



wwPDB EM Validation Summary Report ⓘ

Mar 20, 2026 – 01:56 PM EDT

PDB ID : 7SOM / pdb_00007som
EMDB ID : EMD-25361
Title : Ciliary C2 central pair apparatus isolated from *Chlamydomonas reinhardtii*
Authors : Gui, M.; Wang, X.; Dutcher, S.K.; Brown, A.; Zhang, R.
Deposited on : 2021-11-01
Resolution : 3.70 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

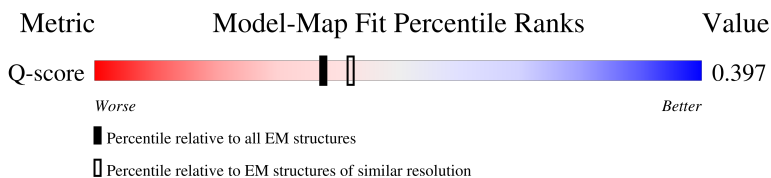
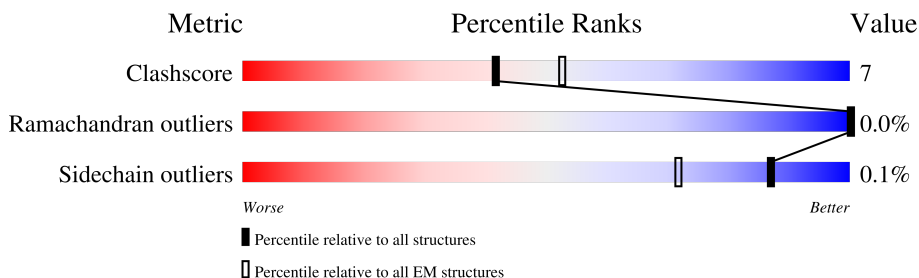
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 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.



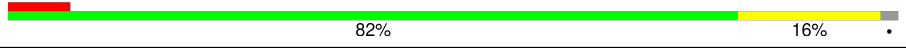
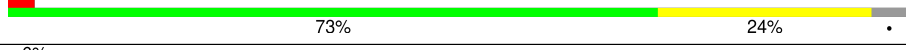
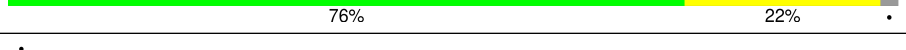
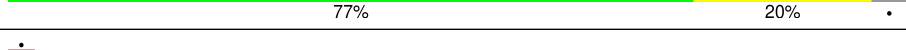
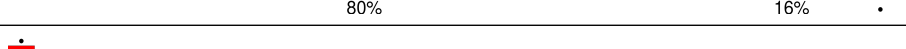
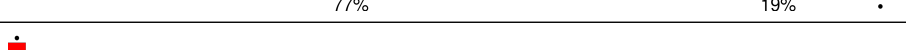
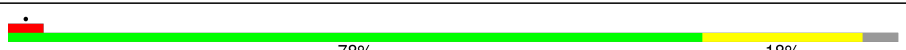
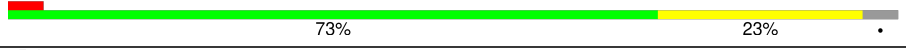
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11569 (3.20 - 4.20)

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

Mol	Chain	Length	Quality of chain
1	AA	443	
1	AC	443	
1	AE	443	
1	AG	443	

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Mol	Chain	Length	Quality of chain
1	AI	443	
1	AK	443	
1	BA	443	
1	BC	443	
1	BE	443	
1	BG	443	
1	BI	443	
1	BK	443	
1	CA	443	
1	CC	443	
1	CE	443	
1	CG	443	
1	CI	443	
1	CK	443	
1	DC	443	
1	DE	443	
1	DG	443	
1	DI	443	
1	DK	443	
1	EA	443	
1	EC	443	
1	EE	443	
1	EG	443	
1	EI	443	
1	EK	443	

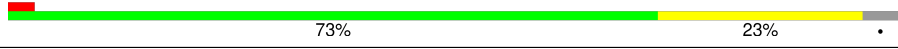
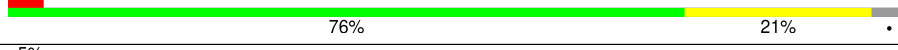
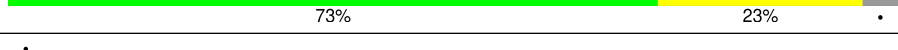
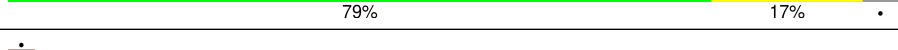
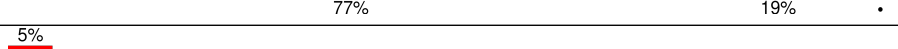
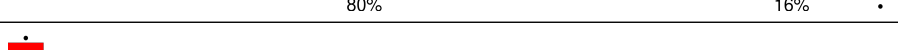
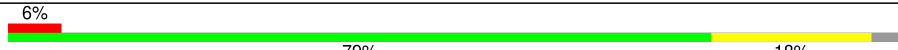
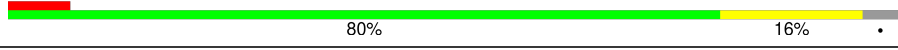
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Mol	Chain	Length	Quality of chain
1	FA	443	
1	FC	443	
1	FE	443	
1	FG	443	
1	FI	443	
1	FK	443	
1	GC	443	
1	GE	443	
1	GG	443	
1	GI	443	
1	GK	443	
1	GM	443	
1	HC	443	
1	HE	443	
1	HG	443	
1	HI	443	
1	HK	443	
1	HM	443	
1	IC	443	
1	IE	443	
1	IG	443	
1	II	443	
1	IK	443	
1	IM	443	
1	JC	443	

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Mol	Chain	Length	Quality of chain
1	JE	443	
1	JG	443	
1	JI	443	
1	JK	443	
1	JM	443	
1	KC	443	
1	KE	443	
1	KG	443	
1	KI	443	
1	KK	443	
1	LC	443	
1	LE	443	
1	LG	443	
1	LI	443	
1	LK	443	
1	MC	443	
1	ME	443	
1	MG	443	
1	MI	443	
1	MK	443	
2	AB	451	
2	AD	451	
2	AF	451	
2	AH	451	
2	AJ	451	

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Mol	Chain	Length	Quality of chain
2	AL	451	
2	BB	451	
2	BD	451	
2	BF	451	
2	BH	451	
2	BJ	451	
2	BL	451	
2	CB	451	
2	CD	451	
2	CF	451	
2	CH	451	
2	CJ	451	
2	DB	451	
2	DD	451	
2	DF	451	
2	DH	451	
2	DJ	451	
2	DL	451	
2	EB	451	
2	ED	451	
2	EF	451	
2	EH	451	
2	EJ	451	
2	EL	451	
2	FB	451	

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Mol	Chain	Length	Quality of chain
2	FD	451	
2	FF	451	
2	FH	451	
2	FJ	451	
2	FL	451	
2	GD	451	
2	GF	451	
2	GH	451	
2	GJ	451	
2	GL	451	
2	HD	451	
2	HF	451	
2	HH	451	
2	HJ	451	
2	HL	451	
2	ID	451	
2	IF	451	
2	IH	451	
2	IJ	451	
2	IL	451	
2	JB	451	
2	JD	451	
2	JF	451	
2	JH	451	
2	JJ	451	

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Mol	Chain	Length	Quality of chain
2	JL	451	
2	KB	451	
2	KD	451	
2	KF	451	
2	KH	451	
2	KJ	451	
2	KL	451	
2	LB	451	
2	LD	451	
2	LF	451	
2	LH	451	
2	LJ	451	
2	LL	451	
2	MB	451	
2	MD	451	
2	MF	451	
2	MH	451	
2	MJ	451	
2	ML	451	
3	a	618	
3	b	618	
3	c	618	
3	d	618	
4	e	201	
4	f	201	

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Mol	Chain	Length	Quality of chain
4	g	201	
5	h	758	
5	i	758	
5	j	758	
6	k	528	
6	l	528	
6	s	528	
7	m	421	
7	n	421	
7	o	421	
8	p	89	
8	q	89	
8	r	89	
9	A	190	
9	B	190	
9	C	190	
10	P	606	
10	Q	606	
10	R	606	
10	S	606	
10	Z	606	
10	aa	606	
10	cc	606	
11	T	93	
11	U	93	

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Mol	Chain	Length	Quality of chain
11	V	93	
11	W	93	
12	D	2257	
12	E	2257	
12	bb	2257	
13	F	1074	
13	G	1074	
13	H	1074	
13	I	1074	
14	J	976	
14	K	976	
15	L	222	
15	M	222	
15	N	222	
15	O	222	
15	X	222	
15	Y	222	
16	A1	48	
17	A2	77	
17	A4	77	
18	A3	47	

2 Entry composition [i](#)

There are 21 unique types of molecules in this entry. The entry contains 618760 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 Tubulin beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AA	431	Total	C	N	O	S	0	0
			3379	2121	579	649	30		
1	AC	430	Total	C	N	O	S	0	0
			3370	2116	578	646	30		
1	AE	431	Total	C	N	O	S	0	0
			3379	2121	579	649	30		
1	AG	431	Total	C	N	O	S	0	0
			3379	2121	579	649	30		
1	AI	431	Total	C	N	O	S	0	0
			3379	2121	579	649	30		
1	AK	431	Total	C	N	O	S	0	0
			3379	2121	579	649	30		
1	BA	432	Total	C	N	O	S	0	0
			3388	2126	580	652	30		
1	BC	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	BE	432	Total	C	N	O	S	0	0
			3388	2126	580	652	30		
1	BG	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	BI	432	Total	C	N	O	S	0	0
			3388	2126	580	652	30		
1	BK	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	CC	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	CE	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	CG	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	CI	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	CK	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	DC	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	DE	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	DG	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	DI	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	DK	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	EA	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	EC	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	EE	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	EG	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	EI	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	EK	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	FA	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	FC	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	FE	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	FG	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	FI	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	FK	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	GC	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	GE	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	GG	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	GI	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	GK	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	GM	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	HC	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	HE	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	HG	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	HI	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	HK	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	HM	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	IC	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	IE	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	IG	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	II	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	IK	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	IM	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	JC	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	JE	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	JG	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	JI	426	Total	C	N	O	S	0	0
			3346	2103	574	639	30		
1	JK	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	JM	426	Total	C	N	O	S	0	0
			3346	2103	574	639	30		
1	KC	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	KE	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	KG	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	KI	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	KK	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	LC	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	LE	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	LG	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	LI	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	LK	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	MC	431	Total	C	N	O	S	0	0
			3379	2121	579	649	30		
1	ME	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	MG	431	Total	C	N	O	S	0	0
			3379	2121	579	649	30		
1	MI	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	MK	431	Total	C	N	O	S	0	0
			3379	2121	579	649	30		
1	CA	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		

- Molecule 2 is a protein called Tubulin alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AB	432	Total	C	N	O	S	0	0
			3355	2124	570	639	22		
2	AD	432	Total	C	N	O	S	0	0
			3355	2123	570	640	22		
2	AF	432	Total	C	N	O	S	0	0
			3355	2124	570	639	22		
2	AH	430	Total	C	N	O	S	0	0
			3341	2116	568	635	22		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	AJ	432	Total 3355	C 2124	N 570	O 639	S 22	0	0
2	AL	430	Total 3341	C 2116	N 568	O 635	S 22	0	0
2	BB	438	Total 3393	C 2146	N 577	O 648	S 22	0	0
2	BD	430	Total 3341	C 2116	N 568	O 635	S 22	0	0
2	BF	438	Total 3393	C 2146	N 577	O 648	S 22	0	0
2	BH	430	Total 3341	C 2116	N 568	O 635	S 22	0	0
2	BJ	438	Total 3393	C 2146	N 577	O 648	S 22	0	0
2	BL	430	Total 3341	C 2116	N 568	O 635	S 22	0	0
2	CB	429	Total 3335	C 2113	N 567	O 633	S 22	0	0
2	CD	429	Total 3335	C 2113	N 567	O 633	S 22	0	0
2	CF	429	Total 3335	C 2113	N 567	O 633	S 22	0	0
2	CH	429	Total 3335	C 2113	N 567	O 633	S 22	0	0
2	CJ	430	Total 3341	C 2116	N 568	O 635	S 22	0	0
2	DB	430	Total 3341	C 2116	N 568	O 635	S 22	0	0
2	DD	429	Total 3335	C 2113	N 567	O 633	S 22	0	0
2	DF	430	Total 3341	C 2116	N 568	O 635	S 22	0	0
2	DH	430	Total 3341	C 2116	N 568	O 635	S 22	0	0
2	DJ	430	Total 3341	C 2116	N 568	O 635	S 22	0	0
2	DL	430	Total 3341	C 2116	N 568	O 635	S 22	0	0
2	EB	438	Total 3393	C 2146	N 577	O 648	S 22	0	0
2	ED	429	Total 3335	C 2113	N 567	O 633	S 22	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	EF	439	Total	C	N	O	S	0	0
			3399	2149	578	650	22		
2	EH	429	Total	C	N	O	S	0	0
			3335	2113	567	633	22		
2	EJ	438	Total	C	N	O	S	0	0
			3393	2146	577	648	22		
2	EL	429	Total	C	N	O	S	0	0
			3335	2113	567	633	22		
2	FB	430	Total	C	N	O	S	0	0
			3341	2116	568	635	22		
2	FD	430	Total	C	N	O	S	0	0
			3341	2116	568	635	22		
2	FF	430	Total	C	N	O	S	0	0
			3341	2116	568	635	22		
2	FH	430	Total	C	N	O	S	0	0
			3341	2116	568	635	22		
2	FJ	430	Total	C	N	O	S	0	0
			3341	2116	568	635	22		
2	FL	430	Total	C	N	O	S	0	0
			3341	2116	568	635	22		
2	GD	430	Total	C	N	O	S	0	0
			3341	2116	568	635	22		
2	GF	430	Total	C	N	O	S	0	0
			3341	2116	568	635	22		
2	GH	430	Total	C	N	O	S	0	0
			3341	2116	568	635	22		
2	GJ	430	Total	C	N	O	S	0	0
			3341	2116	568	635	22		
2	GL	430	Total	C	N	O	S	0	0
			3341	2116	568	635	22		
2	HD	430	Total	C	N	O	S	0	0
			3341	2116	568	635	22		
2	HF	430	Total	C	N	O	S	0	0
			3341	2116	568	635	22		
2	HH	430	Total	C	N	O	S	0	0
			3341	2116	568	635	22		
2	HJ	428	Total	C	N	O	S	0	0
			3326	2108	566	630	22		
2	HL	430	Total	C	N	O	S	0	0
			3341	2116	568	635	22		
2	ID	429	Total	C	N	O	S	0	0
			3335	2113	567	633	22		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	IF	430	Total 3341	C 2116	N 568	O 635	S 22	0	0
2	IH	429	Total 3335	C 2113	N 567	O 633	S 22	0	0
2	IJ	430	Total 3341	C 2116	N 568	O 635	S 22	0	0
2	IL	429	Total 3335	C 2113	N 567	O 633	S 22	0	0
2	JB	430	Total 3341	C 2116	N 568	O 635	S 22	0	0
2	JD	430	Total 3341	C 2116	N 568	O 635	S 22	0	0
2	JF	430	Total 3341	C 2116	N 568	O 635	S 22	0	0
2	JH	430	Total 3341	C 2116	N 568	O 635	S 22	0	0
2	JJ	429	Total 3335	C 2113	N 567	O 633	S 22	0	0
2	JL	429	Total 3335	C 2113	N 567	O 633	S 22	0	0
2	KB	429	Total 3335	C 2113	N 567	O 633	S 22	0	0
2	KD	430	Total 3341	C 2116	N 568	O 635	S 22	0	0
2	KF	429	Total 3335	C 2113	N 567	O 633	S 22	0	0
2	KH	430	Total 3341	C 2116	N 568	O 635	S 22	0	0
2	KJ	429	Total 3335	C 2113	N 567	O 633	S 22	0	0
2	KL	430	Total 3341	C 2116	N 568	O 635	S 22	0	0
2	LB	430	Total 3341	C 2116	N 568	O 635	S 22	0	0
2	LD	430	Total 3341	C 2116	N 568	O 635	S 22	0	0
2	LF	430	Total 3341	C 2116	N 568	O 635	S 22	0	0
2	LH	430	Total 3341	C 2116	N 568	O 635	S 22	0	0
2	LJ	430	Total 3341	C 2116	N 568	O 635	S 22	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	LL	430	Total	C	N	O	S	0	0
			3341	2116	568	635	22		
2	MB	430	Total	C	N	O	S	0	0
			3341	2116	568	635	22		
2	MD	439	Total	C	N	O	S	0	0
			3399	2149	578	650	22		
2	MF	430	Total	C	N	O	S	0	0
			3341	2116	568	635	22		
2	MH	440	Total	C	N	O	S	0	0
			3404	2152	579	651	22		
2	MJ	430	Total	C	N	O	S	0	0
			3341	2116	568	635	22		
2	ML	440	Total	C	N	O	S	0	0
			3404	2152	579	651	22		

- Molecule 3 is a protein called Cilia- and flagella-associated protein 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	a	325	Total	C	N	O	S	0	0
			2380	1491	422	453	14		
3	b	617	Total	C	N	O	S	0	0
			4537	2823	824	857	33		
3	c	617	Total	C	N	O	S	0	0
			4537	2823	824	857	33		
3	d	295	Total	C	N	O	S	0	0
			2180	1345	407	409	19		

- Molecule 4 is a protein called Unknown protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	e	186	Total	C	N	O	S	0	0
			1464	886	289	286	3		
4	f	186	Total	C	N	O	S	0	0
			1464	886	289	286	3		
4	g	145	Total	C	N	O	S	0	0
			1136	690	220	223	3		

- Molecule 5 is a protein called Unknown protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	h	585	Total	C	N	O	S	0	0
			4525	2788	856	866	15		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	i	585	Total	C	N	O	S	0	0
			4525	2788	856	866	15		
5	j	585	Total	C	N	O	S	0	0
			4525	2788	856	866	15		

- Molecule 6 is a protein called Unknown protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	k	388	Total	C	N	O	S	0	0
			3017	1857	582	572	6		
6	l	388	Total	C	N	O	S	0	0
			3017	1857	582	572	6		
6	s	285	Total	C	N	O	S	0	0
			2208	1369	420	415	4		

- Molecule 7 is a protein called FAP65.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	m	352	Total	C	N	O	S	0	0
			2737	1685	532	512	8		
7	n	352	Total	C	N	O	S	0	0
			2737	1685	532	512	8		
7	o	352	Total	C	N	O	S	0	0
			2737	1685	532	512	8		

- Molecule 8 is a protein called FAP70.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	p	88	Total	C	N	O	S	0	0
			698	432	135	129	2		
8	q	88	Total	C	N	O	S	0	0
			698	432	135	129	2		
8	r	88	Total	C	N	O	S	0	0
			698	432	135	129	2		

- Molecule 9 is a protein called FAP147.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	A	186	Total	C	N	O	S	0	0
			1530	982	266	275	7		
9	B	186	Total	C	N	O	S	0	0
			1530	982	266	275	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
9	C	186	Total	C	N	O	S	0	0
			1530	982	266	275	7		

- Molecule 10 is a protein called FAP178.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	P	433	Total	C	N	O	S	0	0
			2493	1507	495	486	5		
10	Q	432	Total	C	N	O	S	0	0
			2488	1504	494	485	5		
10	R	433	Total	C	N	O	S	0	0
			2493	1507	495	486	5		
10	S	432	Total	C	N	O	S	0	0
			2488	1504	494	485	5		
10	aa	292	Total	C	N	O		0	0
			1435	850	292	293			
10	cc	89	Total	C	N	O	S	0	0
			758	475	147	131	5		
10	Z	92	Total	C	N	O	S	0	0
			775	486	150	134	5		

- Molecule 11 is a protein called Flagellar WD repeat-containing protein Pf20.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	T	63	Total	C	N	O	0	0
			312	186	63	63		
11	U	58	Total	C	N	O	0	0
			287	171	58	58		
11	V	67	Total	C	N	O	0	0
			332	198	67	67		
11	W	63	Total	C	N	O	0	0
			312	186	63	63		

- Molecule 12 is a protein called Flagellar associated protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	bb	175	Total	C	N	O	S	0	0
			1065	650	211	202	2		
12	D	1516	Total	C	N	O		0	0
			7474	4442	1516	1516			
12	E	1516	Total	C	N	O		0	0
			7474	4442	1516	1516			

- Molecule 13 is a protein called FAP196.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	F	982	Total	C	N	O	0	0
			4832	2868	982	982		
13	G	993	Total	C	N	O	0	0
			4884	2898	993	993		
13	H	982	Total	C	N	O	0	0
			4832	2868	982	982		
13	I	993	Total	C	N	O	0	0
			4884	2898	993	993		

- Molecule 14 is a protein called FAP213.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	J	666	Total	C	N	O	S	0	0
			3874	2350	768	752	4		
14	K	666	Total	C	N	O	S	0	0
			3874	2350	768	752	4		

- Molecule 15 is a protein called FAP225.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	107	Total	C	N	O	S	0	0
			841	534	154	149	4		
15	Y	107	Total	C	N	O	S	0	0
			841	534	154	149	4		
15	L	107	Total	C	N	O	S	0	0
			841	534	154	149	4		
15	M	107	Total	C	N	O	S	0	0
			841	534	154	149	4		
15	N	107	Total	C	N	O	S	0	0
			841	534	154	149	4		
15	X	107	Total	C	N	O	S	0	0
			841	534	154	149	4		

- Molecule 16 is a protein called FAP239.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	A1	48	Total	C	N	O	0	0
			240	144	48	48		

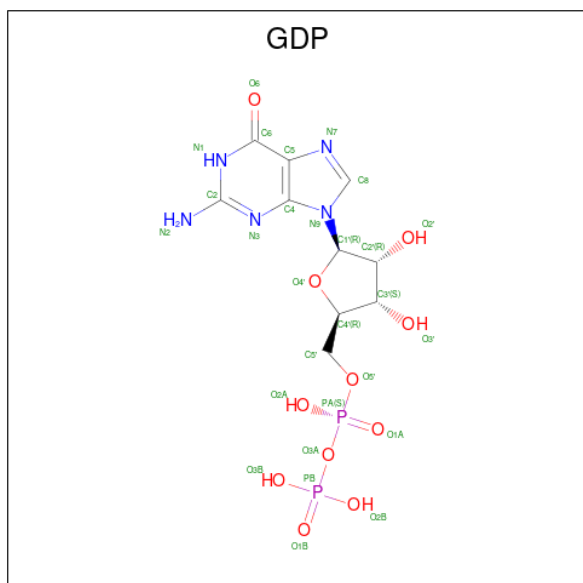
- Molecule 17 is a protein called FAP388.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	A2	77	Total	C	N	O	0	0
			385	231	77	77		
17	A4	77	Total	C	N	O	0	0
			385	231	77	77		

- Molecule 18 is a protein called FAP424.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	A3	47	Total	C	N	O	0	0
			235	141	47	47		

- Molecule 19 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					AltConf
19	AA	1	Total	C	N	O	P	0
			28	10	5	11	2	
19	AC	1	Total	C	N	O	P	0
			28	10	5	11	2	
19	AE	1	Total	C	N	O	P	0
			28	10	5	11	2	
19	AG	1	Total	C	N	O	P	0
			28	10	5	11	2	
19	AI	1	Total	C	N	O	P	0
			28	10	5	11	2	
19	AK	1	Total	C	N	O	P	0
			28	10	5	11	2	
19	BA	1	Total	C	N	O	P	0
			28	10	5	11	2	

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Mol	Chain	Residues	Atoms					AltConf
19	BC	1	Total 28	C 10	N 5	O 11	P 2	0
19	BE	1	Total 28	C 10	N 5	O 11	P 2	0
19	BG	1	Total 28	C 10	N 5	O 11	P 2	0
19	BI	1	Total 28	C 10	N 5	O 11	P 2	0
19	BK	1	Total 28	C 10	N 5	O 11	P 2	0
19	CC	1	Total 28	C 10	N 5	O 11	P 2	0
19	CE	1	Total 28	C 10	N 5	O 11	P 2	0
19	CG	1	Total 28	C 10	N 5	O 11	P 2	0
19	CI	1	Total 28	C 10	N 5	O 11	P 2	0
19	CK	1	Total 28	C 10	N 5	O 11	P 2	0
19	DC	1	Total 28	C 10	N 5	O 11	P 2	0
19	DE	1	Total 28	C 10	N 5	O 11	P 2	0
19	DG	1	Total 28	C 10	N 5	O 11	P 2	0
19	DI	1	Total 28	C 10	N 5	O 11	P 2	0
19	DK	1	Total 28	C 10	N 5	O 11	P 2	0
19	EA	1	Total 28	C 10	N 5	O 11	P 2	0
19	EC	1	Total 28	C 10	N 5	O 11	P 2	0
19	EE	1	Total 28	C 10	N 5	O 11	P 2	0
19	EG	1	Total 28	C 10	N 5	O 11	P 2	0
19	EI	1	Total 28	C 10	N 5	O 11	P 2	0
19	EK	1	Total 28	C 10	N 5	O 11	P 2	0

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Mol	Chain	Residues	Atoms					AltConf
19	FA	1	Total 28	C 10	N 5	O 11	P 2	0
19	FC	1	Total 28	C 10	N 5	O 11	P 2	0
19	FE	1	Total 28	C 10	N 5	O 11	P 2	0
19	FG	1	Total 28	C 10	N 5	O 11	P 2	0
19	FI	1	Total 28	C 10	N 5	O 11	P 2	0
19	FK	1	Total 28	C 10	N 5	O 11	P 2	0
19	GC	1	Total 28	C 10	N 5	O 11	P 2	0
19	GE	1	Total 28	C 10	N 5	O 11	P 2	0
19	GG	1	Total 28	C 10	N 5	O 11	P 2	0
19	GI	1	Total 28	C 10	N 5	O 11	P 2	0
19	GK	1	Total 28	C 10	N 5	O 11	P 2	0
19	GM	1	Total 28	C 10	N 5	O 11	P 2	0
19	HC	1	Total 28	C 10	N 5	O 11	P 2	0
19	HE	1	Total 28	C 10	N 5	O 11	P 2	0
19	HG	1	Total 28	C 10	N 5	O 11	P 2	0
19	HI	1	Total 28	C 10	N 5	O 11	P 2	0
19	HK	1	Total 28	C 10	N 5	O 11	P 2	0
19	HM	1	Total 28	C 10	N 5	O 11	P 2	0
19	IC	1	Total 28	C 10	N 5	O 11	P 2	0
19	IE	1	Total 28	C 10	N 5	O 11	P 2	0
19	IG	1	Total 28	C 10	N 5	O 11	P 2	0

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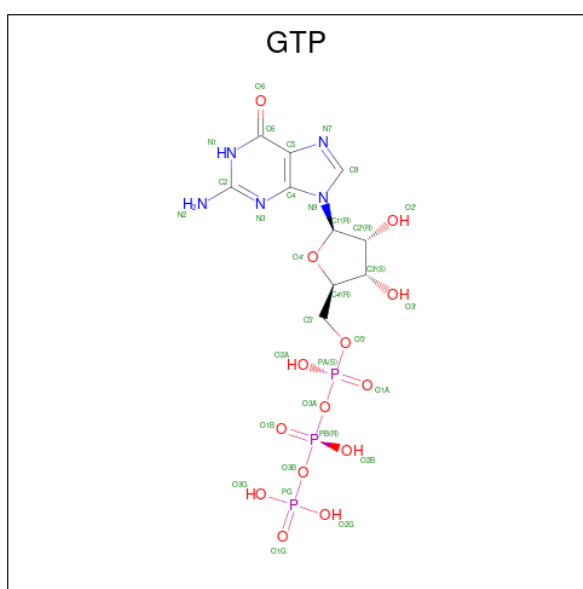
Mol	Chain	Residues	Atoms					AltConf
19	II	1	Total 28	C 10	N 5	O 11	P 2	0
19	IK	1	Total 28	C 10	N 5	O 11	P 2	0
19	IM	1	Total 28	C 10	N 5	O 11	P 2	0
19	JC	1	Total 28	C 10	N 5	O 11	P 2	0
19	JE	1	Total 28	C 10	N 5	O 11	P 2	0
19	JG	1	Total 28	C 10	N 5	O 11	P 2	0
19	JI	1	Total 28	C 10	N 5	O 11	P 2	0
19	JK	1	Total 28	C 10	N 5	O 11	P 2	0
19	JM	1	Total 28	C 10	N 5	O 11	P 2	0
19	KC	1	Total 28	C 10	N 5	O 11	P 2	0
19	KE	1	Total 28	C 10	N 5	O 11	P 2	0
19	KG	1	Total 28	C 10	N 5	O 11	P 2	0
19	KI	1	Total 28	C 10	N 5	O 11	P 2	0
19	KK	1	Total 28	C 10	N 5	O 11	P 2	0
19	LC	1	Total 28	C 10	N 5	O 11	P 2	0
19	LE	1	Total 28	C 10	N 5	O 11	P 2	0
19	LG	1	Total 28	C 10	N 5	O 11	P 2	0
19	LI	1	Total 28	C 10	N 5	O 11	P 2	0
19	LK	1	Total 28	C 10	N 5	O 11	P 2	0
19	MC	1	Total 28	C 10	N 5	O 11	P 2	0
19	ME	1	Total 28	C 10	N 5	O 11	P 2	0

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Mol	Chain	Residues	Atoms					AltConf
19	MG	1	Total	C	N	O	P	0
			28	10	5	11	2	
19	MI	1	Total	C	N	O	P	0
			28	10	5	11	2	
19	MK	1	Total	C	N	O	P	0
			28	10	5	11	2	
19	CA	1	Total	C	N	O	P	0
			28	10	5	11	2	

- Molecule 20 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					AltConf
20	AB	1	Total	C	N	O	P	0
			32	10	5	14	3	
20	AD	1	Total	C	N	O	P	0
			32	10	5	14	3	
20	AF	1	Total	C	N	O	P	0
			32	10	5	14	3	
20	AH	1	Total	C	N	O	P	0
			32	10	5	14	3	
20	AJ	1	Total	C	N	O	P	0
			32	10	5	14	3	
20	AL	1	Total	C	N	O	P	0
			32	10	5	14	3	
20	BB	1	Total	C	N	O	P	0
			32	10	5	14	3	

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Mol	Chain	Residues	Atoms					AltConf
20	BD	1	Total 32	C 10	N 5	O 14	P 3	0
20	BF	1	Total 32	C 10	N 5	O 14	P 3	0
20	BH	1	Total 32	C 10	N 5	O 14	P 3	0
20	BJ	1	Total 32	C 10	N 5	O 14	P 3	0
20	BL	1	Total 32	C 10	N 5	O 14	P 3	0
20	CB	1	Total 32	C 10	N 5	O 14	P 3	0
20	CD	1	Total 32	C 10	N 5	O 14	P 3	0
20	CF	1	Total 32	C 10	N 5	O 14	P 3	0
20	CH	1	Total 32	C 10	N 5	O 14	P 3	0
20	CJ	1	Total 32	C 10	N 5	O 14	P 3	0
20	DB	1	Total 32	C 10	N 5	O 14	P 3	0
20	DD	1	Total 32	C 10	N 5	O 14	P 3	0
20	DF	1	Total 32	C 10	N 5	O 14	P 3	0
20	DH	1	Total 32	C 10	N 5	O 14	P 3	0
20	DJ	1	Total 32	C 10	N 5	O 14	P 3	0
20	DL	1	Total 32	C 10	N 5	O 14	P 3	0
20	EB	1	Total 32	C 10	N 5	O 14	P 3	0
20	ED	1	Total 32	C 10	N 5	O 14	P 3	0
20	EF	1	Total 32	C 10	N 5	O 14	P 3	0
20	EH	1	Total 32	C 10	N 5	O 14	P 3	0
20	EJ	1	Total 32	C 10	N 5	O 14	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
20	EL	1	Total 32	C 10	N 5	O 14	P 3	0
20	FB	1	Total 32	C 10	N 5	O 14	P 3	0
20	FD	1	Total 32	C 10	N 5	O 14	P 3	0
20	FF	1	Total 32	C 10	N 5	O 14	P 3	0
20	FH	1	Total 32	C 10	N 5	O 14	P 3	0
20	FJ	1	Total 32	C 10	N 5	O 14	P 3	0
20	FL	1	Total 32	C 10	N 5	O 14	P 3	0
20	GD	1	Total 32	C 10	N 5	O 14	P 3	0
20	GF	1	Total 32	C 10	N 5	O 14	P 3	0
20	GH	1	Total 32	C 10	N 5	O 14	P 3	0
20	GJ	1	Total 32	C 10	N 5	O 14	P 3	0
20	GL	1	Total 32	C 10	N 5	O 14	P 3	0
20	HD	1	Total 32	C 10	N 5	O 14	P 3	0
20	HF	1	Total 32	C 10	N 5	O 14	P 3	0
20	HI	1	Total 32	C 10	N 5	O 14	P 3	0
20	HJ	1	Total 32	C 10	N 5	O 14	P 3	0
20	HL	1	Total 32	C 10	N 5	O 14	P 3	0
20	ID	1	Total 32	C 10	N 5	O 14	P 3	0
20	IF	1	Total 32	C 10	N 5	O 14	P 3	0
20	IH	1	Total 32	C 10	N 5	O 14	P 3	0
20	IJ	1	Total 32	C 10	N 5	O 14	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
20	IL	1	Total 32	C 10	N 5	O 14	P 3	0
20	JB	1	Total 32	C 10	N 5	O 14	P 3	0
20	JD	1	Total 32	C 10	N 5	O 14	P 3	0
20	JF	1	Total 32	C 10	N 5	O 14	P 3	0
20	JH	1	Total 32	C 10	N 5	O 14	P 3	0
20	JJ	1	Total 32	C 10	N 5	O 14	P 3	0
20	JL	1	Total 32	C 10	N 5	O 14	P 3	0
20	KB	1	Total 32	C 10	N 5	O 14	P 3	0
20	KD	1	Total 32	C 10	N 5	O 14	P 3	0
20	KF	1	Total 32	C 10	N 5	O 14	P 3	0
20	KH	1	Total 32	C 10	N 5	O 14	P 3	0
20	KJ	1	Total 32	C 10	N 5	O 14	P 3	0
20	KL	1	Total 32	C 10	N 5	O 14	P 3	0
20	LB	1	Total 32	C 10	N 5	O 14	P 3	0
20	LD	1	Total 32	C 10	N 5	O 14	P 3	0
20	LF	1	Total 32	C 10	N 5	O 14	P 3	0
20	LH	1	Total 32	C 10	N 5	O 14	P 3	0
20	LJ	1	Total 32	C 10	N 5	O 14	P 3	0
20	LL	1	Total 32	C 10	N 5	O 14	P 3	0
20	MB	1	Total 32	C 10	N 5	O 14	P 3	0
20	MD	1	Total 32	C 10	N 5	O 14	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
20	MF	1	Total	C	N	O	P	0
			32	10	5	14	3	
20	MH	1	Total	C	N	O	P	0
			32	10	5	14	3	
20	MJ	1	Total	C	N	O	P	0
			32	10	5	14	3	
20	ML	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 21 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
21	AB	1	Total	Mg	0
			1	1	
21	AD	1	Total	Mg	0
			1	1	
21	AF	1	Total	Mg	0
			1	1	
21	AH	1	Total	Mg	0
			1	1	
21	AJ	1	Total	Mg	0
			1	1	
21	AL	1	Total	Mg	0
			1	1	
21	BB	1	Total	Mg	0
			1	1	
21	BD	1	Total	Mg	0
			1	1	
21	BF	1	Total	Mg	0
			1	1	
21	BH	1	Total	Mg	0
			1	1	
21	BJ	1	Total	Mg	0
			1	1	
21	BL	1	Total	Mg	0
			1	1	
21	CB	1	Total	Mg	0
			1	1	
21	CD	1	Total	Mg	0
			1	1	
21	CF	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
21	CH	1	Total 1	Mg 1	0
21	CJ	1	Total 1	Mg 1	0
21	DB	1	Total 1	Mg 1	0
21	DD	1	Total 1	Mg 1	0
21	DF	1	Total 1	Mg 1	0
21	DH	1	Total 1	Mg 1	0
21	DJ	1	Total 1	Mg 1	0
21	DL	1	Total 1	Mg 1	0
21	EB	1	Total 1	Mg 1	0
21	EE	1	Total 1	Mg 1	0
21	EF	1	Total 1	Mg 1	0
21	EH	1	Total 1	Mg 1	0
21	EJ	1	Total 1	Mg 1	0
21	EL	1	Total 1	Mg 1	0
21	FB	1	Total 1	Mg 1	0
21	FD	1	Total 1	Mg 1	0
21	FF	1	Total 1	Mg 1	0
21	FH	1	Total 1	Mg 1	0
21	FJ	1	Total 1	Mg 1	0
21	FL	1	Total 1	Mg 1	0
21	GD	1	Total 1	Mg 1	0

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Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
21	GF	1	1	1	0
21	GH	1	1	1	0
21	GJ	1	1	1	0
21	GL	1	1	1	0
21	HD	1	1	1	0
21	HF	1	1	1	0
21	HH	1	1	1	0
21	HJ	1	1	1	0
21	HL	1	1	1	0
21	ID	1	1	1	0
21	IF	1	1	1	0
21	IH	1	1	1	0
21	IJ	1	1	1	0
21	IL	1	1	1	0
21	JB	1	1	1	0
21	JD	1	1	1	0
21	JF	1	1	1	0
21	JH	1	1	1	0
21	JJ	1	1	1	0
21	JL	1	1	1	0
21	KB	1	1	1	0

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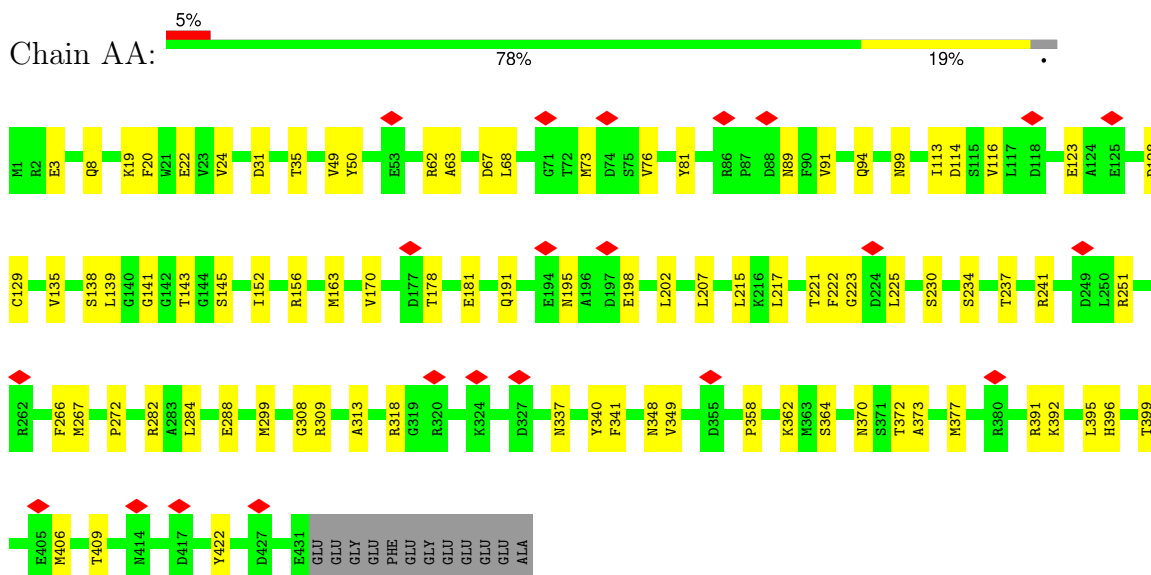
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Mol	Chain	Residues	Atoms		AltConf
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21	KF	1	Total 1	Mg 1	0
21	KI	1	Total 1	Mg 1	0
21	KJ	1	Total 1	Mg 1	0
21	KL	1	Total 1	Mg 1	0
21	LB	1	Total 1	Mg 1	0
21	LD	1	Total 1	Mg 1	0
21	LF	1	Total 1	Mg 1	0
21	LH	1	Total 1	Mg 1	0
21	LJ	1	Total 1	Mg 1	0
21	LL	1	Total 1	Mg 1	0
21	MB	1	Total 1	Mg 1	0
21	MD	1	Total 1	Mg 1	0
21	MF	1	Total 1	Mg 1	0
21	MH	1	Total 1	Mg 1	0
21	MJ	1	Total 1	Mg 1	0
21	ML	1	Total 1	Mg 1	0

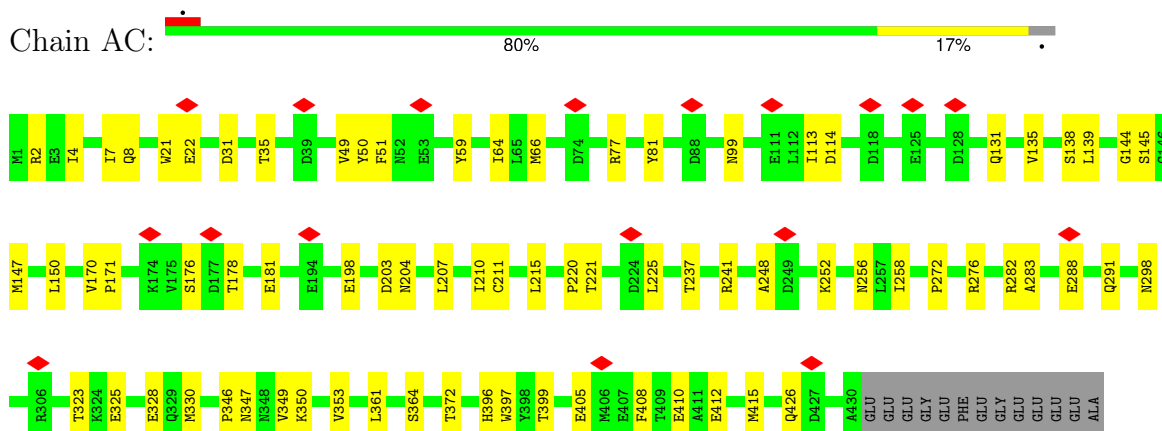
3 Residue-property plots

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.

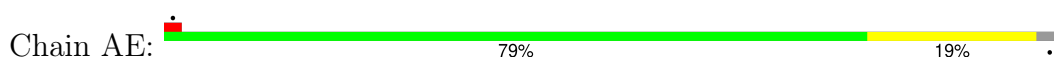
- Molecule 1: Tubulin beta

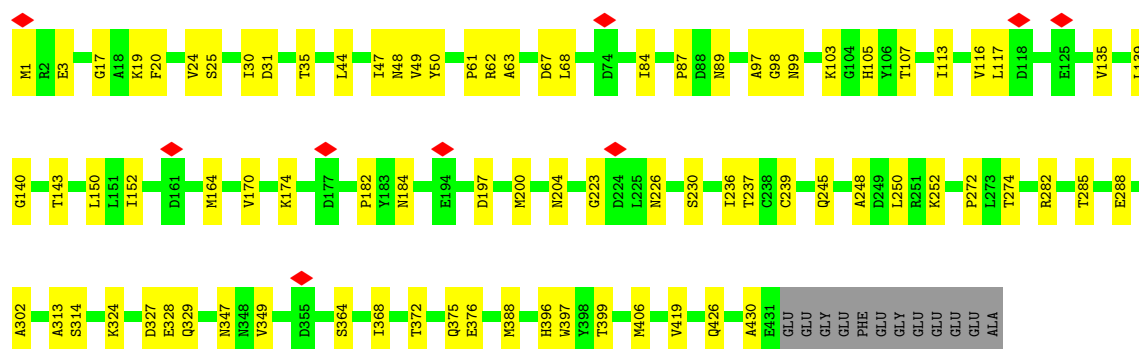


- Molecule 1: Tubulin beta



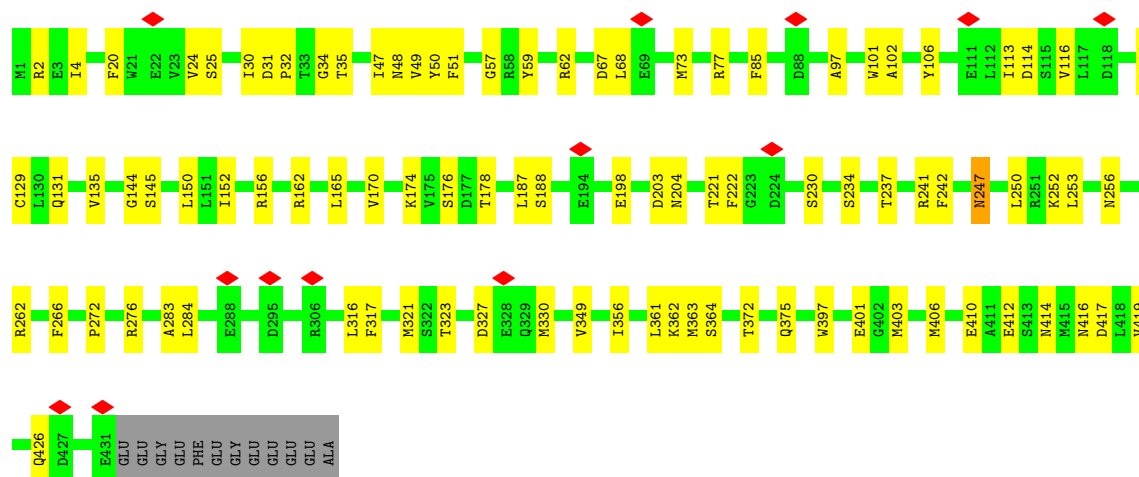
- Molecule 1: Tubulin beta





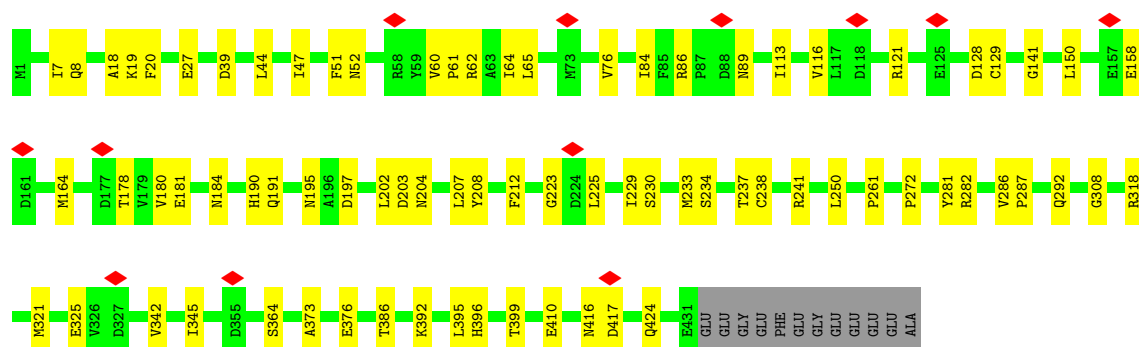
• Molecule 1: Tubulin beta

Chain AG: 76% 21% .



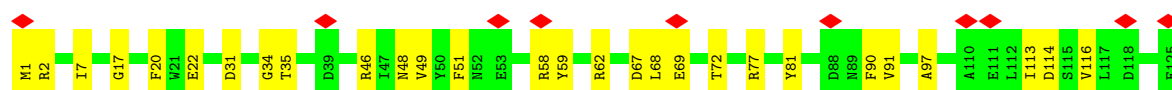
• Molecule 1: Tubulin beta

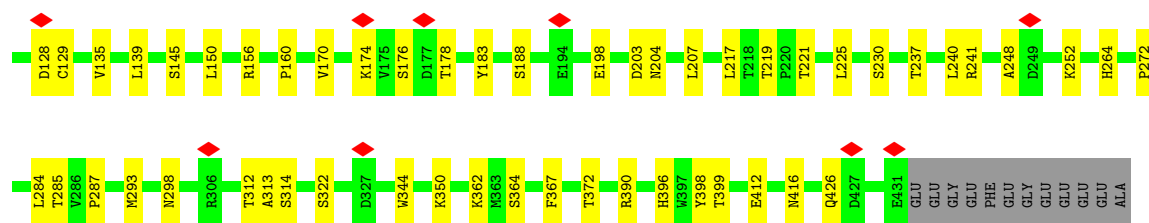
Chain AI: 80% 18% .



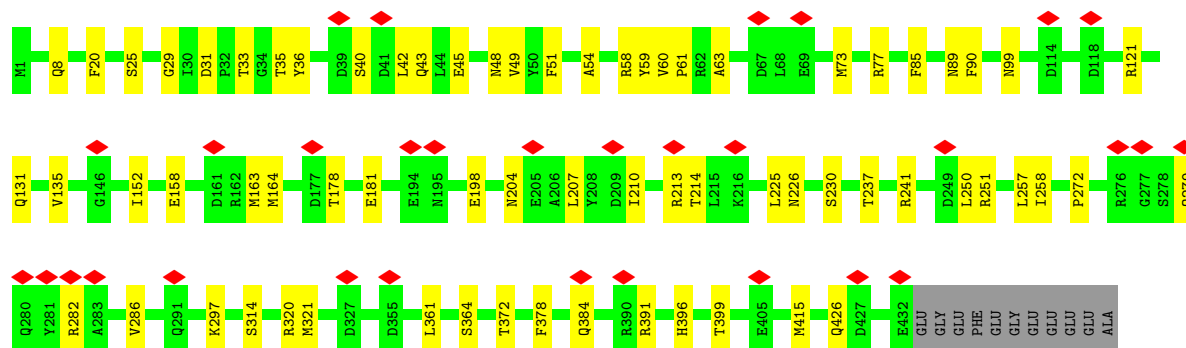
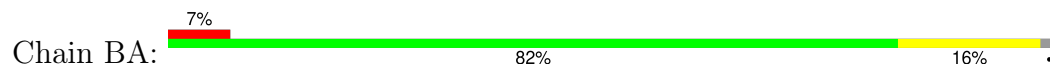
• Molecule 1: Tubulin beta

Chain AK: 79% 18% .

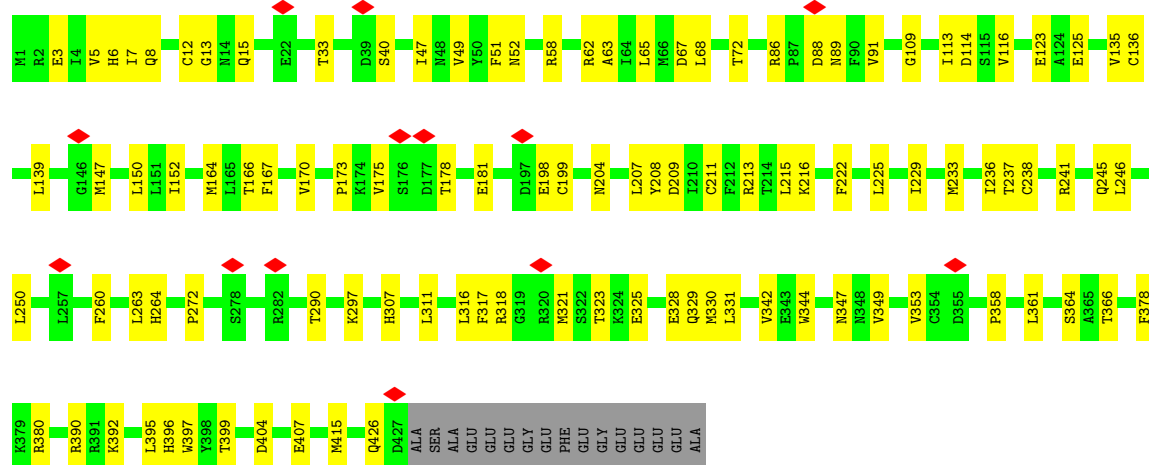




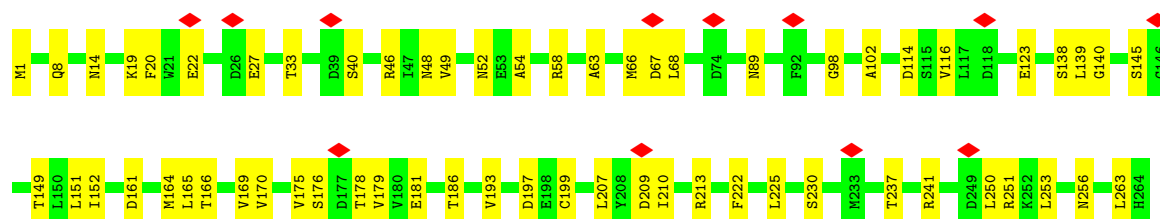
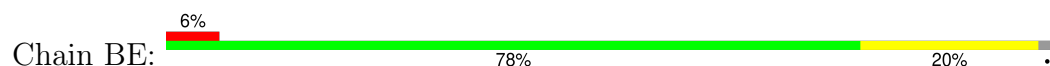
• Molecule 1: Tubulin beta

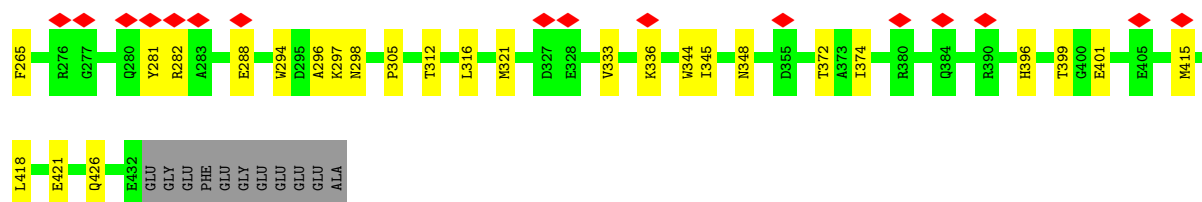


• Molecule 1: Tubulin beta



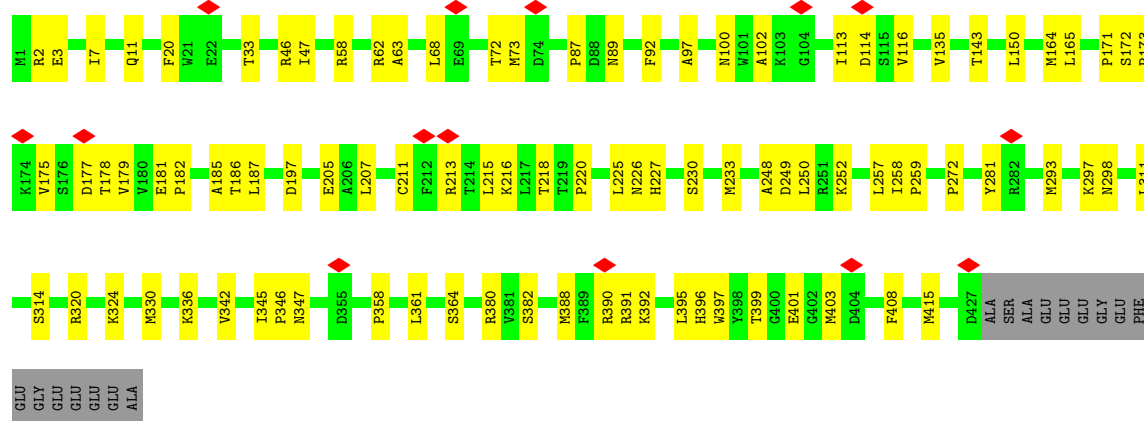
• Molecule 1: Tubulin beta





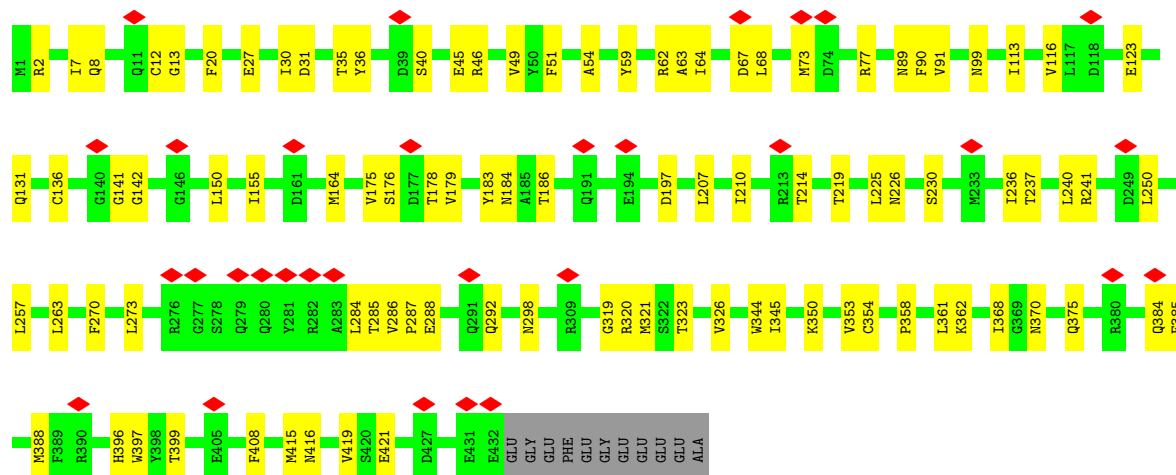
• Molecule 1: Tubulin beta

Chain BG: 75% 21%



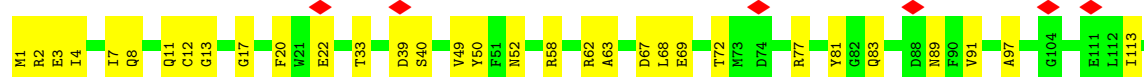
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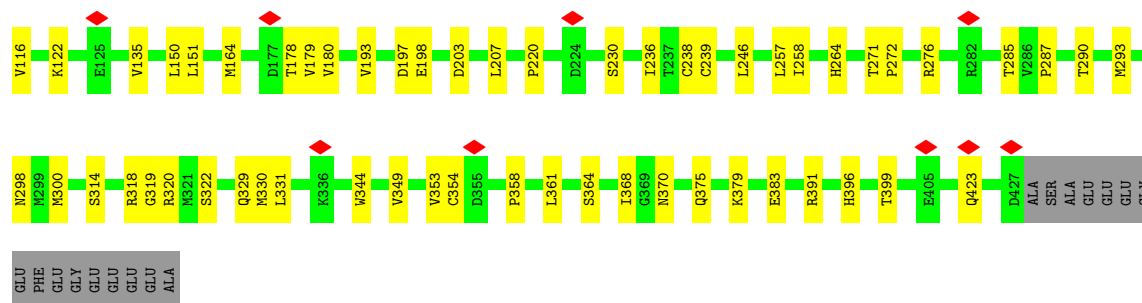
Chain BI: 7% 76% 22%



• Molecule 1: Tubulin beta

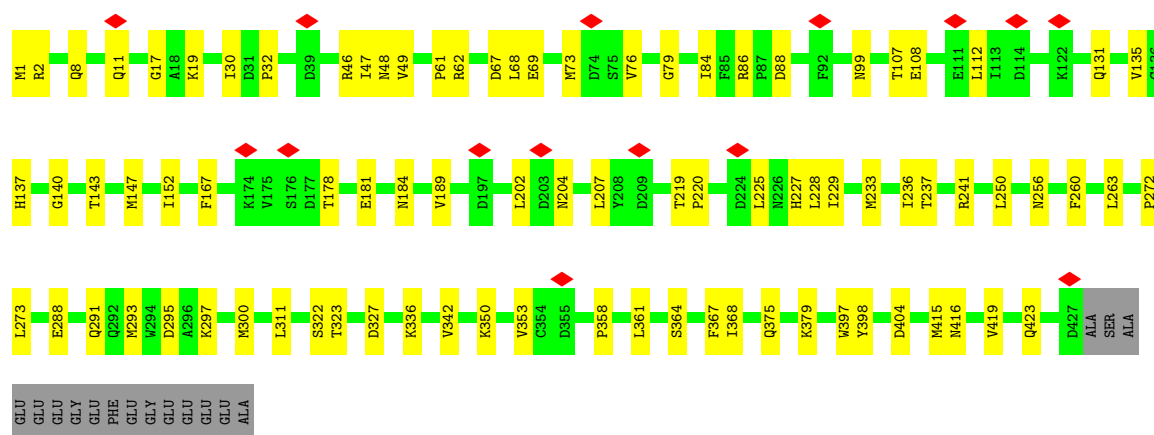
Chain BK: 77% 20%





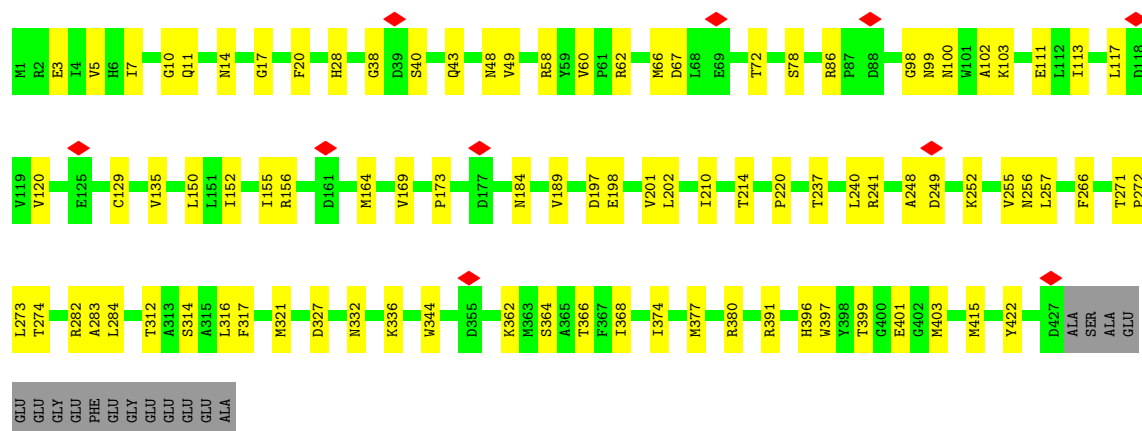
• Molecule 1: Tubulin beta

Chain CC: 77% 19%



• Molecule 1: Tubulin beta

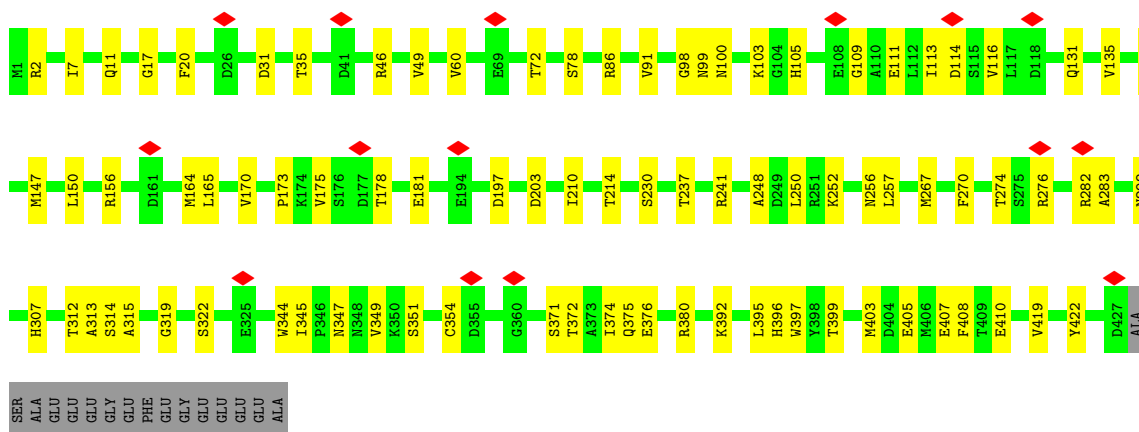
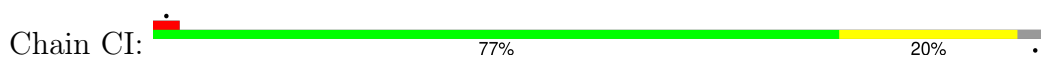
Chain CE: 76% 20%



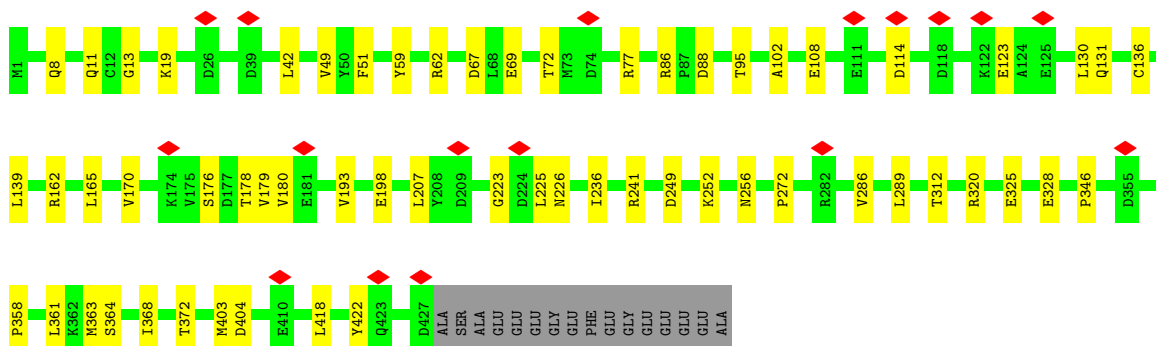
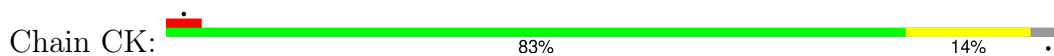
• Molecule 1: Tubulin beta

Chain CG: 77% 20%

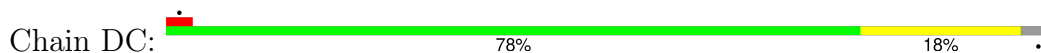
- Molecule 1: Tubulin beta

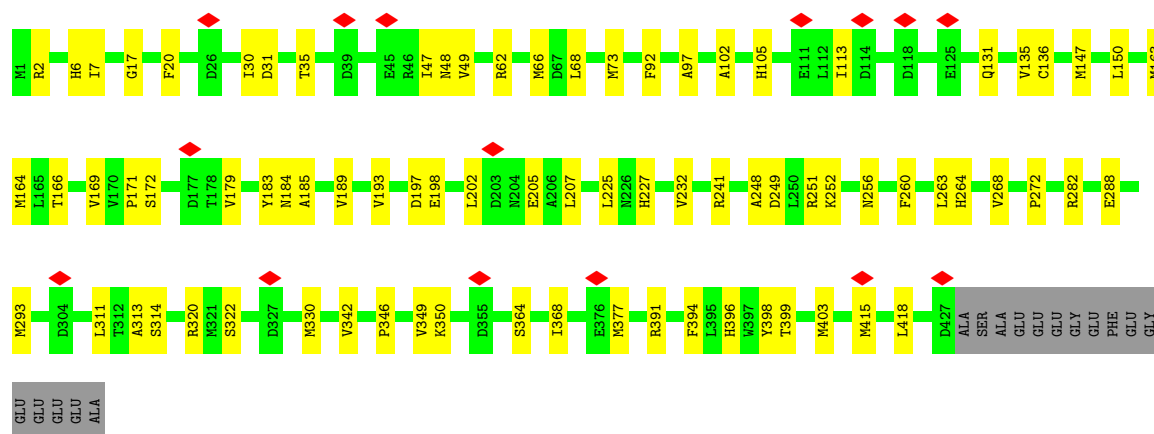


- Molecule 1: Tubulin beta



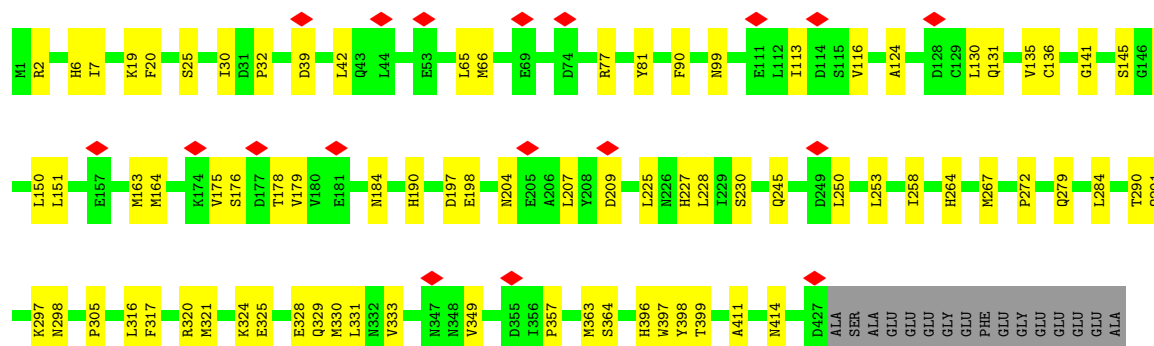
- Molecule 1: Tubulin beta





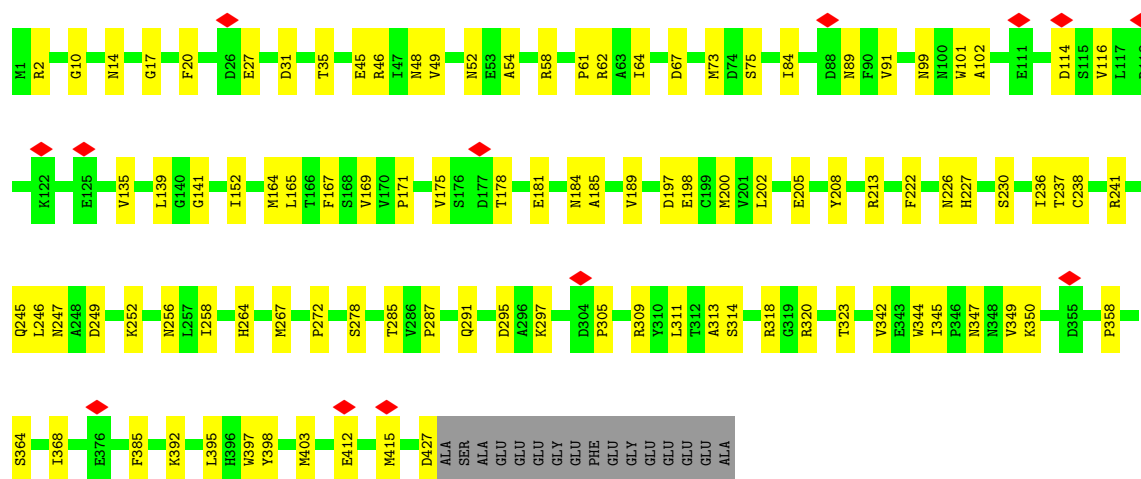
• Molecule 1: Tubulin beta

Chain DE: 78% 18%



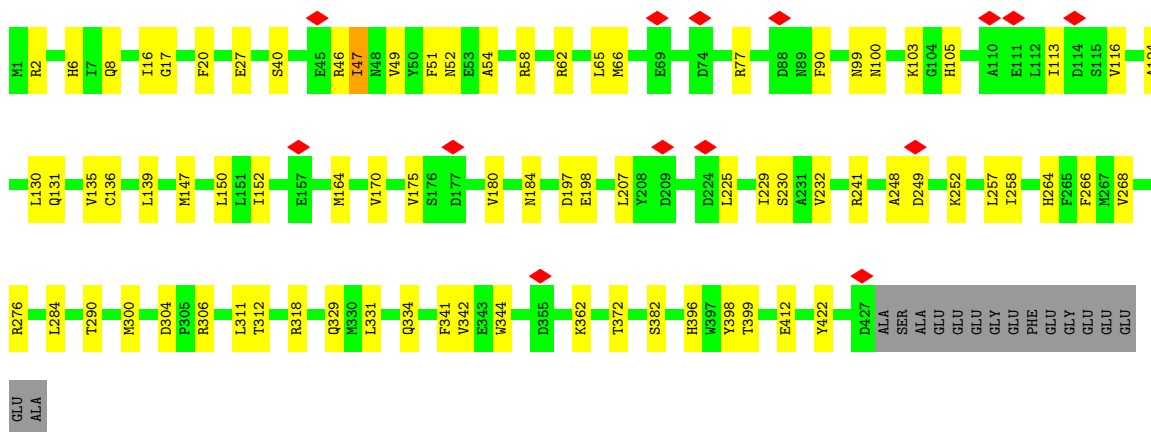
• Molecule 1: Tubulin beta

Chain DG: 74% 23%

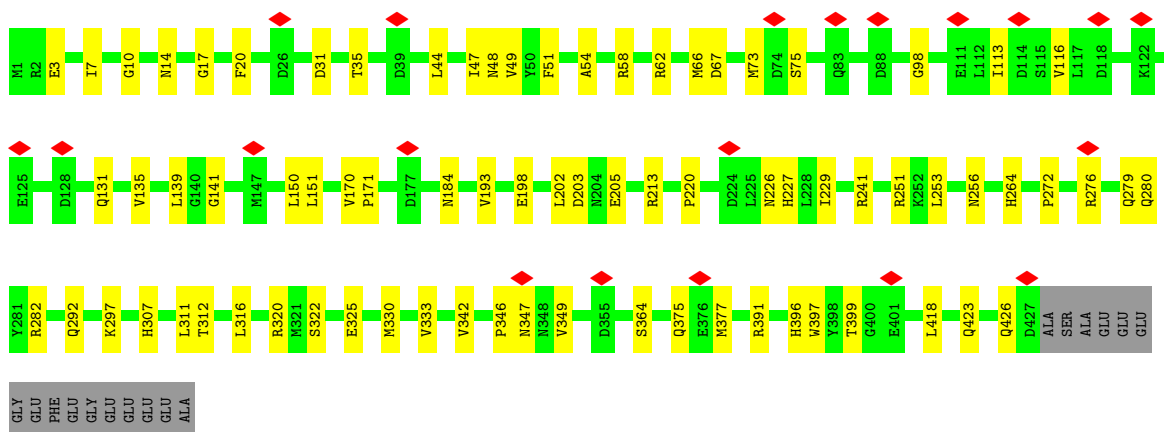
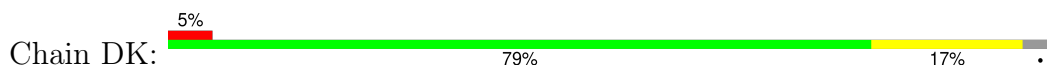


• Molecule 1: Tubulin beta

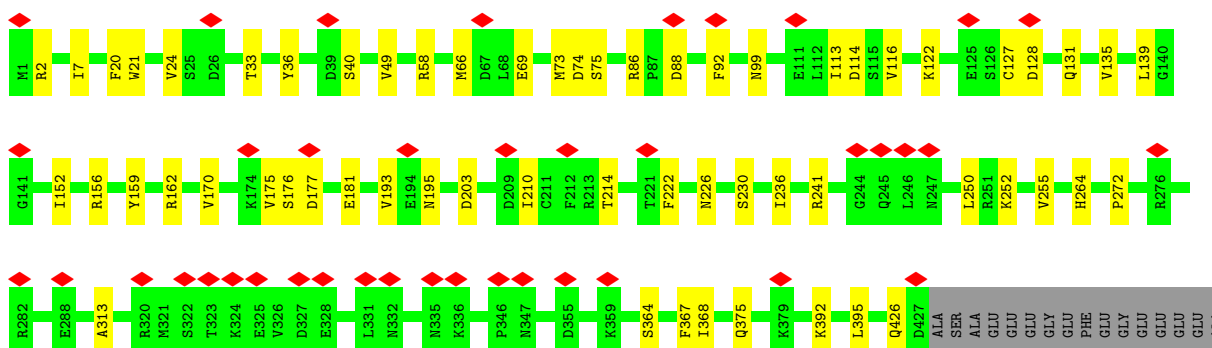
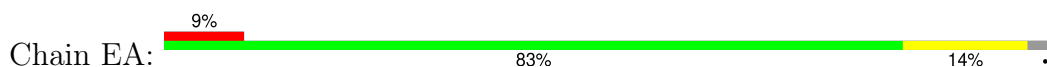
Chain DI: 79% 18%



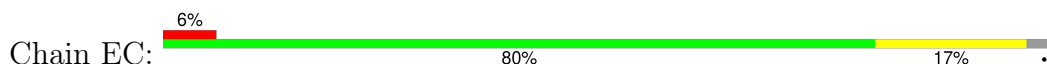
• Molecule 1: Tubulin beta

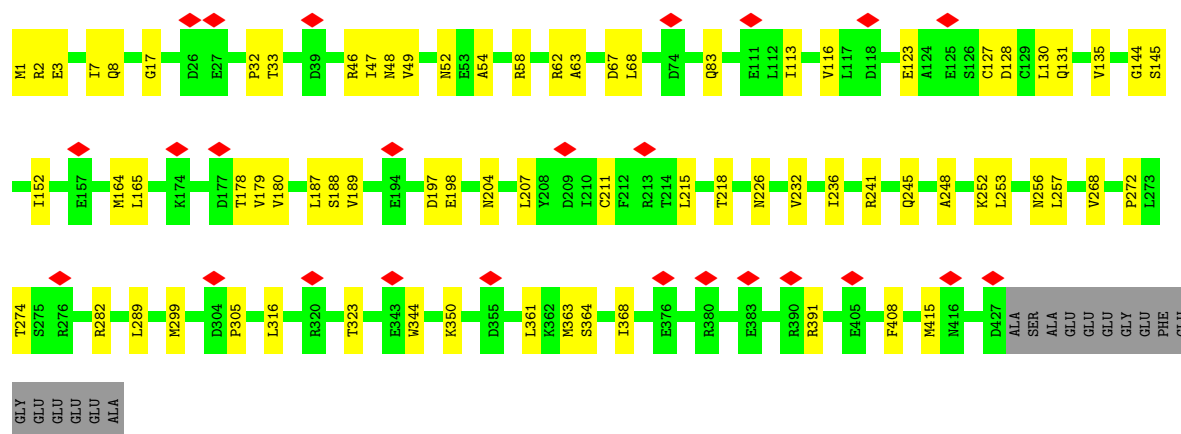


• Molecule 1: Tubulin beta

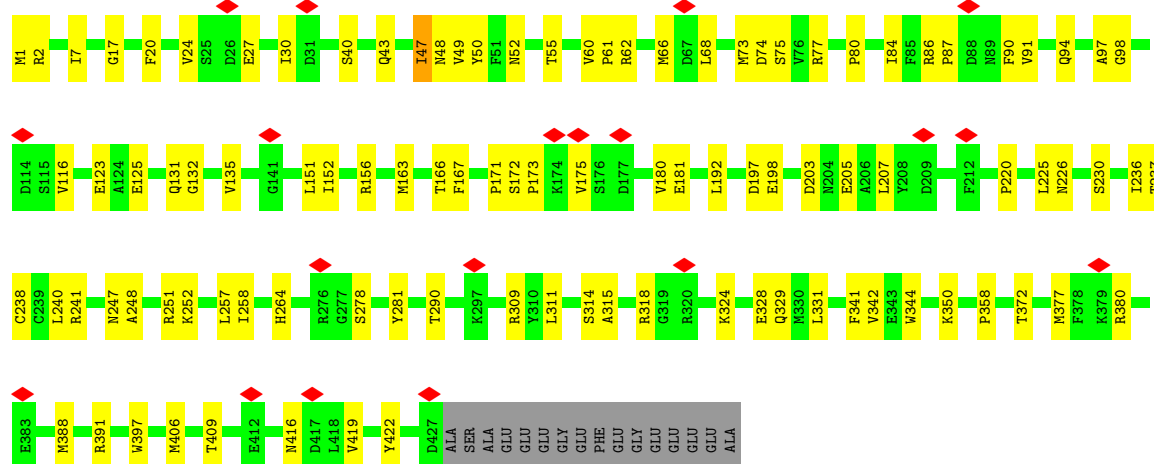
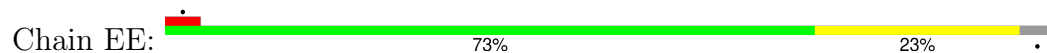


• Molecule 1: Tubulin beta

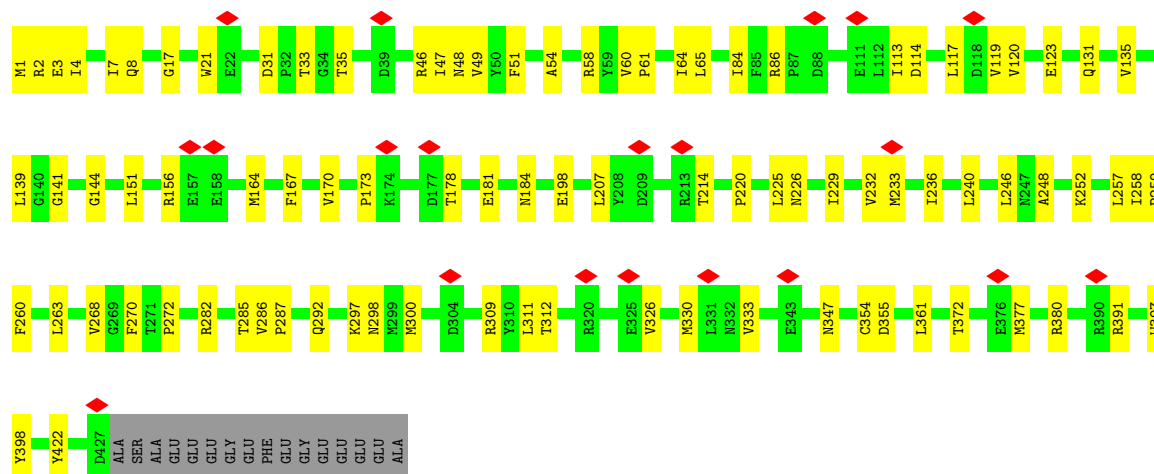
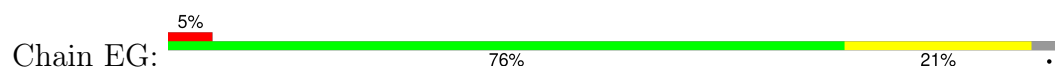




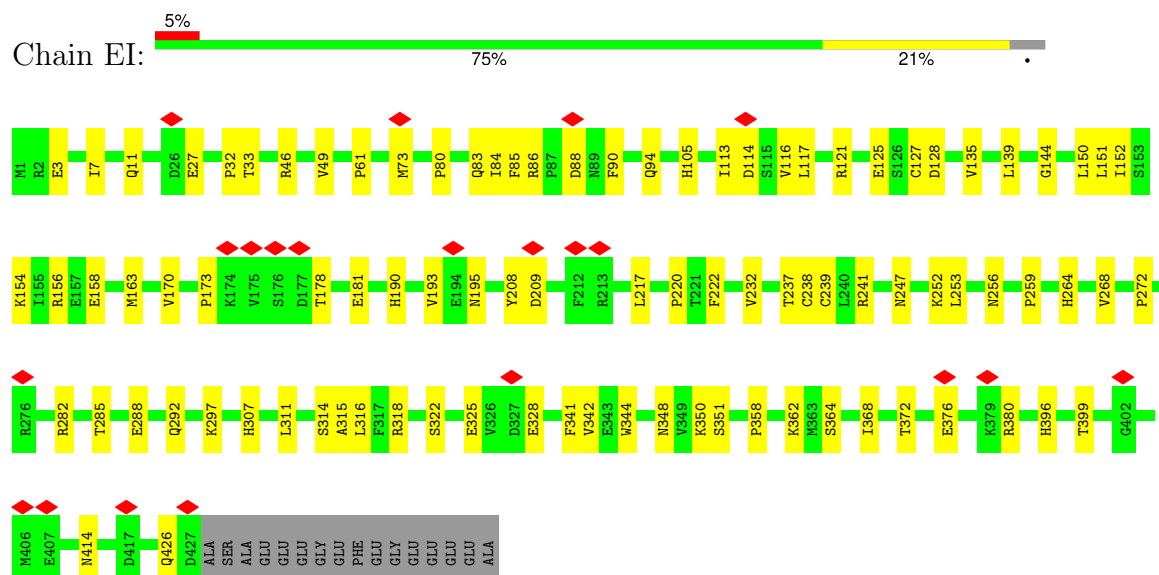
• Molecule 1: Tubulin beta



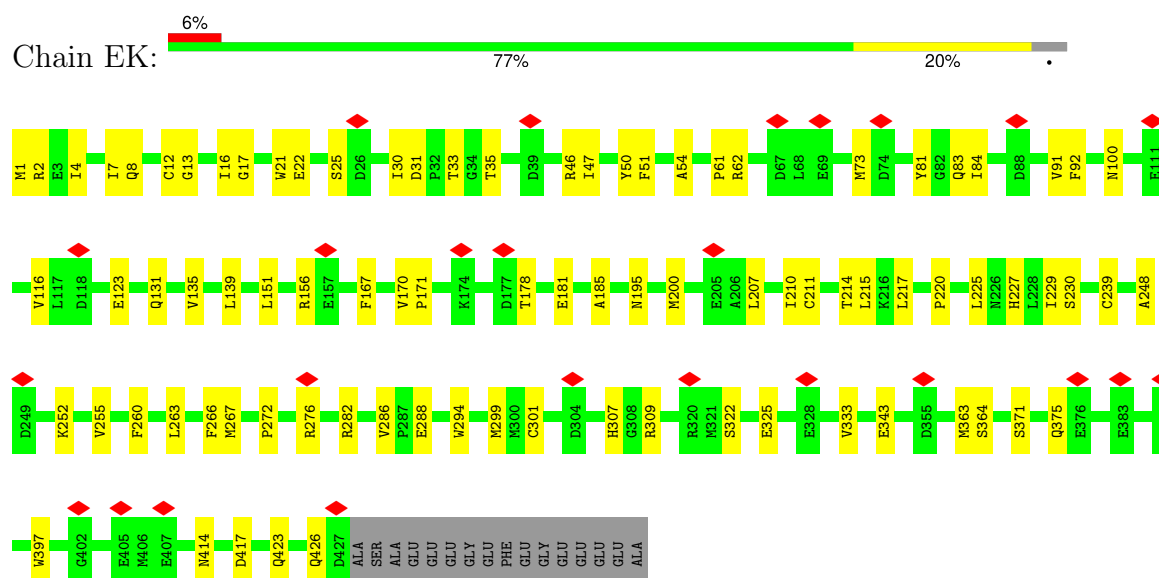
• Molecule 1: Tubulin beta



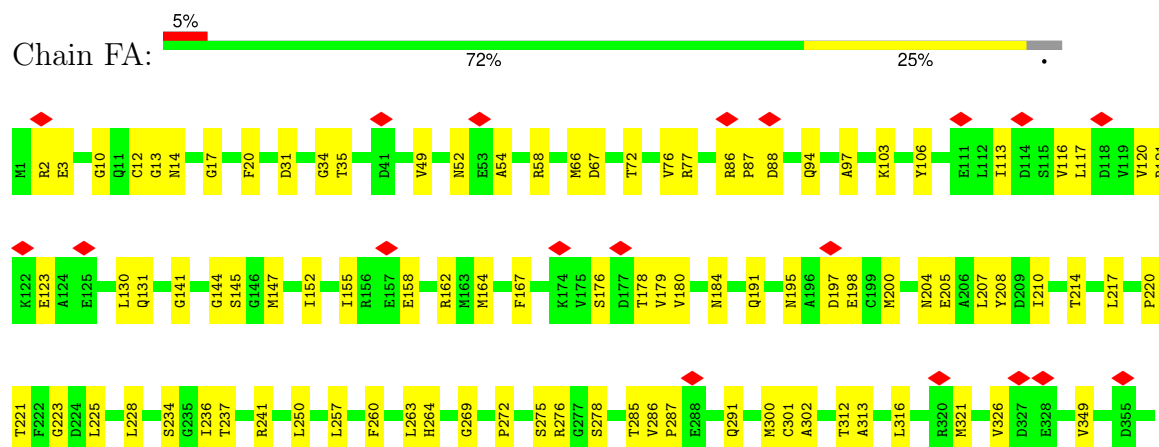
- Molecule 1: Tubulin beta

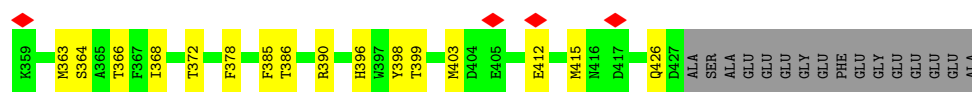


- Molecule 1: Tubulin beta

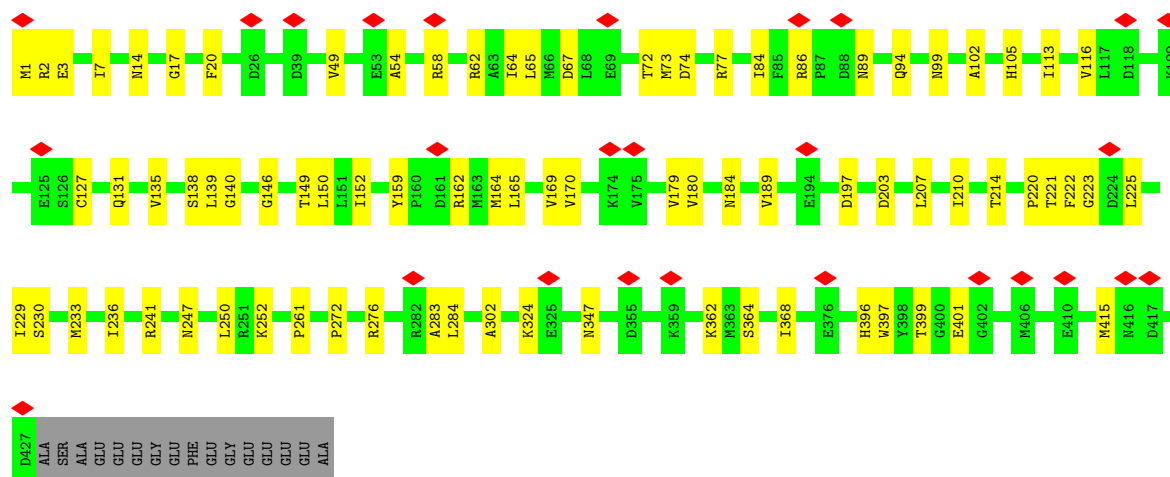
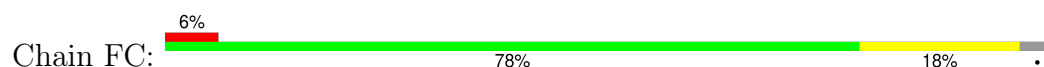


- Molecule 1: Tubulin beta

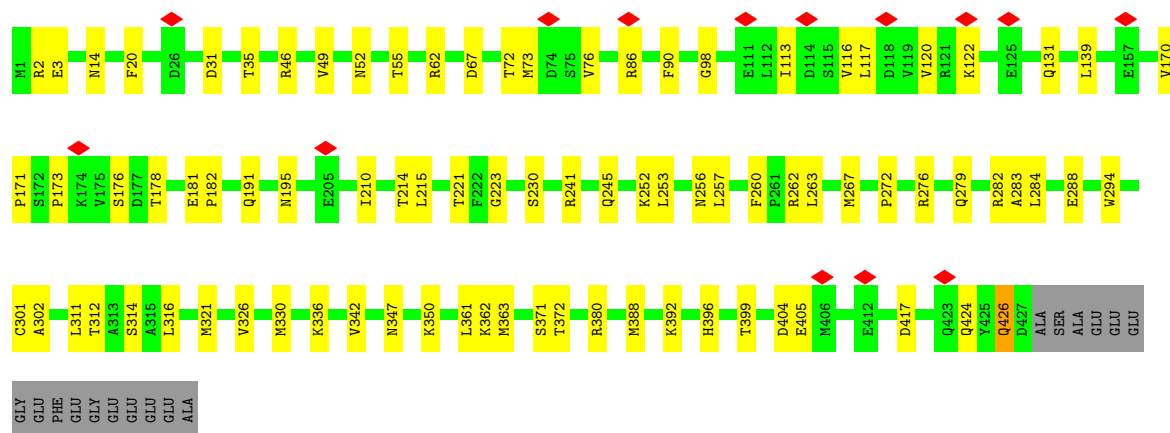
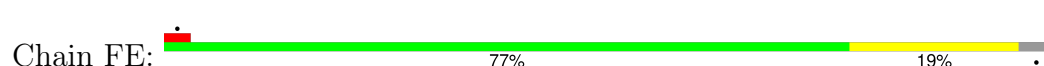




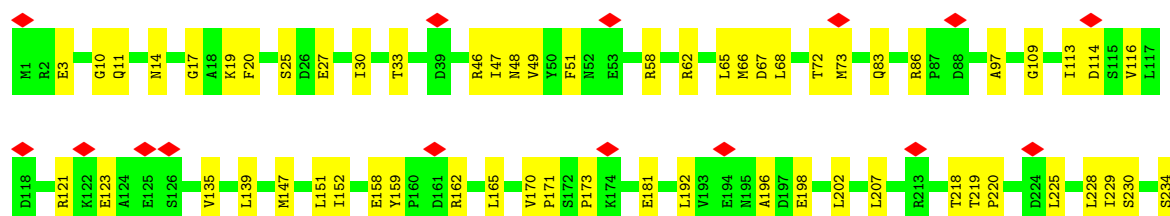
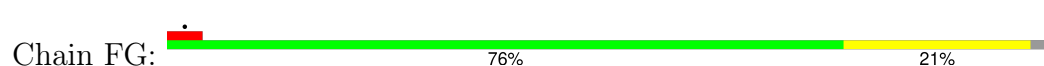
• Molecule 1: Tubulin beta

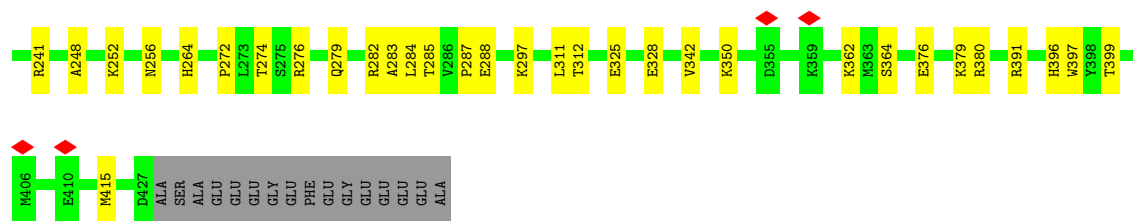


• Molecule 1: Tubulin beta

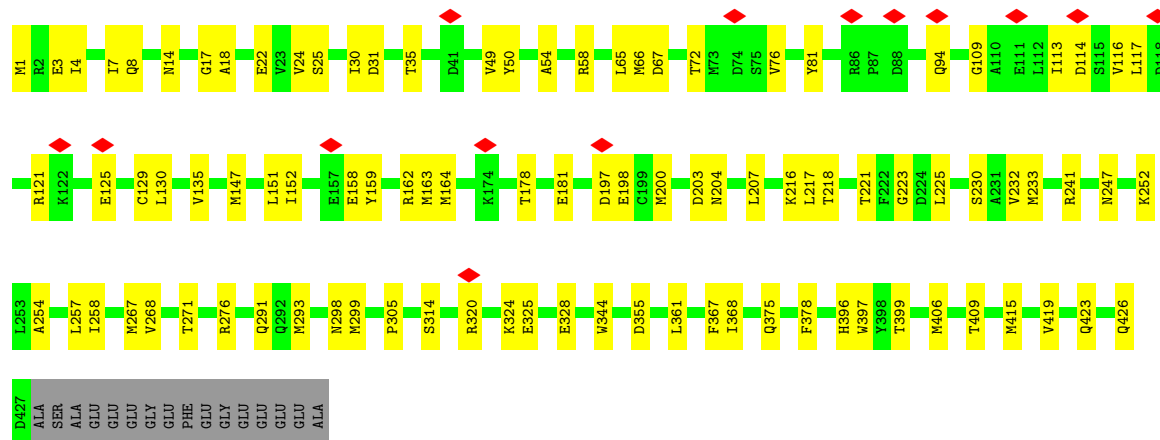
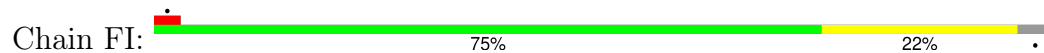


• Molecule 1: Tubulin beta

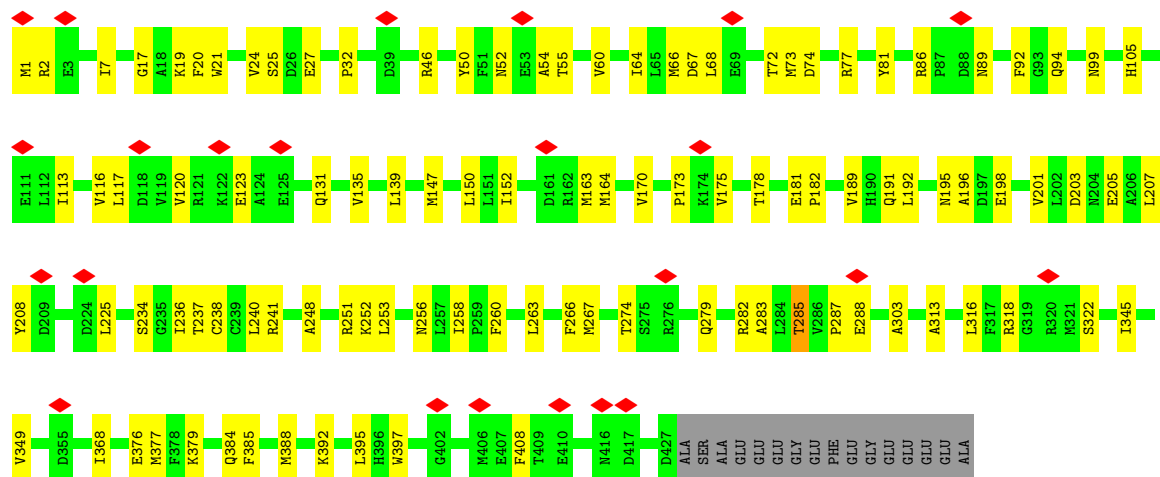
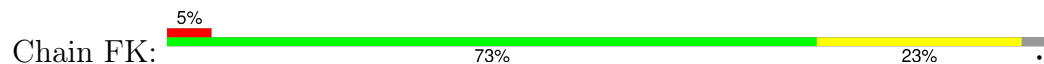




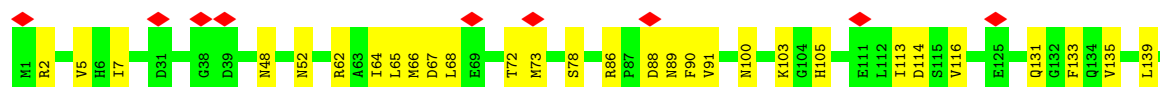
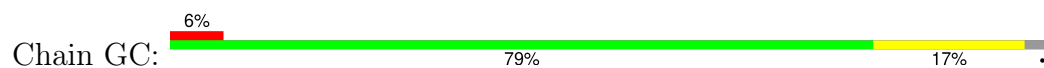
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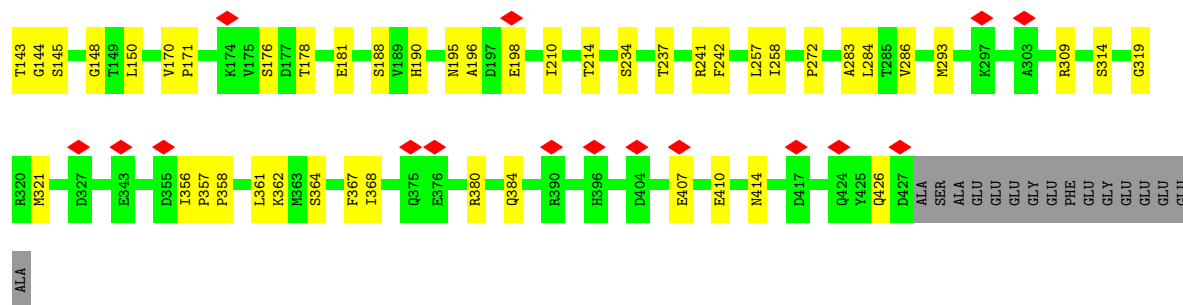


• Molecule 1: Tubulin beta

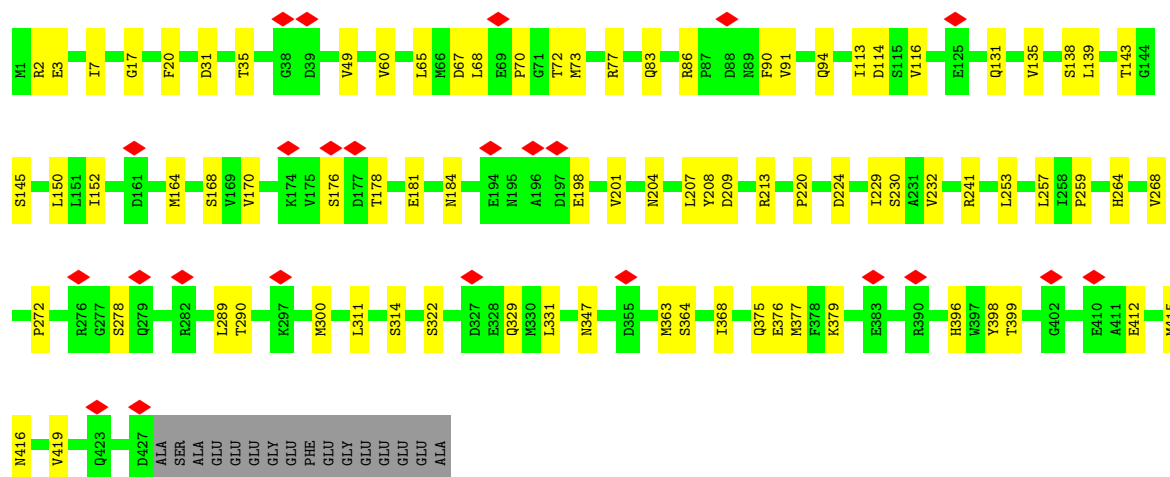
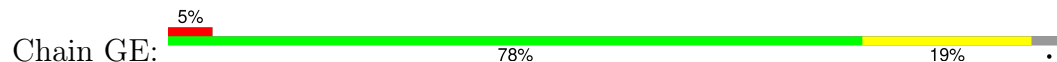


• Molecule 1: Tubulin beta

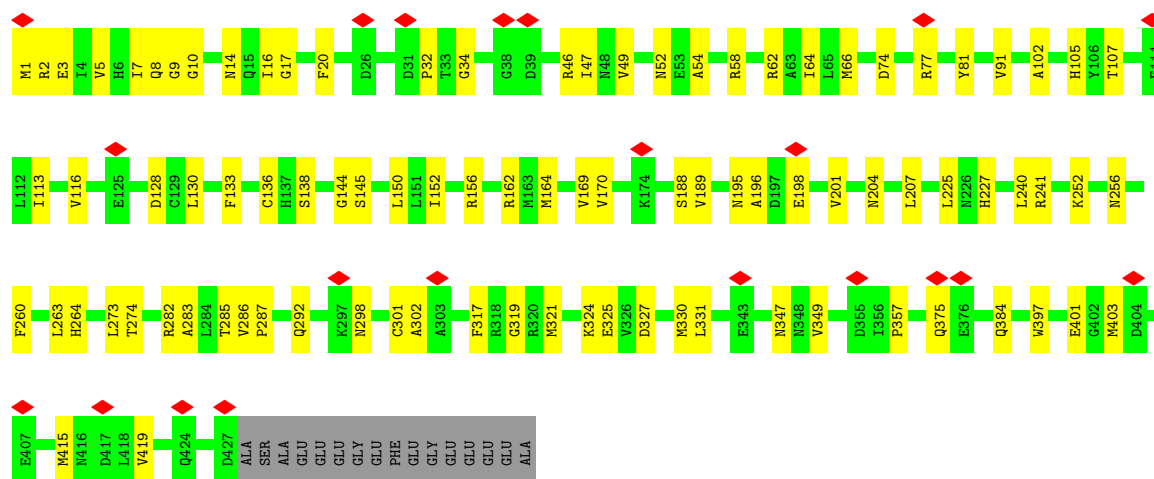
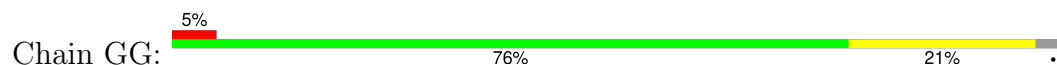




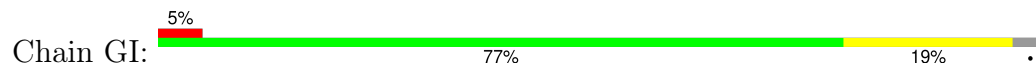
- Molecule 1: Tubulin beta

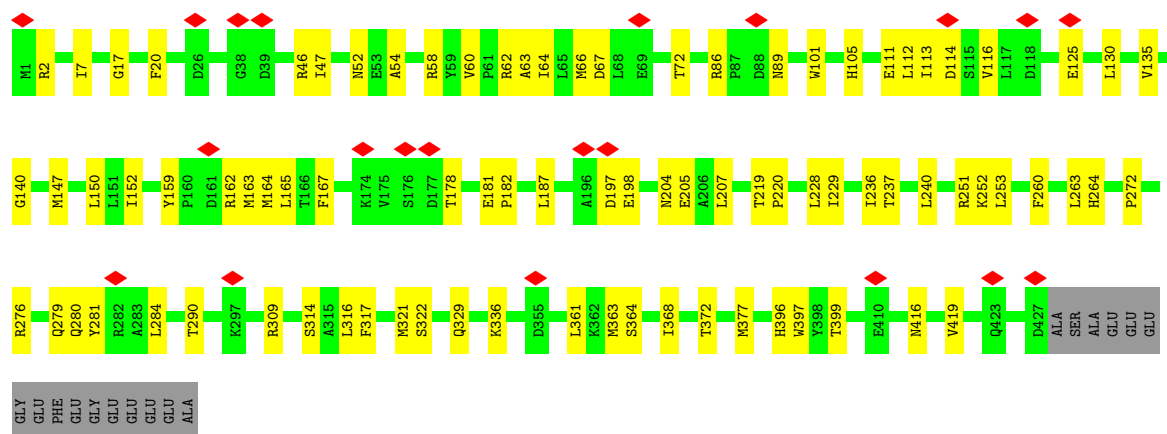


- Molecule 1: Tubulin beta

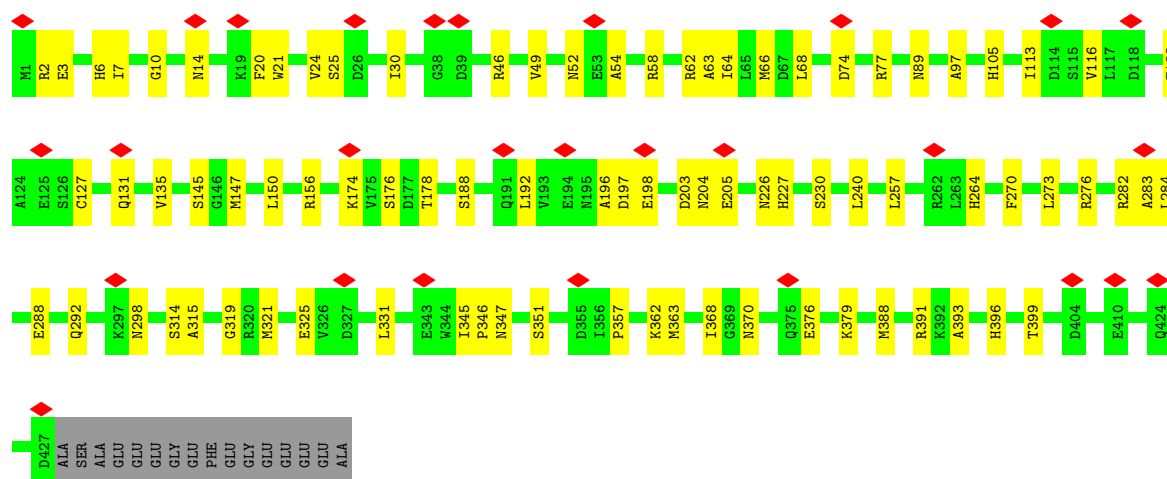
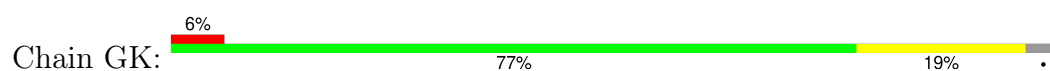


- Molecule 1: Tubulin beta

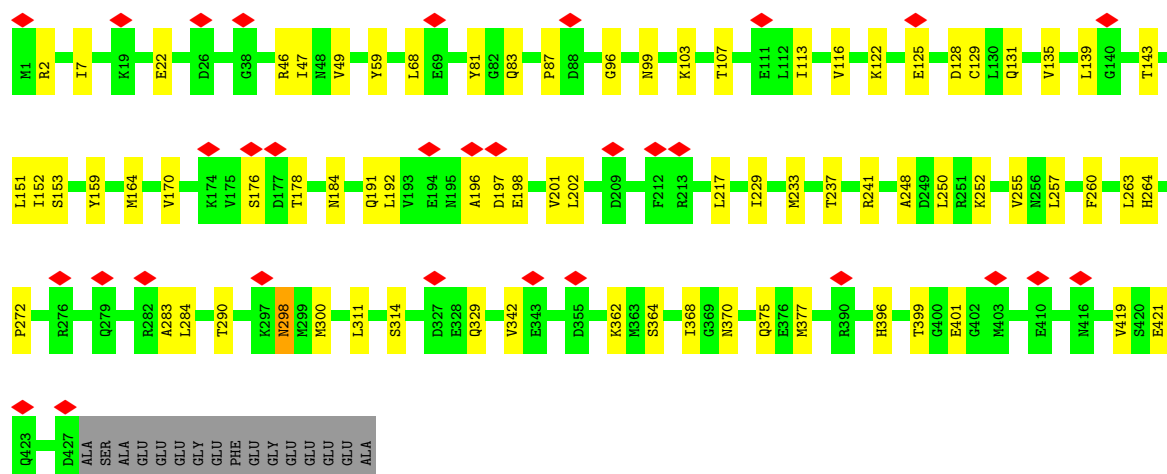
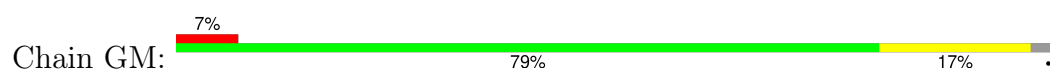




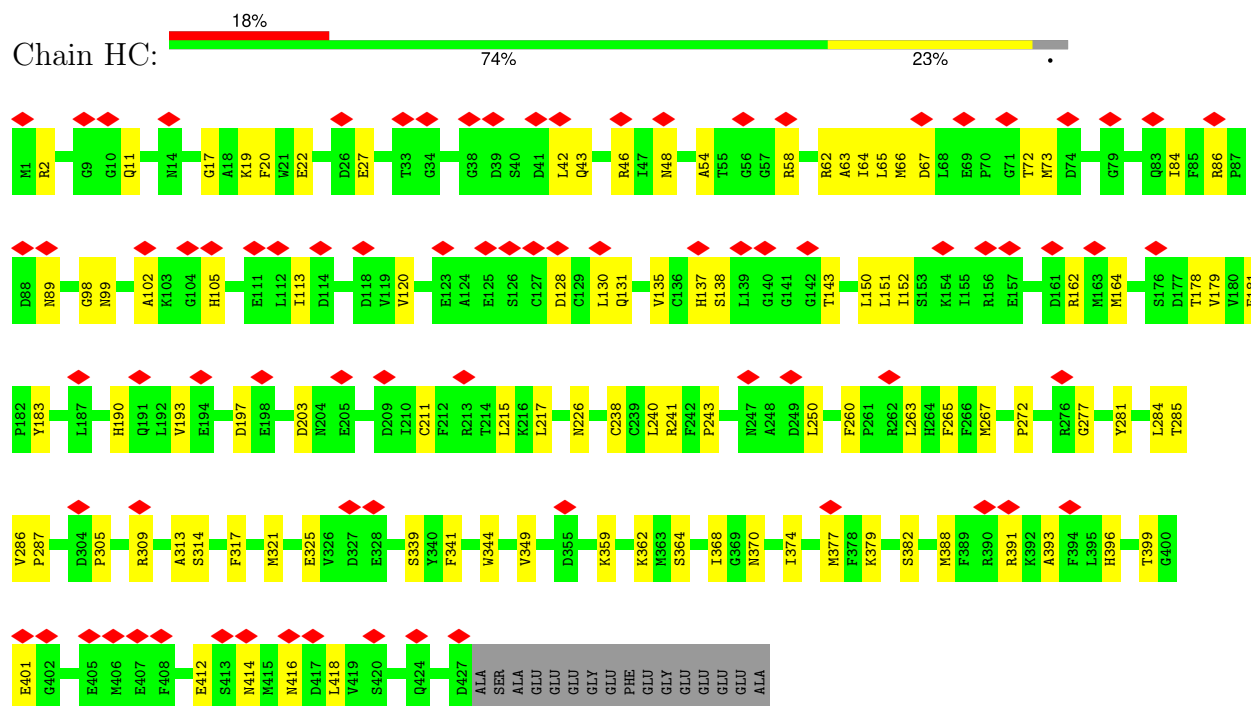
• Molecule 1: Tubulin beta



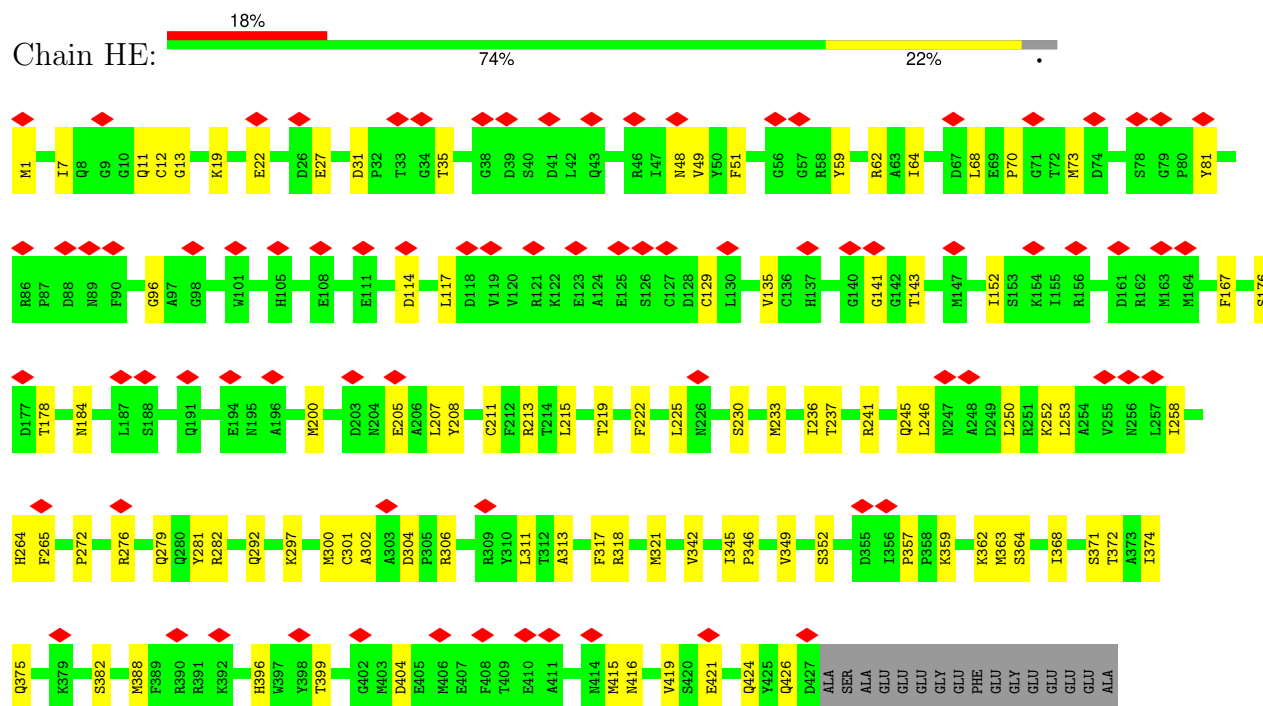
• Molecule 1: Tubulin beta



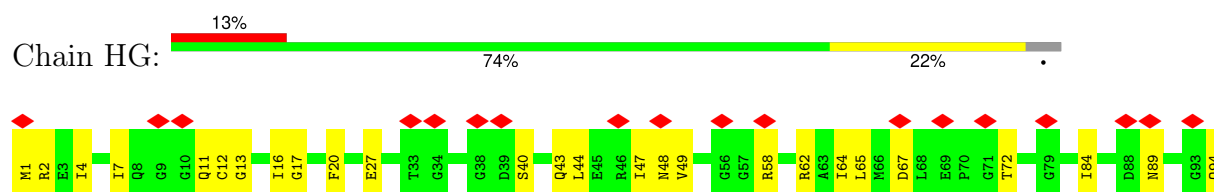
- Molecule 1: Tubulin beta

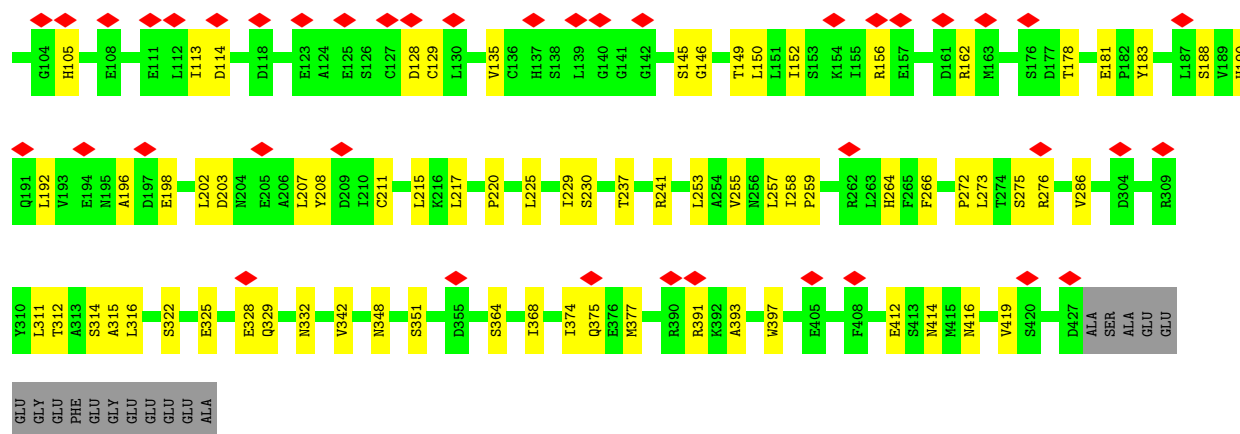


- Molecule 1: Tubulin beta

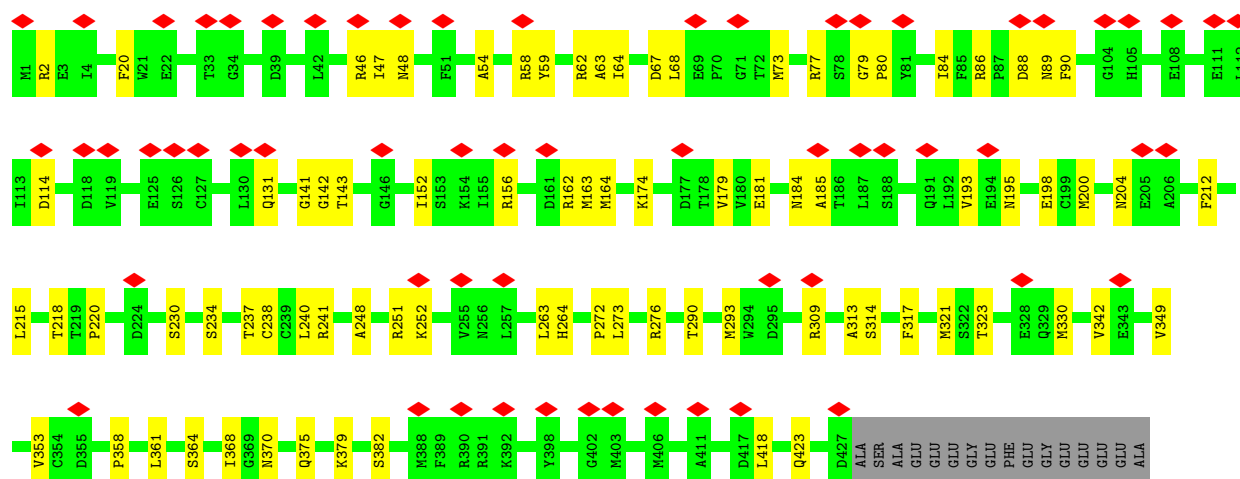
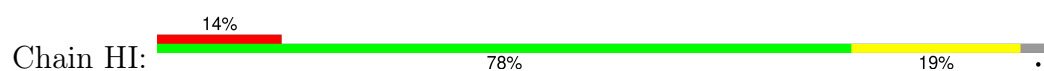


- Molecule 1: Tubulin beta

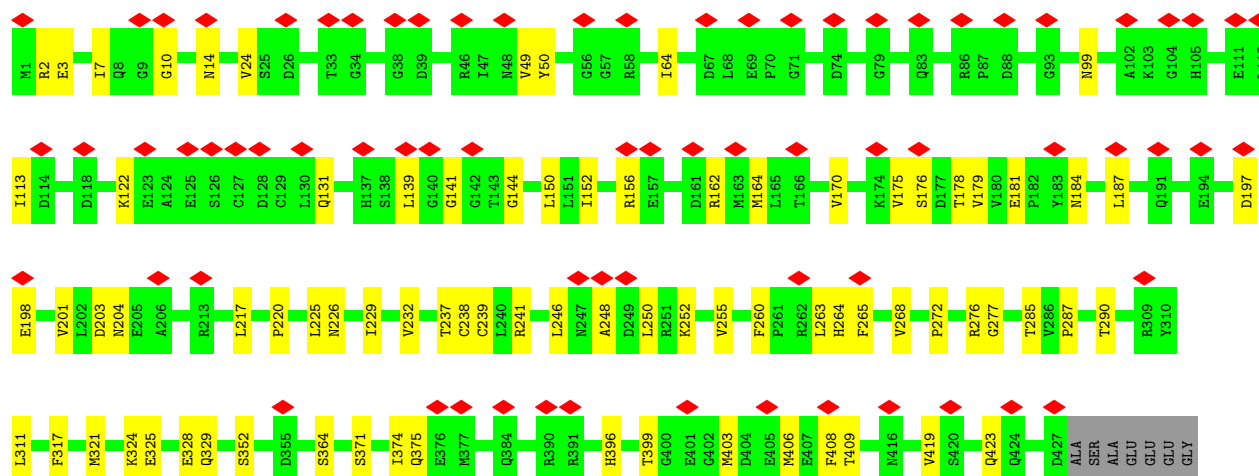
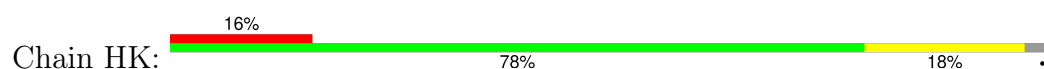




