



wwPDB EM Validation Summary Report ⓘ

Jul 28, 2025 – 12:14 AM EDT

PDB ID : 9NTM / pdb_00009ntm
EMDB ID : EMD-49760
Title : SPEF1 bound to 14-pf microtubule
Authors : Legal, T.; Bui, K.H.
Deposited on : 2025-03-18
Resolution : 7.10 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.dev126
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

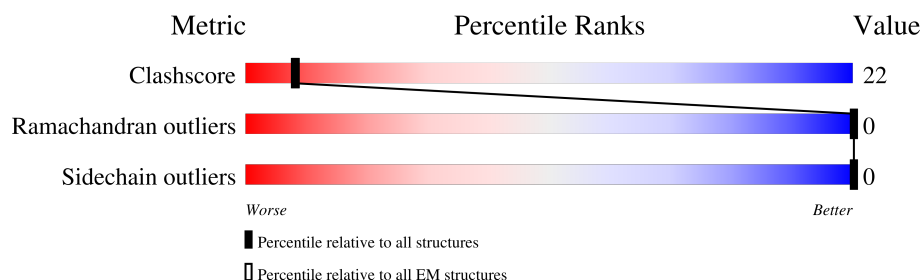
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 7.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.









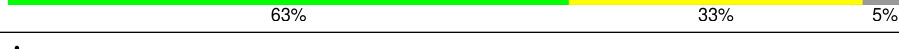
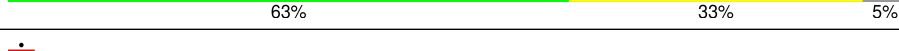
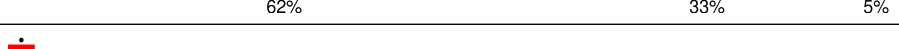
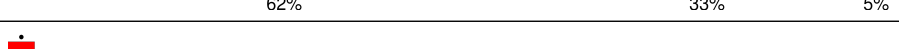
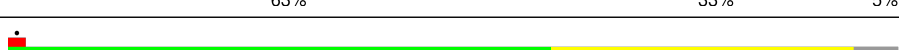

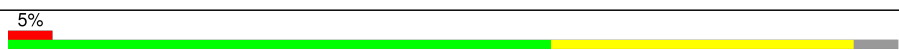

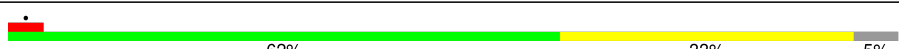





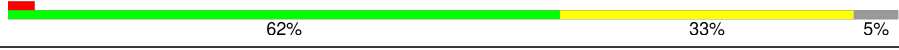
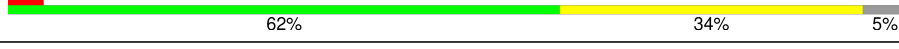



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	1A	393	
1	1B	393	
1	1C	393	
1	1D	393	
1	1E	393	
2	AA	451	
2	AC	451	
2	AE	451	







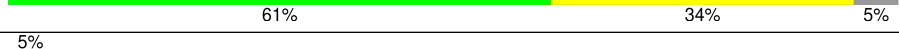
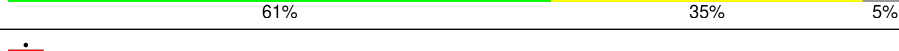
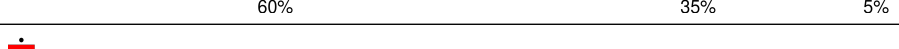
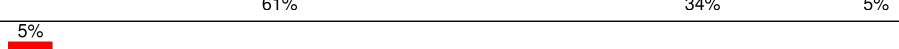
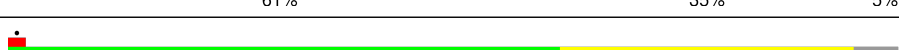

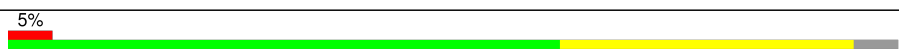

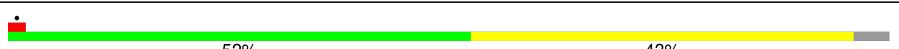





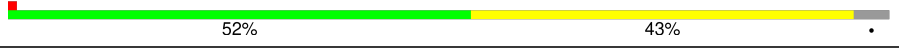
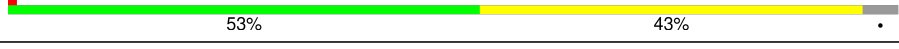



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Mol	Chain	Length	Quality of chain
2	BA	451	
2	BC	451	
2	BE	451	
2	CA	451	
2	CC	451	
2	CE	451	
2	DA	451	
2	DC	451	
2	DE	451	
2	EA	451	
2	EC	451	
2	EE	451	
2	FA	451	
2	FC	451	
2	FE	451	
2	GA	451	
2	GC	451	
2	GE	451	
2	HA	451	
2	HC	451	
2	HE	451	
2	IA	451	
2	IC	451	
2	IE	451	
2	JA	451	





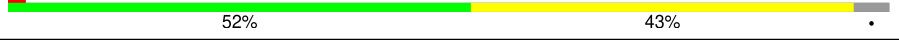



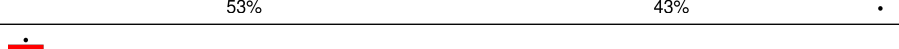
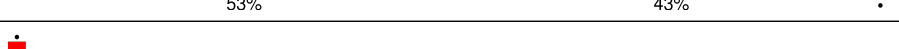



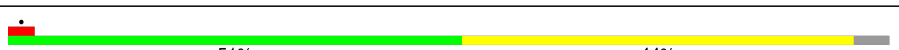
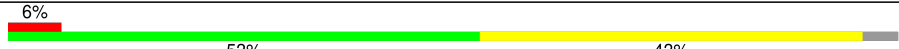





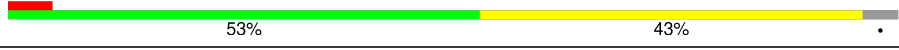
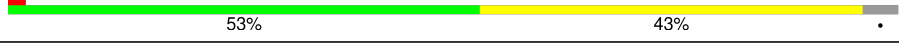



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Mol	Chain	Length	Quality of chain
2	JC	451	
2	JE	451	
2	KA	451	
2	KC	451	
2	KE	451	
2	LA	451	
2	LC	451	
2	LE	451	
2	MA	451	
2	MC	451	
2	ME	451	
2	NA	451	
2	NC	451	
2	NE	451	
3	AB	445	
3	AD	445	
3	AF	445	
3	BB	445	
3	BD	445	
3	BF	445	
3	CB	445	
3	CD	445	
3	CF	445	
3	DB	445	
3	DD	445	


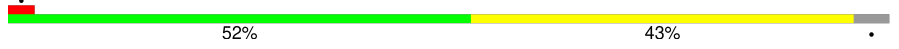


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Mol	Chain	Length	Quality of chain
3	DF	445	
3	EB	445	
3	ED	445	
3	EF	445	
3	FB	445	
3	FD	445	
3	FF	445	
3	GB	445	
3	GD	445	
3	GF	445	
3	HB	445	
3	HD	445	
3	HF	445	
3	IB	445	
3	ID	445	
3	IF	445	
3	JB	445	
3	JD	445	
3	JF	445	
3	KB	445	
3	KD	445	
3	KF	445	
3	LB	445	
3	LD	445	
3	LF	445	

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Mol	Chain	Length	Quality of chain
3	MB	445	
3	MD	445	
3	MF	445	
3	NB	445	
3	ND	445	
3	NF	445	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GTP	JE	501	-	-	X	-
4	GTP	KC	501	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 292618 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 flagellar protein 1,G protein/GFP fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1A	120	Total	C	N	O	S	0	0
			992	630	186	171	5		
1	1B	120	Total	C	N	O	S	0	0
			992	630	186	171	5		
1	1C	120	Total	C	N	O	S	0	0
			992	630	186	171	5		
1	1D	120	Total	C	N	O	S	0	0
			992	630	186	171	5		
1	1E	120	Total	C	N	O	S	0	0
			992	630	186	171	5		

There are 145 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1A	-2	PRO	-	expression tag	UNP Q9Y4P9
1A	-1	THR	-	expression tag	UNP Q9Y4P9
1A	0	MET	-	expression tag	UNP Q9Y4P9
1A	1	GLY	-	expression tag	UNP Q9Y4P9
1A	2	SER	-	expression tag	UNP Q9Y4P9
1A	3	SER	-	expression tag	UNP Q9Y4P9
1A	4	GLY	-	expression tag	UNP Q9Y4P9
1A	5	SER	-	expression tag	UNP Q9Y4P9
1A	6	SER	-	expression tag	UNP Q9Y4P9
1A	7	GLY	-	expression tag	UNP Q9Y4P9
1A	133	SER	-	linker	UNP Q9Y4P9
1A	134	SER	-	linker	UNP Q9Y4P9
1A	135	PRO	-	linker	UNP Q9Y4P9
1A	136	GLN	-	linker	UNP Q9Y4P9
1A	137	GLN	-	linker	UNP Q9Y4P9
1A	377	GLY	-	expression tag	UNP B7UCZ6
1A	378	SER	-	expression tag	UNP B7UCZ6
1A	379	ALA	-	expression tag	UNP B7UCZ6
1A	380	ALA	-	expression tag	UNP B7UCZ6
1A	381	ALA	-	expression tag	UNP B7UCZ6

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Chain	Residue	Modelled	Actual	Comment	Reference
1A	382	ALA	-	expression tag	UNP B7UCZ6
1A	383	TRP	-	expression tag	UNP B7UCZ6
1A	384	SER	-	expression tag	UNP B7UCZ6
1A	385	HIS	-	expression tag	UNP B7UCZ6
1A	386	PRO	-	expression tag	UNP B7UCZ6
1A	387	GLN	-	expression tag	UNP B7UCZ6
1A	388	PHE	-	expression tag	UNP B7UCZ6
1A	389	GLU	-	expression tag	UNP B7UCZ6
1A	390	LYS	-	expression tag	UNP B7UCZ6
1B	-2	PRO	-	expression tag	UNP Q9Y4P9
1B	-1	THR	-	expression tag	UNP Q9Y4P9
1B	0	MET	-	expression tag	UNP Q9Y4P9
1B	1	GLY	-	expression tag	UNP Q9Y4P9
1B	2	SER	-	expression tag	UNP Q9Y4P9
1B	3	SER	-	expression tag	UNP Q9Y4P9
1B	4	GLY	-	expression tag	UNP Q9Y4P9
1B	5	SER	-	expression tag	UNP Q9Y4P9
1B	6	SER	-	expression tag	UNP Q9Y4P9
1B	7	GLY	-	expression tag	UNP Q9Y4P9
1B	133	SER	-	linker	UNP Q9Y4P9
1B	134	SER	-	linker	UNP Q9Y4P9
1B	135	PRO	-	linker	UNP Q9Y4P9
1B	136	GLN	-	linker	UNP Q9Y4P9
1B	137	GLN	-	linker	UNP Q9Y4P9
1B	377	GLY	-	expression tag	UNP B7UCZ6
1B	378	SER	-	expression tag	UNP B7UCZ6
1B	379	ALA	-	expression tag	UNP B7UCZ6
1B	380	ALA	-	expression tag	UNP B7UCZ6
1B	381	ALA	-	expression tag	UNP B7UCZ6
1B	382	ALA	-	expression tag	UNP B7UCZ6
1B	383	TRP	-	expression tag	UNP B7UCZ6
1B	384	SER	-	expression tag	UNP B7UCZ6
1B	385	HIS	-	expression tag	UNP B7UCZ6
1B	386	PRO	-	expression tag	UNP B7UCZ6
1B	387	GLN	-	expression tag	UNP B7UCZ6
1B	388	PHE	-	expression tag	UNP B7UCZ6
1B	389	GLU	-	expression tag	UNP B7UCZ6
1B	390	LYS	-	expression tag	UNP B7UCZ6
1C	-2	PRO	-	expression tag	UNP Q9Y4P9
1C	-1	THR	-	expression tag	UNP Q9Y4P9
1C	0	MET	-	expression tag	UNP Q9Y4P9
1C	1	GLY	-	expression tag	UNP Q9Y4P9

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Chain	Residue	Modelled	Actual	Comment	Reference
1C	2	SER	-	expression tag	UNP Q9Y4P9
1C	3	SER	-	expression tag	UNP Q9Y4P9
1C	4	GLY	-	expression tag	UNP Q9Y4P9
1C	5	SER	-	expression tag	UNP Q9Y4P9
1C	6	SER	-	expression tag	UNP Q9Y4P9
1C	7	GLY	-	expression tag	UNP Q9Y4P9
1C	133	SER	-	linker	UNP Q9Y4P9
1C	134	SER	-	linker	UNP Q9Y4P9
1C	135	PRO	-	linker	UNP Q9Y4P9
1C	136	GLN	-	linker	UNP Q9Y4P9
1C	137	GLN	-	linker	UNP Q9Y4P9
1C	377	GLY	-	expression tag	UNP B7UCZ6
1C	378	SER	-	expression tag	UNP B7UCZ6
1C	379	ALA	-	expression tag	UNP B7UCZ6
1C	380	ALA	-	expression tag	UNP B7UCZ6
1C	381	ALA	-	expression tag	UNP B7UCZ6
1C	382	ALA	-	expression tag	UNP B7UCZ6
1C	383	TRP	-	expression tag	UNP B7UCZ6
1C	384	SER	-	expression tag	UNP B7UCZ6
1C	385	HIS	-	expression tag	UNP B7UCZ6
1C	386	PRO	-	expression tag	UNP B7UCZ6
1C	387	GLN	-	expression tag	UNP B7UCZ6
1C	388	PHE	-	expression tag	UNP B7UCZ6
1C	389	GLU	-	expression tag	UNP B7UCZ6
1C	390	LYS	-	expression tag	UNP B7UCZ6
1D	-2	PRO	-	expression tag	UNP Q9Y4P9
1D	-1	THR	-	expression tag	UNP Q9Y4P9
1D	0	MET	-	expression tag	UNP Q9Y4P9
1D	1	GLY	-	expression tag	UNP Q9Y4P9
1D	2	SER	-	expression tag	UNP Q9Y4P9
1D	3	SER	-	expression tag	UNP Q9Y4P9
1D	4	GLY	-	expression tag	UNP Q9Y4P9
1D	5	SER	-	expression tag	UNP Q9Y4P9
1D	6	SER	-	expression tag	UNP Q9Y4P9
1D	7	GLY	-	expression tag	UNP Q9Y4P9
1D	133	SER	-	linker	UNP Q9Y4P9
1D	134	SER	-	linker	UNP Q9Y4P9
1D	135	PRO	-	linker	UNP Q9Y4P9
1D	136	GLN	-	linker	UNP Q9Y4P9
1D	137	GLN	-	linker	UNP Q9Y4P9
1D	377	GLY	-	expression tag	UNP B7UCZ6
1D	378	SER	-	expression tag	UNP B7UCZ6

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Chain	Residue	Modelled	Actual	Comment	Reference
1D	379	ALA	-	expression tag	UNP B7UCZ6
1D	380	ALA	-	expression tag	UNP B7UCZ6
1D	381	ALA	-	expression tag	UNP B7UCZ6
1D	382	ALA	-	expression tag	UNP B7UCZ6
1D	383	TRP	-	expression tag	UNP B7UCZ6
1D	384	SER	-	expression tag	UNP B7UCZ6
1D	385	HIS	-	expression tag	UNP B7UCZ6
1D	386	PRO	-	expression tag	UNP B7UCZ6
1D	387	GLN	-	expression tag	UNP B7UCZ6
1D	388	PHE	-	expression tag	UNP B7UCZ6
1D	389	GLU	-	expression tag	UNP B7UCZ6
1D	390	LYS	-	expression tag	UNP B7UCZ6
1E	-2	PRO	-	expression tag	UNP Q9Y4P9
1E	-1	THR	-	expression tag	UNP Q9Y4P9
1E	0	MET	-	expression tag	UNP Q9Y4P9
1E	1	GLY	-	expression tag	UNP Q9Y4P9
1E	2	SER	-	expression tag	UNP Q9Y4P9
1E	3	SER	-	expression tag	UNP Q9Y4P9
1E	4	GLY	-	expression tag	UNP Q9Y4P9
1E	5	SER	-	expression tag	UNP Q9Y4P9
1E	6	SER	-	expression tag	UNP Q9Y4P9
1E	7	GLY	-	expression tag	UNP Q9Y4P9
1E	133	SER	-	linker	UNP Q9Y4P9
1E	134	SER	-	linker	UNP Q9Y4P9
1E	135	PRO	-	linker	UNP Q9Y4P9
1E	136	GLN	-	linker	UNP Q9Y4P9
1E	137	GLN	-	linker	UNP Q9Y4P9
1E	377	GLY	-	expression tag	UNP B7UCZ6
1E	378	SER	-	expression tag	UNP B7UCZ6
1E	379	ALA	-	expression tag	UNP B7UCZ6
1E	380	ALA	-	expression tag	UNP B7UCZ6
1E	381	ALA	-	expression tag	UNP B7UCZ6
1E	382	ALA	-	expression tag	UNP B7UCZ6
1E	383	TRP	-	expression tag	UNP B7UCZ6
1E	384	SER	-	expression tag	UNP B7UCZ6
1E	385	HIS	-	expression tag	UNP B7UCZ6
1E	386	PRO	-	expression tag	UNP B7UCZ6
1E	387	GLN	-	expression tag	UNP B7UCZ6
1E	388	PHE	-	expression tag	UNP B7UCZ6
1E	389	GLU	-	expression tag	UNP B7UCZ6
1E	390	LYS	-	expression tag	UNP B7UCZ6

- Molecule 2 is a protein called Tubulin alpha-1B chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AA	430	Total	C	N	O	S	0	0
			3372	2137	573	640	22		
2	AC	430	Total	C	N	O	S	0	0
			3372	2137	573	640	22		
2	AE	430	Total	C	N	O	S	0	0
			3372	2137	573	640	22		
2	BA	430	Total	C	N	O	S	0	0
			3372	2137	573	640	22		
2	BC	430	Total	C	N	O	S	0	0
			3372	2137	573	640	22		
2	BE	430	Total	C	N	O	S	0	0
			3372	2137	573	640	22		
2	CA	430	Total	C	N	O	S	0	0
			3372	2137	573	640	22		
2	CC	430	Total	C	N	O	S	0	0
			3372	2137	573	640	22		
2	CE	430	Total	C	N	O	S	0	0
			3372	2137	573	640	22		
2	DA	430	Total	C	N	O	S	0	0
			3372	2137	573	640	22		
2	DC	430	Total	C	N	O	S	0	0
			3372	2137	573	640	22		
2	DE	430	Total	C	N	O	S	0	0
			3372	2137	573	640	22		
2	EA	430	Total	C	N	O	S	0	0
			3372	2137	573	640	22		
2	EC	430	Total	C	N	O	S	0	0
			3372	2137	573	640	22		
2	EE	430	Total	C	N	O	S	0	0
			3372	2137	573	640	22		
2	FA	430	Total	C	N	O	S	0	0
			3372	2137	573	640	22		
2	FC	430	Total	C	N	O	S	0	0
			3372	2137	573	640	22		
2	FE	430	Total	C	N	O	S	0	0
			3372	2137	573	640	22		
2	GA	430	Total	C	N	O	S	0	0
			3372	2137	573	640	22		
2	GC	430	Total	C	N	O	S	0	0
			3372	2137	573	640	22		
2	GE	430	Total	C	N	O	S	0	0
			3372	2137	573	640	22		
2	HA	430	Total	C	N	O	S	0	0
			3372	2137	573	640	22		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	HC	430	Total 3372	C 2137	N 573	O 640	S 22	0	0
2	HE	430	Total 3372	C 2137	N 573	O 640	S 22	0	0
2	IA	430	Total 3372	C 2137	N 573	O 640	S 22	0	0
2	IC	430	Total 3372	C 2137	N 573	O 640	S 22	0	0
2	IE	430	Total 3372	C 2137	N 573	O 640	S 22	0	0
2	JA	430	Total 3372	C 2137	N 573	O 640	S 22	0	0
2	JC	430	Total 3372	C 2137	N 573	O 640	S 22	0	0
2	JE	430	Total 3372	C 2137	N 573	O 640	S 22	0	0
2	KA	430	Total 3372	C 2137	N 573	O 640	S 22	0	0
2	KC	430	Total 3372	C 2137	N 573	O 640	S 22	0	0
2	KE	430	Total 3372	C 2137	N 573	O 640	S 22	0	0
2	LA	430	Total 3372	C 2137	N 573	O 640	S 22	0	0
2	LC	430	Total 3372	C 2137	N 573	O 640	S 22	0	0
2	LE	430	Total 3372	C 2137	N 573	O 640	S 22	0	0
2	MA	430	Total 3372	C 2137	N 573	O 640	S 22	0	0
2	MC	430	Total 3372	C 2137	N 573	O 640	S 22	0	0
2	ME	430	Total 3372	C 2137	N 573	O 640	S 22	0	0
2	NA	430	Total 3372	C 2137	N 573	O 640	S 22	0	0
2	NC	430	Total 3372	C 2137	N 573	O 640	S 22	0	0
2	NE	430	Total 3372	C 2137	N 573	O 640	S 22	0	0

- Molecule 3 is a protein called Tubulin beta chain.

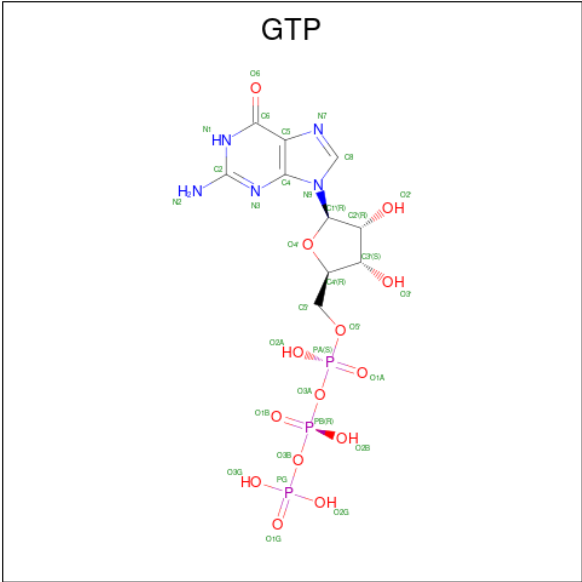
Mol	Chain	Residues	Atoms					AltConf	Trace
3	AB	426	Total	C	N	O	S	0	0
			3354	2107	575	646	26		
3	AD	426	Total	C	N	O	S	0	0
			3354	2107	575	646	26		
3	AF	426	Total	C	N	O	S	0	0
			3354	2107	575	646	26		
3	BB	426	Total	C	N	O	S	0	0
			3354	2107	575	646	26		
3	BD	426	Total	C	N	O	S	0	0
			3354	2107	575	646	26		
3	BF	426	Total	C	N	O	S	0	0
			3354	2107	575	646	26		
3	CB	426	Total	C	N	O	S	0	0
			3354	2107	575	646	26		
3	CD	426	Total	C	N	O	S	0	0
			3354	2107	575	646	26		
3	CF	426	Total	C	N	O	S	0	0
			3354	2107	575	646	26		
3	DB	426	Total	C	N	O	S	0	0
			3354	2107	575	646	26		
3	DD	426	Total	C	N	O	S	0	0
			3354	2107	575	646	26		
3	DF	426	Total	C	N	O	S	0	0
			3354	2107	575	646	26		
3	EB	426	Total	C	N	O	S	0	0
			3354	2107	575	646	26		
3	ED	426	Total	C	N	O	S	0	0
			3354	2107	575	646	26		
3	EF	426	Total	C	N	O	S	0	0
			3354	2107	575	646	26		
3	FB	426	Total	C	N	O	S	0	0
			3354	2107	575	646	26		
3	FD	426	Total	C	N	O	S	0	0
			3354	2107	575	646	26		
3	FF	426	Total	C	N	O	S	0	0
			3354	2107	575	646	26		
3	GB	426	Total	C	N	O	S	0	0
			3354	2107	575	646	26		
3	GD	426	Total	C	N	O	S	0	0
			3354	2107	575	646	26		
3	GF	426	Total	C	N	O	S	0	0
			3354	2107	575	646	26		
3	HB	426	Total	C	N	O	S	0	0
			3354	2107	575	646	26		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	HD	426	Total	C	N	O	S	0	0
			3354	2107	575	646	26		
3	HF	426	Total	C	N	O	S	0	0
			3354	2107	575	646	26		
3	IB	426	Total	C	N	O	S	0	0
			3354	2107	575	646	26		
3	ID	426	Total	C	N	O	S	0	0
			3354	2107	575	646	26		
3	IF	426	Total	C	N	O	S	0	0
			3354	2107	575	646	26		
3	JB	426	Total	C	N	O	S	0	0
			3354	2107	575	646	26		
3	JD	426	Total	C	N	O	S	0	0
			3354	2107	575	646	26		
3	JF	426	Total	C	N	O	S	0	0
			3354	2107	575	646	26		
3	KB	426	Total	C	N	O	S	0	0
			3354	2107	575	646	26		
3	KD	426	Total	C	N	O	S	0	0
			3354	2107	575	646	26		
3	KF	426	Total	C	N	O	S	0	0
			3354	2107	575	646	26		
3	LB	426	Total	C	N	O	S	0	0
			3354	2107	575	646	26		
3	LD	426	Total	C	N	O	S	0	0
			3354	2107	575	646	26		
3	LF	426	Total	C	N	O	S	0	0
			3354	2107	575	646	26		
3	MB	426	Total	C	N	O	S	0	0
			3354	2107	575	646	26		
3	MD	426	Total	C	N	O	S	0	0
			3354	2107	575	646	26		
3	MF	426	Total	C	N	O	S	0	0
			3354	2107	575	646	26		
3	NB	426	Total	C	N	O	S	0	0
			3354	2107	575	646	26		
3	ND	426	Total	C	N	O	S	0	0
			3354	2107	575	646	26		
3	NF	426	Total	C	N	O	S	0	0
			3354	2107	575	646	26		

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					AltConf
4	AA	1	Total	C	N	O	P	0
			32	10	5	14	3	
4	AC	1	Total	C	N	O	P	0
			32	10	5	14	3	
4	AE	1	Total	C	N	O	P	0
			32	10	5	14	3	
4	BA	1	Total	C	N	O	P	0
			32	10	5	14	3	
4	BC	1	Total	C	N	O	P	0
			32	10	5	14	3	
4	BE	1	Total	C	N	O	P	0
			32	10	5	14	3	
4	CA	1	Total	C	N	O	P	0
			32	10	5	14	3	
4	CC	1	Total	C	N	O	P	0
			32	10	5	14	3	
4	CE	1	Total	C	N	O	P	0
			32	10	5	14	3	
4	DA	1	Total	C	N	O	P	0
			32	10	5	14	3	
4	DC	1	Total	C	N	O	P	0
			32	10	5	14	3	
4	DE	1	Total	C	N	O	P	0
			32	10	5	14	3	
4	EA	1	Total	C	N	O	P	0
			32	10	5	14	3	
4	EC	1	Total	C	N	O	P	0
			32	10	5	14	3	

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Mol	Chain	Residues	Atoms					AltConf
4	EE	1	Total 32	C 10	N 5	O 14	P 3	0
4	FA	1	Total 32	C 10	N 5	O 14	P 3	0
4	FC	1	Total 32	C 10	N 5	O 14	P 3	0
4	FE	1	Total 32	C 10	N 5	O 14	P 3	0
4	GA	1	Total 32	C 10	N 5	O 14	P 3	0
4	GC	1	Total 32	C 10	N 5	O 14	P 3	0
4	GE	1	Total 32	C 10	N 5	O 14	P 3	0
4	HA	1	Total 32	C 10	N 5	O 14	P 3	0
4	HC	1	Total 32	C 10	N 5	O 14	P 3	0
4	HE	1	Total 32	C 10	N 5	O 14	P 3	0
4	IA	1	Total 32	C 10	N 5	O 14	P 3	0
4	IC	1	Total 32	C 10	N 5	O 14	P 3	0
4	IE	1	Total 32	C 10	N 5	O 14	P 3	0
4	JA	1	Total 32	C 10	N 5	O 14	P 3	0
4	JC	1	Total 32	C 10	N 5	O 14	P 3	0
4	JE	1	Total 32	C 10	N 5	O 14	P 3	0
4	KA	1	Total 32	C 10	N 5	O 14	P 3	0
4	KC	1	Total 32	C 10	N 5	O 14	P 3	0
4	KE	1	Total 32	C 10	N 5	O 14	P 3	0
4	LA	1	Total 32	C 10	N 5	O 14	P 3	0
4	LC	1	Total 32	C 10	N 5	O 14	P 3	0

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

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
5	AA	1	Total	Mg	0
			1	1	
5	AC	1	Total	Mg	0
			1	1	
5	AE	1	Total	Mg	0
			1	1	
5	BA	1	Total	Mg	0
			1	1	
5	BC	1	Total	Mg	0
			1	1	
5	BE	1	Total	Mg	0
			1	1	
5	CA	1	Total	Mg	0
			1	1	
5	CC	1	Total	Mg	0
			1	1	
5	CE	1	Total	Mg	0
			1	1	
5	DA	1	Total	Mg	0
			1	1	
5	DC	1	Total	Mg	0
			1	1	
5	DE	1	Total	Mg	0
			1	1	

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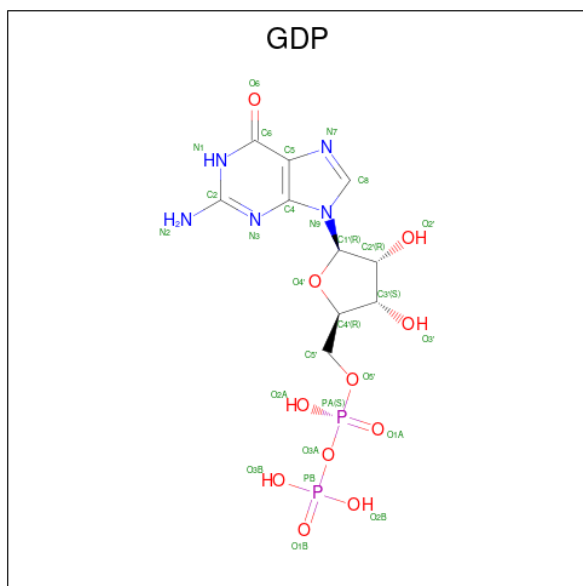
Mol	Chain	Residues	Atoms		AltConf
5	EA	1	Total 1	Mg 1	0
5	EC	1	Total 1	Mg 1	0
5	EE	1	Total 1	Mg 1	0
5	FA	1	Total 1	Mg 1	0
5	FC	1	Total 1	Mg 1	0
5	FE	1	Total 1	Mg 1	0
5	GA	1	Total 1	Mg 1	0
5	GC	1	Total 1	Mg 1	0
5	GE	1	Total 1	Mg 1	0
5	HA	1	Total 1	Mg 1	0
5	HC	1	Total 1	Mg 1	0
5	HE	1	Total 1	Mg 1	0
5	IA	1	Total 1	Mg 1	0
5	IC	1	Total 1	Mg 1	0
5	IE	1	Total 1	Mg 1	0
5	JA	1	Total 1	Mg 1	0
5	JC	1	Total 1	Mg 1	0
5	JE	1	Total 1	Mg 1	0
5	KA	1	Total 1	Mg 1	0
5	KC	1	Total 1	Mg 1	0
5	KE	1	Total 1	Mg 1	0

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Mol	Chain	Residues	Atoms		AltConf
5	LA	1	Total	Mg	0
			1	1	
5	LC	1	Total	Mg	0
			1	1	
5	LE	1	Total	Mg	0
			1	1	
5	MA	1	Total	Mg	0
			1	1	
5	MC	1	Total	Mg	0
			1	1	
5	ME	1	Total	Mg	0
			1	1	
5	NA	1	Total	Mg	0
			1	1	
5	NC	1	Total	Mg	0
			1	1	
5	NE	1	Total	Mg	0
			1	1	

- Molecule 6 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



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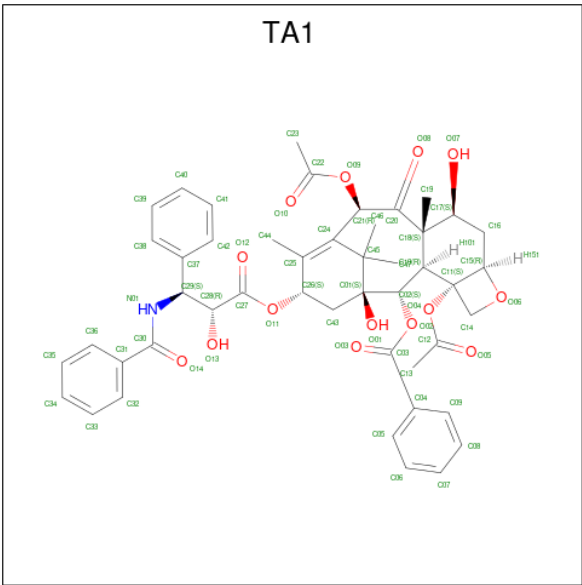
Mol	Chain	Residues	Atoms					AltConf
6	AF	1	Total	C	N	O	P	0
			28	10	5	11	2	
6	BB	1	Total	C	N	O	P	0
			28	10	5	11	2	
6	BD	1	Total	C	N	O	P	0
			28	10	5	11	2	
6	BF	1	Total	C	N	O	P	0
			28	10	5	11	2	
6	CB	1	Total	C	N	O	P	0
			28	10	5	11	2	
6	CD	1	Total	C	N	O	P	0
			28	10	5	11	2	
6	CF	1	Total	C	N	O	P	0
			28	10	5	11	2	
6	DB	1	Total	C	N	O	P	0
			28	10	5	11	2	
6	DD	1	Total	C	N	O	P	0
			28	10	5	11	2	
6	DF	1	Total	C	N	O	P	0
			28	10	5	11	2	
6	EB	1	Total	C	N	O	P	0
			28	10	5	11	2	
6	ED	1	Total	C	N	O	P	0
			28	10	5	11	2	
6	EF	1	Total	C	N	O	P	0
			28	10	5	11	2	
6	FB	1	Total	C	N	O	P	0
			28	10	5	11	2	
6	FD	1	Total	C	N	O	P	0
			28	10	5	11	2	
6	FF	1	Total	C	N	O	P	0
			28	10	5	11	2	
6	GB	1	Total	C	N	O	P	0
			28	10	5	11	2	
6	GD	1	Total	C	N	O	P	0
			28	10	5	11	2	
6	GF	1	Total	C	N	O	P	0
			28	10	5	11	2	
6	HB	1	Total	C	N	O	P	0
			28	10	5	11	2	
6	HD	1	Total	C	N	O	P	0
			28	10	5	11	2	

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Mol	Chain	Residues	Atoms					AltConf
6	HF	1	Total	C	N	O	P	0
			28	10	5	11	2	
6	IB	1	Total	C	N	O	P	0
			28	10	5	11	2	
6	ID	1	Total	C	N	O	P	0
			28	10	5	11	2	
6	IF	1	Total	C	N	O	P	0
			28	10	5	11	2	
6	JB	1	Total	C	N	O	P	0
			28	10	5	11	2	
6	JD	1	Total	C	N	O	P	0
			28	10	5	11	2	
6	JF	1	Total	C	N	O	P	0
			28	10	5	11	2	
6	KB	1	Total	C	N	O	P	0
			28	10	5	11	2	
6	KD	1	Total	C	N	O	P	0
			28	10	5	11	2	
6	KF	1	Total	C	N	O	P	0
			28	10	5	11	2	
6	LB	1	Total	C	N	O	P	0
			28	10	5	11	2	
6	LD	1	Total	C	N	O	P	0
			28	10	5	11	2	
6	LF	1	Total	C	N	O	P	0
			28	10	5	11	2	
6	MB	1	Total	C	N	O	P	0
			28	10	5	11	2	
6	MD	1	Total	C	N	O	P	0
			28	10	5	11	2	
6	MF	1	Total	C	N	O	P	0
			28	10	5	11	2	
6	NB	1	Total	C	N	O	P	0
			28	10	5	11	2	
6	ND	1	Total	C	N	O	P	0
			28	10	5	11	2	
6	NF	1	Total	C	N	O	P	0
			28	10	5	11	2	

- Molecule 7 is TAXOL (CCD ID: TA1) (formula: $C_{47}H_{51}NO_{14}$).



Mol	Chain	Residues	Atoms				AltConf
7	AB	1	Total	C	N	O	0
			62	47	1	14	
7	AD	1	Total	C	N	O	0
			62	47	1	14	
7	AF	1	Total	C	N	O	0
			62	47	1	14	
7	BB	1	Total	C	N	O	0
			62	47	1	14	
7	BD	1	Total	C	N	O	0
			62	47	1	14	
7	BF	1	Total	C	N	O	0
			62	47	1	14	
7	CB	1	Total	C	N	O	0
			62	47	1	14	
7	CD	1	Total	C	N	O	0
			62	47	1	14	
7	CF	1	Total	C	N	O	0
			62	47	1	14	
7	DB	1	Total	C	N	O	0
			62	47	1	14	
7	DD	1	Total	C	N	O	0
			62	47	1	14	
7	DF	1	Total	C	N	O	0
			62	47	1	14	
7	EB	1	Total	C	N	O	0
			62	47	1	14	
7	ED	1	Total	C	N	O	0
			62	47	1	14	

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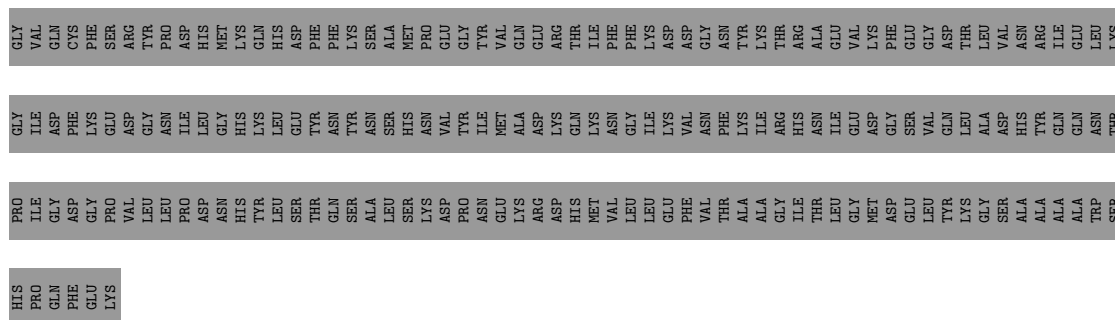
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Mol	Chain	Residues	Atoms				AltConf
7	EF	1	Total 62	C 47	N 1	O 14	0
7	FB	1	Total 62	C 47	N 1	O 14	0
7	FD	1	Total 62	C 47	N 1	O 14	0
7	FF	1	Total 62	C 47	N 1	O 14	0
7	GB	1	Total 62	C 47	N 1	O 14	0
7	GD	1	Total 62	C 47	N 1	O 14	0
7	GF	1	Total 62	C 47	N 1	O 14	0
7	HB	1	Total 62	C 47	N 1	O 14	0
7	HD	1	Total 62	C 47	N 1	O 14	0
7	HF	1	Total 62	C 47	N 1	O 14	0
7	IB	1	Total 62	C 47	N 1	O 14	0
7	ID	1	Total 62	C 47	N 1	O 14	0
7	IF	1	Total 62	C 47	N 1	O 14	0
7	JB	1	Total 62	C 47	N 1	O 14	0
7	JD	1	Total 62	C 47	N 1	O 14	0
7	JF	1	Total 62	C 47	N 1	O 14	0
7	KB	1	Total 62	C 47	N 1	O 14	0
7	KD	1	Total 62	C 47	N 1	O 14	0
7	KF	1	Total 62	C 47	N 1	O 14	0
7	LB	1	Total 62	C 47	N 1	O 14	0
7	LD	1	Total 62	C 47	N 1	O 14	0

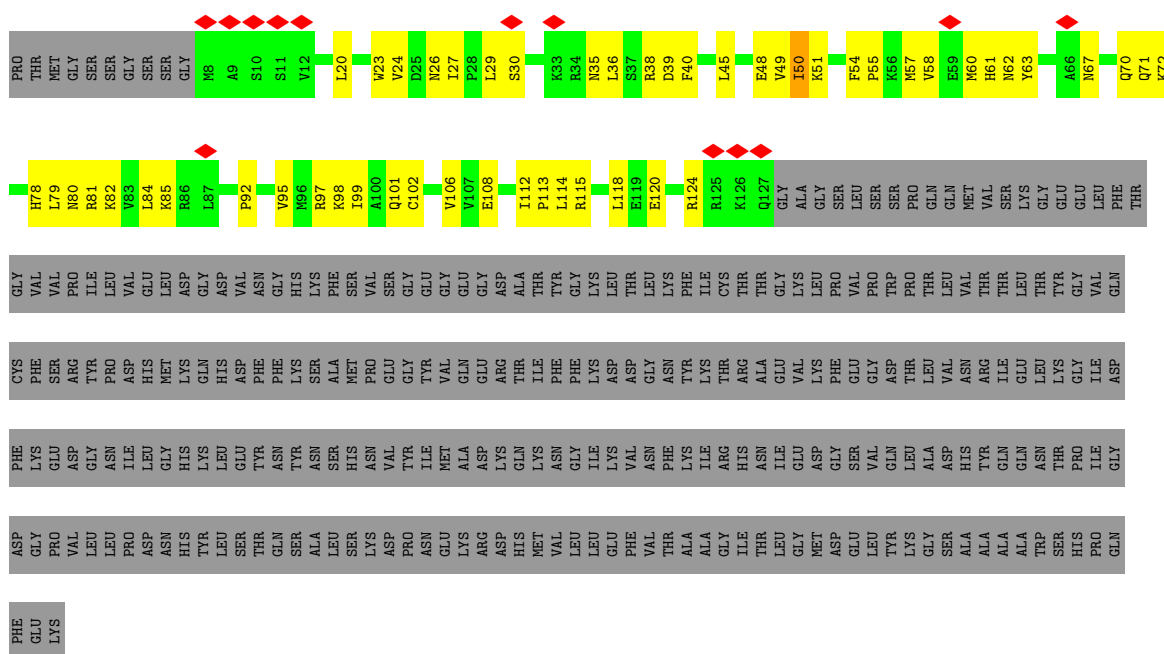
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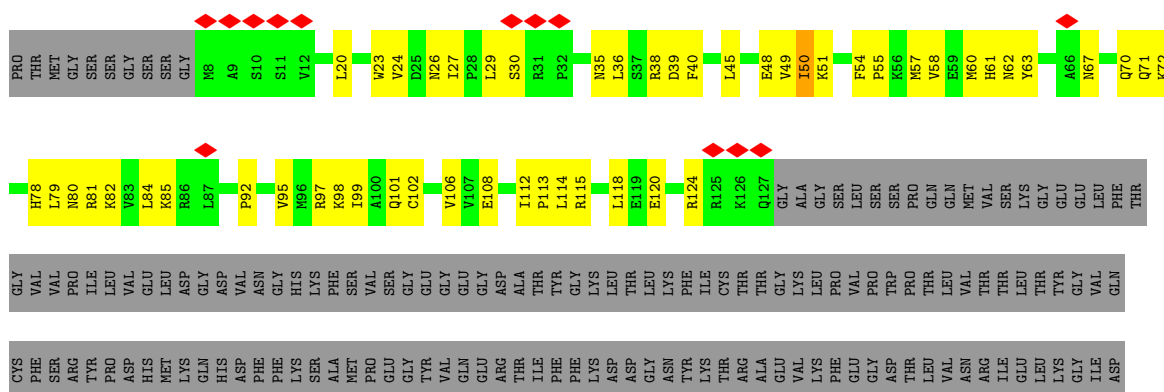
Mol	Chain	Residues	Atoms				AltConf
7	LF	1	Total	C	N	O	0
			62	47	1	14	
7	MB	1	Total	C	N	O	0
			62	47	1	14	
7	MD	1	Total	C	N	O	0
			62	47	1	14	
7	MF	1	Total	C	N	O	0
			62	47	1	14	
7	NB	1	Total	C	N	O	0
			62	47	1	14	
7	ND	1	Total	C	N	O	0
			62	47	1	14	
7	NF	1	Total	C	N	O	0
			62	47	1	14	

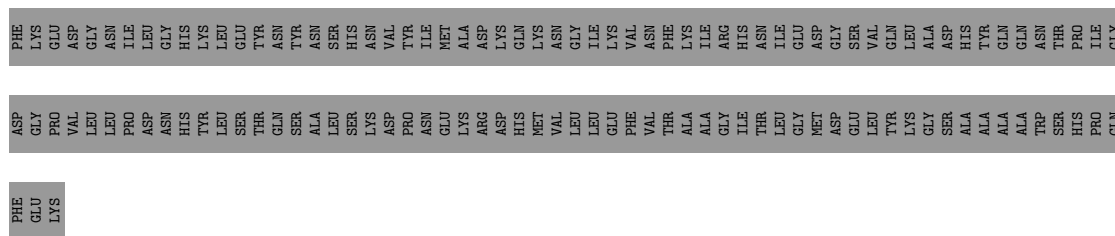


- Molecule 1: Sperm flagellar protein 1,G protein/GFP fusion protein

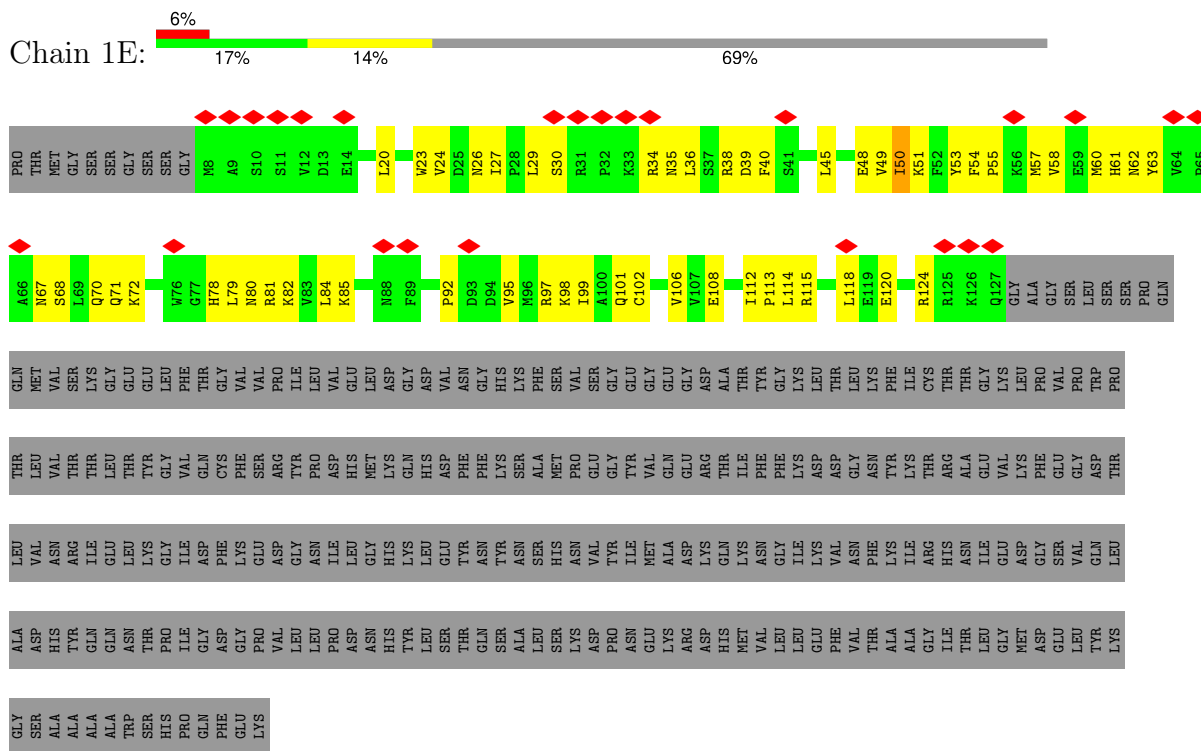


- Molecule 1: Sperm flagellar protein 1, G protein/GFP fusion protein

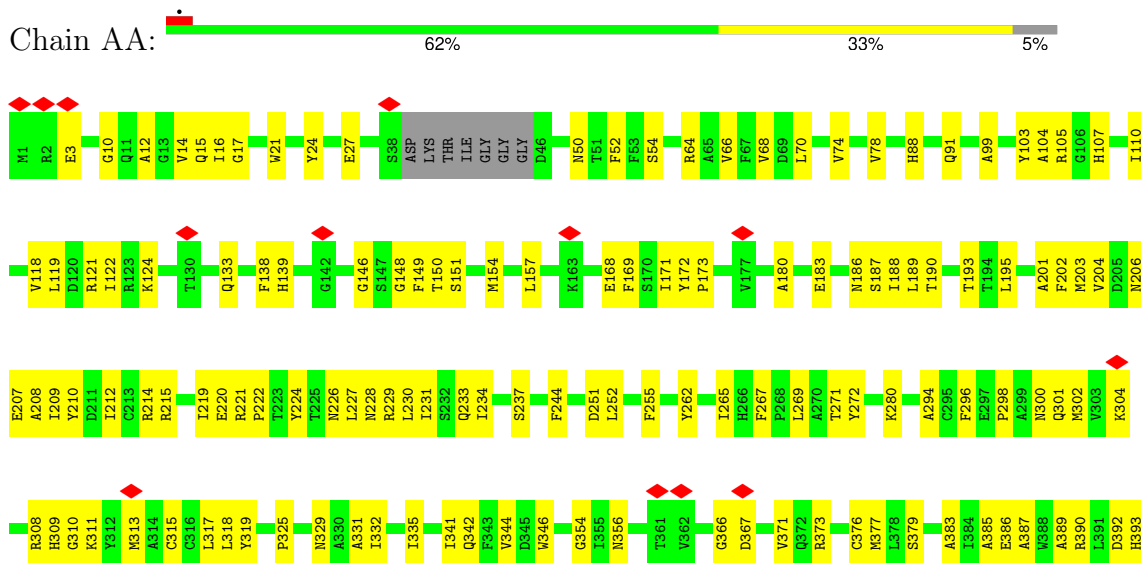




- Molecule 1: Sperm flagellar protein 1, G protein/GFP fusion protein

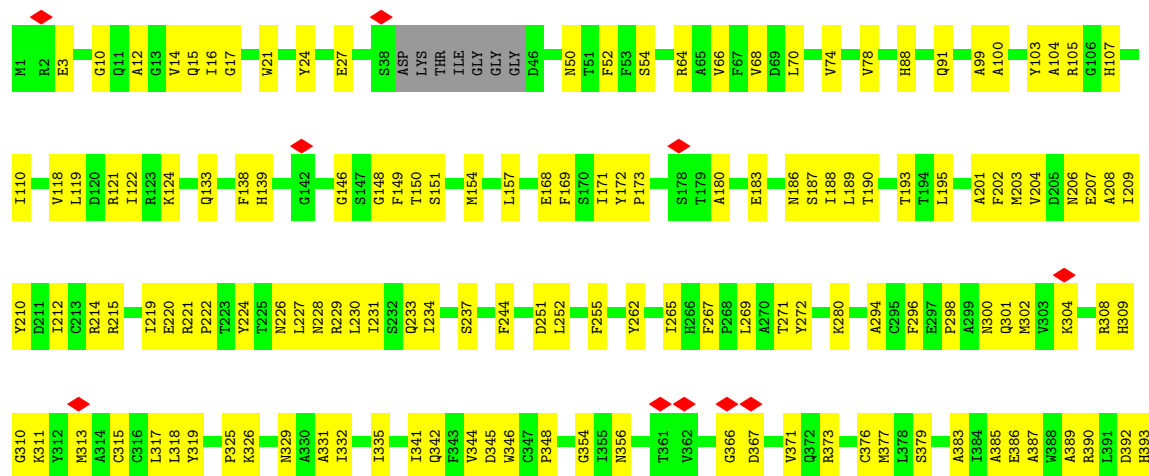


- Molecule 2: Tubulin alpha-1B chain

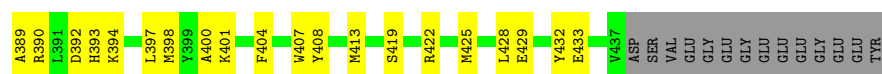
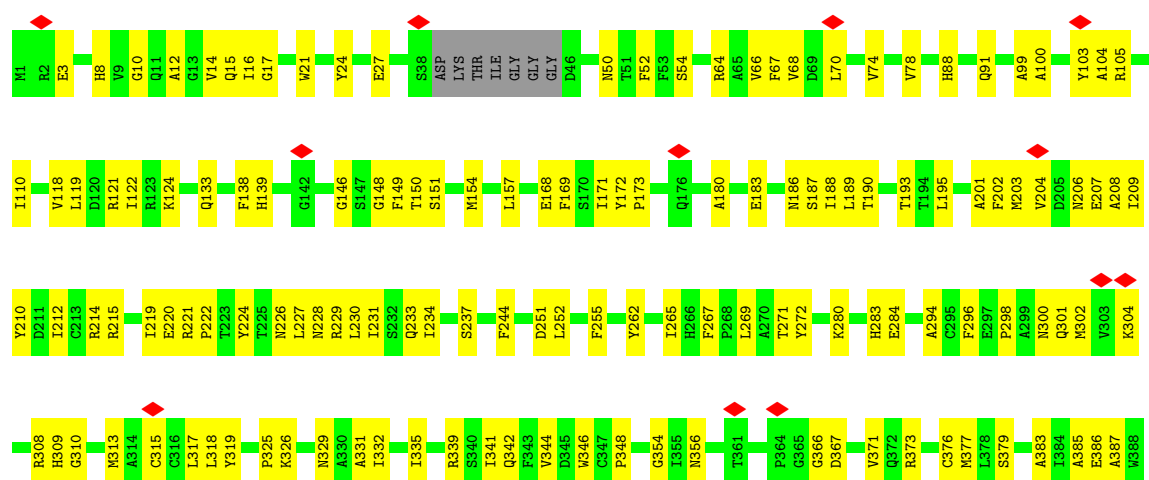




• Molecule 2: Tubulin alpha-1B chain

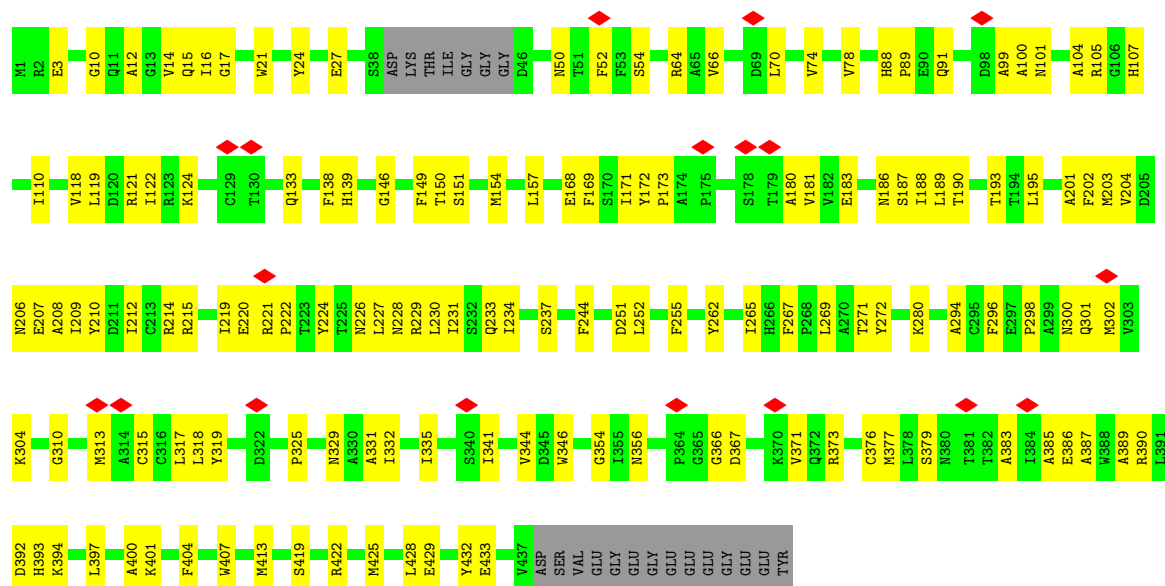


• Molecule 2: Tubulin alpha-1B chain

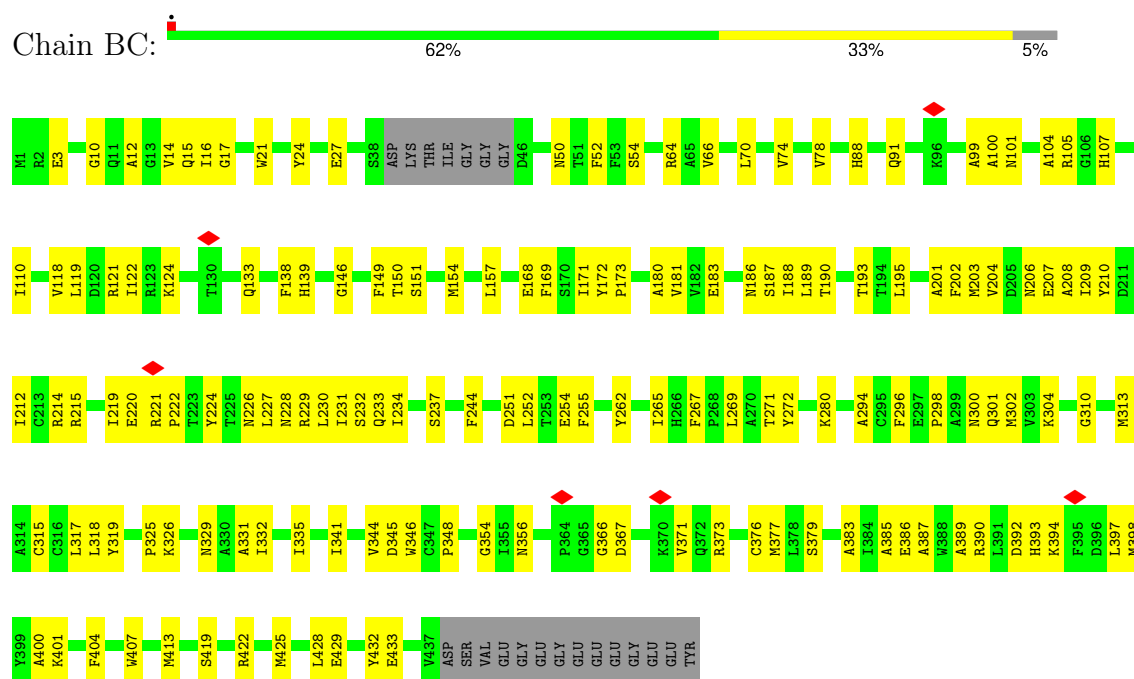


• Molecule 2: Tubulin alpha-1B chain

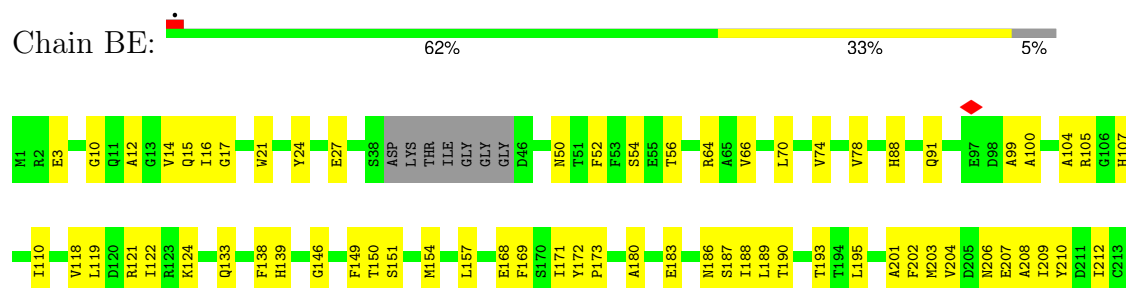


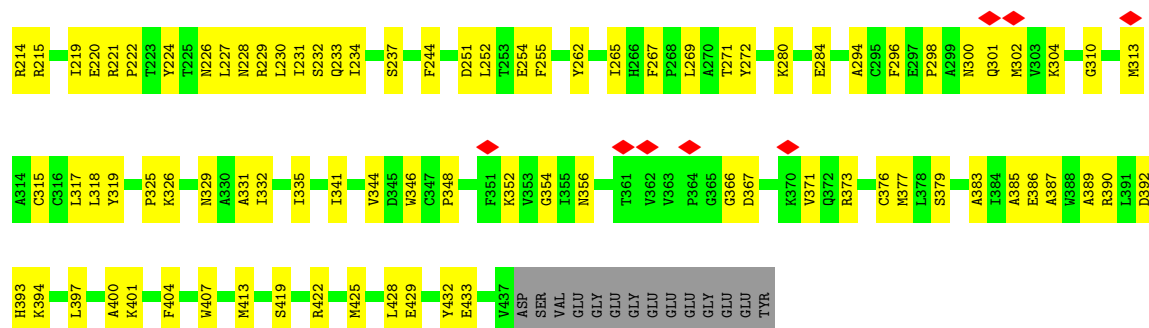


• Molecule 2: Tubulin alpha-1B chain

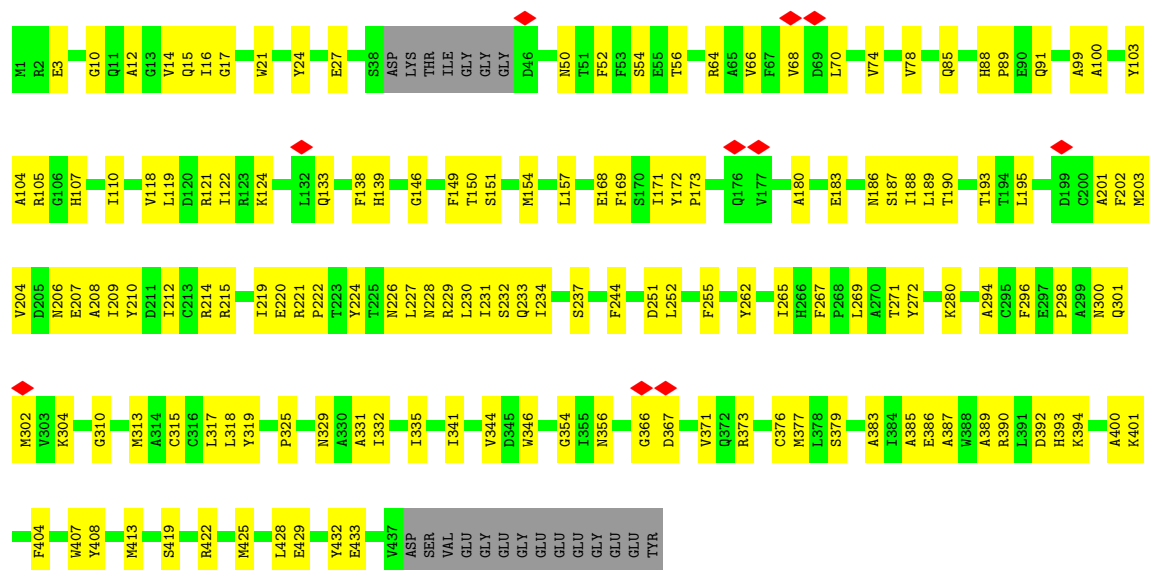


• Molecule 2: Tubulin alpha-1B chain

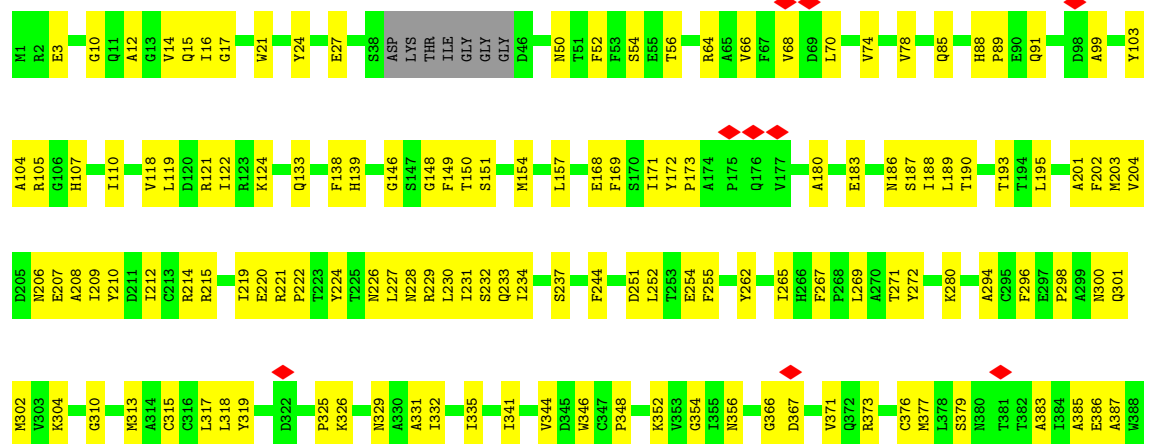




• Molecule 2: Tubulin alpha-1B chain



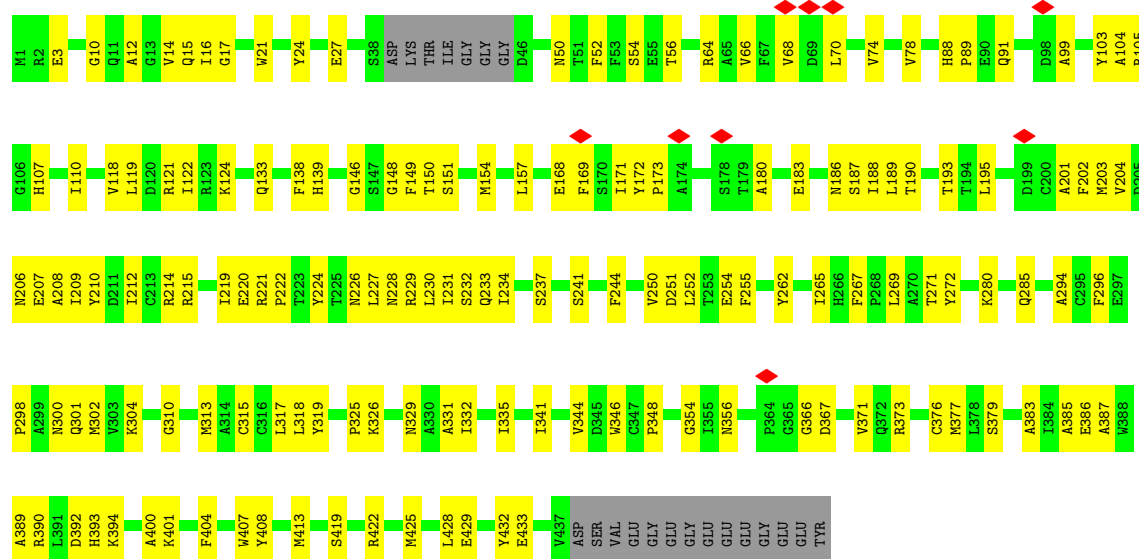
• Molecule 2: Tubulin alpha-1B chain





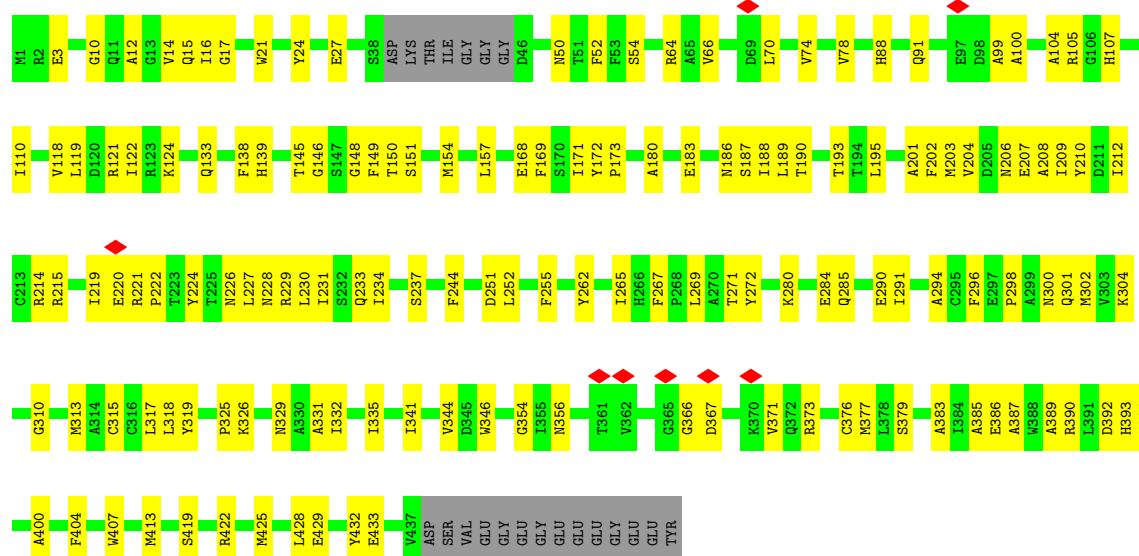
• Molecule 2: Tubulin alpha-1B chain

Chain CE: 61% 34% 5%



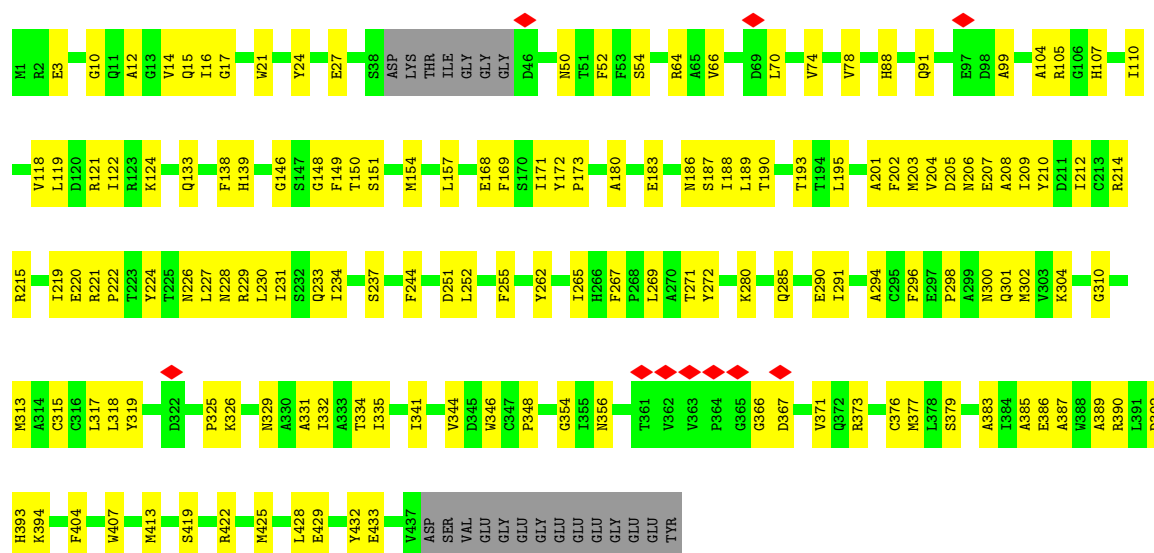
• Molecule 2: Tubulin alpha-1B chain

Chain DA: 63% 33% 5%

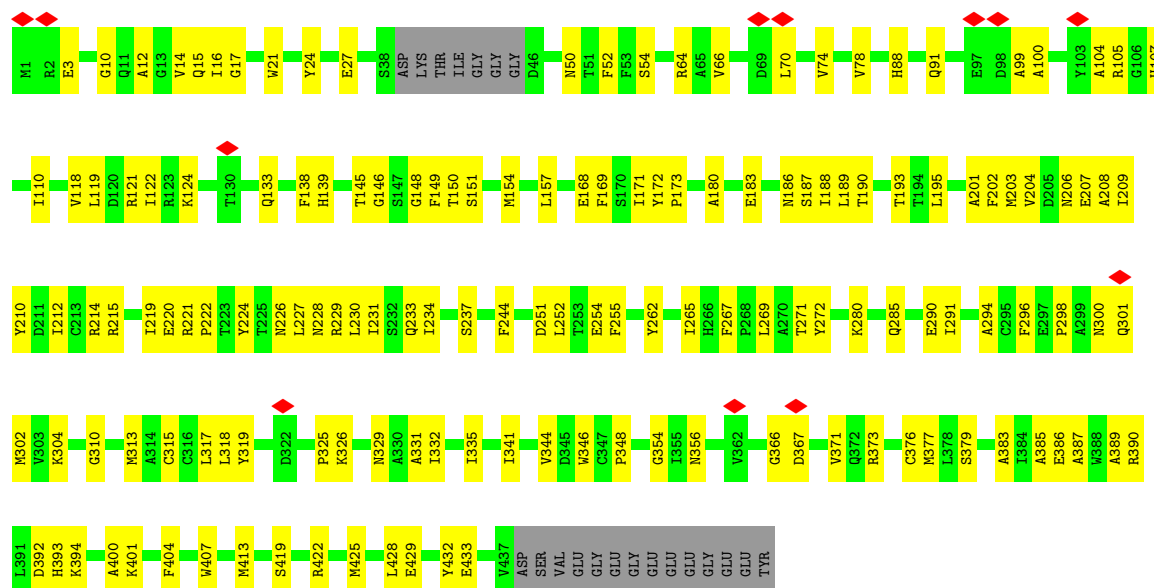


• Molecule 2: Tubulin alpha-1B chain

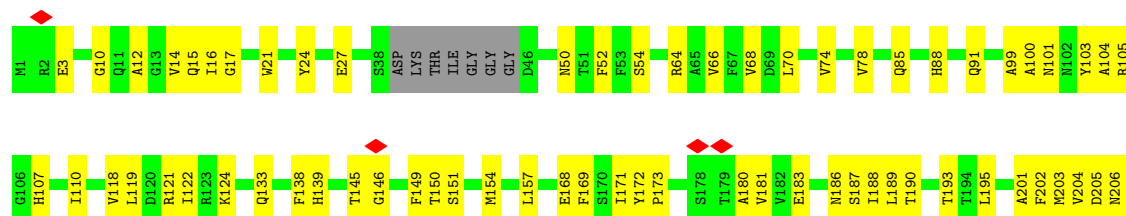
Chain DC: 63% 33% 5%

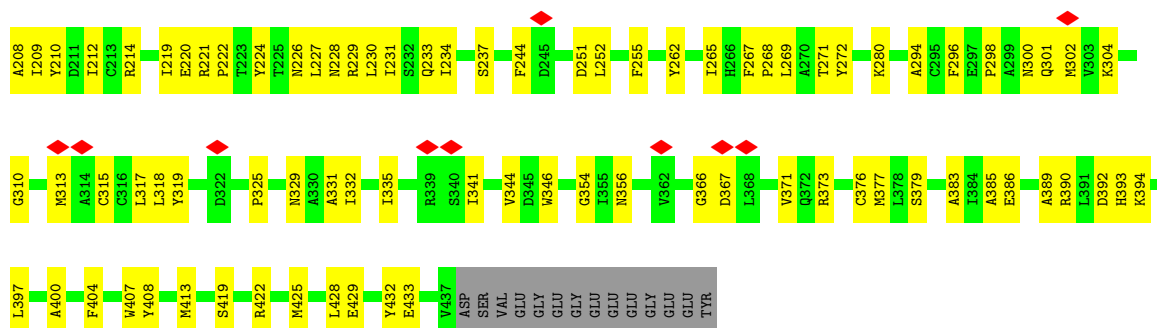


• Molecule 2: Tubulin alpha-1B chain

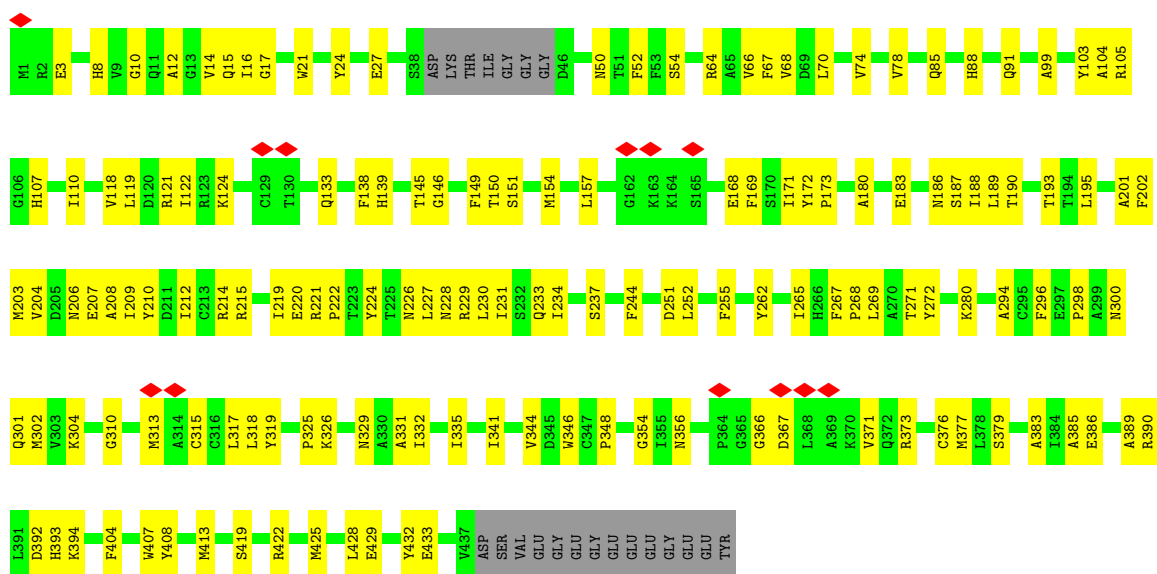


• Molecule 2: Tubulin alpha-1B chain

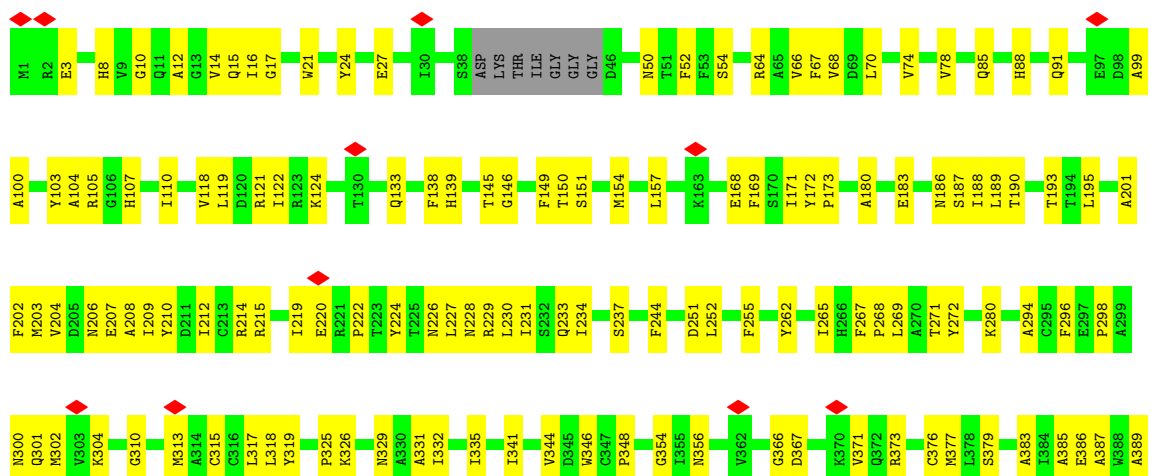




• Molecule 2: Tubulin alpha-1B chain

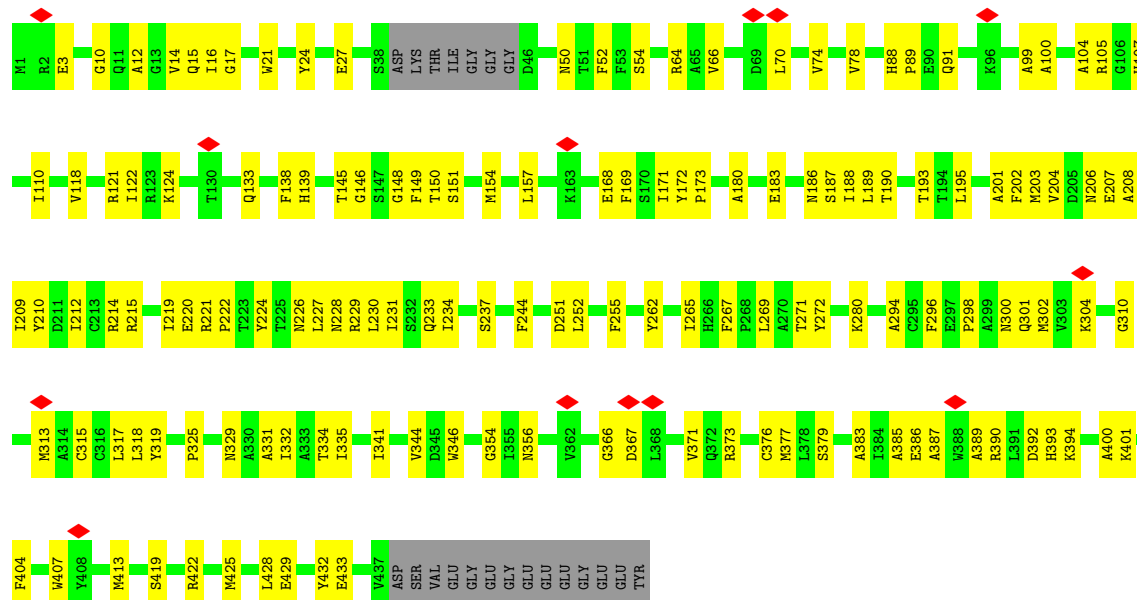


• Molecule 2: Tubulin alpha-1B chain

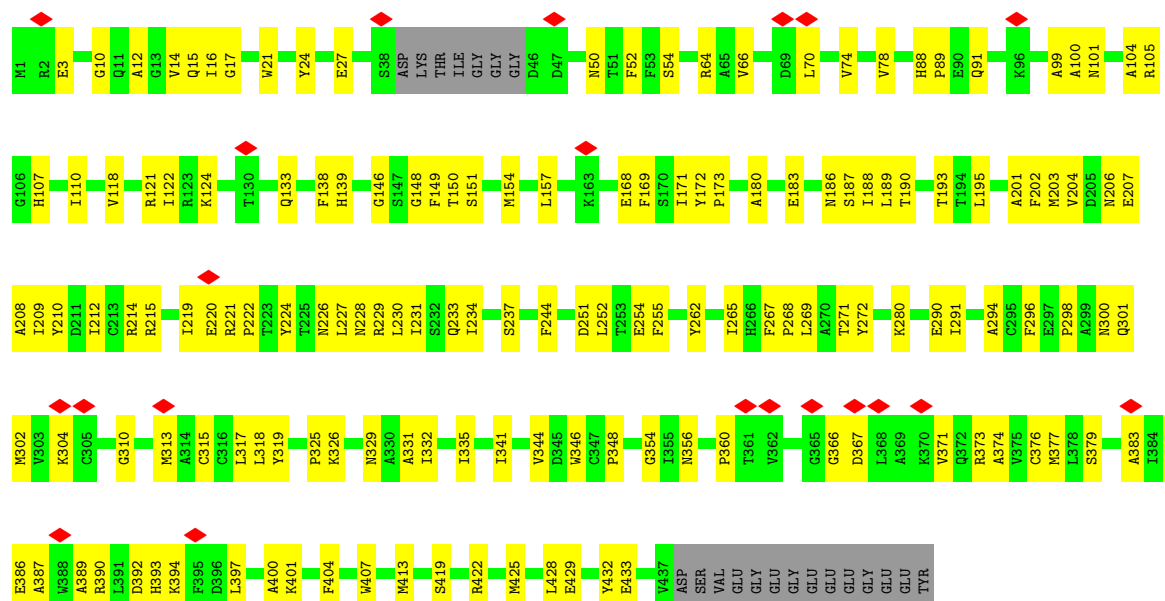




• Molecule 2: Tubulin alpha-1B chain



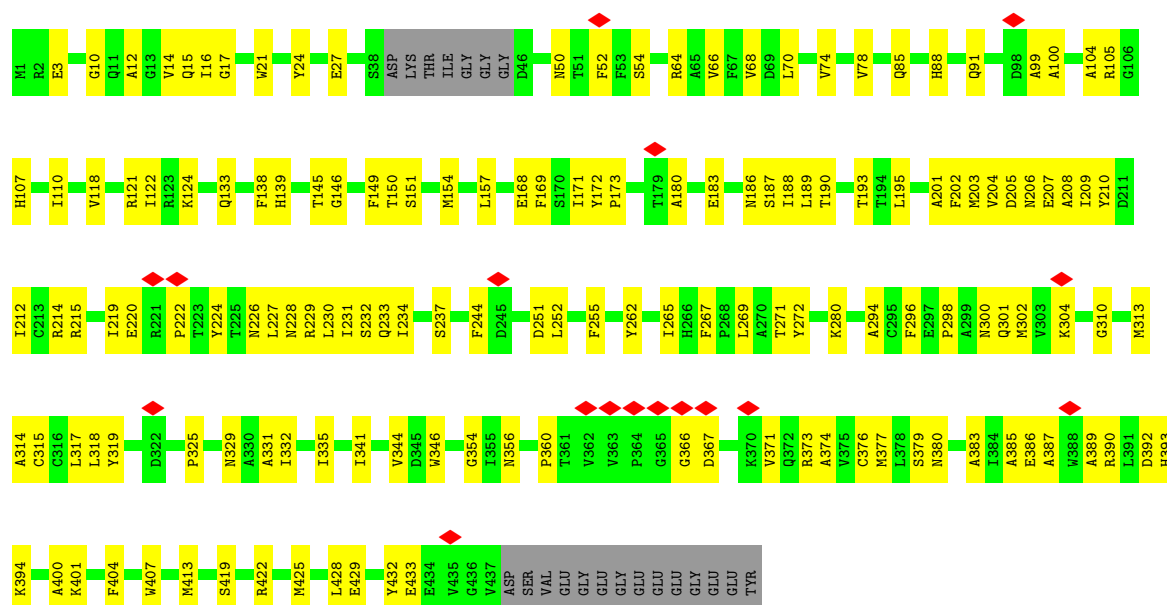
• Molecule 2: Tubulin alpha-1B chain



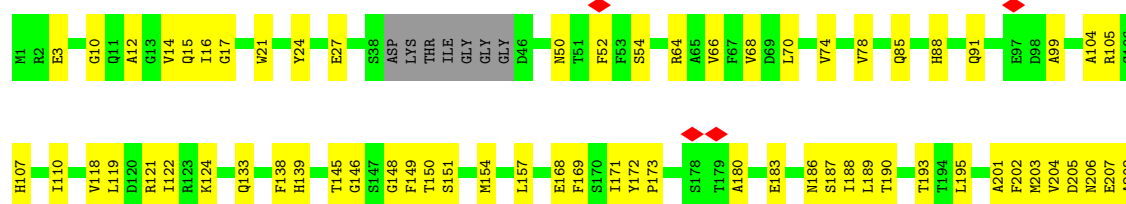
• Molecule 2: Tubulin alpha-1B chain

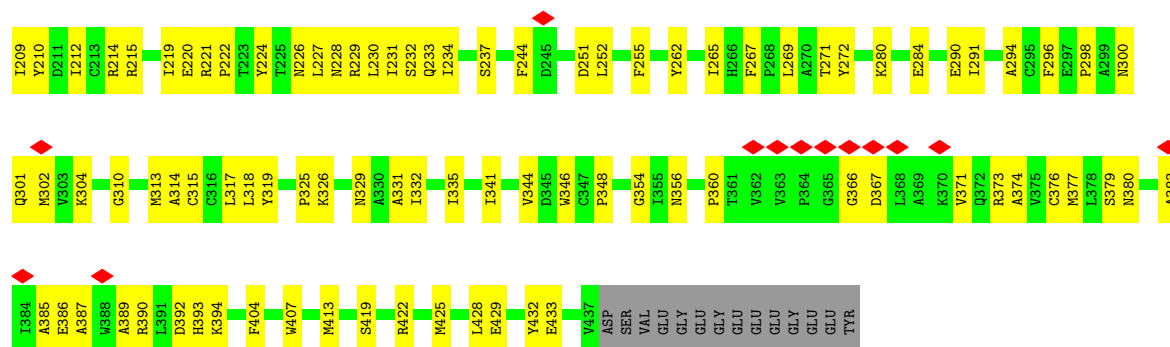


- Molecule 2: Tubulin alpha-1B chain

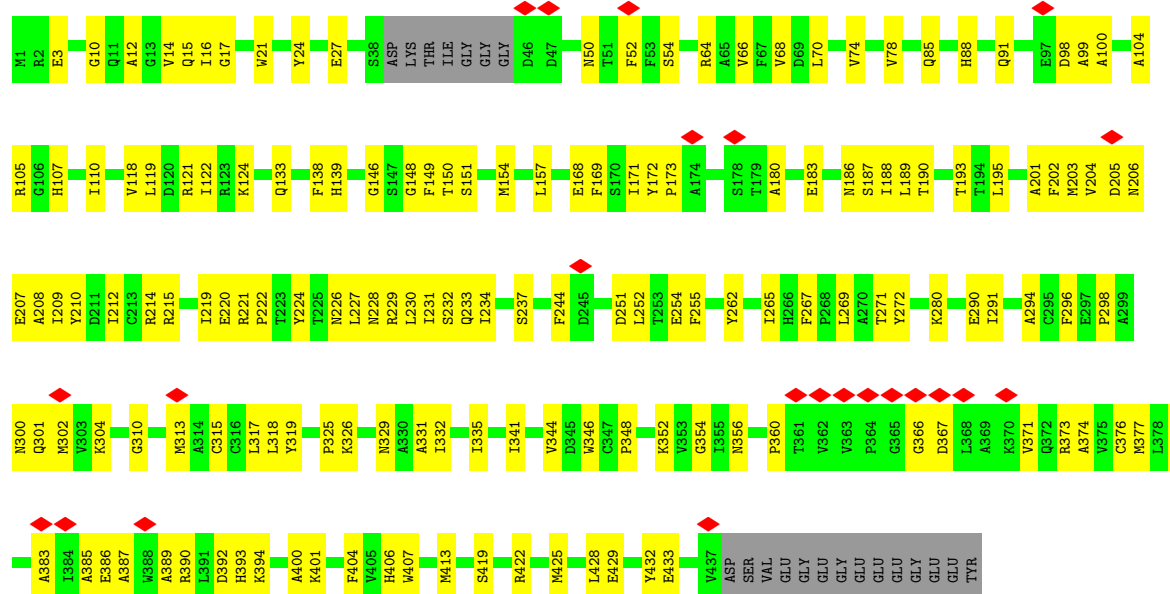


- Molecule 2: Tubulin alpha-1B chain

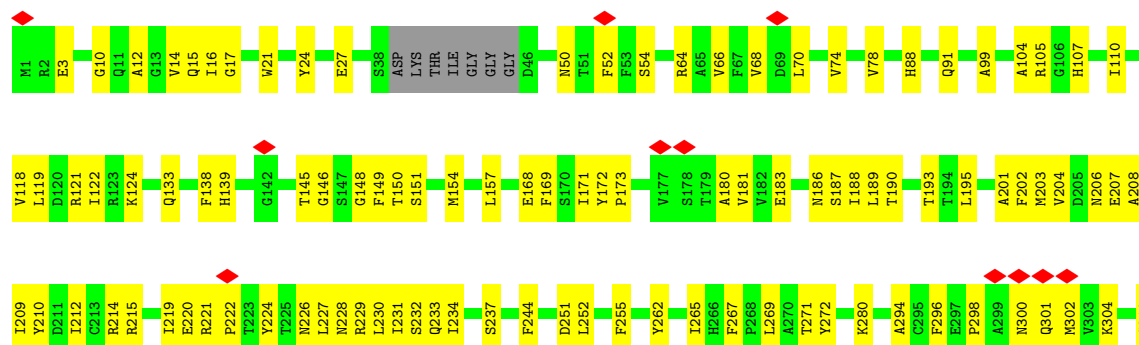


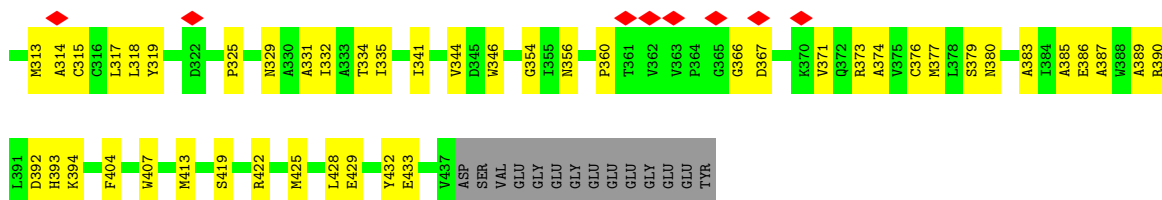


• Molecule 2: Tubulin alpha-1B chain

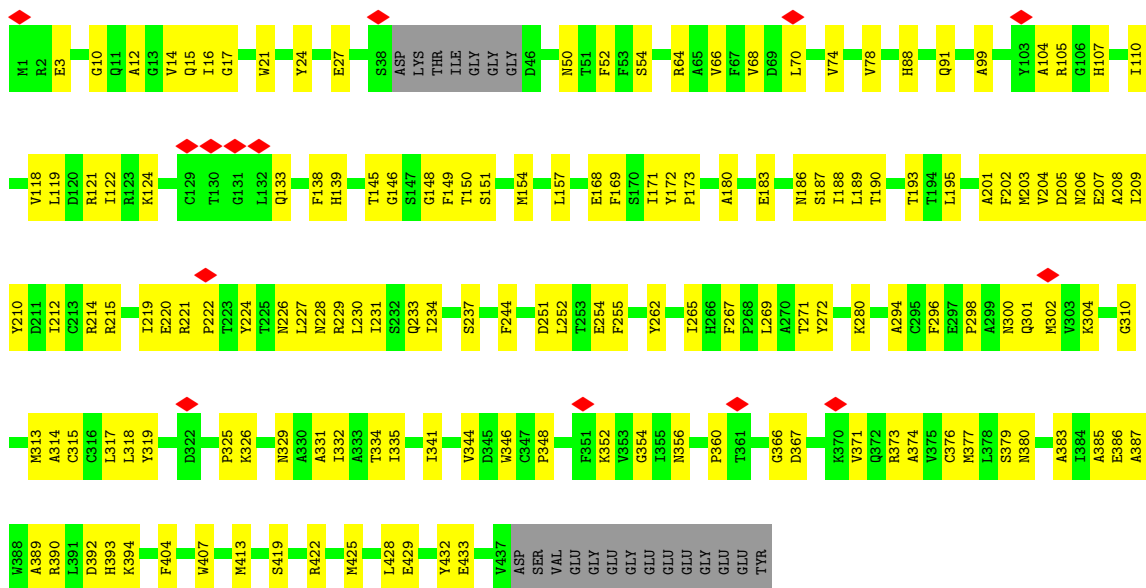


• Molecule 2: Tubulin alpha-1B chain

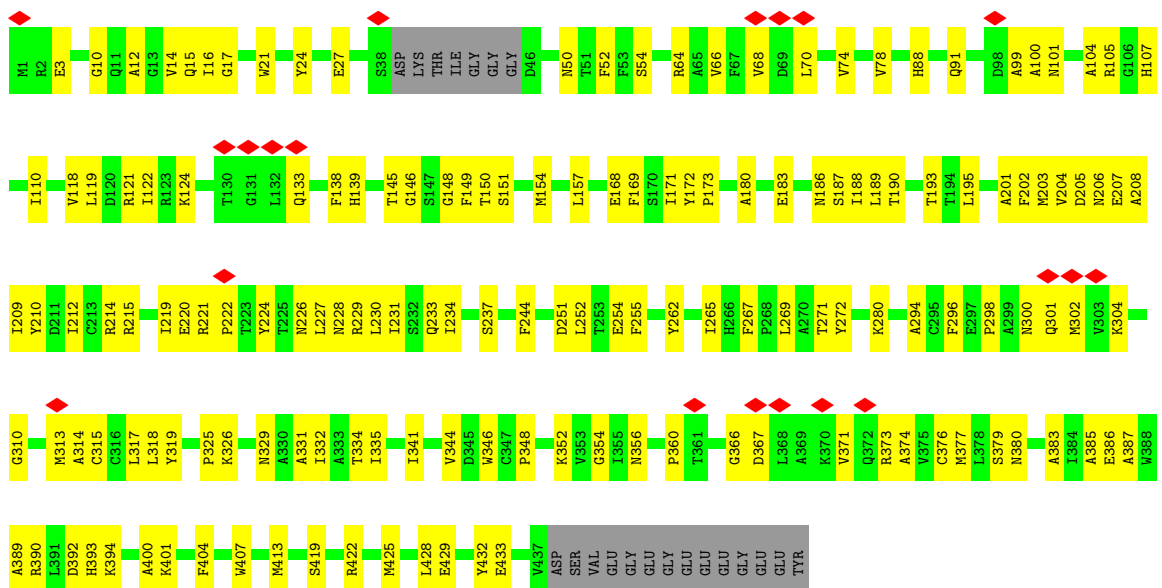




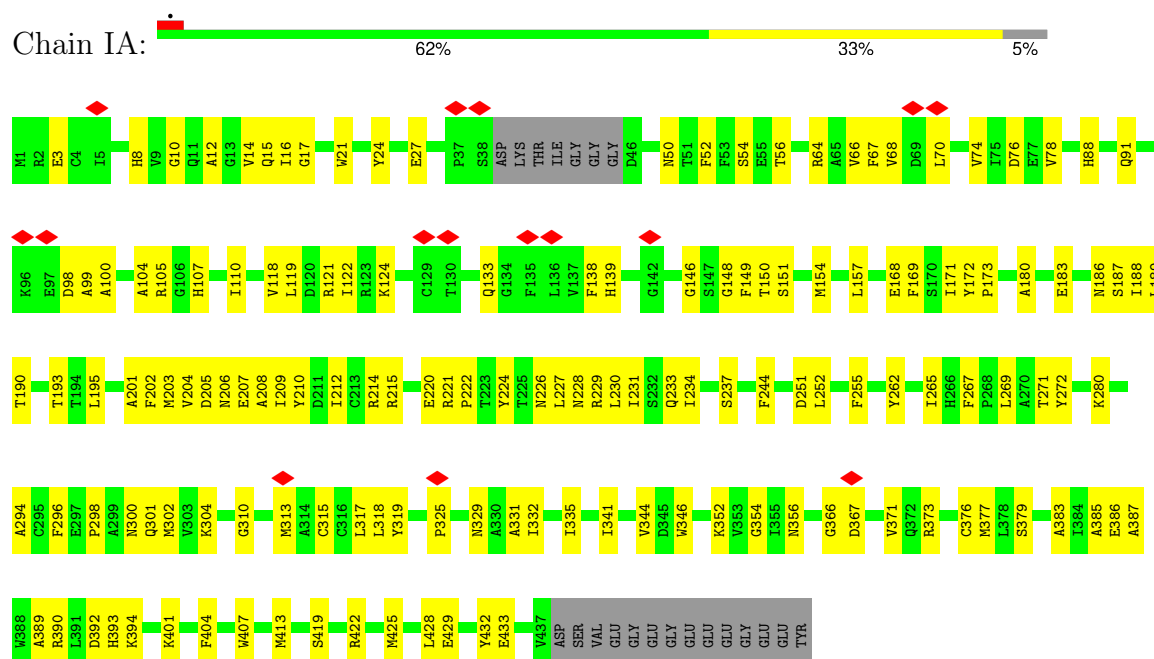
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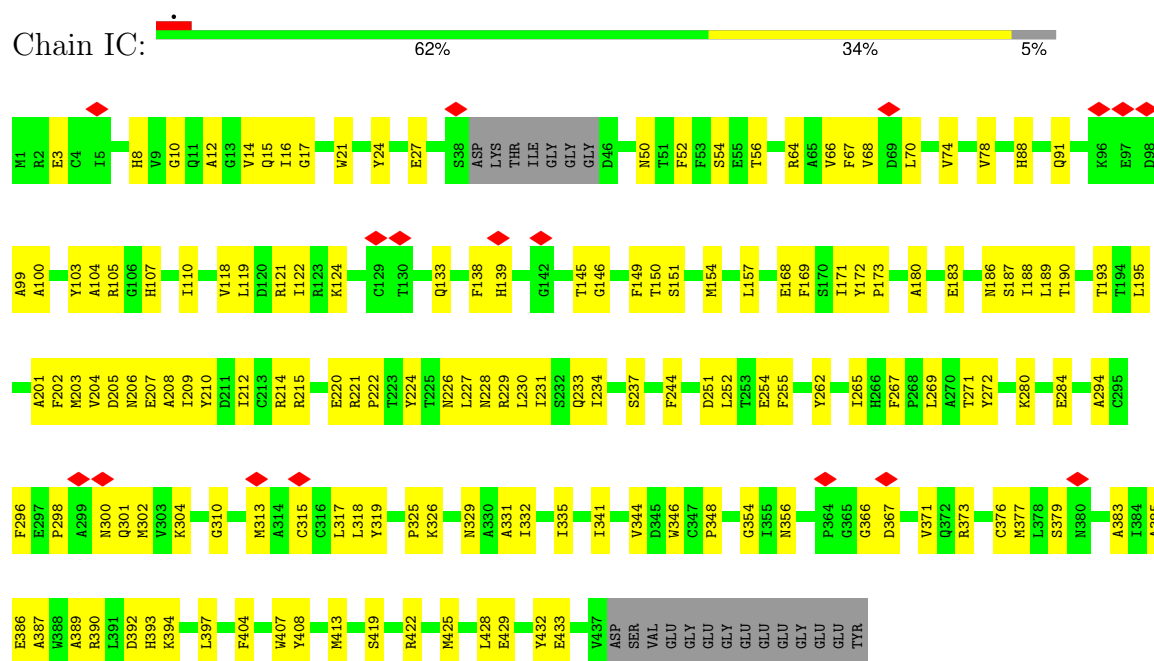
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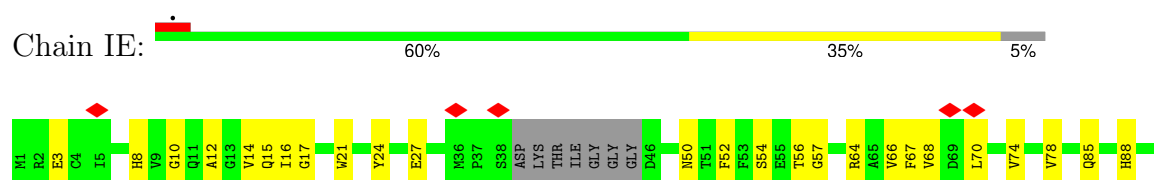
- Molecule 2: Tubulin alpha-1B chain

