



wwPDB EM Validation Summary Report ⓘ

Mar 28, 2026 – 12:58 PM UTC

PDB ID : 7UN1 / pdb_00007un1
EMDB ID : EMD-26611
Title : 8-nm repeat of the human sperm tip singlet microtubule
Authors : Gui, M.; Croft, J.T.; Zabeo, D.; Acharya, V.; Kollman, J.M.; Burgoyne, T.;
Hoog, J.L.; Brown, A.
Deposited on : 2022-04-08
Resolution : 6.00 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:

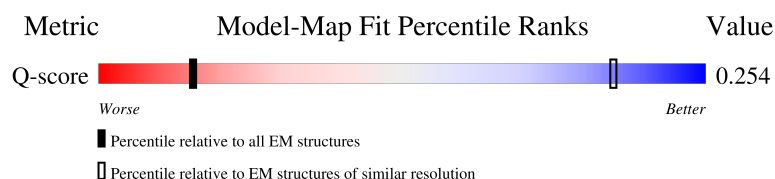
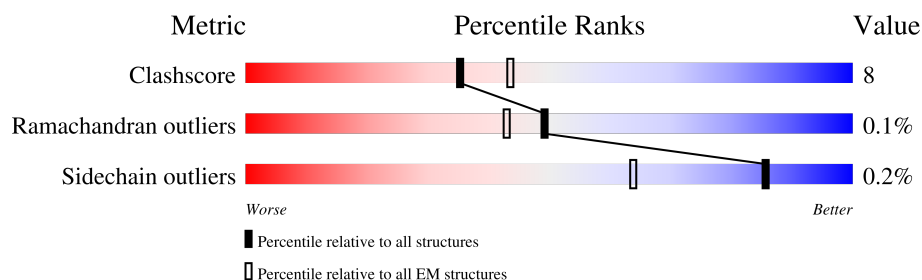
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 6.00 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	525 (5.50 - 6.50)

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	A	222	44% 72% 28%
1	B	222	23% 72% 28%
1	C	222	13% 70% 29%
1	D	222	13% 62% 10% 28%

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Mol	Chain	Length	Quality of chain
1	E	222	
1	F	222	
1	G	222	
1	H	222	
1	I	222	
1	J	222	
1	K	222	
1	L	222	
1	M	222	
1	N	222	
1	O	222	
1	P	222	
1	Q	222	
1	R	222	
1	S	222	
1	T	222	
1	U	222	
1	V	222	
1	W	222	
1	X	222	
1	d	222	
1	e	222	
1	f	222	
1	g	222	
1	h	222	

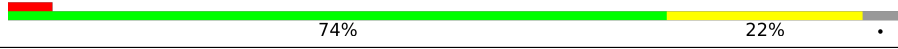
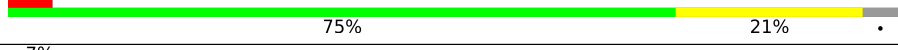
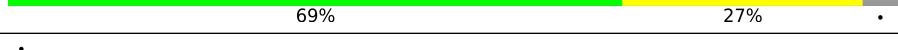
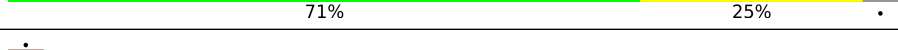
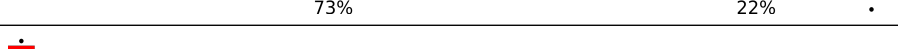
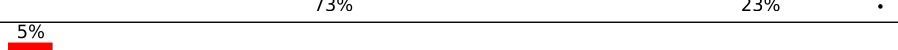
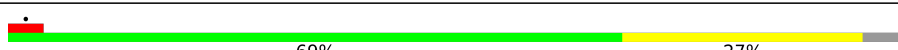
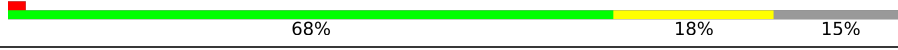
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Mol	Chain	Length	Quality of chain
1	i	222	
1	j	222	
1	k	222	
1	l	222	
2	AB	445	
2	AD	445	
2	AF	445	
2	BA	445	
2	BD	445	
2	BF	445	
2	CB	445	
2	CD	445	
2	CF	445	
2	DB	445	
2	DD	445	
2	DF	445	
2	EB	445	
2	ED	445	
2	EF	445	
2	FD	445	
2	FF	445	
2	FH	445	
2	GD	445	
2	GF	445	
2	GH	445	

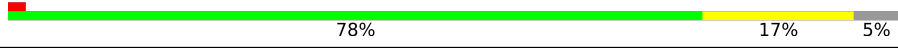
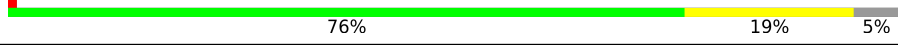
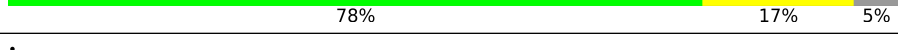
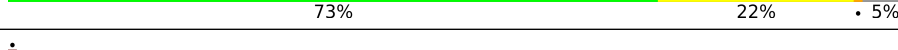
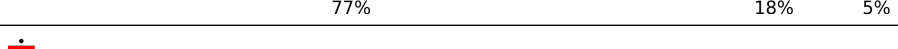
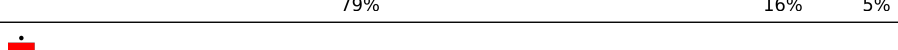
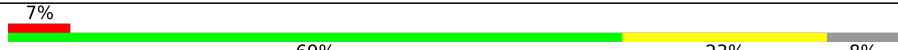
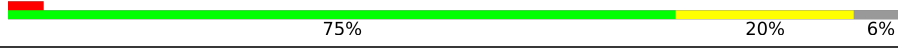
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Mol	Chain	Length	Quality of chain
2	HD	445	
2	HF	445	
2	HH	445	
2	ID	445	
2	IF	445	
2	IH	445	
2	JD	445	
2	JF	445	
2	KD	445	
2	KF	445	
2	KH	445	
2	LB	445	
2	LD	445	
2	LF	445	
2	MB	445	
2	MD	445	
2	MF	445	
3	AC	451	
3	AE	451	
3	BC	451	
3	BE	451	
3	BG	451	
3	CC	451	
3	CE	451	
3	CG	451	

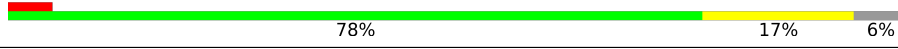
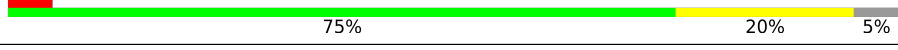
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Mol	Chain	Length	Quality of chain
3	DC	451	
3	DE	451	
3	DG	451	
3	EC	451	
3	EE	451	
3	EG	451	
3	FC	451	
3	FE	451	
3	FG	451	
3	GC	451	
3	GE	451	
3	GG	451	
3	HC	451	
3	HE	451	
3	HG	451	
3	IC	451	
3	IE	451	
3	IG	451	
3	JC	451	
3	JE	451	
3	JG	451	
3	KC	451	
3	KE	451	
3	KG	451	
3	LA	451	

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Mol	Chain	Length	Quality of chain
3	LC	451	
3	LE	451	
3	MA	451	
3	MC	451	
3	ME	451	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 290845 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 Sperm acrosome-associated protein 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	160	Total	C	N	O		0	0
			796	476	160	160			
1	B	160	Total	C	N	O		0	0
			796	476	160	160			
1	C	158	Total	C	N	O		0	0
			786	470	158	158			
1	D	160	Total	C	N	O	S	0	0
			1289	805	231	243	10		
1	E	160	Total	C	N	O	S	0	0
			1289	805	231	243	10		
1	F	157	Total	C	N	O	S	0	0
			1263	788	225	240	10		
1	G	159	Total	C	N	O	S	0	0
			1278	799	227	242	10		
1	H	159	Total	C	N	O	S	0	0
			1278	799	227	242	10		
1	I	159	Total	C	N	O	S	0	0
			1278	799	227	242	10		
1	J	159	Total	C	N	O		0	0
			791	473	159	159			
1	K	159	Total	C	N	O		0	0
			791	473	159	159			
1	L	159	Total	C	N	O		0	0
			791	473	159	159			
1	M	160	Total	C	N	O		0	0
			796	476	160	160			
1	N	156	Total	C	N	O		0	0
			776	464	156	156			
1	O	160	Total	C	N	O		0	0
			796	476	160	160			
1	P	160	Total	C	N	O	S	0	0
			1289	805	231	243	10		
1	Q	157	Total	C	N	O	S	0	0
			1263	788	225	240	10		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	160	Total	C	N	O	S	0	0
			1289	805	231	243	10		
1	S	156	Total	C	N	O	S	0	0
			1254	782	223	239	10		
1	T	159	Total	C	N	O	S	0	0
			1278	799	227	242	10		
1	U	159	Total	C	N	O	S	0	0
			1278	799	227	242	10		
1	V	159	Total	C	N	O		0	0
			791	473	159	159			
1	W	155	Total	C	N	O		0	0
			771	461	155	155			
1	X	160	Total	C	N	O		0	0
			796	476	160	160			
1	d	156	Total	C	N	O	S	0	0
			1254	782	223	239	10		
1	e	157	Total	C	N	O	S	0	0
			1263	788	225	240	10		
1	f	160	Total	C	N	O	S	0	0
			1289	805	231	243	10		
1	g	159	Total	C	N	O	S	0	0
			1278	799	227	242	10		
1	h	156	Total	C	N	O	S	0	0
			1254	782	223	239	10		
1	i	159	Total	C	N	O	S	0	0
			1278	799	227	242	10		
1	j	159	Total	C	N	O		0	0
			791	473	159	159			
1	k	155	Total	C	N	O		0	0
			771	461	155	155			
1	l	152	Total	C	N	O		0	0
			756	452	152	152			

- Molecule 2 is a protein called Tubulin beta-4B chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AB	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
2	AD	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
2	AF	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	BA	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
2	BD	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
2	BF	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
2	CB	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
2	CD	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
2	CF	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
2	DB	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
2	DD	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
2	DF	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
2	EB	411	Total	C	N	O	S	0	0
			3214	2015	549	626	24		
2	ED	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
2	EF	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
2	FD	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
2	FF	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
2	FH	379	Total	C	N	O	S	0	0
			2971	1871	508	570	22		
2	GD	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
2	GF	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
2	GH	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
2	HD	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
2	HF	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
2	HH	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	ID	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
2	IF	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
2	IH	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
2	JD	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
2	JF	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
2	KD	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
2	KF	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
2	KH	403	Total	C	N	O	S	0	0
			3165	1996	539	607	23		
2	LB	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
2	LD	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
2	LF	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
2	MB	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
2	MD	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
2	MF	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		

- Molecule 3 is a protein called Tubulin alpha-1A chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AC	426	Total	C	N	O	S	0	0
			3343	2123	569	629	22		
3	AE	427	Total	C	N	O	S	0	0
			3349	2126	570	631	22		
3	BC	427	Total	C	N	O	S	0	0
			3350	2125	570	633	22		
3	BE	426	Total	C	N	O	S	0	0
			3343	2123	569	629	22		
3	BG	385	Total	C	N	O	S	0	0
			3026	1914	516	575	21		

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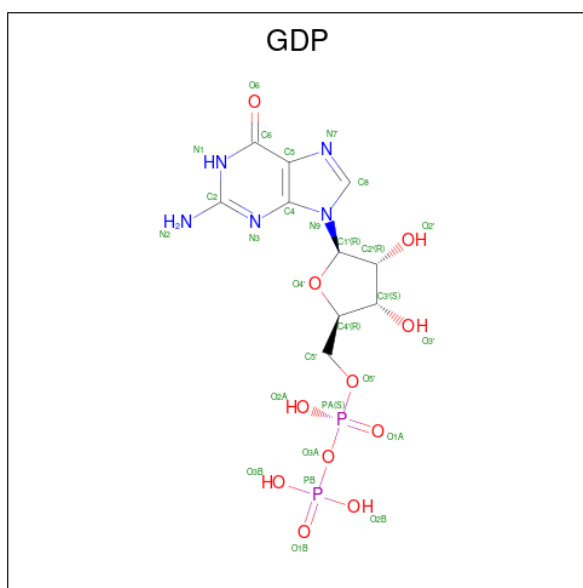
Mol	Chain	Residues	Atoms					AltConf	Trace
3	CC	430	Total	C	N	O	S	0	0
			3369	2136	573	638	22		
3	CE	431	Total	C	N	O	S	0	0
			3377	2140	574	641	22		
3	CG	429	Total	C	N	O	S	0	0
			3363	2133	572	636	22		
3	DC	428	Total	C	N	O	S	0	0
			3357	2130	571	634	22		
3	DE	428	Total	C	N	O	S	0	0
			3357	2130	571	634	22		
3	DG	429	Total	C	N	O	S	0	0
			3363	2133	572	636	22		
3	EC	429	Total	C	N	O	S	0	0
			3363	2133	572	636	22		
3	EE	428	Total	C	N	O	S	0	0
			3356	2128	571	635	22		
3	EG	428	Total	C	N	O	S	0	0
			3357	2130	571	634	22		
3	FC	429	Total	C	N	O	S	0	0
			3365	2134	572	637	22		
3	FE	430	Total	C	N	O	S	0	0
			3369	2136	573	638	22		
3	FG	429	Total	C	N	O	S	0	0
			3363	2133	572	636	22		
3	GC	430	Total	C	N	O	S	0	0
			3371	2137	573	639	22		
3	GE	429	Total	C	N	O	S	0	0
			3364	2132	572	638	22		
3	GG	428	Total	C	N	O	S	0	0
			3356	2127	571	637	21		
3	HC	427	Total	C	N	O	S	0	0
			3350	2125	570	633	22		
3	HE	427	Total	C	N	O	S	0	0
			3349	2126	570	631	22		
3	HG	426	Total	C	N	O	S	0	0
			3342	2121	569	630	22		
3	IC	414	Total	C	N	O	S	0	0
			3239	2051	550	617	21		
3	IE	428	Total	C	N	O	S	0	0
			3357	2130	571	634	22		
3	IG	427	Total	C	N	O	S	0	0
			3350	2125	570	633	22		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	JC	429	Total	C	N	O	S	0	0
			3365	2134	572	637	22		
3	JE	428	Total	C	N	O	S	0	0
			3358	2129	571	636	22		
3	JG	427	Total	C	N	O	S	0	0
			3350	2125	570	633	22		
3	KC	426	Total	C	N	O	S	0	0
			3342	2121	569	630	22		
3	KE	425	Total	C	N	O	S	0	0
			3335	2116	568	629	22		
3	KG	426	Total	C	N	O	S	0	0
			3342	2121	569	630	22		
3	LA	428	Total	C	N	O	S	0	0
			3357	2130	571	634	22		
3	LC	427	Total	C	N	O	S	0	0
			3349	2126	570	631	22		
3	LE	428	Total	C	N	O	S	0	0
			3357	2130	571	634	22		
3	MA	426	Total	C	N	O	S	0	0
			3342	2121	569	630	22		
3	MC	428	Total	C	N	O	S	0	0
			3357	2130	571	634	22		
3	ME	426	Total	C	N	O	S	0	0
			3342	2121	569	630	22		

- Molecule 4 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



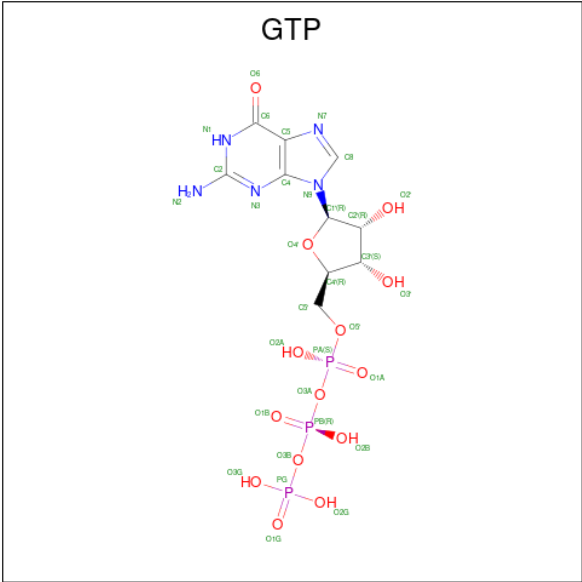
Mol	Chain	Residues	Atoms					AltConf
4	AB	1	Total	C	N	O	P	0
			28	10	5	11	2	
4	AD	1	Total	C	N	O	P	0
			28	10	5	11	2	
4	AF	1	Total	C	N	O	P	0
			28	10	5	11	2	
4	BA	1	Total	C	N	O	P	0
			28	10	5	11	2	
4	BD	1	Total	C	N	O	P	0
			28	10	5	11	2	
4	BF	1	Total	C	N	O	P	0
			28	10	5	11	2	
4	CB	1	Total	C	N	O	P	0
			28	10	5	11	2	
4	CD	1	Total	C	N	O	P	0
			28	10	5	11	2	
4	CF	1	Total	C	N	O	P	0
			28	10	5	11	2	
4	DB	1	Total	C	N	O	P	0
			28	10	5	11	2	
4	DD	1	Total	C	N	O	P	0
			28	10	5	11	2	
4	DF	1	Total	C	N	O	P	0
			28	10	5	11	2	
4	EB	1	Total	C	N	O	P	0
			28	10	5	11	2	
4	ED	1	Total	C	N	O	P	0
			28	10	5	11	2	
4	EF	1	Total	C	N	O	P	0
			28	10	5	11	2	
4	FD	1	Total	C	N	O	P	0
			28	10	5	11	2	
4	FF	1	Total	C	N	O	P	0
			28	10	5	11	2	
4	FH	1	Total	C	N	O	P	0
			28	10	5	11	2	
4	GD	1	Total	C	N	O	P	0
			28	10	5	11	2	
4	GF	1	Total	C	N	O	P	0
			28	10	5	11	2	
4	GH	1	Total	C	N	O	P	0
			28	10	5	11	2	
4	HD	1	Total	C	N	O	P	0
			28	10	5	11	2	

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Mol	Chain	Residues	Atoms					AltConf
4	HF	1	Total	C	N	O	P	0
			28	10	5	11	2	
4	HH	1	Total	C	N	O	P	0
			28	10	5	11	2	
4	ID	1	Total	C	N	O	P	0
			28	10	5	11	2	
4	IF	1	Total	C	N	O	P	0
			28	10	5	11	2	
4	IH	1	Total	C	N	O	P	0
			28	10	5	11	2	
4	JD	1	Total	C	N	O	P	0
			28	10	5	11	2	
4	JF	1	Total	C	N	O	P	0
			28	10	5	11	2	
4	KD	1	Total	C	N	O	P	0
			28	10	5	11	2	
4	KF	1	Total	C	N	O	P	0
			28	10	5	11	2	
4	KH	1	Total	C	N	O	P	0
			28	10	5	11	2	
4	LB	1	Total	C	N	O	P	0
			28	10	5	11	2	
4	LD	1	Total	C	N	O	P	0
			28	10	5	11	2	
4	LF	1	Total	C	N	O	P	0
			28	10	5	11	2	
4	MB	1	Total	C	N	O	P	0
			28	10	5	11	2	
4	MD	1	Total	C	N	O	P	0
			28	10	5	11	2	
4	MF	1	Total	C	N	O	P	0
			28	10	5	11	2	

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



Mol	Chain	Residues	Atoms					AltConf
5	AC	1	Total	C	N	O	P	0
			32	10	5	14	3	
5	AE	1	Total	C	N	O	P	0
			32	10	5	14	3	
5	BC	1	Total	C	N	O	P	0
			32	10	5	14	3	
5	BE	1	Total	C	N	O	P	0
			32	10	5	14	3	
5	BG	1	Total	C	N	O	P	0
			32	10	5	14	3	
5	CC	1	Total	C	N	O	P	0
			32	10	5	14	3	
5	CE	1	Total	C	N	O	P	0
			32	10	5	14	3	
5	CG	1	Total	C	N	O	P	0
			32	10	5	14	3	
5	DC	1	Total	C	N	O	P	0
			32	10	5	14	3	
5	DE	1	Total	C	N	O	P	0
			32	10	5	14	3	
5	DG	1	Total	C	N	O	P	0
			32	10	5	14	3	
5	EC	1	Total	C	N	O	P	0
			32	10	5	14	3	
5	EE	1	Total	C	N	O	P	0
			32	10	5	14	3	
5	EG	1	Total	C	N	O	P	0
			32	10	5	14	3	

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Mol	Chain	Residues	Atoms					AltConf
5	FC	1	Total 32	C 10	N 5	O 14	P 3	0
5	FE	1	Total 32	C 10	N 5	O 14	P 3	0
5	FG	1	Total 32	C 10	N 5	O 14	P 3	0
5	GC	1	Total 32	C 10	N 5	O 14	P 3	0
5	GE	1	Total 32	C 10	N 5	O 14	P 3	0
5	GG	1	Total 32	C 10	N 5	O 14	P 3	0
5	HC	1	Total 32	C 10	N 5	O 14	P 3	0
5	HE	1	Total 32	C 10	N 5	O 14	P 3	0
5	HG	1	Total 32	C 10	N 5	O 14	P 3	0
5	IC	1	Total 32	C 10	N 5	O 14	P 3	0
5	IE	1	Total 32	C 10	N 5	O 14	P 3	0
5	IG	1	Total 32	C 10	N 5	O 14	P 3	0
5	JC	1	Total 32	C 10	N 5	O 14	P 3	0
5	JE	1	Total 32	C 10	N 5	O 14	P 3	0
5	JG	1	Total 32	C 10	N 5	O 14	P 3	0
5	KC	1	Total 32	C 10	N 5	O 14	P 3	0
5	KE	1	Total 32	C 10	N 5	O 14	P 3	0
5	KG	1	Total 32	C 10	N 5	O 14	P 3	0
5	LA	1	Total 32	C 10	N 5	O 14	P 3	0
5	LC	1	Total 32	C 10	N 5	O 14	P 3	0
5	LE	1	Total 32	C 10	N 5	O 14	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
5	MA	1	Total	C	N	O	P	0
			32	10	5	14	3	
5	MC	1	Total	C	N	O	P	0
			32	10	5	14	3	
5	ME	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
6	AC	1	Total	Mg	0
			1	1	
6	AE	1	Total	Mg	0
			1	1	
6	BC	1	Total	Mg	0
			1	1	
6	BE	1	Total	Mg	0
			1	1	
6	BG	1	Total	Mg	0
			1	1	
6	CC	1	Total	Mg	0
			1	1	
6	CE	1	Total	Mg	0
			1	1	
6	CG	1	Total	Mg	0
			1	1	
6	DC	1	Total	Mg	0
			1	1	
6	DE	1	Total	Mg	0
			1	1	
6	DG	1	Total	Mg	0
			1	1	
6	EC	1	Total	Mg	0
			1	1	
6	EE	1	Total	Mg	0
			1	1	
6	EG	1	Total	Mg	0
			1	1	
6	FC	1	Total	Mg	0
			1	1	
6	FE	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
6	FG	1	1	1	0
6	GC	1	1	1	0
6	GE	1	1	1	0
6	GG	1	1	1	0
6	HC	1	1	1	0
6	HE	1	1	1	0
6	HG	1	1	1	0
6	IC	1	1	1	0
6	IE	1	1	1	0
6	IG	1	1	1	0
6	JC	1	1	1	0
6	JE	1	1	1	0
6	JG	1	1	1	0
6	KC	1	1	1	0
6	KE	1	1	1	0
6	KG	1	1	1	0
6	LA	1	1	1	0
6	LC	1	1	1	0
6	LE	1	1	1	0
6	MA	1	1	1	0
6	MC	1	1	1	0

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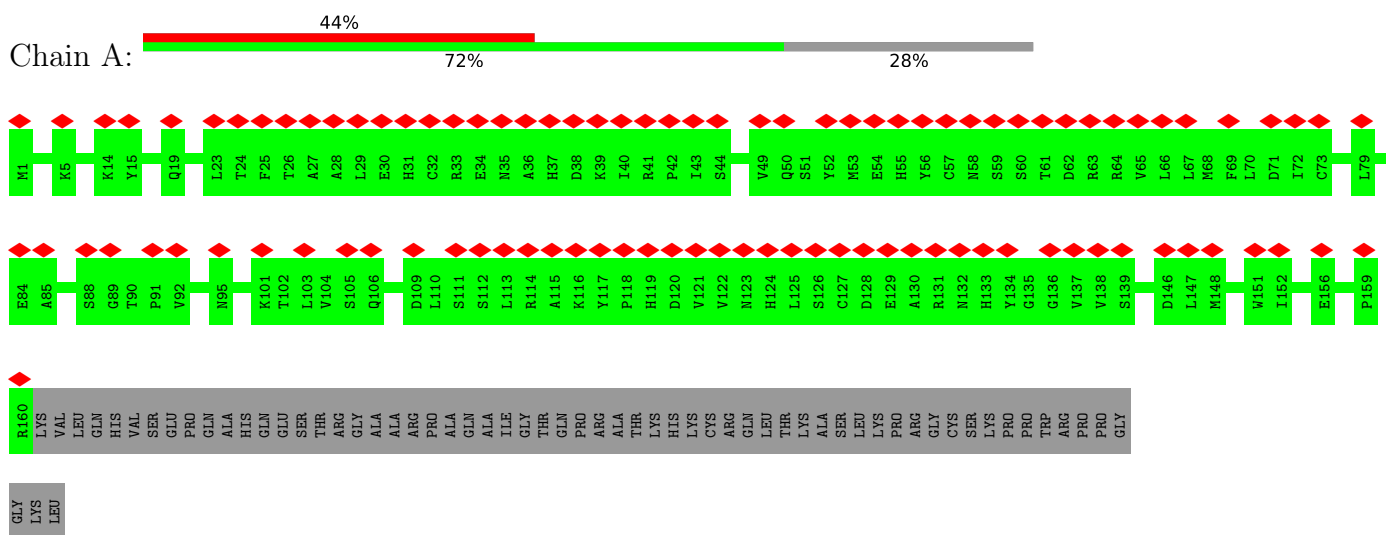
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Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
6	ME	1	1	1	0

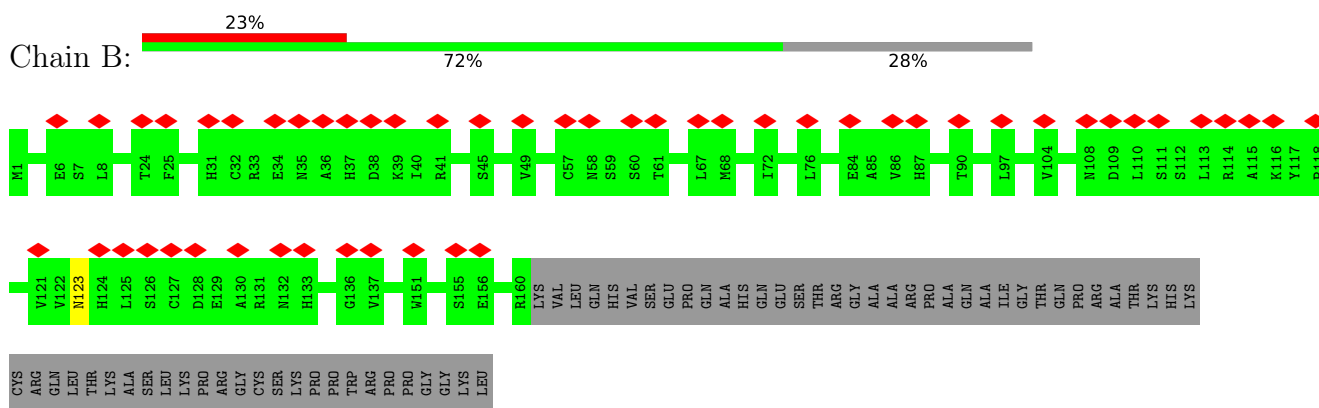
3 Residue-property plots

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.

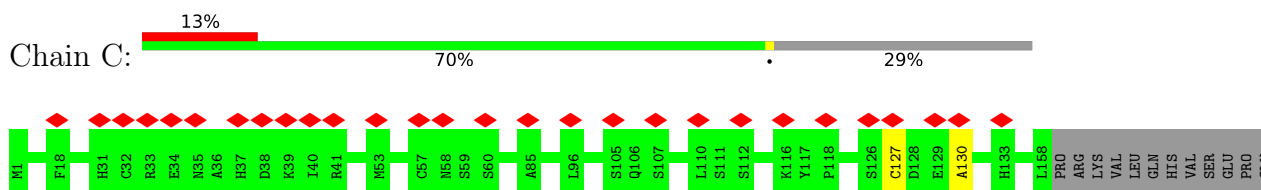
- Molecule 1: Sperm acrosome-associated protein 9



- Molecule 1: Sperm acrosome-associated protein 9



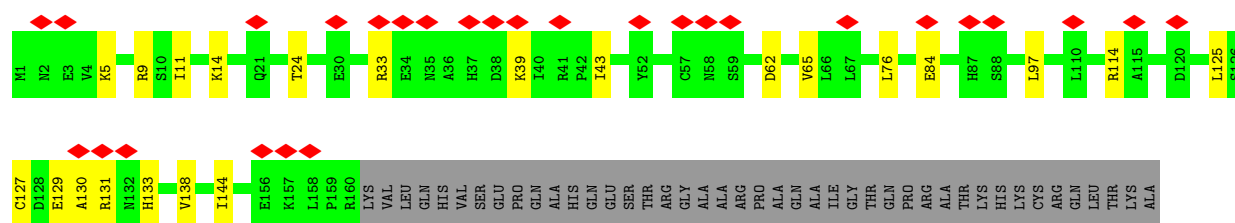
- Molecule 1: Sperm acrosome-associated protein 9



ALA HIS
GLN GLU
SER THR
ARG
GLY
ALA
ARG
PRO
ALA
GLN
ILE
GLY
THR
GLN
PRO
ARG
ALA
THR
LYS
HIS
LYS
CYS
ARG
GLN
LEU
THR
LYS
ALA
SER
LEU
LYS
PRO
ARG
GLY
CYS
SER
LYS
PRO
TRP
ARG
PRO
GLY
LYS
LEU

• Molecule 1: Sperm acrosome-associated protein 9

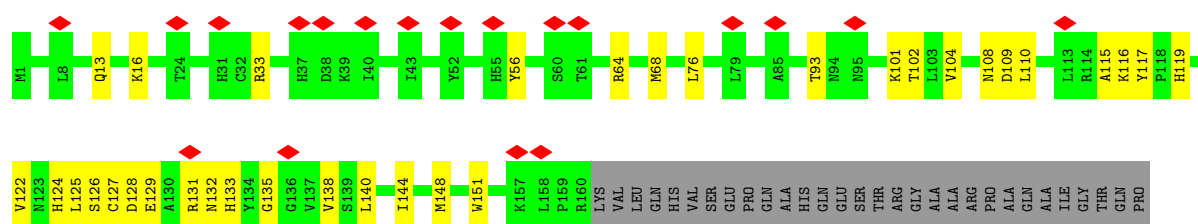
Chain D: 13% 62% 10% 28%



SER
LEU
LYS
PRO
ARG
GLY
CYS
SER
LYS
PRO
TRP
ARG
PRO
PRO
GLY
LYS
LEU

• Molecule 1: Sperm acrosome-associated protein 9

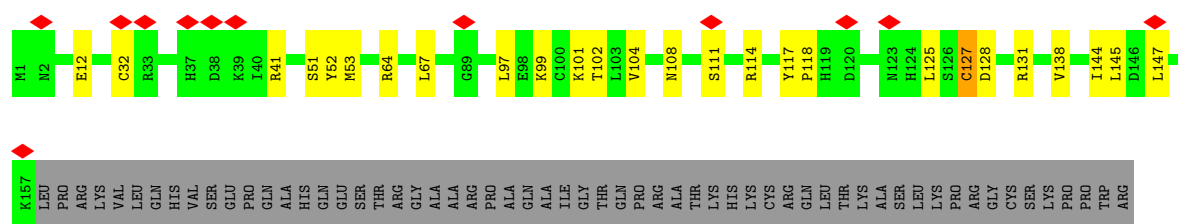
Chain E: 9% 57% 15% 28%



ARG
ALA
THR
LYS
HIS
LYS
CYS
ARG
GLN
LEU
THR
LYS
ALA
SER
LEU
LYS
PRO
ARG
GLY
CYS
SER
LYS
PRO
TRP
ARG
PRO
PRO
GLY
LYS
LEU

• Molecule 1: Sperm acrosome-associated protein 9

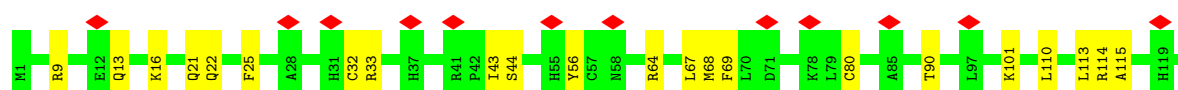
Chain F: 5% 59% 11% 29%



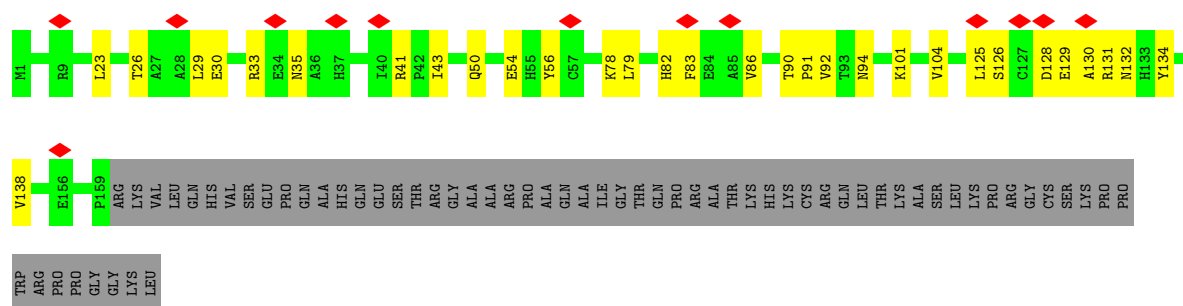
PRO
PRO
GLY
GLY
LYS
LEU

• Molecule 1: Sperm acrosome-associated protein 9

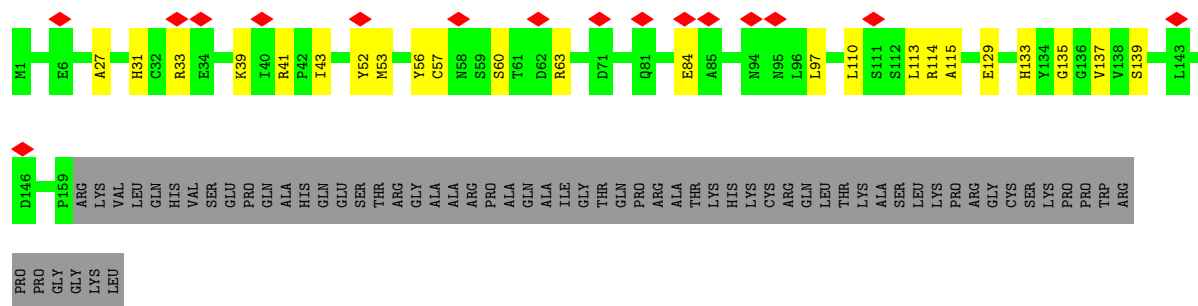
Chain G: 8% 59% 13% 28%



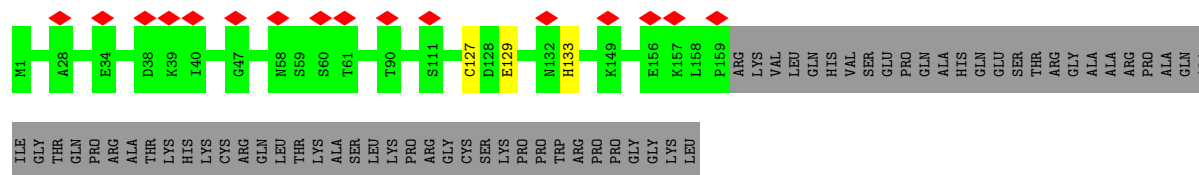
- Molecule 1: Sperm acrosome-associated protein 9



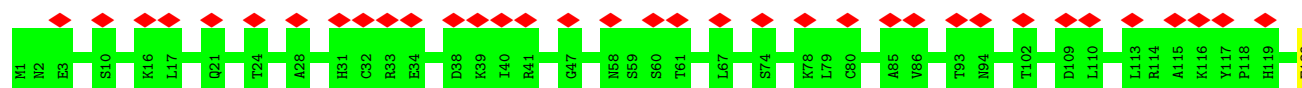
- Molecule 1: Sperm acrosome-associated protein 9

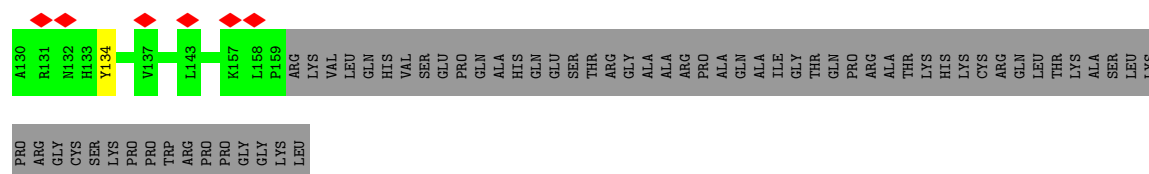


- Molecule 1: Sperm acrosome-associated protein 9

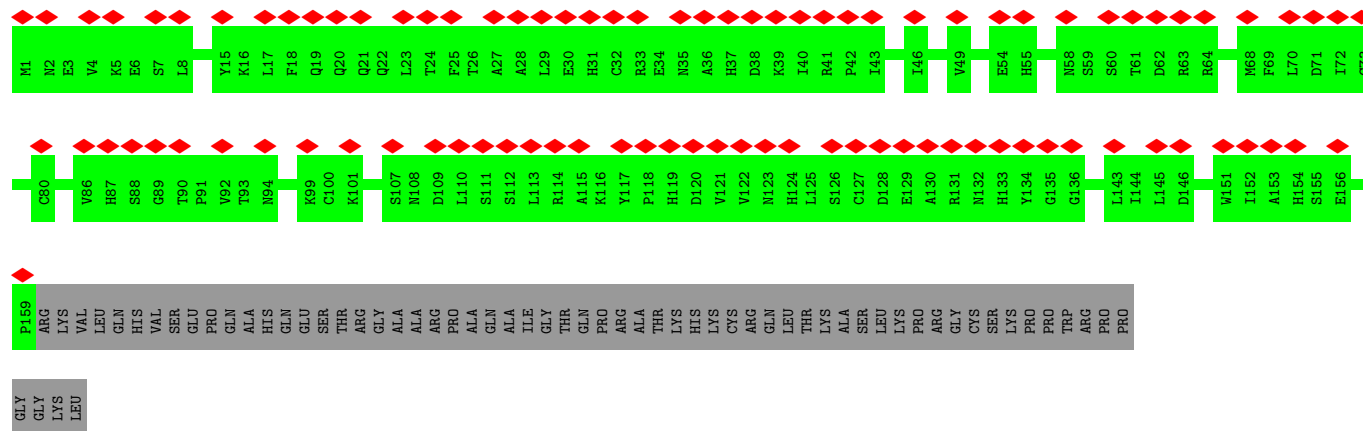


- Molecule 1: Sperm acrosome-associated protein 9

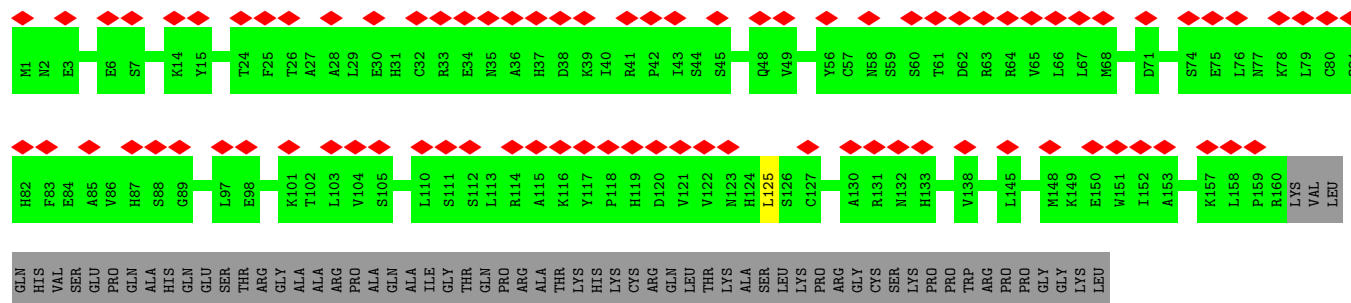
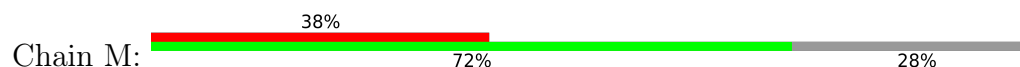




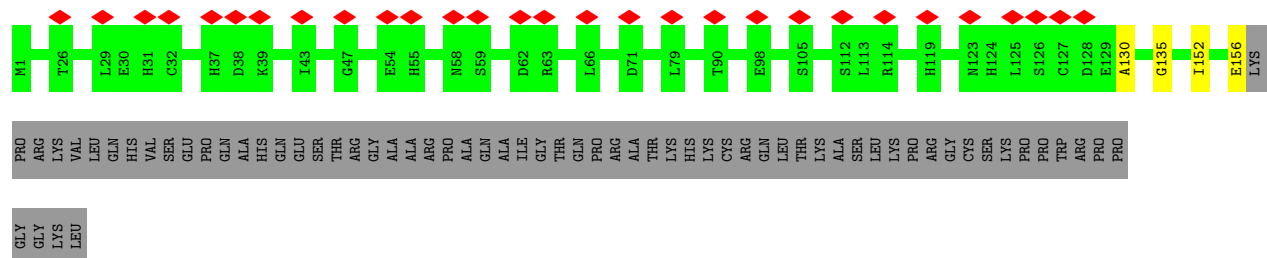
• Molecule 1: Sperm acrosome-associated protein 9



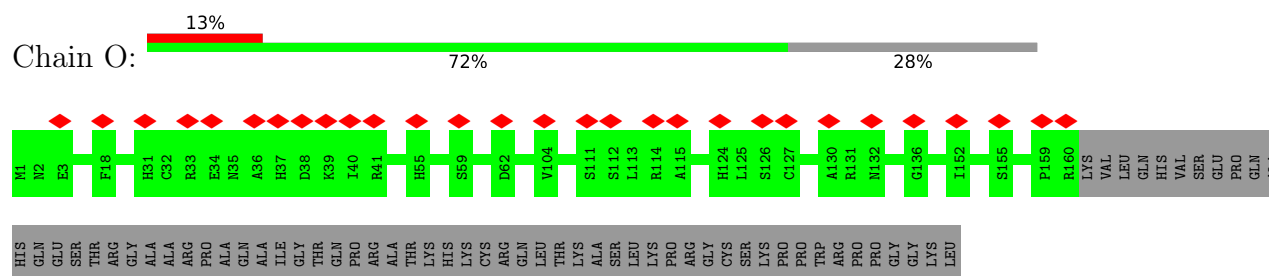
• Molecule 1: Sperm acrosome-associated protein 9



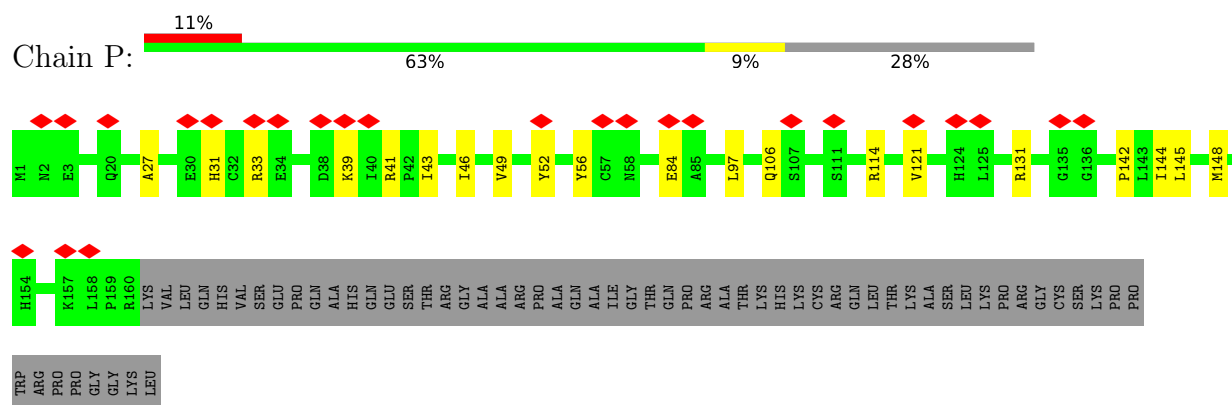
• Molecule 1: Sperm acrosome-associated protein 9



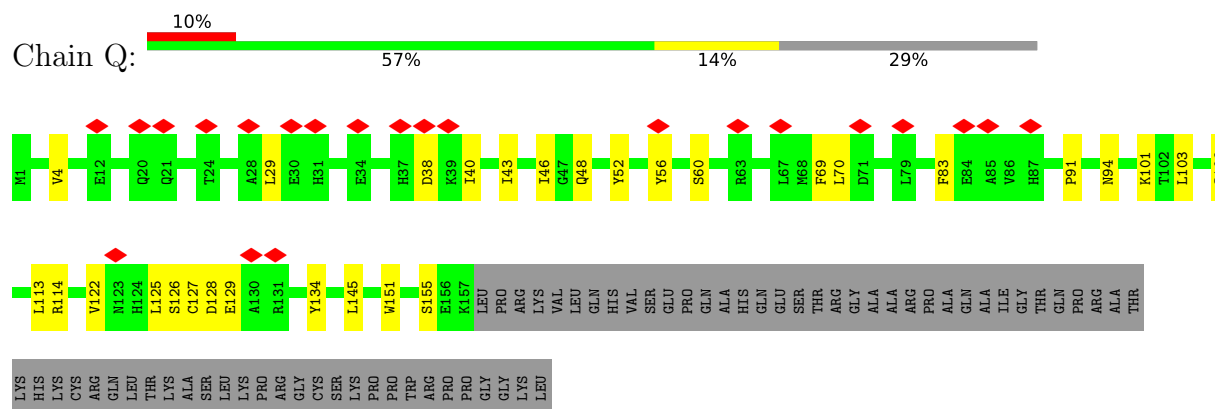
• Molecule 1: Sperm acrosome-associated protein 9



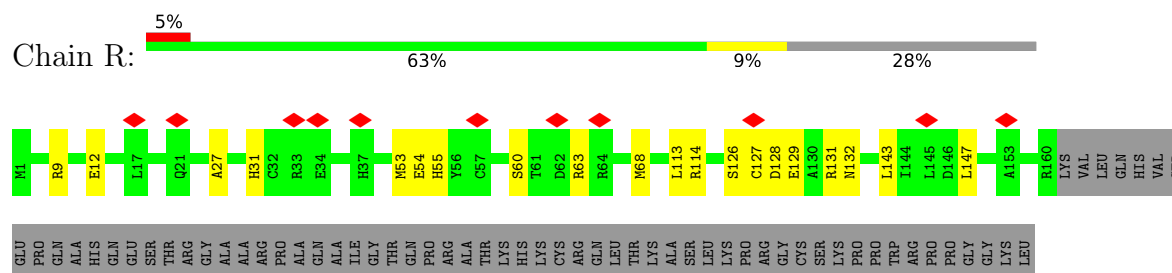
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• Molecule 1: Sperm acrosome-associated protein 9

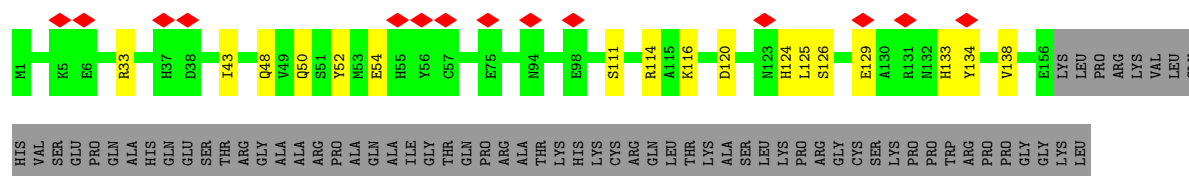


• Molecule 1: Sperm acrosome-associated protein 9

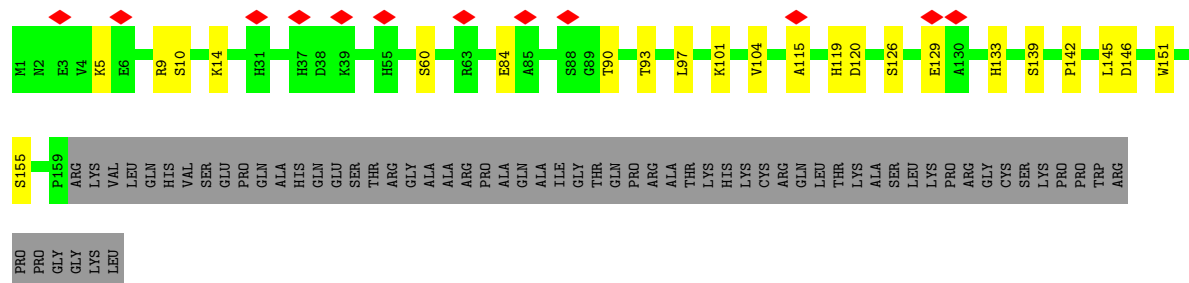


• Molecule 1: Sperm acrosome-associated protein 9

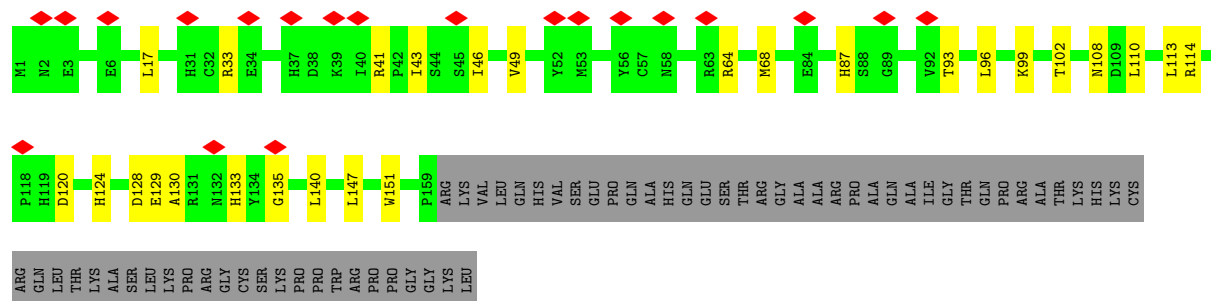




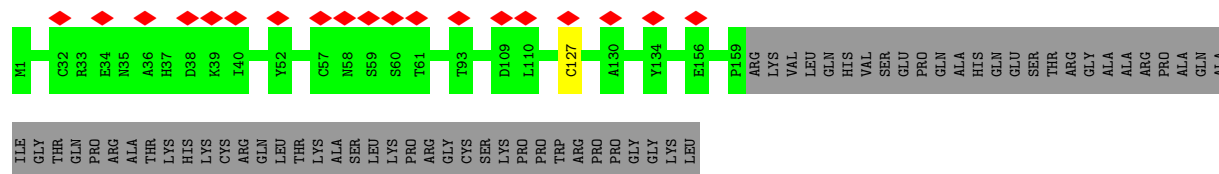
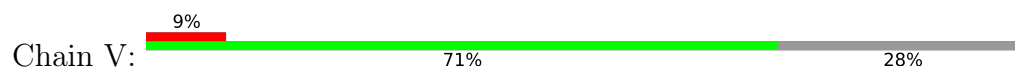
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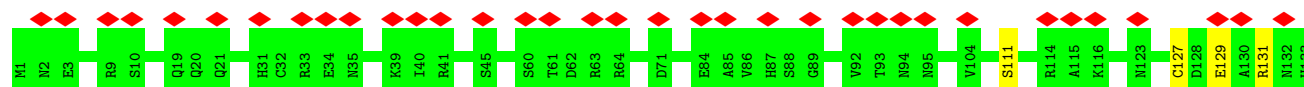
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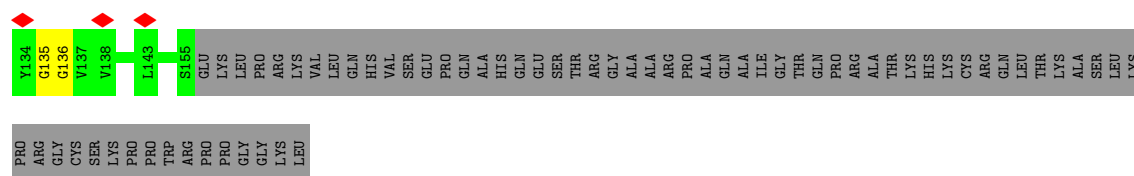


• Molecule 1: Sperm acrosome-associated protein 9

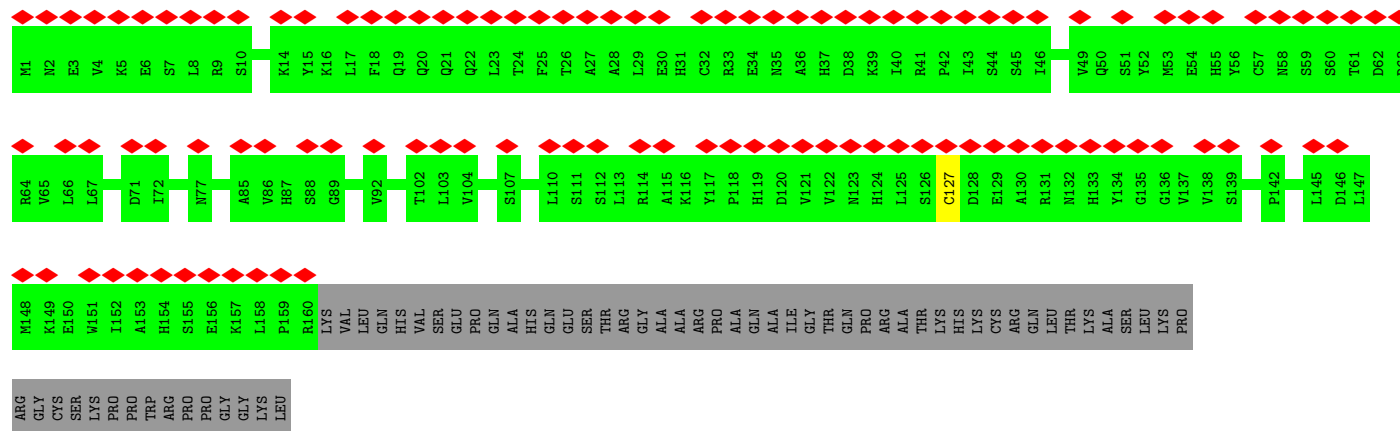


• Molecule 1: Sperm acrosome-associated protein 9

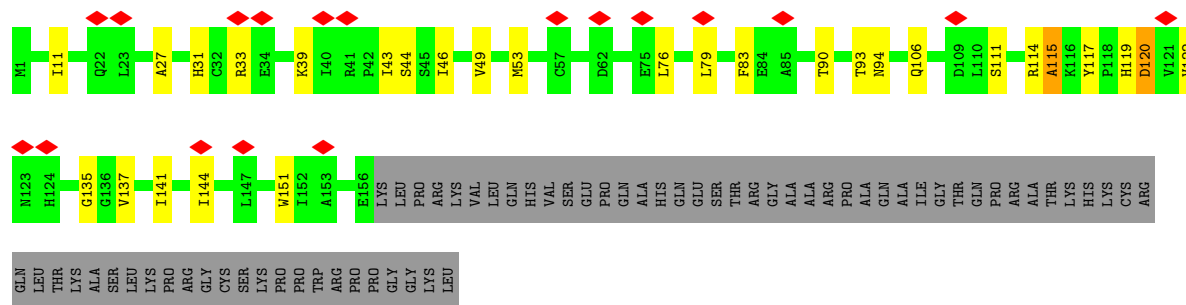




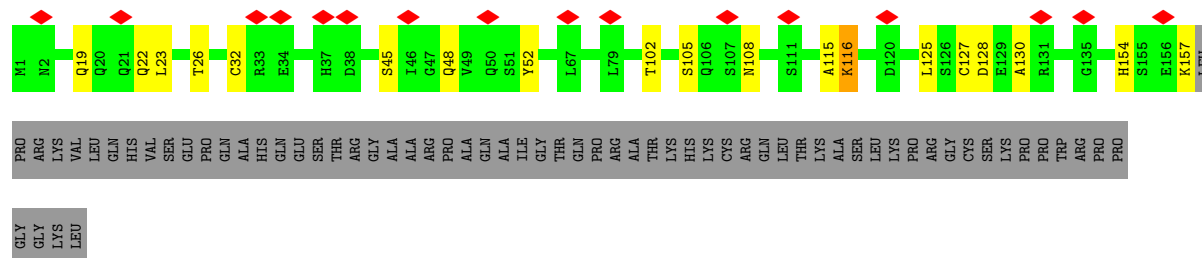
• Molecule 1: Sperm acrosome-associated protein 9



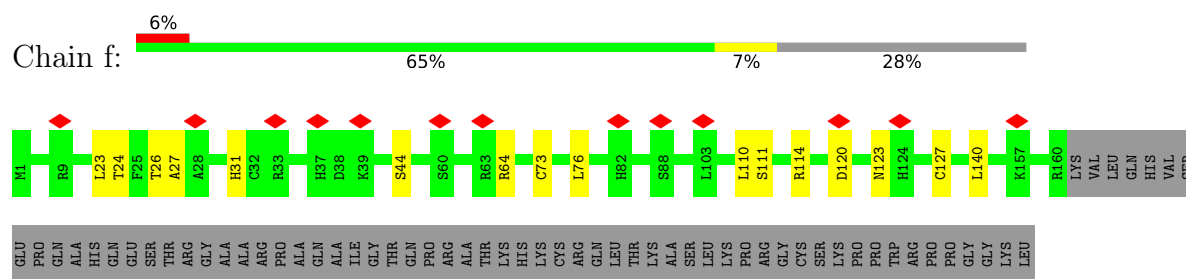
• Molecule 1: Sperm acrosome-associated protein 9



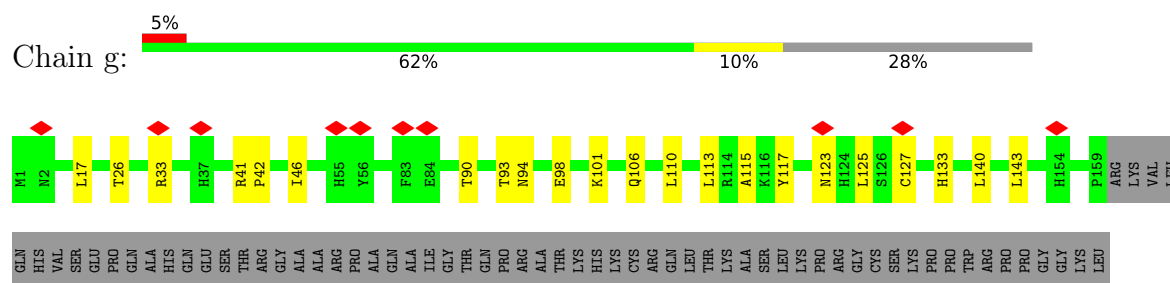
• Molecule 1: Sperm acrosome-associated protein 9



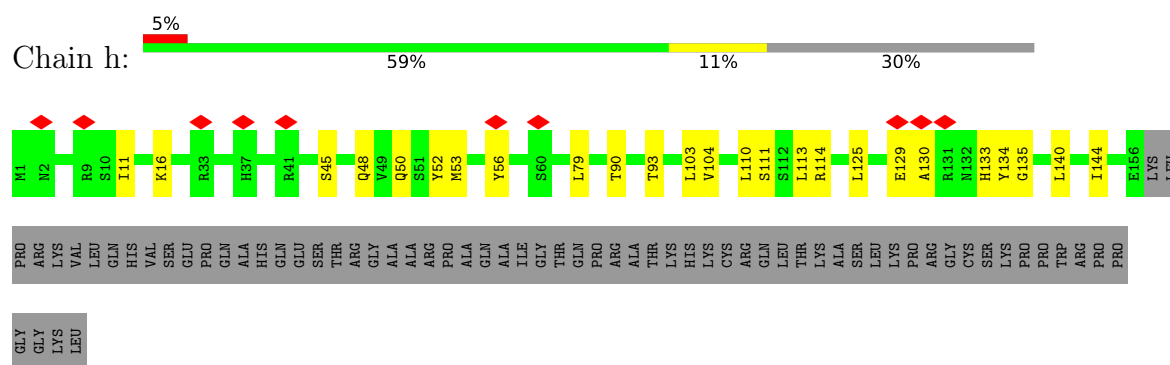
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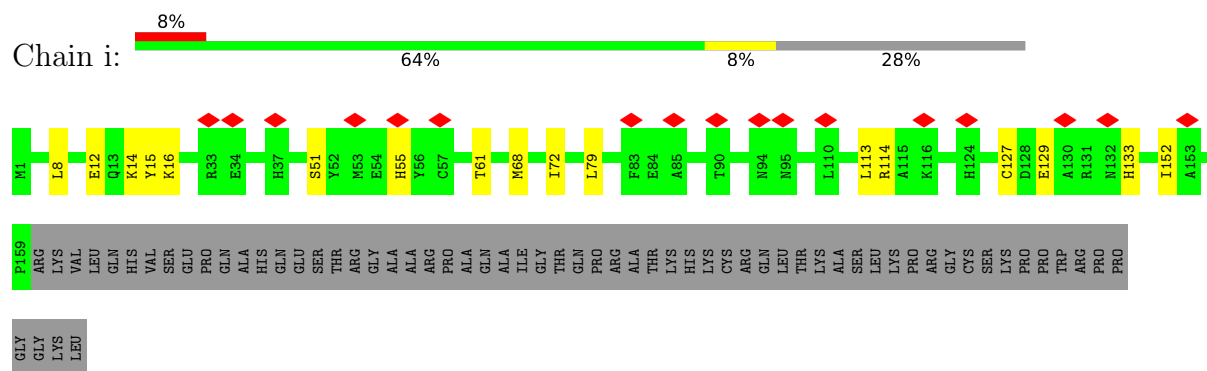
- Molecule 1: Sperm acrosome-associated protein 9



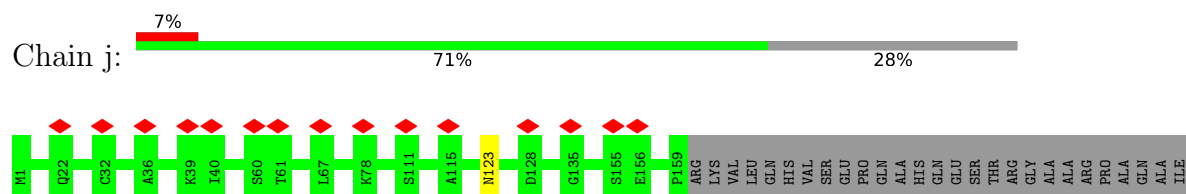
- Molecule 1: Sperm acrosome-associated protein 9



- Molecule 1: Sperm acrosome-associated protein 9



- Molecule 1: Sperm acrosome-associated protein 9



THR GLN PRO PRO ARG ALA THR LYS HIS LYS CYS ARG GLN LEU THR LYS ALA ALA SER SER LYS PRO ARG GLY CYS SER LYS PRO PRO TRP ARG PRO PRO GLY LYS LEU

• Molecule 1: Sperm acrosome-associated protein 9

Chain k: 

M1 S7 Q21 A27 E34 N35 A36 H37 D38 K39 I40 R41 P42 S45 Y56 C57 T61 D62 D71 H82 A85 G89 S111 R114 A115 P118 L125 S126 E129 A130 R131 N132 G135 S155 GLU LYS LEU PRO ARG LYS VAL LEU

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

• Molecule 1: Sperm acrosome-associated protein 9

Chain l: 

M1 N2 L8 I11 E12 Q13 K16 L17 F18 Q19 Q20 Q21 Q22 L23 T24 T25 T26 A27 A28 L29 E30 E31 H31 C32 R33 E34 N35 D38 K39 I40 R41 P42 I43 S44 V49 C57 N58 S59 S60 T61 D62 R63 R64 L67 N68 D71 I72 N77 A85 V86 H87

SS8 Q89 T90 P91 V92 T93 R94 L97 C100 L103 S107 L110 S111 S112 L113 R114 A115 K116 Y117 P118 H119 D120 V121 V122 N123 H124 L125 S126 C127 D128 E129 A130 R131 N132 H133 Y134 G135 V136 D146 E150 W151 I152 ALA HIS SER GLU LYS LEU PRO ARG LYS VAL

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

• Molecule 2: Tubulin beta-4B chain

Chain AB: 

M1 R2 E3 I4 V5 H6 L7 Q8 A9 G10 Q11 C12 G13 W21 Y36 H37 G38 R46 Y50 A54 K58 Y59 V60 F61 R62 L65 M73 R86 F90 V91 F92 A97 G98 N99 N100 K103 C127 D128 C129 L130 Q131 G132 F133 Q134 L135 T136 H137

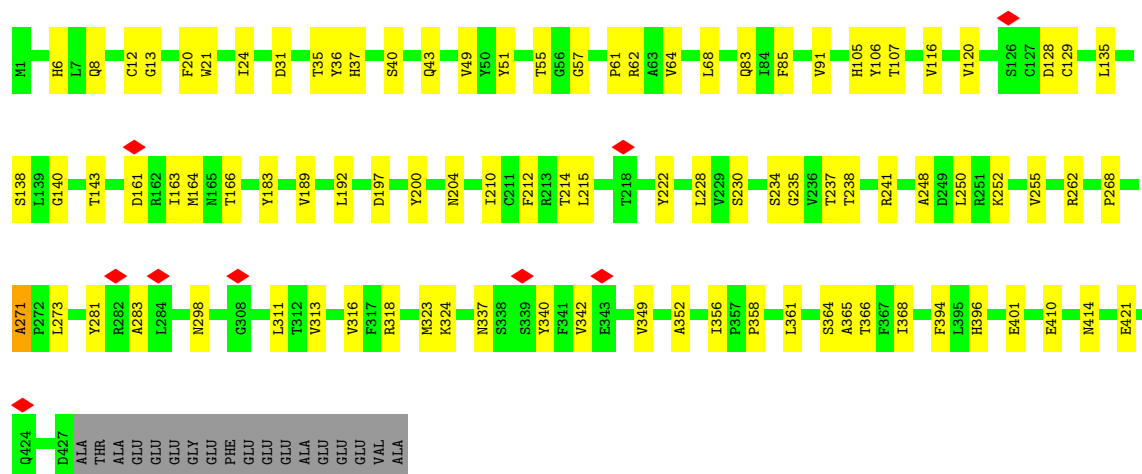
S138 L139 R156 R162 I163 T166 F167 S168 P171 T178 V179 V180 E181 N184 L187 H190 Q191 T199 Y200 Y203 N204 Y208 C211 L215 T218 M233 S234 G235 T238 R241 N247 L250 R251 K252 L253 A254 V255 N256 R262