• Molecule 1: Tubulin beta

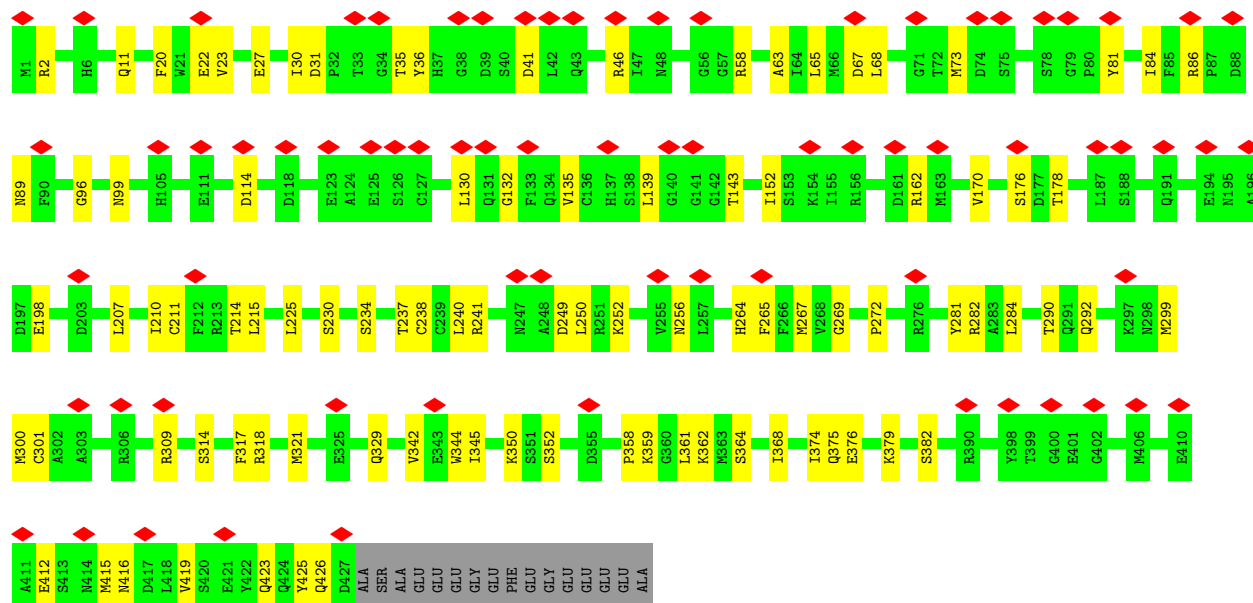
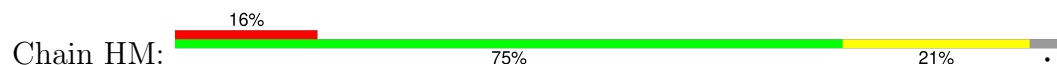


• Molecule 1: Tubulin beta

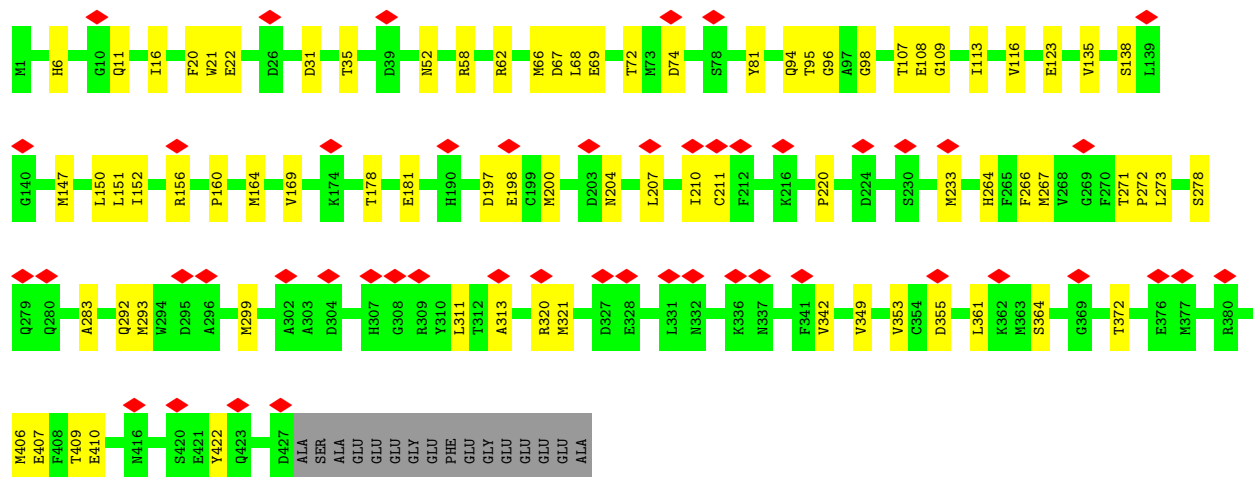
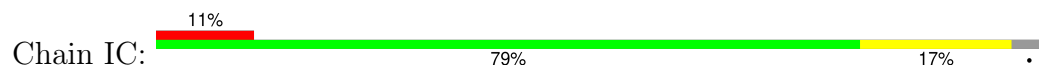


GLU
PHE
GLU
GLY
GLU
GLU
GLU
GLU
ALA

• Molecule 1: Tubulin beta

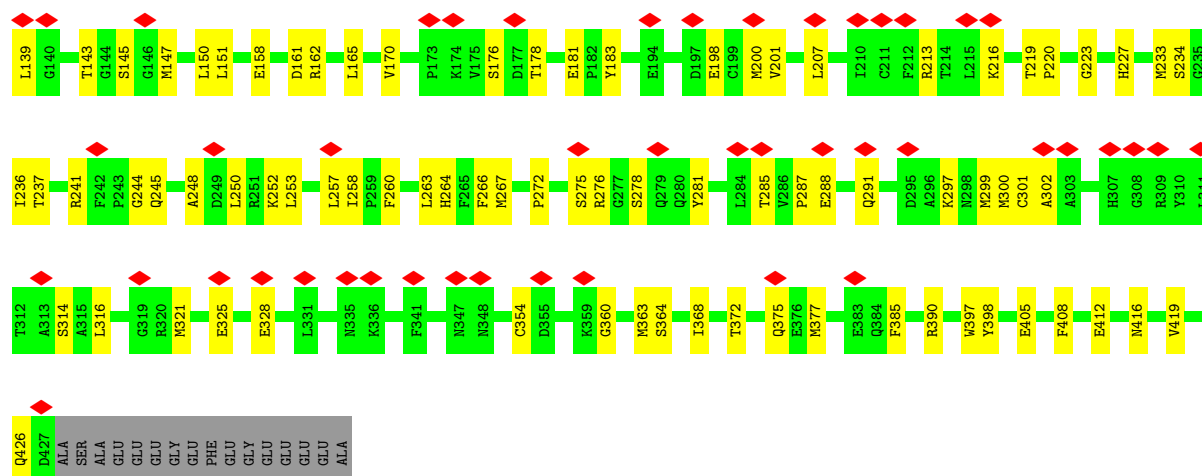


• Molecule 1: Tubulin beta

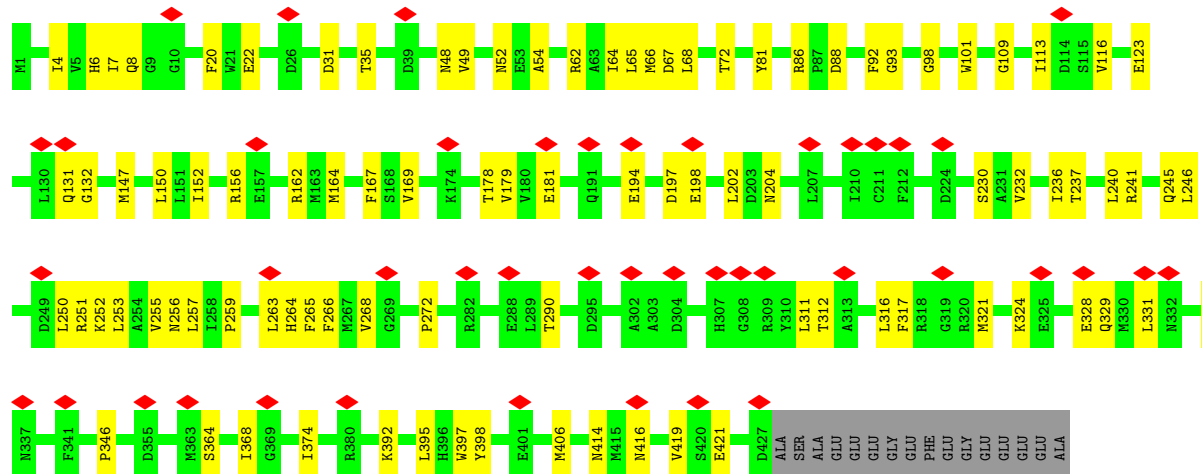
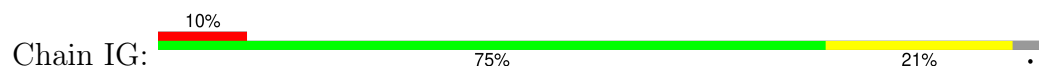


• Molecule 1: Tubulin beta

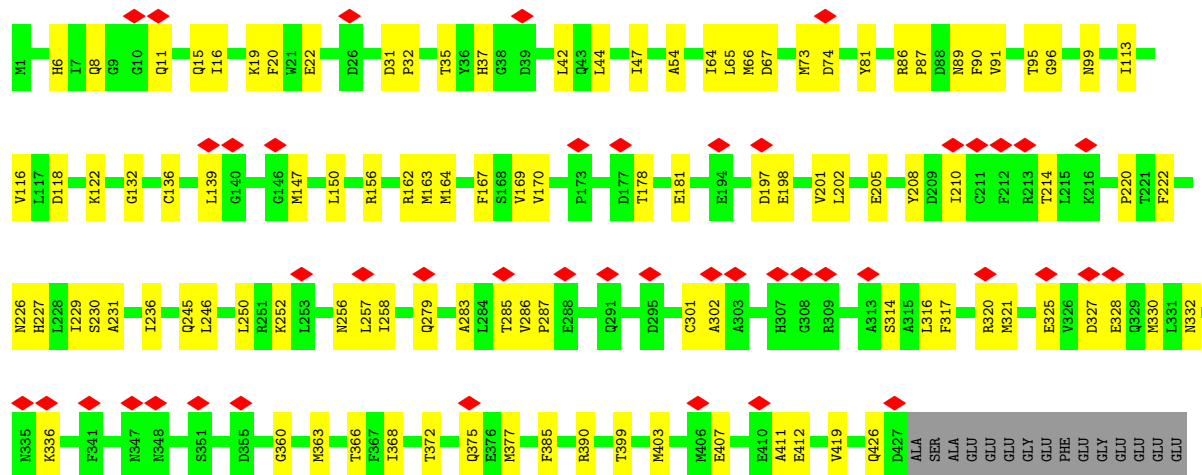




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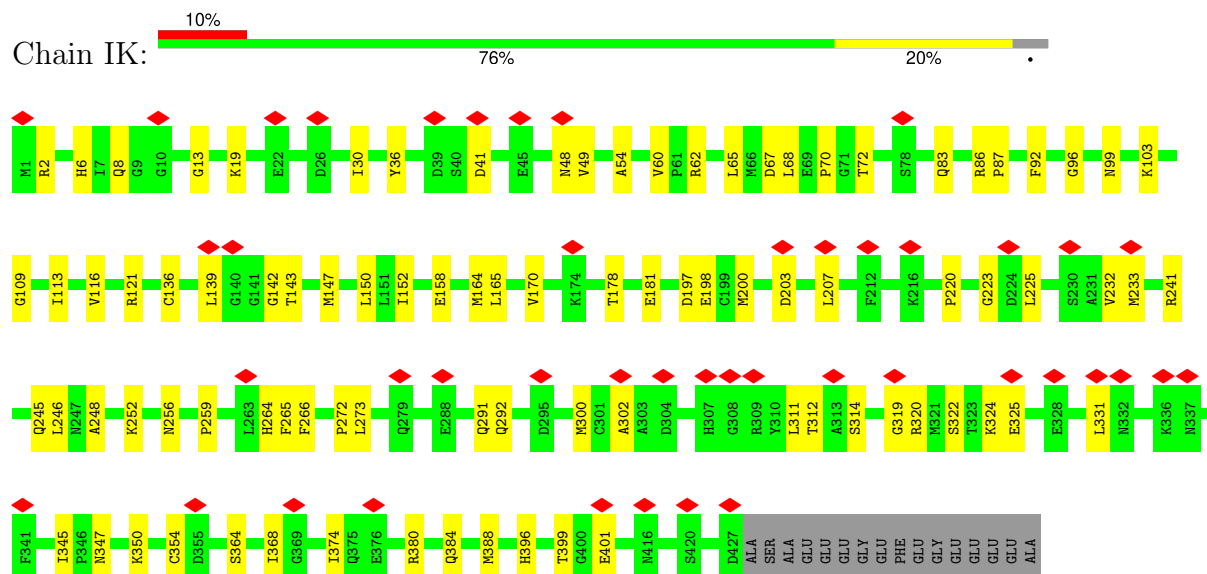


• Molecule 1: Tubulin beta

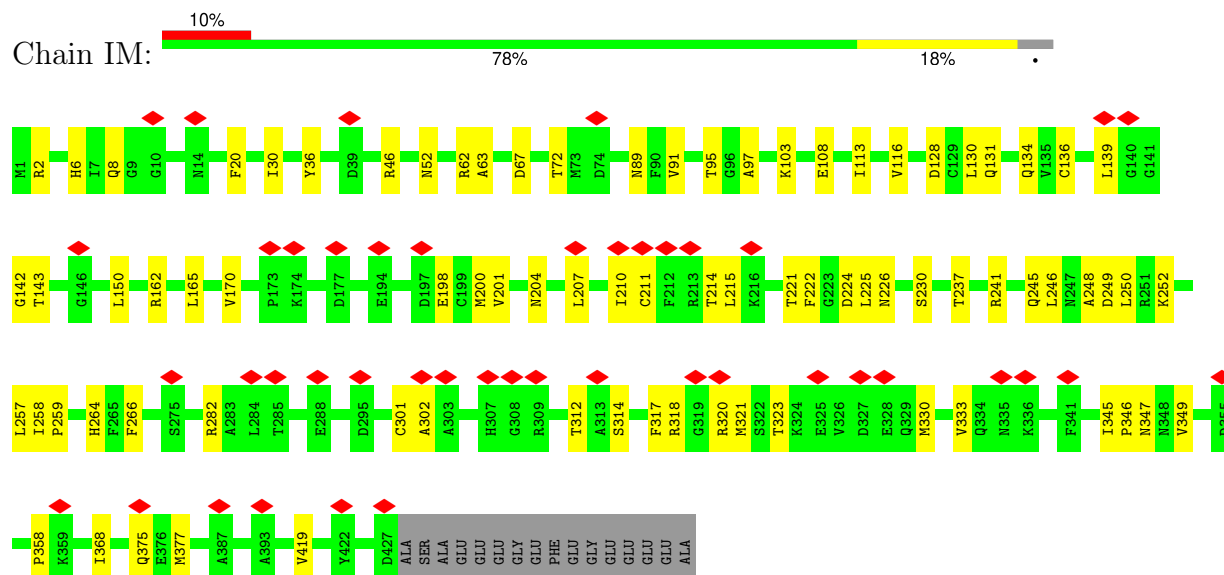


ALA

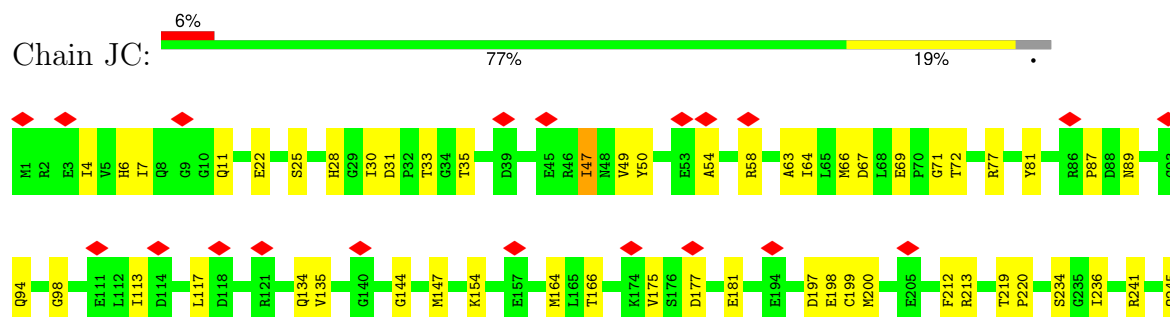
- Molecule 1: Tubulin beta

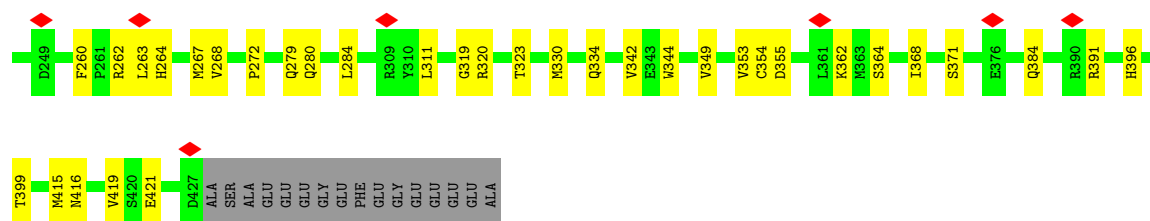


- Molecule 1: Tubulin beta



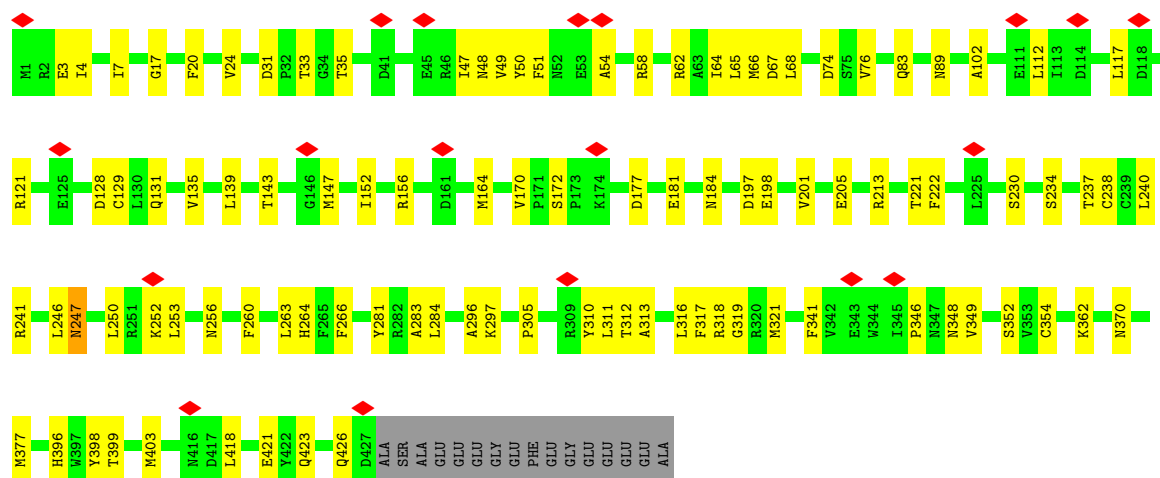
- Molecule 1: Tubulin beta





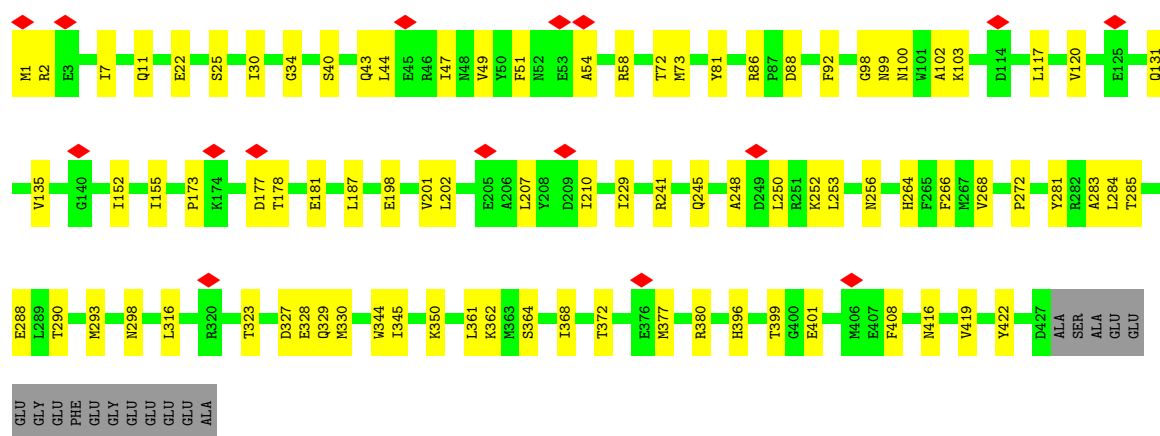
• Molecule 1: Tubulin beta

Chain JE: 74% 22%



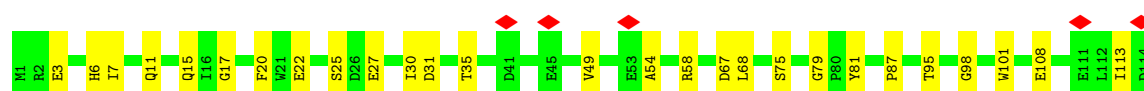
• Molecule 1: Tubulin beta

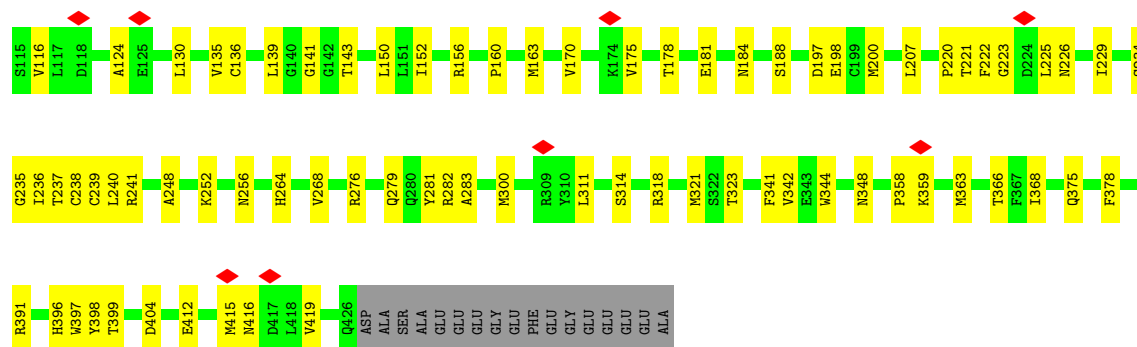
Chain JG: 77% 19%



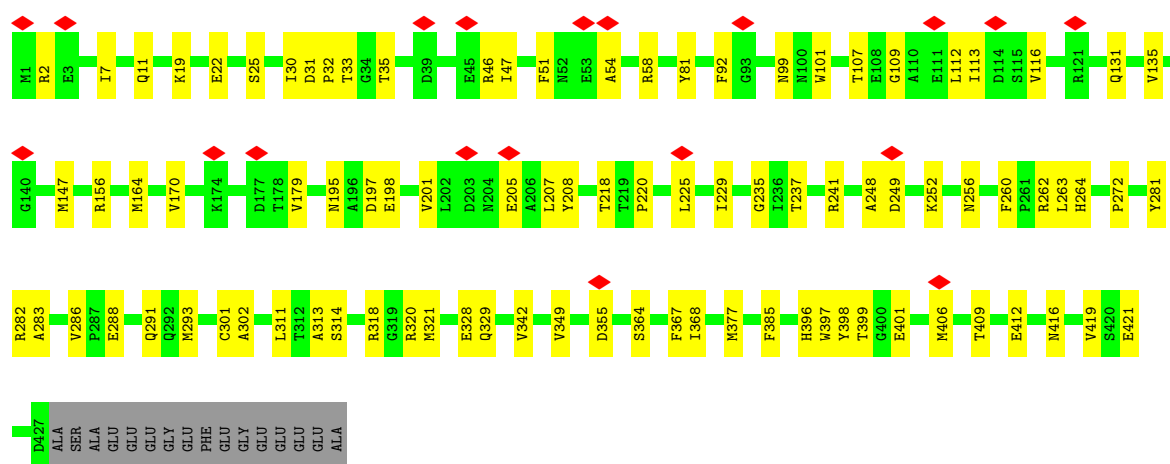
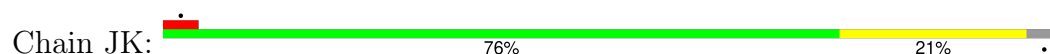
• Molecule 1: Tubulin beta

Chain JI: 73% 23%

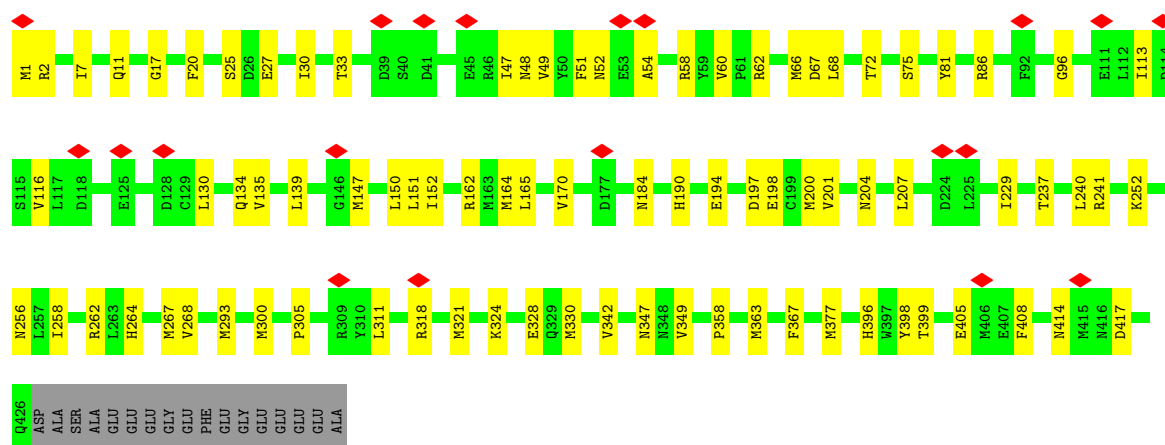
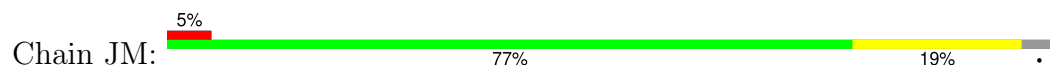




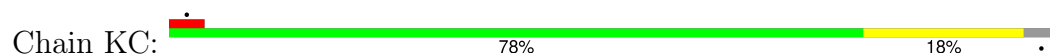
• Molecule 1: Tubulin beta

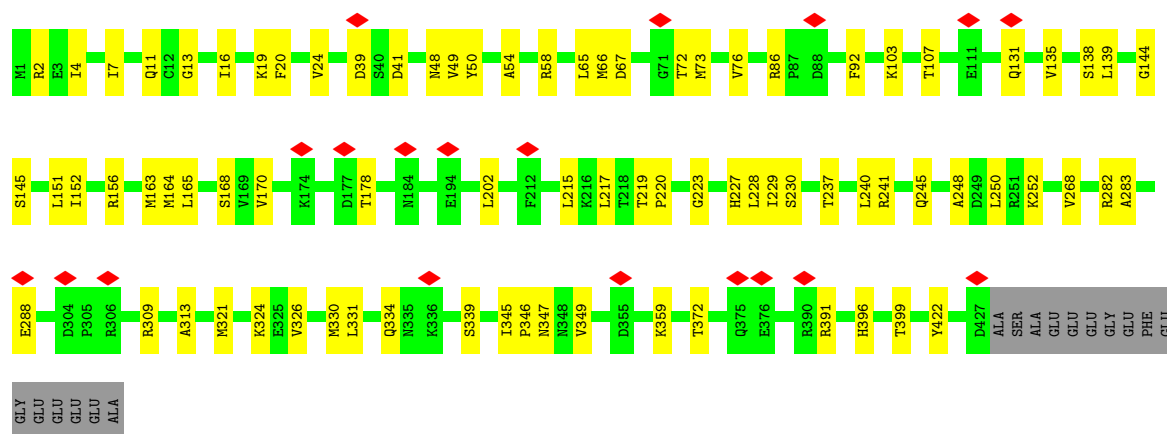


• Molecule 1: Tubulin beta

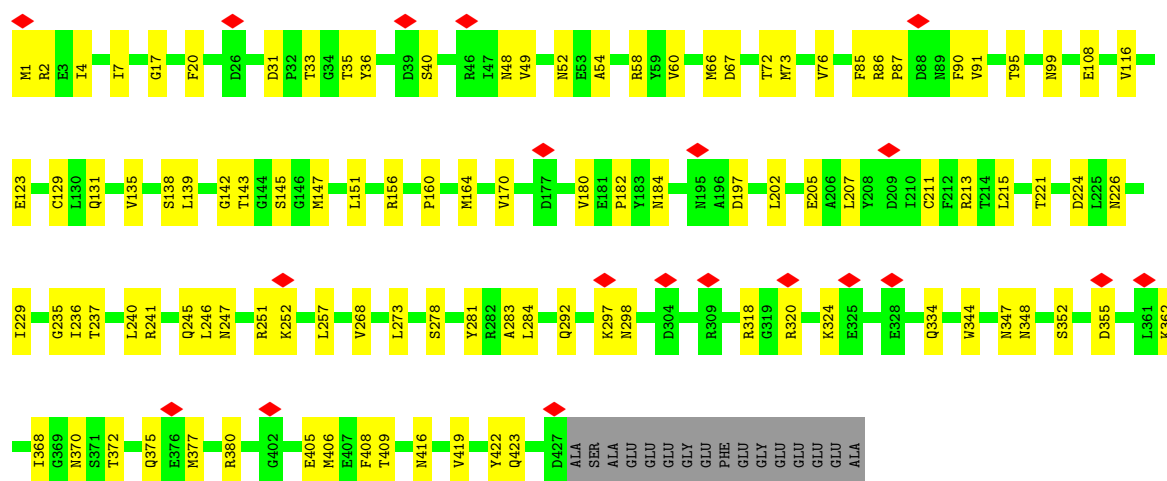
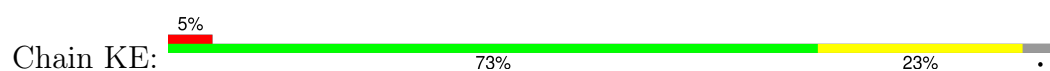


• Molecule 1: Tubulin beta

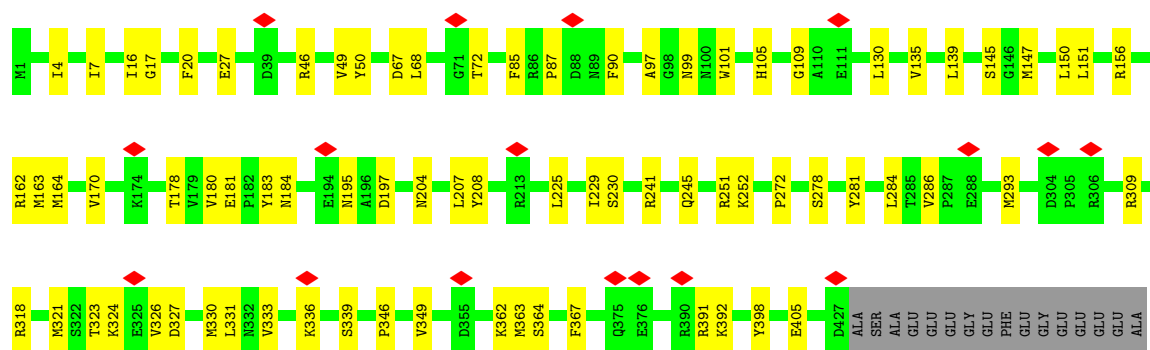
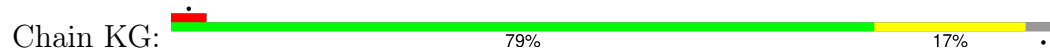




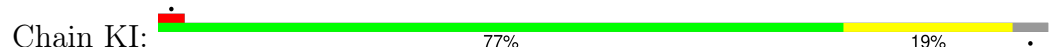
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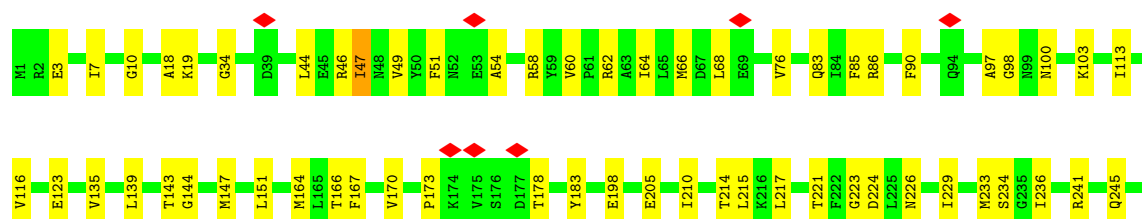


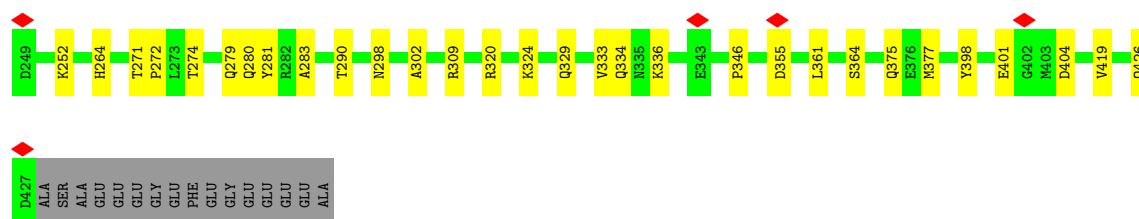
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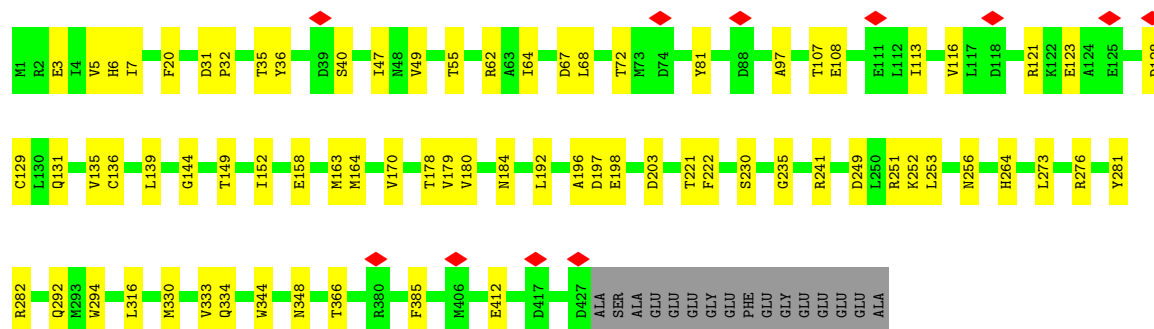
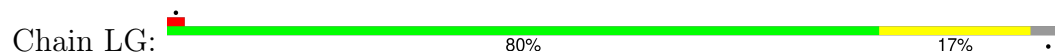
• Molecule 1: Tubulin beta



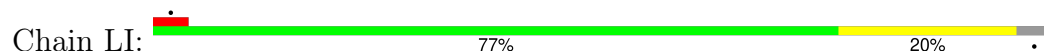




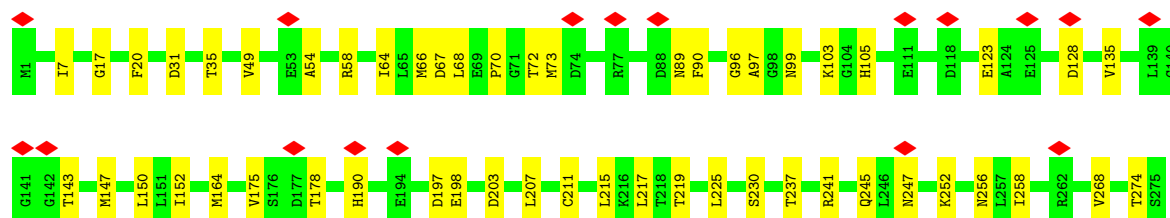
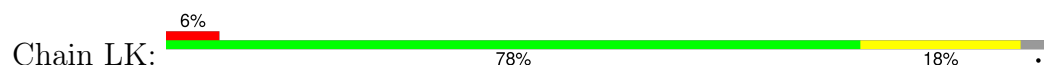
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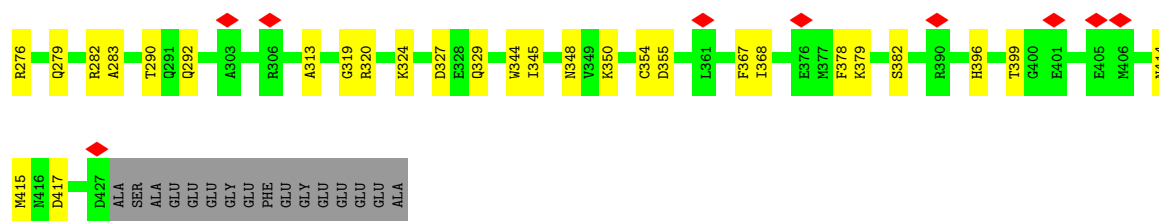


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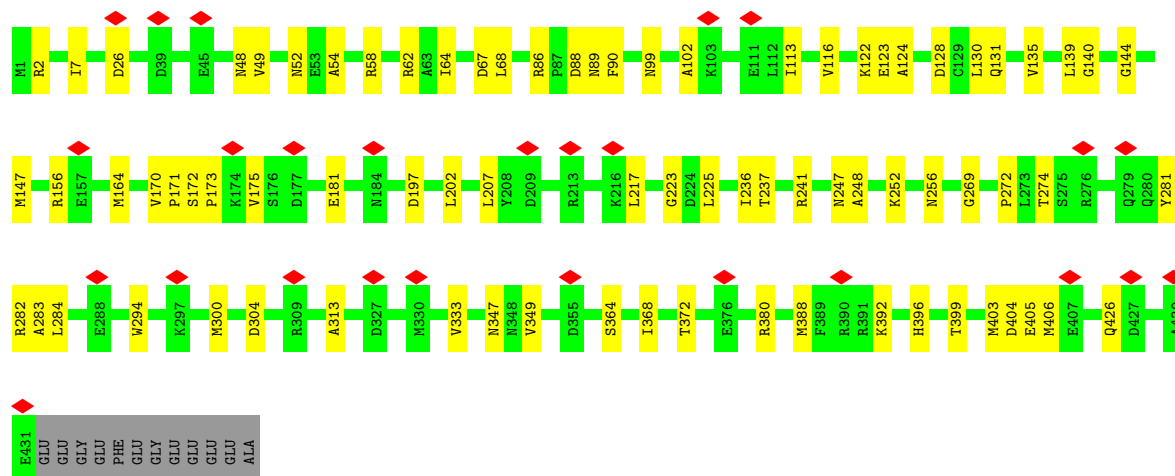
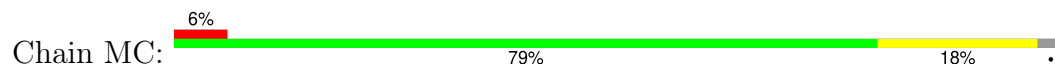


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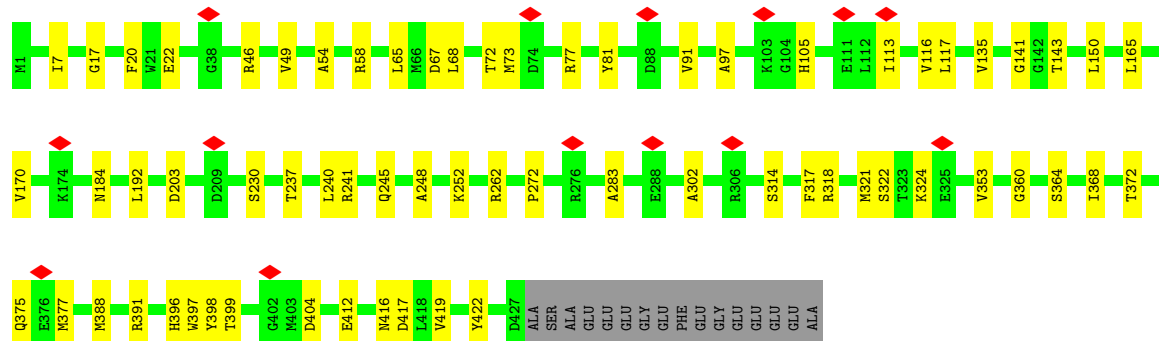
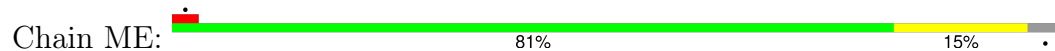




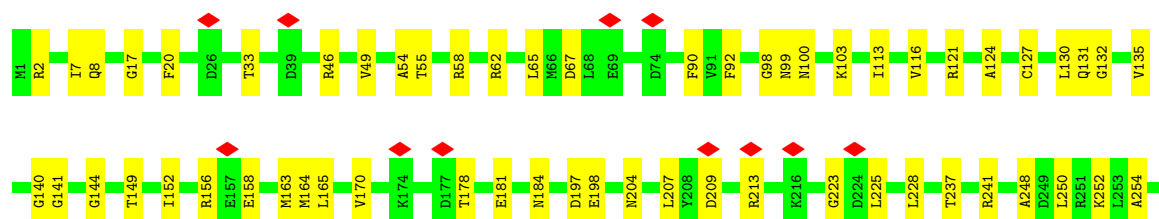
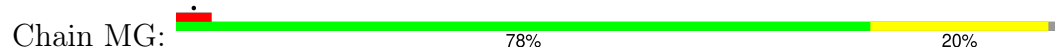
- Molecule 1: Tubulin beta

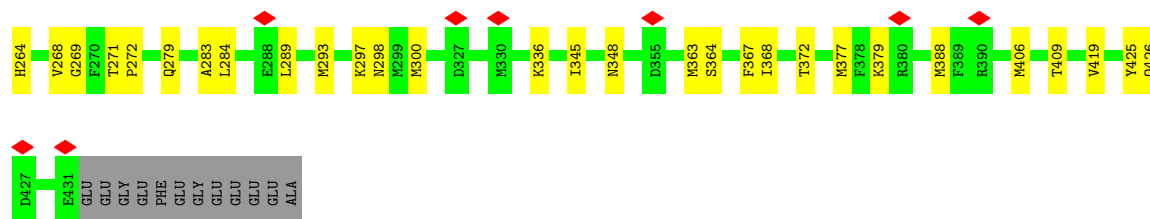


- Molecule 1: Tubulin beta

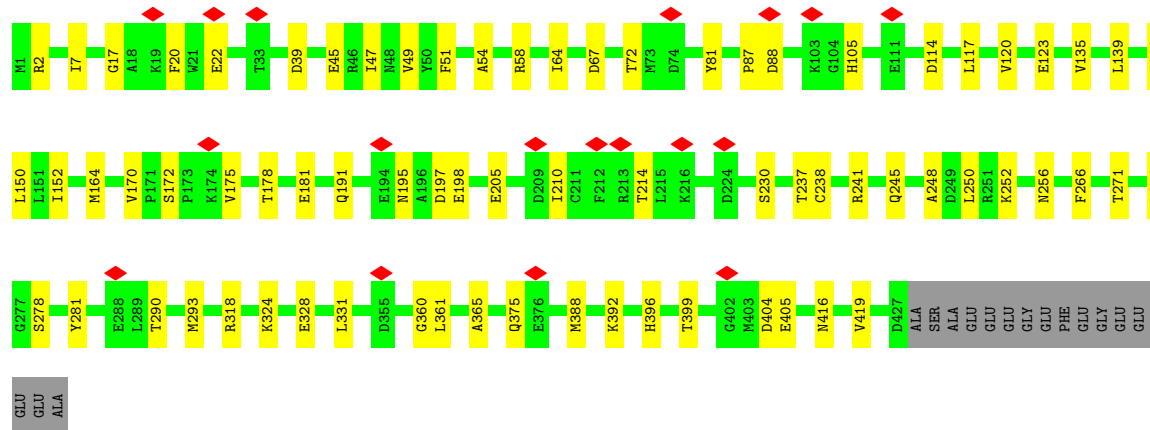
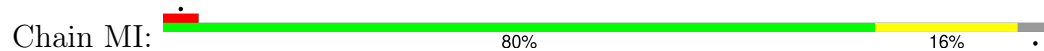


- Molecule 1: Tubulin beta

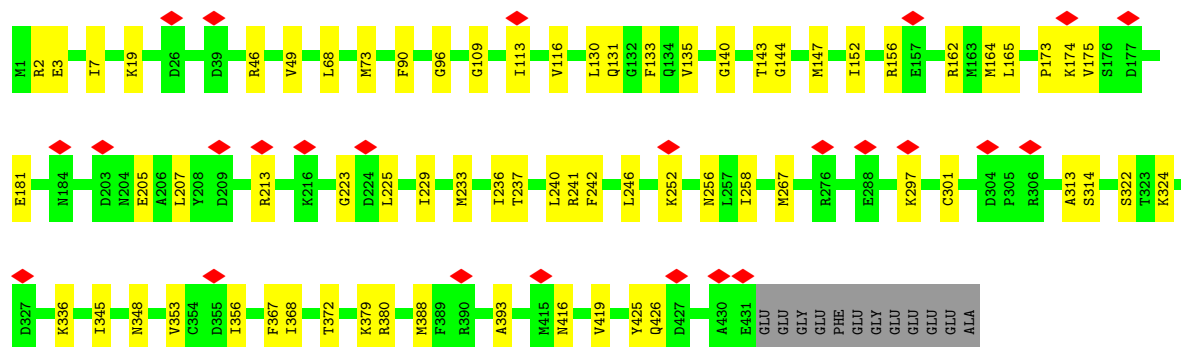
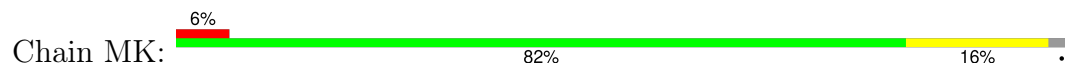




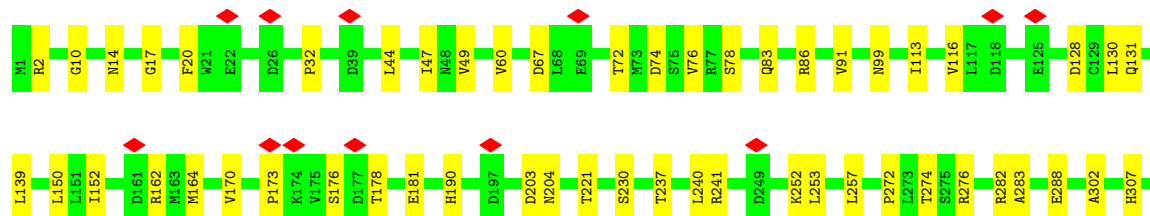
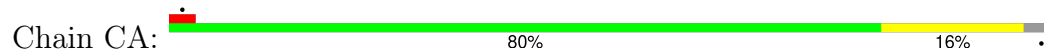
• Molecule 1: Tubulin beta



• Molecule 1: Tubulin beta

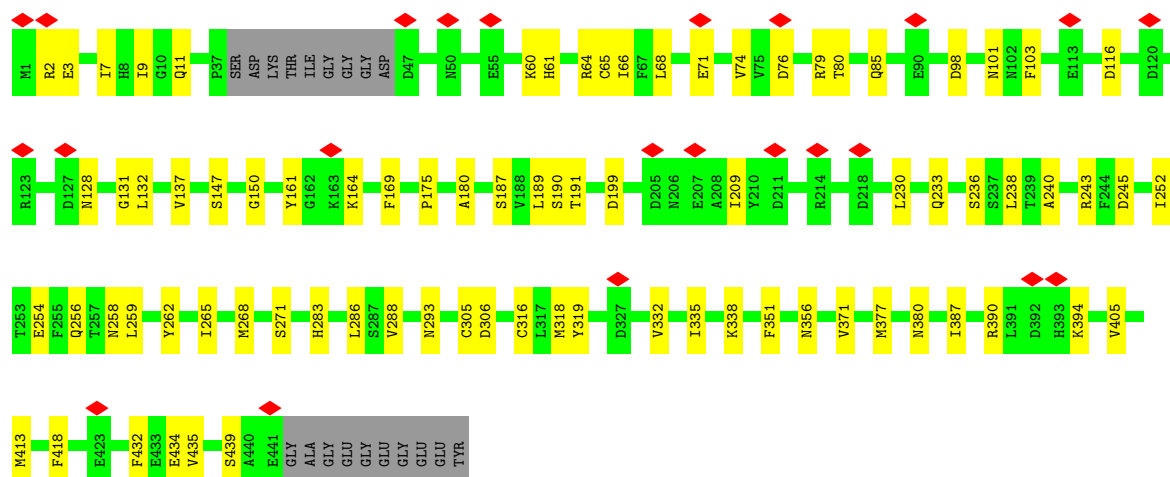
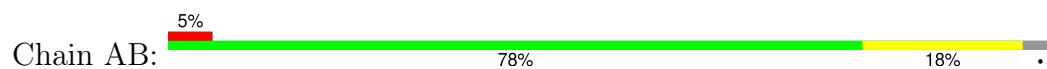


• Molecule 1: Tubulin beta

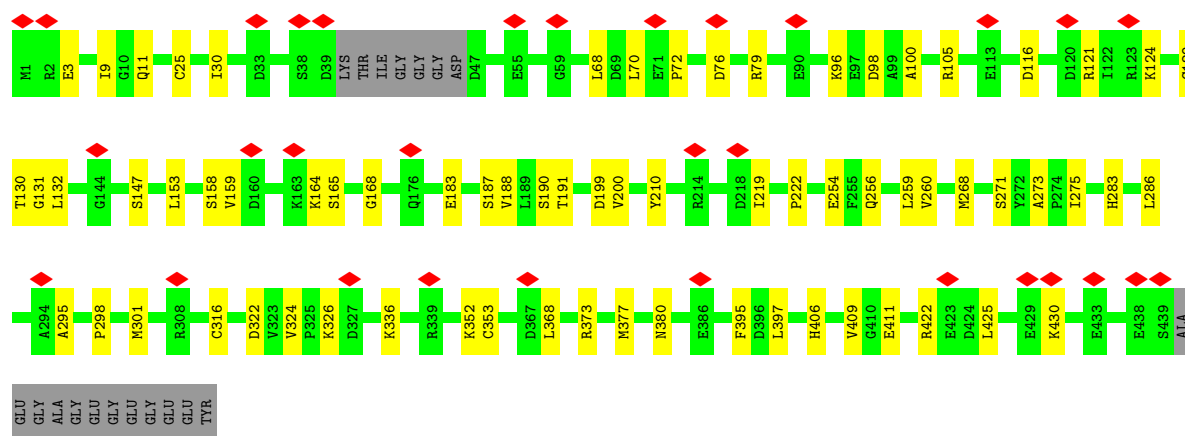
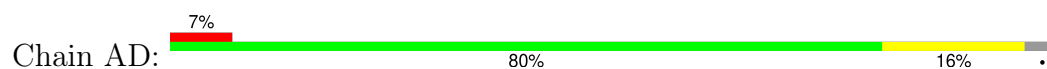




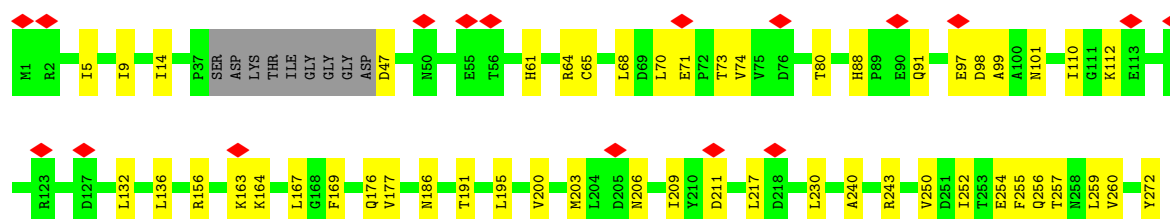
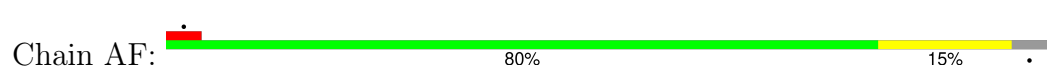
• Molecule 2: Tubulin alpha



• Molecule 2: Tubulin alpha

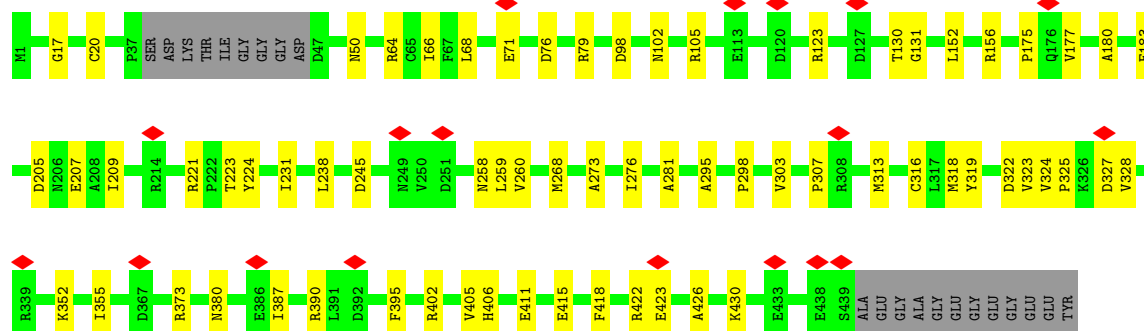
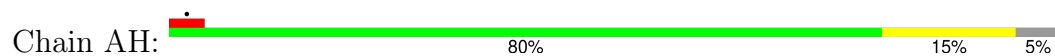


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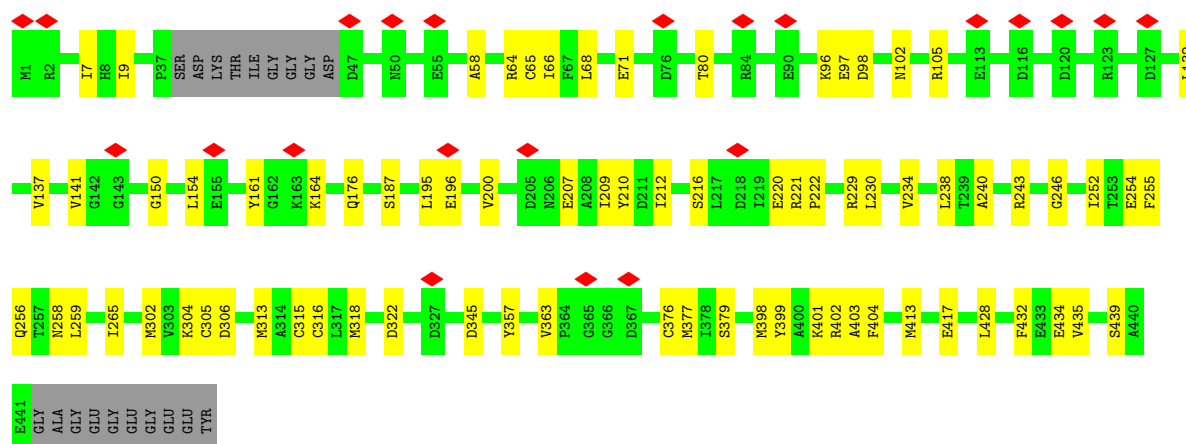
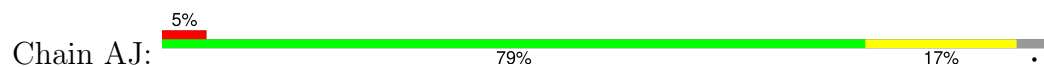




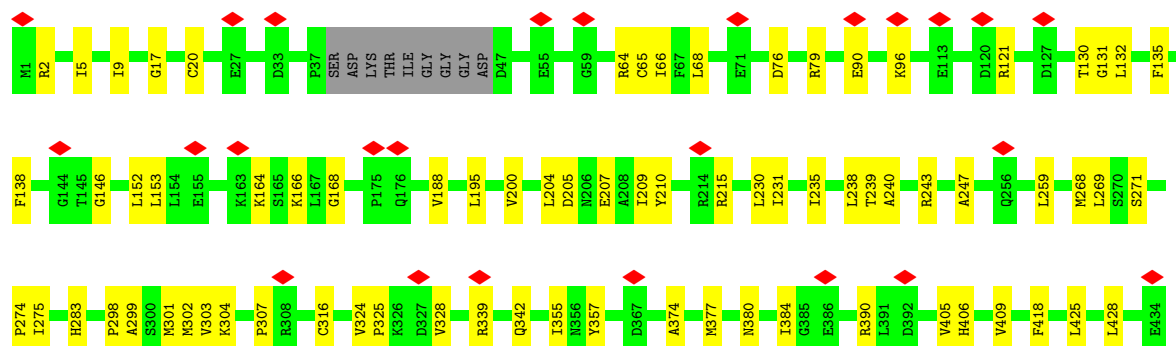
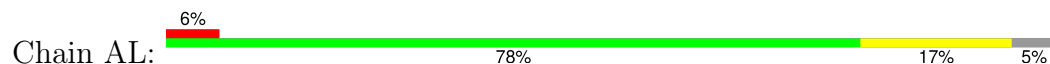
• Molecule 2: Tubulin alpha

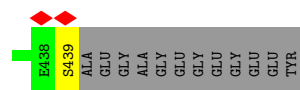


• Molecule 2: Tubulin alpha

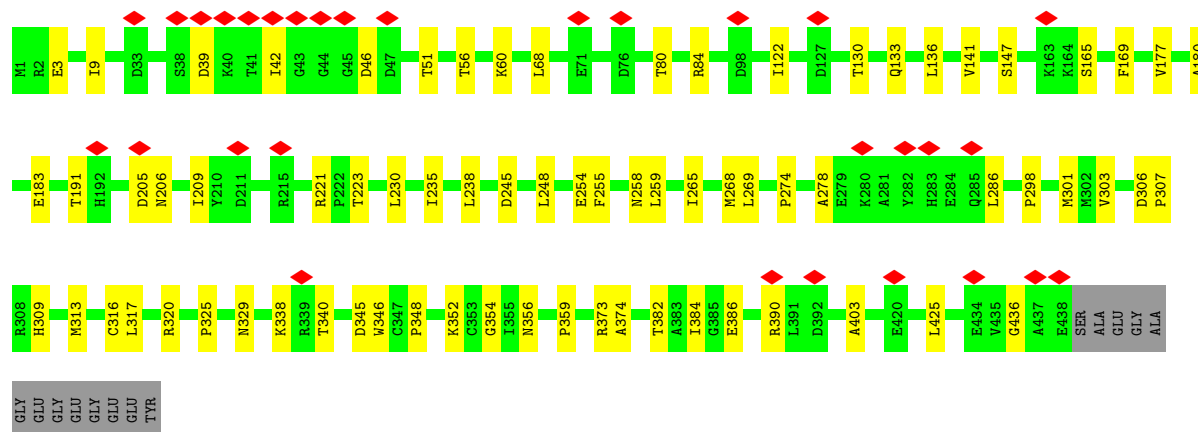
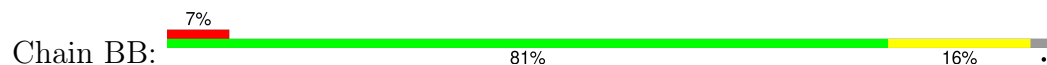


• Molecule 2: Tubulin alpha

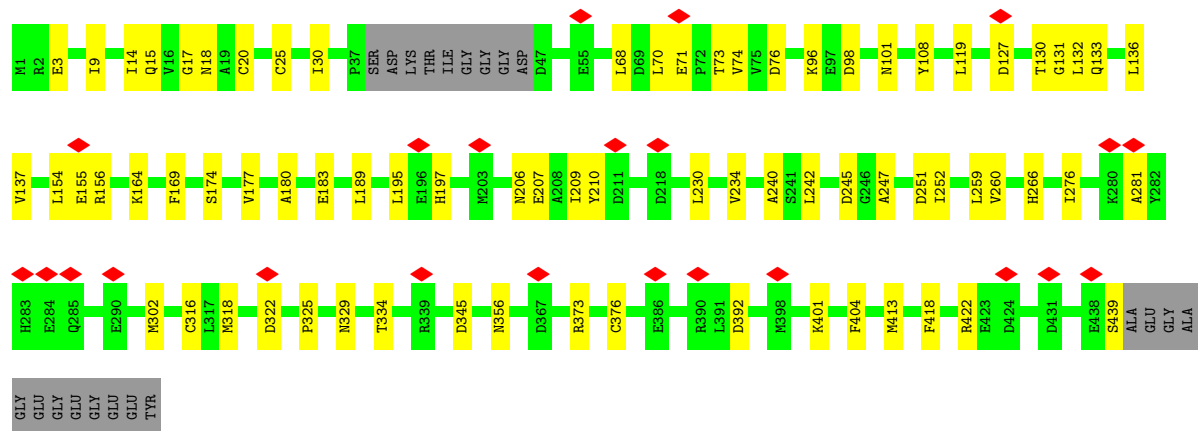
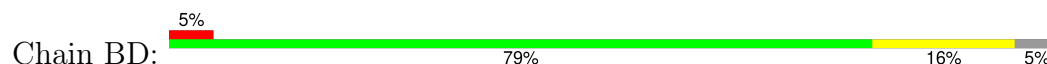




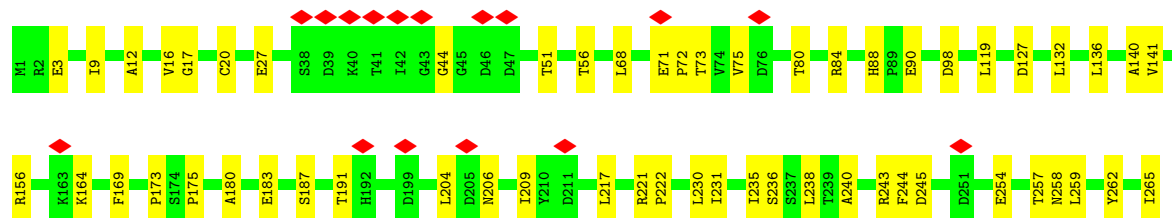
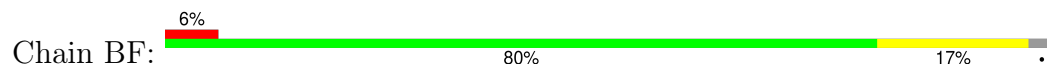
- Molecule 2: Tubulin alpha

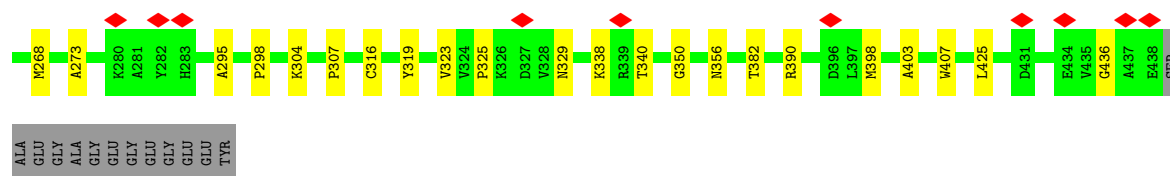


- Molecule 2: Tubulin alpha



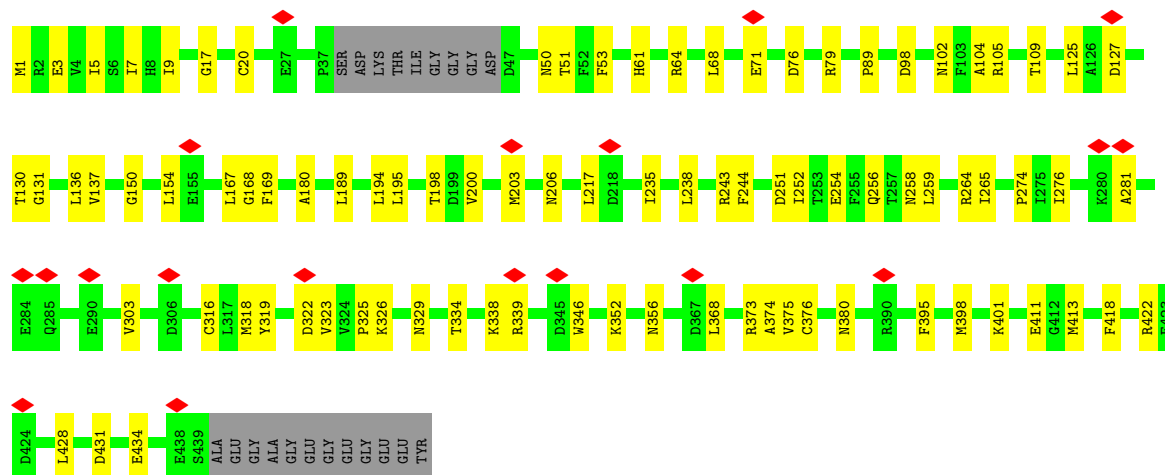
- Molecule 2: Tubulin alpha





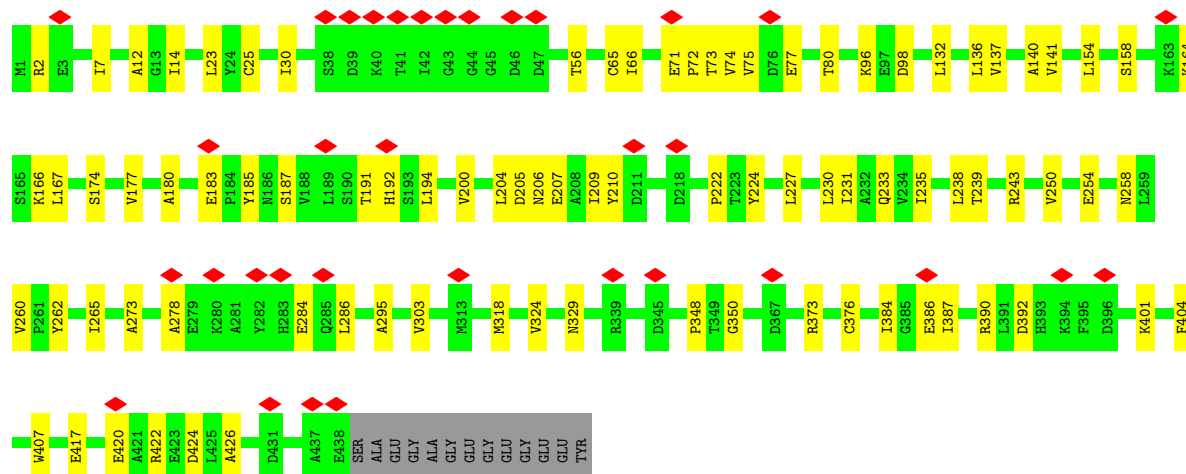
• Molecule 2: Tubulin alpha

Chain BH: 76% 20% 5%



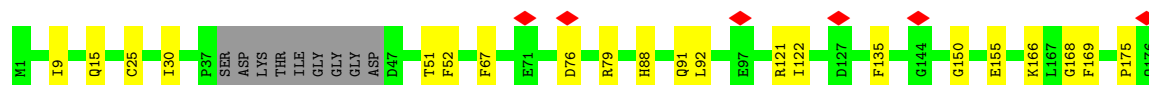
• Molecule 2: Tubulin alpha

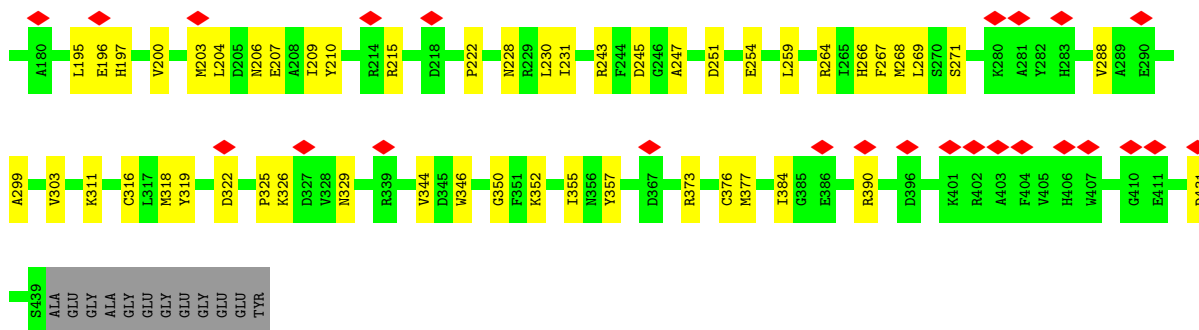
Chain BJ: 8% 78% 19%



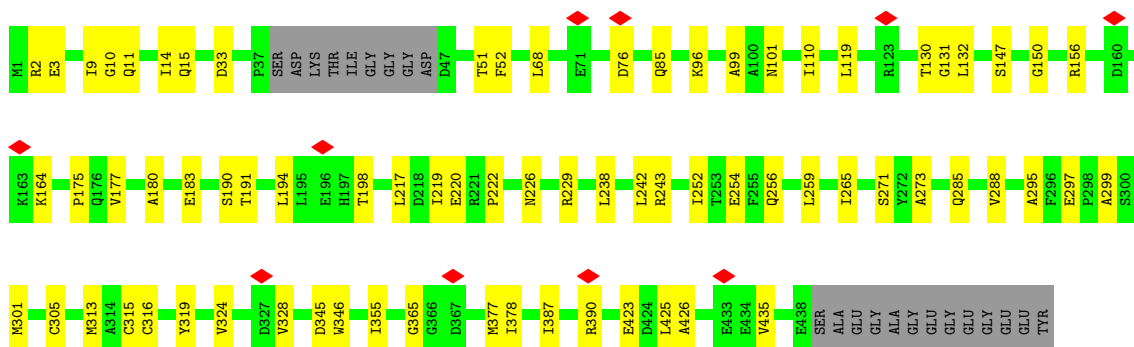
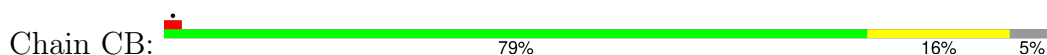
• Molecule 2: Tubulin alpha

Chain BL: 7% 80% 16% 5%

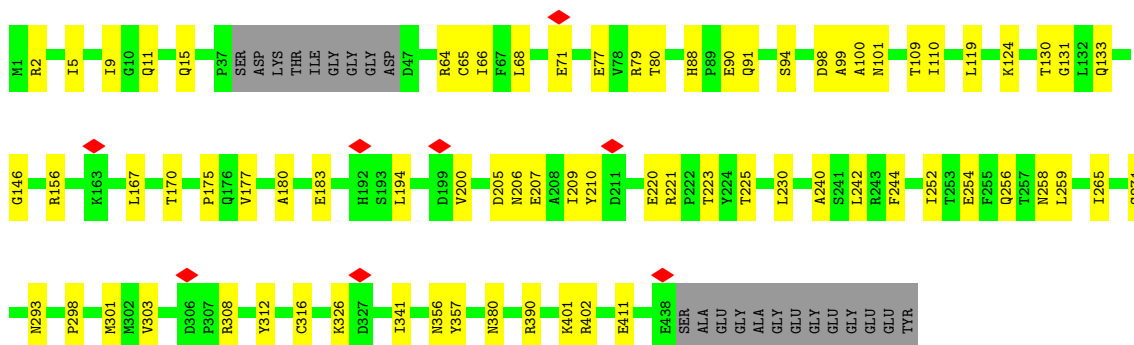
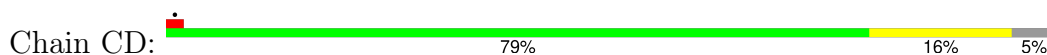




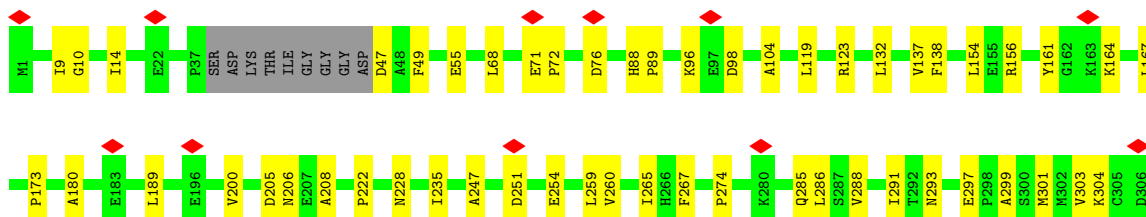
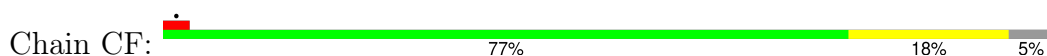
- Molecule 2: Tubulin alpha

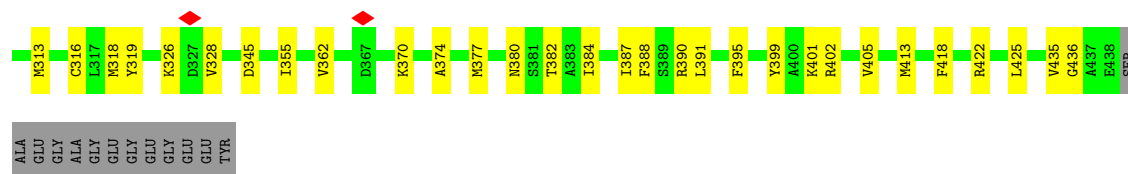


- Molecule 2: Tubulin alpha



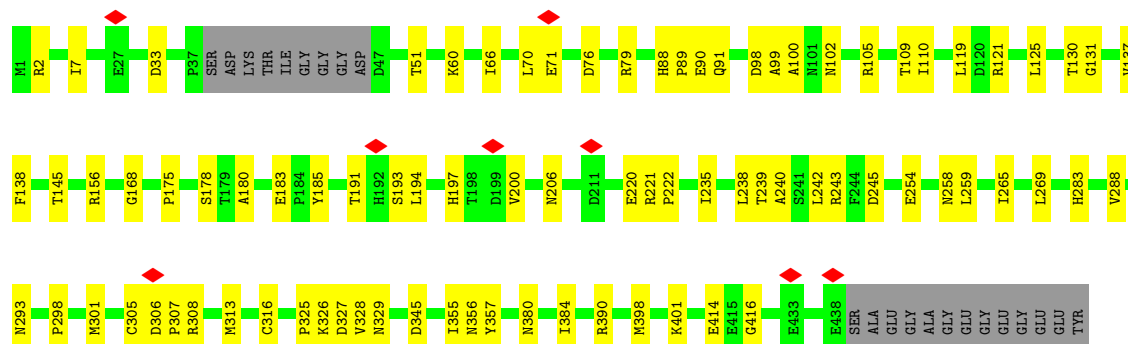
- Molecule 2: Tubulin alpha





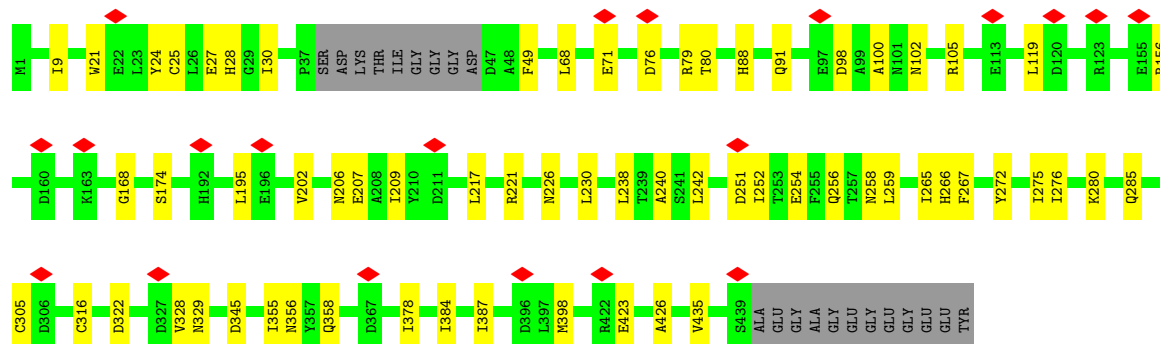
• Molecule 2: Tubulin alpha

Chain CH: 76% 19% 5%



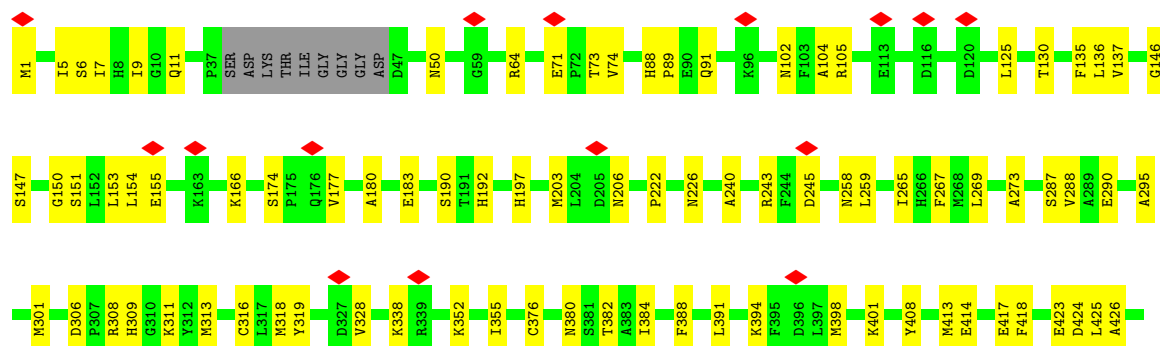
• Molecule 2: Tubulin alpha

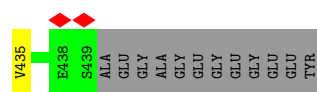
Chain CJ: 81% 14% 5%



• Molecule 2: Tubulin alpha

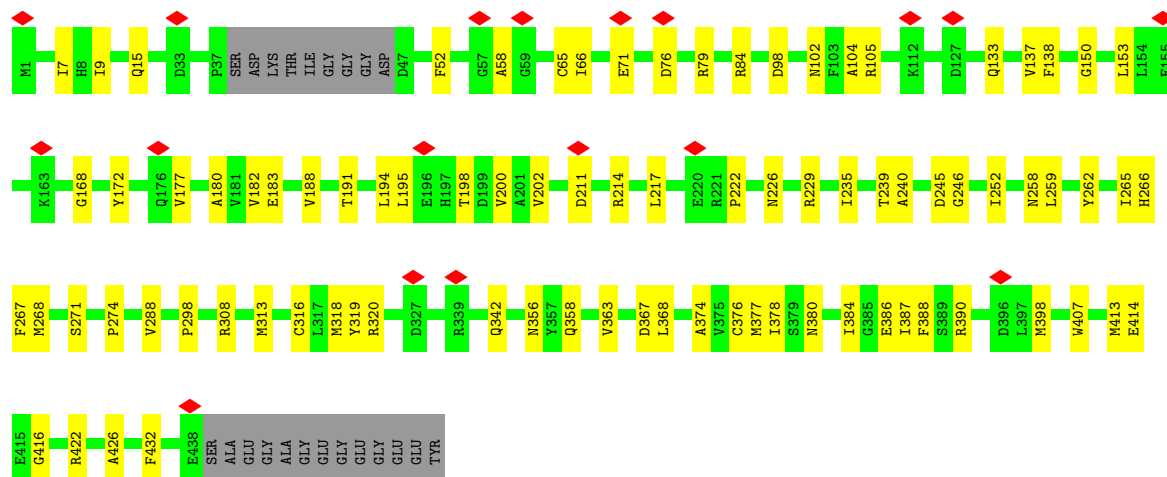
Chain DB: 76% 19% 5%





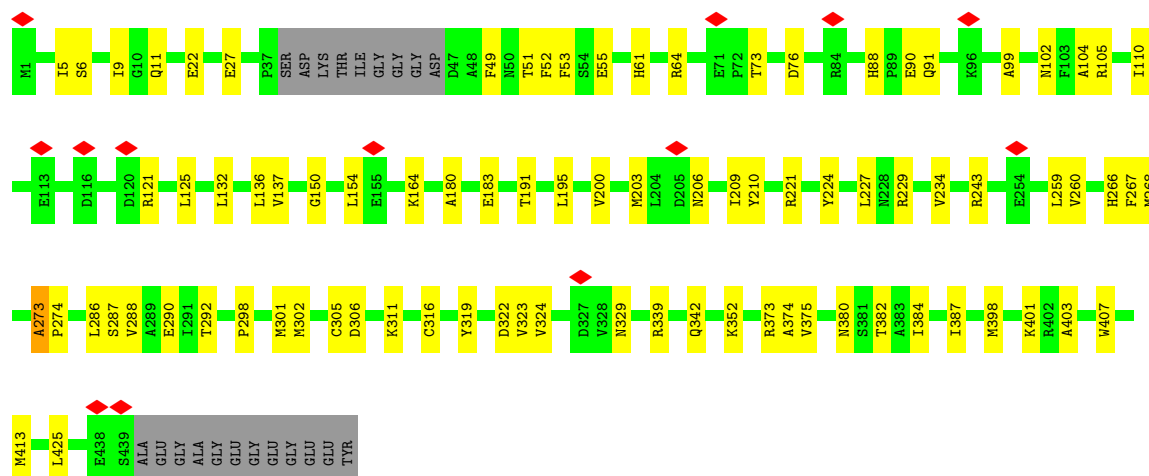
• Molecule 2: Tubulin alpha

Chain DD: 76% 19% 5%



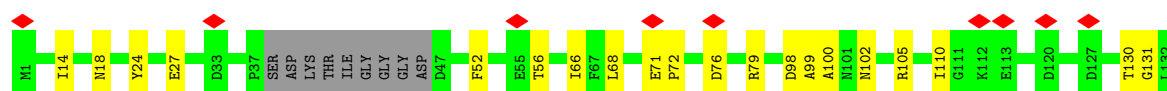
• Molecule 2: Tubulin alpha

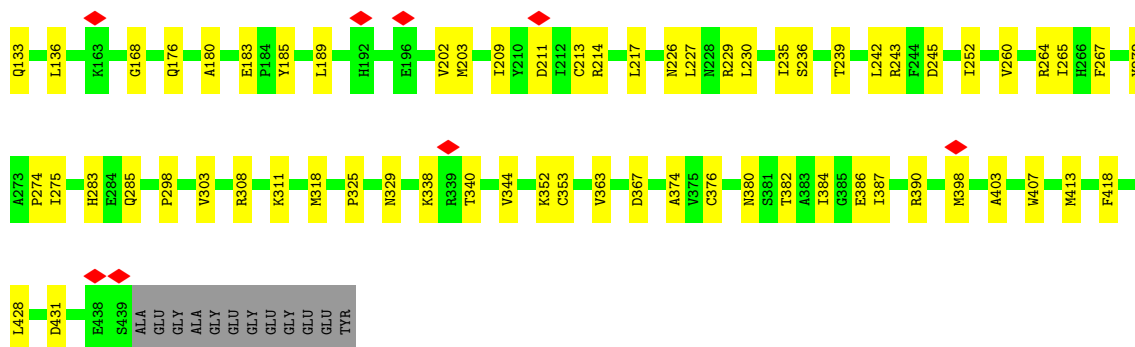
Chain DF: 76% 19% 5%



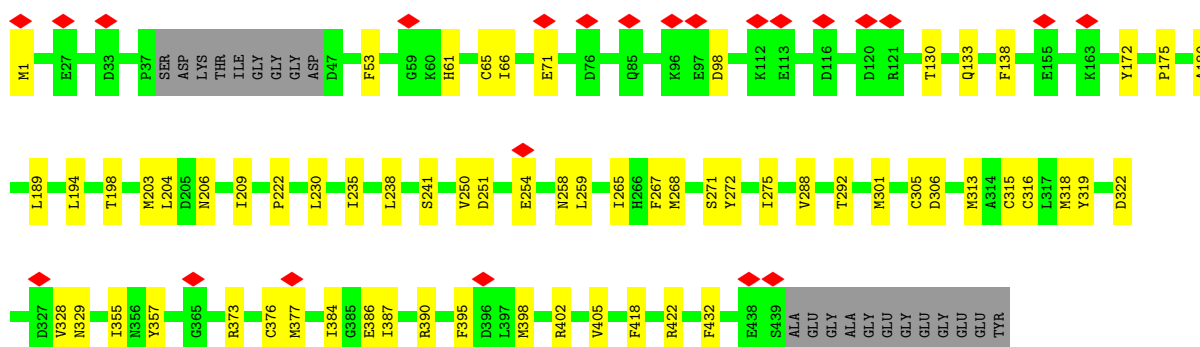
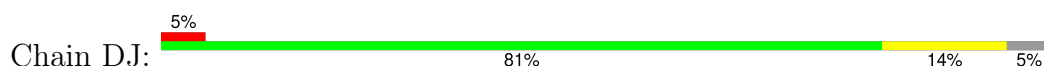
• Molecule 2: Tubulin alpha

Chain DH: 77% 19% 5%

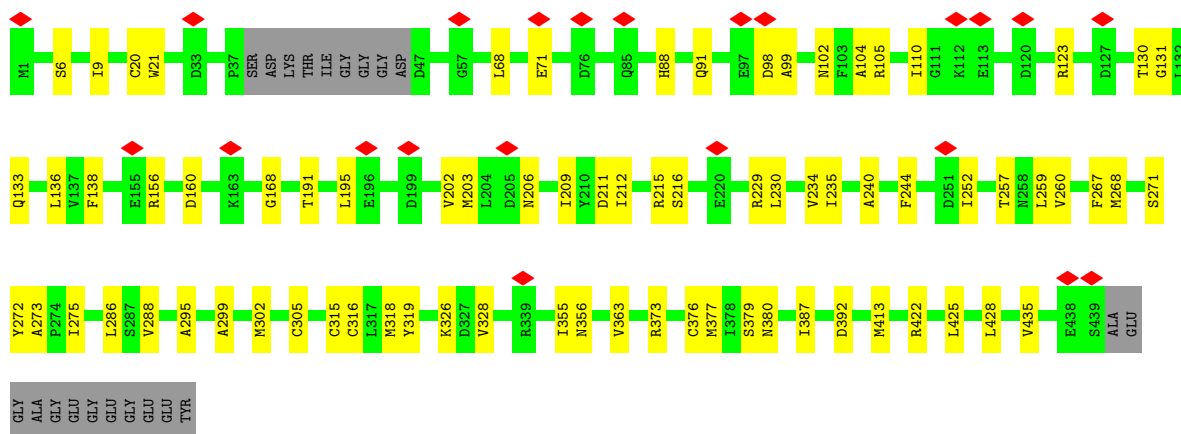
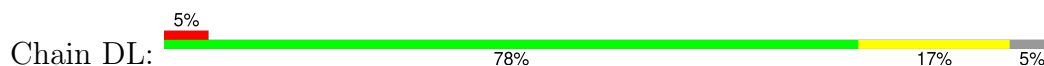




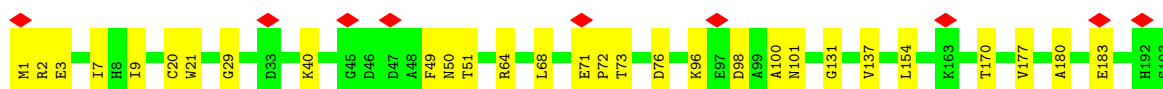
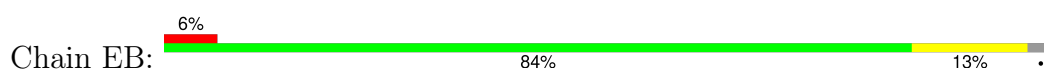
• Molecule 2: Tubulin alpha

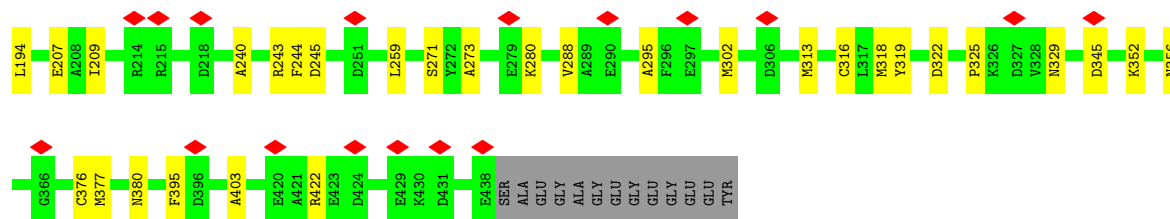


• Molecule 2: Tubulin alpha

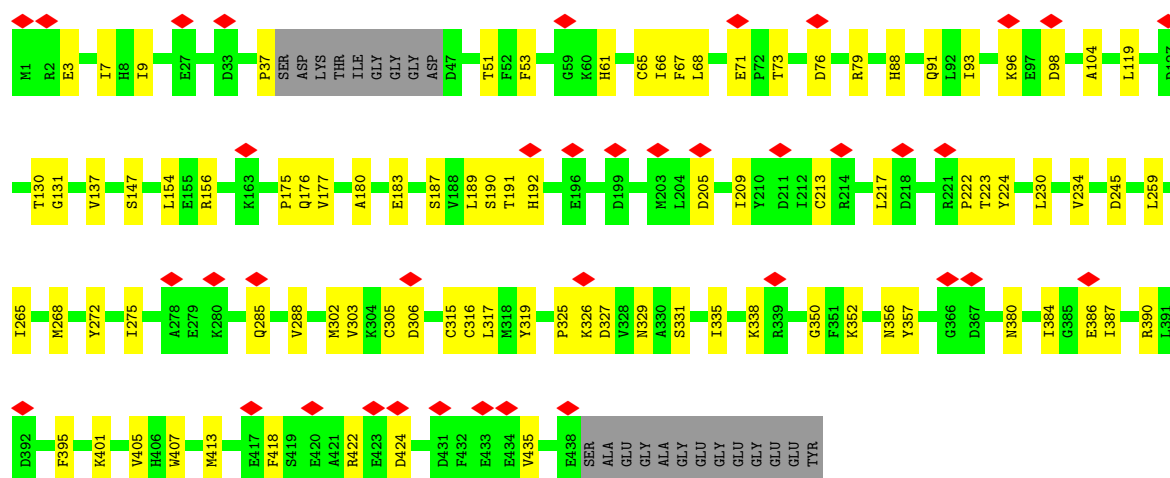
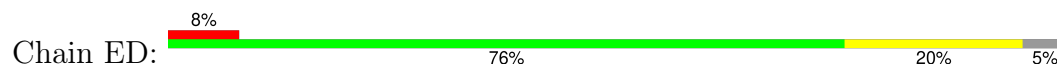


• Molecule 2: Tubulin alpha

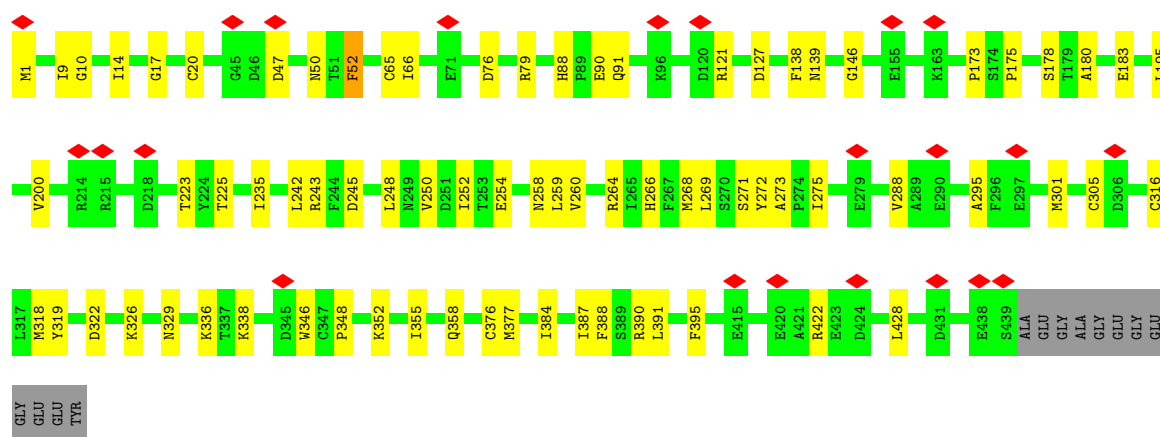
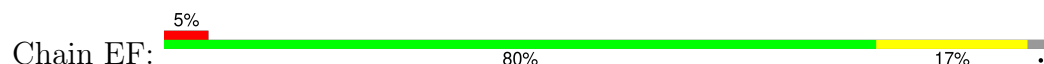




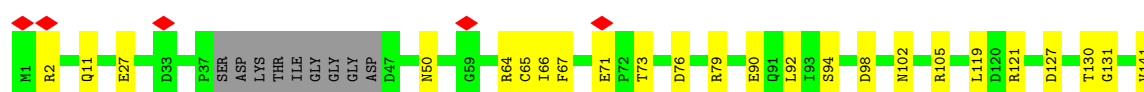
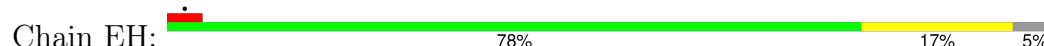
• Molecule 2: Tubulin alpha

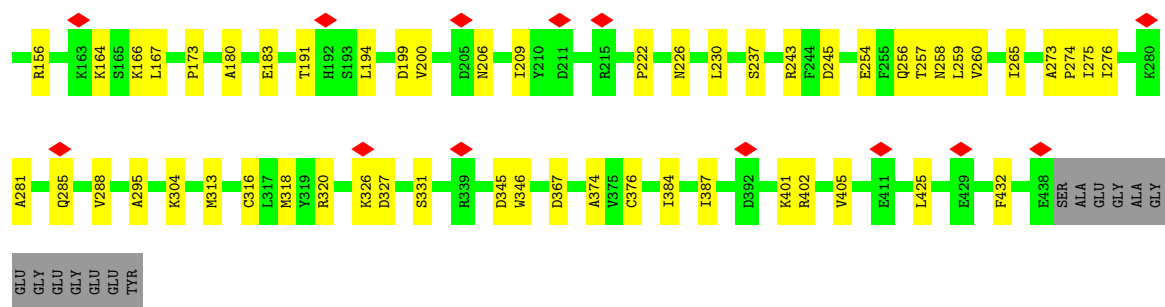


• Molecule 2: Tubulin alpha

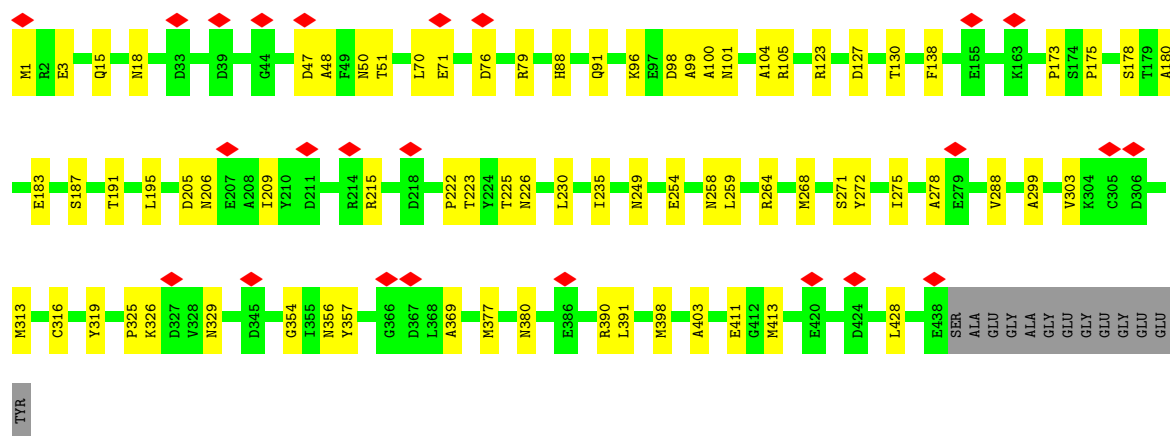
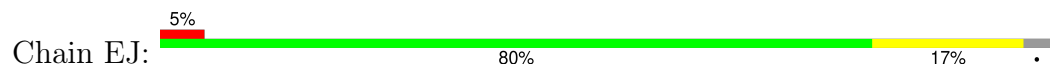


• Molecule 2: Tubulin alpha

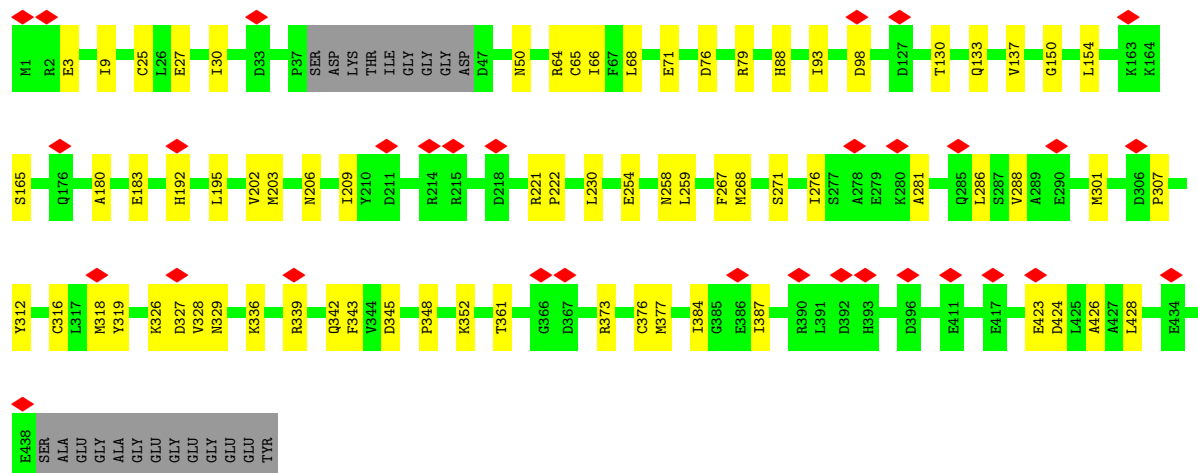
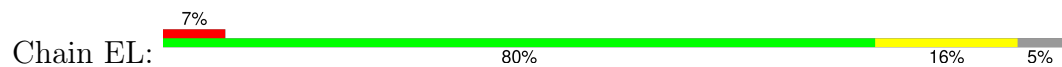




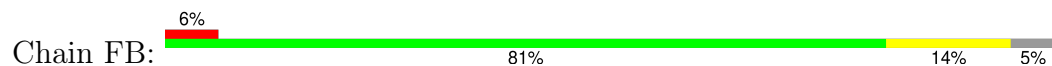
- Molecule 2: Tubulin alpha



- Molecule 2: Tubulin alpha

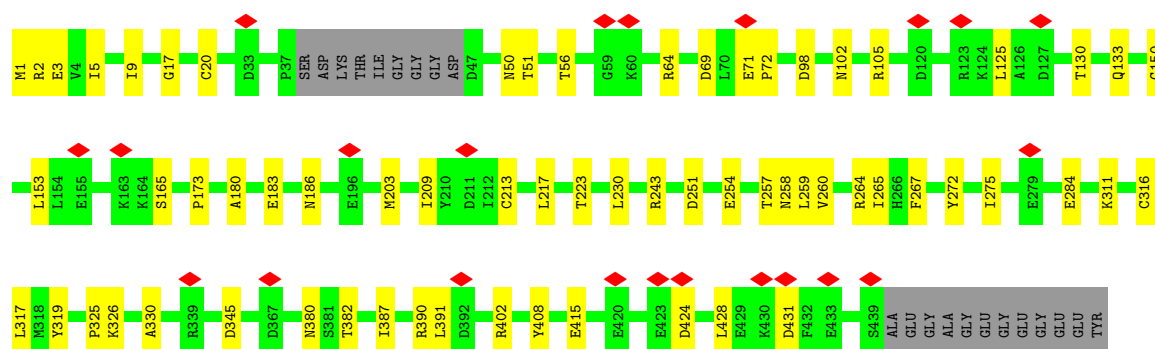
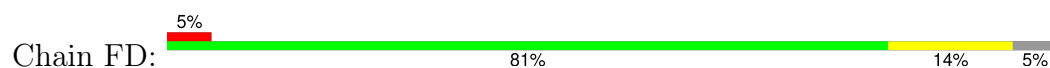


- Molecule 2: Tubulin alpha

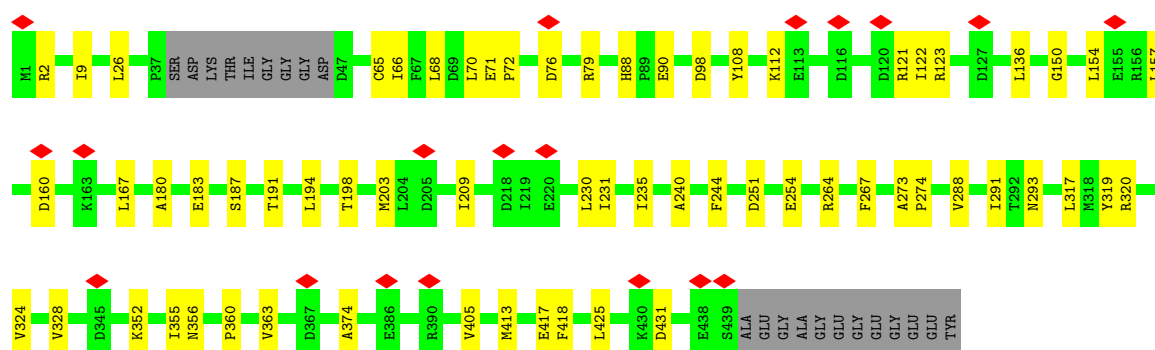
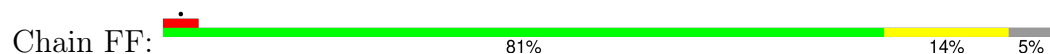




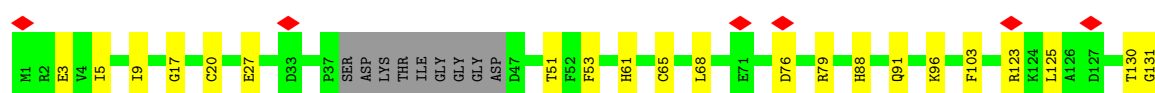
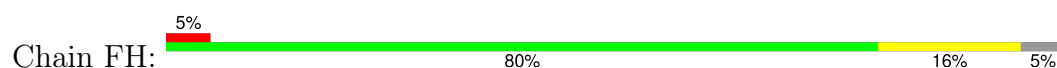
• Molecule 2: Tubulin alpha

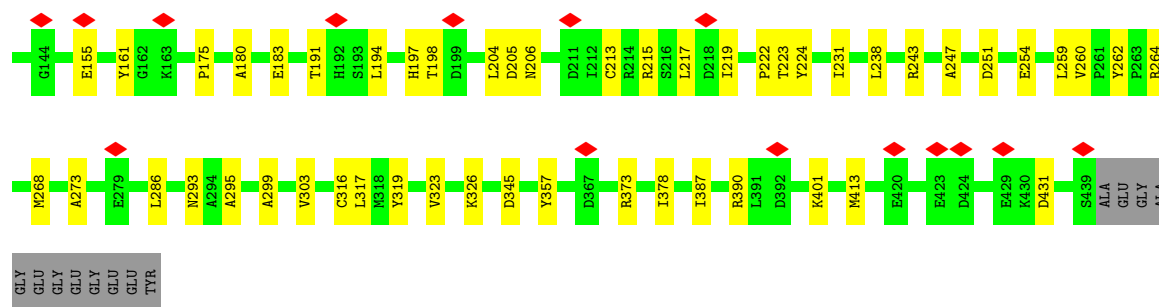


• Molecule 2: Tubulin alpha



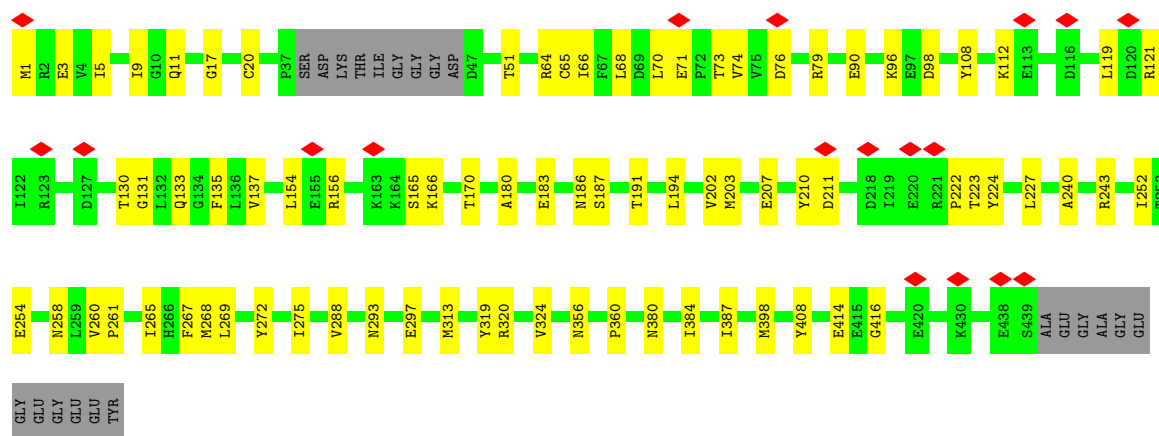
• Molecule 2: Tubulin alpha





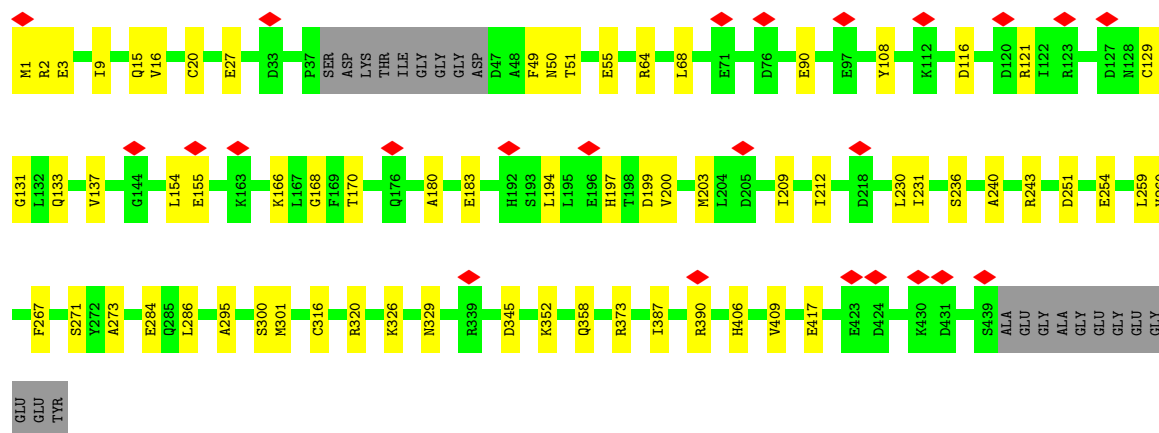
- Molecule 2: Tubulin alpha

Chain FJ: 78% 18% 5%



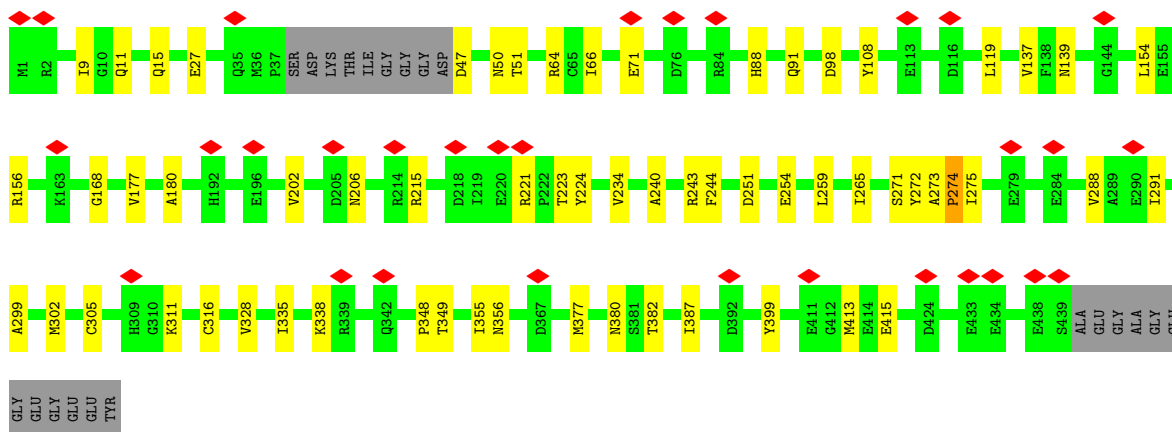
- Molecule 2: Tubulin alpha

Chain FL: 80% 15% 5%



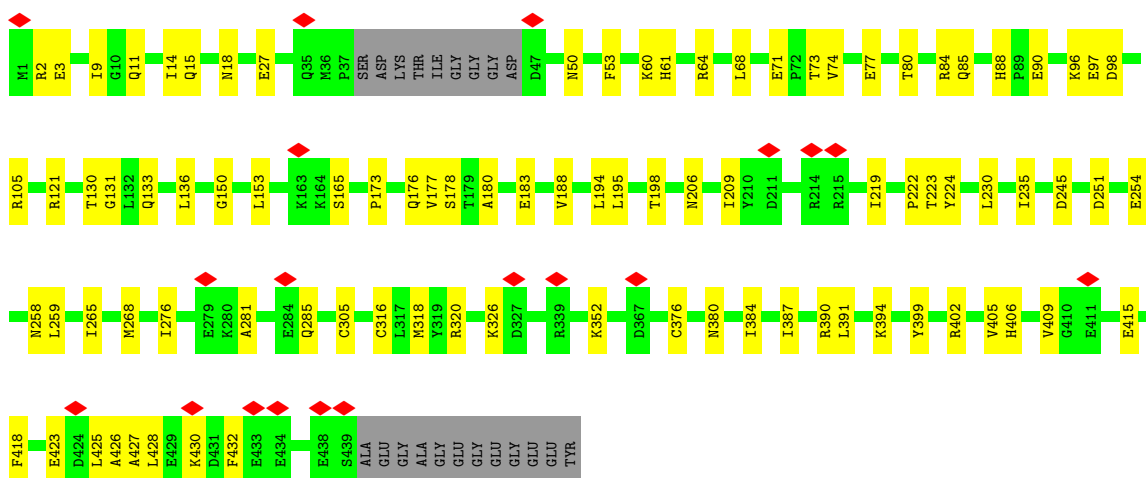
- Molecule 2: Tubulin alpha

Chain GD: 82% 14% 5%



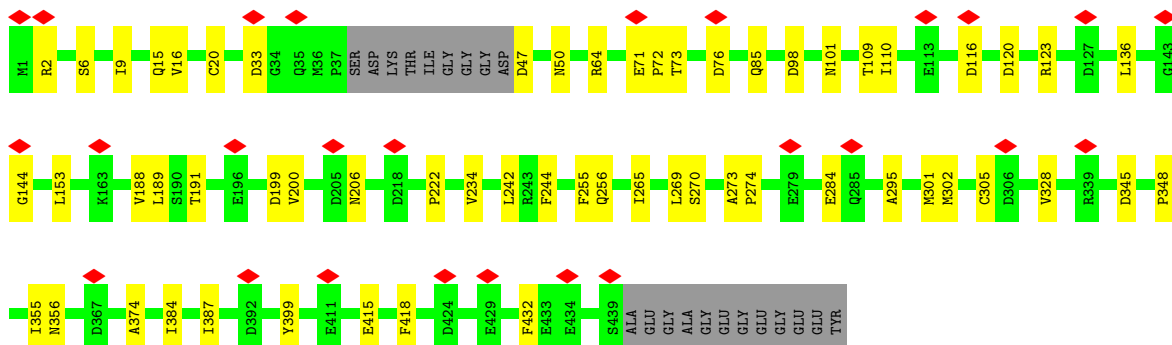
• Molecule 2: Tubulin alpha

Chain GF: 75% 20% 5%



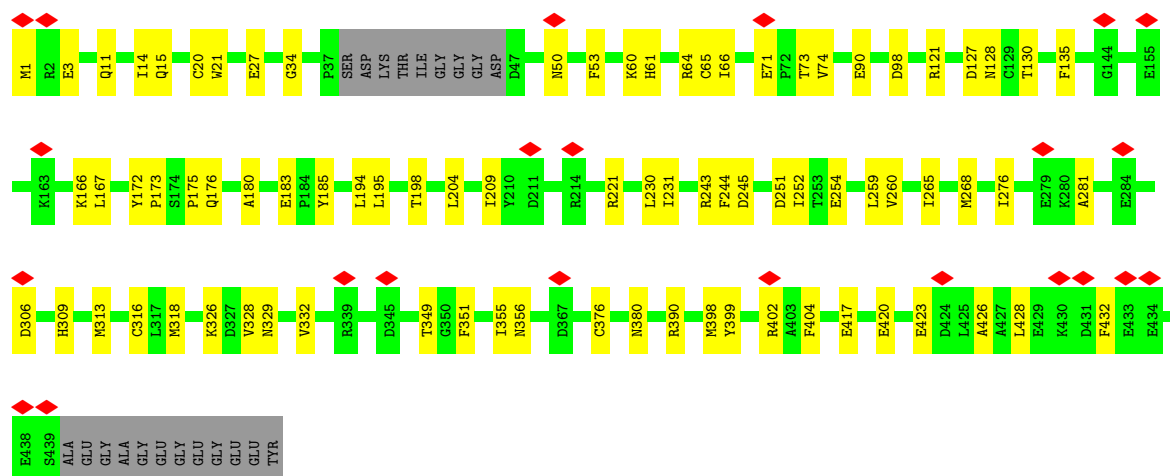
• Molecule 2: Tubulin alpha

Chain GH: 6% 82% 13% 5%

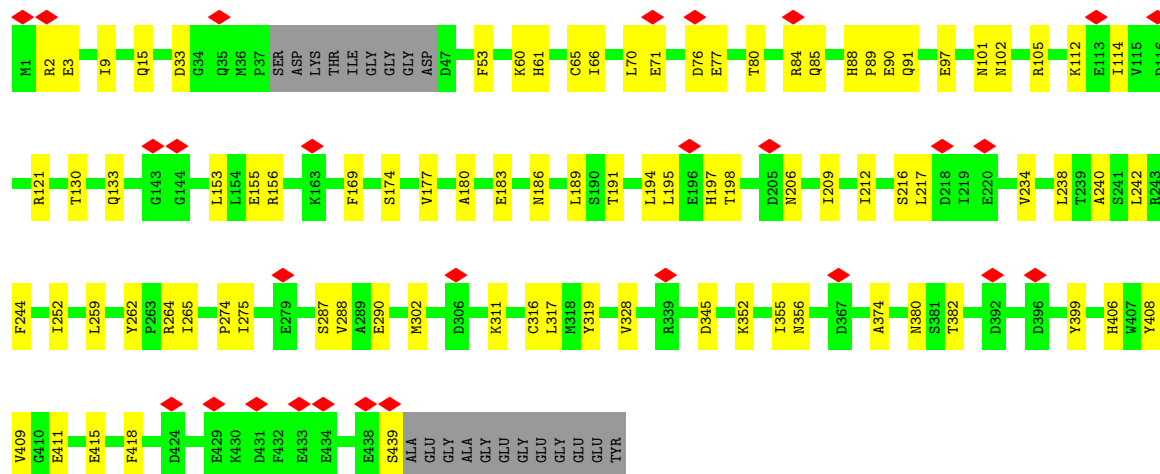
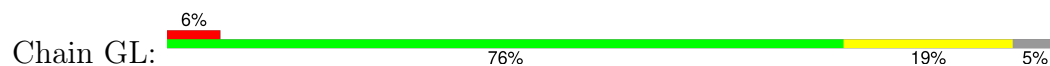


• Molecule 2: Tubulin alpha

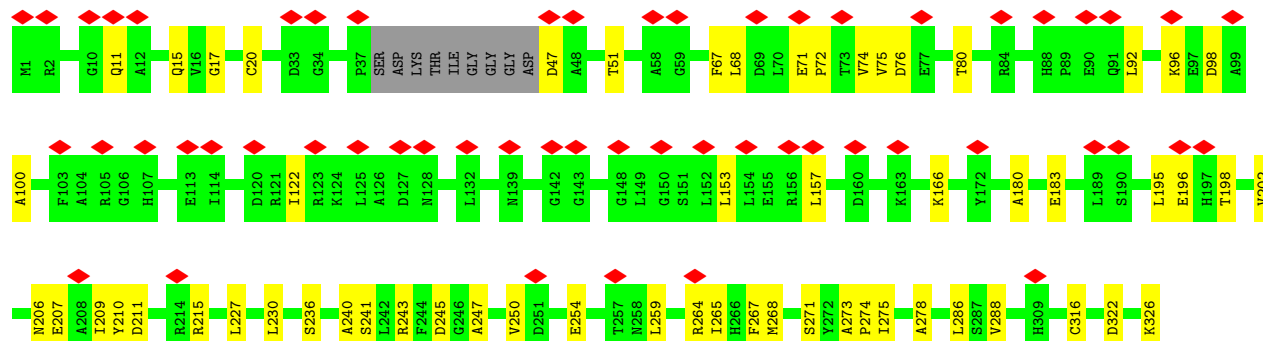
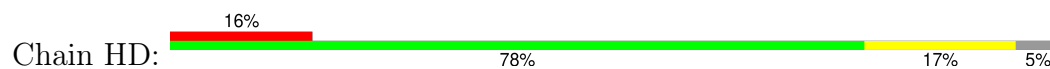
Chain GJ: 5% 77% 18% 5%

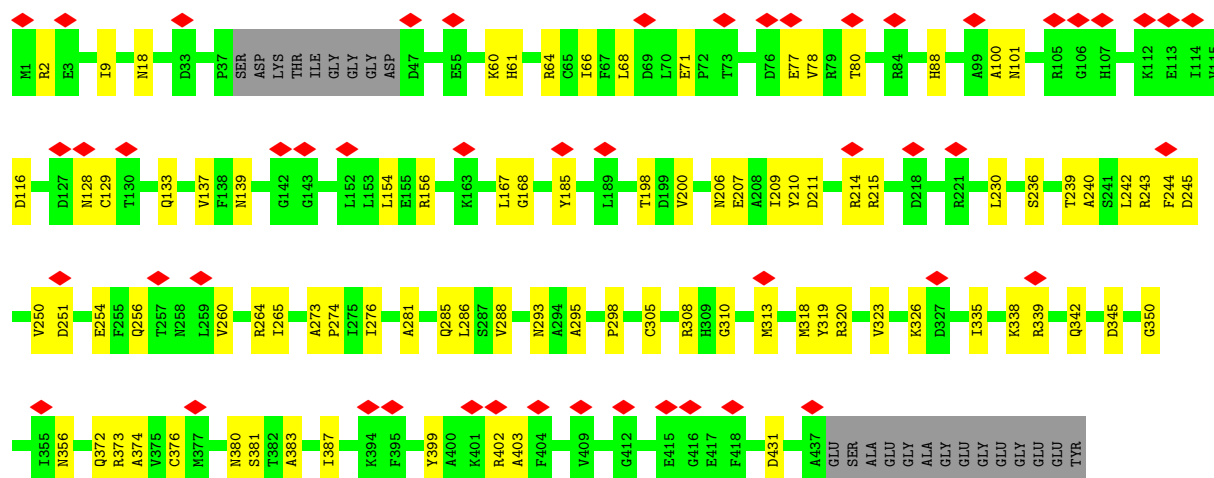


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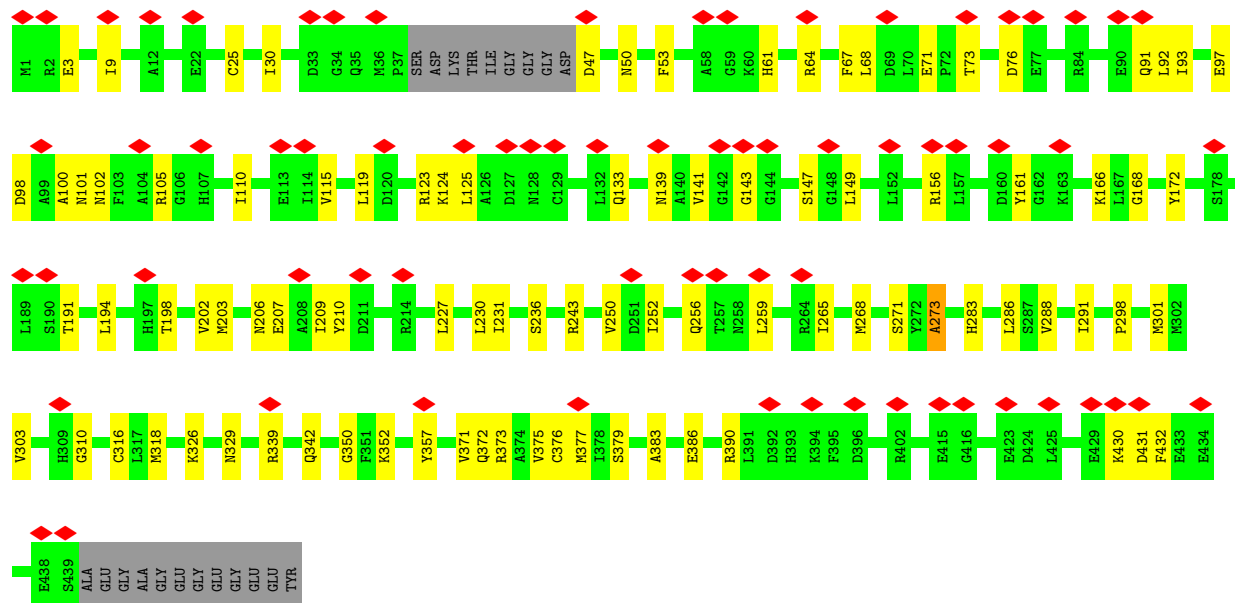
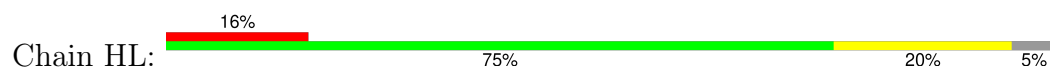