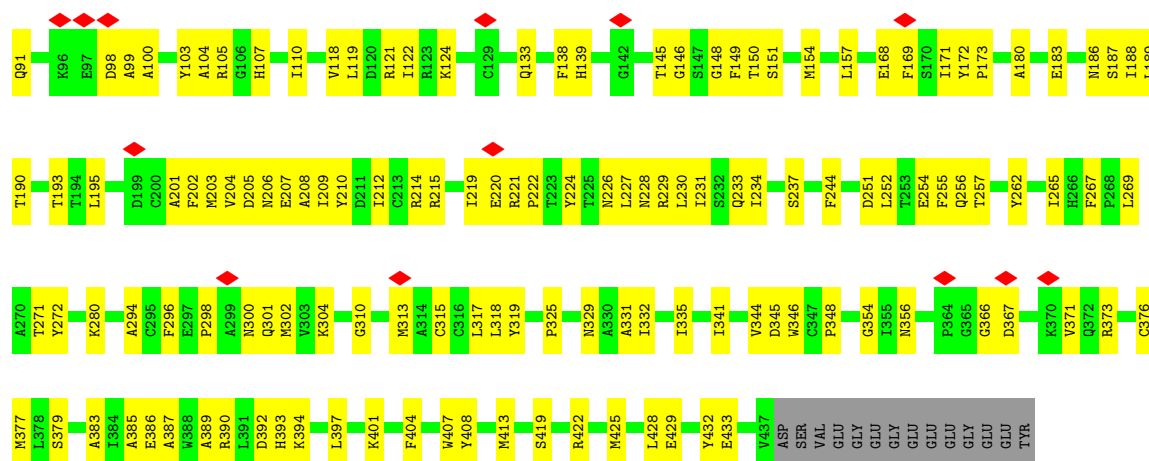


- Molecule 2: Tubulin alpha-1B chain

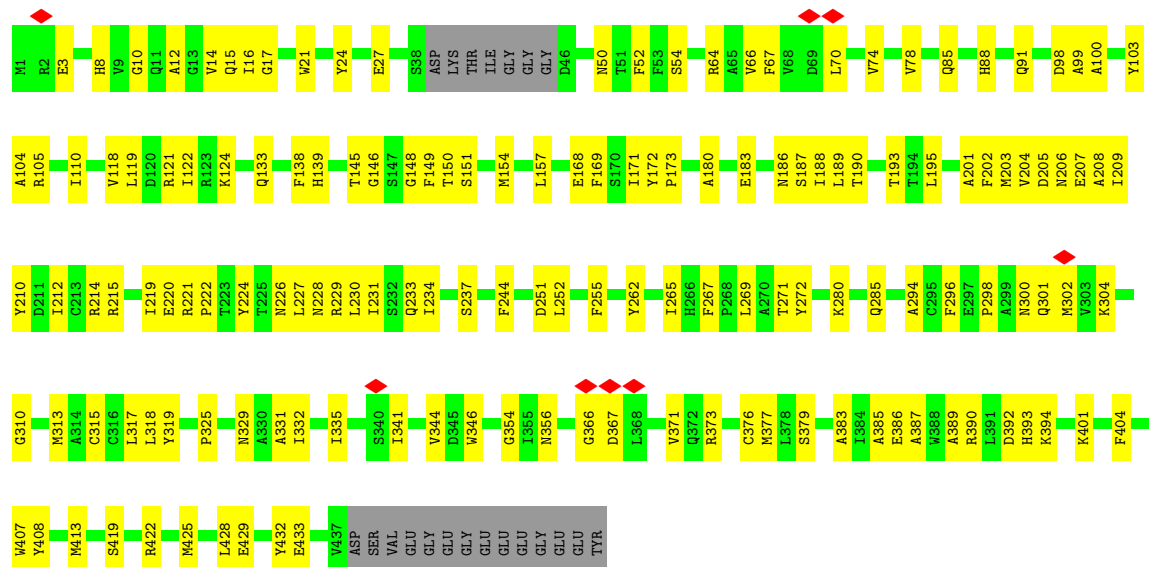


- Molecule 2: Tubulin alpha-1B chain

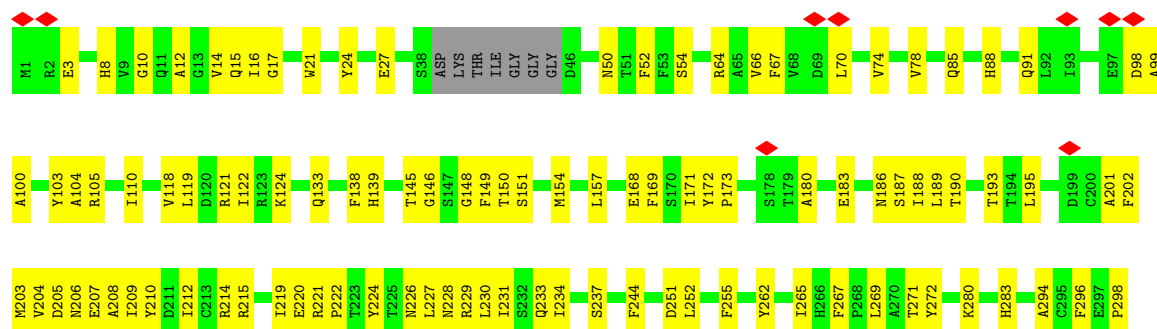


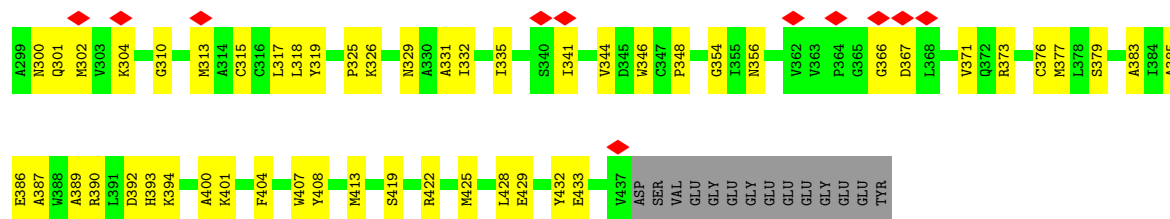


• Molecule 2: Tubulin alpha-1B chain

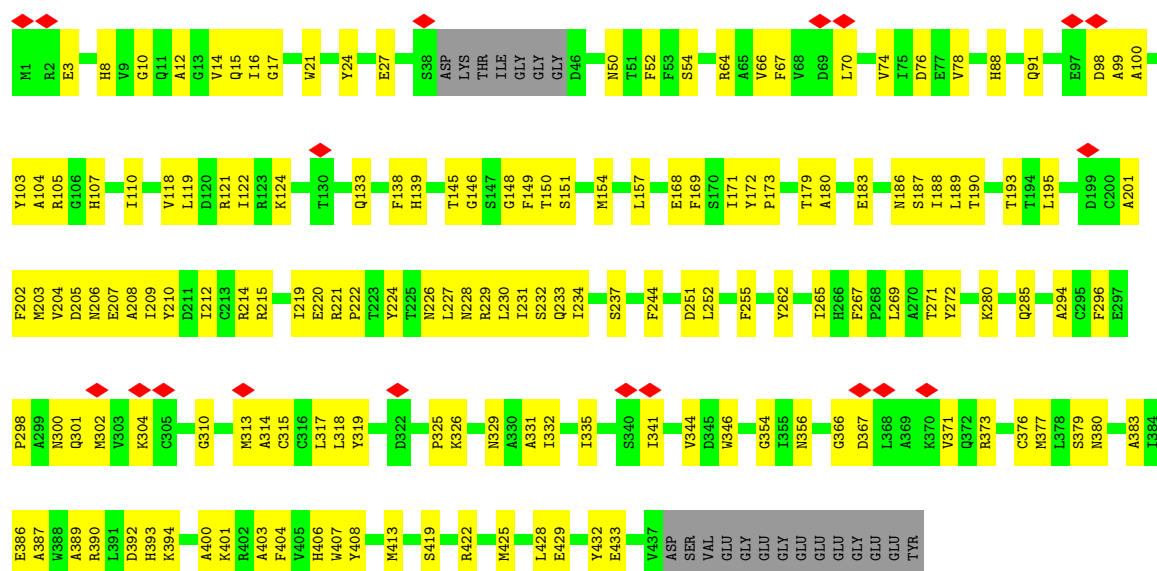


• Molecule 2: Tubulin alpha-1B chain

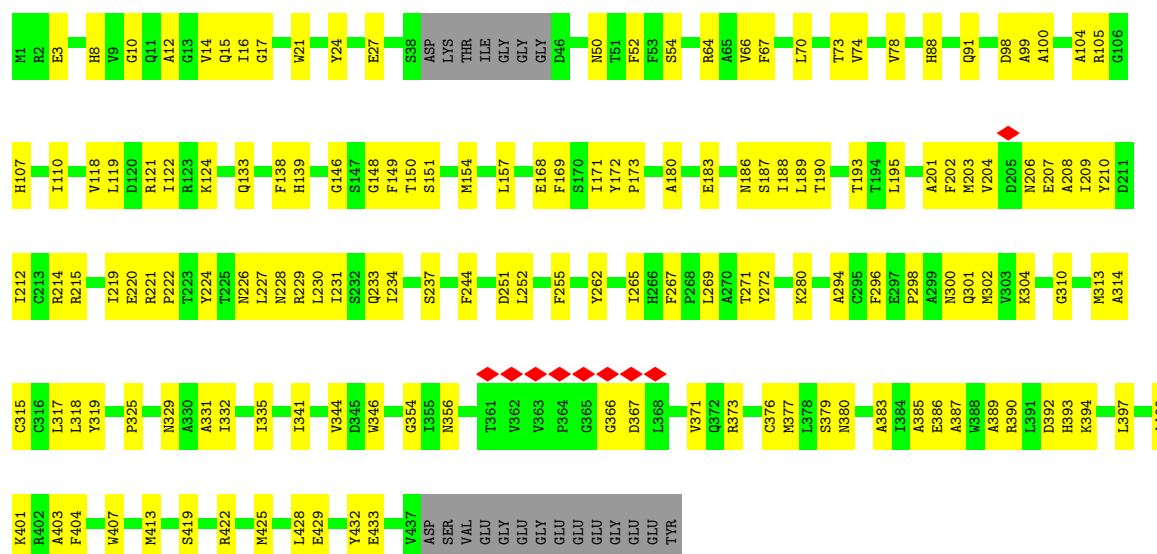




• Molecule 2: Tubulin alpha-1B chain

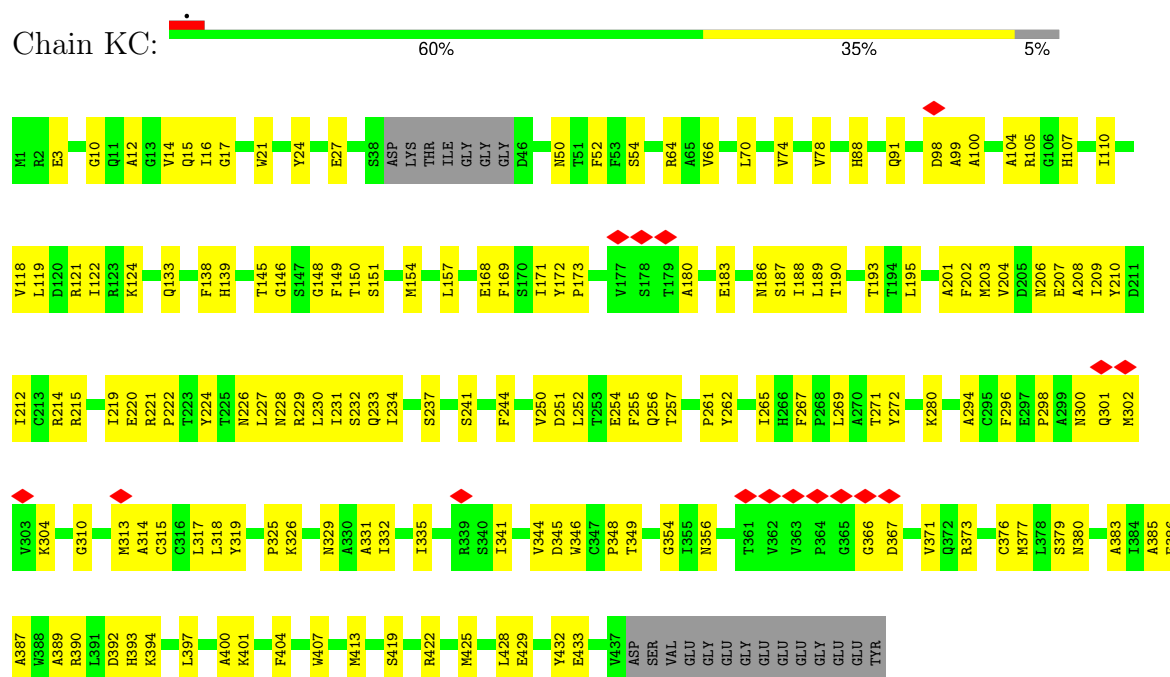


• Molecule 2: Tubulin alpha-1B chain



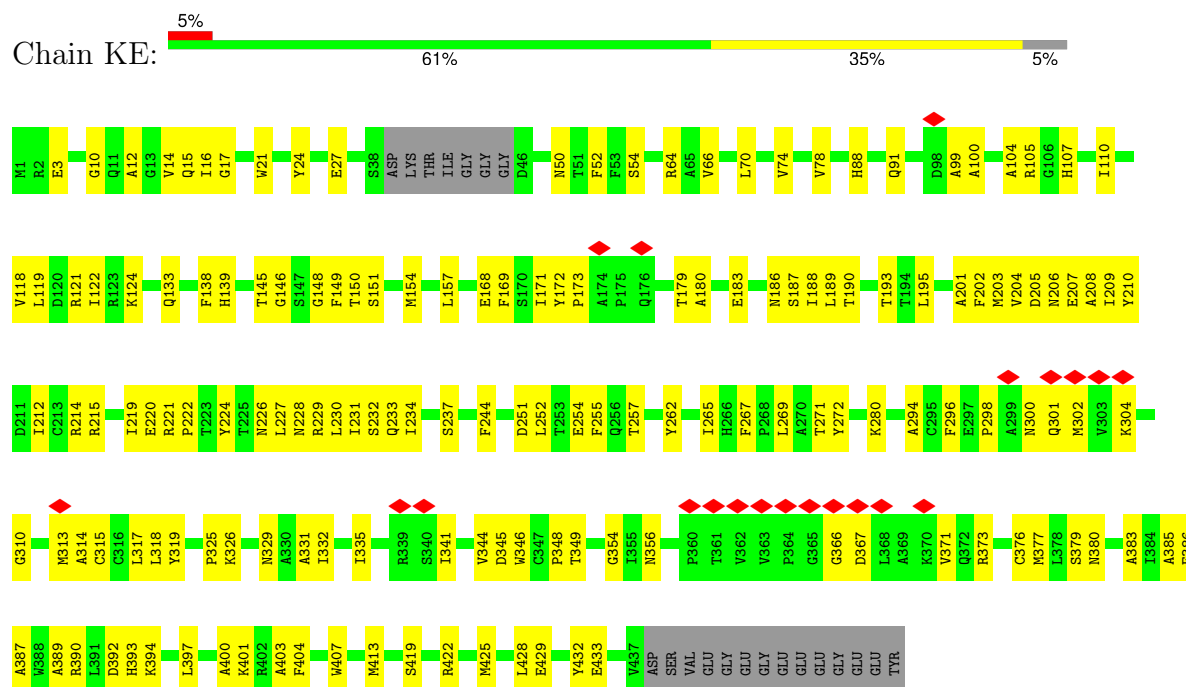
• Molecule 2: Tubulin alpha-1B chain

Chain KC:



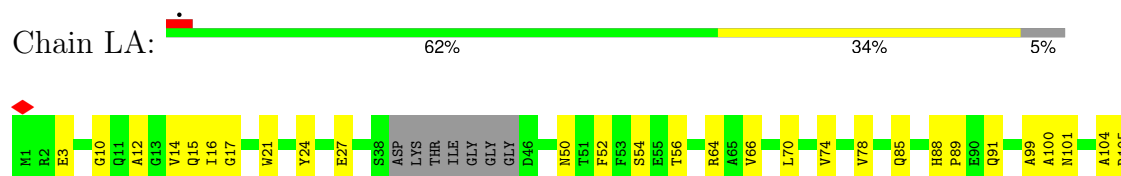
- Molecule 2: Tubulin alpha-1B chain

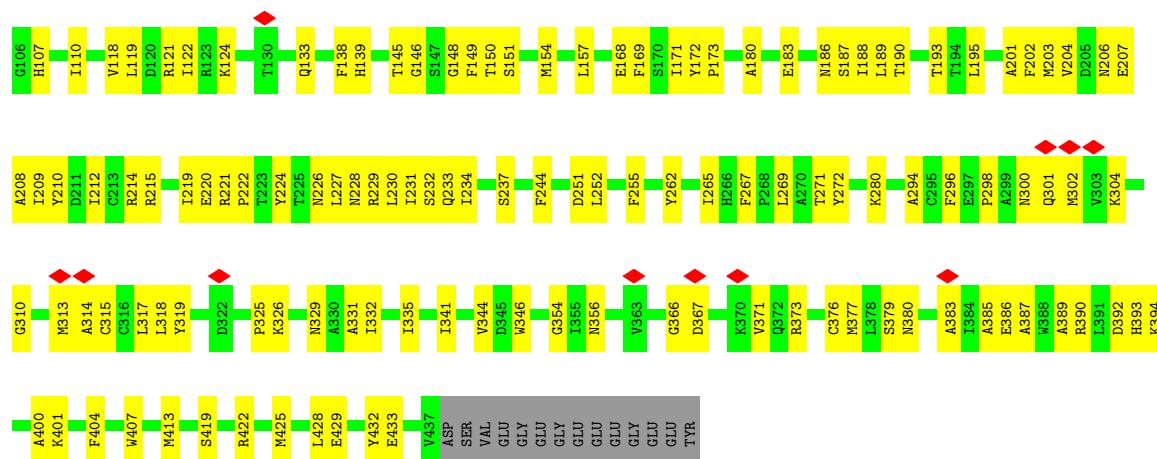
Chain KE:



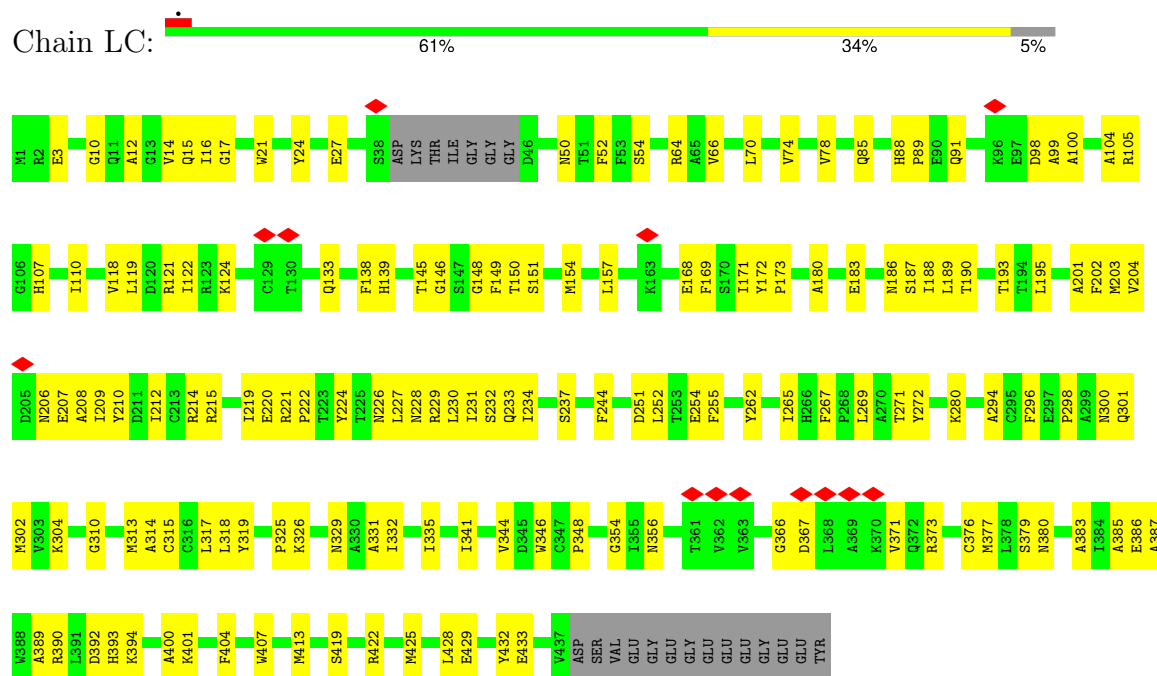
- Molecule 2: Tubulin alpha-1B chain

Chain LA:

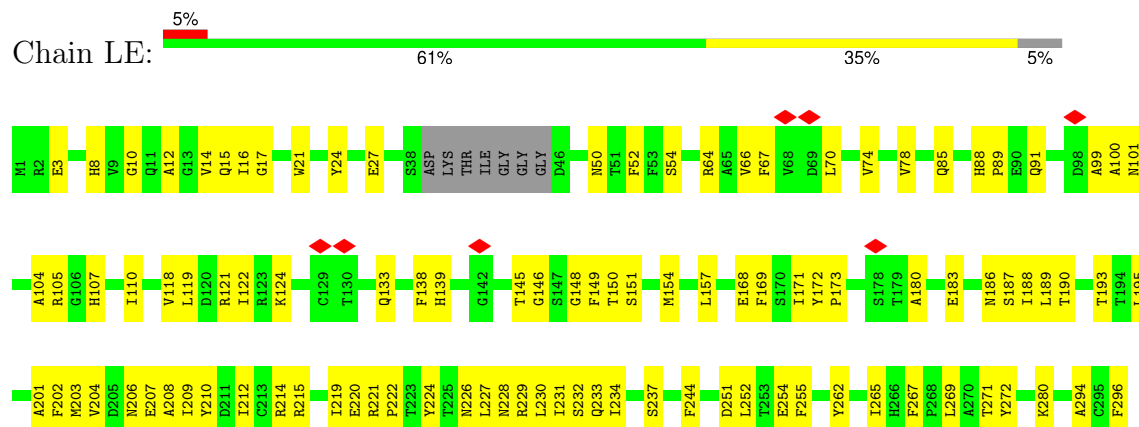


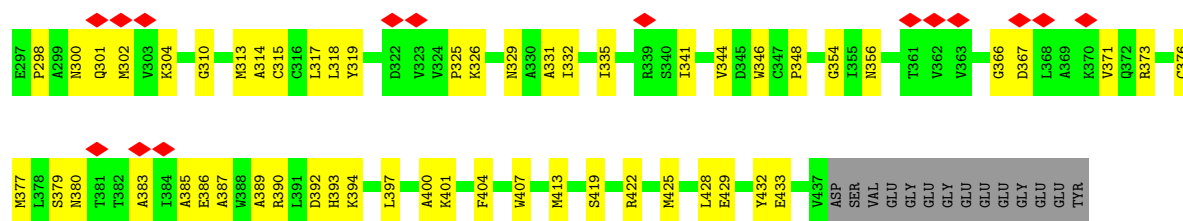


• Molecule 2: Tubulin alpha-1B chain



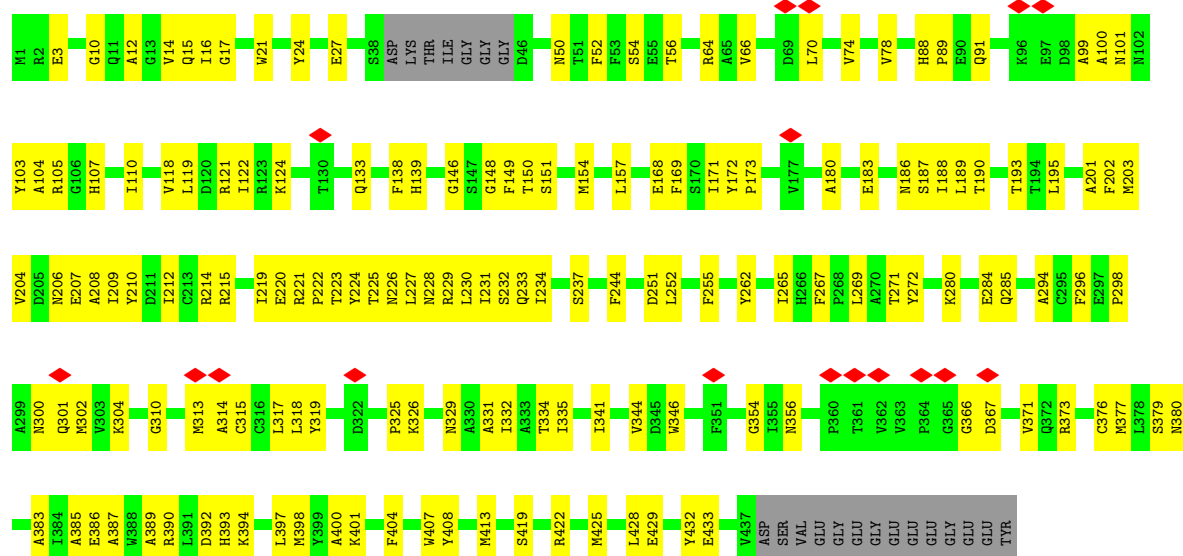
• Molecule 2: Tubulin alpha-1B chain





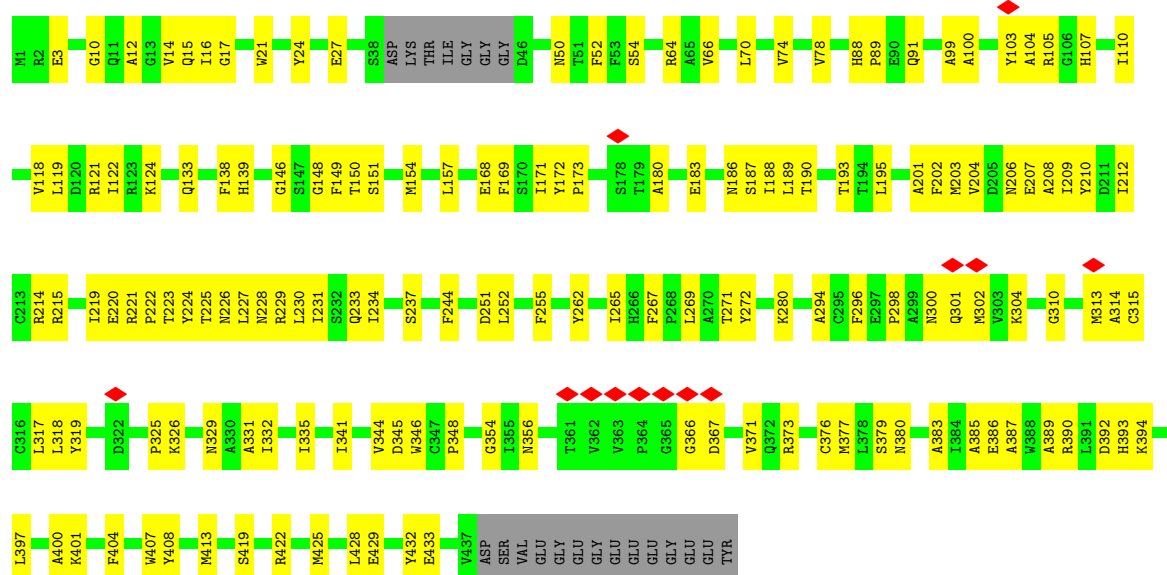
• Molecule 2: Tubulin alpha-1B chain

Chain MA: 60% 35% 5%

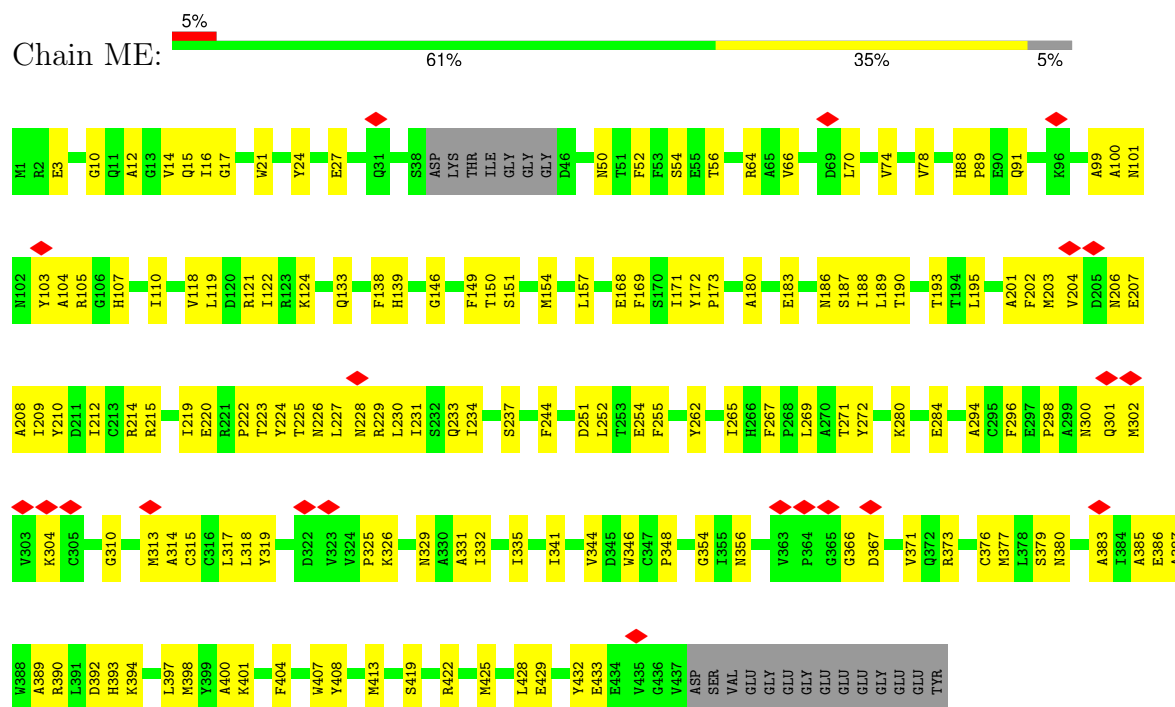


• Molecule 2: Tubulin alpha-1B chain

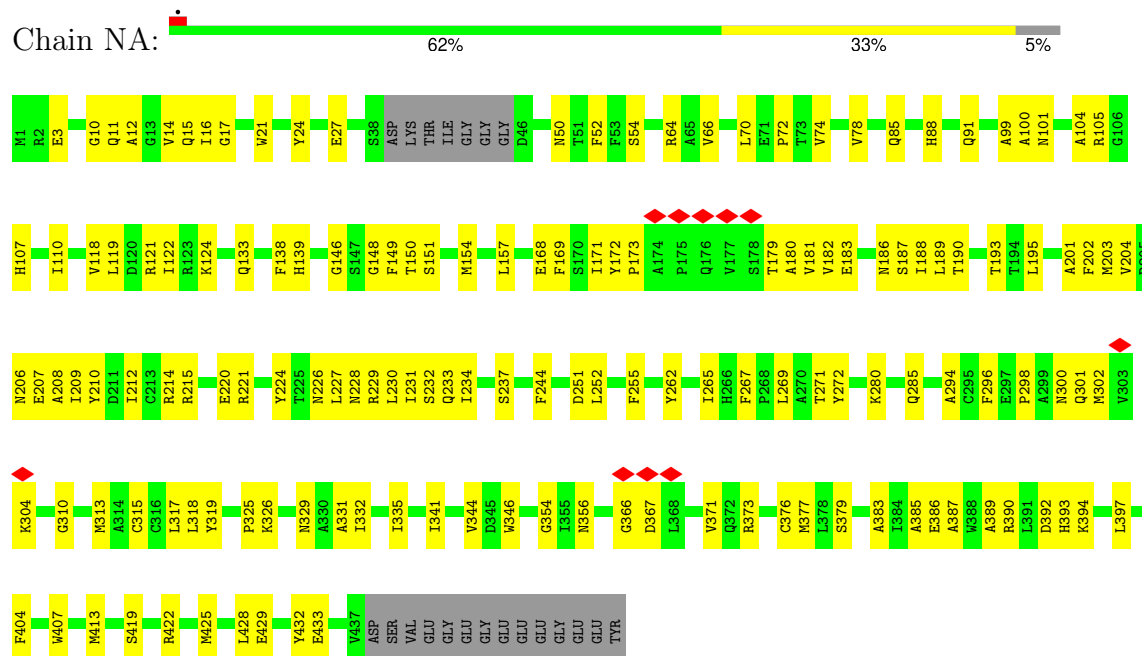
Chain MC: 61% 34% 5%



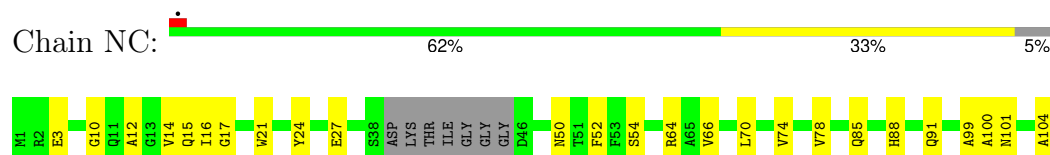
- Molecule 2: Tubulin alpha-1B chain

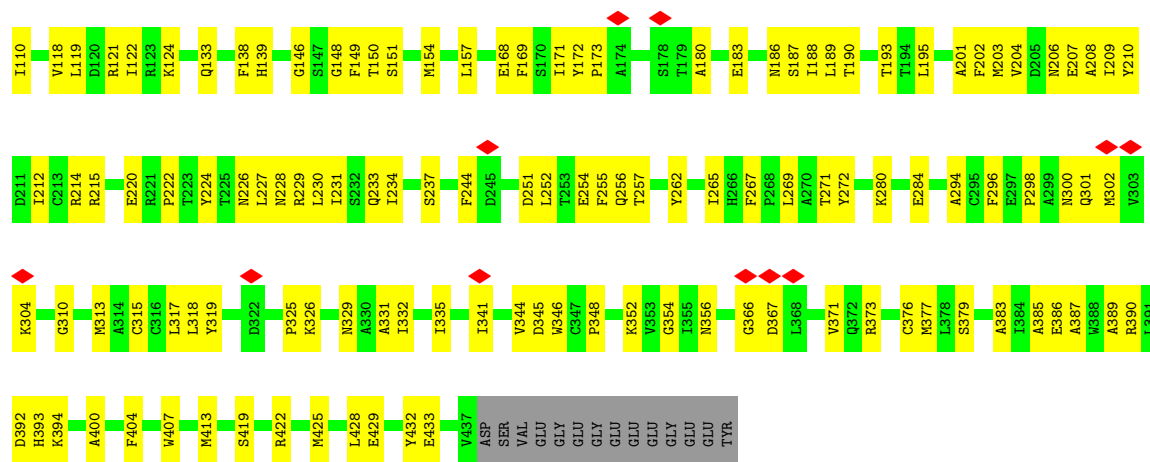


- Molecule 2: Tubulin alpha-1B chain

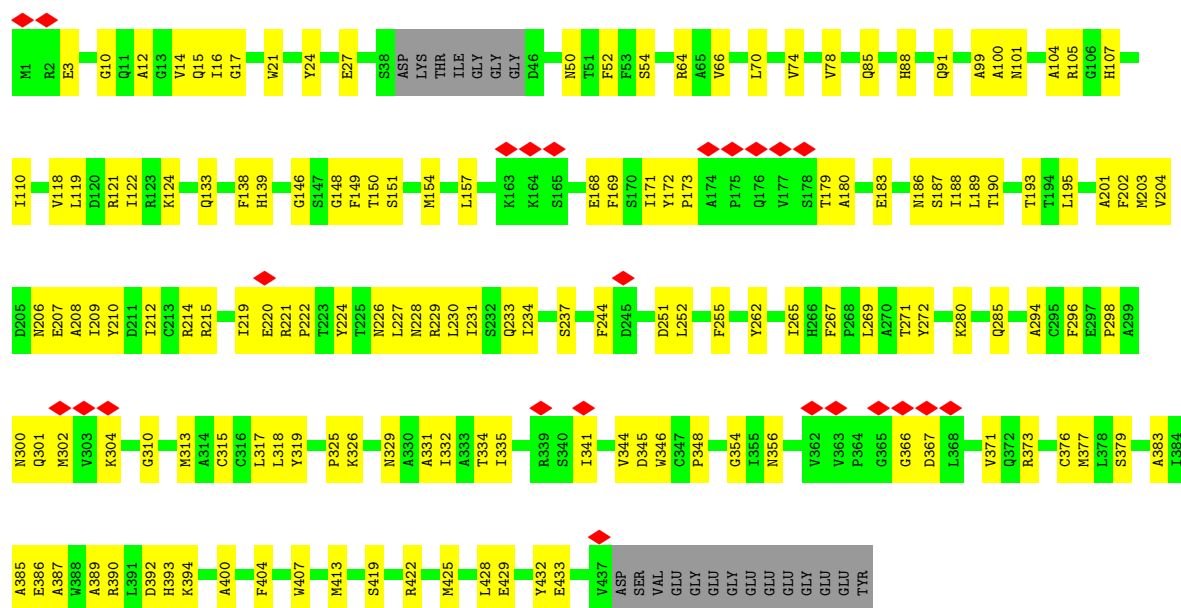


- Molecule 2: Tubulin alpha-1B chain

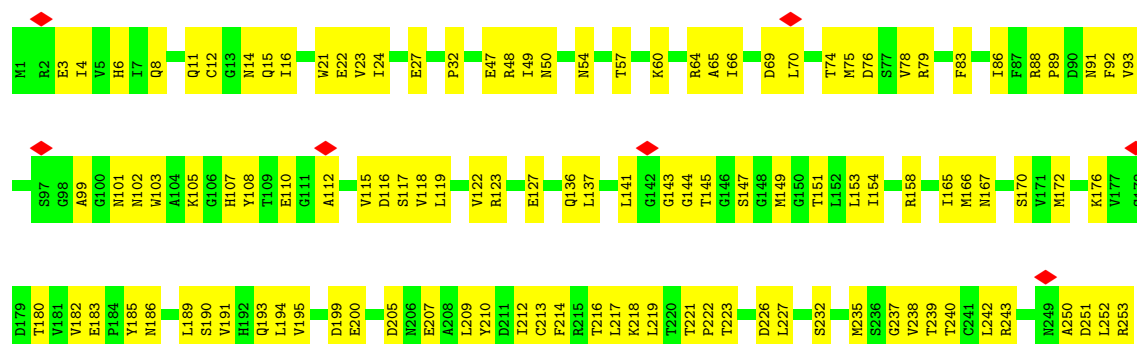




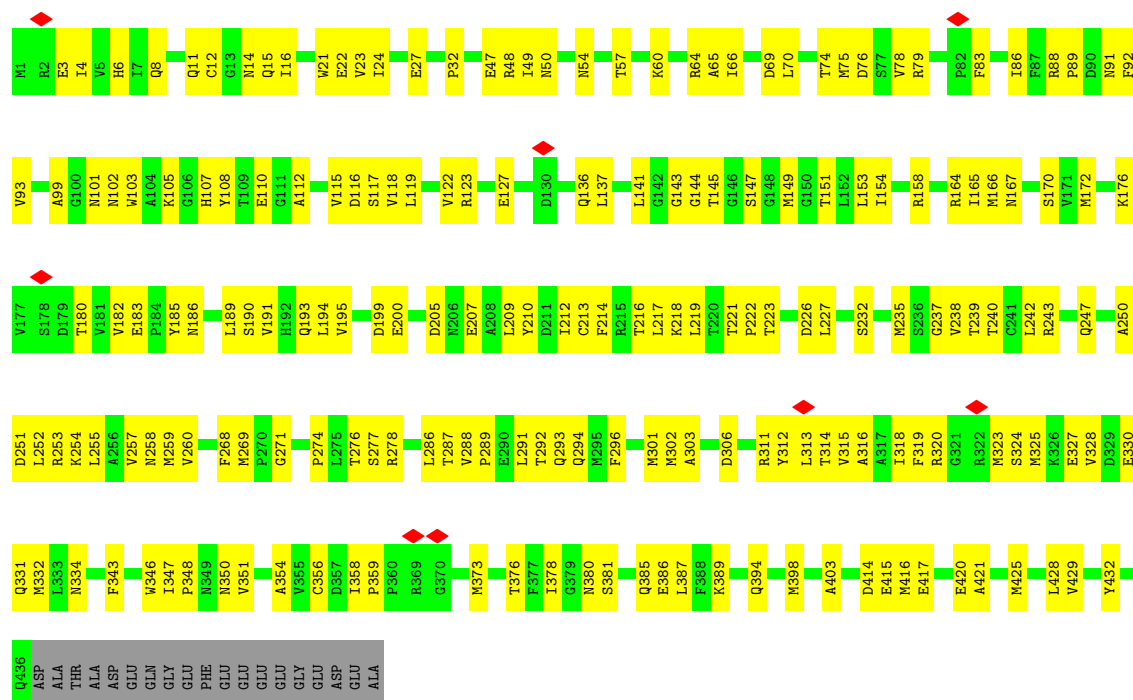
• Molecule 2: Tubulin alpha-1B chain



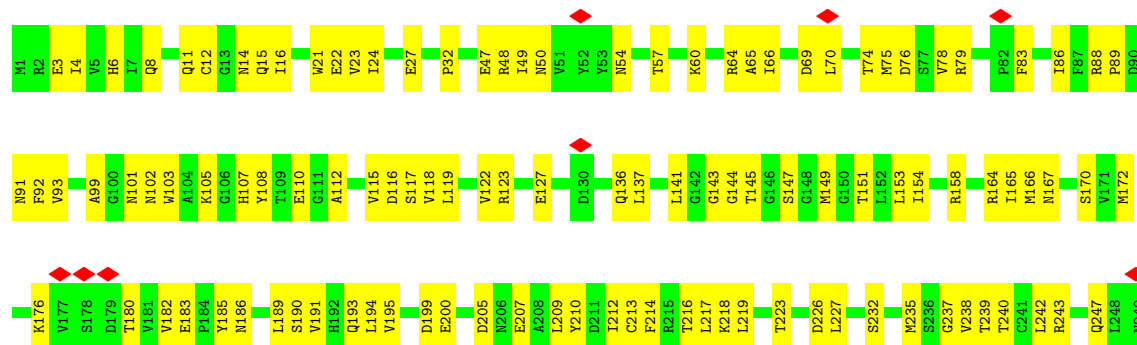
• Molecule 3: Tubulin beta chain



- Molecule 3: Tubulin beta chain

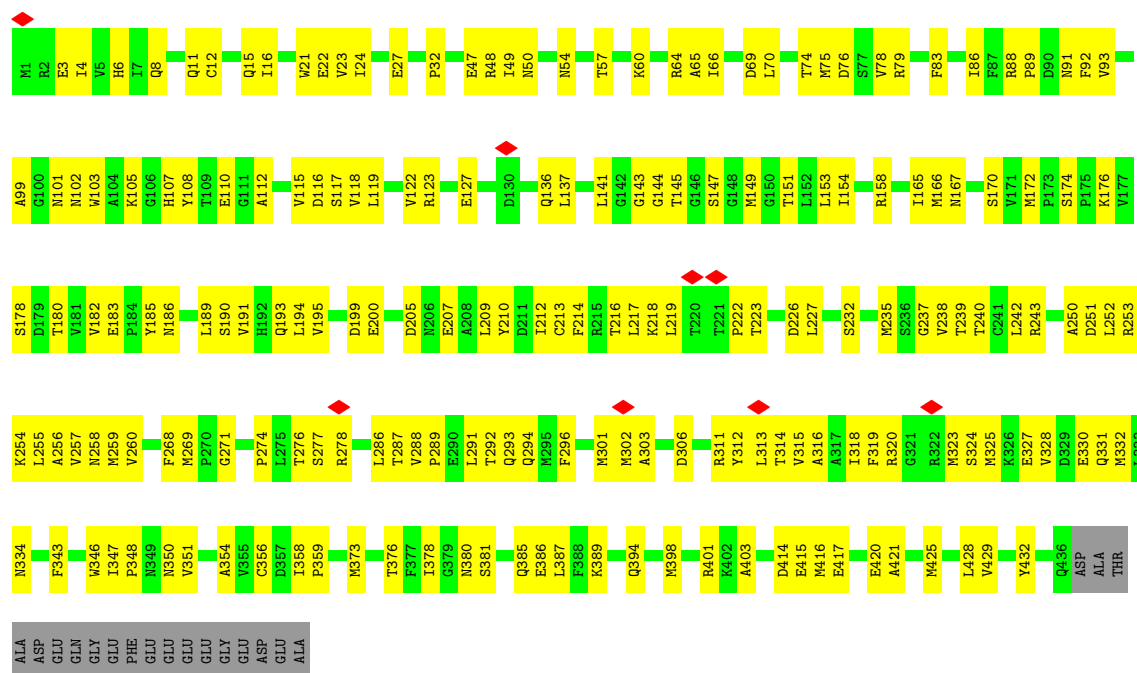


- Molecule 3: Tubulin beta chain



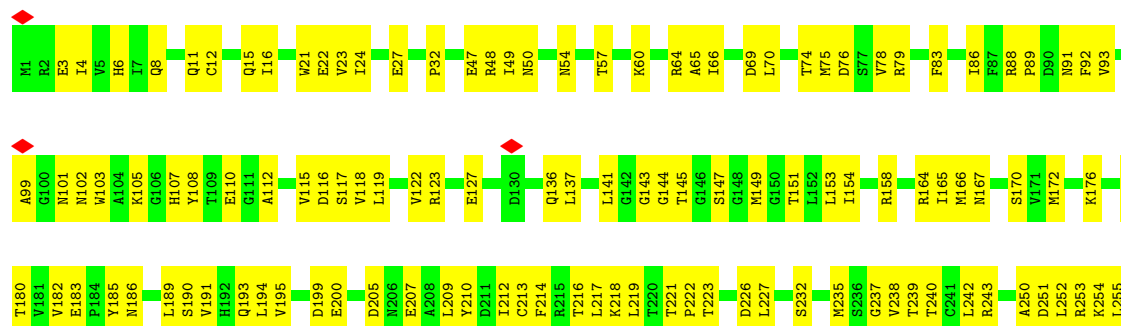
- Molecule 3: Tubulin beta chain

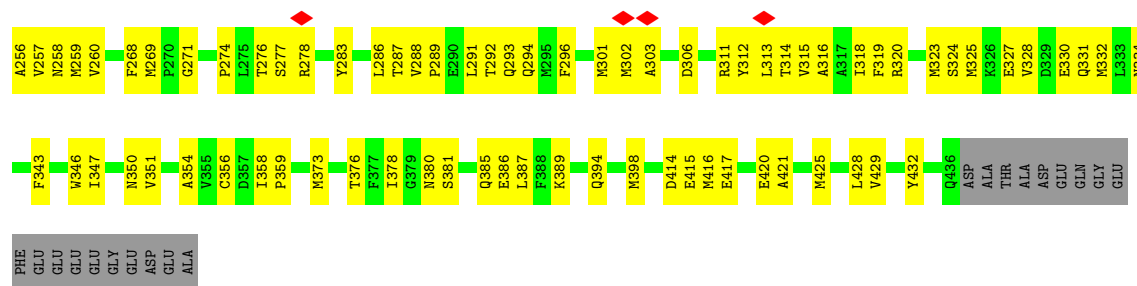
Chain BB:  52% 43%



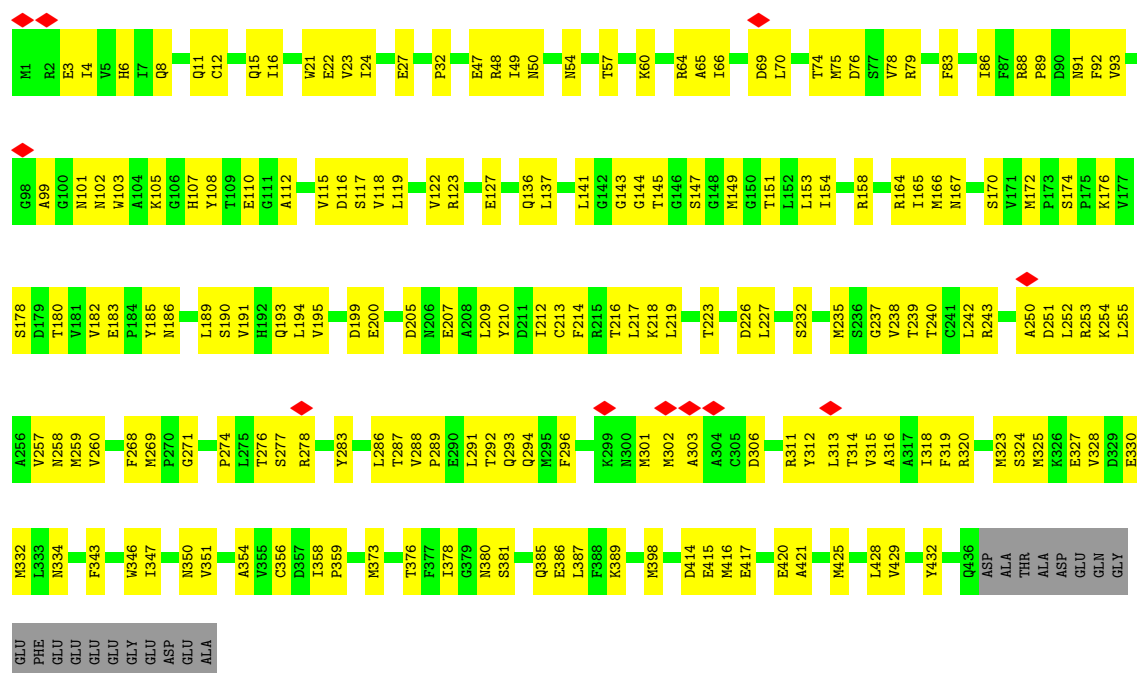
- Molecule 3: Tubulin beta chain

Chain BD:  53% 43%

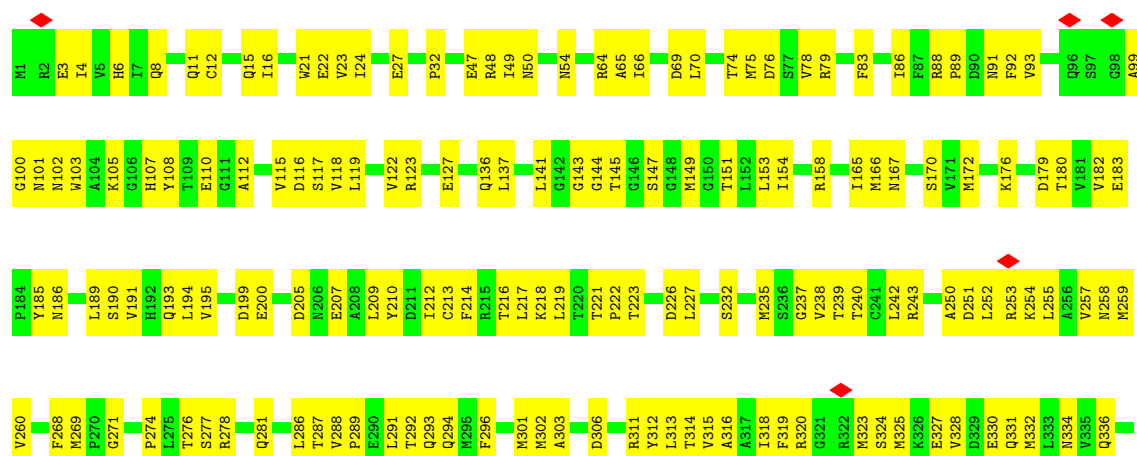


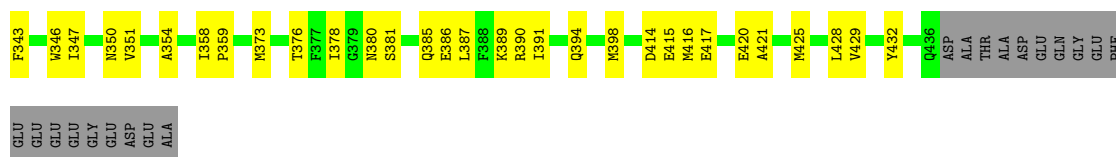


• Molecule 3: Tubulin beta chain

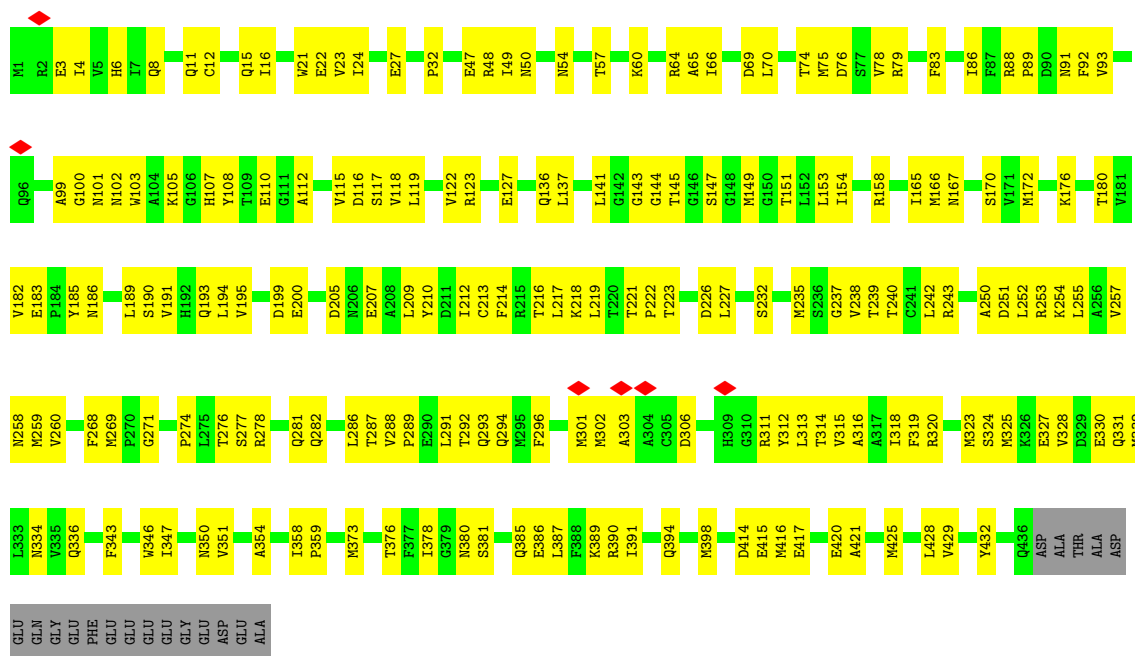


• Molecule 3: Tubulin beta chain

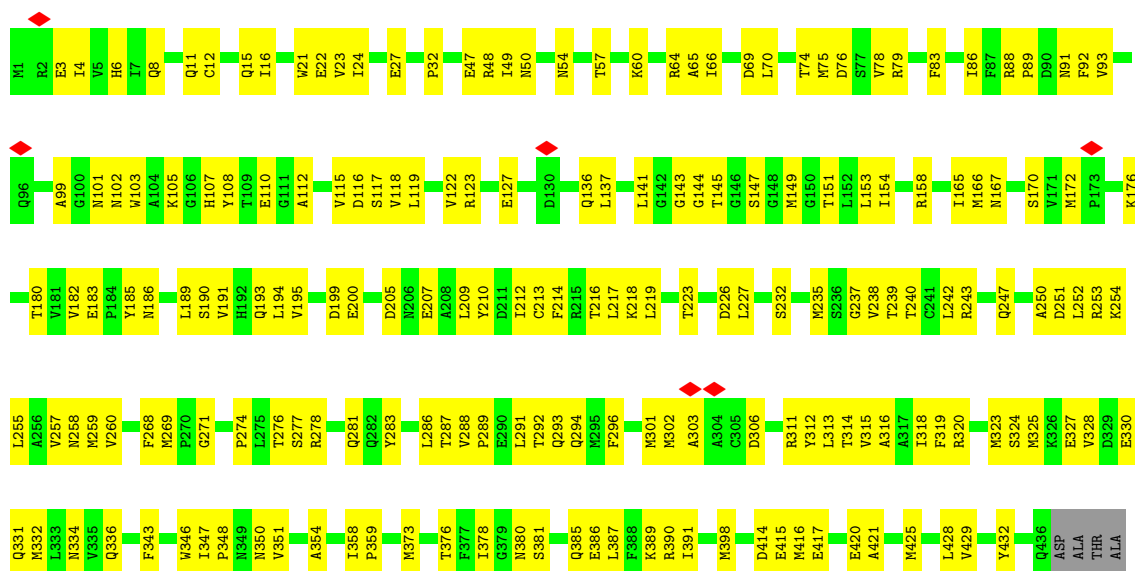




• Molecule 3: Tubulin beta chain

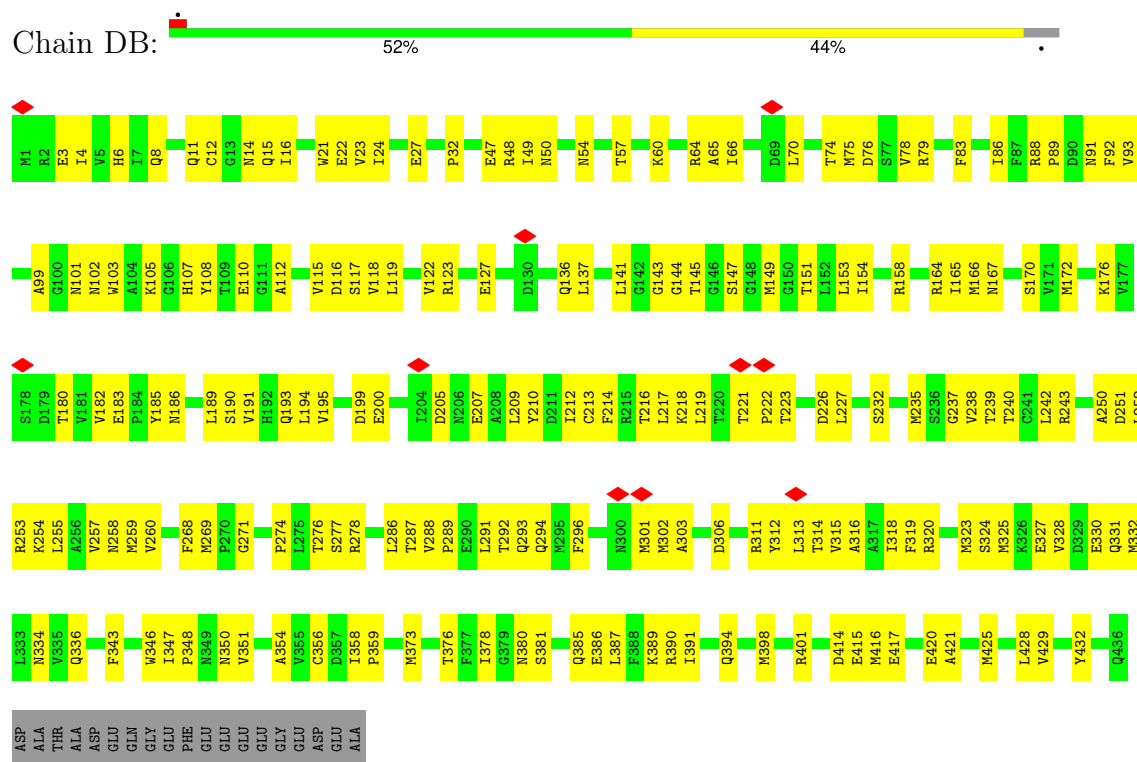


• Molecule 3: Tubulin beta chain

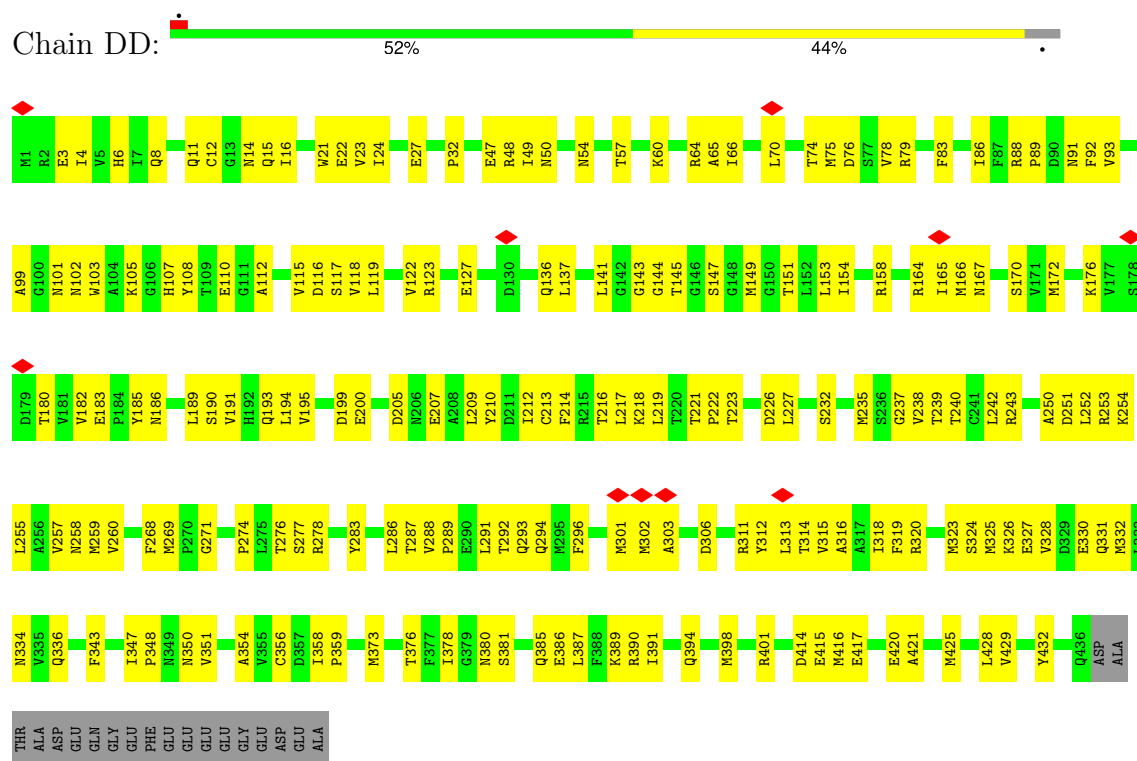


ASP
GLU
GLN
GLY
GLU
PHE
GLU
GLU
GLU
ASP
GLU
ALA

• Molecule 3: Tubulin beta chain

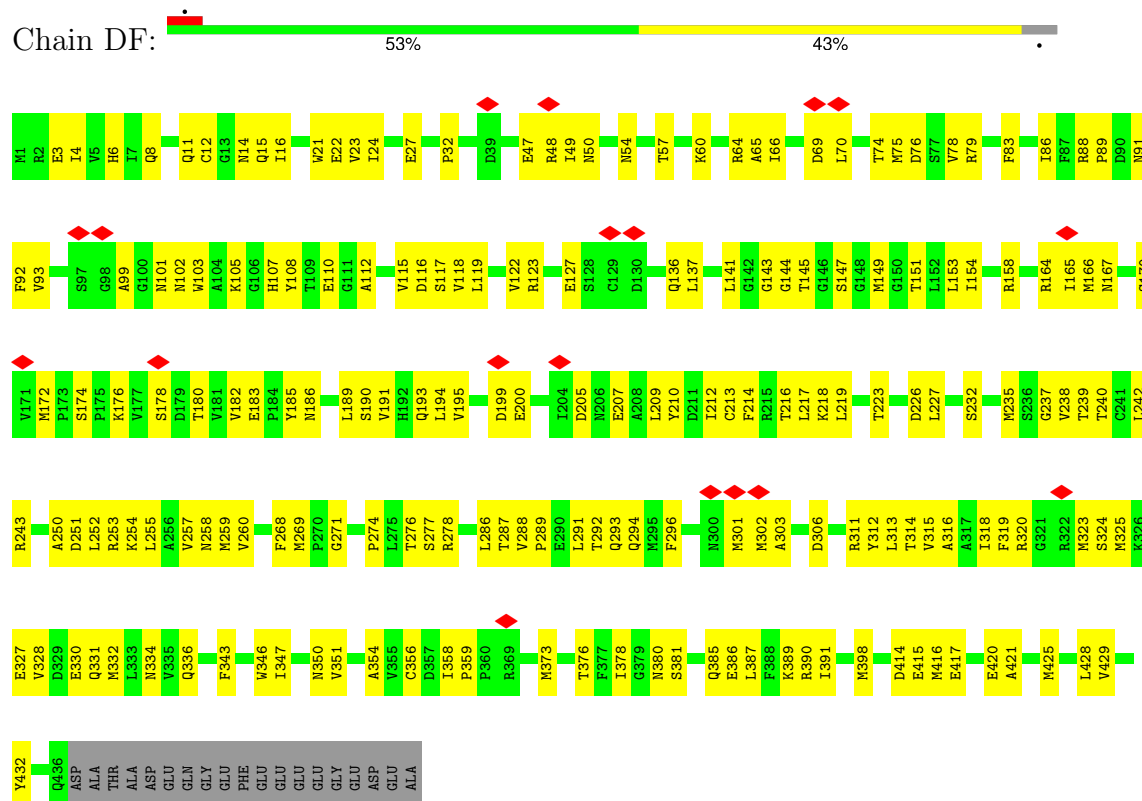


• Molecule 3: Tubulin beta chain



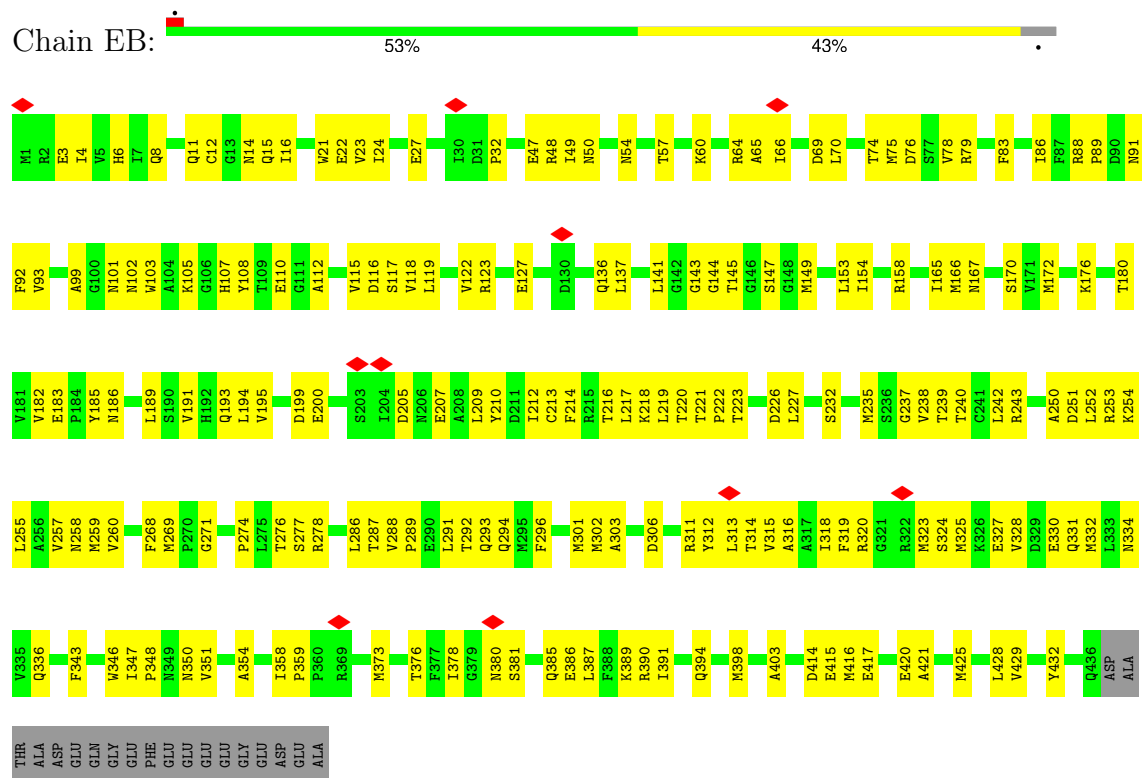
- Molecule 3: Tubulin beta chain

Chain DF:

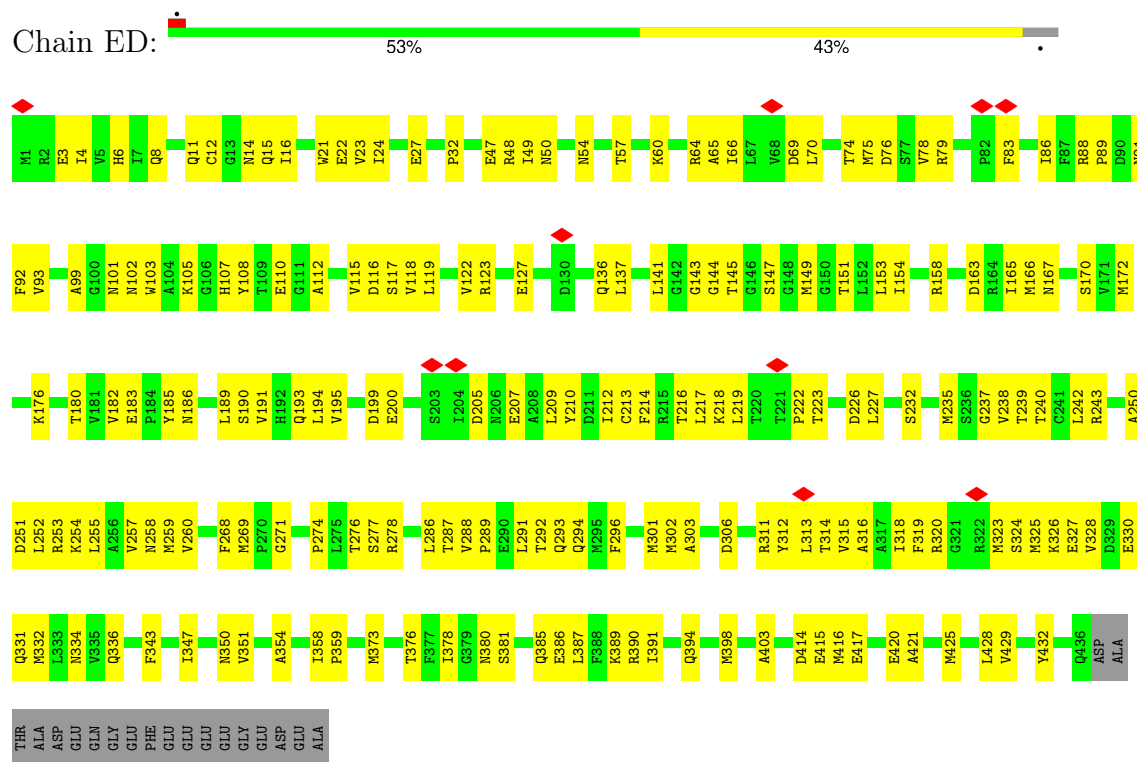


- Molecule 3: Tubulin beta chain

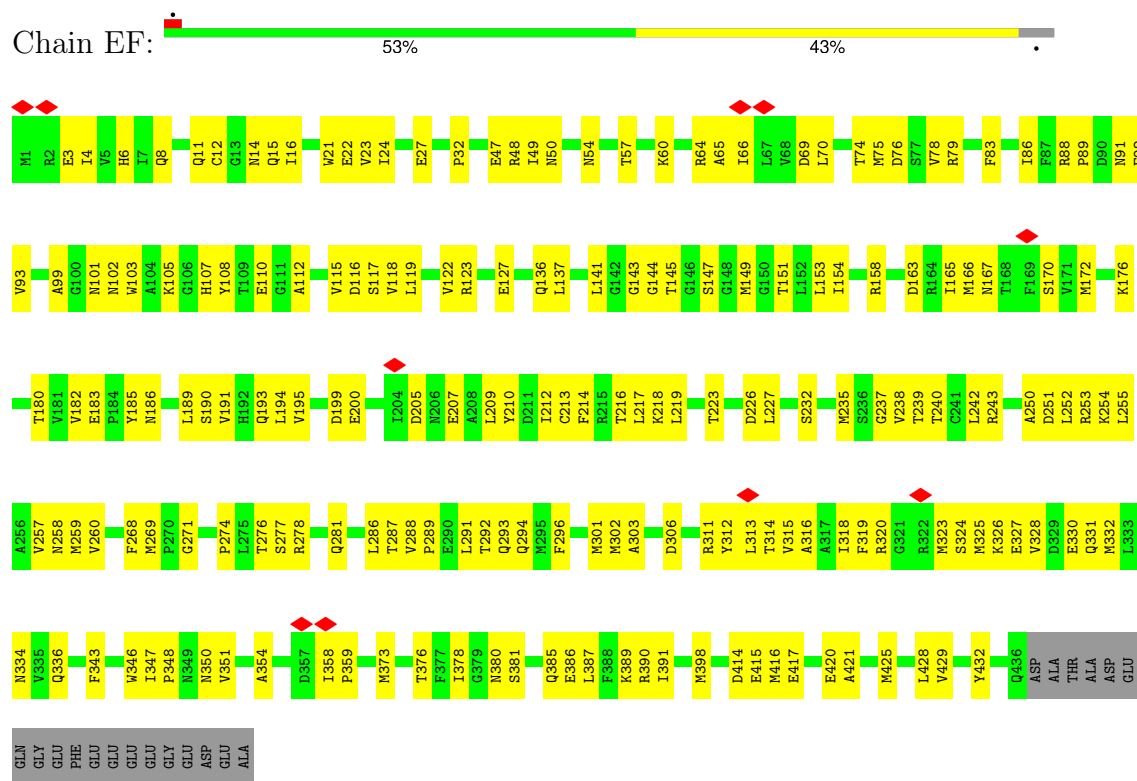
Chain EB:



- Molecule 3: Tubulin beta chain

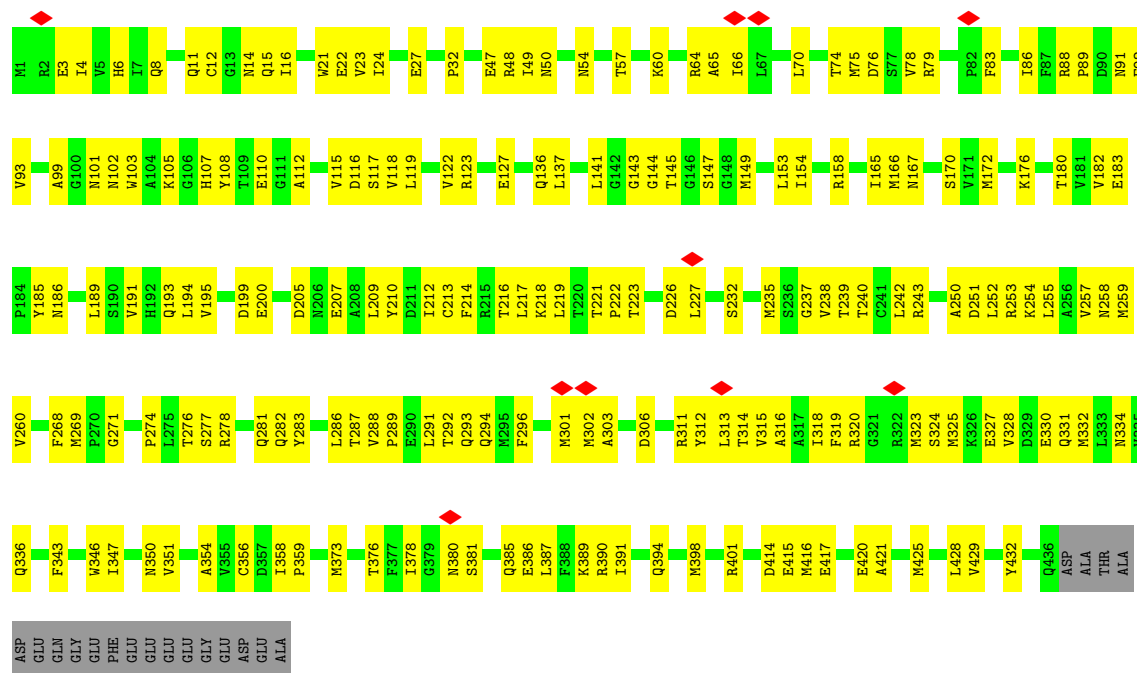


• Molecule 3: Tubulin beta chain



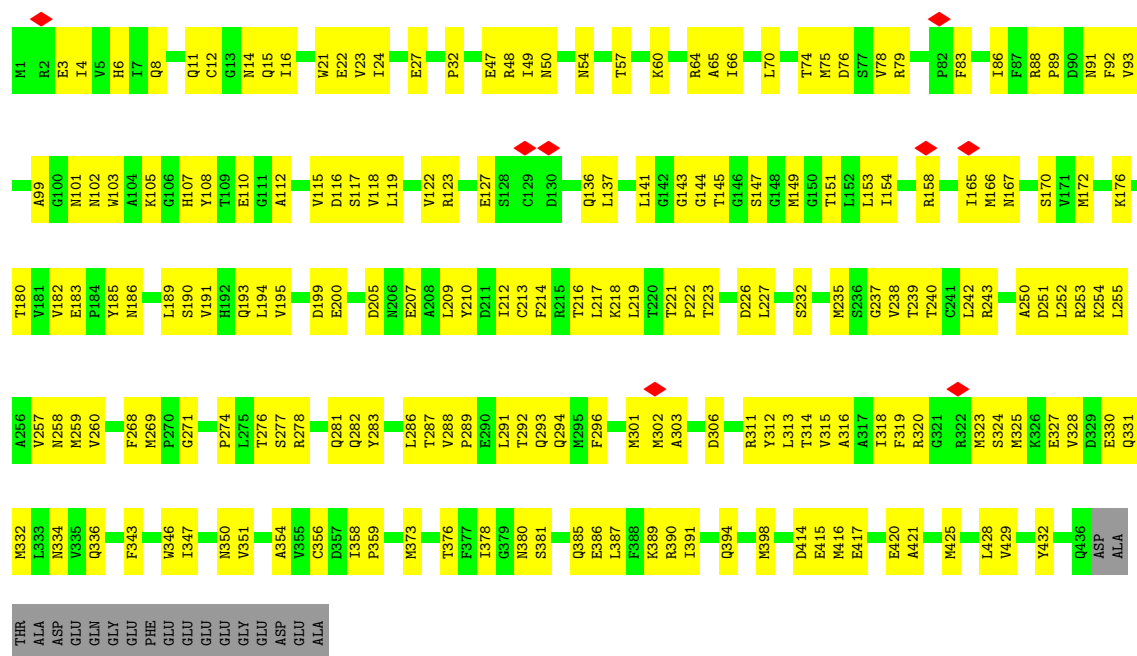
• Molecule 3: Tubulin beta chain





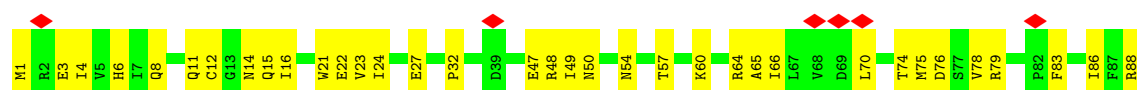
• Molecule 3: Tubulin beta chain

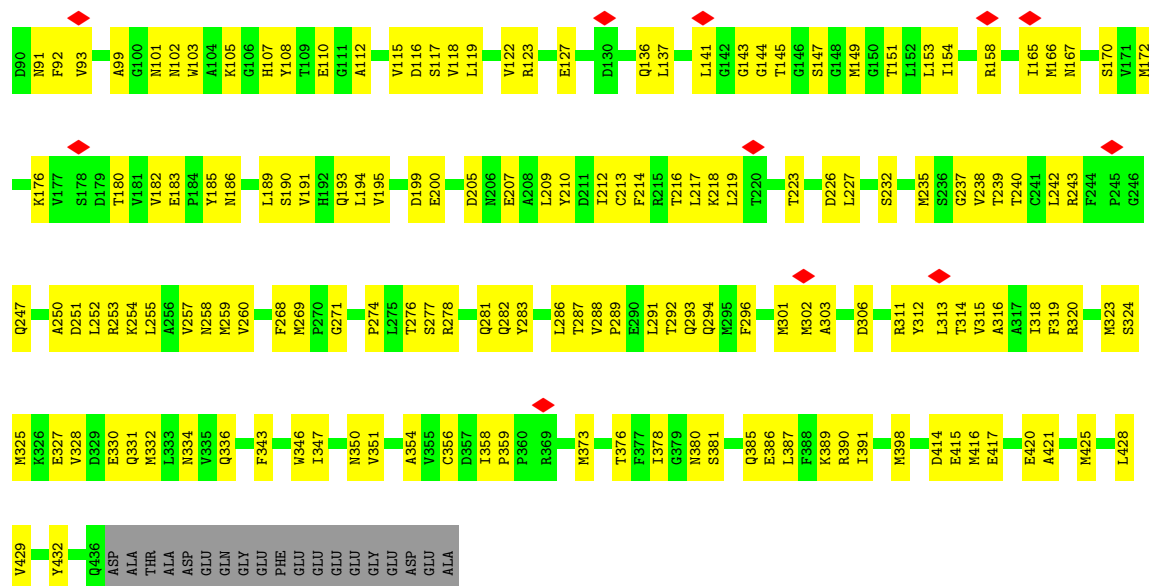
Chain FD: 52% 44%



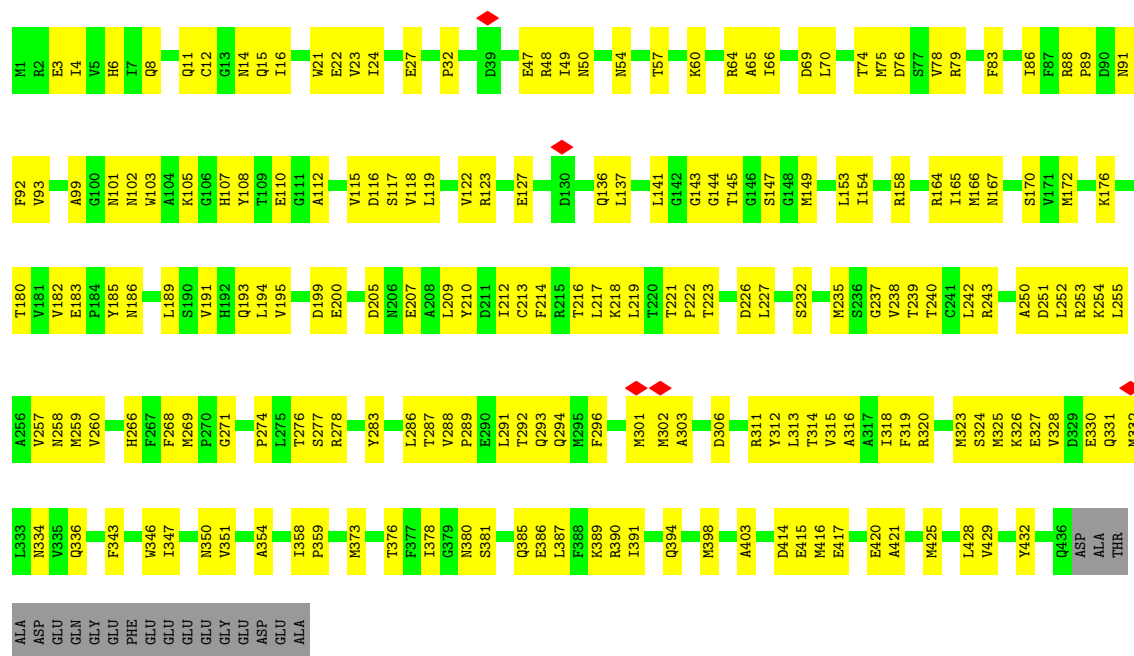
• Molecule 3: Tubulin beta chain

Chain FF: 52% 43%



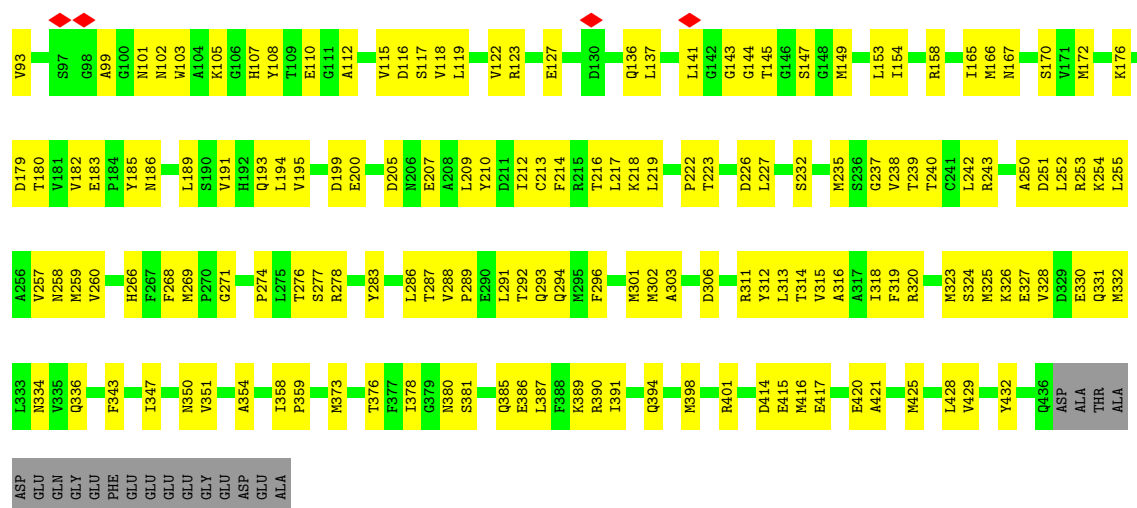


- Molecule 3: Tubulin beta chain



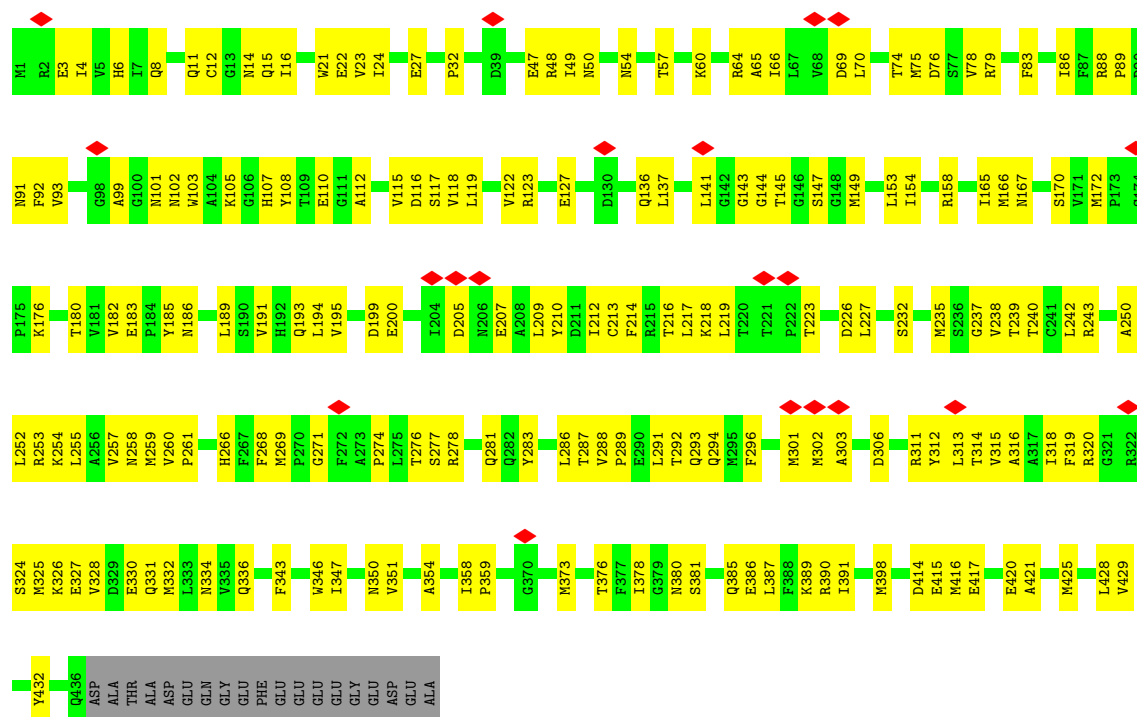
- Molecule 3: Tubulin beta chain





• Molecule 3: Tubulin beta chain

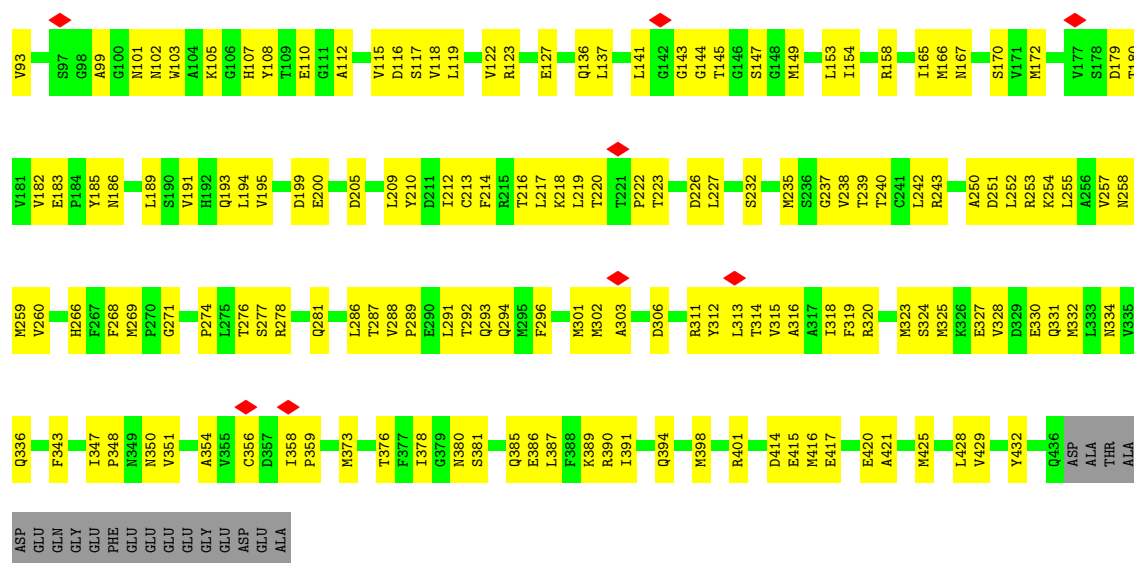
Chain GF: 53% 43%



• Molecule 3: Tubulin beta chain

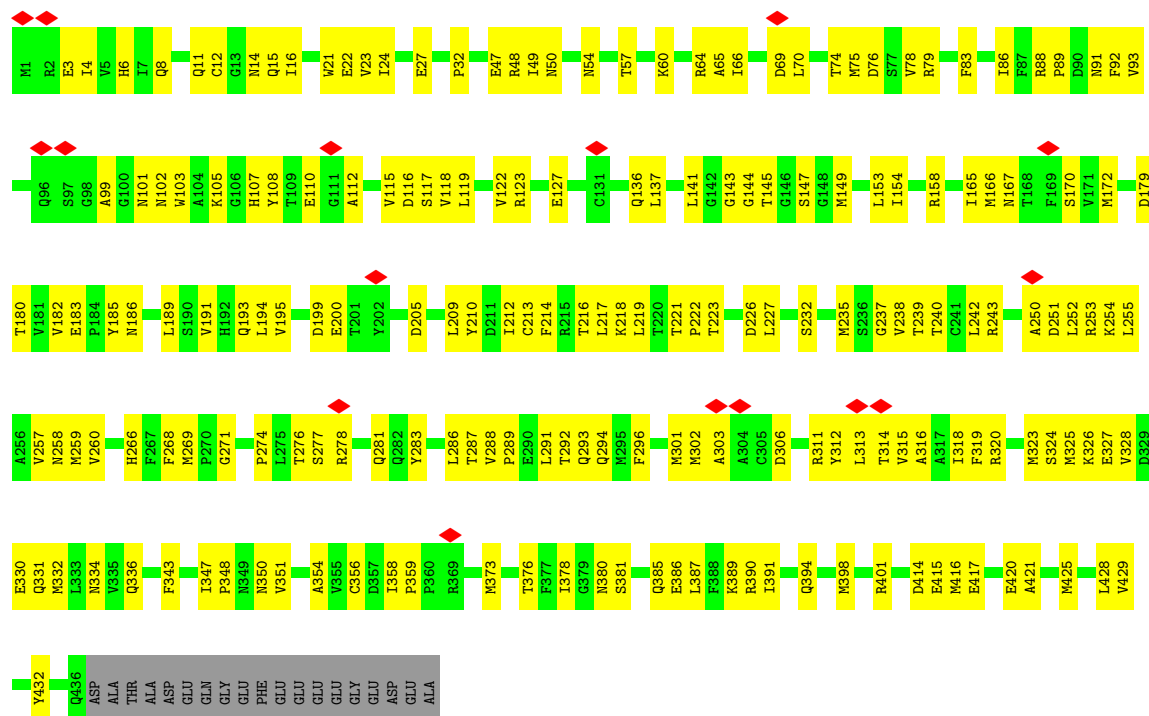
Chain HB: 53% 43%





• Molecule 3: Tubulin beta chain

Chain HD: 52% 44%



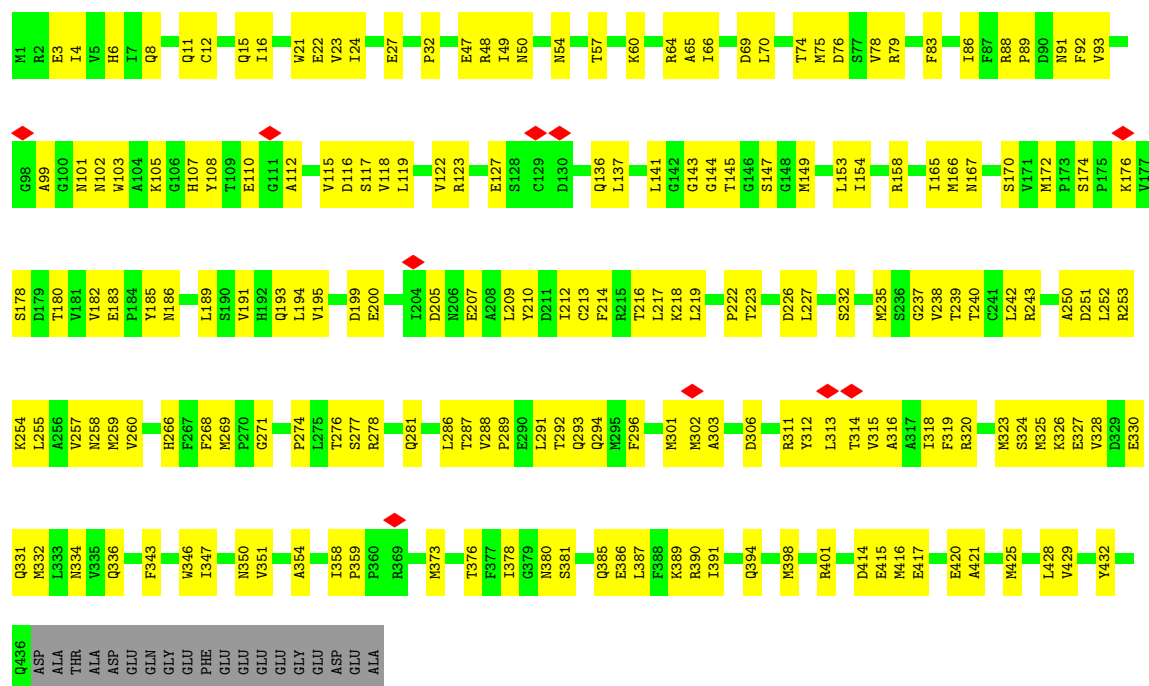
• Molecule 3: Tubulin beta chain

Chain HF: 54% 42%



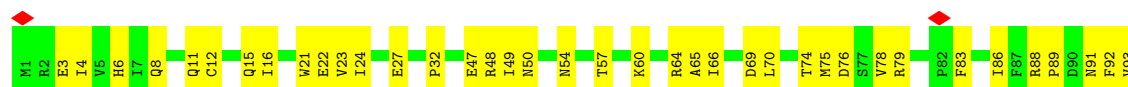
- Molecule 3: Tubulin beta chain

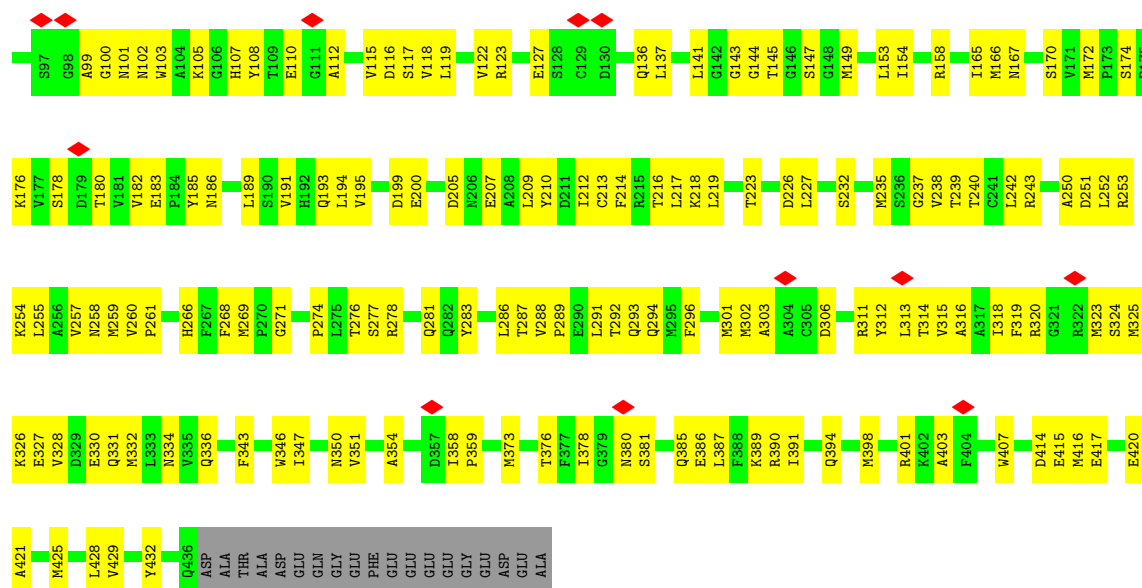
Chain IB:



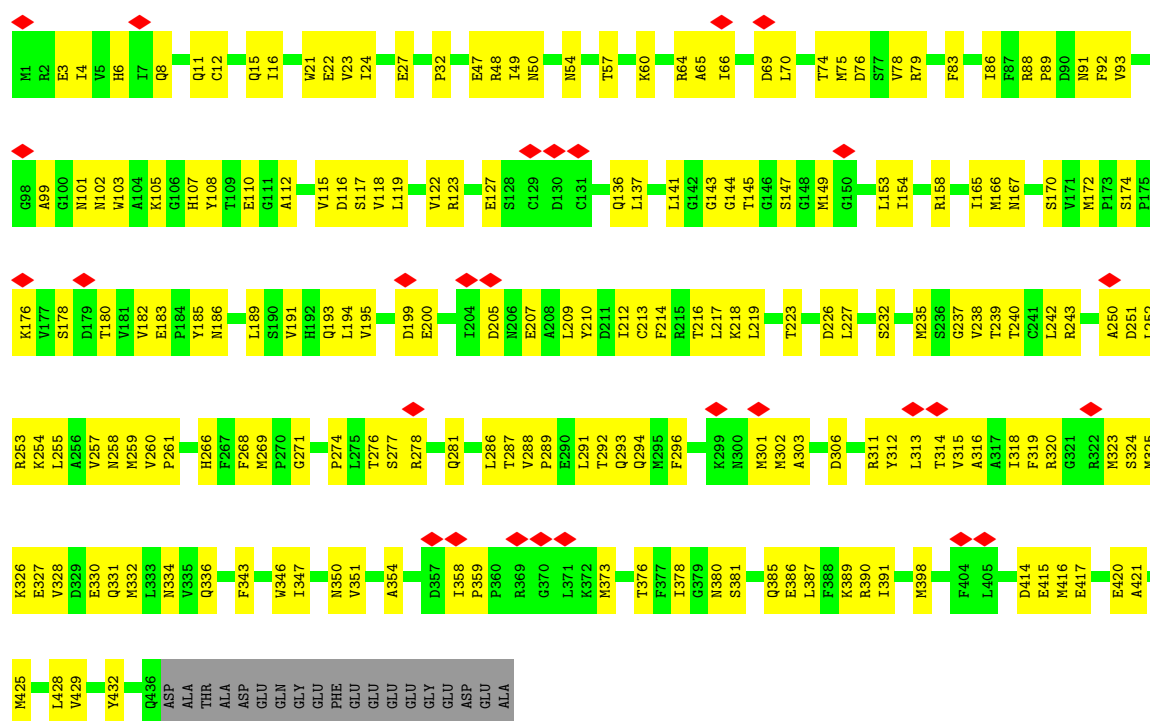
- Molecule 3: Tubulin beta chain

Chain ID:

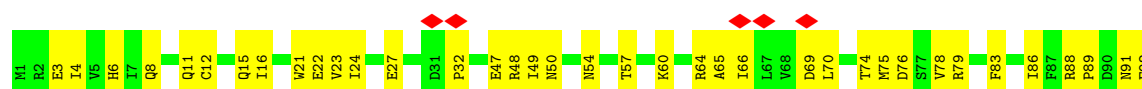




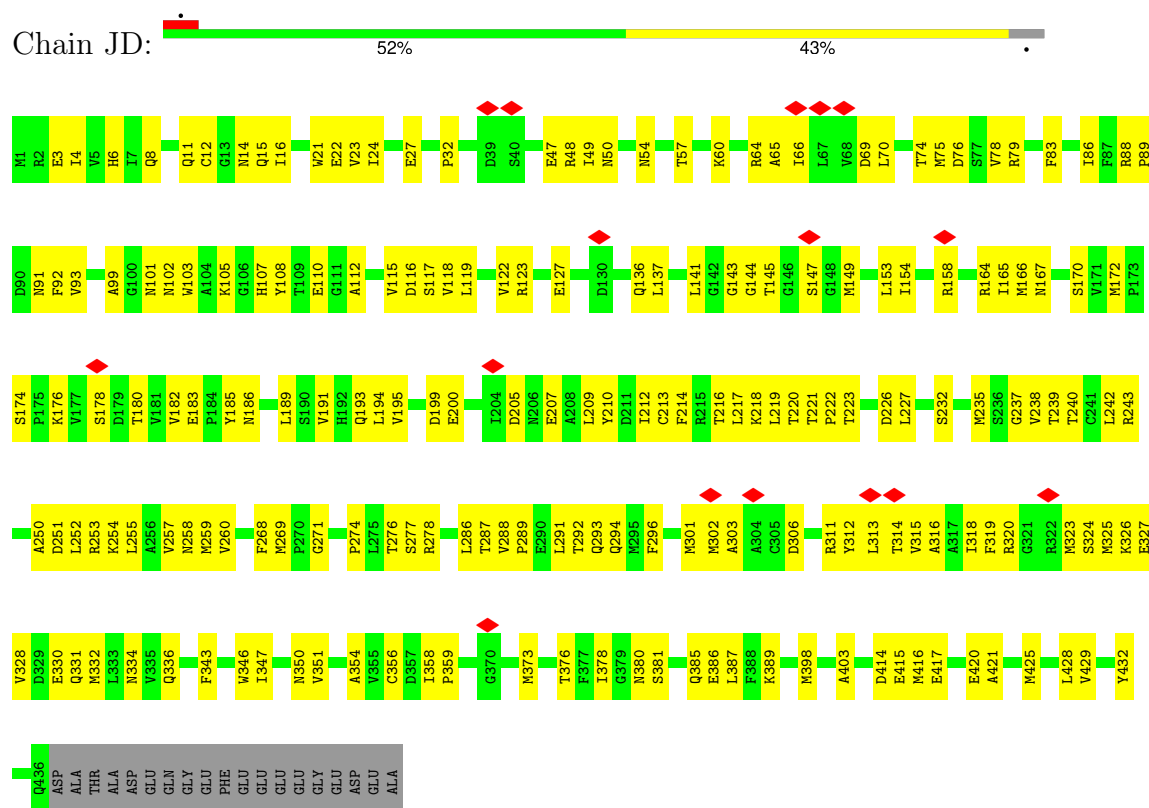
• Molecule 3: Tubulin beta chain



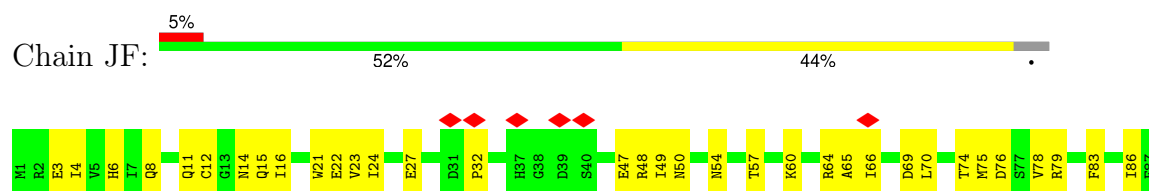
• Molecule 3: Tubulin beta chain

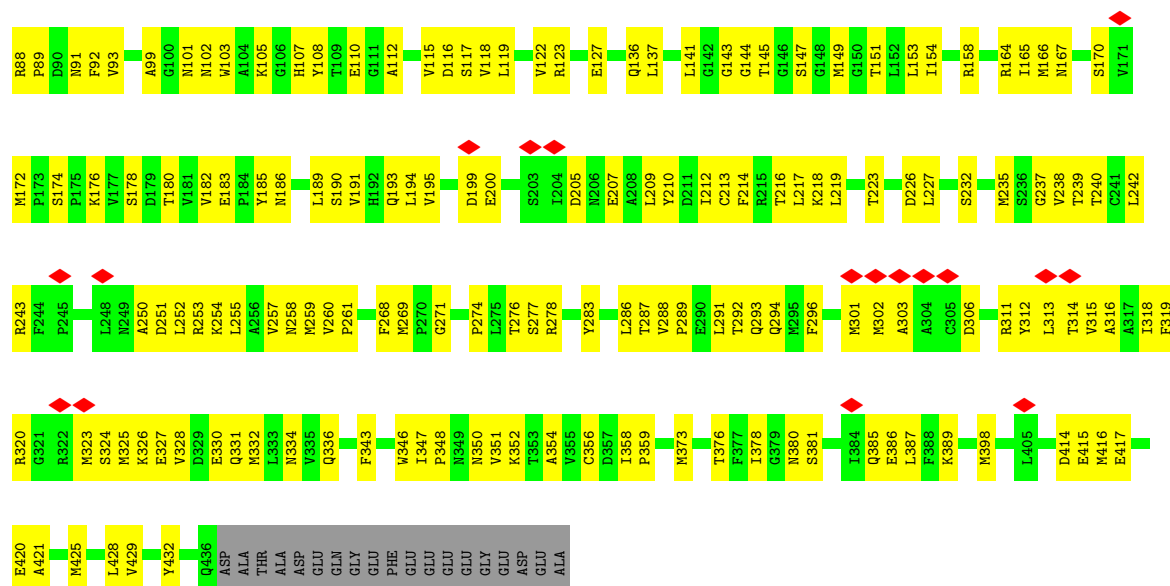


- Molecule 3: Tubulin beta chain

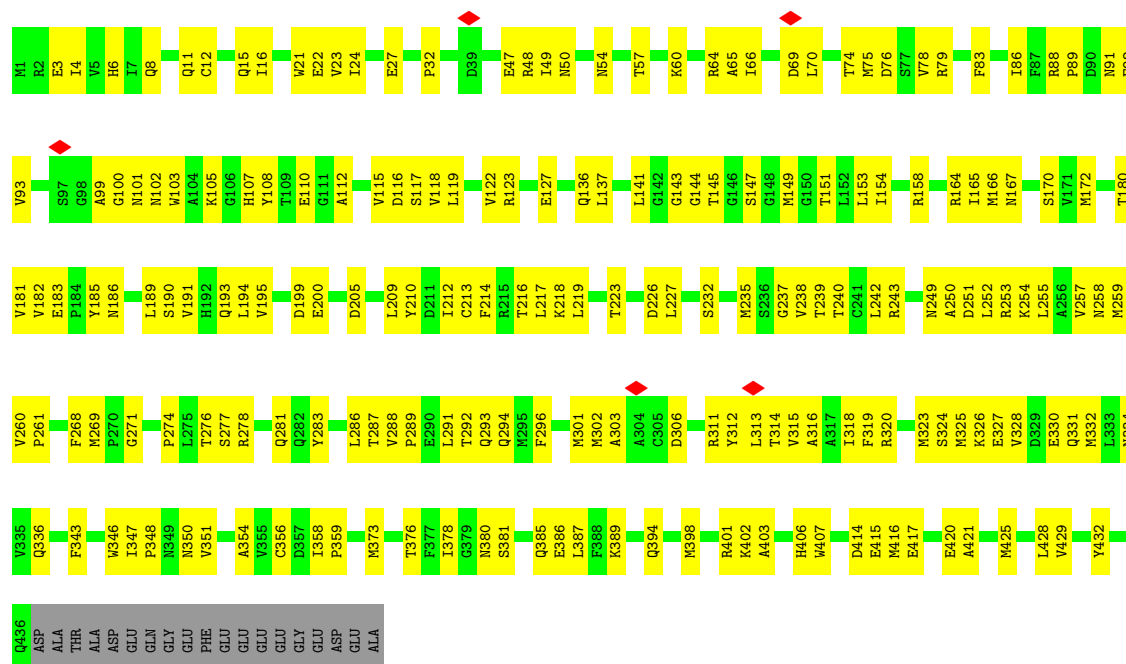


- Molecule 3: Tubulin beta chain

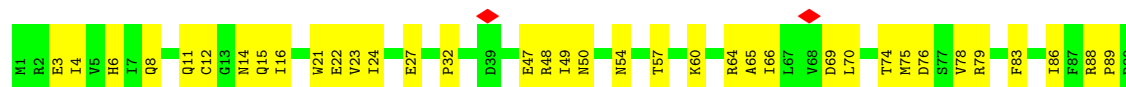


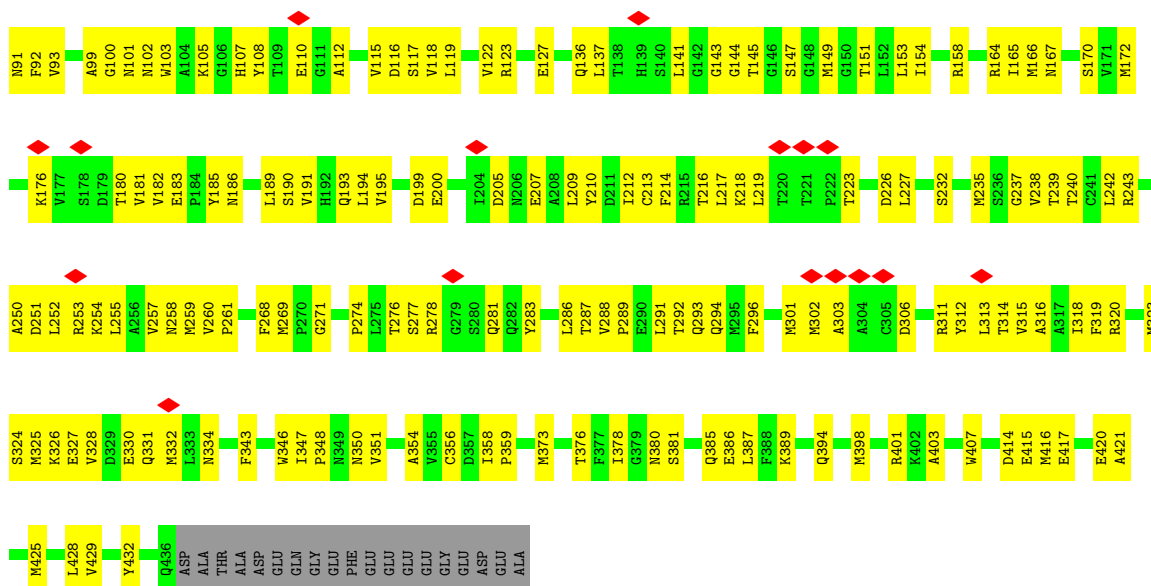


• Molecule 3: Tubulin beta chain

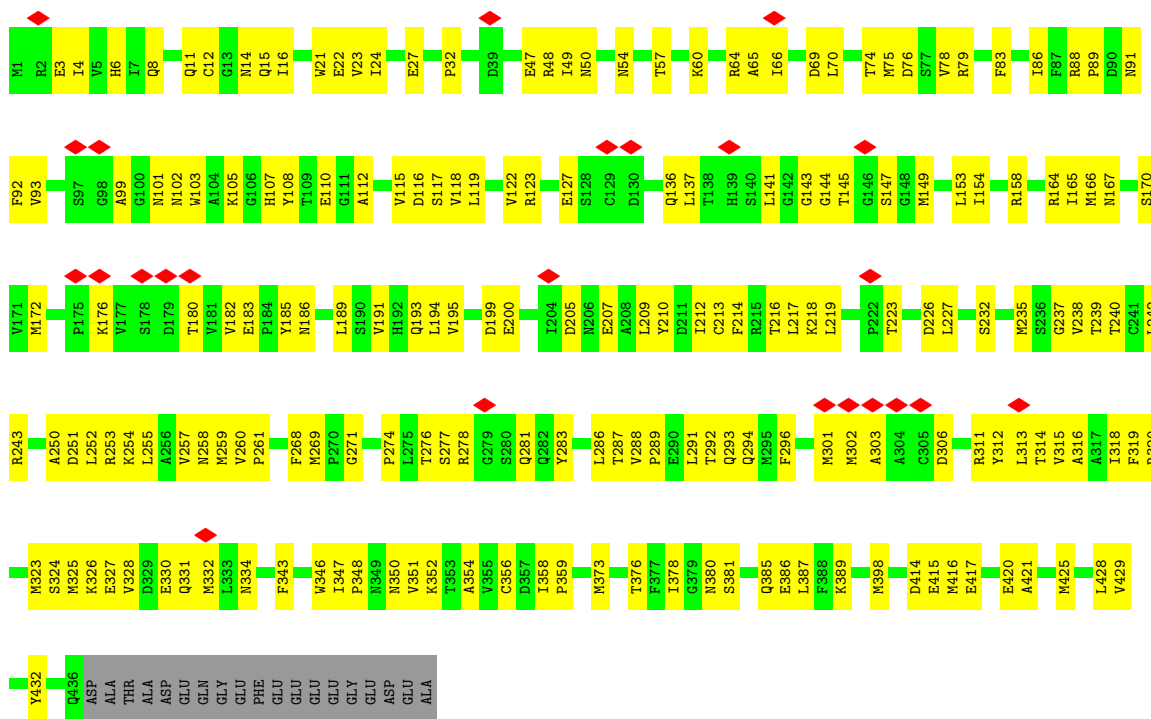


• Molecule 3: Tubulin beta chain

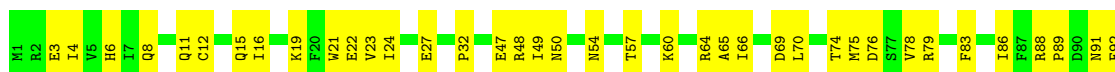


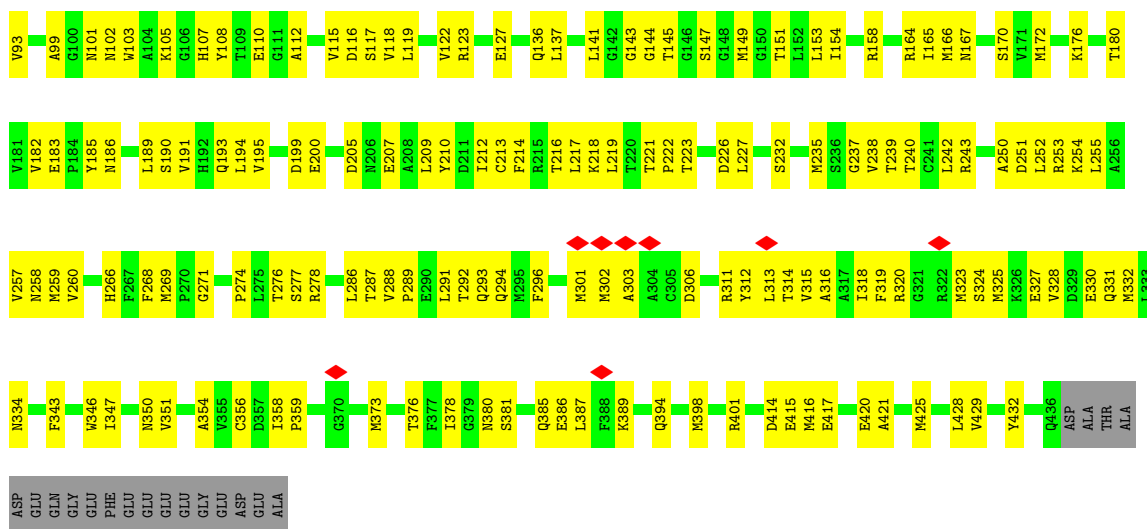


• Molecule 3: Tubulin beta chain



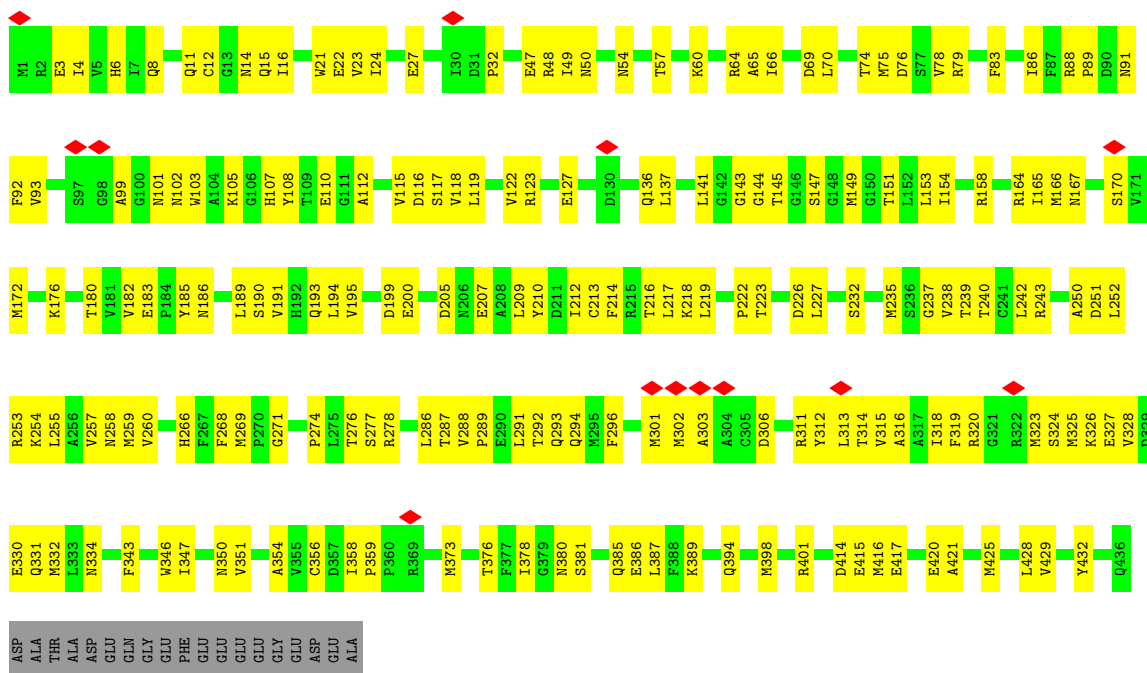
• Molecule 3: Tubulin beta chain





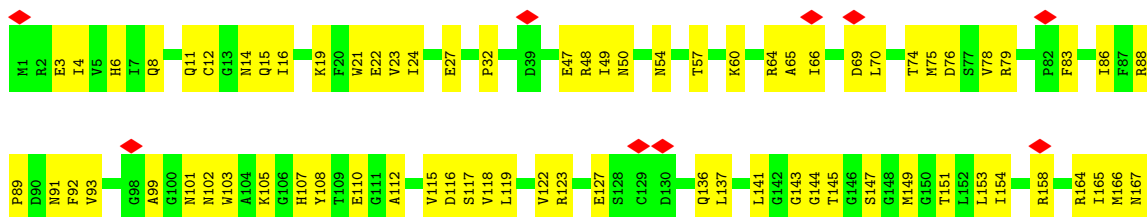
• Molecule 3: Tubulin beta chain

Chain LD: 53% 43%

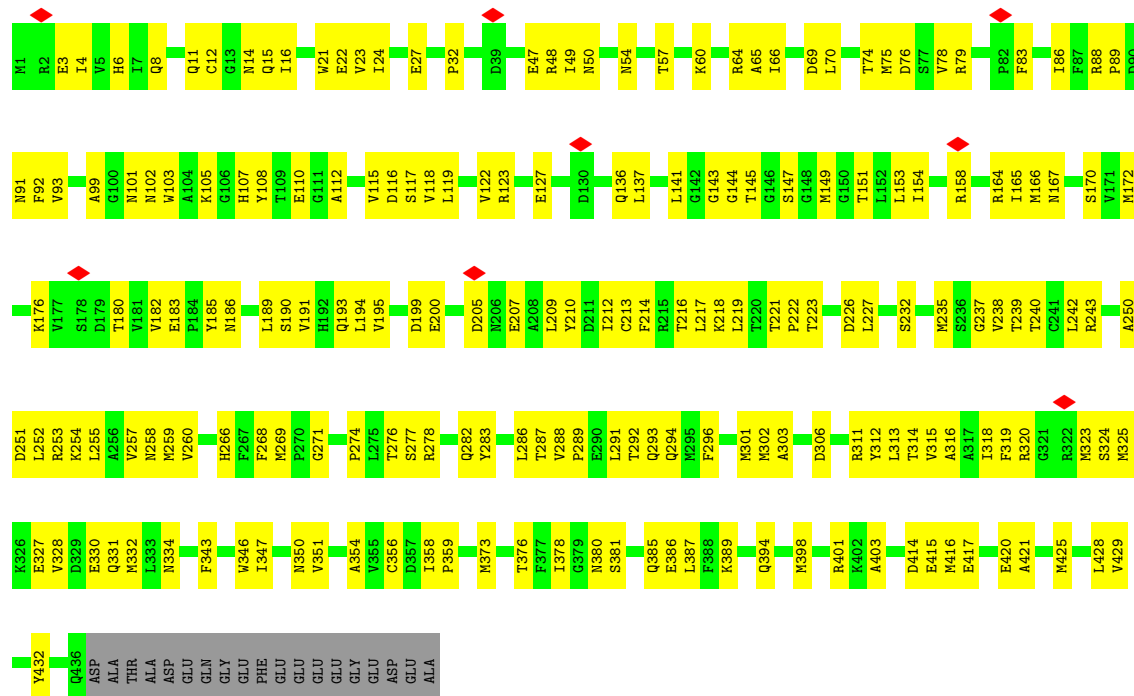


• Molecule 3: Tubulin beta chain

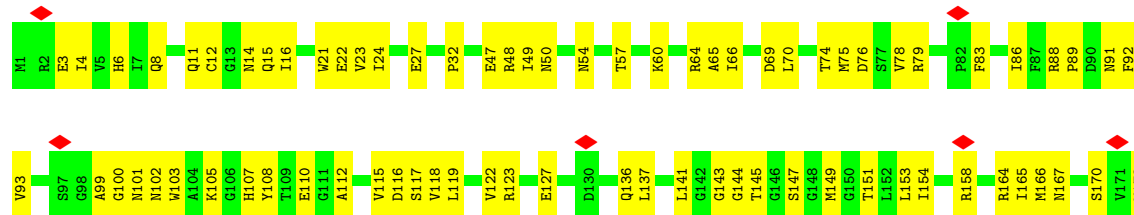
Chain LF: 5% 42%

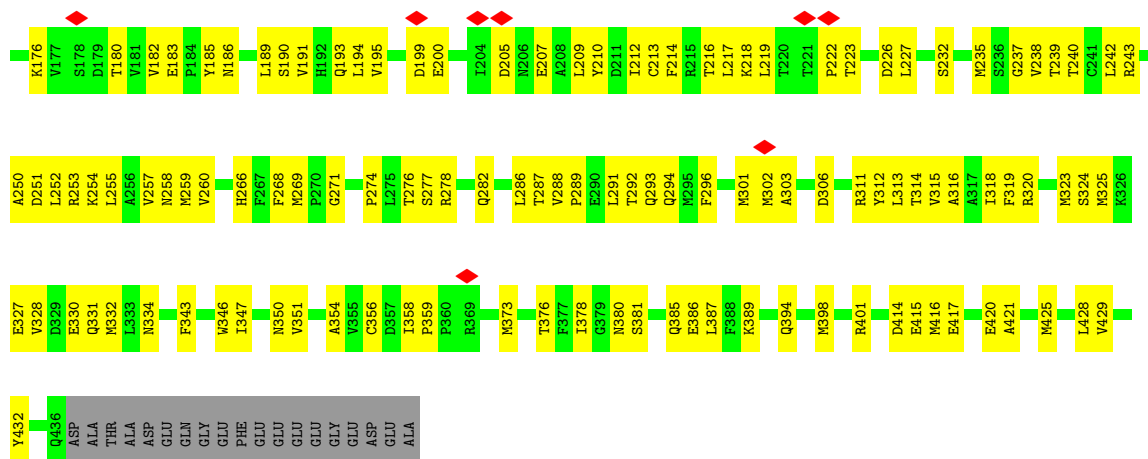


- Molecule 3: Tubulin beta chain

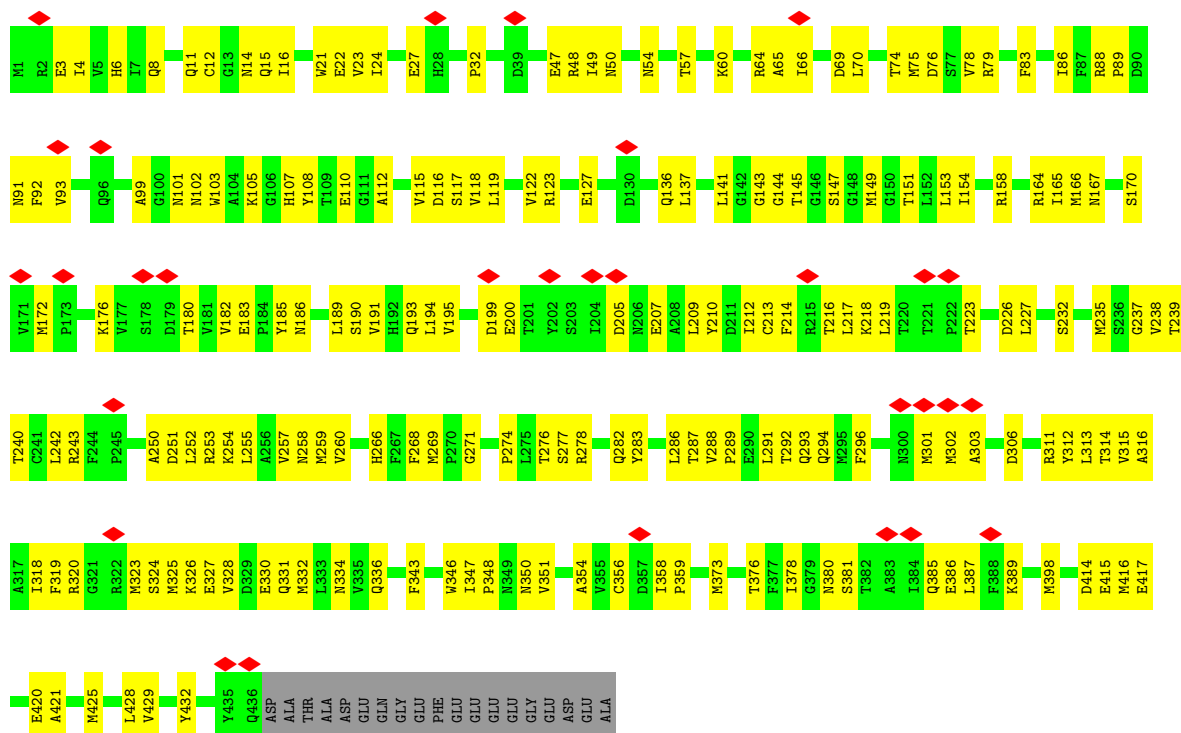


- Molecule 3: Tubulin beta chain

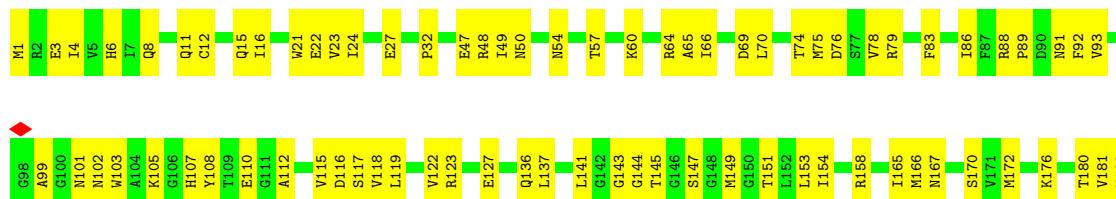


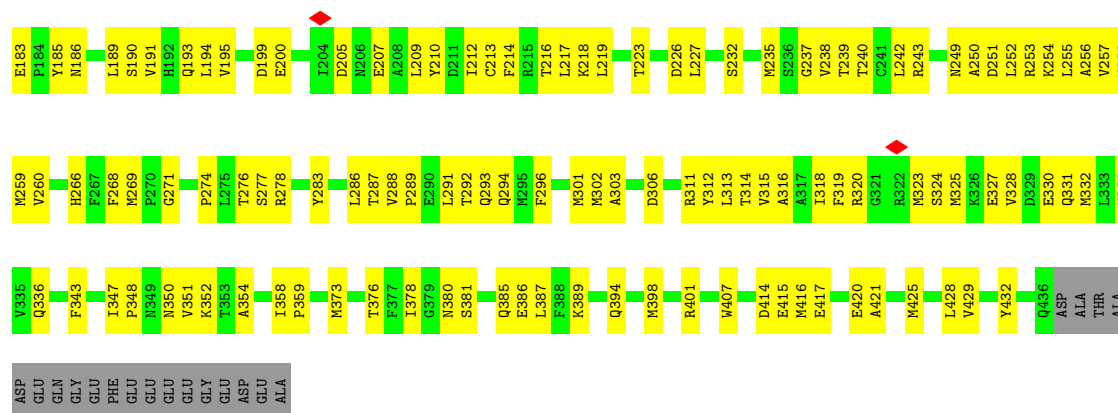


• Molecule 3: Tubulin beta chain

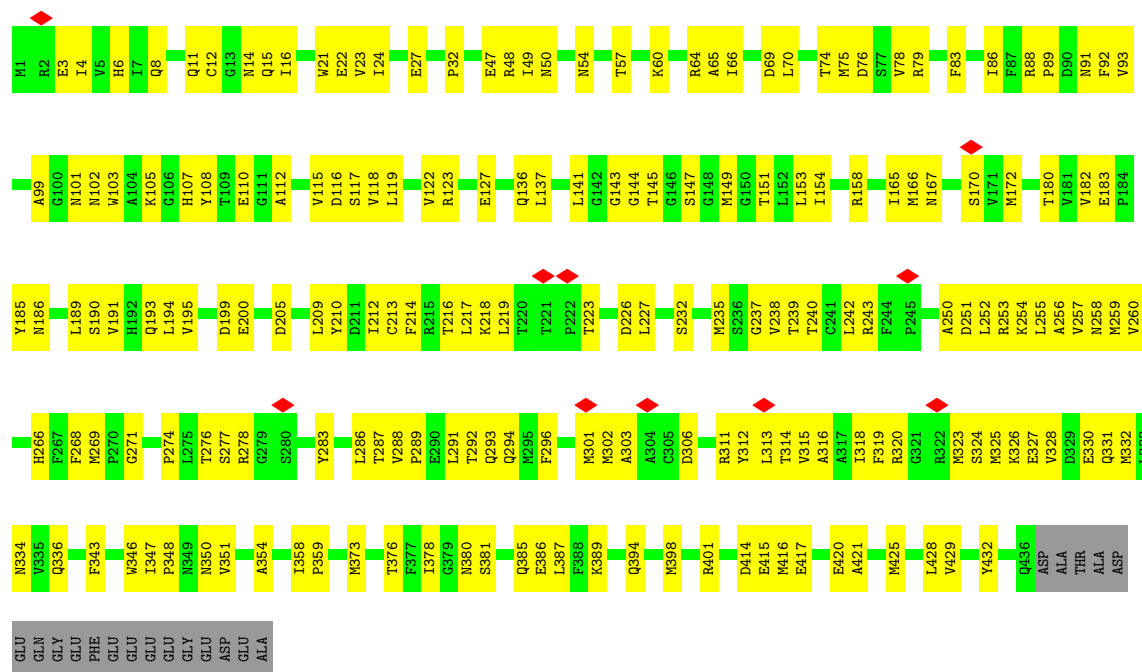


• Molecule 3: Tubulin beta chain

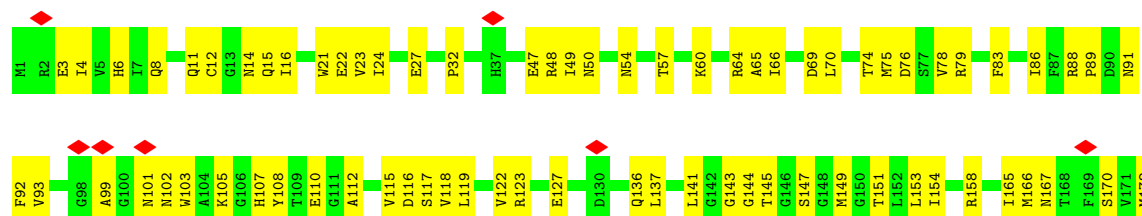


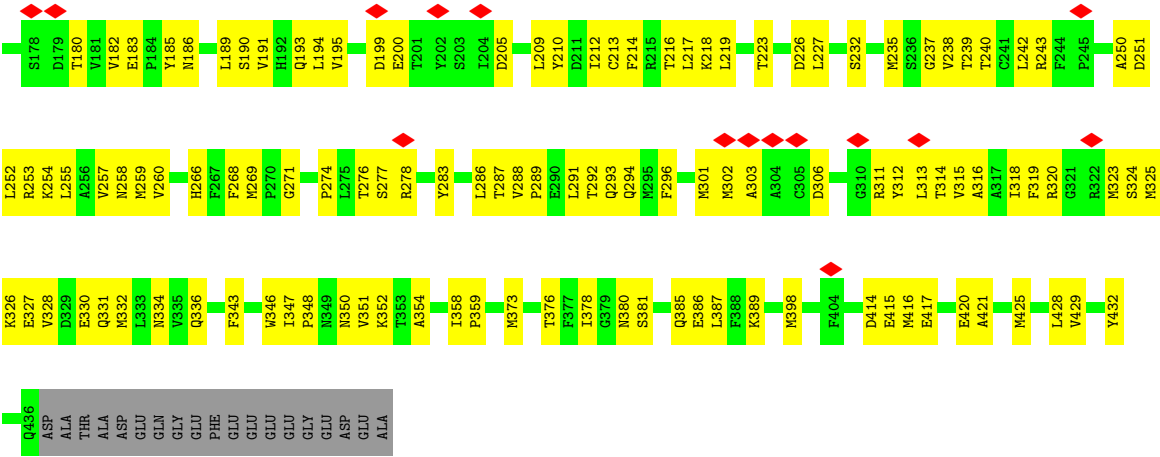


• Molecule 3: Tubulin beta chain



• Molecule 3: Tubulin beta chain





4 Experimental information

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, Not provided	
Number of subtomograms used	9625	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	164	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.363	Depositor
Minimum map value	-0.000	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.042	Depositor
Recommended contour level	0.0398	Depositor
Map size (\AA)	801.36, 801.36, 801.36	wwPDB
Map dimensions	378, 378, 378	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	2.12, 2.12, 2.12	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, GTP, GDP, TA1

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	1A	0.28	0/1012	0.66	1/1365 (0.1%)
1	1B	0.28	0/1012	0.66	1/1365 (0.1%)
1	1C	0.28	0/1012	0.66	1/1365 (0.1%)
1	1D	0.28	0/1012	0.66	1/1365 (0.1%)
1	1E	0.28	0/1012	0.66	1/1365 (0.1%)
2	AA	0.17	0/3449	0.48	0/4682
2	AC	0.17	0/3449	0.48	0/4682
2	AE	0.18	0/3449	0.48	0/4682
2	BA	0.18	0/3449	0.48	0/4682
2	BC	0.17	0/3449	0.48	0/4682
2	BE	0.18	0/3449	0.48	0/4682
2	CA	0.17	0/3449	0.48	0/4682
2	CC	0.18	0/3449	0.48	0/4682
2	CE	0.17	0/3449	0.48	0/4682
2	DA	0.18	0/3449	0.48	0/4682
2	DC	0.17	0/3449	0.48	0/4682
2	DE	0.18	0/3449	0.48	0/4682
2	EA	0.17	0/3449	0.48	0/4682
2	EC	0.17	0/3449	0.48	0/4682
2	EE	0.17	0/3449	0.48	0/4682
2	FA	0.17	0/3449	0.48	0/4682
2	FC	0.17	0/3449	0.48	0/4682
2	FE	0.18	0/3449	0.48	0/4682
2	GA	0.18	0/3449	0.48	0/4682
2	GC	0.17	0/3449	0.48	0/4682
2	GE	0.18	0/3449	0.48	0/4682
2	HA	0.17	0/3449	0.48	0/4682
2	HC	0.18	0/3449	0.48	0/4682
2	HE	0.17	0/3449	0.49	0/4682
2	IA	0.17	0/3449	0.48	0/4682
2	IC	0.17	0/3449	0.48	0/4682
2	IE	0.17	0/3449	0.48	0/4682

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	JA	0.17	0/3449	0.48	0/4682
2	JC	0.17	0/3449	0.48	0/4682
2	JE	0.18	0/3449	0.48	0/4682
2	KA	0.17	0/3449	0.48	0/4682
2	KC	0.17	0/3449	0.48	0/4682
2	KE	0.17	0/3449	0.48	0/4682
2	LA	0.17	0/3449	0.48	0/4682
2	LC	0.17	0/3449	0.49	0/4682
2	LE	0.17	0/3449	0.48	0/4682
2	MA	0.17	0/3449	0.48	0/4682
2	MC	0.17	0/3449	0.48	0/4682
2	ME	0.17	0/3449	0.49	0/4682
2	NA	0.17	0/3449	0.48	0/4682
2	NC	0.17	0/3449	0.49	0/4682
2	NE	0.17	0/3449	0.48	0/4682
3	AB	0.18	0/3429	0.49	2/4643 (0.0%)
3	AD	0.18	0/3429	0.49	2/4643 (0.0%)
3	AF	0.18	0/3429	0.49	2/4643 (0.0%)
3	BB	0.18	0/3429	0.49	2/4643 (0.0%)
3	BD	0.18	0/3429	0.49	2/4643 (0.0%)
3	BF	0.18	0/3429	0.49	2/4643 (0.0%)
3	CB	0.18	0/3429	0.49	2/4643 (0.0%)
3	CD	0.18	0/3429	0.49	2/4643 (0.0%)
3	CF	0.18	0/3429	0.49	2/4643 (0.0%)
3	DB	0.18	0/3429	0.49	2/4643 (0.0%)
3	DD	0.18	0/3429	0.49	2/4643 (0.0%)
3	DF	0.18	0/3429	0.49	2/4643 (0.0%)
3	EB	0.18	0/3429	0.49	2/4643 (0.0%)
3	ED	0.18	0/3429	0.49	2/4643 (0.0%)
3	EF	0.18	0/3429	0.49	2/4643 (0.0%)
3	FB	0.18	0/3429	0.49	2/4643 (0.0%)
3	FD	0.18	0/3429	0.49	2/4643 (0.0%)
3	FF	0.18	0/3429	0.49	2/4643 (0.0%)
3	GB	0.18	0/3429	0.49	2/4643 (0.0%)
3	GD	0.18	0/3429	0.49	2/4643 (0.0%)
3	GF	0.18	0/3429	0.49	2/4643 (0.0%)
3	HB	0.18	0/3429	0.49	2/4643 (0.0%)
3	HD	0.18	0/3429	0.49	2/4643 (0.0%)
3	HF	0.18	0/3429	0.49	2/4643 (0.0%)
3	IB	0.18	0/3429	0.49	2/4643 (0.0%)
3	ID	0.18	0/3429	0.49	2/4643 (0.0%)
3	IF	0.18	0/3429	0.49	2/4643 (0.0%)
3	JB	0.18	0/3429	0.49	2/4643 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	JD	0.18	0/3429	0.49	2/4643 (0.0%)
3	JF	0.18	0/3429	0.49	2/4643 (0.0%)
3	KB	0.18	0/3429	0.49	2/4643 (0.0%)
3	KD	0.18	0/3429	0.49	2/4643 (0.0%)
3	KF	0.18	0/3429	0.49	2/4643 (0.0%)
3	LB	0.18	0/3429	0.49	2/4643 (0.0%)
3	LD	0.18	0/3429	0.49	2/4643 (0.0%)
3	LF	0.18	0/3429	0.49	2/4643 (0.0%)
3	MB	0.18	0/3429	0.49	2/4643 (0.0%)
3	MD	0.18	0/3429	0.49	2/4643 (0.0%)
3	MF	0.18	0/3429	0.49	2/4643 (0.0%)
3	NB	0.18	0/3429	0.49	2/4643 (0.0%)
3	ND	0.18	0/3429	0.49	2/4643 (0.0%)
3	NF	0.18	0/3429	0.49	2/4643 (0.0%)
All	All	0.18	0/293936	0.49	89/398475 (0.0%)

There are no bond length outliers.

The worst 5 of 89 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	GB	287	THR	CA-C-N	5.78	123.88	120.24
3	GB	287	THR	C-N-CA	5.78	123.88	120.24
3	LD	287	THR	CA-C-N	5.73	123.85	120.24
3	LD	287	THR	C-N-CA	5.73	123.85	120.24
3	CF	287	THR	CA-C-N	5.72	123.84	120.24

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	1A	992	0	1022	70	0
1	1B	992	0	1022	70	0
1	1C	992	0	1022	74	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1D	992	0	1022	54	0
1	1E	992	0	1022	62	0
2	AA	3372	0	3286	139	0
2	AC	3372	0	3286	158	0
2	AE	3372	0	3286	175	0
2	BA	3372	0	3286	127	0
2	BC	3372	0	3286	139	0
2	BE	3372	0	3286	129	0
2	CA	3372	0	3286	128	0
2	CC	3372	0	3286	136	0
2	CE	3372	0	3286	134	0
2	DA	3372	0	3286	125	0
2	DC	3372	0	3286	125	0
2	DE	3372	0	3286	133	0
2	EA	3372	0	3286	123	0
2	EC	3372	0	3286	131	0
2	EE	3372	0	3286	138	0
2	FA	3372	0	3286	128	0
2	FC	3372	0	3286	141	0
2	FE	3372	0	3286	143	0
2	GA	3372	0	3286	124	0
2	GC	3372	0	3286	136	0
2	GE	3372	0	3286	147	0
2	HA	3372	0	3286	118	0
2	HC	3372	0	3286	131	0
2	HE	3372	0	3286	139	0
2	IA	3372	0	3286	127	0
2	IC	3372	0	3286	133	0
2	IE	3372	0	3286	164	0
2	JA	3372	0	3286	127	0
2	JC	3372	0	3286	144	0
2	JE	3372	0	3286	167	0
2	KA	3372	0	3286	145	0
2	KC	3372	0	3286	158	0
2	KE	3372	0	3286	154	0
2	LA	3372	0	3286	132	0
2	LC	3372	0	3286	138	0
2	LE	3372	0	3286	142	0
2	MA	3372	0	3286	139	0
2	MC	3372	0	3286	147	0
2	ME	3372	0	3286	156	0
2	NA	3372	0	3286	141	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	NC	3372	0	3286	153	0
2	NE	3372	0	3286	139	0
3	AB	3354	0	3236	167	0
3	AD	3354	0	3236	168	0
3	AF	3354	0	3236	162	0
3	BB	3354	0	3236	169	0
3	BD	3354	0	3236	179	0
3	BF	3354	0	3236	157	0
3	CB	3354	0	3236	165	0
3	CD	3354	0	3236	163	0
3	CF	3354	0	3236	151	0
3	DB	3354	0	3236	163	0
3	DD	3354	0	3236	161	0
3	DF	3354	0	3236	161	0
3	EB	3354	0	3236	170	0
3	ED	3354	0	3236	157	0
3	EF	3354	0	3236	180	0
3	FB	3354	0	3236	177	0
3	FD	3354	0	3236	170	0
3	FF	3354	0	3236	180	0
3	GB	3354	0	3236	169	0
3	GD	3354	0	3236	166	0
3	GF	3354	0	3236	170	0
3	HB	3354	0	3236	159	0
3	HD	3354	0	3236	167	0
3	HF	3354	0	3236	162	0
3	IB	3354	0	3236	166	0
3	ID	3354	0	3236	177	0
3	IF	3354	0	3236	174	0
3	JB	3354	0	3236	167	0
3	JD	3354	0	3236	175	0
3	JF	3354	0	3236	186	0
3	KB	3354	0	3236	206	0
3	KD	3354	0	3236	186	0
3	KF	3354	0	3236	172	0
3	LB	3354	0	3236	169	0
3	LD	3354	0	3236	170	0
3	LF	3354	0	3236	177	0
3	MB	3354	0	3236	187	0
3	MD	3354	0	3236	167	0
3	MF	3354	0	3236	196	0
3	NB	3354	0	3236	216	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	ND	3354	0	3236	169	0
3	NF	3354	0	3236	172	0
4	AA	32	0	12	4	0
4	AC	32	0	12	7	0
4	AE	32	0	12	5	0
4	BA	32	0	12	5	0
4	BC	32	0	12	5	0
4	BE	32	0	12	5	0
4	CA	32	0	12	4	0
4	CC	32	0	12	4	0
4	CE	32	0	12	4	0
4	DA	32	0	12	8	0
4	DC	32	0	12	6	0
4	DE	32	0	12	7	0
4	EA	32	0	12	6	0
4	EC	32	0	12	6	0
4	EE	32	0	12	8	0
4	FA	32	0	12	7	0
4	FC	32	0	12	6	0
4	FE	32	0	12	6	0
4	GA	32	0	12	6	0
4	GC	32	0	12	7	0
4	GE	32	0	12	4	0
4	HA	32	0	12	5	0
4	HC	32	0	12	5	0
4	HE	32	0	12	5	0
4	IA	32	0	12	5	0
4	IC	32	0	12	6	0
4	IE	32	0	12	6	0
4	JA	32	0	12	6	0
4	JC	32	0	12	8	0
4	JE	32	0	12	9	0
4	KA	32	0	12	8	0
4	KC	32	0	12	9	0
4	KE	32	0	12	8	0
4	LA	32	0	12	6	0
4	LC	32	0	12	7	0
4	LE	32	0	12	6	0
4	MA	32	0	12	5	0
4	MC	32	0	12	6	0
4	ME	32	0	12	7	0
4	NA	32	0	12	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	NC	32	0	12	7	0
4	NE	32	0	12	7	0
5	AA	1	0	0	0	0
5	AC	1	0	0	0	0
5	AE	1	0	0	0	0
5	BA	1	0	0	0	0
5	BC	1	0	0	0	0
5	BE	1	0	0	0	0
5	CA	1	0	0	0	0
5	CC	1	0	0	0	0
5	CE	1	0	0	0	0
5	DA	1	0	0	0	0
5	DC	1	0	0	0	0
5	DE	1	0	0	0	0
5	EA	1	0	0	0	0
5	EC	1	0	0	0	0
5	EE	1	0	0	0	0
5	FA	1	0	0	0	0
5	FC	1	0	0	0	0
5	FE	1	0	0	0	0
5	GA	1	0	0	0	0
5	GC	1	0	0	0	0
5	GE	1	0	0	0	0
5	HA	1	0	0	0	0
5	HC	1	0	0	0	0
5	HE	1	0	0	0	0
5	IA	1	0	0	0	0
5	IC	1	0	0	0	0
5	IE	1	0	0	0	0
5	JA	1	0	0	0	0
5	JC	1	0	0	0	0
5	JE	1	0	0	0	0
5	KA	1	0	0	0	0
5	KC	1	0	0	0	0
5	KE	1	0	0	0	0
5	LA	1	0	0	0	0
5	LC	1	0	0	0	0
5	LE	1	0	0	0	0
5	MA	1	0	0	0	0
5	MC	1	0	0	0	0
5	ME	1	0	0	0	0
5	NA	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	NC	1	0	0	0	0
5	NE	1	0	0	0	0
6	AB	28	0	12	5	0
6	AD	28	0	12	5	0
6	AF	28	0	12	5	0
6	BB	28	0	12	5	0
6	BD	28	0	12	5	0
6	BF	28	0	12	5	0
6	CB	28	0	12	5	0
6	CD	28	0	12	5	0
6	CF	28	0	12	5	0
6	DB	28	0	12	5	0
6	DD	28	0	12	5	0
6	DF	28	0	12	5	0
6	EB	28	0	12	5	0
6	ED	28	0	12	5	0
6	EF	28	0	12	5	0
6	FB	28	0	12	5	0
6	FD	28	0	12	5	0
6	FF	28	0	12	5	0
6	GB	28	0	12	5	0
6	GD	28	0	12	5	0
6	GF	28	0	12	5	0
6	HB	28	0	12	5	0
6	HD	28	0	12	5	0
6	HF	28	0	12	5	0
6	IB	28	0	12	5	0
6	ID	28	0	12	5	0
6	IF	28	0	12	5	0
6	JB	28	0	12	5	0
6	JD	28	0	12	5	0
6	JF	28	0	12	5	0
6	KB	28	0	12	5	0
6	KD	28	0	12	5	0
6	KF	28	0	12	6	0
6	LB	28	0	12	5	0
6	LD	28	0	12	5	0
6	LF	28	0	12	5	0
6	MB	28	0	12	5	0
6	MD	28	0	12	5	0
6	MF	28	0	12	5	0
6	NB	28	0	12	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	ND	28	0	12	5	0
6	NF	28	0	12	5	0
7	AB	62	0	51	6	0
7	AD	62	0	51	6	0
7	AF	62	0	51	6	0
7	BB	62	0	51	6	0
7	BD	62	0	51	7	0
7	BF	62	0	51	6	0
7	CB	62	0	51	6	0
7	CD	62	0	51	6	0
7	CF	62	0	51	6	0
7	DB	62	0	51	6	0
7	DD	62	0	51	6	0
7	DF	62	0	51	6	0
7	EB	62	0	51	7	0
7	ED	62	0	51	6	0
7	EF	62	0	51	8	0
7	FB	62	0	51	7	0
7	FD	62	0	51	7	0
7	FF	62	0	51	7	0
7	GB	62	0	51	7	0
7	GD	62	0	51	7	0
7	GF	62	0	51	7	0
7	HB	62	0	51	7	0
7	HD	62	0	51	7	0
7	HF	62	0	51	7	0
7	IB	62	0	51	7	0
7	ID	62	0	51	8	0
7	IF	62	0	51	7	0
7	JB	62	0	51	7	0
7	JD	62	0	51	7	0
7	JF	62	0	51	7	0
7	KB	62	0	51	7	0
7	KD	62	0	51	7	0
7	KF	62	0	51	7	0
7	LB	62	0	51	7	0
7	LD	62	0	51	6	0
7	LF	62	0	51	6	0
7	MB	62	0	51	7	0
7	MD	62	0	51	6	0
7	MF	62	0	51	6	0
7	NB	62	0	51	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	ND	62	0	51	6	0
7	NF	62	0	51	6	0
All	All	292618	0	282184	12387	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 22.

The worst 5 of 12387 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:AE:283:HIS:O	3:NB:88:ARG:NH2	1.69	1.25
3:JD:221:THR:HA	2:JE:326:LYS:HZ3	1.01	1.14
2:IE:221:ARG:NH2	3:IF:327:GLU:OE2	1.82	1.13
3:JD:221:THR:HA	2:JE:326:LYS:NZ	1.61	1.12
2:ME:224:TYR:CE1	3:MF:325:MET:HG3	1.84	1.12

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	1A	118/393 (30%)	113 (96%)	5 (4%)	0	100	100
1	1B	118/393 (30%)	113 (96%)	5 (4%)	0	100	100
1	1C	118/393 (30%)	113 (96%)	5 (4%)	0	100	100
1	1D	118/393 (30%)	113 (96%)	5 (4%)	0	100	100
1	1E	118/393 (30%)	113 (96%)	5 (4%)	0	100	100
2	AA	426/451 (94%)	412 (97%)	14 (3%)	0	100	100
2	AC	426/451 (94%)	412 (97%)	14 (3%)	0	100	100
2	AE	426/451 (94%)	412 (97%)	14 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	BA	426/451 (94%)	412 (97%)	14 (3%)	0	100	100
2	BC	426/451 (94%)	412 (97%)	14 (3%)	0	100	100
2	BE	426/451 (94%)	412 (97%)	14 (3%)	0	100	100
2	CA	426/451 (94%)	412 (97%)	14 (3%)	0	100	100
2	CC	426/451 (94%)	412 (97%)	14 (3%)	0	100	100
2	CE	426/451 (94%)	412 (97%)	14 (3%)	0	100	100
2	DA	426/451 (94%)	412 (97%)	14 (3%)	0	100	100
2	DC	426/451 (94%)	412 (97%)	14 (3%)	0	100	100
2	DE	426/451 (94%)	412 (97%)	14 (3%)	0	100	100
2	EA	426/451 (94%)	412 (97%)	14 (3%)	0	100	100
2	EC	426/451 (94%)	412 (97%)	14 (3%)	0	100	100
2	EE	426/451 (94%)	412 (97%)	14 (3%)	0	100	100
2	FA	426/451 (94%)	412 (97%)	14 (3%)	0	100	100
2	FC	426/451 (94%)	412 (97%)	14 (3%)	0	100	100
2	FE	426/451 (94%)	412 (97%)	14 (3%)	0	100	100
2	GA	426/451 (94%)	412 (97%)	14 (3%)	0	100	100
2	GC	426/451 (94%)	412 (97%)	14 (3%)	0	100	100
2	GE	426/451 (94%)	412 (97%)	14 (3%)	0	100	100
2	HA	426/451 (94%)	412 (97%)	14 (3%)	0	100	100
2	HC	426/451 (94%)	412 (97%)	14 (3%)	0	100	100
2	HE	426/451 (94%)	412 (97%)	14 (3%)	0	100	100
2	IA	426/451 (94%)	412 (97%)	14 (3%)	0	100	100
2	IC	426/451 (94%)	412 (97%)	14 (3%)	0	100	100
2	IE	426/451 (94%)	412 (97%)	14 (3%)	0	100	100
2	JA	426/451 (94%)	412 (97%)	14 (3%)	0	100	100
2	JC	426/451 (94%)	412 (97%)	14 (3%)	0	100	100
2	JE	426/451 (94%)	412 (97%)	14 (3%)	0	100	100
2	KA	426/451 (94%)	412 (97%)	14 (3%)	0	100	100
2	KC	426/451 (94%)	412 (97%)	14 (3%)	0	100	100
2	KE	426/451 (94%)	412 (97%)	14 (3%)	0	100	100
2	LA	426/451 (94%)	412 (97%)	14 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	LC	426/451 (94%)	412 (97%)	14 (3%)	0	100	100
2	LE	426/451 (94%)	412 (97%)	14 (3%)	0	100	100
2	MA	426/451 (94%)	412 (97%)	14 (3%)	0	100	100
2	MC	426/451 (94%)	412 (97%)	14 (3%)	0	100	100
2	ME	426/451 (94%)	412 (97%)	14 (3%)	0	100	100
2	NA	426/451 (94%)	412 (97%)	14 (3%)	0	100	100
2	NC	426/451 (94%)	412 (97%)	14 (3%)	0	100	100
2	NE	426/451 (94%)	412 (97%)	14 (3%)	0	100	100
3	AB	424/445 (95%)	409 (96%)	15 (4%)	0	100	100
3	AD	424/445 (95%)	409 (96%)	15 (4%)	0	100	100
3	AF	424/445 (95%)	409 (96%)	15 (4%)	0	100	100
3	BB	424/445 (95%)	409 (96%)	15 (4%)	0	100	100
3	BD	424/445 (95%)	409 (96%)	15 (4%)	0	100	100
3	BF	424/445 (95%)	409 (96%)	15 (4%)	0	100	100
3	CB	424/445 (95%)	409 (96%)	15 (4%)	0	100	100
3	CD	424/445 (95%)	409 (96%)	15 (4%)	0	100	100
3	CF	424/445 (95%)	409 (96%)	15 (4%)	0	100	100
3	DB	424/445 (95%)	409 (96%)	15 (4%)	0	100	100
3	DD	424/445 (95%)	409 (96%)	15 (4%)	0	100	100
3	DF	424/445 (95%)	409 (96%)	15 (4%)	0	100	100
3	EB	424/445 (95%)	409 (96%)	15 (4%)	0	100	100
3	ED	424/445 (95%)	409 (96%)	15 (4%)	0	100	100
3	EF	424/445 (95%)	409 (96%)	15 (4%)	0	100	100
3	FB	424/445 (95%)	409 (96%)	15 (4%)	0	100	100
3	FD	424/445 (95%)	409 (96%)	15 (4%)	0	100	100
3	FF	424/445 (95%)	409 (96%)	15 (4%)	0	100	100
3	GB	424/445 (95%)	409 (96%)	15 (4%)	0	100	100
3	GD	424/445 (95%)	409 (96%)	15 (4%)	0	100	100
3	GF	424/445 (95%)	409 (96%)	15 (4%)	0	100	100
3	HB	424/445 (95%)	409 (96%)	15 (4%)	0	100	100
3	HD	424/445 (95%)	409 (96%)	15 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	HF	424/445 (95%)	409 (96%)	15 (4%)	0	100	100
3	IB	424/445 (95%)	409 (96%)	15 (4%)	0	100	100
3	ID	424/445 (95%)	409 (96%)	15 (4%)	0	100	100
3	IF	424/445 (95%)	409 (96%)	15 (4%)	0	100	100
3	JB	424/445 (95%)	409 (96%)	15 (4%)	0	100	100
3	JD	424/445 (95%)	409 (96%)	15 (4%)	0	100	100
3	JF	424/445 (95%)	409 (96%)	15 (4%)	0	100	100
3	KB	424/445 (95%)	409 (96%)	15 (4%)	0	100	100
3	KD	424/445 (95%)	409 (96%)	15 (4%)	0	100	100
3	KF	424/445 (95%)	409 (96%)	15 (4%)	0	100	100
3	LB	424/445 (95%)	409 (96%)	15 (4%)	0	100	100
3	LD	424/445 (95%)	409 (96%)	15 (4%)	0	100	100
3	LF	424/445 (95%)	409 (96%)	15 (4%)	0	100	100
3	MB	424/445 (95%)	409 (96%)	15 (4%)	0	100	100
3	MD	424/445 (95%)	409 (96%)	15 (4%)	0	100	100
3	MF	424/445 (95%)	409 (96%)	15 (4%)	0	100	100
3	NB	424/445 (95%)	409 (96%)	15 (4%)	0	100	100
3	ND	424/445 (95%)	409 (96%)	15 (4%)	0	100	100
3	NF	424/445 (95%)	409 (96%)	15 (4%)	0	100	100
All	All	36290/39597 (92%)	35047 (97%)	1243 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	1A	111/343 (32%)	111 (100%)	0	100	100
1	1B	111/343 (32%)	111 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1C	111/343 (32%)	111 (100%)	0	100	100
1	1D	111/343 (32%)	111 (100%)	0	100	100
1	1E	111/343 (32%)	111 (100%)	0	100	100
2	AA	364/379 (96%)	364 (100%)	0	100	100
2	AC	364/379 (96%)	364 (100%)	0	100	100
2	AE	364/379 (96%)	364 (100%)	0	100	100
2	BA	364/379 (96%)	364 (100%)	0	100	100
2	BC	364/379 (96%)	364 (100%)	0	100	100
2	BE	364/379 (96%)	364 (100%)	0	100	100
2	CA	364/379 (96%)	364 (100%)	0	100	100
2	CC	364/379 (96%)	364 (100%)	0	100	100
2	CE	364/379 (96%)	364 (100%)	0	100	100
2	DA	364/379 (96%)	364 (100%)	0	100	100
2	DC	364/379 (96%)	364 (100%)	0	100	100
2	DE	364/379 (96%)	364 (100%)	0	100	100
2	EA	364/379 (96%)	364 (100%)	0	100	100
2	EC	364/379 (96%)	364 (100%)	0	100	100
2	EE	364/379 (96%)	364 (100%)	0	100	100
2	FA	364/379 (96%)	364 (100%)	0	100	100
2	FC	364/379 (96%)	364 (100%)	0	100	100
2	FE	364/379 (96%)	364 (100%)	0	100	100
2	GA	364/379 (96%)	364 (100%)	0	100	100
2	GC	364/379 (96%)	364 (100%)	0	100	100
2	GE	364/379 (96%)	364 (100%)	0	100	100
2	HA	364/379 (96%)	364 (100%)	0	100	100
2	HC	364/379 (96%)	364 (100%)	0	100	100
2	HE	364/379 (96%)	364 (100%)	0	100	100
2	IA	364/379 (96%)	364 (100%)	0	100	100
2	IC	364/379 (96%)	364 (100%)	0	100	100
2	IE	364/379 (96%)	364 (100%)	0	100	100
2	JA	364/379 (96%)	364 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	JC	364/379 (96%)	364 (100%)	0	100	100
2	JE	364/379 (96%)	364 (100%)	0	100	100
2	KA	364/379 (96%)	364 (100%)	0	100	100
2	KC	364/379 (96%)	364 (100%)	0	100	100
2	KE	364/379 (96%)	364 (100%)	0	100	100
2	LA	364/379 (96%)	364 (100%)	0	100	100
2	LC	364/379 (96%)	364 (100%)	0	100	100
2	LE	364/379 (96%)	364 (100%)	0	100	100
2	MA	364/379 (96%)	364 (100%)	0	100	100
2	MC	364/379 (96%)	364 (100%)	0	100	100
2	ME	364/379 (96%)	364 (100%)	0	100	100
2	NA	364/379 (96%)	364 (100%)	0	100	100
2	NC	364/379 (96%)	364 (100%)	0	100	100
2	NE	364/379 (96%)	364 (100%)	0	100	100
3	AB	368/383 (96%)	368 (100%)	0	100	100
3	AD	368/383 (96%)	368 (100%)	0	100	100
3	AF	368/383 (96%)	368 (100%)	0	100	100
3	BB	368/383 (96%)	368 (100%)	0	100	100
3	BD	368/383 (96%)	368 (100%)	0	100	100
3	BF	368/383 (96%)	368 (100%)	0	100	100
3	CB	368/383 (96%)	368 (100%)	0	100	100
3	CD	368/383 (96%)	368 (100%)	0	100	100
3	CF	368/383 (96%)	368 (100%)	0	100	100
3	DB	368/383 (96%)	368 (100%)	0	100	100
3	DD	368/383 (96%)	368 (100%)	0	100	100
3	DF	368/383 (96%)	368 (100%)	0	100	100
3	EB	368/383 (96%)	368 (100%)	0	100	100
3	ED	368/383 (96%)	368 (100%)	0	100	100
3	EF	368/383 (96%)	368 (100%)	0	100	100
3	FB	368/383 (96%)	368 (100%)	0	100	100
3	FD	368/383 (96%)	368 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	FF	368/383 (96%)	368 (100%)	0	100	100
3	GB	368/383 (96%)	368 (100%)	0	100	100
3	GD	368/383 (96%)	368 (100%)	0	100	100
3	GF	368/383 (96%)	368 (100%)	0	100	100
3	HB	368/383 (96%)	368 (100%)	0	100	100
3	HD	368/383 (96%)	368 (100%)	0	100	100
3	HF	368/383 (96%)	368 (100%)	0	100	100
3	IB	368/383 (96%)	368 (100%)	0	100	100
3	ID	368/383 (96%)	368 (100%)	0	100	100
3	IF	368/383 (96%)	368 (100%)	0	100	100
3	JB	368/383 (96%)	368 (100%)	0	100	100
3	JD	368/383 (96%)	368 (100%)	0	100	100
3	JF	368/383 (96%)	368 (100%)	0	100	100
3	KB	368/383 (96%)	368 (100%)	0	100	100
3	KD	368/383 (96%)	368 (100%)	0	100	100
3	KF	368/383 (96%)	368 (100%)	0	100	100
3	LB	368/383 (96%)	368 (100%)	0	100	100
3	LD	368/383 (96%)	368 (100%)	0	100	100
3	LF	368/383 (96%)	368 (100%)	0	100	100
3	MB	368/383 (96%)	368 (100%)	0	100	100
3	MD	368/383 (96%)	368 (100%)	0	100	100
3	MF	368/383 (96%)	368 (100%)	0	100	100
3	NB	368/383 (96%)	368 (100%)	0	100	100
3	ND	368/383 (96%)	368 (100%)	0	100	100
3	NF	368/383 (96%)	368 (100%)	0	100	100
All	All	31299/33719 (93%)	31299 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 375 such sidechains are listed below:

Mol	Chain	Res	Type
2	IE	258	ASN

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Mol	Chain	Res	Type
3	KD	331	GLN
3	IF	331	GLN
2	JE	329	ASN
3	LB	107	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 168 ligands modelled in this entry, 42 are monoatomic - leaving 126 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	$\# Z > 2$
7	TA1	JB	502	-	68,68,68	0.68	1 (1%)	105,105,105	1.73	19 (18%)
6	GDP	EF	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.06	2 (6%)
6	GDP	MF	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.06	2 (6%)
4	GTP	FA	501	5	29,34,34	1.28	4 (13%)	35,54,54	1.25	4 (11%)
4	GTP	HA	501	5	29,34,34	1.28	4 (13%)	35,54,54	1.25	4 (11%)
6	GDP	KB	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.07	2 (6%)
6	GDP	IB	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.06	2 (6%)
6	GDP	DD	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.06	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GTP	NA	501	5	29,34,34	1.28	4 (13%)	35,54,54	1.25	4 (11%)
4	GTP	CE	501	5	29,34,34	1.28	4 (13%)	35,54,54	1.25	4 (11%)
7	TA1	KF	502	-	68,68,68	0.68	1 (1%)	105,105,105	1.73	19 (18%)
6	GDP	CB	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.06	2 (6%)
4	GTP	JC	501	5	29,34,34	1.28	4 (13%)	35,54,54	1.25	4 (11%)
6	GDP	DB	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.06	2 (6%)
6	GDP	JF	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.06	2 (6%)
7	TA1	JD	502	-	68,68,68	0.68	1 (1%)	105,105,105	1.73	19 (18%)
6	GDP	ND	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.06	2 (6%)
4	GTP	DE	501	5	29,34,34	1.28	4 (13%)	35,54,54	1.25	4 (11%)
6	GDP	ID	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.06	2 (6%)
6	GDP	LF	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.06	2 (6%)
6	GDP	NB	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.06	2 (6%)
7	TA1	MF	502	-	68,68,68	0.68	1 (1%)	105,105,105	1.73	18 (17%)
6	GDP	AD	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.05	2 (6%)
4	GTP	EC	501	5	29,34,34	1.27	4 (13%)	35,54,54	1.25	4 (11%)
4	GTP	GC	501	5	29,34,34	1.28	4 (13%)	35,54,54	1.25	4 (11%)
4	GTP	DA	501	5	29,34,34	1.28	4 (13%)	35,54,54	1.25	4 (11%)
6	GDP	CD	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.06	2 (6%)
4	GTP	LA	501	5	29,34,34	1.28	4 (13%)	35,54,54	1.25	4 (11%)
6	GDP	GF	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.06	2 (6%)
7	TA1	DB	502	-	68,68,68	0.68	1 (1%)	105,105,105	1.73	18 (17%)
7	TA1	ND	502	-	68,68,68	0.68	1 (1%)	105,105,105	1.73	19 (18%)
4	GTP	MA	501	5	29,34,34	1.28	4 (13%)	35,54,54	1.25	4 (11%)
4	GTP	CA	501	5	29,34,34	1.27	4 (13%)	35,54,54	1.25	4 (11%)
4	GTP	GA	501	5	29,34,34	1.28	4 (13%)	35,54,54	1.25	4 (11%)
4	GTP	AA	501	5	29,34,34	1.27	4 (13%)	35,54,54	1.25	4 (11%)
7	TA1	HD	502	-	68,68,68	0.68	1 (1%)	105,105,105	1.73	18 (17%)
4	GTP	BE	501	5	29,34,34	1.28	4 (13%)	35,54,54	1.26	4 (11%)
6	GDP	MD	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.06	2 (6%)
6	GDP	HF	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.06	2 (6%)
4	GTP	LC	501	5	29,34,34	1.28	4 (13%)	35,54,54	1.25	4 (11%)
4	GTP	AE	501	5	29,34,34	1.28	4 (13%)	35,54,54	1.25	4 (11%)
7	TA1	EB	502	-	68,68,68	0.68	1 (1%)	105,105,105	1.73	19 (18%)
7	TA1	BF	502	-	68,68,68	0.68	1 (1%)	105,105,105	1.73	19 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	GDP	GB	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.06	2 (6%)
7	TA1	EF	502	-	68,68,68	0.68	1 (1%)	105,105,105	1.73	19 (18%)
4	GTP	MC	501	5	29,34,34	1.27	4 (13%)	35,54,54	1.25	4 (11%)
4	GTP	EE	501	5	29,34,34	1.28	4 (13%)	35,54,54	1.25	4 (11%)
6	GDP	ED	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.06	2 (6%)
7	TA1	LD	502	-	68,68,68	0.68	1 (1%)	105,105,105	1.73	18 (17%)
4	GTP	KE	501	5	29,34,34	1.28	4 (13%)	35,54,54	1.25	4 (11%)
4	GTP	BC	501	5	29,34,34	1.28	4 (13%)	35,54,54	1.25	4 (11%)
7	TA1	GF	502	-	68,68,68	0.68	1 (1%)	105,105,105	1.73	19 (18%)
6	GDP	CF	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.06	2 (6%)
6	GDP	AB	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.06	2 (6%)
6	GDP	DF	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.06	2 (6%)
6	GDP	JD	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.06	2 (6%)
7	TA1	MD	502	-	68,68,68	0.68	1 (1%)	105,105,105	1.73	19 (18%)
6	GDP	FB	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.06	2 (6%)
7	TA1	DD	502	-	68,68,68	0.68	1 (1%)	105,105,105	1.73	19 (18%)
7	TA1	IB	502	-	68,68,68	0.68	1 (1%)	105,105,105	1.73	18 (17%)
6	GDP	IF	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.06	2 (6%)
7	TA1	HF	502	-	68,68,68	0.68	1 (1%)	105,105,105	1.73	19 (18%)
4	GTP	LE	501	5	29,34,34	1.28	4 (13%)	35,54,54	1.25	4 (11%)
4	GTP	GE	501	5	29,34,34	1.27	4 (13%)	35,54,54	1.26	4 (11%)
4	GTP	JA	501	5	29,34,34	1.27	4 (13%)	35,54,54	1.25	4 (11%)
6	GDP	MB	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.06	2 (6%)
7	TA1	LF	502	-	68,68,68	0.68	1 (1%)	105,105,105	1.73	19 (18%)
7	TA1	GB	502	-	68,68,68	0.68	1 (1%)	105,105,105	1.73	18 (17%)
6	GDP	HB	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.06	2 (6%)
7	TA1	AD	502	-	68,68,68	0.68	1 (1%)	105,105,105	1.73	19 (18%)
7	TA1	ED	502	-	68,68,68	0.68	1 (1%)	105,105,105	1.73	18 (17%)
4	GTP	IE	501	5	29,34,34	1.28	4 (13%)	35,54,54	1.25	4 (11%)
4	GTP	KA	501	5	29,34,34	1.28	4 (13%)	35,54,54	1.25	4 (11%)
6	GDP	HD	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.06	2 (6%)
7	TA1	NF	502	-	68,68,68	0.68	1 (1%)	105,105,105	1.73	19 (18%)
4	GTP	DC	501	5	29,34,34	1.28	4 (13%)	35,54,54	1.25	4 (11%)
4	GTP	CC	501	5	29,34,34	1.27	4 (13%)	35,54,54	1.25	4 (11%)
7	TA1	CD	502	-	68,68,68	0.68	1 (1%)	105,105,105	1.73	18 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	GDP	KF	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.06	2 (6%)
7	TA1	CF	502	-	68,68,68	0.68	1 (1%)	105,105,105	1.73	18 (17%)
4	GTP	KC	501	5	29,34,34	1.28	4 (13%)	35,54,54	1.25	4 (11%)
7	TA1	DF	502	-	68,68,68	0.68	1 (1%)	105,105,105	1.73	19 (18%)
7	TA1	FF	502	-	68,68,68	0.68	1 (1%)	105,105,105	1.73	18 (17%)
6	GDP	LB	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.06	2 (6%)
7	TA1	LB	502	-	68,68,68	0.68	1 (1%)	105,105,105	1.73	19 (18%)
7	TA1	KB	502	-	68,68,68	0.68	1 (1%)	105,105,105	1.73	19 (18%)
4	GTP	HE	501	5	29,34,34	1.28	4 (13%)	35,54,54	1.25	4 (11%)
4	GTP	IA	501	5	29,34,34	1.27	4 (13%)	35,54,54	1.25	4 (11%)
6	GDP	JB	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.06	2 (6%)
4	GTP	AC	501	5	29,34,34	1.28	4 (13%)	35,54,54	1.25	4 (11%)
4	GTP	HC	501	5	29,34,34	1.27	4 (13%)	35,54,54	1.25	4 (11%)
7	TA1	HB	502	-	68,68,68	0.68	1 (1%)	105,105,105	1.73	18 (17%)
6	GDP	BB	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.06	2 (6%)
7	TA1	ID	502	-	68,68,68	0.68	1 (1%)	105,105,105	1.73	19 (18%)
6	GDP	FD	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.06	2 (6%)
7	TA1	BB	502	-	68,68,68	0.68	1 (1%)	105,105,105	1.73	18 (17%)
7	TA1	GD	502	-	68,68,68	0.68	1 (1%)	105,105,105	1.73	18 (17%)
4	GTP	EA	501	5	29,34,34	1.28	4 (13%)	35,54,54	1.25	4 (11%)
4	GTP	JE	501	5	29,34,34	1.28	4 (13%)	35,54,54	1.25	4 (11%)
4	GTP	FC	501	5	29,34,34	1.28	4 (13%)	35,54,54	1.25	4 (11%)
6	GDP	KD	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.06	2 (6%)
4	GTP	IC	501	5	29,34,34	1.28	4 (13%)	35,54,54	1.25	4 (11%)
6	GDP	LD	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.06	2 (6%)
4	GTP	NE	501	5	29,34,34	1.28	4 (13%)	35,54,54	1.26	4 (11%)
7	TA1	AB	502	-	68,68,68	0.68	1 (1%)	105,105,105	1.73	19 (18%)
7	TA1	IF	502	-	68,68,68	0.68	1 (1%)	105,105,105	1.73	18 (17%)
6	GDP	GD	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.06	2 (6%)
6	GDP	NF	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.06	2 (6%)
7	TA1	FD	502	-	68,68,68	0.68	1 (1%)	105,105,105	1.73	19 (18%)
7	TA1	NB	502	-	68,68,68	0.68	1 (1%)	105,105,105	1.73	19 (18%)
7	TA1	CB	502	-	68,68,68	0.68	1 (1%)	105,105,105	1.73	18 (17%)
7	TA1	JF	502	-	68,68,68	0.67	1 (1%)	105,105,105	1.73	19 (18%)
7	TA1	AF	502	-	68,68,68	0.68	1 (1%)	105,105,105	1.73	19 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	TA1	FB	502	-	68,68,68	0.68	1 (1%)	105,105,105	1.73	19 (18%)
6	GDP	BF	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.06	2 (6%)
7	TA1	KD	502	-	68,68,68	0.67	1 (1%)	105,105,105	1.73	19 (18%)
6	GDP	AF	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.06	2 (6%)
7	TA1	MB	502	-	68,68,68	0.68	1 (1%)	105,105,105	1.73	18 (17%)
4	GTP	FE	501	5	29,34,34	1.27	4 (13%)	35,54,54	1.25	4 (11%)
6	GDP	BD	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.06	2 (6%)
7	TA1	BD	502	-	68,68,68	0.68	1 (1%)	105,105,105	1.73	19 (18%)
4	GTP	BA	501	5	29,34,34	1.28	4 (13%)	35,54,54	1.25	4 (11%)
4	GTP	ME	501	5	29,34,34	1.28	4 (13%)	35,54,54	1.25	4 (11%)
6	GDP	FF	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.06	2 (6%)
6	GDP	EB	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.06	2 (6%)
4	GTP	NC	501	5	29,34,34	1.28	4 (13%)	35,54,54	1.25	4 (11%)

