



wwPDB EM Validation Summary Report ⓘ

Nov 22, 2022 – 11:04 PM JST

PDB ID : 7EXT
EMDB ID : EMD-31373
Title : Cryo-EM structure of cyanobacterial phycobilisome from *Synechococcus* sp. PCC 7002
Authors : Zheng, L.; Zheng, Z.; Li, X.; Wang, G.; Zhang, K.; Wei, P.; Zhao, J.; Gao, N.
Deposited on : 2021-05-28
Resolution : 3.50 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:

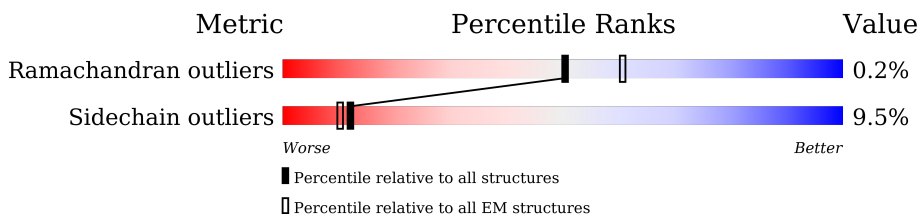
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

1 Overall quality at a glance

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

The reported resolution of this entry is 3.50 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)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	A1	248	
1	A2	248	
1	A4	248	
1	A5	248	
1	A6	248	
1	A8	248	
2	B1	162	
2	B2	162	
2	B4	162	

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Mol	Chain	Length	Quality of chain
2	B5	162	98% 94% 6%
2	B6	162	64% 90% 10%
2	B8	162	93% 90% 10%
2	D1	162	100% 94% 6%
2	D2	162	93% 90% 10%
2	D4	162	100% 89% 10%
2	D5	162	100% 94% 6%
2	D6	162	94% 90% 10%
2	D8	162	100% 90% 10%
2	F1	162	99% 94% 6%
2	F2	162	85% 90% 10%
2	F4	162	97% 89% 10%
2	F5	162	99% 94% 6%
2	F6	162	83% 90% 10%
2	F8	162	97% 89% 10%
2	H1	162	99% 94% 6%
2	H2	162	90% 90% 10%
2	H4	162	99% 88% 11%
2	H5	162	100% 94% 6%
2	H6	162	91% 90% 10%
2	H8	162	100% 88% 11%
2	J1	162	98% 94% 6%
2	J2	162	74% 90% 10%
2	J4	162	94% 89% 10%
2	J5	162	99% 94% 6%

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Mol	Chain	Length	Quality of chain
2	J6	162	74% 90% 10%
2	J8	162	92% 89% 10%
2	L1	162	99% 94% 6%
2	L2	162	95% 90% 10%
2	L4	162	98% 91% 9%
2	L5	162	99% 94% 6%
2	L6	162	96% 90% 10%
2	L8	162	96% 90% 9%
2	O1	162	99% 94% 6%
2	O2	162	100% 90% 10%
2	O4	162	100% 89% 10%
2	O5	162	99% 94% 6%
2	O6	162	100% 90% 10%
2	O8	162	100% 89% 10%
2	Q1	162	100% 94% 6%
2	Q2	162	100% 90% 10%
2	Q4	162	100% 90% 10%
2	Q5	162	100% 94% 6%
2	Q6	162	99% 90% 10%
2	Q8	162	100% 90% 10%
2	S1	162	100% 94% 6%
2	S2	162	100% 90% 10%
2	S4	162	100% 91% 9%
2	S5	162	100% 94% 6%
2	S6	162	100% 90% 10%

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Mol	Chain	Length	Quality of chain
2	S8	162	100% 91% 9%
2	U1	162	100% 94% 6%
2	U2	162	100% 90% 10%
2	U4	162	100% 90% 9%
2	U5	162	100% 94% 6%
2	U6	162	100% 90% 10%
2	U8	162	100% 90% 9%
2	W1	162	100% 94% 6%
2	W2	162	100% 90% 10%
2	W4	162	100% 90% 9%
2	W5	162	100% 94% 6%
2	W6	162	100% 90% 10%
2	W8	162	100% 90% 9%
2	Y1	162	100% 94% 6%
2	Y2	162	100% 90% 10%
2	Y4	162	100% 90% 9%
2	Y5	162	100% 94% 6%
2	Y6	162	100% 90% 10%
2	Y8	162	100% 90% 9%
3	C1	172	100% 91% 9%
3	C2	172	81% 85% 13%
3	C4	172	99% 92% 8%
3	C5	172	100% 91% 9%
3	C6	172	83% 85% 14%
3	C8	172	98% 92% 7%

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Mol	Chain	Length	Quality of chain
3	E1	172	100% 91% 9%
3	E2	172	93% 87% 12%
3	E4	172	100% 92% 8%
3	E5	172	100% 91% 9%
3	E6	172	94% 87% 12%
3	E8	172	100% 92% 8%
3	G1	172	98% 92% 8%
3	G2	172	56% 87% 12%
3	G4	172	95% 92% 8%
3	G5	172	98% 92% 8%
3	G6	172	58% 88% 11%
3	G8	172	95% 92% 8%
3	I1	172	99% 91% 9%
3	I2	172	78% 88% 11%
3	I4	172	96% 92% 7%
3	I5	172	99% 91% 9%
3	I6	172	81% 88% 11%
3	I8	172	99% 92% 7%
3	K1	172	100% 91% 9%
3	K2	172	88% 89% 11%
3	K4	172	97% 92% 7%
3	K5	172	100% 91% 9%
3	K6	172	89% 89% 11%
3	K8	172	97% 92% 7%
3	M1	172	100% 91% 9%

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Mol	Chain	Length	Quality of chain
3	M2	172	91% 89% 10% .
3	M4	172	99% 92% 8%
3	M5	172	100% 91% 9%
3	M6	172	91% 89% 10% .
3	M8	172	99% 92% 8%
3	P1	172	100% 91% 9%
3	P2	172	100% 87% 12% ..
3	P4	172	100% 94% 6% .
3	P5	172	100% 91% 9%
3	P6	172	100% 87% 12% ..
3	P8	172	100% 94% 6% .
3	R1	172	100% 91% 9%
3	R2	172	97% 88% 12% .
3	R4	172	100% 94% 6% .
3	R5	172	100% 91% 9%
3	R6	172	98% 88% 12% .
3	R8	172	100% 94% 6% .
3	T1	172	100% 91% 9%
3	T2	172	100% 87% 12% .
3	T4	172	100% 94% 6% .
3	T5	172	100% 91% 9%
3	T6	172	100% 87% 12% .
3	T8	172	100% 94% 6% .
3	V1	172	100% 91% 9%
3	V2	172	99% 87% 12% .

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Mol	Chain	Length	Quality of chain
3	V4	172	100% 92% 7%
3	V5	172	100% 91% 9%
3	V6	172	100% 87% 12%
3	V8	172	100% 92% 7%
3	X1	172	100% 91% 9%
3	X2	172	100% 88% 12%
3	X4	172	100% 94% 6%
3	X5	172	100% 91% 9%
3	X6	172	100% 88% 11%
3	X8	172	100% 94% 6%
3	Z1	172	100% 91% 9%
3	Z2	172	100% 87% 12%
3	Z4	172	100% 92% 7%
3	Z5	172	100% 91% 9%
3	Z6	172	99% 87% 12%
3	Z8	172	100% 92% 7%
4	N1	290	99% 97%
4	N2	290	91% 94% 5%
4	N4	290	97% 97%
4	N5	290	99% 97%
4	N6	290	89% 94% 5%
4	N8	290	96% 97%
4	a1	290	22% 78%
4	a2	290	22% 78%
4	a4	290	21% 79%

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Mol	Chain	Length	Quality of chain
4	a5	290	22% 78%
4	a6	290	22% 21% 78%
4	a8	290	21% 20% 79%
5	03	886	85% 8% 7%
5	13	886	84% 9% 7%
6	23	67	13% 94%
6	33	67	15% 94%
6	G7	67	91% 93%
6	N7	67	91% 96%
6	U7	67	94%
6	b7	67	6% 93%
7	A7	161	96% 89% 10%
7	C7	161	91% 89% 10%
7	E7	161	93% 89% 10%
7	G3	161	90% 9%
7	H7	161	97% 89% 11%
7	I3	161	90% 9%
7	J7	161	92% 89% 10%
7	K3	161	89% 10%
7	L7	161	89% 10%
7	N3	161	90% 9%
7	O7	161	7% 89% 10%
7	P3	161	90% 9%
7	Q7	161	89% 10%
7	R3	161	27% 90% 9%

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Mol	Chain	Length	Quality of chain
7	S7	161	
7	T3	161	
7	V7	161	
7	X3	161	
7	X7	161	
7	Z3	161	
7	Z7	161	
7	b3	161	
7	d3	161	
7	f3	161	
7	i3	161	
7	k3	161	
7	o3	161	
7	q3	161	
7	s3	161	
7	u3	161	
7	w3	161	
7	y3	161	
8	B7	161	
8	D7	161	
8	F7	161	
8	H3	161	
8	I7	161	
8	J3	161	
8	K7	161	

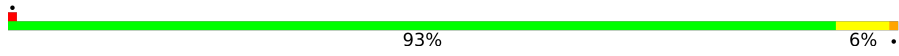
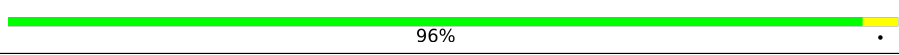
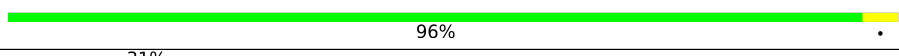
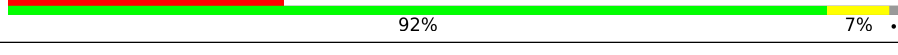
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Mol	Chain	Length	Quality of chain
8	L3	161	93% 6%
8	M3	161	93% 6%
8	M7	161	88% 12% 99%
8	O3	161	93% 6%
8	P7	161	88% 12% 7%
8	R7	161	88% 12%
8	S3	161	93% 6% 41%
8	T7	161	88% 12% 6%
8	U3	161	93% 6% 50%
8	W3	161	93% 6% 36%
8	W7	161	88% 12% 7%
8	Y3	161	94% 6%
8	Y7	161	88% 12%
8	a3	161	93% 6%
8	a7	161	88% 12% 6%
8	c3	161	93% 6%
8	e3	161	93% 6%
8	h3	161	93% 6%
8	j3	161	93% 6% 48%
8	l3	161	93% 6% 50%
8	n3	161	93% 6% 34%
8	p3	161	93% 6%
8	r3	161	93% 6%
8	t3	161	93% 6%
8	v3	161	93% 6%

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Mol	Chain	Length	Quality of chain
8	x3	161	 93% 6% .
8	z3	161	 93% 6% .
9	Q3	169	 96% .
9	g3	169	 96% .
10	V3	161	 31% 92% 7% .
10	m3	161	 31% 92% 7% .

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 322286 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 Phycobilisome rod-core linker polypeptide CpcG.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A1	225	Total 1841	C 1168	N 325	O 343	S 5	0	0
1	A2	228	Total 1865	C 1185	N 329	O 346	S 5	0	0
1	A4	225	Total 1841	C 1168	N 325	O 343	S 5	0	0
1	A5	225	Total 1841	C 1168	N 325	O 343	S 5	0	0
1	A6	228	Total 1865	C 1185	N 329	O 346	S 5	0	0
1	A8	225	Total 1841	C 1168	N 325	O 343	S 5	0	0

- Molecule 2 is a protein called C-phycoerythrin subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B1	162	Total 1240	C 781	N 210	O 244	S 5	0	0
2	D1	162	Total 1240	C 781	N 210	O 244	S 5	0	0
2	F1	162	Total 1240	C 781	N 210	O 244	S 5	0	0
2	H1	162	Total 1240	C 781	N 210	O 244	S 5	0	0
2	J1	162	Total 1240	C 781	N 210	O 244	S 5	0	0
2	L1	162	Total 1240	C 781	N 210	O 244	S 5	0	0
2	O1	161	Total 1232	C 776	N 209	O 243	S 4	0	0
2	Q1	162	Total 1240	C 781	N 210	O 244	S 5	0	0
2	S1	162	Total 1240	C 781	N 210	O 244	S 5	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	U1	162	Total	C	N	O	S	0	0
			1240	781	210	244	5		
2	W1	162	Total	C	N	O	S	0	0
			1240	781	210	244	5		
2	Y1	162	Total	C	N	O	S	0	0
			1240	781	210	244	5		
2	B2	162	Total	C	N	O	S	0	0
			1240	781	210	244	5		
2	D2	162	Total	C	N	O	S	0	0
			1240	781	210	244	5		
2	F2	162	Total	C	N	O	S	0	0
			1240	781	210	244	5		
2	H2	162	Total	C	N	O	S	0	0
			1240	781	210	244	5		
2	J2	162	Total	C	N	O	S	0	0
			1240	781	210	244	5		
2	L2	162	Total	C	N	O	S	0	0
			1240	781	210	244	5		
2	O2	162	Total	C	N	O	S	0	0
			1240	781	210	244	5		
2	Q2	162	Total	C	N	O	S	0	0
			1240	781	210	244	5		
2	S2	162	Total	C	N	O	S	0	0
			1240	781	210	244	5		
2	U2	162	Total	C	N	O	S	0	0
			1240	781	210	244	5		
2	W2	162	Total	C	N	O	S	0	0
			1240	781	210	244	5		
2	Y2	162	Total	C	N	O	S	0	0
			1240	781	210	244	5		
2	B4	162	Total	C	N	O	S	0	0
			1240	781	210	244	5		
2	D4	162	Total	C	N	O	S	0	0
			1240	781	210	244	5		
2	F4	162	Total	C	N	O	S	0	0
			1240	781	210	244	5		
2	H4	162	Total	C	N	O	S	0	0
			1240	781	210	244	5		
2	J4	162	Total	C	N	O	S	0	0
			1240	781	210	244	5		
2	L4	162	Total	C	N	O	S	0	0
			1240	781	210	244	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	O4	162	Total	C	N	O	S	0	0
			1240	781	210	244	5		
2	Q4	162	Total	C	N	O	S	0	0
			1240	781	210	244	5		
2	S4	162	Total	C	N	O	S	0	0
			1240	781	210	244	5		
2	U4	162	Total	C	N	O	S	0	0
			1240	781	210	244	5		
2	W4	162	Total	C	N	O	S	0	0
			1240	781	210	244	5		
2	Y4	162	Total	C	N	O	S	0	0
			1240	781	210	244	5		
2	B5	162	Total	C	N	O	S	0	0
			1240	781	210	244	5		
2	D5	162	Total	C	N	O	S	0	0
			1240	781	210	244	5		
2	F5	162	Total	C	N	O	S	0	0
			1240	781	210	244	5		
2	H5	162	Total	C	N	O	S	0	0
			1240	781	210	244	5		
2	J5	162	Total	C	N	O	S	0	0
			1240	781	210	244	5		
2	L5	162	Total	C	N	O	S	0	0
			1240	781	210	244	5		
2	O5	161	Total	C	N	O	S	0	0
			1232	776	209	243	4		
2	Q5	162	Total	C	N	O	S	0	0
			1240	781	210	244	5		
2	S5	162	Total	C	N	O	S	0	0
			1240	781	210	244	5		
2	U5	162	Total	C	N	O	S	0	0
			1240	781	210	244	5		
2	W5	162	Total	C	N	O	S	0	0
			1240	781	210	244	5		
2	Y5	162	Total	C	N	O	S	0	0
			1240	781	210	244	5		
2	B6	162	Total	C	N	O	S	0	0
			1240	781	210	244	5		
2	D6	162	Total	C	N	O	S	0	0
			1240	781	210	244	5		
2	F6	162	Total	C	N	O	S	0	0
			1240	781	210	244	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	H6	162	Total 1240	C 781	N 210	O 244	S 5	0	0
2	J6	162	Total 1240	C 781	N 210	O 244	S 5	0	0
2	L6	162	Total 1240	C 781	N 210	O 244	S 5	0	0
2	O6	162	Total 1240	C 781	N 210	O 244	S 5	0	0
2	Q6	162	Total 1240	C 781	N 210	O 244	S 5	0	0
2	S6	162	Total 1240	C 781	N 210	O 244	S 5	0	0
2	U6	162	Total 1240	C 781	N 210	O 244	S 5	0	0
2	W6	162	Total 1240	C 781	N 210	O 244	S 5	0	0
2	Y6	162	Total 1240	C 781	N 210	O 244	S 5	0	0
2	B8	162	Total 1240	C 781	N 210	O 244	S 5	0	0
2	D8	162	Total 1240	C 781	N 210	O 244	S 5	0	0
2	F8	162	Total 1240	C 781	N 210	O 244	S 5	0	0
2	H8	162	Total 1240	C 781	N 210	O 244	S 5	0	0
2	J8	162	Total 1240	C 781	N 210	O 244	S 5	0	0
2	L8	162	Total 1240	C 781	N 210	O 244	S 5	0	0
2	O8	162	Total 1240	C 781	N 210	O 244	S 5	0	0
2	Q8	162	Total 1240	C 781	N 210	O 244	S 5	0	0
2	S8	162	Total 1240	C 781	N 210	O 244	S 5	0	0
2	U8	162	Total 1240	C 781	N 210	O 244	S 5	0	0
2	W8	162	Total 1240	C 781	N 210	O 244	S 5	0	0
2	Y8	162	Total 1240	C 781	N 210	O 244	S 5	0	0

- Molecule 3 is a protein called C-phycoyanin subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C1	172	1281	794	227	251	9	0	0
3	E1	172	1281	794	227	251	9	0	0
3	G1	172	1281	794	227	251	9	0	0
3	I1	172	1281	794	227	251	9	0	0
3	K1	172	1281	794	227	251	9	0	0
3	M1	172	1281	794	227	251	9	0	0
3	P1	172	1281	794	227	251	9	0	0
3	R1	172	1281	794	227	251	9	0	0
3	T1	172	1281	794	227	251	9	0	0
3	V1	172	1281	794	227	251	9	0	0
3	X1	172	1281	794	227	251	9	0	0
3	Z1	172	1281	794	227	251	9	0	0
3	C2	172	1281	794	227	251	9	0	0
3	E2	172	1281	794	227	251	9	0	0
3	G2	172	1281	794	227	251	9	0	0
3	I2	172	1281	794	227	251	9	0	0
3	K2	172	1281	794	227	251	9	0	0
3	M2	172	1281	794	227	251	9	0	0
3	P2	172	1281	794	227	251	9	0	0
3	R2	172	1281	794	227	251	9	0	0
3	T2	172	1281	794	227	251	9	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	V2	172	1281	794	227	251	9	0	0
3	X2	172	1281	794	227	251	9	0	0
3	Z2	172	1281	794	227	251	9	0	0
3	C4	172	1281	794	227	251	9	0	0
3	E4	172	1281	794	227	251	9	0	0
3	G4	172	1281	794	227	251	9	0	0
3	I4	172	1281	794	227	251	9	0	0
3	K4	172	1281	794	227	251	9	0	0
3	M4	172	1281	794	227	251	9	0	0
3	P4	172	1281	794	227	251	9	0	0
3	R4	172	1281	794	227	251	9	0	0
3	T4	172	1281	794	227	251	9	0	0
3	V4	172	1281	794	227	251	9	0	0
3	X4	172	1281	794	227	251	9	0	0
3	Z4	172	1281	794	227	251	9	0	0
3	C5	172	1281	794	227	251	9	0	0
3	E5	172	1281	794	227	251	9	0	0
3	G5	172	1281	794	227	251	9	0	0
3	I5	172	1281	794	227	251	9	0	0
3	K5	172	1281	794	227	251	9	0	0
3	M5	172	1281	794	227	251	9	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	P5	172	Total	C	N	O	S	0	0
			1281	794	227	251	9		
3	R5	172	Total	C	N	O	S	0	0
			1281	794	227	251	9		
3	T5	172	Total	C	N	O	S	0	0
			1281	794	227	251	9		
3	V5	172	Total	C	N	O	S	0	0
			1281	794	227	251	9		
3	X5	172	Total	C	N	O	S	0	0
			1281	794	227	251	9		
3	Z5	172	Total	C	N	O	S	0	0
			1281	794	227	251	9		
3	C6	172	Total	C	N	O	S	0	0
			1281	794	227	251	9		
3	E6	172	Total	C	N	O	S	0	0
			1281	794	227	251	9		
3	G6	172	Total	C	N	O	S	0	0
			1281	794	227	251	9		
3	I6	172	Total	C	N	O	S	0	0
			1281	794	227	251	9		
3	K6	172	Total	C	N	O	S	0	0
			1281	794	227	251	9		
3	M6	172	Total	C	N	O	S	0	0
			1281	794	227	251	9		
3	P6	172	Total	C	N	O	S	0	0
			1281	794	227	251	9		
3	R6	172	Total	C	N	O	S	0	0
			1281	794	227	251	9		
3	T6	172	Total	C	N	O	S	0	0
			1281	794	227	251	9		
3	V6	172	Total	C	N	O	S	0	0
			1281	794	227	251	9		
3	X6	172	Total	C	N	O	S	0	0
			1281	794	227	251	9		
3	Z6	172	Total	C	N	O	S	0	0
			1281	794	227	251	9		
3	C8	172	Total	C	N	O	S	0	0
			1281	794	227	251	9		
3	E8	172	Total	C	N	O	S	0	0
			1281	794	227	251	9		
3	G8	172	Total	C	N	O	S	0	0
			1281	794	227	251	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	I8	172	Total	C	N	O	S	0	0
			1281	794	227	251	9		
3	K8	172	Total	C	N	O	S	0	0
			1281	794	227	251	9		
3	M8	172	Total	C	N	O	S	0	0
			1281	794	227	251	9		
3	P8	172	Total	C	N	O	S	0	0
			1281	794	227	251	9		
3	R8	172	Total	C	N	O	S	0	0
			1281	794	227	251	9		
3	T8	172	Total	C	N	O	S	0	0
			1281	794	227	251	9		
3	V8	172	Total	C	N	O	S	0	0
			1281	794	227	251	9		
3	X8	172	Total	C	N	O	S	0	0
			1281	794	227	251	9		
3	Z8	172	Total	C	N	O	S	0	0
			1281	794	227	251	9		

- Molecule 4 is a protein called Phycobilisome 32.3 kDa linker polypeptide, phycocyanin-associated, rod.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	N1	289	Total	C	N	O	S	0	0
			2270	1413	416	438	3		
4	a1	64	Total	C	N	O	S	0	0
			487	301	96	89	1		
4	N2	289	Total	C	N	O	S	0	0
			2270	1413	416	438	3		
4	a2	64	Total	C	N	O	S	0	0
			487	301	96	89	1		
4	N4	289	Total	C	N	O	S	0	0
			2270	1413	416	438	3		
4	a4	61	Total	C	N	O	S	0	0
			469	290	93	85	1		
4	N5	289	Total	C	N	O	S	0	0
			2270	1413	416	438	3		
4	a5	64	Total	C	N	O	S	0	0
			487	301	96	89	1		
4	N6	289	Total	C	N	O	S	0	0
			2270	1413	416	438	3		
4	a6	64	Total	C	N	O	S	0	0
			487	301	96	89	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	N8	289	Total	C	N	O	S	0	0
			2270	1413	416	438	3		
4	a8	61	Total	C	N	O	S	0	0
			469	290	93	85	1		

- Molecule 5 is a protein called Phycobiliprotein ApcE.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	03	826	Total	C	N	O	S	0	0
			6594	4183	1160	1235	16		
5	13	826	Total	C	N	O	S	0	0
			6594	4183	1160	1235	16		

- Molecule 6 is a protein called Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	23	65	Total	C	N	O	S	0	0
			529	335	99	91	4		
6	33	65	Total	C	N	O	S	0	0
			529	335	99	91	4		
6	G7	65	Total	C	N	O	S	0	0
			529	335	99	91	4		
6	N7	66	Total	C	N	O	S	0	0
			537	340	100	92	5		
6	U7	65	Total	C	N	O	S	0	0
			529	335	99	91	4		
6	b7	65	Total	C	N	O	S	0	0
			529	335	99	91	4		

- Molecule 7 is a protein called Allophycocyanin alpha subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G3	160	Total	C	N	O	S	0	0
			1199	748	203	240	8		
7	I3	160	Total	C	N	O	S	0	0
			1199	748	203	240	8		
7	K3	160	Total	C	N	O	S	0	0
			1199	748	203	240	8		
7	N3	160	Total	C	N	O	S	0	0
			1199	748	203	240	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
7	P3	160	Total 1199	C 748	N 203	O 240	S 8	0	0
7	R3	160	Total 1199	C 748	N 203	O 240	S 8	0	0
7	T3	160	Total 1199	C 748	N 203	O 240	S 8	0	0
7	X3	160	Total 1199	C 748	N 203	O 240	S 8	0	0
7	Z3	160	Total 1199	C 748	N 203	O 240	S 8	0	0
7	b3	160	Total 1199	C 748	N 203	O 240	S 8	0	0
7	d3	160	Total 1199	C 748	N 203	O 240	S 8	0	0
7	f3	160	Total 1199	C 748	N 203	O 240	S 8	0	0
7	i3	160	Total 1199	C 748	N 203	O 240	S 8	0	0
7	k3	160	Total 1199	C 748	N 203	O 240	S 8	0	0
7	o3	160	Total 1199	C 748	N 203	O 240	S 8	0	0
7	q3	160	Total 1199	C 748	N 203	O 240	S 8	0	0
7	s3	160	Total 1199	C 748	N 203	O 240	S 8	0	0
7	u3	160	Total 1199	C 748	N 203	O 240	S 8	0	0
7	w3	160	Total 1199	C 748	N 203	O 240	S 8	0	0
7	y3	160	Total 1199	C 748	N 203	O 240	S 8	0	0
7	A7	160	Total 1199	C 748	N 203	O 240	S 8	0	0
7	C7	160	Total 1199	C 748	N 203	O 240	S 8	0	0
7	E7	160	Total 1199	C 748	N 203	O 240	S 8	0	0
7	H7	160	Total 1199	C 748	N 203	O 240	S 8	0	0
7	J7	160	Total 1199	C 748	N 203	O 240	S 8	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
7	L7	160	Total	C	N	O	S	0	0
			1199	748	203	240	8		
7	O7	160	Total	C	N	O	S	0	0
			1199	748	203	240	8		
7	Q7	160	Total	C	N	O	S	0	0
			1199	748	203	240	8		
7	S7	160	Total	C	N	O	S	0	0
			1199	748	203	240	8		
7	V7	160	Total	C	N	O	S	0	0
			1199	748	203	240	8		
7	X7	160	Total	C	N	O	S	0	0
			1199	748	203	240	8		
7	Z7	160	Total	C	N	O	S	0	0
			1199	748	203	240	8		

- Molecule 8 is a protein called Allophycocyanin beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H3	161	Total	C	N	O	S	0	0
			1205	756	204	237	8		
8	J3	161	Total	C	N	O	S	0	0
			1205	756	204	237	8		
8	L3	161	Total	C	N	O	S	0	0
			1205	756	204	237	8		
8	M3	161	Total	C	N	O	S	0	0
			1205	756	204	237	8		
8	O3	161	Total	C	N	O	S	0	0
			1205	756	204	237	8		
8	S3	161	Total	C	N	O	S	0	0
			1205	756	204	237	8		
8	U3	161	Total	C	N	O	S	0	0
			1205	756	204	237	8		
8	W3	161	Total	C	N	O	S	0	0
			1205	756	204	237	8		
8	Y3	161	Total	C	N	O	S	0	0
			1205	756	204	237	8		
8	a3	161	Total	C	N	O	S	0	0
			1205	756	204	237	8		
8	c3	161	Total	C	N	O	S	0	0
			1205	756	204	237	8		
8	e3	161	Total	C	N	O	S	0	0
			1205	756	204	237	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
8	h3	161	Total 1205	C 756	N 204	O 237	S 8	0	0
8	j3	161	Total 1205	C 756	N 204	O 237	S 8	0	0
8	l3	161	Total 1205	C 756	N 204	O 237	S 8	0	0
8	n3	161	Total 1205	C 756	N 204	O 237	S 8	0	0
8	p3	161	Total 1205	C 756	N 204	O 237	S 8	0	0
8	r3	161	Total 1205	C 756	N 204	O 237	S 8	0	0
8	t3	161	Total 1205	C 756	N 204	O 237	S 8	0	0
8	v3	161	Total 1205	C 756	N 204	O 237	S 8	0	0
8	x3	161	Total 1205	C 756	N 204	O 237	S 8	0	0
8	z3	161	Total 1205	C 756	N 204	O 237	S 8	0	0
8	B7	161	Total 1205	C 756	N 204	O 237	S 8	0	0
8	D7	161	Total 1205	C 756	N 204	O 237	S 8	0	0
8	F7	161	Total 1205	C 756	N 204	O 237	S 8	0	0
8	I7	161	Total 1205	C 756	N 204	O 237	S 8	0	0
8	K7	161	Total 1205	C 756	N 204	O 237	S 8	0	0
8	M7	161	Total 1205	C 756	N 204	O 237	S 8	0	0
8	P7	161	Total 1205	C 756	N 204	O 237	S 8	0	0
8	R7	161	Total 1205	C 756	N 204	O 237	S 8	0	0
8	T7	161	Total 1205	C 756	N 204	O 237	S 8	0	0
8	W7	161	Total 1205	C 756	N 204	O 237	S 8	0	0
8	Y7	161	Total 1205	C 756	N 204	O 237	S 8	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	a7	161	Total	C	N	O	S	0	0
			1205	756	204	237	8		

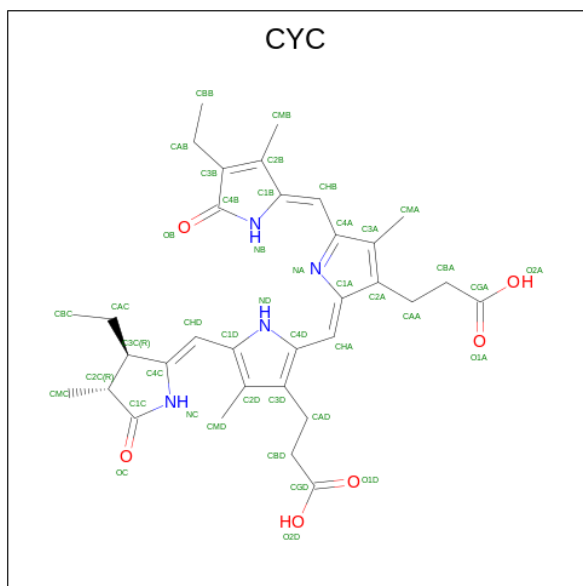
- Molecule 9 is a protein called Allophycocyanin subunit beta-18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	Q3	169	Total	C	N	O	S	0	0
			1314	825	225	257	7		
9	g3	169	Total	C	N	O	S	0	0
			1314	825	225	257	7		

- Molecule 10 is a protein called Allophycocyanin subunit alpha-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	V3	160	Total	C	N	O	S	0	0
			1235	782	213	235	5		
10	m3	160	Total	C	N	O	S	0	0
			1235	782	213	235	5		

- Molecule 11 is PHYCOCYANOBILIN (three-letter code: CYC) (formula: $C_{33}H_{40}N_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
11	A1	1	Total	C	N	O	0
			86	66	8	12	