P265 F266 M267 P268 A271 P272 S278 R282 A283 L284 W293 A301 G308 R309 A314 R318 E325 V326 D327 E328 L331 N337 Y340 E343 W344 I345 C354 D355 P358 S364 F367 I368 T372 S382 D404 E405 M406 T409

R414 M415 M416 D417 Q426 D427 ALA THR ALA GLU GLU GLY GLU PHE GLU GLU ALA ALA GLU VAL ALA

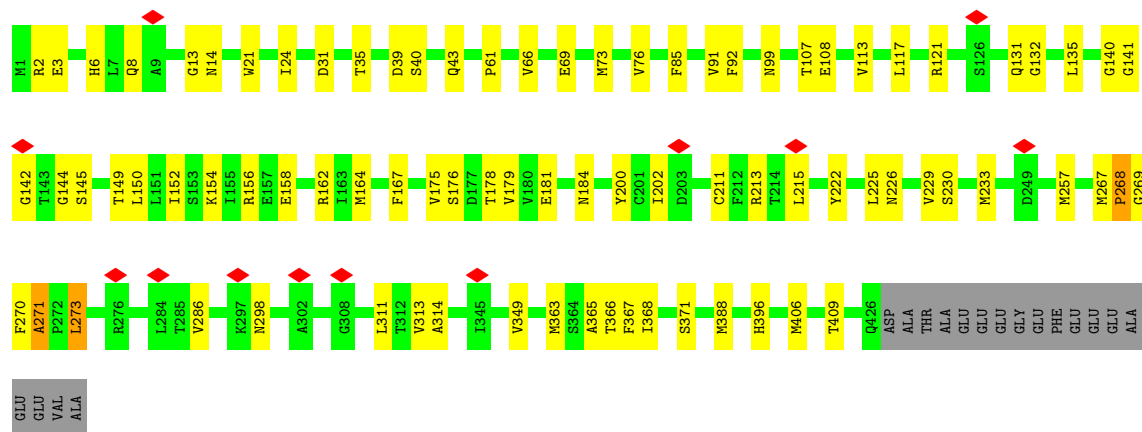
• Molecule 2: Tubulin beta-4B chain

Chain AD: 



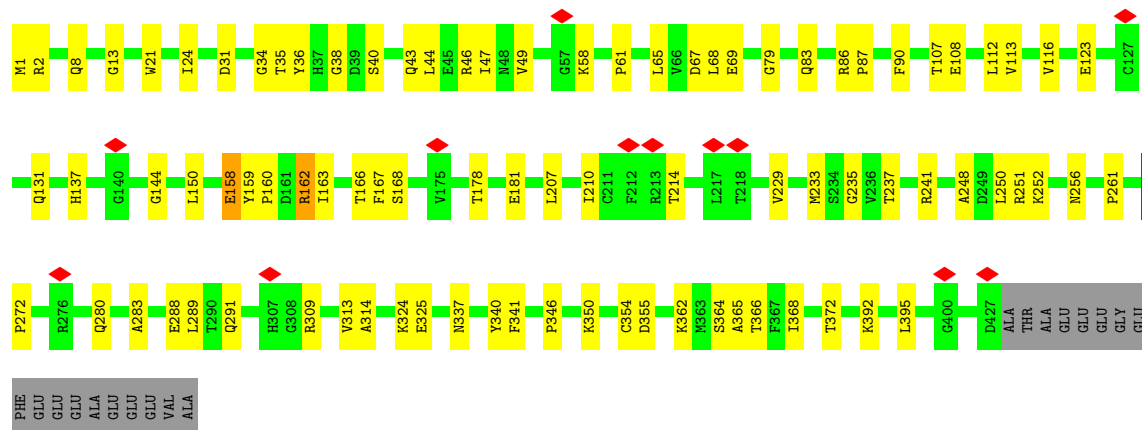
- Molecule 2: Tubulin beta-4B chain

Chain AF: 77% 18%



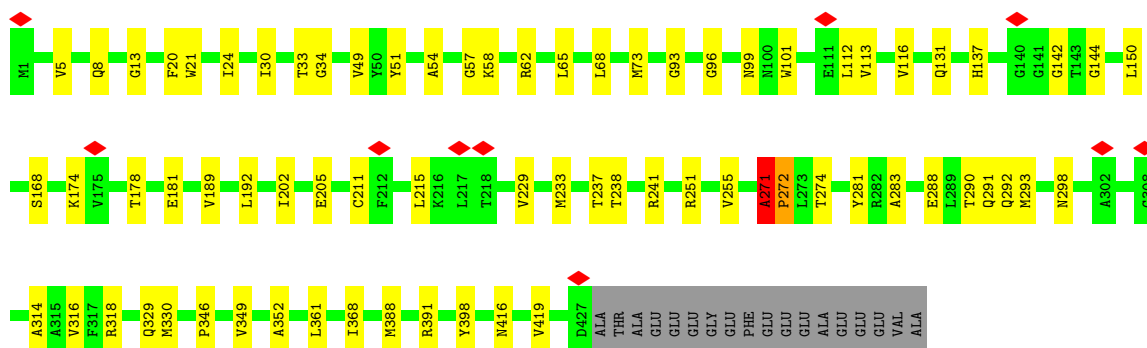
- Molecule 2: Tubulin beta-4B chain

Chain BA: 76% 19%



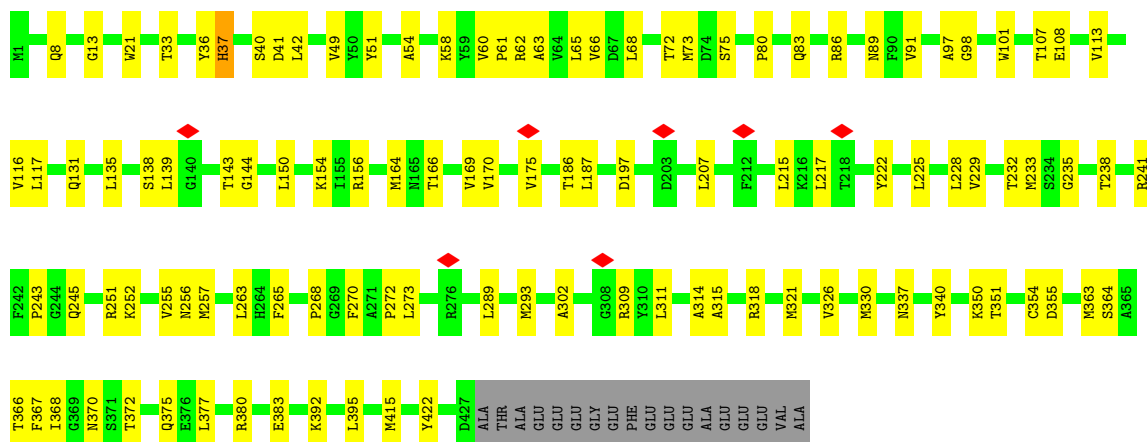
- Molecule 2: Tubulin beta-4B chain

Chain BD:  80% 16%



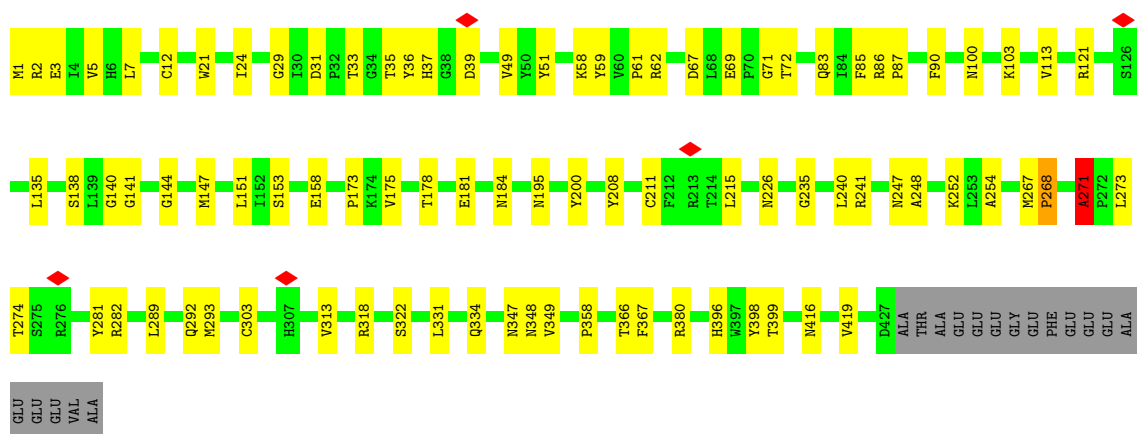
• Molecule 2: Tubulin beta-4B chain

Chain BF:  71% 24%



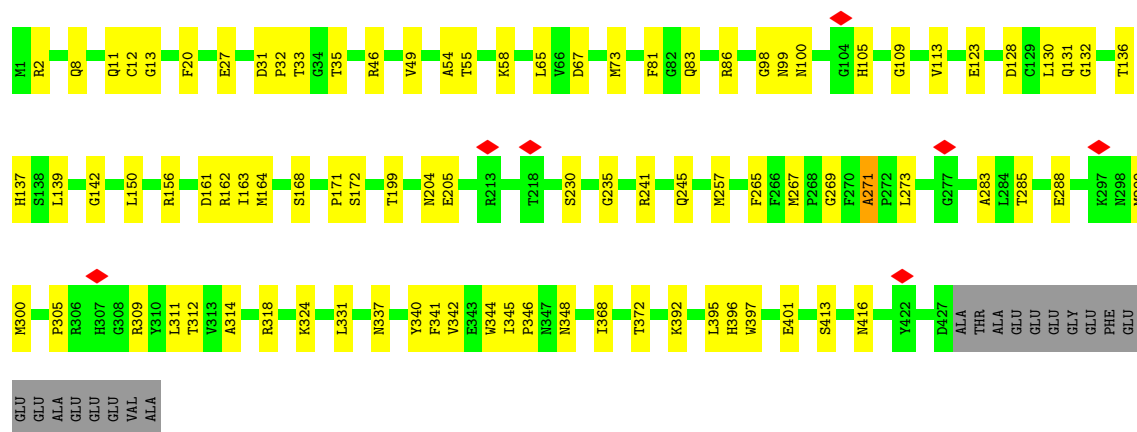
• Molecule 2: Tubulin beta-4B chain

Chain CB:  76% 20%

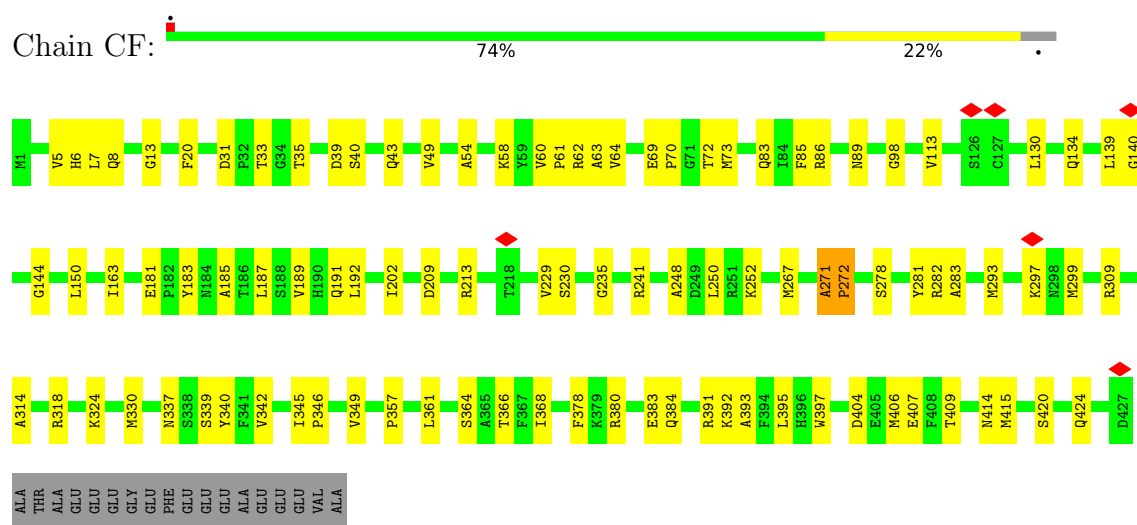


• Molecule 2: Tubulin beta-4B chain

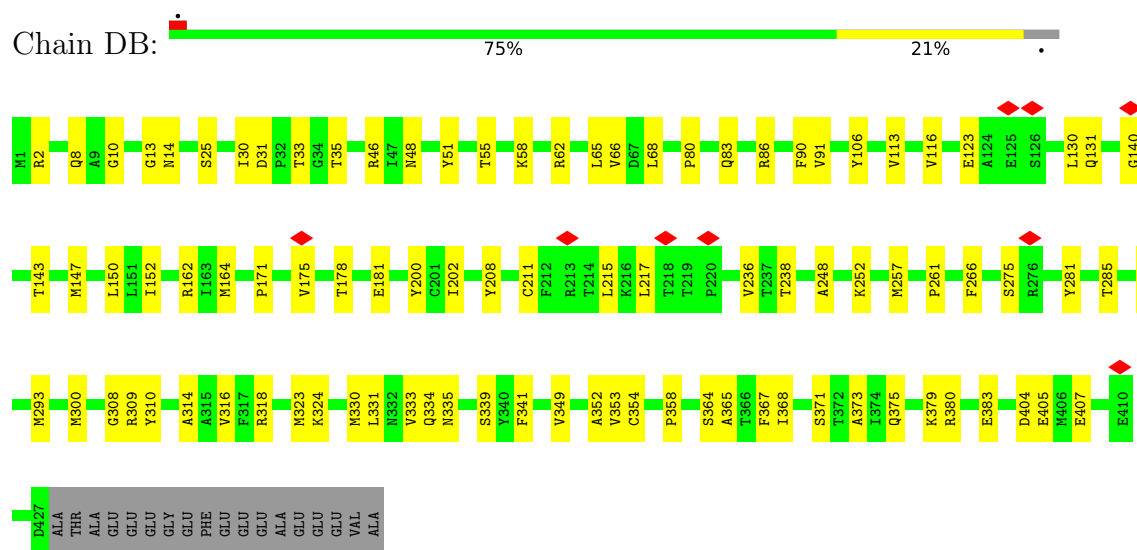
Chain CD:  76% 20%



• Molecule 2: Tubulin beta-4B chain

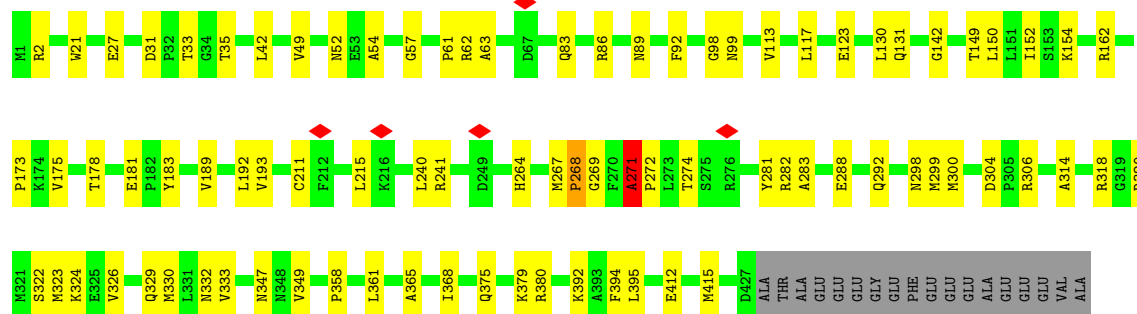


• Molecule 2: Tubulin beta-4B chain



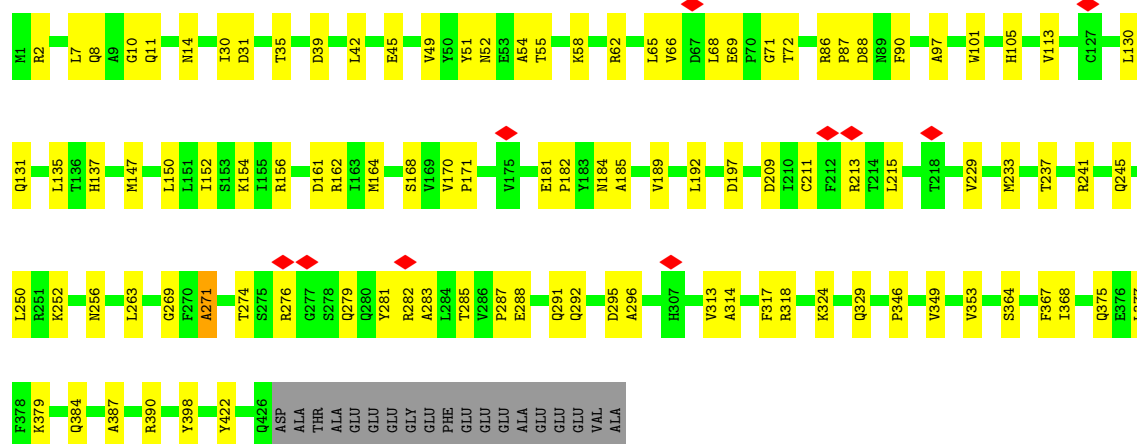
• Molecule 2: Tubulin beta-4B chain

Chain DD:  77% 19% .



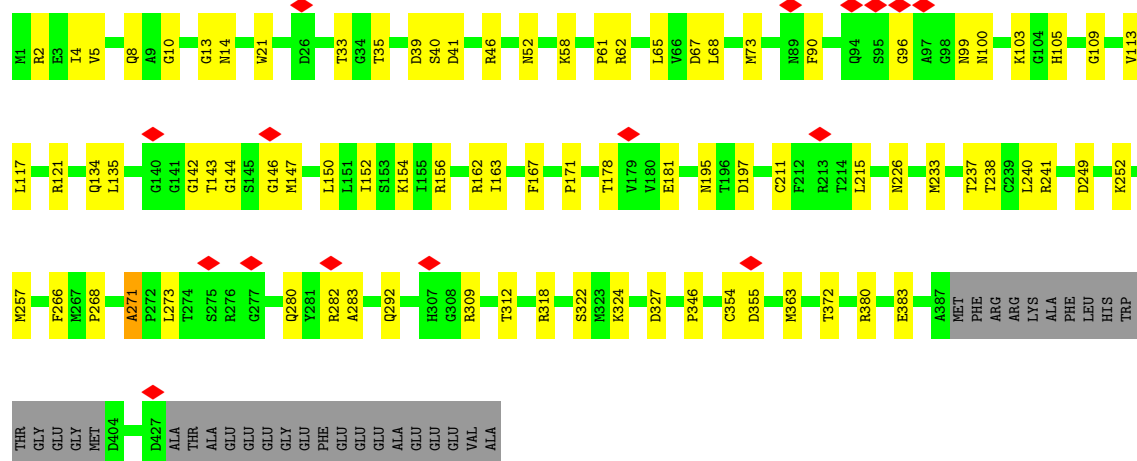
• Molecule 2: Tubulin beta-4B chain

Chain DF:  73% 23% .

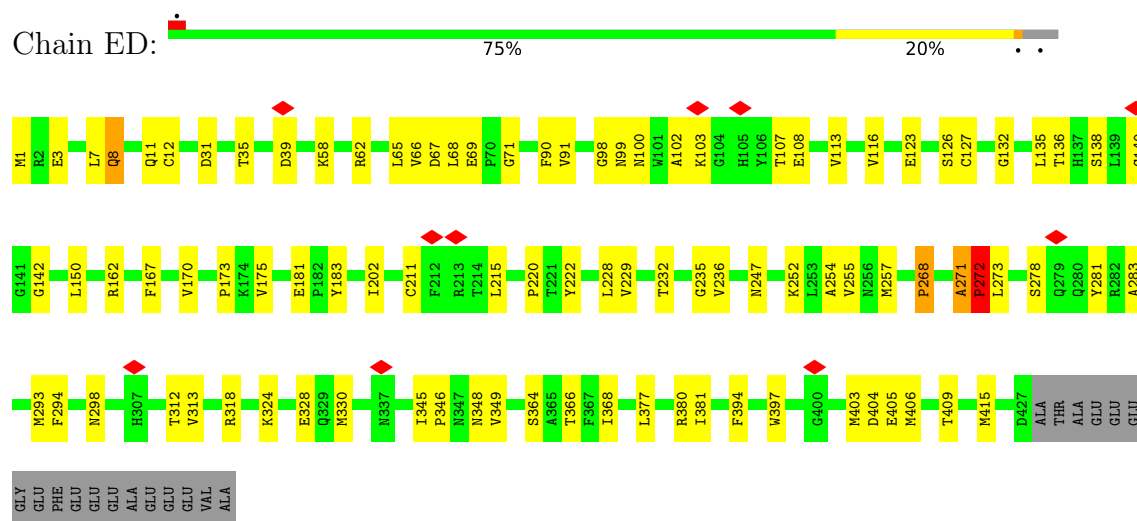


• Molecule 2: Tubulin beta-4B chain

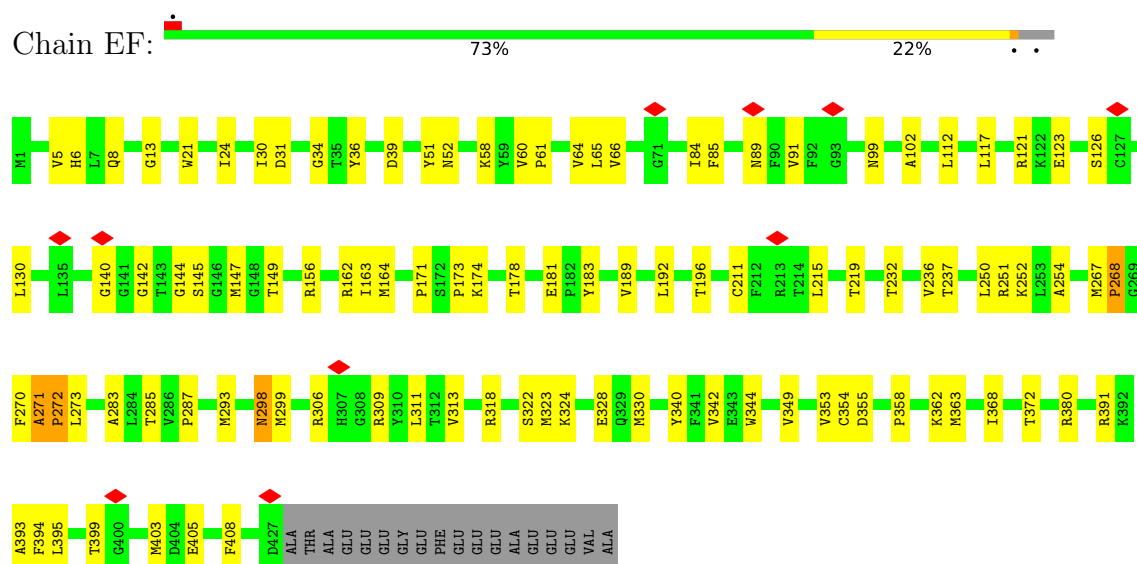
Chain EB:  74% 18% 8% .



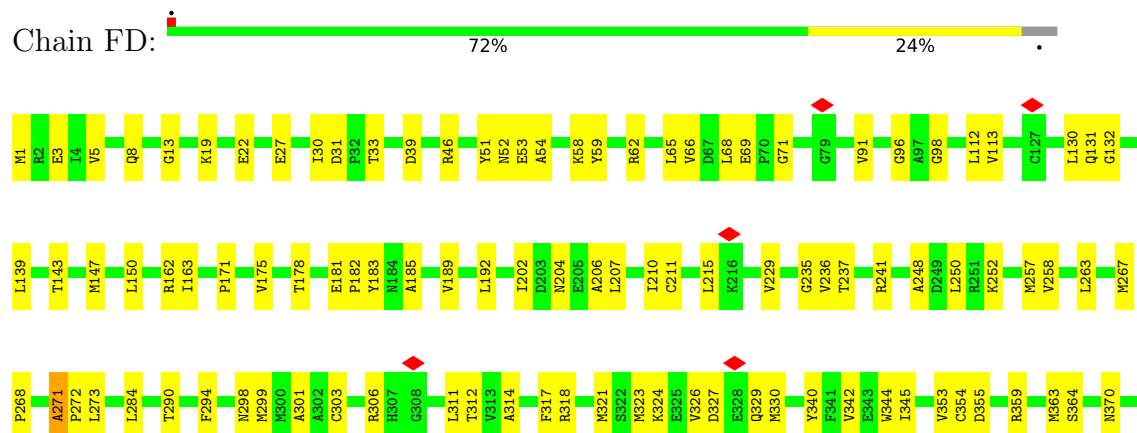
• Molecule 2: Tubulin beta-4B chain



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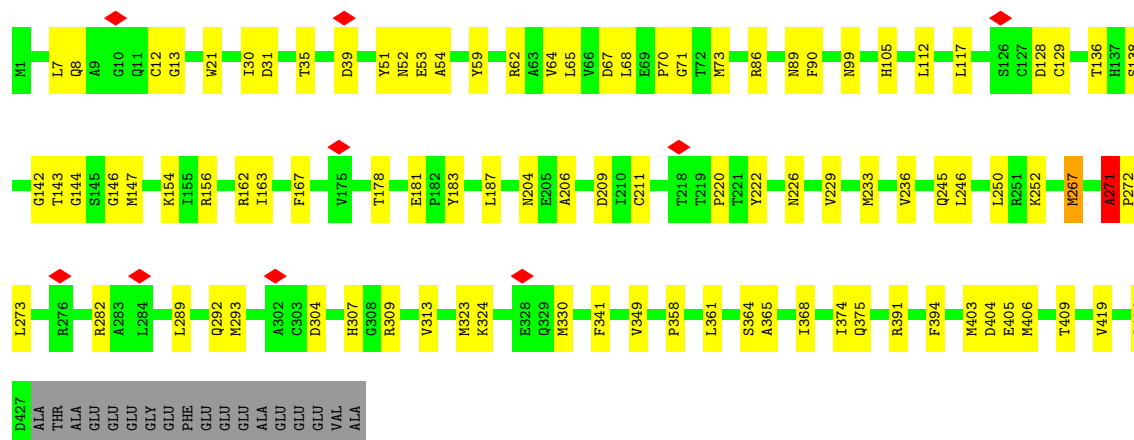
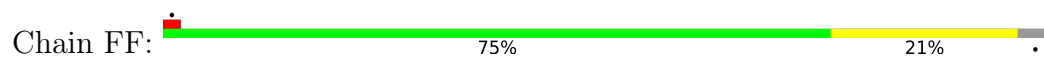


• Molecule 2: Tubulin beta-4B chain

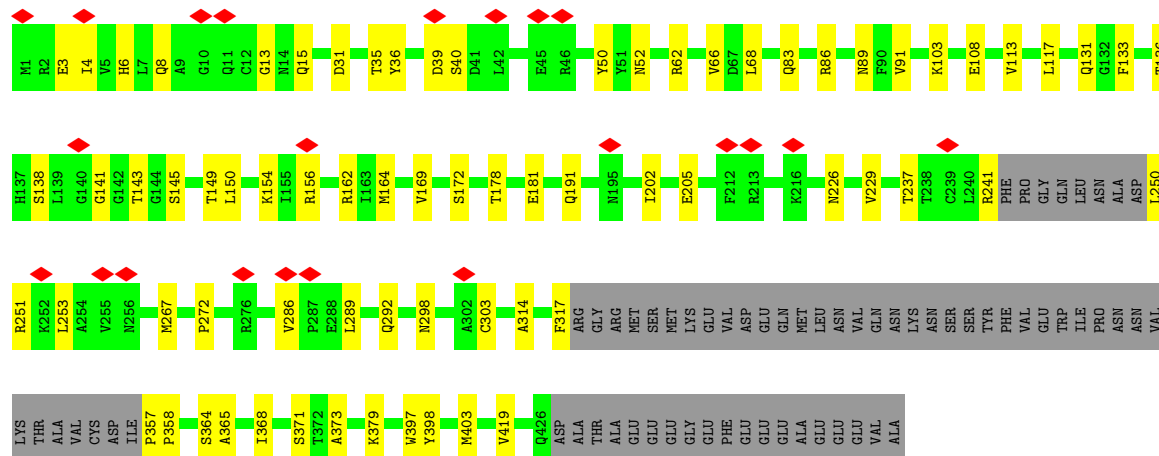




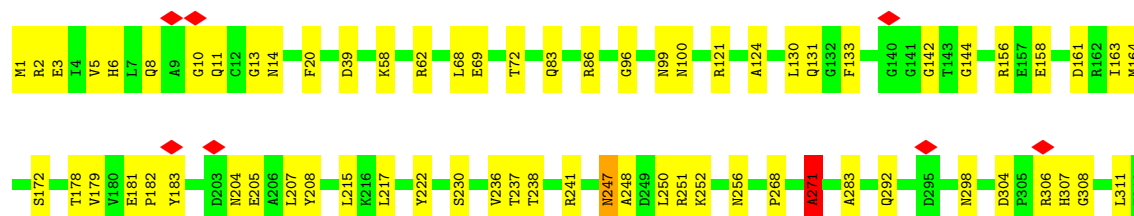
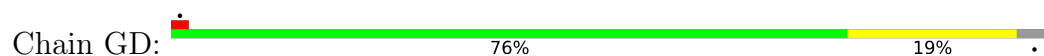
• Molecule 2: Tubulin beta-4B chain



• Molecule 2: Tubulin beta-4B chain

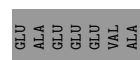
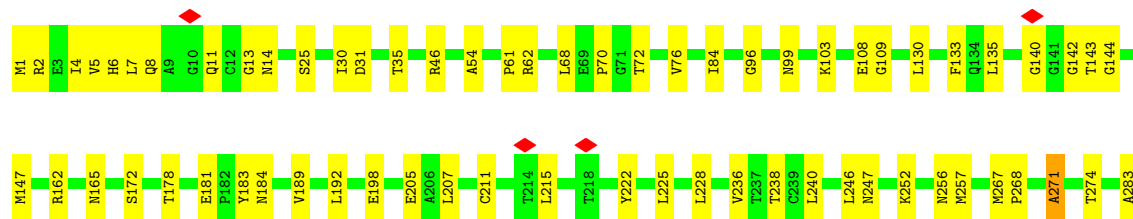
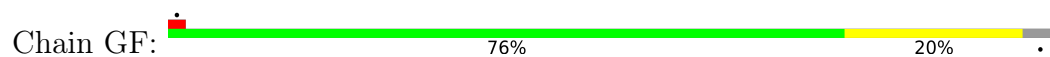


• Molecule 2: Tubulin beta-4B chain

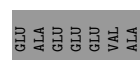
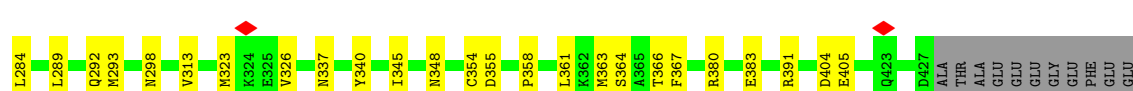
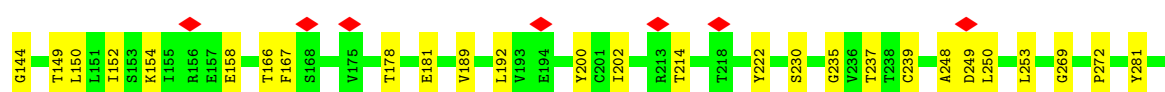
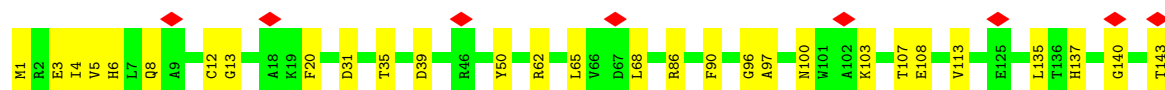
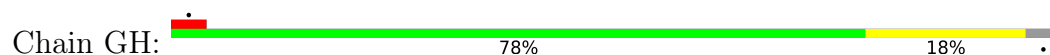




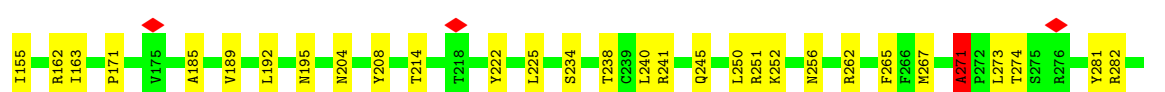
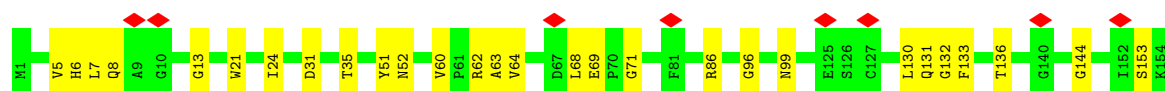
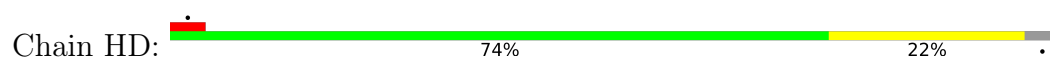
• Molecule 2: Tubulin beta-4B chain

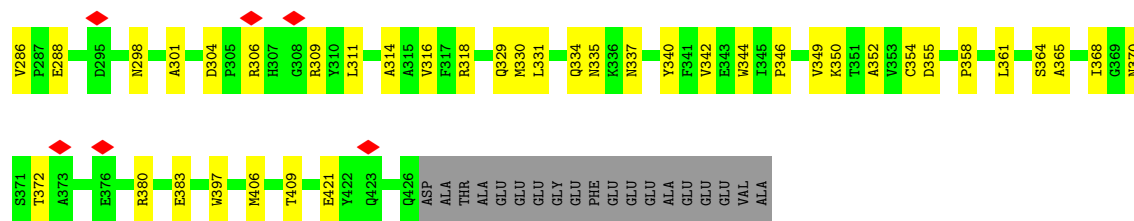


• Molecule 2: Tubulin beta-4B chain

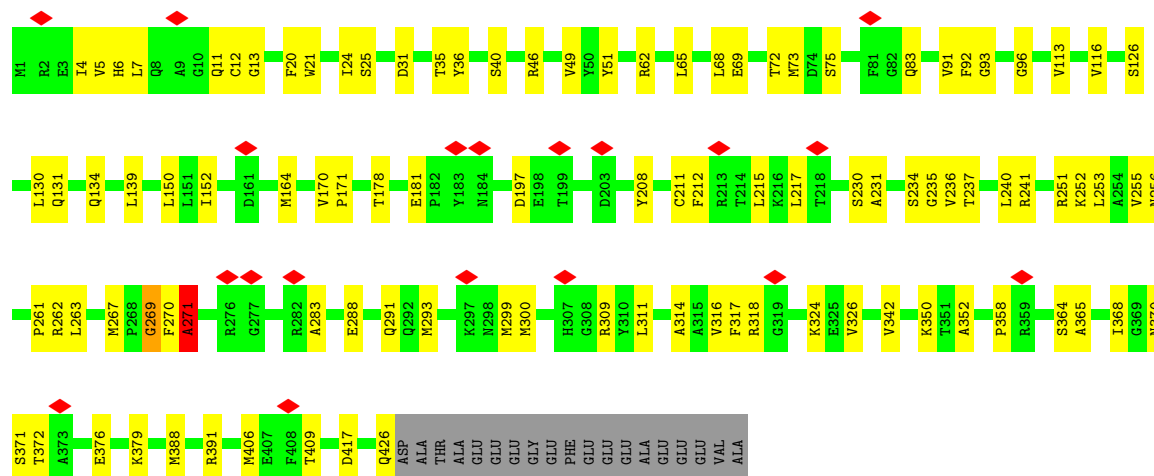
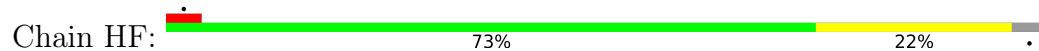


• Molecule 2: Tubulin beta-4B chain

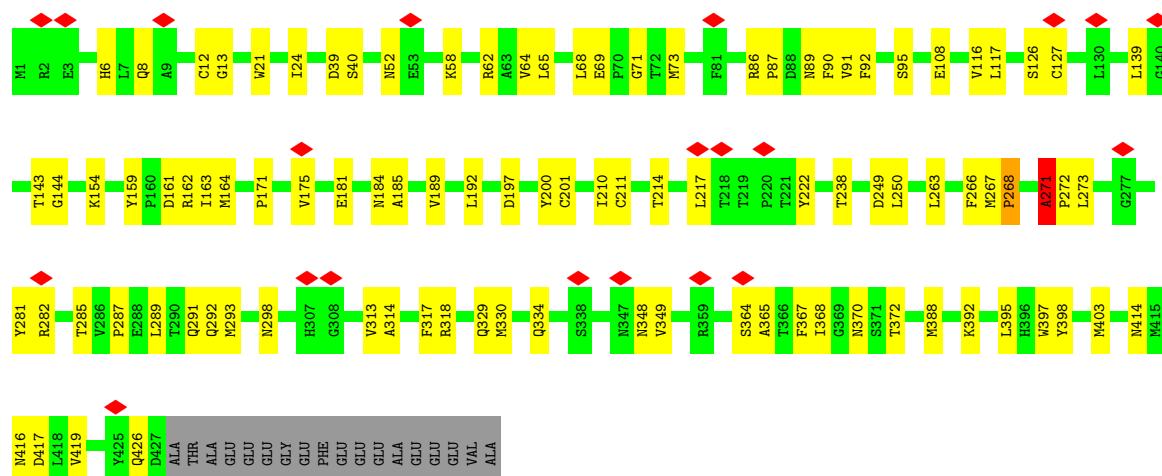
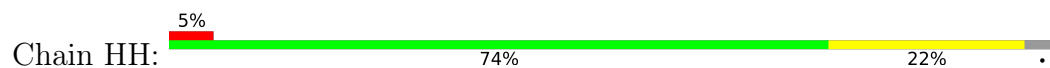




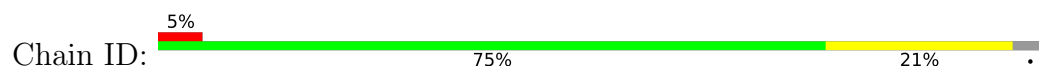
• Molecule 2: Tubulin beta-4B chain

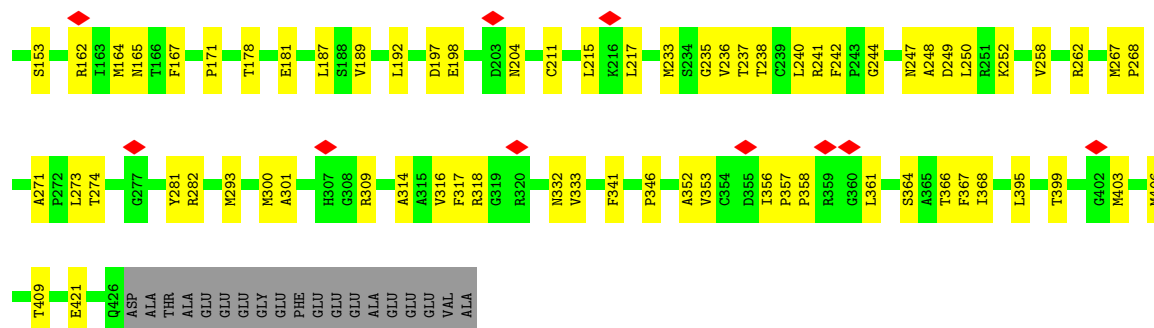


• Molecule 2: Tubulin beta-4B chain



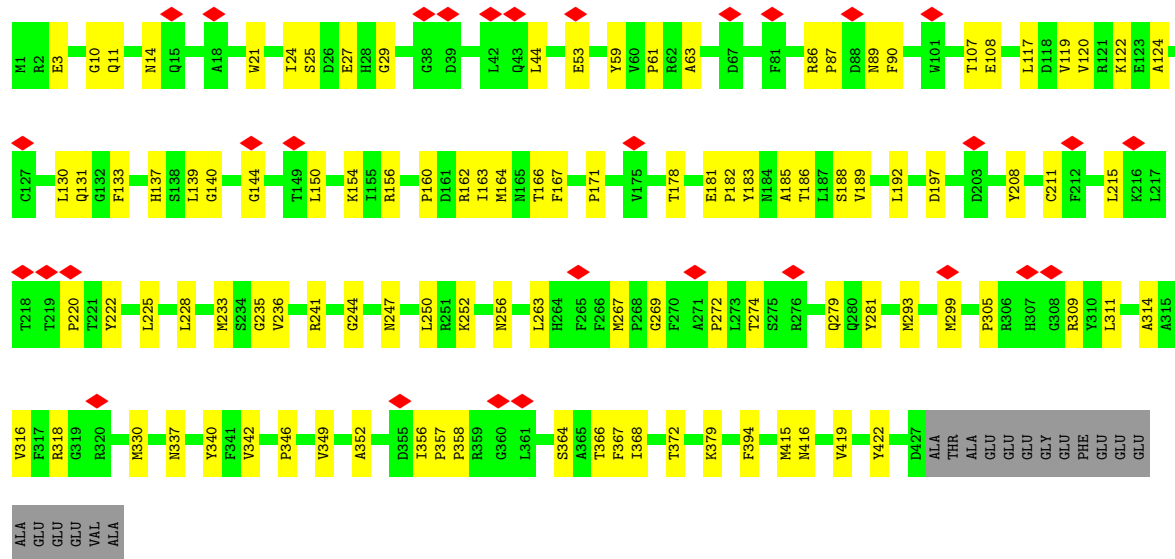
• Molecule 2: Tubulin beta-4B chain





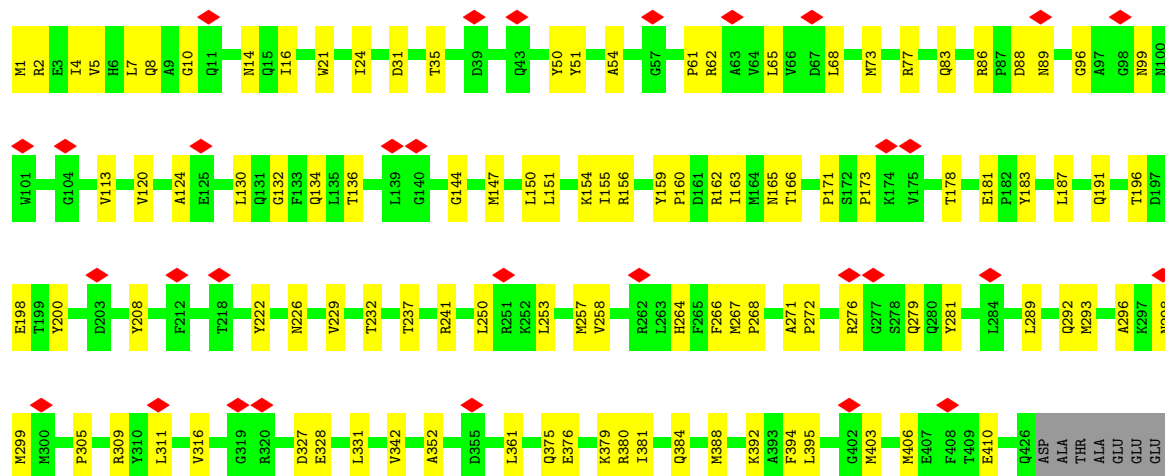
• Molecule 2: Tubulin beta-4B chain

Chain IF: 7% 73% 23%



• Molecule 2: Tubulin beta-4B chain

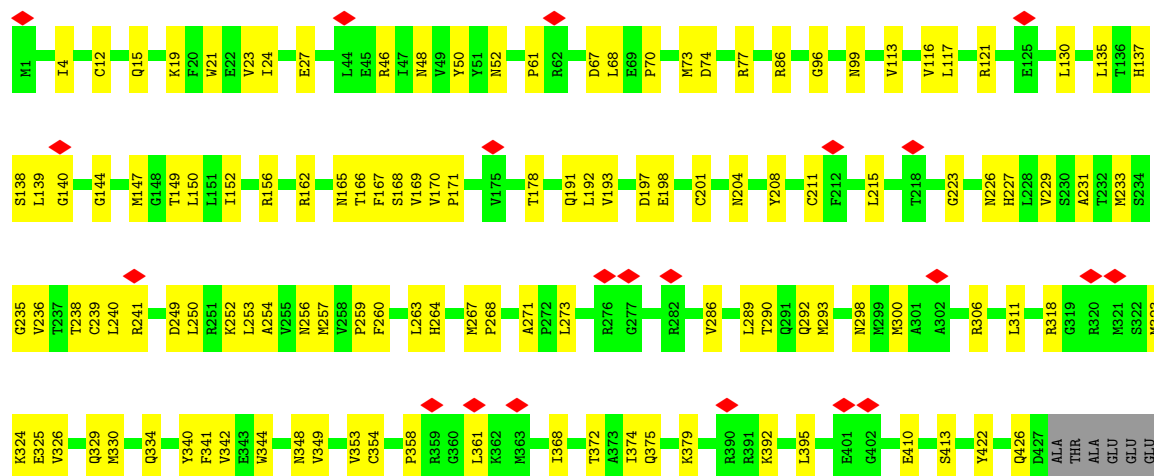
Chain IH: 7% 72% 24%



GLY
GLU
PHE
GLU
GLU
GLU
ALA
GLU
GLU
VAL
ALA

• Molecule 2: Tubulin beta-4B chain

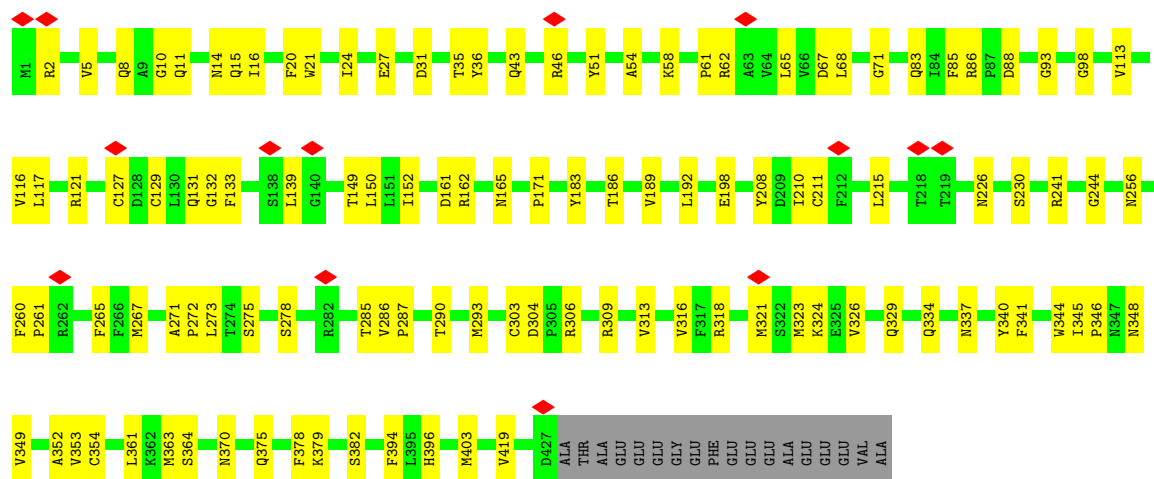
Chain JD:  5% 69% 27%



GLY
GLU
PHE
GLU
GLU
GLU
ALA
GLU
GLU
VAL
ALA

• Molecule 2: Tubulin beta-4B chain

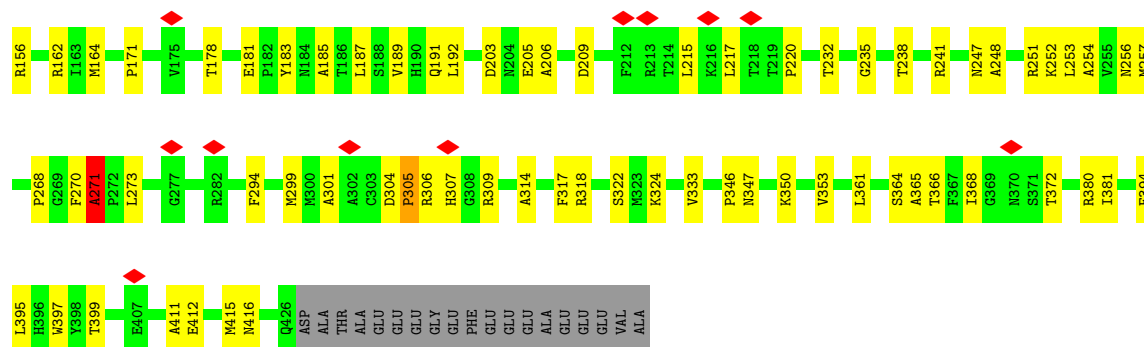
Chain JF:  71% 25%



• Molecule 2: Tubulin beta-4B chain

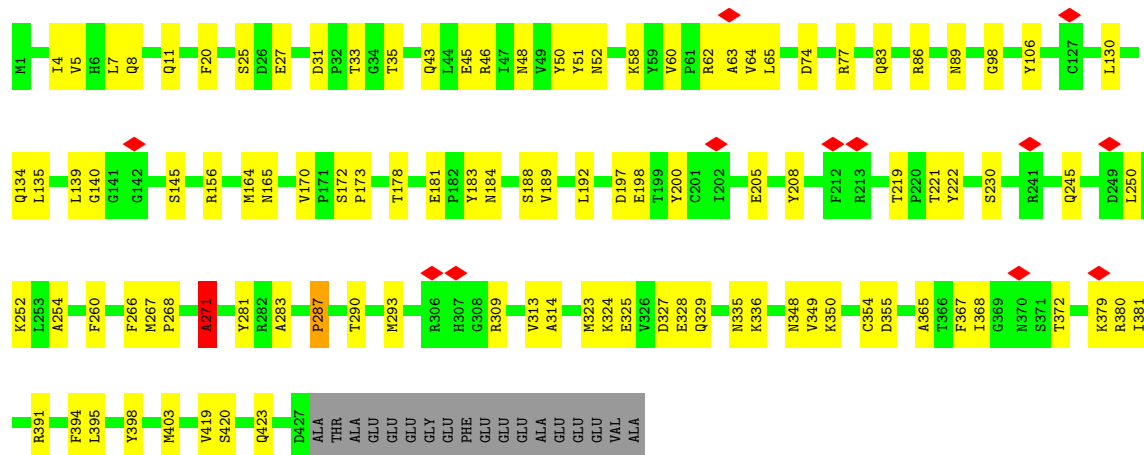
Chain KD:  73% 22%





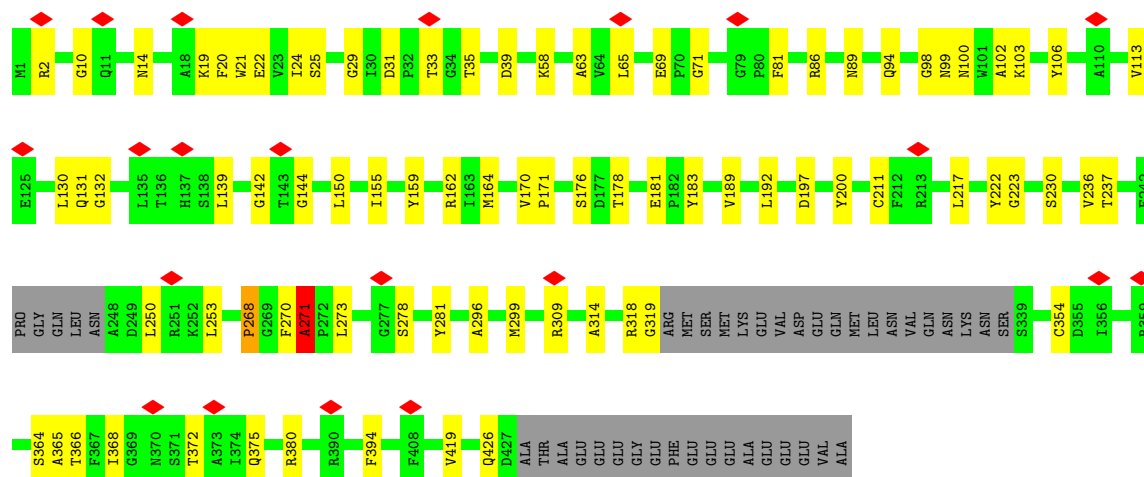
• Molecule 2: Tubulin beta-4B chain

Chain KF: 73% 23% .



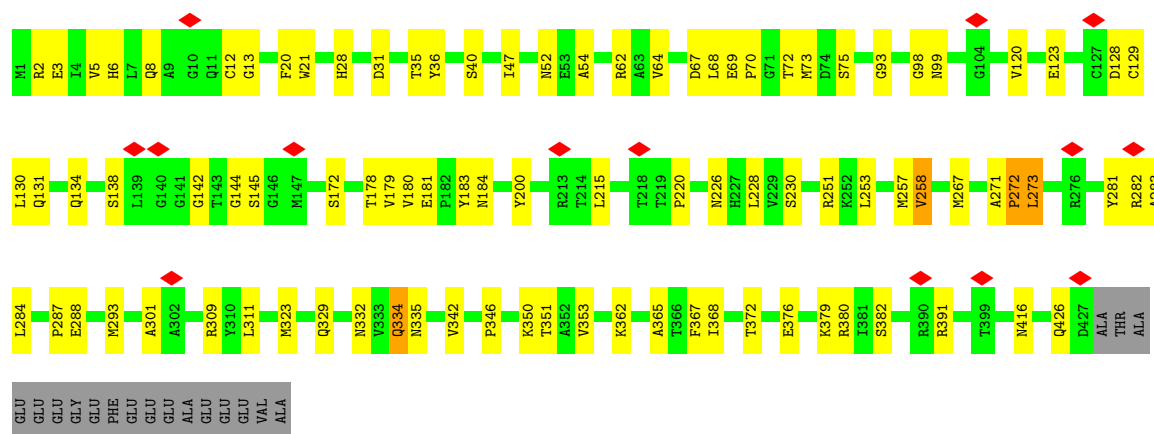
• Molecule 2: Tubulin beta-4B chain

Chain KH: 5% 72% 18% 9%

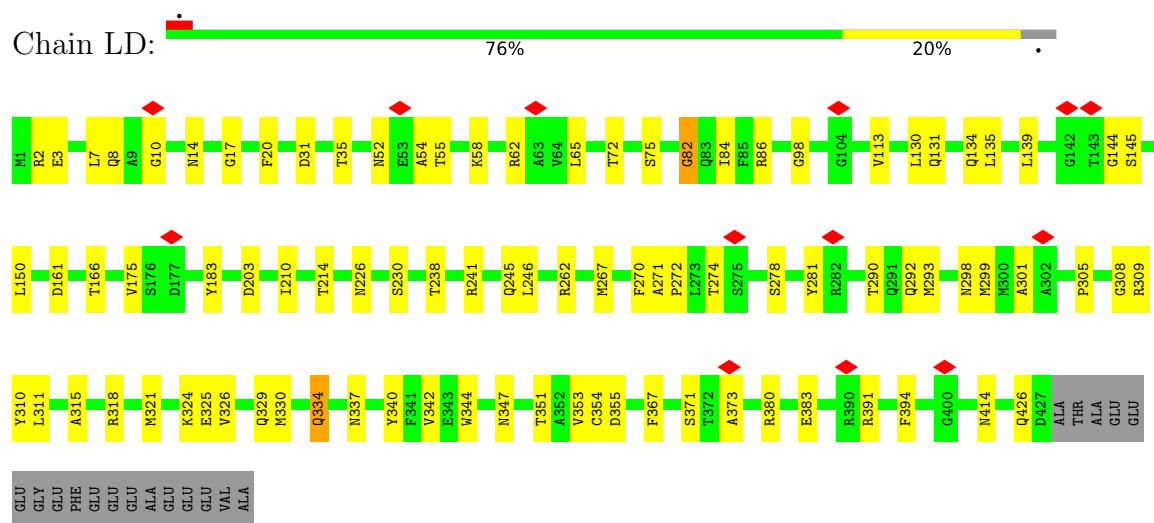


• Molecule 2: Tubulin beta-4B chain

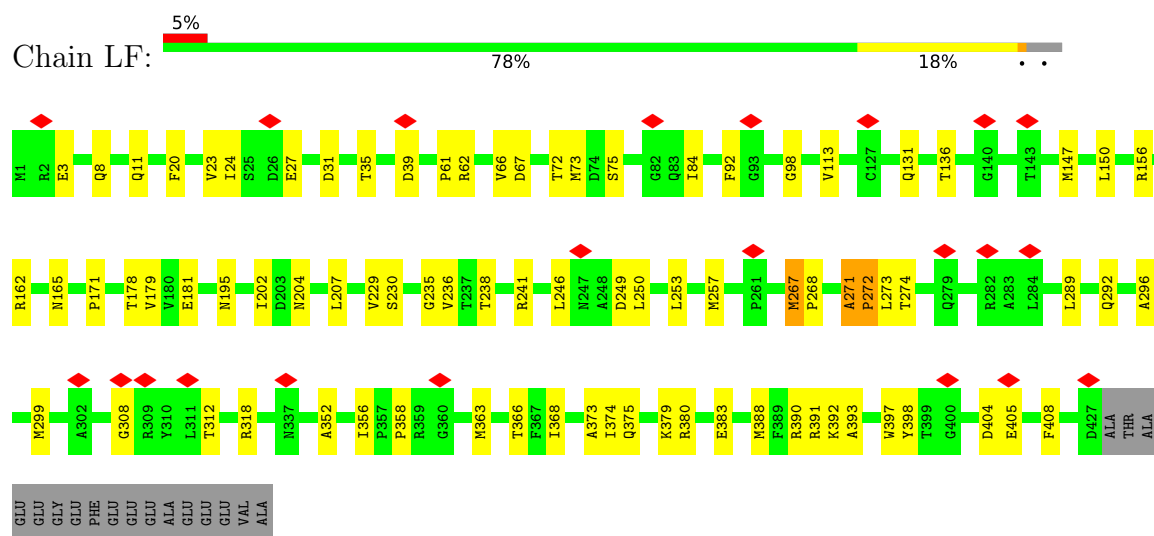
Chain LB: 75% 20% . .



