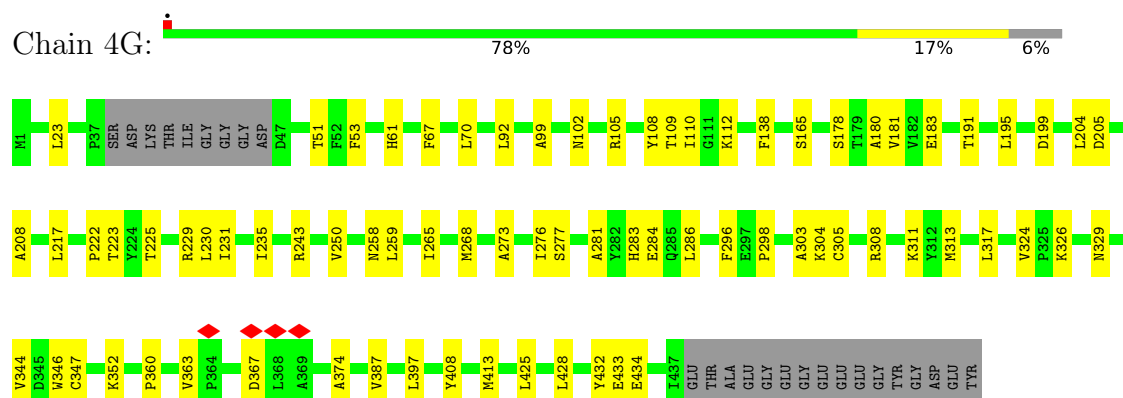




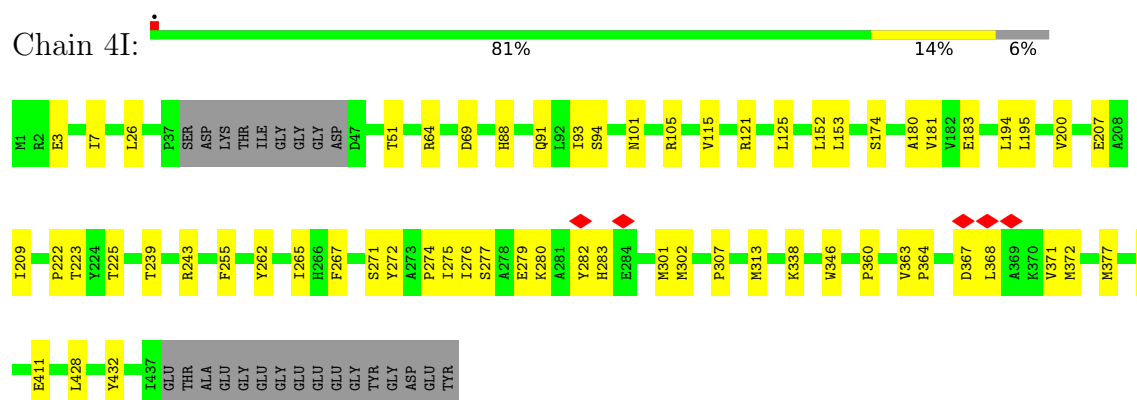
- Molecule 3: Tubulin alpha chain



- Molecule 3: Tubulin alpha chain

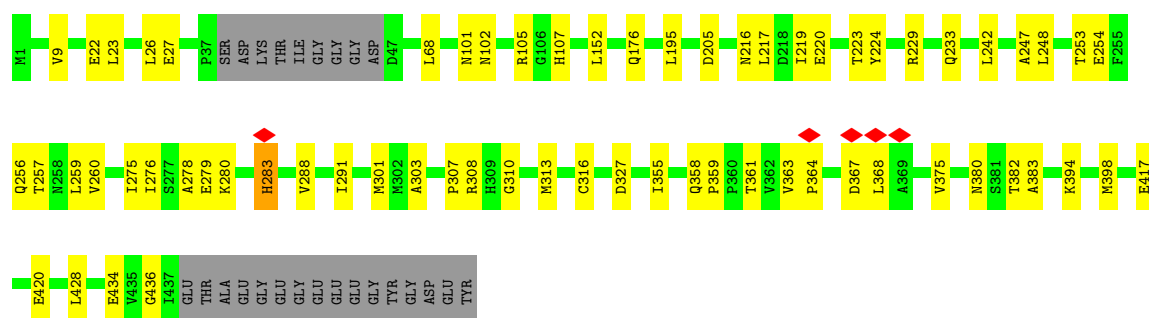


- Molecule 3: Tubulin alpha chain



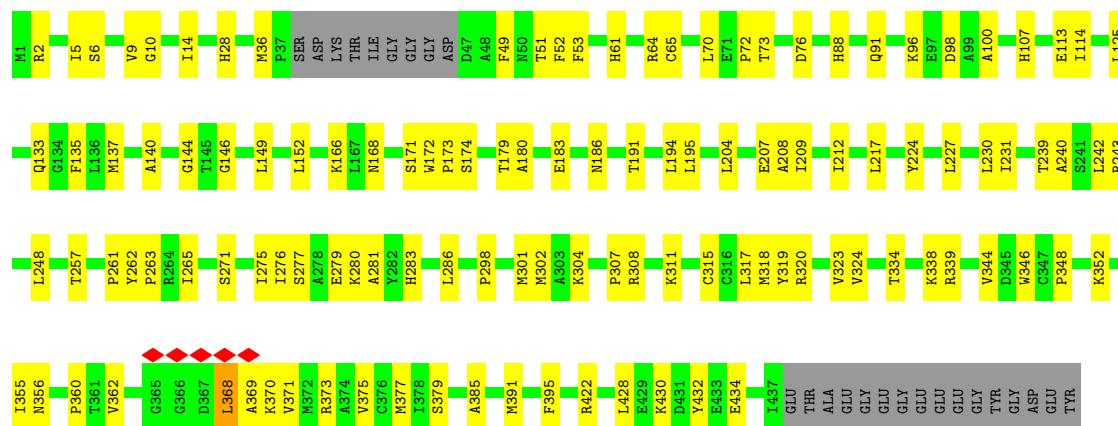
- Molecule 3: Tubulin alpha chain

Chain 4K: 



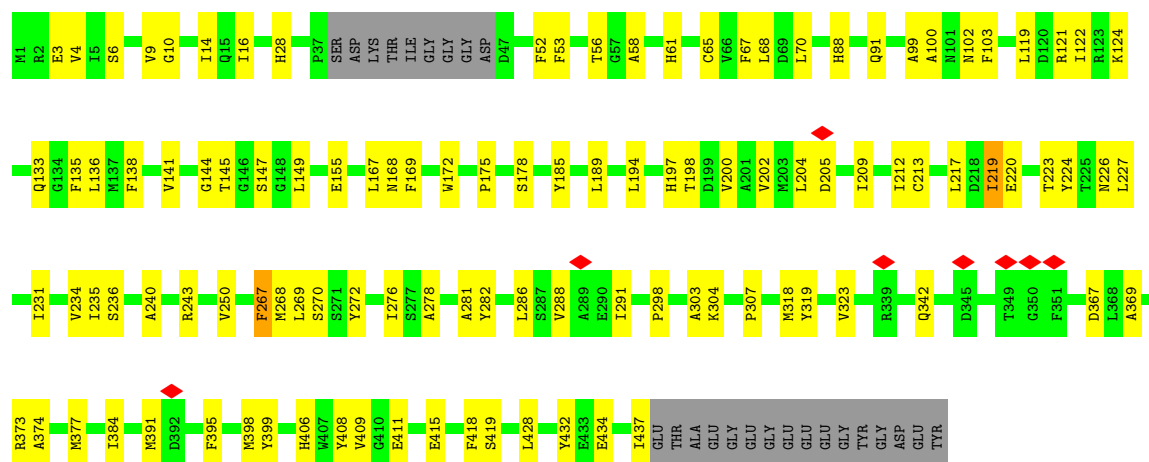
• Molecule 3: Tubulin alpha chain

Chain 4M: 



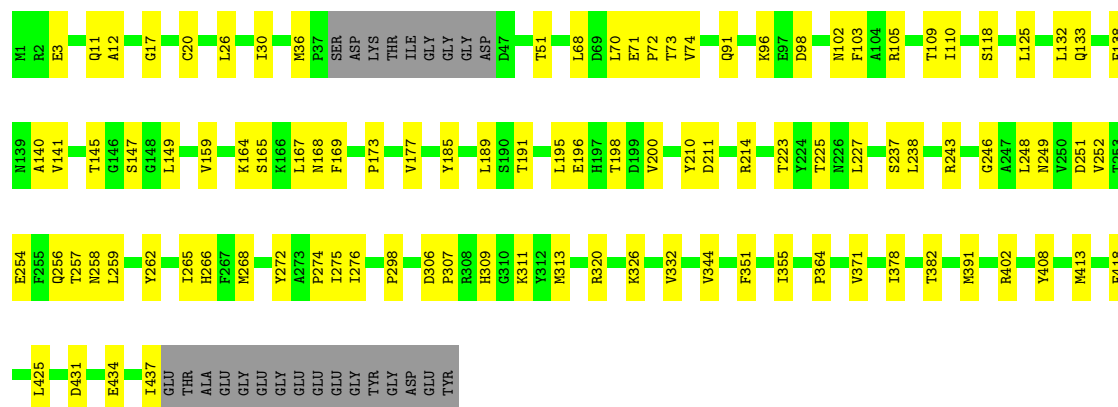
• Molecule 3: Tubulin alpha chain

Chain 5A: 



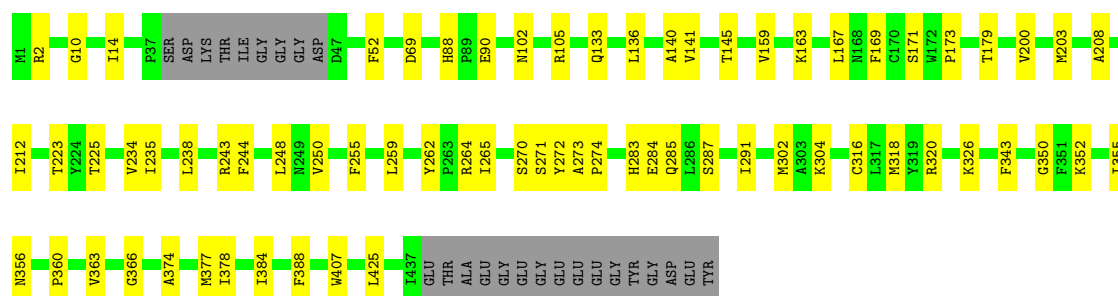
• Molecule 3: Tubulin alpha chain

Chain 5C: 



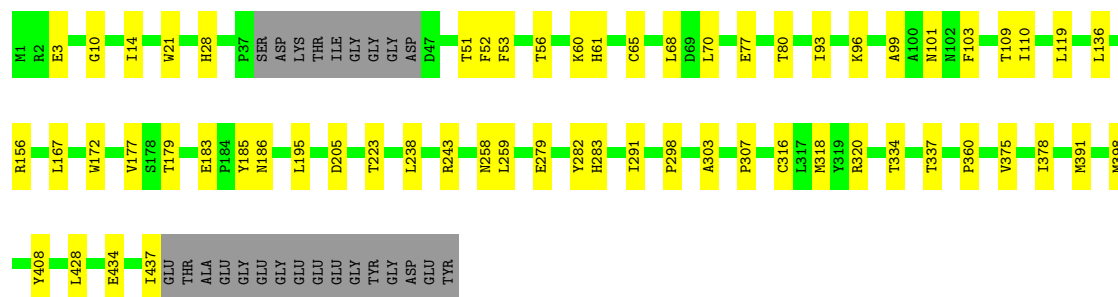
• Molecule 3: Tubulin alpha chain

Chain 5E: 79% 15% 6%



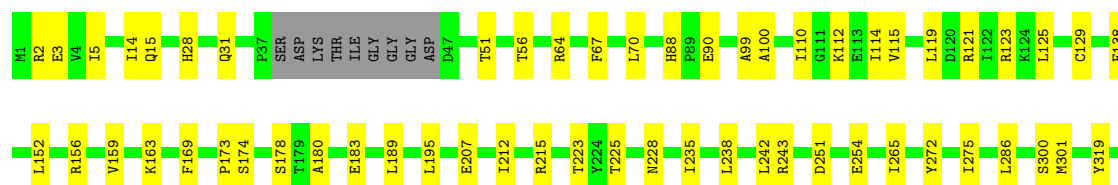
• Molecule 3: Tubulin alpha chain

Chain 5G: 81% 13% 6%



• Molecule 3: Tubulin alpha chain

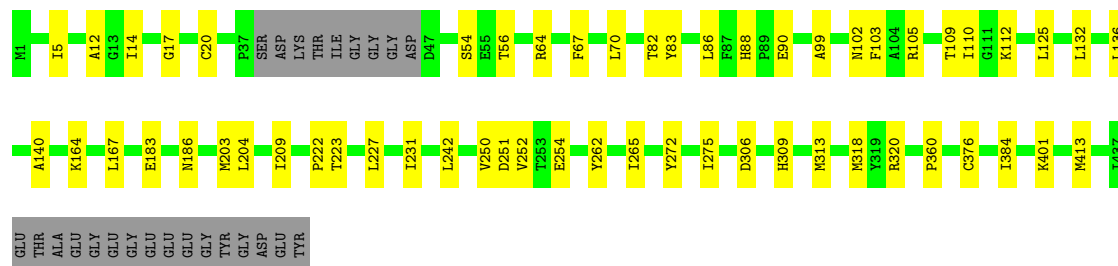
Chain 5I: 79% 16% 6%





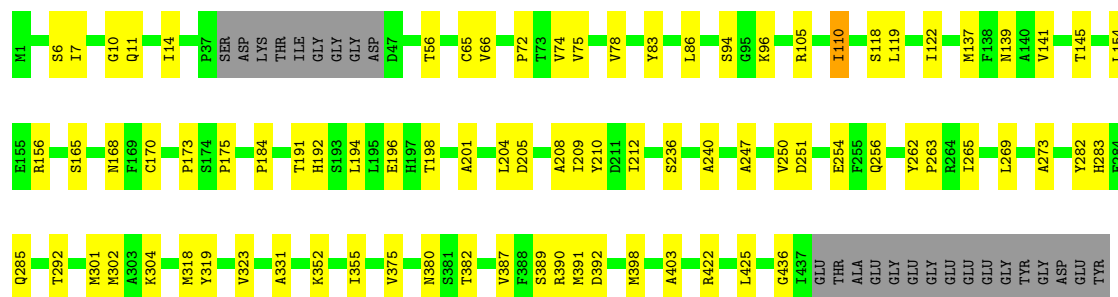
- Molecule 3: Tubulin alpha chain

Chain 5K: 82% 12% 6%



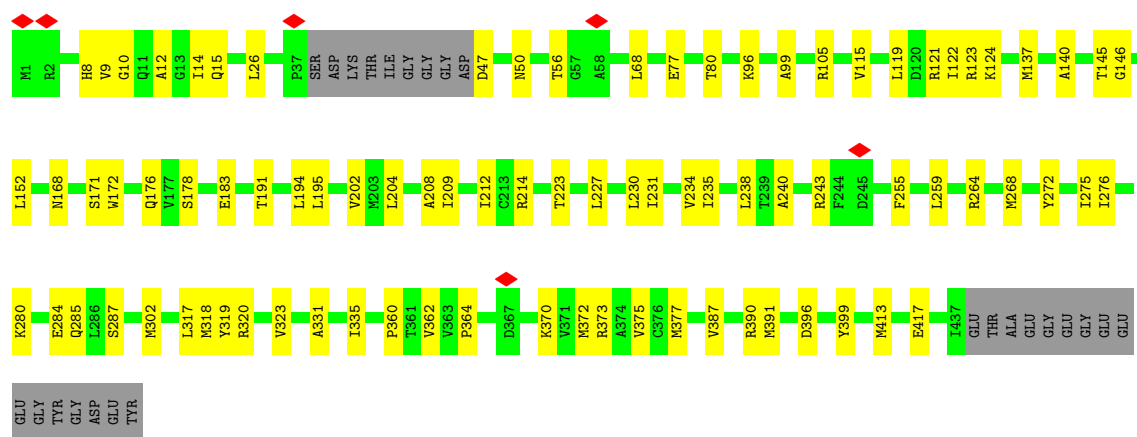
- Molecule 3: Tubulin alpha chain

Chain 5M: 76% 18% 6%



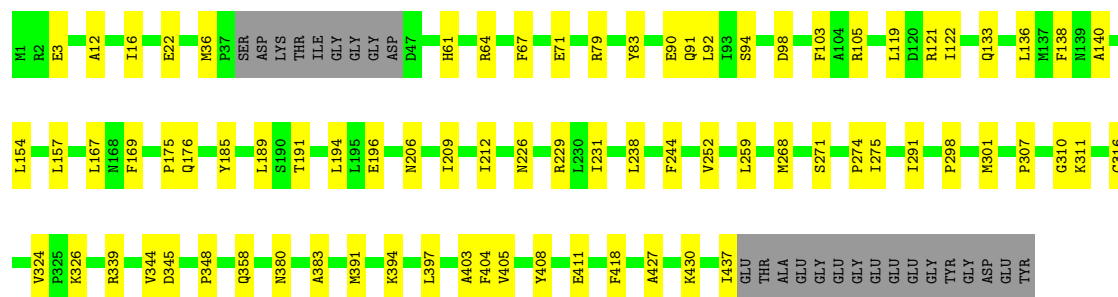
- Molecule 3: Tubulin alpha chain

Chain 6A: 76% 19% 6%



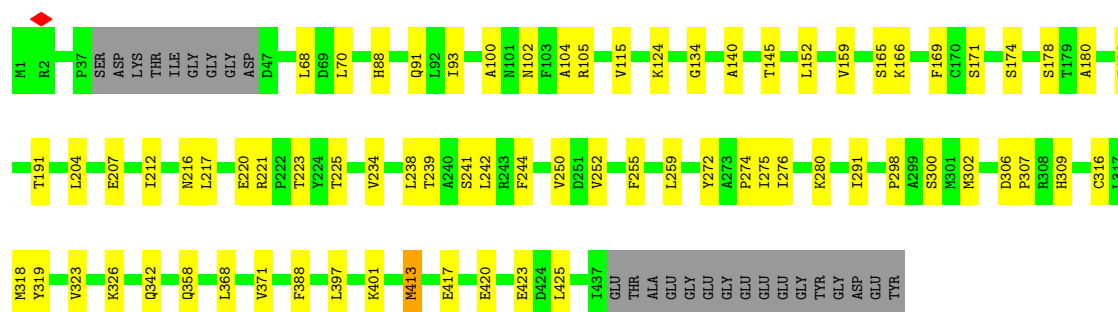
- Molecule 3: Tubulin alpha chain

Chain 6C: 77% 17% 6%



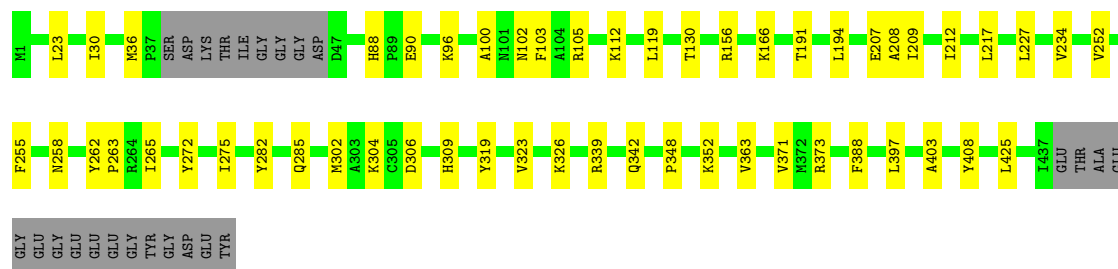
• Molecule 3: Tubulin alpha chain

Chain 6E: 78% 16% 6%



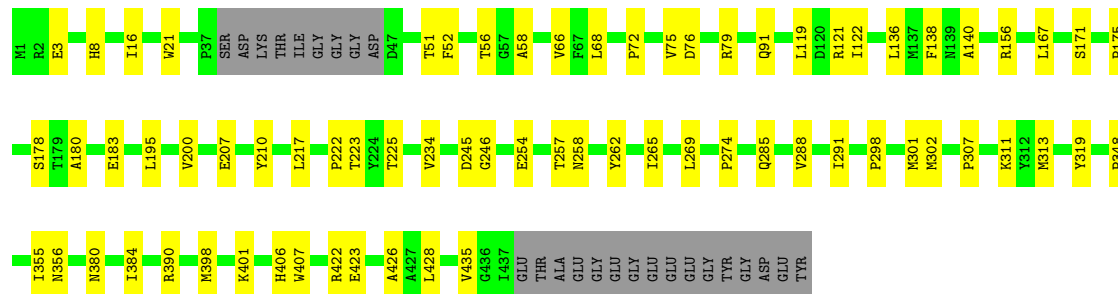
• Molecule 3: Tubulin alpha chain

Chain 6G: 83% 12% 6%



• Molecule 3: Tubulin alpha chain

Chain 6I: 79% 16% 6%

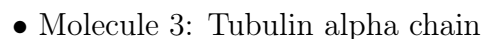


• Molecule 3: Tubulin alpha chain

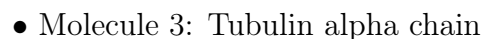
App Type	Percentage
Shopping app	80%
Social media app	15%
Productivity app	6%



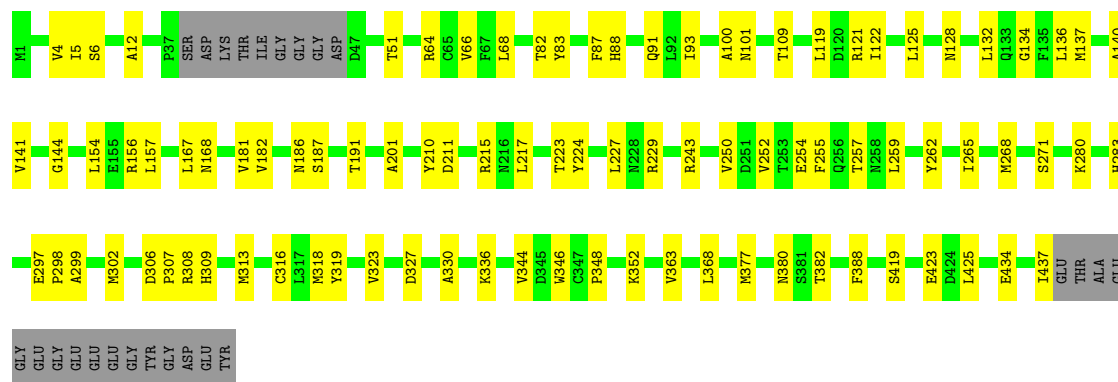
Response	Percentage
Yes, the U.S. is a democracy	66%
No, the U.S. is not a democracy	29%
Don't know	6%



Response	Percentage
Yes	80%
No	15%
Don't know	6%

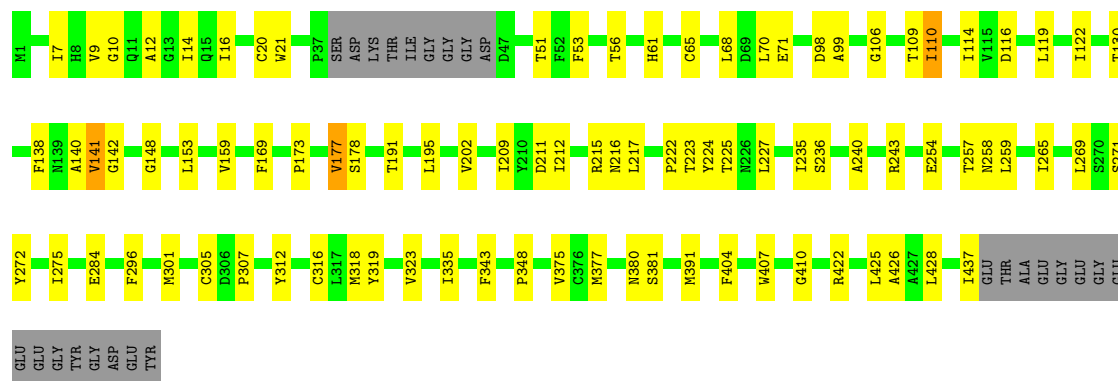


App Type	Percentage
Shopping app	74%
Social media app	20%
Productivity app	6%



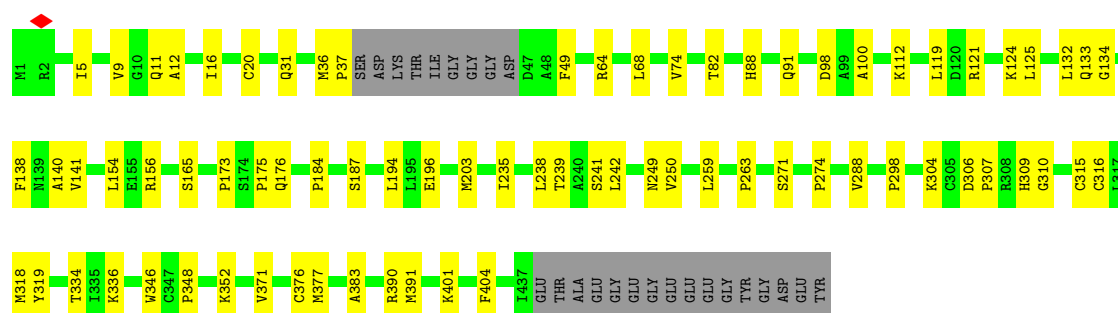
• Molecule 3: Tubulin alpha chain

Chain 7E: 75% 19% 6%



• Molecule 3: Tubulin alpha chain

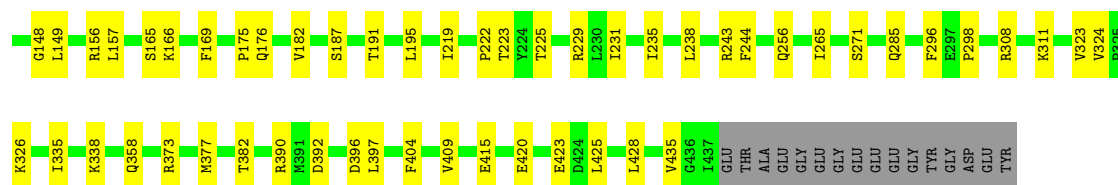
Chain 7G: 78% 17% 6%



• Molecule 3: Tubulin alpha chain

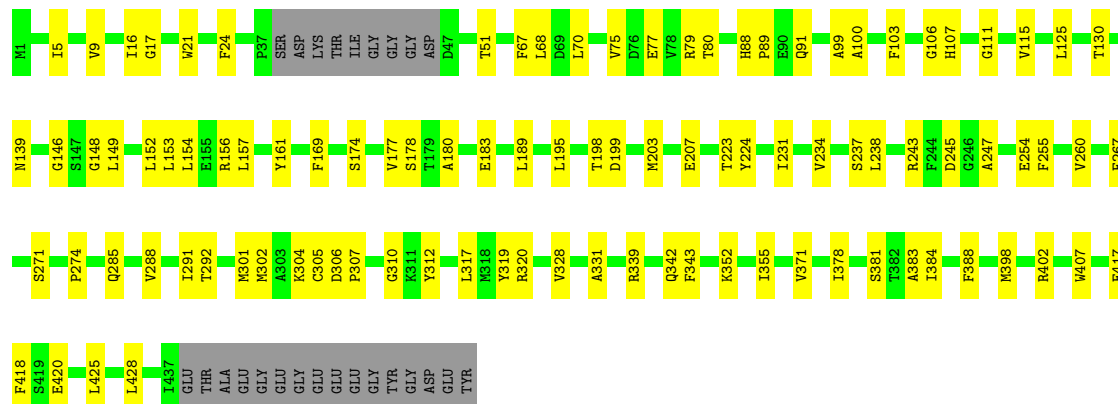
Chain 7I: 77% 17% 6%





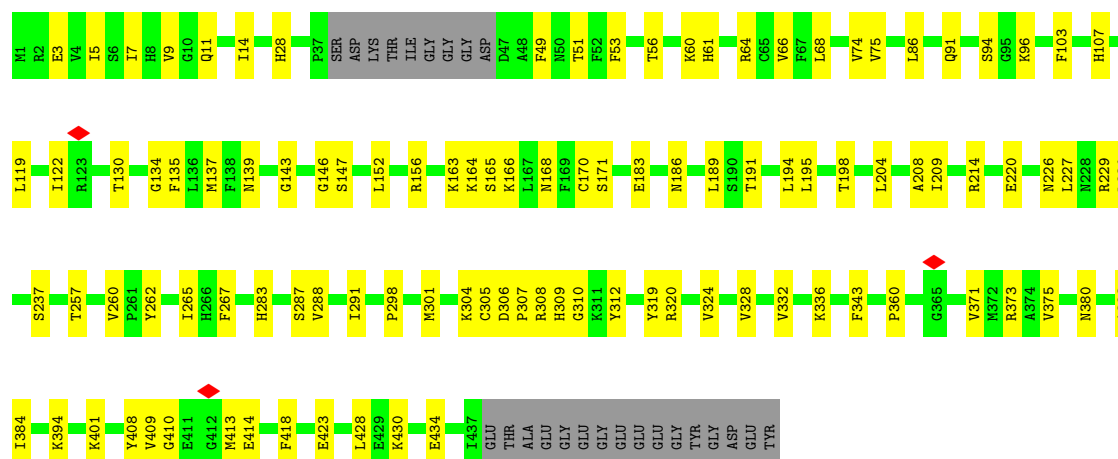
• Molecule 3: Tubulin alpha chain

Chain 7K: 73% 22% 6%



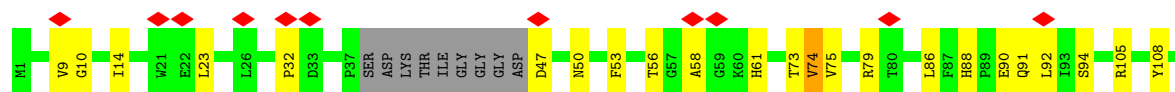
• Molecule 3: Tubulin alpha chain

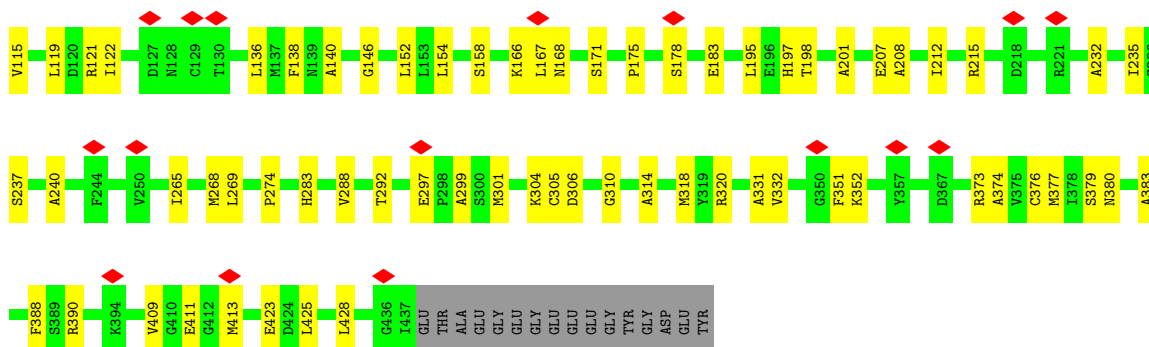
Chain 7M: 71% 23% 6%



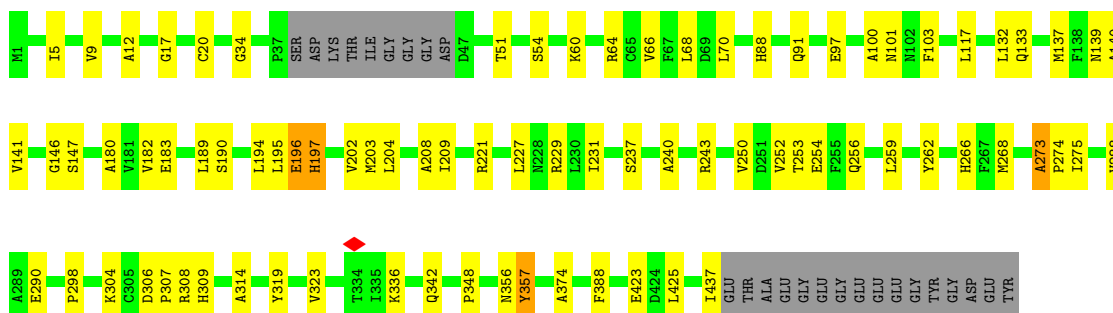
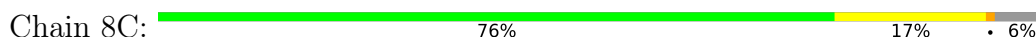
• Molecule 3: Tubulin alpha chain

Chain 8A: 6% 75% 19% 6%

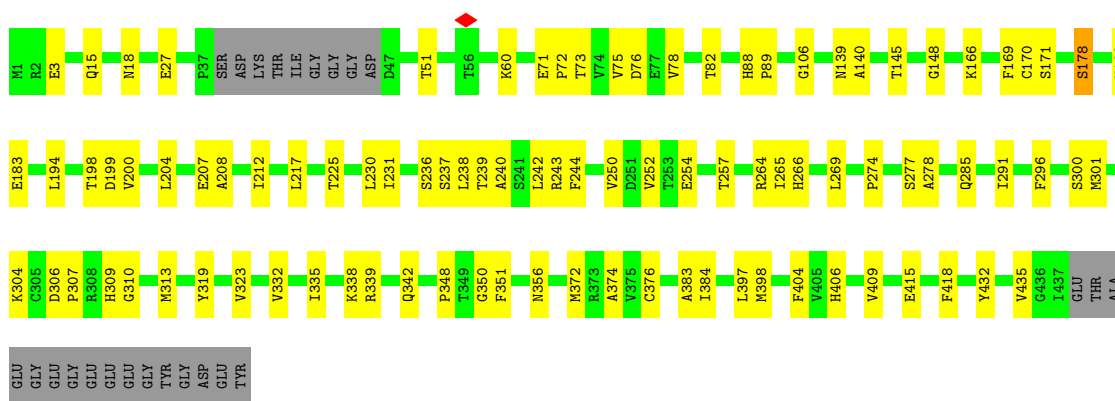




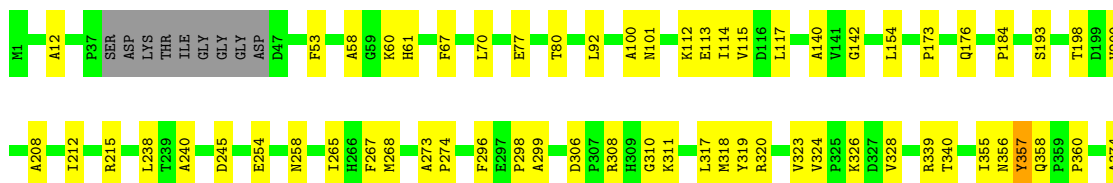
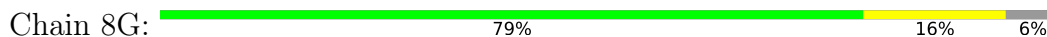
- Molecule 3: Tubulin alpha chain



- Molecule 3: Tubulin alpha chain



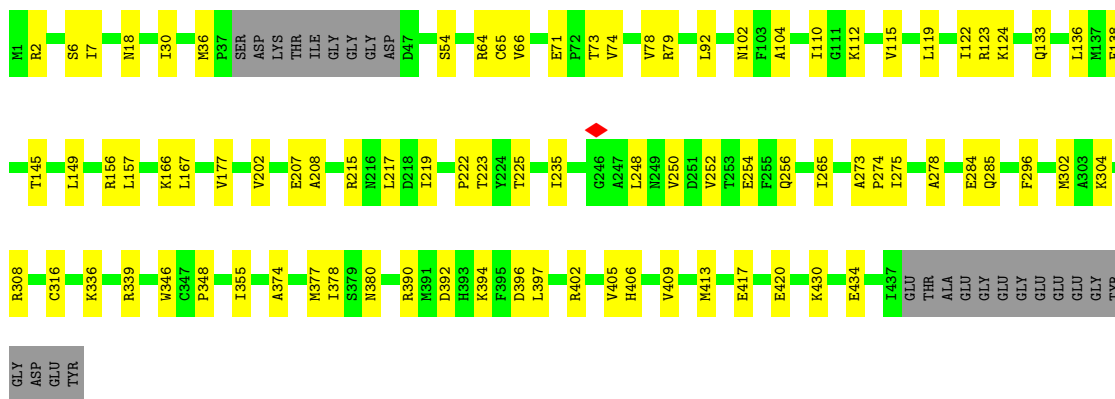
- Molecule 3: Tubulin alpha chain





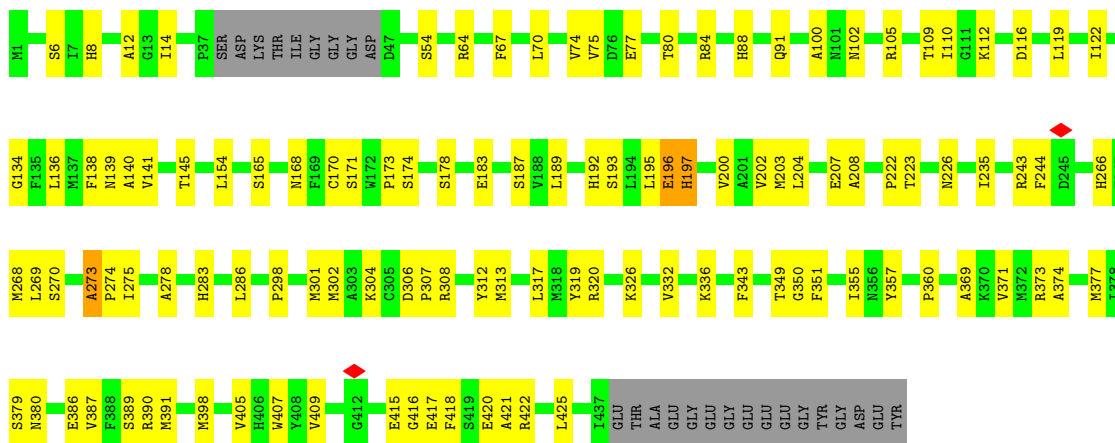
• Molecule 3: Tubulin alpha chain

Chain 8I: 76% 19% 6%



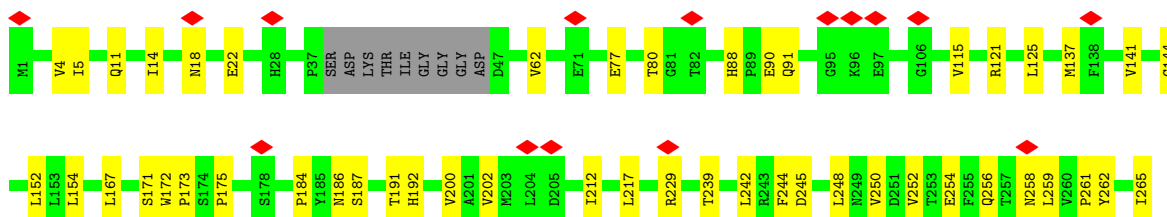
• Molecule 3: Tubulin alpha chain

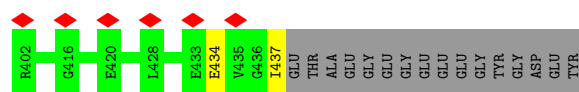
Chain 8K: 69% 25% 6%



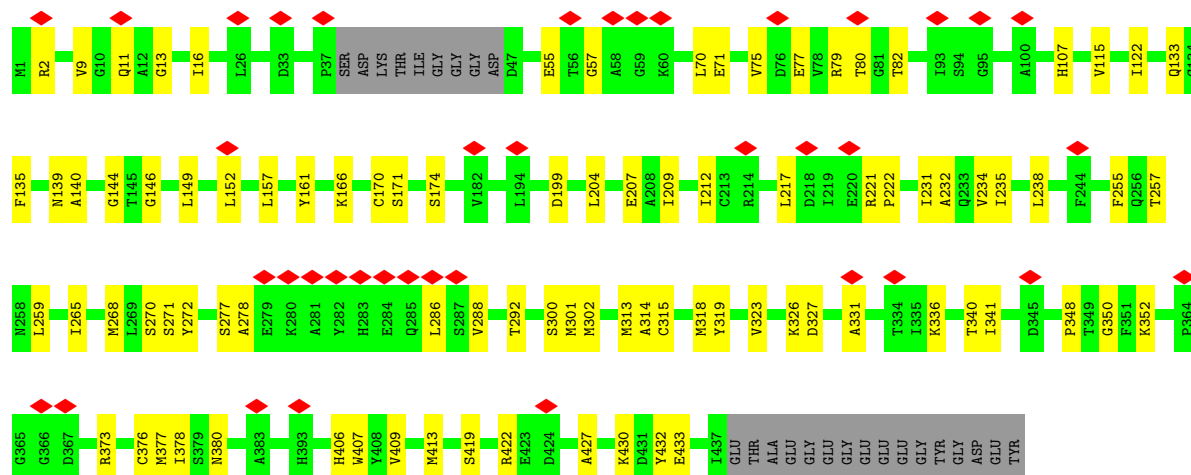
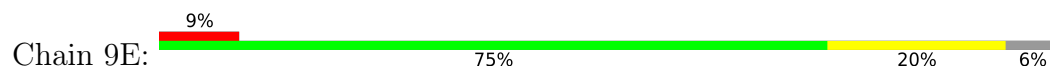
• Molecule 3: Tubulin alpha chain

Chain 8M: 5% 76% 18% 6%

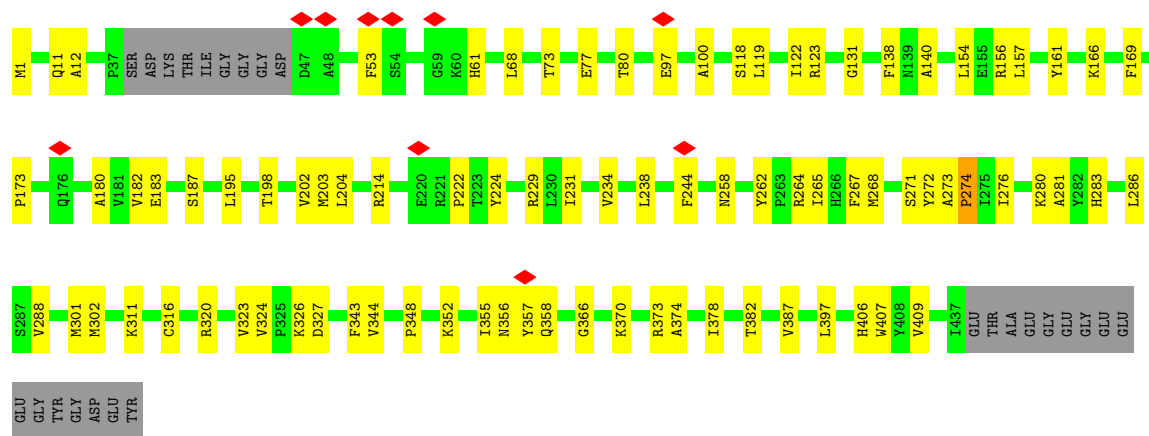
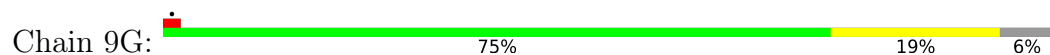




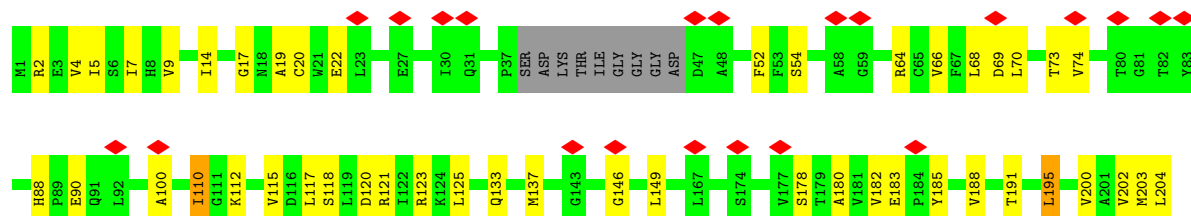
• Molecule 3: Tubulin alpha chain

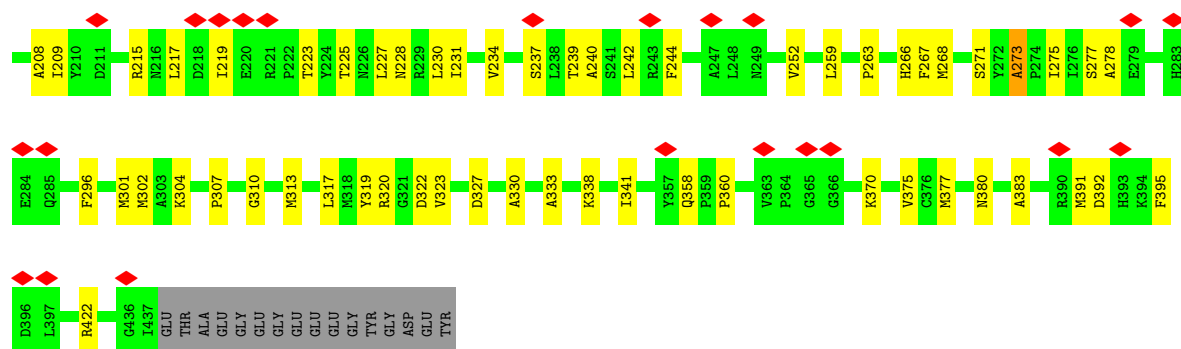


• Molecule 3: Tubulin alpha chain

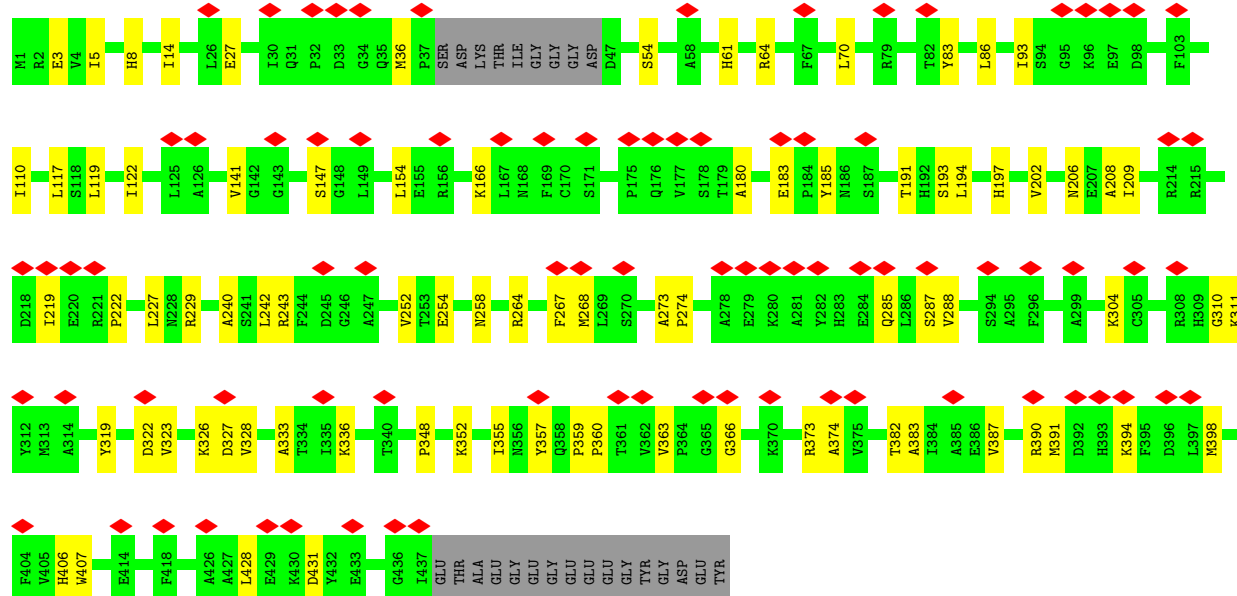
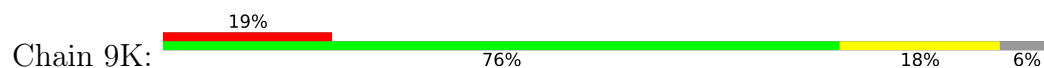


• Molecule 3: Tubulin alpha chain

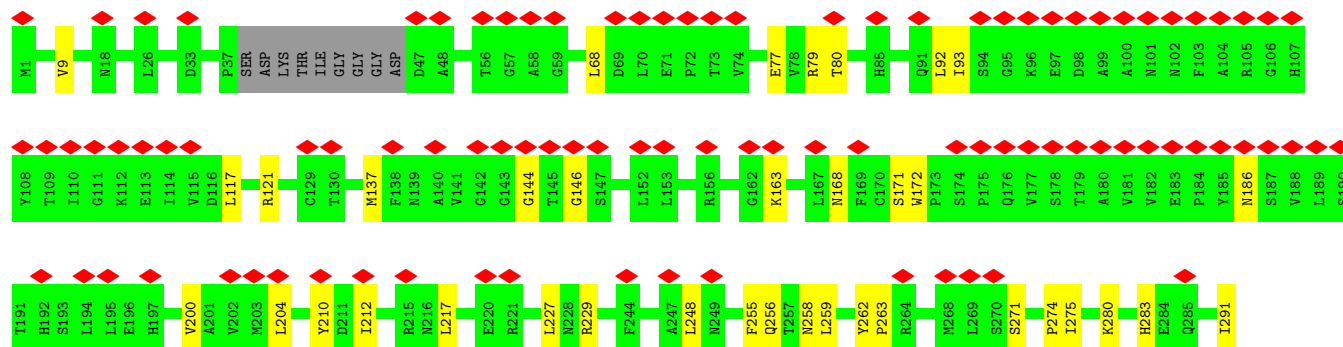
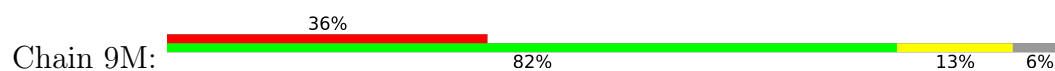


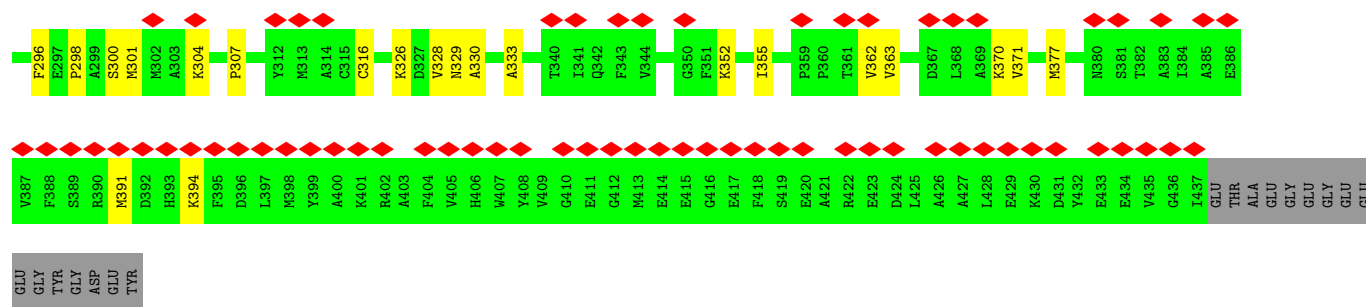


• Molecule 3: Tubulin alpha chain

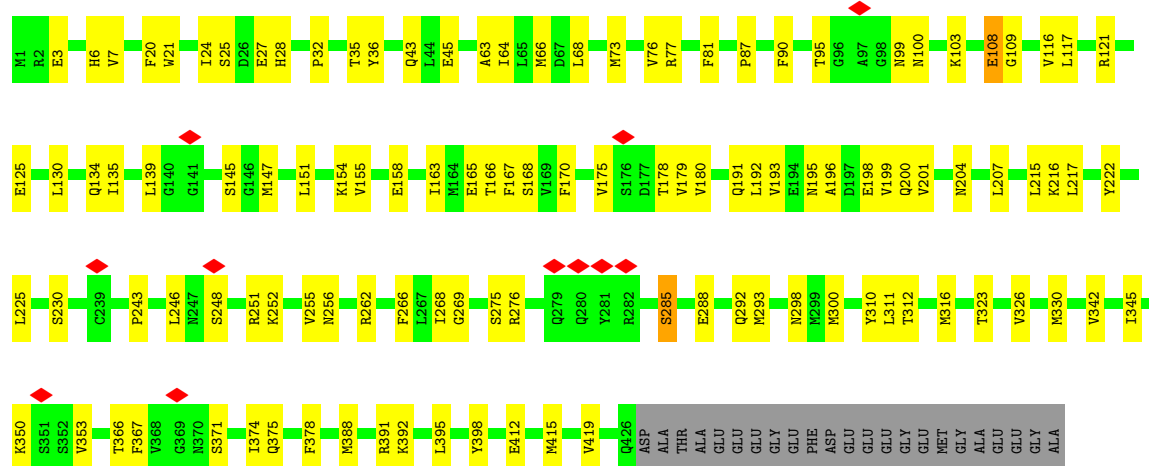


• Molecule 3: Tubulin alpha chain

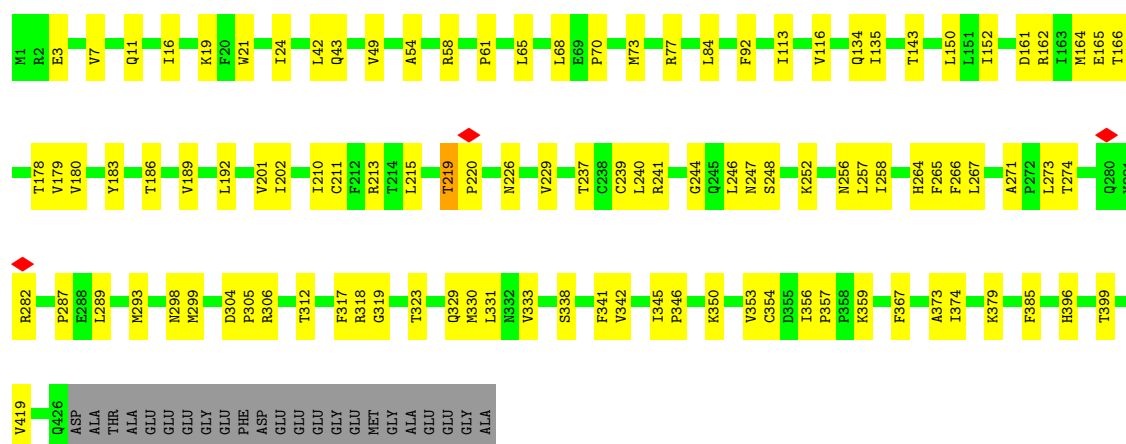
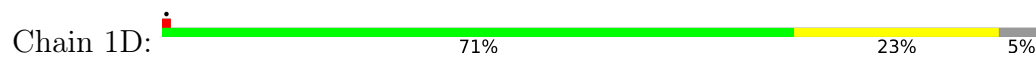




• Molecule 4: Tubulin beta chain



• Molecule 4: Tubulin beta chain

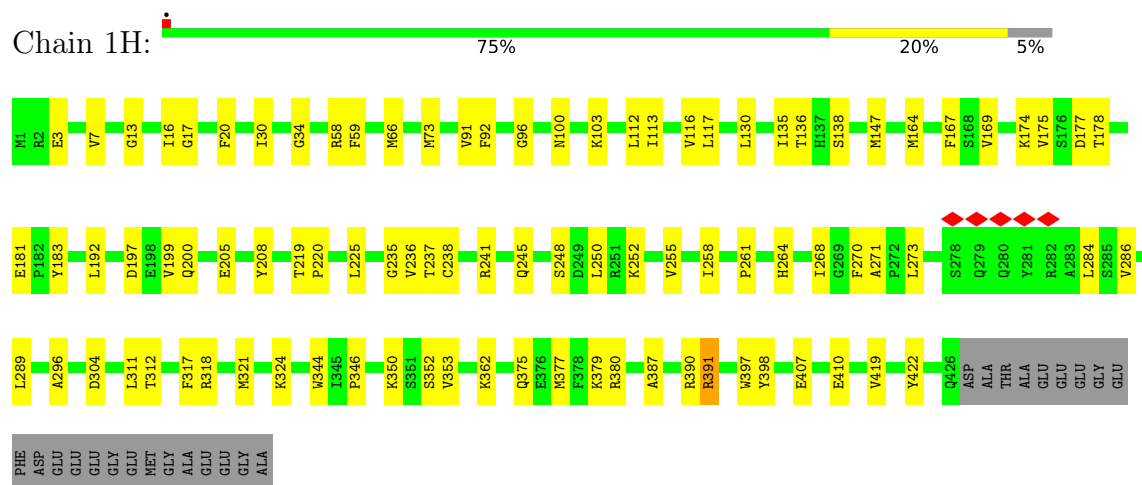


• Molecule 4: Tubulin beta chain

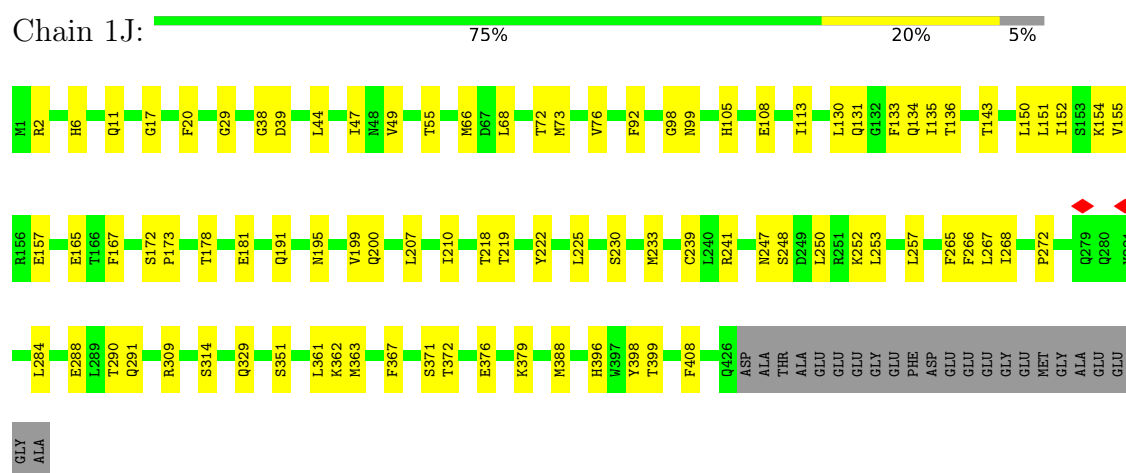




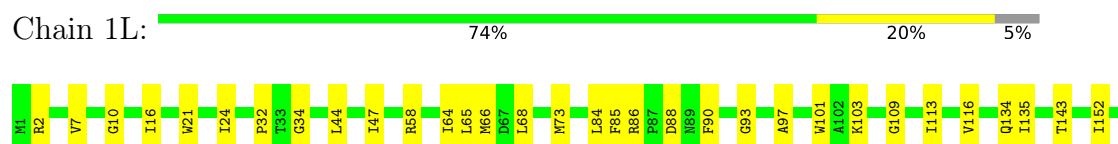
- Molecule 4: Tubulin beta chain



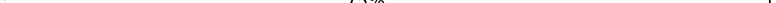
- Molecule 4: Tubulin beta chain

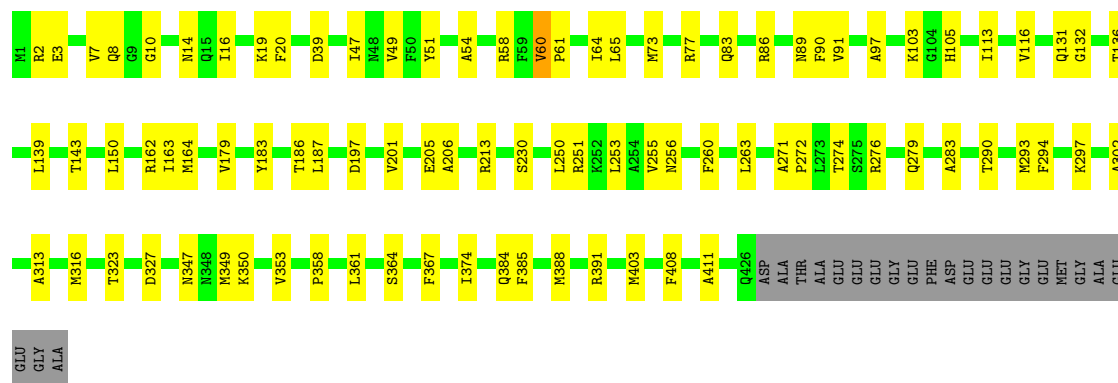


- Molecule 4: Tubulin beta chain



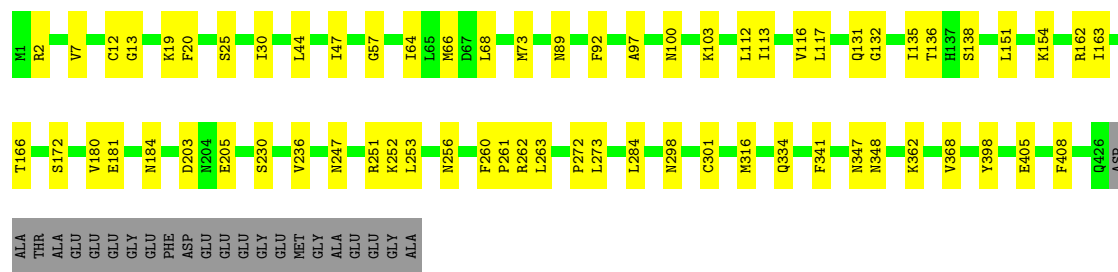
- Molecule 4: Tubulin beta chain

Chain 2F:  75% 19% 5%

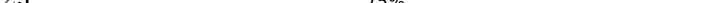


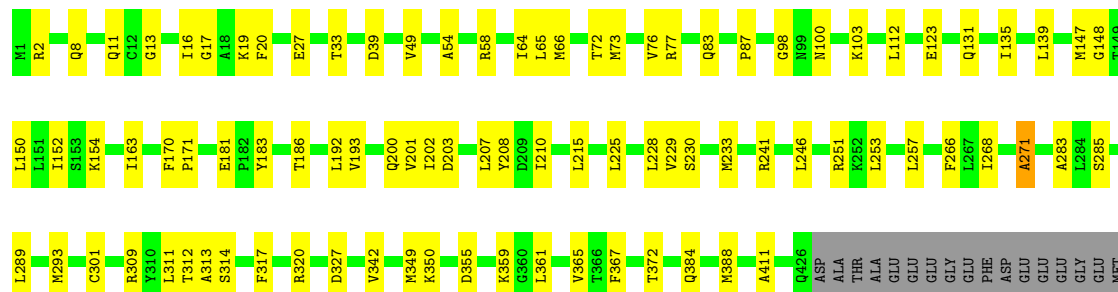
- Molecule 4: Tubulin beta chain

Chain 2H:  80% 15% 5%



- Molecule 4: Tubulin beta chain

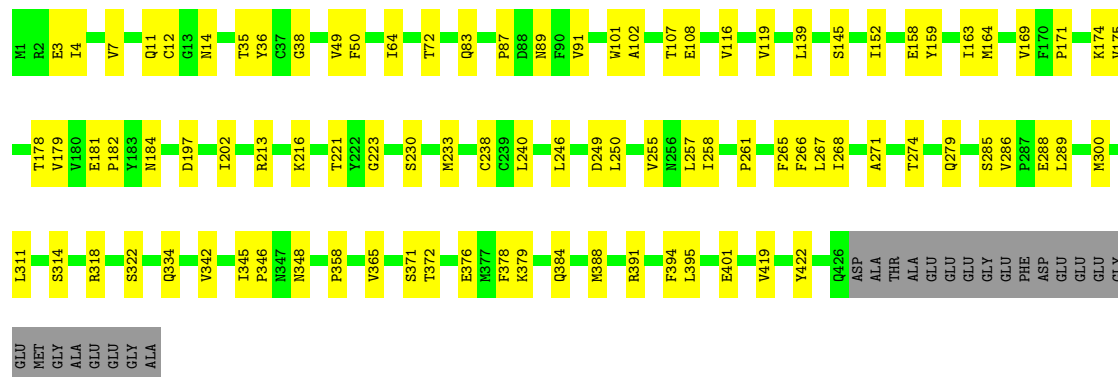
Chain 2J:  75% 20% 5%



GLY
ALA
GLU
GLU
GLY
ALA

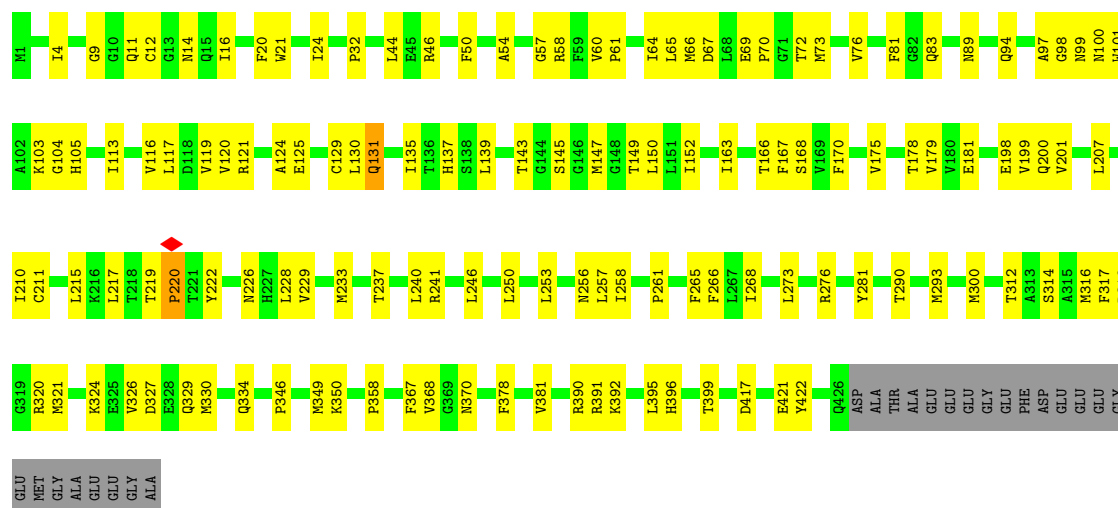
• Molecule 4: Tubulin beta chain

Chain 2L:  74% 20% 5%



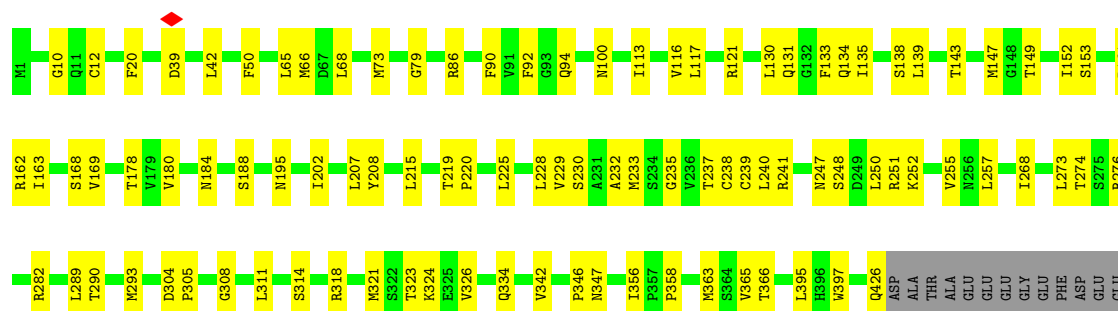
• Molecule 4: Tubulin beta chain

Chain 3B:  65% 29% 5%



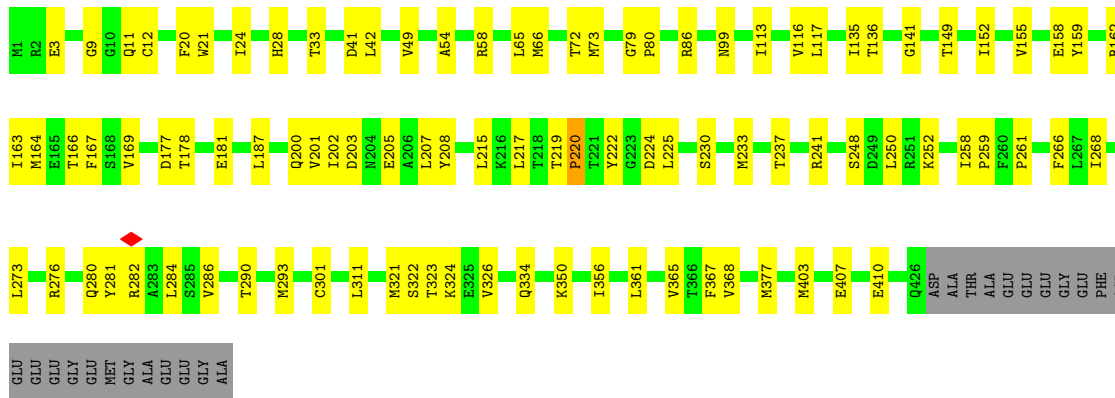
• Molecule 4: Tubulin beta chain

Chain 3D:  73% 22% 5%

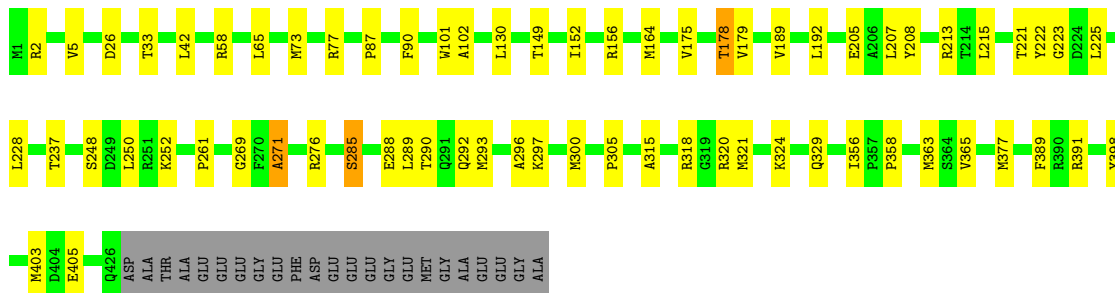


GLU
GLY
GLU
MET
GLY
ALA
GLU
GLY
ALA

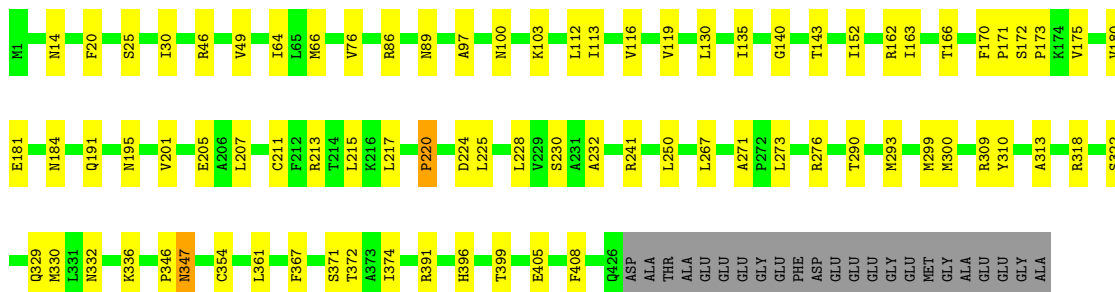
• Molecule 4: Tubulin beta chain

Chain 3F:  73% 21% 5%

• Molecule 4: Tubulin beta chain

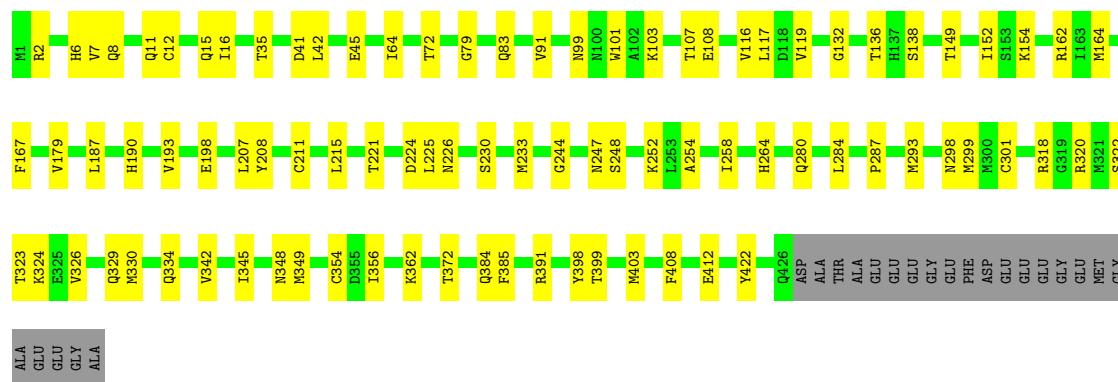
Chain 3H:  80% 14% 5%

• Molecule 4: Tubulin beta chain

Chain 3J:  77% 18% 5%

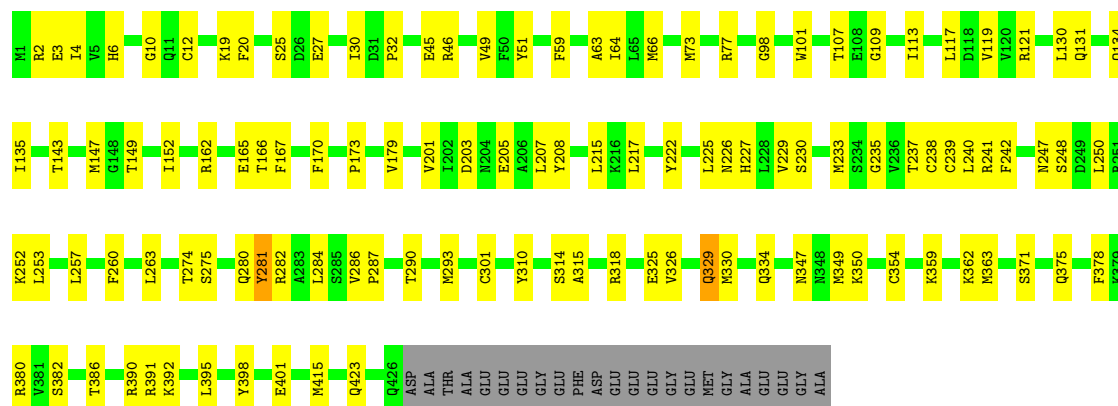
• Molecule 4: Tubulin beta chain

Chain 3L:  75% 20% 5%



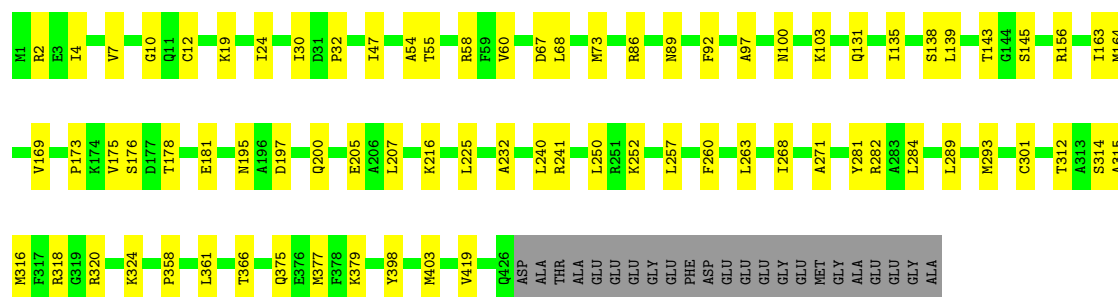
• Molecule 4: Tubulin beta chain

Chain 4B: 69% 25% 5%



• Molecule 4: Tubulin beta chain

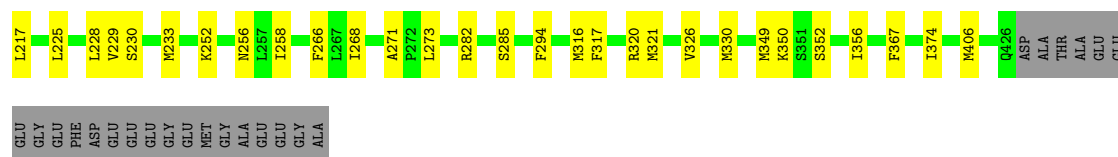
Chain 4D: 78% 17% 5%



• Molecule 4: Tubulin beta chain

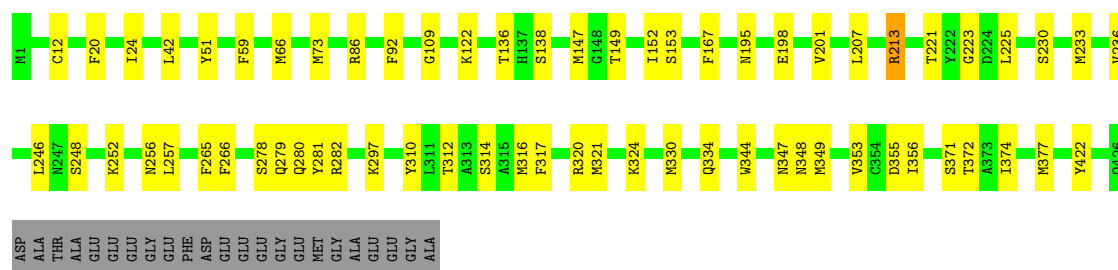
Chain 4F: 81% 13% 5%





• Molecule 4: Tubulin beta chain

Chain 4H: 80% 14% 5%



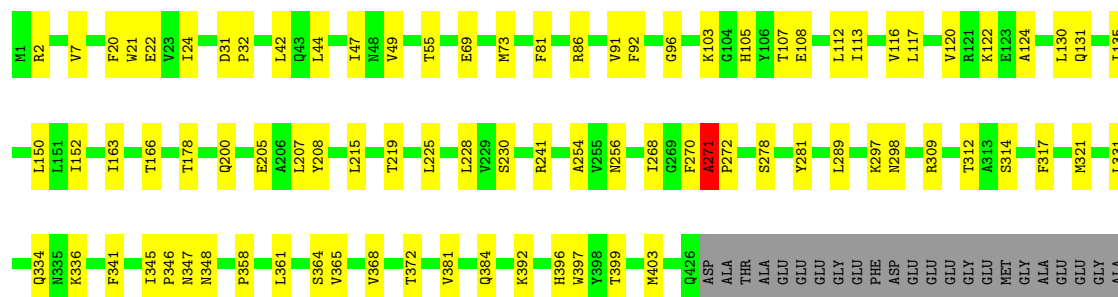
• Molecule 4: Tubulin beta chain

Chain 4J: 81% 14% 5%



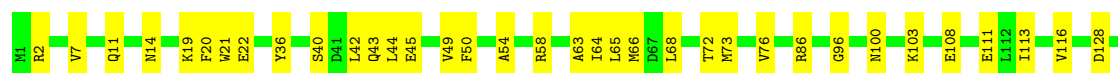
• Molecule 4: Tubulin beta chain

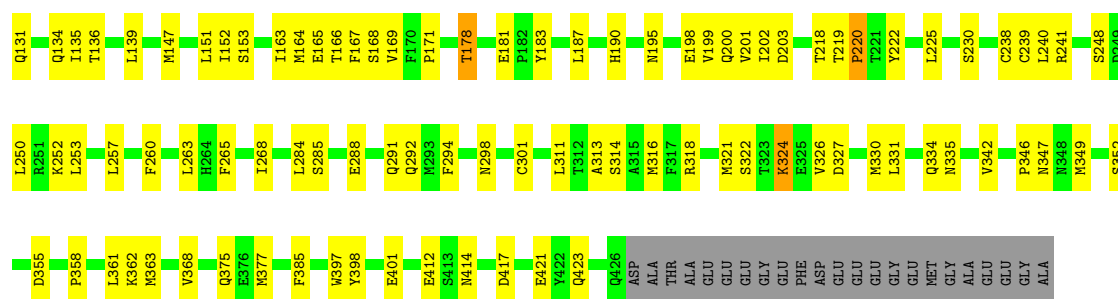
Chain 4L: 76% 19% 5%



• Molecule 4: Tubulin beta chain

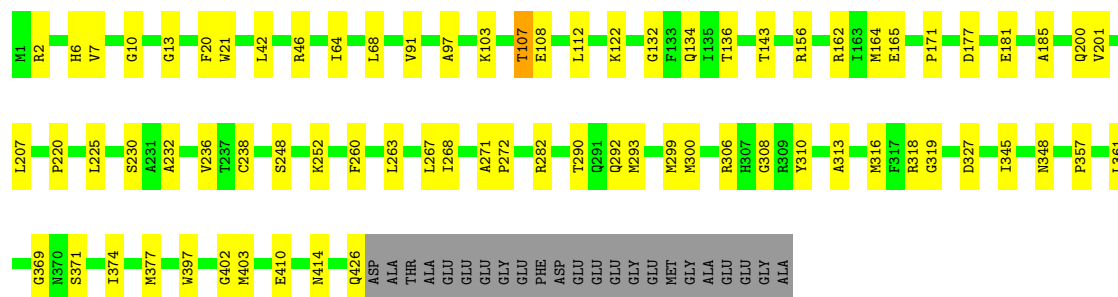
Chain 5B: 67% 28% 5%





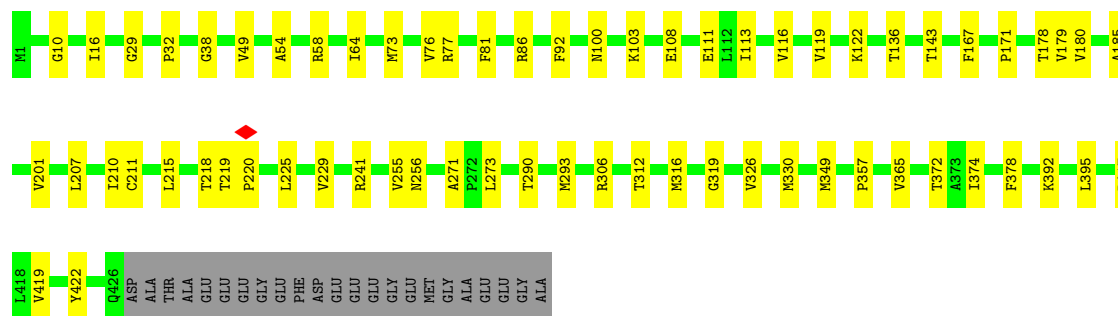
- Molecule 4: Tubulin beta chain

Chain 5D: 78% 16% 5%



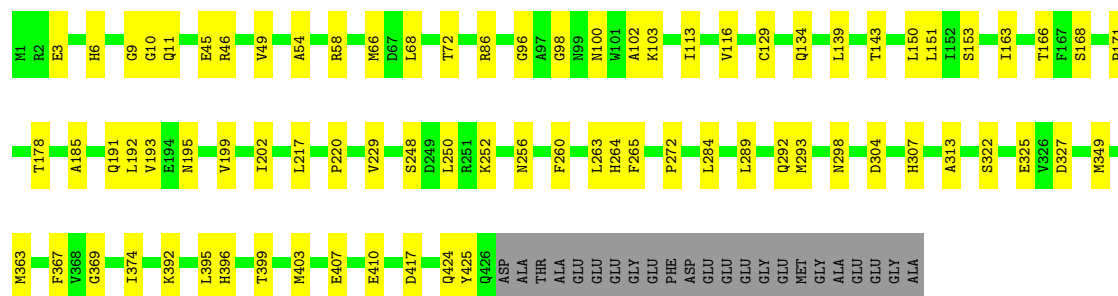
- Molecule 4: Tubulin beta chain

Chain 5F: 80% 14% 5%



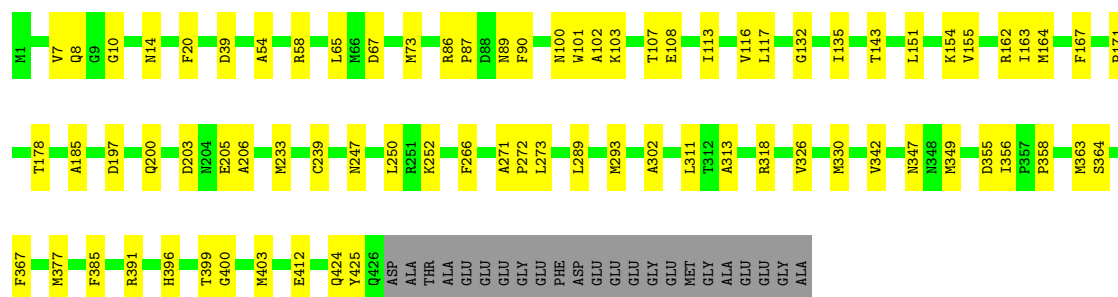
- Molecule 4: Tubulin beta chain

Chain 5H: 78% 17% 5%



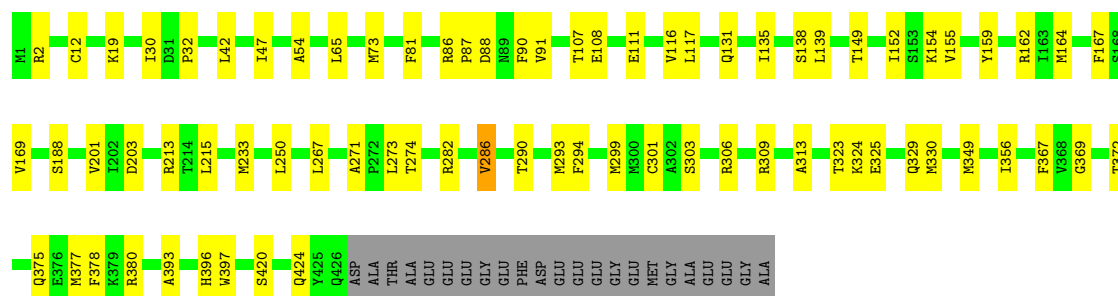
- Molecule 4: Tubulin beta chain

Chain 5J:  78% 17% 5%



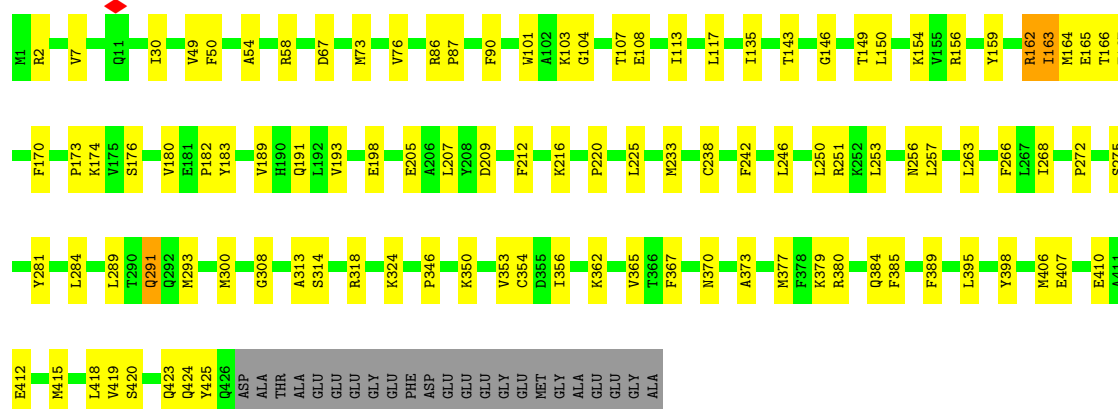
• Molecule 4: Tubulin beta chain

Chain 5L:  78% 16% 5%



• Molecule 4: Tubulin beta chain

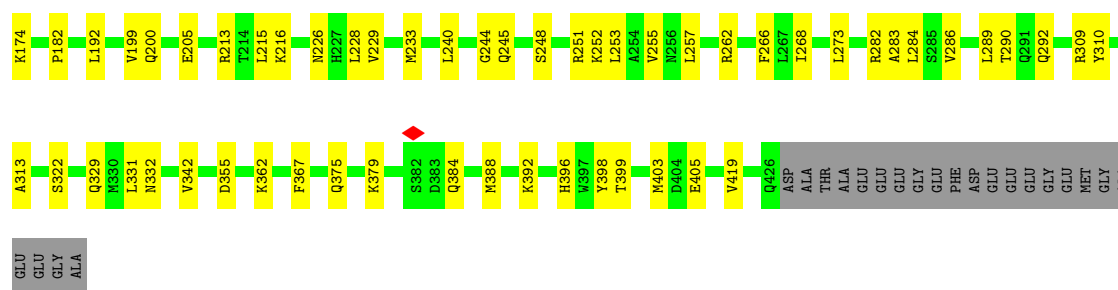
Chain 5N:  71% 23% 5%



• Molecule 4: Tubulin beta chain

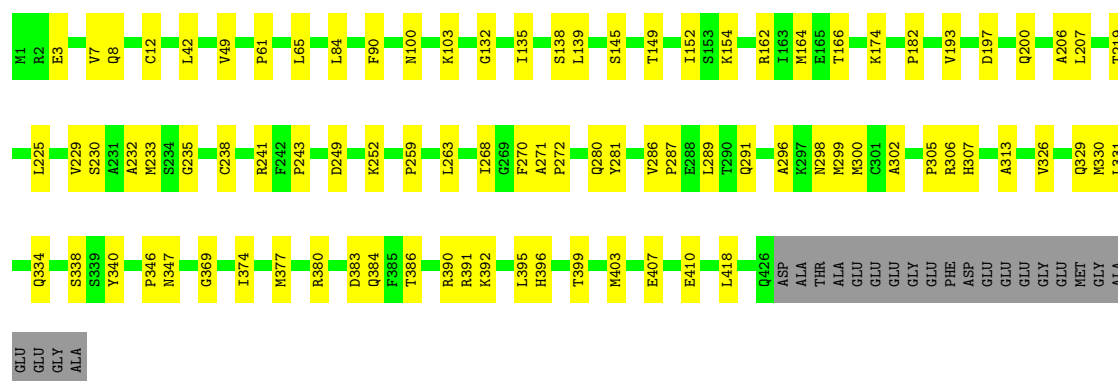
Chain 6B:  75% 20% 5%





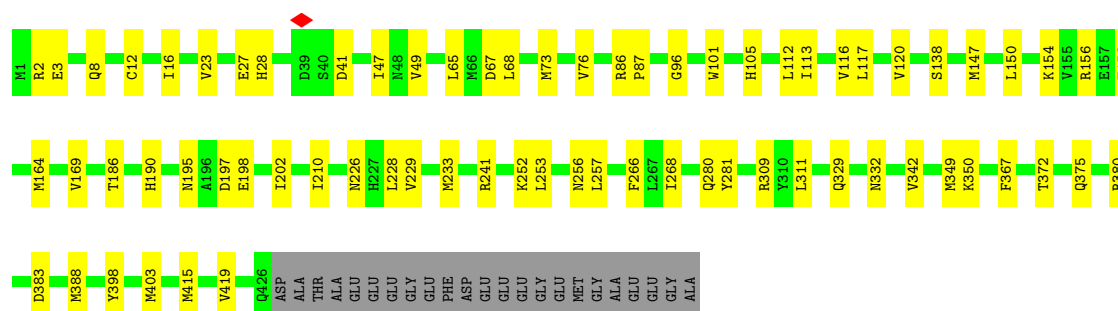
• Molecule 4: Tubulin beta chain

Chain 6D: 75% 20% 5%



• Molecule 4: Tubulin beta chain

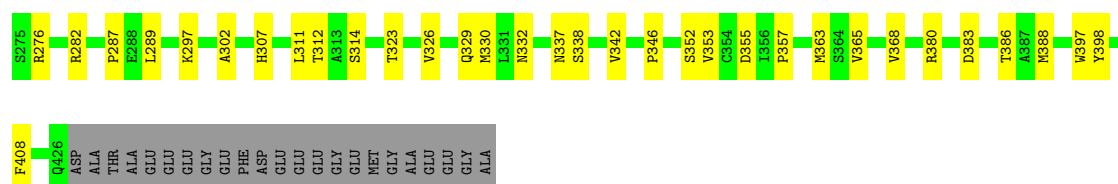
Chain 6F: 79% 16% 5%



• Molecule 4: Tubulin beta chain

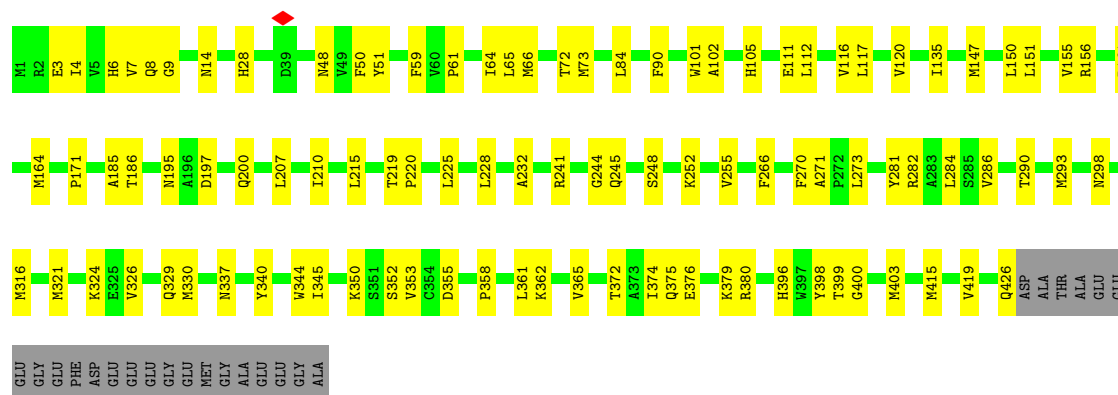
Chain 6H: 73% 22% 5%





• Molecule 4: Tubulin beta chain

Chain 6J: 73% 22% 5%



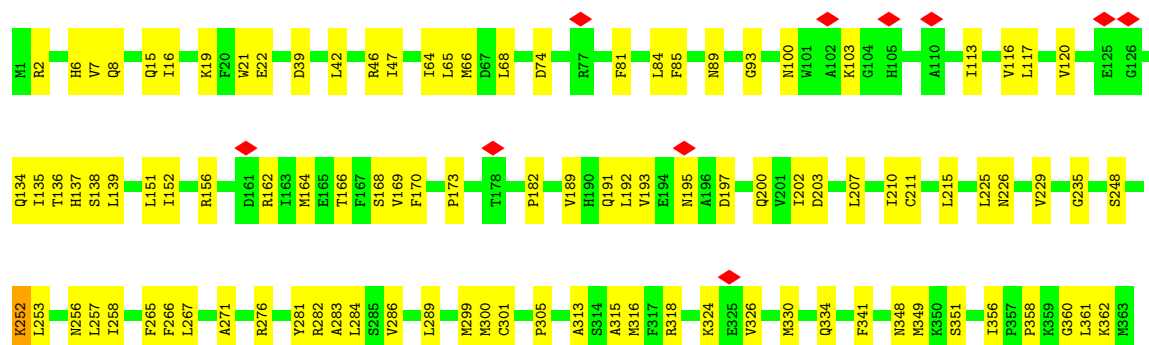
• Molecule 4: Tubulin beta chain

Chain 6L: 76% 19% 5%



• Molecule 4: Tubulin beta chain

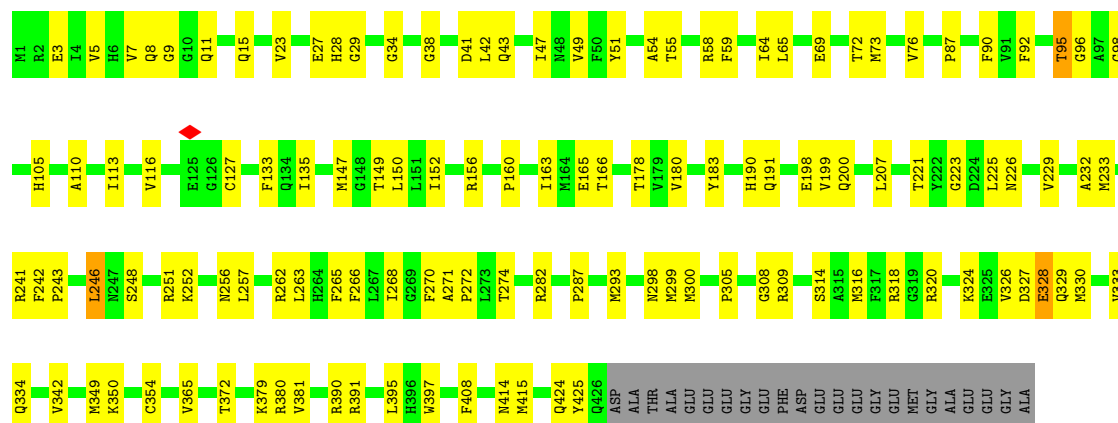
Chain 6N: 69% 26% 5%





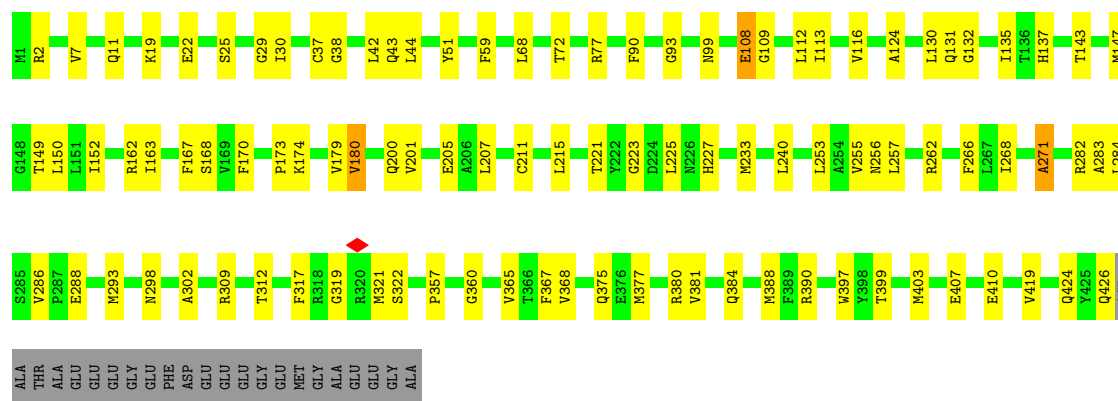
• Molecule 4: Tubulin beta chain

Chain 7B: 67% 27% 5%



• Molecule 4: Tubulin beta chain

Chain 7D: 73% 22% 5%



• Molecule 4: Tubulin beta chain

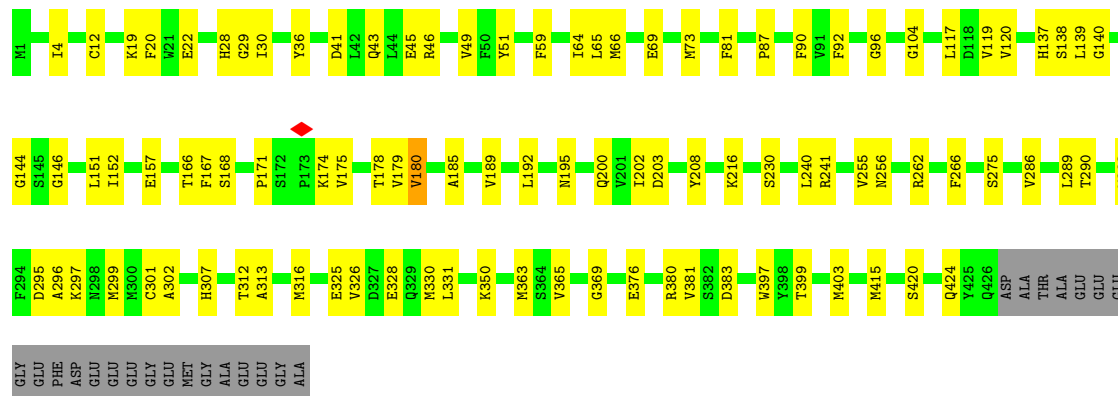
Chain 7F: 75% 20% 5%



GLU
MET
GLY
ALA
GLU
GLU
GLY
ALA

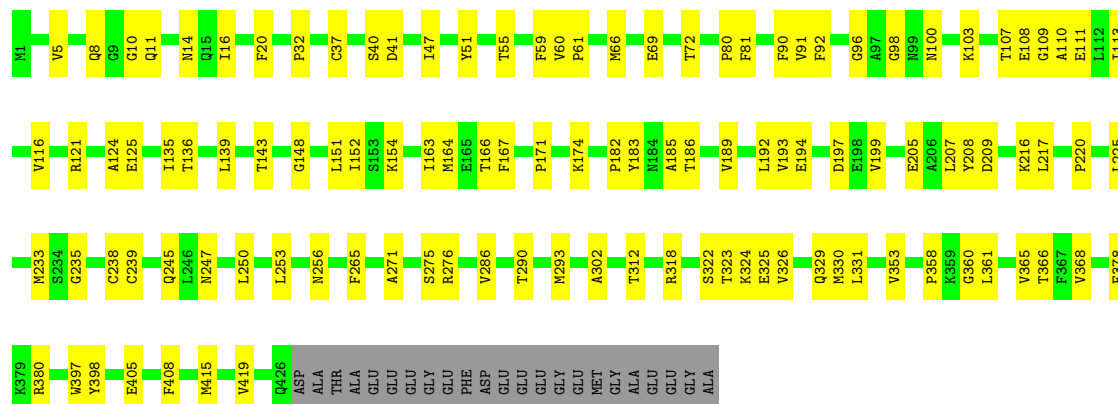
• Molecule 4: Tubulin beta chain

Chain 7H: 73% 22% 5%



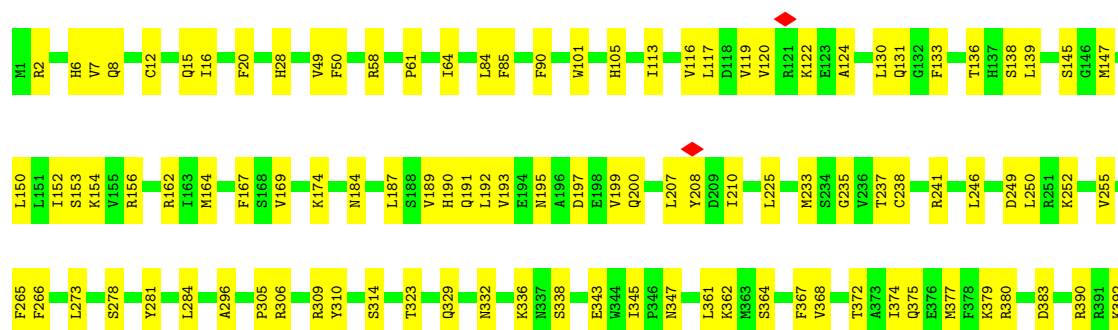
• Molecule 4: Tubulin beta chain

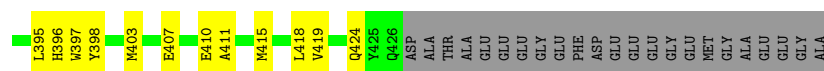
Chain 7J: 70% 25% 5%



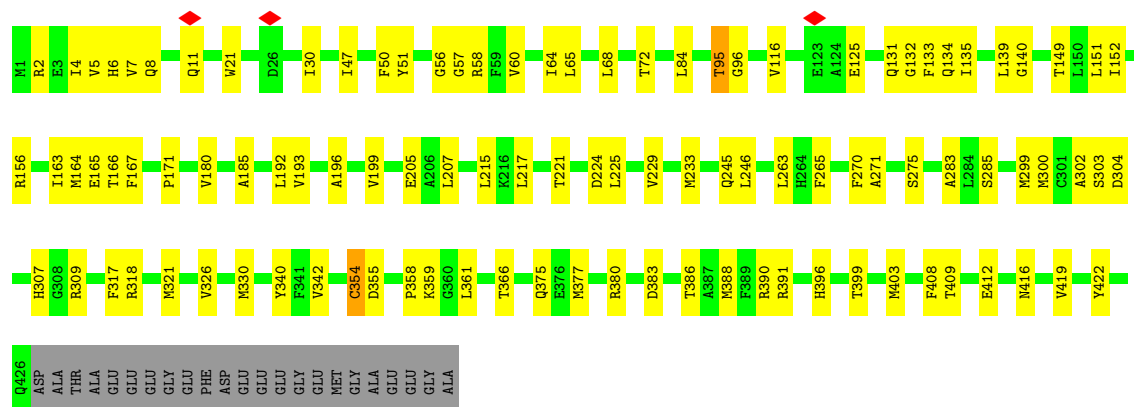
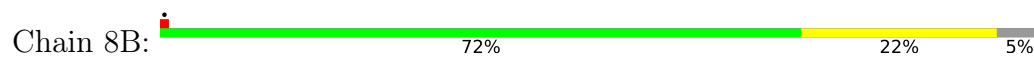
• Molecule 4: Tubulin beta chain

Chain 7L: 69% 26% 5%

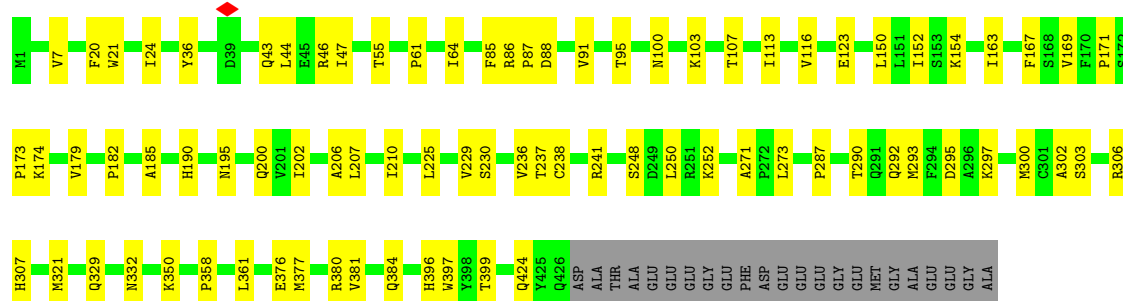
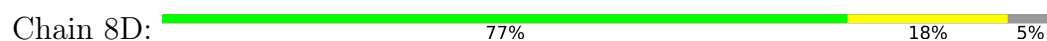




- Molecule 4: Tubulin beta chain



- Molecule 4: Tubulin beta chain

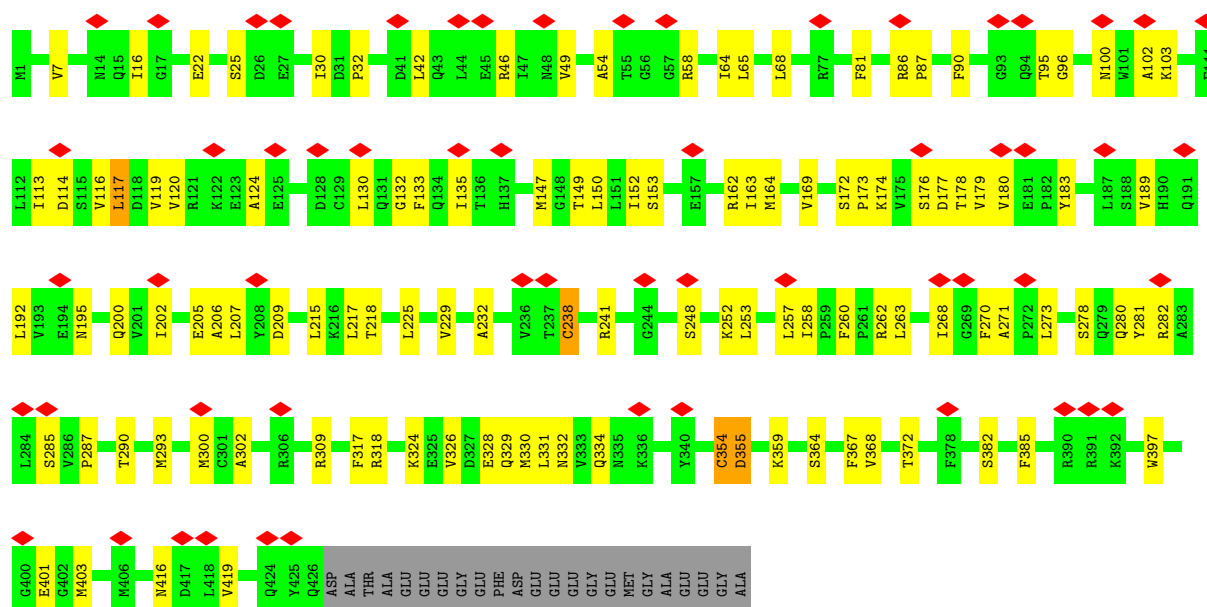


- Molecule 4: Tubulin beta chain



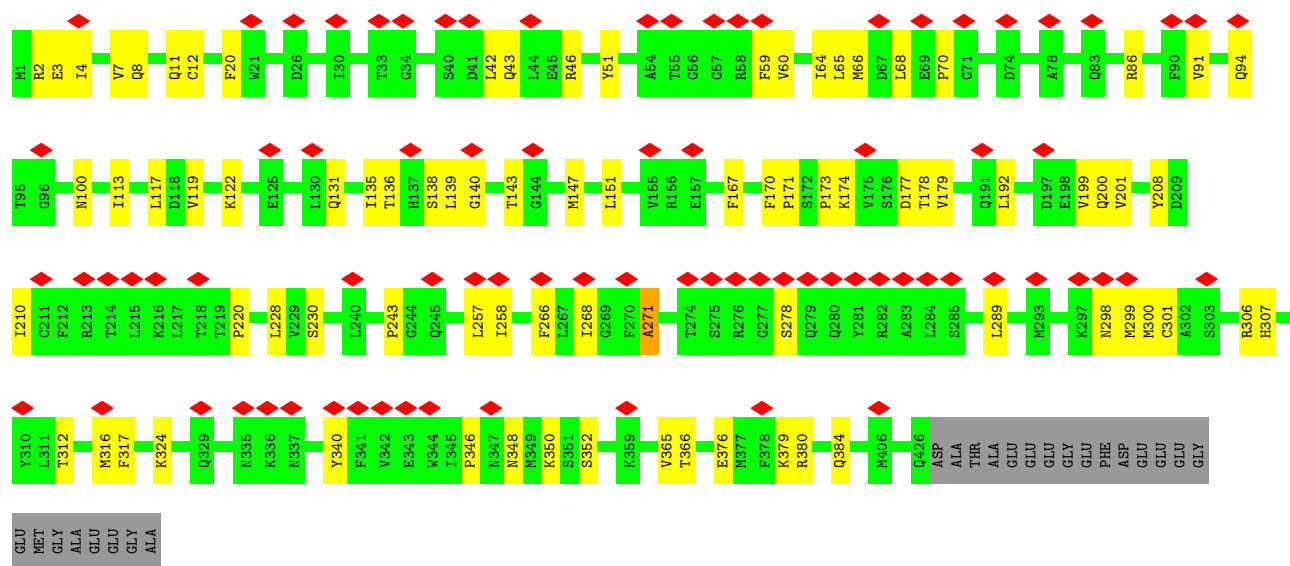
- Molecule 4: Tubulin beta chain

Chain 9B: 