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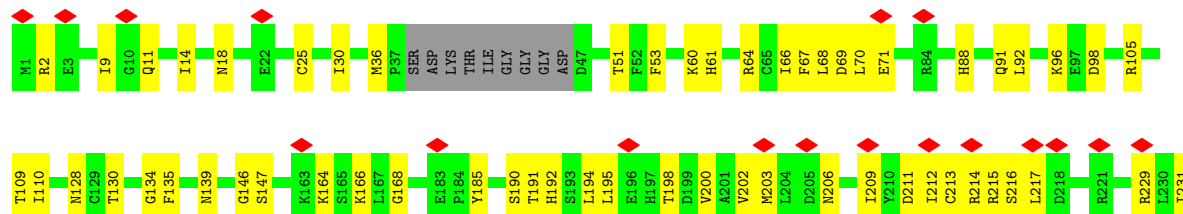
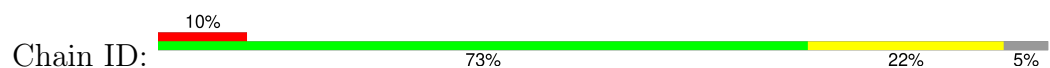


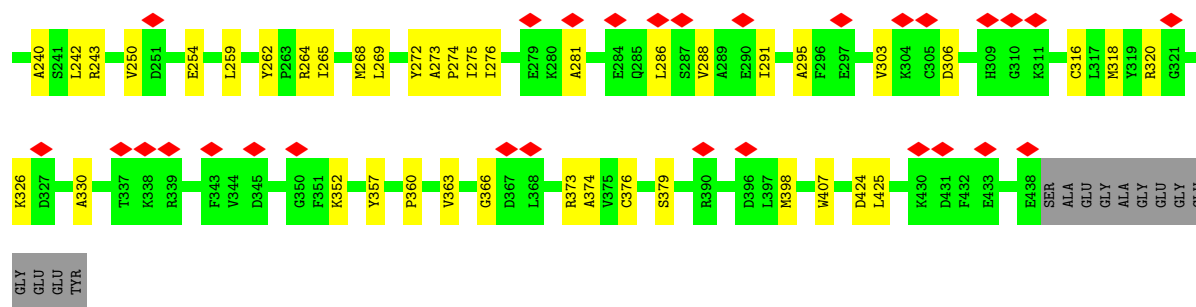


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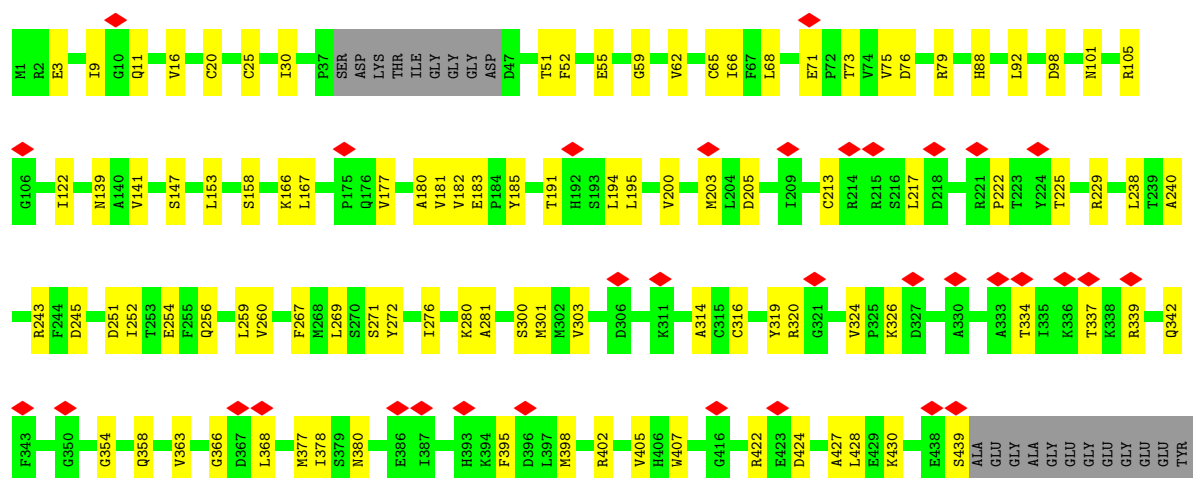
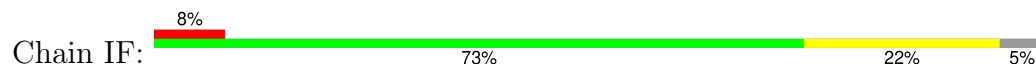


• Molecule 2: Tubulin alpha

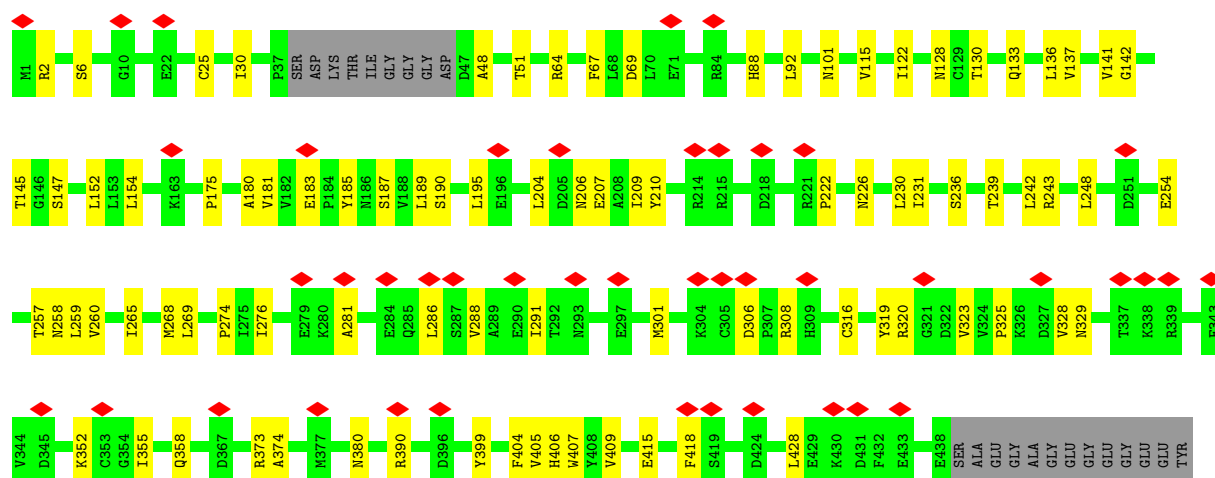
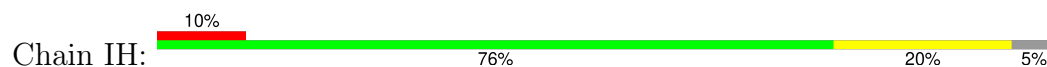




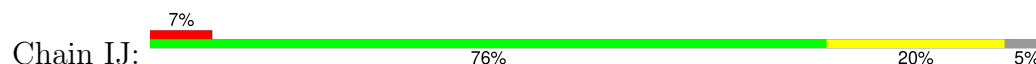
• Molecule 2: Tubulin alpha

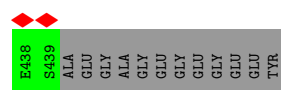


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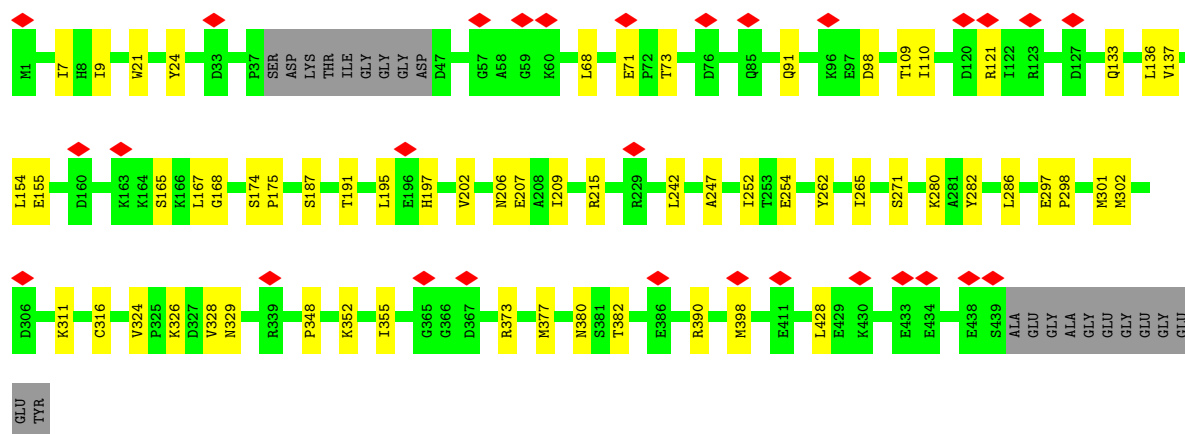
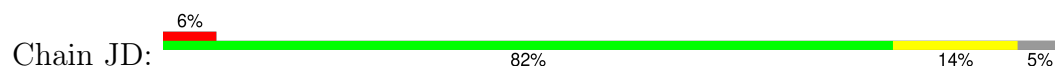


• Molecule 2: Tubulin alpha

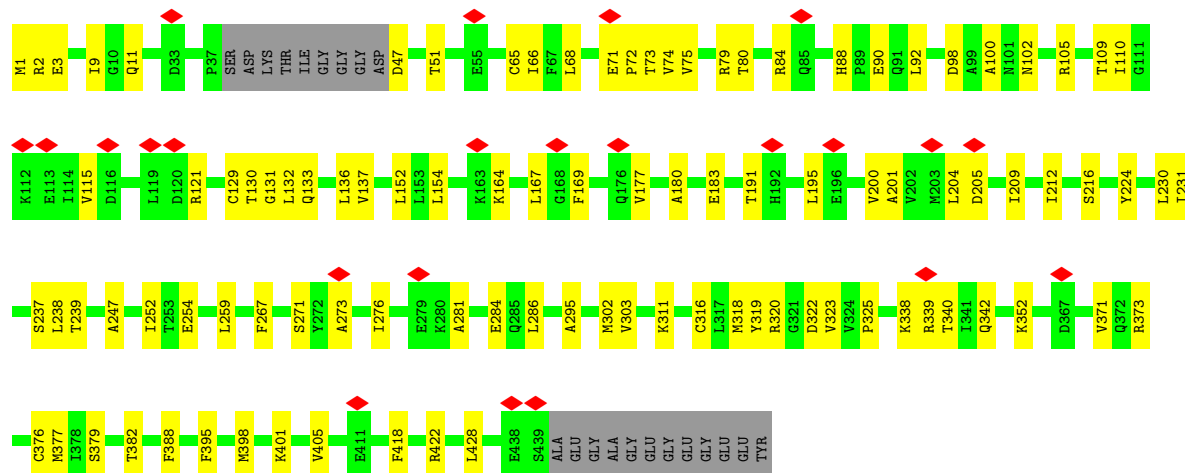
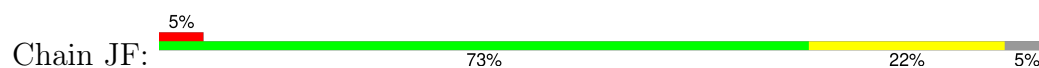




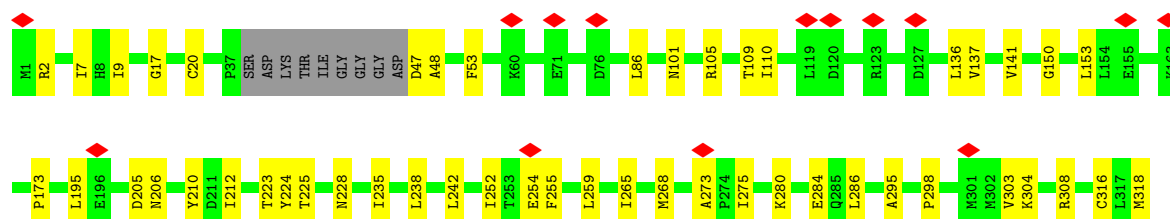
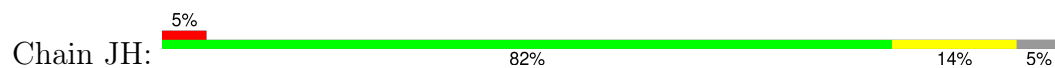
• Molecule 2: Tubulin alpha



• Molecule 2: Tubulin alpha



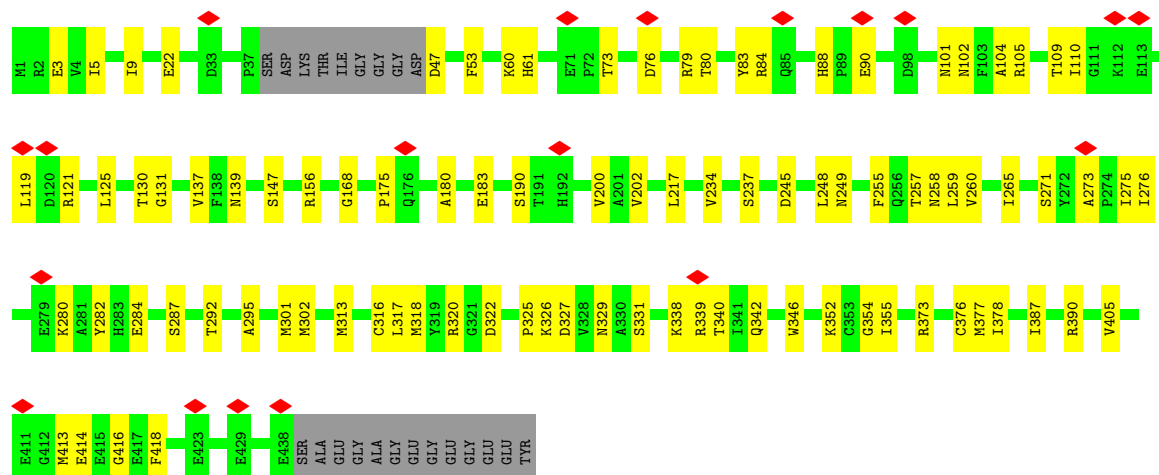
• Molecule 2: Tubulin alpha





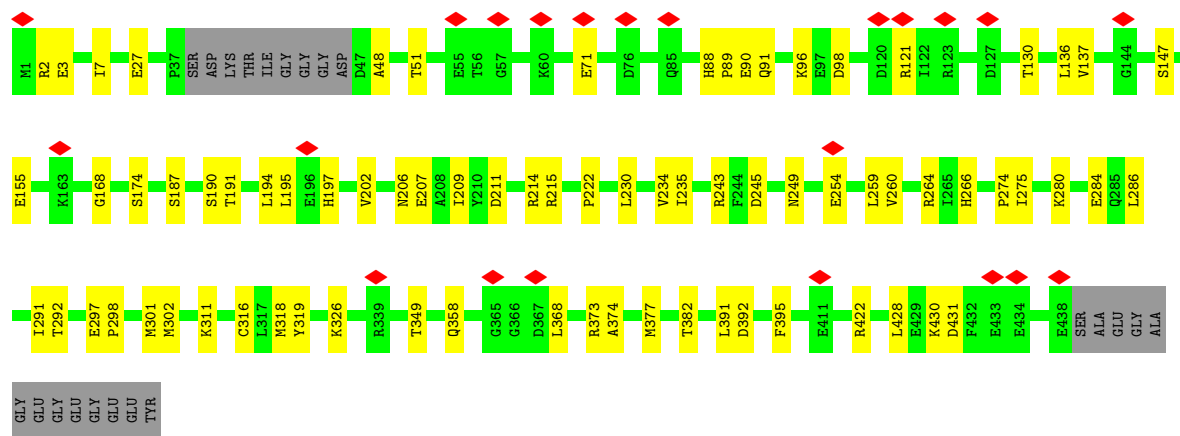
• Molecule 2: Tubulin alpha

Chain JJ: 75% 20% 5%



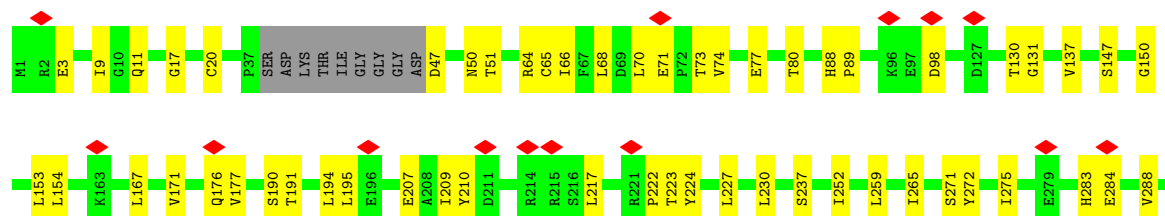
• Molecule 2: Tubulin alpha

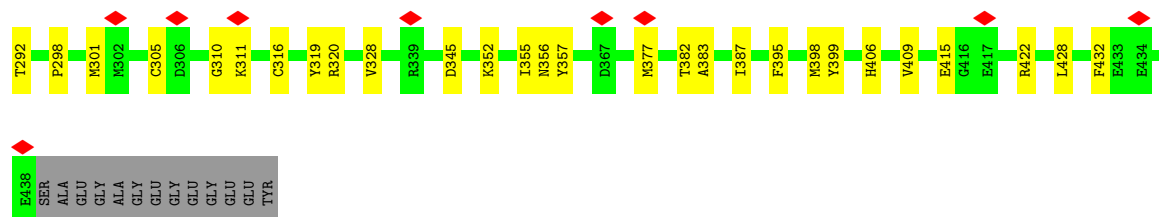
Chain JL: 78% 17% 5%



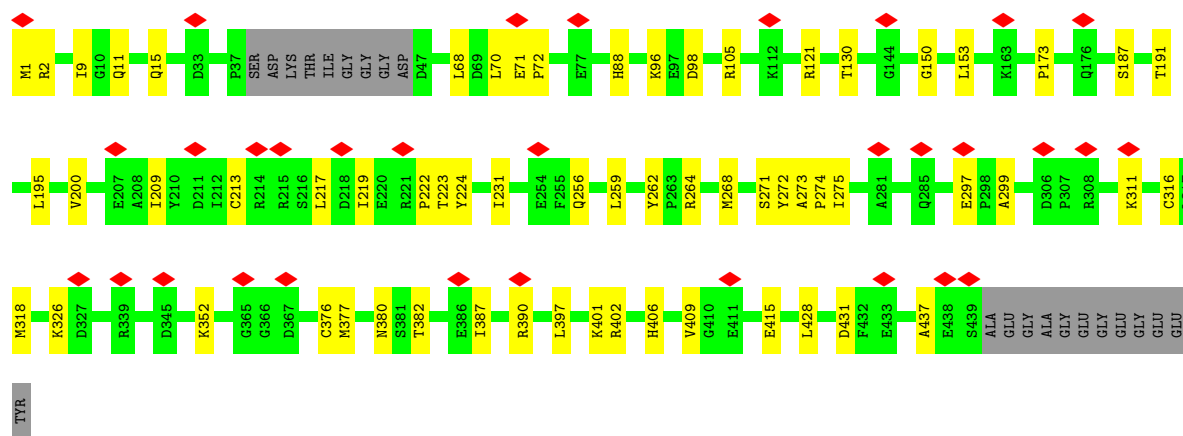
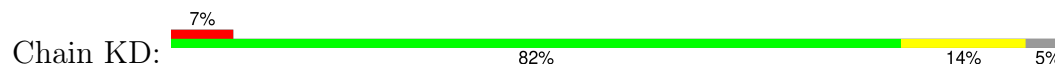
• Molecule 2: Tubulin alpha

Chain KB: 77% 18% 5%

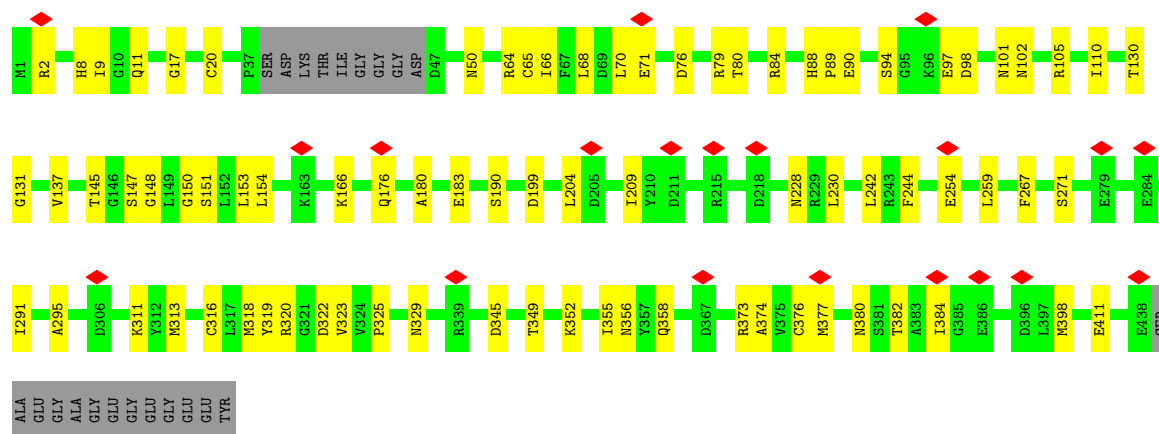
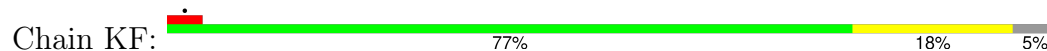




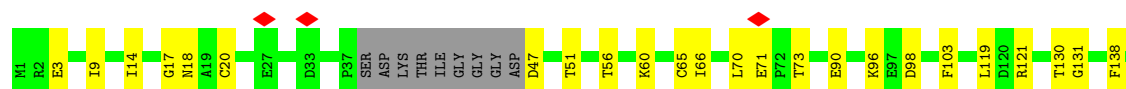
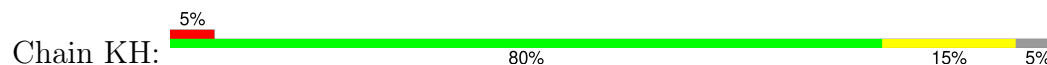
- Molecule 2: Tubulin alpha

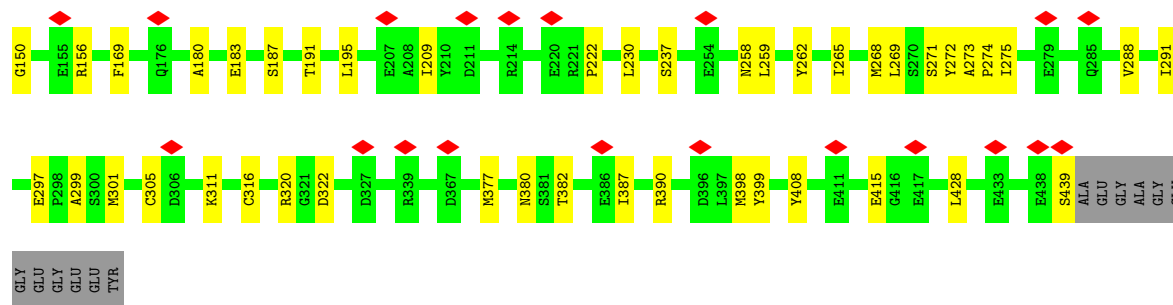


- Molecule 2: Tubulin alpha

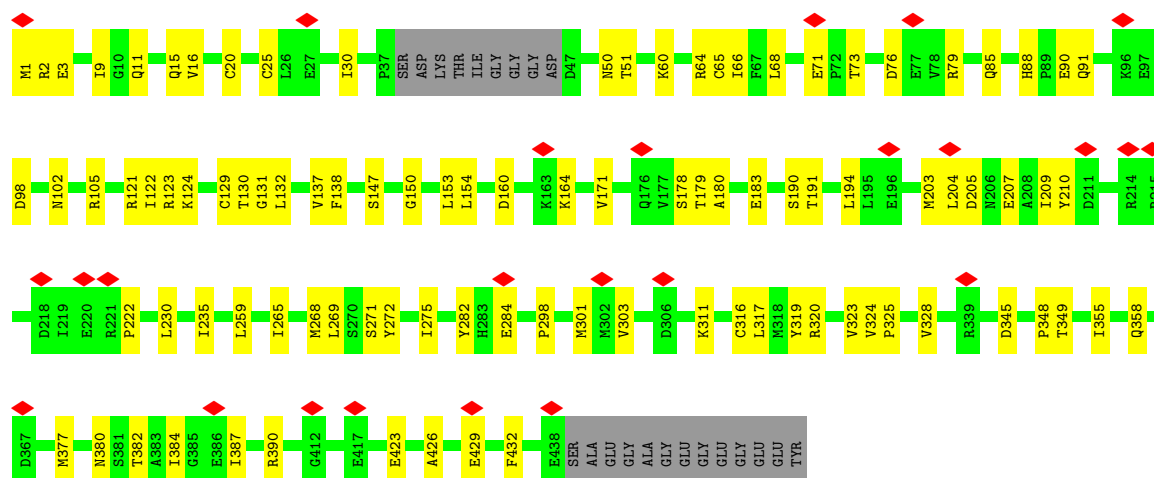
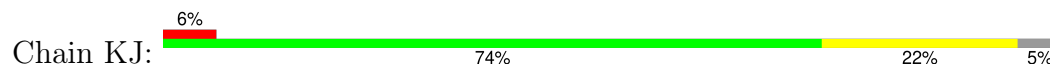


- Molecule 2: Tubulin alpha

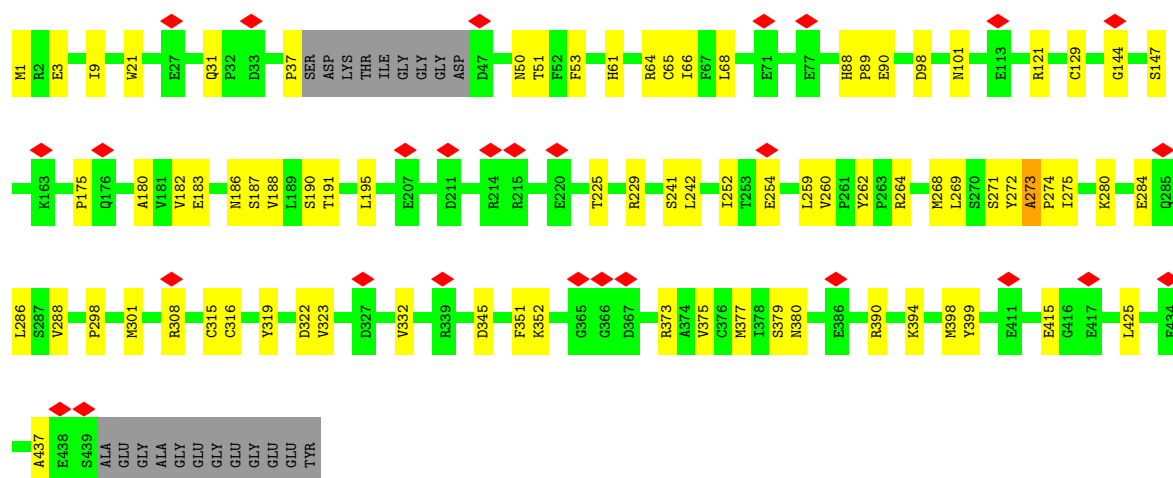
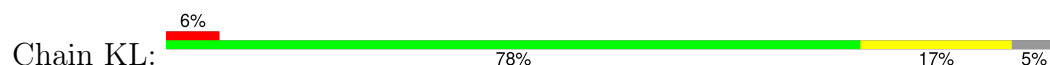




• Molecule 2: Tubulin alpha

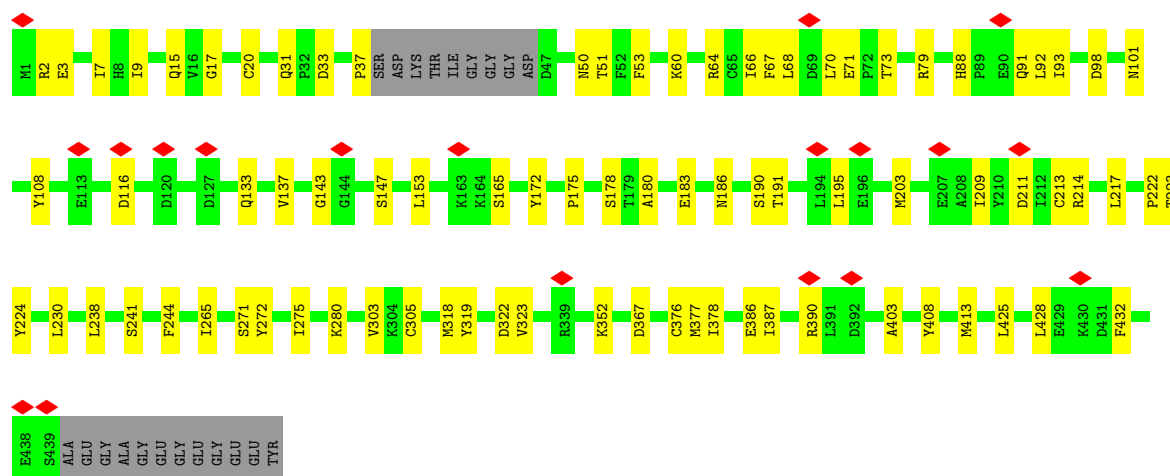


• Molecule 2: Tubulin alpha

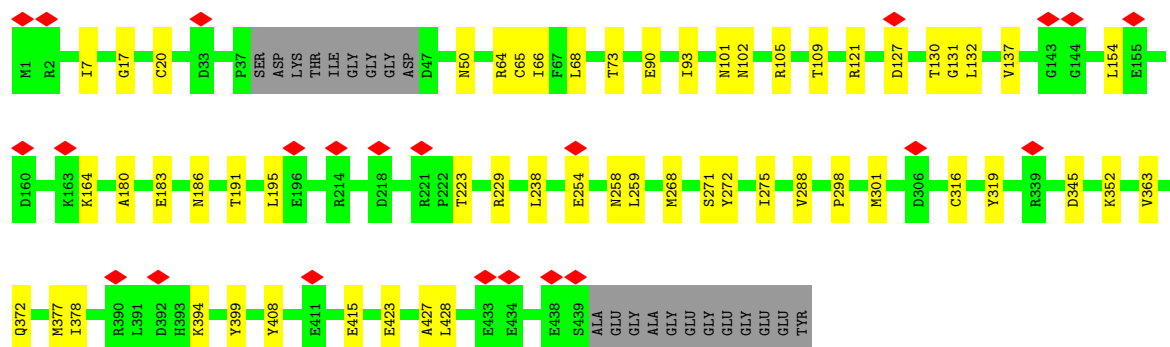
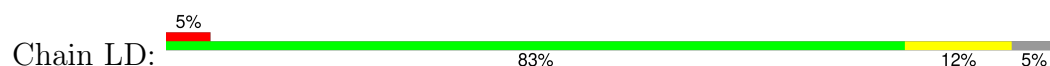


• Molecule 2: Tubulin alpha

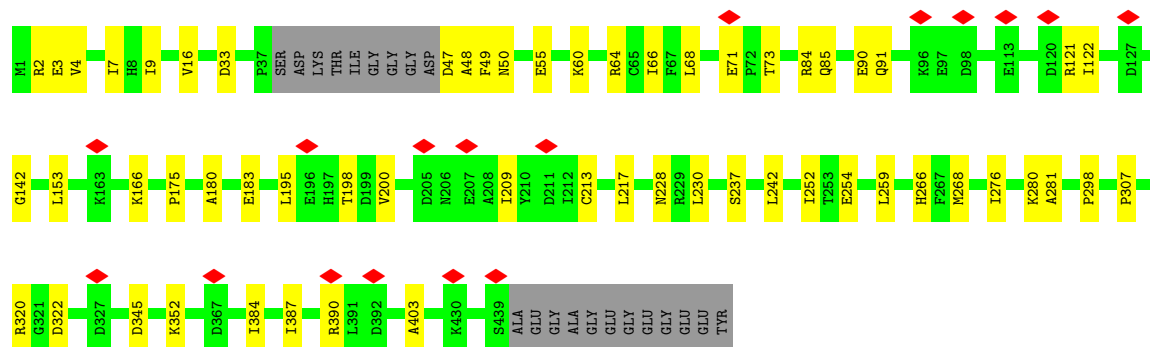
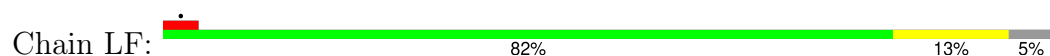




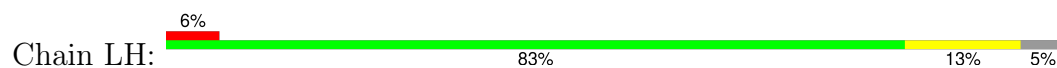
• Molecule 2: Tubulin alpha

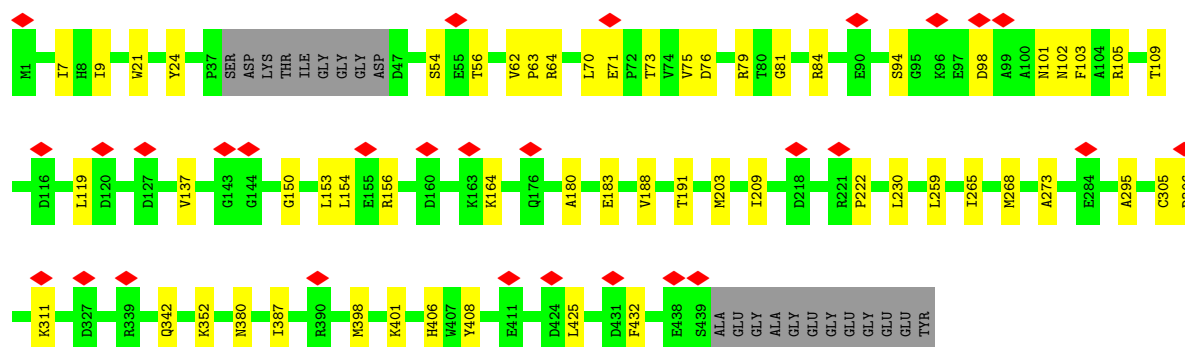


• Molecule 2: Tubulin alpha

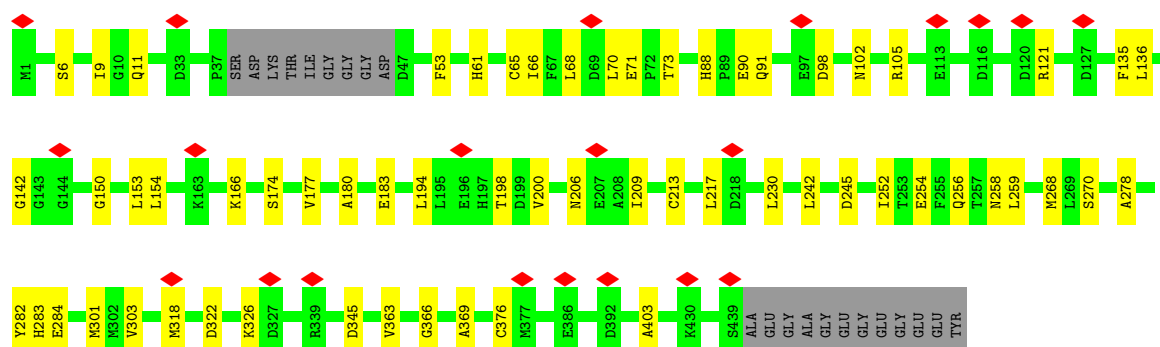
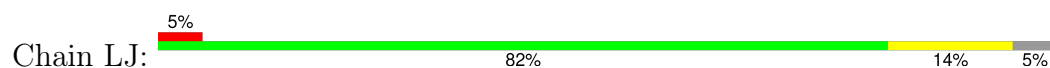


• Molecule 2: Tubulin alpha

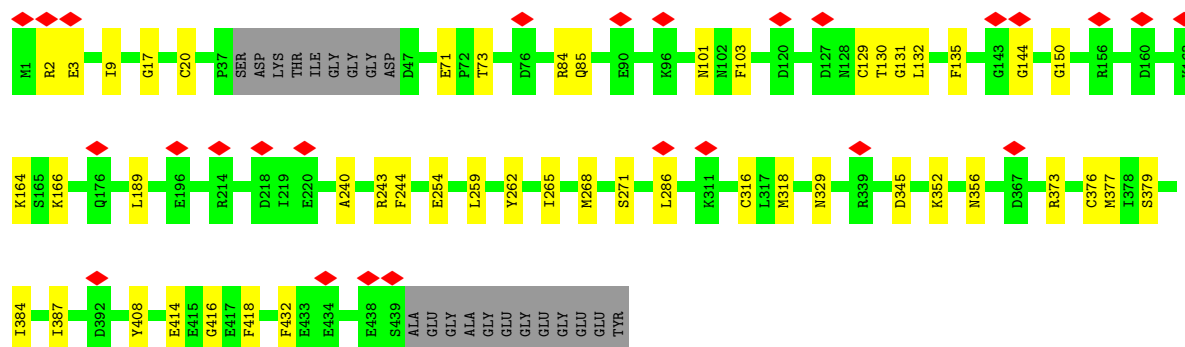
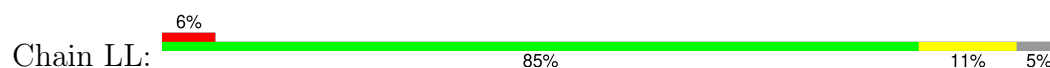




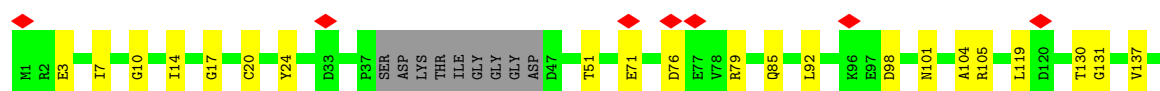
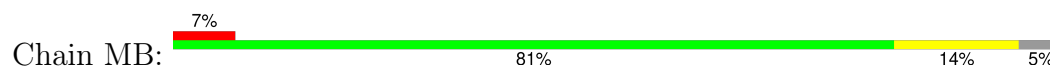
• Molecule 2: Tubulin alpha

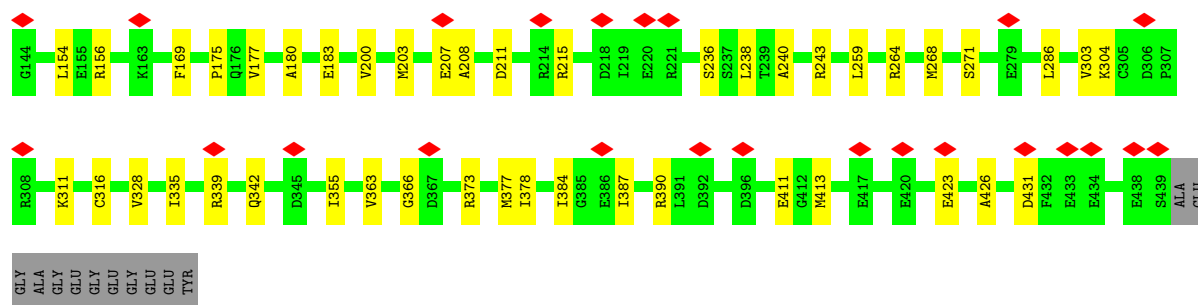


• Molecule 2: Tubulin alpha

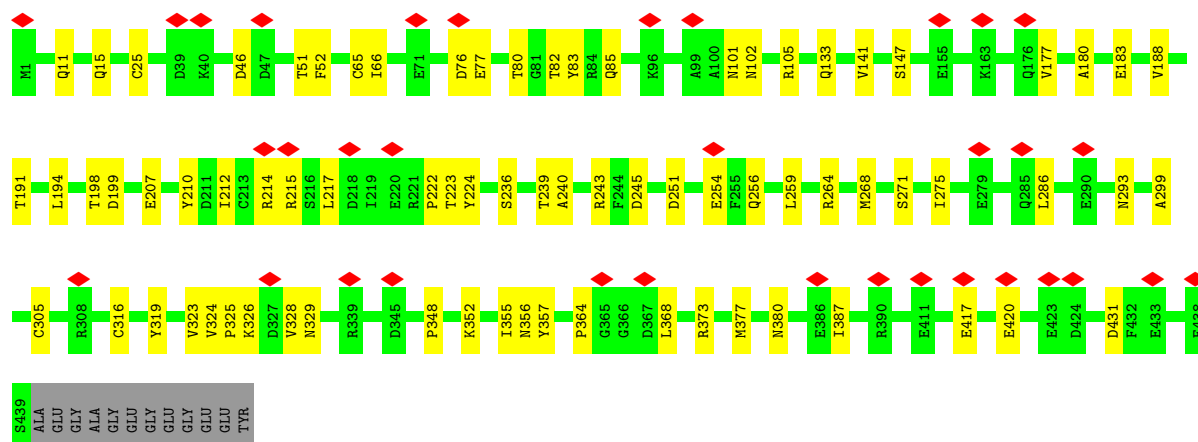
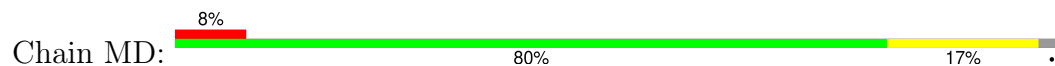


• Molecule 2: Tubulin alpha

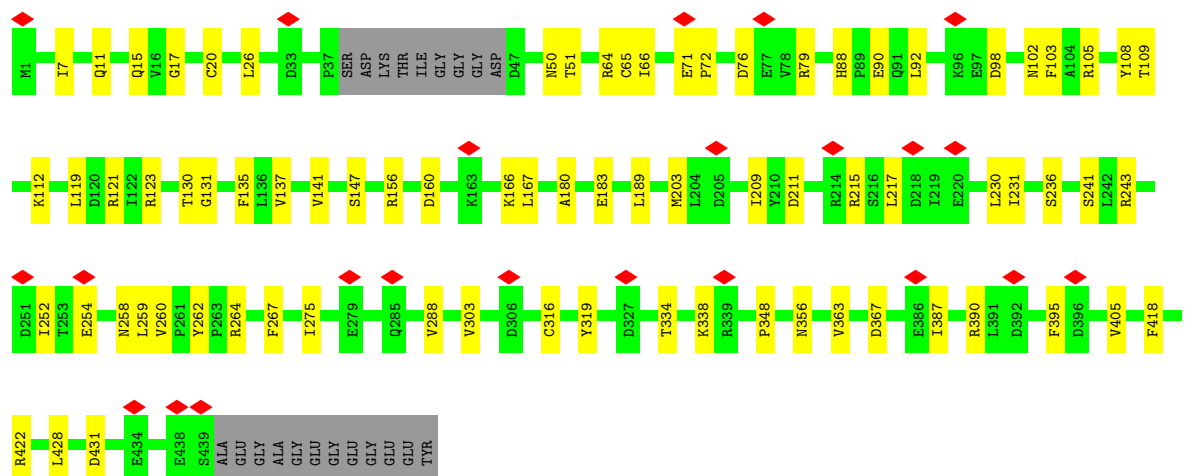
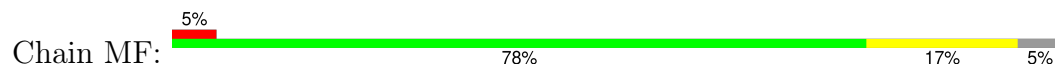




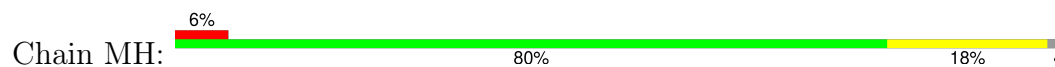
• Molecule 2: Tubulin alpha

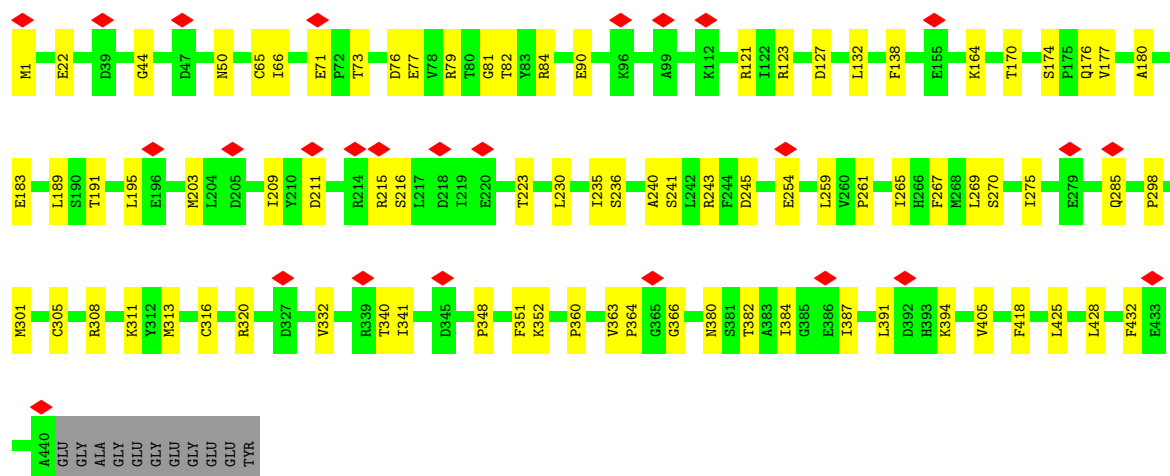


• Molecule 2: Tubulin alpha

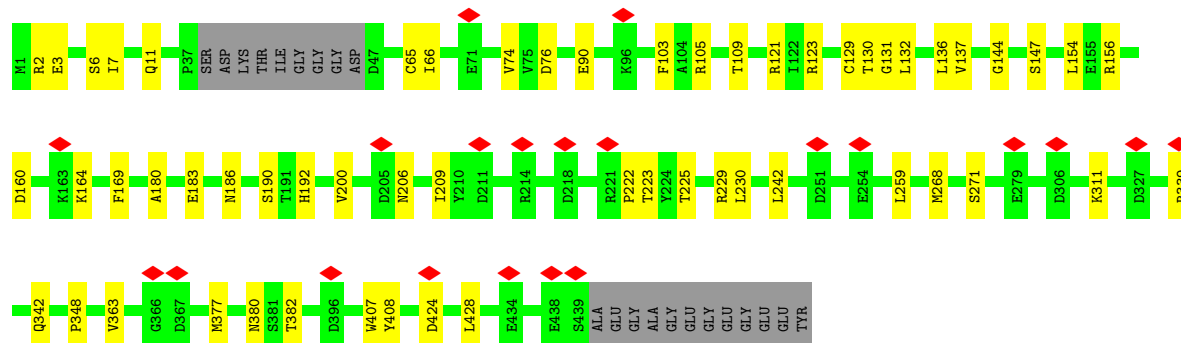
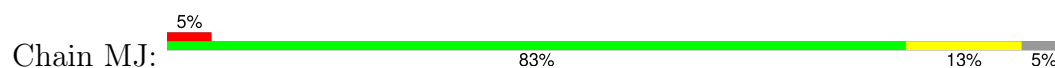


• Molecule 2: Tubulin alpha

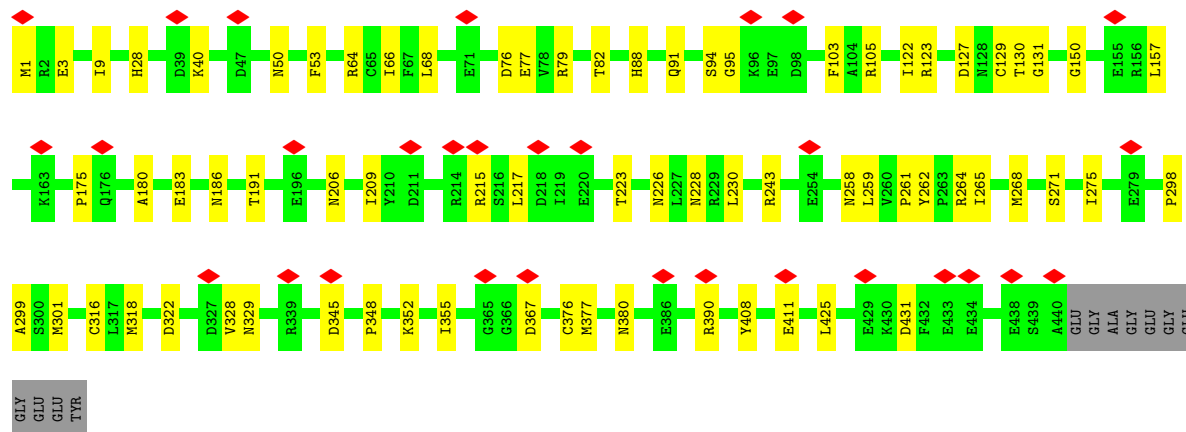
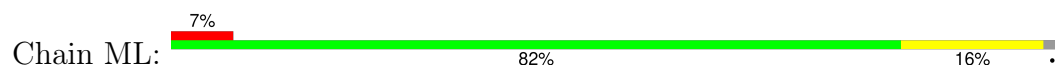




• Molecule 2: Tubulin alpha

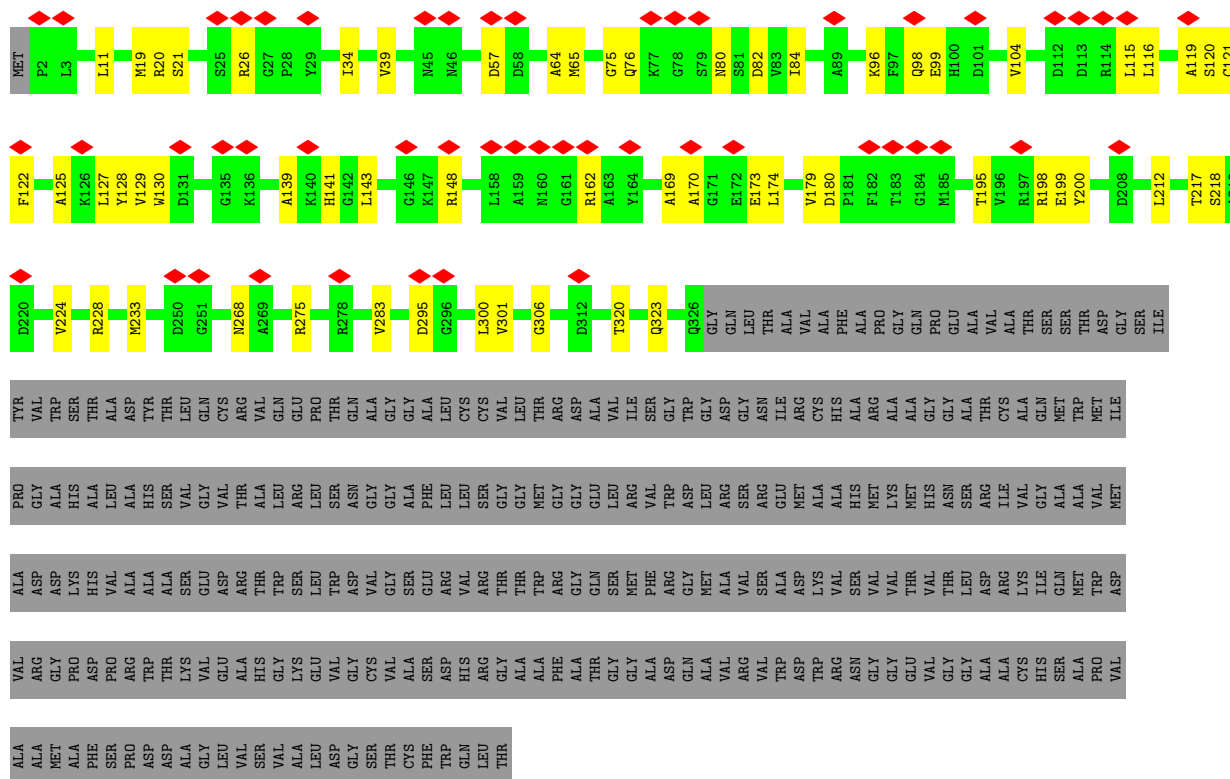


• Molecule 2: Tubulin alpha

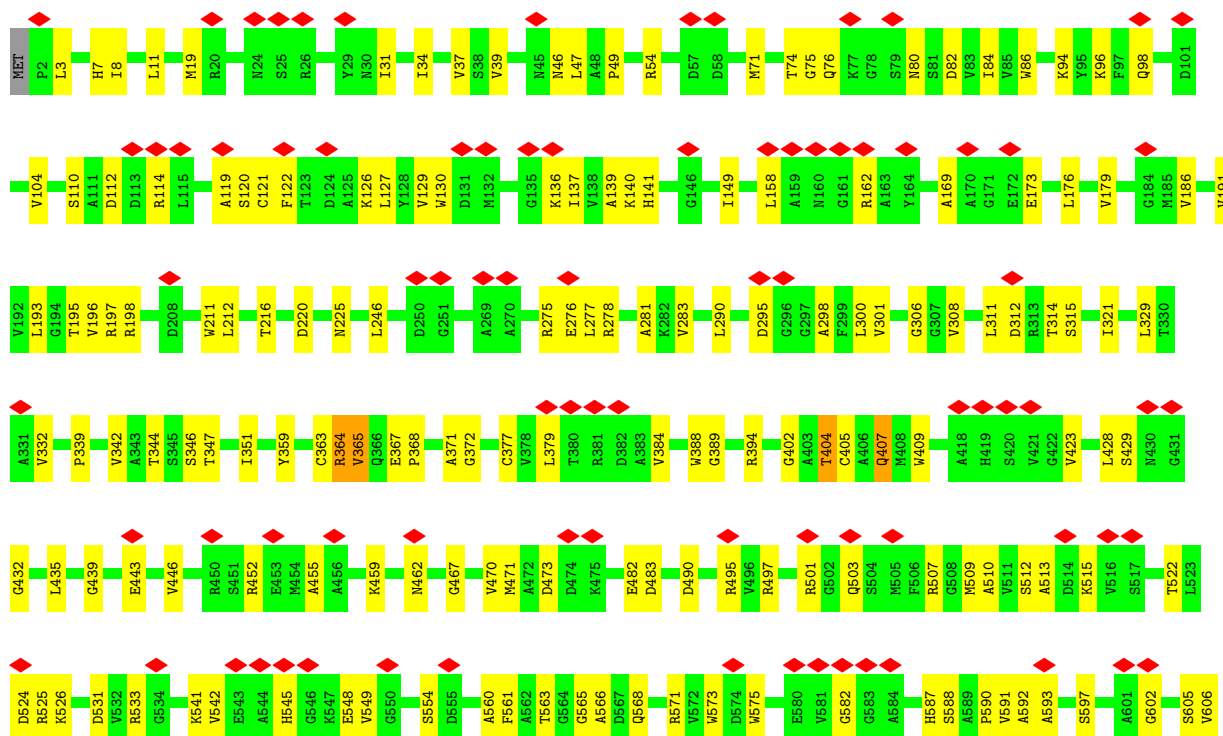


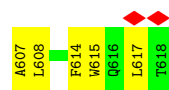
• Molecule 3: Cilia- and flagella-associated protein 20



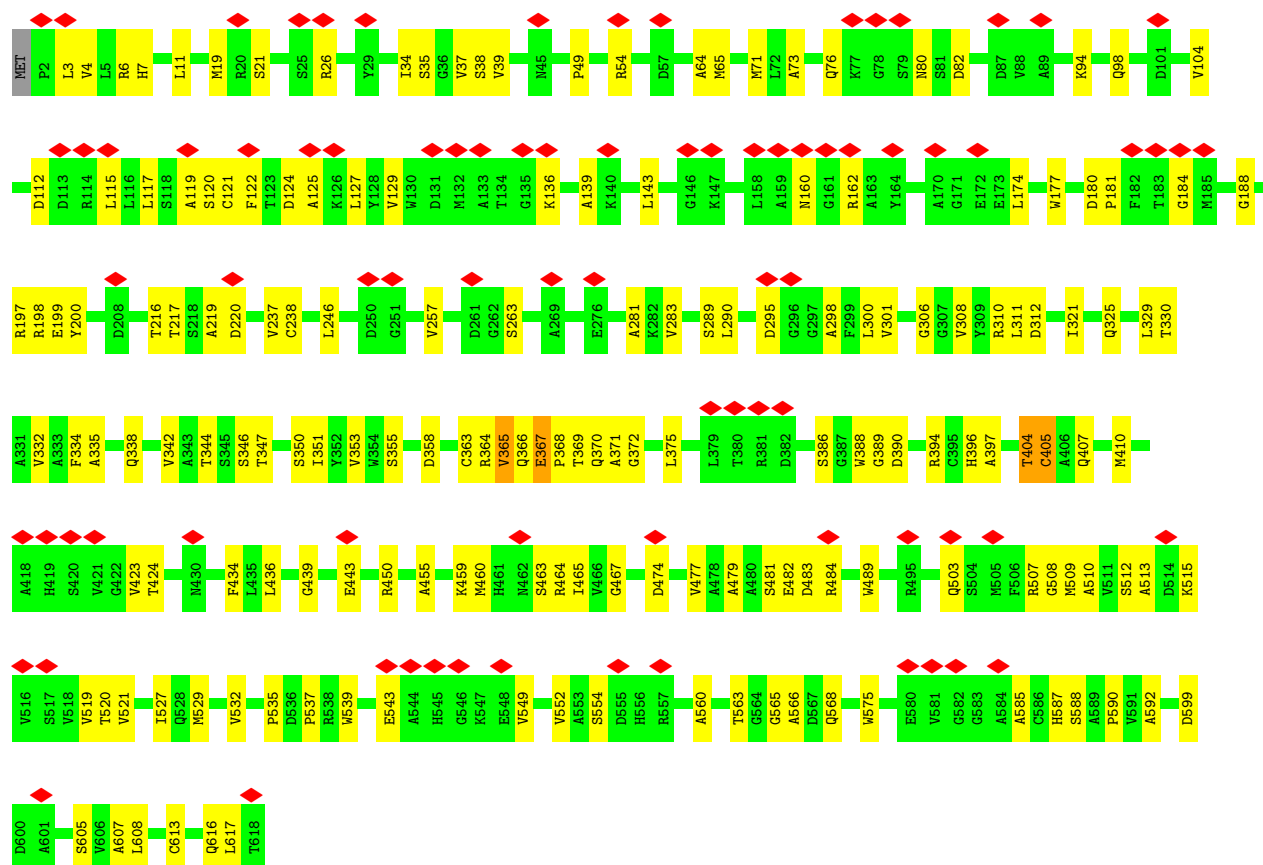


• Molecule 3: Cilia- and flagella-associated protein 20

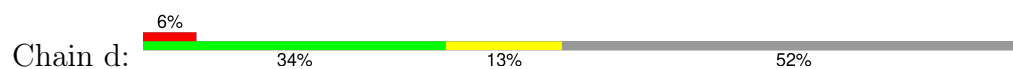


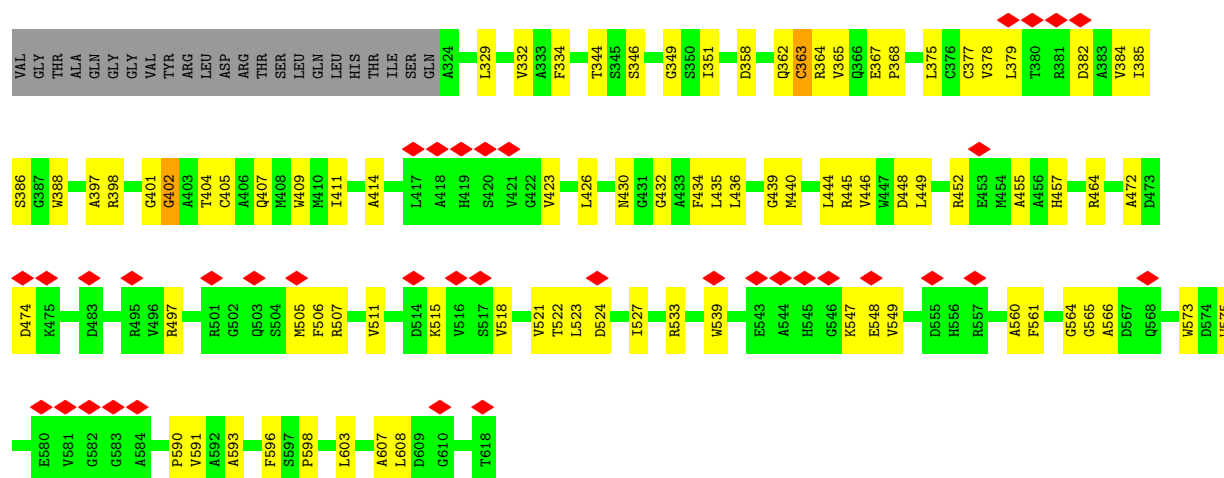


• Molecule 3: Cilia- and flagella-associated protein 20

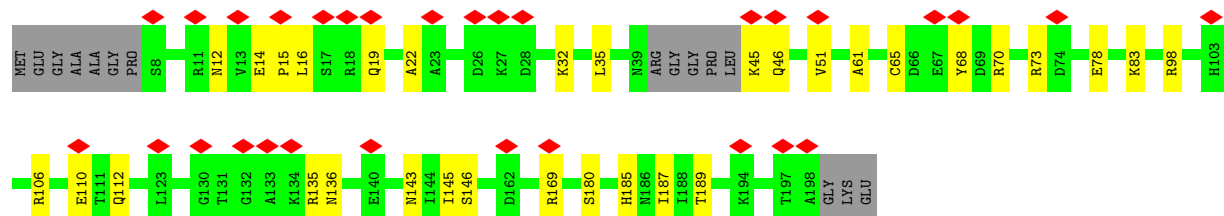


• Molecule 3: Cilia- and flagella-associated protein 20

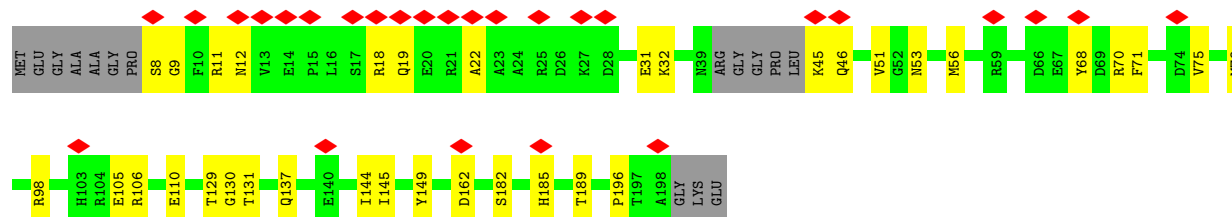
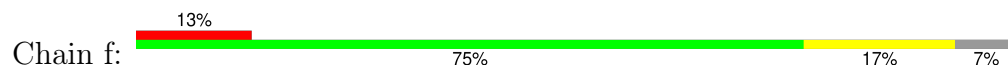




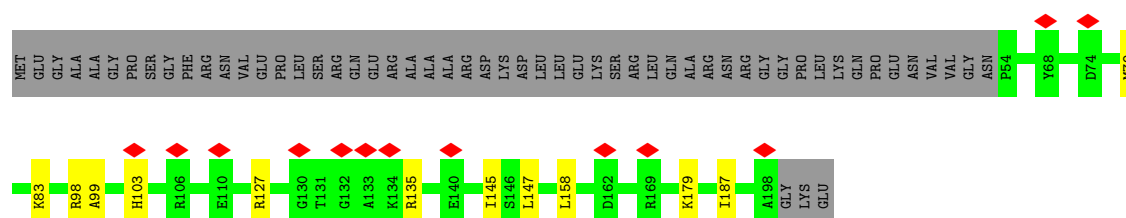
• Molecule 4: Unknown protein



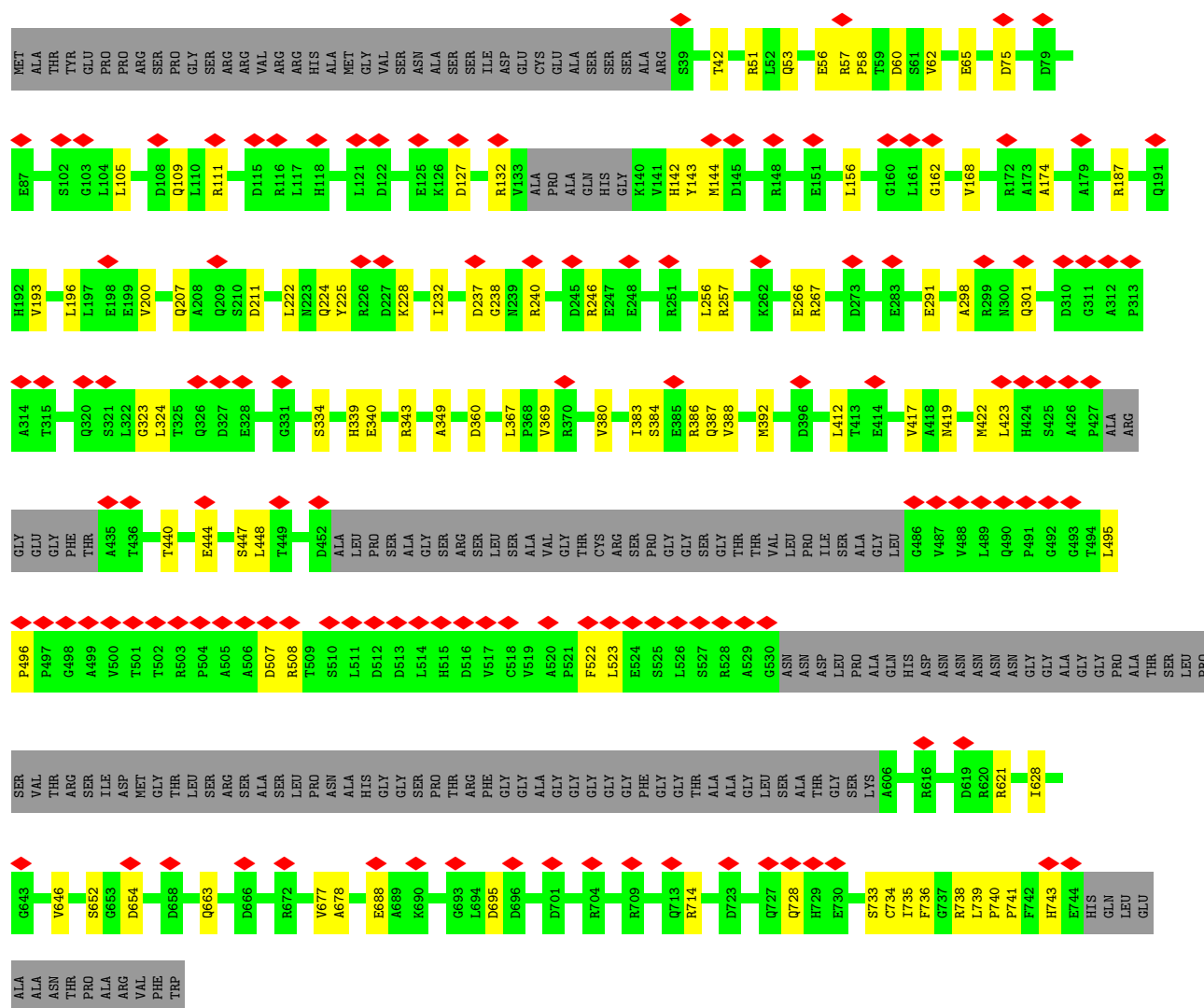
• Molecule 4: Unknown protein



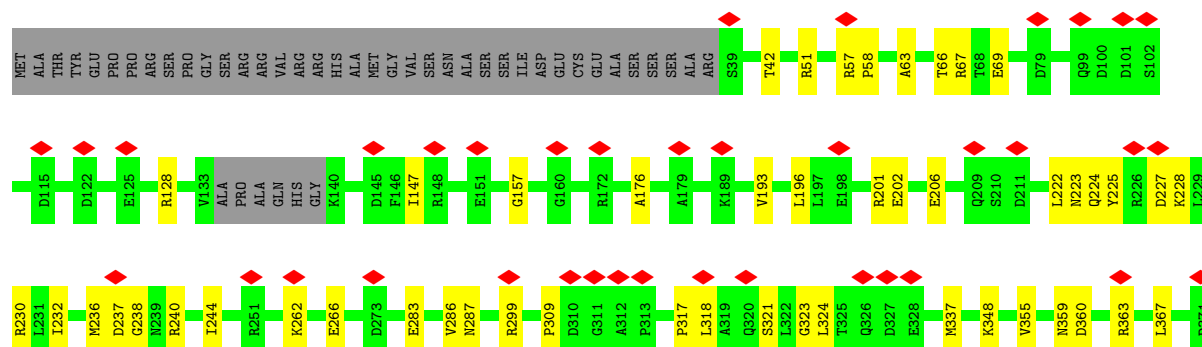
• Molecule 4: Unknown protein

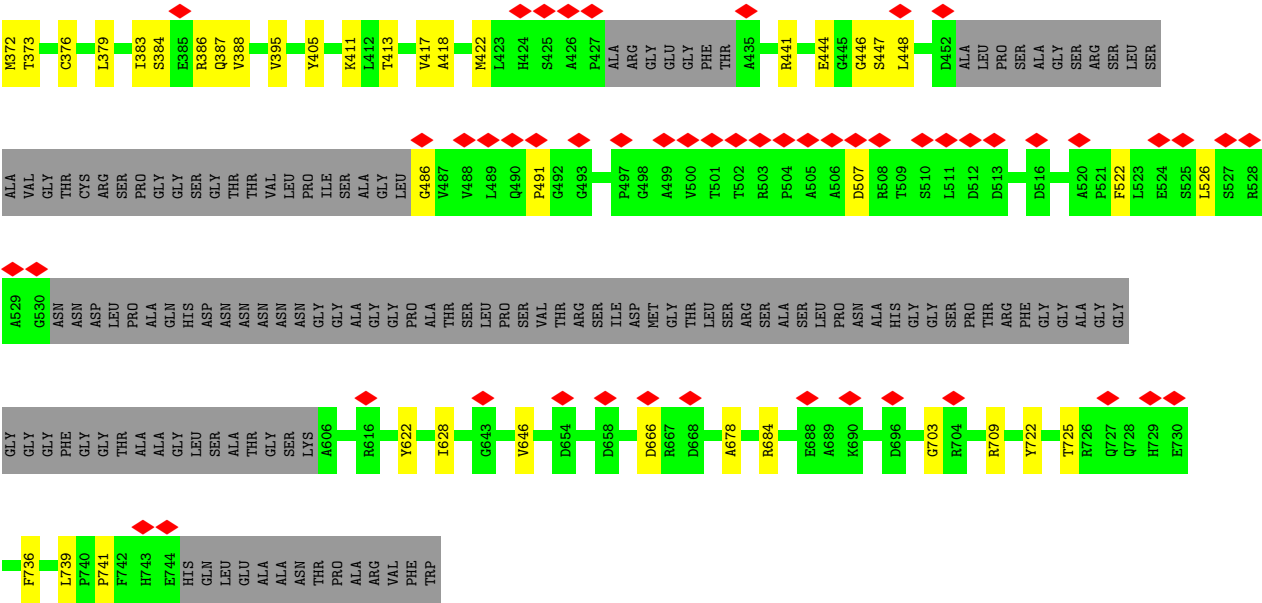


• Molecule 5: Unknown protein

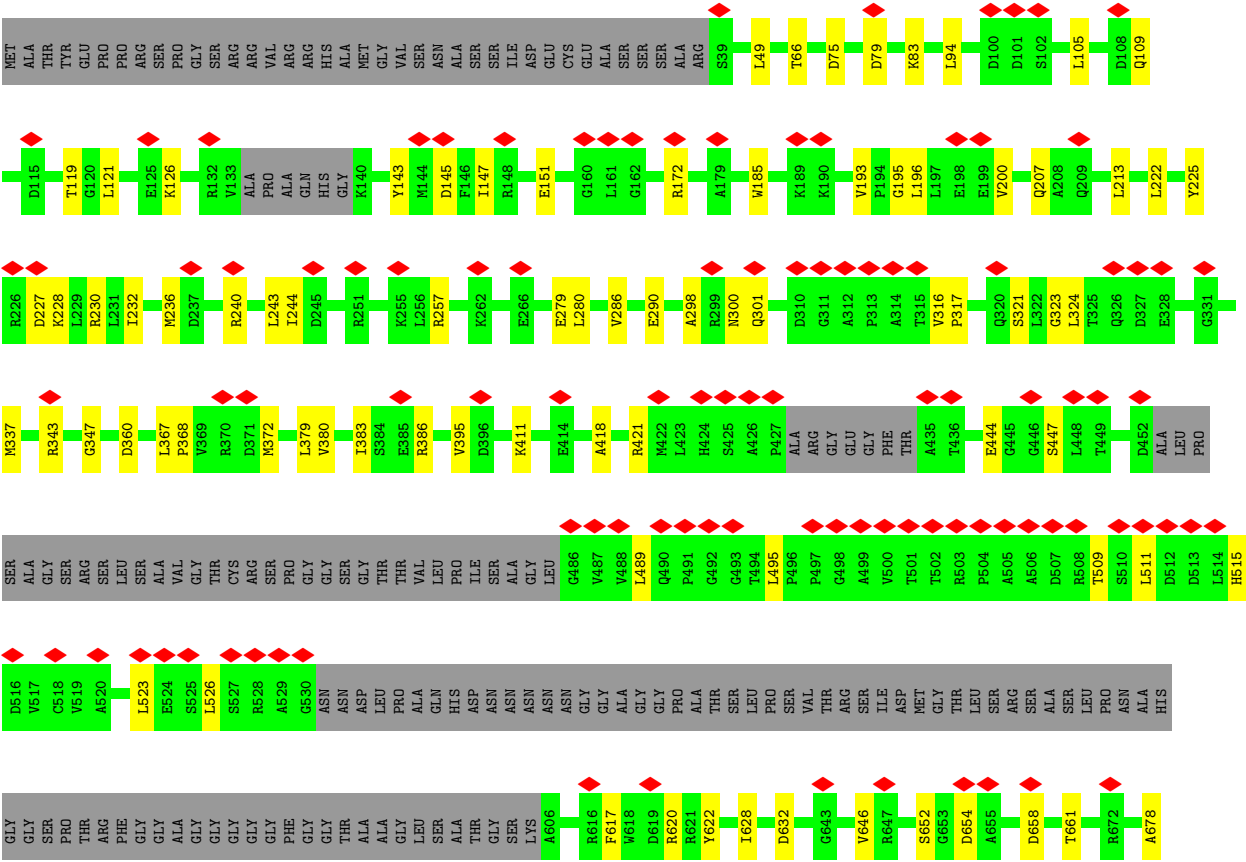


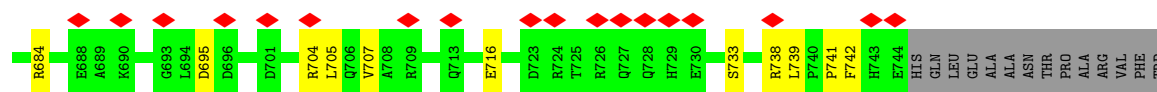
• Molecule 5: Unknown protein



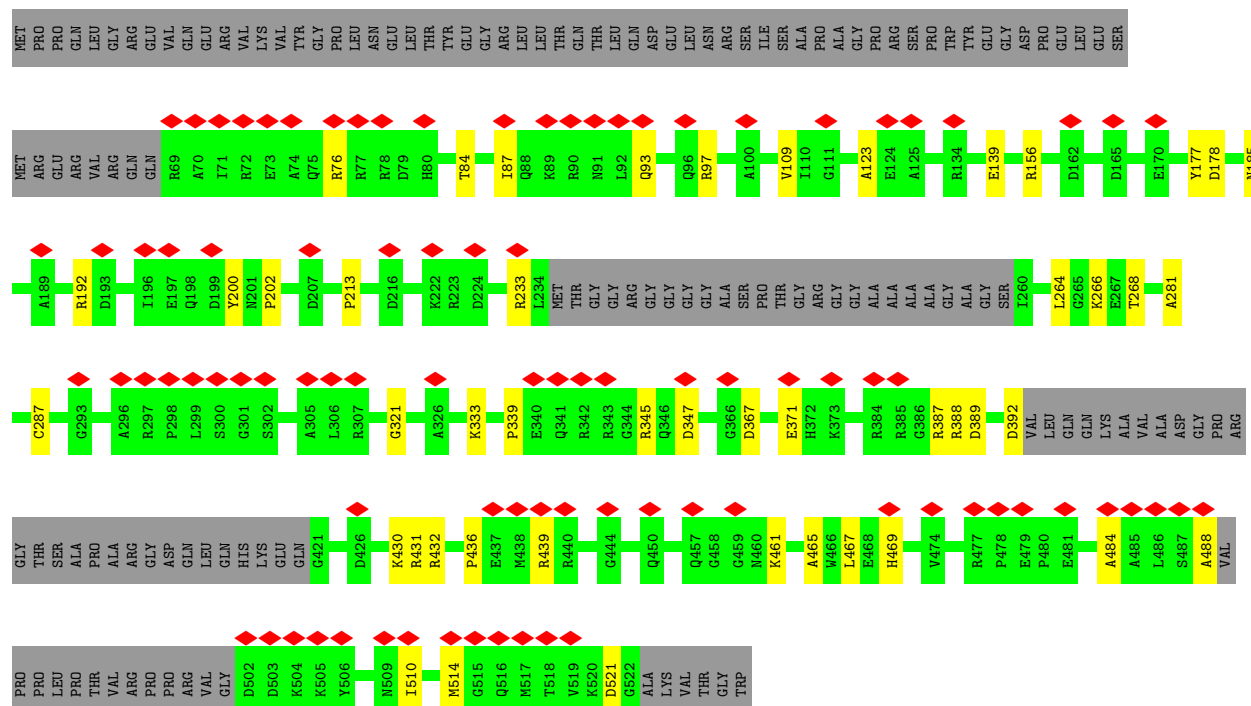


• Molecule 5: Unknown protein

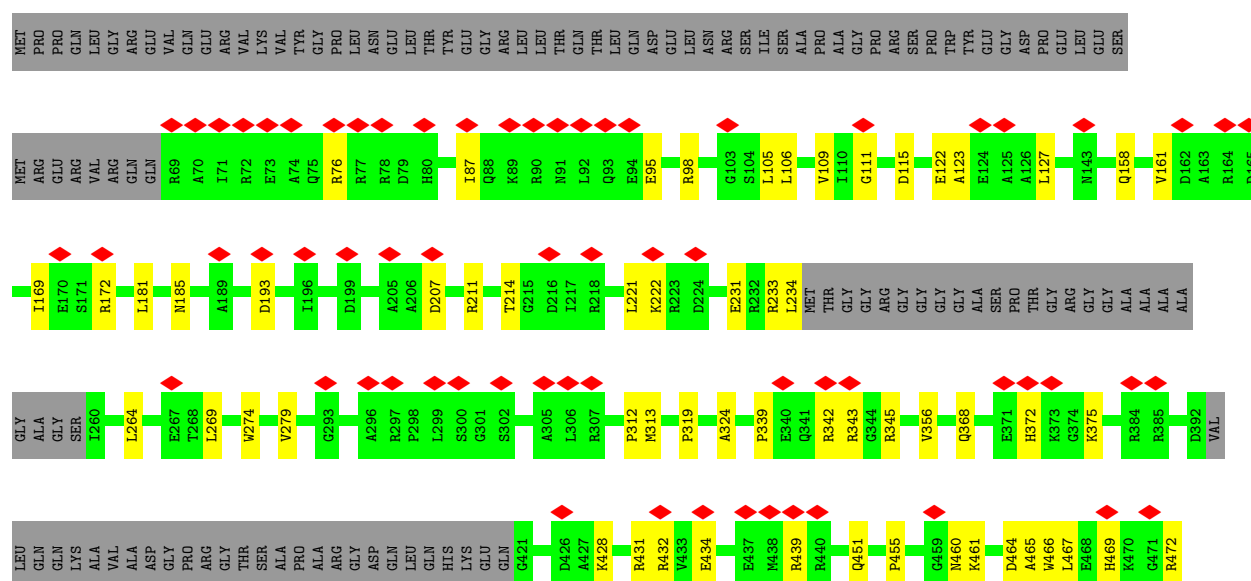


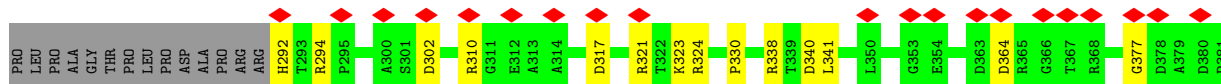


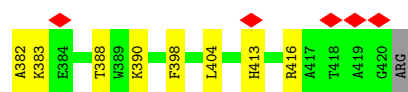
• Molecule 6: Unknown protein



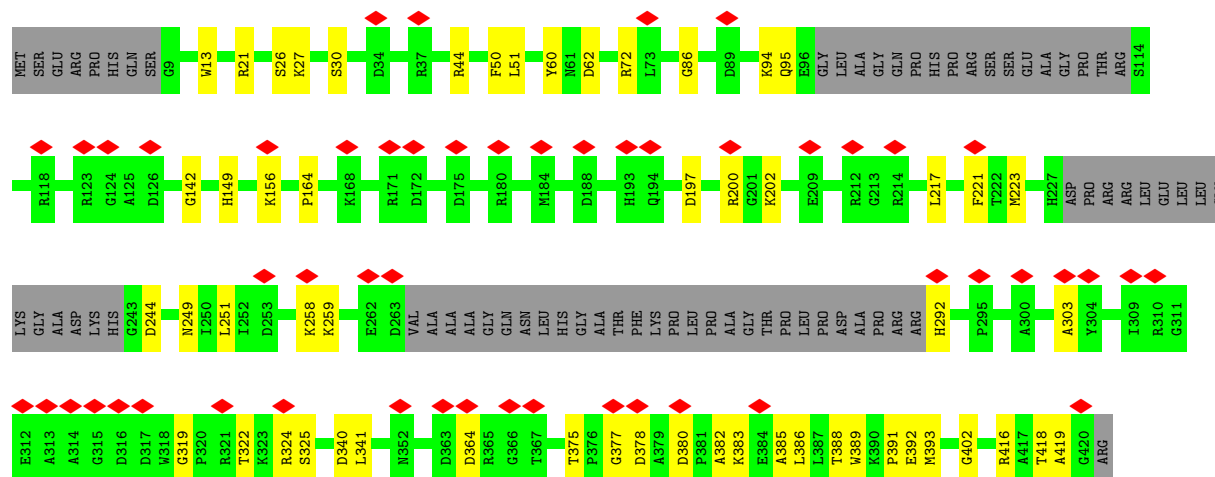
• Molecule 6: Unknown protein



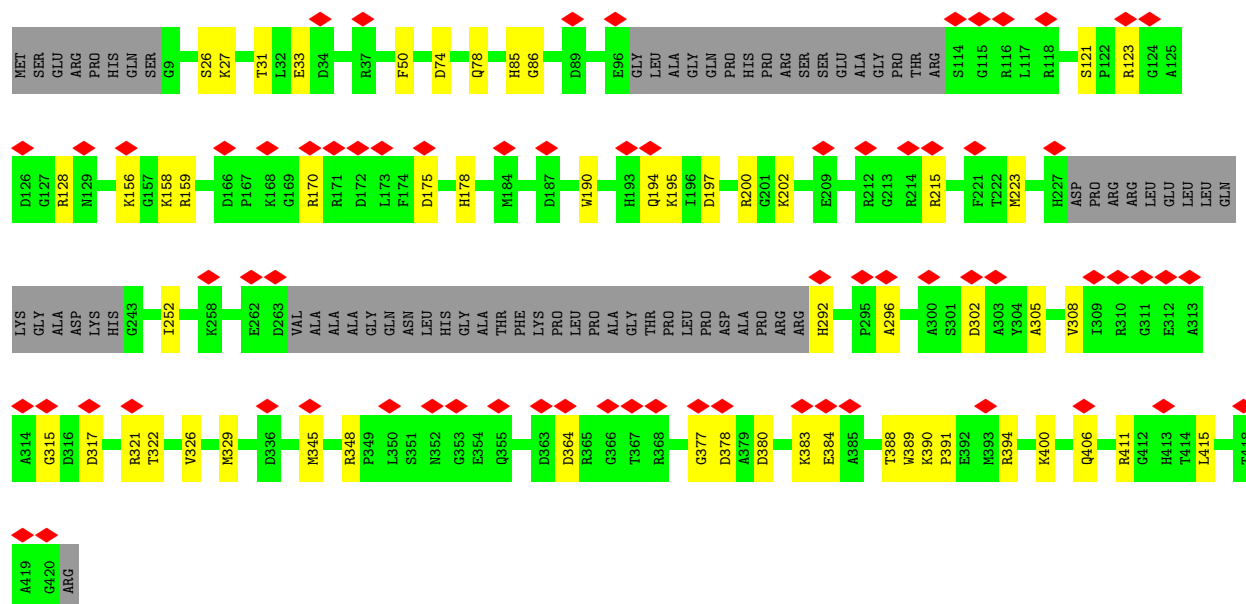




• Molecule 7: FAP65

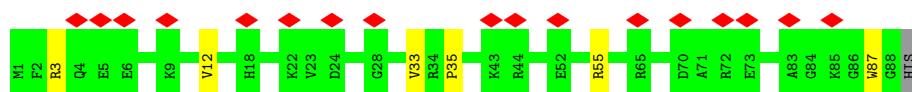


• Molecule 7: FAP65

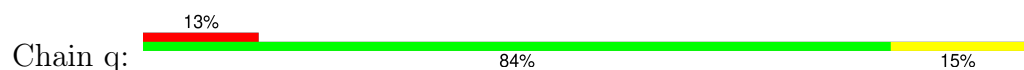


• Molecule 8: FAP70

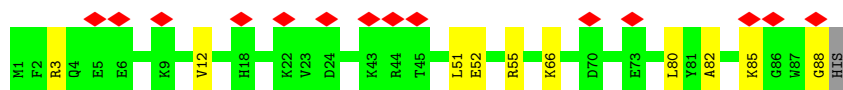
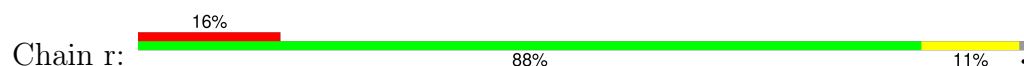




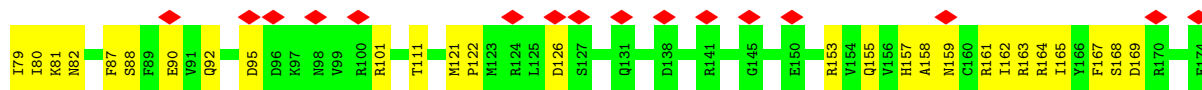
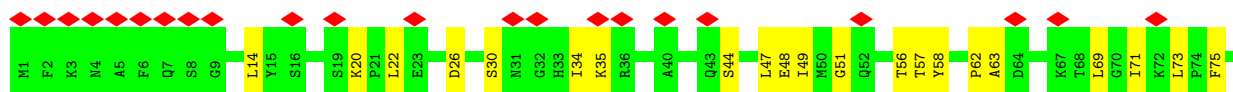
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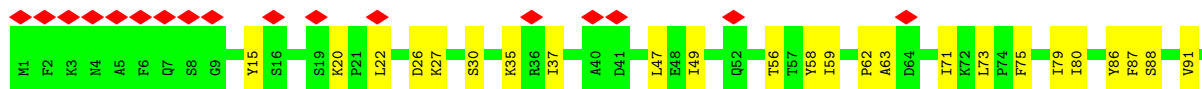
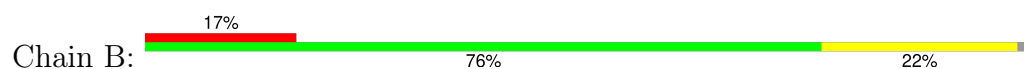
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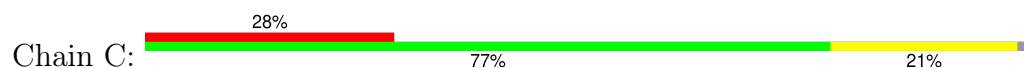
• Molecule 9: FAP147



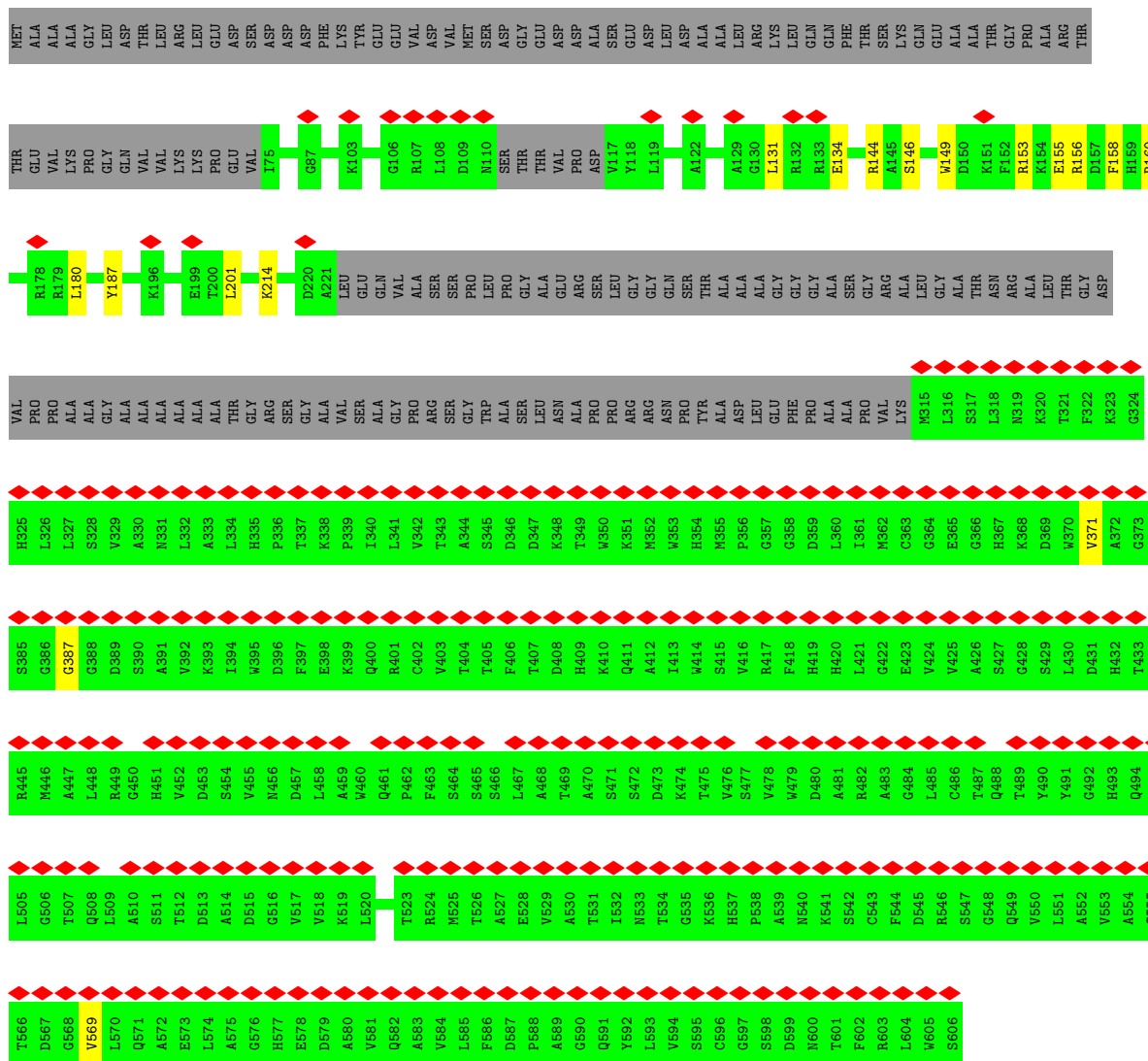
• Molecule 9: FAP147



• Molecule 9: FAP147

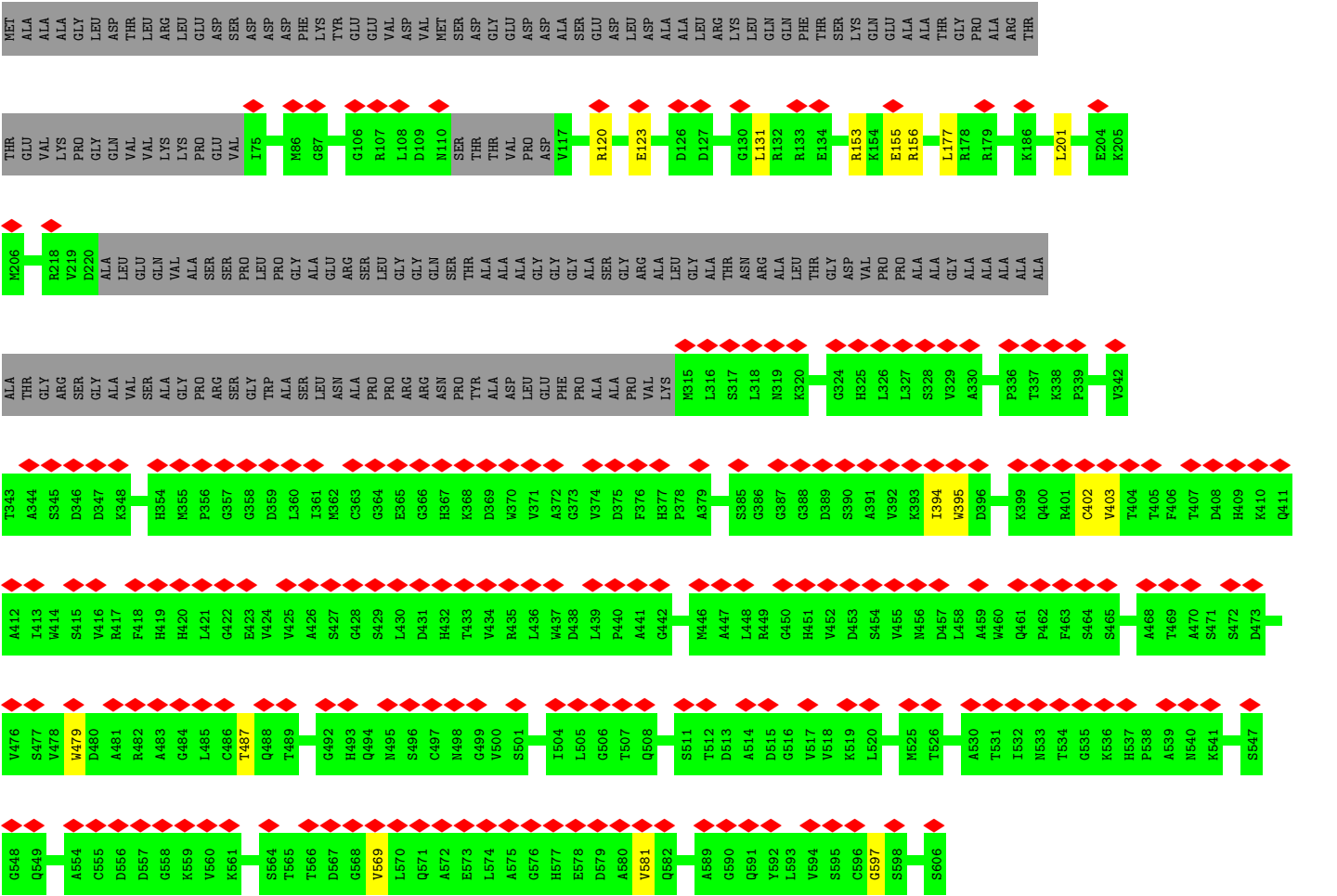


- Molecule 10: FAP178

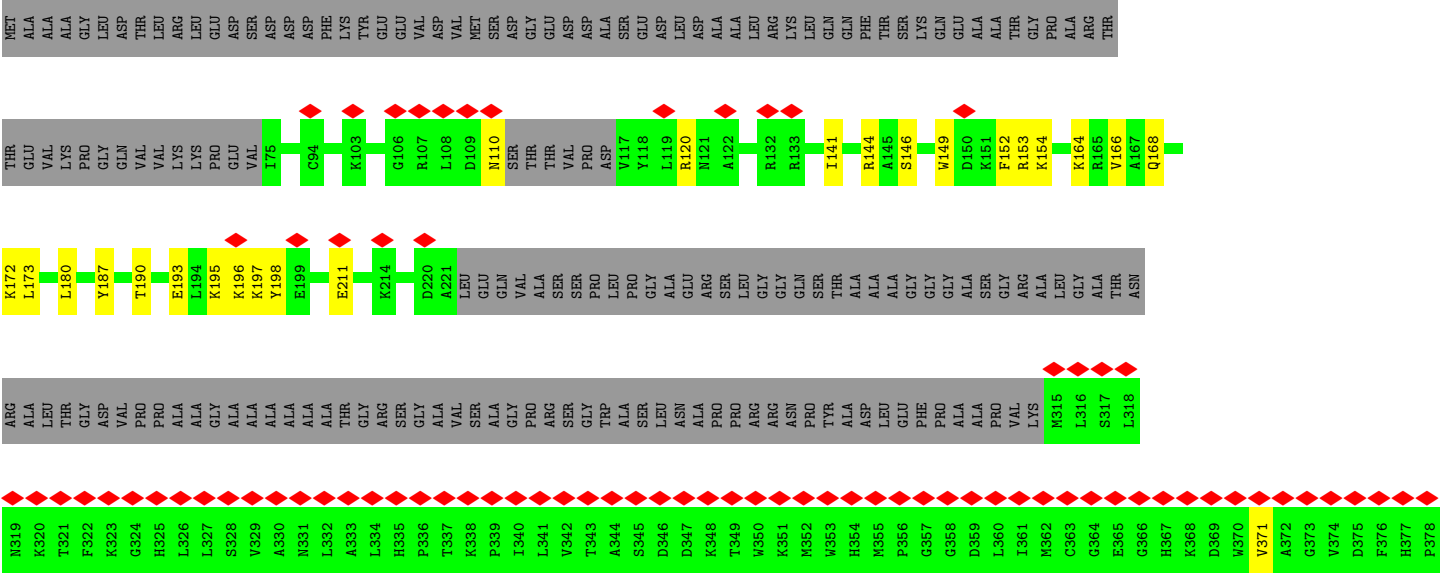


- Molecule 10: FAP178





• Molecule 10: FAP178





A575	G506	L436	A372	ASN
G576	T507	M437	G373	PRO
H577	Q508	D438	V374	TYR
E578		L439	D375	ASP
D579	T512	P440	F376	LEU
A580	D513	A441	H377	GLU
V581	A514	G442	P378	PRO
Q582	D515		A379	ALA
A589	G516	M446	S385	ALA
G590	V517	A447	G386	PRO
Q591	V518		G387	VAL
Y592	K519	G450	G388	LYS
L593	M625	H451	D389	M315
V594	T526	V452	S390	L316
	A527	D453	A391	S317
	E528	S454	V392	L318
	V529	V455	K393	M319
	A530	M456	T394	K320
	T531	D457	K395	
	I532	L458	D396	G324
	M533	A459	F397	H325
	T534	M460	E398	L326
	G535	Q461	K399	L327
	K536	P462	Q400	S328
	H537	F463	R401	V329
	P538	S464	C402	A330
	A539	S465	V403	
	N540		T404	P336
	K541	A468	T405	T337
	S542	T469	F406	K338
	C543	A470	T407	P339
		S471	D408	
		S472	H409	V342
		D473	K410	T343
			Q411	A344
		V476	A412	S345
		S477	I413	D346
		V478	M414	D347
		D480	S415	K348
		A481	V416	
		D482	R417	H354
		A483	H419	M355
		G484	H420	P356
		L485	L421	G357
		C486	G422	G358
			E423	D359
		T489	V424	L360
			V425	I361
		G492	A426	M362
		H493	S427	G363
		Q494	G428	G364
		M495	S429	E365
		S496	L430	G366
		C497	D431	H367
		M498	H432	K368
		G499	T433	D369
			I504	M370
			L505	V371

Chain cc: 14% 85%



[illegible]

- Molecule 10: FAP178

[illegible][illegible]

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

TRP	ASP	THR	THR	ARG	MET	THR	ALA	GLU	VAL	VAL	ALA	ALA	THR	THR	ILE	ASN	THR	GLY	HIS	HIS	PRO	ALA	ASN	LYS	LYS	CYS	PHE	CYS	ASP	ARG	SER	GLY	GLN	VAL	VAL	LEU	ALA	VAL	VAL	ALA	ALA	CYS	ASP	ASP	GLY	GLY	LYS	LYS	VAL	VAL	LYS	TYP	SER	THR	THR	ASP	GLY	VAL	LEU	GLN	ALA	ALA	GLU	LEU	ALA	GLY	HIS	ASP	ALA
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VAL	GLN	ALA	VAL	LEU	PHE	ASP	PRO	ALA	GLY	GLN	TYR	LEU	VAL	SER	CYS	GLY	SER	ASP	ASN	THR	PHE	ARG	LEU	TRP	SER
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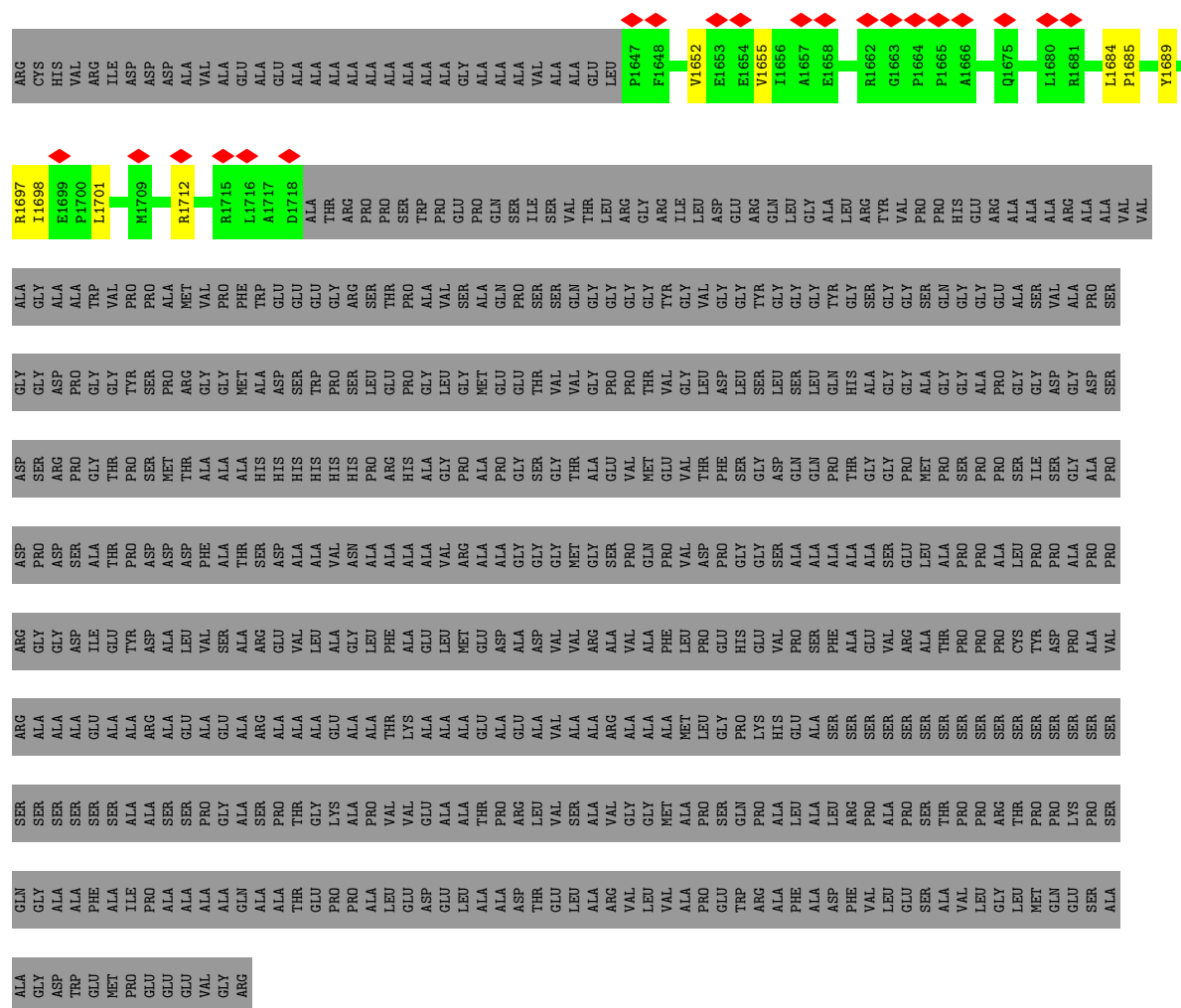
- Molecule 11: Flagellar WD repeat-containing protein Pf20



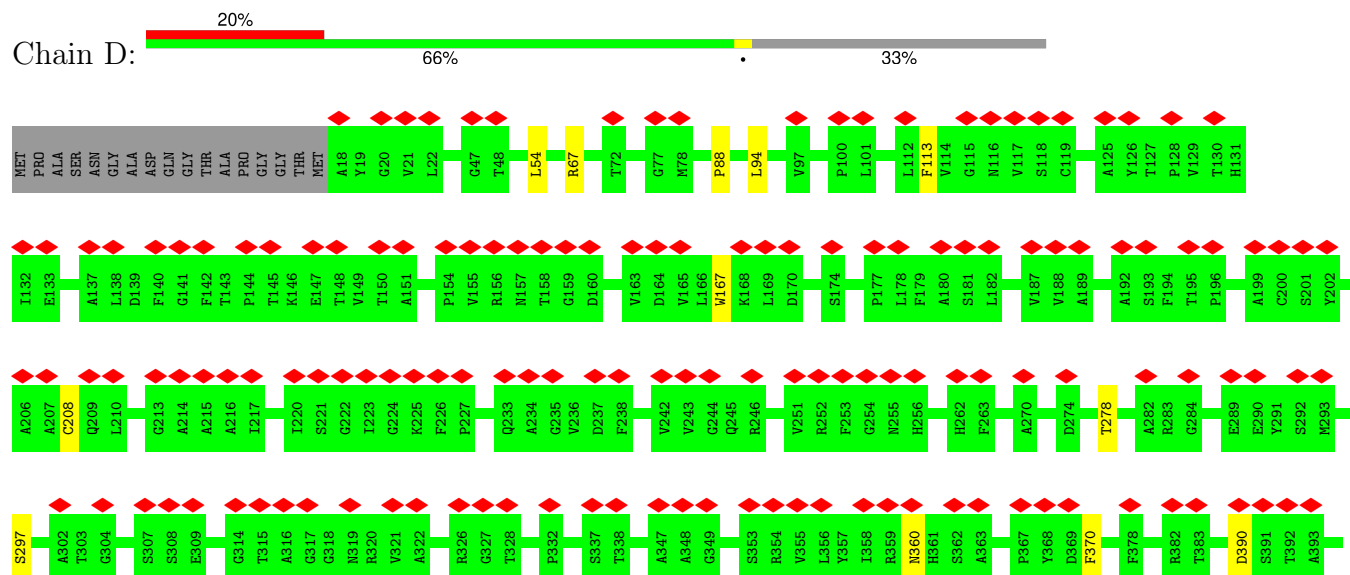
SER	LEU	GLU	ALA	ALA	ALA	GLU	THR	ALA	MET	S2	E3	S4	T8	G17	A18	I19	D20	V21	L22	V23	L26	Y30	E31	E32	P33	A39	Q45	C46	L47	G48	SER	PRO	THR	PRO	A53	E54	Y55	E56	V59	G64	I65	Q66	K67	Q68	LEU	GLU	GLU	ALA	ASN	GLN	LEU	ILE	ALA	GLU	LEU	GLN	SER	ARG	VAL
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- Molecule 11: Flagellar WD repeat-containing protein Pf20





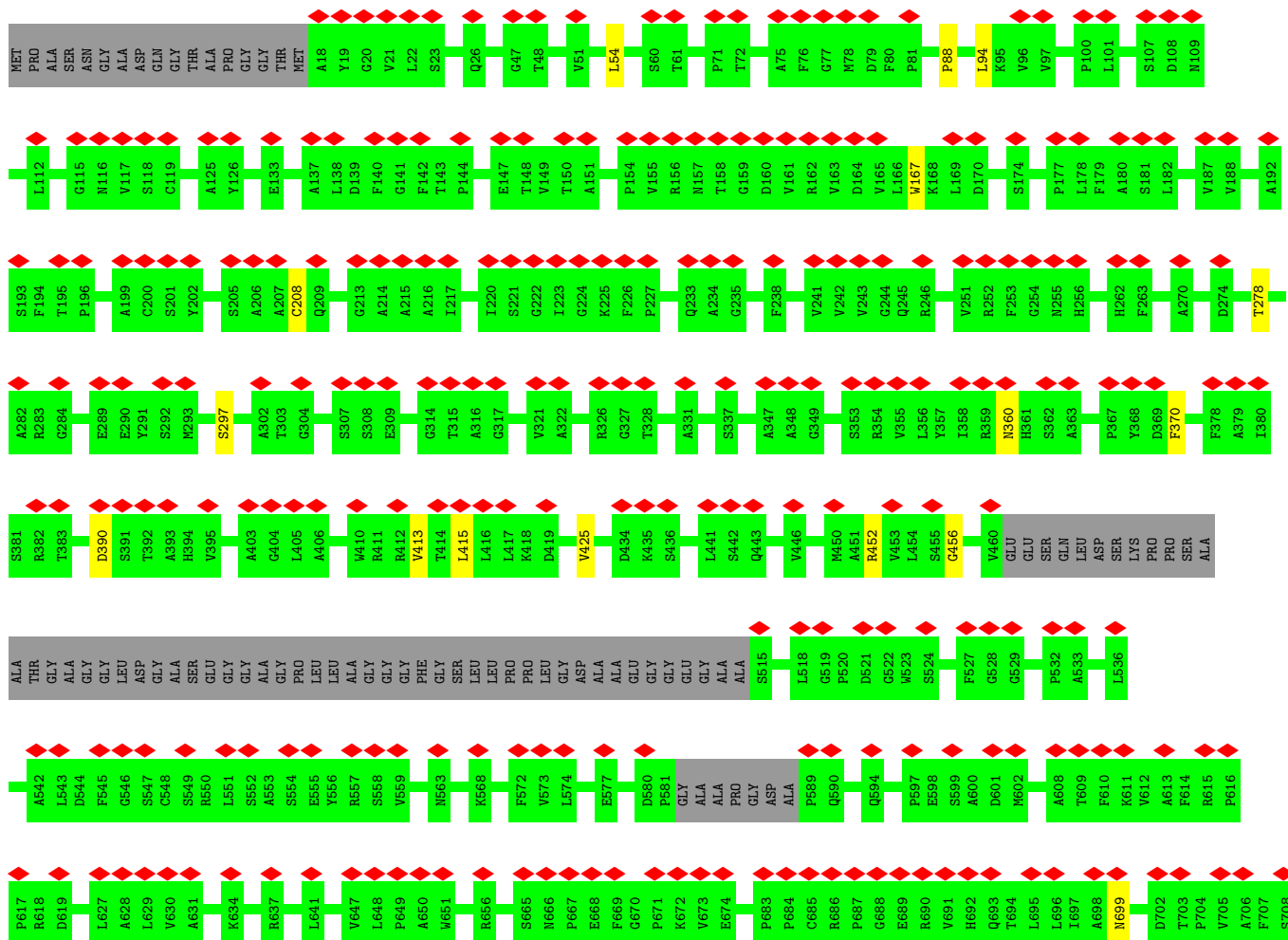
- Molecule 12: Flagellar associated protein





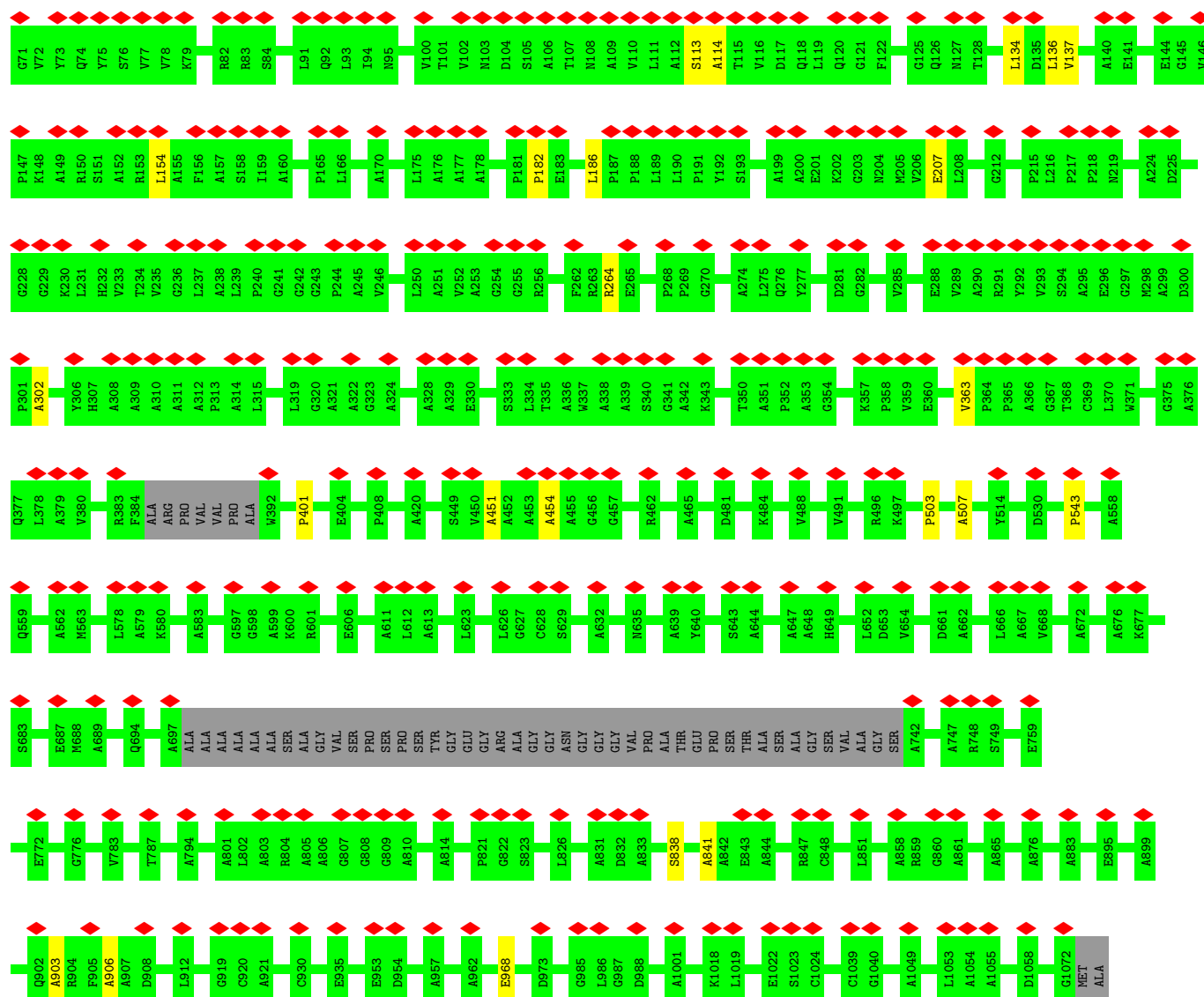
MET	ALA	SER	ALA	GLU	THR	THR	THR
PRO	ILE	ALA	ALA	TYR	GLU	THR	THR
GLU	GLU	ALA	ARG	ASP	ALA	PRO	PRO
GLU	ALA	SER	GLU	LEU	ASP	ASP	ASP
VAL	ALA	PRO	ALA	VAL	PHE	ALA	ALA
ARG	ALA	GLY	GLU	SER	ALA	ALA	ALA
	GLN	ALA	GLN	ALA	THR	THR	ALA
	ALA	SER	ARG	ARG	SER	SER	HIS
	ALA	PRO	ALA	GLU	ASP	ASP	HIS
	THR	THR	ALA	VAL	VAL	ALA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

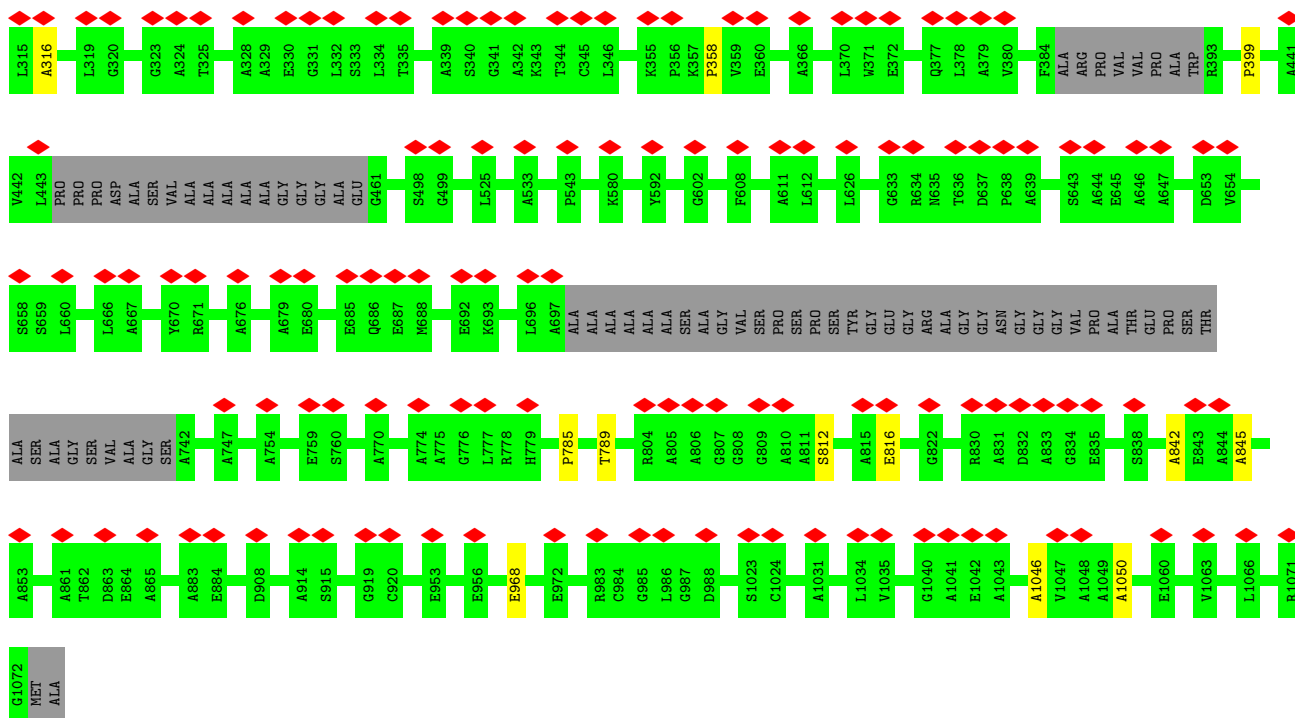
- Molecule 12: Flagellar associated protein



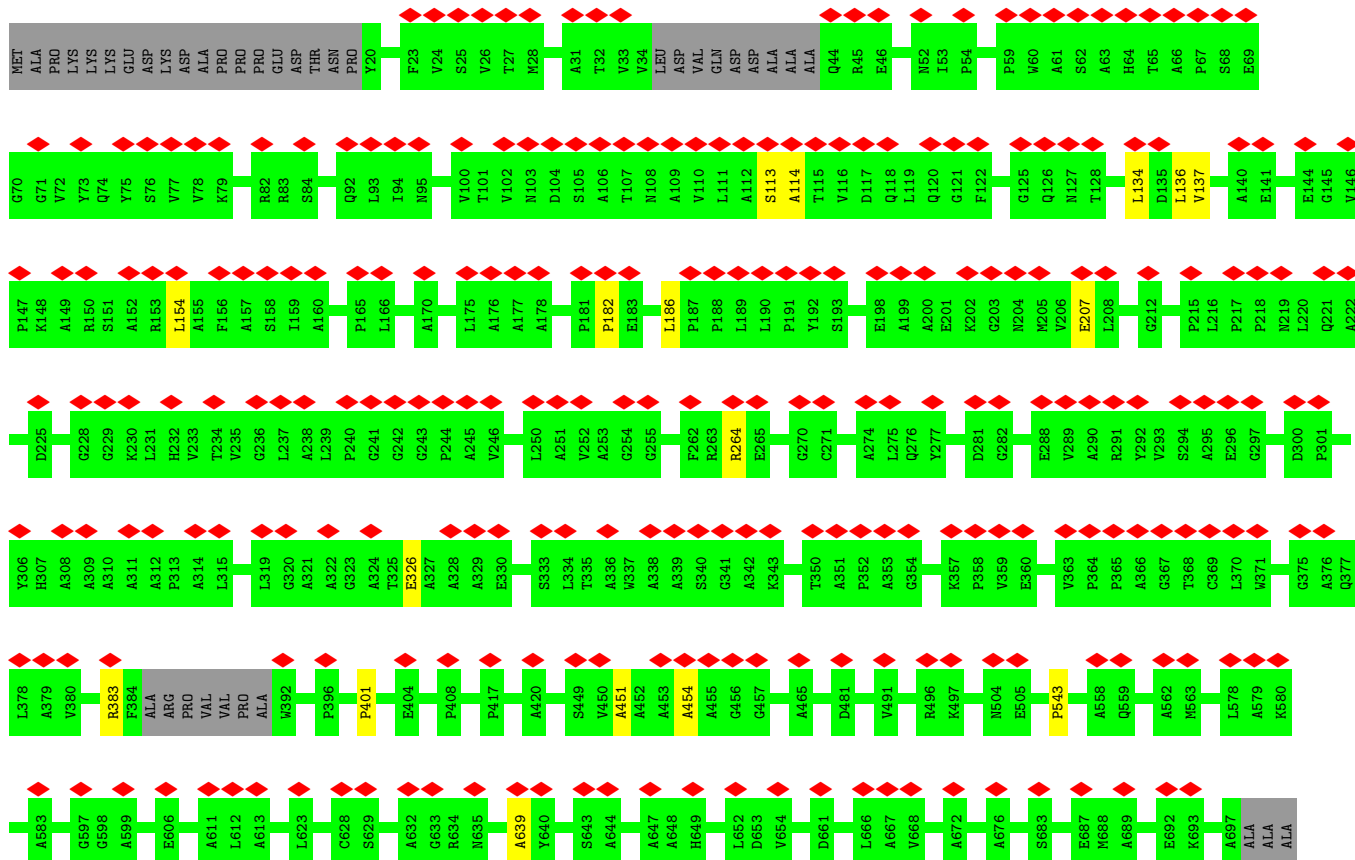
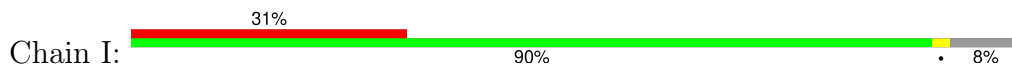