• Molecule 2: Tubulin beta-4B chain

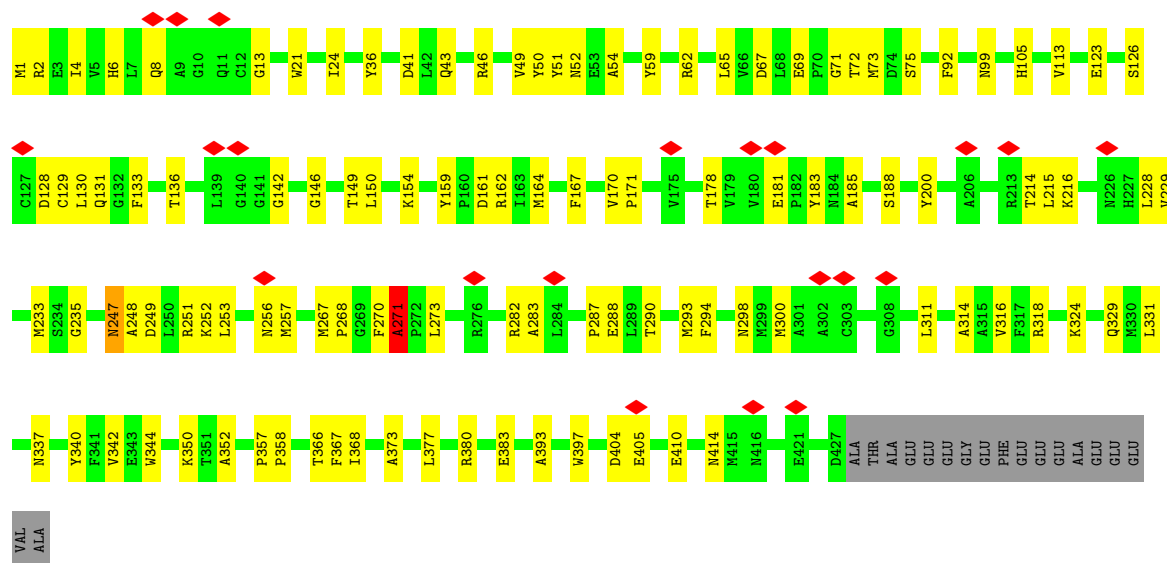


• Molecule 2: Tubulin beta-4B chain



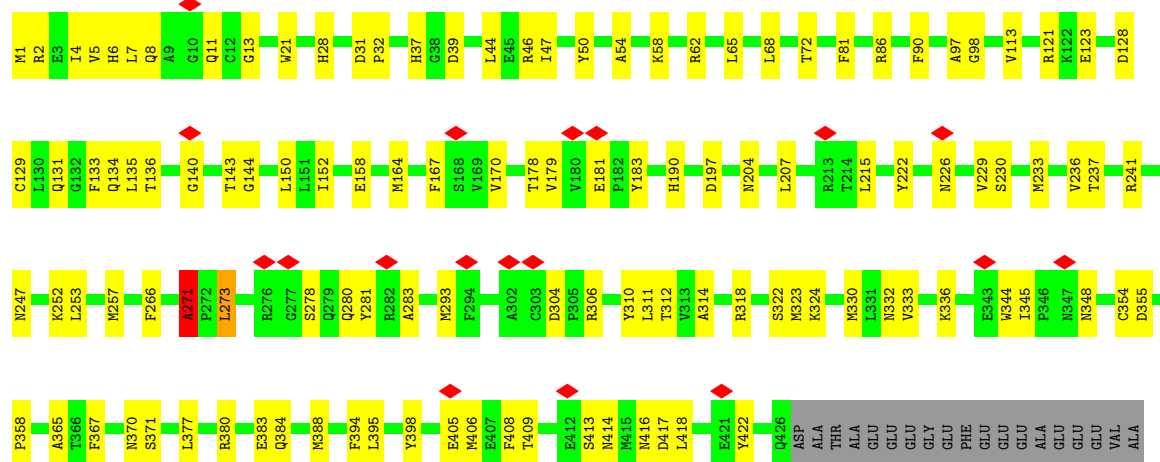
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Chain MB: 



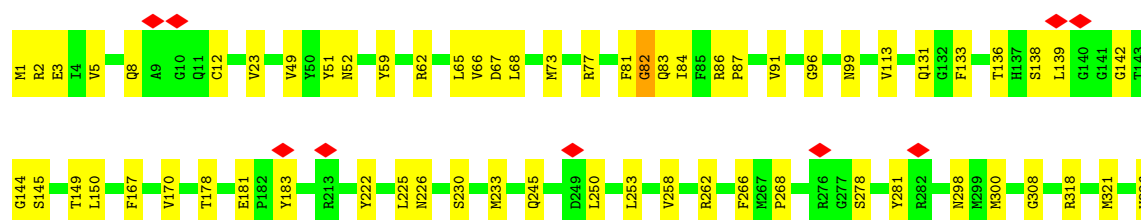
• Molecule 2: Tubulin beta-4B chain

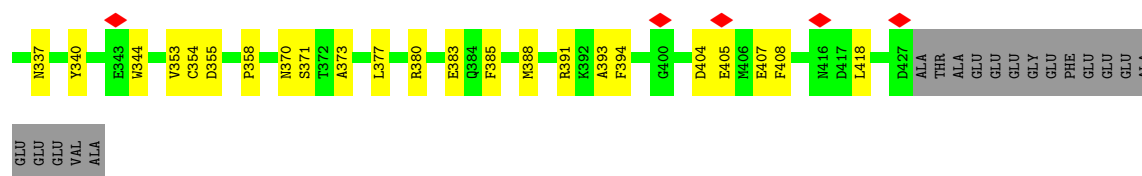
Chain MD: 



• Molecule 2: Tubulin beta-4B chain

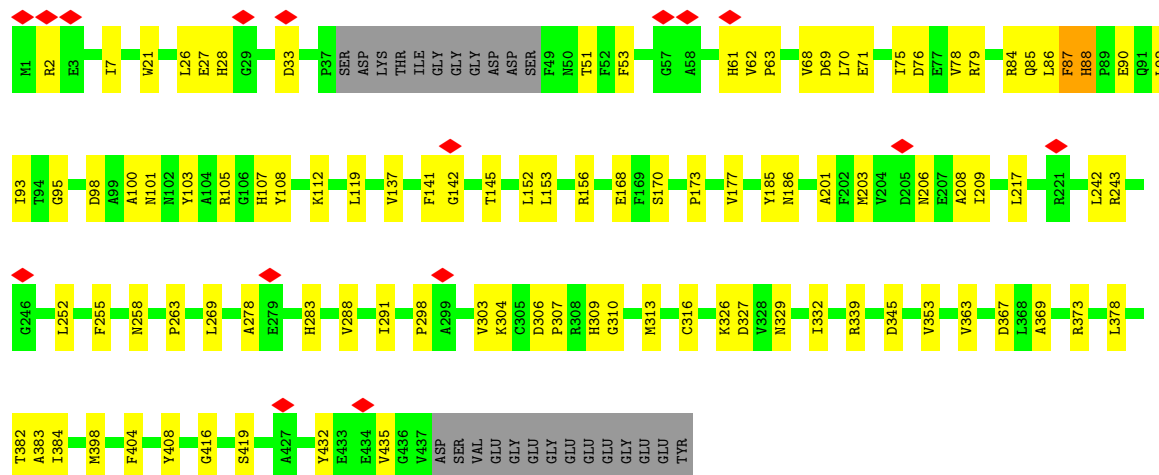
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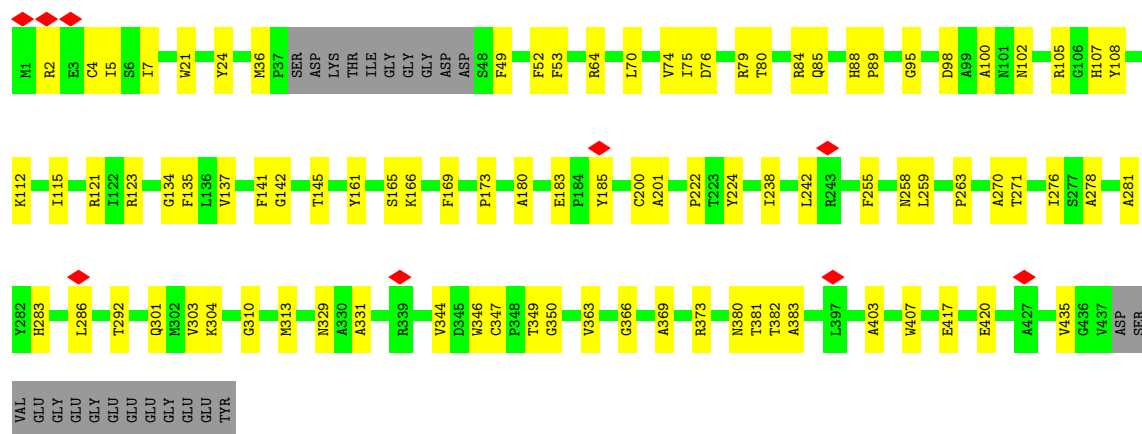
• Molecule 3: Tubulin alpha-1A chain

Chain AC: 73% 22% 6%



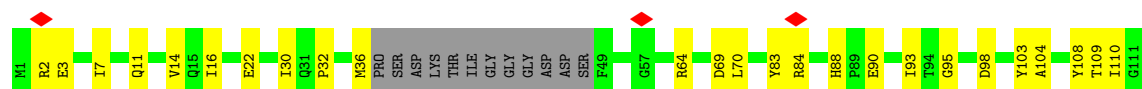
• Molecule 3: Tubulin alpha-1A chain

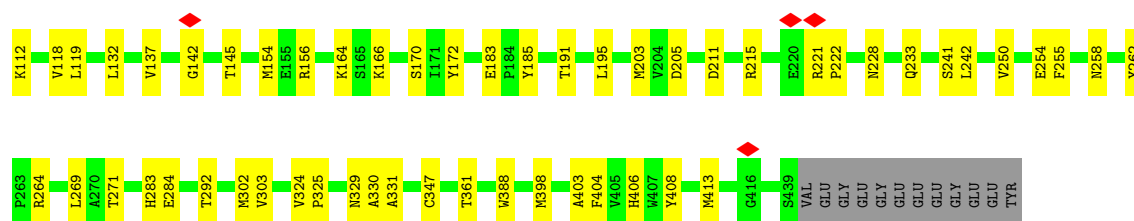
Chain AE: 75% 20% 5%



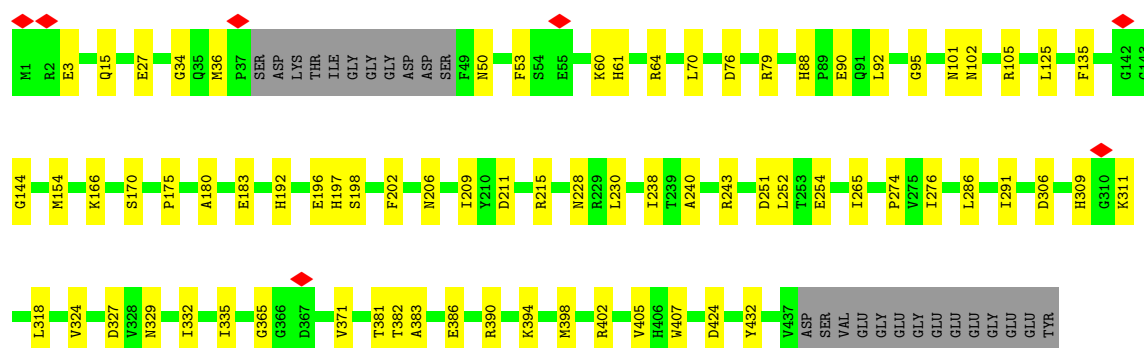
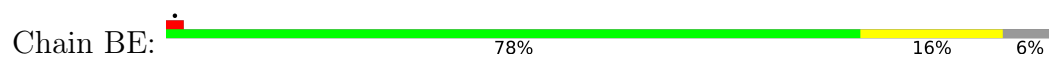
• Molecule 3: Tubulin alpha-1A chain

Chain BC: 77% 18% 5%

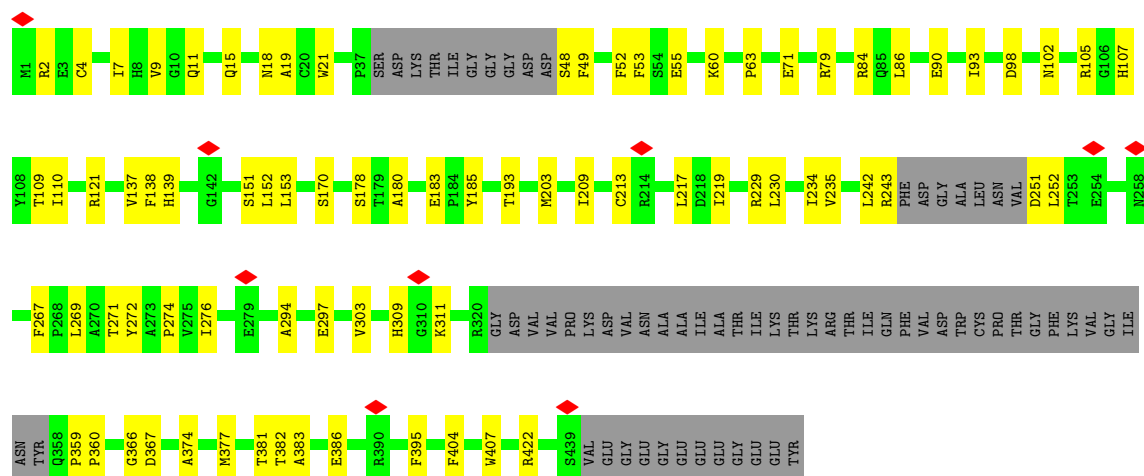




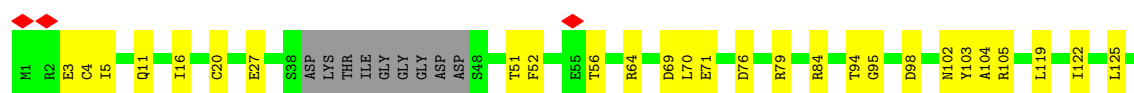
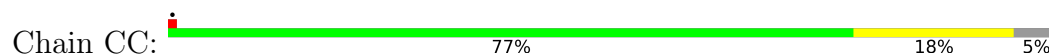
• Molecule 3: Tubulin alpha-1A chain



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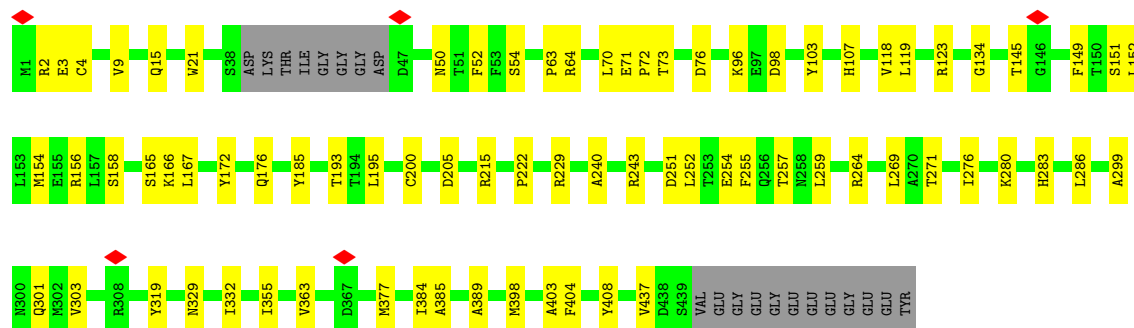
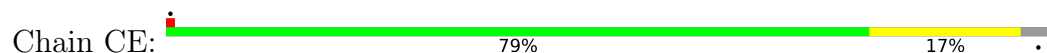


• Molecule 3: Tubulin alpha-1A chain

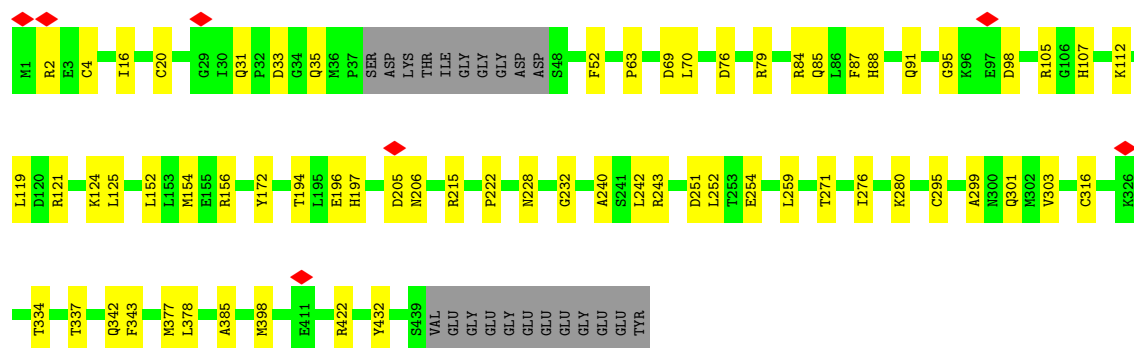
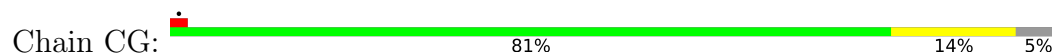




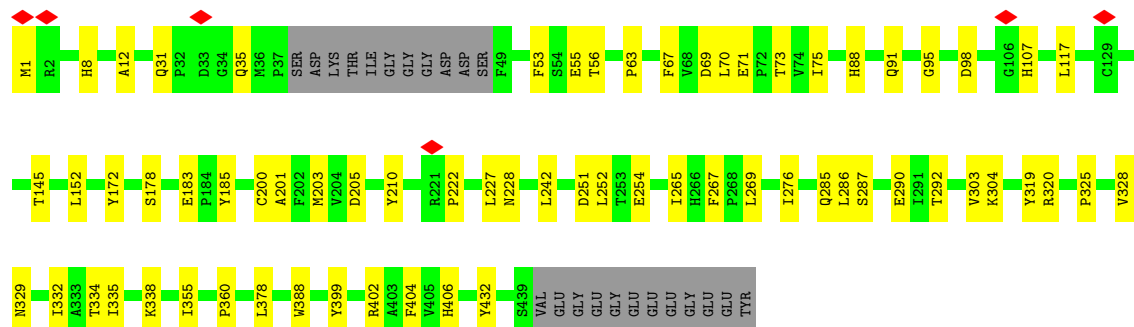
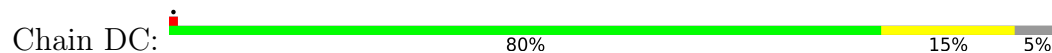
• Molecule 3: Tubulin alpha-1A chain



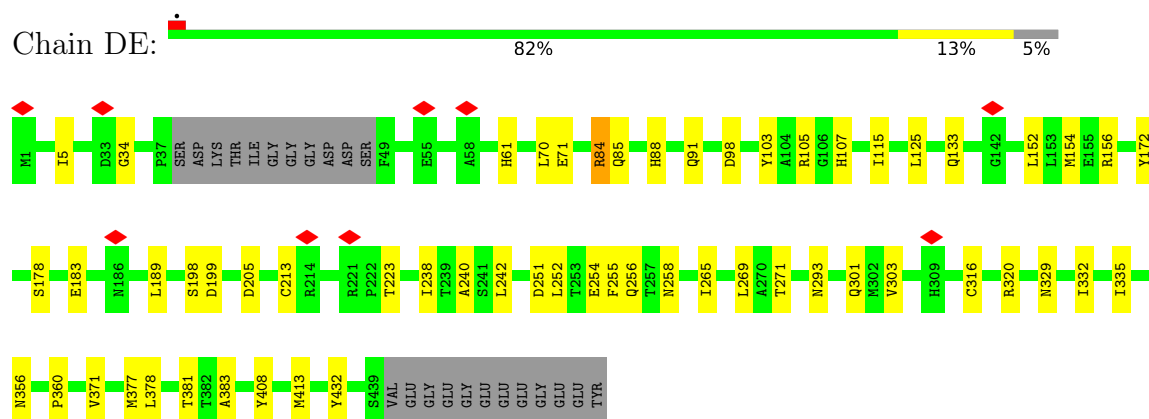
• Molecule 3: Tubulin alpha-1A chain



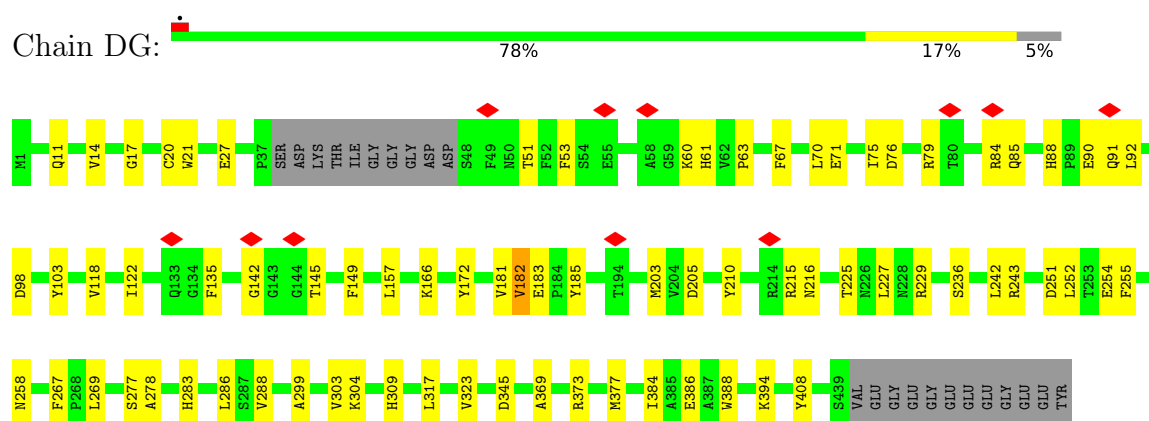
• Molecule 3: Tubulin alpha-1A chain



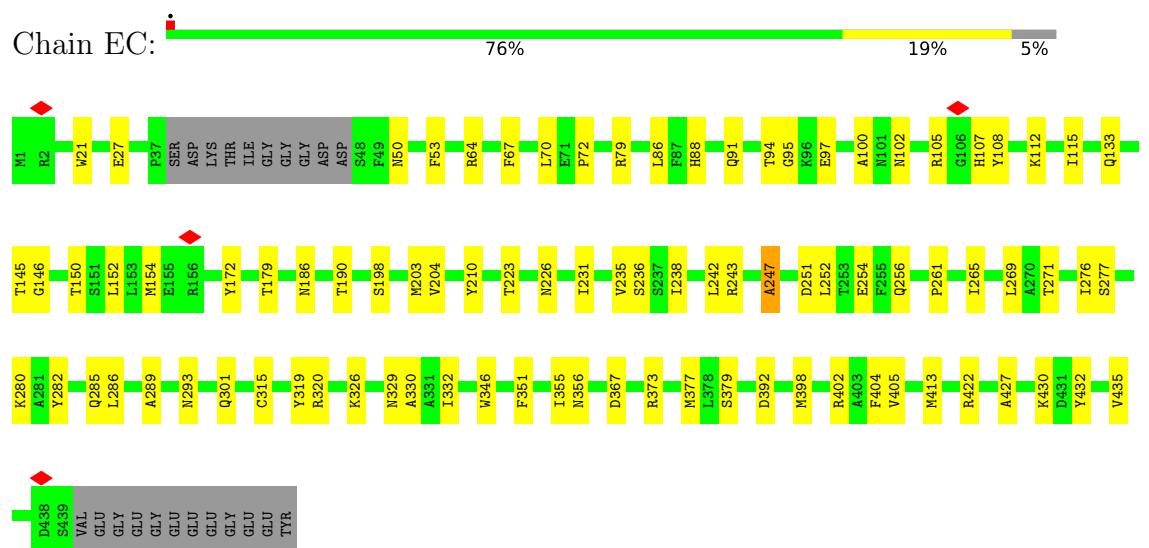
- Molecule 3: Tubulin alpha-1A chain



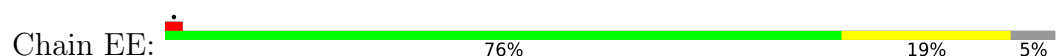
- Molecule 3: Tubulin alpha-1A chain

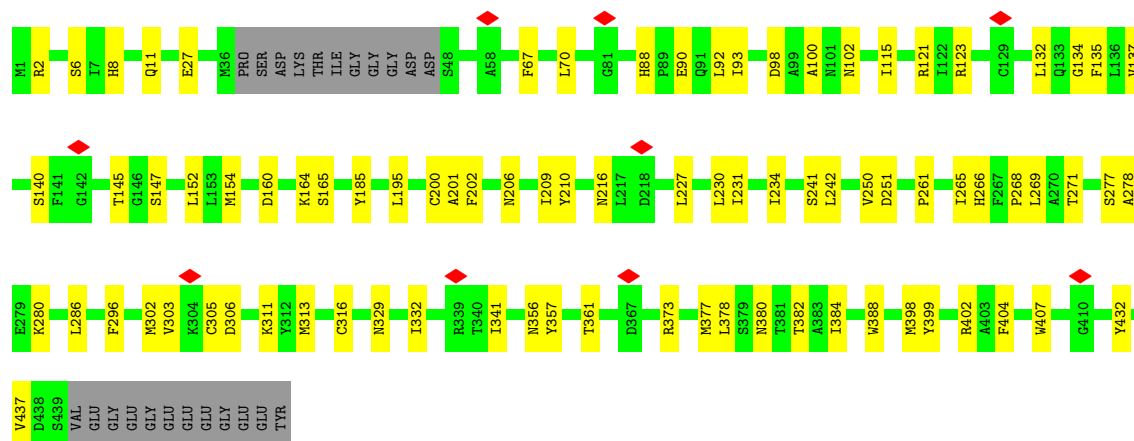


- Molecule 3: Tubulin alpha-1A chain

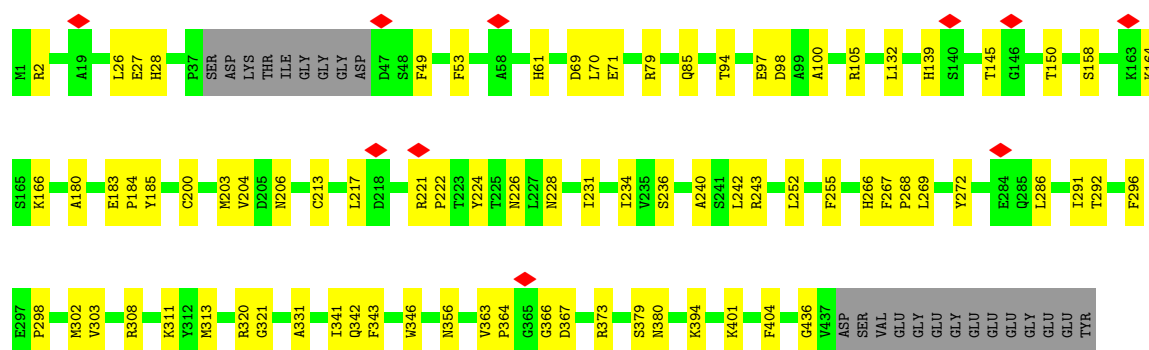
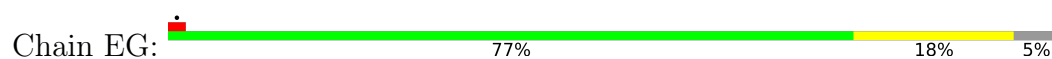


- Molecule 3: Tubulin alpha-1A chain

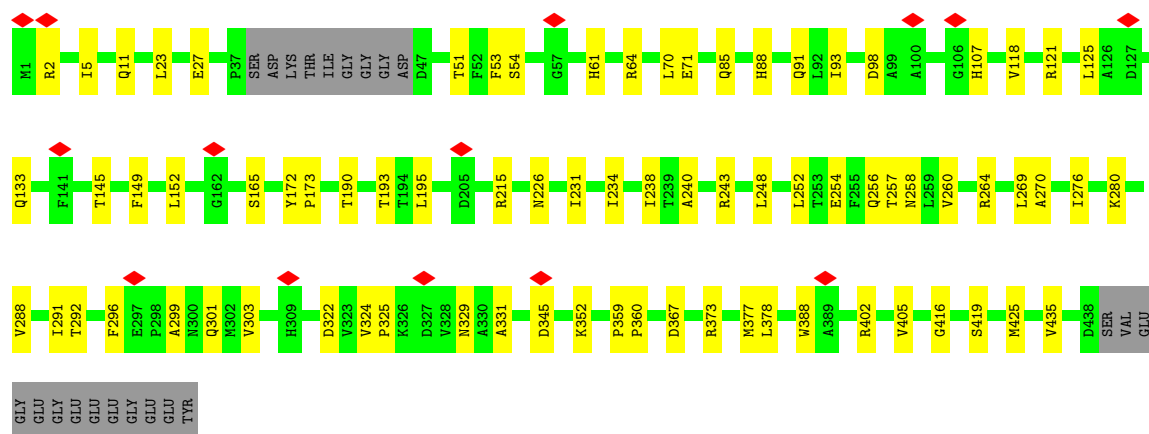
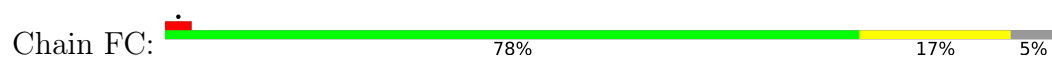




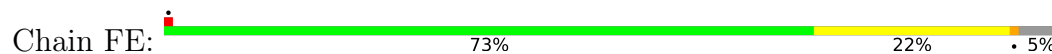
• Molecule 3: Tubulin alpha-1A chain

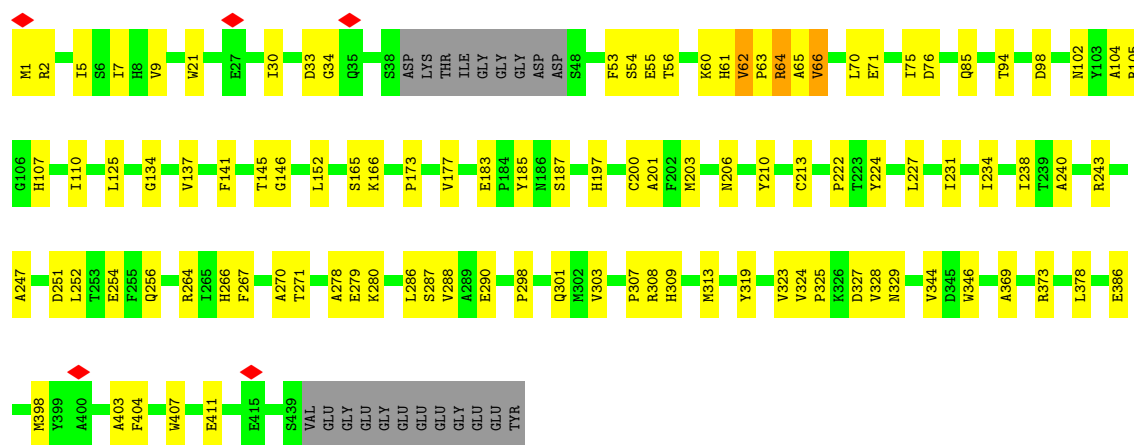


• Molecule 3: Tubulin alpha-1A chain

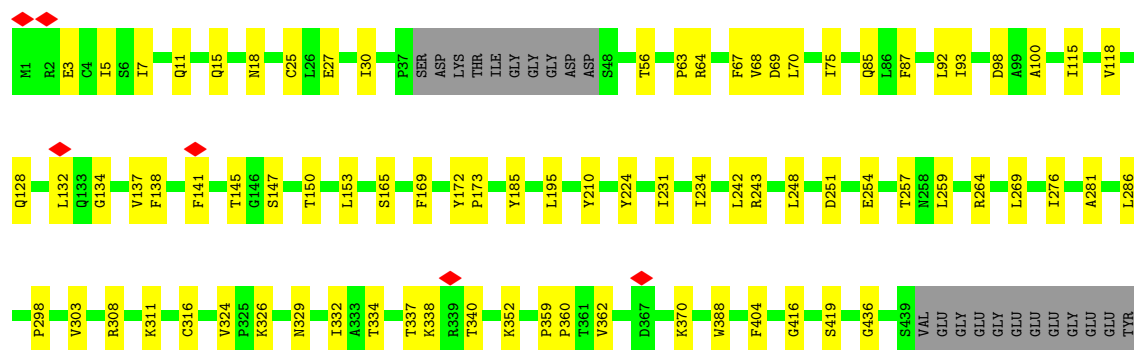
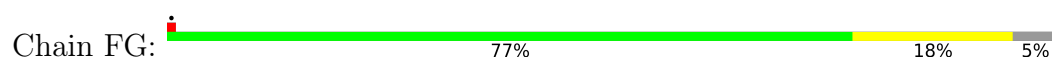


• Molecule 3: Tubulin alpha-1A chain

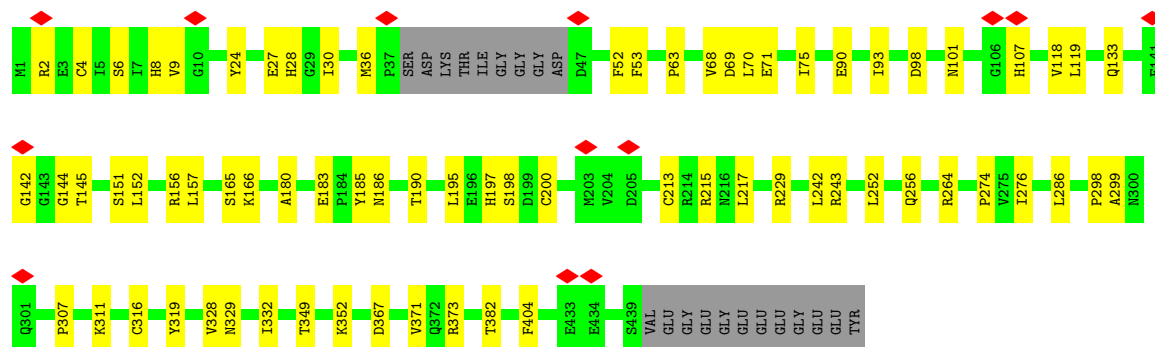
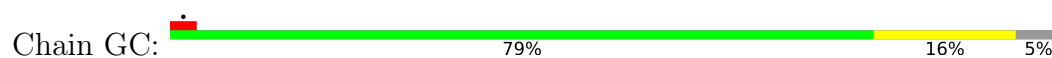




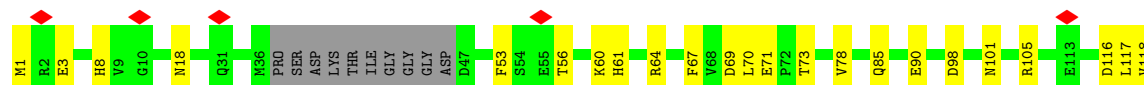
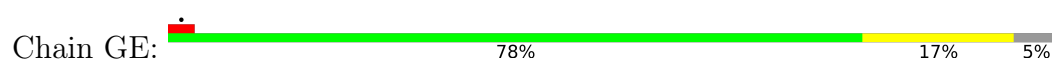
- Molecule 3: Tubulin alpha-1A chain

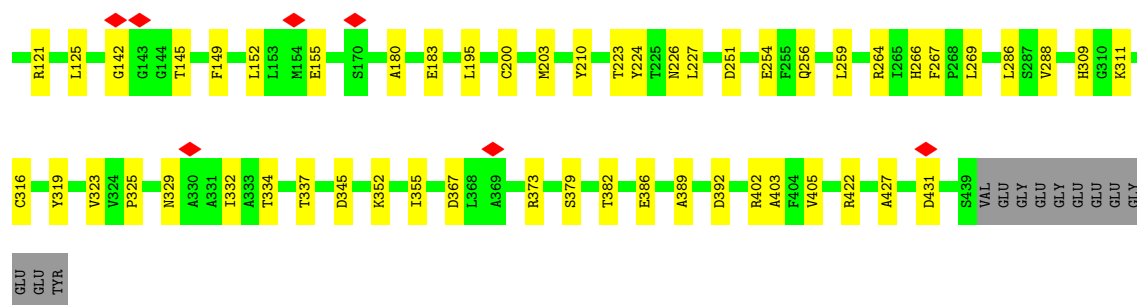


- Molecule 3: Tubulin alpha-1A chain

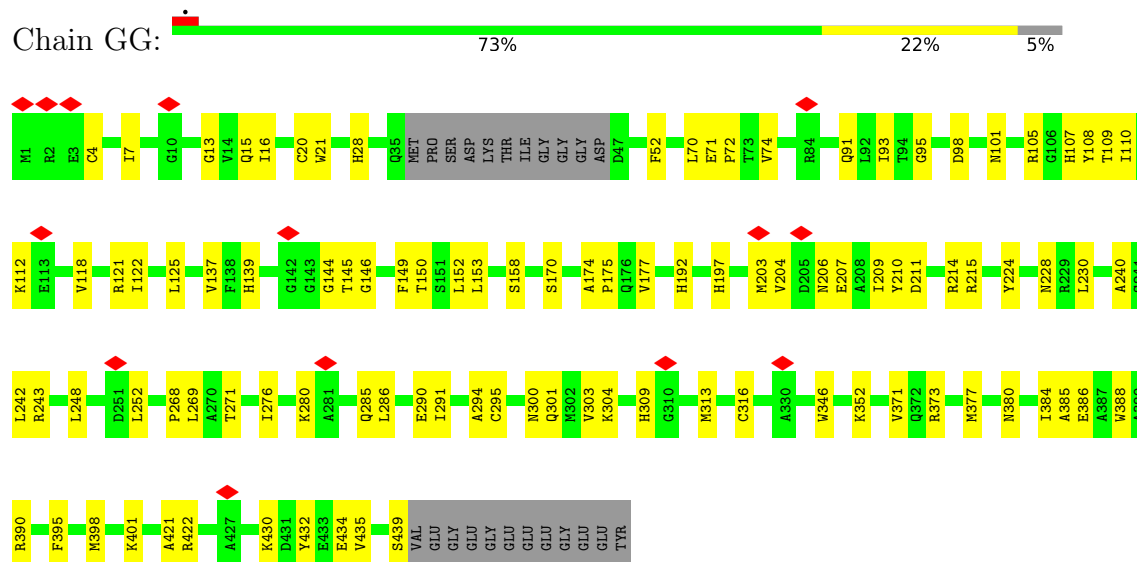


- Molecule 3: Tubulin alpha-1A chain

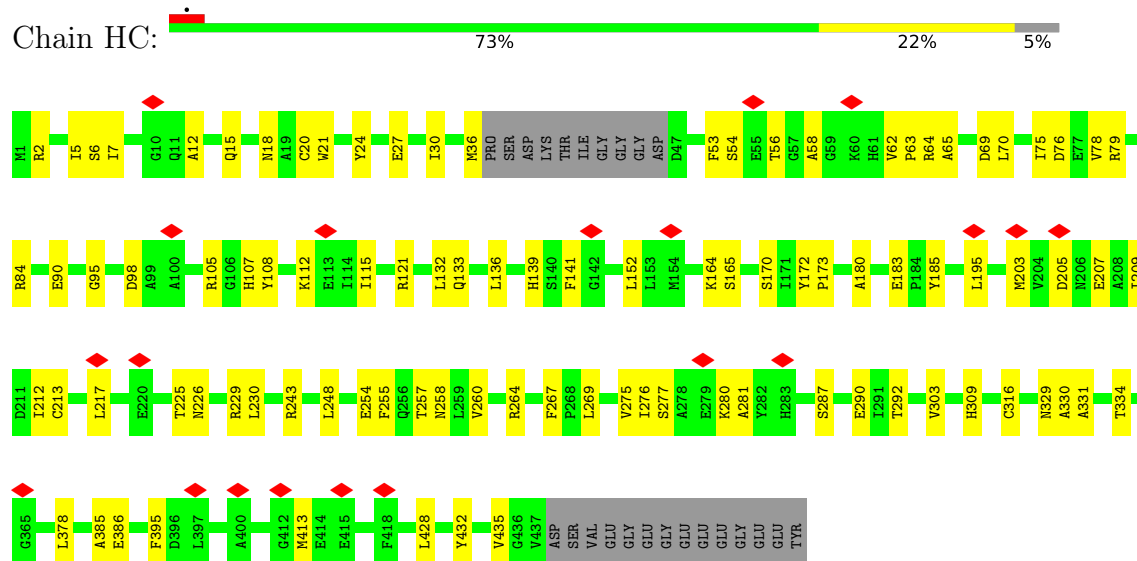




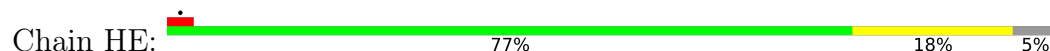
• Molecule 3: Tubulin alpha-1A chain

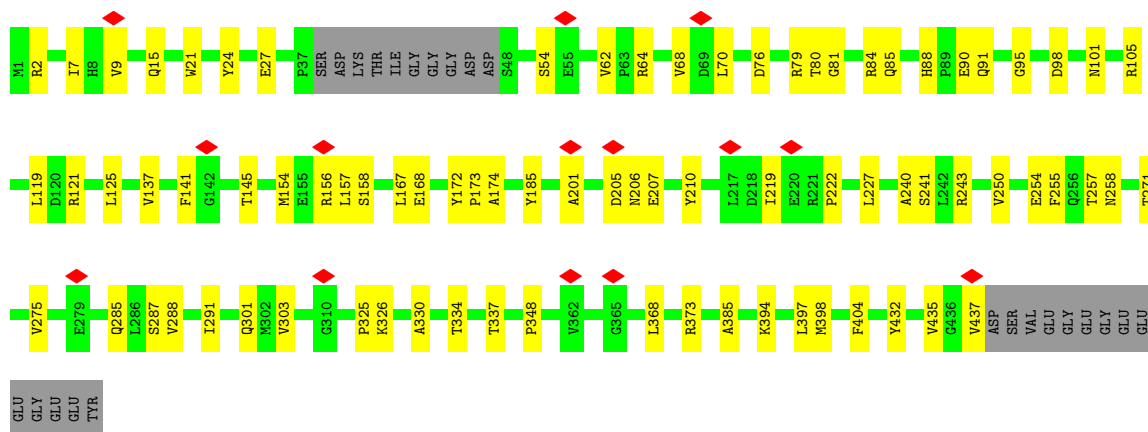


• Molecule 3: Tubulin alpha-1A chain



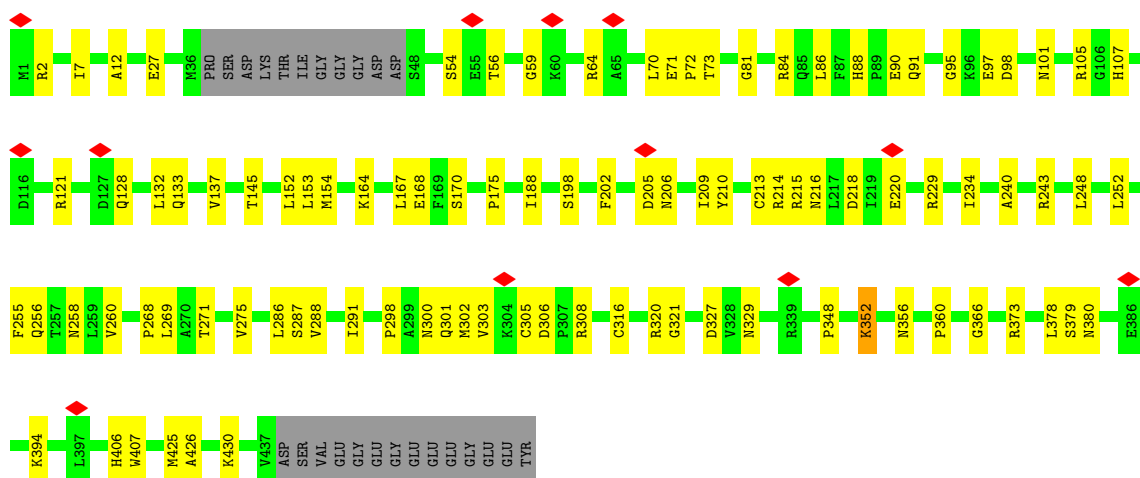
• Molecule 3: Tubulin alpha-1A chain





• Molecule 3: Tubulin alpha-1A chain

Chain HG: 73% 21% 6%



• Molecule 3: Tubulin alpha-1A chain

Chain IC: 69% 23% 8%

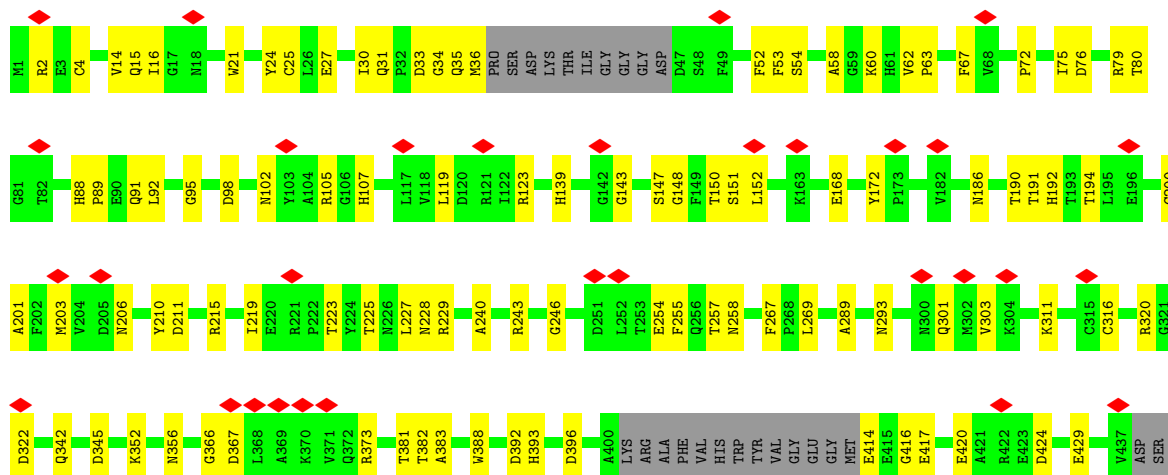
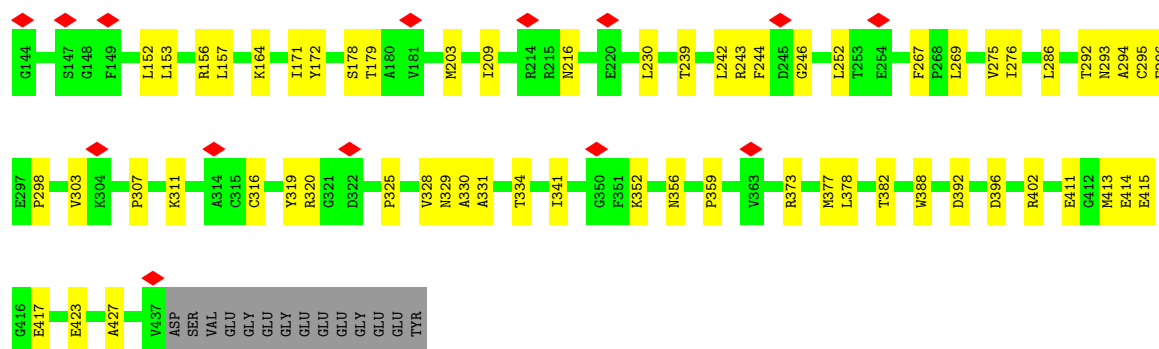
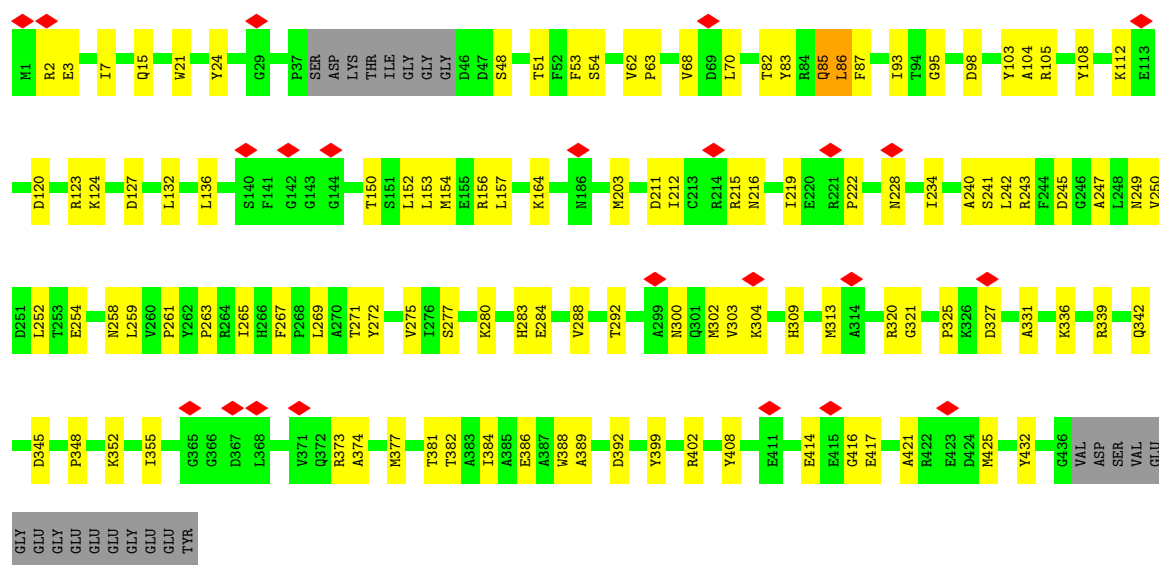
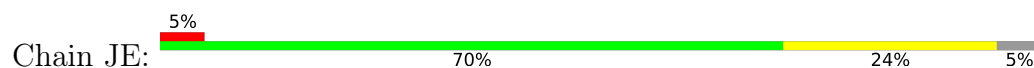


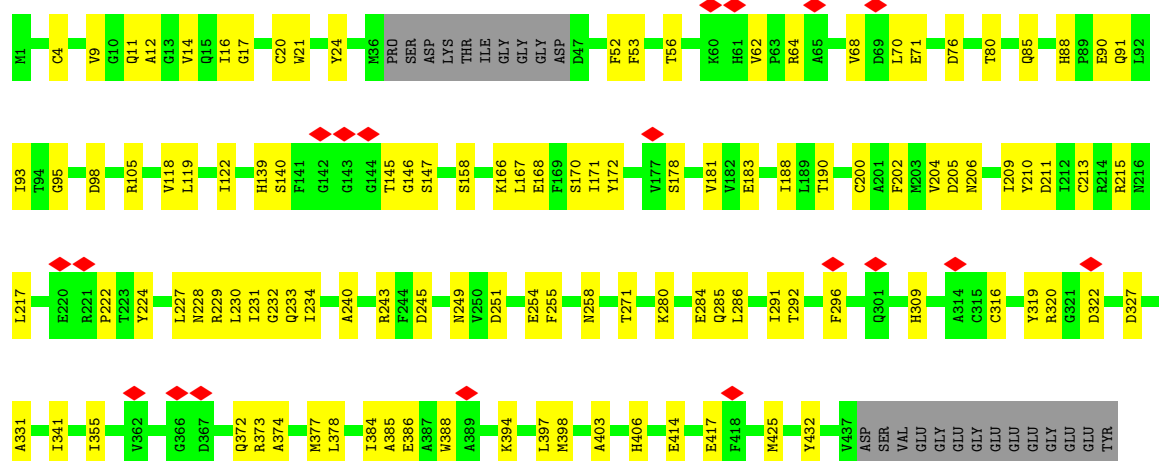
Figure 1: Distribution of amino acid types across 14 protein families. The chart shows the number of amino acids (x-axis, 0 to 20) for each family (y-axis). The families are color-coded: yellow for most families, grey for LYS, THR, ILE, GLY, and L70, and green for D46. Red diamonds are placed above the bars for M1, R2, E3, A65, D69, L70, A100, and C129.



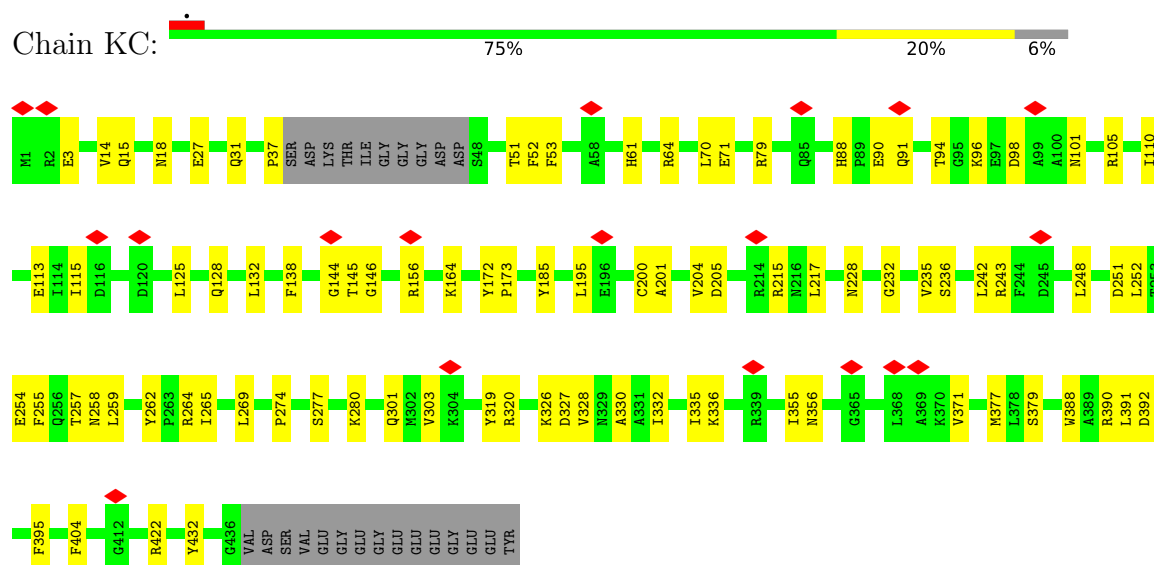
• Molecule 3: Tubulin alpha-1A chain



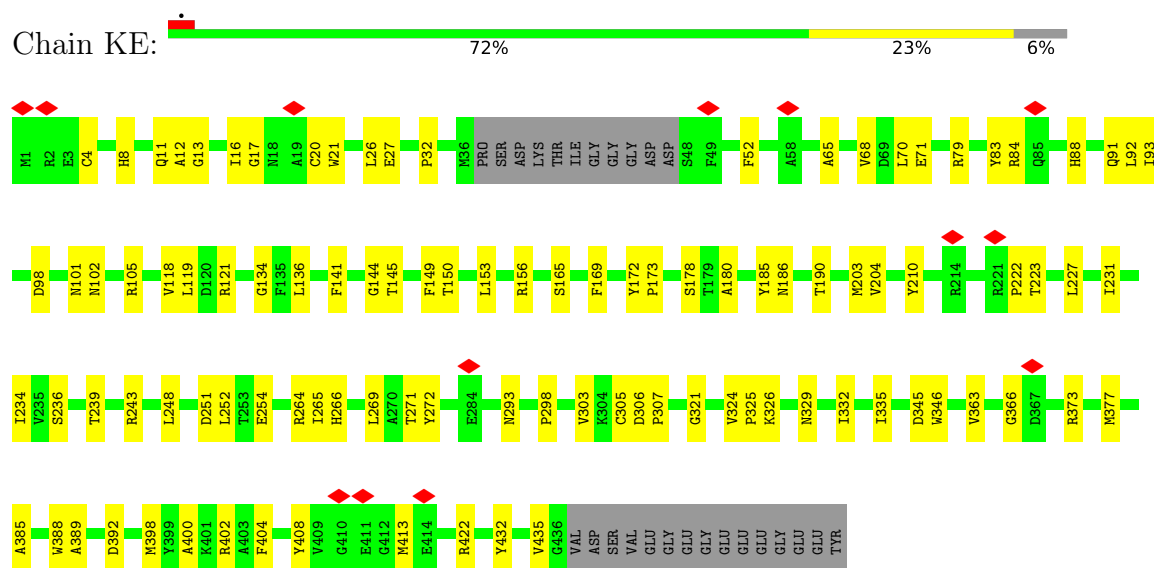
• Molecule 3: Tubulin alpha-1A chain



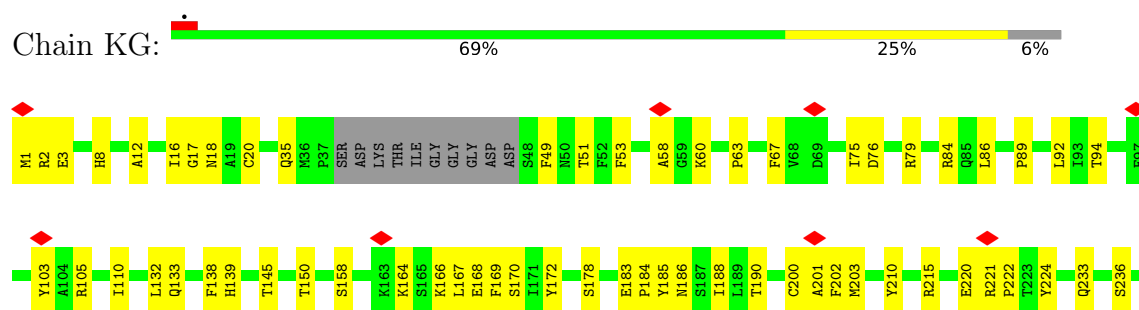
- Molecule 3: Tubulin alpha-1A chain

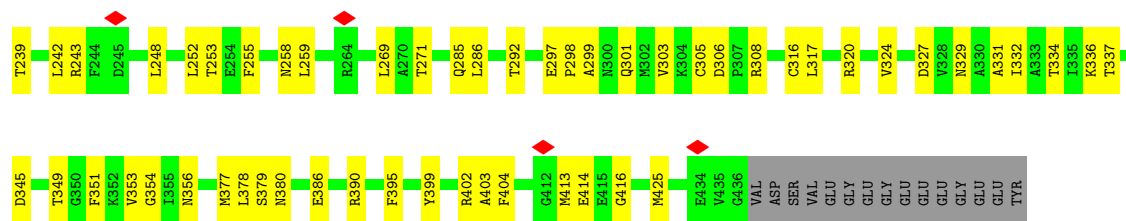


- Molecule 3: Tubulin alpha-1A chain



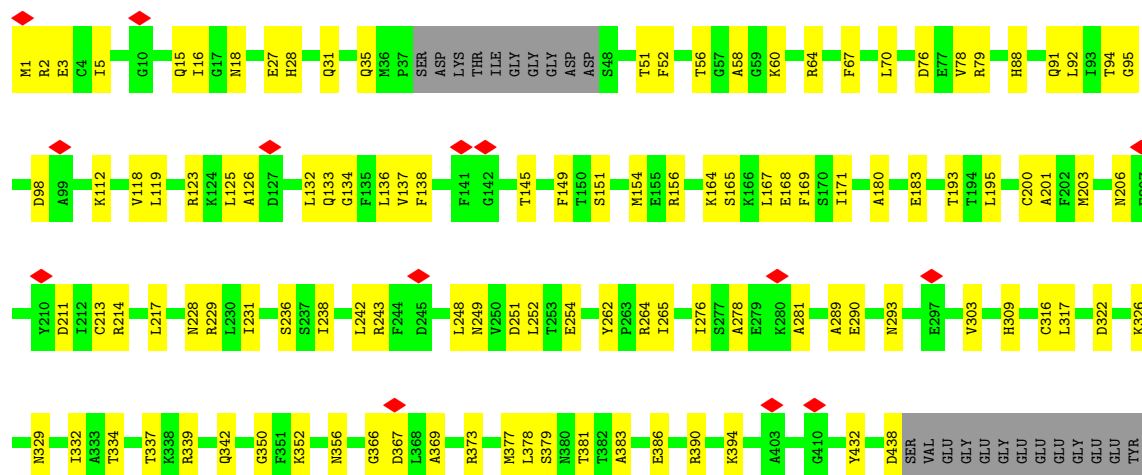
- Molecule 3: Tubulin alpha-1A chain





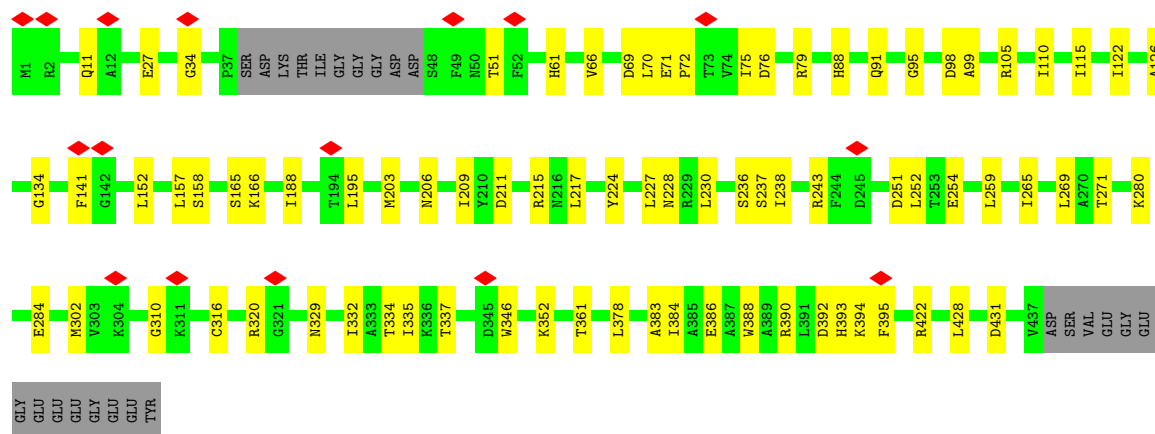
• Molecule 3: Tubulin alpha-1A chain

Chain LA: 70% 25% 5%



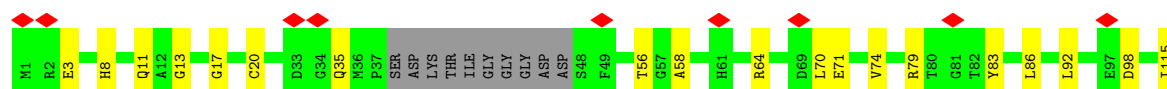
• Molecule 3: Tubulin alpha-1A chain

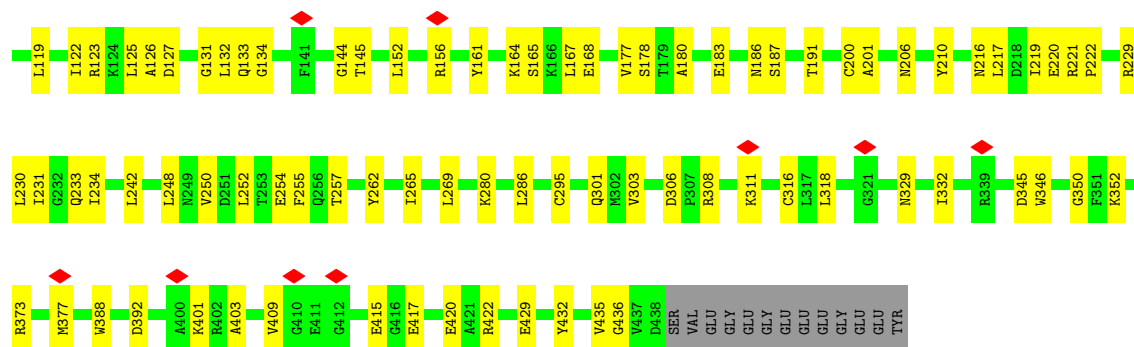
Chain LC: 77% 18% 5%



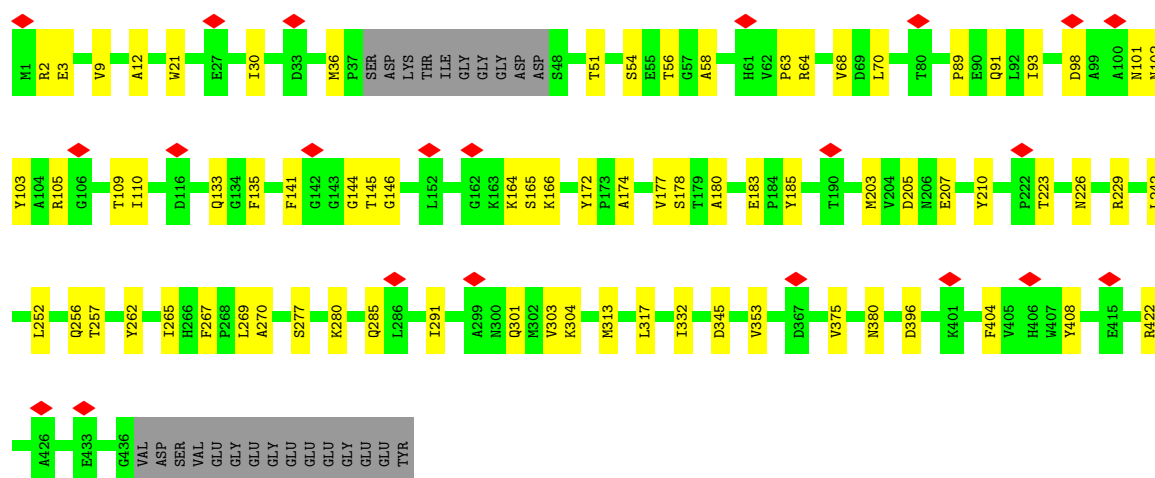
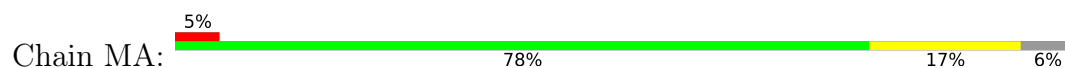
• Molecule 3: Tubulin alpha-1A chain

Chain LE: 73% 22% 5%

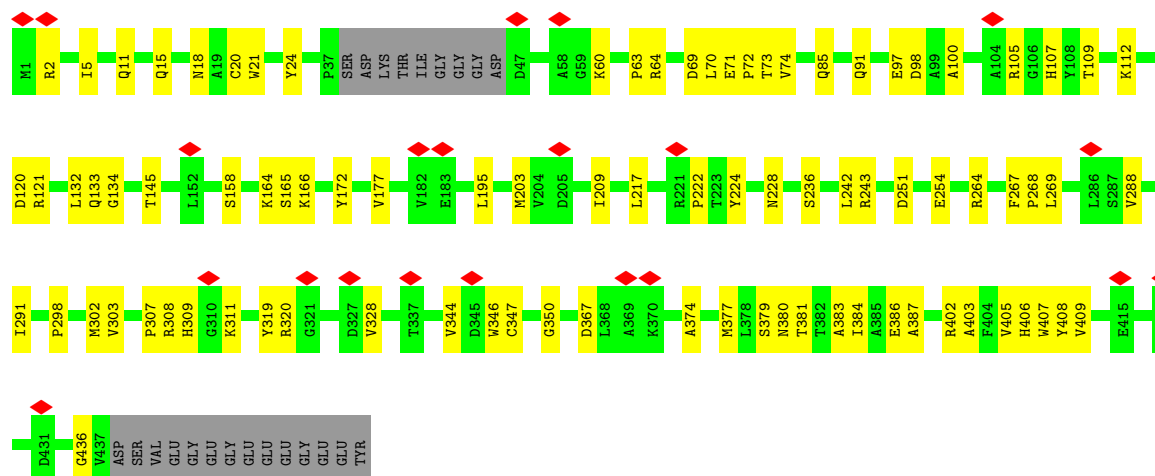
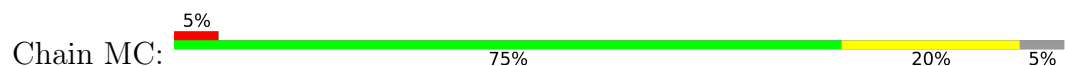




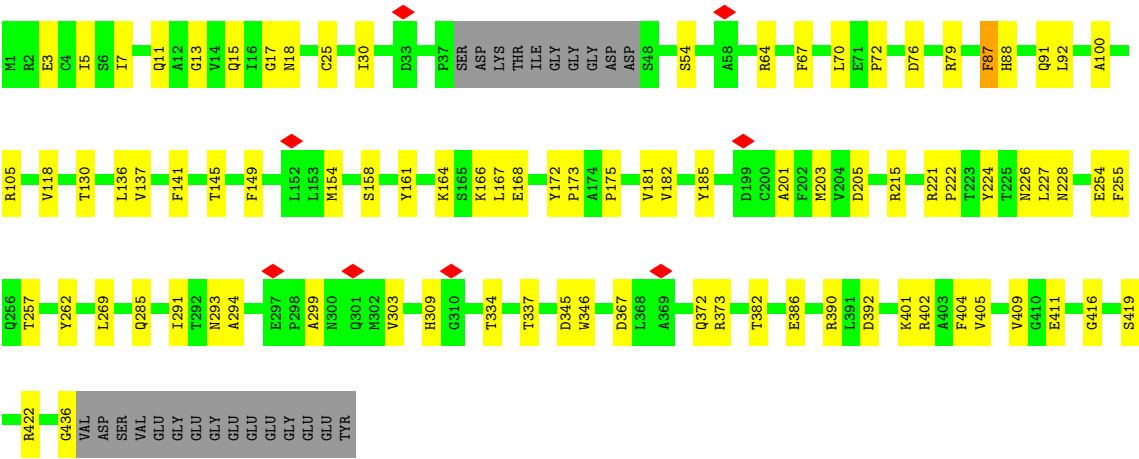
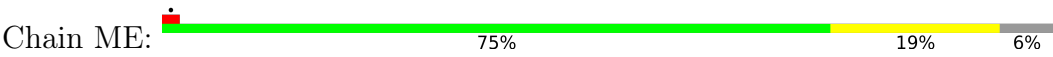
• Molecule 3: Tubulin alpha-1A chain



• Molecule 3: Tubulin alpha-1A chain



• Molecule 3: Tubulin alpha-1A chain



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	21990	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.386	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.015	Depositor
Map value standard deviation	0.090	Depositor
Recommended contour level	0.05	Depositor
Map size ($\text{\AA}$)	404.63998, 404.63998, 404.63998	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.843, 0.843, 0.843	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.12	0/795	0.32	0/1109
1	B	0.11	0/795	0.37	0/1109
1	C	0.12	0/785	0.42	0/1095
1	D	0.17	0/1313	0.44	0/1772
1	E	0.22	0/1313	0.53	3/1772 (0.2%)
1	F	0.18	0/1286	0.47	1/1735 (0.1%)
1	G	0.19	0/1302	0.48	0/1758
1	H	0.15	0/1302	0.41	0/1758
1	I	0.18	0/1302	0.41	0/1758
1	J	0.14	0/790	0.40	0/1102
1	K	0.13	0/790	0.31	0/1102
1	L	0.11	0/790	0.31	0/1102
1	M	0.12	0/795	0.32	0/1109
1	N	0.14	0/775	0.45	0/1081
1	O	0.13	0/795	0.33	0/1109
1	P	0.19	0/1313	0.52	0/1772
1	Q	0.19	0/1286	0.48	0/1735
1	R	0.18	0/1313	0.47	0/1772
1	S	0.17	0/1277	0.43	0/1724
1	T	0.19	0/1302	0.49	0/1758
1	U	0.20	0/1302	0.49	0/1758
1	V	0.13	0/790	0.34	0/1102
1	W	0.11	0/770	0.31	0/1074
1	X	0.11	0/795	0.31	0/1109
1	d	0.23	0/1277	0.61	3/1724 (0.2%)
1	e	0.25	0/1286	0.57	2/1735 (0.1%)
1	f	0.17	0/1313	0.44	0/1772
1	g	0.27	0/1302	0.54	3/1758 (0.2%)
1	h	0.16	0/1277	0.44	0/1724
1	i	0.19	0/1302	0.49	0/1758
1	j	0.13	0/790	0.35	0/1102
1	k	0.13	0/770	0.34	0/1074

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	l	0.12	0/755	0.31	0/1053
2	AB	0.26	0/3431	0.54	3/4649 (0.1%)
2	AD	0.23	0/3431	0.51	2/4649 (0.0%)
2	AF	0.22	0/3423	0.54	8/4638 (0.2%)
2	BA	0.25	0/3431	0.56	6/4649 (0.1%)
2	BD	0.24	0/3431	0.51	4/4649 (0.1%)
2	BF	0.22	0/3431	0.51	0/4649
2	CB	0.21	0/3431	0.52	4/4649 (0.1%)
2	CD	0.20	0/3431	0.48	4/4649 (0.1%)
2	CF	0.23	0/3431	0.53	3/4649 (0.1%)
2	DB	0.19	0/3431	0.47	0/4649
2	DD	0.24	0/3431	0.52	4/4649 (0.1%)
2	DF	0.22	0/3423	0.50	3/4638 (0.1%)
2	EB	0.20	0/3282	0.48	2/4449 (0.0%)
2	ED	0.27	0/3431	0.55	4/4649 (0.1%)
2	EF	0.23	0/3431	0.56	6/4649 (0.1%)
2	FD	0.24	0/3431	0.54	2/4649 (0.0%)
2	FF	0.23	0/3431	0.52	5/4649 (0.1%)
2	FH	0.18	0/3037	0.45	0/4112
2	GD	0.22	0/3431	0.47	2/4649 (0.0%)
2	GF	0.21	0/3431	0.49	4/4649 (0.1%)
2	GH	0.17	0/3431	0.43	0/4649
2	HD	0.23	0/3423	0.48	1/4638 (0.0%)
2	HF	0.21	0/3423	0.50	5/4638 (0.1%)
2	HH	0.22	1/3431 (0.0%)	0.51	4/4649 (0.1%)
2	ID	0.18	0/3423	0.46	0/4638
2	IF	0.19	0/3431	0.52	1/4649 (0.0%)
2	IH	0.20	0/3423	0.47	1/4638 (0.0%)
2	JD	0.20	0/3431	0.47	0/4649
2	JF	0.23	0/3431	0.54	3/4649 (0.1%)
2	KD	0.23	0/3423	0.53	4/4638 (0.1%)
2	KF	0.25	0/3431	0.57	6/4649 (0.1%)
2	KH	0.20	0/3237	0.52	4/4387 (0.1%)
2	LB	0.25	0/3431	0.53	4/4649 (0.1%)
2	LD	0.24	0/3431	0.54	7/4649 (0.2%)
2	LF	0.23	0/3431	0.53	5/4649 (0.1%)
2	MB	0.23	0/3431	0.52	1/4649 (0.0%)
2	MD	0.23	0/3423	0.50	3/4638 (0.1%)
2	MF	0.22	0/3431	0.52	2/4649 (0.0%)
3	AC	0.26	0/3420	0.53	6/4643 (0.1%)
3	AE	0.20	0/3426	0.45	1/4651 (0.0%)
3	BC	0.19	0/3426	0.44	0/4650
3	BE	0.18	0/3420	0.41	0/4643

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	BG	0.17	0/3093	0.44	0/4193
3	CC	0.19	0/3446	0.47	0/4678
3	CE	0.18	0/3454	0.44	0/4689
3	CG	0.17	0/3440	0.43	0/4670
3	DC	0.19	0/3434	0.43	0/4662
3	DE	0.22	0/3434	0.46	1/4662 (0.0%)
3	DG	0.17	0/3440	0.43	1/4670 (0.0%)
3	EC	0.21	0/3440	0.47	1/4670 (0.0%)
3	EE	0.19	0/3432	0.44	0/4658
3	EG	0.18	0/3434	0.43	0/4662
3	FC	0.18	0/3442	0.43	0/4673
3	FE	0.23	0/3446	0.50	1/4678 (0.0%)
3	FG	0.18	0/3440	0.44	0/4670
3	GC	0.17	0/3448	0.44	0/4681
3	GE	0.17	0/3440	0.46	0/4669
3	GG	0.18	0/3432	0.46	0/4659
3	HC	0.17	0/3426	0.45	0/4650
3	HE	0.17	0/3426	0.43	0/4651
3	HG	0.19	0/3418	0.48	1/4639 (0.0%)
3	IC	0.17	0/3309	0.44	0/4491
3	IE	0.17	0/3434	0.45	0/4662
3	IG	0.17	0/3426	0.41	0/4650
3	JC	0.17	0/3442	0.44	1/4673 (0.0%)
3	JE	0.22	0/3435	0.52	3/4663 (0.1%)
3	JG	0.17	0/3426	0.42	0/4650
3	KC	0.18	0/3419	0.44	0/4641
3	KE	0.17	0/3411	0.41	0/4629
3	KG	0.18	0/3419	0.42	0/4641
3	LA	0.17	0/3434	0.42	0/4662
3	LC	0.19	0/3426	0.45	0/4651
3	LE	0.18	0/3434	0.45	0/4662
3	MA	0.18	0/3419	0.45	1/4641 (0.0%)
3	MC	0.20	0/3434	0.46	0/4662
3	ME	0.19	0/3419	0.49	2/4641 (0.0%)
All	All	0.20	1/294669 (0.0%)	0.48	148/399940 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	HH	272	PRO	CA-C	-5.33	1.48	1.52

The worst 5 of 148 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	LB	257	MET	N-CA-C	13.11	125.65	111.36
2	LD	271	ALA	N-CA-C	12.73	130.40	108.75
2	EF	271	ALA	N-CA-C	12.39	129.81	108.75
2	KF	254	ALA	N-CA-C	10.67	122.48	111.07
2	FF	271	ALA	N-CA-C	10.49	132.99	109.81

There are no chirality outliers.