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
11	A1	1	86	66	8	12	0
11	B1	1	43	33	4	6	0
11	C1	1	86	66	8	12	0
11	C1	1	86	66	8	12	0
11	D1	1	43	33	4	6	0
11	F1	1	43	33	4	6	0
11	G1	1	86	66	8	12	0
11	G1	1	86	66	8	12	0
11	H1	1	43	33	4	6	0
11	I1	1	86	66	8	12	0
11	I1	1	86	66	8	12	0
11	J1	1	43	33	4	6	0
11	K1	1	86	66	8	12	0
11	K1	1	86	66	8	12	0
11	L1	1	43	33	4	6	0
11	M1	1	86	66	8	12	0
11	M1	1	86	66	8	12	0
11	N1	1	43	33	4	6	0
11	O1	1	43	33	4	6	0
11	P1	1	86	66	8	12	0
11	P1	1	86	66	8	12	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
11	Q1	1	43	33	4	6	0
11	R1	1	86	66	8	12	0
11	R1	1	86	66	8	12	0
11	S1	1	43	33	4	6	0
11	T1	1	43	33	4	6	0
11	U1	1	86	66	8	12	0
11	U1	1	86	66	8	12	0
11	V1	1	86	66	8	12	0
11	V1	1	86	66	8	12	0
11	X1	1	129	99	12	18	0
11	X1	1	129	99	12	18	0
11	X1	1	129	99	12	18	0
11	Z1	1	86	66	8	12	0
11	Z1	1	86	66	8	12	0
11	A2	1	43	33	4	6	0
11	B2	1	43	33	4	6	0
11	C2	1	86	66	8	12	0
11	C2	1	86	66	8	12	0
11	D2	1	43	33	4	6	0
11	E2	1	129	99	12	18	0
11	E2	1	129	99	12	18	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
11	E2	1	Total 129	C 99	N 12	O 18	0
11	G2	1	Total 43	C 33	N 4	O 6	0
11	H2	1	Total 43	C 33	N 4	O 6	0
11	I2	1	Total 129	C 99	N 12	O 18	0
11	I2	1	Total 129	C 99	N 12	O 18	0
11	I2	1	Total 129	C 99	N 12	O 18	0
11	K2	1	Total 129	C 99	N 12	O 18	0
11	K2	1	Total 129	C 99	N 12	O 18	0
11	K2	1	Total 129	C 99	N 12	O 18	0
11	M2	1	Total 86	C 66	N 8	O 12	0
11	M2	1	Total 86	C 66	N 8	O 12	0
11	N2	1	Total 86	C 66	N 8	O 12	0
11	N2	1	Total 86	C 66	N 8	O 12	0
11	P2	1	Total 86	C 66	N 8	O 12	0
11	P2	1	Total 86	C 66	N 8	O 12	0
11	Q2	1	Total 43	C 33	N 4	O 6	0
11	R2	1	Total 43	C 33	N 4	O 6	0
11	S2	1	Total 43	C 33	N 4	O 6	0
11	T2	1	Total 86	C 66	N 8	O 12	0
11	T2	1	Total 86	C 66	N 8	O 12	0
11	V2	1	Total 86	C 66	N 8	O 12	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
11	V2	1	Total 86	C 66	N 8	O 12	0
11	W2	1	Total 43	C 33	N 4	O 6	0
11	X2	1	Total 129	C 99	N 12	O 18	0
11	X2	1	Total 129	C 99	N 12	O 18	0
11	X2	1	Total 129	C 99	N 12	O 18	0
11	Z2	1	Total 129	C 99	N 12	O 18	0
11	Z2	1	Total 129	C 99	N 12	O 18	0
11	Z2	1	Total 129	C 99	N 12	O 18	0
11	03	1	Total 86	C 66	N 8	O 12	0
11	03	1	Total 86	C 66	N 8	O 12	0
11	13	1	Total 172	C 132	N 16	O 24	0
11	13	1	Total 172	C 132	N 16	O 24	0
11	13	1	Total 172	C 132	N 16	O 24	0
11	13	1	Total 172	C 132	N 16	O 24	0
11	G3	1	Total 43	C 33	N 4	O 6	0
11	H3	1	Total 43	C 33	N 4	O 6	0
11	I3	1	Total 43	C 33	N 4	O 6	0
11	J3	1	Total 43	C 33	N 4	O 6	0
11	K3	1	Total 43	C 33	N 4	O 6	0
11	M3	1	Total 43	C 33	N 4	O 6	0
11	N3	1	Total 43	C 33	N 4	O 6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
11	O3	1	43	33	4	6	0
11	P3	1	43	33	4	6	0
11	Q3	1	43	33	4	6	0
11	R3	1	43	33	4	6	0
11	S3	1	43	33	4	6	0
11	T3	1	43	33	4	6	0
11	U3	1	43	33	4	6	0
11	V3	1	43	33	4	6	0
11	W3	1	43	33	4	6	0
11	X3	1	43	33	4	6	0
11	Z3	1	43	33	4	6	0
11	b3	1	43	33	4	6	0
11	c3	1	43	33	4	6	0
11	d3	1	43	33	4	6	0
11	e3	1	43	33	4	6	0
11	f3	1	43	33	4	6	0
11	g3	1	43	33	4	6	0
11	i3	1	43	33	4	6	0
11	j3	1	43	33	4	6	0
11	k3	1	43	33	4	6	0
11	l3	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
11	m3	1	43	33	4	6	0
11	n3	1	43	33	4	6	0
11	o3	1	43	33	4	6	0
11	p3	1	43	33	4	6	0
11	q3	1	43	33	4	6	0
11	r3	1	43	33	4	6	0
11	s3	1	43	33	4	6	0
11	t3	1	43	33	4	6	0
11	u3	1	43	33	4	6	0
11	v3	1	43	33	4	6	0
11	w3	1	43	33	4	6	0
11	x3	1	43	33	4	6	0
11	y3	1	43	33	4	6	0
11	z3	1	43	33	4	6	0
11	A4	1	43	33	4	6	0
11	C4	1	43	33	4	6	0
11	D4	1	43	33	4	6	0
11	E4	1	129	99	12	18	0
11	E4	1	129	99	12	18	0
11	E4	1	129	99	12	18	0
11	F4	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
11	G4	1	86	66	8	12	0
11	G4	1	86	66	8	12	0
11	I4	1	129	99	12	18	0
11	I4	1	129	99	12	18	0
11	I4	1	129	99	12	18	0
11	K4	1	86	66	8	12	0
11	K4	1	86	66	8	12	0
11	L4	1	86	66	8	12	0
11	L4	1	86	66	8	12	0
11	M4	1	86	66	8	12	0
11	M4	1	86	66	8	12	0
11	N4	1	43	33	4	6	0
11	O4	1	43	33	4	6	0
11	P4	1	129	99	12	18	0
11	P4	1	129	99	12	18	0
11	P4	1	129	99	12	18	0
11	R4	1	43	33	4	6	0
11	S4	1	43	33	4	6	0
11	T4	1	86	66	8	12	0
11	T4	1	86	66	8	12	0
11	U4	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
11	V4	1	86	66	8	12	0
11	V4	1	86	66	8	12	0
11	W4	1	43	33	4	6	0
11	X4	1	86	66	8	12	0
11	X4	1	86	66	8	12	0
11	Y4	1	43	33	4	6	0
11	Z4	1	86	66	8	12	0
11	Z4	1	86	66	8	12	0
11	A5	1	86	66	8	12	0
11	A5	1	86	66	8	12	0
11	B5	1	43	33	4	6	0
11	C5	1	86	66	8	12	0
11	C5	1	86	66	8	12	0
11	D5	1	43	33	4	6	0
11	F5	1	43	33	4	6	0
11	G5	1	86	66	8	12	0
11	G5	1	86	66	8	12	0
11	H5	1	43	33	4	6	0
11	I5	1	86	66	8	12	0
11	I5	1	86	66	8	12	0
11	J5	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
11	K5	1	Total 86	C 66	N 8	O 12	0
11	K5	1	Total 86	C 66	N 8	O 12	0
11	L5	1	Total 43	C 33	N 4	O 6	0
11	M5	1	Total 86	C 66	N 8	O 12	0
11	M5	1	Total 86	C 66	N 8	O 12	0
11	N5	1	Total 43	C 33	N 4	O 6	0
11	O5	1	Total 43	C 33	N 4	O 6	0
11	P5	1	Total 86	C 66	N 8	O 12	0
11	P5	1	Total 86	C 66	N 8	O 12	0
11	Q5	1	Total 43	C 33	N 4	O 6	0
11	R5	1	Total 86	C 66	N 8	O 12	0
11	R5	1	Total 86	C 66	N 8	O 12	0
11	S5	1	Total 43	C 33	N 4	O 6	0
11	T5	1	Total 43	C 33	N 4	O 6	0
11	U5	1	Total 86	C 66	N 8	O 12	0
11	U5	1	Total 86	C 66	N 8	O 12	0
11	V5	1	Total 86	C 66	N 8	O 12	0
11	V5	1	Total 86	C 66	N 8	O 12	0
11	X5	1	Total 129	C 99	N 12	O 18	0
11	X5	1	Total 129	C 99	N 12	O 18	0
11	X5	1	Total 129	C 99	N 12	O 18	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
11	Z5	1	Total 86	C 66	N 8	O 12	0
11	Z5	1	Total 86	C 66	N 8	O 12	0
11	A6	1	Total 43	C 33	N 4	O 6	0
11	B6	1	Total 43	C 33	N 4	O 6	0
11	C6	1	Total 129	C 99	N 12	O 18	0
11	C6	1	Total 129	C 99	N 12	O 18	0
11	C6	1	Total 129	C 99	N 12	O 18	0
11	E6	1	Total 86	C 66	N 8	O 12	0
11	E6	1	Total 86	C 66	N 8	O 12	0
11	F6	1	Total 43	C 33	N 4	O 6	0
11	G6	1	Total 43	C 33	N 4	O 6	0
11	H6	1	Total 43	C 33	N 4	O 6	0
11	I6	1	Total 86	C 66	N 8	O 12	0
11	I6	1	Total 86	C 66	N 8	O 12	0
11	J6	1	Total 43	C 33	N 4	O 6	0
11	K6	1	Total 86	C 66	N 8	O 12	0
11	K6	1	Total 86	C 66	N 8	O 12	0
11	L6	1	Total 43	C 33	N 4	O 6	0
11	M6	1	Total 86	C 66	N 8	O 12	0
11	M6	1	Total 86	C 66	N 8	O 12	0
11	N6	1	Total 86	C 66	N 8	O 12	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
11	N6	1	86	66	8	12	0
11	O6	1	43	33	4	6	0
11	P6	1	86	66	8	12	0
11	P6	1	86	66	8	12	0
11	Q6	1	43	33	4	6	0
11	R6	1	86	66	8	12	0
11	R6	1	86	66	8	12	0
11	T6	1	43	33	4	6	0
11	U6	1	43	33	4	6	0
11	V6	1	86	66	8	12	0
11	V6	1	86	66	8	12	0
11	W6	1	43	33	4	6	0
11	X6	1	86	66	8	12	0
11	X6	1	86	66	8	12	0
11	Y6	1	43	33	4	6	0
11	Z6	1	86	66	8	12	0
11	Z6	1	86	66	8	12	0
11	A7	1	43	33	4	6	0
11	B7	1	43	33	4	6	0
11	C7	1	43	33	4	6	0
11	D7	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
11	E7	1	43	33	4	6	0
11	F7	1	43	33	4	6	0
11	H7	1	43	33	4	6	0
11	I7	1	43	33	4	6	0
11	J7	1	43	33	4	6	0
11	K7	1	43	33	4	6	0
11	L7	1	43	33	4	6	0
11	M7	1	43	33	4	6	0
11	O7	1	43	33	4	6	0
11	P7	1	43	33	4	6	0
11	Q7	1	43	33	4	6	0
11	R7	1	43	33	4	6	0
11	S7	1	43	33	4	6	0
11	T7	1	43	33	4	6	0
11	V7	1	43	33	4	6	0
11	W7	1	43	33	4	6	0
11	X7	1	43	33	4	6	0
11	Y7	1	43	33	4	6	0
11	Z7	1	43	33	4	6	0
11	a7	1	43	33	4	6	0
11	A8	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
11	C8	1	Total 43	C 33	N 4	O 6	0
11	D8	1	Total 43	C 33	N 4	O 6	0
11	E8	1	Total 129	C 99	N 12	O 18	0
11	E8	1	Total 129	C 99	N 12	O 18	0
11	E8	1	Total 129	C 99	N 12	O 18	0
11	F8	1	Total 43	C 33	N 4	O 6	0
11	G8	1	Total 86	C 66	N 8	O 12	0
11	G8	1	Total 86	C 66	N 8	O 12	0
11	I8	1	Total 129	C 99	N 12	O 18	0
11	I8	1	Total 129	C 99	N 12	O 18	0
11	I8	1	Total 129	C 99	N 12	O 18	0
11	K8	1	Total 86	C 66	N 8	O 12	0
11	K8	1	Total 86	C 66	N 8	O 12	0
11	L8	1	Total 86	C 66	N 8	O 12	0
11	L8	1	Total 86	C 66	N 8	O 12	0
11	M8	1	Total 86	C 66	N 8	O 12	0
11	M8	1	Total 86	C 66	N 8	O 12	0
11	N8	1	Total 43	C 33	N 4	O 6	0
11	O8	1	Total 43	C 33	N 4	O 6	0
11	P8	1	Total 129	C 99	N 12	O 18	0
11	P8	1	Total 129	C 99	N 12	O 18	0

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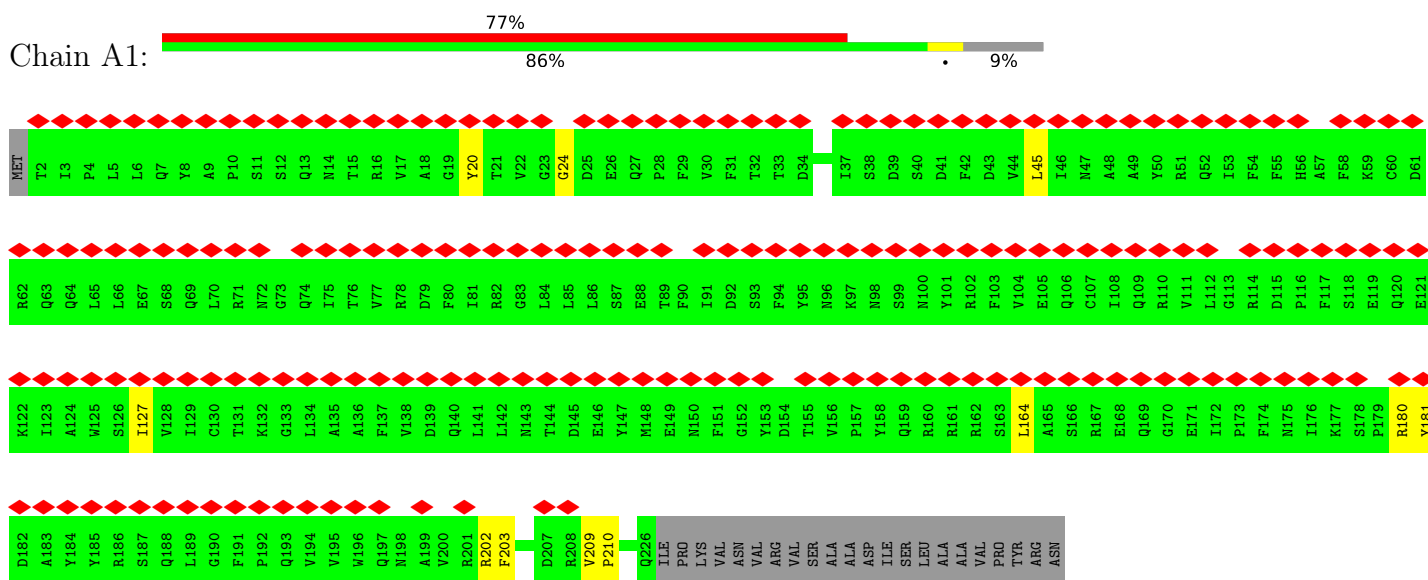
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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
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11	R8	1	Total 43	C 33	N 4	O 6	0
11	S8	1	Total 43	C 33	N 4	O 6	0
11	T8	1	Total 86	C 66	N 8	O 12	0
11	T8	1	Total 86	C 66	N 8	O 12	0
11	U8	1	Total 43	C 33	N 4	O 6	0
11	V8	1	Total 86	C 66	N 8	O 12	0
11	V8	1	Total 86	C 66	N 8	O 12	0
11	W8	1	Total 43	C 33	N 4	O 6	0
11	X8	1	Total 86	C 66	N 8	O 12	0
11	X8	1	Total 86	C 66	N 8	O 12	0
11	Y8	1	Total 43	C 33	N 4	O 6	0
11	Z8	1	Total 86	C 66	N 8	O 12	0
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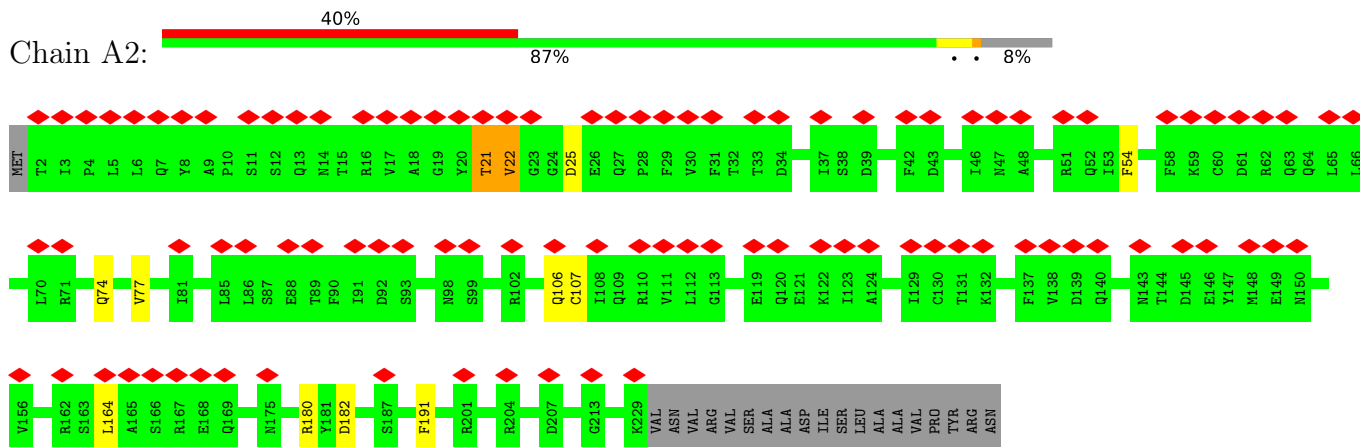
3 Residue-property plots

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

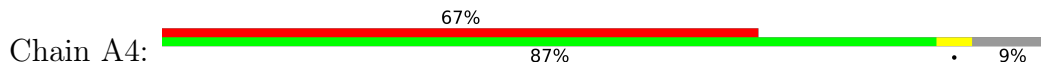
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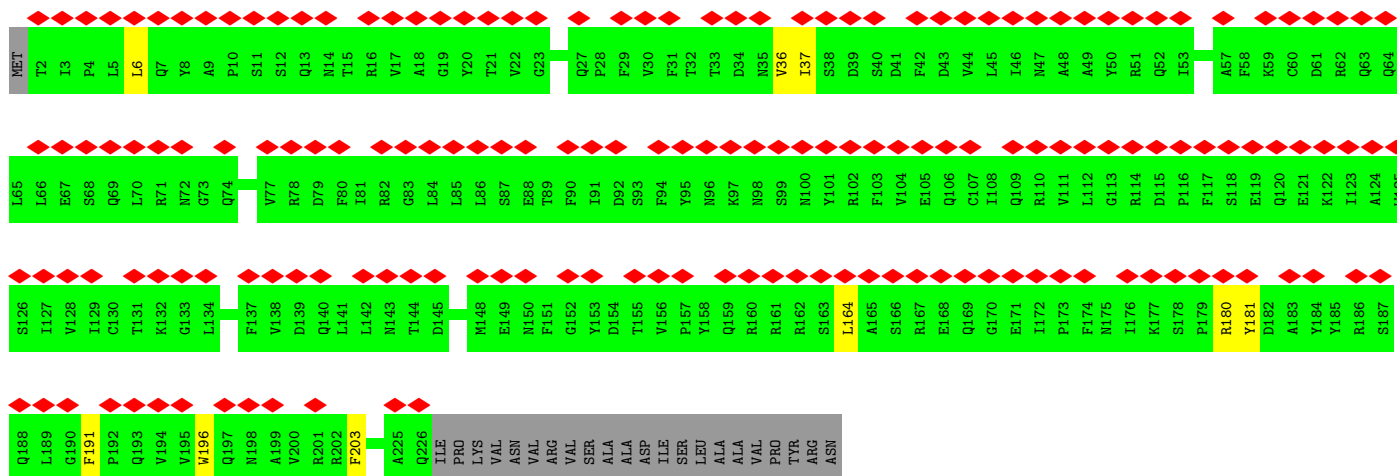


- Molecule 1: Phycobilisome rod-core linker polypeptide CpcG

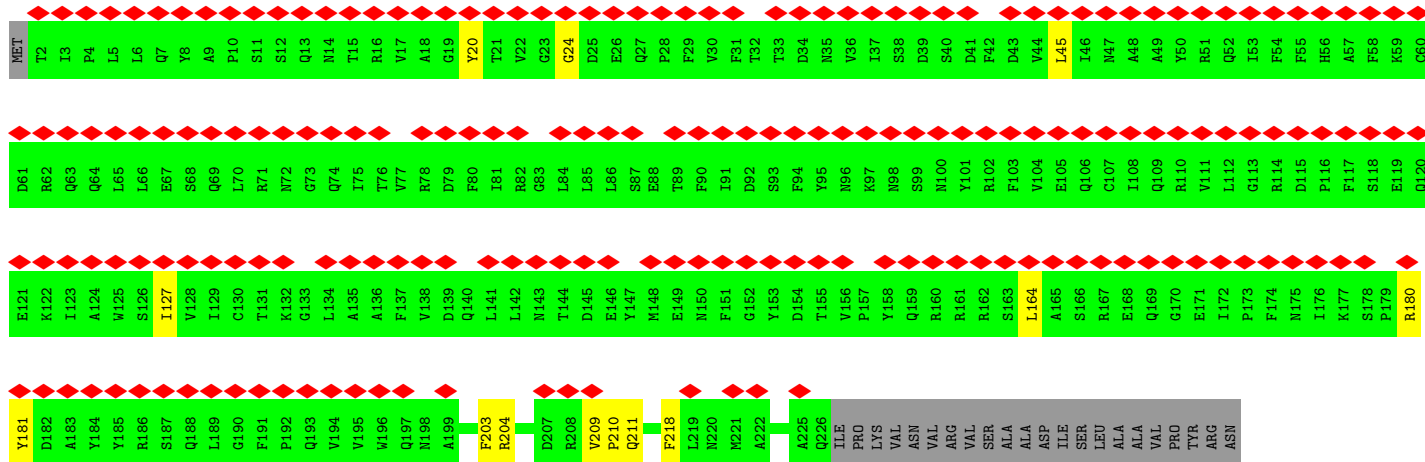
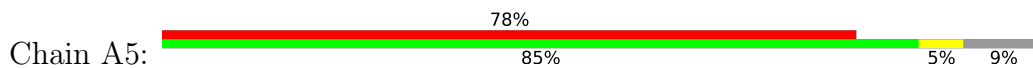


- Molecule 1: Phycobilisome rod-core linker polypeptide CpcG

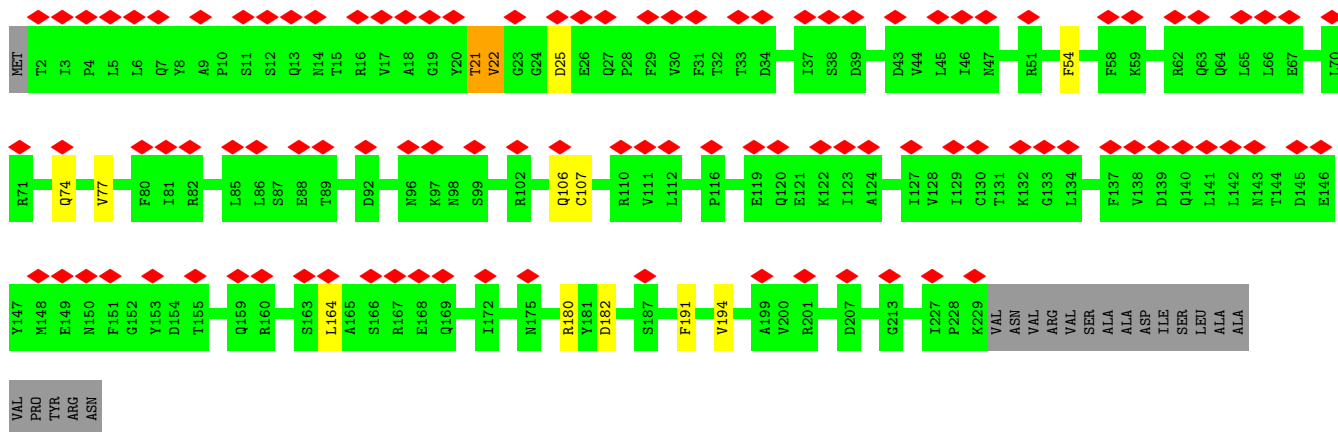
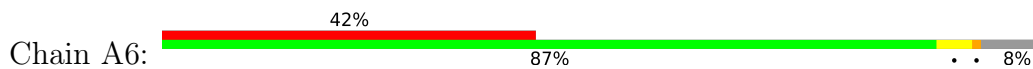




• Molecule 1: Phycobilisome rod-core linker polypeptide CpcG

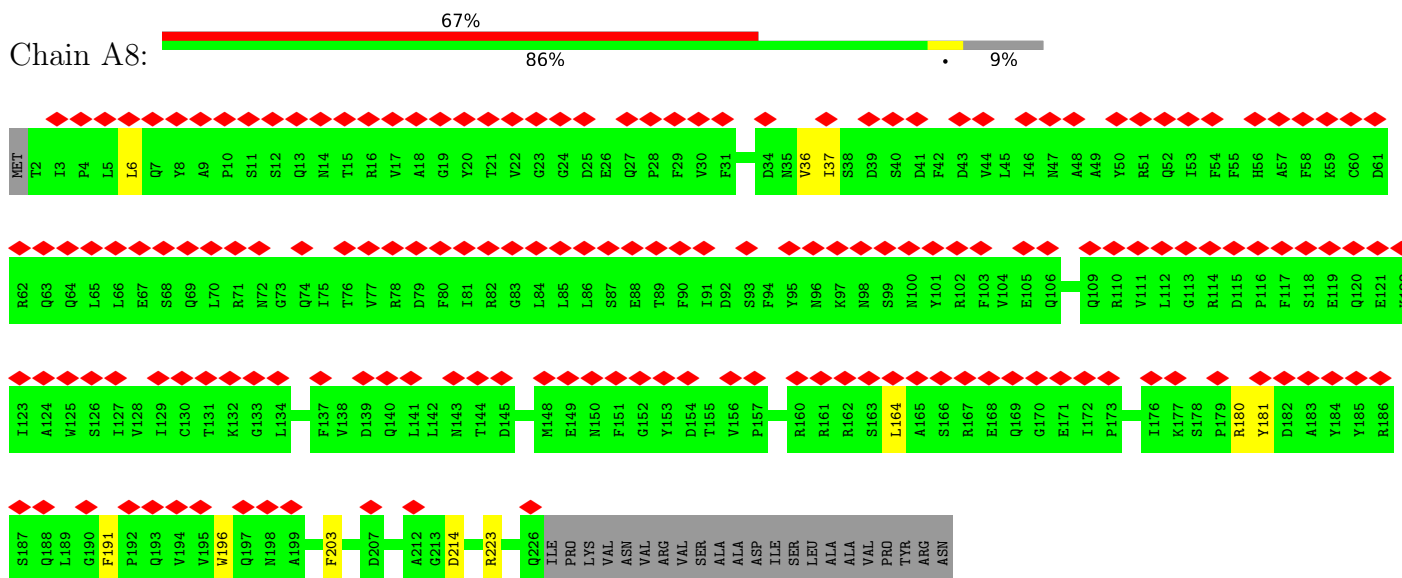


• Molecule 1: Phycobilisome rod-core linker polypeptide CpcG



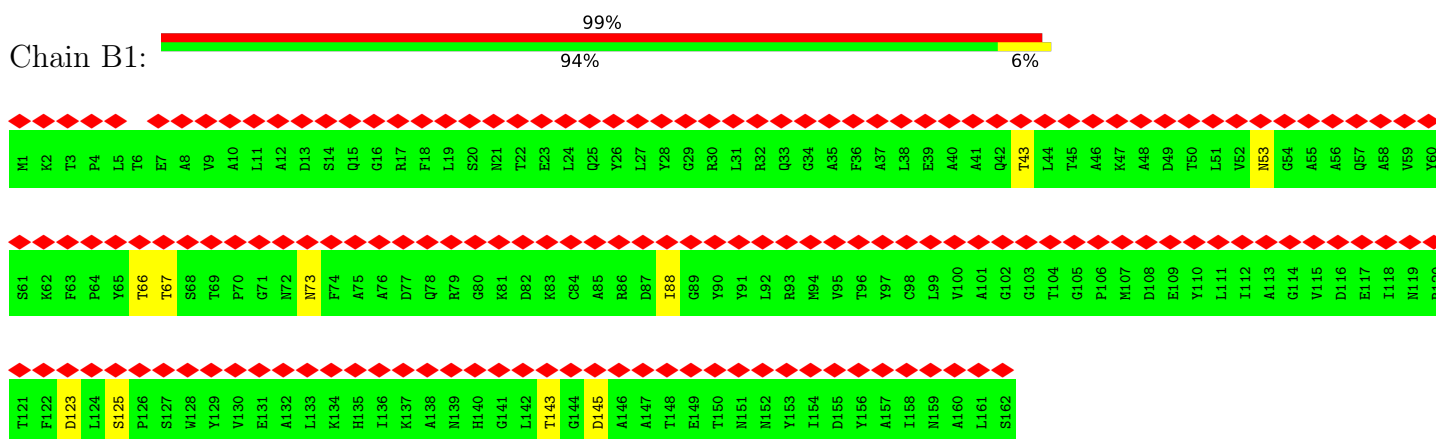
- Molecule 1: Phycobilisome rod-core linker polypeptide CpcG

Chain A8:



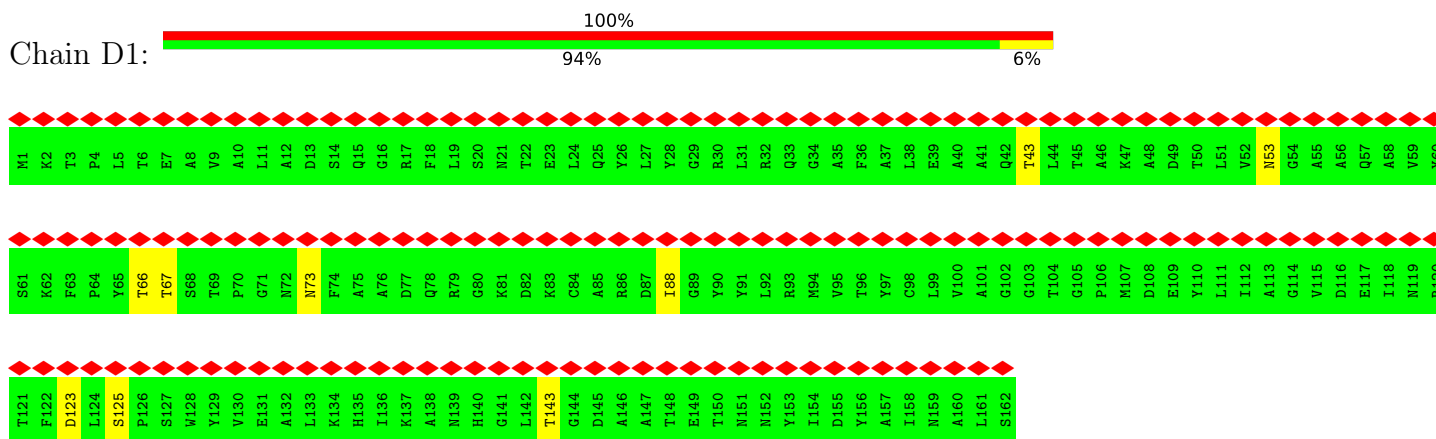
- Molecule 2: C-phycoerythrin subunit alpha

Chain B1:

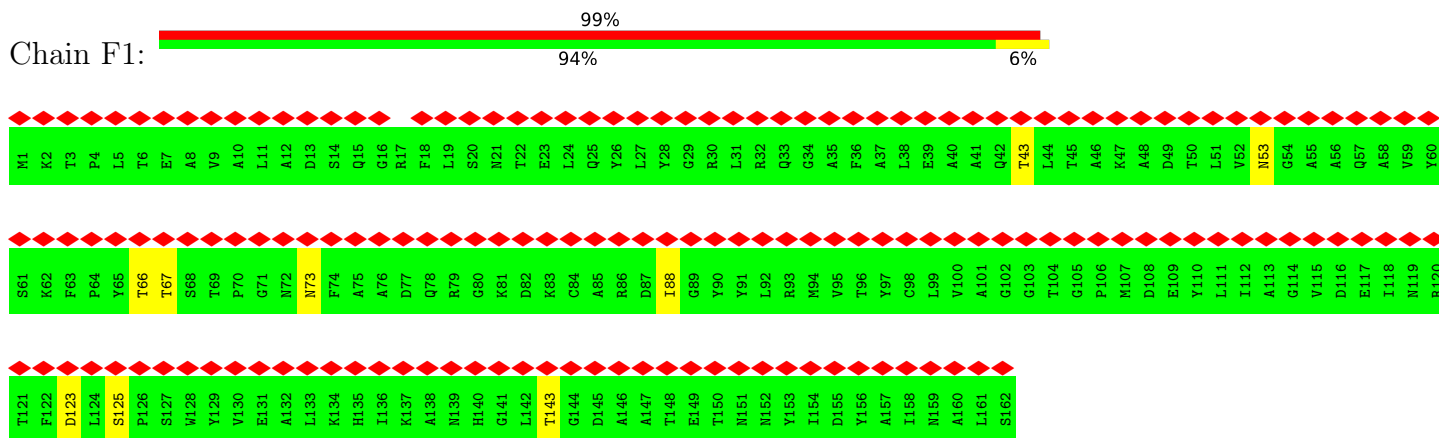


- Molecule 2: C-phycoerythrin subunit alpha

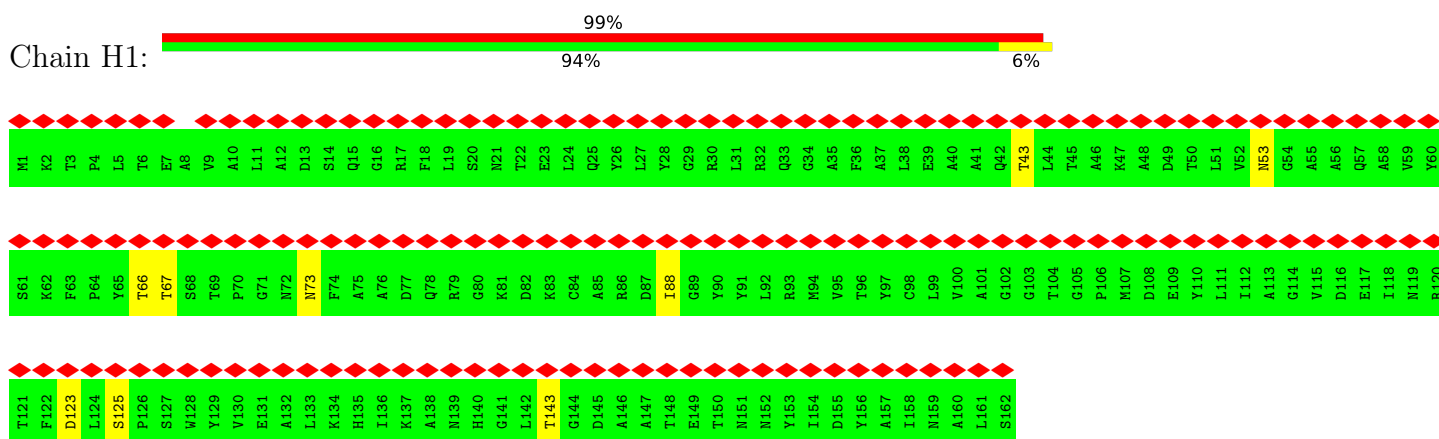
Chain D1:



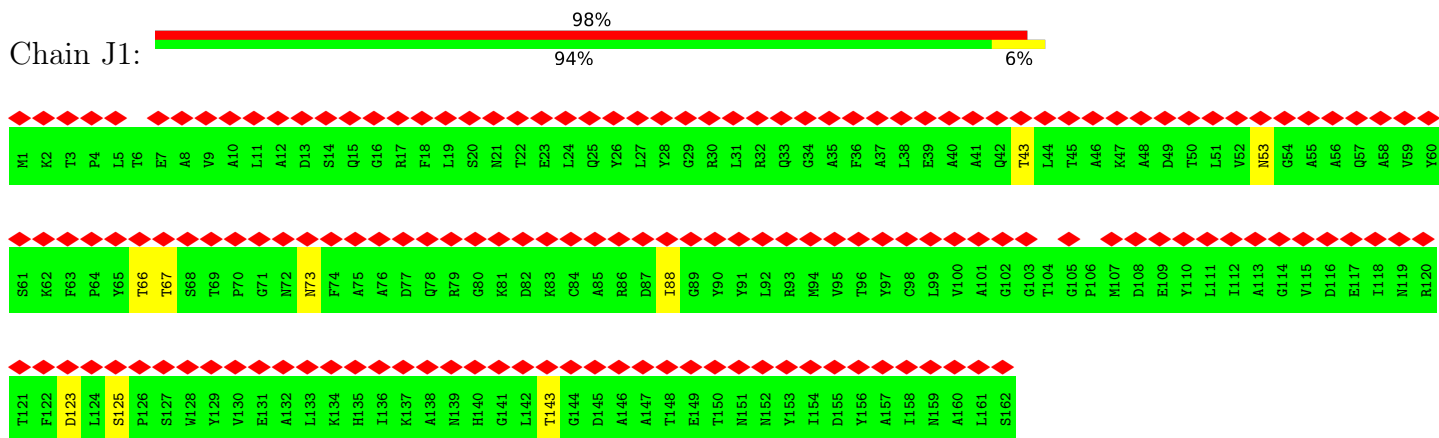
- Molecule 2: C-phycoerythrin subunit alpha



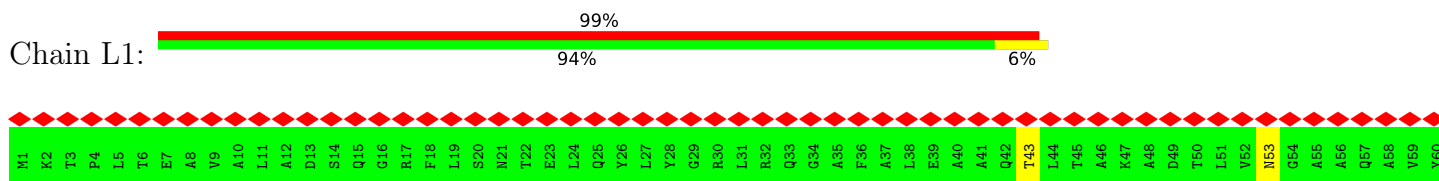
• Molecule 2: C-phycoerythrin subunit alpha

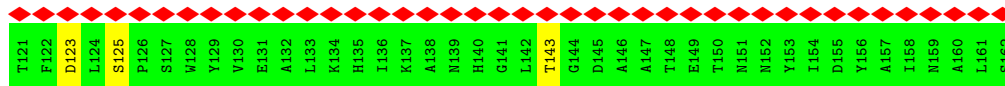
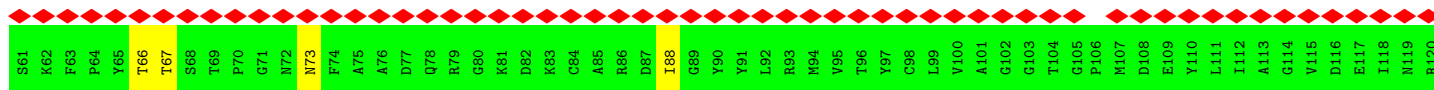


• Molecule 2: C-phycoerythrin subunit alpha

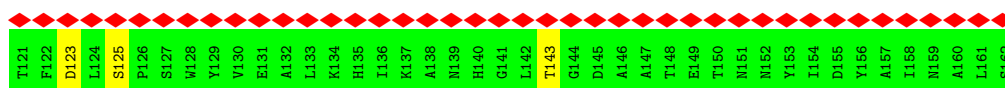
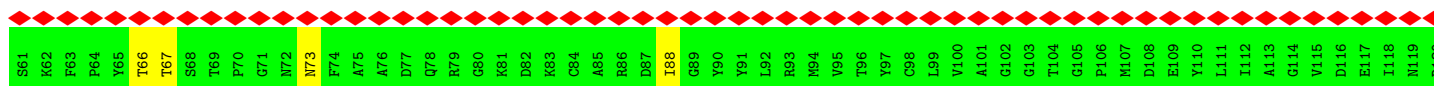
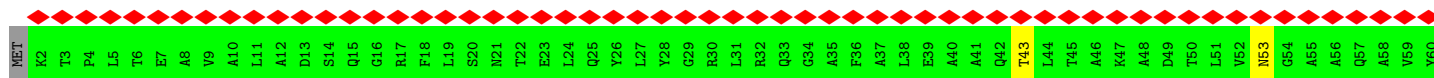


• Molecule 2: C-phycoerythrin subunit alpha

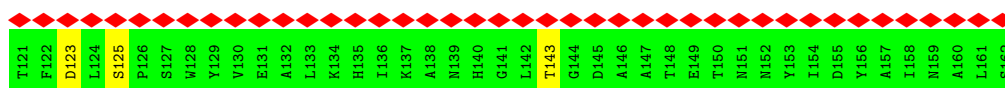
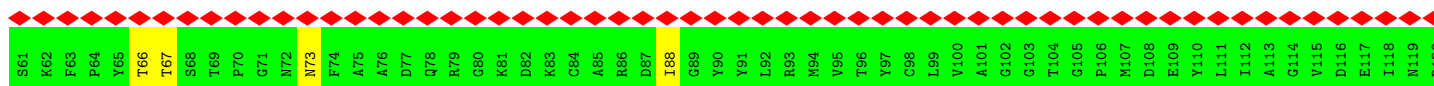
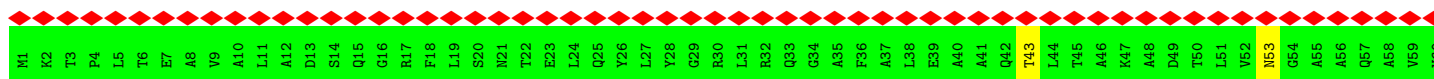




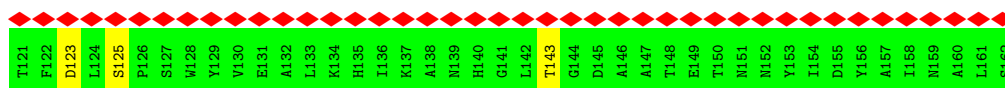
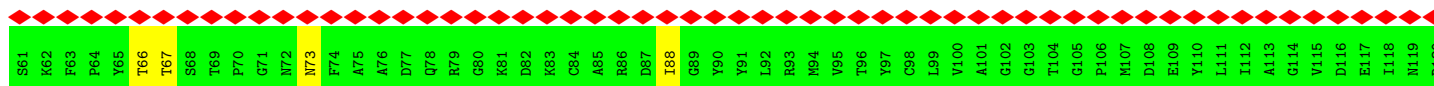
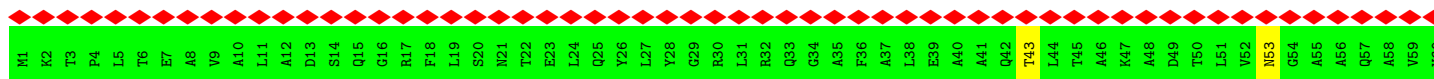
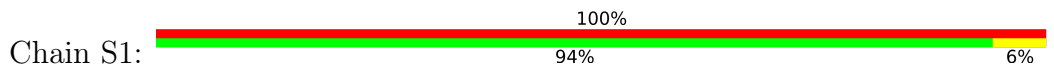
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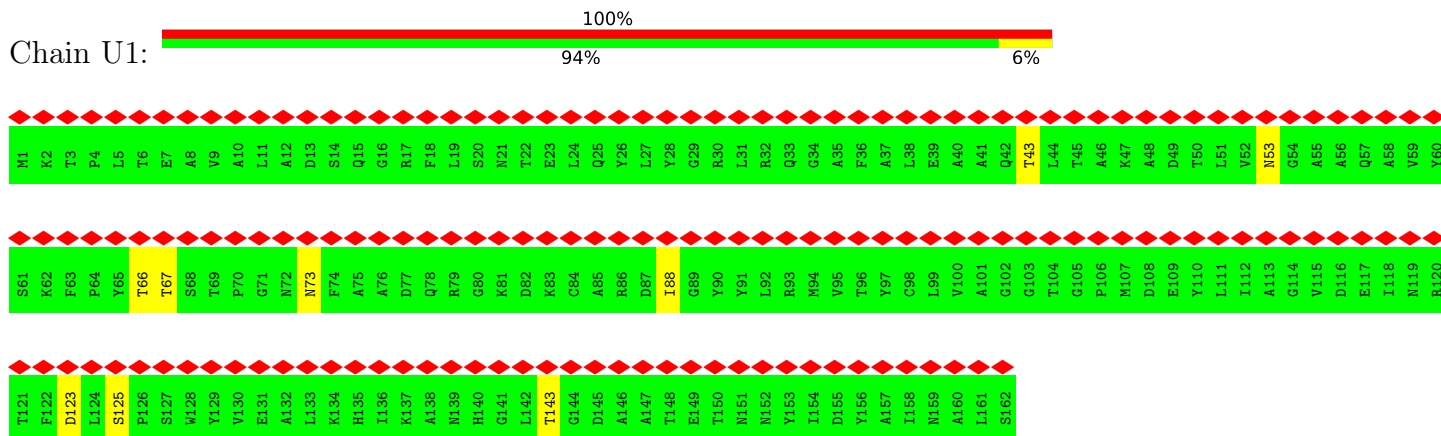
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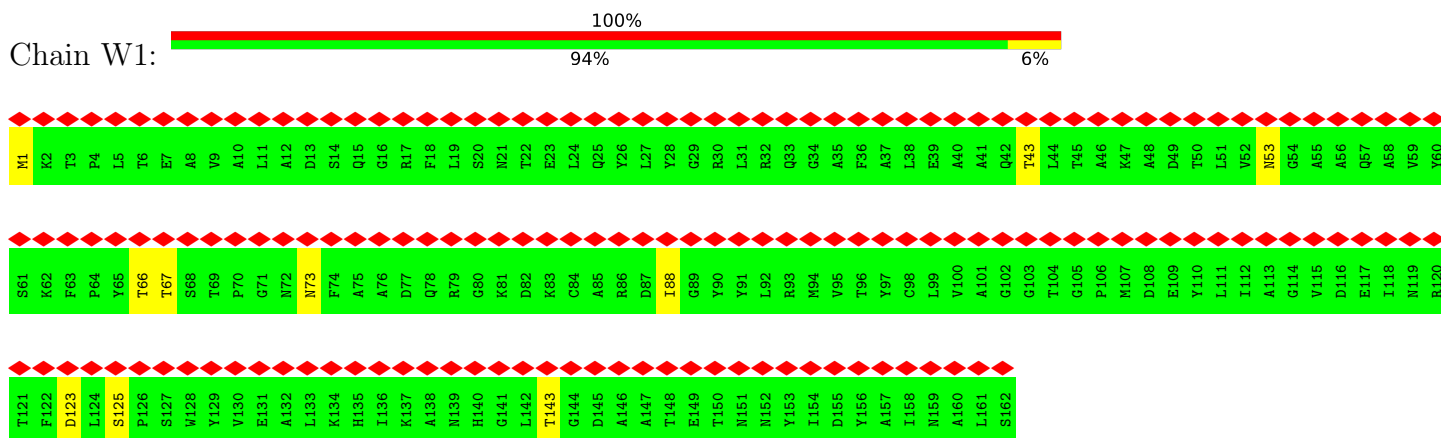
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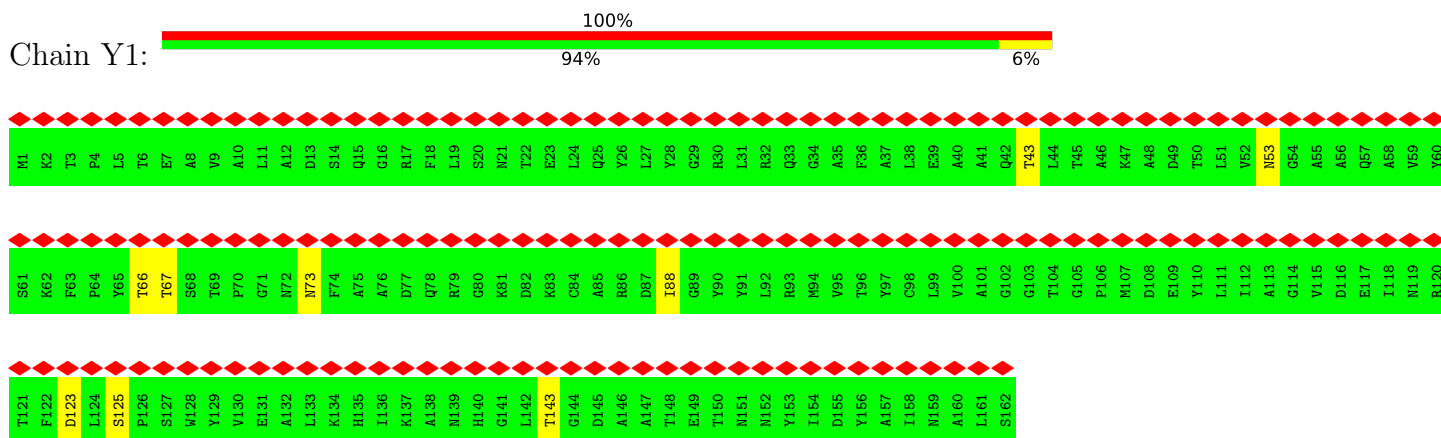
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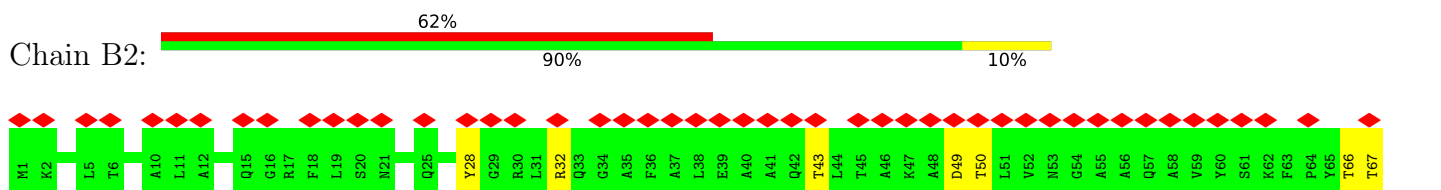
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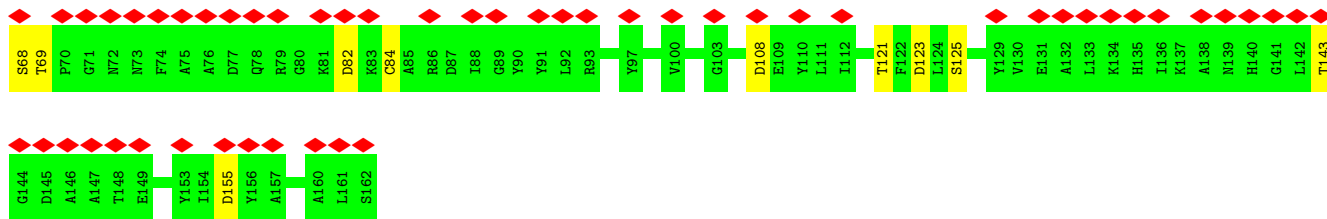


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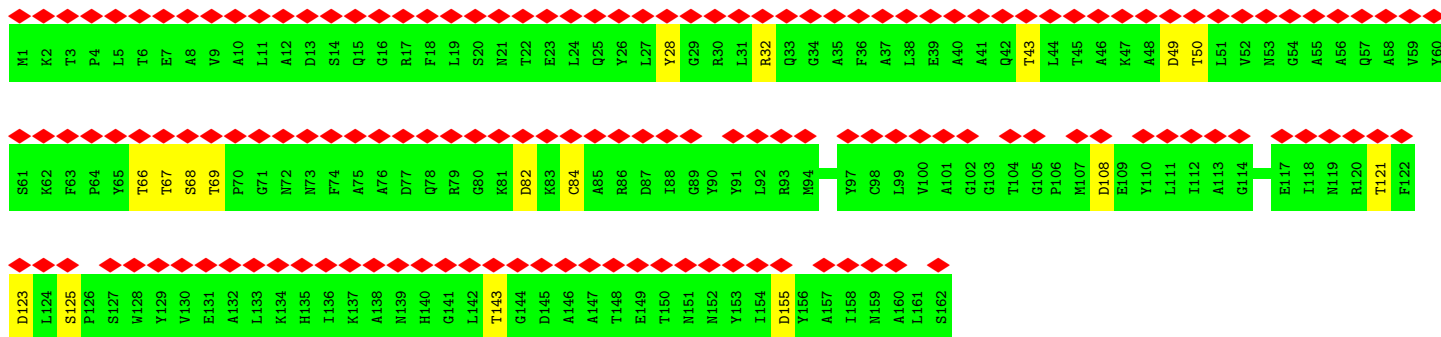
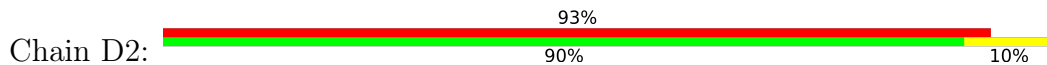


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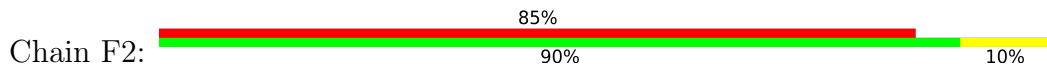




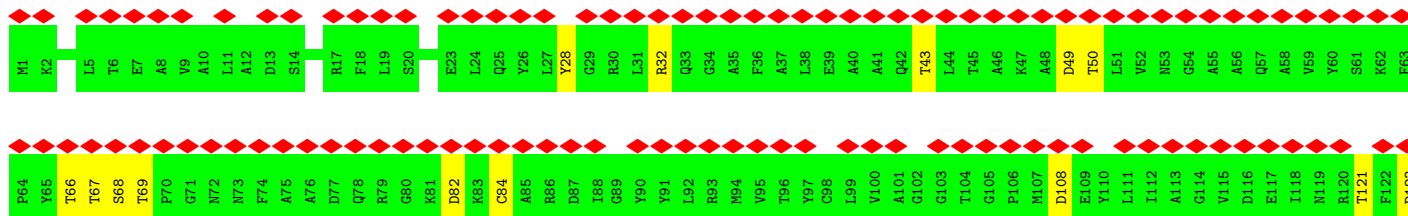
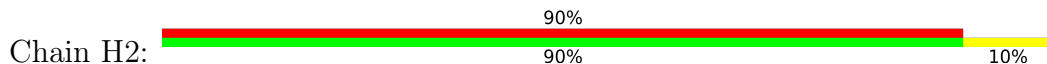
• Molecule 2: C-phycoerythrin subunit alpha



• Molecule 2: C-phycoerythrin subunit alpha

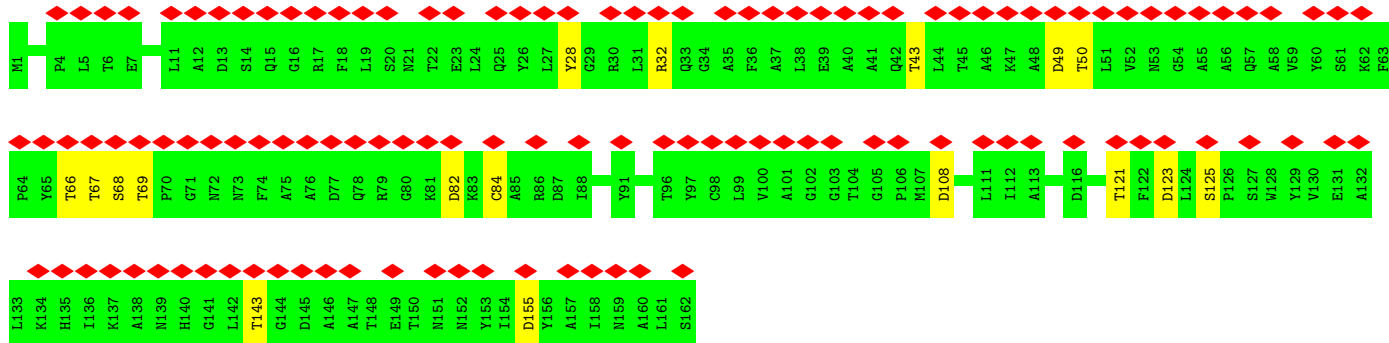
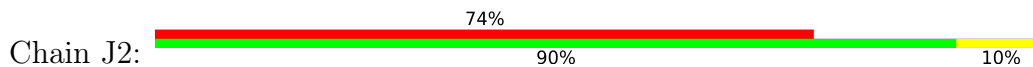


• Molecule 2: C-phycoerythrin subunit alpha

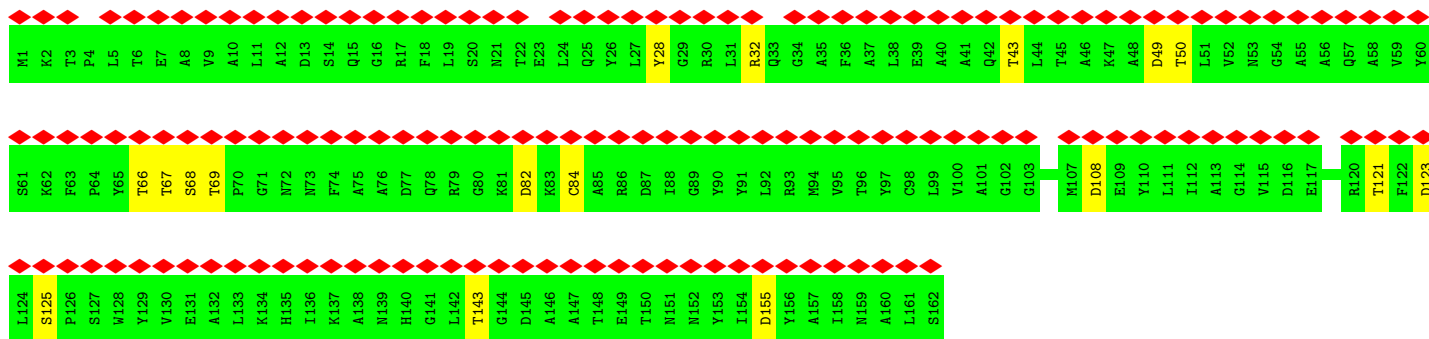
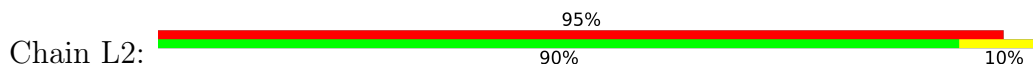




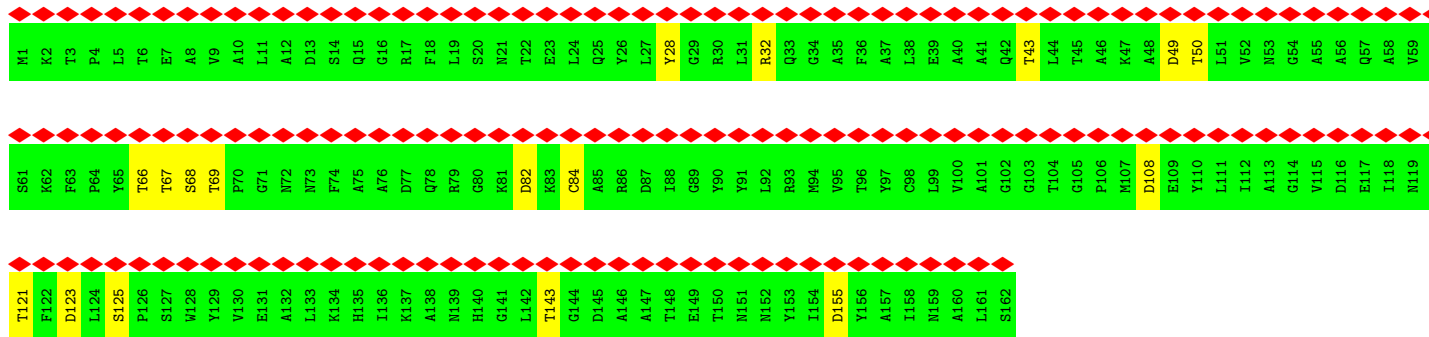
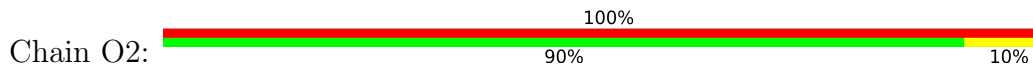
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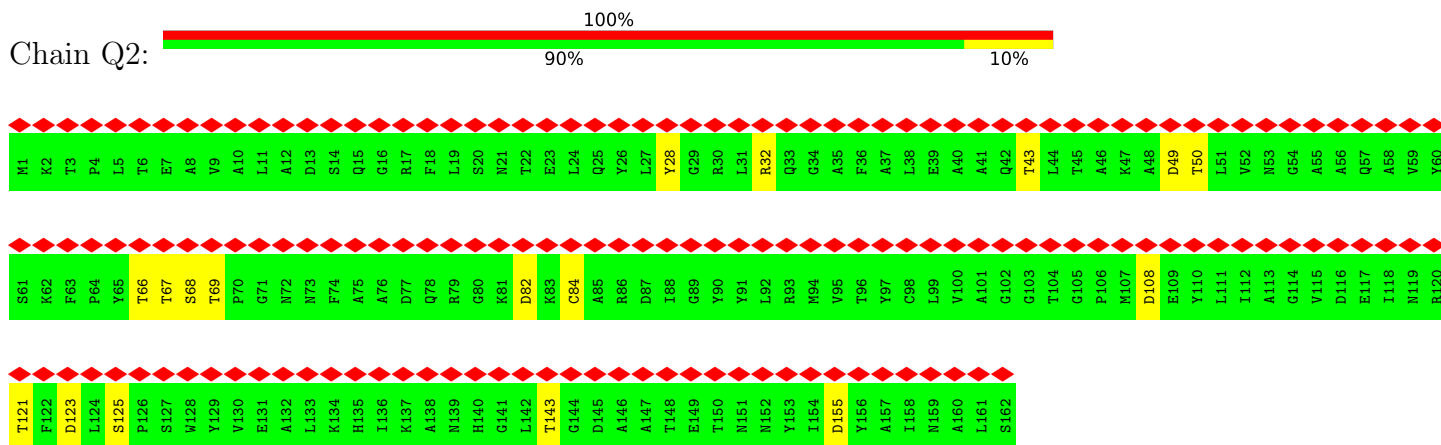
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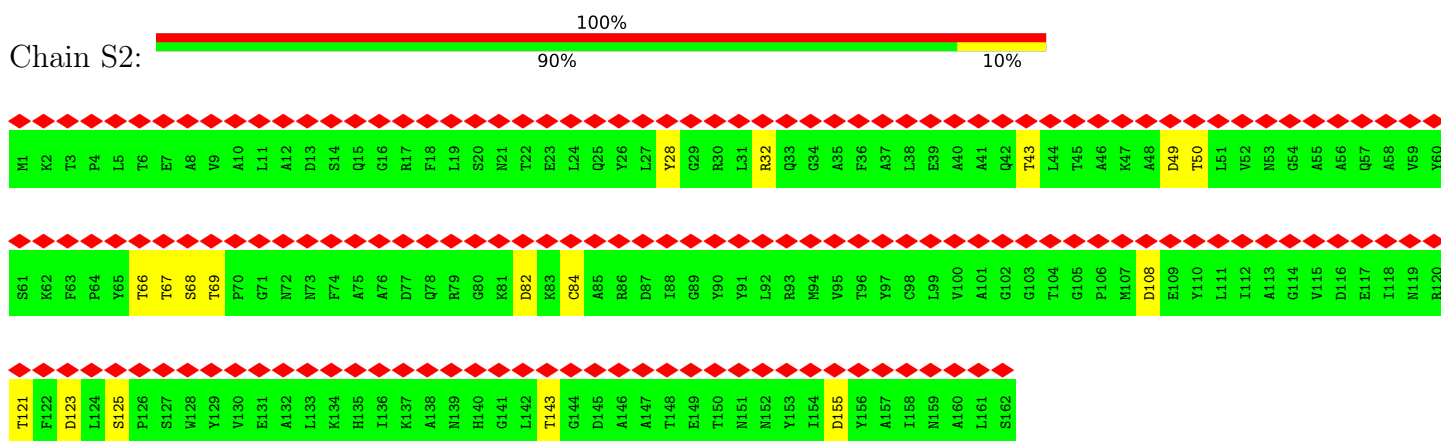
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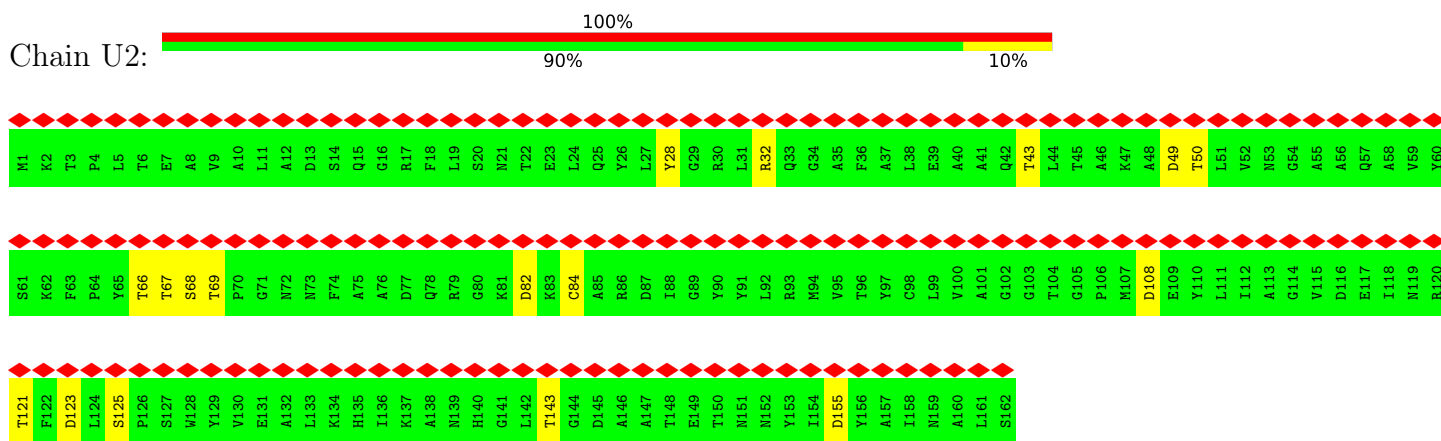
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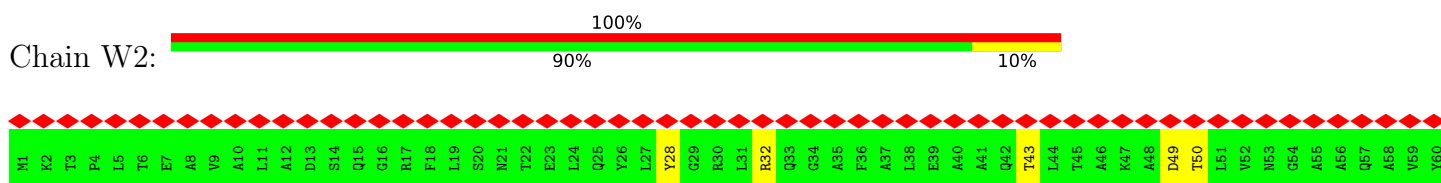
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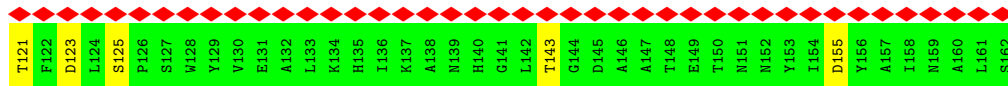
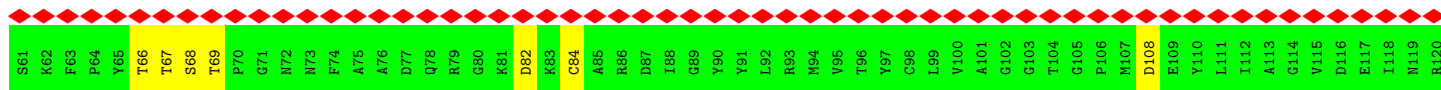