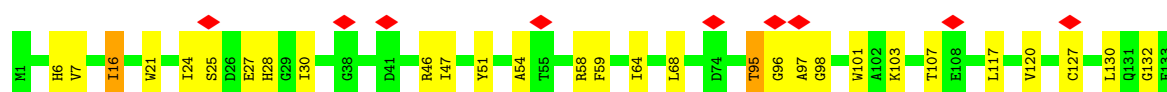
• Molecule 4: Tubulin beta chain

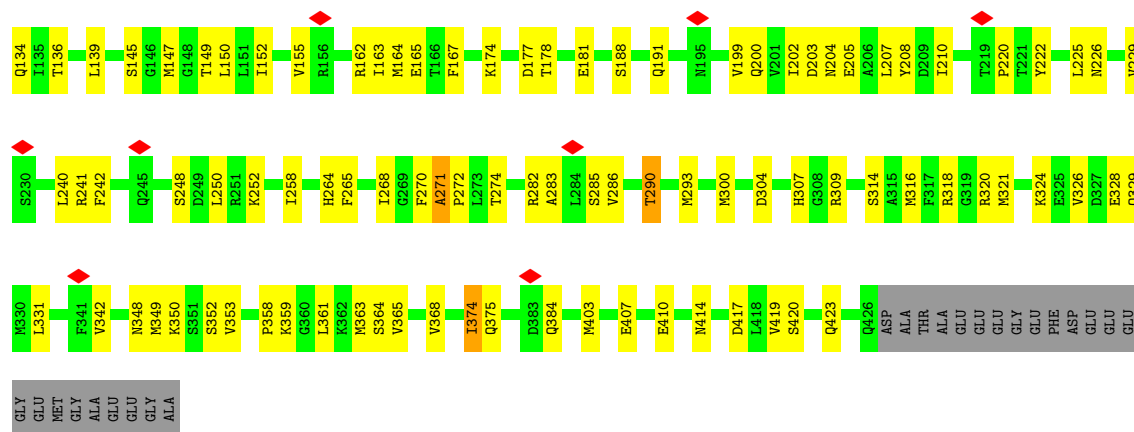
Chain 9D: 



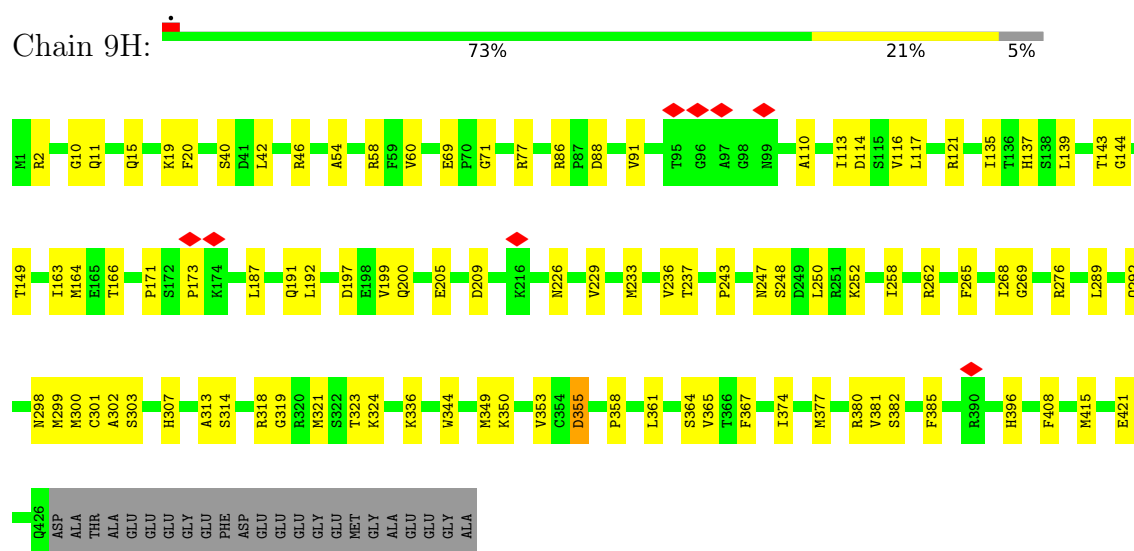
• Molecule 4: Tubulin beta chain

Chain 9F: 

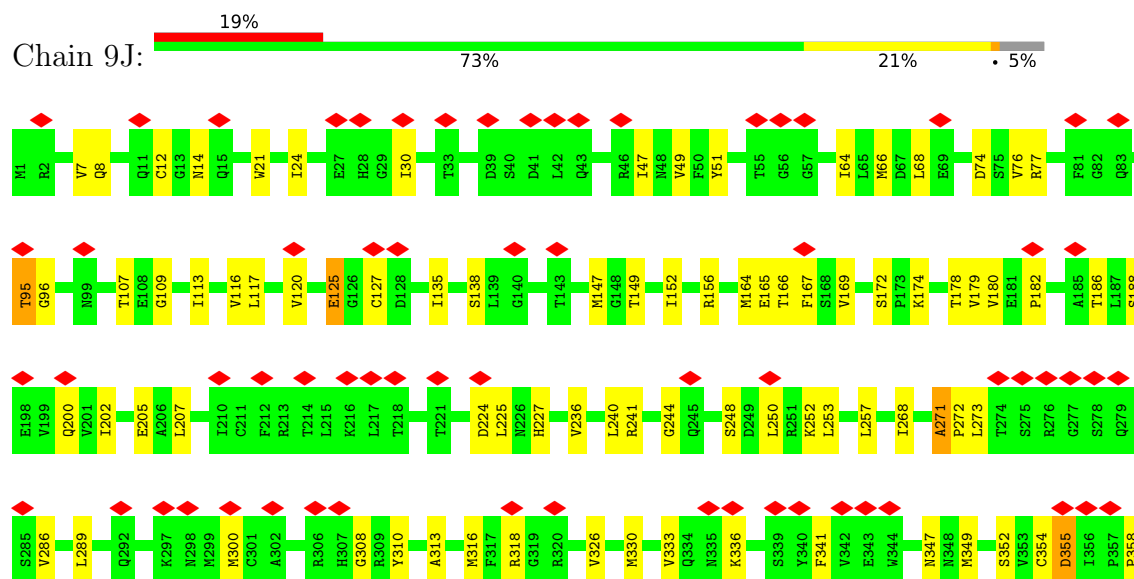


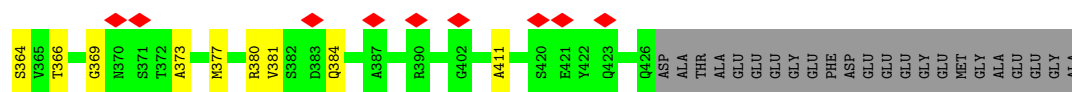


• Molecule 4: Tubulin beta chain

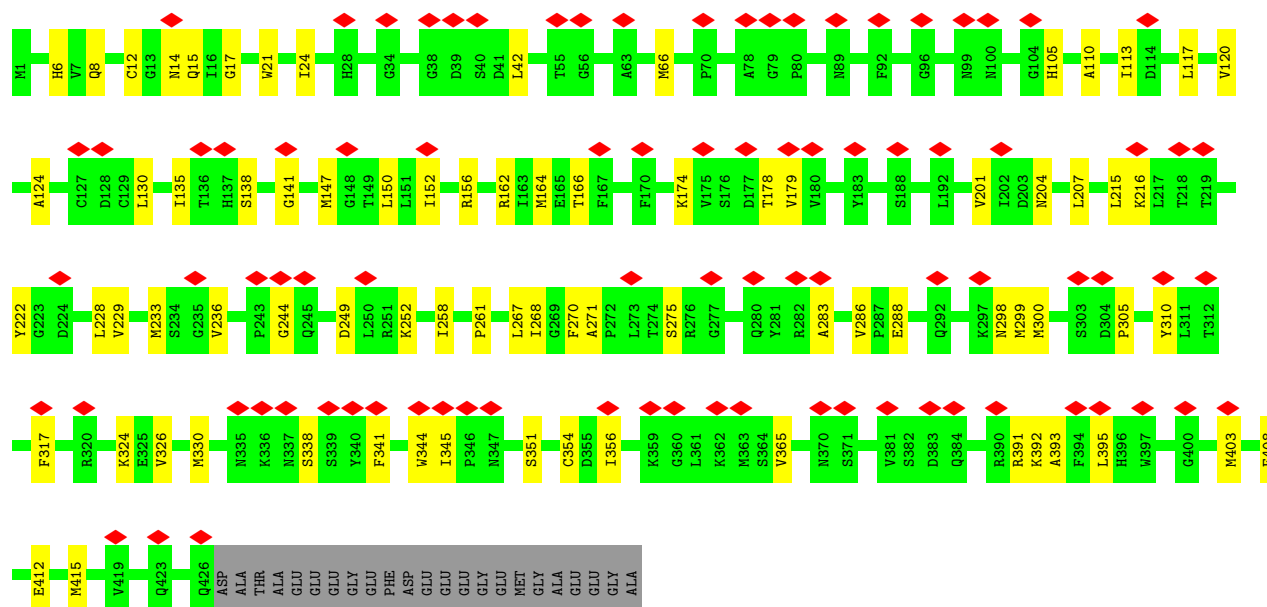
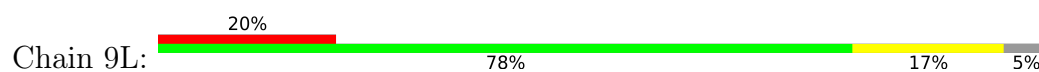


• Molecule 4: Tubulin beta chain

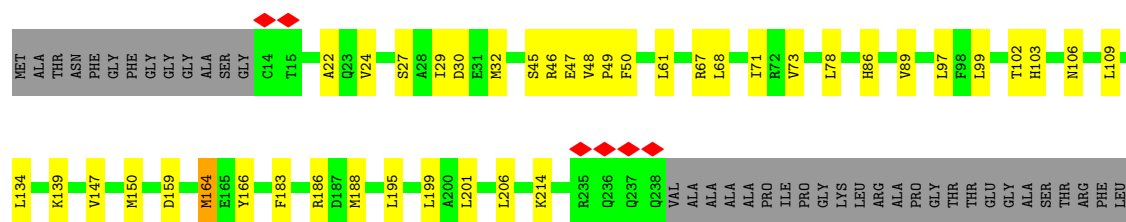




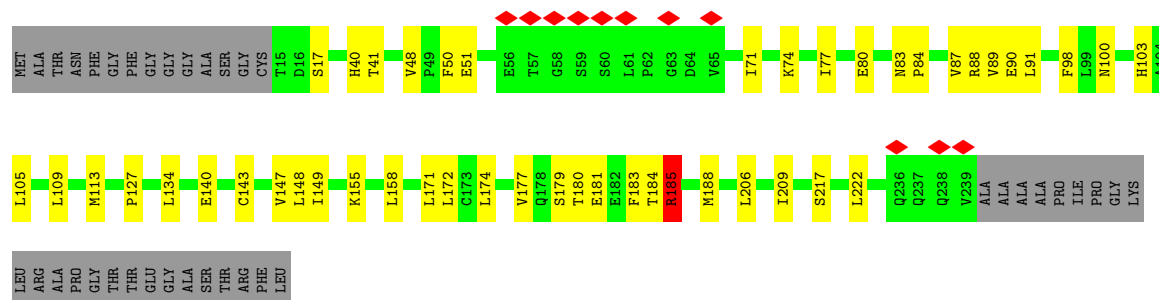
• Molecule 4: Tubulin beta chain



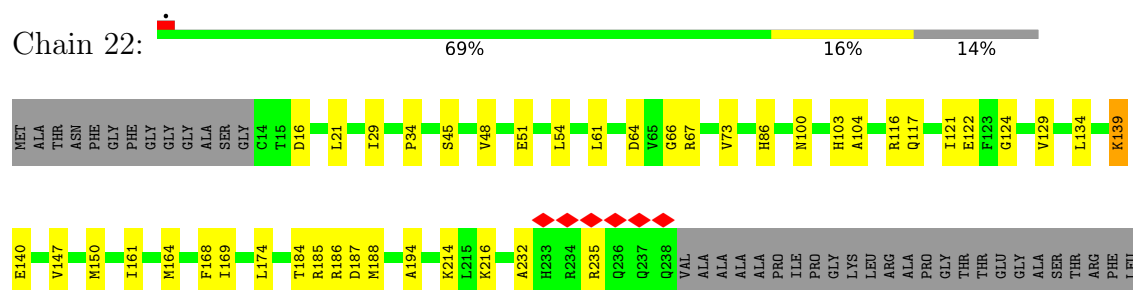
• Molecule 5: Spindle assembly abnormal protein 6 N-terminal domain-containing protein



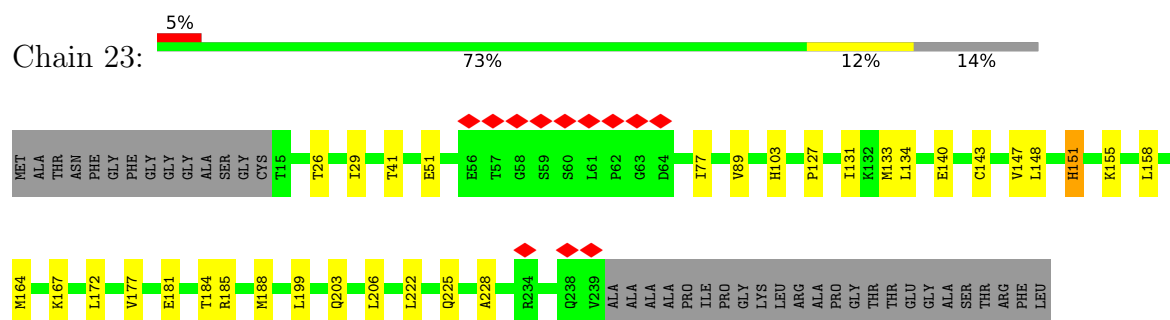
• Molecule 5: Spindle assembly abnormal protein 6 N-terminal domain-containing protein



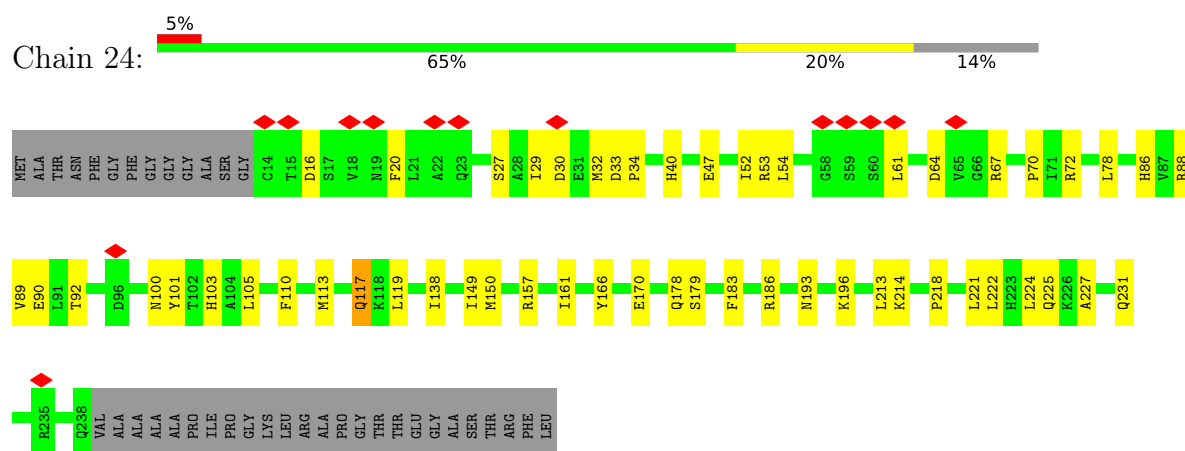
- Molecule 5: Spindle assembly abnormal protein 6 N-terminal domain-containing protein



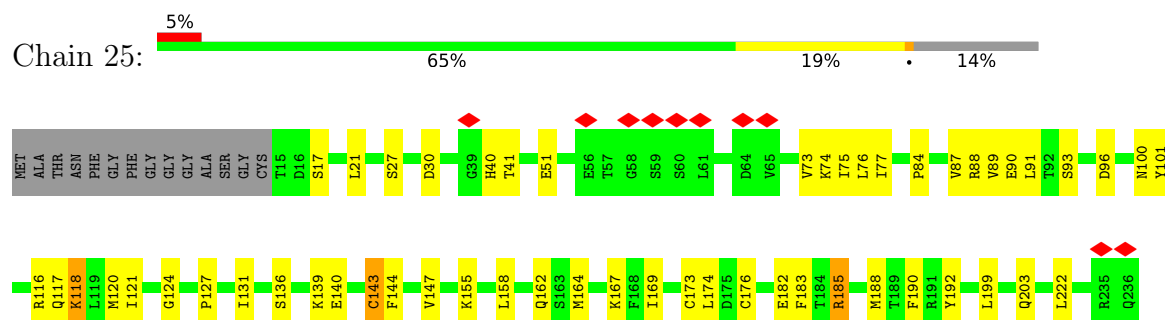
- Molecule 5: Spindle assembly abnormal protein 6 N-terminal domain-containing protein

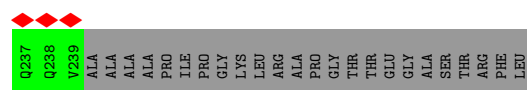


- Molecule 5: Spindle assembly abnormal protein 6 N-terminal domain-containing protein

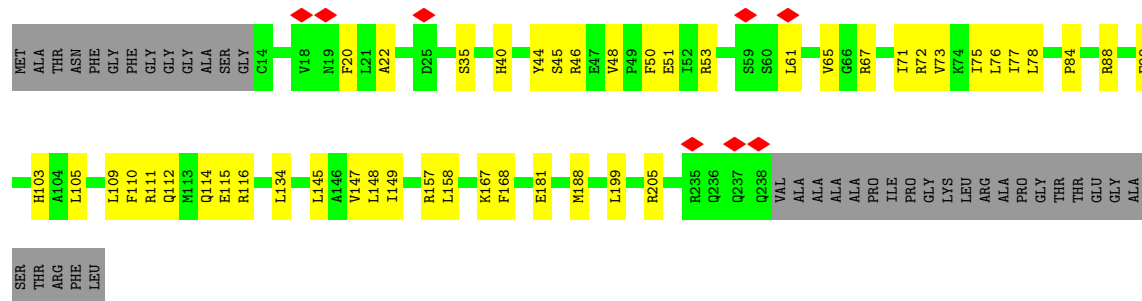


- Molecule 5: Spindle assembly abnormal protein 6 N-terminal domain-containing protein

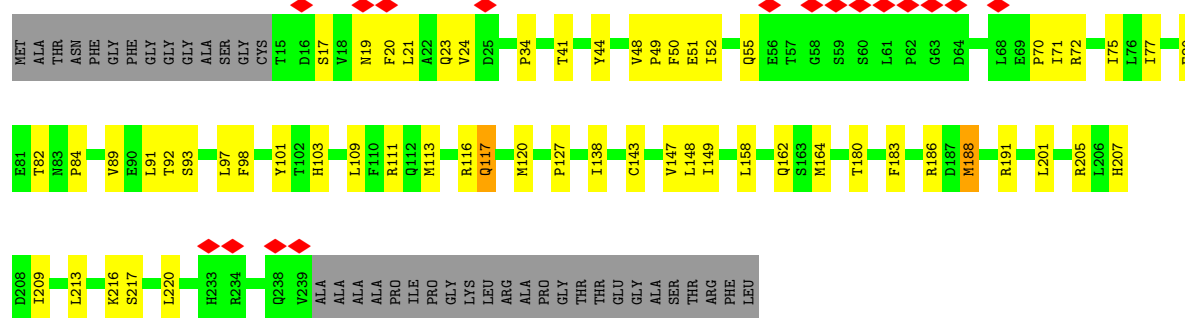




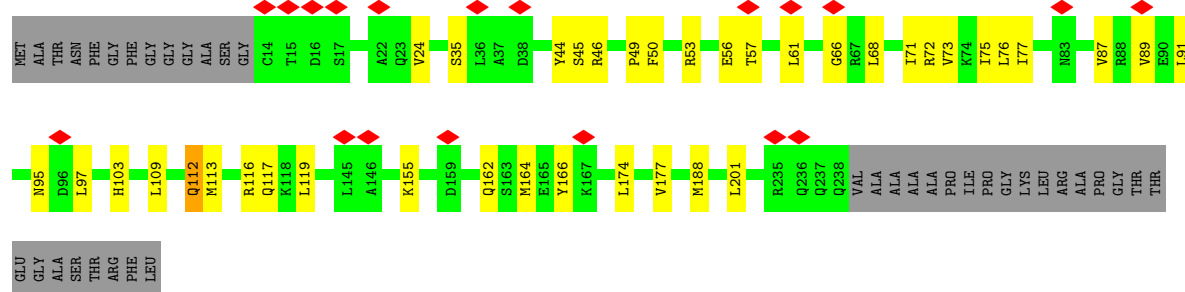
- Molecule 5: Spindle assembly abnormal protein 6 N-terminal domain-containing protein



- Molecule 5: Spindle assembly abnormal protein 6 N-terminal domain-containing protein

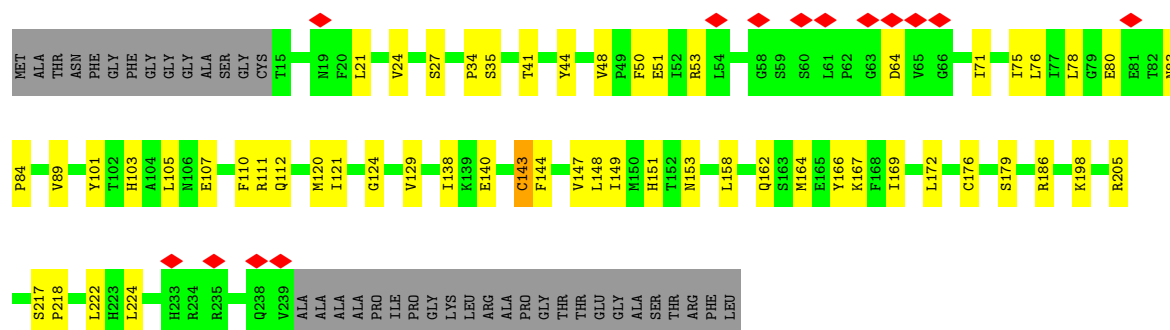


- Molecule 5: Spindle assembly abnormal protein 6 N-terminal domain-containing protein



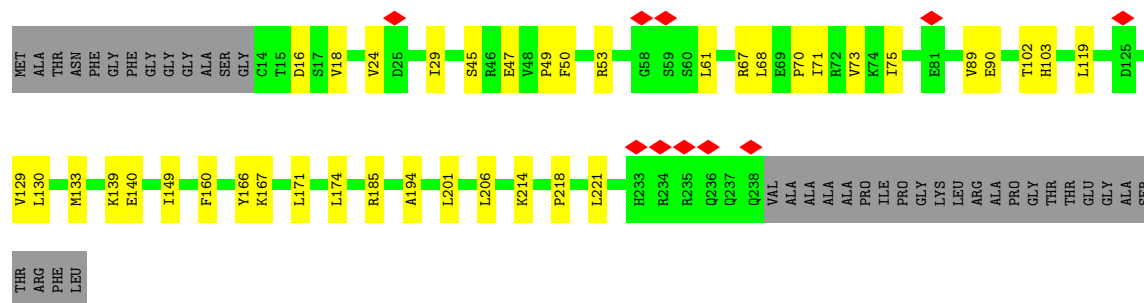
- Molecule 5: Spindle assembly abnormal protein 6 N-terminal domain-containing protein





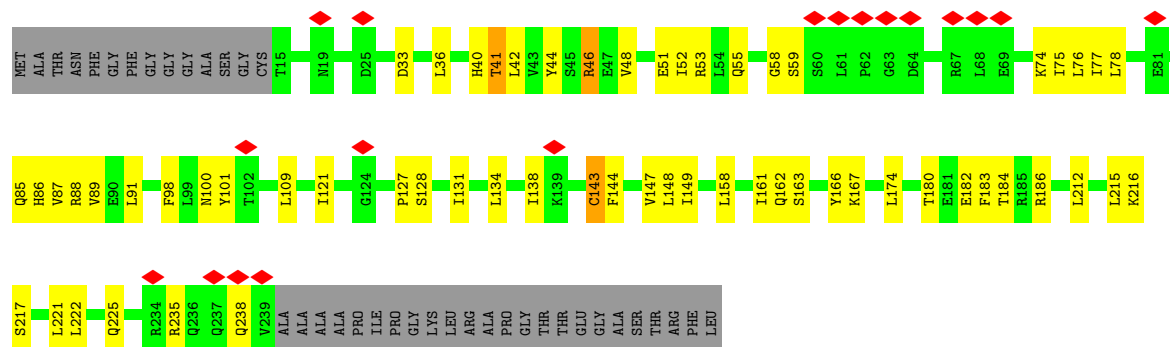
- Molecule 5: Spindle assembly abnormal protein 6 N-terminal domain-containing protein

Chain 30: 71% 15% 14%



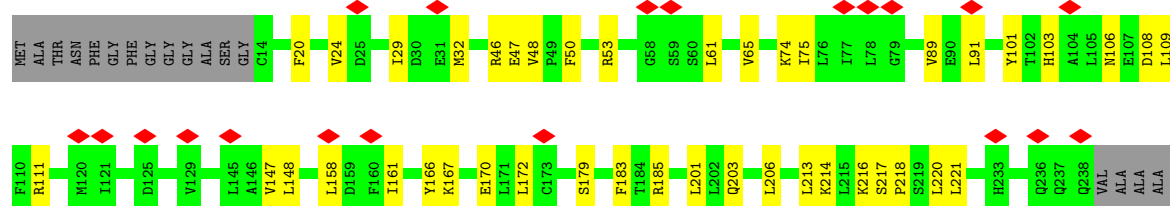
- Molecule 5: Spindle assembly abnormal protein 6 N-terminal domain-containing protein

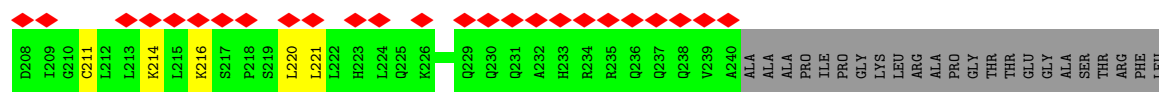
Chain 31: 7% 62% 22% 14%



- Molecule 5: Spindle assembly abnormal protein 6 N-terminal domain-containing protein

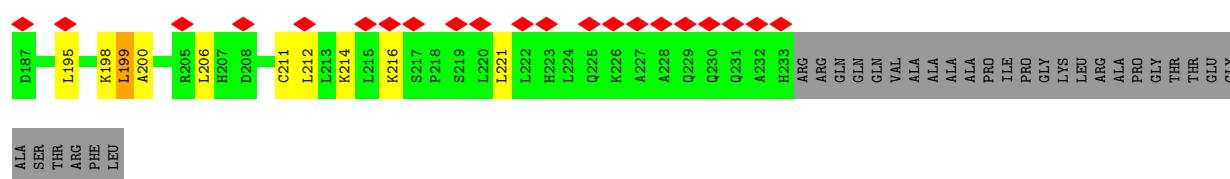
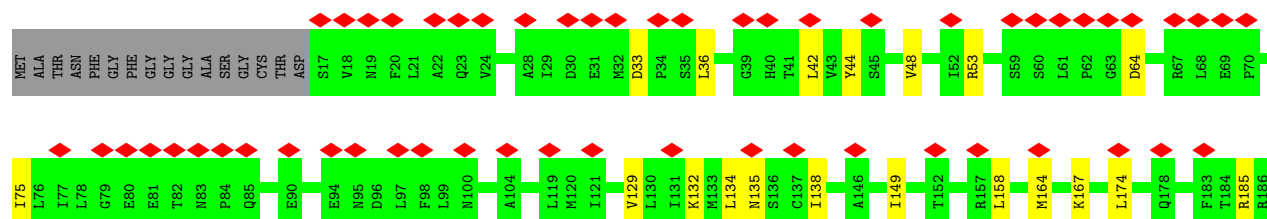
Chain 32: 8% 70% 16% 14%





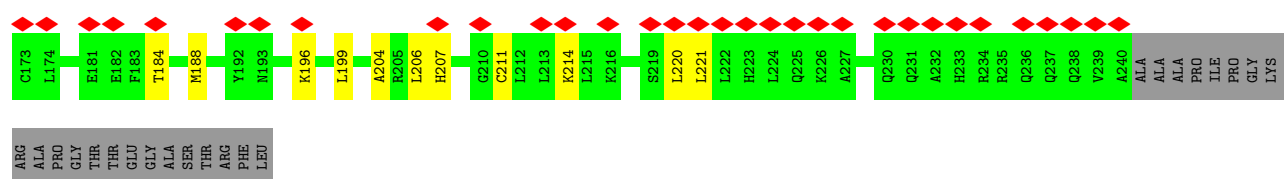
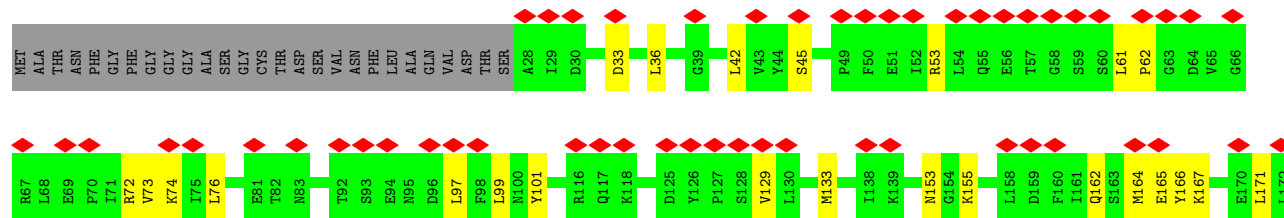
- Molecule 5: Spindle assembly abnormal protein 6 N-terminal domain-containing protein

Chain 37: 29% 71% 11% 17%



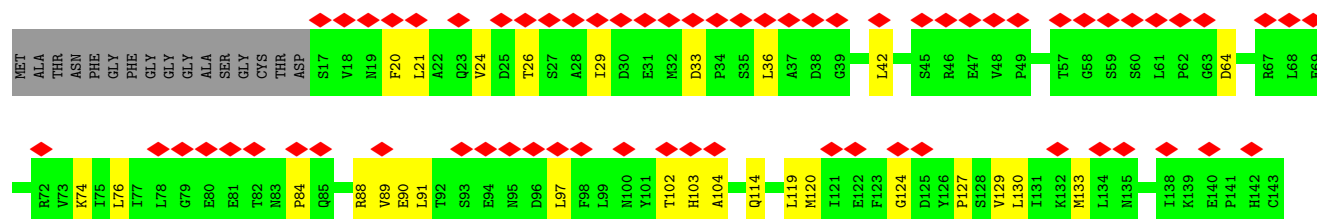
- Molecule 5: Spindle assembly abnormal protein 6 N-terminal domain-containing protein

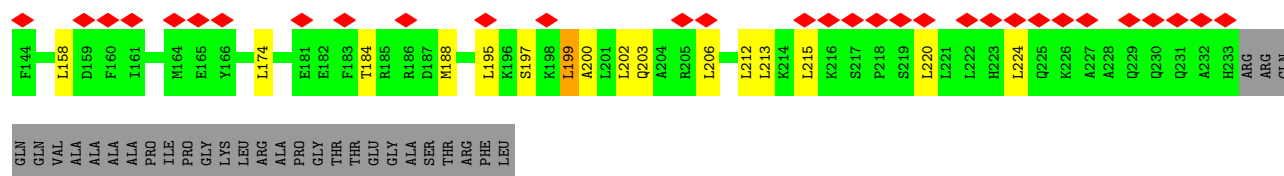
Chain 38: 32% 68% 13% 19%



- Molecule 5: Spindle assembly abnormal protein 6 N-terminal domain-containing protein

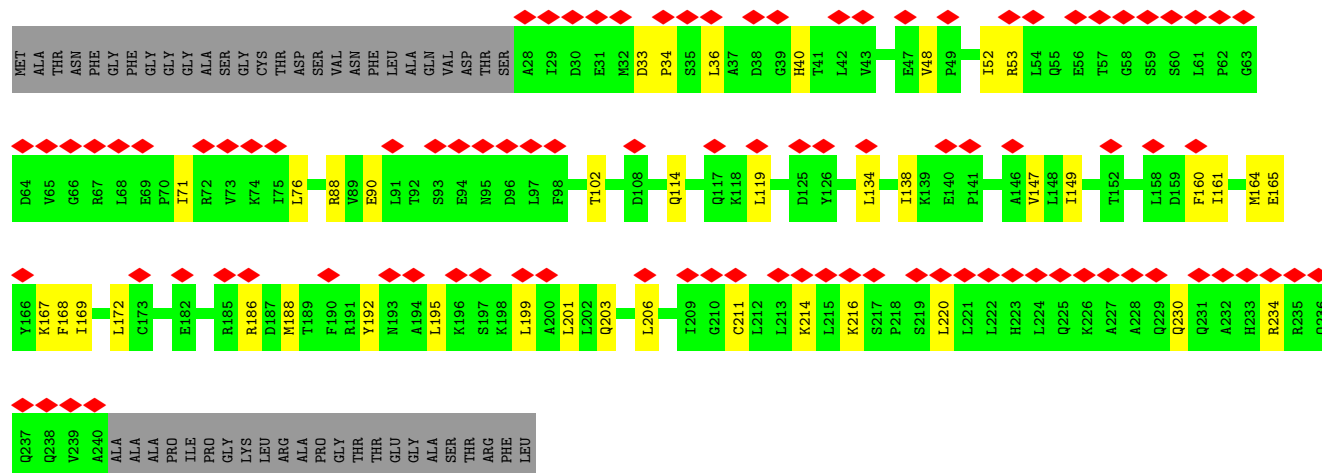
Chain 39: 37% 66% 16% 17%





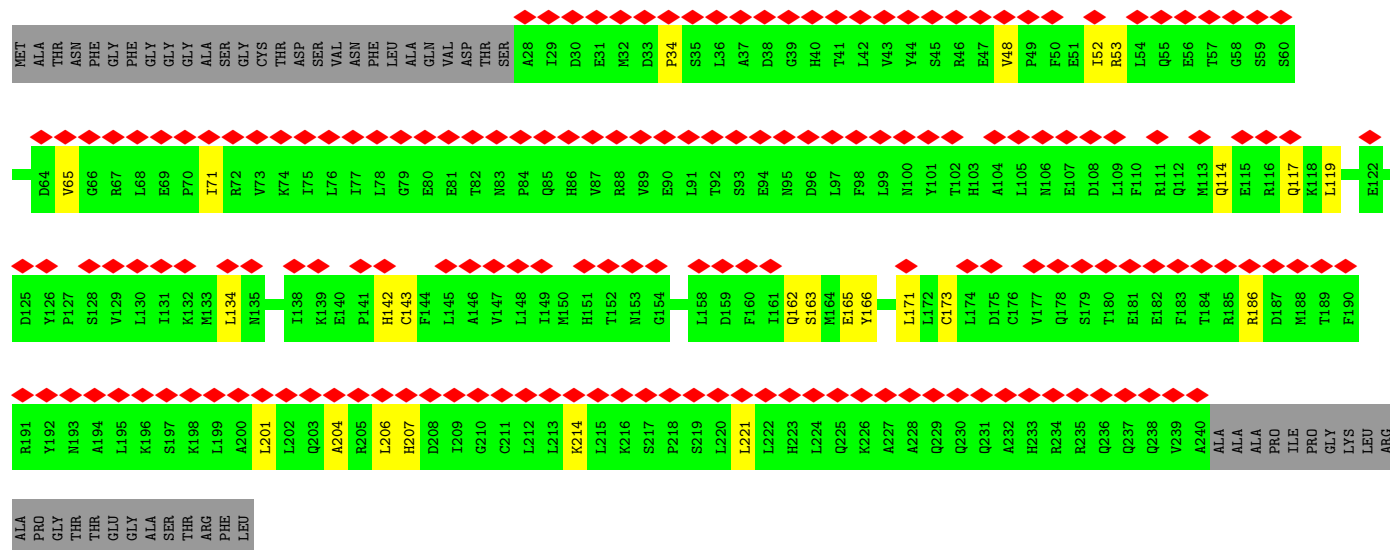
- Molecule 5: Spindle assembly abnormal protein 6 N-terminal domain-containing protein

Chain 40: 36% 66% 15% 19%



- Molecule 5: Spindle assembly abnormal protein 6 N-terminal domain-containing protein

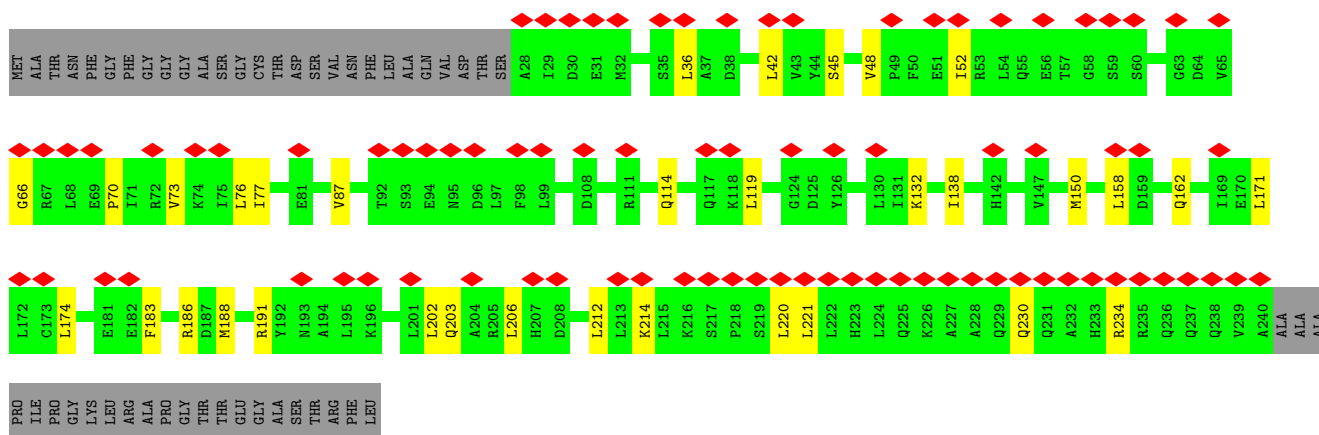
Chain 42: 67% 71% 10% 19%



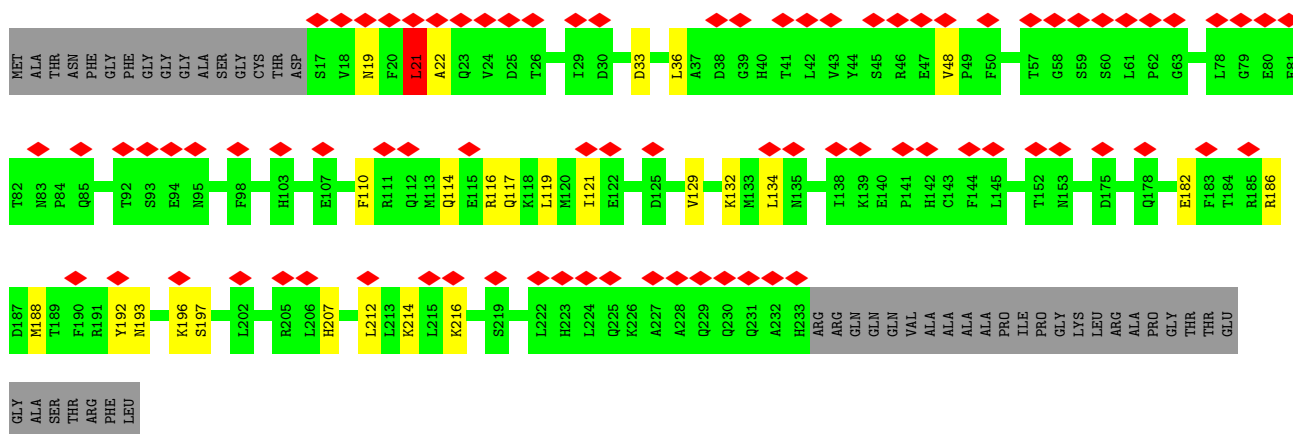
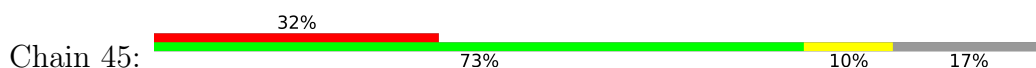
- Molecule 5: Spindle assembly abnormal protein 6 N-terminal domain-containing protein

Chain 43: 33% 68% 14% 17%

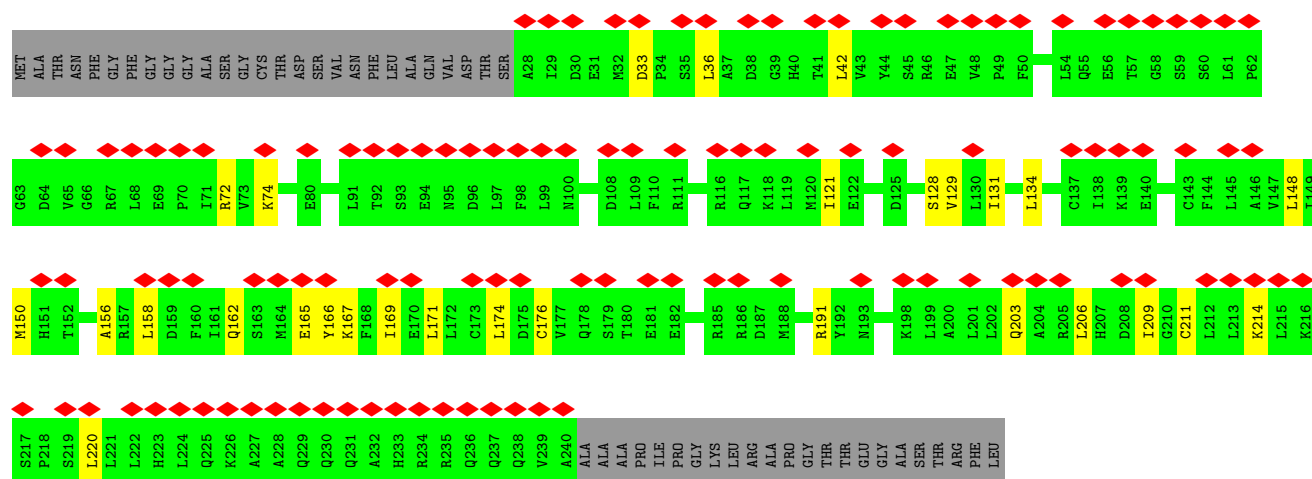
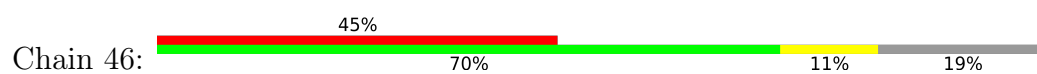
- Molecule 5: Spindle assembly abnormal protein 6 N-terminal domain-containing protein



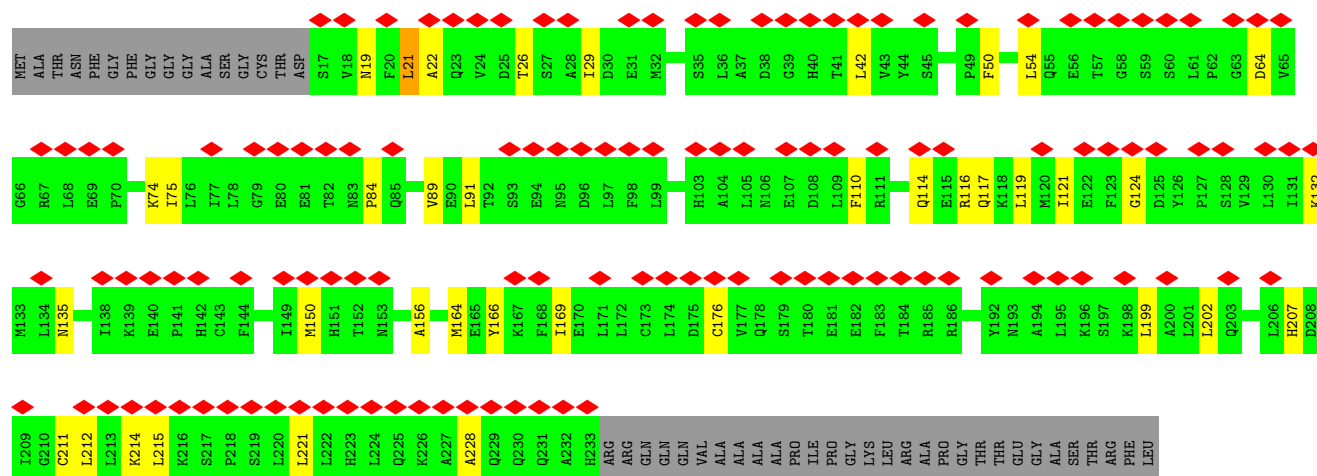
- Molecule 5: Spindle assembly abnormal protein 6 N-terminal domain-containing protein



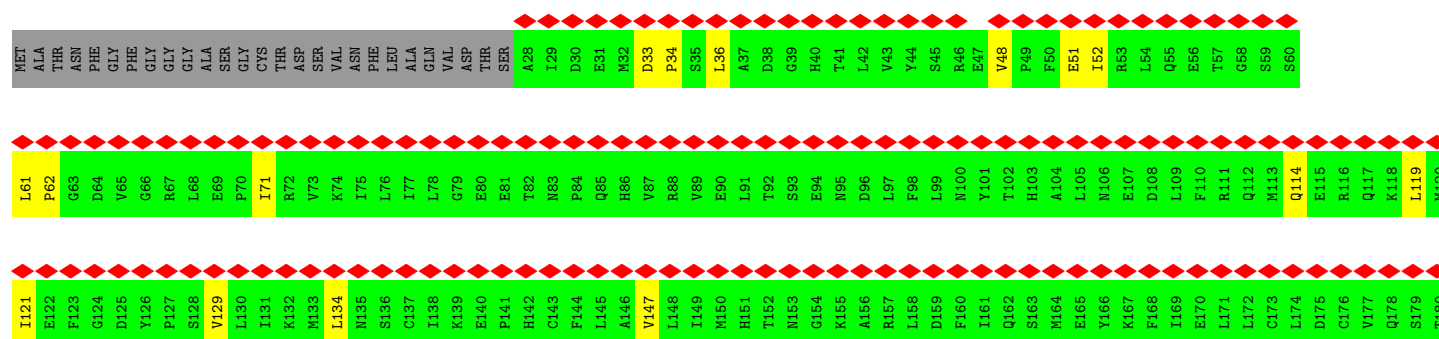
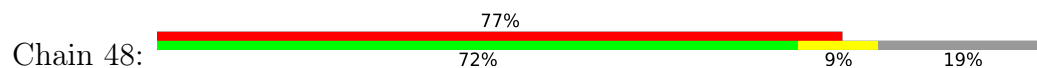
- Molecule 5: Spindle assembly abnormal protein 6 N-terminal domain-containing protein

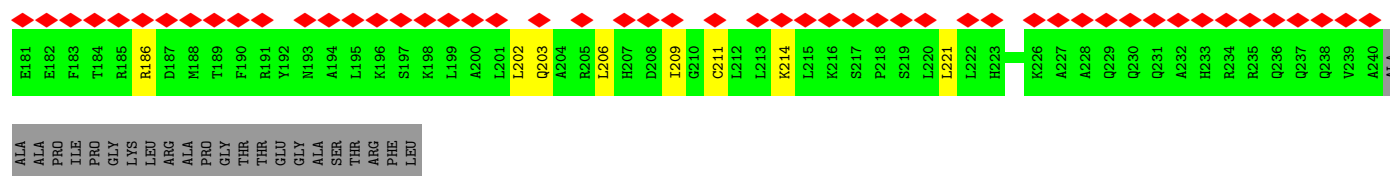


- Molecule 5: Spindle assembly abnormal protein 6 N-terminal domain-containing protein

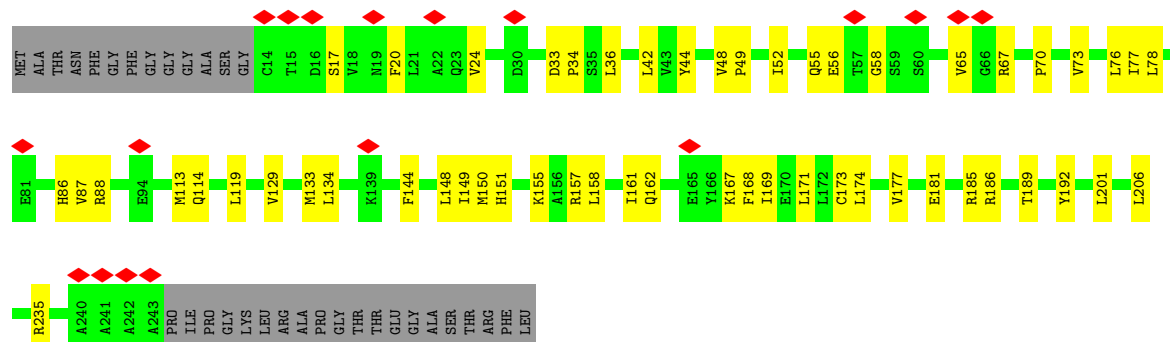


- Molecule 5: Spindle assembly abnormal protein 6 N-terminal domain-containing protein

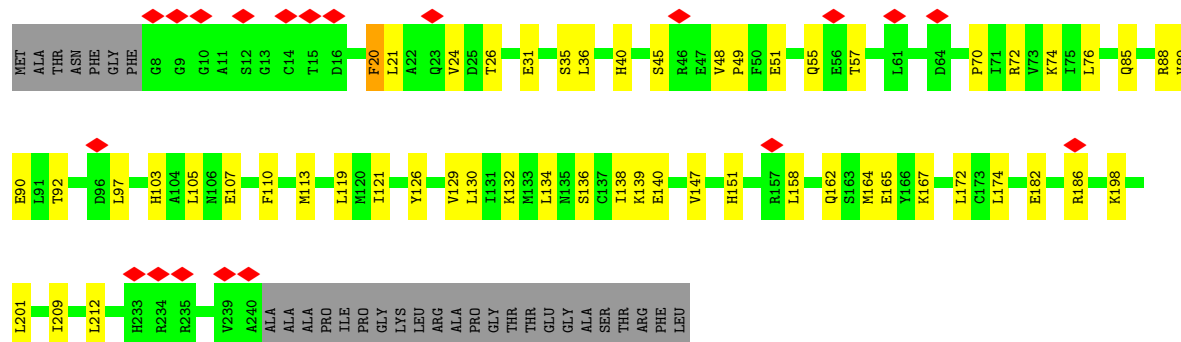




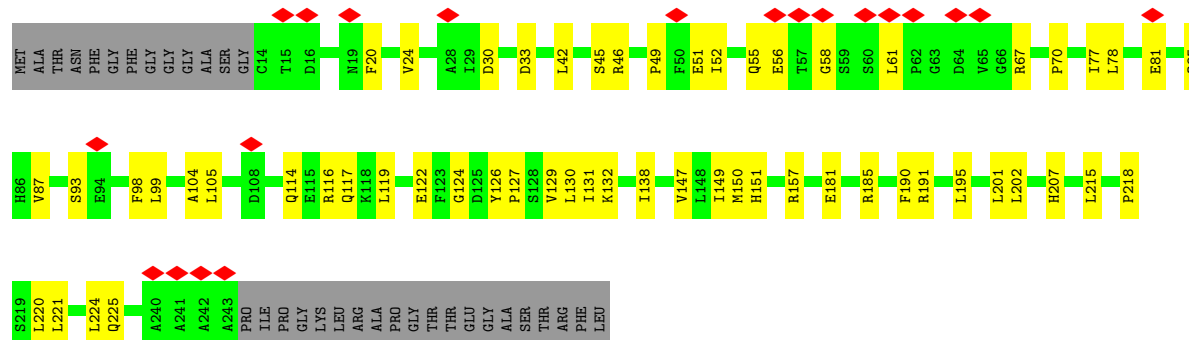
- Molecule 5: Spindle assembly abnormal protein 6 N-terminal domain-containing protein



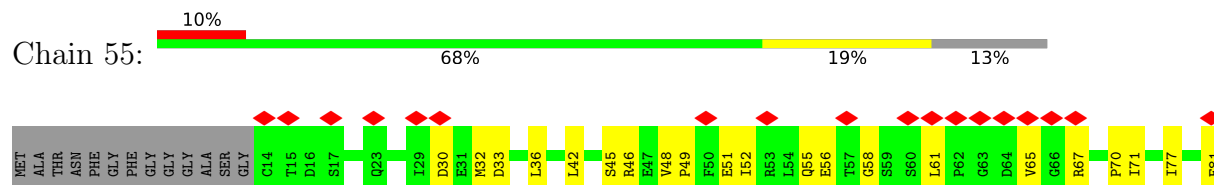
- Molecule 5: Spindle assembly abnormal protein 6 N-terminal domain-containing protein

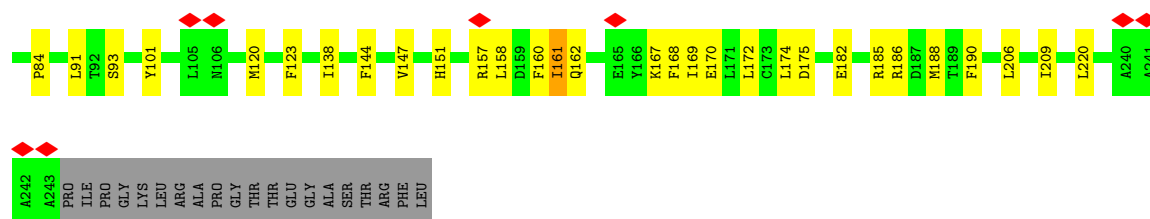


- Molecule 5: Spindle assembly abnormal protein 6 N-terminal domain-containing protein

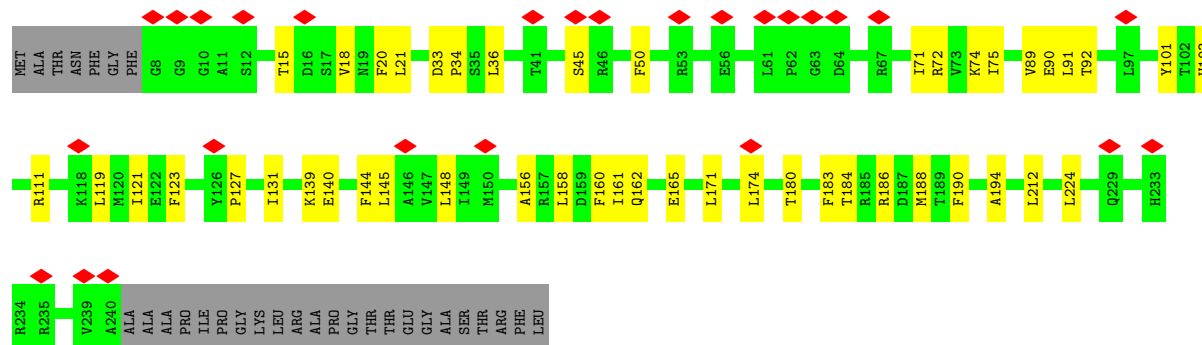
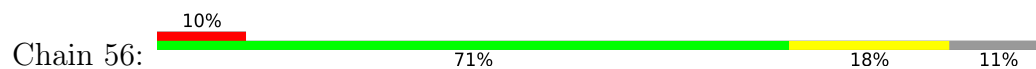


- Chain 52:

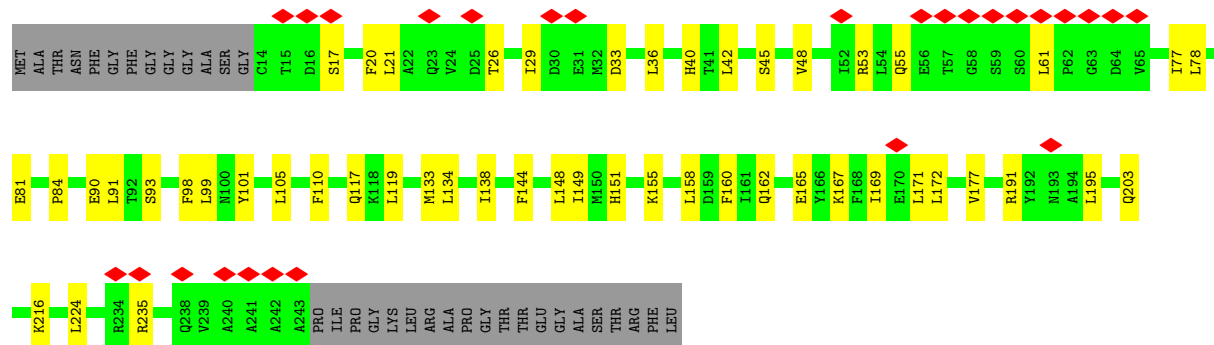




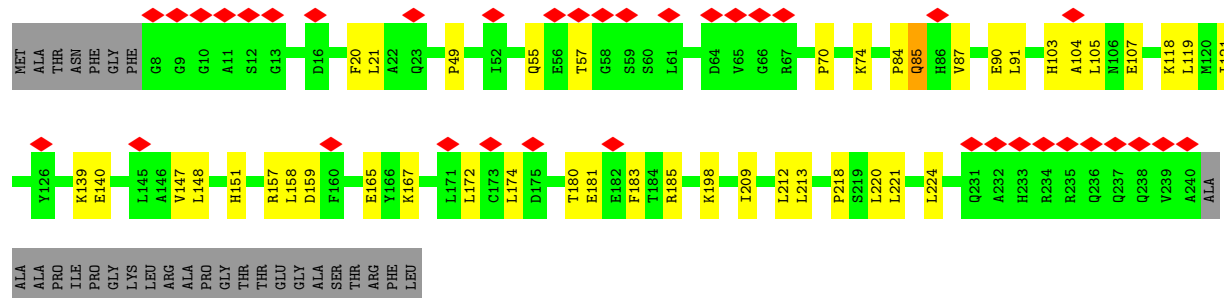
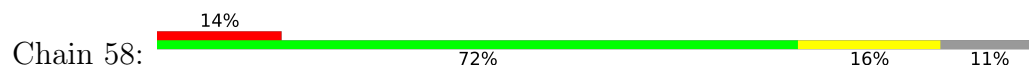
- Molecule 5: Spindle assembly abnormal protein 6 N-terminal domain-containing protein



- Molecule 5: Spindle assembly abnormal protein 6 N-terminal domain-containing protein



- Molecule 5: Spindle assembly abnormal protein 6 N-terminal domain-containing protein



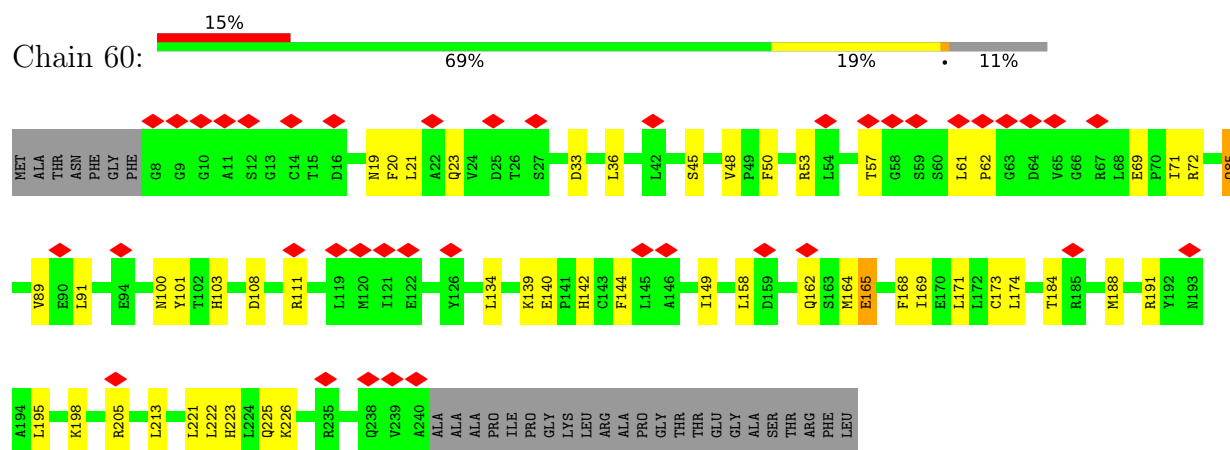
- Molecule 5: Spindle assembly abnormal protein 6 N-terminal domain-containing protein

Chain 59:



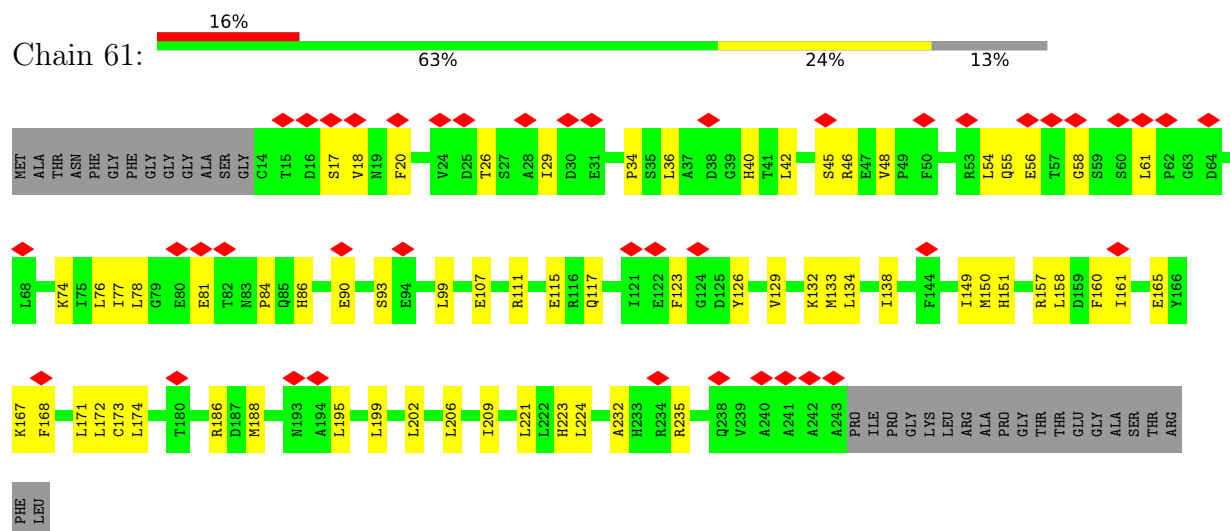
- Molecule 5: Spindle assembly abnormal protein 6 N-terminal domain-containing protein

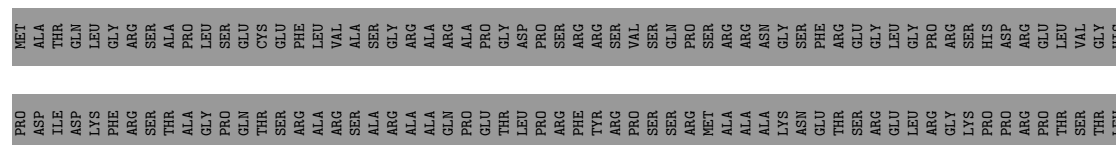
Chain 60:

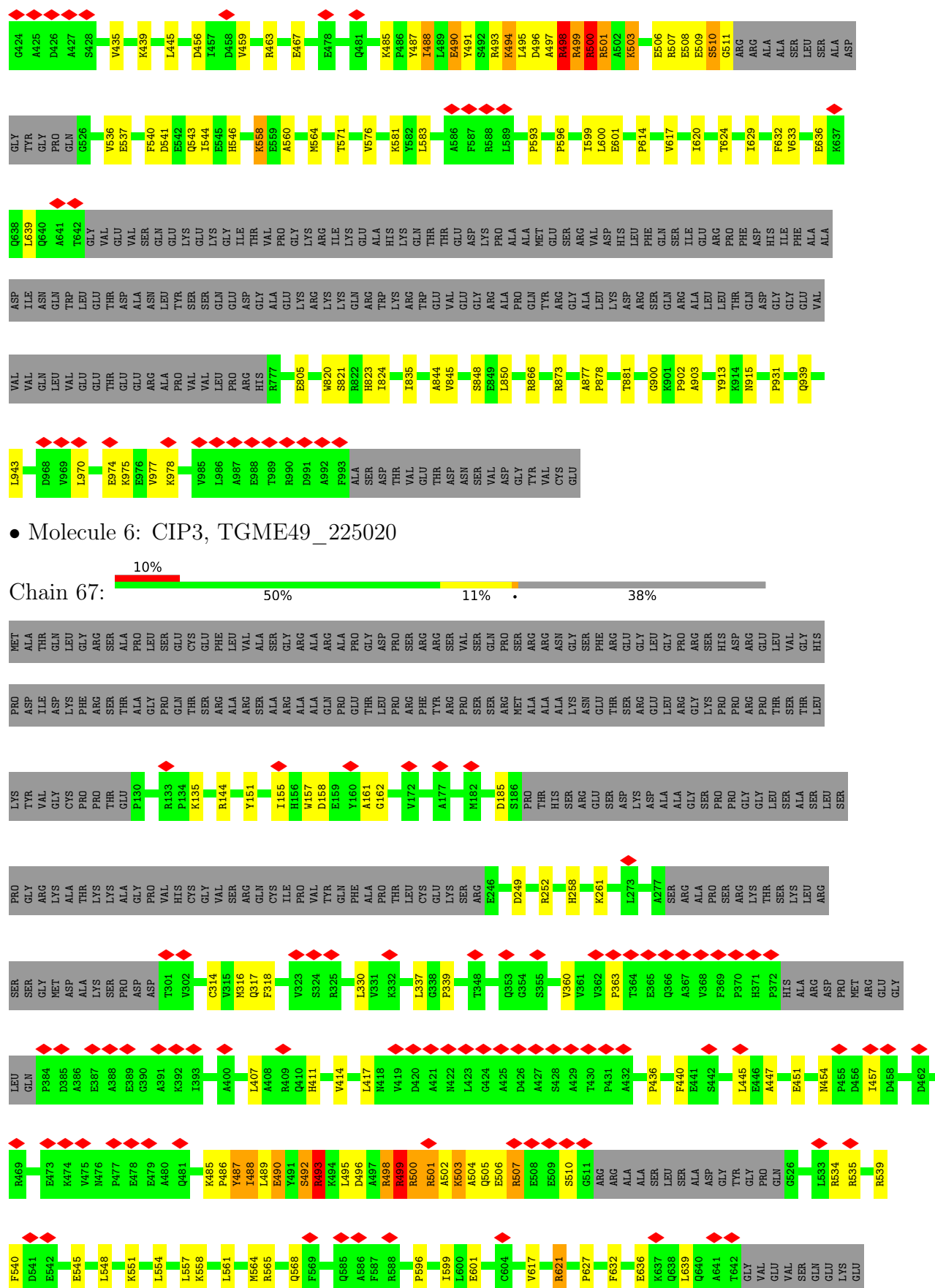


- Molecule 5: Spindle assembly abnormal protein 6 N-terminal domain-containing protein

Chain 61:

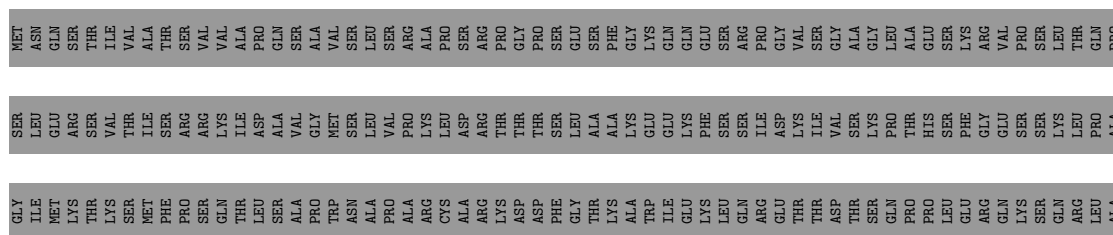
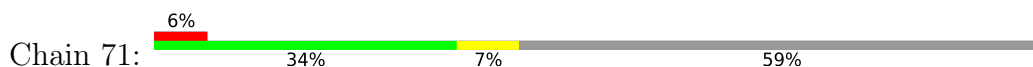
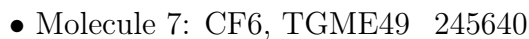


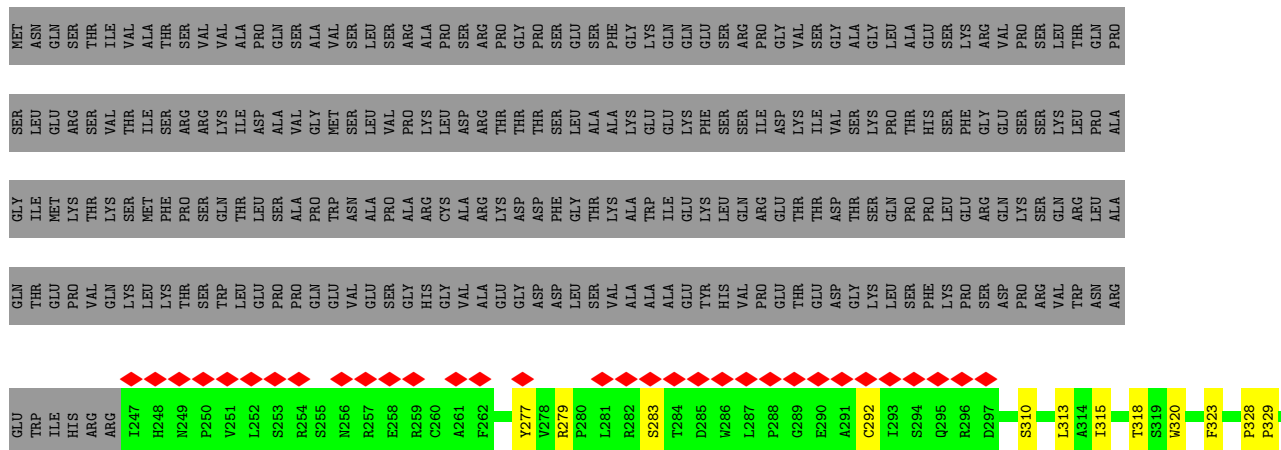


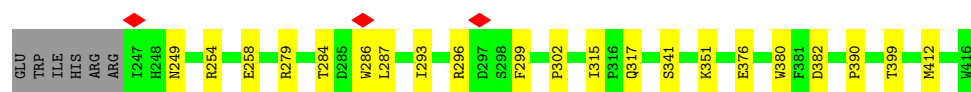


• Molecule 6: CIP3, TGME49_225020

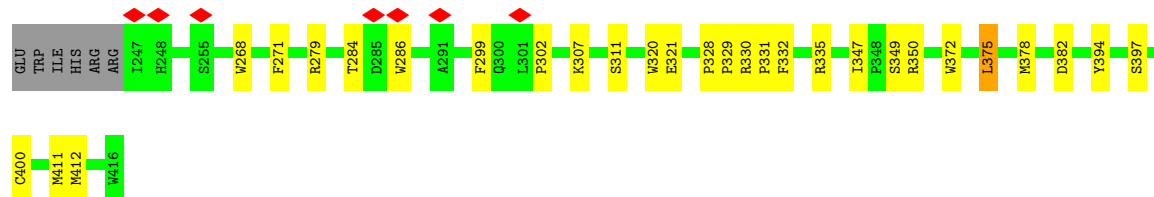
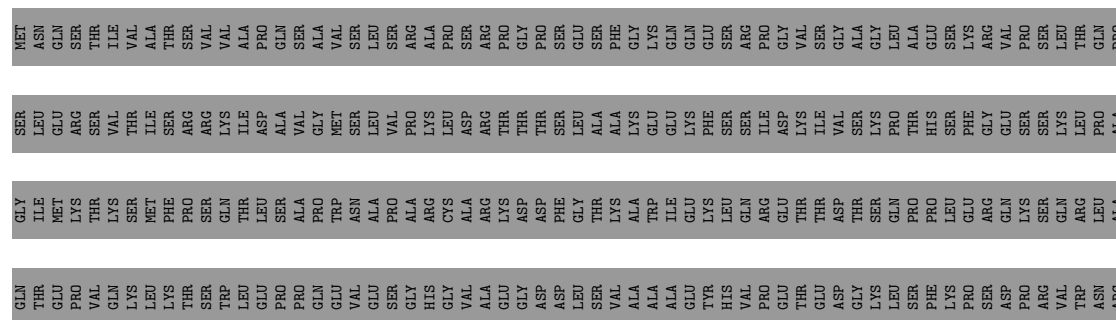
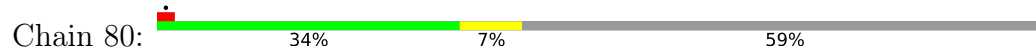
Chain 69: 50% 11% 38%



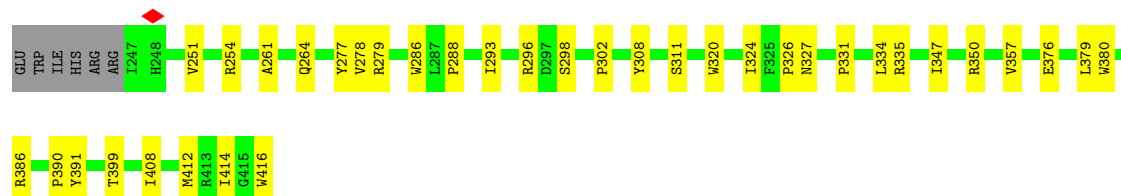
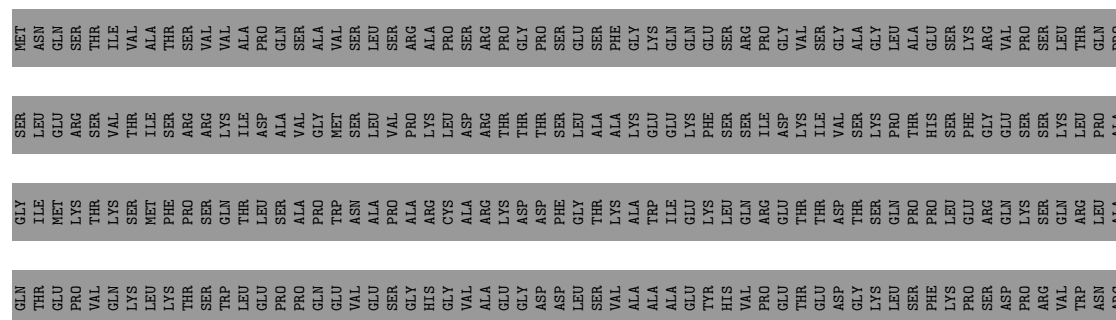




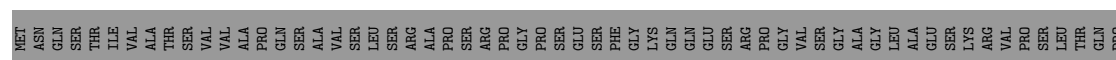
• Molecule 7: CF6, TGME49_245640



• Molecule 7: CF6, TGME49_245640

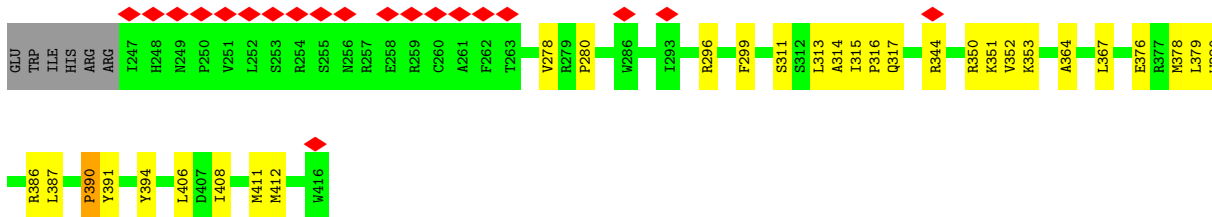
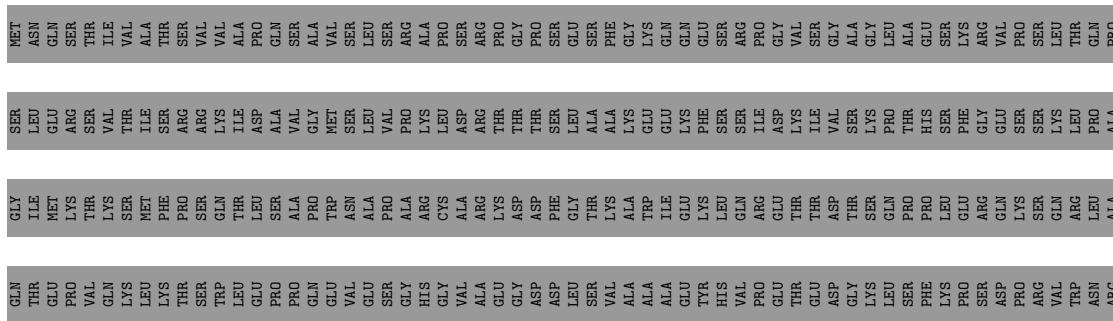
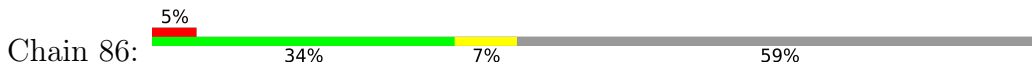


• Molecule 7: CF6, TGME49_245640

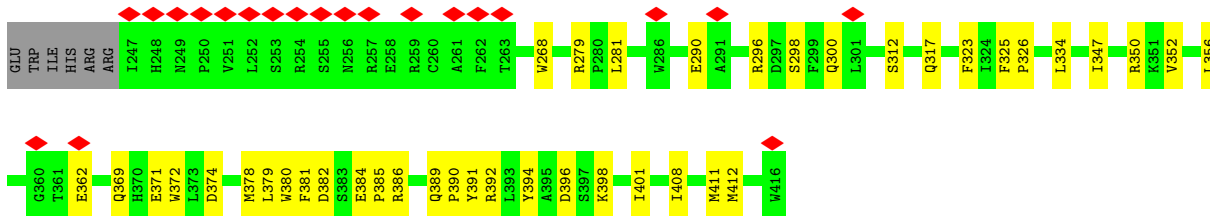
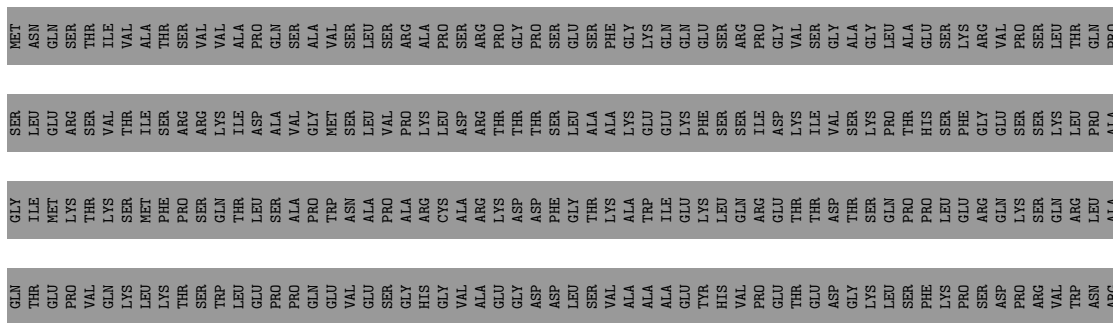
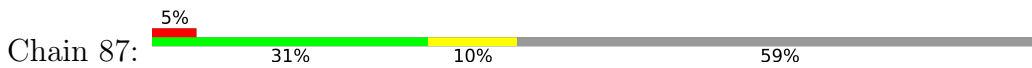




- Molecule 7: CF6, TGME49_245640



- Molecule 7: CF6, TGME49_245640



- Molecule 7: CF6, TGME49_245640

Frequency	Percentage
Daily	32%
Weekly	8%
Monthly	59%

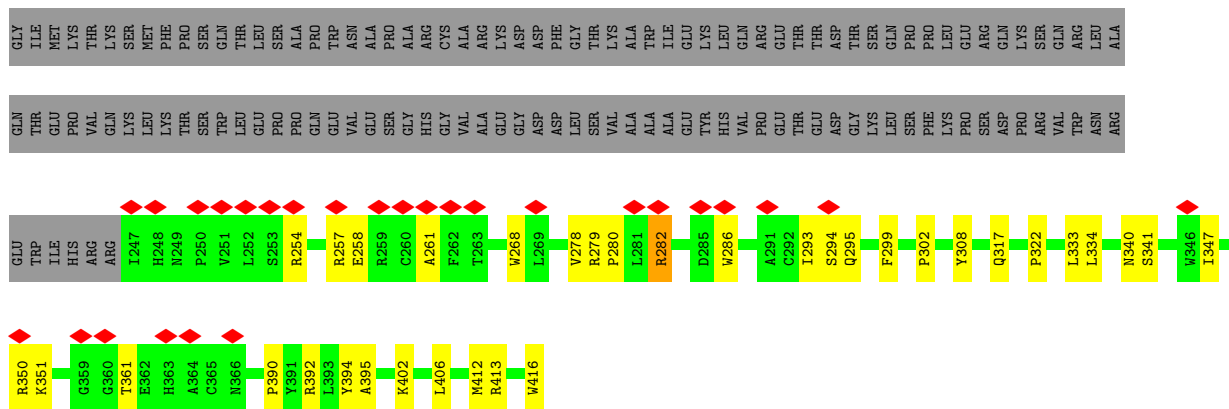
- Molecule 7: CF6, TGME49 245640

Frequency	Percentage
Daily	32%
Weekly	9%
Monthly	59%

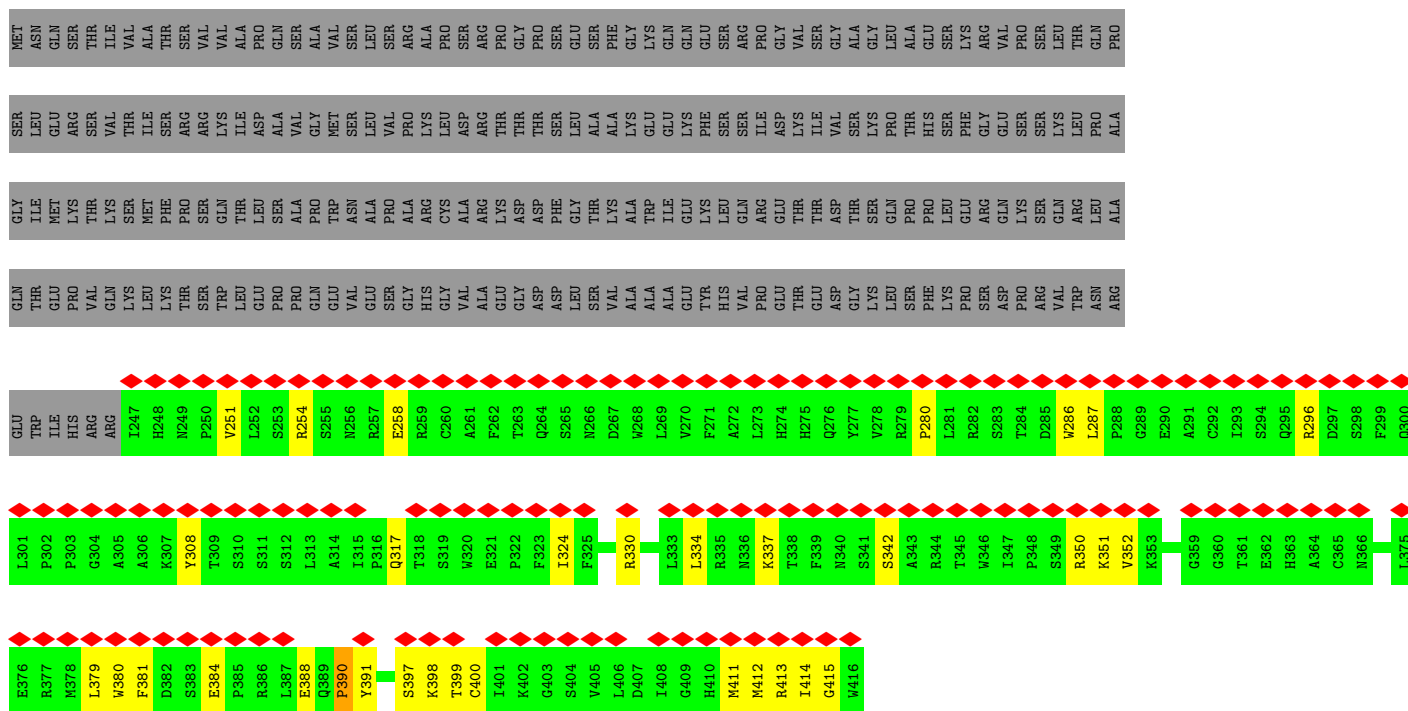
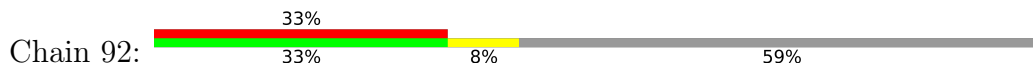
- Molecule 7: CF6, TGME49 245640

Frequency	Percentage
Very often	6%
Often	32%
Sometimes	8%
Never	59%

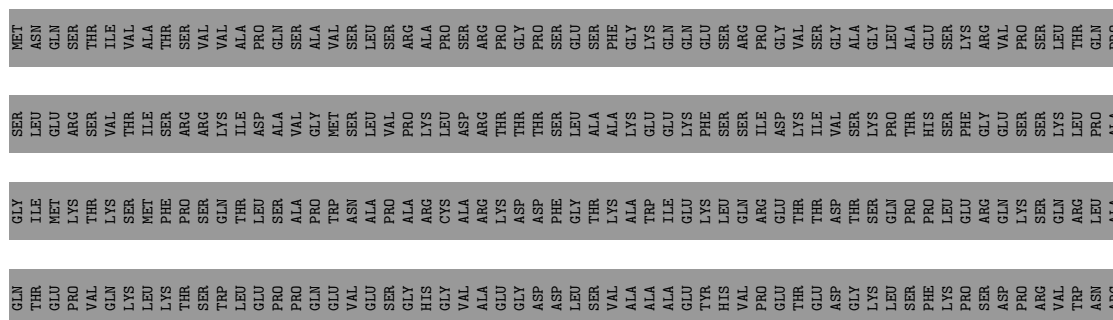
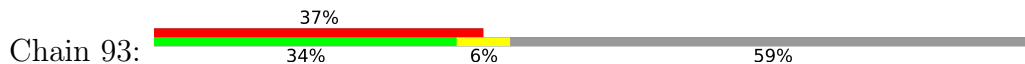
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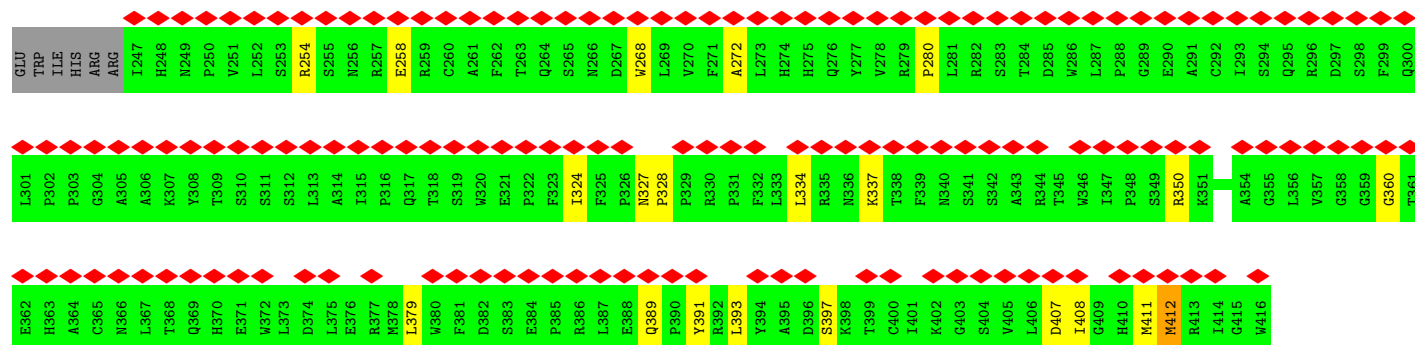


- Molecule 7: CF6, TGME49_245640

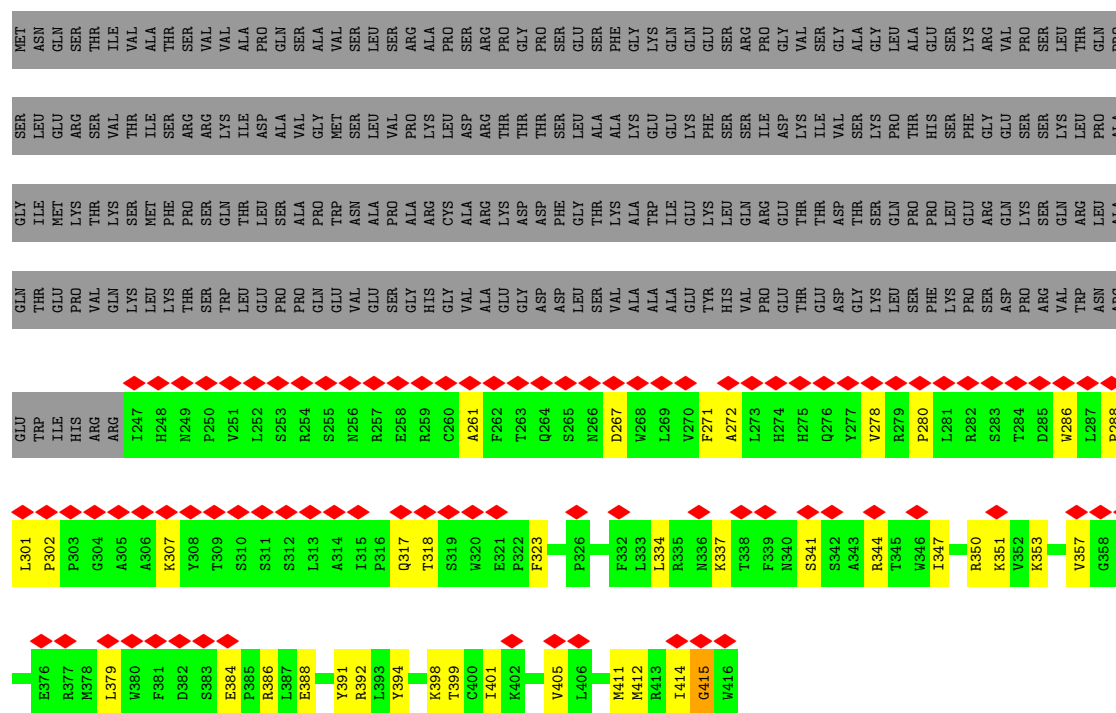
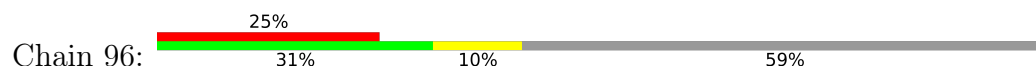


- Molecule 7: CF6, TGME49_245640

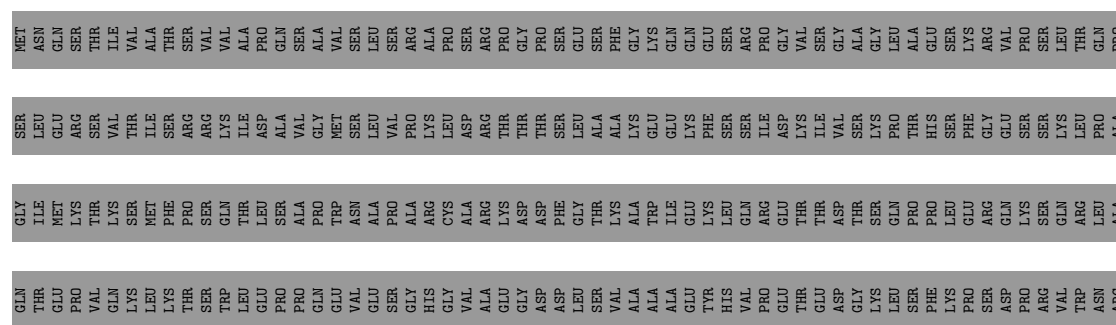
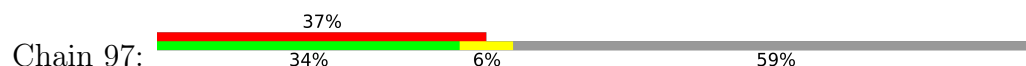


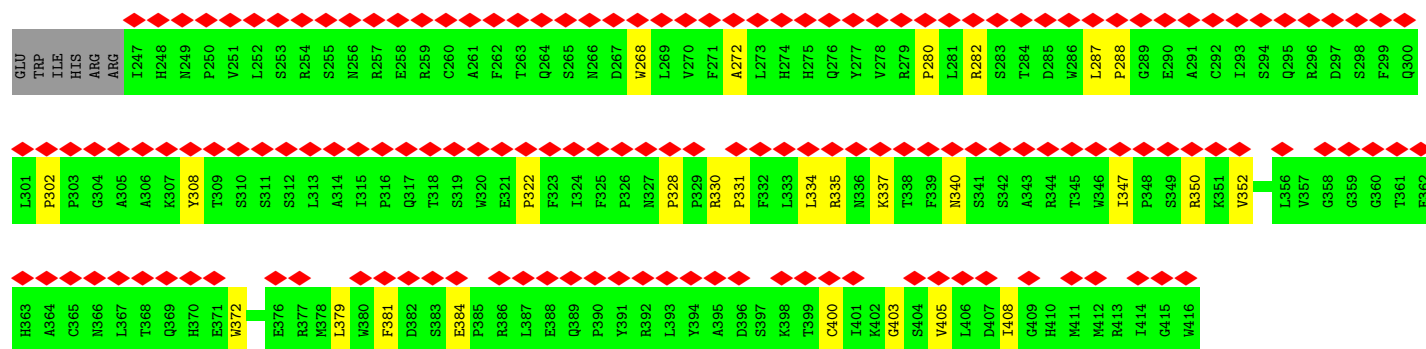


• Molecule 7: CF6, TGME49_245640



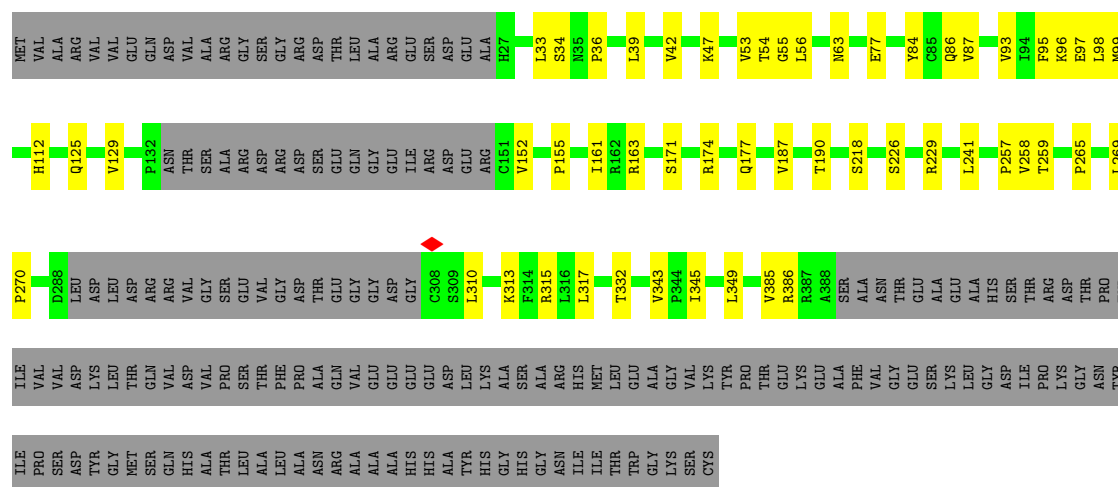
• Molecule 7: CF6, TGME49_245640





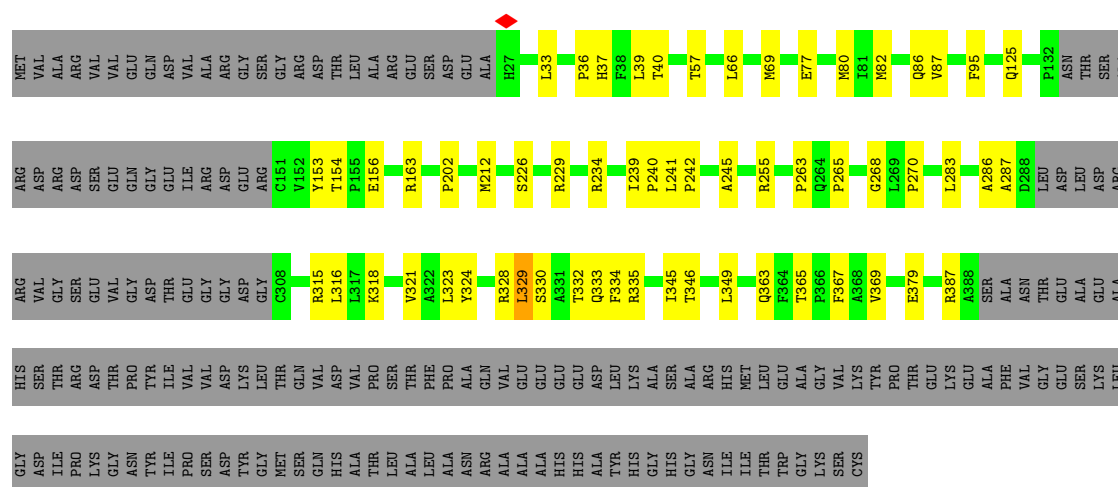
• Molecule 8: CF₄, TGME49_246720

Chain A1: 54% 11% 35%



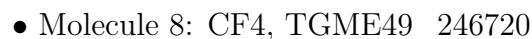
• Molecule 8: CF₄, TGME49_246720

Chain A2: 53% 12% 35%

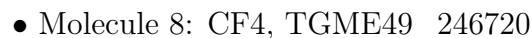


• Molecule 8: CF₄, TGME49_246720

Category	Percentage
Very bad	37%
Bad	9%
Good	54%

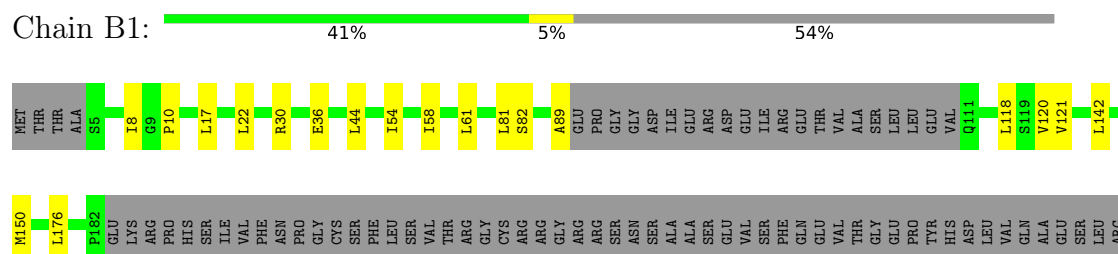
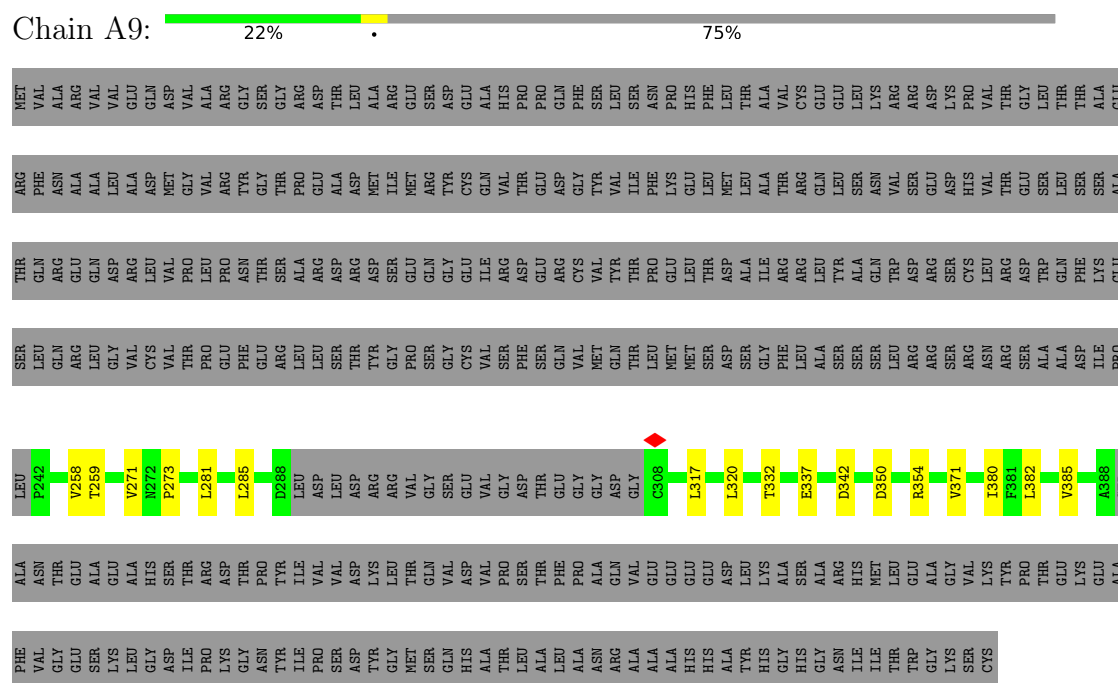


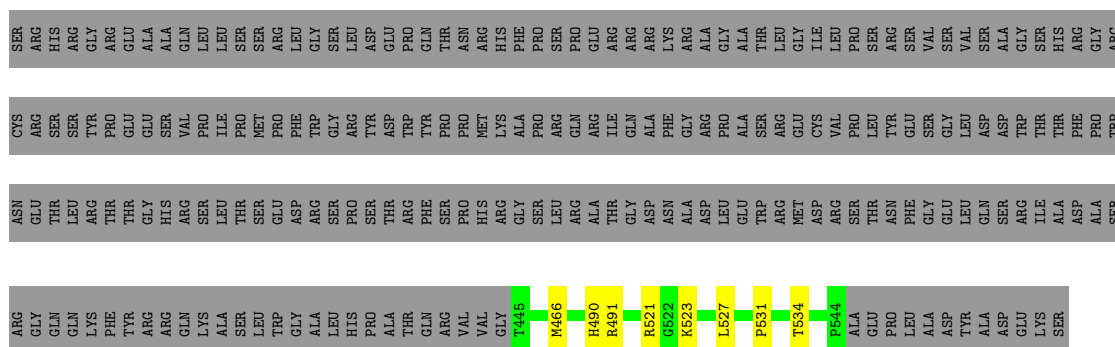
Response	Percentage
Yes	23%
No	5%
Not sure	72%



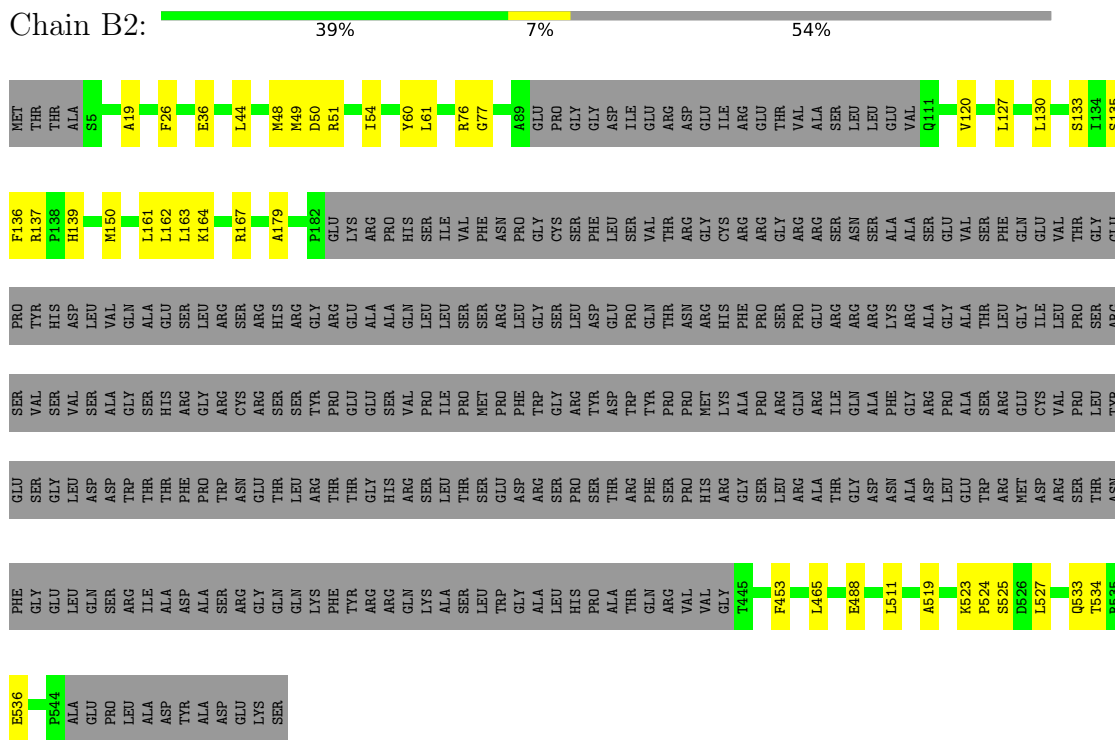
Response	Percentage
Used	57%
Not used	8%
Don't know	35%