There are no planarity outliers.

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	A	796	0	342	0	0
1	B	796	0	342	1	0
1	C	786	0	339	1	0
1	D	1289	0	1284	14	0
1	E	1289	0	1284	18	0
1	F	1263	0	1253	15	0
1	G	1278	0	1271	19	0
1	H	1278	0	1271	17	0
1	I	1278	0	1271	17	0
1	J	791	0	340	2	0
1	K	791	0	340	1	0
1	L	791	0	340	0	0
1	M	796	0	342	1	0
1	N	776	0	335	2	0
1	O	796	0	342	0	0
1	P	1289	0	1284	12	0
1	Q	1263	0	1253	22	0
1	R	1289	0	1284	13	0
1	S	1254	0	1240	10	0
1	T	1278	0	1271	14	0
1	U	1278	0	1271	17	0
1	V	791	0	340	2	0
1	W	771	0	333	3	0
1	X	796	0	342	1	0
1	d	1254	0	1240	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	e	1263	0	1253	10	0
1	f	1289	0	1284	10	0
1	g	1278	0	1271	12	0
1	h	1254	0	1240	15	0
1	i	1278	0	1271	12	0
1	j	791	0	340	1	0
1	k	771	0	333	0	0
1	l	756	0	324	1	0
2	AB	3356	0	3240	65	0
2	AD	3356	0	3240	60	0
2	AF	3348	0	3236	52	0
2	BA	3356	0	3240	62	0
2	BD	3356	0	3240	52	0
2	BF	3356	0	3240	77	0
2	CB	3356	0	3240	59	0
2	CD	3356	0	3240	58	0
2	CF	3356	0	3240	65	0
2	DB	3356	0	3240	59	0
2	DD	3356	0	3240	53	0
2	DF	3348	0	3236	60	0
2	EB	3214	0	3103	54	0
2	ED	3356	0	3240	62	0
2	EF	3356	0	3240	65	0
2	FD	3356	0	3240	70	0
2	FF	3356	0	3240	64	0
2	FH	2971	0	2870	42	0
2	GD	3356	0	3240	59	0
2	GF	3356	0	3240	58	0
2	GH	3356	0	3240	51	0
2	HD	3348	0	3236	65	0
2	HF	3348	0	3236	71	0
2	HH	3356	0	3240	65	0
2	ID	3348	0	3236	61	0
2	IF	3356	0	3240	66	0
2	IH	3348	0	3236	68	0
2	JD	3356	0	3240	73	0
2	JF	3356	0	3240	77	0
2	KD	3348	0	3236	69	0
2	KF	3356	0	3240	72	0
2	KH	3165	0	3048	50	0
2	LB	3356	0	3240	64	0
2	LD	3356	0	3240	61	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	LF	3356	0	3240	53	0
2	MB	3356	0	3240	78	0
2	MD	3348	0	3236	84	0
2	MF	3356	0	3240	50	0
3	AC	3343	0	3268	66	0
3	AE	3349	0	3273	64	0
3	BC	3350	0	3270	52	0
3	BE	3343	0	3268	48	0
3	BG	3026	0	2939	50	0
3	CC	3369	0	3287	56	0
3	CE	3377	0	3291	53	0
3	CG	3363	0	3282	42	0
3	DC	3357	0	3277	47	0
3	DE	3357	0	3277	36	0
3	DG	3363	0	3282	47	0
3	EC	3363	0	3282	62	0
3	EE	3356	0	3275	52	0
3	EG	3357	0	3277	50	0
3	FC	3365	0	3281	50	0
3	FE	3369	0	3287	71	0
3	FG	3363	0	3282	50	0
3	GC	3371	0	3286	47	0
3	GE	3364	0	3279	54	0
3	GG	3356	0	3270	74	0
3	HC	3350	0	3270	68	0
3	HE	3349	0	3273	54	0
3	HG	3342	0	3266	67	0
3	IC	3239	0	3164	67	0
3	IE	3357	0	3277	73	0
3	IG	3350	0	3270	66	0
3	JC	3365	0	3281	47	0
3	JE	3358	0	3272	76	0
3	JG	3350	0	3269	73	0
3	KC	3342	0	3264	61	0
3	KE	3335	0	3257	72	0
3	KG	3342	0	3264	73	0
3	LA	3357	0	3277	72	0
3	LC	3349	0	3273	57	0
3	LE	3357	0	3277	66	0
3	MA	3342	0	3264	49	0
3	MC	3357	0	3277	59	0
3	ME	3342	0	3264	56	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	AB	28	0	12	3	0
4	AD	28	0	12	3	0
4	AF	28	0	12	3	0
4	BA	28	0	12	1	0
4	BD	28	0	12	1	0
4	BF	28	0	12	1	0
4	CB	28	0	12	3	0
4	CD	28	0	12	2	0
4	CF	28	0	12	1	0
4	DB	28	0	12	0	0
4	DD	28	0	12	0	0
4	DF	28	0	12	0	0
4	EB	28	0	12	2	0
4	ED	28	0	12	0	0
4	EF	28	0	12	1	0
4	FD	28	0	12	1	0
4	FF	28	0	12	2	0
4	FH	28	0	12	1	0
4	GD	28	0	12	1	0
4	GF	28	0	12	1	0
4	GH	28	0	12	4	0
4	HD	28	0	12	3	0
4	HF	28	0	12	1	0
4	HH	28	0	12	2	0
4	ID	28	0	12	3	0
4	IF	28	0	12	1	0
4	IH	28	0	12	1	0
4	JD	28	0	12	4	0
4	JF	28	0	12	1	0
4	KD	28	0	12	2	0
4	KF	28	0	12	1	0
4	KH	28	0	12	1	0
4	LB	28	0	12	4	0
4	LD	28	0	12	3	0
4	LF	28	0	12	2	0
4	MB	28	0	12	0	0
4	MD	28	0	12	1	0
4	MF	28	0	12	1	0
5	AC	32	0	12	1	0
5	AE	32	0	12	1	0
5	BC	32	0	12	2	0
5	BE	32	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	BG	32	0	12	3	0
5	CC	32	0	12	1	0
5	CE	32	0	12	0	0
5	CG	32	0	12	3	0
5	DC	32	0	12	2	0
5	DE	32	0	12	0	0
5	DG	32	0	12	1	0
5	EC	32	0	12	3	0
5	EE	32	0	12	1	0
5	EG	32	0	12	1	0
5	FC	32	0	12	1	0
5	FE	32	0	12	1	0
5	FG	32	0	12	1	0
5	GC	32	0	12	0	0
5	GE	32	0	12	3	0
5	GG	32	0	12	1	0
5	HC	32	0	12	1	0
5	HE	32	0	12	2	0
5	HG	32	0	12	3	0
5	IC	32	0	12	1	0
5	IE	32	0	12	2	0
5	IG	32	0	12	0	0
5	JC	32	0	12	0	0
5	JE	32	0	12	1	0
5	JG	32	0	12	0	0
5	KC	32	0	12	3	0
5	KE	32	0	12	1	0
5	KG	32	0	12	1	0
5	LA	32	0	12	2	0
5	LC	32	0	12	2	0
5	LE	32	0	12	3	0
5	MA	32	0	12	1	0
5	MC	32	0	12	0	0
5	ME	32	0	12	1	0
6	AC	1	0	0	0	0
6	AE	1	0	0	0	0
6	BC	1	0	0	0	0
6	BE	1	0	0	0	0
6	BG	1	0	0	0	0
6	CC	1	0	0	0	0
6	CE	1	0	0	0	0
6	CG	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	DC	1	0	0	0	0
6	DE	1	0	0	0	0
6	DG	1	0	0	0	0
6	EC	1	0	0	0	0
6	EE	1	0	0	0	0
6	EG	1	0	0	0	0
6	FC	1	0	0	0	0
6	FE	1	0	0	0	0
6	FG	1	0	0	0	0
6	GC	1	0	0	0	0
6	GE	1	0	0	0	0
6	GG	1	0	0	0	0
6	HC	1	0	0	0	0
6	HE	1	0	0	0	0
6	HG	1	0	0	0	0
6	IC	1	0	0	0	0
6	IE	1	0	0	0	0
6	IG	1	0	0	0	0
6	JC	1	0	0	0	0
6	JE	1	0	0	0	0
6	JG	1	0	0	0	0
6	KC	1	0	0	0	0
6	KE	1	0	0	0	0
6	KG	1	0	0	0	0
6	LA	1	0	0	0	0
6	LC	1	0	0	0	0
6	LE	1	0	0	0	0
6	MA	1	0	0	0	0
6	MC	1	0	0	0	0
6	ME	1	0	0	0	0
All	All	290845	0	275163	4494	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 4494 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:KF:271:ALA:HB3	2:KF:365:ALA:HB3	1.49	0.94
2:BA:271:ALA:HB3	2:BA:365:ALA:HB3	1.54	0.90
2:AD:271:ALA:HB3	2:AD:365:ALA:HB3	1.54	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:IF:86:ARG:HH22	3:JE:283:HIS:HB3	1.40	0.86
2:HD:214:THR:HG21	2:HD:273:LEU:HB3	1.61	0.81

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	A	158/222 (71%)	155 (98%)	3 (2%)	0	100	100
1	B	158/222 (71%)	155 (98%)	3 (2%)	0	100	100
1	C	156/222 (70%)	149 (96%)	7 (4%)	0	100	100
1	D	158/222 (71%)	150 (95%)	8 (5%)	0	100	100
1	E	158/222 (71%)	150 (95%)	8 (5%)	0	100	100
1	F	155/222 (70%)	150 (97%)	5 (3%)	0	100	100
1	G	157/222 (71%)	151 (96%)	6 (4%)	0	100	100
1	H	157/222 (71%)	153 (98%)	4 (2%)	0	100	100
1	I	157/222 (71%)	153 (98%)	4 (2%)	0	100	100
1	J	157/222 (71%)	147 (94%)	10 (6%)	0	100	100
1	K	157/222 (71%)	154 (98%)	3 (2%)	0	100	100
1	L	157/222 (71%)	153 (98%)	4 (2%)	0	100	100
1	M	158/222 (71%)	155 (98%)	3 (2%)	0	100	100
1	N	154/222 (69%)	146 (95%)	8 (5%)	0	100	100
1	O	158/222 (71%)	154 (98%)	4 (2%)	0	100	100
1	P	158/222 (71%)	158 (100%)	0	0	100	100
1	Q	155/222 (70%)	152 (98%)	3 (2%)	0	100	100
1	R	158/222 (71%)	151 (96%)	7 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	S	154/222 (69%)	149 (97%)	5 (3%)	0	100	100
1	T	157/222 (71%)	152 (97%)	5 (3%)	0	100	100
1	U	157/222 (71%)	152 (97%)	5 (3%)	0	100	100
1	V	157/222 (71%)	150 (96%)	7 (4%)	0	100	100
1	W	153/222 (69%)	149 (97%)	4 (3%)	0	100	100
1	X	158/222 (71%)	152 (96%)	6 (4%)	0	100	100
1	d	154/222 (69%)	146 (95%)	8 (5%)	0	100	100
1	e	155/222 (70%)	148 (96%)	7 (4%)	0	100	100
1	f	158/222 (71%)	151 (96%)	7 (4%)	0	100	100
1	g	157/222 (71%)	150 (96%)	7 (4%)	0	100	100
1	h	154/222 (69%)	145 (94%)	9 (6%)	0	100	100
1	i	157/222 (71%)	152 (97%)	5 (3%)	0	100	100
1	j	157/222 (71%)	147 (94%)	10 (6%)	0	100	100
1	k	153/222 (69%)	149 (97%)	4 (3%)	0	100	100
1	l	150/222 (68%)	145 (97%)	5 (3%)	0	100	100
2	AB	425/445 (96%)	408 (96%)	17 (4%)	0	100	100
2	AD	425/445 (96%)	405 (95%)	20 (5%)	0	100	100
2	AF	424/445 (95%)	399 (94%)	25 (6%)	0	100	100
2	BA	425/445 (96%)	407 (96%)	16 (4%)	2 (0%)	24	63
2	BD	425/445 (96%)	406 (96%)	18 (4%)	1 (0%)	43	77
2	BF	425/445 (96%)	403 (95%)	22 (5%)	0	100	100
2	CB	425/445 (96%)	405 (95%)	19 (4%)	1 (0%)	43	77
2	CD	425/445 (96%)	398 (94%)	26 (6%)	1 (0%)	43	77
2	CF	425/445 (96%)	407 (96%)	17 (4%)	1 (0%)	43	77
2	DB	425/445 (96%)	412 (97%)	13 (3%)	0	100	100
2	DD	425/445 (96%)	407 (96%)	17 (4%)	1 (0%)	43	77
2	DF	424/445 (95%)	397 (94%)	26 (6%)	1 (0%)	43	77
2	EB	407/445 (92%)	387 (95%)	19 (5%)	1 (0%)	43	77
2	ED	425/445 (96%)	408 (96%)	16 (4%)	1 (0%)	43	77
2	EF	425/445 (96%)	400 (94%)	24 (6%)	1 (0%)	43	77
2	FD	425/445 (96%)	405 (95%)	19 (4%)	1 (0%)	43	77

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	FF	425/445 (96%)	406 (96%)	18 (4%)	1 (0%)	43	77
2	FH	373/445 (84%)	353 (95%)	20 (5%)	0	100	100
2	GD	425/445 (96%)	409 (96%)	15 (4%)	1 (0%)	43	77
2	GF	425/445 (96%)	406 (96%)	18 (4%)	1 (0%)	43	77
2	GH	425/445 (96%)	402 (95%)	23 (5%)	0	100	100
2	HD	424/445 (95%)	400 (94%)	23 (5%)	1 (0%)	43	77
2	HF	424/445 (95%)	399 (94%)	24 (6%)	1 (0%)	43	77
2	HH	425/445 (96%)	407 (96%)	17 (4%)	1 (0%)	43	77
2	ID	424/445 (95%)	403 (95%)	21 (5%)	0	100	100
2	IF	425/445 (96%)	389 (92%)	36 (8%)	0	100	100
2	IH	424/445 (95%)	402 (95%)	22 (5%)	0	100	100
2	JD	425/445 (96%)	399 (94%)	26 (6%)	0	100	100
2	JF	425/445 (96%)	402 (95%)	23 (5%)	0	100	100
2	KD	424/445 (95%)	403 (95%)	20 (5%)	1 (0%)	43	77
2	KF	425/445 (96%)	403 (95%)	21 (5%)	1 (0%)	43	77
2	KH	397/445 (89%)	374 (94%)	22 (6%)	1 (0%)	36	72
2	LB	425/445 (96%)	402 (95%)	22 (5%)	1 (0%)	43	77
2	LD	425/445 (96%)	406 (96%)	19 (4%)	0	100	100
2	LF	425/445 (96%)	404 (95%)	19 (4%)	2 (0%)	24	63
2	MB	425/445 (96%)	405 (95%)	19 (4%)	1 (0%)	43	77
2	MD	424/445 (95%)	405 (96%)	18 (4%)	1 (0%)	43	77
2	MF	425/445 (96%)	404 (95%)	20 (5%)	1 (0%)	43	77
3	AC	422/451 (94%)	409 (97%)	13 (3%)	0	100	100
3	AE	423/451 (94%)	409 (97%)	14 (3%)	0	100	100
3	BC	423/451 (94%)	411 (97%)	12 (3%)	0	100	100
3	BE	422/451 (94%)	403 (96%)	19 (4%)	0	100	100
3	BG	377/451 (84%)	367 (97%)	10 (3%)	0	100	100
3	CC	426/451 (94%)	415 (97%)	11 (3%)	0	100	100
3	CE	427/451 (95%)	410 (96%)	17 (4%)	0	100	100
3	CG	425/451 (94%)	412 (97%)	13 (3%)	0	100	100
3	DC	424/451 (94%)	411 (97%)	13 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	DE	424/451 (94%)	404 (95%)	20 (5%)	0	100	100
3	DG	425/451 (94%)	407 (96%)	18 (4%)	0	100	100
3	EC	425/451 (94%)	418 (98%)	7 (2%)	0	100	100
3	EE	424/451 (94%)	410 (97%)	14 (3%)	0	100	100
3	EG	424/451 (94%)	402 (95%)	22 (5%)	0	100	100
3	FC	425/451 (94%)	412 (97%)	13 (3%)	0	100	100
3	FE	426/451 (94%)	408 (96%)	18 (4%)	0	100	100
3	FG	425/451 (94%)	412 (97%)	13 (3%)	0	100	100
3	GC	426/451 (94%)	416 (98%)	10 (2%)	0	100	100
3	GE	425/451 (94%)	406 (96%)	19 (4%)	0	100	100
3	GG	424/451 (94%)	410 (97%)	14 (3%)	0	100	100
3	HC	423/451 (94%)	410 (97%)	13 (3%)	0	100	100
3	HE	423/451 (94%)	412 (97%)	11 (3%)	0	100	100
3	HG	422/451 (94%)	406 (96%)	16 (4%)	0	100	100
3	IC	408/451 (90%)	393 (96%)	15 (4%)	0	100	100
3	IE	424/451 (94%)	409 (96%)	15 (4%)	0	100	100
3	IG	423/451 (94%)	408 (96%)	15 (4%)	0	100	100
3	JC	425/451 (94%)	407 (96%)	18 (4%)	0	100	100
3	JE	424/451 (94%)	403 (95%)	21 (5%)	0	100	100
3	JG	423/451 (94%)	404 (96%)	19 (4%)	0	100	100
3	KC	422/451 (94%)	411 (97%)	11 (3%)	0	100	100
3	KE	421/451 (93%)	406 (96%)	15 (4%)	0	100	100
3	KG	422/451 (94%)	411 (97%)	11 (3%)	0	100	100
3	LA	424/451 (94%)	402 (95%)	22 (5%)	0	100	100
3	LC	423/451 (94%)	407 (96%)	16 (4%)	0	100	100
3	LE	424/451 (94%)	409 (96%)	15 (4%)	0	100	100
3	MA	422/451 (94%)	407 (96%)	15 (4%)	0	100	100
3	MC	424/451 (94%)	405 (96%)	19 (4%)	0	100	100
3	ME	422/451 (94%)	408 (97%)	14 (3%)	0	100	100
All	All	37242/41374 (90%)	35680 (96%)	1535 (4%)	27 (0%)	49	83

5 of 27 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	BA	158	GLU
2	LF	268	PRO
2	ED	272	PRO
2	MF	83	GLN
2	CB	271	ALA

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	D	149/199 (75%)	149 (100%)	0	100	100
1	E	149/199 (75%)	148 (99%)	1 (1%)	76	81
1	F	146/199 (73%)	146 (100%)	0	100	100
1	G	148/199 (74%)	148 (100%)	0	100	100
1	H	148/199 (74%)	148 (100%)	0	100	100
1	I	148/199 (74%)	148 (100%)	0	100	100
1	P	149/199 (75%)	149 (100%)	0	100	100
1	Q	146/199 (73%)	146 (100%)	0	100	100
1	R	149/199 (75%)	149 (100%)	0	100	100
1	S	145/199 (73%)	145 (100%)	0	100	100
1	T	148/199 (74%)	148 (100%)	0	100	100
1	U	148/199 (74%)	148 (100%)	0	100	100
1	d	145/199 (73%)	144 (99%)	1 (1%)	76	81
1	e	146/199 (73%)	146 (100%)	0	100	100
1	f	149/199 (75%)	149 (100%)	0	100	100
1	g	148/199 (74%)	148 (100%)	0	100	100
1	h	145/199 (73%)	145 (100%)	0	100	100
1	i	148/199 (74%)	148 (100%)	0	100	100
2	AB	367/380 (97%)	366 (100%)	1 (0%)	86	85
2	AD	367/380 (97%)	367 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AF	366/380 (96%)	365 (100%)	1 (0%)	86	85
2	BA	367/380 (97%)	366 (100%)	1 (0%)	86	85
2	BD	367/380 (97%)	365 (100%)	2 (0%)	81	83
2	BF	367/380 (97%)	366 (100%)	1 (0%)	86	85
2	CB	367/380 (97%)	366 (100%)	1 (0%)	86	85
2	CD	367/380 (97%)	367 (100%)	0	100	100
2	CF	367/380 (97%)	367 (100%)	0	100	100
2	DB	367/380 (97%)	367 (100%)	0	100	100
2	DD	367/380 (97%)	366 (100%)	1 (0%)	86	85
2	DF	366/380 (96%)	364 (100%)	2 (0%)	81	83
2	EB	354/380 (93%)	352 (99%)	2 (1%)	78	82
2	ED	367/380 (97%)	366 (100%)	1 (0%)	86	85
2	EF	367/380 (97%)	366 (100%)	1 (0%)	86	85
2	FD	367/380 (97%)	367 (100%)	0	100	100
2	FF	367/380 (97%)	366 (100%)	1 (0%)	86	85
2	FH	323/380 (85%)	323 (100%)	0	100	100
2	GD	367/380 (97%)	366 (100%)	1 (0%)	86	85
2	GF	367/380 (97%)	366 (100%)	1 (0%)	86	85
2	GH	367/380 (97%)	367 (100%)	0	100	100
2	HD	366/380 (96%)	365 (100%)	1 (0%)	86	85
2	HF	366/380 (96%)	366 (100%)	0	100	100
2	HH	367/380 (97%)	366 (100%)	1 (0%)	86	85
2	ID	366/380 (96%)	366 (100%)	0	100	100
2	IF	367/380 (97%)	367 (100%)	0	100	100
2	IH	366/380 (96%)	366 (100%)	0	100	100
2	JD	367/380 (97%)	365 (100%)	2 (0%)	81	83
2	JF	367/380 (97%)	367 (100%)	0	100	100
2	KD	366/380 (96%)	365 (100%)	1 (0%)	86	85
2	KF	367/380 (97%)	367 (100%)	0	100	100
2	KH	344/380 (90%)	343 (100%)	1 (0%)	86	85
2	LB	367/380 (97%)	363 (99%)	4 (1%)	65	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	LD	367/380 (97%)	365 (100%)	2 (0%)	81	83
2	LF	367/380 (97%)	366 (100%)	1 (0%)	86	85
2	MB	367/380 (97%)	366 (100%)	1 (0%)	86	85
2	MD	366/380 (96%)	365 (100%)	1 (0%)	86	85
2	MF	367/380 (97%)	367 (100%)	0	100	100
3	AC	359/378 (95%)	357 (99%)	2 (1%)	78	82
3	AE	360/378 (95%)	360 (100%)	0	100	100
3	BC	360/378 (95%)	360 (100%)	0	100	100
3	BE	359/378 (95%)	359 (100%)	0	100	100
3	BG	326/378 (86%)	326 (100%)	0	100	100
3	CC	363/378 (96%)	363 (100%)	0	100	100
3	CE	364/378 (96%)	363 (100%)	1 (0%)	86	85
3	CG	362/378 (96%)	362 (100%)	0	100	100
3	DC	361/378 (96%)	361 (100%)	0	100	100
3	DE	361/378 (96%)	359 (99%)	2 (1%)	78	82
3	DG	362/378 (96%)	362 (100%)	0	100	100
3	EC	362/378 (96%)	362 (100%)	0	100	100
3	EE	361/378 (96%)	361 (100%)	0	100	100
3	EG	361/378 (96%)	361 (100%)	0	100	100
3	FC	362/378 (96%)	362 (100%)	0	100	100
3	FE	363/378 (96%)	359 (99%)	4 (1%)	65	76
3	FG	362/378 (96%)	361 (100%)	1 (0%)	86	85
3	GC	363/378 (96%)	363 (100%)	0	100	100
3	GE	362/378 (96%)	361 (100%)	1 (0%)	86	85
3	GG	361/378 (96%)	361 (100%)	0	100	100
3	HC	360/378 (95%)	360 (100%)	0	100	100
3	HE	360/378 (95%)	360 (100%)	0	100	100
3	HG	359/378 (95%)	358 (100%)	1 (0%)	86	85
3	IC	350/378 (93%)	350 (100%)	0	100	100
3	IE	361/378 (96%)	361 (100%)	0	100	100
3	IG	360/378 (95%)	360 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	JC	362/378 (96%)	362 (100%)	0	100	100
3	JE	361/378 (96%)	360 (100%)	1 (0%)	86	85
3	JG	360/378 (95%)	360 (100%)	0	100	100
3	KC	359/378 (95%)	359 (100%)	0	100	100
3	KE	358/378 (95%)	357 (100%)	1 (0%)	86	85
3	KG	359/378 (95%)	358 (100%)	1 (0%)	86	85
3	LA	361/378 (96%)	361 (100%)	0	100	100
3	LC	360/378 (95%)	360 (100%)	0	100	100
3	LE	361/378 (96%)	361 (100%)	0	100	100
3	MA	359/378 (95%)	358 (100%)	1 (0%)	86	85
3	MC	361/378 (96%)	361 (100%)	0	100	100
3	ME	359/378 (95%)	359 (100%)	0	100	100
All	All	30176/32386 (93%)	30126 (100%)	50 (0%)	85	86

5 of 50 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	GF	274	THR
2	KD	273	LEU
1	d	119	HIS
2	HD	274	THR
2	JD	99	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 410 such sidechains are listed below:

Mol	Chain	Res	Type
2	HH	291	GLN
2	JF	14	ASN
1	f	132	ASN
3	IC	35	GLN
2	IF	134	GLN

5.3.3 RNA ⓘ

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 114 ligands modelled in this entry, 38 are monoatomic - leaving 76 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$
4	GDP	HF	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.72	7 (15%)
4	GDP	ID	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.81	8 (17%)
4	GDP	MB	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.79	8 (17%)
5	GTP	KG	501	6	33,34,34	0.97	1 (3%)	50,54,54	1.60	8 (16%)
4	GDP	LF	501	-	29,30,30	1.21	3 (10%)	45,47,47	1.80	9 (20%)
4	GDP	FH	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.77	7 (15%)
4	GDP	GH	501	-	29,30,30	1.13	3 (10%)	45,47,47	1.80	7 (15%)
5	GTP	BC	501	6	33,34,34	0.93	2 (6%)	50,54,54	1.57	8 (16%)
4	GDP	CB	501	-	29,30,30	1.13	3 (10%)	45,47,47	1.77	6 (13%)
4	GDP	FF	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.79	6 (13%)
5	GTP	FE	501	6	33,34,34	0.94	1 (3%)	50,54,54	1.57	8 (16%)
5	GTP	LC	501	6	33,34,34	0.92	2 (6%)	50,54,54	1.62	8 (16%)
4	GDP	DB	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.78	7 (15%)
5	GTP	EC	501	6	33,34,34	0.92	1 (3%)	50,54,54	1.62	8 (16%)
5	GTP	HG	501	6	33,34,34	0.92	1 (3%)	50,54,54	1.57	9 (18%)
4	GDP	GD	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.72	6 (13%)
5	GTP	LE	501	6	33,34,34	0.95	2 (6%)	50,54,54	1.60	8 (16%)
4	GDP	BD	501	-	29,30,30	1.18	3 (10%)	45,47,47	1.79	7 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GDP	HD	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.73	6 (13%)
5	GTP	JC	501	6	33,34,34	0.94	1 (3%)	50,54,54	1.59	8 (16%)
5	GTP	GC	501	6	33,34,34	0.89	1 (3%)	50,54,54	1.58	8 (16%)
5	GTP	MA	501	6	33,34,34	0.95	2 (6%)	50,54,54	1.56	8 (16%)
5	GTP	LA	501	6	33,34,34	0.95	2 (6%)	50,54,54	1.61	8 (16%)
4	GDP	CF	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.71	6 (13%)
4	GDP	AB	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.79	7 (15%)
5	GTP	CE	501	6	33,34,34	0.98	2 (6%)	50,54,54	1.59	8 (16%)
5	GTP	BG	501	6	33,34,34	0.89	1 (3%)	50,54,54	1.51	8 (16%)
4	GDP	BA	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.75	6 (13%)
4	GDP	GF	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	6 (13%)
4	GDP	KD	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	5 (11%)
4	GDP	ED	501	-	29,30,30	1.13	3 (10%)	45,47,47	1.80	7 (15%)
5	GTP	MC	501	6	33,34,34	1.03	4 (12%)	50,54,54	1.67	10 (20%)
5	GTP	IG	501	6	33,34,34	0.96	2 (6%)	50,54,54	1.62	10 (20%)
5	GTP	DC	501	6	33,34,34	0.96	1 (3%)	50,54,54	1.55	8 (16%)
5	GTP	GG	501	6	33,34,34	0.90	2 (6%)	50,54,54	1.58	8 (16%)
4	GDP	KH	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
4	GDP	LD	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.75	7 (15%)
5	GTP	FC	501	6	33,34,34	0.93	2 (6%)	50,54,54	1.56	8 (16%)
5	GTP	FG	501	6	33,34,34	0.94	0	50,54,54	1.52	8 (16%)
5	GTP	HC	501	6	33,34,34	0.93	2 (6%)	50,54,54	1.54	8 (16%)
5	GTP	HE	501	6	33,34,34	0.91	2 (6%)	50,54,54	1.55	8 (16%)
5	GTP	AE	501	6	33,34,34	0.92	2 (6%)	50,54,54	1.59	10 (20%)
4	GDP	EB	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.76	6 (13%)
5	GTP	JG	501	6	33,34,34	1.01	3 (9%)	50,54,54	1.64	9 (18%)
5	GTP	GE	501	6	33,34,34	0.90	1 (3%)	50,54,54	1.59	8 (16%)
4	GDP	LB	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.74	6 (13%)
4	GDP	CD	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.74	6 (13%)
5	GTP	AC	501	6	33,34,34	0.91	2 (6%)	50,54,54	1.65	9 (18%)
5	GTP	CC	501	6	33,34,34	0.94	1 (3%)	50,54,54	1.56	9 (18%)
5	GTP	IC	501	6	33,34,34	0.94	1 (3%)	50,54,54	1.55	9 (18%)
4	GDP	KF	501	-	29,30,30	1.19	3 (10%)	45,47,47	1.79	7 (15%)
5	GTP	DG	501	6	33,34,34	0.95	1 (3%)	50,54,54	1.59	8 (16%)
4	GDP	JF	501	-	29,30,30	1.18	3 (10%)	45,47,47	1.80	7 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GDP	MD	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.73	6 (13%)
5	GTP	CG	501	6	33,34,34	0.95	2 (6%)	50,54,54	1.55	8 (16%)
4	GDP	HH	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.75	8 (17%)
4	GDP	DD	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.75	6 (13%)
4	GDP	AD	501	-	29,30,30	1.18	3 (10%)	45,47,47	1.77	7 (15%)
5	GTP	KE	501	6	33,34,34	1.06	3 (9%)	50,54,54	1.56	8 (16%)
4	GDP	AF	501	-	29,30,30	1.16	4 (13%)	45,47,47	1.65	7 (15%)
5	GTP	ME	501	6	33,34,34	0.98	2 (6%)	50,54,54	1.66	9 (18%)
4	GDP	DF	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.73	6 (13%)
4	GDP	IH	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
4	GDP	JD	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.79	7 (15%)
5	GTP	BE	501	6	33,34,34	0.90	2 (6%)	50,54,54	1.56	8 (16%)
5	GTP	EG	501	6	33,34,34	0.98	2 (6%)	50,54,54	1.61	9 (18%)
4	GDP	MF	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.76	7 (15%)
4	GDP	FD	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.79	6 (13%)
4	GDP	EF	501	-	29,30,30	1.13	3 (10%)	45,47,47	1.74	6 (13%)
4	GDP	IF	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.76	6 (13%)
4	GDP	BF	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.74	7 (15%)
5	GTP	EE	501	6	33,34,34	0.94	2 (6%)	50,54,54	1.62	8 (16%)
5	GTP	IE	501	6	33,34,34	0.93	1 (3%)	50,54,54	1.55	8 (16%)
5	GTP	DE	501	6	33,34,34	0.95	2 (6%)	50,54,54	1.57	8 (16%)
5	GTP	JE	501	6	33,34,34	0.94	1 (3%)	50,54,54	1.60	8 (16%)
5	GTP	KC	501	6	33,34,34	1.01	3 (9%)	50,54,54	1.65	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
4	GDP	HF	501	-	-	3/16/32/32	0/3/3/3
4	GDP	ID	501	-	-	4/16/32/32	0/3/3/3
4	GDP	MB	501	-	-	2/16/32/32	0/3/3/3
5	GTP	KG	501	6	-	5/22/38/38	0/3/3/3
4	GDP	LF	501	-	-	4/16/32/32	0/3/3/3
4	GDP	FH	501	-	-	3/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GDP	GH	501	-	-	3/16/32/32	0/3/3/3
5	GTP	BC	501	6	-	3/22/38/38	0/3/3/3
4	GDP	CB	501	-	-	2/16/32/32	0/3/3/3
4	GDP	FF	501	-	-	2/16/32/32	0/3/3/3
5	GTP	FE	501	6	-	6/22/38/38	0/3/3/3
5	GTP	LC	501	6	-	2/22/38/38	0/3/3/3
4	GDP	DB	501	-	-	2/16/32/32	0/3/3/3
5	GTP	EC	501	6	-	5/22/38/38	0/3/3/3
5	GTP	HG	501	6	-	5/22/38/38	0/3/3/3
4	GDP	GD	501	-	-	4/16/32/32	0/3/3/3
5	GTP	LE	501	6	-	6/22/38/38	0/3/3/3
4	GDP	BD	501	-	-	2/16/32/32	0/3/3/3
4	GDP	HD	501	-	-	2/16/32/32	0/3/3/3
5	GTP	JC	501	6	-	6/22/38/38	0/3/3/3
5	GTP	GC	501	6	-	6/22/38/38	0/3/3/3
5	GTP	MA	501	6	-	0/22/38/38	0/3/3/3
5	GTP	LA	501	6	-	6/22/38/38	0/3/3/3
4	GDP	CF	501	-	-	1/16/32/32	0/3/3/3
4	GDP	AB	501	-	-	1/16/32/32	0/3/3/3
5	GTP	CE	501	6	-	5/22/38/38	0/3/3/3
5	GTP	BG	501	6	-	6/22/38/38	0/3/3/3
4	GDP	BA	501	-	-	3/16/32/32	0/3/3/3
4	GDP	GF	501	-	-	3/16/32/32	0/3/3/3
4	GDP	KD	501	-	-	1/16/32/32	0/3/3/3
4	GDP	ED	501	-	-	3/16/32/32	0/3/3/3
5	GTP	MC	501	6	-	5/22/38/38	0/3/3/3
5	GTP	IG	501	6	-	2/22/38/38	0/3/3/3
5	GTP	DC	501	6	-	7/22/38/38	0/3/3/3
5	GTP	GG	501	6	-	4/22/38/38	0/3/3/3
4	GDP	KH	501	-	-	2/16/32/32	0/3/3/3
4	GDP	LD	501	-	-	2/16/32/32	0/3/3/3
5	GTP	FC	501	6	-	4/22/38/38	0/3/3/3
5	GTP	FG	501	6	-	7/22/38/38	0/3/3/3
5	GTP	HC	501	6	-	7/22/38/38	0/3/3/3
5	GTP	HE	501	6	-	7/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GTP	AE	501	6	-	3/22/38/38	0/3/3/3
4	GDP	EB	501	-	-	3/16/32/32	0/3/3/3
5	GTP	JG	501	6	-	3/22/38/38	0/3/3/3
5	GTP	GE	501	6	-	7/22/38/38	0/3/3/3
4	GDP	LB	501	-	-	4/16/32/32	0/3/3/3
4	GDP	CD	501	-	-	1/16/32/32	0/3/3/3
5	GTP	AC	501	6	-	3/22/38/38	0/3/3/3
5	GTP	CC	501	6	-	4/22/38/38	0/3/3/3
5	GTP	IC	501	6	-	9/22/38/38	0/3/3/3
4	GDP	KF	501	-	-	1/16/32/32	0/3/3/3
5	GTP	DG	501	6	-	6/22/38/38	0/3/3/3
4	GDP	JF	501	-	-	4/16/32/32	0/3/3/3
4	GDP	MD	501	-	-	2/16/32/32	0/3/3/3
5	GTP	CG	501	6	-	6/22/38/38	0/3/3/3
4	GDP	HH	501	-	-	2/16/32/32	0/3/3/3
4	GDP	DD	501	-	-	2/16/32/32	0/3/3/3
4	GDP	AD	501	-	-	3/16/32/32	0/3/3/3
5	GTP	KE	501	6	-	4/22/38/38	0/3/3/3
4	GDP	AF	501	-	-	5/16/32/32	0/3/3/3
5	GTP	ME	501	6	-	5/22/38/38	0/3/3/3
4	GDP	DF	501	-	-	1/16/32/32	0/3/3/3
4	GDP	IH	501	-	-	1/16/32/32	0/3/3/3
4	GDP	JD	501	-	-	2/16/32/32	0/3/3/3
5	GTP	BE	501	6	-	4/22/38/38	0/3/3/3
5	GTP	EG	501	6	-	5/22/38/38	0/3/3/3
4	GDP	MF	501	-	-	2/16/32/32	0/3/3/3
4	GDP	FD	501	-	-	1/16/32/32	0/3/3/3
4	GDP	EF	501	-	-	2/16/32/32	0/3/3/3
4	GDP	IF	501	-	-	4/16/32/32	0/3/3/3
4	GDP	BF	501	-	-	2/16/32/32	0/3/3/3
5	GTP	EE	501	6	-	7/22/38/38	0/3/3/3
5	GTP	IE	501	6	-	8/22/38/38	0/3/3/3
5	GTP	DE	501	6	-	7/22/38/38	0/3/3/3
5	GTP	JE	501	6	-	7/22/38/38	0/3/3/3
5	GTP	KC	501	6	-	5/22/38/38	0/3/3/3

The worst 5 of 180 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	AB	501	GDP	C5-C4	3.04	1.47	1.38
4	IF	501	GDP	C5-C4	3.03	1.47	1.38
4	HF	501	GDP	C5-C4	3.03	1.47	1.38
4	HH	501	GDP	C5-C4	3.03	1.47	1.38
4	KH	501	GDP	C5-C4	3.03	1.47	1.38

The worst 5 of 571 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	AB	501	GDP	C5-C4-N3	-6.29	118.38	128.39
4	AD	501	GDP	C5-C4-N3	-6.29	118.38	128.39
4	DB	501	GDP	C5-C4-N3	-6.28	118.40	128.39
4	KD	501	GDP	C5-C4-N3	-6.27	118.41	128.39
4	BD	501	GDP	C5-C4-N3	-6.25	118.44	128.39

There are no chirality outliers.

5 of 288 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	AB	501	GDP	C5'-O5'-PA-O1A
4	AD	501	GDP	C5'-O5'-PA-O1A
4	AF	501	GDP	C5'-O5'-PA-O3A
4	AF	501	GDP	C5'-O5'-PA-O2A
4	AF	501	GDP	O4'-C4'-C5'-O5'

There are no ring outliers.

63 monomers are involved in 112 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	HF	501	GDP	1	0
4	ID	501	GDP	3	0
5	KG	501	GTP	1	0
4	LF	501	GDP	2	0
4	FH	501	GDP	1	0
4	GH	501	GDP	4	0
5	BC	501	GTP	2	0
4	CB	501	GDP	3	0
4	FF	501	GDP	2	0
5	FE	501	GTP	1	0
5	LC	501	GTP	2	0

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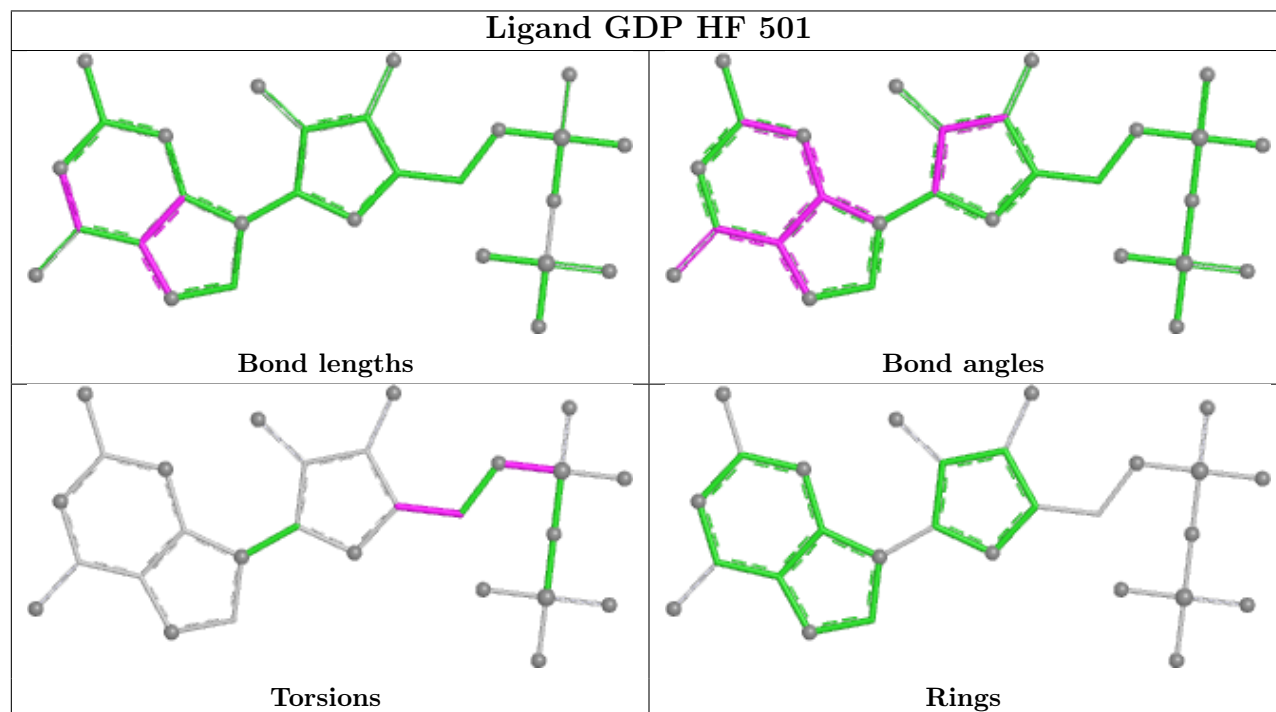
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	EC	501	GTP	3	0
5	HG	501	GTP	3	0
4	GD	501	GDP	1	0
5	LE	501	GTP	3	0
4	BD	501	GDP	1	0
4	HD	501	GDP	3	0
5	MA	501	GTP	1	0
5	LA	501	GTP	2	0
4	CF	501	GDP	1	0
4	AB	501	GDP	3	0
5	BG	501	GTP	3	0
4	BA	501	GDP	1	0
4	GF	501	GDP	1	0
4	KD	501	GDP	2	0
5	DC	501	GTP	2	0
5	GG	501	GTP	1	0
4	KH	501	GDP	1	0
4	LD	501	GDP	3	0
5	FC	501	GTP	1	0
5	FG	501	GTP	1	0
5	HC	501	GTP	1	0
5	HE	501	GTP	2	0
5	AE	501	GTP	1	0
4	EB	501	GDP	2	0
5	GE	501	GTP	3	0
4	LB	501	GDP	4	0
4	CD	501	GDP	2	0
5	AC	501	GTP	1	0
5	CC	501	GTP	1	0
5	IC	501	GTP	1	0
4	KF	501	GDP	1	0
5	DG	501	GTP	1	0
4	JF	501	GDP	1	0
4	MD	501	GDP	1	0
5	CG	501	GTP	3	0
4	HH	501	GDP	2	0
4	AD	501	GDP	3	0
5	KE	501	GTP	1	0
4	AF	501	GDP	3	0
5	ME	501	GTP	1	0
4	IH	501	GDP	1	0
4	JD	501	GDP	4	0

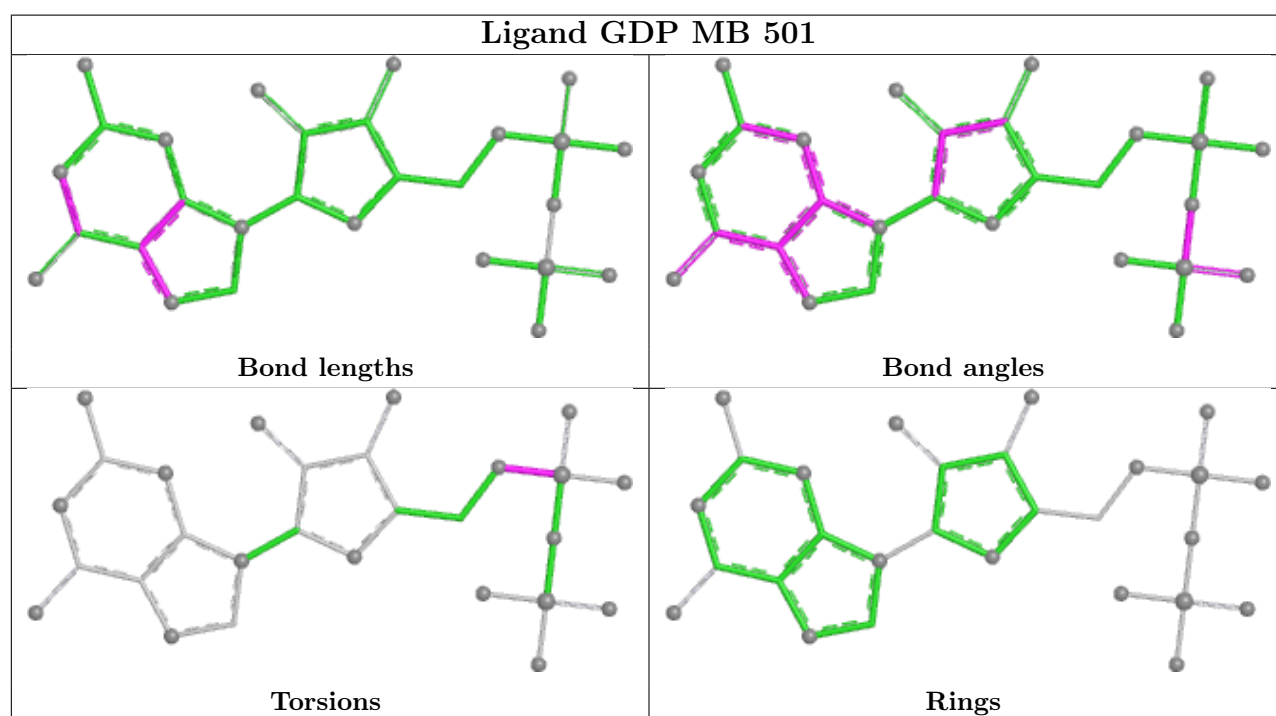
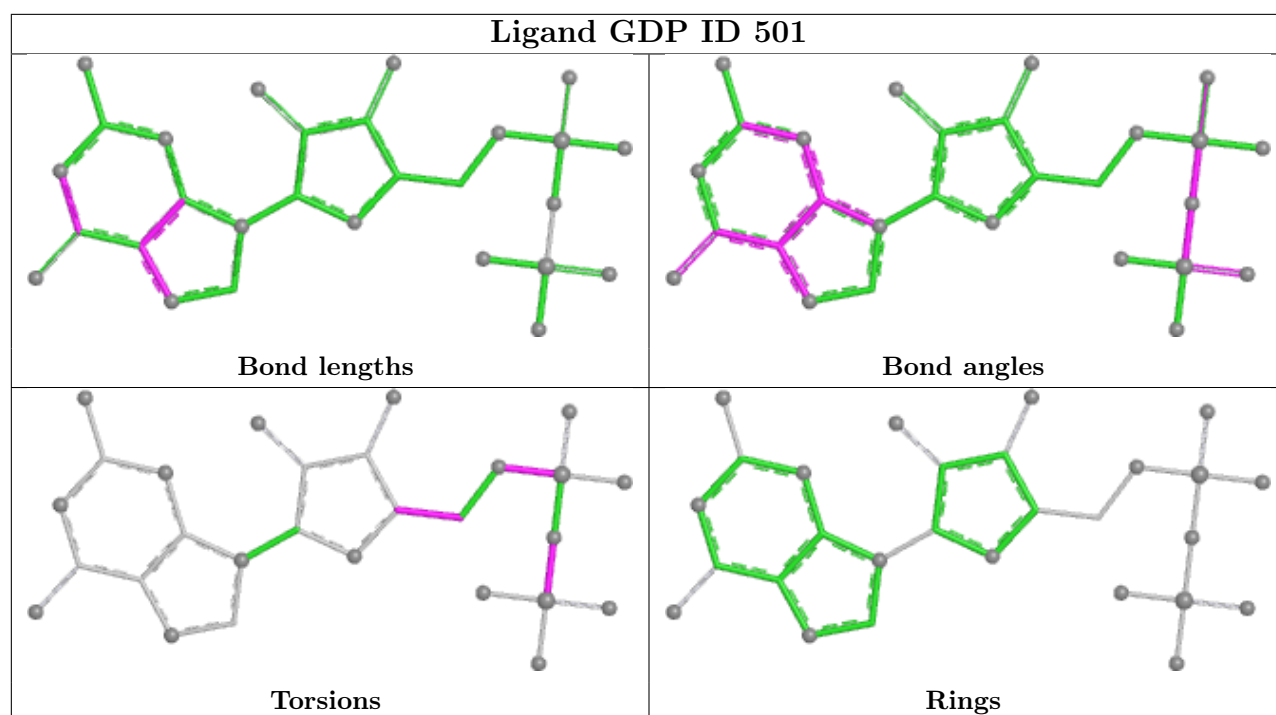
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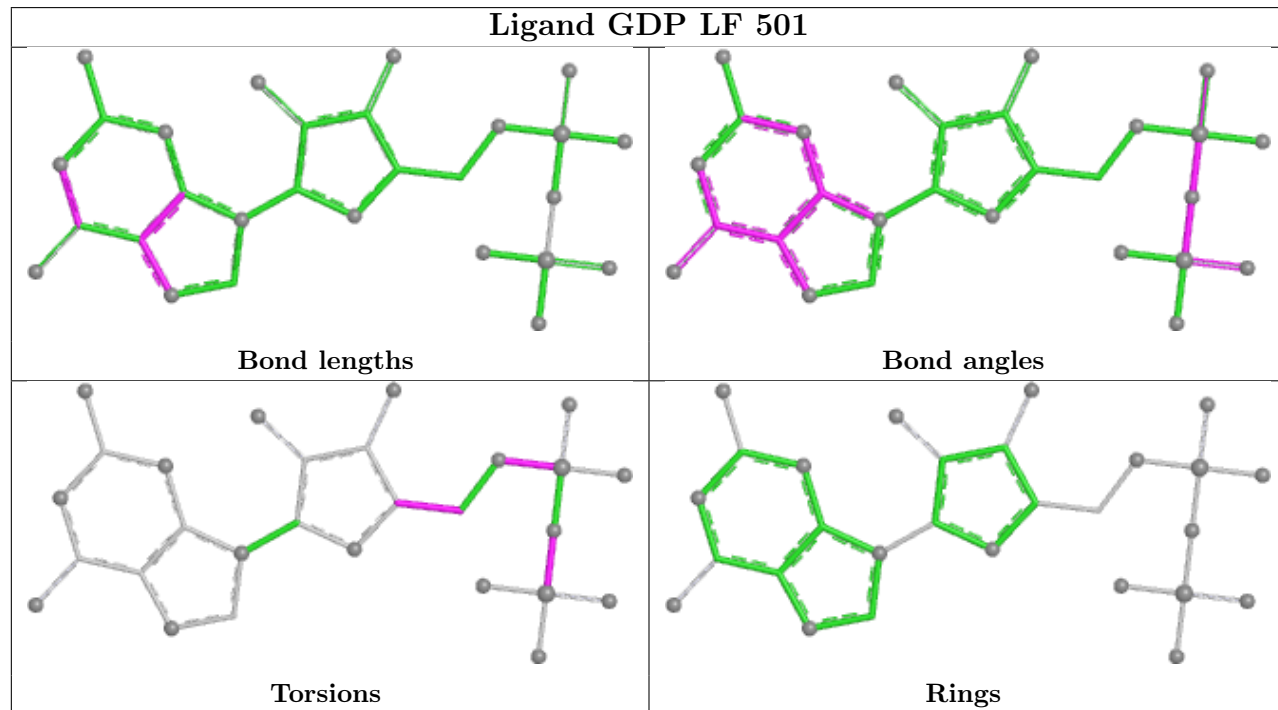
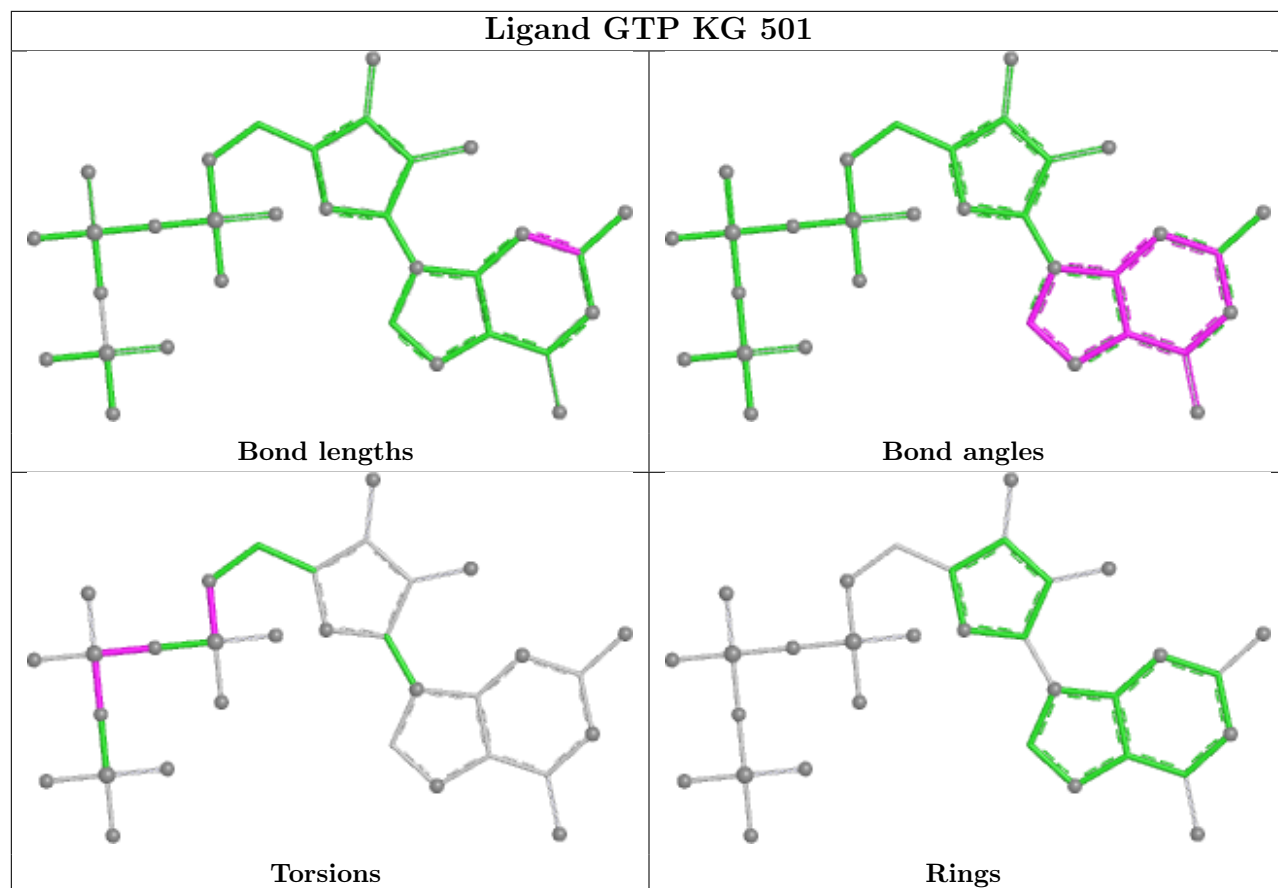
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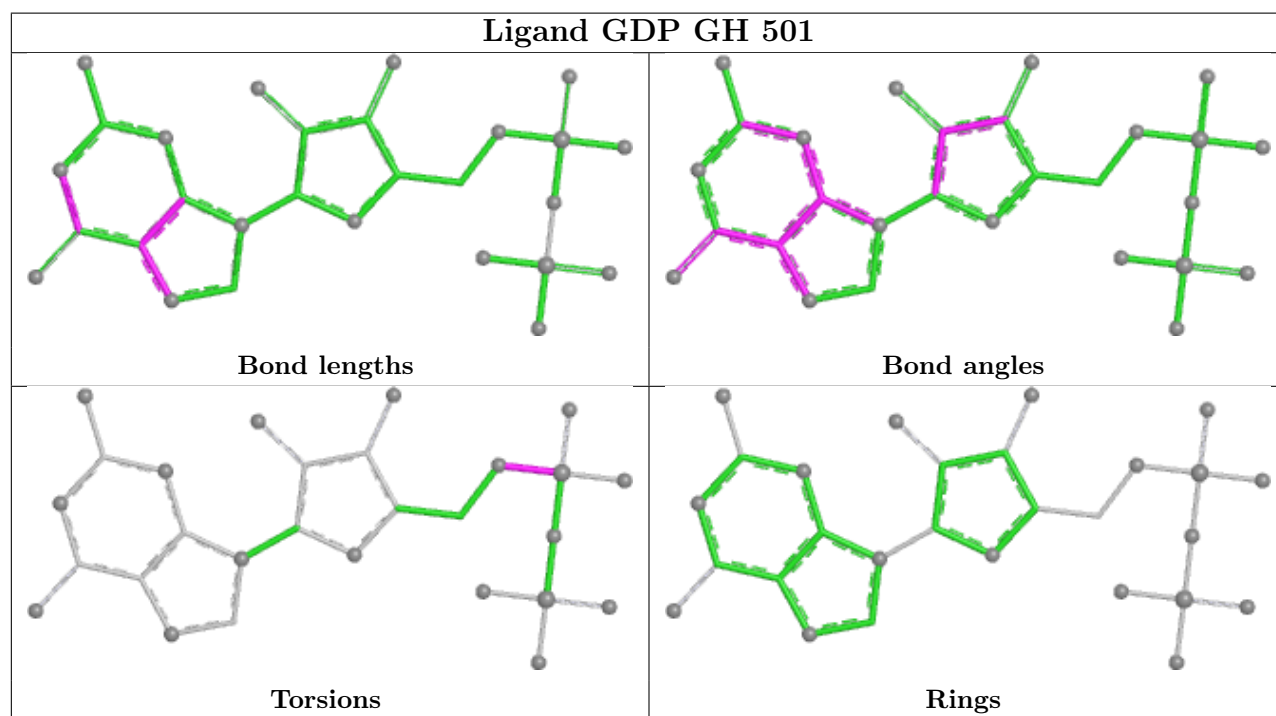
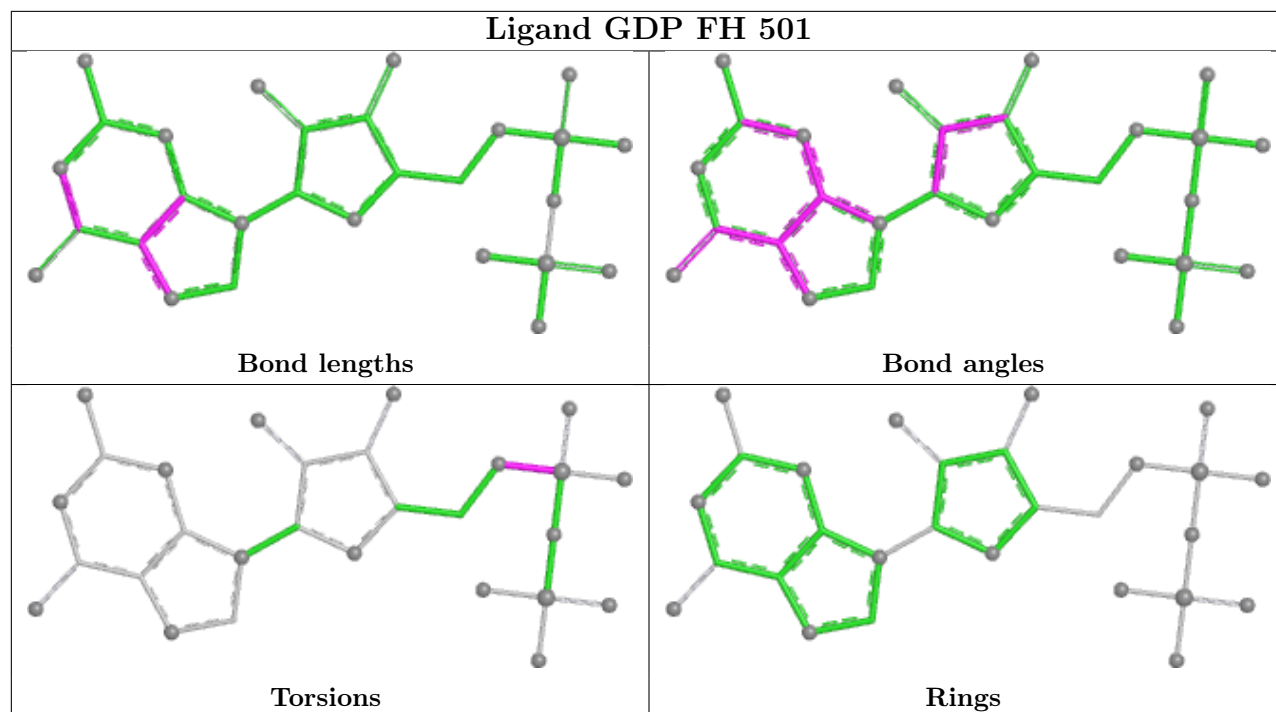
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	EG	501	GTP	1	0
4	MF	501	GDP	1	0
4	FD	501	GDP	1	0
4	EF	501	GDP	1	0
4	IF	501	GDP	1	0
4	BF	501	GDP	1	0
5	EE	501	GTP	1	0
5	IE	501	GTP	2	0
5	JE	501	GTP	1	0
5	KC	501	GTP	3	0