• Molecule 2: C-phycoeyanin subunit alpha

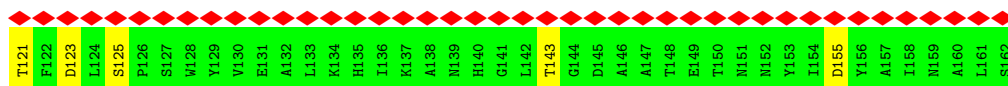
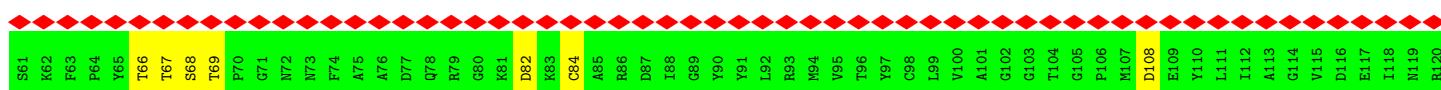
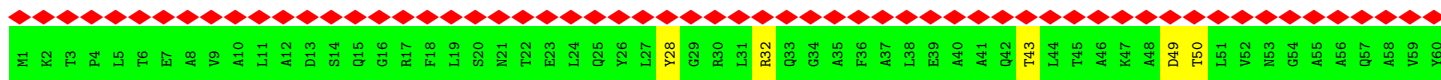
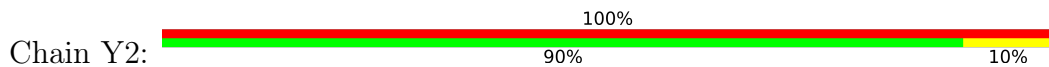


• Molecule 2: C-phycoeyanin subunit alpha

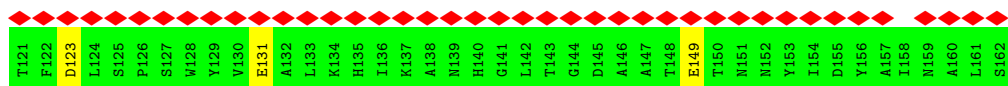
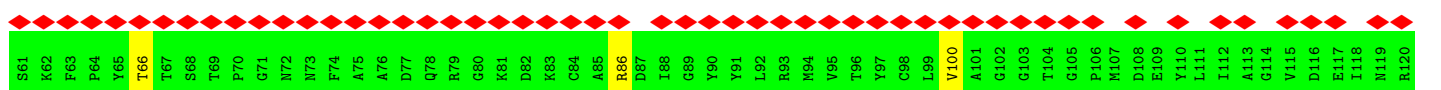
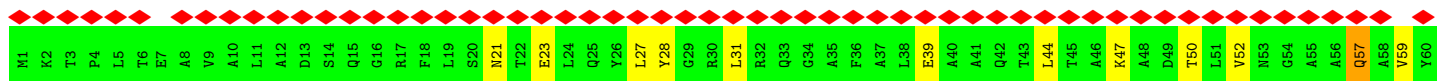
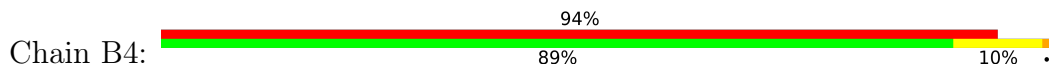




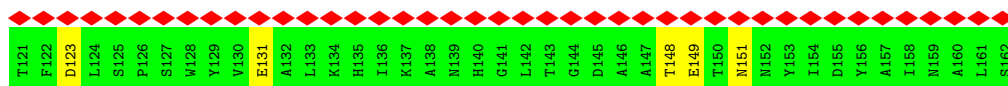
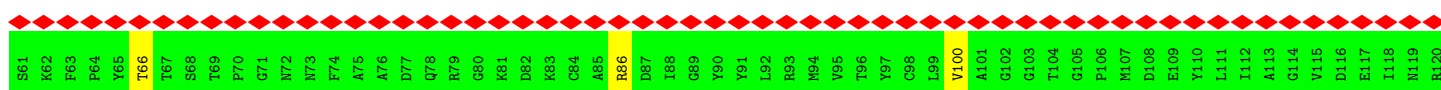
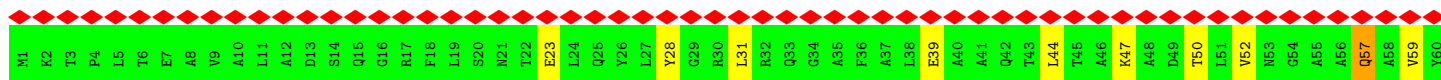
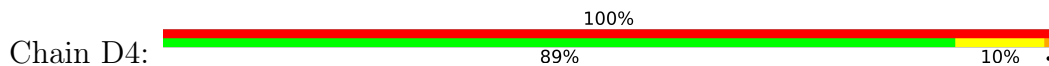
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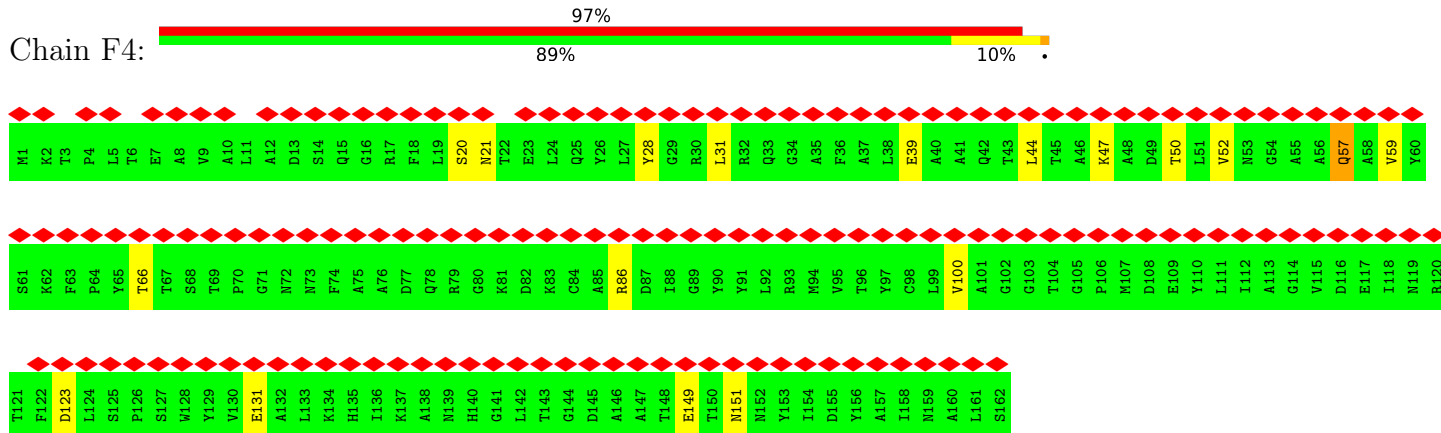
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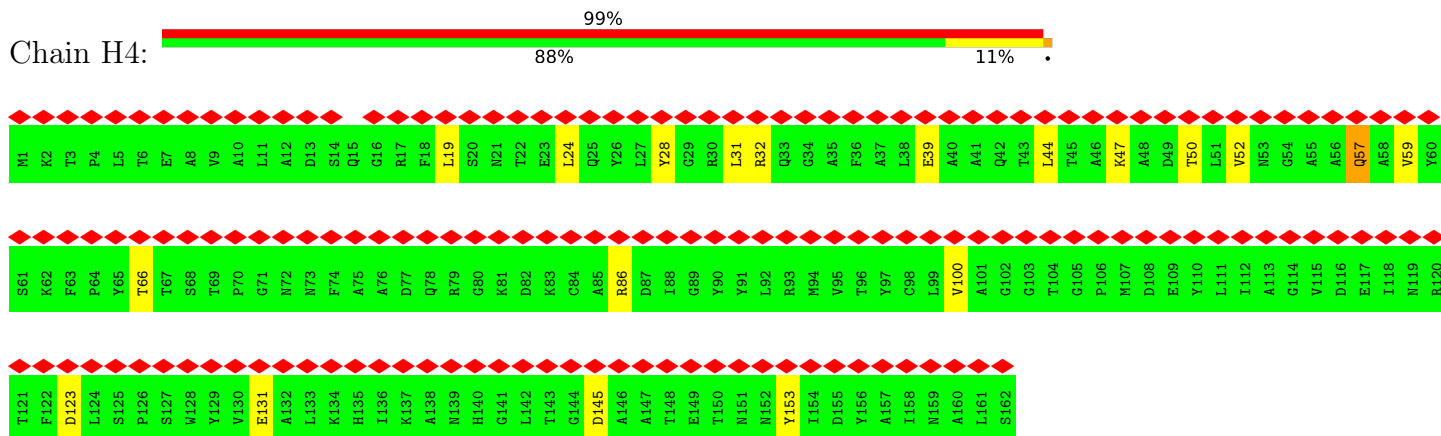
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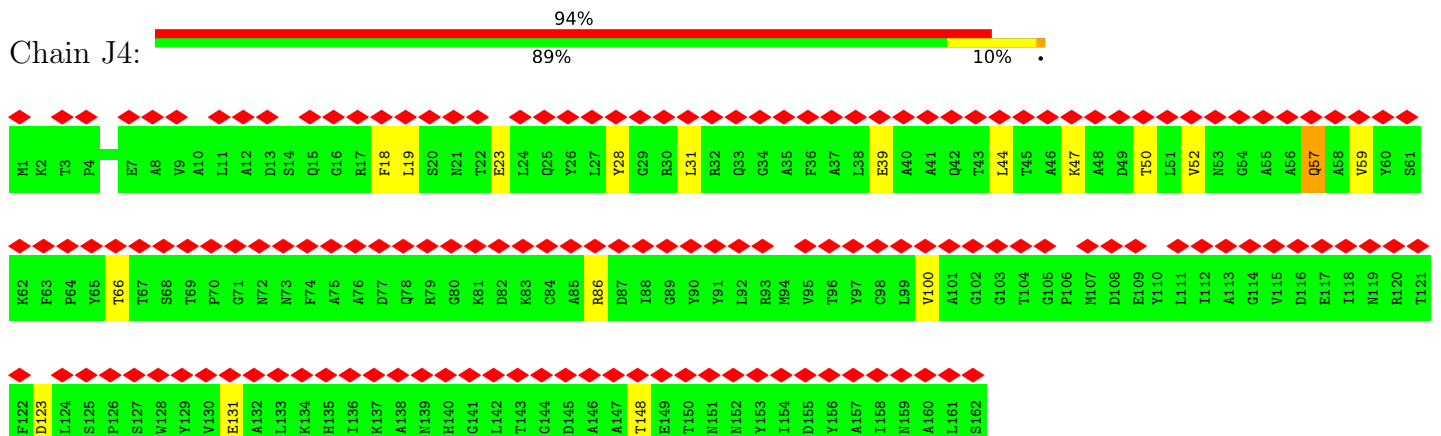
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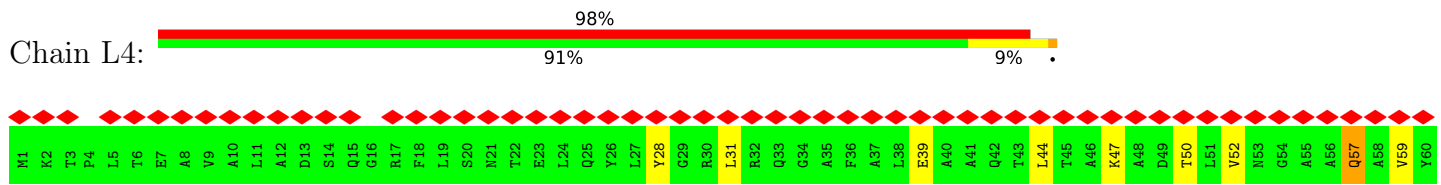
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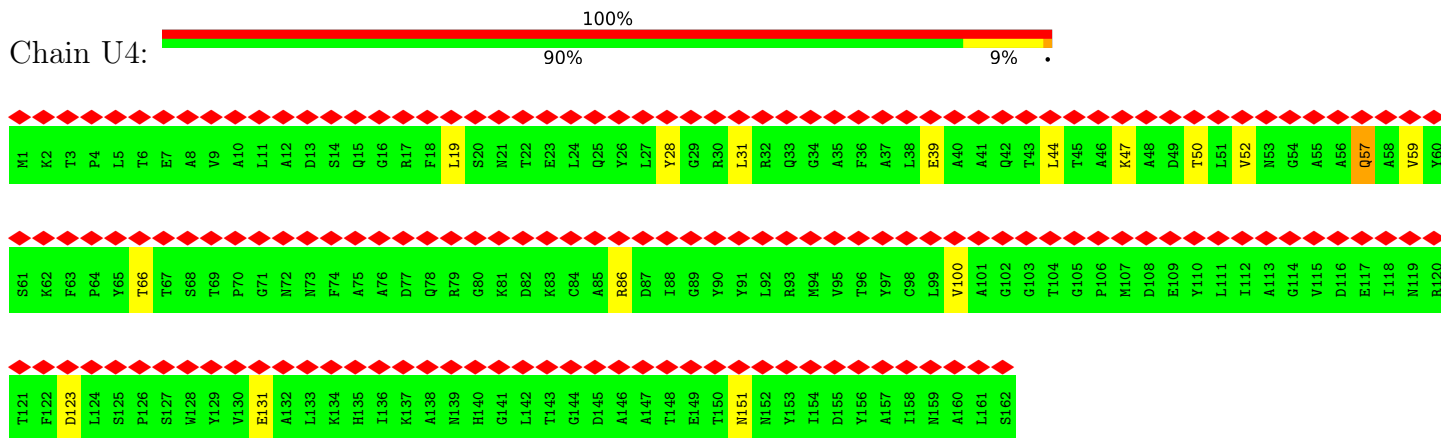
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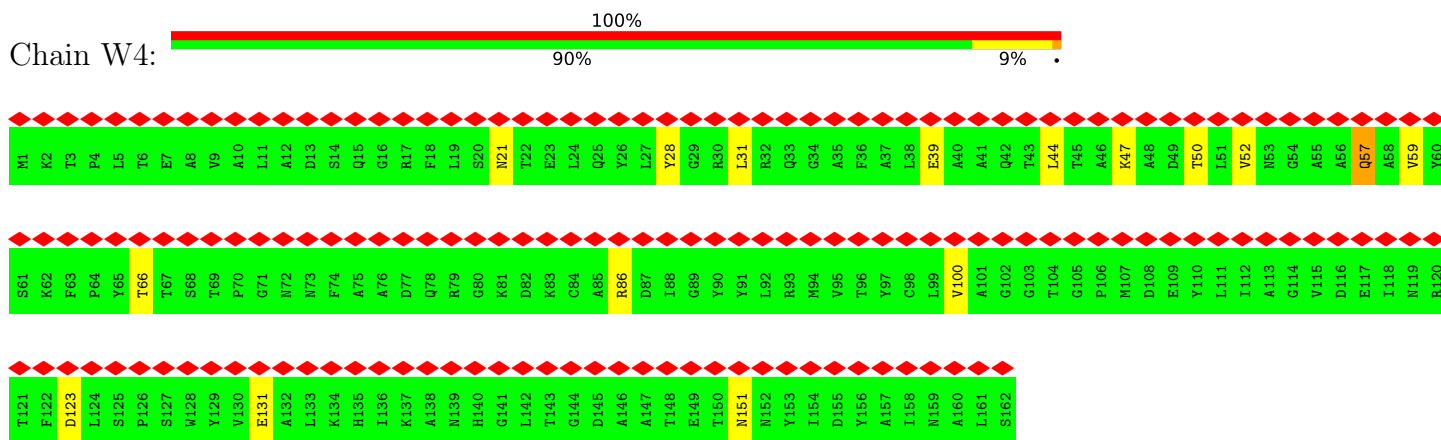
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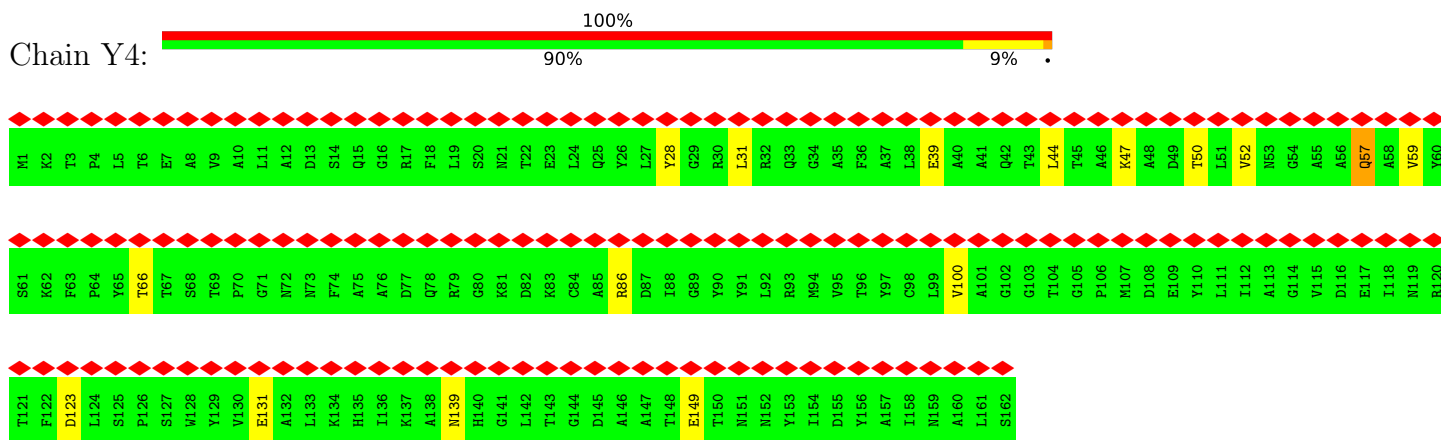
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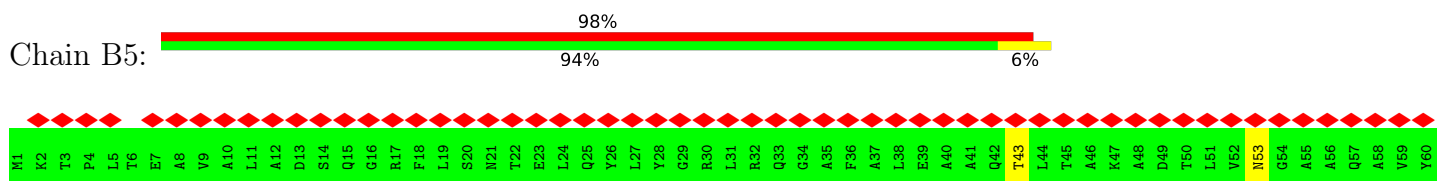
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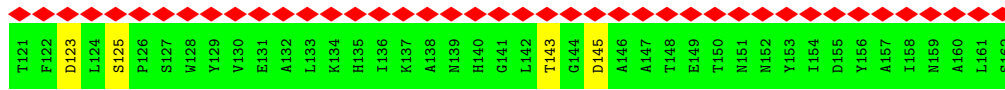
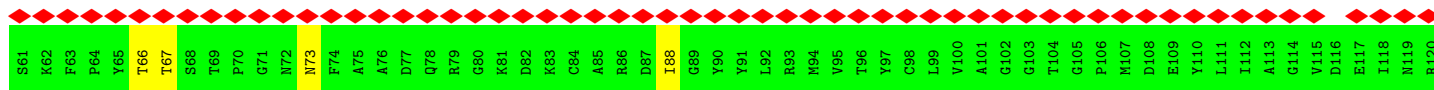


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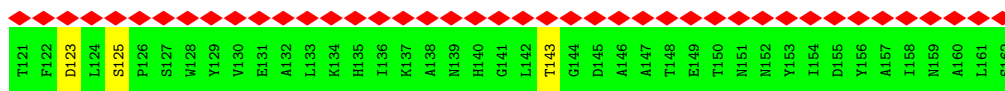
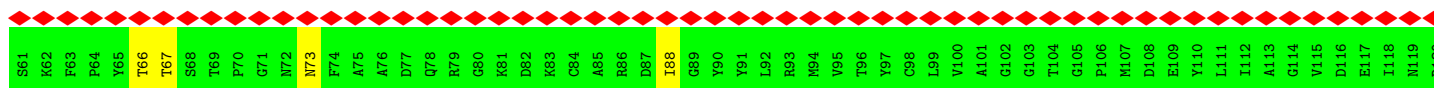
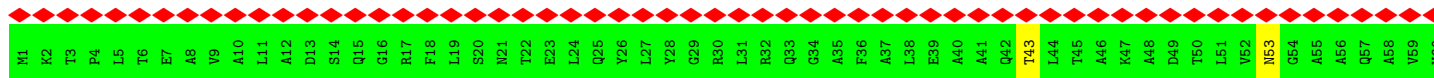


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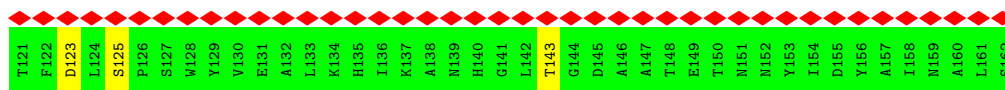
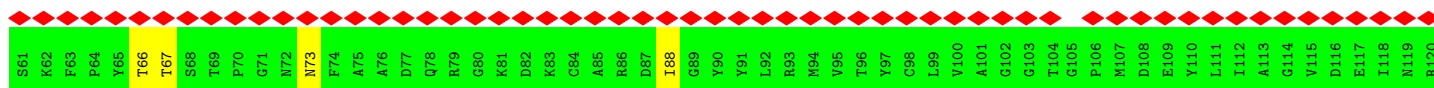
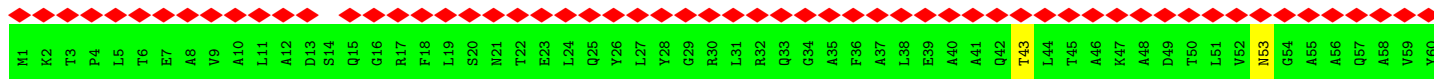




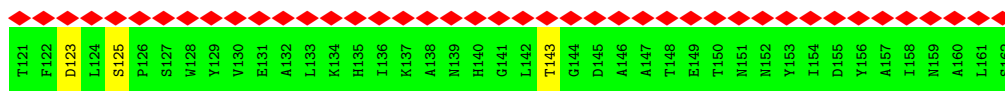
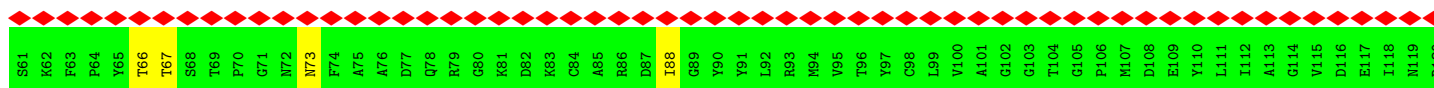
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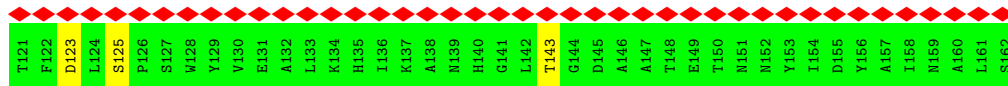
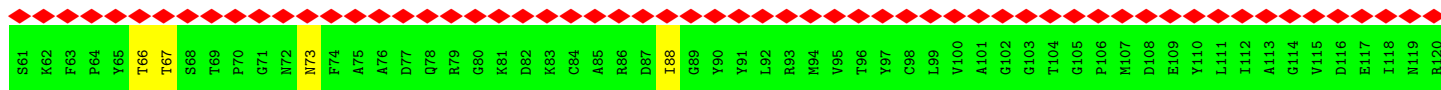


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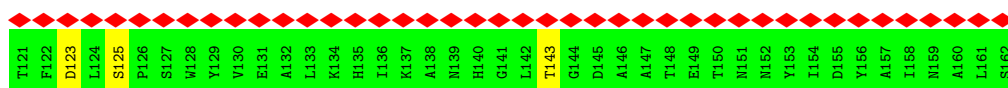
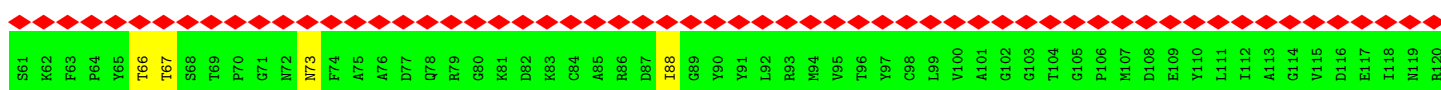
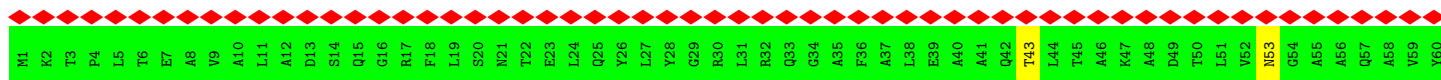


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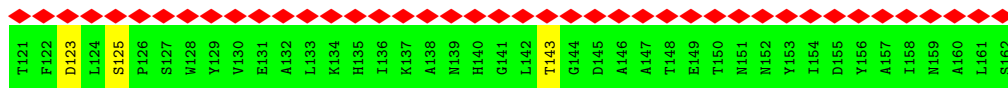
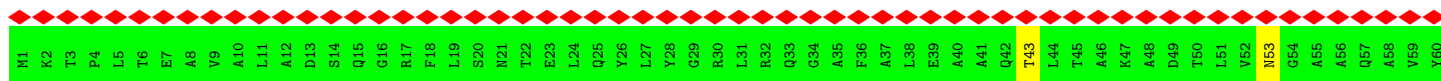




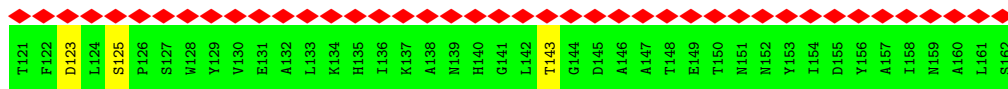
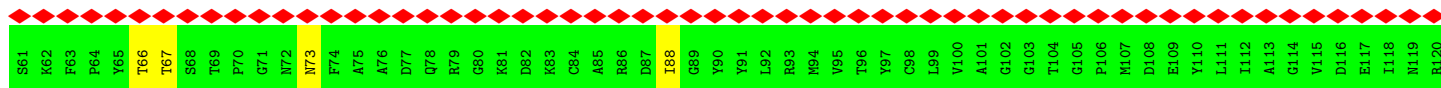
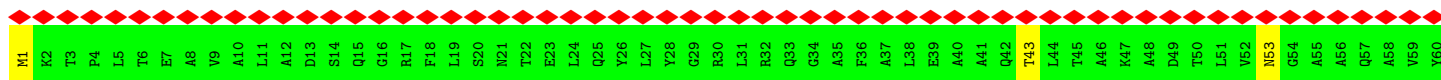
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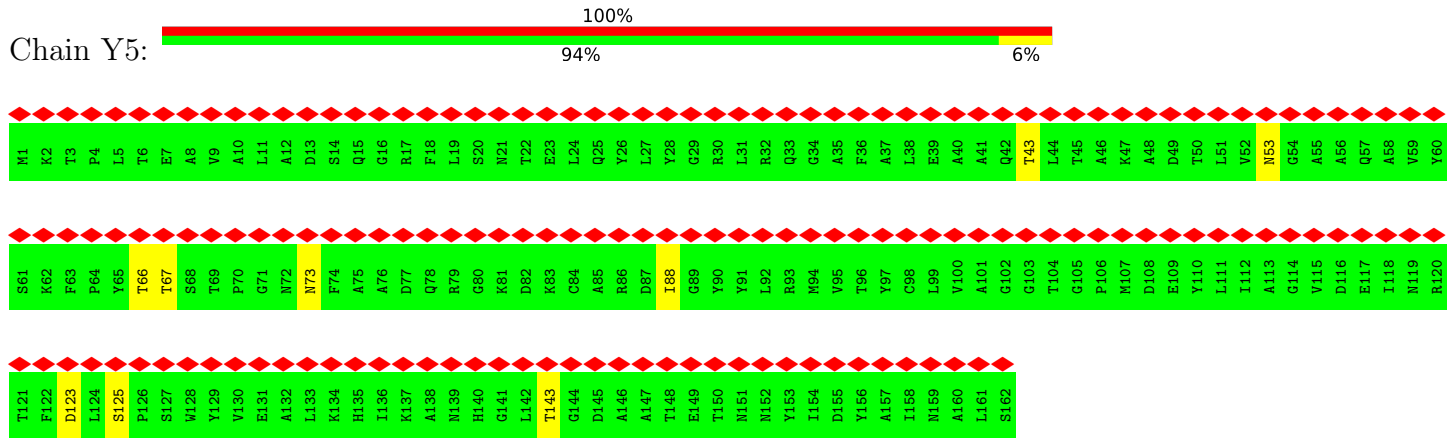
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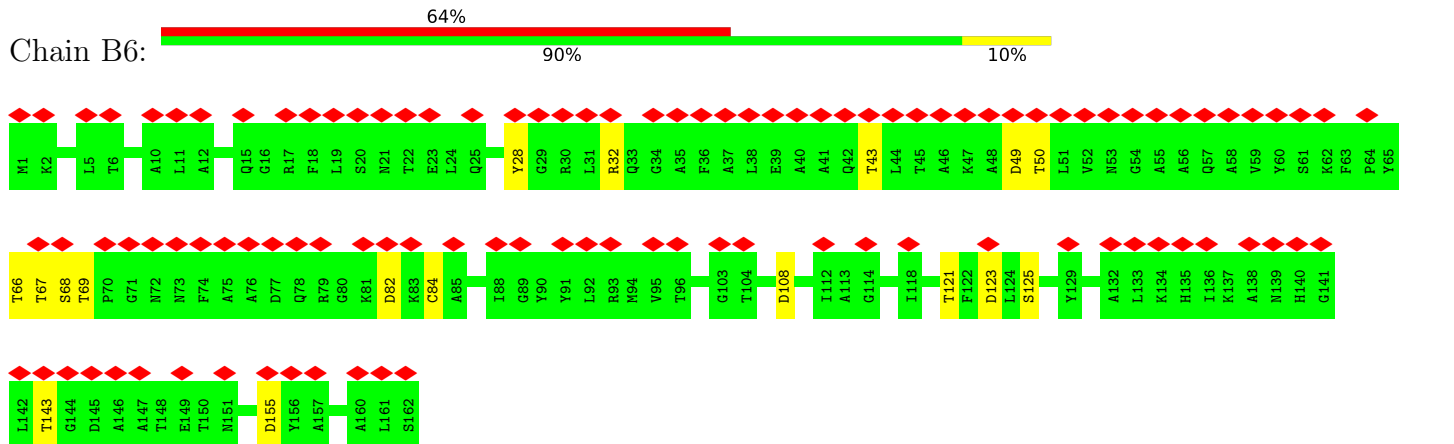
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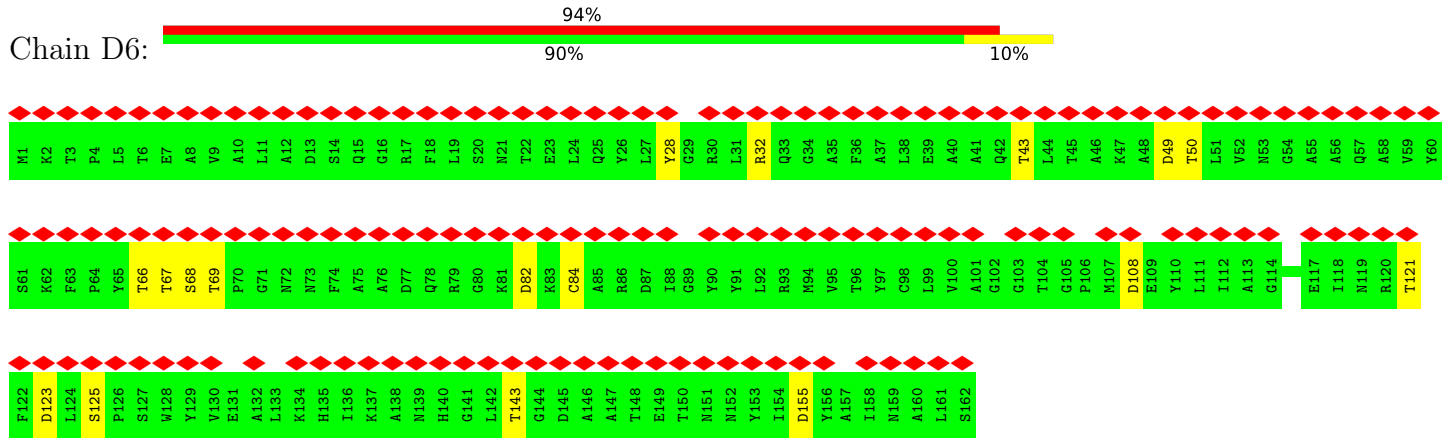
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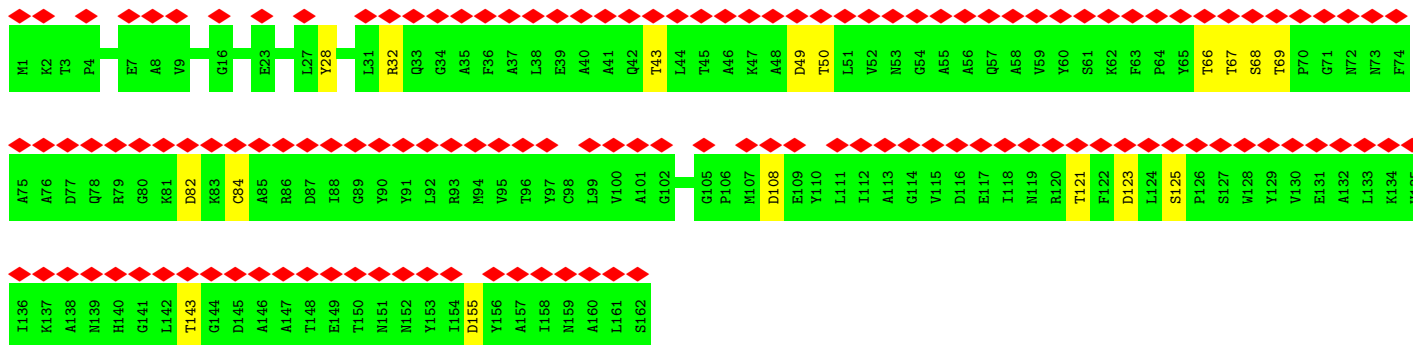