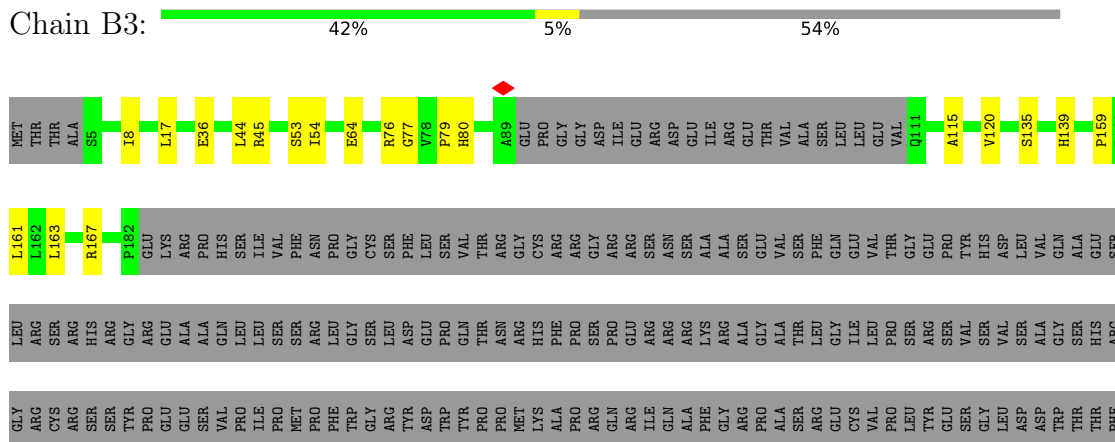


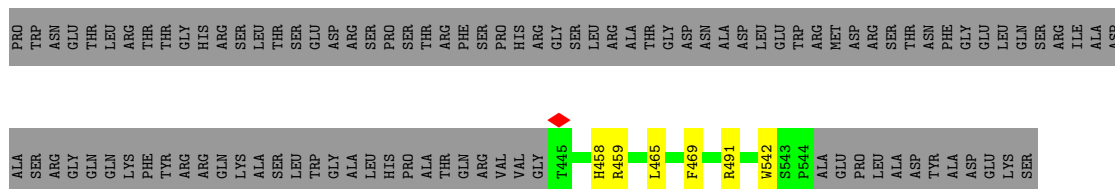


- Molecule 9: CF3, TGME49_255895

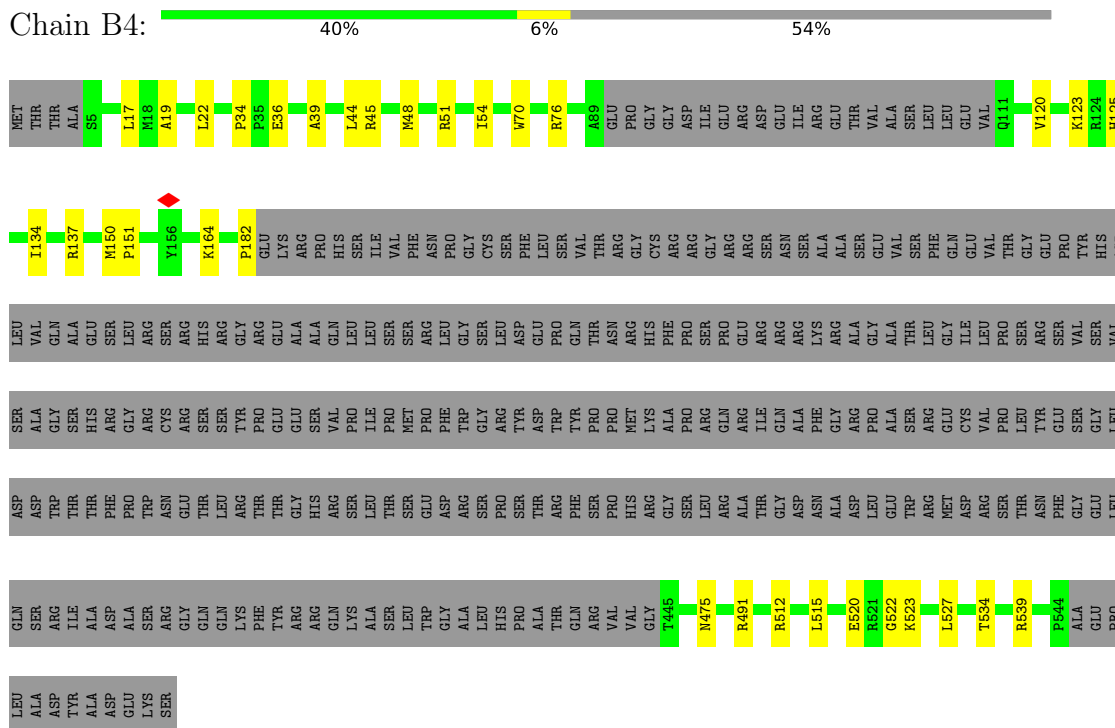


- Molecule 9: CF3, TGME49_255895

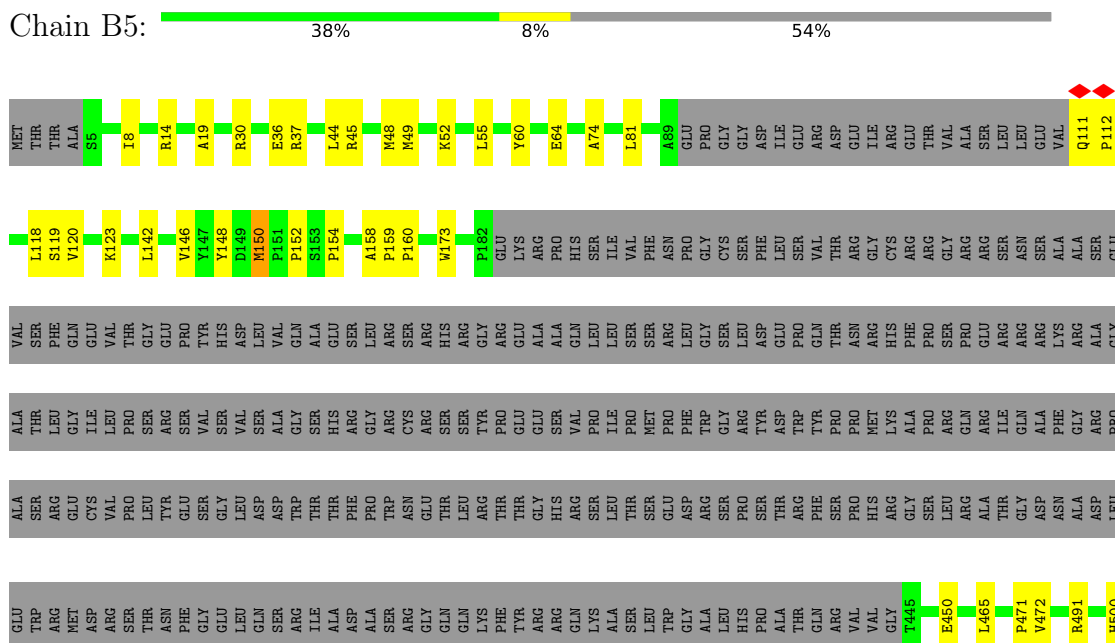




- Molecule 9: CF3, TGME49 255895



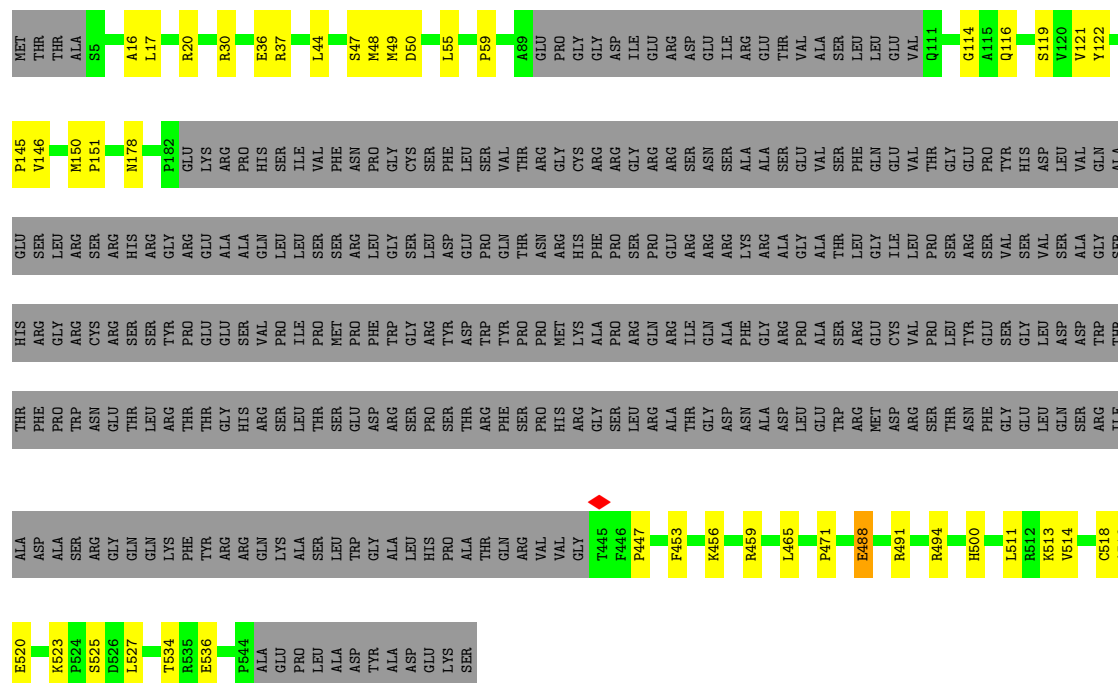
- Molecule 9: CF3, TGME49 255895





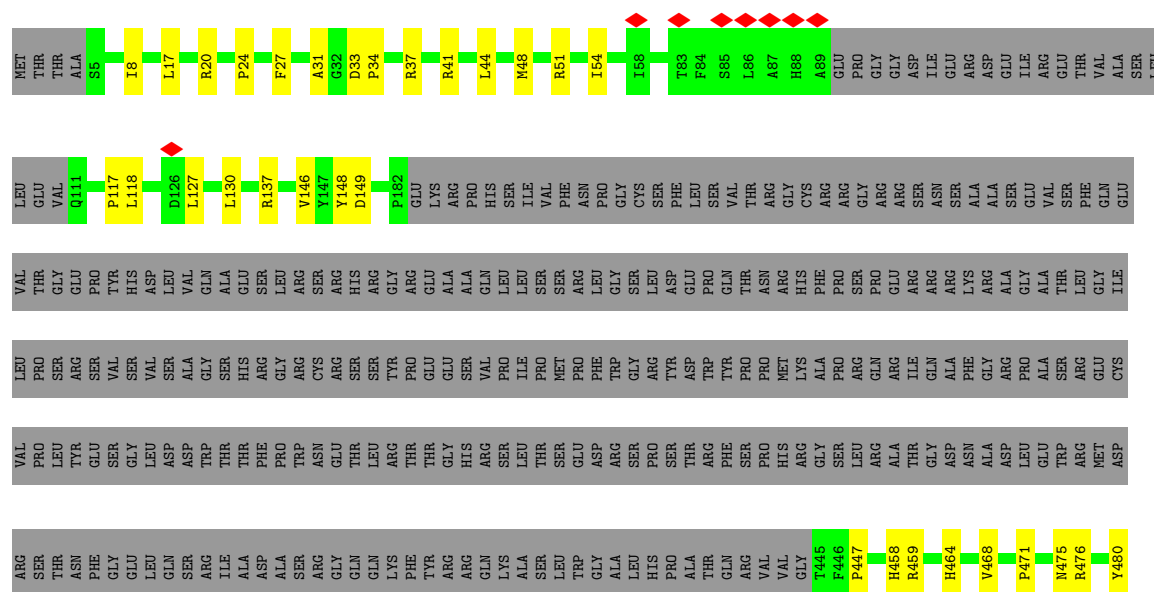
• Molecule 9: CF3, TGME49_255895

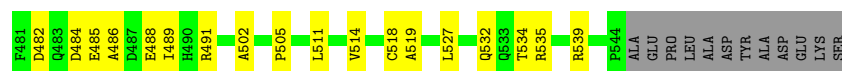
Chain B6: 38% 8% 54%



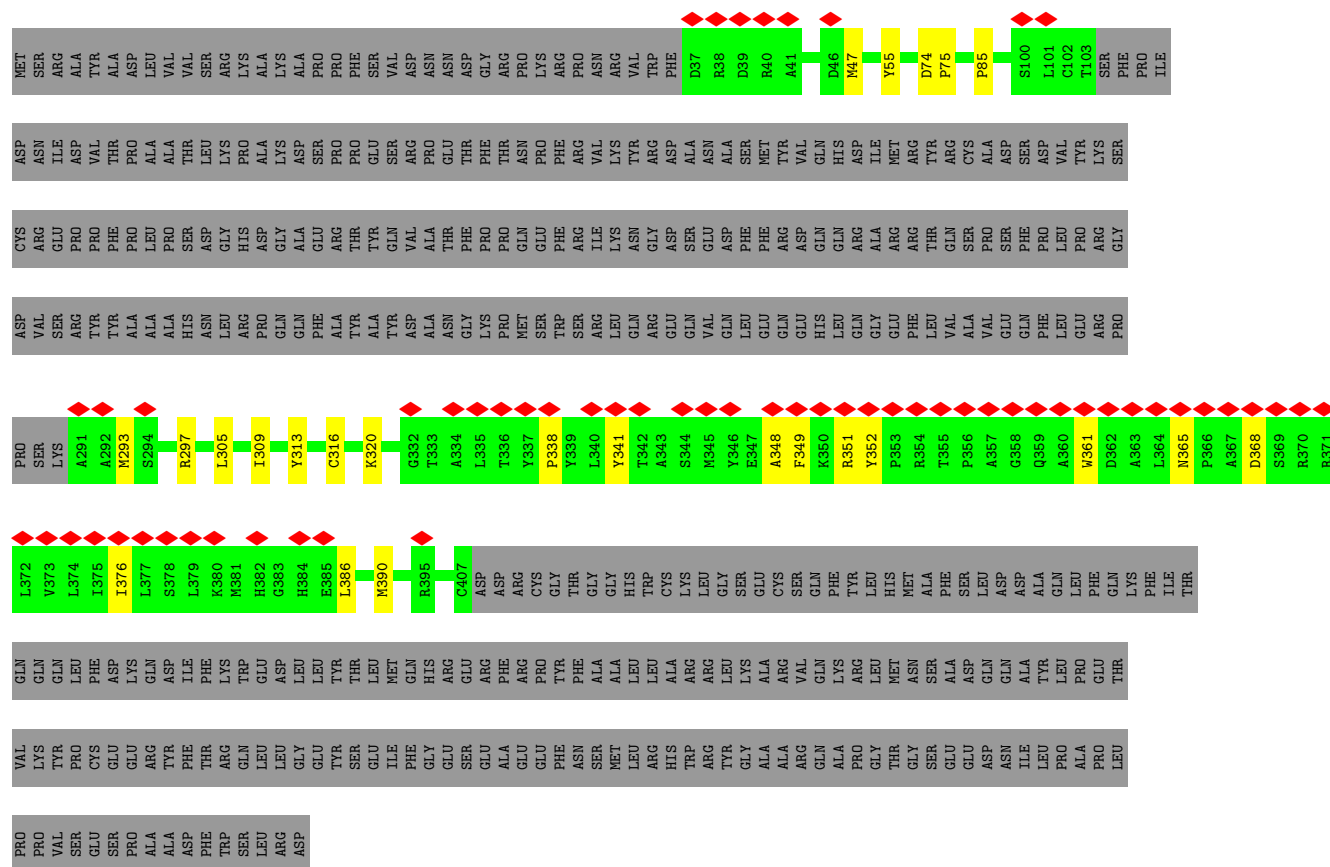
• Molecule 9: CF3, TGME49_255895

Chain B7: 37% 9% 54%

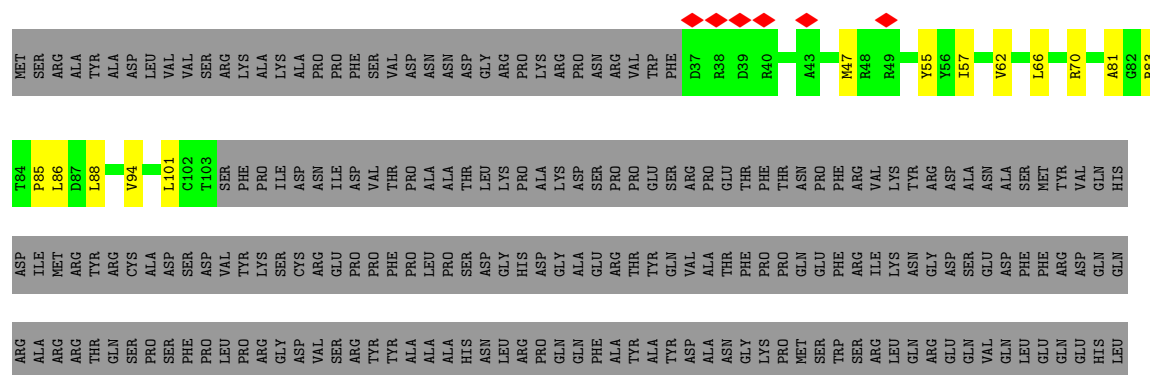




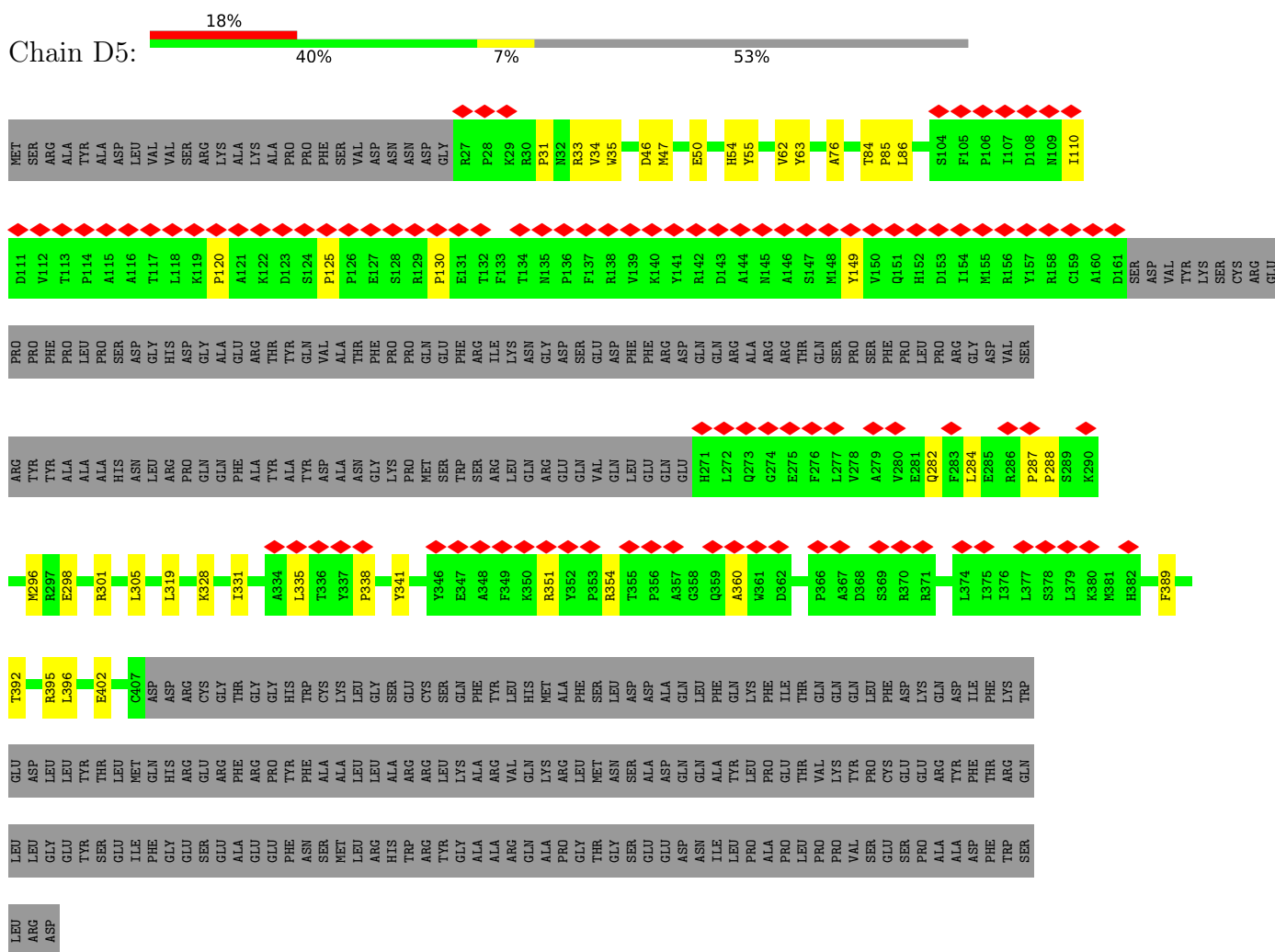
• Molecule 10: CPH1, TGME49_266630



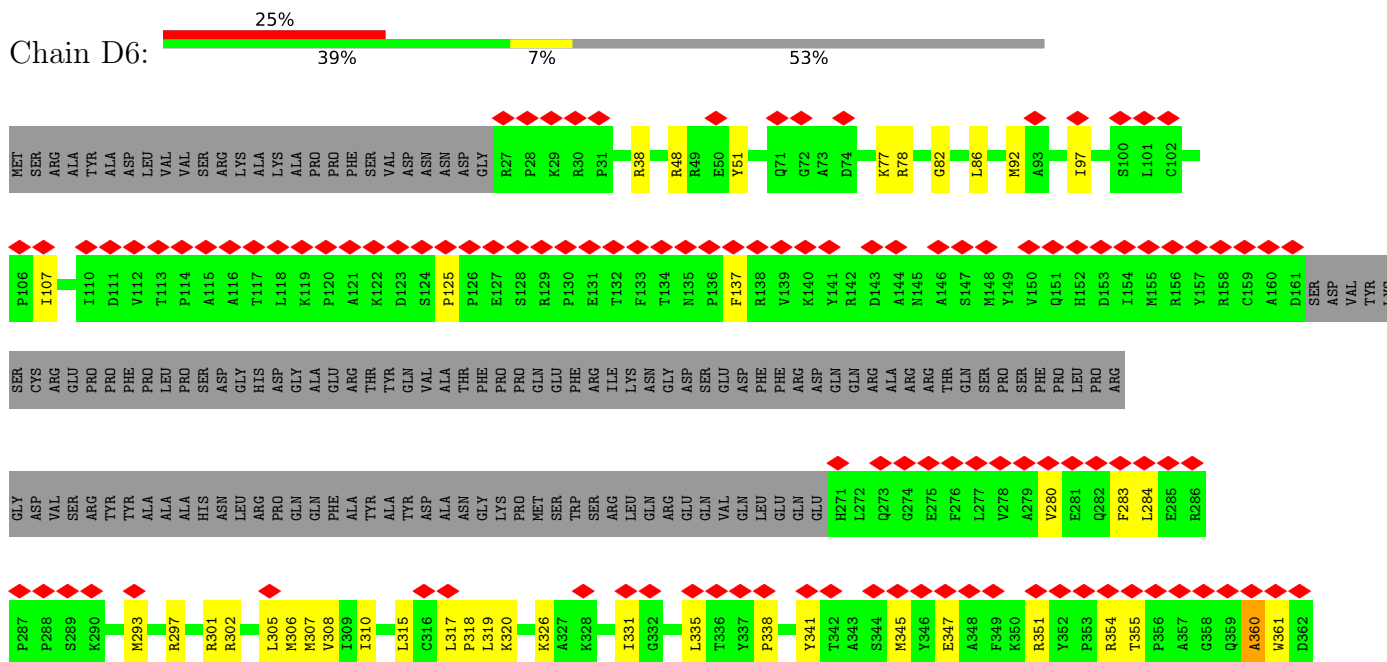
• Molecule 10: CPH1, TGME49_266630



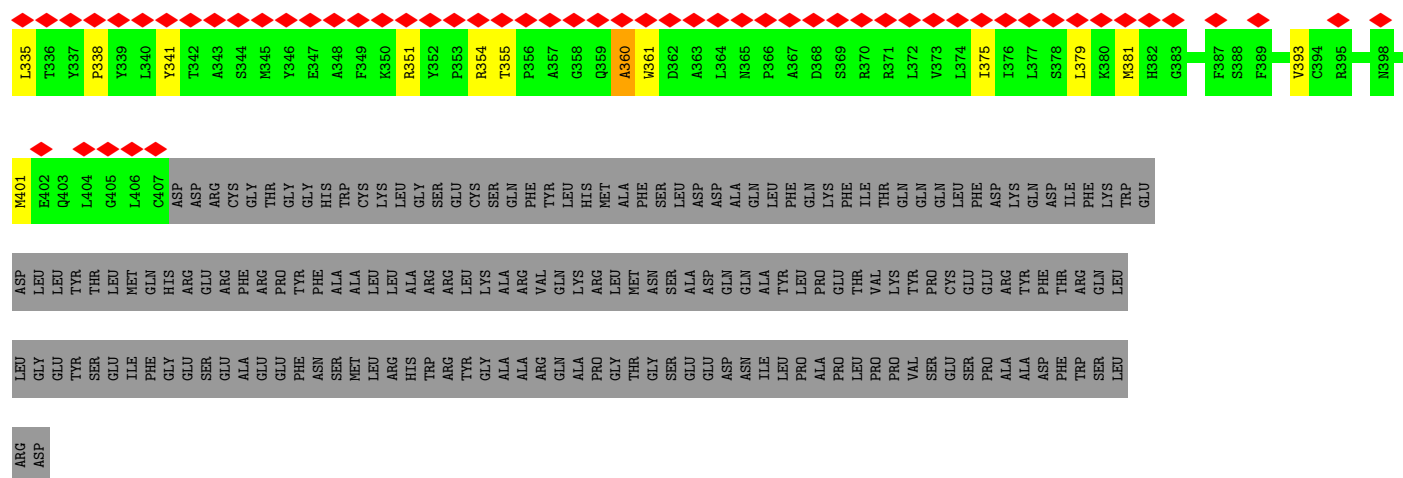




- Molecule 10: CPH1, TGME49 266630

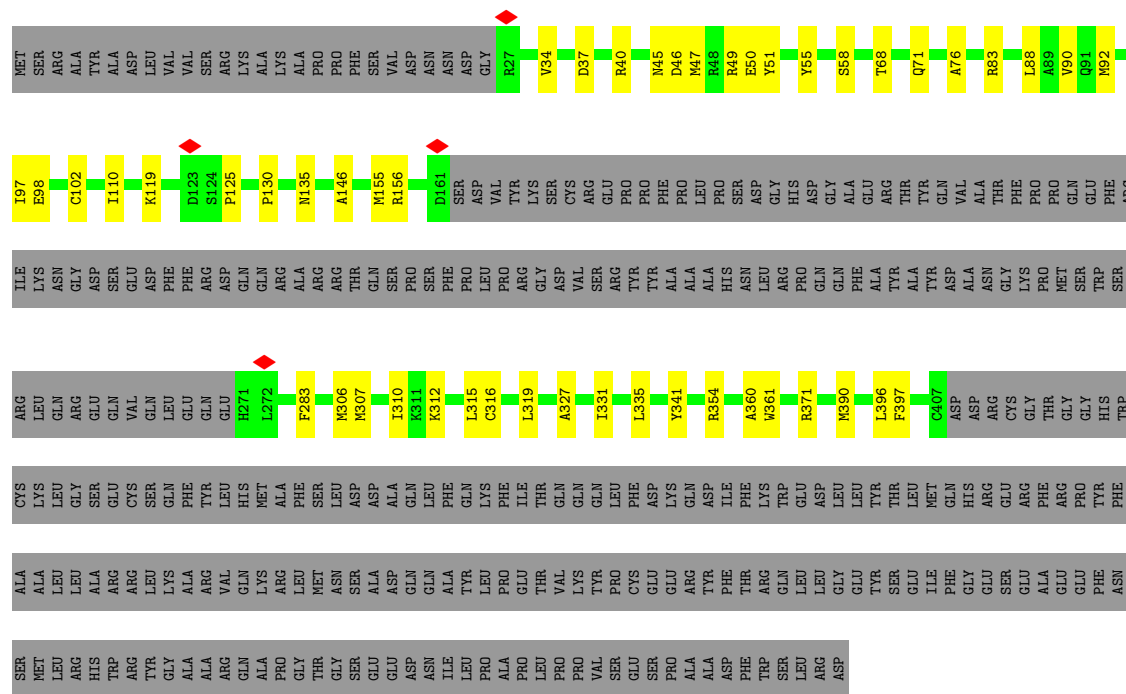






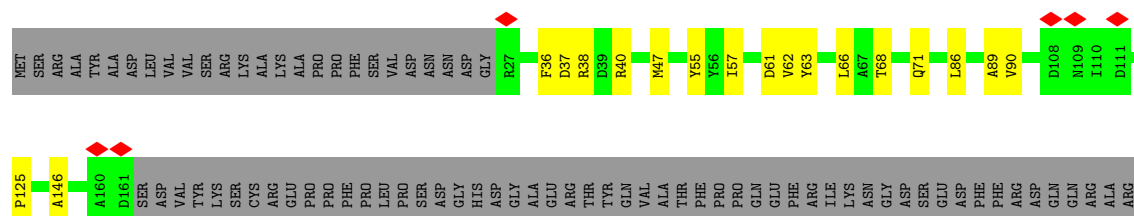
• Molecule 10: CPH1, TGME49_266630

Chain E4: 38% 8% 53%



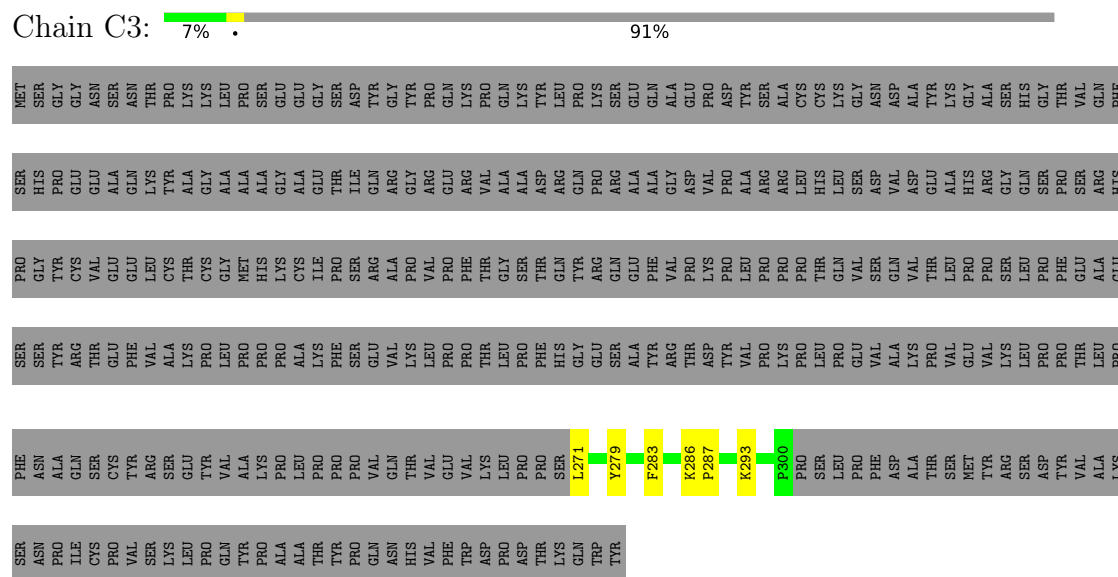
• Molecule 10: CPH1, TGME49_266630

Chain E5: 41% 6% 53%

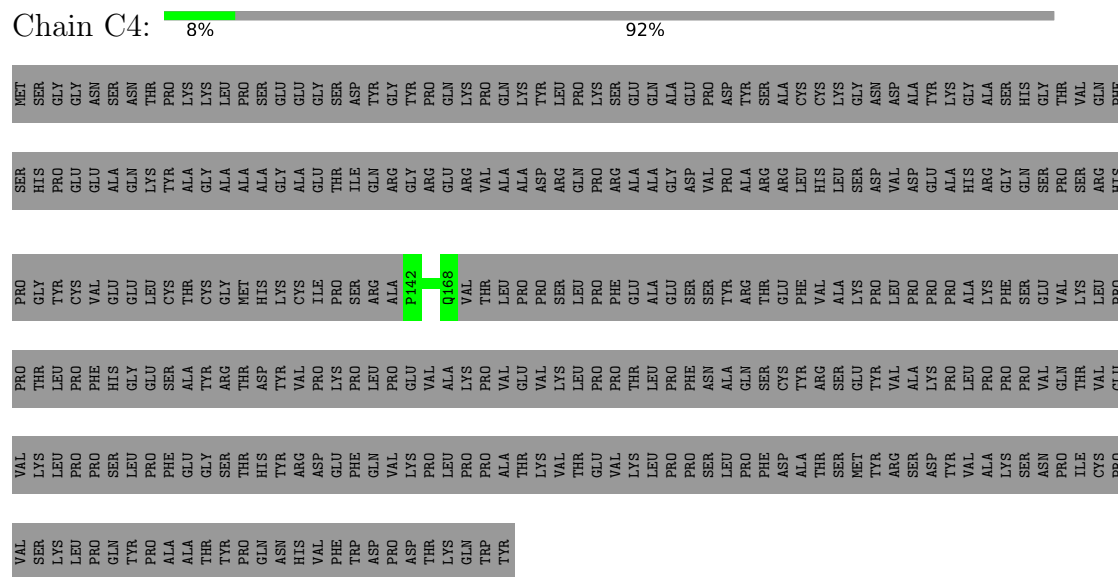




● Molecule 11: Microtubule associated protein SPM1

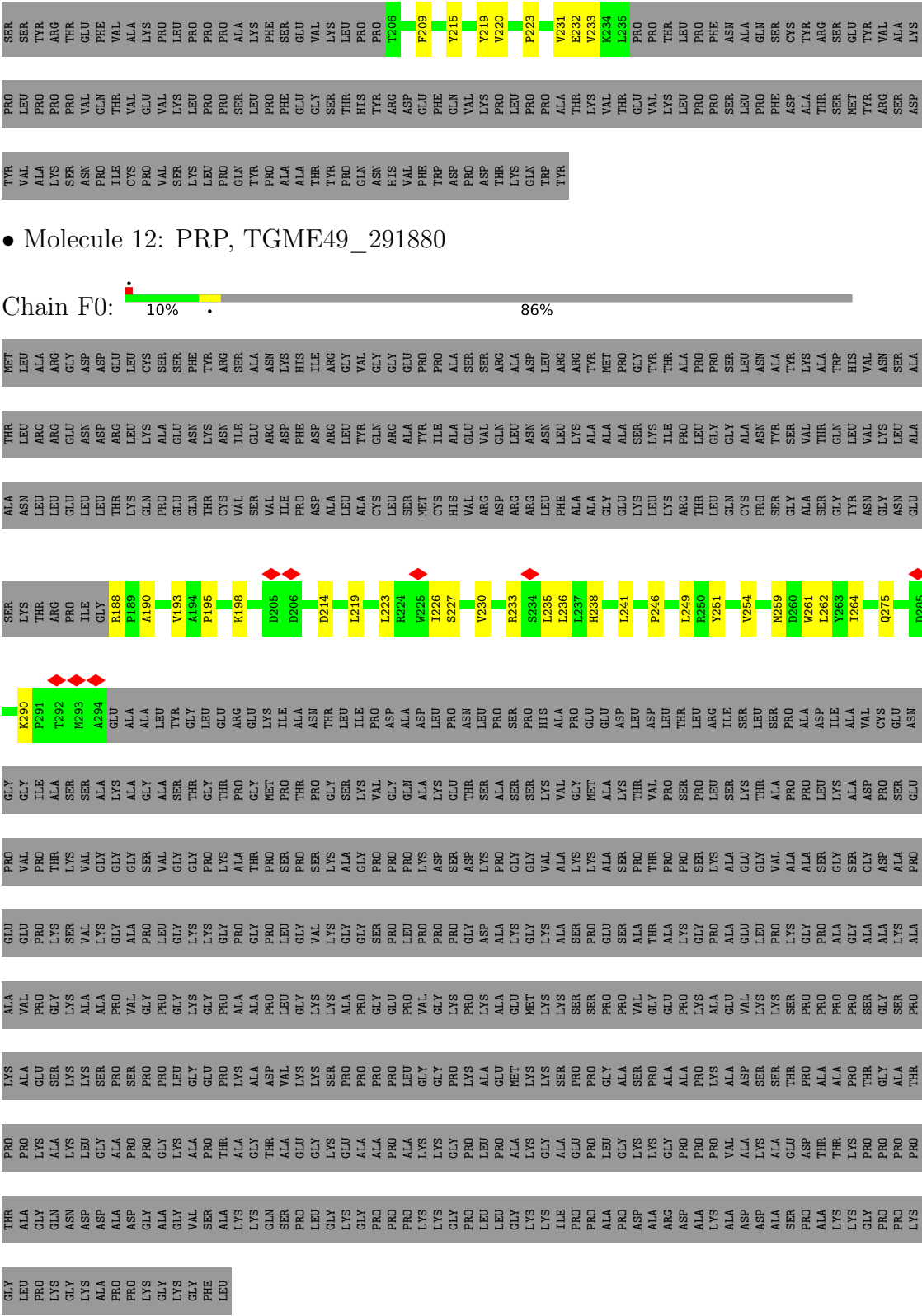


● Molecule 11: Microtubule associated protein SPM1



● Molecule 11: Microtubule associated protein SPM1

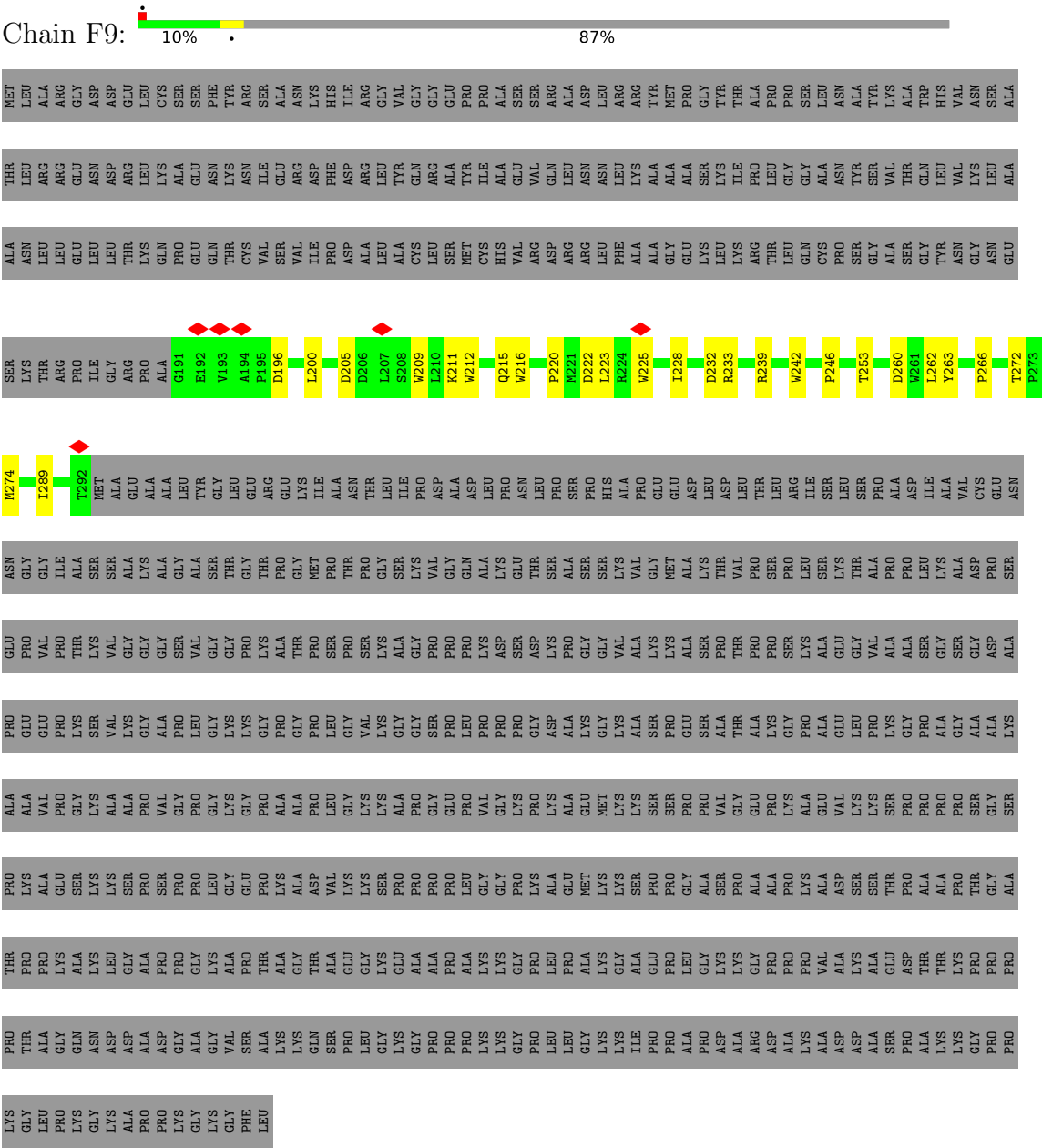




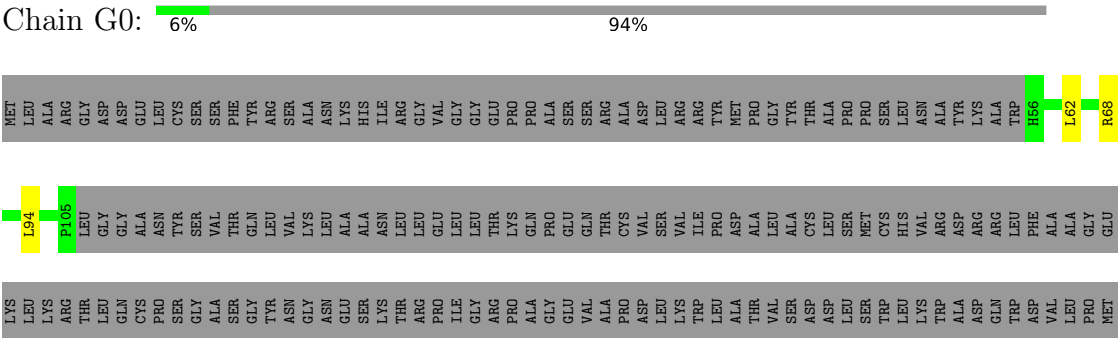
• Molecule 12: PRP, TGME49_291880



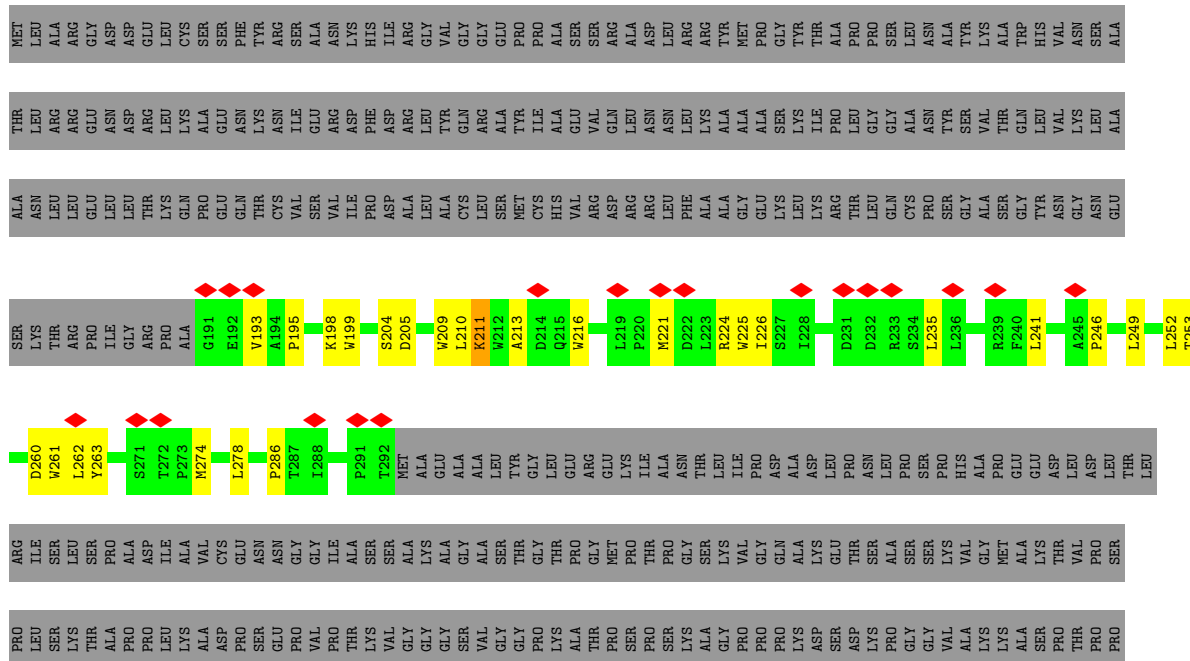
● Molecule 12: PRP, TGME49_291880



● Molecule 12: PRP, TGME49_291880



[illegible][illegible]

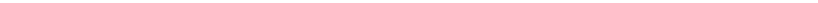


THR	LEU	ARG	ARG	GLU	ASN	ASP	ARG	LEU	LYS	ALA	GLU	ASN	ASN	LYS	ILE	ILE	GLU	ARG	GLU	ASP	PHE	ASP	ASP	ARG	ARG	LEU	TYR	GLN	ALA	ARG	ALA	TYR	TYR	ILE	ALA	GLU	VAL	GLN	LEU	ASN	ASN	LEU	LYS	ALA	ALA	ALA	ALA	SER	LYS	ILE	PRO	LEU	GLY	GLY	ALA	ASN	TYR	SER	VAL	GLN	LEU	VAL	LYS	LEU
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[illegible]

- Molecule 12: PRP, TGME49_291880

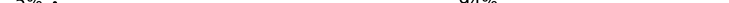
Chain H0: 

[illegible]

PRO	LEU	LEU	LEU	LYS	LYS	ILE	PRO	PRO	PRO	ASP	ALA	ALA	ARG	ASP	ALA	LYS	ALA	ASP	ASP	ALA	SER	PRO	ALA	LYS	LYS	GLY	PRO	PRO	LYS	GLY	LEU	PRO	LYS	GLY	LYS	ALA	PRO	PRO	LYS	GLY	LYS	GLY	GLY	PHE	LEU
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Chain H1: 97%

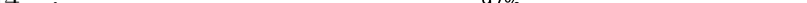
LEU	LEU	GLY	LYS	ILE	PRO	PRO	ALA	PRO	ASP	ALA	ARG	ASP	ALA	LYS	ALA	ASP	ASP	ALA	SER	PRO	ALA	LYS	LYS	GLY	PRO	PRO	LYS	GLY	LEU	PRO	LYS	GLY	LYS	ALA	PRO	PRO	LYS	GLY	LYS	GLY	LEU	PHU	LEU
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Chain H2:  5% • 94%

[illegible]

[illegible]

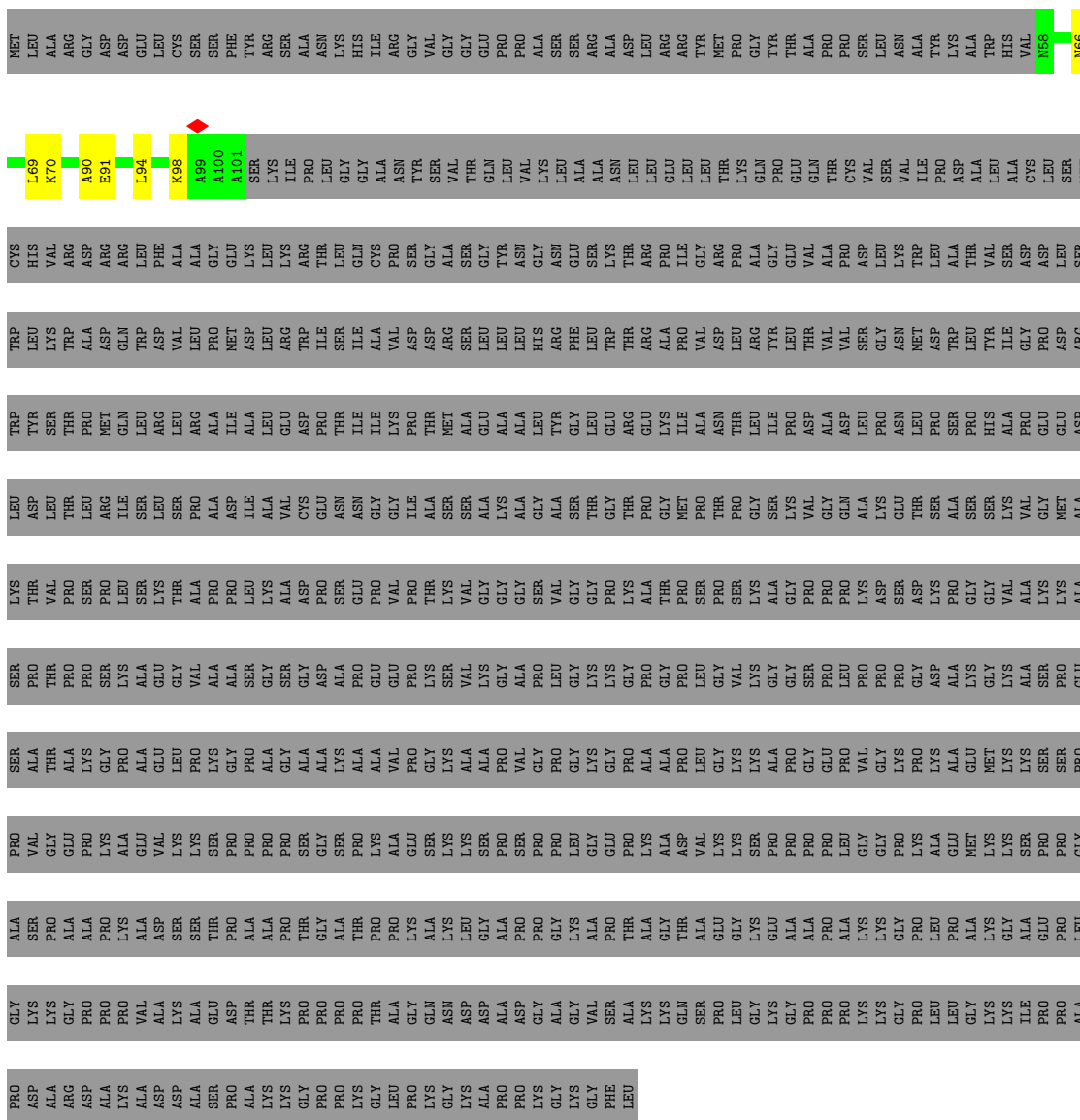
- Molecule 12: PRP, TGME49_291880

Chain H4:  97%

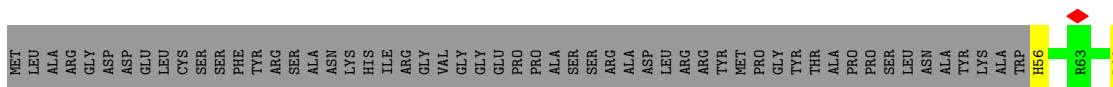
[illegible]

LYS
GLY
PRO
LEU
LEU
GLY
LYS
LYS
TLE
PRO
PRO
ALA
ALA
ASP
ALA
ALA
ARG
ASP
ALA
LYS
ALA
ASP
ASP
ASP
SER
PRO
ALA
LYS
LYS
GLY
PRO
PRO
LYS
LYS
GLY
LEU
PRO
LYS
GLY
LYS
ALA
PRO
PRO
LYS
GLY
LYS
GLY
PHE
LEU

Chain H5: 5% • 94%

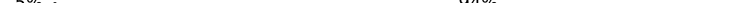


Chain H6: 6% . 94%



[illegible]

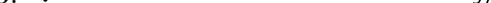
- Molecule 12: PRP, TGME49_291880

Chain H8:  5% 94%

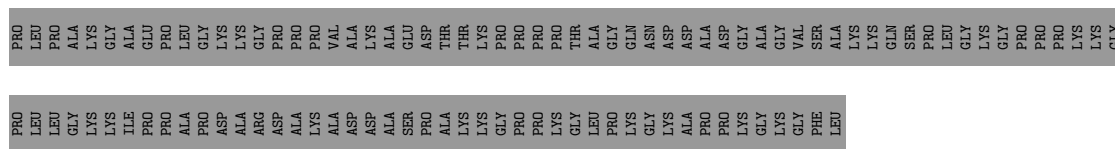
[illegible]

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

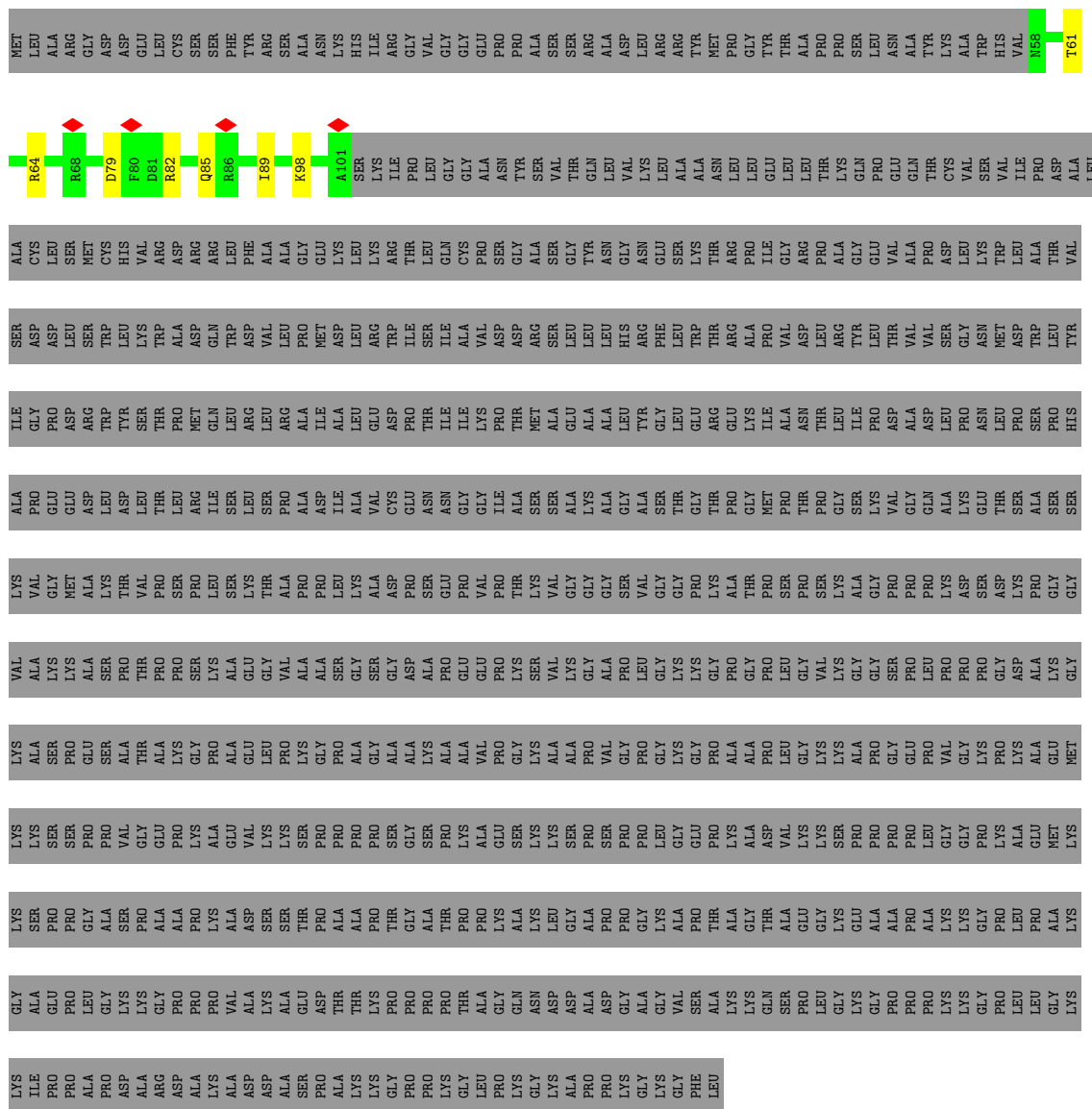
- Molecule 12: PRP, TGME49_291880

Chain I3:  97%

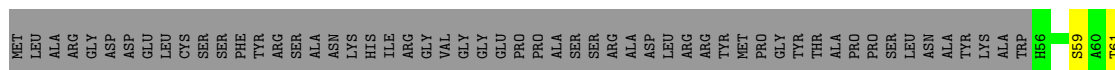
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ALA	GLU	ALA	PRO	ALA	GLY	PRO	SER	GLU	GLU	THR	LEU	LYS	ASN	LEU	THR
GLU	MET	LYS	GLY	GLU	GLY	GLY	ALA	GLU	GLU	ARG	ARG	THR	LEU	ARG	ALA
LYS	LYS	LYS	VAL	LYS	VAL	VAL	LYS	ILE	ILE	PRO	PRO	ILE	LEU	ASN	GLY
SER	LYS	ALA	LYS	GLY	VAL	LYS	VAL	ALA	ALA	VAL	ASP	GLY	LEU	ASP	ASP
PRO	PRO	SER	LYS	ALA	LYS	LYS	GLY	ASN	ASN	ASP	GLU	ARG	THR	ARG	GLY
PRO	PRO	SER	PRO	GLY	ALA	MET	THR	LEU	THR	LEU	LEU	PRO	LYS	LYS	CYS
GLY	GLY	ALA	ALA	ALA	ALA	ALA	ALA	ILE	ILE	ARG	GLU	ALA	PRO	ALA	SER
ALA	SER	SER	PRO	PRO	THR	SER	THR	PRO	THR	LEU	GLY	VAL	GLN	GLU	SER
PRO	PRO	ALA	VAL	GLY	THR	THR	VAL	D313	D313	THR	THR	VAL	GLN	ASN	PHE
ALA	ALA	ALA	PRO	GLU	ALA	PRO	PRO	L329	L329	VAL	VAL	ALA	THR	LYS	TYR
PRO	PRO	GLY	SER	LYS	GLY	SER	PRO	ILE	ILE	SER	SER	VAL	ILE	ASN	THR
LYS	LYS	ALA	LEU	ALA	LEU	LYS	LEU	I335	I335	GLY	GLY	SER	SER	ALA	ALA
ASP	ASP	GLU	LYS	ALA	ALA	GLY	SER	S336	S336	ASN	ASN	LYS	VAL	ASN	LYS
SER	SER	LEU	THR	GLY	GLY	GLY	THR	LEU	LEU	MET	MET	TRP	ILE	ARG	THR
SER	SER	PRO	LYS	LYS	VAL	VAL	THR	SER	ASP	THR	THR	ALA	PRO	PHE	ILE
THR	THR	LYS	PRO	PRO	ALA	ALA	PRO	PRO	ALA	LEU	LEU	THR	ALA	ARG	ARG
PRO	PRO	GLY	GLY	GLY	GLY	GLY	GLY	ILE	ILE	TYR	TYR	VAL	ALA	GLY	GLY
ALA	ALA	PRO	SER	PRO	SER	SER	LEU	ILE	ILE	ILE	GLY	SER	ALA	VAL	VAL
PRO	PRO	ALA	GLY	ALA	GLY	GLY	LYS	VAL	VAL	PRO	PRO	ASP	CYS	GLN	GLY
THR	THR	PRO	GLY	GLY	GLY	GLY	THR	ASN	ASN	TYR	TYR	LEU	HIS	ALA	ALA
PRO	PRO	ALA	GLU	LYS	GLU	GLU	PRO	GLY	GLY	SER	THR	TRP	VAL	GLU	GLU
LYS	LYS	GLY	VAL	GLY	GLY	GLY	PRO	CYS	CYS	ARG	ARG	SER	MET	GLY	GLY
GLY	GLY	ALA	ASP	GLY	GLY	GLY	ASP	VAL	VAL	PRO	PRO	LEU	ASP	ALA	ALA
LYS	LYS	LYS	SER	LYS	VAL	SER	LYS	ALA	ALA	GLN	GLN	ASN	ARG	ASN	LEU
LEU	LEU	ALA	VAL	LYS	LYS	VAL	VAL	SER	SER	LEU	LEU	ASN	ASN	ASN	LEU
ALA	ALA	PRO	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ARG	ARG	PHE	PHE	LEU	LEU
PRO	PRO	PRO	GLY	GLY	GLY	GLY	VAL	ALA	ALA	LEU	LEU	LYS	LYS	LYS	THR
THR	THR	PRO	ALA	LYS	PRO	PRO	ALA	LYS	LYS	ARG	ARG	TYR	TYR	ALA	ALA
GLY	GLY	ALA	PRO	PRO	PRO	PRO	SER	GLY	GLY	PRO	PRO	GLY	GLY	ALA	MET
LYS	LYS	LEU	PRO	LEU	GLY	GLY	VAL	ALA	ALA	ILE	ILE	MET	PRO	ALA	GLY
ALA	ALA	GLY	LYS	GLY	LYS	LYS	GLY	SER	SER	ALA	ALA	ASP	LYS	SER	GLY
PRO	PRO	GLY	GLY	GLY	GLY	GLY	PRO	THR	THR	LEU	LEU	LEU	LEU	TYR	TYR
GLY	GLY	GLY	PRO	PRO	PRO	PRO	PRO	THR	THR	GLU	GLU	ARG	LYS	ILE	ILE
THR	THR	ASP	ALA	VAL	PRO	LEU	PRO	GLY	GLY	THR	THR	ILE	GLY	GLY	GLY
ALA	ALA	VAL	ASP	VAL	LEU	LEU	SER	PRO	PRO	ILE	ILE	ILE	CYS	ALA	ALA
GLY	GLY	LYS	LYS	LYS	GLY	GLY	VAL	THR	THR	LYS	LYS	VAL	ASN	ASN	LEU
LYS	LYS	GLY	GLY	GLY	GLY	GLY	GLY	THR	THR	GLY	GLY	VAL	PRO	ASN	ASN
GLY	GLY	PRO	GLY	PRO	PRO</										



- Molecule 12: PRP, TGME49_291880



- Molecule 12: PRP, TGME49_291880



[illegible]

- Molecule 12: PRP, TGME49_291880

Chain I7: 5% . 94%



- Molecule 12: PRP, TGME49_291880

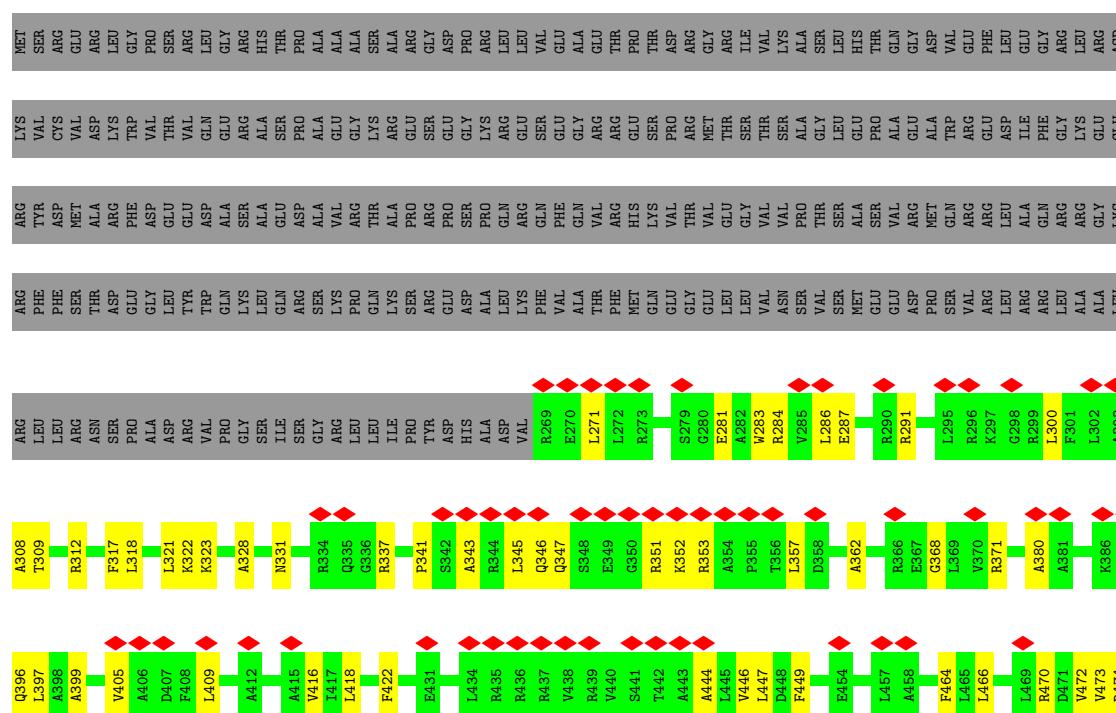
Chain I8: 6% 94%

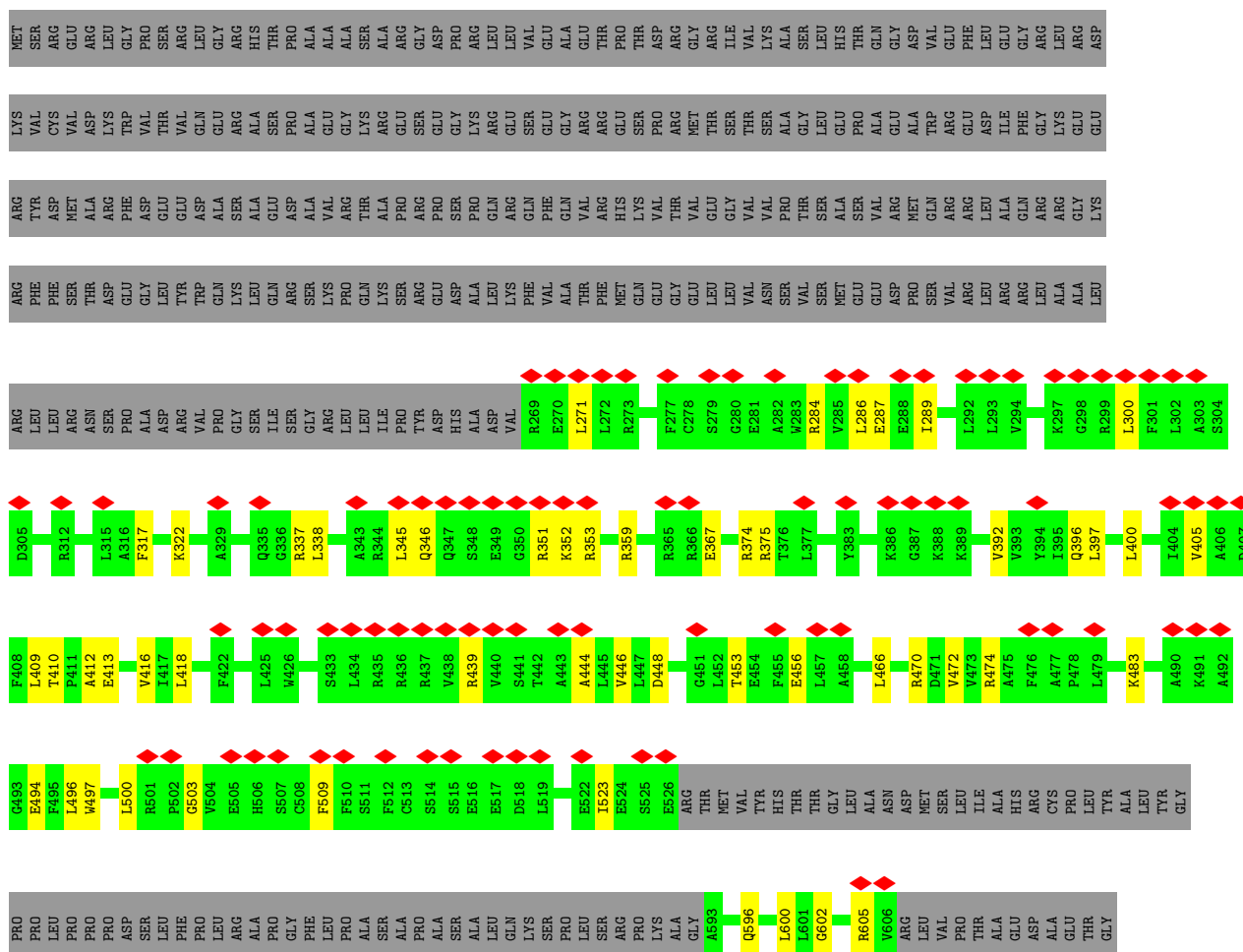
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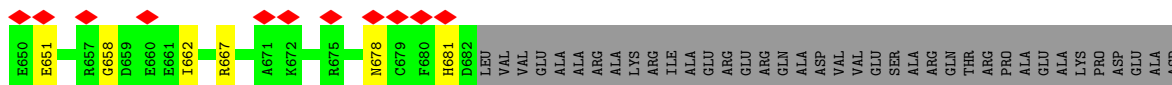
- Molecule 12: PRP, TGME49 291880

Chain I9: 97%

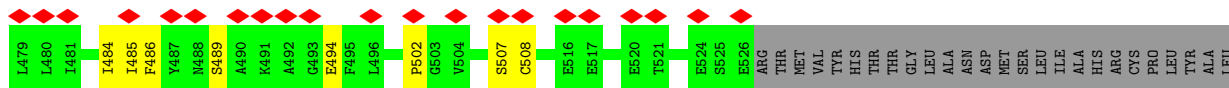
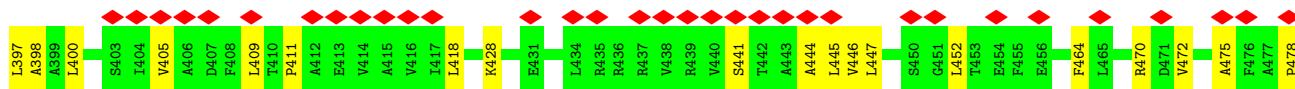
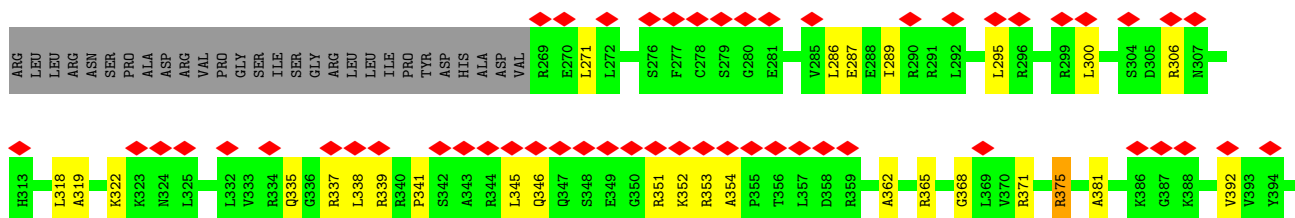
Met	Leu	Ala	Ala	Ala	Arg	Gly	Asp	Asp	Leu	Cys	Ser	Ser	Phe	Tyr	Arg	Ser	Ala	Ala	Asn	Lys	His	Ile	Arg	Gly	Val	Gly	Gly	Leu	Pro	Pro	Ala	Ser	Ser	Arg	Ala	Arg	Asp	Leu	Arg	Arg	Tyr	Pro	Ala	Pro	Pro	Ser	Ser	Leu	Asn	Ala	Tyr	Lys	Ala	Ala	Trp	His	Val	Asn	Asn	Ser	Ala
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Chain J6:

[illegible]

THR	GLY	PRO	PRO	LEU	PRO	PRO	ASP	SER	LEU	PHE	PRO	LEU	ARG	ALA	ALA	GLY	PHE	PRO	LEU	ALA	SER	ALA	ALA	ALA	GLN	LYS	SER	PRO	LEU	SER	ARG	PRO	PRO	ALA	ALA	GLY	ASP	GLU	ALA	ALA	GLU	THR	GLY	SER
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LEU	PRO	ARG	ALA	PRO	PHE	PHE	ARG	THR	ALA	GLY	GLU	SER	ARG	GLU	GLU	GLU	GLU	ASN	ALA	ALA	GLY	LEU	ALA	ARG	GLY	GLY	E647	E648	E649	E650	E651	E652	E653	E654	E655	E656	D659	E660	E661	E662			E678	F680	H681	D682	LEU	VAL	VAL	GLU	ALA	ALA	ARG	ALA	LYS	ARG	ILE	ALA	GLU
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GLU	ARG	GLN	ALA	ASP	VAL	VAL	GLU	SER	ALA	ALA	ARG	GLN	THR	ARG	PRO	ALA	GLU	ASP	LYS	ALA	ALA	PRO	GLU	GLU	GLU	LEU	ASP	LEU	ASP	SER	VAL	ASP	VAL	ILE	ASP	PRO	ASP	ALA	ASN	LEU	GLY	PRO	SER	GLU	GLY	CYS	ALA	ALA	ALA	VAL	VAL	ALA	GLN
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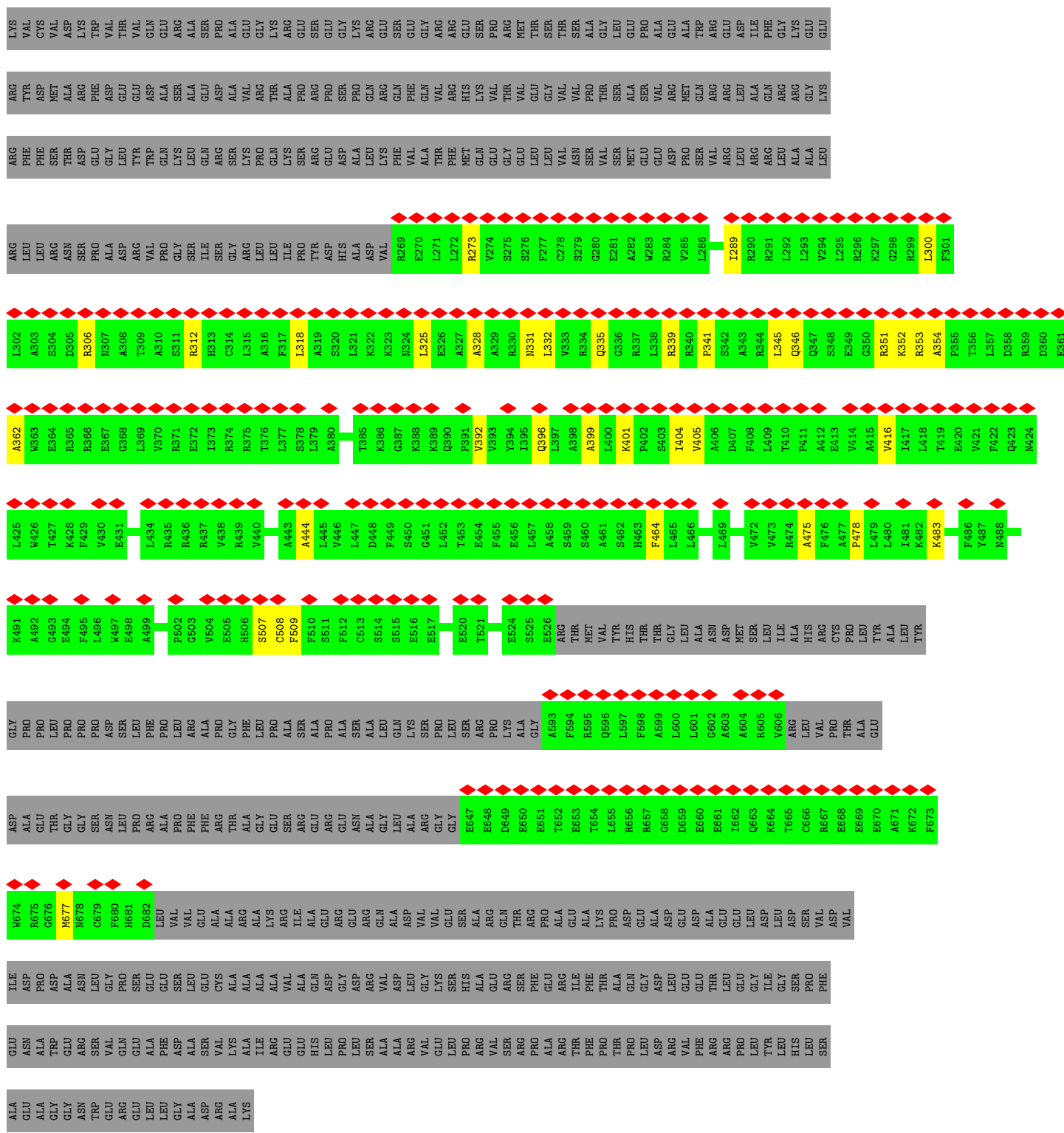
ASP GLY ASP ARG VAL ASP LEU GLY LYS SER HIS ALA GLU ARG SER PHE GLU ARG ILE PHE THR ALA GLN GLY ASP LEU GLU GLY THR THR LEU GLU GLY ILE GLY SER PRO PHE GLU ASN ALA TRP ALA GLU ARG SER VAL GLN GLN GLU ALA PHE ASP ALA VAL LYS ARG ALA ILE ARG GLU GLU HIS

LEU	PRO	LEU	SER	ALA	ALA	ARG	VAL	GLY	LEU	PRO	ARG	VAL	SER	ARG	PRO	ALA	ARG	THR	PHE	PRO	PRO	THR	LEU	ASP	ARG	VAL	PHE	ARG	ARG	PRO	LEU	TYR	HIS	LEU	LEU	ALA	ALA	ALA	GLY	GLY	ASN	TRP	GLY	ARG	GLU	LEU	LEU	GLY	ASP	ALA	TYR
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Chain J7:

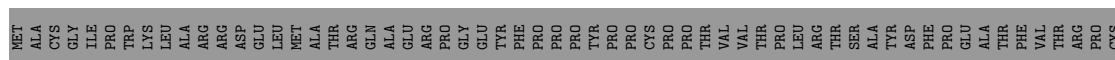


MET	SER	ARG	ARG	GLU	ARG	ARG	LEU	GLY	PRO	SER	ARG	ARG	LEU	GLY	ARG	HIS	THR	PRO	ALA	ALA	ALA	SER	ALA	ALA	ARG	GLY	ASP	PRO	PRO	LEU	LEU	VAL	GLU	GLU	ALA	THR	PRO	THR	THR	ASP	ARG	GLY	ARG	ILE	ILE	VAL	LYS	ALA	SER	SER	LEU	HIS	HIS	THR	THR	GLN	GLY	GLN	ASP	VAL	GLU	PHE	LEU	LEU	GLY	GLY	ARG	ARG	LEU	LEU	ARG	ASP
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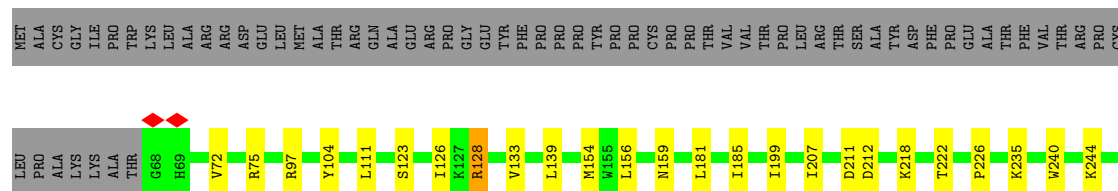
- Molecule 14: DCX, TGME49 256030

Chain K0:

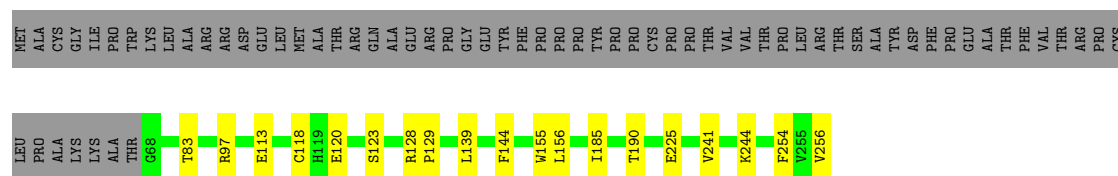




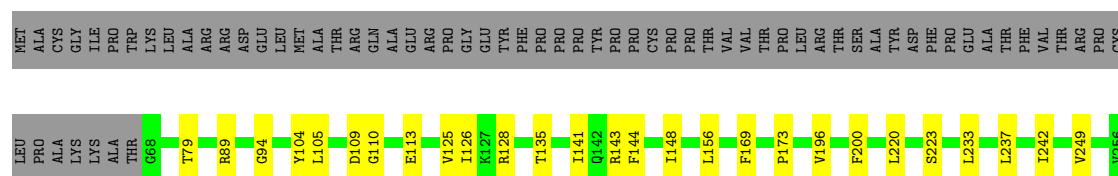
- Molecule 14: DCX, TGME49_256030



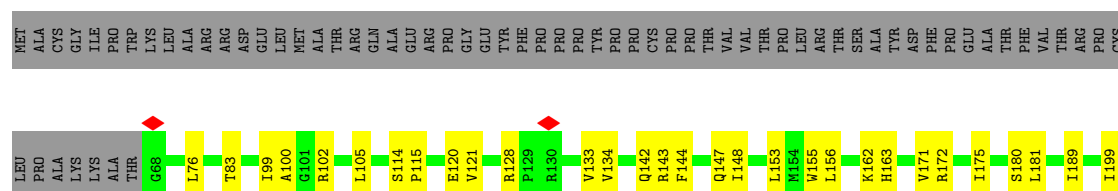
- Molecule 14: DCX, TGME49_256030



- Molecule 14: DCX, TGME49_256030



- Molecule 14: DCX, TGME49_256030



- Molecule 14: DCX, TGME49_256030

Chain K5:  64% 10% 26%

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

LEU PRO ALA GLY LYS ALA THR G68 F73 T79 F90 G94 I99 A100 Y104 L105 Y106 D109 G110 L111 S114 R117 Q142 R143 F144 L156 M178 L181 Y182 I185 I199 I207 I210 I242 I247 V256

- Molecule 14: DCX, TGME49_256030

Chain K6:  62% 11% 26%

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

LEU PRO ALA GLY LYS ALA THR G68 H69 T63 R89 R97 G98 I99 L105 G110 L111 T112 P115 C118 S123 R128 Q142 R143 F144 L156 F169 R172 I185 T190 P191 V196 I207 D212 A217 K218 Y219 P226 P227 A228 I242 F254 V255 V256

- Molecule 14: DCX, TGME49_256030

Chain K7:  68% 6% 26%

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

LEU PRO ALA GLY LYS ALA THR G68 H69 K70 W71 V72 R75 A80 Y81 R87 D91 E92 K131 P132 Q142 R143 W155 L156 P168 I185 I192 I207 I213 T222 S223 G224 V241 P250 V256

- Molecule 14: DCX, TGME49_256030

Chain K8:  64% 9% 26%

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

LEU PRO ALA GLY LYS ALA THR G68 R97 G98 I99 R102 L105 P115 C118 S123 V133 I148 M154 W155 M159 P173 Y174 I175 S180 L181 Y182 Q183 Q184 I192 I199 T222 K235 V241 K244 V256

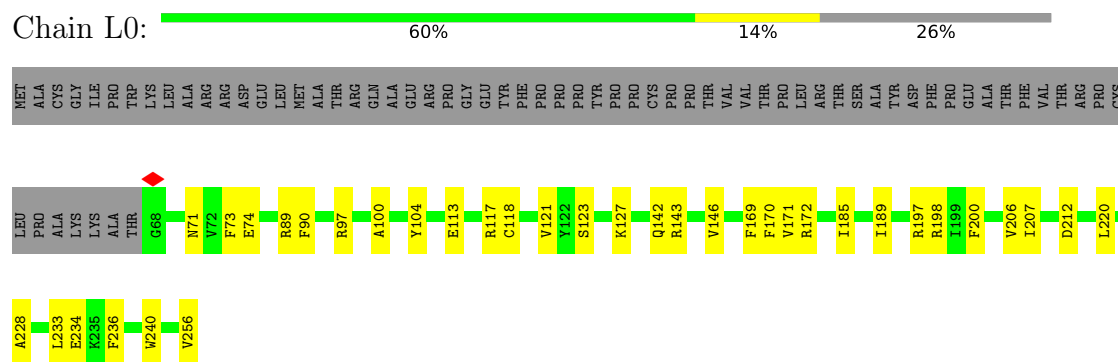
- Molecule 14: DCX, TGME49_256030

Chain K9:  67% 7% 26%

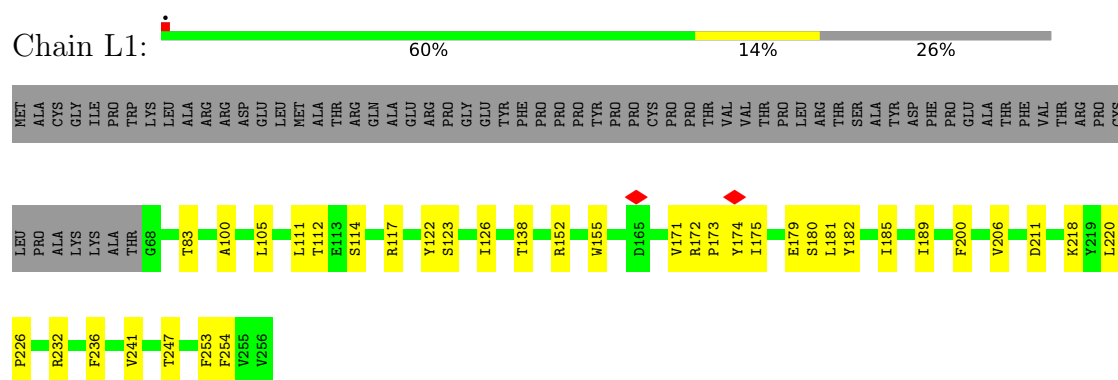
MET ALA CYS GLY ILE PRO TRP LYS LEU ALA ARG ASP GLU MET THR ARG GLN ALA GLU ARG PRO GLY GLU TYR PHE PRO PRO TYR PRO PRO PRO THR VAL THR PRO LEU ARG THR SER ALA TYR ASP PHE PRO GLU ALA THR PHE VAL THR ARG CYS

LEU PRO ALA GLY LYS ALA THR G68 H69 K70 L76 H86 I99 A100 G101 R102 L105 L111 T112 V133 M154 W155 L156 M159 L181 I185 G216 L220 P226 V256

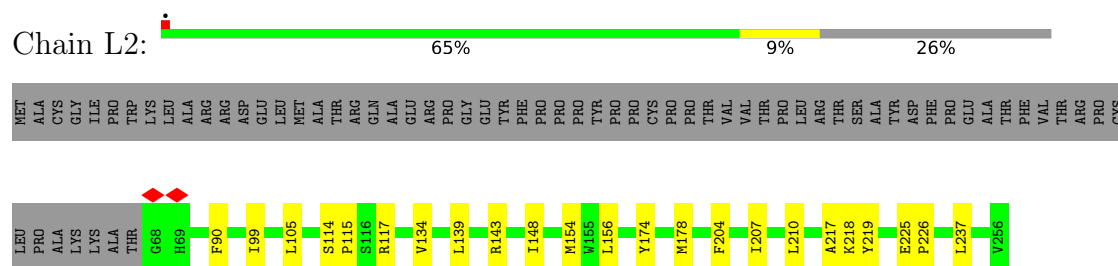
- Molecule 14: DCX, TGME49_256030



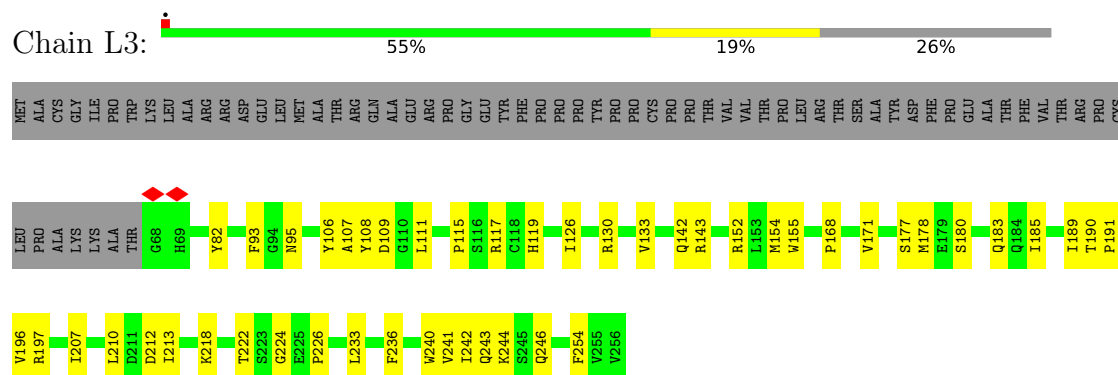
- Molecule 14: DCX, TGME49_256030



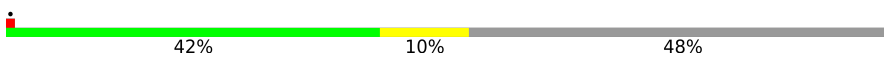
- Molecule 14: DCX, TGME49_256030



- Molecule 14: DCX, TGME49_256030



- Molecule 14: DCX, TGME49_256030

Chain L4: 

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

LEU PRO LYS LYS ALA THR GLY HIS LYS ASN VAL PHE GLU ARG LEU THR ASP THR THR ALA TYR THR TYR GLY SER HIS ARG GLU ARG PHE ASP PHE GLU PHE ASP GLU

VAL TYR SER V125 R130 V133 G137 T136 L139 G140 I141 Q142 R143 R172 M178 Y182 I185 T186 I189 T190 P191 L220 C221 T222 E225 A228 A229 Y230 L233 F236 L237 I242 Q246 T247 K248 V255 V256

- Molecule 14: DCX, TGME49_256030

Chain L5: 

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

LEU PRO LYS LYS ALA THR G68 V72 R75 R89 R102 L111 T112 E113 C118 T138 Q142 R143 F144 Q147 R152 L153 M154 W155 L156 V171 M178 Y178 Q183 T186 I192 P195 I207 C221 T222 E225 F236 L237 P250

F254 V255 V256

- Molecule 14: DCX, TGME49_256030

Chain L6: 

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

LEU PRO LYS LYS ALA THR G66 F73 Y82 T83 R89 R97 Y104 L106 E113 E117 C118 H119 S123 P129 R143 L148 I148 P151 L156 F169 R172 P173 Y174 I175 E179 Q183 T186 P191 V196 P227 L233

T247 P253 V256

- Molecule 14: DCX, TGME49_256030

Chain L7: 

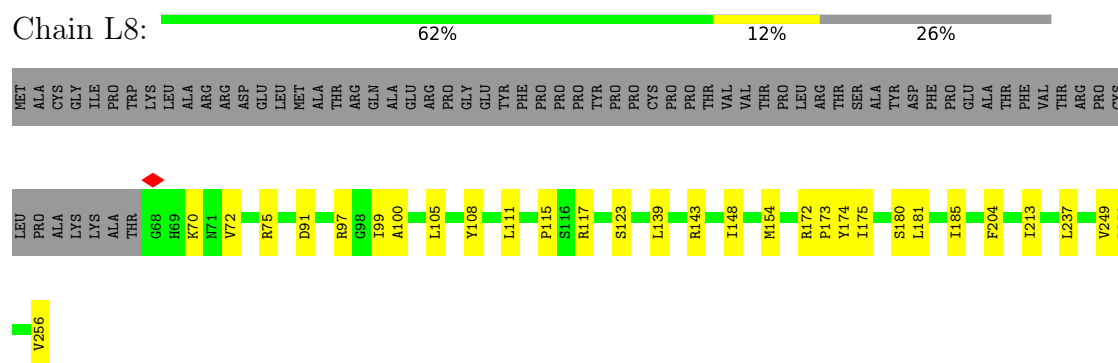
MET ALA CYS GLY ILE PRO TRP LYS LEU ALA ARG ASP GLU LEU MET ALA THR THR ARG GLN ALA GLU ARG PRO GLY GLU TYR PHE ARG PRO PRO TYR PRO PRO CYS PRO PRO THR VAL THR THR LEU THR SER ALA ASP PHE PRO GLU ALA THR PHE VAL THR ARG CYS

LEU PRO LYS LYS ALA THR G68 H86 R89 A100 L105 L111 T112 E113 S114 P115 Y122 I126 P129 Q142 W155 L156 Y157 R158 R172 I175 M178 L181 Y182 I185 I189 I192 R198 V206 L210 T222 P227

A228 W240 V241 K244 S245 Q246 V256

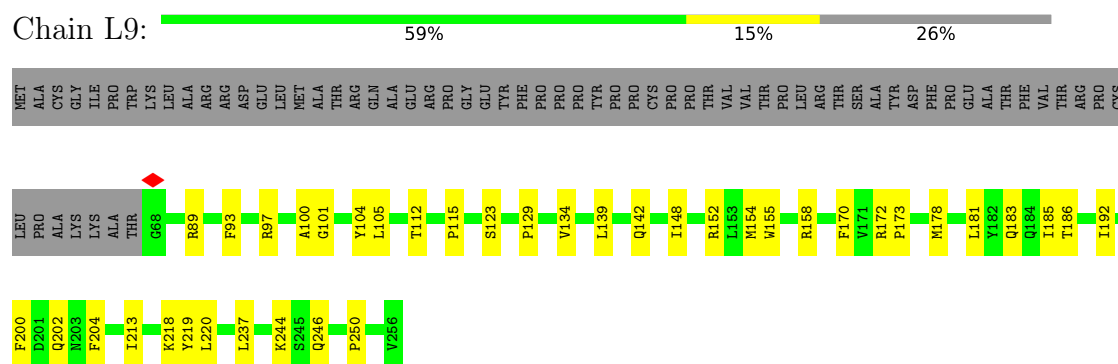
- Molecule 14: DCX, TGME49_256030

Chain L8:



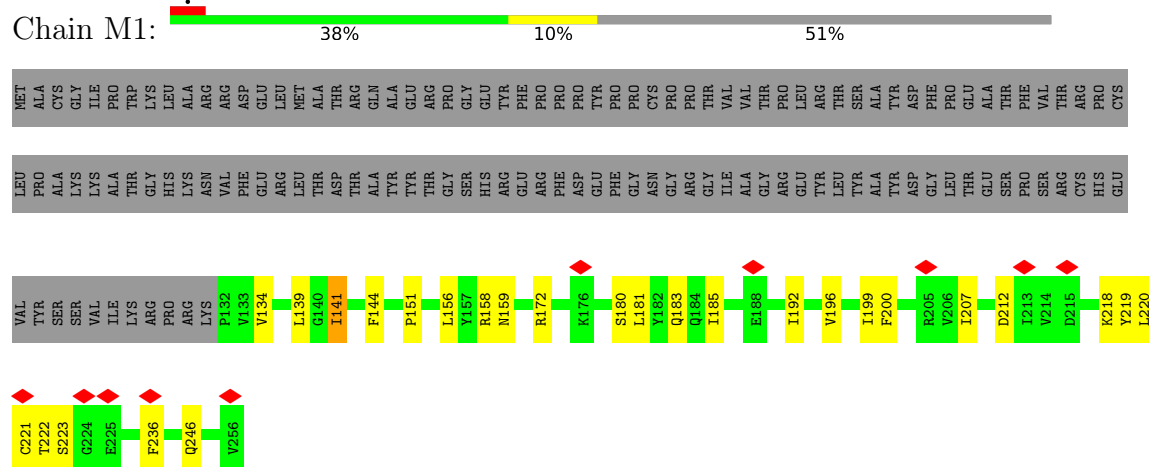
- Molecule 14: DCX, TGME49_256030

Chain L9:



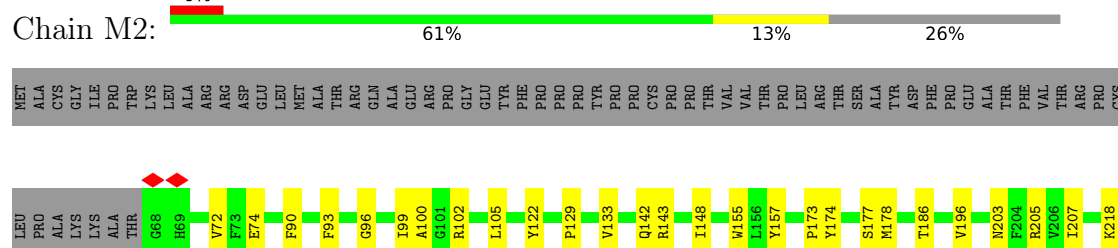
- Molecule 14: DCX, TGME49_256030

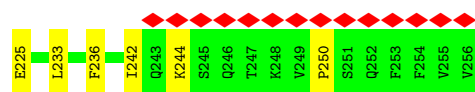
Chain M1:



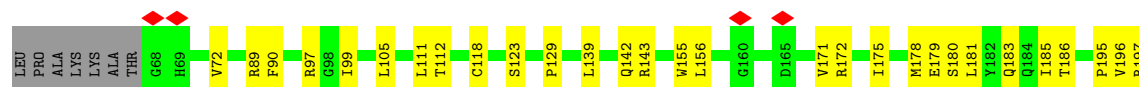
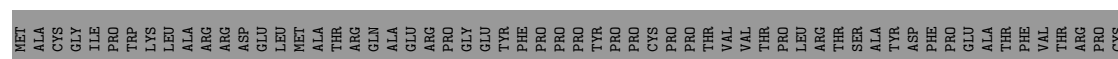
- Molecule 14: DCX, TGME49_256030

Chain M2:

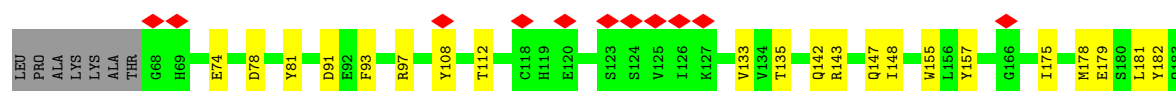
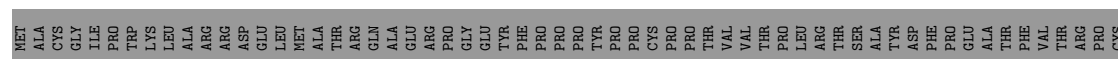




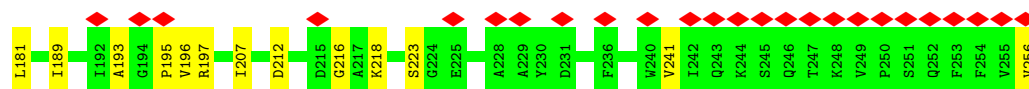
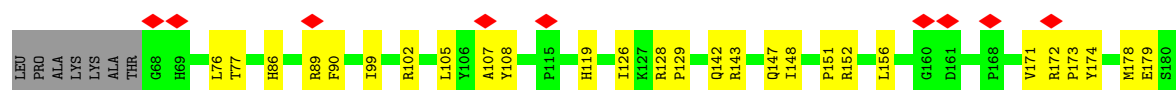
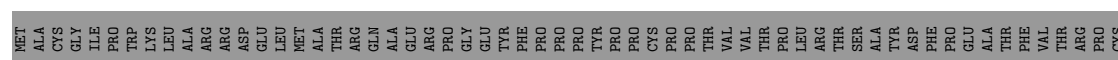
- Molecule 14: DCX, TGME49_256030



- Molecule 14: DCX, TGME49_256030

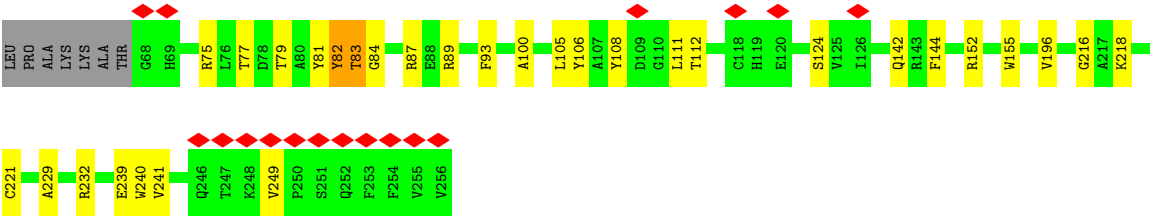


- Molecule 14: DCX, TGME49_256030

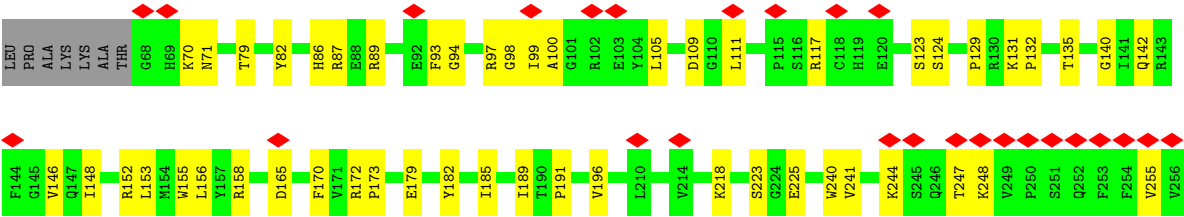
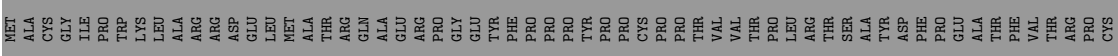


- Molecule 14: DCX, TGME49_256030





• Molecule 14: DCX, TGME49_256030



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	95409	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	5000	Depositor
Maximum defocus (nm)	25000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.352	Depositor
Minimum map value	-0.059	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.056	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	686.08, 686.08, 686.08	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.34, 1.34, 1.34	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	1	0.28	0/892	0.73	0/1200
1	2	0.30	0/892	0.81	0/1200
1	A	0.29	0/2440	0.65	2/3258 (0.1%)
1	B	0.34	1/2020 (0.0%)	0.68	2/2701 (0.1%)
1	C	0.44	0/1249	0.79	2/1669 (0.1%)
1	D	0.37	0/997	0.89	7/1326 (0.5%)
1	E	0.30	0/2245	0.65	0/3005
1	F	0.29	0/2485	0.65	0/3319
1	G	0.39	0/1427	0.90	9/1912 (0.5%)
1	H	0.32	0/963	0.67	0/1281
1	I	0.60	0/3038	0.88	1/4054 (0.0%)
1	J	0.64	0/2986	0.97	5/3984 (0.1%)
1	K	0.31	0/1652	0.74	5/2205 (0.2%)
1	L	0.30	0/1693	0.71	0/2260
1	M	0.71	0/1795	1.03	3/2392 (0.1%)
1	N	0.77	0/1731	1.07	1/2308 (0.0%)
1	O	0.96	0/467	1.29	1/622 (0.2%)
1	P	0.94	0/445	1.35	1/592 (0.2%)
1	Q	0.28	0/2898	0.61	0/3867
1	R	0.29	0/2109	0.65	0/2815
1	S	0.29	0/1481	0.73	4/1976 (0.2%)
1	T	0.23	0/651	0.64	0/867
1	U	0.28	0/3121	0.68	8/4165 (0.2%)
1	V	0.26	0/2135	0.60	0/2852
1	W	0.25	0/1664	0.56	2/2220 (0.1%)
1	X	0.28	0/754	0.60	0/1005
1	Y	0.67	1/2983 (0.0%)	0.96	3/3982 (0.1%)
1	Z	0.35	0/2036	0.74	2/2720 (0.1%)
1	a	0.90	3/1568 (0.2%)	1.15	1/2089 (0.0%)
1	b	0.29	0/739	0.62	0/982
1	c	0.75	2/3012 (0.1%)	0.97	4/4021 (0.1%)
1	d	0.34	0/2076	0.73	1/2774 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	e	0.29	0/732	0.77	1/973 (0.1%)
1	f	1.16	5/1594 (0.3%)	1.38	9/2124 (0.4%)
1	g	0.25	0/745	0.71	2/1017 (0.2%)
1	h	0.31	0/745	0.89	2/1017 (0.2%)
1	i	0.30	0/745	0.77	0/1017
1	j	0.31	0/745	0.82	2/1017 (0.2%)
1	k	0.25	0/745	0.74	0/1017
1	l	0.26	0/745	0.83	0/1017
1	m	0.28	0/745	0.81	2/1017 (0.2%)
1	n	0.26	0/706	0.63	0/949
1	o	0.27	0/706	0.76	0/949
1	p	0.27	0/706	0.70	2/949 (0.2%)
1	q	0.30	0/706	0.76	0/949
1	r	0.32	0/706	0.73	0/949
1	s	0.31	1/706 (0.1%)	0.59	0/949
1	t	0.23	0/706	0.59	0/949
1	u	0.24	0/892	0.62	0/1200
1	v	0.21	0/892	0.56	1/1200 (0.1%)
1	w	0.29	0/892	0.69	0/1200
1	x	0.29	0/892	0.74	1/1200 (0.1%)
1	y	0.22	0/892	0.66	1/1200 (0.1%)
1	z	0.23	0/892	0.64	1/1200 (0.1%)
2	10	0.25	0/1508	0.63	2/1999 (0.1%)
2	11	0.28	0/1527	0.69	0/2024
2	12	0.30	0/1508	0.83	4/1999 (0.2%)
2	13	0.29	0/1527	0.71	4/2024 (0.2%)
2	14	0.28	0/1508	0.67	0/1999
2	15	0.27	0/772	0.63	2/1020 (0.2%)
2	16	0.29	0/843	0.83	4/1114 (0.4%)
2	3	0.30	0/1527	0.75	5/2024 (0.2%)
2	4	0.28	0/1508	0.68	0/1999
2	5	0.33	0/1527	0.81	3/2024 (0.1%)
2	6	0.35	0/1508	0.90	5/1999 (0.3%)
2	7	0.28	0/1527	0.68	3/2024 (0.1%)
2	8	0.29	0/1508	0.73	1/1999 (0.1%)
2	9	0.29	0/1527	0.70	2/2024 (0.1%)
3	1A	0.27	0/3398	0.66	1/4606 (0.0%)
3	1C	0.24	0/3398	0.61	0/4606
3	1E	0.25	0/3398	0.66	1/4606 (0.0%)
3	1G	0.21	0/3398	0.55	0/4606
3	1I	0.23	0/3398	0.56	0/4606
3	1K	0.22	0/3398	0.55	0/4606
3	1M	0.29	0/3398	0.78	8/4606 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	2A	0.29	0/3398	0.74	2/4606 (0.0%)
3	2C	0.23	0/3398	0.58	1/4606 (0.0%)
3	2E	0.28	0/3398	0.74	4/4606 (0.1%)
3	2G	0.19	0/3398	0.51	2/4606 (0.0%)
3	2I	0.22	0/3398	0.56	0/4606
3	2K	0.22	0/3398	0.53	0/4606
3	2M	0.27	0/3398	0.68	2/4606 (0.0%)
3	3A	0.29	0/3398	0.75	1/4606 (0.0%)
3	3C	0.22	0/3398	0.56	0/4606
3	3E	0.22	0/3398	0.57	2/4606 (0.0%)
3	3G	0.18	0/3398	0.46	0/4606
3	3I	0.21	0/3398	0.56	3/4606 (0.1%)
3	3K	0.21	0/3398	0.54	0/4606
3	3M	0.26	0/3398	0.63	2/4606 (0.0%)
3	4A	0.24	0/3398	0.62	2/4606 (0.0%)
3	4C	0.22	0/3398	0.56	0/4606
3	4E	0.24	0/3398	0.60	0/4606
3	4G	0.20	0/3398	0.52	0/4606
3	4I	0.22	0/3398	0.56	0/4606
3	4K	0.22	0/3398	0.56	0/4606
3	4M	0.27	0/3398	0.70	2/4606 (0.0%)
3	5A	0.26	0/3398	0.69	2/4606 (0.0%)
3	5C	0.20	0/3398	0.52	0/4606
3	5E	0.20	0/3398	0.51	0/4606
3	5G	0.19	0/3398	0.47	0/4606
3	5I	0.20	0/3398	0.52	0/4606
3	5K	0.19	0/3398	0.49	0/4606
3	5M	0.26	0/3398	0.72	2/4606 (0.0%)
3	6A	0.23	0/3398	0.60	0/4606
3	6C	0.22	0/3398	0.58	0/4606
3	6E	0.22	0/3398	0.57	2/4606 (0.0%)
3	6G	0.22	0/3398	0.52	2/4606 (0.0%)
3	6I	0.22	0/3398	0.55	3/4606 (0.1%)
3	6K	0.22	0/3398	0.53	2/4606 (0.0%)
3	6M	0.25	0/3398	0.67	3/4606 (0.1%)
3	7A	0.23	0/3398	0.59	0/4606
3	7C	0.22	0/3398	0.59	0/4606
3	7E	0.26	0/3398	0.63	0/4606
3	7G	0.21	0/3398	0.55	0/4606
3	7I	0.23	0/3398	0.57	0/4606
3	7K	0.22	0/3398	0.58	0/4606
3	7M	0.26	0/3398	0.69	1/4606 (0.0%)
3	8A	0.23	0/3398	0.58	2/4606 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	8C	0.23	0/3398	0.62	1/4606 (0.0%)
3	8E	0.26	0/3398	0.65	4/4606 (0.1%)
3	8G	0.22	0/3398	0.57	1/4606 (0.0%)
3	8I	0.24	0/3398	0.66	2/4606 (0.0%)
3	8K	0.25	0/3398	0.66	3/4606 (0.1%)
3	8M	0.22	0/3398	0.62	2/4606 (0.0%)
3	9A	0.19	0/3398	0.49	1/4606 (0.0%)
3	9C	0.19	0/3398	0.52	1/4606 (0.0%)
3	9E	0.23	0/3398	0.58	1/4606 (0.0%)
3	9G	0.21	0/3398	0.61	1/4606 (0.0%)
3	9I	0.26	0/3398	0.69	4/4606 (0.1%)
3	9K	0.21	0/3398	0.59	1/4606 (0.0%)
3	9M	0.19	0/3398	0.53	0/4606
4	1B	0.26	0/3404	0.68	3/4606 (0.1%)
4	1D	0.24	0/3404	0.64	0/4606
4	1F	0.23	0/3404	0.61	0/4606
4	1H	0.22	0/3404	0.60	3/4606 (0.1%)
4	1J	0.24	0/3404	0.63	0/4606
4	1L	0.23	0/3404	0.63	3/4606 (0.1%)
4	1N	0.25	0/3404	0.69	2/4606 (0.0%)
4	2B	0.27	0/3404	0.70	1/4606 (0.0%)
4	2D	0.24	0/3404	0.63	2/4606 (0.0%)
4	2F	0.23	0/3404	0.60	0/4606
4	2H	0.20	0/3404	0.50	1/4606 (0.0%)
4	2J	0.24	0/3404	0.61	2/4606 (0.0%)
4	2L	0.22	0/3404	0.61	1/4606 (0.0%)
4	3B	0.27	0/3404	0.72	2/4606 (0.0%)
4	3D	0.21	0/3404	0.54	0/4606
4	3F	0.24	0/3404	0.55	0/4606
4	3H	0.20	0/3404	0.54	2/4606 (0.0%)
4	3J	0.23	0/3404	0.60	0/4606
4	3L	0.22	0/3404	0.56	1/4606 (0.0%)
4	4B	0.25	0/3404	0.65	1/4606 (0.0%)
4	4D	0.18	0/3404	0.50	0/4606
4	4F	0.24	0/3404	0.58	2/4606 (0.0%)
4	4H	0.19	0/3404	0.52	2/4606 (0.0%)
4	4J	0.25	0/3404	0.61	0/4606
4	4L	0.23	0/3404	0.61	3/4606 (0.1%)
4	5B	0.30	0/3404	0.74	3/4606 (0.1%)
4	5D	0.21	0/3404	0.55	3/4606 (0.1%)
4	5F	0.21	0/3404	0.55	0/4606
4	5H	0.18	0/3404	0.47	0/4606
4	5J	0.23	0/3404	0.60	0/4606

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
4	5L	0.23	1/3404 (0.0%)	0.52	1/4606 (0.0%)
4	5N	0.28	0/3404	0.76	6/4606 (0.1%)
4	6B	0.26	0/3404	0.70	0/4606
4	6D	0.22	0/3404	0.55	0/4606
4	6F	0.22	0/3404	0.57	0/4606
4	6H	0.21	0/3404	0.53	0/4606
4	6J	0.25	0/3404	0.61	1/4606 (0.0%)
4	6L	0.22	0/3404	0.59	0/4606
4	6N	0.27	0/3404	0.66	1/4606 (0.0%)
4	7B	0.29	0/3404	0.75	7/4606 (0.2%)
4	7D	0.24	0/3404	0.64	0/4606
4	7F	0.24	0/3404	0.64	1/4606 (0.0%)
4	7H	0.22	0/3404	0.56	0/4606
4	7J	0.27	0/3404	0.68	2/4606 (0.0%)
4	7L	0.25	0/3404	0.66	0/4606
4	8B	0.27	0/3404	0.71	5/4606 (0.1%)
4	8D	0.26	0/3404	0.64	0/4606
4	8F	0.26	0/3404	0.69	1/4606 (0.0%)
4	8H	0.23	0/3404	0.59	0/4606
4	8J	0.25	0/3404	0.68	1/4606 (0.0%)
4	8L	0.24	0/3404	0.66	0/4606
4	9B	0.31	0/3404	0.72	7/4606 (0.2%)
4	9D	0.21	0/3404	0.59	2/4606 (0.0%)
4	9F	0.25	0/3404	0.67	9/4606 (0.2%)
4	9H	0.23	0/3404	0.62	2/4606 (0.0%)
4	9J	0.25	0/3404	0.65	2/4606 (0.0%)
4	9L	0.22	0/3404	0.56	0/4606
5	20	0.29	0/1844	0.74	0/2487
5	21	0.26	0/1845	0.74	3/2489 (0.1%)
5	22	0.26	0/1844	0.67	1/2487 (0.0%)
5	23	0.25	0/1845	0.70	0/2489
5	24	0.29	0/1844	0.78	0/2487
5	25	0.29	0/1845	0.75	3/2489 (0.1%)
5	26	0.27	0/1844	0.74	1/2487 (0.0%)
5	27	0.28	0/1845	0.71	1/2489 (0.0%)
5	28	0.27	0/1844	0.71	1/2487 (0.0%)
5	29	0.26	0/1845	0.67	0/2489
5	30	0.25	0/1844	0.67	0/2487
5	31	0.27	0/1845	0.70	0/2489
5	32	0.27	0/1844	0.71	0/2487
5	33	0.19	0/1344	0.58	0/1818
5	35	0.21	0/1774	0.51	0/2394
5	36	0.21	0/1752	0.51	0/2361

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
5	37	0.23	0/1774	0.62	2/2394 (0.1%)
5	38	0.21	0/1752	0.51	0/2361
5	39	0.20	0/1774	0.58	3/2394 (0.1%)
5	40	0.21	0/1752	0.48	0/2361
5	42	0.17	0/1752	0.38	0/2361
5	43	0.20	0/1774	0.52	0/2394
5	44	0.21	0/1752	0.44	0/2361
5	45	0.21	0/1774	0.54	2/2394 (0.1%)
5	46	0.18	0/1752	0.39	0/2361
5	47	0.17	0/1774	0.47	1/2394 (0.0%)
5	48	0.17	0/1752	0.34	0/2361
5	49	0.25	0/1871	0.64	0/2525
5	50	0.25	0/1883	0.70	0/2539
5	51	0.25	0/1871	0.65	0/2525
5	52	0.22	0/1883	0.64	0/2539
5	53	0.25	0/1871	0.65	0/2525
5	54	0.27	0/1883	0.67	3/2539 (0.1%)
5	55	0.24	0/1871	0.65	1/2525 (0.0%)
5	56	0.27	0/1883	0.70	1/2539 (0.0%)
5	57	0.24	0/1871	0.63	0/2525
5	58	0.23	0/1883	0.62	3/2539 (0.1%)
5	59	0.23	0/1871	0.63	0/2525
5	60	0.24	0/1883	0.68	1/2539 (0.0%)
5	61	0.24	0/1871	0.64	1/2525 (0.0%)
5	62	0.23	0/1883	0.59	0/2539
6	63	0.22	0/5165	0.60	1/6980 (0.0%)
6	64	0.29	0/5165	0.61	0/6980
6	65	0.29	0/5165	0.62	0/6980
6	66	0.30	0/5165	0.65	1/6980 (0.0%)
6	67	0.33	1/5165 (0.0%)	0.69	5/6980 (0.1%)
6	68	0.32	0/5165	0.70	1/6980 (0.0%)
6	69	0.31	0/5165	0.67	0/6980
7	71	0.20	0/1427	0.51	0/1942
7	72	0.20	0/1427	0.55	0/1942
7	73	0.25	0/1427	0.66	0/1942
7	75	0.20	0/1427	0.58	2/1942 (0.1%)
7	76	0.20	0/1427	0.52	0/1942
7	77	0.22	0/1427	0.62	4/1942 (0.2%)
7	78	0.22	0/1427	0.55	0/1942
7	79	0.31	1/1427 (0.1%)	0.57	1/1942 (0.1%)
7	80	0.25	0/1427	0.63	1/1942 (0.1%)
7	82	0.21	0/1427	0.50	0/1942
7	83	0.22	0/1427	0.59	0/1942

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
7	84	0.23	0/1427	0.60	0/1942
7	85	0.27	0/1427	0.63	0/1942
7	86	0.24	0/1427	0.67	2/1942 (0.1%)
7	87	0.28	0/1427	0.69	0/1942
7	89	0.27	0/1427	0.61	0/1942
7	90	0.28	0/1427	0.64	0/1942
7	91	0.23	0/1427	0.60	0/1942
7	92	0.23	0/1427	0.60	0/1942
7	93	0.19	0/1427	0.52	0/1942
7	94	0.19	0/1427	0.48	0/1942
7	95	0.20	0/1427	0.53	1/1942 (0.1%)
7	96	0.19	0/1427	0.52	0/1942
7	97	0.31	1/1427 (0.1%)	0.52	1/1942 (0.1%)
8	A1	0.19	0/2638	0.48	0/3582
8	A2	0.22	0/2638	0.59	1/3582 (0.0%)
8	A3	0.23	0/1888	0.59	1/2568 (0.0%)
8	A4	0.27	0/1031	0.77	1/1404 (0.1%)
8	A5	0.20	0/2638	0.49	0/3582
8	A6	0.21	0/2638	0.52	0/3582
8	A7	0.25	0/2638	0.55	0/3582
8	A8	0.22	0/2638	0.49	0/3582
8	A9	0.18	0/1045	0.45	0/1423
9	B1	0.22	0/2119	0.58	0/2878
9	B2	0.21	0/2119	0.54	3/2878 (0.1%)
9	B3	0.20	0/2119	0.54	0/2878
9	B4	0.22	0/2119	0.55	0/2878
9	B5	0.24	0/2119	0.64	1/2878 (0.0%)
9	B6	0.29	1/2119 (0.0%)	0.65	2/2878 (0.1%)
9	B7	0.25	0/2119	0.66	1/2878 (0.0%)
10	C0	0.22	0/1499	0.56	0/2021
10	C6	0.21	0/1499	0.57	0/2021
10	C7	0.25	0/1499	0.63	1/2021 (0.0%)
10	C8	0.27	0/1499	0.66	0/2021
10	C9	0.25	0/1499	0.68	0/2021
10	D0	0.21	0/2249	0.54	0/3042
10	D1	0.25	0/1499	0.62	0/2021
10	D2	0.25	0/1499	0.67	1/2021 (0.0%)
10	D3	0.21	0/2249	0.53	0/3042
10	D4	0.20	0/2249	0.53	0/3042
10	D5	0.23	0/2249	0.59	1/3042 (0.0%)
10	D6	0.22	0/2249	0.53	0/3042
10	D7	0.22	0/2249	0.58	0/3042
10	D8	0.23	0/2249	0.59	0/3042

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
10	D9	0.24	0/2249	0.60	0/3042
10	E0	0.22	0/2249	0.56	0/3042
10	E1	0.22	0/2249	0.54	1/3042 (0.0%)
10	E2	0.26	0/2249	0.68	3/3042 (0.1%)
10	E3	0.23	0/2249	0.59	1/3042 (0.0%)
10	E4	0.24	0/2249	0.60	0/3042
10	E5	0.27	0/2249	0.59	1/3042 (0.0%)
10	E6	0.25	0/2249	0.61	1/3042 (0.0%)
10	E7	0.24	0/2249	0.63	1/3042 (0.0%)
10	E8	0.23	0/2249	0.61	1/3042 (0.0%)
10	E9	0.21	0/2249	0.57	3/3042 (0.1%)
10	F1	0.23	0/2249	0.57	0/3042
10	F2	0.28	0/2249	0.69	3/3042 (0.1%)
10	F3	0.26	0/2249	0.66	4/3042 (0.1%)
11	C1	0.29	0/244	0.42	0/335
11	C2	0.12	0/246	0.36	0/334
11	C3	0.22	0/250	0.58	0/341
11	C4	0.30	0/223	0.51	0/307
11	C5	0.18	0/247	0.55	0/338
12	F0	0.25	0/911	0.69	0/1250
12	F5	0.27	0/874	0.83	0/1200
12	F6	0.26	0/911	0.66	1/1250 (0.1%)
12	F7	0.25	0/874	0.73	1/1200 (0.1%)
12	F8	0.23	0/911	0.60	0/1250
12	F9	0.24	0/874	0.65	0/1200
12	G0	0.21	0/416	0.48	0/558
12	G1	0.24	0/874	0.70	0/1200
12	G2	0.26	0/911	0.71	0/1250
12	G3	0.24	0/874	0.71	0/1200
12	G4	0.24	0/911	0.66	2/1250 (0.2%)
12	G5	0.27	0/874	0.71	2/1200 (0.2%)
12	G6	0.27	0/911	0.70	1/1250 (0.1%)
12	G7	0.27	0/874	0.76	1/1200 (0.1%)
12	G8	0.23	0/911	0.64	1/1250 (0.1%)
12	G9	0.25	0/367	0.71	1/491 (0.2%)
12	H0	0.25	0/188	0.55	0/259
12	H1	0.24	0/188	0.68	0/259
12	H2	0.24	0/367	0.67	1/491 (0.2%)
12	H3	0.23	0/416	0.50	0/558
12	H4	0.21	0/188	0.50	0/259
12	H5	0.26	0/367	0.71	0/491
12	H6	0.25	0/416	0.57	0/558
12	H7	0.23	0/188	0.74	0/259

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
12	H8	0.19	0/367	0.36	0/491
12	H9	0.31	0/416	0.75	1/558 (0.2%)
12	I1	0.31	0/367	0.81	1/491 (0.2%)
12	I2	0.23	0/416	0.56	0/558
12	I3	0.21	0/188	0.60	0/259
12	I4	0.27	0/367	0.69	0/491
12	I5	0.32	0/416	0.78	0/558
12	I6	0.23	0/188	0.64	0/259
12	I7	0.24	0/367	0.64	0/491
12	I8	0.23	0/416	0.54	0/558
12	I9	0.21	0/188	0.56	0/259
13	J1	0.21	0/2529	0.54	1/3401 (0.0%)
13	J2	0.22	0/2529	0.56	2/3401 (0.1%)
13	J3	0.22	0/2529	0.51	0/3401
13	J4	0.20	0/2529	0.50	0/3401
13	J5	0.23	0/2529	0.56	2/3401 (0.1%)
13	J6	0.20	0/2529	0.51	1/3401 (0.0%)
13	J7	0.16	0/2529	0.40	0/3401
14	K0	0.22	0/1579	0.61	0/2139
14	K1	0.21	0/1579	0.50	0/2139
14	K2	0.19	0/1579	0.48	0/2139
14	K3	0.23	0/1579	0.61	0/2139
14	K4	0.21	0/1579	0.57	0/2139
14	K5	0.21	0/1579	0.52	0/2139
14	K6	0.22	0/1579	0.54	0/2139
14	K7	0.19	0/1579	0.47	0/2139
14	K8	0.19	0/1579	0.48	0/2139
14	K9	0.19	0/1579	0.47	0/2139
14	L0	0.22	0/1579	0.57	1/2139 (0.0%)
14	L1	0.24	0/1579	0.62	0/2139
14	L2	0.18	0/1579	0.46	0/2139
14	L3	0.22	0/1579	0.57	0/2139
14	L4	0.20	0/1102	0.55	0/1496
14	L5	0.19	0/1579	0.50	0/2139
14	L6	0.20	0/1579	0.52	0/2139
14	L7	0.22	0/1579	0.59	0/2139
14	L8	0.22	0/1579	0.58	0/2139
14	L9	0.22	0/1579	0.54	0/2139
14	M1	0.23	0/1039	0.64	1/1412 (0.1%)
14	M2	0.21	0/1579	0.52	0/2139
14	M3	0.22	0/1579	0.54	0/2139
14	M4	0.20	0/1579	0.53	0/2139
14	M5	0.22	0/1579	0.58	0/2139

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
14	M6	0.20	0/1579	0.54	0/2139
14	M7	0.22	0/1579	0.60	2/2139 (0.1%)
All	All	0.27	18/819485 (0.0%)	0.63	385/1107855 (0.0%)

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	1	0	2
1	2	0	1
1	C	0	3
1	F	0	1
1	G	0	1
1	I	0	13
1	J	0	12
1	L	0	2
1	M	0	9
1	N	0	12
1	O	0	4
1	P	0	5
1	S	0	1
1	Y	0	12
1	Z	0	1
1	a	0	13
1	c	0	13
1	d	0	1
1	f	0	21
1	g	0	1
1	h	0	2
1	i	0	2
1	j	0	1
1	k	0	1
1	l	0	2
1	m	0	2
1	p	0	1
1	u	0	1
1	v	0	2
1	w	0	2
1	x	0	1
1	y	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	z	0	1
2	3	0	1
3	1A	0	3
3	1E	0	1
3	1G	0	1
3	1K	0	2
3	1M	0	1
3	2C	0	1
3	2E	0	1
3	2G	0	1
3	2I	0	2
3	2M	0	1
3	3A	0	2
3	3C	0	1
3	3E	0	1
3	3I	0	1
3	3K	0	2
3	4A	0	2
3	4C	0	1
3	4E	0	1
3	4G	0	1
3	4K	0	1
3	5A	0	1
3	5E	0	1
3	5M	0	3
3	6C	0	1
3	6G	0	1
3	7E	0	2
3	8C	0	5
3	8G	0	2
3	8I	0	2
3	8K	0	4
3	8M	0	1
3	9C	0	2
3	9E	0	1
3	9G	0	3
3	9I	0	3
3	9K	0	2
4	1B	0	1
4	1D	0	2
4	1H	0	2
4	1L	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
4	1N	0	1
4	2F	0	2
4	2J	0	1
4	2L	0	2
4	3H	0	1
4	3J	0	1
4	4B	0	2
4	4D	0	1
4	4F	0	2
4	4H	0	2
4	4J	0	2
4	4L	0	1
4	5D	0	2
4	5F	0	1
4	5J	0	1
4	5L	0	1
4	6H	0	1
4	7B	0	2
4	7D	0	1
4	7H	0	1
4	8B	0	1
4	8D	0	1
4	8F	0	1
4	8J	0	2
4	8L	0	1
4	9B	0	2
4	9D	0	2
4	9F	0	4
4	9J	0	2
5	20	0	1
5	21	0	2
5	22	0	1
5	23	0	2
5	24	0	1
5	25	0	2
5	27	0	2
5	29	0	2
5	31	0	3
5	33	0	1
5	50	0	1
6	63	0	1
6	64	0	5

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Mol	Chain	#Chirality outliers	#Planarity outliers
6	65	0	6
6	66	0	6
6	67	0	6
6	68	0	7
6	69	0	5
7	72	0	1
7	79	0	1
7	84	0	1
7	87	0	1
7	89	0	2
7	90	0	3
7	91	0	1
7	92	0	3
7	93	0	2
7	95	0	2
7	96	0	1
7	97	0	1
8	A1	0	1
8	A3	0	1
8	A4	0	1
8	A5	0	1
8	A6	0	1
8	A7	0	1
8	A8	0	1
9	B5	0	1
9	B6	0	1
9	B7	0	2
10	D0	0	1
10	D1	0	2
10	D3	0	2
10	D4	0	2
10	D5	0	1
10	D6	0	2
10	D7	0	2
10	D8	0	2
10	D9	0	3
10	E1	0	1
10	E2	0	1
10	E3	0	3
10	E4	0	1
10	E5	0	1
10	E6	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
10	E8	0	2
10	E9	0	2
10	F2	0	1
10	F3	0	2
12	F5	0	1
12	F7	0	1
12	F9	0	1
12	G1	0	2
12	G2	0	1
12	G3	0	2
12	G5	0	1
12	G7	0	1
13	J6	0	1
14	K1	0	1
14	K3	0	1
14	K4	0	1
14	K6	0	1
14	M4	0	1
All	All	0	393

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	67	855	PRO	CA-C	-9.07	1.46	1.51
7	97	302	PRO	CA-C	-8.48	1.46	1.52
7	79	302	PRO	CA-C	-8.25	1.47	1.51
9	B6	151	PRO	CA-C	6.89	1.56	1.52
4	5L	286	VAL	CA-CB	-6.63	1.49	1.53

The worst 5 of 385 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	5N	30	ILE	CA-C-N	10.00	139.95	120.94
4	5N	30	ILE	C-N-CA	10.00	139.95	120.94
1	K	361	LEU	CA-CB-CG	8.38	145.63	116.30
4	5B	324	LYS	CG-CD-CE	-8.28	92.26	111.30
1	J	618	ARG	N-CA-C	-8.18	102.44	111.36

There are no chirality outliers.