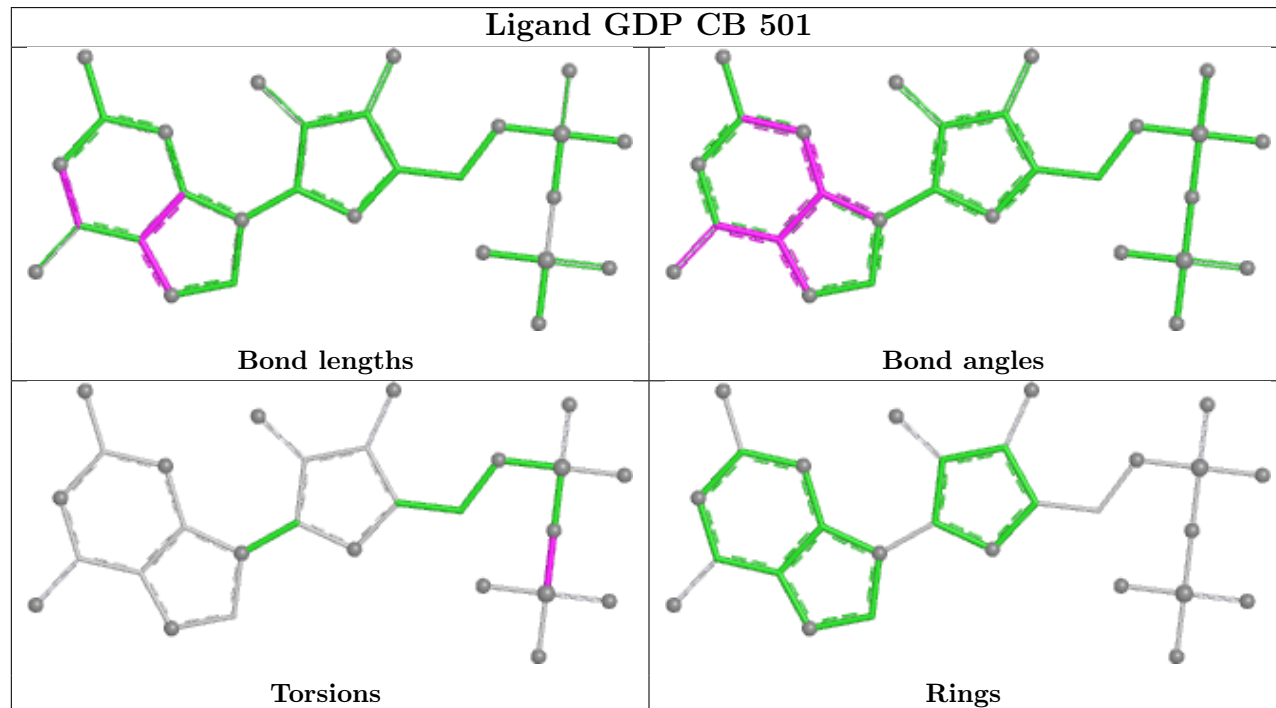
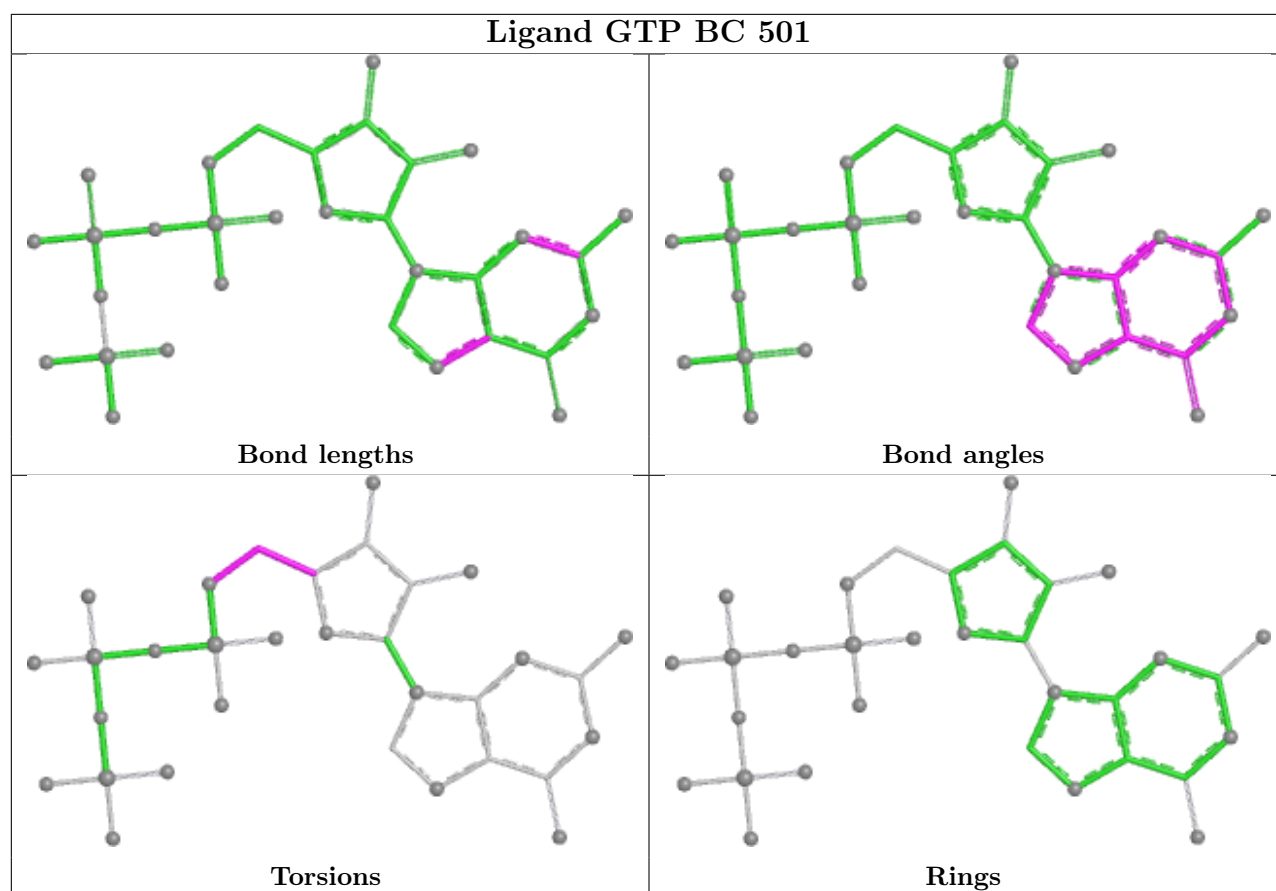
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

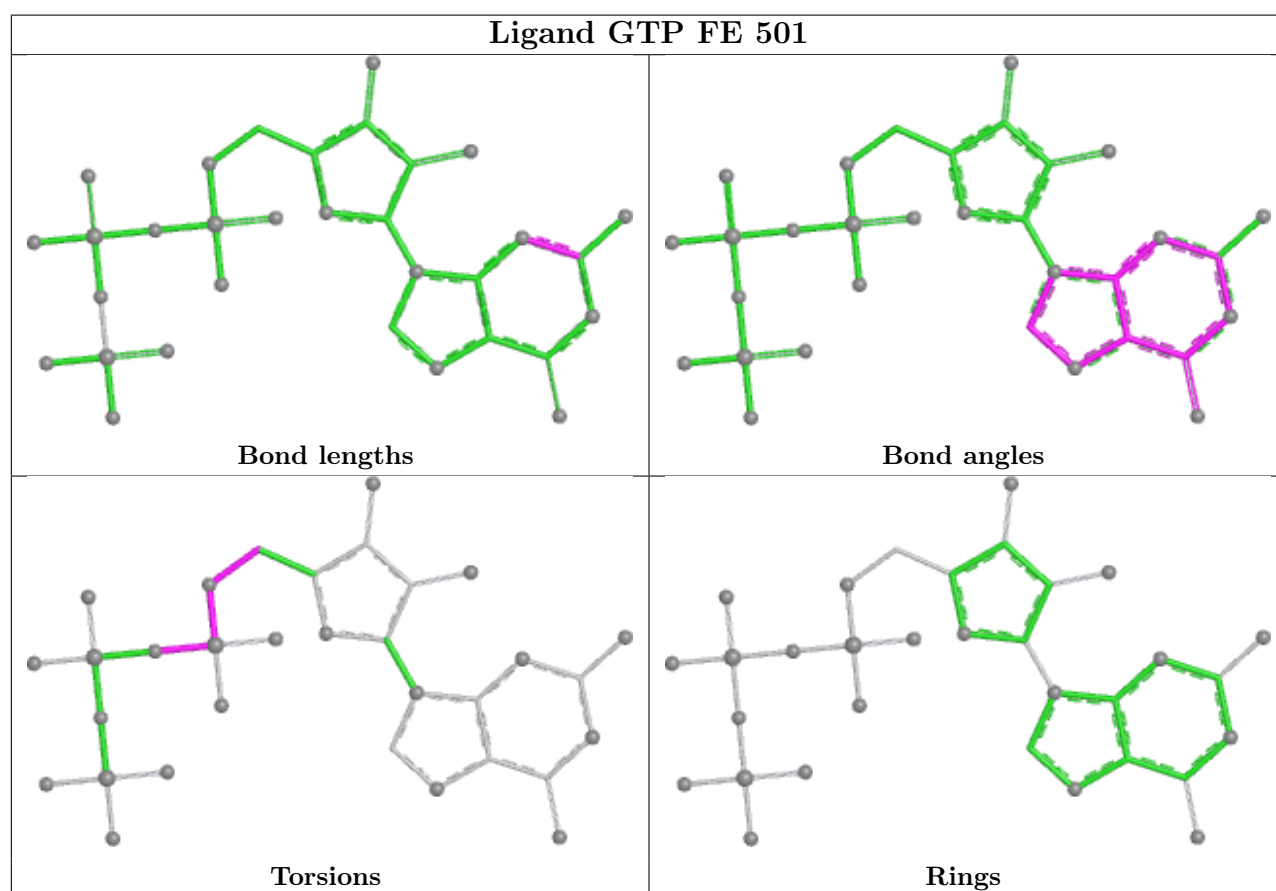
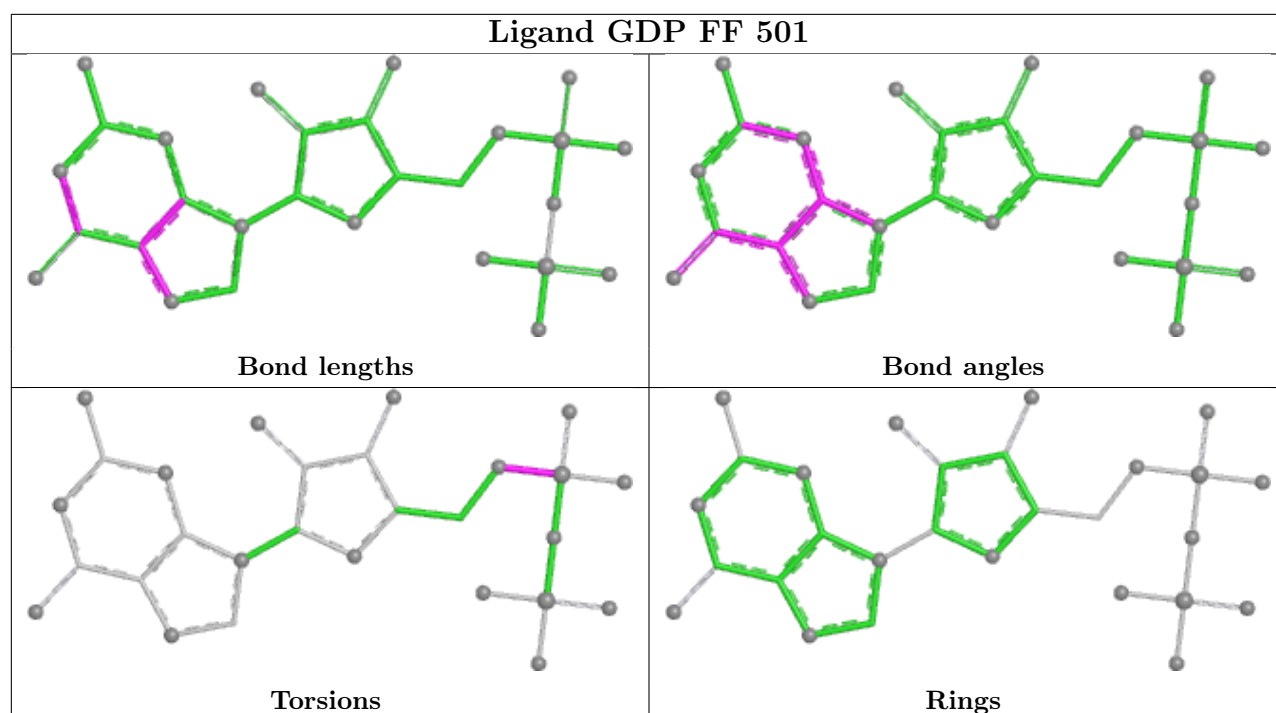


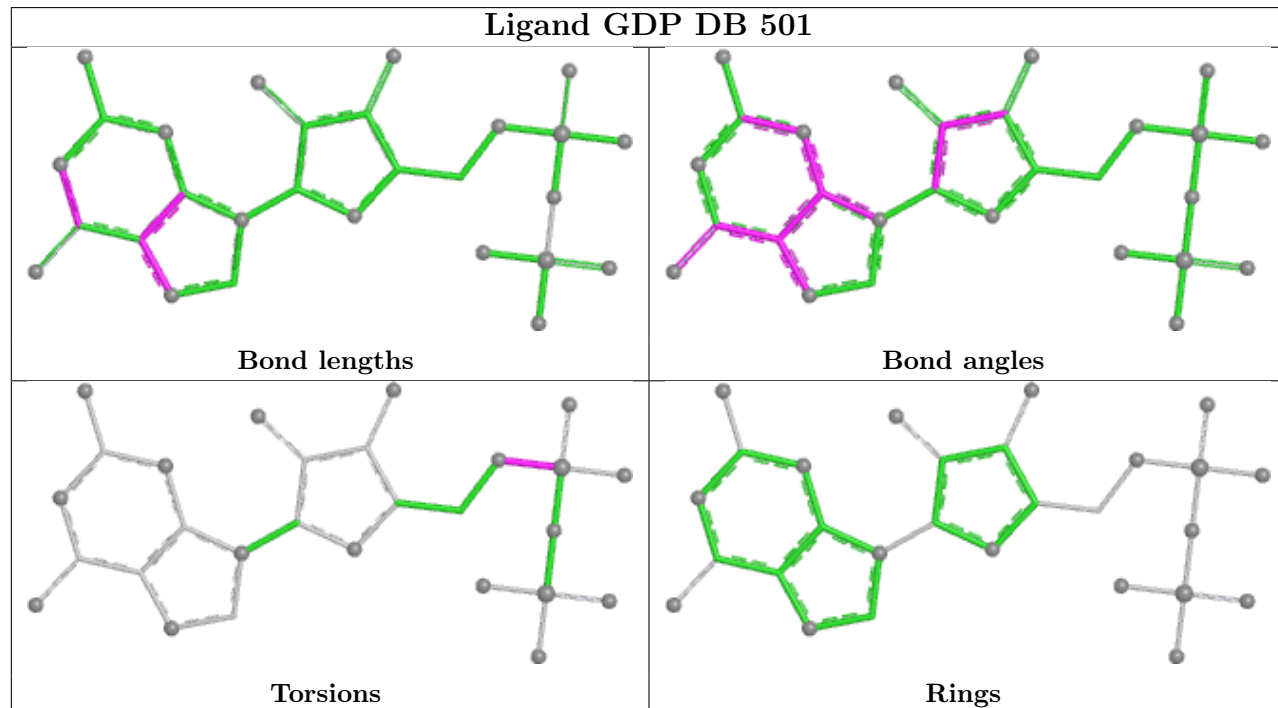
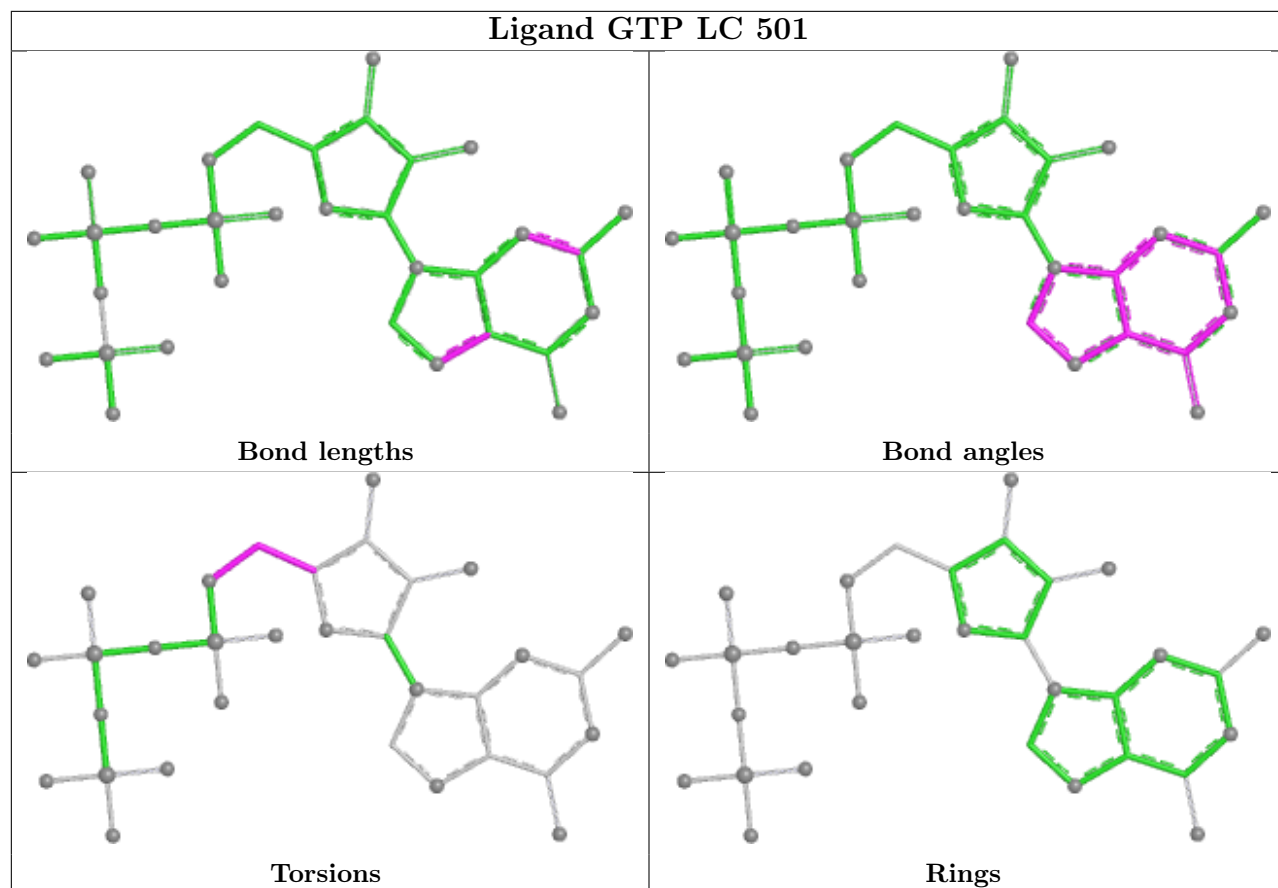




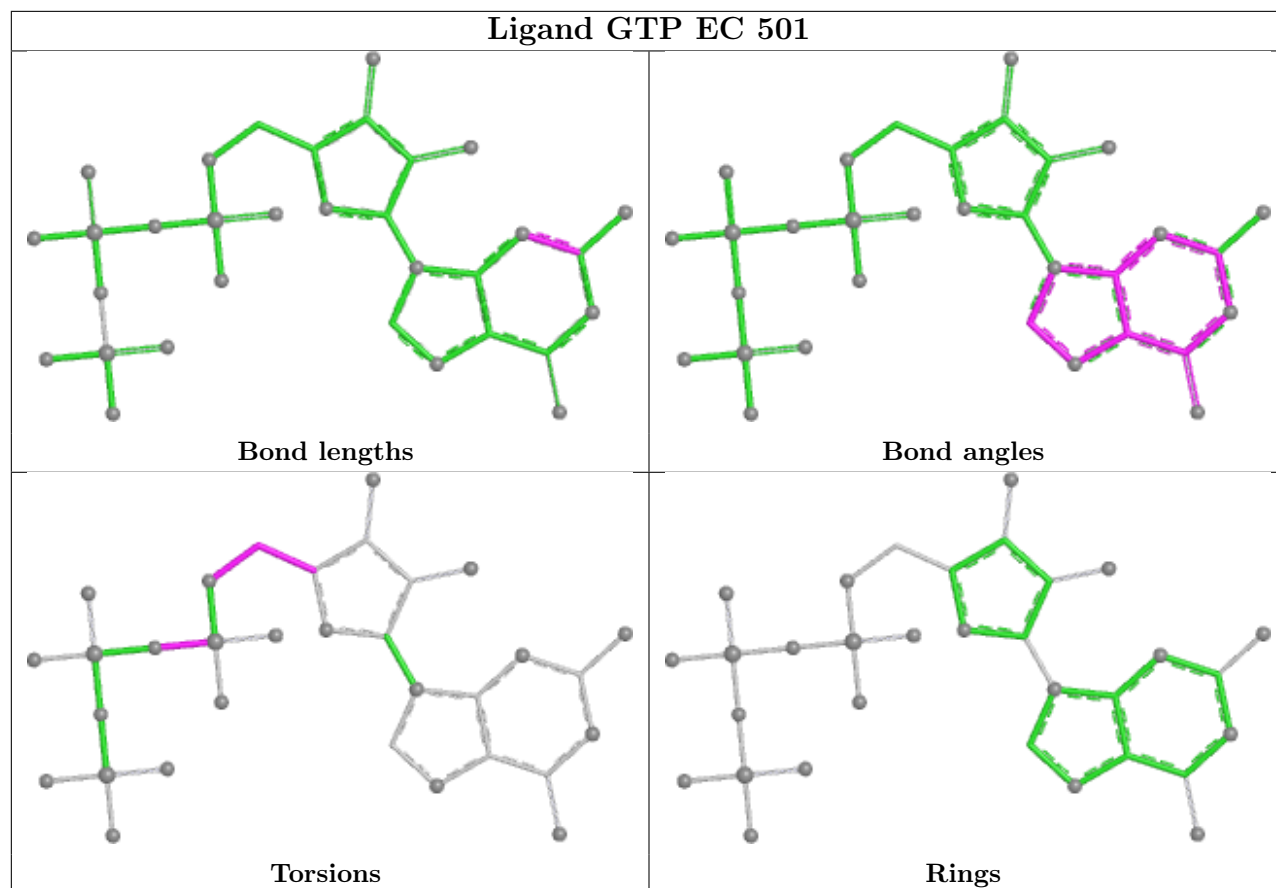




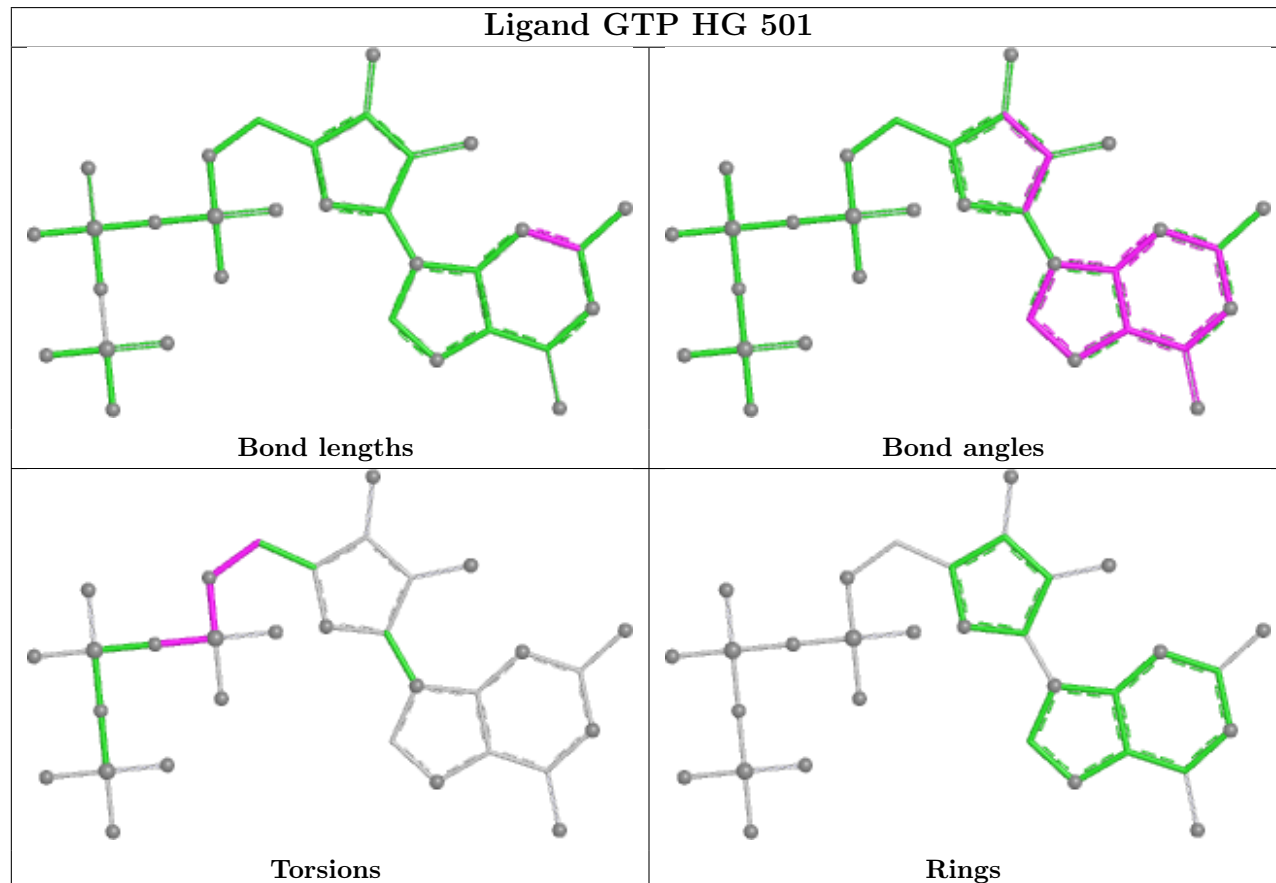


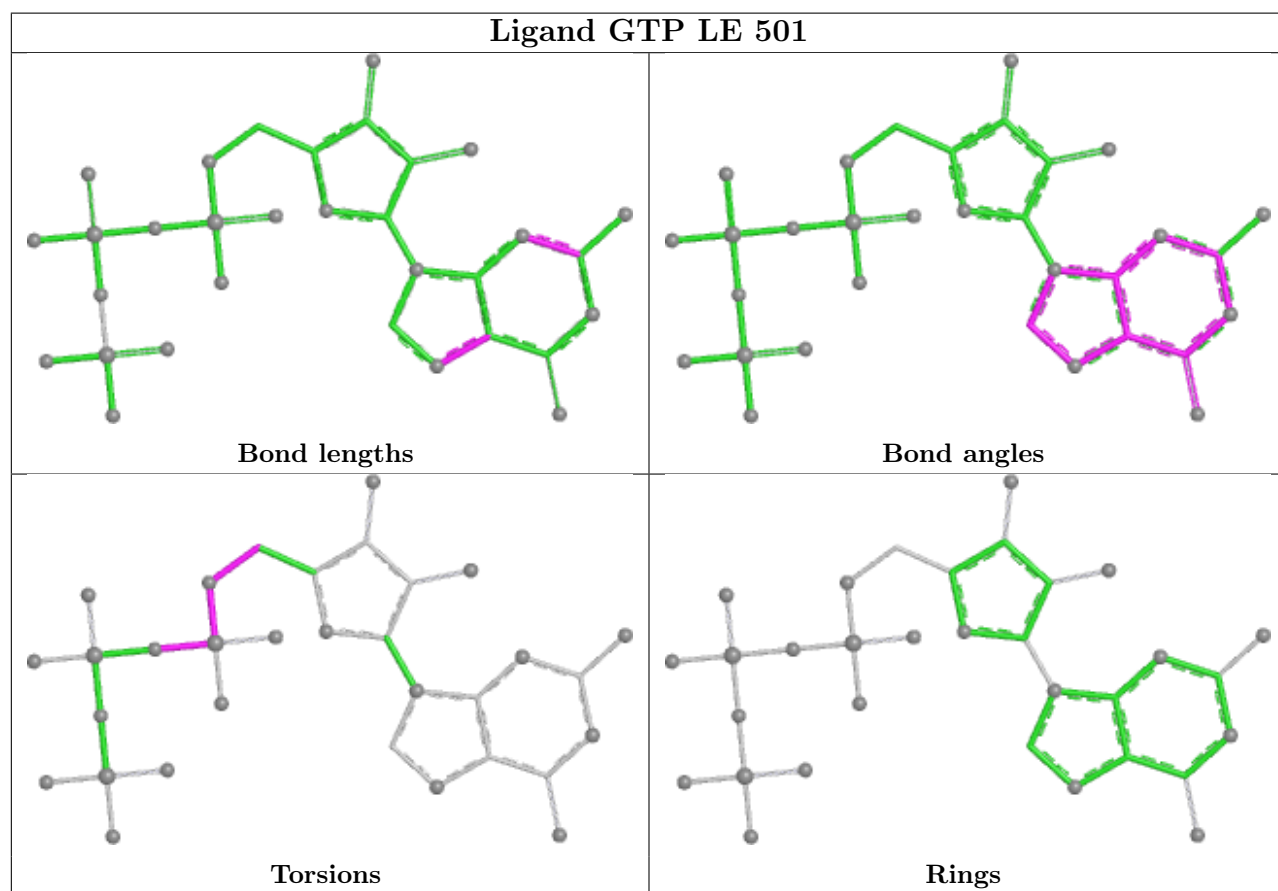
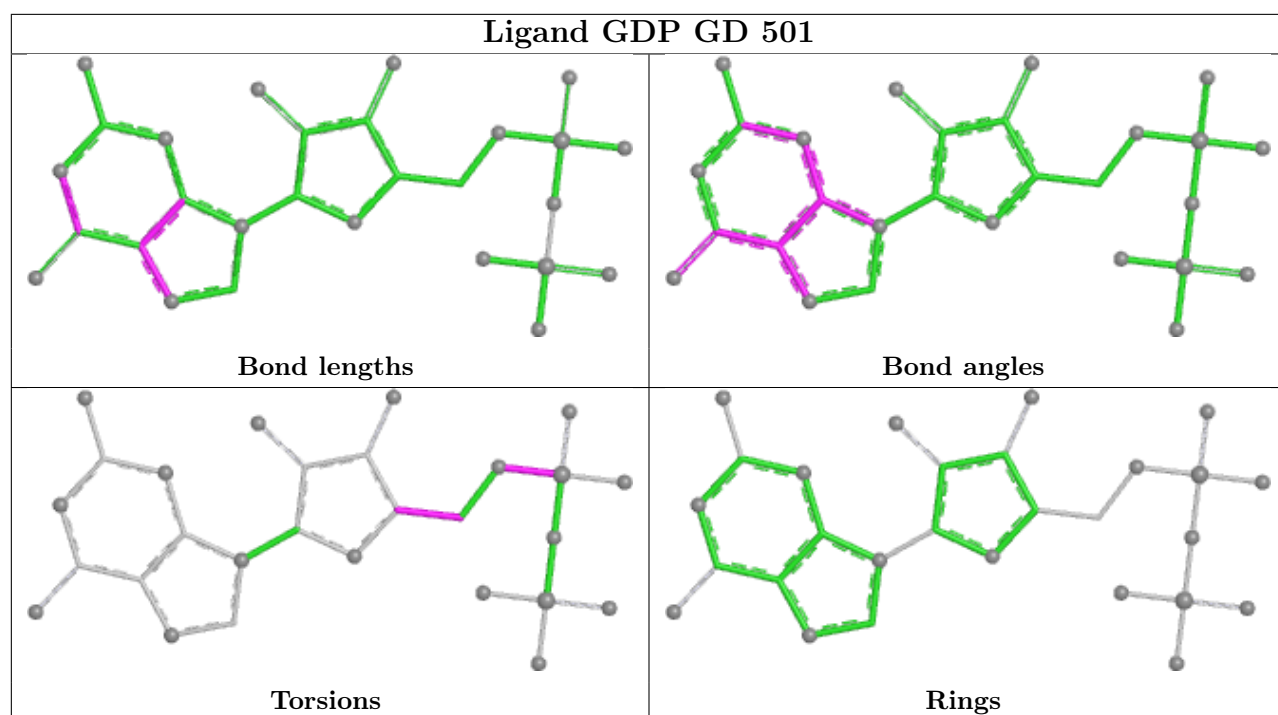


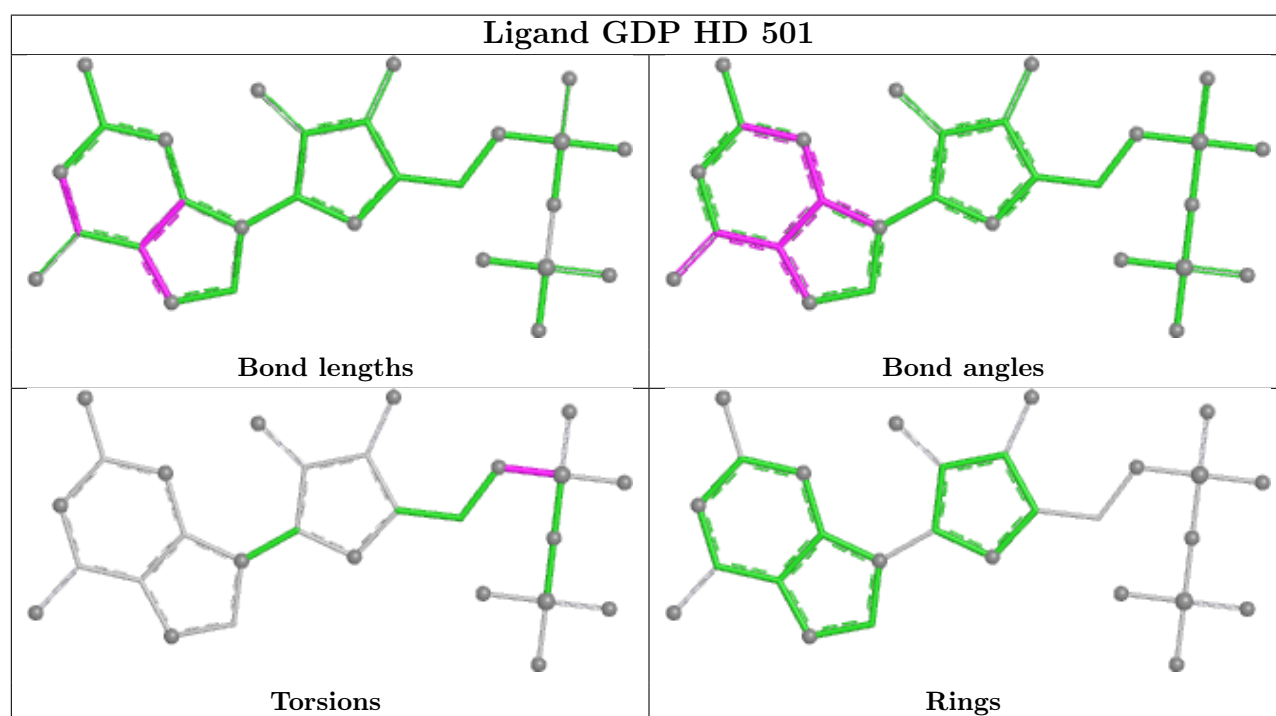
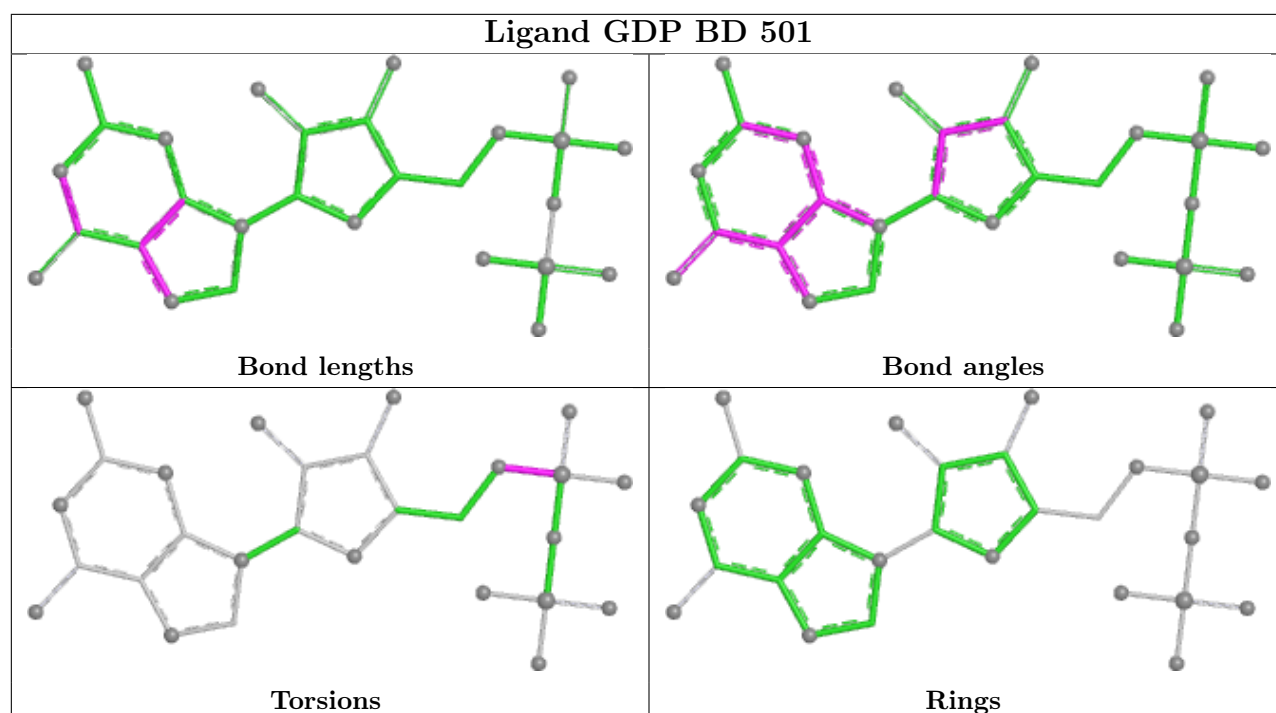
Ligand GTP EC 501



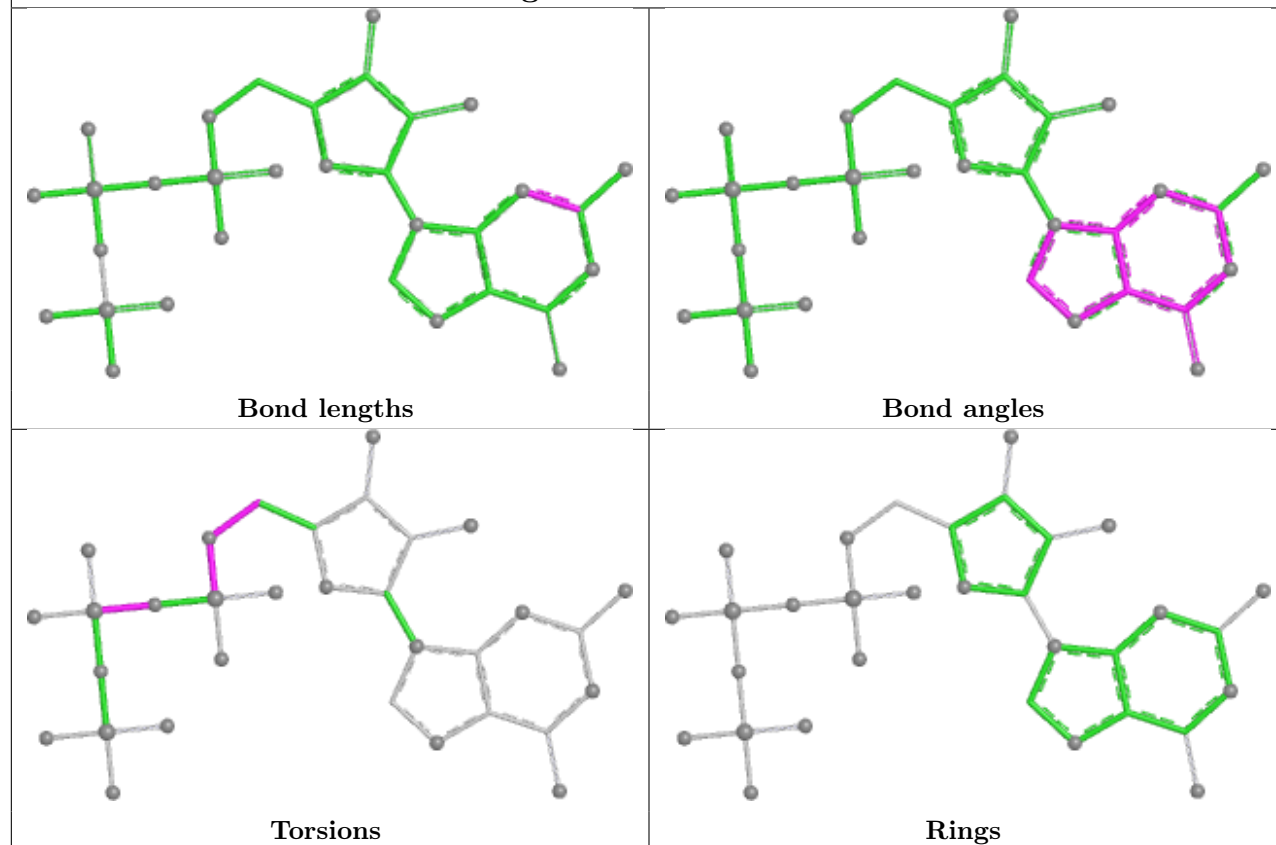
Ligand GTP HG 501



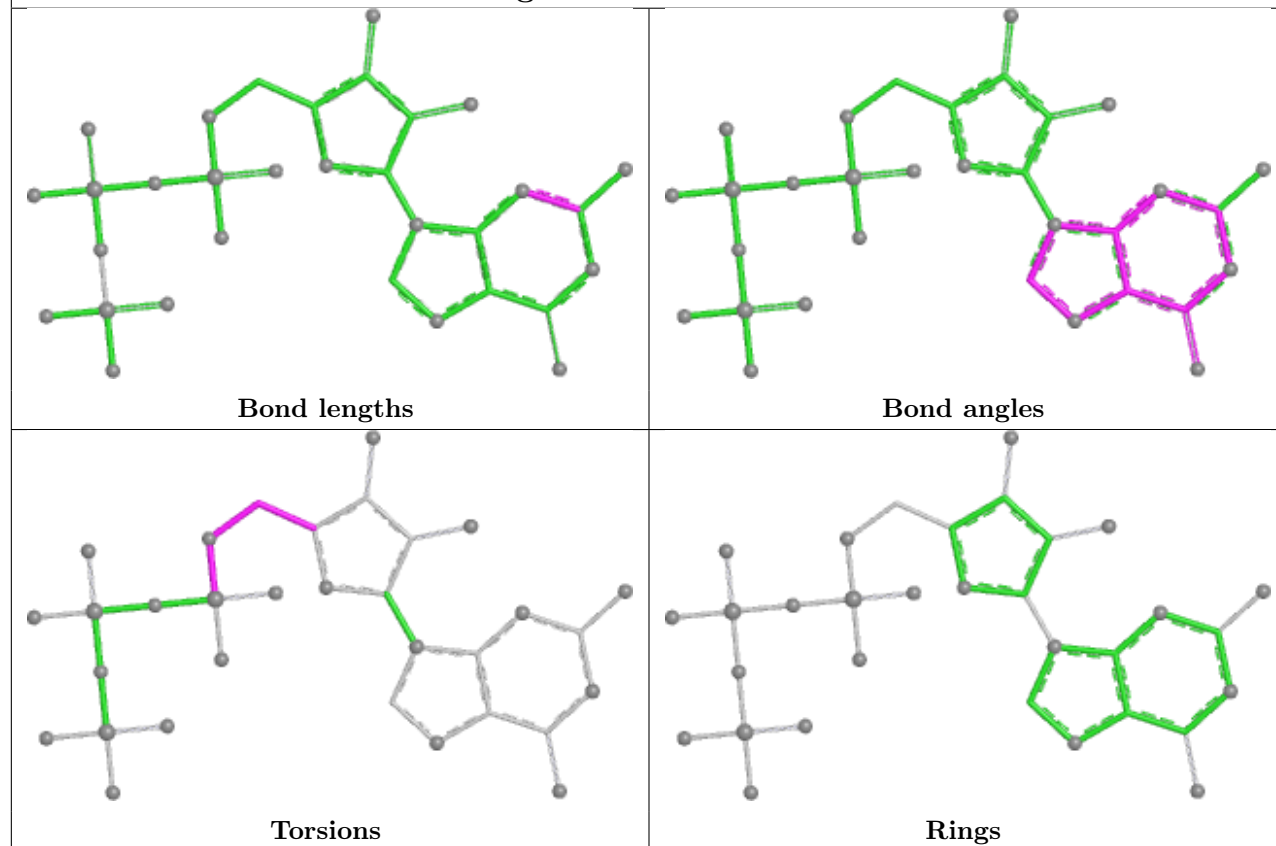




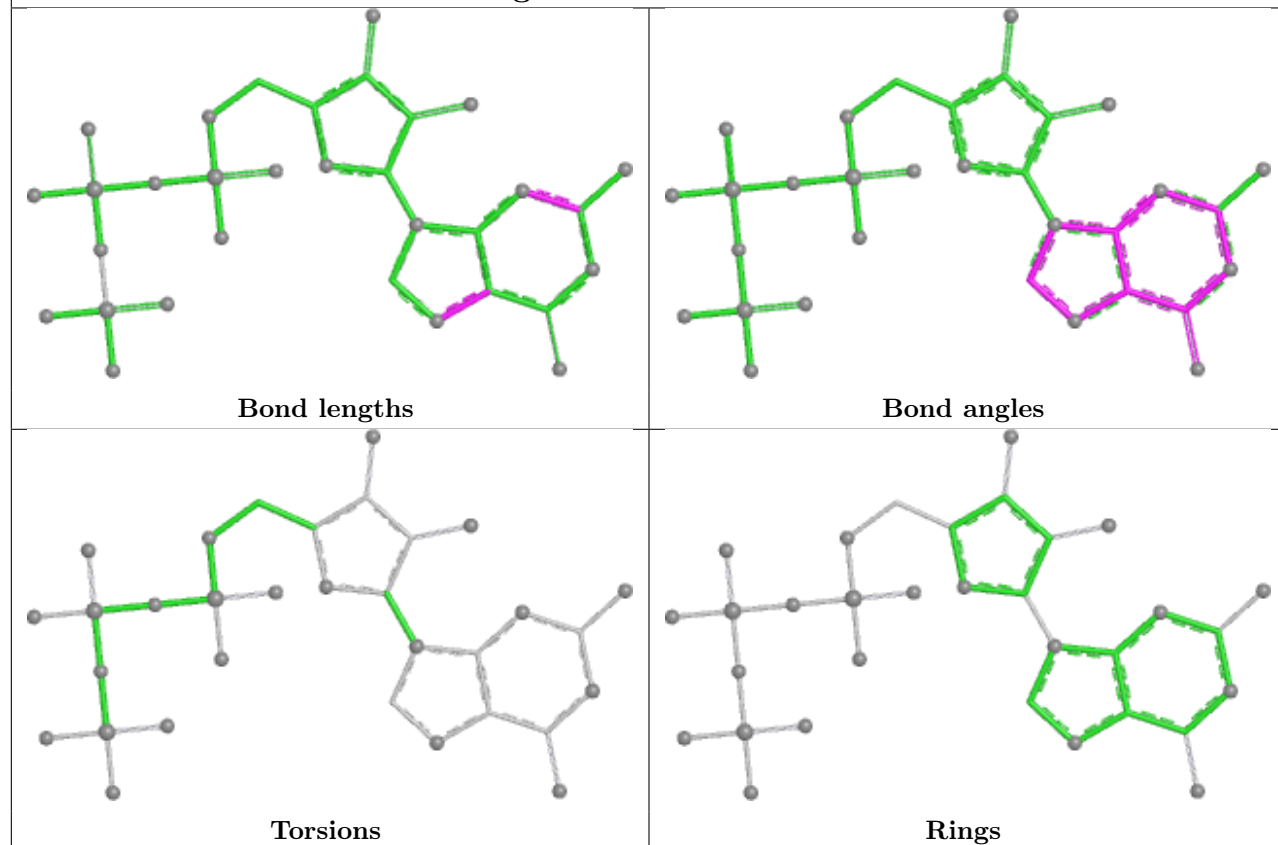
Ligand GTP JC 501



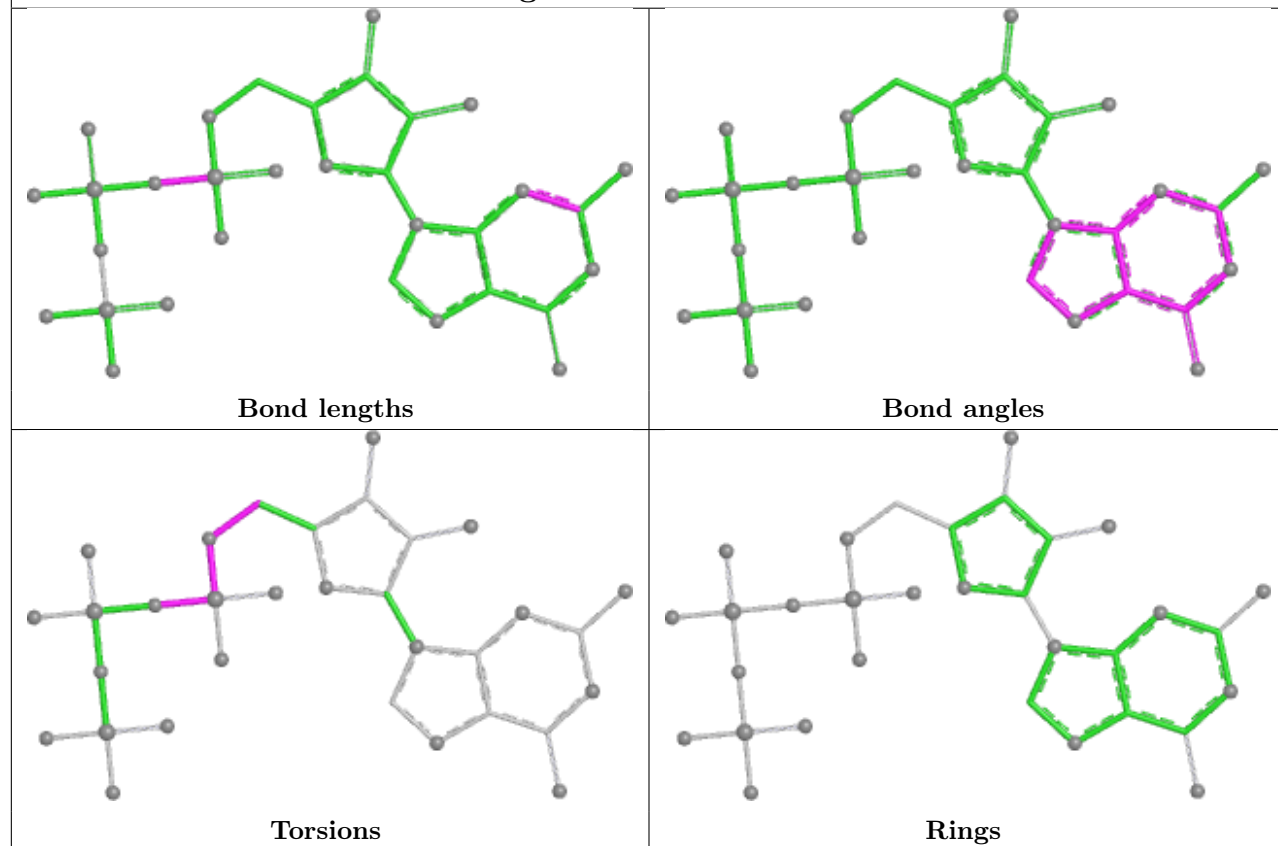
Ligand GTP GC 501

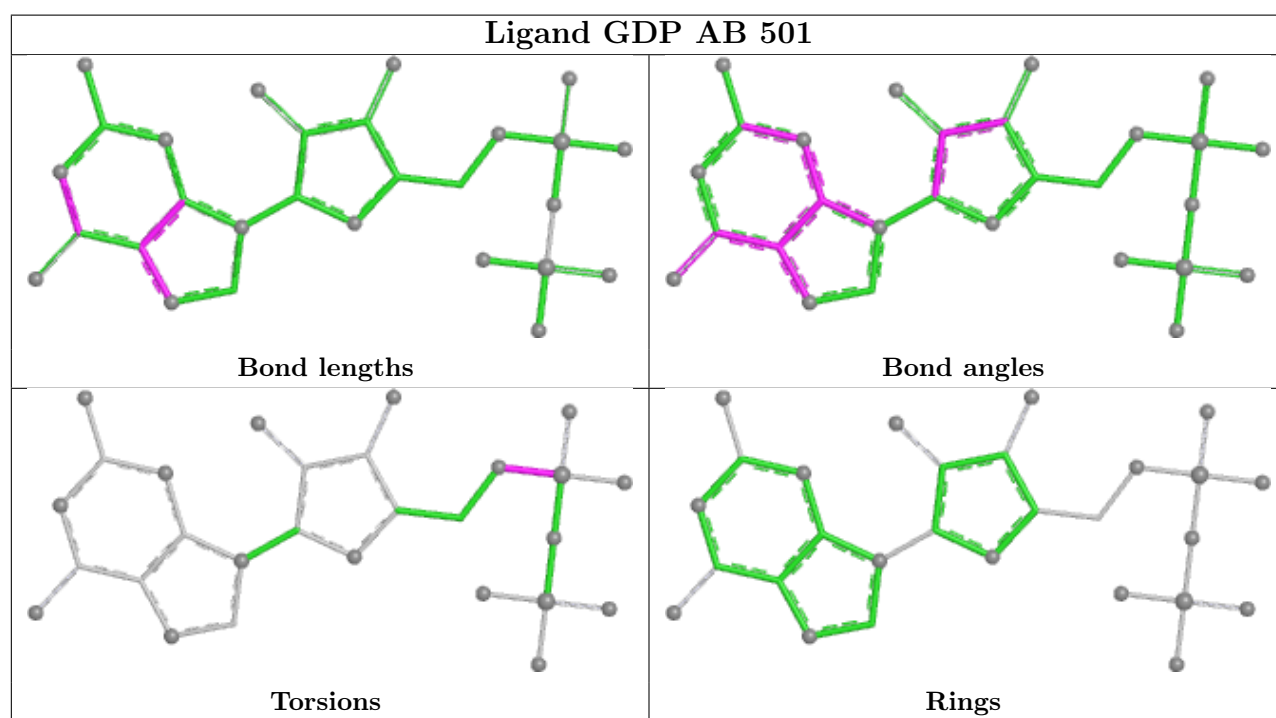
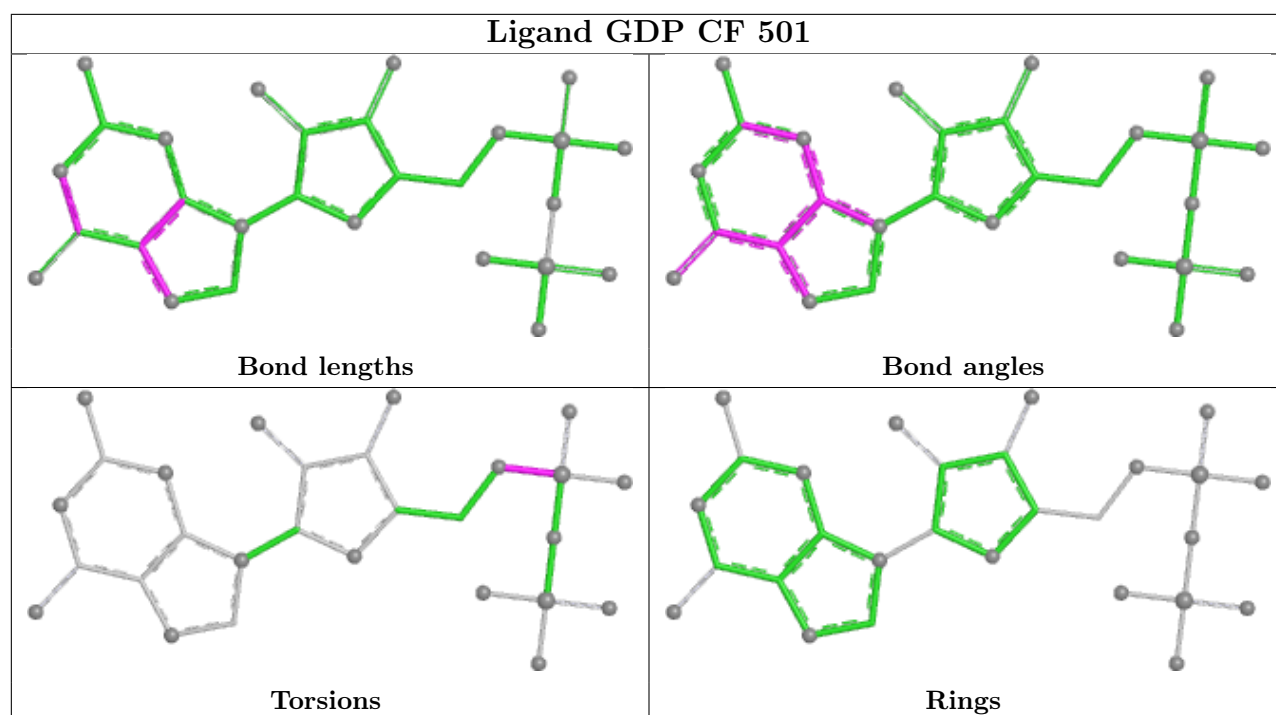


Ligand GTP MA 501

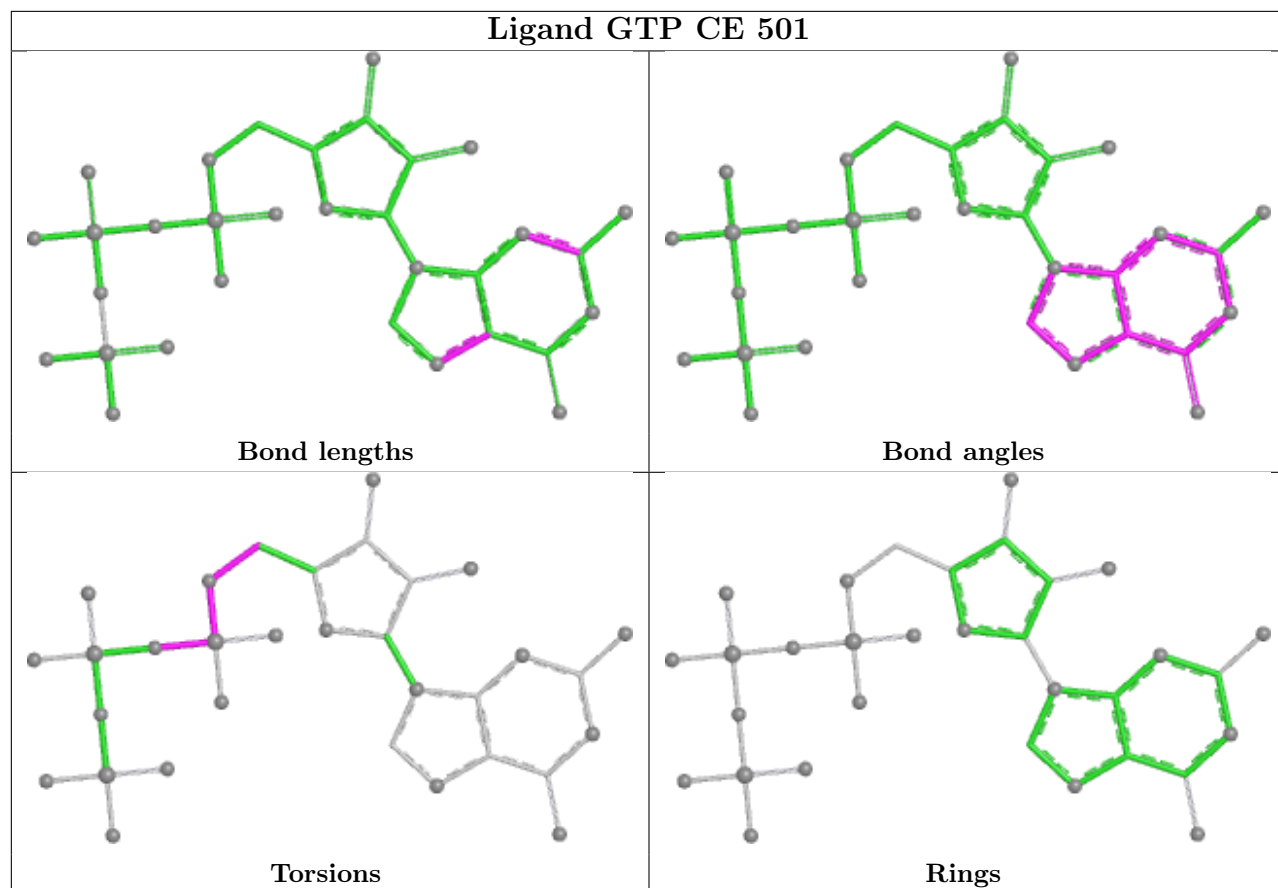


Ligand GTP LA 501

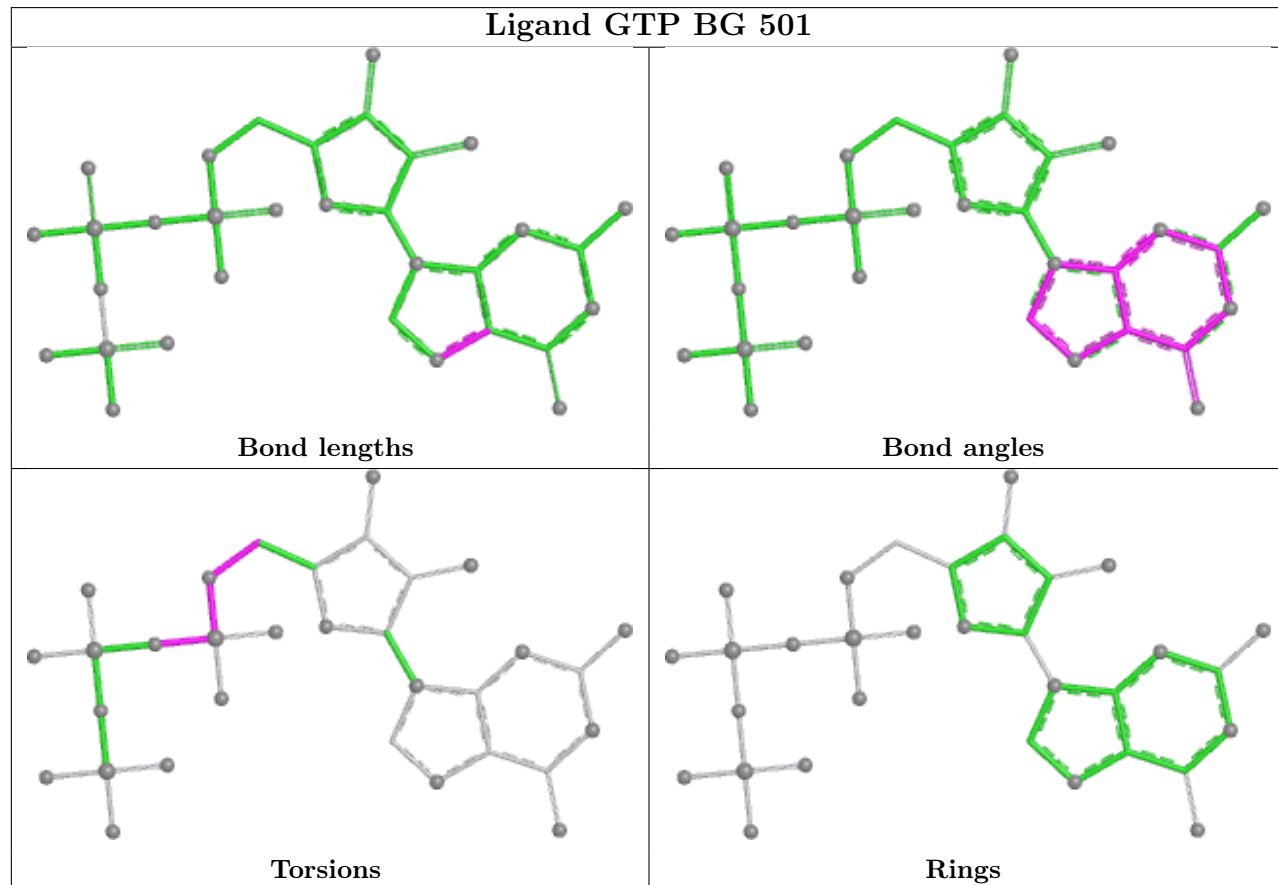


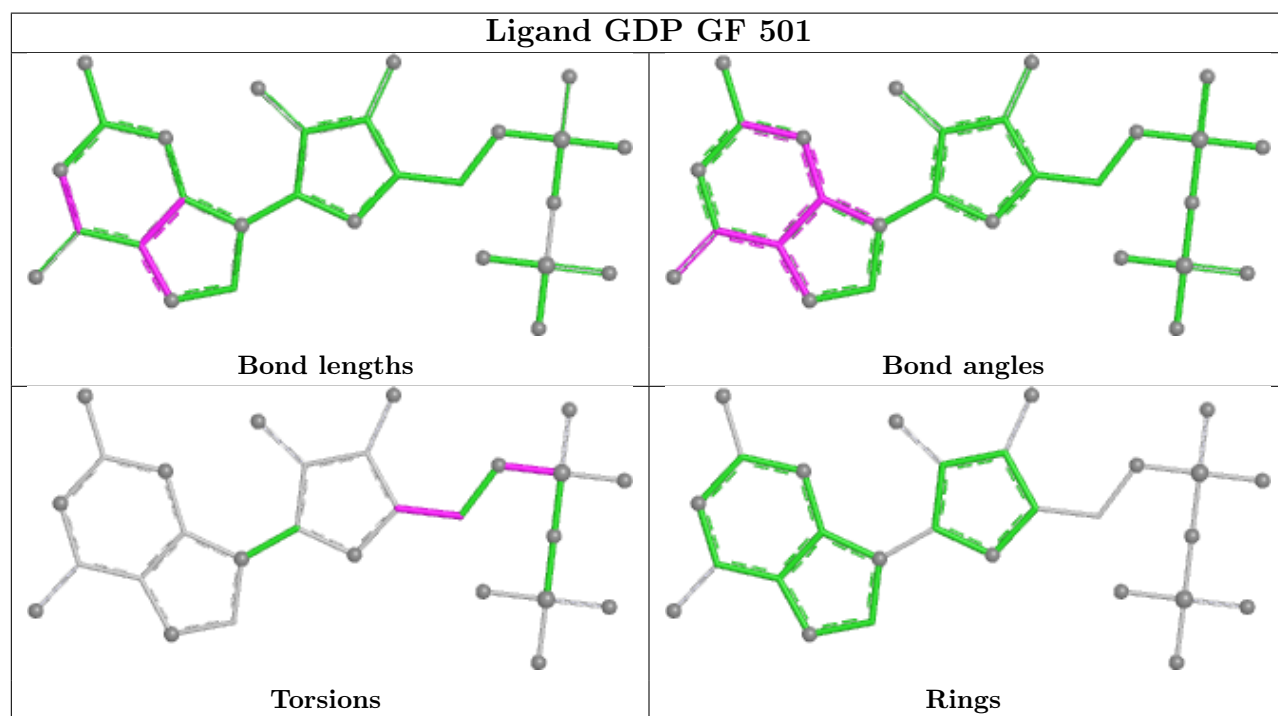
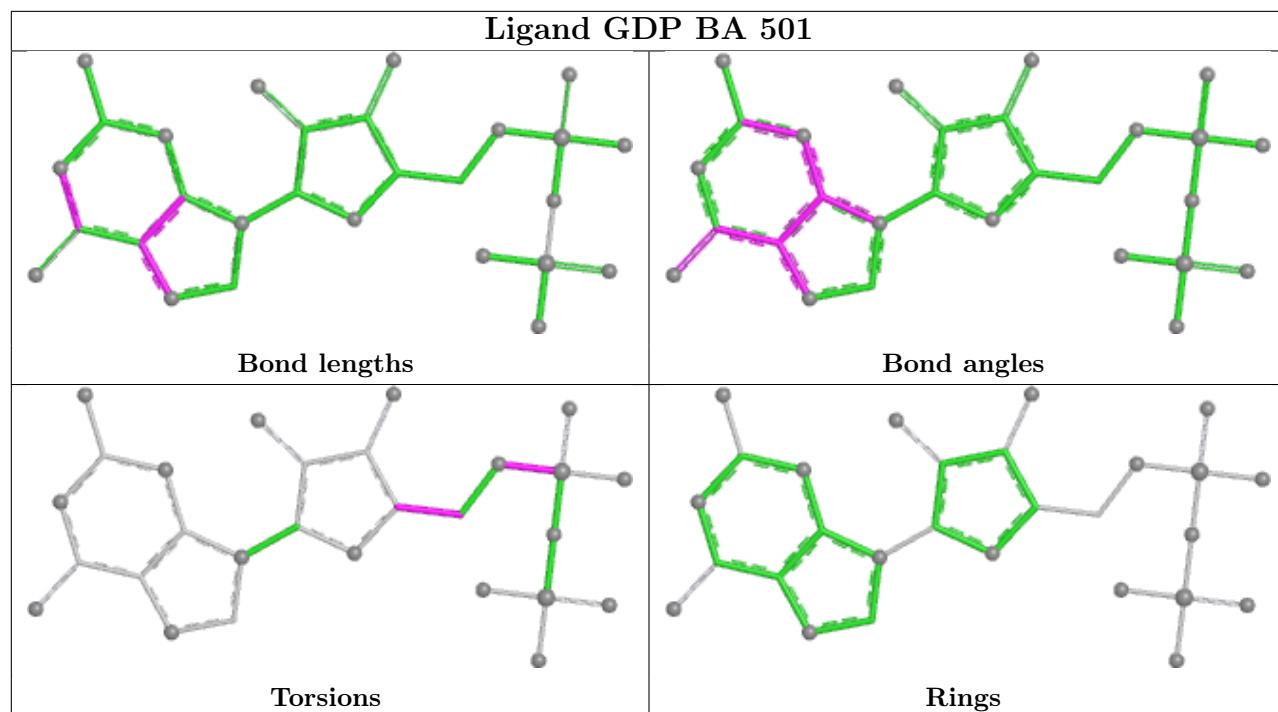