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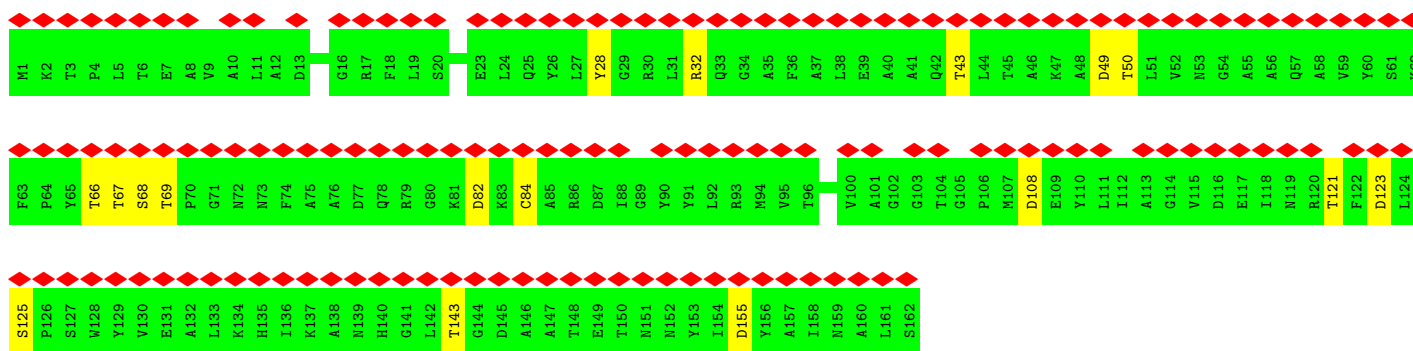
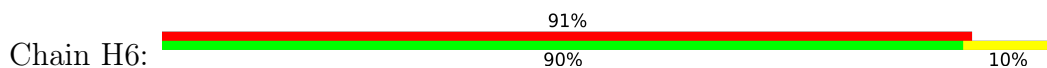


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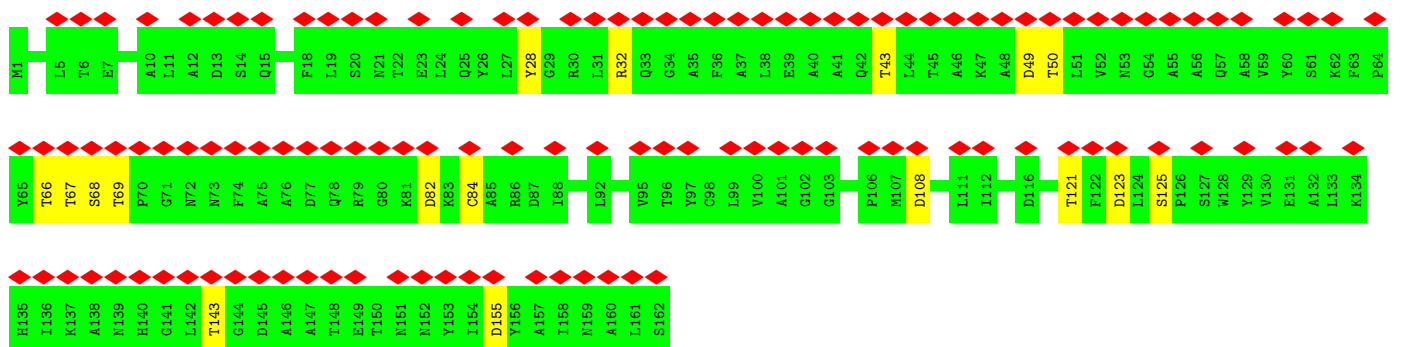
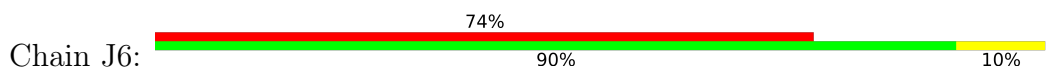




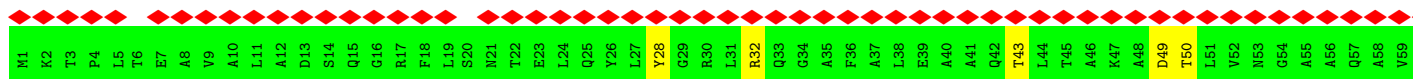
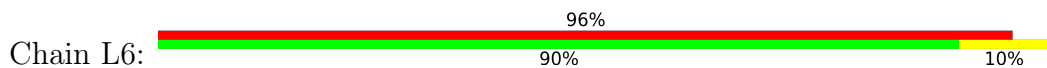
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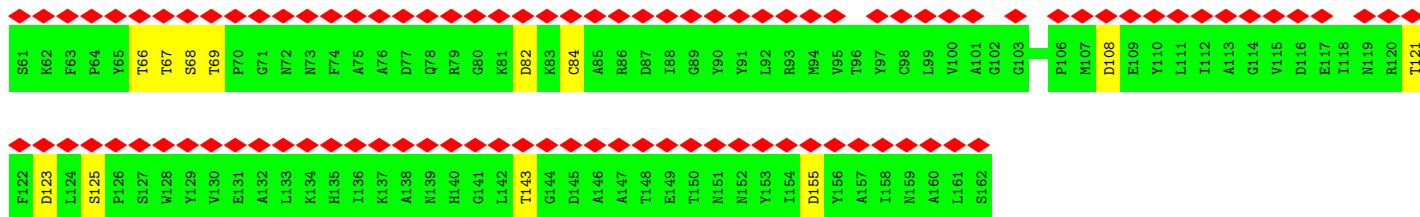


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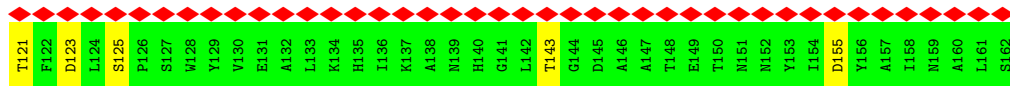
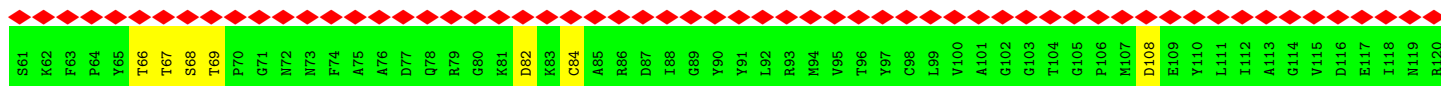
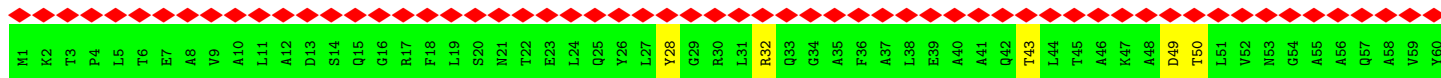
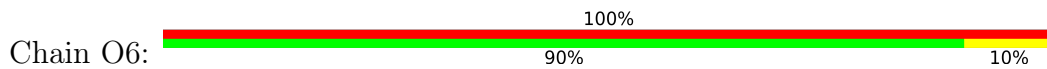


• Molecule 2: C-phycoerythrin subunit alpha

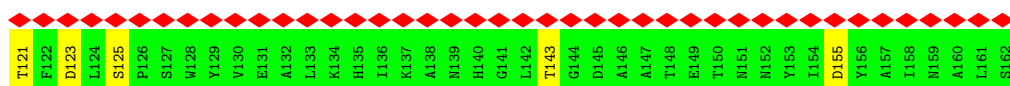
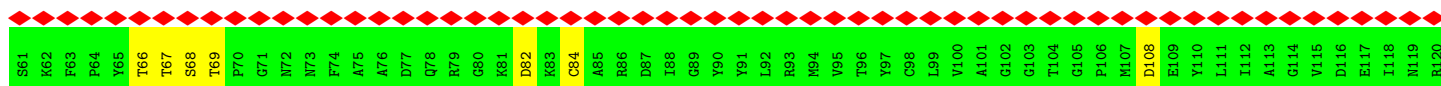
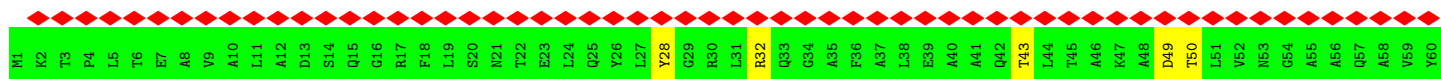
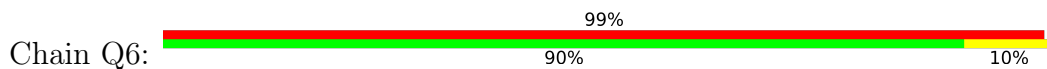




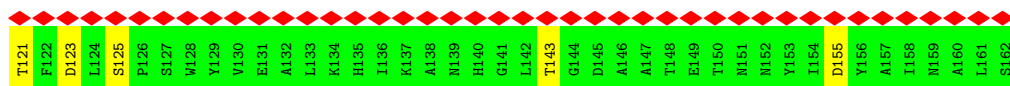
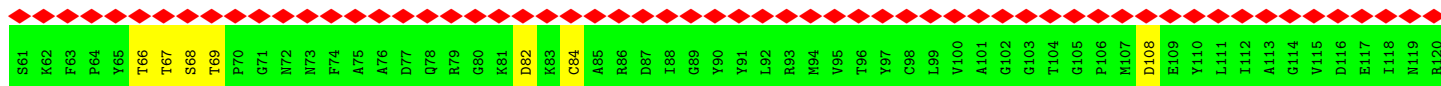
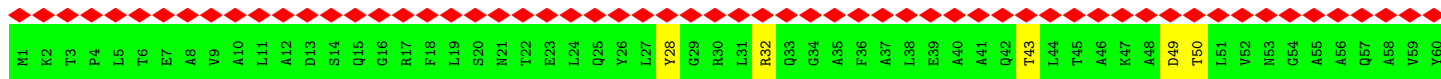
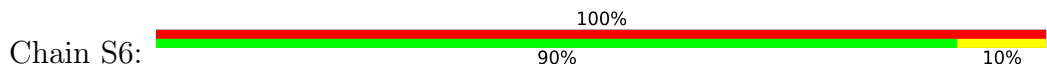
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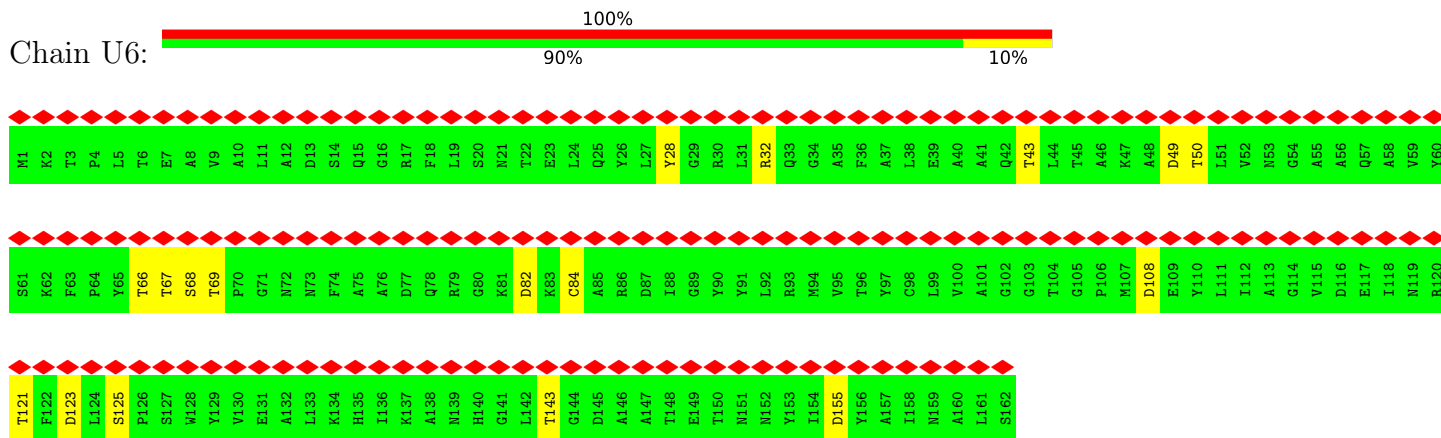
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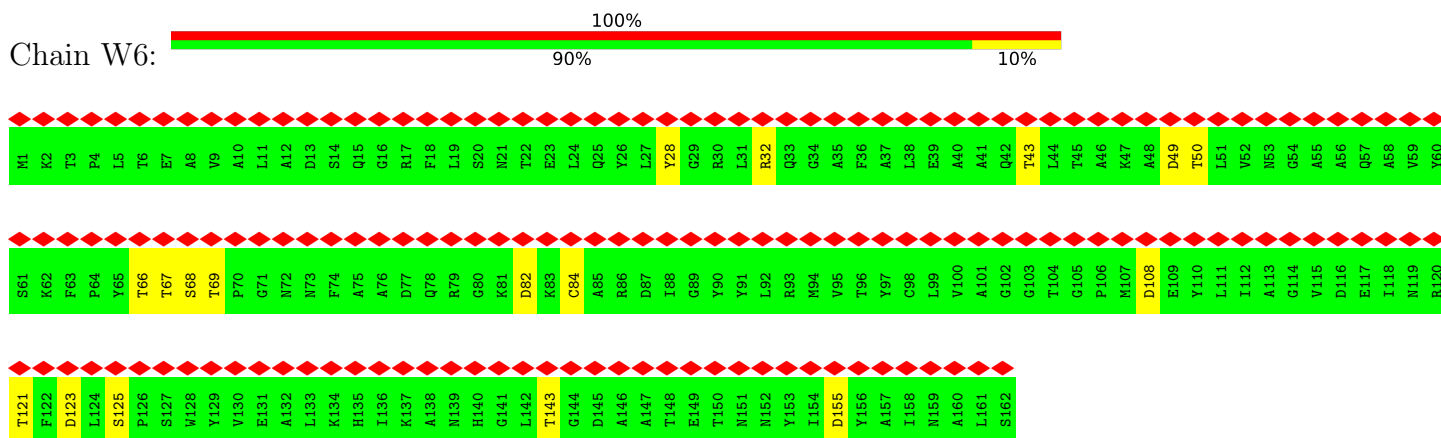
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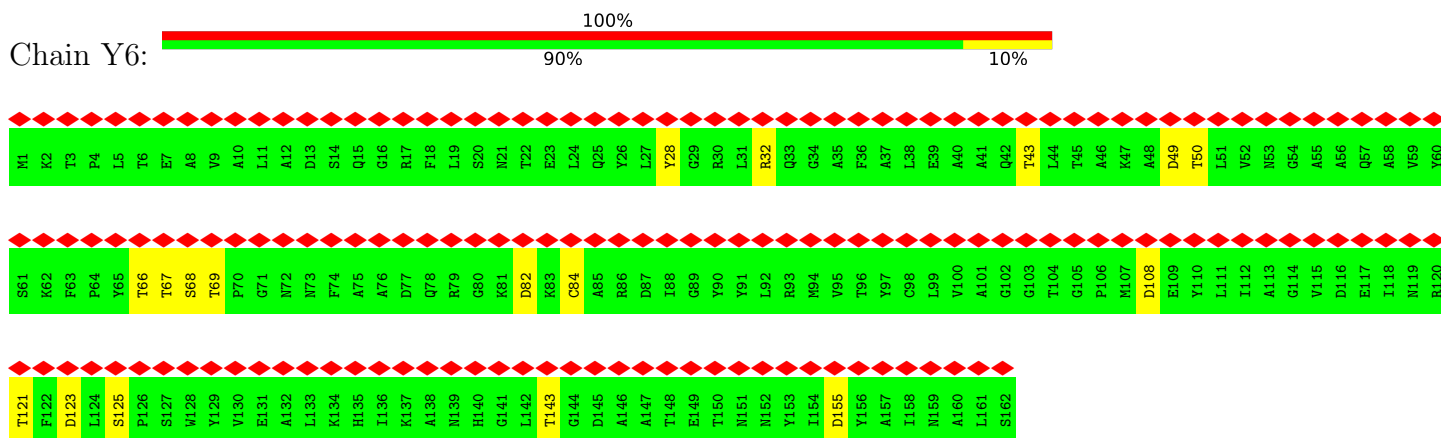
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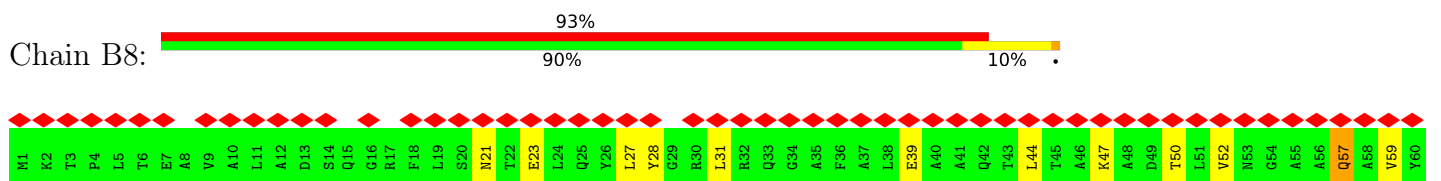
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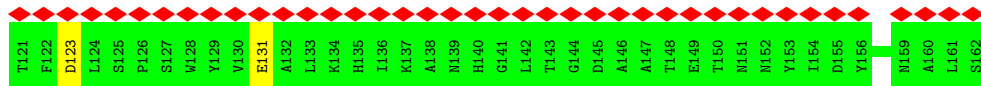
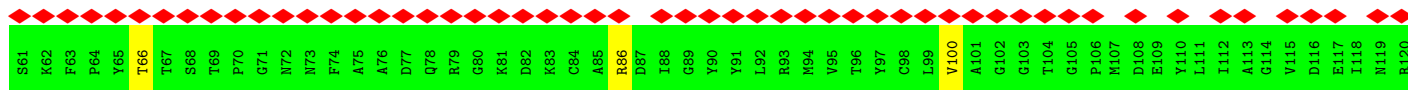


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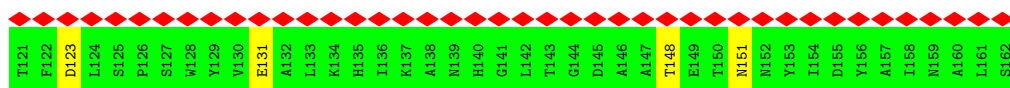
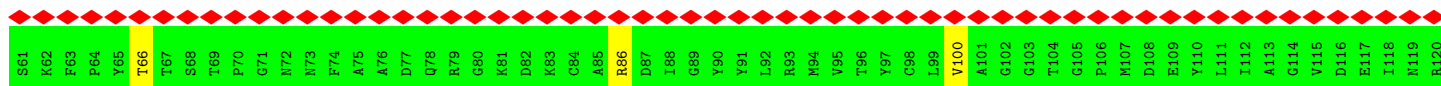
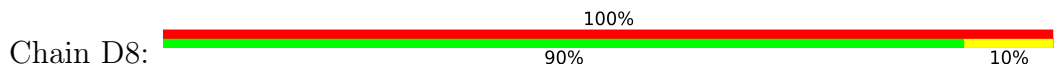


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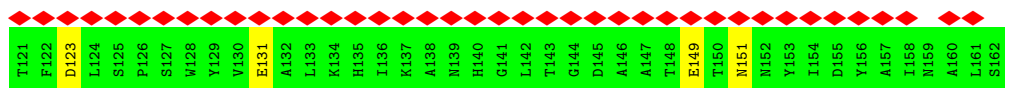
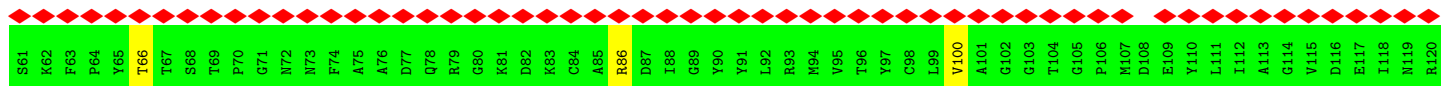
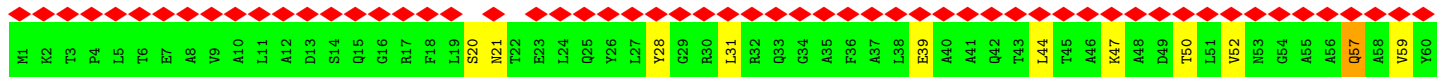
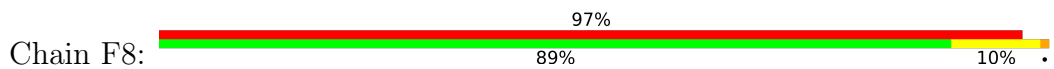




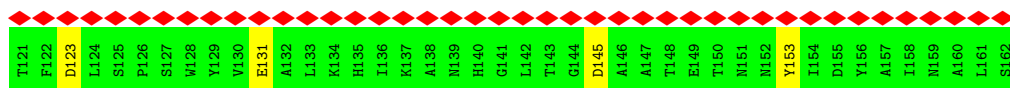
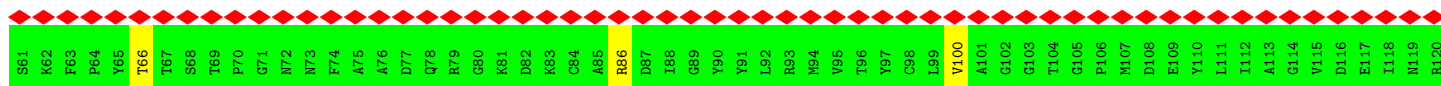
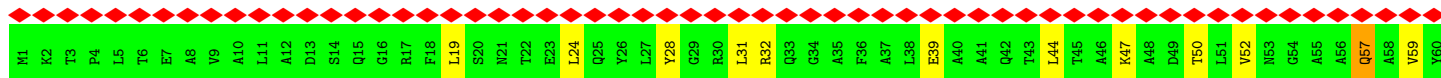
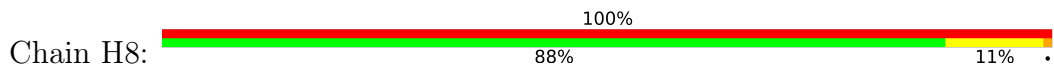
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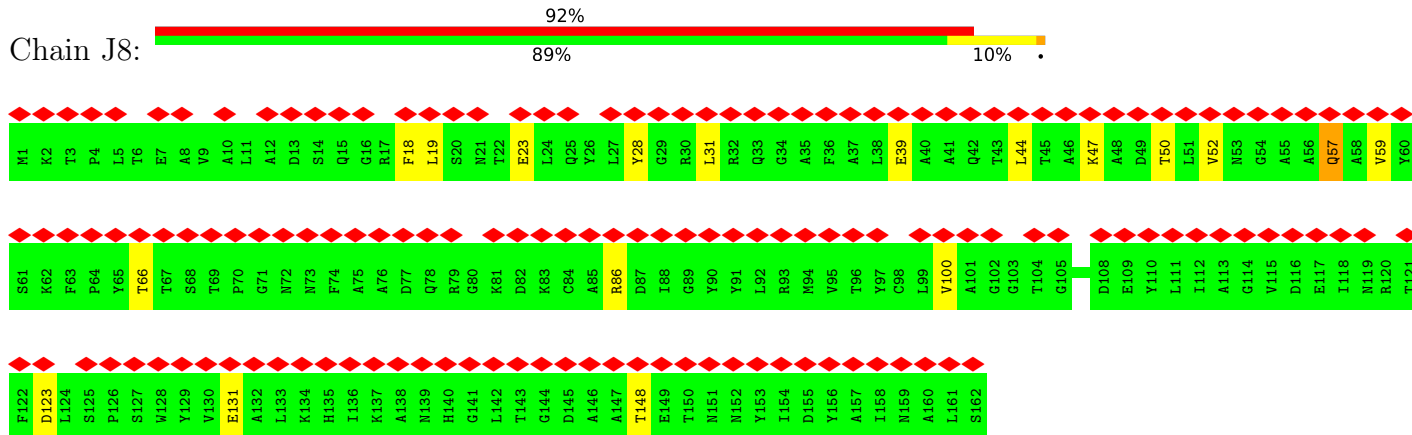
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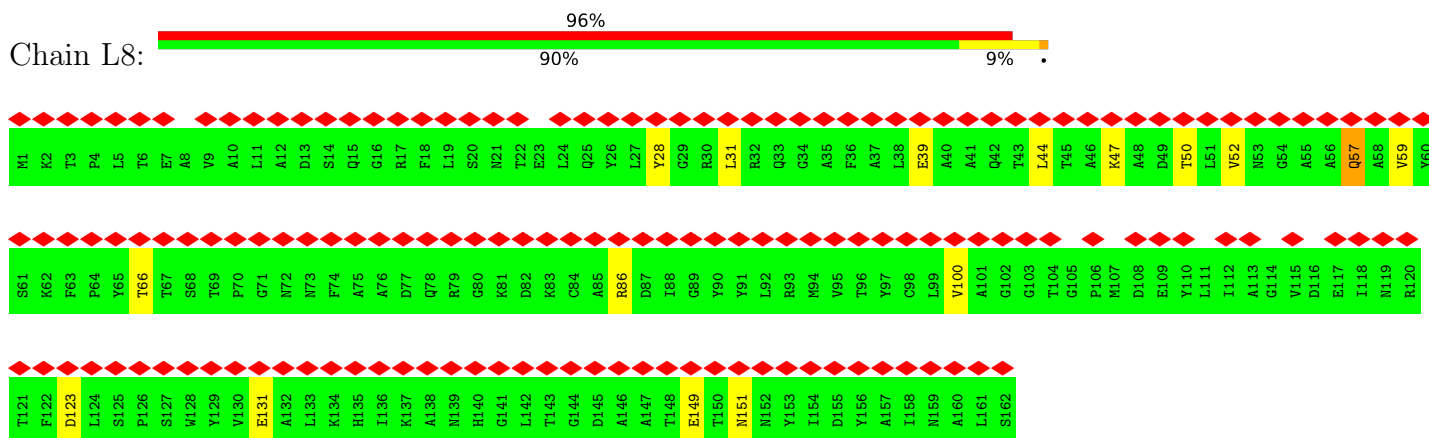
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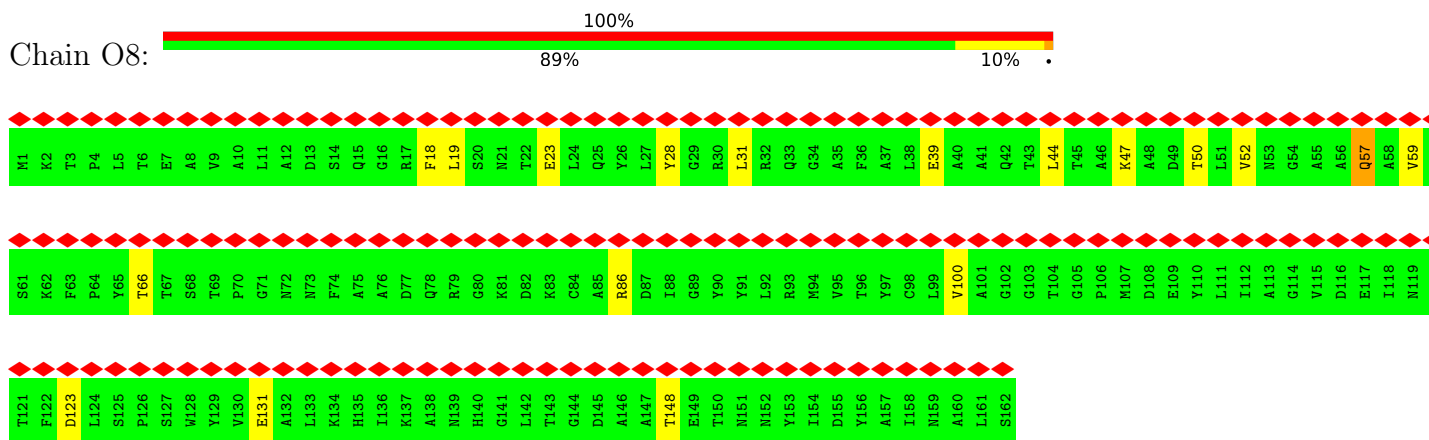
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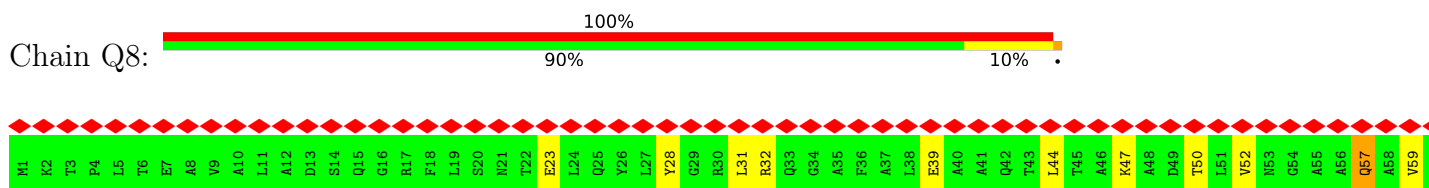
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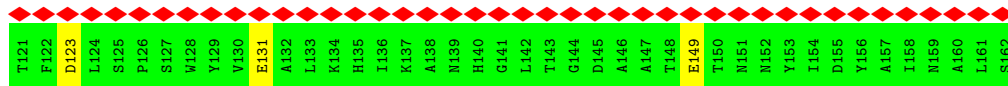
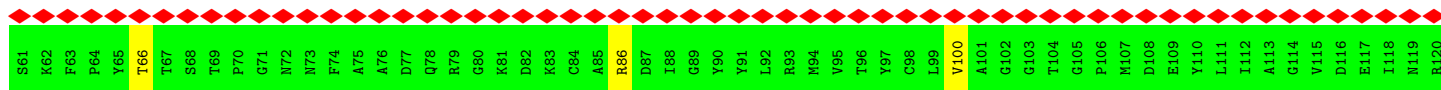


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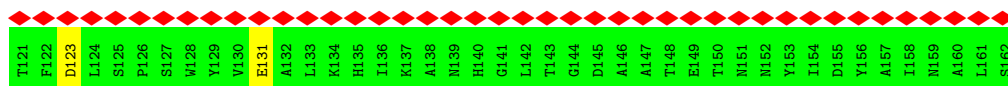
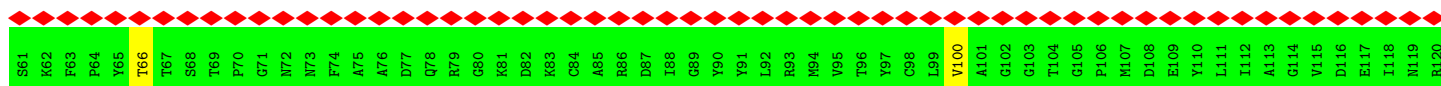
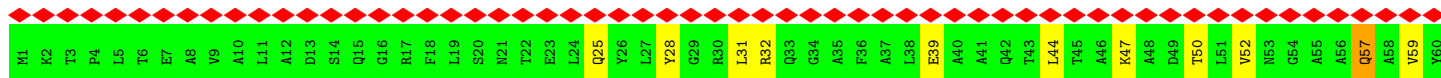
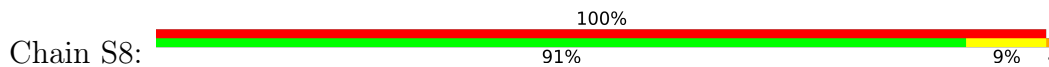