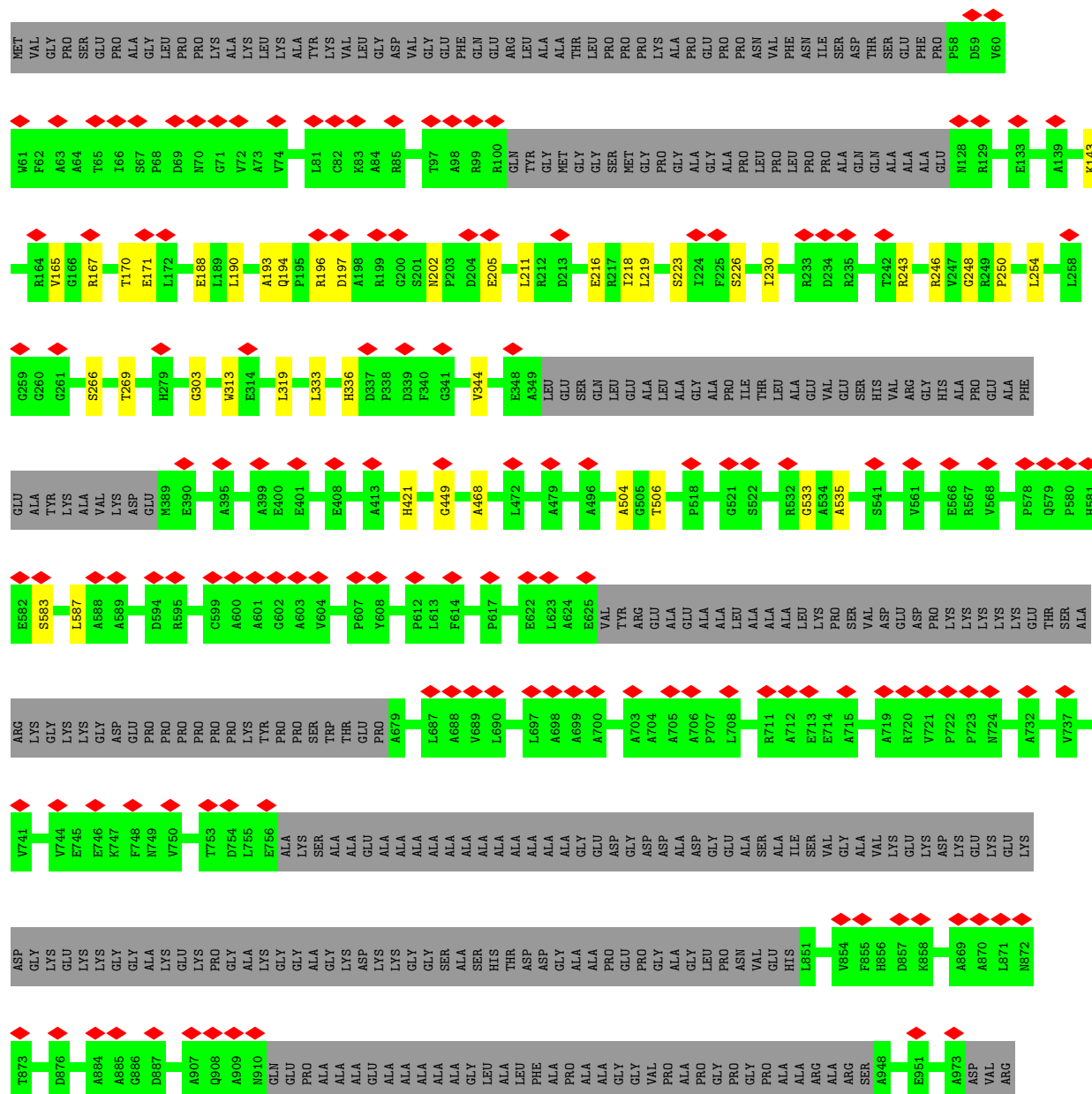
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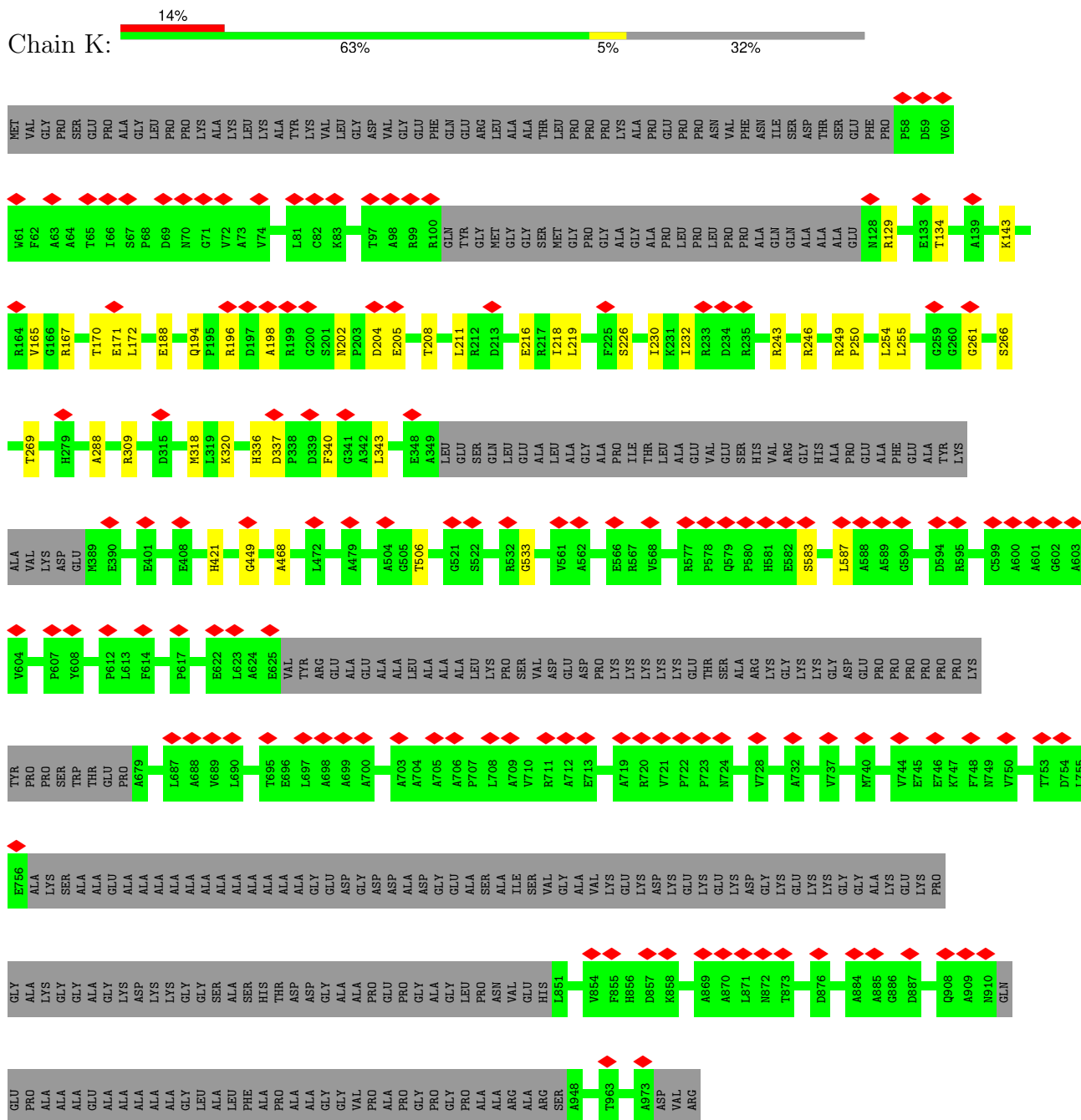


• Molecule 13: FAP196

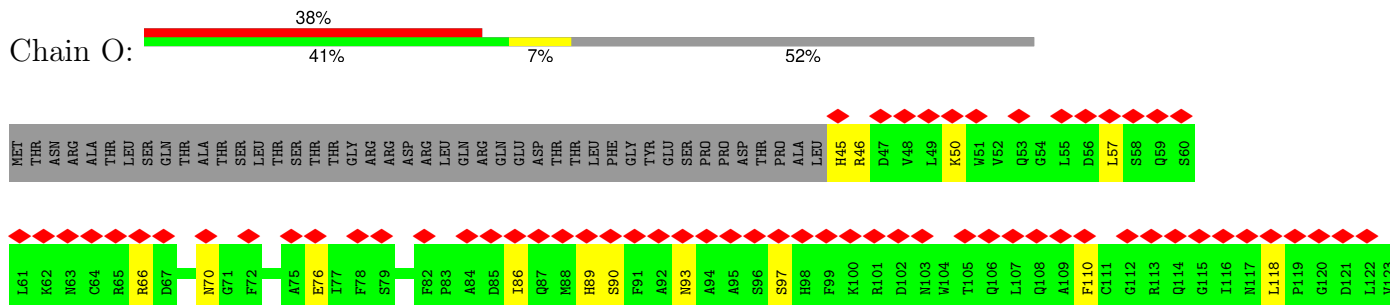


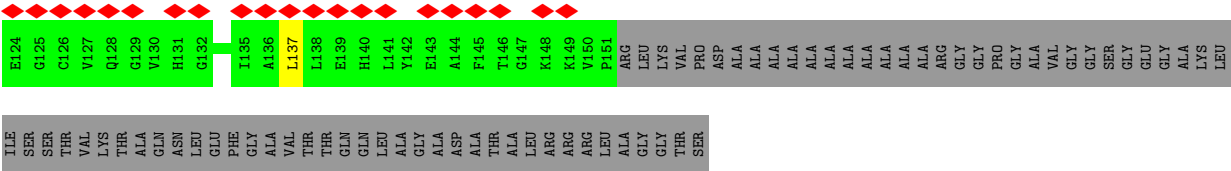


Chain K:

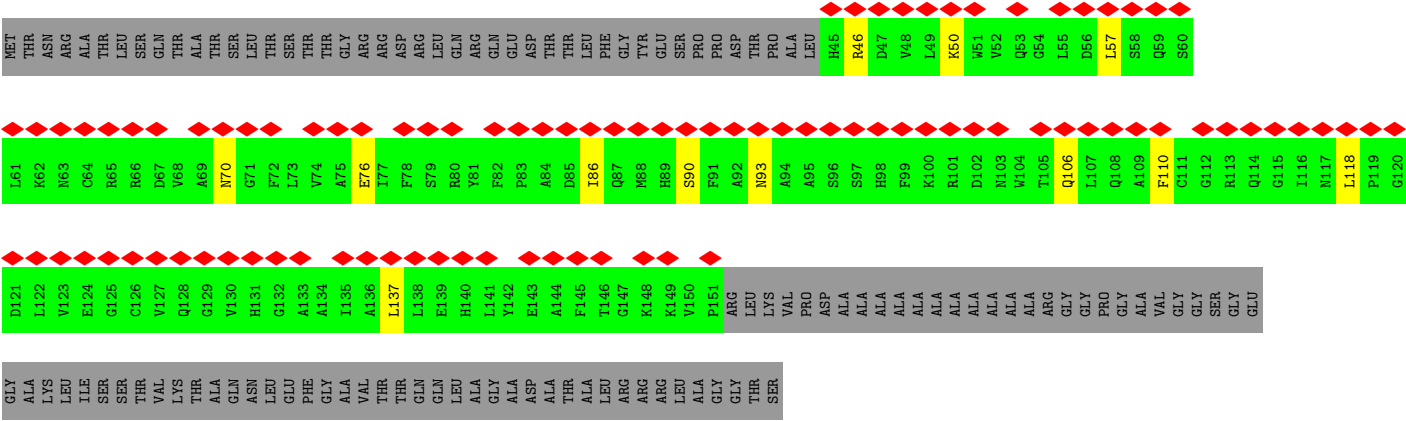
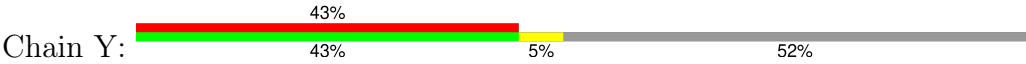


Chain O:

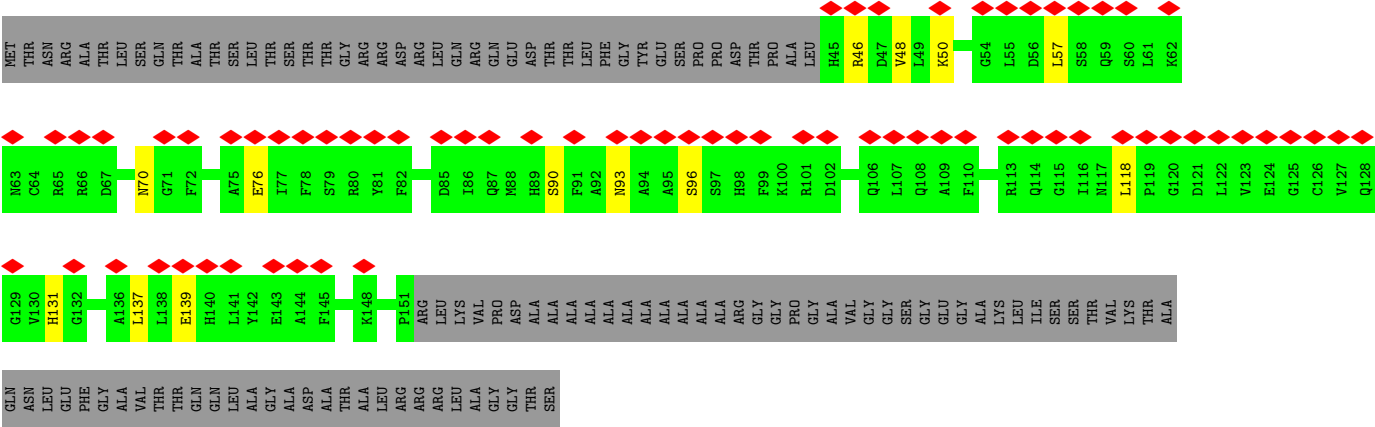
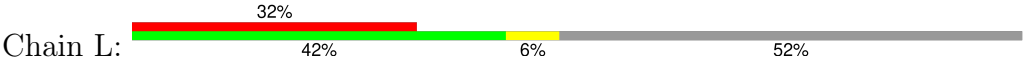




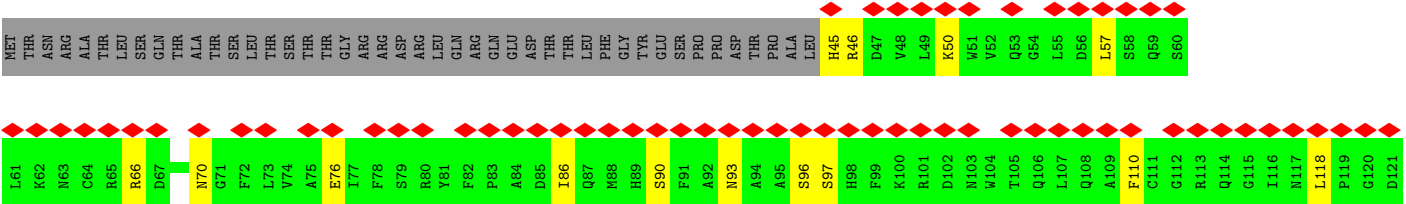
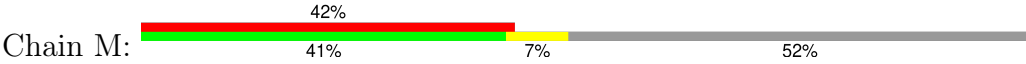
• Molecule 15: FAP225



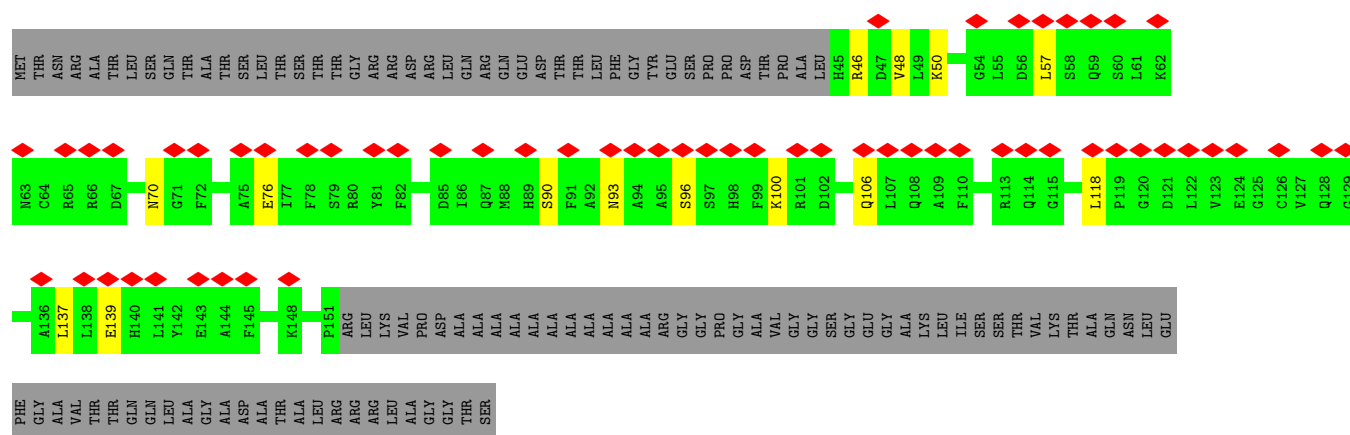
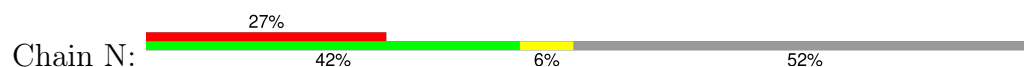
• Molecule 15: FAP225



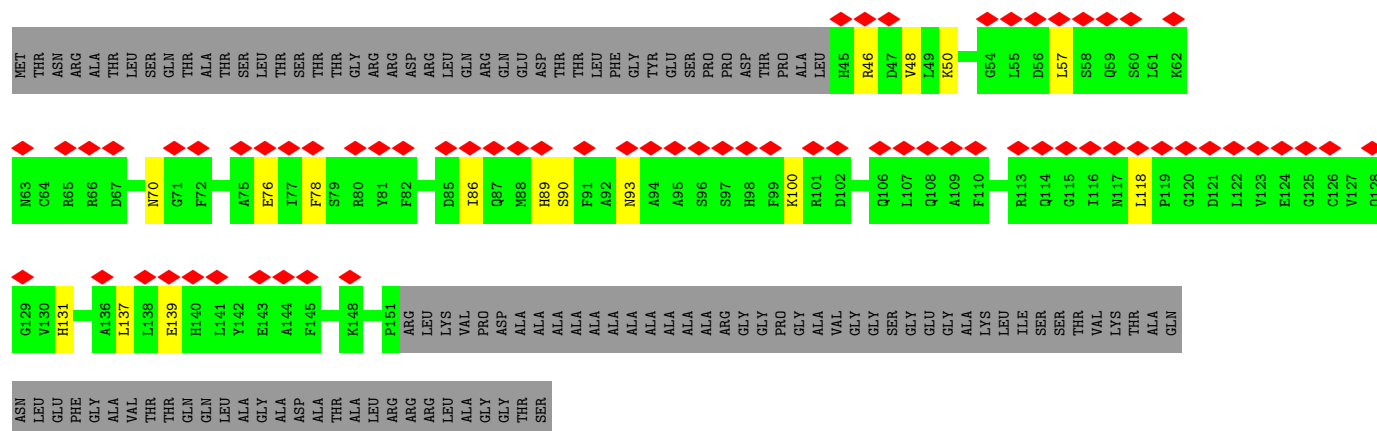
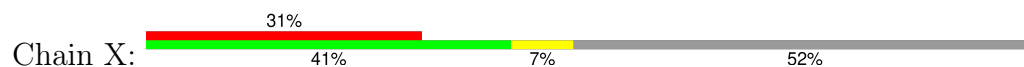
• Molecule 15: FAP225



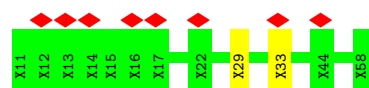
- Molecule 15: FAP225



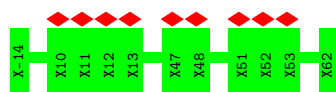
- Molecule 15: FAP225



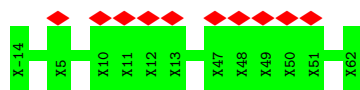
- Molecule 16: FAP239



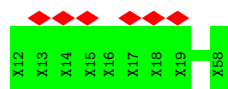
- Molecule 17: FAP388



- Molecule 17: FAP388



- Molecule 18: FAP424



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	104806	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	39.6	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.998	Depositor
Minimum map value	0.000	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.050	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	711.68, 711.68, 711.68	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.39, 1.39, 1.39	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, MG, 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	AA	0.15	0/3453	0.36	0/4673
1	AC	0.15	0/3444	0.37	0/4661
1	AE	0.17	0/3453	0.41	0/4673
1	AG	0.18	0/3453	0.40	0/4673
1	AI	0.15	0/3453	0.36	0/4673
1	AK	0.14	0/3453	0.35	0/4673
1	BA	0.14	0/3462	0.36	0/4685
1	BC	0.15	0/3428	0.35	0/4639
1	BE	0.17	0/3462	0.38	0/4685
1	BG	0.17	0/3428	0.40	1/4639 (0.0%)
1	BI	0.15	0/3462	0.36	0/4685
1	BK	0.14	0/3428	0.38	0/4639
1	CA	0.14	0/3428	0.35	0/4639
1	CC	0.16	0/3428	0.38	0/4639
1	CE	0.17	0/3428	0.38	0/4639
1	CG	0.17	0/3428	0.37	0/4639
1	CI	0.15	0/3428	0.37	0/4639
1	CK	0.15	0/3428	0.36	0/4639
1	DC	0.15	0/3428	0.35	0/4639
1	DE	0.16	0/3428	0.37	0/4639
1	DG	0.18	0/3428	0.36	0/4639
1	DI	0.17	0/3428	0.40	1/4639 (0.0%)
1	DK	0.15	0/3428	0.38	0/4639
1	EA	0.14	0/3428	0.35	0/4639
1	EC	0.14	0/3428	0.37	1/4639 (0.0%)
1	EE	0.17	0/3428	0.37	1/4639 (0.0%)
1	EG	0.17	0/3428	0.39	0/4639
1	EI	0.15	0/3428	0.35	0/4639
1	EK	0.15	0/3428	0.38	0/4639
1	FA	0.15	0/3428	0.37	0/4639
1	FC	0.15	0/3428	0.35	0/4639
1	FE	0.17	0/3428	0.40	0/4639

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	FG	0.16	0/3428	0.37	0/4639
1	FI	0.15	0/3428	0.35	0/4639
1	FK	0.15	0/3428	0.38	2/4639 (0.0%)
1	GC	0.15	0/3428	0.36	0/4639
1	GE	0.15	0/3428	0.36	0/4639
1	GG	0.16	0/3428	0.42	1/4639 (0.0%)
1	GI	0.16	0/3428	0.37	1/4639 (0.0%)
1	GK	0.15	0/3428	0.37	0/4639
1	GM	0.14	0/3428	0.37	0/4639
1	HC	0.14	0/3428	0.37	0/4639
1	HE	0.15	0/3428	0.39	0/4639
1	HG	0.17	0/3428	0.41	0/4639
1	HI	0.15	0/3428	0.40	0/4639
1	HK	0.14	0/3428	0.38	0/4639
1	HM	0.14	0/3428	0.38	0/4639
1	IC	0.14	0/3428	0.37	0/4639
1	IE	0.15	0/3428	0.39	0/4639
1	IG	0.16	0/3428	0.39	0/4639
1	II	0.16	0/3428	0.38	0/4639
1	IK	0.15	0/3428	0.35	0/4639
1	IM	0.14	0/3428	0.37	0/4639
1	JC	0.13	0/3428	0.36	1/4639 (0.0%)
1	JE	0.15	0/3428	0.38	0/4639
1	JG	0.15	0/3428	0.36	0/4639
1	JI	0.18	0/3420	0.41	0/4628
1	JK	0.15	0/3428	0.38	0/4639
1	JM	0.14	0/3420	0.36	0/4628
1	KC	0.15	0/3428	0.36	0/4639
1	KE	0.16	0/3428	0.39	0/4639
1	KG	0.17	0/3428	0.38	0/4639
1	KI	0.17	0/3428	0.40	0/4639
1	KK	0.14	0/3428	0.36	0/4639
1	LC	0.15	0/3428	0.35	0/4639
1	LE	0.16	0/3428	0.38	1/4639 (0.0%)
1	LG	0.16	0/3428	0.37	1/4639 (0.0%)
1	LI	0.17	0/3428	0.39	0/4639
1	LK	0.13	0/3428	0.35	0/4639
1	MC	0.15	0/3453	0.36	0/4673
1	ME	0.16	0/3428	0.39	0/4639
1	MG	0.17	0/3453	0.37	0/4673
1	MI	0.17	0/3428	0.37	0/4639
1	MK	0.16	0/3453	0.37	0/4673
2	AB	0.15	0/3426	0.38	0/4644

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	AD	0.14	0/3426	0.36	0/4644
2	AF	0.16	0/3426	0.38	0/4644
2	AH	0.17	0/3412	0.40	0/4625
2	AJ	0.14	0/3426	0.34	0/4644
2	AL	0.13	0/3412	0.35	0/4625
2	BB	0.14	0/3465	0.38	0/4697
2	BD	0.15	0/3412	0.37	0/4625
2	BF	0.17	0/3465	0.42	2/4697 (0.0%)
2	BH	0.16	0/3412	0.39	0/4625
2	BJ	0.15	0/3465	0.40	0/4697
2	BL	0.14	0/3412	0.37	0/4625
2	CB	0.15	0/3406	0.37	0/4617
2	CD	0.16	0/3406	0.38	0/4617
2	CF	0.15	0/3406	0.37	0/4617
2	CH	0.16	0/3406	0.40	0/4617
2	CJ	0.15	0/3412	0.37	0/4625
2	DB	0.16	0/3412	0.39	0/4625
2	DD	0.16	0/3406	0.39	0/4617
2	DF	0.17	0/3412	0.39	0/4625
2	DH	0.17	0/3412	0.38	0/4625
2	DJ	0.14	0/3412	0.37	0/4625
2	DL	0.15	0/3412	0.38	0/4625
2	EB	0.15	0/3465	0.37	0/4697
2	ED	0.14	0/3406	0.38	0/4617
2	EF	0.16	0/3471	0.37	0/4705
2	EH	0.17	0/3406	0.38	0/4617
2	EJ	0.15	0/3465	0.38	0/4697
2	EL	0.14	0/3406	0.37	0/4617
2	FB	0.14	0/3412	0.37	0/4625
2	FD	0.14	0/3412	0.37	0/4625
2	FF	0.16	0/3412	0.38	0/4625
2	FH	0.17	0/3412	0.41	0/4625
2	FJ	0.14	0/3412	0.38	0/4625
2	FL	0.14	0/3412	0.37	0/4625
2	GD	0.15	0/3412	0.40	0/4625
2	GF	0.15	0/3412	0.41	0/4625
2	GH	0.16	0/3412	0.39	0/4625
2	GJ	0.16	0/3412	0.40	0/4625
2	GL	0.15	0/3412	0.38	0/4625
2	HD	0.15	0/3412	0.38	0/4625
2	HF	0.14	0/3412	0.39	0/4625
2	HH	0.15	0/3412	0.39	0/4625
2	HJ	0.14	0/3397	0.39	0/4605

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	HL	0.14	0/3412	0.36	0/4625
2	ID	0.15	0/3406	0.40	0/4617
2	IF	0.15	0/3412	0.39	0/4625
2	IH	0.15	0/3406	0.37	0/4617
2	IJ	0.15	0/3412	0.38	0/4625
2	IL	0.14	0/3406	0.40	0/4617
2	JB	0.14	0/3412	0.38	0/4625
2	JD	0.14	0/3412	0.36	0/4625
2	JF	0.16	0/3412	0.37	0/4625
2	JH	0.16	0/3412	0.37	0/4625
2	JJ	0.15	0/3406	0.38	0/4617
2	JL	0.15	0/3406	0.39	0/4617
2	KB	0.14	0/3406	0.36	0/4617
2	KD	0.15	0/3412	0.38	0/4625
2	KF	0.16	0/3406	0.38	0/4617
2	KH	0.17	0/3412	0.40	0/4625
2	KJ	0.14	0/3406	0.38	0/4617
2	KL	0.15	0/3412	0.37	0/4625
2	LB	0.14	0/3412	0.37	0/4625
2	LD	0.15	0/3412	0.39	0/4625
2	LF	0.16	0/3412	0.39	0/4625
2	LH	0.16	0/3412	0.39	0/4625
2	LJ	0.15	0/3412	0.37	0/4625
2	LL	0.14	0/3412	0.35	0/4625
2	MB	0.14	0/3412	0.36	0/4625
2	MD	0.15	0/3471	0.36	0/4705
2	MF	0.17	0/3412	0.39	0/4625
2	MH	0.17	0/3476	0.38	0/4712
2	MJ	0.15	0/3412	0.36	0/4625
2	ML	0.15	0/3476	0.39	0/4712
3	a	0.15	0/2428	0.43	0/3300
3	b	0.19	0/4634	0.53	1/6298 (0.0%)
3	c	0.20	0/4634	0.56	4/6298 (0.1%)
3	d	0.21	0/2228	0.60	3/3026 (0.1%)
4	e	0.17	0/1484	0.41	0/1994
4	f	0.15	0/1484	0.36	0/1994
4	g	0.16	0/1154	0.38	0/1553
5	h	0.16	0/4608	0.41	0/6234
5	i	0.17	0/4608	0.42	0/6234
5	j	0.15	0/4608	0.40	0/6234
6	k	0.17	0/3072	0.45	0/4147
6	l	0.16	0/3072	0.46	0/4147
6	s	0.16	0/2253	0.42	0/3048

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
7	m	0.15	0/2808	0.44	0/3798
7	n	0.18	0/2808	0.51	0/3798
7	o	0.16	0/2808	0.43	0/3798
8	p	0.14	0/714	0.46	0/962
8	q	0.16	0/714	0.42	0/962
8	r	0.13	0/714	0.37	0/962
9	A	0.15	0/1564	0.43	0/2113
9	B	0.15	0/1564	0.42	0/2113
9	C	0.15	0/1564	0.43	0/2113
10	P	0.15	0/2503	0.40	0/3420
10	Q	0.15	0/2498	0.39	0/3413
10	R	0.16	0/2503	0.39	0/3420
10	S	0.15	0/2498	0.41	0/3413
10	Z	0.09	0/786	0.29	0/1041
10	aa	0.09	0/1434	0.30	0/1989
10	cc	0.09	0/769	0.28	0/1018
11	T	0.11	0/310	0.34	0/429
11	U	0.12	0/285	0.30	0/394
11	V	0.13	0/331	0.40	0/460
11	W	0.10	0/311	0.30	0/432
12	D	0.12	0/7465	0.30	0/10373
12	E	0.13	0/7465	0.31	0/10373
12	bb	0.18	0/1076	0.44	0/1482
13	F	0.12	0/4827	0.33	0/6703
13	G	0.12	0/4880	0.33	0/6777
13	H	0.13	0/4827	0.35	0/6703
13	I	0.13	0/4880	0.34	1/6777 (0.0%)
14	J	0.14	0/3904	0.35	0/5372
14	K	0.14	0/3904	0.37	0/5372
15	L	0.13	0/861	0.37	0/1163
15	M	0.13	0/861	0.34	0/1163
15	N	0.14	0/861	0.36	0/1163
15	O	0.13	0/861	0.35	0/1163
15	X	0.14	0/861	0.37	0/1163
15	Y	0.13	0/861	0.37	0/1163
All	All	0.15	0/625065	0.38	22/848033 (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
2	DB	0	1
2	DF	0	1
2	GD	0	1
2	HD	0	1
2	HL	0	1
2	KD	0	1
2	KH	0	1
2	KL	0	1
3	c	0	1
3	d	0	1
13	G	0	1
13	H	0	1
13	I	0	1
All	All	0	13

There are no bond length outliers.

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BG	47	ILE	N-CA-C	-6.72	106.24	112.96
1	DI	47	ILE	N-CA-C	-6.31	106.03	113.42
1	EC	47	ILE	N-CA-C	-6.25	106.70	112.96
1	EE	47	ILE	N-CA-C	-6.04	106.92	112.96
3	c	404	THR	N-CA-C	-5.92	100.30	109.24

There are no chirality outliers.

5 of 13 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	DB	401	LYS	Peptide
2	DF	273	ALA	Peptide
2	GD	273	ALA	Peptide
2	HD	273	ALA	Peptide
2	HL	273	ALA	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	3379	0	3265	53	0
1	AC	3370	0	3259	54	0
1	AE	3379	0	3265	56	0
1	AG	3379	0	3265	70	0
1	AI	3379	0	3265	51	0
1	AK	3379	0	3265	49	0
1	BA	3388	0	3271	43	0
1	BC	3354	0	3244	70	0
1	BE	3388	0	3271	58	0
1	BG	3354	0	3244	69	0
1	BI	3388	0	3271	64	0
1	BK	3354	0	3244	64	0
1	CA	3354	0	3244	49	0
1	CC	3354	0	3244	62	0
1	CE	3354	0	3244	62	0
1	CG	3354	0	3244	59	0
1	CI	3354	0	3244	59	0
1	CK	3354	0	3244	36	0
1	DC	3354	0	3244	47	0
1	DE	3354	0	3244	51	0
1	DG	3354	0	3244	70	0
1	DI	3354	0	3244	55	0
1	DK	3354	0	3244	49	0
1	EA	3354	0	3244	38	0
1	EC	3354	0	3244	52	0
1	EE	3354	0	3244	72	0
1	EG	3354	0	3244	57	0
1	EI	3354	0	3244	61	0
1	EK	3354	0	3244	54	0
1	FA	3354	0	3244	65	0
1	FC	3354	0	3244	61	0
1	FE	3354	0	3244	54	0
1	FG	3354	0	3244	61	0
1	FI	3354	0	3244	64	0
1	FK	3354	0	3244	69	0
1	GC	3354	0	3244	48	0
1	GE	3354	0	3244	55	0
1	GG	3354	0	3244	61	0
1	GI	3354	0	3244	60	0
1	GK	3354	0	3244	56	0
1	GM	3354	0	3244	48	0
1	HC	3354	0	3244	66	0
1	HE	3354	0	3244	64	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	HG	3354	0	3244	64	0
1	HI	3354	0	3242	55	0
1	HK	3354	0	3244	56	0
1	HM	3354	0	3244	60	0
1	IC	3354	0	3244	52	0
1	IE	3354	0	3244	73	0
1	IG	3354	0	3244	64	0
1	II	3354	0	3244	69	0
1	IK	3354	0	3244	69	0
1	IM	3354	0	3244	57	0
1	JC	3354	0	3243	61	0
1	JE	3354	0	3244	62	0
1	JG	3354	0	3244	55	0
1	JI	3346	0	3240	75	0
1	JK	3354	0	3244	59	0
1	JM	3346	0	3240	55	0
1	KC	3354	0	3244	61	0
1	KE	3354	0	3244	67	0
1	KG	3354	0	3244	50	0
1	KI	3354	0	3244	53	0
1	KK	3354	0	3244	57	0
1	LC	3354	0	3244	51	0
1	LE	3354	0	3244	60	0
1	LG	3354	0	3244	46	0
1	LI	3354	0	3244	55	0
1	LK	3354	0	3244	51	0
1	MC	3379	0	3265	57	0
1	ME	3354	0	3244	46	0
1	MG	3379	0	3265	59	0
1	MI	3354	0	3244	49	0
1	MK	3379	0	3265	48	0
2	AB	3355	0	3293	56	0
2	AD	3355	0	3291	51	0
2	AF	3355	0	3293	48	0
2	AH	3341	0	3282	42	0
2	AJ	3355	0	3293	53	0
2	AL	3341	0	3282	46	0
2	BB	3393	0	3331	49	0
2	BD	3341	0	3282	48	0
2	BF	3393	0	3331	58	0
2	BH	3341	0	3282	63	0
2	BJ	3393	0	3331	56	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	BL	3341	0	3282	44	0
2	CB	3335	0	3277	53	0
2	CD	3335	0	3277	52	0
2	CF	3335	0	3277	57	0
2	CH	3335	0	3277	56	0
2	CJ	3341	0	3282	42	0
2	DB	3341	0	3282	52	0
2	DD	3335	0	3277	55	0
2	DF	3341	0	3282	63	0
2	DH	3341	0	3282	52	0
2	DJ	3341	0	3282	43	0
2	DL	3341	0	3282	43	0
2	EB	3393	0	3331	44	0
2	ED	3335	0	3277	61	0
2	EF	3399	0	3336	52	0
2	EH	3335	0	3277	52	0
2	EJ	3393	0	3331	52	0
2	EL	3335	0	3277	39	0
2	FB	3341	0	3282	45	0
2	FD	3341	0	3282	44	0
2	FF	3341	0	3282	42	0
2	FH	3341	0	3282	48	0
2	FJ	3341	0	3282	49	0
2	FL	3341	0	3282	45	0
2	GD	3341	0	3282	39	0
2	GF	3341	0	3282	63	0
2	GH	3341	0	3282	42	0
2	GJ	3341	0	3282	52	0
2	GL	3341	0	3282	55	0
2	HD	3341	0	3282	55	0
2	HF	3341	0	3282	64	0
2	HH	3341	0	3282	53	0
2	HJ	3326	0	3271	63	0
2	HL	3341	0	3282	65	0
2	ID	3335	0	3277	63	0
2	IF	3341	0	3282	62	0
2	IH	3335	0	3277	58	0
2	IJ	3341	0	3282	67	0
2	IL	3335	0	3277	56	0
2	JB	3341	0	3282	48	0
2	JD	3341	0	3282	40	0
2	JF	3341	0	3282	62	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	JH	3341	0	3282	40	0
2	JJ	3335	0	3277	64	0
2	JL	3335	0	3277	51	0
2	KB	3335	0	3277	52	0
2	KD	3341	0	3282	44	0
2	KF	3335	0	3277	53	0
2	KH	3341	0	3282	40	0
2	KJ	3335	0	3277	66	0
2	KL	3341	0	3282	48	0
2	LB	3341	0	3282	57	0
2	LD	3341	0	3282	33	0
2	LF	3341	0	3282	36	0
2	LH	3341	0	3282	37	0
2	LJ	3341	0	3282	45	0
2	LL	3341	0	3282	30	0
2	MB	3341	0	3282	38	0
2	MD	3399	0	3336	55	0
2	MF	3341	0	3282	49	0
2	MH	3404	0	3341	53	0
2	MJ	3341	0	3282	36	0
2	ML	3404	0	3341	44	0
3	a	2380	0	2348	41	0
3	b	4537	0	4426	106	0
3	c	4537	0	4426	102	0
3	d	2180	0	2098	52	0
4	e	1464	0	1434	28	0
4	f	1464	0	1434	28	0
4	g	1136	0	1104	10	0
5	h	4525	0	4445	73	0
5	i	4525	0	4445	59	0
5	j	4525	0	4445	71	0
6	k	3017	0	2979	40	0
6	l	3017	0	2979	65	0
6	s	2208	0	2181	27	0
7	m	2737	0	2635	54	0
7	n	2737	0	2635	54	0
7	o	2737	0	2635	51	0
8	p	698	0	692	7	0
8	q	698	0	692	11	0
8	r	698	0	692	7	0
9	A	1530	0	1544	35	0
9	B	1530	0	1544	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	C	1530	0	1544	22	0
10	P	2493	0	1678	16	0
10	Q	2488	0	1673	12	0
10	R	2493	0	1678	24	0
10	S	2488	0	1673	19	0
10	Z	775	0	813	6	0
10	aa	1435	0	688	4	0
10	cc	758	0	794	4	0
11	T	312	0	143	0	0
11	U	287	0	133	0	0
11	V	332	0	150	0	0
11	W	312	0	142	0	0
12	D	7474	0	3576	21	0
12	E	7474	0	3576	22	0
12	bb	1065	0	775	10	0
13	F	4832	0	2578	12	0
13	G	4884	0	2623	11	0
13	H	4832	0	2578	13	0
13	I	4884	0	2623	11	0
14	J	3874	0	2852	31	0
14	K	3874	0	2852	35	0
15	L	841	0	820	9	0
15	M	841	0	820	10	0
15	N	841	0	820	10	0
15	O	841	0	820	11	0
15	X	841	0	820	11	0
15	Y	841	0	820	8	0
16	A1	240	0	50	1	0
17	A2	385	0	87	0	0
17	A4	385	0	88	0	0
18	A3	235	0	50	0	0
19	AA	28	0	12	0	0
19	AC	28	0	12	2	0
19	AE	28	0	12	2	0
19	AG	28	0	12	2	0
19	AI	28	0	12	1	0
19	AK	28	0	12	1	0
19	BA	28	0	12	2	0
19	BC	28	0	12	0	0
19	BE	28	0	12	0	0
19	BG	28	0	12	1	0
19	BI	28	0	12	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	BK	28	0	12	0	0
19	CA	28	0	12	1	0
19	CC	28	0	12	1	0
19	CE	28	0	12	0	0
19	CG	28	0	12	2	0
19	CI	28	0	12	0	0
19	CK	28	0	12	1	0
19	DC	28	0	12	0	0
19	DE	28	0	12	1	0
19	DG	28	0	12	1	0
19	DI	28	0	12	0	0
19	DK	28	0	12	1	0
19	EA	28	0	12	1	0
19	EC	28	0	12	3	0
19	EE	28	0	12	2	0
19	EG	28	0	12	2	0
19	EI	28	0	12	1	0
19	EK	28	0	12	0	0
19	FA	28	0	12	2	0
19	FC	28	0	12	0	0
19	FE	28	0	12	0	0
19	FG	28	0	12	0	0
19	FI	28	0	12	1	0
19	FK	28	0	12	0	0
19	GC	28	0	12	1	0
19	GE	28	0	12	2	0
19	GG	28	0	12	2	0
19	GI	28	0	12	1	0
19	GK	28	0	12	2	0
19	GM	28	0	12	0	0
19	HC	28	0	12	2	0
19	HE	28	0	12	2	0
19	HG	28	0	12	1	0
19	HI	28	0	12	3	0
19	HK	28	0	12	2	0
19	HM	28	0	12	2	0
19	IC	28	0	12	2	0
19	IE	28	0	12	1	0
19	IG	28	0	12	1	0
19	II	28	0	12	1	0
19	IK	28	0	12	2	0
19	IM	28	0	12	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	JC	28	0	12	1	0
19	JE	28	0	12	1	0
19	JG	28	0	12	1	0
19	JI	28	0	12	1	0
19	JK	28	0	12	0	0
19	JM	28	0	12	0	0
19	KC	28	0	12	1	0
19	KE	28	0	12	3	0
19	KG	28	0	12	1	0
19	KI	28	0	12	0	0
19	KK	28	0	12	2	0
19	LC	28	0	12	1	0
19	LE	28	0	12	2	0
19	LG	28	0	12	1	0
19	LI	28	0	12	1	0
19	LK	28	0	12	0	0
19	MC	28	0	12	1	0
19	ME	28	0	12	0	0
19	MG	28	0	12	2	0
19	MI	28	0	12	0	0
19	MK	28	0	12	1	0
20	AB	32	0	12	0	0
20	AD	32	0	12	1	0
20	AF	32	0	12	1	0
20	AH	32	0	12	0	0
20	AJ	32	0	12	0	0
20	AL	32	0	12	0	0
20	BB	32	0	12	1	0
20	BD	32	0	12	1	0
20	BF	32	0	12	1	0
20	BH	32	0	12	1	0
20	BJ	32	0	12	1	0
20	BL	32	0	12	1	0
20	CB	32	0	12	3	0
20	CD	32	0	12	1	0
20	CF	32	0	12	3	0
20	CH	32	0	12	1	0
20	CJ	32	0	12	2	0
20	DB	32	0	12	1	0
20	DD	32	0	12	1	0
20	DF	32	0	12	2	0
20	DH	32	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	DJ	32	0	12	2	0
20	DL	32	0	12	1	0
20	EB	32	0	12	0	0
20	ED	32	0	12	0	0
20	EF	32	0	12	1	0
20	EH	32	0	12	1	0
20	EJ	32	0	12	1	0
20	EL	32	0	12	1	0
20	FB	32	0	12	0	0
20	FD	32	0	12	0	0
20	FF	32	0	12	0	0
20	FH	32	0	12	1	0
20	FJ	32	0	12	0	0
20	FL	32	0	12	1	0
20	GD	32	0	12	2	0
20	GF	32	0	12	2	0
20	GH	32	0	12	3	0
20	GJ	32	0	12	1	0
20	GL	32	0	12	3	0
20	HD	32	0	12	2	0
20	HF	32	0	12	2	0
20	HI	32	0	12	2	0
20	HJ	32	0	12	2	0
20	HL	32	0	12	3	0
20	ID	32	0	12	1	0
20	IF	32	0	12	2	0
20	IH	32	0	12	2	0
20	IJ	32	0	12	2	0
20	IL	32	0	12	2	0
20	JB	32	0	12	1	0
20	JD	32	0	12	2	0
20	JF	32	0	12	1	0
20	JH	32	0	12	1	0
20	JJ	32	0	12	0	0
20	JL	32	0	12	1	0
20	KB	32	0	12	1	0
20	KD	32	0	12	2	0
20	KF	32	0	12	2	0
20	KH	32	0	12	0	0
20	KJ	32	0	12	1	0
20	KL	32	0	12	0	0
20	LB	32	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	LD	32	0	12	1	0
20	LF	32	0	12	1	0
20	LH	32	0	12	1	0
20	LJ	32	0	12	1	0
20	LL	32	0	12	0	0
20	MB	32	0	12	0	0
20	MD	32	0	12	3	0
20	MF	32	0	12	1	0
20	MH	32	0	12	0	0
20	MJ	32	0	12	2	0
20	ML	32	0	12	2	0
21	AB	1	0	0	0	0
21	AD	1	0	0	0	0
21	AF	1	0	0	0	0
21	AH	1	0	0	0	0
21	AJ	1	0	0	0	0
21	AL	1	0	0	0	0
21	BB	1	0	0	0	0
21	BD	1	0	0	0	0
21	BF	1	0	0	0	0
21	BH	1	0	0	0	0
21	BJ	1	0	0	0	0
21	BL	1	0	0	0	0
21	CB	1	0	0	0	0
21	CD	1	0	0	0	0
21	CF	1	0	0	0	0
21	CH	1	0	0	0	0
21	CJ	1	0	0	0	0
21	DB	1	0	0	0	0
21	DD	1	0	0	0	0
21	DF	1	0	0	0	0
21	DH	1	0	0	0	0
21	DJ	1	0	0	0	0
21	DL	1	0	0	0	0
21	EB	1	0	0	0	0
21	EE	1	0	0	0	0
21	EF	1	0	0	0	0
21	EH	1	0	0	0	0
21	EJ	1	0	0	0	0
21	EL	1	0	0	0	0
21	FB	1	0	0	0	0
21	FD	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	FF	1	0	0	0	0
21	FH	1	0	0	0	0
21	FJ	1	0	0	0	0
21	FL	1	0	0	0	0
21	GD	1	0	0	0	0
21	GF	1	0	0	0	0
21	GH	1	0	0	0	0
21	GJ	1	0	0	0	0
21	GL	1	0	0	0	0
21	HD	1	0	0	0	0
21	HF	1	0	0	0	0
21	HH	1	0	0	0	0
21	HJ	1	0	0	0	0
21	HL	1	0	0	0	0
21	ID	1	0	0	0	0
21	IF	1	0	0	0	0
21	IH	1	0	0	0	0
21	IJ	1	0	0	0	0
21	IL	1	0	0	0	0
21	JB	1	0	0	0	0
21	JD	1	0	0	0	0
21	JF	1	0	0	0	0
21	JH	1	0	0	0	0
21	JJ	1	0	0	0	0
21	JL	1	0	0	0	0
21	KB	1	0	0	0	0
21	KD	1	0	0	0	0
21	KF	1	0	0	0	0
21	KI	1	0	0	0	0
21	KJ	1	0	0	0	0
21	KL	1	0	0	0	0
21	LB	1	0	0	0	0
21	LD	1	0	0	0	0
21	LF	1	0	0	0	0
21	LH	1	0	0	0	0
21	LJ	1	0	0	0	0
21	LL	1	0	0	0	0
21	MB	1	0	0	0	0
21	MD	1	0	0	0	0
21	MF	1	0	0	0	0
21	MH	1	0	0	0	0
21	MJ	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	ML	1	0	0	0	0
All	All	618760	0	577525	8163	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 7.

The worst 5 of 8163 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)
2:CF:259:LEU:HD21	2:CF:316:CYS:HB2	1.66	0.78
3:c:184:GLY:H	4:f:11:ARG:HH21	1.29	0.78
9:A:75:PHE:HB2	9:A:168:SER:O	1.84	0.78
2:MD:259:LEU:HD11	2:MD:316:CYS:HB2	1.67	0.76
1:DE:317:PHE:HB3	1:DE:321:MET:HE1	1.67	0.76

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AA	429/443 (97%)	417 (97%)	12 (3%)	0	100	100
1	AC	428/443 (97%)	412 (96%)	16 (4%)	0	100	100
1	AE	429/443 (97%)	414 (96%)	15 (4%)	0	100	100
1	AG	429/443 (97%)	417 (97%)	12 (3%)	0	100	100
1	AI	429/443 (97%)	416 (97%)	13 (3%)	0	100	100
1	AK	429/443 (97%)	415 (97%)	14 (3%)	0	100	100
1	BA	430/443 (97%)	421 (98%)	9 (2%)	0	100	100
1	BC	425/443 (96%)	416 (98%)	9 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	BE	430/443 (97%)	417 (97%)	13 (3%)	0	100	100
1	BG	425/443 (96%)	415 (98%)	10 (2%)	0	100	100
1	BI	430/443 (97%)	418 (97%)	12 (3%)	0	100	100
1	BK	425/443 (96%)	411 (97%)	14 (3%)	0	100	100
1	CA	425/443 (96%)	413 (97%)	12 (3%)	0	100	100
1	CC	425/443 (96%)	410 (96%)	15 (4%)	0	100	100
1	CE	425/443 (96%)	416 (98%)	9 (2%)	0	100	100
1	CG	425/443 (96%)	411 (97%)	14 (3%)	0	100	100
1	CI	425/443 (96%)	415 (98%)	10 (2%)	0	100	100
1	CK	425/443 (96%)	410 (96%)	15 (4%)	0	100	100
1	DC	425/443 (96%)	415 (98%)	10 (2%)	0	100	100
1	DE	425/443 (96%)	413 (97%)	12 (3%)	0	100	100
1	DG	425/443 (96%)	415 (98%)	10 (2%)	0	100	100
1	DI	425/443 (96%)	411 (97%)	14 (3%)	0	100	100
1	DK	425/443 (96%)	412 (97%)	13 (3%)	0	100	100
1	EA	425/443 (96%)	413 (97%)	12 (3%)	0	100	100
1	EC	425/443 (96%)	410 (96%)	15 (4%)	0	100	100
1	EE	425/443 (96%)	409 (96%)	16 (4%)	0	100	100
1	EG	425/443 (96%)	412 (97%)	13 (3%)	0	100	100
1	EI	425/443 (96%)	415 (98%)	10 (2%)	0	100	100
1	EK	425/443 (96%)	413 (97%)	12 (3%)	0	100	100
1	FA	425/443 (96%)	408 (96%)	17 (4%)	0	100	100
1	FC	425/443 (96%)	412 (97%)	13 (3%)	0	100	100
1	FE	425/443 (96%)	408 (96%)	17 (4%)	0	100	100
1	FG	425/443 (96%)	413 (97%)	12 (3%)	0	100	100
1	FI	425/443 (96%)	412 (97%)	13 (3%)	0	100	100
1	FK	425/443 (96%)	407 (96%)	18 (4%)	0	100	100
1	GC	425/443 (96%)	410 (96%)	15 (4%)	0	100	100
1	GE	425/443 (96%)	413 (97%)	12 (3%)	0	100	100
1	GG	425/443 (96%)	411 (97%)	14 (3%)	0	100	100
1	GI	425/443 (96%)	413 (97%)	12 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	GK	425/443 (96%)	413 (97%)	12 (3%)	0	100	100
1	GM	425/443 (96%)	409 (96%)	16 (4%)	0	100	100
1	HC	425/443 (96%)	411 (97%)	14 (3%)	0	100	100
1	HE	425/443 (96%)	405 (95%)	20 (5%)	0	100	100
1	HG	425/443 (96%)	408 (96%)	17 (4%)	0	100	100
1	HI	425/443 (96%)	414 (97%)	11 (3%)	0	100	100
1	HK	425/443 (96%)	414 (97%)	11 (3%)	0	100	100
1	HM	425/443 (96%)	407 (96%)	18 (4%)	0	100	100
1	IC	425/443 (96%)	414 (97%)	11 (3%)	0	100	100
1	IE	425/443 (96%)	409 (96%)	16 (4%)	0	100	100
1	IG	425/443 (96%)	414 (97%)	11 (3%)	0	100	100
1	II	425/443 (96%)	411 (97%)	14 (3%)	0	100	100
1	IK	425/443 (96%)	413 (97%)	12 (3%)	0	100	100
1	IM	425/443 (96%)	409 (96%)	16 (4%)	0	100	100
1	JC	425/443 (96%)	409 (96%)	16 (4%)	0	100	100
1	JE	425/443 (96%)	409 (96%)	16 (4%)	0	100	100
1	JG	425/443 (96%)	413 (97%)	12 (3%)	0	100	100
1	JI	424/443 (96%)	407 (96%)	17 (4%)	0	100	100
1	JK	425/443 (96%)	411 (97%)	14 (3%)	0	100	100
1	JM	424/443 (96%)	412 (97%)	12 (3%)	0	100	100
1	KC	425/443 (96%)	410 (96%)	15 (4%)	0	100	100
1	KE	425/443 (96%)	414 (97%)	11 (3%)	0	100	100
1	KG	425/443 (96%)	413 (97%)	12 (3%)	0	100	100
1	KI	425/443 (96%)	408 (96%)	17 (4%)	0	100	100
1	KK	425/443 (96%)	412 (97%)	13 (3%)	0	100	100
1	LC	425/443 (96%)	414 (97%)	11 (3%)	0	100	100
1	LE	425/443 (96%)	412 (97%)	13 (3%)	0	100	100
1	LG	425/443 (96%)	411 (97%)	14 (3%)	0	100	100
1	LI	425/443 (96%)	414 (97%)	11 (3%)	0	100	100
1	LK	425/443 (96%)	412 (97%)	13 (3%)	0	100	100
1	MC	429/443 (97%)	413 (96%)	16 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	ME	425/443 (96%)	406 (96%)	19 (4%)	0	100	100
1	MG	429/443 (97%)	414 (96%)	15 (4%)	0	100	100
1	MI	425/443 (96%)	409 (96%)	16 (4%)	0	100	100
1	MK	429/443 (97%)	418 (97%)	11 (3%)	0	100	100
2	AB	428/451 (95%)	415 (97%)	13 (3%)	0	100	100
2	AD	428/451 (95%)	411 (96%)	17 (4%)	0	100	100
2	AF	428/451 (95%)	413 (96%)	15 (4%)	0	100	100
2	AH	426/451 (94%)	411 (96%)	15 (4%)	0	100	100
2	AJ	428/451 (95%)	418 (98%)	10 (2%)	0	100	100
2	AL	426/451 (94%)	414 (97%)	12 (3%)	0	100	100
2	BB	436/451 (97%)	422 (97%)	14 (3%)	0	100	100
2	BD	426/451 (94%)	412 (97%)	14 (3%)	0	100	100
2	BF	436/451 (97%)	418 (96%)	18 (4%)	0	100	100
2	BH	426/451 (94%)	408 (96%)	18 (4%)	0	100	100
2	BJ	436/451 (97%)	420 (96%)	16 (4%)	0	100	100
2	BL	426/451 (94%)	411 (96%)	15 (4%)	0	100	100
2	CB	425/451 (94%)	409 (96%)	16 (4%)	0	100	100
2	CD	425/451 (94%)	413 (97%)	12 (3%)	0	100	100
2	CF	425/451 (94%)	411 (97%)	14 (3%)	0	100	100
2	CH	425/451 (94%)	410 (96%)	15 (4%)	0	100	100
2	CJ	426/451 (94%)	412 (97%)	14 (3%)	0	100	100
2	DB	426/451 (94%)	411 (96%)	15 (4%)	0	100	100
2	DD	425/451 (94%)	412 (97%)	13 (3%)	0	100	100
2	DF	426/451 (94%)	408 (96%)	18 (4%)	0	100	100
2	DH	426/451 (94%)	414 (97%)	12 (3%)	0	100	100
2	DJ	426/451 (94%)	412 (97%)	14 (3%)	0	100	100
2	DL	426/451 (94%)	413 (97%)	13 (3%)	0	100	100
2	EB	436/451 (97%)	421 (97%)	15 (3%)	0	100	100
2	ED	425/451 (94%)	407 (96%)	18 (4%)	0	100	100
2	EF	437/451 (97%)	419 (96%)	17 (4%)	1 (0%)	43	72
2	EH	425/451 (94%)	411 (97%)	14 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	EJ	436/451 (97%)	420 (96%)	16 (4%)	0	100	100
2	EL	425/451 (94%)	412 (97%)	13 (3%)	0	100	100
2	FB	426/451 (94%)	413 (97%)	13 (3%)	0	100	100
2	FD	426/451 (94%)	406 (95%)	20 (5%)	0	100	100
2	FF	426/451 (94%)	415 (97%)	11 (3%)	0	100	100
2	FH	426/451 (94%)	409 (96%)	17 (4%)	0	100	100
2	FJ	426/451 (94%)	409 (96%)	17 (4%)	0	100	100
2	FL	426/451 (94%)	413 (97%)	13 (3%)	0	100	100
2	GD	426/451 (94%)	411 (96%)	14 (3%)	1 (0%)	43	72
2	GF	426/451 (94%)	407 (96%)	19 (4%)	0	100	100
2	GH	426/451 (94%)	417 (98%)	9 (2%)	0	100	100
2	GJ	426/451 (94%)	409 (96%)	17 (4%)	0	100	100
2	GL	426/451 (94%)	409 (96%)	17 (4%)	0	100	100
2	HD	426/451 (94%)	412 (97%)	13 (3%)	1 (0%)	43	72
2	HF	426/451 (94%)	409 (96%)	17 (4%)	0	100	100
2	HH	426/451 (94%)	409 (96%)	17 (4%)	0	100	100
2	HJ	424/451 (94%)	406 (96%)	18 (4%)	0	100	100
2	HL	426/451 (94%)	412 (97%)	14 (3%)	0	100	100
2	ID	425/451 (94%)	411 (97%)	14 (3%)	0	100	100
2	IF	426/451 (94%)	415 (97%)	11 (3%)	0	100	100
2	IH	425/451 (94%)	408 (96%)	17 (4%)	0	100	100
2	IJ	426/451 (94%)	410 (96%)	16 (4%)	0	100	100
2	IL	425/451 (94%)	407 (96%)	18 (4%)	0	100	100
2	JB	426/451 (94%)	413 (97%)	13 (3%)	0	100	100
2	JD	426/451 (94%)	411 (96%)	15 (4%)	0	100	100
2	JF	426/451 (94%)	416 (98%)	10 (2%)	0	100	100
2	JH	426/451 (94%)	413 (97%)	13 (3%)	0	100	100
2	JJ	425/451 (94%)	411 (97%)	14 (3%)	0	100	100
2	JL	425/451 (94%)	408 (96%)	17 (4%)	0	100	100
2	KB	425/451 (94%)	410 (96%)	15 (4%)	0	100	100
2	KD	426/451 (94%)	414 (97%)	11 (3%)	1 (0%)	43	72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	KF	425/451 (94%)	410 (96%)	15 (4%)	0	100	100
2	KH	426/451 (94%)	411 (96%)	14 (3%)	1 (0%)	43	72
2	KJ	425/451 (94%)	406 (96%)	19 (4%)	0	100	100
2	KL	426/451 (94%)	415 (97%)	10 (2%)	1 (0%)	43	72
2	LB	426/451 (94%)	410 (96%)	16 (4%)	0	100	100
2	LD	426/451 (94%)	412 (97%)	14 (3%)	0	100	100
2	LF	426/451 (94%)	412 (97%)	14 (3%)	0	100	100
2	LH	426/451 (94%)	409 (96%)	17 (4%)	0	100	100
2	LJ	426/451 (94%)	412 (97%)	14 (3%)	0	100	100
2	LL	426/451 (94%)	412 (97%)	14 (3%)	0	100	100
2	MB	426/451 (94%)	407 (96%)	19 (4%)	0	100	100
2	MD	437/451 (97%)	422 (97%)	15 (3%)	0	100	100
2	MF	426/451 (94%)	414 (97%)	12 (3%)	0	100	100
2	MH	438/451 (97%)	422 (96%)	16 (4%)	0	100	100
2	MJ	426/451 (94%)	412 (97%)	14 (3%)	0	100	100
2	ML	438/451 (97%)	424 (97%)	14 (3%)	0	100	100
3	a	323/618 (52%)	295 (91%)	28 (9%)	0	100	100
3	b	615/618 (100%)	558 (91%)	55 (9%)	2 (0%)	36	65
3	c	615/618 (100%)	551 (90%)	62 (10%)	2 (0%)	36	65
3	d	293/618 (47%)	259 (88%)	32 (11%)	2 (1%)	18	50
4	e	182/201 (90%)	172 (94%)	10 (6%)	0	100	100
4	f	182/201 (90%)	170 (93%)	12 (7%)	0	100	100
4	g	143/201 (71%)	134 (94%)	9 (6%)	0	100	100
5	h	575/758 (76%)	549 (96%)	26 (4%)	0	100	100
5	i	575/758 (76%)	547 (95%)	28 (5%)	0	100	100
5	j	575/758 (76%)	546 (95%)	29 (5%)	0	100	100
6	k	380/528 (72%)	355 (93%)	25 (7%)	0	100	100
6	l	380/528 (72%)	357 (94%)	23 (6%)	0	100	100
6	s	279/528 (53%)	267 (96%)	12 (4%)	0	100	100
7	m	344/421 (82%)	319 (93%)	23 (7%)	2 (1%)	21	52
7	n	344/421 (82%)	311 (90%)	32 (9%)	1 (0%)	36	65

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	o	344/421 (82%)	323 (94%)	21 (6%)	0	100	100
8	p	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
8	q	86/89 (97%)	80 (93%)	6 (7%)	0	100	100
8	r	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
9	A	184/190 (97%)	175 (95%)	9 (5%)	0	100	100
9	B	184/190 (97%)	173 (94%)	11 (6%)	0	100	100
9	C	184/190 (97%)	173 (94%)	11 (6%)	0	100	100
10	P	427/606 (70%)	420 (98%)	6 (1%)	1 (0%)	43	72
10	Q	426/606 (70%)	415 (97%)	10 (2%)	1 (0%)	43	72
10	R	427/606 (70%)	418 (98%)	8 (2%)	1 (0%)	43	72
10	S	426/606 (70%)	417 (98%)	8 (2%)	1 (0%)	43	72
10	Z	90/606 (15%)	89 (99%)	1 (1%)	0	100	100
10	aa	290/606 (48%)	283 (98%)	6 (2%)	1 (0%)	36	65
10	cc	87/606 (14%)	87 (100%)	0	0	100	100
11	T	59/93 (63%)	55 (93%)	4 (7%)	0	100	100
11	U	54/93 (58%)	53 (98%)	1 (2%)	0	100	100
11	V	65/93 (70%)	60 (92%)	5 (8%)	0	100	100
11	W	61/93 (66%)	57 (93%)	4 (7%)	0	100	100
12	D	1498/2257 (66%)	1457 (97%)	40 (3%)	1 (0%)	48	78
12	E	1498/2257 (66%)	1459 (97%)	37 (2%)	2 (0%)	48	78
12	bb	171/2257 (8%)	161 (94%)	10 (6%)	0	100	100
13	F	972/1074 (90%)	931 (96%)	40 (4%)	1 (0%)	48	78
13	G	985/1074 (92%)	942 (96%)	41 (4%)	2 (0%)	43	72
13	H	972/1074 (90%)	938 (96%)	33 (3%)	1 (0%)	48	78
13	I	985/1074 (92%)	939 (95%)	43 (4%)	3 (0%)	36	65
14	J	654/976 (67%)	634 (97%)	19 (3%)	1 (0%)	43	72
14	K	654/976 (67%)	633 (97%)	20 (3%)	1 (0%)	43	72
15	L	105/222 (47%)	100 (95%)	5 (5%)	0	100	100
15	M	105/222 (47%)	101 (96%)	4 (4%)	0	100	100
15	N	105/222 (47%)	102 (97%)	3 (3%)	0	100	100
15	O	105/222 (47%)	101 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	X	105/222 (47%)	101 (96%)	4 (4%)	0	100	100
15	Y	105/222 (47%)	101 (96%)	4 (4%)	0	100	100
All	All	81498/94154 (87%)	78546 (96%)	2920 (4%)	32 (0%)	100	100

5 of 32 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	GD	274	PRO
2	HD	274	PRO
2	KD	274	PRO
2	KH	274	PRO
2	KL	274	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AA	370/379 (98%)	370 (100%)	0	100	100
1	AC	369/379 (97%)	369 (100%)	0	100	100
1	AE	370/379 (98%)	370 (100%)	0	100	100
1	AG	370/379 (98%)	369 (100%)	1 (0%)	86	83
1	AI	370/379 (98%)	370 (100%)	0	100	100
1	AK	370/379 (98%)	369 (100%)	1 (0%)	86	83
1	BA	371/379 (98%)	371 (100%)	0	100	100
1	BC	368/379 (97%)	368 (100%)	0	100	100
1	BE	371/379 (98%)	371 (100%)	0	100	100
1	BG	368/379 (97%)	368 (100%)	0	100	100
1	BI	371/379 (98%)	371 (100%)	0	100	100
1	BK	368/379 (97%)	368 (100%)	0	100	100
1	CA	368/379 (97%)	368 (100%)	0	100	100
1	CC	368/379 (97%)	368 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	CE	368/379 (97%)	368 (100%)	0	100	100
1	CG	368/379 (97%)	368 (100%)	0	100	100
1	CI	368/379 (97%)	368 (100%)	0	100	100
1	CK	368/379 (97%)	368 (100%)	0	100	100
1	DC	368/379 (97%)	368 (100%)	0	100	100
1	DE	368/379 (97%)	367 (100%)	1 (0%)	86	83
1	DG	368/379 (97%)	368 (100%)	0	100	100
1	DI	368/379 (97%)	368 (100%)	0	100	100
1	DK	368/379 (97%)	368 (100%)	0	100	100
1	EA	368/379 (97%)	368 (100%)	0	100	100
1	EC	368/379 (97%)	368 (100%)	0	100	100
1	EE	368/379 (97%)	368 (100%)	0	100	100
1	EG	368/379 (97%)	368 (100%)	0	100	100
1	EI	368/379 (97%)	368 (100%)	0	100	100
1	EK	368/379 (97%)	368 (100%)	0	100	100
1	FA	368/379 (97%)	368 (100%)	0	100	100
1	FC	368/379 (97%)	368 (100%)	0	100	100
1	FE	368/379 (97%)	367 (100%)	1 (0%)	86	83
1	FG	368/379 (97%)	368 (100%)	0	100	100
1	FI	368/379 (97%)	368 (100%)	0	100	100
1	FK	368/379 (97%)	368 (100%)	0	100	100
1	GC	368/379 (97%)	368 (100%)	0	100	100
1	GE	368/379 (97%)	368 (100%)	0	100	100
1	GG	368/379 (97%)	368 (100%)	0	100	100
1	GI	368/379 (97%)	368 (100%)	0	100	100
1	GK	368/379 (97%)	368 (100%)	0	100	100
1	GM	368/379 (97%)	367 (100%)	1 (0%)	86	83
1	HC	368/379 (97%)	368 (100%)	0	100	100
1	HE	368/379 (97%)	368 (100%)	0	100	100
1	HG	368/379 (97%)	368 (100%)	0	100	100
1	HI	368/379 (97%)	368 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	HK	368/379 (97%)	368 (100%)	0	100	100
1	HM	368/379 (97%)	368 (100%)	0	100	100
1	IC	368/379 (97%)	368 (100%)	0	100	100
1	IE	368/379 (97%)	368 (100%)	0	100	100
1	IG	368/379 (97%)	368 (100%)	0	100	100
1	II	368/379 (97%)	368 (100%)	0	100	100
1	IK	368/379 (97%)	368 (100%)	0	100	100
1	IM	368/379 (97%)	368 (100%)	0	100	100
1	JC	368/379 (97%)	367 (100%)	1 (0%)	86	83
1	JE	368/379 (97%)	367 (100%)	1 (0%)	86	83
1	JG	368/379 (97%)	368 (100%)	0	100	100
1	JI	367/379 (97%)	367 (100%)	0	100	100
1	JK	368/379 (97%)	368 (100%)	0	100	100
1	JM	367/379 (97%)	367 (100%)	0	100	100
1	KC	368/379 (97%)	368 (100%)	0	100	100
1	KE	368/379 (97%)	368 (100%)	0	100	100
1	KG	368/379 (97%)	368 (100%)	0	100	100
1	KI	368/379 (97%)	368 (100%)	0	100	100
1	KK	368/379 (97%)	368 (100%)	0	100	100
1	LC	368/379 (97%)	368 (100%)	0	100	100
1	LE	368/379 (97%)	367 (100%)	1 (0%)	86	83
1	LG	368/379 (97%)	368 (100%)	0	100	100
1	LI	368/379 (97%)	368 (100%)	0	100	100
1	LK	368/379 (97%)	368 (100%)	0	100	100
1	MC	370/379 (98%)	370 (100%)	0	100	100
1	ME	368/379 (97%)	368 (100%)	0	100	100
1	MG	370/379 (98%)	370 (100%)	0	100	100
1	MI	368/379 (97%)	368 (100%)	0	100	100
1	MK	370/379 (98%)	370 (100%)	0	100	100
2	AB	363/374 (97%)	363 (100%)	0	100	100
2	AD	364/374 (97%)	364 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AF	363/374 (97%)	363 (100%)	0	100	100
2	AH	362/374 (97%)	362 (100%)	0	100	100
2	AJ	363/374 (97%)	363 (100%)	0	100	100
2	AL	362/374 (97%)	362 (100%)	0	100	100
2	BB	367/374 (98%)	367 (100%)	0	100	100
2	BD	362/374 (97%)	362 (100%)	0	100	100
2	BF	367/374 (98%)	367 (100%)	0	100	100
2	BH	362/374 (97%)	362 (100%)	0	100	100
2	BJ	367/374 (98%)	367 (100%)	0	100	100
2	BL	362/374 (97%)	362 (100%)	0	100	100
2	CB	361/374 (96%)	361 (100%)	0	100	100
2	CD	361/374 (96%)	361 (100%)	0	100	100
2	CF	361/374 (96%)	361 (100%)	0	100	100
2	CH	361/374 (96%)	361 (100%)	0	100	100
2	CJ	362/374 (97%)	362 (100%)	0	100	100
2	DB	362/374 (97%)	362 (100%)	0	100	100
2	DD	361/374 (96%)	361 (100%)	0	100	100
2	DF	362/374 (97%)	362 (100%)	0	100	100
2	DH	362/374 (97%)	362 (100%)	0	100	100
2	DJ	362/374 (97%)	362 (100%)	0	100	100
2	DL	362/374 (97%)	362 (100%)	0	100	100
2	EB	367/374 (98%)	367 (100%)	0	100	100
2	ED	361/374 (96%)	361 (100%)	0	100	100
2	EF	368/374 (98%)	368 (100%)	0	100	100
2	EH	361/374 (96%)	361 (100%)	0	100	100
2	EJ	367/374 (98%)	367 (100%)	0	100	100
2	EL	361/374 (96%)	361 (100%)	0	100	100
2	FB	362/374 (97%)	362 (100%)	0	100	100
2	FD	362/374 (97%)	362 (100%)	0	100	100
2	FF	362/374 (97%)	362 (100%)	0	100	100
2	FH	362/374 (97%)	362 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	FJ	362/374 (97%)	362 (100%)	0	100	100
2	FL	362/374 (97%)	362 (100%)	0	100	100
2	GD	362/374 (97%)	362 (100%)	0	100	100
2	GF	362/374 (97%)	362 (100%)	0	100	100
2	GH	362/374 (97%)	362 (100%)	0	100	100
2	GJ	362/374 (97%)	362 (100%)	0	100	100
2	GL	362/374 (97%)	362 (100%)	0	100	100
2	HD	362/374 (97%)	362 (100%)	0	100	100
2	HF	362/374 (97%)	362 (100%)	0	100	100
2	HH	362/374 (97%)	362 (100%)	0	100	100
2	HJ	360/374 (96%)	360 (100%)	0	100	100
2	HL	362/374 (97%)	362 (100%)	0	100	100
2	ID	361/374 (96%)	361 (100%)	0	100	100
2	IF	362/374 (97%)	362 (100%)	0	100	100
2	IH	361/374 (96%)	361 (100%)	0	100	100
2	IJ	362/374 (97%)	362 (100%)	0	100	100
2	IL	361/374 (96%)	361 (100%)	0	100	100
2	JB	362/374 (97%)	362 (100%)	0	100	100
2	JD	362/374 (97%)	362 (100%)	0	100	100
2	JF	362/374 (97%)	362 (100%)	0	100	100
2	JH	362/374 (97%)	362 (100%)	0	100	100
2	JJ	361/374 (96%)	361 (100%)	0	100	100
2	JL	361/374 (96%)	361 (100%)	0	100	100
2	KB	361/374 (96%)	361 (100%)	0	100	100
2	KD	362/374 (97%)	362 (100%)	0	100	100
2	KF	361/374 (96%)	361 (100%)	0	100	100
2	KH	362/374 (97%)	362 (100%)	0	100	100
2	KJ	361/374 (96%)	361 (100%)	0	100	100
2	KL	362/374 (97%)	362 (100%)	0	100	100
2	LB	362/374 (97%)	362 (100%)	0	100	100
2	LD	362/374 (97%)	361 (100%)	1 (0%)	86	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	LF	362/374 (97%)	362 (100%)	0	100	100
2	LH	362/374 (97%)	362 (100%)	0	100	100
2	LJ	362/374 (97%)	362 (100%)	0	100	100
2	LL	362/374 (97%)	362 (100%)	0	100	100
2	MB	362/374 (97%)	362 (100%)	0	100	100
2	MD	368/374 (98%)	368 (100%)	0	100	100
2	MF	362/374 (97%)	362 (100%)	0	100	100
2	MH	368/374 (98%)	368 (100%)	0	100	100
2	MJ	362/374 (97%)	362 (100%)	0	100	100
2	ML	368/374 (98%)	368 (100%)	0	100	100
3	a	247/462 (54%)	247 (100%)	0	100	100
3	b	461/462 (100%)	454 (98%)	7 (2%)	57	68
3	c	461/462 (100%)	454 (98%)	7 (2%)	57	68
3	d	216/462 (47%)	209 (97%)	7 (3%)	34	56
4	e	151/159 (95%)	151 (100%)	0	100	100
4	f	151/159 (95%)	151 (100%)	0	100	100
4	g	116/159 (73%)	116 (100%)	0	100	100
5	h	478/598 (80%)	478 (100%)	0	100	100
5	i	478/598 (80%)	478 (100%)	0	100	100
5	j	478/598 (80%)	478 (100%)	0	100	100
6	k	304/410 (74%)	304 (100%)	0	100	100
6	l	304/410 (74%)	304 (100%)	0	100	100
6	s	224/410 (55%)	224 (100%)	0	100	100
7	m	278/331 (84%)	278 (100%)	0	100	100
7	n	278/331 (84%)	278 (100%)	0	100	100
7	o	278/331 (84%)	277 (100%)	1 (0%)	84	81
8	p	72/73 (99%)	72 (100%)	0	100	100
8	q	72/73 (99%)	72 (100%)	0	100	100
8	r	72/73 (99%)	72 (100%)	0	100	100
9	A	172/176 (98%)	172 (100%)	0	100	100
9	B	172/176 (98%)	172 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	C	172/176 (98%)	172 (100%)	0	100	100
10	P	91/482 (19%)	91 (100%)	0	100	100
10	Q	91/482 (19%)	91 (100%)	0	100	100
10	R	91/482 (19%)	91 (100%)	0	100	100
10	S	91/482 (19%)	91 (100%)	0	100	100
10	Z	80/482 (17%)	80 (100%)	0	100	100
10	cc	79/482 (16%)	79 (100%)	0	100	100
12	bb	57/1666 (3%)	57 (100%)	0	100	100
14	J	165/697 (24%)	165 (100%)	0	100	100
14	K	165/697 (24%)	165 (100%)	0	100	100
15	L	87/166 (52%)	87 (100%)	0	100	100
15	M	87/166 (52%)	87 (100%)	0	100	100
15	N	87/166 (52%)	87 (100%)	0	100	100
15	O	87/166 (52%)	87 (100%)	0	100	100
15	X	87/166 (52%)	87 (100%)	0	100	100
15	Y	87/166 (52%)	87 (100%)	0	100	100
All	All	61147/69759 (88%)	61116 (100%)	31 (0%)	87	88

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	b	405	CYS
3	d	398	ARG
3	c	364	ARG
3	d	407	GLN
3	d	363	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 651 such sidechains are listed below:

Mol	Chain	Res	Type
2	KD	107	HIS
1	MG	99	ASN
1	KG	247	ASN
2	KD	102	ASN
2	LF	102	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 222 ligands modelled in this entry, 74 are monoatomic - leaving 148 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$
19	GDP	KG	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.75	6 (13%)
19	GDP	LC	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.80	7 (15%)
20	GTP	HF	501	21	33,34,34	0.92	1 (3%)	50,54,54	1.59	9 (18%)
19	GDP	EE	502	-	29,30,30	1.16	3 (10%)	45,47,47	1.73	6 (13%)
20	GTP	DF	501	21	33,34,34	0.91	1 (3%)	50,54,54	1.56	8 (16%)
20	GTP	CJ	501	21	33,34,34	0.89	1 (3%)	50,54,54	1.58	9 (18%)
20	GTP	JF	501	21	33,34,34	0.88	1 (3%)	50,54,54	1.58	10 (20%)
19	GDP	GG	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.78	6 (13%)
19	GDP	LG	501	-	29,30,30	1.13	3 (10%)	45,47,47	1.74	7 (15%)
19	GDP	HG	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	6 (13%)
19	GDP	FA	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
20	GTP	LD	501	21	33,34,34	0.92	1 (3%)	50,54,54	1.60	10 (20%)
19	GDP	FC	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	6 (13%)
19	GDP	AE	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.72	7 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	GTP	EF	501	21	33,34,34	0.95	2 (6%)	50,54,54	1.63	10 (20%)
19	GDP	HK	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.76	6 (13%)
20	GTP	CH	501	21	33,34,34	0.91	1 (3%)	50,54,54	1.58	9 (18%)
19	GDP	JE	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.73	6 (13%)
19	GDP	ME	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.74	6 (13%)
19	GDP	EG	501	-	29,30,30	1.15	4 (13%)	45,47,47	1.70	7 (15%)
19	GDP	AC	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	6 (13%)
20	GTP	EH	501	21	33,34,34	0.89	1 (3%)	50,54,54	1.60	9 (18%)
19	GDP	IE	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.72	6 (13%)
19	GDP	CA	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
19	GDP	CI	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	7 (15%)
20	GTP	AF	501	21	33,34,34	0.91	1 (3%)	50,54,54	1.57	8 (16%)
20	GTP	KL	501	21	33,34,34	0.93	1 (3%)	50,54,54	1.60	9 (18%)
20	GTP	EJ	501	21	33,34,34	0.93	1 (3%)	50,54,54	1.61	10 (20%)
20	GTP	KH	501	21	33,34,34	0.91	1 (3%)	50,54,54	1.59	9 (18%)
20	GTP	AD	501	21	33,34,34	0.90	1 (3%)	50,54,54	1.56	9 (18%)
19	GDP	AA	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
19	GDP	MI	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	6 (13%)
19	GDP	MG	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.74	6 (13%)
19	GDP	JC	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.73	6 (13%)
20	GTP	EL	501	21	33,34,34	0.90	1 (3%)	50,54,54	1.56	9 (18%)
20	GTP	LH	501	21	33,34,34	0.89	1 (3%)	50,54,54	1.53	8 (16%)
19	GDP	BC	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	7 (15%)
19	GDP	KI	502	-	29,30,30	1.16	3 (10%)	45,47,47	1.74	7 (15%)
20	GTP	GF	501	21	33,34,34	0.87	1 (3%)	50,54,54	1.58	9 (18%)
19	GDP	GK	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.71	6 (13%)
19	GDP	DK	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.72	6 (13%)
19	GDP	GE	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	6 (13%)
20	GTP	MD	501	21	33,34,34	0.87	1 (3%)	50,54,54	1.59	9 (18%)
20	GTP	FD	501	21	33,34,34	0.92	1 (3%)	50,54,54	1.59	9 (18%)
20	GTP	CF	501	21	33,34,34	0.89	1 (3%)	50,54,54	1.58	8 (16%)
19	GDP	FE	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.73	7 (15%)
19	GDP	GI	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.78	7 (15%)
19	GDP	KC	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.74	6 (13%)
19	GDP	CE	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	6 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	GTP	AL	501	21	33,34,34	0.91	1 (3%)	50,54,54	1.56	8 (16%)
20	GTP	FB	501	21	33,34,34	0.90	1 (3%)	50,54,54	1.56	9 (18%)
20	GTP	DD	501	21	33,34,34	0.91	0	50,54,54	1.58	8 (16%)
20	GTP	HJ	501	21	33,34,34	0.91	1 (3%)	50,54,54	1.59	9 (18%)
20	GTP	JH	501	21	33,34,34	0.93	1 (3%)	50,54,54	1.61	8 (16%)
20	GTP	MJ	501	21	33,34,34	0.93	1 (3%)	50,54,54	1.61	9 (18%)
19	GDP	KK	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.73	6 (13%)
19	GDP	HE	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.72	6 (13%)
19	GDP	LK	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	6 (13%)
20	GTP	MB	501	21	33,34,34	0.94	1 (3%)	50,54,54	1.61	10 (20%)
20	GTP	DL	501	21	33,34,34	0.91	1 (3%)	50,54,54	1.57	9 (18%)
19	GDP	DE	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.78	6 (13%)
20	GTP	LB	501	21	33,34,34	0.91	1 (3%)	50,54,54	1.57	9 (18%)
20	GTP	BF	501	21	33,34,34	0.90	1 (3%)	50,54,54	1.60	9 (18%)
20	GTP	HL	501	21	33,34,34	0.90	1 (3%)	50,54,54	1.62	9 (18%)
20	GTP	FH	501	21	33,34,34	0.92	1 (3%)	50,54,54	1.59	9 (18%)
20	GTP	GH	501	21	33,34,34	0.90	1 (3%)	50,54,54	1.61	9 (18%)
19	GDP	FK	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	6 (13%)
19	GDP	DC	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.74	6 (13%)
20	GTP	BL	501	21	33,34,34	0.94	1 (3%)	50,54,54	1.59	9 (18%)
19	GDP	CK	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.74	7 (15%)
20	GTP	IJ	501	21	33,34,34	0.90	1 (3%)	50,54,54	1.57	9 (18%)
19	GDP	GM	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	6 (13%)
19	GDP	IC	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.77	7 (15%)
20	GTP	EB	501	21	33,34,34	0.94	1 (3%)	50,54,54	1.62	10 (20%)
19	GDP	IK	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.74	6 (13%)
19	GDP	BG	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.70	7 (15%)
19	GDP	FI	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.74	6 (13%)
20	GTP	GL	501	21	33,34,34	0.94	1 (3%)	50,54,54	1.61	9 (18%)
19	GDP	HM	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
20	GTP	BH	501	21	33,34,34	0.89	1 (3%)	50,54,54	1.60	9 (18%)
20	GTP	AJ	501	21	33,34,34	0.91	1 (3%)	50,54,54	1.57	9 (18%)
20	GTP	FL	501	21	33,34,34	0.92	1 (3%)	50,54,54	1.59	9 (18%)
20	GTP	DB	501	21	33,34,34	0.92	1 (3%)	50,54,54	1.59	10 (20%)
20	GTP	IF	501	21	33,34,34	0.91	2 (6%)	50,54,54	1.57	9 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	GDP	II	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.77	7 (15%)
20	GTP	GJ	501	21	33,34,34	0.88	1 (3%)	50,54,54	1.57	9 (18%)
19	GDP	BI	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.74	6 (13%)
20	GTP	CD	501	21	33,34,34	0.92	1 (3%)	50,54,54	1.64	10 (20%)
20	GTP	KB	501	21	33,34,34	0.88	1 (3%)	50,54,54	1.58	8 (16%)
19	GDP	EC	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.72	7 (15%)
19	GDP	HC	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.75	7 (15%)
20	GTP	BB	501	21	33,34,34	0.90	1 (3%)	50,54,54	1.60	9 (18%)
20	GTP	HI	501	21	33,34,34	0.89	1 (3%)	50,54,54	1.57	9 (18%)
20	GTP	ID	501	21	33,34,34	0.93	1 (3%)	50,54,54	1.56	9 (18%)
20	GTP	JB	501	21	33,34,34	0.88	1 (3%)	50,54,54	1.55	9 (18%)
19	GDP	EK	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.74	7 (15%)
20	GTP	ED	501	21	33,34,34	0.90	1 (3%)	50,54,54	1.54	9 (18%)
20	GTP	BD	501	21	33,34,34	0.89	1 (3%)	50,54,54	1.59	8 (16%)
19	GDP	EI	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	6 (13%)
19	GDP	GC	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.78	7 (15%)
20	GTP	KF	501	21	33,34,34	0.89	1 (3%)	50,54,54	1.58	8 (16%)
19	GDP	AK	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.71	6 (13%)
19	GDP	JK	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.78	7 (15%)
20	GTP	KD	501	21	33,34,34	0.90	1 (3%)	50,54,54	1.57	8 (16%)
19	GDP	JI	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	6 (13%)
19	GDP	JM	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.76	7 (15%)
20	GTP	IH	501	21	33,34,34	0.92	1 (3%)	50,54,54	1.59	9 (18%)
20	GTP	CB	501	21	33,34,34	0.90	1 (3%)	50,54,54	1.61	9 (18%)
19	GDP	AI	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	6 (13%)
19	GDP	BK	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
19	GDP	EA	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	6 (13%)
20	GTP	MH	501	21	33,34,34	0.88	1 (3%)	50,54,54	1.58	9 (18%)
19	GDP	IG	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.73	6 (13%)
20	GTP	ML	501	21	33,34,34	0.89	1 (3%)	50,54,54	1.59	9 (18%)
20	GTP	FF	501	21	33,34,34	0.92	1 (3%)	50,54,54	1.59	8 (16%)
20	GTP	MF	501	21	33,34,34	0.92	1 (3%)	50,54,54	1.57	9 (18%)
19	GDP	CG	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.70	6 (13%)
19	GDP	KE	501	-	29,30,30	1.15	4 (13%)	45,47,47	1.74	5 (11%)
20	GTP	LL	501	21	33,34,34	0.92	1 (3%)	50,54,54	1.57	9 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	GDP	HI	502	-	29,30,30	1.16	3 (10%)	45,47,47	1.74	6 (13%)
19	GDP	LE	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.72	6 (13%)
19	GDP	LI	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.79	6 (13%)
20	GTP	HD	501	21	33,34,34	0.92	1 (3%)	50,54,54	1.59	9 (18%)
19	GDP	IM	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.73	7 (15%)
20	GTP	IL	501	21	33,34,34	0.90	1 (3%)	50,54,54	1.57	9 (18%)
20	GTP	AH	501	21	33,34,34	0.92	1 (3%)	50,54,54	1.62	9 (18%)
20	GTP	LJ	501	21	33,34,34	0.89	1 (3%)	50,54,54	1.57	9 (18%)
20	GTP	DH	501	21	33,34,34	0.88	0	50,54,54	1.55	9 (18%)
19	GDP	BE	501	-	29,30,30	1.19	3 (10%)	45,47,47	1.72	5 (11%)
19	GDP	DG	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.72	7 (15%)
19	GDP	AG	501	-	29,30,30	1.18	3 (10%)	45,47,47	1.77	6 (13%)
19	GDP	FG	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.73	6 (13%)
20	GTP	DJ	501	21	33,34,34	0.90	1 (3%)	50,54,54	1.56	8 (16%)
20	GTP	JJ	501	21	33,34,34	0.90	1 (3%)	50,54,54	1.58	9 (18%)
19	GDP	CC	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.75	7 (15%)
19	GDP	BA	501	-	29,30,30	1.13	3 (10%)	45,47,47	1.69	6 (13%)
20	GTP	KJ	501	21	33,34,34	0.91	1 (3%)	50,54,54	1.56	8 (16%)
20	GTP	AB	501	21	33,34,34	0.92	1 (3%)	50,54,54	1.58	9 (18%)
19	GDP	JG	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.74	7 (15%)
19	GDP	MK	501	-	29,30,30	1.12	3 (10%)	45,47,47	1.74	6 (13%)
20	GTP	FJ	501	21	33,34,34	0.90	1 (3%)	50,54,54	1.58	9 (18%)
20	GTP	BJ	501	21	33,34,34	0.89	1 (3%)	50,54,54	1.58	9 (18%)
20	GTP	JD	501	21	33,34,34	0.94	1 (3%)	50,54,54	1.59	10 (20%)
19	GDP	MC	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.73	6 (13%)
20	GTP	GD	501	21	33,34,34	0.91	1 (3%)	50,54,54	1.59	9 (18%)
20	GTP	JL	501	21	33,34,34	0.91	1 (3%)	50,54,54	1.56	9 (18%)
19	GDP	DI	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.70	6 (13%)
20	GTP	LF	501	21	33,34,34	0.88	1 (3%)	50,54,54	1.57	9 (18%)

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
19	GDP	KG	501	-	-	1/16/32/32	0/3/3/3
19	GDP	LC	501	-	-	0/16/32/32	0/3/3/3
20	GTP	HF	501	21	-	5/22/38/38	0/3/3/3
19	GDP	EE	502	-	-	7/16/32/32	0/3/3/3
20	GTP	DF	501	21	-	4/22/38/38	0/3/3/3
20	GTP	CJ	501	21	-	4/22/38/38	0/3/3/3
20	GTP	JF	501	21	-	1/22/38/38	0/3/3/3
19	GDP	GG	501	-	-	0/16/32/32	0/3/3/3
19	GDP	LG	501	-	-	0/16/32/32	0/3/3/3
19	GDP	HG	501	-	-	1/16/32/32	0/3/3/3
19	GDP	FA	501	-	-	1/16/32/32	0/3/3/3
20	GTP	LD	501	21	-	6/22/38/38	0/3/3/3
19	GDP	FC	501	-	-	1/16/32/32	0/3/3/3
19	GDP	AE	501	-	-	0/16/32/32	0/3/3/3
20	GTP	EF	501	21	-	7/22/38/38	0/3/3/3
19	GDP	HK	501	-	-	2/16/32/32	0/3/3/3
20	GTP	CH	501	21	-	5/22/38/38	0/3/3/3
19	GDP	JE	501	-	-	3/16/32/32	0/3/3/3
19	GDP	ME	501	-	-	3/16/32/32	0/3/3/3
19	GDP	EG	501	-	-	4/16/32/32	0/3/3/3
19	GDP	AC	501	-	-	1/16/32/32	0/3/3/3
20	GTP	EH	501	21	-	7/22/38/38	0/3/3/3
19	GDP	IE	501	-	-	3/16/32/32	0/3/3/3
19	GDP	CA	501	-	-	0/16/32/32	0/3/3/3
19	GDP	CI	501	-	-	2/16/32/32	0/3/3/3
20	GTP	AF	501	21	-	3/22/38/38	0/3/3/3
20	GTP	KL	501	21	-	8/22/38/38	0/3/3/3
20	GTP	EJ	501	21	-	6/22/38/38	0/3/3/3
20	GTP	KH	501	21	-	3/22/38/38	0/3/3/3
20	GTP	AD	501	21	-	5/22/38/38	0/3/3/3
19	GDP	AA	501	-	-	0/16/32/32	0/3/3/3
19	GDP	MI	501	-	-	4/16/32/32	0/3/3/3
19	GDP	MG	501	-	-	0/16/32/32	0/3/3/3
19	GDP	JC	501	-	-	1/16/32/32	0/3/3/3
20	GTP	EL	501	21	-	5/22/38/38	0/3/3/3
20	GTP	LH	501	21	-	4/22/38/38	0/3/3/3
19	GDP	BC	501	-	-	3/16/32/32	0/3/3/3
19	GDP	KI	502	-	-	5/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	GTP	GF	501	21	-	6/22/38/38	0/3/3/3
19	GDP	GK	501	-	-	0/16/32/32	0/3/3/3
19	GDP	DK	501	-	-	2/16/32/32	0/3/3/3
19	GDP	GE	501	-	-	2/16/32/32	0/3/3/3
20	GTP	MD	501	21	-	4/22/38/38	0/3/3/3
20	GTP	FD	501	21	-	2/22/38/38	0/3/3/3
20	GTP	CF	501	21	-	3/22/38/38	0/3/3/3
19	GDP	FE	501	-	-	1/16/32/32	0/3/3/3
19	GDP	GI	501	-	-	1/16/32/32	0/3/3/3
19	GDP	KC	501	-	-	1/16/32/32	0/3/3/3
19	GDP	CE	501	-	-	0/16/32/32	0/3/3/3
20	GTP	AL	501	21	-	4/22/38/38	0/3/3/3
20	GTP	FB	501	21	-	5/22/38/38	0/3/3/3
20	GTP	DD	501	21	-	8/22/38/38	0/3/3/3
20	GTP	HJ	501	21	-	4/22/38/38	0/3/3/3
20	GTP	JH	501	21	-	6/22/38/38	0/3/3/3
20	GTP	MJ	501	21	-	4/22/38/38	0/3/3/3
19	GDP	KK	501	-	-	0/16/32/32	0/3/3/3
19	GDP	HE	501	-	-	5/16/32/32	0/3/3/3
19	GDP	LK	501	-	-	0/16/32/32	0/3/3/3
20	GTP	MB	501	21	-	5/22/38/38	0/3/3/3
20	GTP	DL	501	21	-	6/22/38/38	0/3/3/3
19	GDP	DE	501	-	-	2/16/32/32	0/3/3/3
20	GTP	LB	501	21	-	3/22/38/38	0/3/3/3
20	GTP	BF	501	21	-	3/22/38/38	0/3/3/3
20	GTP	HL	501	21	-	7/22/38/38	0/3/3/3
20	GTP	FH	501	21	-	4/22/38/38	0/3/3/3
20	GTP	GH	501	21	-	6/22/38/38	0/3/3/3
19	GDP	FK	501	-	-	2/16/32/32	0/3/3/3
19	GDP	DC	501	-	-	2/16/32/32	0/3/3/3
20	GTP	BL	501	21	-	6/22/38/38	0/3/3/3
19	GDP	CK	501	-	-	6/16/32/32	0/3/3/3
20	GTP	IJ	501	21	-	4/22/38/38	0/3/3/3
19	GDP	GM	501	-	-	2/16/32/32	0/3/3/3
19	GDP	IC	501	-	-	5/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	GTP	EB	501	21	-	4/22/38/38	0/3/3/3
19	GDP	IK	501	-	-	3/16/32/32	0/3/3/3
19	GDP	BG	501	-	-	2/16/32/32	0/3/3/3
19	GDP	FI	501	-	-	0/16/32/32	0/3/3/3
20	GTP	GL	501	21	-	6/22/38/38	0/3/3/3
19	GDP	HM	501	-	-	4/16/32/32	0/3/3/3
20	GTP	BH	501	21	-	5/22/38/38	0/3/3/3
20	GTP	AJ	501	21	-	6/22/38/38	0/3/3/3
20	GTP	FL	501	21	-	4/22/38/38	0/3/3/3
20	GTP	DB	501	21	-	6/22/38/38	0/3/3/3
20	GTP	IF	501	21	-	6/22/38/38	0/3/3/3
19	GDP	II	501	-	-	7/16/32/32	0/3/3/3
20	GTP	GJ	501	21	-	5/22/38/38	0/3/3/3
19	GDP	BI	501	-	-	3/16/32/32	0/3/3/3
20	GTP	CD	501	21	-	8/22/38/38	0/3/3/3
20	GTP	KB	501	21	-	5/22/38/38	0/3/3/3
19	GDP	EC	501	-	-	1/16/32/32	0/3/3/3
19	GDP	HC	501	-	-	3/16/32/32	0/3/3/3
20	GTP	BB	501	21	-	3/22/38/38	0/3/3/3
20	GTP	HI	501	21	-	3/22/38/38	0/3/3/3
20	GTP	ID	501	21	-	3/22/38/38	0/3/3/3
20	GTP	JB	501	21	-	7/22/38/38	0/3/3/3
19	GDP	EK	501	-	-	1/16/32/32	0/3/3/3
20	GTP	ED	501	21	-	3/22/38/38	0/3/3/3
20	GTP	BD	501	21	-	5/22/38/38	0/3/3/3
19	GDP	EI	501	-	-	0/16/32/32	0/3/3/3
19	GDP	GC	501	-	-	0/16/32/32	0/3/3/3
20	GTP	KF	501	21	-	5/22/38/38	0/3/3/3
19	GDP	AK	501	-	-	4/16/32/32	0/3/3/3
19	GDP	JK	501	-	-	2/16/32/32	0/3/3/3
20	GTP	KD	501	21	-	5/22/38/38	0/3/3/3
19	GDP	JI	501	-	-	2/16/32/32	0/3/3/3
19	GDP	JM	501	-	-	0/16/32/32	0/3/3/3
20	GTP	IH	501	21	-	6/22/38/38	0/3/3/3
20	GTP	CB	501	21	-	6/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	GDP	AI	501	-	-	1/16/32/32	0/3/3/3
19	GDP	BK	501	-	-	3/16/32/32	0/3/3/3
19	GDP	EA	501	-	-	6/16/32/32	0/3/3/3
20	GTP	MH	501	21	-	7/22/38/38	0/3/3/3
19	GDP	IG	501	-	-	0/16/32/32	0/3/3/3
20	GTP	ML	501	21	-	4/22/38/38	0/3/3/3
20	GTP	FF	501	21	-	5/22/38/38	0/3/3/3
20	GTP	MF	501	21	-	5/22/38/38	0/3/3/3
19	GDP	CG	501	-	-	3/16/32/32	0/3/3/3
19	GDP	KE	501	-	-	7/16/32/32	0/3/3/3
20	GTP	LL	501	21	-	6/22/38/38	0/3/3/3
19	GDP	HI	502	-	-	2/16/32/32	0/3/3/3
19	GDP	LE	501	-	-	1/16/32/32	0/3/3/3
19	GDP	LI	501	-	-	0/16/32/32	0/3/3/3
20	GTP	HD	501	21	-	5/22/38/38	0/3/3/3
19	GDP	IM	501	-	-	4/16/32/32	0/3/3/3
20	GTP	IL	501	21	-	6/22/38/38	0/3/3/3
20	GTP	AH	501	21	-	7/22/38/38	0/3/3/3
20	GTP	LJ	501	21	-	6/22/38/38	0/3/3/3
20	GTP	DH	501	21	-	7/22/38/38	0/3/3/3
19	GDP	BE	501	-	-	2/16/32/32	0/3/3/3
19	GDP	DG	501	-	-	2/16/32/32	0/3/3/3
19	GDP	AG	501	-	-	0/16/32/32	0/3/3/3
19	GDP	FG	501	-	-	1/16/32/32	0/3/3/3
20	GTP	DJ	501	21	-	5/22/38/38	0/3/3/3
20	GTP	JJ	501	21	-	6/22/38/38	0/3/3/3
19	GDP	CC	501	-	-	4/16/32/32	0/3/3/3
19	GDP	BA	501	-	-	7/16/32/32	0/3/3/3
20	GTP	KJ	501	21	-	5/22/38/38	0/3/3/3
20	GTP	AB	501	21	-	4/22/38/38	0/3/3/3
19	GDP	JG	501	-	-	5/16/32/32	0/3/3/3
19	GDP	MK	501	-	-	0/16/32/32	0/3/3/3
20	GTP	FJ	501	21	-	4/22/38/38	0/3/3/3
20	GTP	BJ	501	21	-	1/22/38/38	0/3/3/3
20	GTP	JD	501	21	-	3/22/38/38	0/3/3/3
19	GDP	MC	501	-	-	0/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	GTP	GD	501	21	-	4/22/38/38	0/3/3/3
20	GTP	JL	501	21	-	7/22/38/38	0/3/3/3
19	GDP	DI	501	-	-	2/16/32/32	0/3/3/3
20	GTP	LF	501	21	-	4/22/38/38	0/3/3/3

The worst 5 of 298 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	GI	501	GDP	C5-C4	3.05	1.47	1.38
19	JM	501	GDP	C5-C4	3.05	1.47	1.38
19	GE	501	GDP	C5-C4	3.05	1.47	1.38
19	IC	501	GDP	C5-C4	3.04	1.47	1.38
19	BK	501	GDP	C5-C4	3.04	1.47	1.38

The worst 5 of 1131 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	GI	501	GDP	C5-C4-N3	-6.36	118.28	128.39
19	LC	501	GDP	C5-C4-N3	-6.31	118.35	128.39
19	AG	501	GDP	C5-C4-N3	-6.29	118.38	128.39
19	GG	501	GDP	C5-C4-N3	-6.27	118.41	128.39
19	DE	501	GDP	C5-C4-N3	-6.26	118.44	128.39

There are no chirality outliers.

5 of 520 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	AK	501	GDP	C5'-O5'-PA-O3A
19	BA	501	GDP	C5'-O5'-PA-O3A
19	BA	501	GDP	C5'-O5'-PA-O2A
19	BA	501	GDP	O4'-C4'-C5'-O5'
19	BC	501	GDP	PA-O3A-PB-O2B

There are no ring outliers.

111 monomers are involved in 172 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	KG	501	GDP	1	0
19	LC	501	GDP	1	0
20	HF	501	GTP	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	EE	502	GDP	2	0
20	DF	501	GTP	2	0
20	CJ	501	GTP	2	0
20	JF	501	GTP	1	0
19	GG	501	GDP	2	0
19	LG	501	GDP	1	0
19	HG	501	GDP	1	0
19	FA	501	GDP	2	0
20	LD	501	GTP	1	0
19	AE	501	GDP	2	0
20	EF	501	GTP	1	0
19	HK	501	GDP	2	0
20	CH	501	GTP	1	0
19	JE	501	GDP	1	0
19	EG	501	GDP	2	0
19	AC	501	GDP	2	0
20	EH	501	GTP	1	0
19	IE	501	GDP	1	0
19	CA	501	GDP	1	0
20	AF	501	GTP	1	0
20	EJ	501	GTP	1	0
20	AD	501	GTP	1	0
19	MG	501	GDP	2	0
19	JC	501	GDP	1	0
20	EL	501	GTP	1	0
20	LH	501	GTP	1	0
20	GF	501	GTP	2	0
19	GK	501	GDP	2	0
19	DK	501	GDP	1	0
19	GE	501	GDP	2	0
20	MD	501	GTP	3	0
20	CF	501	GTP	3	0
19	GI	501	GDP	1	0
19	KC	501	GDP	1	0
20	DD	501	GTP	1	0
20	HJ	501	GTP	2	0
20	JH	501	GTP	1	0
20	MJ	501	GTP	2	0
19	KK	501	GDP	2	0
19	HE	501	GDP	2	0
20	DL	501	GTP	1	0
19	DE	501	GDP	1	0

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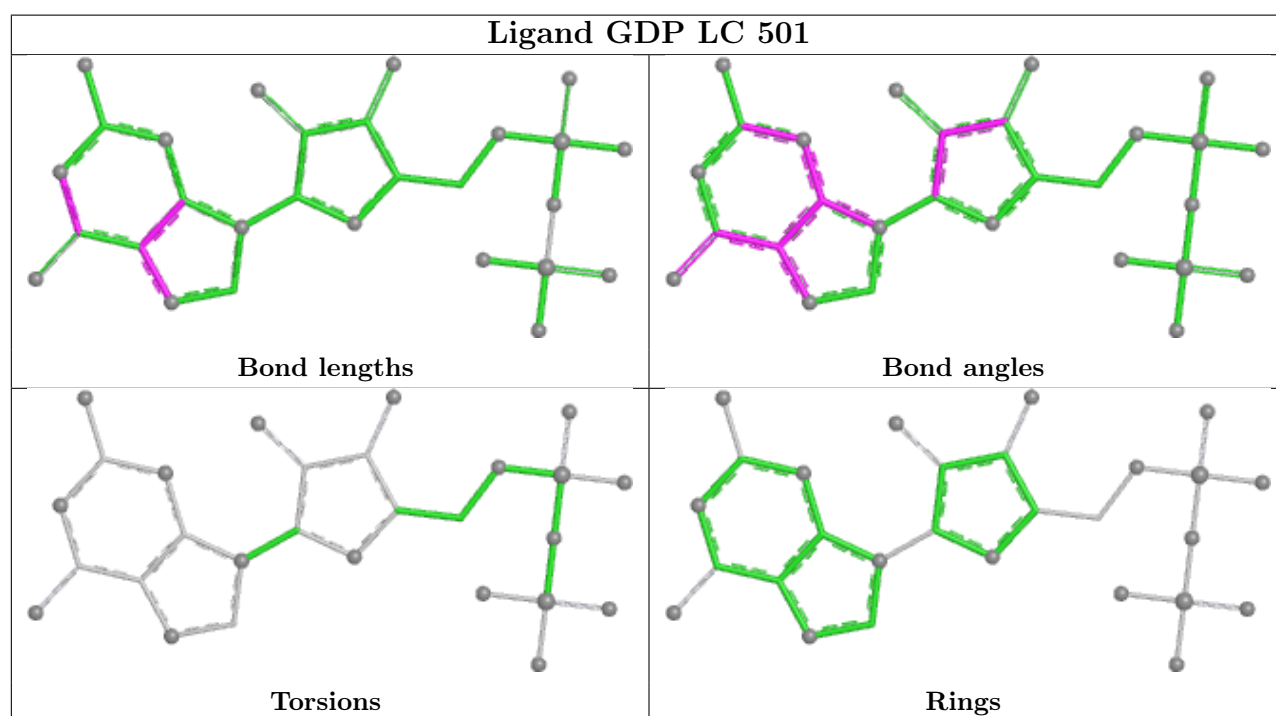
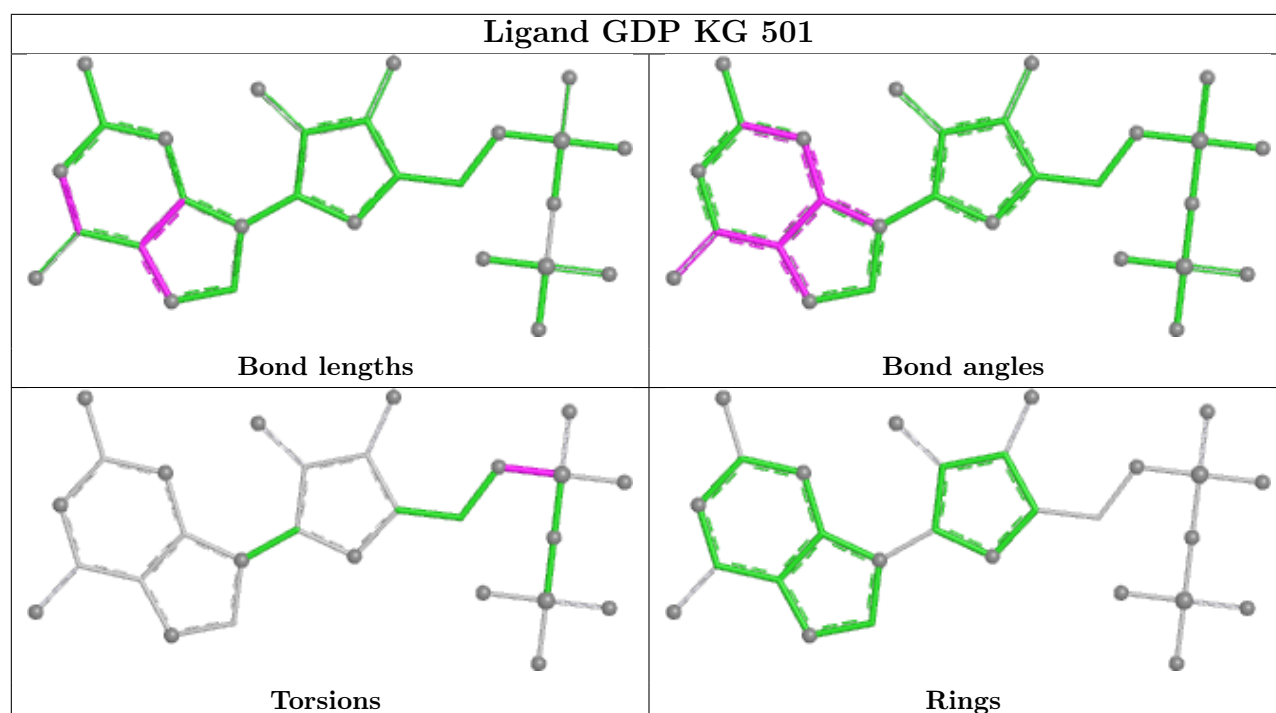
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	LB	501	GTP	1	0
20	BF	501	GTP	1	0
20	HL	501	GTP	3	0
20	FH	501	GTP	1	0
20	GH	501	GTP	3	0
20	BL	501	GTP	1	0
19	CK	501	GDP	1	0
20	IJ	501	GTP	2	0
19	IC	501	GDP	2	0
19	IK	501	GDP	2	0
19	BG	501	GDP	1	0
19	FI	501	GDP	1	0
20	GL	501	GTP	3	0
19	HM	501	GDP	2	0
20	BH	501	GTP	1	0
20	FL	501	GTP	1	0
20	DB	501	GTP	1	0
20	IF	501	GTP	2	0
19	II	501	GDP	1	0
20	GJ	501	GTP	1	0
19	BI	501	GDP	3	0
20	CD	501	GTP	1	0
20	KB	501	GTP	1	0
19	EC	501	GDP	3	0
19	HC	501	GDP	2	0
20	BB	501	GTP	1	0
20	HI	501	GTP	2	0
20	ID	501	GTP	1	0
20	JB	501	GTP	1	0
20	BD	501	GTP	1	0
19	EI	501	GDP	1	0
19	GC	501	GDP	1	0
20	KF	501	GTP	2	0
19	AK	501	GDP	1	0
20	KD	501	GTP	2	0
19	JI	501	GDP	1	0
20	IH	501	GTP	2	0
20	CB	501	GTP	3	0
19	AI	501	GDP	1	0
19	EA	501	GDP	1	0
19	IG	501	GDP	1	0
20	ML	501	GTP	2	0

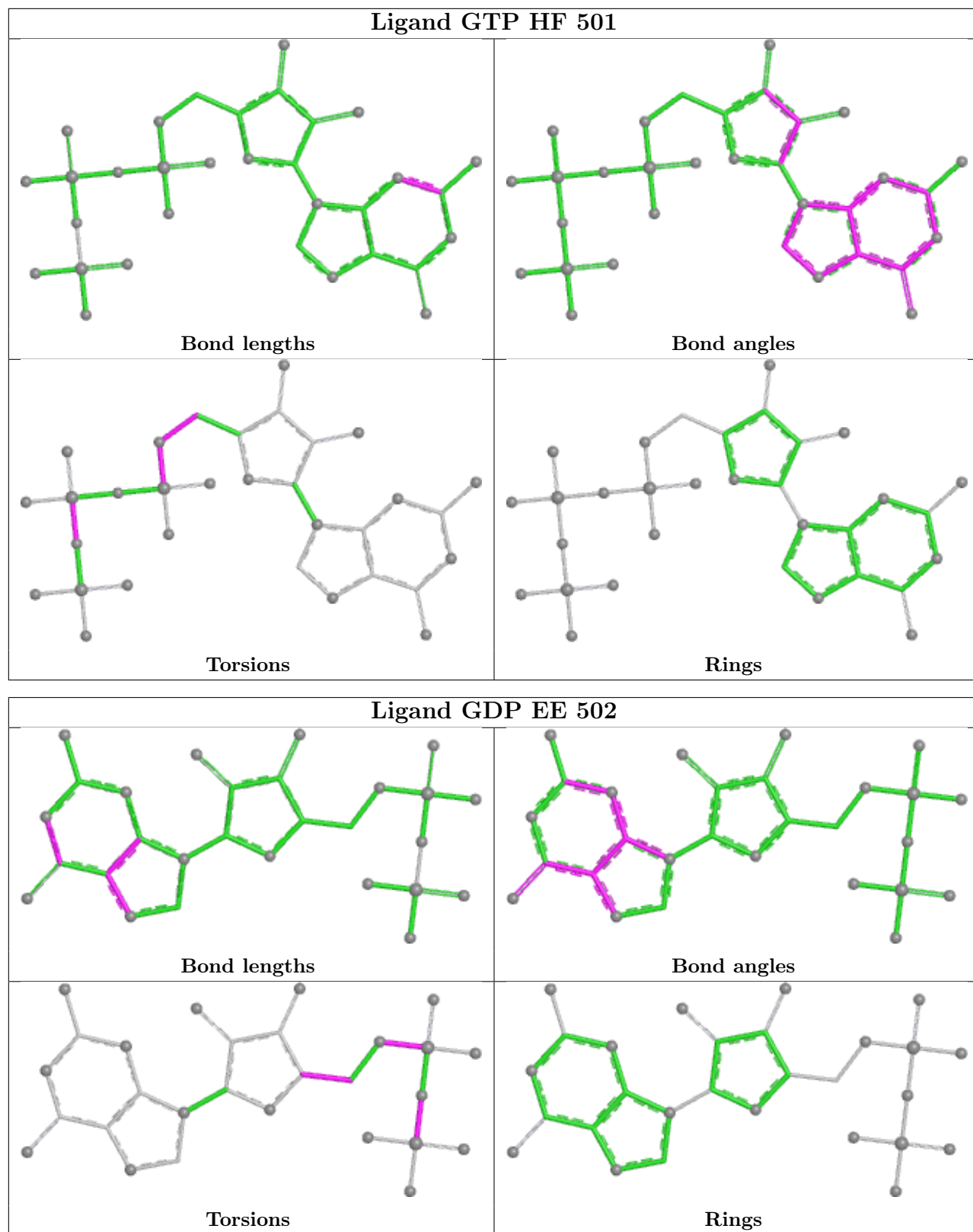
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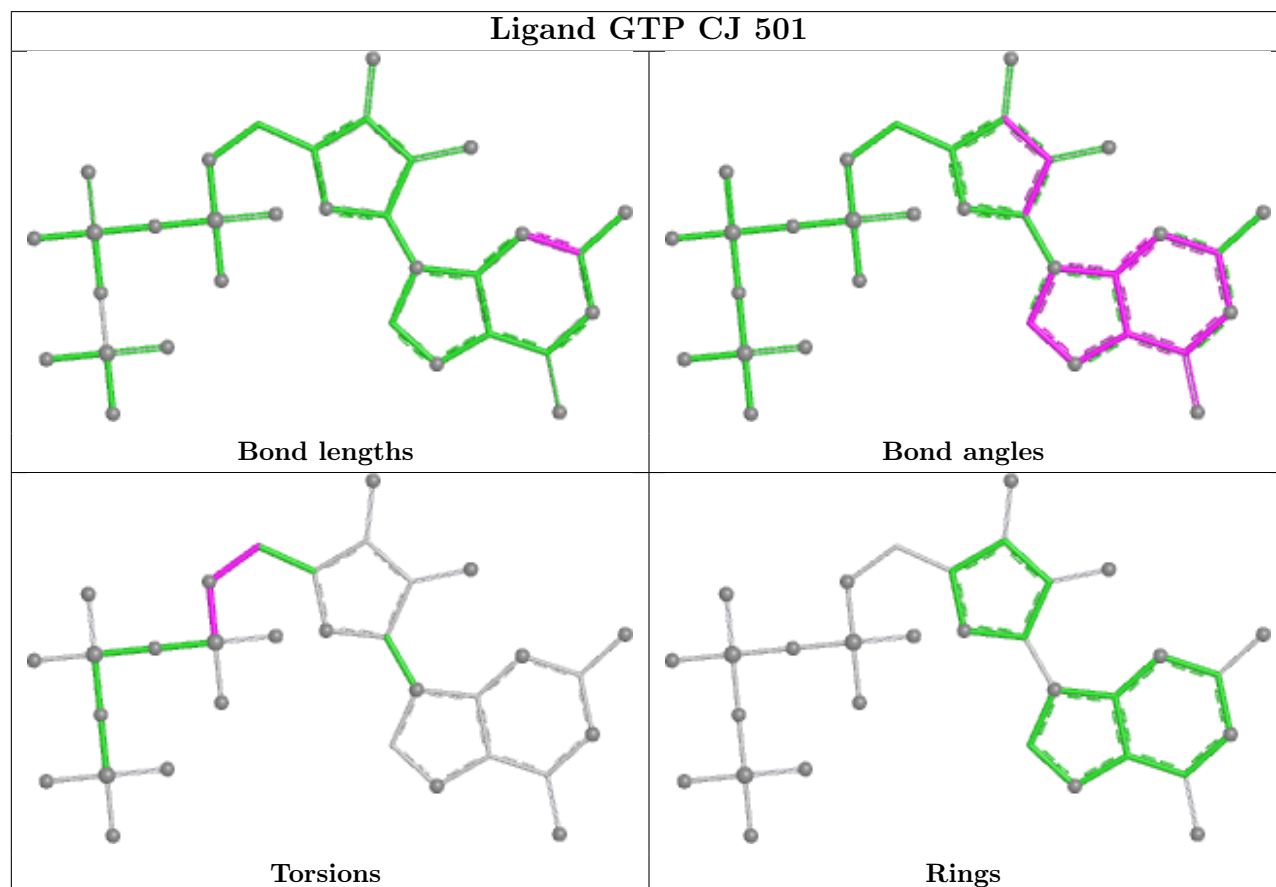
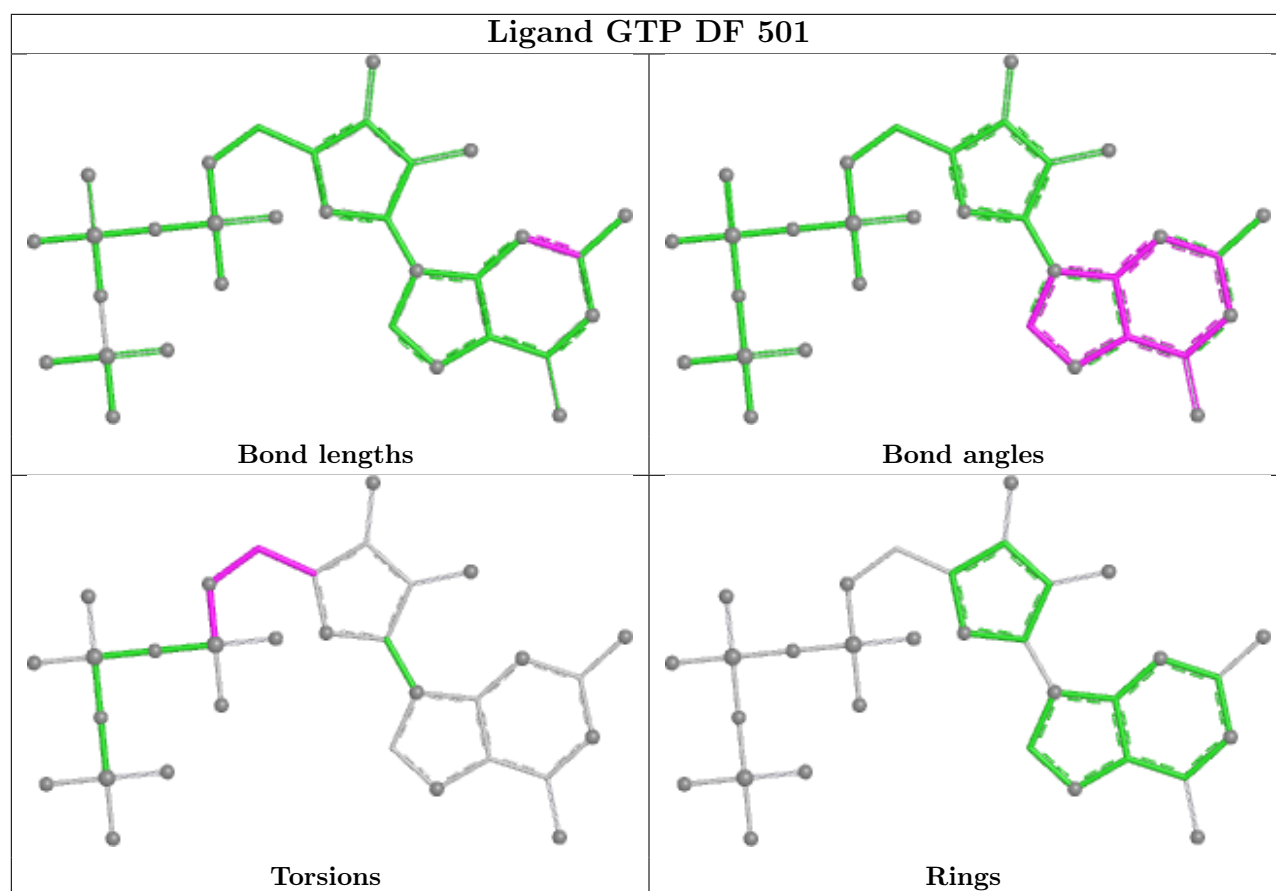
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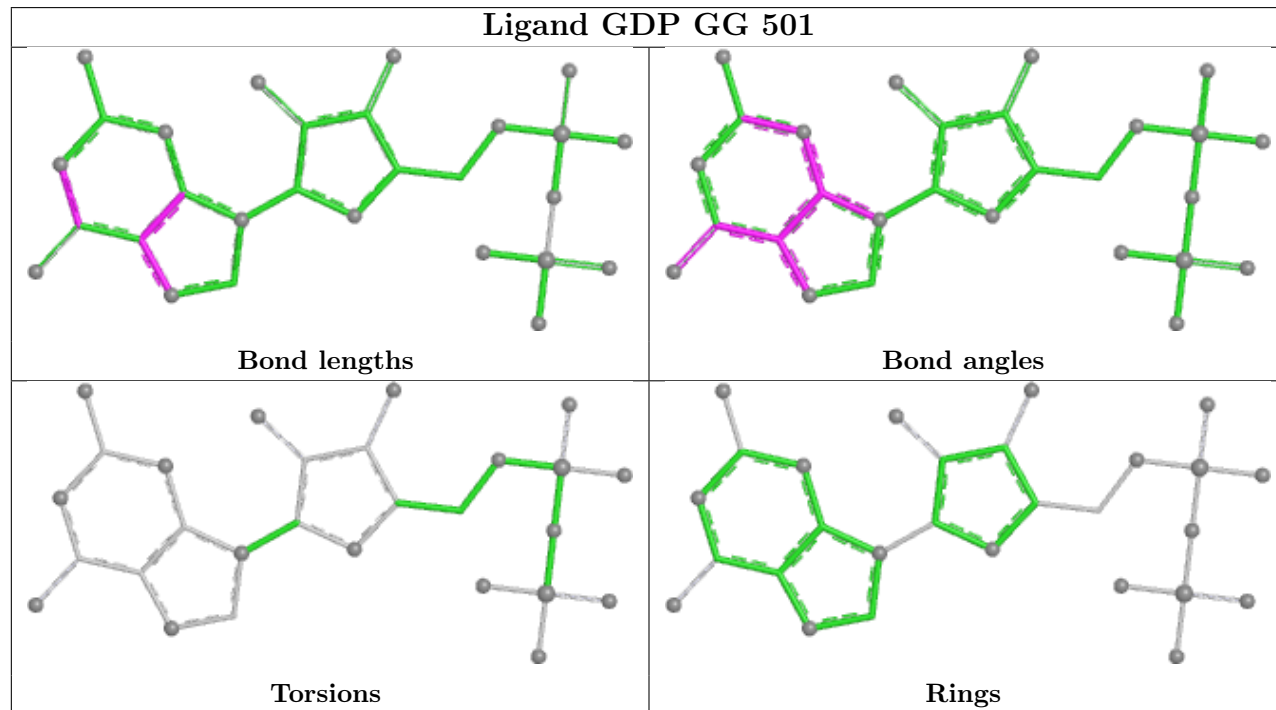
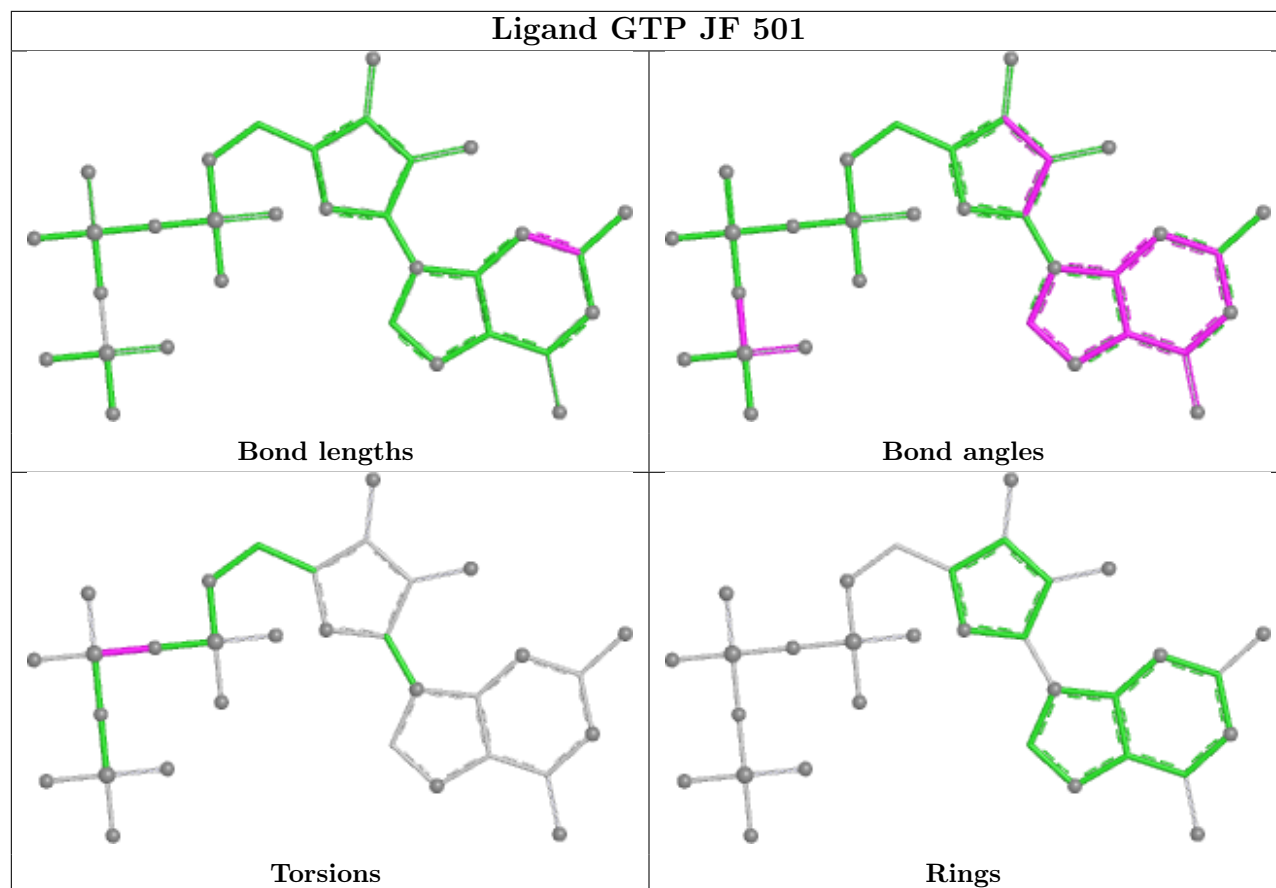
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	MF	501	GTP	1	0
19	CG	501	GDP	2	0
19	KE	501	GDP	3	0
19	HI	502	GDP	3	0
19	LE	501	GDP	2	0
19	LI	501	GDP	1	0
20	HD	501	GTP	2	0
19	IM	501	GDP	4	0
20	IL	501	GTP	2	0
20	LJ	501	GTP	1	0
19	DG	501	GDP	1	0
19	AG	501	GDP	2	0
20	DJ	501	GTP	2	0
19	CC	501	GDP	1	0
19	BA	501	GDP	2	0
20	KJ	501	GTP	1	0
19	JG	501	GDP	1	0
19	MK	501	GDP	1	0
20	BJ	501	GTP	1	0
20	JD	501	GTP	2	0
19	MC	501	GDP	1	0
20	GD	501	GTP	2	0
20	JL	501	GTP	1	0
20	LF	501	GTP	1	0