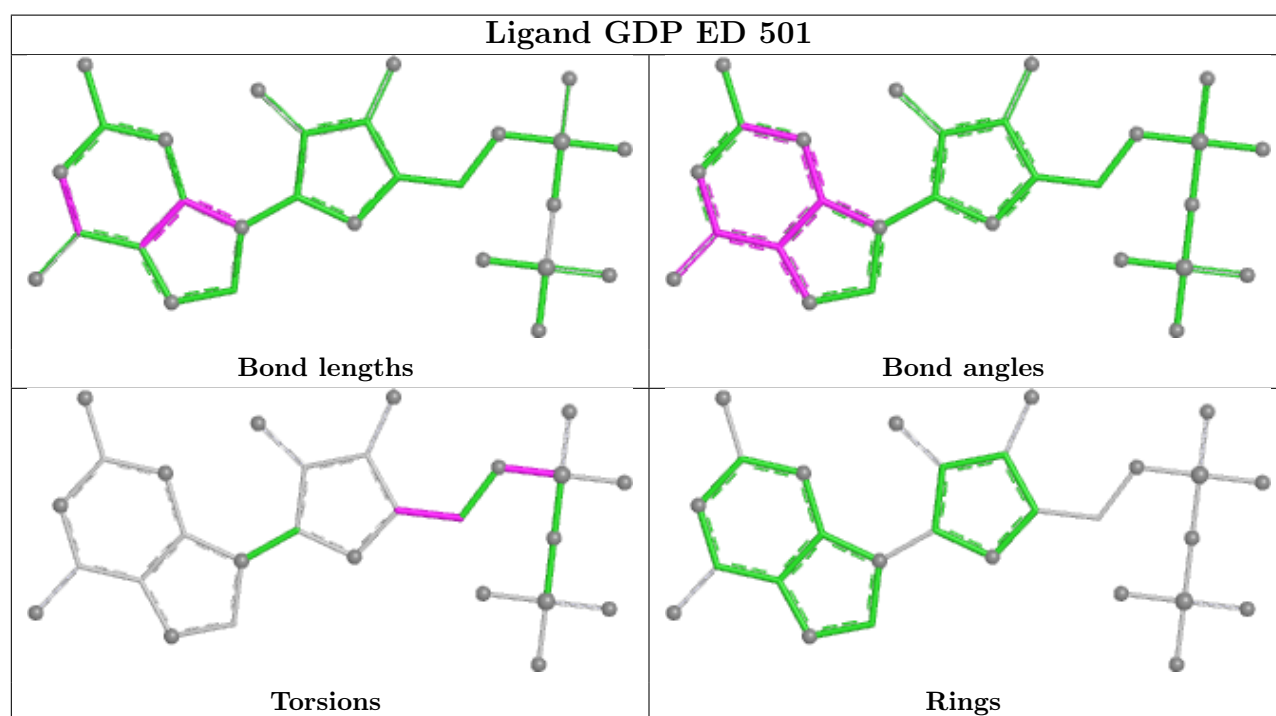
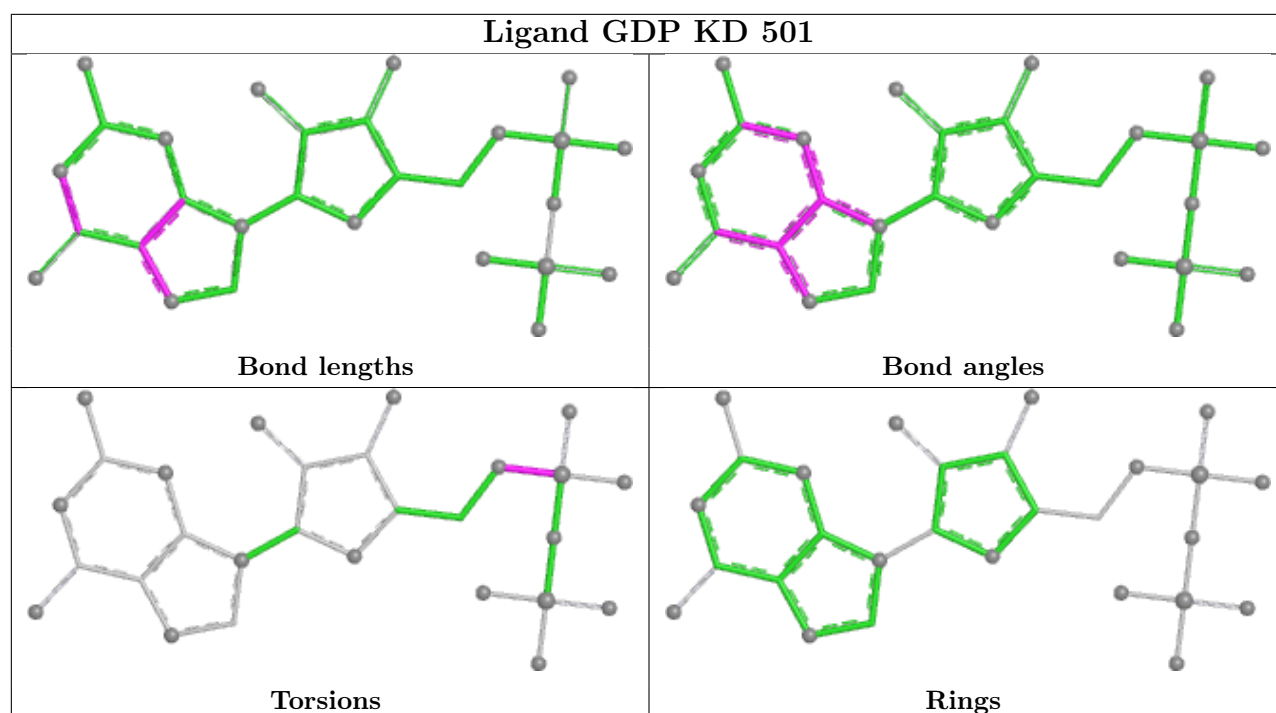
Ligand GTP CE 501



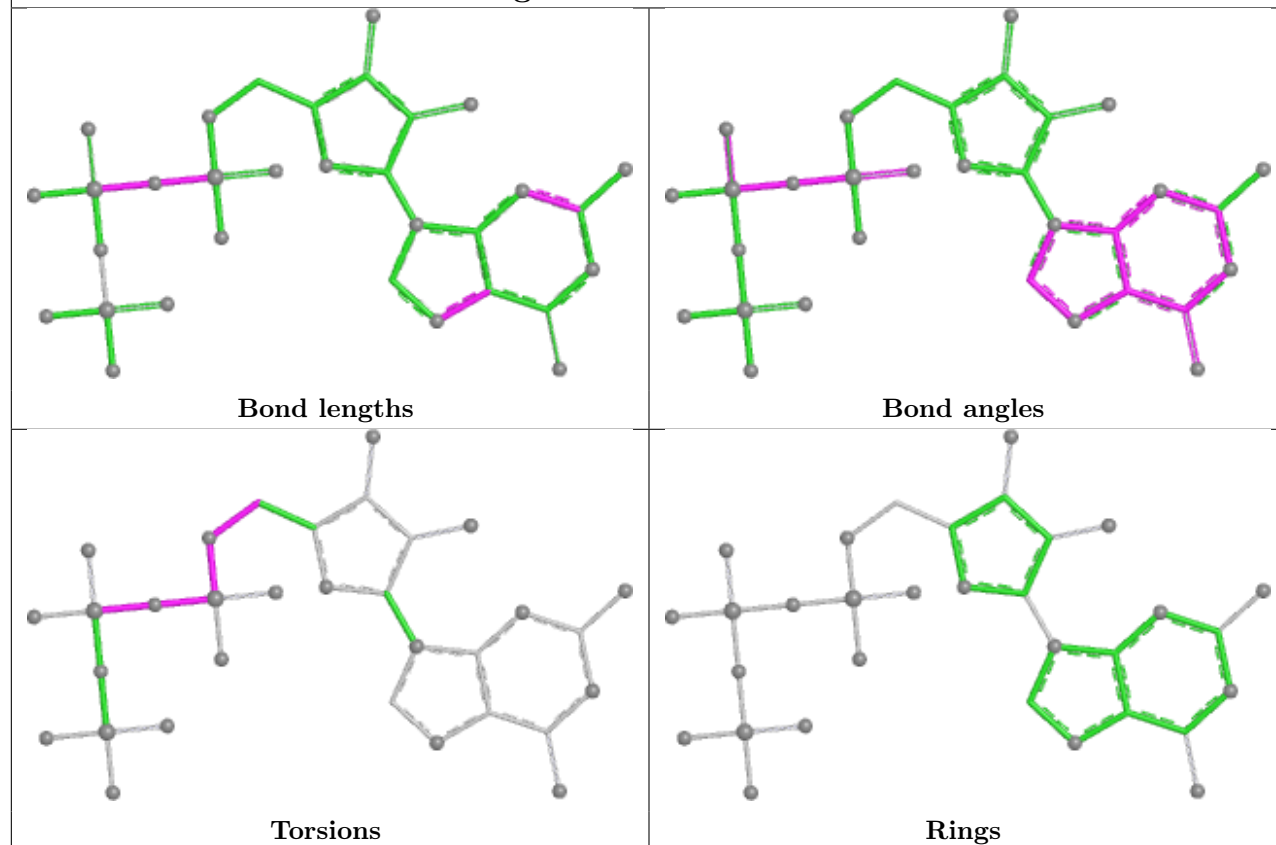
Ligand GTP BG 501



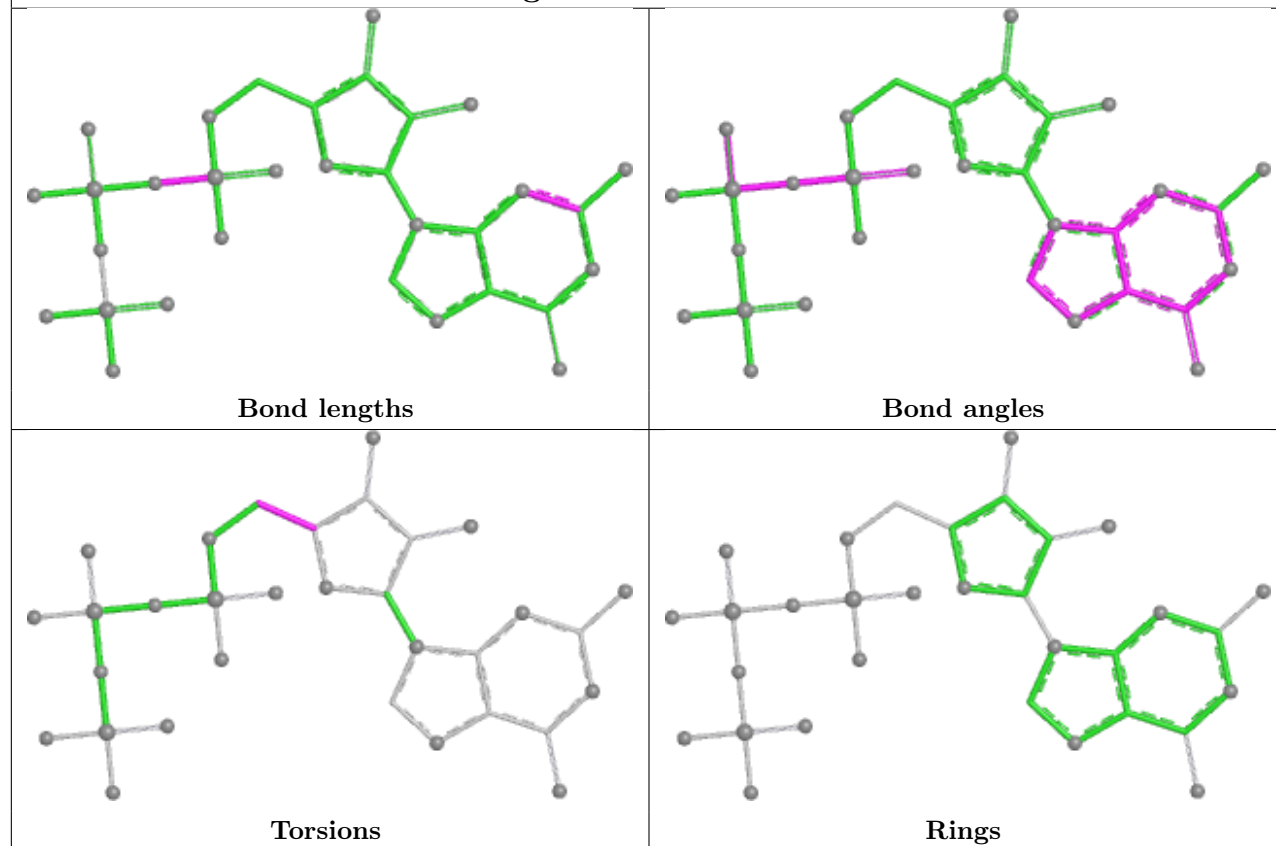




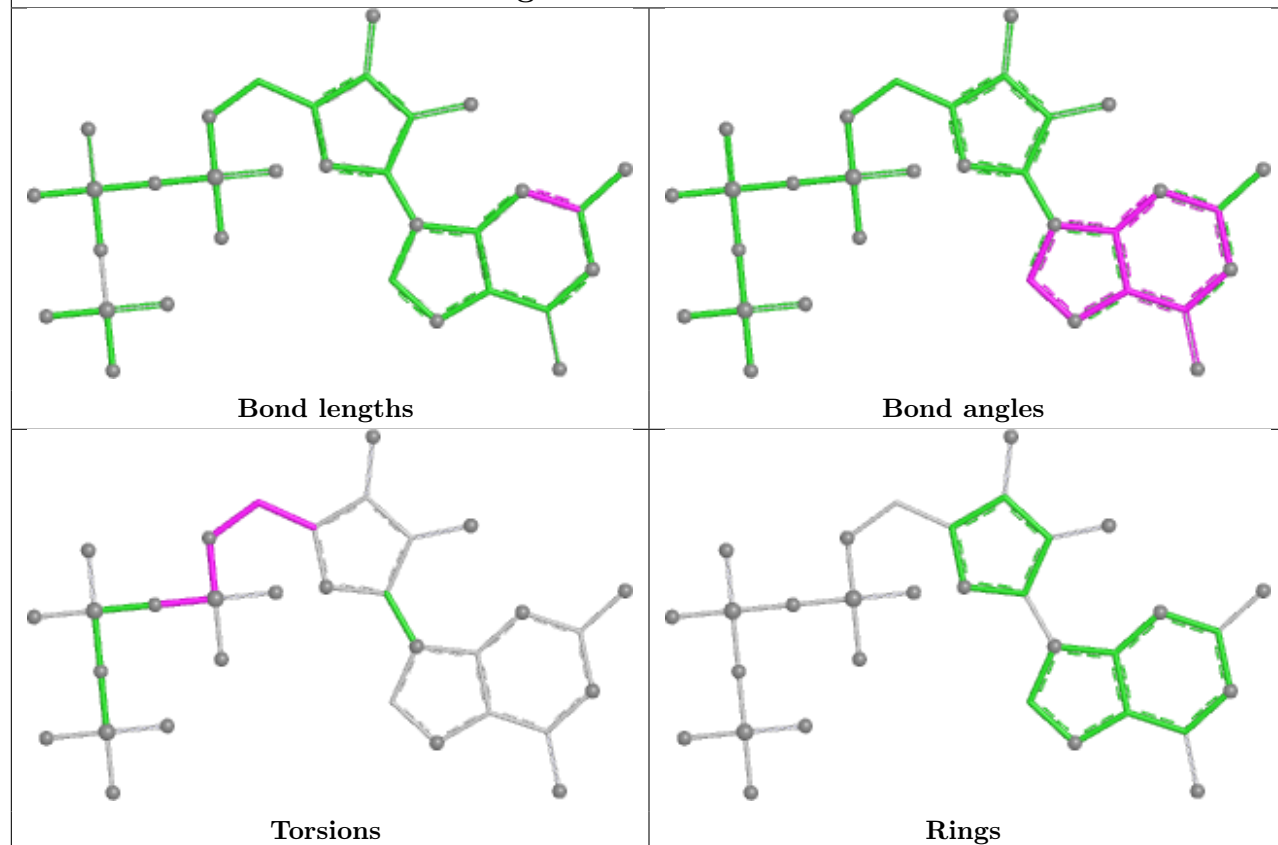
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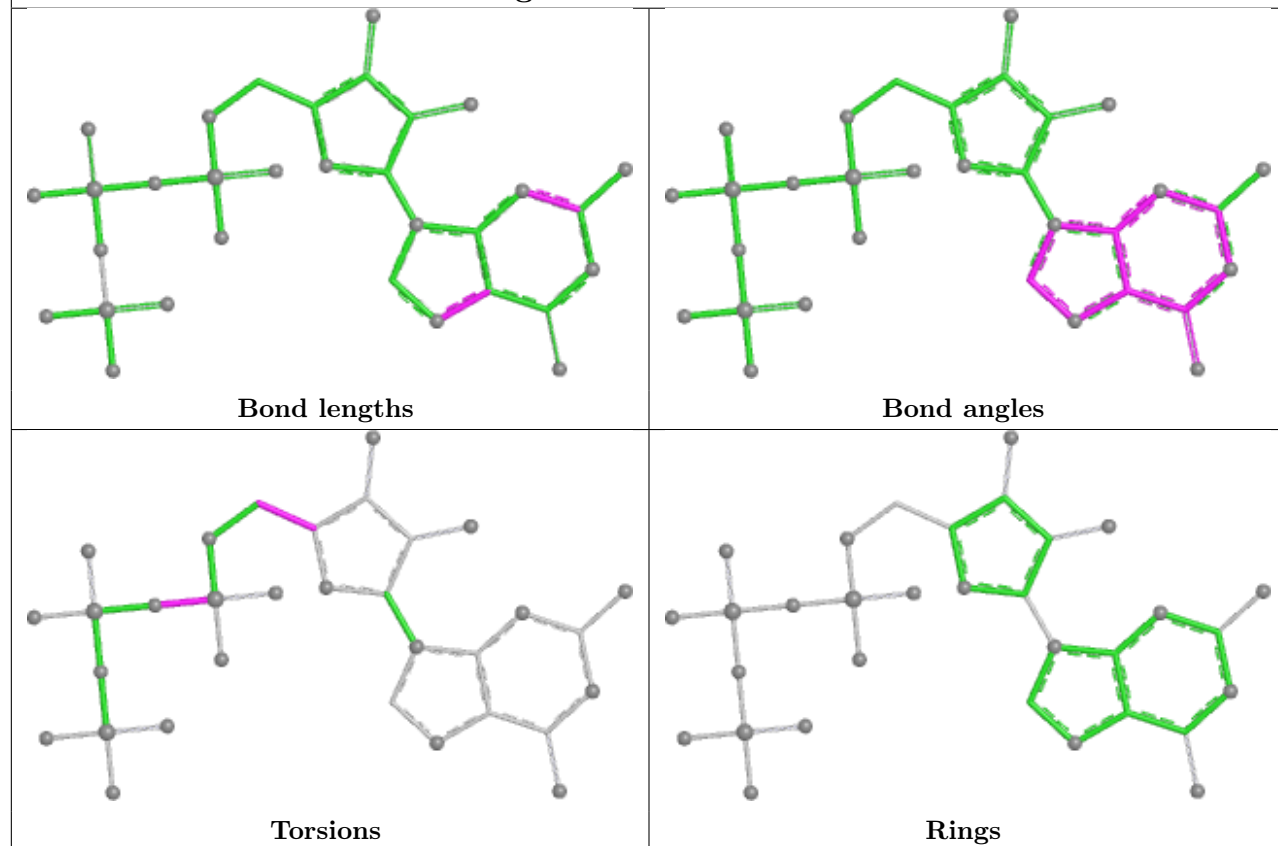
Ligand GTP IG 501

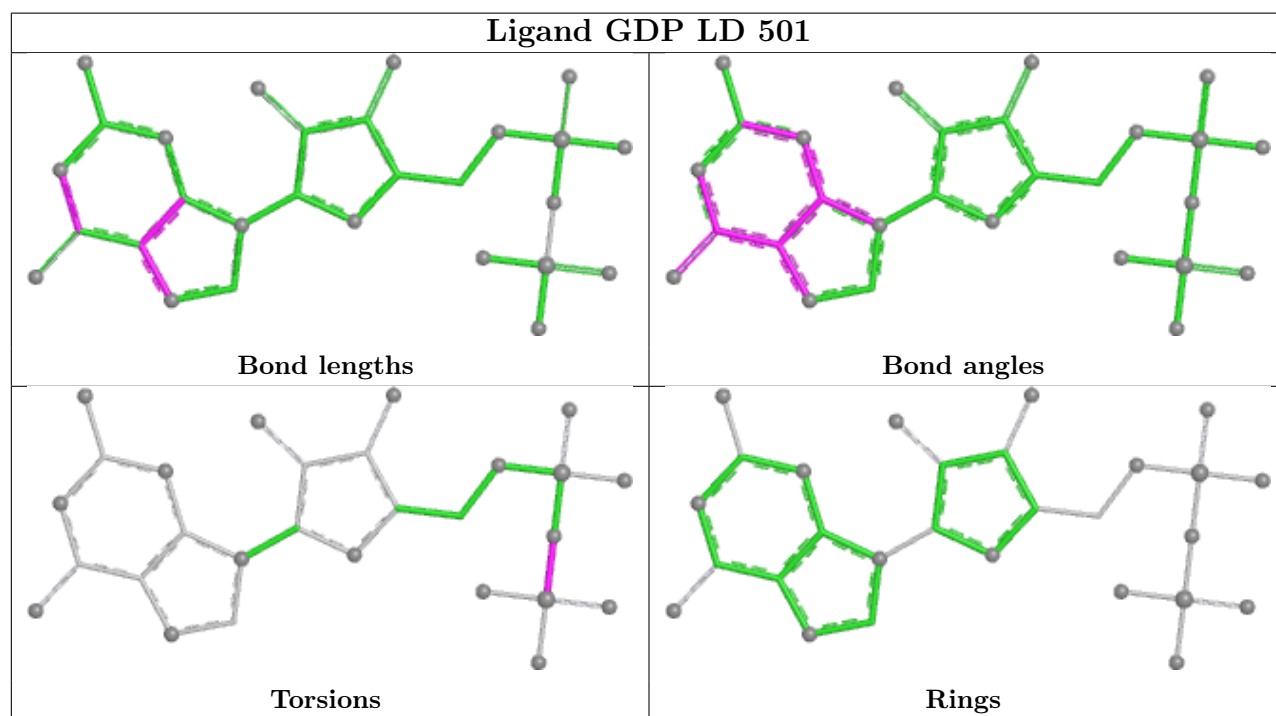
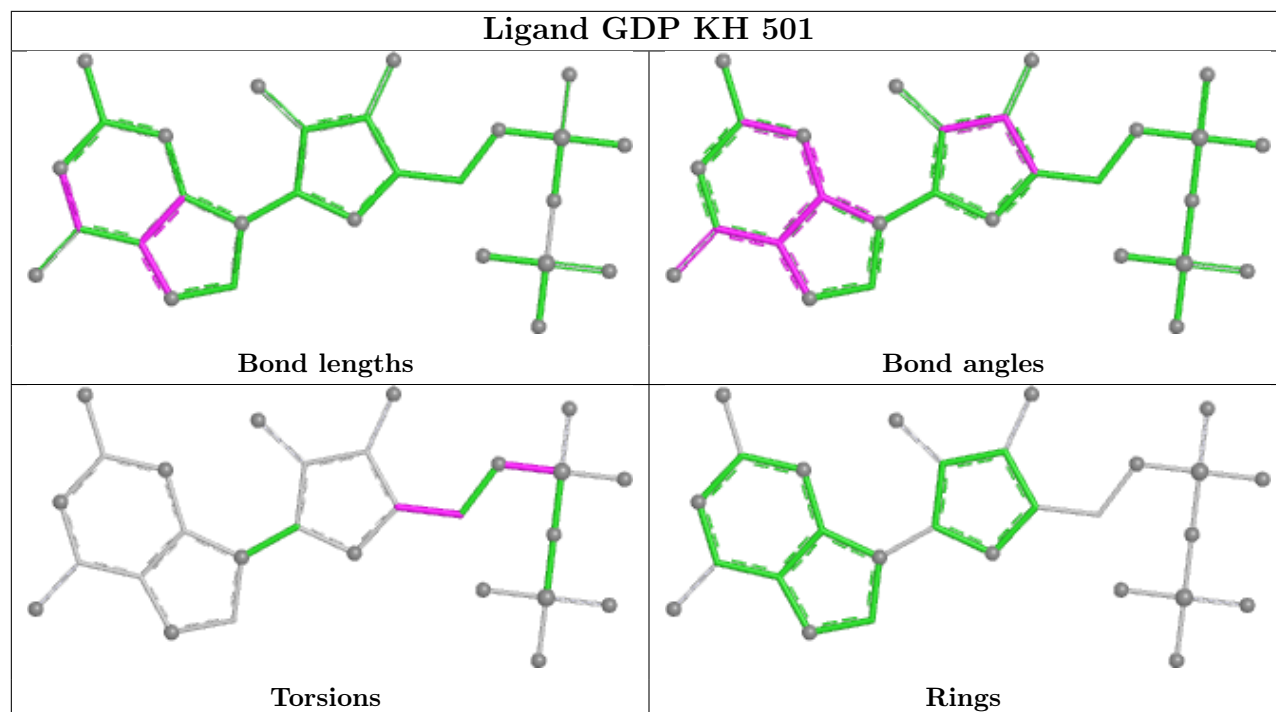


Ligand GTP DC 501

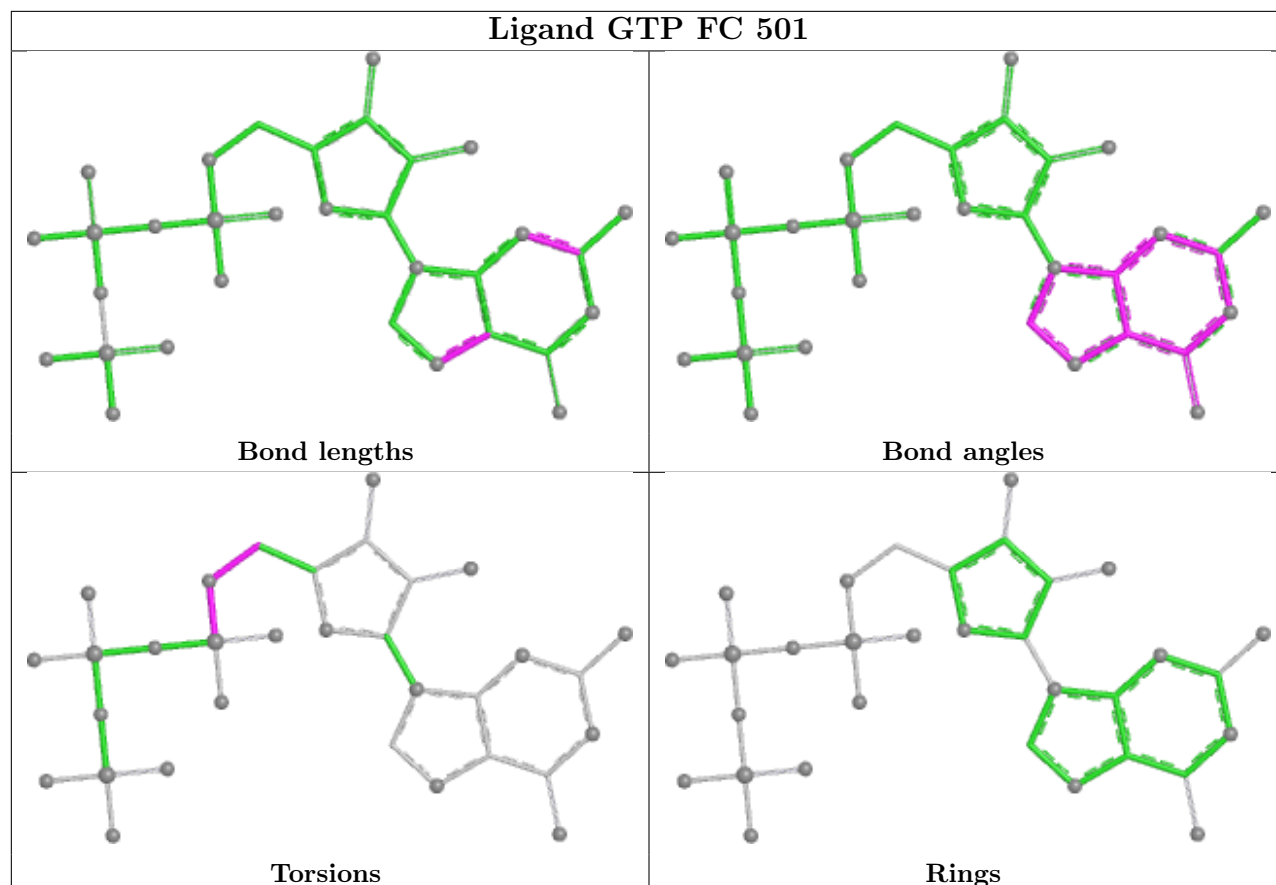


Ligand GTP GG 501

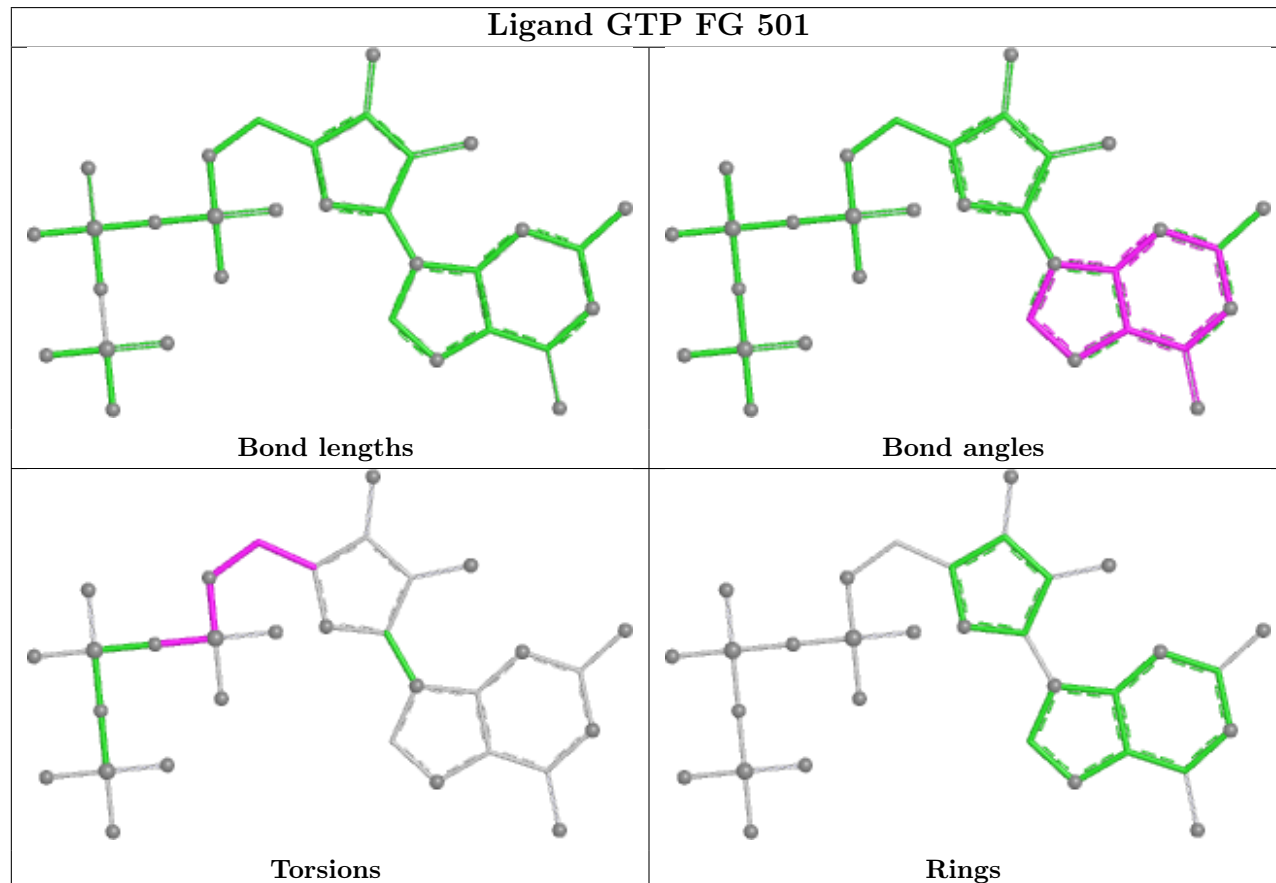




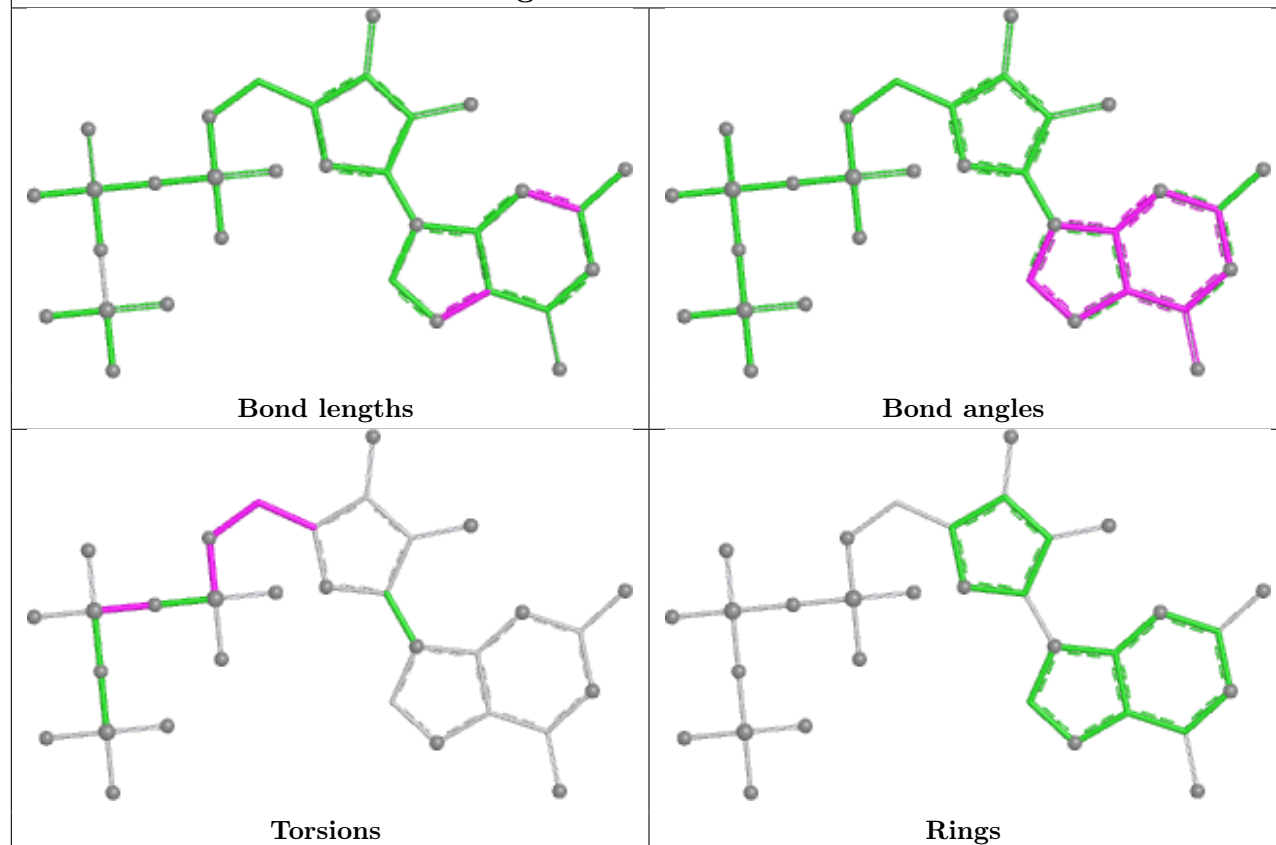
Ligand GTP FC 501



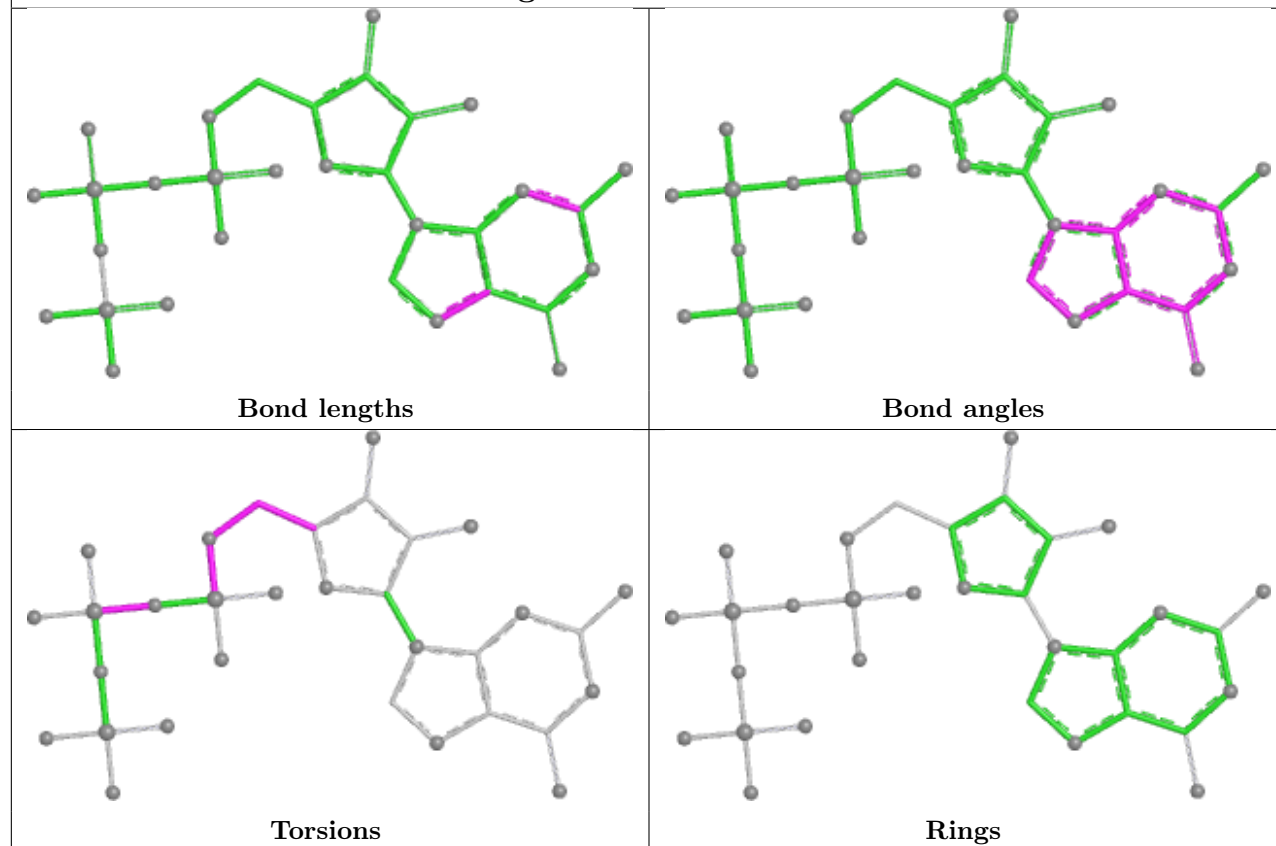
Ligand GTP FG 501

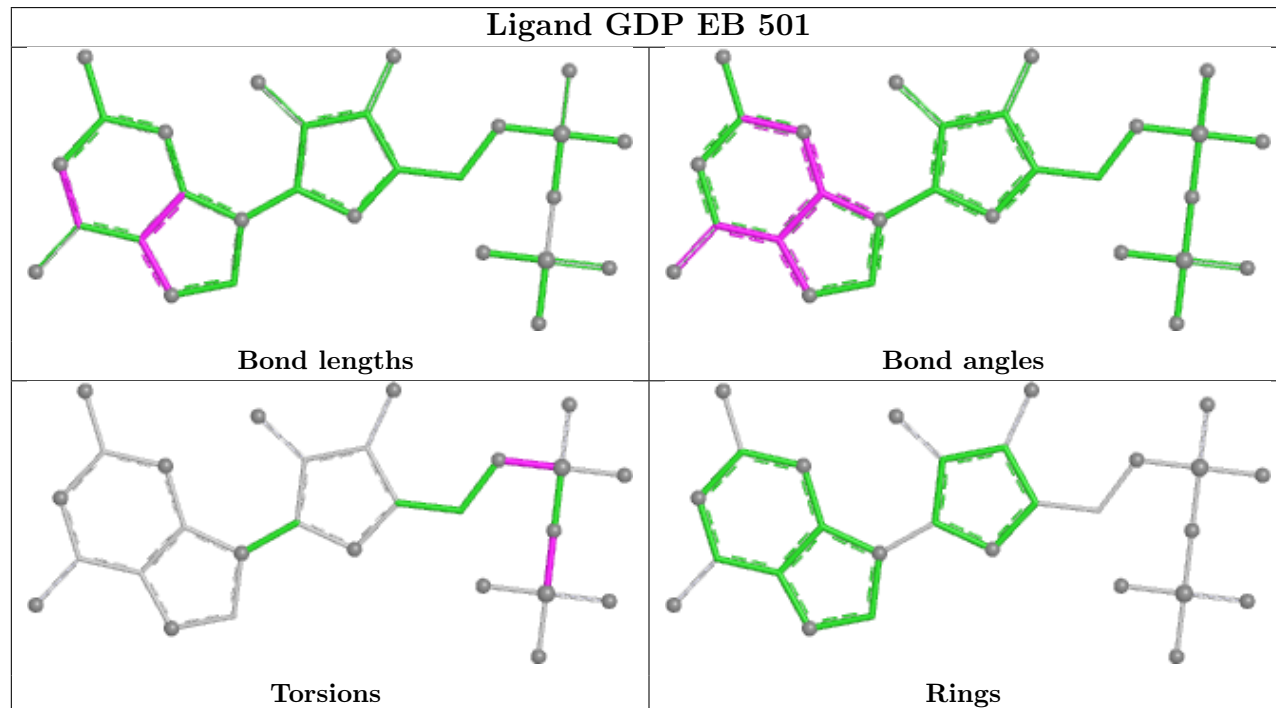
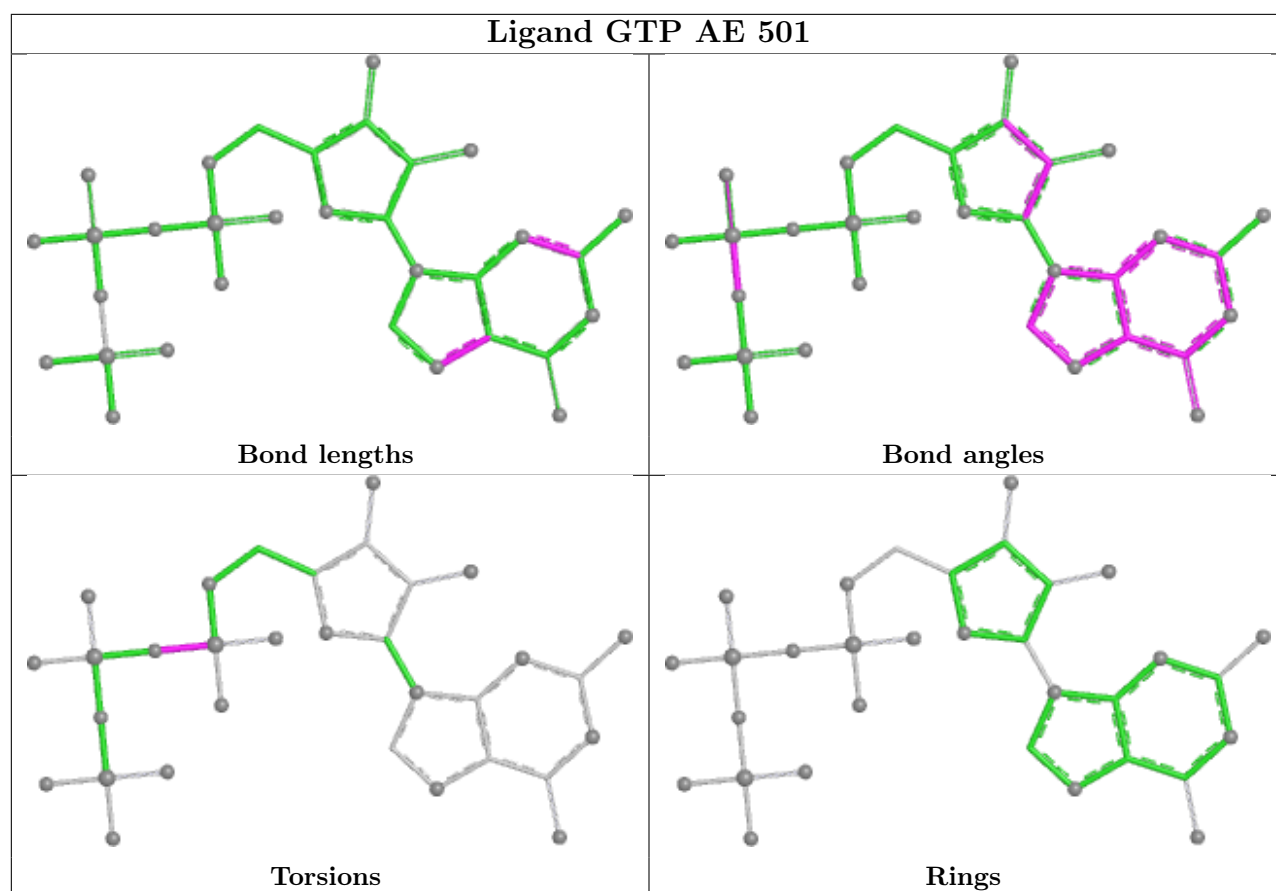


Ligand GTP HC 501

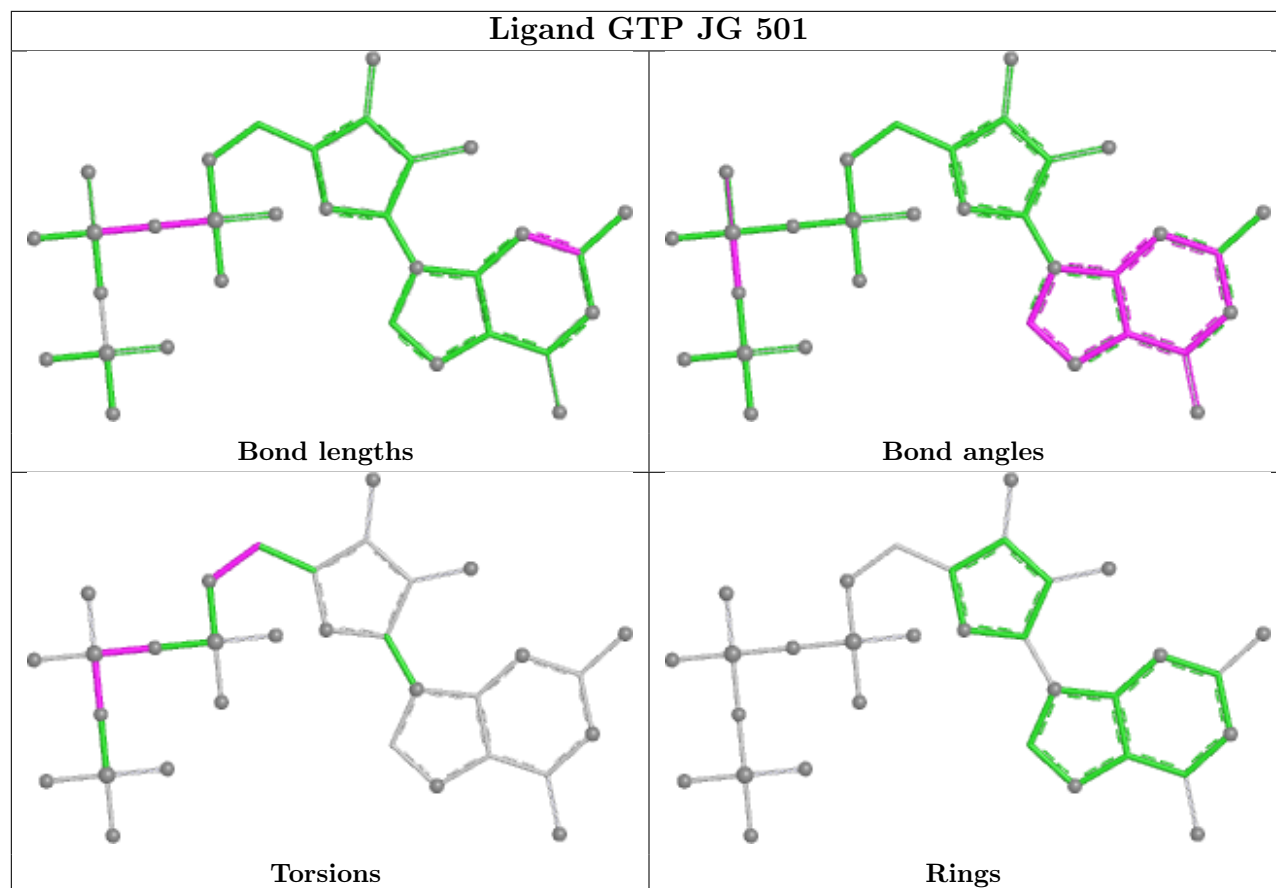


Ligand GTP HE 501

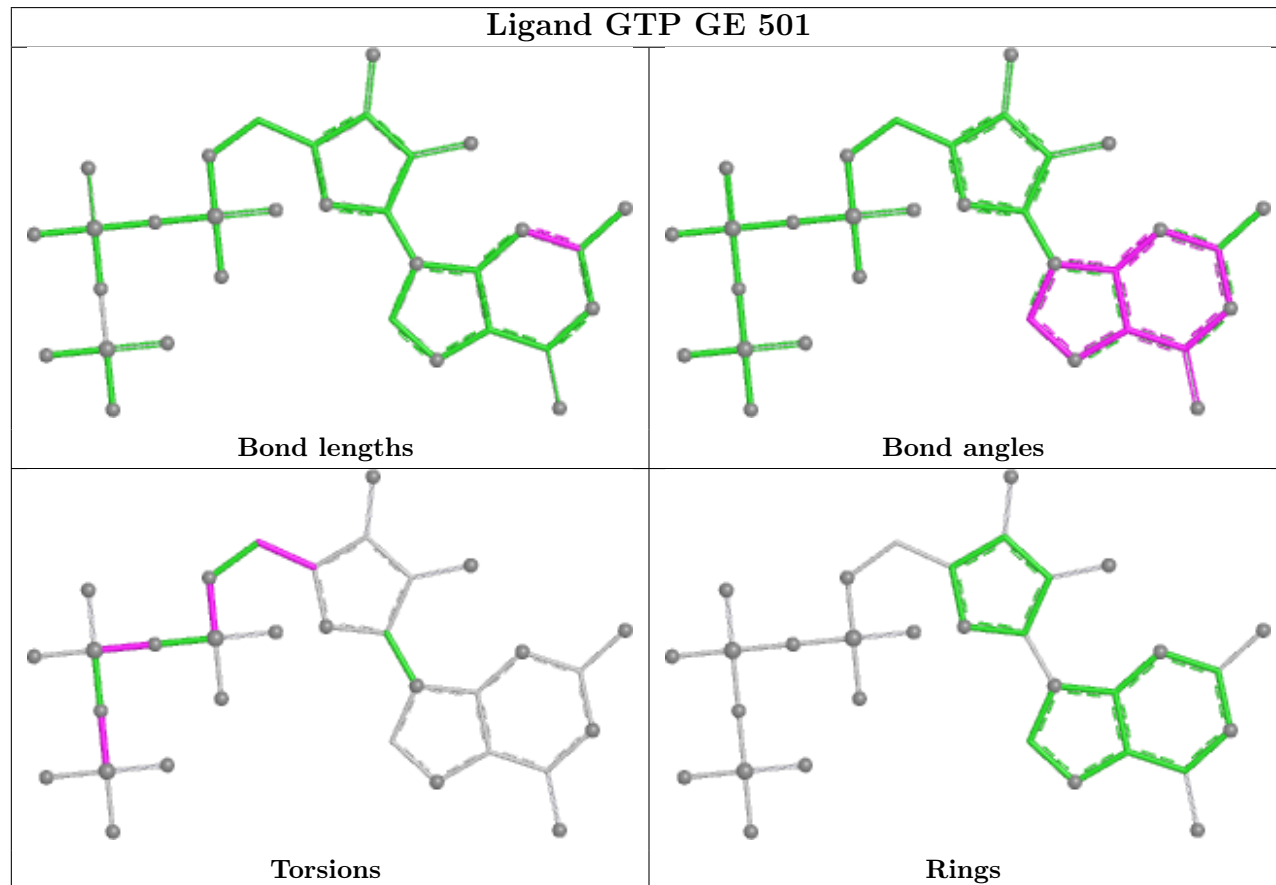


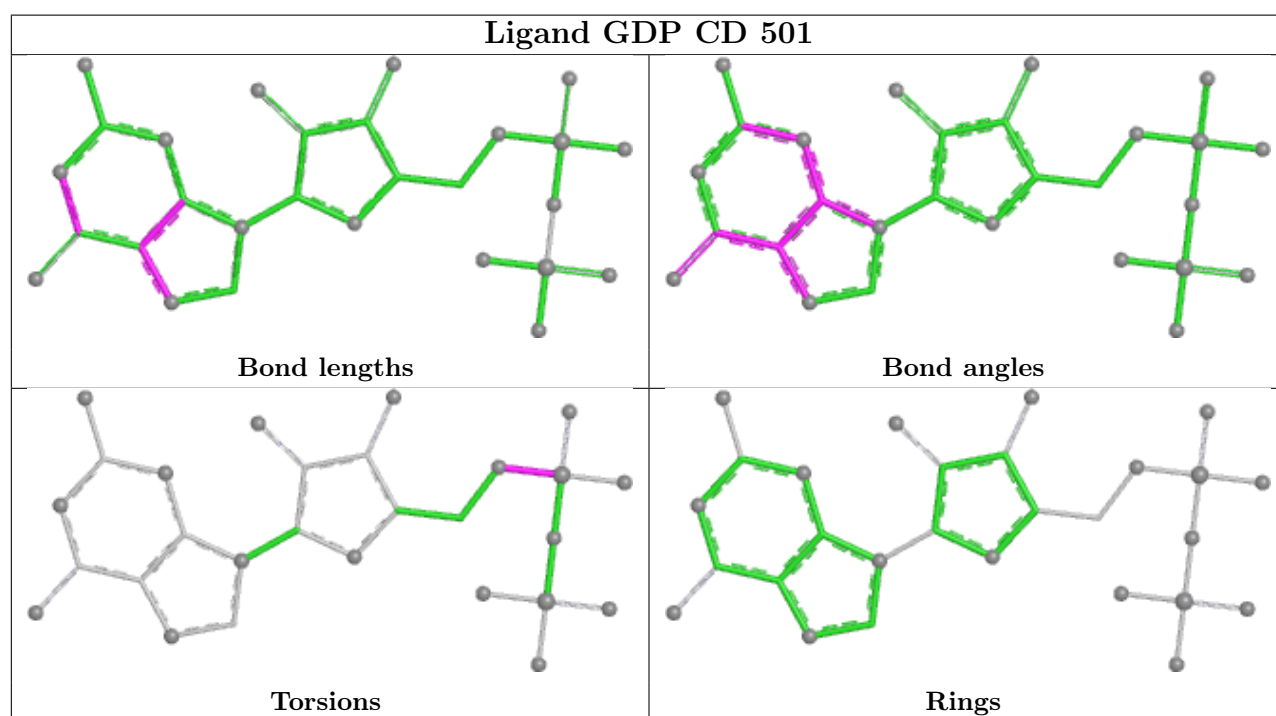
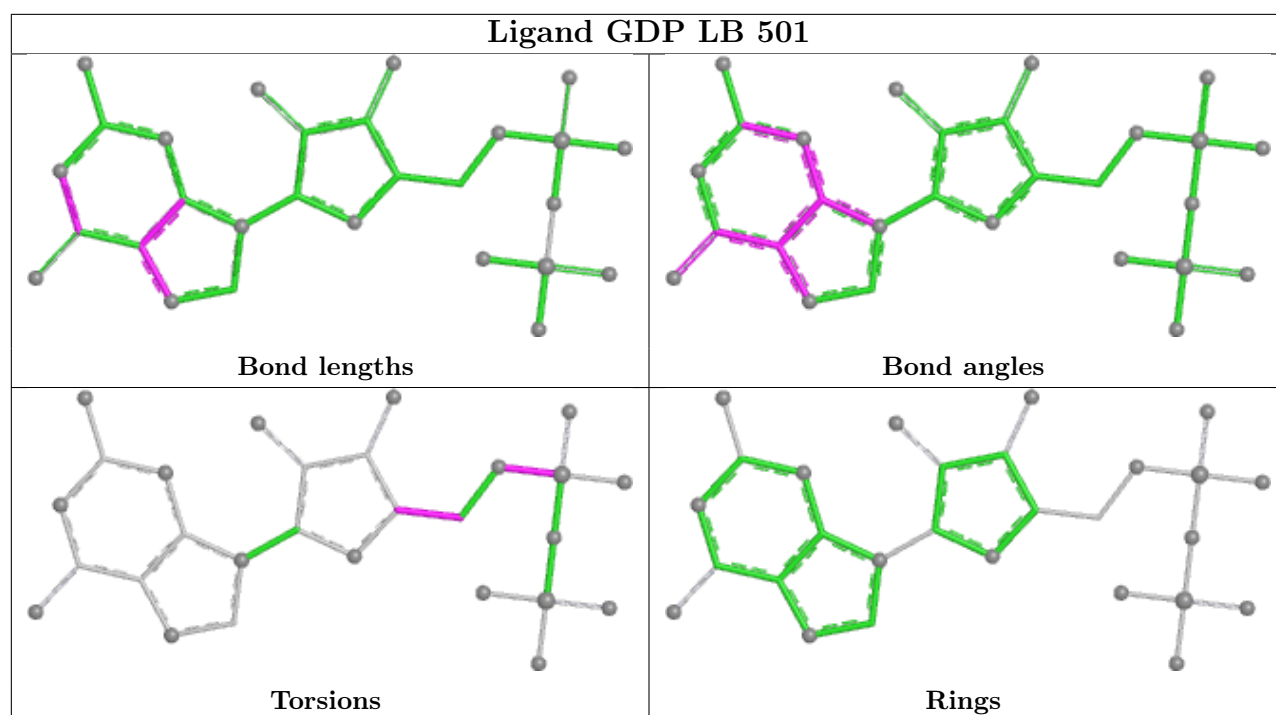


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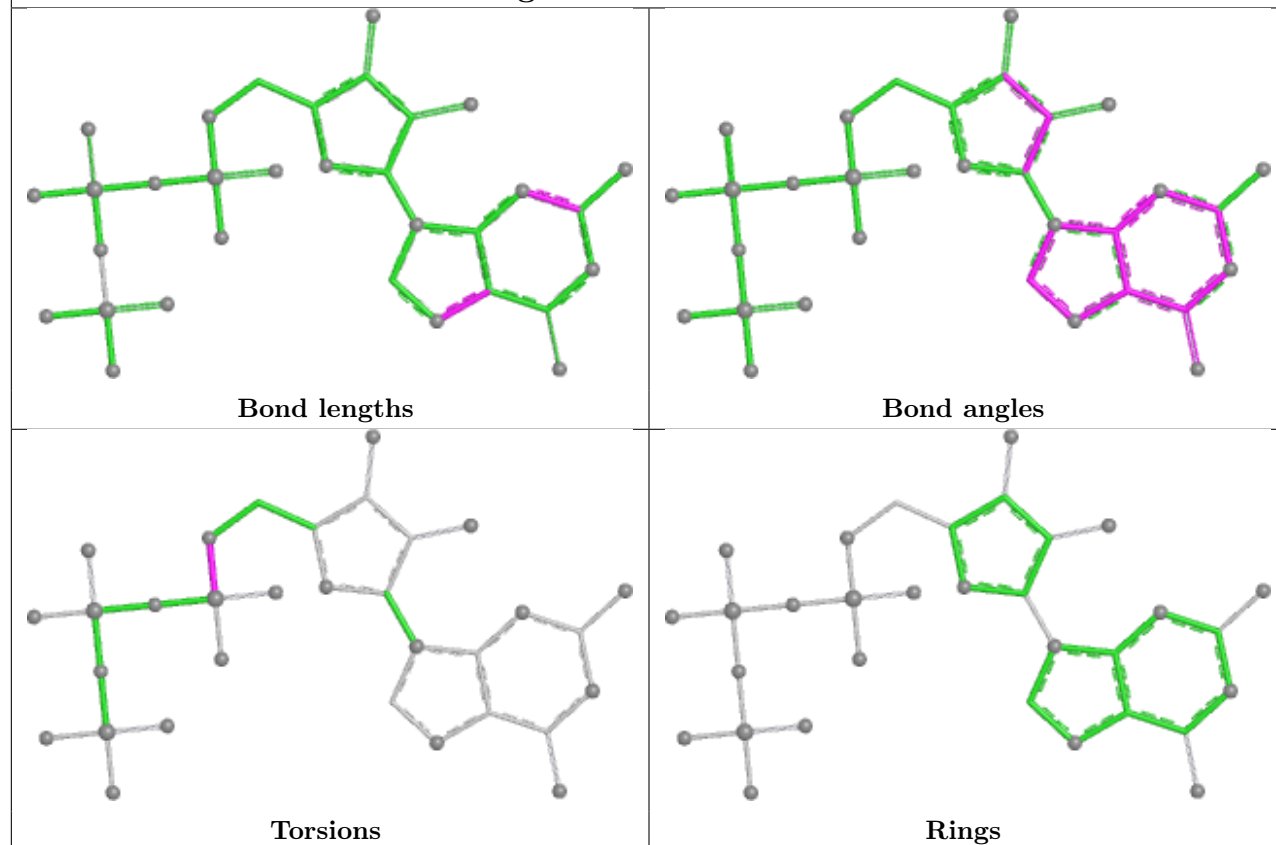


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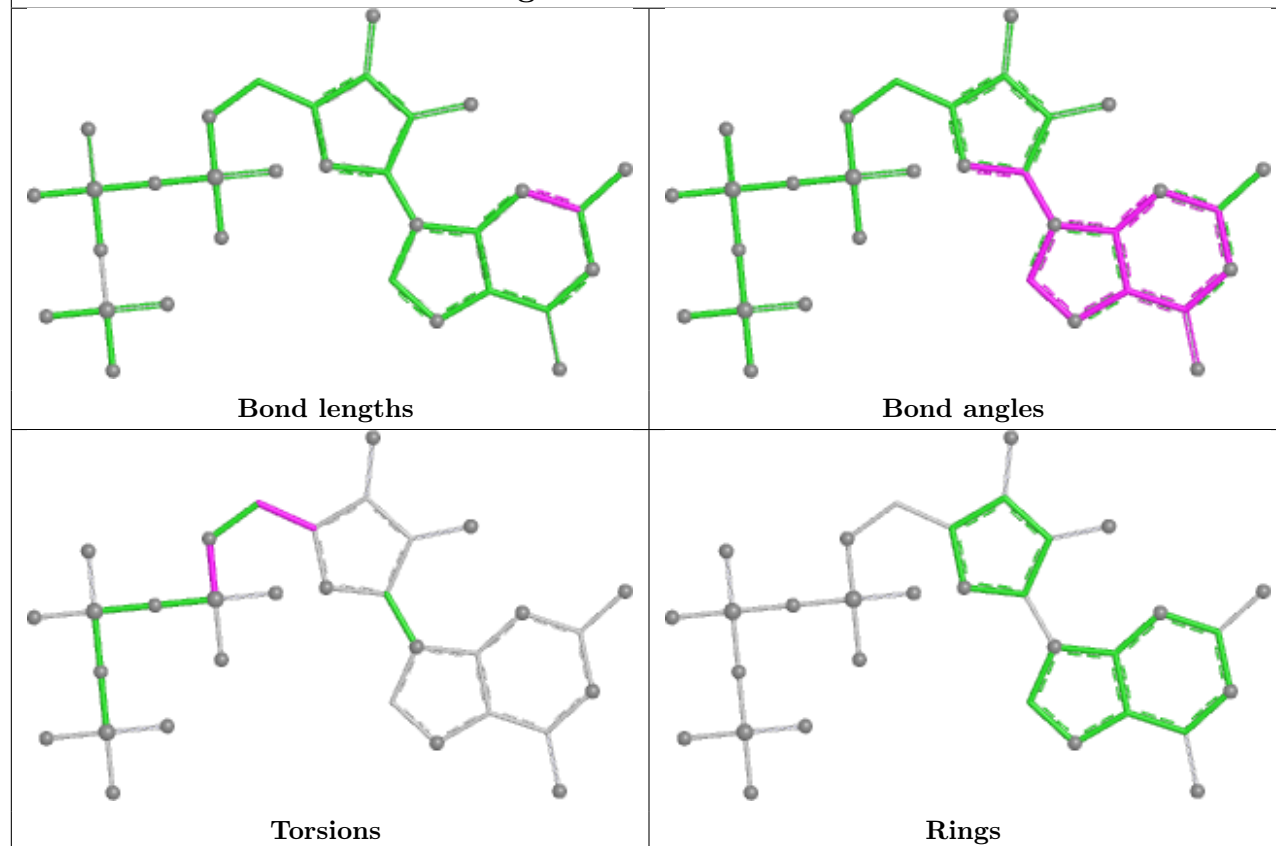