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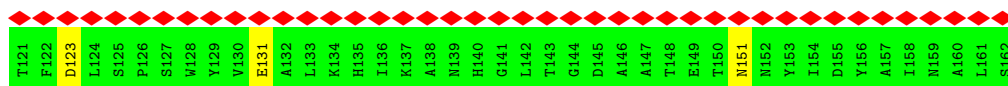
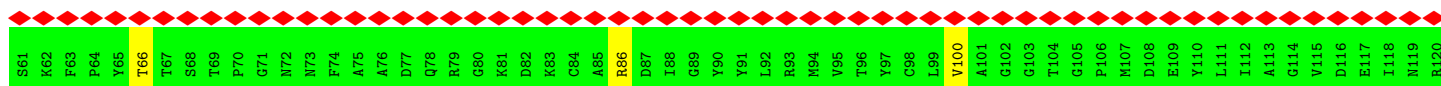
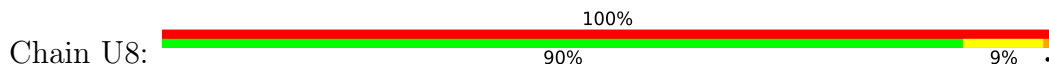




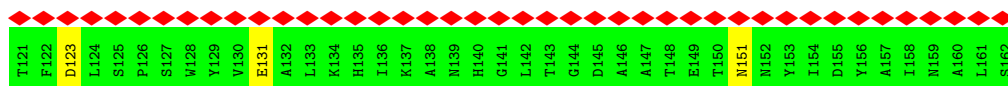
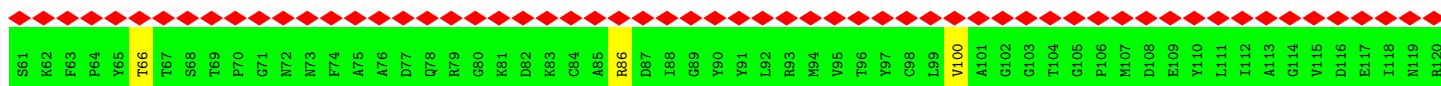
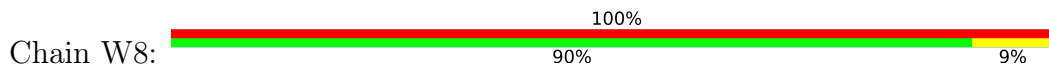
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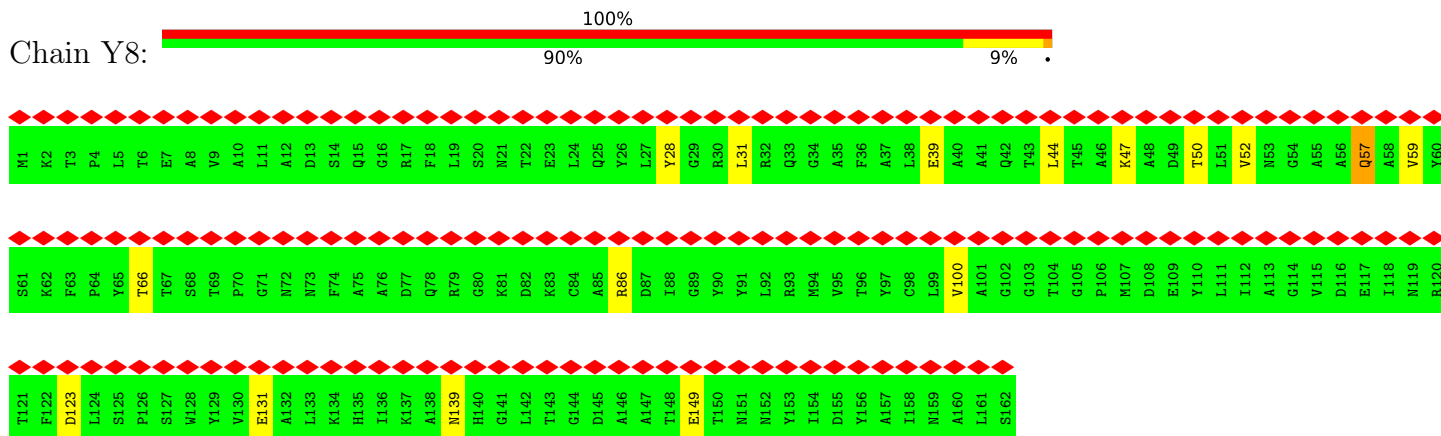
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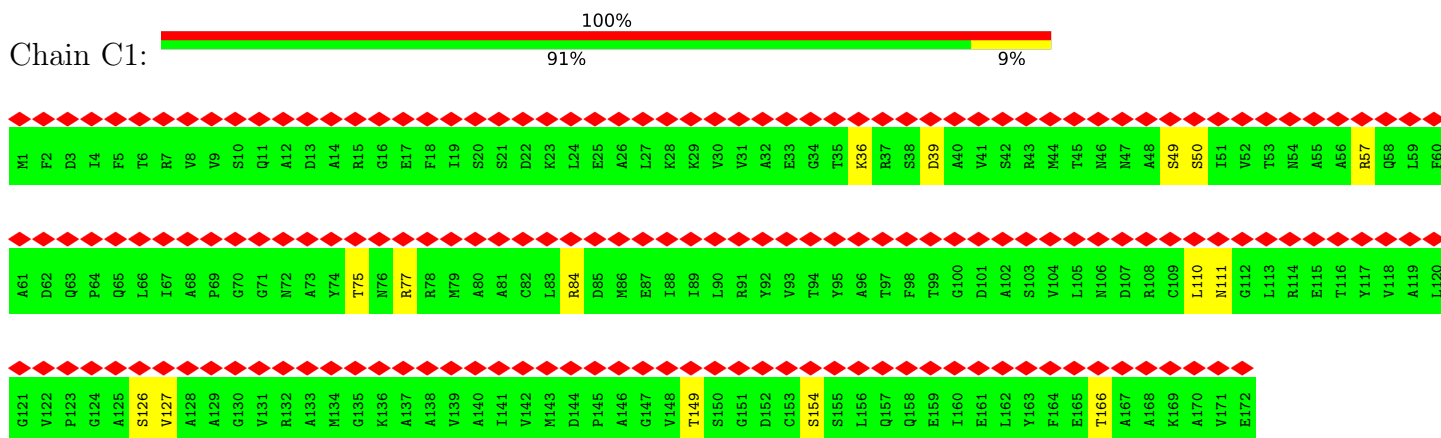
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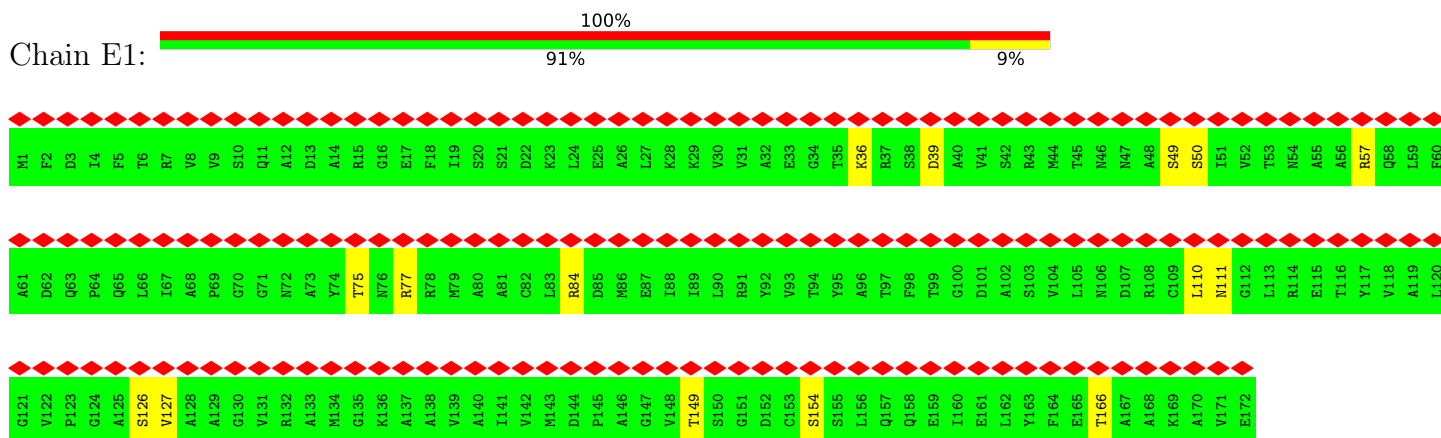
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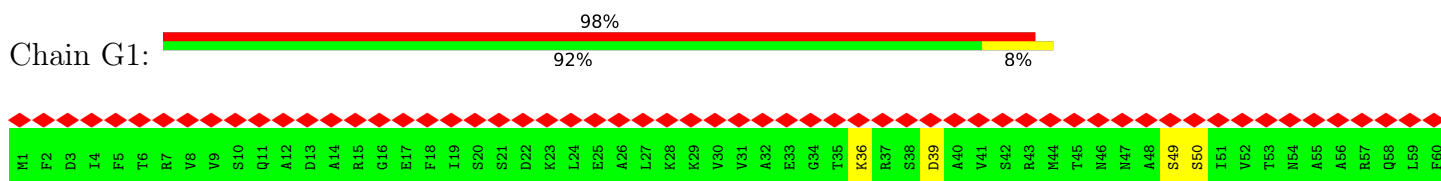
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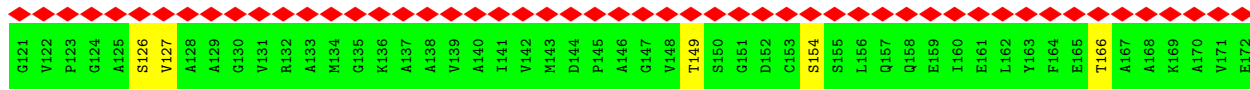
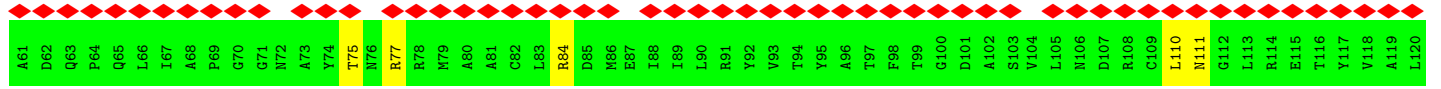


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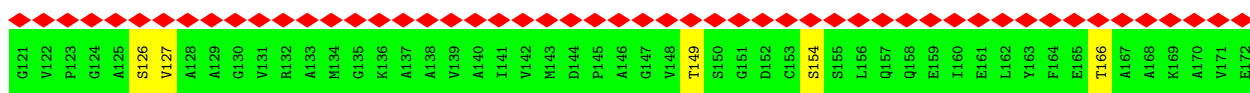
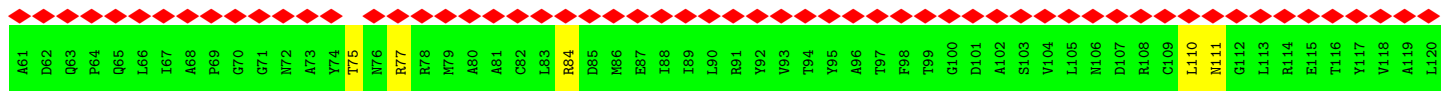
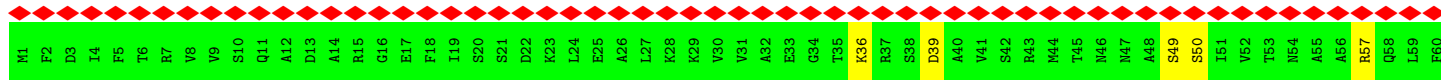
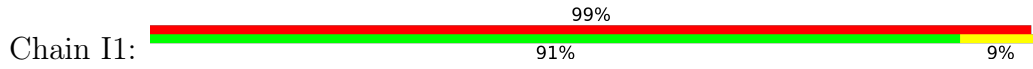


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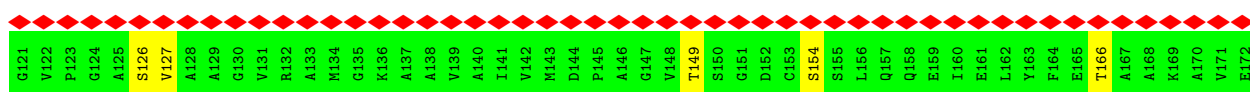
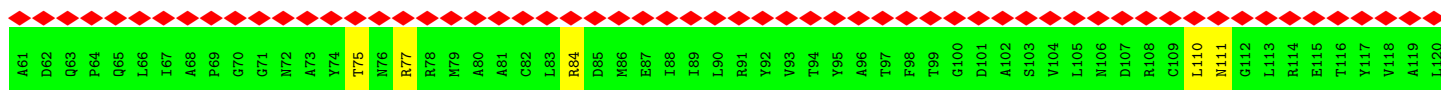
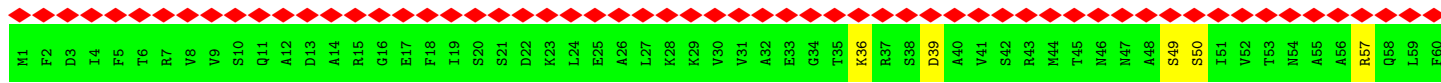




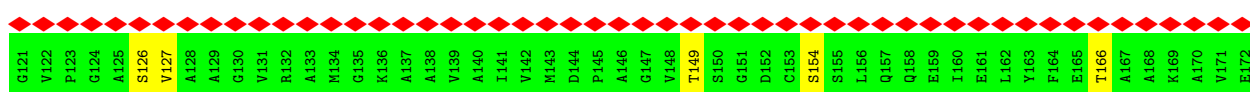
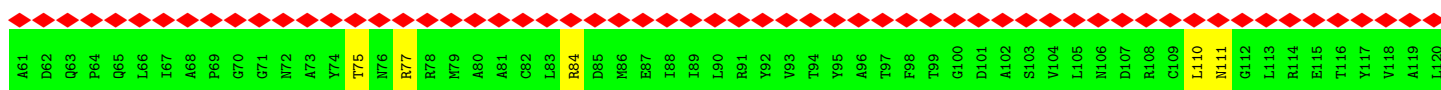
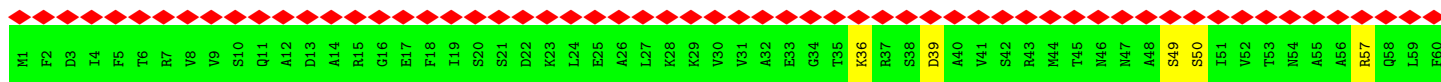
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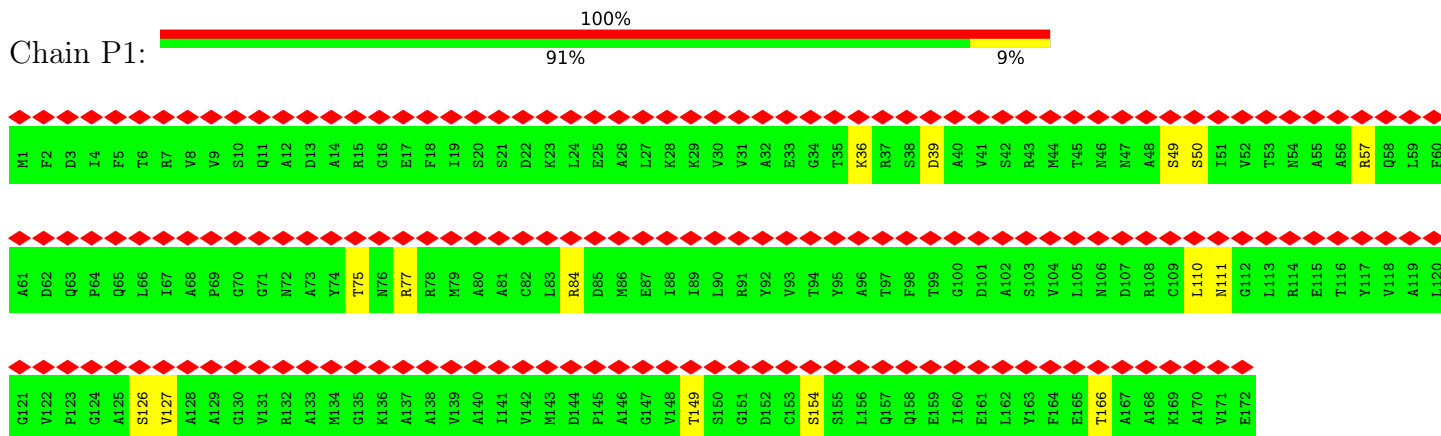
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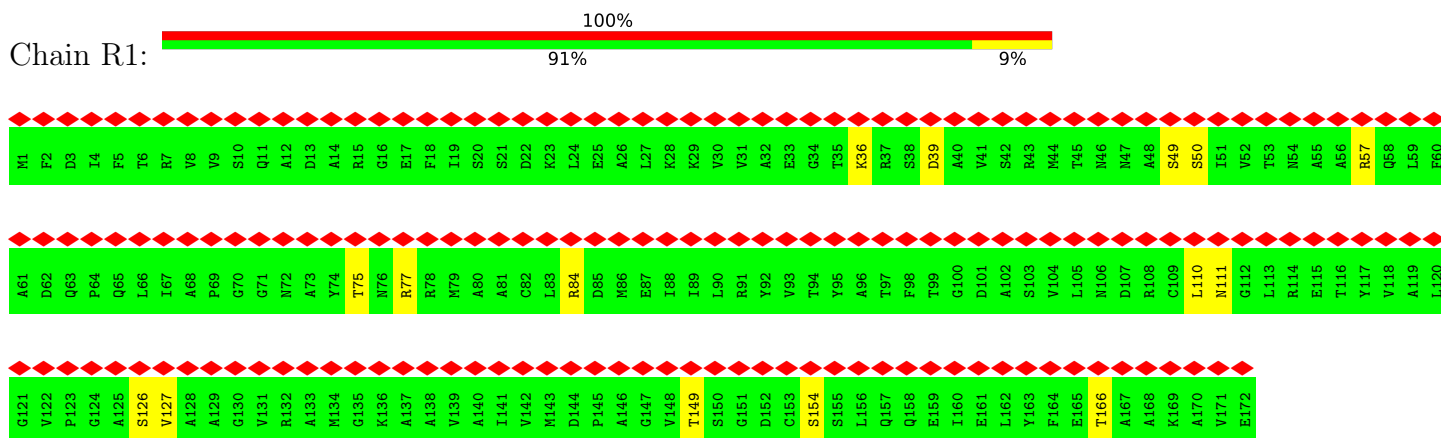
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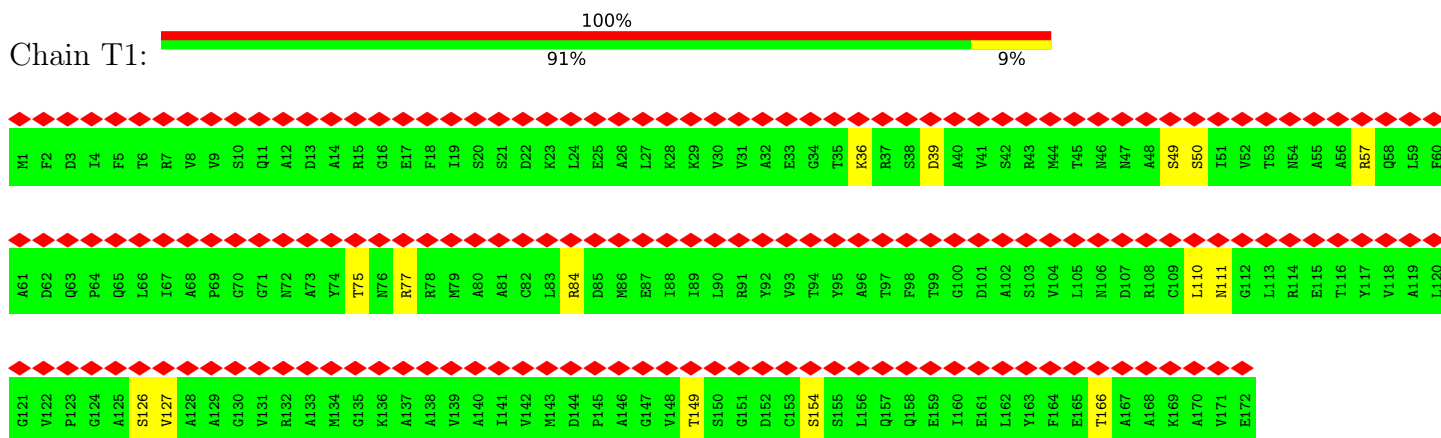
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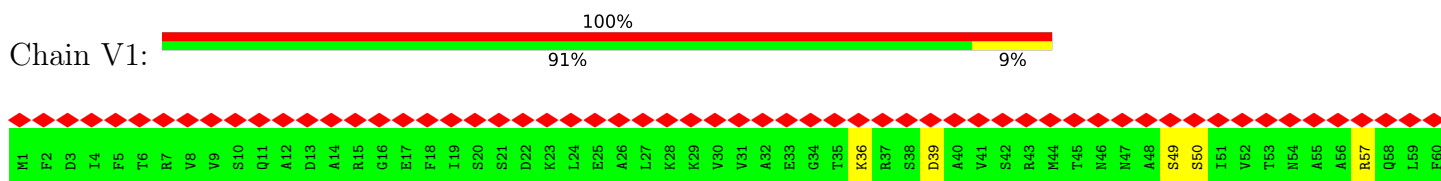
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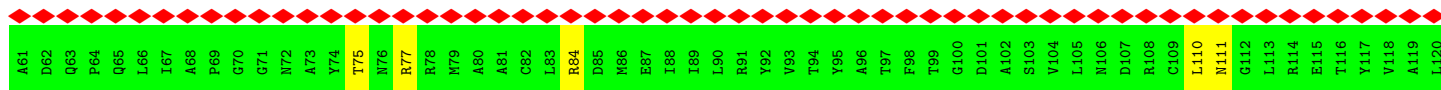


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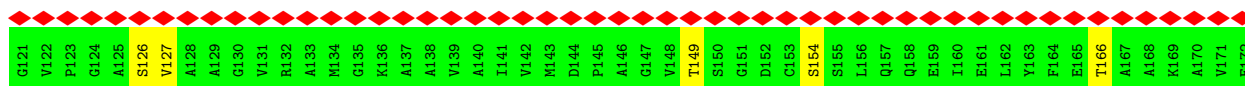
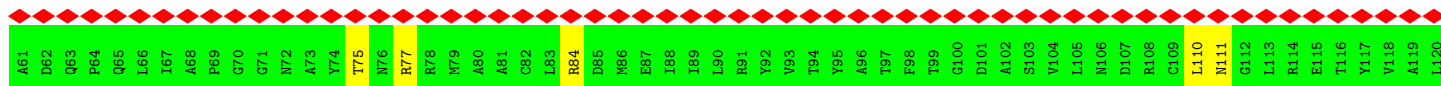
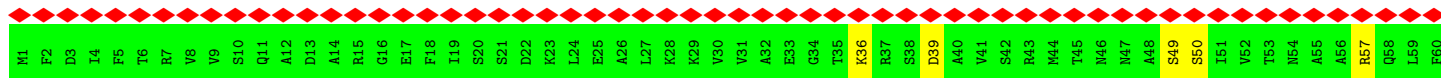
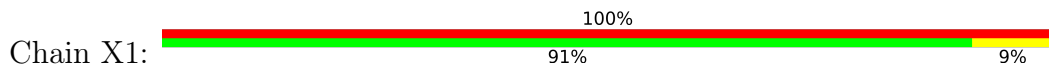


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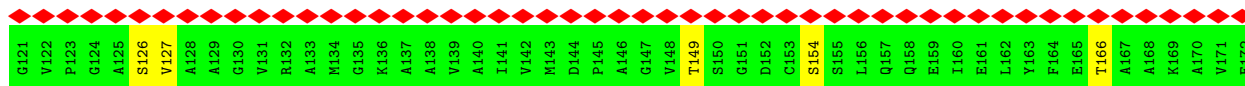
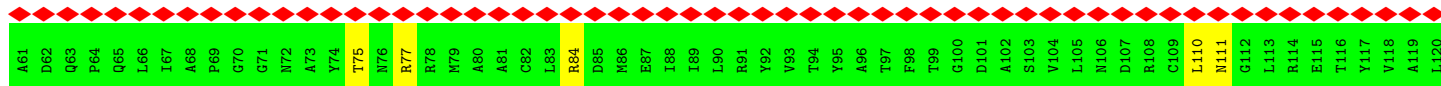
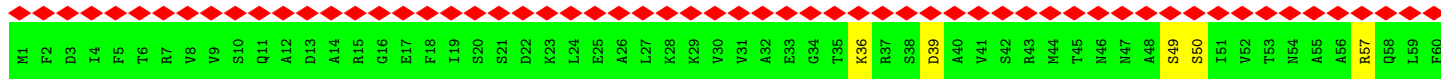
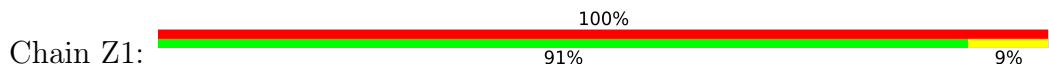




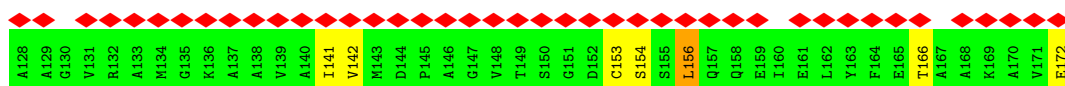
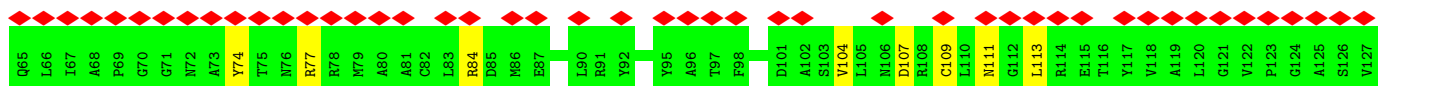
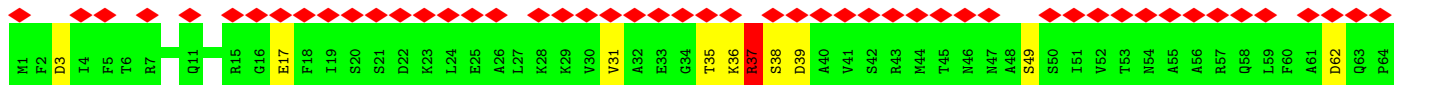
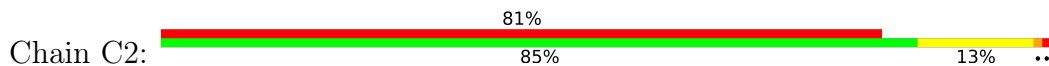
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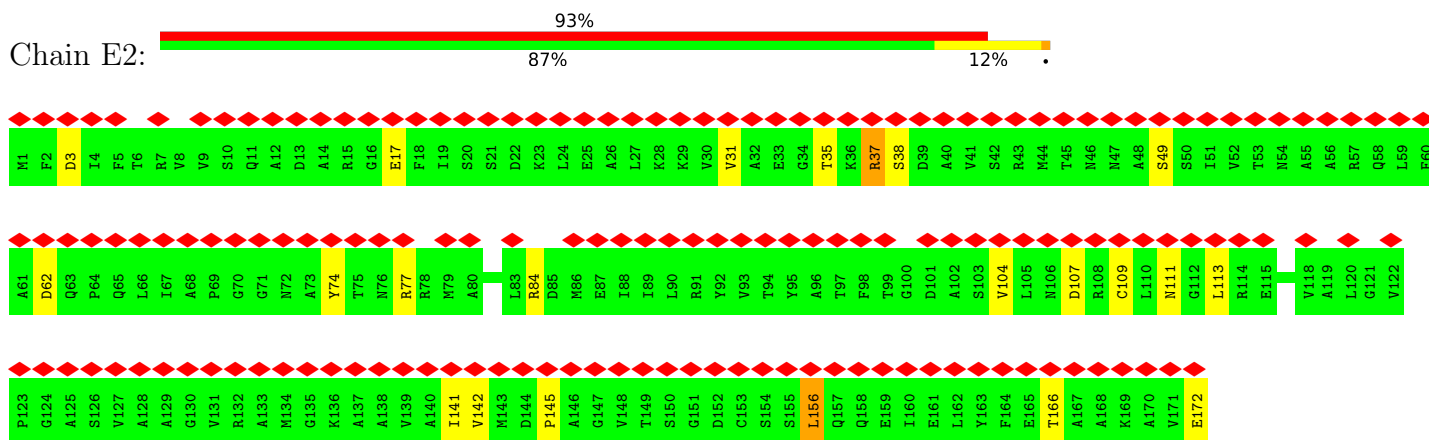
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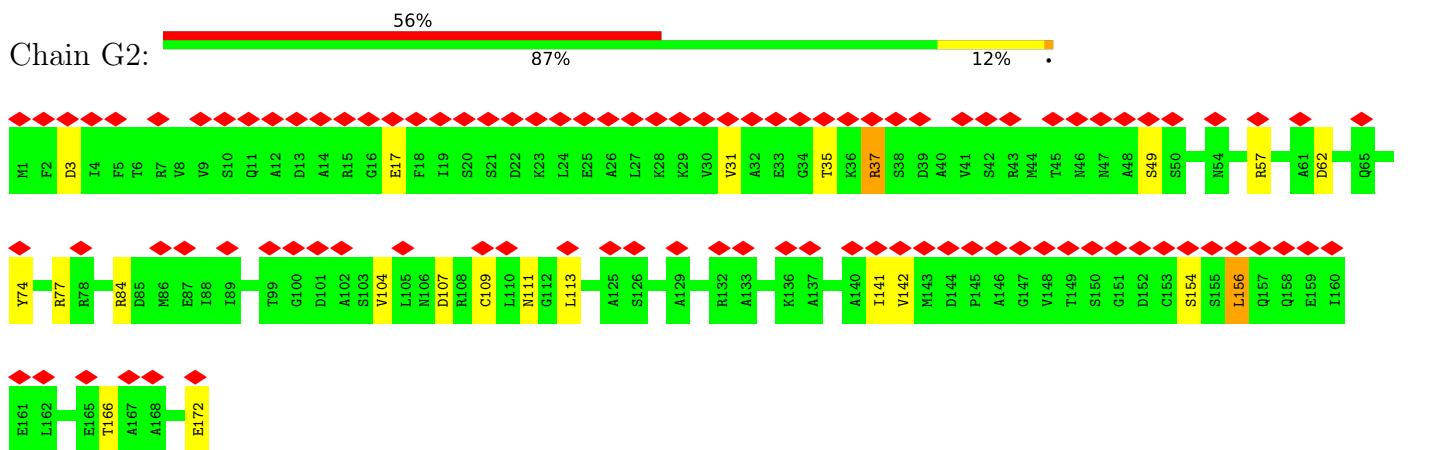
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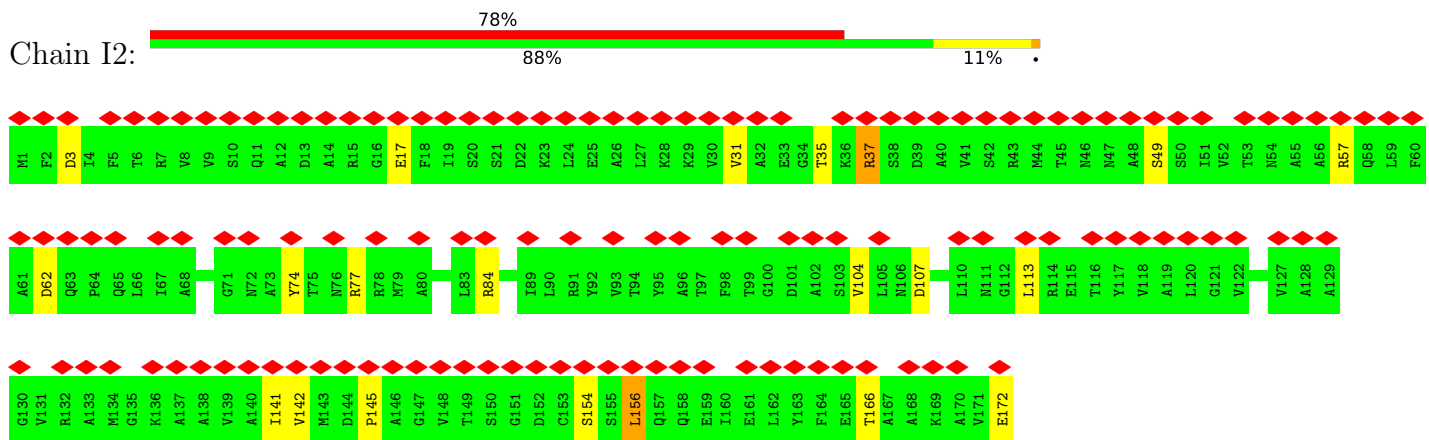
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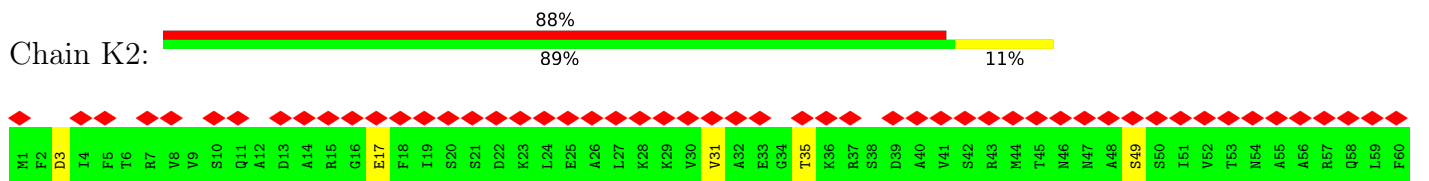
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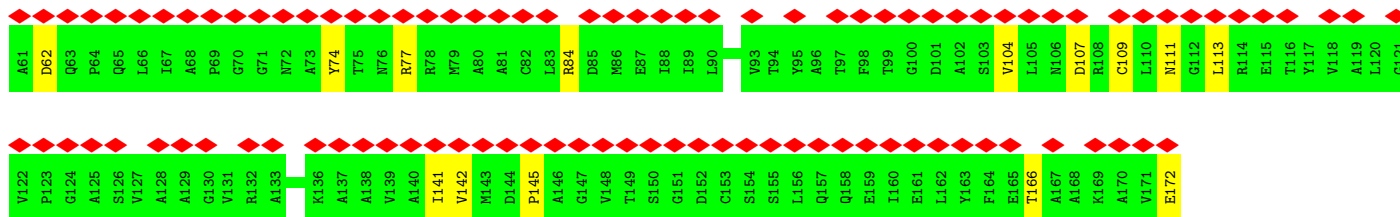