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
7	TA1	JB	502	-	-	7/41/127/127	0/7/7/7
6	GDP	EF	501	-	-	4/12/32/32	0/3/3/3
6	GDP	MF	501	-	-	4/12/32/32	0/3/3/3
4	GTP	FA	501	5	-	6/18/38/38	0/3/3/3
4	GTP	HA	501	5	-	6/18/38/38	0/3/3/3
6	GDP	KB	501	-	-	4/12/32/32	0/3/3/3
6	GDP	IB	501	-	-	4/12/32/32	0/3/3/3
6	GDP	DD	501	-	-	4/12/32/32	0/3/3/3
4	GTP	NA	501	5	-	6/18/38/38	0/3/3/3
4	GTP	CE	501	5	-	6/18/38/38	0/3/3/3
7	TA1	KF	502	-	-	7/41/127/127	0/7/7/7
6	GDP	CB	501	-	-	4/12/32/32	0/3/3/3
4	GTP	JC	501	5	-	6/18/38/38	0/3/3/3
6	GDP	DB	501	-	-	4/12/32/32	0/3/3/3
6	GDP	JF	501	-	-	4/12/32/32	0/3/3/3
7	TA1	JD	502	-	-	7/41/127/127	0/7/7/7

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GDP	ND	501	-	-	4/12/32/32	0/3/3/3
4	GTP	DE	501	5	-	6/18/38/38	0/3/3/3
6	GDP	ID	501	-	-	4/12/32/32	0/3/3/3
6	GDP	LF	501	-	-	4/12/32/32	0/3/3/3
6	GDP	NB	501	-	-	4/12/32/32	0/3/3/3
7	TA1	MF	502	-	-	7/41/127/127	0/7/7/7
6	GDP	AD	501	-	-	4/12/32/32	0/3/3/3
4	GTP	EC	501	5	-	6/18/38/38	0/3/3/3
4	GTP	GC	501	5	-	6/18/38/38	0/3/3/3
4	GTP	DA	501	5	-	6/18/38/38	0/3/3/3
6	GDP	CD	501	-	-	4/12/32/32	0/3/3/3
4	GTP	LA	501	5	-	6/18/38/38	0/3/3/3
6	GDP	GF	501	-	-	4/12/32/32	0/3/3/3
7	TA1	DB	502	-	-	7/41/127/127	0/7/7/7
7	TA1	ND	502	-	-	7/41/127/127	0/7/7/7
4	GTP	MA	501	5	-	6/18/38/38	0/3/3/3
4	GTP	CA	501	5	-	6/18/38/38	0/3/3/3
4	GTP	GA	501	5	-	6/18/38/38	0/3/3/3
4	GTP	AA	501	5	-	6/18/38/38	0/3/3/3
7	TA1	HD	502	-	-	7/41/127/127	0/7/7/7
4	GTP	BE	501	5	-	6/18/38/38	0/3/3/3
6	GDP	MD	501	-	-	4/12/32/32	0/3/3/3
6	GDP	HF	501	-	-	4/12/32/32	0/3/3/3
4	GTP	LC	501	5	-	6/18/38/38	0/3/3/3
4	GTP	AE	501	5	-	6/18/38/38	0/3/3/3
7	TA1	EB	502	-	-	7/41/127/127	0/7/7/7
7	TA1	BF	502	-	-	7/41/127/127	0/7/7/7
6	GDP	GB	501	-	-	4/12/32/32	0/3/3/3
7	TA1	EF	502	-	-	7/41/127/127	0/7/7/7
4	GTP	MC	501	5	-	6/18/38/38	0/3/3/3
4	GTP	EE	501	5	-	6/18/38/38	0/3/3/3
6	GDP	ED	501	-	-	4/12/32/32	0/3/3/3
7	TA1	LD	502	-	-	7/41/127/127	0/7/7/7
4	GTP	KE	501	5	-	6/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GTP	BC	501	5	-	6/18/38/38	0/3/3/3
7	TA1	GF	502	-	-	7/41/127/127	0/7/7/7
6	GDP	CF	501	-	-	4/12/32/32	0/3/3/3
6	GDP	AB	501	-	-	4/12/32/32	0/3/3/3
6	GDP	DF	501	-	-	4/12/32/32	0/3/3/3
6	GDP	JD	501	-	-	4/12/32/32	0/3/3/3
7	TA1	MD	502	-	-	7/41/127/127	0/7/7/7
6	GDP	FB	501	-	-	4/12/32/32	0/3/3/3
7	TA1	DD	502	-	-	7/41/127/127	0/7/7/7
7	TA1	IB	502	-	-	7/41/127/127	0/7/7/7
6	GDP	IF	501	-	-	4/12/32/32	0/3/3/3
7	TA1	HF	502	-	-	7/41/127/127	0/7/7/7
4	GTP	LE	501	5	-	6/18/38/38	0/3/3/3
4	GTP	GE	501	5	-	6/18/38/38	0/3/3/3
4	GTP	JA	501	5	-	6/18/38/38	0/3/3/3
6	GDP	MB	501	-	-	4/12/32/32	0/3/3/3
7	TA1	LF	502	-	-	7/41/127/127	0/7/7/7
7	TA1	GB	502	-	-	7/41/127/127	0/7/7/7
6	GDP	HB	501	-	-	4/12/32/32	0/3/3/3
7	TA1	AD	502	-	-	7/41/127/127	0/7/7/7
7	TA1	ED	502	-	-	7/41/127/127	0/7/7/7
4	GTP	IE	501	5	-	6/18/38/38	0/3/3/3
4	GTP	KA	501	5	-	6/18/38/38	0/3/3/3
6	GDP	HD	501	-	-	4/12/32/32	0/3/3/3
7	TA1	NF	502	-	-	7/41/127/127	0/7/7/7
4	GTP	DC	501	5	-	6/18/38/38	0/3/3/3
4	GTP	CC	501	5	-	6/18/38/38	0/3/3/3
7	TA1	CD	502	-	-	7/41/127/127	0/7/7/7
6	GDP	KF	501	-	-	4/12/32/32	0/3/3/3
7	TA1	CF	502	-	-	7/41/127/127	0/7/7/7
4	GTP	KC	501	5	-	6/18/38/38	0/3/3/3
7	TA1	DF	502	-	-	7/41/127/127	0/7/7/7
7	TA1	FF	502	-	-	7/41/127/127	0/7/7/7
6	GDP	LB	501	-	-	4/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	TA1	LB	502	-	-	7/41/127/127	0/7/7/7
7	TA1	KB	502	-	-	7/41/127/127	0/7/7/7
4	GTP	HE	501	5	-	6/18/38/38	0/3/3/3
4	GTP	IA	501	5	-	6/18/38/38	0/3/3/3
6	GDP	JB	501	-	-	4/12/32/32	0/3/3/3
4	GTP	AC	501	5	-	6/18/38/38	0/3/3/3
4	GTP	HC	501	5	-	6/18/38/38	0/3/3/3
7	TA1	HB	502	-	-	7/41/127/127	0/7/7/7
6	GDP	BB	501	-	-	4/12/32/32	0/3/3/3
7	TA1	ID	502	-	-	7/41/127/127	0/7/7/7
6	GDP	FD	501	-	-	4/12/32/32	0/3/3/3
7	TA1	BB	502	-	-	7/41/127/127	0/7/7/7
7	TA1	GD	502	-	-	7/41/127/127	0/7/7/7
4	GTP	EA	501	5	-	6/18/38/38	0/3/3/3
4	GTP	JE	501	5	-	6/18/38/38	0/3/3/3
4	GTP	FC	501	5	-	6/18/38/38	0/3/3/3
6	GDP	KD	501	-	-	4/12/32/32	0/3/3/3
4	GTP	IC	501	5	-	6/18/38/38	0/3/3/3
6	GDP	LD	501	-	-	4/12/32/32	0/3/3/3
4	GTP	NE	501	5	-	6/18/38/38	0/3/3/3
7	TA1	AB	502	-	-	7/41/127/127	0/7/7/7
7	TA1	IF	502	-	-	7/41/127/127	0/7/7/7
6	GDP	GD	501	-	-	4/12/32/32	0/3/3/3
6	GDP	NF	501	-	-	4/12/32/32	0/3/3/3
7	TA1	FD	502	-	-	7/41/127/127	0/7/7/7
7	TA1	NB	502	-	-	7/41/127/127	0/7/7/7
7	TA1	CB	502	-	-	7/41/127/127	0/7/7/7
7	TA1	JF	502	-	-	7/41/127/127	0/7/7/7
7	TA1	AF	502	-	-	7/41/127/127	0/7/7/7
7	TA1	FB	502	-	-	7/41/127/127	0/7/7/7
6	GDP	BF	501	-	-	4/12/32/32	0/3/3/3
7	TA1	KD	502	-	-	7/41/127/127	0/7/7/7
6	GDP	AF	501	-	-	4/12/32/32	0/3/3/3
7	TA1	MB	502	-	-	7/41/127/127	0/7/7/7

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GTP	FE	501	5	-	6/18/38/38	0/3/3/3
6	GDP	BD	501	-	-	4/12/32/32	0/3/3/3
7	TA1	BD	502	-	-	7/41/127/127	0/7/7/7
4	GTP	BA	501	5	-	6/18/38/38	0/3/3/3
4	GTP	ME	501	5	-	6/18/38/38	0/3/3/3
6	GDP	FF	501	-	-	4/12/32/32	0/3/3/3
6	GDP	EB	501	-	-	4/12/32/32	0/3/3/3
4	GTP	NC	501	5	-	6/18/38/38	0/3/3/3

The worst 5 of 252 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	AE	501	GTP	C5-C6	-4.14	1.39	1.47
4	BE	501	GTP	C5-C6	-4.14	1.39	1.47
4	LA	501	GTP	C5-C6	-4.14	1.39	1.47
4	JA	501	GTP	C5-C6	-4.13	1.39	1.47
4	DC	501	GTP	C5-C6	-4.12	1.39	1.47

The worst 5 of 1034 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	GB	502	TA1	C10-C18-C20	-6.26	105.97	116.30
7	AF	502	TA1	C10-C18-C20	-6.26	105.97	116.30
7	GF	502	TA1	C10-C18-C20	-6.25	105.98	116.30
7	BB	502	TA1	C10-C18-C20	-6.25	105.98	116.30
7	FB	502	TA1	C10-C18-C20	-6.25	105.99	116.30

There are no chirality outliers.

5 of 714 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	AA	501	GTP	C5'-O5'-PA-O3A
4	AA	501	GTP	C5'-O5'-PA-O1A
4	AC	501	GTP	C5'-O5'-PA-O3A
4	AC	501	GTP	C5'-O5'-PA-O1A
4	AE	501	GTP	C5'-O5'-PA-O3A

There are no ring outliers.

126 monomers are involved in 745 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	JB	502	TA1	7	0
6	EF	501	GDP	5	0
6	MF	501	GDP	5	0
4	FA	501	GTP	7	0
4	HA	501	GTP	5	0
6	KB	501	GDP	5	0
6	IB	501	GDP	5	0
6	DD	501	GDP	5	0
4	NA	501	GTP	6	0
4	CE	501	GTP	4	0
7	KF	502	TA1	7	0
6	CB	501	GDP	5	0
4	JC	501	GTP	8	0
6	DB	501	GDP	5	0
6	JF	501	GDP	5	0
7	JD	502	TA1	7	0
6	ND	501	GDP	5	0
4	DE	501	GTP	7	0
6	ID	501	GDP	5	0
6	LF	501	GDP	5	0
6	NB	501	GDP	5	0
7	MF	502	TA1	6	0
6	AD	501	GDP	5	0
4	EC	501	GTP	6	0
4	GC	501	GTP	7	0
4	DA	501	GTP	8	0
6	CD	501	GDP	5	0
4	LA	501	GTP	6	0
6	GF	501	GDP	5	0
7	DB	502	TA1	6	0
7	ND	502	TA1	6	0
4	MA	501	GTP	5	0
4	CA	501	GTP	4	0
4	GA	501	GTP	6	0
4	AA	501	GTP	4	0
7	HD	502	TA1	7	0
4	BE	501	GTP	5	0
6	MD	501	GDP	5	0
6	HF	501	GDP	5	0
4	LC	501	GTP	7	0
4	AE	501	GTP	5	0
7	EB	502	TA1	7	0
7	BF	502	TA1	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	GB	501	GDP	5	0
7	EF	502	TA1	8	0
4	MC	501	GTP	6	0
4	EE	501	GTP	8	0
6	ED	501	GDP	5	0
7	LD	502	TA1	6	0
4	KE	501	GTP	8	0
4	BC	501	GTP	5	0
7	GF	502	TA1	7	0
6	CF	501	GDP	5	0
6	AB	501	GDP	5	0
6	DF	501	GDP	5	0
6	JD	501	GDP	5	0
7	MD	502	TA1	6	0
6	FB	501	GDP	5	0
7	DD	502	TA1	6	0
7	IB	502	TA1	7	0
6	IF	501	GDP	5	0
7	HF	502	TA1	7	0
4	LE	501	GTP	6	0
4	GE	501	GTP	4	0
4	JA	501	GTP	6	0
6	MB	501	GDP	5	0
7	LF	502	TA1	6	0
7	GB	502	TA1	7	0
6	HB	501	GDP	5	0
7	AD	502	TA1	6	0
7	ED	502	TA1	6	0
4	IE	501	GTP	6	0
4	KA	501	GTP	8	0
6	HD	501	GDP	5	0
7	NF	502	TA1	6	0
4	DC	501	GTP	6	0
4	CC	501	GTP	4	0
7	CD	502	TA1	6	0
6	KF	501	GDP	6	0
7	CF	502	TA1	6	0
4	KC	501	GTP	9	0
7	DF	502	TA1	6	0
7	FF	502	TA1	7	0
6	LB	501	GDP	5	0
7	LB	502	TA1	7	0

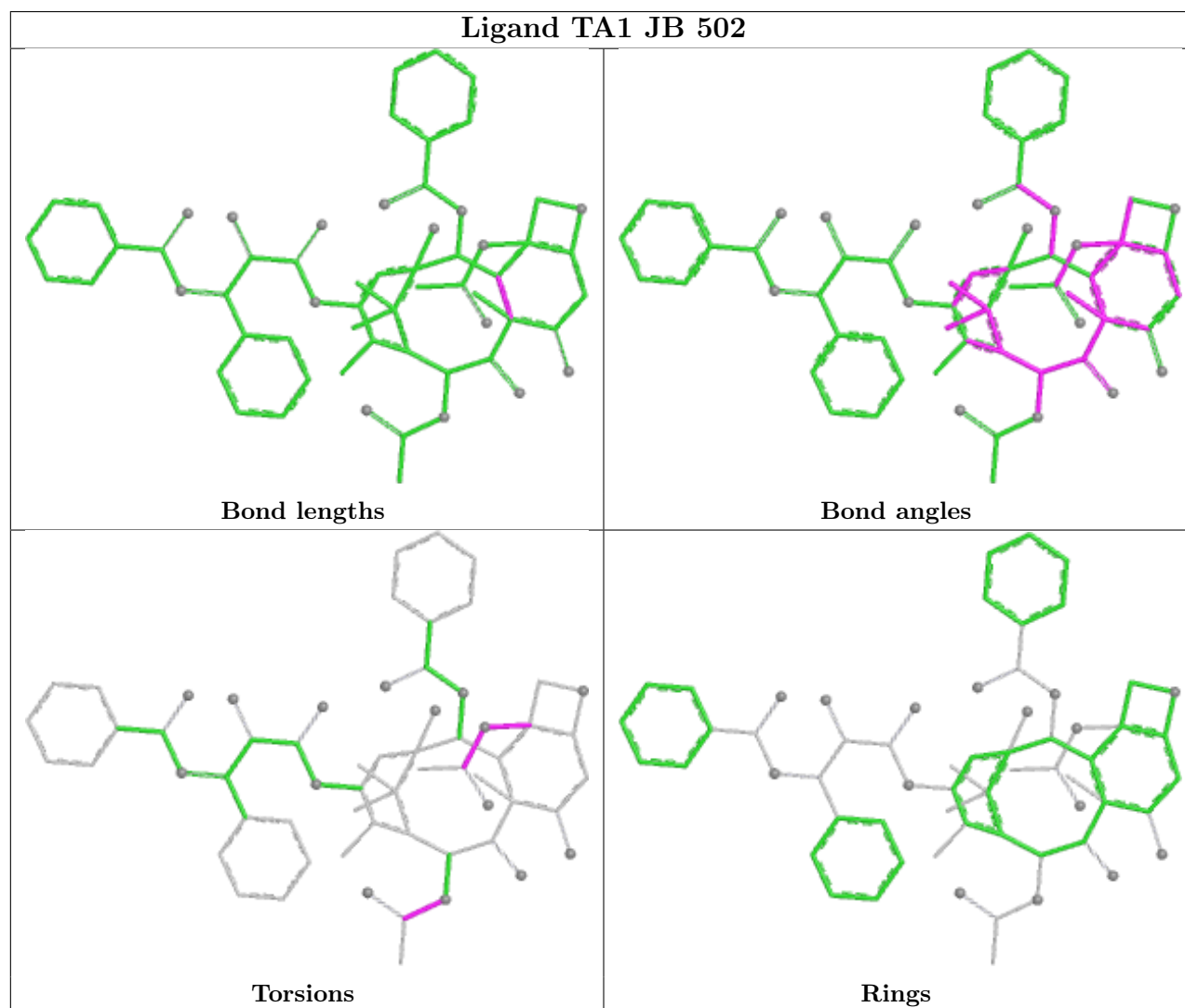
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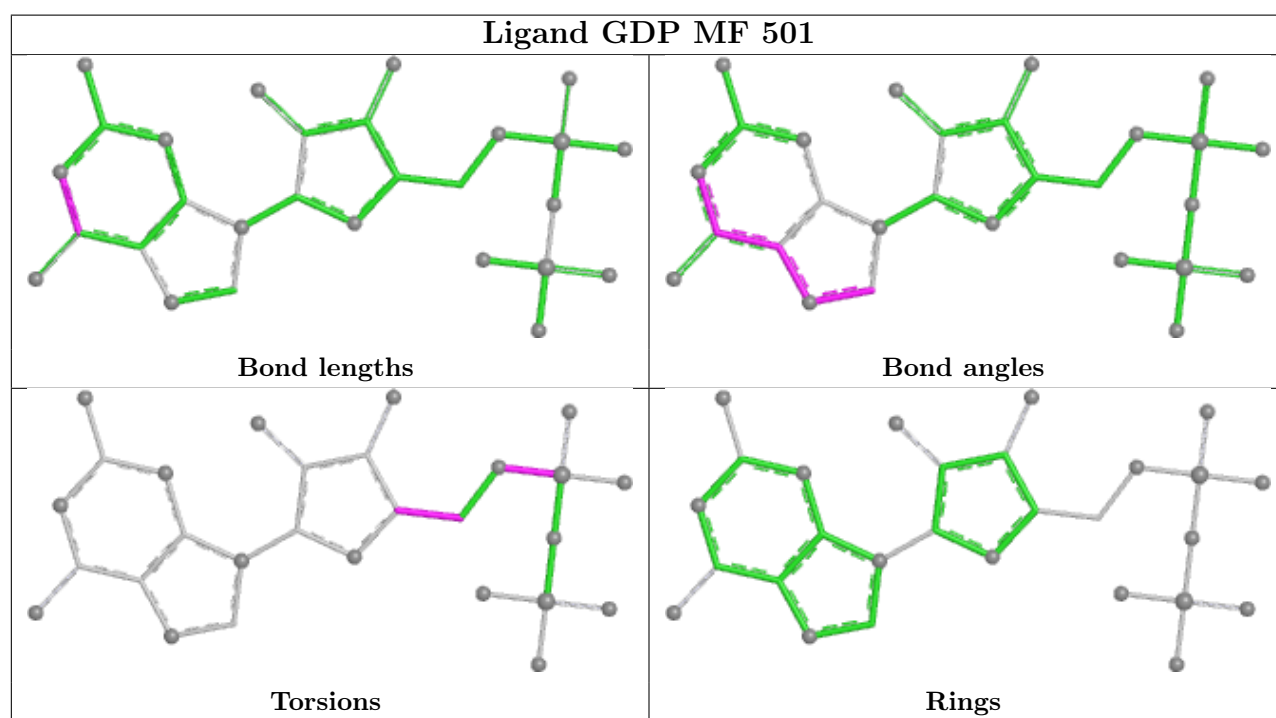
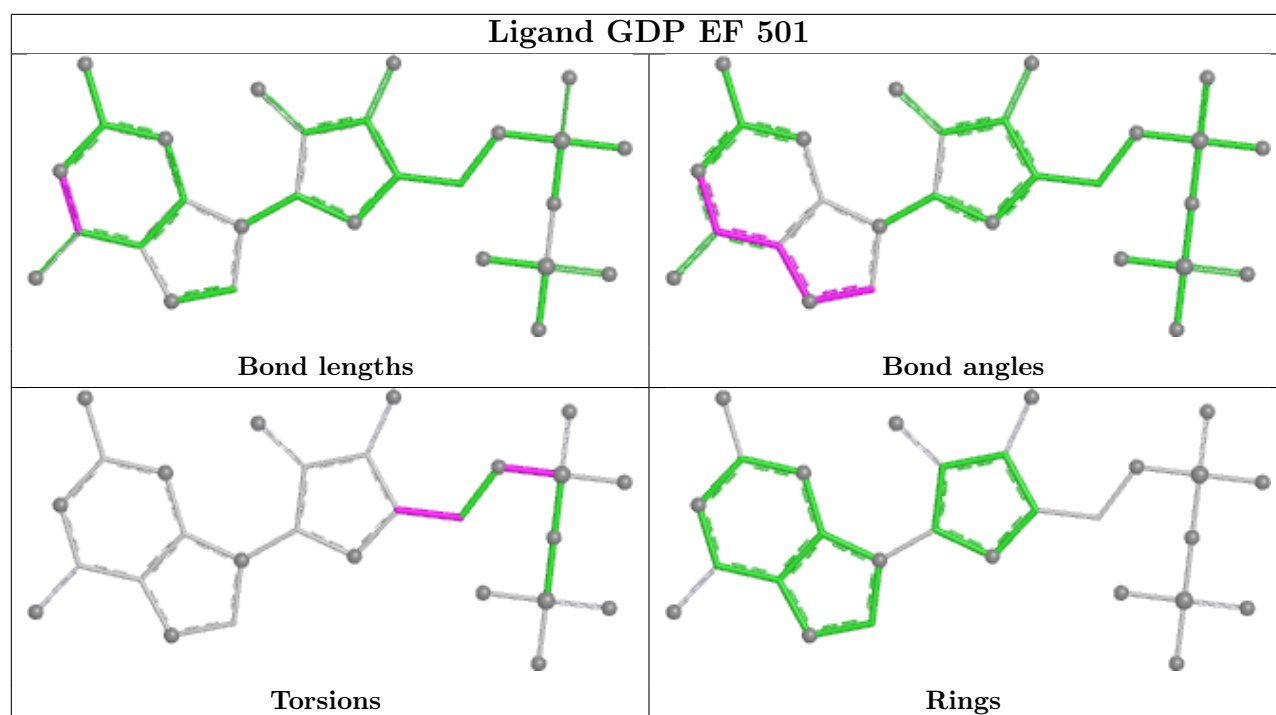
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	KB	502	TA1	7	0
4	HE	501	GTP	5	0
4	IA	501	GTP	5	0
6	JB	501	GDP	5	0
4	AC	501	GTP	7	0
4	HC	501	GTP	5	0
7	HB	502	TA1	7	0
6	BB	501	GDP	5	0
7	ID	502	TA1	8	0
6	FD	501	GDP	5	0
7	BB	502	TA1	6	0
7	GD	502	TA1	7	0
4	EA	501	GTP	6	0
4	JE	501	GTP	9	0
4	FC	501	GTP	6	0
6	KD	501	GDP	5	0
4	IC	501	GTP	6	0
6	LD	501	GDP	5	0
4	NE	501	GTP	7	0
7	AB	502	TA1	6	0
7	IF	502	TA1	7	0
6	GD	501	GDP	5	0
6	NF	501	GDP	5	0
7	FD	502	TA1	7	0
7	NB	502	TA1	6	0
7	CB	502	TA1	6	0
7	JF	502	TA1	7	0
7	AF	502	TA1	6	0
7	FB	502	TA1	7	0
6	BF	501	GDP	5	0
7	KD	502	TA1	7	0
6	AF	501	GDP	5	0
7	MB	502	TA1	7	0
4	FE	501	GTP	6	0
6	BD	501	GDP	5	0
7	BD	502	TA1	7	0
4	BA	501	GTP	5	0
4	ME	501	GTP	7	0
6	FF	501	GDP	5	0
6	EB	501	GDP	5	0
4	NC	501	GTP	7	0

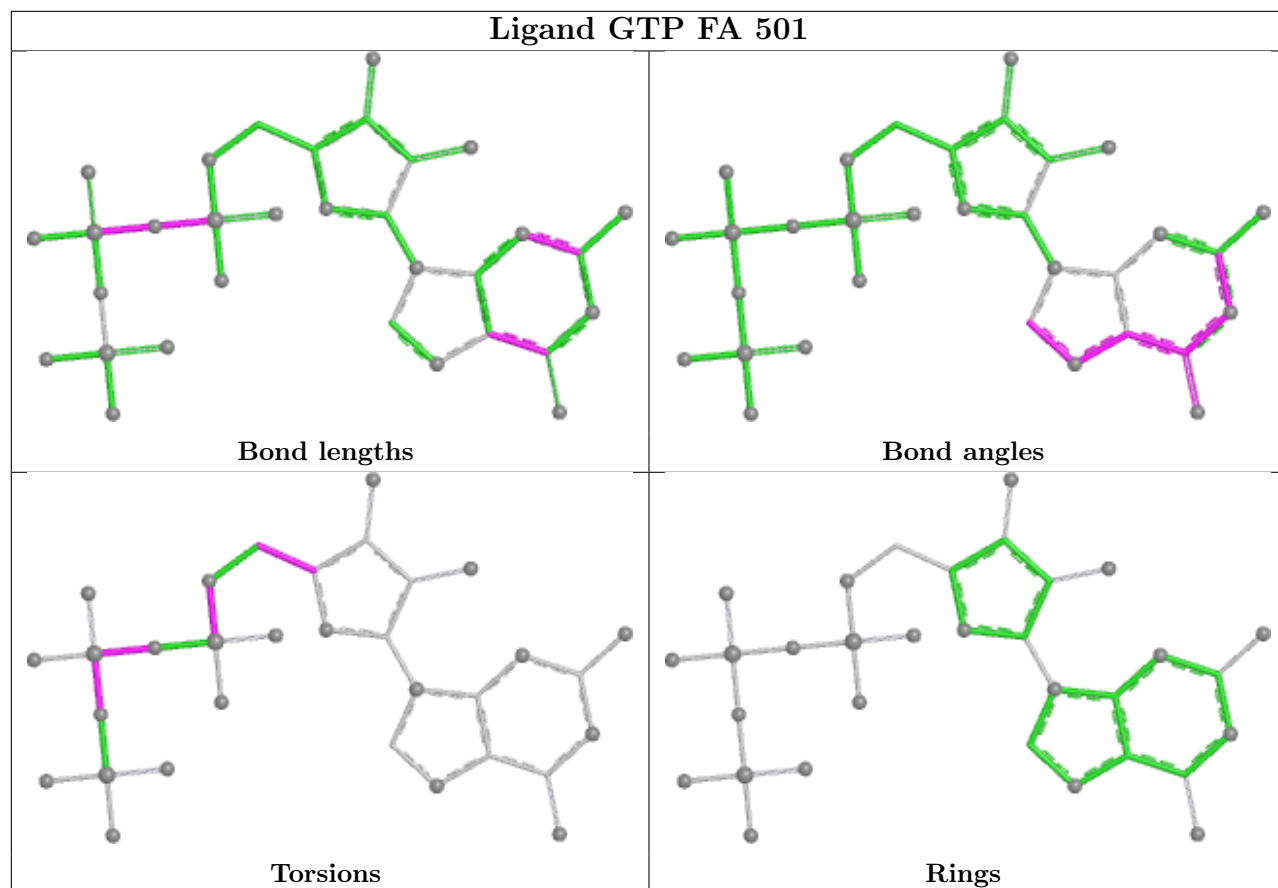
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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.

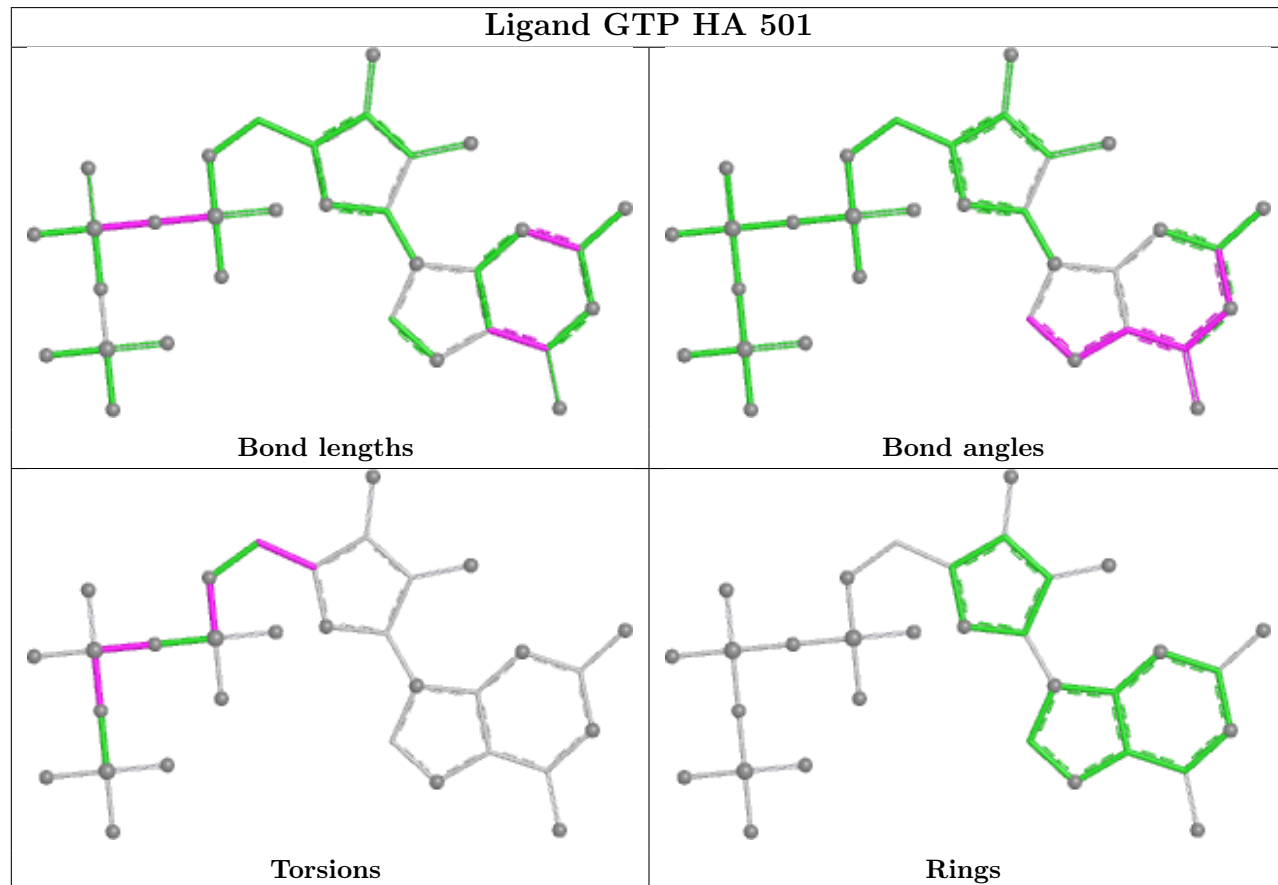


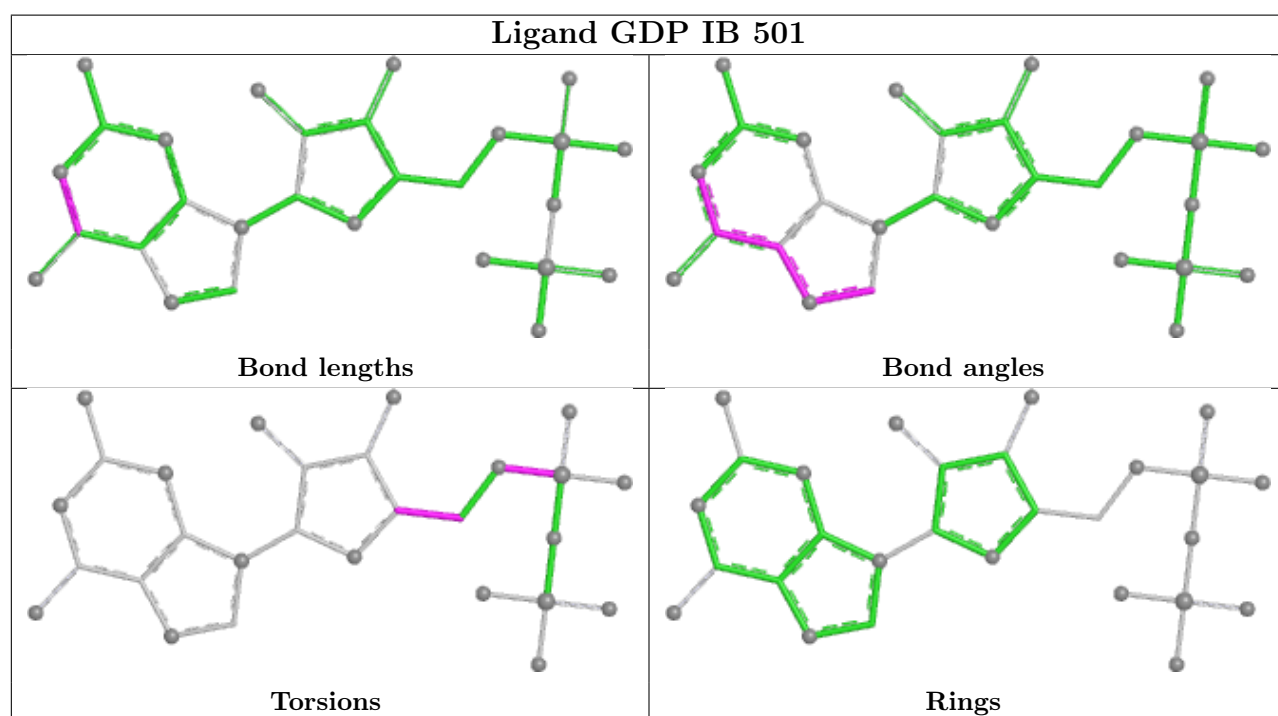
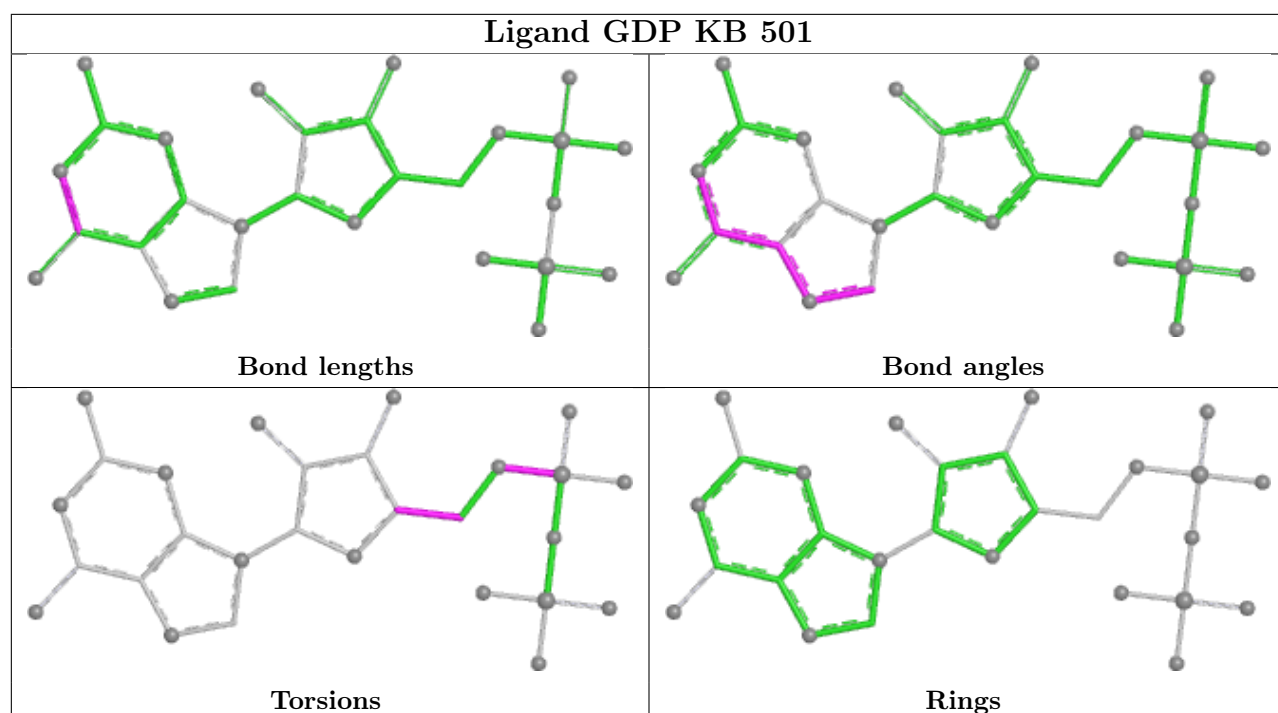


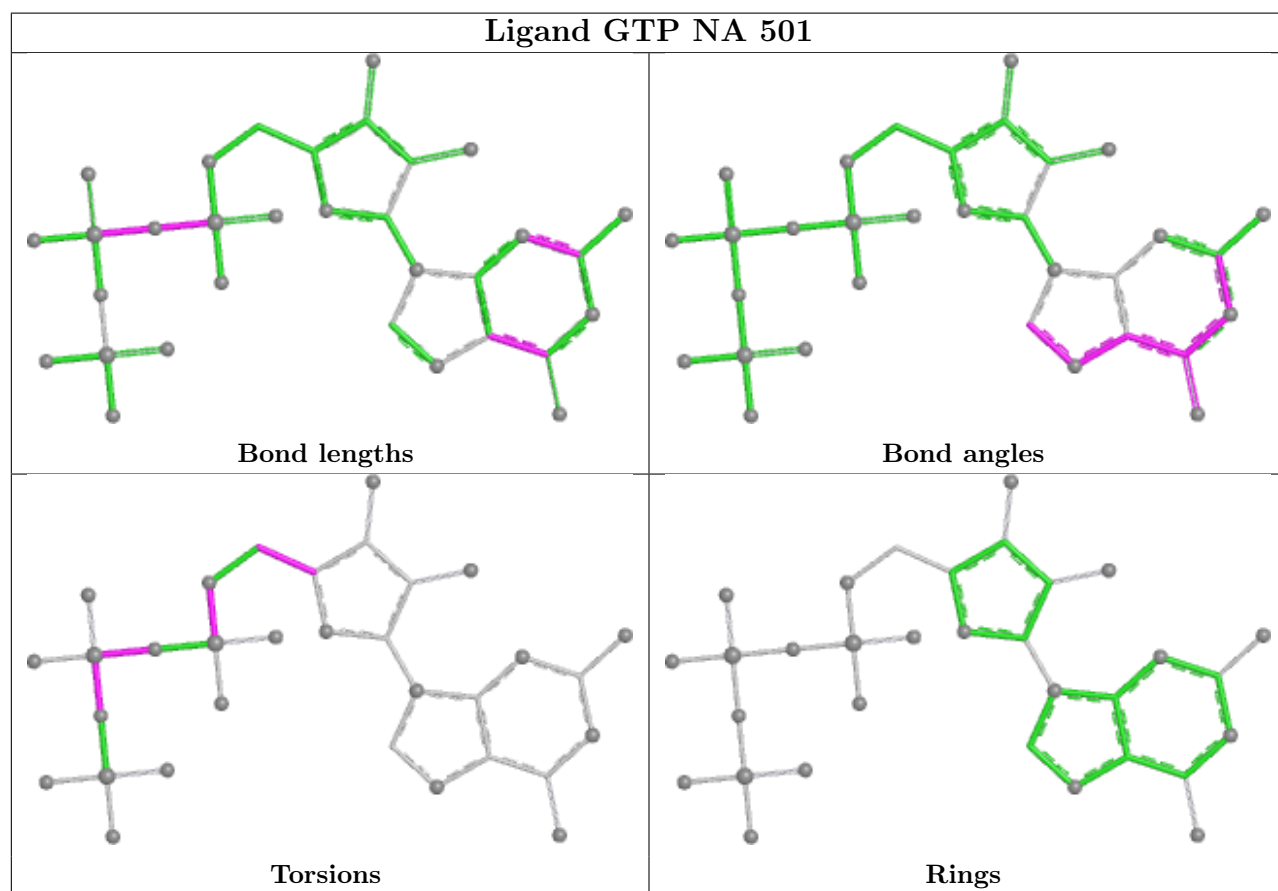
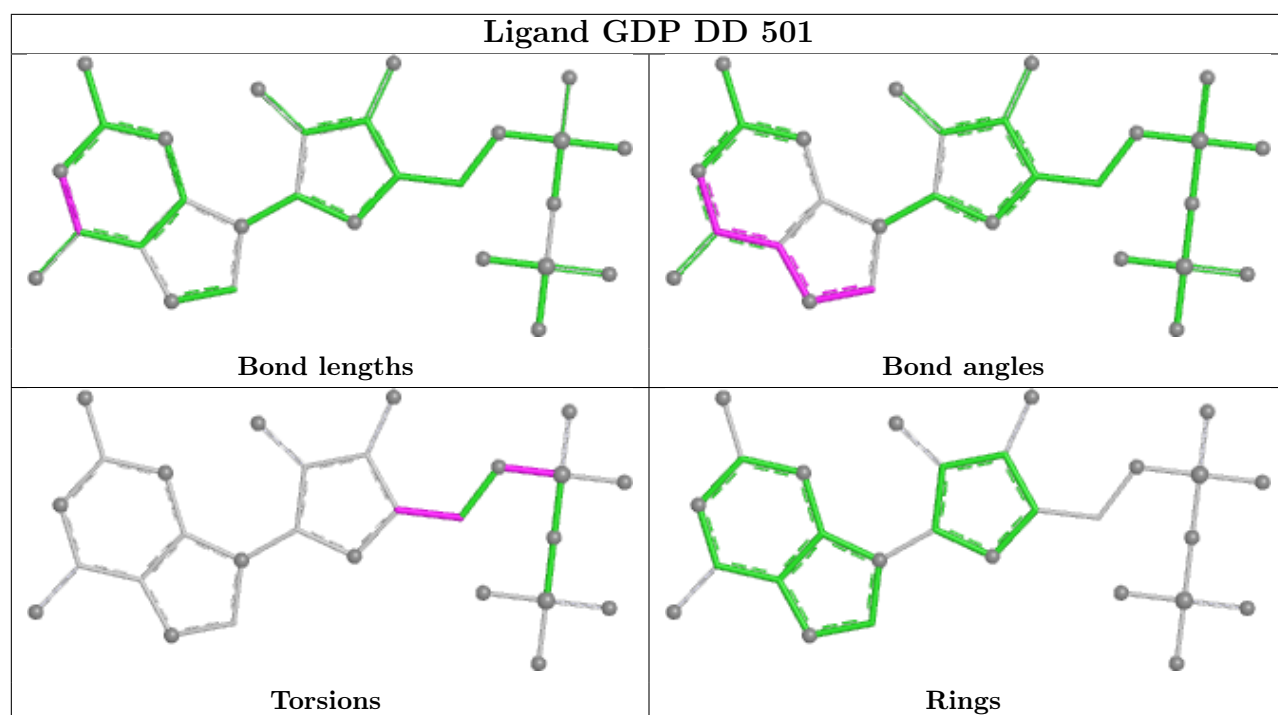
Ligand GTP FA 501

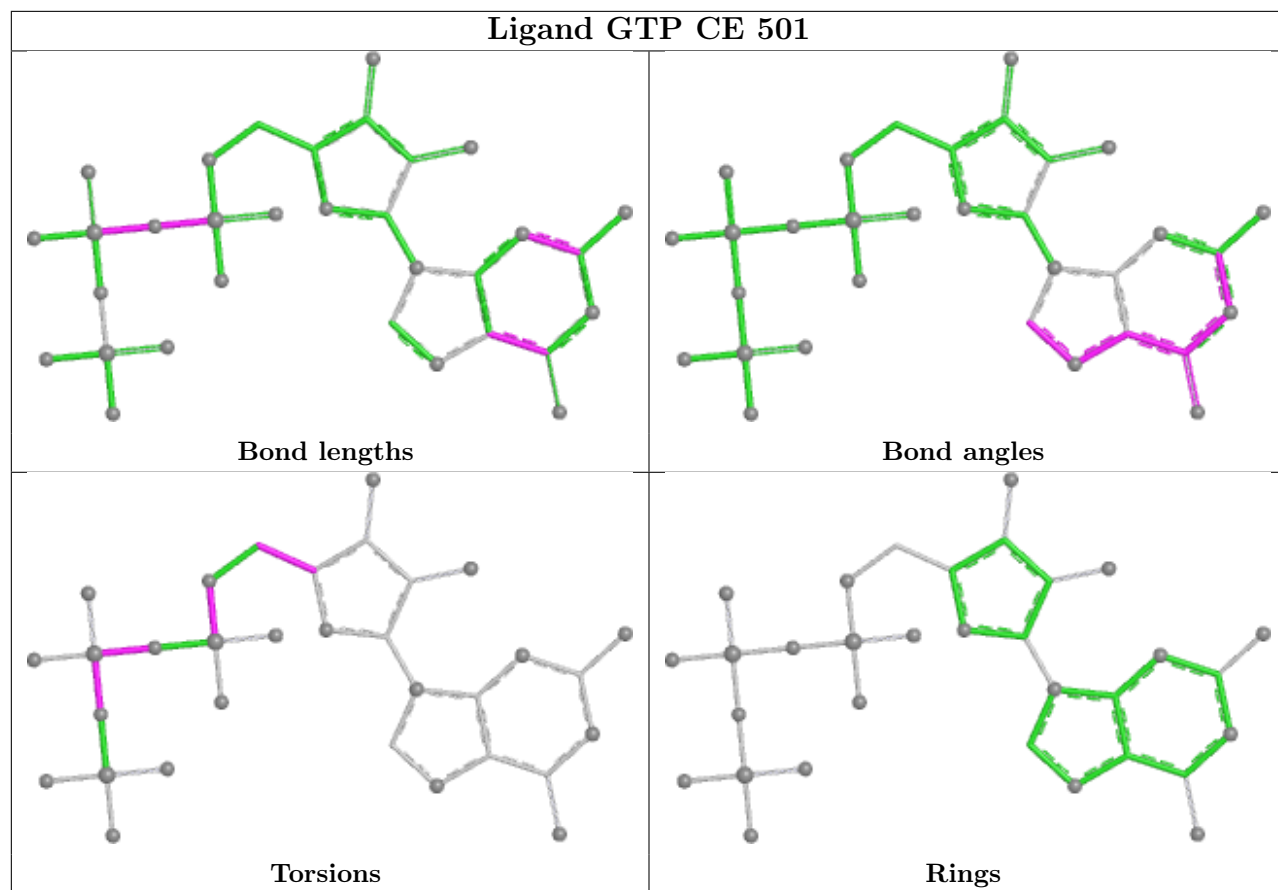


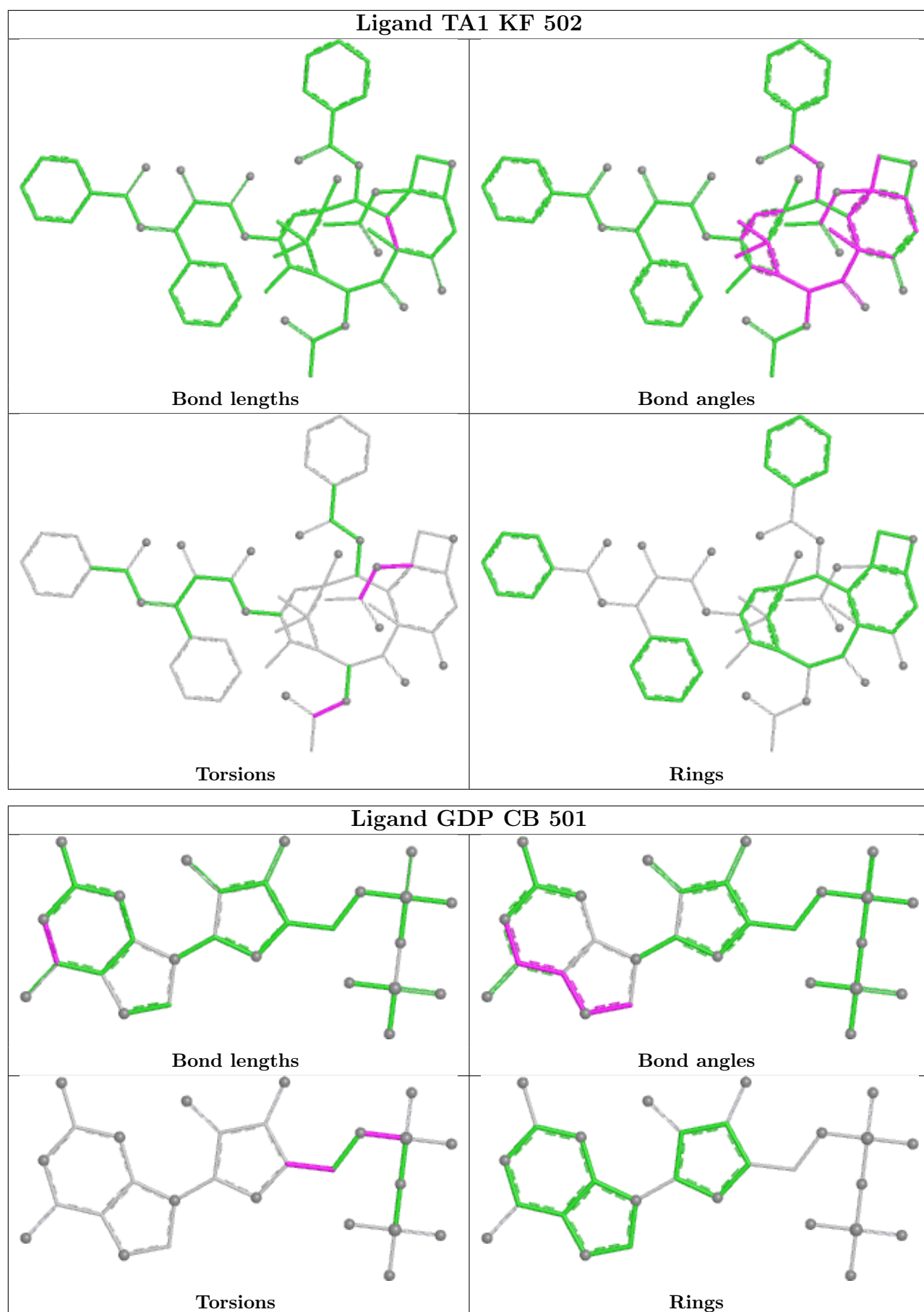
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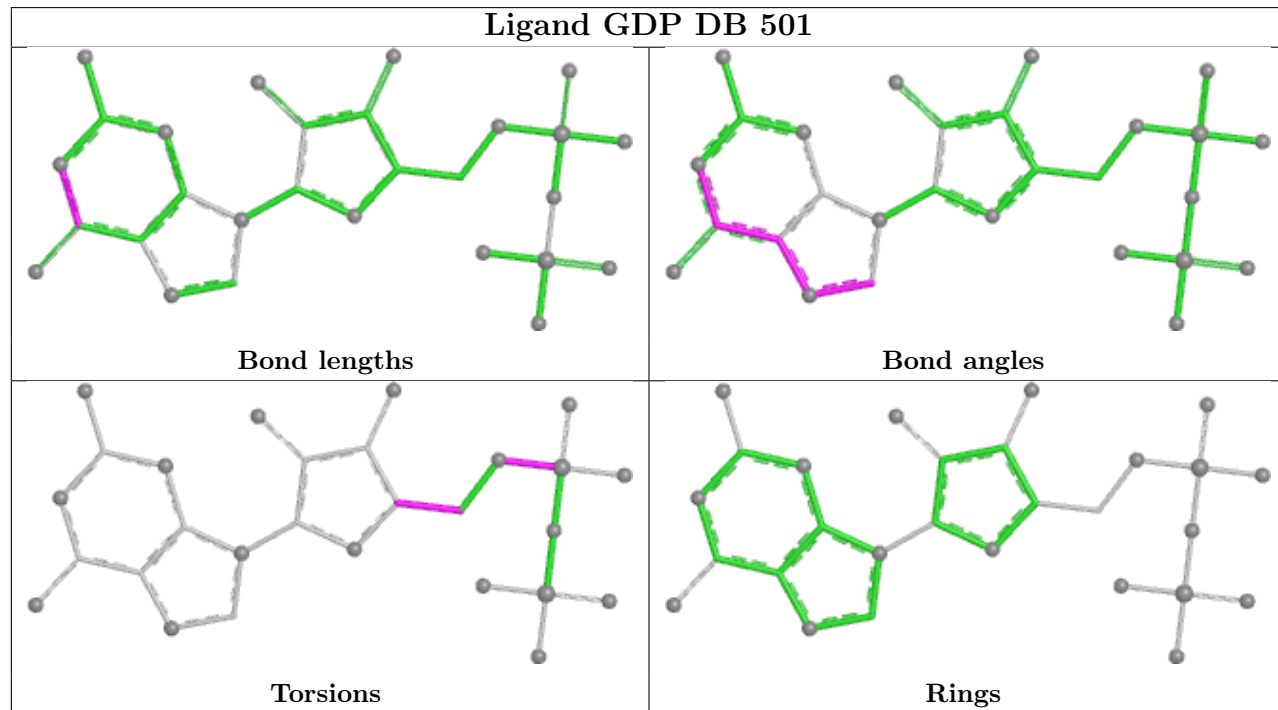
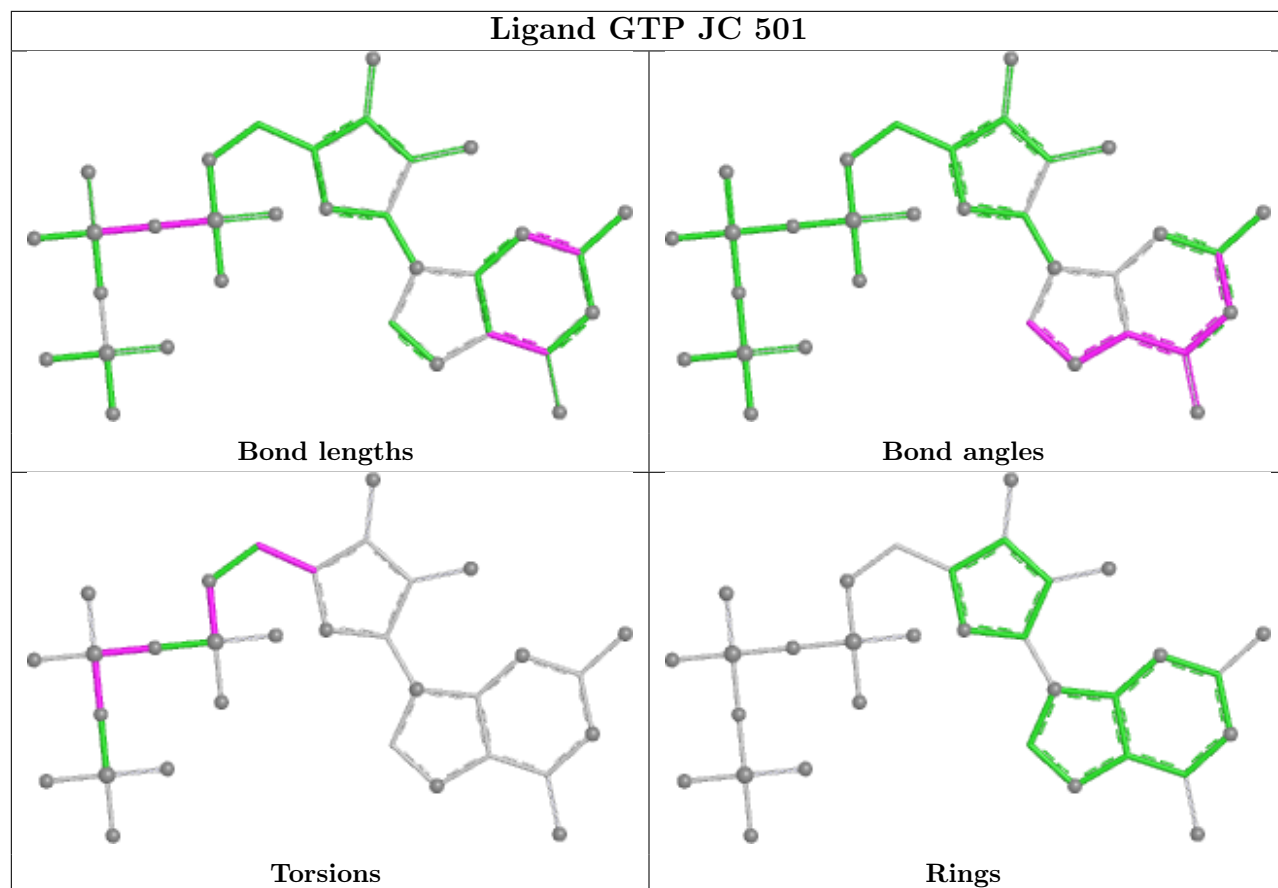


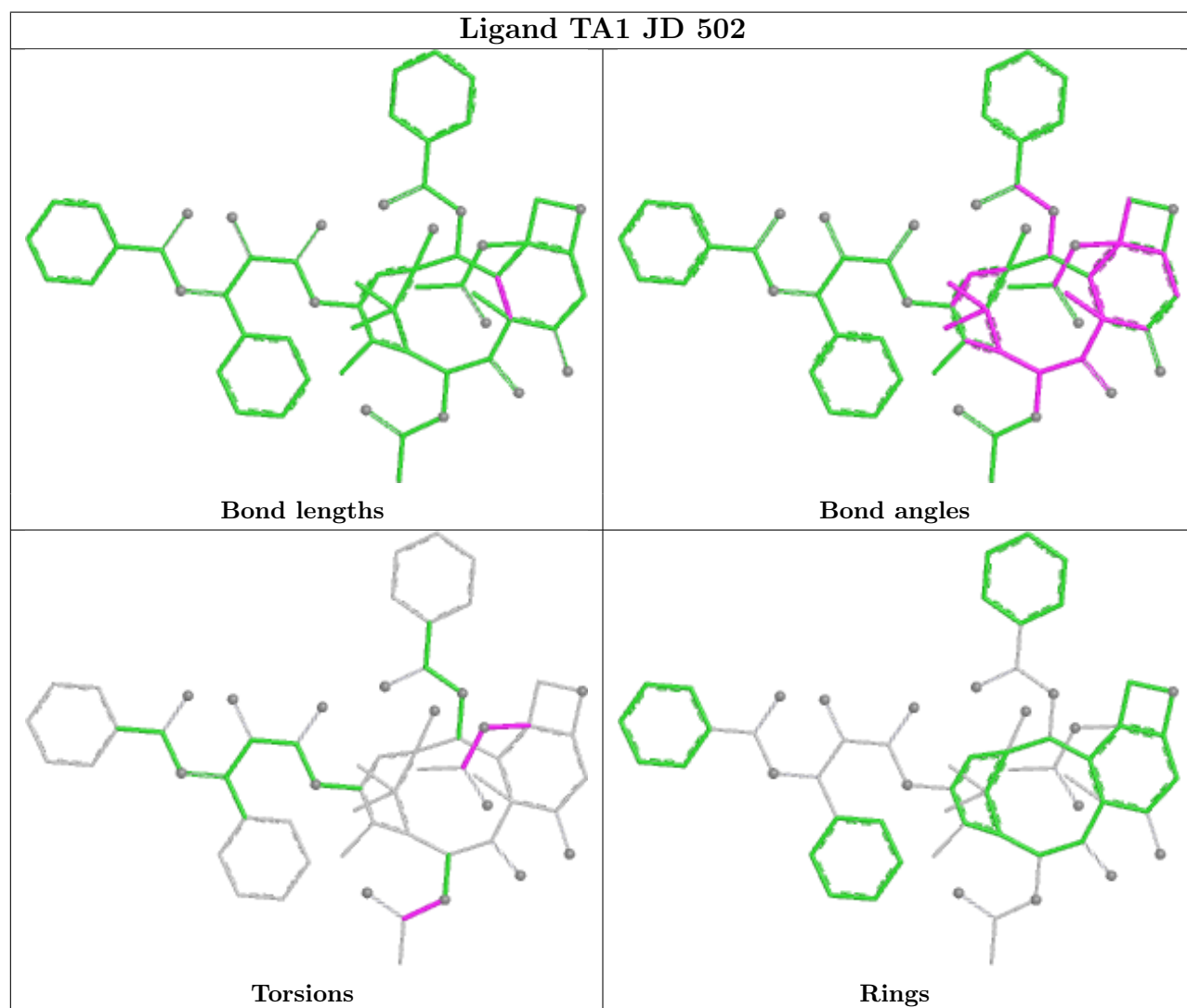
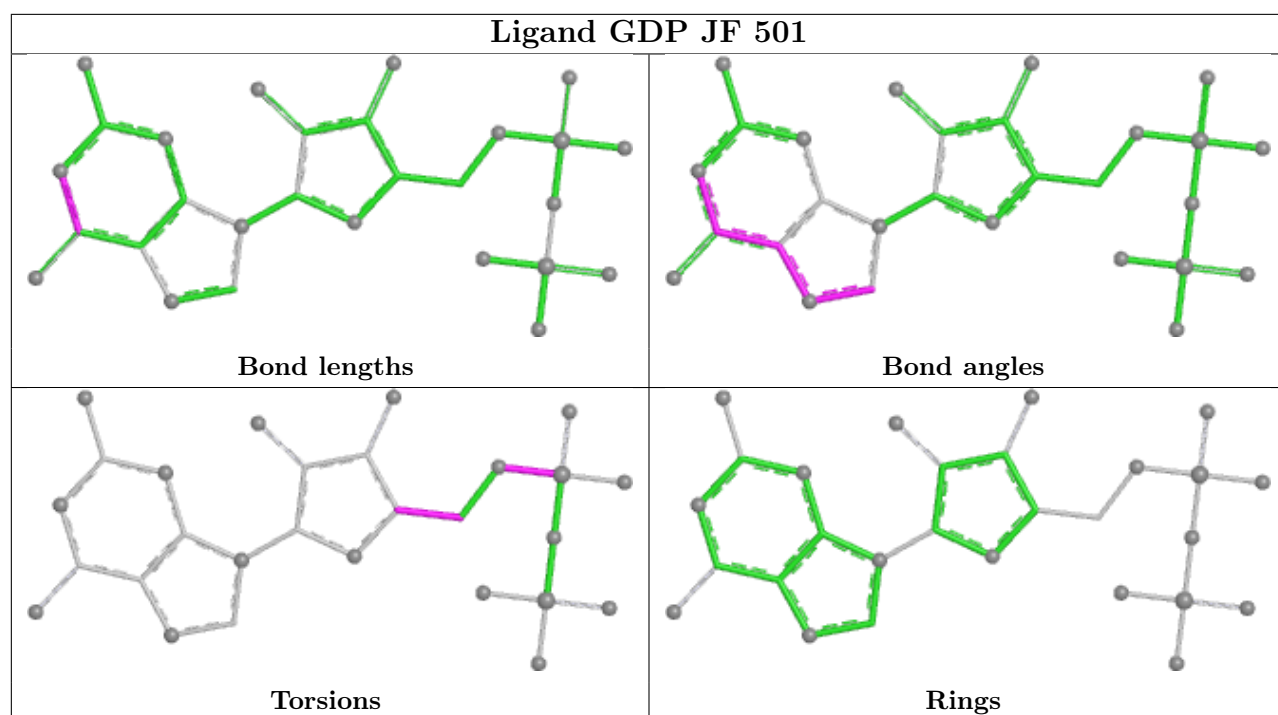




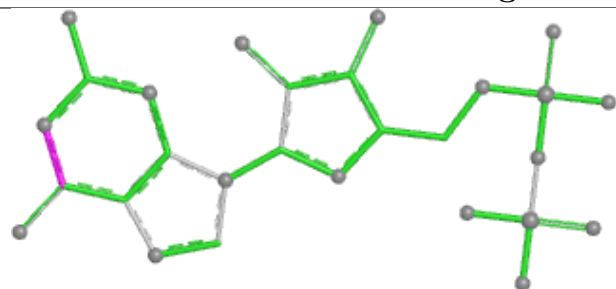




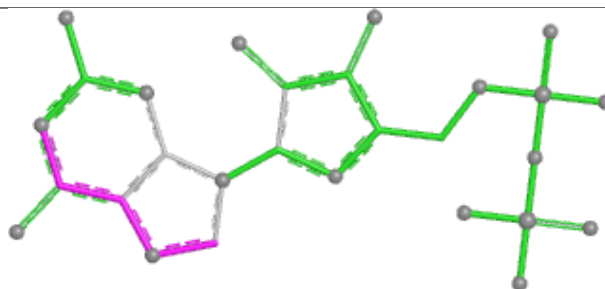




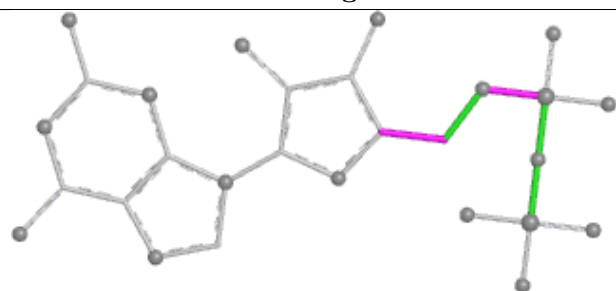
Ligand GDP ND 501



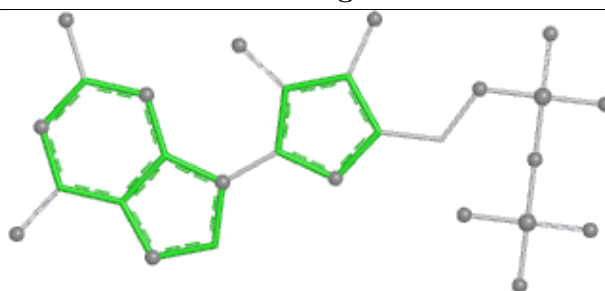
Bond lengths



Bond angles

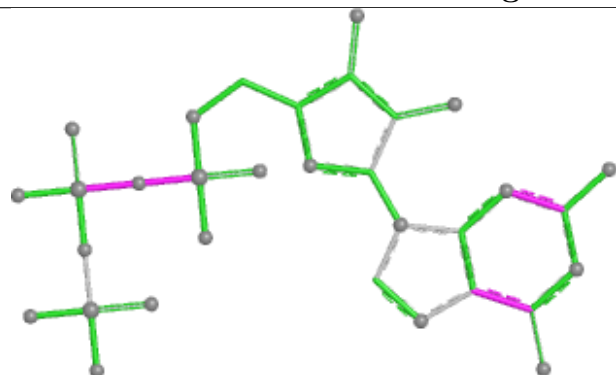


Torsions

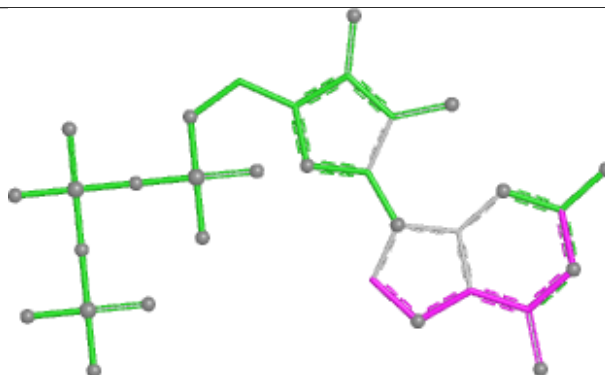


Rings

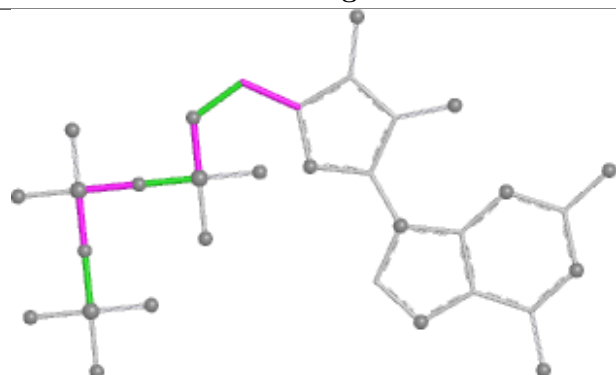
Ligand GTP DE 501



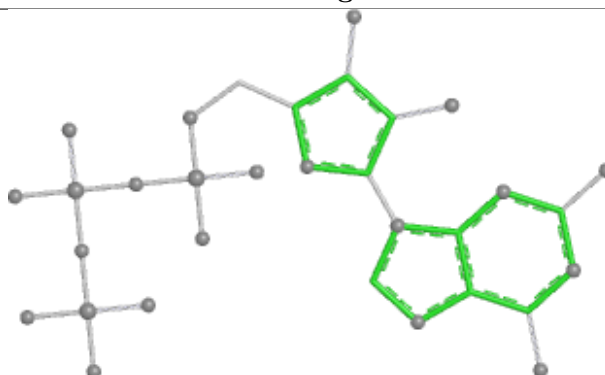
Bond lengths



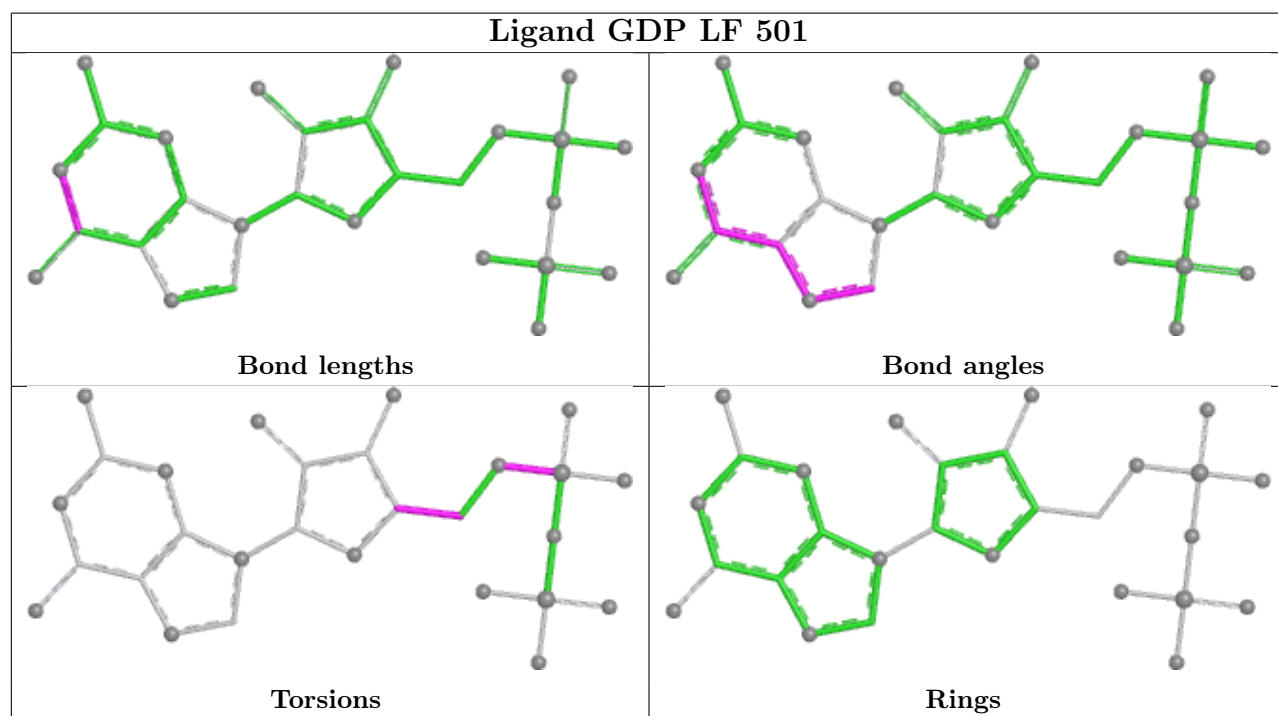
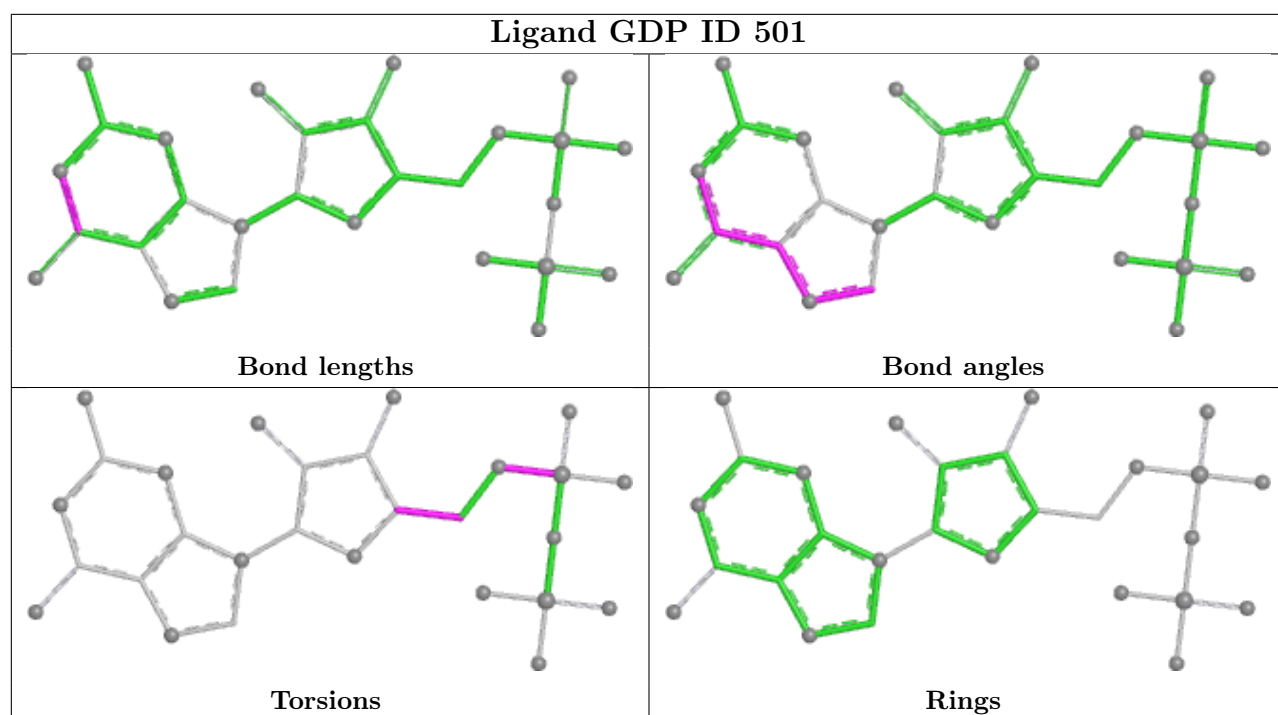
Bond angles

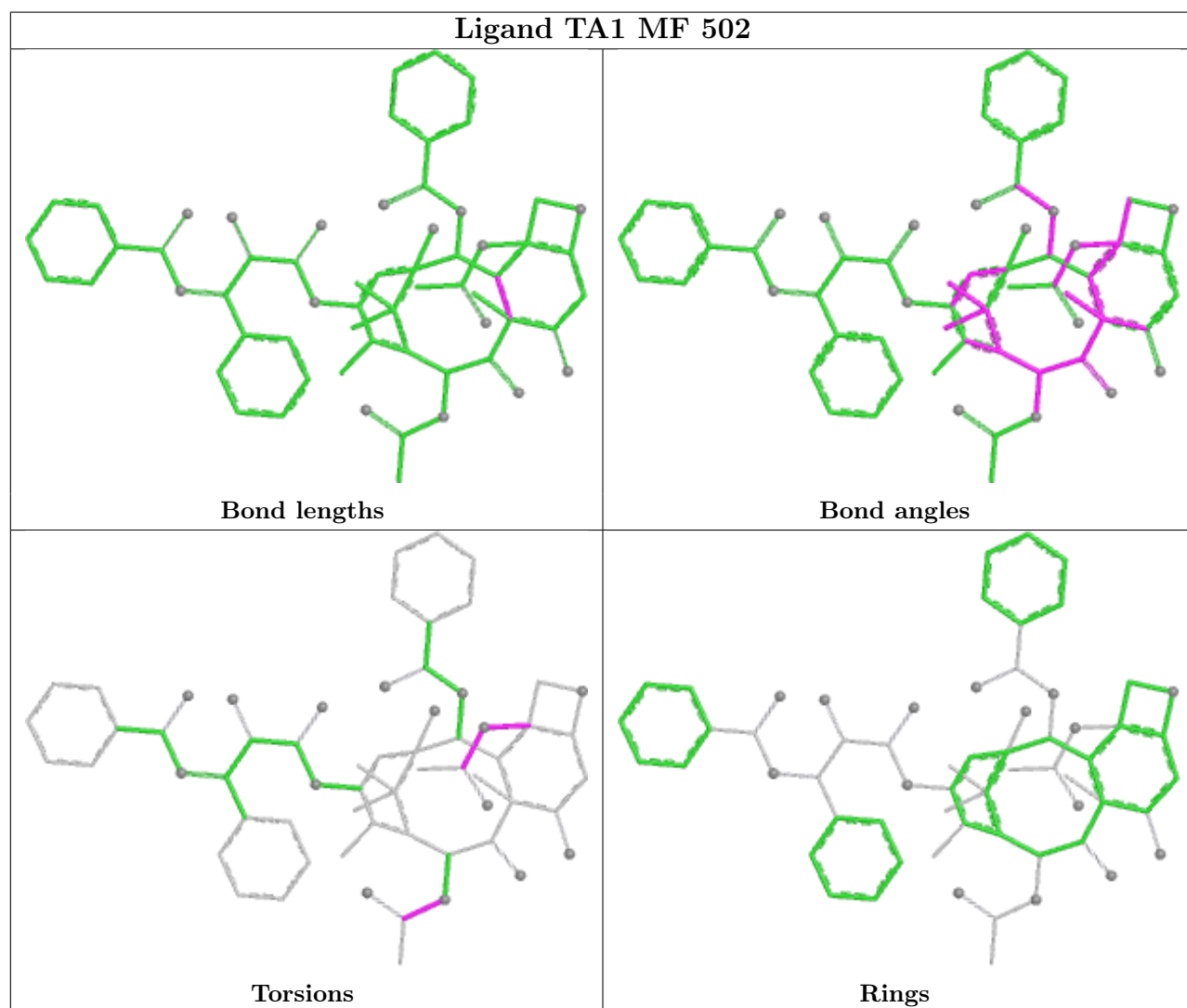
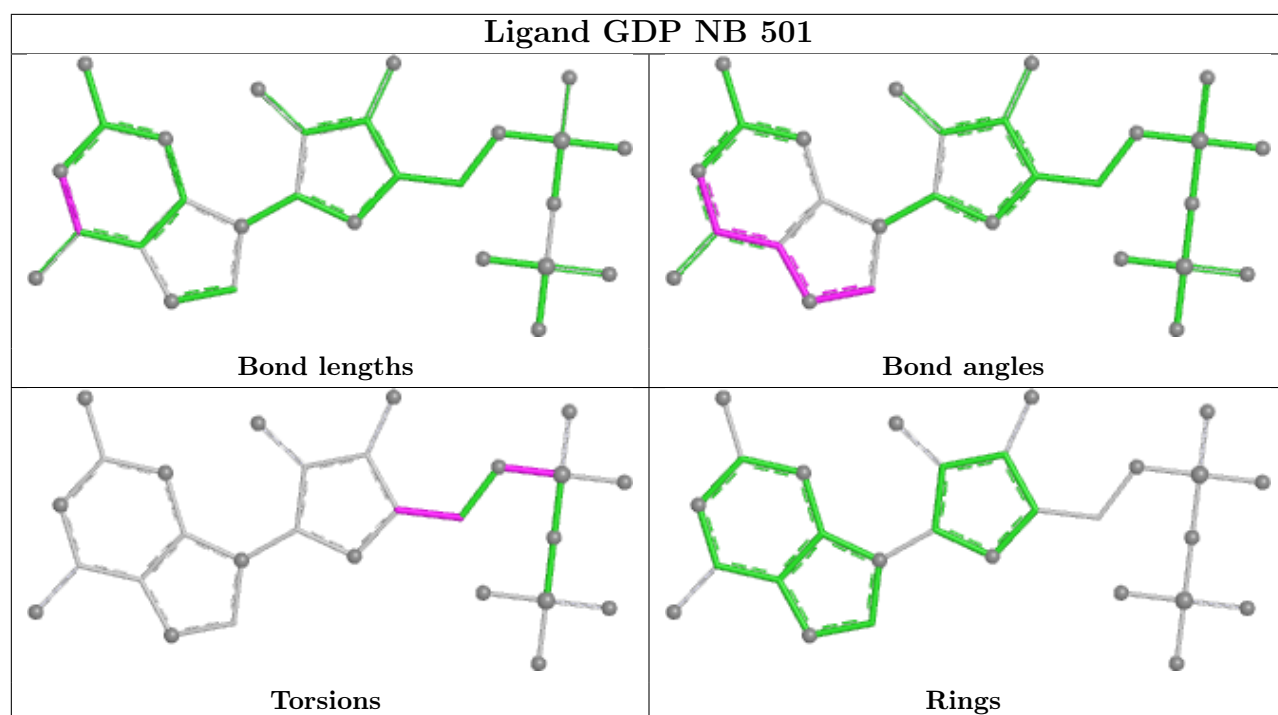


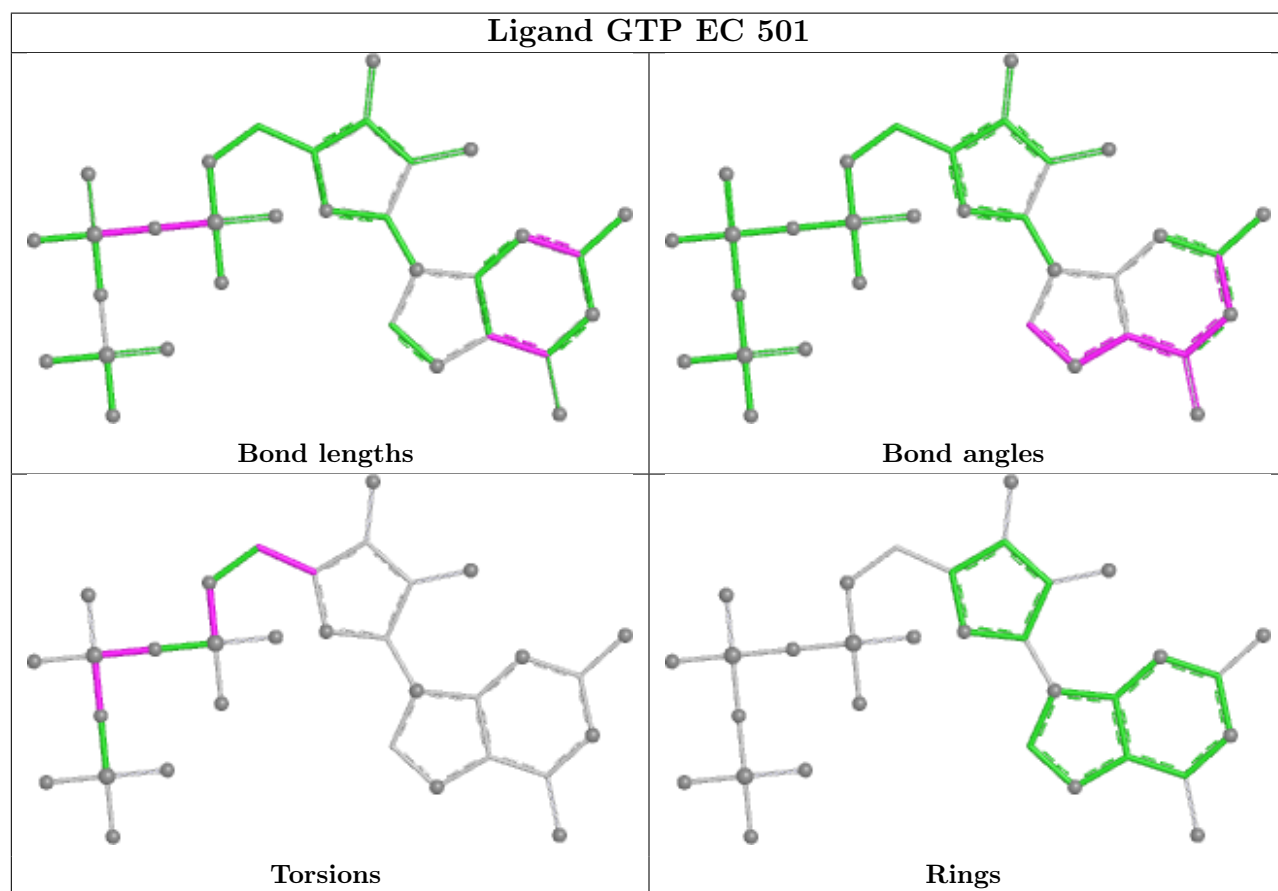
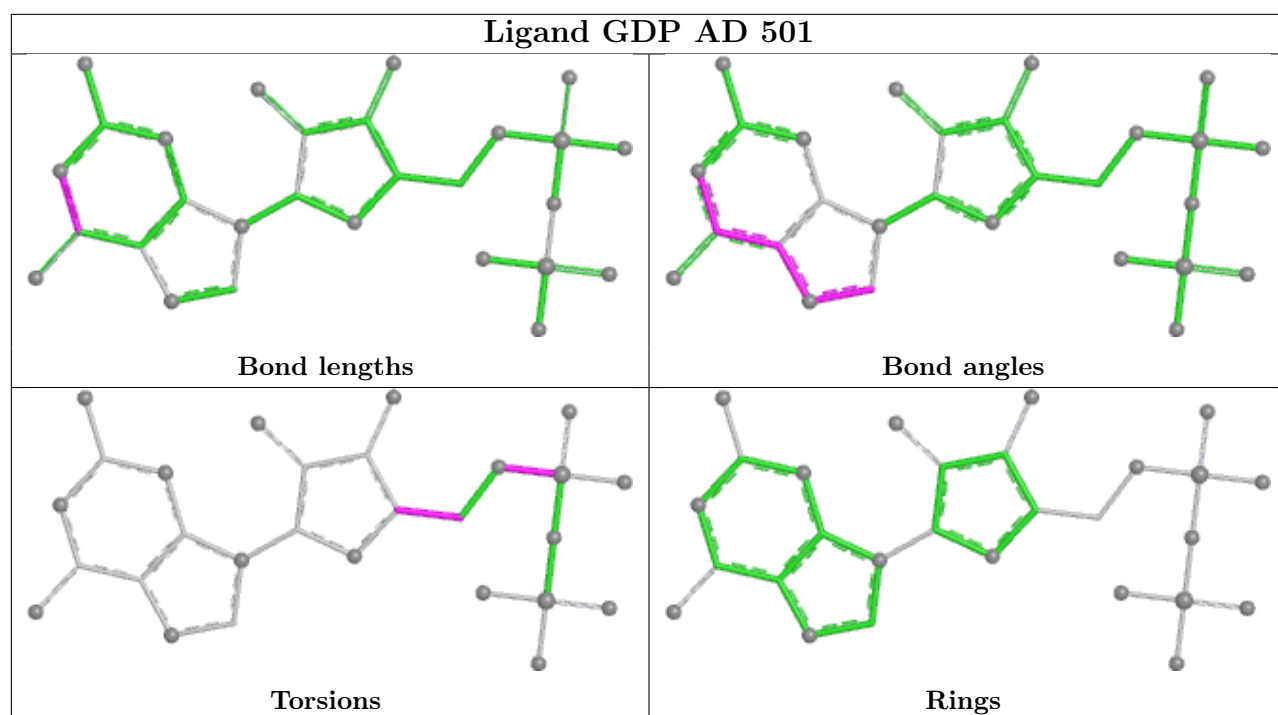
Torsions