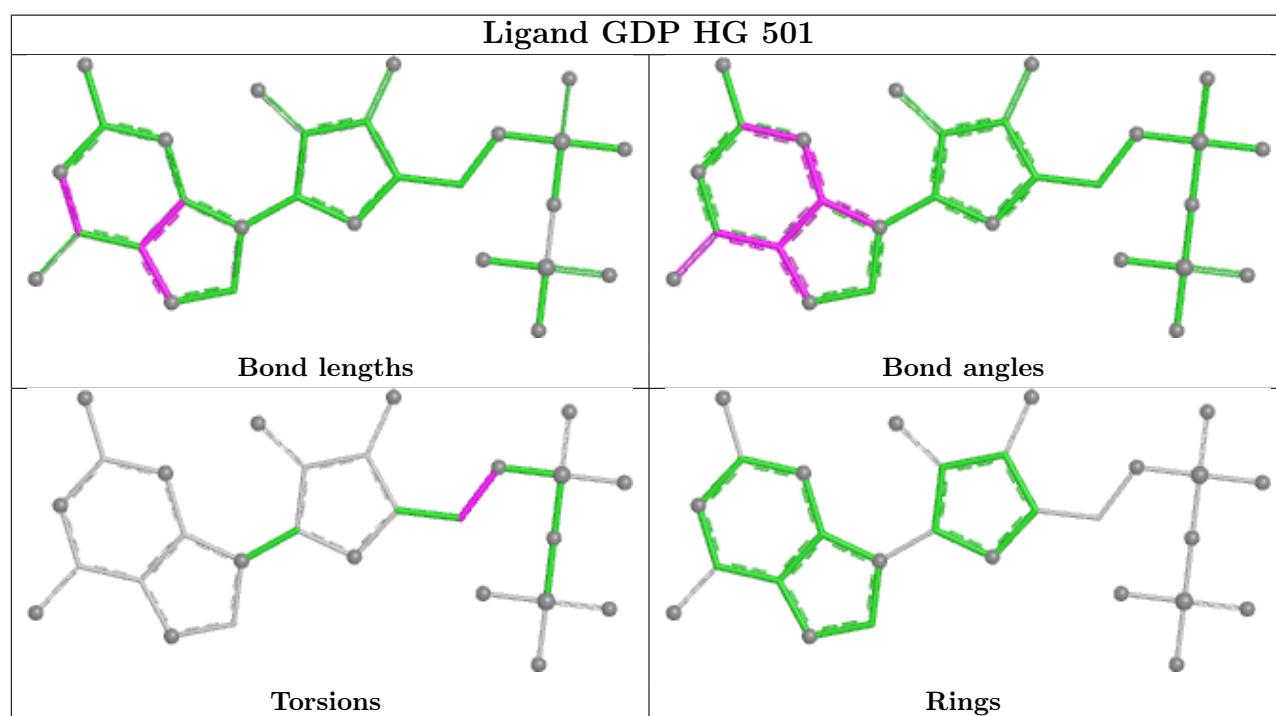
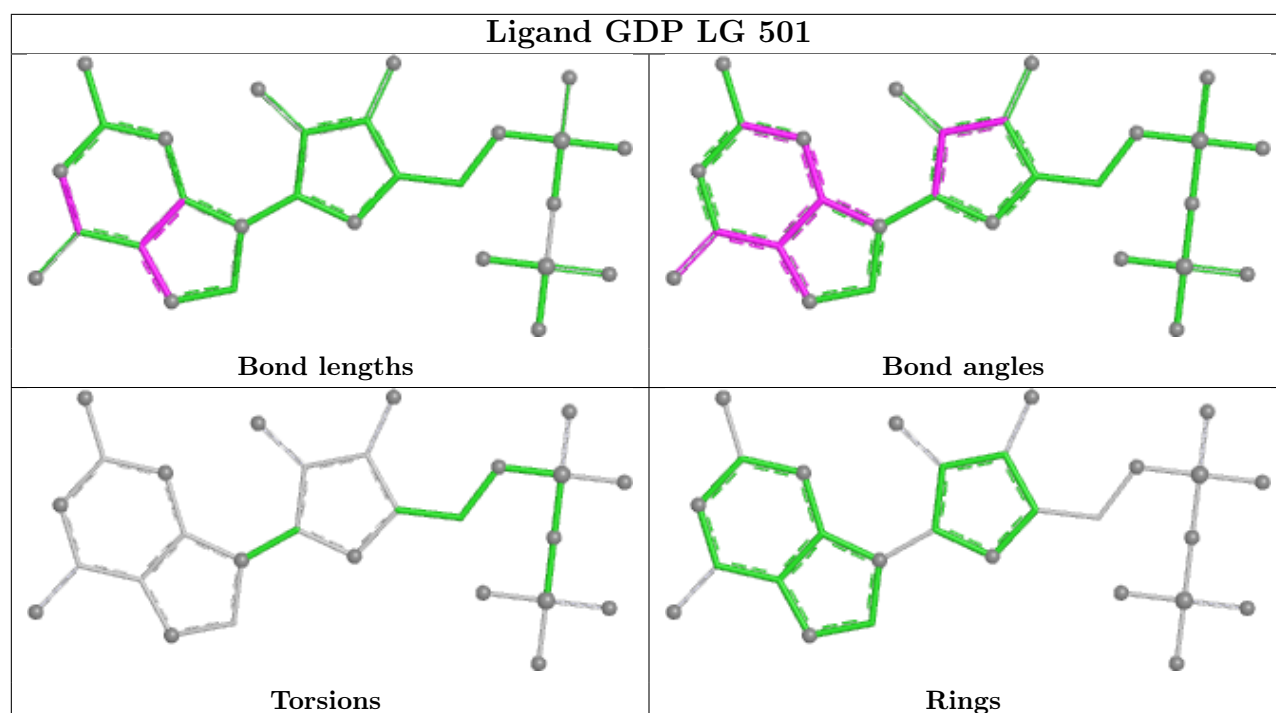
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

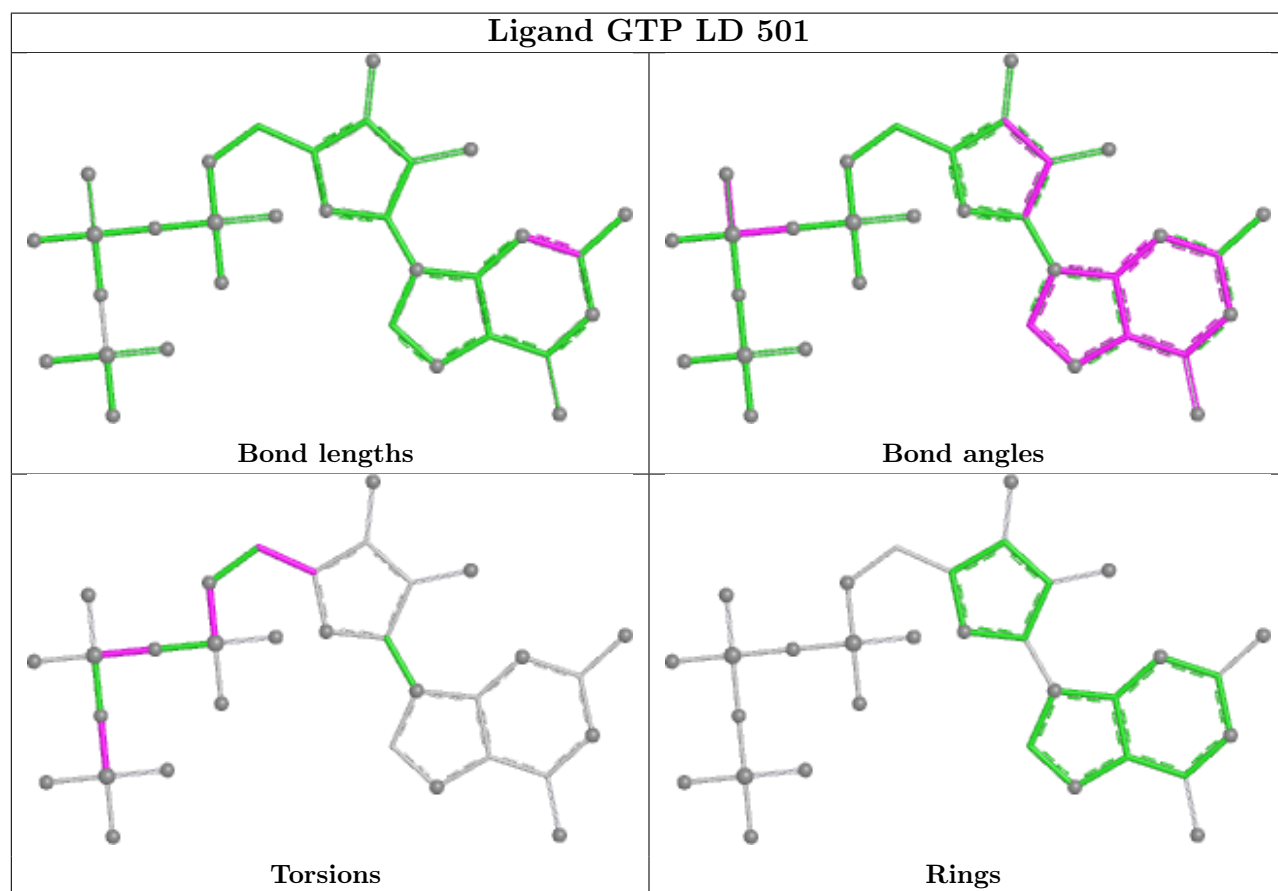
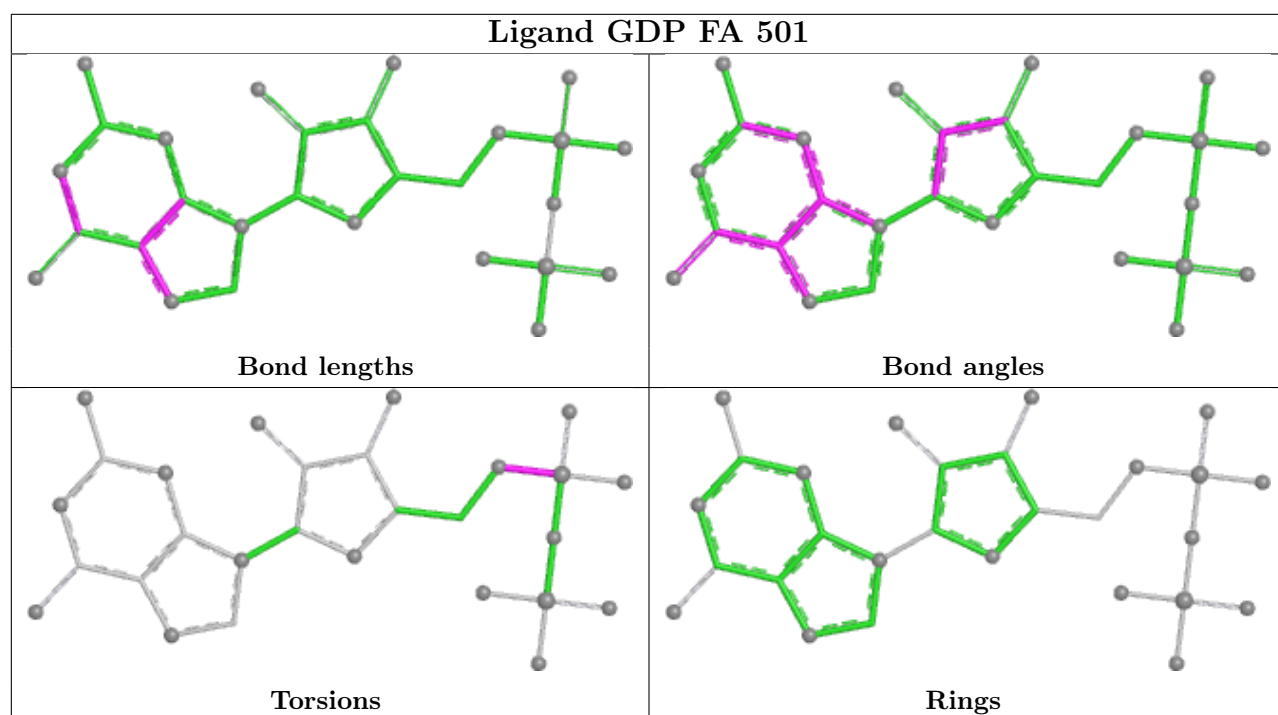


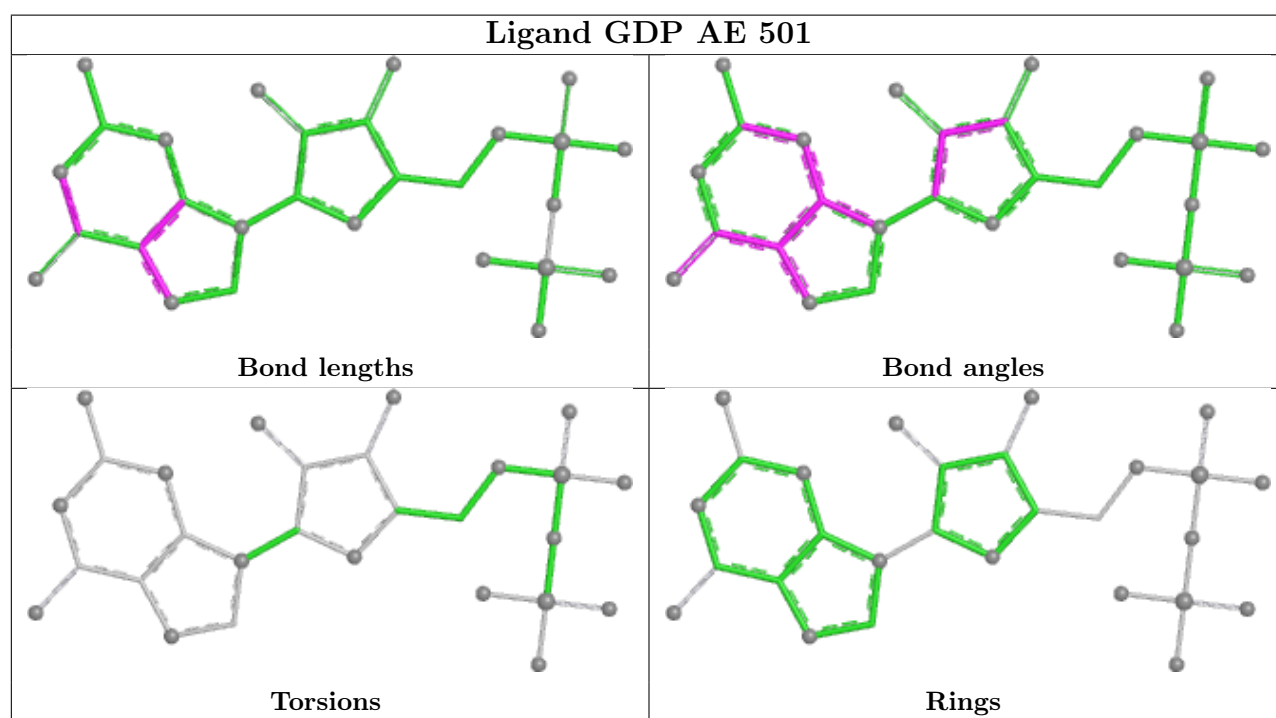
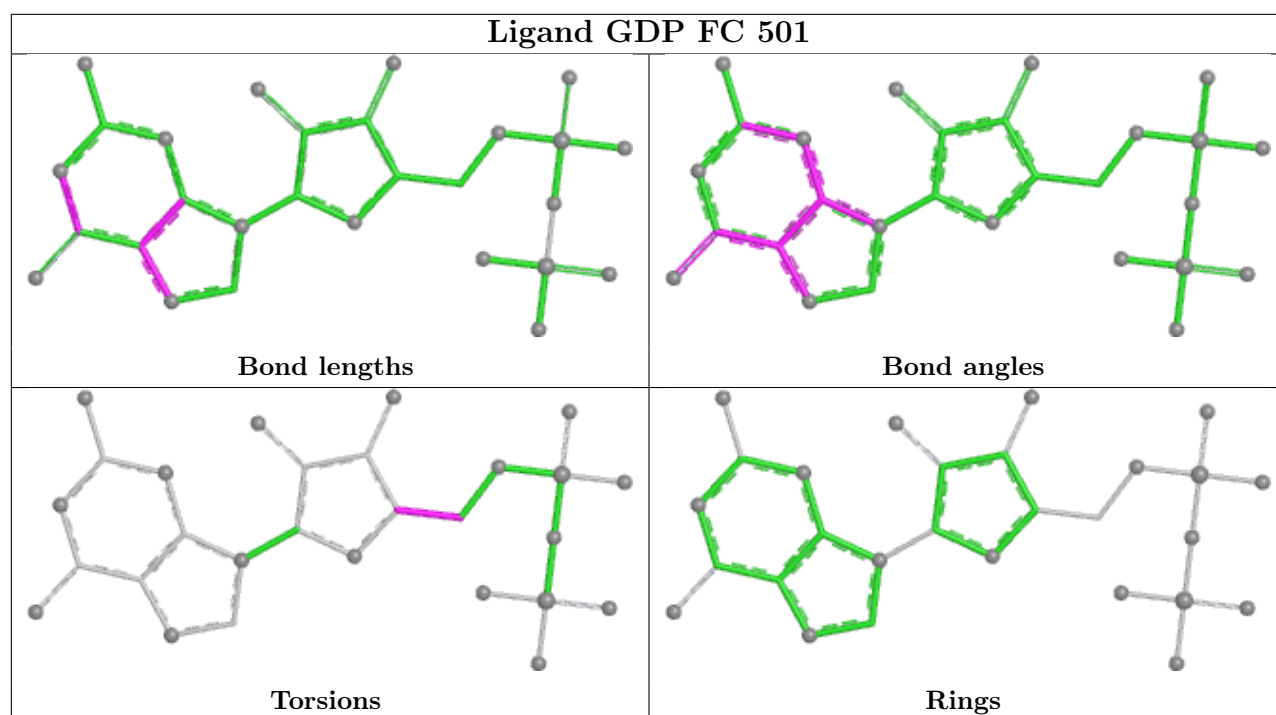


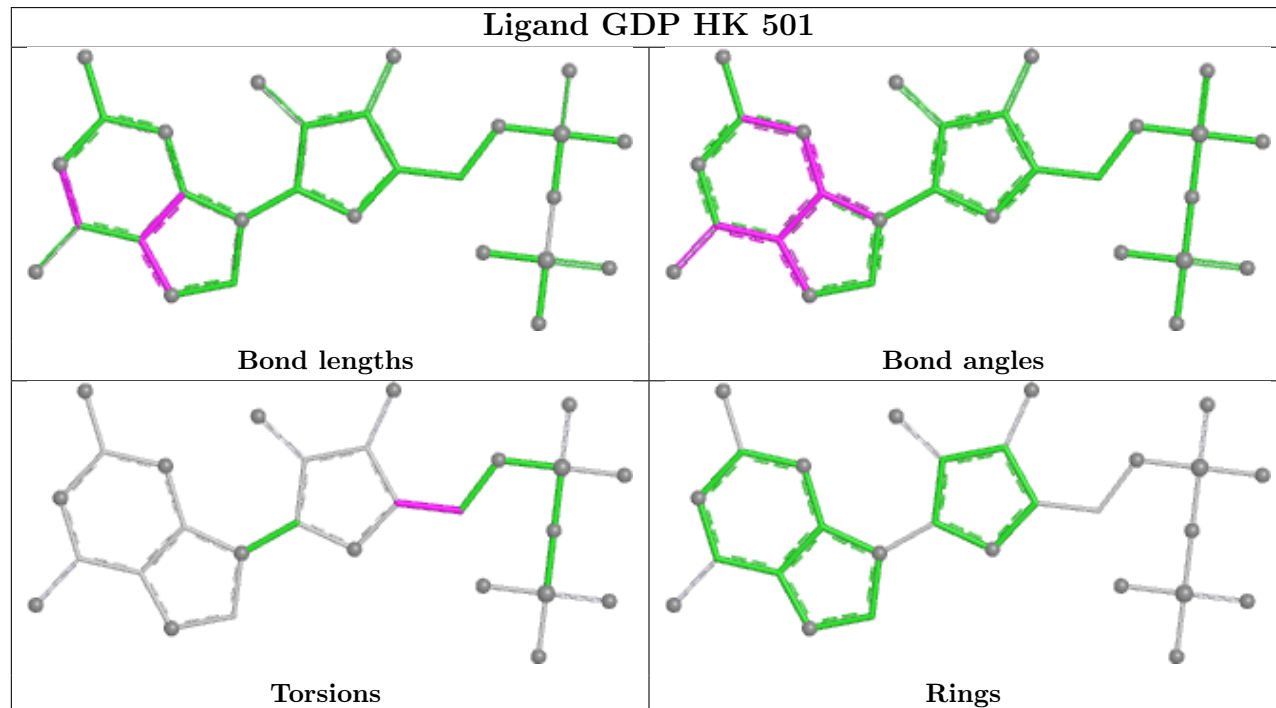
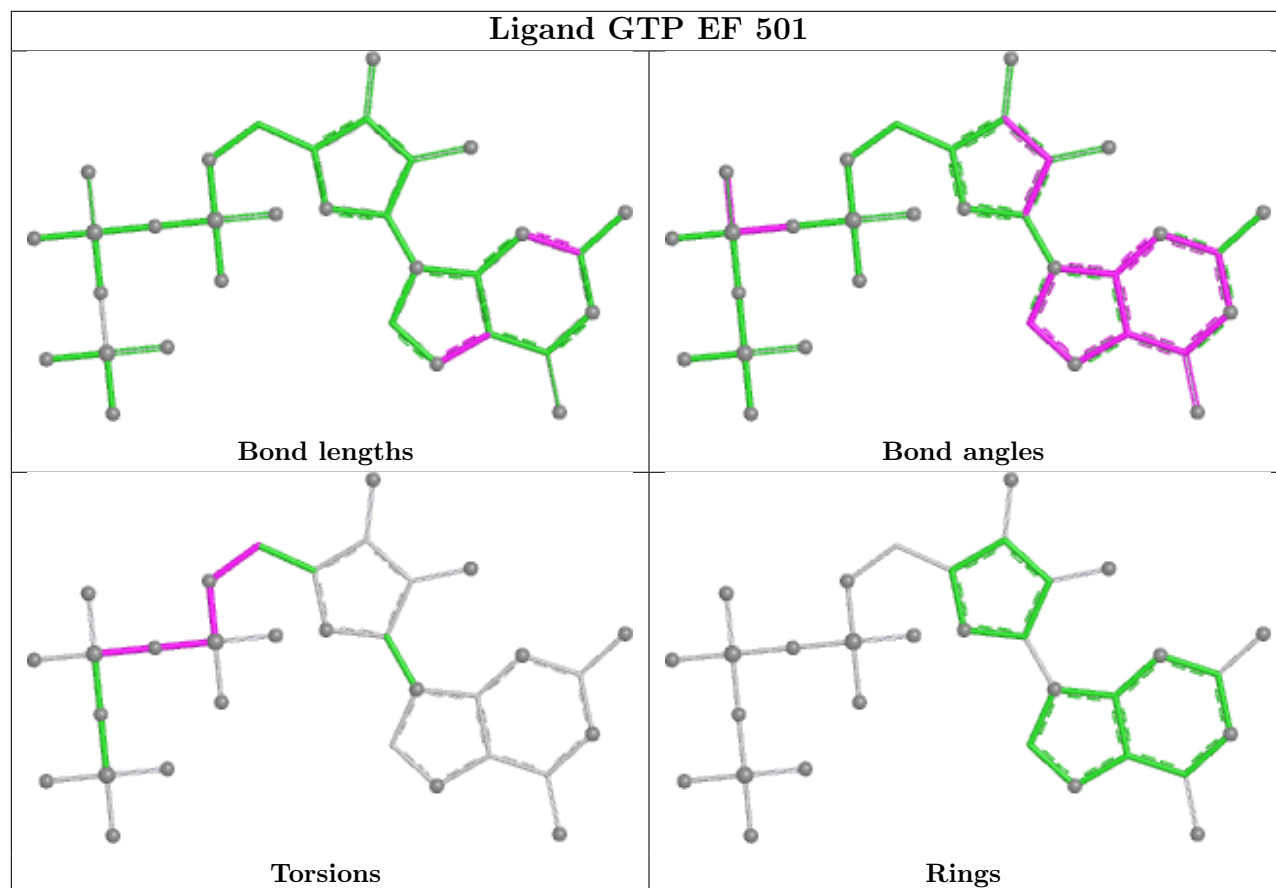


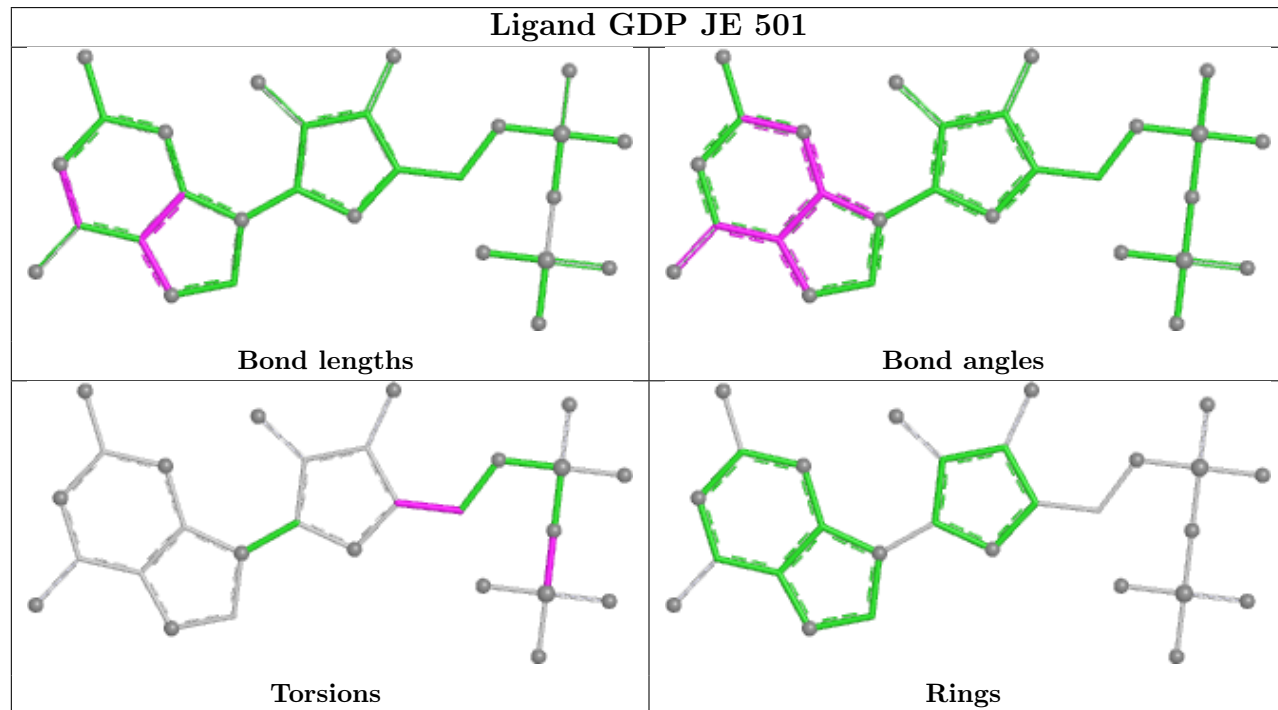
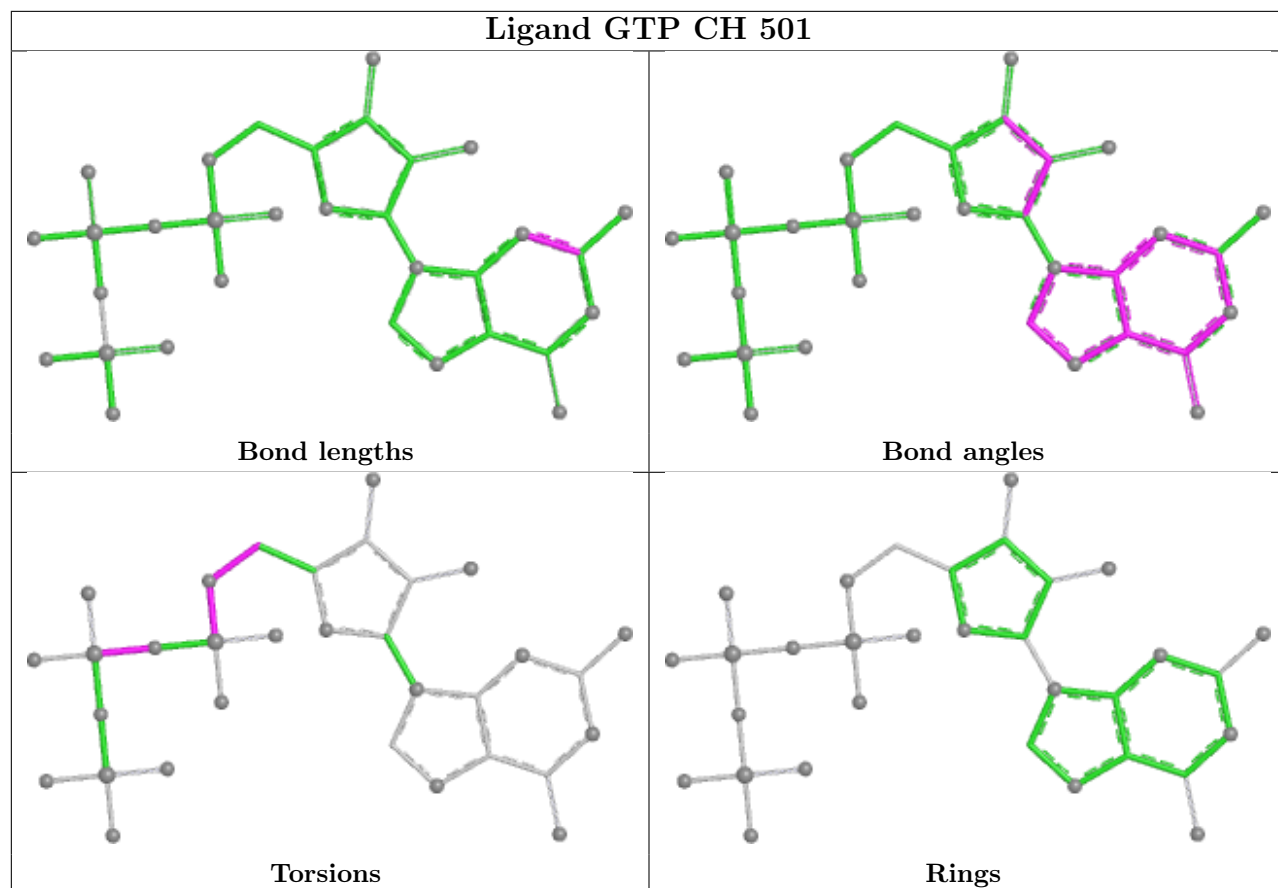


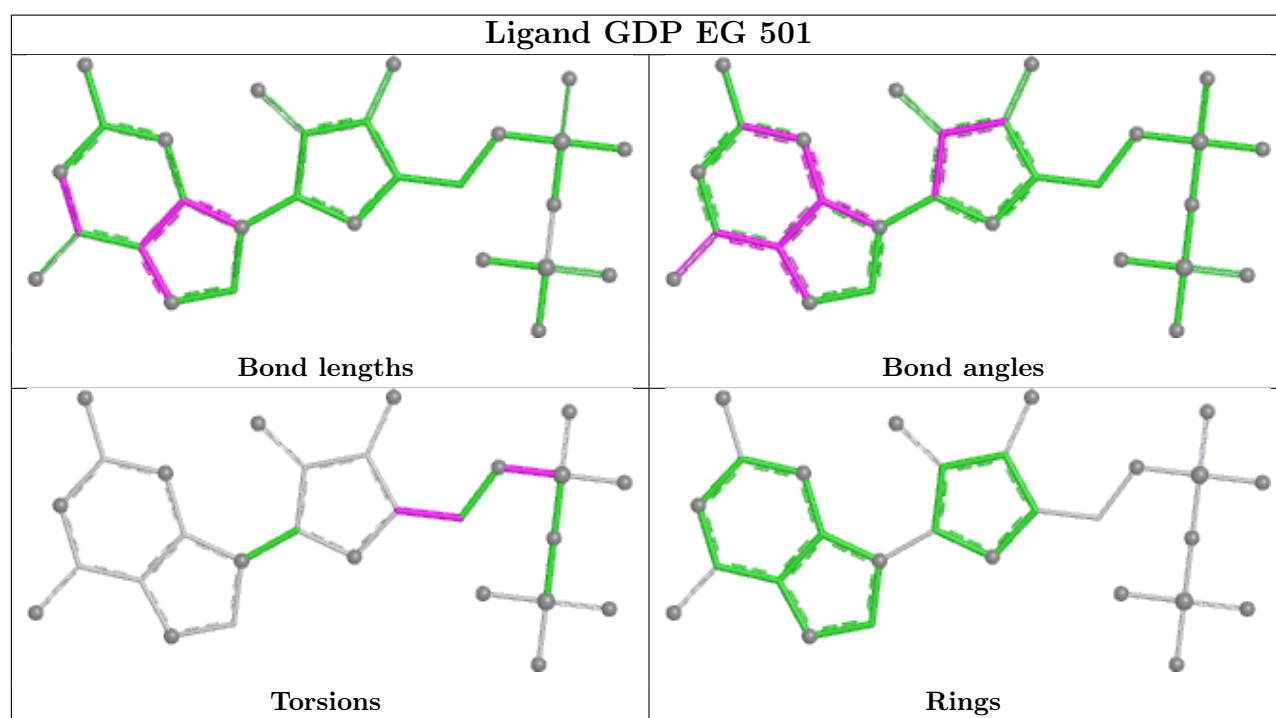
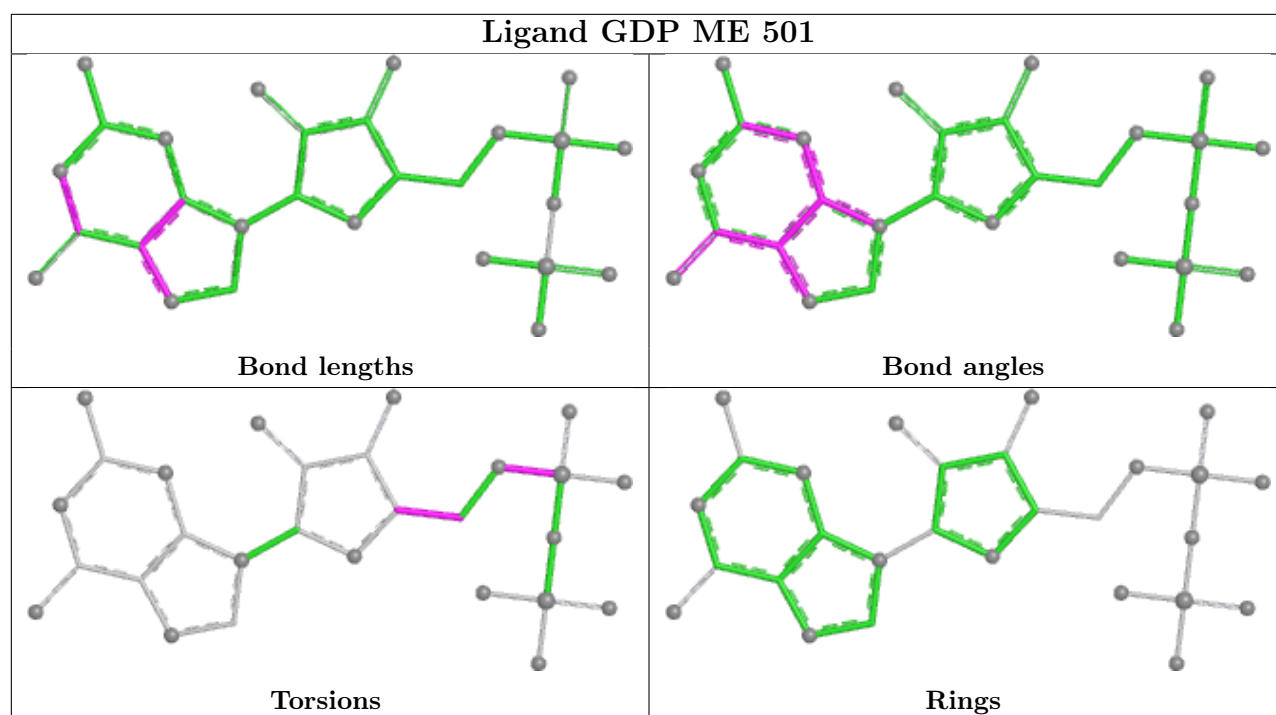


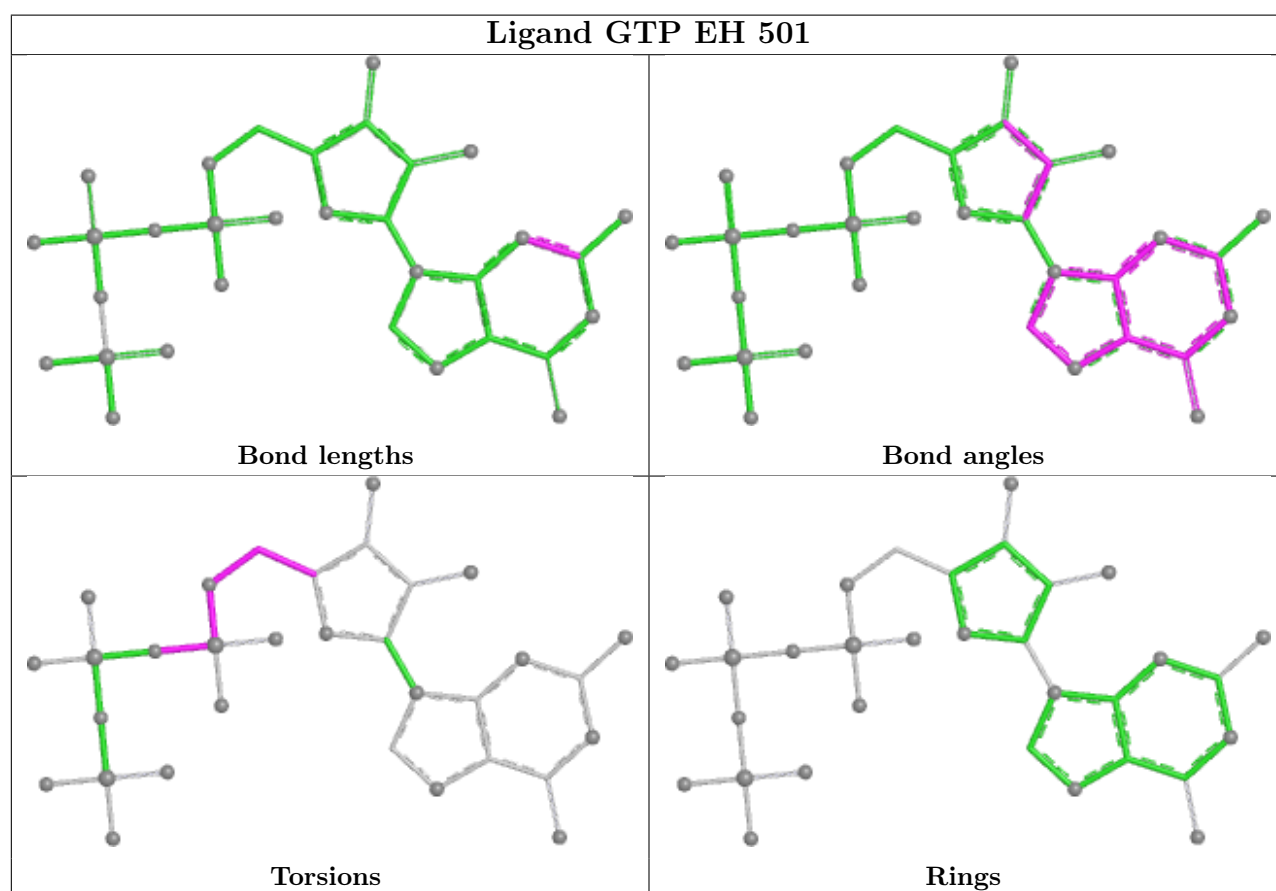
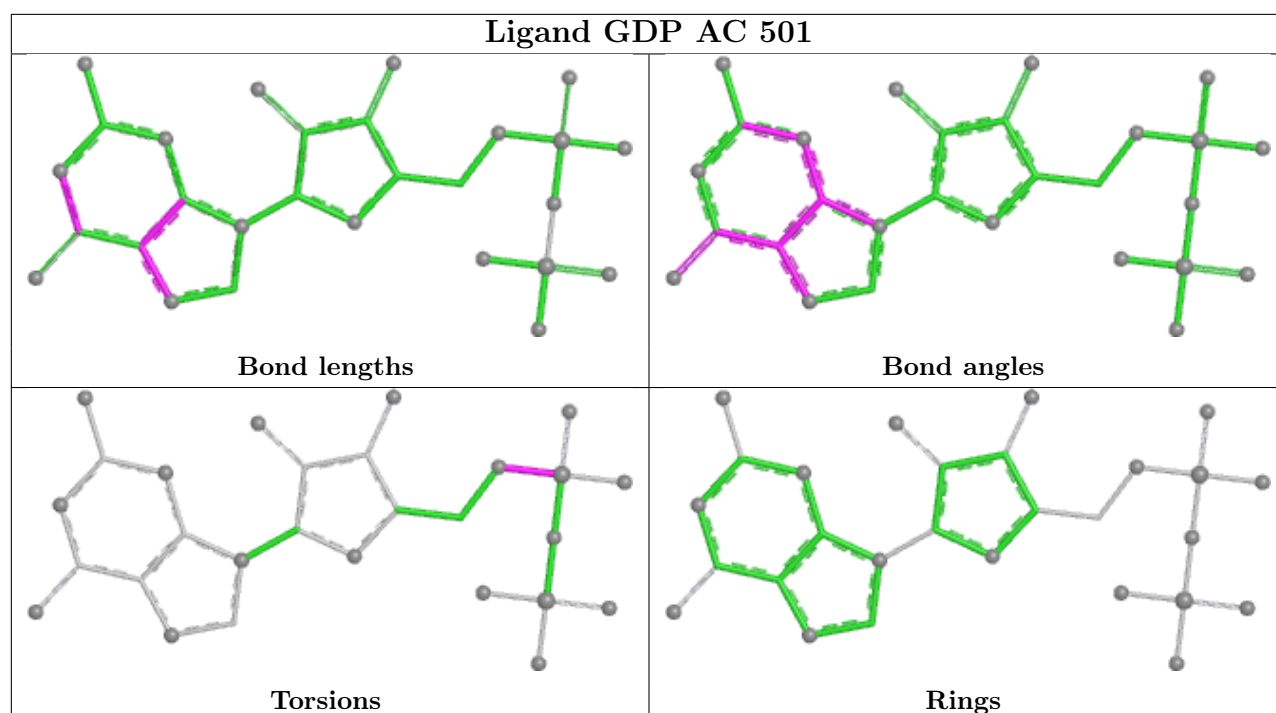


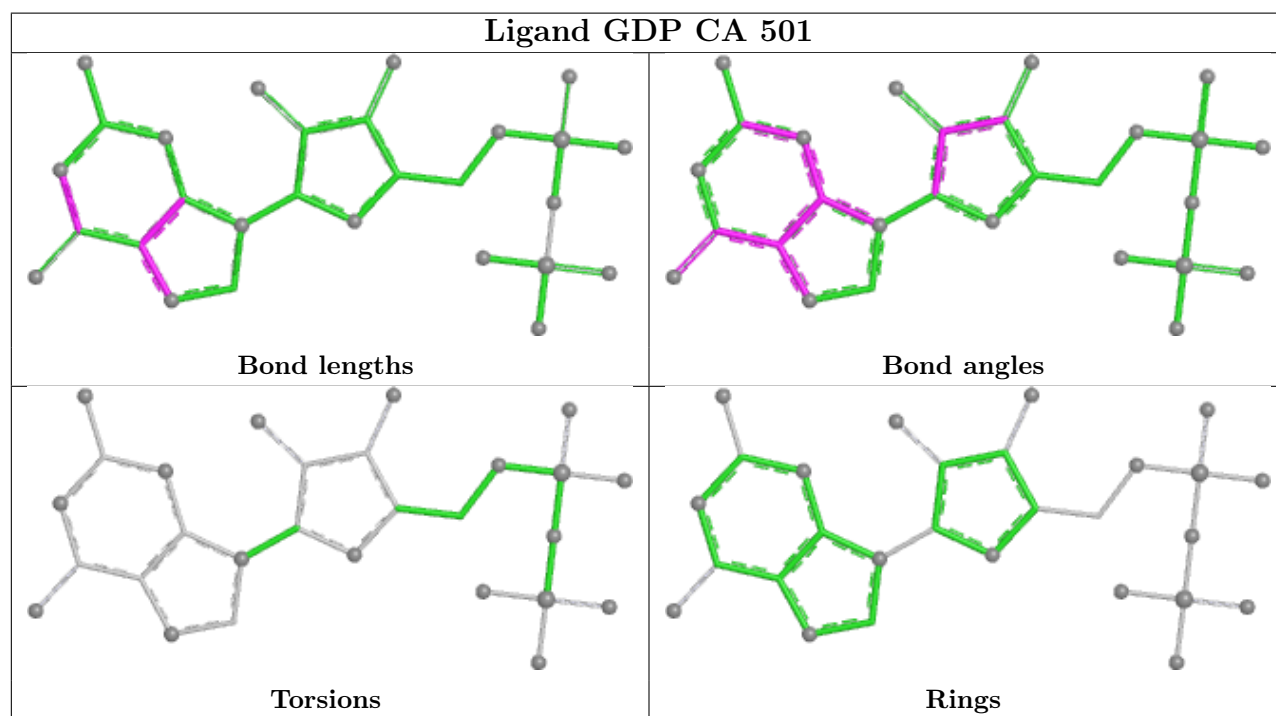
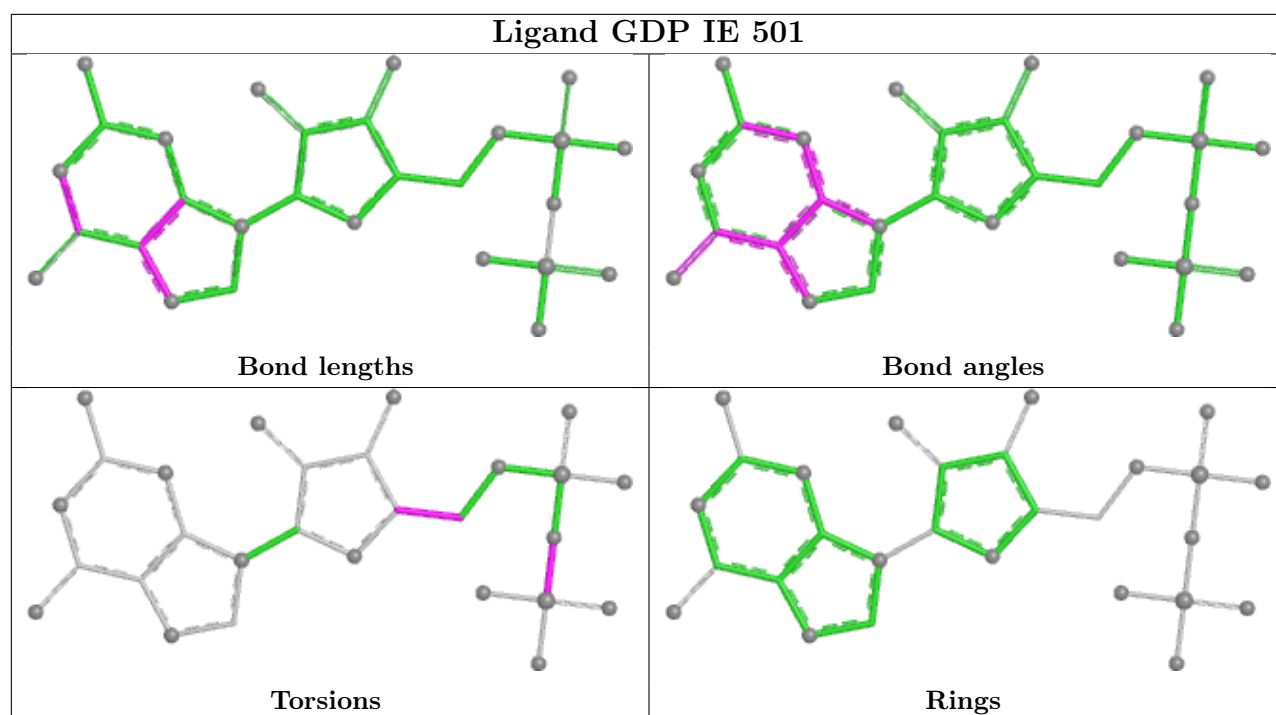


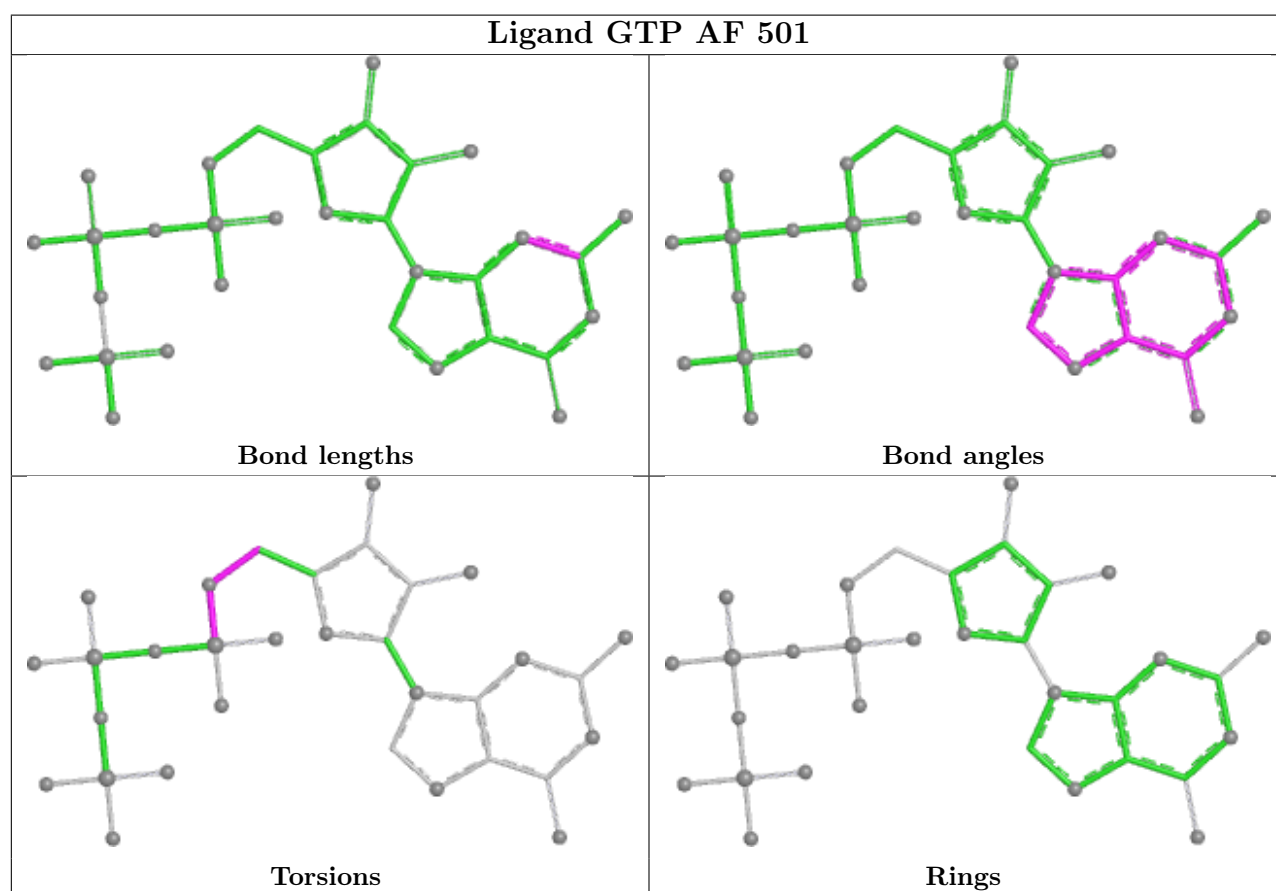
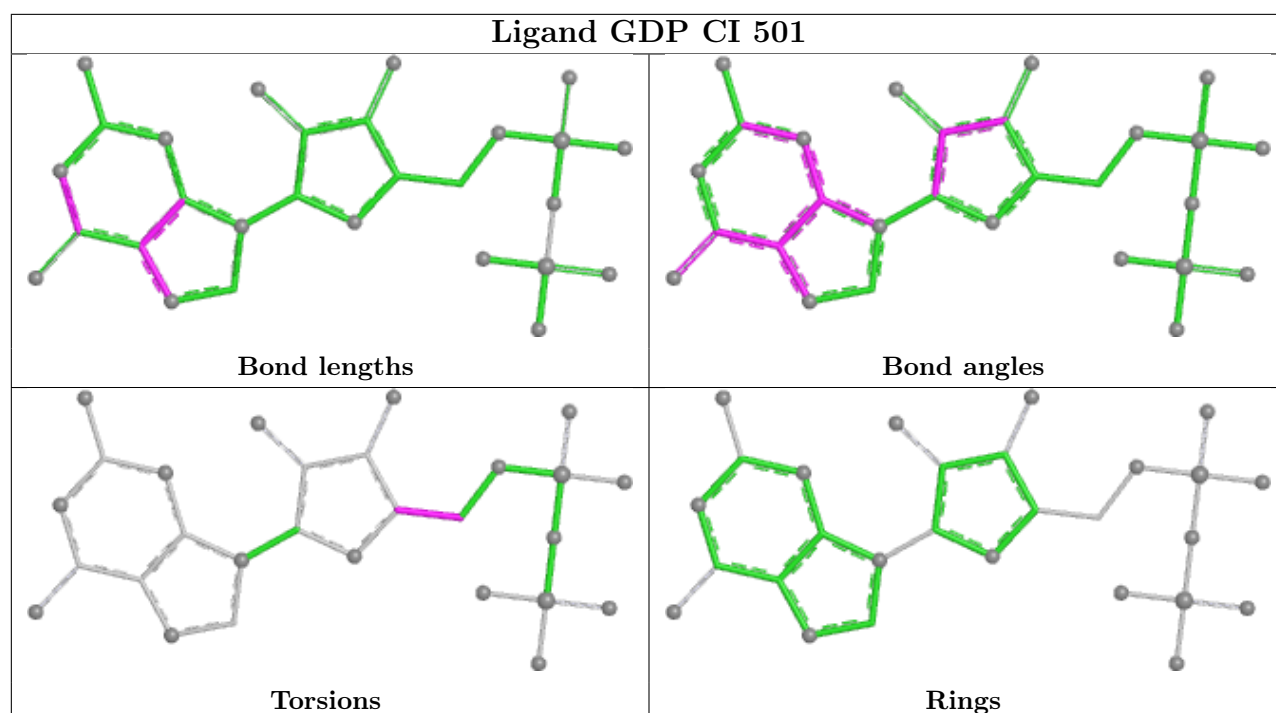




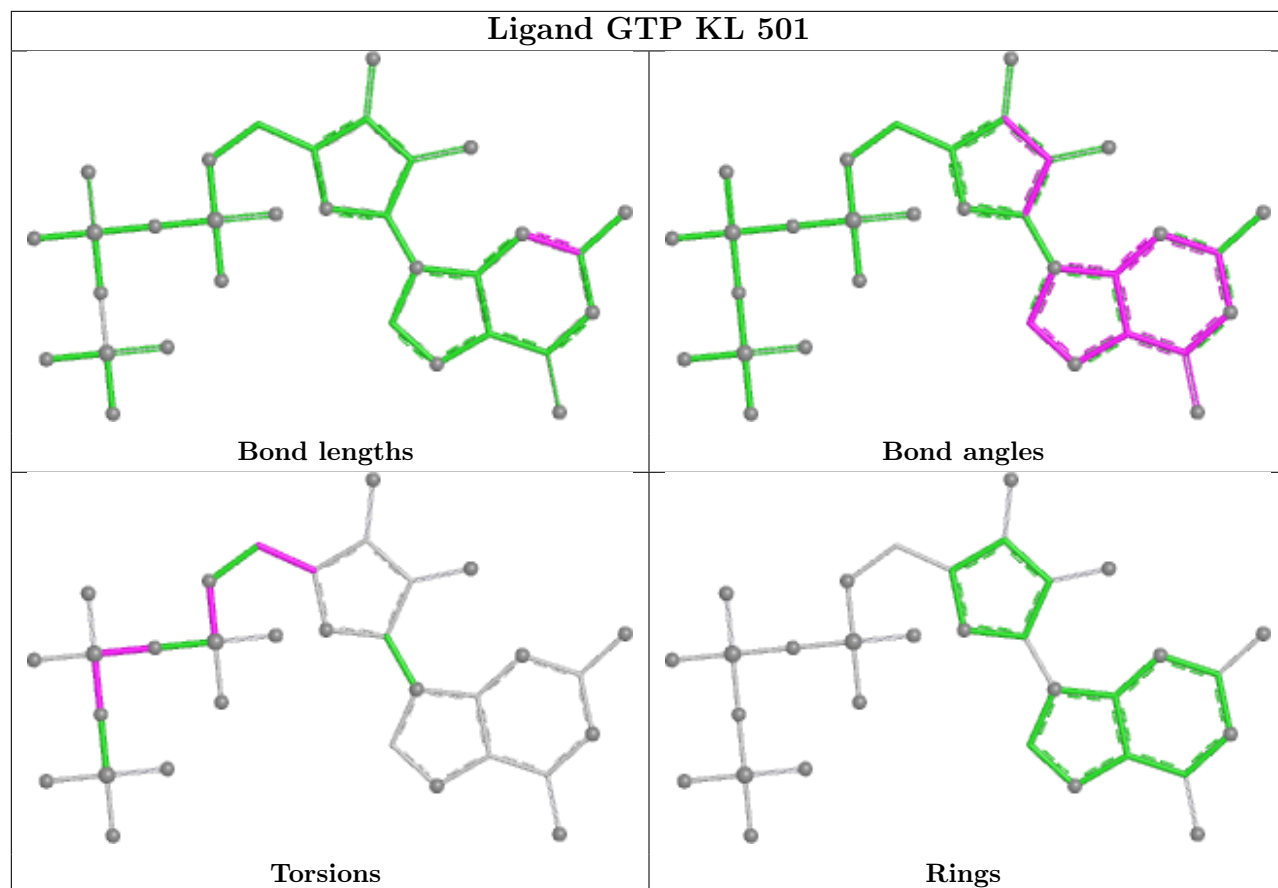




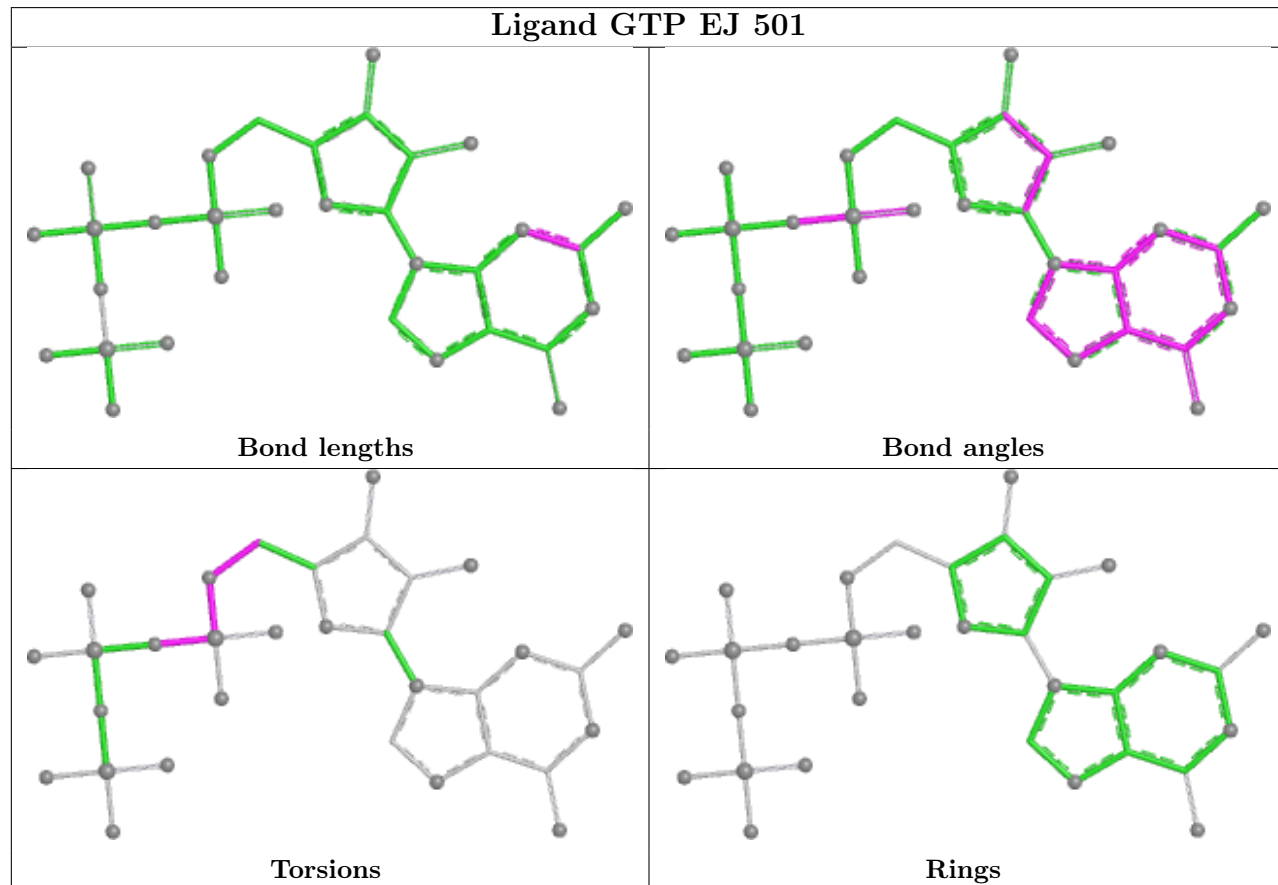




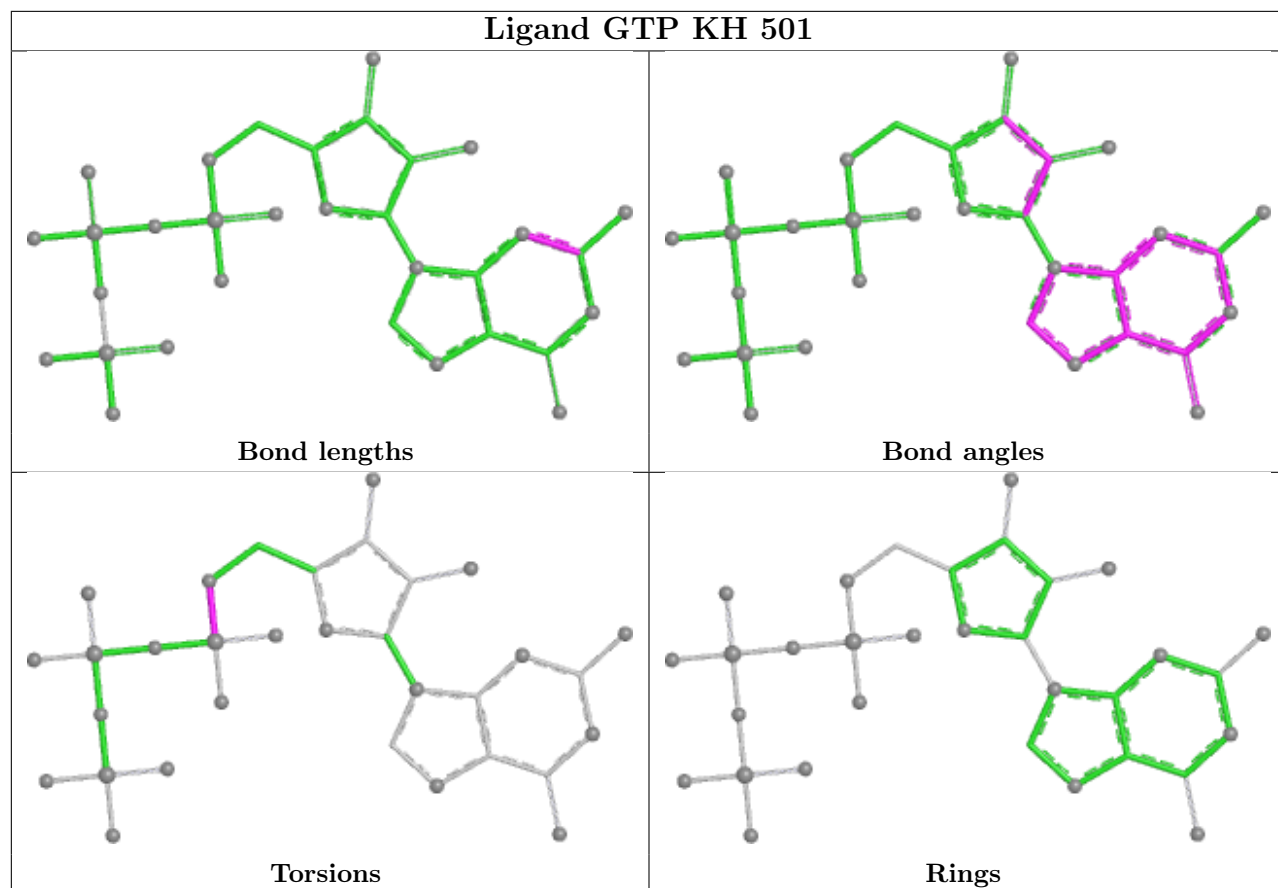
Ligand GTP KL 501



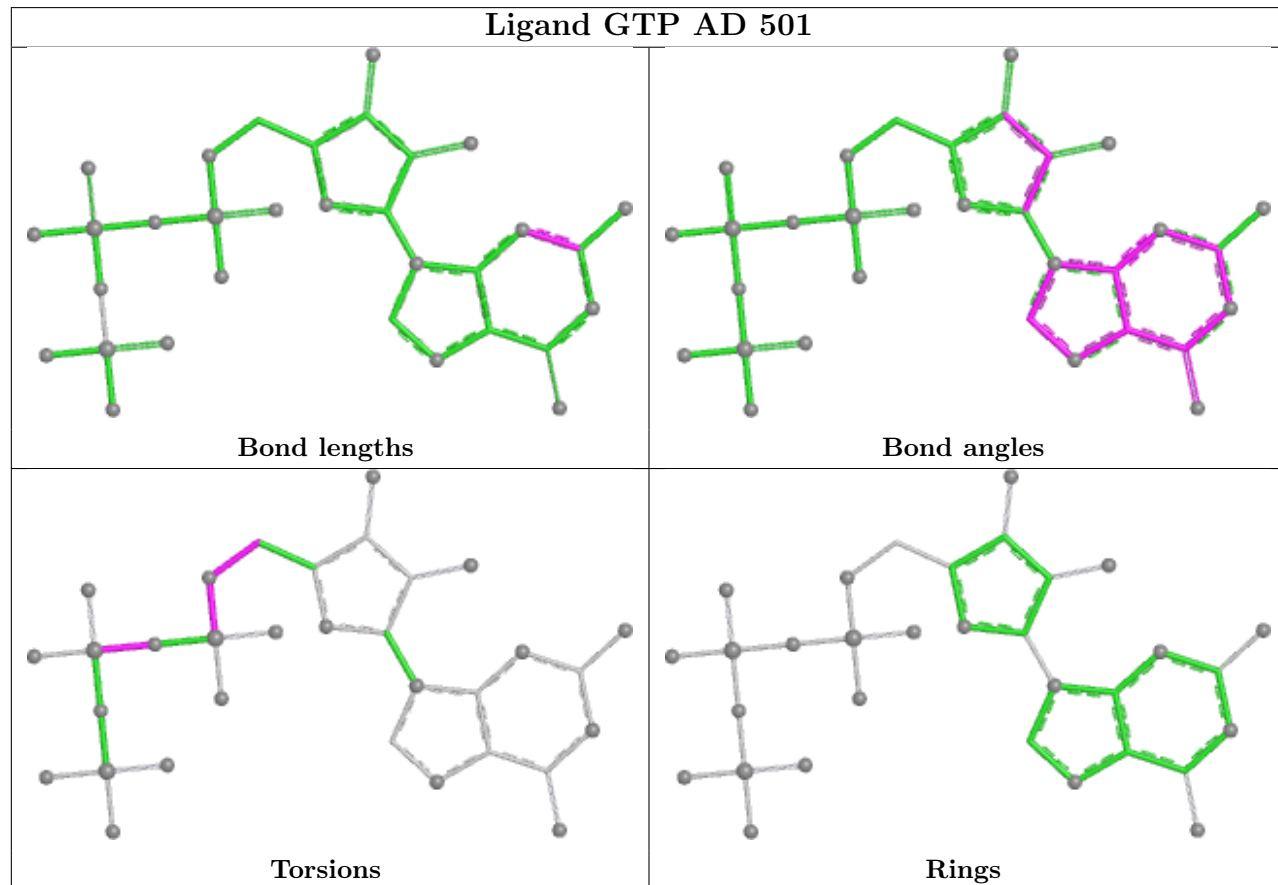
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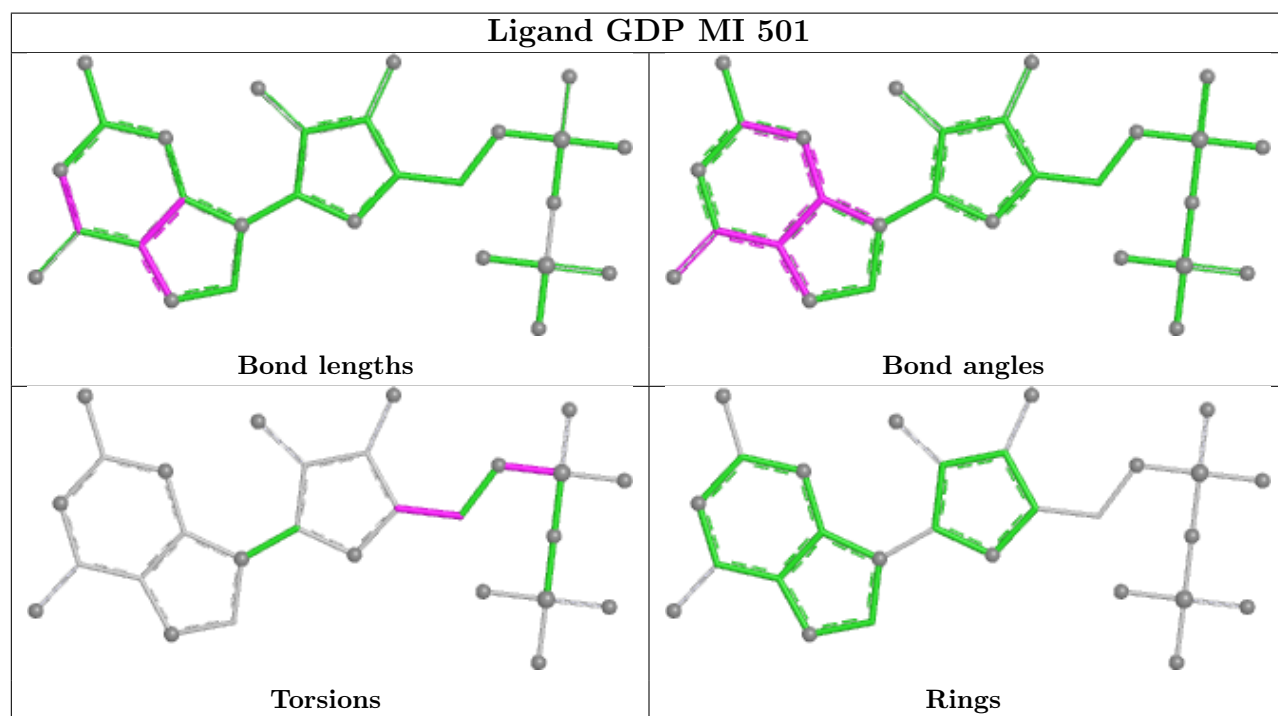
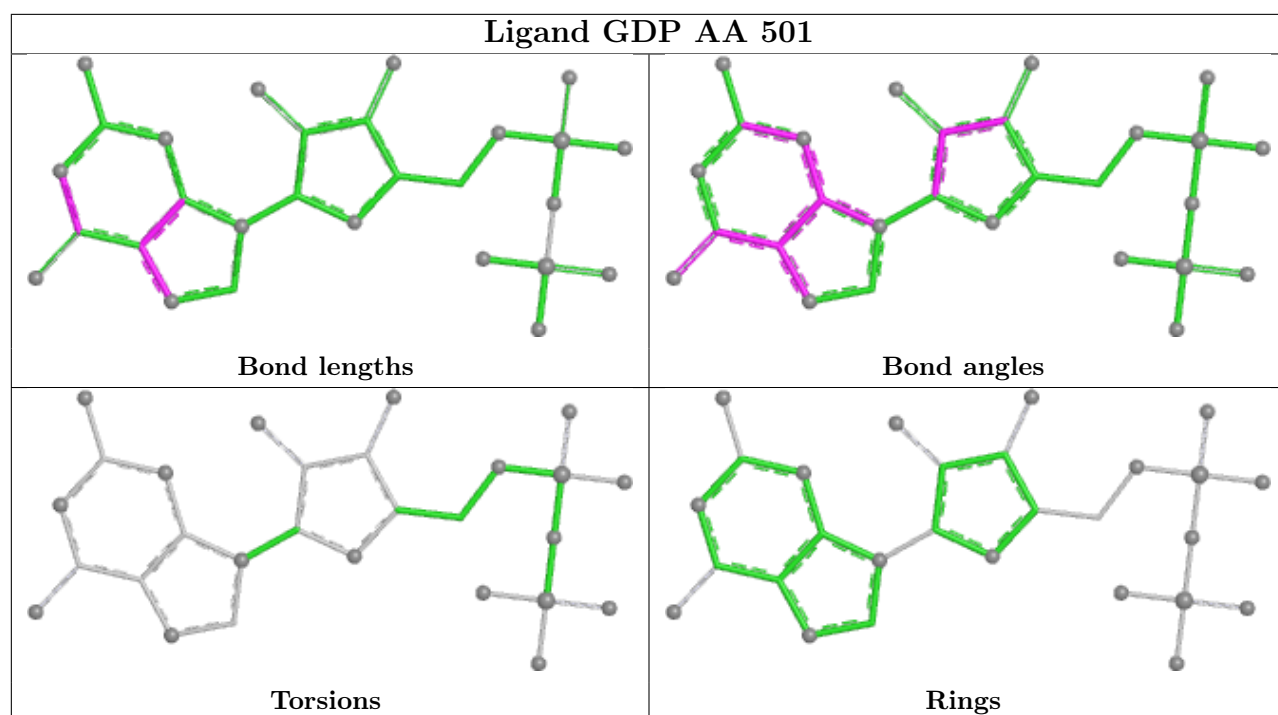


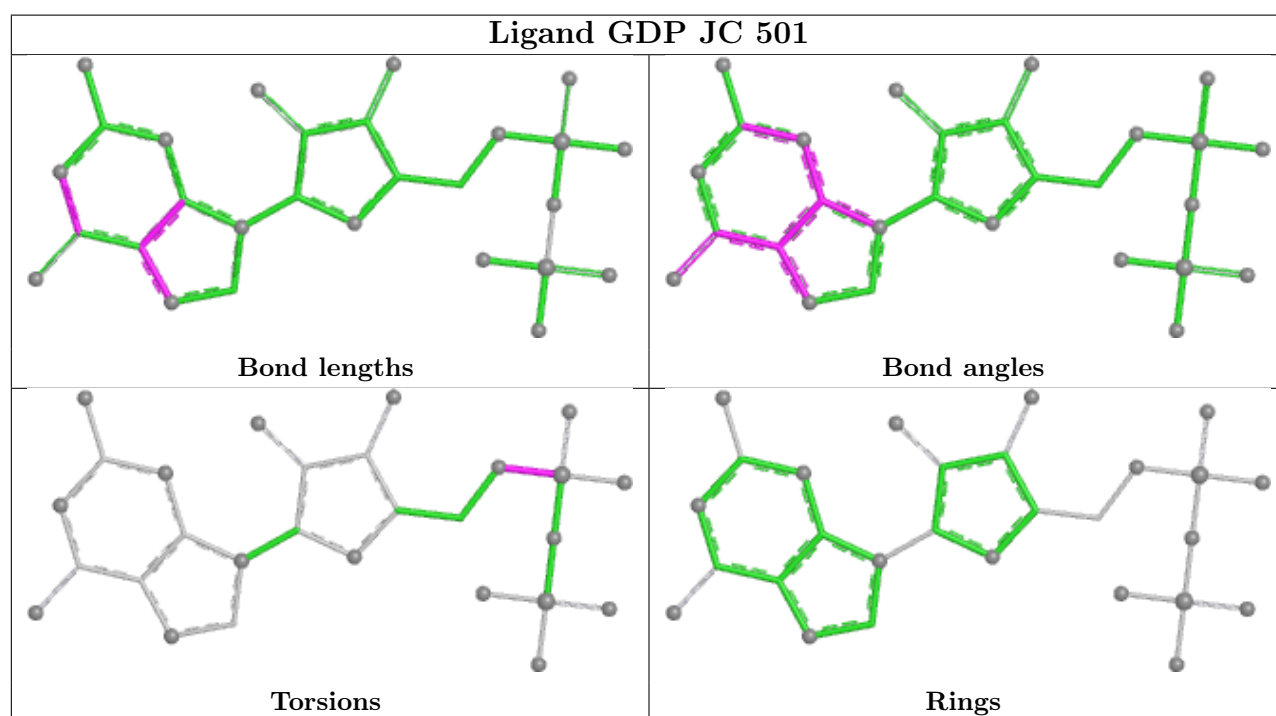
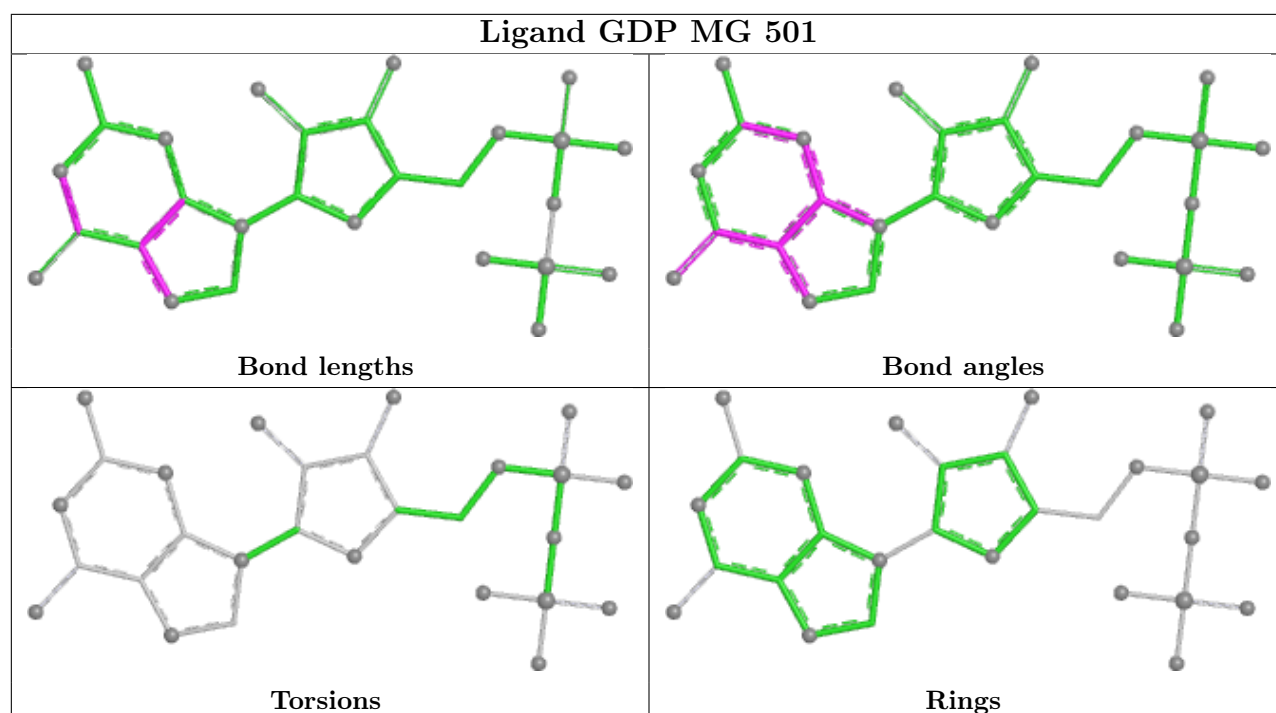
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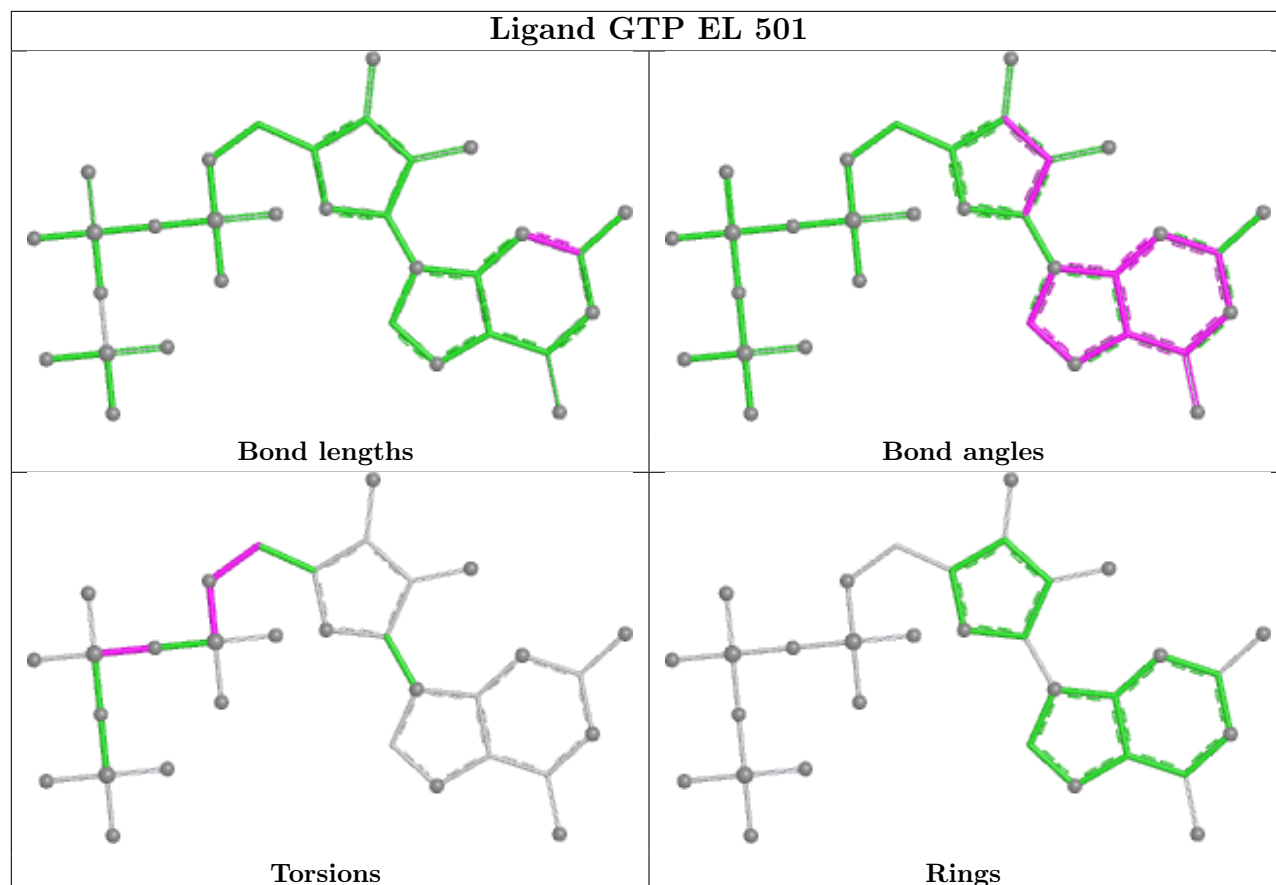
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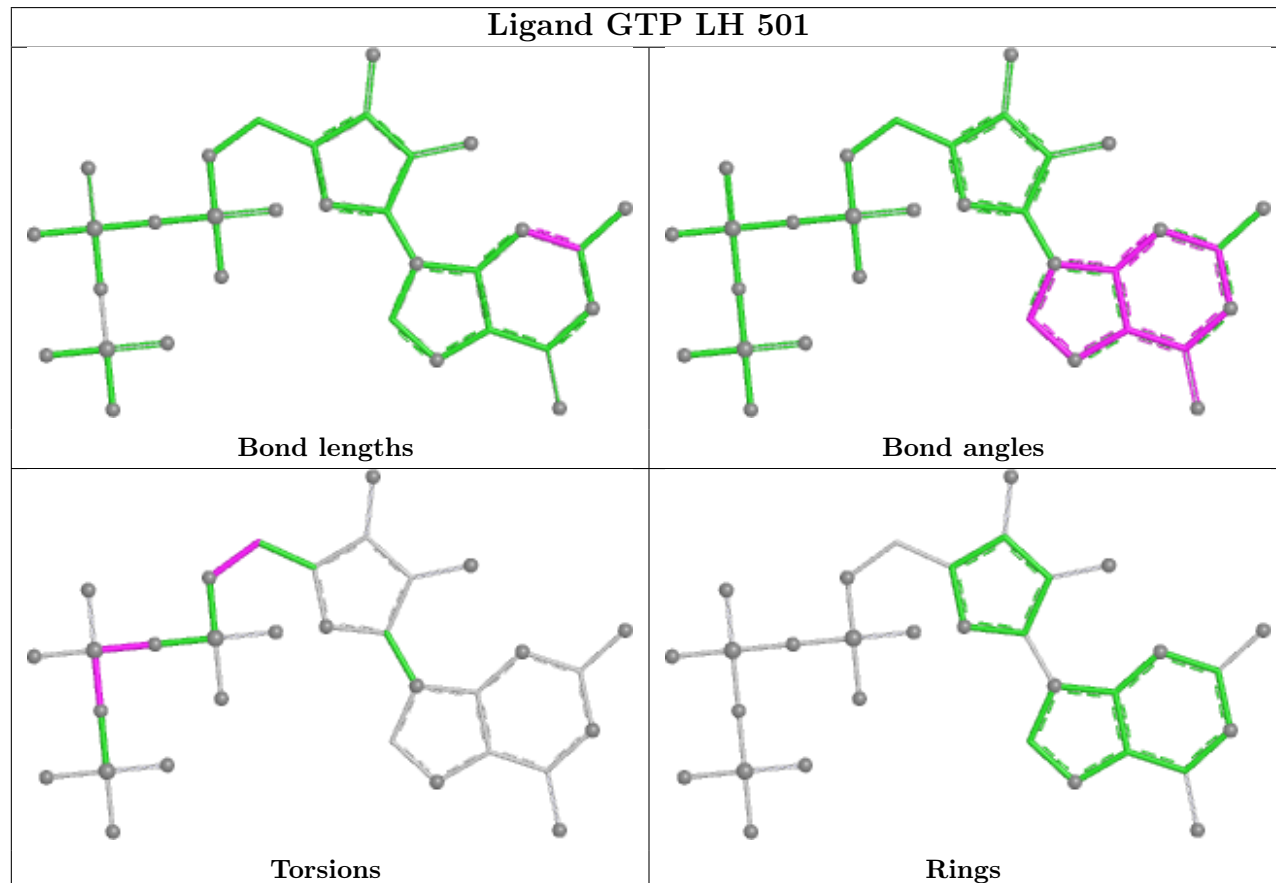


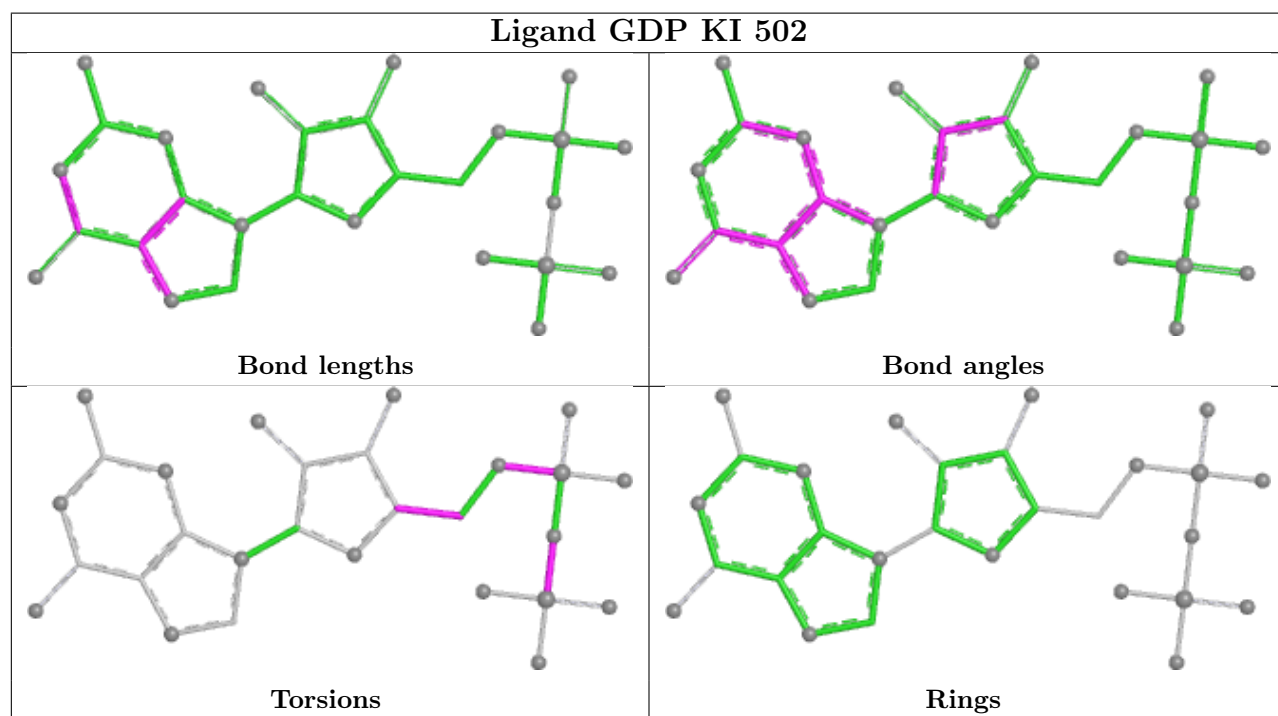
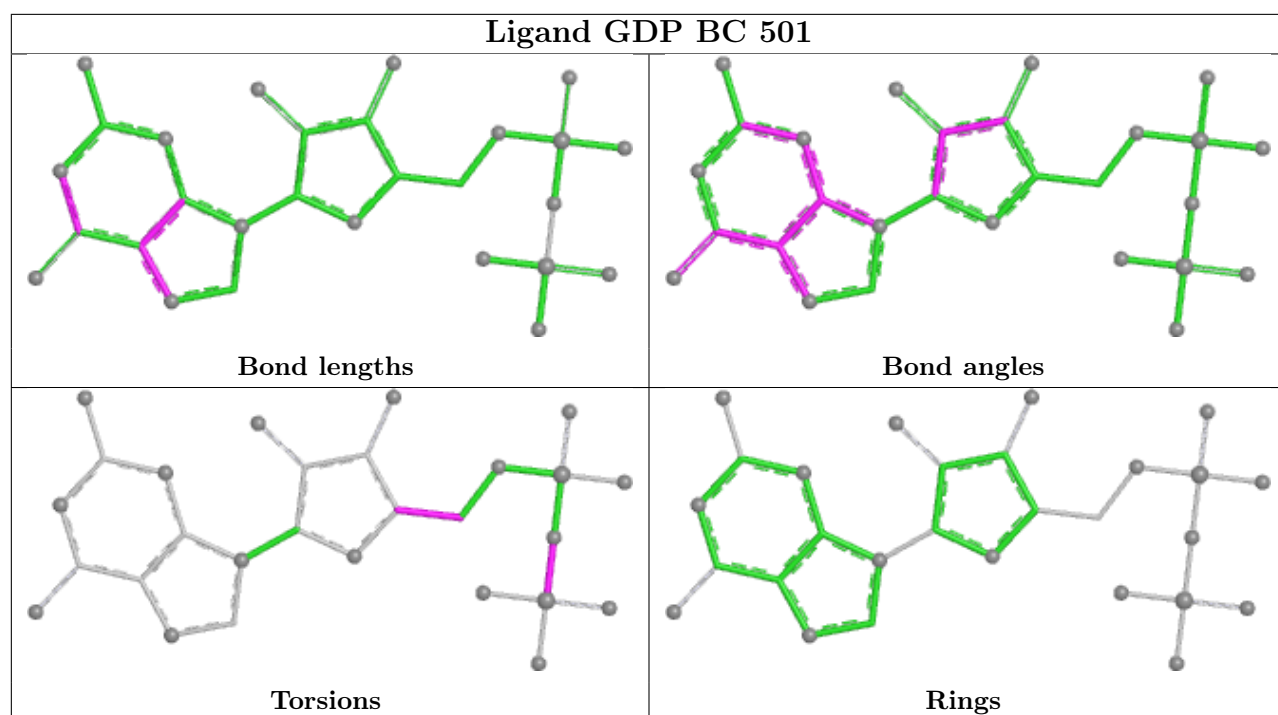


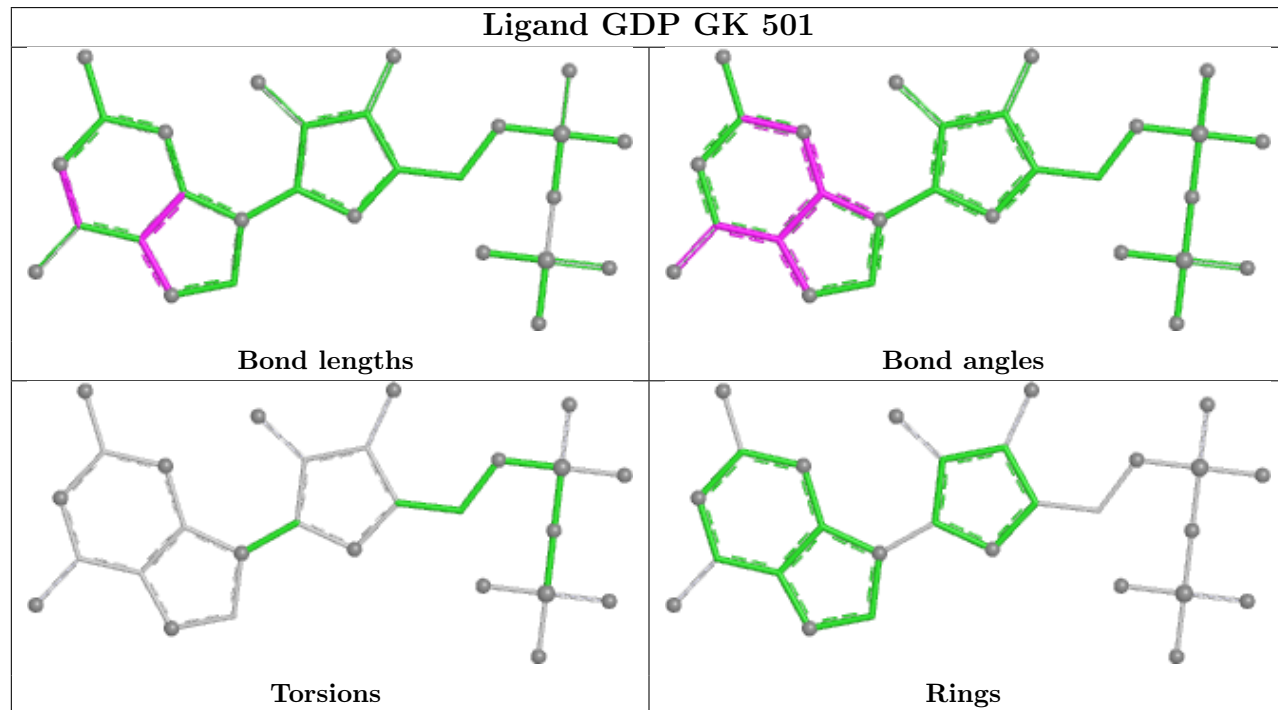
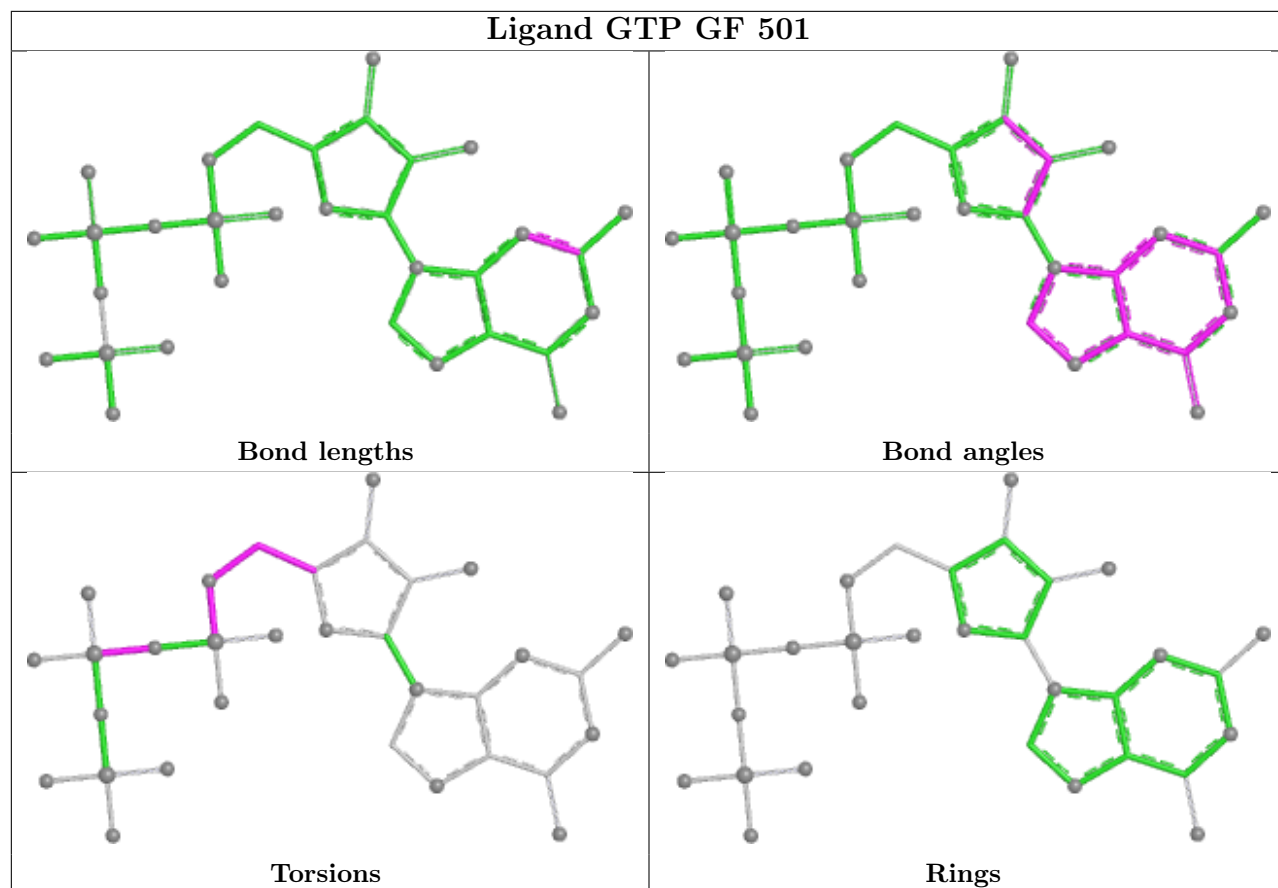
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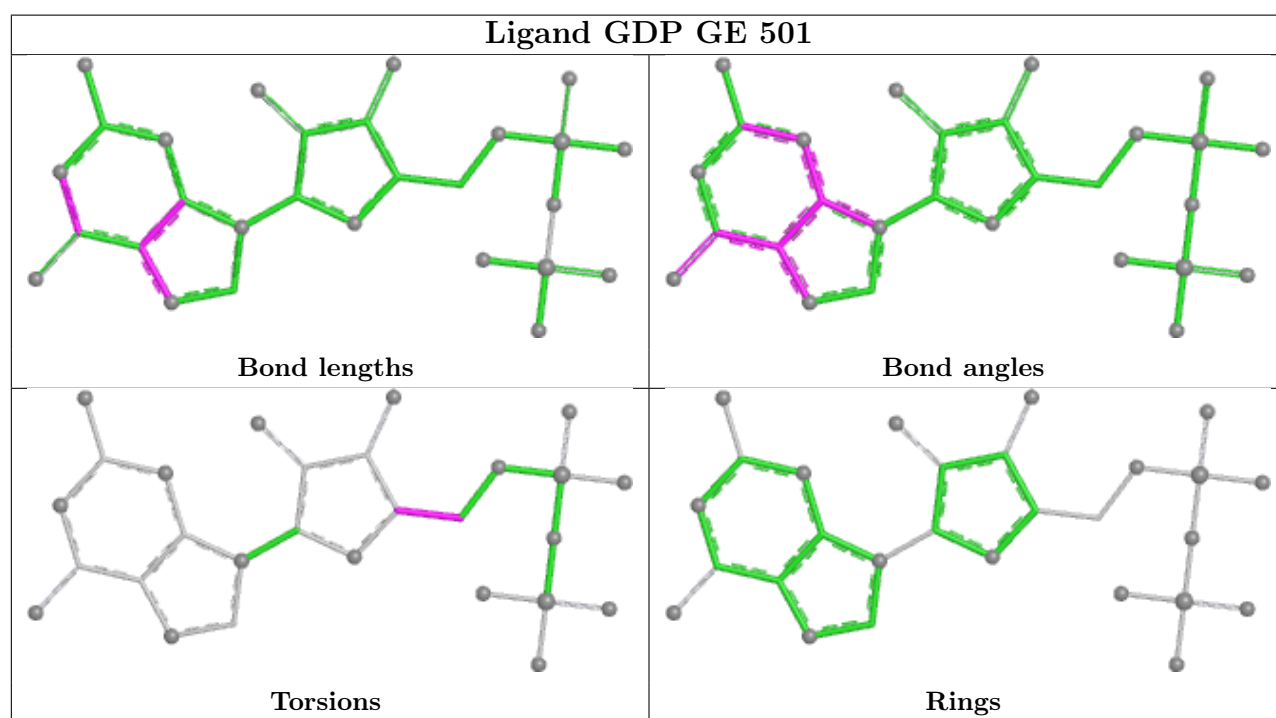
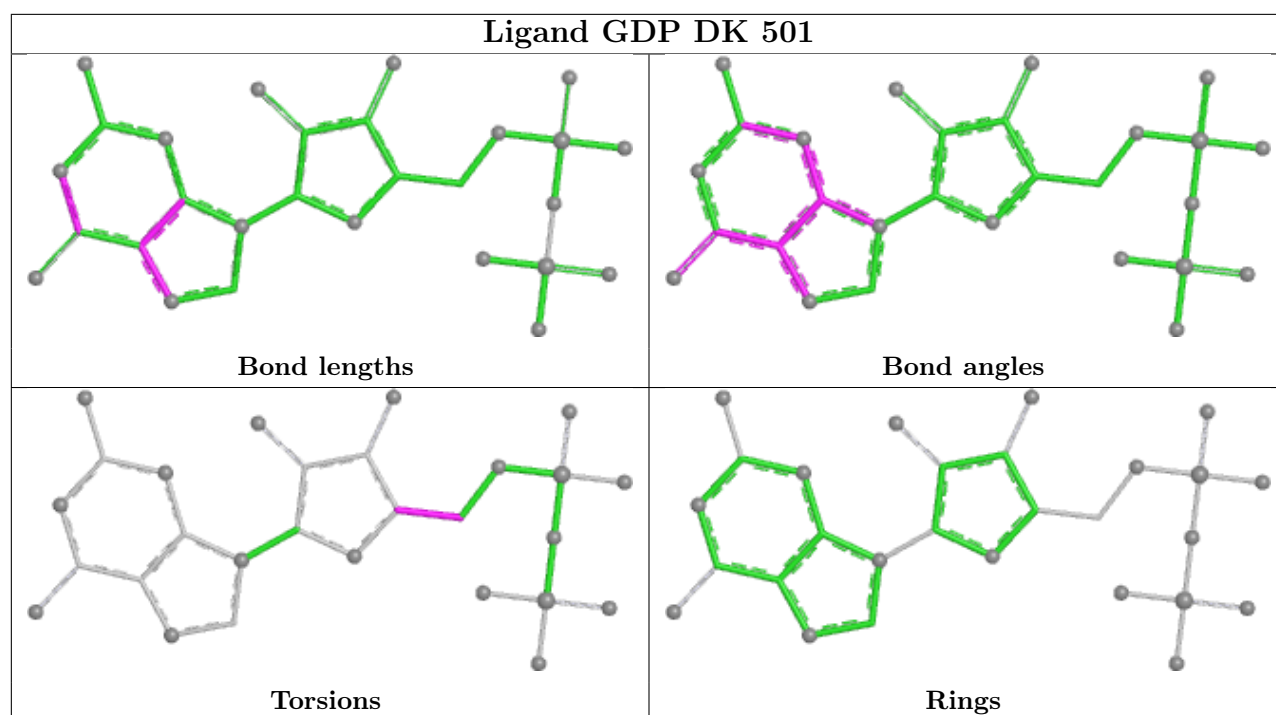


Ligand GTP LH 501

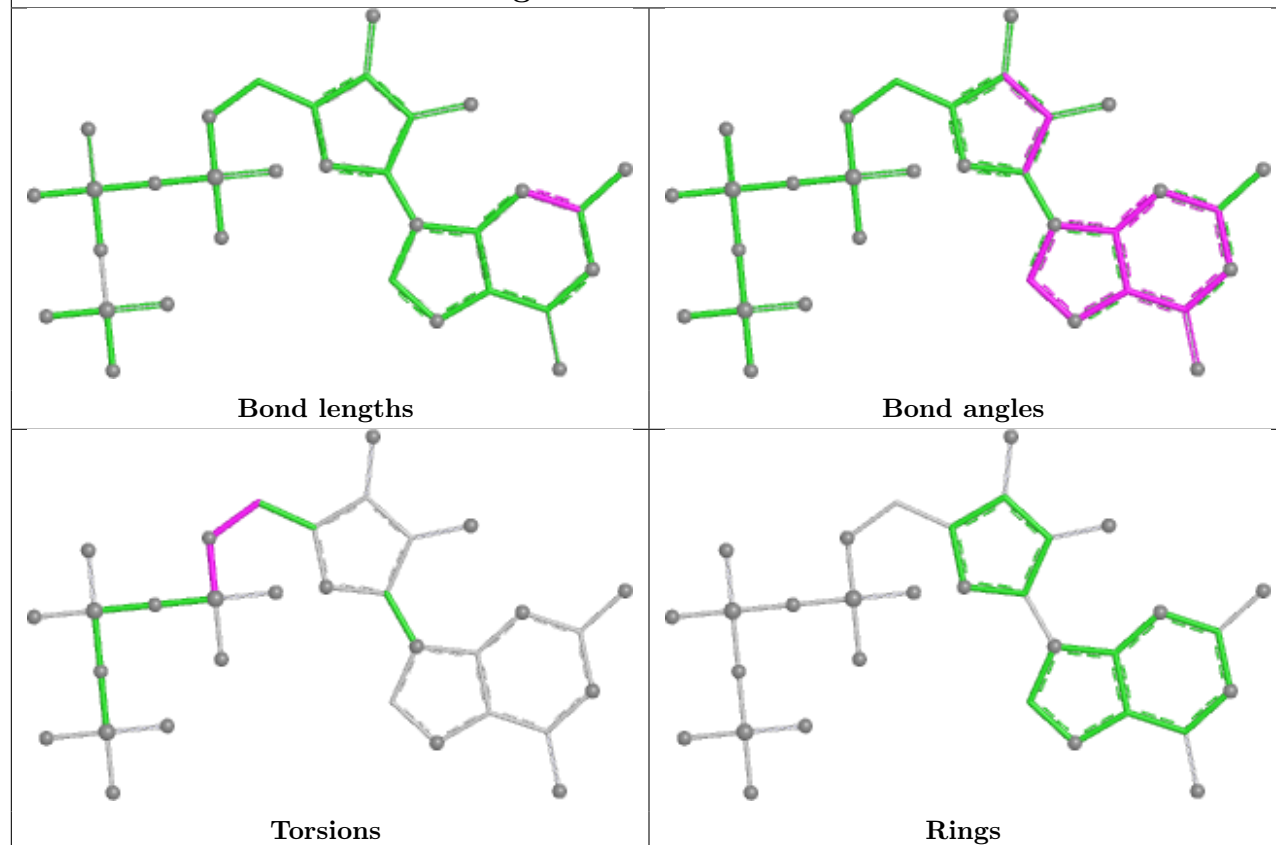




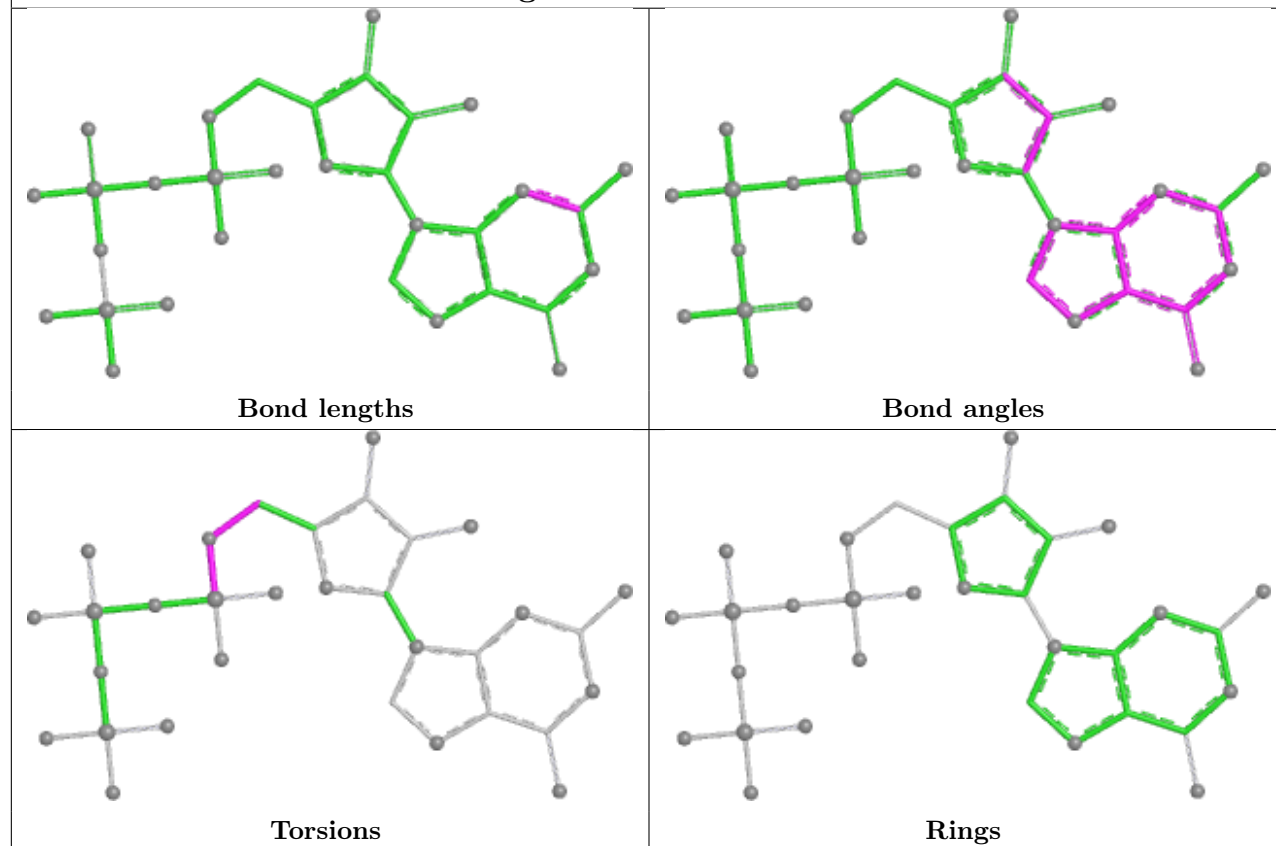


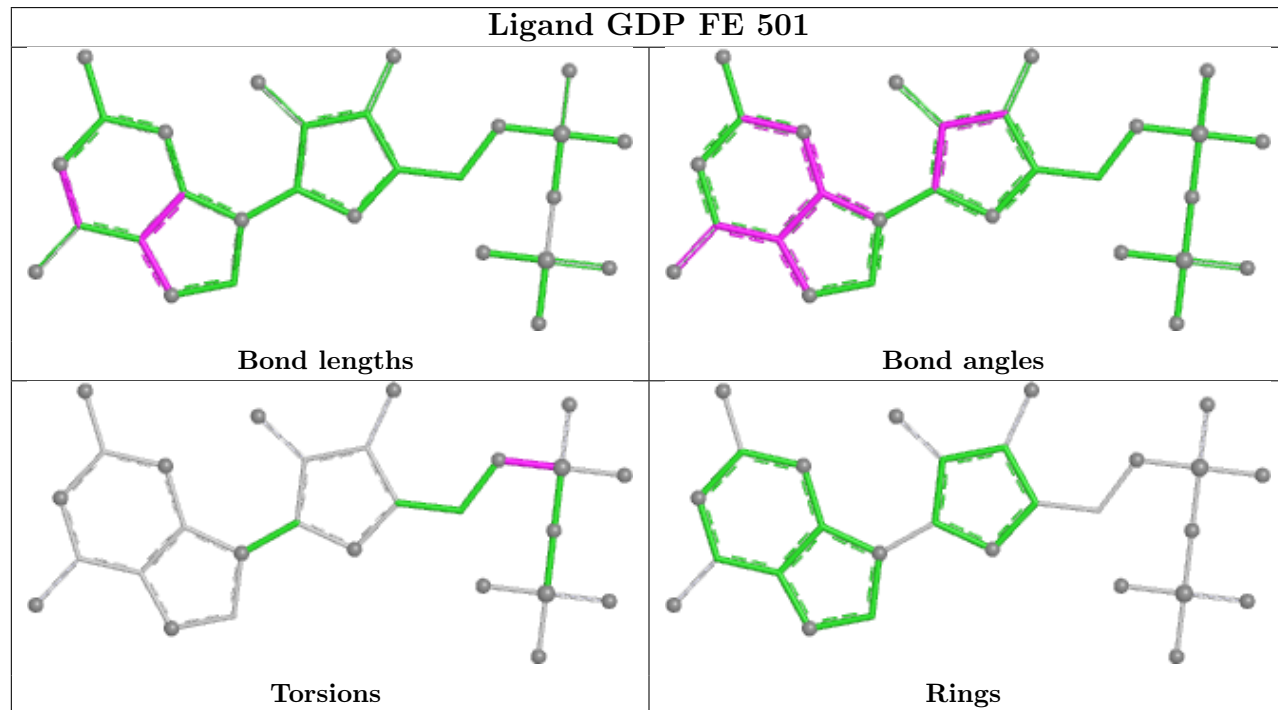
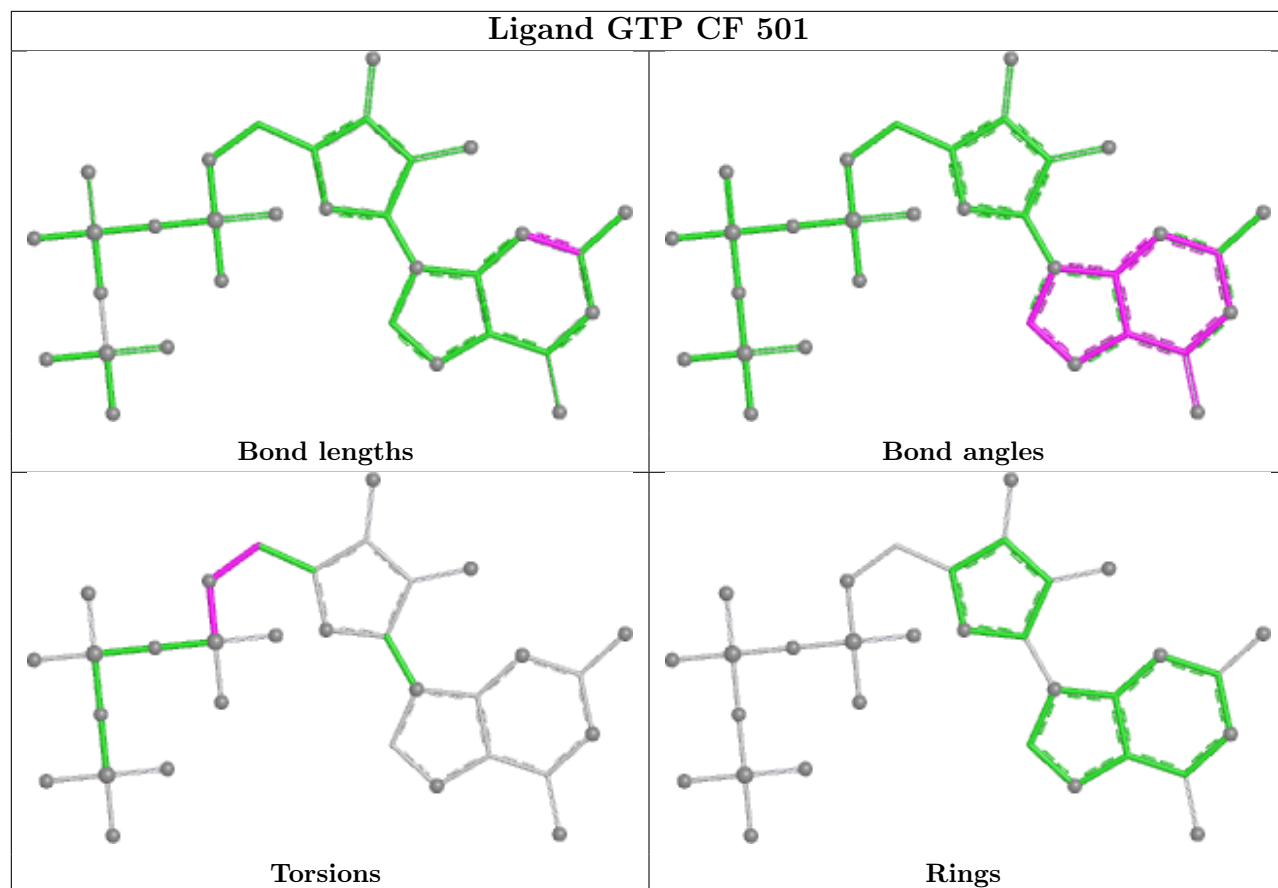