5 of 393 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	316	LEU	Peptide
1	C	379	ARG	Sidechain
1	C	387	ILE	Peptide
1	F	499	ARG	Sidechain
1	G	429	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	881	0	906	11	0
1	2	881	0	906	23	0
1	A	2425	0	2423	48	0
1	B	1998	0	1977	35	0
1	C	1232	0	1211	30	0
1	D	993	0	1005	25	0
1	E	2215	0	2180	34	0
1	F	2469	0	2470	33	0
1	G	1403	0	1365	35	0
1	H	959	0	978	26	0
1	I	3014	0	3010	102	0
1	J	2963	0	2965	124	0
1	K	1637	0	1630	31	0
1	L	1678	0	1669	33	0
1	M	1786	0	1796	78	0
1	N	1723	0	1738	77	0
1	O	465	0	465	25	0
1	P	444	0	446	26	0
1	Q	2876	0	2882	50	0
1	R	2096	0	2111	29	0
1	S	1468	0	1460	22	0
1	T	647	0	652	19	0
1	U	3096	0	3078	50	0
1	V	2121	0	2126	29	0
1	W	1649	0	1638	18	0
1	X	749	0	761	16	0
1	Y	2959	0	2962	104	0
1	Z	2017	0	2003	35	0
1	a	1559	0	1569	109	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	b	731	0	710	9	0
1	c	2988	0	2987	133	0
1	d	2057	0	2040	34	0
1	e	725	0	706	10	0
1	f	1586	0	1591	125	0
1	g	729	0	717	11	0
1	h	729	0	717	21	0
1	i	729	0	717	28	0
1	j	729	0	717	18	0
1	k	729	0	717	10	0
1	l	729	0	717	26	0
1	m	729	0	717	24	0
1	n	699	0	733	10	0
1	o	699	0	733	17	0
1	p	699	0	733	16	0
1	q	699	0	733	16	0
1	r	699	0	733	9	0
1	s	699	0	733	11	0
1	t	699	0	733	16	0
1	u	881	0	906	17	0
1	v	881	0	906	13	0
1	w	881	0	906	10	0
1	x	881	0	906	18	0
1	y	881	0	906	14	0
1	z	881	0	906	11	0
2	10	1493	0	1518	22	0
2	11	1512	0	1542	18	0
2	12	1493	0	1518	35	0
2	13	1512	0	1542	18	0
2	14	1493	0	1518	20	0
2	15	764	0	797	6	0
2	16	834	0	863	13	0
2	3	1512	0	1542	21	0
2	4	1493	0	1518	21	0
2	5	1512	0	1542	19	0
2	6	1493	0	1518	30	0
2	7	1512	0	1542	18	0
2	8	1493	0	1518	30	0
2	9	1512	0	1542	22	0
3	1A	3325	0	3251	78	0
3	1C	3325	0	3252	62	0
3	1E	3325	0	3249	82	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	1G	3325	0	3252	56	0
3	1I	3325	0	3252	44	0
3	1K	3325	0	3252	58	0
3	1M	3325	0	3252	80	0
3	2A	3325	0	3252	73	0
3	2C	3325	0	3250	68	0
3	2E	3325	0	3250	69	0
3	2G	3325	0	3252	52	0
3	2I	3325	0	3251	61	0
3	2K	3325	0	3252	54	0
3	2M	3325	0	3252	63	0
3	3A	3325	0	3251	90	0
3	3C	3325	0	3252	72	0
3	3E	3325	0	3252	48	0
3	3G	3325	0	3252	35	0
3	3I	3325	0	3251	43	0
3	3K	3325	0	3252	54	0
3	3M	3325	0	3252	76	0
3	4A	3325	0	3252	66	0
3	4C	3325	0	3252	61	0
3	4E	3325	0	3252	43	0
3	4G	3325	0	3251	46	0
3	4I	3325	0	3252	36	0
3	4K	3325	0	3252	41	0
3	4M	3325	0	3252	81	0
3	5A	3325	0	3252	82	0
3	5C	3325	0	3252	64	0
3	5E	3325	0	3251	43	0
3	5G	3325	0	3252	40	0
3	5I	3325	0	3252	46	0
3	5K	3325	0	3252	34	0
3	5M	3325	0	3252	51	0
3	6A	3325	0	3251	57	0
3	6C	3325	0	3252	48	0
3	6E	3325	0	3251	45	0
3	6G	3325	0	3252	37	0
3	6I	3325	0	3252	50	0
3	6K	3325	0	3252	41	0
3	6M	3325	0	3252	92	0
3	7A	3325	0	3252	42	0
3	7C	3325	0	3252	60	0
3	7E	3325	0	3252	61	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	7G	3325	0	3252	46	0
3	7I	3325	0	3252	46	0
3	7K	3325	0	3252	74	0
3	7M	3325	0	3252	76	0
3	8A	3325	0	3251	55	0
3	8C	3325	0	3252	53	0
3	8E	3325	0	3252	65	0
3	8G	3325	0	3252	47	0
3	8I	3325	0	3252	53	0
3	8K	3325	0	3252	72	0
3	8M	3325	0	3252	49	0
3	9A	3325	0	3252	56	0
3	9C	3325	0	3252	51	0
3	9E	3325	0	3251	59	0
3	9G	3325	0	3252	56	0
3	9I	3325	0	3252	65	0
3	9K	3325	0	3252	53	0
3	9M	3325	0	3252	39	0
4	1B	3331	0	3207	78	0
4	1D	3331	0	3209	72	0
4	1F	3331	0	3205	68	0
4	1H	3331	0	3209	58	0
4	1J	3331	0	3207	58	0
4	1L	3331	0	3209	62	0
4	1N	3331	0	3207	54	0
4	2B	3331	0	3207	84	0
4	2D	3331	0	3209	71	0
4	2F	3331	0	3207	64	0
4	2H	3331	0	3209	42	0
4	2J	3331	0	3207	57	0
4	2L	3331	0	3209	58	0
4	3B	3331	0	3207	96	0
4	3D	3331	0	3209	66	0
4	3F	3331	0	3207	71	0
4	3H	3331	0	3209	48	0
4	3J	3331	0	3207	54	0
4	3L	3331	0	3209	64	0
4	4B	3331	0	3207	75	0
4	4D	3331	0	3209	52	0
4	4F	3331	0	3207	41	0
4	4H	3331	0	3209	44	0
4	4J	3331	0	3207	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	4L	3331	0	3209	55	0
4	5B	3331	0	3207	86	0
4	5D	3331	0	3209	45	0
4	5F	3331	0	3207	37	0
4	5H	3331	0	3209	48	0
4	5J	3331	0	3207	50	0
4	5L	3331	0	3209	49	0
4	5N	3331	0	3207	72	0
4	6B	3331	0	3207	69	0
4	6D	3331	0	3209	56	0
4	6F	3331	0	3207	49	0
4	6H	3331	0	3209	65	0
4	6J	3331	0	3207	67	0
4	6L	3331	0	3209	54	0
4	6N	3331	0	3205	88	0
4	7B	3331	0	3207	83	0
4	7D	3331	0	3209	71	0
4	7F	3331	0	3207	63	0
4	7H	3331	0	3209	59	0
4	7J	3331	0	3207	76	0
4	7L	3331	0	3209	87	0
4	8B	3331	0	3207	62	0
4	8D	3331	0	3209	55	0
4	8F	3331	0	3207	80	0
4	8H	3331	0	3209	52	0
4	8J	3331	0	3207	79	0
4	8L	3331	0	3209	95	0
4	9B	3331	0	3207	72	0
4	9D	3331	0	3206	56	0
4	9F	3331	0	3207	77	0
4	9H	3331	0	3209	64	0
4	9J	3331	0	3207	60	0
4	9L	3331	0	3207	54	0
5	20	1814	0	1830	30	0
5	21	1815	0	1834	31	0
5	22	1814	0	1830	24	0
5	23	1815	0	1834	23	0
5	24	1814	0	1830	37	0
5	25	1815	0	1834	40	0
5	26	1814	0	1830	32	0
5	27	1815	0	1834	39	0
5	28	1814	0	1830	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	29	1815	0	1834	36	0
5	30	1814	0	1830	24	0
5	31	1815	0	1834	45	0
5	32	1814	0	1830	30	0
5	33	1321	0	1311	24	0
5	35	1744	0	1764	37	0
5	36	1723	0	1750	17	0
5	37	1744	0	1764	20	0
5	38	1723	0	1750	28	0
5	39	1744	0	1764	34	0
5	40	1723	0	1750	30	0
5	42	1723	0	1750	15	0
5	43	1744	0	1764	30	0
5	44	1723	0	1750	26	0
5	45	1744	0	1764	16	0
5	46	1723	0	1750	20	0
5	47	1744	0	1764	28	0
5	48	1723	0	1750	14	0
5	49	1841	0	1859	35	0
5	50	1853	0	1866	38	0
5	51	1841	0	1859	38	0
5	52	1853	0	1866	41	0
5	53	1841	0	1859	37	0
5	54	1853	0	1866	27	0
5	55	1841	0	1859	35	0
5	56	1853	0	1866	28	0
5	57	1841	0	1859	34	0
5	58	1853	0	1866	28	0
5	59	1841	0	1859	26	0
5	60	1853	0	1866	31	0
5	61	1841	0	1859	43	0
5	62	1853	0	1866	45	0
6	63	5055	0	5022	69	0
6	64	5055	0	5022	65	0
6	65	5055	0	5022	69	0
6	66	5055	0	5022	88	0
6	67	5055	0	5022	87	0
6	68	5055	0	5022	87	0
6	69	5055	0	5022	81	0
7	71	1382	0	1347	25	0
7	72	1382	0	1347	23	0
7	73	1382	0	1347	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	75	1382	0	1347	30	0
7	76	1382	0	1347	19	0
7	77	1382	0	1347	32	0
7	78	1382	0	1347	25	0
7	79	1382	0	1347	16	0
7	80	1382	0	1347	27	0
7	82	1382	0	1347	25	0
7	83	1382	0	1347	38	0
7	84	1382	0	1347	32	0
7	85	1382	0	1347	21	0
7	86	1382	0	1347	23	0
7	87	1382	0	1347	31	0
7	89	1382	0	1347	25	0
7	90	1382	0	1347	27	0
7	91	1382	0	1347	31	0
7	92	1382	0	1347	26	0
7	93	1382	0	1347	23	0
7	94	1382	0	1347	21	0
7	95	1382	0	1347	18	0
7	96	1382	0	1347	30	0
7	97	1382	0	1347	20	0
8	A1	2582	0	2580	36	0
8	A2	2582	0	2580	45	0
8	A3	1844	0	1818	38	0
8	A4	1016	0	899	19	0
8	A5	2582	0	2580	39	0
8	A6	2582	0	2580	34	0
8	A7	2582	0	2580	44	0
8	A8	2582	0	2580	28	0
8	A9	1020	0	1043	11	0
9	B1	2055	0	2002	19	0
9	B2	2055	0	2002	30	0
9	B3	2055	0	2002	24	0
9	B4	2055	0	2002	24	0
9	B5	2055	0	2002	41	0
9	B6	2055	0	2002	35	0
9	B7	2055	0	2002	40	0
10	C0	1471	0	1499	13	0
10	C6	1471	0	1499	26	0
10	C7	1471	0	1499	23	0
10	C8	1471	0	1499	31	0
10	C9	1471	0	1499	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	D0	2197	0	2210	23	0
10	D1	1471	0	1499	23	0
10	D2	1471	0	1499	24	0
10	D3	2197	0	2210	20	0
10	D4	2197	0	2210	16	0
10	D5	2197	0	2210	26	0
10	D6	2197	0	2210	28	0
10	D7	2197	0	2210	23	0
10	D8	2197	0	2210	25	0
10	D9	2197	0	2210	35	0
10	E0	2197	0	2210	21	0
10	E1	2197	0	2210	27	0
10	E2	2197	0	2210	35	0
10	E3	2197	0	2210	30	0
10	E4	2197	0	2210	31	0
10	E5	2197	0	2210	23	0
10	E6	2197	0	2210	39	0
10	E7	2197	0	2210	24	0
10	E8	2197	0	2210	26	0
10	E9	2197	0	2210	25	0
10	F1	2197	0	2210	24	0
10	F2	2197	0	2210	42	0
10	F3	2197	0	2210	30	0
11	C1	237	0	242	2	0
11	C2	238	0	239	2	0
11	C3	242	0	244	5	0
11	C4	214	0	212	0	0
11	C5	239	0	243	6	0
12	F0	883	0	883	15	0
12	F5	847	0	844	14	0
12	F6	883	0	883	21	0
12	F7	847	0	844	14	0
12	F8	883	0	883	14	0
12	F9	847	0	844	19	0
12	G0	412	0	416	3	0
12	G1	847	0	844	19	0
12	G2	883	0	883	22	0
12	G3	847	0	844	15	0
12	G4	883	0	883	16	0
12	G5	847	0	844	16	0
12	G6	883	0	883	17	0
12	G7	847	0	844	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	G8	883	0	883	18	0
12	G9	365	0	364	3	0
12	H0	184	0	174	2	0
12	H1	184	0	174	3	0
12	H2	365	0	364	5	0
12	H3	412	0	416	2	0
12	H4	184	0	174	3	0
12	H5	365	0	364	6	0
12	H6	412	0	416	5	0
12	H7	184	0	174	5	0
12	H8	365	0	364	3	0
12	H9	412	0	416	6	0
12	I1	365	0	364	2	0
12	I2	412	0	416	3	0
12	I3	184	0	174	2	0
12	I4	365	0	364	4	0
12	I5	412	0	416	5	0
12	I6	184	0	174	2	0
12	I7	365	0	364	4	0
12	I8	412	0	416	4	0
12	I9	184	0	174	5	0
13	J1	2488	0	2518	42	0
13	J2	2488	0	2518	44	0
13	J3	2488	0	2518	34	0
13	J4	2488	0	2518	29	0
13	J5	2488	0	2518	34	0
13	J6	2488	0	2518	39	0
13	J7	2488	0	2518	22	0
14	K0	1537	0	1507	20	0
14	K1	1537	0	1507	22	0
14	K2	1537	0	1507	16	0
14	K3	1537	0	1507	23	0
14	K4	1537	0	1507	31	0
14	K5	1537	0	1507	18	0
14	K6	1537	0	1507	29	0
14	K7	1537	0	1507	12	0
14	K8	1537	0	1507	17	0
14	K9	1537	0	1507	15	0
14	L0	1537	0	1507	29	0
14	L1	1537	0	1507	29	0
14	L2	1537	0	1507	17	0
14	L3	1537	0	1507	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	L4	1073	0	1091	20	0
14	L5	1537	0	1507	24	0
14	L6	1537	0	1507	23	0
14	L7	1537	0	1507	30	0
14	L8	1537	0	1507	21	0
14	L9	1537	0	1507	28	0
14	M1	1011	0	1013	18	0
14	M2	1537	0	1507	32	0
14	M3	1537	0	1507	34	0
14	M4	1537	0	1507	27	0
14	M5	1537	0	1507	29	0
14	M6	1537	0	1507	22	0
14	M7	1537	0	1507	37	0
15	1A	32	0	12	1	0
15	1C	32	0	12	0	0
15	1E	32	0	12	0	0
15	1G	32	0	12	0	0
15	1I	32	0	12	0	0
15	1K	32	0	12	0	0
15	1M	32	0	12	0	0
15	2A	32	0	12	2	0
15	2C	32	0	12	1	0
15	2E	32	0	12	0	0
15	2G	32	0	12	0	0
15	2I	32	0	12	0	0
15	2K	32	0	12	0	0
15	2M	32	0	12	0	0
15	3A	32	0	12	0	0
15	3C	32	0	12	0	0
15	3E	32	0	12	0	0
15	3G	32	0	12	0	0
15	3I	32	0	12	0	0
15	3K	32	0	12	0	0
15	3M	32	0	12	0	0
15	4A	32	0	12	0	0
15	4C	32	0	12	0	0
15	4E	32	0	12	0	0
15	4G	32	0	12	0	0
15	4I	32	0	12	0	0
15	4K	32	0	12	0	0
15	4M	32	0	12	0	0
15	5A	32	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	5C	32	0	12	0	0
15	5E	32	0	12	0	0
15	5G	32	0	12	0	0
15	5I	32	0	12	0	0
15	5K	32	0	12	0	0
15	5M	32	0	12	0	0
15	6A	32	0	12	0	0
15	6C	32	0	12	1	0
15	6E	32	0	12	0	0
15	6G	32	0	12	0	0
15	6I	32	0	12	0	0
15	6K	32	0	12	0	0
15	6N	32	0	12	0	0
15	7A	32	0	12	0	0
15	7C	32	0	12	0	0
15	7E	32	0	12	0	0
15	7G	32	0	12	0	0
15	7I	32	0	12	0	0
15	7K	32	0	12	0	0
15	7M	32	0	12	0	0
15	8A	32	0	12	0	0
15	8C	32	0	12	0	0
15	8E	32	0	12	0	0
15	8G	32	0	12	0	0
15	8I	32	0	12	0	0
15	8K	32	0	12	0	0
15	8M	32	0	12	0	0
15	9A	32	0	12	0	0
15	9C	32	0	12	0	0
15	9E	32	0	12	0	0
15	9G	32	0	12	0	0
15	9I	32	0	12	0	0
15	9K	32	0	12	1	0
15	9M	32	0	12	0	0
16	1A	1	0	0	0	0
16	1C	1	0	0	0	0
16	1E	1	0	0	0	0
16	1G	1	0	0	0	0
16	1I	1	0	0	0	0
16	1K	1	0	0	0	0
16	2A	1	0	0	0	0
16	2C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	2E	1	0	0	0	0
16	2G	1	0	0	0	0
16	2I	1	0	0	0	0
16	2K	1	0	0	0	0
16	3A	1	0	0	0	0
16	3C	1	0	0	0	0
16	3E	1	0	0	0	0
16	3G	1	0	0	0	0
16	3I	1	0	0	0	0
16	3K	1	0	0	0	0
16	4A	1	0	0	0	0
16	4C	1	0	0	0	0
16	4E	1	0	0	0	0
16	4G	1	0	0	0	0
16	4I	1	0	0	0	0
16	4K	1	0	0	0	0
16	5A	1	0	0	0	0
16	5C	1	0	0	0	0
16	5E	1	0	0	0	0
16	5G	1	0	0	0	0
16	5I	1	0	0	0	0
16	5K	1	0	0	0	0
16	6A	1	0	0	0	0
16	6C	1	0	0	0	0
16	6E	1	0	0	0	0
16	6G	1	0	0	0	0
16	6I	1	0	0	0	0
16	6K	1	0	0	0	0
16	7B	1	0	0	0	0
16	7C	1	0	0	0	0
16	7E	1	0	0	0	0
16	7G	1	0	0	0	0
16	7I	1	0	0	0	0
16	7K	1	0	0	0	0
16	8A	1	0	0	0	0
16	8C	1	0	0	0	0
16	8E	1	0	0	1	0
16	8G	1	0	0	0	0
16	8I	1	0	0	0	0
16	8K	1	0	0	0	0
16	9A	1	0	0	0	0
16	9C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	9E	1	0	0	0	0
16	9G	1	0	0	0	0
16	9I	1	0	0	0	0
16	9K	1	0	0	0	0
17	1B	28	0	12	1	0
17	1D	28	0	12	2	0
17	1F	28	0	12	1	0
17	1H	28	0	12	0	0
17	1J	28	0	12	0	0
17	1L	28	0	12	0	0
17	1N	28	0	12	0	0
17	2B	28	0	12	2	0
17	2D	28	0	12	0	0
17	2F	28	0	12	1	0
17	2H	28	0	12	2	0
17	2J	28	0	12	0	0
17	2L	28	0	12	1	0
17	3B	28	0	12	2	0
17	3D	28	0	12	0	0
17	3F	28	0	12	1	0
17	3H	28	0	12	0	0
17	3J	28	0	12	2	0
17	3L	28	0	12	2	0
17	4B	28	0	12	1	0
17	4D	28	0	12	1	0
17	4F	28	0	12	0	0
17	4H	28	0	12	0	0
17	4J	28	0	12	1	0
17	4L	28	0	12	0	0
17	5B	28	0	12	0	0
17	5D	28	0	12	0	0
17	5F	28	0	12	0	0
17	5H	28	0	12	0	0
17	5J	28	0	12	0	0
17	5L	28	0	12	2	0
17	5N	28	0	12	0	0
17	6B	28	0	12	0	0
17	6D	28	0	12	0	0
17	6F	28	0	12	0	0
17	6H	28	0	12	0	0
17	6J	28	0	12	0	0
17	6L	28	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	6N	28	0	12	1	0
17	7B	28	0	12	0	0
17	7D	28	0	12	0	0
17	7F	28	0	12	0	0
17	7H	28	0	12	0	0
17	7J	28	0	12	0	0
17	7L	28	0	12	0	0
17	8B	28	0	12	1	0
17	8D	28	0	12	0	0
17	8F	28	0	12	0	0
17	8H	28	0	12	0	0
17	8J	28	0	12	0	0
17	8L	28	0	12	0	0
17	9B	28	0	12	0	0
17	9D	28	0	11	0	0
17	9F	28	0	12	0	0
17	9H	28	0	12	0	0
17	9J	28	0	12	0	0
17	9L	28	0	12	1	0
All	All	806376	0	792189	12039	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 8.

The worst 5 of 12039 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)
1:M:682:LYS:HE2	1:l:795:LEU:CD2	1.42	1.49
1:J:577:GLN:NE2	1:J:578:ARG:HD2	1.63	1.14
1:a:607:LEU:HB2	1:f:607:LEU:HB3	1.30	1.14
1:M:682:LYS:CE	1:l:795:LEU:CD2	2.27	1.11
1:a:558:LEU:HD22	1:f:558:LEU:HB3	1.33	1.10

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	110/954 (12%)	96 (87%)	12 (11%)	2 (2%)	6	25
1	2	110/954 (12%)	95 (86%)	14 (13%)	1 (1%)	14	41
1	A	290/954 (30%)	286 (99%)	4 (1%)	0	100	100
1	B	239/954 (25%)	232 (97%)	7 (3%)	0	100	100
1	C	146/954 (15%)	137 (94%)	9 (6%)	0	100	100
1	D	116/954 (12%)	116 (100%)	0	0	100	100
1	E	267/954 (28%)	255 (96%)	11 (4%)	1 (0%)	30	59
1	F	297/954 (31%)	293 (99%)	4 (1%)	0	100	100
1	G	168/954 (18%)	154 (92%)	11 (6%)	3 (2%)	6	25
1	H	112/954 (12%)	112 (100%)	0	0	100	100
1	I	358/954 (38%)	354 (99%)	4 (1%)	0	100	100
1	J	352/954 (37%)	346 (98%)	6 (2%)	0	100	100
1	K	195/954 (20%)	194 (100%)	1 (0%)	0	100	100
1	L	200/954 (21%)	198 (99%)	2 (1%)	0	100	100
1	M	211/954 (22%)	207 (98%)	4 (2%)	0	100	100
1	N	204/954 (21%)	197 (97%)	7 (3%)	0	100	100
1	O	55/954 (6%)	50 (91%)	5 (9%)	0	100	100
1	P	52/954 (6%)	46 (88%)	6 (12%)	0	100	100
1	Q	340/954 (36%)	336 (99%)	2 (1%)	2 (1%)	21	50
1	R	250/954 (26%)	242 (97%)	8 (3%)	0	100	100
1	S	173/954 (18%)	167 (96%)	6 (4%)	0	100	100
1	T	75/954 (8%)	75 (100%)	0	0	100	100
1	U	370/954 (39%)	367 (99%)	3 (1%)	0	100	100
1	V	256/954 (27%)	255 (100%)	1 (0%)	0	100	100
1	W	196/954 (20%)	196 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	X	88/954 (9%)	86 (98%)	2 (2%)	0	100	100
1	Y	352/954 (37%)	345 (98%)	7 (2%)	0	100	100
1	Z	241/954 (25%)	241 (100%)	0	0	100	100
1	a	183/954 (19%)	176 (96%)	7 (4%)	0	100	100
1	b	83/954 (9%)	83 (100%)	0	0	100	100
1	c	357/954 (37%)	334 (94%)	18 (5%)	5 (1%)	9	31
1	d	246/954 (26%)	245 (100%)	1 (0%)	0	100	100
1	e	83/954 (9%)	82 (99%)	1 (1%)	0	100	100
1	f	188/954 (20%)	162 (86%)	21 (11%)	5 (3%)	4	18
1	g	98/954 (10%)	85 (87%)	12 (12%)	1 (1%)	12	38
1	h	98/954 (10%)	69 (70%)	29 (30%)	0	100	100
1	i	98/954 (10%)	89 (91%)	8 (8%)	1 (1%)	12	38
1	j	98/954 (10%)	82 (84%)	14 (14%)	2 (2%)	6	23
1	k	98/954 (10%)	82 (84%)	16 (16%)	0	100	100
1	l	98/954 (10%)	72 (74%)	26 (26%)	0	100	100
1	m	98/954 (10%)	71 (72%)	26 (26%)	1 (1%)	12	38
1	n	86/954 (9%)	75 (87%)	10 (12%)	1 (1%)	10	34
1	o	86/954 (9%)	74 (86%)	11 (13%)	1 (1%)	10	34
1	p	86/954 (9%)	75 (87%)	8 (9%)	3 (4%)	3	14
1	q	86/954 (9%)	73 (85%)	11 (13%)	2 (2%)	5	20
1	r	86/954 (9%)	76 (88%)	6 (7%)	4 (5%)	2	10
1	s	86/954 (9%)	76 (88%)	8 (9%)	2 (2%)	5	20
1	t	86/954 (9%)	73 (85%)	9 (10%)	4 (5%)	2	10
1	u	110/954 (12%)	95 (86%)	13 (12%)	2 (2%)	6	25
1	v	110/954 (12%)	96 (87%)	13 (12%)	1 (1%)	14	41
1	w	110/954 (12%)	95 (86%)	13 (12%)	2 (2%)	6	25
1	x	110/954 (12%)	95 (86%)	12 (11%)	3 (3%)	4	18
1	y	110/954 (12%)	94 (86%)	16 (14%)	0	100	100
1	z	110/954 (12%)	94 (86%)	15 (14%)	1 (1%)	14	41
2	10	173/410 (42%)	168 (97%)	4 (2%)	1 (1%)	21	50
2	11	175/410 (43%)	171 (98%)	2 (1%)	2 (1%)	11	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	12	173/410 (42%)	169 (98%)	3 (2%)	1 (1%)	21	50
2	13	175/410 (43%)	172 (98%)	3 (2%)	0	100	100
2	14	173/410 (42%)	170 (98%)	2 (1%)	1 (1%)	21	50
2	15	86/410 (21%)	85 (99%)	1 (1%)	0	100	100
2	16	95/410 (23%)	91 (96%)	3 (3%)	1 (1%)	11	36
2	3	175/410 (43%)	173 (99%)	2 (1%)	0	100	100
2	4	173/410 (42%)	169 (98%)	3 (2%)	1 (1%)	21	50
2	5	175/410 (43%)	172 (98%)	1 (1%)	2 (1%)	11	36
2	6	173/410 (42%)	168 (97%)	4 (2%)	1 (1%)	21	50
2	7	175/410 (43%)	172 (98%)	2 (1%)	1 (1%)	21	50
2	8	173/410 (42%)	167 (96%)	5 (3%)	1 (1%)	21	50
2	9	175/410 (43%)	171 (98%)	2 (1%)	2 (1%)	11	36
3	1A	424/453 (94%)	383 (90%)	40 (9%)	1 (0%)	43	70
3	1C	424/453 (94%)	388 (92%)	34 (8%)	2 (0%)	24	54
3	1E	424/453 (94%)	386 (91%)	37 (9%)	1 (0%)	43	70
3	1G	424/453 (94%)	388 (92%)	35 (8%)	1 (0%)	43	70
3	1I	424/453 (94%)	393 (93%)	29 (7%)	2 (0%)	24	54
3	1K	424/453 (94%)	391 (92%)	33 (8%)	0	100	100
3	1M	424/453 (94%)	378 (89%)	45 (11%)	1 (0%)	43	70
3	2A	424/453 (94%)	371 (88%)	51 (12%)	2 (0%)	24	54
3	2C	424/453 (94%)	395 (93%)	29 (7%)	0	100	100
3	2E	424/453 (94%)	393 (93%)	29 (7%)	2 (0%)	24	54
3	2G	424/453 (94%)	395 (93%)	29 (7%)	0	100	100
3	2I	424/453 (94%)	405 (96%)	19 (4%)	0	100	100
3	2K	424/453 (94%)	392 (92%)	32 (8%)	0	100	100
3	2M	424/453 (94%)	385 (91%)	39 (9%)	0	100	100
3	3A	424/453 (94%)	397 (94%)	25 (6%)	2 (0%)	24	54
3	3C	424/453 (94%)	397 (94%)	27 (6%)	0	100	100
3	3E	424/453 (94%)	405 (96%)	18 (4%)	1 (0%)	43	70
3	3G	424/453 (94%)	402 (95%)	22 (5%)	0	100	100
3	3I	424/453 (94%)	400 (94%)	24 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	3K	424/453 (94%)	397 (94%)	25 (6%)	2 (0%)	24	54
3	3M	424/453 (94%)	394 (93%)	28 (7%)	2 (0%)	24	54
3	4A	424/453 (94%)	379 (89%)	45 (11%)	0	100	100
3	4C	424/453 (94%)	393 (93%)	31 (7%)	0	100	100
3	4E	424/453 (94%)	385 (91%)	38 (9%)	1 (0%)	43	70
3	4G	424/453 (94%)	393 (93%)	31 (7%)	0	100	100
3	4I	424/453 (94%)	389 (92%)	34 (8%)	1 (0%)	43	70
3	4K	424/453 (94%)	394 (93%)	29 (7%)	1 (0%)	43	70
3	4M	424/453 (94%)	386 (91%)	36 (8%)	2 (0%)	24	54
3	5A	424/453 (94%)	393 (93%)	28 (7%)	3 (1%)	18	47
3	5C	424/453 (94%)	400 (94%)	24 (6%)	0	100	100
3	5E	424/453 (94%)	392 (92%)	31 (7%)	1 (0%)	43	70
3	5G	424/453 (94%)	400 (94%)	23 (5%)	1 (0%)	43	70
3	5I	424/453 (94%)	400 (94%)	23 (5%)	1 (0%)	43	70
3	5K	424/453 (94%)	396 (93%)	27 (6%)	1 (0%)	43	70
3	5M	424/453 (94%)	382 (90%)	40 (9%)	2 (0%)	24	54
3	6A	424/453 (94%)	408 (96%)	16 (4%)	0	100	100
3	6C	424/453 (94%)	403 (95%)	21 (5%)	0	100	100
3	6E	424/453 (94%)	407 (96%)	17 (4%)	0	100	100
3	6G	424/453 (94%)	394 (93%)	30 (7%)	0	100	100
3	6I	424/453 (94%)	402 (95%)	22 (5%)	0	100	100
3	6K	424/453 (94%)	403 (95%)	21 (5%)	0	100	100
3	6M	424/453 (94%)	399 (94%)	24 (6%)	1 (0%)	43	70
3	7A	424/453 (94%)	402 (95%)	22 (5%)	0	100	100
3	7C	424/453 (94%)	383 (90%)	40 (9%)	1 (0%)	43	70
3	7E	424/453 (94%)	395 (93%)	27 (6%)	2 (0%)	24	54
3	7G	424/453 (94%)	376 (89%)	46 (11%)	2 (0%)	24	54
3	7I	424/453 (94%)	391 (92%)	32 (8%)	1 (0%)	43	70
3	7K	424/453 (94%)	393 (93%)	31 (7%)	0	100	100
3	7M	424/453 (94%)	392 (92%)	32 (8%)	0	100	100
3	8A	424/453 (94%)	404 (95%)	20 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	8C	424/453 (94%)	380 (90%)	43 (10%)	1 (0%)	43	70
3	8E	424/453 (94%)	385 (91%)	37 (9%)	2 (0%)	24	54
3	8G	424/453 (94%)	383 (90%)	41 (10%)	0	100	100
3	8I	424/453 (94%)	377 (89%)	45 (11%)	2 (0%)	24	54
3	8K	424/453 (94%)	380 (90%)	42 (10%)	2 (0%)	24	54
3	8M	424/453 (94%)	397 (94%)	26 (6%)	1 (0%)	43	70
3	9A	424/453 (94%)	409 (96%)	15 (4%)	0	100	100
3	9C	424/453 (94%)	383 (90%)	41 (10%)	0	100	100
3	9E	424/453 (94%)	387 (91%)	35 (8%)	2 (0%)	24	54
3	9G	424/453 (94%)	382 (90%)	41 (10%)	1 (0%)	43	70
3	9I	424/453 (94%)	374 (88%)	48 (11%)	2 (0%)	24	54
3	9K	424/453 (94%)	388 (92%)	36 (8%)	0	100	100
3	9M	424/453 (94%)	398 (94%)	26 (6%)	0	100	100
4	1B	424/449 (94%)	395 (93%)	29 (7%)	0	100	100
4	1D	424/449 (94%)	379 (89%)	44 (10%)	1 (0%)	43	70
4	1F	424/449 (94%)	382 (90%)	42 (10%)	0	100	100
4	1H	424/449 (94%)	382 (90%)	41 (10%)	1 (0%)	43	70
4	1J	424/449 (94%)	391 (92%)	31 (7%)	2 (0%)	24	54
4	1L	424/449 (94%)	386 (91%)	36 (8%)	2 (0%)	24	54
4	1N	424/449 (94%)	385 (91%)	39 (9%)	0	100	100
4	2B	424/449 (94%)	389 (92%)	35 (8%)	0	100	100
4	2D	424/449 (94%)	389 (92%)	35 (8%)	0	100	100
4	2F	424/449 (94%)	389 (92%)	35 (8%)	0	100	100
4	2H	424/449 (94%)	392 (92%)	32 (8%)	0	100	100
4	2J	424/449 (94%)	392 (92%)	31 (7%)	1 (0%)	43	70
4	2L	424/449 (94%)	394 (93%)	29 (7%)	1 (0%)	43	70
4	3B	424/449 (94%)	383 (90%)	39 (9%)	2 (0%)	24	54
4	3D	424/449 (94%)	387 (91%)	37 (9%)	0	100	100
4	3F	424/449 (94%)	395 (93%)	28 (7%)	1 (0%)	43	70
4	3H	424/449 (94%)	392 (92%)	31 (7%)	1 (0%)	43	70
4	3J	424/449 (94%)	394 (93%)	29 (7%)	1 (0%)	43	70

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	3L	424/449 (94%)	396 (93%)	28 (7%)	0	100	100
4	4B	424/449 (94%)	395 (93%)	29 (7%)	0	100	100
4	4D	424/449 (94%)	393 (93%)	31 (7%)	0	100	100
4	4F	424/449 (94%)	398 (94%)	26 (6%)	0	100	100
4	4H	424/449 (94%)	410 (97%)	14 (3%)	0	100	100
4	4J	424/449 (94%)	401 (95%)	23 (5%)	0	100	100
4	4L	424/449 (94%)	391 (92%)	32 (8%)	1 (0%)	43	70
4	5B	424/449 (94%)	380 (90%)	39 (9%)	5 (1%)	10	34
4	5D	424/449 (94%)	397 (94%)	26 (6%)	1 (0%)	43	70
4	5F	424/449 (94%)	402 (95%)	20 (5%)	2 (0%)	24	54
4	5H	424/449 (94%)	401 (95%)	22 (5%)	1 (0%)	43	70
4	5J	424/449 (94%)	393 (93%)	29 (7%)	2 (0%)	24	54
4	5L	424/449 (94%)	391 (92%)	33 (8%)	0	100	100
4	5N	424/449 (94%)	381 (90%)	42 (10%)	1 (0%)	43	70
4	6B	424/449 (94%)	399 (94%)	25 (6%)	0	100	100
4	6D	424/449 (94%)	406 (96%)	18 (4%)	0	100	100
4	6F	424/449 (94%)	407 (96%)	17 (4%)	0	100	100
4	6H	424/449 (94%)	408 (96%)	16 (4%)	0	100	100
4	6J	424/449 (94%)	405 (96%)	19 (4%)	0	100	100
4	6L	424/449 (94%)	402 (95%)	22 (5%)	0	100	100
4	6N	424/449 (94%)	399 (94%)	25 (6%)	0	100	100
4	7B	424/449 (94%)	386 (91%)	36 (8%)	2 (0%)	24	54
4	7D	424/449 (94%)	377 (89%)	45 (11%)	2 (0%)	24	54
4	7F	424/449 (94%)	382 (90%)	41 (10%)	1 (0%)	43	70
4	7H	424/449 (94%)	387 (91%)	35 (8%)	2 (0%)	24	54
4	7J	424/449 (94%)	379 (89%)	44 (10%)	1 (0%)	43	70
4	7L	424/449 (94%)	388 (92%)	34 (8%)	2 (0%)	24	54
4	8B	424/449 (94%)	375 (88%)	46 (11%)	3 (1%)	18	47
4	8D	424/449 (94%)	375 (88%)	46 (11%)	3 (1%)	18	47
4	8F	424/449 (94%)	377 (89%)	45 (11%)	2 (0%)	24	54
4	8H	424/449 (94%)	387 (91%)	35 (8%)	2 (0%)	24	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	8J	424/449 (94%)	387 (91%)	33 (8%)	4 (1%)	14	41
4	8L	424/449 (94%)	371 (88%)	52 (12%)	1 (0%)	43	70
4	9B	424/449 (94%)	373 (88%)	48 (11%)	3 (1%)	18	47
4	9D	424/449 (94%)	379 (89%)	42 (10%)	3 (1%)	18	47
4	9F	424/449 (94%)	383 (90%)	39 (9%)	2 (0%)	24	54
4	9H	424/449 (94%)	385 (91%)	37 (9%)	2 (0%)	24	54
4	9J	424/449 (94%)	388 (92%)	31 (7%)	5 (1%)	10	34
4	9L	424/449 (94%)	383 (90%)	41 (10%)	0	100	100
5	20	223/263 (85%)	194 (87%)	28 (13%)	1 (0%)	30	59
5	21	223/263 (85%)	197 (88%)	26 (12%)	0	100	100
5	22	223/263 (85%)	199 (89%)	22 (10%)	2 (1%)	14	41
5	23	223/263 (85%)	201 (90%)	22 (10%)	0	100	100
5	24	223/263 (85%)	194 (87%)	27 (12%)	2 (1%)	14	41
5	25	223/263 (85%)	198 (89%)	24 (11%)	1 (0%)	30	59
5	26	223/263 (85%)	197 (88%)	25 (11%)	1 (0%)	30	59
5	27	223/263 (85%)	195 (87%)	28 (13%)	0	100	100
5	28	223/263 (85%)	199 (89%)	23 (10%)	1 (0%)	30	59
5	29	223/263 (85%)	196 (88%)	26 (12%)	1 (0%)	30	59
5	30	223/263 (85%)	197 (88%)	24 (11%)	2 (1%)	14	41
5	31	223/263 (85%)	199 (89%)	24 (11%)	0	100	100
5	32	223/263 (85%)	200 (90%)	22 (10%)	1 (0%)	30	59
5	33	163/263 (62%)	143 (88%)	20 (12%)	0	100	100
5	35	215/263 (82%)	205 (95%)	9 (4%)	1 (0%)	24	54
5	36	211/263 (80%)	205 (97%)	6 (3%)	0	100	100
5	37	215/263 (82%)	202 (94%)	12 (6%)	1 (0%)	24	54
5	38	211/263 (80%)	201 (95%)	10 (5%)	0	100	100
5	39	215/263 (82%)	205 (95%)	8 (4%)	2 (1%)	14	41
5	40	211/263 (80%)	203 (96%)	8 (4%)	0	100	100
5	42	211/263 (80%)	205 (97%)	6 (3%)	0	100	100
5	43	215/263 (82%)	203 (94%)	11 (5%)	1 (0%)	24	54
5	44	211/263 (80%)	206 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	45	215/263 (82%)	207 (96%)	7 (3%)	1 (0%)	24	54
5	46	211/263 (80%)	204 (97%)	7 (3%)	0	100	100
5	47	215/263 (82%)	204 (95%)	10 (5%)	1 (0%)	24	54
5	48	211/263 (80%)	206 (98%)	5 (2%)	0	100	100
5	49	228/263 (87%)	207 (91%)	21 (9%)	0	100	100
5	50	231/263 (88%)	208 (90%)	21 (9%)	2 (1%)	14	41
5	51	228/263 (87%)	203 (89%)	24 (10%)	1 (0%)	30	59
5	52	231/263 (88%)	201 (87%)	29 (13%)	1 (0%)	30	59
5	53	228/263 (87%)	206 (90%)	20 (9%)	2 (1%)	14	41
5	54	231/263 (88%)	209 (90%)	21 (9%)	1 (0%)	30	59
5	55	228/263 (87%)	208 (91%)	19 (8%)	1 (0%)	30	59
5	56	231/263 (88%)	211 (91%)	19 (8%)	1 (0%)	30	59
5	57	228/263 (87%)	205 (90%)	21 (9%)	2 (1%)	14	41
5	58	231/263 (88%)	208 (90%)	21 (9%)	2 (1%)	14	41
5	59	228/263 (87%)	209 (92%)	17 (8%)	2 (1%)	14	41
5	60	231/263 (88%)	210 (91%)	18 (8%)	3 (1%)	9	32
5	61	228/263 (87%)	207 (91%)	19 (8%)	2 (1%)	14	41
5	62	231/263 (88%)	210 (91%)	20 (9%)	1 (0%)	30	59
6	63	611/1010 (60%)	553 (90%)	56 (9%)	2 (0%)	36	64
6	64	611/1010 (60%)	556 (91%)	53 (9%)	2 (0%)	36	64
6	65	611/1010 (60%)	550 (90%)	59 (10%)	2 (0%)	36	64
6	66	611/1010 (60%)	545 (89%)	64 (10%)	2 (0%)	36	64
6	67	611/1010 (60%)	552 (90%)	57 (9%)	2 (0%)	36	64
6	68	611/1010 (60%)	534 (87%)	76 (12%)	1 (0%)	43	70
6	69	611/1010 (60%)	546 (89%)	61 (10%)	4 (1%)	18	47
7	71	168/416 (40%)	155 (92%)	13 (8%)	0	100	100
7	72	168/416 (40%)	152 (90%)	16 (10%)	0	100	100
7	73	168/416 (40%)	158 (94%)	10 (6%)	0	100	100
7	75	168/416 (40%)	152 (90%)	15 (9%)	1 (1%)	21	50
7	76	168/416 (40%)	150 (89%)	17 (10%)	1 (1%)	21	50
7	77	168/416 (40%)	153 (91%)	15 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	78	168/416 (40%)	154 (92%)	14 (8%)	0	100	100
7	79	168/416 (40%)	153 (91%)	14 (8%)	1 (1%)	21	50
7	80	168/416 (40%)	149 (89%)	19 (11%)	0	100	100
7	82	168/416 (40%)	152 (90%)	16 (10%)	0	100	100
7	83	168/416 (40%)	152 (90%)	16 (10%)	0	100	100
7	84	168/416 (40%)	153 (91%)	15 (9%)	0	100	100
7	85	168/416 (40%)	150 (89%)	18 (11%)	0	100	100
7	86	168/416 (40%)	151 (90%)	16 (10%)	1 (1%)	21	50
7	87	168/416 (40%)	150 (89%)	17 (10%)	1 (1%)	21	50
7	89	168/416 (40%)	153 (91%)	14 (8%)	1 (1%)	21	50
7	90	168/416 (40%)	154 (92%)	13 (8%)	1 (1%)	21	50
7	91	168/416 (40%)	151 (90%)	16 (10%)	1 (1%)	21	50
7	92	168/416 (40%)	146 (87%)	22 (13%)	0	100	100
7	93	168/416 (40%)	149 (89%)	19 (11%)	0	100	100
7	94	168/416 (40%)	147 (88%)	21 (12%)	0	100	100
7	95	168/416 (40%)	147 (88%)	21 (12%)	0	100	100
7	96	168/416 (40%)	151 (90%)	17 (10%)	0	100	100
7	97	168/416 (40%)	148 (88%)	20 (12%)	0	100	100
8	A1	319/502 (64%)	300 (94%)	18 (6%)	1 (0%)	36	64
8	A2	319/502 (64%)	299 (94%)	16 (5%)	4 (1%)	9	32
8	A3	228/502 (45%)	204 (90%)	23 (10%)	1 (0%)	30	59
8	A4	138/502 (28%)	120 (87%)	18 (13%)	0	100	100
8	A5	319/502 (64%)	293 (92%)	26 (8%)	0	100	100
8	A6	319/502 (64%)	295 (92%)	24 (8%)	0	100	100
8	A7	319/502 (64%)	298 (93%)	20 (6%)	1 (0%)	36	64
8	A8	319/502 (64%)	299 (94%)	19 (6%)	1 (0%)	36	64
8	A9	124/502 (25%)	119 (96%)	5 (4%)	0	100	100
9	B1	251/556 (45%)	227 (90%)	24 (10%)	0	100	100
9	B2	251/556 (45%)	234 (93%)	16 (6%)	1 (0%)	30	59
9	B3	251/556 (45%)	231 (92%)	20 (8%)	0	100	100
9	B4	251/556 (45%)	230 (92%)	21 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	B5	251/556 (45%)	224 (89%)	26 (10%)	1 (0%)	30	59
9	B6	251/556 (45%)	221 (88%)	29 (12%)	1 (0%)	30	59
9	B7	251/556 (45%)	222 (88%)	29 (12%)	0	100	100
10	C0	180/582 (31%)	170 (94%)	10 (6%)	0	100	100
10	C6	180/582 (31%)	171 (95%)	9 (5%)	0	100	100
10	C7	180/582 (31%)	171 (95%)	9 (5%)	0	100	100
10	C8	180/582 (31%)	165 (92%)	15 (8%)	0	100	100
10	C9	180/582 (31%)	171 (95%)	9 (5%)	0	100	100
10	D0	268/582 (46%)	243 (91%)	25 (9%)	0	100	100
10	D1	180/582 (31%)	168 (93%)	12 (7%)	0	100	100
10	D2	180/582 (31%)	174 (97%)	5 (3%)	1 (1%)	21	50
10	D3	268/582 (46%)	240 (90%)	28 (10%)	0	100	100
10	D4	268/582 (46%)	244 (91%)	24 (9%)	0	100	100
10	D5	268/582 (46%)	244 (91%)	24 (9%)	0	100	100
10	D6	268/582 (46%)	243 (91%)	25 (9%)	0	100	100
10	D7	268/582 (46%)	246 (92%)	22 (8%)	0	100	100
10	D8	268/582 (46%)	246 (92%)	22 (8%)	0	100	100
10	D9	268/582 (46%)	245 (91%)	23 (9%)	0	100	100
10	E0	268/582 (46%)	248 (92%)	20 (8%)	0	100	100
10	E1	268/582 (46%)	244 (91%)	24 (9%)	0	100	100
10	E2	268/582 (46%)	242 (90%)	26 (10%)	0	100	100
10	E3	268/582 (46%)	244 (91%)	24 (9%)	0	100	100
10	E4	268/582 (46%)	243 (91%)	25 (9%)	0	100	100
10	E5	268/582 (46%)	243 (91%)	25 (9%)	0	100	100
10	E6	268/582 (46%)	241 (90%)	27 (10%)	0	100	100
10	E7	268/582 (46%)	250 (93%)	18 (7%)	0	100	100
10	E8	268/582 (46%)	244 (91%)	24 (9%)	0	100	100
10	E9	268/582 (46%)	250 (93%)	18 (7%)	0	100	100
10	F1	268/582 (46%)	244 (91%)	24 (9%)	0	100	100
10	F2	268/582 (46%)	248 (92%)	20 (8%)	0	100	100
10	F3	268/582 (46%)	246 (92%)	22 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	C1	28/351 (8%)	26 (93%)	2 (7%)	0	100	100
11	C2	28/351 (8%)	26 (93%)	2 (7%)	0	100	100
11	C3	28/351 (8%)	27 (96%)	1 (4%)	0	100	100
11	C4	25/351 (7%)	24 (96%)	1 (4%)	0	100	100
11	C5	28/351 (8%)	25 (89%)	3 (11%)	0	100	100
12	F0	105/783 (13%)	90 (86%)	13 (12%)	2 (2%)	6	24
12	F5	100/783 (13%)	90 (90%)	8 (8%)	2 (2%)	6	23
12	F6	105/783 (13%)	89 (85%)	15 (14%)	1 (1%)	12	38
12	F7	100/783 (13%)	91 (91%)	6 (6%)	3 (3%)	3	16
12	F8	105/783 (13%)	89 (85%)	14 (13%)	2 (2%)	6	24
12	F9	100/783 (13%)	90 (90%)	8 (8%)	2 (2%)	6	23
12	G0	48/783 (6%)	48 (100%)	0	0	100	100
12	G1	100/783 (13%)	90 (90%)	7 (7%)	3 (3%)	3	16
12	G2	105/783 (13%)	89 (85%)	14 (13%)	2 (2%)	6	24
12	G3	100/783 (13%)	89 (89%)	8 (8%)	3 (3%)	3	16
12	G4	105/783 (13%)	90 (86%)	13 (12%)	2 (2%)	6	24
12	G5	100/783 (13%)	89 (89%)	9 (9%)	2 (2%)	6	23
12	G6	105/783 (13%)	91 (87%)	13 (12%)	1 (1%)	12	38
12	G7	100/783 (13%)	92 (92%)	6 (6%)	2 (2%)	6	23
12	G8	105/783 (13%)	91 (87%)	12 (11%)	2 (2%)	6	24
12	G9	42/783 (5%)	42 (100%)	0	0	100	100
12	H0	22/783 (3%)	21 (96%)	1 (4%)	0	100	100
12	H1	22/783 (3%)	21 (96%)	1 (4%)	0	100	100
12	H2	42/783 (5%)	42 (100%)	0	0	100	100
12	H3	48/783 (6%)	48 (100%)	0	0	100	100
12	H4	22/783 (3%)	19 (86%)	3 (14%)	0	100	100
12	H5	42/783 (5%)	42 (100%)	0	0	100	100
12	H6	48/783 (6%)	48 (100%)	0	0	100	100
12	H7	22/783 (3%)	22 (100%)	0	0	100	100
12	H8	42/783 (5%)	42 (100%)	0	0	100	100
12	H9	48/783 (6%)	48 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	I1	42/783 (5%)	42 (100%)	0	0	100	100
12	I2	48/783 (6%)	48 (100%)	0	0	100	100
12	I3	22/783 (3%)	20 (91%)	2 (9%)	0	100	100
12	I4	42/783 (5%)	42 (100%)	0	0	100	100
12	I5	48/783 (6%)	47 (98%)	1 (2%)	0	100	100
12	I6	22/783 (3%)	20 (91%)	2 (9%)	0	100	100
12	I7	42/783 (5%)	42 (100%)	0	0	100	100
12	I8	48/783 (6%)	48 (100%)	0	0	100	100
12	I9	22/783 (3%)	21 (96%)	1 (4%)	0	100	100
13	J1	302/871 (35%)	288 (95%)	13 (4%)	1 (0%)	36	64
13	J2	302/871 (35%)	288 (95%)	13 (4%)	1 (0%)	36	64
13	J3	302/871 (35%)	289 (96%)	13 (4%)	0	100	100
13	J4	302/871 (35%)	294 (97%)	7 (2%)	1 (0%)	36	64
13	J5	302/871 (35%)	290 (96%)	11 (4%)	1 (0%)	36	64
13	J6	302/871 (35%)	291 (96%)	11 (4%)	0	100	100
13	J7	302/871 (35%)	290 (96%)	12 (4%)	0	100	100
14	K0	187/256 (73%)	177 (95%)	10 (5%)	0	100	100
14	K1	187/256 (73%)	175 (94%)	12 (6%)	0	100	100
14	K2	187/256 (73%)	172 (92%)	14 (8%)	1 (0%)	24	54
14	K3	187/256 (73%)	176 (94%)	11 (6%)	0	100	100
14	K4	187/256 (73%)	174 (93%)	12 (6%)	1 (0%)	24	54
14	K5	187/256 (73%)	175 (94%)	11 (6%)	1 (0%)	24	54
14	K6	187/256 (73%)	175 (94%)	12 (6%)	0	100	100
14	K7	187/256 (73%)	175 (94%)	12 (6%)	0	100	100
14	K8	187/256 (73%)	175 (94%)	12 (6%)	0	100	100
14	K9	187/256 (73%)	177 (95%)	10 (5%)	0	100	100
14	L0	187/256 (73%)	178 (95%)	9 (5%)	0	100	100
14	L1	187/256 (73%)	174 (93%)	13 (7%)	0	100	100
14	L2	187/256 (73%)	174 (93%)	13 (7%)	0	100	100
14	L3	187/256 (73%)	172 (92%)	15 (8%)	0	100	100
14	L4	130/256 (51%)	122 (94%)	8 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	L5	187/256 (73%)	179 (96%)	8 (4%)	0	100	100
14	L6	187/256 (73%)	179 (96%)	8 (4%)	0	100	100
14	L7	187/256 (73%)	176 (94%)	11 (6%)	0	100	100
14	L8	187/256 (73%)	173 (92%)	14 (8%)	0	100	100
14	L9	187/256 (73%)	178 (95%)	9 (5%)	0	100	100
14	M1	123/256 (48%)	114 (93%)	8 (6%)	1 (1%)	16	44
14	M2	187/256 (73%)	174 (93%)	13 (7%)	0	100	100
14	M3	187/256 (73%)	172 (92%)	15 (8%)	0	100	100
14	M4	187/256 (73%)	172 (92%)	15 (8%)	0	100	100
14	M5	187/256 (73%)	169 (90%)	18 (10%)	0	100	100
14	M6	187/256 (73%)	172 (92%)	14 (8%)	1 (0%)	24	54
14	M7	187/256 (73%)	171 (91%)	15 (8%)	1 (0%)	24	54
All	All	99858/206100 (48%)	92192 (92%)	7369 (7%)	297 (0%)	37	64

5 of 297 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	10	200	GLN
2	11	189	GLU
4	1L	278	SER
4	1L	280	GLN
5	39	21	LEU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	93/790 (12%)	93 (100%)	0	100	100
1	2	93/790 (12%)	93 (100%)	0	100	100
1	A	259/790 (33%)	259 (100%)	0	100	100
1	B	208/790 (26%)	208 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	129/790 (16%)	129 (100%)	0	100	100
1	D	109/790 (14%)	109 (100%)	0	100	100
1	E	229/790 (29%)	229 (100%)	0	100	100
1	F	264/790 (33%)	264 (100%)	0	100	100
1	G	146/790 (18%)	146 (100%)	0	100	100
1	H	105/790 (13%)	105 (100%)	0	100	100
1	I	317/790 (40%)	271 (86%)	46 (14%)	3	13
1	J	313/790 (40%)	262 (84%)	51 (16%)	2	10
1	K	171/790 (22%)	171 (100%)	0	100	100
1	L	176/790 (22%)	174 (99%)	2 (1%)	65	75
1	M	189/790 (24%)	153 (81%)	36 (19%)	1	7
1	N	183/790 (23%)	141 (77%)	42 (23%)	1	4
1	O	49/790 (6%)	26 (53%)	23 (47%)	0	0
1	P	48/790 (6%)	33 (69%)	15 (31%)	0	0
1	Q	304/790 (38%)	304 (100%)	0	100	100
1	R	222/790 (28%)	222 (100%)	0	100	100
1	S	154/790 (20%)	154 (100%)	0	100	100
1	T	71/790 (9%)	71 (100%)	0	100	100
1	U	327/790 (41%)	327 (100%)	0	100	100
1	V	224/790 (28%)	223 (100%)	1 (0%)	84	84
1	W	173/790 (22%)	173 (100%)	0	100	100
1	X	81/790 (10%)	81 (100%)	0	100	100
1	Y	311/790 (39%)	282 (91%)	29 (9%)	8	28
1	Z	209/790 (26%)	209 (100%)	0	100	100
1	a	164/790 (21%)	126 (77%)	38 (23%)	1	3
1	b	76/790 (10%)	76 (100%)	0	100	100
1	c	316/790 (40%)	265 (84%)	51 (16%)	2	10
1	d	214/790 (27%)	214 (100%)	0	100	100
1	e	76/790 (10%)	76 (100%)	0	100	100
1	f	169/790 (21%)	110 (65%)	59 (35%)	0	0
1	g	84/790 (11%)	84 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	h	84/790 (11%)	83 (99%)	1 (1%)	63	74
1	i	84/790 (11%)	84 (100%)	0	100	100
1	j	84/790 (11%)	84 (100%)	0	100	100
1	k	84/790 (11%)	84 (100%)	0	100	100
1	l	84/790 (11%)	84 (100%)	0	100	100
1	m	84/790 (11%)	84 (100%)	0	100	100
1	n	76/790 (10%)	76 (100%)	0	100	100
1	o	76/790 (10%)	76 (100%)	0	100	100
1	p	76/790 (10%)	76 (100%)	0	100	100
1	q	76/790 (10%)	76 (100%)	0	100	100
1	r	76/790 (10%)	76 (100%)	0	100	100
1	s	76/790 (10%)	76 (100%)	0	100	100
1	t	76/790 (10%)	76 (100%)	0	100	100
1	u	93/790 (12%)	93 (100%)	0	100	100
1	v	93/790 (12%)	93 (100%)	0	100	100
1	w	93/790 (12%)	93 (100%)	0	100	100
1	x	93/790 (12%)	93 (100%)	0	100	100
1	y	93/790 (12%)	93 (100%)	0	100	100
1	z	93/790 (12%)	93 (100%)	0	100	100
2	10	155/355 (44%)	155 (100%)	0	100	100
2	11	157/355 (44%)	157 (100%)	0	100	100
2	12	155/355 (44%)	155 (100%)	0	100	100
2	13	157/355 (44%)	157 (100%)	0	100	100
2	14	155/355 (44%)	155 (100%)	0	100	100
2	15	80/355 (22%)	80 (100%)	0	100	100
2	16	87/355 (24%)	87 (100%)	0	100	100
2	3	157/355 (44%)	157 (100%)	0	100	100
2	4	155/355 (44%)	155 (100%)	0	100	100
2	5	157/355 (44%)	157 (100%)	0	100	100
2	6	155/355 (44%)	154 (99%)	1 (1%)	78	80
2	7	157/355 (44%)	157 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	8	155/355 (44%)	155 (100%)	0	100	100
2	9	157/355 (44%)	157 (100%)	0	100	100
3	1A	359/379 (95%)	359 (100%)	0	100	100
3	1C	359/379 (95%)	359 (100%)	0	100	100
3	1E	359/379 (95%)	359 (100%)	0	100	100
3	1G	359/379 (95%)	359 (100%)	0	100	100
3	1I	359/379 (95%)	359 (100%)	0	100	100
3	1K	359/379 (95%)	359 (100%)	0	100	100
3	1M	359/379 (95%)	359 (100%)	0	100	100
3	2A	359/379 (95%)	359 (100%)	0	100	100
3	2C	359/379 (95%)	359 (100%)	0	100	100
3	2E	359/379 (95%)	358 (100%)	1 (0%)	86	85
3	2G	359/379 (95%)	359 (100%)	0	100	100
3	2I	359/379 (95%)	359 (100%)	0	100	100
3	2K	359/379 (95%)	359 (100%)	0	100	100
3	2M	359/379 (95%)	359 (100%)	0	100	100
3	3A	359/379 (95%)	359 (100%)	0	100	100
3	3C	359/379 (95%)	359 (100%)	0	100	100
3	3E	359/379 (95%)	359 (100%)	0	100	100
3	3G	359/379 (95%)	359 (100%)	0	100	100
3	3I	359/379 (95%)	359 (100%)	0	100	100
3	3K	359/379 (95%)	359 (100%)	0	100	100
3	3M	359/379 (95%)	359 (100%)	0	100	100
3	4A	359/379 (95%)	359 (100%)	0	100	100
3	4C	359/379 (95%)	359 (100%)	0	100	100
3	4E	359/379 (95%)	359 (100%)	0	100	100
3	4G	359/379 (95%)	359 (100%)	0	100	100
3	4I	359/379 (95%)	359 (100%)	0	100	100
3	4K	359/379 (95%)	359 (100%)	0	100	100
3	4M	359/379 (95%)	359 (100%)	0	100	100
3	5A	359/379 (95%)	358 (100%)	1 (0%)	86	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	5C	359/379 (95%)	359 (100%)	0	100	100
3	5E	359/379 (95%)	359 (100%)	0	100	100
3	5G	359/379 (95%)	359 (100%)	0	100	100
3	5I	359/379 (95%)	358 (100%)	1 (0%)	86	85
3	5K	359/379 (95%)	359 (100%)	0	100	100
3	5M	359/379 (95%)	359 (100%)	0	100	100
3	6A	359/379 (95%)	359 (100%)	0	100	100
3	6C	359/379 (95%)	359 (100%)	0	100	100
3	6E	359/379 (95%)	359 (100%)	0	100	100
3	6G	359/379 (95%)	359 (100%)	0	100	100
3	6I	359/379 (95%)	359 (100%)	0	100	100
3	6K	359/379 (95%)	359 (100%)	0	100	100
3	6M	359/379 (95%)	359 (100%)	0	100	100
3	7A	359/379 (95%)	359 (100%)	0	100	100
3	7C	359/379 (95%)	359 (100%)	0	100	100
3	7E	359/379 (95%)	359 (100%)	0	100	100
3	7G	359/379 (95%)	359 (100%)	0	100	100
3	7I	359/379 (95%)	359 (100%)	0	100	100
3	7K	359/379 (95%)	359 (100%)	0	100	100
3	7M	359/379 (95%)	359 (100%)	0	100	100
3	8A	359/379 (95%)	358 (100%)	1 (0%)	86	85
3	8C	359/379 (95%)	359 (100%)	0	100	100
3	8E	359/379 (95%)	359 (100%)	0	100	100
3	8G	359/379 (95%)	359 (100%)	0	100	100
3	8I	359/379 (95%)	359 (100%)	0	100	100
3	8K	359/379 (95%)	359 (100%)	0	100	100
3	8M	359/379 (95%)	359 (100%)	0	100	100
3	9A	359/379 (95%)	359 (100%)	0	100	100
3	9C	359/379 (95%)	359 (100%)	0	100	100
3	9E	359/379 (95%)	359 (100%)	0	100	100
3	9G	359/379 (95%)	359 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	9I	359/379 (95%)	359 (100%)	0	100	100
3	9K	359/379 (95%)	359 (100%)	0	100	100
3	9M	359/379 (95%)	359 (100%)	0	100	100
4	1B	364/381 (96%)	364 (100%)	0	100	100
4	1D	364/381 (96%)	364 (100%)	0	100	100
4	1F	364/381 (96%)	364 (100%)	0	100	100
4	1H	364/381 (96%)	364 (100%)	0	100	100
4	1J	364/381 (96%)	364 (100%)	0	100	100
4	1L	364/381 (96%)	364 (100%)	0	100	100
4	1N	364/381 (96%)	364 (100%)	0	100	100
4	2B	364/381 (96%)	364 (100%)	0	100	100
4	2D	364/381 (96%)	364 (100%)	0	100	100
4	2F	364/381 (96%)	364 (100%)	0	100	100
4	2H	364/381 (96%)	364 (100%)	0	100	100
4	2J	364/381 (96%)	364 (100%)	0	100	100
4	2L	364/381 (96%)	364 (100%)	0	100	100
4	3B	364/381 (96%)	363 (100%)	1 (0%)	86	85
4	3D	364/381 (96%)	364 (100%)	0	100	100
4	3F	364/381 (96%)	363 (100%)	1 (0%)	86	85
4	3H	364/381 (96%)	364 (100%)	0	100	100
4	3J	364/381 (96%)	363 (100%)	1 (0%)	86	85
4	3L	364/381 (96%)	364 (100%)	0	100	100
4	4B	364/381 (96%)	364 (100%)	0	100	100
4	4D	364/381 (96%)	364 (100%)	0	100	100
4	4F	364/381 (96%)	364 (100%)	0	100	100
4	4H	364/381 (96%)	364 (100%)	0	100	100
4	4J	364/381 (96%)	364 (100%)	0	100	100
4	4L	364/381 (96%)	364 (100%)	0	100	100
4	5B	364/381 (96%)	364 (100%)	0	100	100
4	5D	364/381 (96%)	364 (100%)	0	100	100
4	5F	364/381 (96%)	364 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	5H	364/381 (96%)	364 (100%)	0	100	100
4	5J	364/381 (96%)	364 (100%)	0	100	100
4	5L	364/381 (96%)	364 (100%)	0	100	100
4	5N	364/381 (96%)	363 (100%)	1 (0%)	86	85
4	6B	364/381 (96%)	364 (100%)	0	100	100
4	6D	364/381 (96%)	364 (100%)	0	100	100
4	6F	364/381 (96%)	364 (100%)	0	100	100
4	6H	364/381 (96%)	364 (100%)	0	100	100
4	6J	364/381 (96%)	364 (100%)	0	100	100
4	6L	364/381 (96%)	364 (100%)	0	100	100
4	6N	364/381 (96%)	364 (100%)	0	100	100
4	7B	364/381 (96%)	364 (100%)	0	100	100
4	7D	364/381 (96%)	364 (100%)	0	100	100
4	7F	364/381 (96%)	364 (100%)	0	100	100
4	7H	364/381 (96%)	364 (100%)	0	100	100
4	7J	364/381 (96%)	364 (100%)	0	100	100
4	7L	364/381 (96%)	364 (100%)	0	100	100
4	8B	364/381 (96%)	364 (100%)	0	100	100
4	8D	364/381 (96%)	364 (100%)	0	100	100
4	8F	364/381 (96%)	363 (100%)	1 (0%)	86	85
4	8H	364/381 (96%)	364 (100%)	0	100	100
4	8J	364/381 (96%)	362 (100%)	2 (0%)	81	82
4	8L	364/381 (96%)	364 (100%)	0	100	100
4	9B	364/381 (96%)	364 (100%)	0	100	100
4	9D	364/381 (96%)	364 (100%)	0	100	100
4	9F	364/381 (96%)	364 (100%)	0	100	100
4	9H	364/381 (96%)	364 (100%)	0	100	100
4	9J	364/381 (96%)	364 (100%)	0	100	100
4	9L	364/381 (96%)	364 (100%)	0	100	100
5	20	205/227 (90%)	205 (100%)	0	100	100
5	21	205/227 (90%)	205 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	22	205/227 (90%)	205 (100%)	0	100	100
5	23	205/227 (90%)	205 (100%)	0	100	100
5	24	205/227 (90%)	205 (100%)	0	100	100
5	25	205/227 (90%)	205 (100%)	0	100	100
5	26	205/227 (90%)	205 (100%)	0	100	100
5	27	205/227 (90%)	204 (100%)	1 (0%)	81	82
5	28	205/227 (90%)	205 (100%)	0	100	100
5	29	205/227 (90%)	204 (100%)	1 (0%)	81	82
5	30	205/227 (90%)	205 (100%)	0	100	100
5	31	205/227 (90%)	205 (100%)	0	100	100
5	32	205/227 (90%)	205 (100%)	0	100	100
5	33	152/227 (67%)	152 (100%)	0	100	100
5	35	197/227 (87%)	197 (100%)	0	100	100
5	36	193/227 (85%)	193 (100%)	0	100	100
5	37	197/227 (87%)	197 (100%)	0	100	100
5	38	193/227 (85%)	193 (100%)	0	100	100
5	39	197/227 (87%)	197 (100%)	0	100	100
5	40	193/227 (85%)	193 (100%)	0	100	100
5	42	193/227 (85%)	193 (100%)	0	100	100
5	43	197/227 (87%)	197 (100%)	0	100	100
5	44	193/227 (85%)	193 (100%)	0	100	100
5	45	197/227 (87%)	197 (100%)	0	100	100
5	46	193/227 (85%)	193 (100%)	0	100	100
5	47	197/227 (87%)	197 (100%)	0	100	100
5	48	193/227 (85%)	193 (100%)	0	100	100
5	49	206/227 (91%)	206 (100%)	0	100	100
5	50	207/227 (91%)	207 (100%)	0	100	100
5	51	206/227 (91%)	206 (100%)	0	100	100
5	52	207/227 (91%)	207 (100%)	0	100	100
5	53	206/227 (91%)	206 (100%)	0	100	100
5	54	207/227 (91%)	207 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	55	206/227 (91%)	206 (100%)	0	100	100
5	56	207/227 (91%)	207 (100%)	0	100	100
5	57	206/227 (91%)	206 (100%)	0	100	100
5	58	207/227 (91%)	207 (100%)	0	100	100
5	59	206/227 (91%)	206 (100%)	0	100	100
5	60	207/227 (91%)	207 (100%)	0	100	100
5	61	206/227 (91%)	206 (100%)	0	100	100
5	62	207/227 (91%)	206 (100%)	1 (0%)	81	82
6	63	541/863 (63%)	541 (100%)	0	100	100
6	64	541/863 (63%)	531 (98%)	10 (2%)	51	69
6	65	541/863 (63%)	529 (98%)	12 (2%)	45	67
6	66	541/863 (63%)	530 (98%)	11 (2%)	48	68
6	67	541/863 (63%)	528 (98%)	13 (2%)	43	65
6	68	541/863 (63%)	528 (98%)	13 (2%)	43	65
6	69	541/863 (63%)	528 (98%)	13 (2%)	43	65
7	71	151/364 (42%)	151 (100%)	0	100	100
7	72	151/364 (42%)	151 (100%)	0	100	100
7	73	151/364 (42%)	151 (100%)	0	100	100
7	75	151/364 (42%)	151 (100%)	0	100	100
7	76	151/364 (42%)	151 (100%)	0	100	100
7	77	151/364 (42%)	151 (100%)	0	100	100
7	78	151/364 (42%)	151 (100%)	0	100	100
7	79	151/364 (42%)	151 (100%)	0	100	100
7	80	151/364 (42%)	151 (100%)	0	100	100
7	82	151/364 (42%)	151 (100%)	0	100	100
7	83	151/364 (42%)	151 (100%)	0	100	100
7	84	151/364 (42%)	151 (100%)	0	100	100
7	85	151/364 (42%)	151 (100%)	0	100	100
7	86	151/364 (42%)	151 (100%)	0	100	100
7	87	151/364 (42%)	151 (100%)	0	100	100
7	89	151/364 (42%)	151 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	90	151/364 (42%)	151 (100%)	0	100	100
7	91	151/364 (42%)	151 (100%)	0	100	100
7	92	151/364 (42%)	151 (100%)	0	100	100
7	93	151/364 (42%)	151 (100%)	0	100	100
7	94	151/364 (42%)	151 (100%)	0	100	100
7	95	151/364 (42%)	151 (100%)	0	100	100
7	96	151/364 (42%)	151 (100%)	0	100	100
7	97	151/364 (42%)	151 (100%)	0	100	100
8	A1	287/428 (67%)	287 (100%)	0	100	100
8	A2	287/428 (67%)	287 (100%)	0	100	100
8	A3	209/428 (49%)	209 (100%)	0	100	100
8	A4	94/428 (22%)	94 (100%)	0	100	100
8	A5	287/428 (67%)	287 (100%)	0	100	100
8	A6	287/428 (67%)	287 (100%)	0	100	100
8	A7	287/428 (67%)	287 (100%)	0	100	100
8	A8	287/428 (67%)	287 (100%)	0	100	100
8	A9	111/428 (26%)	111 (100%)	0	100	100
9	B1	225/479 (47%)	225 (100%)	0	100	100
9	B2	225/479 (47%)	225 (100%)	0	100	100
9	B3	225/479 (47%)	225 (100%)	0	100	100
9	B4	225/479 (47%)	225 (100%)	0	100	100
9	B5	225/479 (47%)	225 (100%)	0	100	100
9	B6	225/479 (47%)	225 (100%)	0	100	100
9	B7	225/479 (47%)	225 (100%)	0	100	100
10	C0	154/501 (31%)	154 (100%)	0	100	100
10	C6	154/501 (31%)	154 (100%)	0	100	100
10	C7	154/501 (31%)	154 (100%)	0	100	100
10	C8	154/501 (31%)	154 (100%)	0	100	100
10	C9	154/501 (31%)	154 (100%)	0	100	100
10	D0	234/501 (47%)	234 (100%)	0	100	100
10	D1	154/501 (31%)	154 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	D2	154/501 (31%)	154 (100%)	0	100	100
10	D3	234/501 (47%)	234 (100%)	0	100	100
10	D4	234/501 (47%)	234 (100%)	0	100	100
10	D5	234/501 (47%)	234 (100%)	0	100	100
10	D6	234/501 (47%)	234 (100%)	0	100	100
10	D7	234/501 (47%)	234 (100%)	0	100	100
10	D8	234/501 (47%)	234 (100%)	0	100	100
10	D9	234/501 (47%)	234 (100%)	0	100	100
10	E0	234/501 (47%)	234 (100%)	0	100	100
10	E1	234/501 (47%)	234 (100%)	0	100	100
10	E2	234/501 (47%)	234 (100%)	0	100	100
10	E3	234/501 (47%)	234 (100%)	0	100	100
10	E4	234/501 (47%)	234 (100%)	0	100	100
10	E5	234/501 (47%)	234 (100%)	0	100	100
10	E6	234/501 (47%)	234 (100%)	0	100	100
10	E7	234/501 (47%)	234 (100%)	0	100	100
10	E8	234/501 (47%)	234 (100%)	0	100	100
10	E9	234/501 (47%)	234 (100%)	0	100	100
10	F1	234/501 (47%)	234 (100%)	0	100	100
10	F2	234/501 (47%)	234 (100%)	0	100	100
10	F3	234/501 (47%)	234 (100%)	0	100	100
11	C1	28/305 (9%)	28 (100%)	0	100	100
11	C2	27/305 (9%)	27 (100%)	0	100	100
11	C3	28/305 (9%)	28 (100%)	0	100	100
11	C4	26/305 (8%)	26 (100%)	0	100	100
11	C5	27/305 (9%)	27 (100%)	0	100	100
12	F0	95/596 (16%)	95 (100%)	0	100	100
12	F5	92/596 (15%)	92 (100%)	0	100	100
12	F6	95/596 (16%)	95 (100%)	0	100	100
12	F7	92/596 (15%)	92 (100%)	0	100	100
12	F8	95/596 (16%)	95 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	F9	92/596 (15%)	92 (100%)	0	100	100
12	G0	43/596 (7%)	43 (100%)	0	100	100
12	G1	92/596 (15%)	92 (100%)	0	100	100
12	G2	95/596 (16%)	95 (100%)	0	100	100
12	G3	92/596 (15%)	92 (100%)	0	100	100
12	G4	95/596 (16%)	95 (100%)	0	100	100
12	G5	92/596 (15%)	92 (100%)	0	100	100
12	G6	95/596 (16%)	95 (100%)	0	100	100
12	G7	92/596 (15%)	92 (100%)	0	100	100
12	G8	95/596 (16%)	95 (100%)	0	100	100
12	G9	37/596 (6%)	37 (100%)	0	100	100
12	H0	22/596 (4%)	22 (100%)	0	100	100
12	H1	22/596 (4%)	22 (100%)	0	100	100
12	H2	37/596 (6%)	37 (100%)	0	100	100
12	H3	43/596 (7%)	43 (100%)	0	100	100
12	H4	22/596 (4%)	22 (100%)	0	100	100
12	H5	37/596 (6%)	37 (100%)	0	100	100
12	H6	43/596 (7%)	43 (100%)	0	100	100
12	H7	22/596 (4%)	22 (100%)	0	100	100
12	H8	37/596 (6%)	37 (100%)	0	100	100
12	H9	43/596 (7%)	43 (100%)	0	100	100
12	I1	37/596 (6%)	37 (100%)	0	100	100
12	I2	43/596 (7%)	43 (100%)	0	100	100
12	I3	22/596 (4%)	22 (100%)	0	100	100
12	I4	37/596 (6%)	37 (100%)	0	100	100
12	I5	43/596 (7%)	34 (79%)	9 (21%)	1	5
12	I6	22/596 (4%)	22 (100%)	0	100	100
12	I7	37/596 (6%)	37 (100%)	0	100	100
12	I8	43/596 (7%)	43 (100%)	0	100	100
12	I9	22/596 (4%)	22 (100%)	0	100	100
13	J1	262/721 (36%)	262 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	J2	262/721 (36%)	262 (100%)	0	100	100
13	J3	262/721 (36%)	262 (100%)	0	100	100
13	J4	262/721 (36%)	262 (100%)	0	100	100
13	J5	262/721 (36%)	262 (100%)	0	100	100
13	J6	262/721 (36%)	262 (100%)	0	100	100
13	J7	262/721 (36%)	262 (100%)	0	100	100
14	K0	166/223 (74%)	166 (100%)	0	100	100
14	K1	166/223 (74%)	166 (100%)	0	100	100
14	K2	166/223 (74%)	166 (100%)	0	100	100
14	K3	166/223 (74%)	166 (100%)	0	100	100
14	K4	166/223 (74%)	166 (100%)	0	100	100
14	K5	166/223 (74%)	165 (99%)	1 (1%)	78	80
14	K6	166/223 (74%)	166 (100%)	0	100	100
14	K7	166/223 (74%)	166 (100%)	0	100	100
14	K8	166/223 (74%)	166 (100%)	0	100	100
14	K9	166/223 (74%)	166 (100%)	0	100	100
14	L0	166/223 (74%)	166 (100%)	0	100	100
14	L1	166/223 (74%)	166 (100%)	0	100	100
14	L2	166/223 (74%)	166 (100%)	0	100	100
14	L3	166/223 (74%)	165 (99%)	1 (1%)	78	80
14	L4	119/223 (53%)	119 (100%)	0	100	100
14	L5	166/223 (74%)	166 (100%)	0	100	100
14	L6	166/223 (74%)	166 (100%)	0	100	100
14	L7	166/223 (74%)	166 (100%)	0	100	100
14	L8	166/223 (74%)	166 (100%)	0	100	100
14	L9	166/223 (74%)	166 (100%)	0	100	100
14	M1	112/223 (50%)	112 (100%)	0	100	100
14	M2	166/223 (74%)	166 (100%)	0	100	100
14	M3	166/223 (74%)	166 (100%)	0	100	100
14	M4	166/223 (74%)	166 (100%)	0	100	100
14	M5	166/223 (74%)	166 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	M6	166/223 (74%)	160 (96%)	6 (4%)	31	58
14	M7	166/223 (74%)	166 (100%)	0	100	100
All	All	86983/171994 (51%)	86485 (99%)	498 (1%)	76	80

5 of 498 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Y	624	GLN
1	f	533	ARG
6	66	503	LYS
1	f	512	LYS
1	f	613	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 1216 such sidechains are listed below:

Mol	Chain	Res	Type
3	8K	85	HIS
14	K6	252	GLN
7	95	248	HIS
3	8K	50	ASN
8	A2	278	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 174 ligands modelled in this entry, 54 are monoatomic - leaving 120 for Mogul analysis.

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$
15	GTP	7G	501	16	33,34,34	0.96	1 (3%)	50,54,54	1.55	8 (16%)
17	GDP	9J	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.79	7 (15%)
15	GTP	6C	501	16	33,34,34	0.90	1 (3%)	50,54,54	1.58	9 (18%)
17	GDP	8J	501	-	29,30,30	1.19	3 (10%)	45,47,47	1.81	7 (15%)
15	GTP	9E	501	16	33,34,34	1.04	4 (12%)	50,54,54	1.56	9 (18%)
17	GDP	7D	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.80	7 (15%)
15	GTP	4I	501	16	33,34,34	0.95	0	50,54,54	1.50	9 (18%)
15	GTP	9K	501	16	33,34,34	1.01	3 (9%)	50,54,54	1.65	11 (22%)
15	GTP	3C	501	16	33,34,34	0.91	1 (3%)	50,54,54	1.60	8 (16%)
15	GTP	1C	501	16	33,34,34	0.95	1 (3%)	50,54,54	1.61	8 (16%)
15	GTP	9M	501	-	33,34,34	0.94	1 (3%)	50,54,54	1.58	9 (18%)
17	GDP	6N	502	-	29,30,30	1.15	3 (10%)	45,47,47	1.78	7 (15%)
15	GTP	9C	501	-	33,34,34	0.92	1 (3%)	50,54,54	1.56	9 (18%)
17	GDP	2H	501	-	29,30,30	1.18	3 (10%)	45,47,47	1.79	9 (20%)
17	GDP	4F	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.80	7 (15%)
17	GDP	1H	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.74	6 (13%)
15	GTP	5C	501	16	33,34,34	0.91	1 (3%)	50,54,54	1.60	9 (18%)
17	GDP	4H	501	-	29,30,30	1.18	3 (10%)	45,47,47	1.83	9 (20%)
17	GDP	1J	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.84	7 (15%)
17	GDP	3F	501	-	29,30,30	1.19	3 (10%)	45,47,47	1.81	6 (13%)
15	GTP	7M	501	-	33,34,34	0.97	1 (3%)	50,54,54	1.60	8 (16%)
17	GDP	7H	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.81	7 (15%)
17	GDP	2D	501	-	29,30,30	1.19	3 (10%)	45,47,47	1.83	7 (15%)
15	GTP	6E	501	16	33,34,34	0.91	1 (3%)	50,54,54	1.58	9 (18%)
15	GTP	6K	501	16	33,34,34	0.86	1 (3%)	50,54,54	1.59	10 (20%)
15	GTP	3M	501	-	33,34,34	0.96	2 (6%)	50,54,54	1.57	8 (16%)
17	GDP	3D	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.83	7 (15%)
15	GTP	2M	501	-	33,34,34	0.93	1 (3%)	50,54,54	1.61	9 (18%)
15	GTP	1A	501	16	33,34,34	1.14	4 (12%)	50,54,54	1.58	10 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	GTP	4K	501	16	33,34,34	0.91	1 (3%)	50,54,54	1.62	9 (18%)
15	GTP	6I	501	16	33,34,34	0.94	1 (3%)	50,54,54	1.55	8 (16%)
15	GTP	6N	501	-	33,34,34	1.06	2 (6%)	50,54,54	1.63	10 (20%)
17	GDP	3B	501	-	29,30,30	1.18	3 (10%)	45,47,47	1.81	7 (15%)
17	GDP	5D	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.84	7 (15%)
15	GTP	5M	501	-	33,34,34	0.91	0	50,54,54	1.56	8 (16%)
15	GTP	3I	501	16	33,34,34	0.91	1 (3%)	50,54,54	1.56	8 (16%)
17	GDP	4D	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.82	7 (15%)
17	GDP	7J	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.88	8 (17%)
15	GTP	4G	501	16	33,34,34	0.89	1 (3%)	50,54,54	1.55	8 (16%)
17	GDP	9H	501	-	29,30,30	1.19	4 (13%)	45,47,47	1.85	8 (17%)
15	GTP	3A	501	16	33,34,34	0.92	1 (3%)	50,54,54	1.62	8 (16%)
15	GTP	2G	501	16	33,34,34	0.92	1 (3%)	50,54,54	1.59	8 (16%)
15	GTP	4E	501	16	33,34,34	0.96	1 (3%)	50,54,54	1.55	10 (20%)
17	GDP	6L	501	-	29,30,30	1.19	3 (10%)	45,47,47	1.78	7 (15%)
15	GTP	7C	501	16	33,34,34	0.88	1 (3%)	50,54,54	1.63	9 (18%)
17	GDP	2B	501	-	29,30,30	1.15	2 (6%)	45,47,47	1.78	7 (15%)
15	GTP	9G	501	-	33,34,34	0.99	2 (6%)	50,54,54	1.59	8 (16%)
17	GDP	5B	501	-	29,30,30	1.20	3 (10%)	45,47,47	1.79	7 (15%)
17	GDP	4J	501	-	29,30,30	1.18	3 (10%)	45,47,47	1.88	7 (15%)
17	GDP	9D	501	-	29,30,30	1.20	4 (13%)	45,47,47	1.84	8 (17%)
17	GDP	8F	501	-	29,30,30	1.18	4 (13%)	45,47,47	1.76	8 (17%)
17	GDP	4B	501	-	29,30,30	1.20	3 (10%)	45,47,47	1.88	9 (20%)
17	GDP	6J	501	-	29,30,30	1.18	3 (10%)	45,47,47	1.83	6 (13%)
17	GDP	6F	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.92	8 (17%)
15	GTP	3E	501	16	33,34,34	0.96	1 (3%)	50,54,54	1.59	9 (18%)
17	GDP	8D	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.82	7 (15%)
15	GTP	1M	501	-	33,34,34	0.93	1 (3%)	50,54,54	1.59	8 (16%)
15	GTP	8G	501	-	33,34,34	0.90	1 (3%)	50,54,54	1.57	10 (20%)
15	GTP	7K	501	16	33,34,34	0.99	2 (6%)	50,54,54	1.59	9 (18%)
15	GTP	2C	501	16	33,34,34	0.89	1 (3%)	50,54,54	1.62	9 (18%)
15	GTP	9A	501	16	33,34,34	0.97	2 (6%)	50,54,54	1.57	9 (18%)
15	GTP	8K	501	-	33,34,34	0.95	2 (6%)	50,54,54	1.62	9 (18%)
15	GTP	5A	501	16	33,34,34	0.95	1 (3%)	50,54,54	1.59	8 (16%)
15	GTP	3G	501	16	33,34,34	0.94	1 (3%)	50,54,54	1.55	8 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	GTP	8C	501	-	33,34,34	0.86	0	50,54,54	1.57	8 (16%)
15	GTP	5K	501	16	33,34,34	0.94	1 (3%)	50,54,54	1.55	9 (18%)
15	GTP	2I	501	16	33,34,34	0.90	1 (3%)	50,54,54	1.60	9 (18%)
15	GTP	8A	501	16	33,34,34	0.93	1 (3%)	50,54,54	1.51	8 (16%)
15	GTP	1G	501	16	33,34,34	0.87	1 (3%)	50,54,54	1.62	10 (20%)
17	GDP	5J	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	6 (13%)
15	GTP	1K	501	16	33,34,34	0.93	1 (3%)	50,54,54	1.62	9 (18%)
15	GTP	5I	501	16	33,34,34	0.90	1 (3%)	50,54,54	1.59	8 (16%)
17	GDP	3L	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.81	7 (15%)
15	GTP	7A	501	16	33,34,34	0.94	2 (6%)	50,54,54	1.55	8 (16%)
17	GDP	9F	501	-	29,30,30	1.18	3 (10%)	45,47,47	1.83	8 (17%)
17	GDP	7L	501	-	29,30,30	1.18	3 (10%)	45,47,47	1.80	7 (15%)
15	GTP	2A	501	16	33,34,34	1.03	3 (9%)	50,54,54	1.74	10 (20%)
17	GDP	5N	501	-	29,30,30	1.19	3 (10%)	45,47,47	1.85	8 (17%)
15	GTP	4A	501	16	33,34,34	0.98	1 (3%)	50,54,54	1.63	10 (20%)
17	GDP	2F	501	-	29,30,30	1.19	3 (10%)	45,47,47	1.77	6 (13%)
15	GTP	6A	501	16	33,34,34	0.88	1 (3%)	50,54,54	1.56	9 (18%)
15	GTP	4C	501	16	33,34,34	0.87	1 (3%)	50,54,54	1.59	9 (18%)
15	GTP	5G	501	16	33,34,34	0.89	1 (3%)	50,54,54	1.58	9 (18%)
15	GTP	8M	501	-	33,34,34	1.00	2 (6%)	50,54,54	1.59	8 (16%)
17	GDP	9L	501	-	29,30,30	1.19	3 (10%)	45,47,47	1.74	8 (17%)
15	GTP	2E	501	16	33,34,34	0.97	3 (9%)	50,54,54	1.60	8 (16%)
15	GTP	8E	501	16	33,34,34	1.00	1 (3%)	50,54,54	1.59	8 (16%)
17	GDP	8L	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.83	8 (17%)
17	GDP	9B	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.85	7 (15%)
15	GTP	1E	501	16	33,34,34	0.88	1 (3%)	50,54,54	1.60	9 (18%)
17	GDP	1L	501	-	29,30,30	1.19	3 (10%)	45,47,47	1.80	6 (13%)
17	GDP	1D	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.80	7 (15%)
15	GTP	7E	501	16	33,34,34	0.96	1 (3%)	50,54,54	1.55	8 (16%)
15	GTP	6G	501	16	33,34,34	0.91	1 (3%)	50,54,54	1.61	9 (18%)
15	GTP	5E	501	16	33,34,34	0.92	1 (3%)	50,54,54	1.58	9 (18%)
17	GDP	6H	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.83	7 (15%)
17	GDP	8H	501	-	29,30,30	1.18	3 (10%)	45,47,47	1.77	7 (15%)
17	GDP	5H	501	-	29,30,30	1.18	3 (10%)	45,47,47	1.79	9 (20%)
17	GDP	8B	501	-	29,30,30	1.18	4 (13%)	45,47,47	1.80	9 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	GDP	6D	501	-	29,30,30	1.18	3 (10%)	45,47,47	1.82	7 (15%)
15	GTP	2K	501	16	33,34,34	0.92	1 (3%)	50,54,54	1.59	9 (18%)
15	GTP	9I	501	16	33,34,34	1.00	3 (9%)	50,54,54	1.63	8 (16%)
17	GDP	2J	501	-	29,30,30	1.20	3 (10%)	45,47,47	1.88	7 (15%)
17	GDP	1N	501	-	29,30,30	1.19	4 (13%)	45,47,47	1.85	9 (20%)
17	GDP	7F	501	-	29,30,30	1.18	3 (10%)	45,47,47	1.84	9 (20%)
17	GDP	5L	501	-	29,30,30	1.18	3 (10%)	45,47,47	1.77	6 (13%)
15	GTP	7I	501	16	33,34,34	0.93	1 (3%)	50,54,54	1.58	9 (18%)
15	GTP	8I	501	16	33,34,34	0.90	1 (3%)	50,54,54	1.61	8 (16%)
17	GDP	1B	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.74	6 (13%)
17	GDP	7B	502	-	29,30,30	1.17	3 (10%)	45,47,47	1.96	10 (22%)
17	GDP	6B	501	-	29,30,30	1.21	3 (10%)	45,47,47	1.85	10 (22%)
17	GDP	4L	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.79	7 (15%)
15	GTP	4M	501	-	33,34,34	0.92	1 (3%)	50,54,54	1.51	8 (16%)
15	GTP	1I	501	16	33,34,34	0.93	1 (3%)	50,54,54	1.56	8 (16%)
17	GDP	5F	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.83	7 (15%)
15	GTP	3K	501	16	33,34,34	0.90	1 (3%)	50,54,54	1.59	8 (16%)
17	GDP	2L	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	7 (15%)
17	GDP	3H	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.81	7 (15%)
17	GDP	3J	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.77	7 (15%)
17	GDP	1F	501	-	29,30,30	1.19	3 (10%)	45,47,47	1.74	6 (13%)

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
15	GTP	7G	501	16	-	4/22/38/38	0/3/3/3
17	GDP	9J	501	-	-	3/16/32/32	0/3/3/3
15	GTP	6C	501	16	-	6/22/38/38	0/3/3/3
17	GDP	8J	501	-	-	3/16/32/32	0/3/3/3
15	GTP	9E	501	16	-	7/22/38/38	0/3/3/3
17	GDP	7D	501	-	-	3/16/32/32	0/3/3/3
15	GTP	4I	501	16	-	8/22/38/38	0/3/3/3
15	GTP	9K	501	16	-	7/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	GTP	3C	501	16	-	6/22/38/38	0/3/3/3
15	GTP	1C	501	16	-	4/22/38/38	0/3/3/3
15	GTP	9M	501	-	-	8/22/38/38	0/3/3/3
17	GDP	6N	502	-	-	5/16/32/32	0/3/3/3
15	GTP	9C	501	-	-	7/22/38/38	0/3/3/3
17	GDP	2H	501	-	-	9/16/32/32	0/3/3/3
17	GDP	4F	501	-	-	4/16/32/32	0/3/3/3
17	GDP	1H	501	-	-	6/16/32/32	0/3/3/3
15	GTP	5C	501	16	-	5/22/38/38	0/3/3/3
17	GDP	4H	501	-	-	4/16/32/32	0/3/3/3
17	GDP	1J	501	-	-	7/16/32/32	0/3/3/3
17	GDP	3F	501	-	-	5/16/32/32	0/3/3/3
15	GTP	7M	501	-	-	8/22/38/38	0/3/3/3
17	GDP	7H	501	-	-	3/16/32/32	0/3/3/3
17	GDP	2D	501	-	-	4/16/32/32	0/3/3/3
15	GTP	6E	501	16	-	7/22/38/38	0/3/3/3
15	GTP	6K	501	16	-	7/22/38/38	0/3/3/3
15	GTP	3M	501	-	-	6/22/38/38	0/3/3/3
17	GDP	3D	501	-	-	3/16/32/32	0/3/3/3
15	GTP	2M	501	-	-	8/22/38/38	0/3/3/3
15	GTP	1A	501	16	-	6/22/38/38	0/3/3/3
15	GTP	4K	501	16	-	8/22/38/38	0/3/3/3
15	GTP	6I	501	16	-	7/22/38/38	0/3/3/3
15	GTP	6N	501	-	-	5/22/38/38	0/3/3/3
17	GDP	3B	501	-	-	3/16/32/32	0/3/3/3
17	GDP	5D	501	-	-	3/16/32/32	0/3/3/3
15	GTP	5M	501	-	-	9/22/38/38	0/3/3/3
15	GTP	3I	501	16	-	6/22/38/38	0/3/3/3
17	GDP	4D	501	-	-	4/16/32/32	0/3/3/3
17	GDP	7J	501	-	-	6/16/32/32	0/3/3/3
15	GTP	4G	501	16	-	7/22/38/38	0/3/3/3
17	GDP	9H	501	-	-	7/16/32/32	0/3/3/3
15	GTP	3A	501	16	-	7/22/38/38	0/3/3/3
15	GTP	2G	501	16	-	8/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	GTP	4E	501	16	-	8/22/38/38	0/3/3/3
17	GDP	6L	501	-	-	2/16/32/32	0/3/3/3
15	GTP	7C	501	16	-	6/22/38/38	0/3/3/3
17	GDP	2B	501	-	-	6/16/32/32	0/3/3/3
15	GTP	9G	501	-	-	9/22/38/38	0/3/3/3
17	GDP	5B	501	-	-	4/16/32/32	0/3/3/3
17	GDP	4J	501	-	-	5/16/32/32	0/3/3/3
17	GDP	9D	501	-	-	2/16/32/32	0/3/3/3
17	GDP	8F	501	-	-	5/16/32/32	0/3/3/3
17	GDP	4B	501	-	-	4/16/32/32	0/3/3/3
17	GDP	6J	501	-	-	4/16/32/32	0/3/3/3
17	GDP	6F	501	-	-	7/16/32/32	0/3/3/3
15	GTP	3E	501	16	-	10/22/38/38	0/3/3/3
17	GDP	8D	501	-	-	3/16/32/32	0/3/3/3
15	GTP	1M	501	-	-	7/22/38/38	0/3/3/3
15	GTP	8G	501	-	-	9/22/38/38	0/3/3/3
15	GTP	7K	501	16	-	7/22/38/38	0/3/3/3
15	GTP	2C	501	16	-	6/22/38/38	0/3/3/3
15	GTP	9A	501	16	-	6/22/38/38	0/3/3/3
15	GTP	8K	501	-	-	6/22/38/38	0/3/3/3
15	GTP	5A	501	16	-	7/22/38/38	0/3/3/3
15	GTP	3G	501	16	-	4/22/38/38	0/3/3/3
15	GTP	8C	501	-	-	6/22/38/38	0/3/3/3
15	GTP	5K	501	16	-	5/22/38/38	0/3/3/3
15	GTP	2I	501	16	-	7/22/38/38	0/3/3/3
15	GTP	8A	501	16	-	5/22/38/38	0/3/3/3
15	GTP	1G	501	16	-	4/22/38/38	0/3/3/3
17	GDP	5J	501	-	-	4/16/32/32	0/3/3/3
15	GTP	1K	501	16	-	9/22/38/38	0/3/3/3
15	GTP	5I	501	16	-	8/22/38/38	0/3/3/3
17	GDP	3L	501	-	-	6/16/32/32	0/3/3/3
15	GTP	7A	501	16	-	6/22/38/38	0/3/3/3
17	GDP	9F	501	-	-	2/16/32/32	0/3/3/3
17	GDP	7L	501	-	-	3/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	GTP	2A	501	16	-	6/22/38/38	0/3/3/3
17	GDP	5N	501	-	-	4/16/32/32	0/3/3/3
15	GTP	4A	501	16	-	4/22/38/38	0/3/3/3
17	GDP	2F	501	-	-	5/16/32/32	0/3/3/3
15	GTP	6A	501	16	-	6/22/38/38	0/3/3/3
15	GTP	4C	501	16	-	5/22/38/38	0/3/3/3
15	GTP	5G	501	16	-	5/22/38/38	0/3/3/3
15	GTP	8M	501	-	-	5/22/38/38	0/3/3/3
17	GDP	9L	501	-	-	0/16/32/32	0/3/3/3
15	GTP	2E	501	16	-	5/22/38/38	0/3/3/3
15	GTP	8E	501	16	-	6/22/38/38	0/3/3/3
17	GDP	8L	501	-	-	8/16/32/32	0/3/3/3
17	GDP	9B	501	-	-	3/16/32/32	0/3/3/3
15	GTP	1E	501	16	-	7/22/38/38	0/3/3/3
17	GDP	1L	501	-	-	5/16/32/32	0/3/3/3
17	GDP	1D	501	-	-	5/16/32/32	0/3/3/3
15	GTP	7E	501	16	-	4/22/38/38	0/3/3/3
15	GTP	6G	501	16	-	9/22/38/38	0/3/3/3
15	GTP	5E	501	16	-	6/22/38/38	0/3/3/3
17	GDP	6H	501	-	-	4/16/32/32	0/3/3/3
17	GDP	8H	501	-	-	6/16/32/32	0/3/3/3
17	GDP	5H	501	-	-	7/16/32/32	0/3/3/3
17	GDP	8B	501	-	-	7/16/32/32	0/3/3/3
17	GDP	6D	501	-	-	8/16/32/32	0/3/3/3
15	GTP	2K	501	16	-	7/22/38/38	0/3/3/3
15	GTP	9I	501	16	-	7/22/38/38	0/3/3/3
17	GDP	2J	501	-	-	3/16/32/32	0/3/3/3
17	GDP	1N	501	-	-	6/16/32/32	0/3/3/3
17	GDP	7F	501	-	-	5/16/32/32	0/3/3/3
17	GDP	5L	501	-	-	9/16/32/32	0/3/3/3
15	GTP	7I	501	16	-	5/22/38/38	0/3/3/3
15	GTP	8I	501	16	-	7/22/38/38	0/3/3/3
17	GDP	1B	501	-	-	4/16/32/32	0/3/3/3
17	GDP	7B	502	-	-	6/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	GDP	6B	501	-	-	5/16/32/32	0/3/3/3
17	GDP	4L	501	-	-	6/16/32/32	0/3/3/3
15	GTP	4M	501	-	-	7/22/38/38	0/3/3/3
15	GTP	1I	501	16	-	8/22/38/38	0/3/3/3
17	GDP	5F	501	-	-	3/16/32/32	0/3/3/3
15	GTP	3K	501	16	-	6/22/38/38	0/3/3/3
17	GDP	2L	501	-	-	5/16/32/32	0/3/3/3
17	GDP	3H	501	-	-	3/16/32/32	0/3/3/3
17	GDP	3J	501	-	-	5/16/32/32	0/3/3/3
17	GDP	1F	501	-	-	5/16/32/32	0/3/3/3

The worst 5 of 257 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	6N	501	GTP	PB-O3B	3.43	1.63	1.59
17	3L	501	GDP	C5-C4	3.26	1.47	1.38
17	3B	501	GDP	C5-C4	3.25	1.47	1.38
17	5L	501	GDP	C5-C4	3.24	1.47	1.38
17	6L	501	GDP	C5-C4	3.24	1.47	1.38

The worst 5 of 968 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	2J	501	GDP	C5-C4-N3	-6.80	117.58	128.39
17	4B	501	GDP	C5-C4-N3	-6.73	117.68	128.39
17	6F	501	GDP	C5-C4-N3	-6.70	117.73	128.39
17	7B	502	GDP	C5-C4-N3	-6.67	117.77	128.39
17	4J	501	GDP	C5-C4-N3	-6.56	117.95	128.39

There are no chirality outliers.