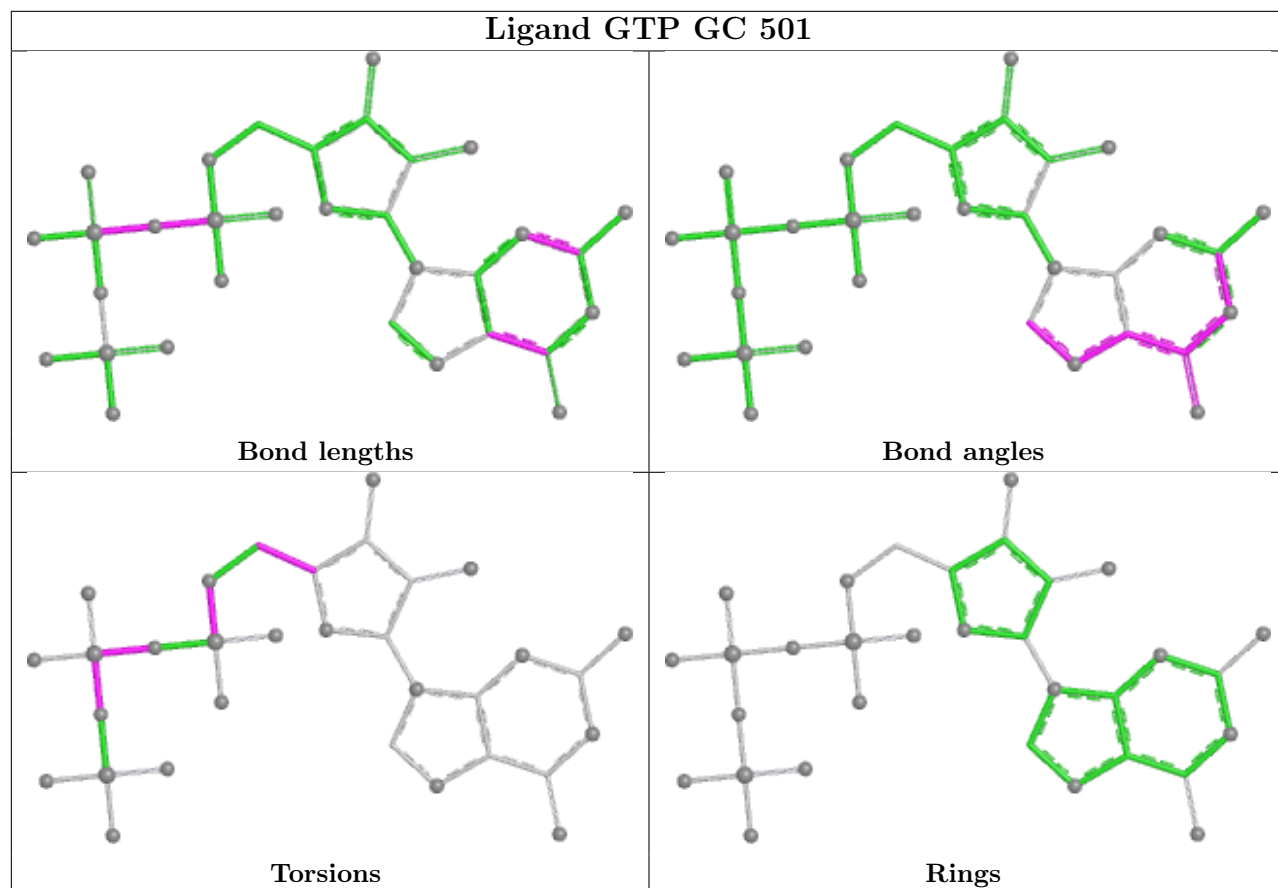
Rings



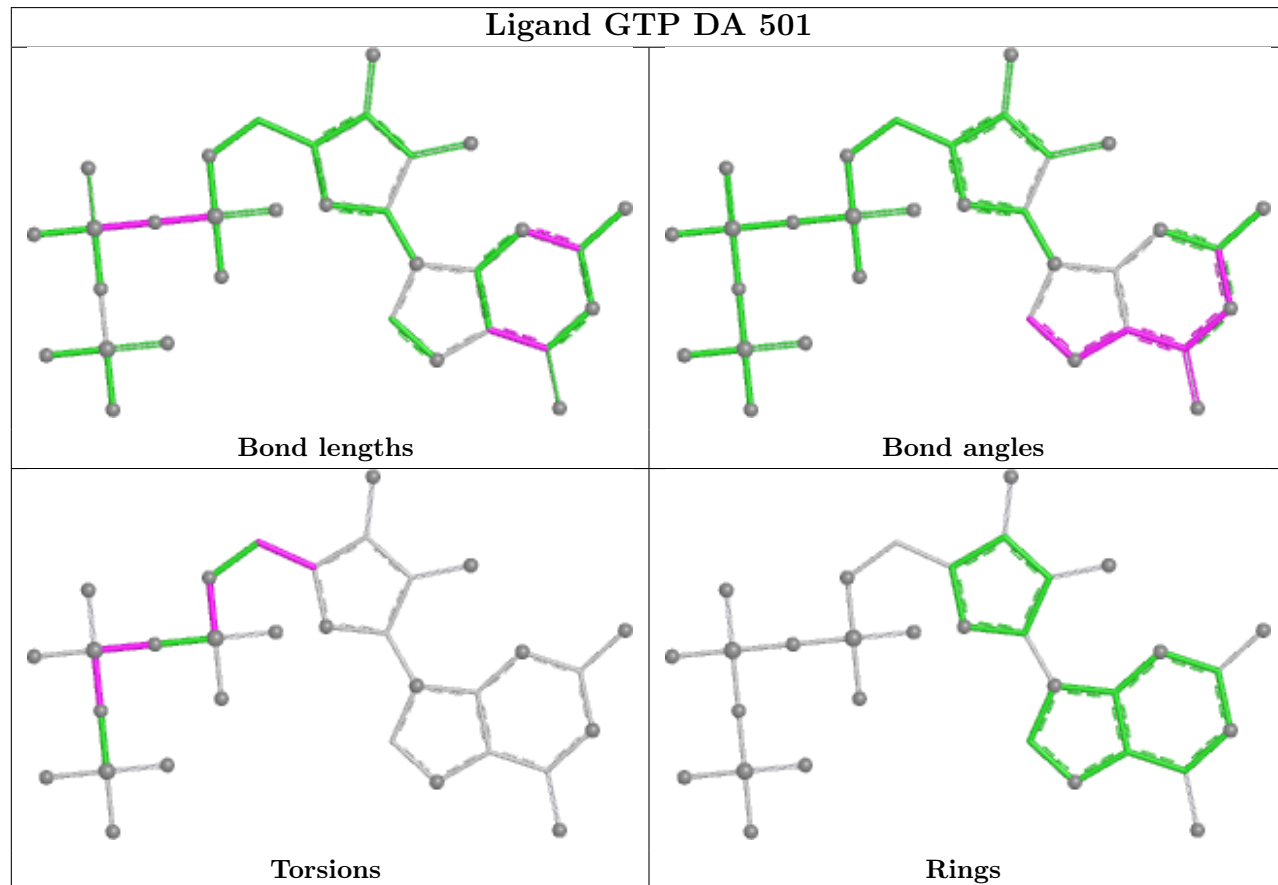


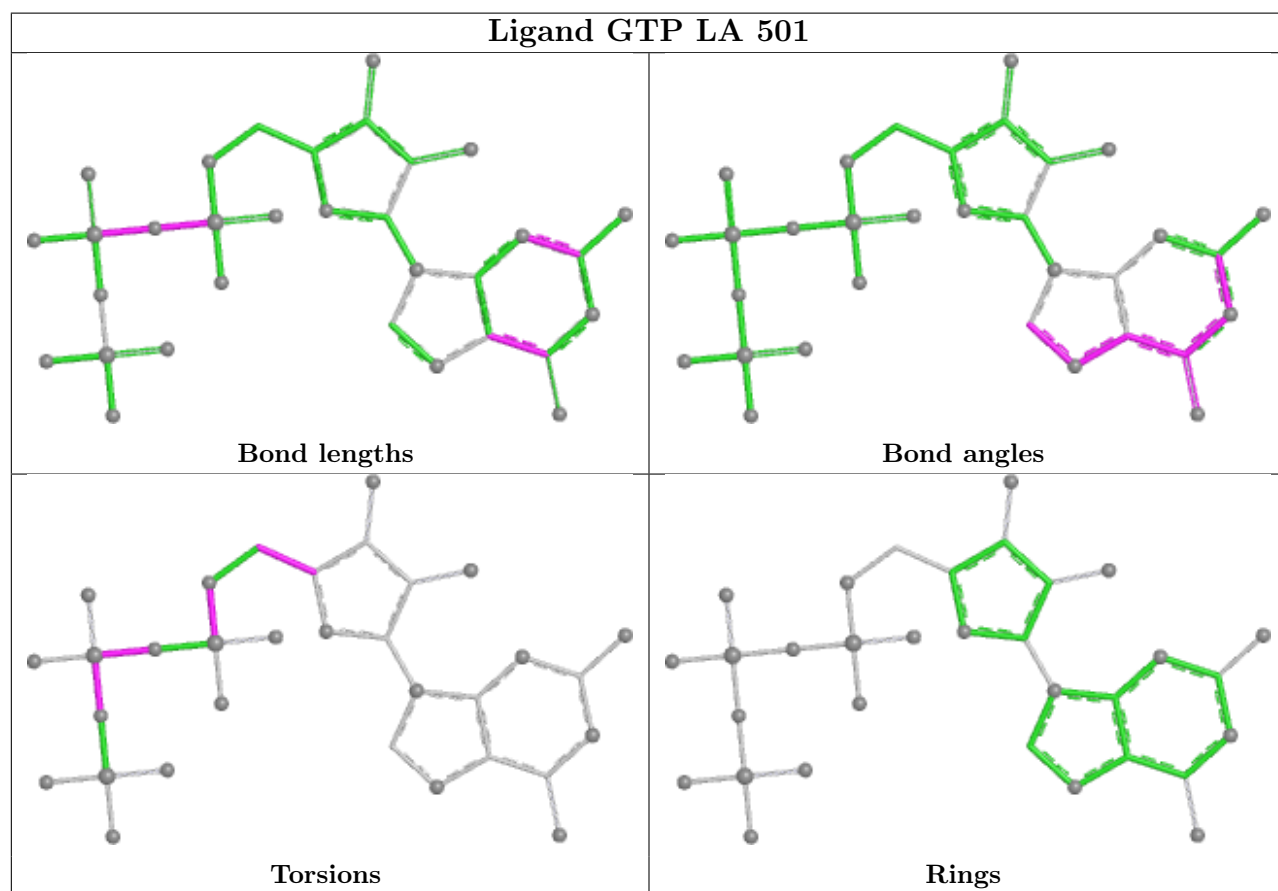
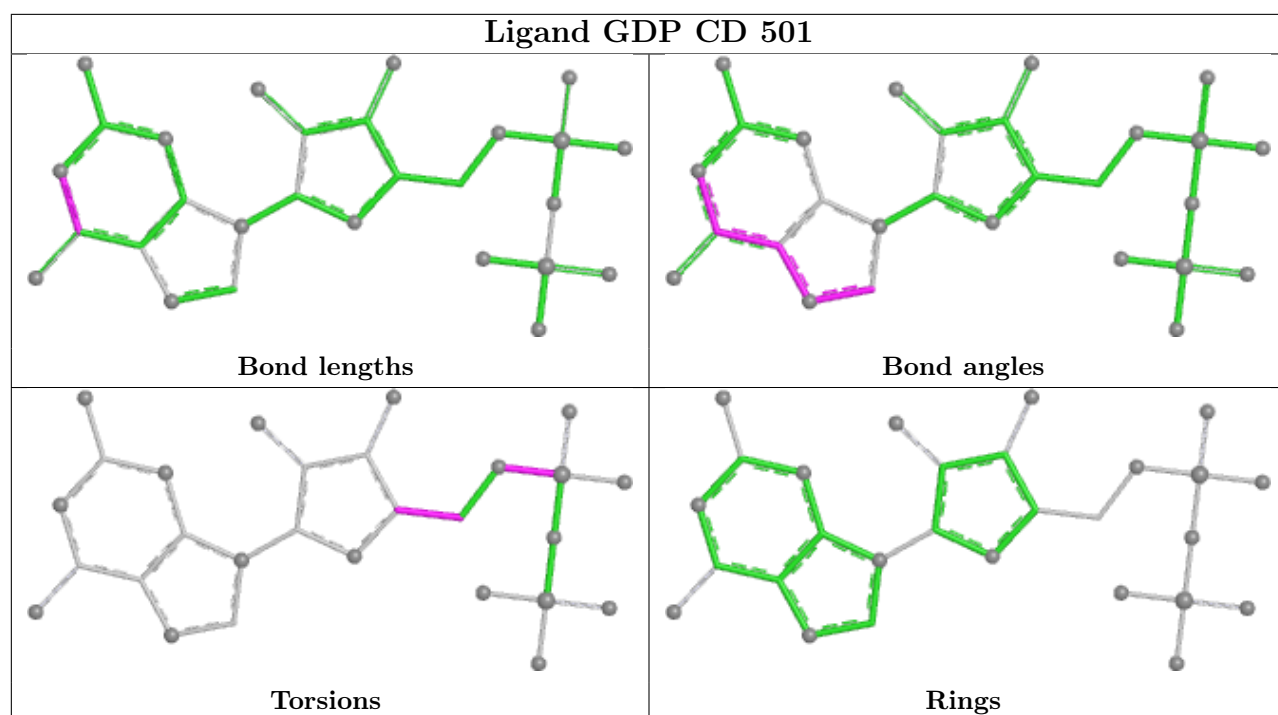


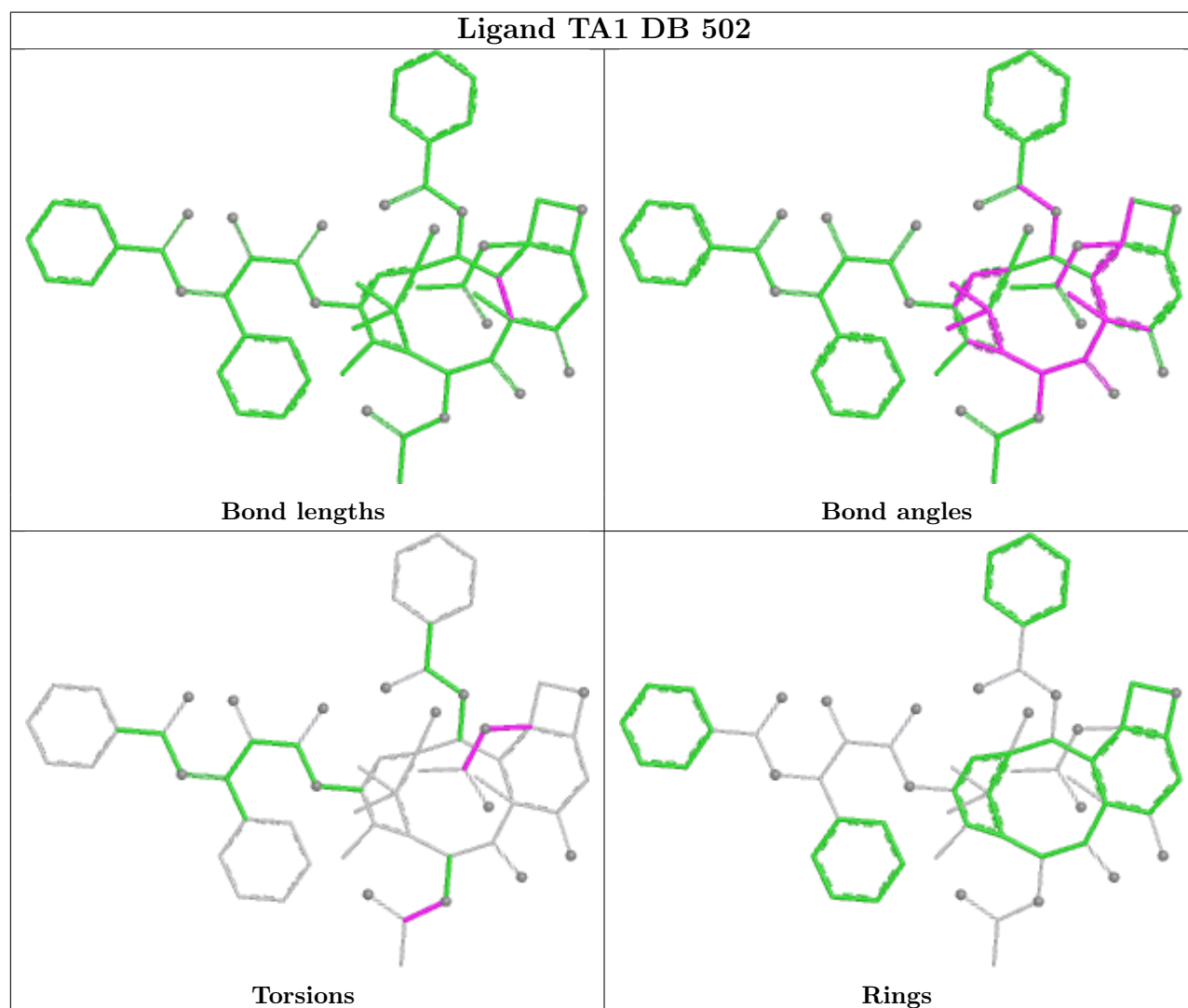
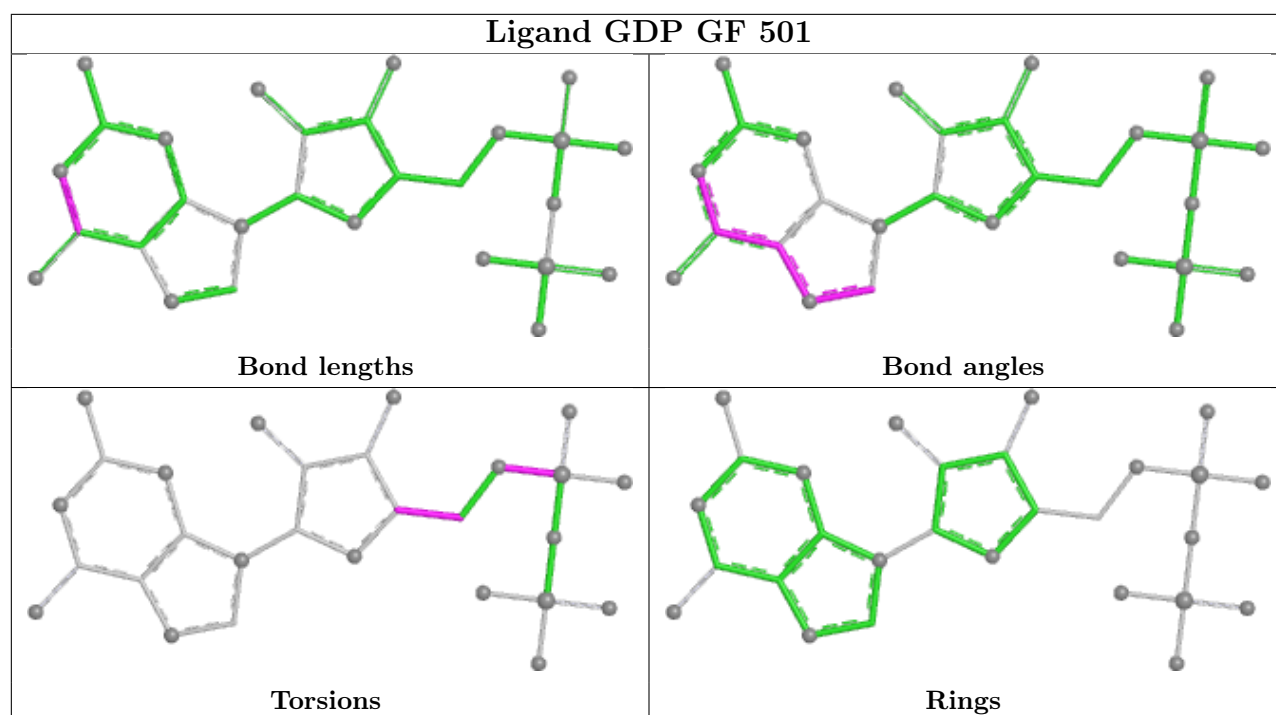
Ligand GTP GC 501



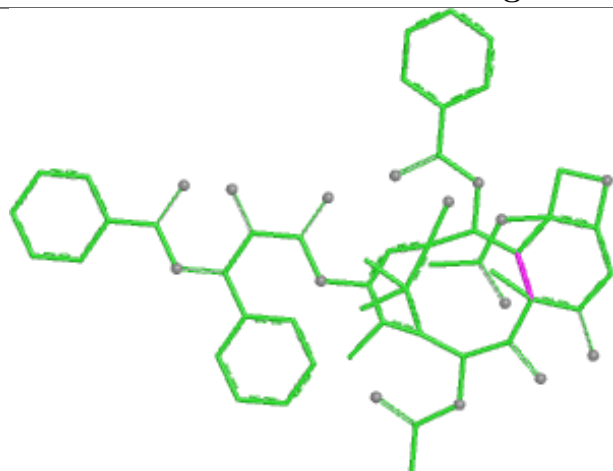
Ligand GTP DA 501



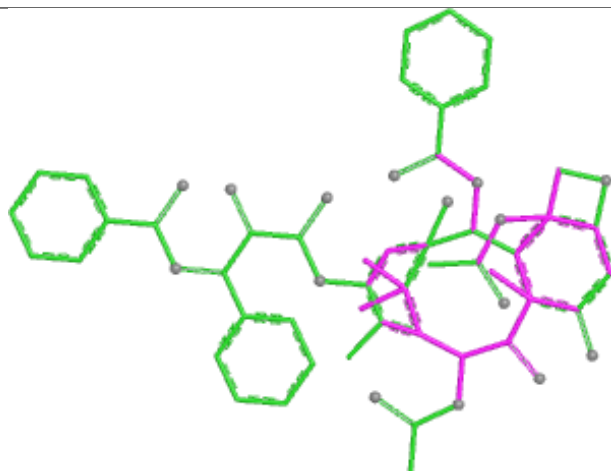




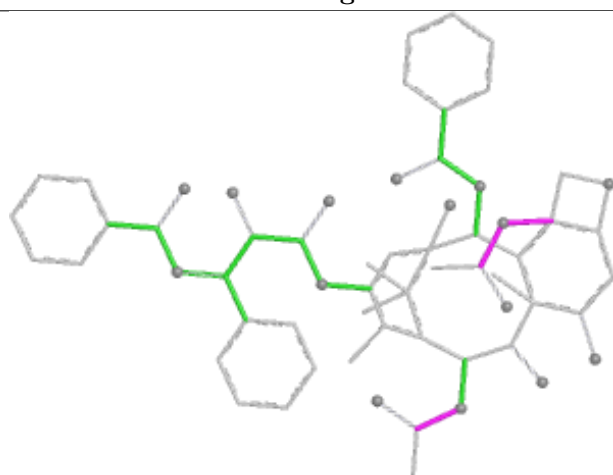
Ligand TA1 ND 502



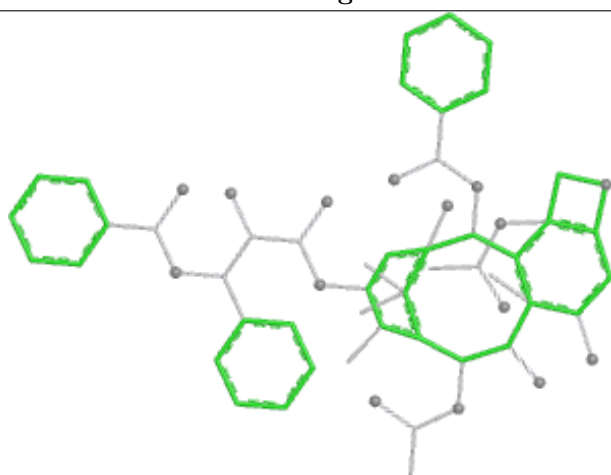
Bond lengths



Bond angles

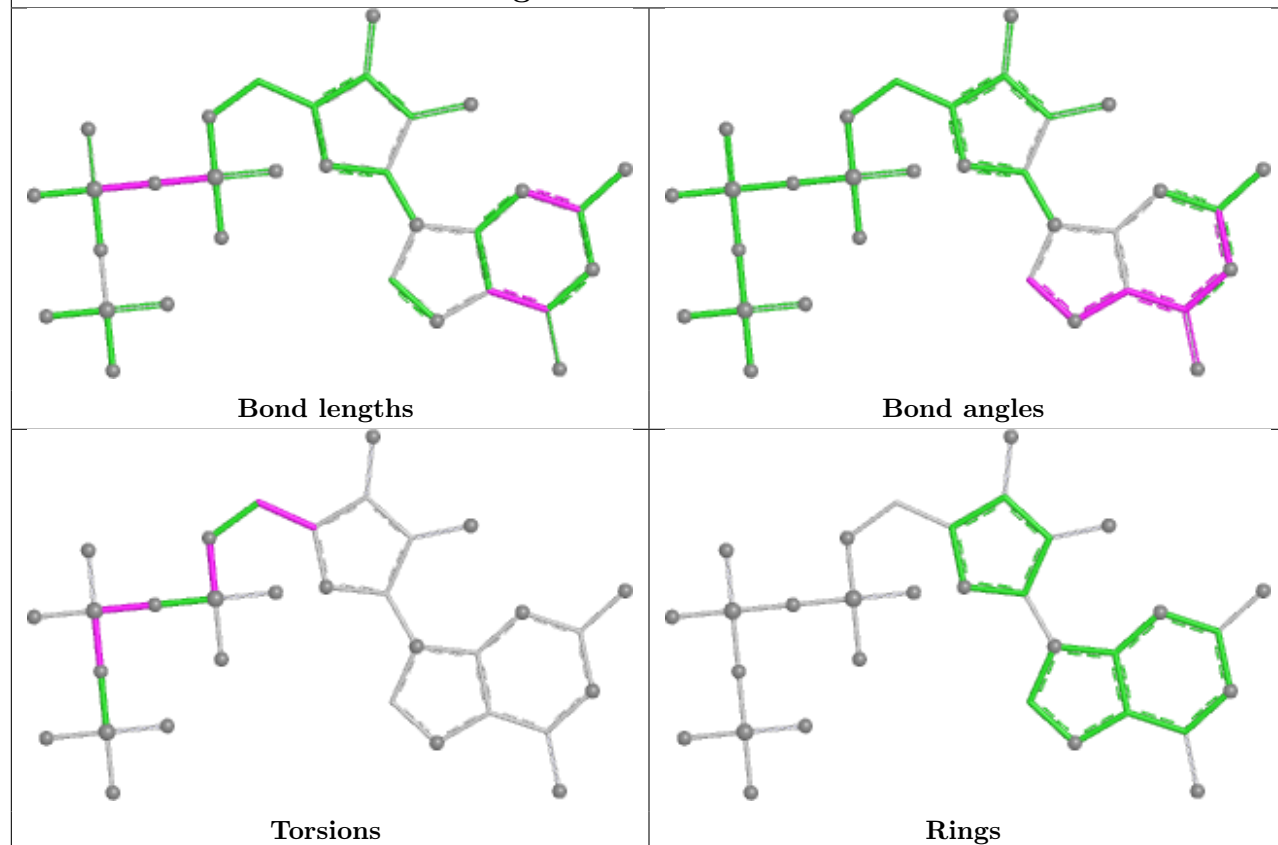


Torsions

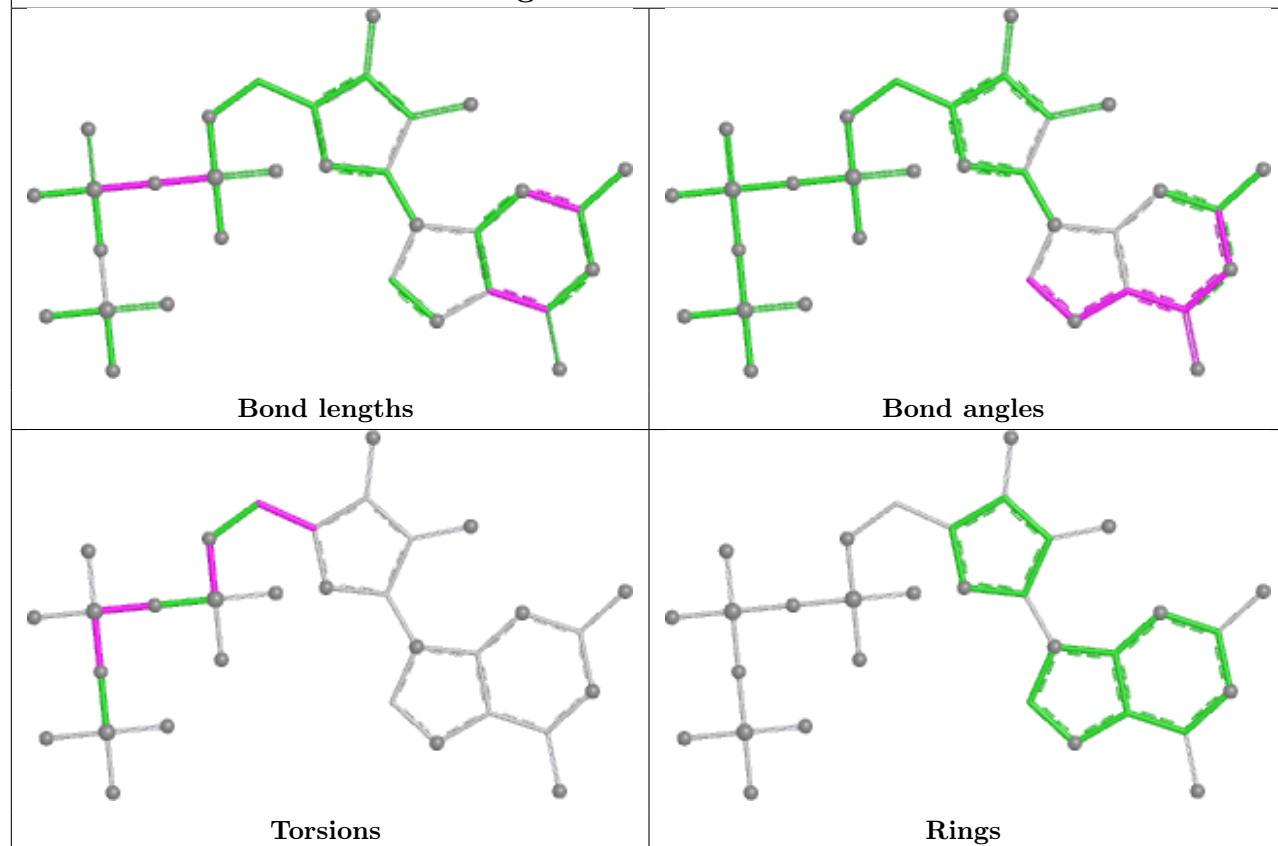


Rings

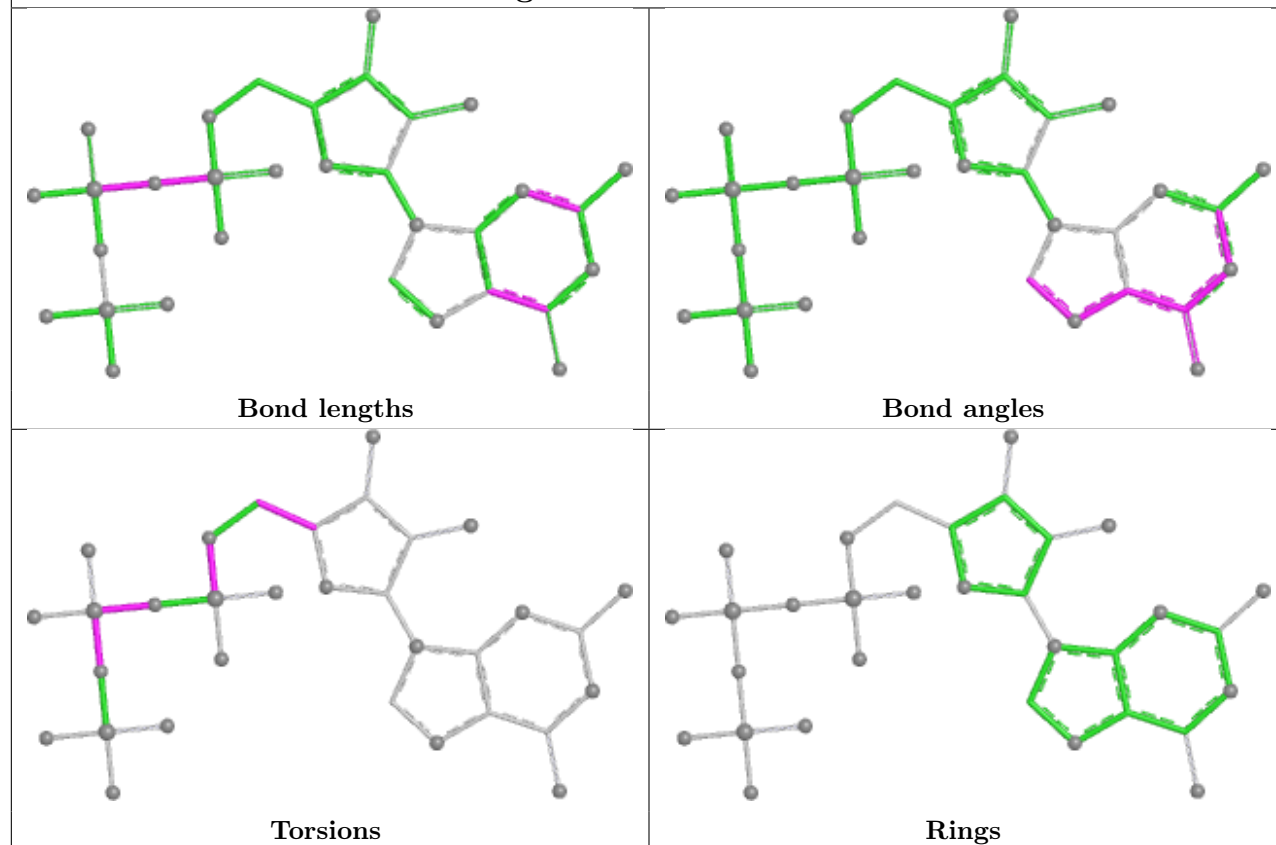
Ligand GTP MA 501



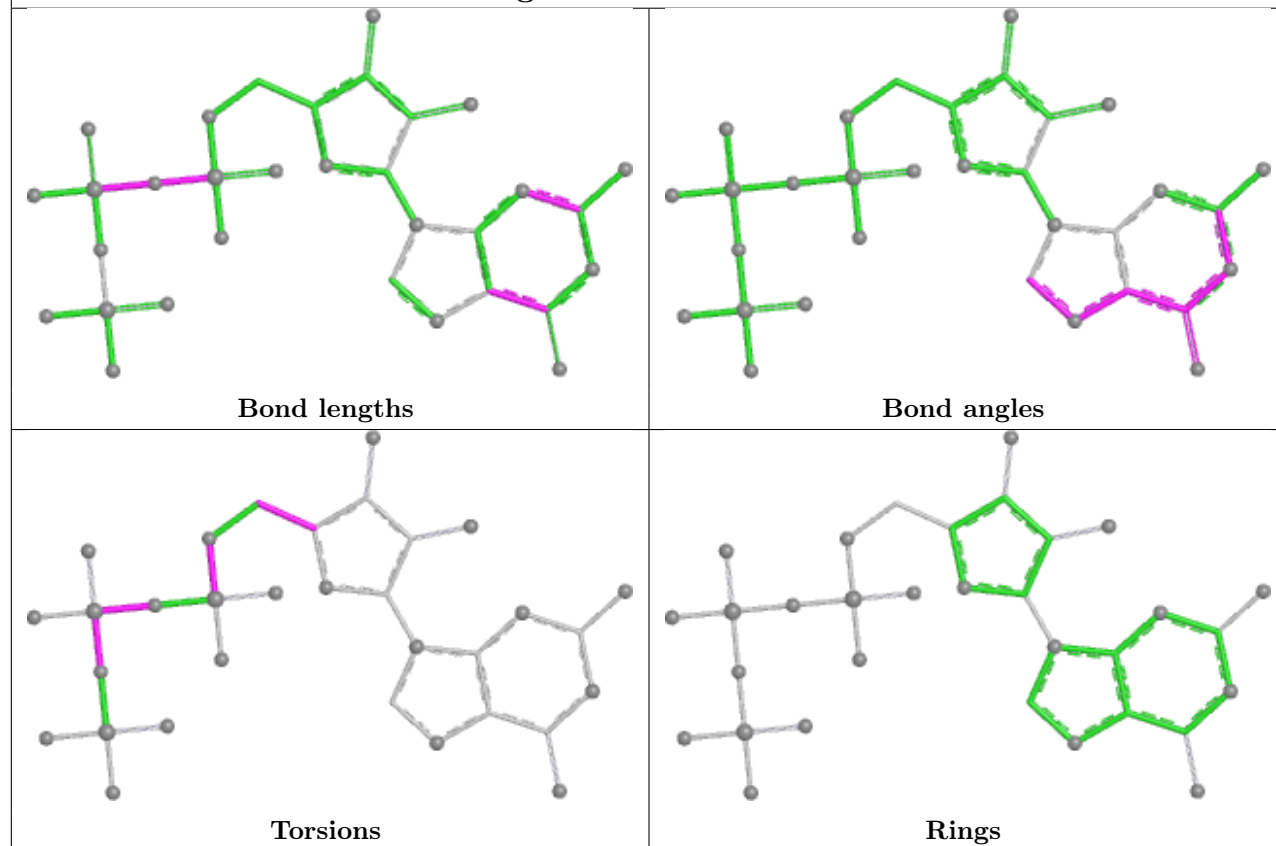
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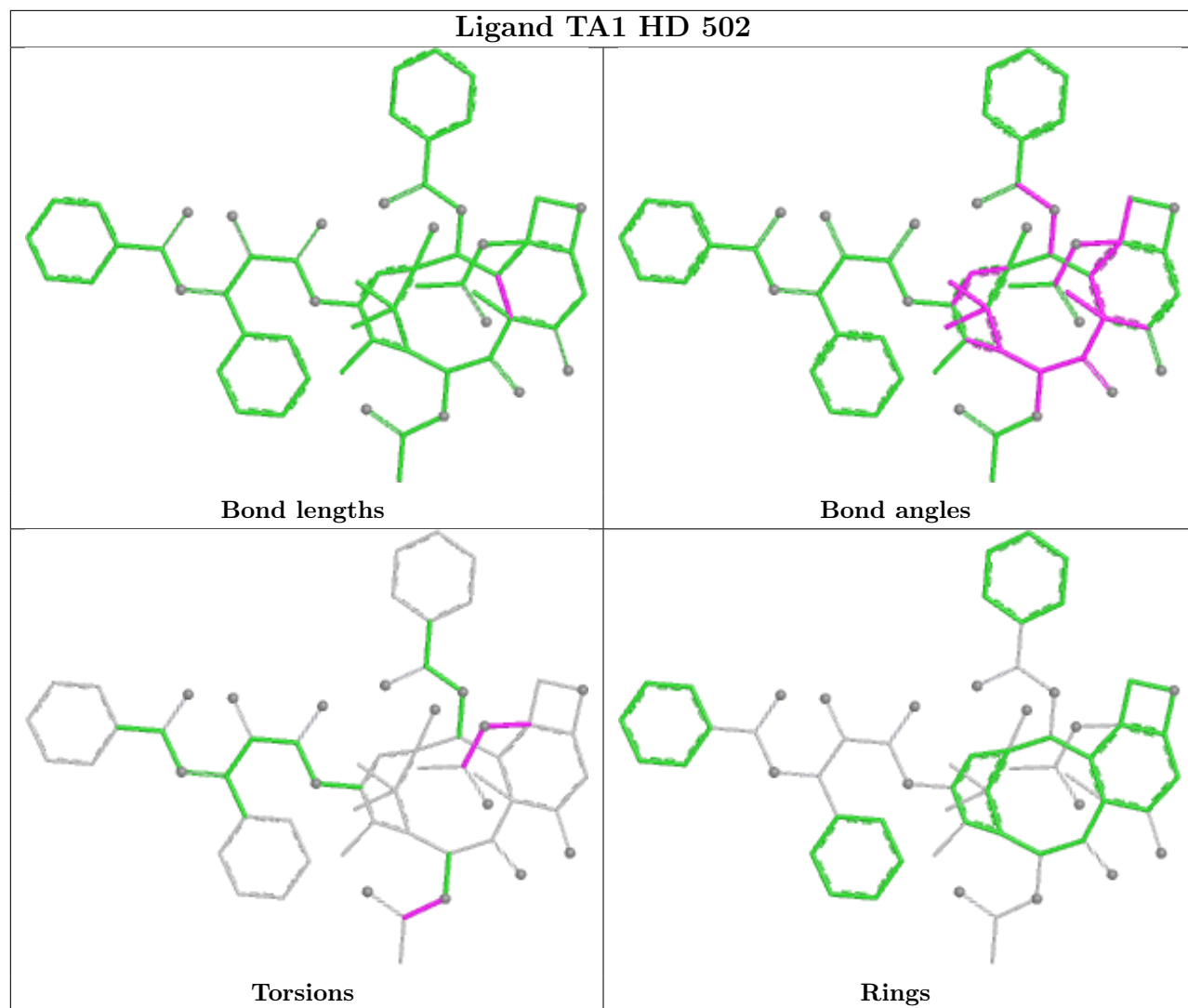


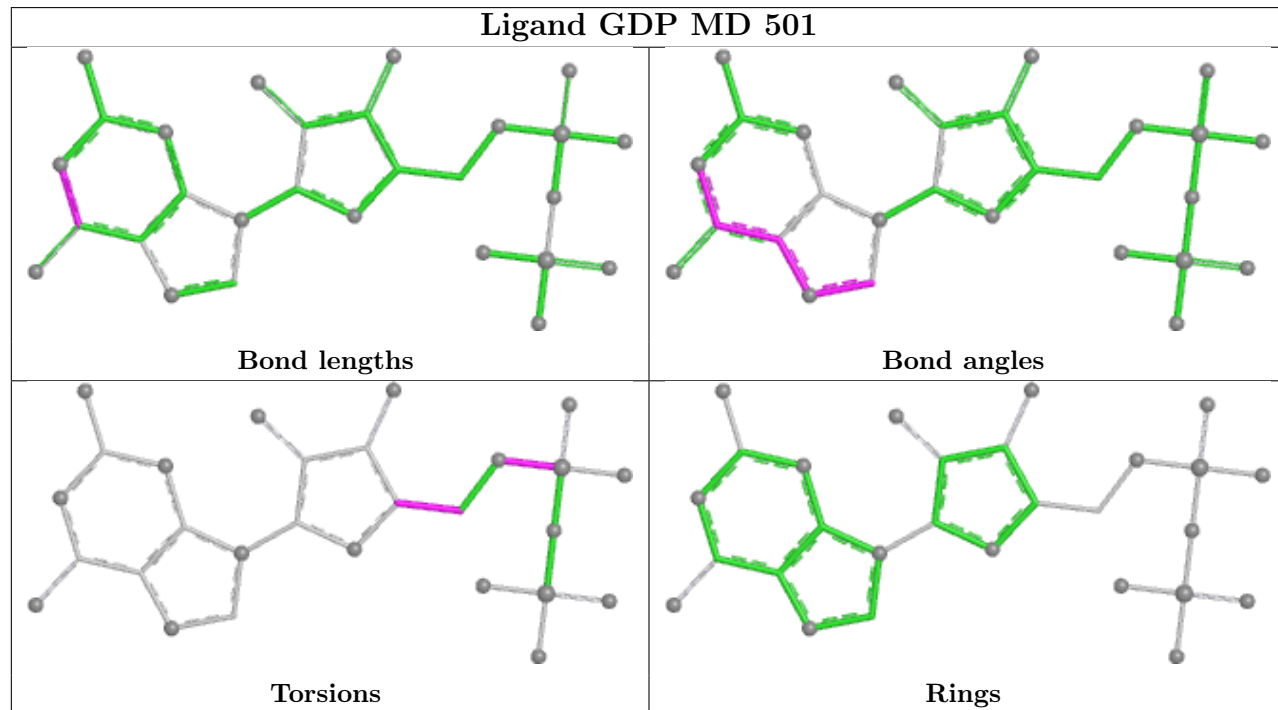
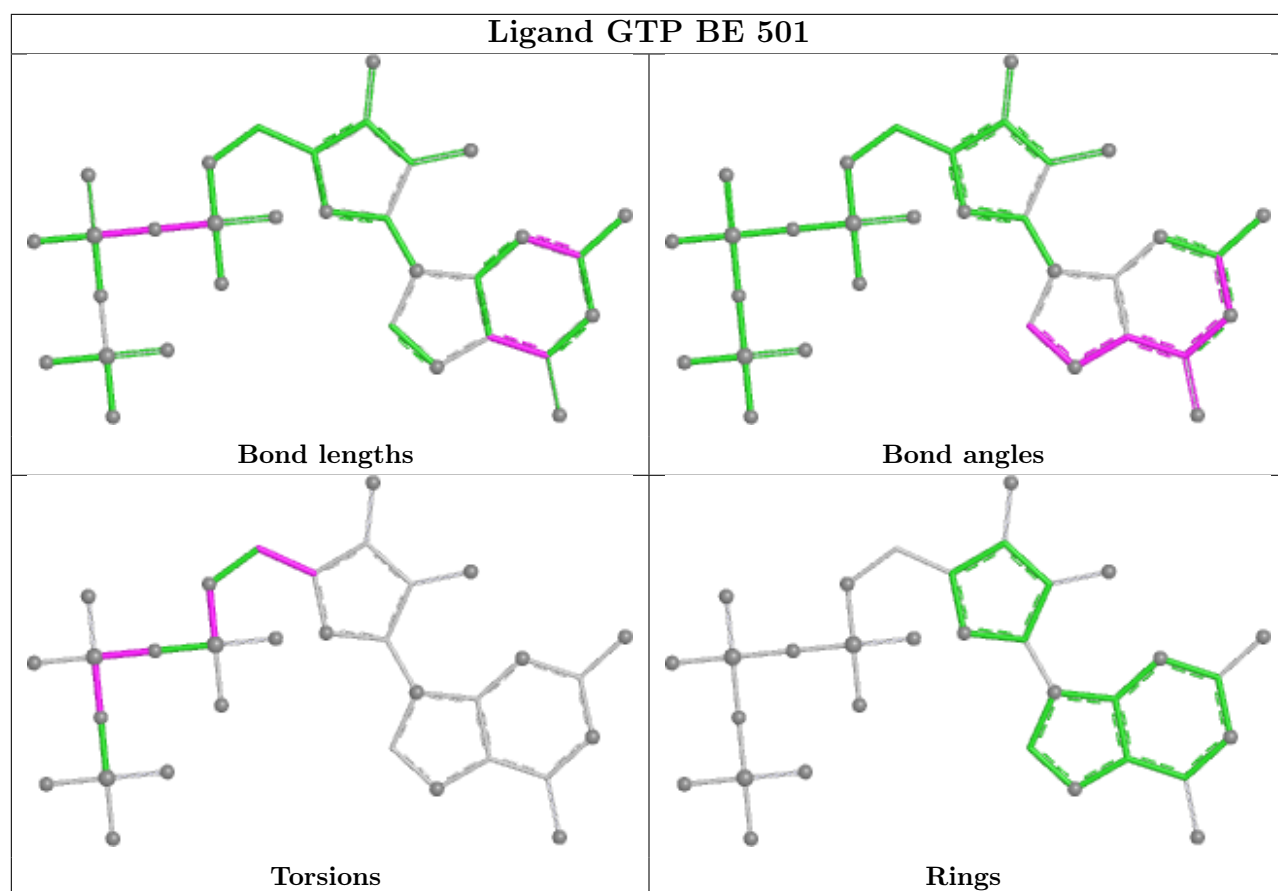
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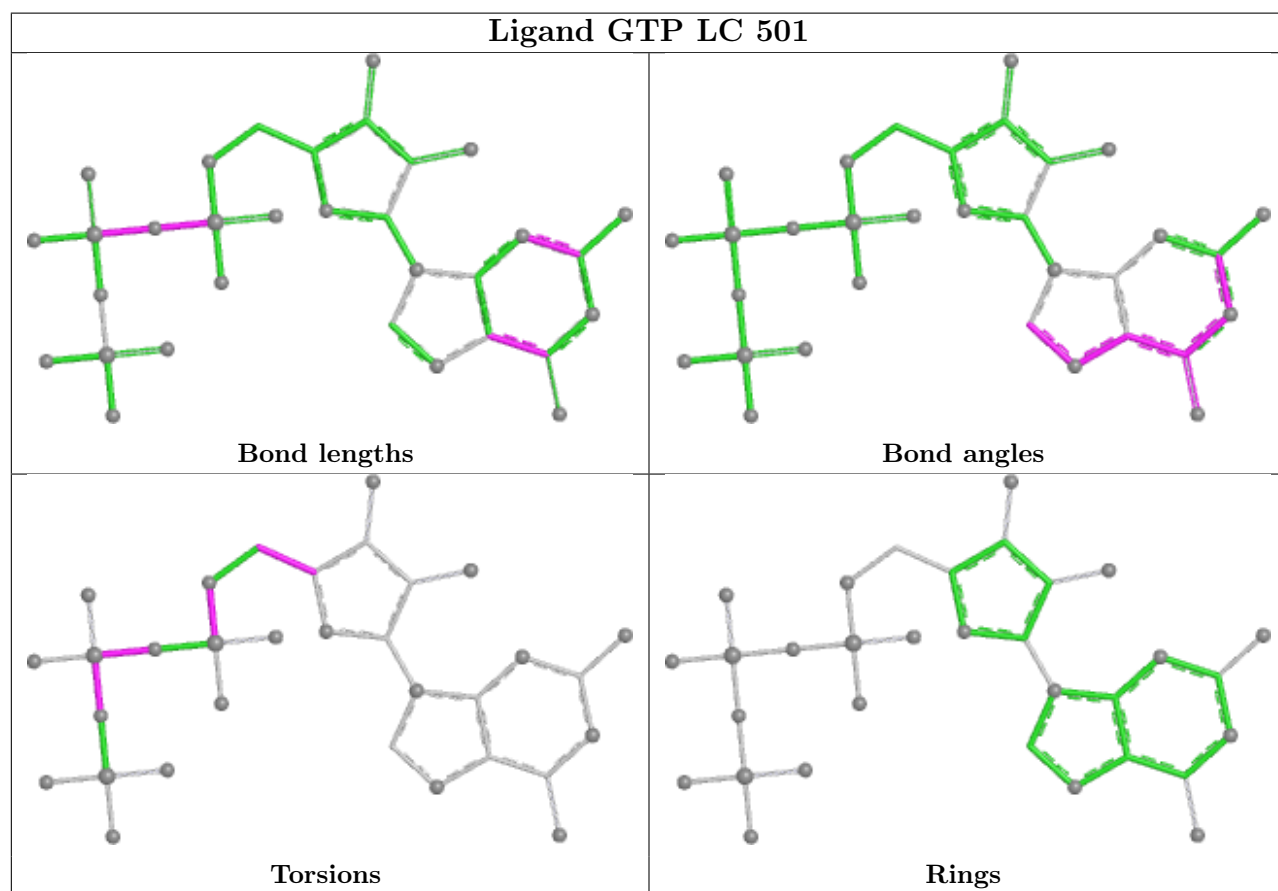
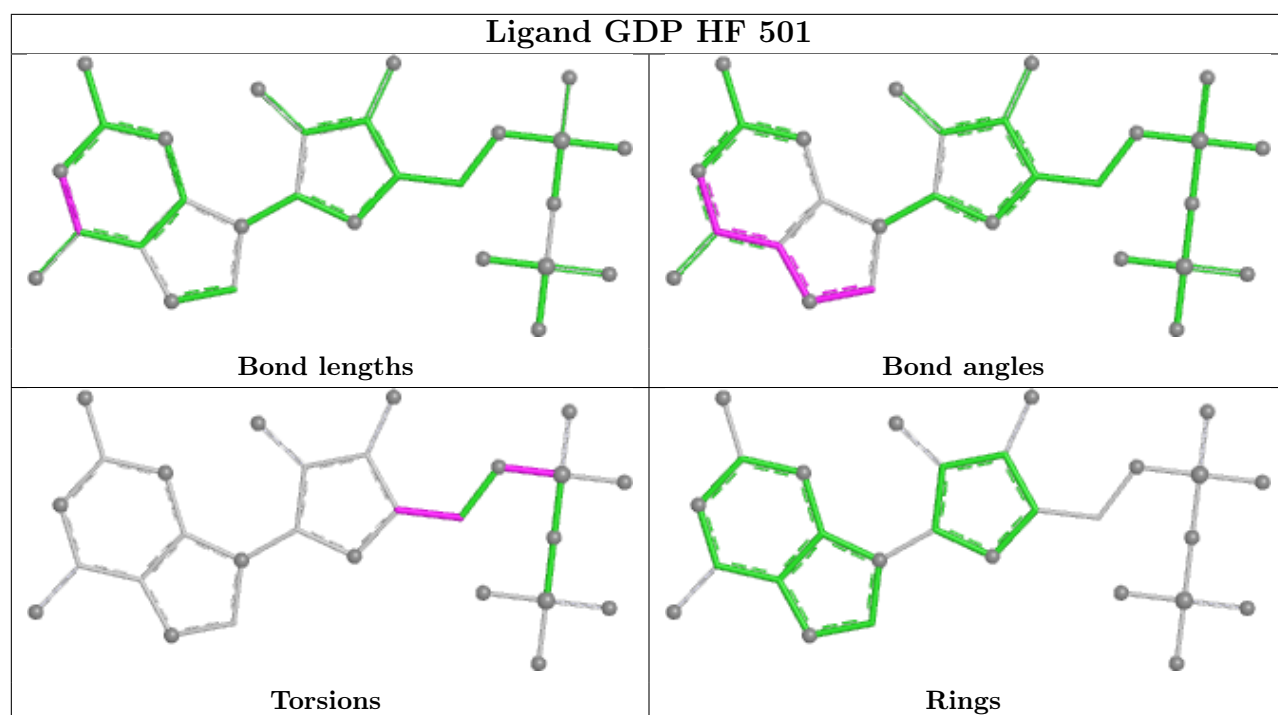


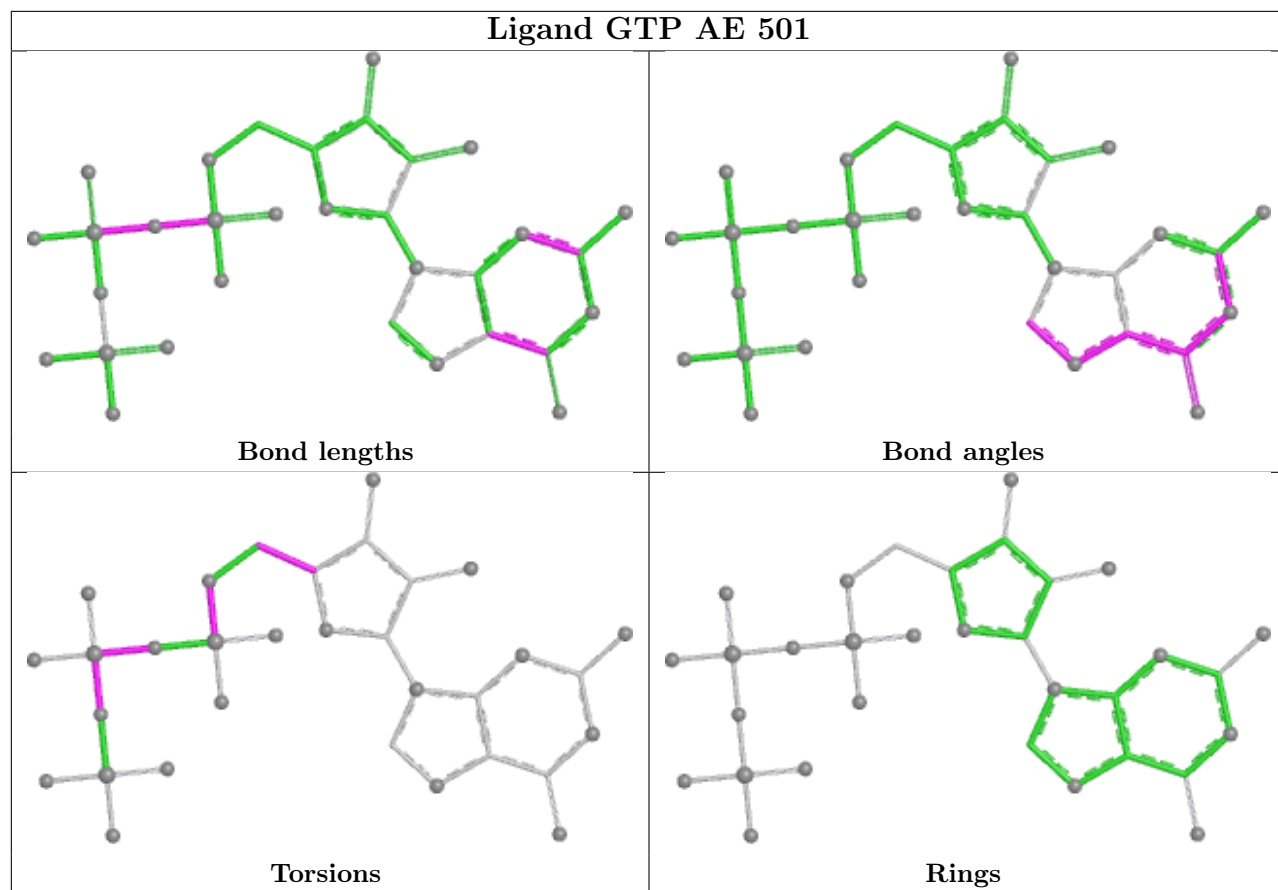
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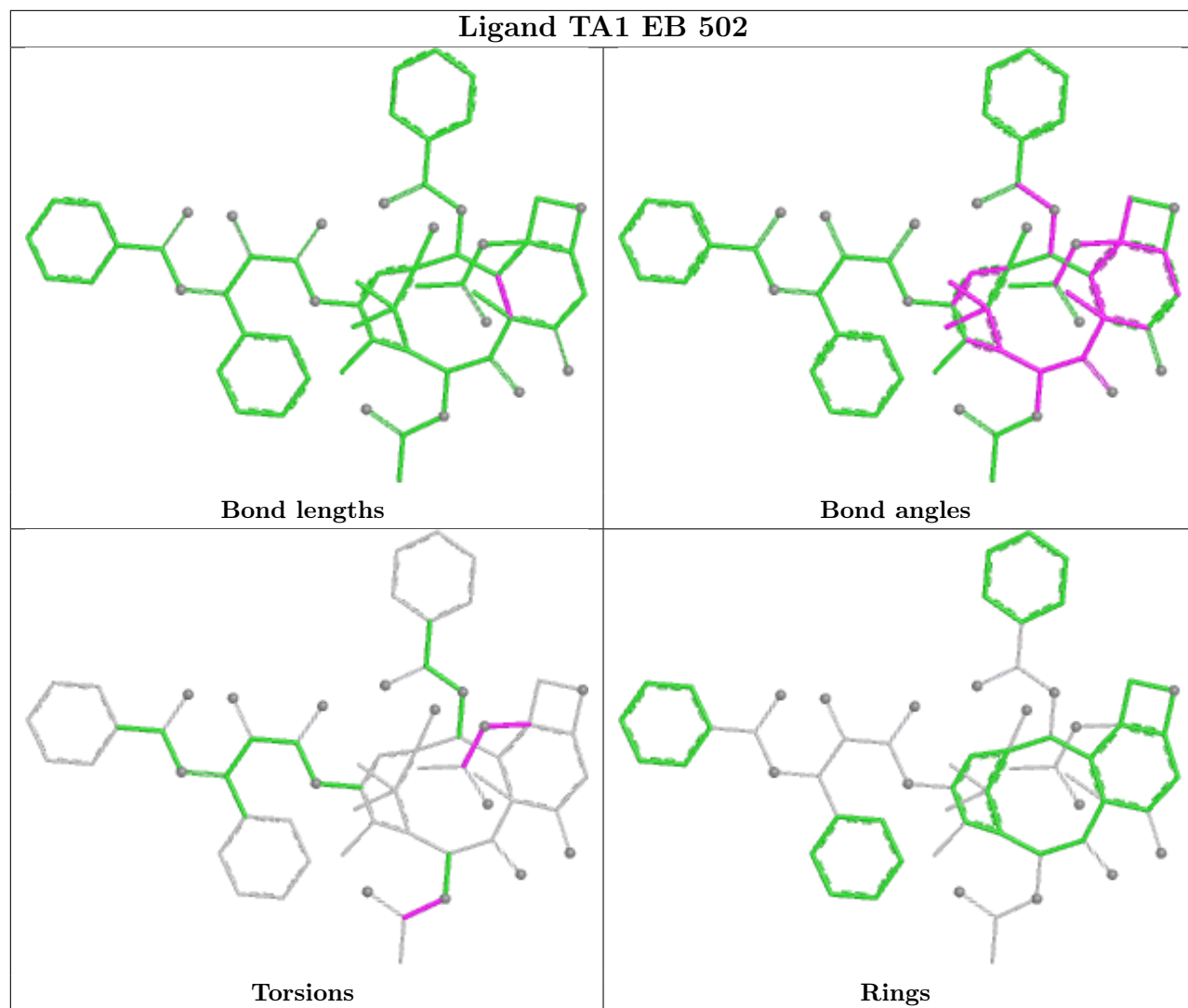


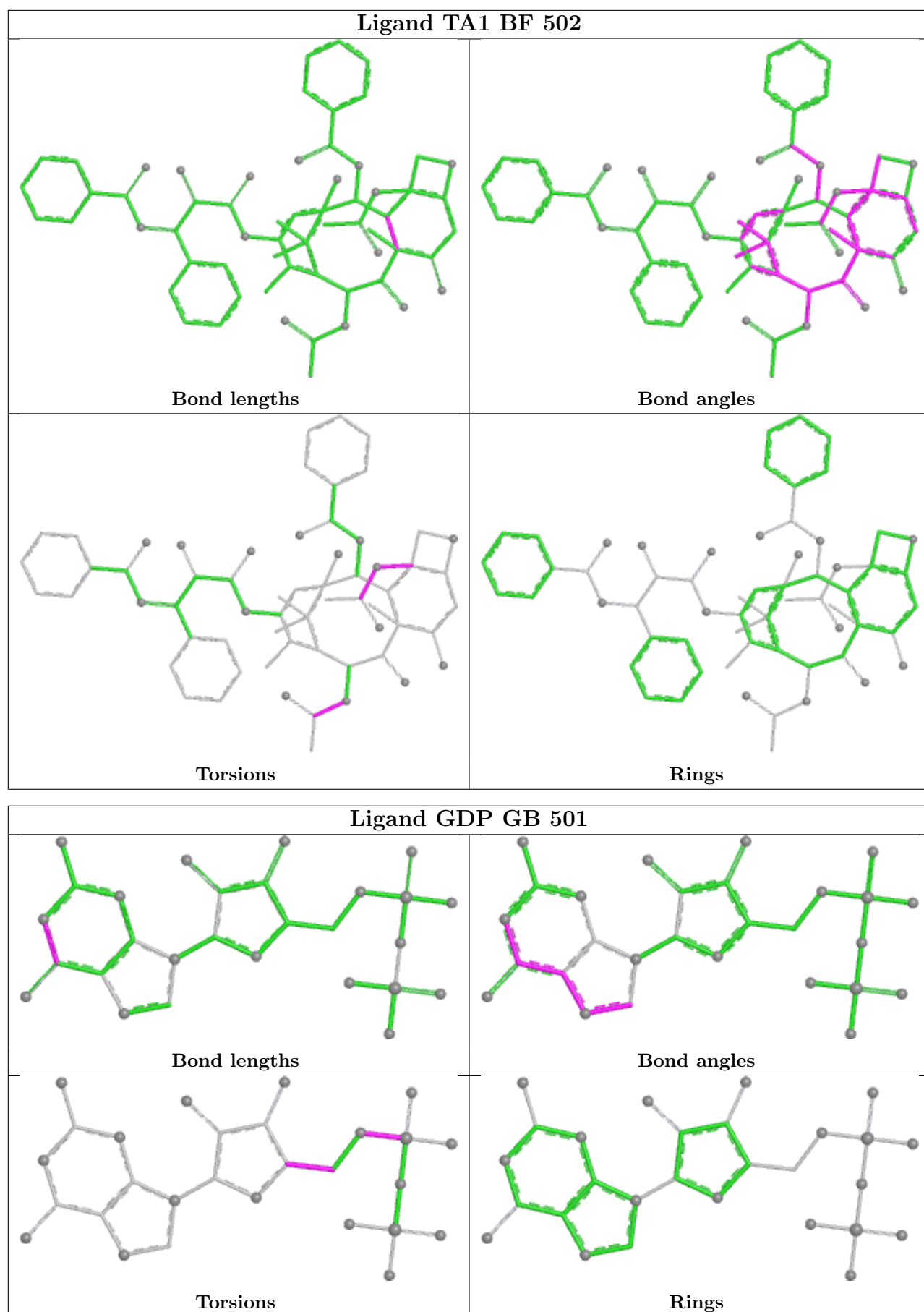


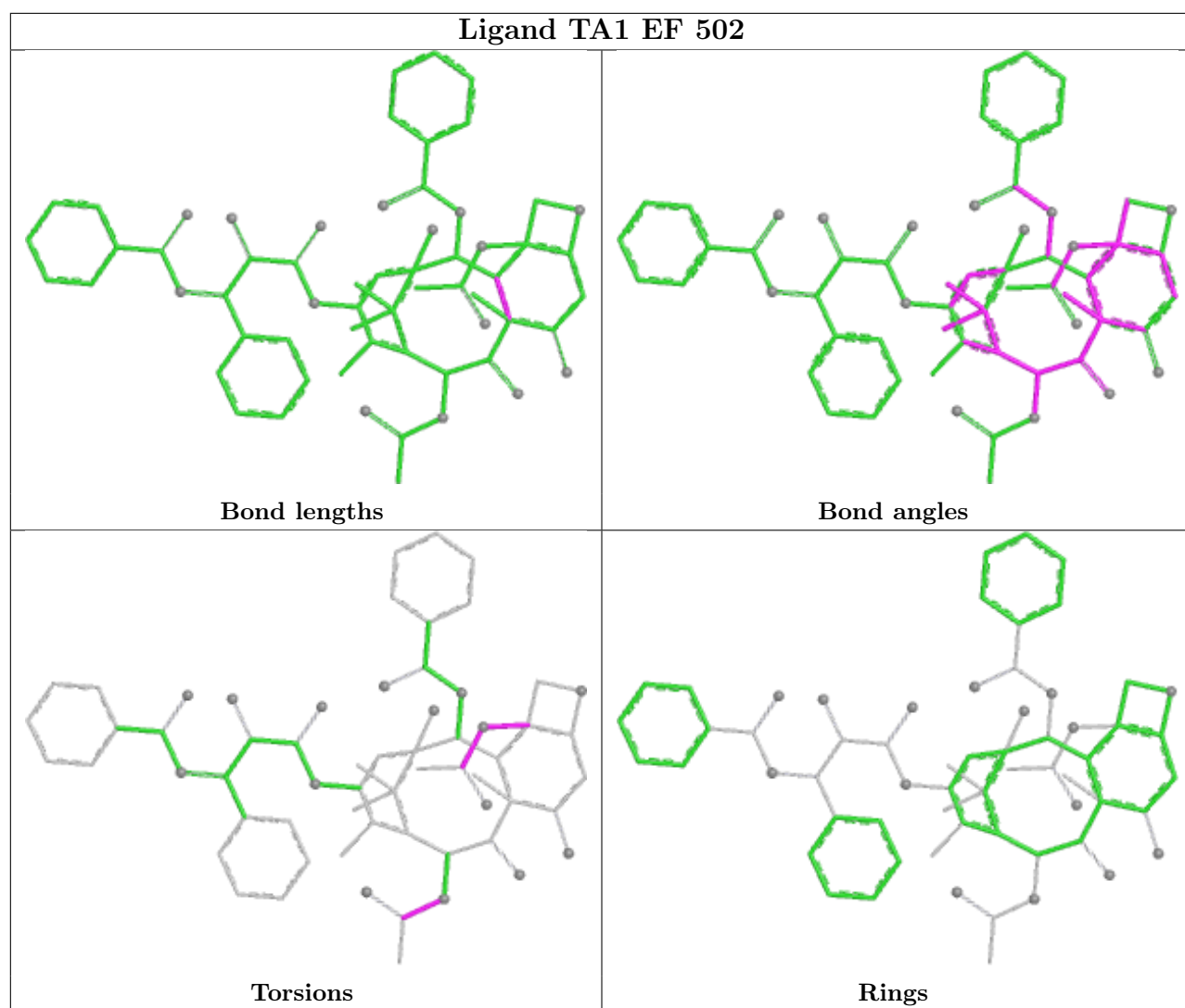




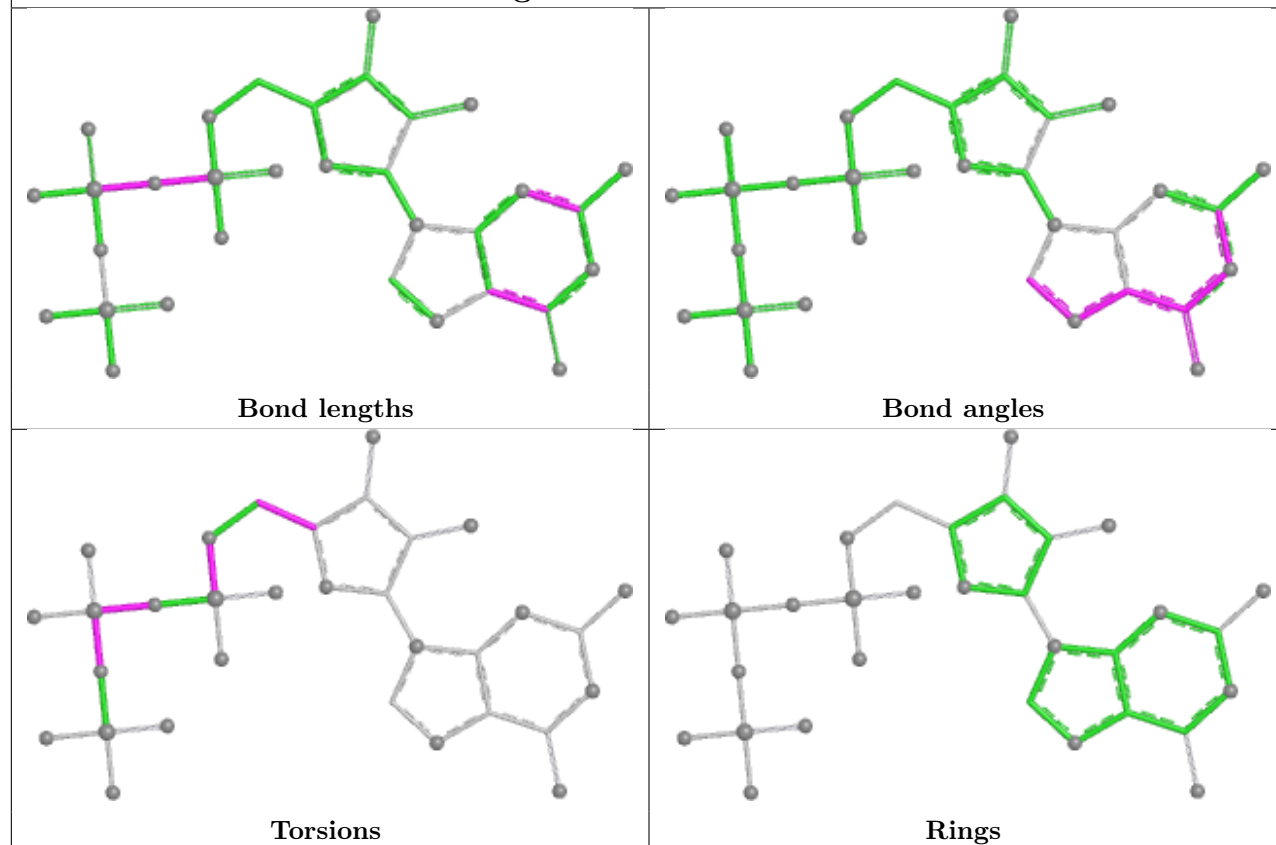




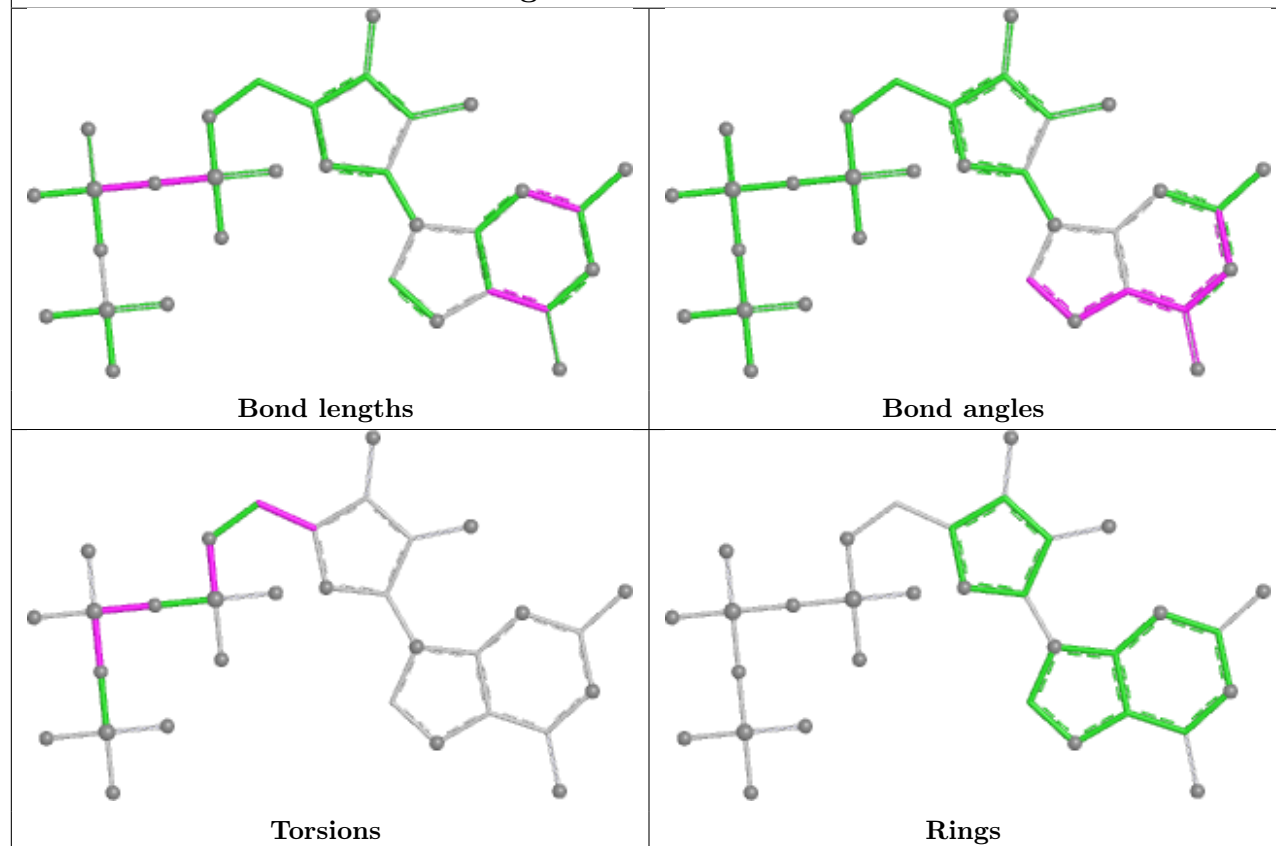


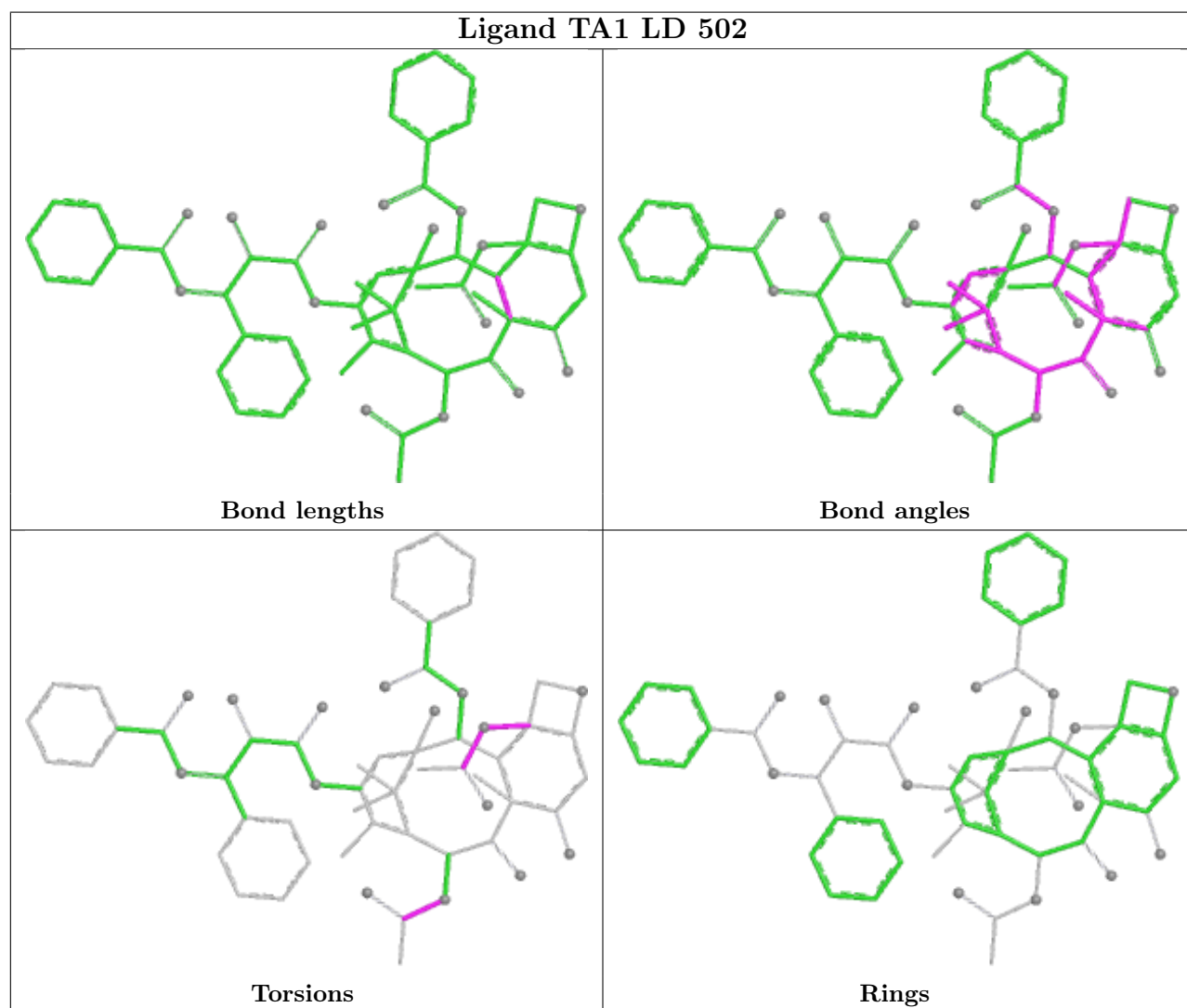
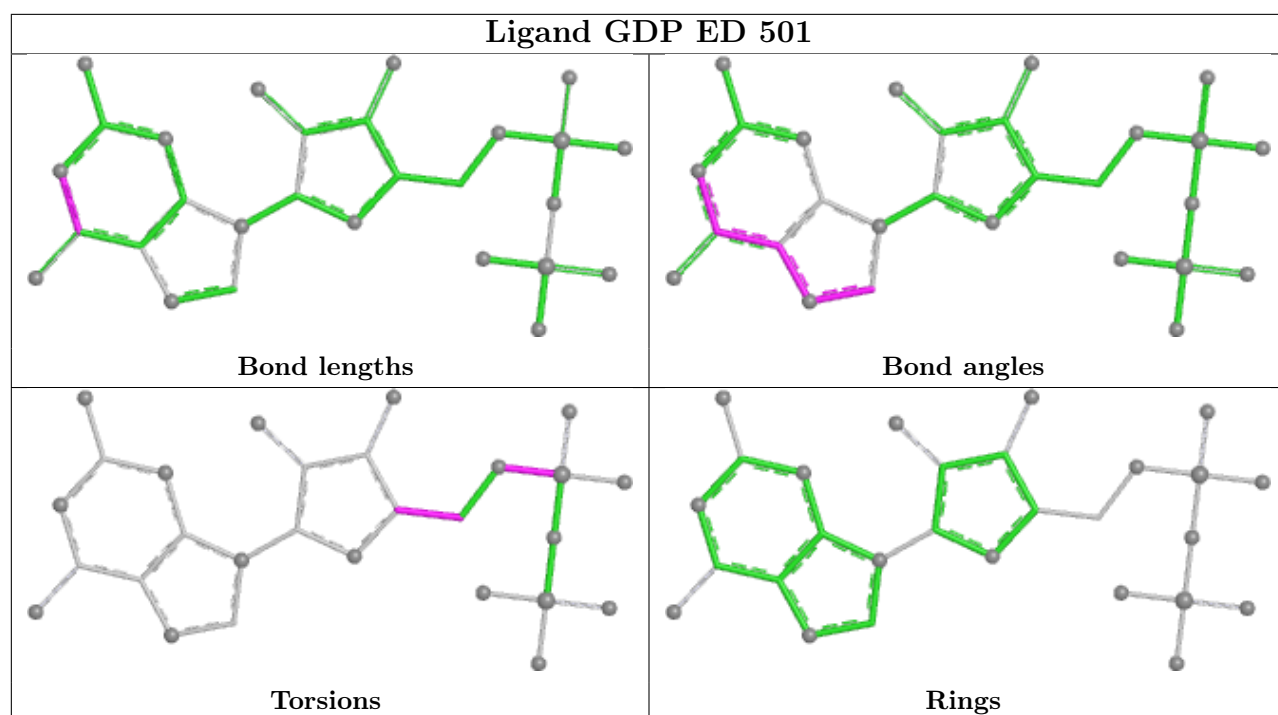