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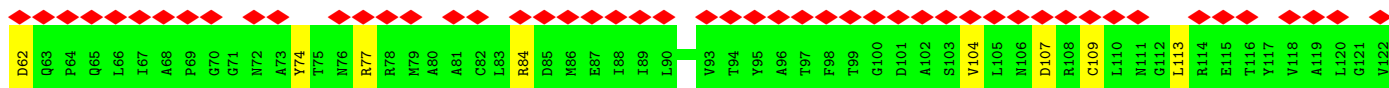
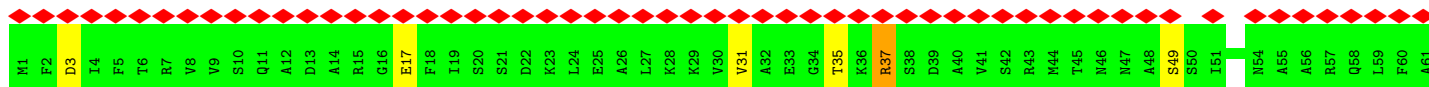
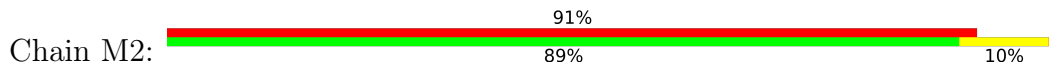


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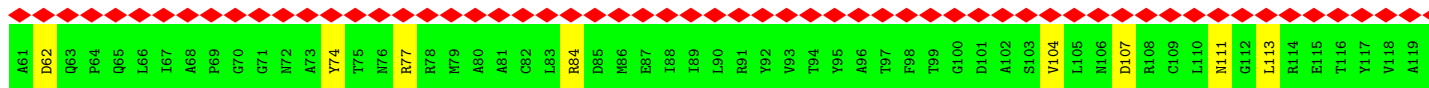
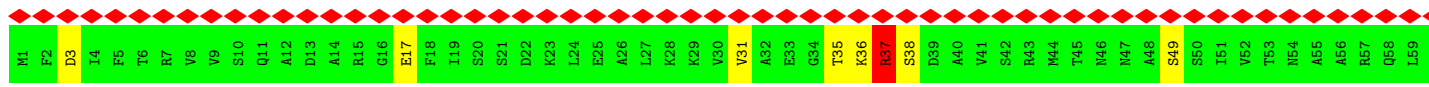
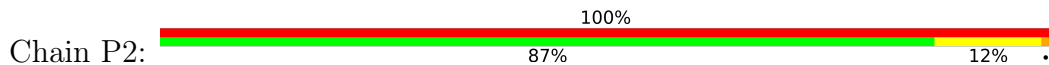




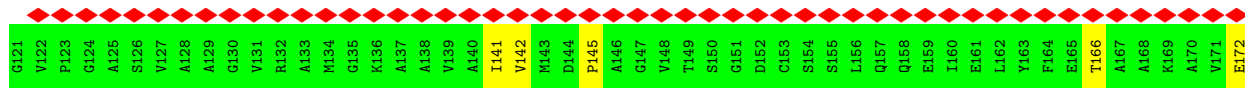
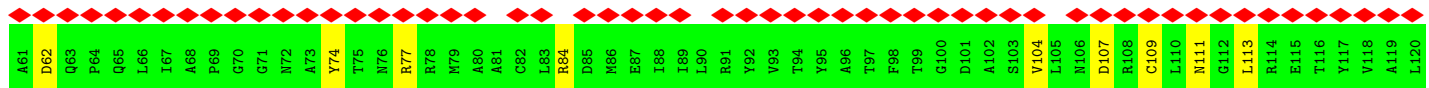
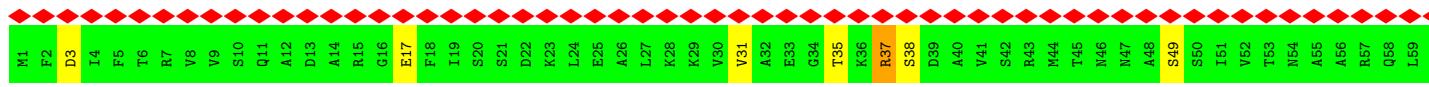
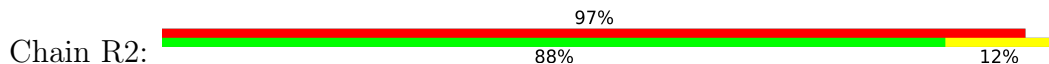
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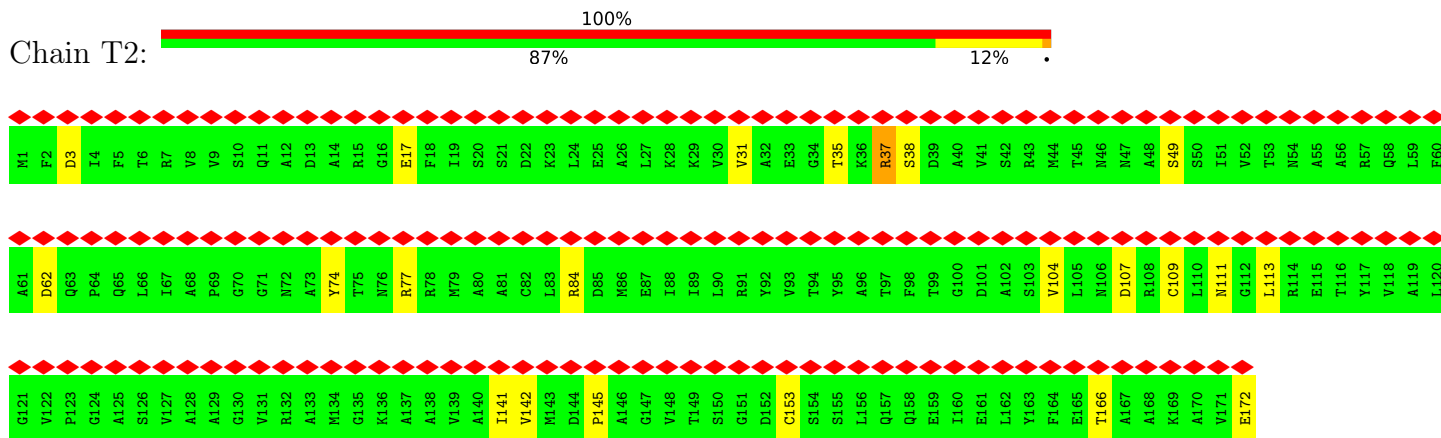
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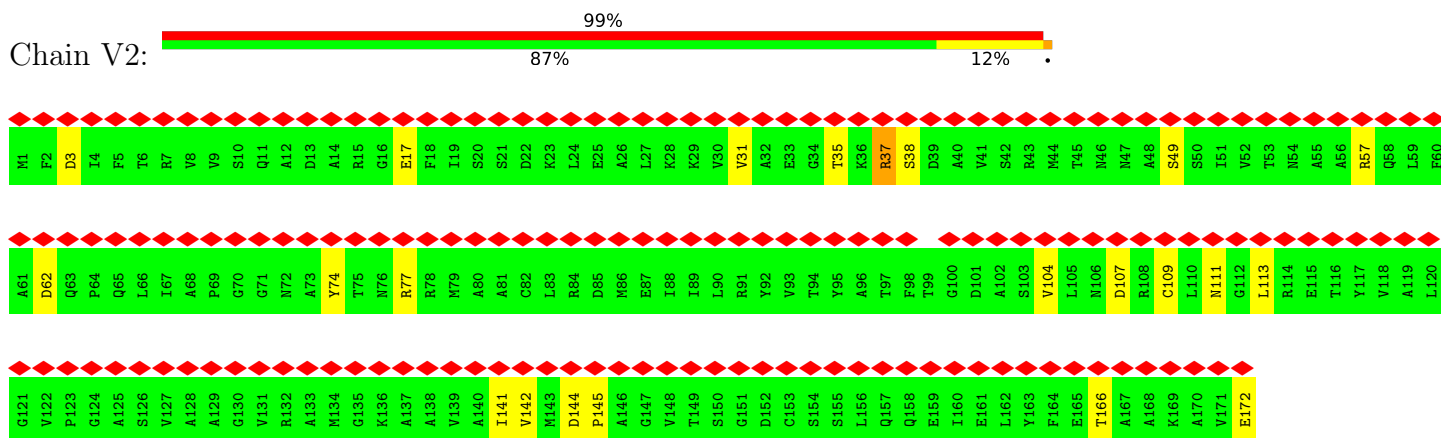
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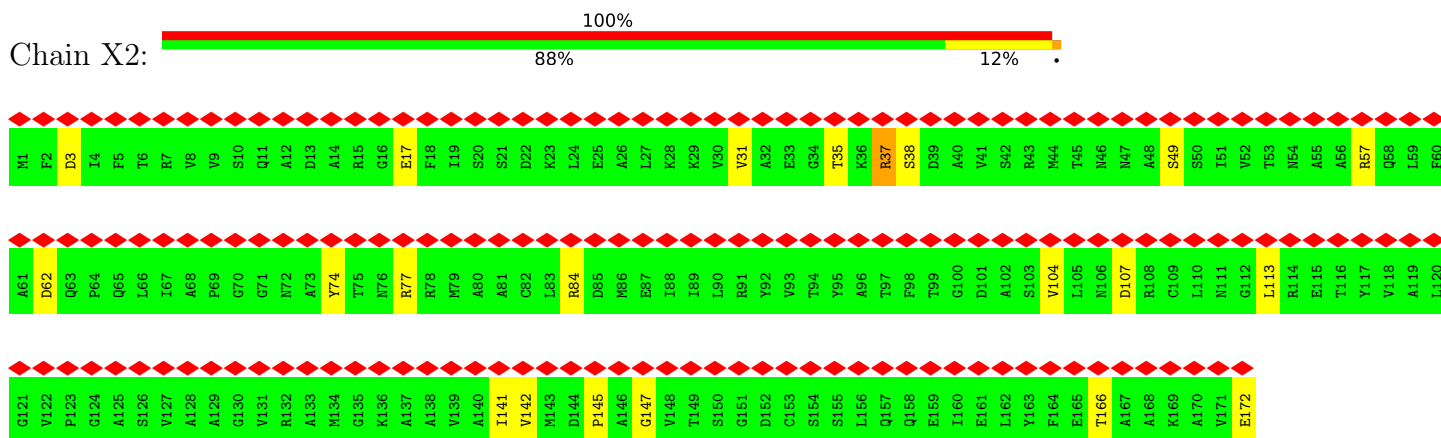
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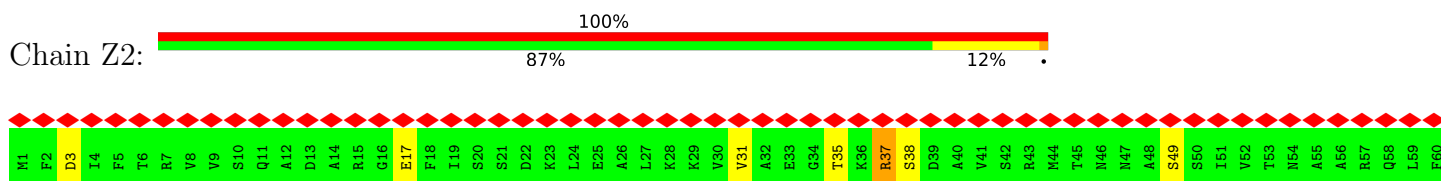
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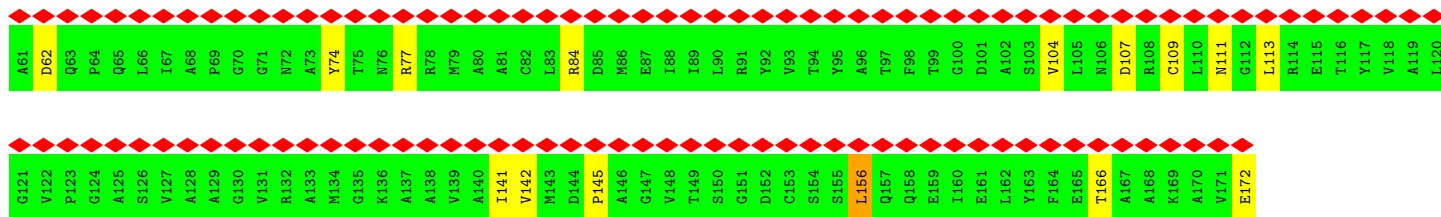


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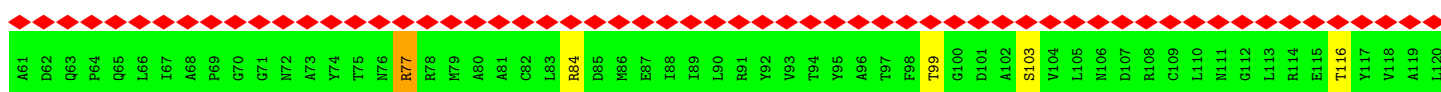
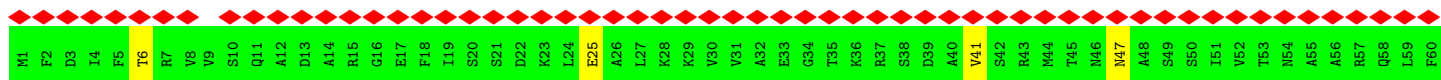
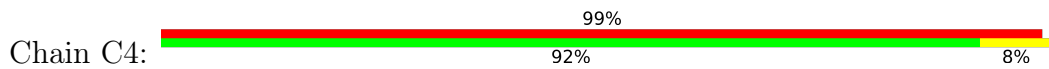


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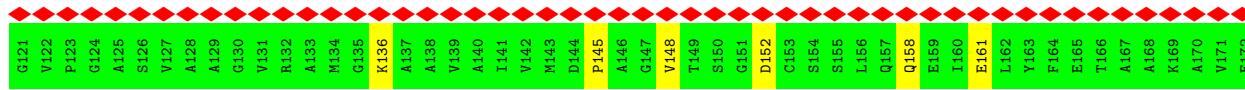
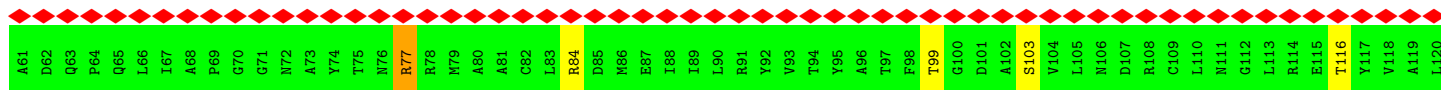
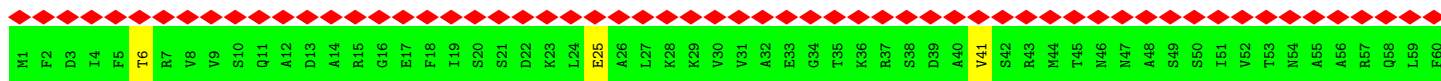
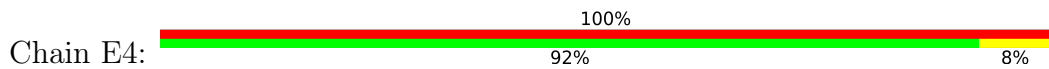




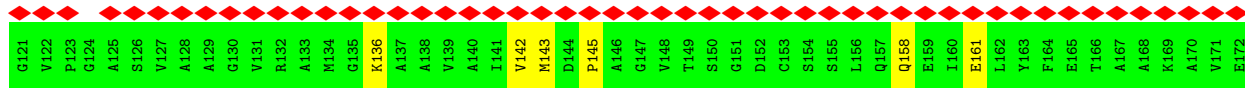
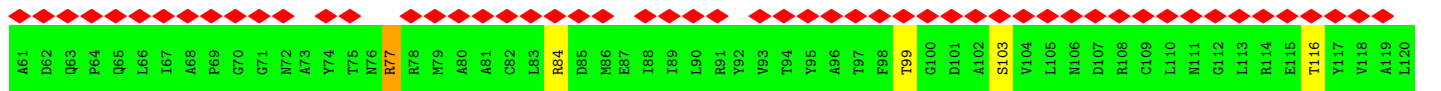
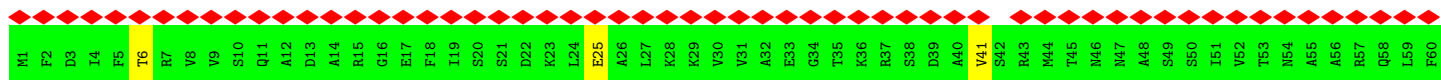
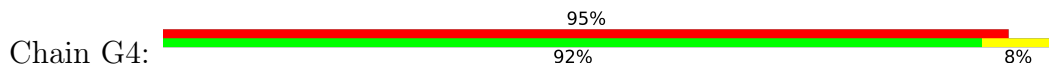
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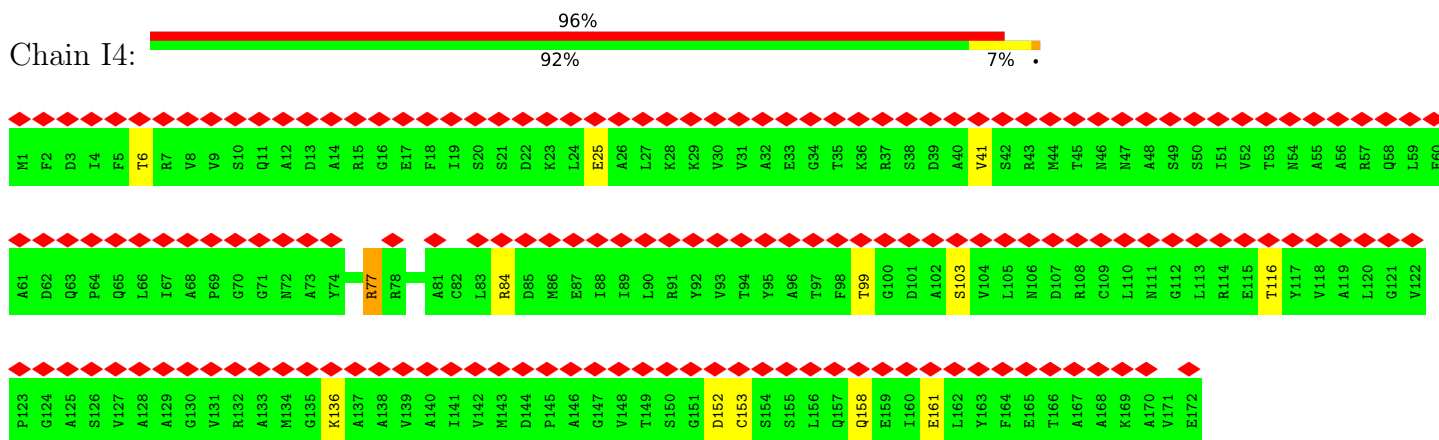
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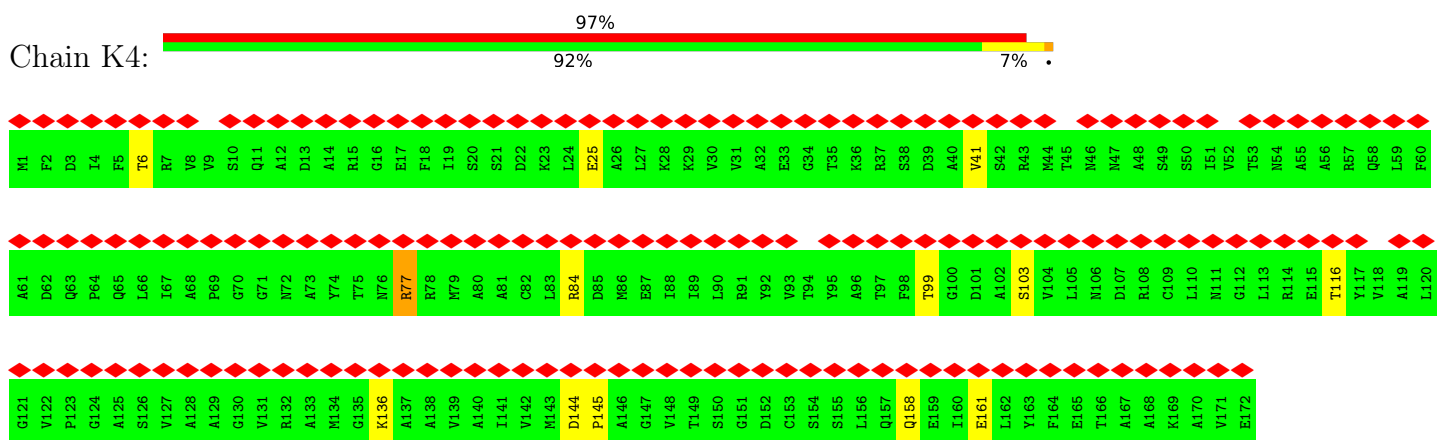
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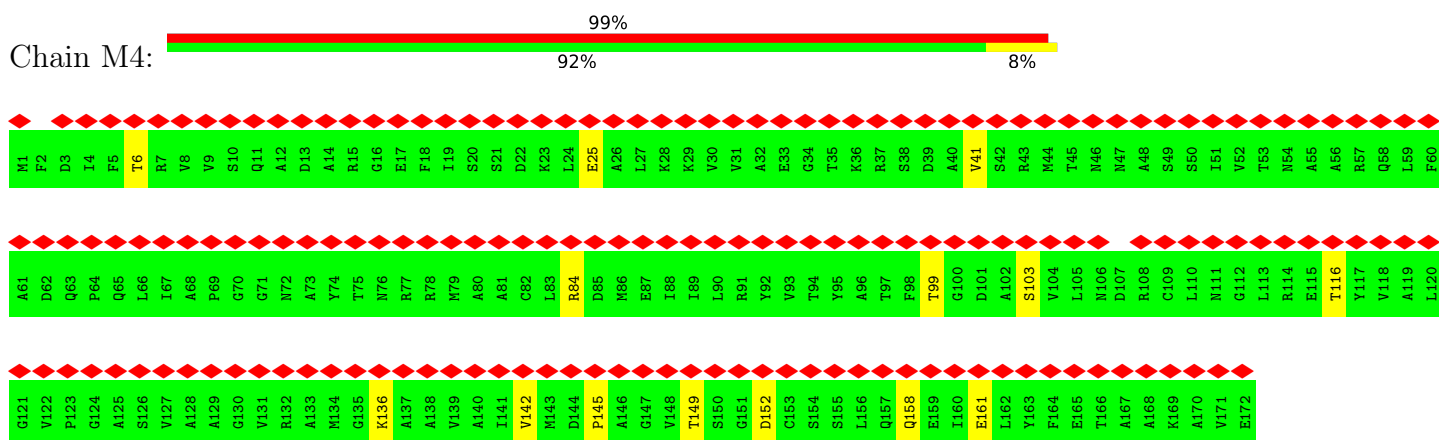
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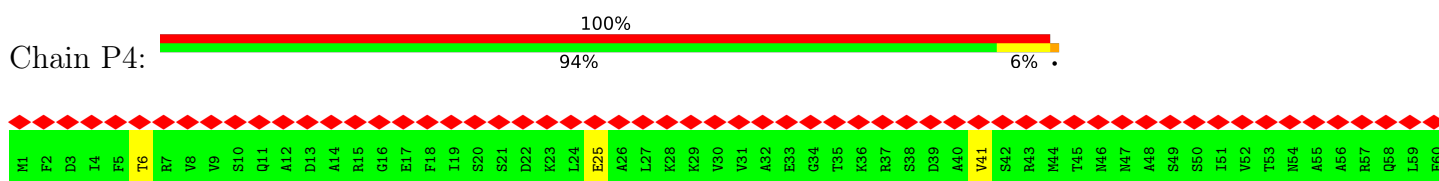
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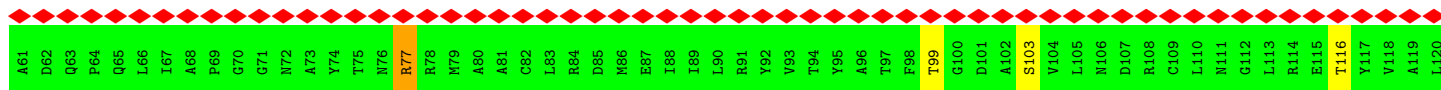


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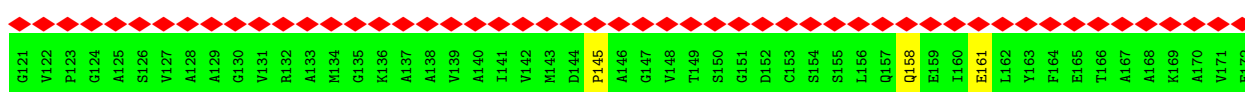
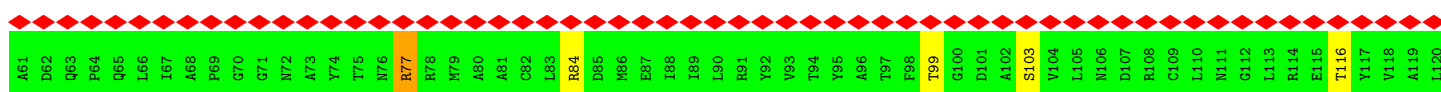
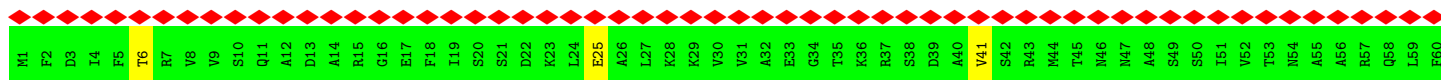


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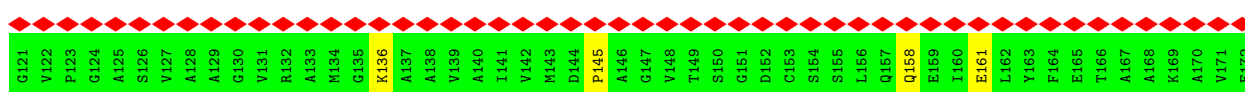
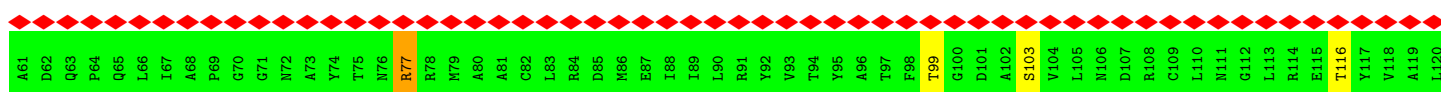
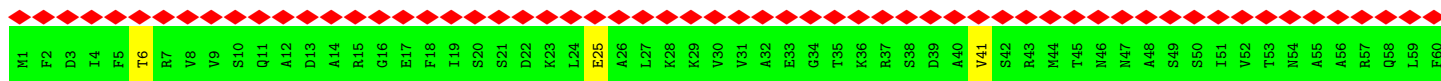