5 of 677 torsion outliers are listed below:

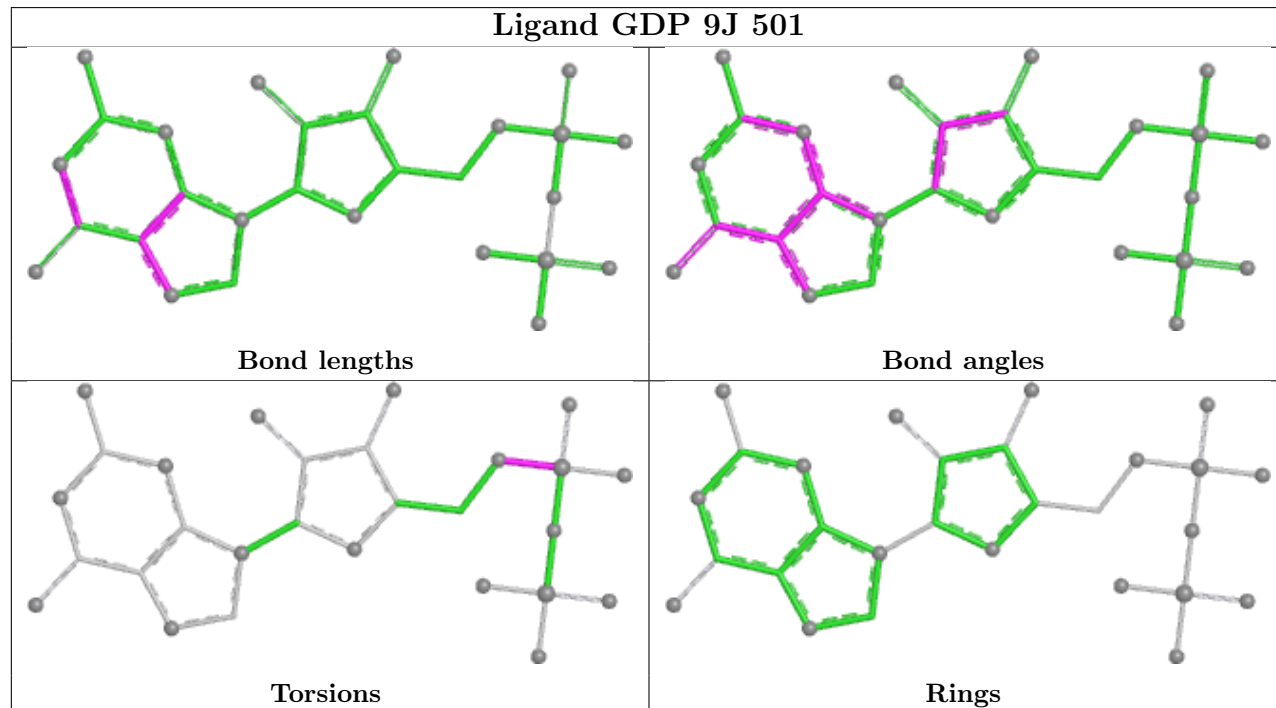
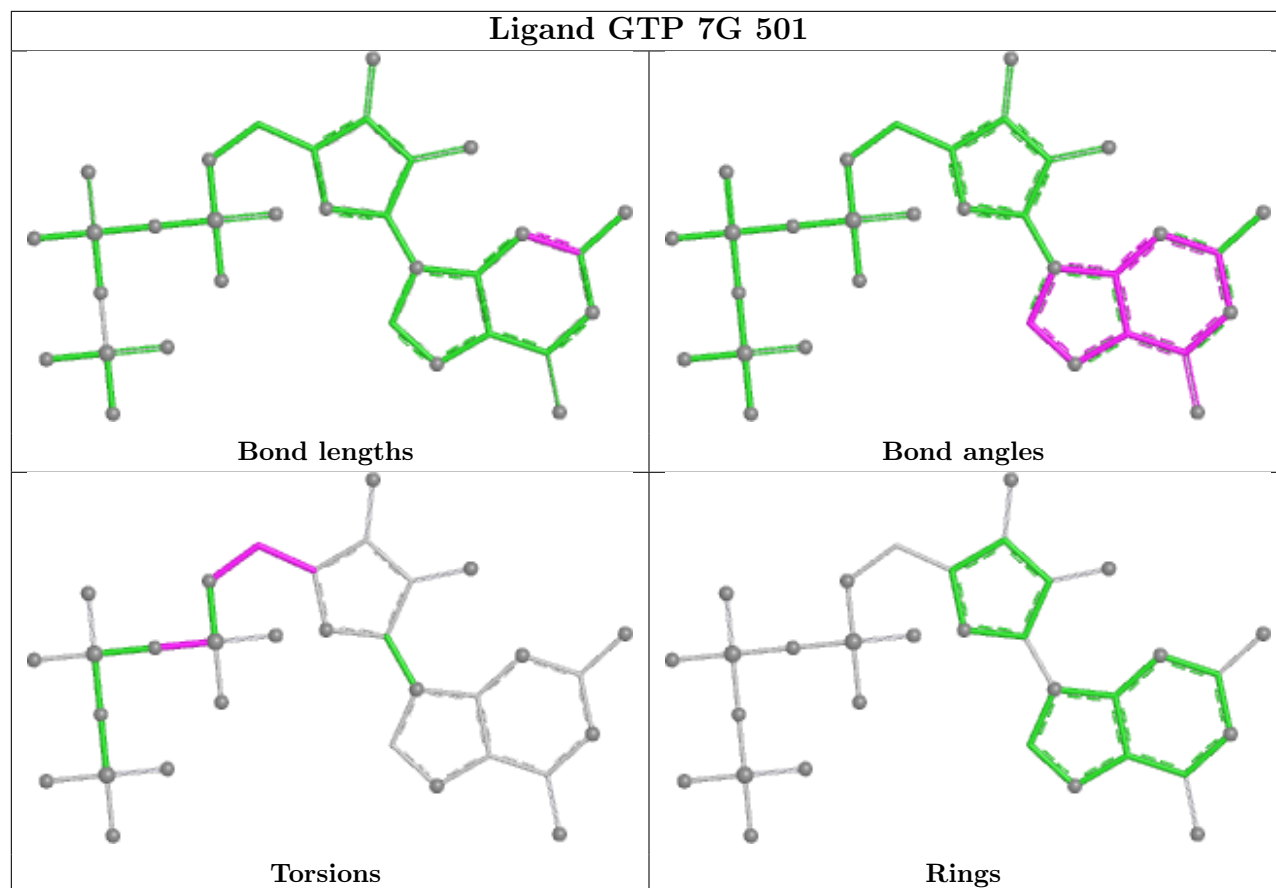
Mol	Chain	Res	Type	Atoms
15	1A	501	GTP	C5'-O5'-PA-O3A
15	1A	501	GTP	C5'-O5'-PA-O1A
15	1A	501	GTP	C5'-O5'-PA-O2A
15	1C	501	GTP	O4'-C4'-C5'-O5'
15	1E	501	GTP	C5'-O5'-PA-O3A

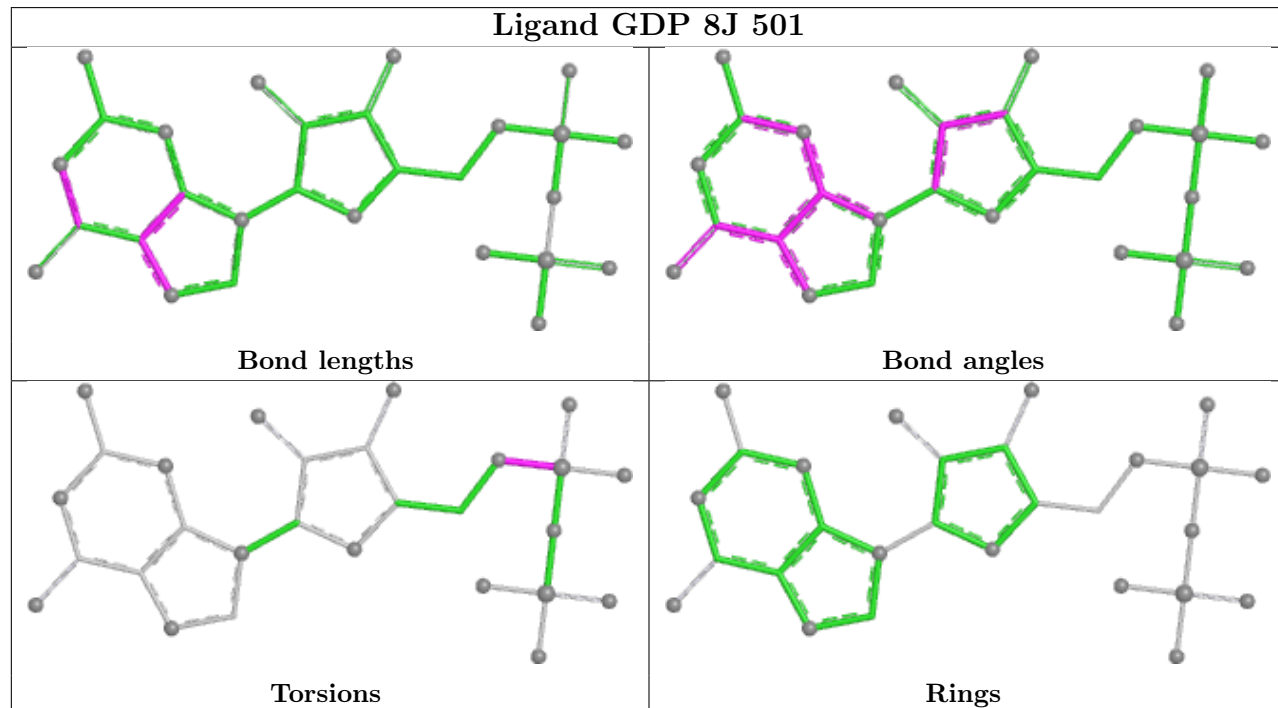
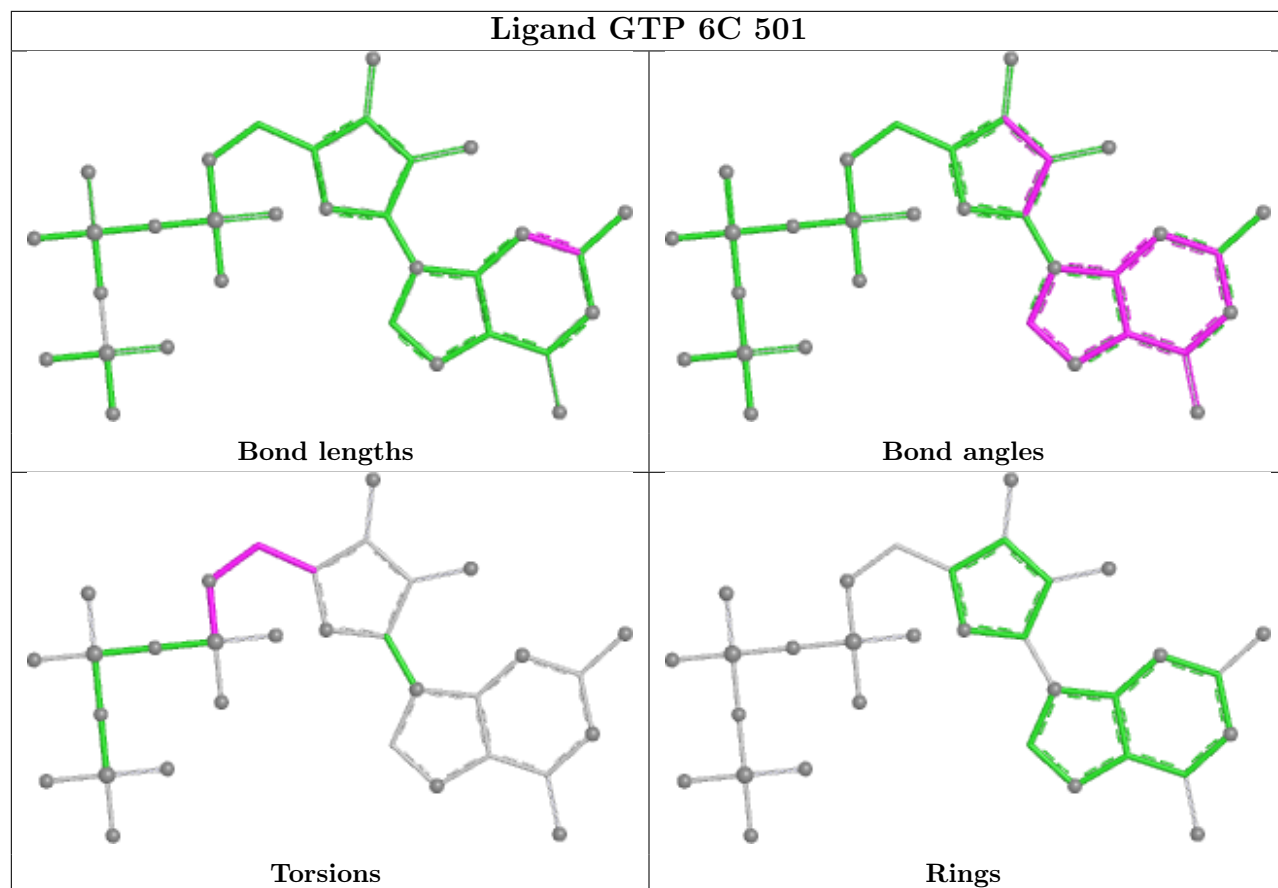
There are no ring outliers.

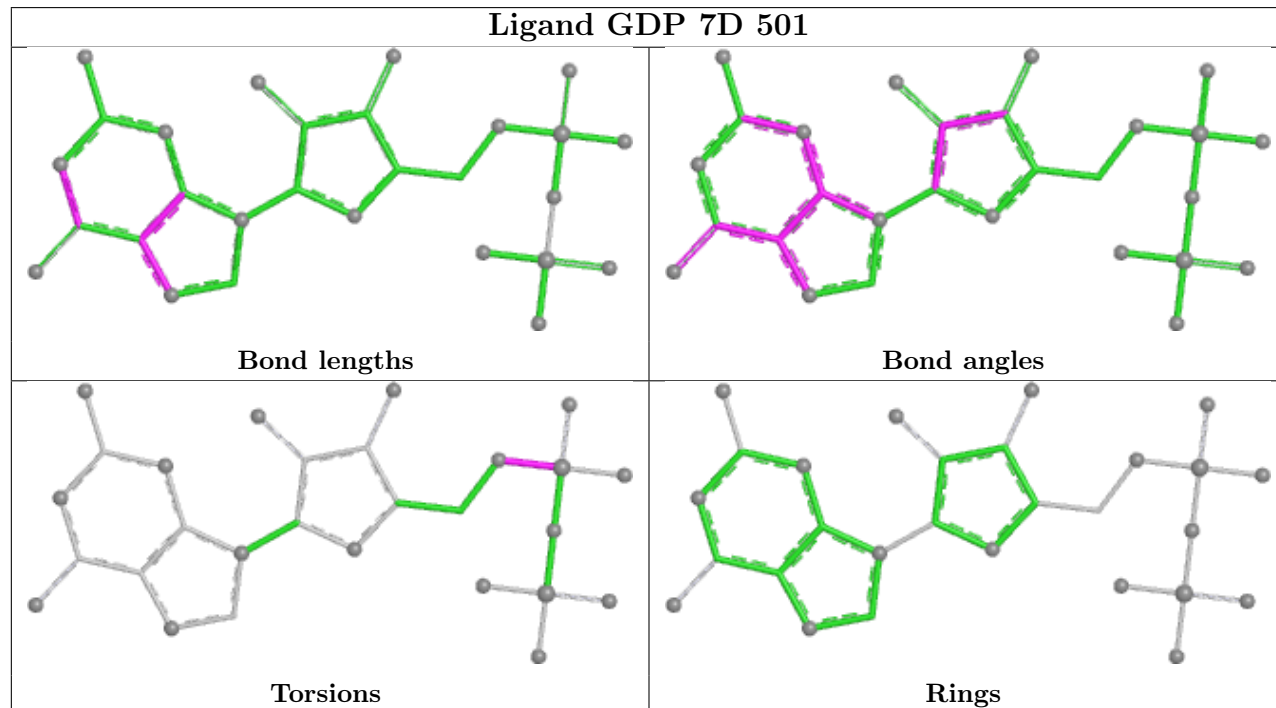
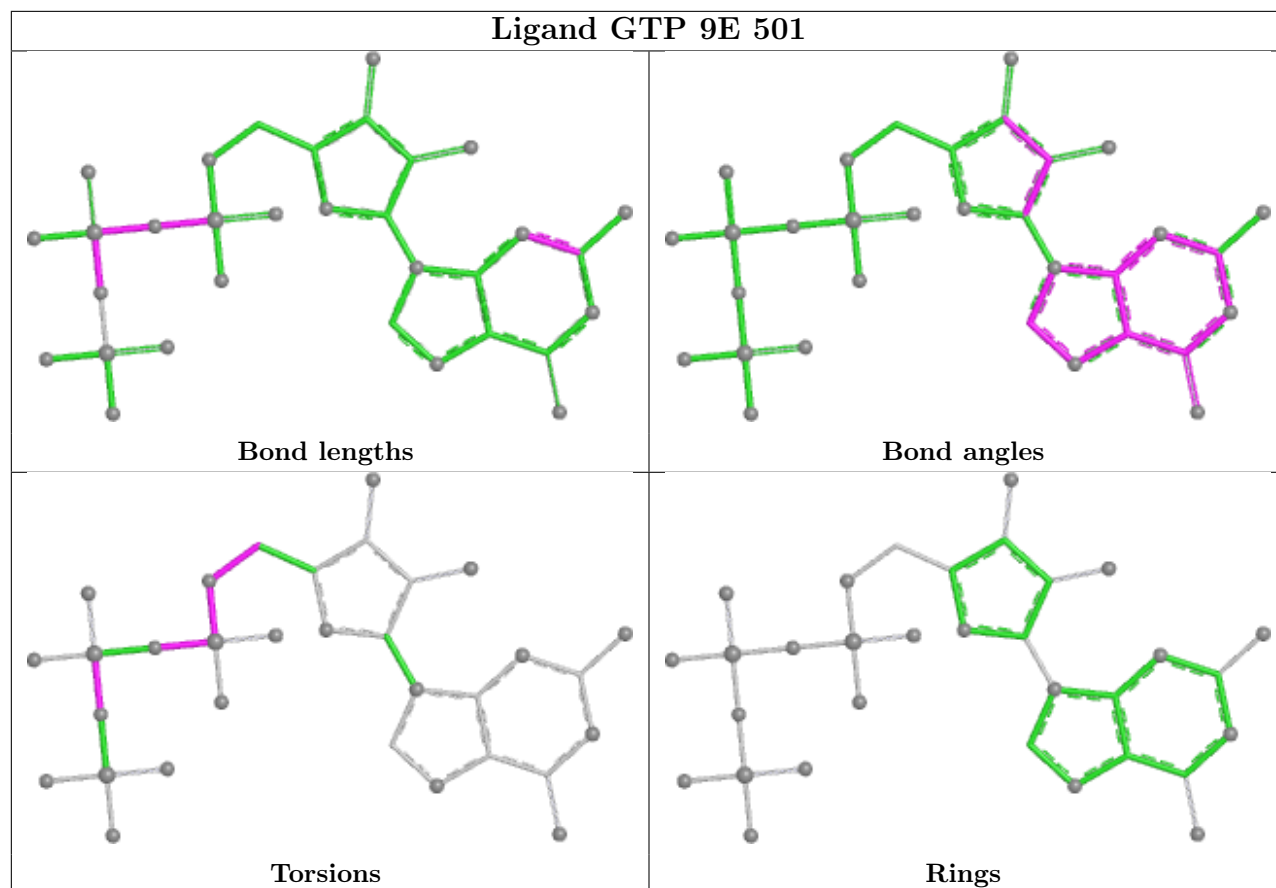
23 monomers are involved in 31 short contacts:

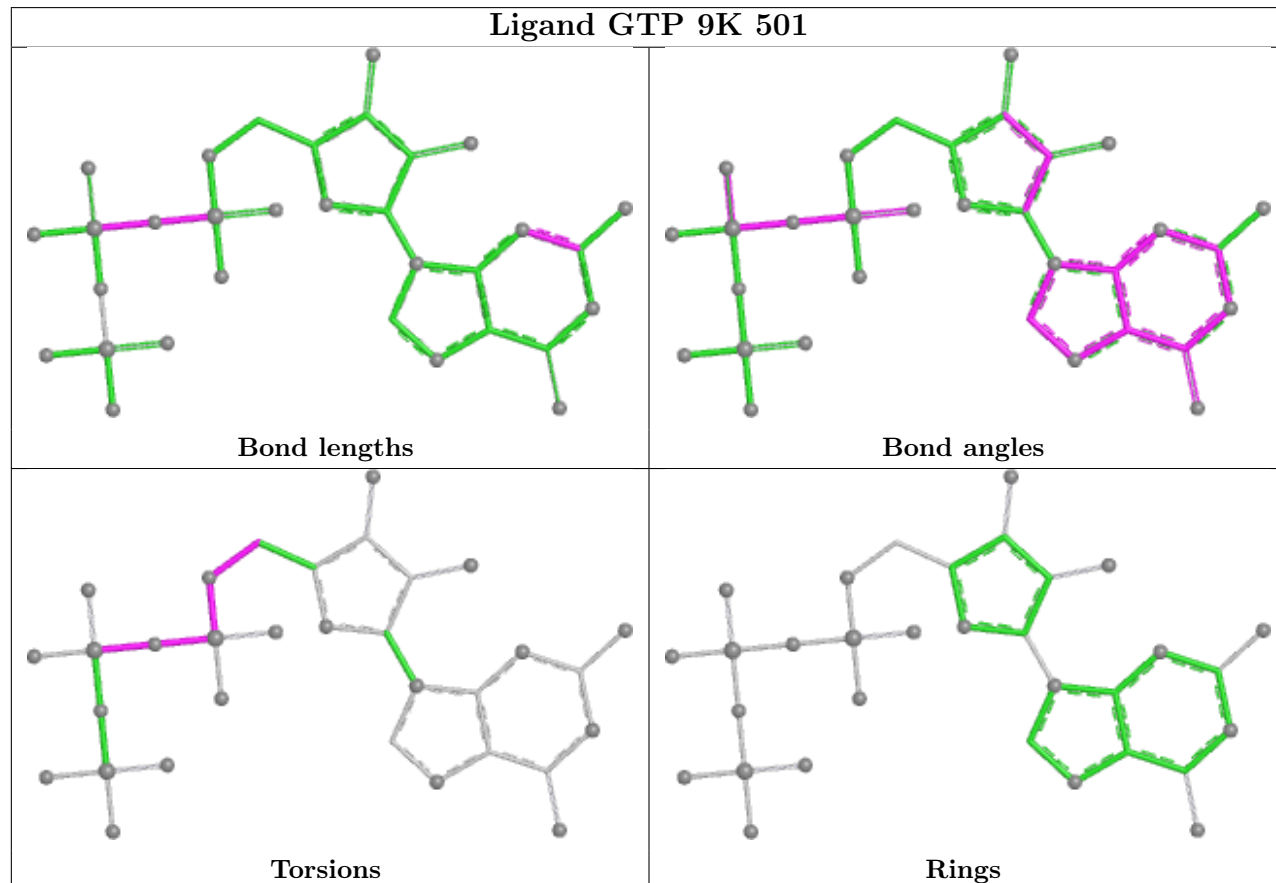
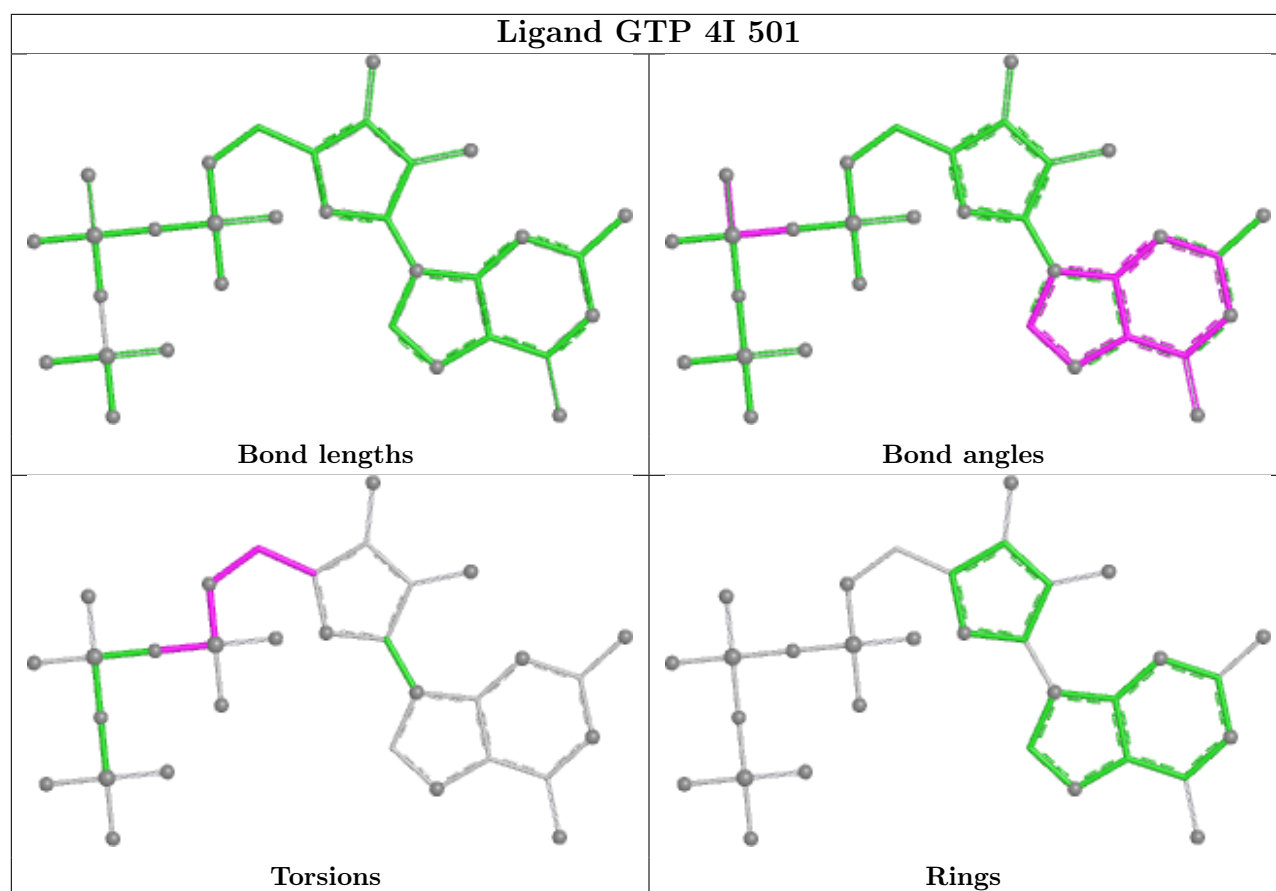
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	6C	501	GTP	1	0
15	9K	501	GTP	1	0
17	6N	502	GDP	1	0
17	2H	501	GDP	2	0
17	3F	501	GDP	1	0
15	1A	501	GTP	1	0
17	3B	501	GDP	2	0
17	4D	501	GDP	1	0
17	2B	501	GDP	2	0
17	4J	501	GDP	1	0
17	4B	501	GDP	1	0
15	2C	501	GTP	1	0
17	3L	501	GDP	2	0
15	2A	501	GTP	2	0
17	2F	501	GDP	1	0
17	9L	501	GDP	1	0
17	1D	501	GDP	2	0
17	8B	501	GDP	1	0
17	5L	501	GDP	2	0
17	1B	501	GDP	1	0
17	2L	501	GDP	1	0
17	3J	501	GDP	2	0
17	1F	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 than 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.

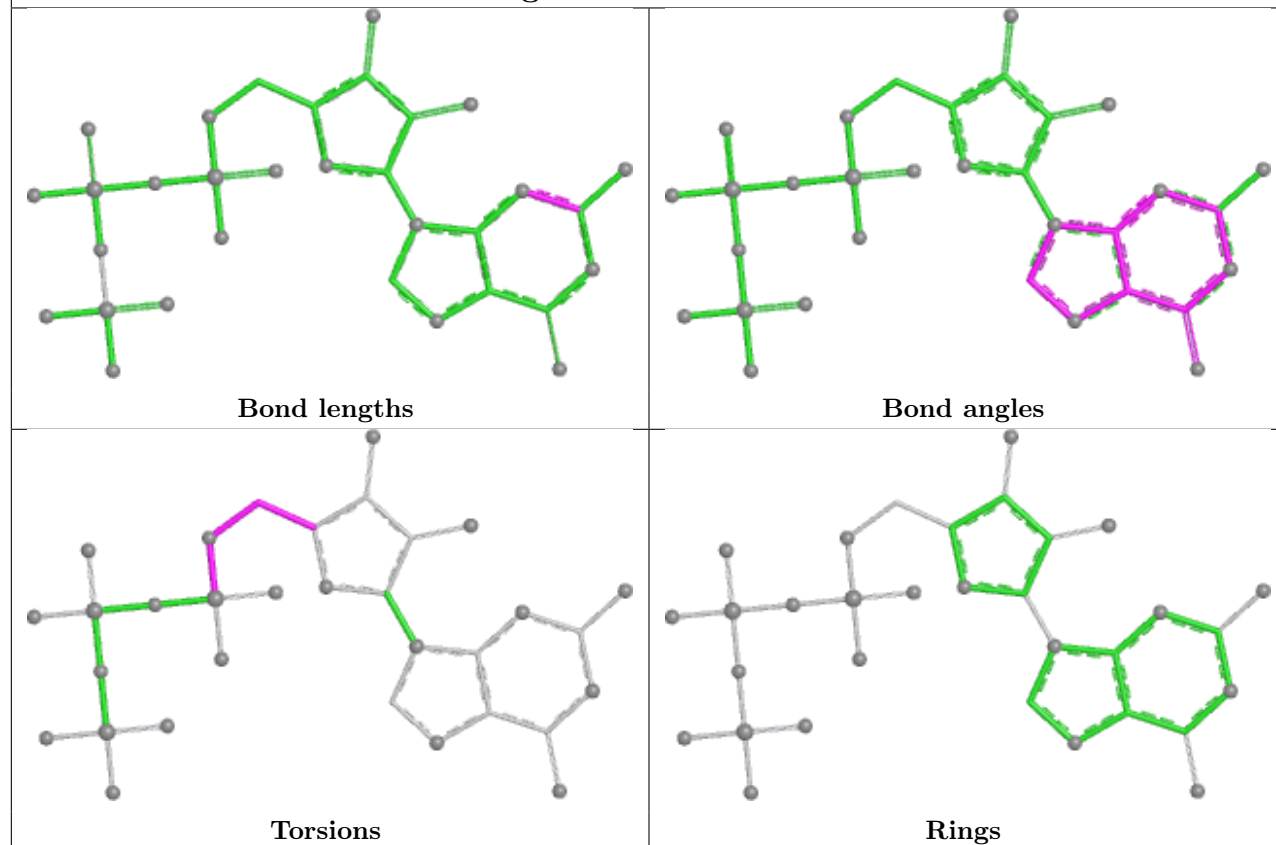




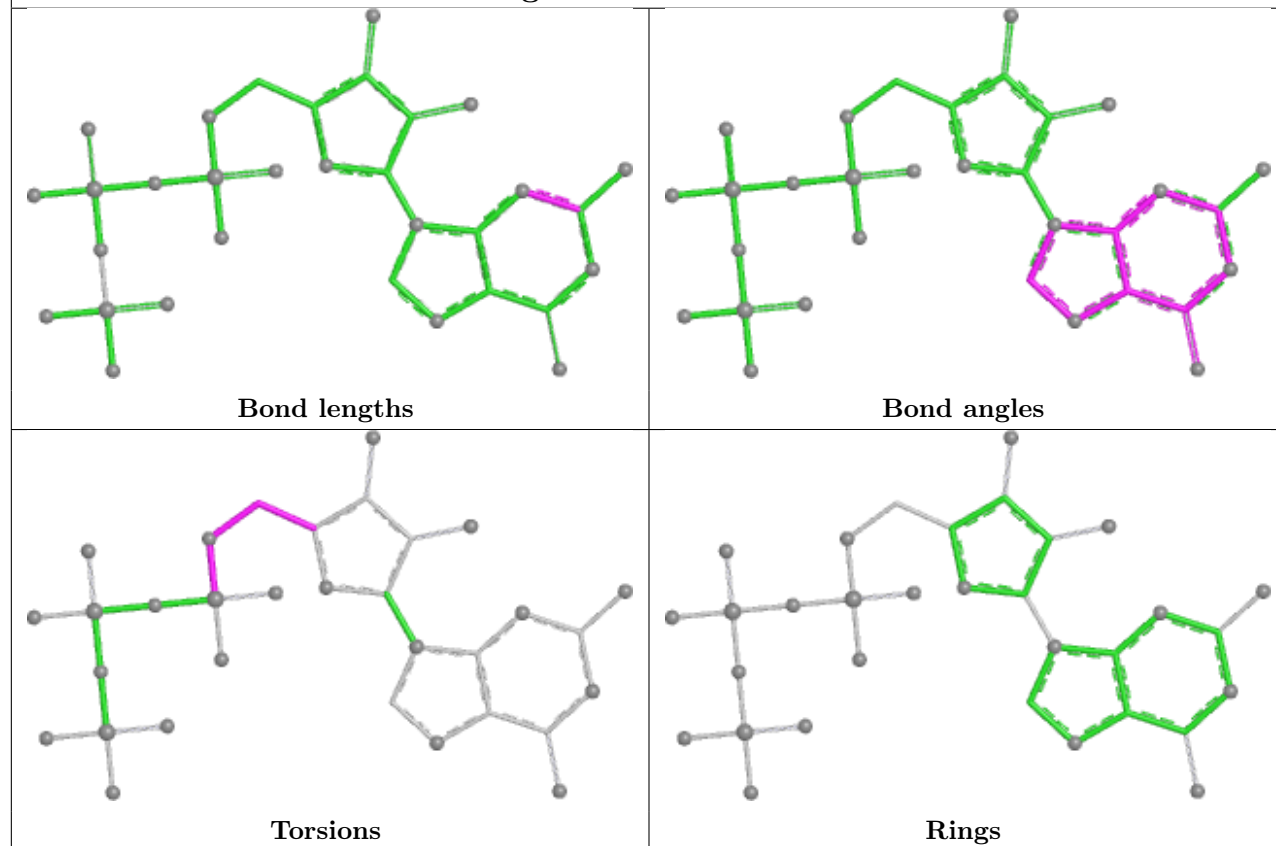


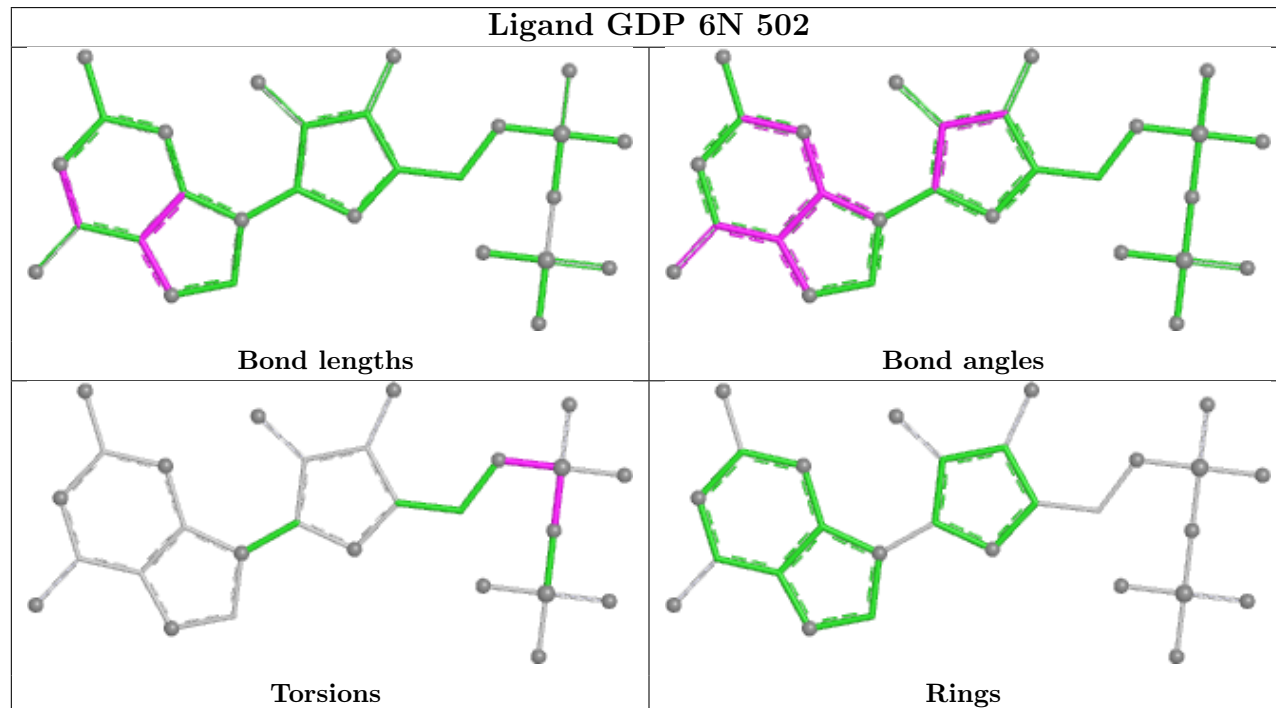
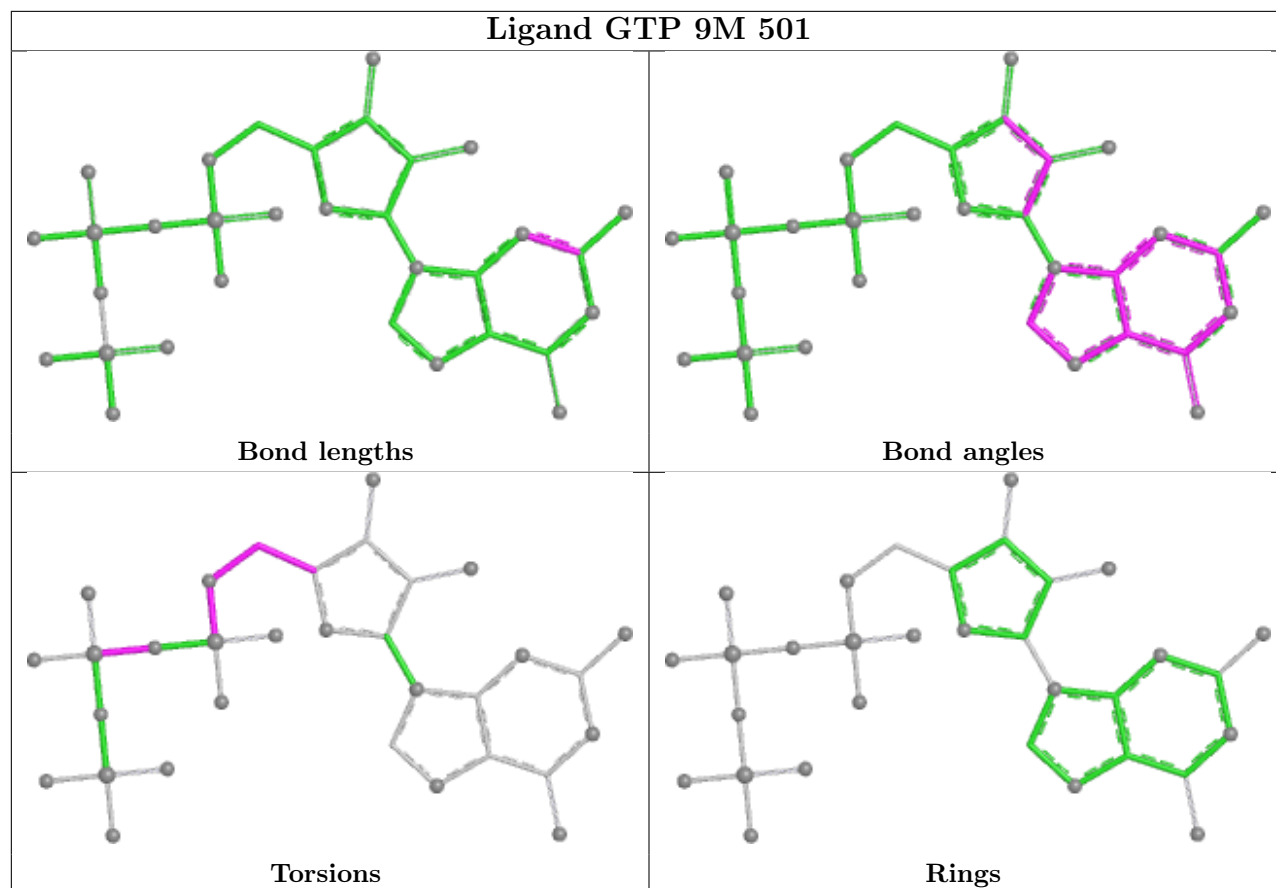


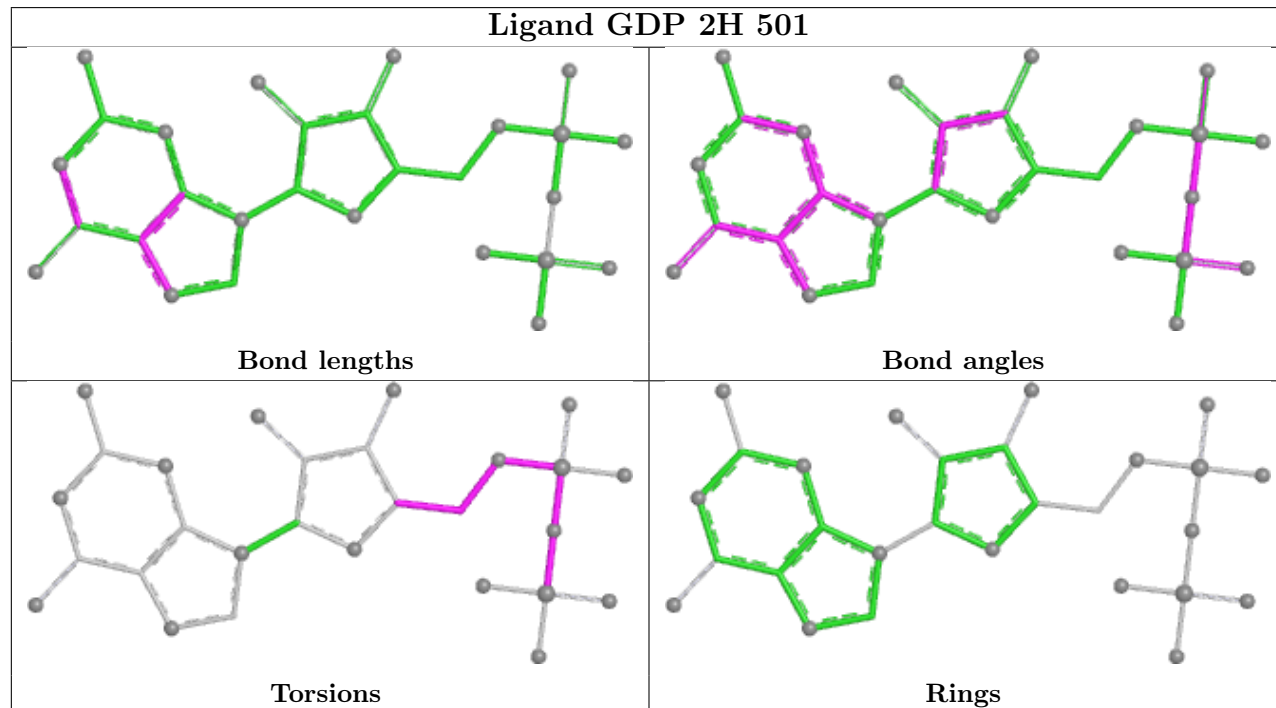
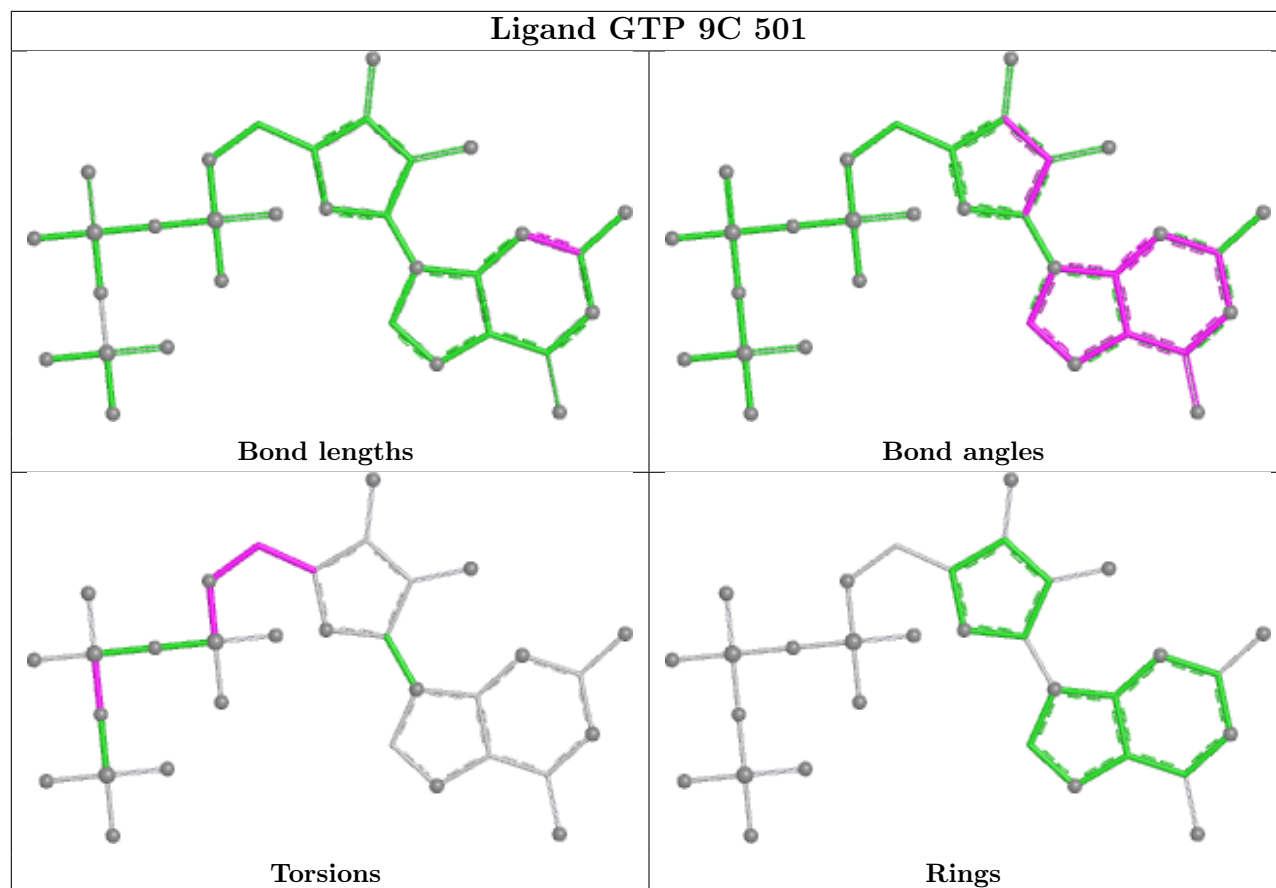
Ligand GTP 3C 501

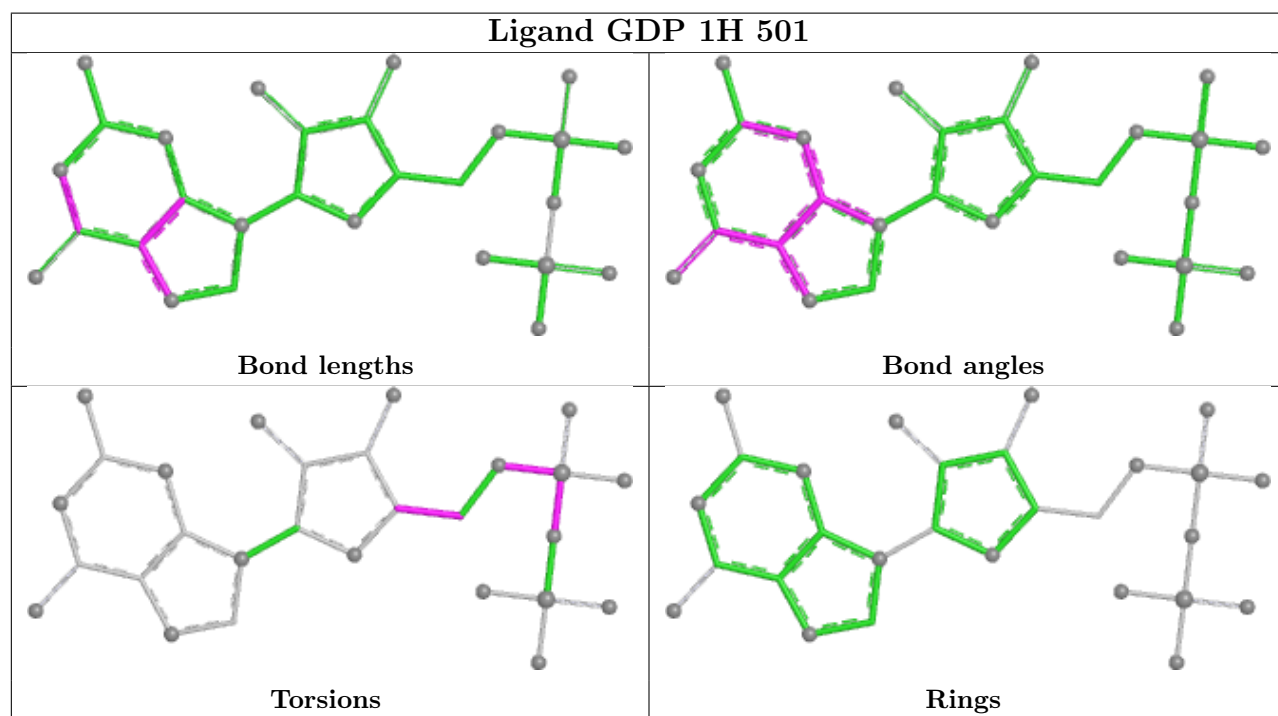
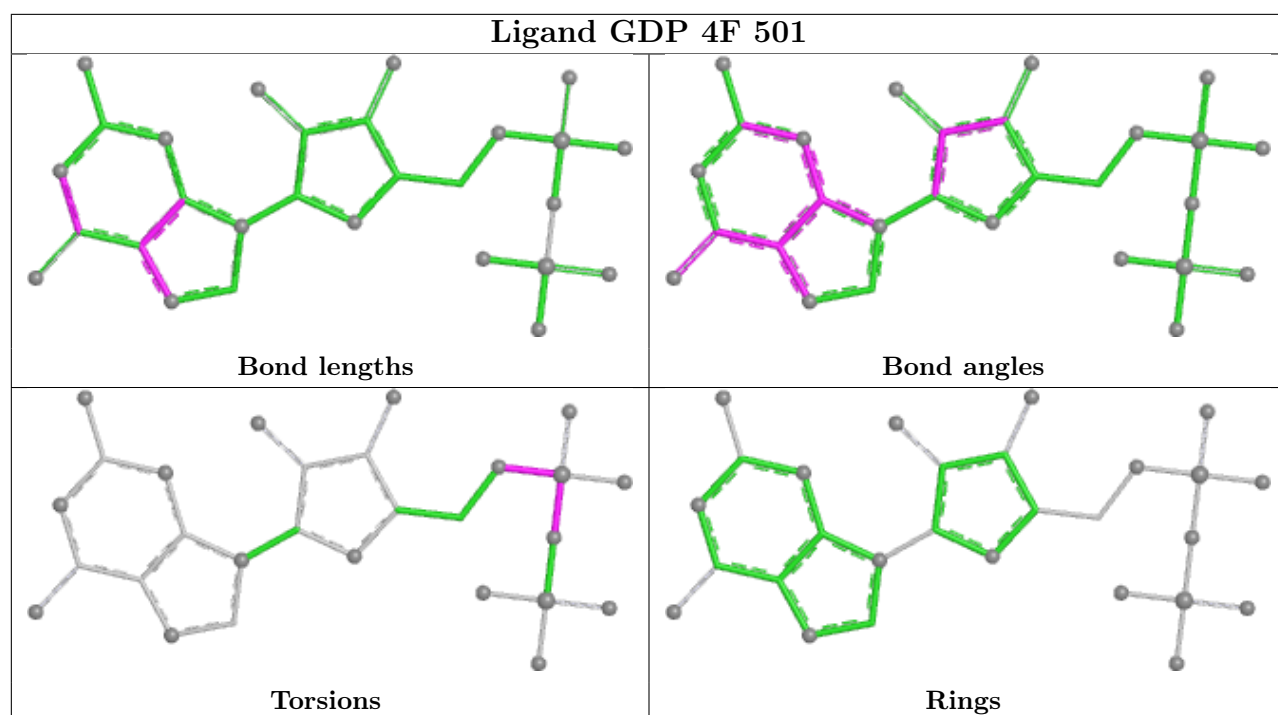


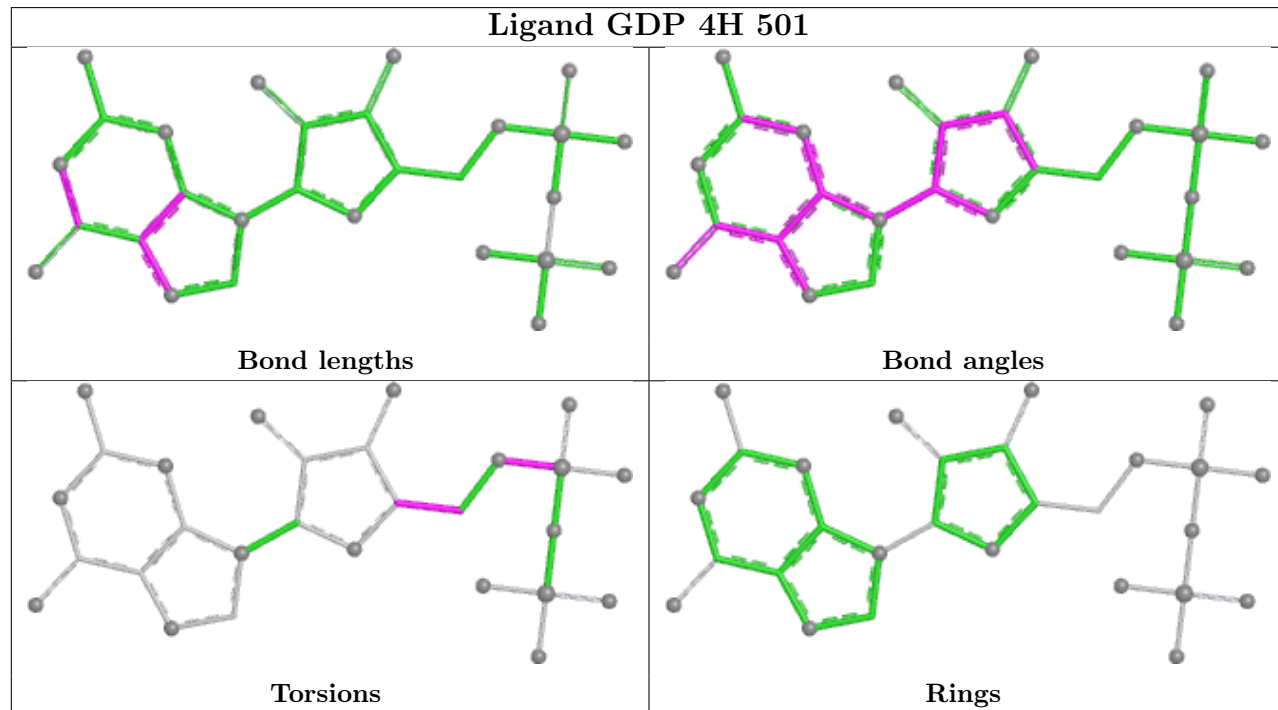
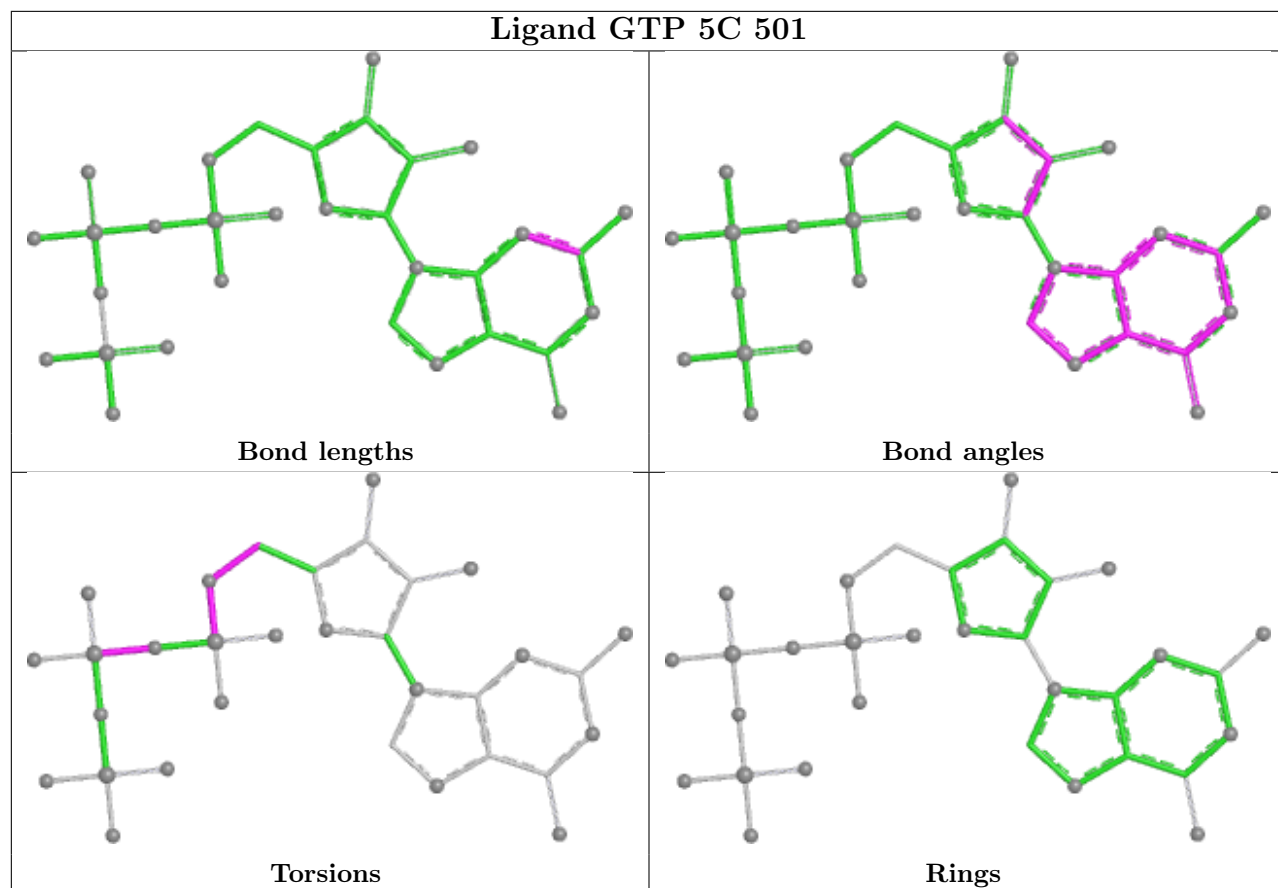
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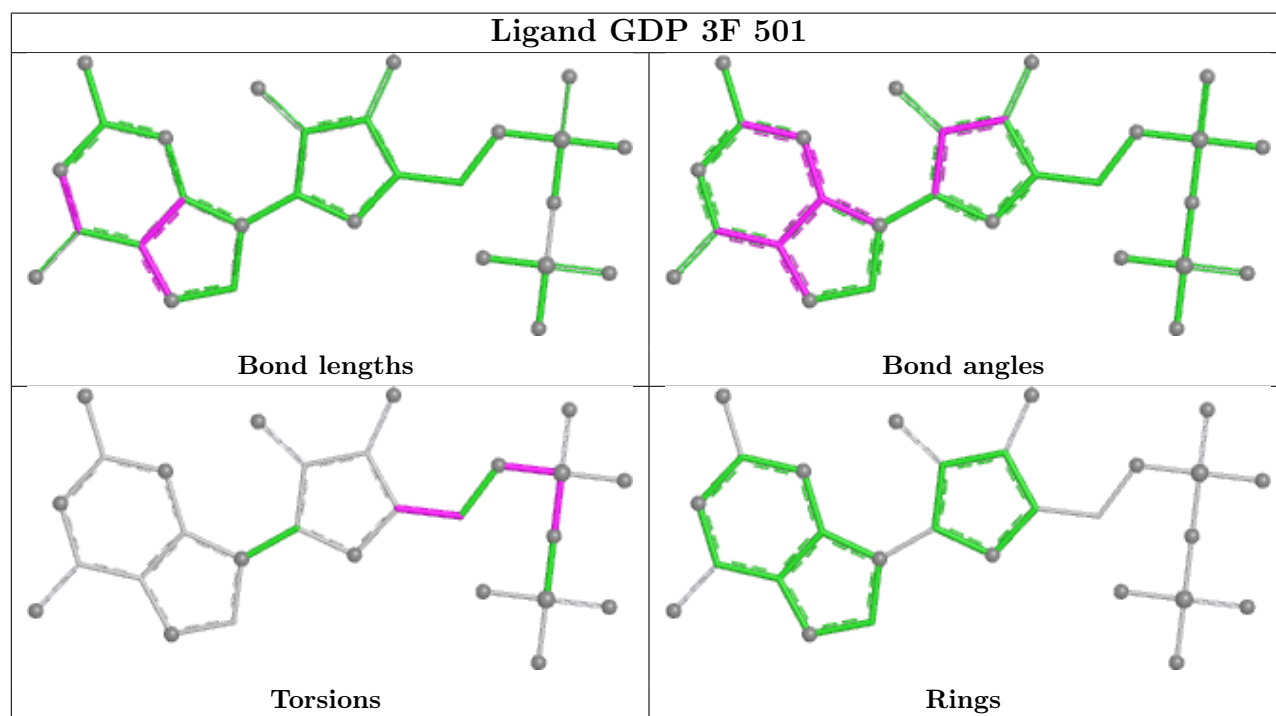
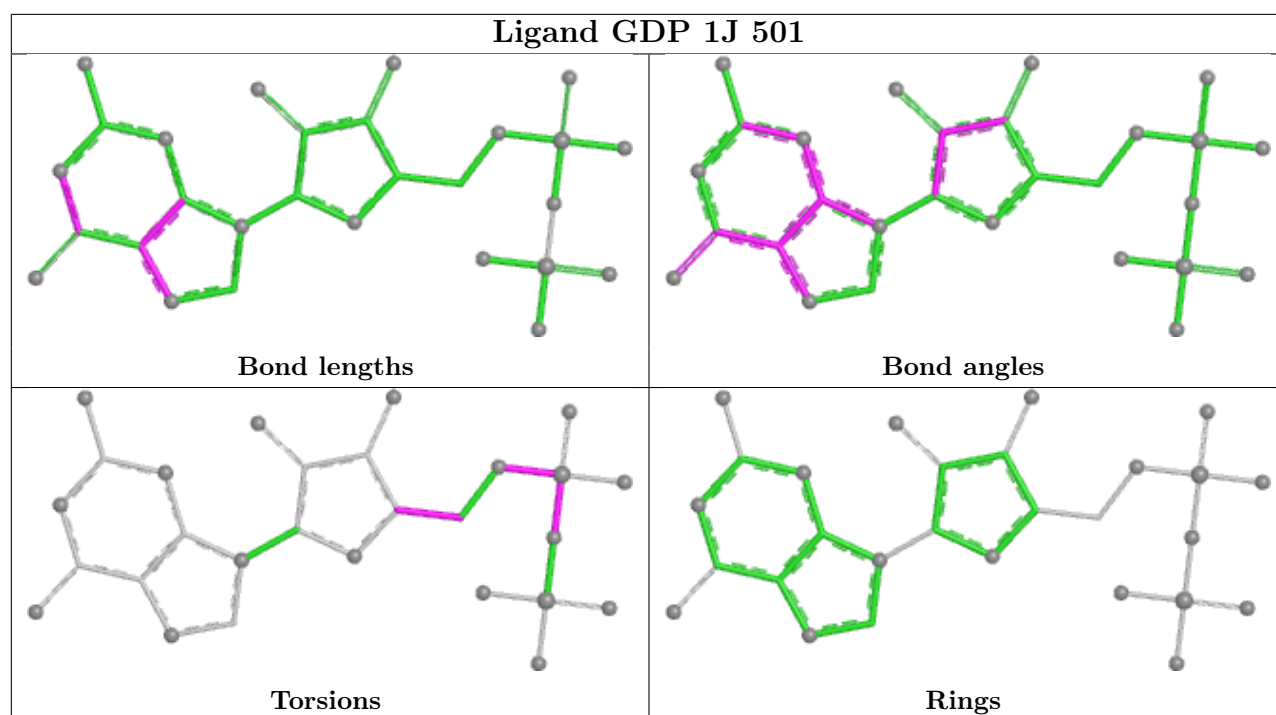




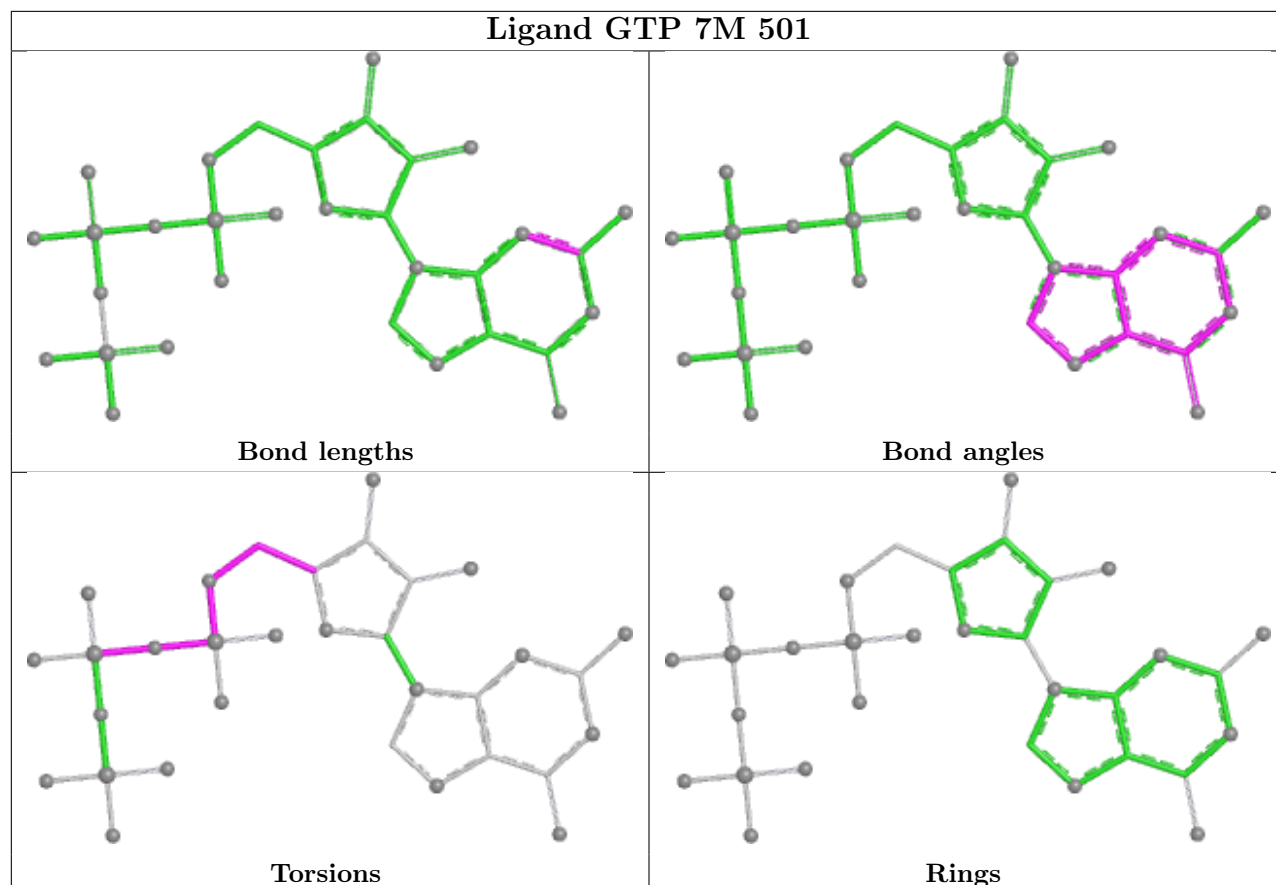




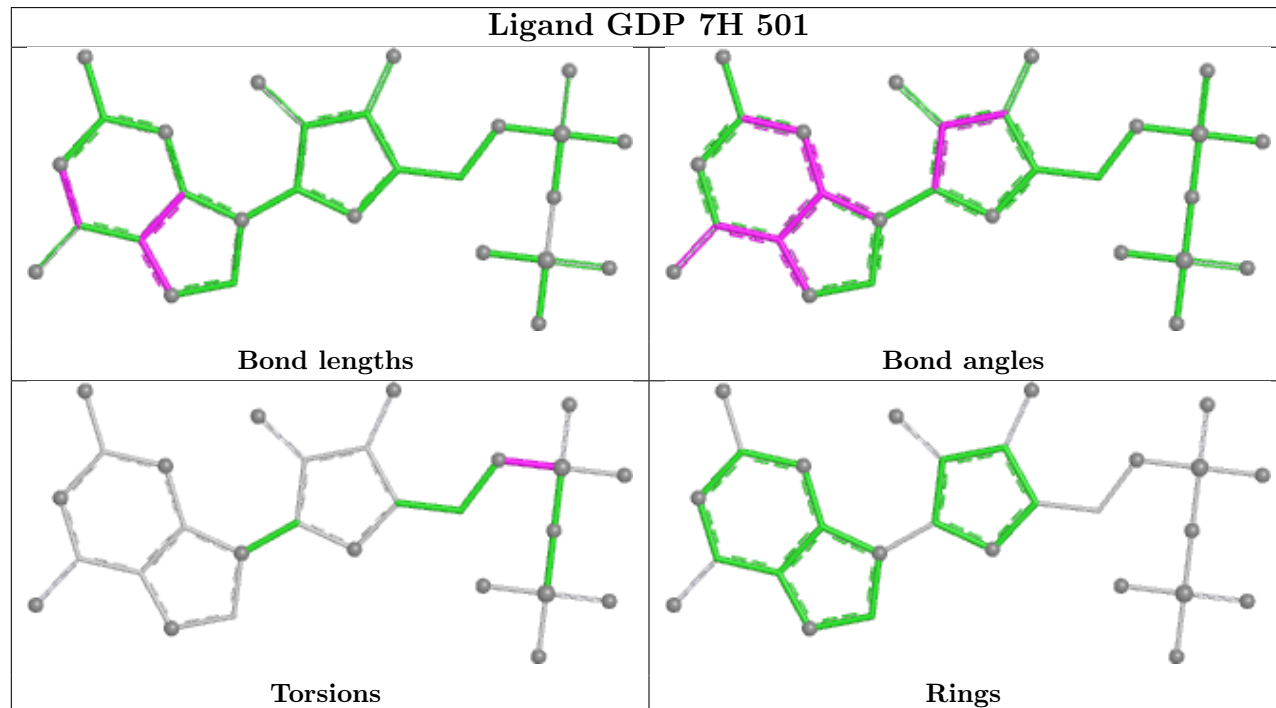


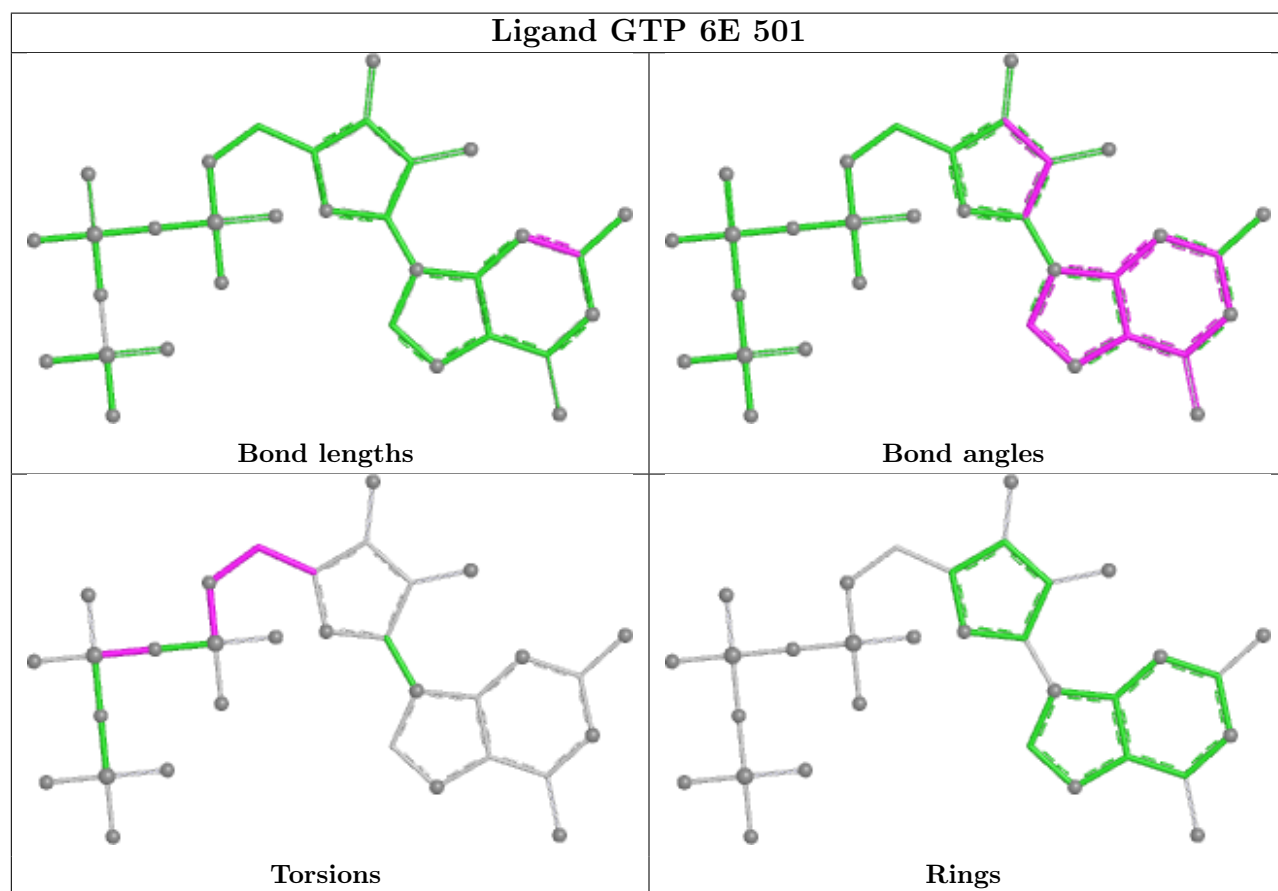
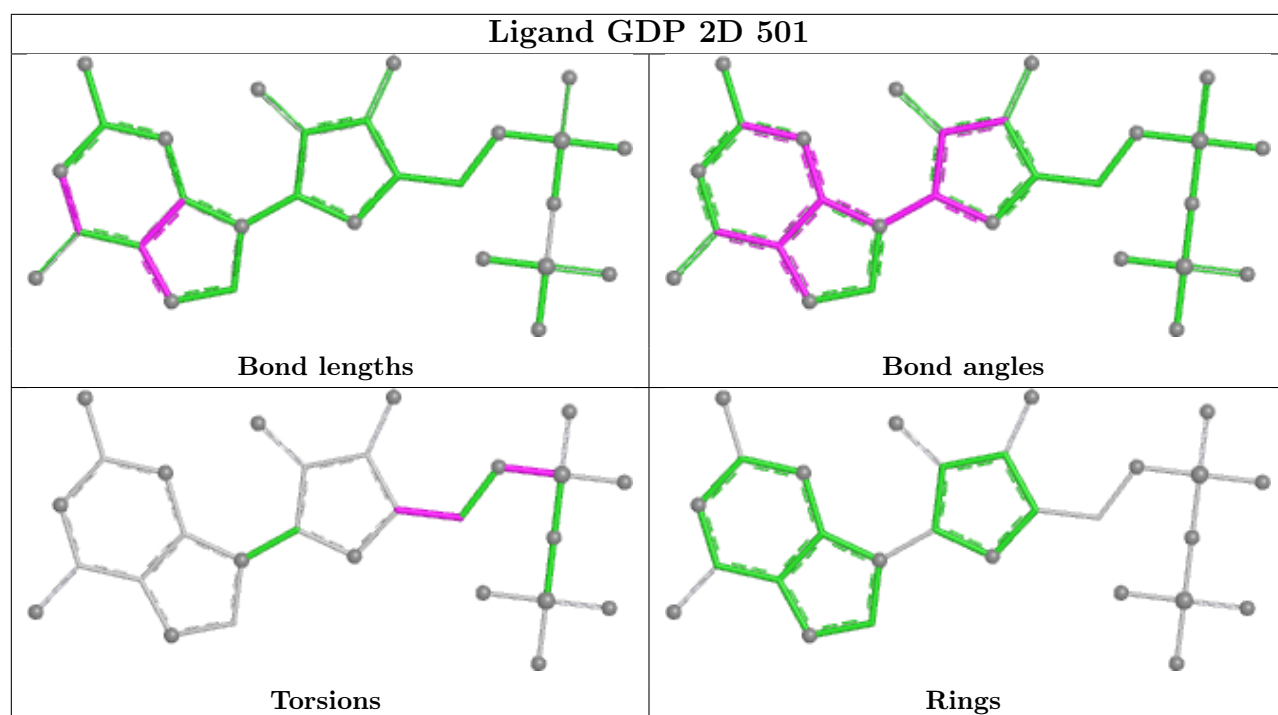


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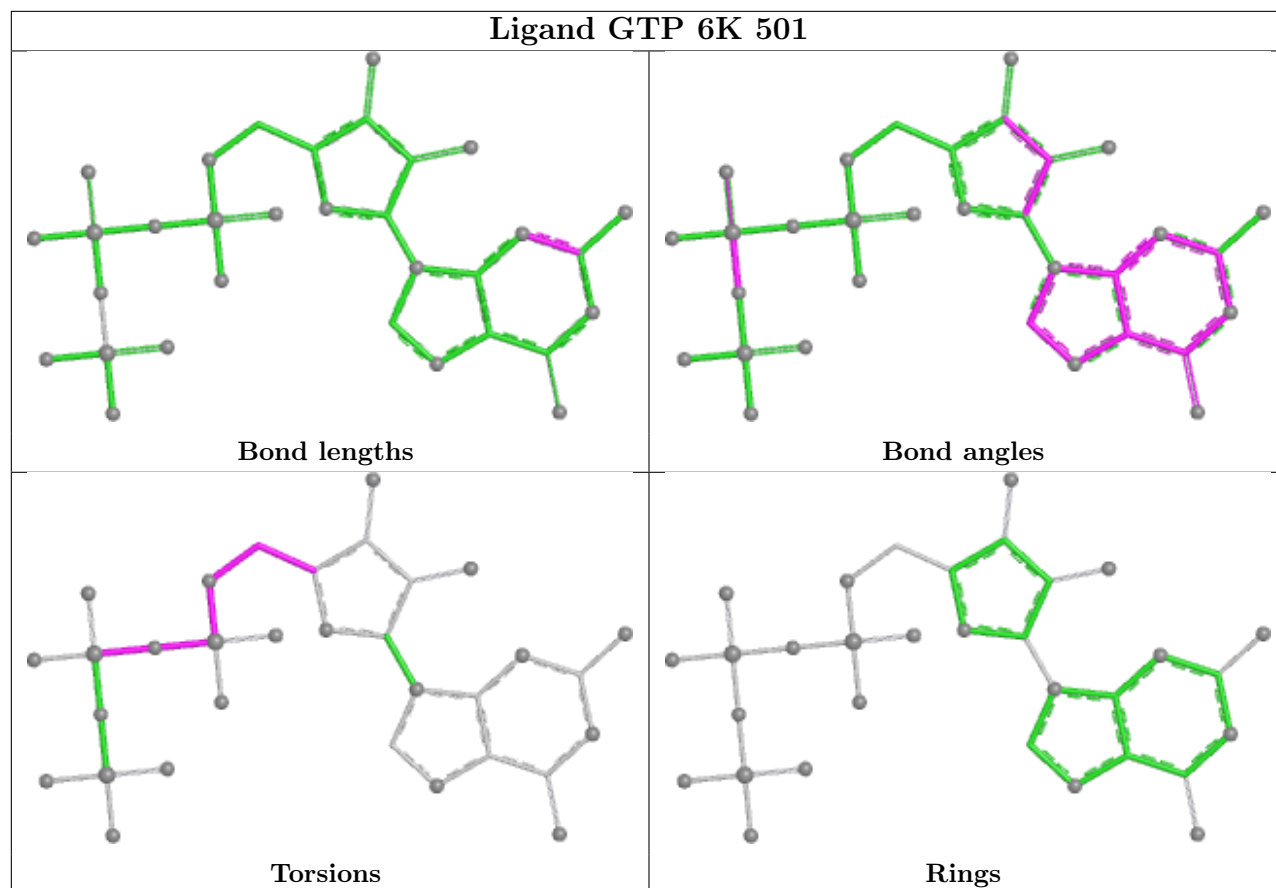


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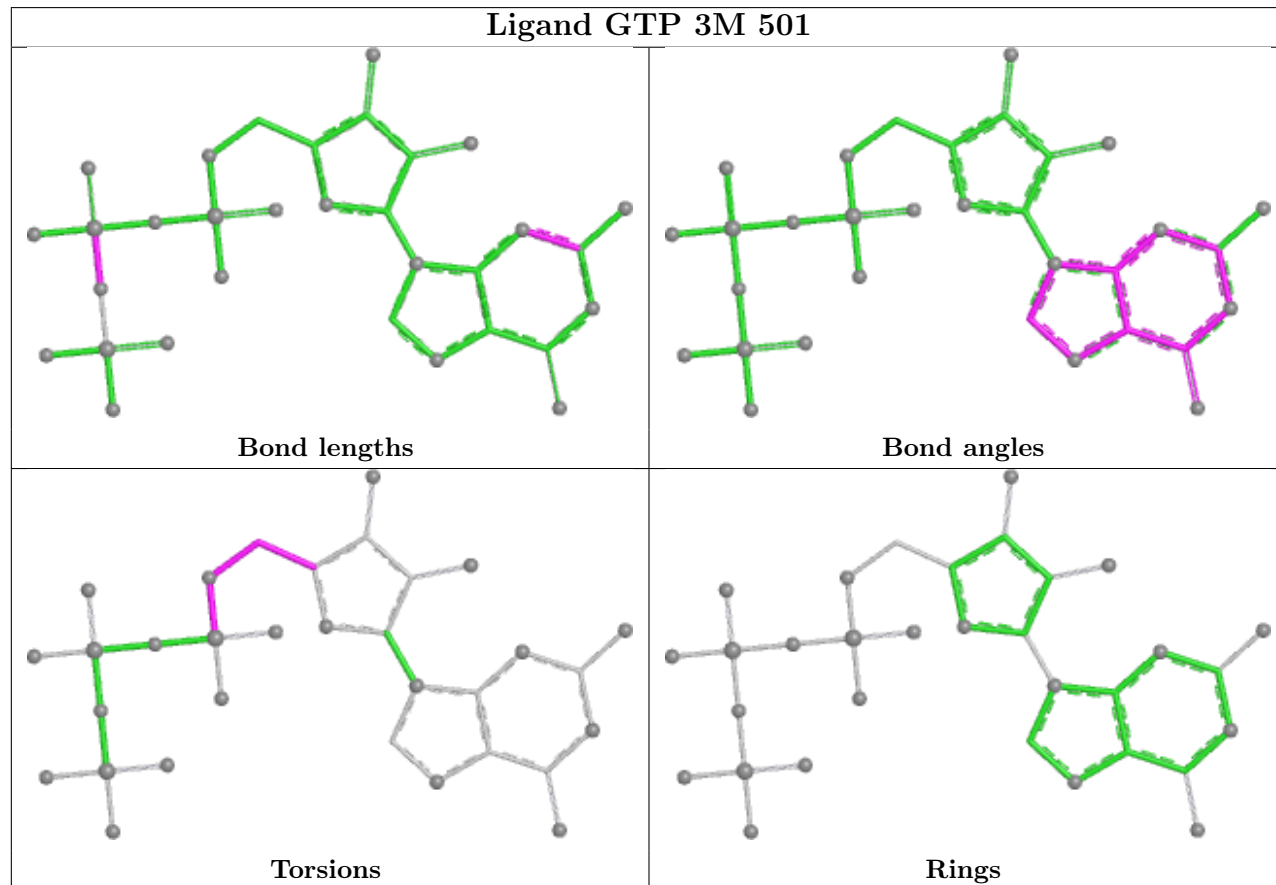


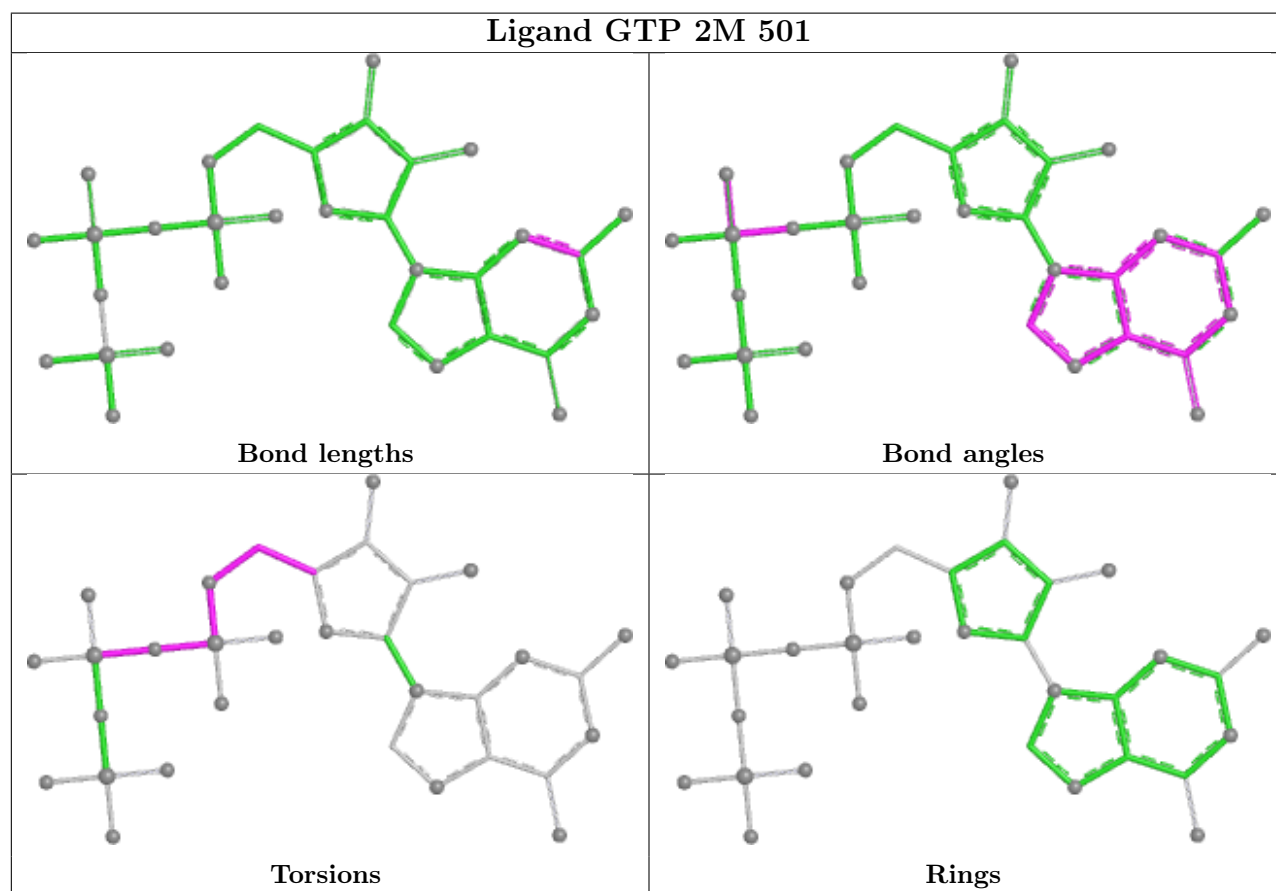
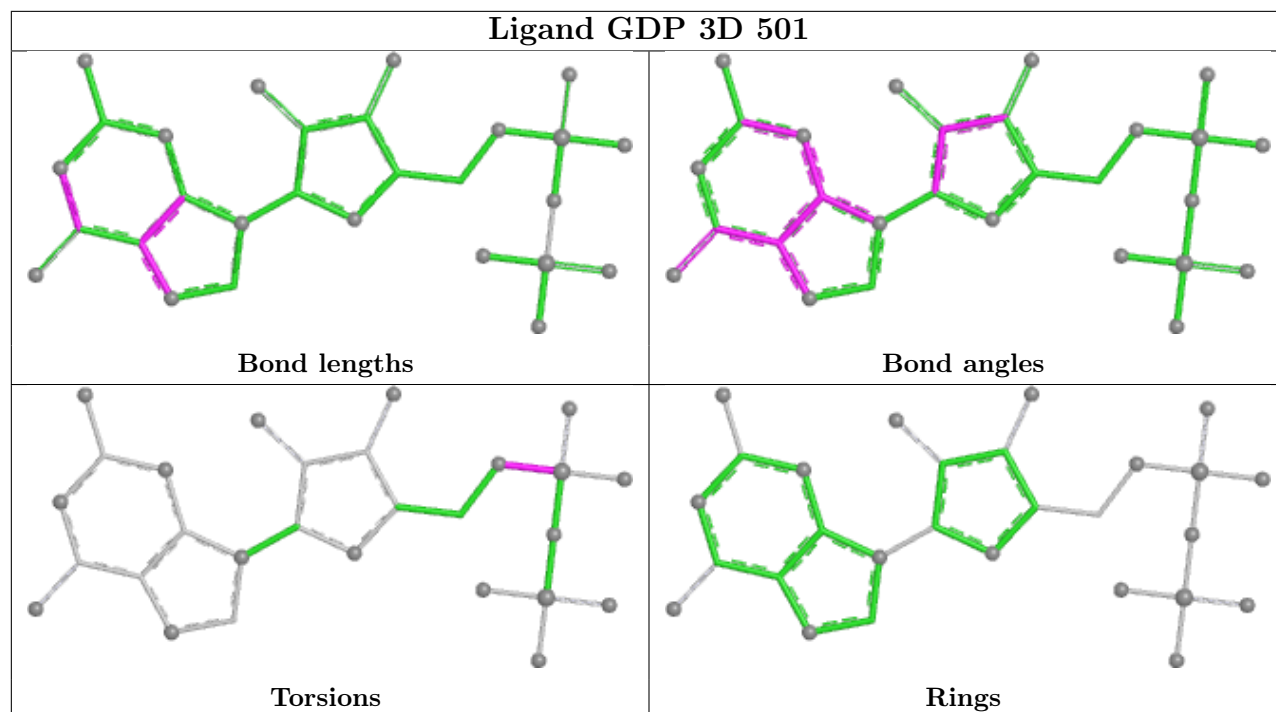


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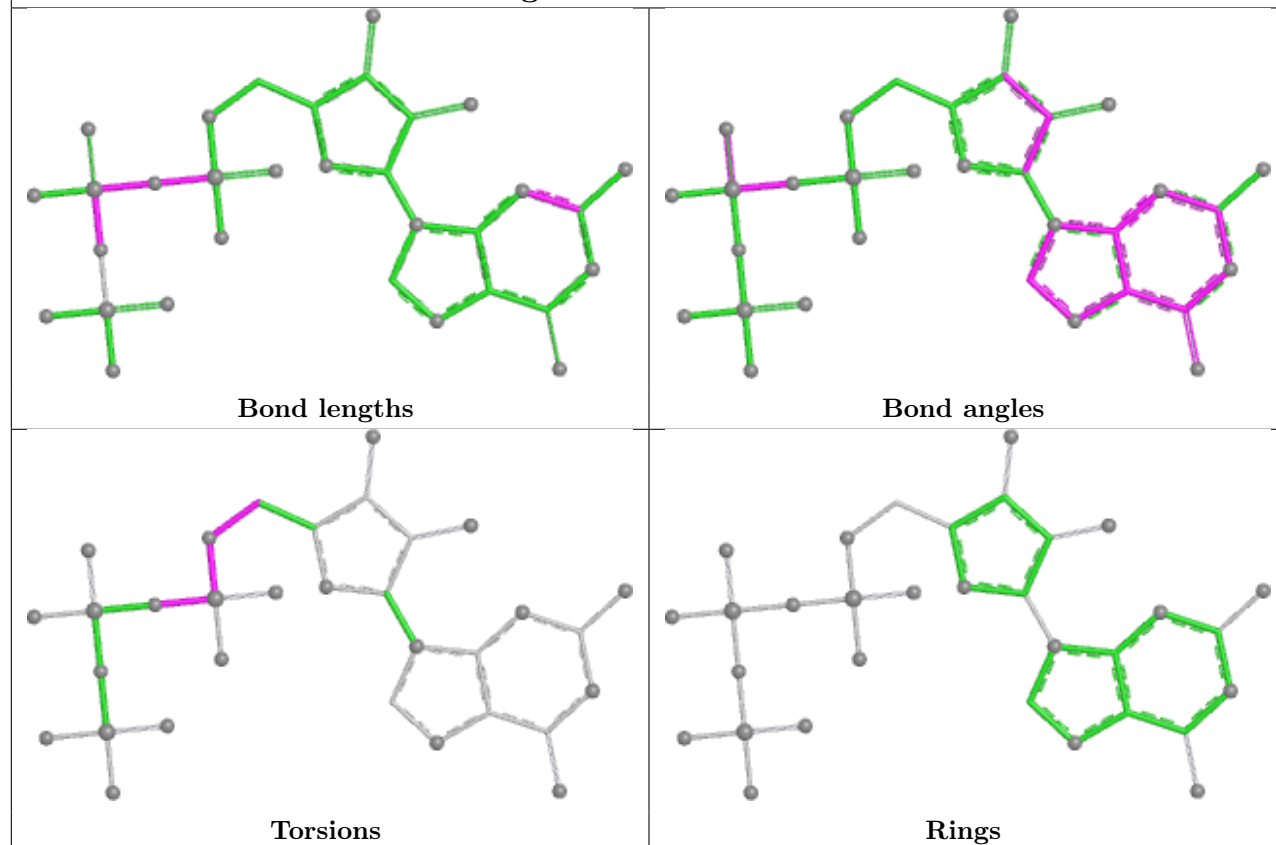


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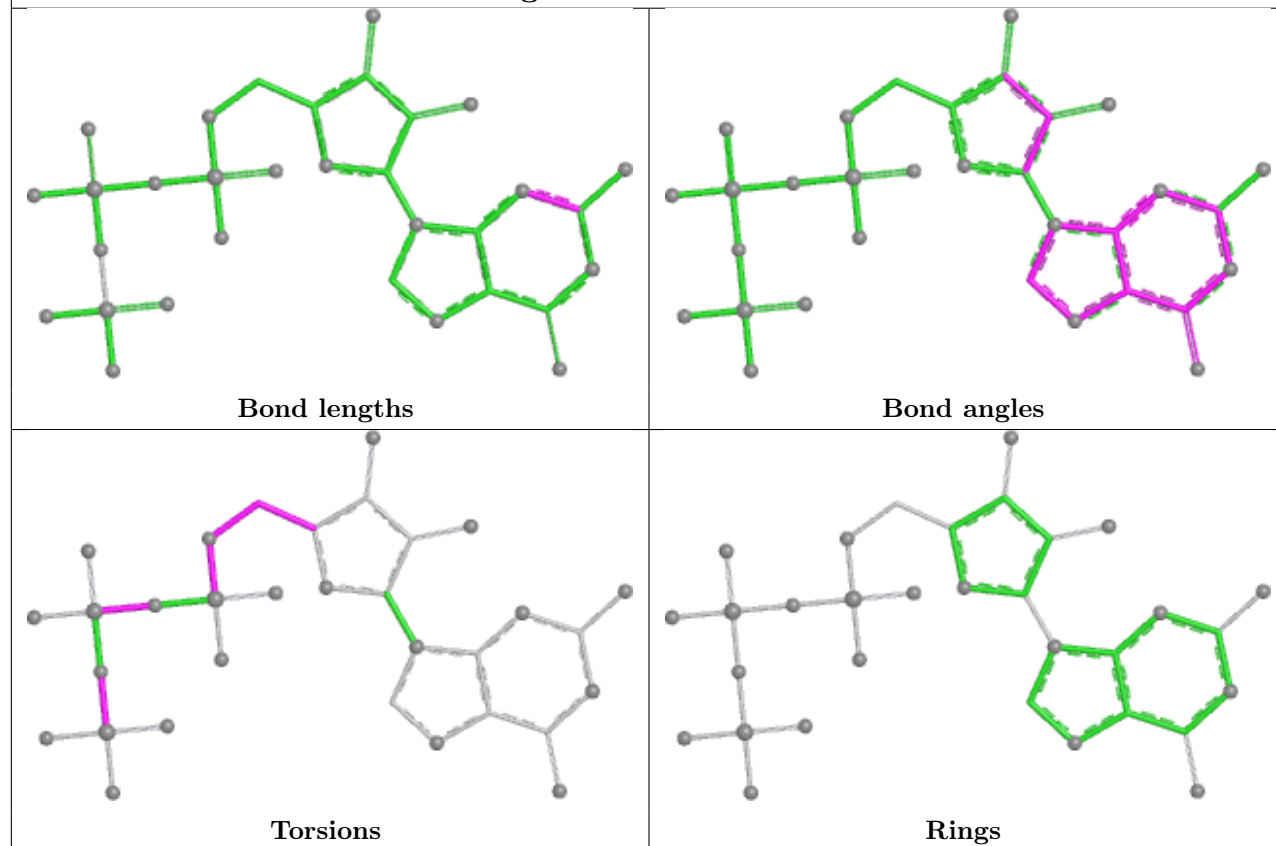


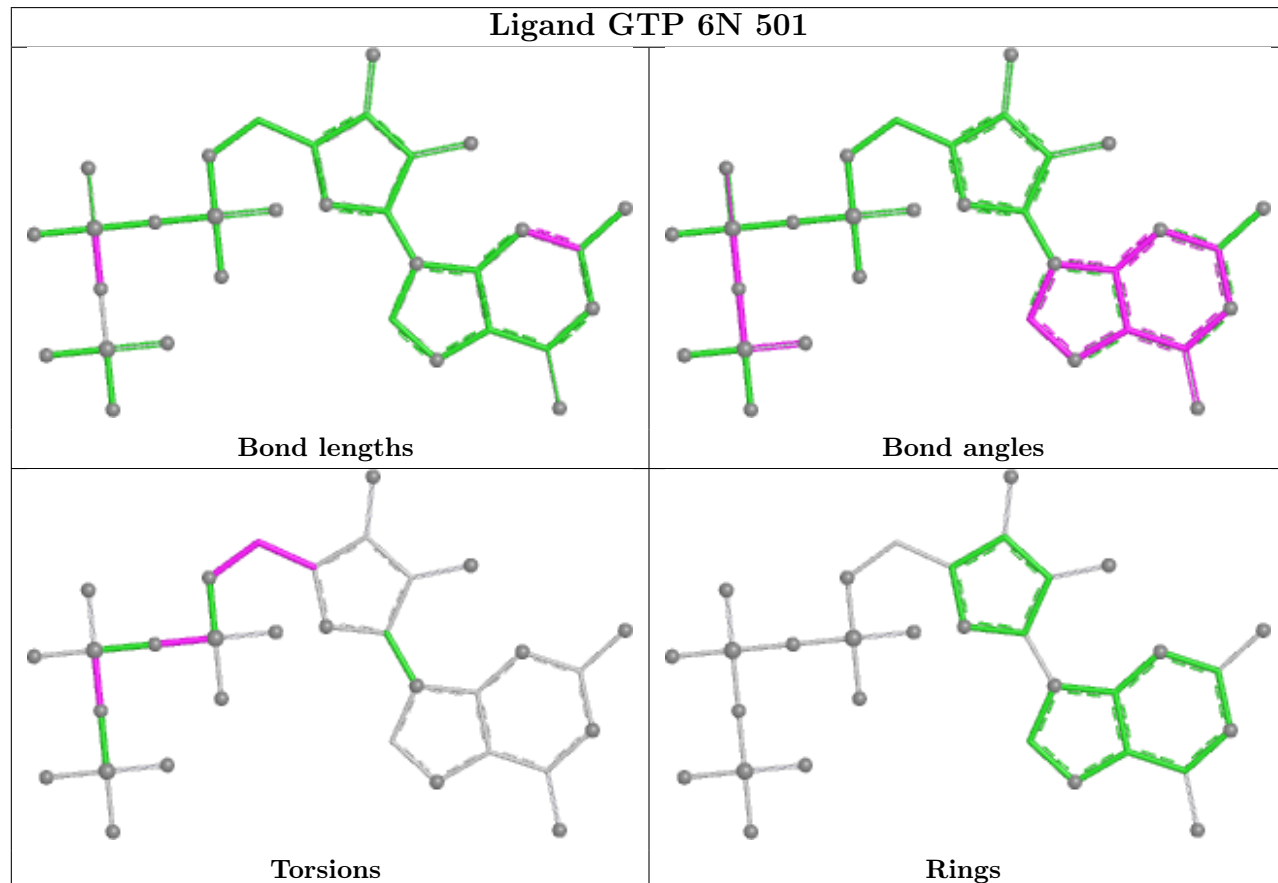
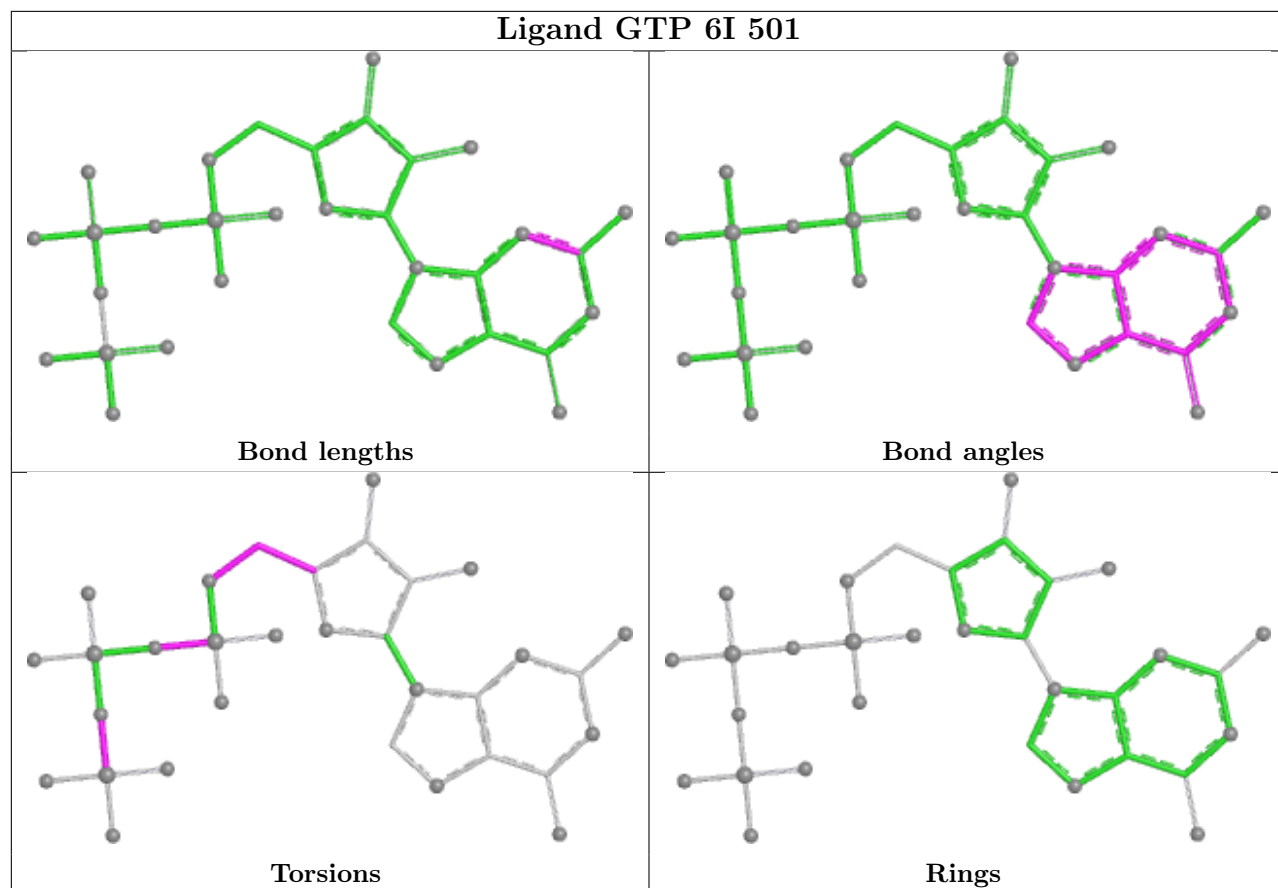