Ligand GTP MC 501

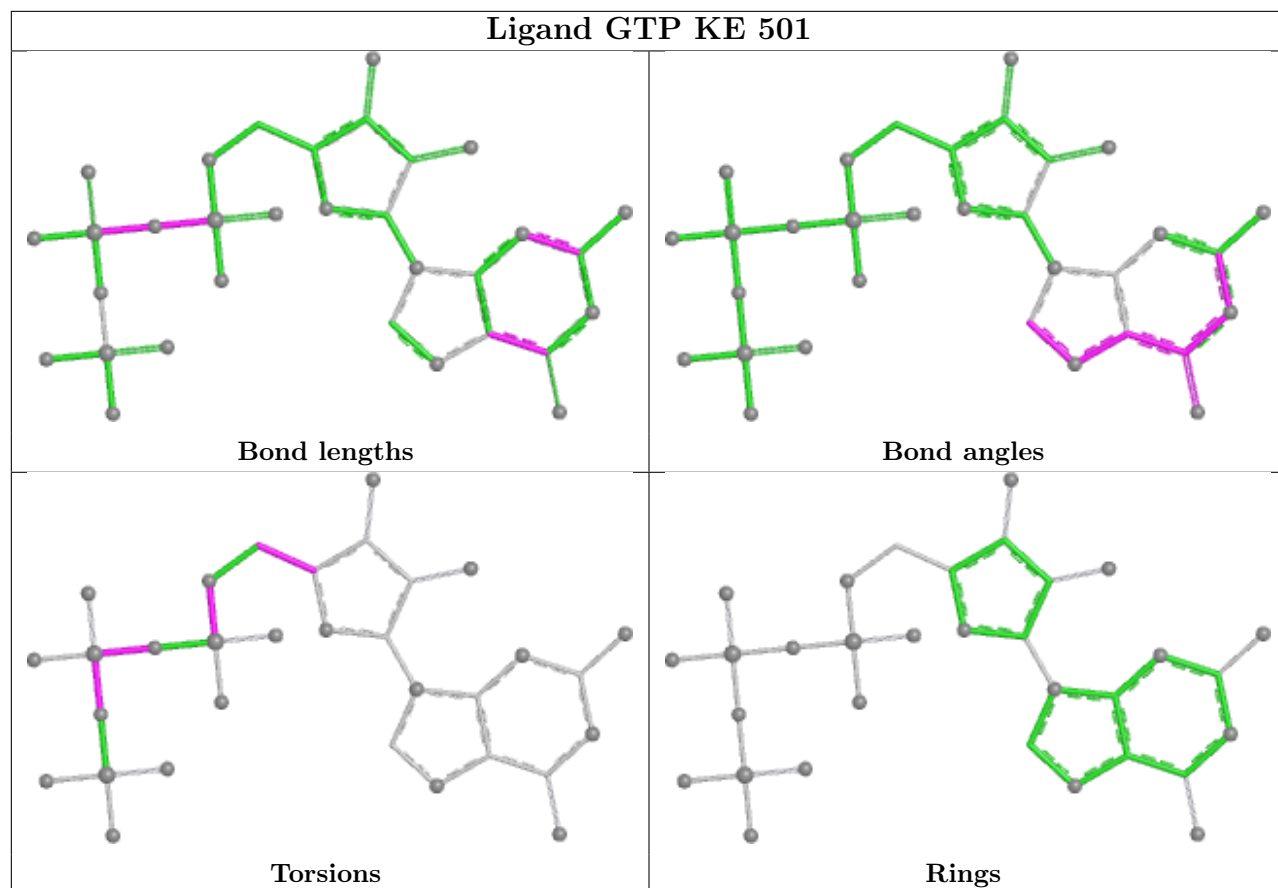


Ligand GTP EE 501

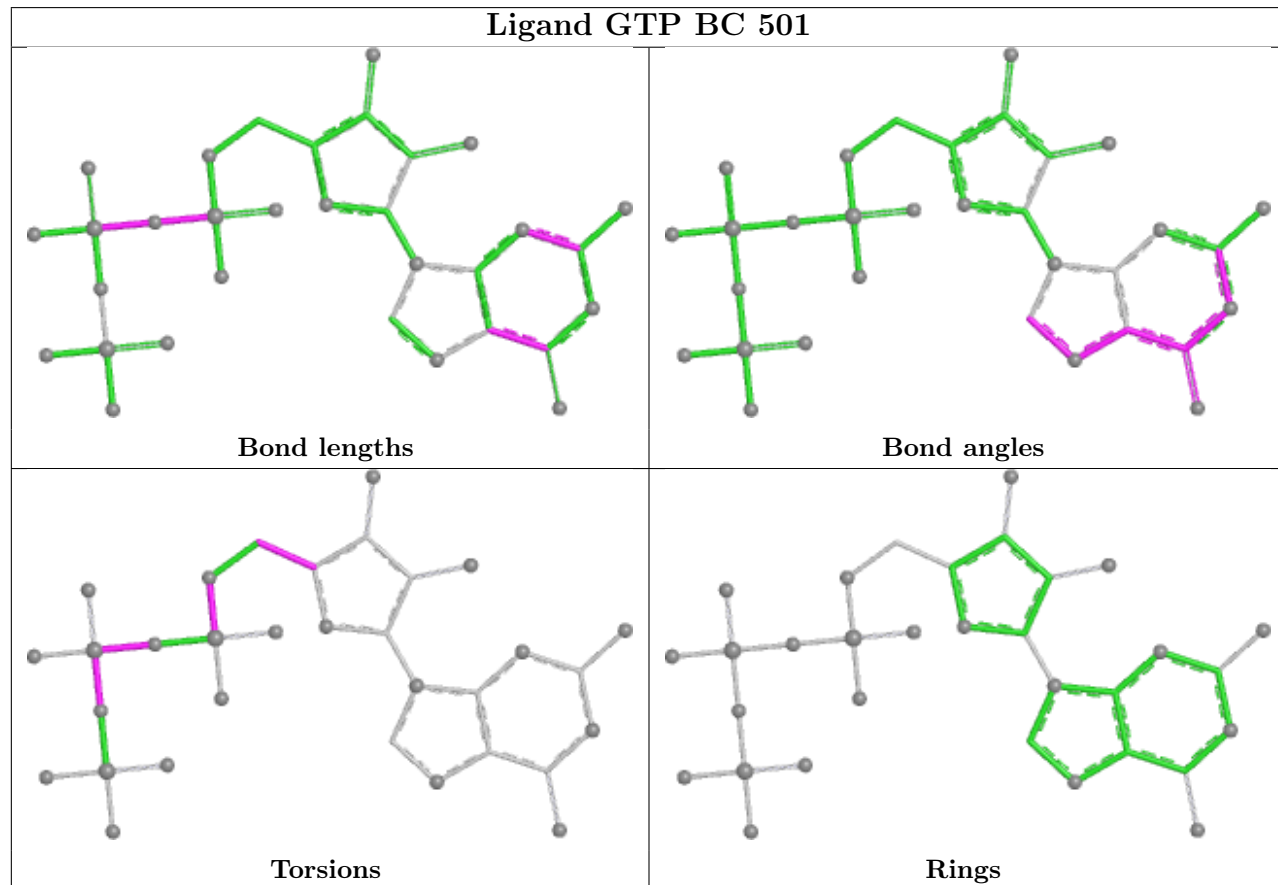


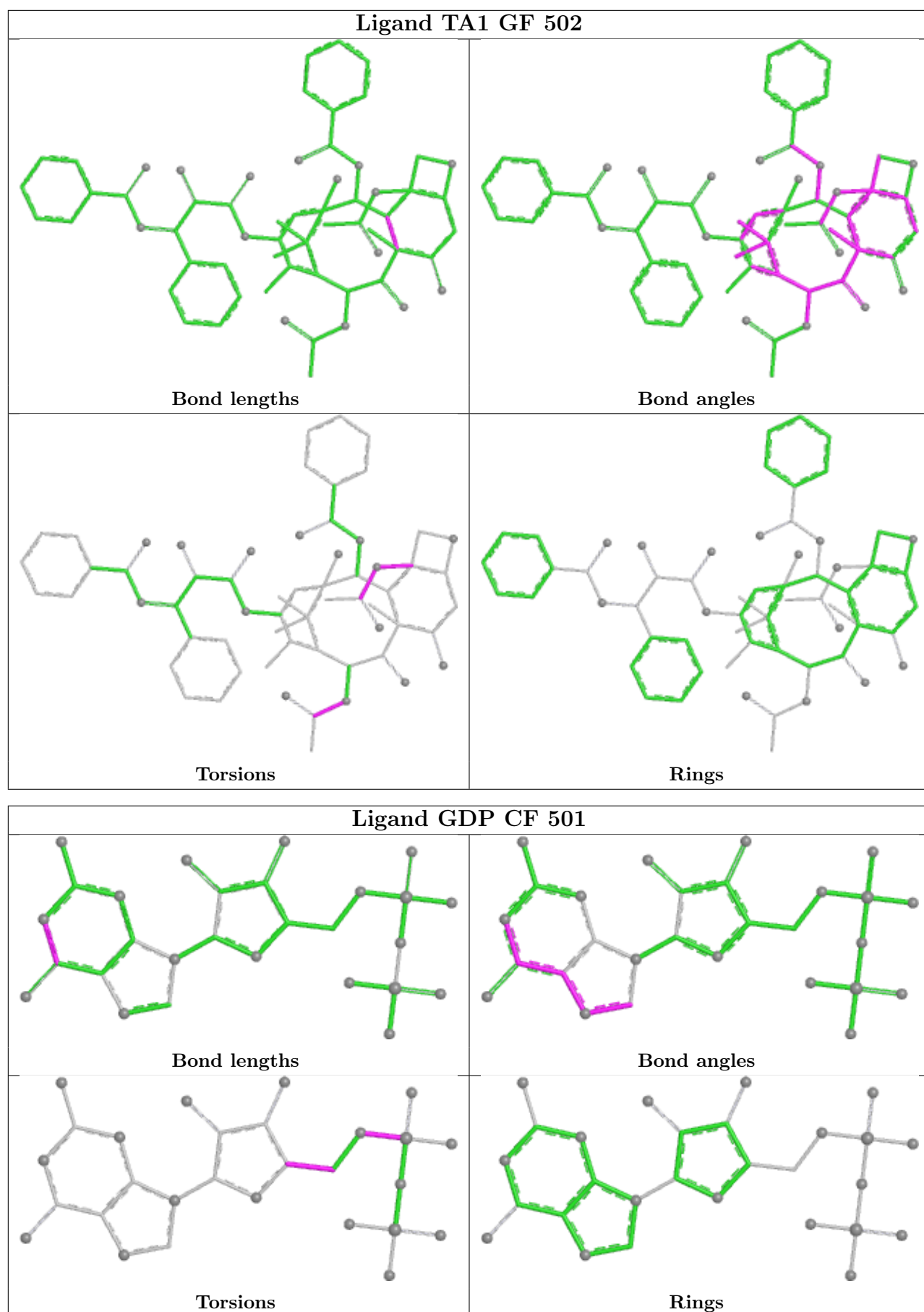


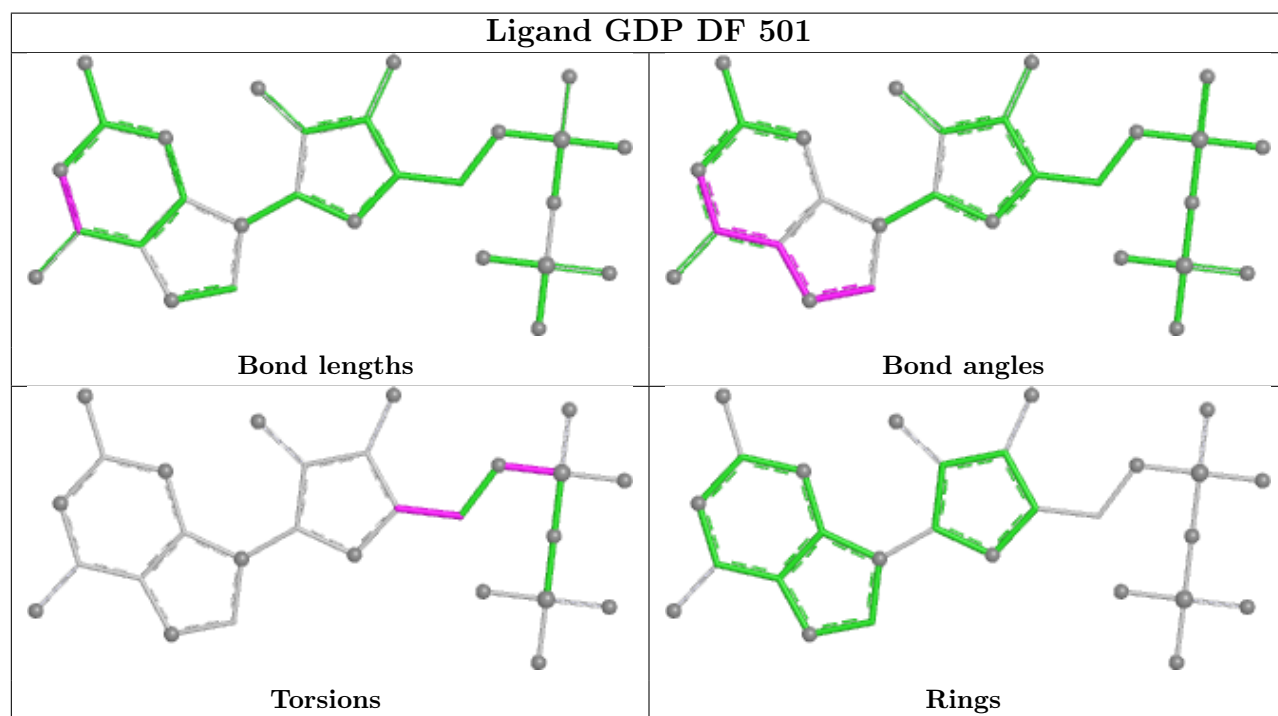
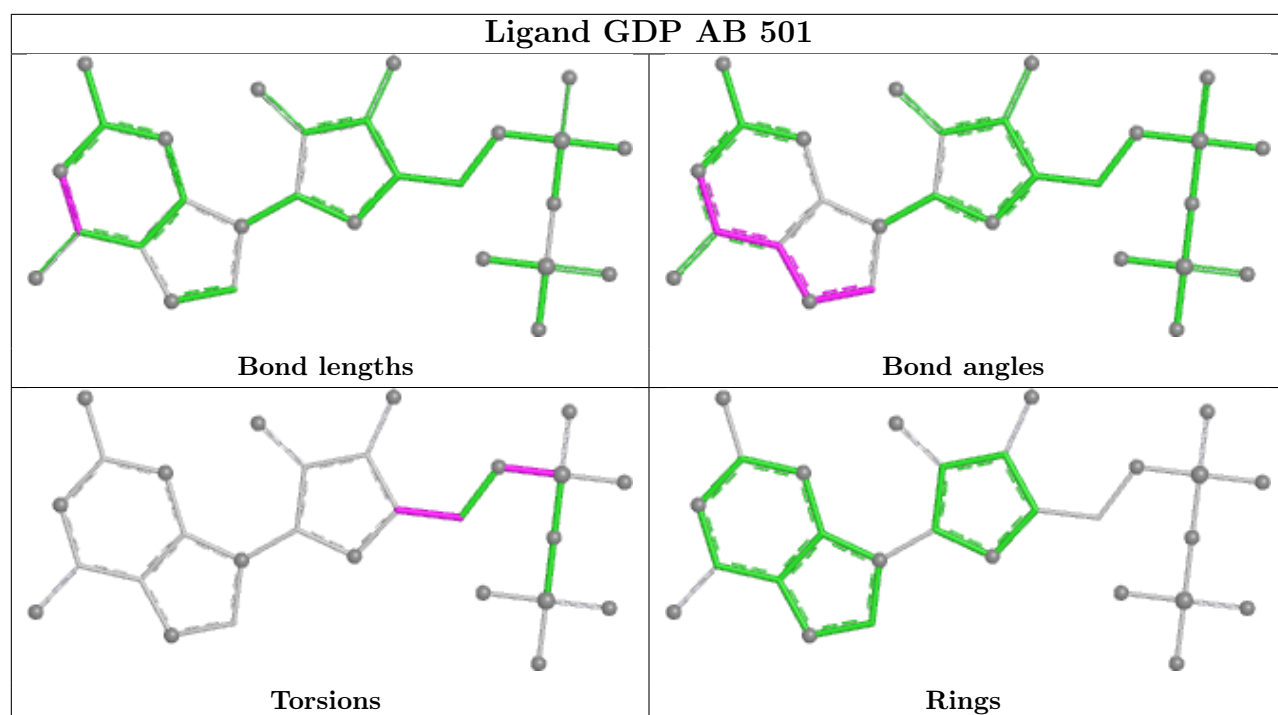
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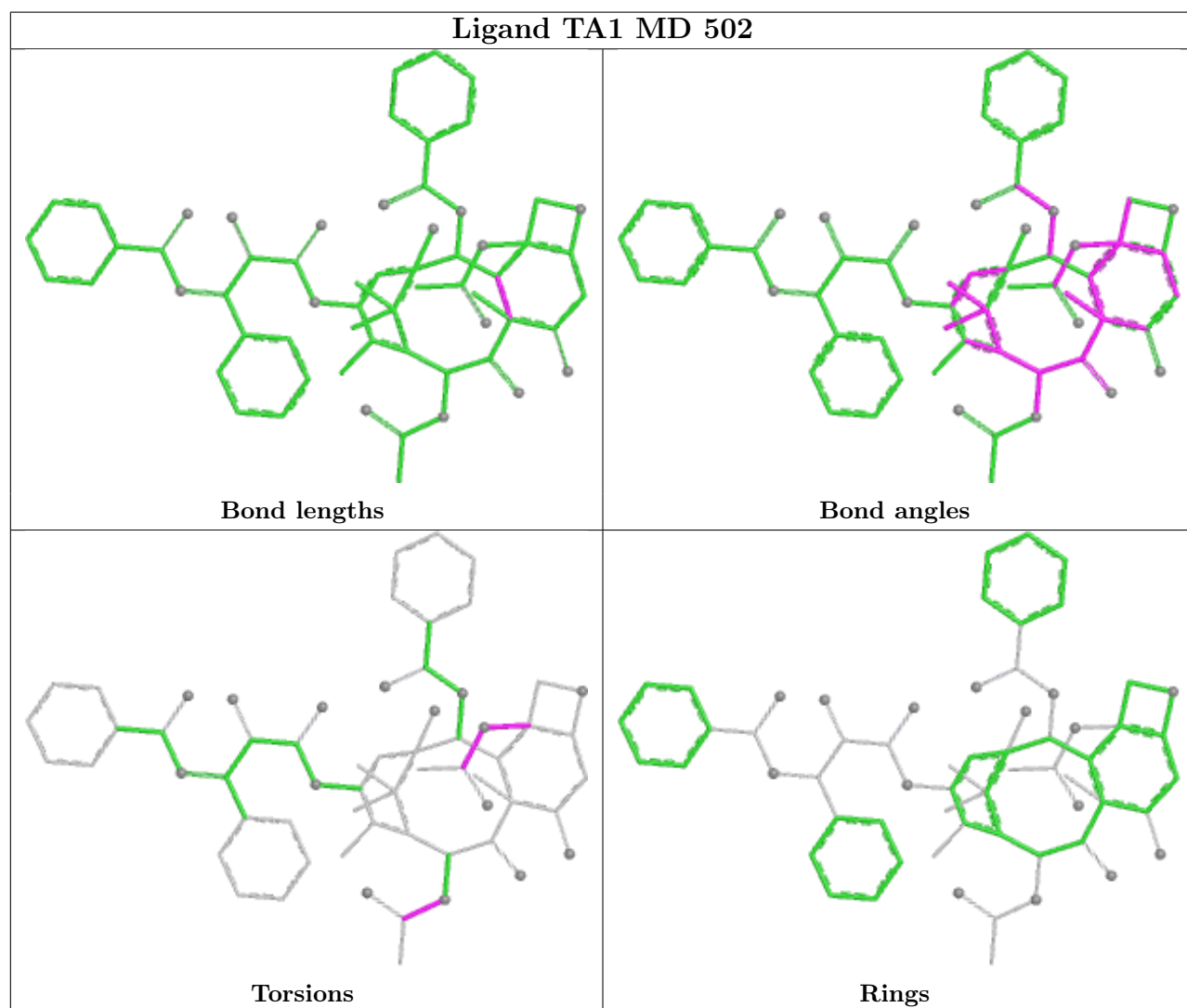
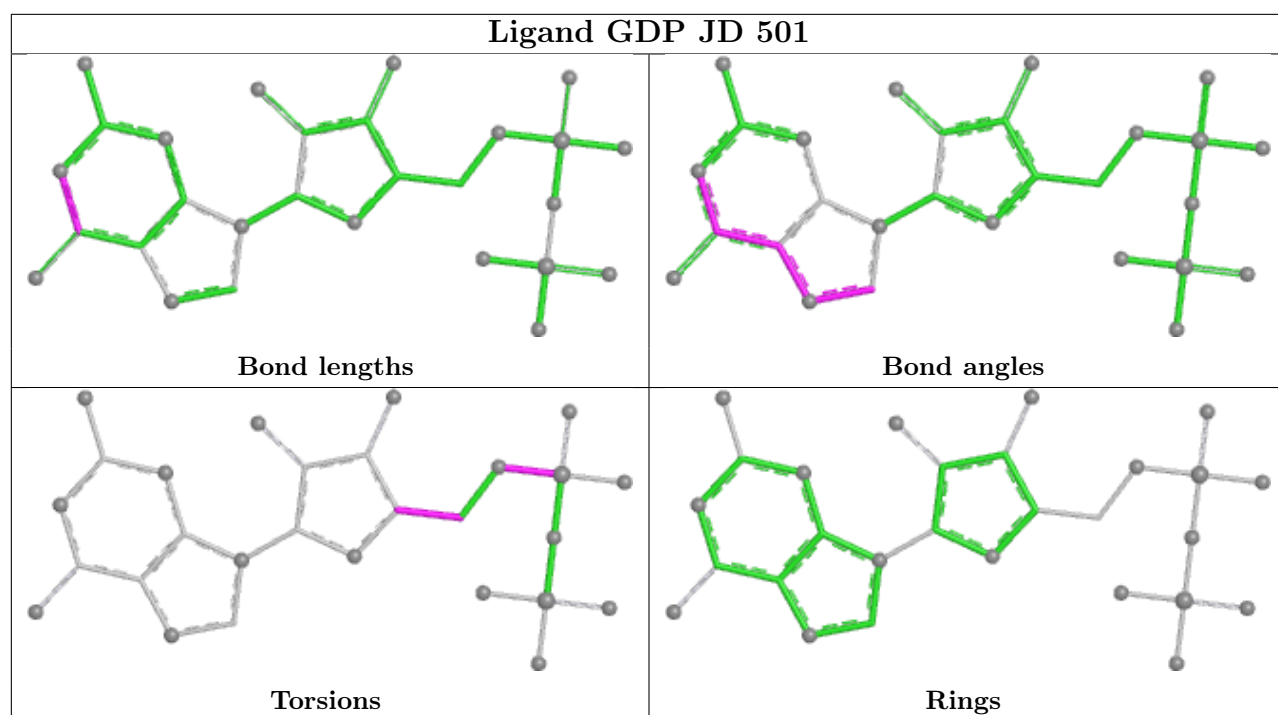


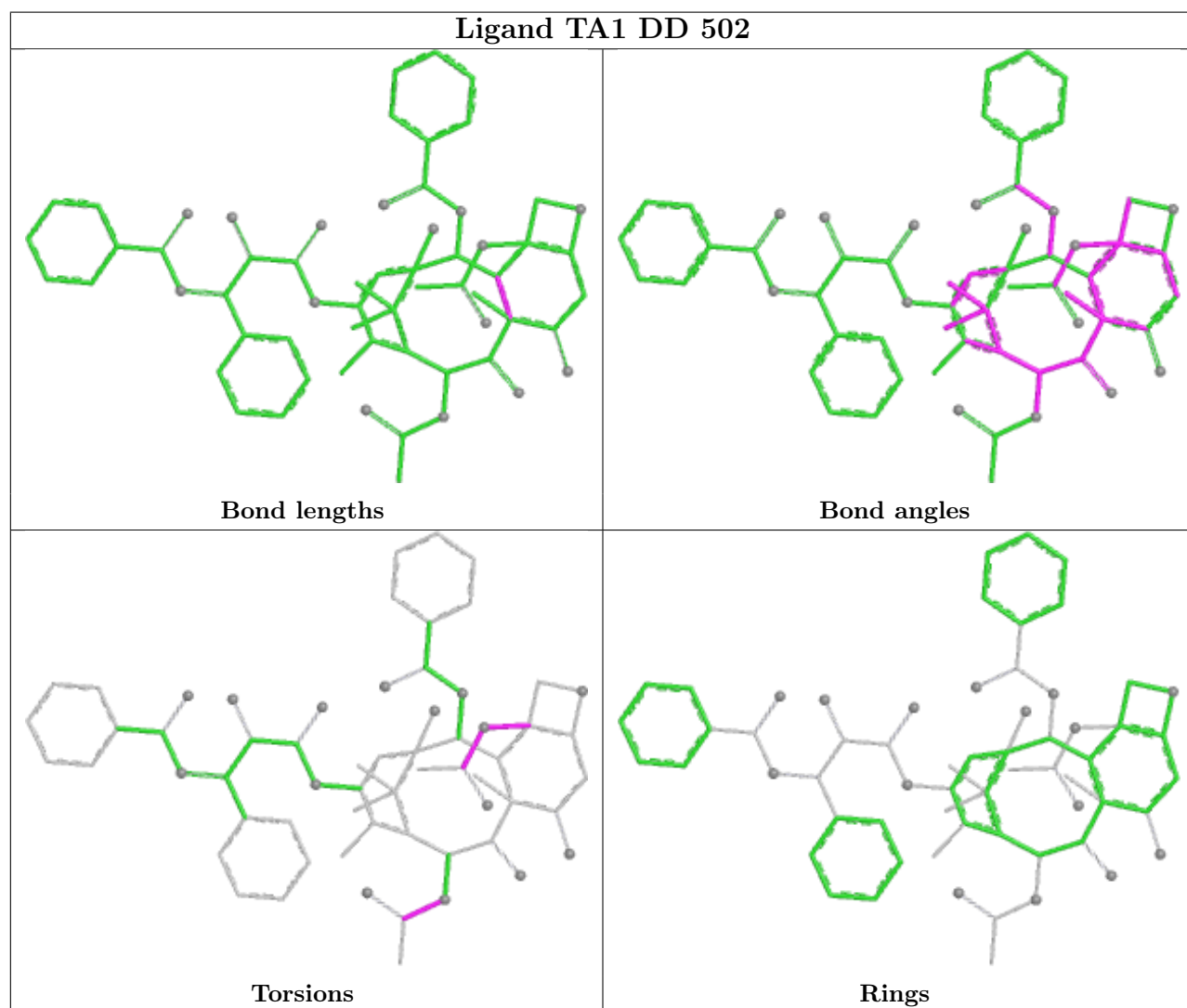
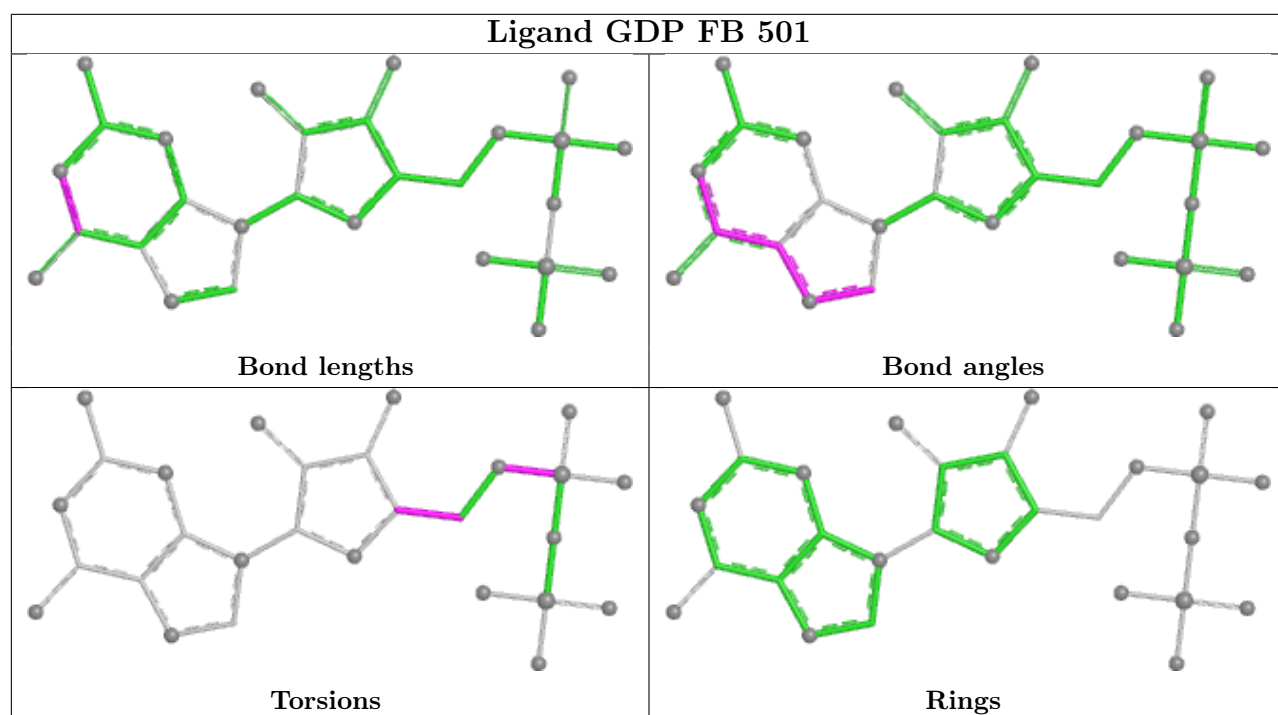
Ligand GTP BC 501

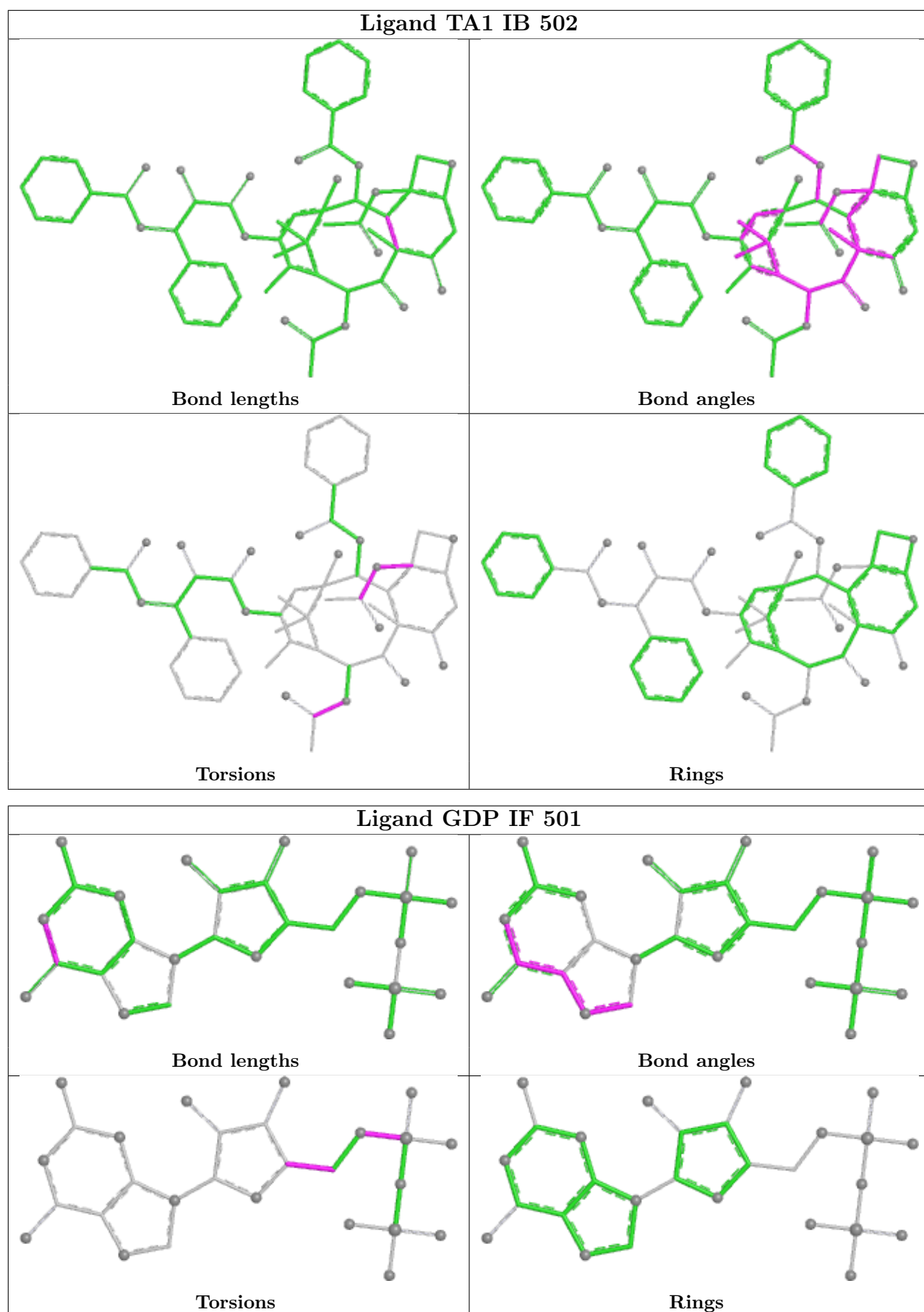


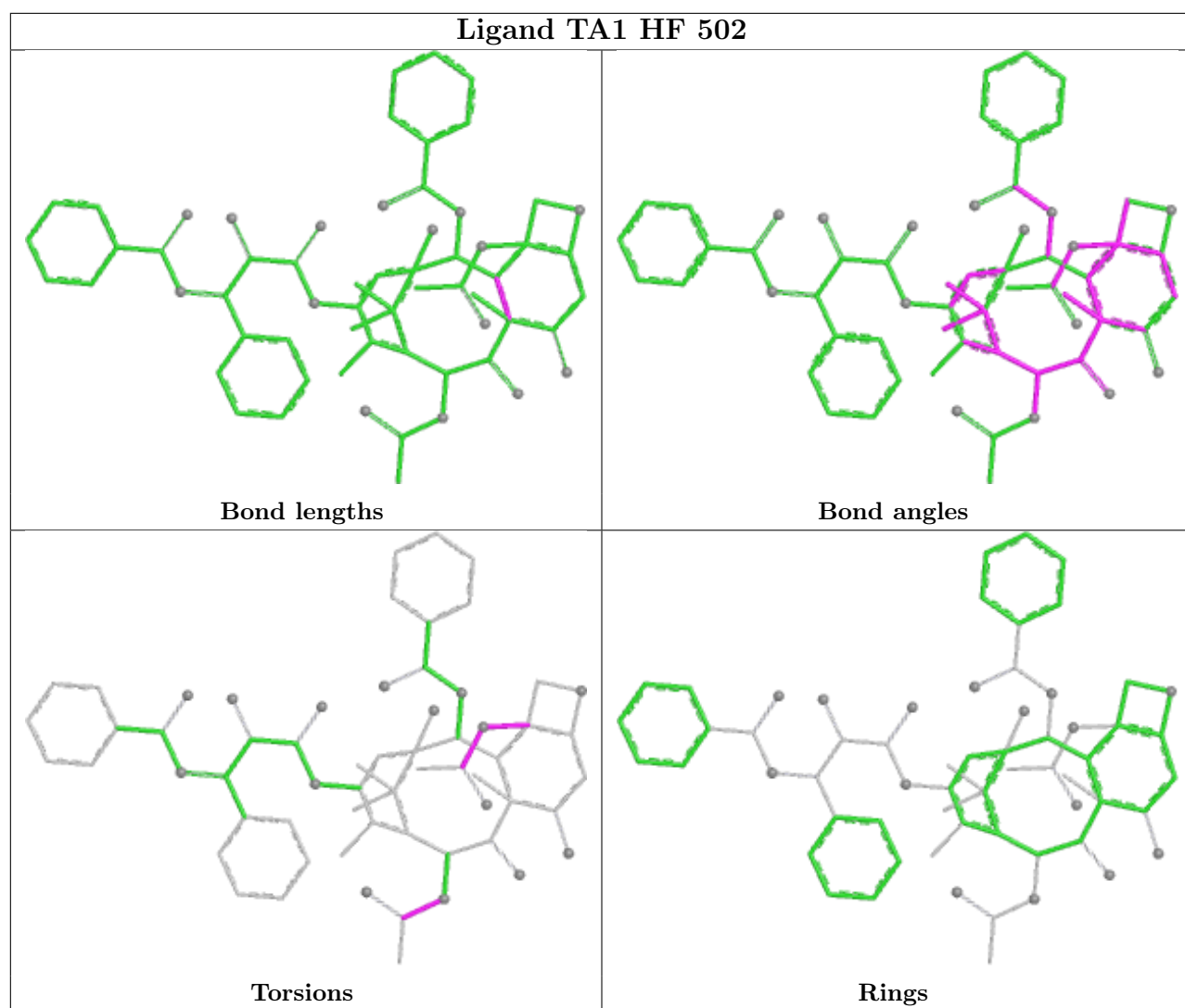




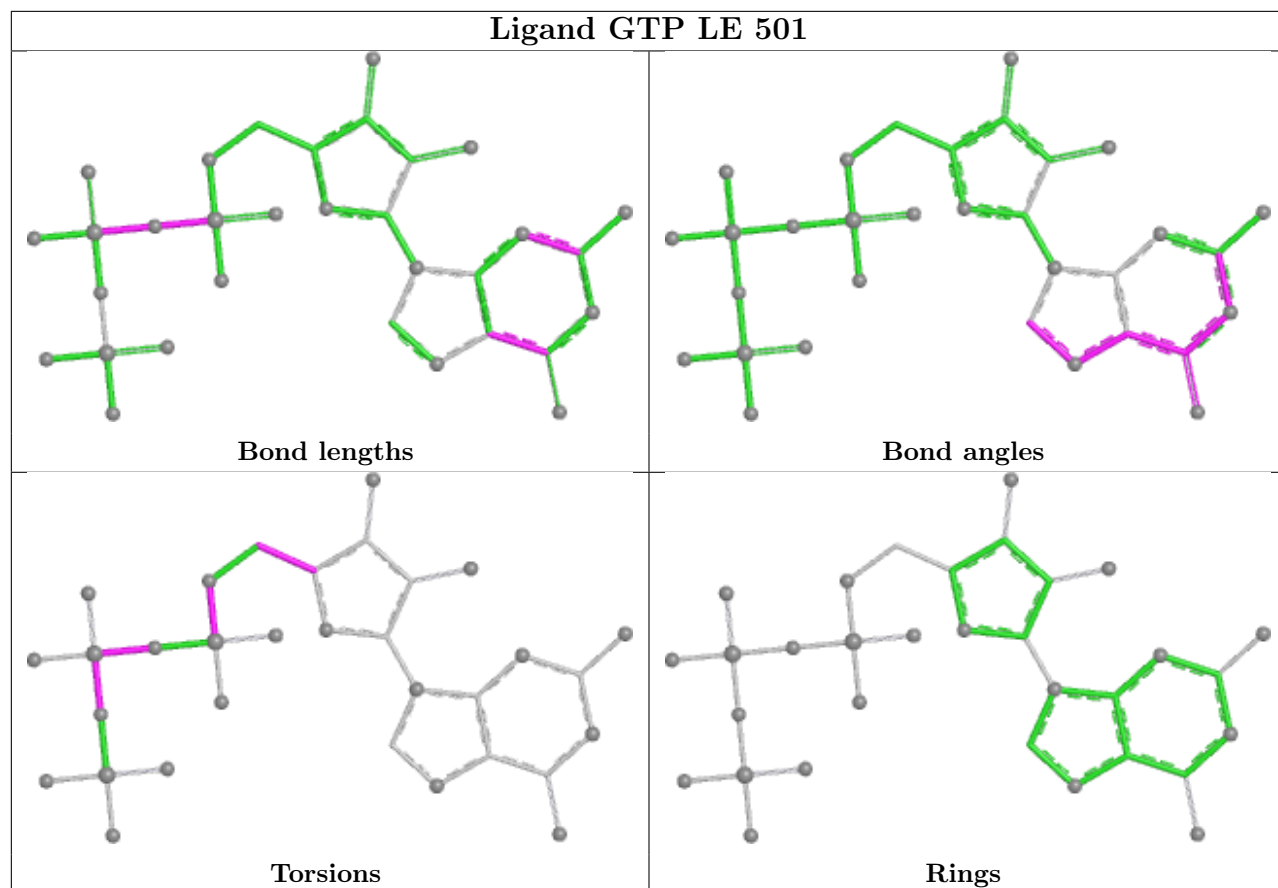




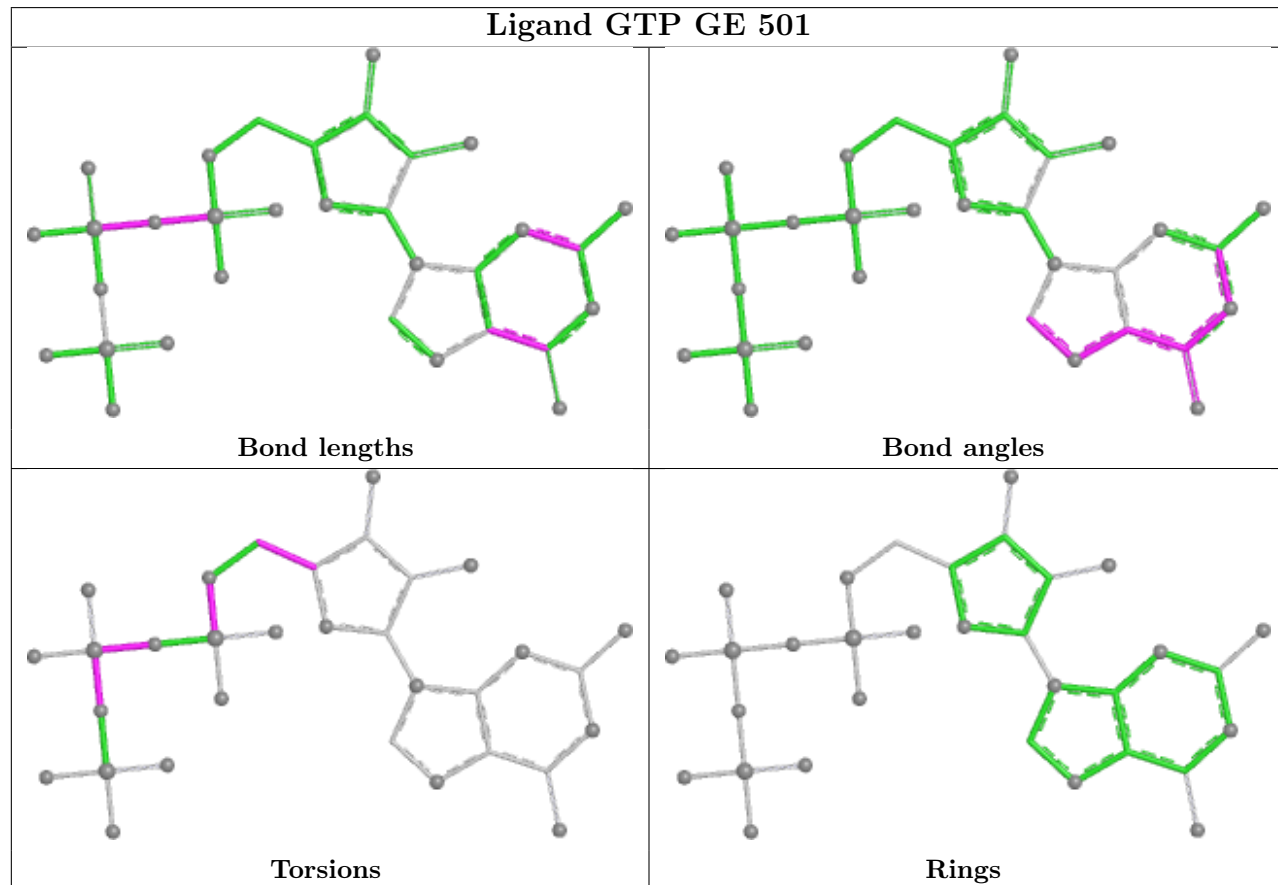




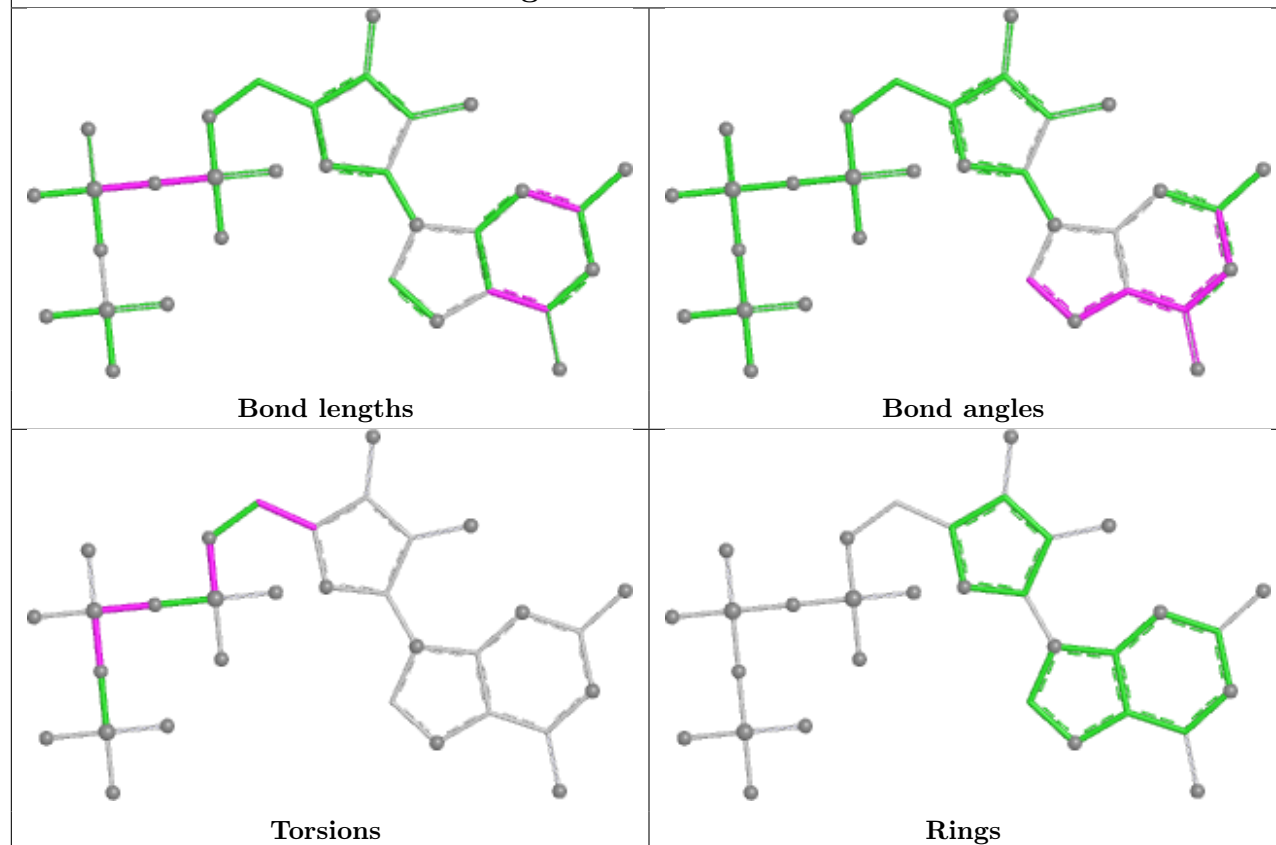
Ligand GTP LE 501



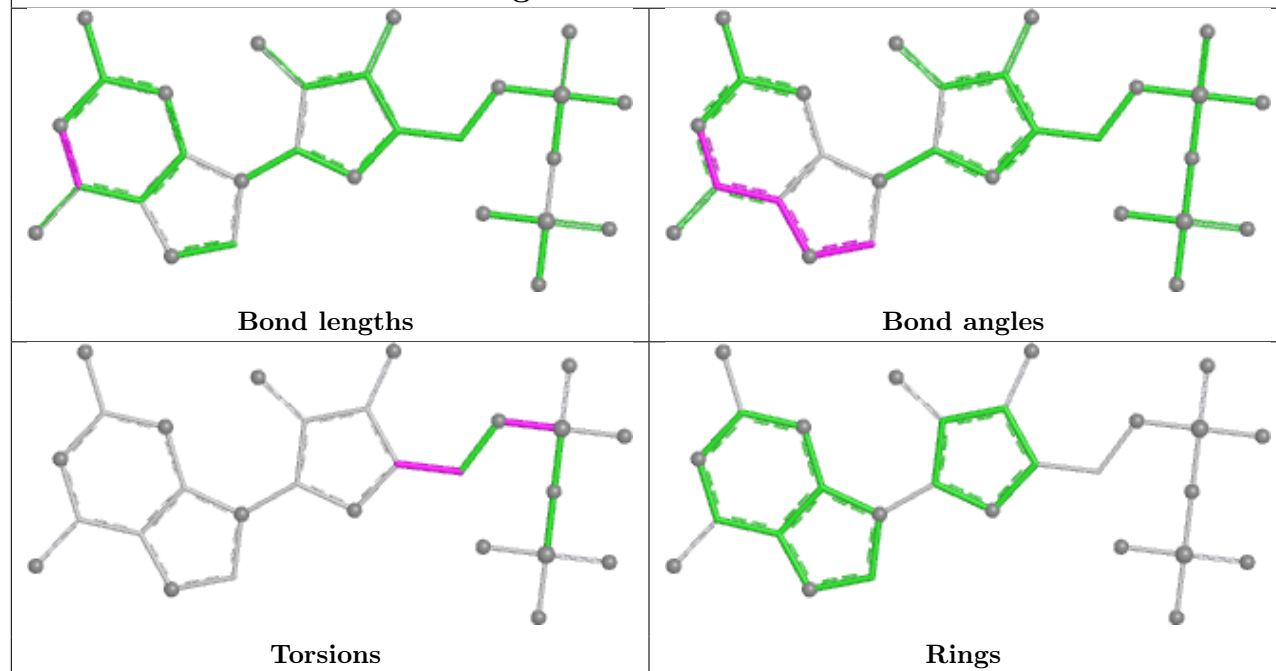
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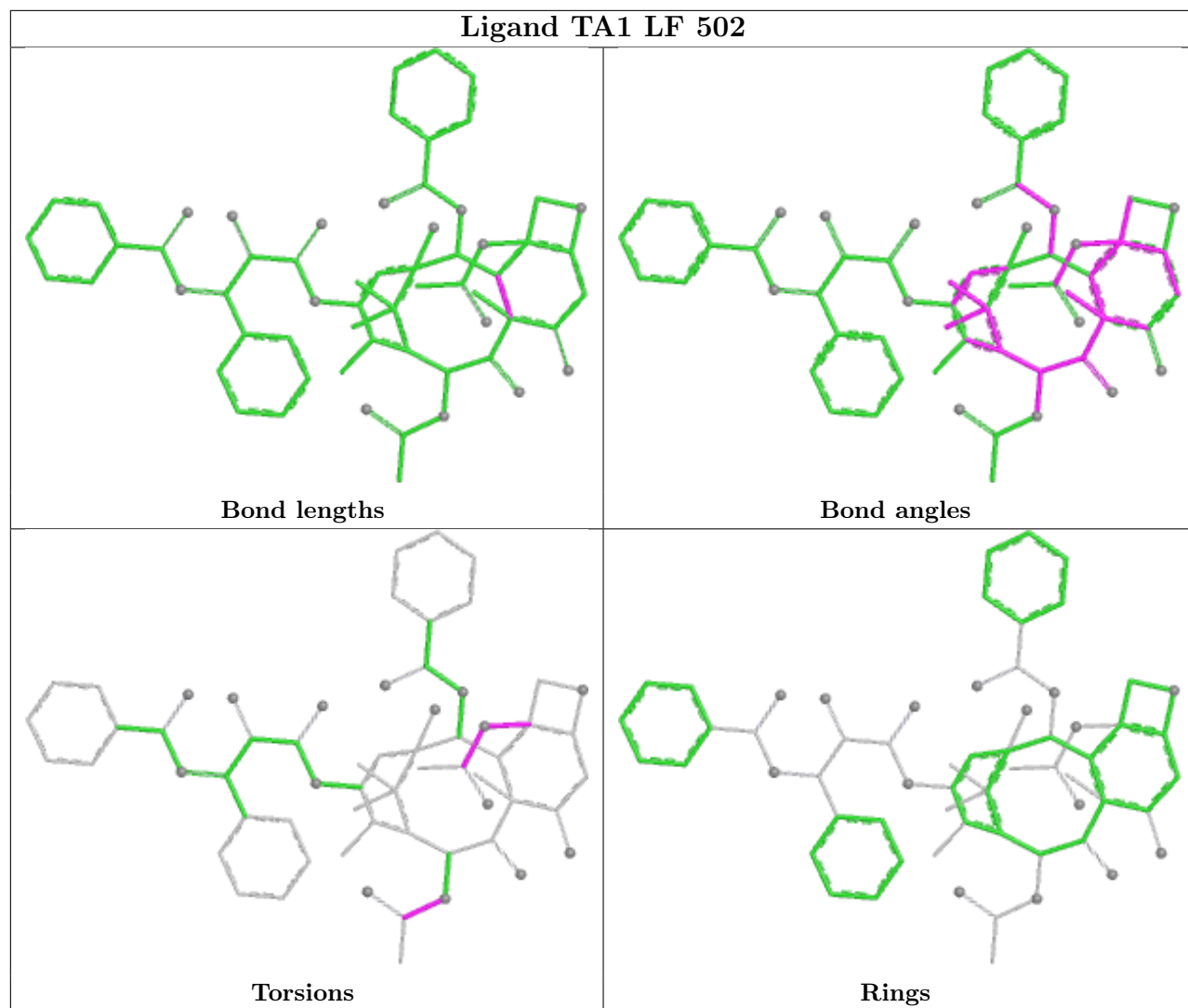


Ligand GTP JA 501

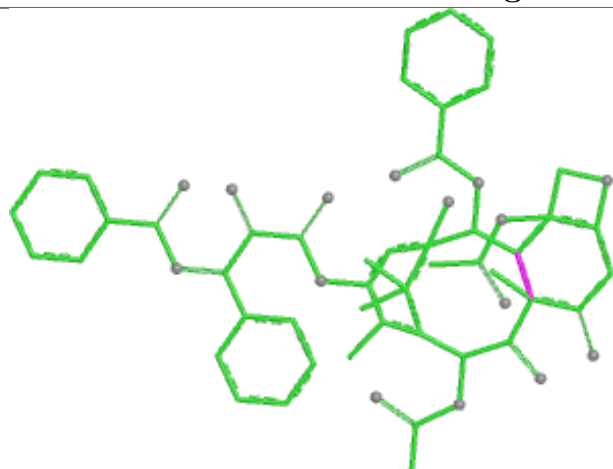


Ligand GDP MB 501

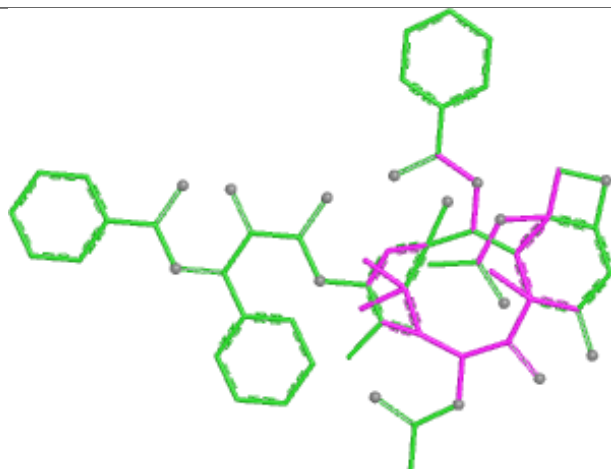




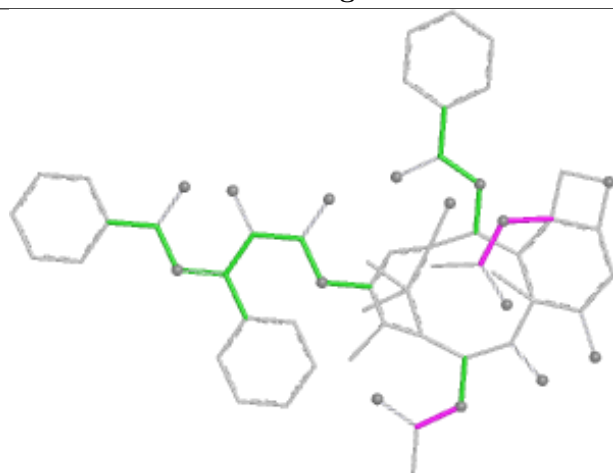
Ligand TA1 GB 502



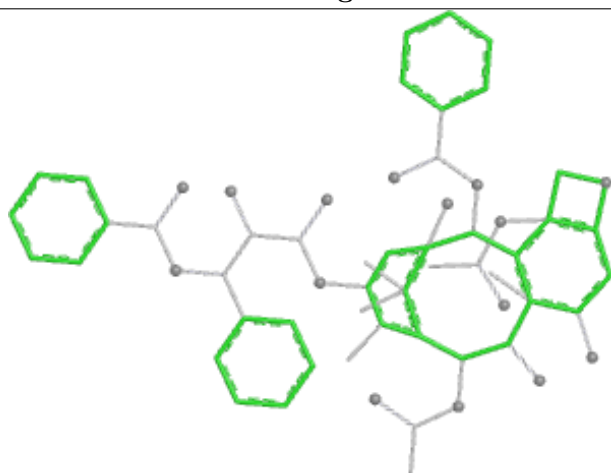
Bond lengths



Bond angles

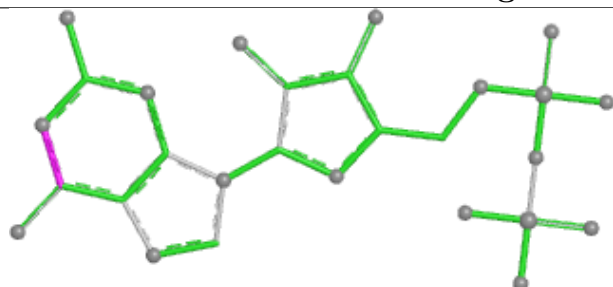


Torsions

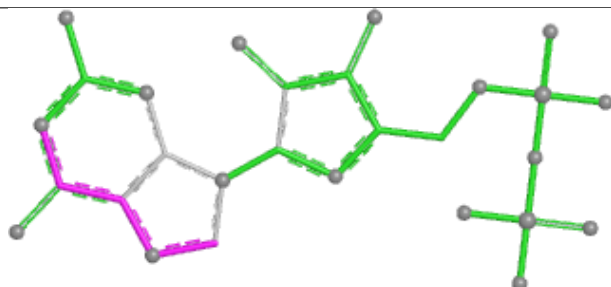


Rings

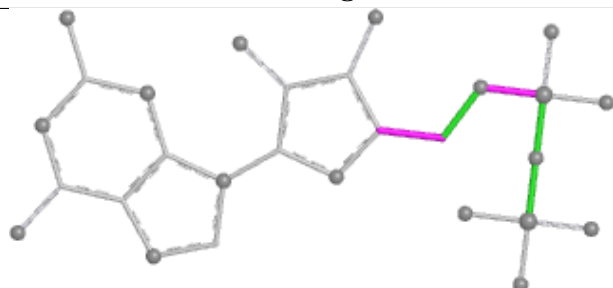
Ligand GDP HB 501



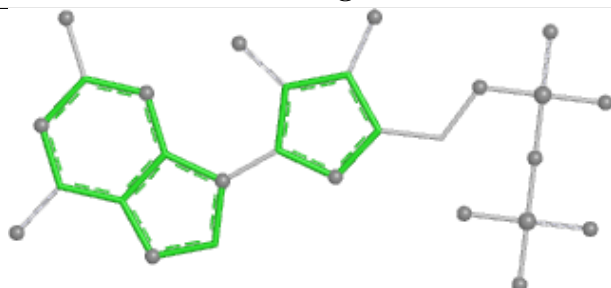
Bond lengths



Bond angles

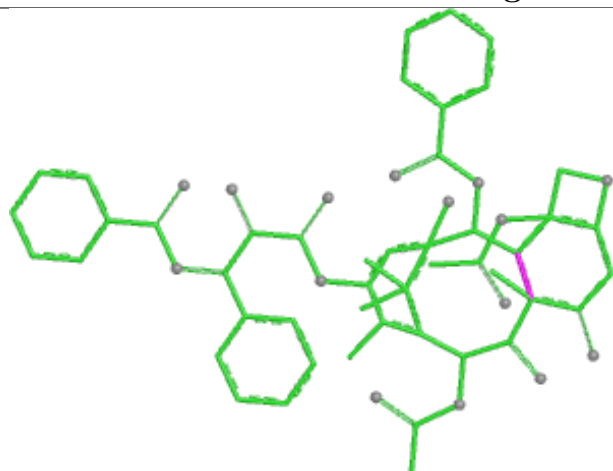


Torsions

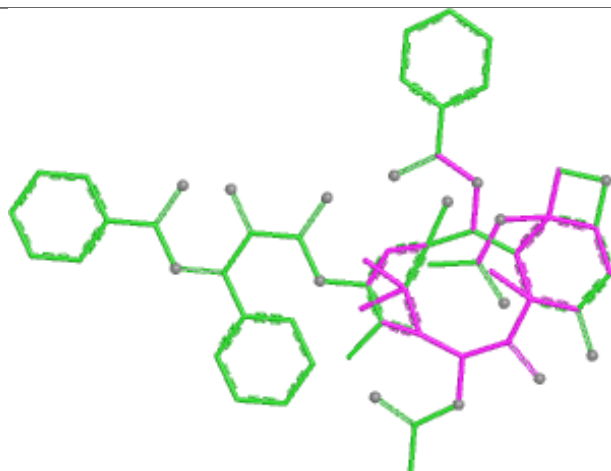


Rings

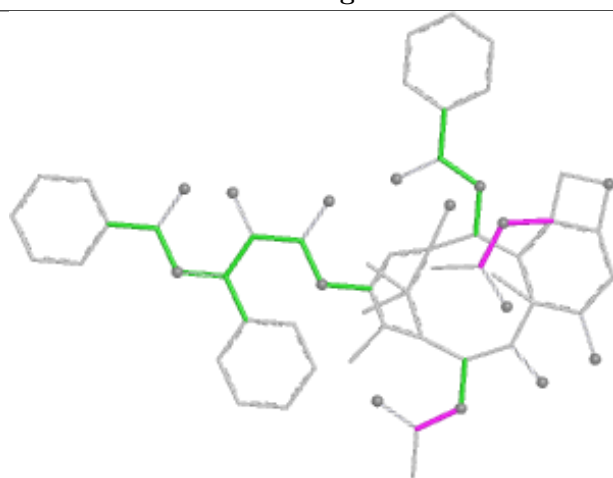
Ligand TA1 AD 502



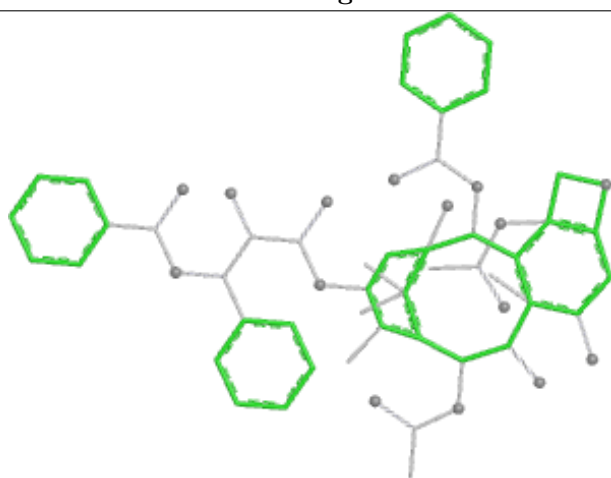
Bond lengths



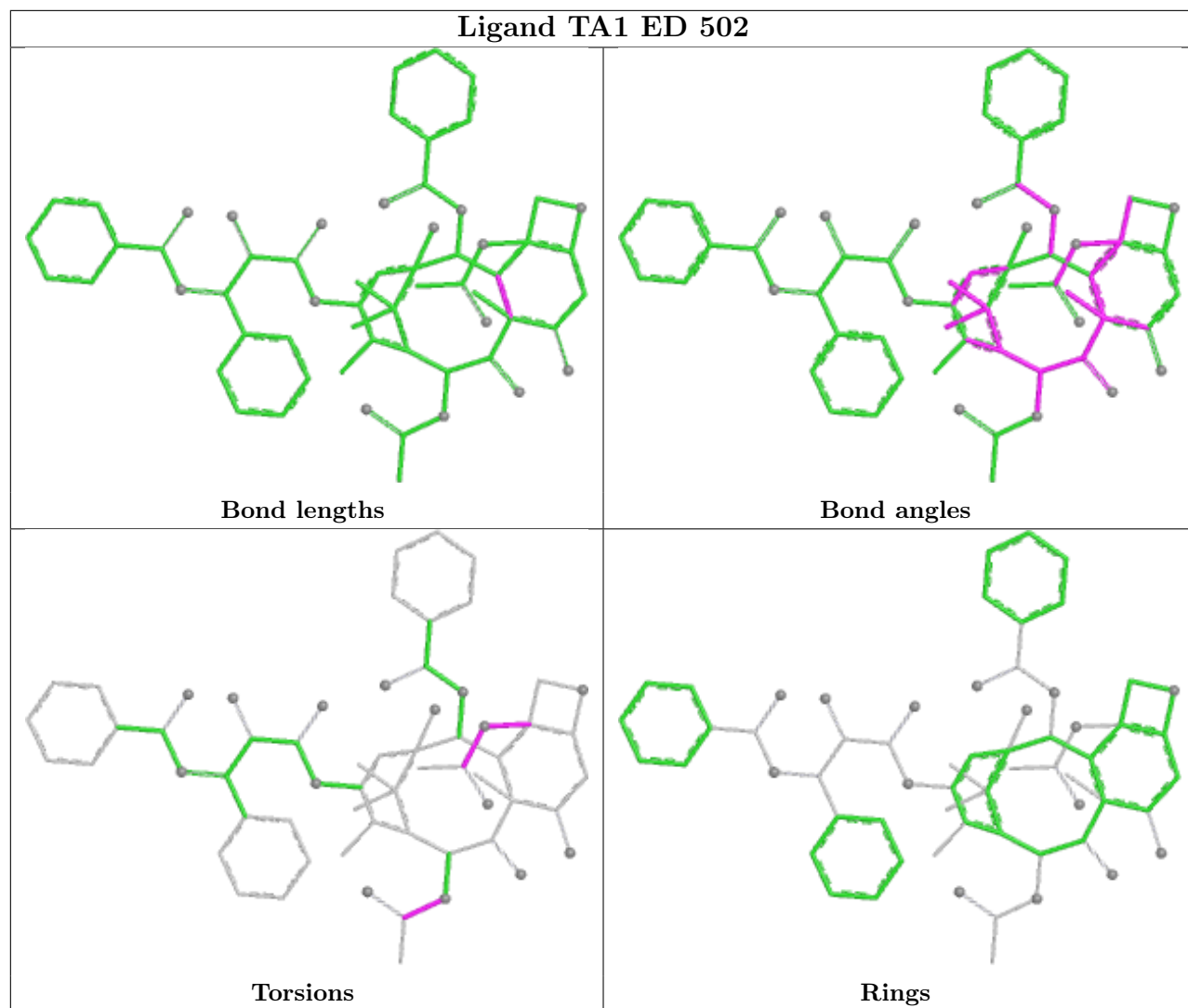
Bond angles

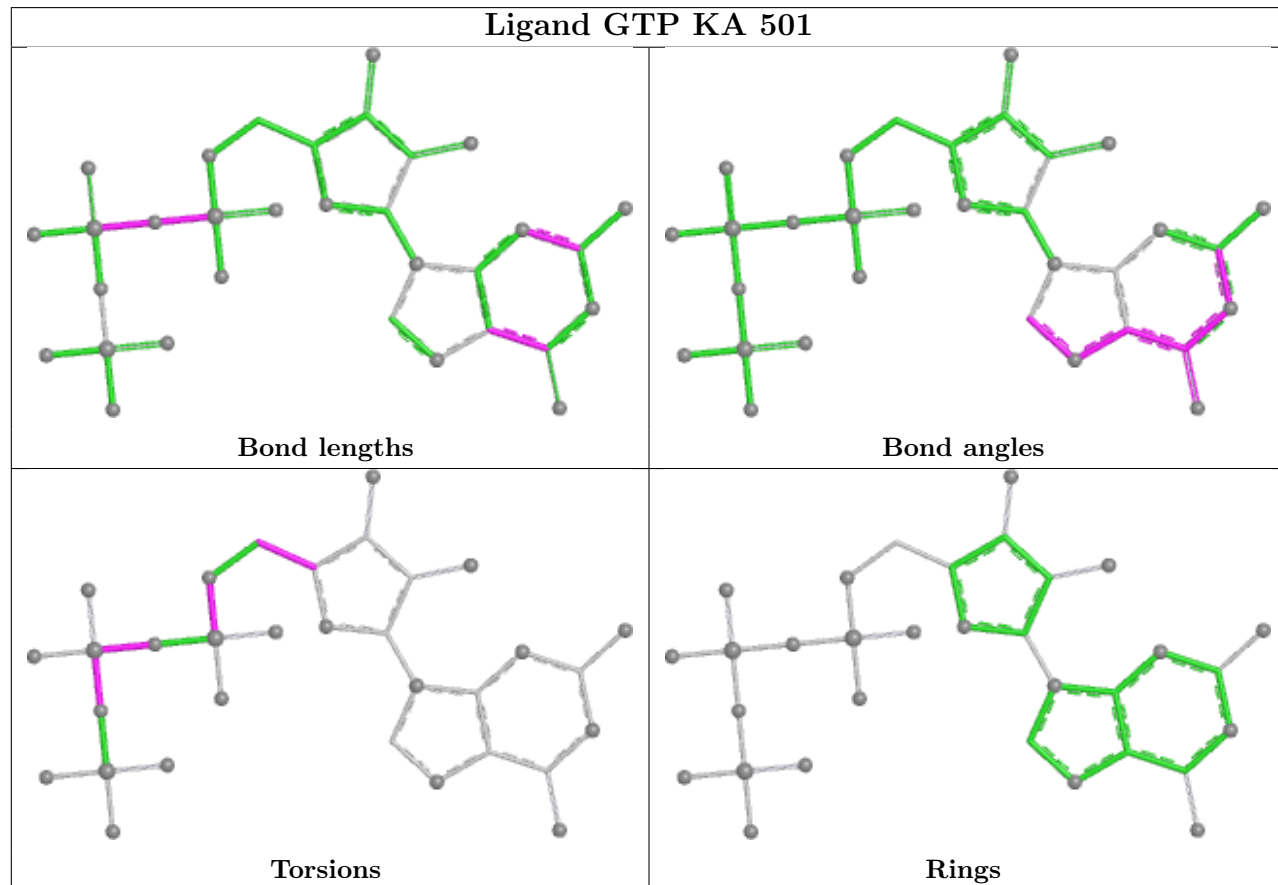
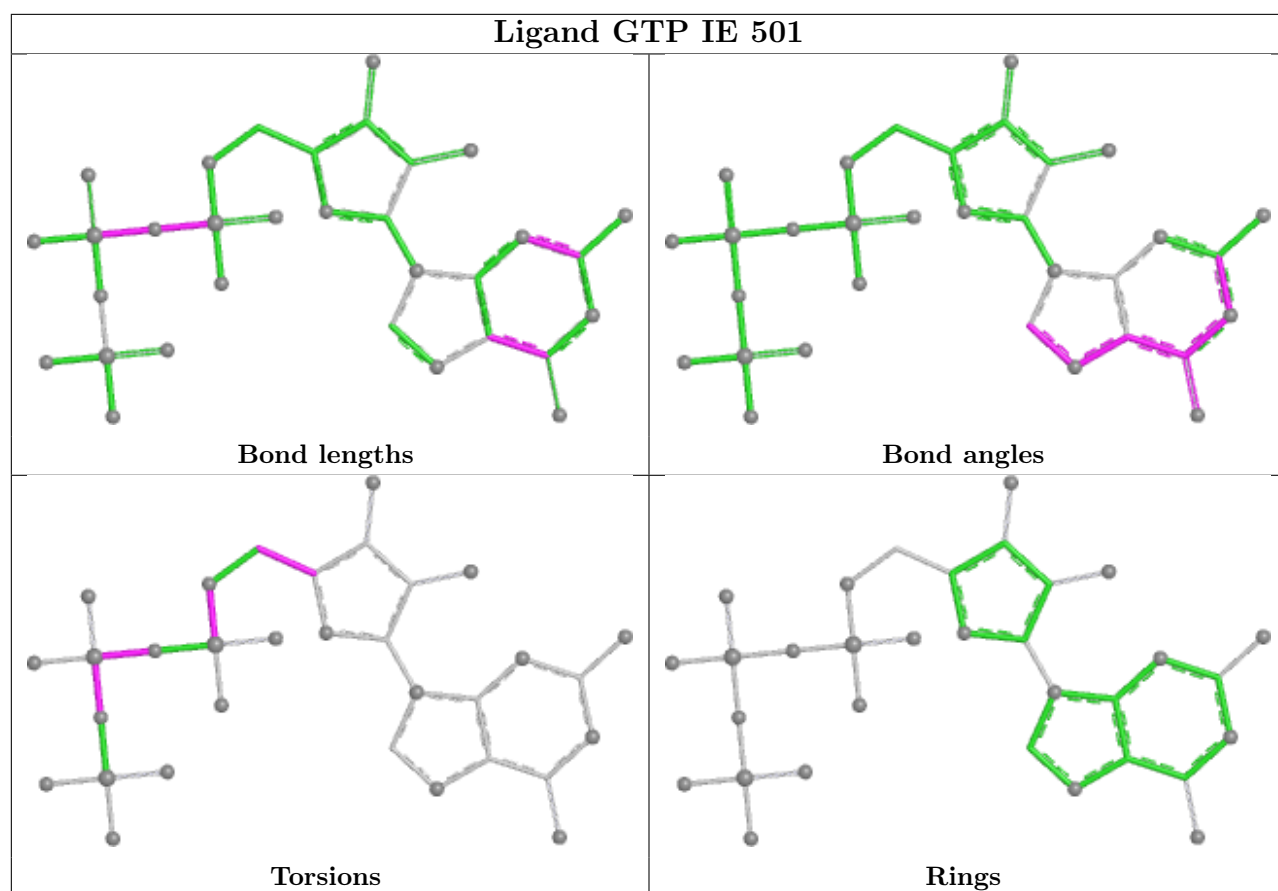


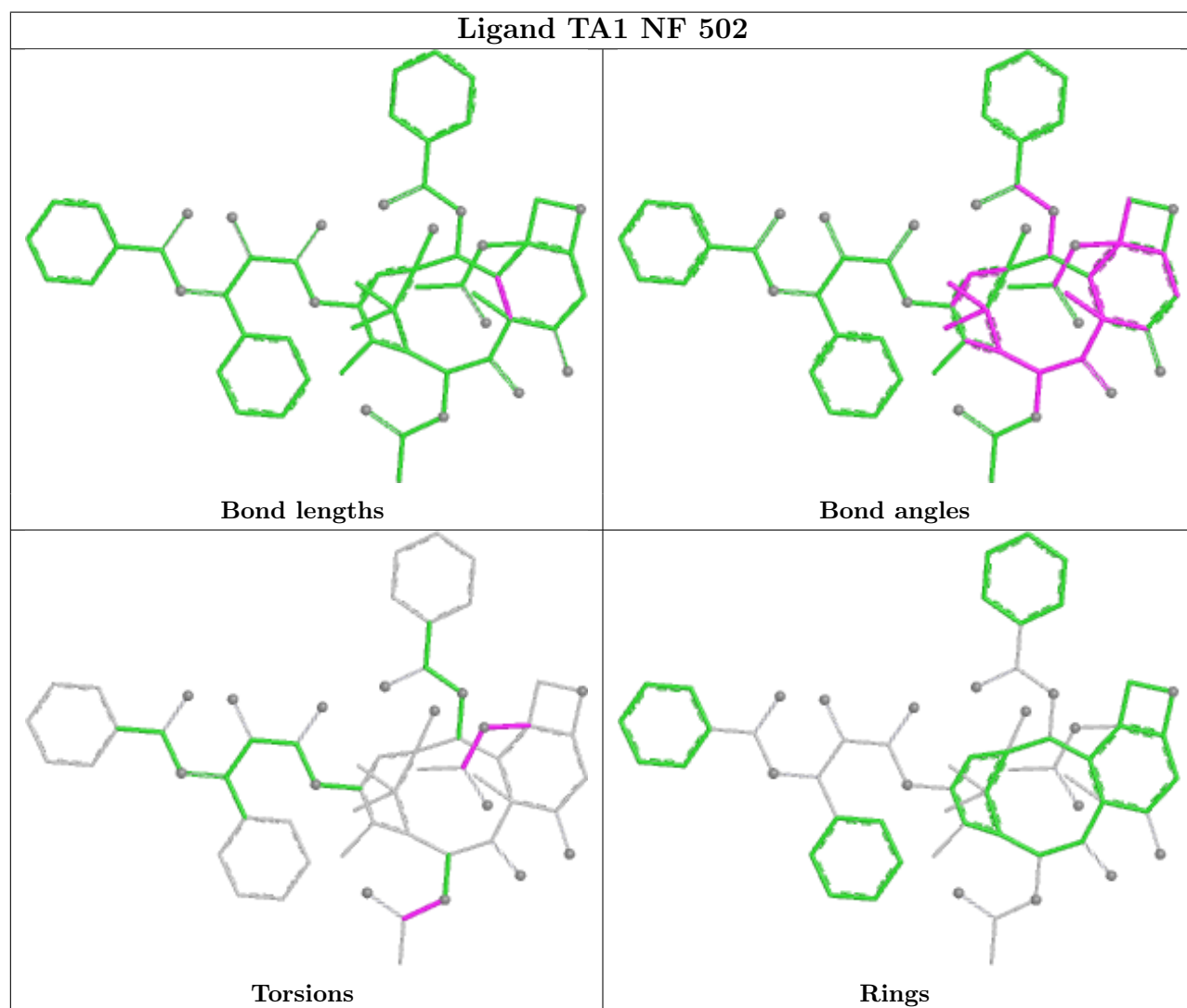
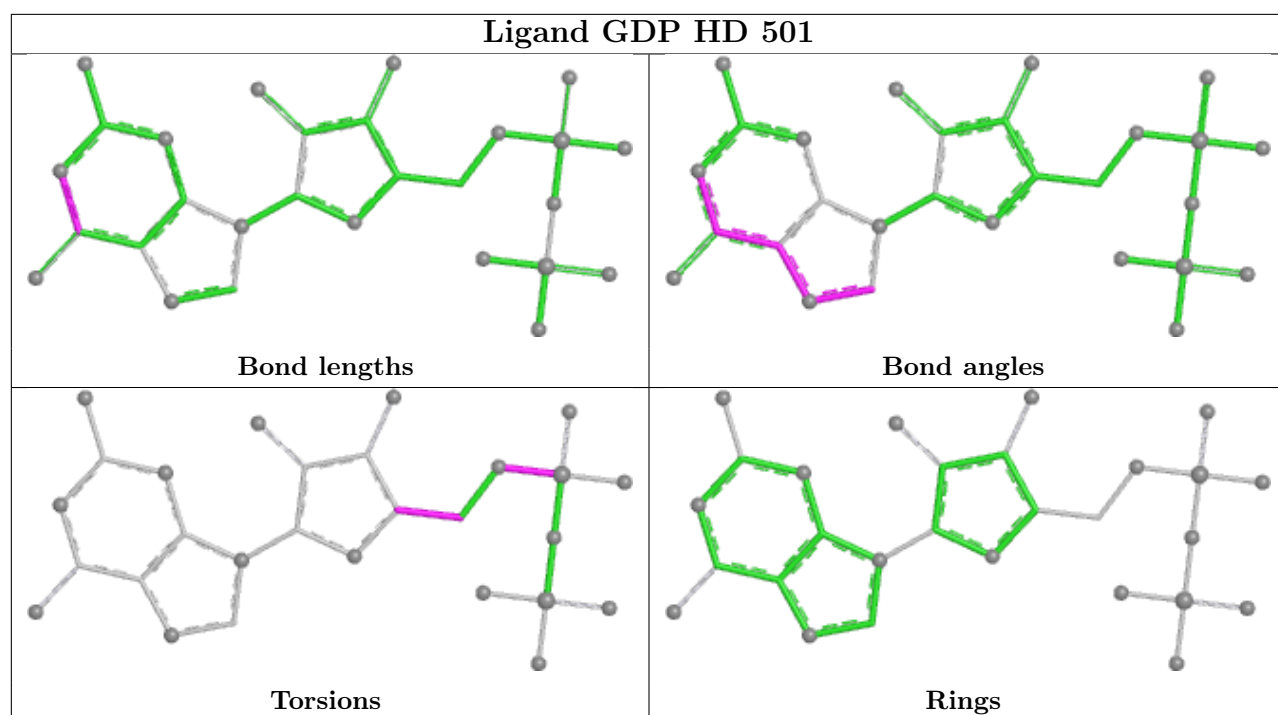
Torsions



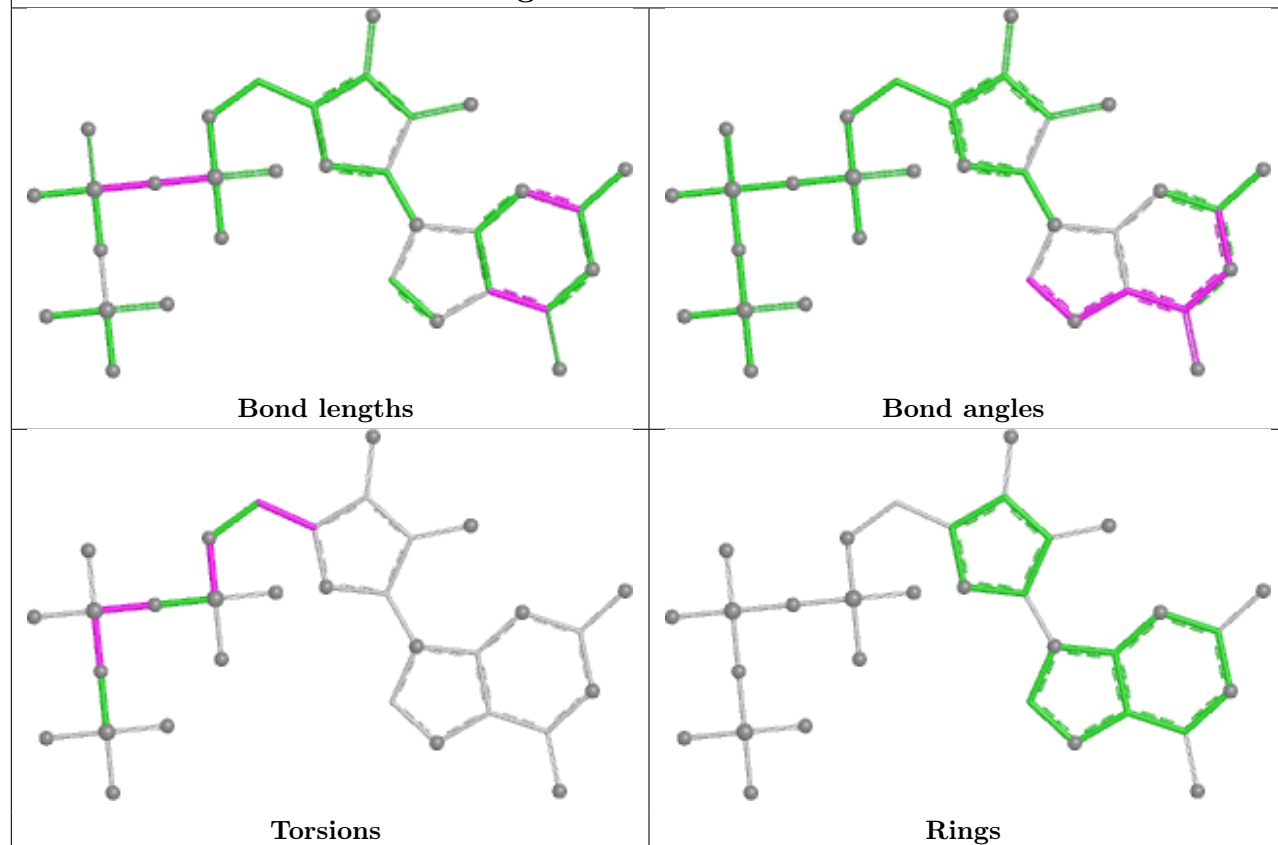
Rings



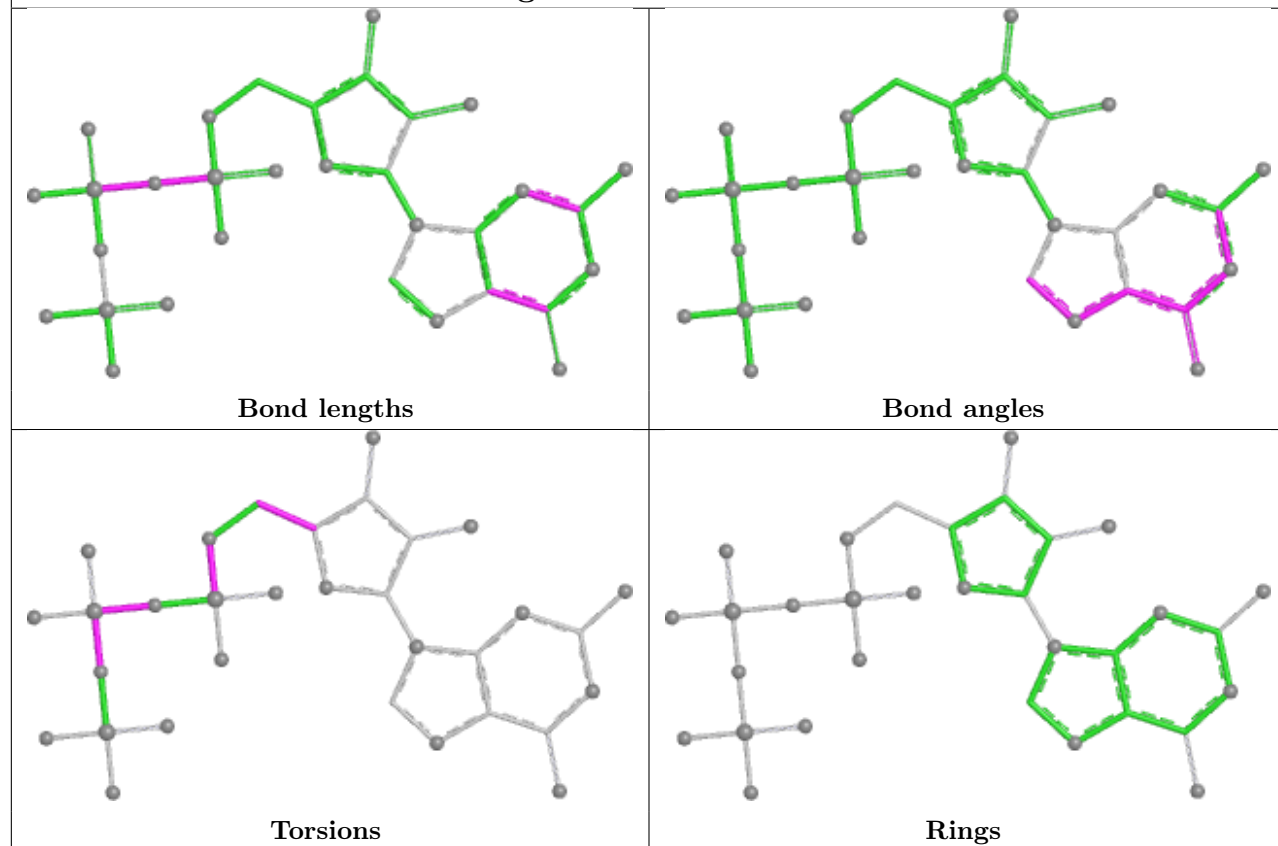


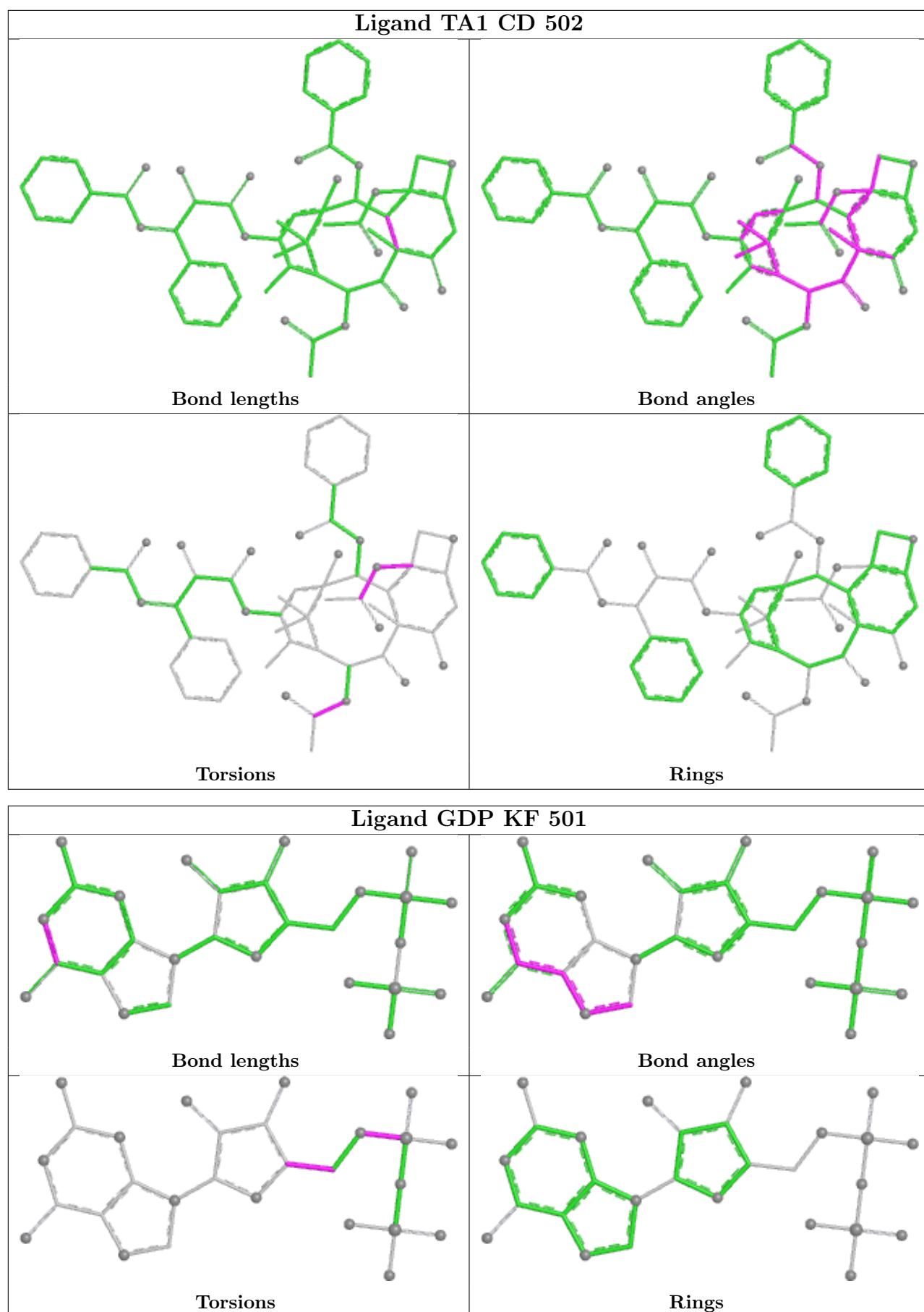


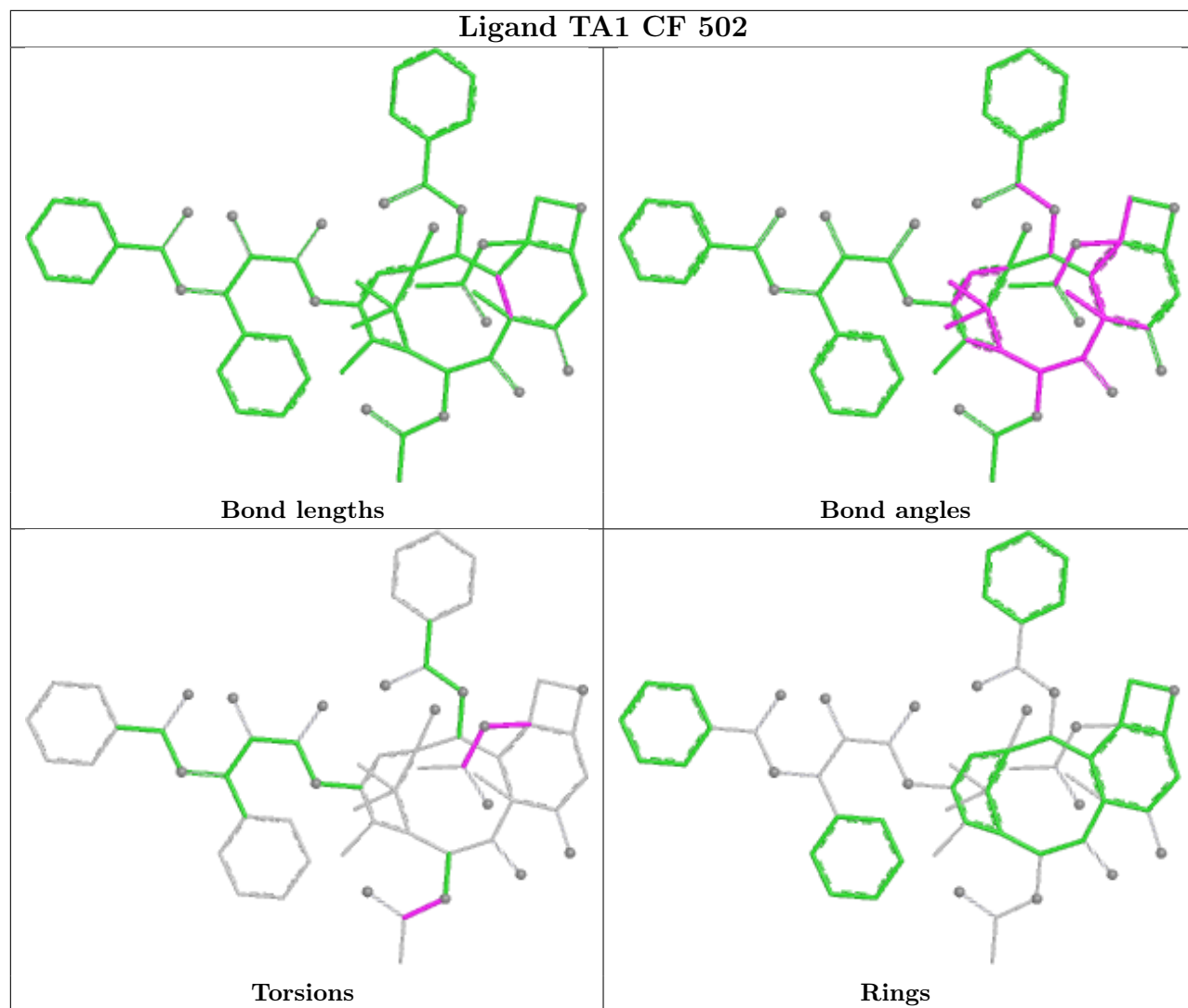
Ligand GTP DC 501

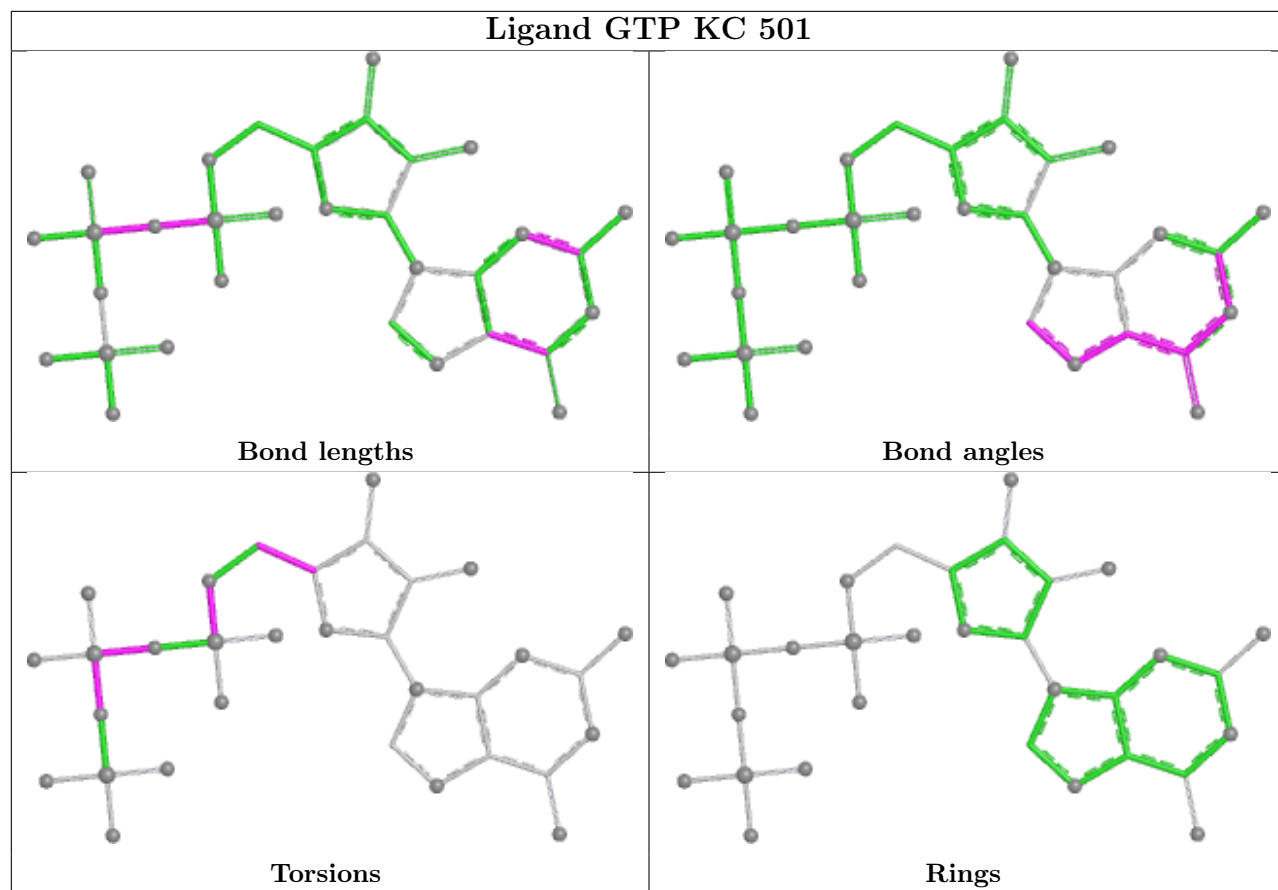


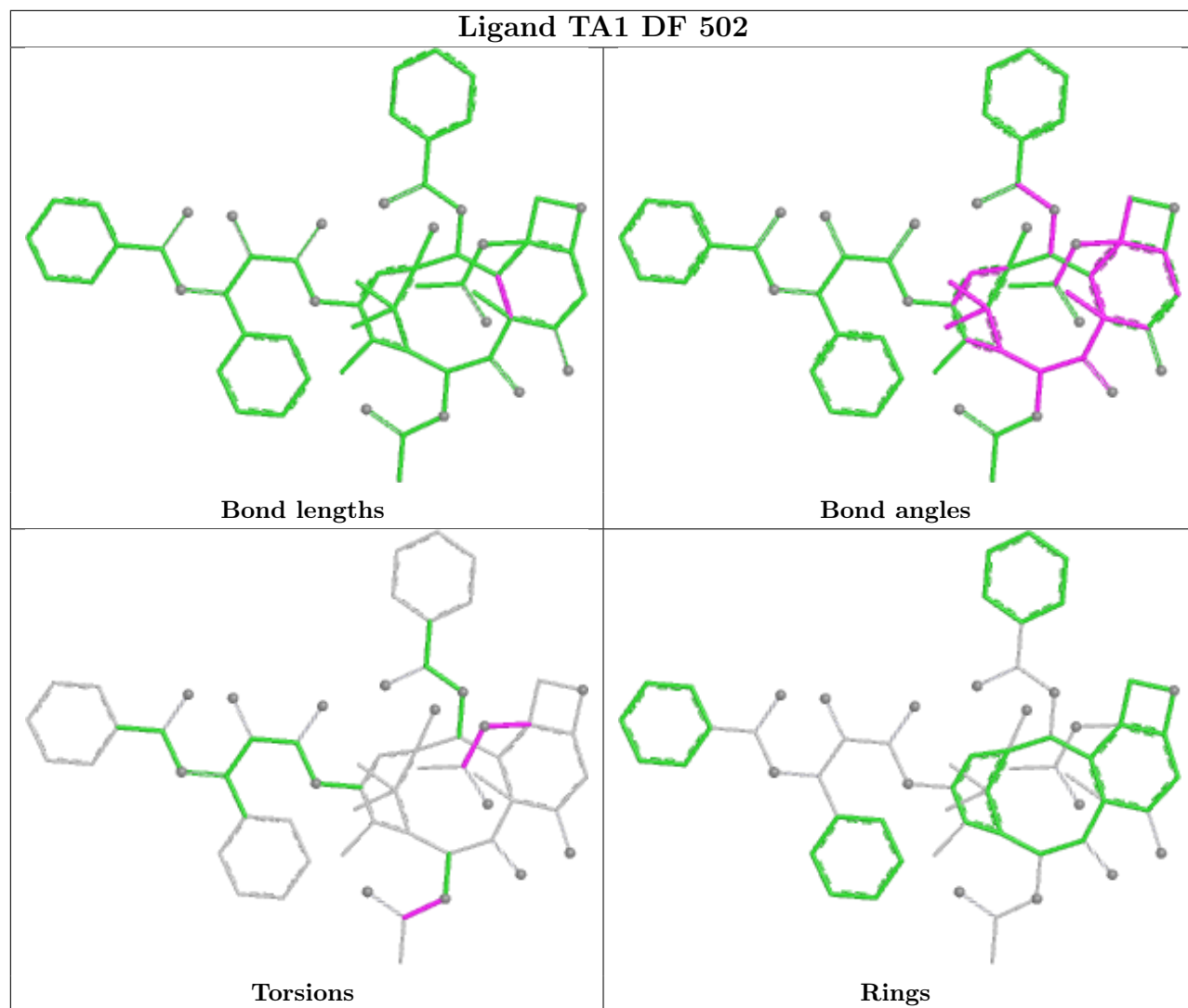
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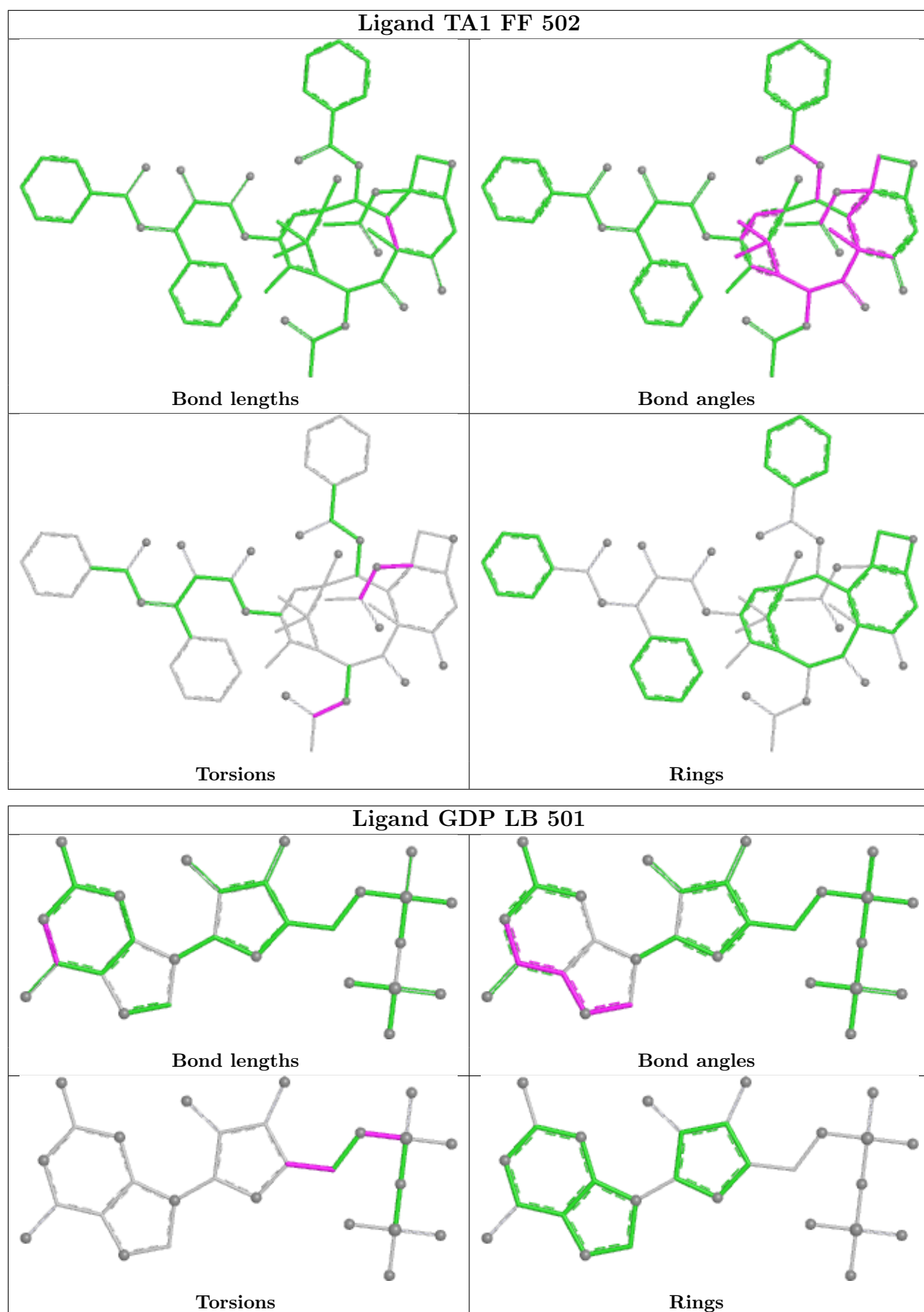