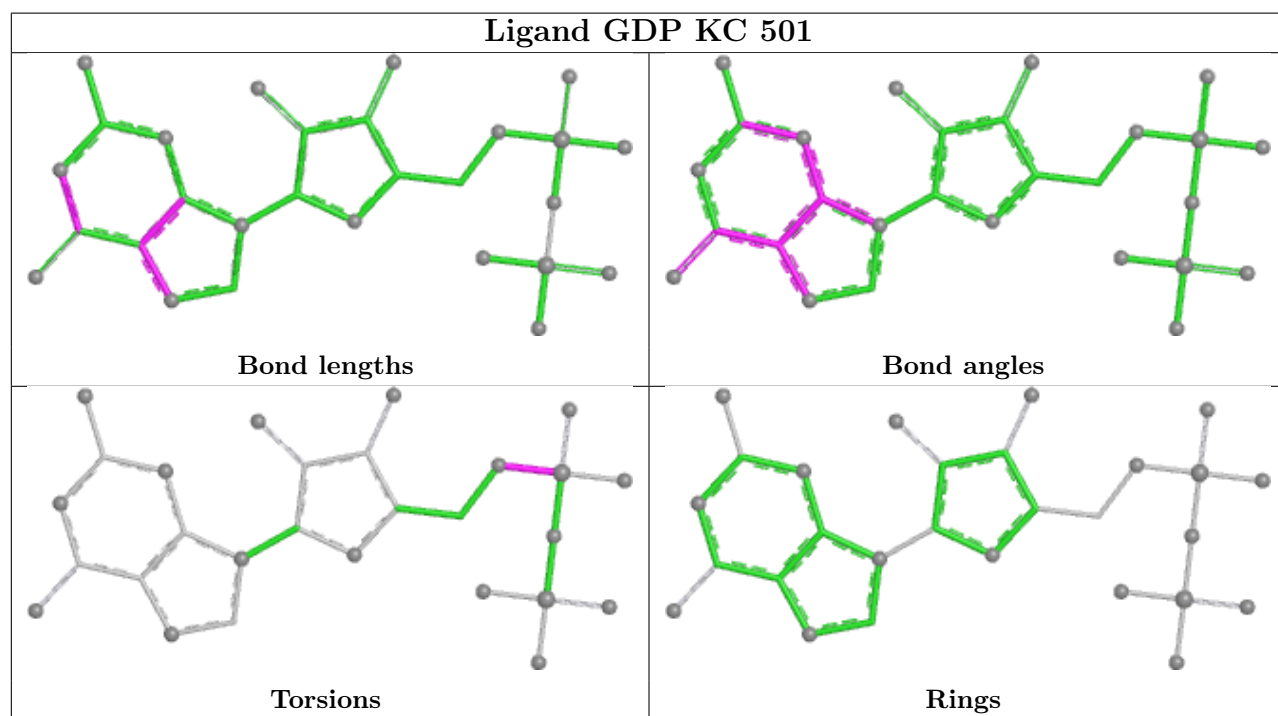
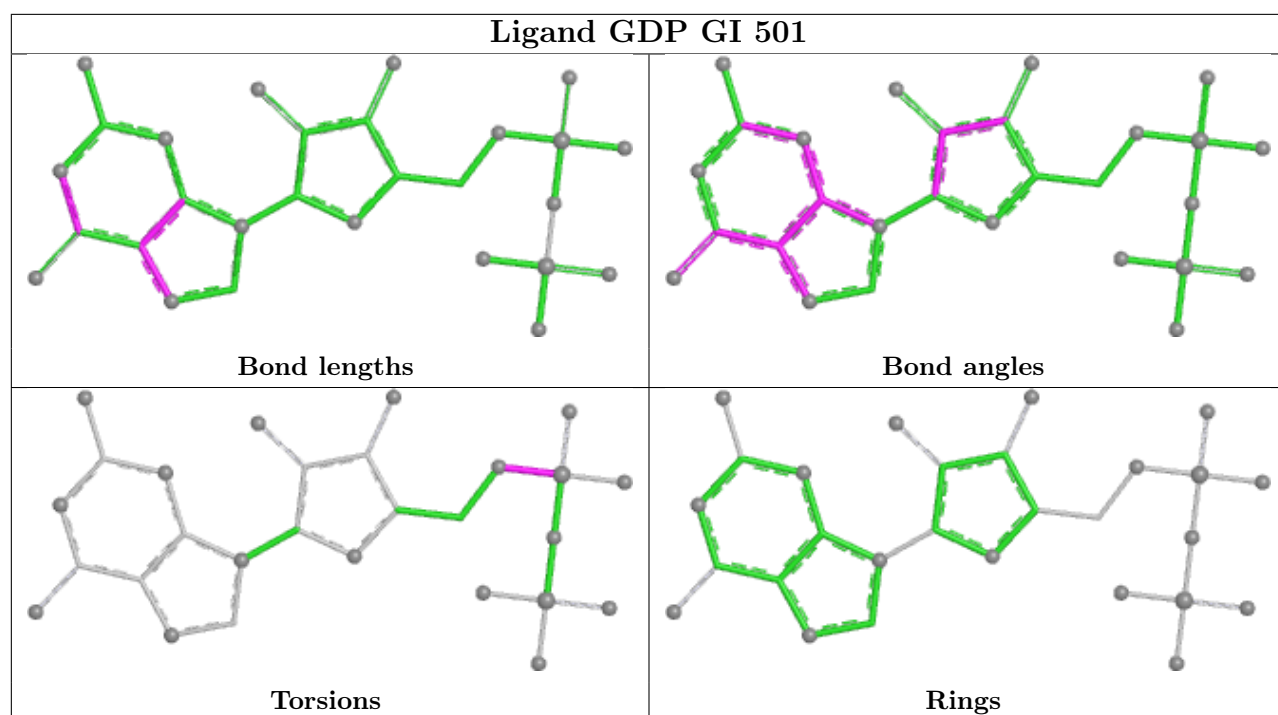
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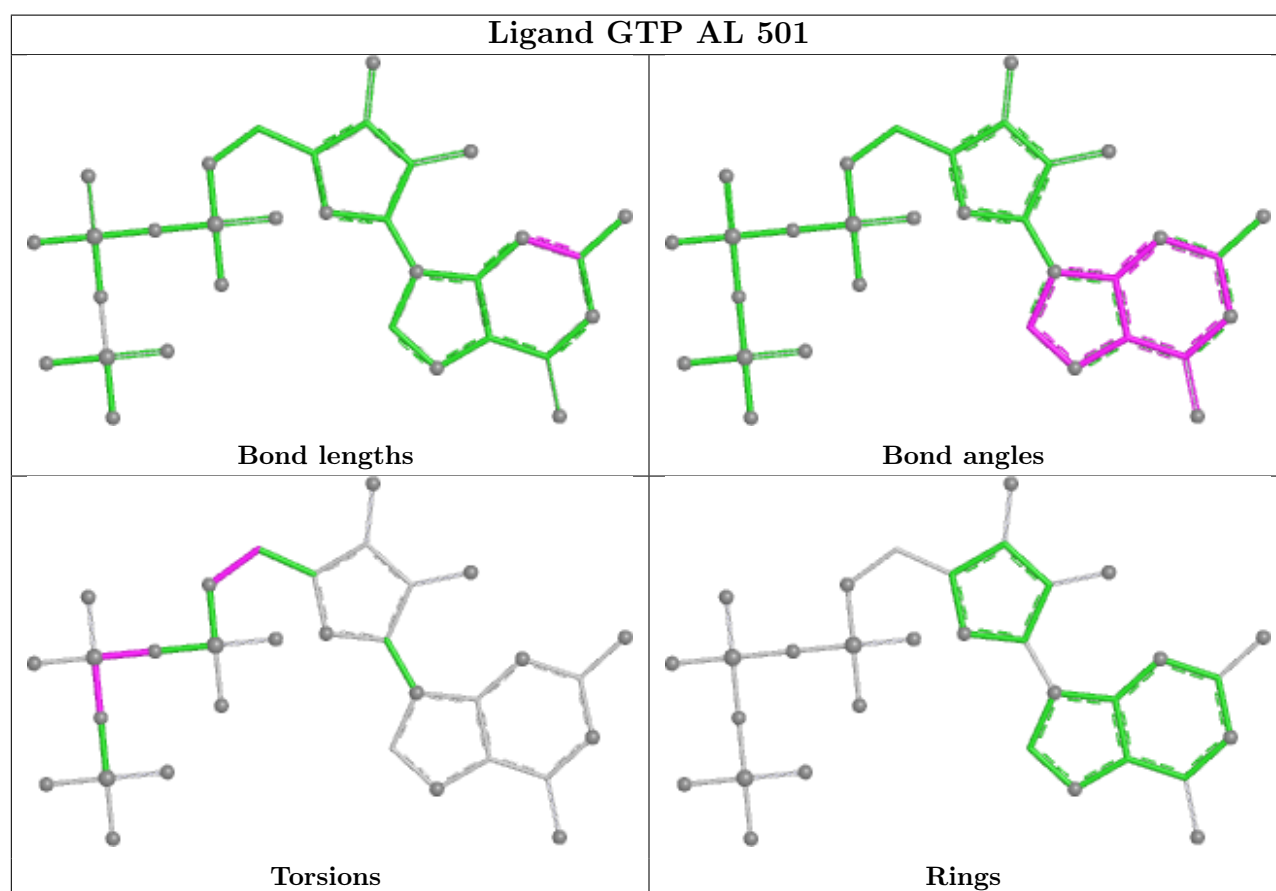
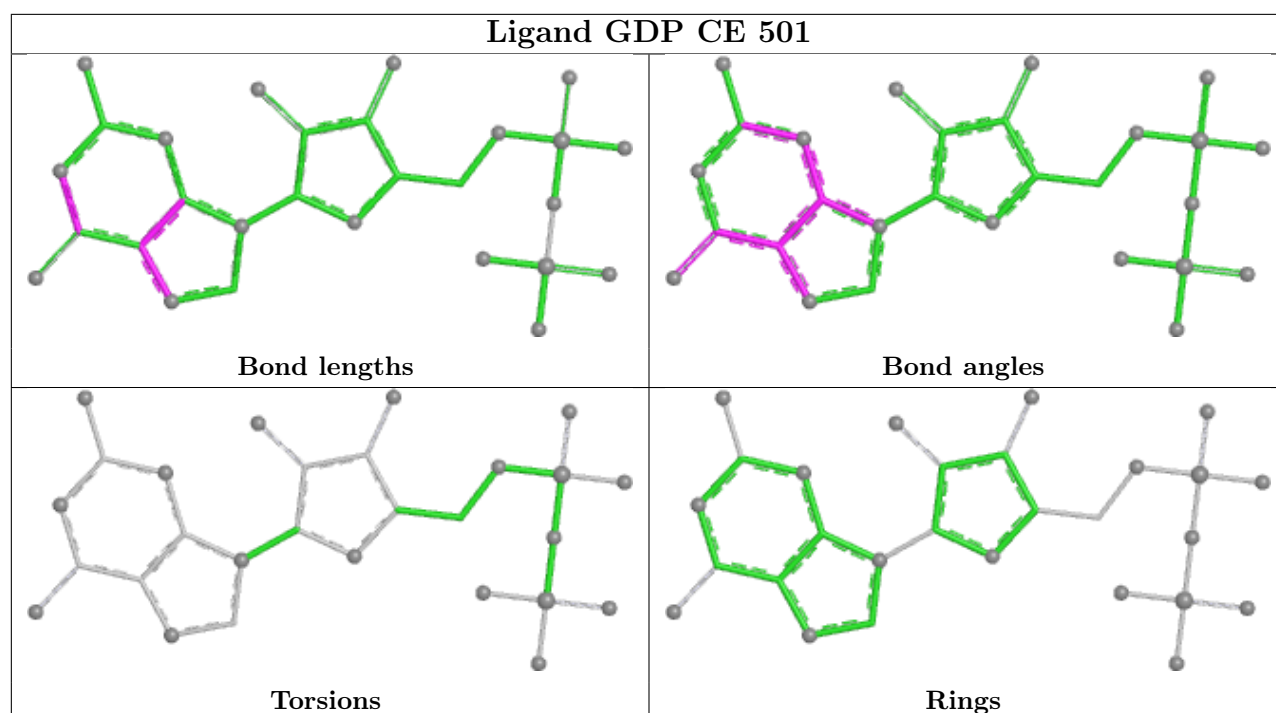


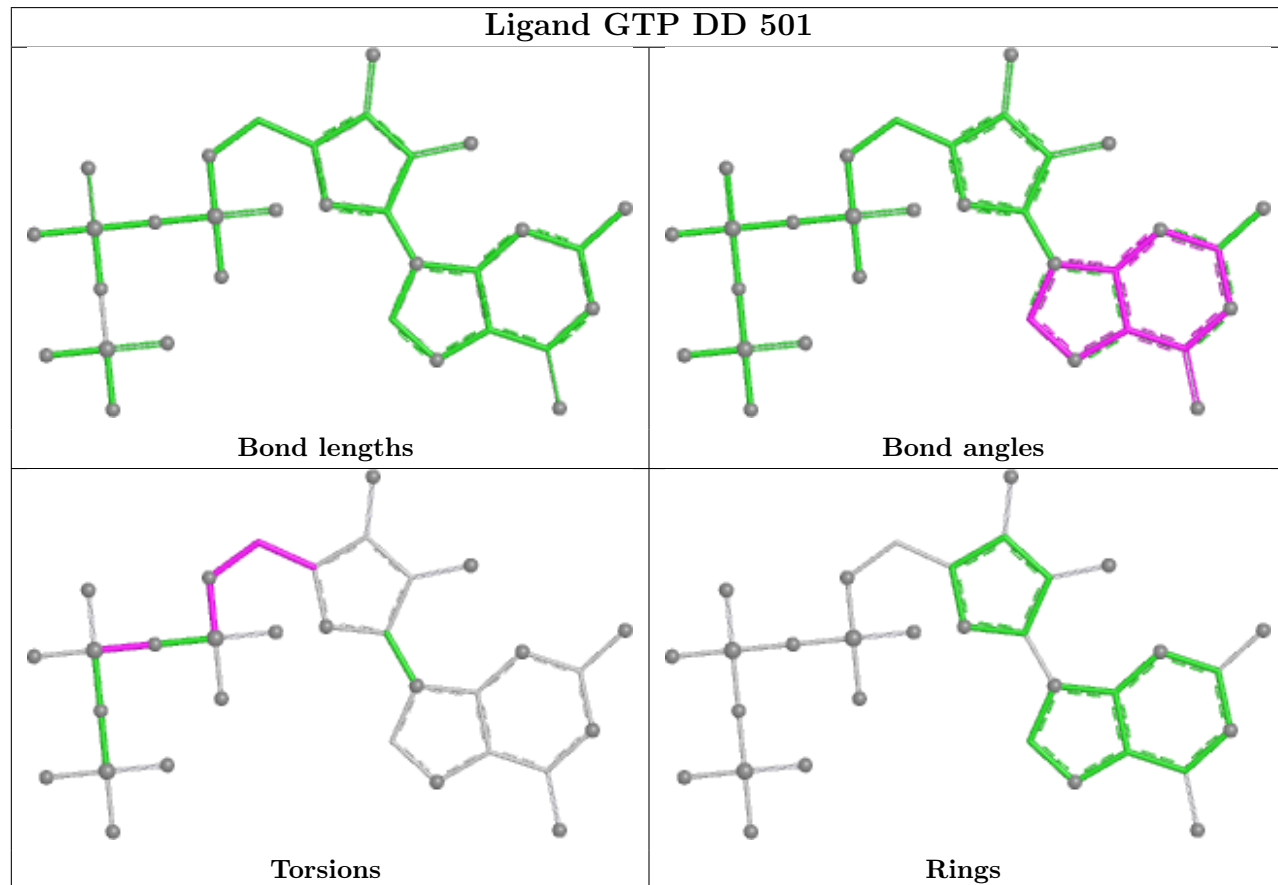
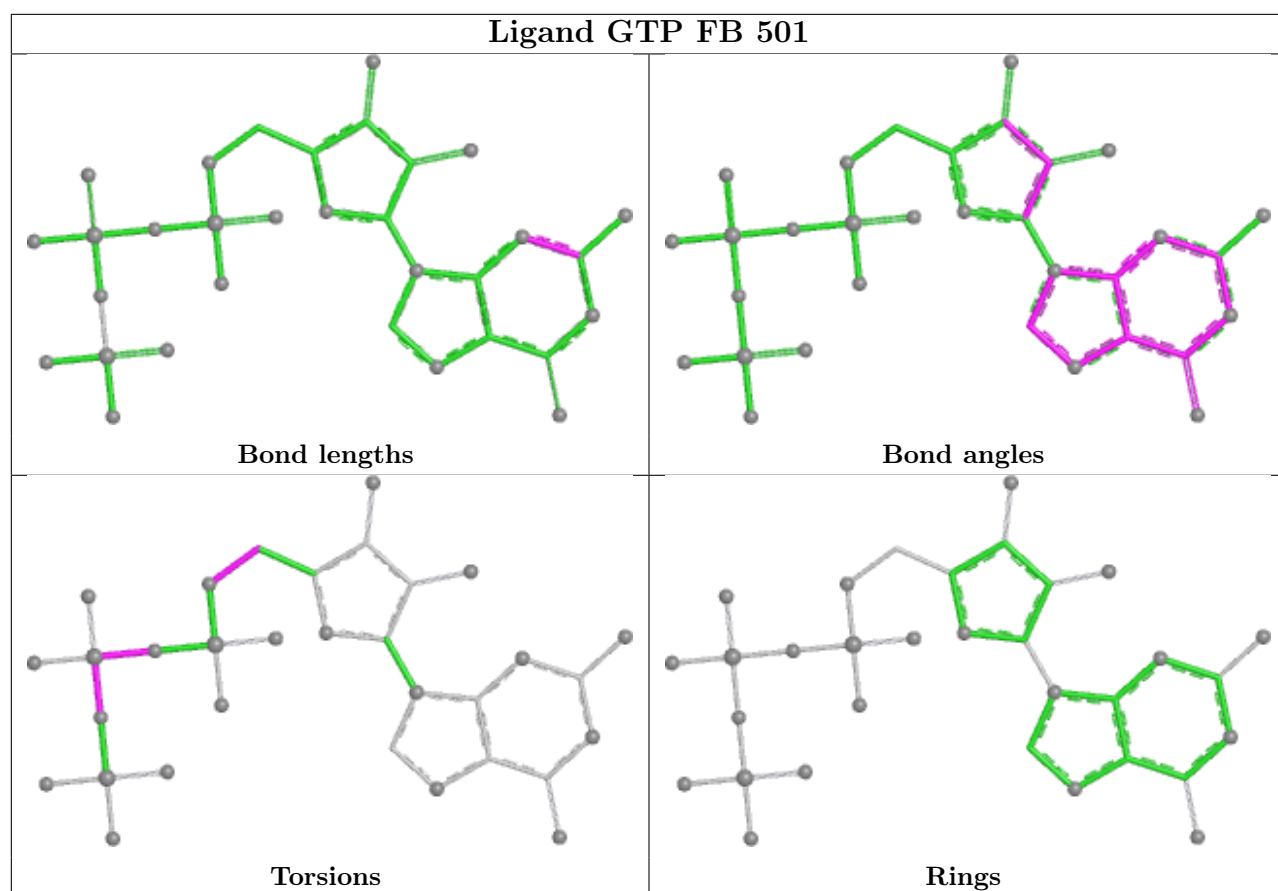
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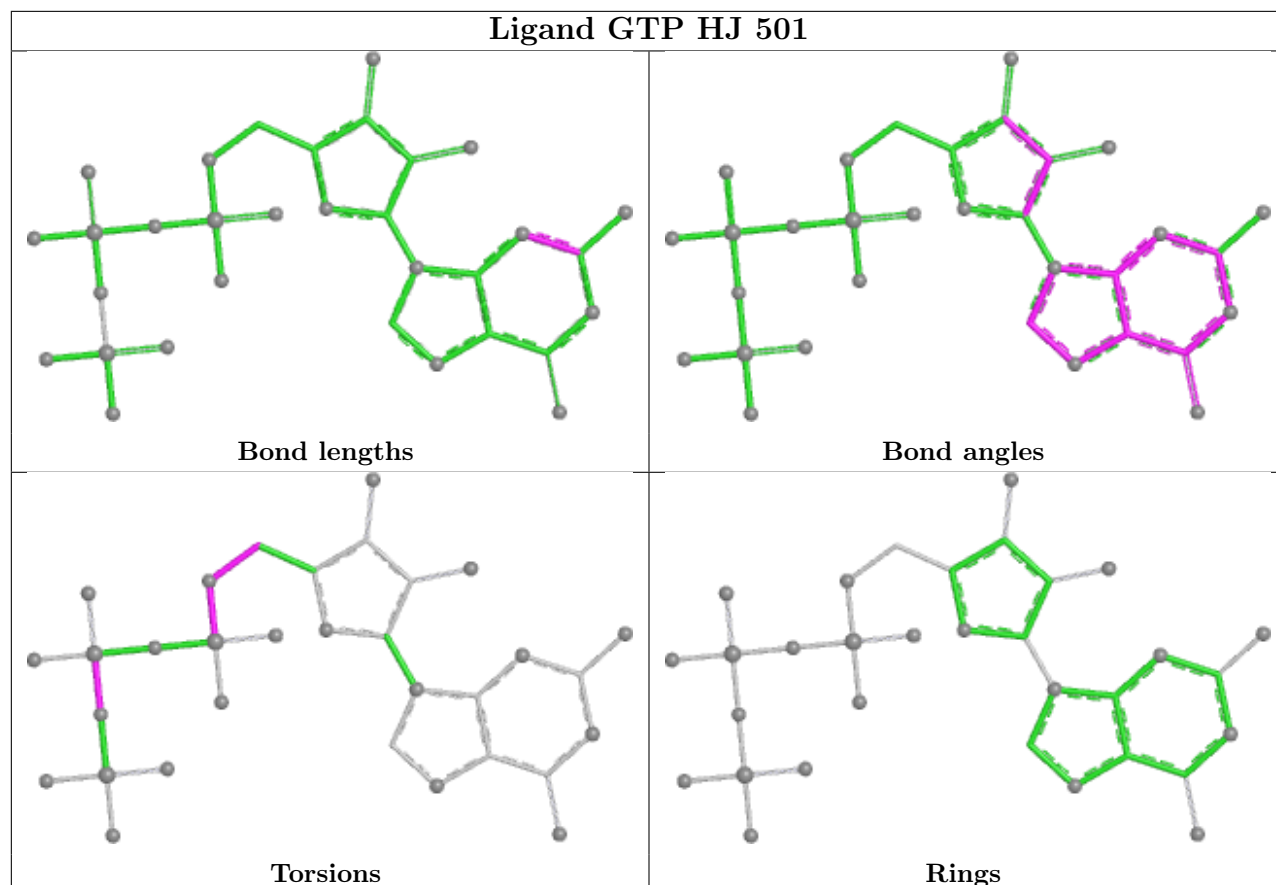




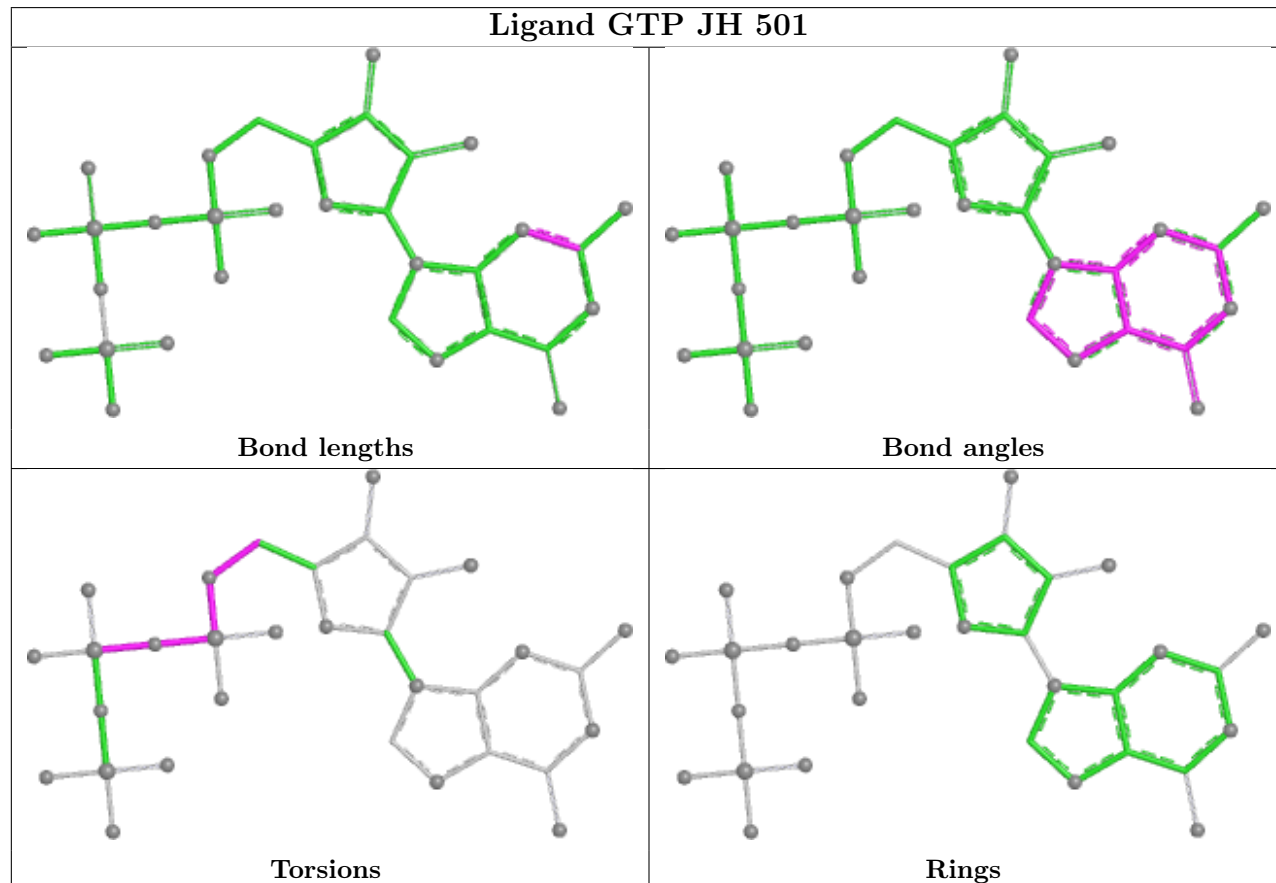


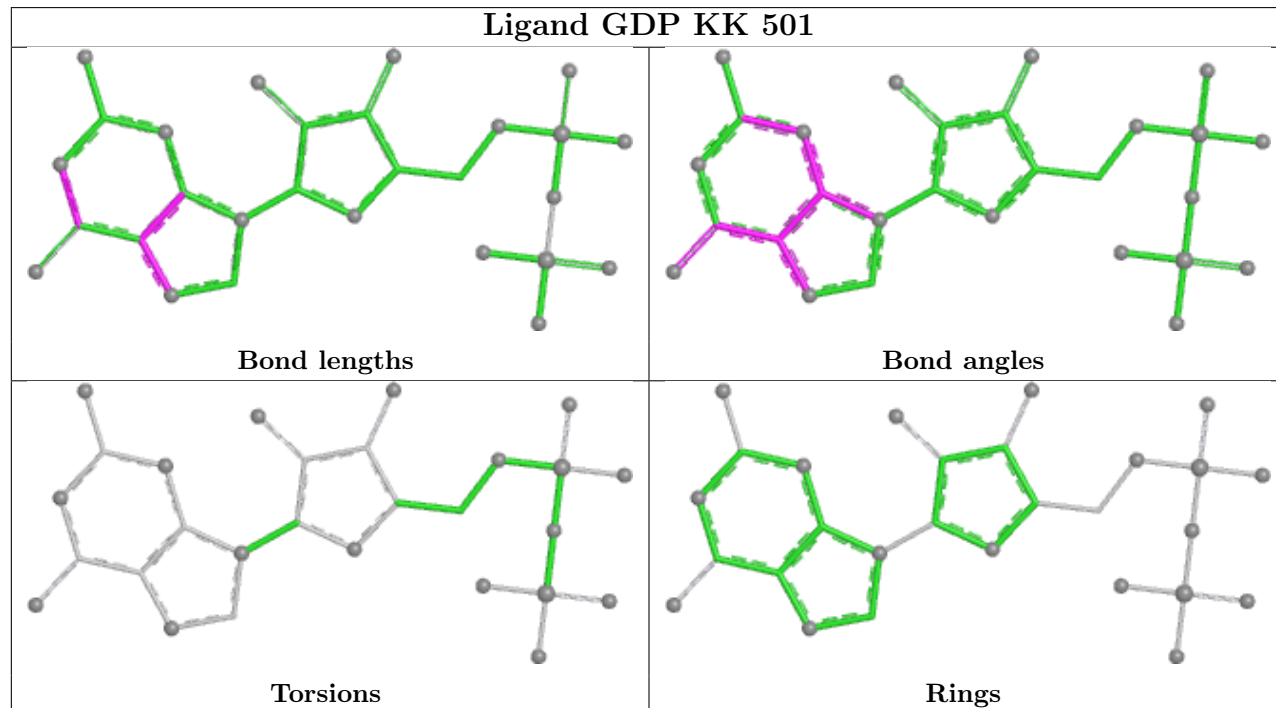
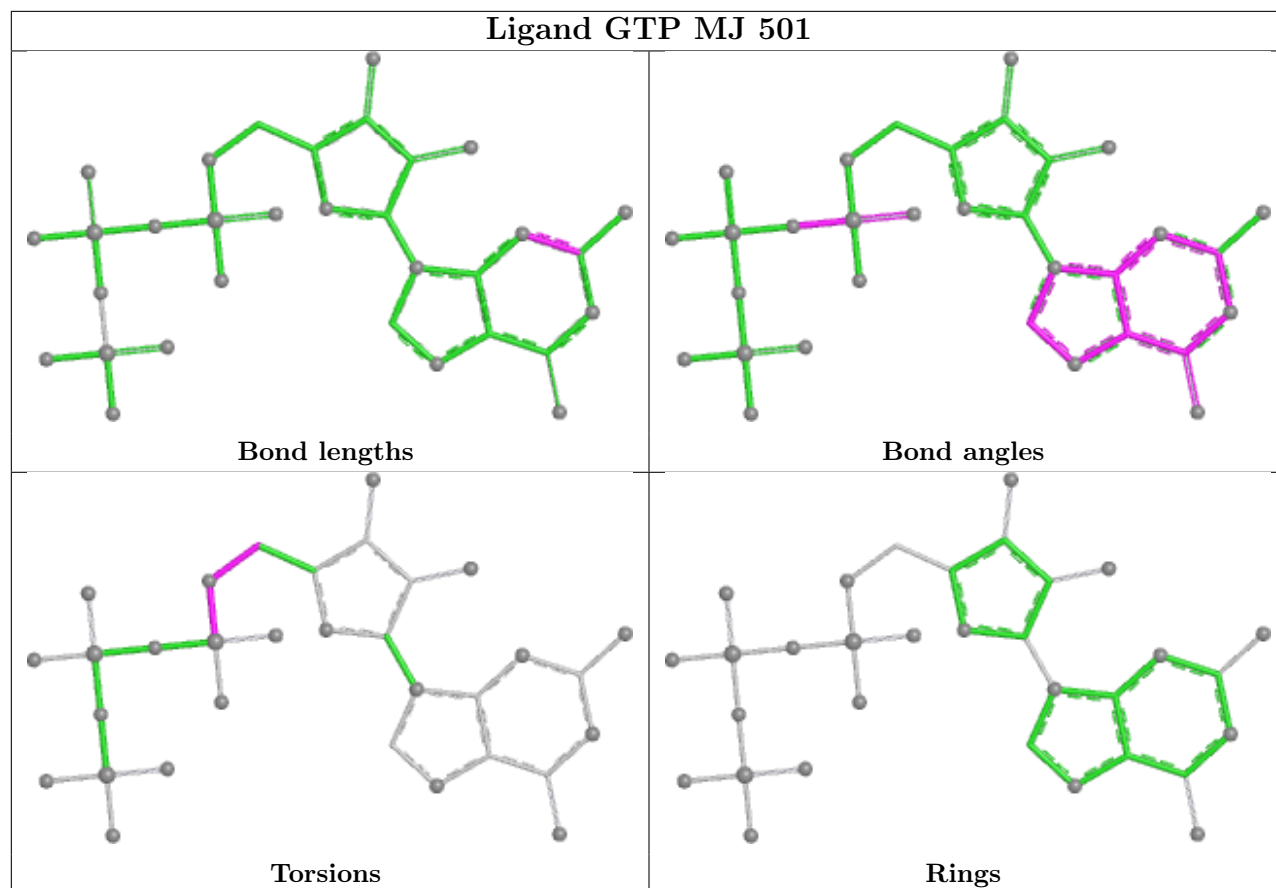


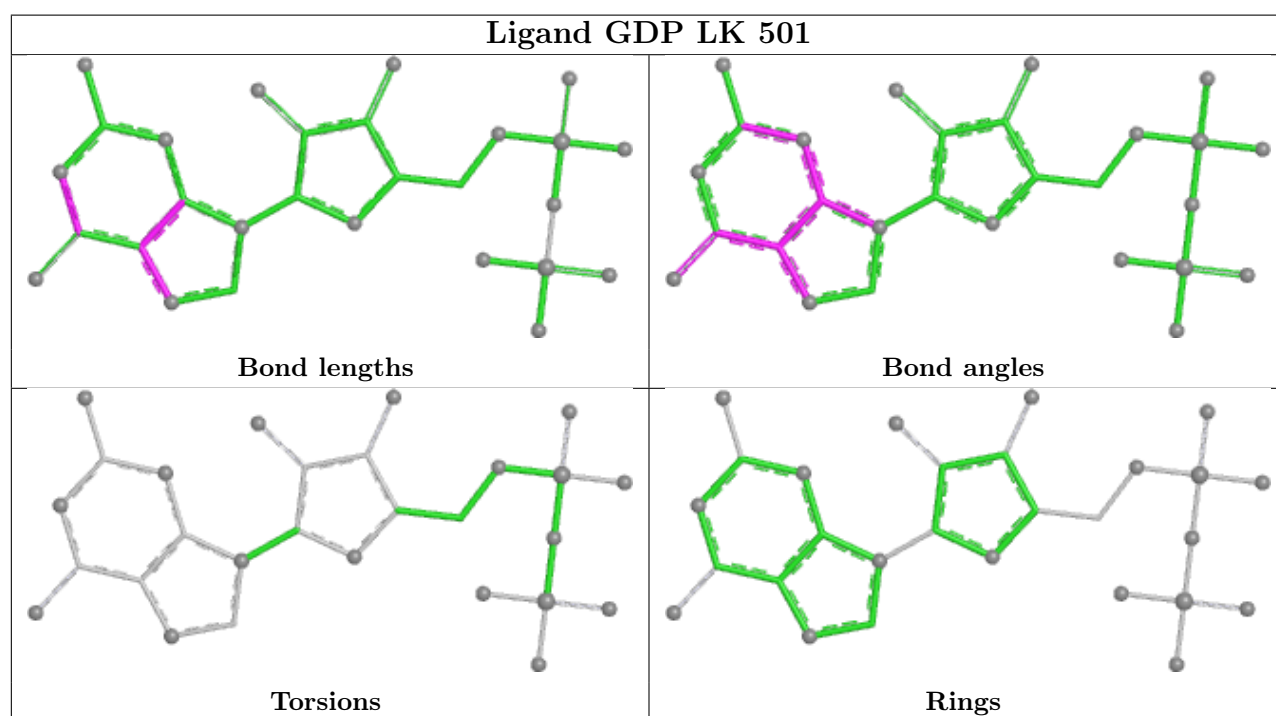
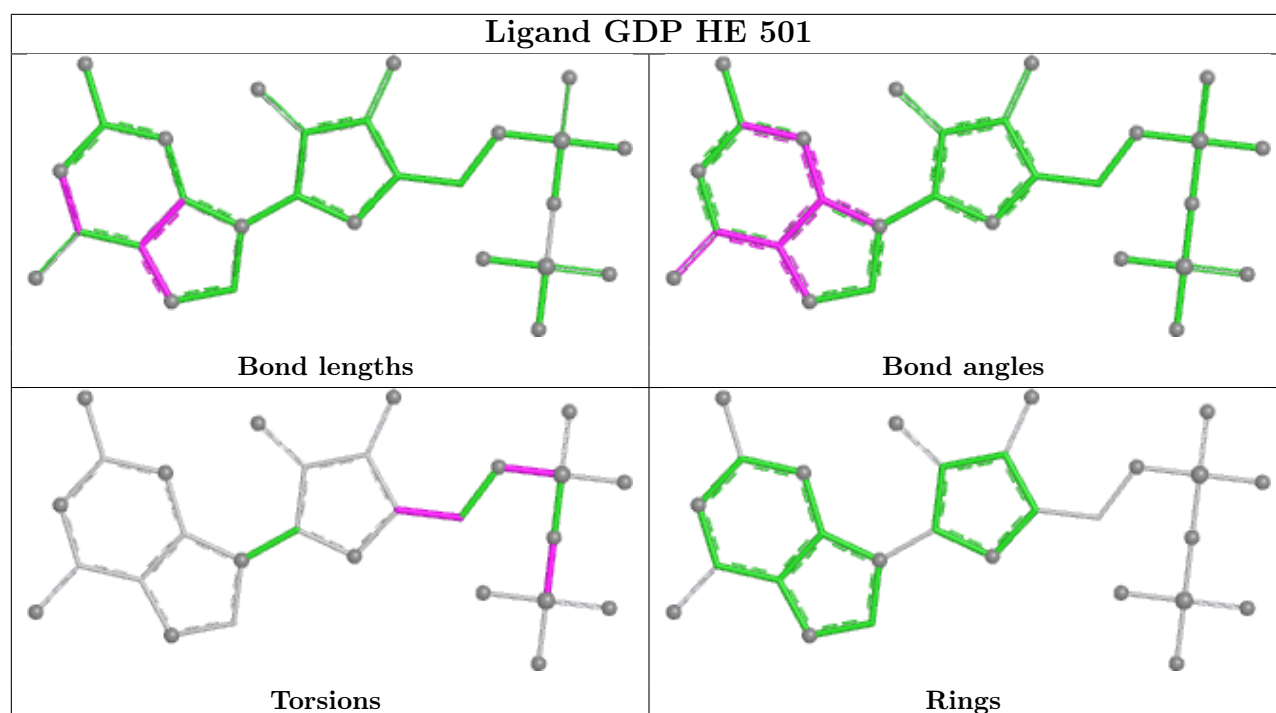
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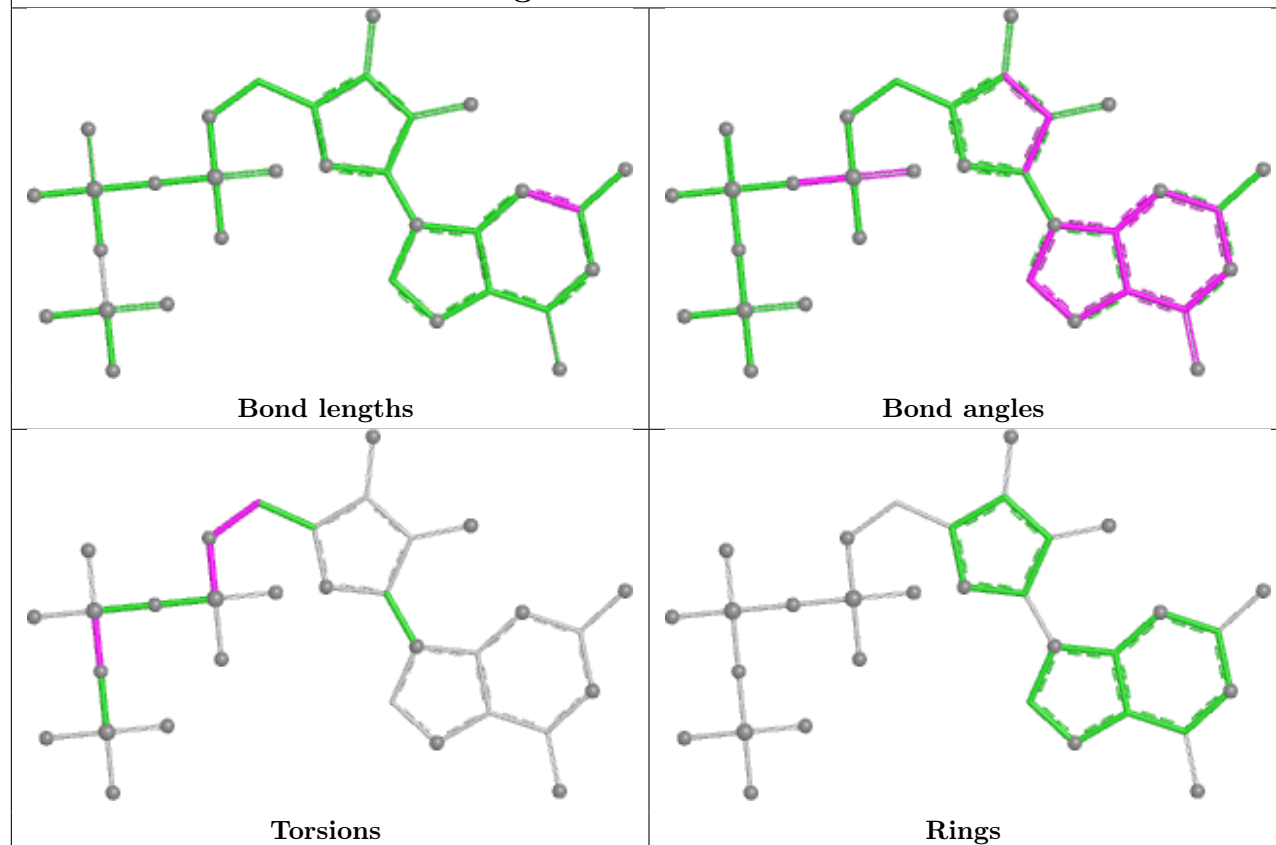
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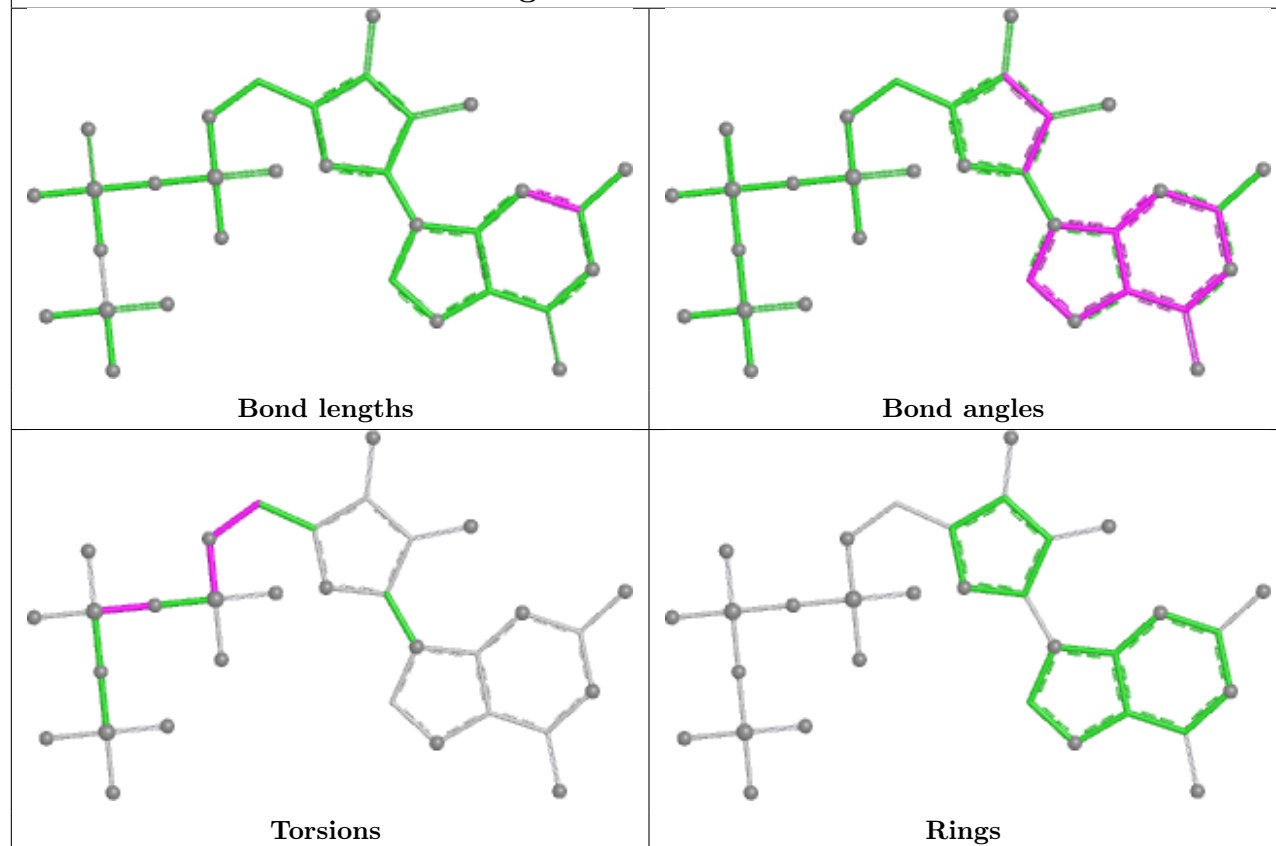


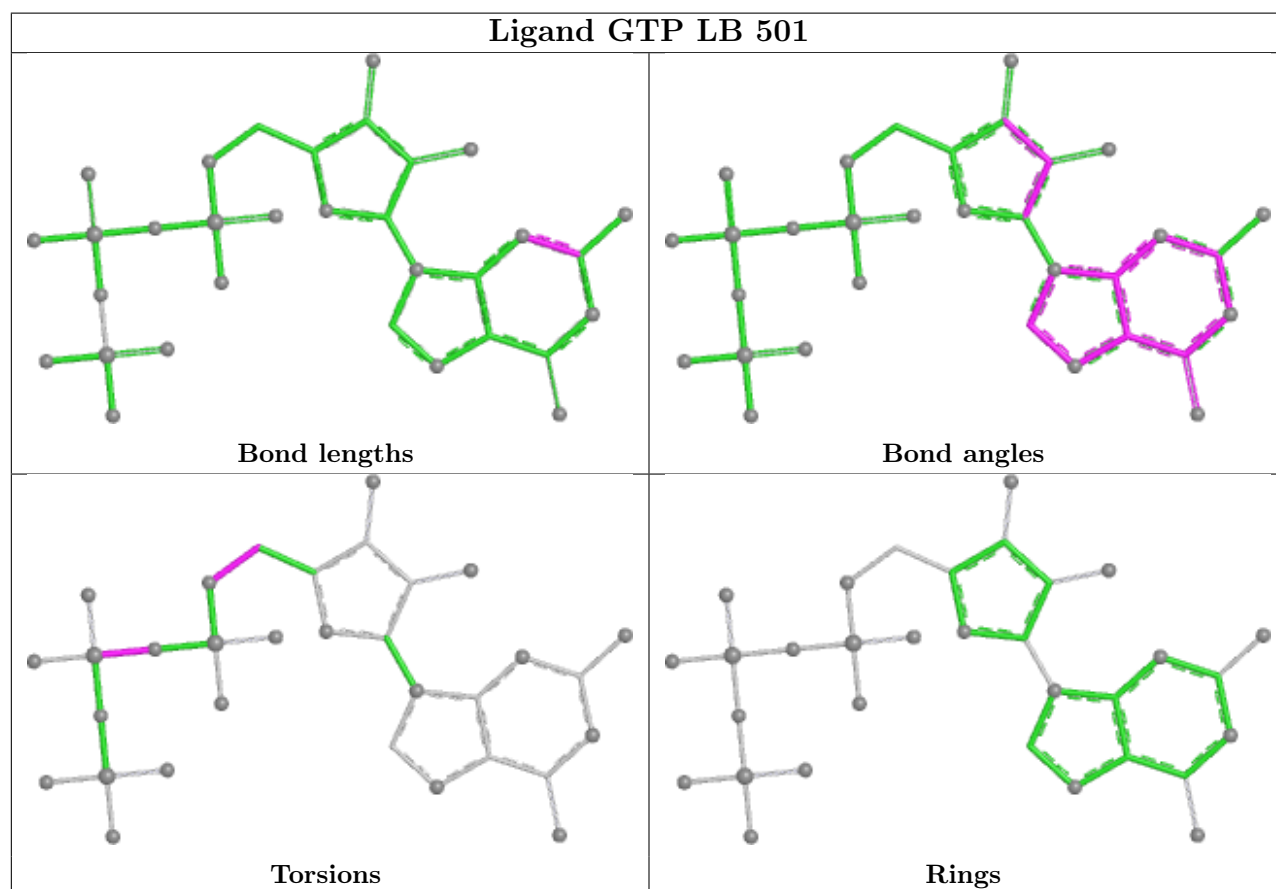
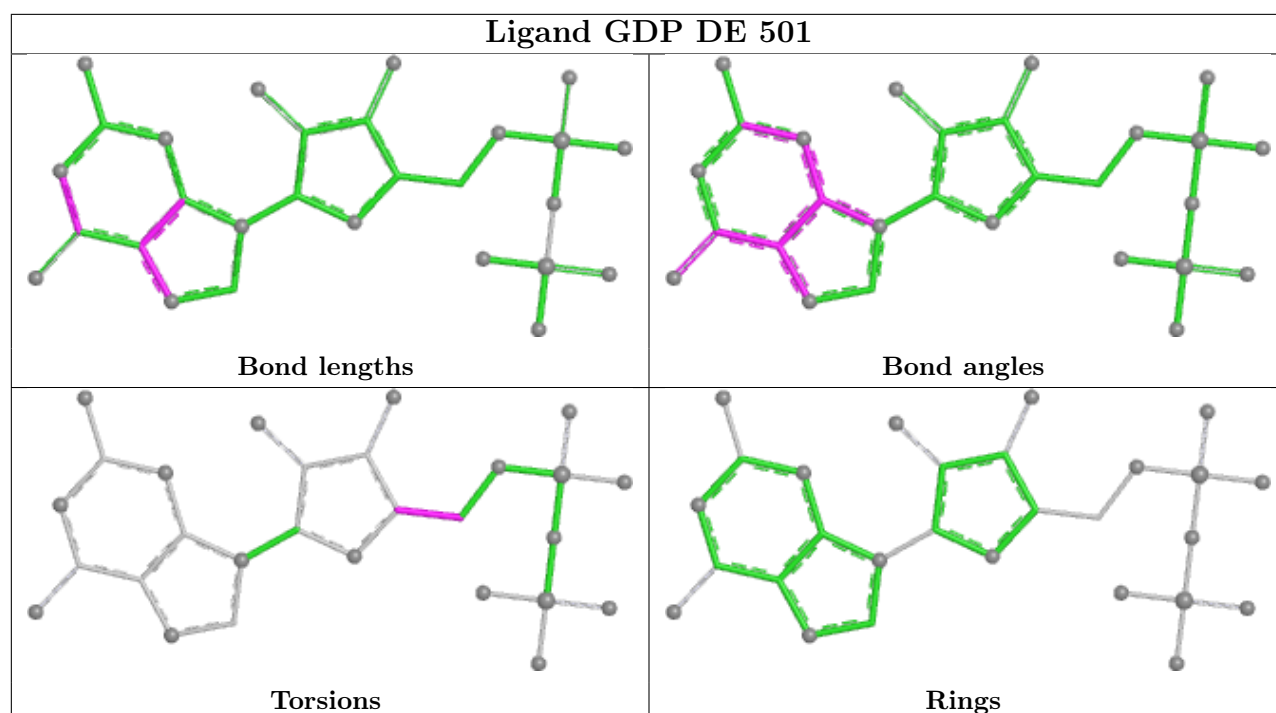


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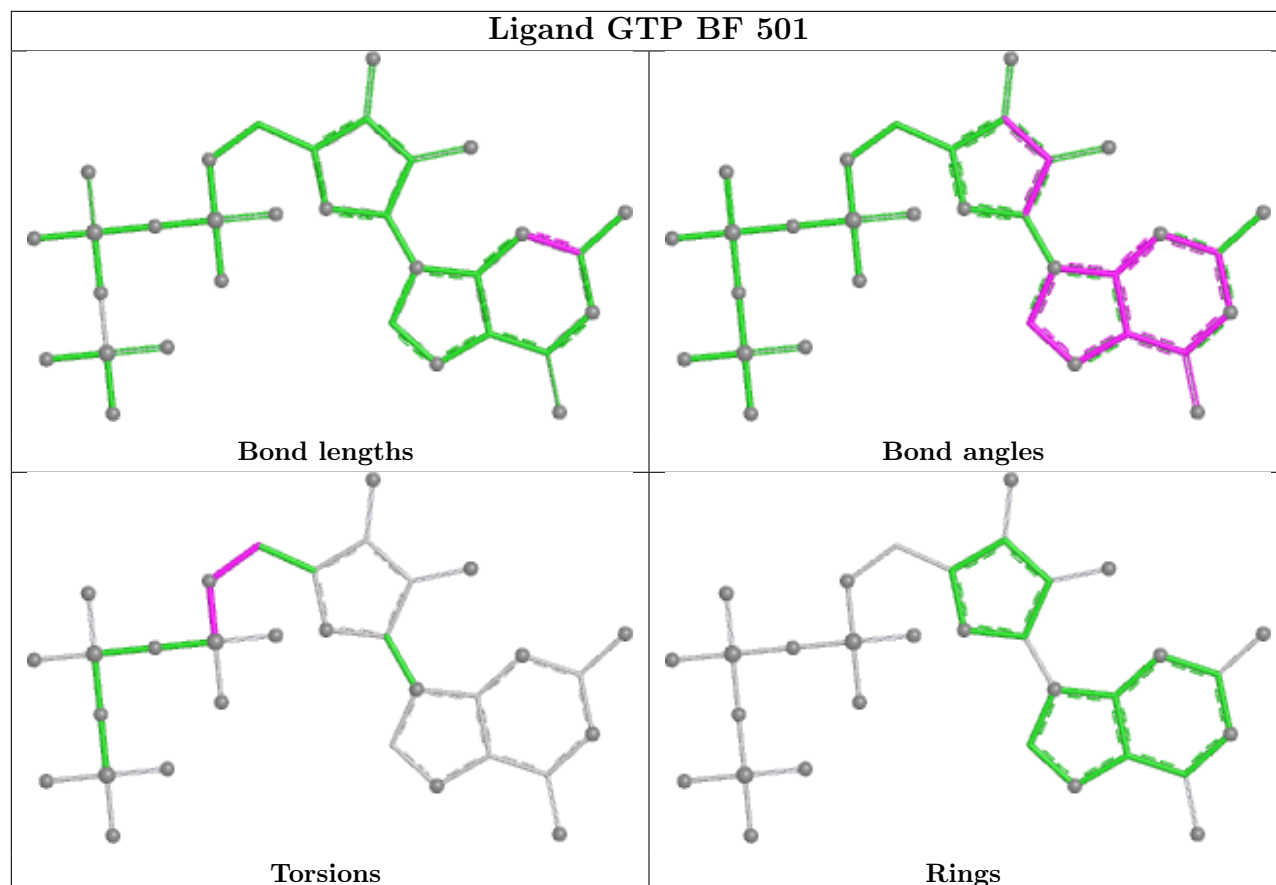


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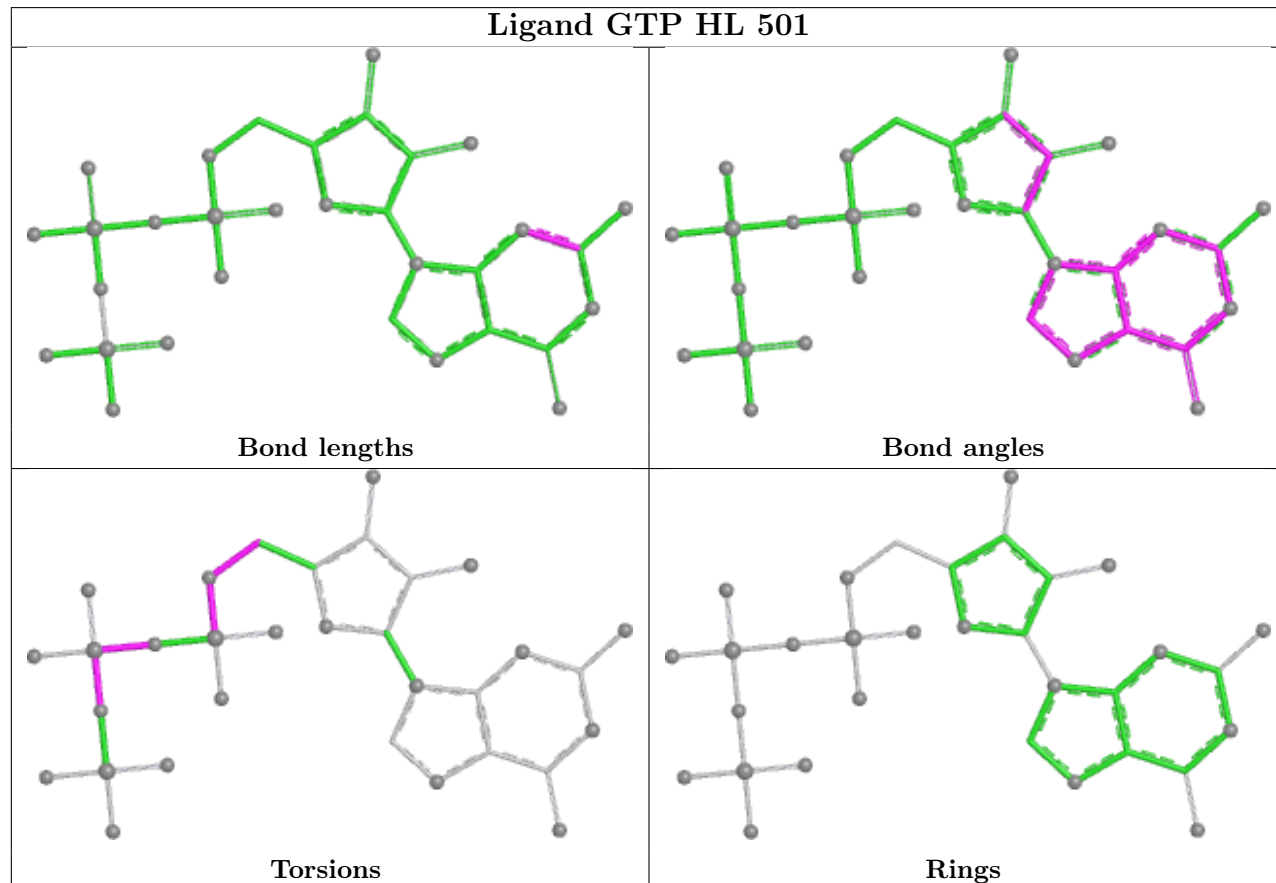




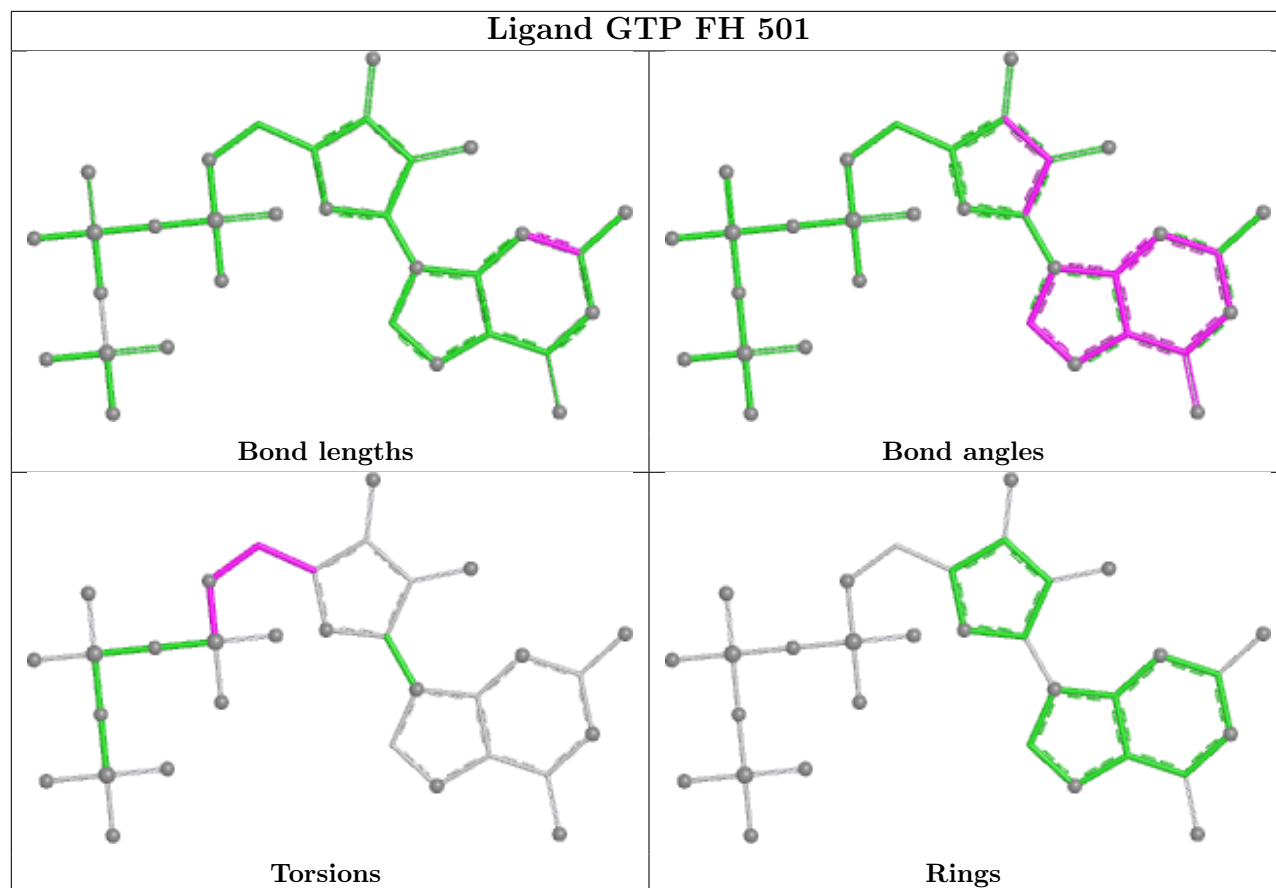
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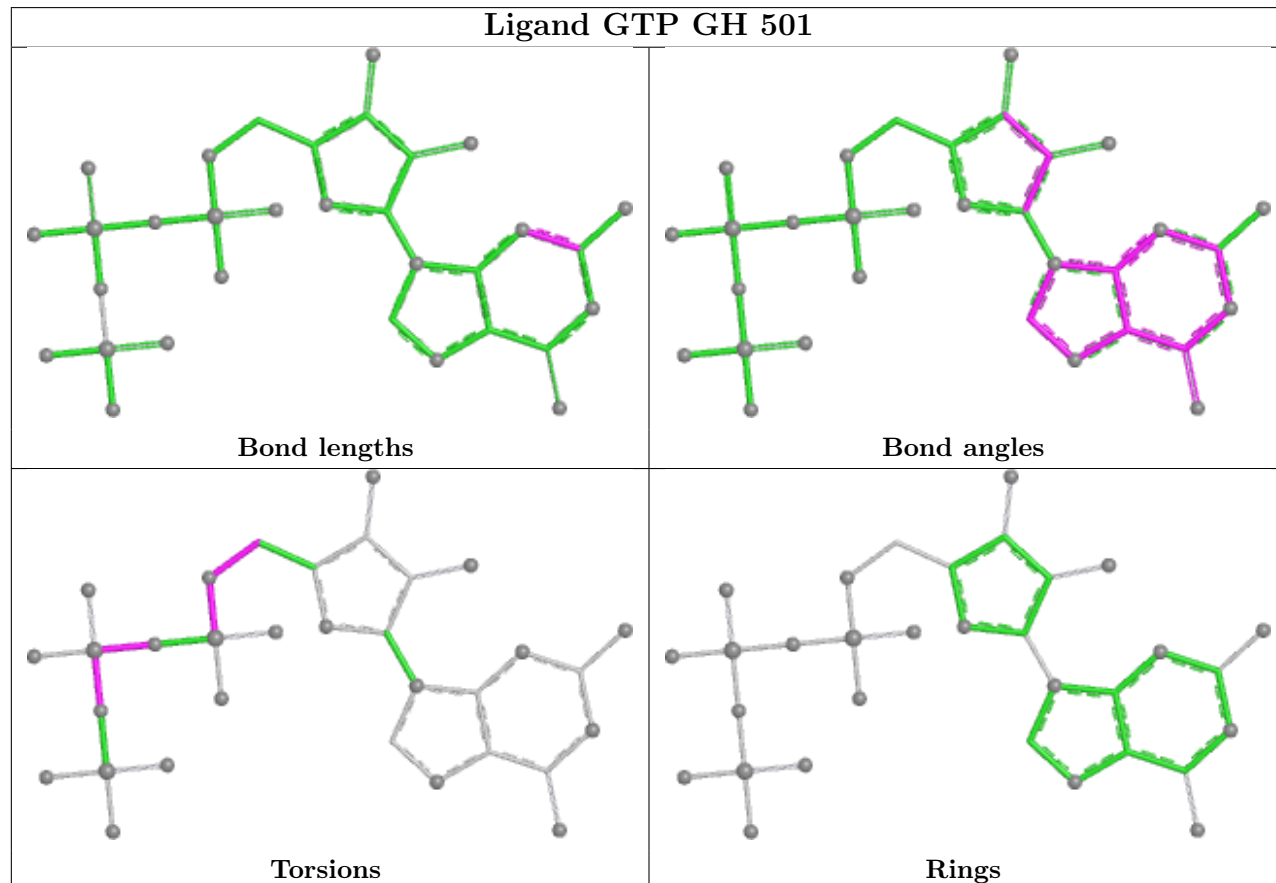
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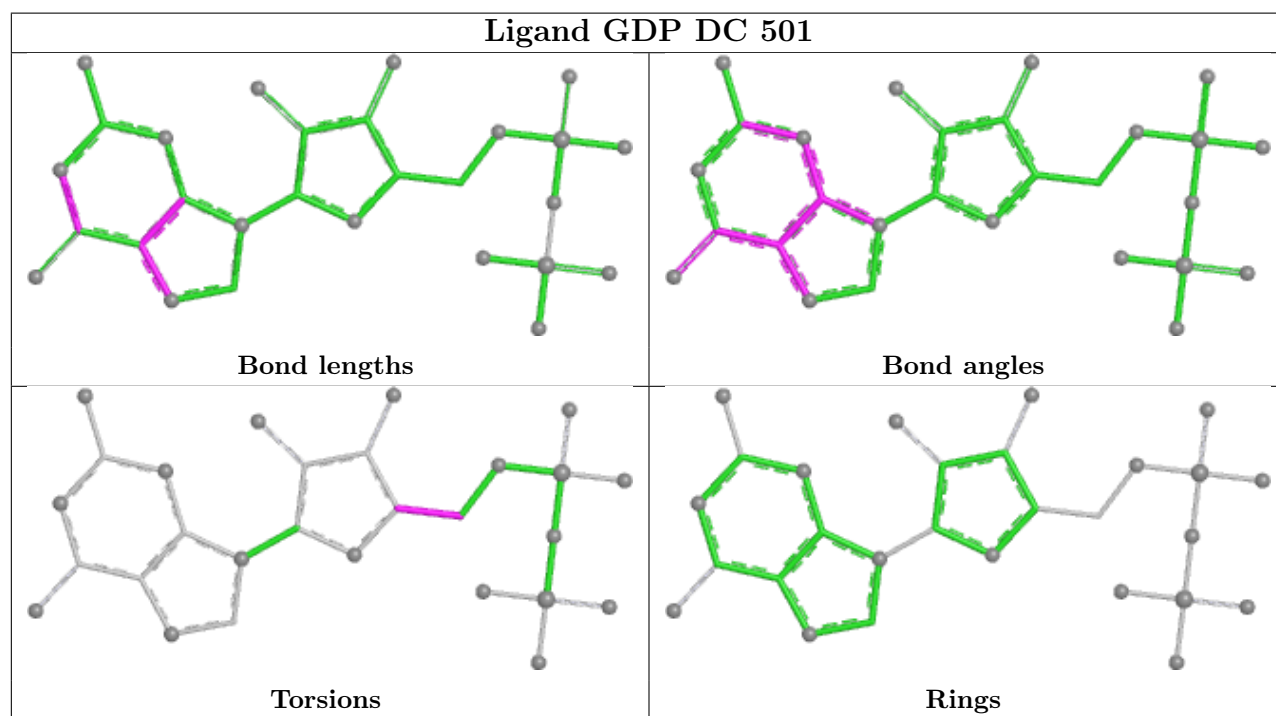
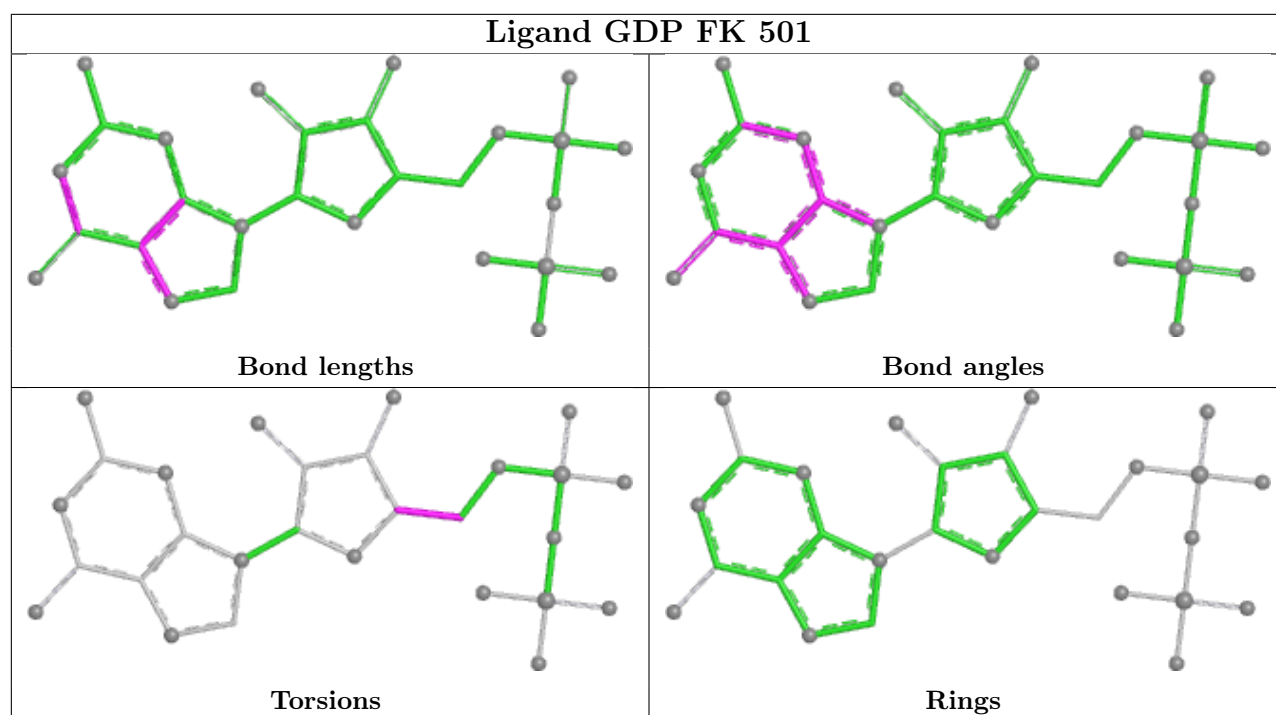


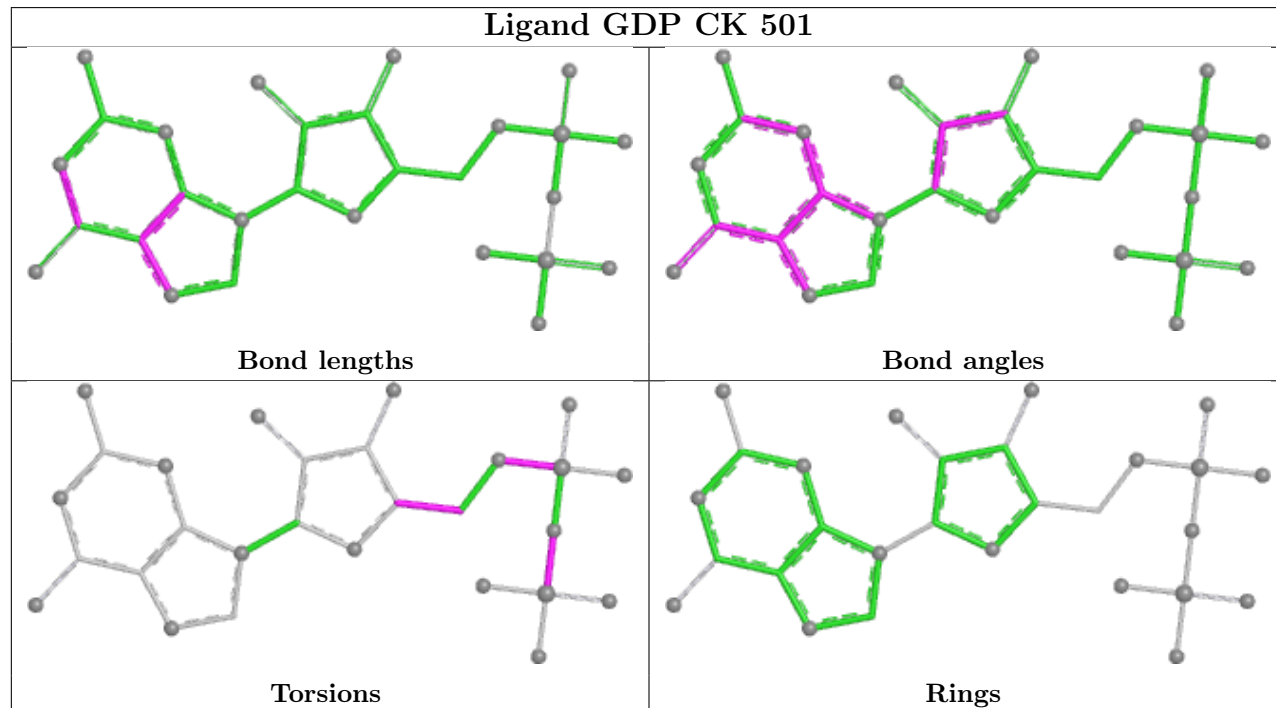
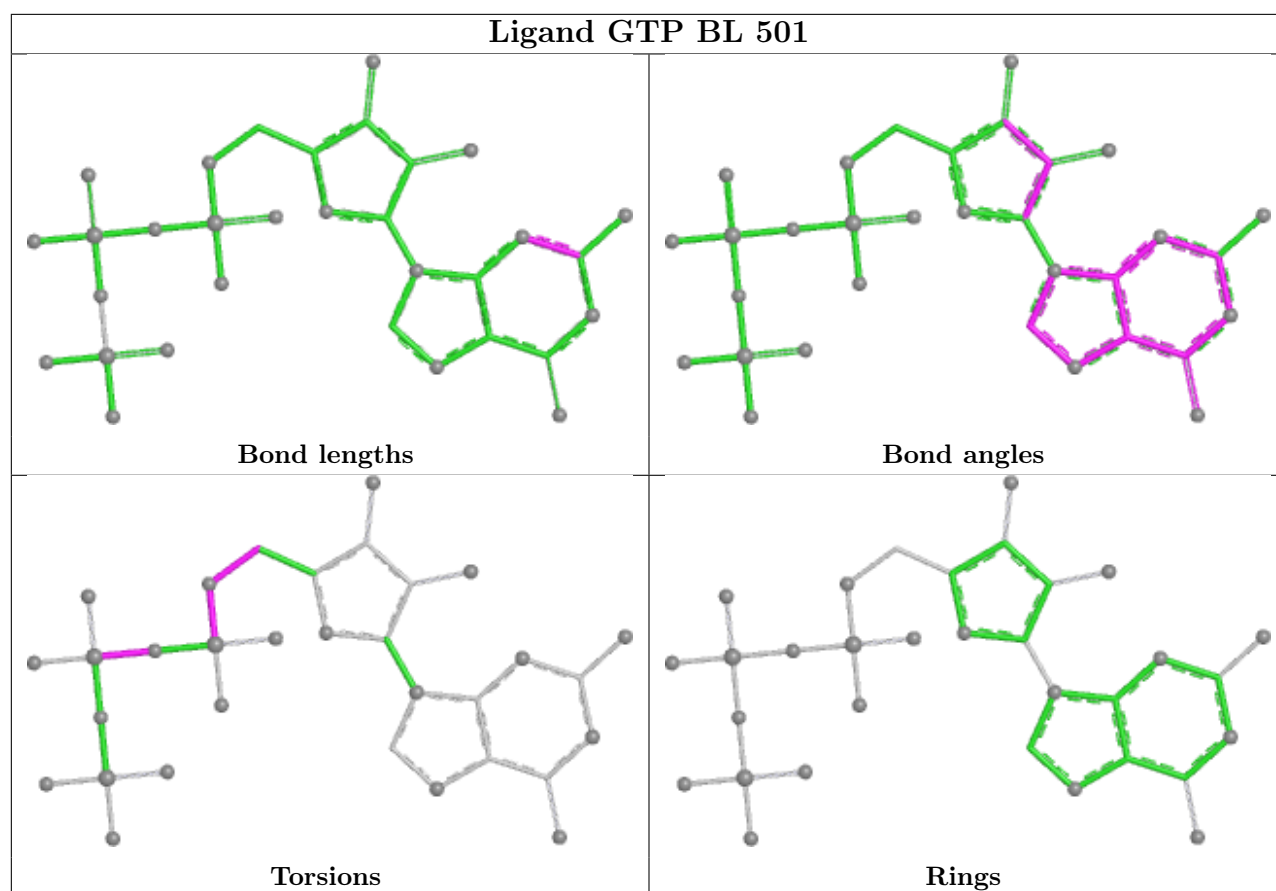
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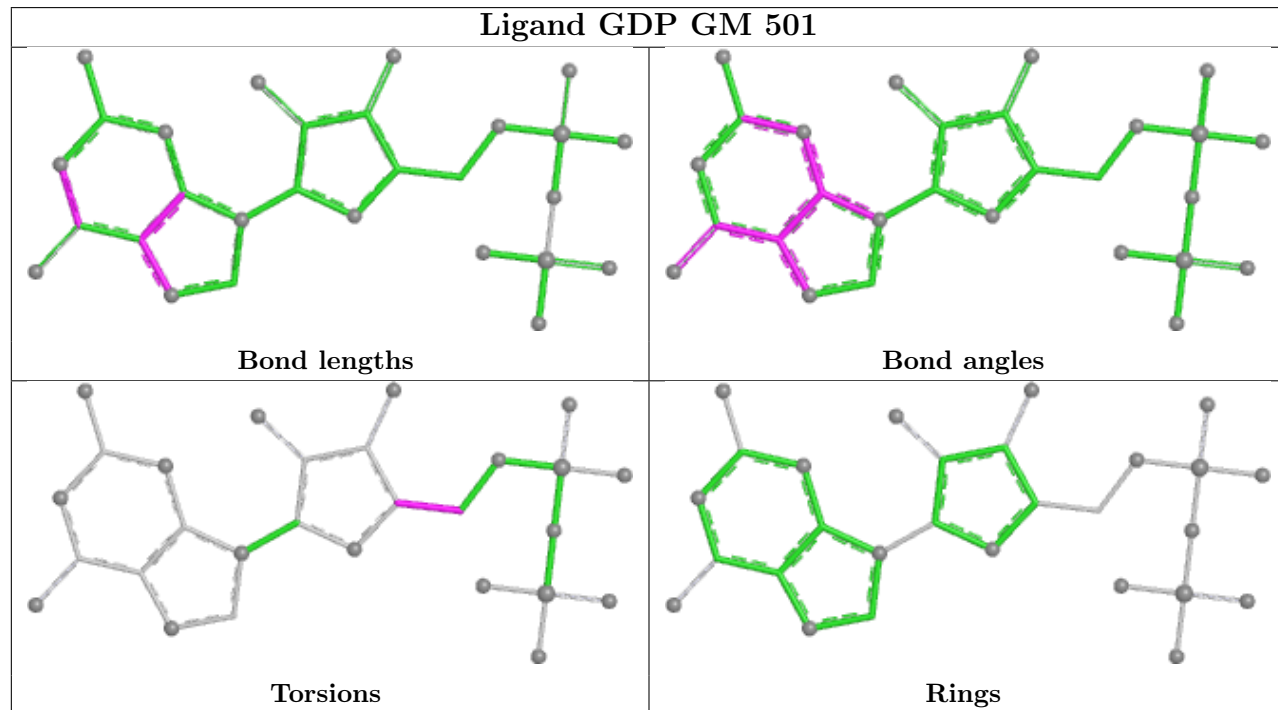
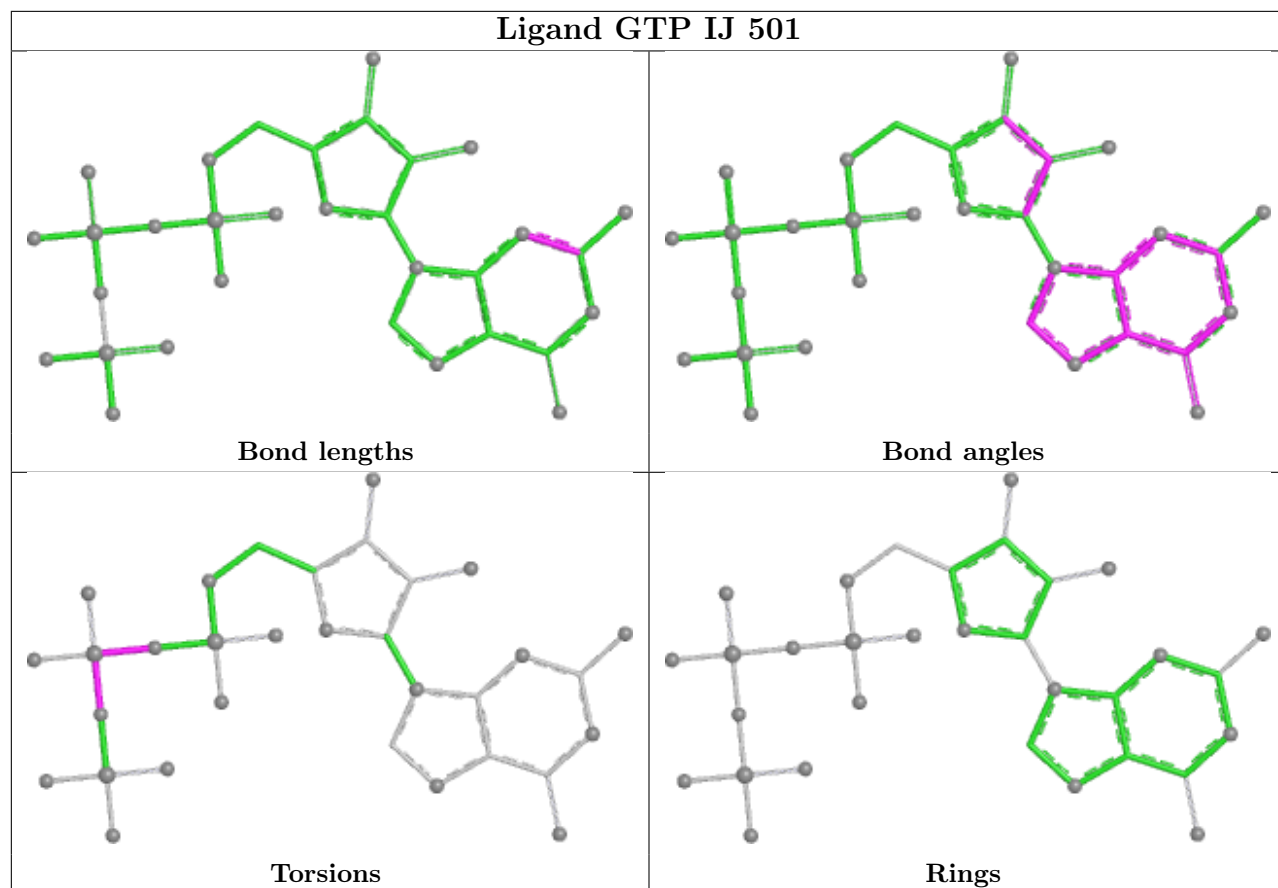


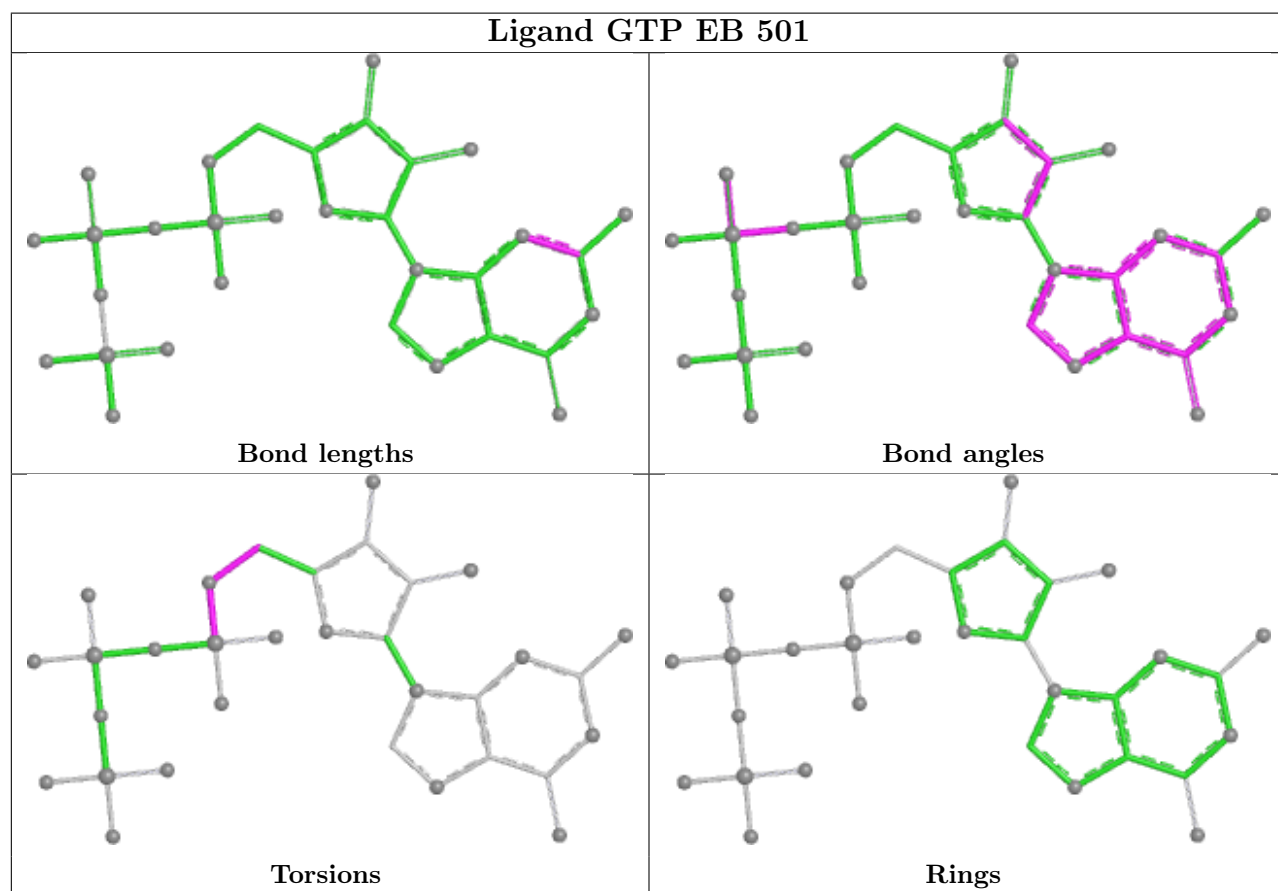
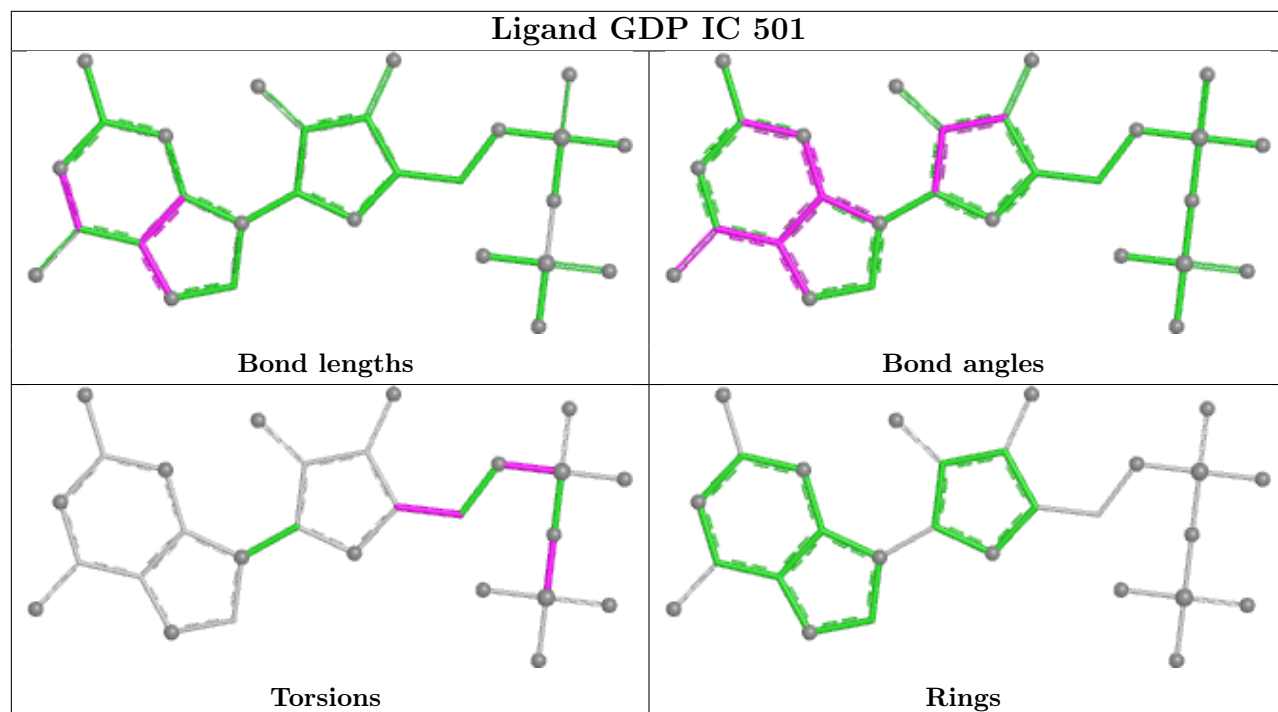
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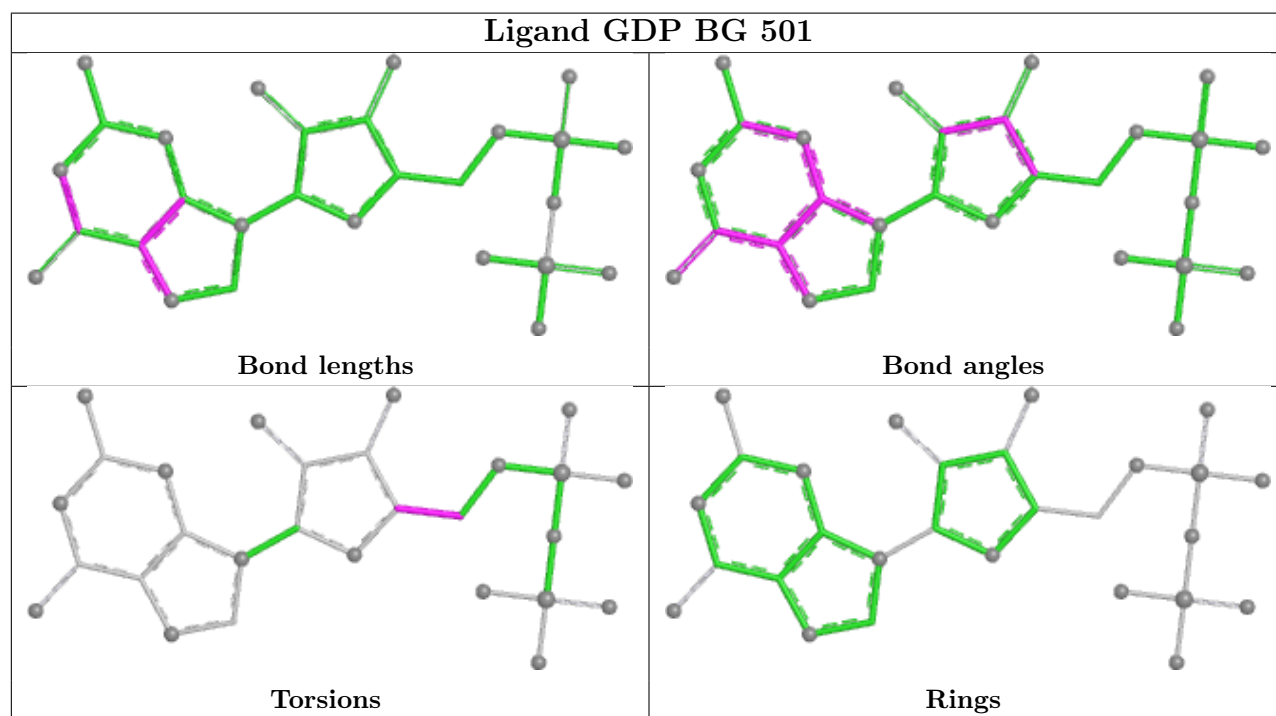
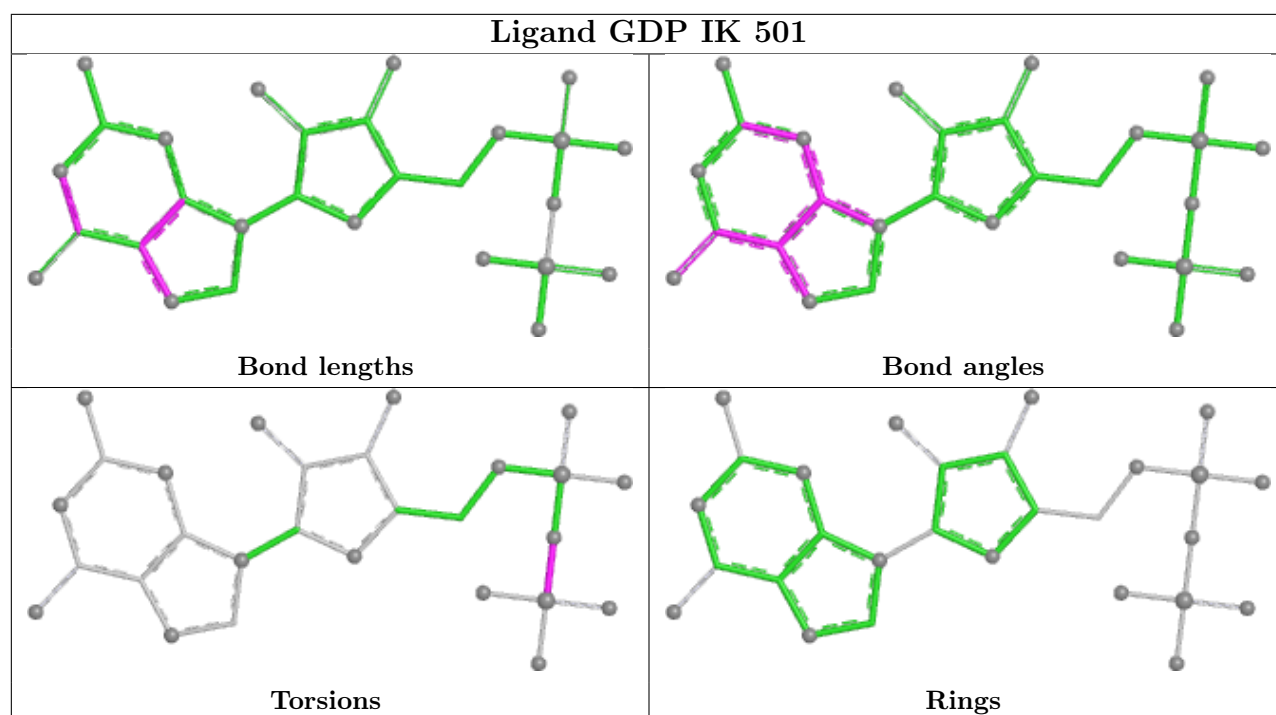


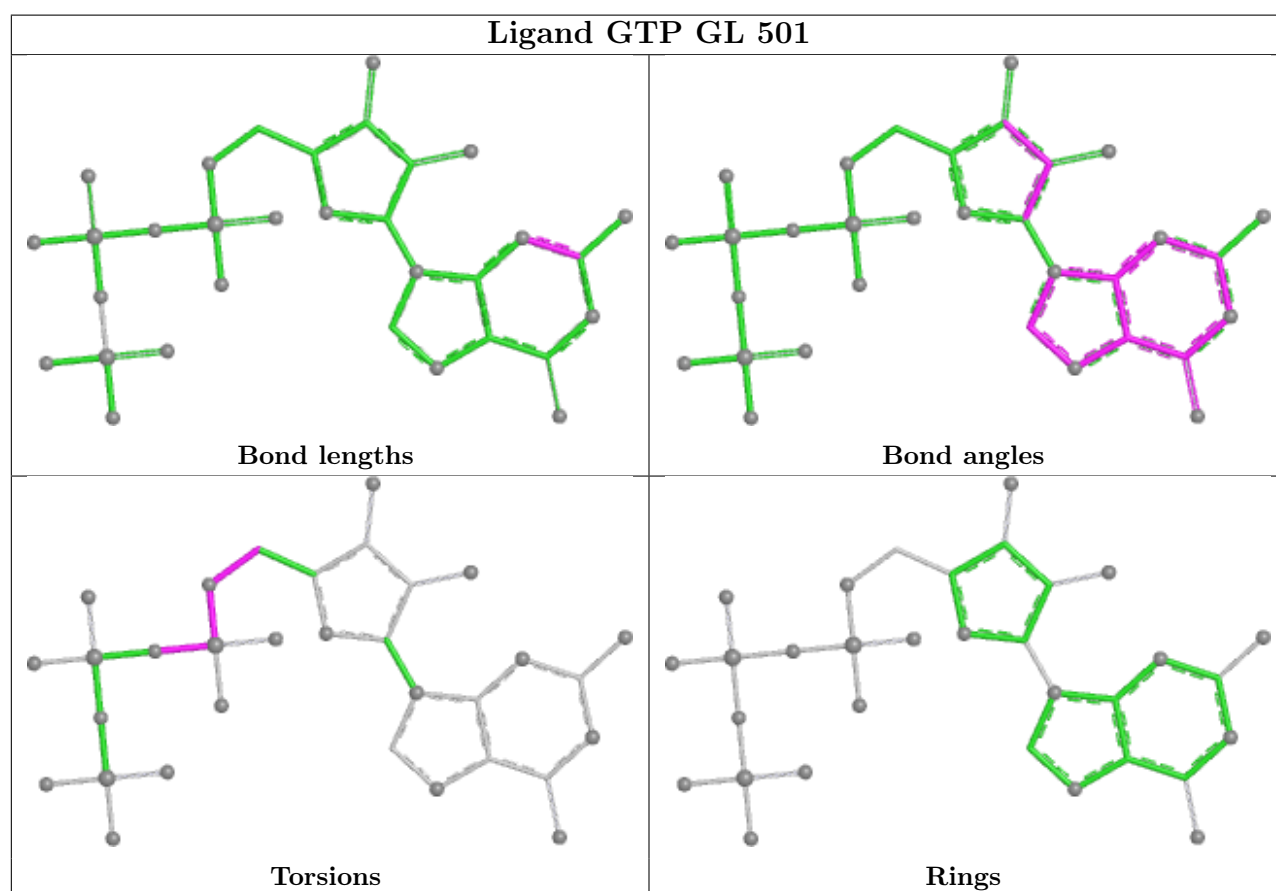
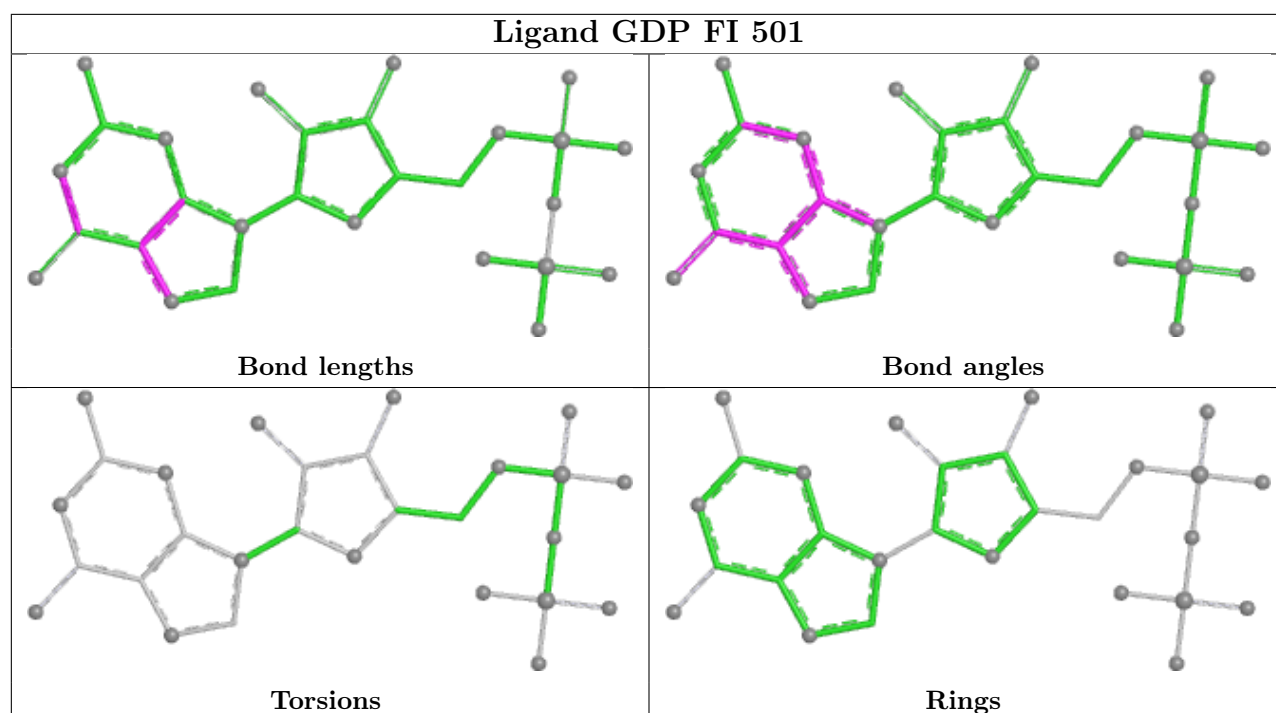


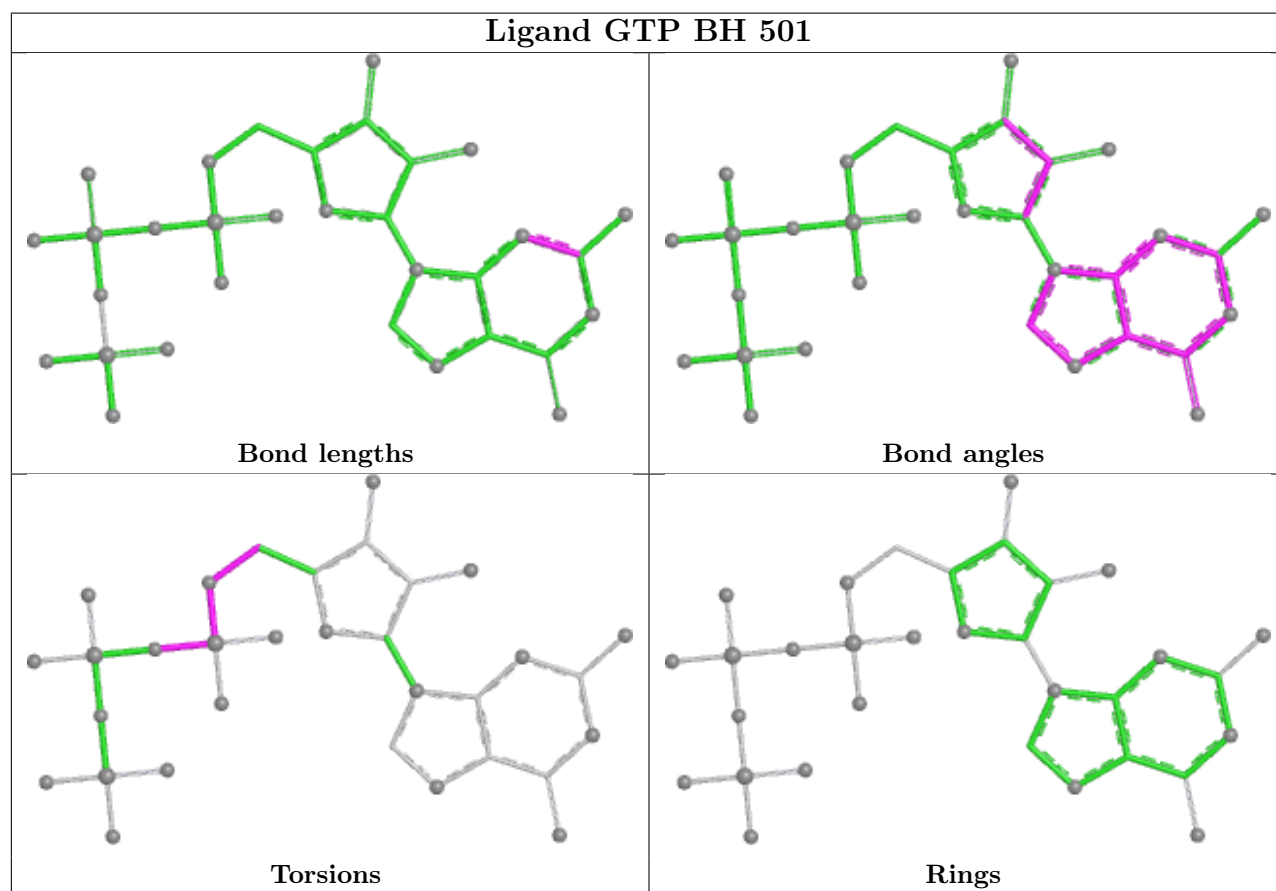
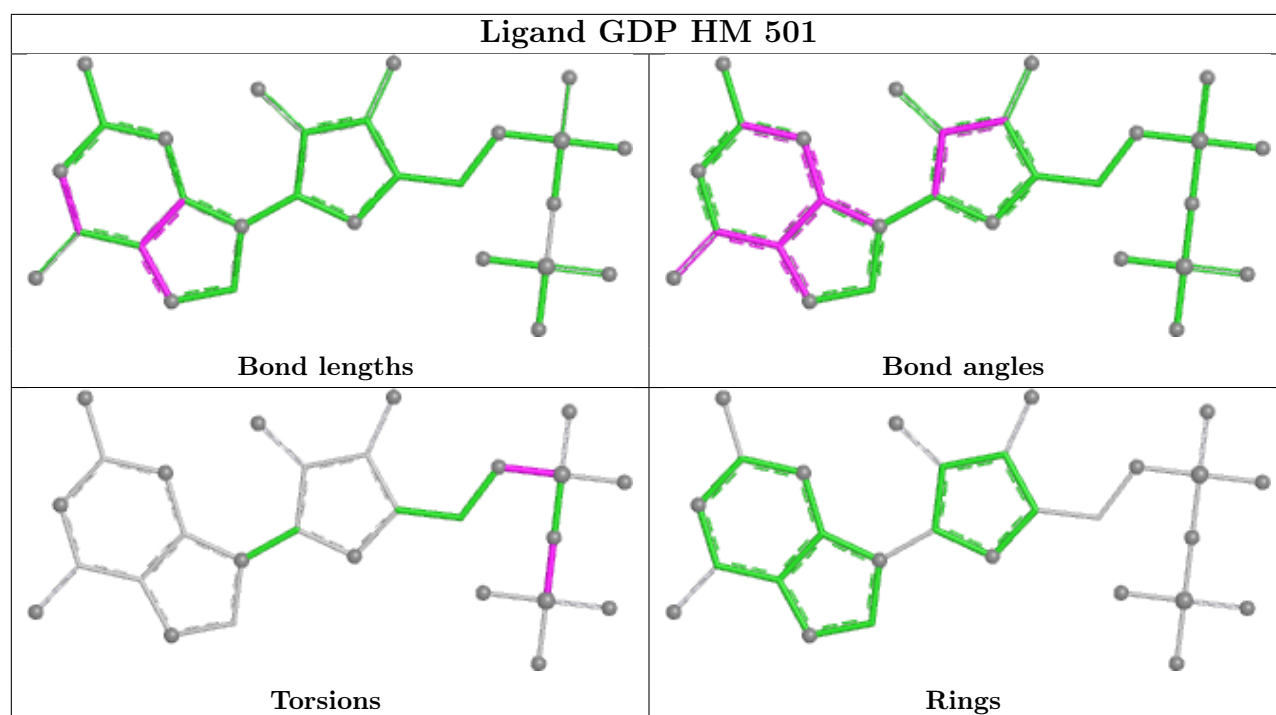