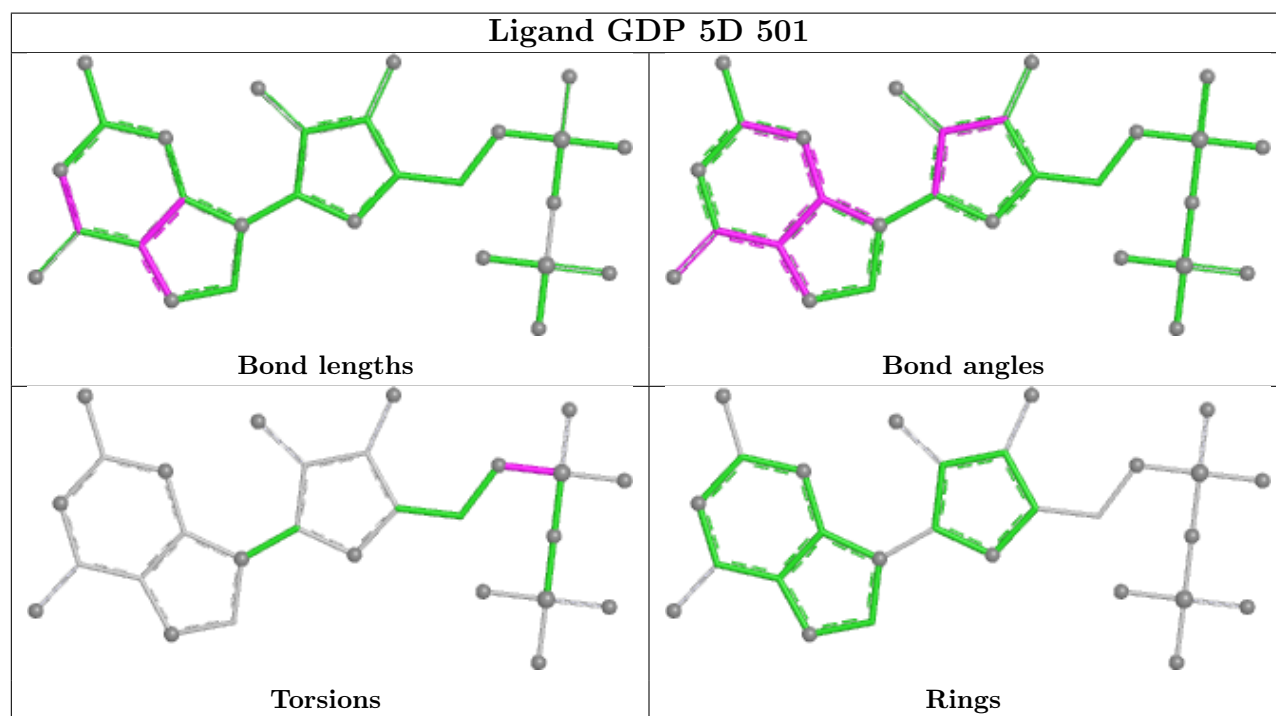
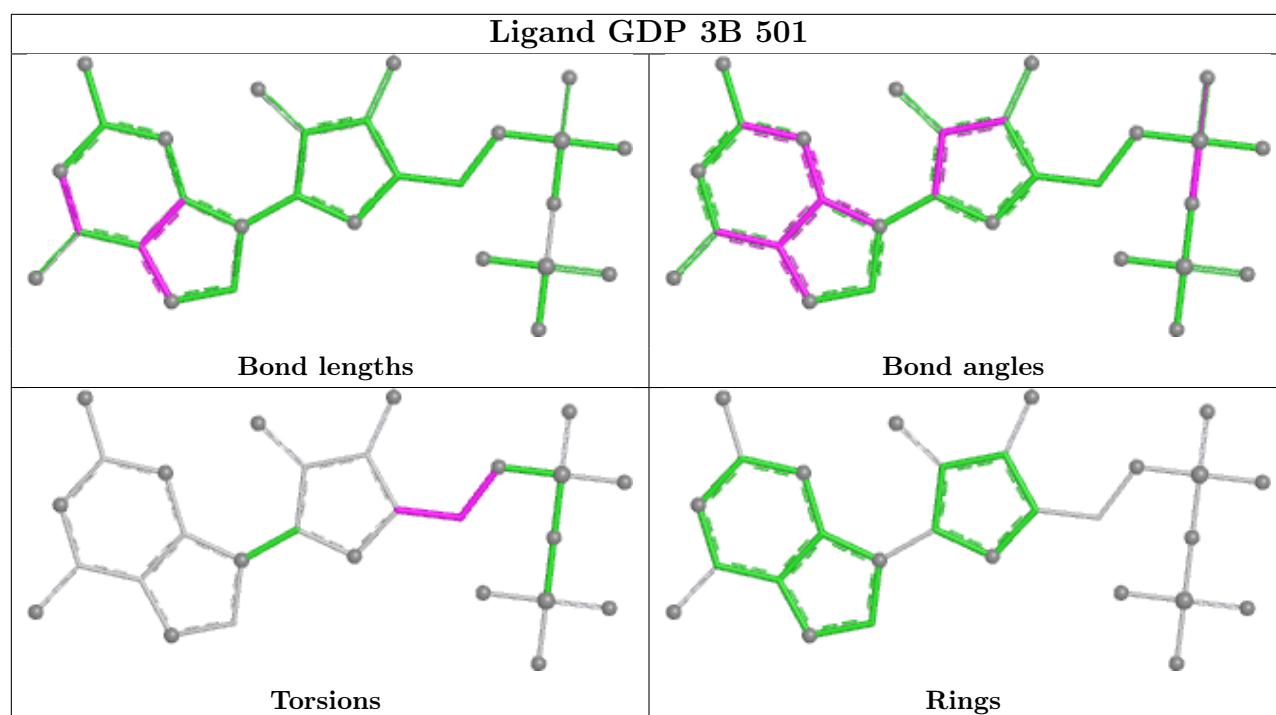
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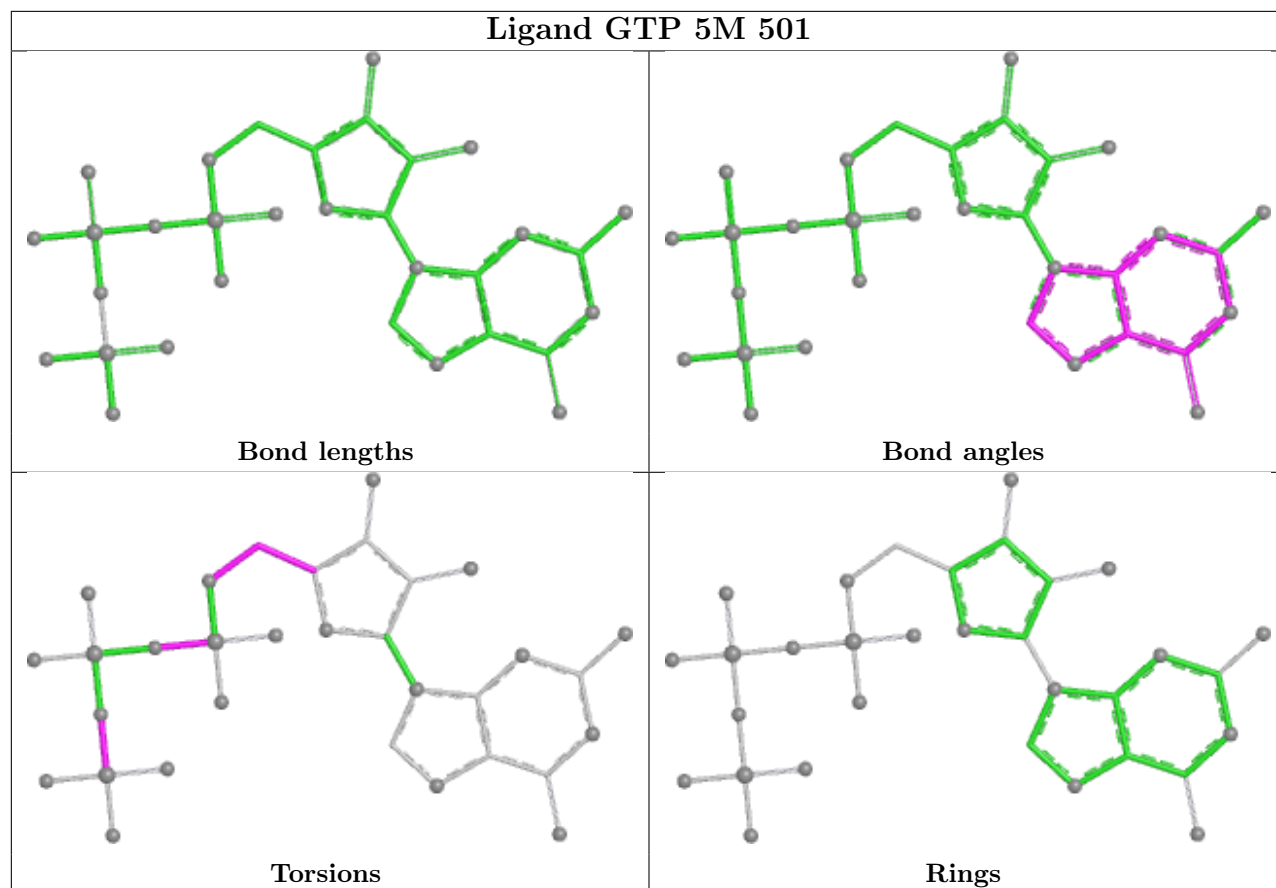
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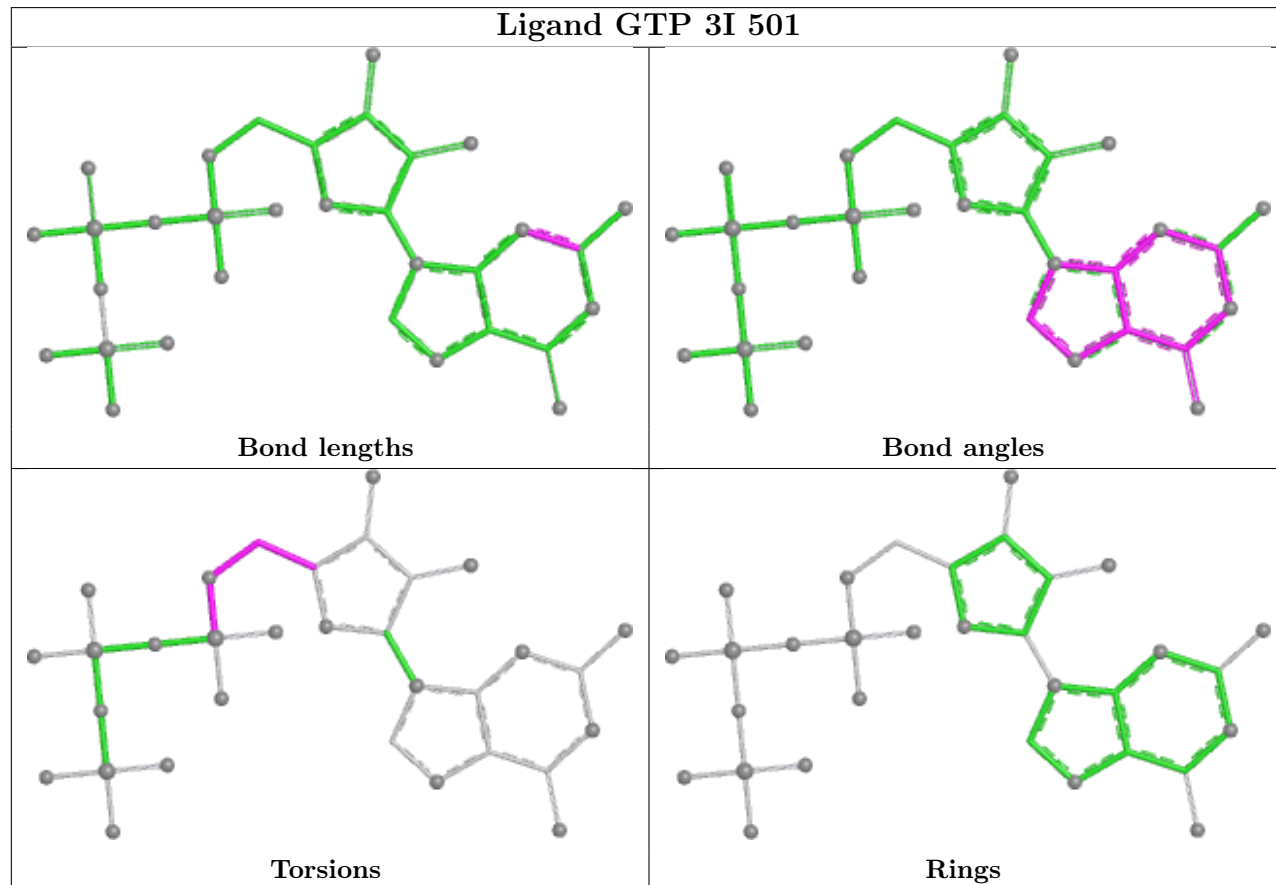


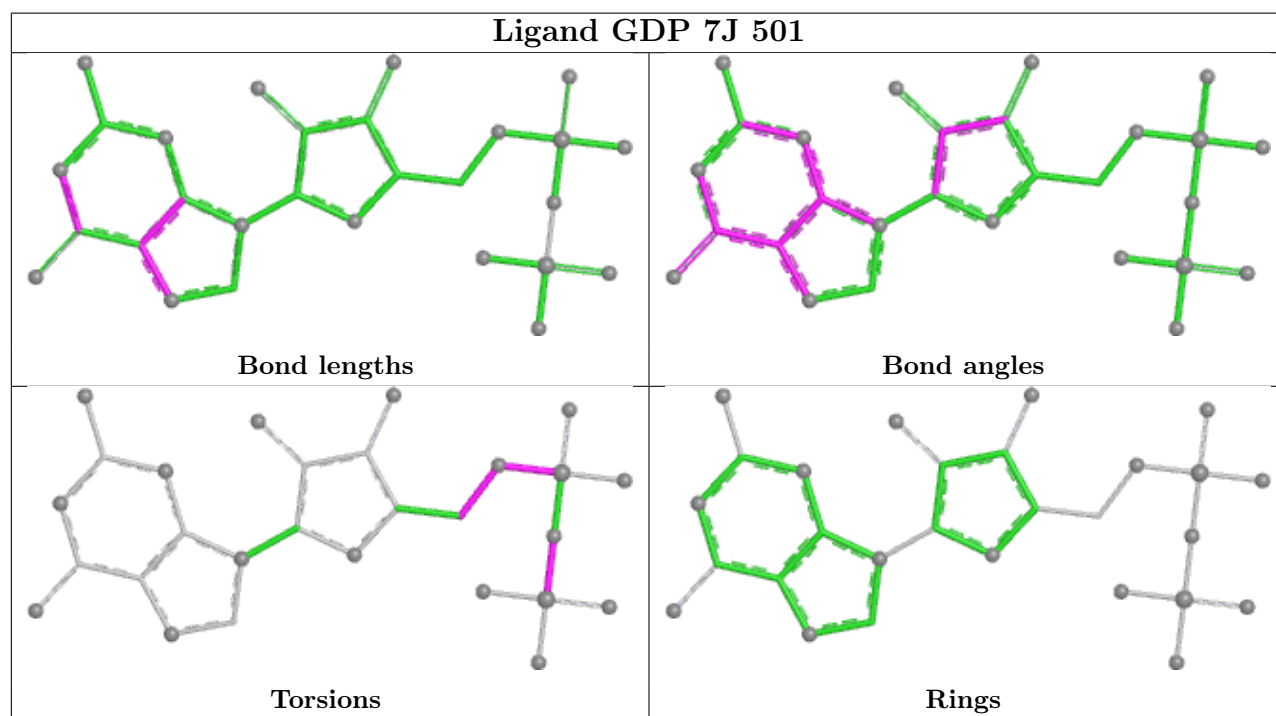
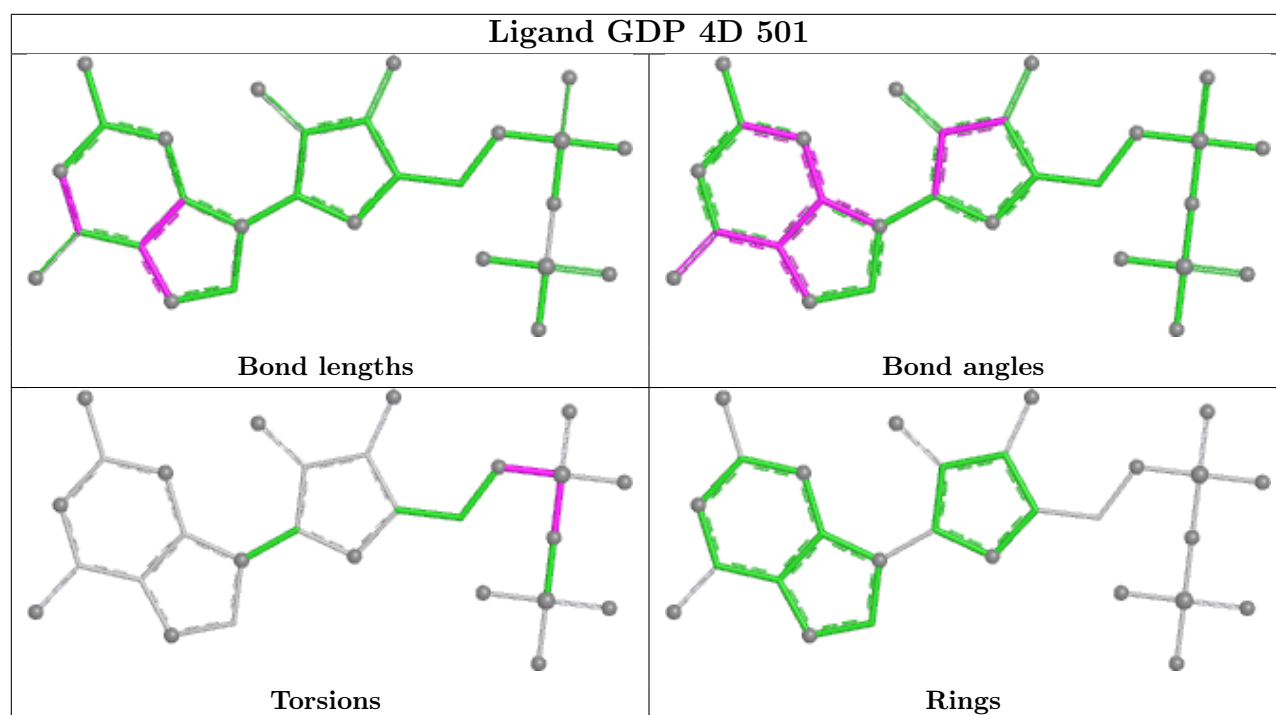


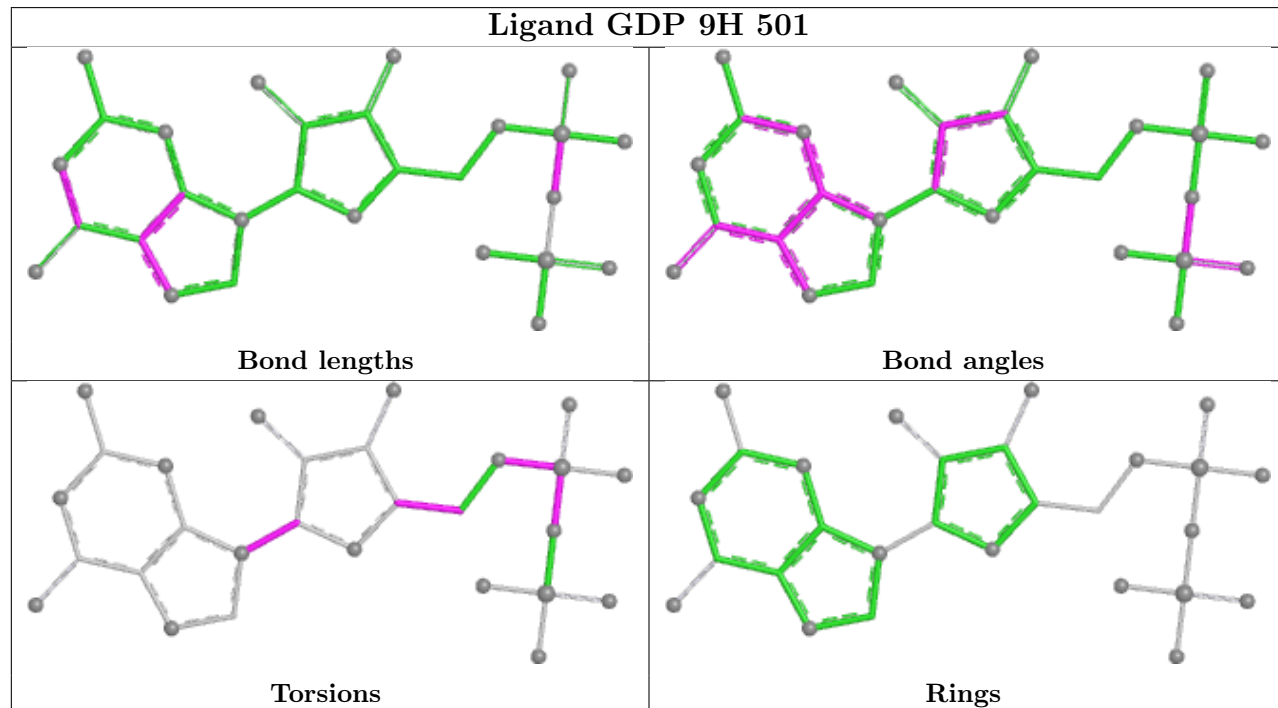
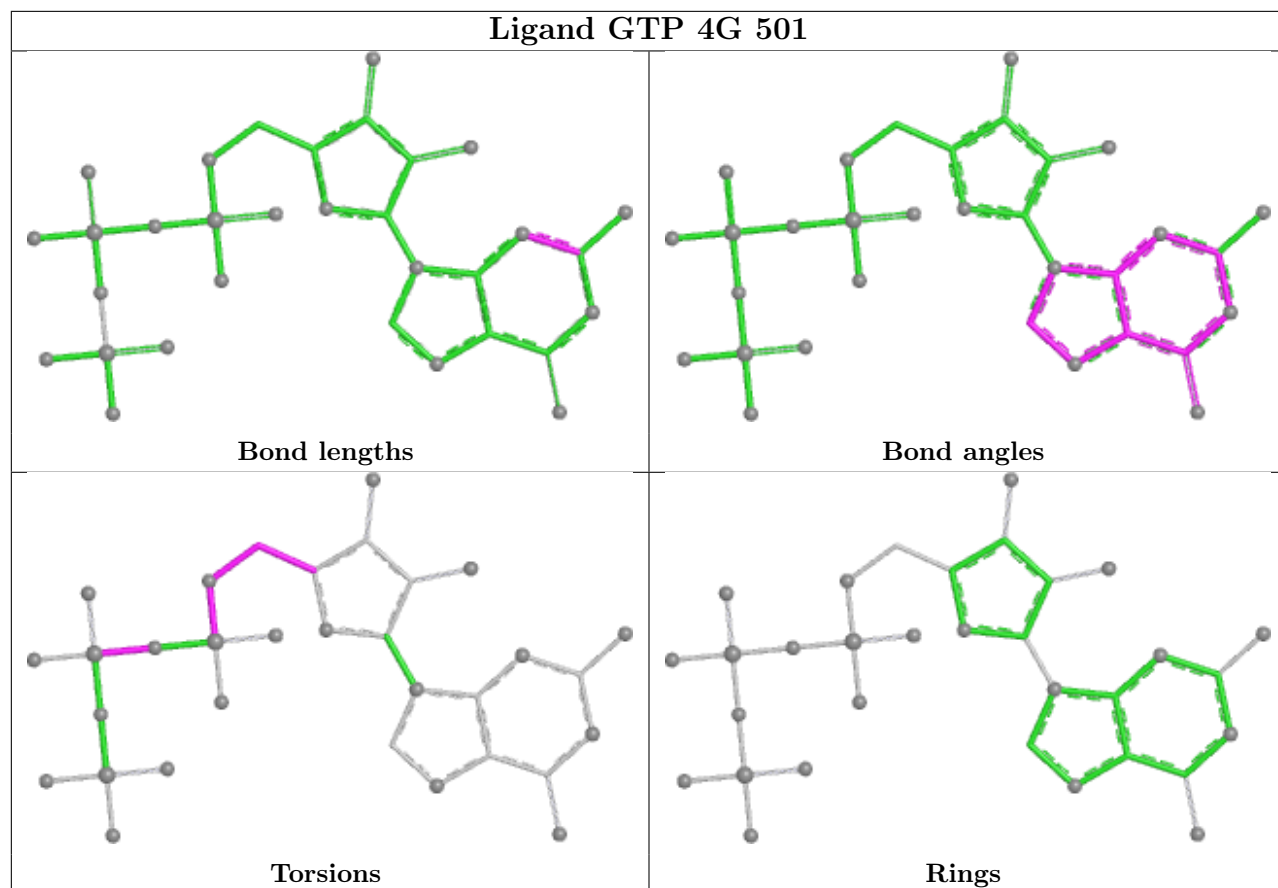
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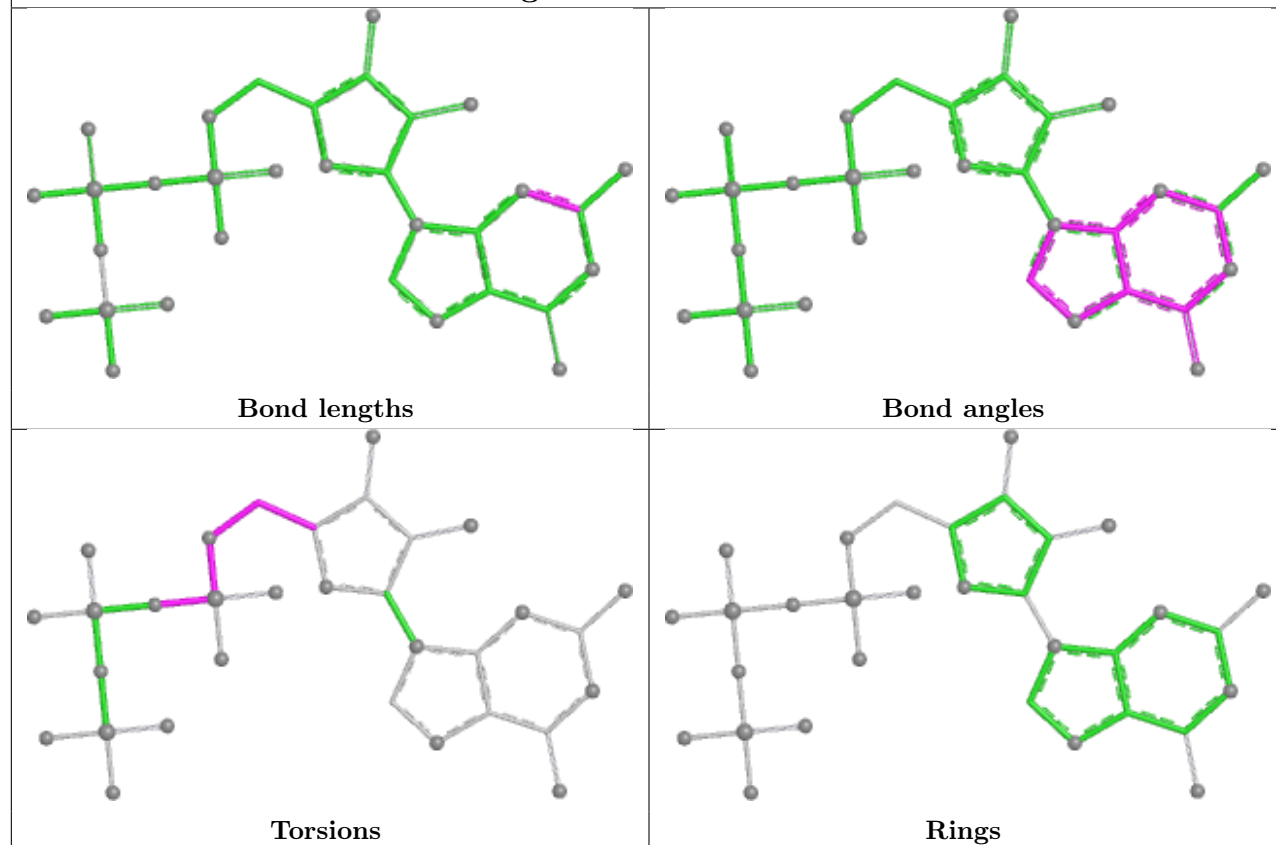
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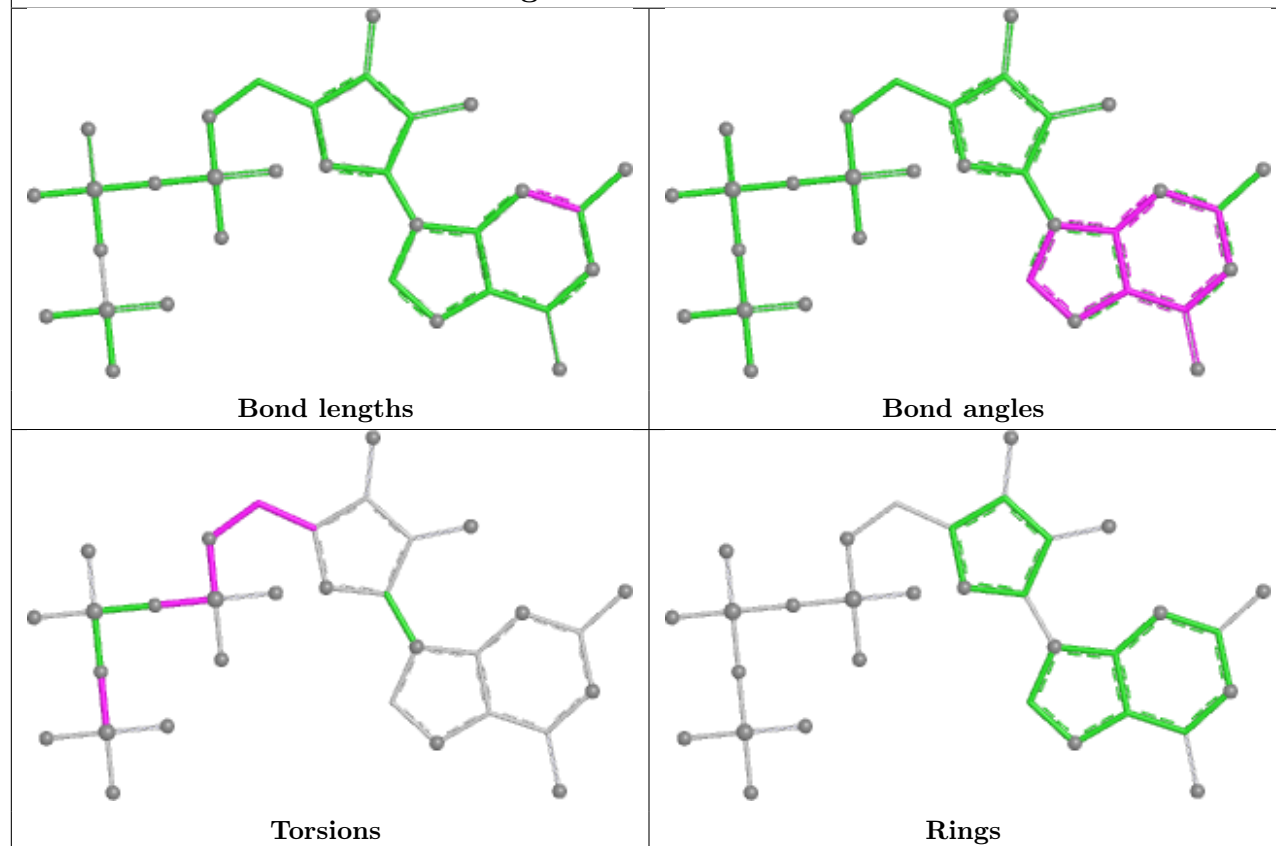


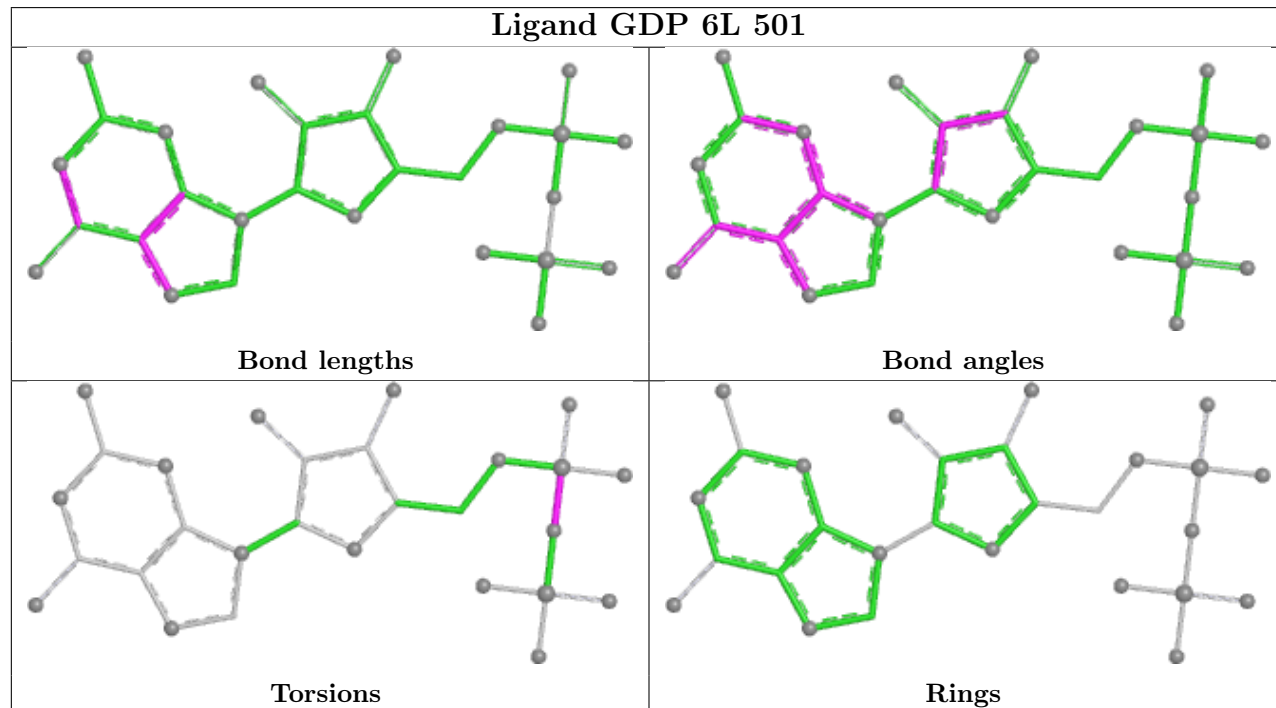
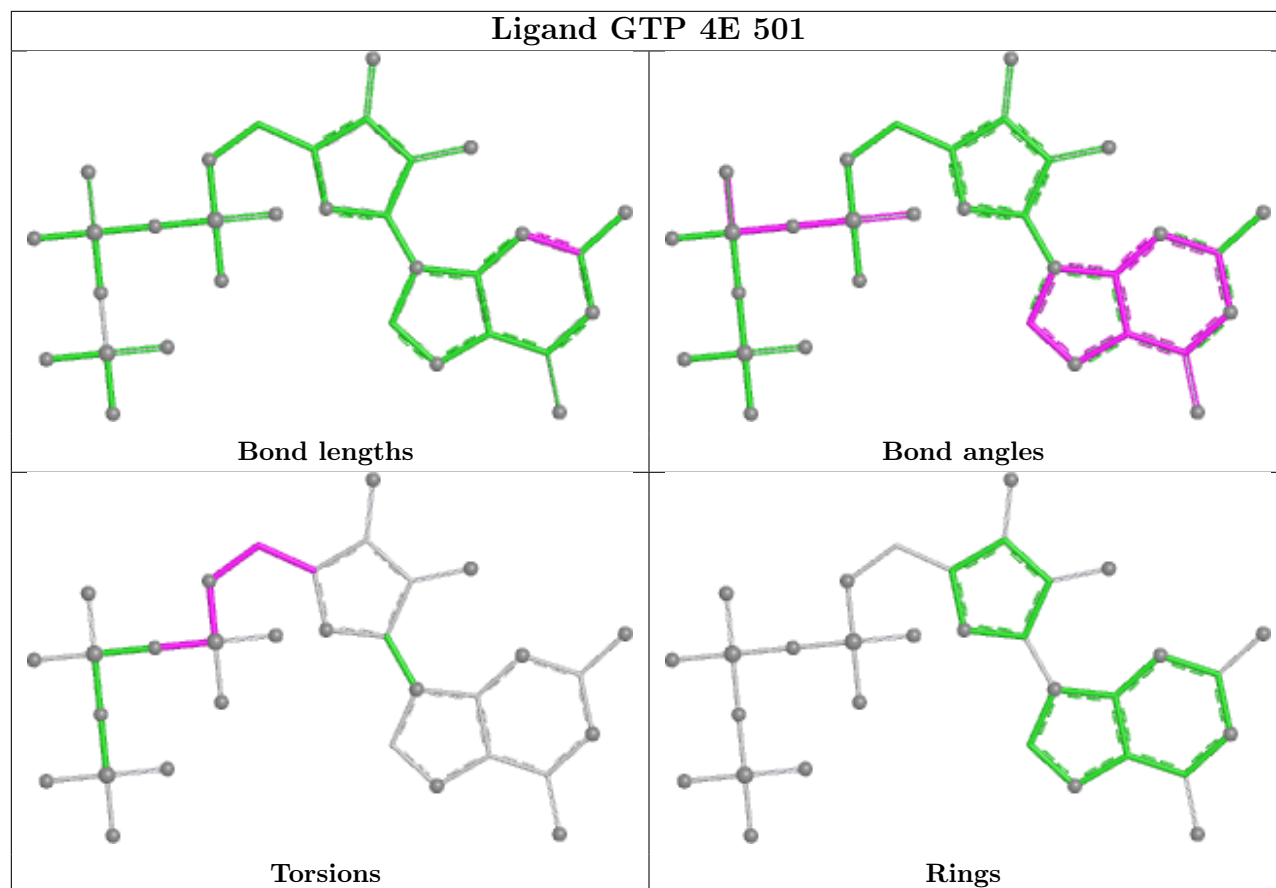


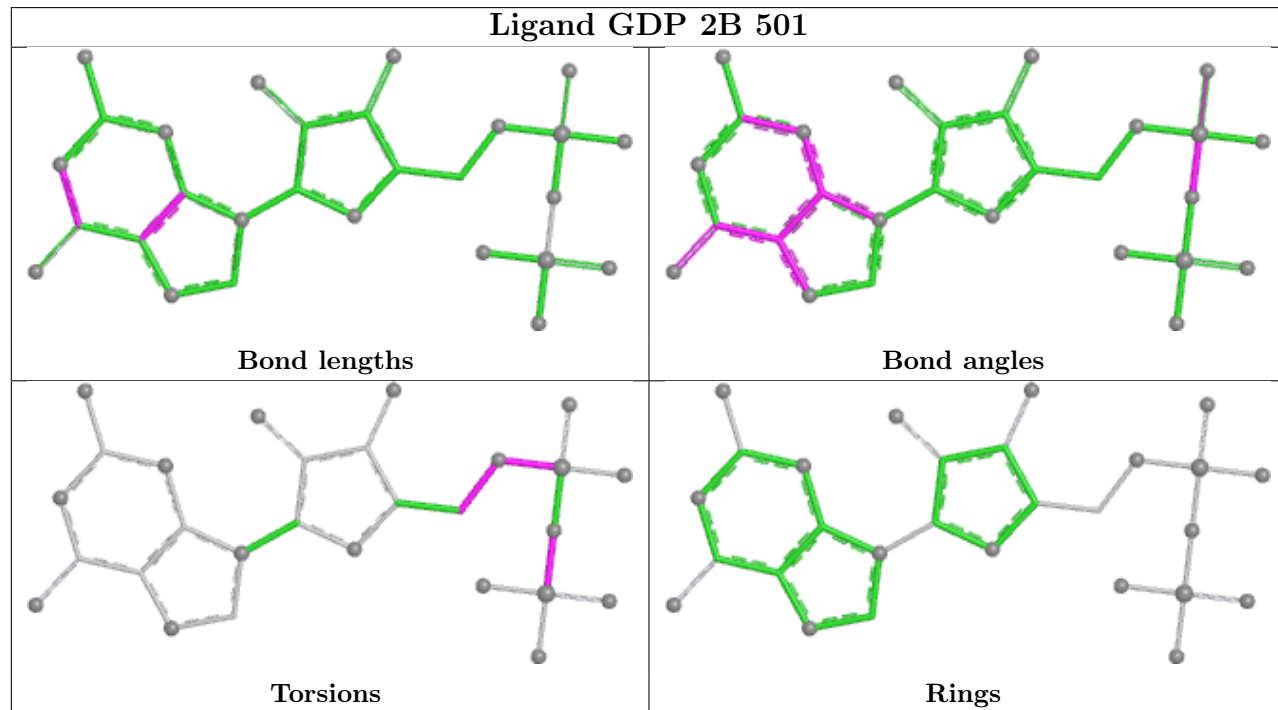
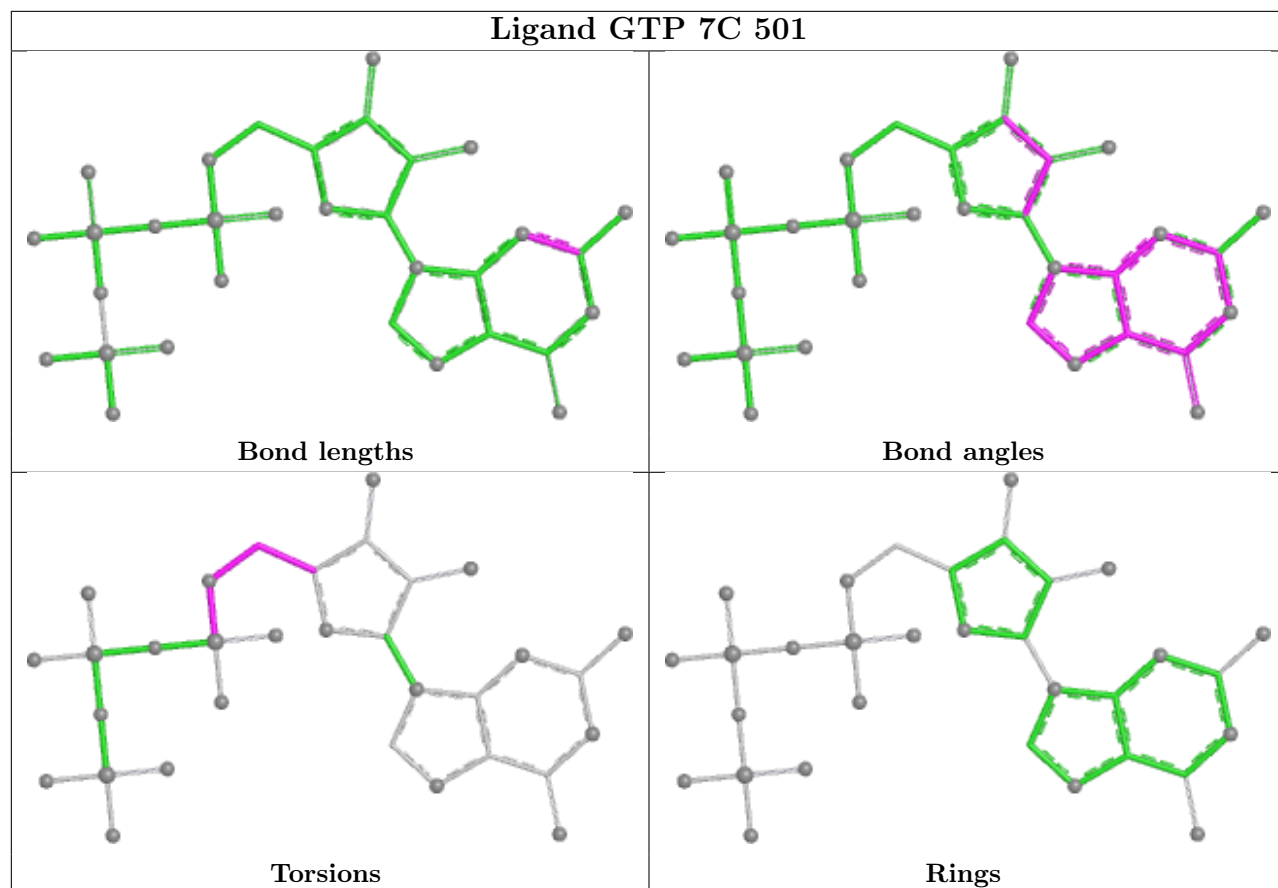
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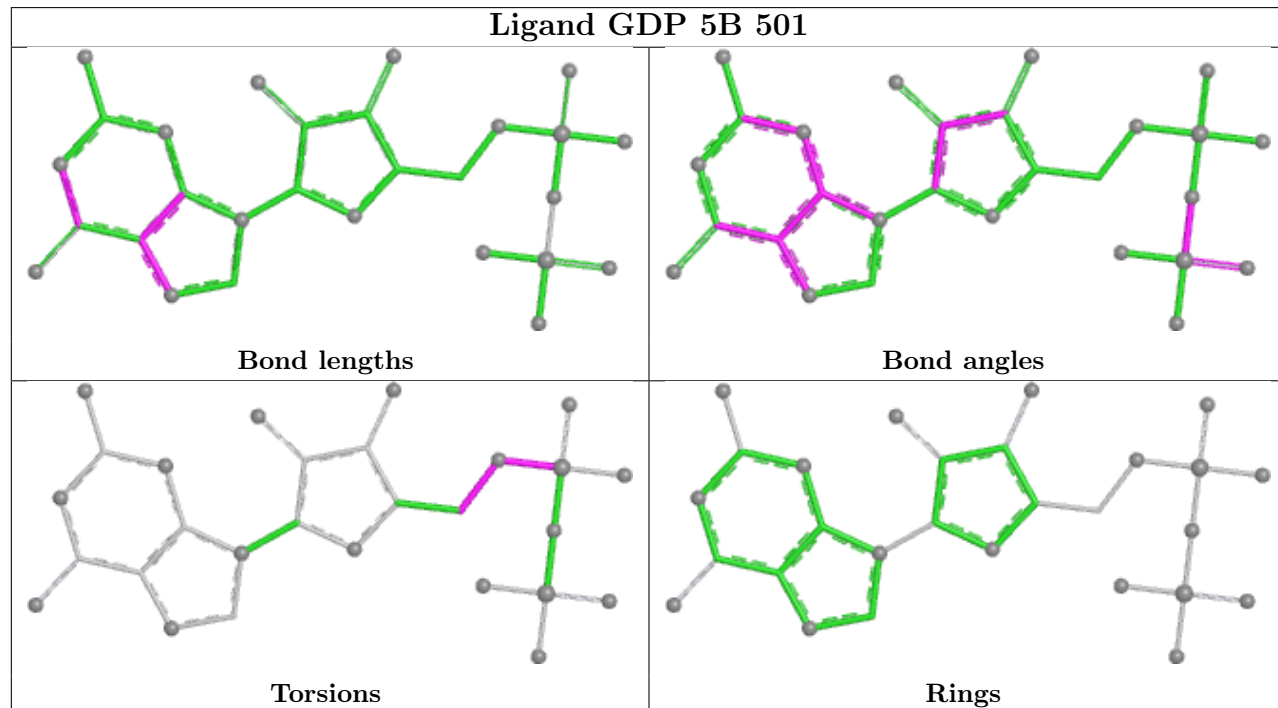
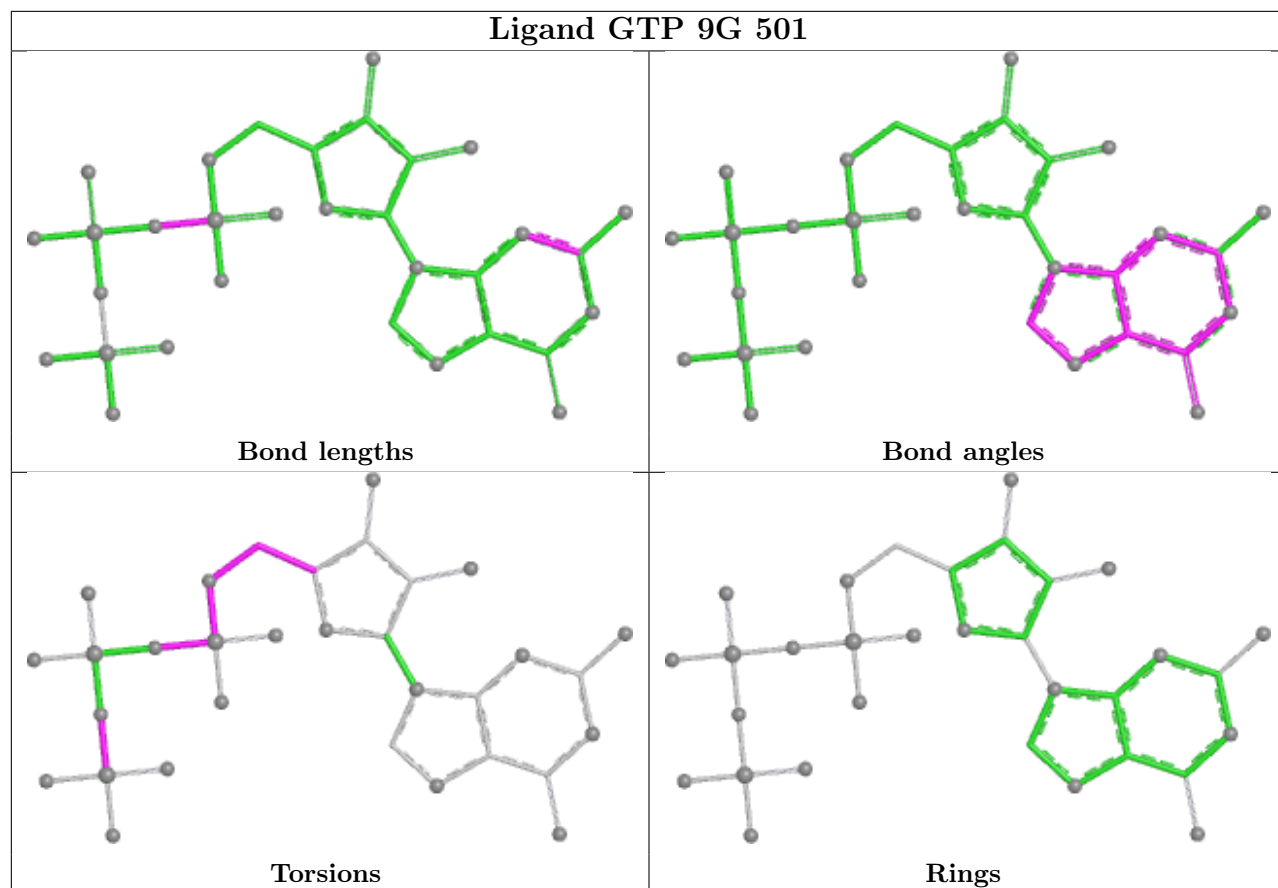


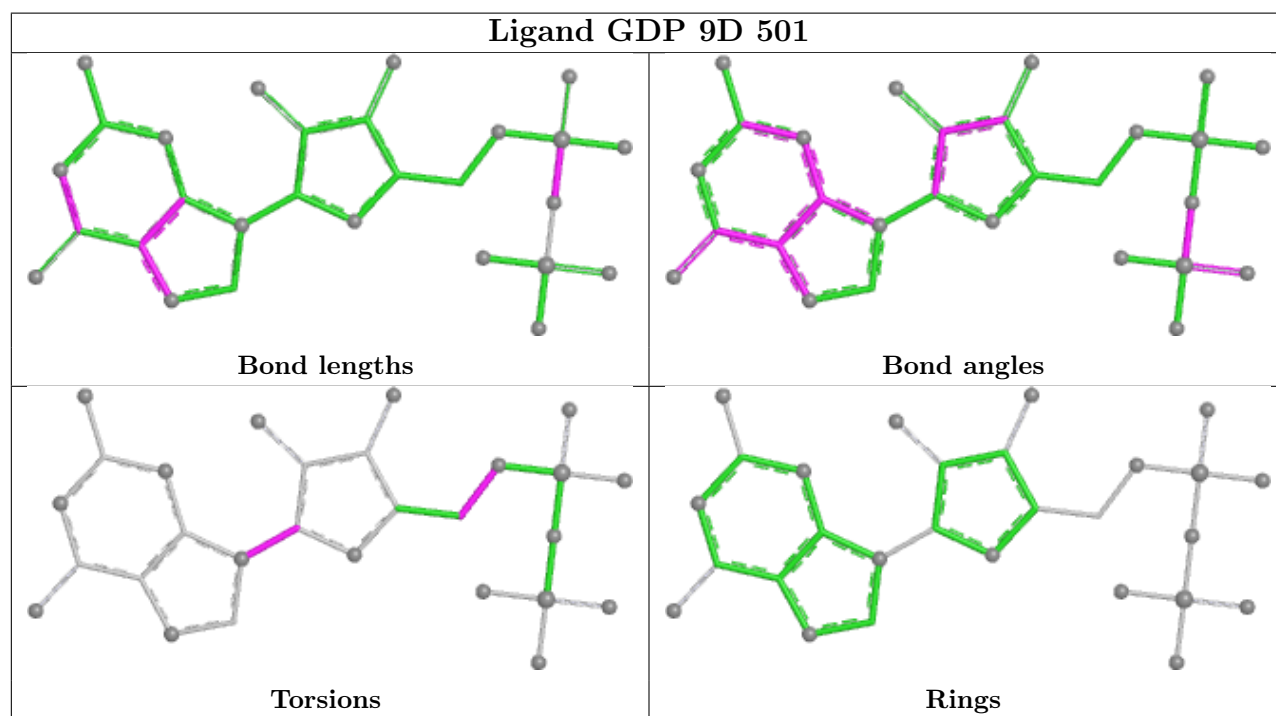
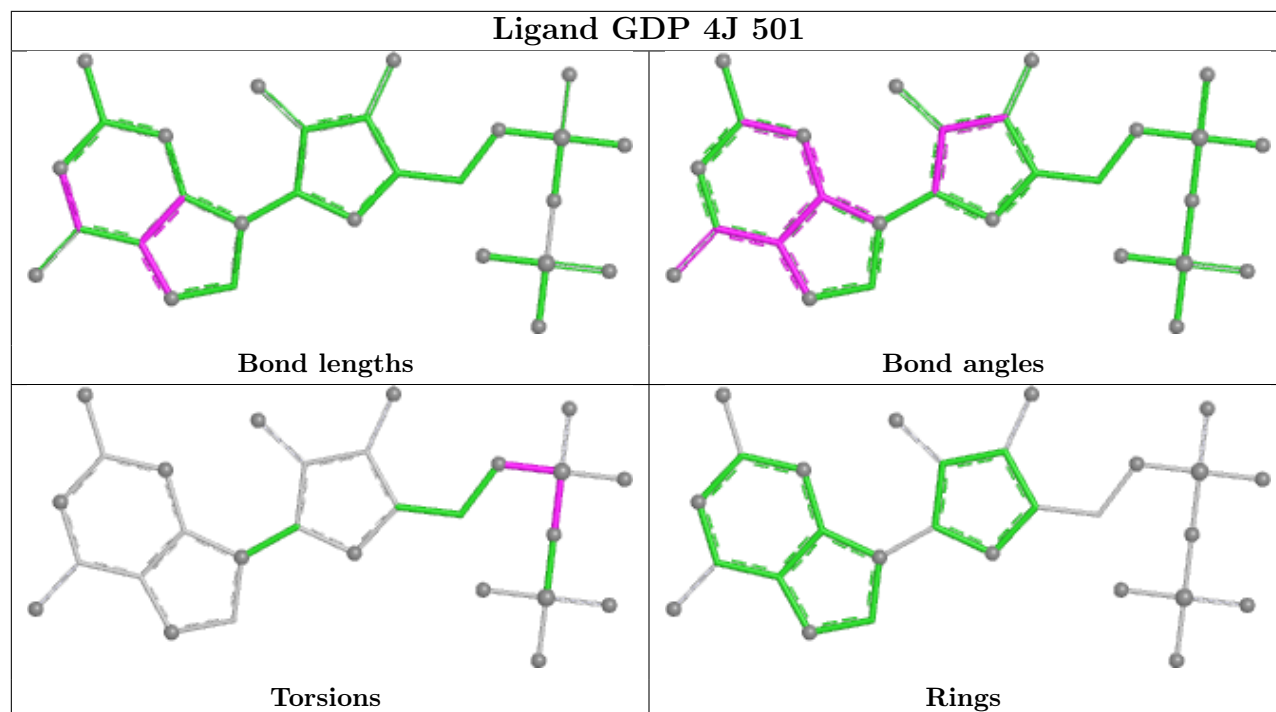
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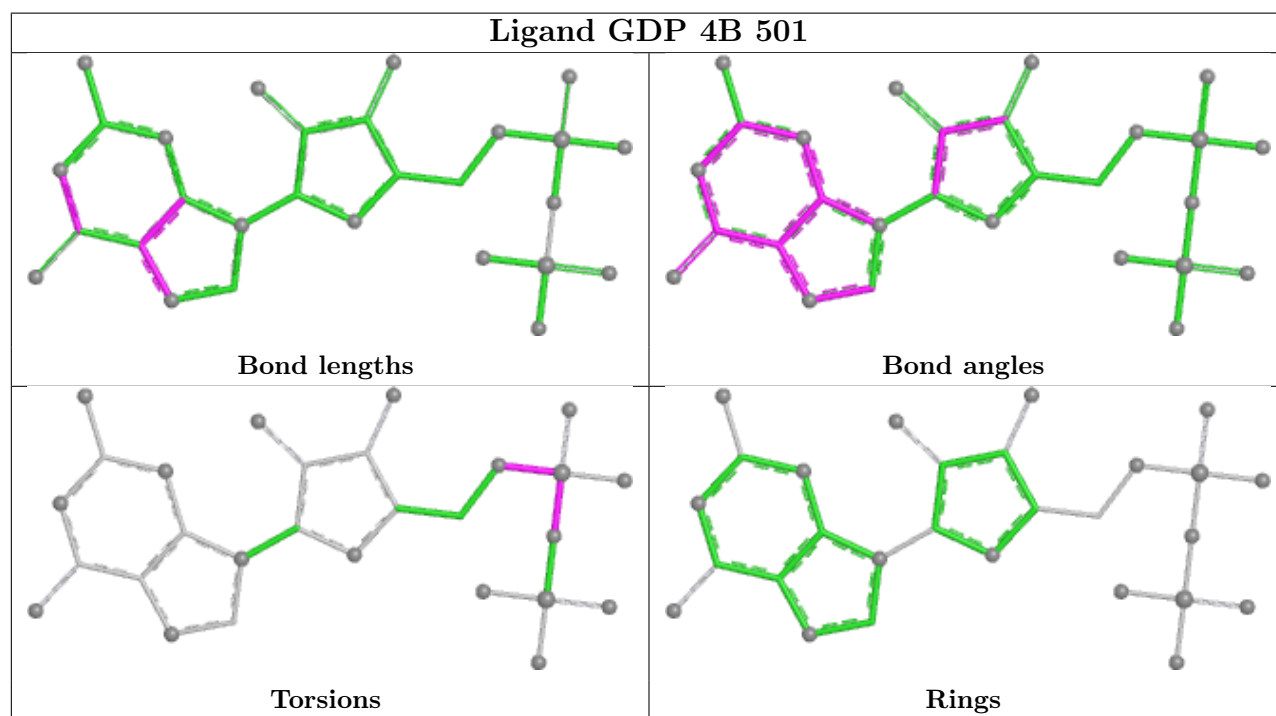
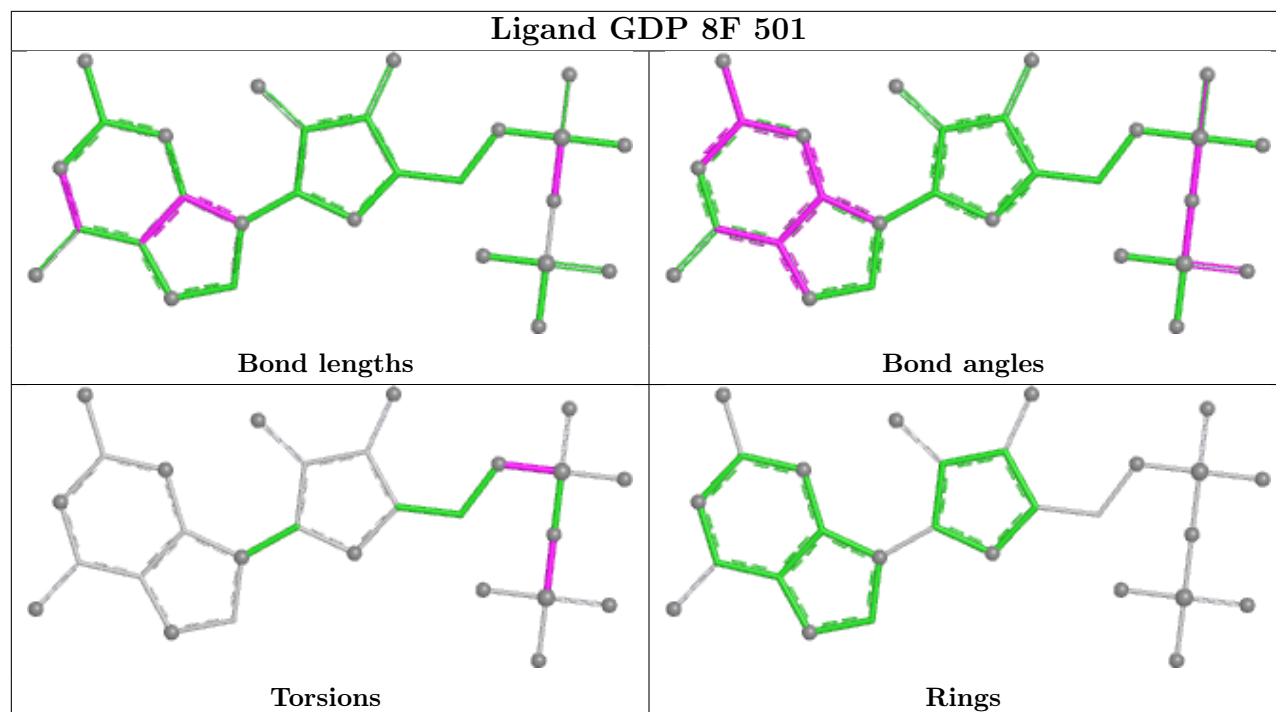


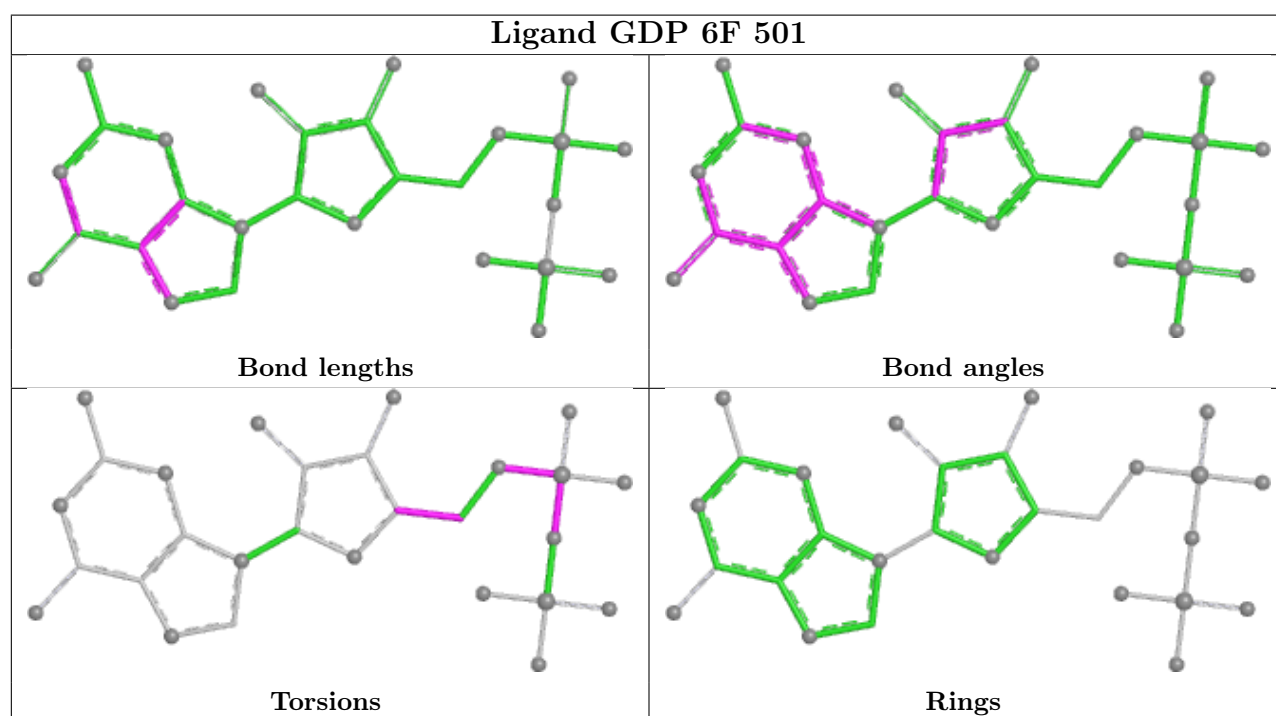
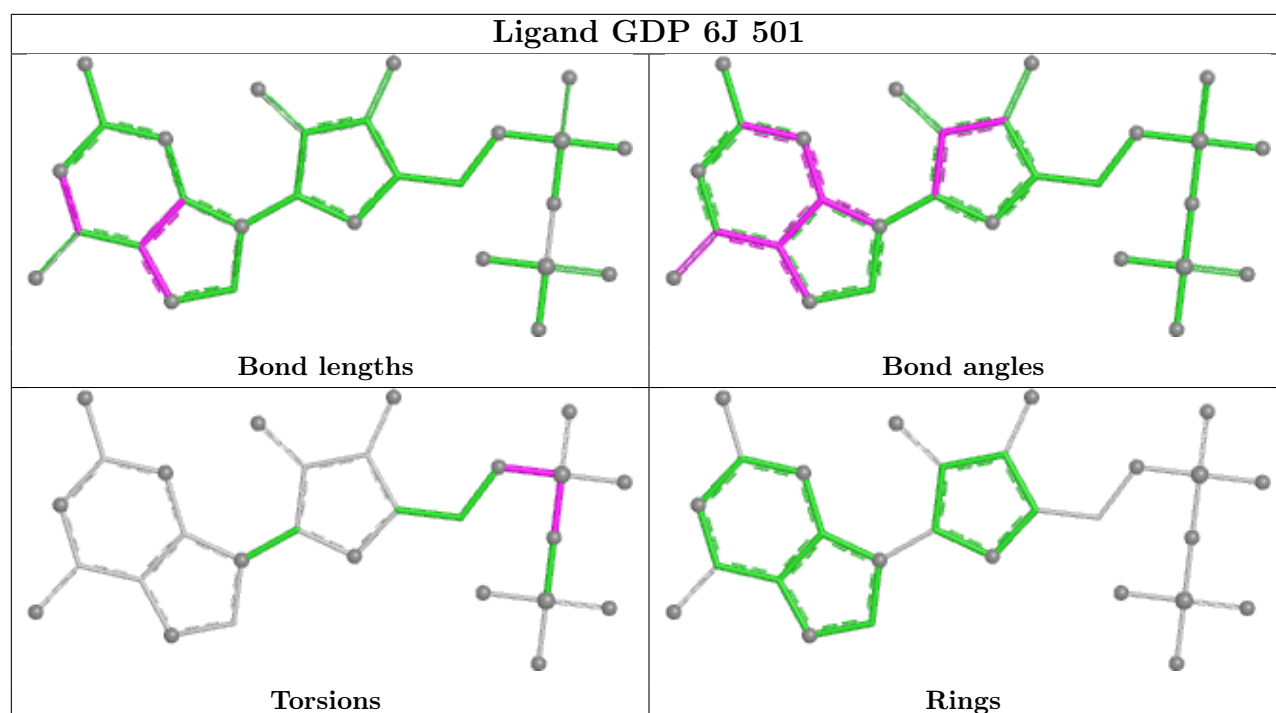


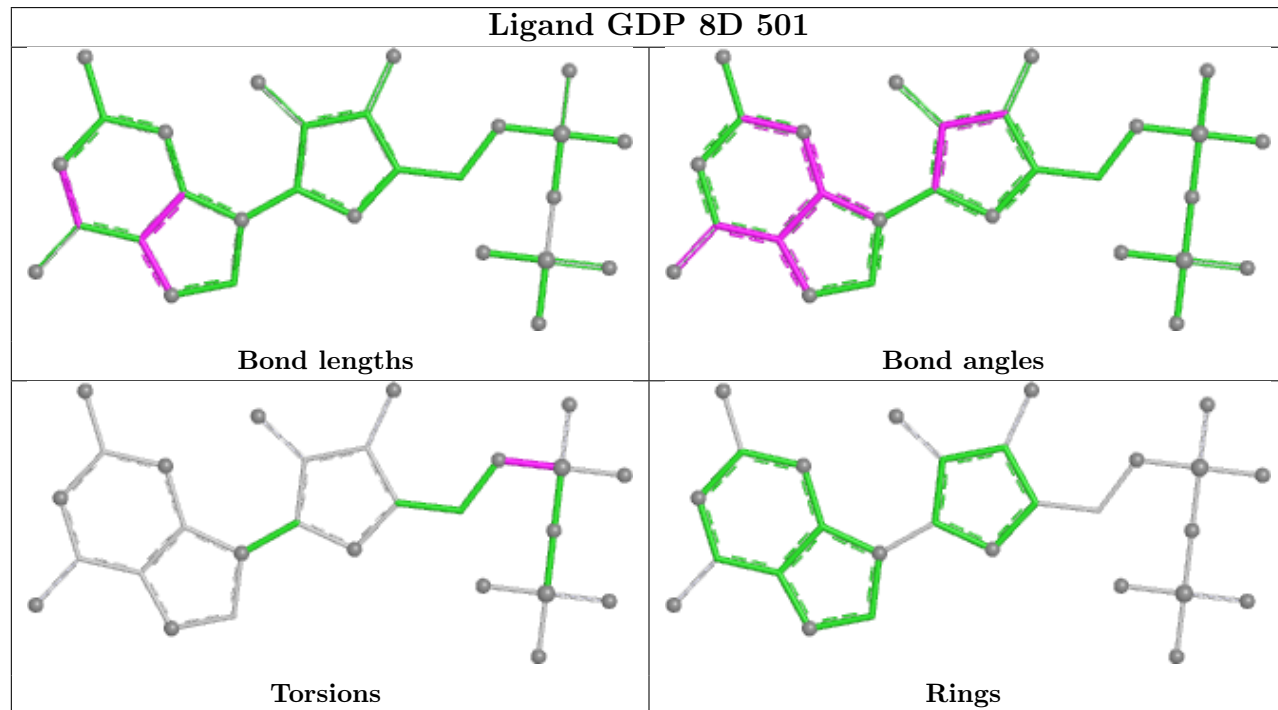
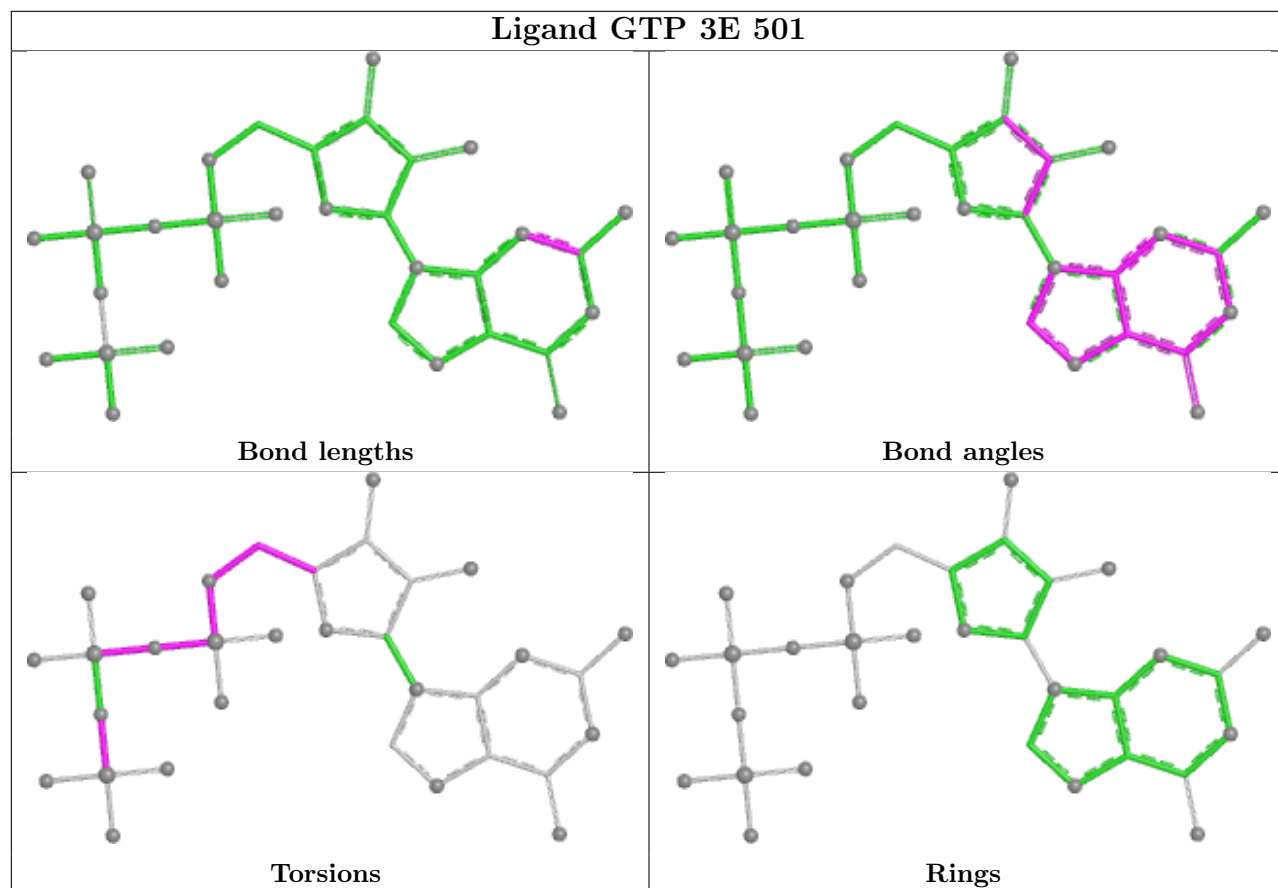




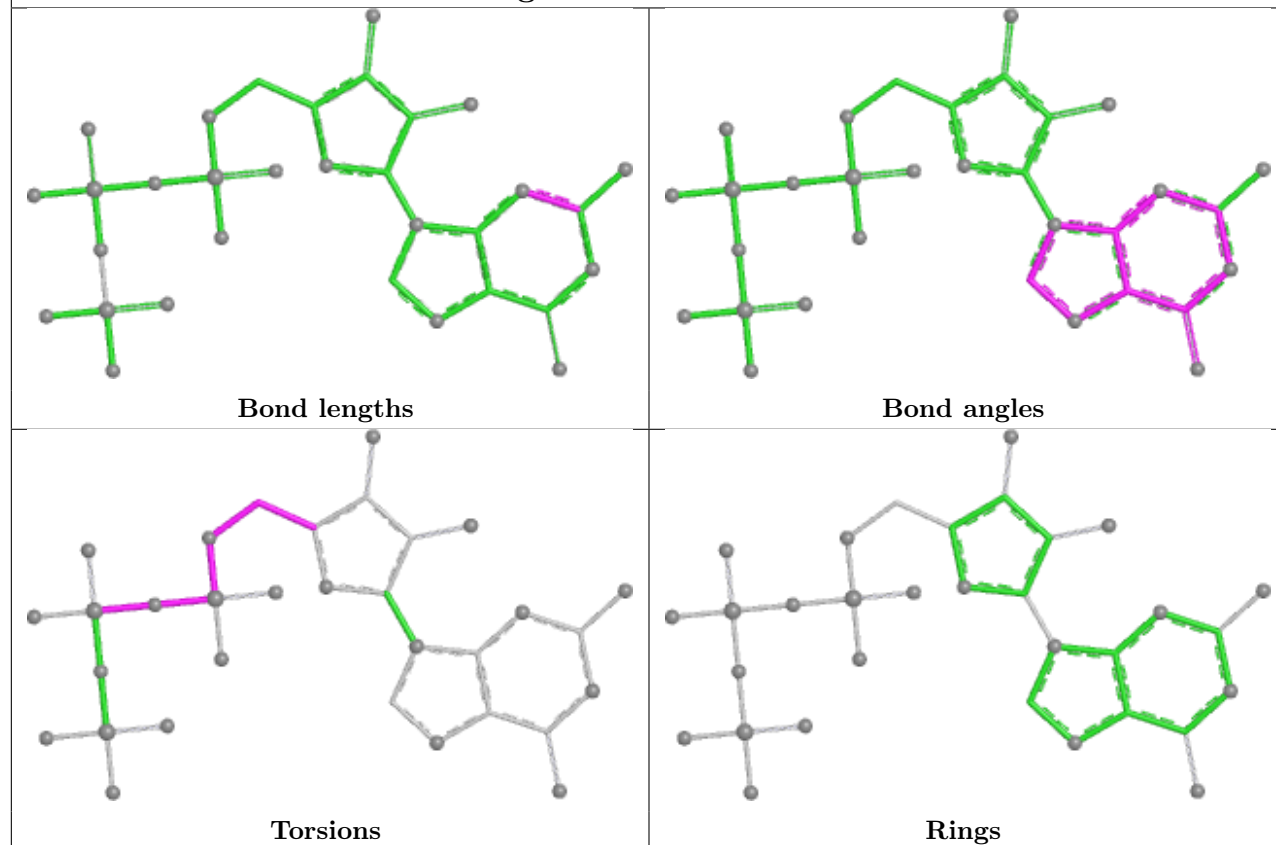




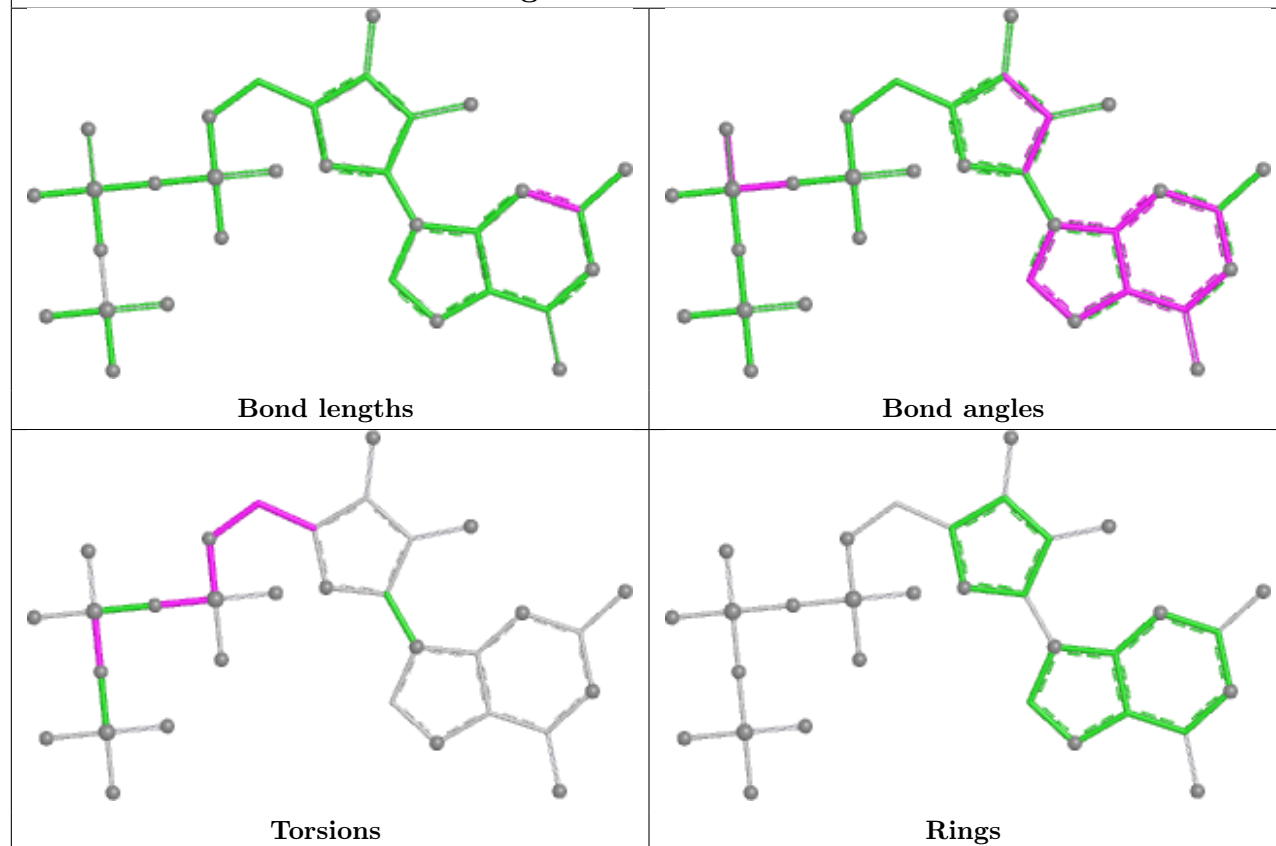




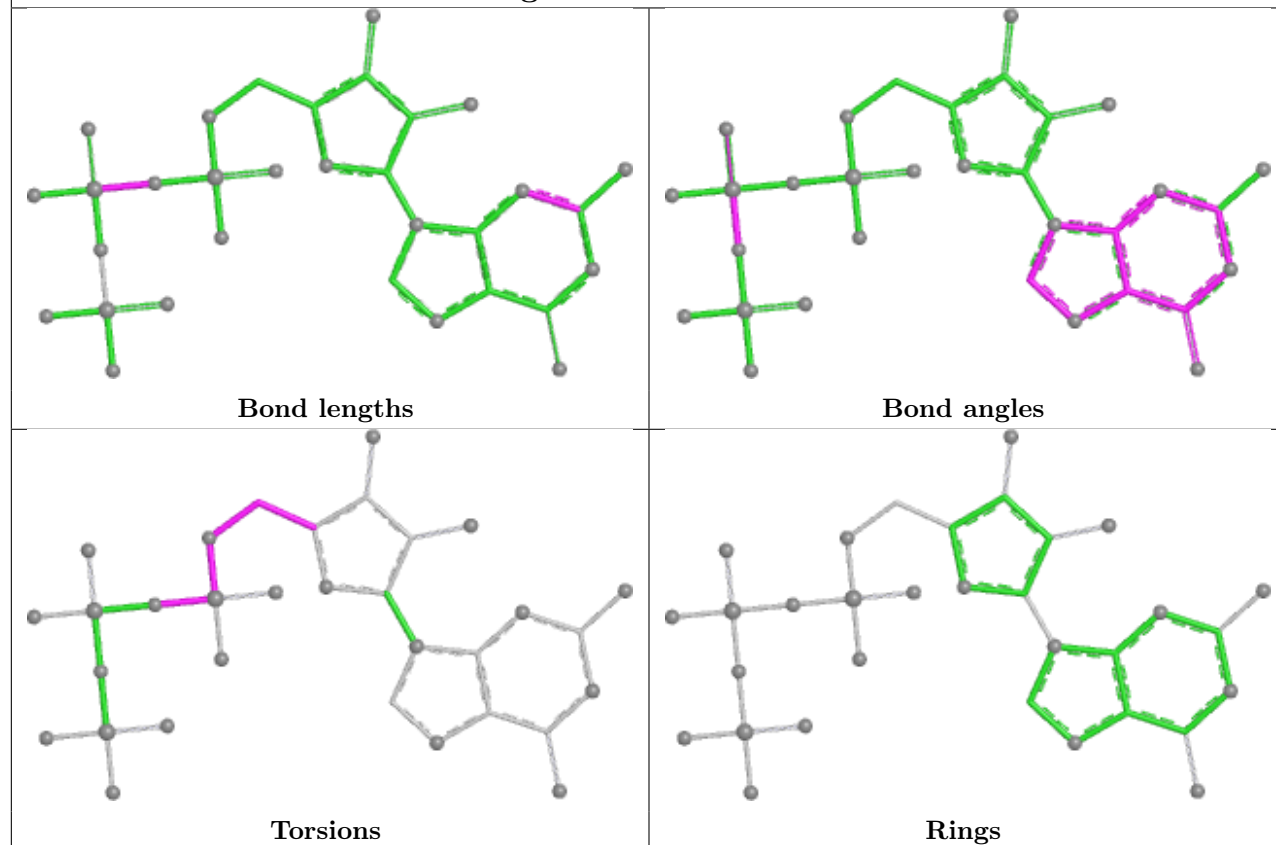
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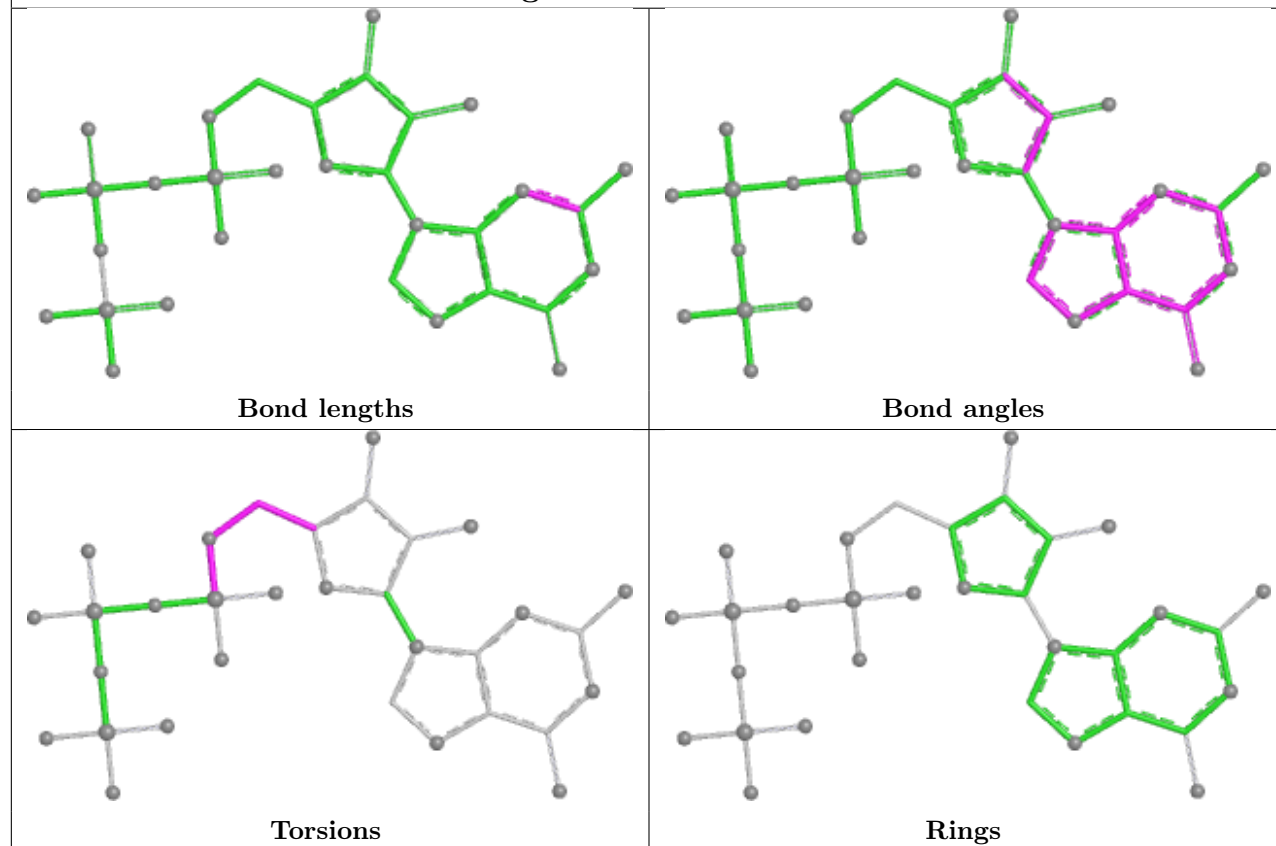
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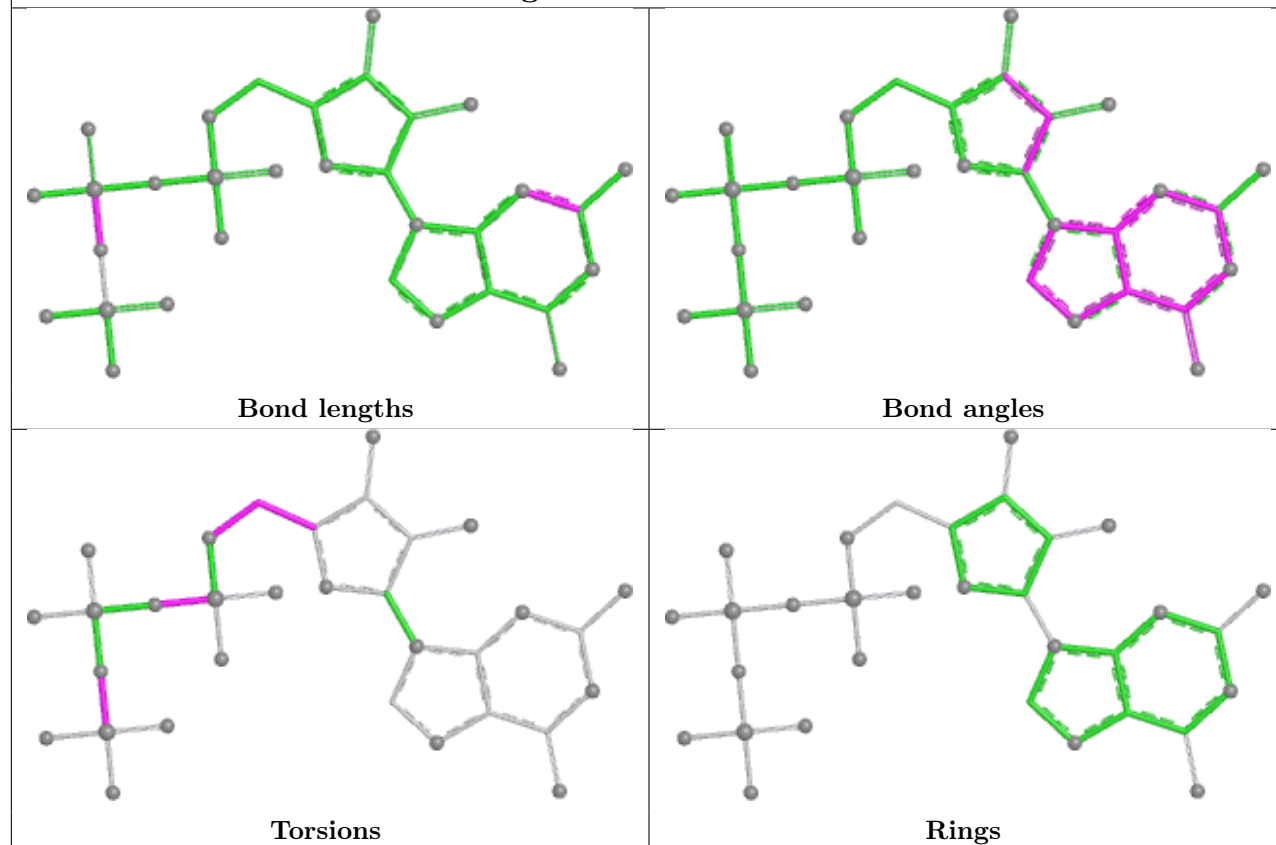
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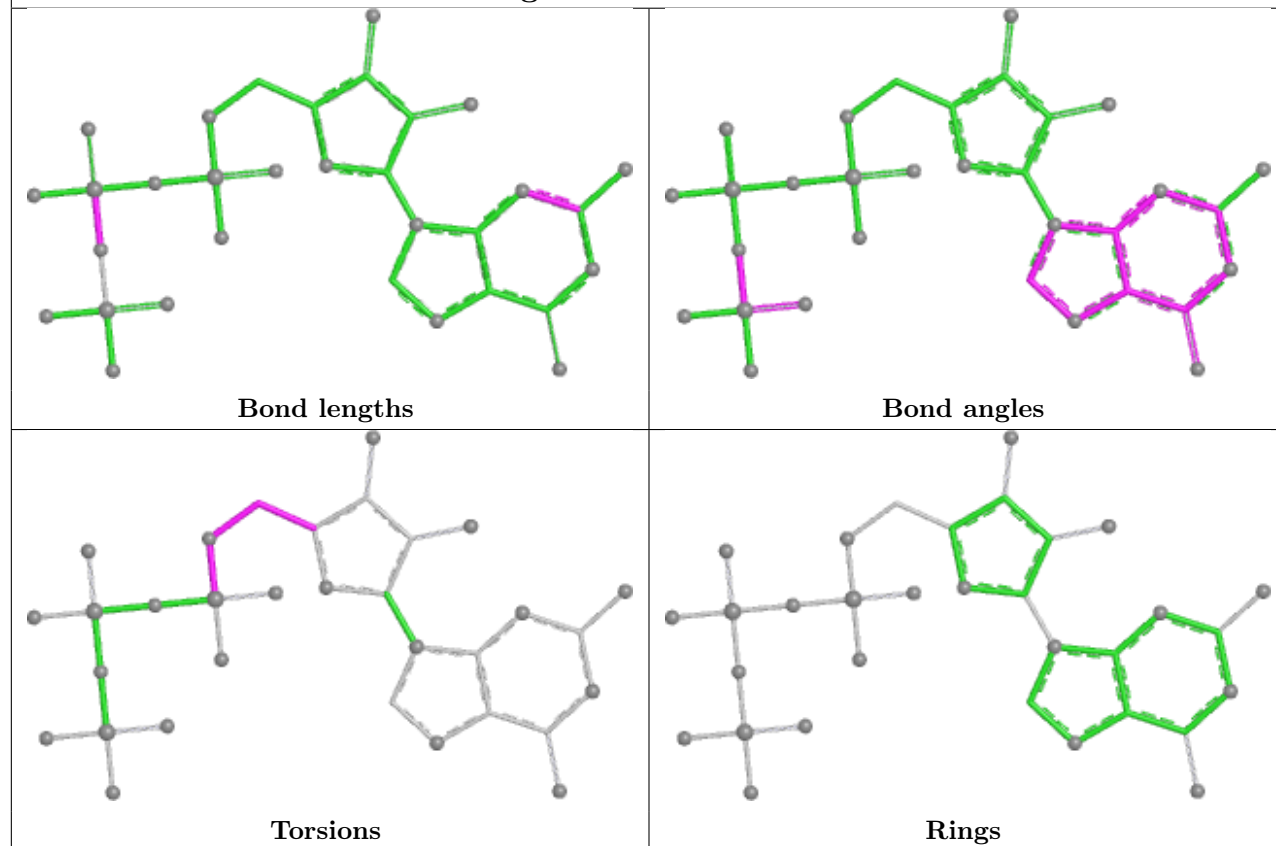
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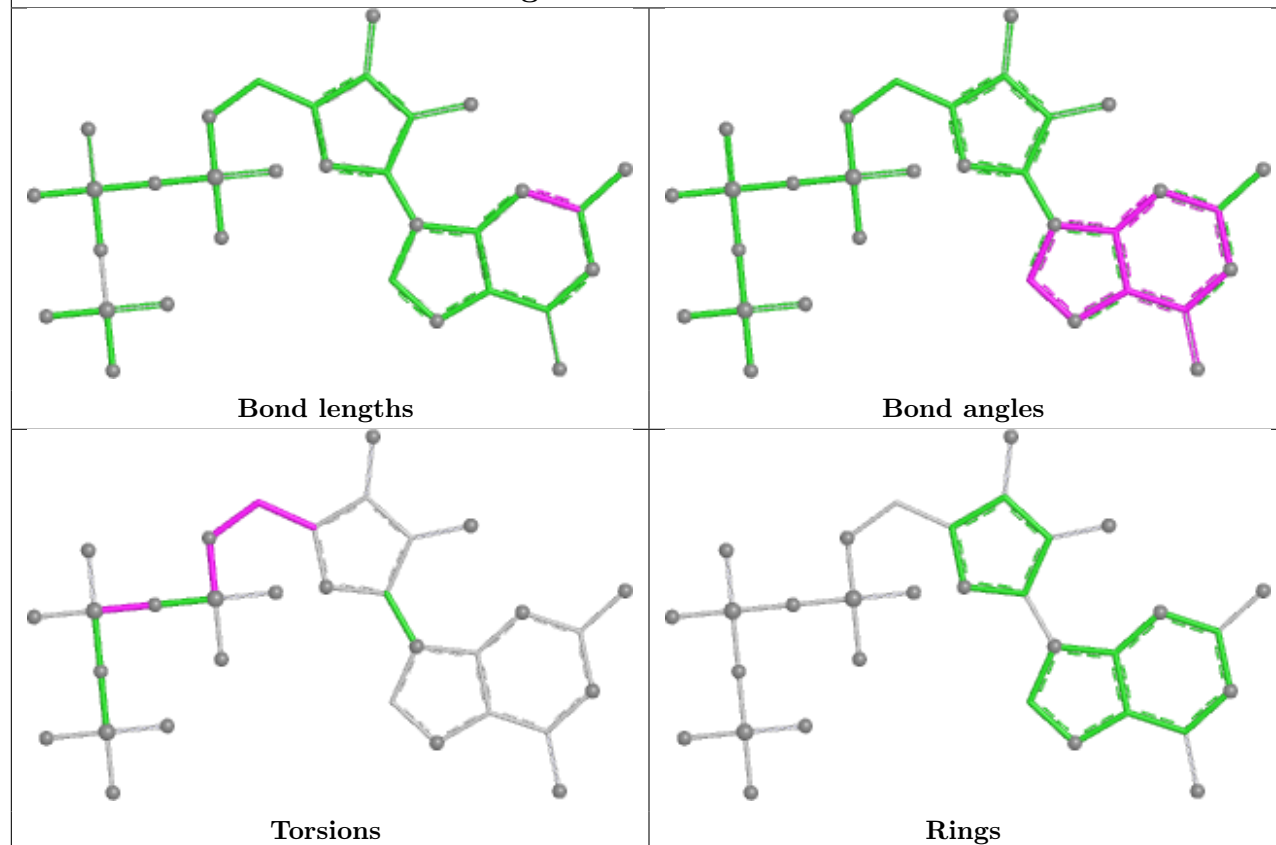
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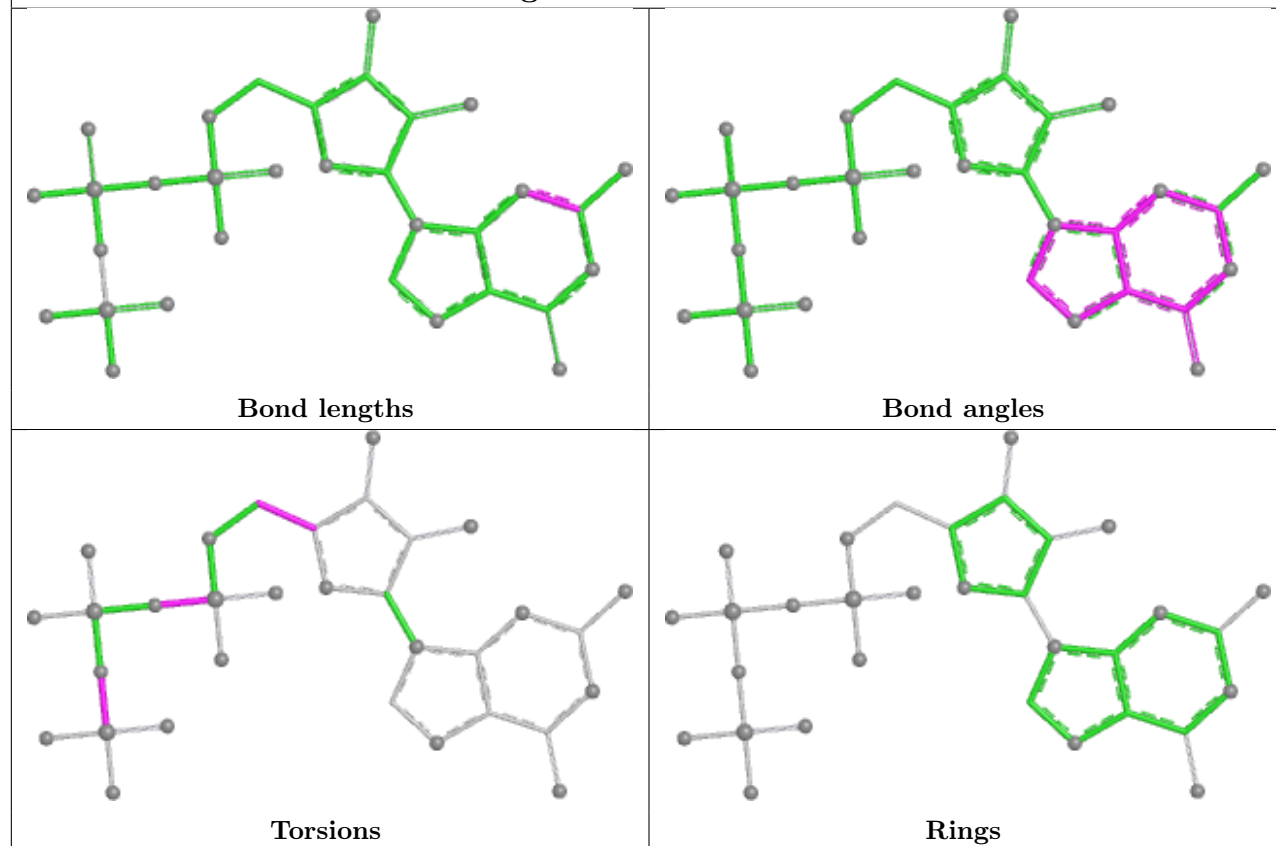
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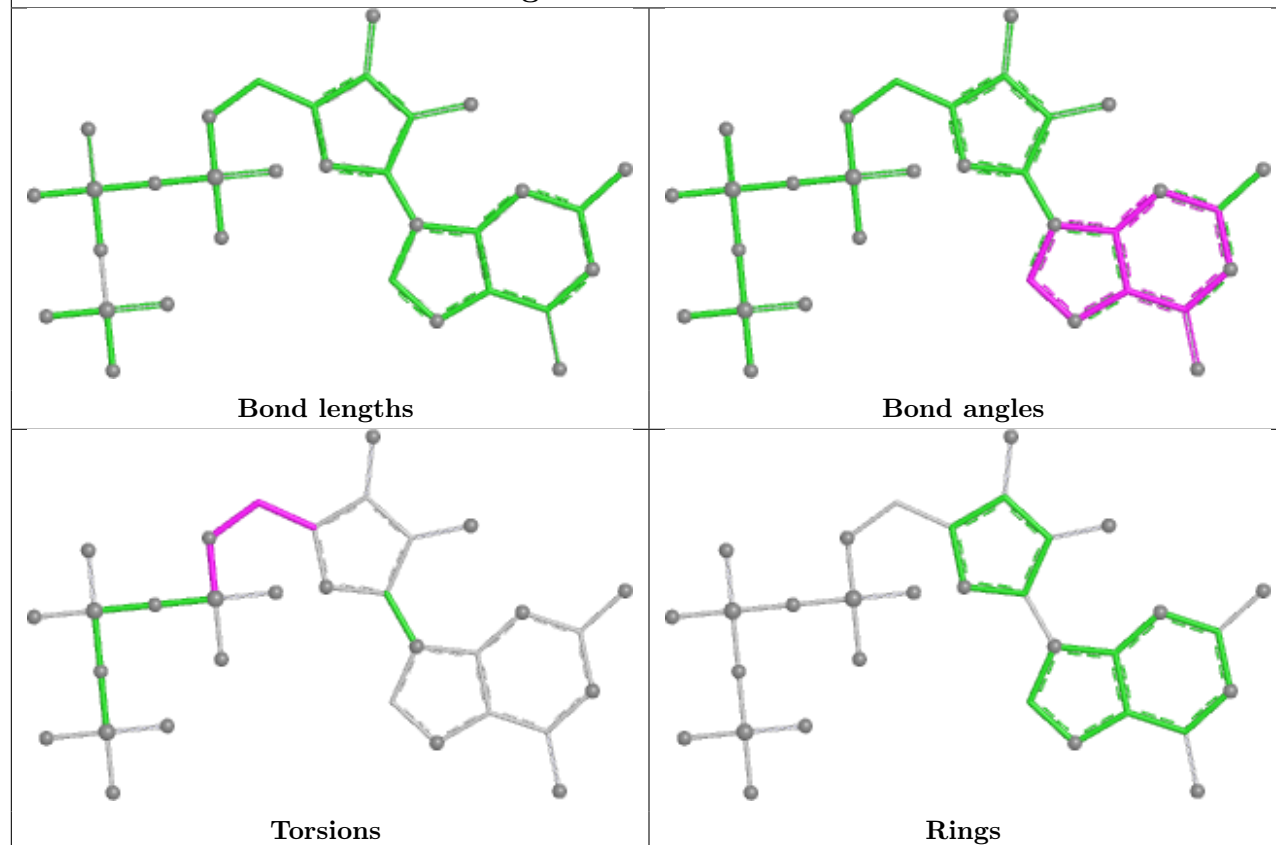
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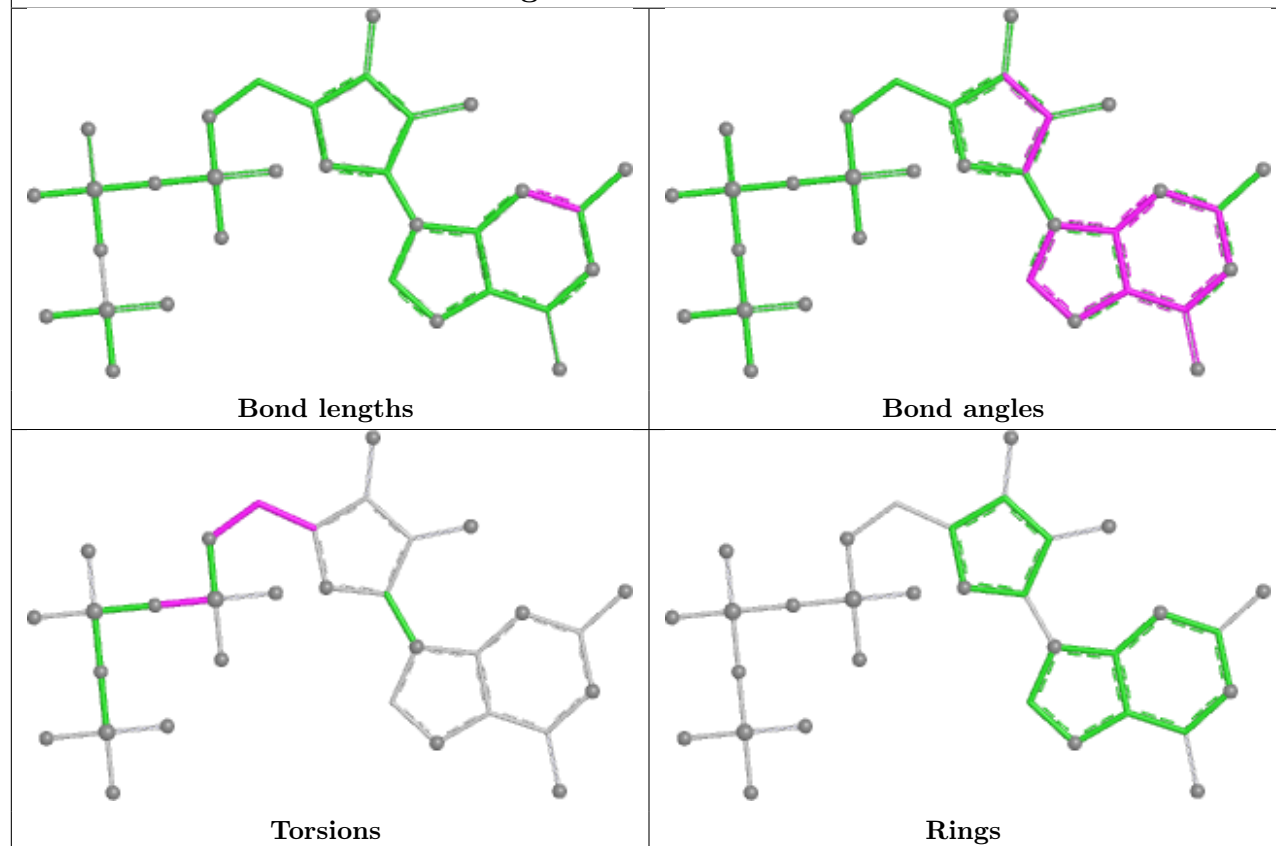
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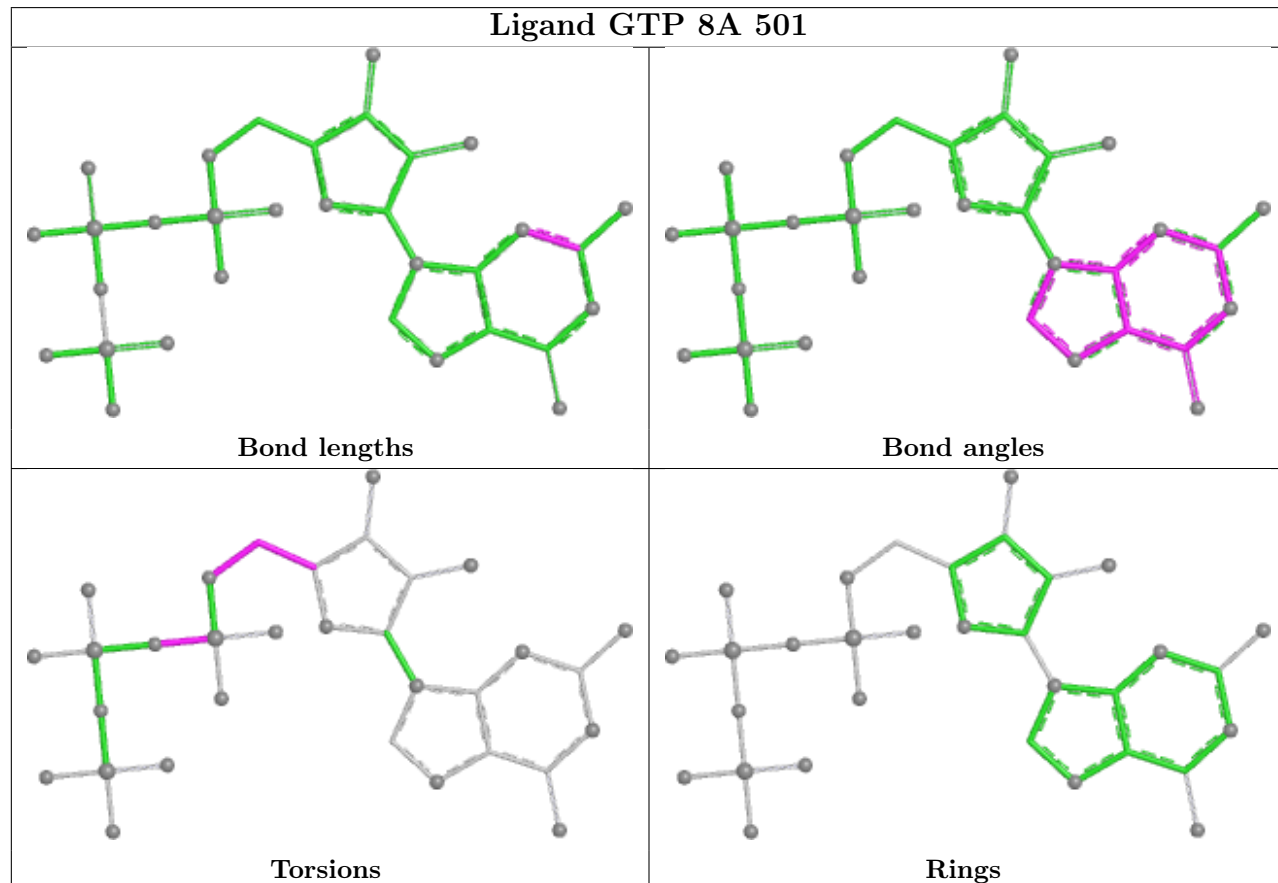
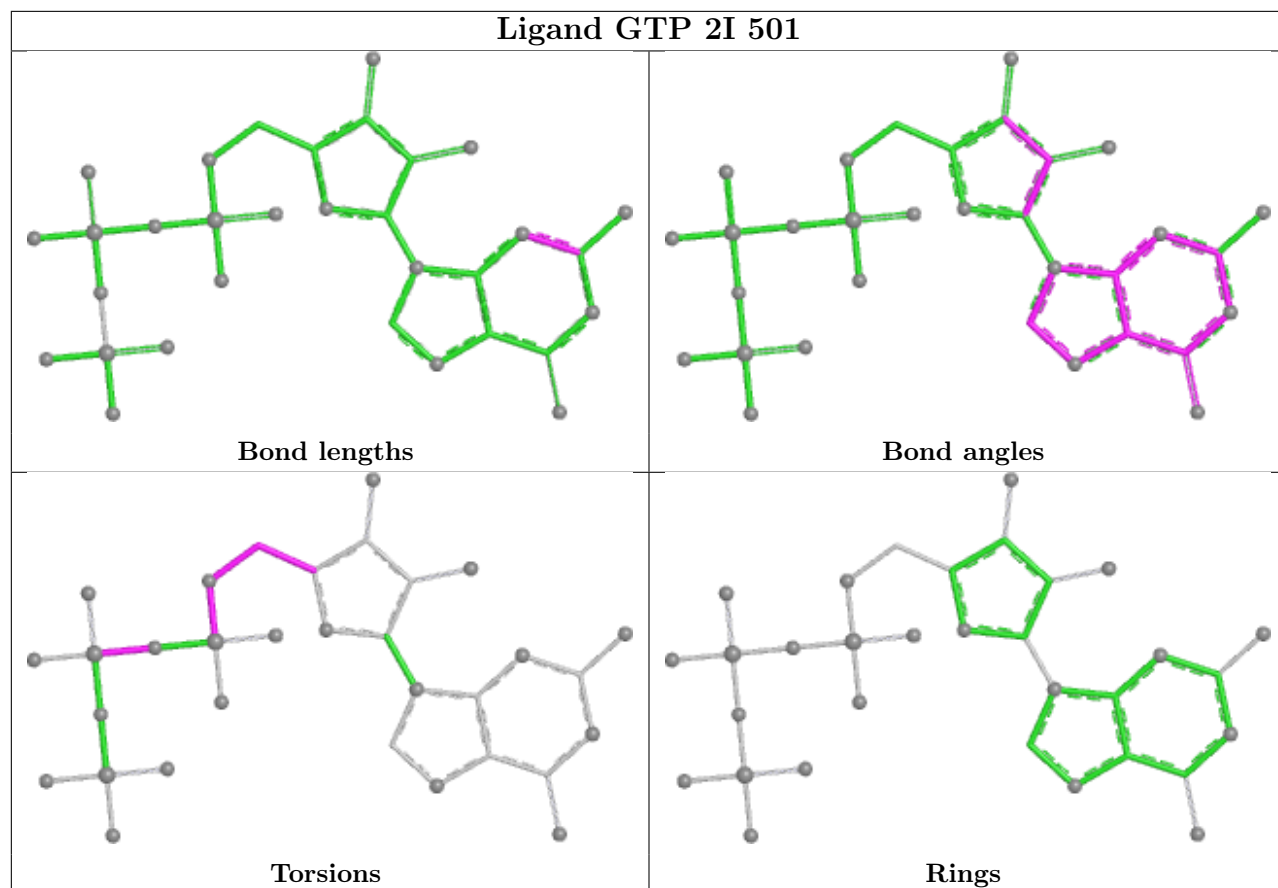