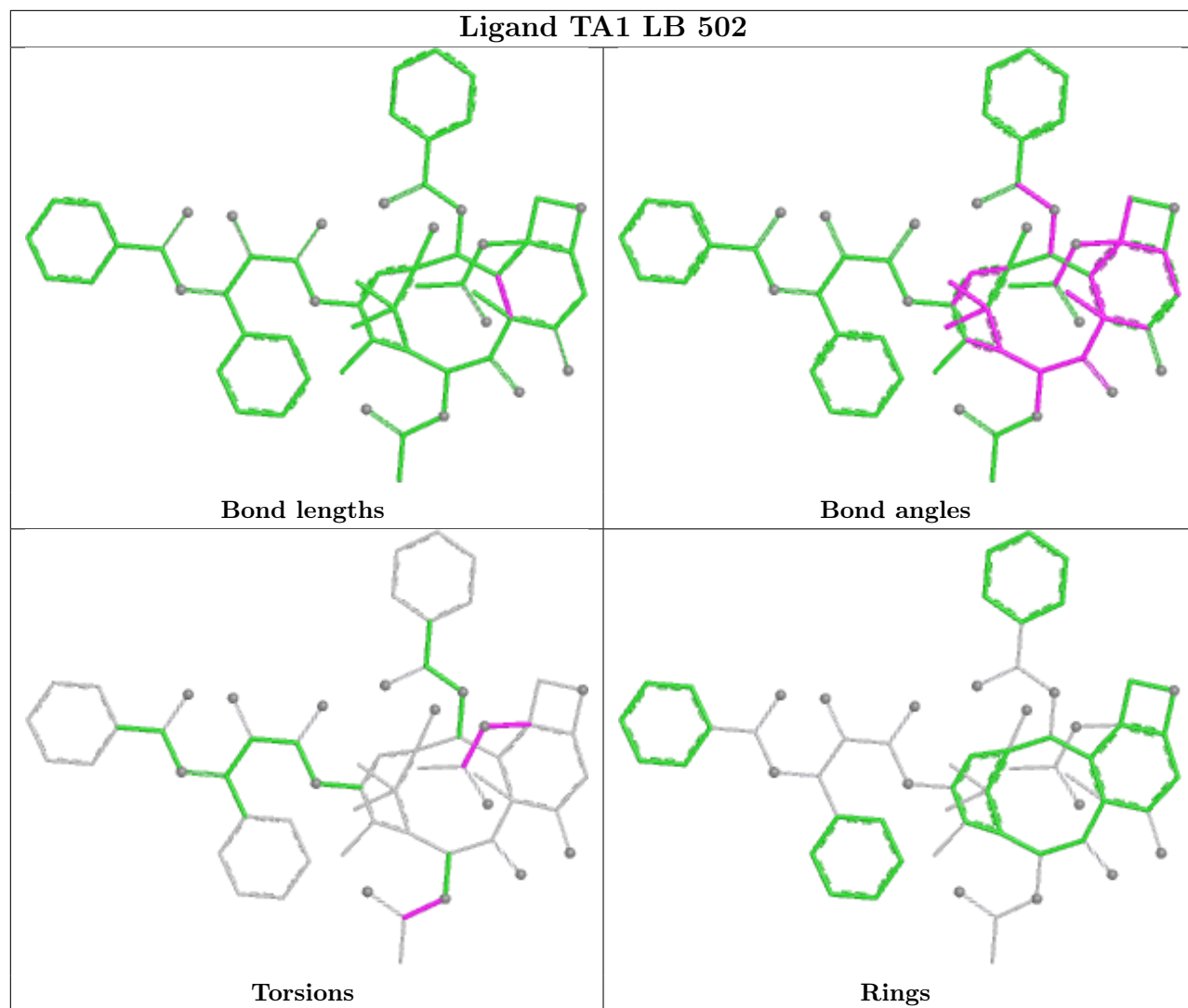




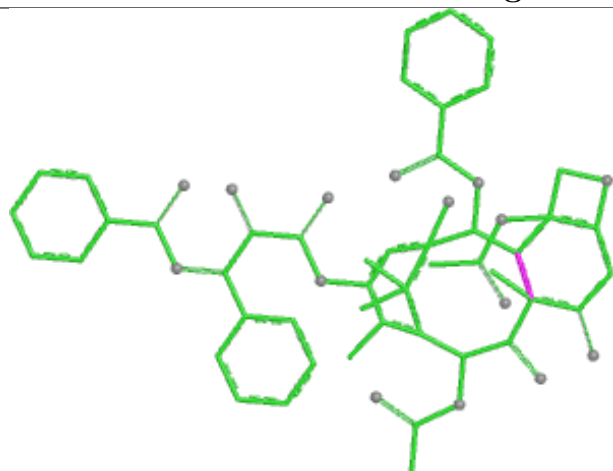




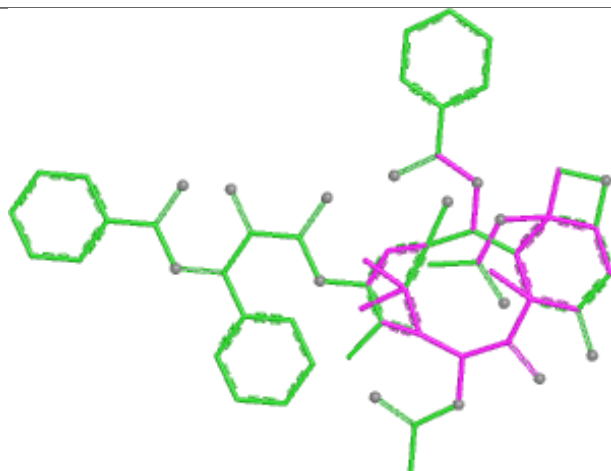




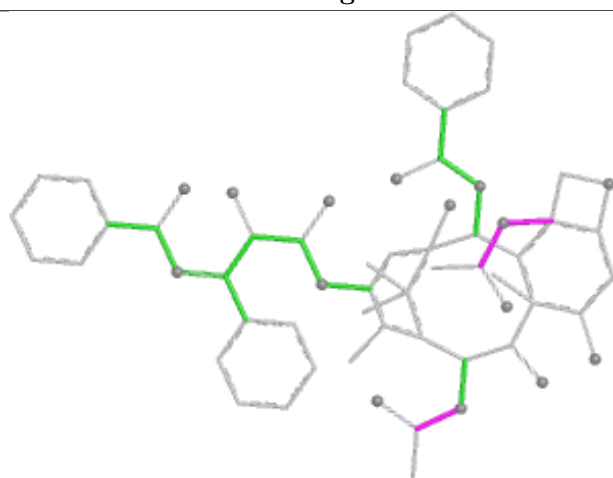
Ligand TA1 KB 502



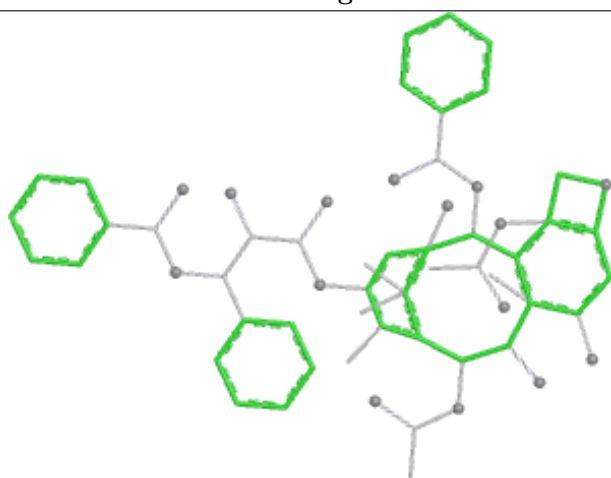
Bond lengths



Bond angles

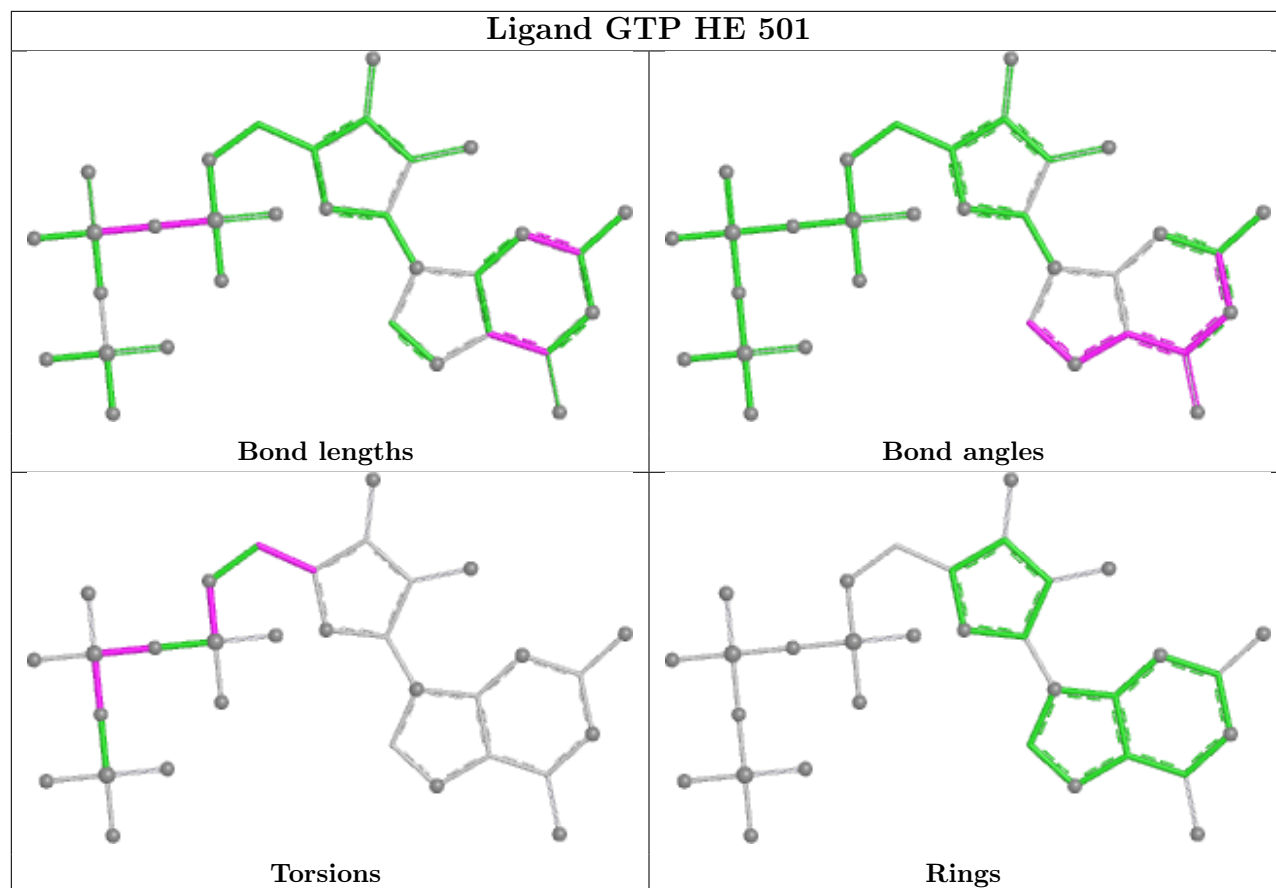


Torsions

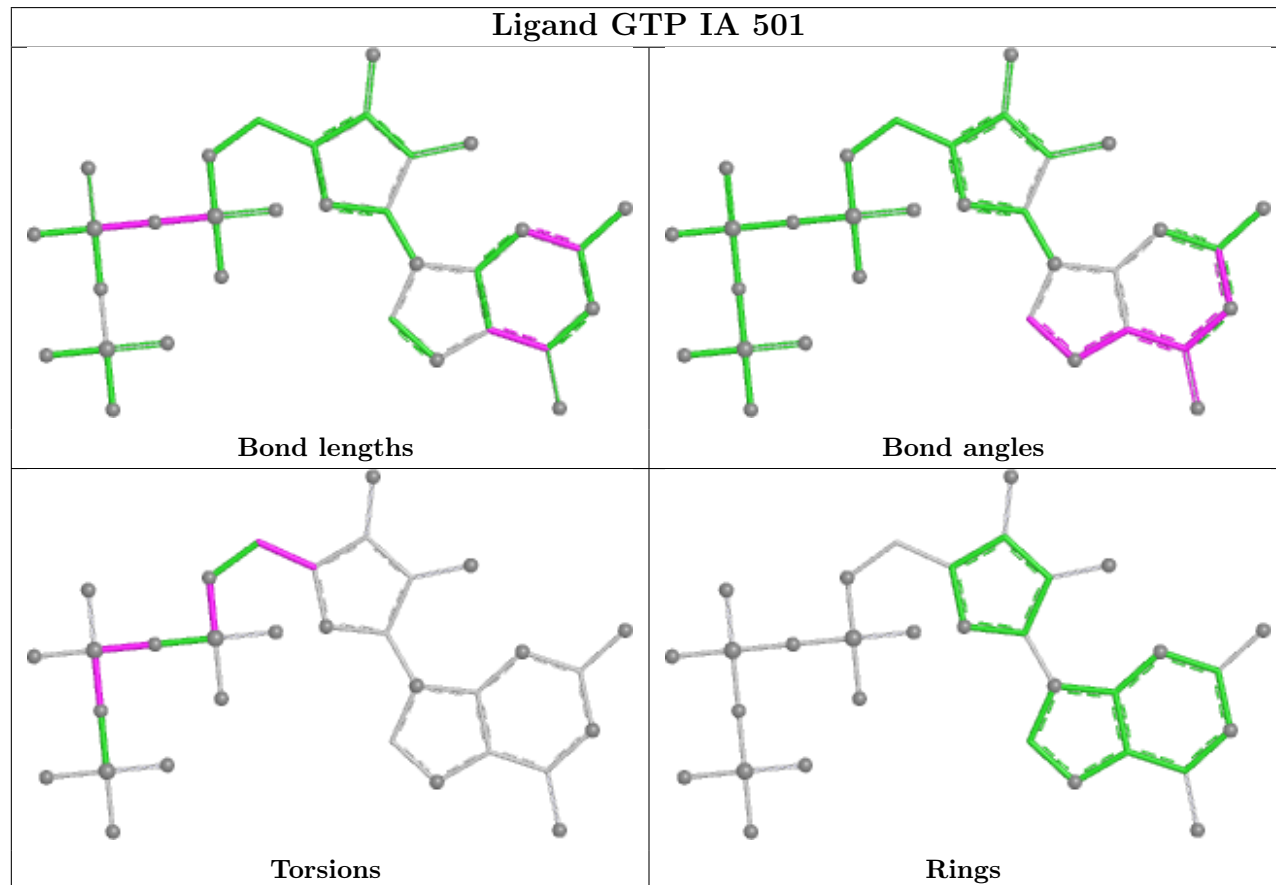


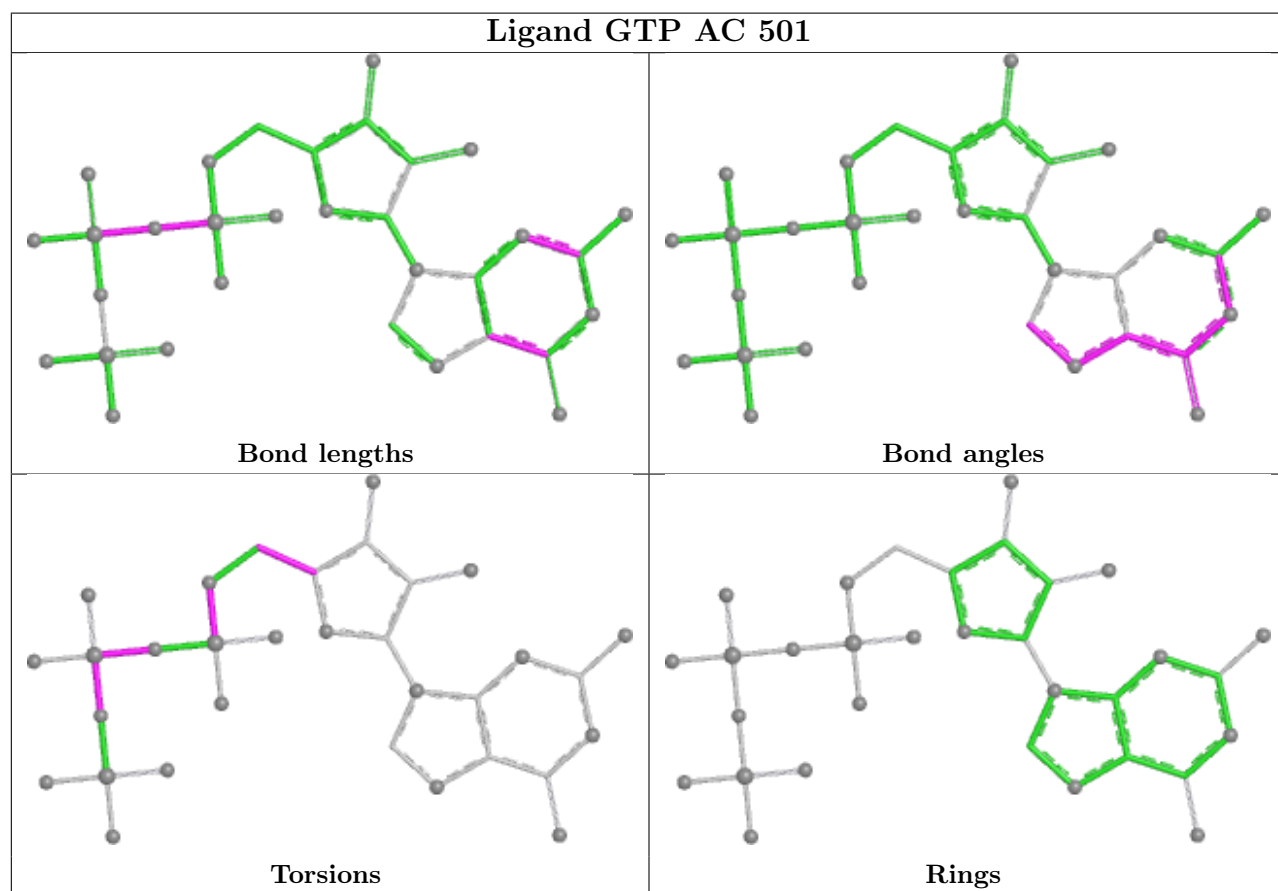
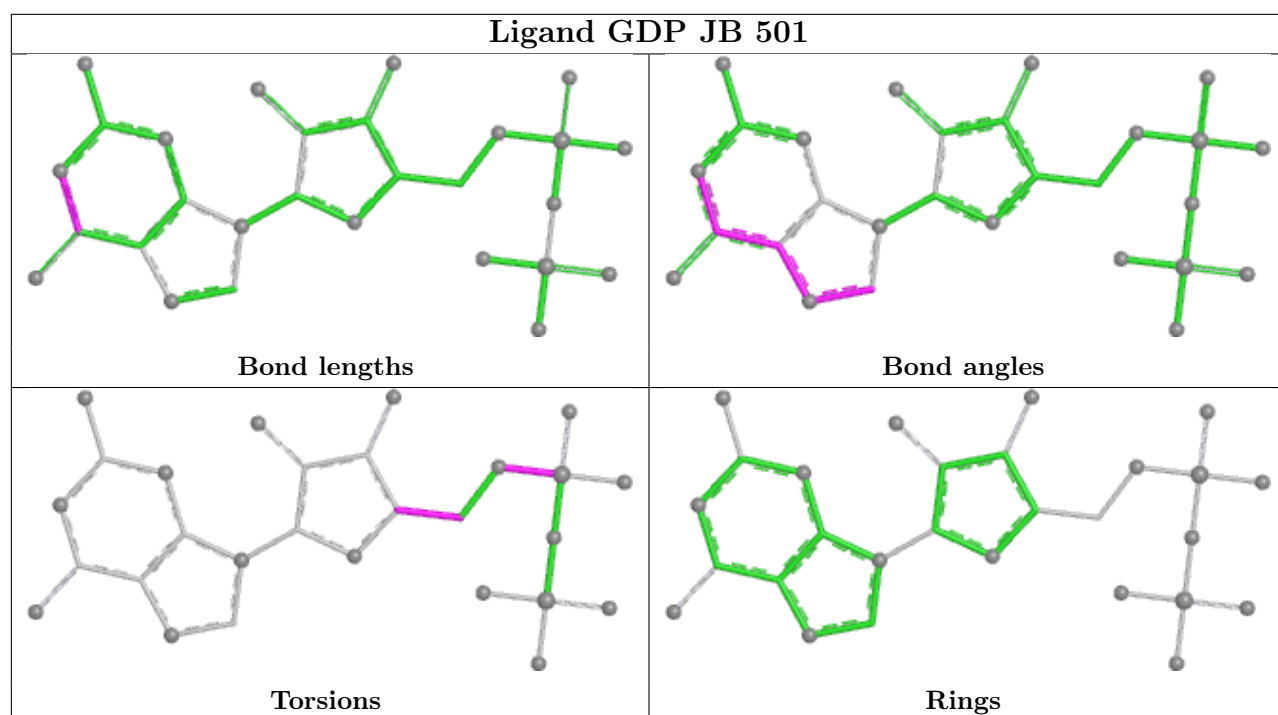
Rings

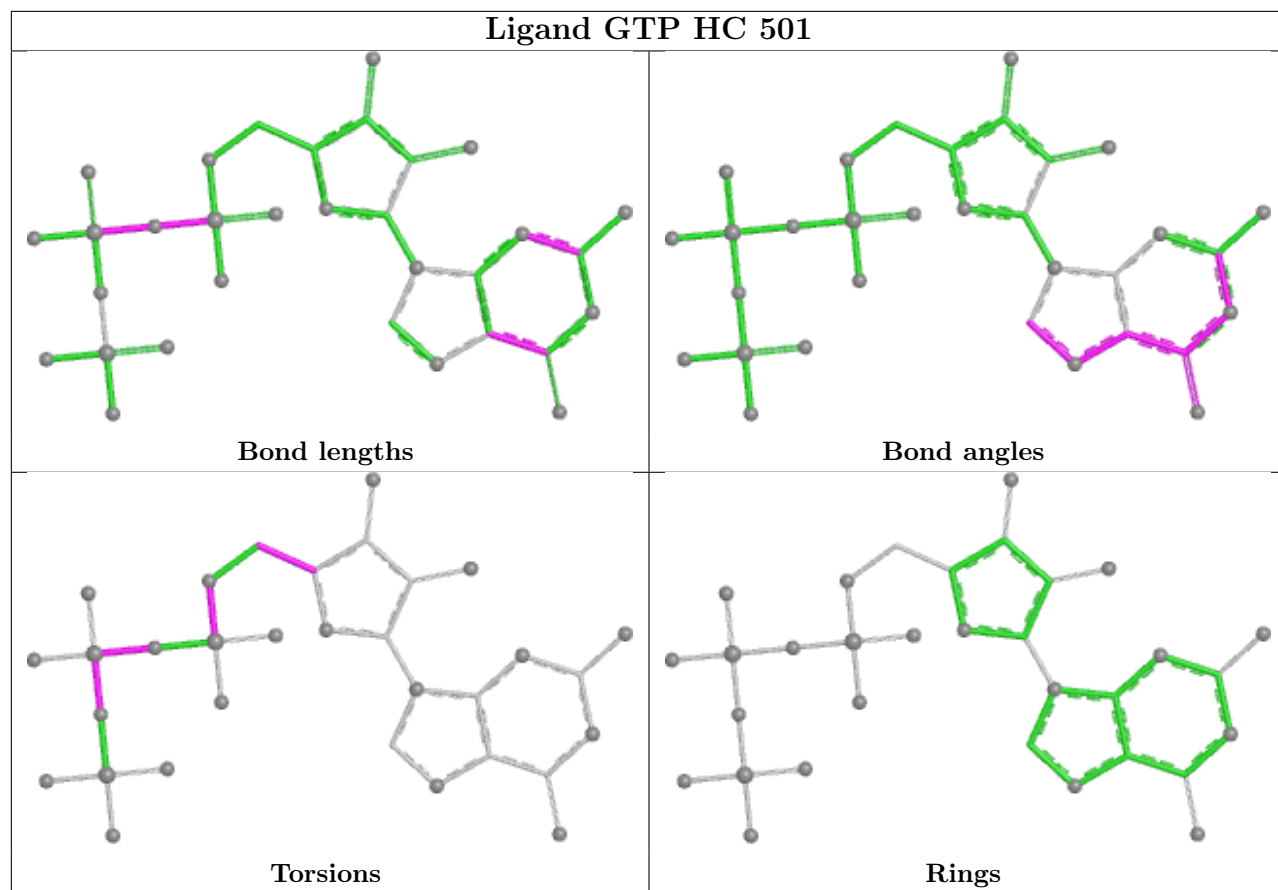
Ligand GTP HE 501



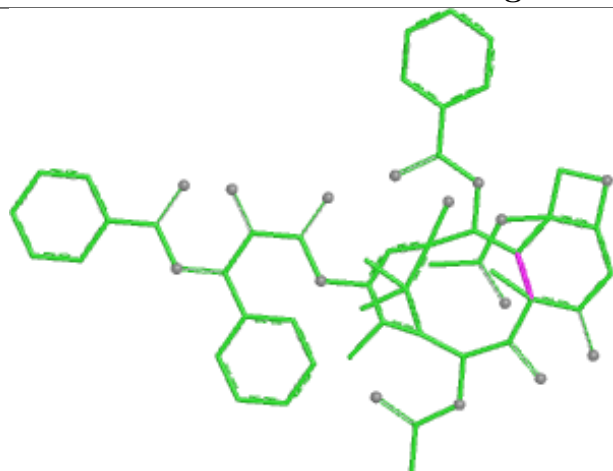
Ligand GTP IA 501



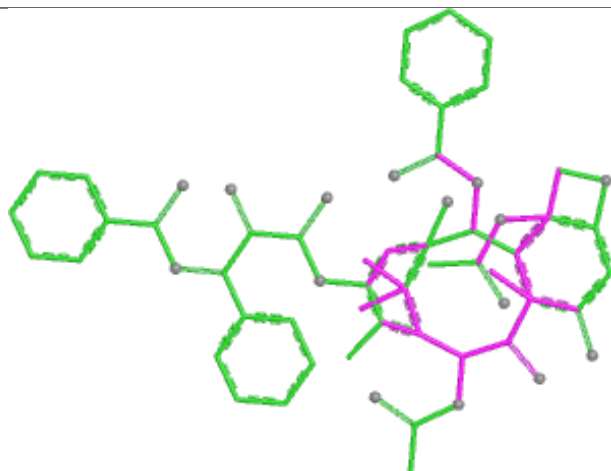




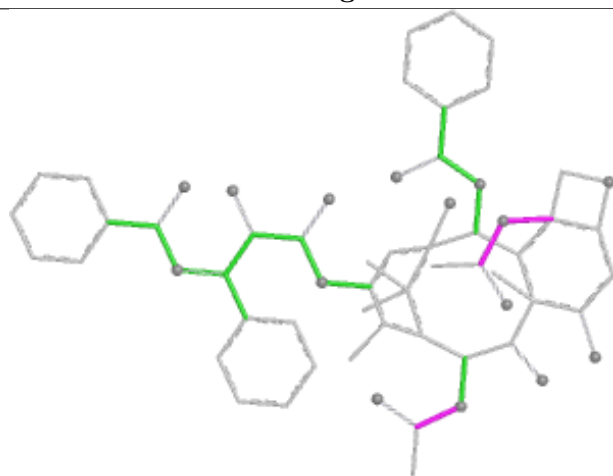
Ligand TA1 HB 502



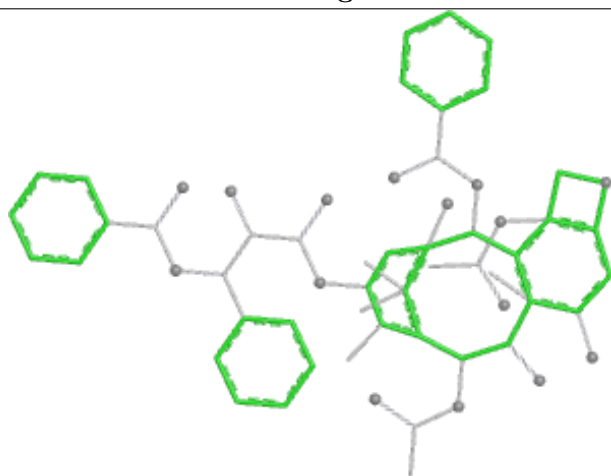
Bond lengths



Bond angles

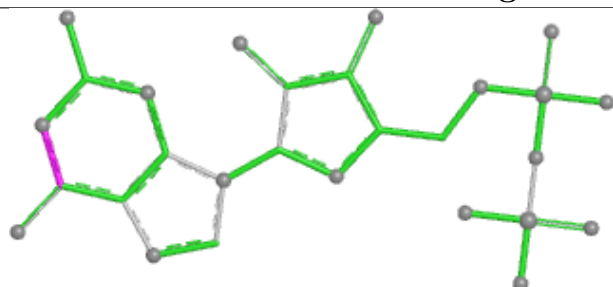


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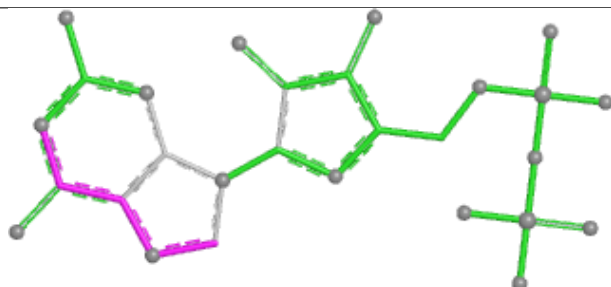


Rings

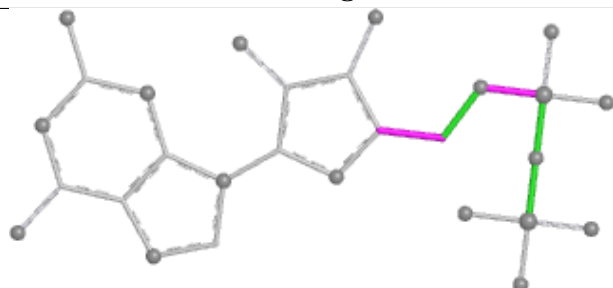
Ligand GDP BB 501



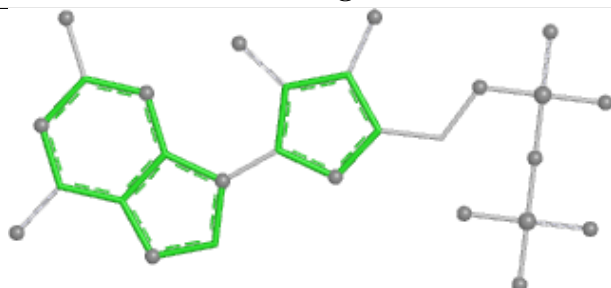
Bond lengths



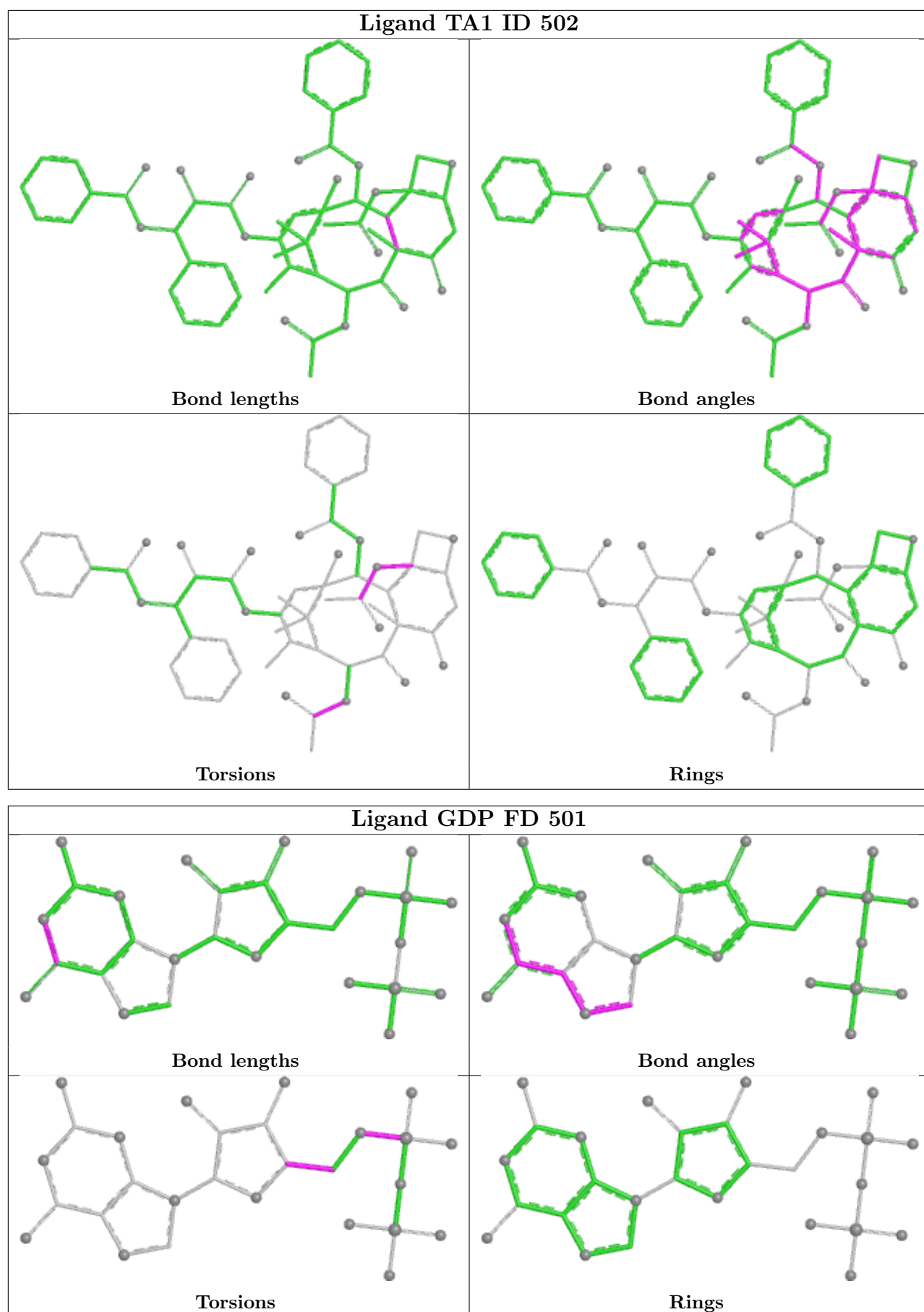
Bond angles

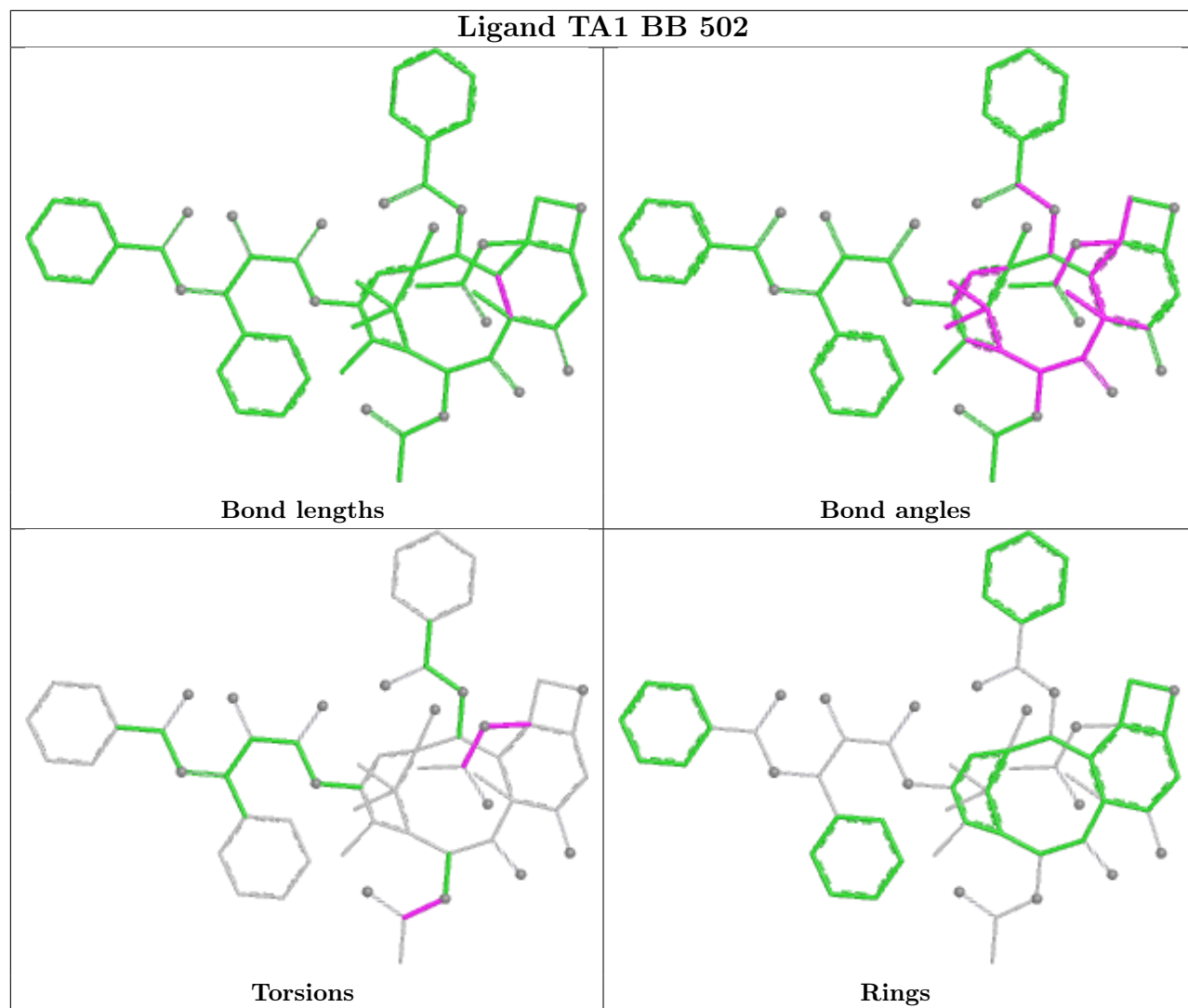


Torsions

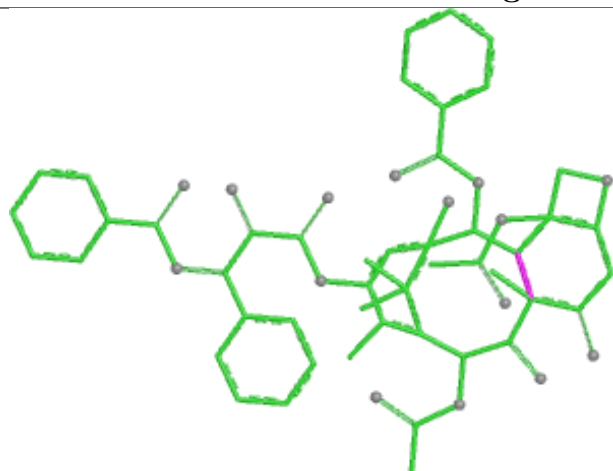


Rings

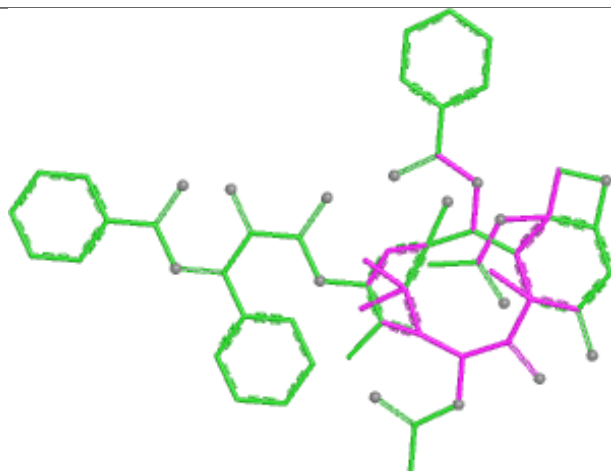




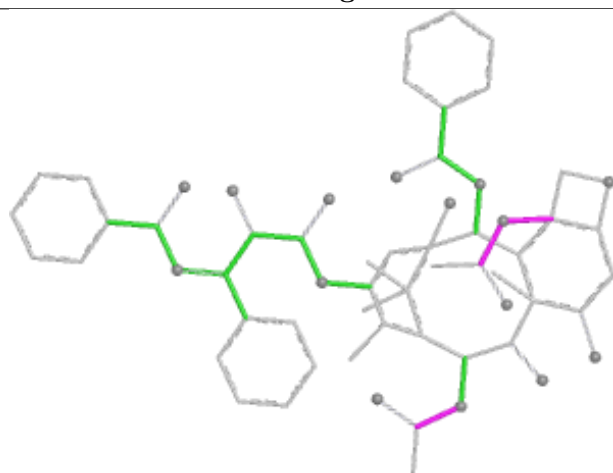
Ligand TA1 GD 502



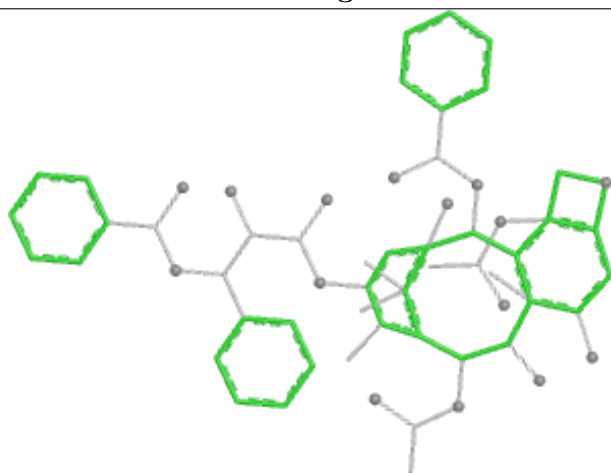
Bond lengths



Bond angles

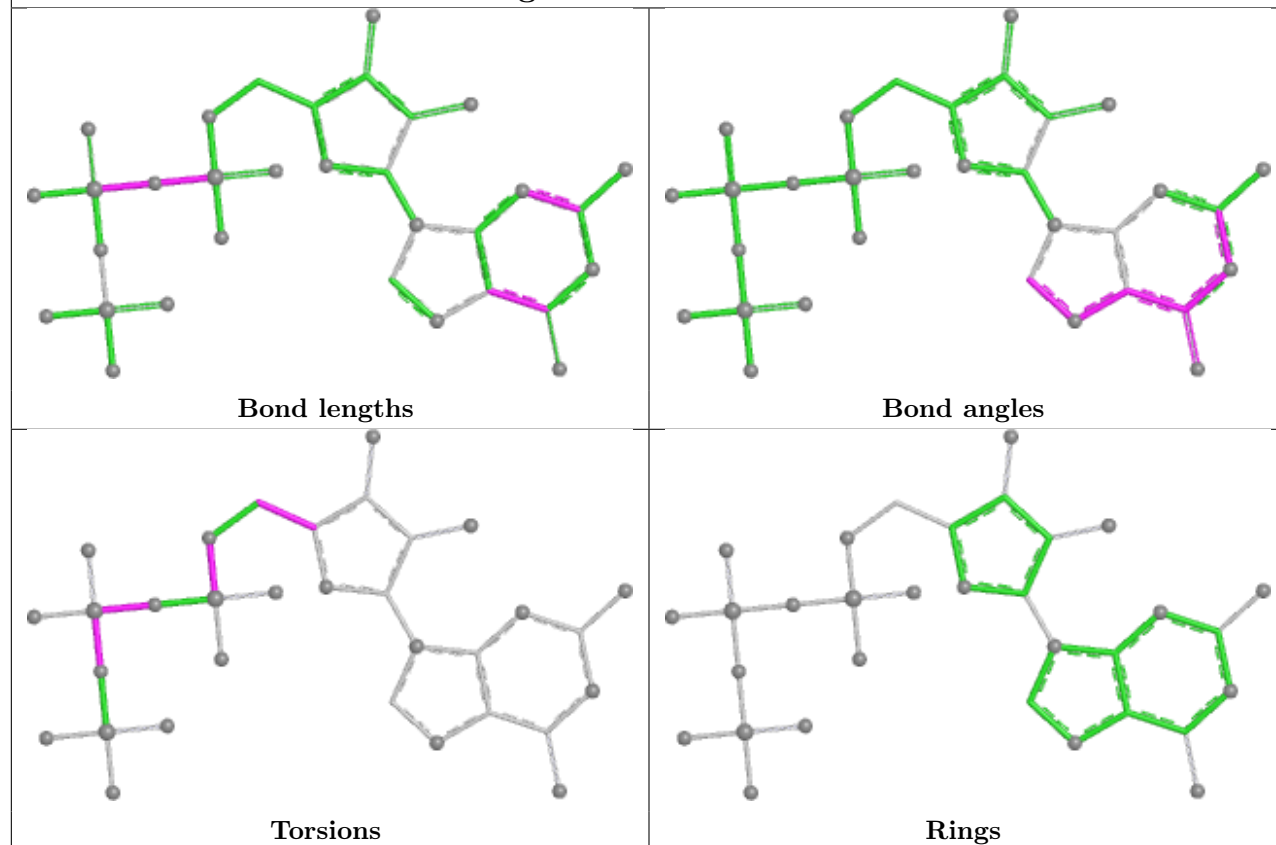


Torsions

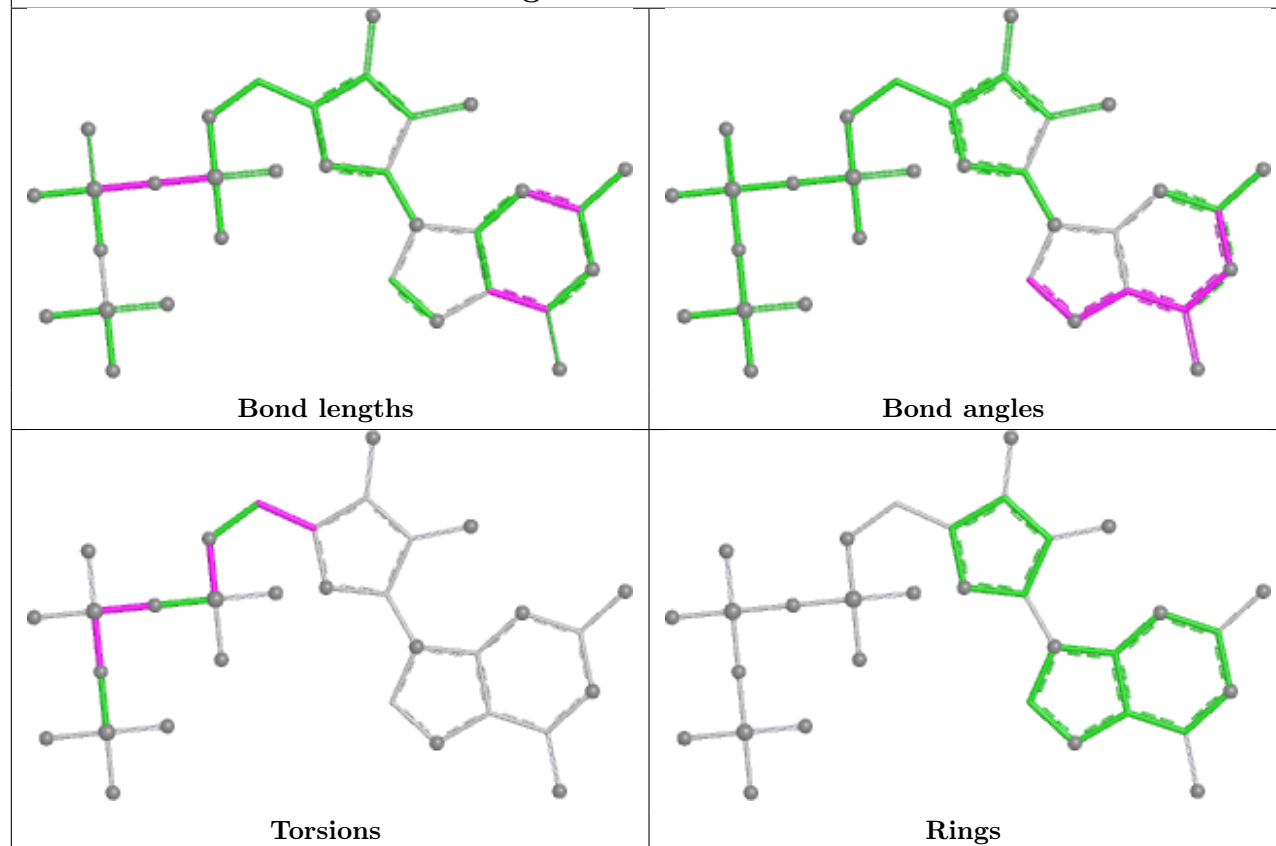


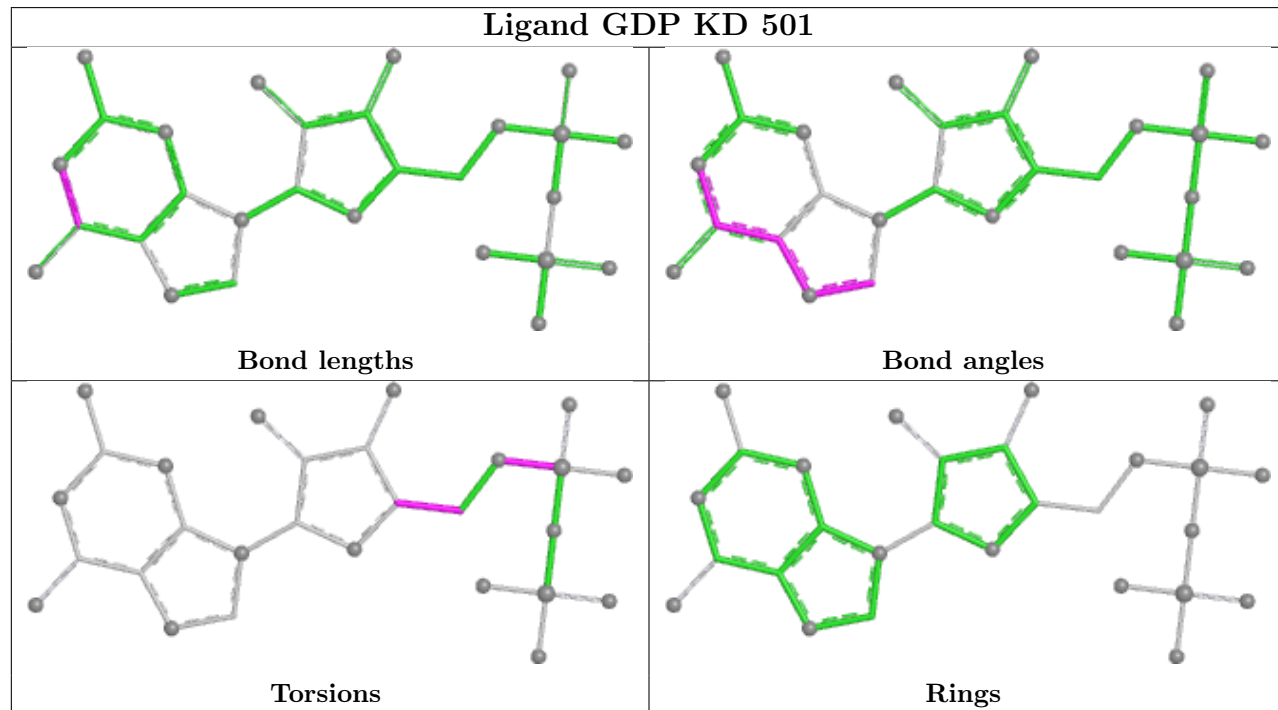
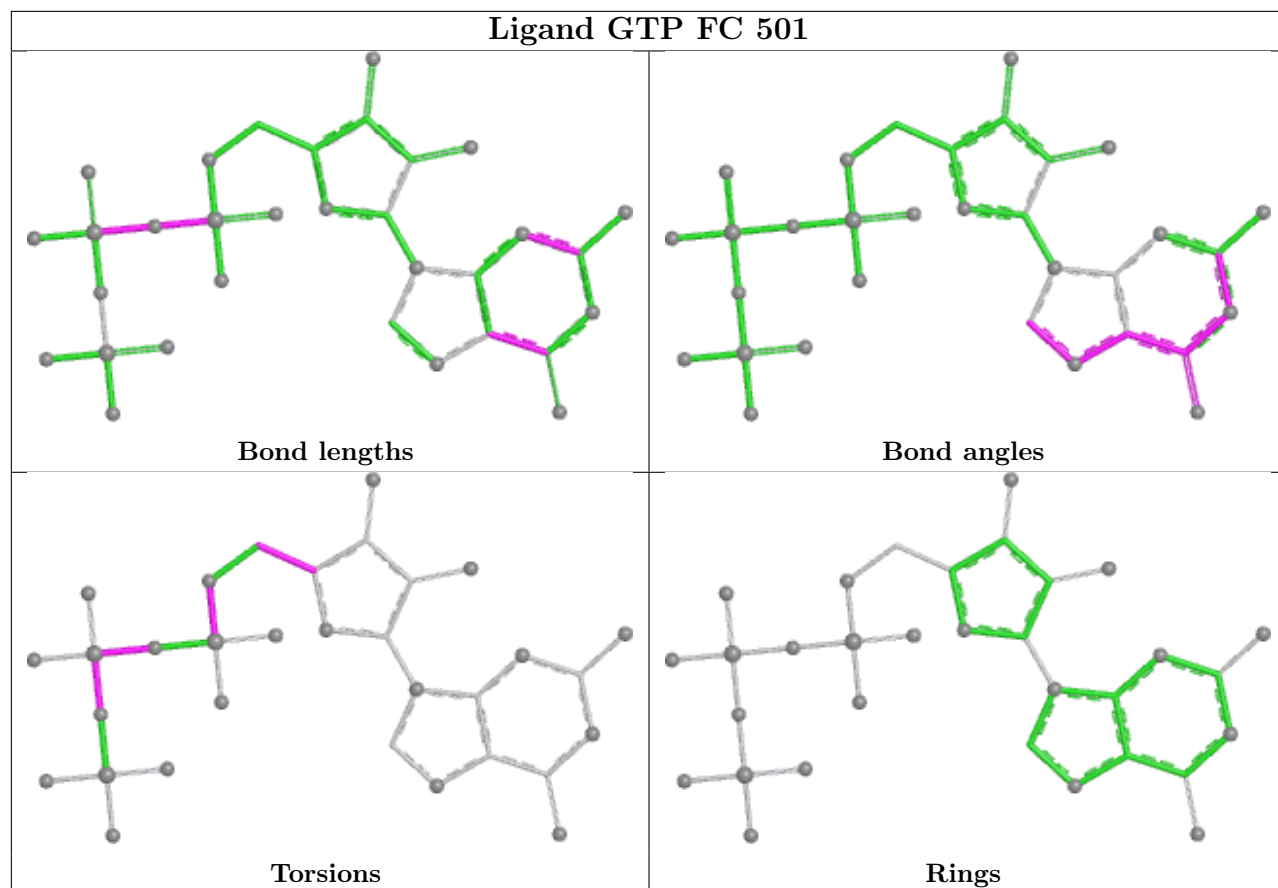
Rings

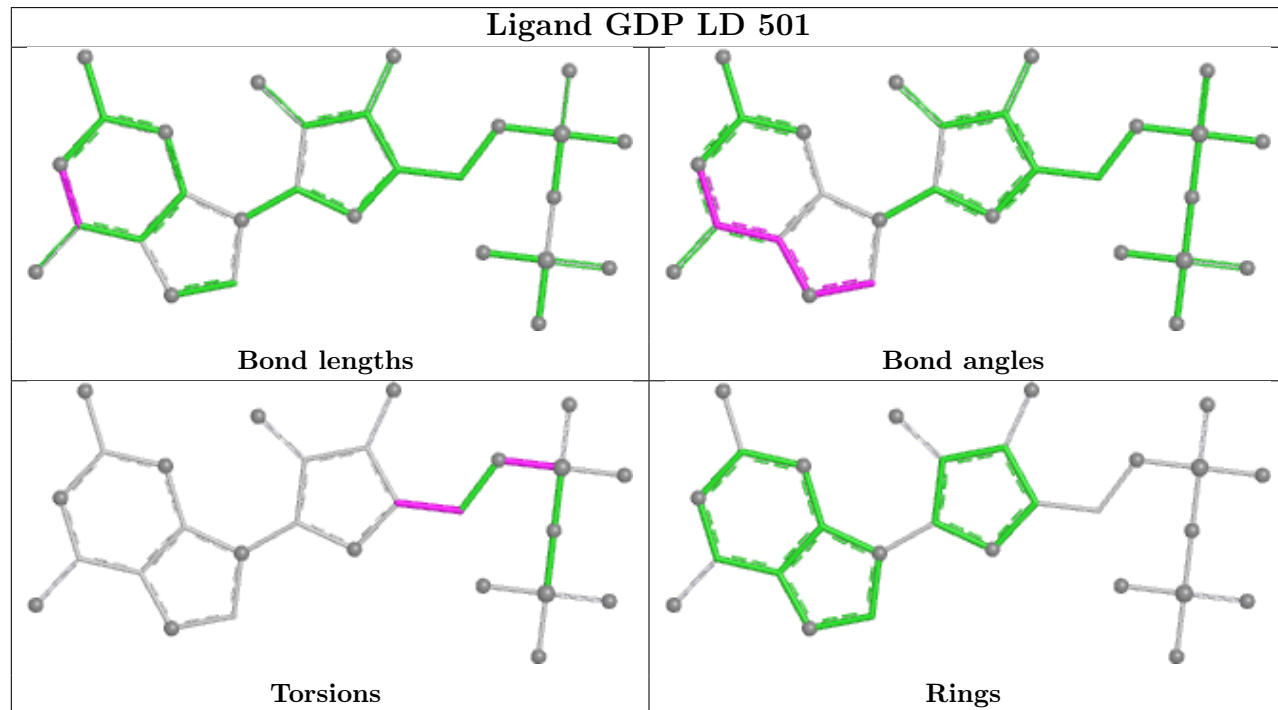
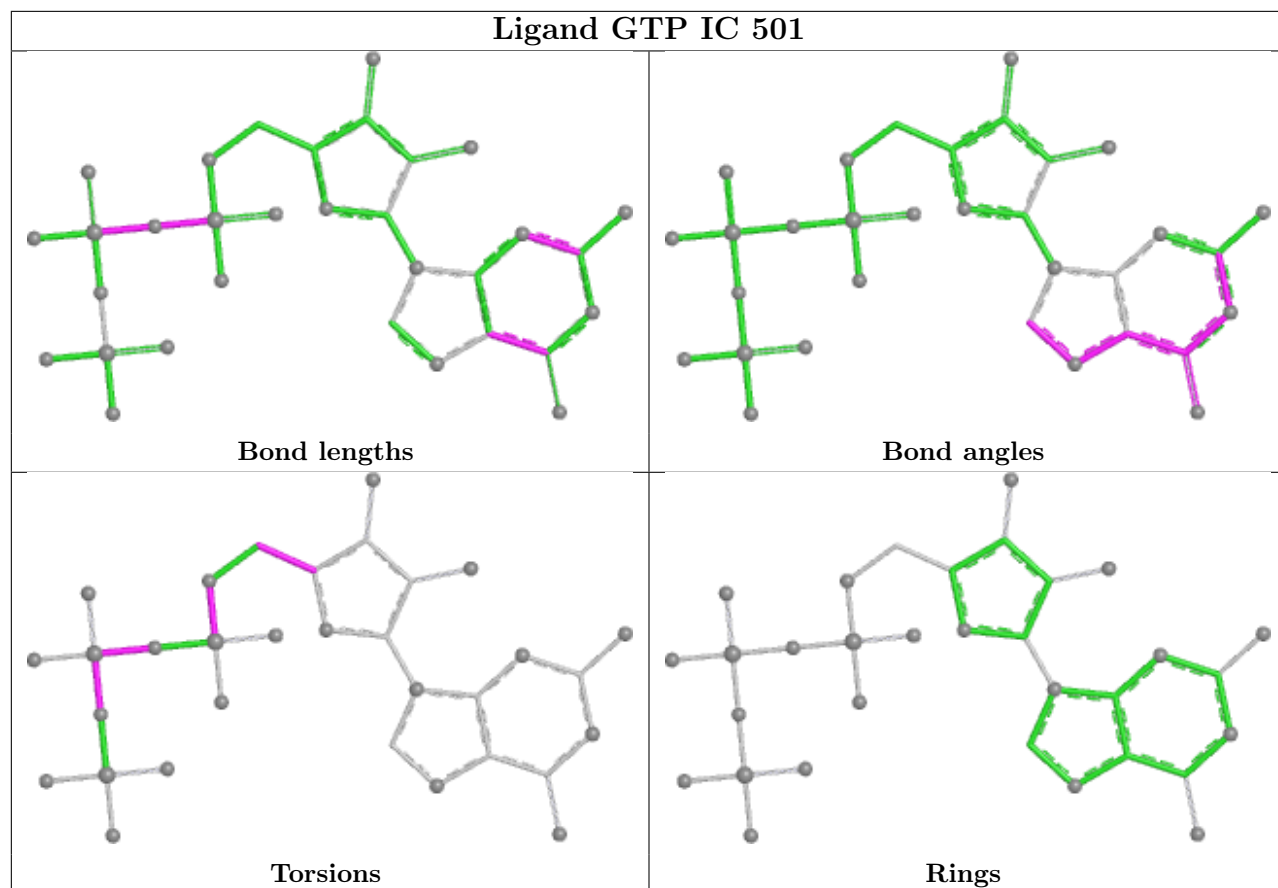
Ligand GTP EA 501

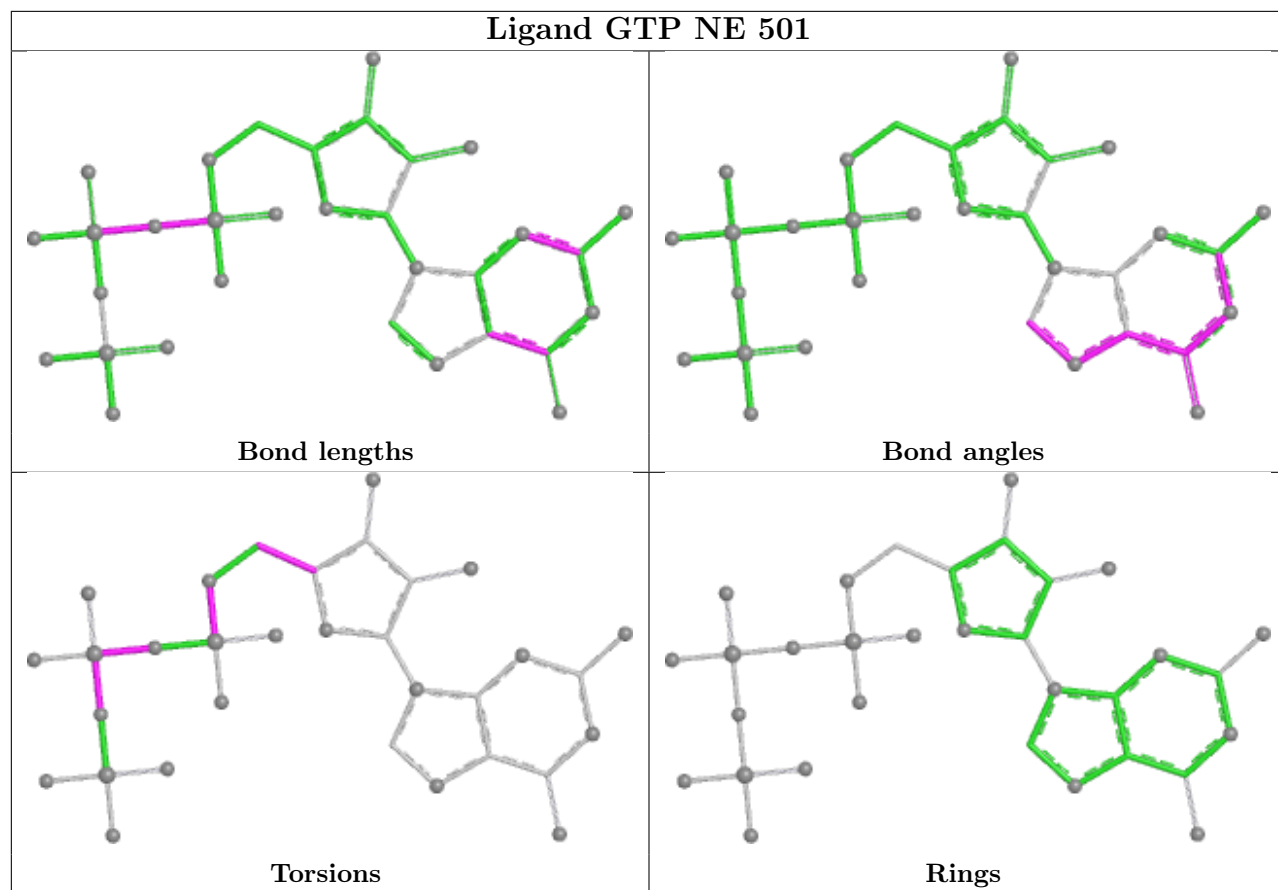


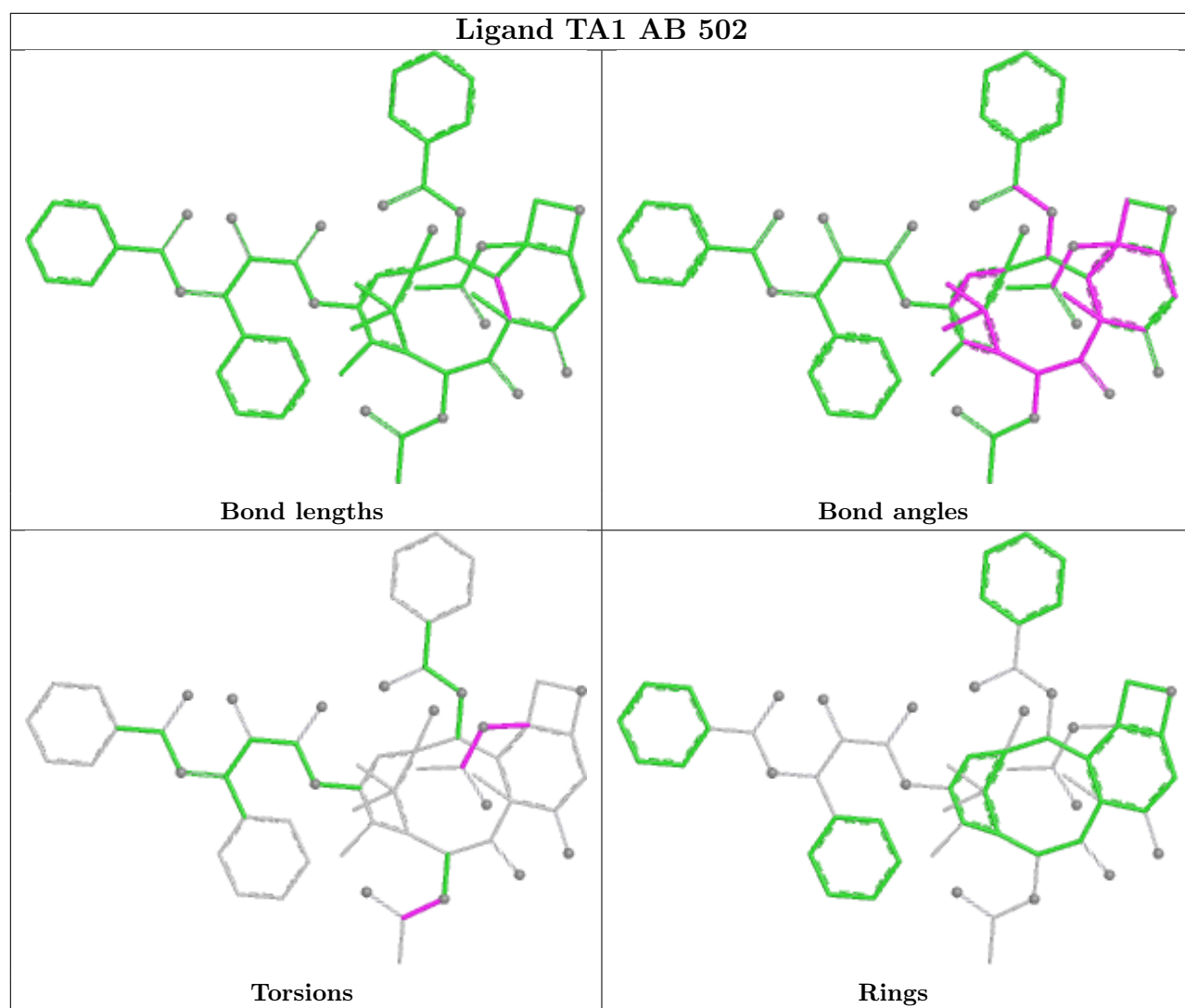
Ligand GTP JE 501

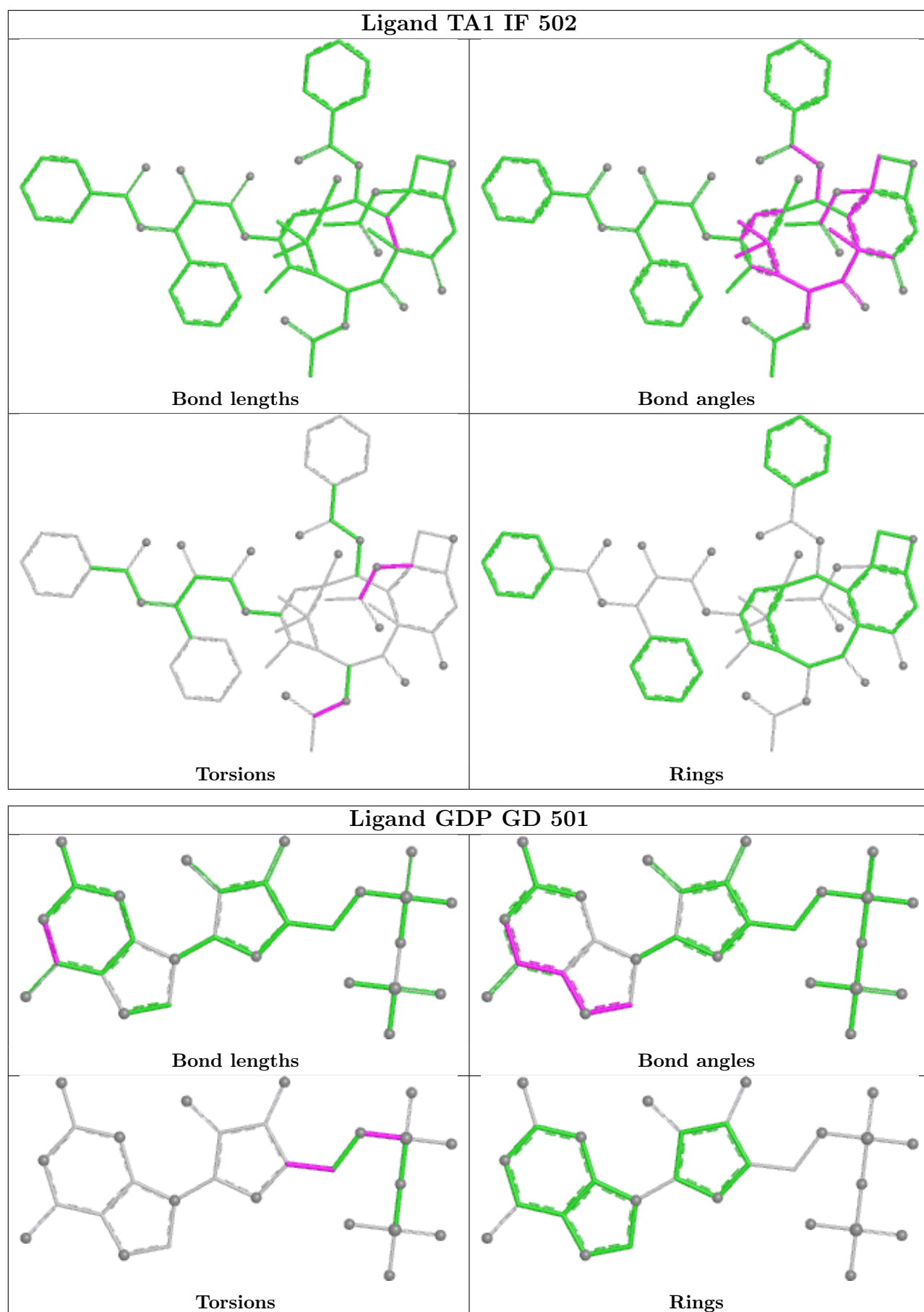


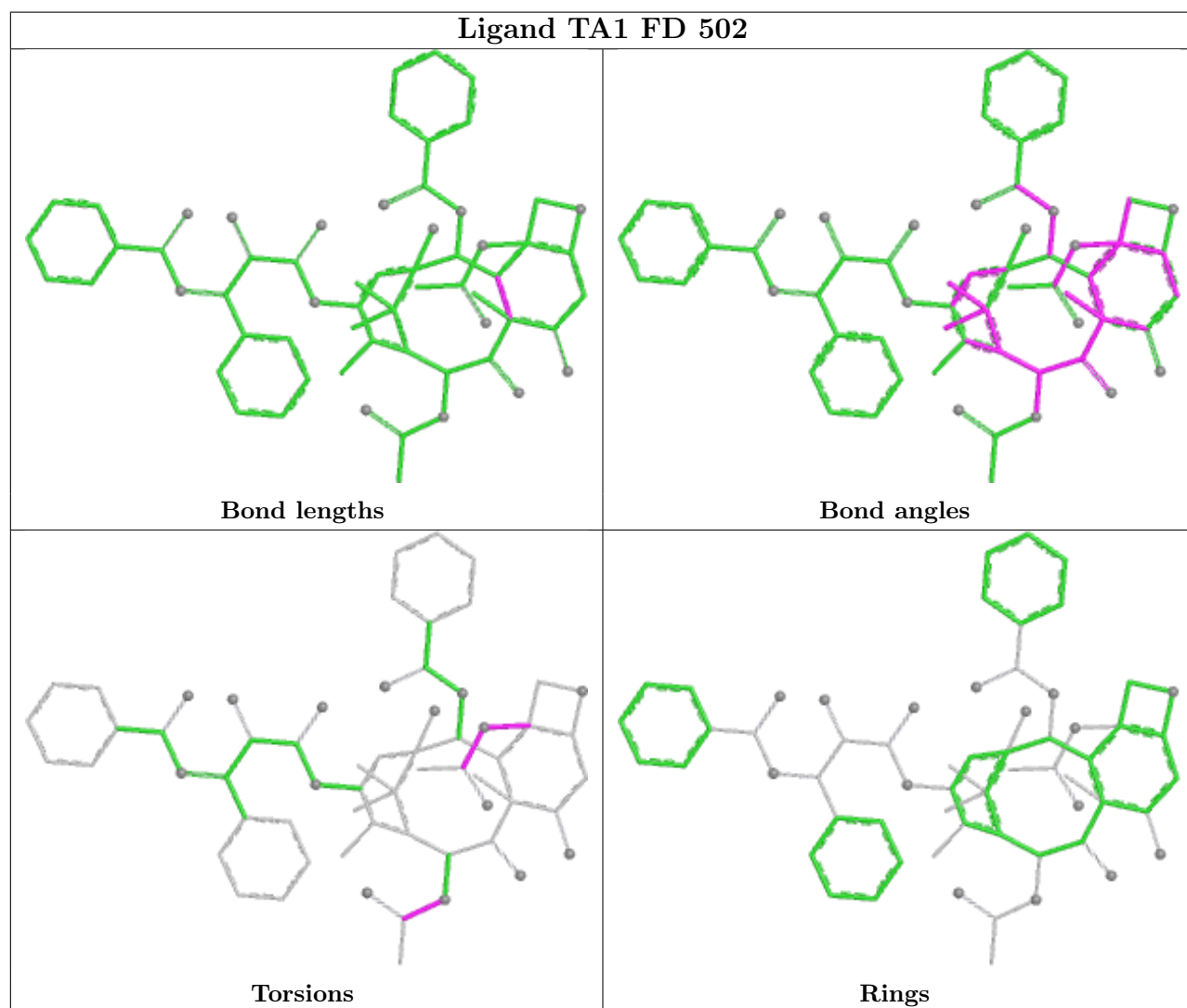
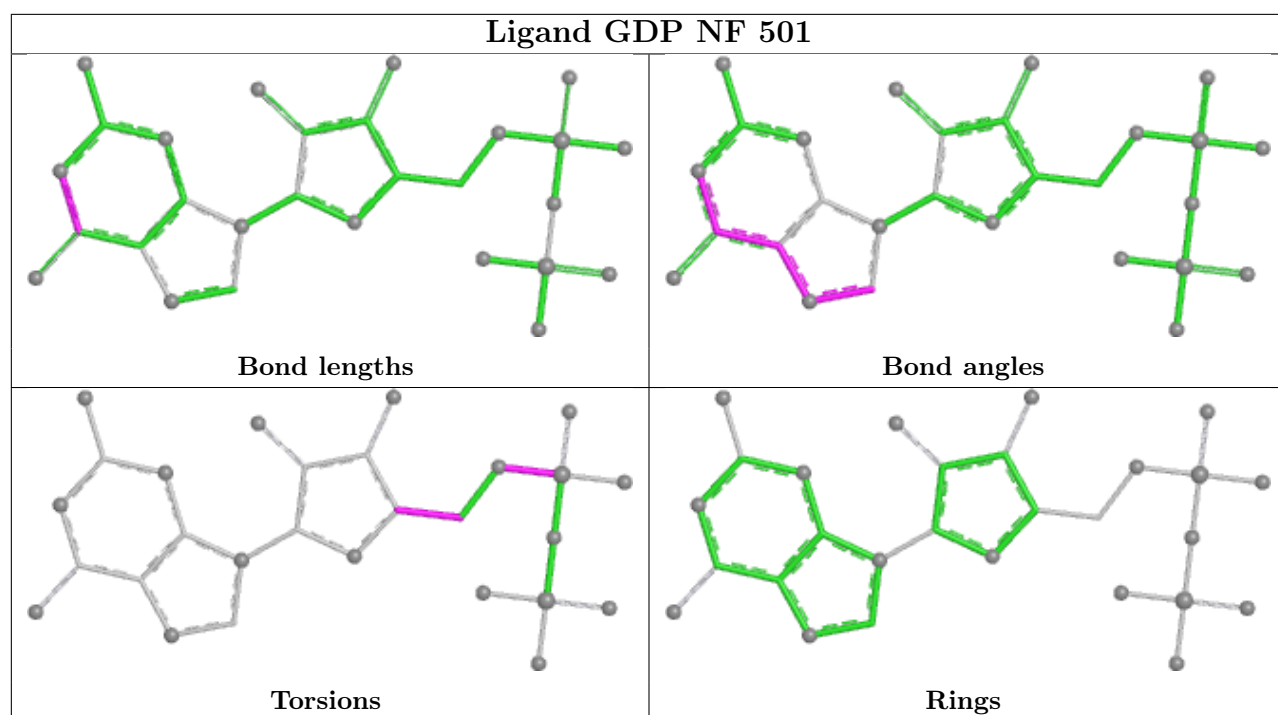