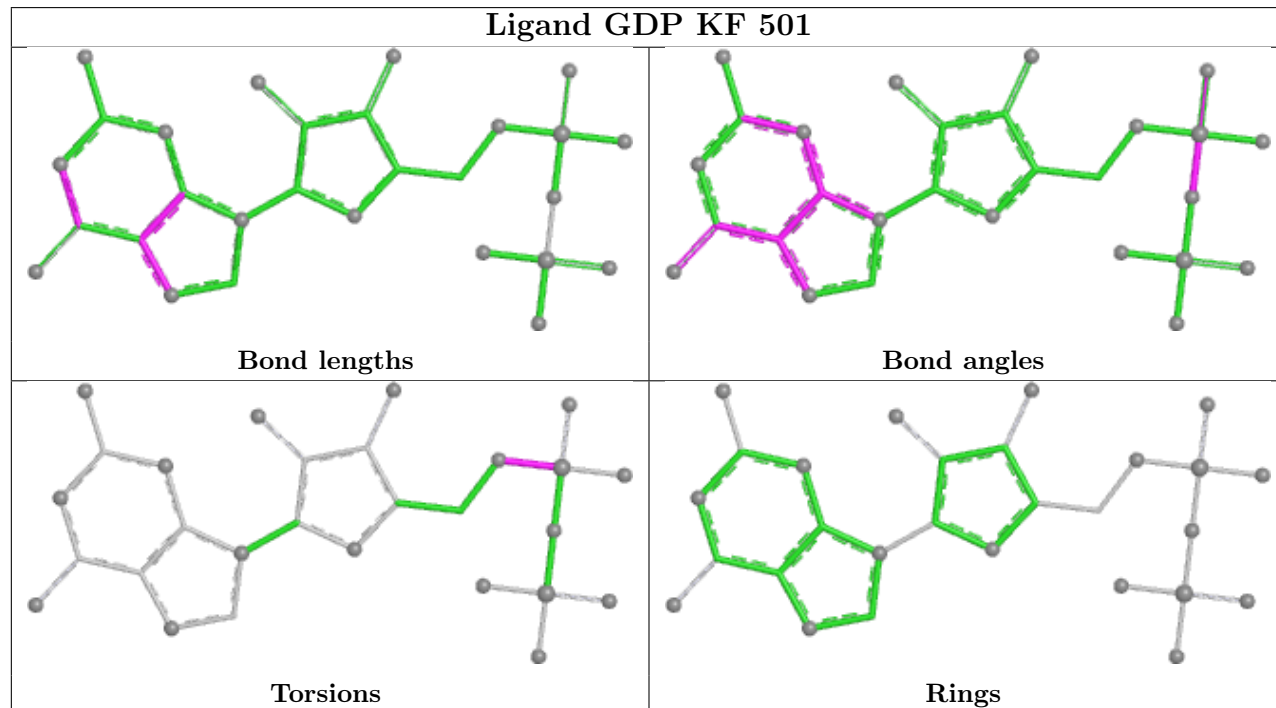
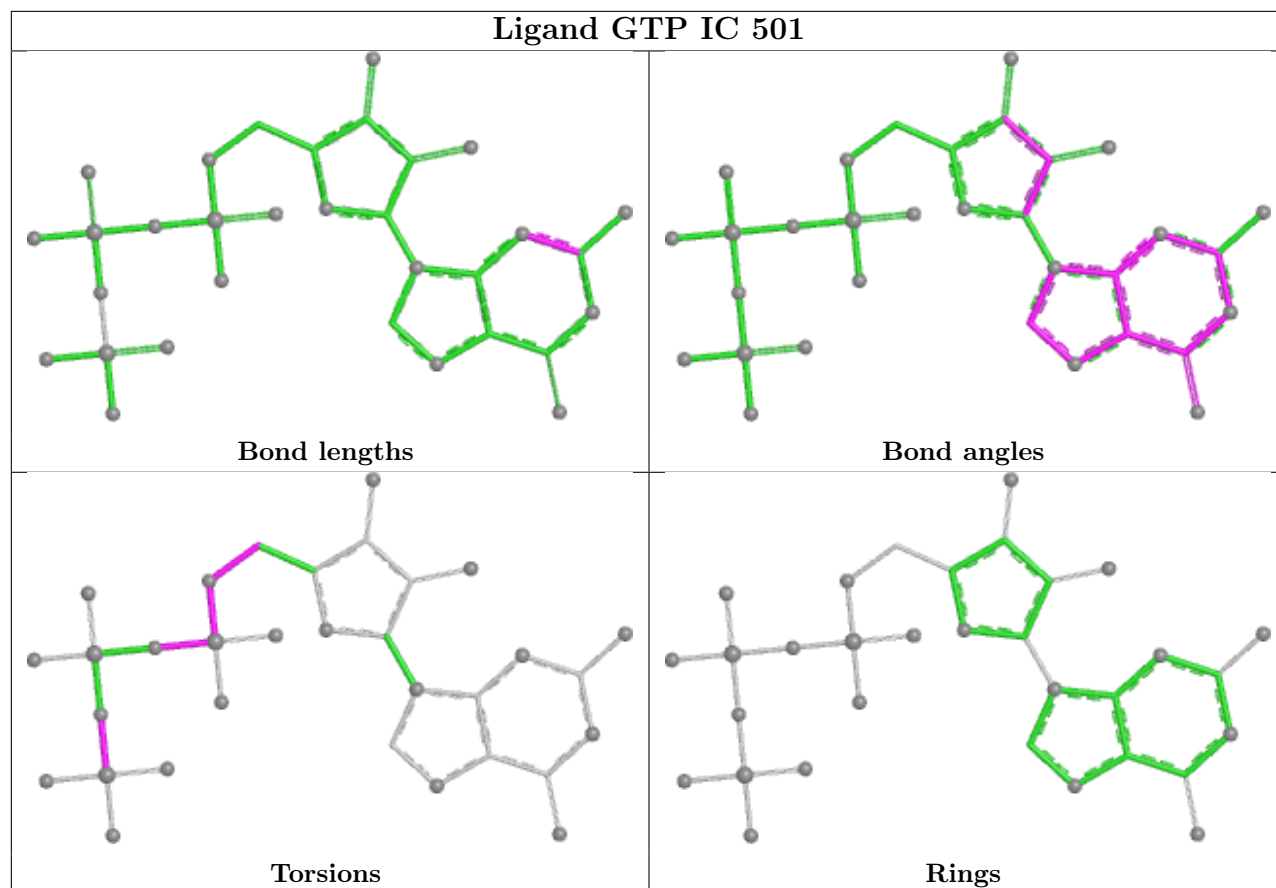


Ligand GTP AC 501

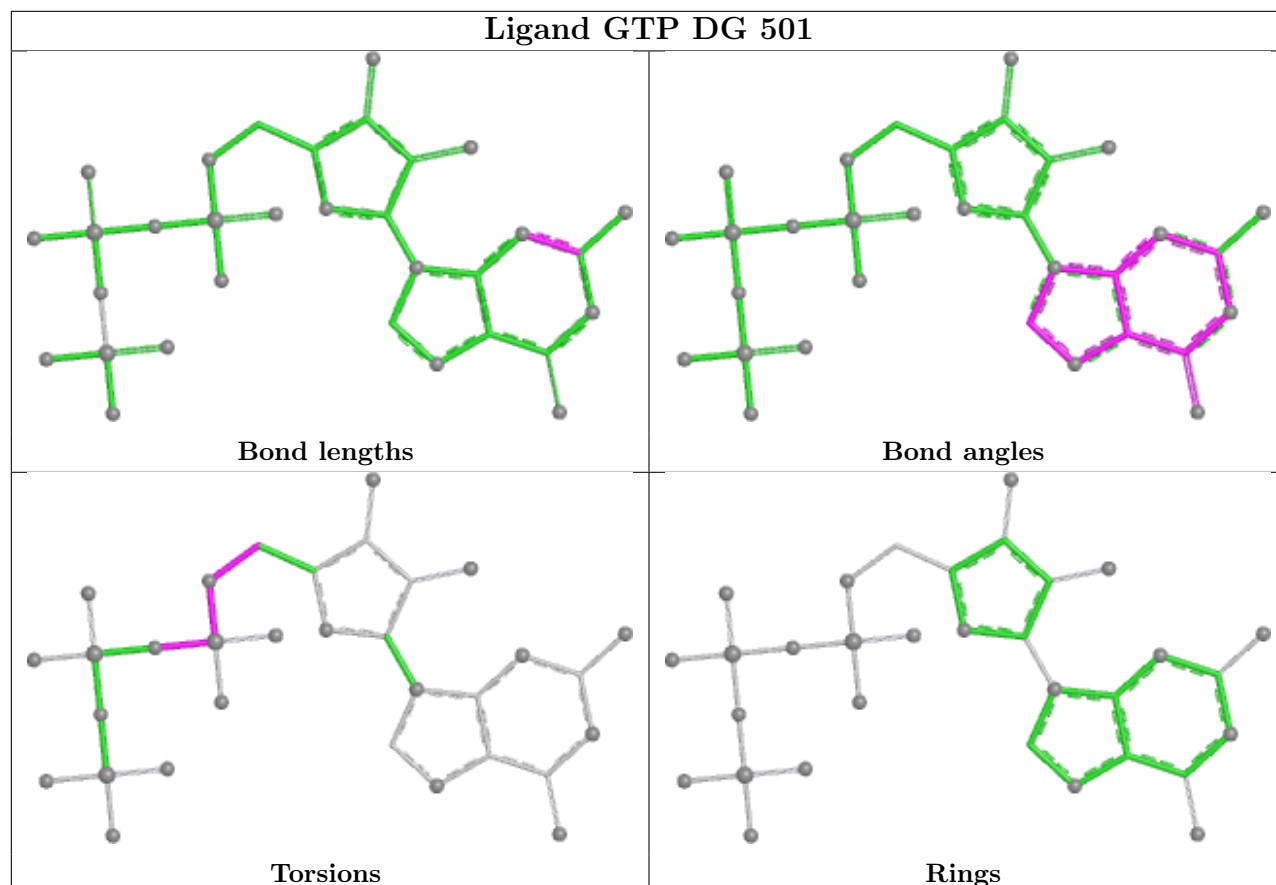


Ligand GTP CC 501

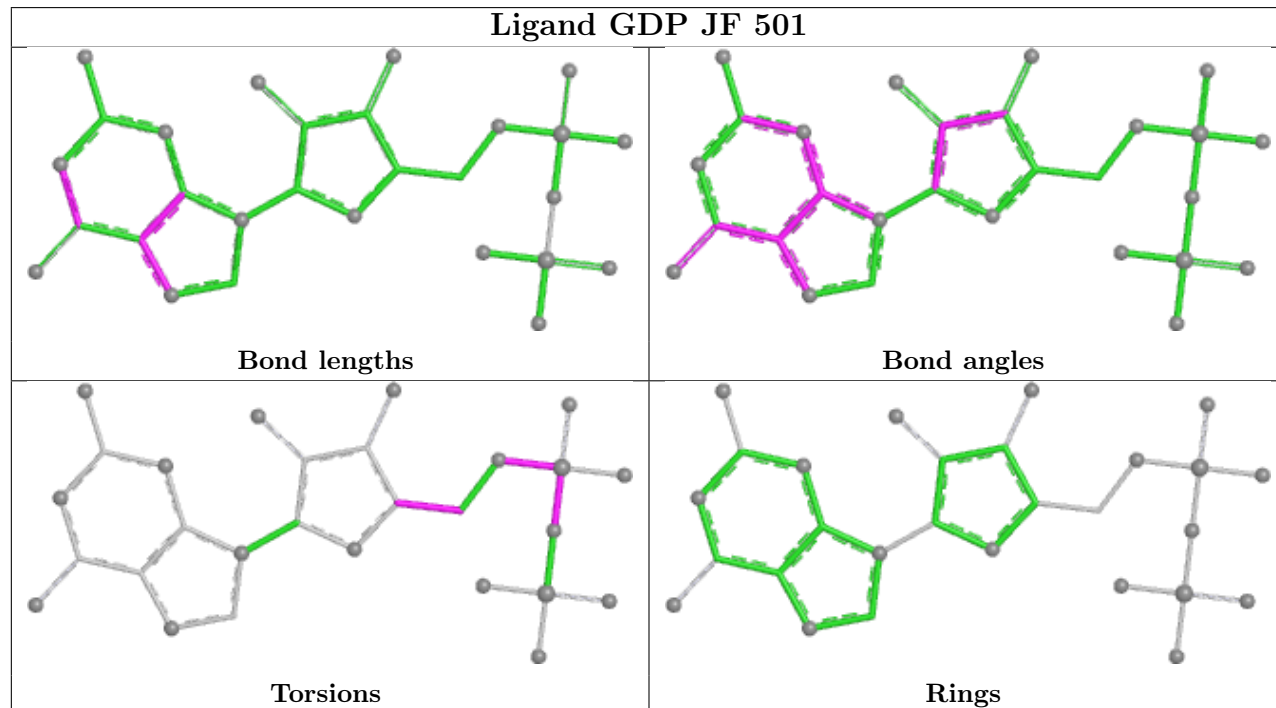


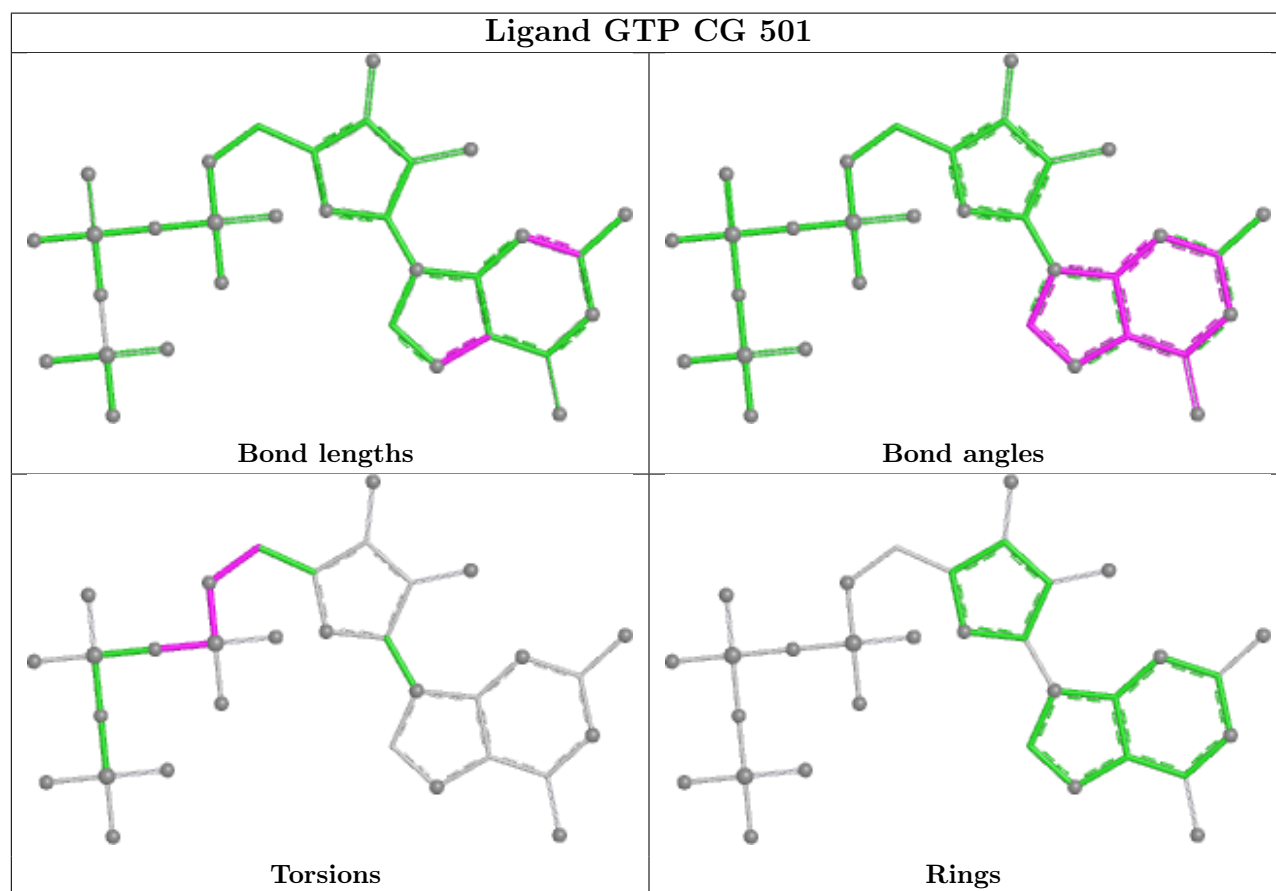
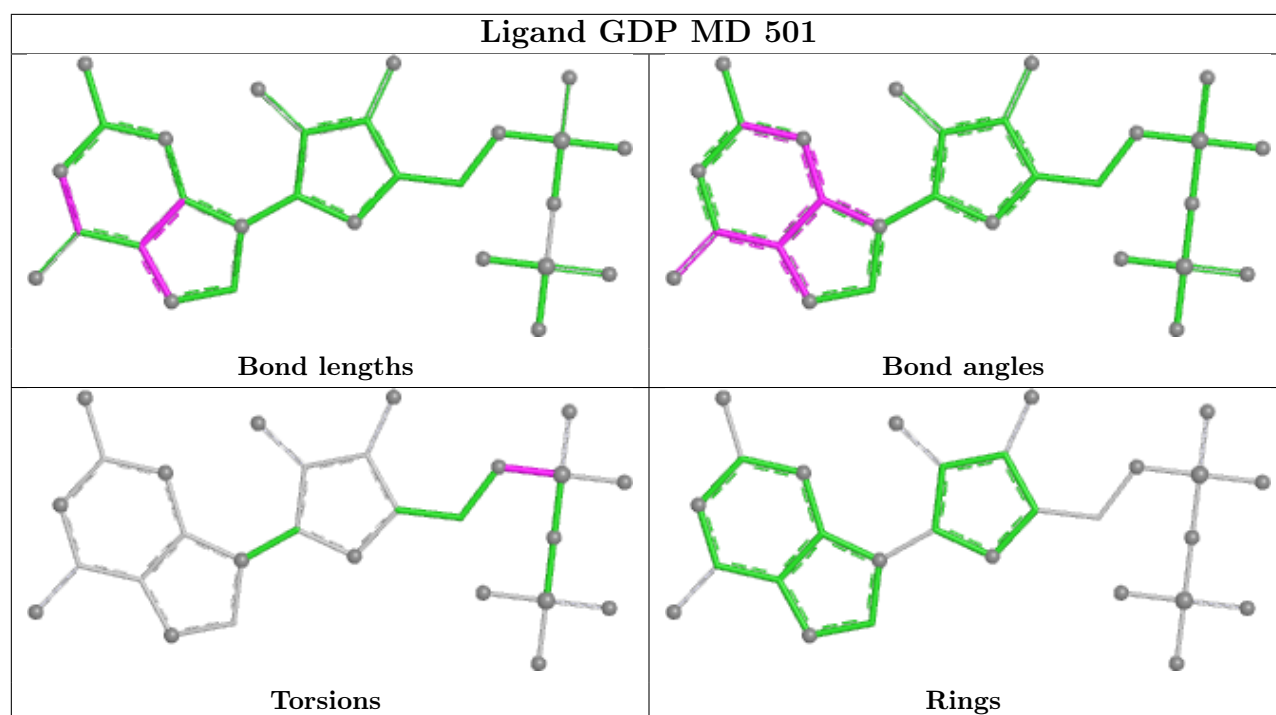


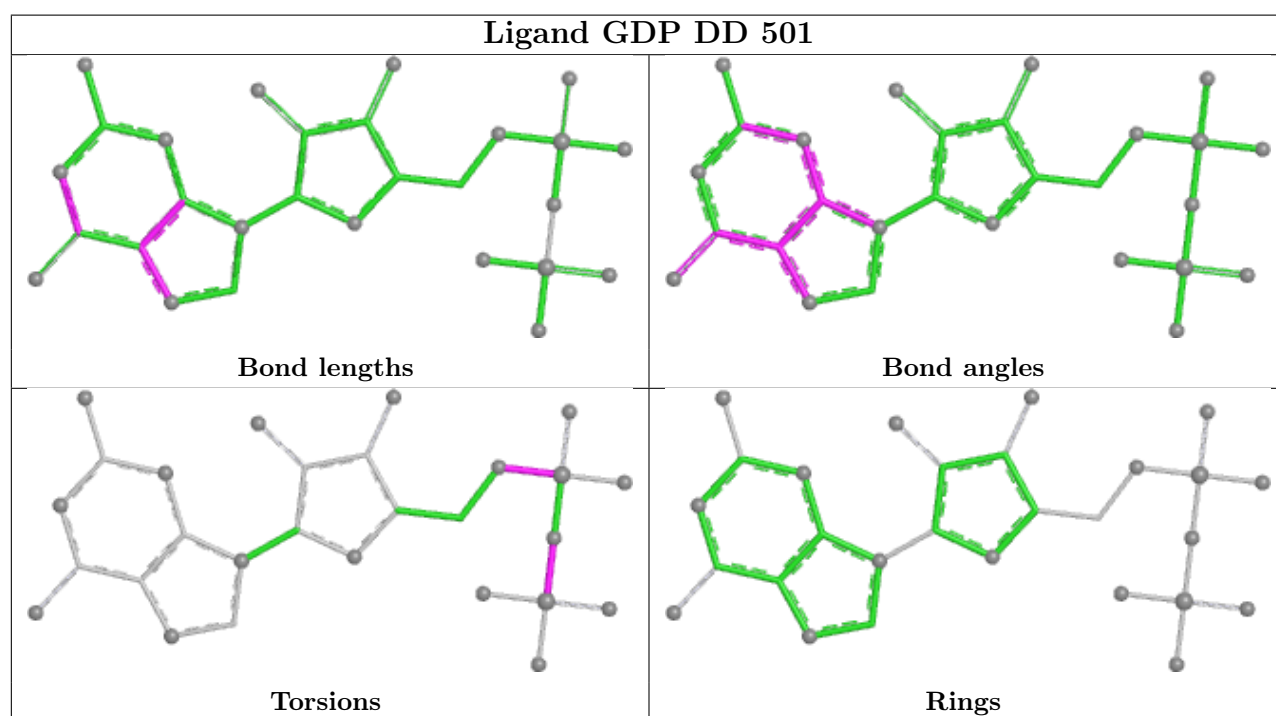
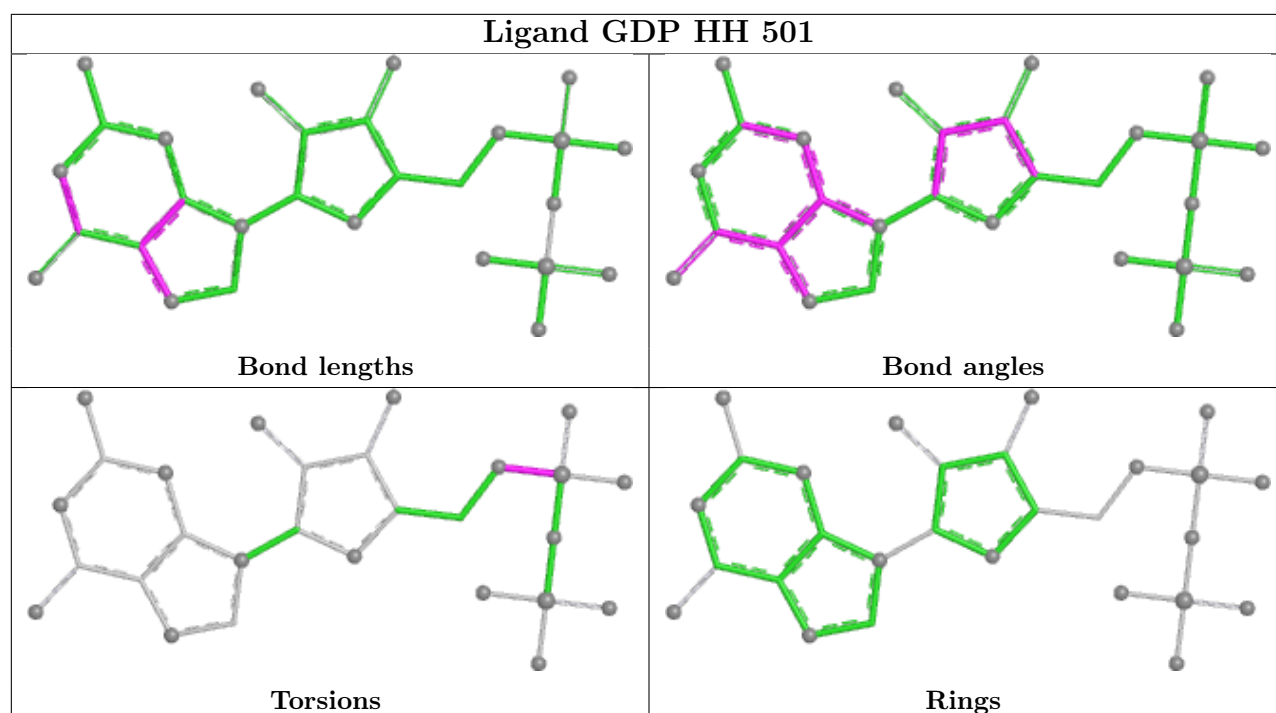
Ligand GTP DG 501

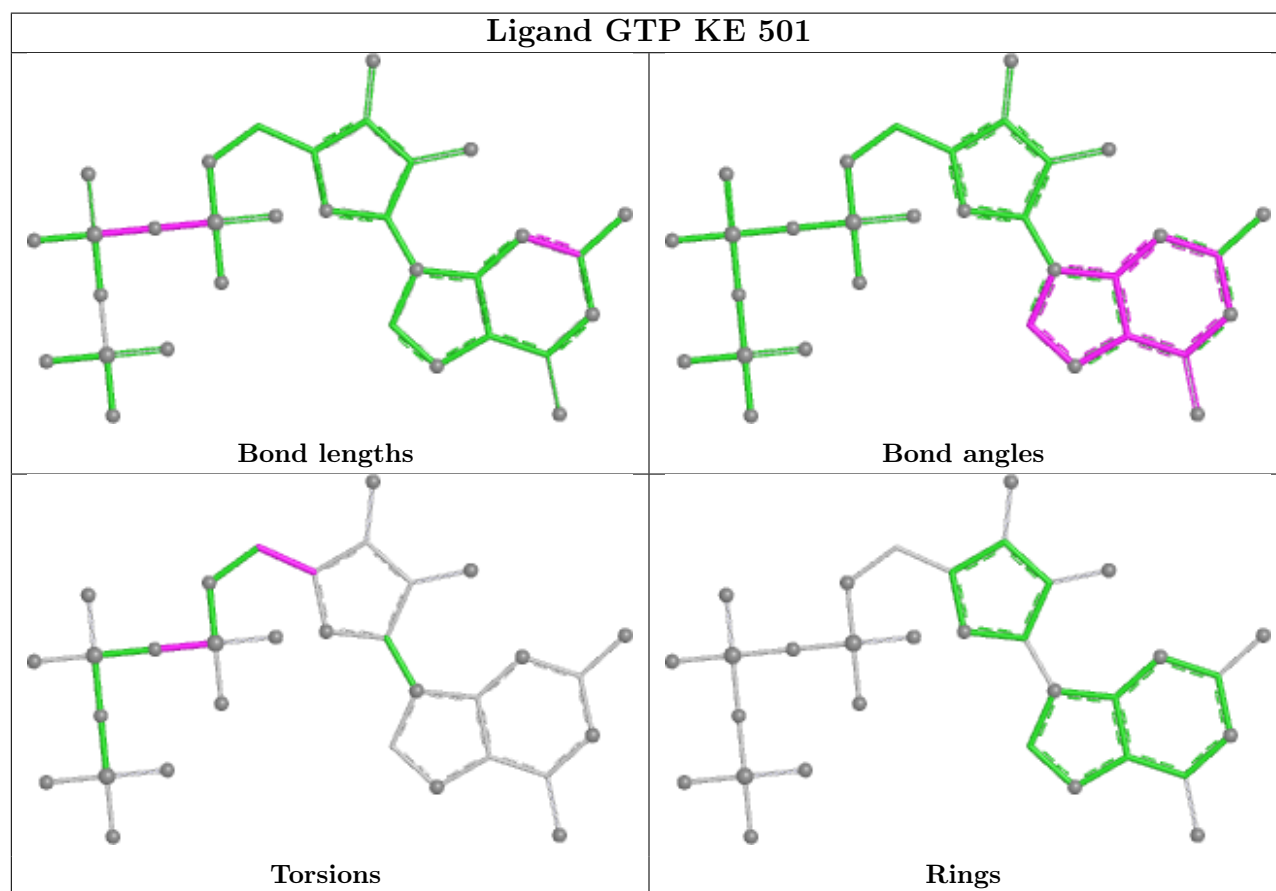
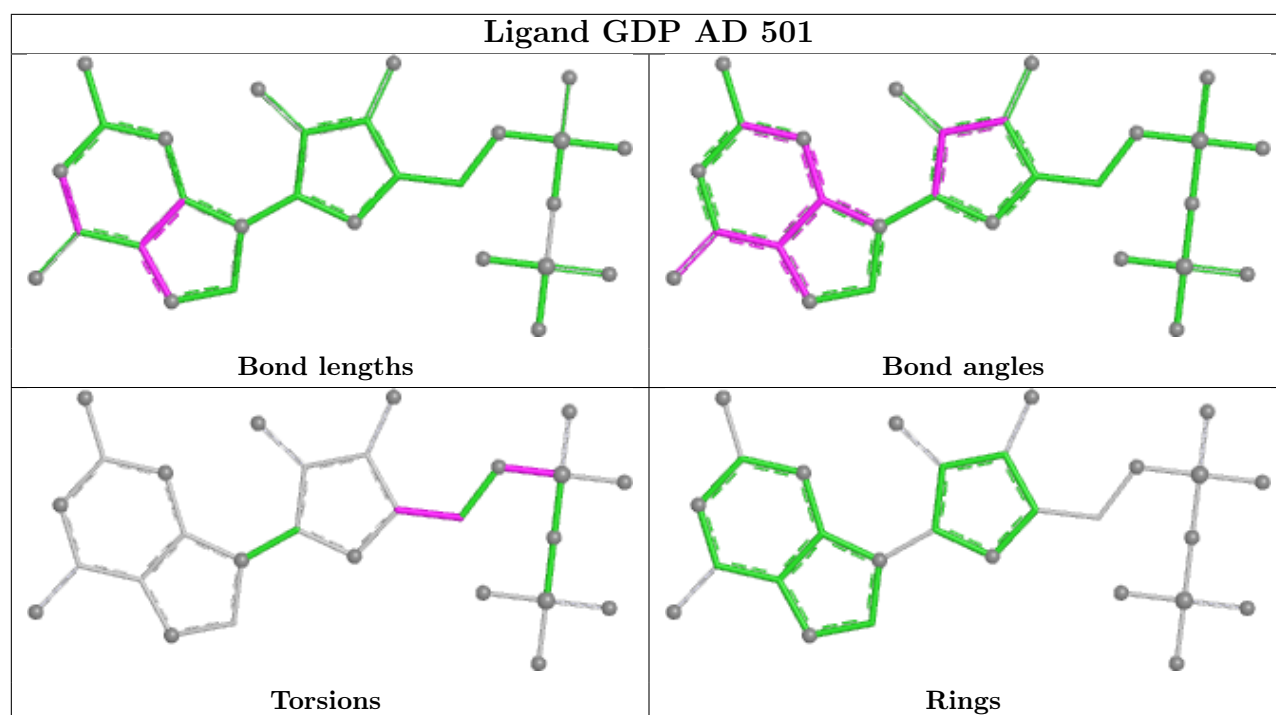


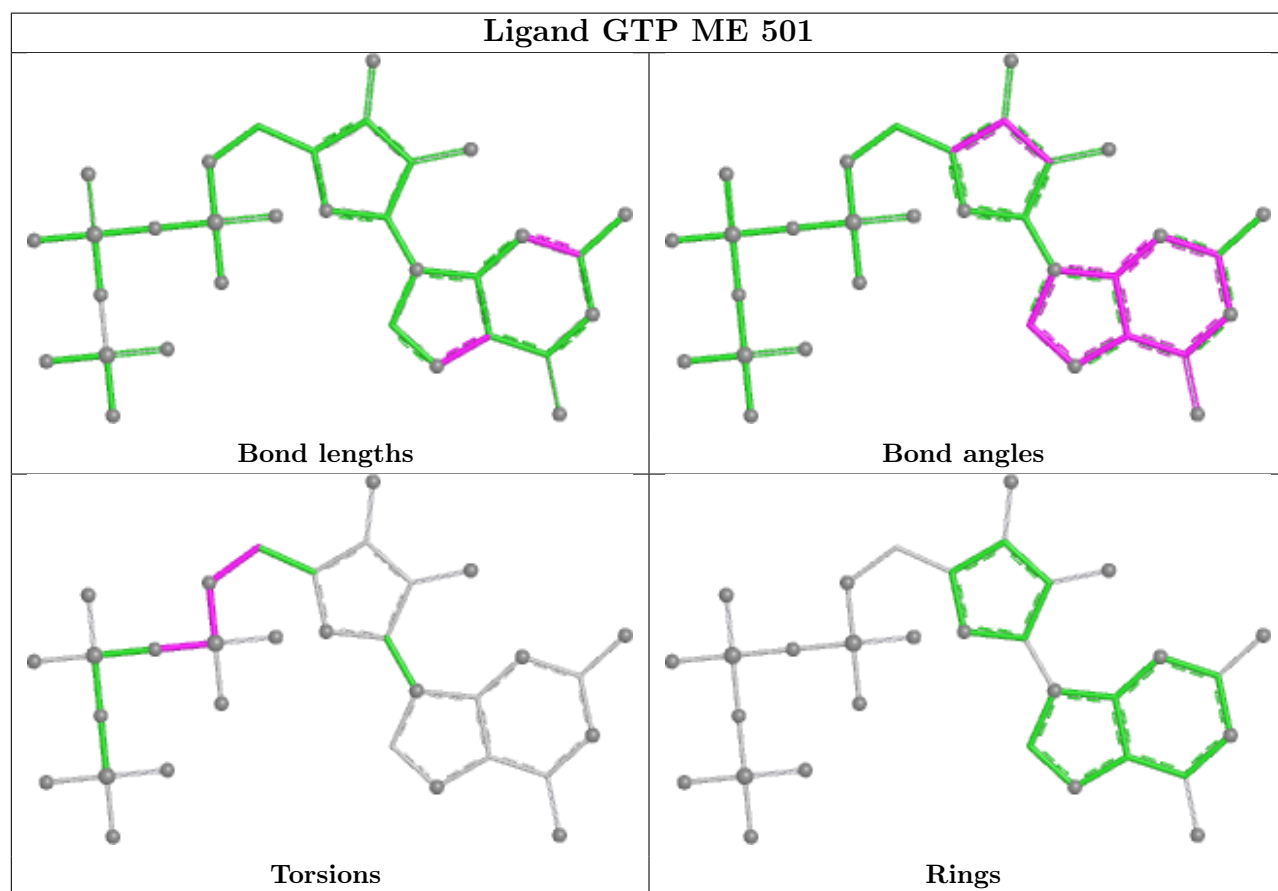
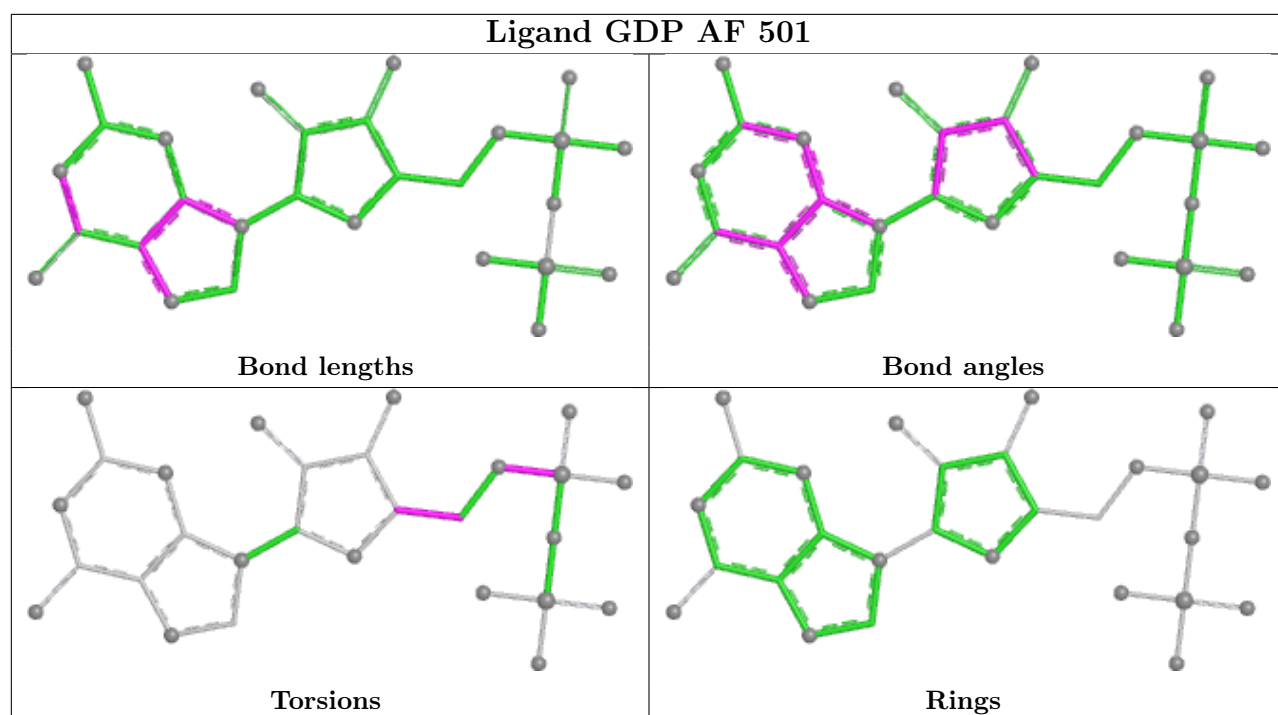
Ligand GDP JF 501

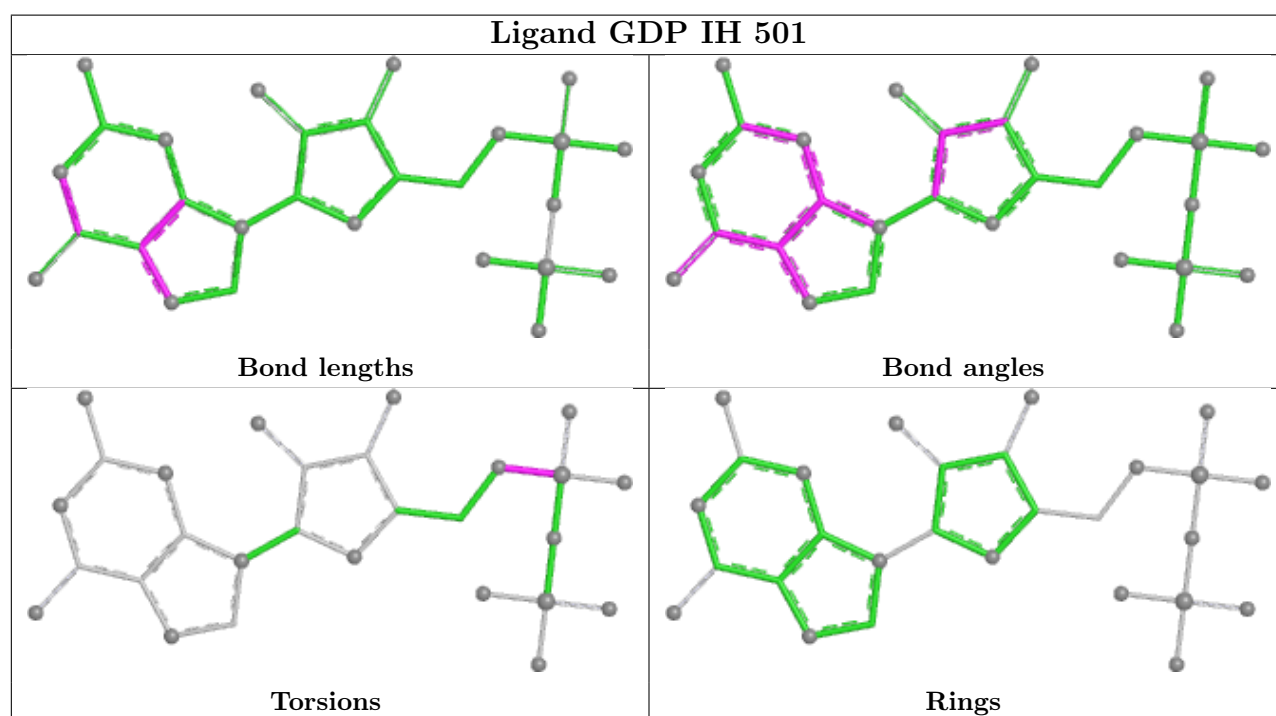
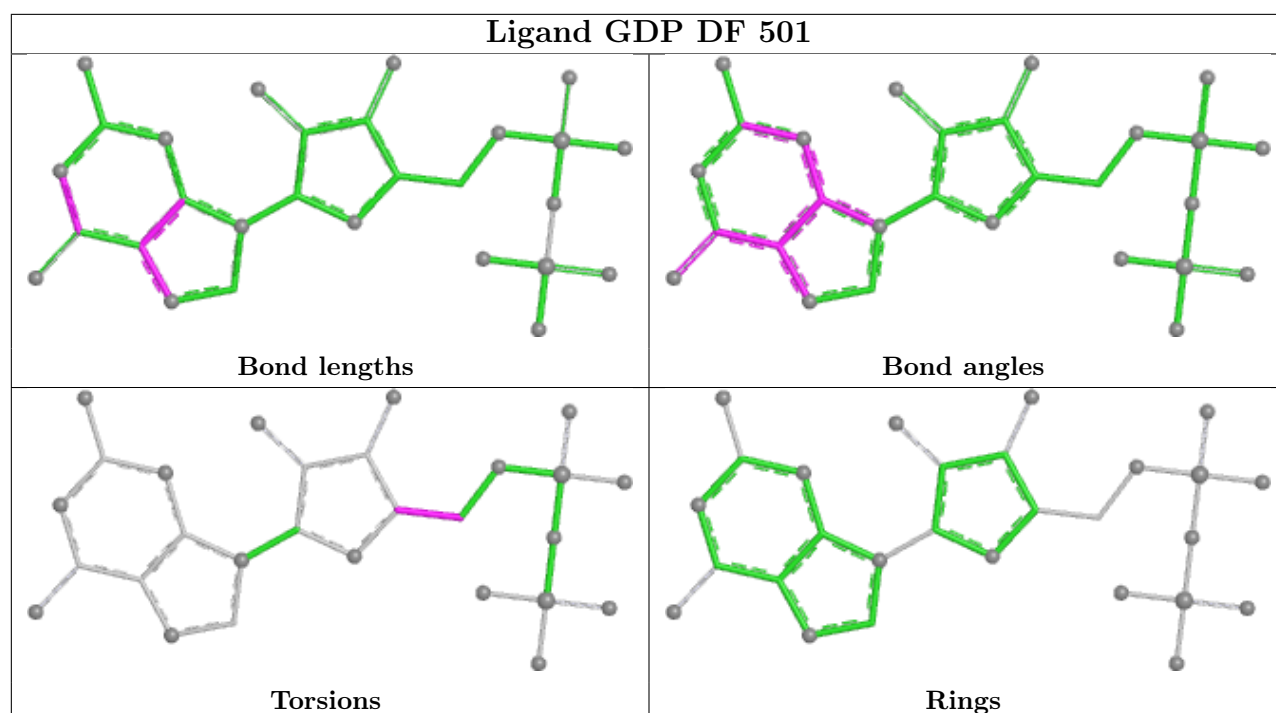


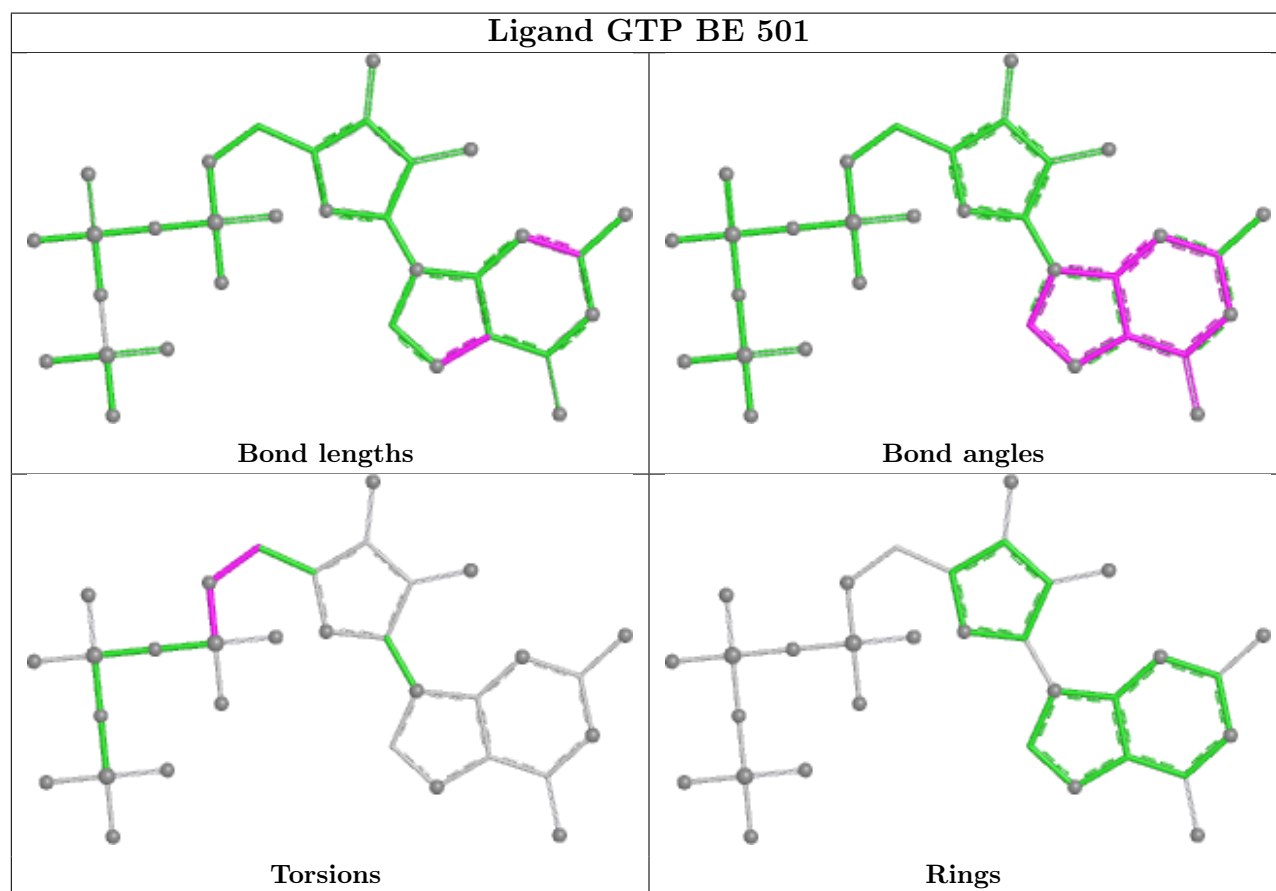
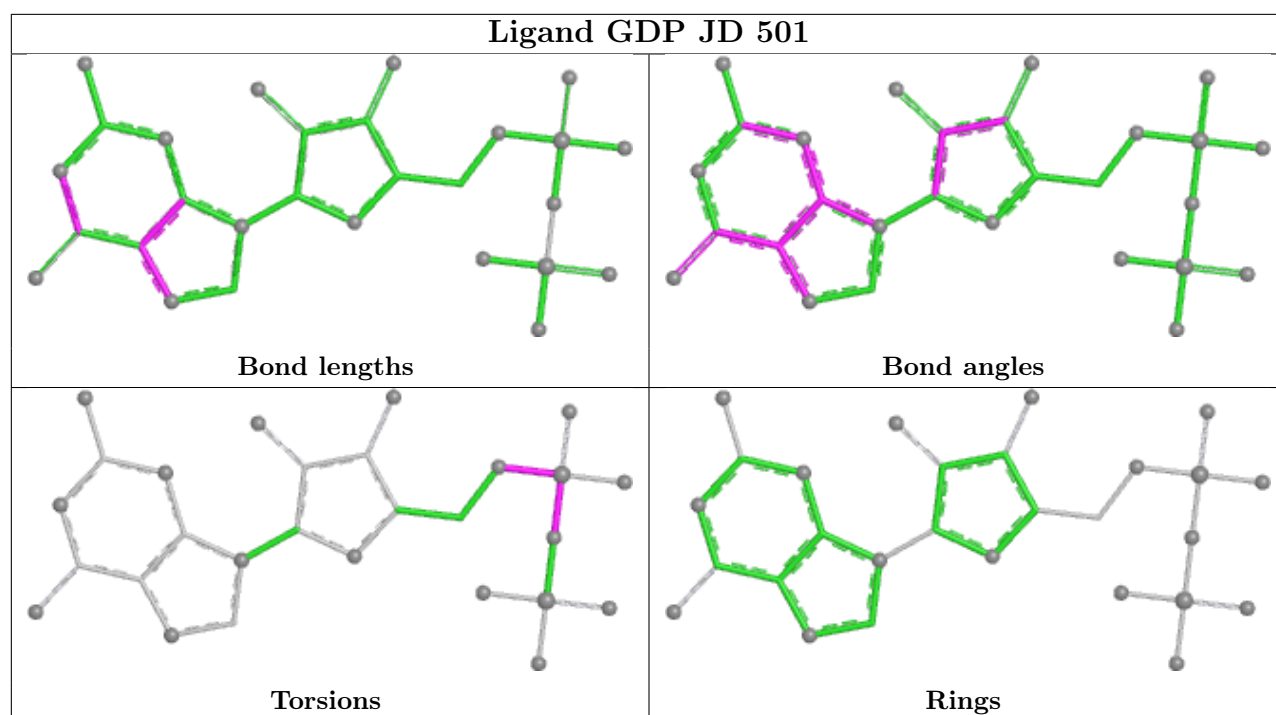


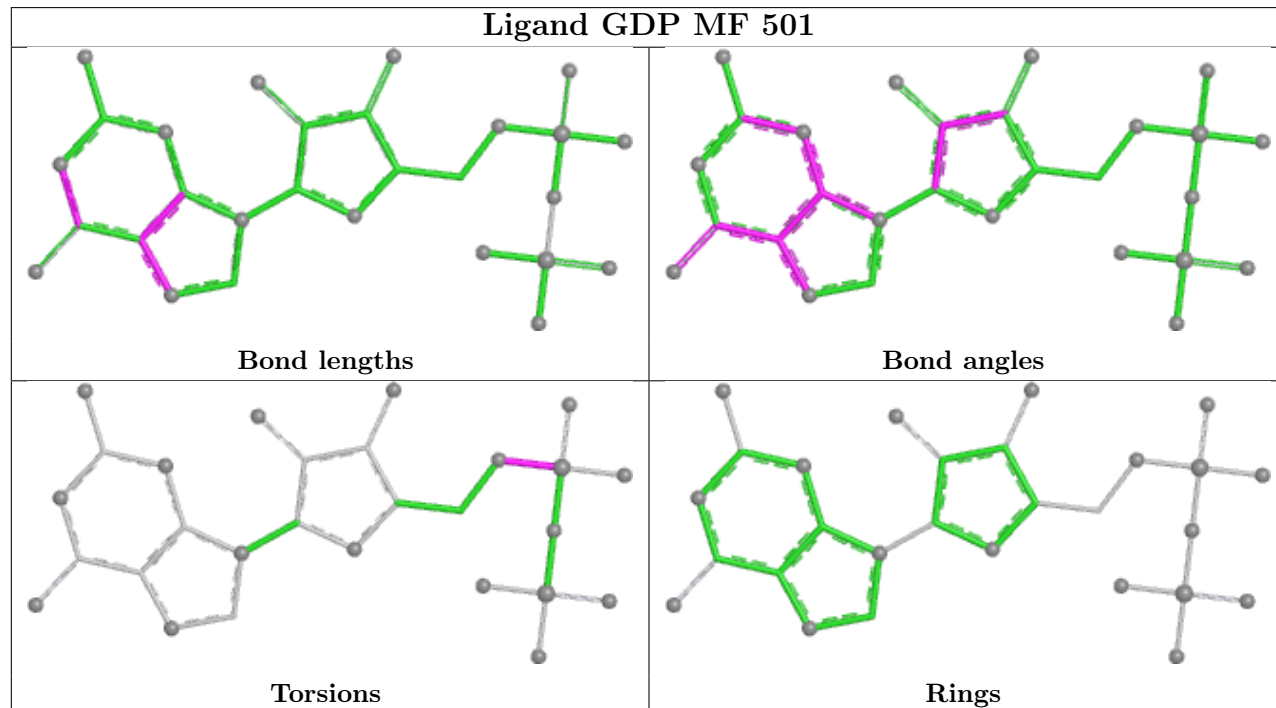
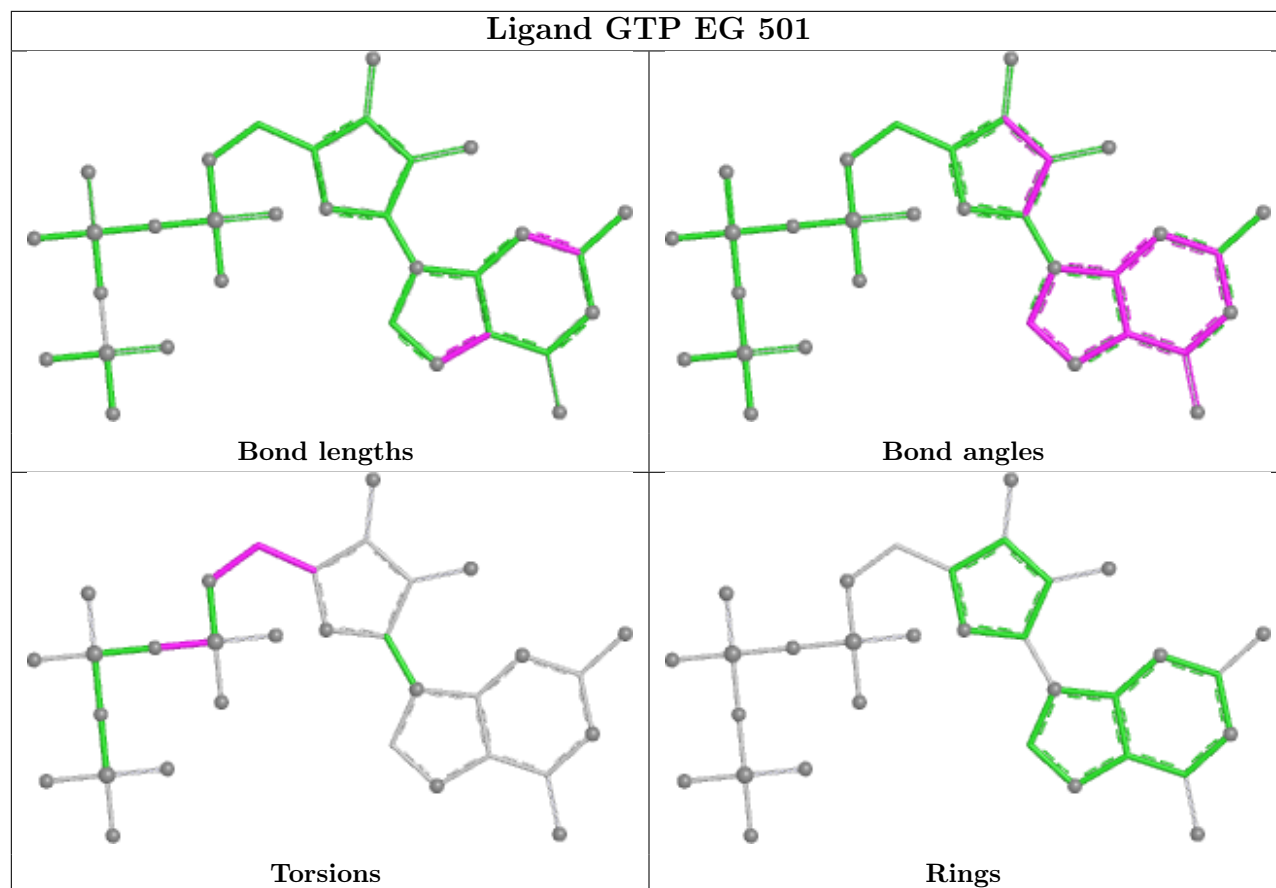


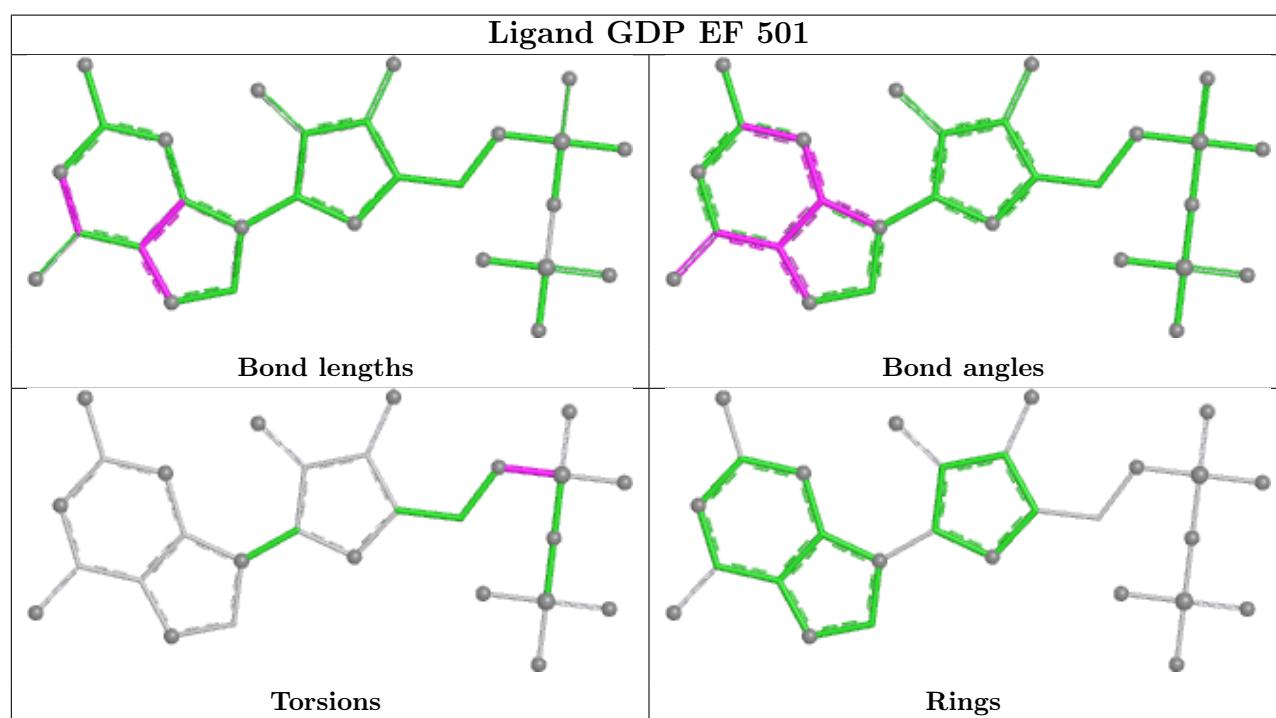
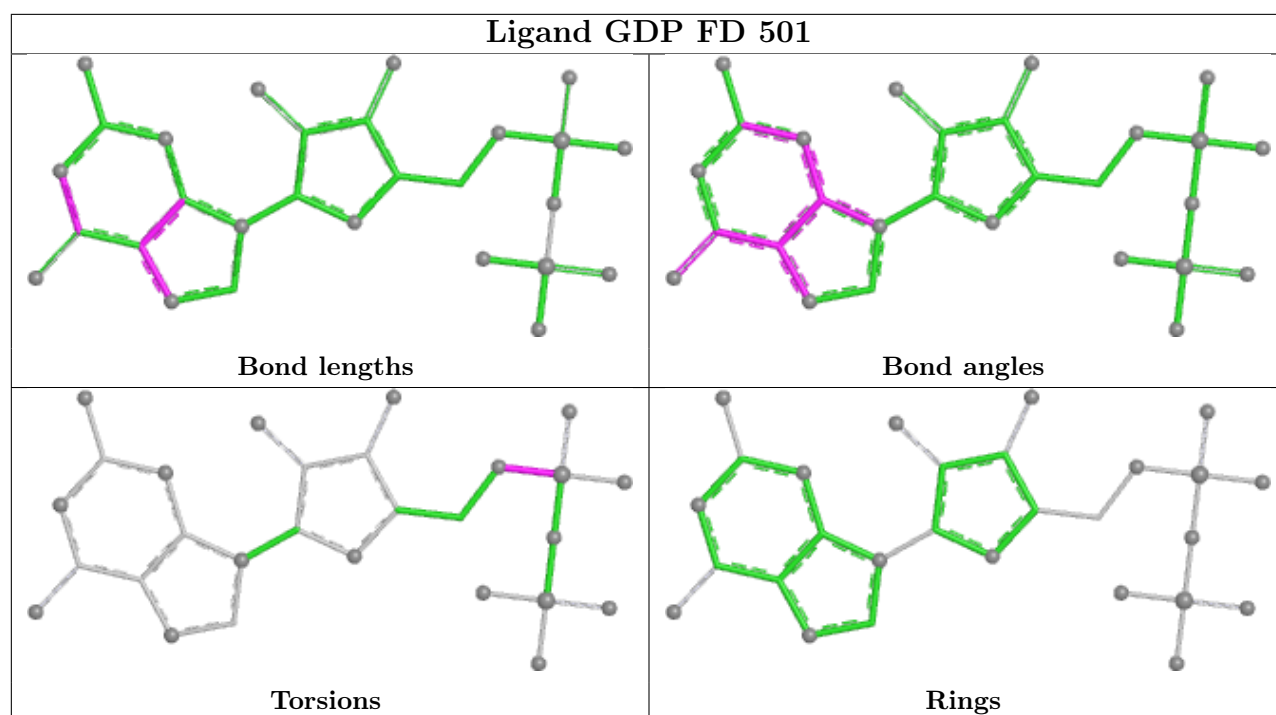