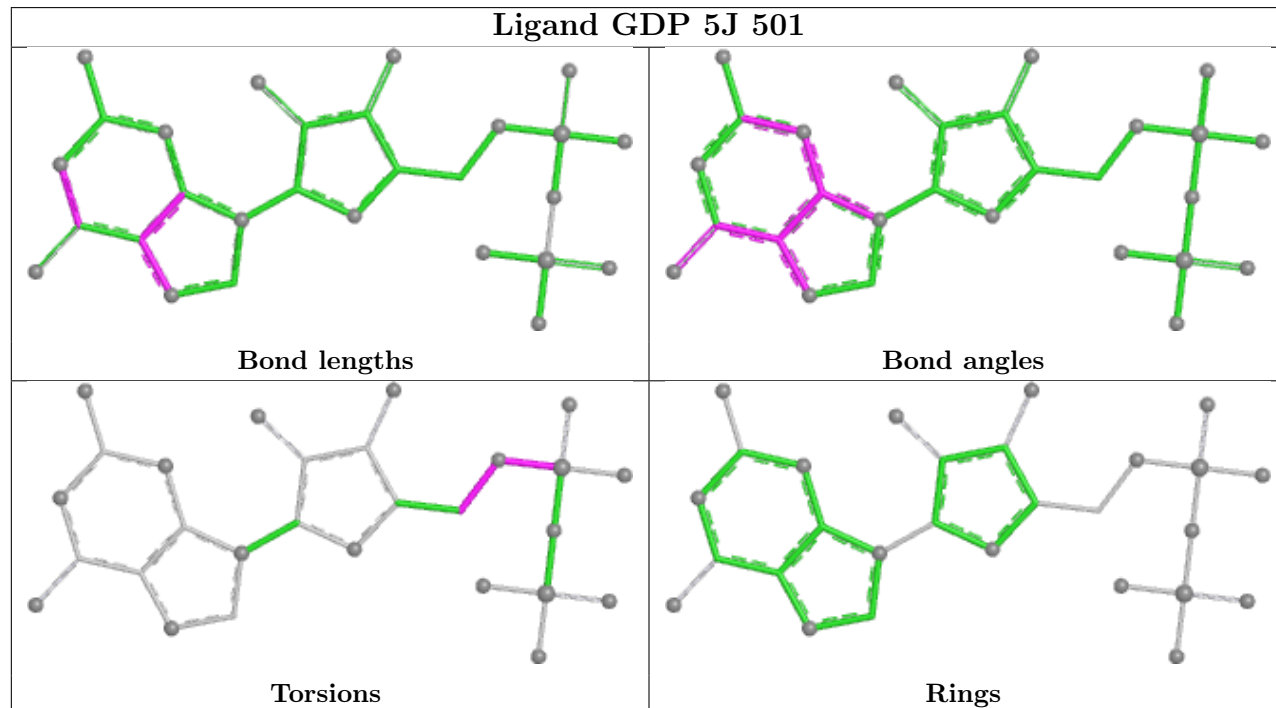
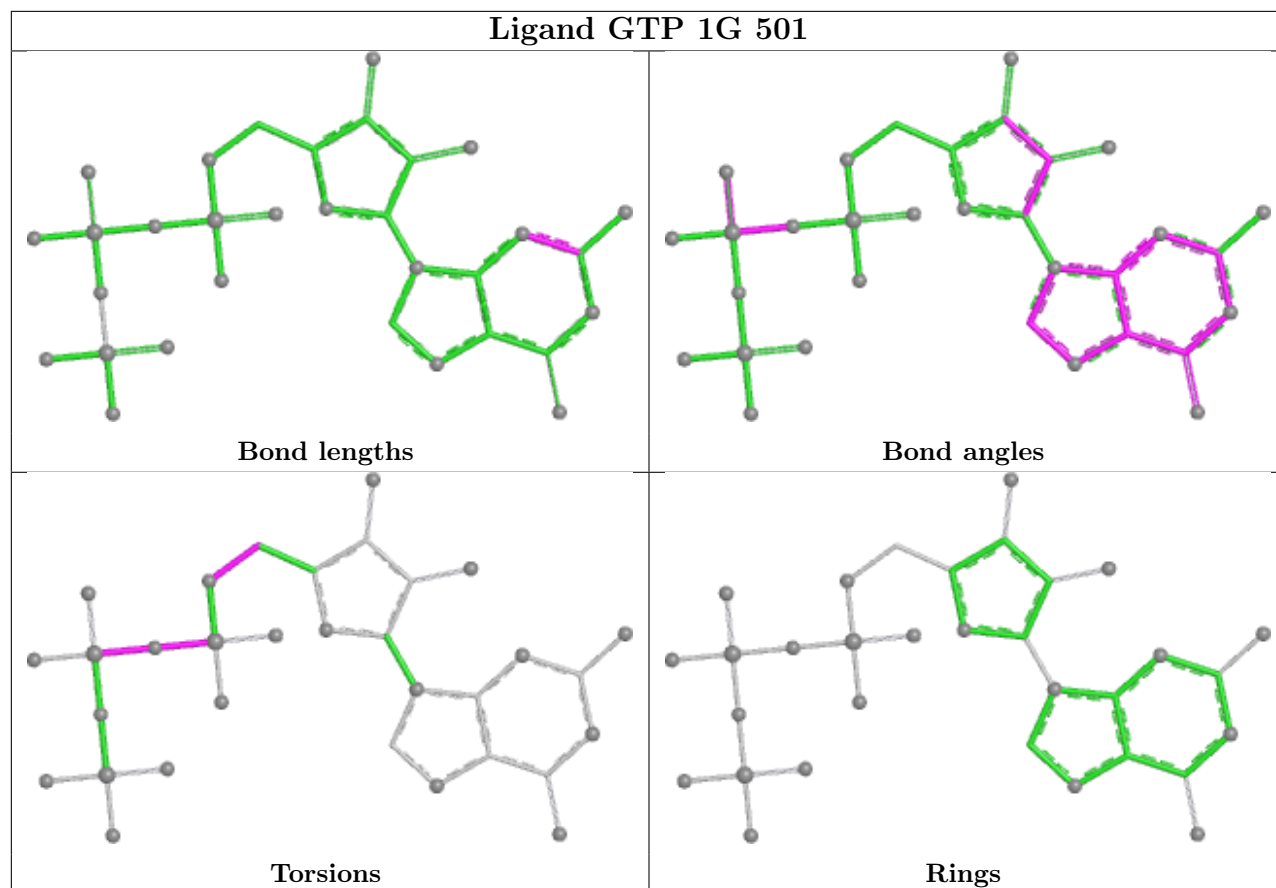
Ligand GTP 8C 501



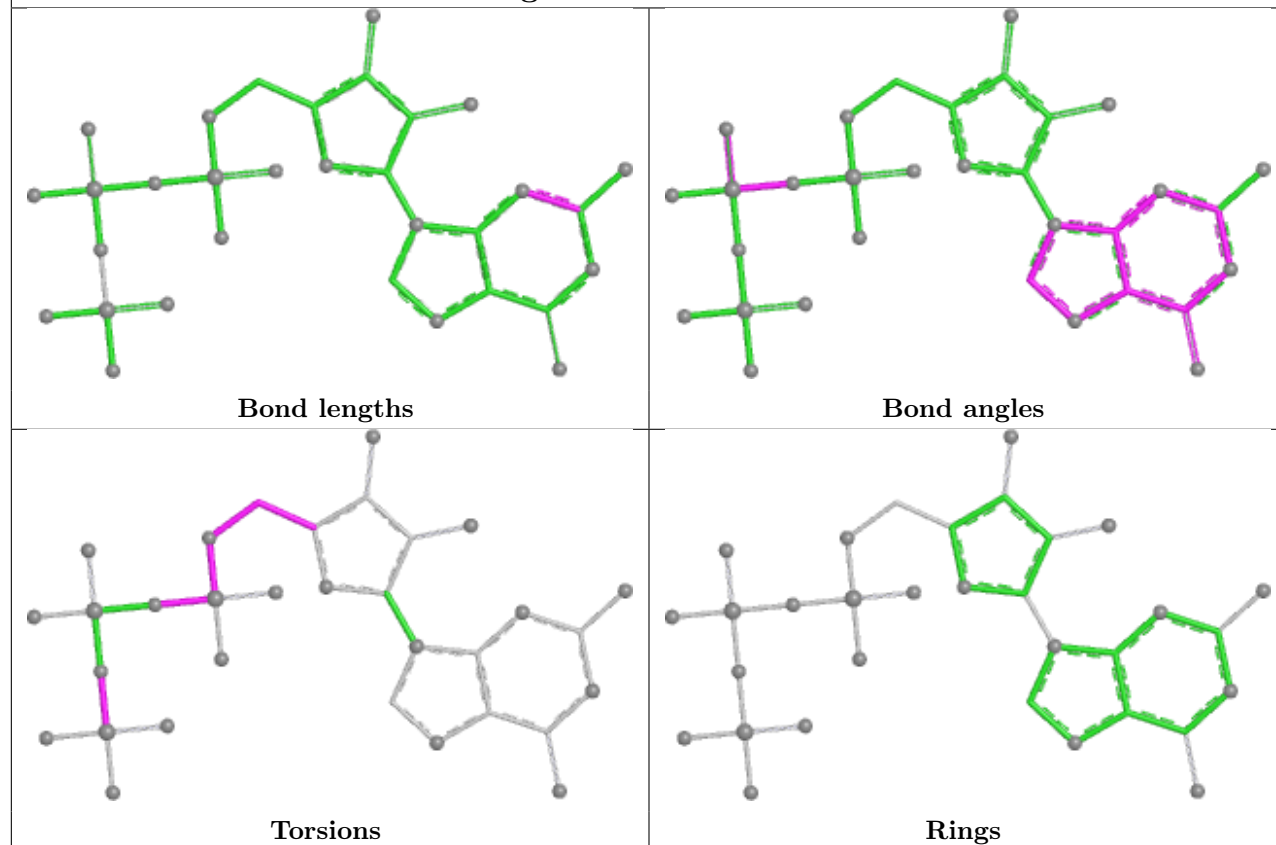
Ligand GTP 5K 501



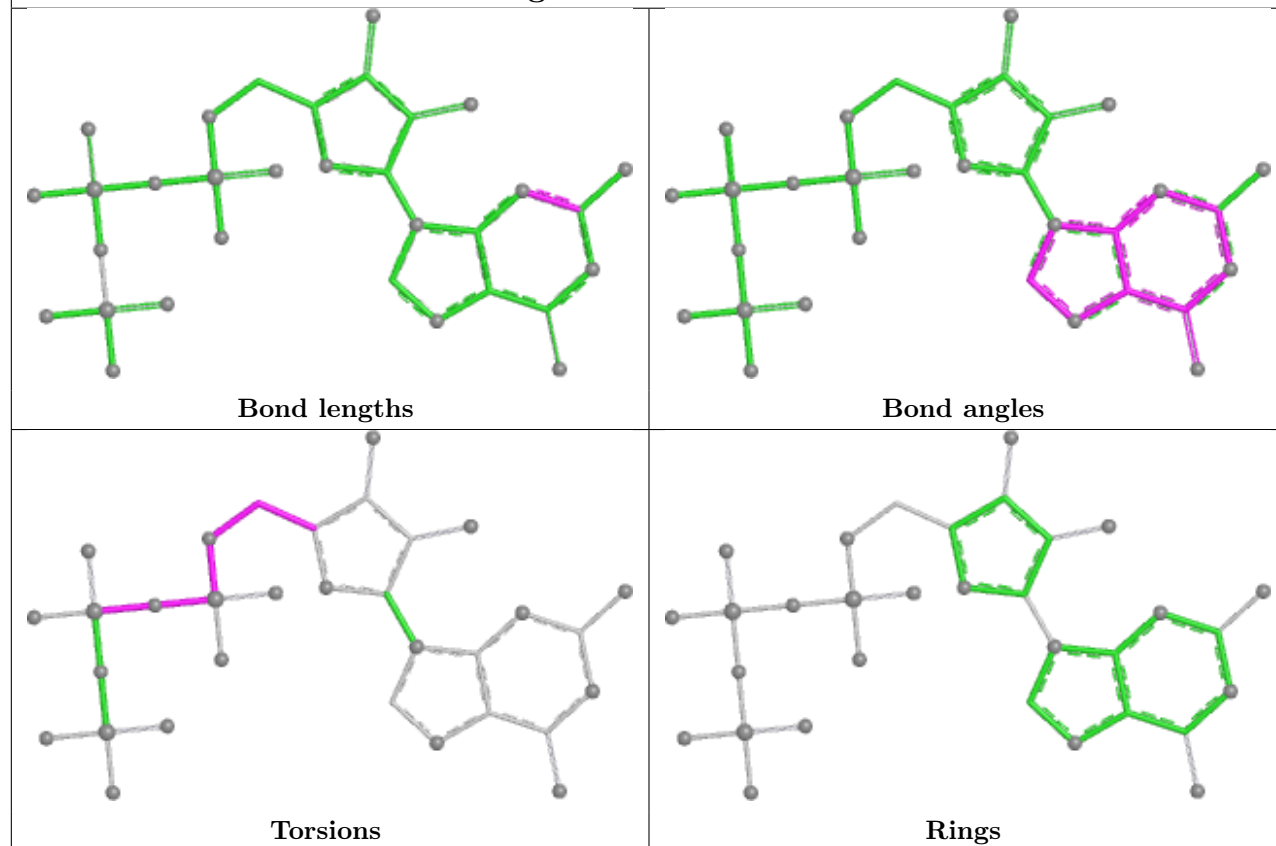


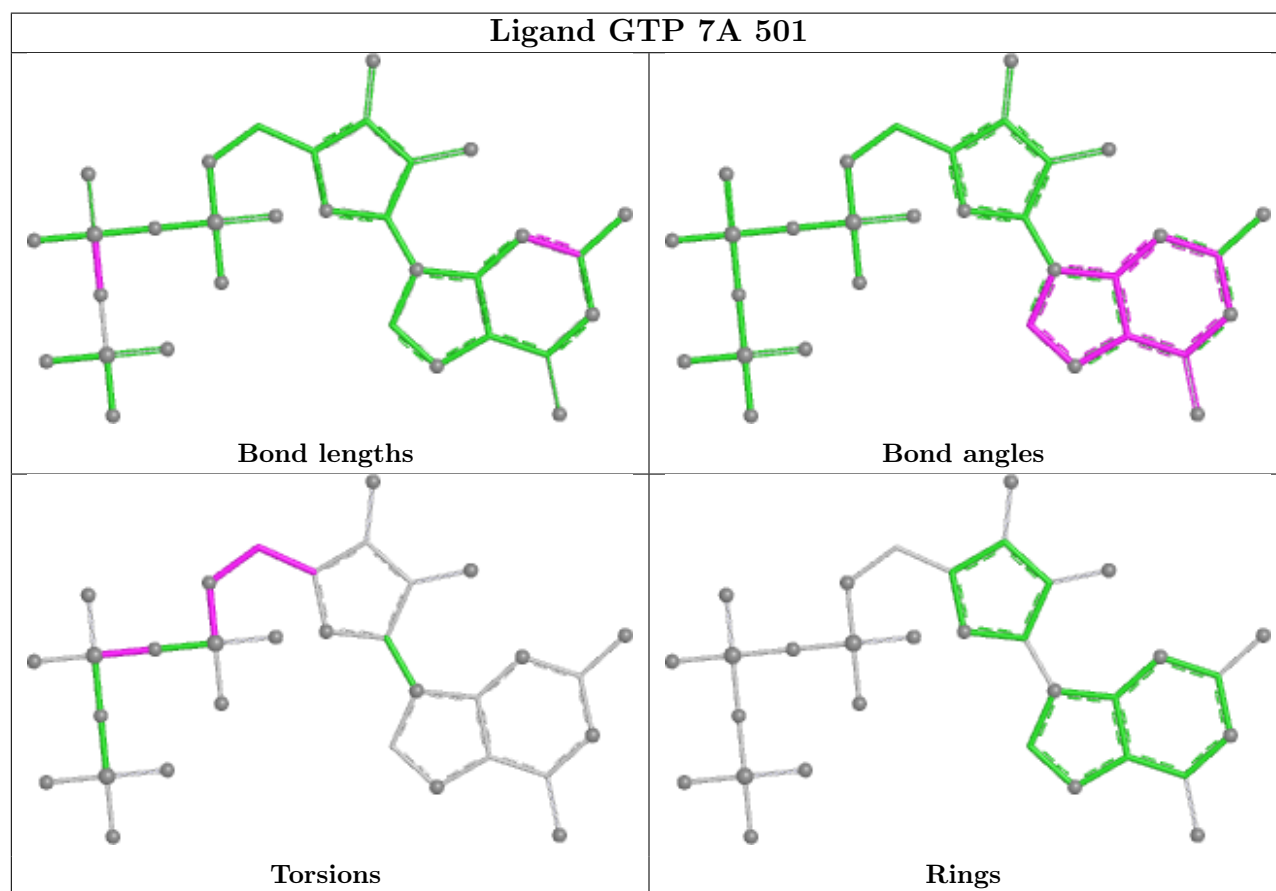
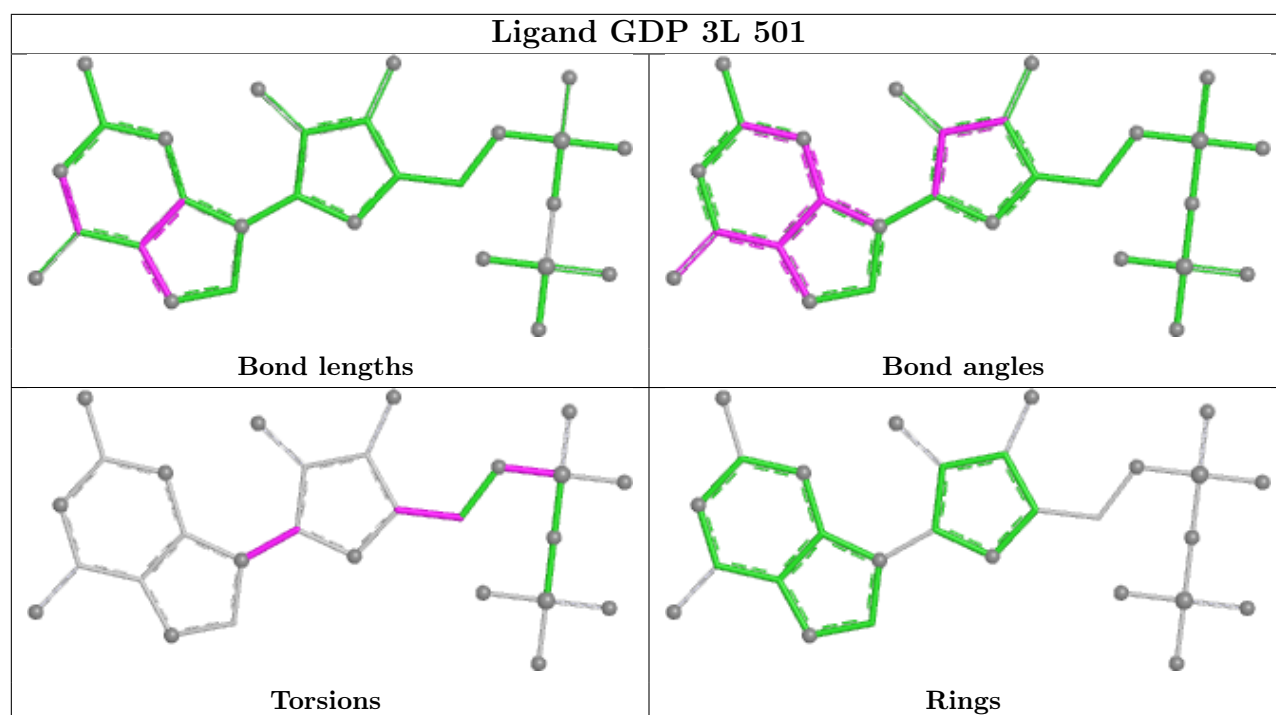


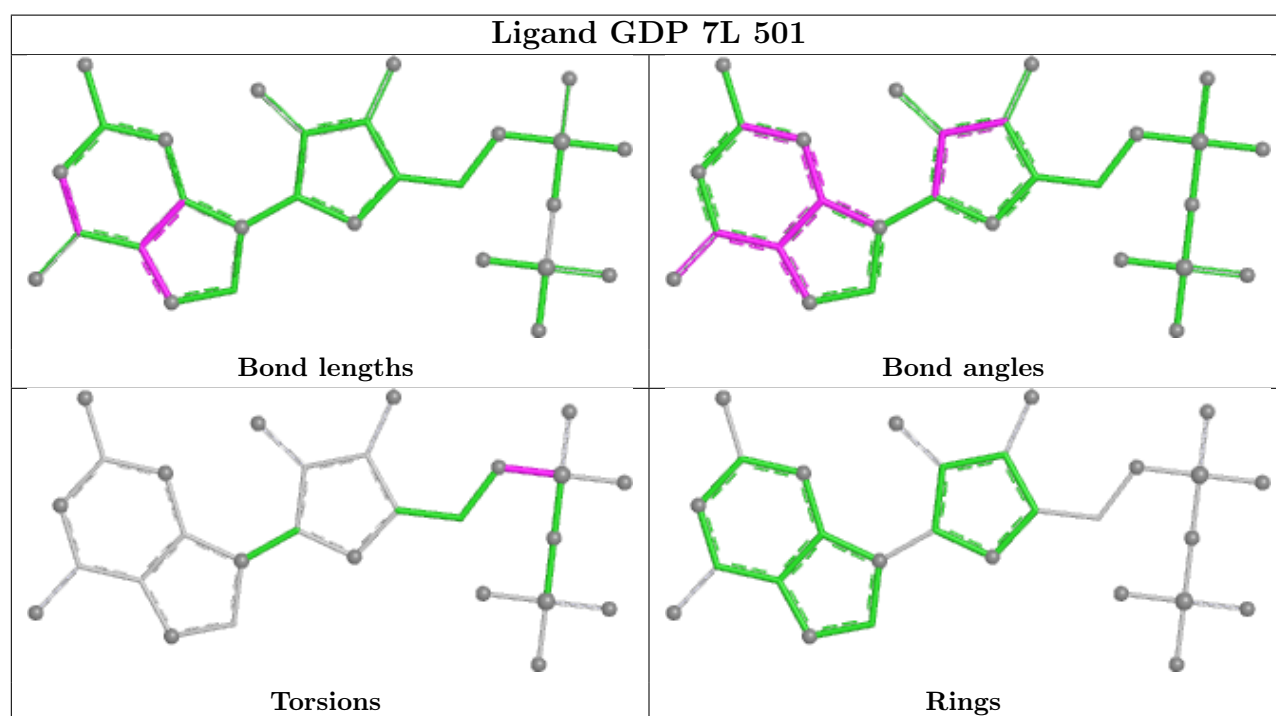
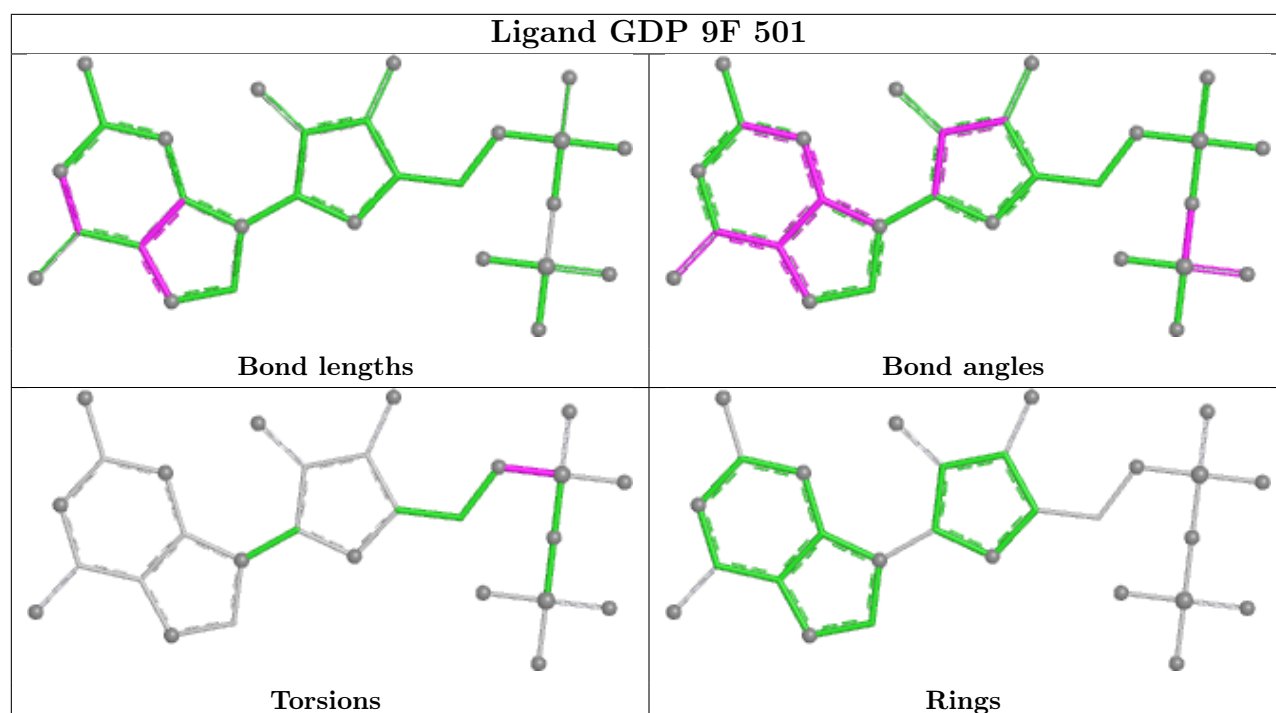
Ligand GTP 1K 501

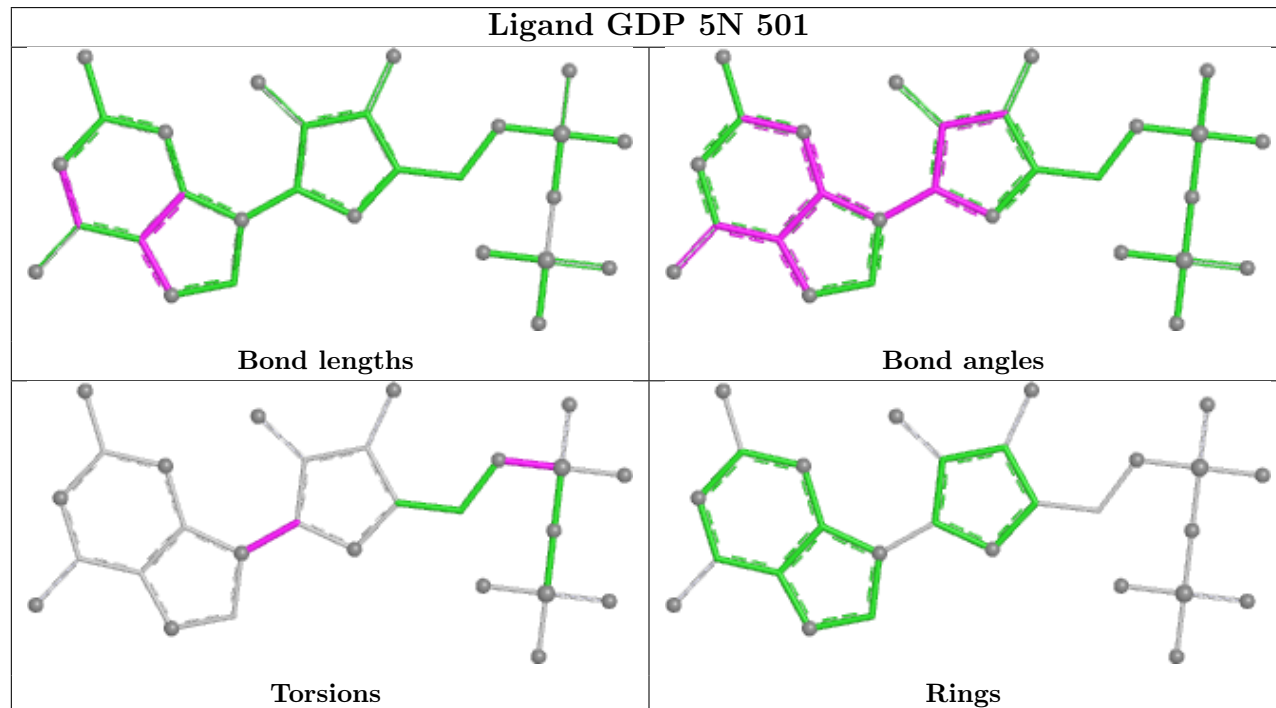
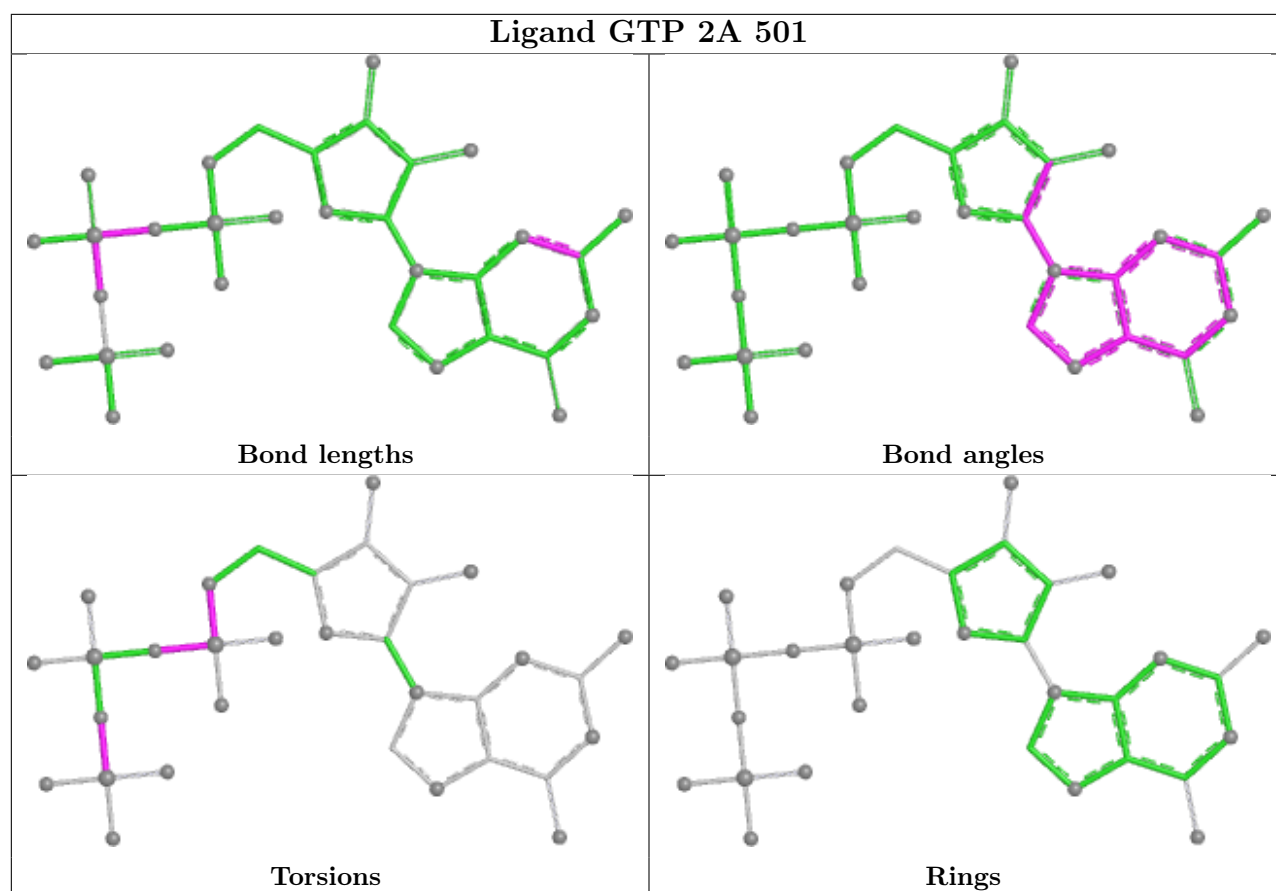


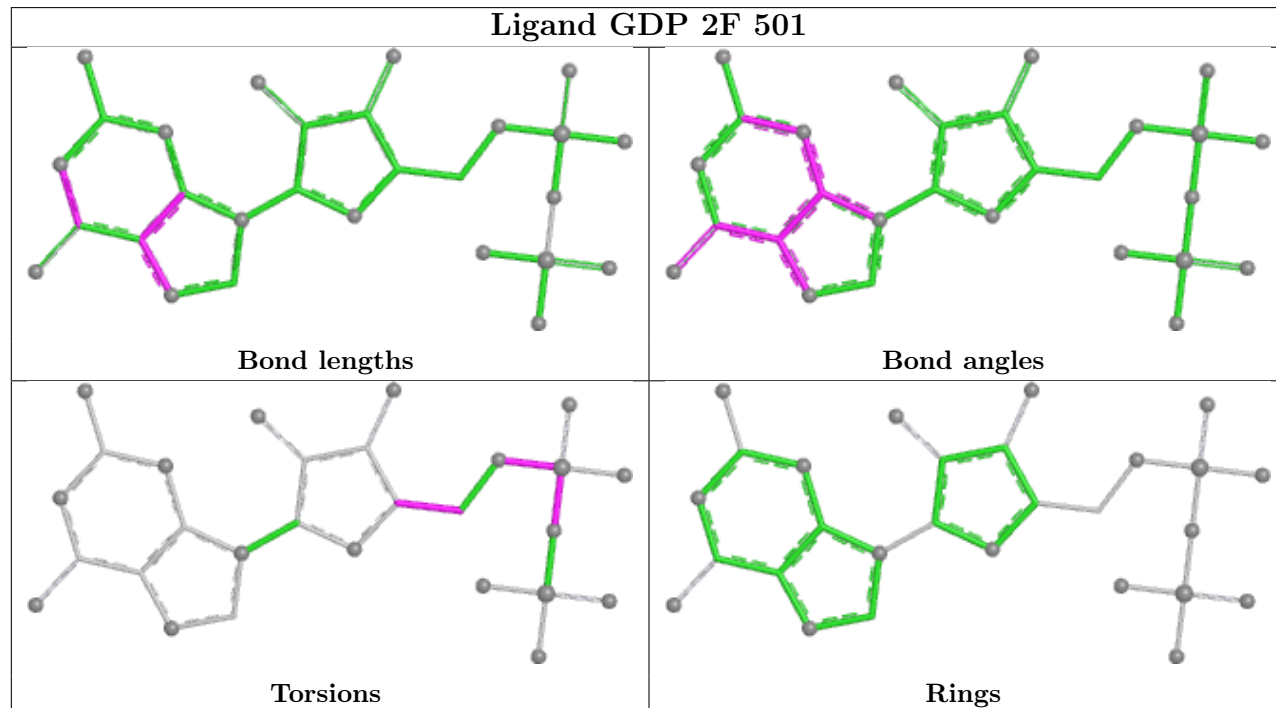
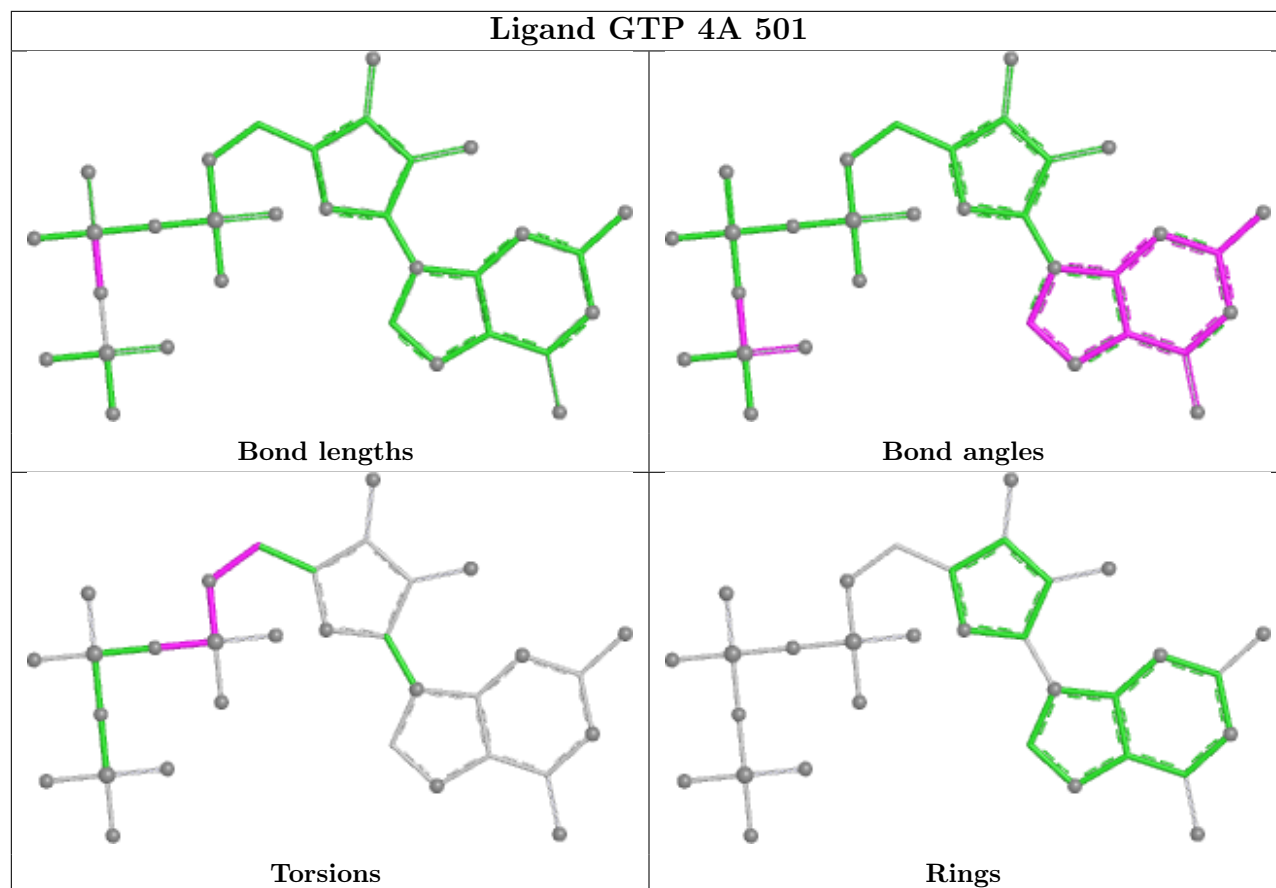
Ligand GTP 5I 501



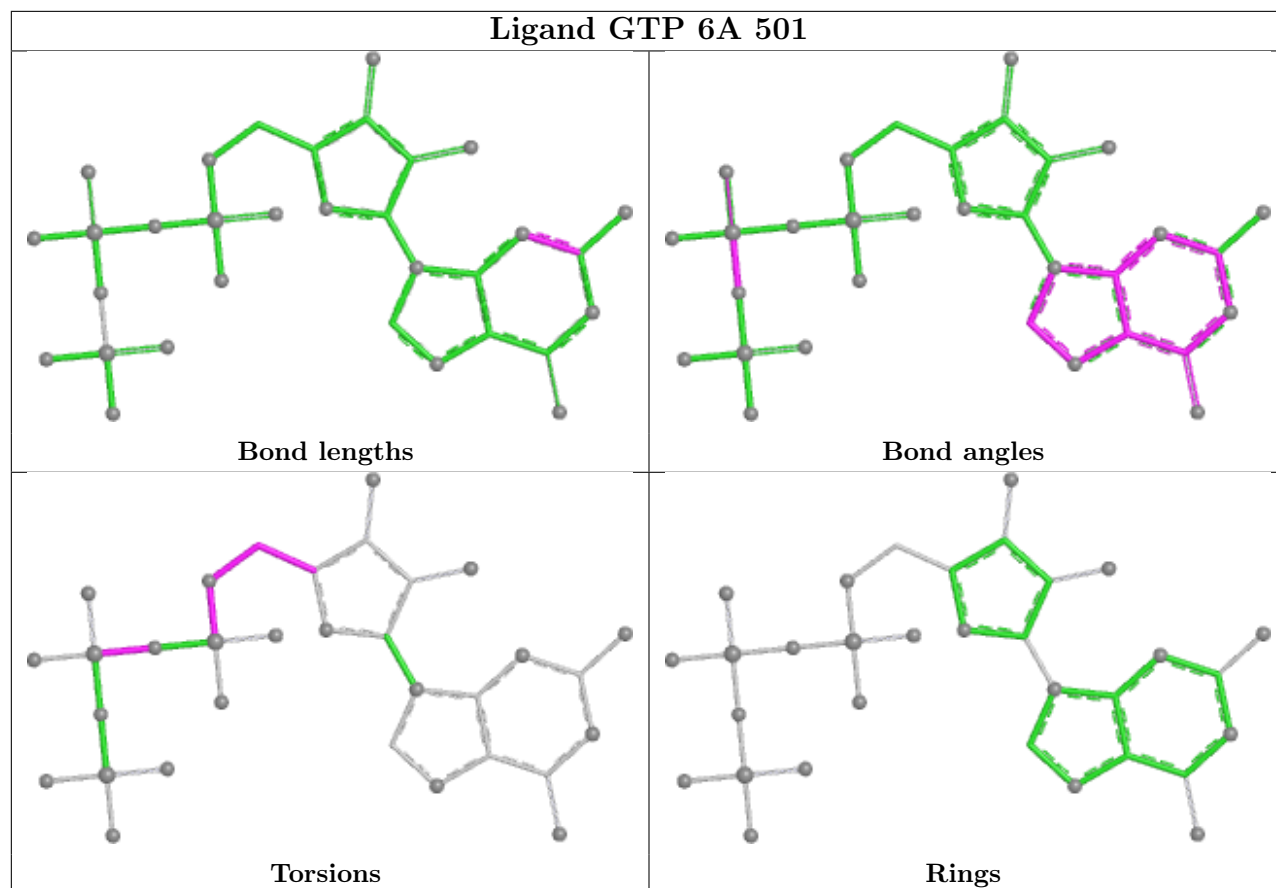




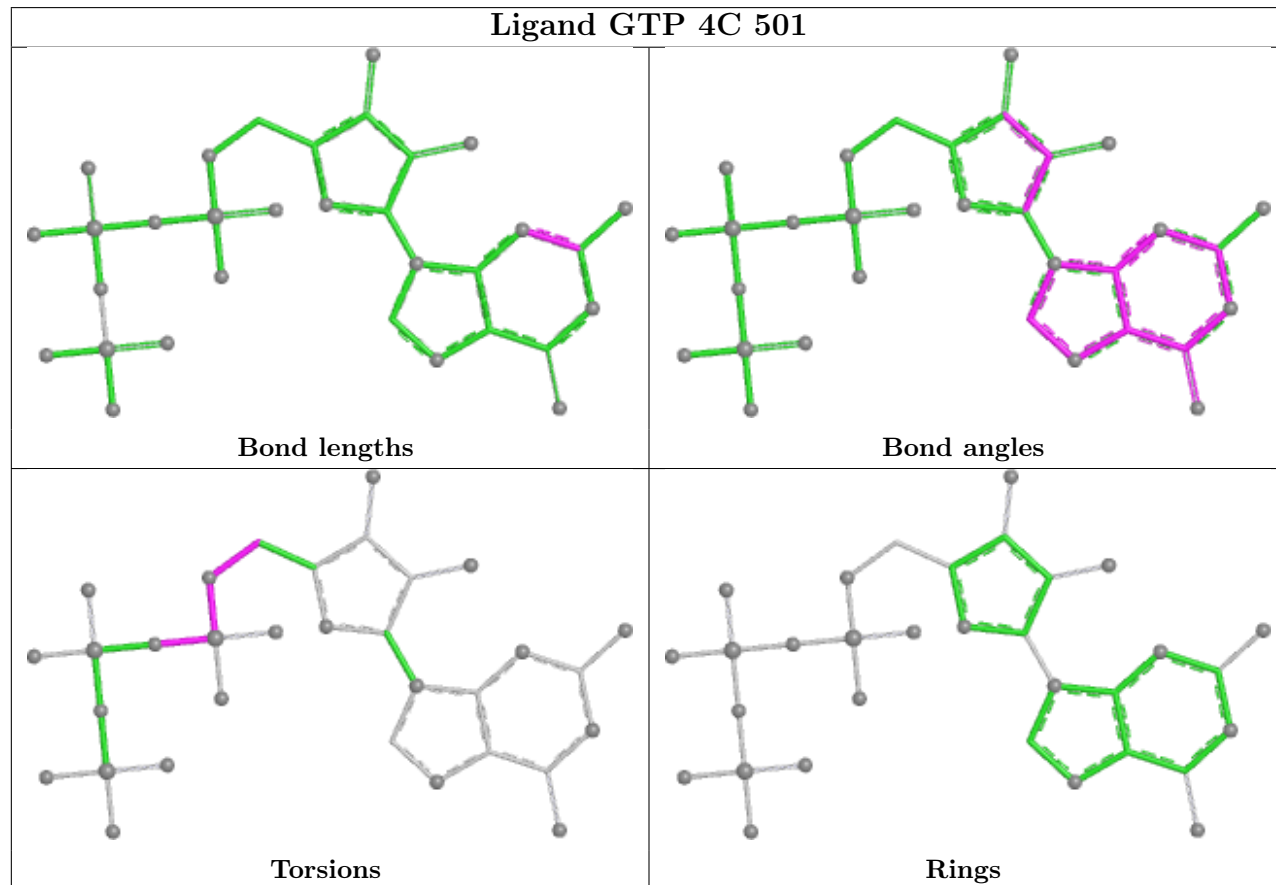




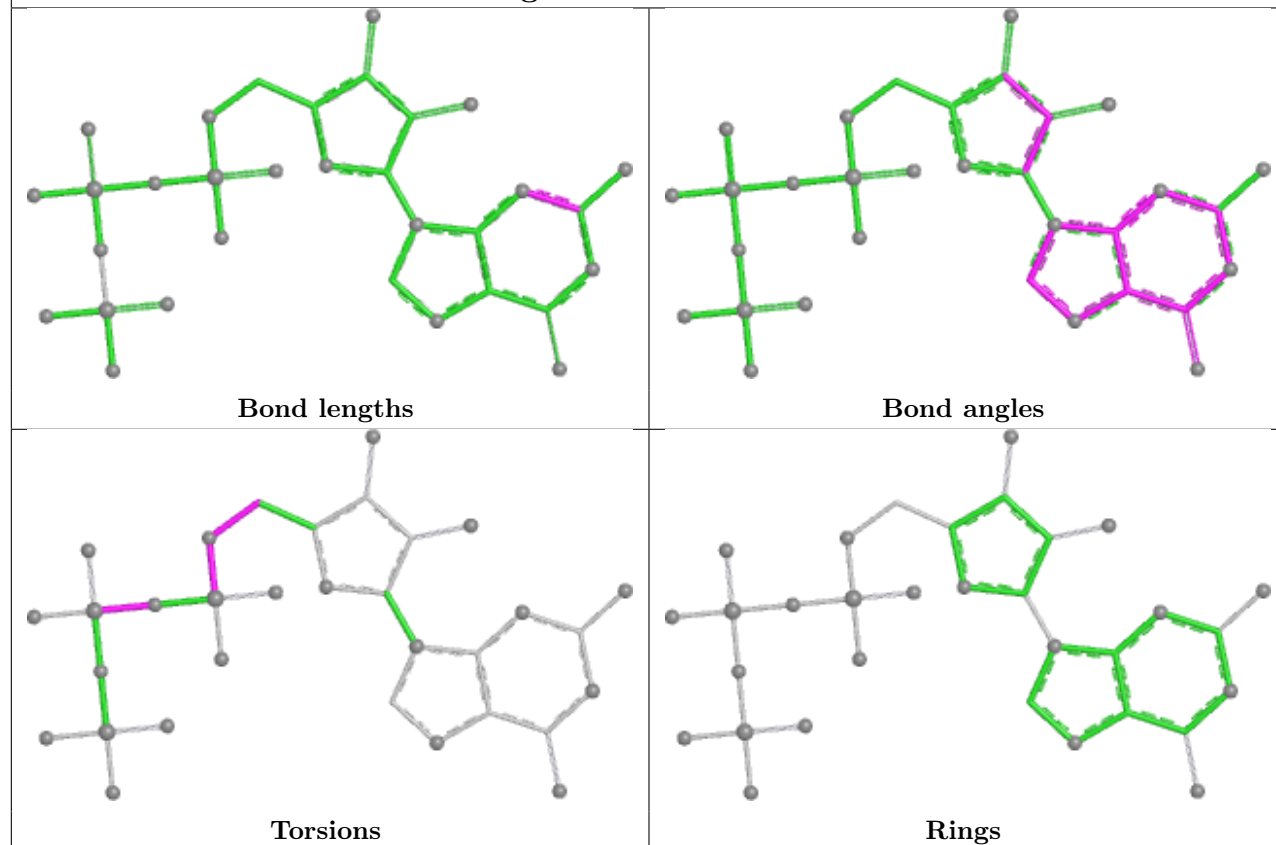
Ligand GTP 6A 501



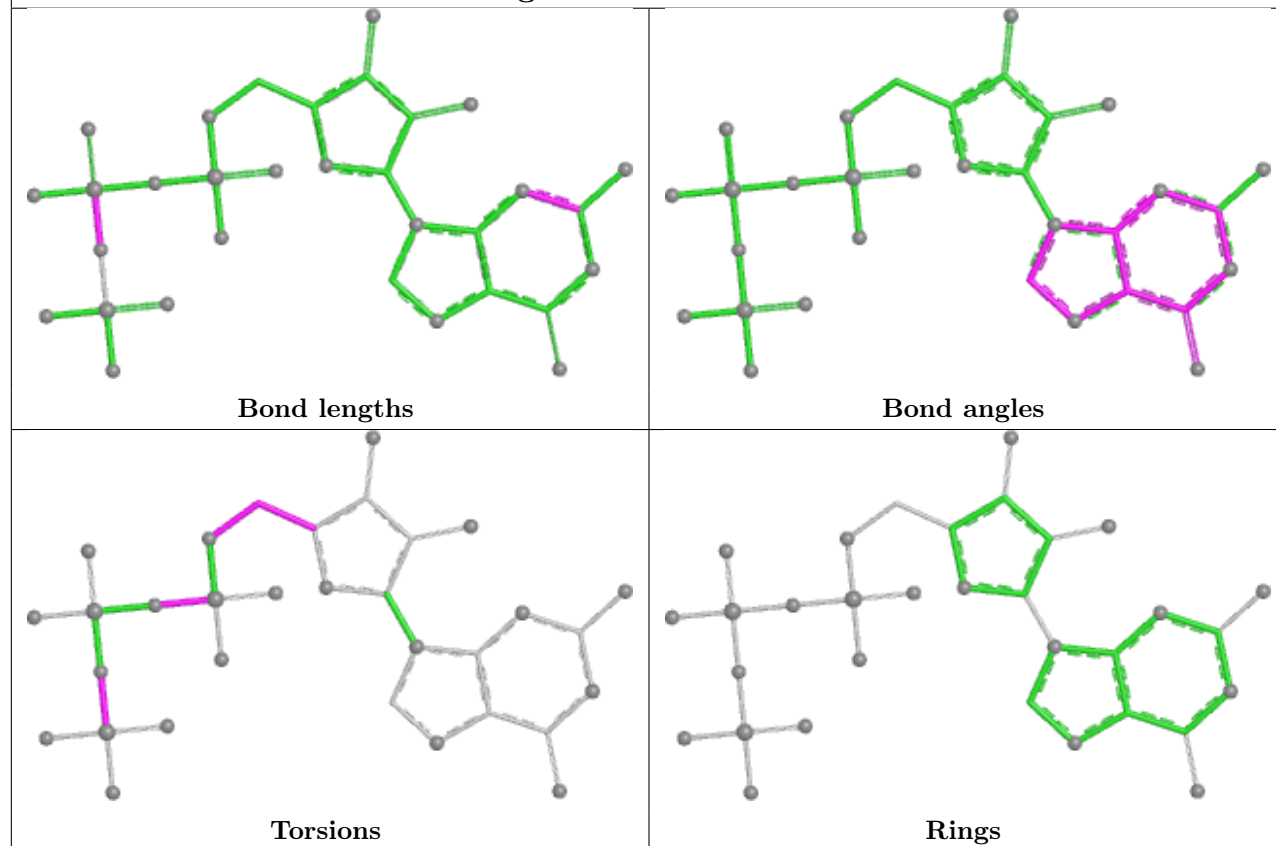
Ligand GTP 4C 501

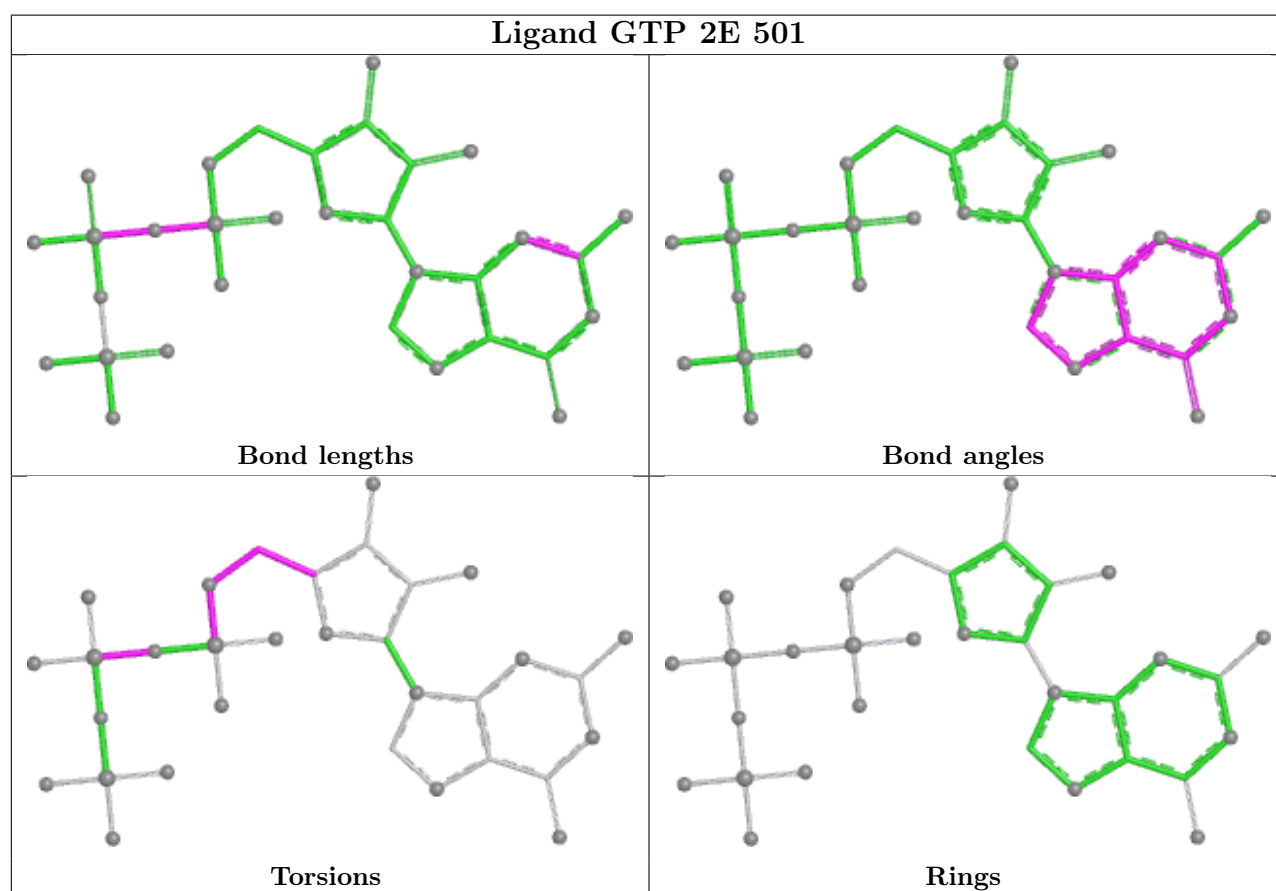
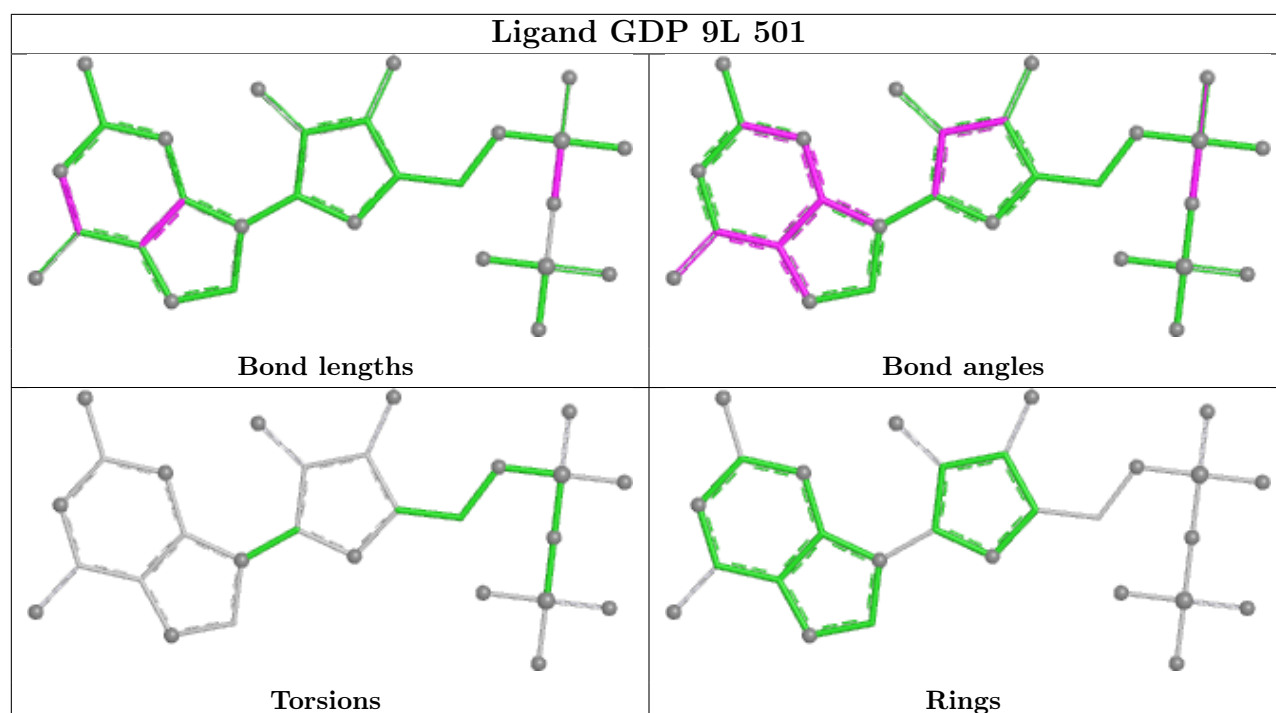


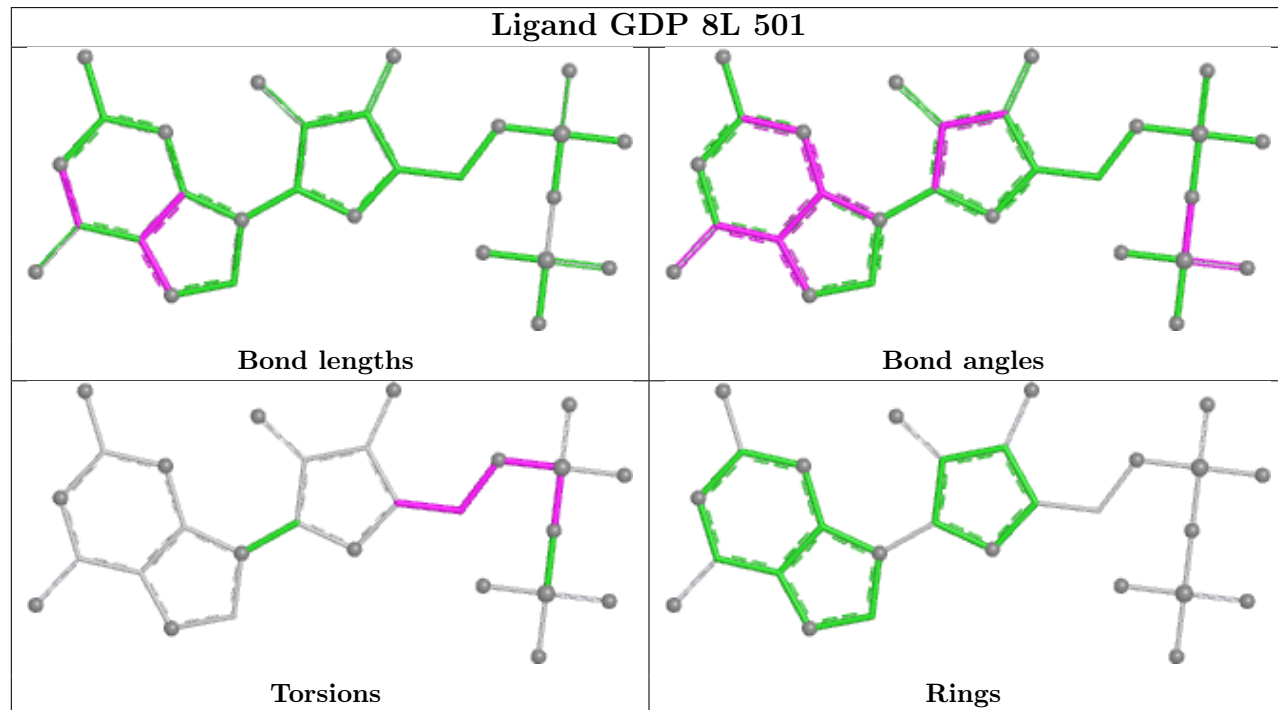
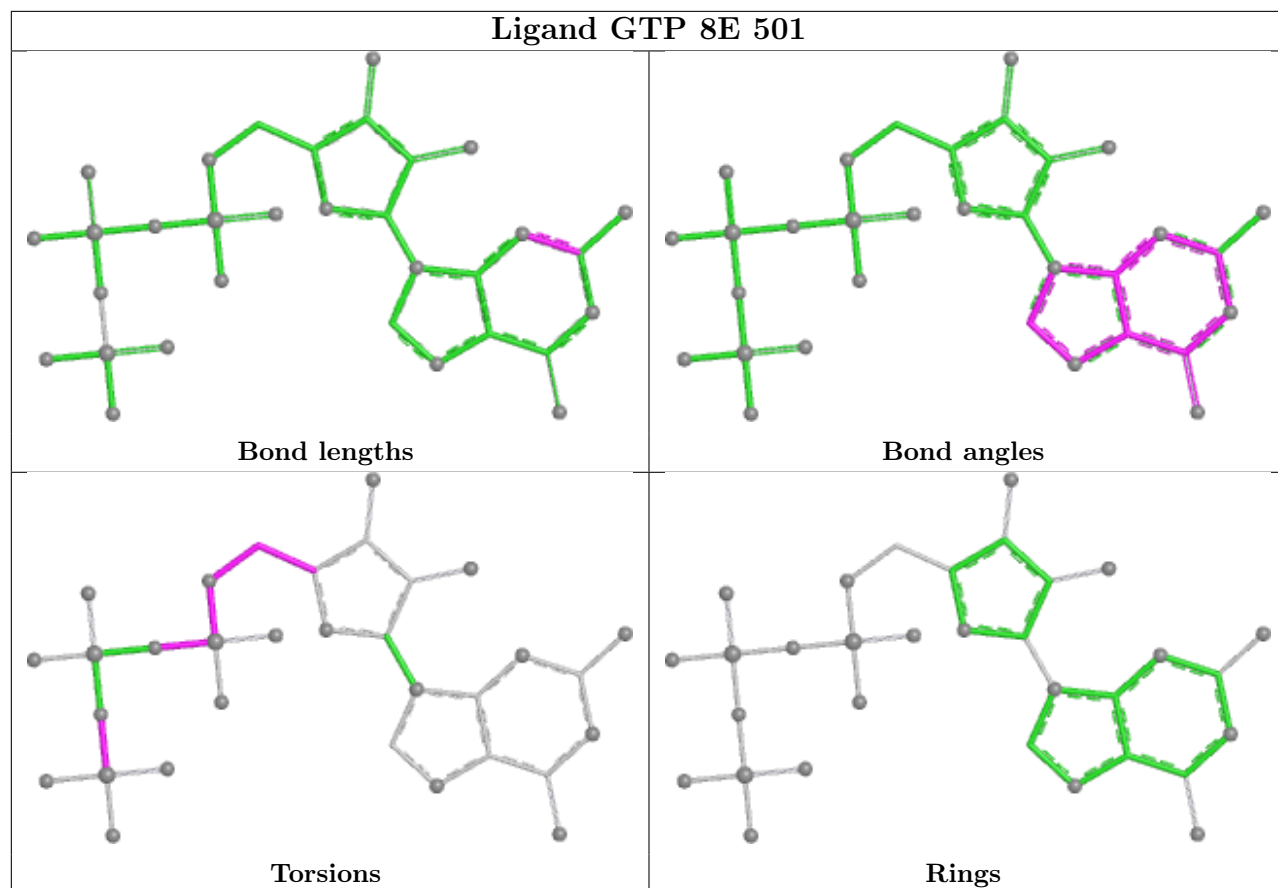
Ligand GTP 5G 501

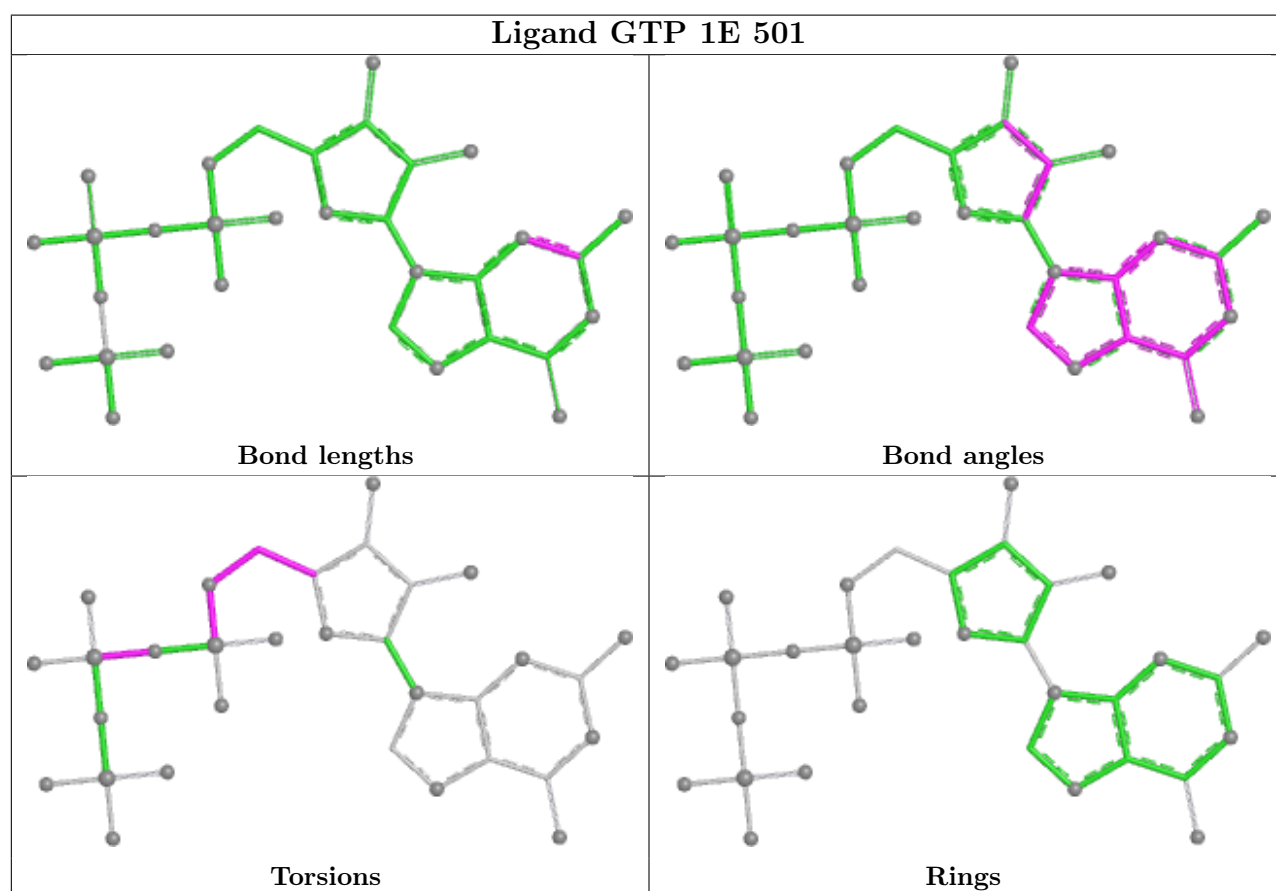
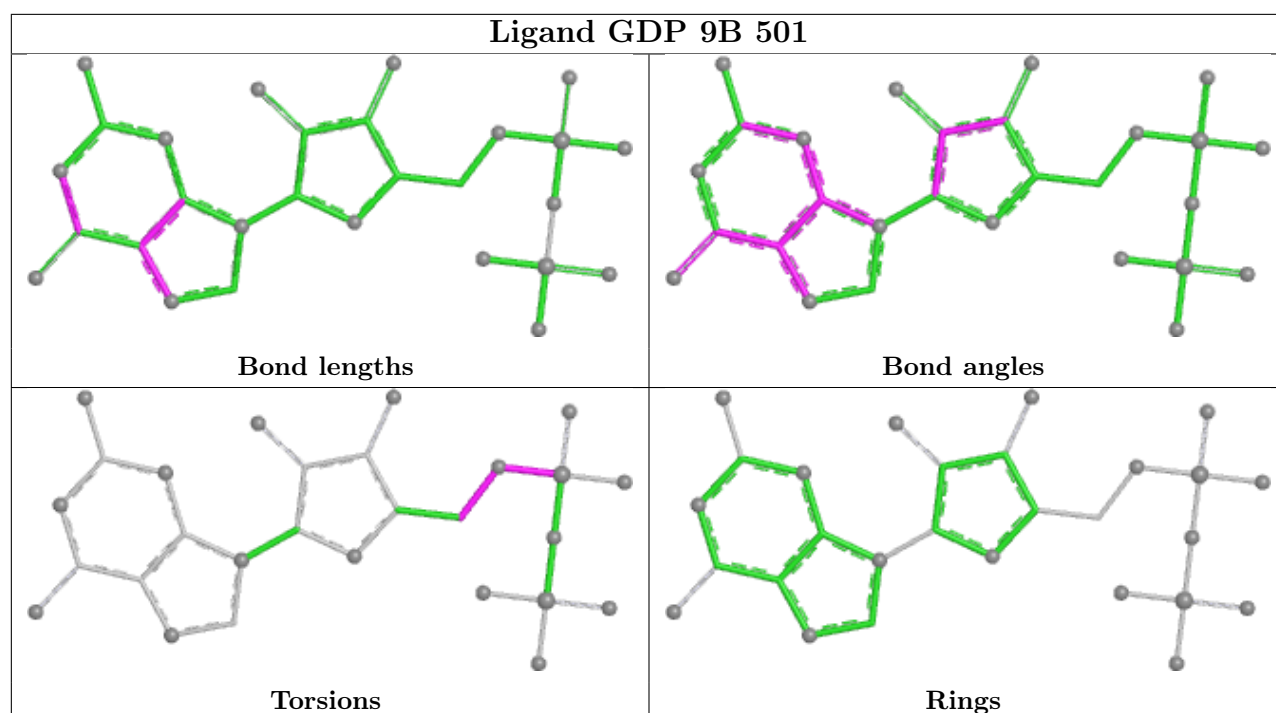


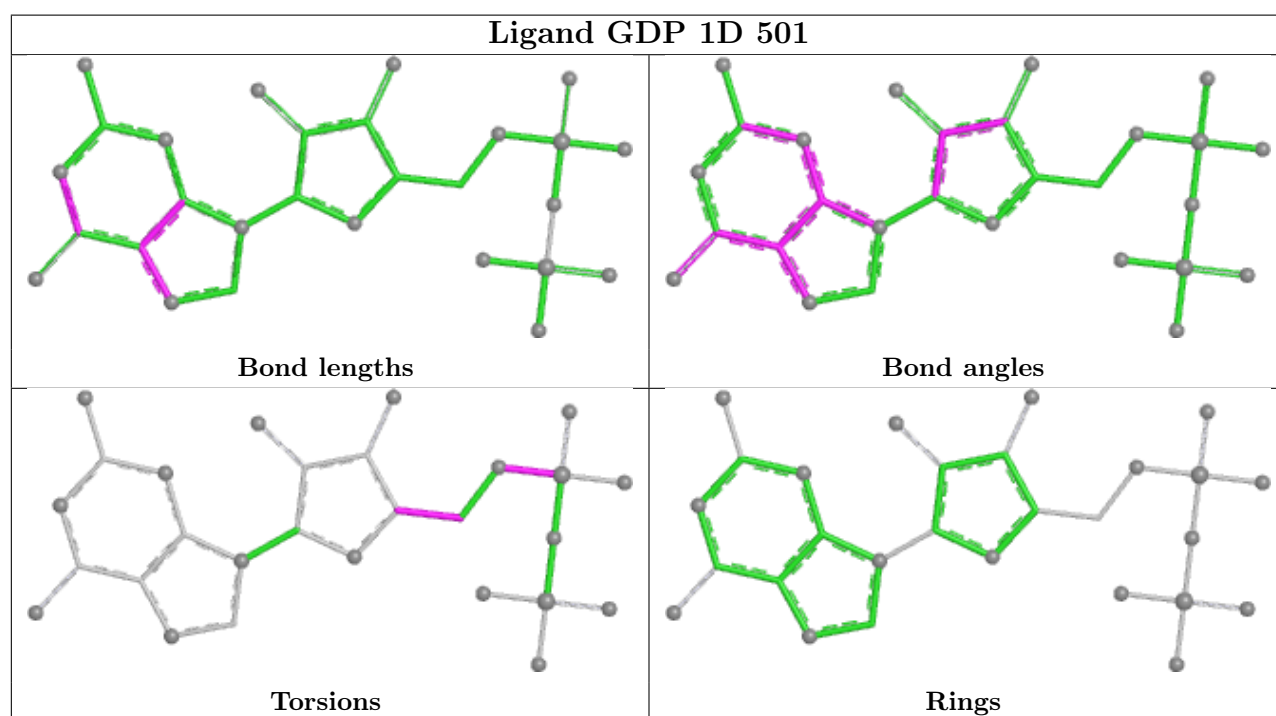
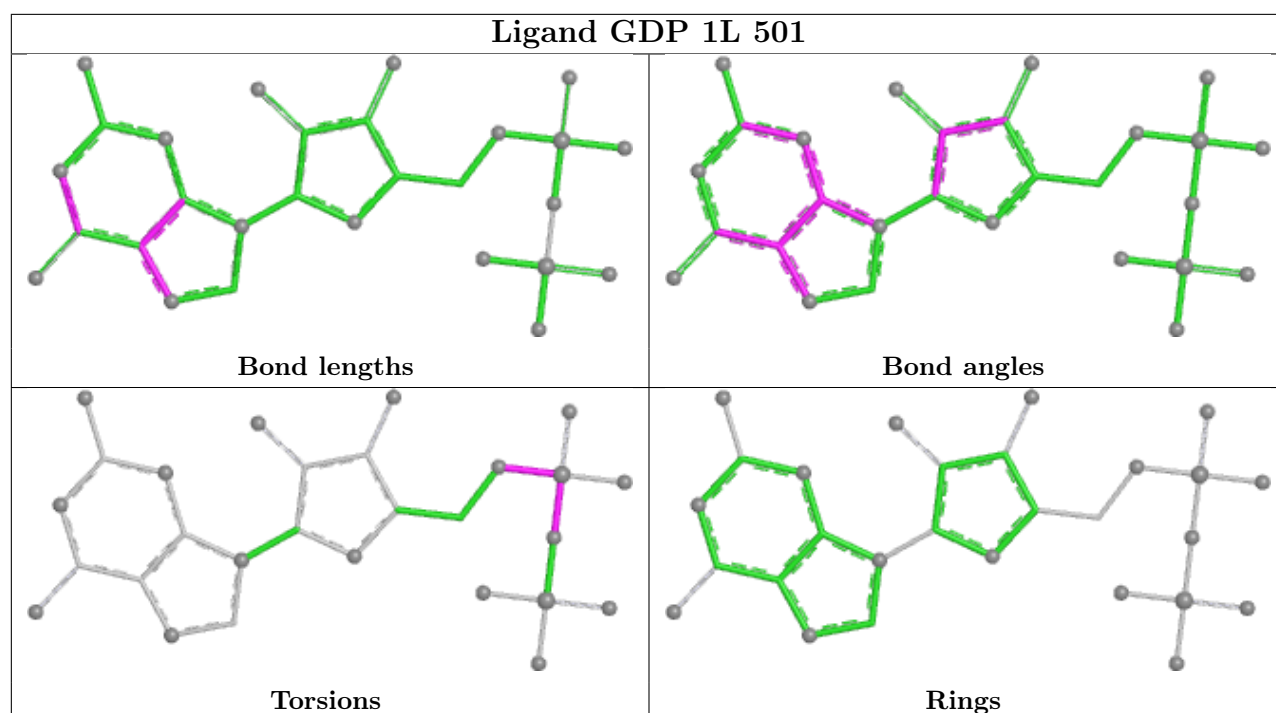
Ligand GTP 8M 501



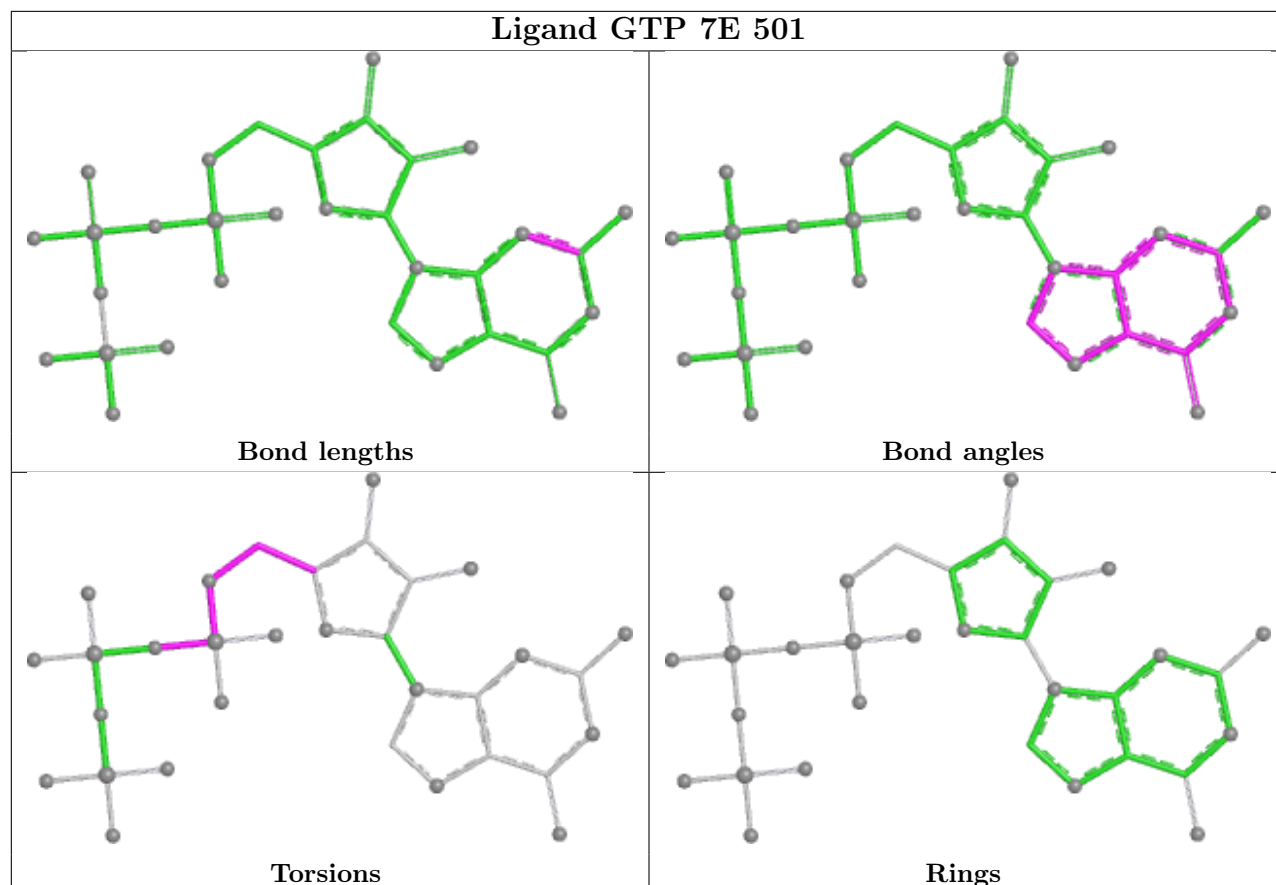




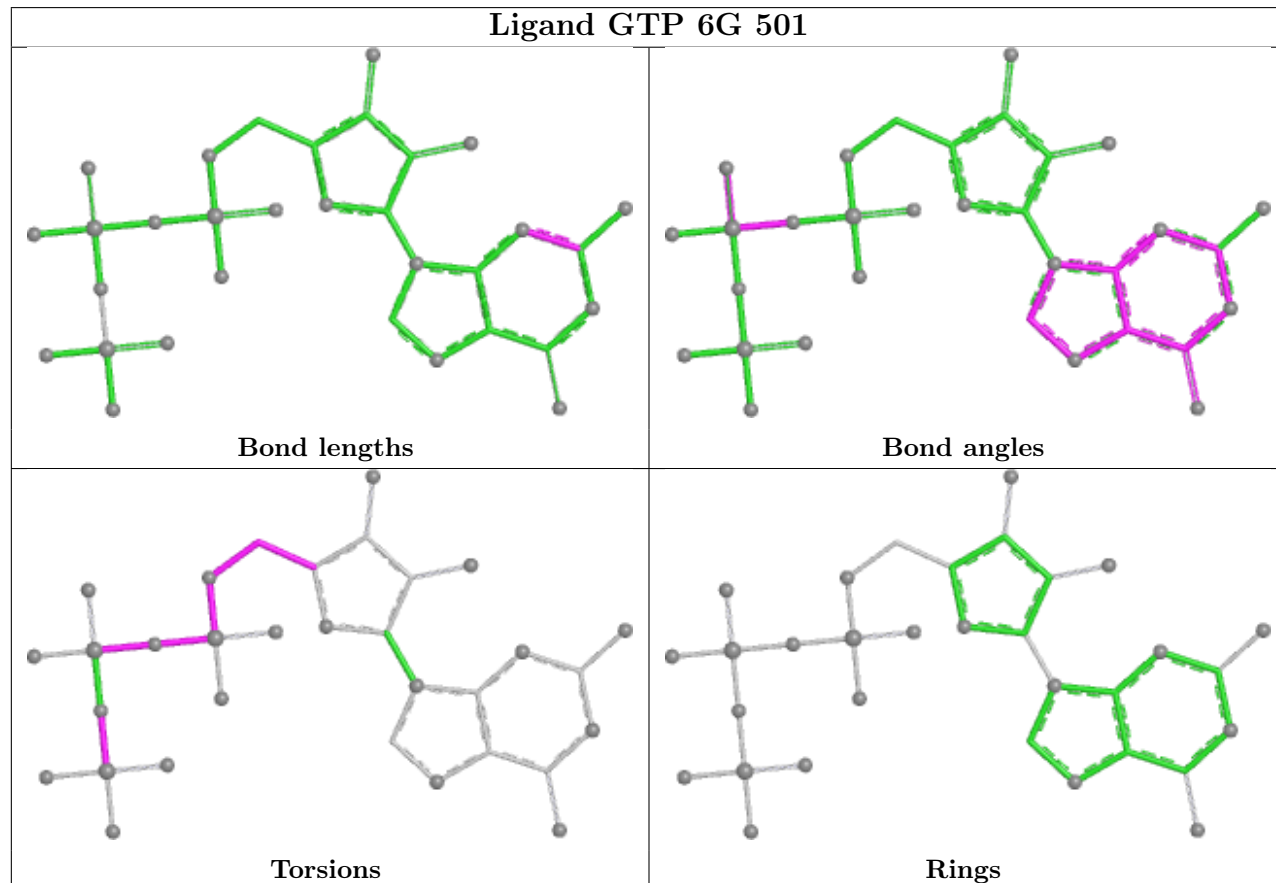


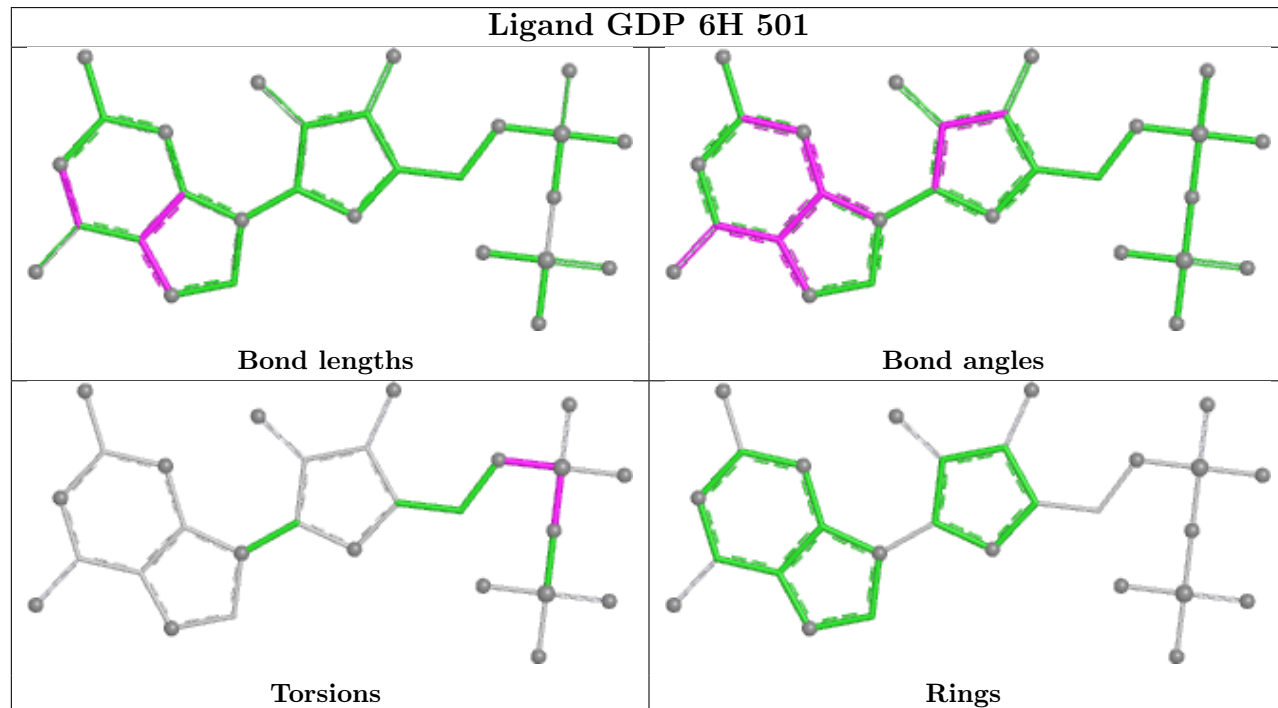
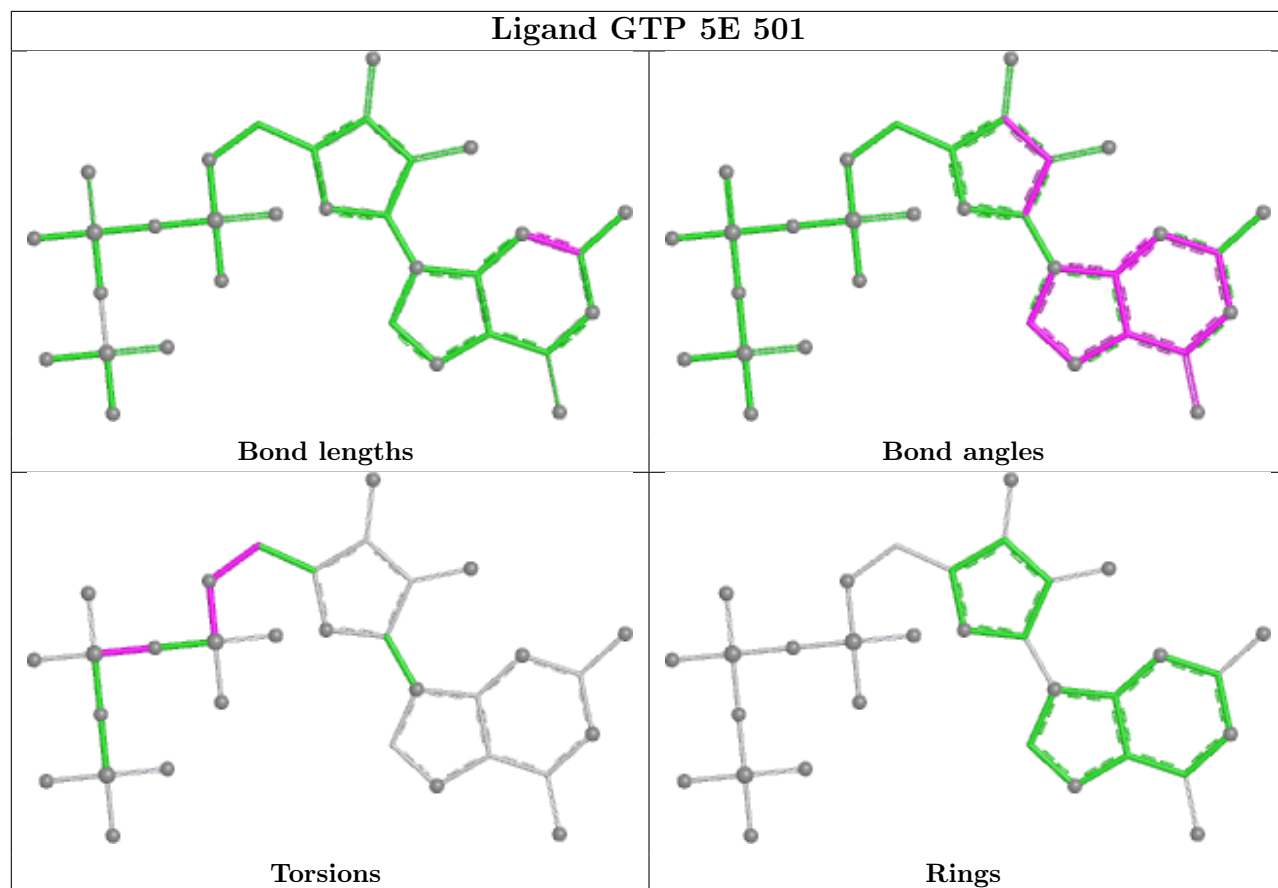


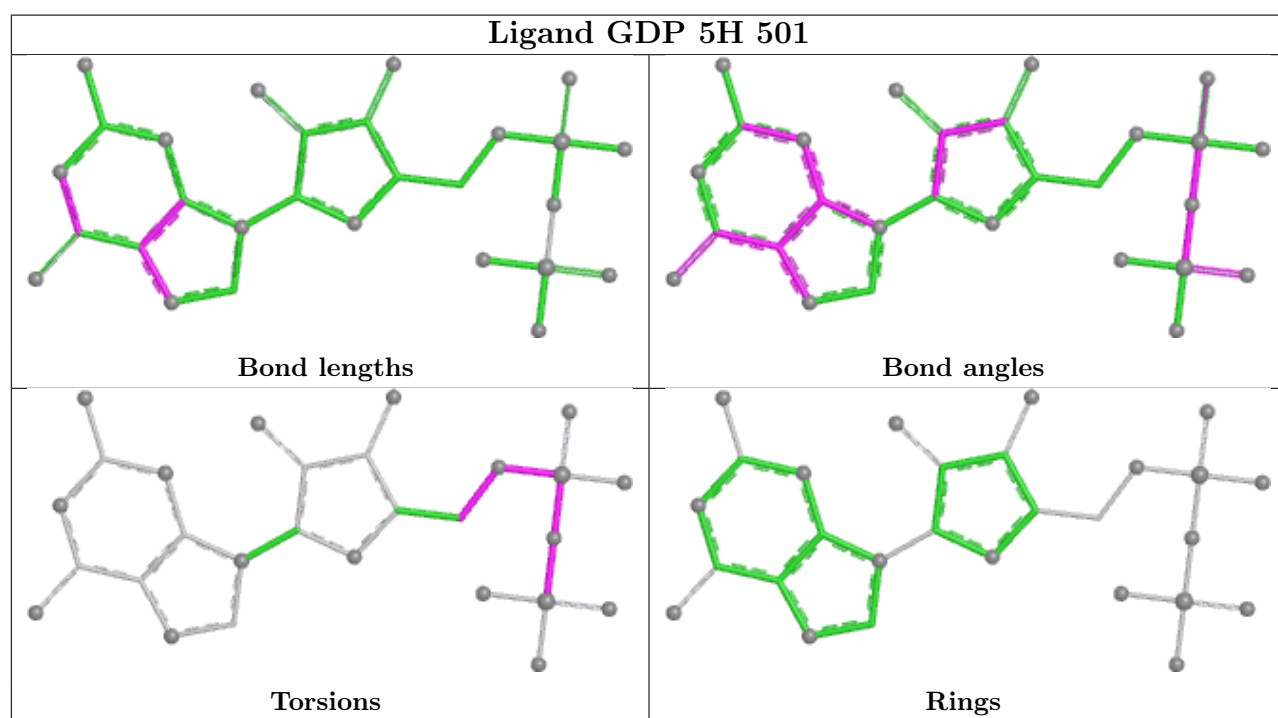
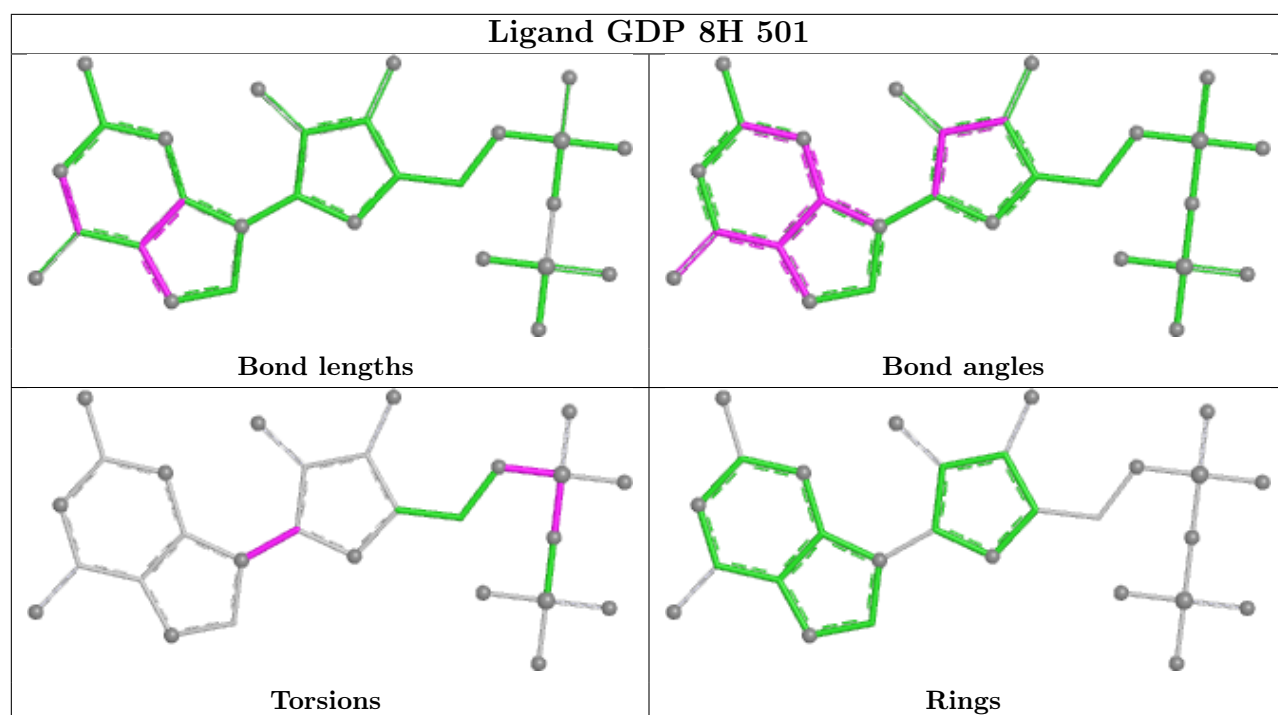
Ligand GTP 7E 501

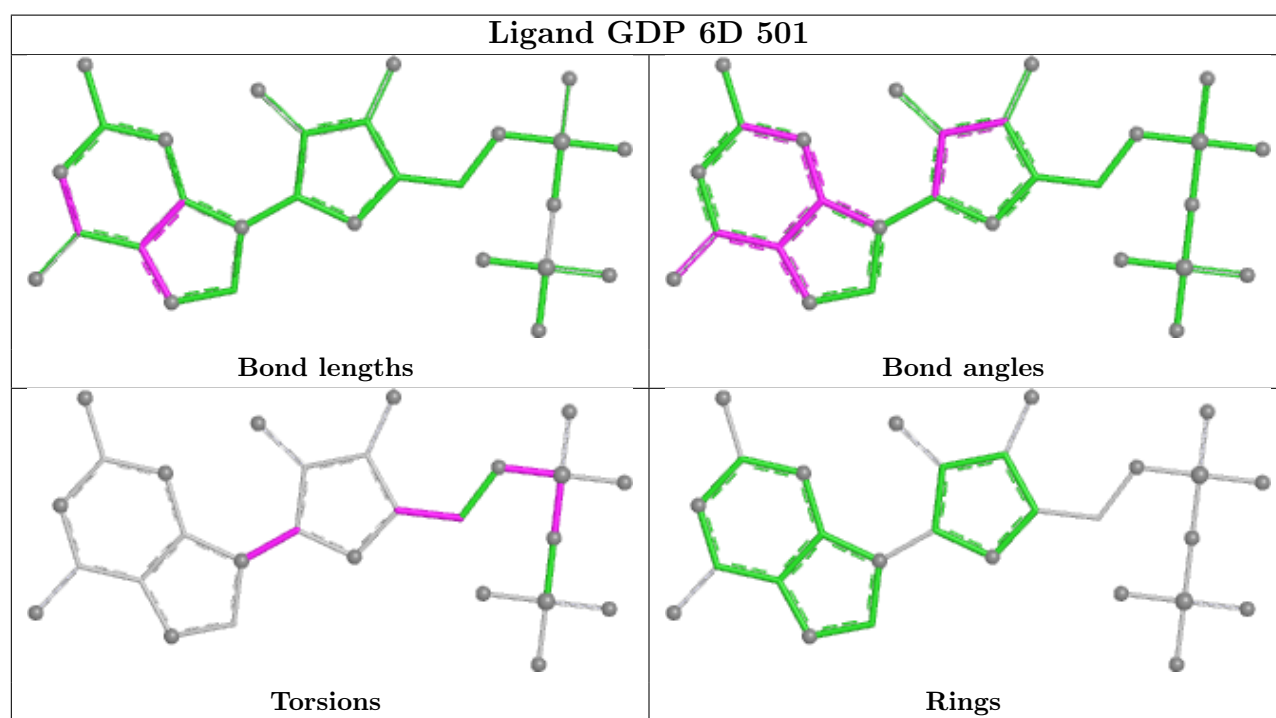
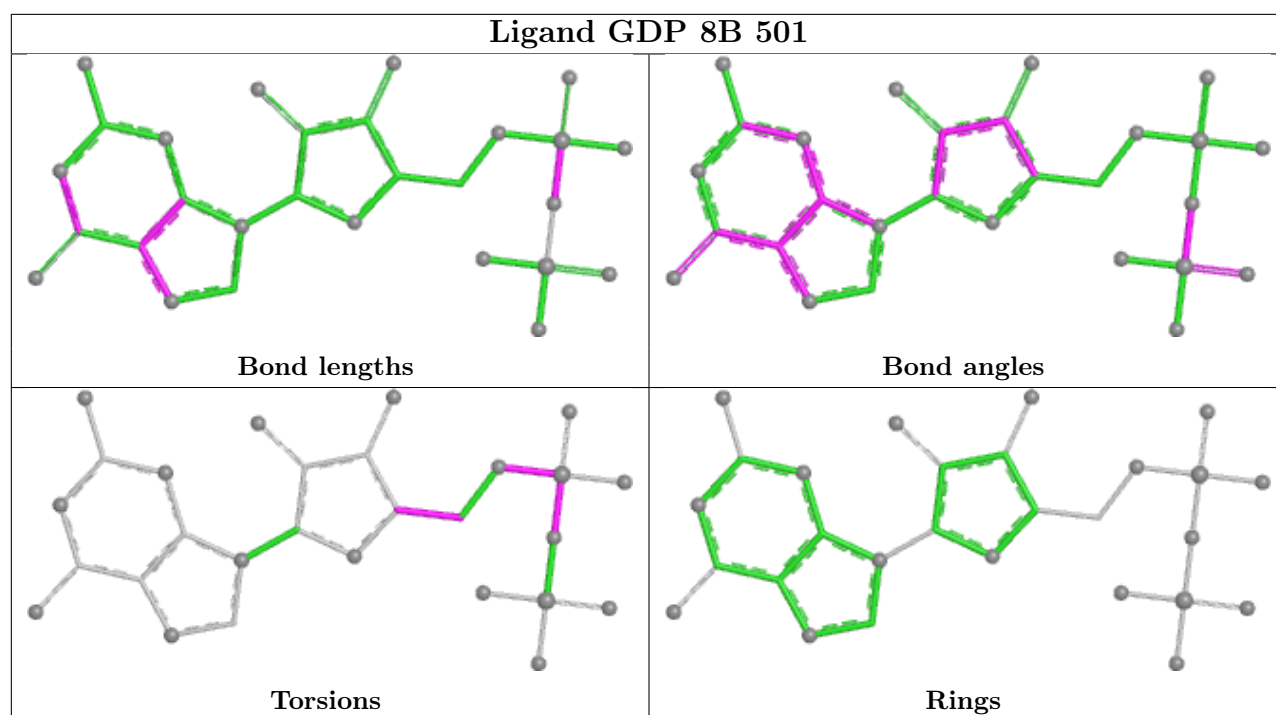