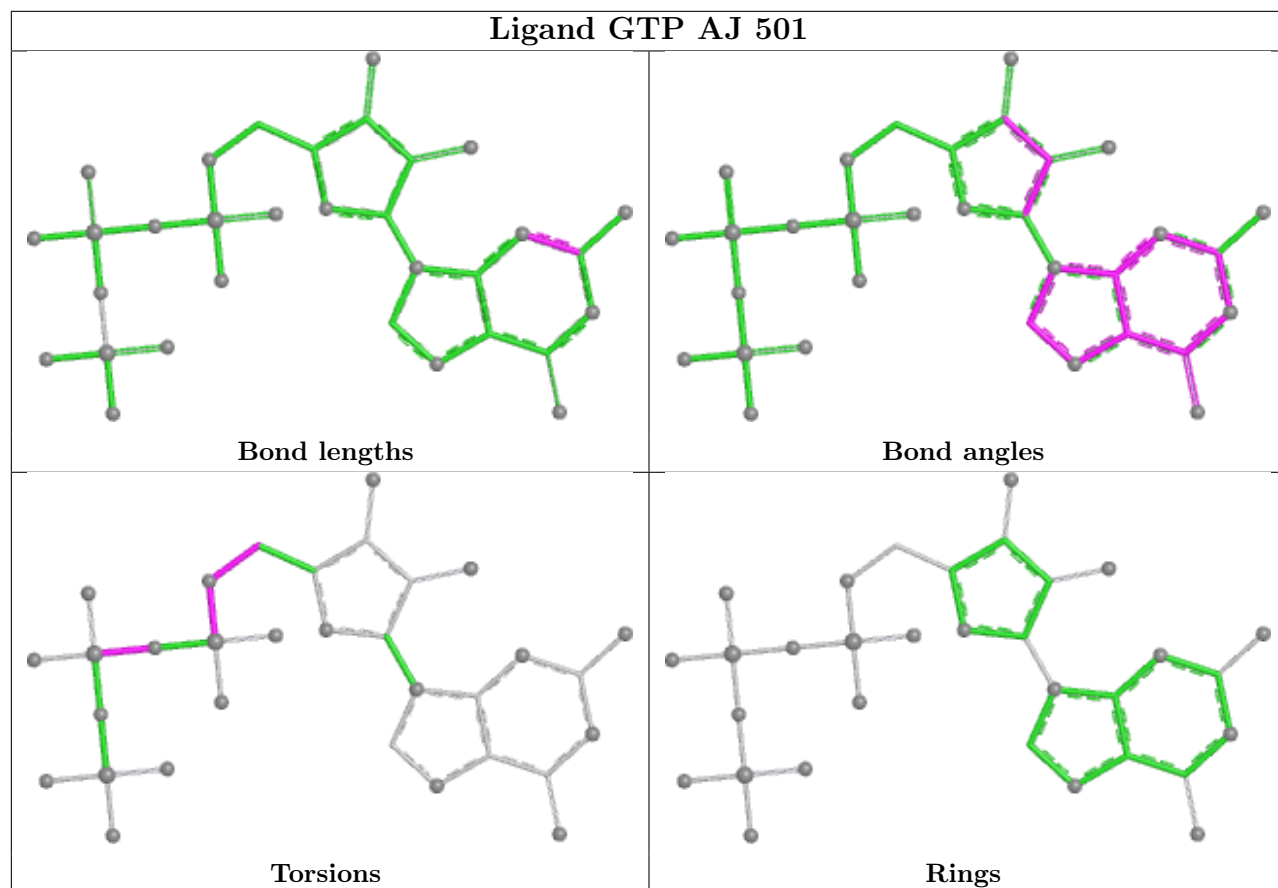




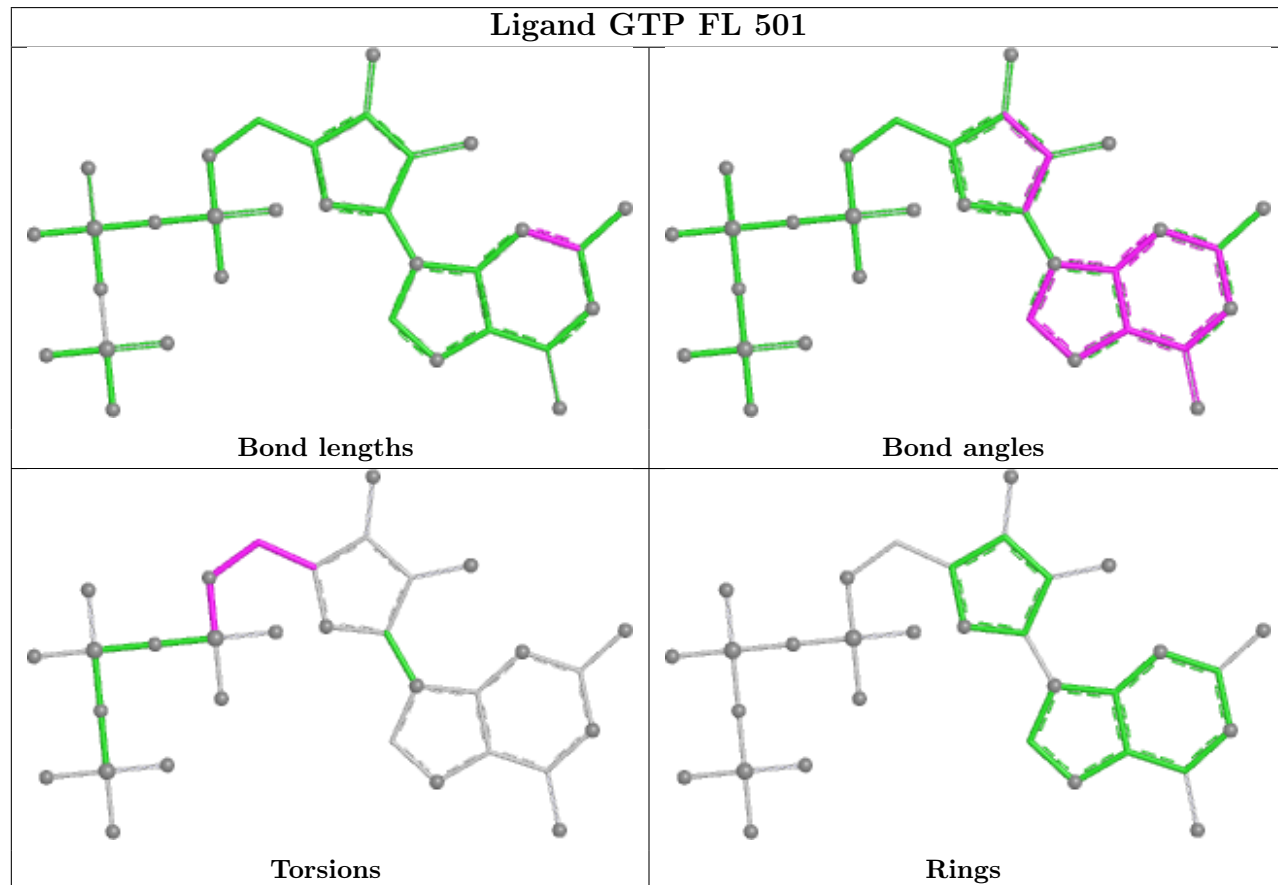




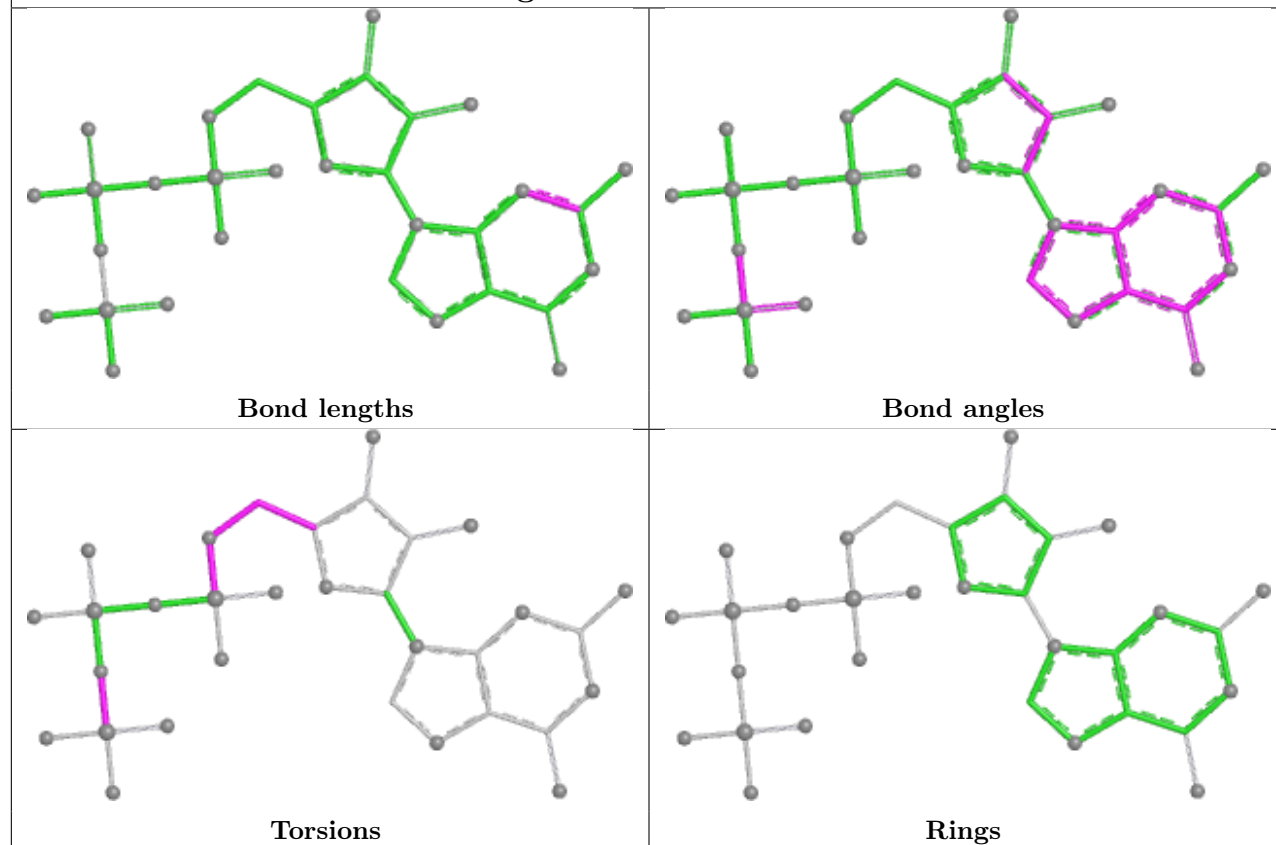
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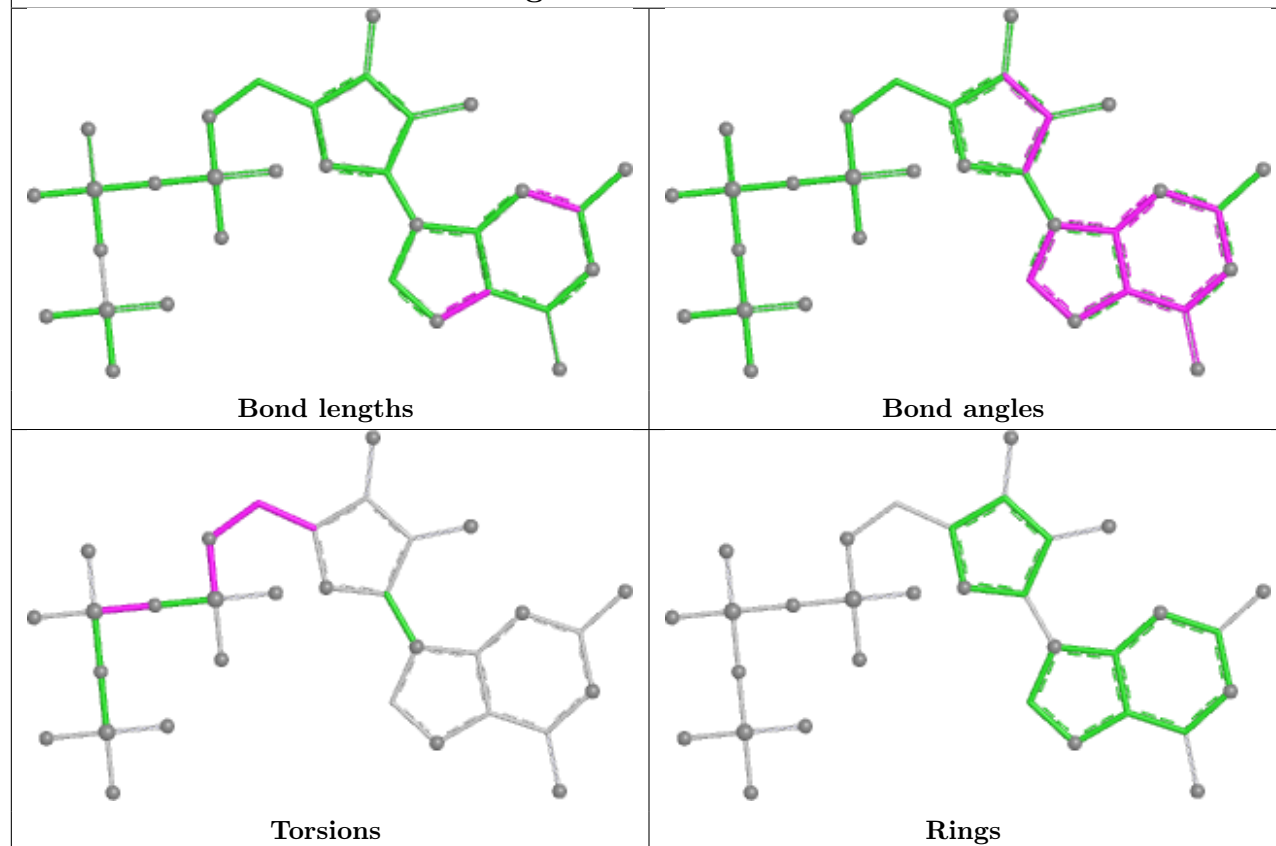
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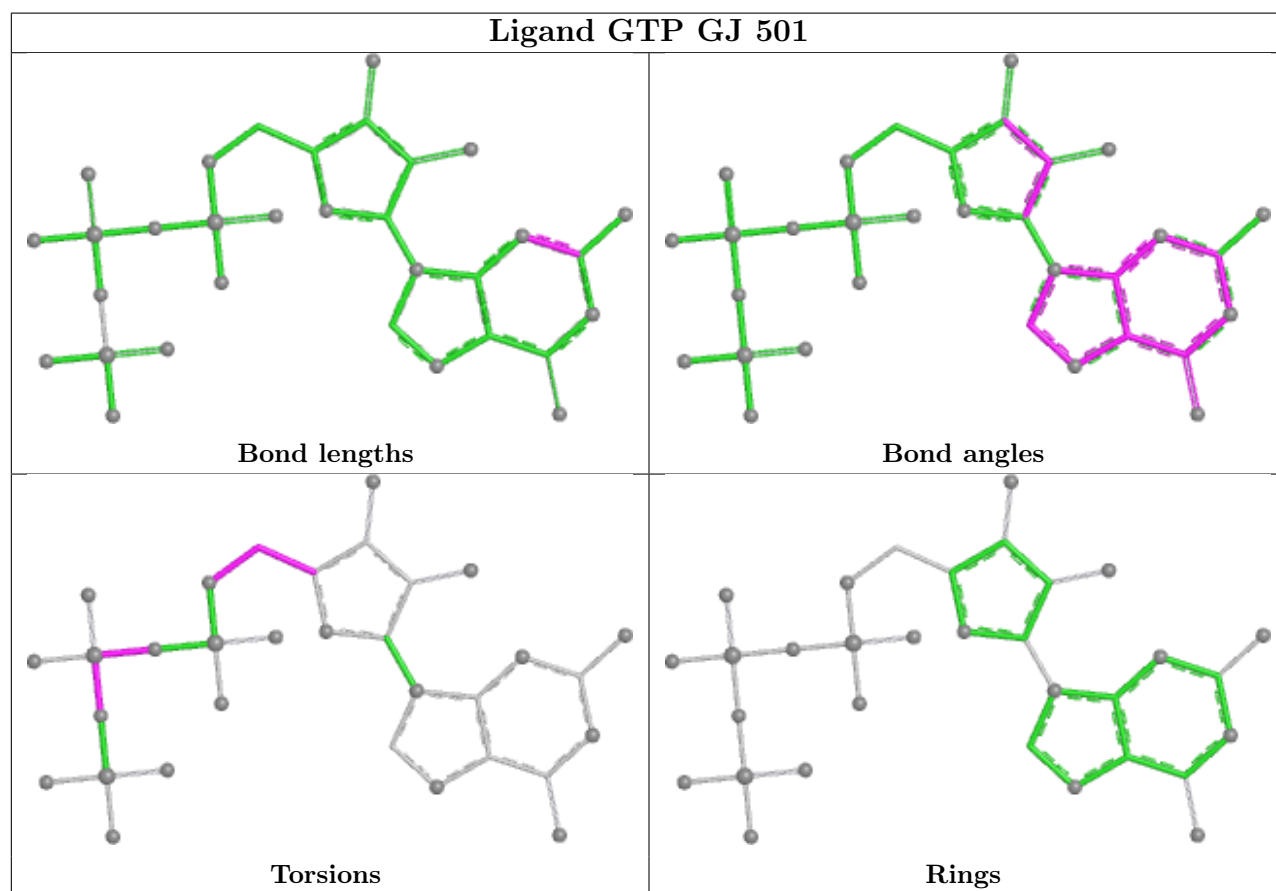
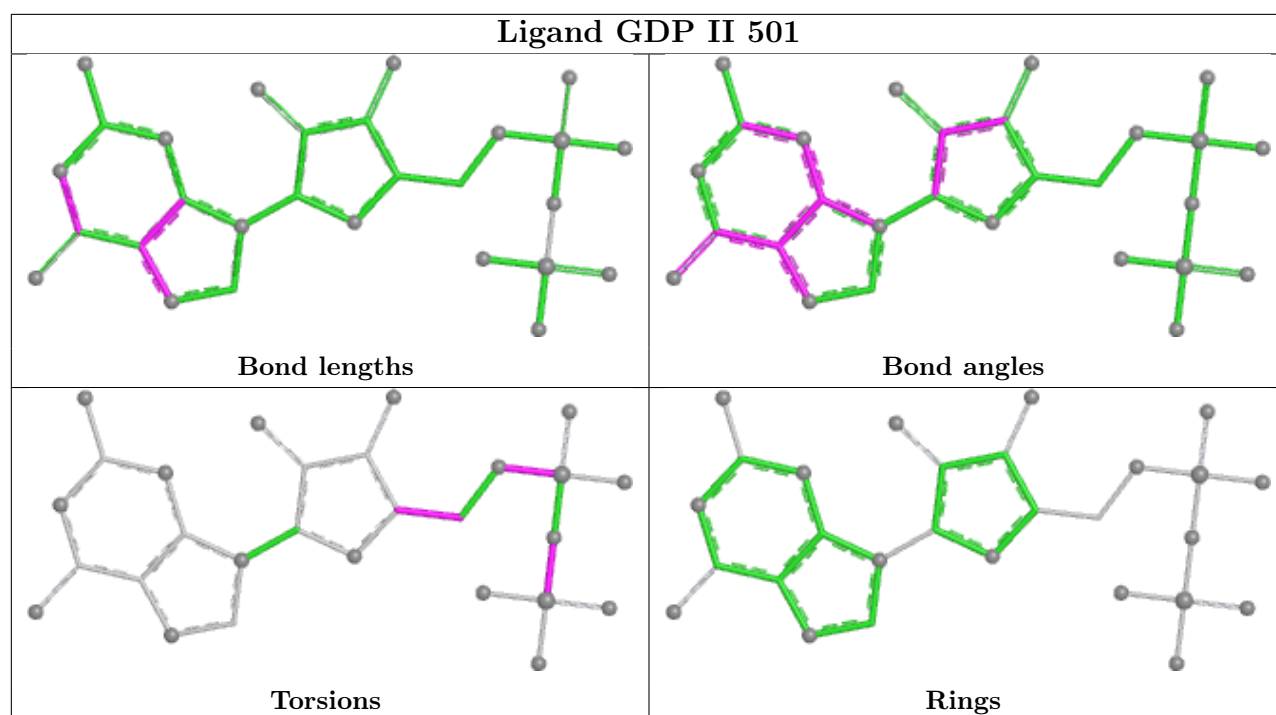


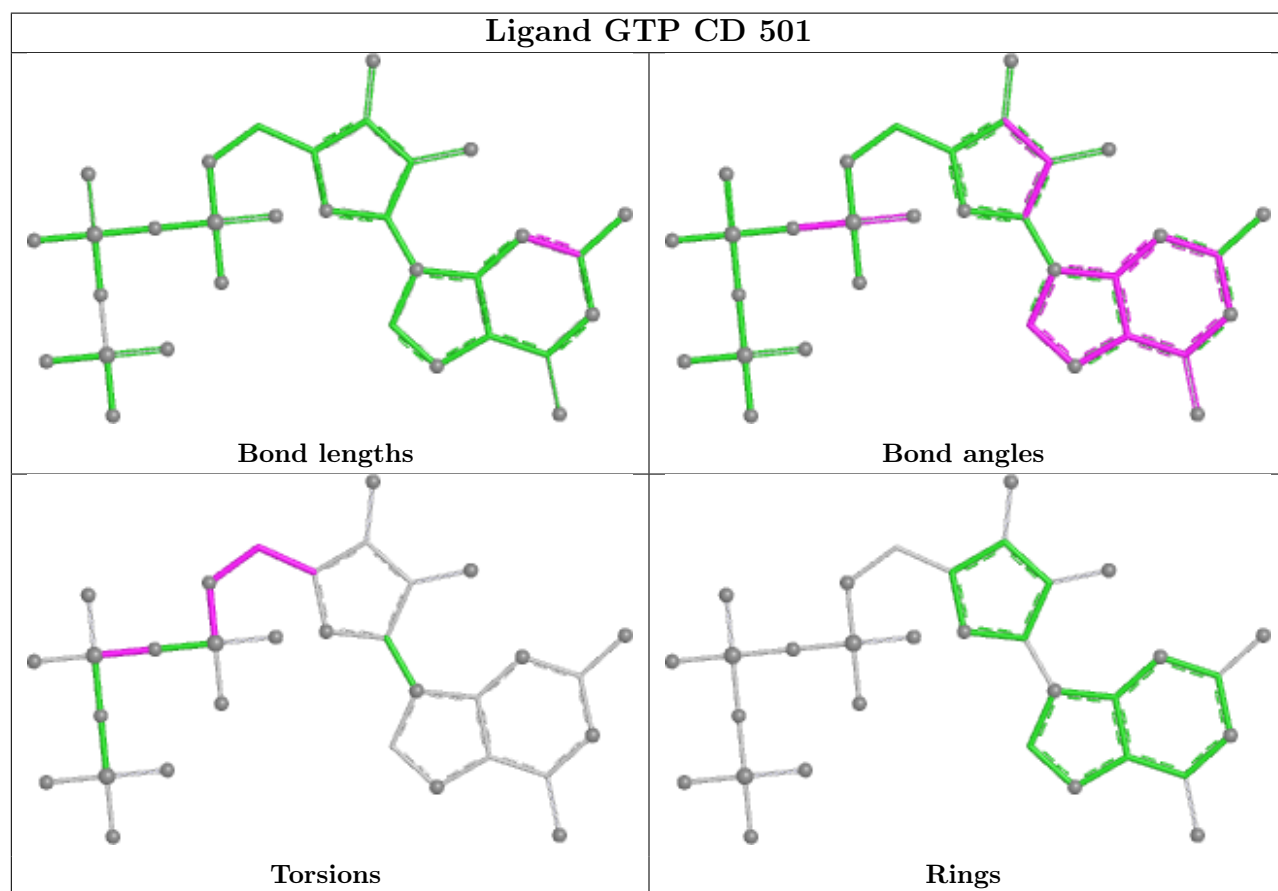
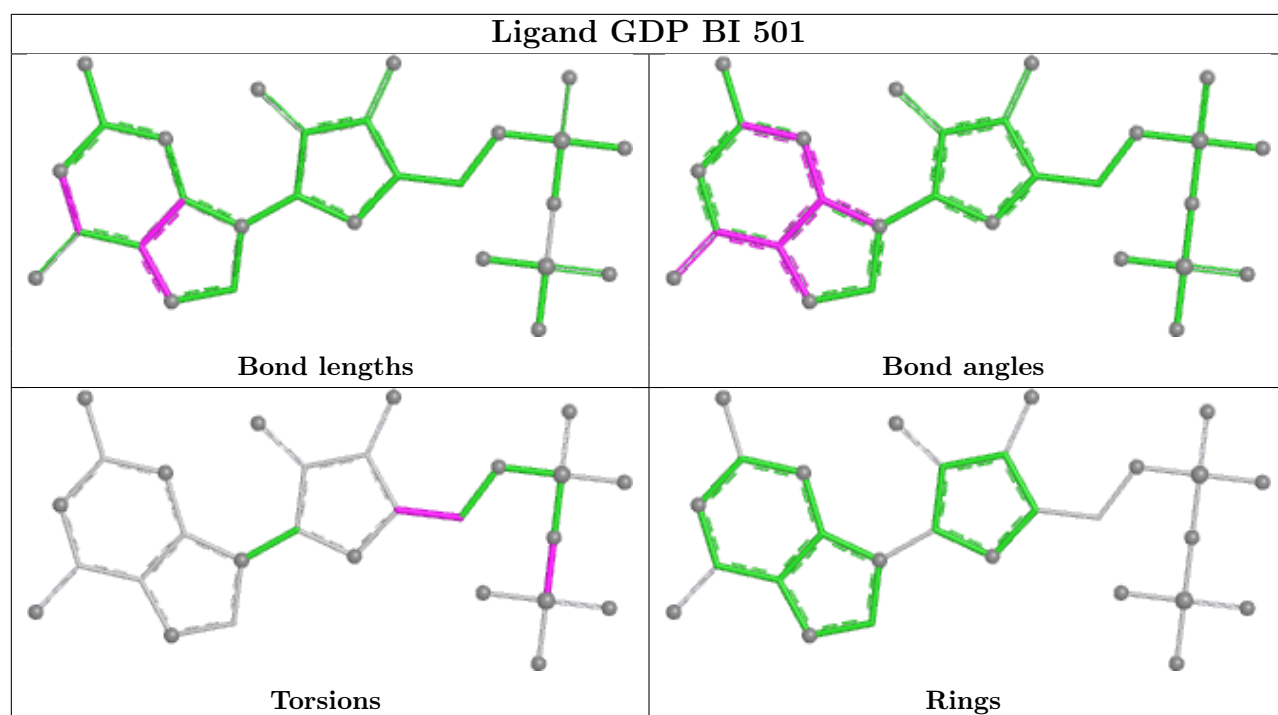
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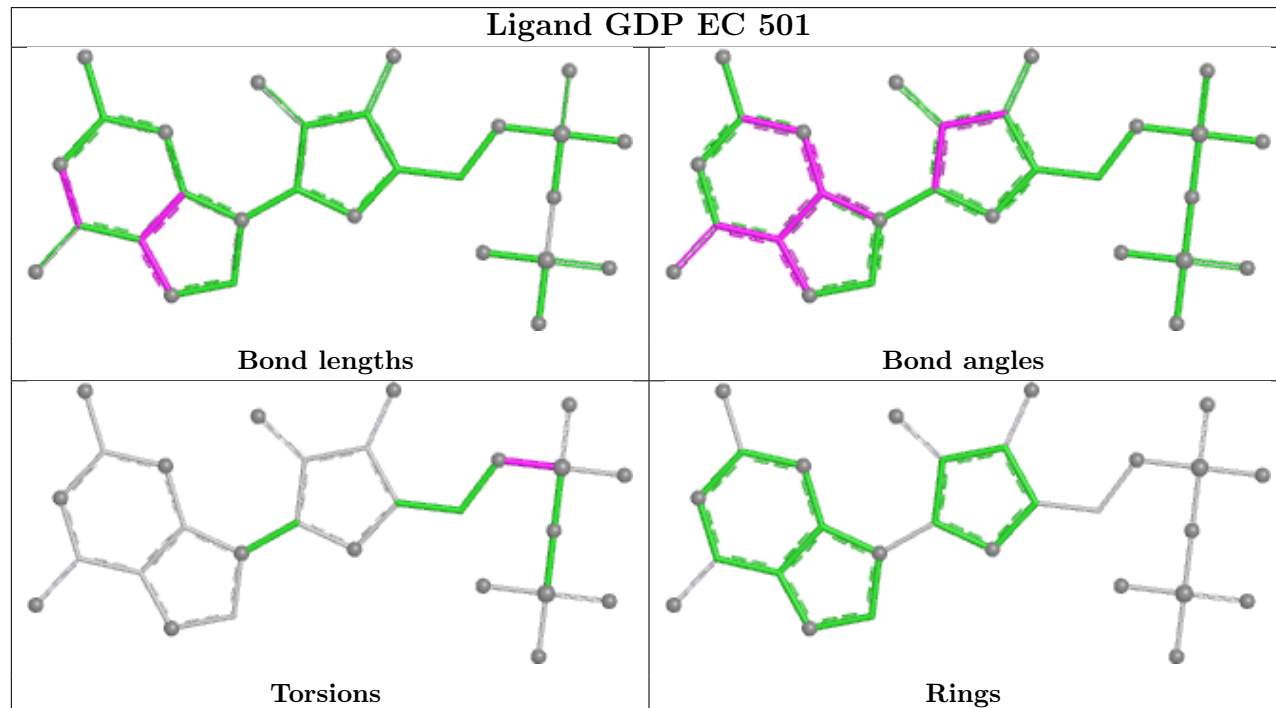
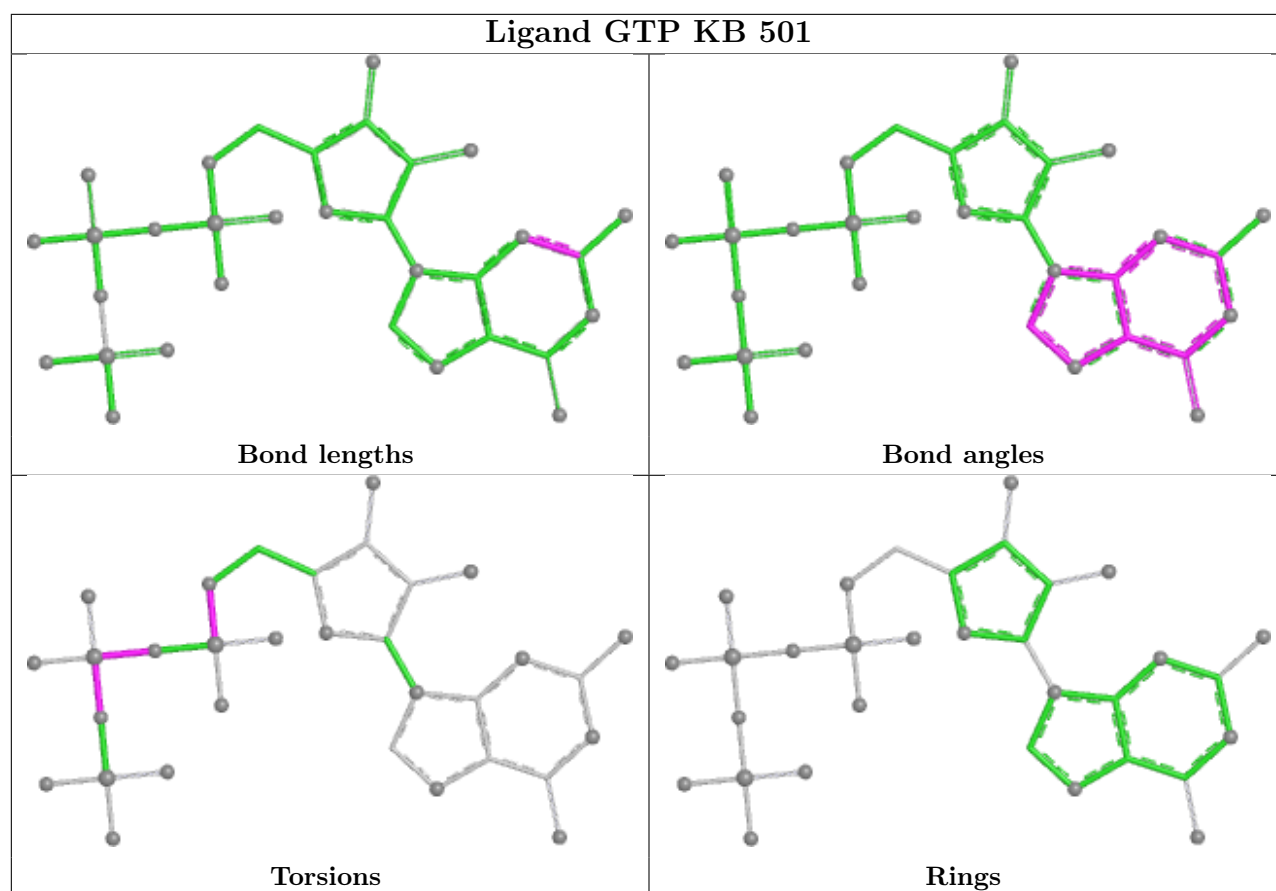


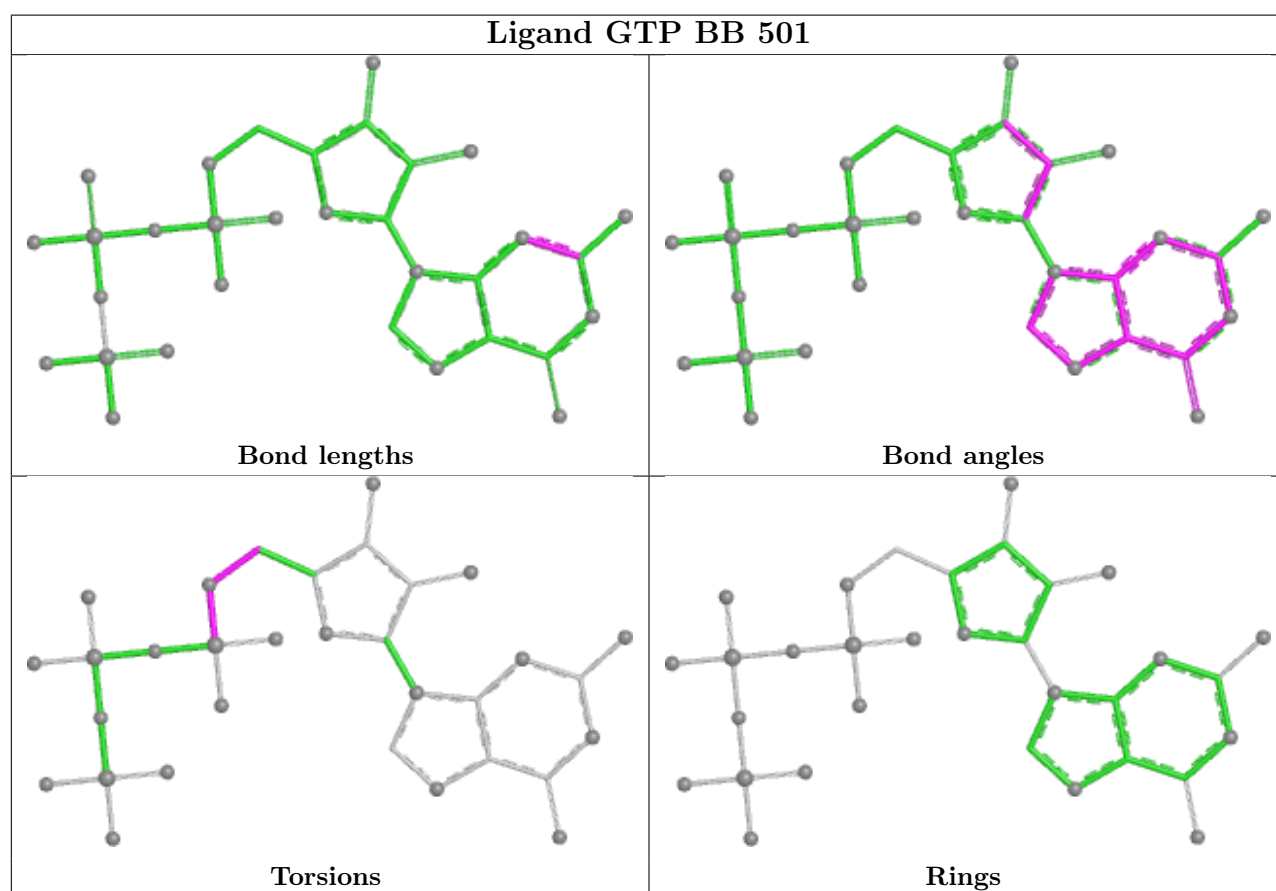
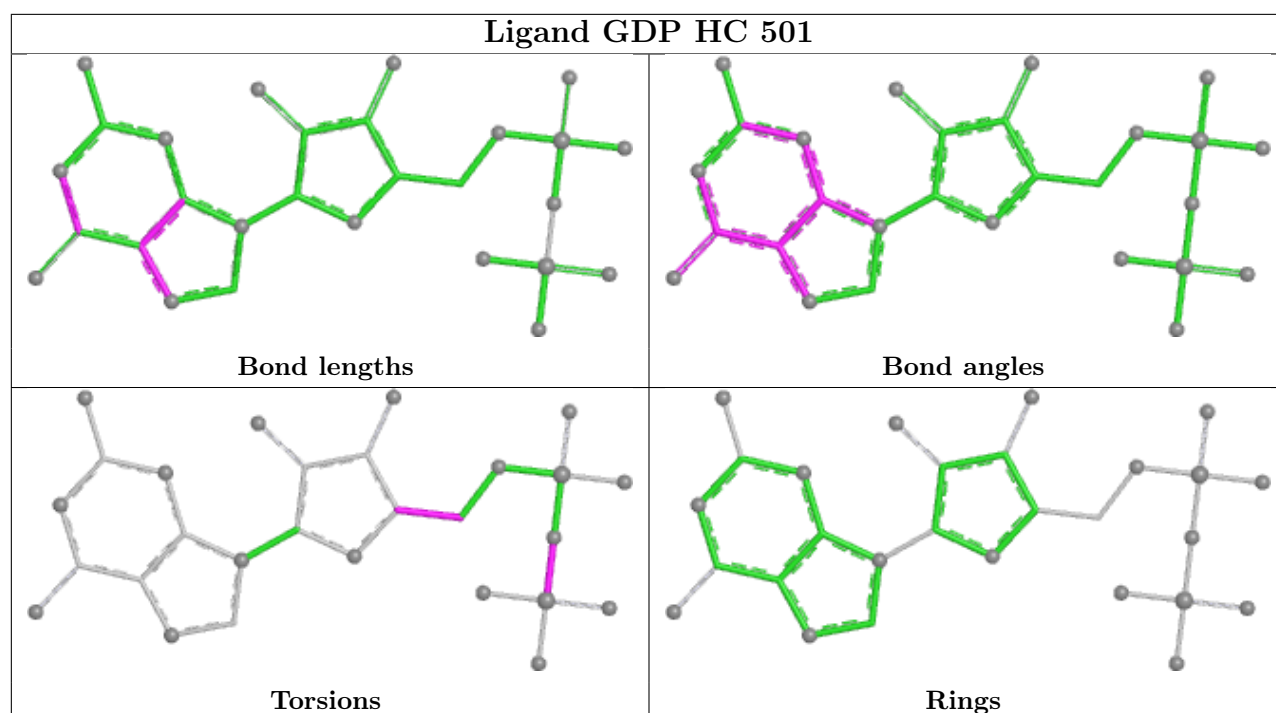
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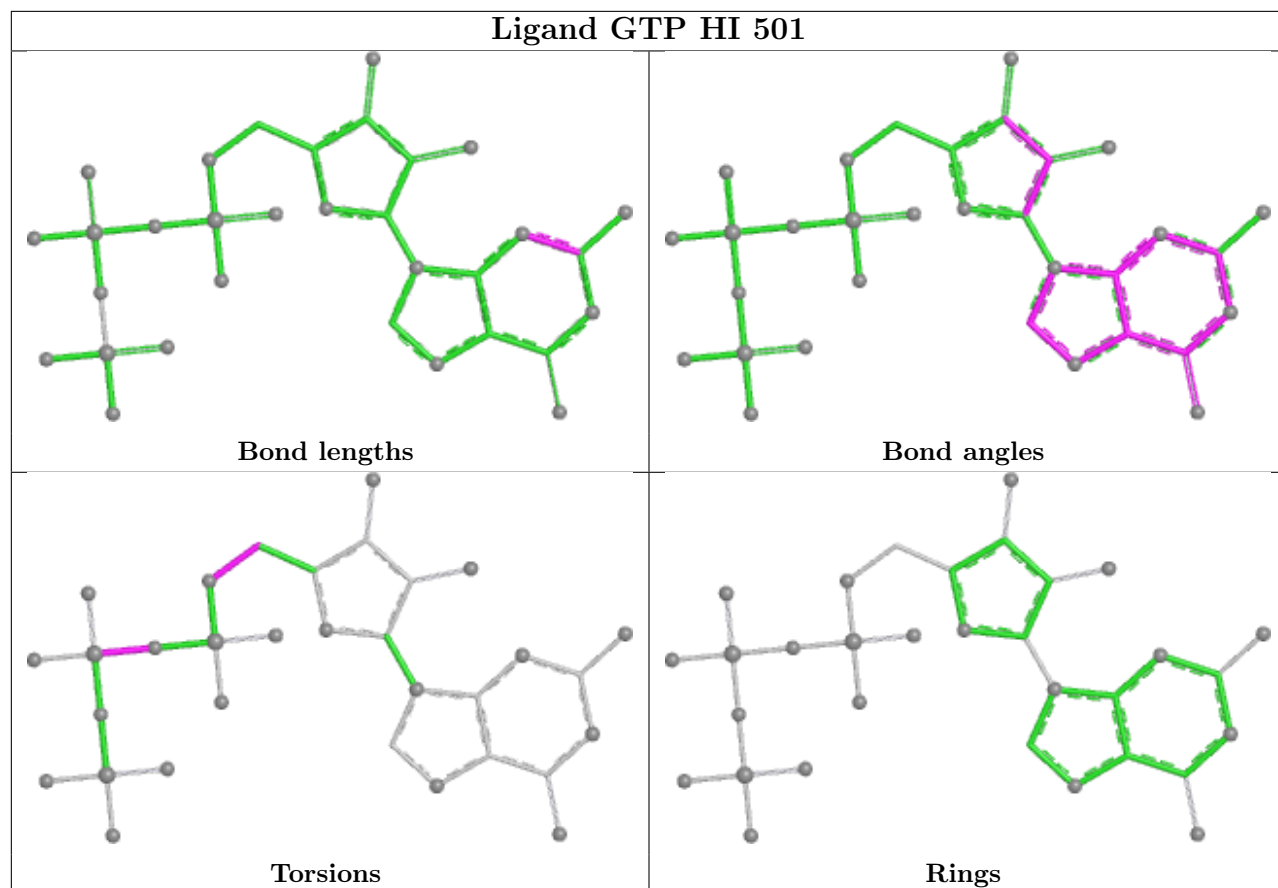




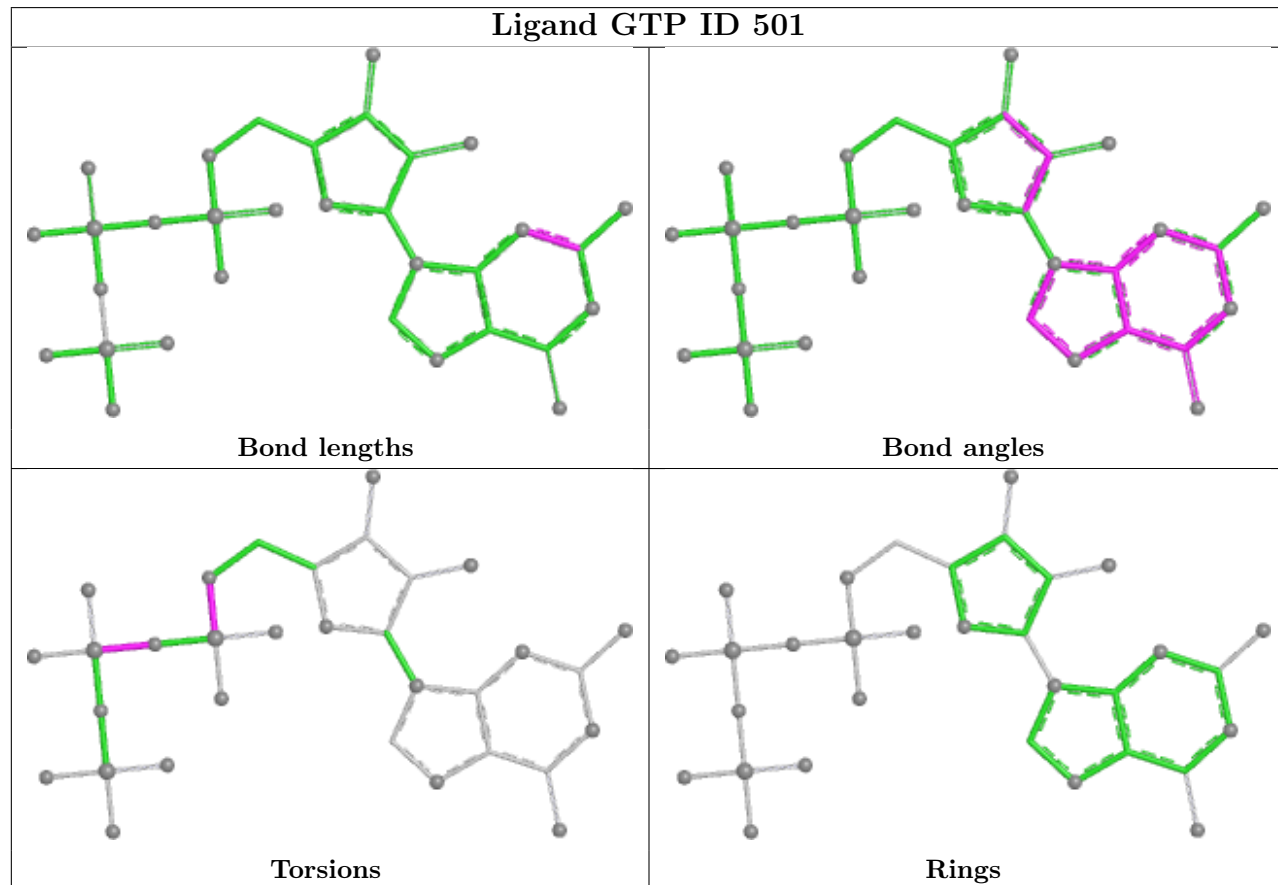


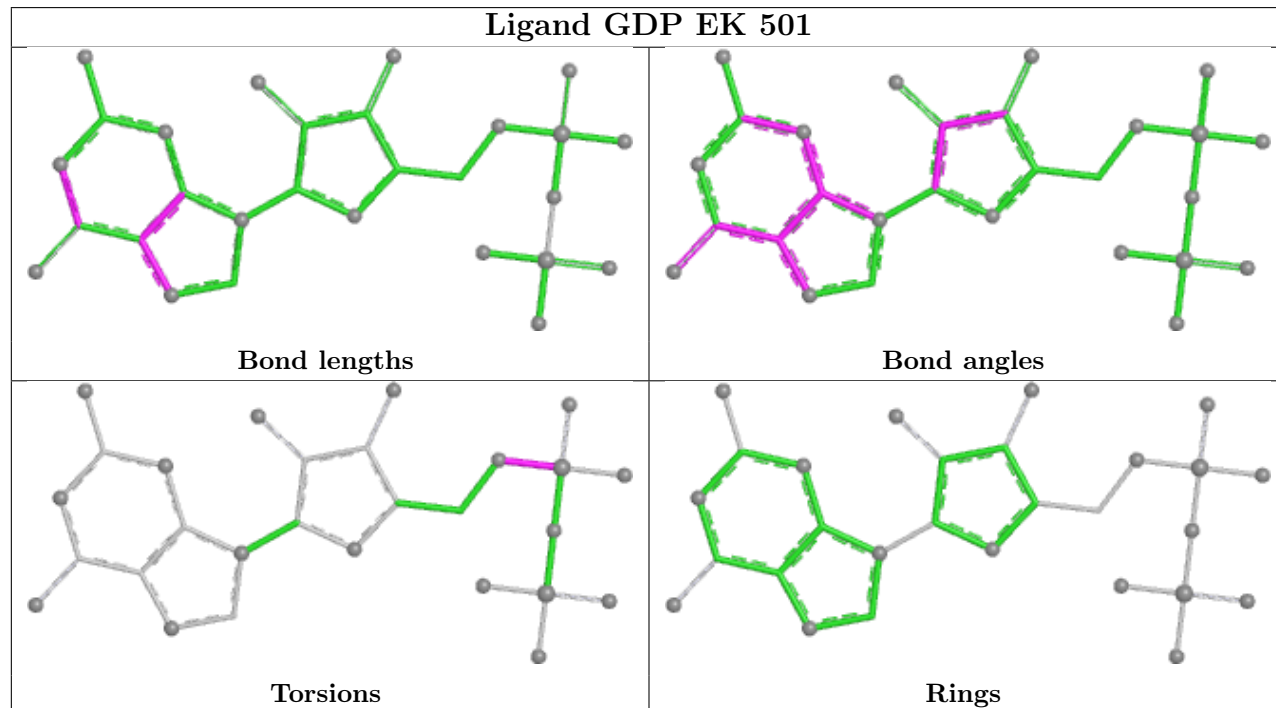
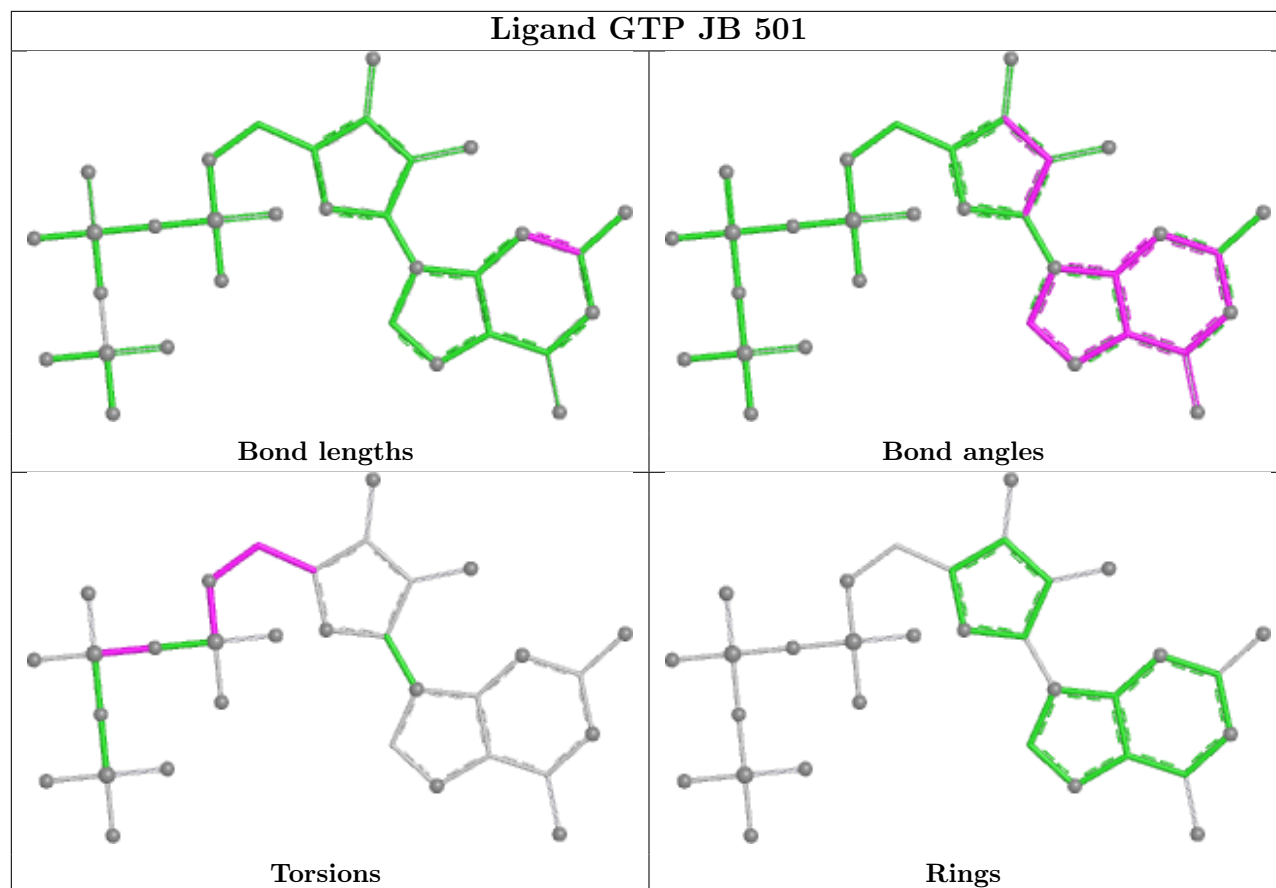


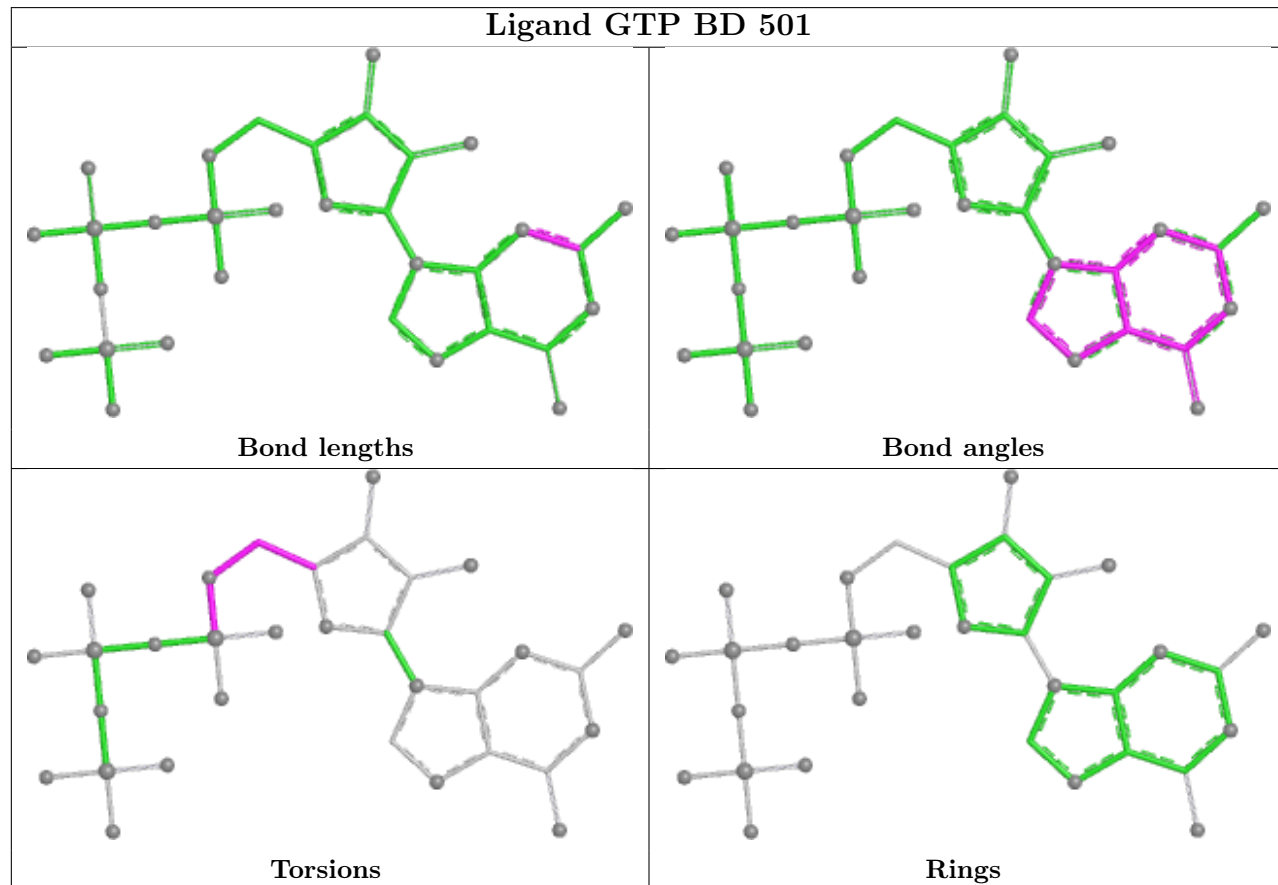
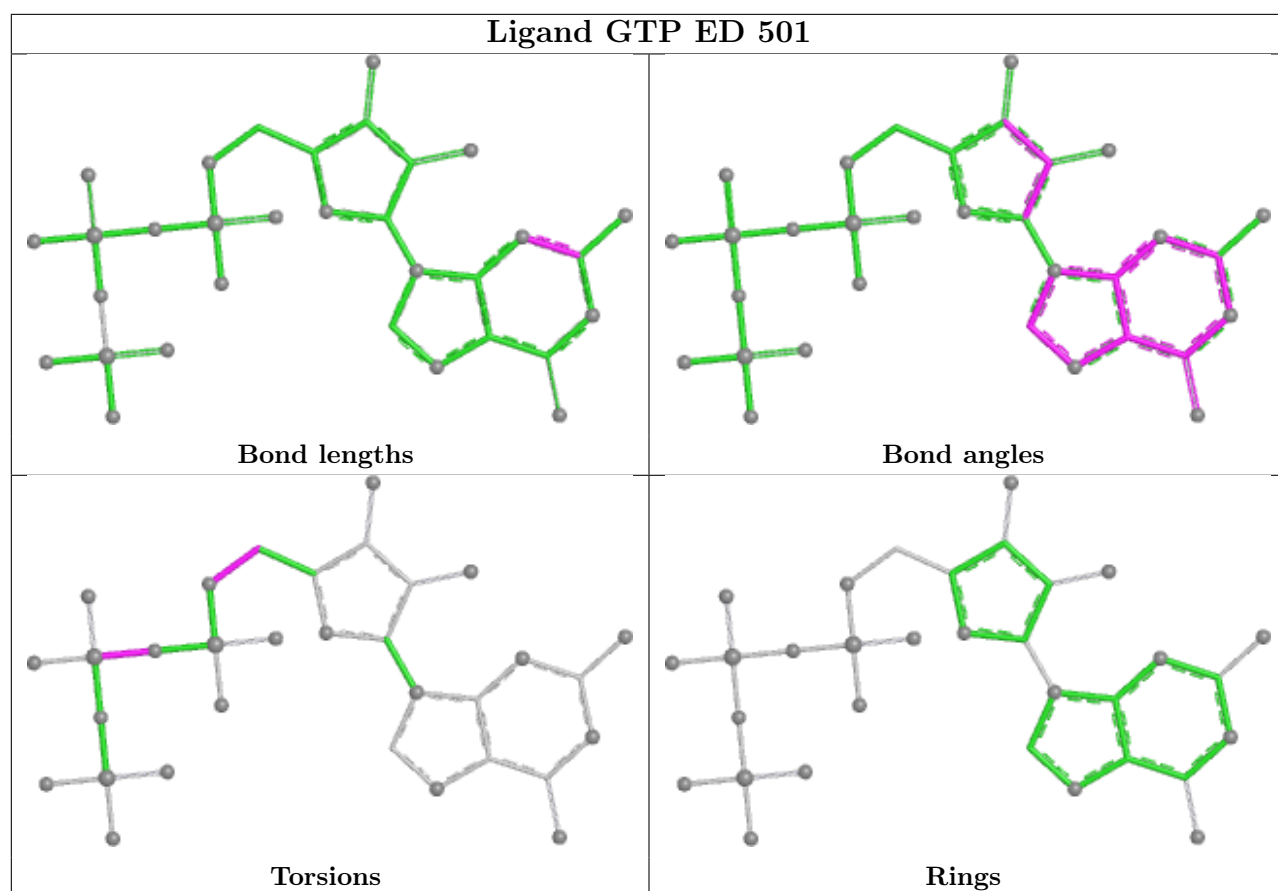
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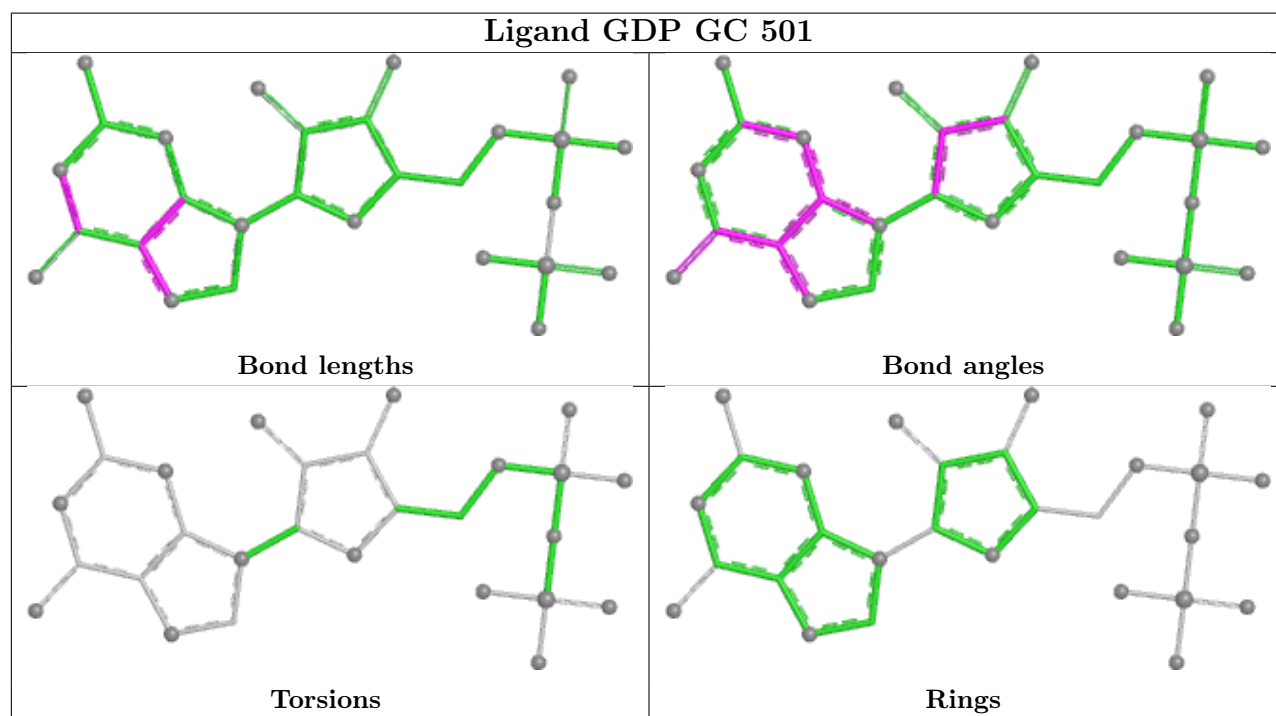
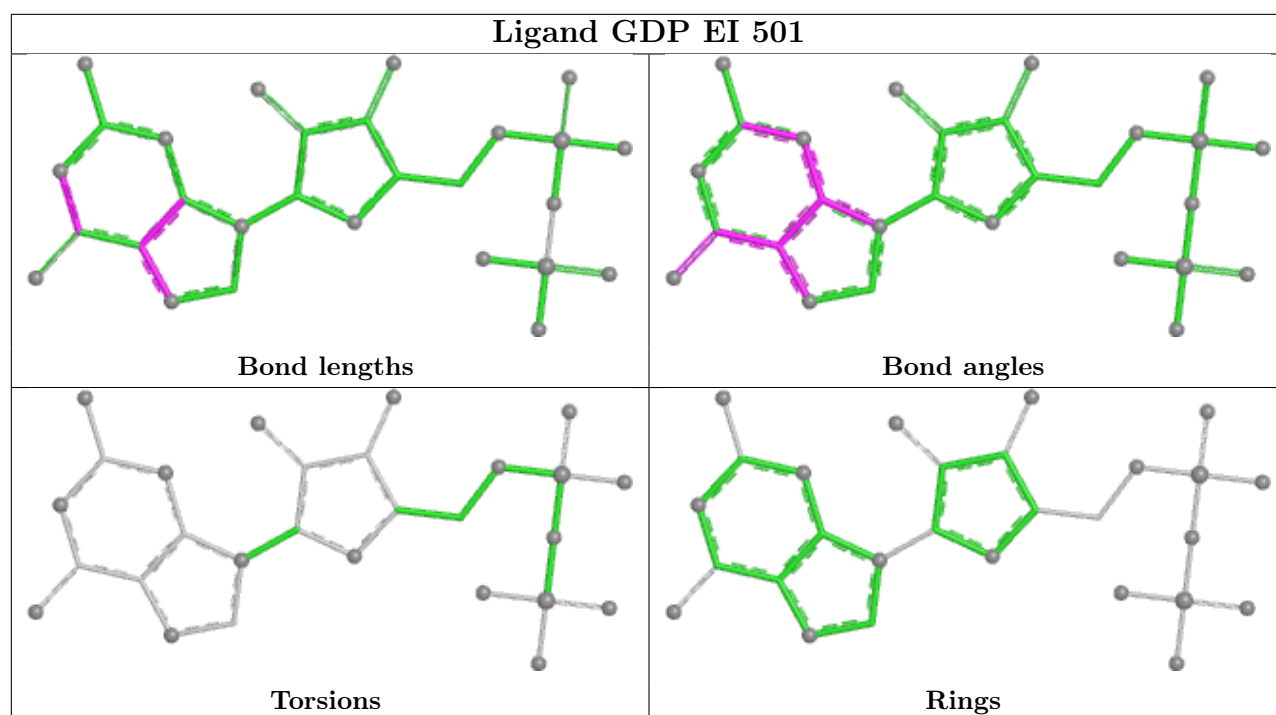


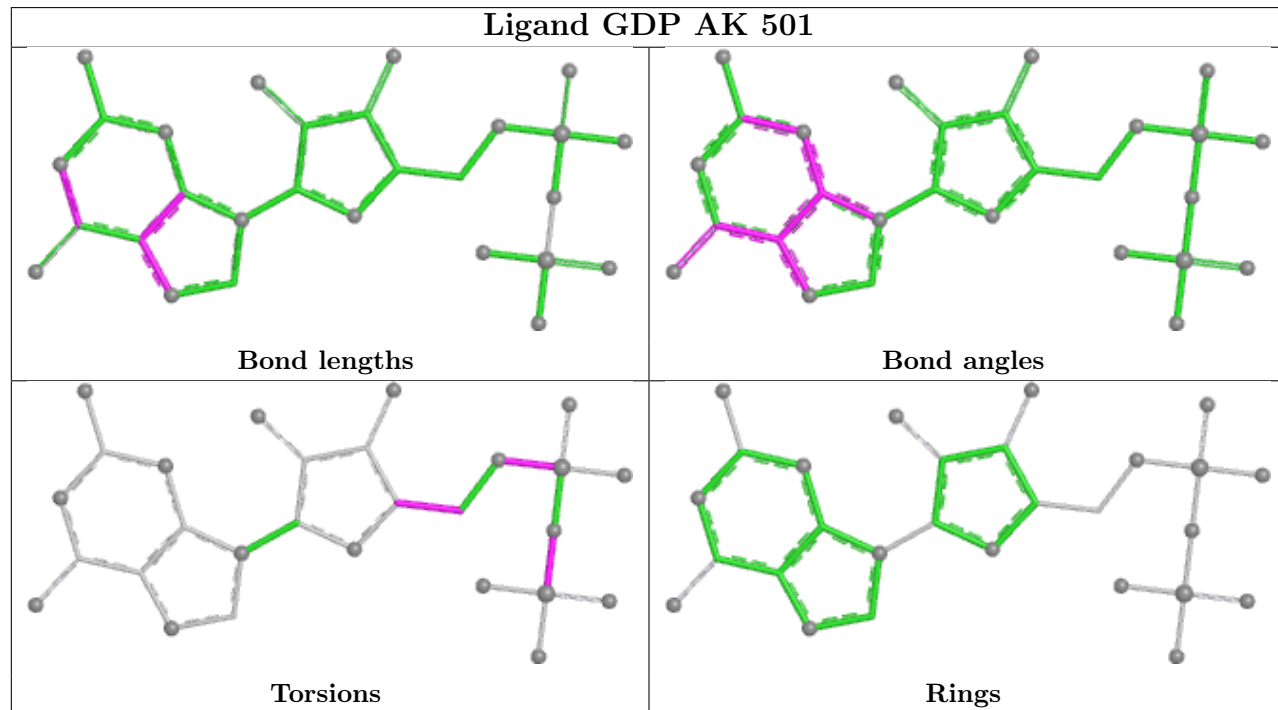
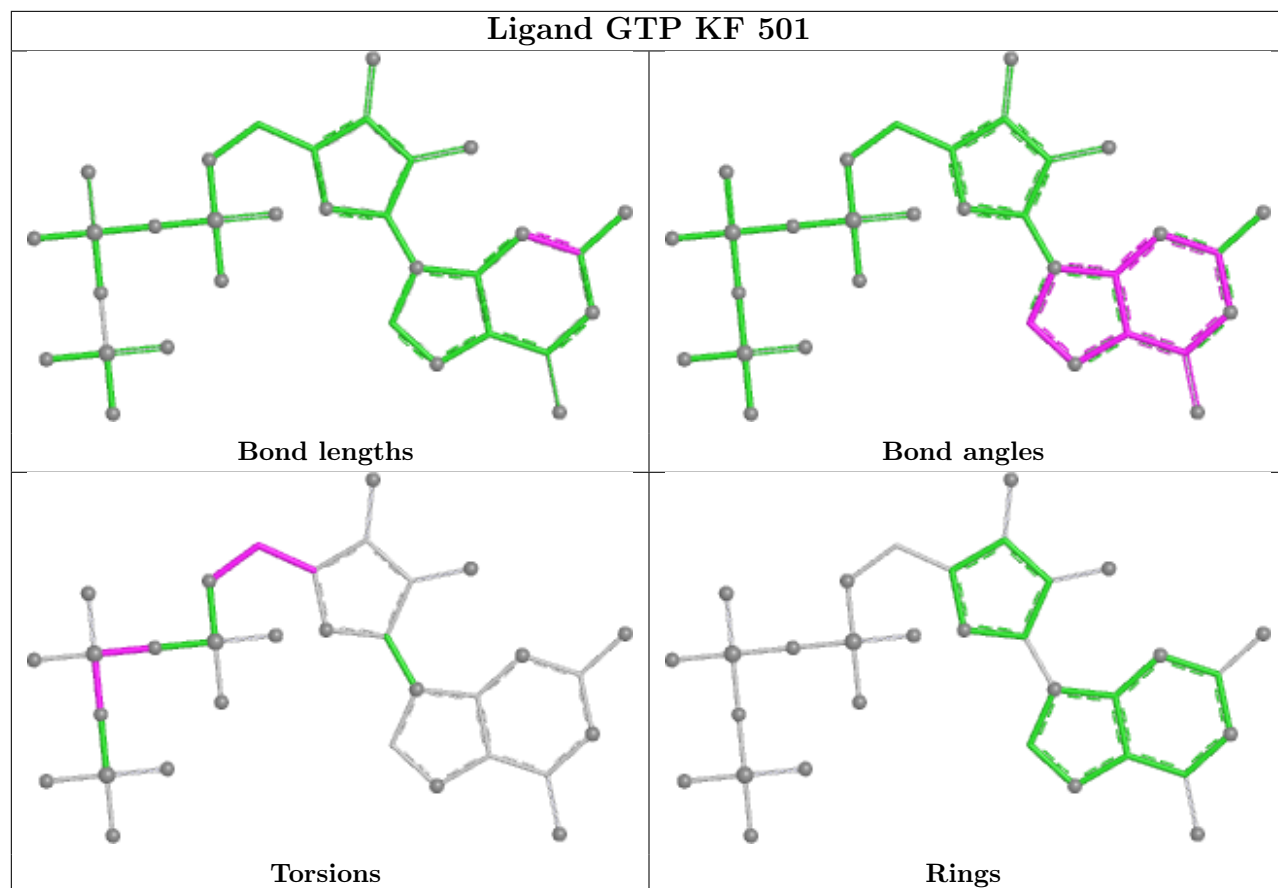
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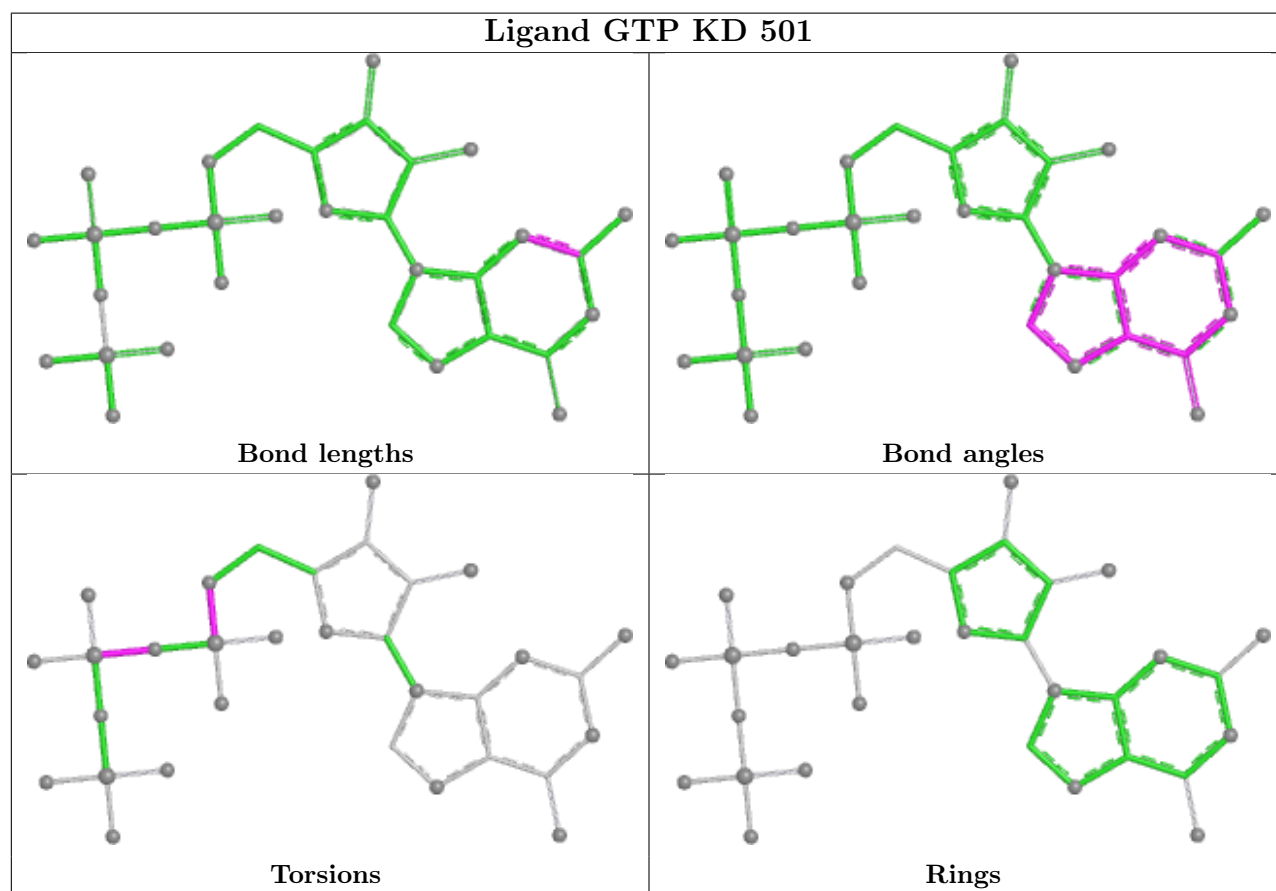
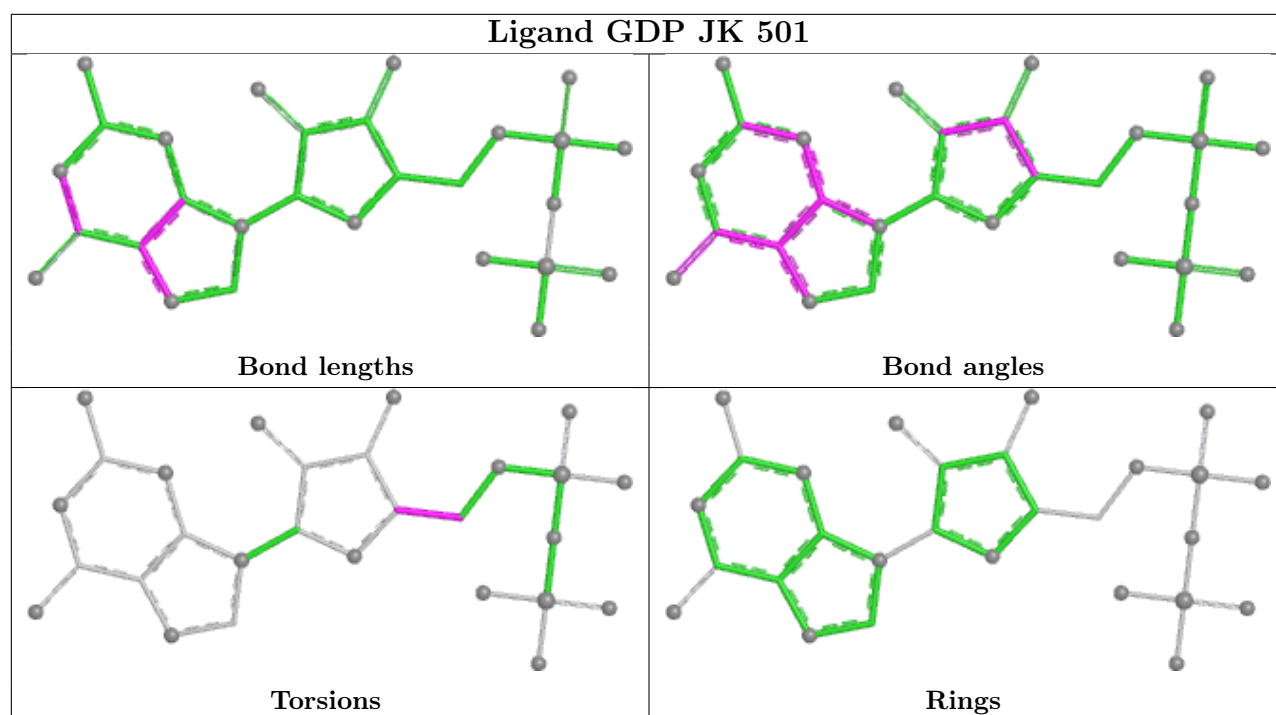


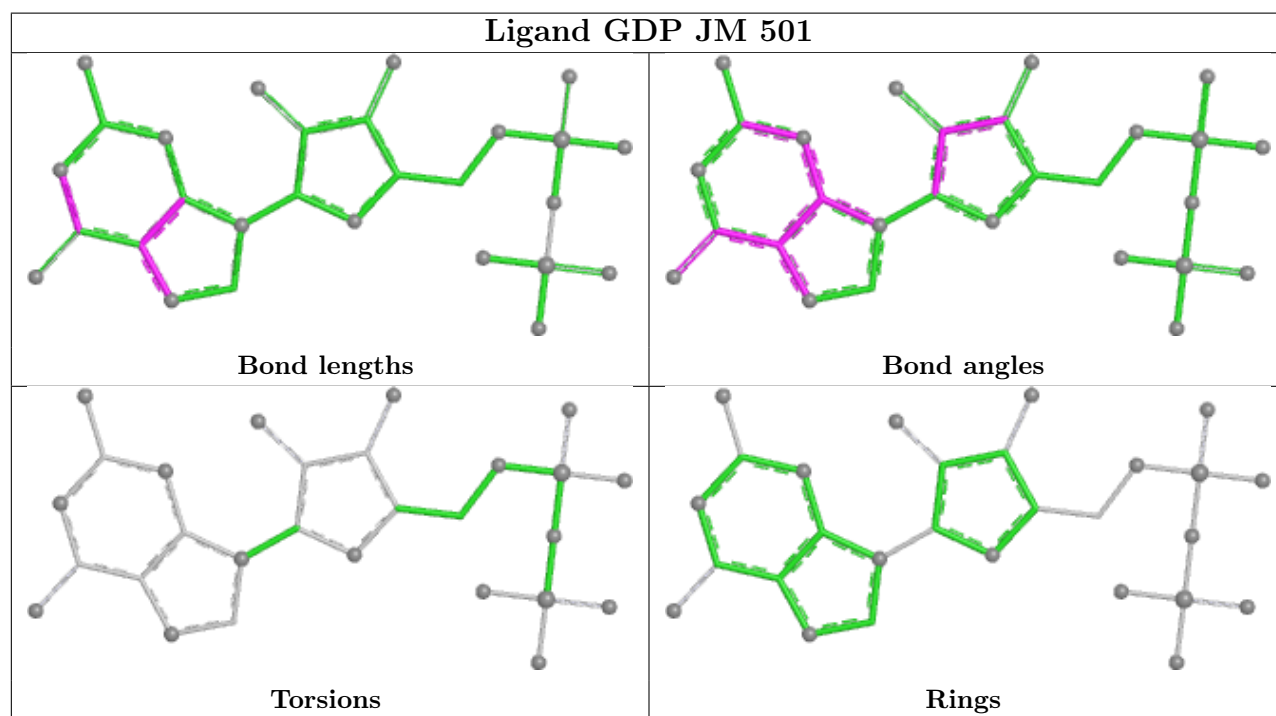
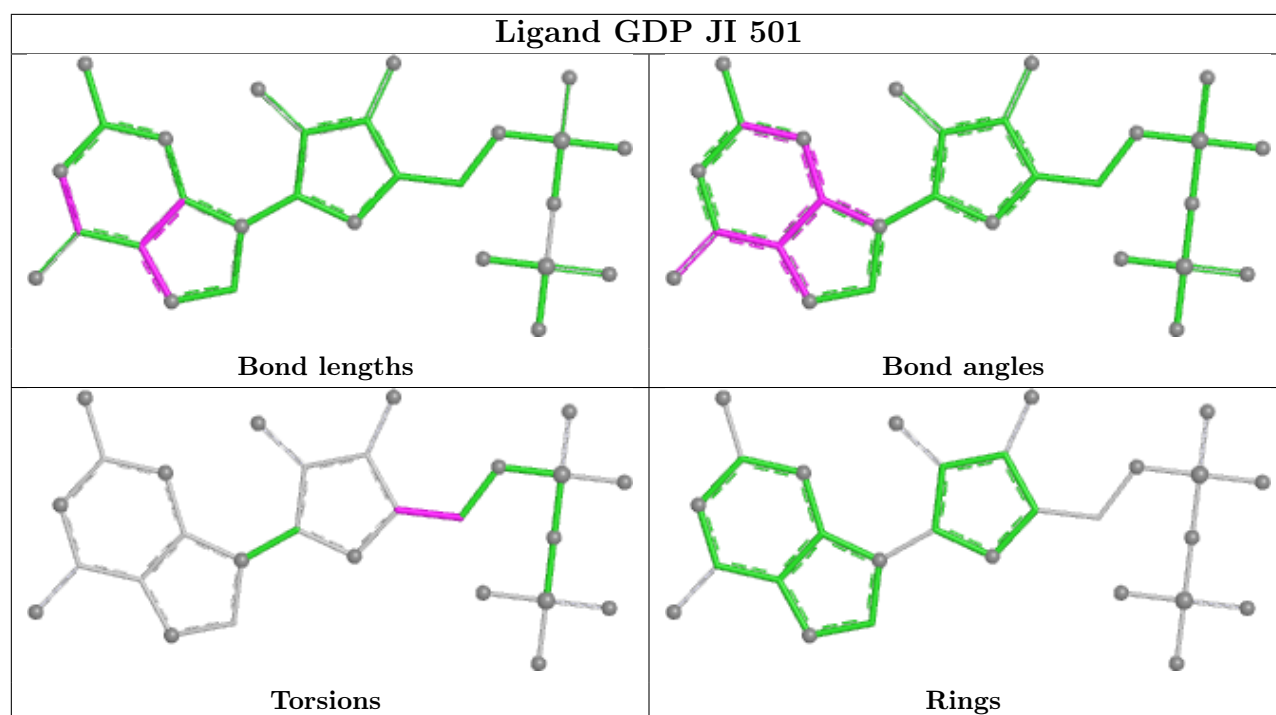




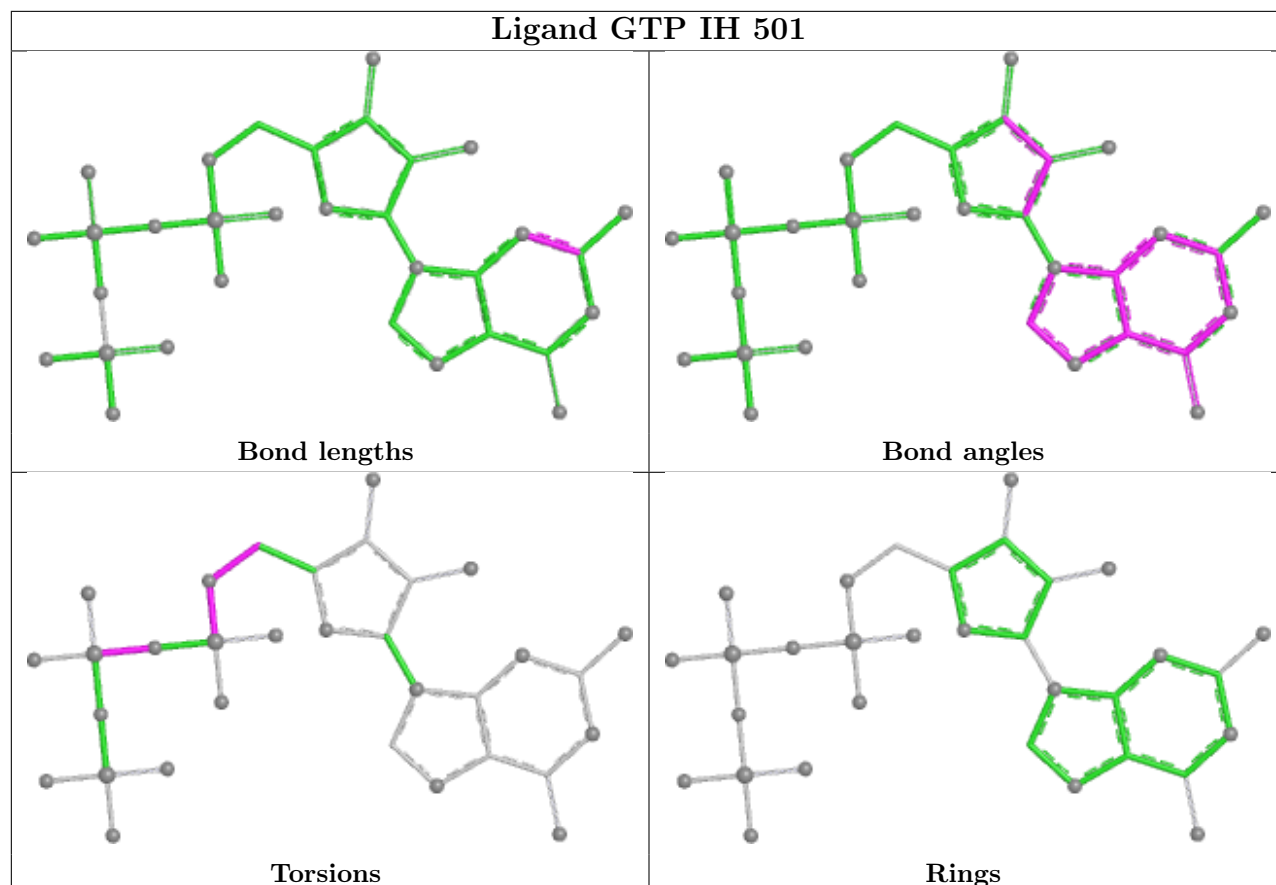




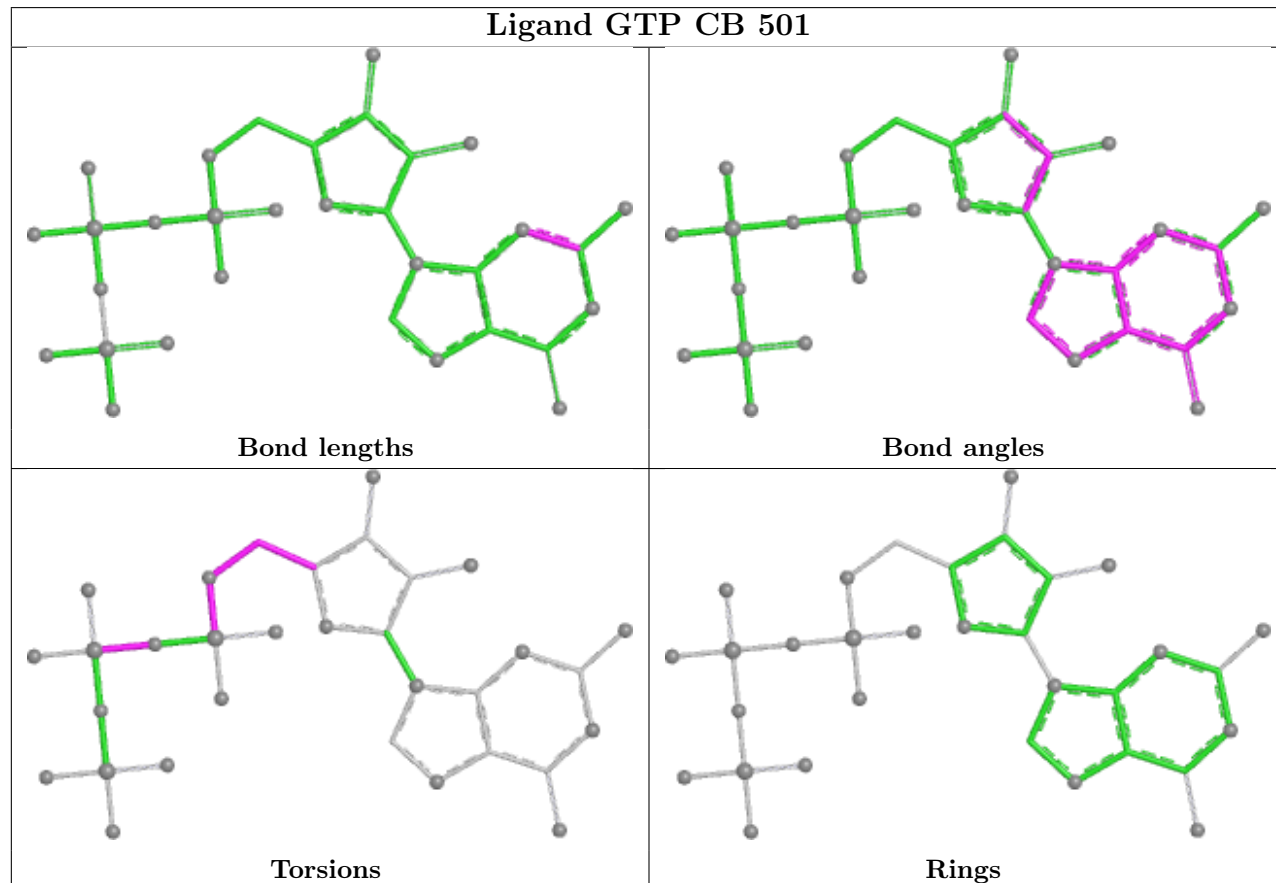


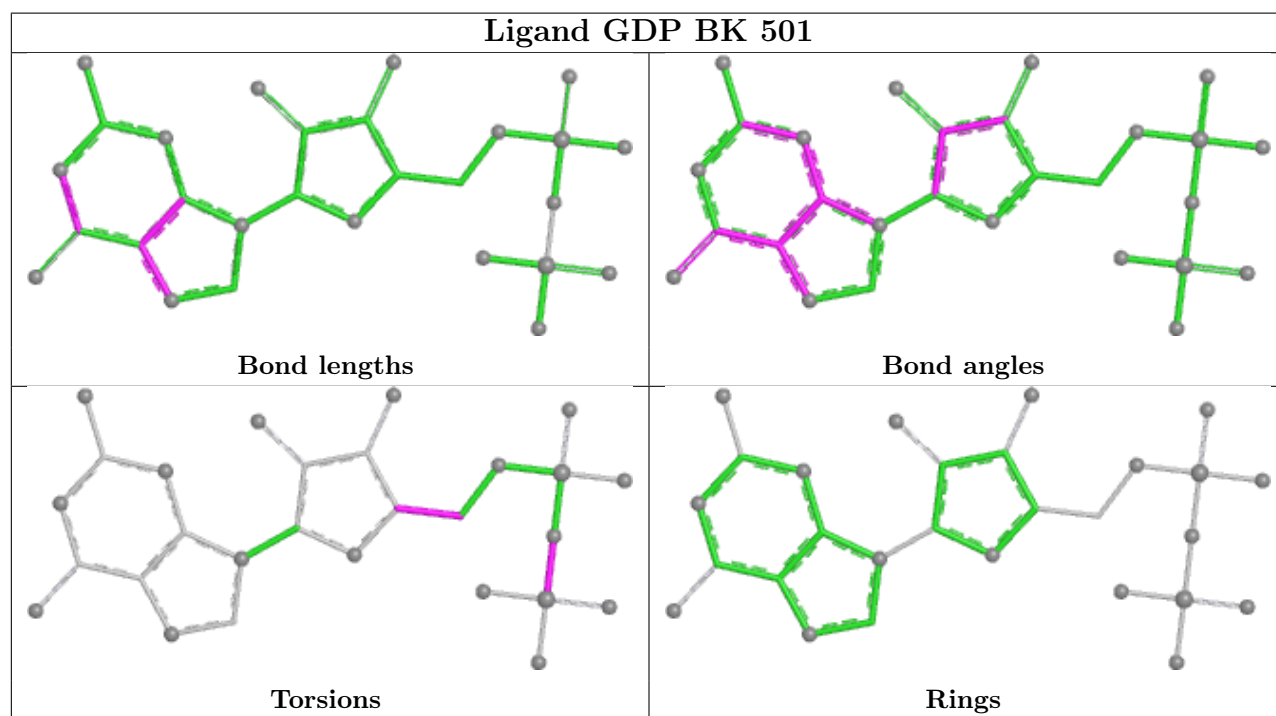
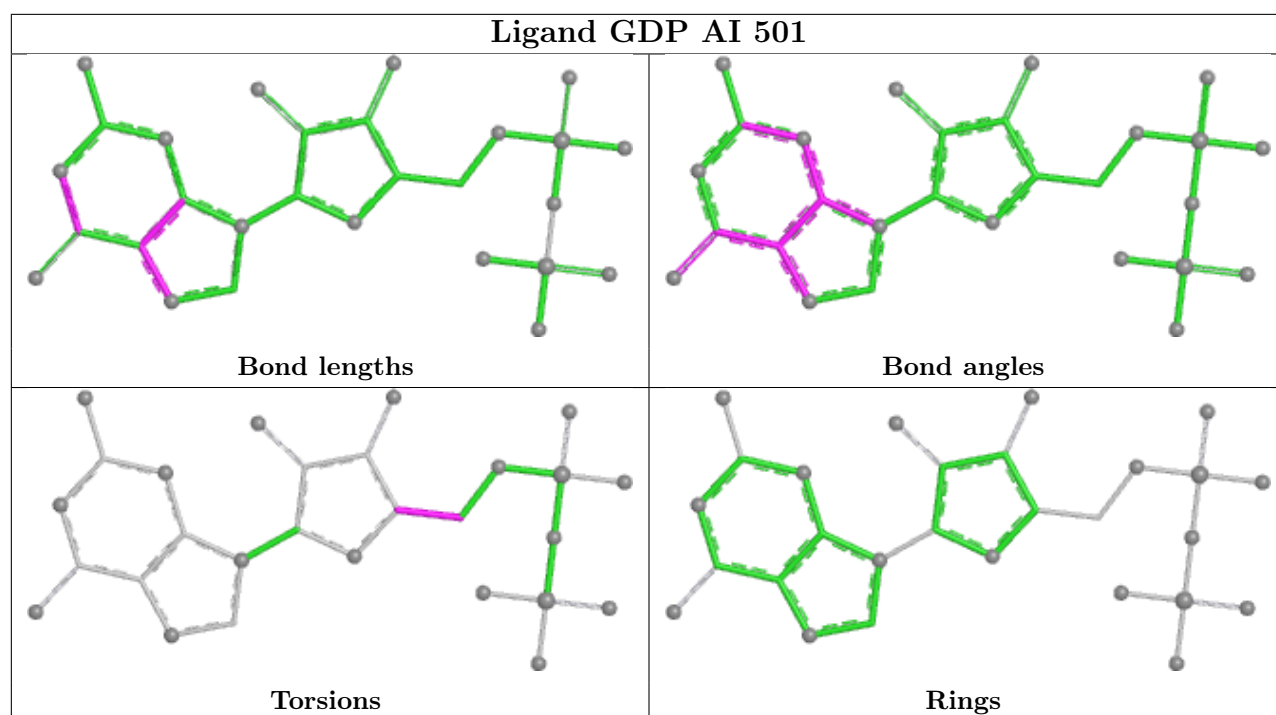


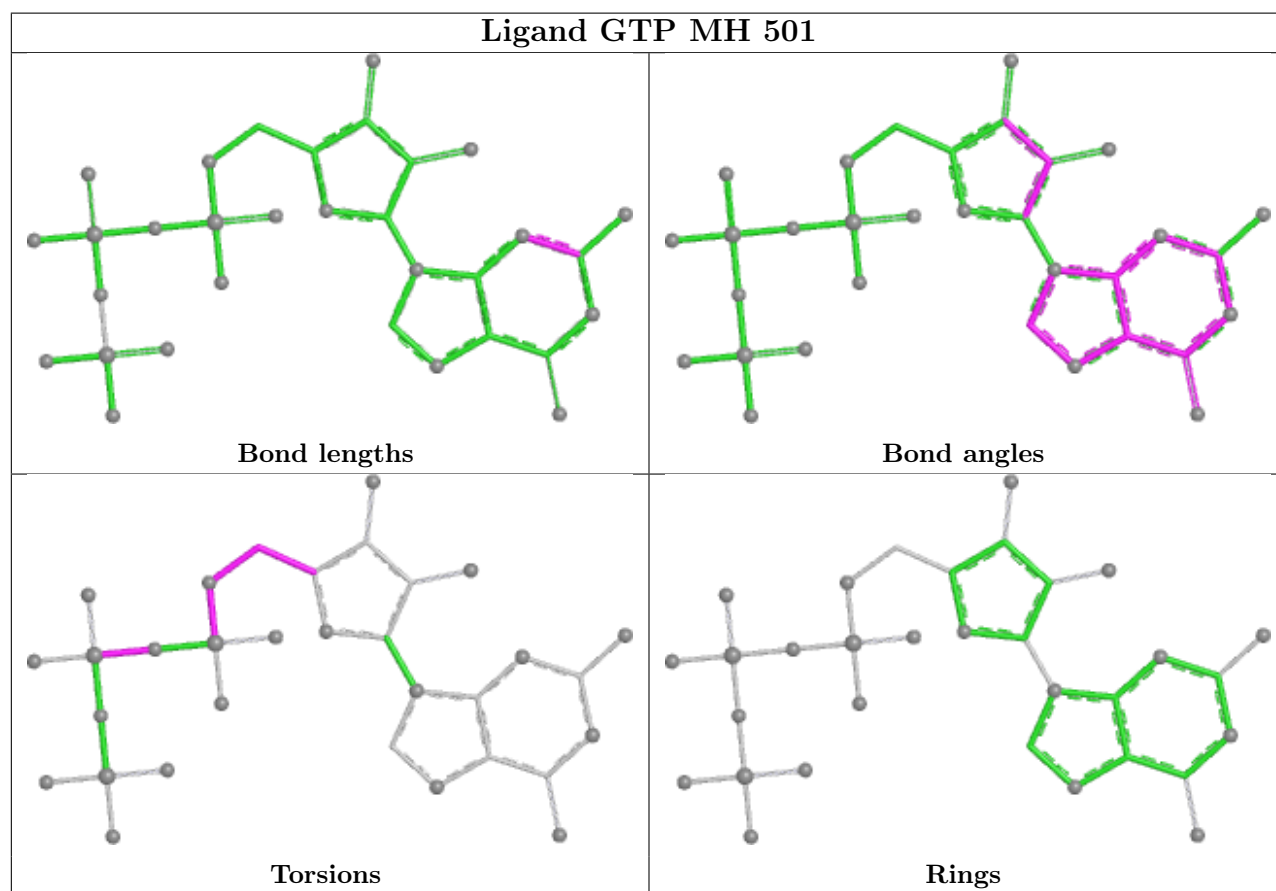
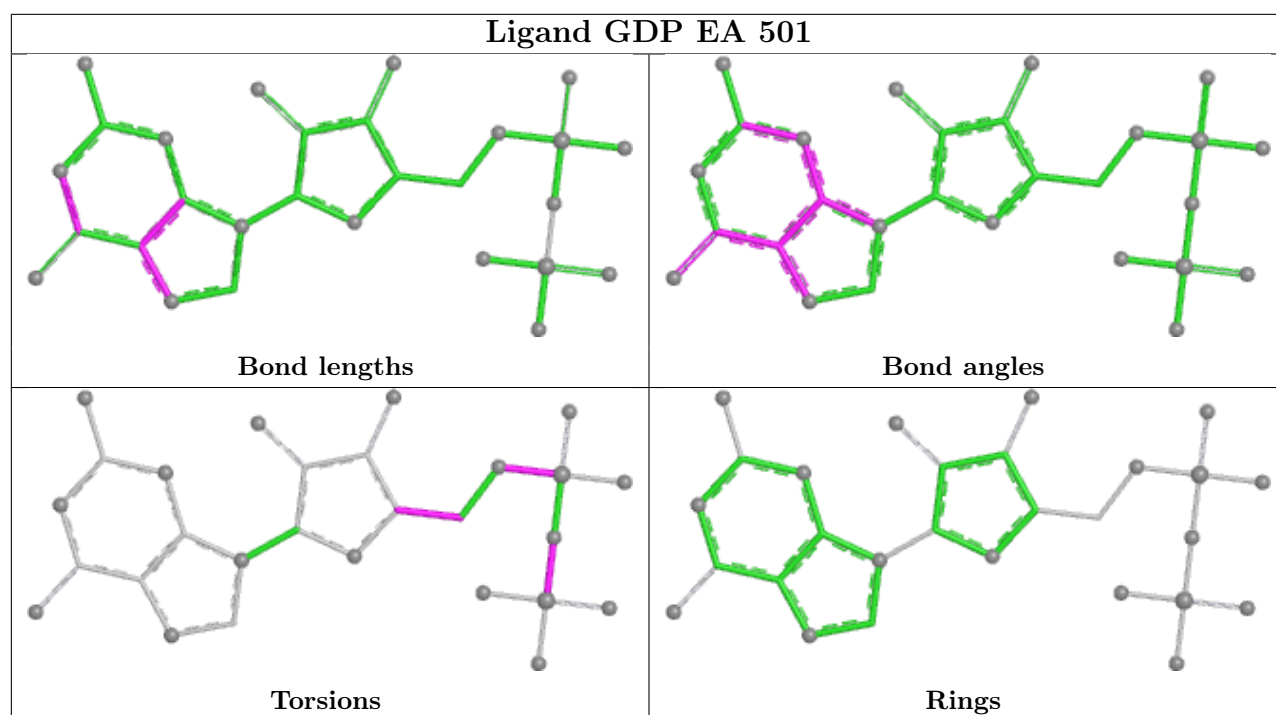
Ligand GTP IH 501

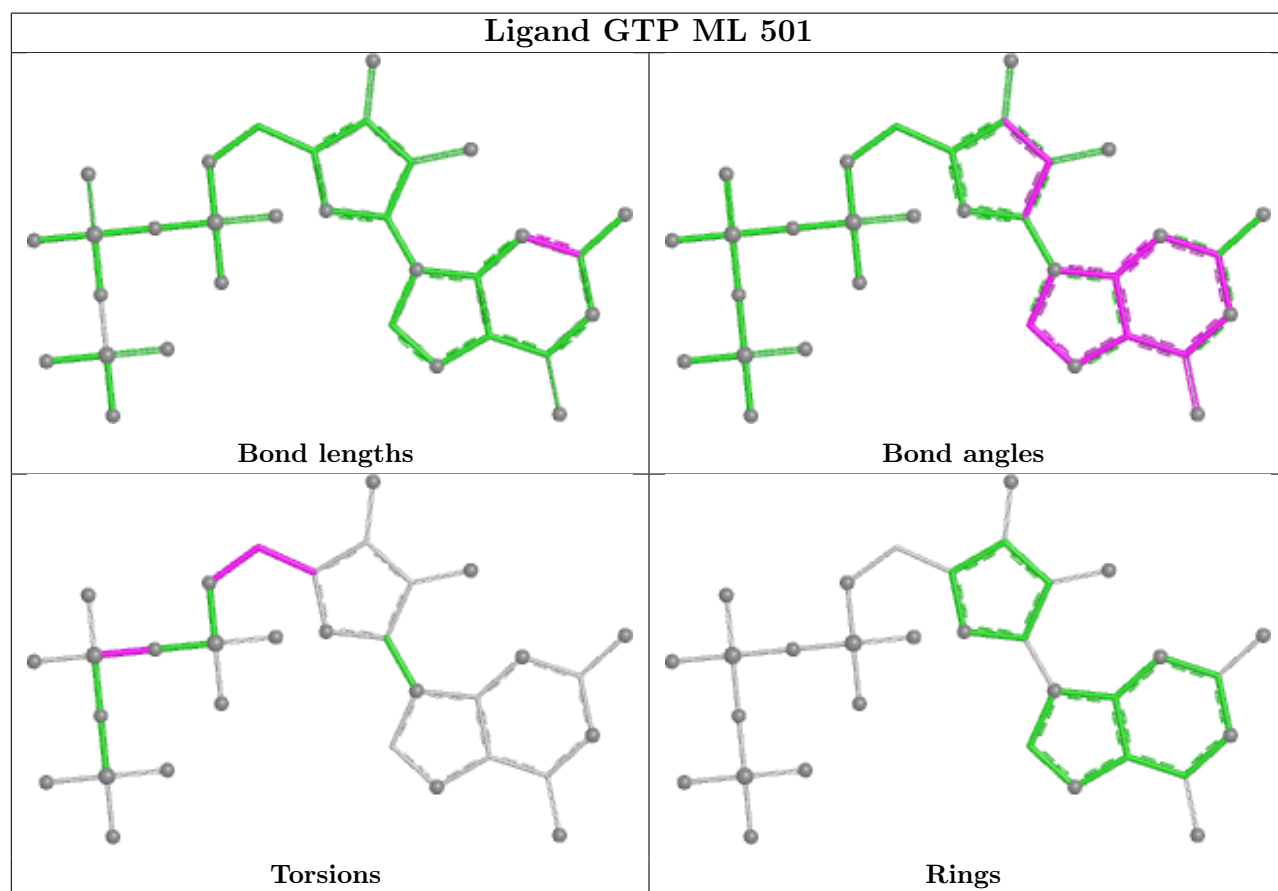
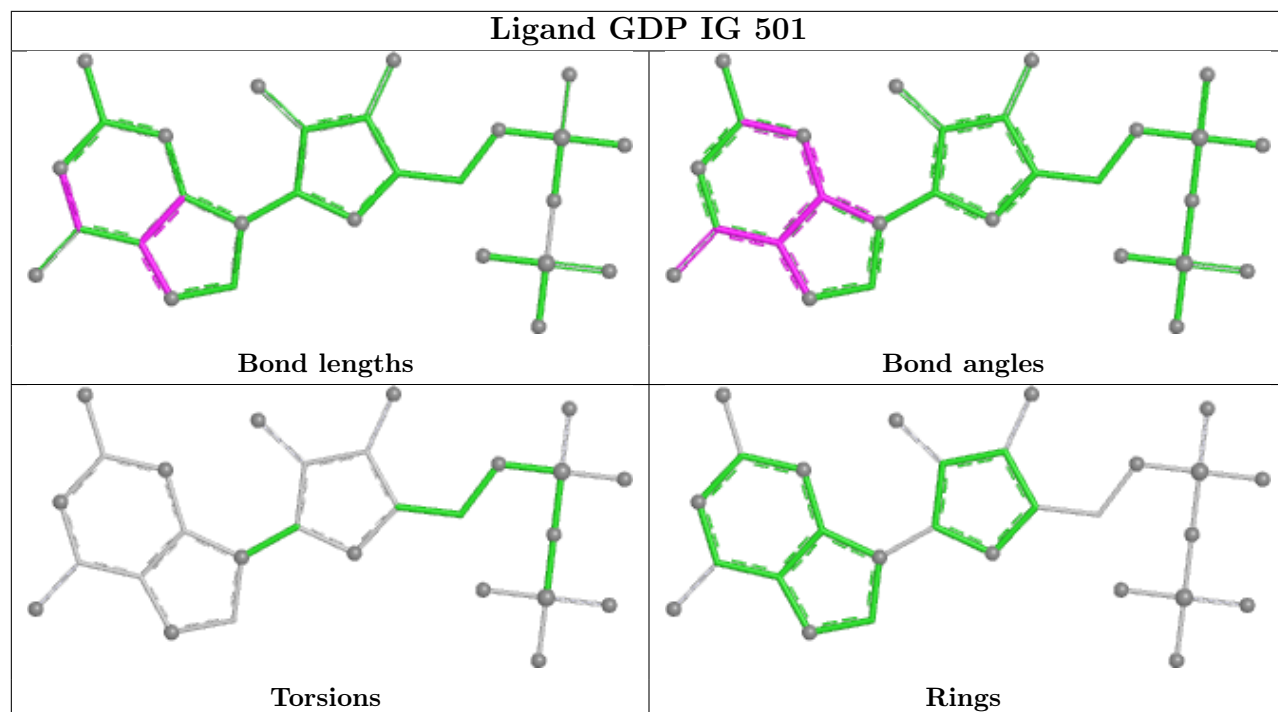


Ligand GTP CB 501

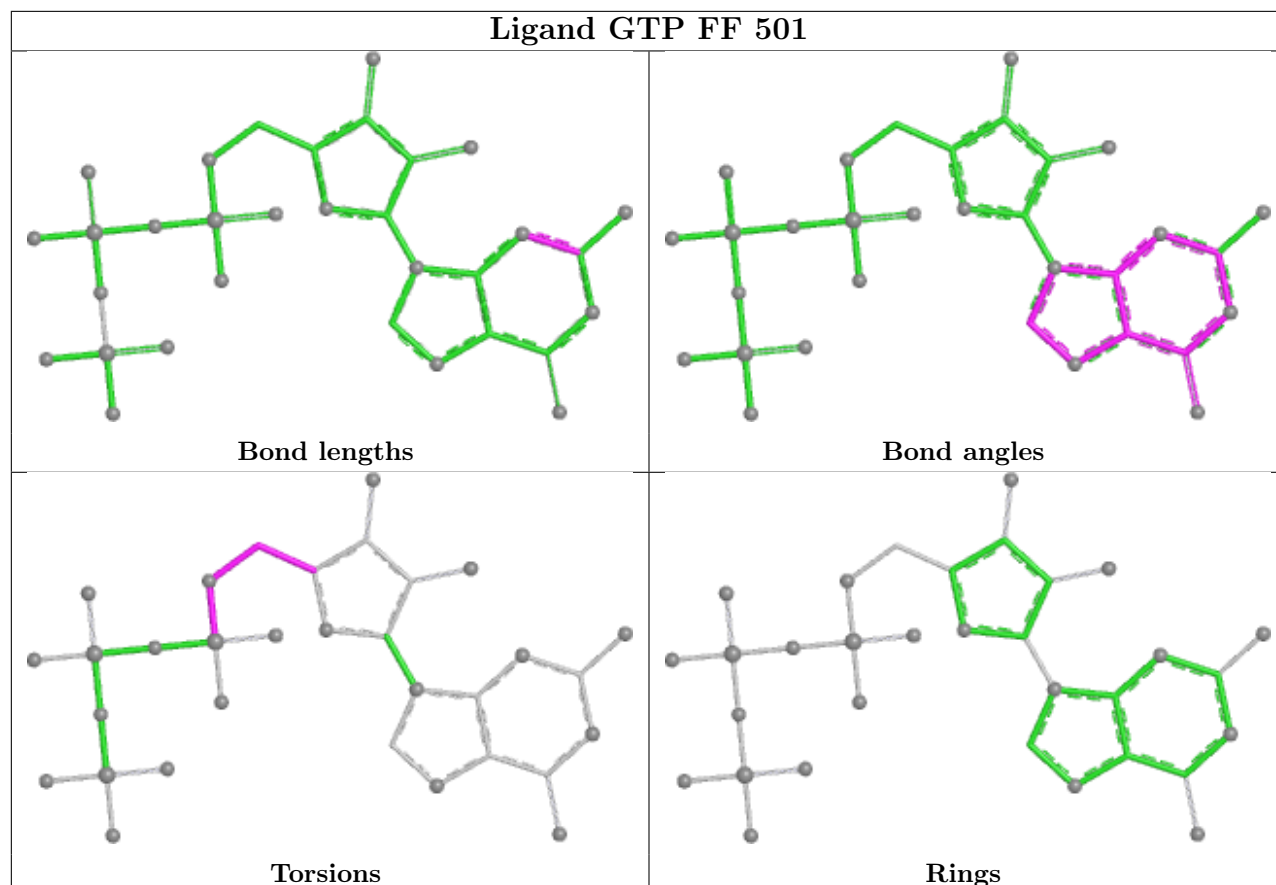




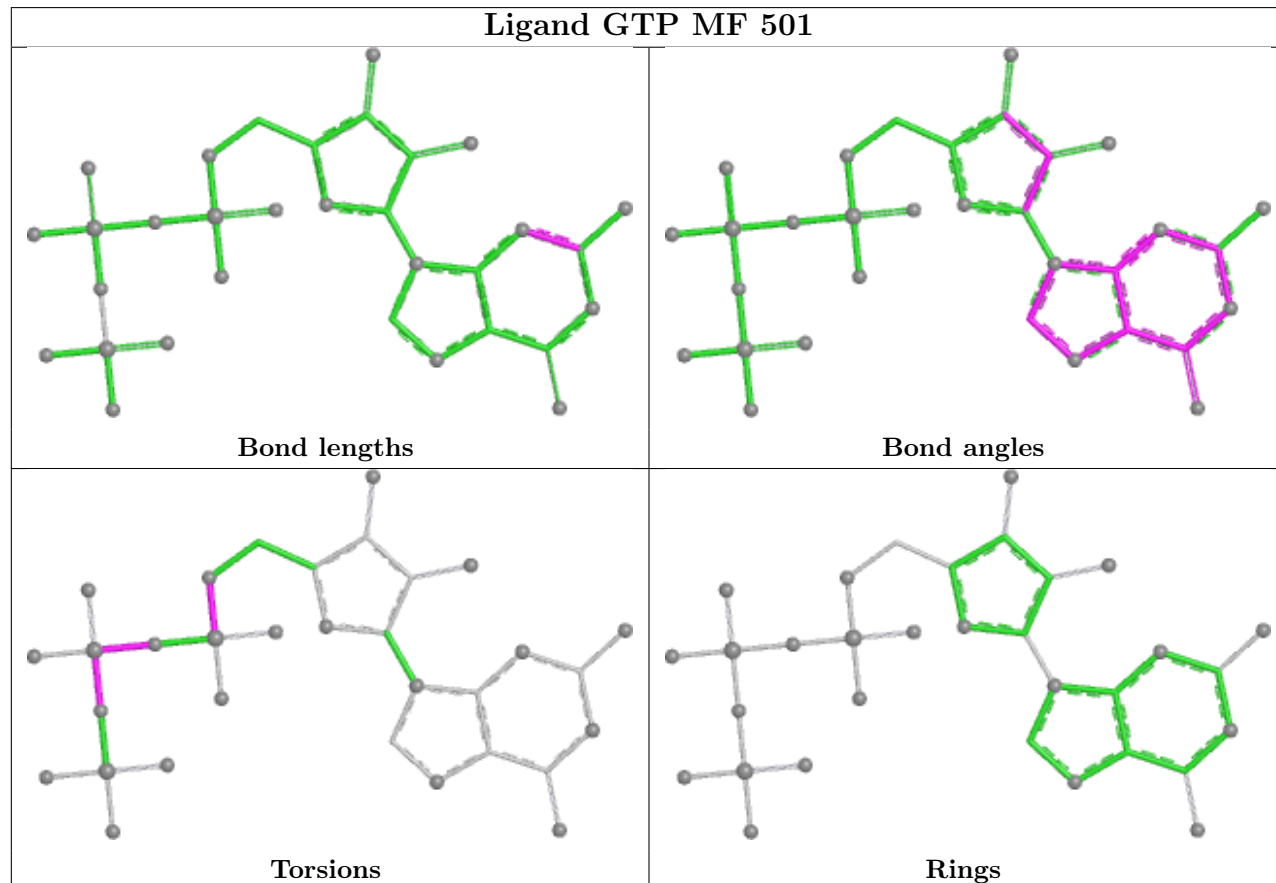


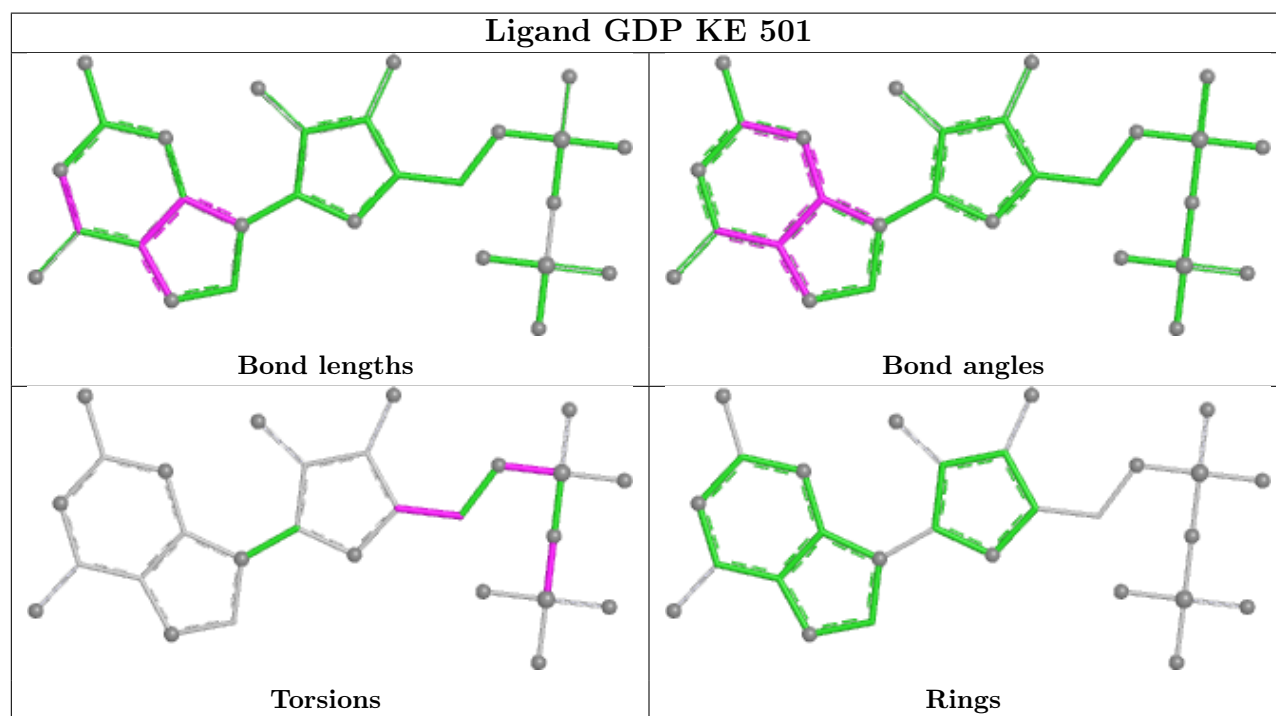
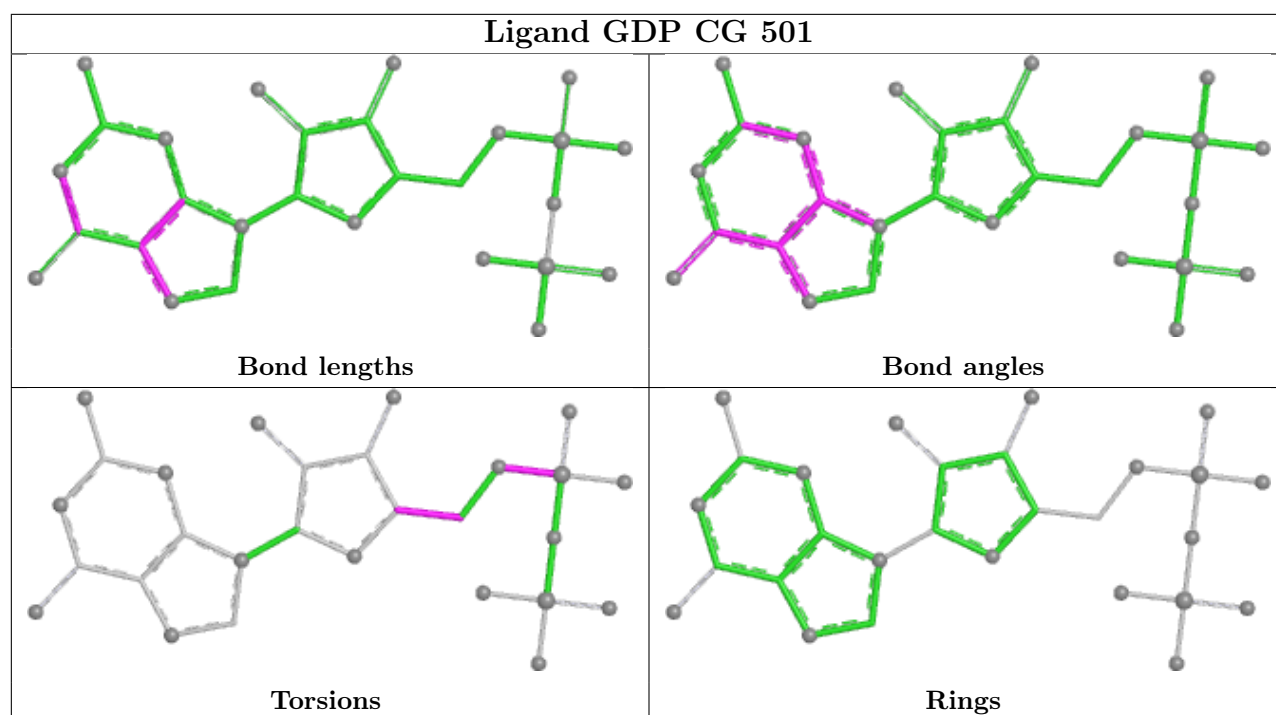


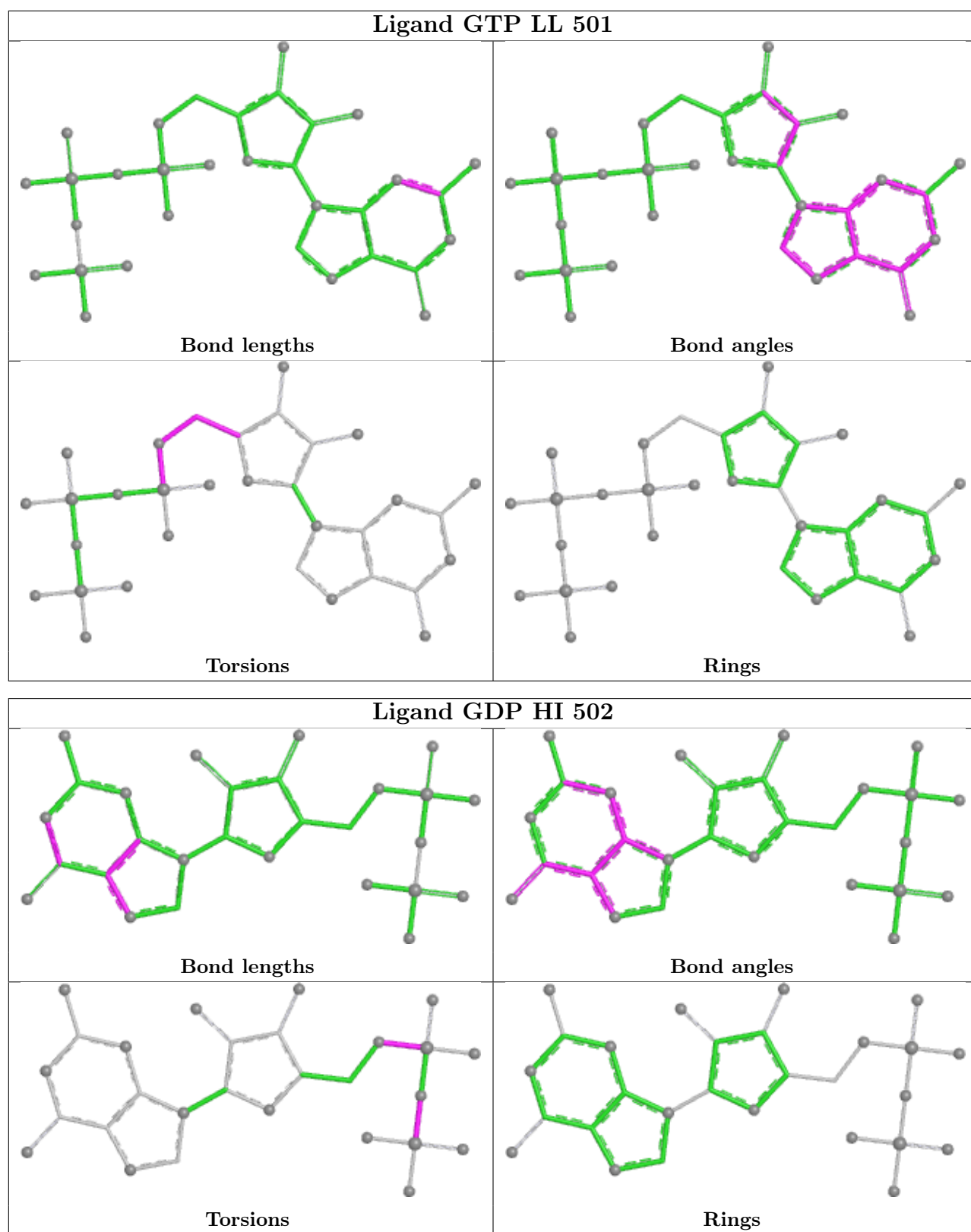
Ligand GTP FF 501

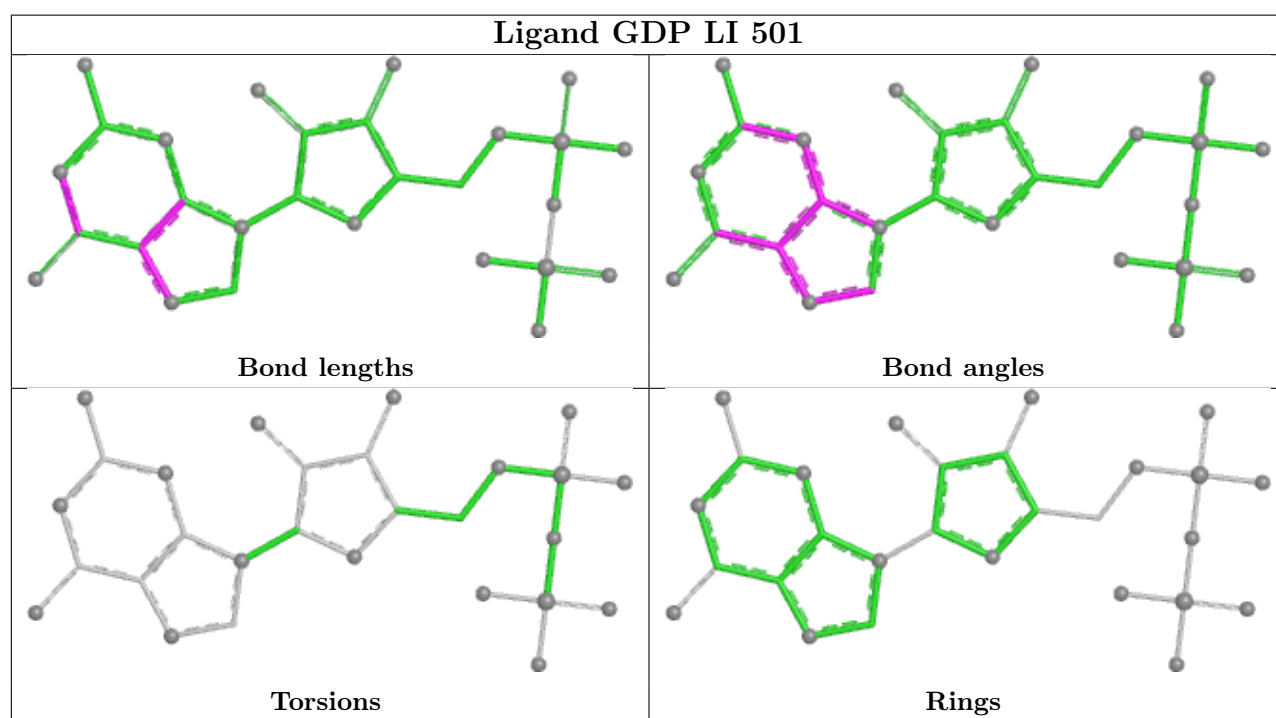
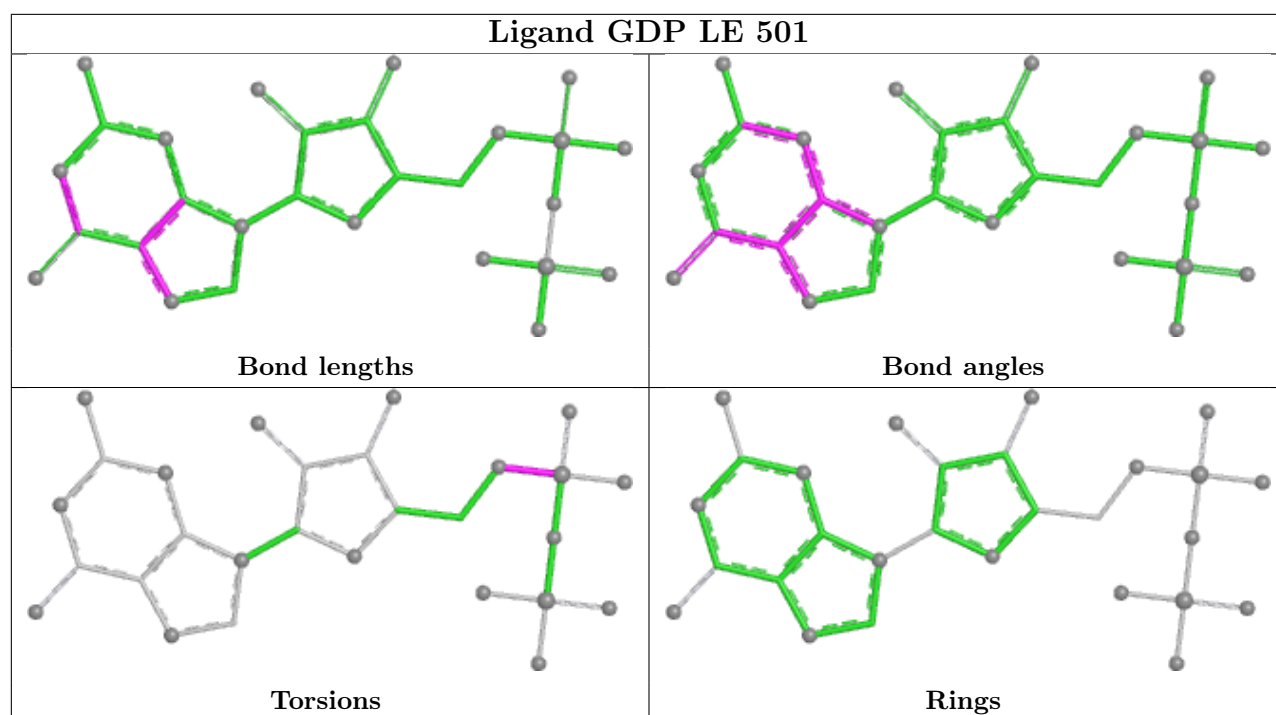