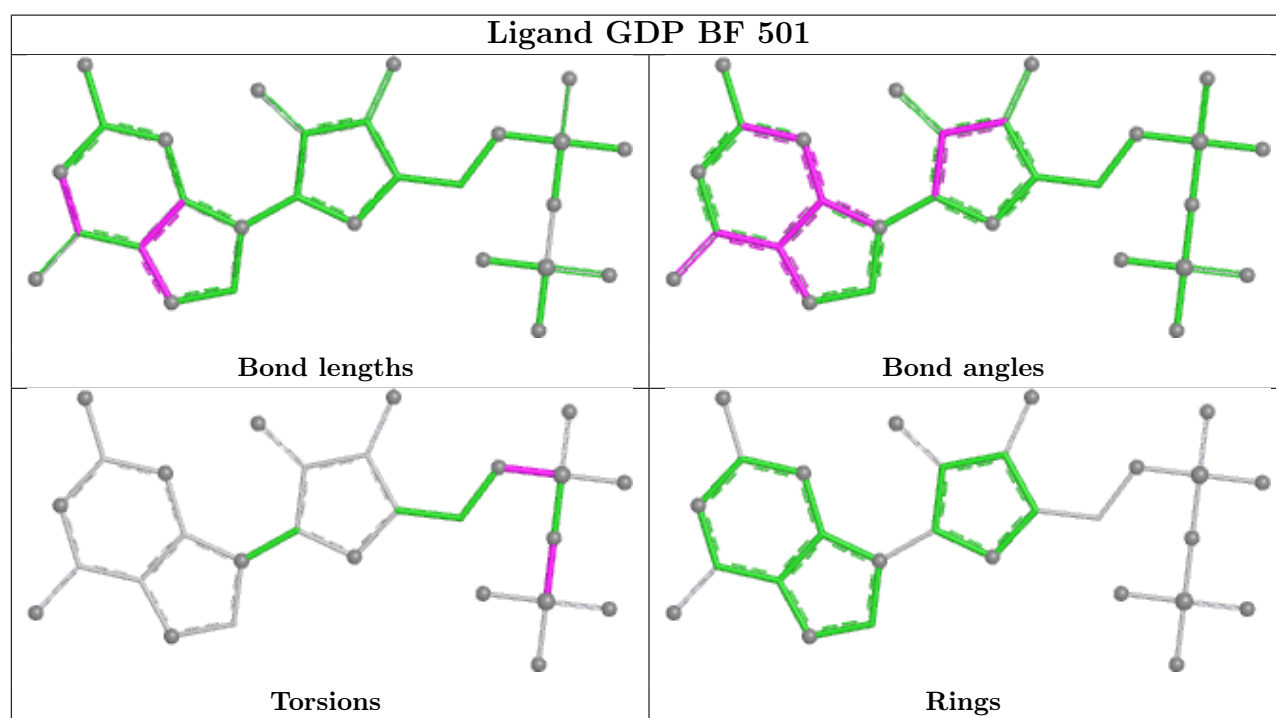
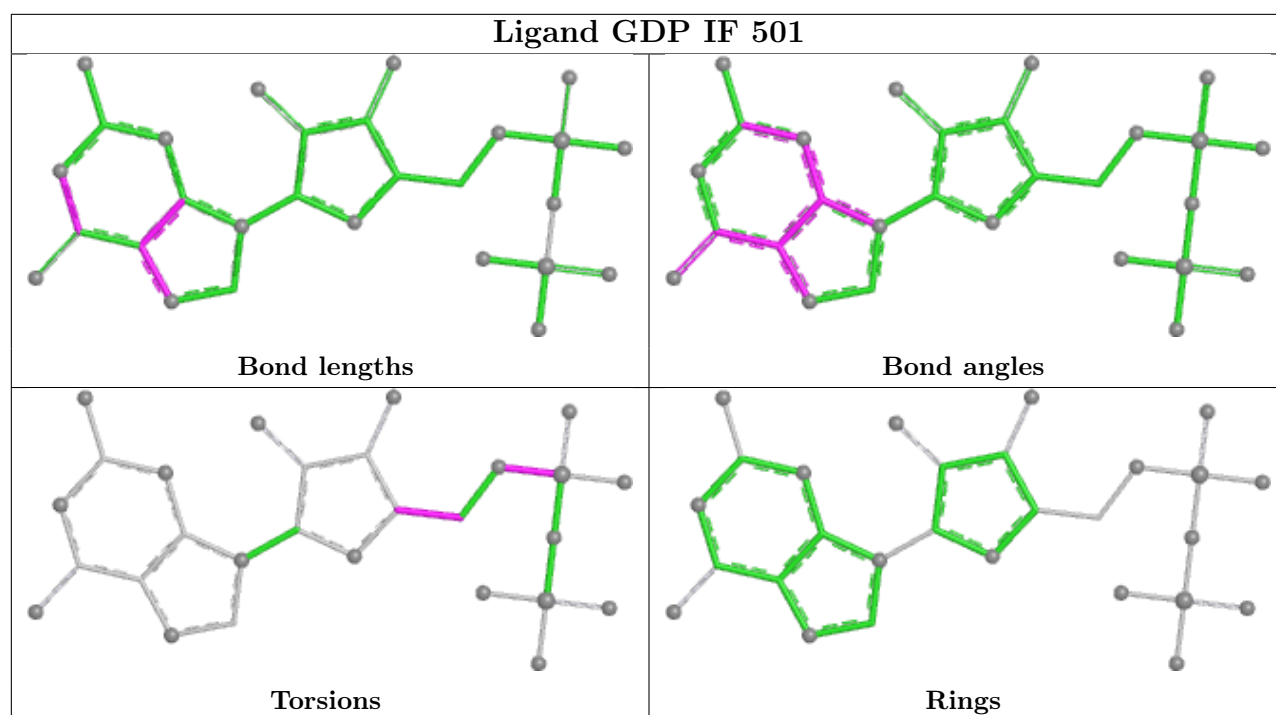




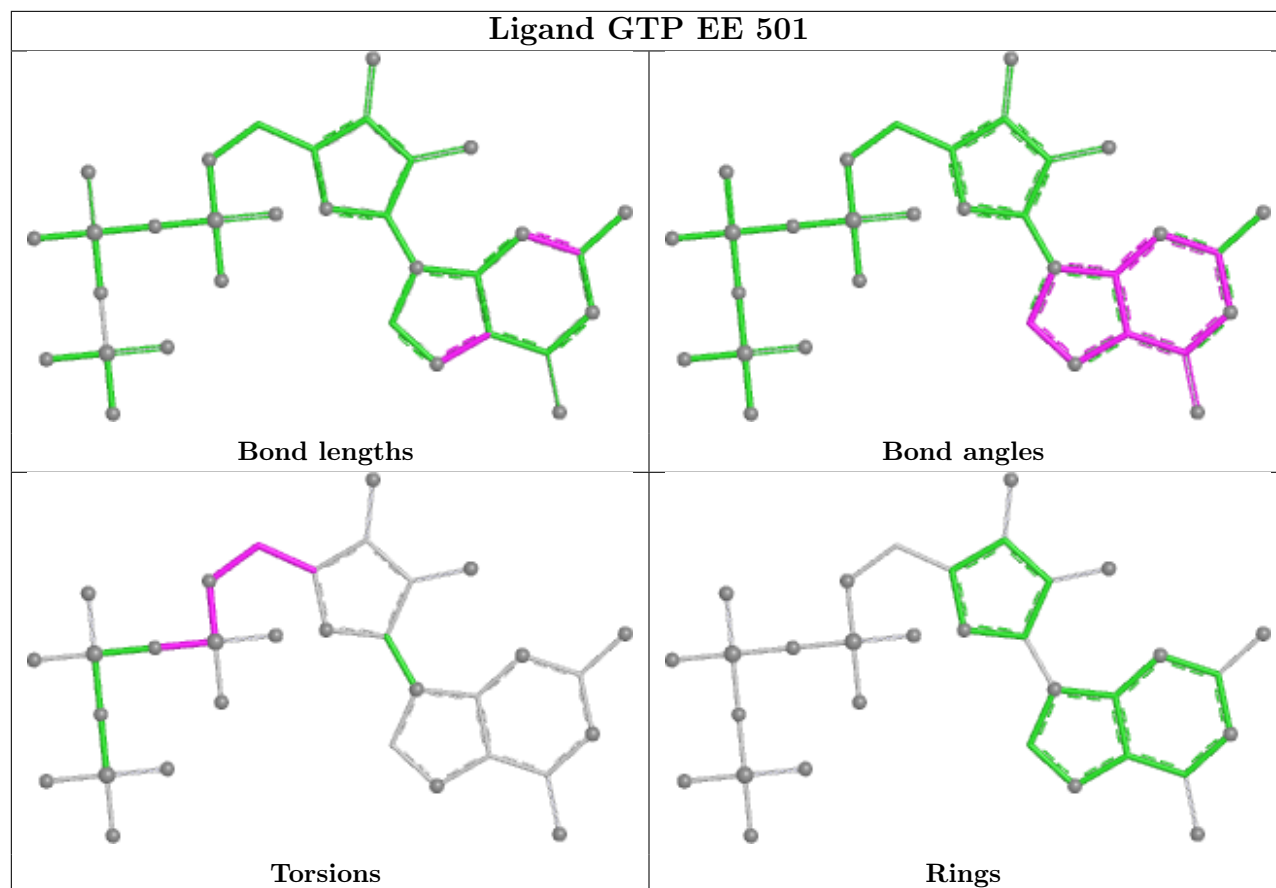




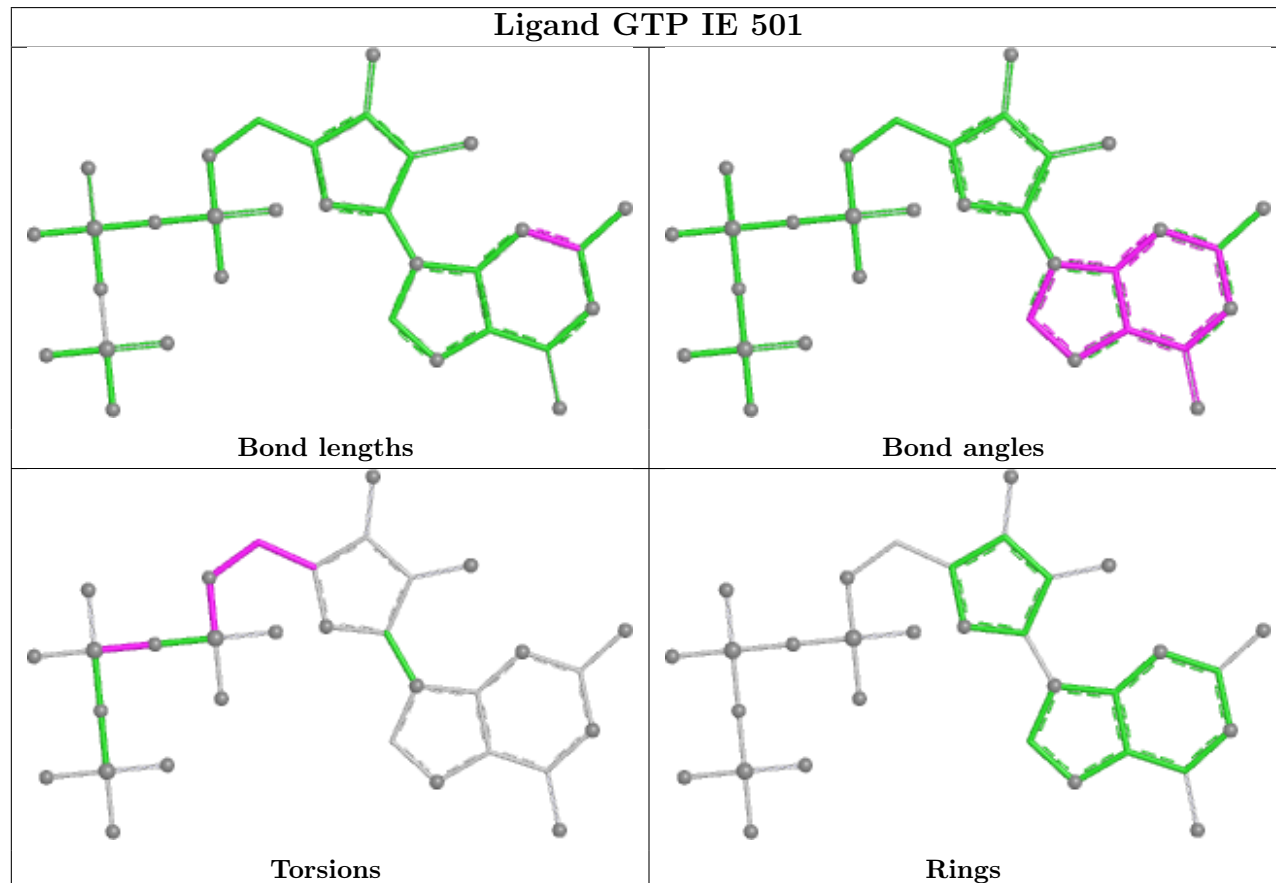




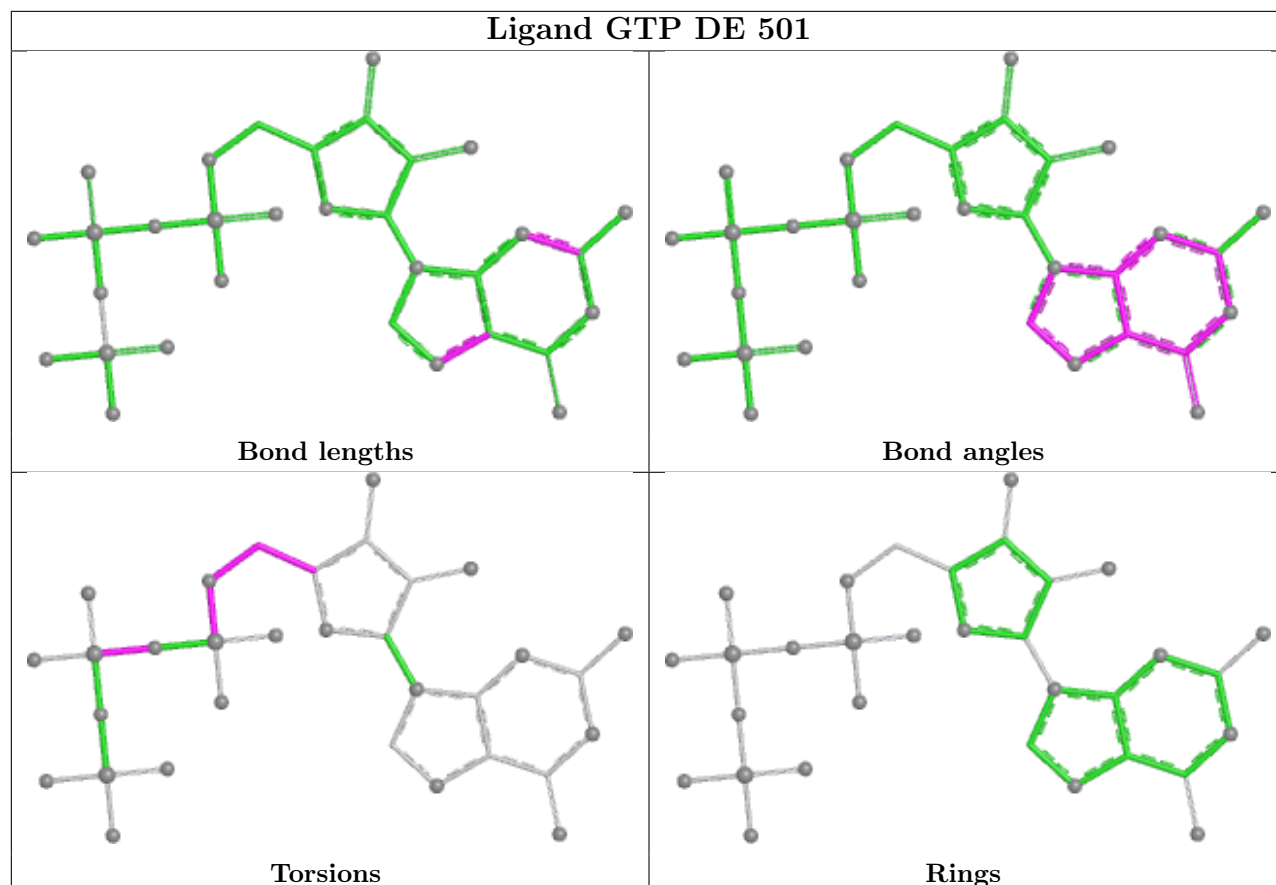
Ligand GTP EE 501



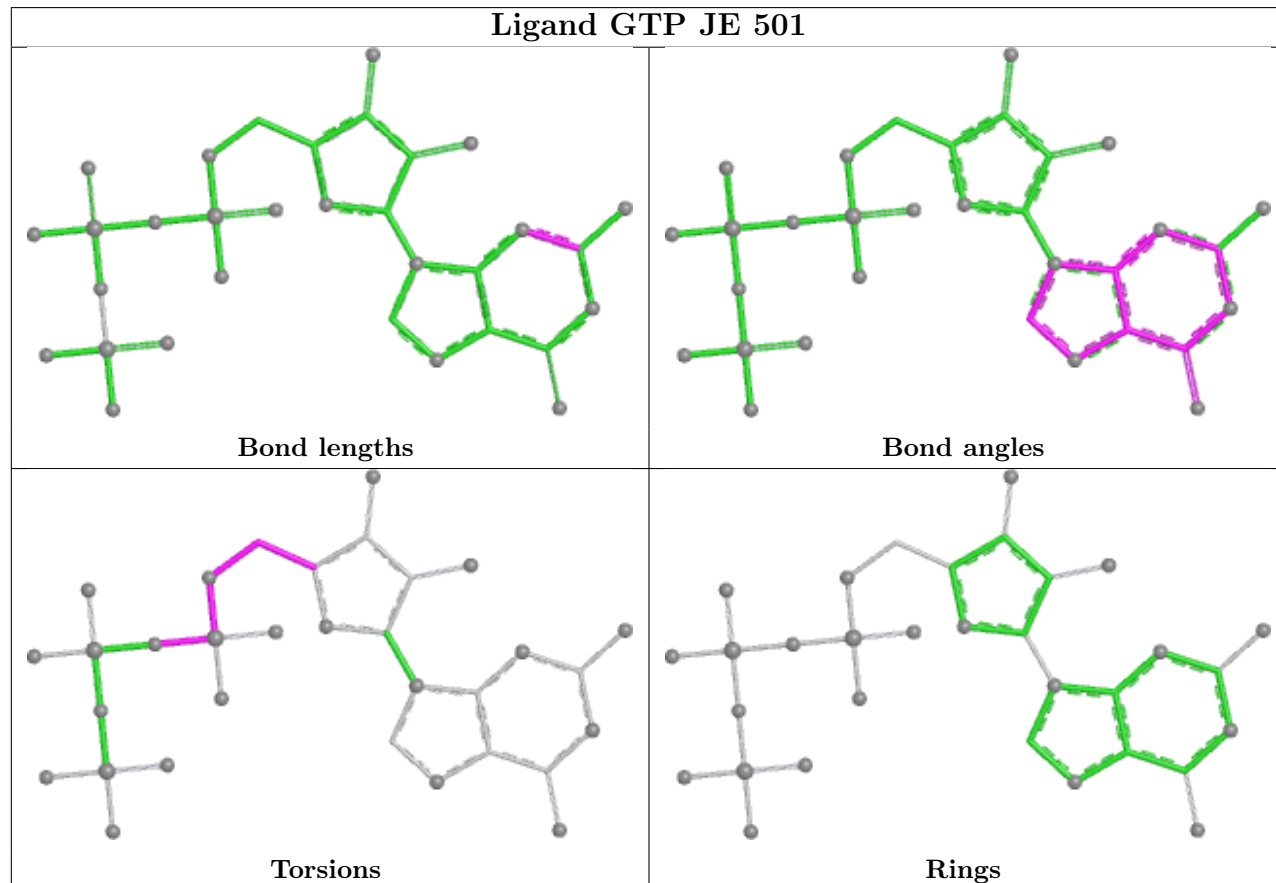
Ligand GTP IE 501

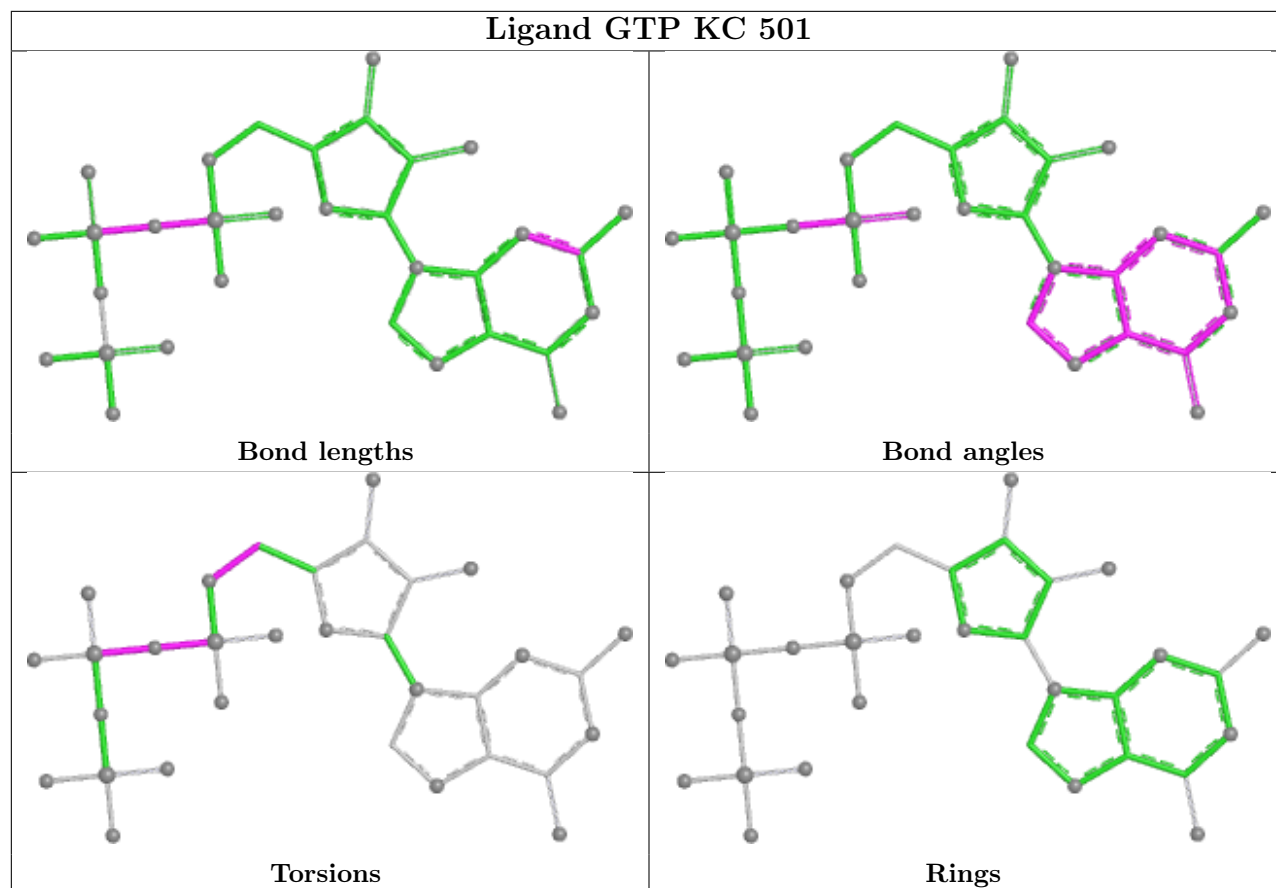


Ligand GTP DE 501



Ligand GTP JE 501





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

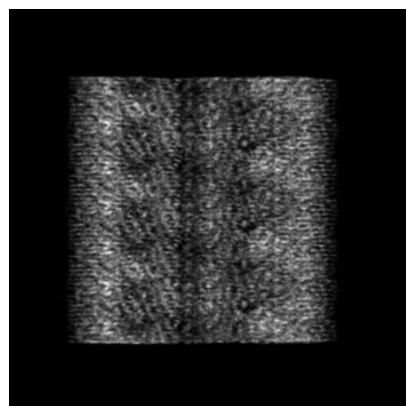
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26611. These allow visual inspection of the internal detail of the map and identification of artifacts.

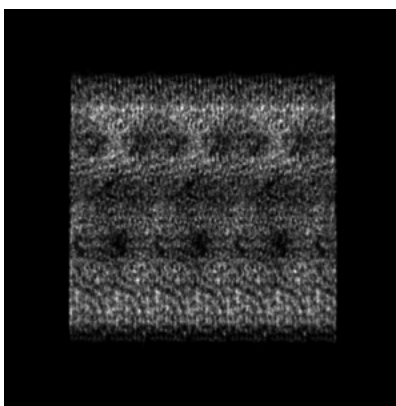
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

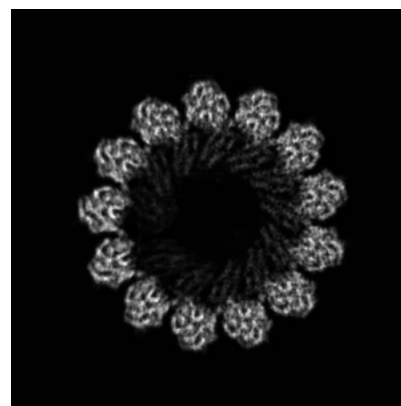
6.1.1 Primary map



X

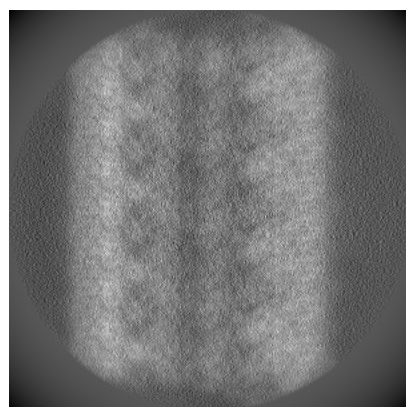


Y

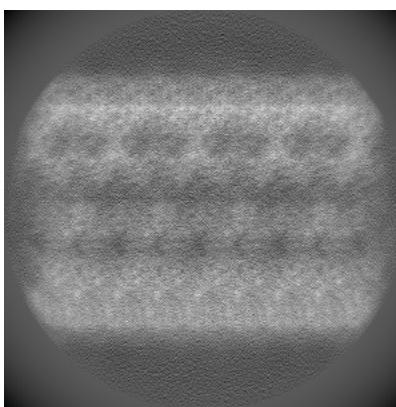


Z

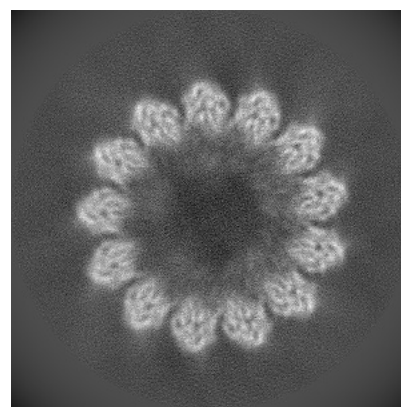
6.1.2 Raw map



X



Y

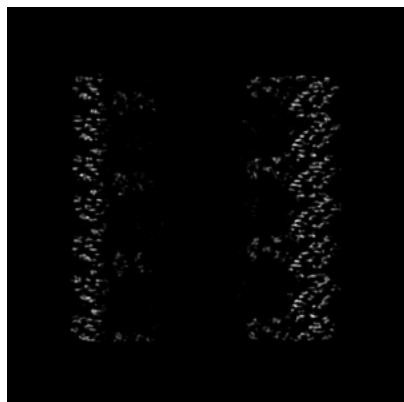


Z

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

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 240

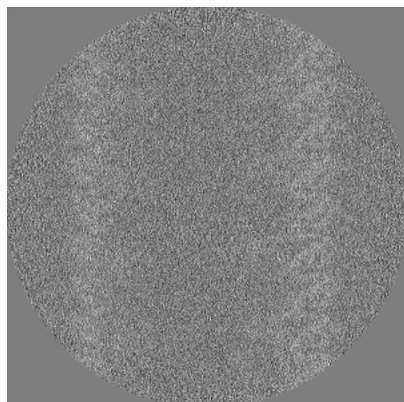


Y Index: 240

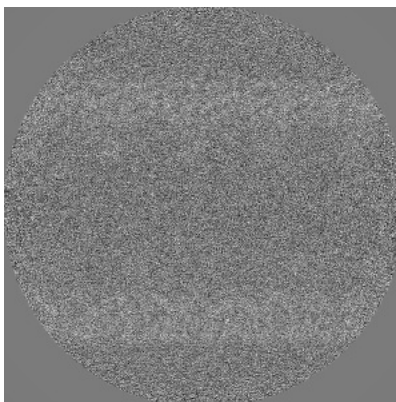


Z Index: 240

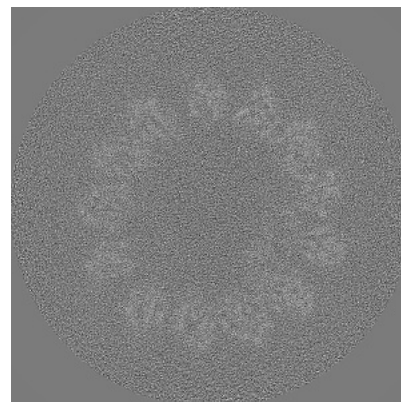
6.2.2 Raw map



X Index: 240



Y Index: 240

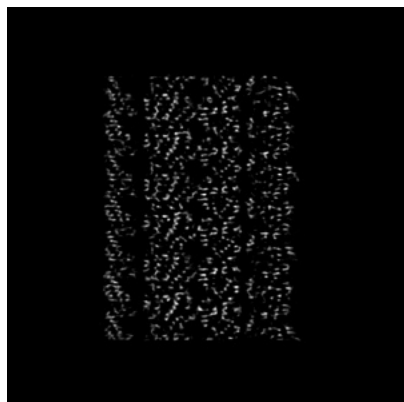


Z Index: 240

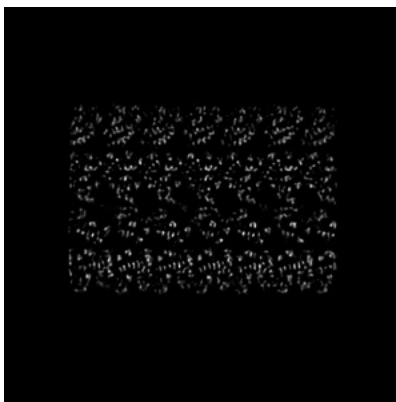
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 359

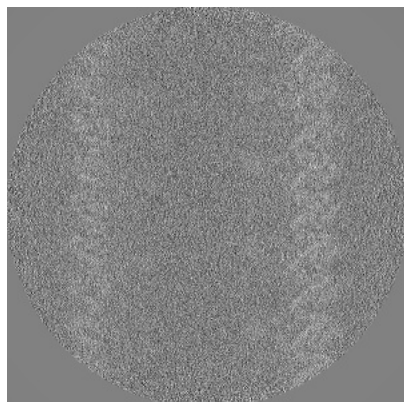


Y Index: 118

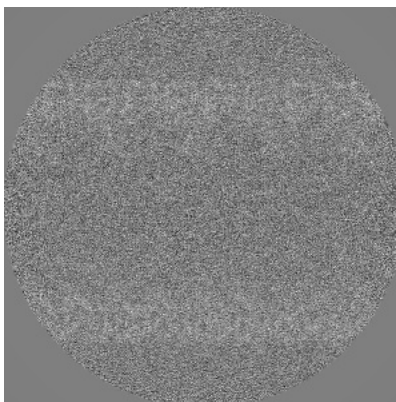


Z Index: 160

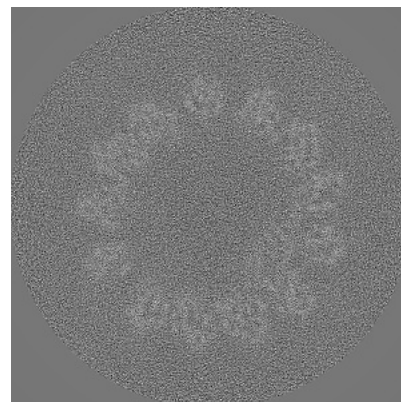
6.3.2 Raw map



X Index: 238



Y Index: 239

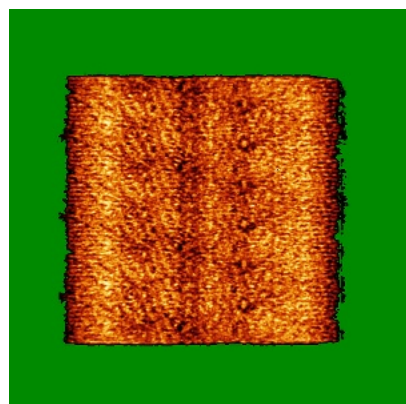


Z Index: 244

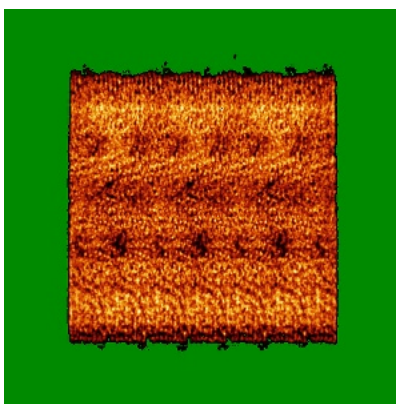
The images above show the largest variance slices of the map in three orthogonal directions.

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

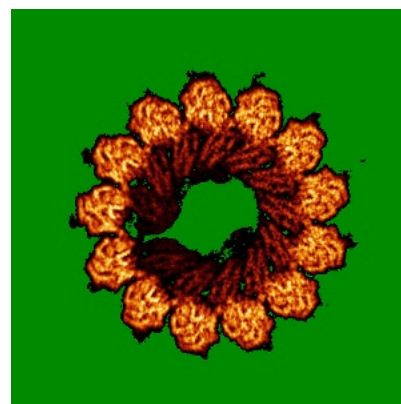
6.4.1 Primary map



X

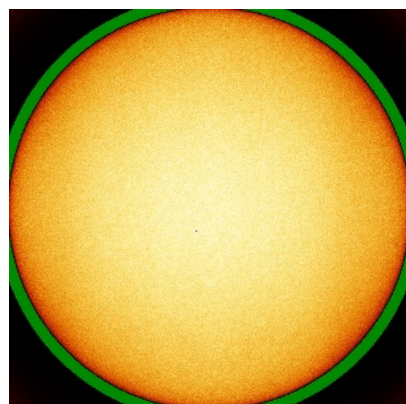


Y

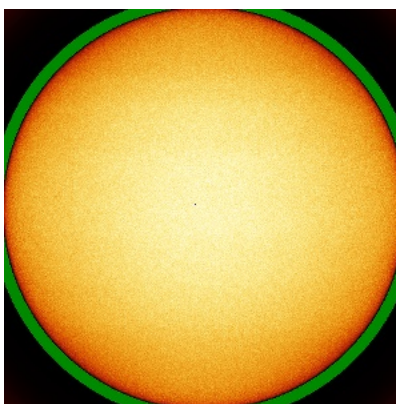


Z

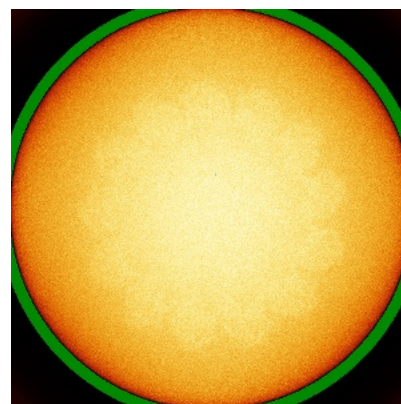
6.4.2 Raw map



X



Y

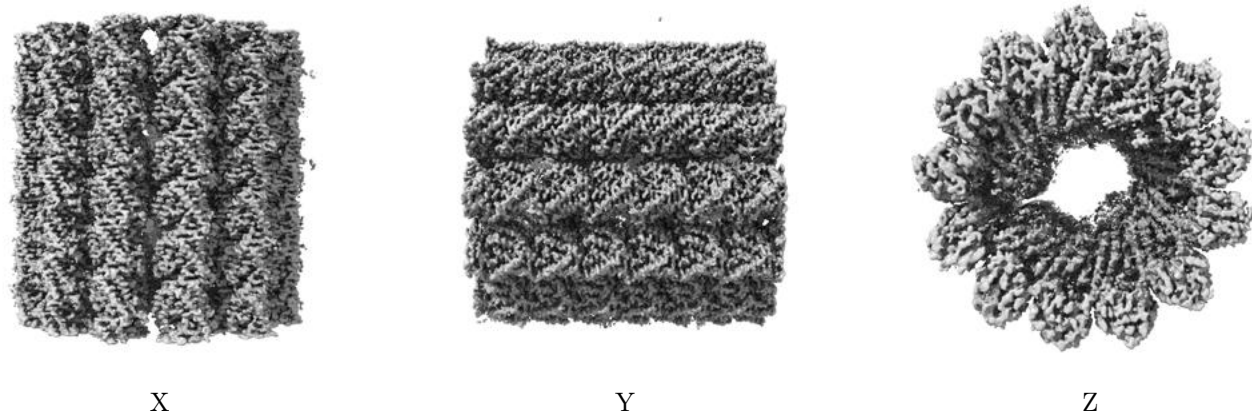


Z

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

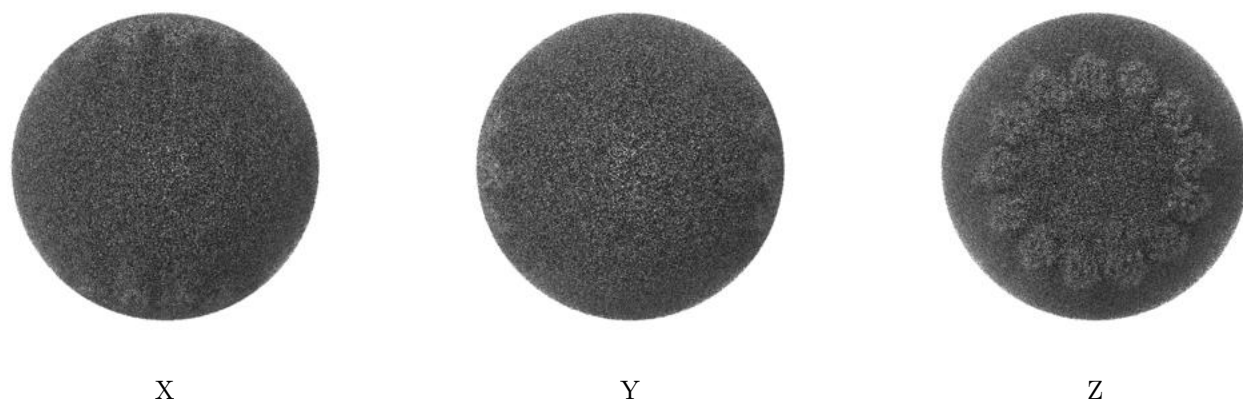
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

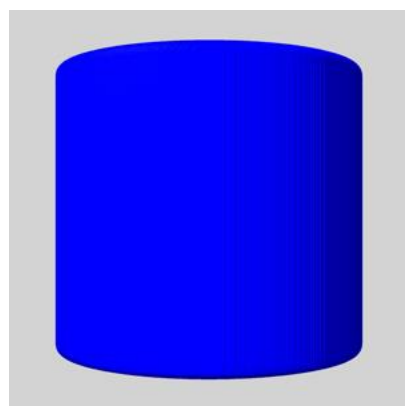
6.6 Mask visualisation [i](#)

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

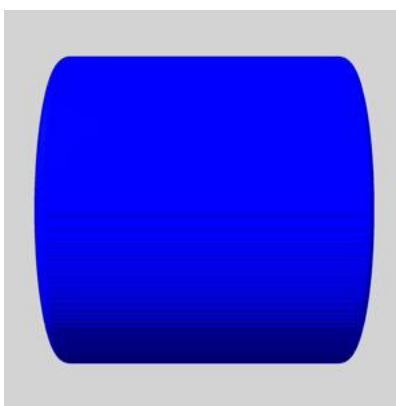
A mask typically either:

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

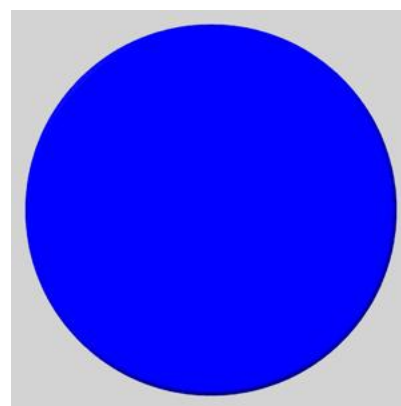
6.6.1 emd_26611_msk_1.map [i](#)



X



Y

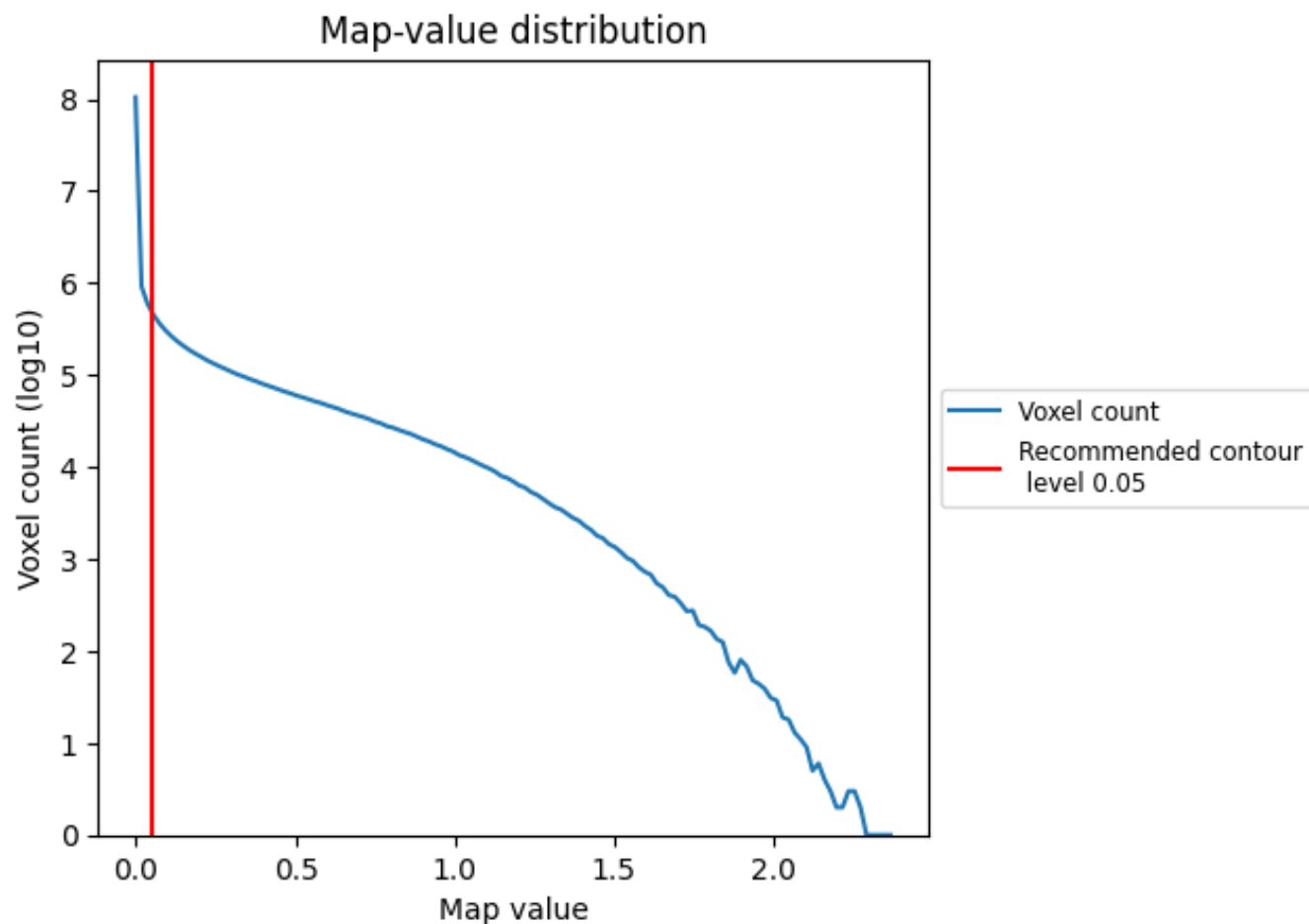


Z

7 Map analysis [i](#)

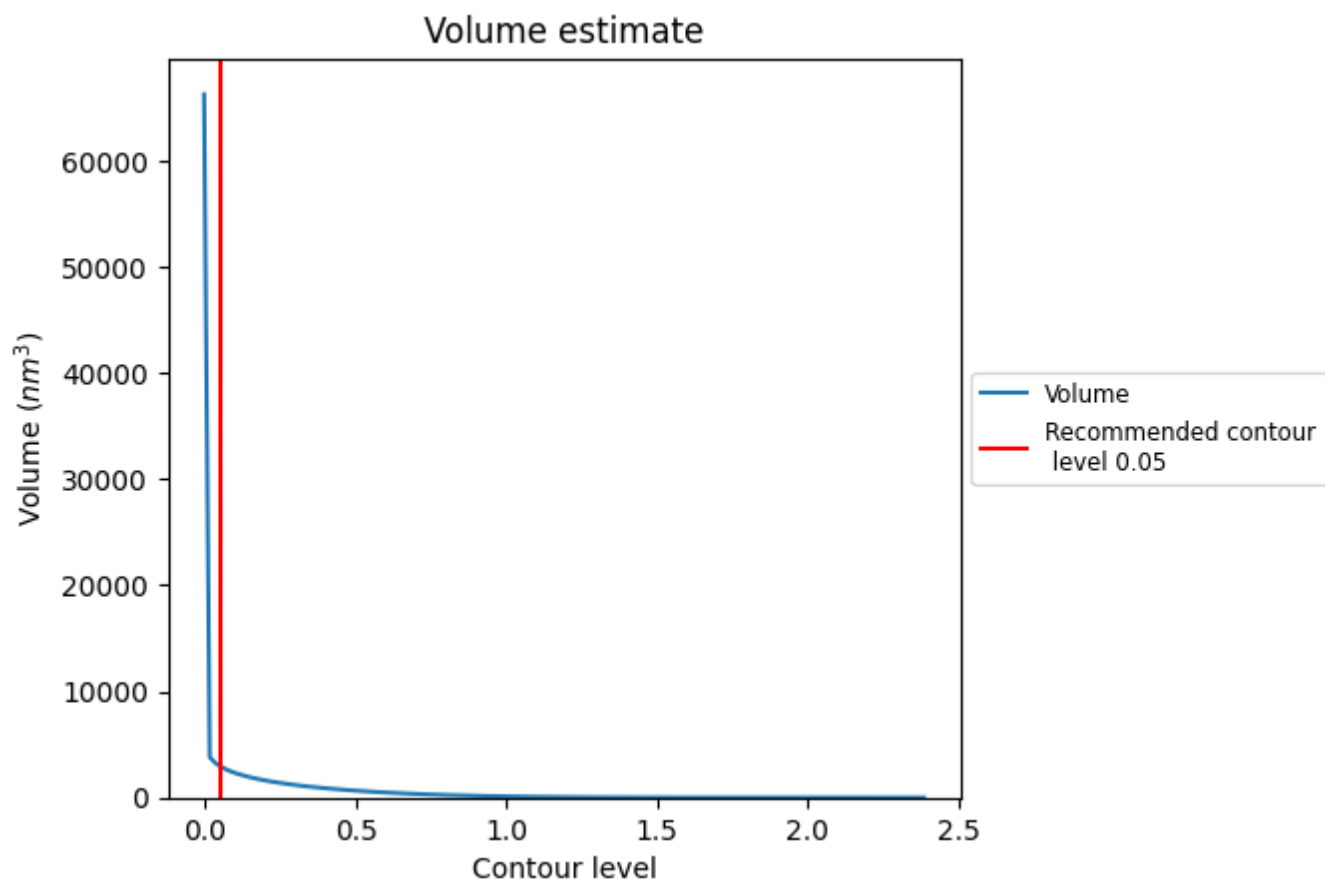
This section contains the results of statistical analysis of the map.

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.

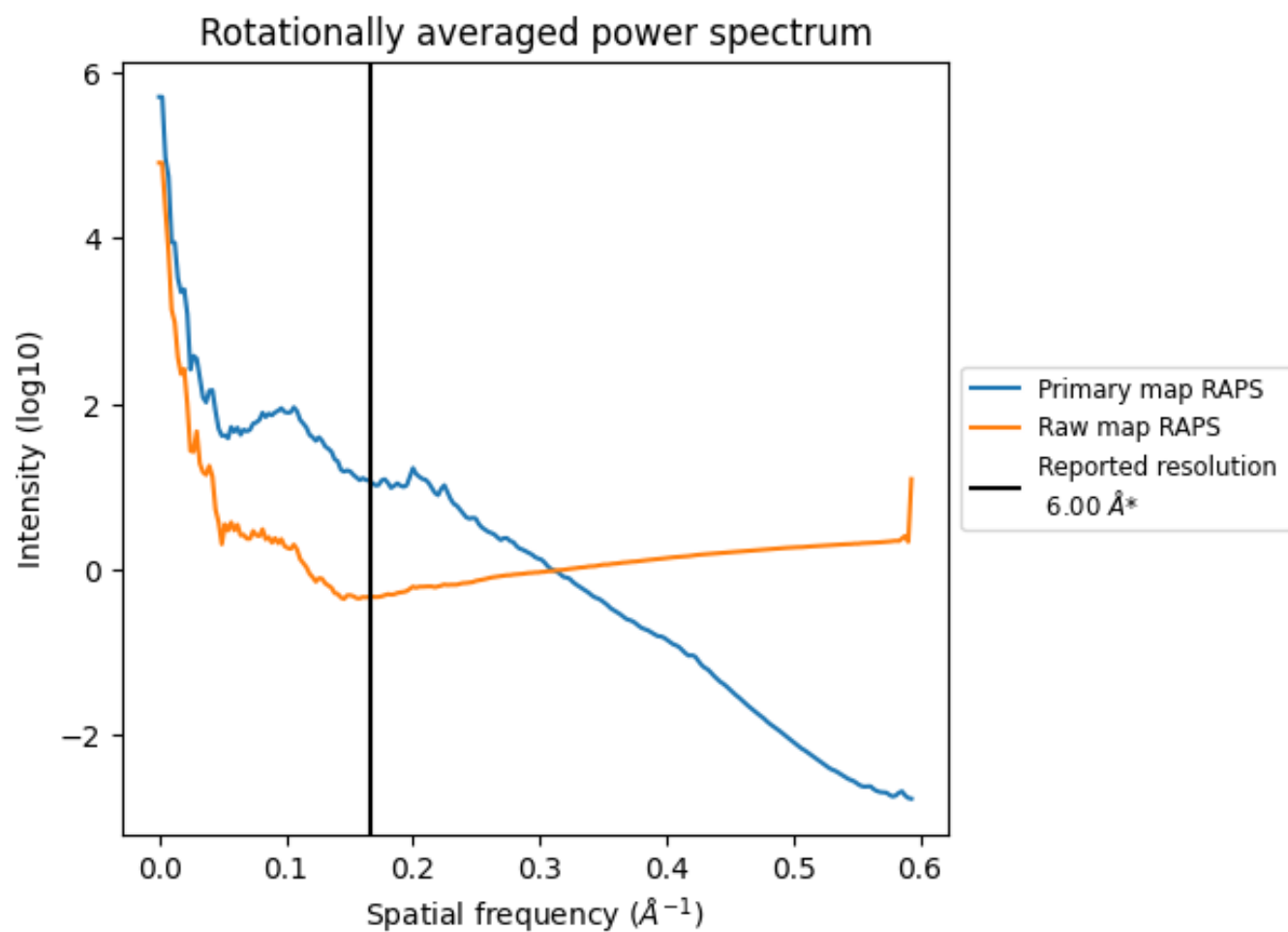
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2981 nm³; this corresponds to an approximate mass of 2692 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 ⓘ

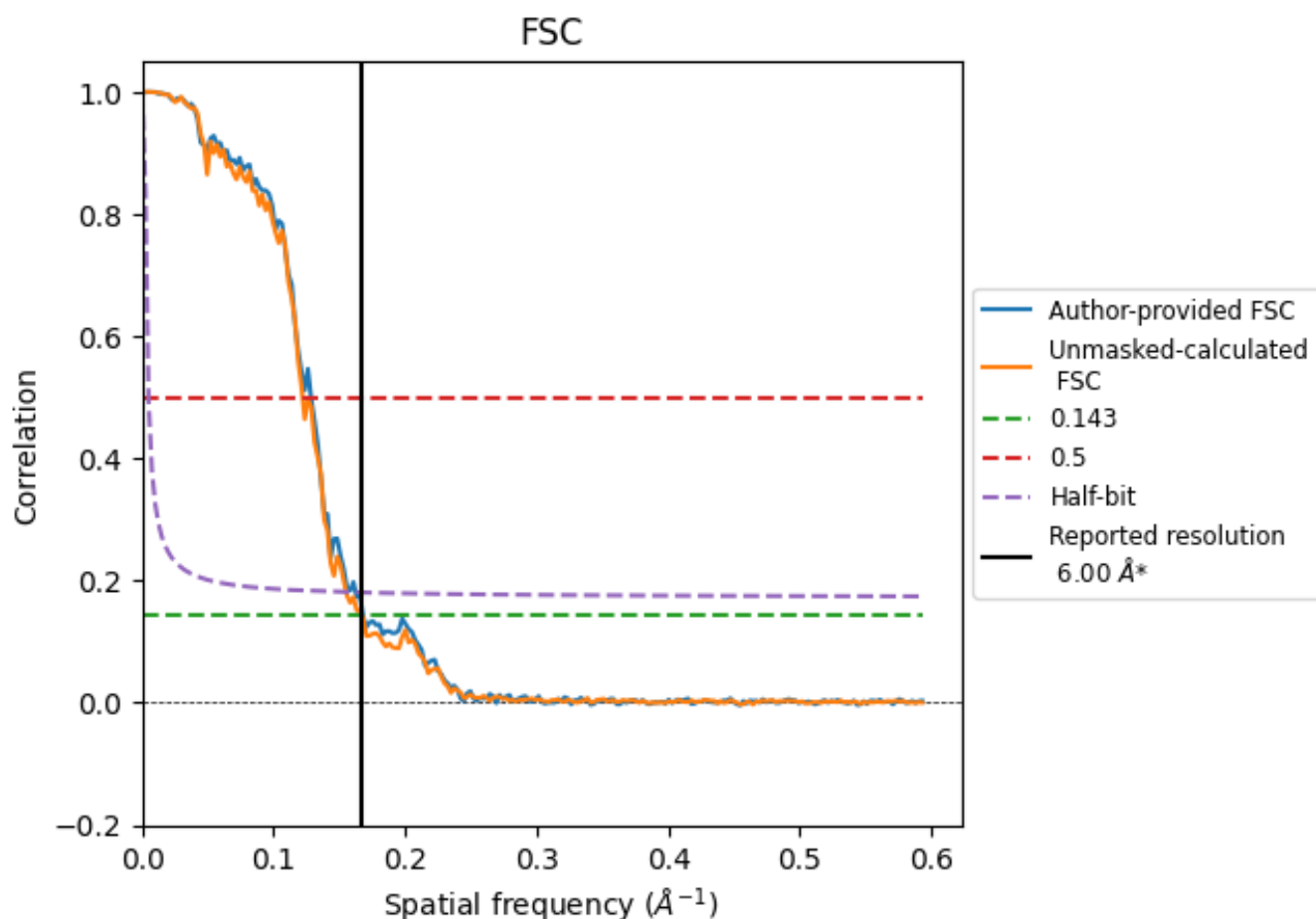


*Reported resolution corresponds to spatial frequency of 0.167 Å⁻¹

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 0.167 Å⁻¹

8.2 Resolution estimates [i](#)

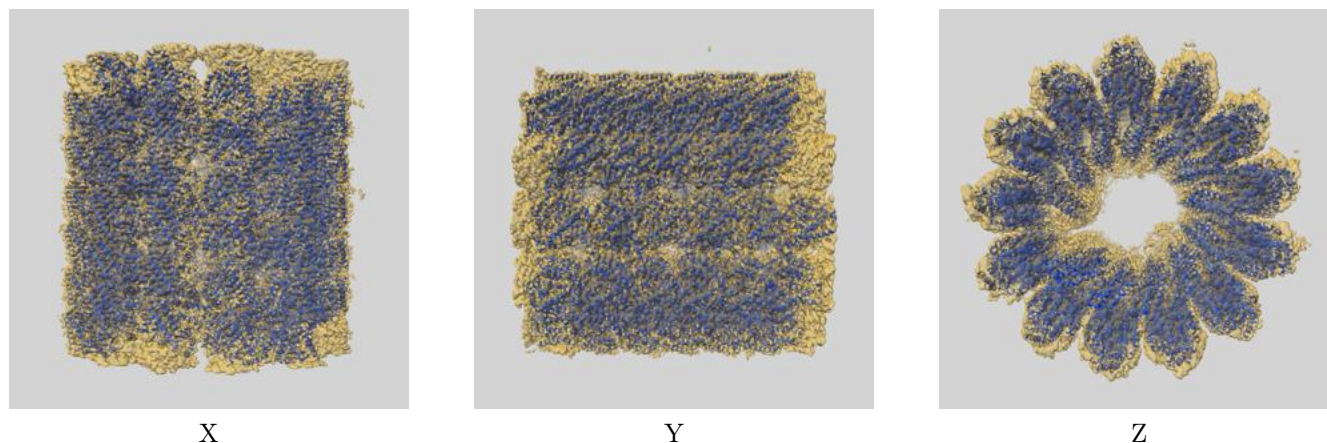
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.00	-	-
Author-provided FSC curve	5.96	7.79	6.16
Unmasked-calculated*	5.98	8.20	6.45

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

9 Map-model fit [i](#)

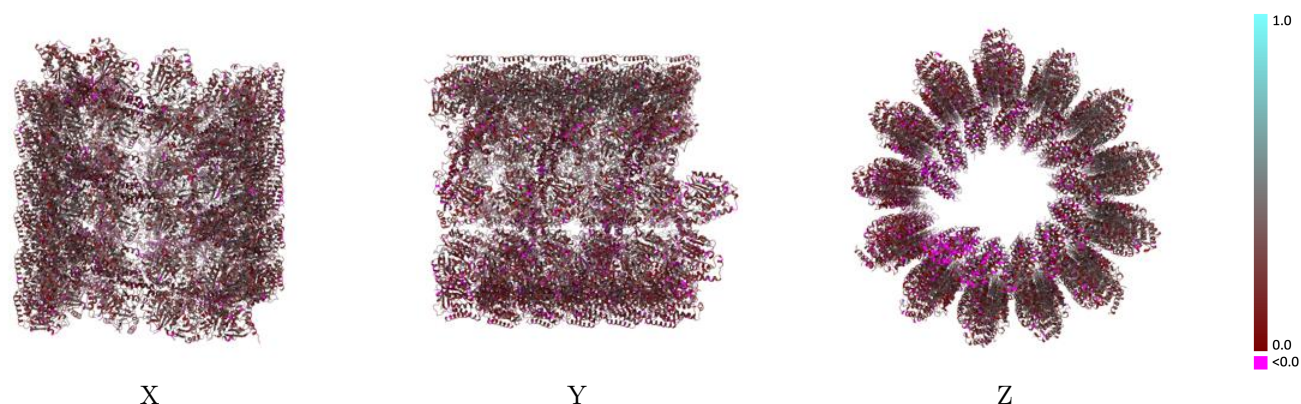
This section contains information regarding the fit between EMDB map EMD-26611 and PDB model 7UN1. Per-residue inclusion information can be found in section [3](#) on page [21](#).

9.1 Map-model overlay [i](#)



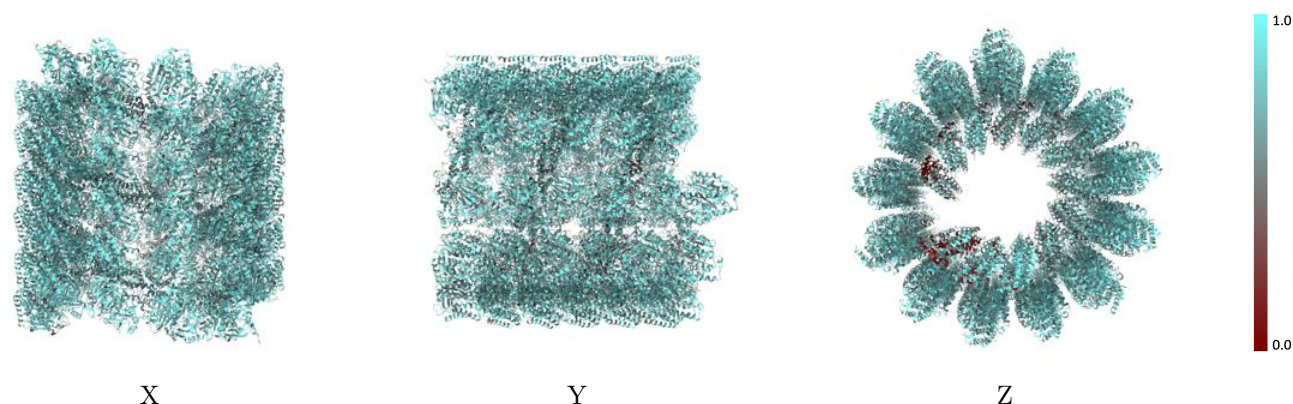
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



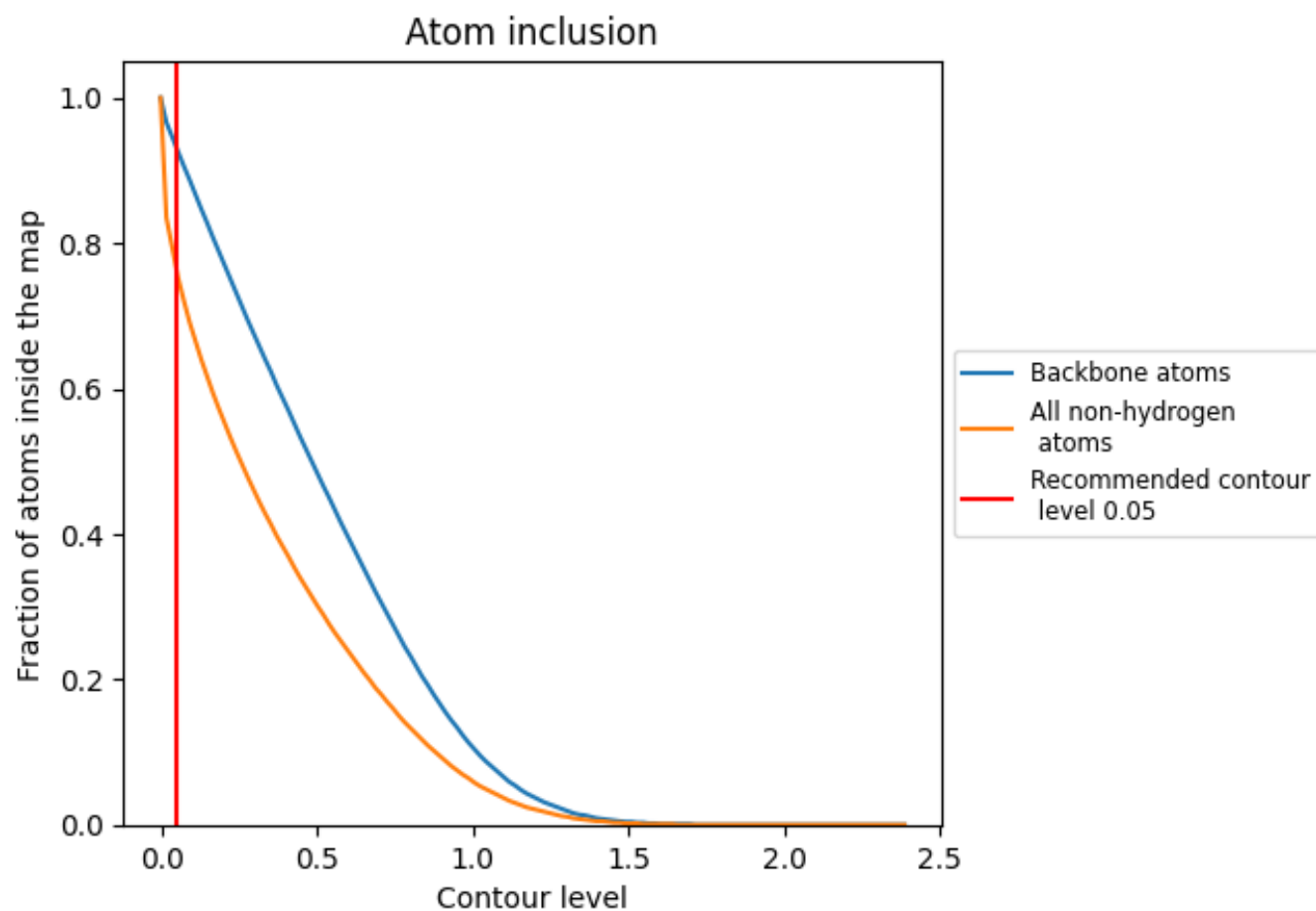
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.05).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 76% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7610	 0.2540
A	 0.4030	 0.0620
AB	 0.7900	 0.2920
AC	 0.7980	 0.2980
AD	 0.8030	 0.3010
AE	 0.8030	 0.2950
AF	 0.7810	 0.2790
B	 0.6180	 0.1090
BA	 0.7960	 0.3010
BC	 0.8140	 0.3250
BD	 0.8060	 0.3210
BE	 0.8090	 0.3180
BF	 0.8070	 0.3040
BG	 0.7870	 0.2760
C	 0.7700	 0.1700
CB	 0.7920	 0.3000
CC	 0.8180	 0.3250
CD	 0.7990	 0.3240
CE	 0.8150	 0.3330
CF	 0.8010	 0.3120
CG	 0.7970	 0.3020
D	 0.6090	 0.1440
DB	 0.7840	 0.2810
DC	 0.8020	 0.3180
DD	 0.8080	 0.3220
DE	 0.7980	 0.3180
DF	 0.8080	 0.3130
DG	 0.7930	 0.2890
E	 0.6830	 0.1840
EB	 0.7800	 0.2850
EC	 0.7860	 0.3030
ED	 0.8070	 0.3020
EE	 0.8040	 0.3100
EF	 0.7930	 0.2920
EG	 0.7870	 0.2900



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Chain	Atom inclusion	Q-score
F	 0.7160	 0.1960
FC	 0.7820	 0.2870
FD	 0.7820	 0.2930
FE	 0.8000	 0.3050
FF	 0.7900	 0.2960
FG	 0.7940	 0.2880
FH	 0.7500	 0.2570
G	 0.7000	 0.2100
GC	 0.7600	 0.2560
GD	 0.7670	 0.2730
GE	 0.7760	 0.2790
GF	 0.7600	 0.2650
GG	 0.7640	 0.2570
GH	 0.7440	 0.2370
H	 0.6760	 0.1900
HC	 0.7510	 0.2230
HD	 0.7590	 0.2430
HE	 0.7670	 0.2500
HF	 0.7590	 0.2420
HG	 0.7760	 0.2490
HH	 0.7470	 0.2160
I	 0.6540	 0.1660
IC	 0.7220	 0.1860
ID	 0.7280	 0.1950
IE	 0.7350	 0.2120
IF	 0.7330	 0.2030
IG	 0.7470	 0.2110
IH	 0.7270	 0.1840
J	 0.8230	 0.2300
JC	 0.7320	 0.1860
JD	 0.7470	 0.2110
JE	 0.7420	 0.2020
JF	 0.7450	 0.2140
JG	 0.7370	 0.1920
K	 0.6880	 0.1610
KC	 0.7550	 0.2210
KD	 0.7590	 0.2250
KE	 0.7550	 0.2450
KF	 0.7590	 0.2210
KG	 0.7630	 0.2290
KH	 0.7380	 0.2000
L	 0.4310	 0.0510

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Chain	Atom inclusion	Q-score
LA	 0.7560	 0.2360
LB	 0.7760	 0.2510
LC	 0.7670	 0.2550
LD	 0.7730	 0.2640
LE	 0.7520	 0.2410
LF	 0.7540	 0.2280
M	 0.4850	 0.0630
MA	 0.7590	 0.2560
MB	 0.7670	 0.2620
MC	 0.7710	 0.2690
MD	 0.7700	 0.2630
ME	 0.7740	 0.2700
MF	 0.7720	 0.2510
N	 0.7290	 0.1880
O	 0.7510	 0.2030
P	 0.6070	 0.1340
Q	 0.6900	 0.1970
R	 0.6950	 0.1950
S	 0.7120	 0.2180
T	 0.6900	 0.1780
U	 0.6640	 0.1820
V	 0.8100	 0.2280
W	 0.7030	 0.1940
X	 0.3390	 0.0160
d	 0.6440	 0.1400
e	 0.6860	 0.1880
f	 0.7090	 0.2040
g	 0.6940	 0.2040
h	 0.6950	 0.1950
i	 0.6700	 0.1830
j	 0.8240	 0.2460
k	 0.7020	 0.1810
l	 0.4420	 0.0520