Ligand GTP 6G 501

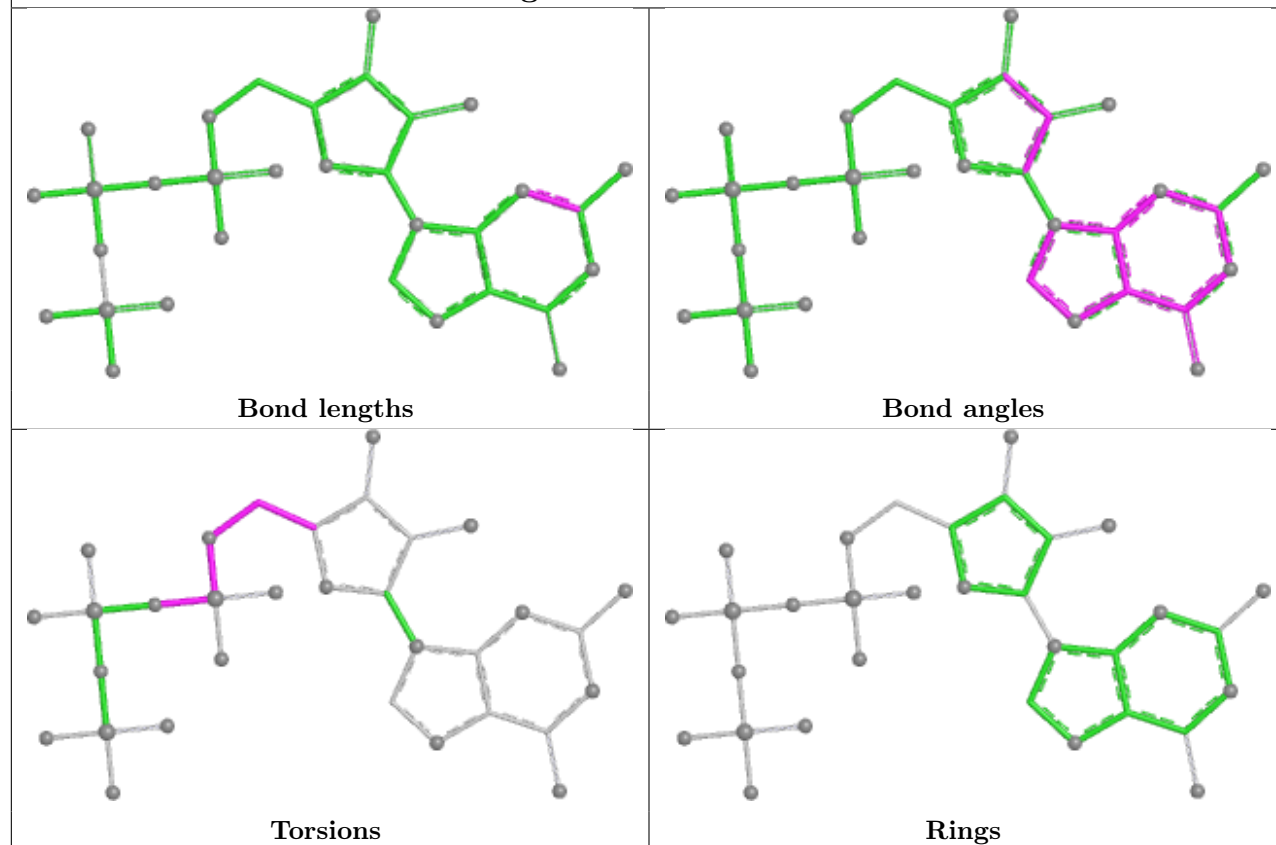




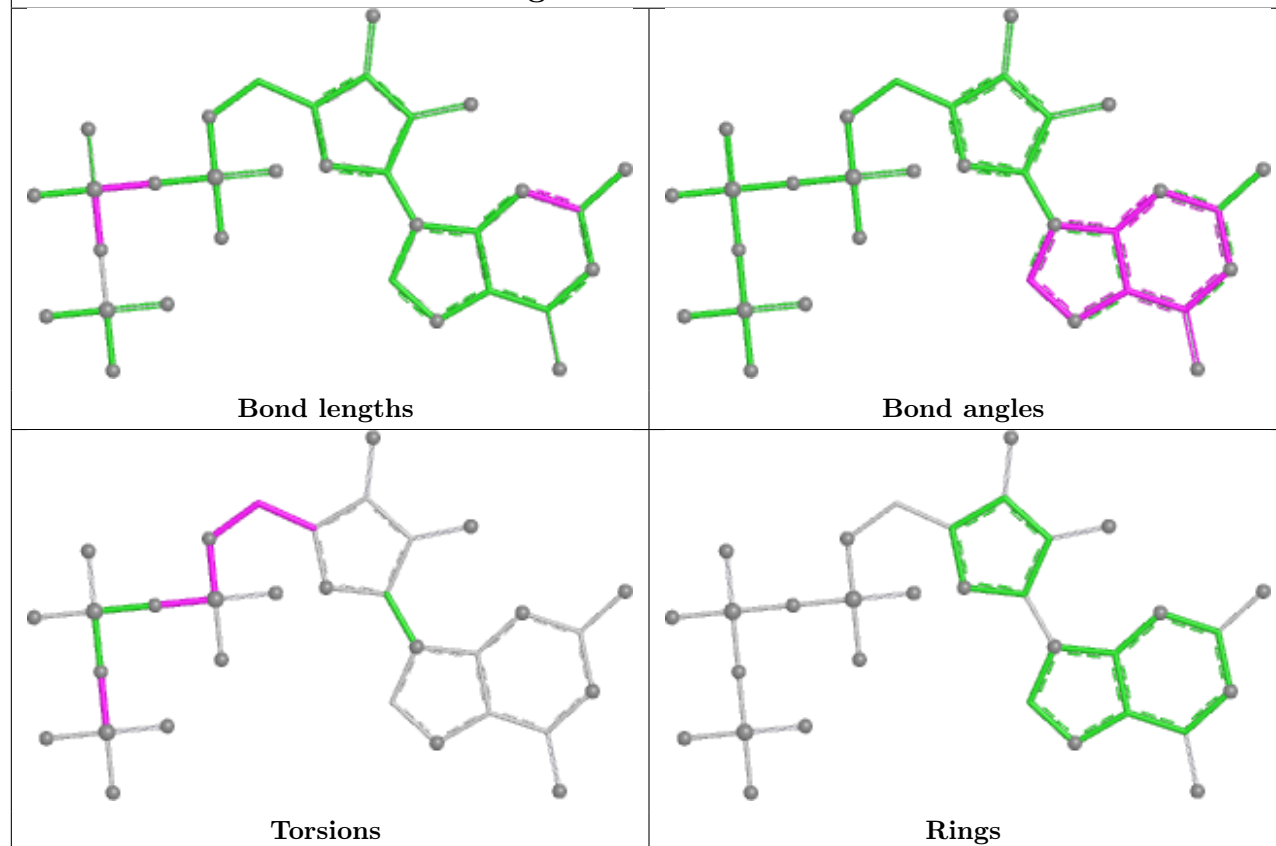


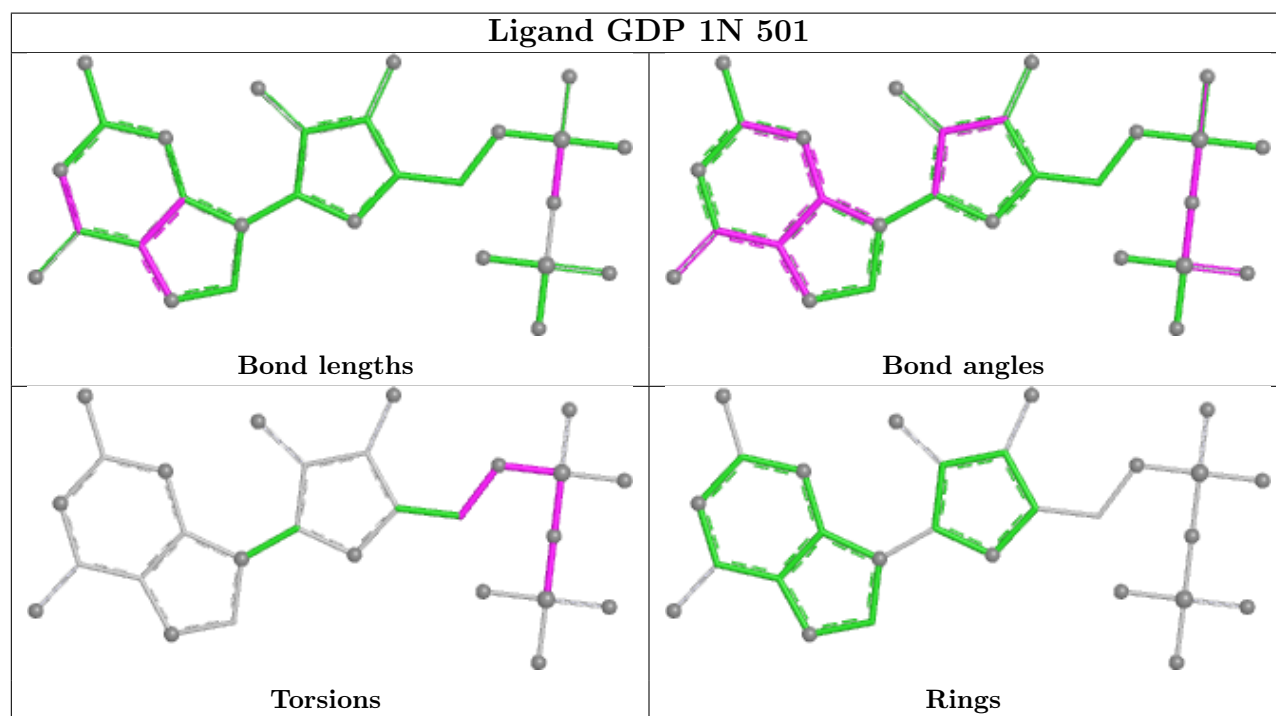
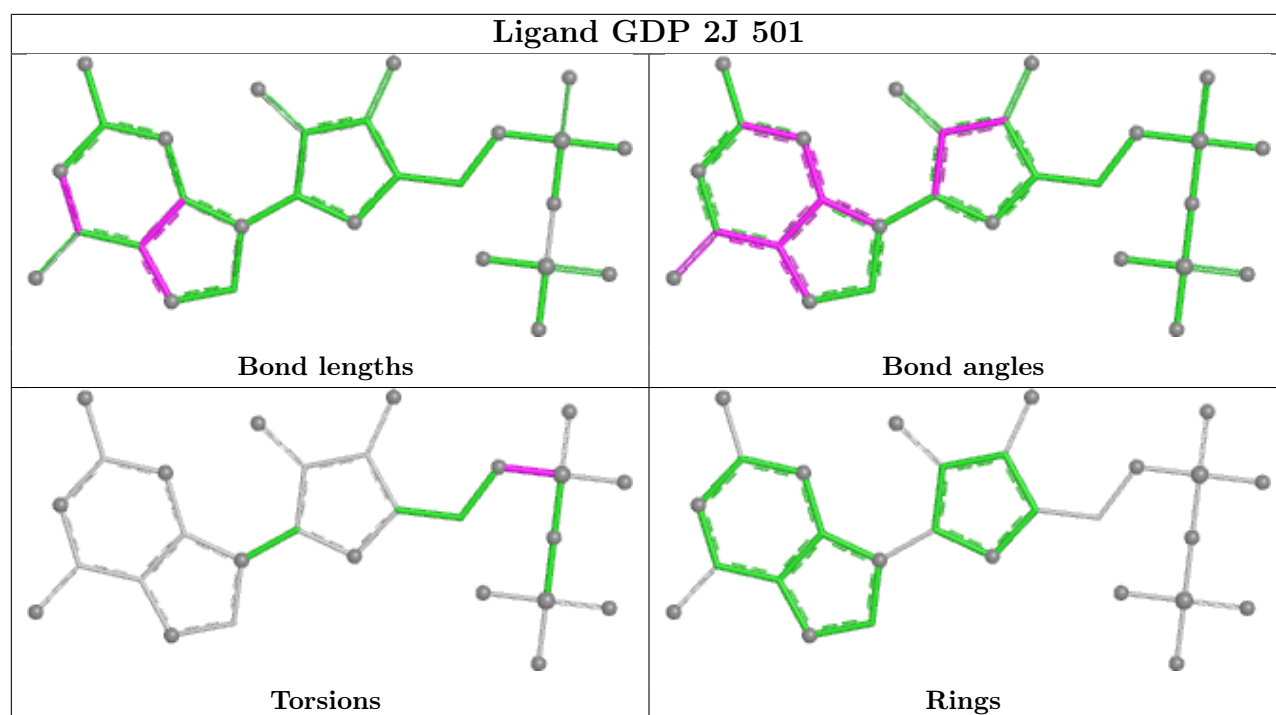


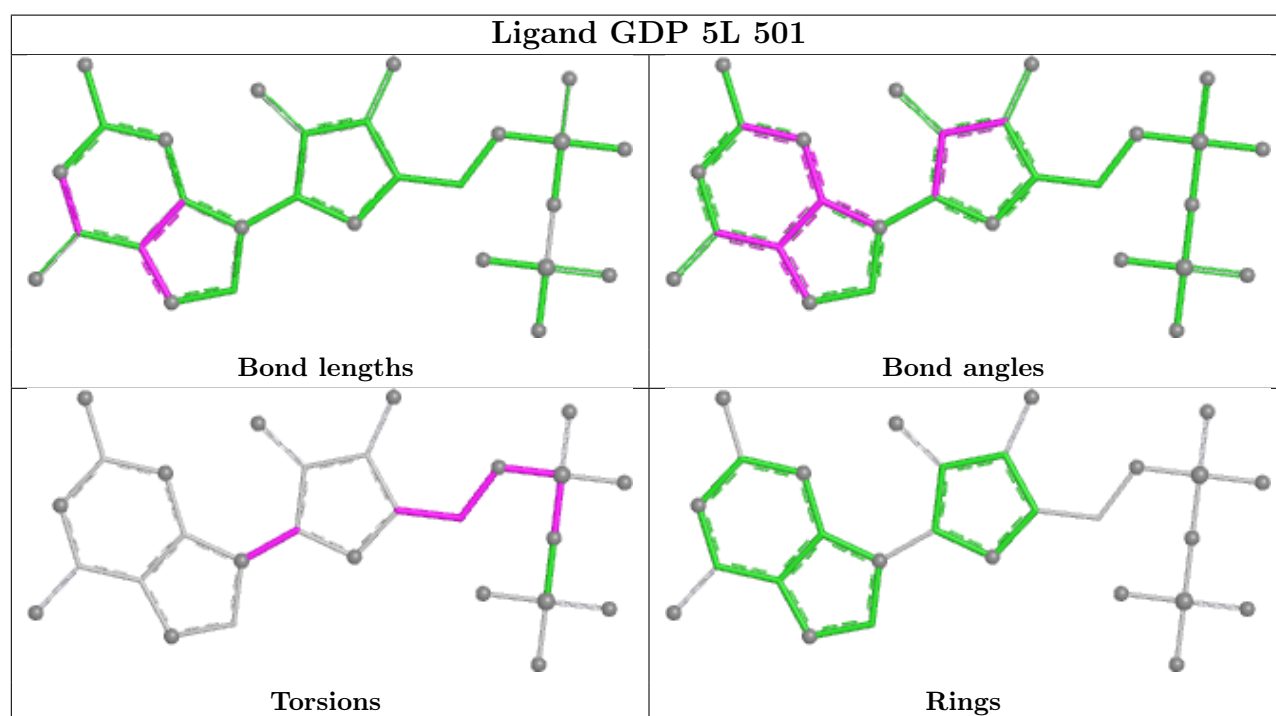
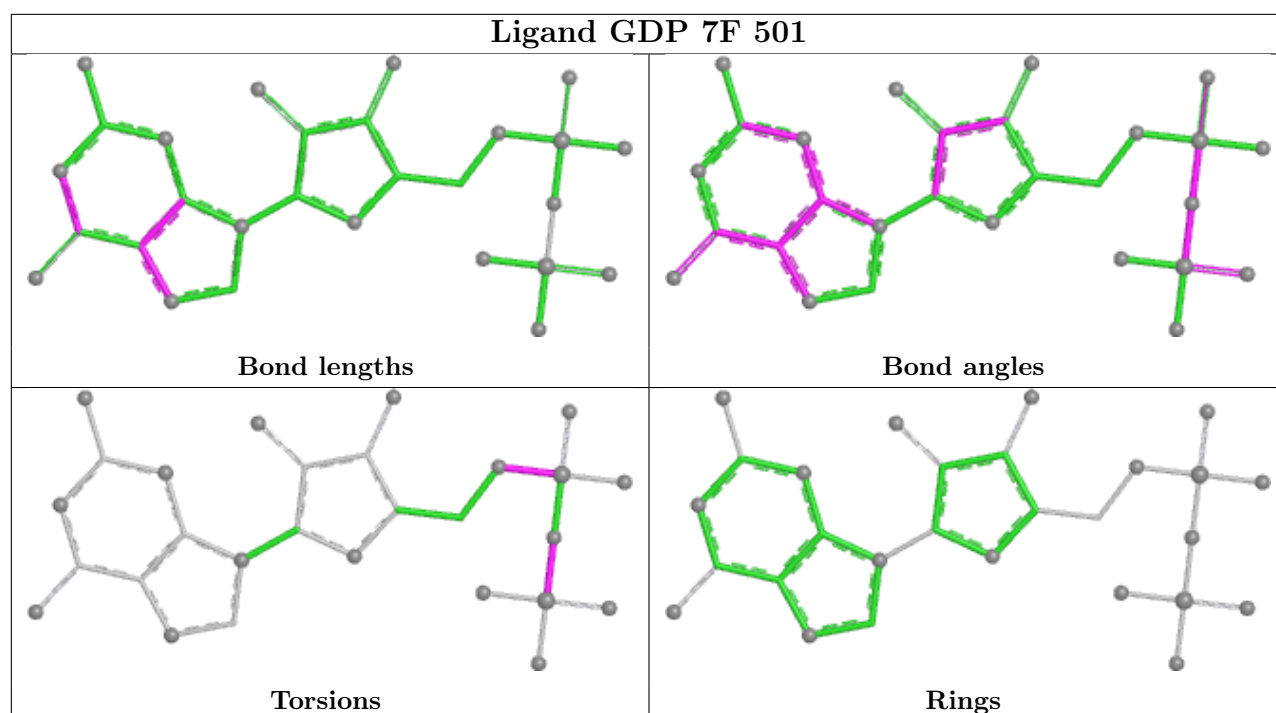
Ligand GTP 2K 501

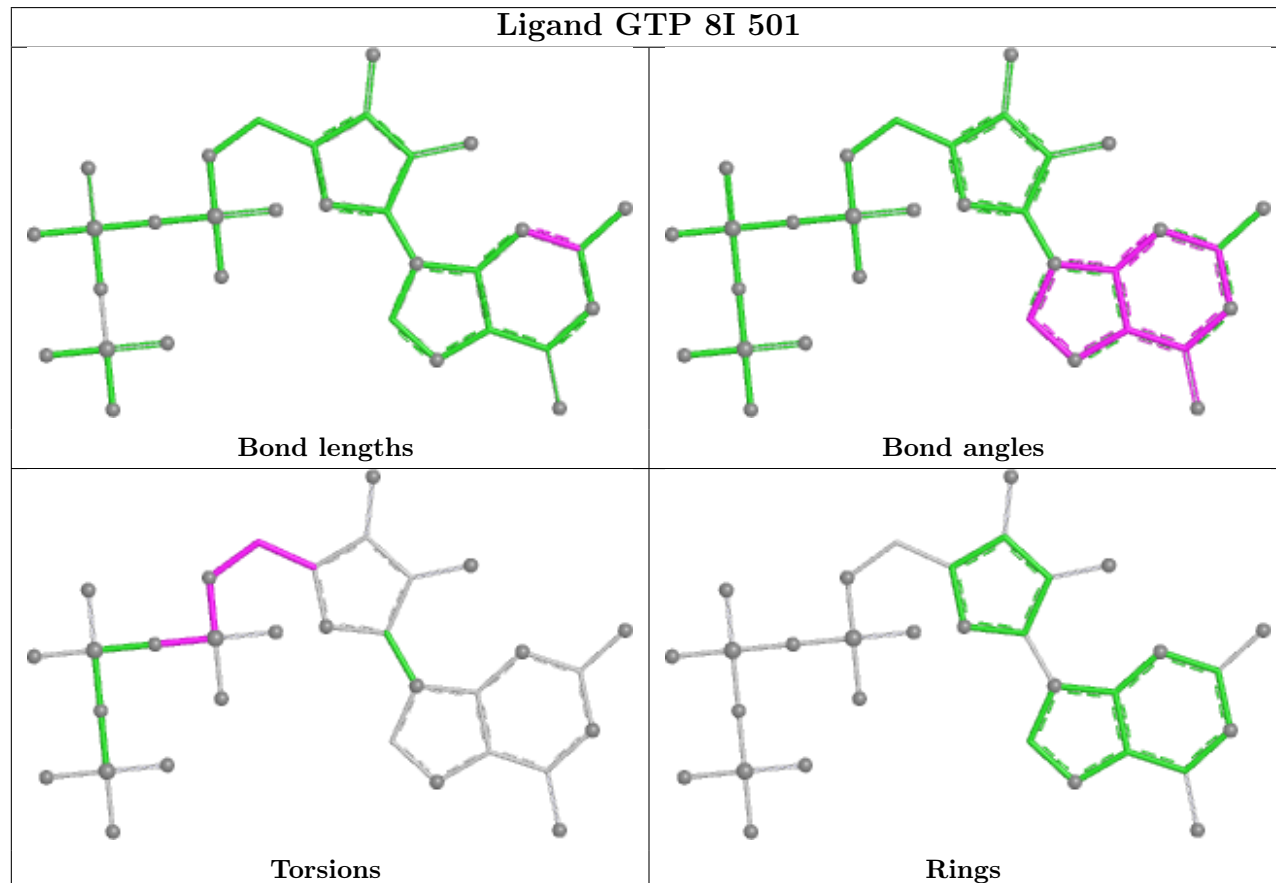
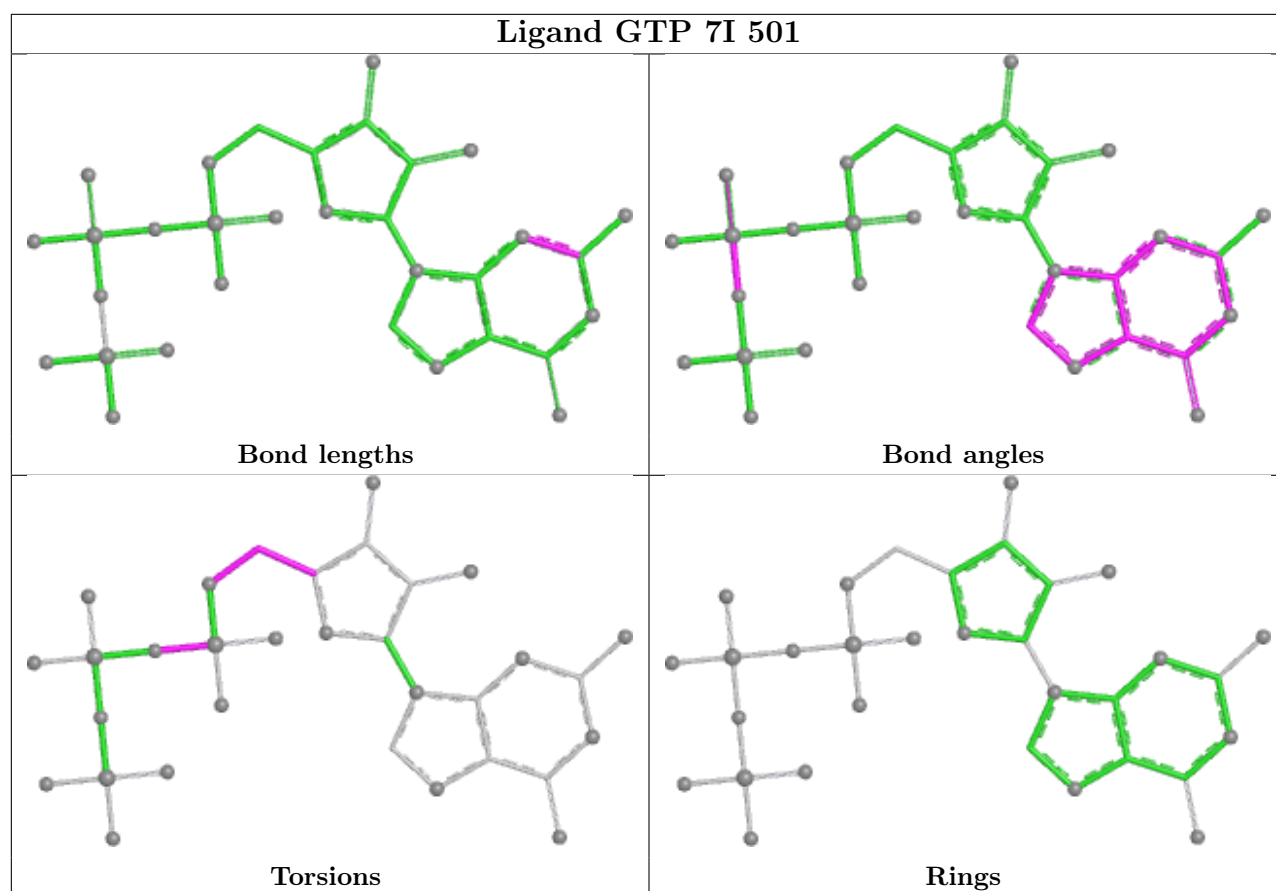


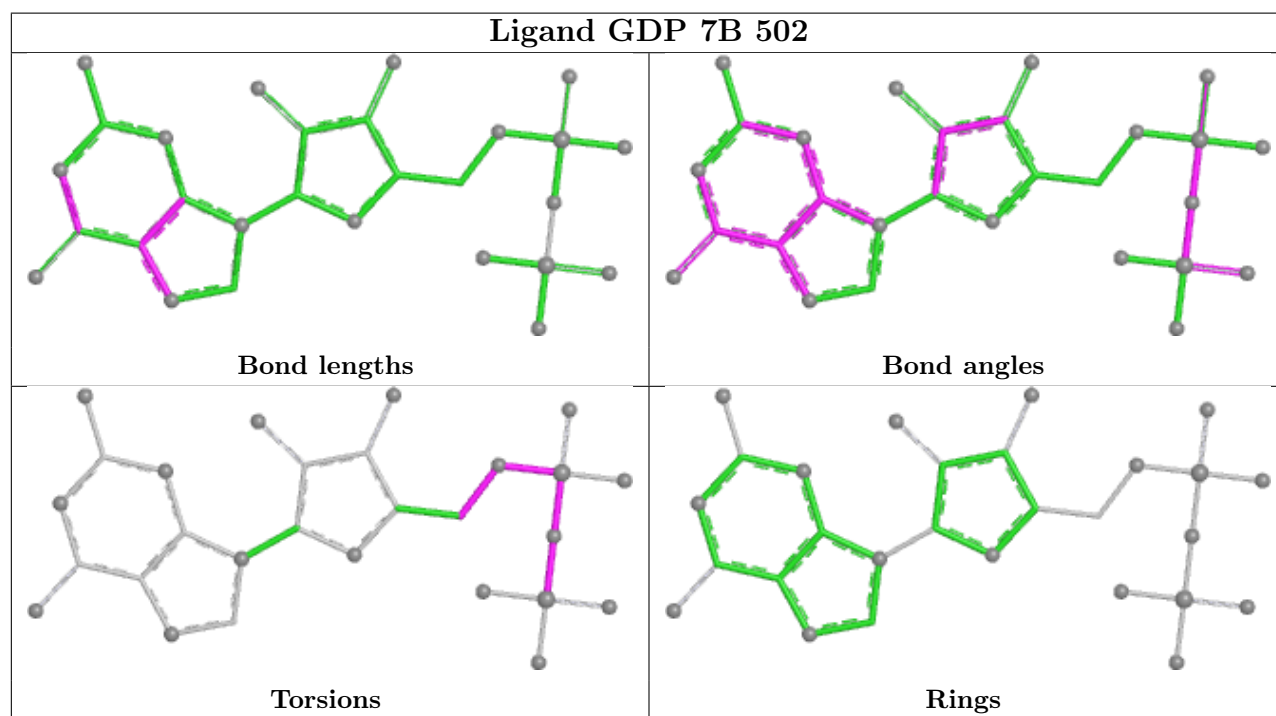
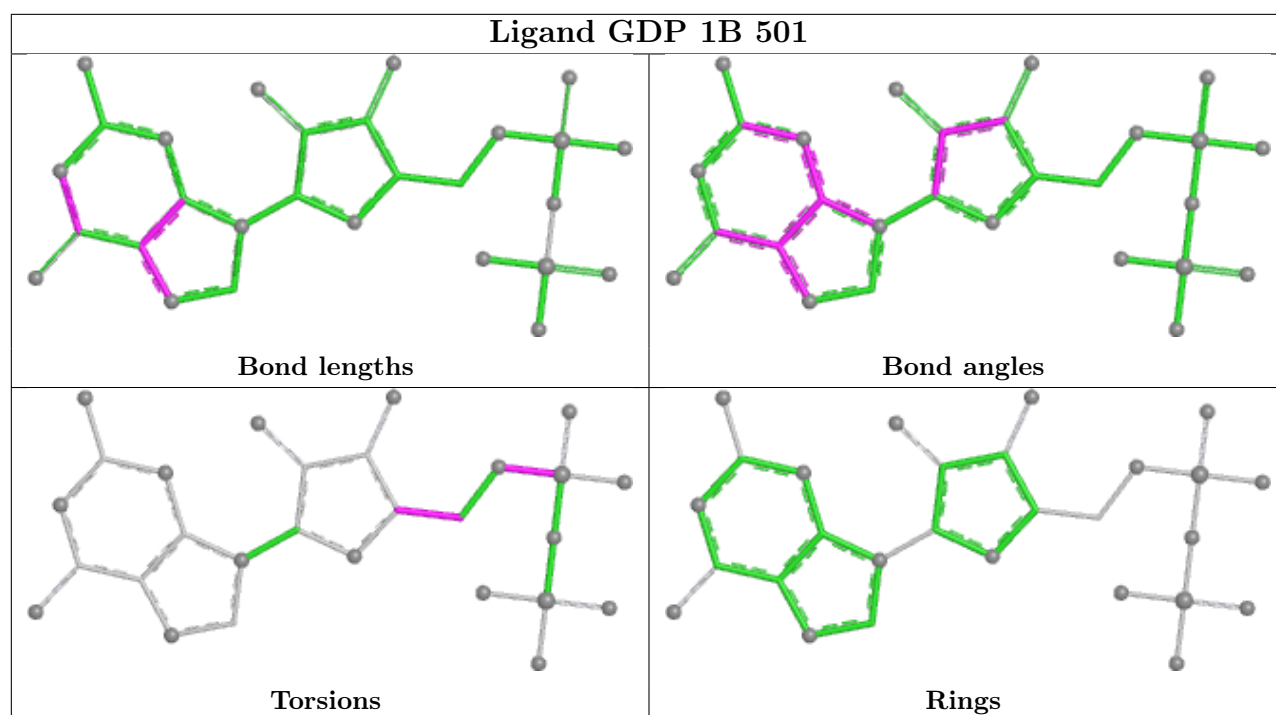
Ligand GTP 9I 501

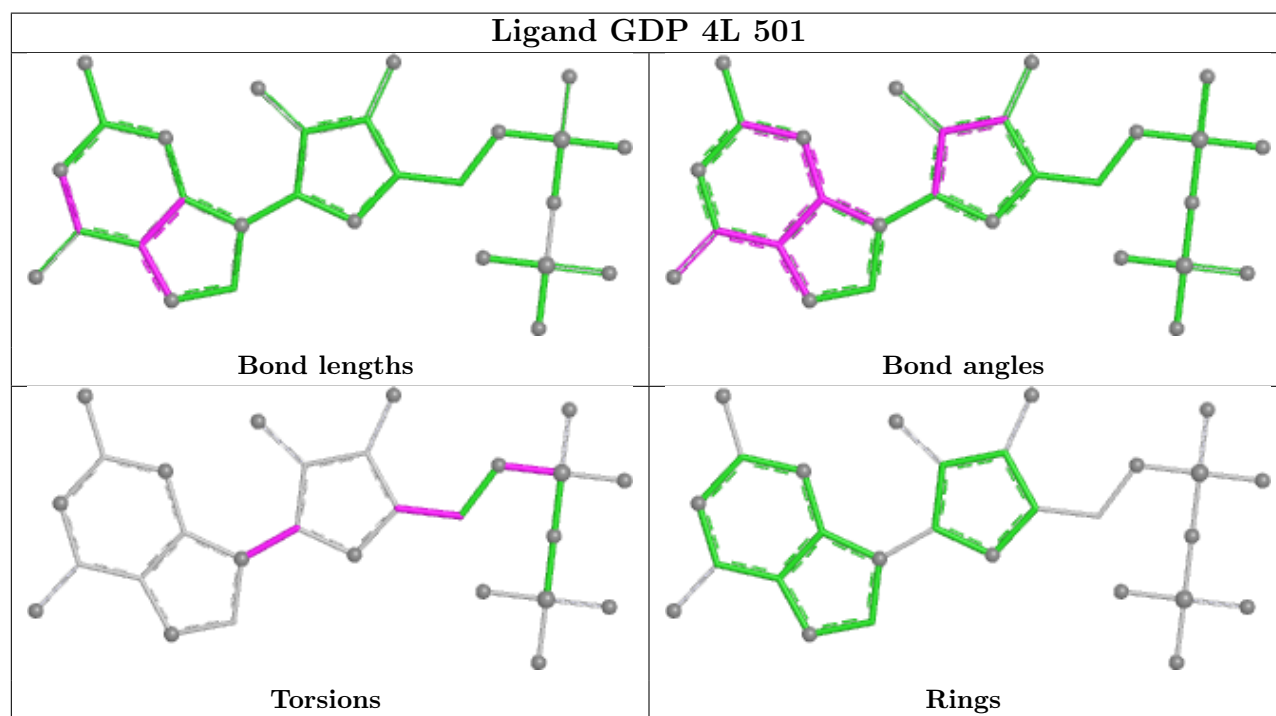
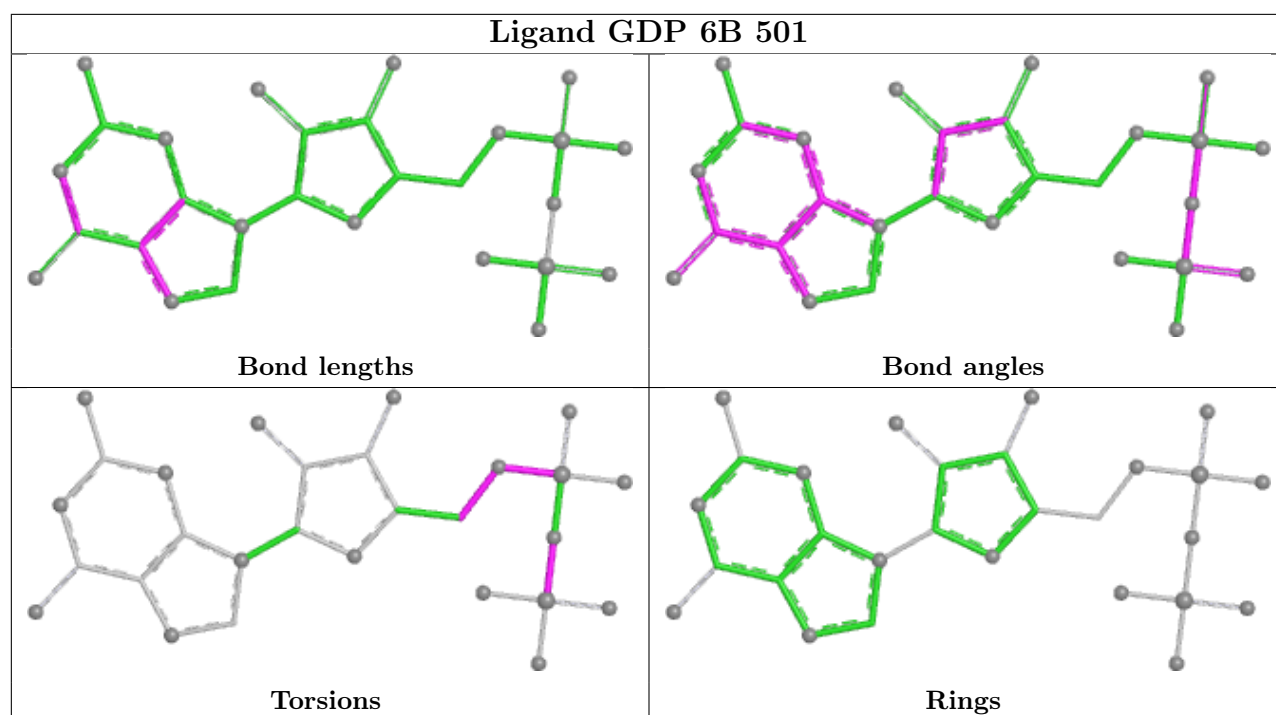




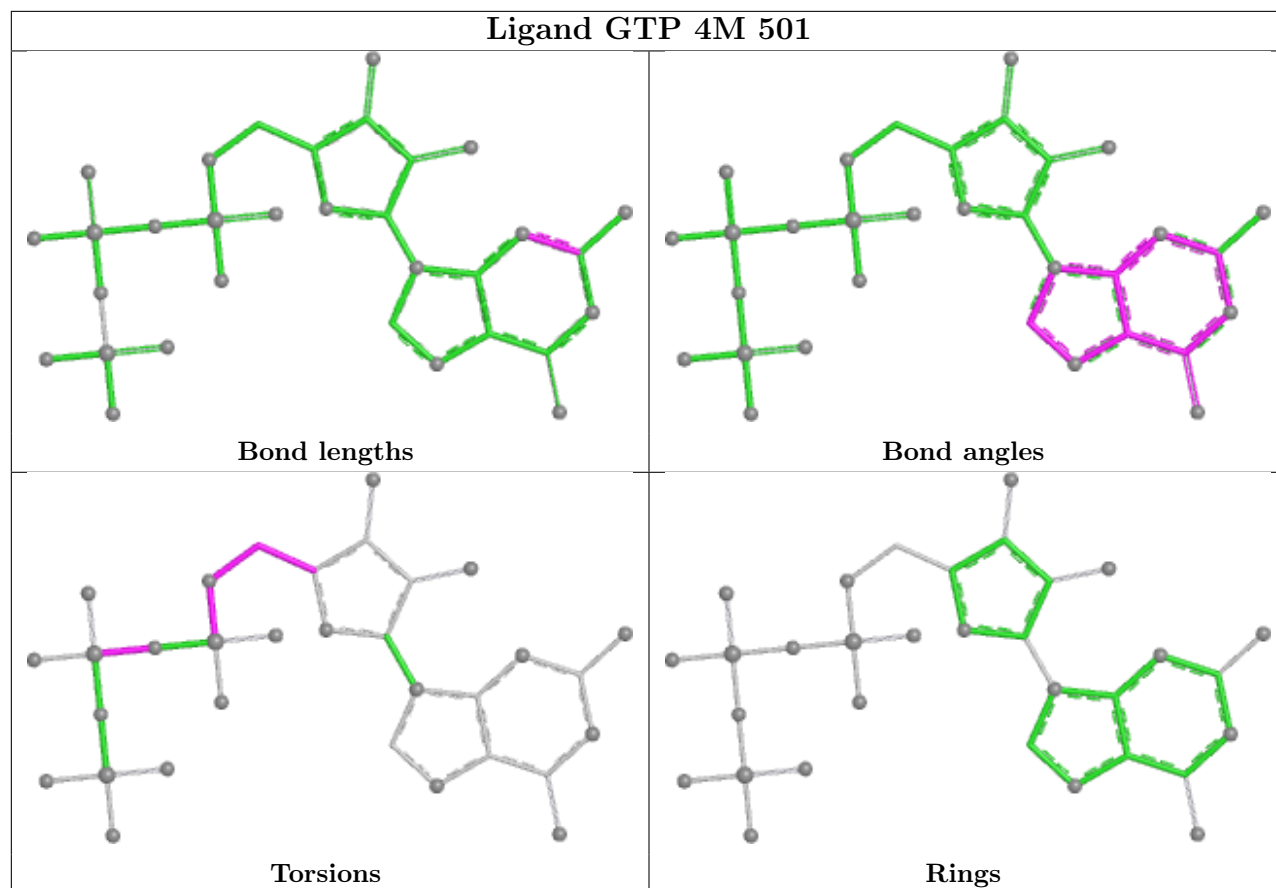




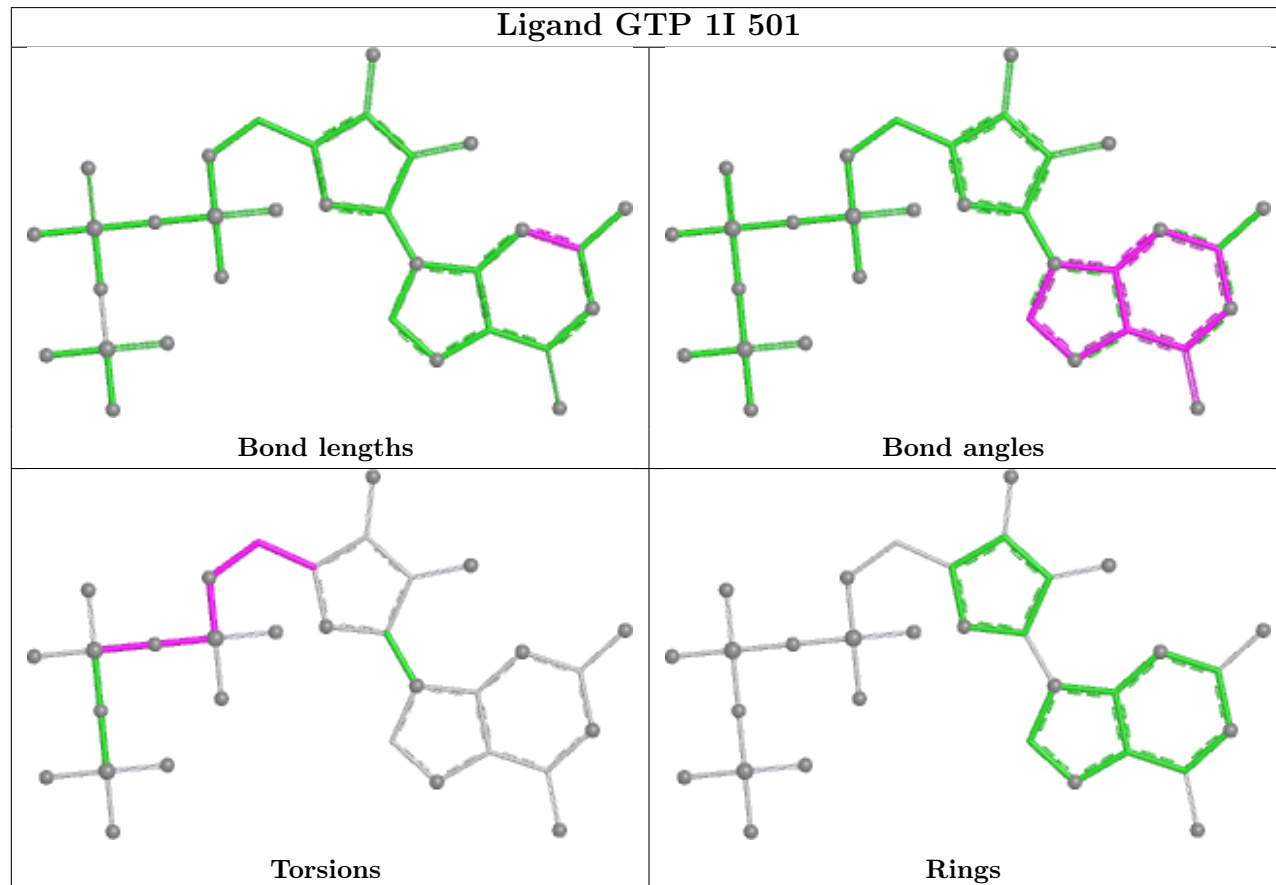


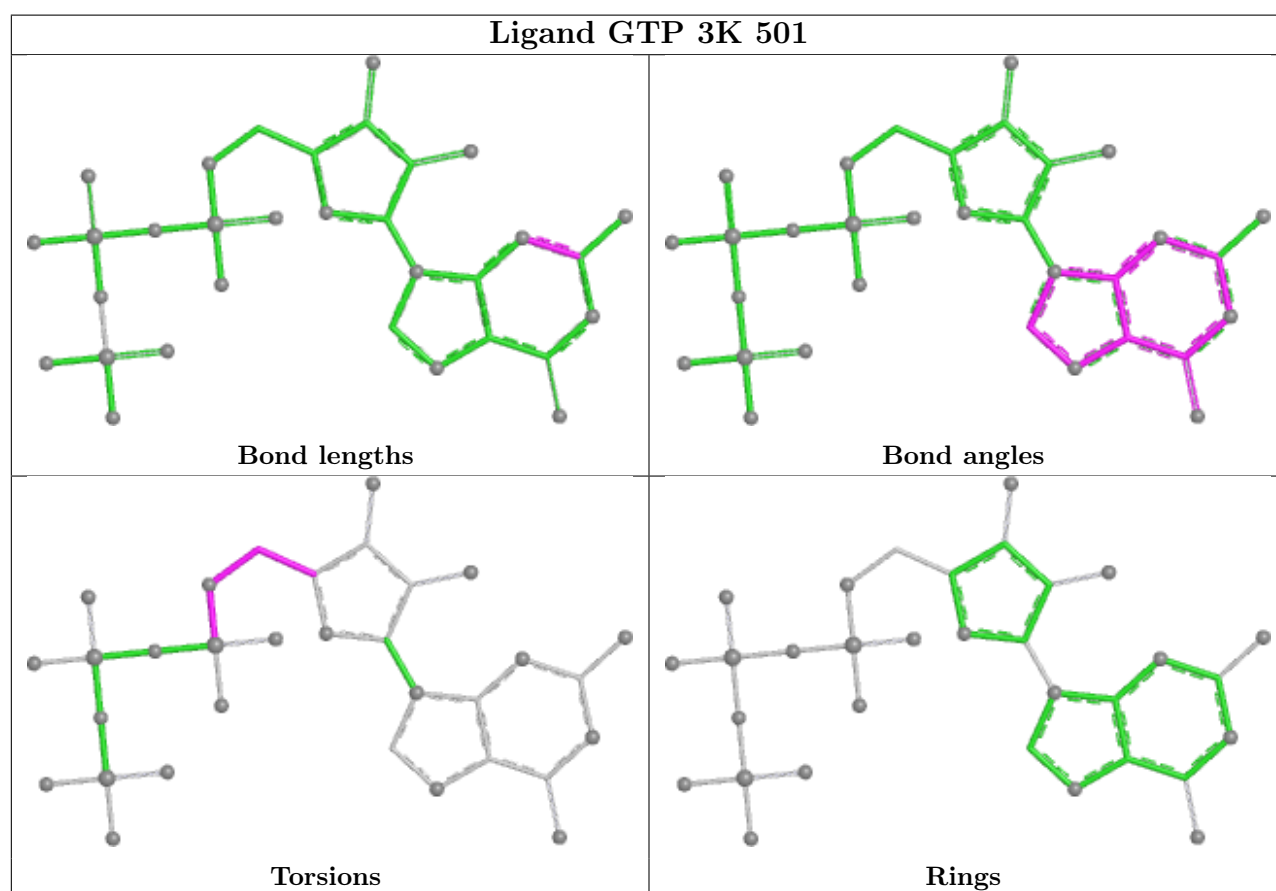
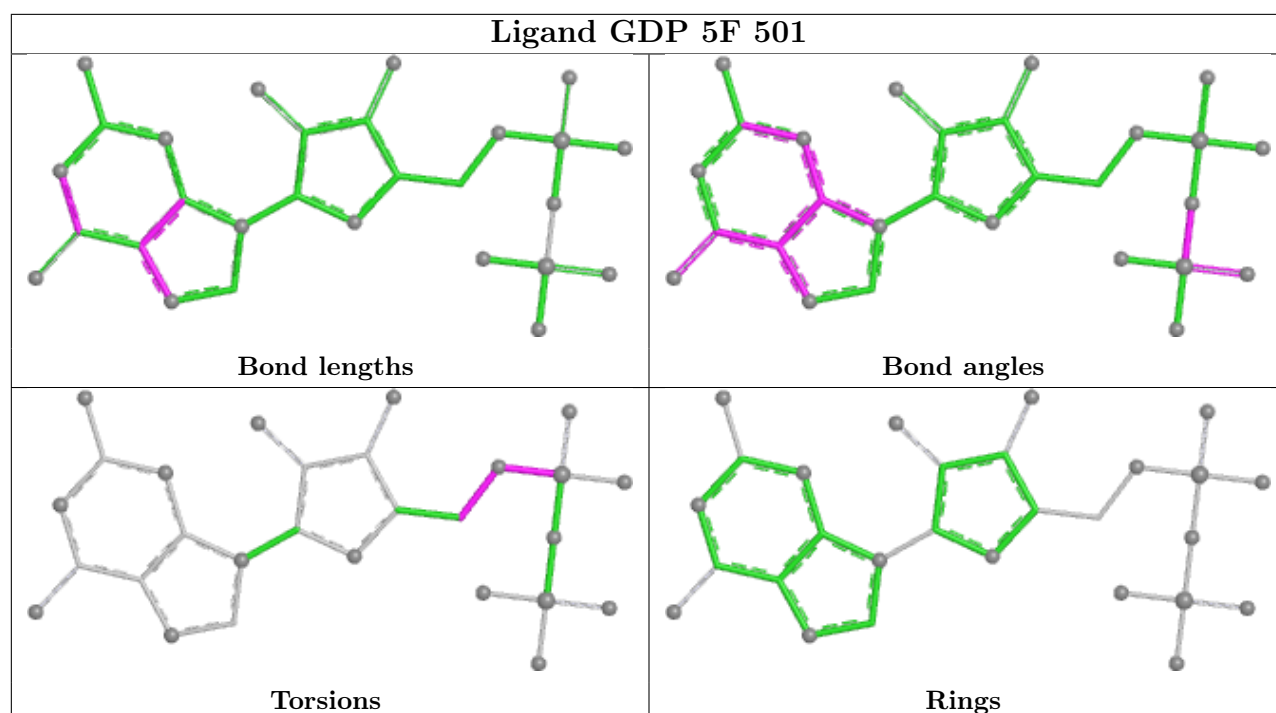


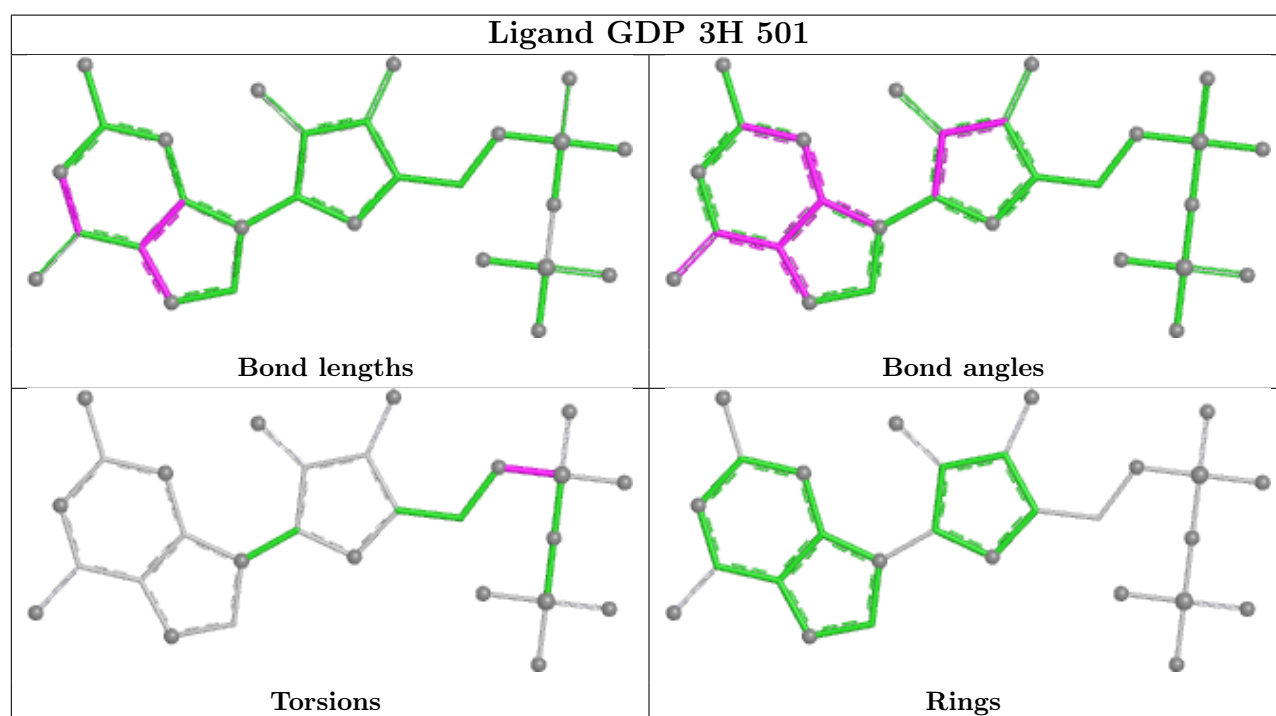
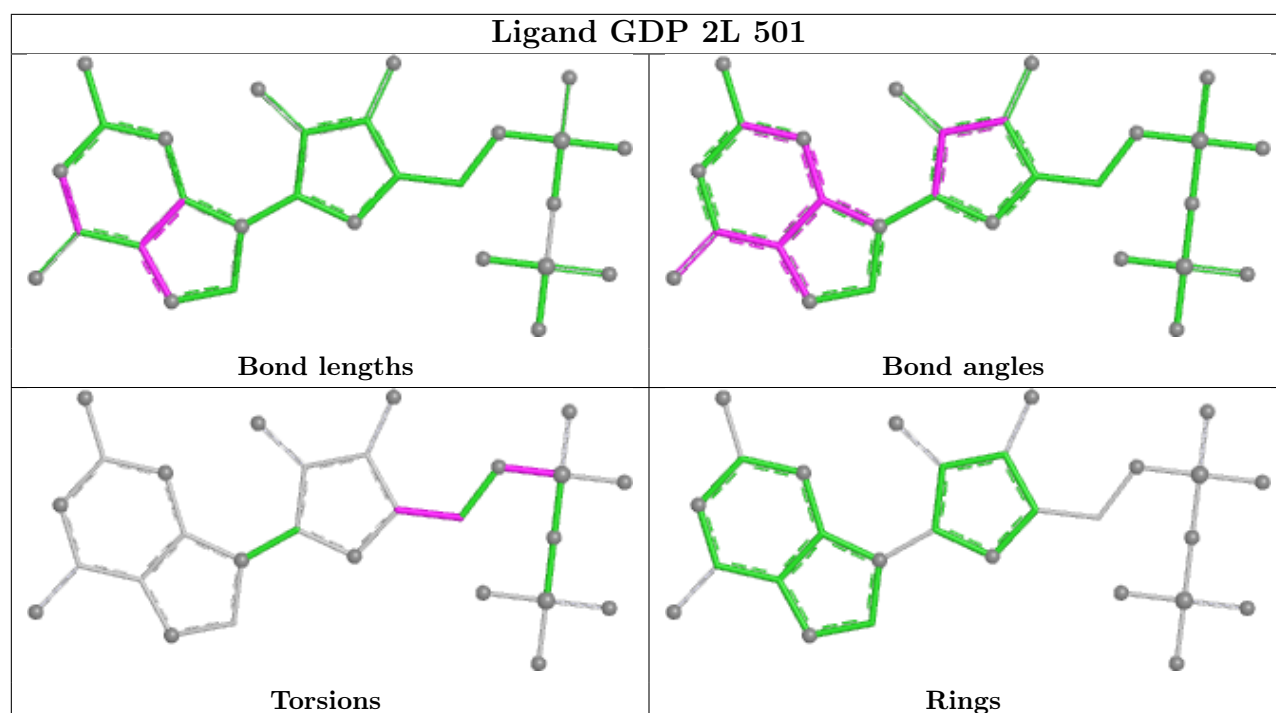
Ligand GTP 4M 501

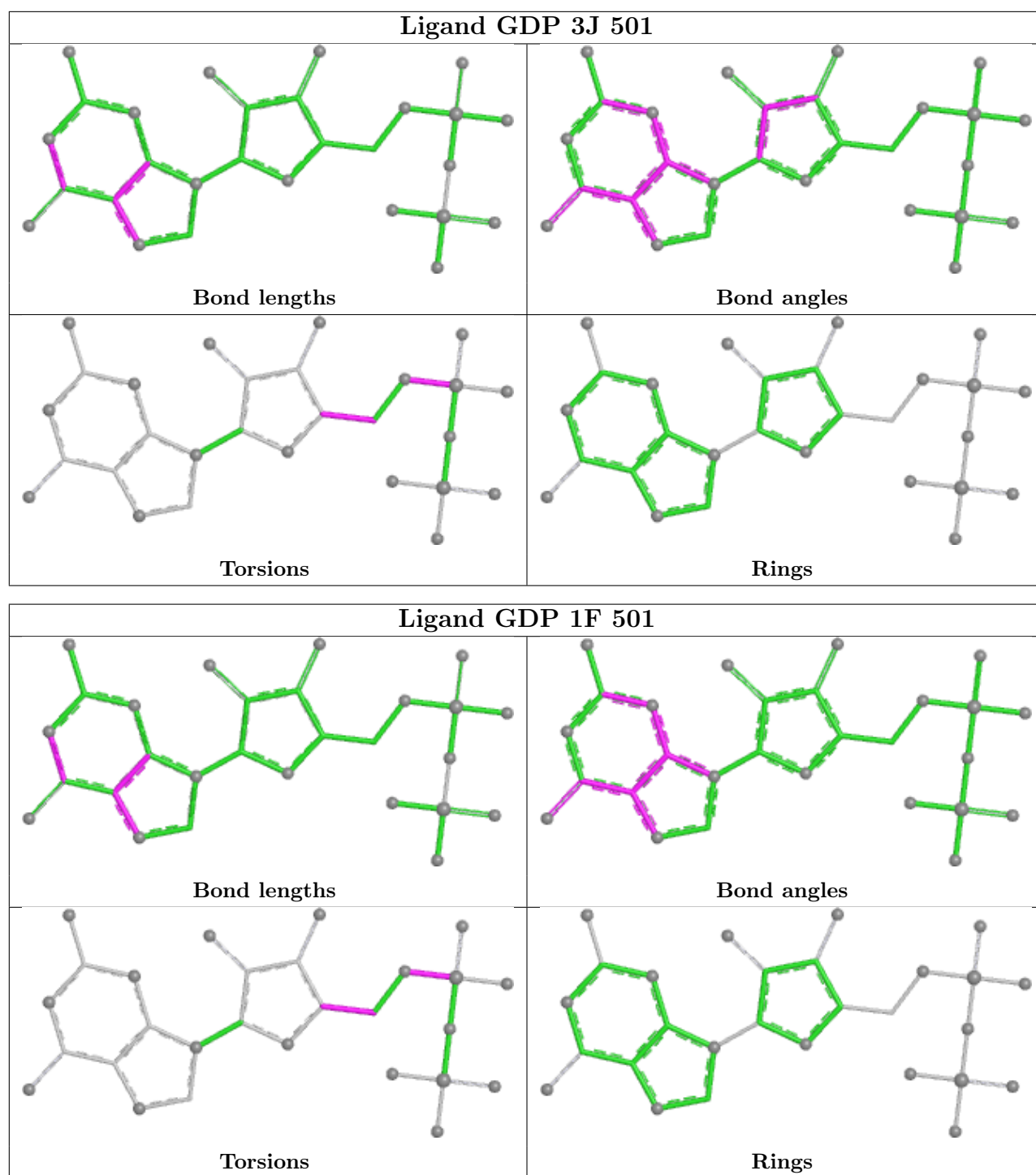


Ligand GTP 1I 501









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

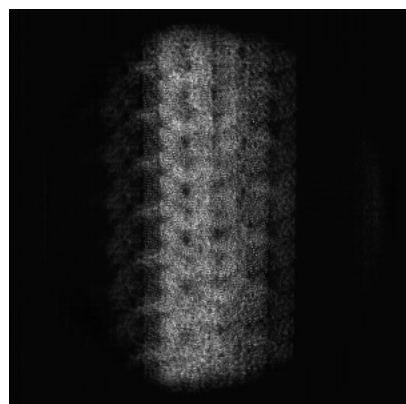
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-72715. These allow visual inspection of the internal detail of the map and identification of artifacts.

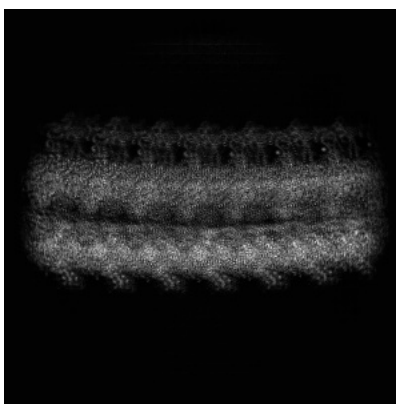
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

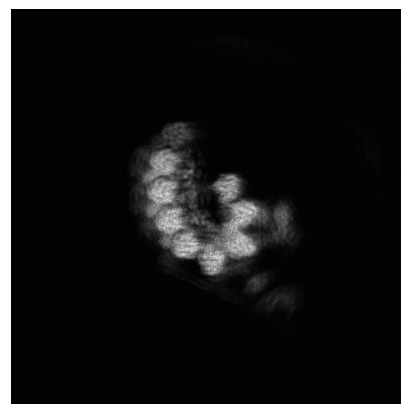
6.1.1 Primary map



X

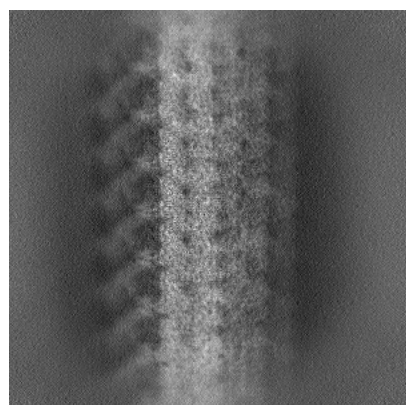


Y

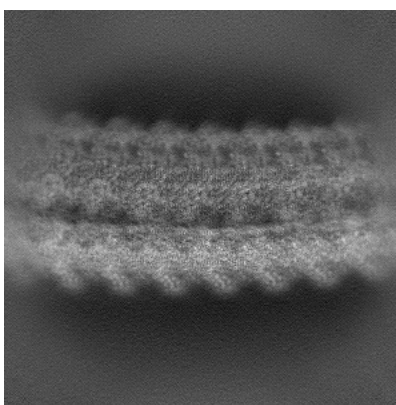


Z

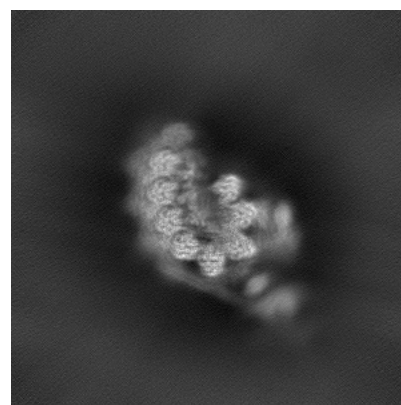
6.1.2 Raw map



X



Y

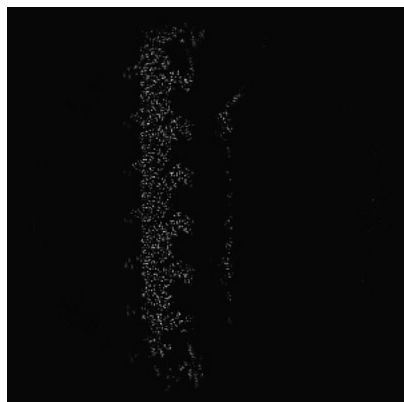


Z

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

6.2 Central slices [i](#)

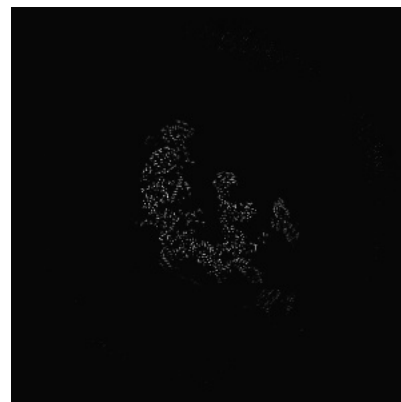
6.2.1 Primary map



X Index: 256

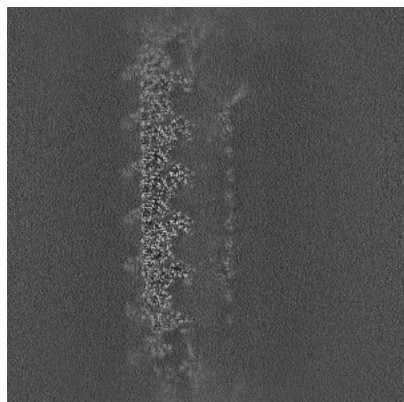


Y Index: 256

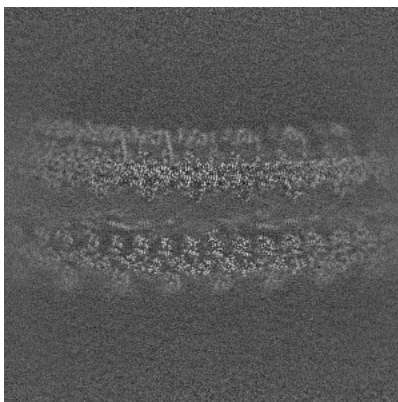


Z Index: 256

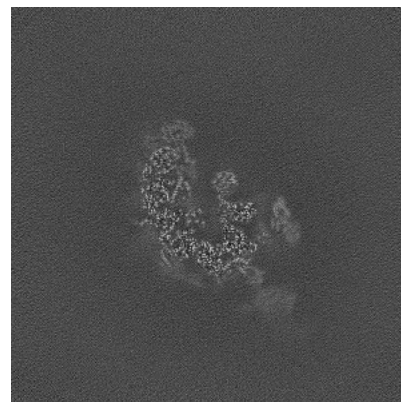
6.2.2 Raw map



X Index: 256



Y Index: 256



Z Index: 256

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: 201

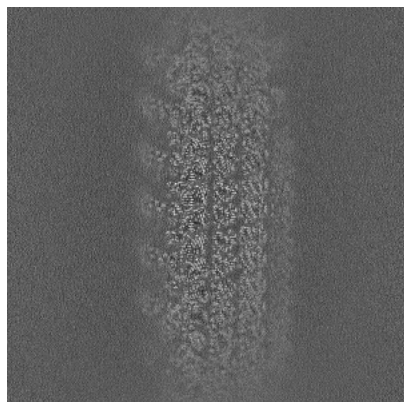


Y Index: 206

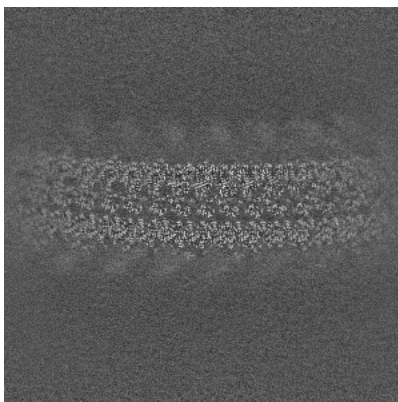


Z Index: 188

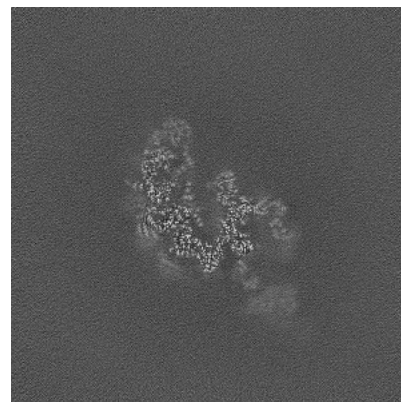
6.3.2 Raw map



X Index: 201



Y Index: 203

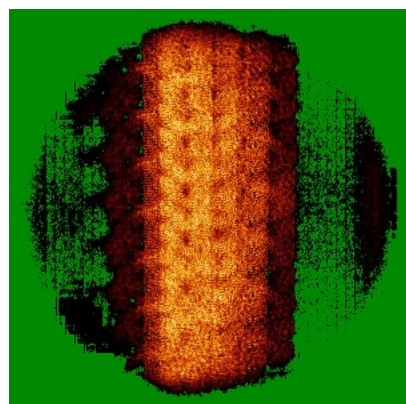


Z Index: 265

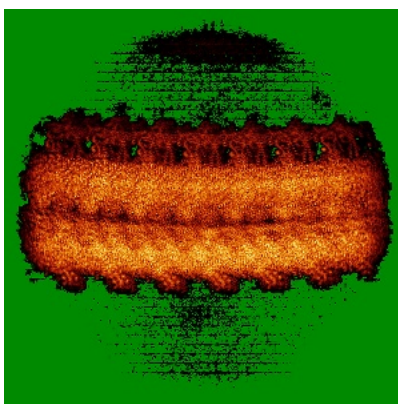
The images above show the largest variance slices of the map in three orthogonal directions.

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

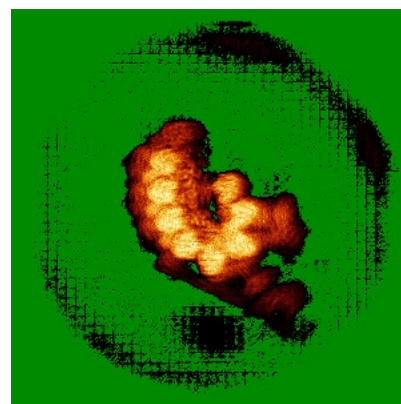
6.4.1 Primary map



X

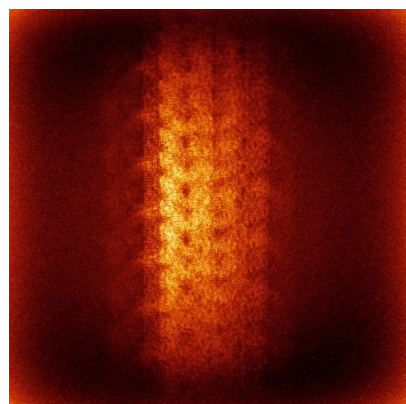


Y

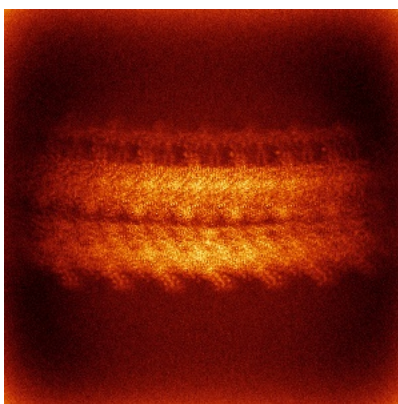


Z

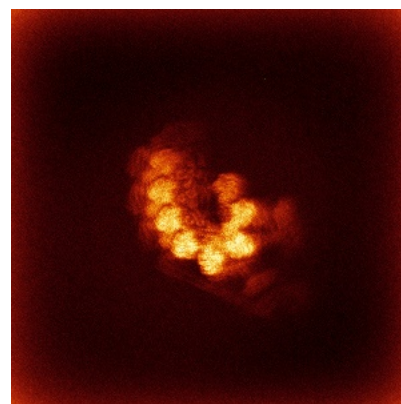
6.4.2 Raw map



X



Y

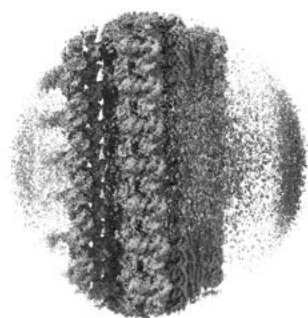


Z

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



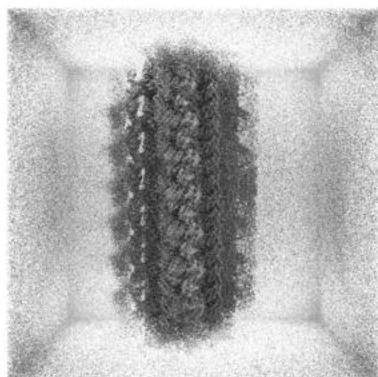
Y



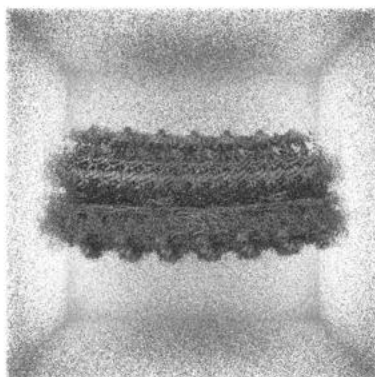
Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

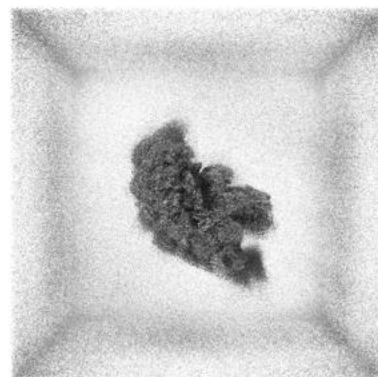
6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

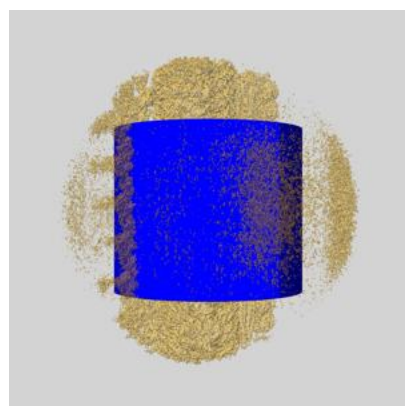
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

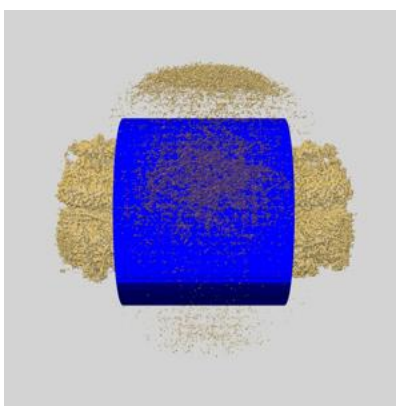
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

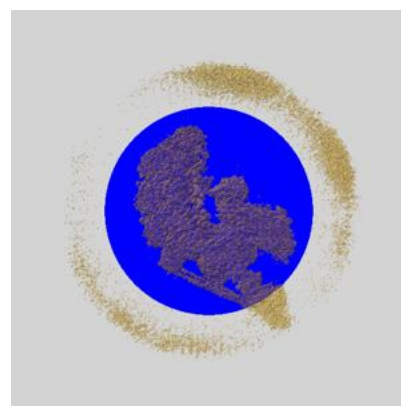
6.6.1 emd_72715_msk_1.map [i](#)



X



Y

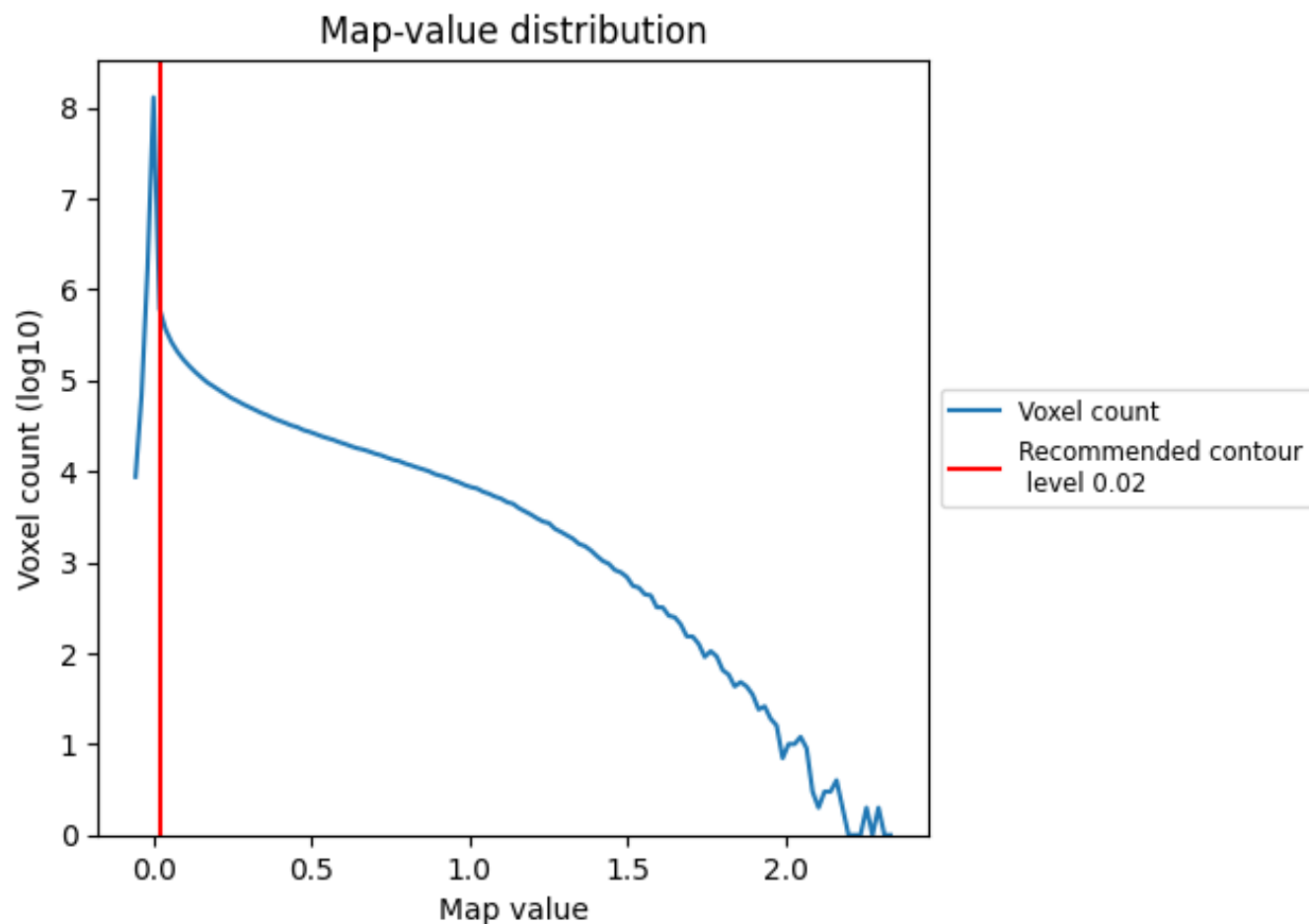


Z

7 Map analysis [i](#)

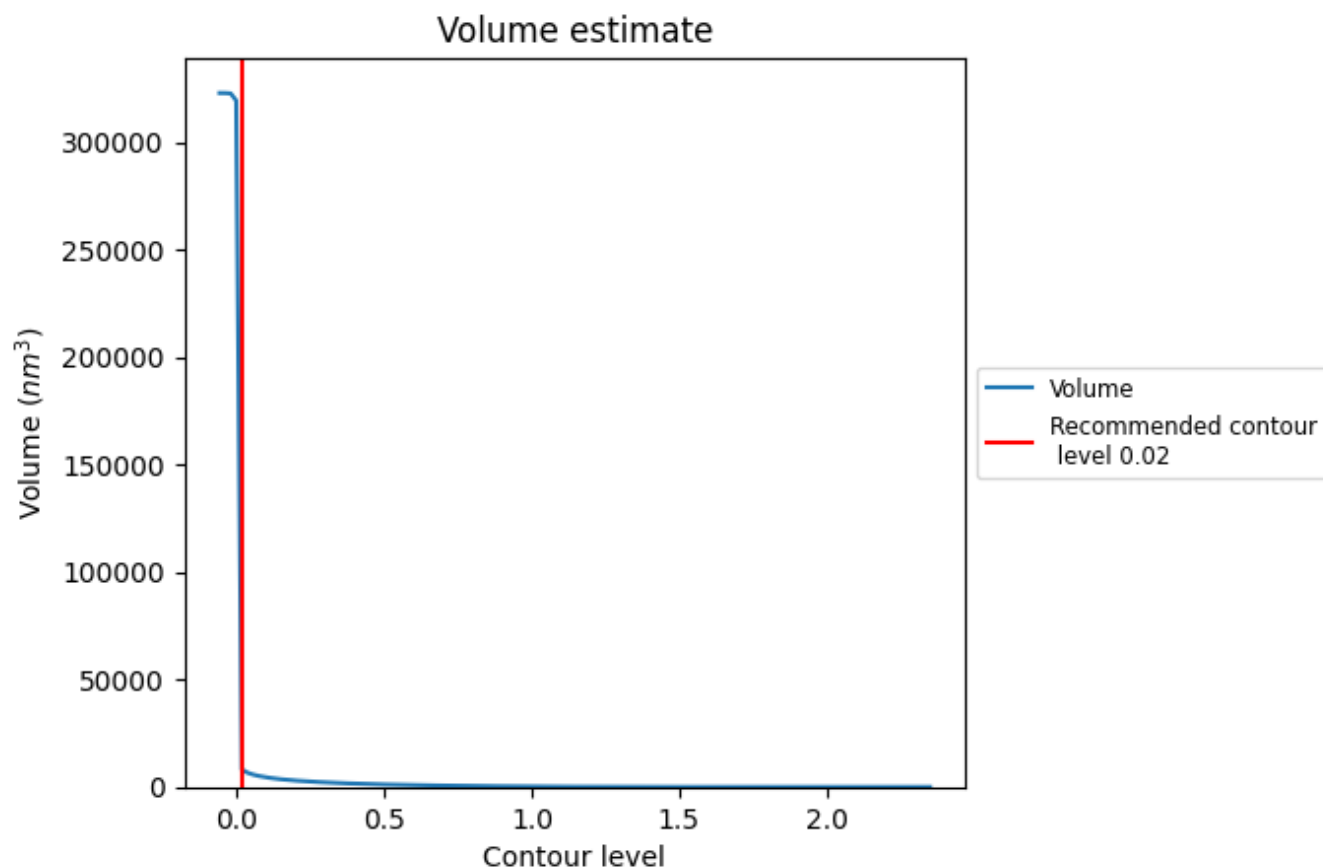
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

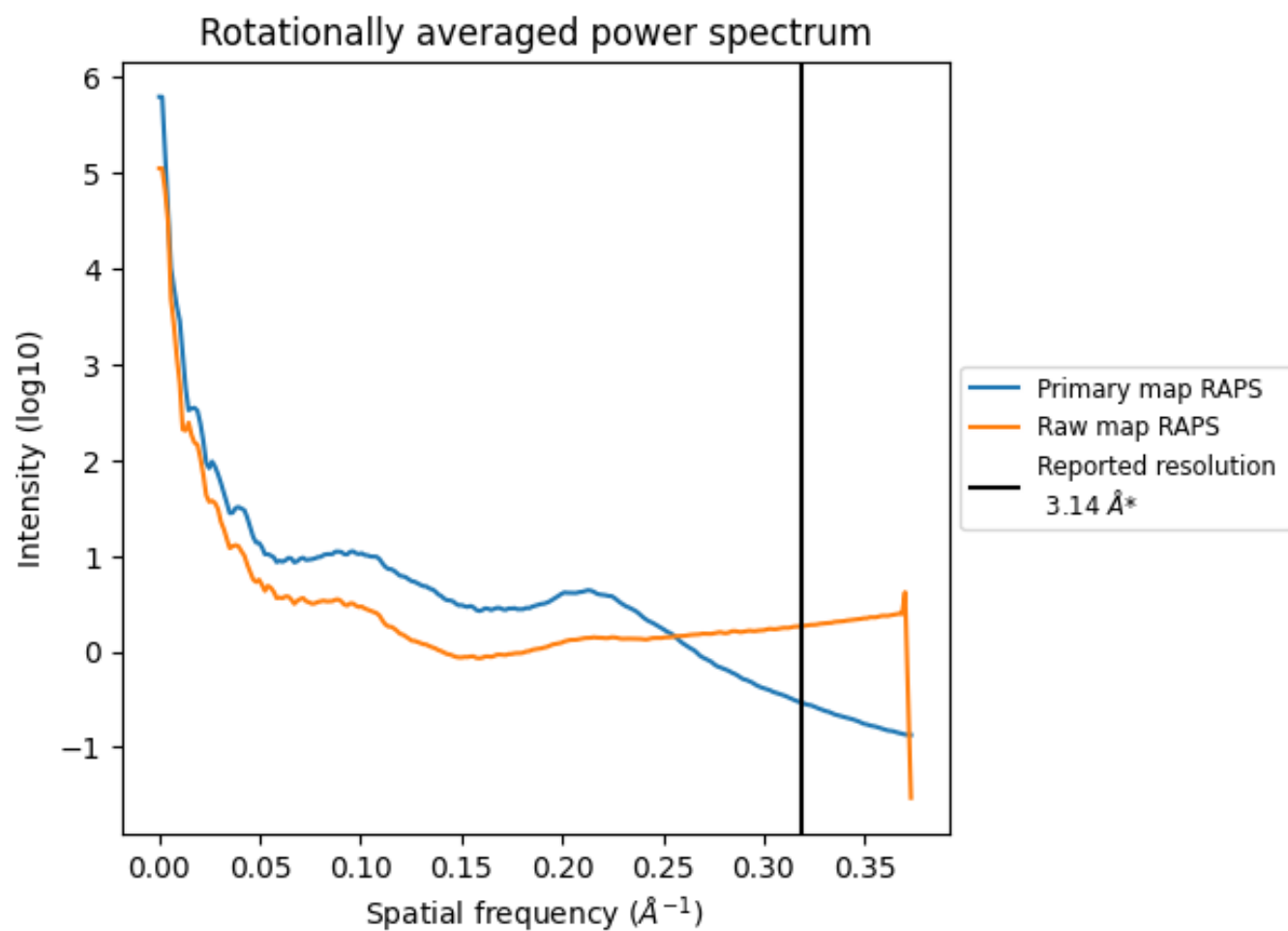
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 7892 nm^3 ; this corresponds to an approximate mass of 7129 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

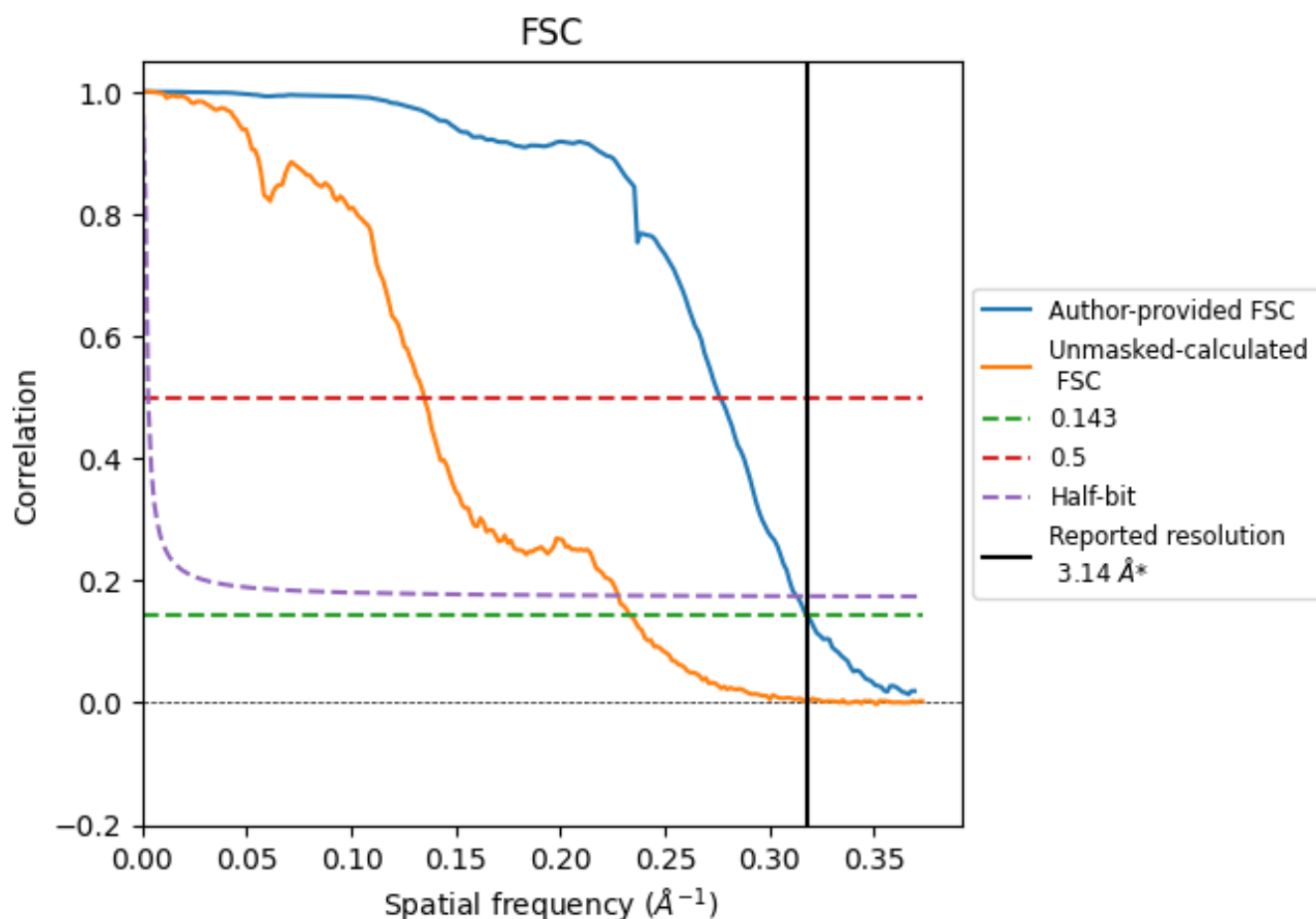


*Reported resolution corresponds to spatial frequency of 0.318 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.318 Å⁻¹

8.2 Resolution estimates [i](#)

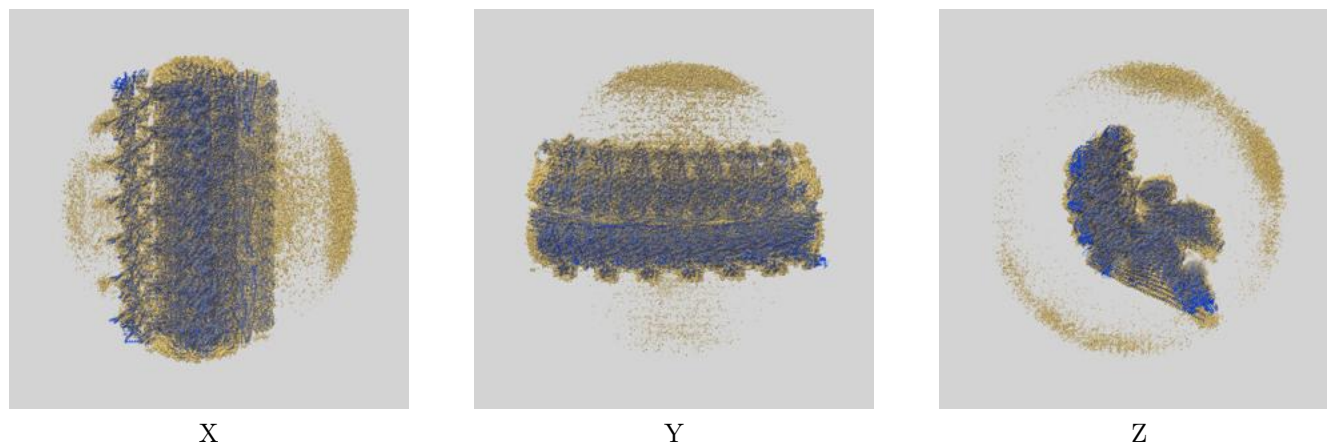
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.14	-	-
Author-provided FSC curve	3.14	3.62	3.19
Unmasked-calculated*	4.29	7.41	4.39

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.29 differs from the reported value 3.14 by more than 10 %

9 Map-model fit [i](#)

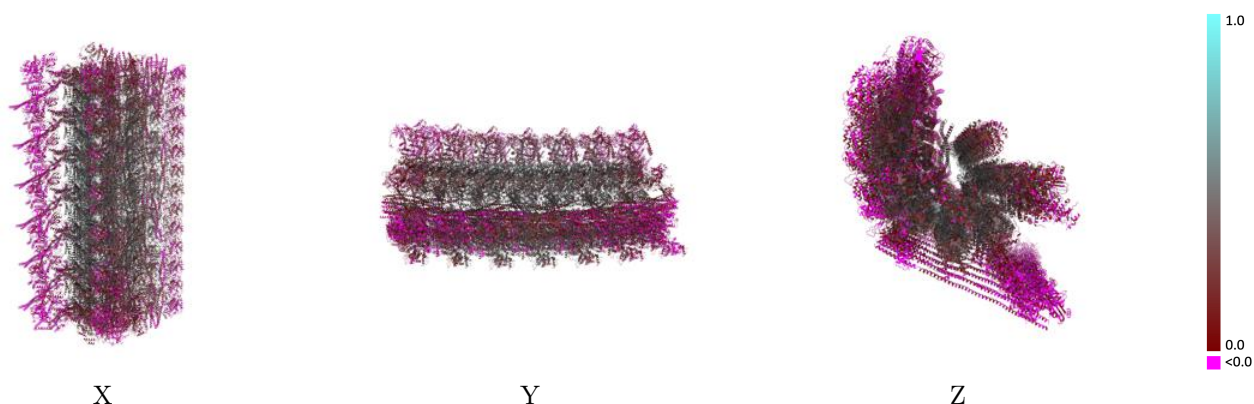
This section contains information regarding the fit between EMDB map EMD-72715 and PDB model 9Y9Z. Per-residue inclusion information can be found in section [3](#) on page [47](#).

9.1 Map-model overlay [i](#)



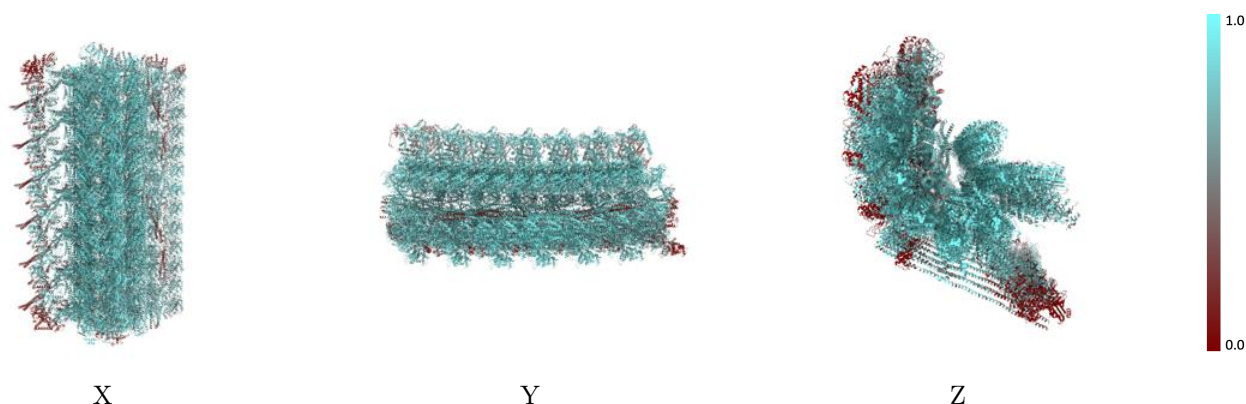
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



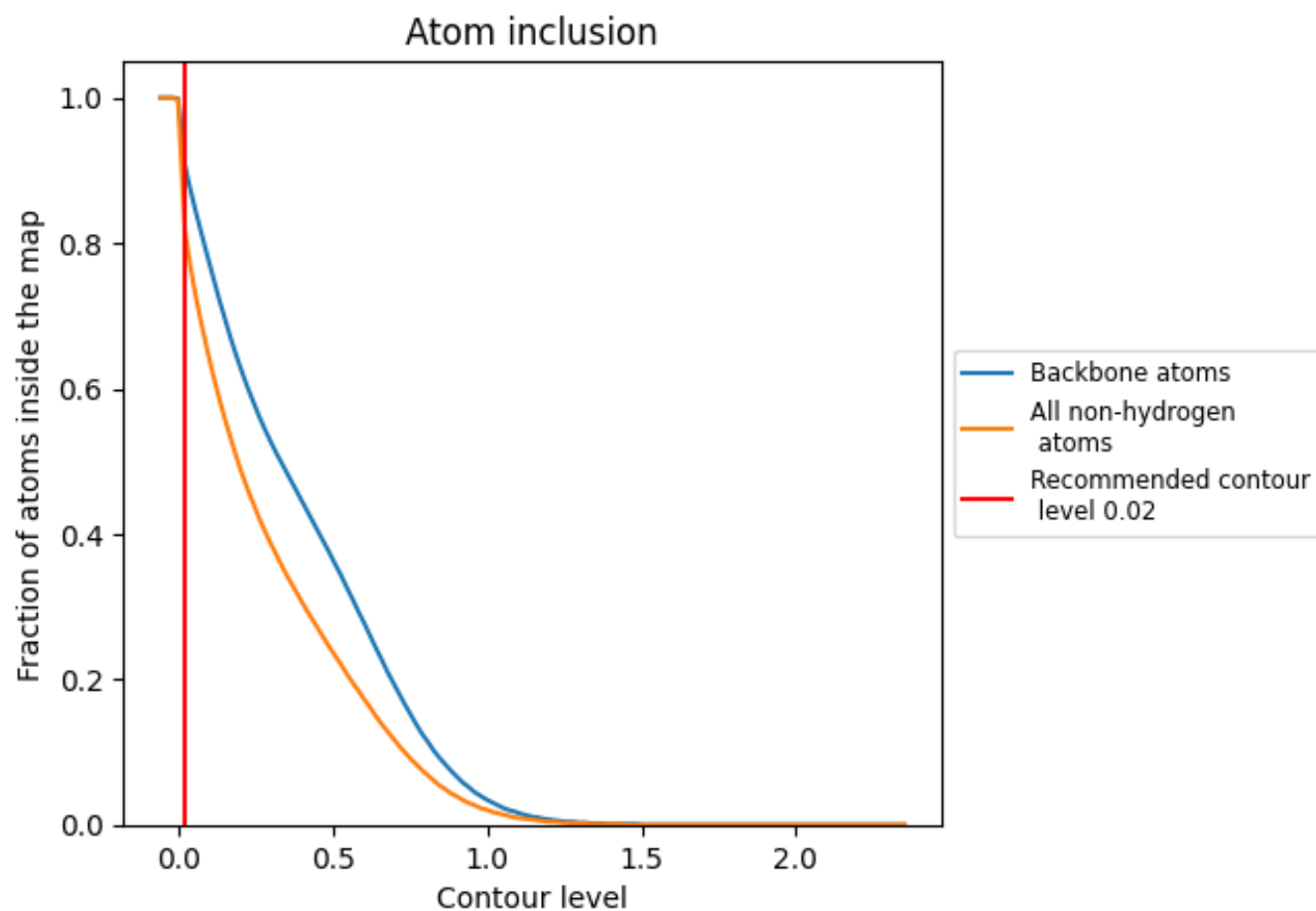
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 82% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8180	 0.2870
1	 0.8720	 0.3290
10	 0.4430	 0.0160
11	 0.5150	 0.0350
12	 0.4880	 0.0270
13	 0.5500	 0.0410
14	 0.4560	 -0.0070
15	 0.5160	 0.0440
16	 0.4690	 0.0150
1A	 0.7850	 0.1560
1B	 0.8330	 0.1940
1C	 0.8930	 0.3150
1D	 0.9090	 0.3450
1E	 0.9340	 0.3860
1F	 0.9380	 0.3940
1G	 0.9340	 0.4010
1H	 0.9200	 0.3940
1I	 0.9410	 0.4180
1J	 0.9340	 0.3980
1K	 0.9430	 0.3970
1L	 0.9380	 0.3620
1M	 0.8900	 0.2710
1N	 0.8280	 0.1970
2	 0.8460	 0.2230
20	 0.8620	 0.2940
21	 0.8360	 0.3120
22	 0.8670	 0.3070
23	 0.8430	 0.3060
24	 0.8190	 0.1780
25	 0.8140	 0.2360
26	 0.8410	 0.2490
27	 0.8250	 0.2400
28	 0.7750	 0.1090
29	 0.7810	 0.1700
2A	 0.8650	 0.2330



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Chain	Atom inclusion	Q-score
2B	 0.9080	 0.3010
2C	 0.9330	 0.3710
2D	 0.9570	 0.4300
2E	 0.9600	 0.4620
2F	 0.9580	 0.4700
2G	 0.9690	 0.4950
2H	 0.9660	 0.4890
2I	 0.9640	 0.4790
2J	 0.9650	 0.4630
2K	 0.9590	 0.4440
2L	 0.9540	 0.4050
2M	 0.9130	 0.3230
3	 0.5800	 0.0980
30	 0.8210	 0.1740
31	 0.7610	 0.1260
32	 0.7620	 0.1160
33	 0.3890	 0.0110
35	 0.5420	 0.0020
36	 0.5410	 0.0060
37	 0.5540	 0.0160
38	 0.5380	 -0.0060
39	 0.4790	 -0.0030
3A	 0.8720	 0.2660
3B	 0.9110	 0.3380
3C	 0.9480	 0.4170
3D	 0.9620	 0.4610
3E	 0.9680	 0.4800
3F	 0.9670	 0.4840
3G	 0.9690	 0.5040
3H	 0.9660	 0.5010
3I	 0.9640	 0.4880
3J	 0.9630	 0.4750
3K	 0.9610	 0.4520
3L	 0.9430	 0.4200
3M	 0.9190	 0.3510
4	 0.4900	 0.0750
40	 0.4900	 0.0070
42	 0.1760	 -0.0320
43	 0.5250	 0.0020
44	 0.5210	 -0.0070
45	 0.4940	 -0.0050
46	 0.4110	 -0.0130

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Chain	Atom inclusion	Q-score
47	 0.3890	 -0.0290
48	 0.0650	 -0.0470
49	 0.7740	 0.2020
4A	 0.8970	 0.3030
4B	 0.9390	 0.3790
4C	 0.9330	 0.4220
4D	 0.9610	 0.4770
4E	 0.9420	 0.4530
4F	 0.9650	 0.4910
4G	 0.9500	 0.4820
4H	 0.9670	 0.4960
4I	 0.9500	 0.4720
4J	 0.9630	 0.4730
4K	 0.9490	 0.4430
4L	 0.9490	 0.4180
4M	 0.9090	 0.3290
5	 0.5690	 0.0520
50	 0.7630	 0.1910
51	 0.7510	 0.1470
52	 0.7430	 0.1530
53	 0.7530	 0.1690
54	 0.7320	 0.1280
55	 0.7450	 0.1250
56	 0.7280	 0.1140
57	 0.7360	 0.1180
58	 0.7000	 0.0940
59	 0.4710	 0.0500
5A	 0.8560	 0.2540
5B	 0.9270	 0.3550
5C	 0.9560	 0.4300
5D	 0.9570	 0.4620
5E	 0.9660	 0.4840
5F	 0.9620	 0.4870
5G	 0.9630	 0.4990
5H	 0.9740	 0.4970
5I	 0.9610	 0.4840
5J	 0.9630	 0.4770
5K	 0.9640	 0.4790
5L	 0.9590	 0.4510
5M	 0.9410	 0.4000
5N	 0.9070	 0.3150
6	 0.4730	 0.0310

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Chain	Atom inclusion	Q-score
60	 0.6670	 0.0600
61	 0.6900	 0.0700
62	 0.5130	 0.0290
63	 0.8780	 0.3680
64	 0.8750	 0.3680
65	 0.8560	 0.3340
66	 0.8170	 0.2500
67	 0.6970	 0.1190
68	 0.8090	 0.2120
69	 0.8590	 0.3140
6A	 0.8670	 0.2540
6B	 0.9250	 0.3390
6C	 0.9570	 0.4230
6D	 0.9520	 0.4420
6E	 0.9570	 0.4650
6F	 0.9490	 0.4530
6G	 0.9670	 0.4830
6H	 0.9550	 0.4650
6I	 0.9610	 0.4780
6J	 0.9550	 0.4390
6K	 0.9570	 0.4390
6L	 0.9420	 0.3770
6M	 0.9130	 0.2980
6N	 0.8310	 0.1840
7	 0.5780	 0.0460
71	 0.7830	 0.3430
72	 0.7040	 0.2800
73	 0.7000	 0.2110
75	 0.7800	 0.3190
76	 0.7140	 0.2890
77	 0.6850	 0.2000
78	 0.9060	 0.4040
79	 0.8820	 0.3640
7A	 0.8720	 0.2280
7B	 0.9150	 0.3050
7C	 0.9440	 0.3950
7D	 0.9480	 0.4220
7E	 0.9580	 0.4530
7F	 0.9590	 0.4620
7G	 0.9580	 0.4760
7H	 0.9590	 0.4650
7I	 0.9580	 0.4610

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Chain	Atom inclusion	Q-score
7J	 0.9640	 0.4380
7K	 0.9530	 0.3960
7L	 0.9210	 0.3240
7M	 0.8860	 0.2420
8	 0.5140	 0.0490
80	 0.8270	 0.2680
82	 0.9110	 0.4050
83	 0.8910	 0.3370
84	 0.8180	 0.2140
85	 0.8330	 0.3480
86	 0.7950	 0.3020
87	 0.7670	 0.2220
89	 0.8370	 0.3400
8A	 0.8010	 0.1570
8B	 0.8540	 0.2150
8C	 0.9060	 0.3060
8D	 0.9190	 0.3400
8E	 0.9450	 0.3940
8F	 0.9500	 0.4250
8G	 0.9580	 0.4370
8H	 0.9480	 0.4200
8I	 0.9490	 0.4070
8J	 0.9420	 0.3680
8K	 0.9100	 0.2910
8L	 0.8660	 0.2120
8M	 0.8000	 0.1350
9	 0.4880	 0.0150
90	 0.7920	 0.2480
91	 0.7230	 0.1270
92	 0.1710	 -0.0220
93	 0.1090	 -0.0430
94	 0.1200	 -0.0540
95	 0.1140	 -0.0670
96	 0.2990	 0.0360
97	 0.0950	 -0.0620
9A	 0.5830	 0.0100
9B	 0.7110	 0.0660
9C	 0.6480	 0.0520
9D	 0.6460	 0.0790
9E	 0.7460	 0.1370
9F	 0.7910	 0.1870
9G	 0.8550	 0.2470

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Chain	Atom inclusion	Q-score
9H	 0.8410	 0.2120
9I	 0.7280	 0.1290
9J	 0.6380	 0.0920
9K	 0.6480	 0.0800
9L	 0.6430	 0.0380
9M	 0.5290	 0.0140
A	 0.8370	 0.2940
A1	 0.9560	 0.4760
A2	 0.9390	 0.4220
A3	 0.9210	 0.3660
A4	 0.9020	 0.2850
A5	 0.9520	 0.4790
A6	 0.9560	 0.4780
A7	 0.9480	 0.4490
A8	 0.8720	 0.3350
A9	 0.8870	 0.3080
B	 0.8900	 0.3430
B1	 0.9640	 0.4850
B2	 0.9570	 0.4850
B3	 0.9540	 0.4670
B4	 0.9460	 0.4480
B5	 0.9350	 0.3930
B6	 0.9220	 0.3770
B7	 0.8390	 0.2290
C	 0.8260	 0.2690
C0	 0.5670	 0.1580
C1	 0.8880	 0.4320
C2	 0.8810	 0.4010
C3	 0.8490	 0.3620
C4	 0.8530	 0.3910
C5	 0.8340	 0.3160
C6	 0.6020	 0.1900
C7	 0.6280	 0.1910
C8	 0.5530	 0.1180
C9	 0.5220	 0.0490
D	 0.8000	 0.2060
D0	 0.9040	 0.4060
D1	 0.5650	 0.1010
D2	 0.5330	 0.0510
D3	 0.5600	 0.2240
D4	 0.5330	 0.2000
D5	 0.5520	 0.1470

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Chain	Atom inclusion	Q-score
D6	 0.4160	 0.0020
D7	 0.5930	 0.2430
D8	 0.5430	 0.1740
D9	 0.4990	 0.0940
E	 0.8200	 0.2770
E0	 0.8910	 0.3420
E1	 0.8690	 0.3200
E2	 0.8060	 0.2010
E3	 0.5130	 0.0690
E4	 0.8920	 0.3760
E5	 0.8680	 0.3160
E6	 0.8200	 0.2020
E7	 0.8570	 0.2700
E8	 0.8930	 0.3720
E9	 0.1590	 -0.0250
F	 0.8450	 0.2850
F0	 0.7550	 0.1350
F1	 0.8710	 0.2800
F2	 0.7510	 0.1320
F3	 0.7660	 0.1470
F5	 0.7740	 0.1530
F6	 0.7590	 0.1540
F7	 0.7890	 0.1280
F8	 0.7350	 0.0780
F9	 0.7910	 0.1830
G	 0.8120	 0.2450
G0	 0.8790	 0.3430
G1	 0.7100	 0.0340
G2	 0.6360	 0.0250
G3	 0.7800	 0.0990
G4	 0.7160	 0.0860
G5	 0.6830	 0.0350
G6	 0.6440	 0.0560
G7	 0.7780	 0.1230
G8	 0.7280	 0.1030
G9	 0.8550	 0.3090
H	 0.8070	 0.2100
H0	 0.9180	 0.4250
H1	 0.8900	 0.4110
H2	 0.8550	 0.2350
H3	 0.8090	 0.2250
H4	 0.8520	 0.3390

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Chain	Atom inclusion	Q-score
H5	 0.7780	 0.1580
H6	 0.7860	 0.1490
H7	 0.8410	 0.2150
H8	 0.9120	 0.3630
H9	 0.8570	 0.3440
I	 0.6290	 0.1280
I1	 0.8180	 0.2370
I2	 0.8220	 0.2690
I3	 0.8790	 0.3430
I4	 0.7090	 0.0610
I5	 0.6730	 0.0850
I6	 0.7420	 0.1420
I7	 0.7810	 0.1420
I8	 0.7710	 0.1170
I9	 0.8190	 0.2740
J	 0.6270	 0.1200
J1	 0.6210	 0.0200
J2	 0.5850	 0.0070
J3	 0.5640	 0.0160
J4	 0.3470	 -0.0280
J5	 0.5730	 0.0130
J6	 0.5170	 0.0080
J7	 0.1640	 -0.0340
K	 0.7370	 0.1660
K0	 0.9500	 0.4320
K1	 0.9460	 0.4710
K2	 0.9510	 0.4620
K3	 0.9420	 0.4270
K4	 0.8920	 0.3100
K5	 0.9430	 0.4550
K6	 0.9290	 0.4030
K7	 0.8170	 0.2320
K8	 0.9540	 0.4850
K9	 0.9500	 0.4710
L	 0.7420	 0.1600
L0	 0.8850	 0.2760
L1	 0.8830	 0.3060
L2	 0.9470	 0.4550
L3	 0.8990	 0.3380
L4	 0.8790	 0.2500
L5	 0.9550	 0.4660
L6	 0.9460	 0.4430

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Chain	Atom inclusion	Q-score
L7	 0.9310	 0.3820
L8	 0.8590	 0.2590
L9	 0.9450	 0.4090
M	 0.5380	 0.1150
M1	 0.7630	 0.1140
M2	 0.8220	 0.3040
M3	 0.8200	 0.2830
M4	 0.7430	 0.1880
M5	 0.6760	 0.1050
M6	 0.7930	 0.2210
M7	 0.7120	 0.1010
N	 0.5870	 0.1330
O	 0.6130	 0.0700
P	 0.5950	 0.1140
Q	 0.8230	 0.2860
R	 0.8310	 0.2940
S	 0.8040	 0.2630
T	 0.8540	 0.2880
U	 0.8140	 0.2840
V	 0.8320	 0.2860
W	 0.7870	 0.2480
X	 0.7960	 0.2570
Y	 0.8310	 0.2760
Z	 0.8280	 0.2860
a	 0.8000	 0.2370
b	 0.6930	 0.1290
c	 0.8250	 0.2730
d	 0.7900	 0.2290
e	 0.7030	 0.1590
f	 0.8230	 0.2610
g	 0.9150	 0.4330
h	 0.8290	 0.2840
i	 0.7590	 0.2010
j	 0.7870	 0.3120
k	 0.7660	 0.3040
l	 0.8310	 0.3250
m	 0.7380	 0.1950
n	 0.8030	 0.2780
o	 0.7440	 0.1950
p	 0.8130	 0.3110
q	 0.7510	 0.1500
r	 0.7510	 0.1240

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Chain	Atom inclusion	Q-score
s	 0.3560	 0.1210
t	 0.2560	 0.0590
u	 0.9140	 0.4200
v	 0.8990	 0.4130
w	 0.9060	 0.3970
x	 0.8980	 0.3460
y	 0.6970	 0.1400
z	 0.8940	 0.3800