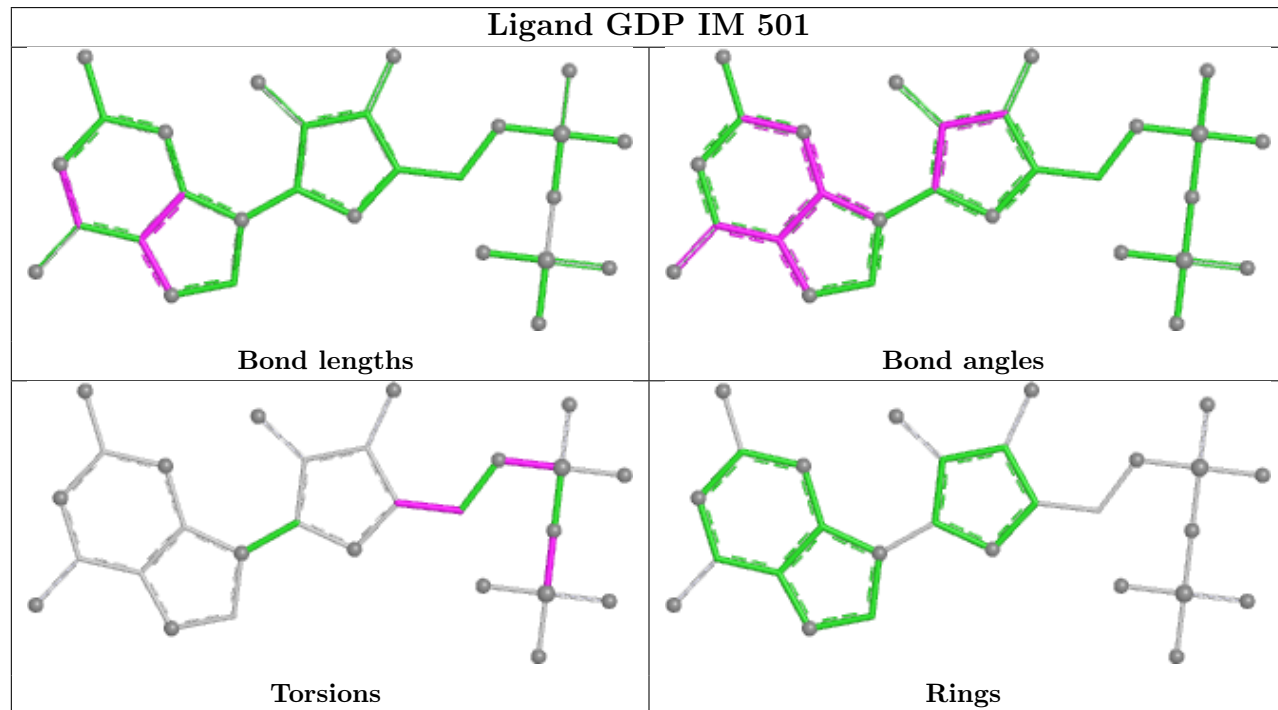
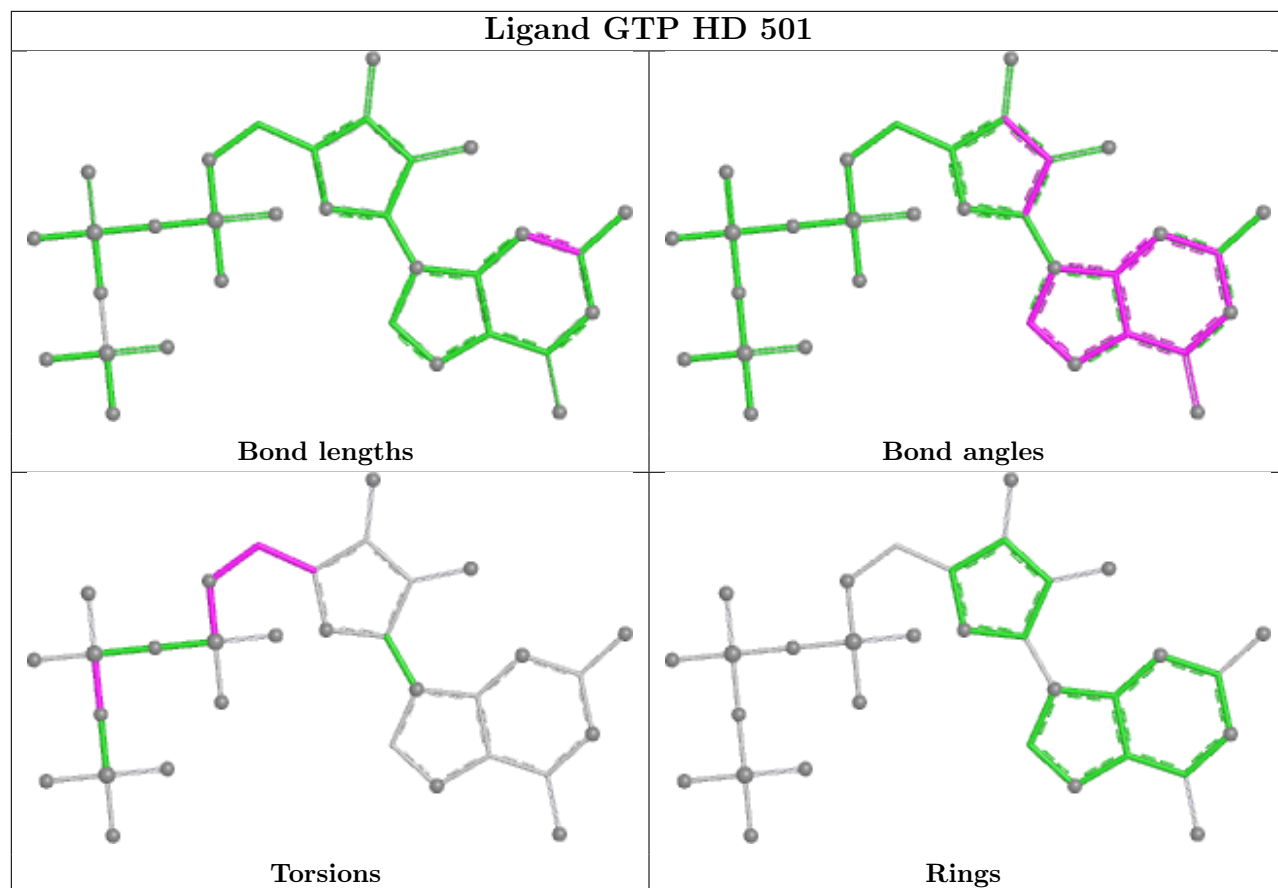
Ligand GTP MF 501

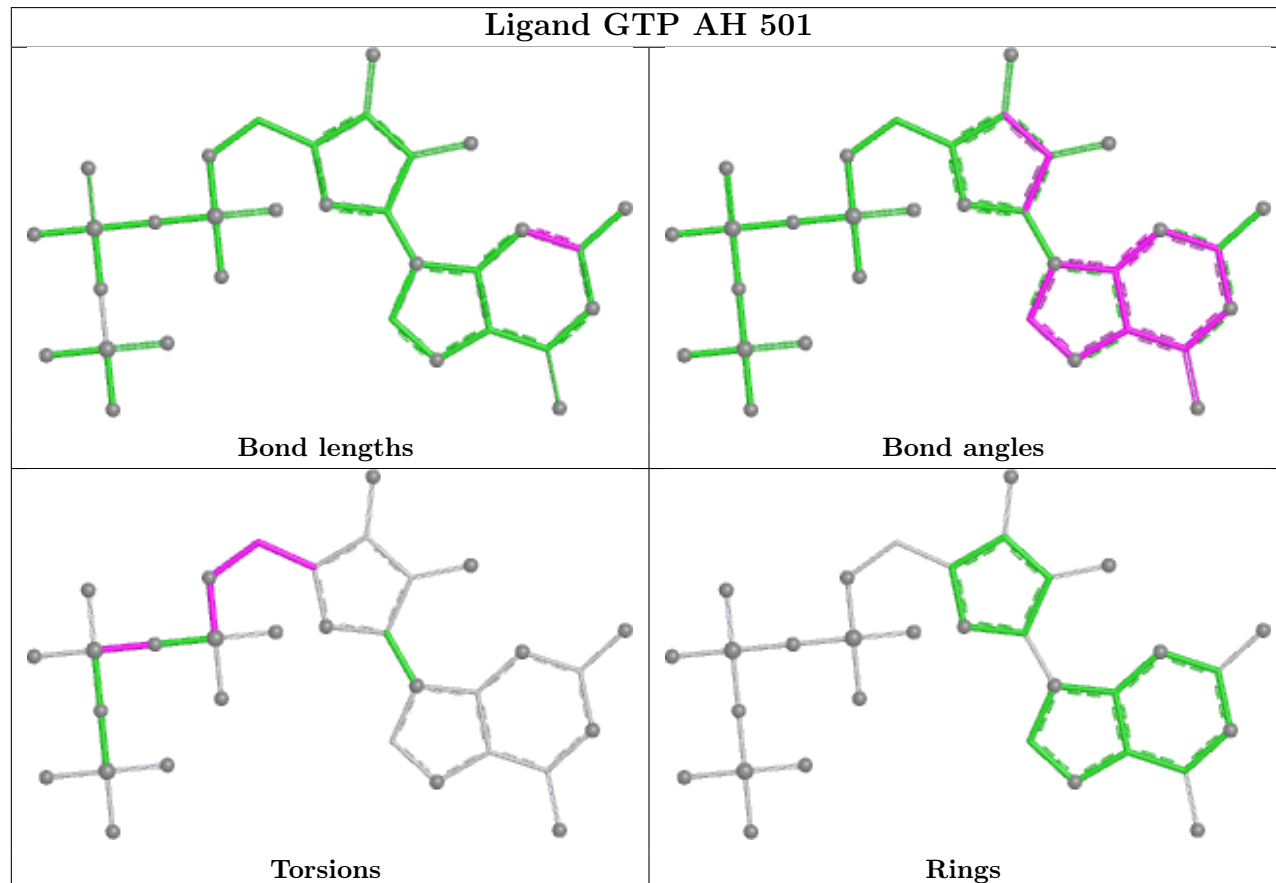
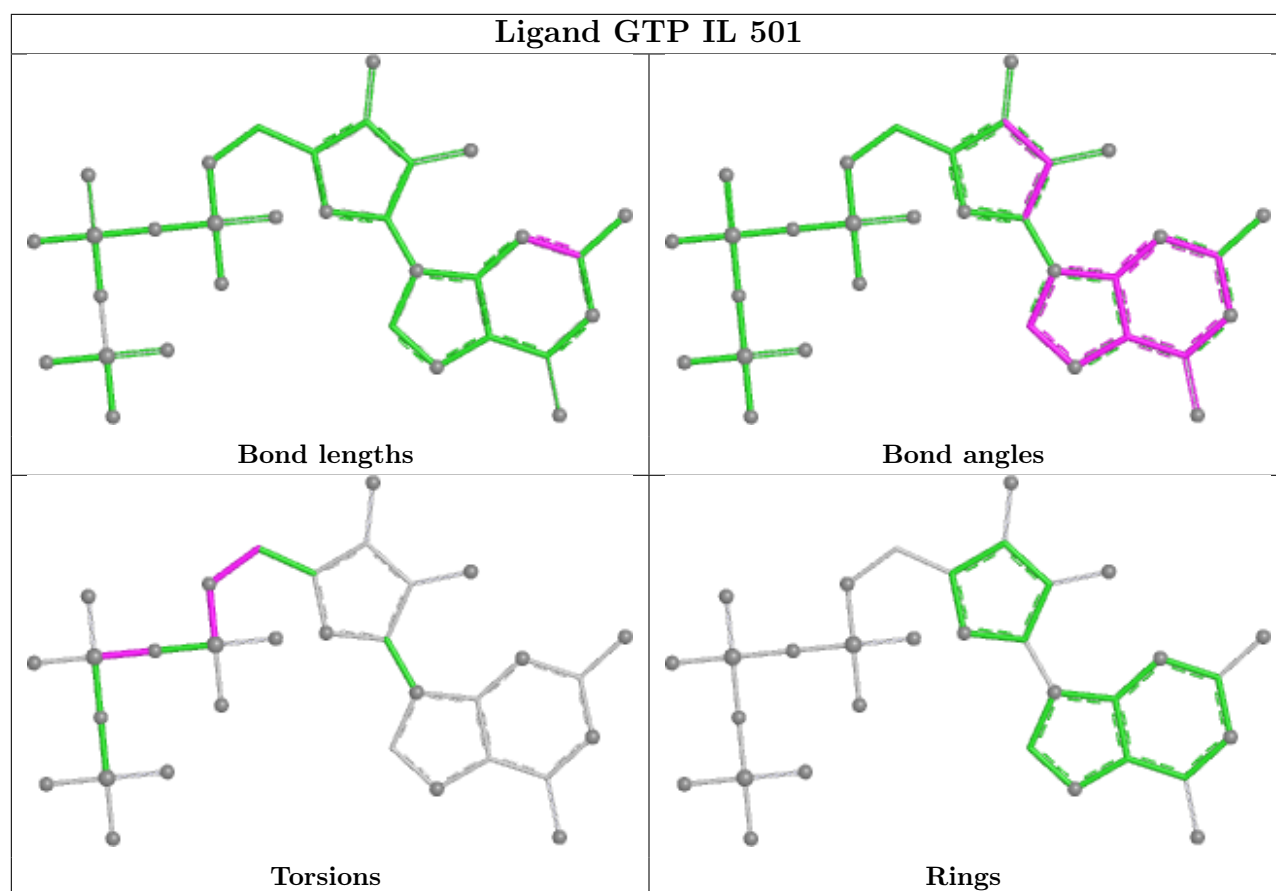




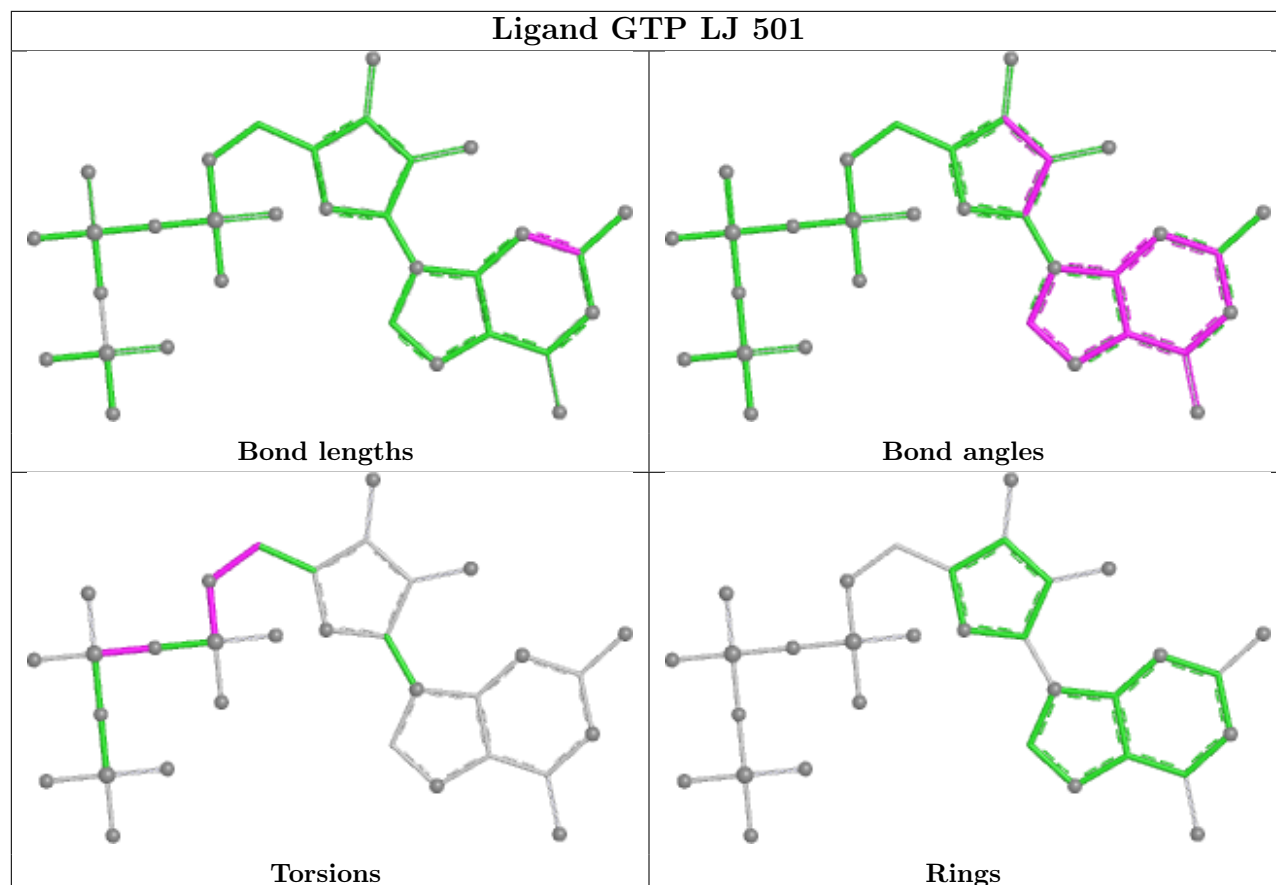




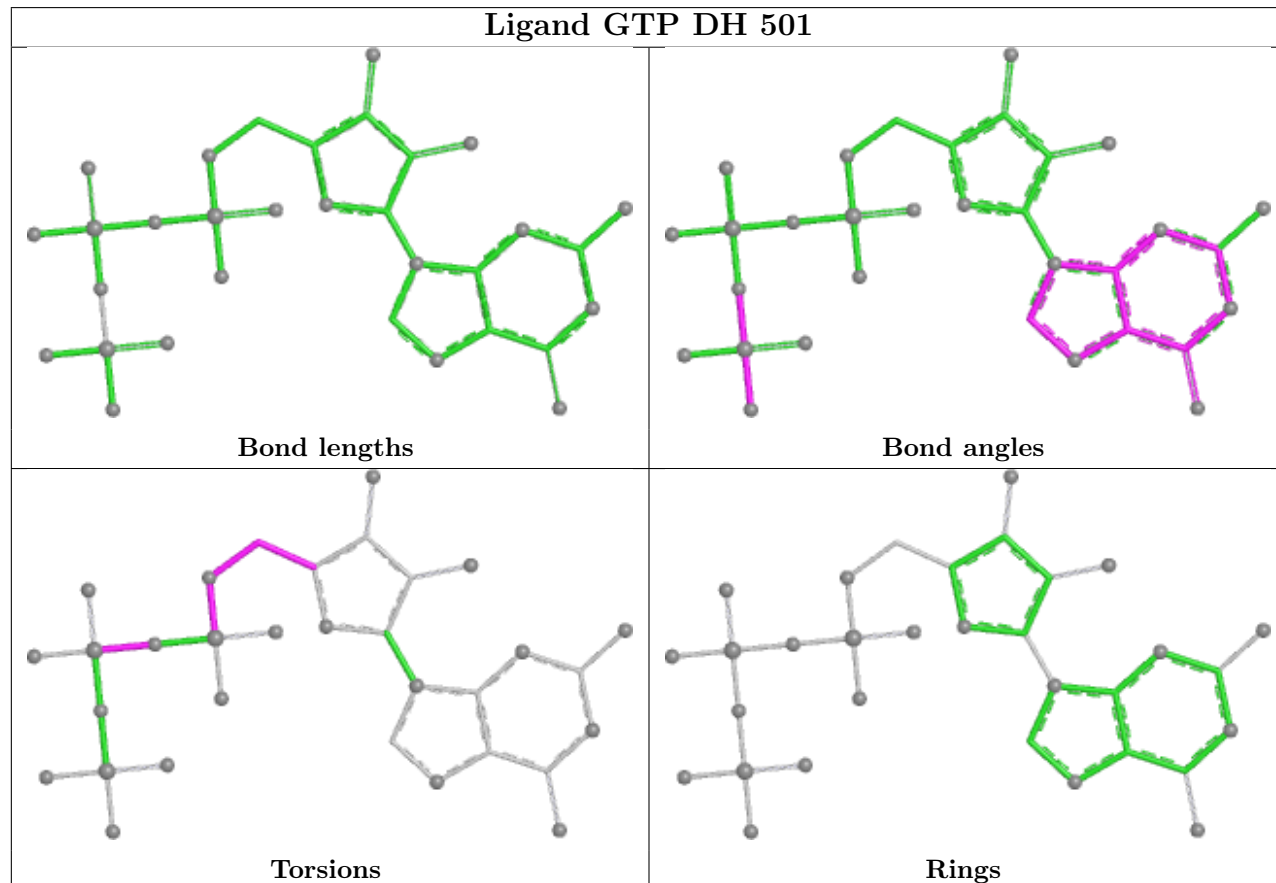


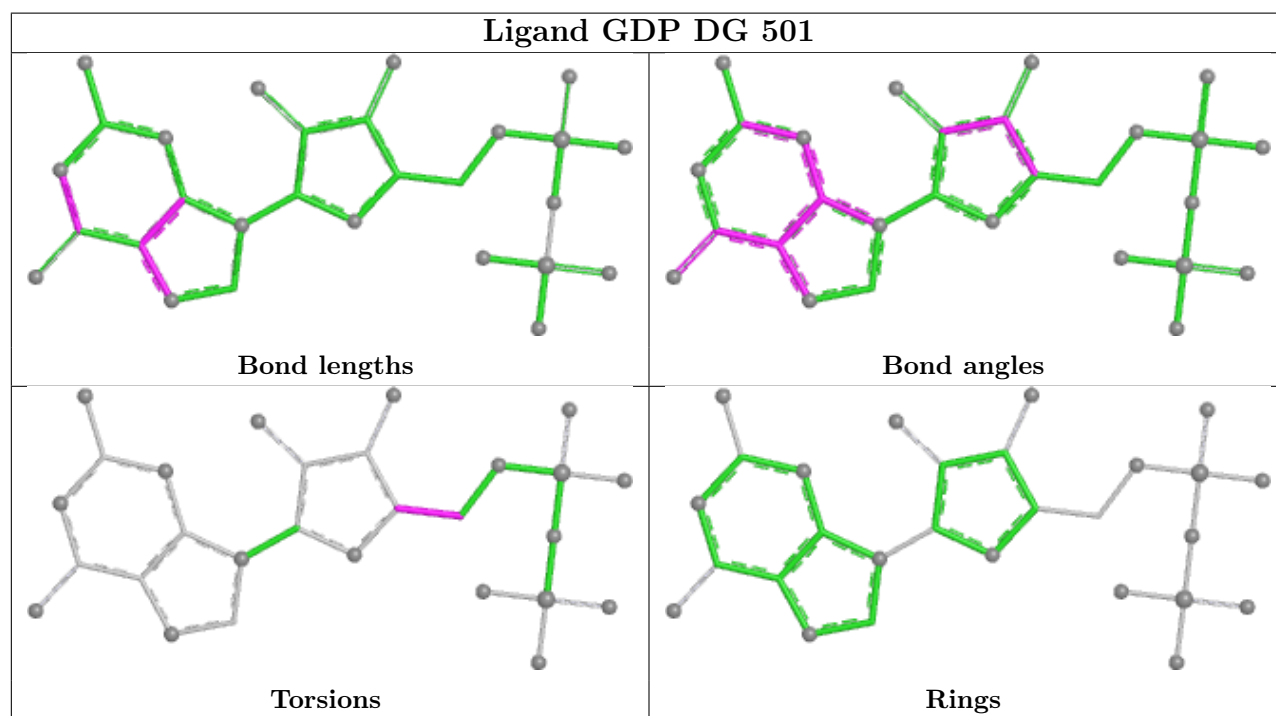
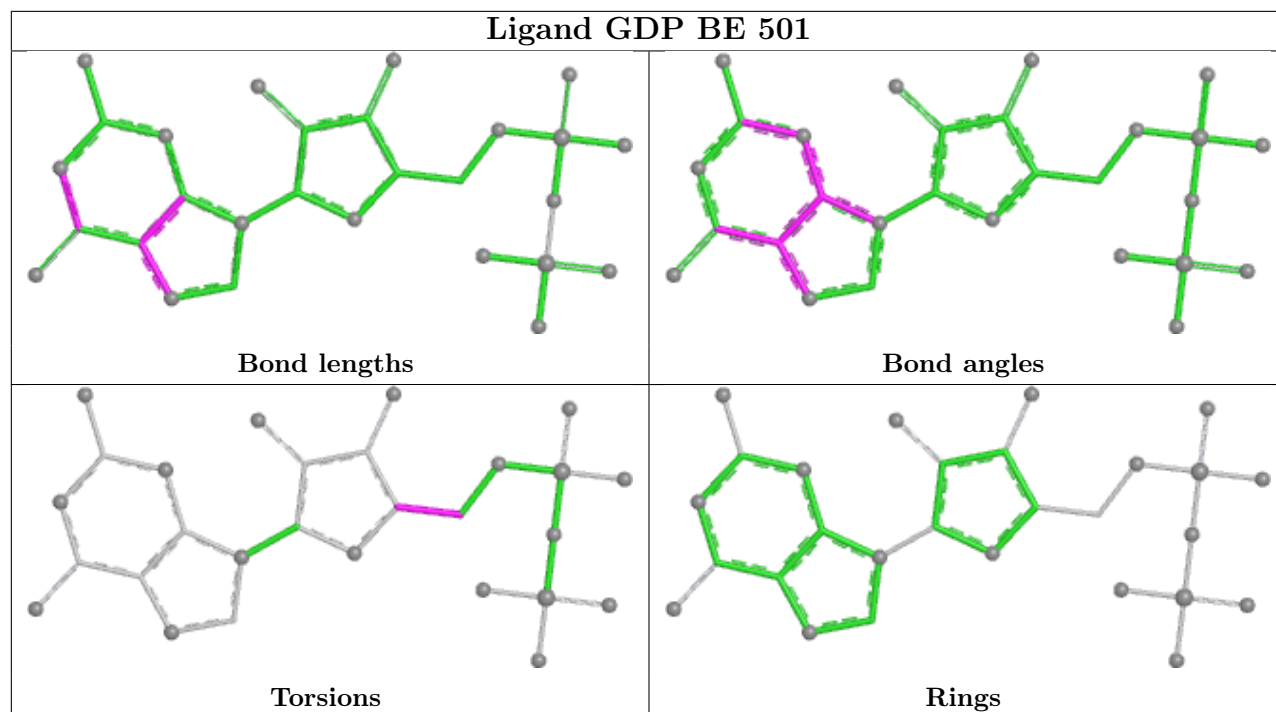


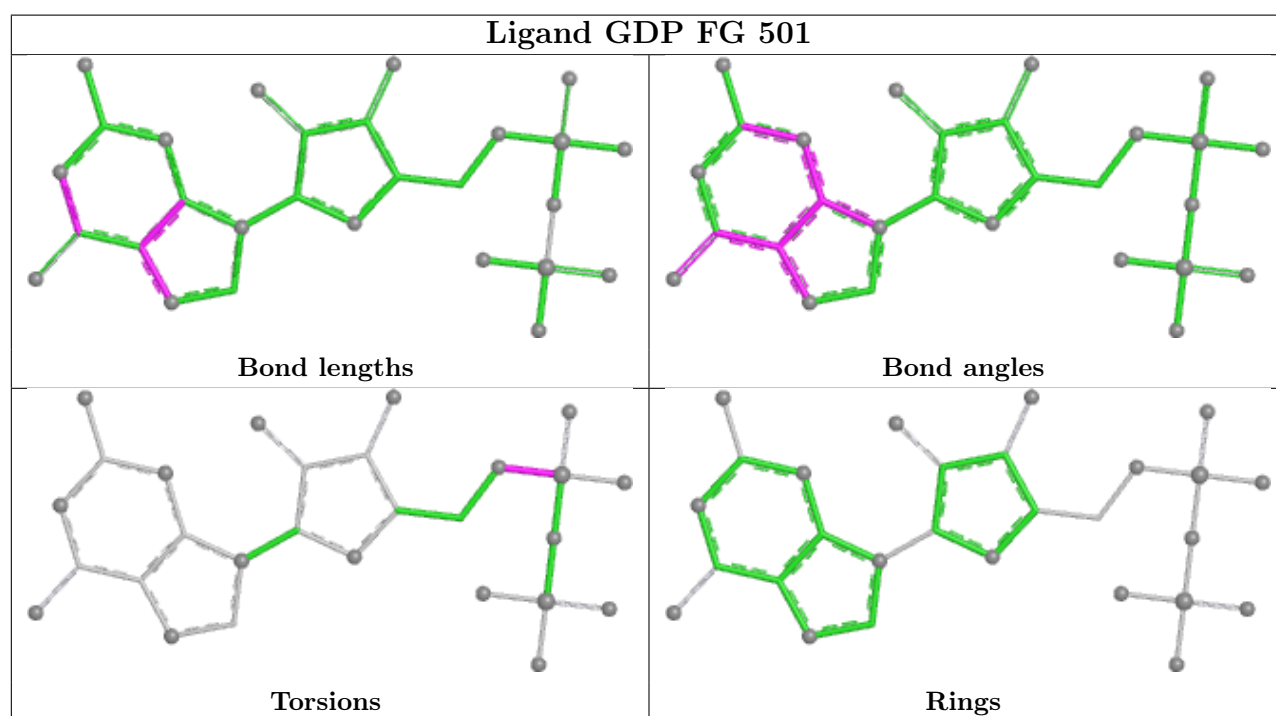
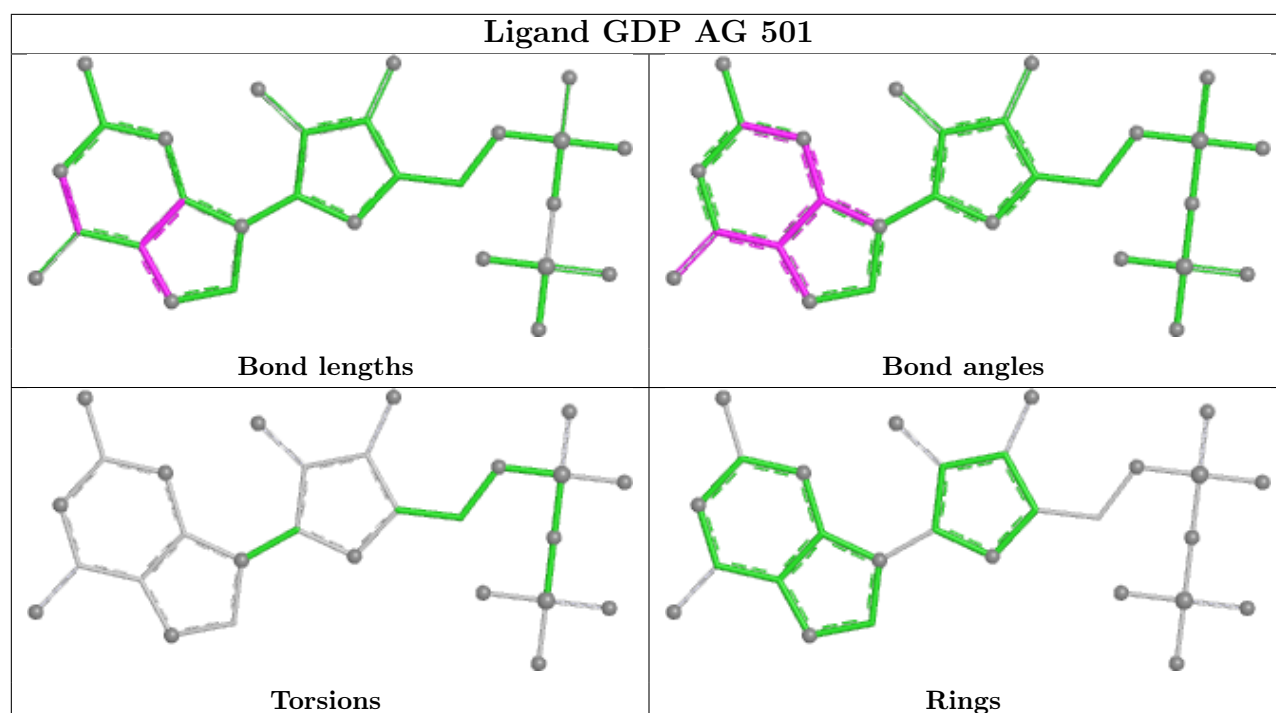
Ligand GTP LJ 501



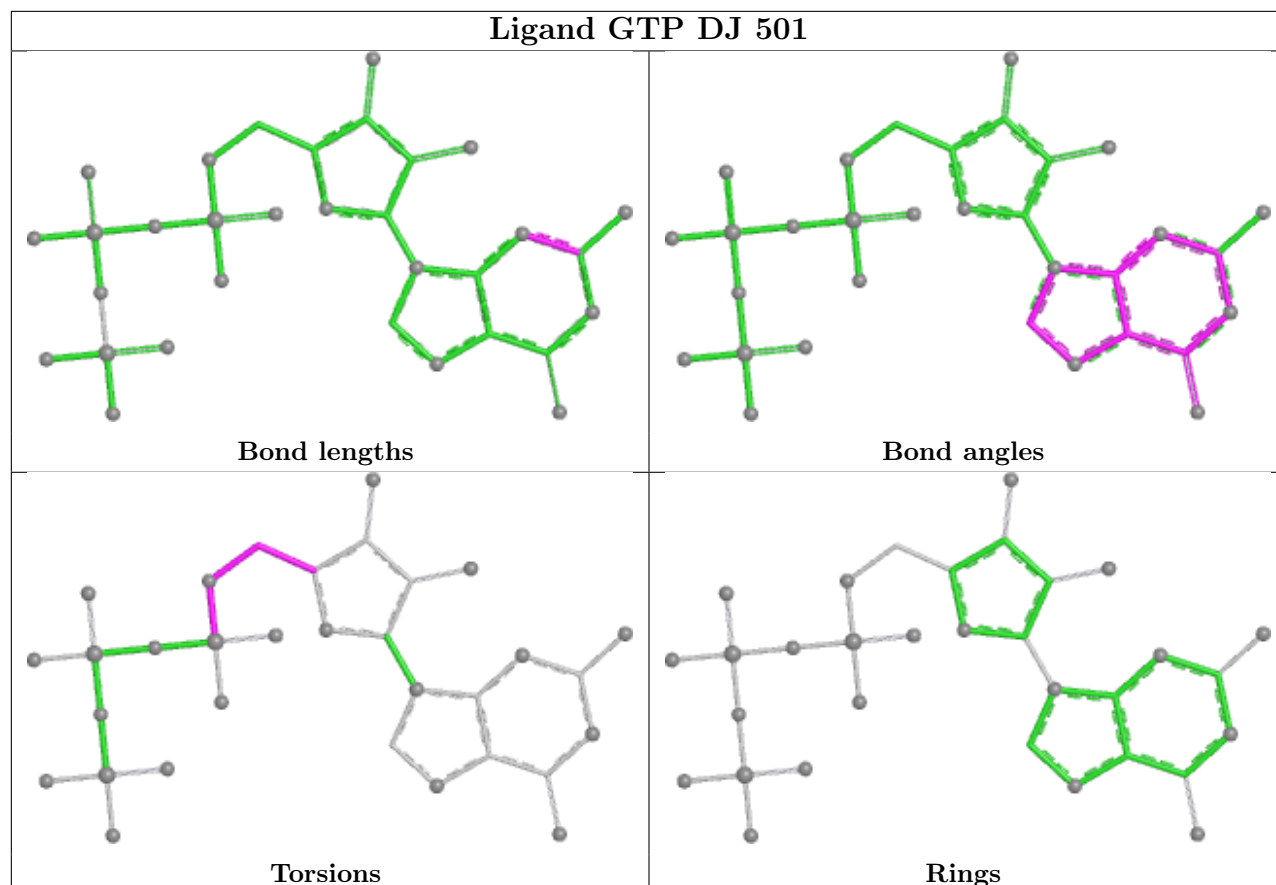
Ligand GTP DH 501



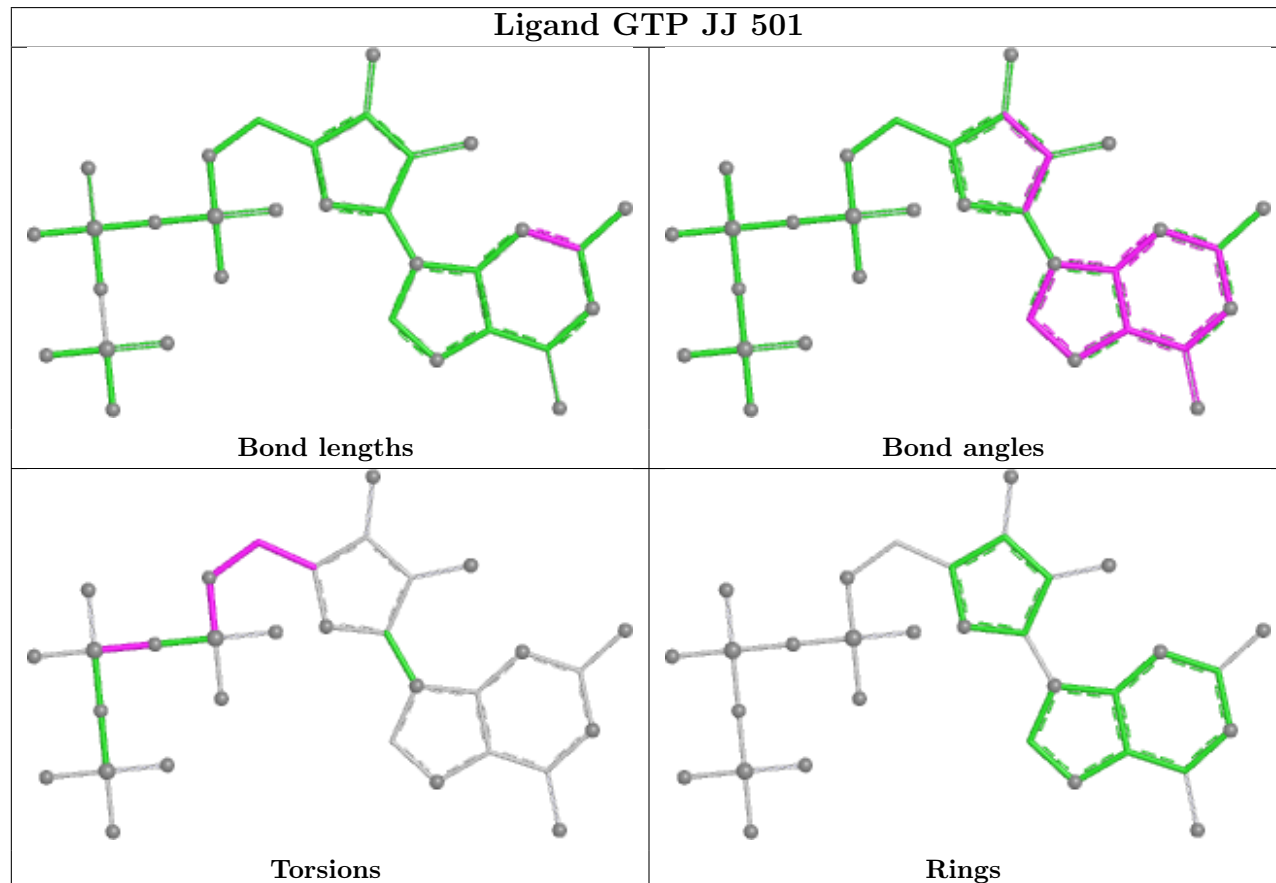


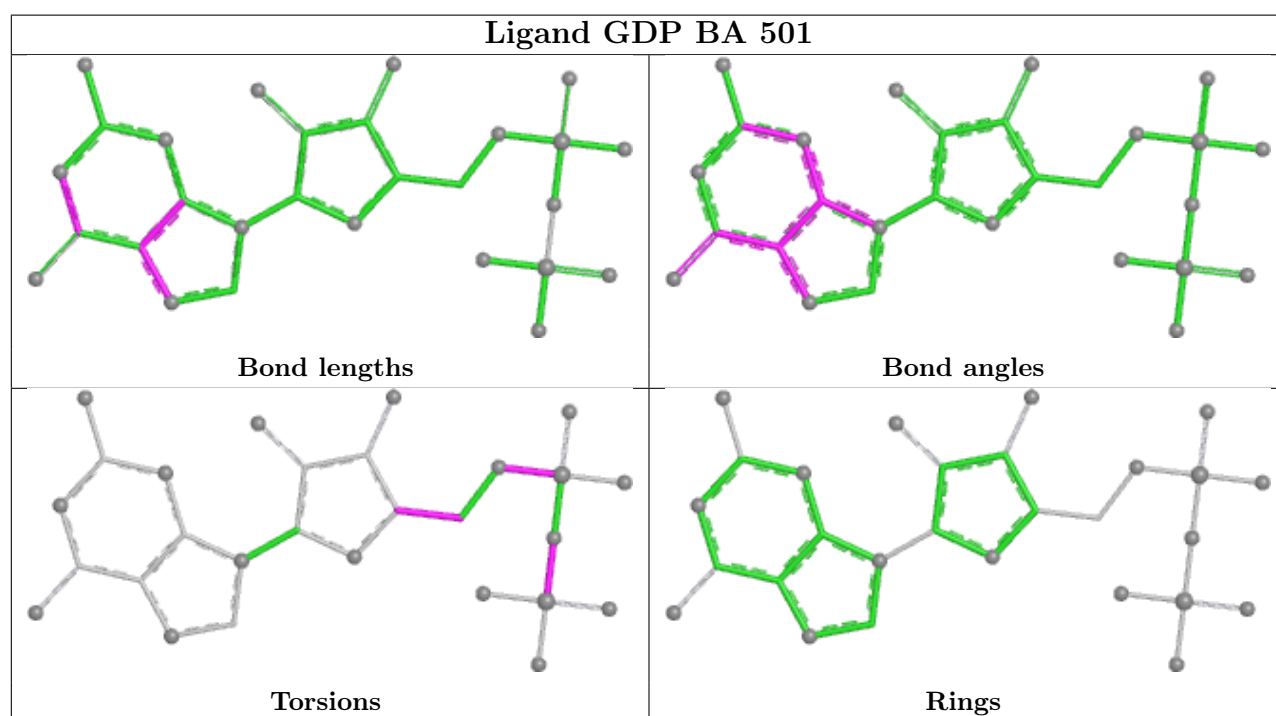
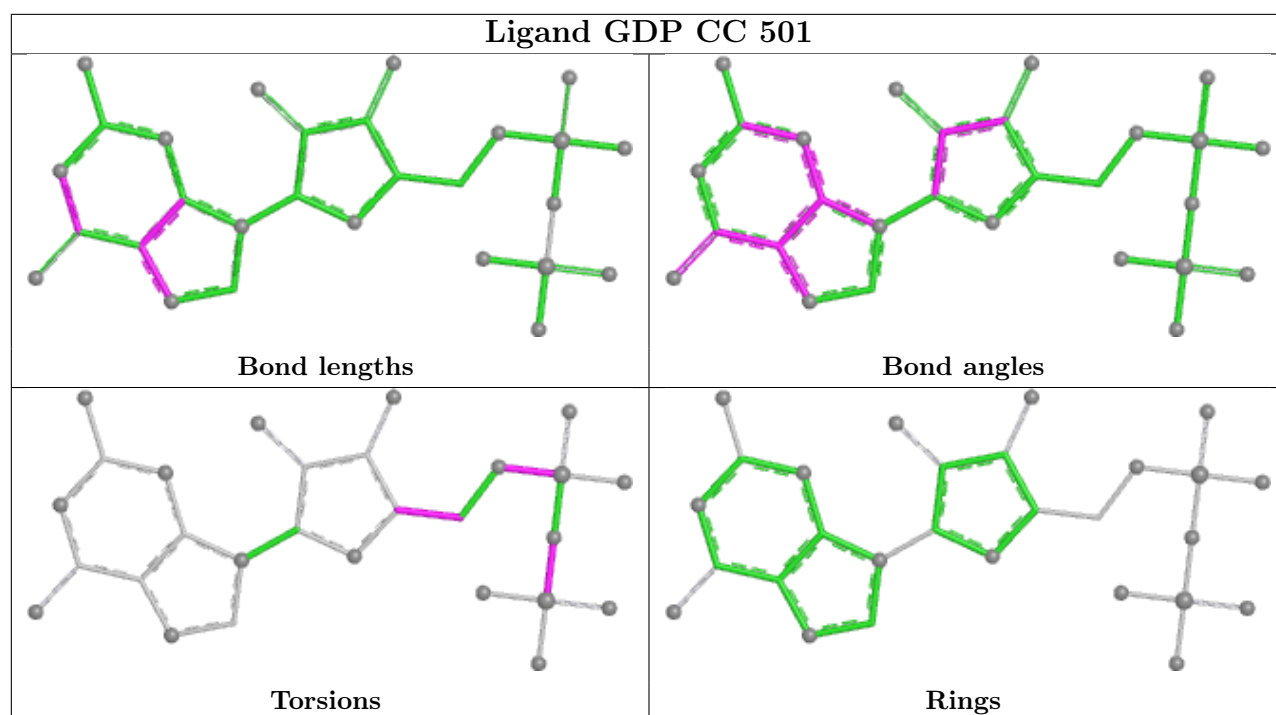


Ligand GTP DJ 501

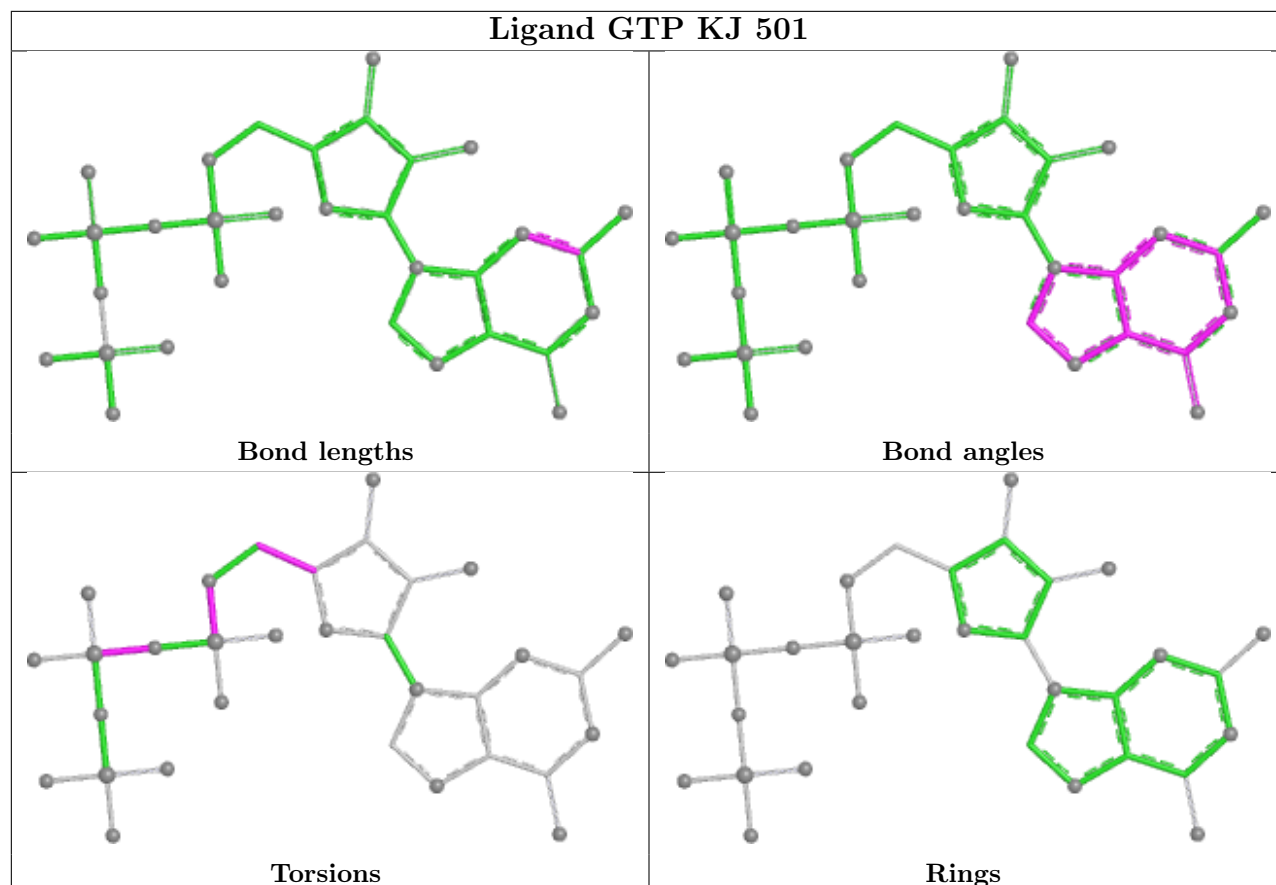


Ligand GTP JJ 501

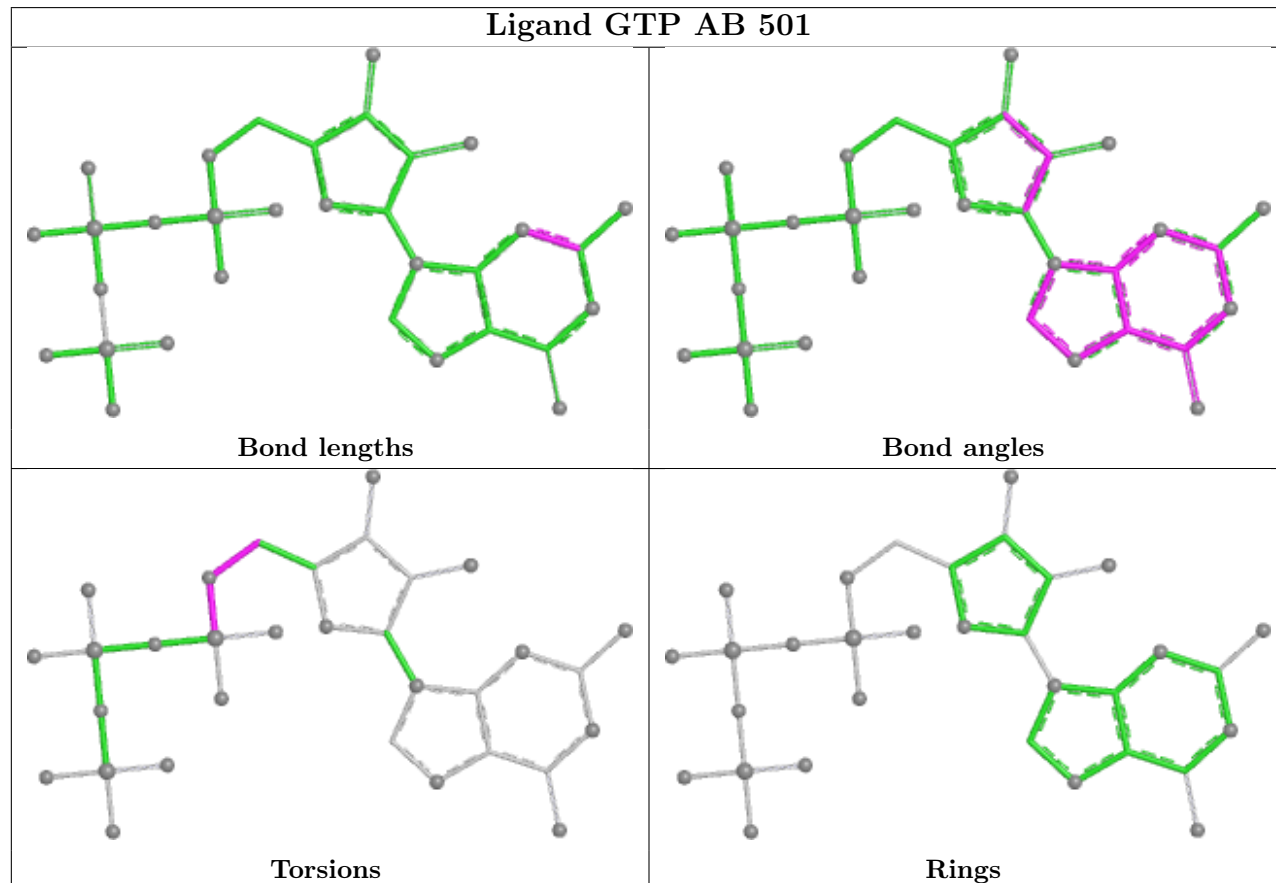


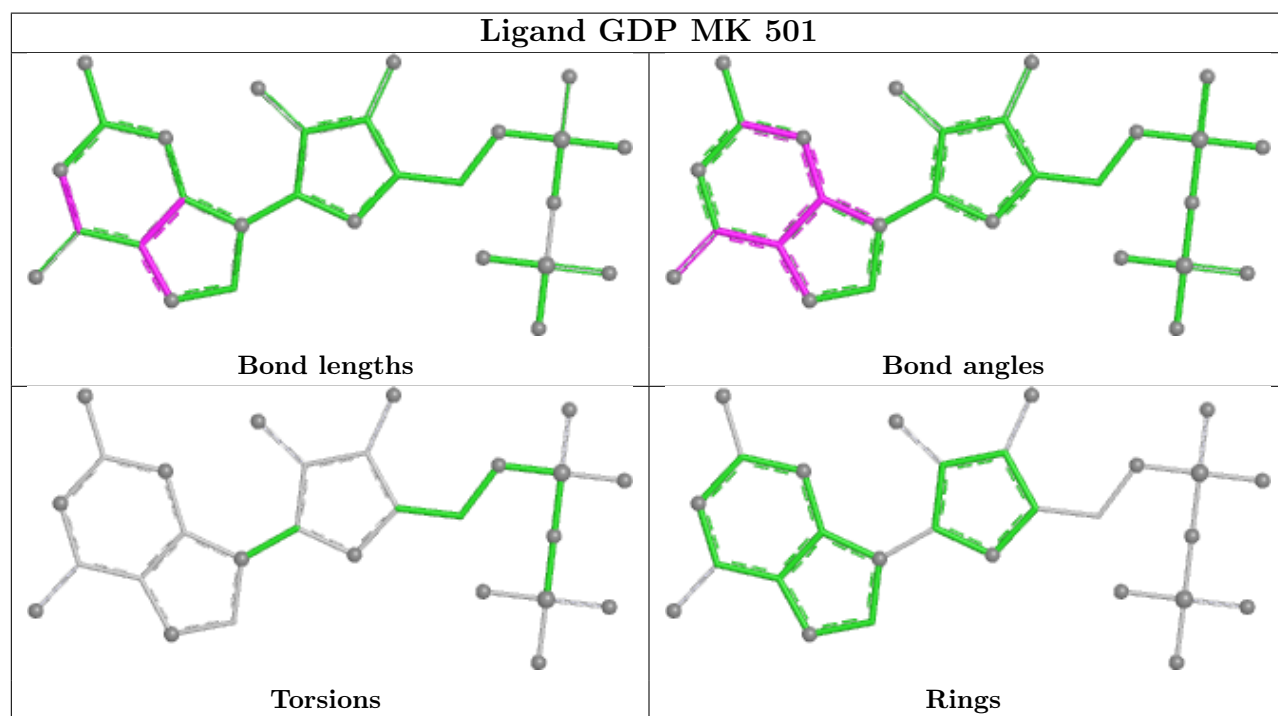
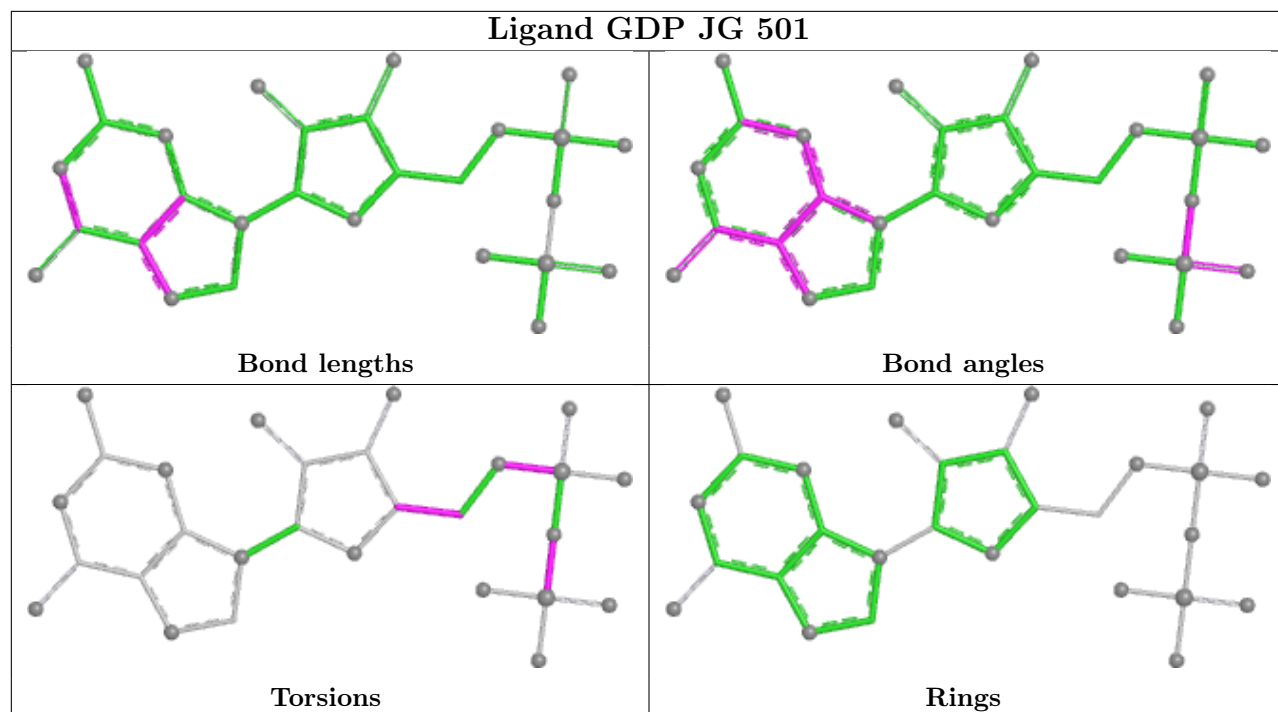


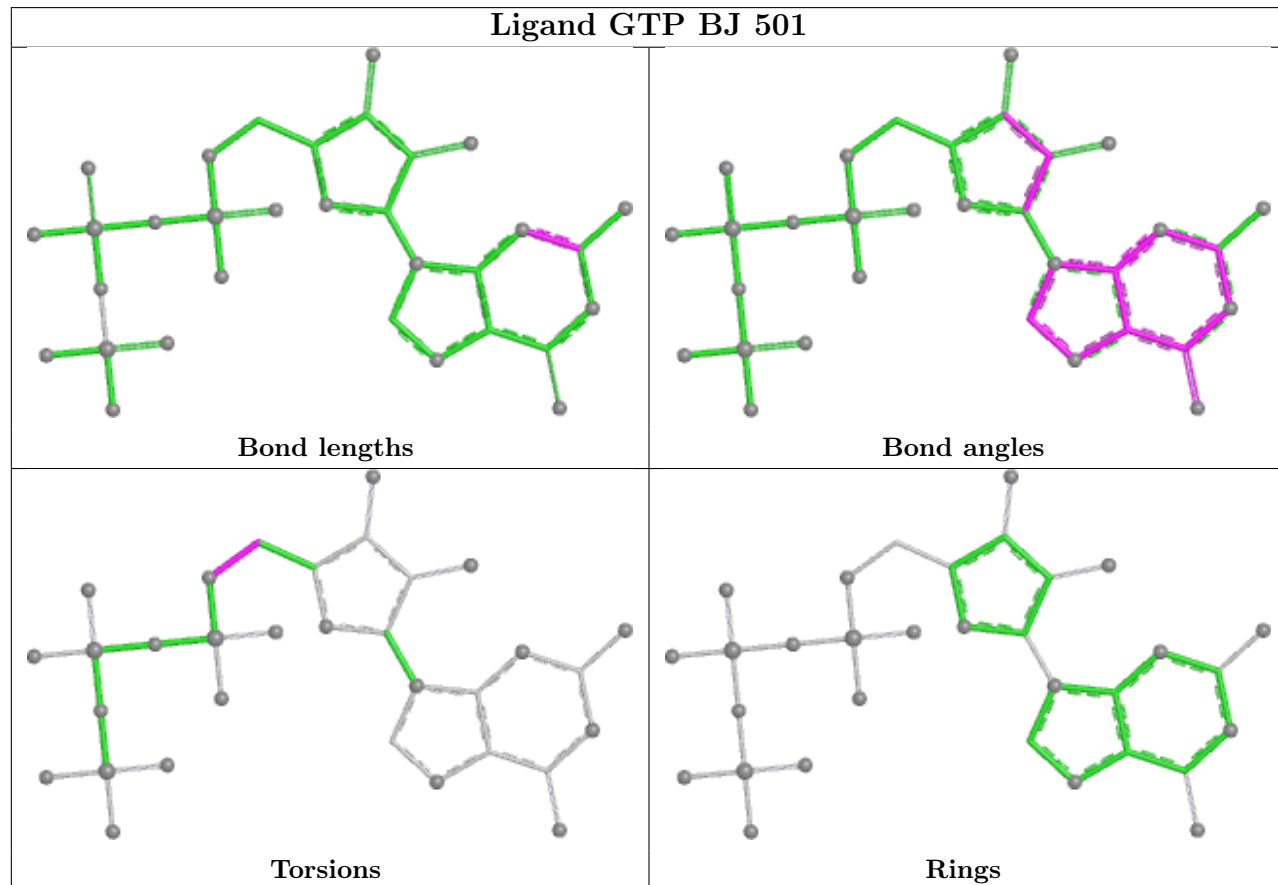
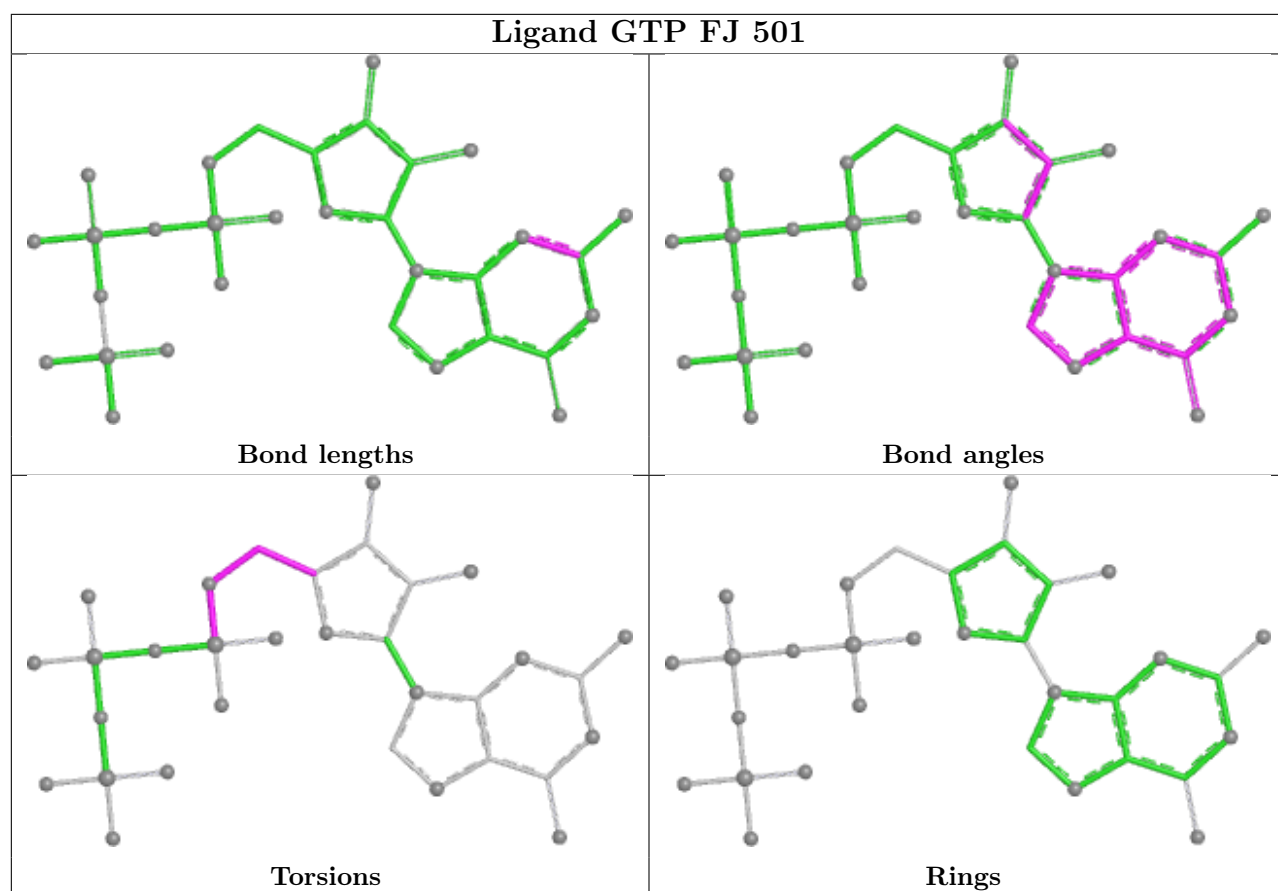
Ligand GTP KJ 501

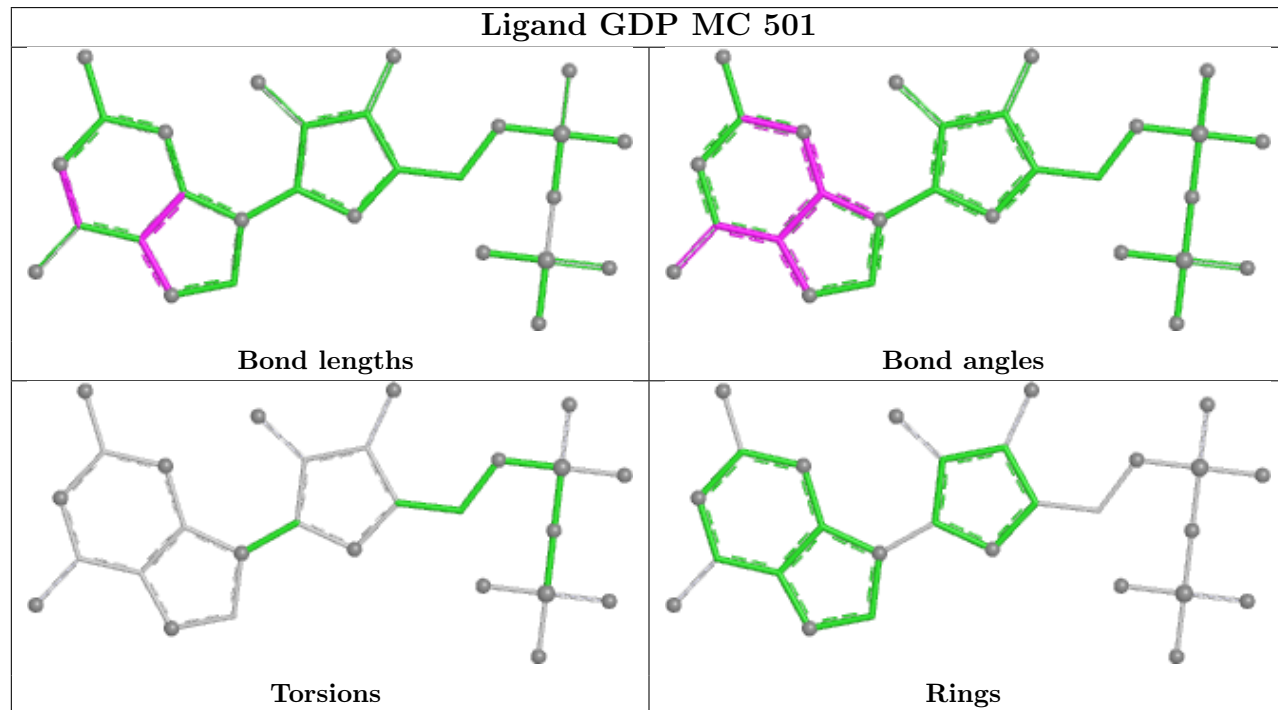
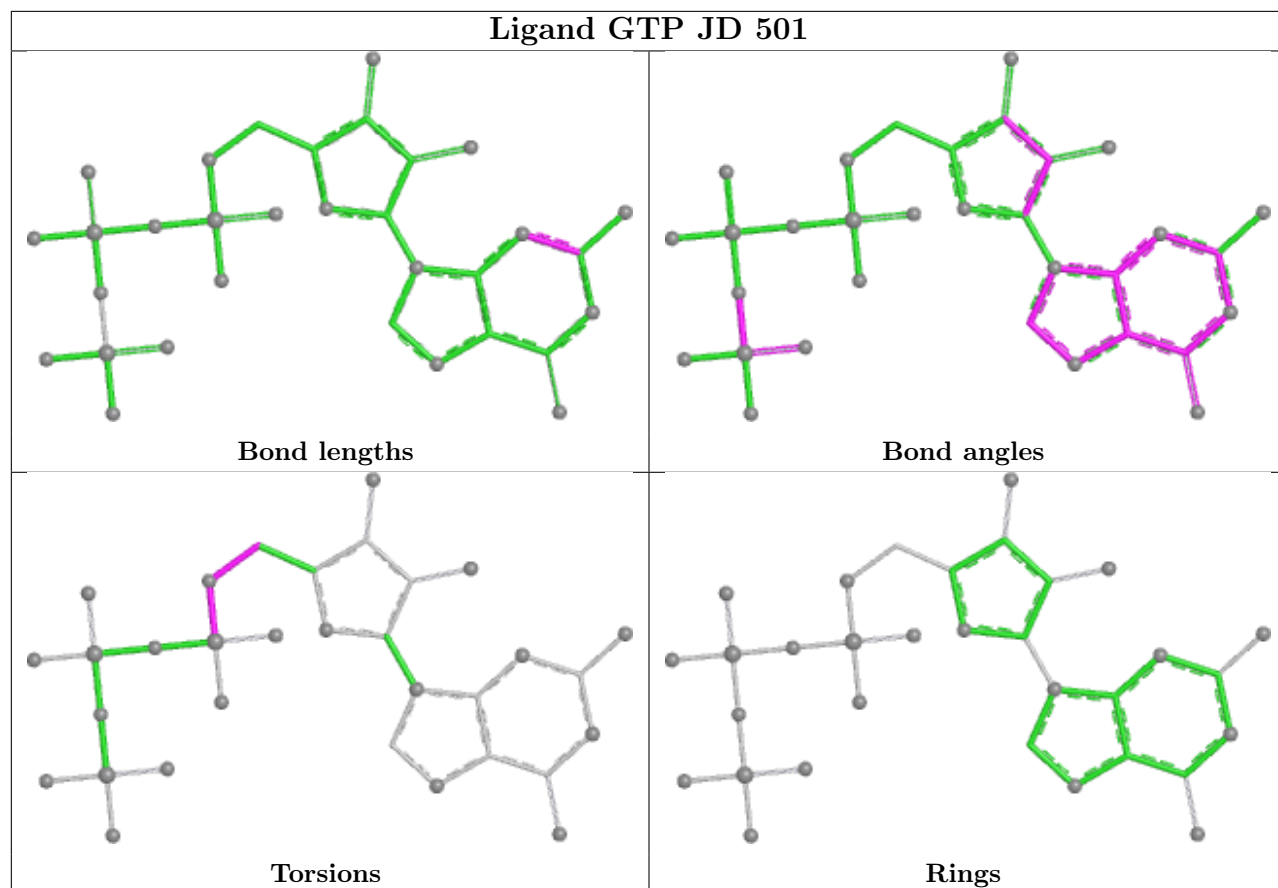


Ligand GTP AB 501

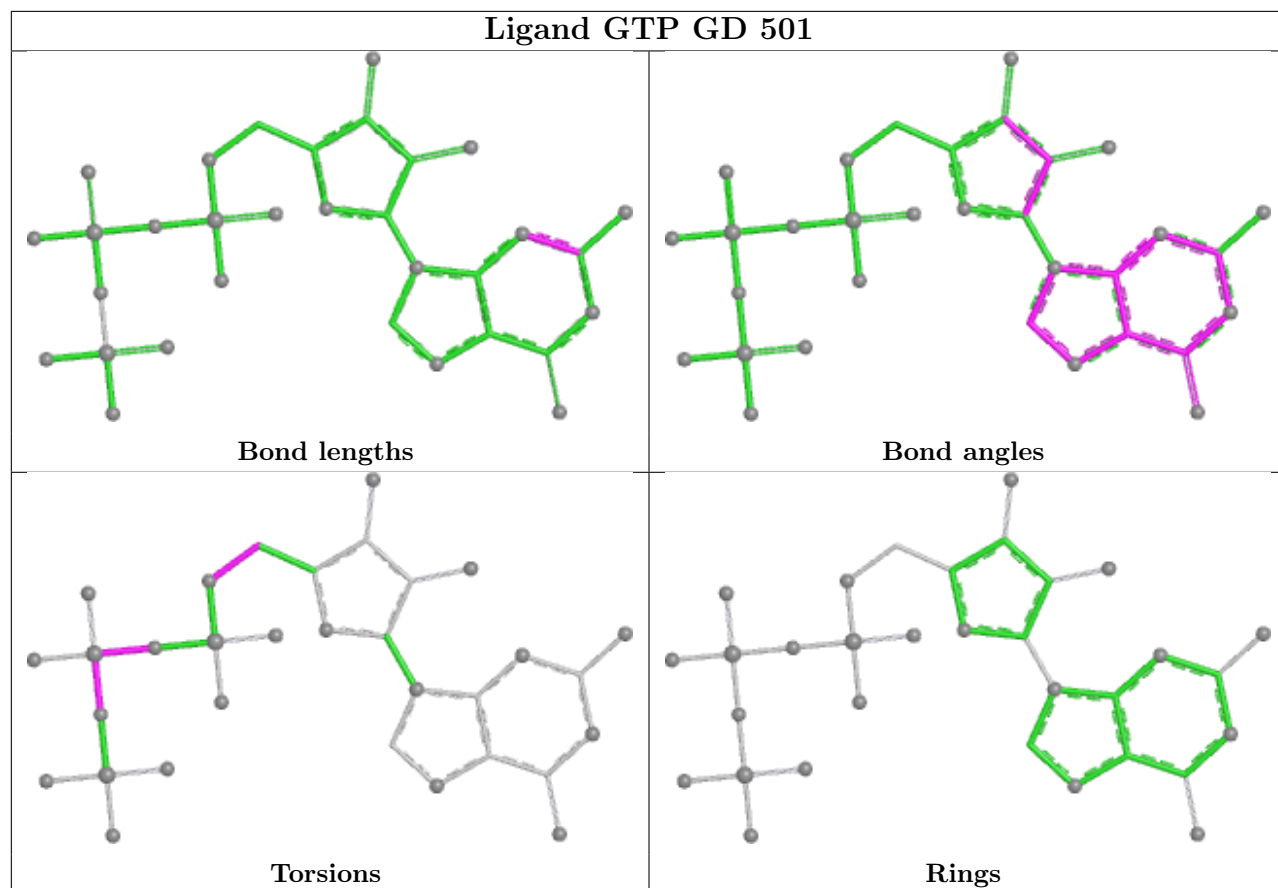




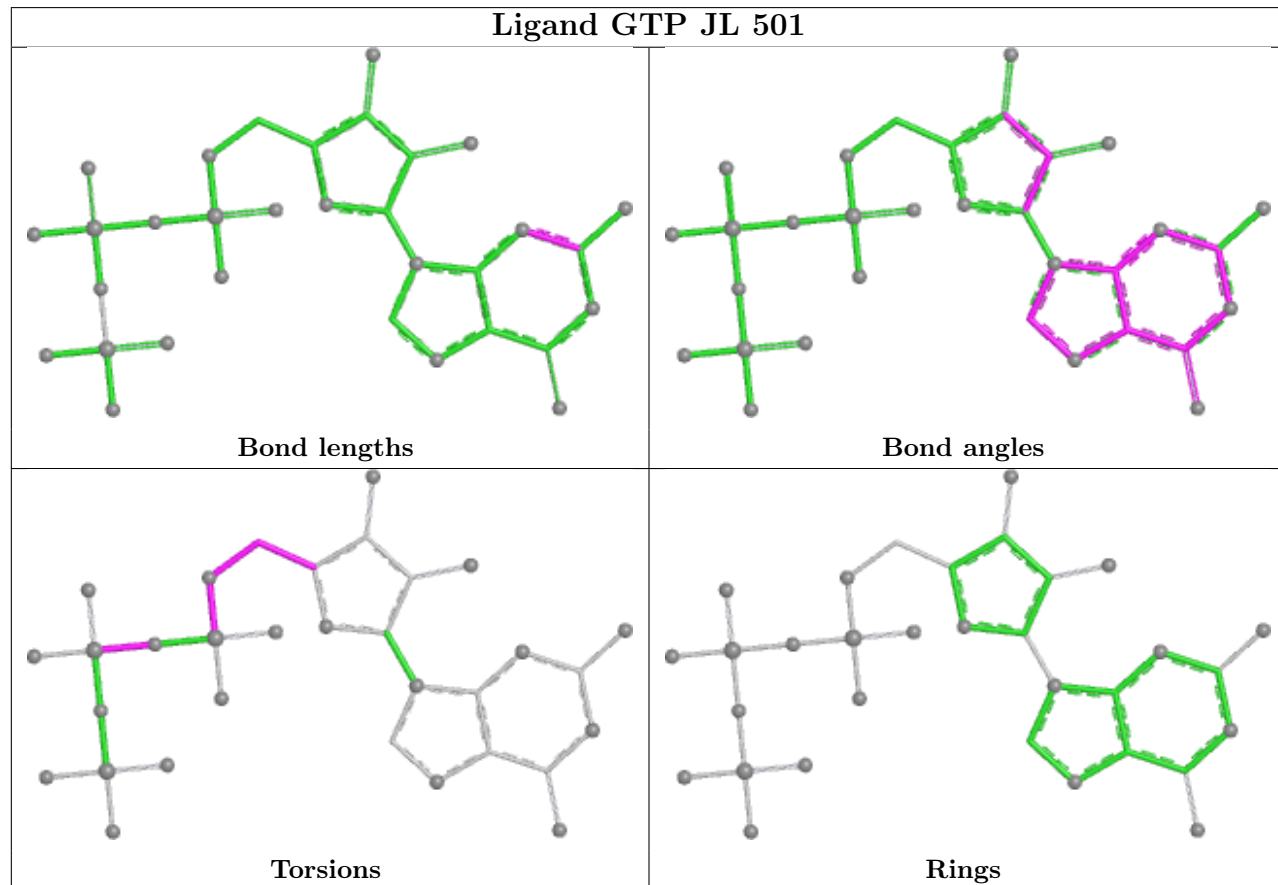


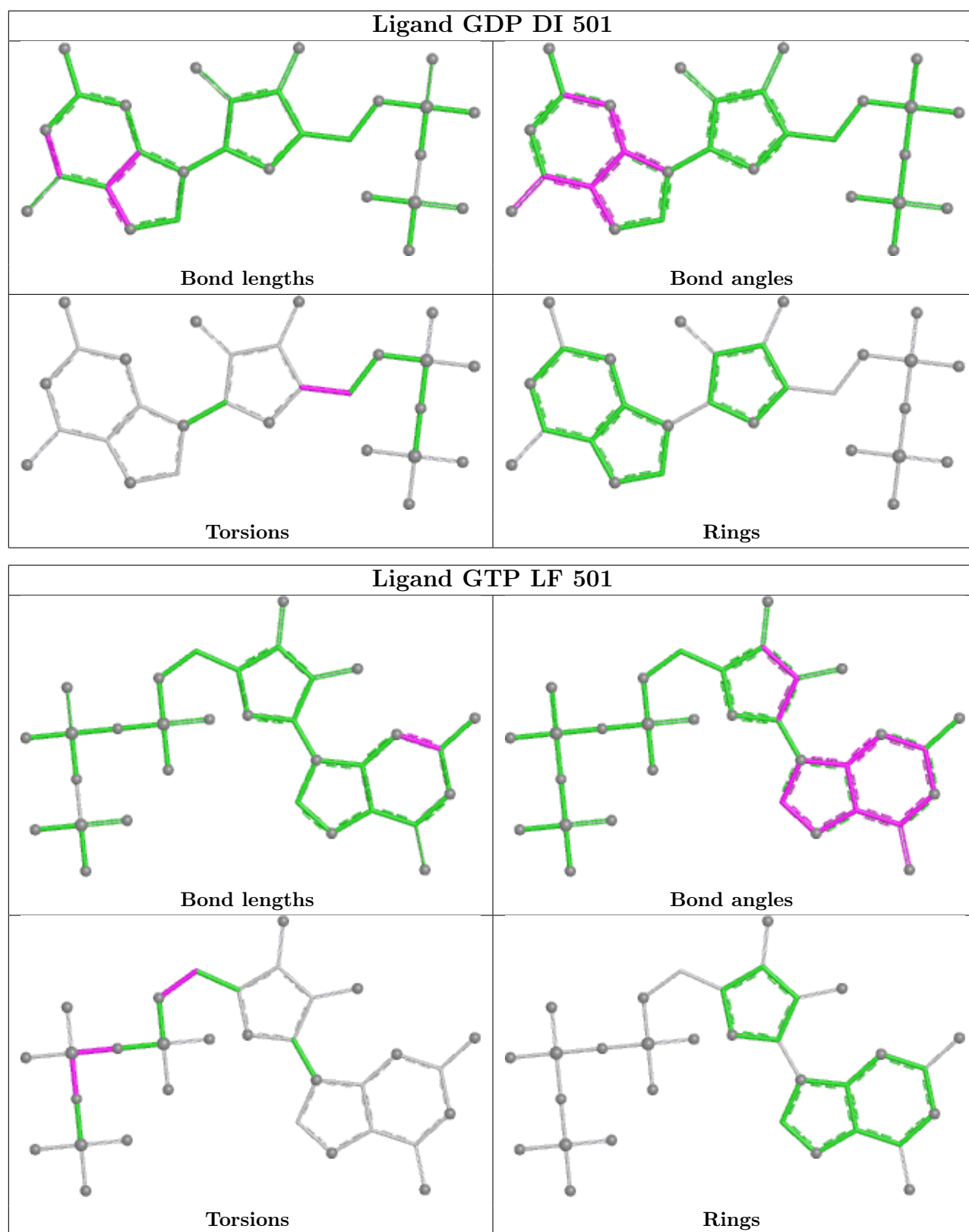


Ligand GTP GD 501



Ligand GTP JL 501





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

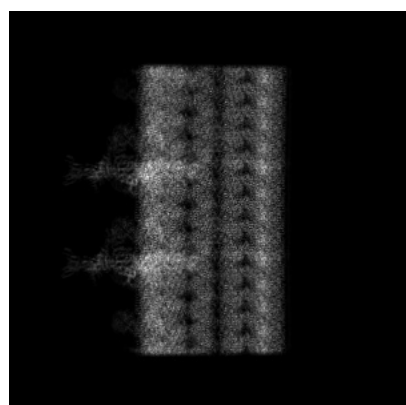
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25361. These allow visual inspection of the internal detail of the map and identification of artifacts.

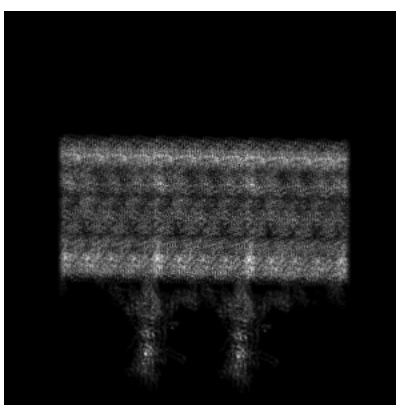
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

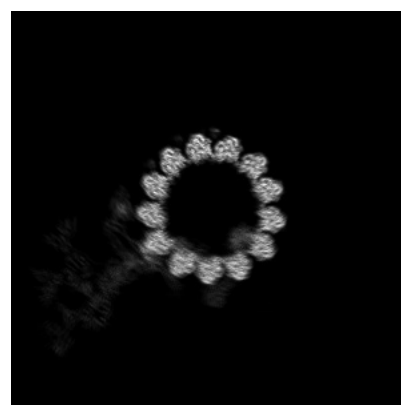
6.1.1 Primary map



X



Y



Z

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

6.2 Central slices [i](#)

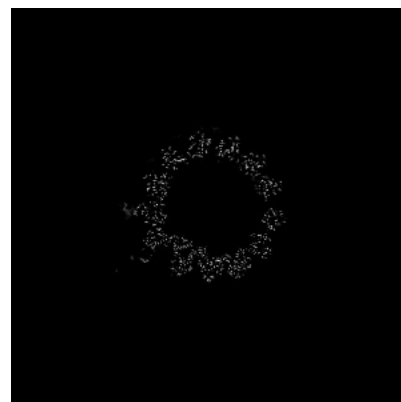
6.2.1 Primary map



X Index: 256



Y Index: 256

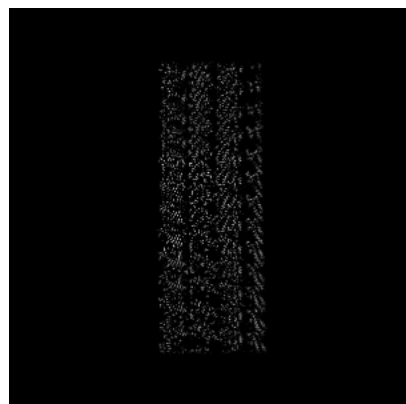


Z Index: 256

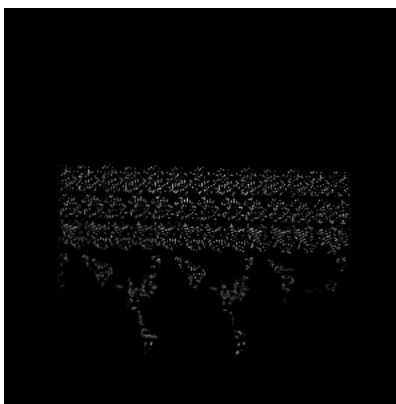
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 324



Y Index: 187

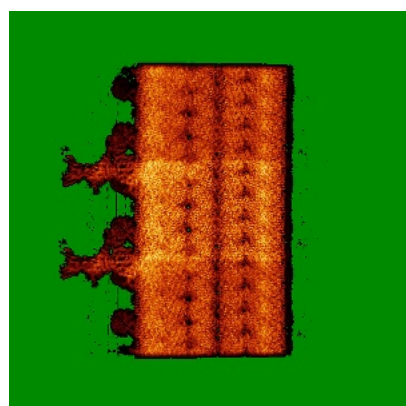


Z Index: 195

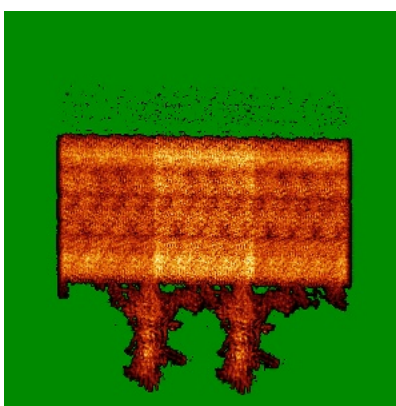
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X



Y

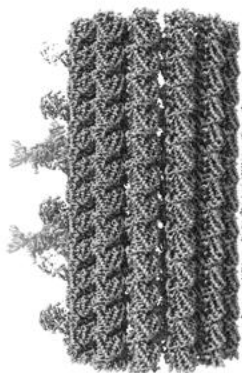


Z

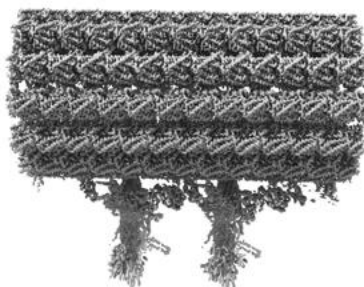
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

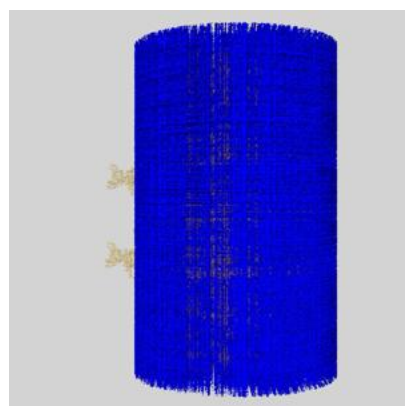
6.6 Mask visualisation [i](#)

This section 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

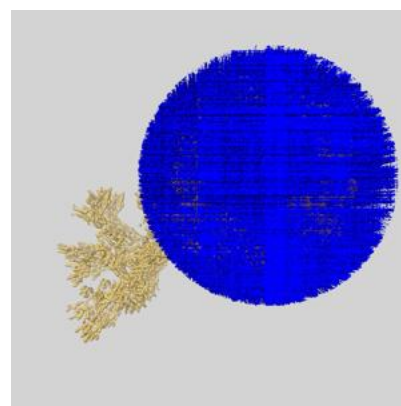
6.6.1 emd_25361_msk_1.map [i](#)



X



Y

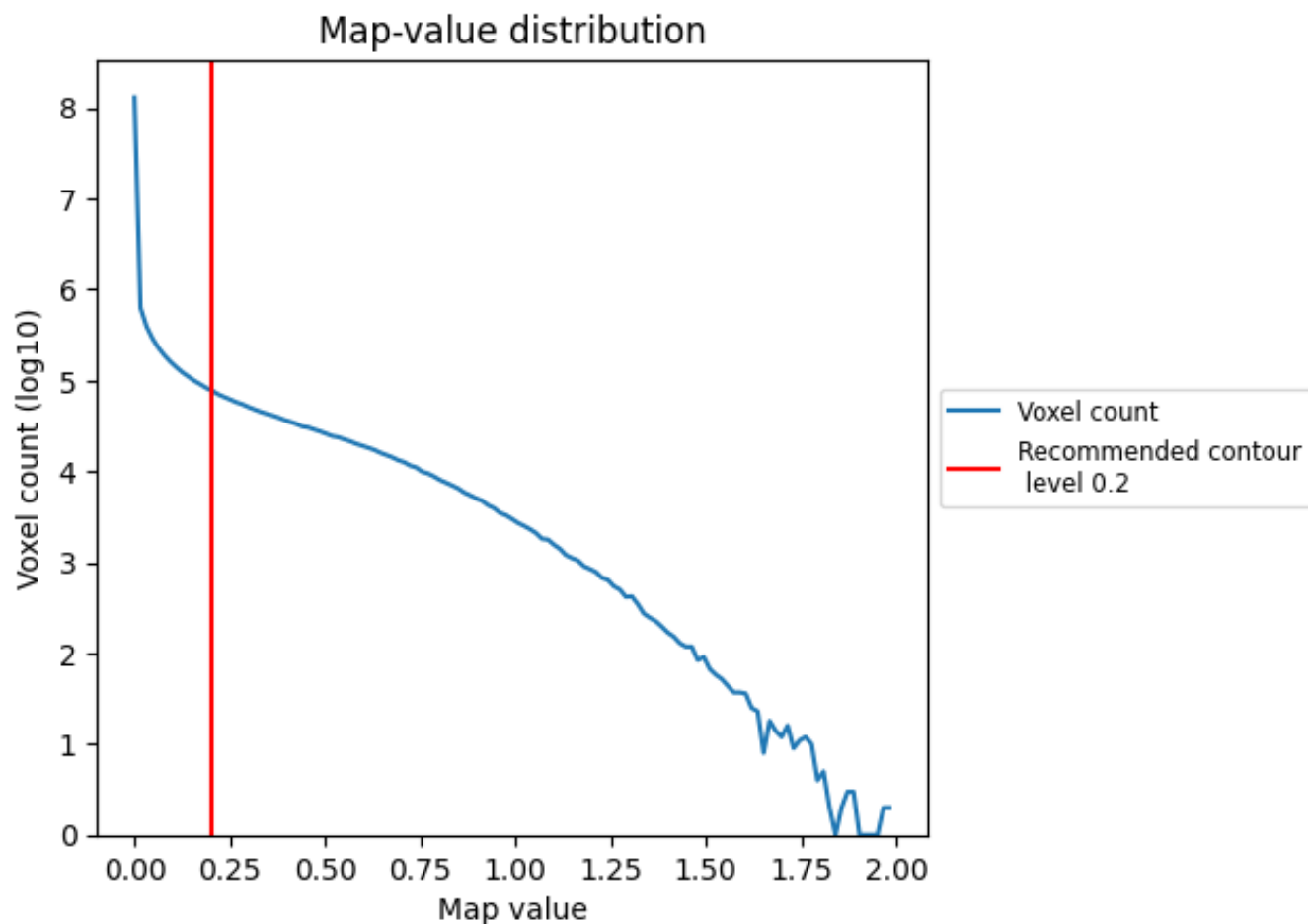


Z

7 Map analysis [i](#)

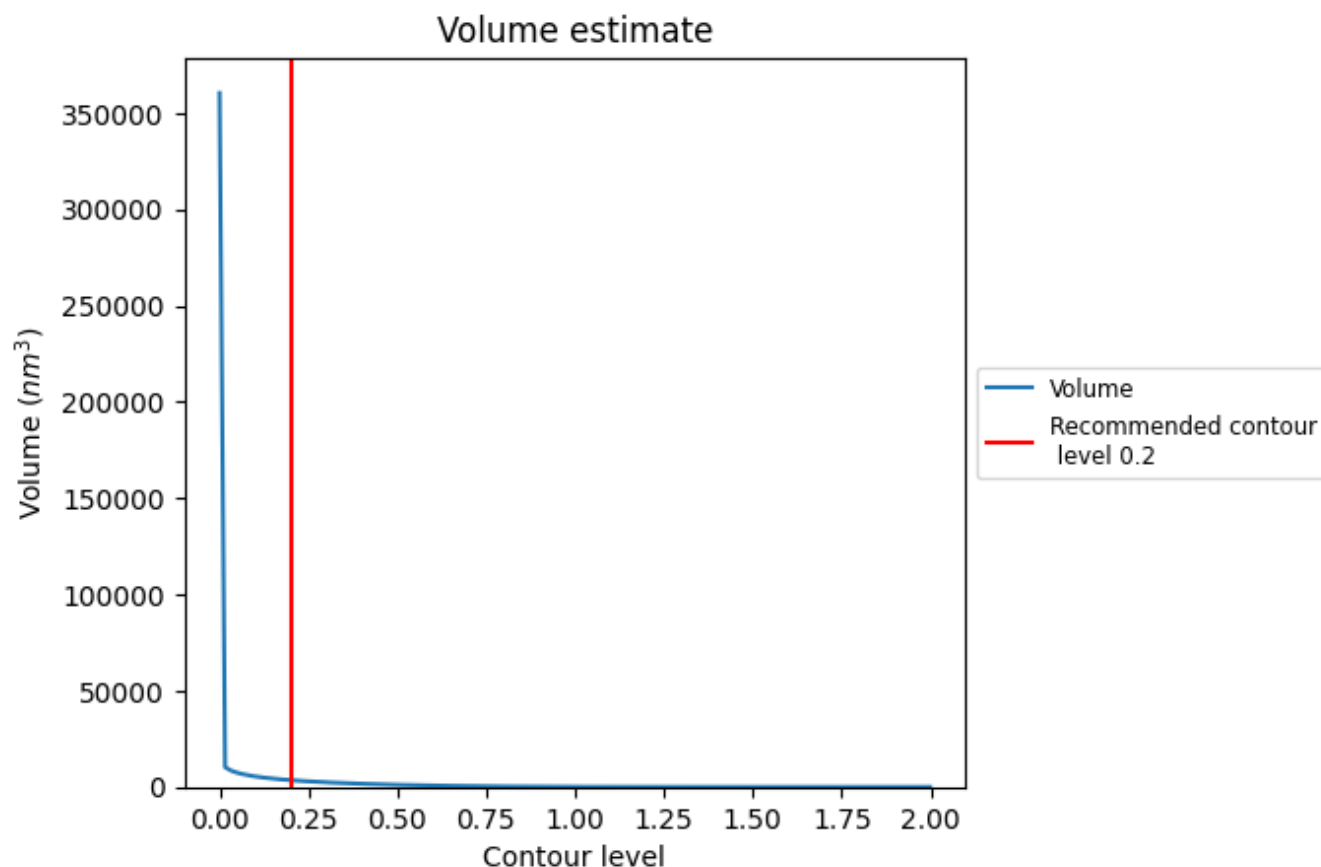
This section contains the results of statistical analysis of the map.

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.

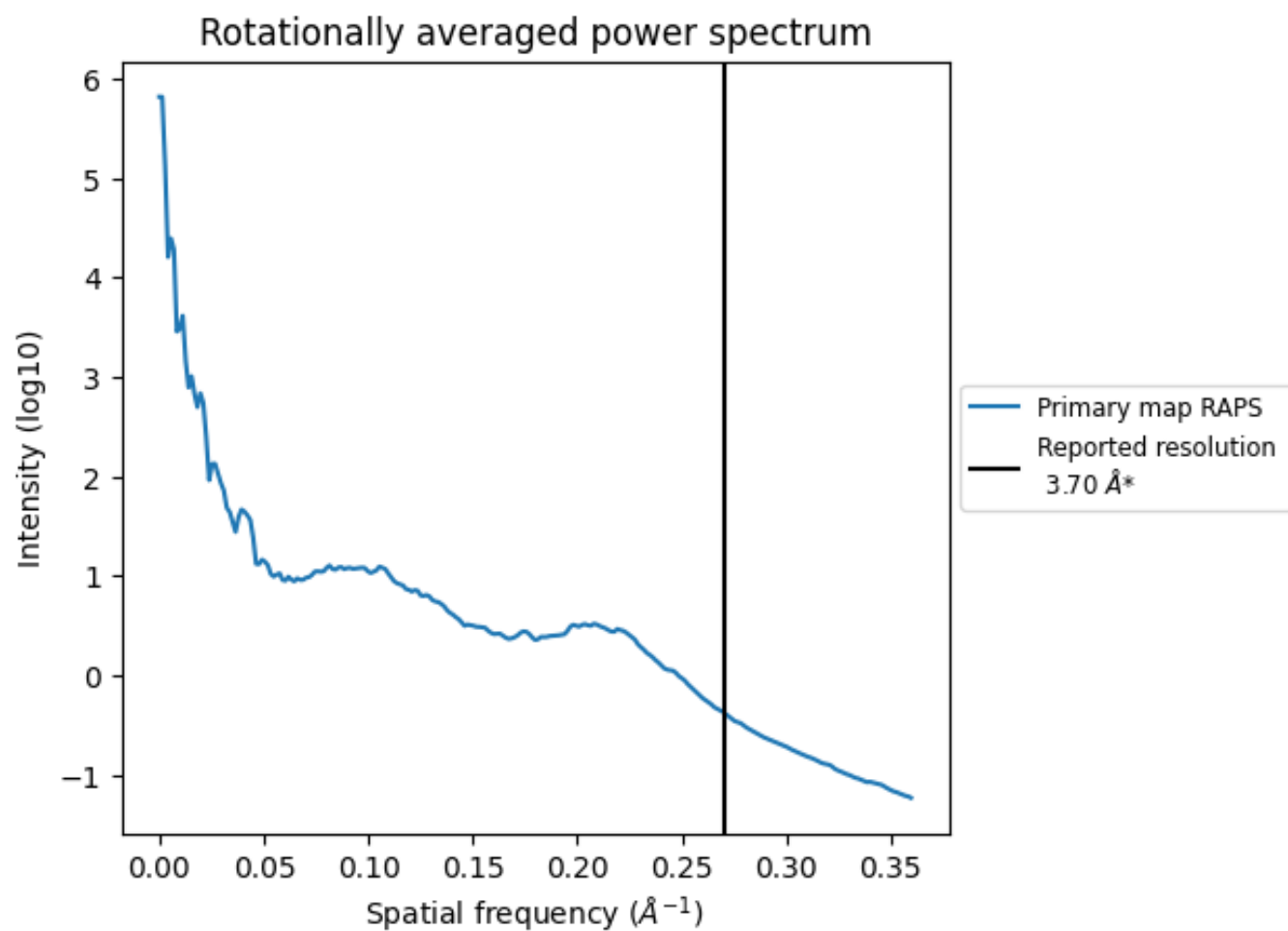
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3525 nm^3 ; this corresponds to an approximate mass of 3184 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 ⓘ

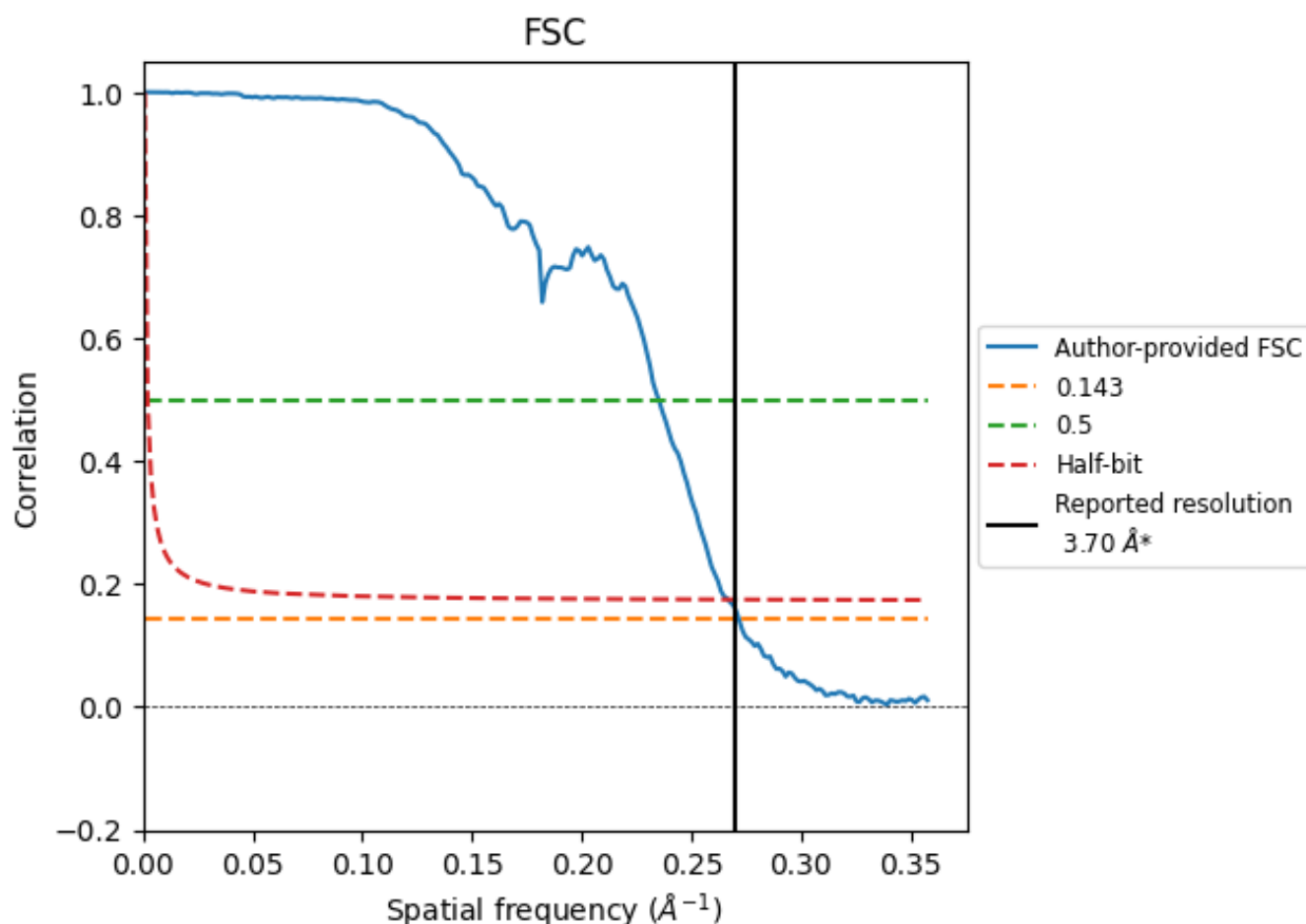


*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

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 0.270 Å⁻¹

8.2 Resolution estimates [i](#)

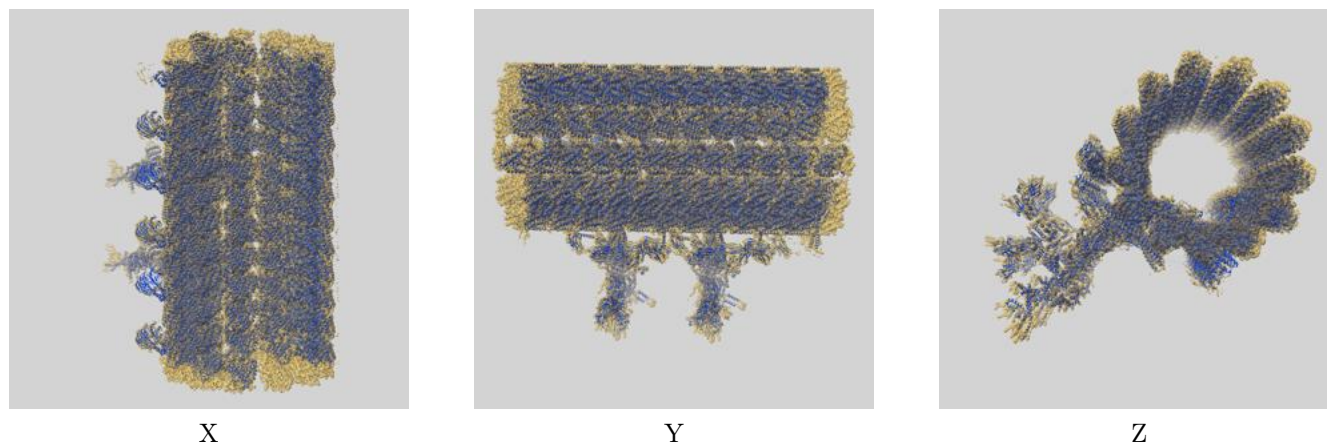
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.68	4.26	3.75
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

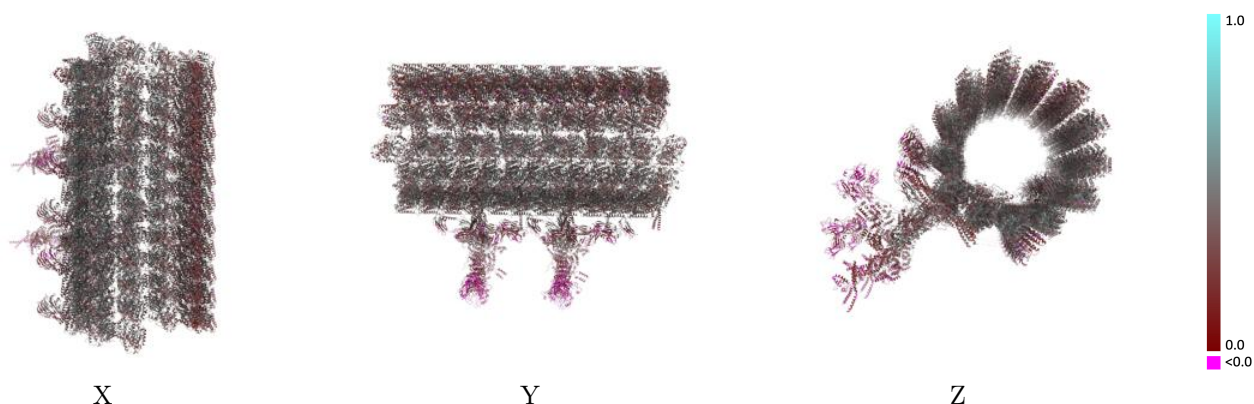
This section contains information regarding the fit between EMDB map EMD-25361 and PDB model 7SOM. Per-residue inclusion information can be found in section [3](#) on page [34](#).

9.1 Map-model overlay [i](#)



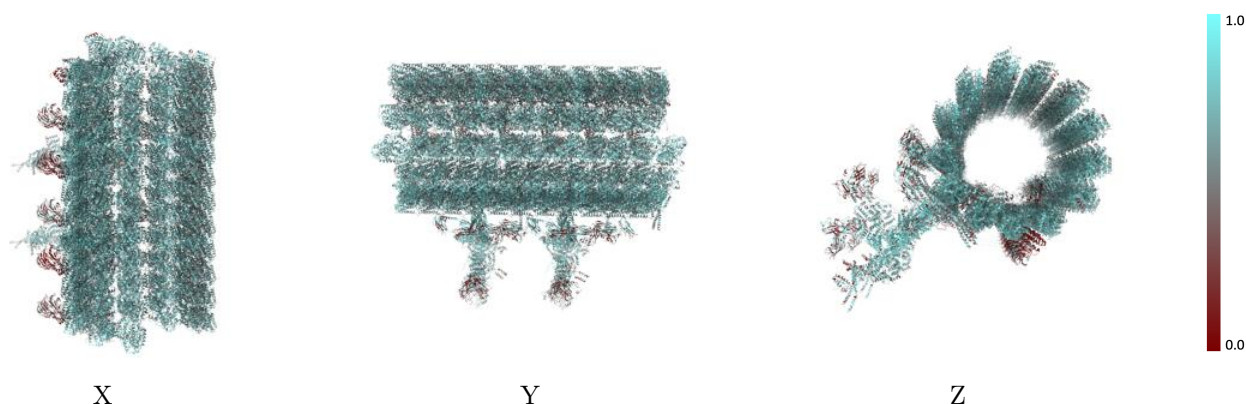
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



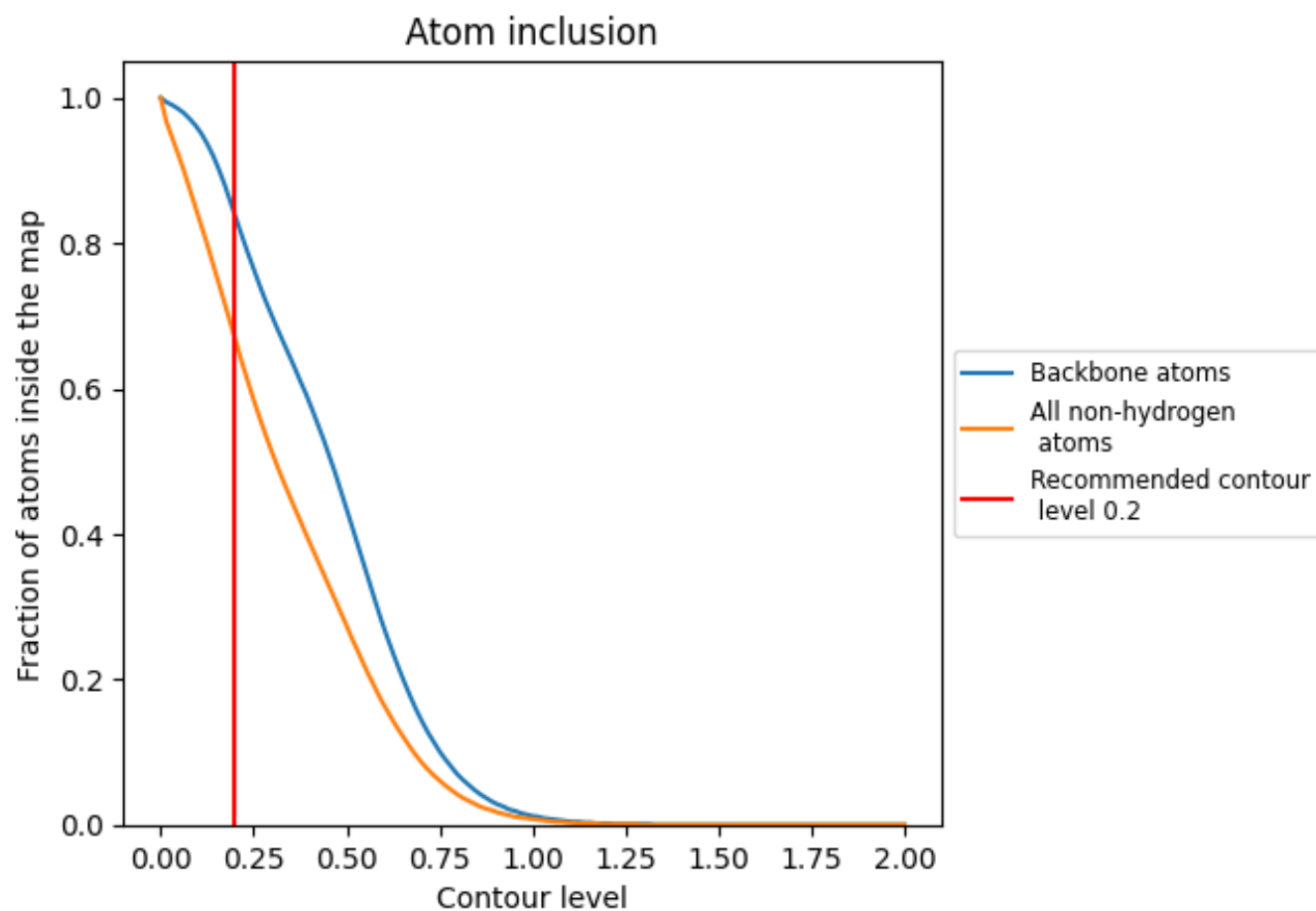
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 67% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6680	 0.3970
A	 0.5370	 0.3720
A1	 0.7080	 0.3380
A2	 0.7560	 0.3430
A3	 0.6890	 0.3320
A4	 0.7560	 0.3440
AA	 0.7110	 0.4210
AB	 0.6970	 0.4310
AC	 0.7070	 0.4310
AD	 0.6910	 0.4120
AE	 0.7460	 0.4430
AF	 0.7100	 0.4510
AG	 0.7180	 0.4580
AH	 0.7170	 0.4440
AI	 0.7320	 0.4270
AJ	 0.6910	 0.4220
AK	 0.7080	 0.4340
AL	 0.7050	 0.4260
B	 0.5720	 0.3900
BA	 0.6860	 0.4220
BB	 0.6850	 0.4320
BC	 0.7140	 0.4210
BD	 0.7180	 0.4200
BE	 0.6910	 0.4320
BF	 0.6950	 0.4430
BG	 0.7160	 0.4420
BH	 0.7270	 0.4280
BI	 0.6760	 0.4110
BJ	 0.6800	 0.4190
BK	 0.7040	 0.4220
BL	 0.6820	 0.4060
C	 0.5090	 0.3720
CA	 0.7170	 0.4420
CB	 0.7160	 0.4480
CC	 0.7270	 0.4430



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Chain	Atom inclusion	Q-score
CD	 0.7450	 0.4440
CE	 0.7270	 0.4590
CF	 0.7240	 0.4630
CG	 0.7350	 0.4530
CH	 0.7510	 0.4430
CI	 0.7100	 0.4460
CJ	 0.7020	 0.4420
CK	 0.7170	 0.4290
D	 0.6240	 0.3360
DB	 0.7140	 0.4430
DC	 0.7080	 0.4470
DD	 0.7130	 0.4340
DE	 0.7310	 0.4370
DF	 0.7240	 0.4520
DG	 0.7150	 0.4540
DH	 0.7160	 0.4470
DI	 0.7310	 0.4380
DJ	 0.7190	 0.4380
DK	 0.6990	 0.4350
DL	 0.7060	 0.4300
E	 0.6190	 0.3340
EA	 0.6710	 0.4220
EB	 0.6900	 0.4320
EC	 0.6740	 0.4160
ED	 0.6820	 0.4240
EE	 0.7230	 0.4390
EF	 0.6990	 0.4510
EG	 0.6860	 0.4430
EH	 0.7040	 0.4480
EI	 0.7140	 0.4270
EJ	 0.6880	 0.4320
EK	 0.6810	 0.4180
EL	 0.6890	 0.4280
F	 0.6240	 0.2290
FA	 0.6920	 0.4160
FB	 0.6900	 0.4140
FC	 0.6790	 0.4070
FD	 0.7000	 0.4140
FE	 0.7140	 0.4310
FF	 0.7050	 0.4430
FG	 0.6980	 0.4370
FH	 0.7180	 0.4280

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Chain	Atom inclusion	Q-score
FI	 0.7100	 0.4180
FJ	 0.7040	 0.4260
FK	 0.6930	 0.4190
FL	 0.6990	 0.4110
G	 0.5950	 0.2040
GC	 0.6890	 0.4070
GD	 0.6850	 0.4050
GE	 0.6800	 0.4060
GF	 0.6950	 0.3960
GG	 0.6920	 0.4160
GH	 0.6920	 0.4210
GI	 0.6940	 0.4220
GJ	 0.6990	 0.3960
GK	 0.6780	 0.3990
GL	 0.6900	 0.4030
GM	 0.6800	 0.4050
H	 0.6260	 0.2310
HC	 0.6110	 0.3320
HD	 0.6100	 0.3270
HE	 0.5890	 0.3120
HF	 0.6550	 0.3230
HG	 0.6290	 0.3460
HH	 0.6330	 0.3450
HI	 0.6210	 0.3420
HJ	 0.6490	 0.3250
HK	 0.6020	 0.3200
HL	 0.6070	 0.3260
HM	 0.6100	 0.3170
I	 0.5910	 0.2010
IC	 0.6260	 0.3490
ID	 0.6470	 0.3550
IE	 0.6300	 0.3400
IF	 0.6850	 0.3480
IG	 0.6490	 0.3670
IH	 0.6610	 0.3670
II	 0.6410	 0.3520
IJ	 0.6810	 0.3490
IK	 0.6320	 0.3540
IL	 0.6510	 0.3560
IM	 0.6360	 0.3440
J	 0.6390	 0.3300
JB	 0.6990	 0.3940

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Chain	Atom inclusion	Q-score
JC	 0.6740	 0.3960
JD	 0.6790	 0.4000
JE	 0.6950	 0.4000
JF	 0.7170	 0.4050
JG	 0.6930	 0.4140
JH	 0.6980	 0.4220
JI	 0.7040	 0.4110
JJ	 0.7100	 0.3960
JK	 0.6850	 0.4040
JL	 0.6900	 0.4050
JM	 0.6900	 0.4000
K	 0.6510	 0.3350
KB	 0.6990	 0.4060
KC	 0.6930	 0.4190
KD	 0.6820	 0.4050
KE	 0.6950	 0.4000
KF	 0.6990	 0.4190
KG	 0.7010	 0.4300
KH	 0.6890	 0.4230
KI	 0.7080	 0.4110
KJ	 0.6890	 0.3970
KK	 0.6890	 0.4110
KL	 0.6820	 0.4090
L	 0.3190	 0.2810
LB	 0.7060	 0.4200
LC	 0.6920	 0.4230
LD	 0.6880	 0.4110
LE	 0.7290	 0.4170
LF	 0.7110	 0.4440
LG	 0.6980	 0.4350
LH	 0.6890	 0.4320
LI	 0.7170	 0.4200
LJ	 0.6940	 0.4140
LK	 0.6770	 0.4070
LL	 0.6930	 0.4100
M	 0.1770	 0.2360
MB	 0.6920	 0.4310
MC	 0.6900	 0.4310
MD	 0.6950	 0.4240
ME	 0.7110	 0.4310
MF	 0.7030	 0.4480
MG	 0.6980	 0.4410

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Chain	Atom inclusion	Q-score
MH	 0.7010	 0.4420
MI	 0.7110	 0.4360
MJ	 0.6990	 0.4350
MK	 0.6900	 0.4260
ML	 0.7000	 0.4310
N	 0.3600	 0.2880
O	 0.2140	 0.2400
P	 0.3020	 0.2320
Q	 0.4590	 0.3420
R	 0.2880	 0.2380
S	 0.4960	 0.3390
T	 0.5320	 0.1890
U	 0.5680	 0.2250
V	 0.4640	 0.1730
W	 0.5580	 0.2060
X	 0.3150	 0.2790
Y	 0.1560	 0.2320
Z	 0.5670	 0.3170
a	 0.5900	 0.3810
aa	 0.3150	 0.3660
b	 0.6280	 0.3910
bb	 0.5450	 0.3360
c	 0.6250	 0.3880
cc	 0.5790	 0.3280
d	 0.6320	 0.3820
e	 0.5810	 0.3700
f	 0.5940	 0.3940
g	 0.6200	 0.3830
h	 0.5590	 0.3980
i	 0.6140	 0.4150
j	 0.5770	 0.3990
k	 0.5840	 0.3510
l	 0.5840	 0.3420
m	 0.5990	 0.3980
n	 0.6230	 0.4130
o	 0.5960	 0.3970
p	 0.5840	 0.4030
q	 0.6150	 0.4130
r	 0.6020	 0.4180
s	 0.5730	 0.3570