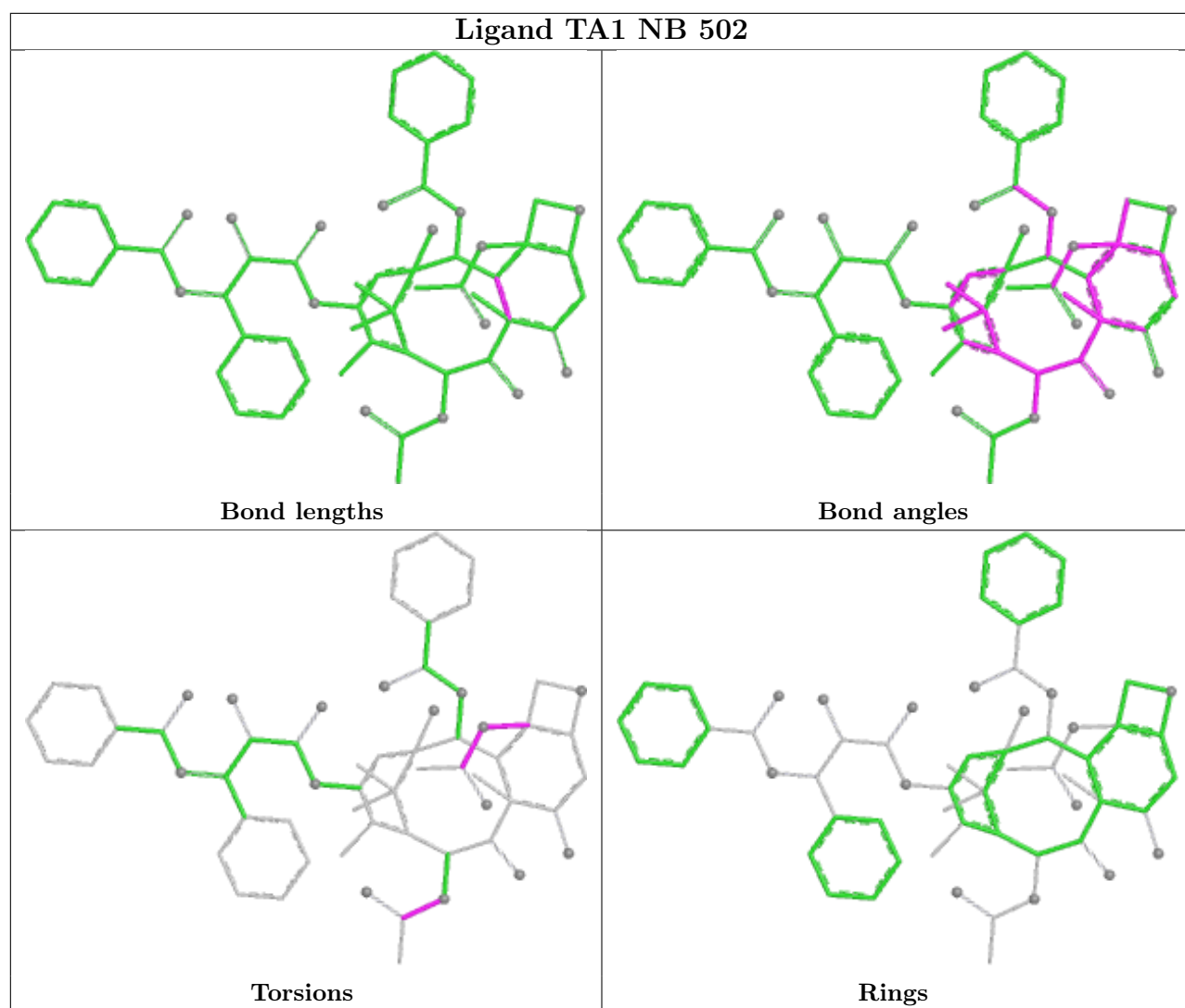


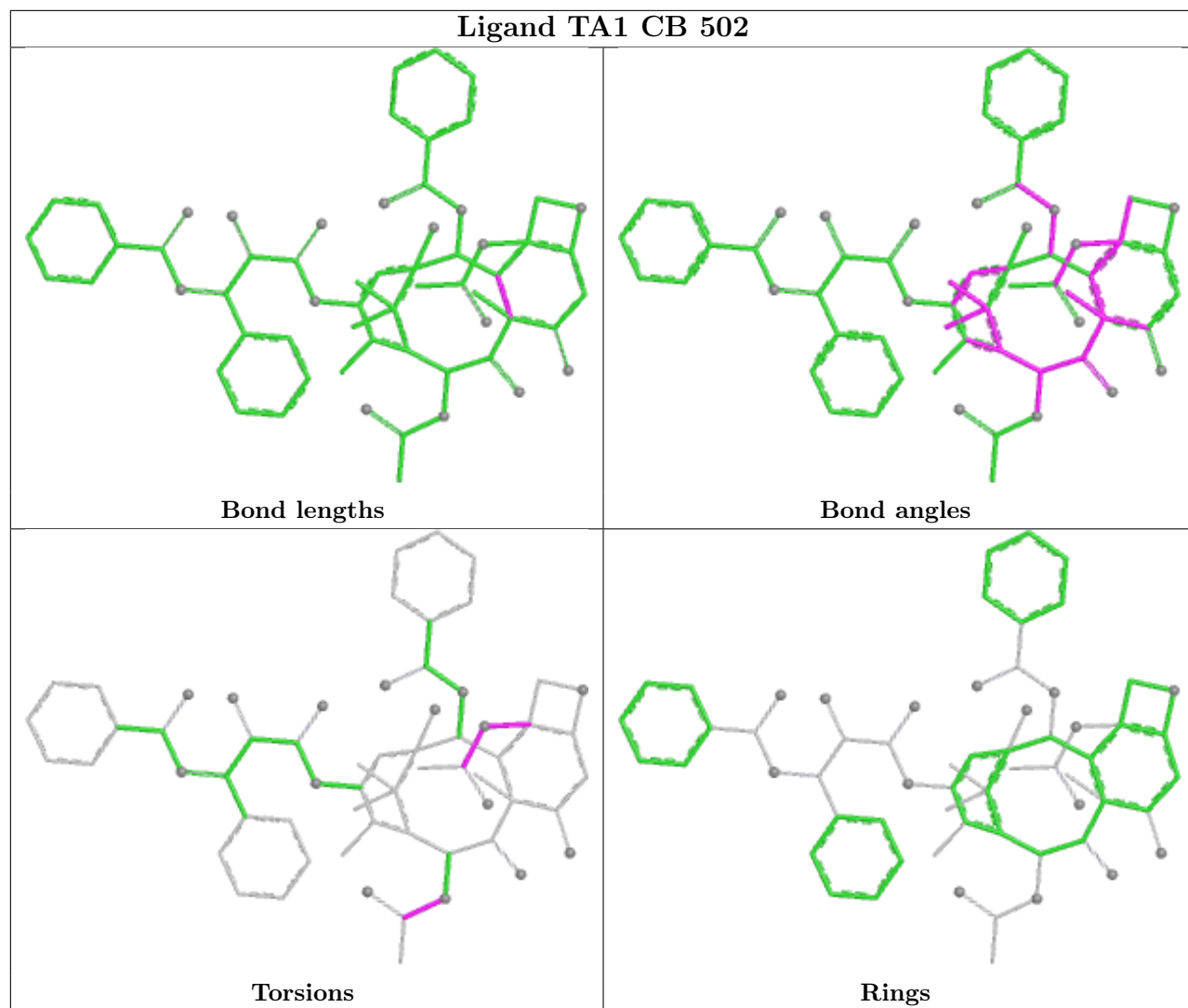


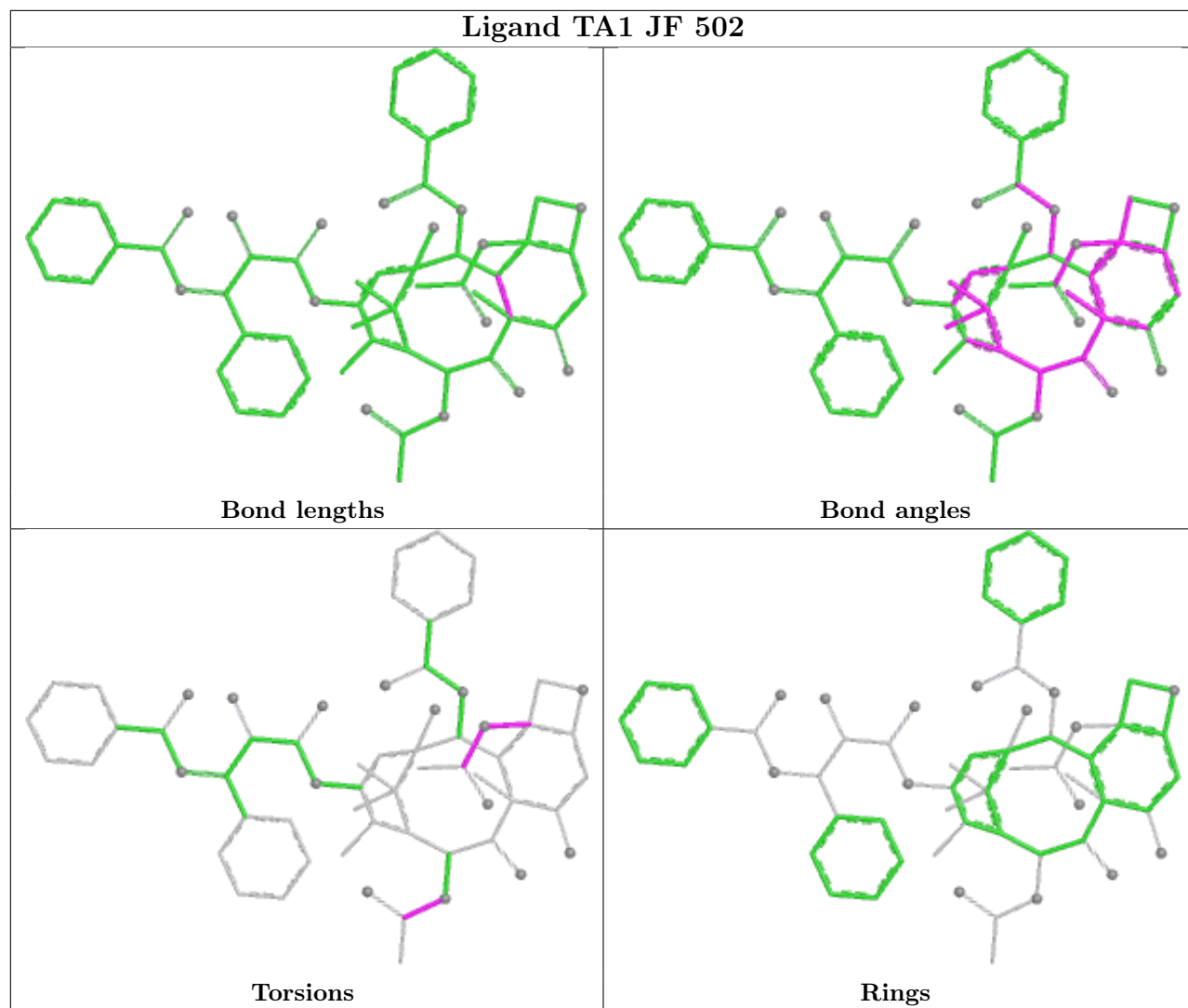


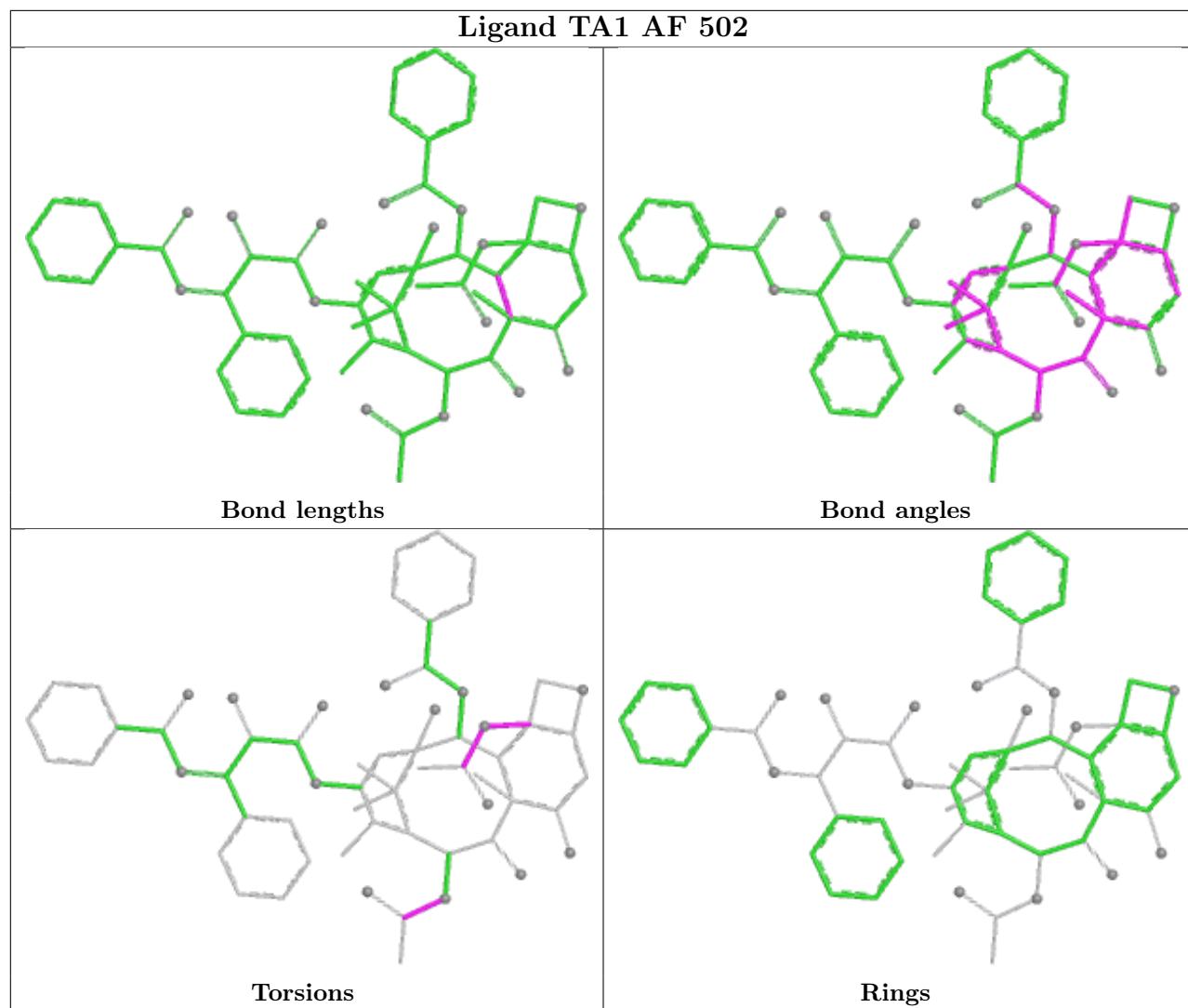


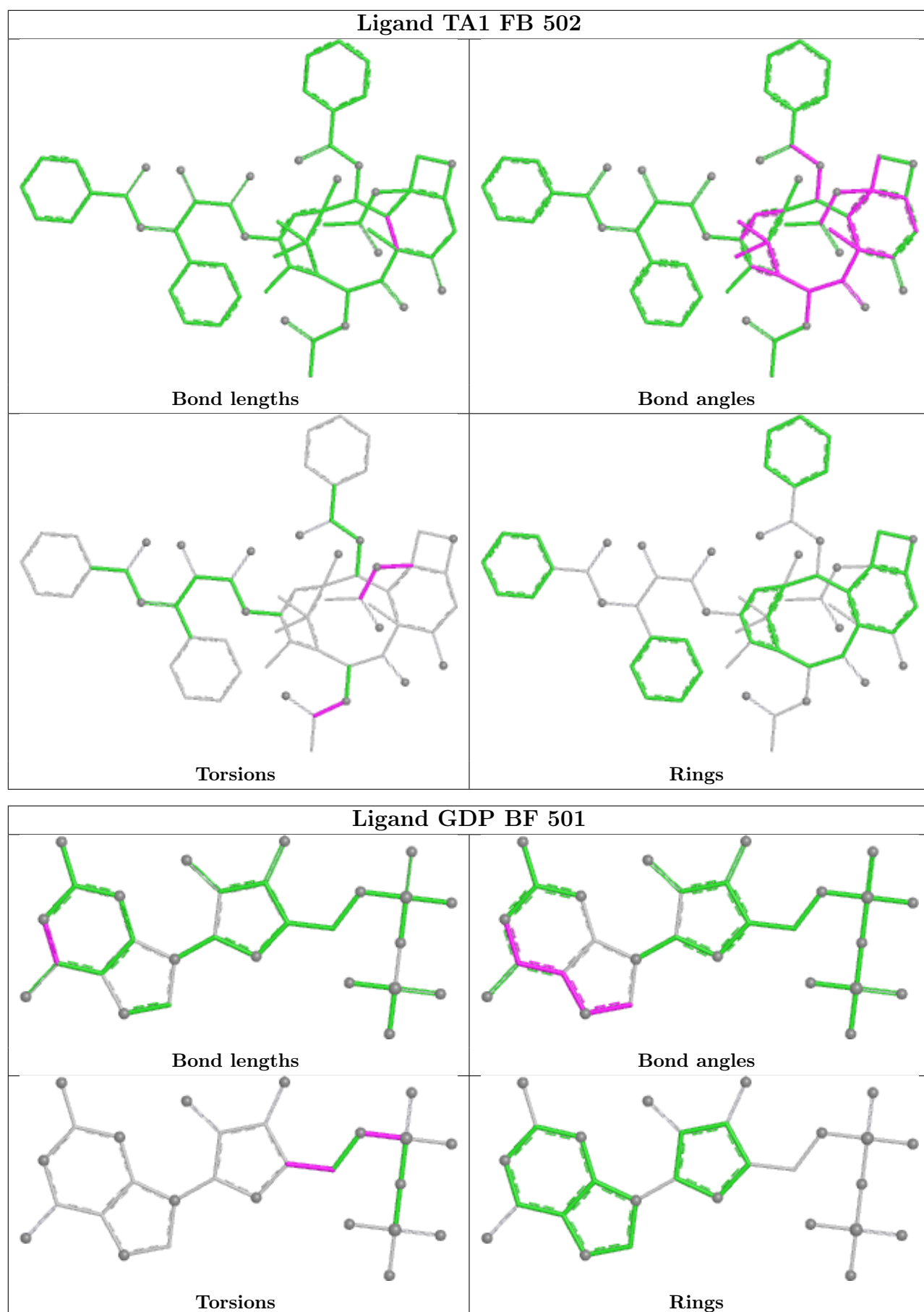




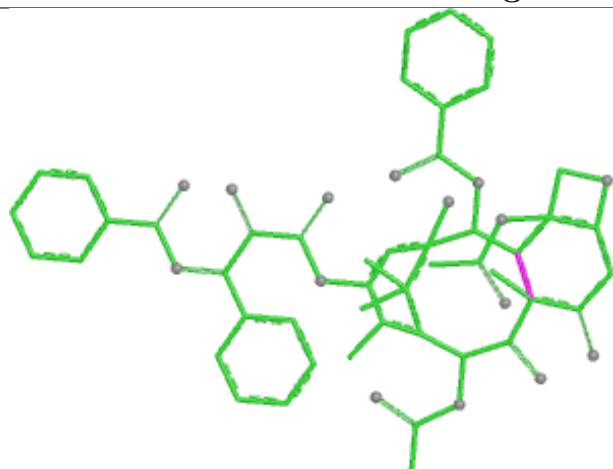




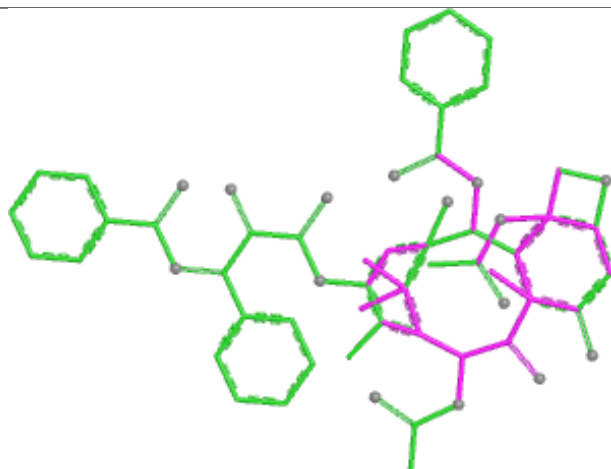




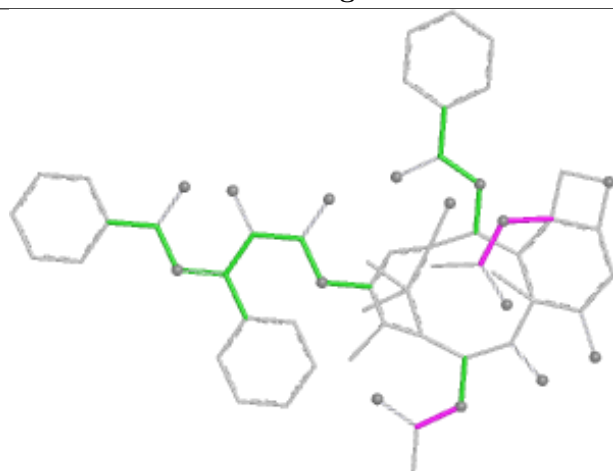
Ligand TA1 KD 502



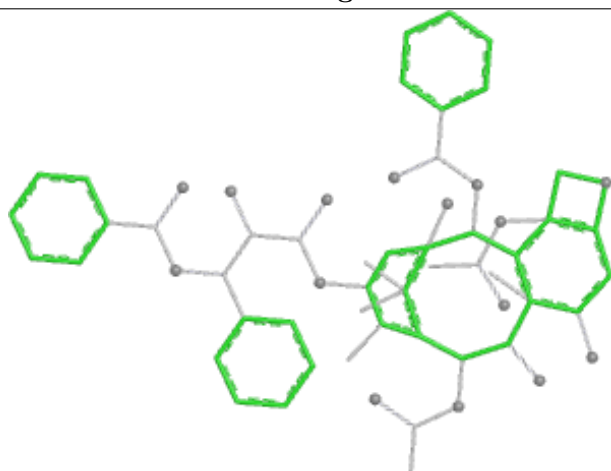
Bond lengths



Bond angles

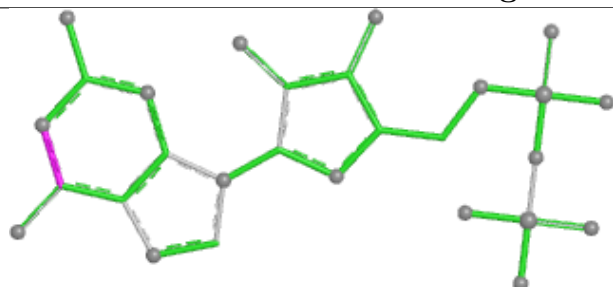


Torsions

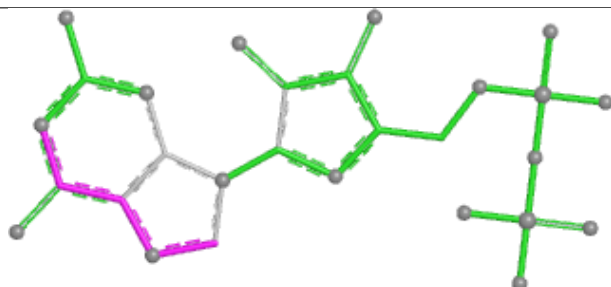


Rings

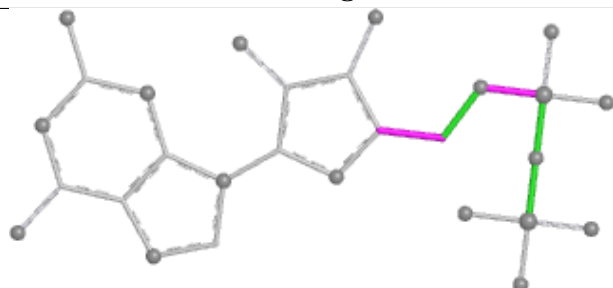
Ligand GDP AF 501



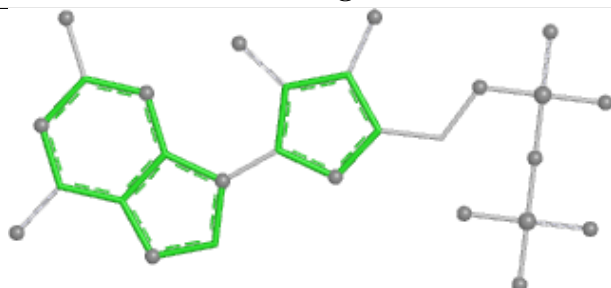
Bond lengths



Bond angles

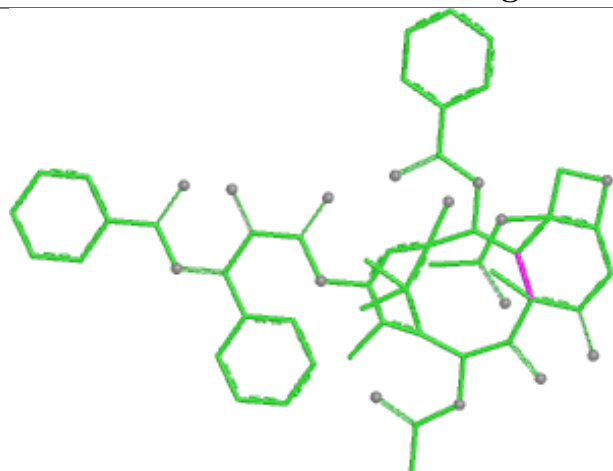


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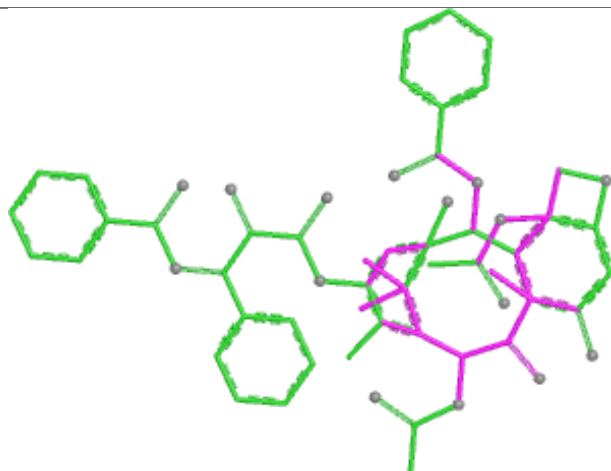


Rings

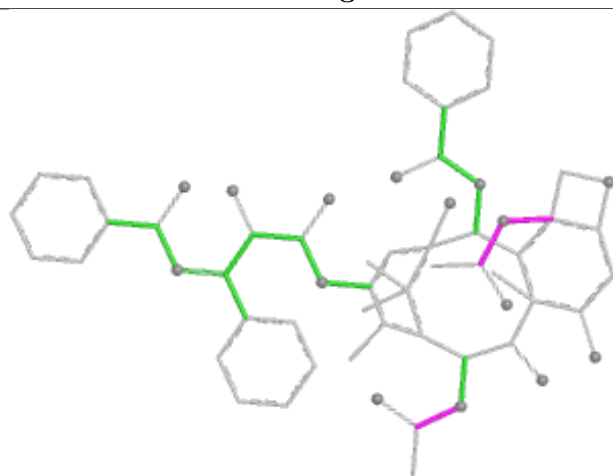
Ligand TA1 MB 502



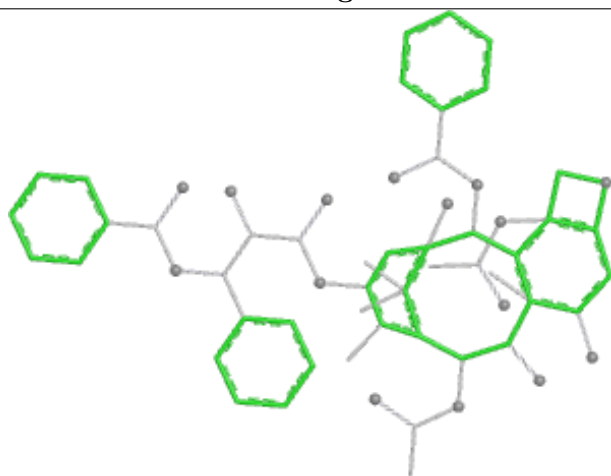
Bond lengths



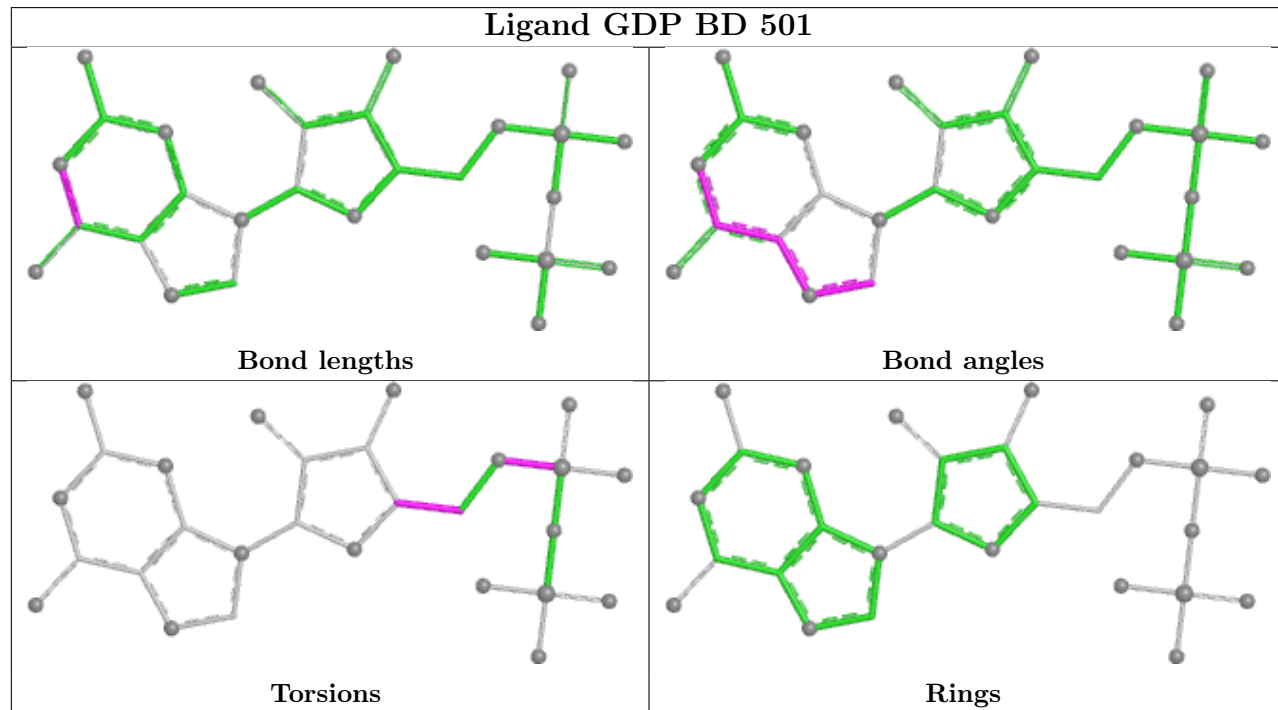
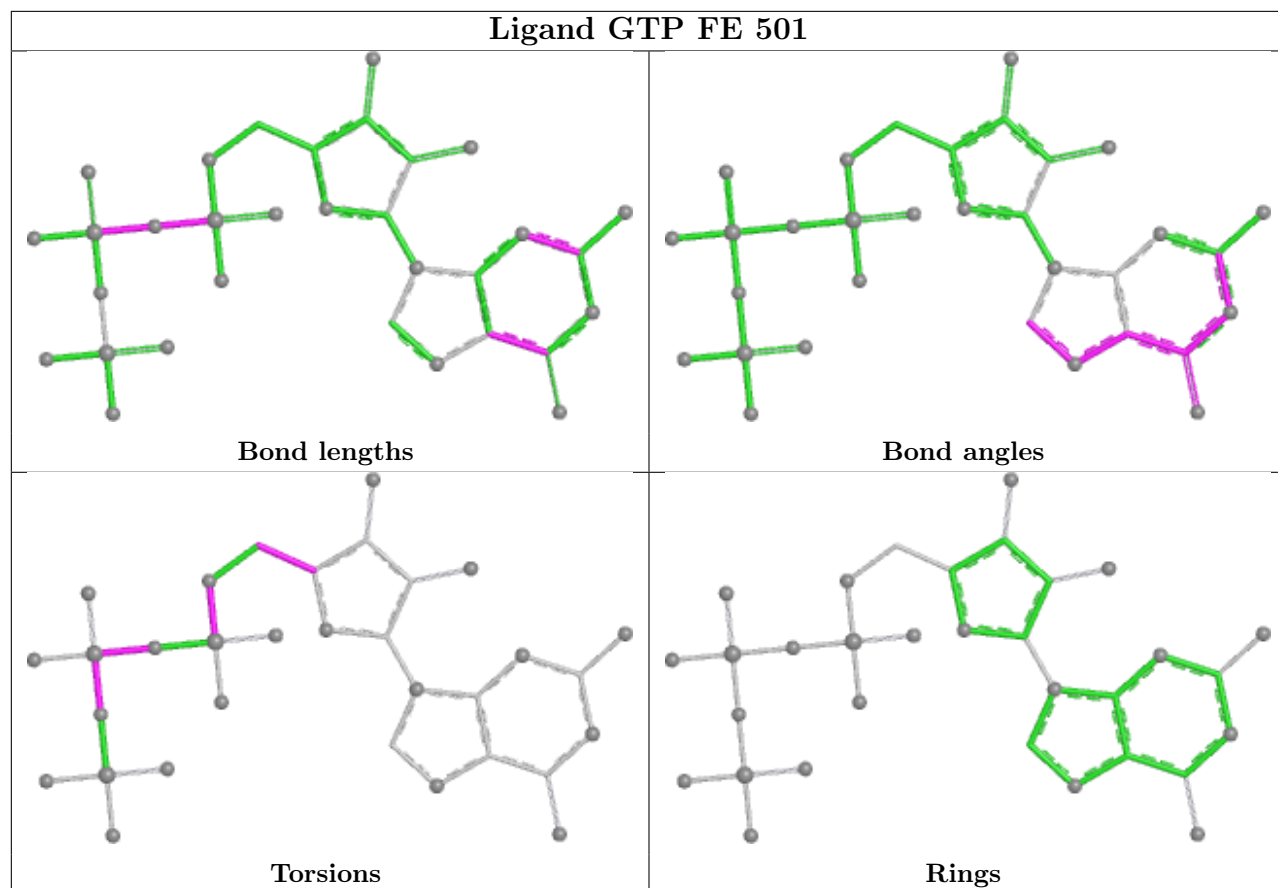
Bond angles

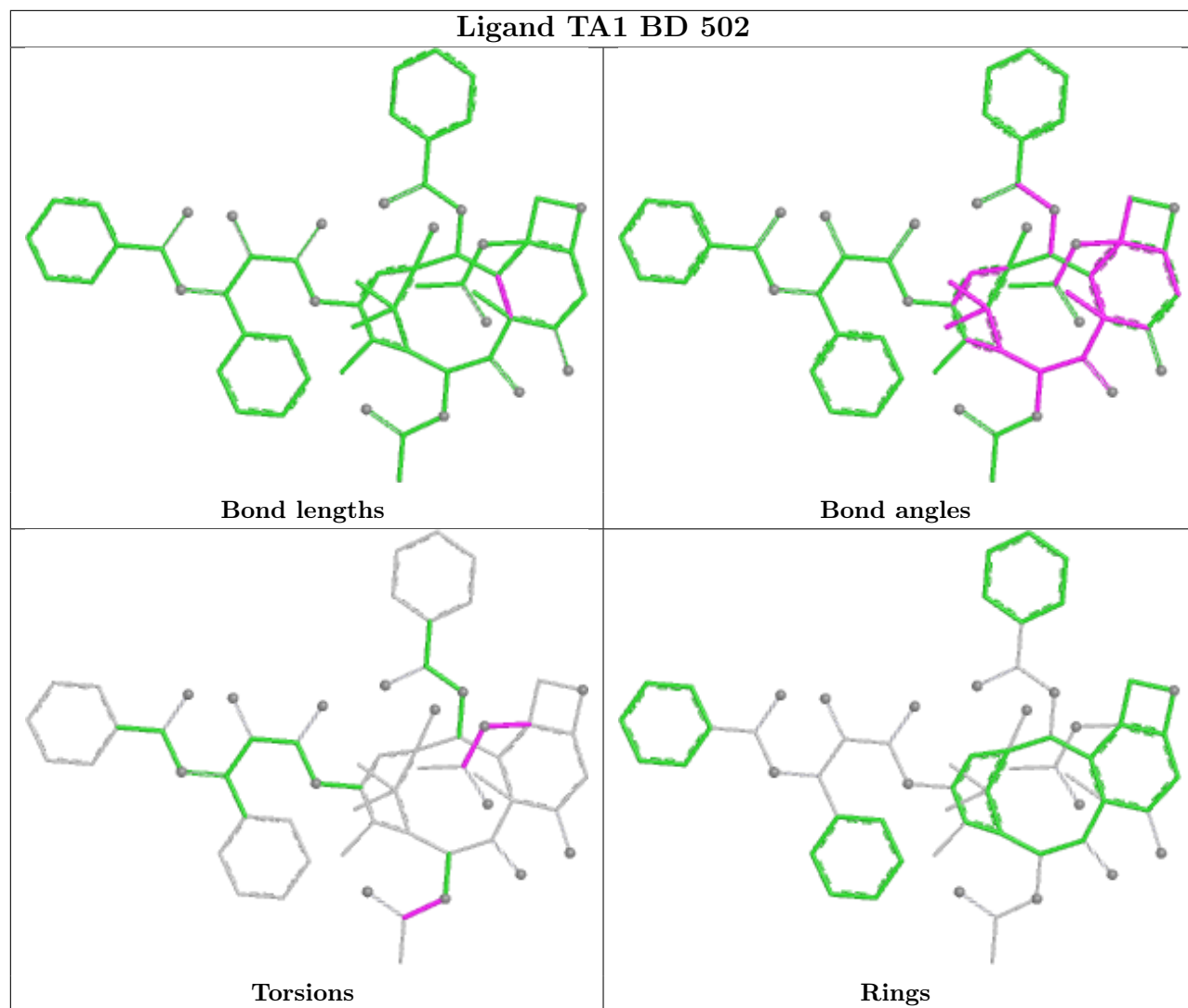


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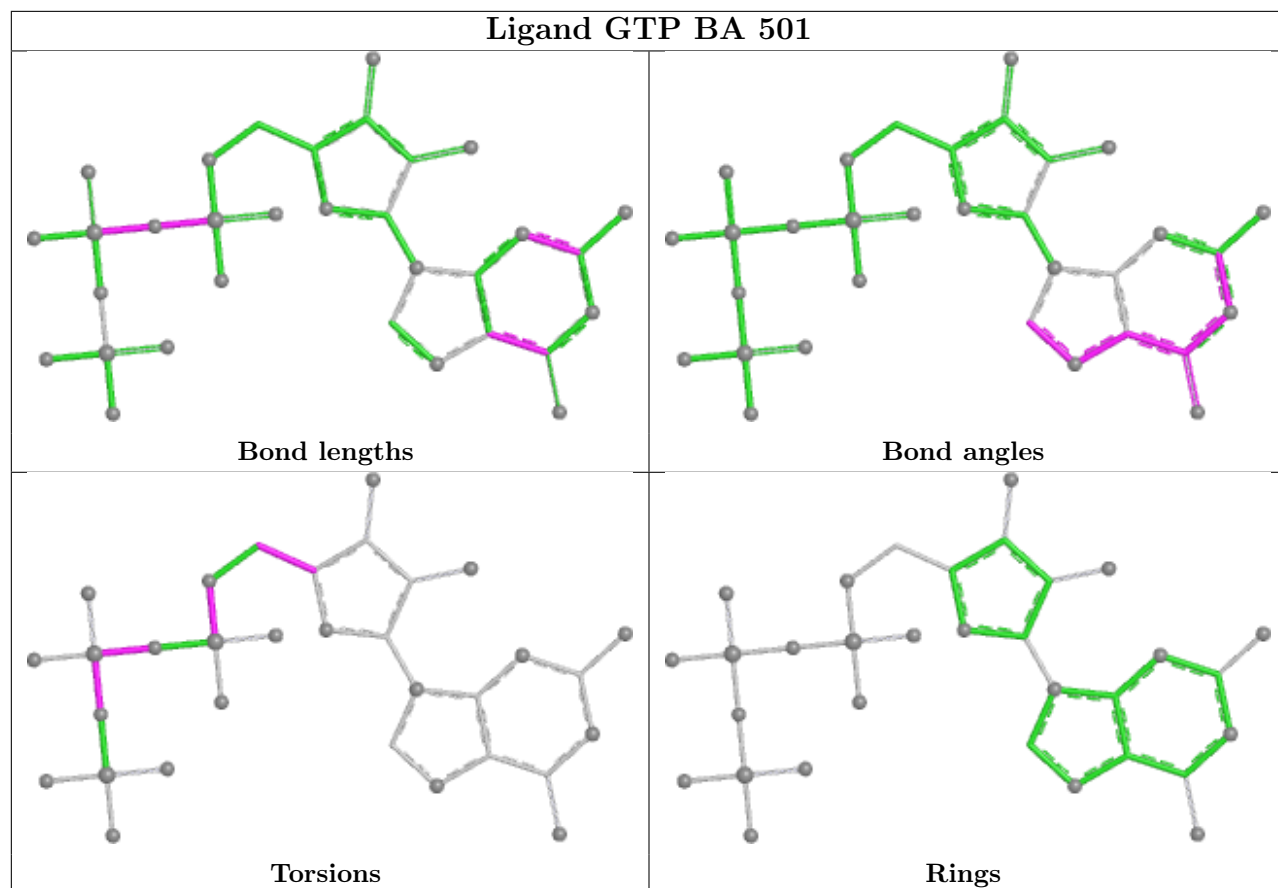


Rings

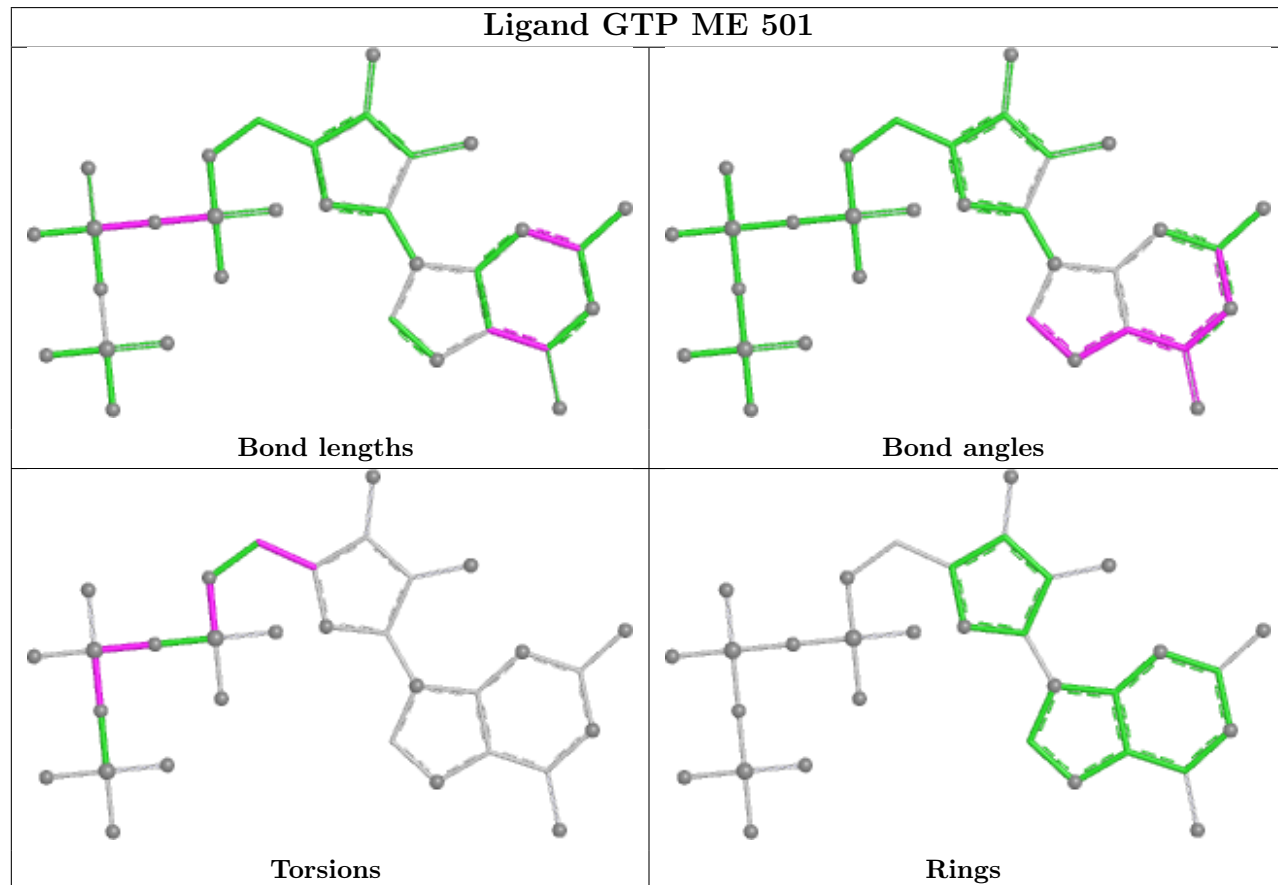


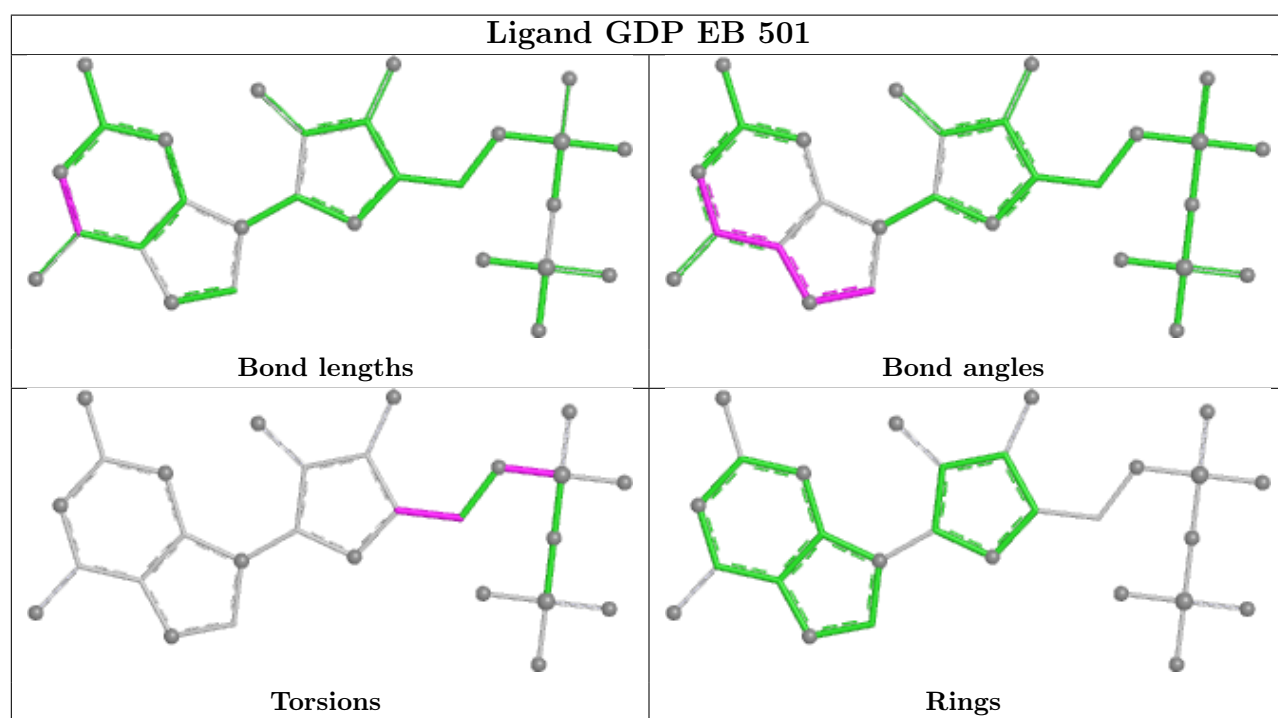
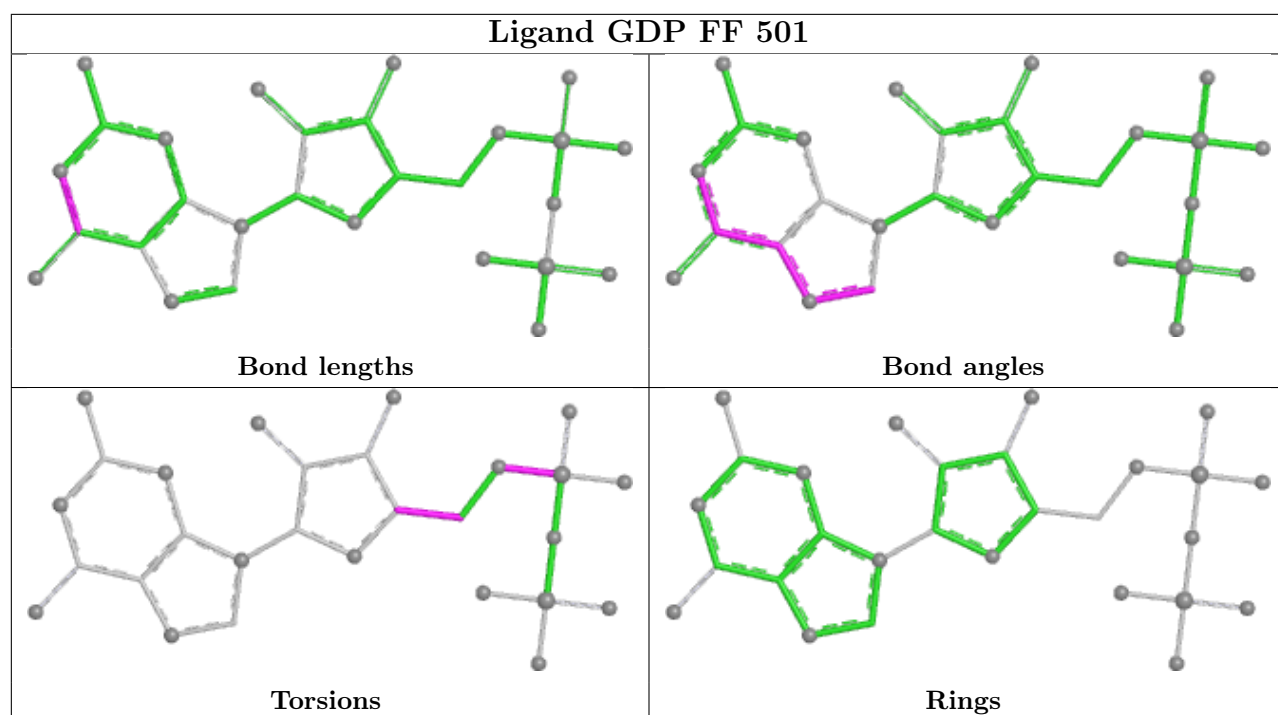


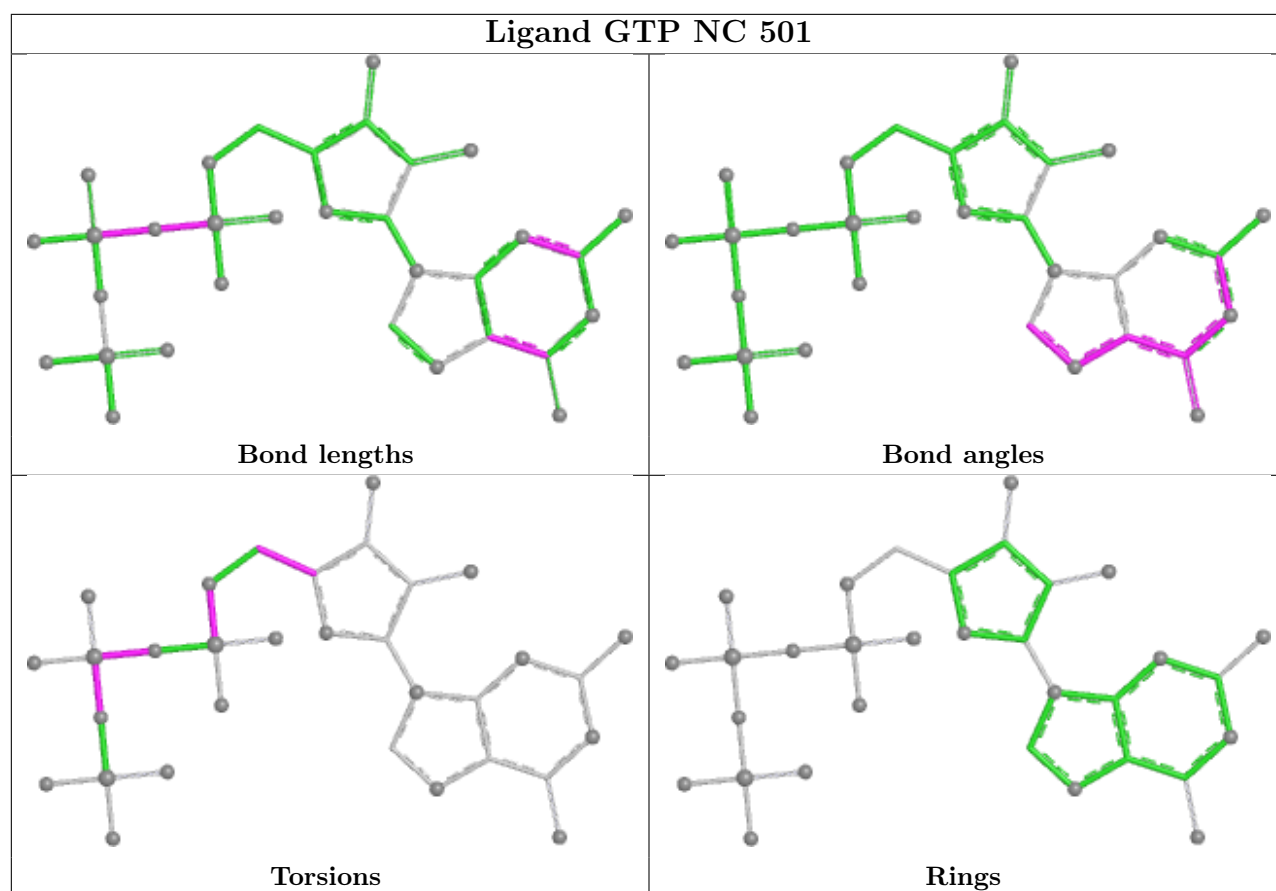
Ligand GTP BA 501



Ligand GTP ME 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.

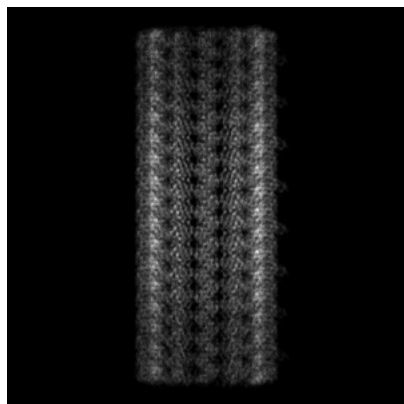
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49760. These allow visual inspection of the internal detail of the map and identification of artifacts.

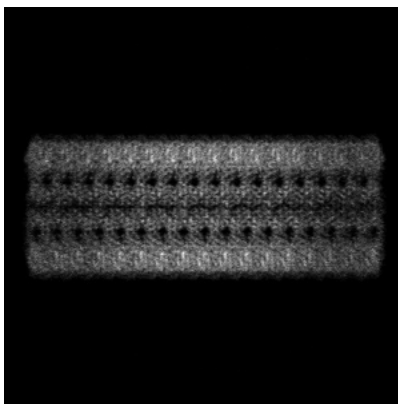
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

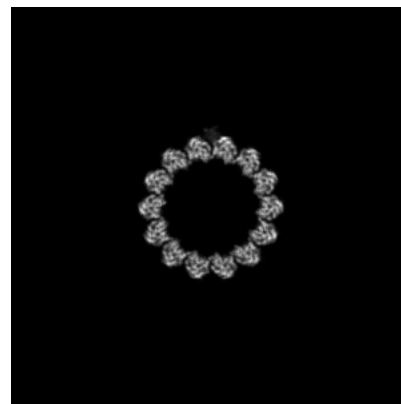
6.1.1 Primary map



X

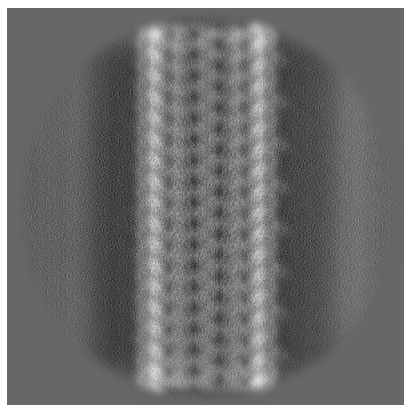


Y

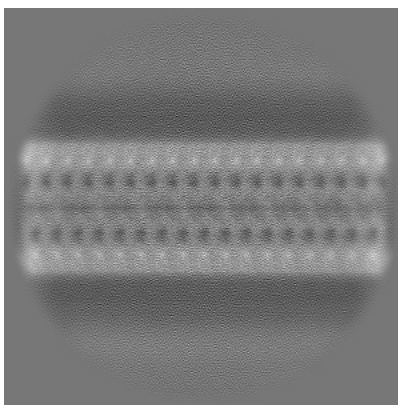


Z

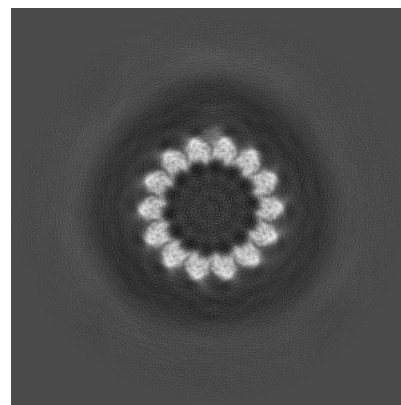
6.1.2 Raw map



X



Y

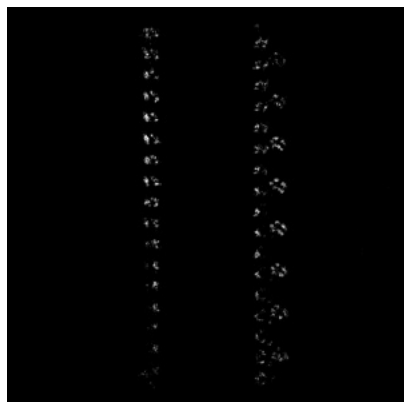


Z

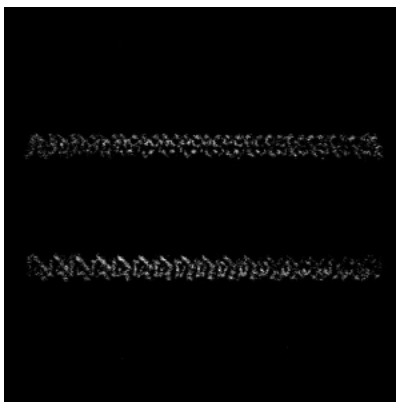
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 189

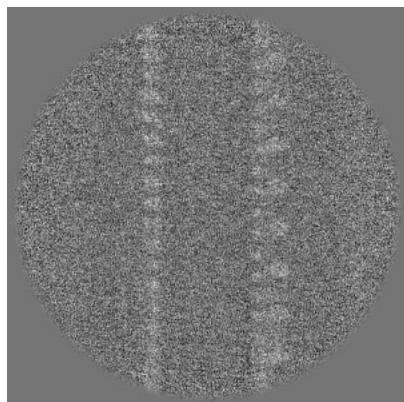


Y Index: 189

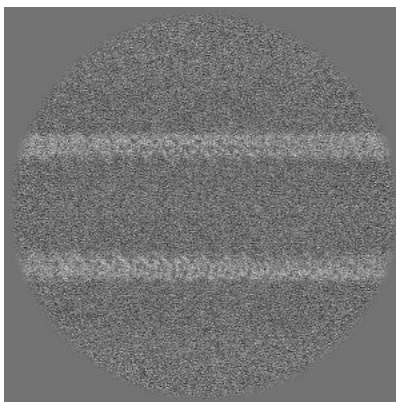


Z Index: 189

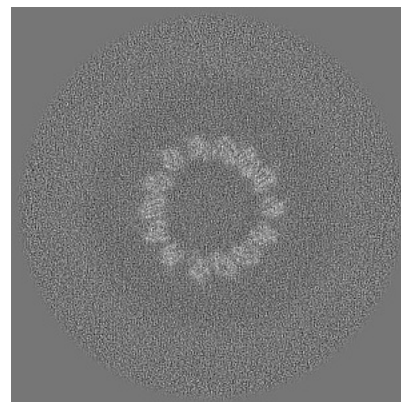
6.2.2 Raw map



X Index: 189



Y Index: 189

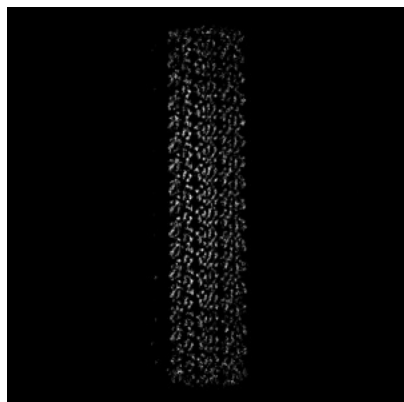


Z Index: 189

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

6.3 Largest variance slices [i](#)

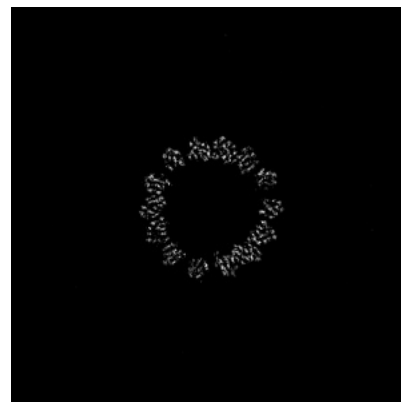
6.3.1 Primary map



X Index: 239

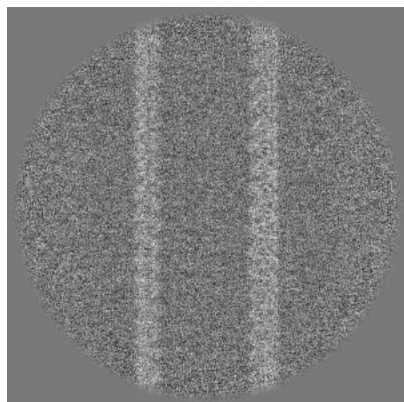


Y Index: 239

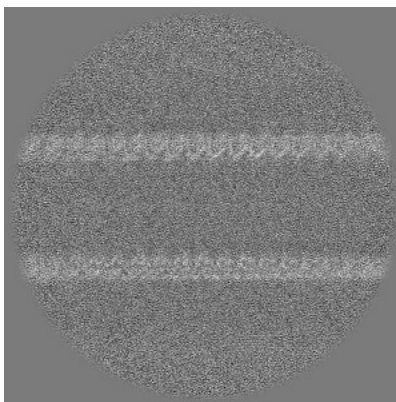


Z Index: 147

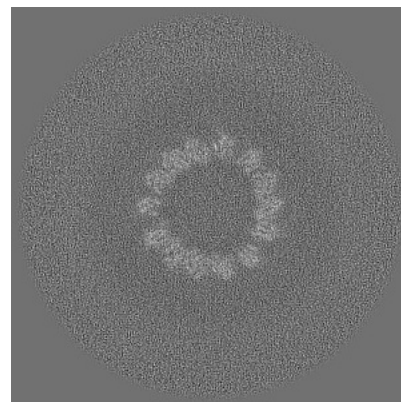
6.3.2 Raw map



X Index: 202



Y Index: 186

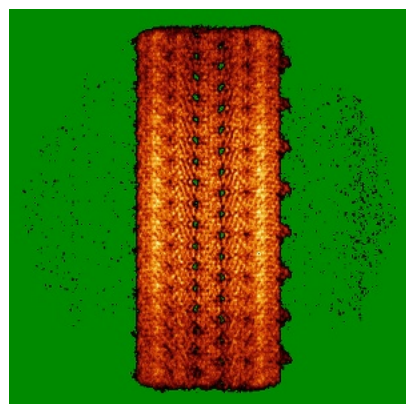


Z Index: 198

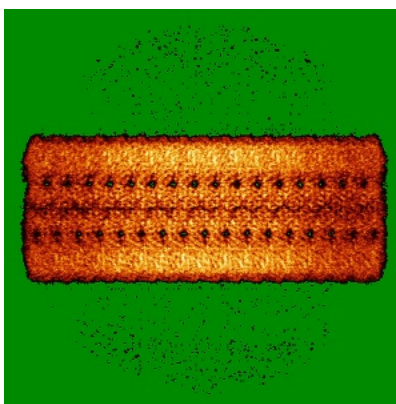
The images above show the largest variance slices of the map in three orthogonal directions.

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

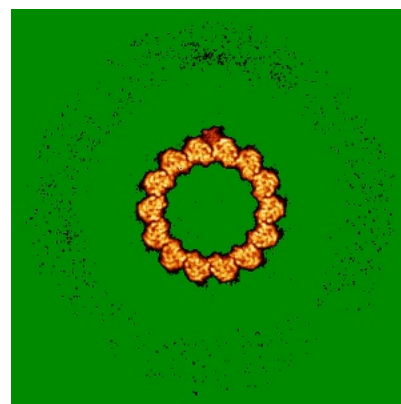
6.4.1 Primary map



X

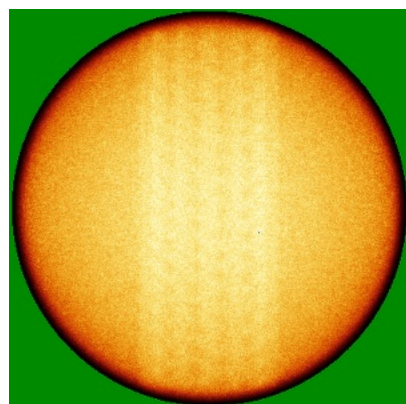


Y

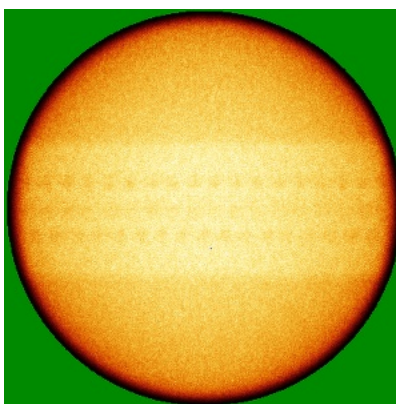


Z

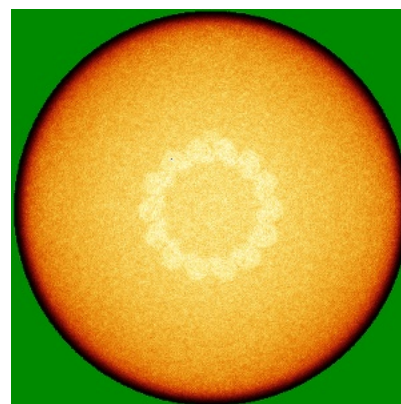
6.4.2 Raw map



X



Y

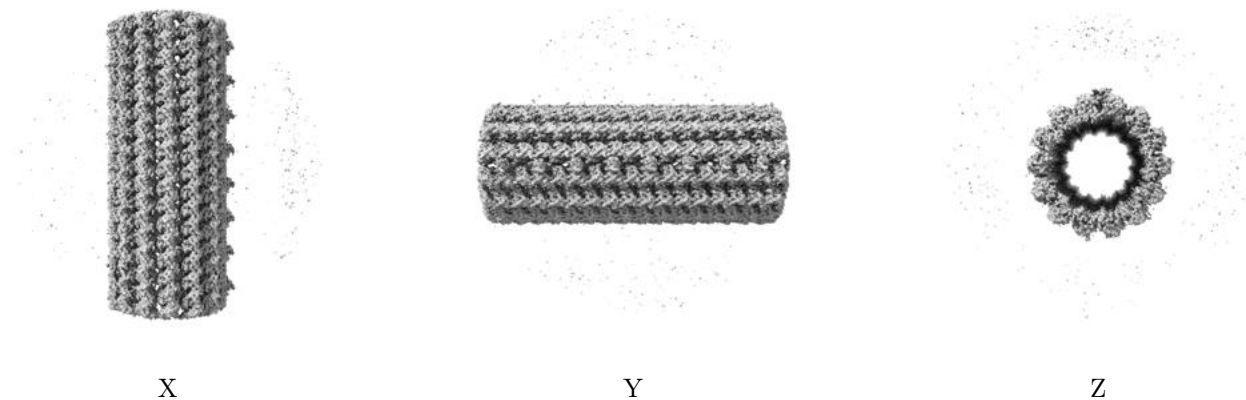


Z

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.

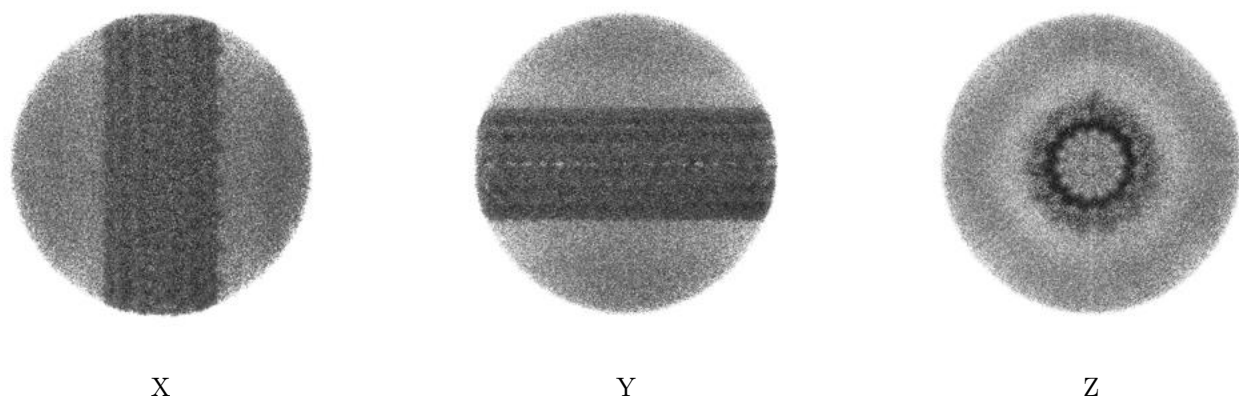
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0398. 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.

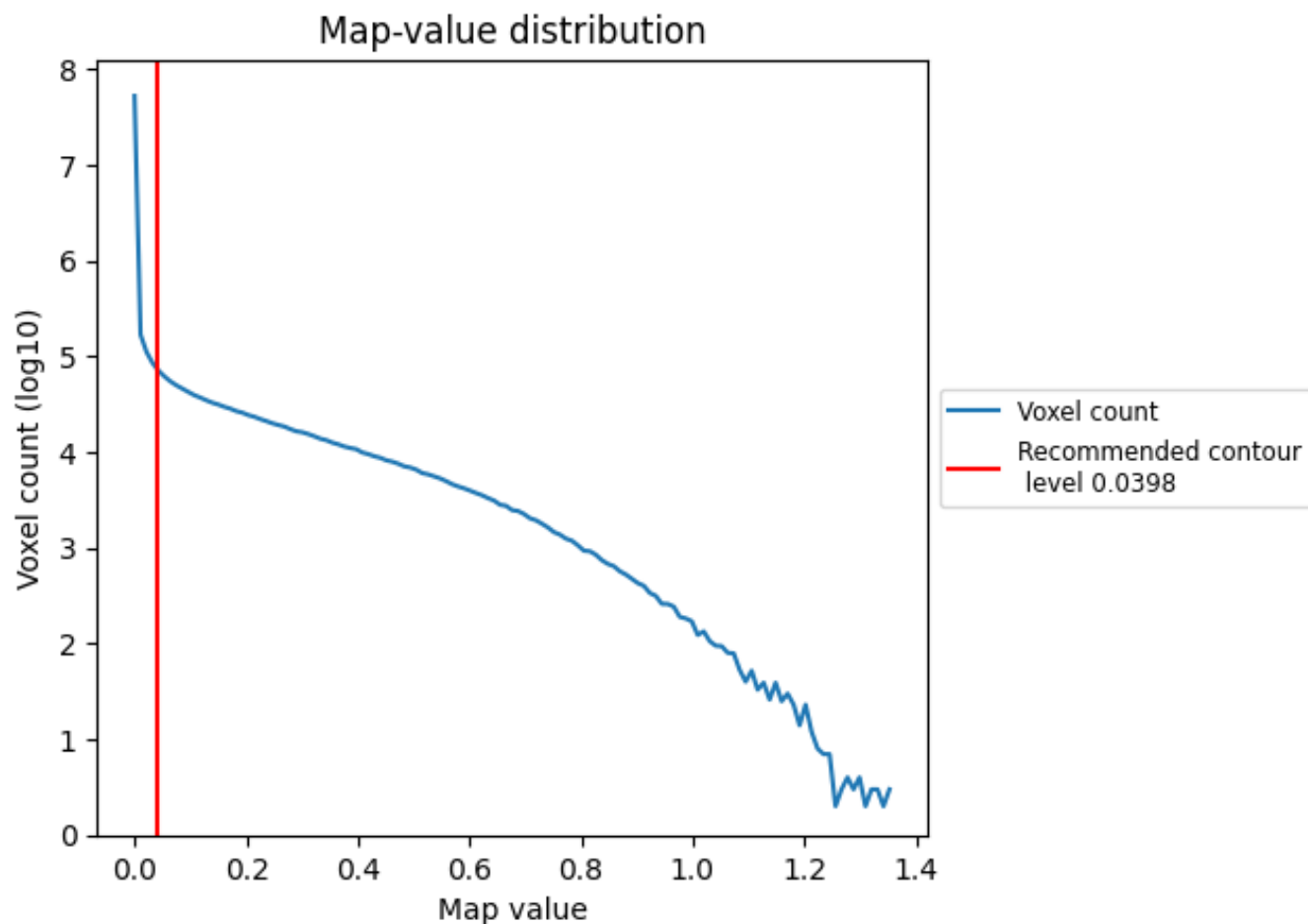
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

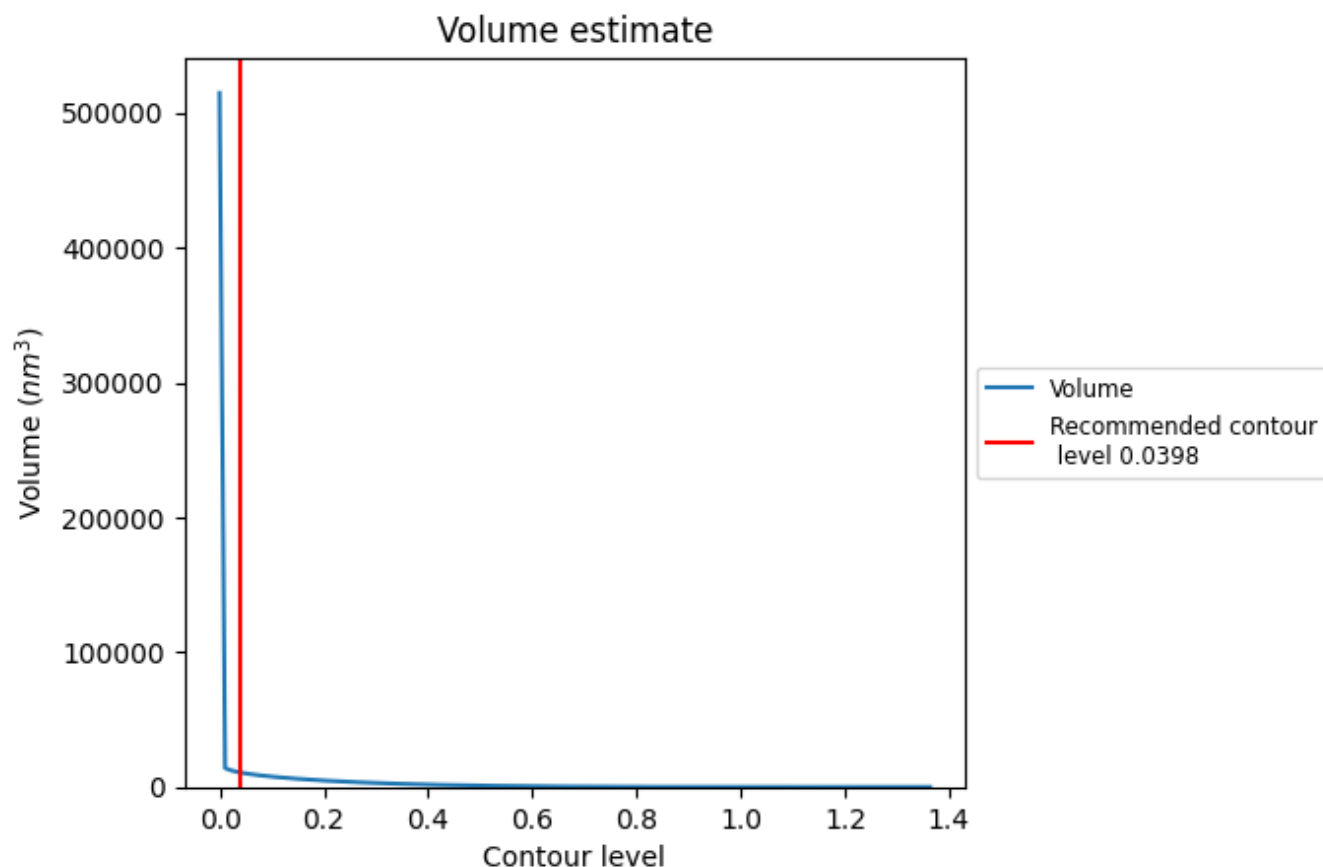
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

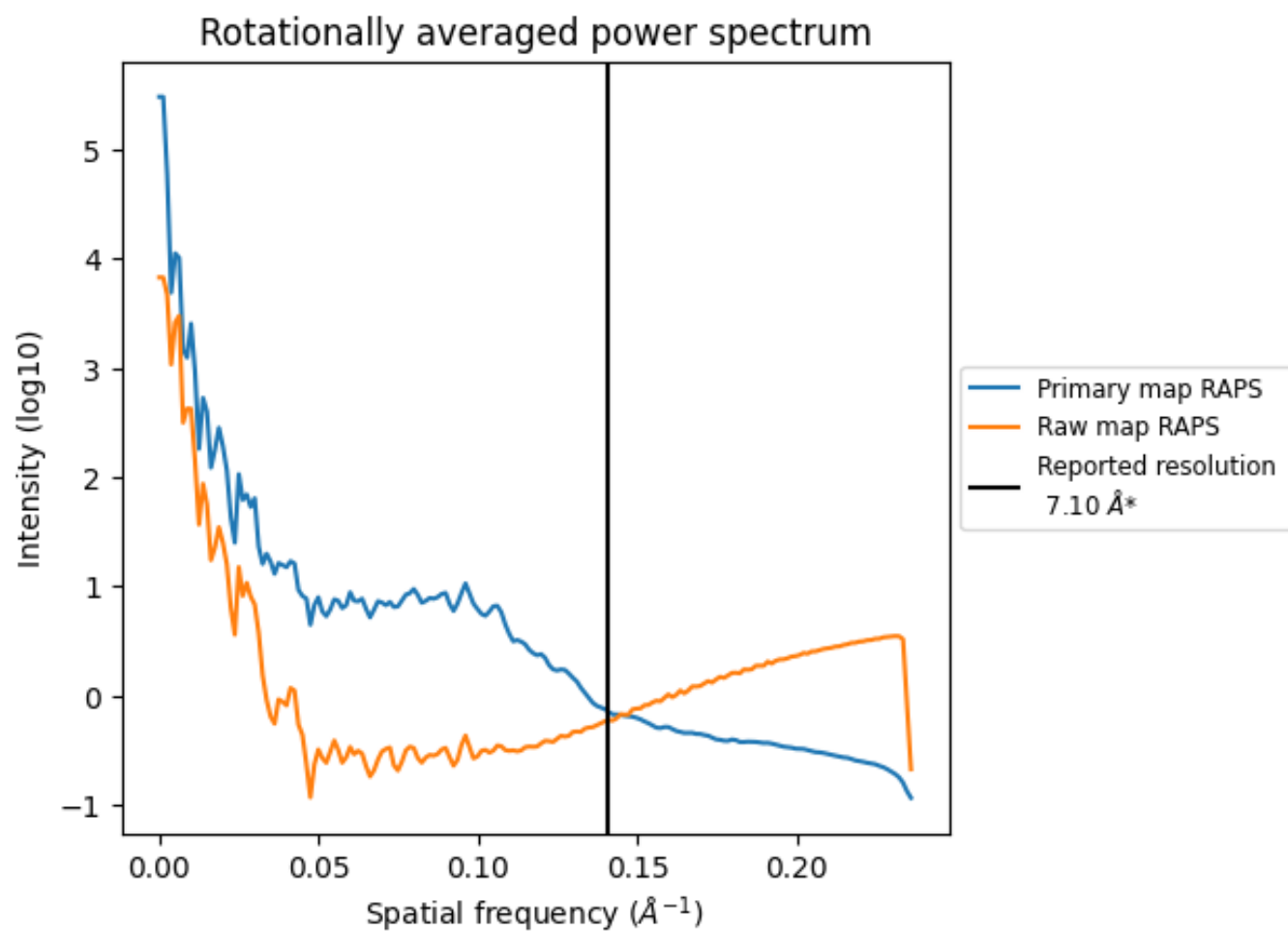
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 10696 nm^3 ; this corresponds to an approximate mass of 9662 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 ⓘ

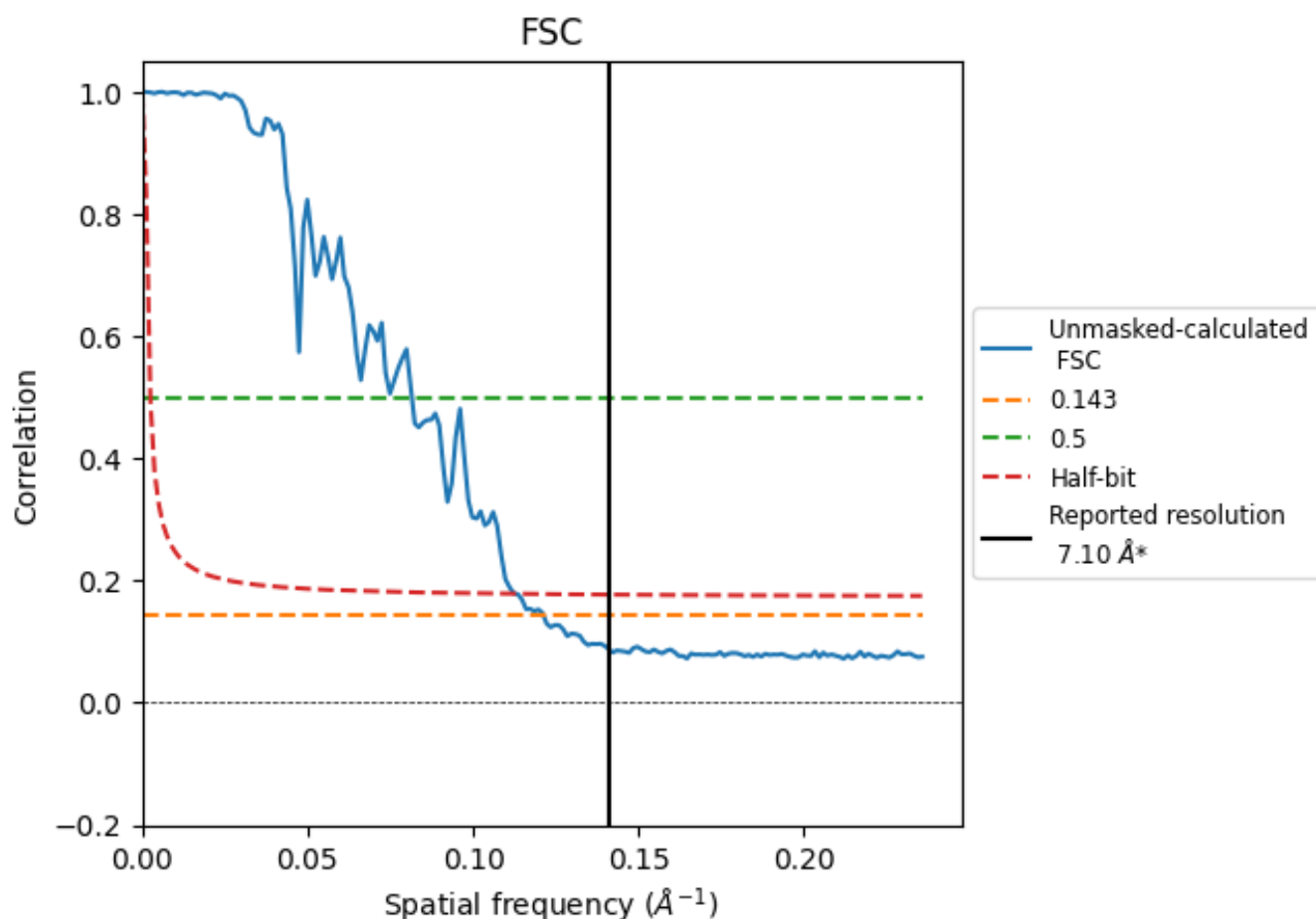


*Reported resolution corresponds to spatial frequency of 0.141 Å⁻¹

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 0.141 Å⁻¹

8.2 Resolution estimates [i](#)

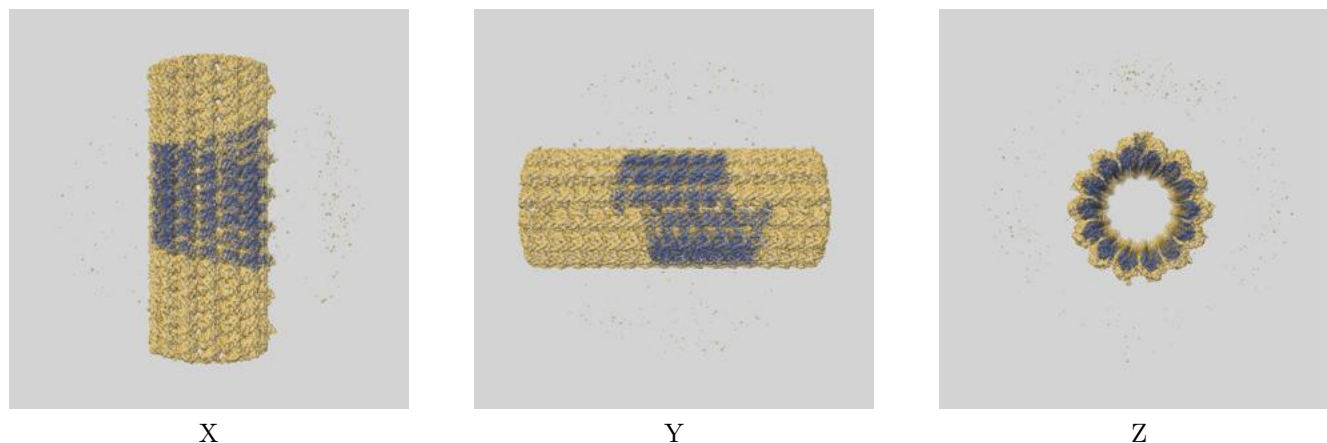
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	7.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	8.24	12.27	8.85

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.24 differs from the reported value 7.1 by more than 10 %

9 Map-model fit [i](#)

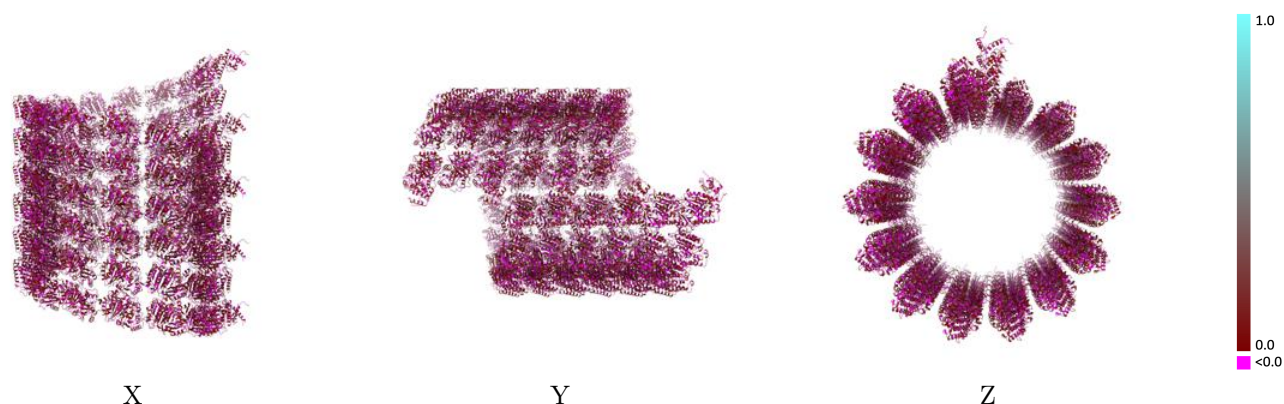
This section contains information regarding the fit between EMDB map EMD-49760 and PDB model 9NTM. Per-residue inclusion information can be found in [section 3](#) on [page 25](#).

9.1 Map-model overlay [i](#)



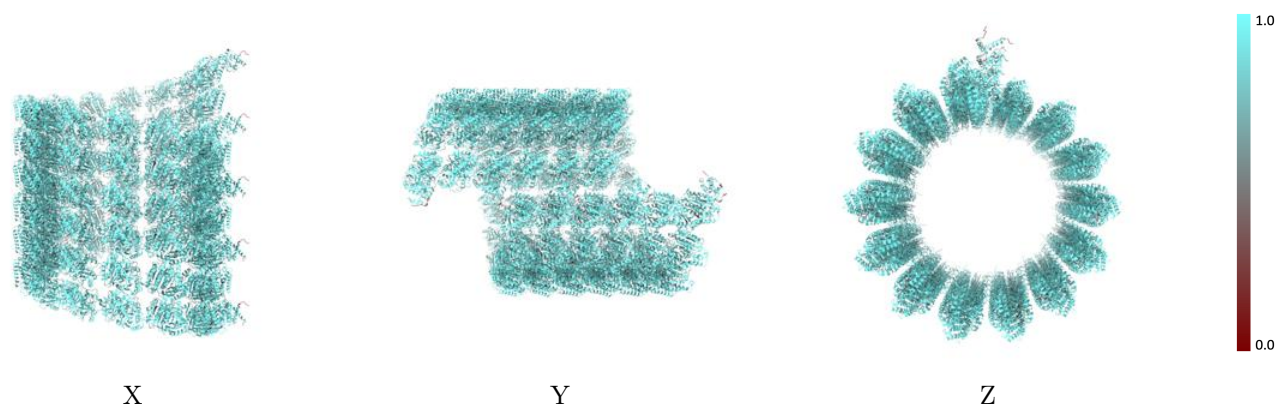
The images above show the 3D surface view of the map at the recommended contour level 0.0398 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



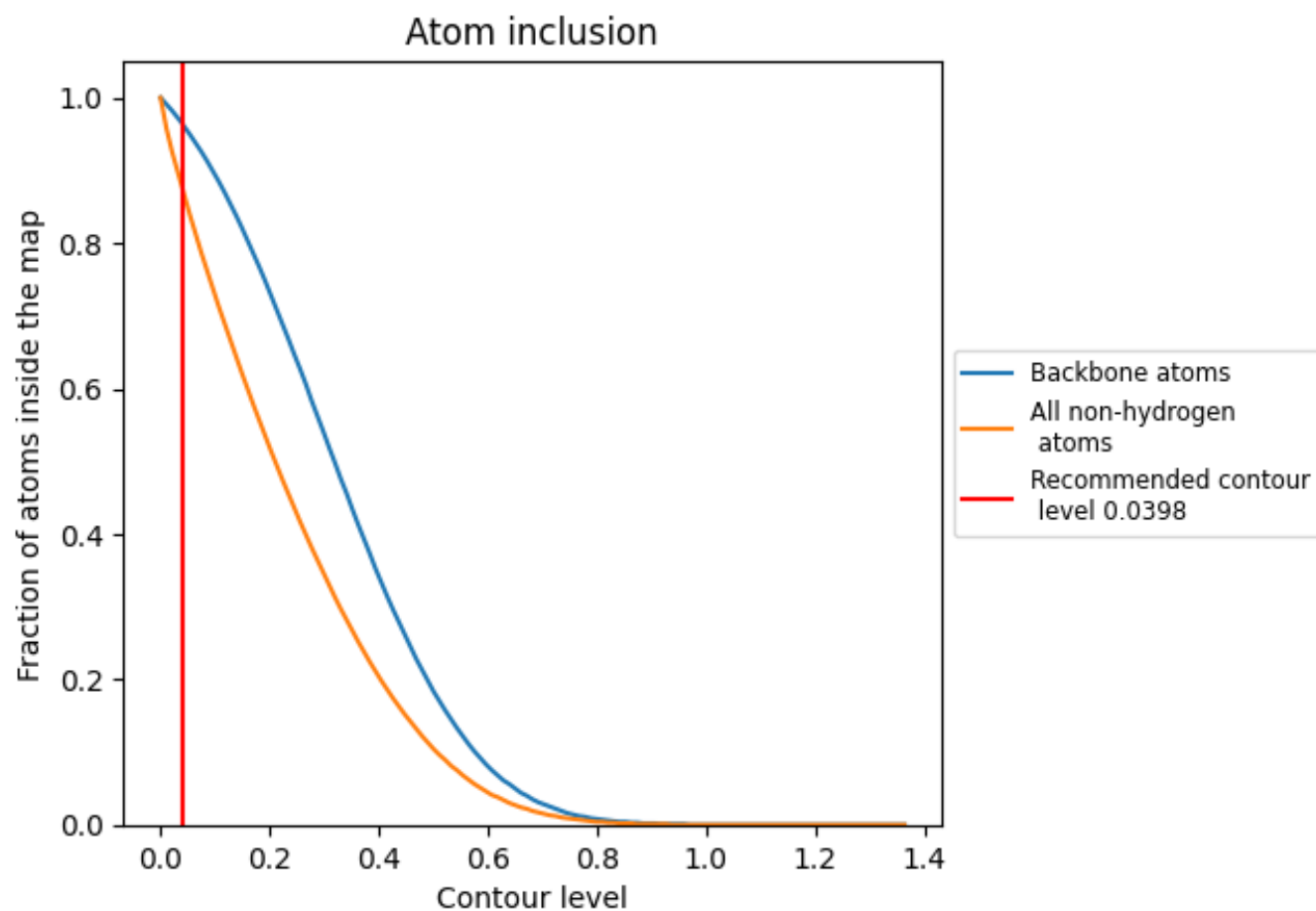
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0398).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 87% 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 (0.0398) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8740	 0.0900
1A	 0.7570	 0.0780
1B	 0.7870	 0.0880
1C	 0.7930	 0.0880
1D	 0.8010	 0.0970
1E	 0.6550	 0.0560
AA	 0.8750	 0.0950
AB	 0.8960	 0.1120
AC	 0.8940	 0.1050
AD	 0.9020	 0.1170
AE	 0.8890	 0.1000
AF	 0.8960	 0.1040
BA	 0.8660	 0.0900
BB	 0.8990	 0.0970
BC	 0.8960	 0.0990
BD	 0.8940	 0.0970
BE	 0.8930	 0.1100
BF	 0.8880	 0.0930
CA	 0.8810	 0.0930
CB	 0.9020	 0.1010
CC	 0.8940	 0.1070
CD	 0.9010	 0.0930
CE	 0.8980	 0.1140
CF	 0.8960	 0.0990
DA	 0.8840	 0.0930
DB	 0.8850	 0.0930
DC	 0.8920	 0.0980
DD	 0.8900	 0.1050
DE	 0.8920	 0.0910
DF	 0.8680	 0.0880
EA	 0.8750	 0.0890
EB	 0.8730	 0.0840
EC	 0.8820	 0.0850
ED	 0.8830	 0.0930
EE	 0.8870	 0.0930





























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Chain	Atom inclusion	Q-score
EF	 0.8690	 0.0780
FA	 0.8740	 0.0760
FB	 0.8740	 0.0750
FC	 0.8690	 0.0800
FD	 0.8850	 0.0830
FE	 0.8640	 0.0740
FF	 0.8500	 0.0690
GA	 0.8610	 0.0810
GB	 0.8850	 0.0930
GC	 0.8700	 0.0850
GD	 0.8790	 0.0920
GE	 0.8520	 0.0730
GF	 0.8440	 0.0820
HA	 0.8680	 0.0970
HB	 0.8850	 0.0930
HC	 0.8770	 0.1030
HD	 0.8770	 0.0890
HE	 0.8770	 0.0980
HF	 0.8440	 0.0810
IA	 0.8680	 0.0830
IB	 0.8750	 0.0920
IC	 0.8730	 0.0830
ID	 0.8730	 0.0870
IE	 0.8530	 0.0780
IF	 0.8430	 0.0700
JA	 0.8840	 0.0910
JB	 0.8960	 0.0920
JC	 0.8750	 0.0890
JD	 0.8670	 0.0830
JE	 0.8670	 0.0850
JF	 0.8500	 0.0650
KA	 0.8850	 0.1050
KB	 0.8890	 0.0960
KC	 0.8820	 0.0960
KD	 0.8680	 0.0840
KE	 0.8640	 0.0910
KF	 0.8440	 0.0820
LA	 0.8840	 0.0980
LB	 0.8860	 0.1020
LC	 0.8740	 0.0900
LD	 0.8790	 0.0940
LE	 0.8530	 0.0810

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Chain	Atom inclusion	Q-score
LF	 0.8460	 0.0760
MA	 0.8680	 0.0870
MB	 0.8810	 0.0800
MC	 0.8750	 0.0910
MD	 0.8640	 0.0860
ME	 0.8500	 0.0800
MF	 0.8200	 0.0560
NA	 0.8810	 0.1050
NB	 0.8970	 0.1050
NC	 0.8760	 0.1010
ND	 0.8780	 0.0920
NE	 0.8670	 0.0840
NF	 0.8360	 0.0750