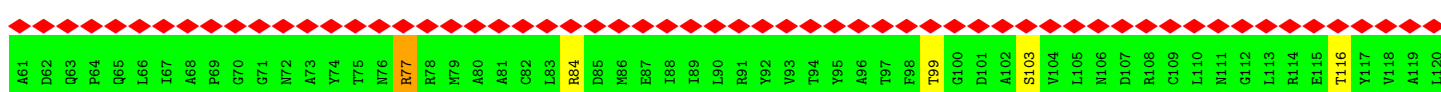
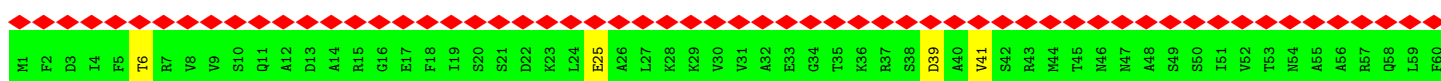
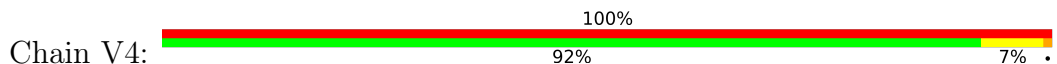
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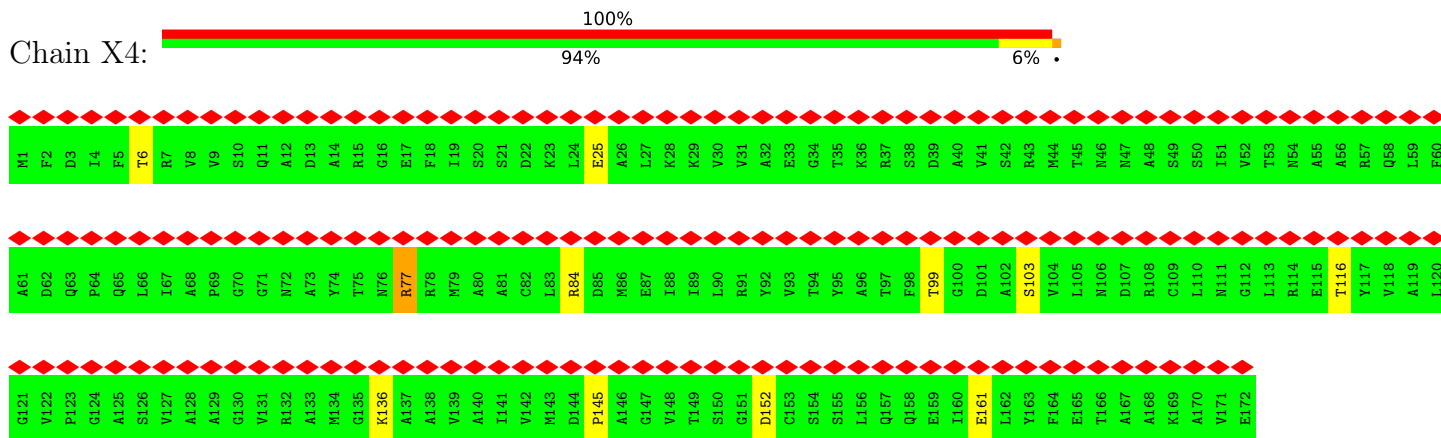
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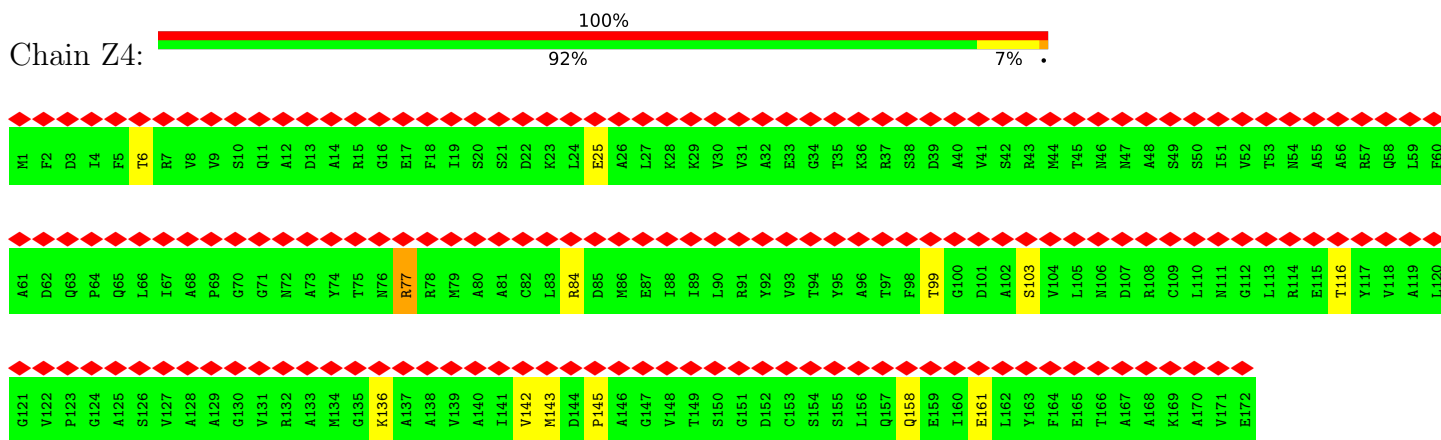
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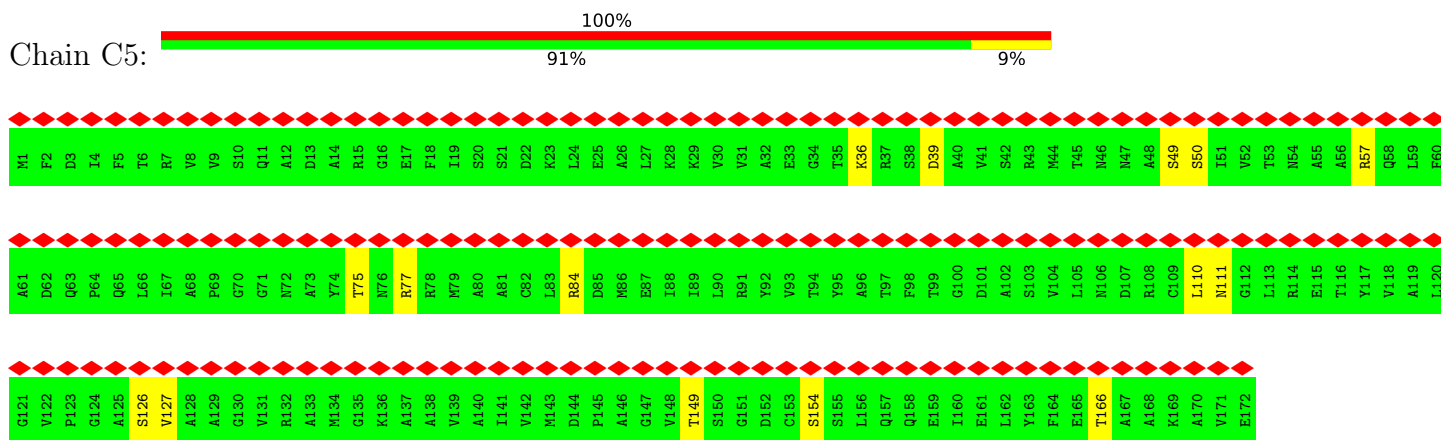
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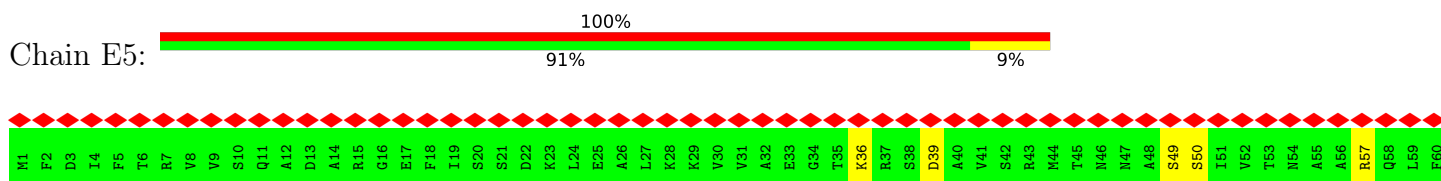
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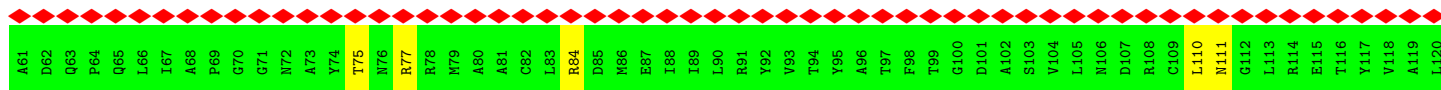


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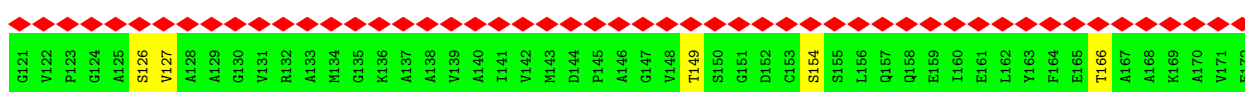
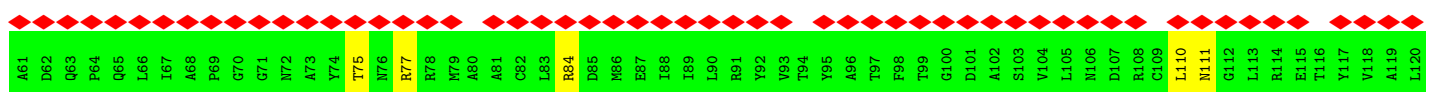
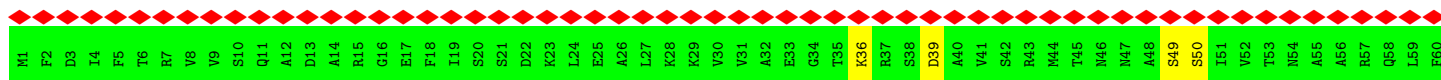
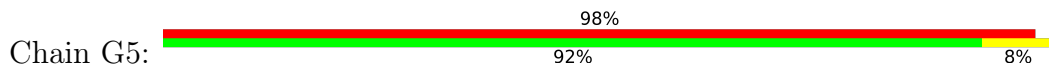


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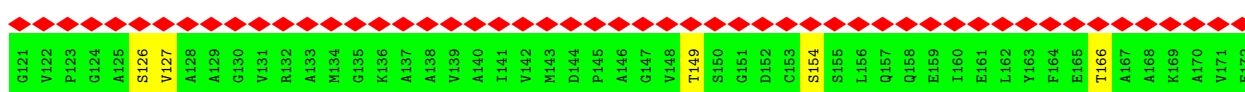
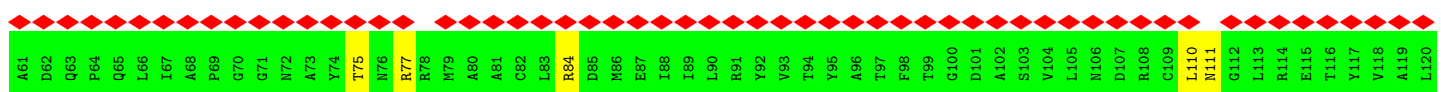
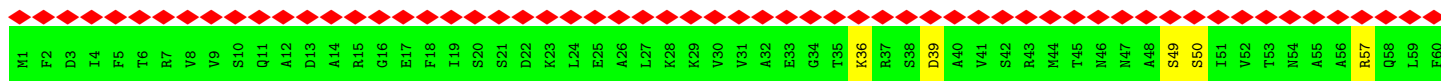
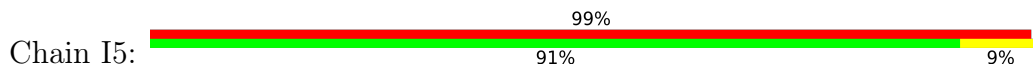




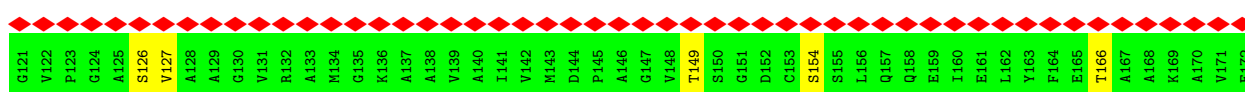
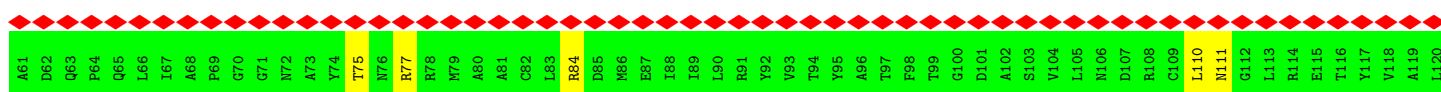
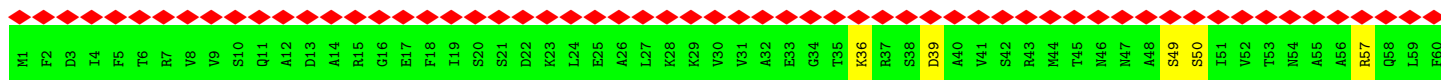
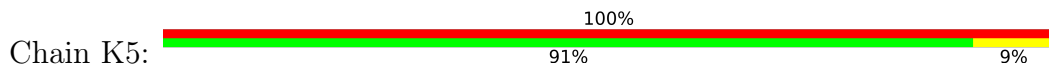
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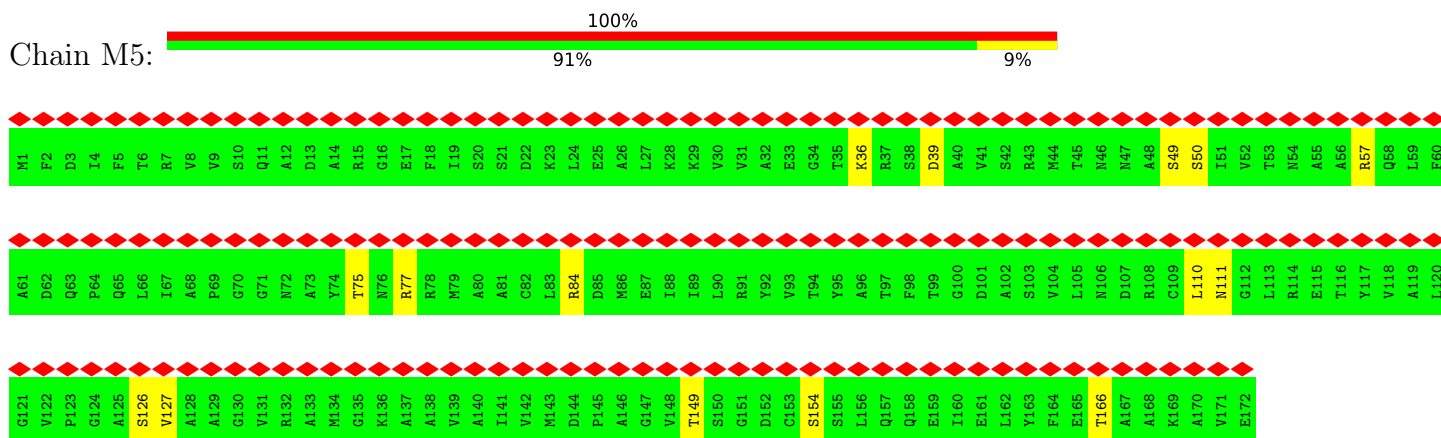
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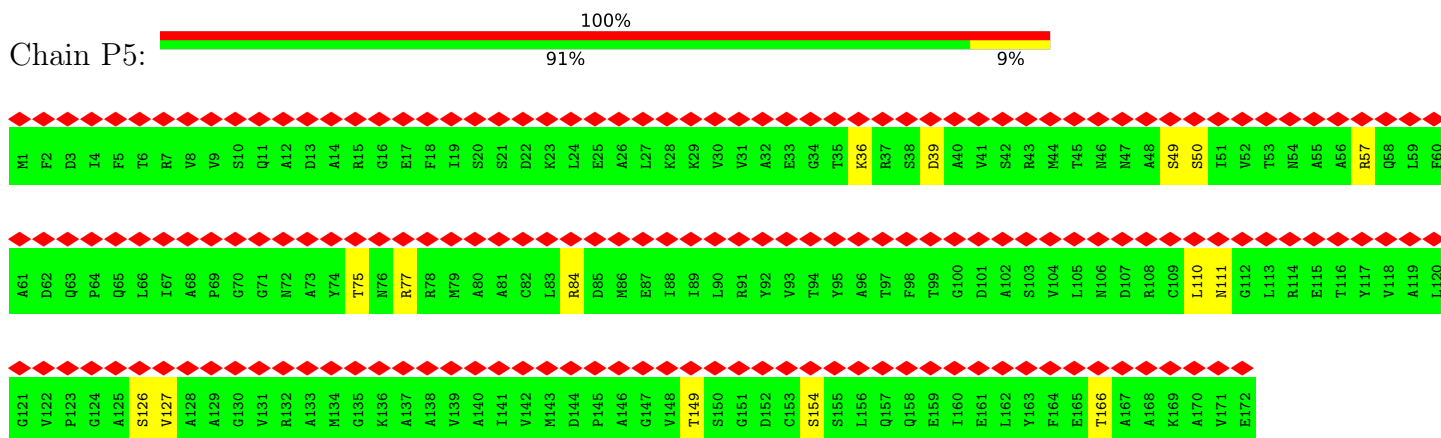
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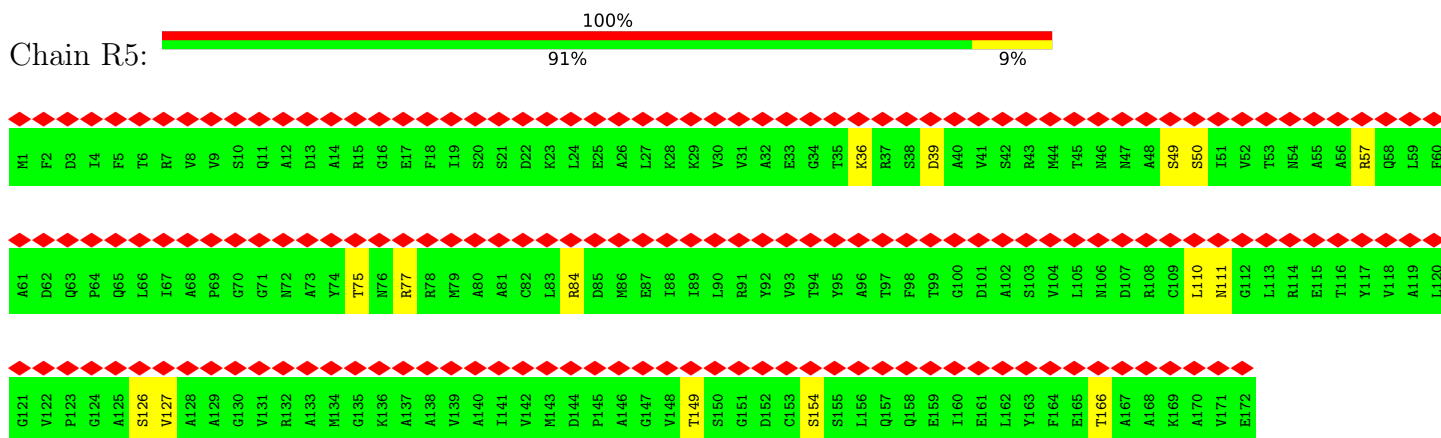
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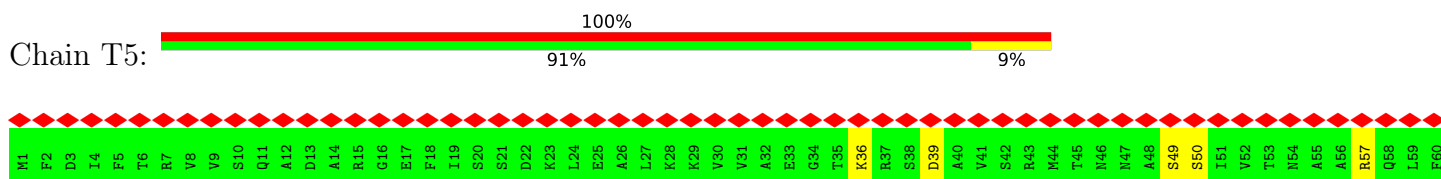
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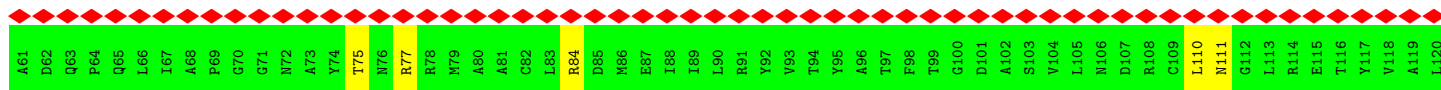


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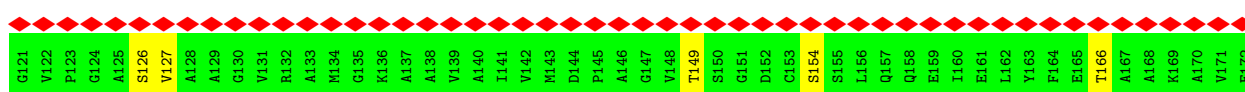
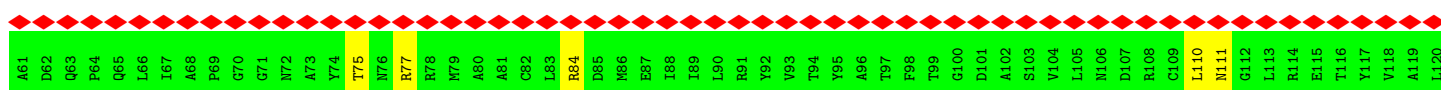
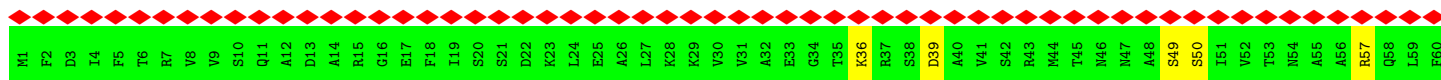
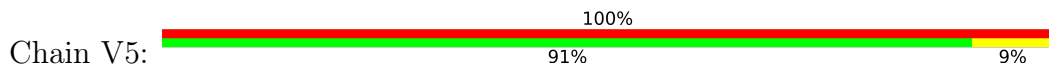


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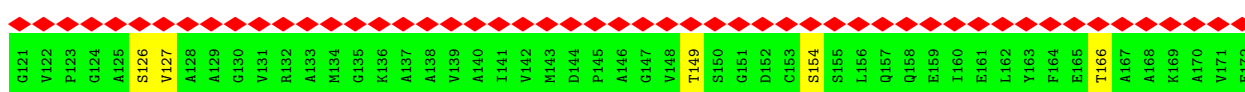
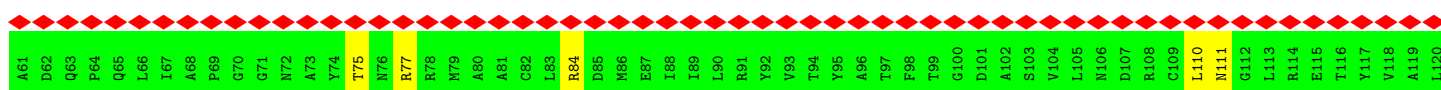
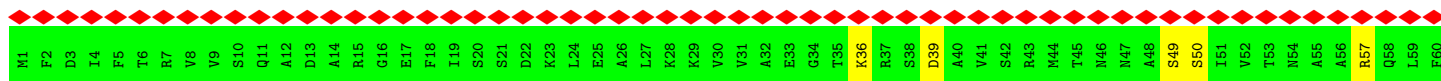
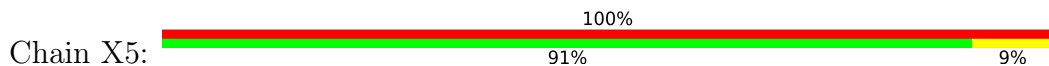




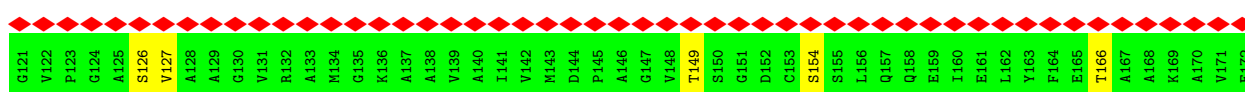
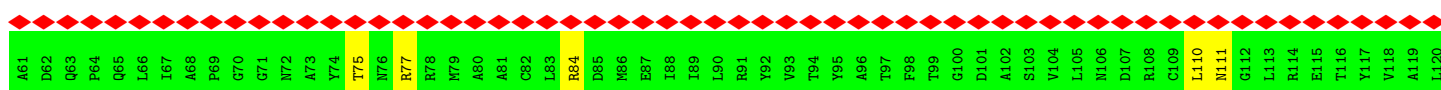
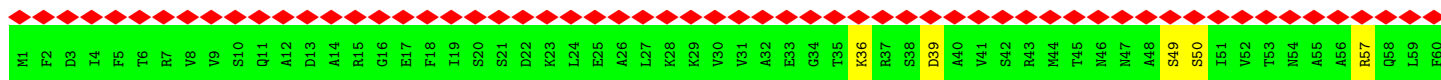
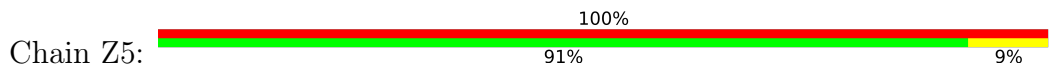
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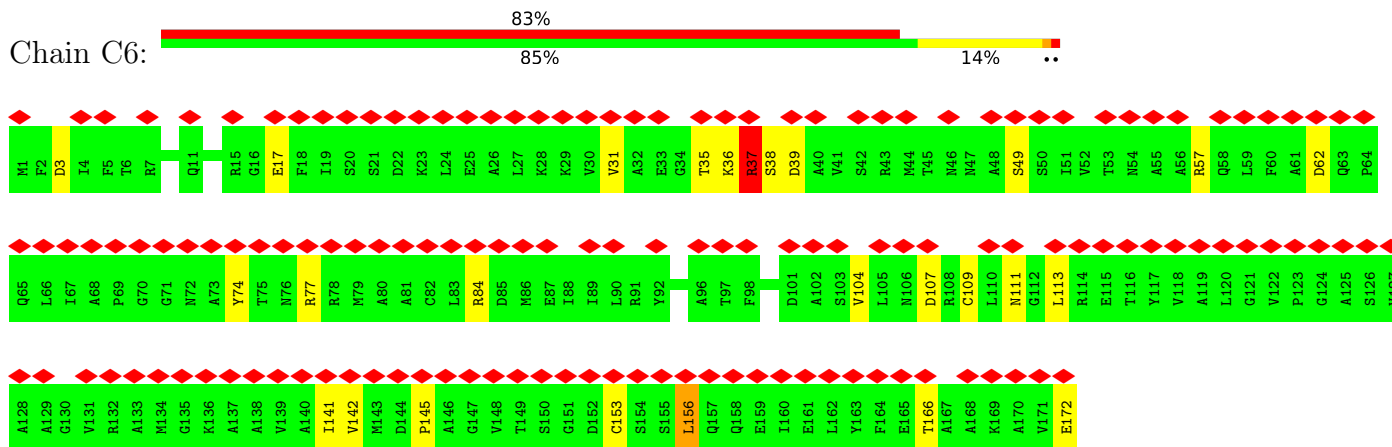
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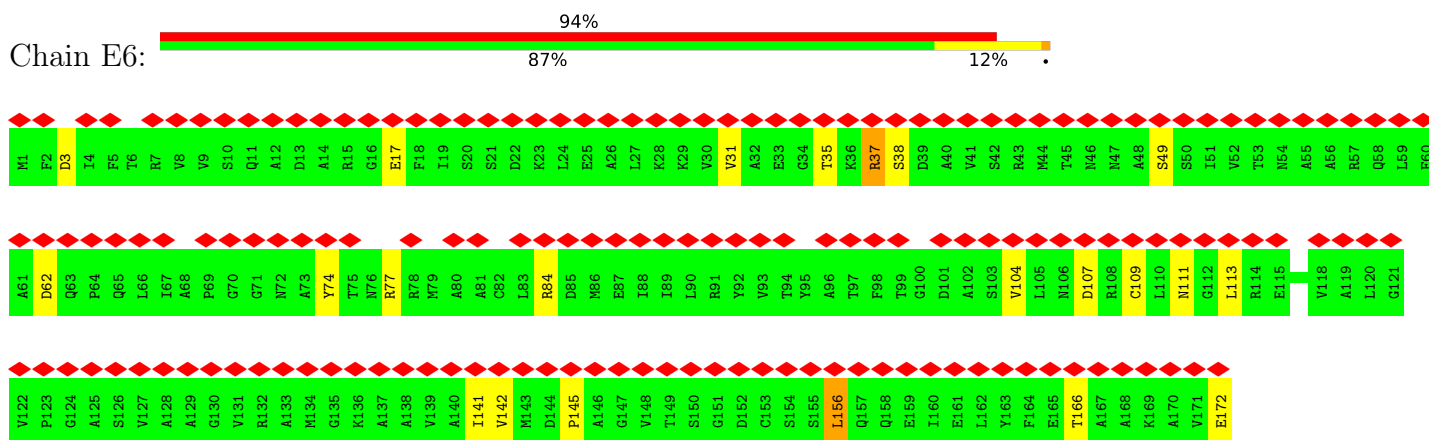
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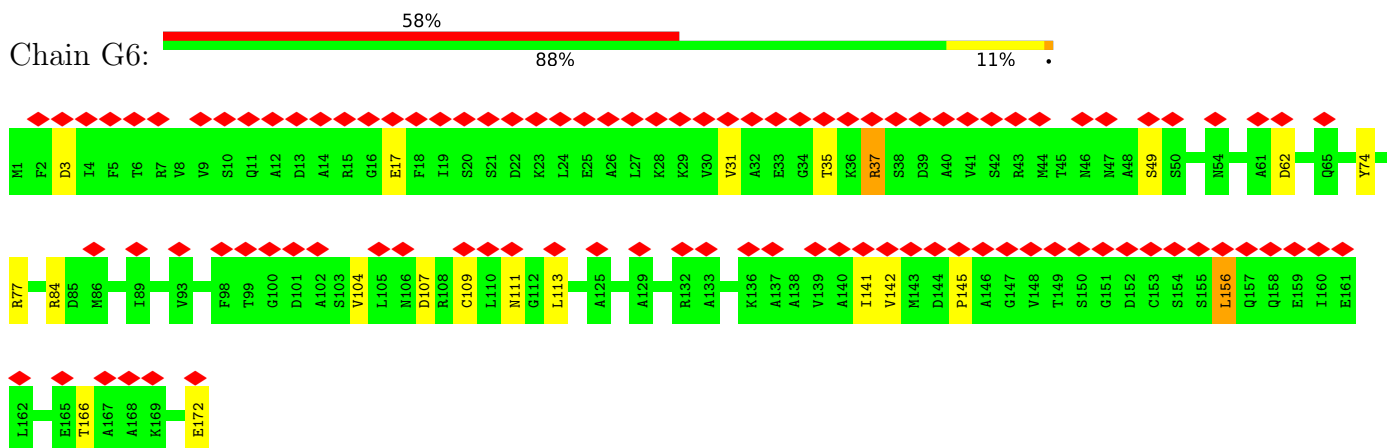
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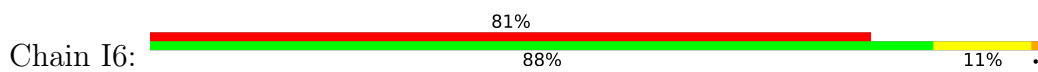
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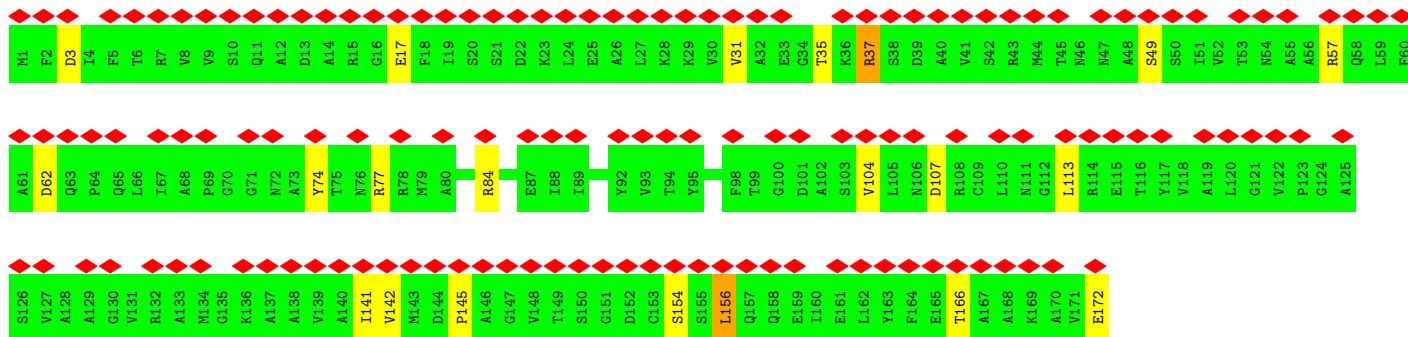


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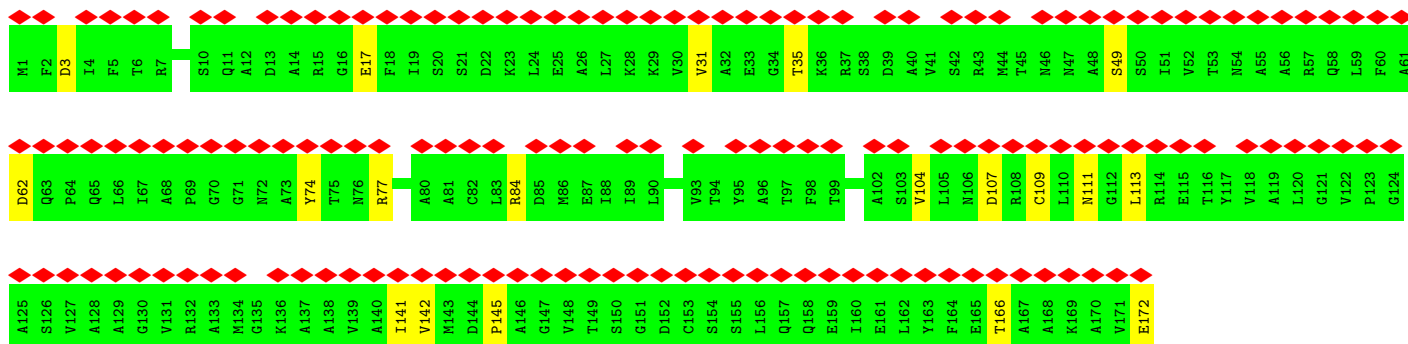
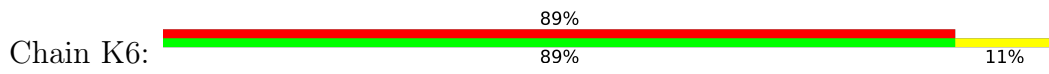


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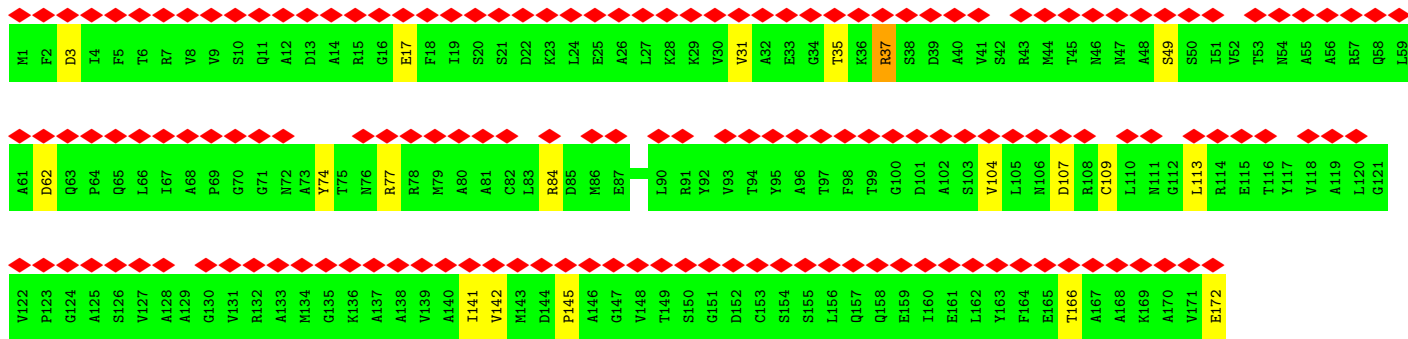
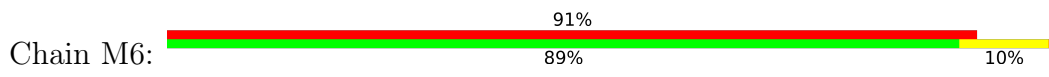




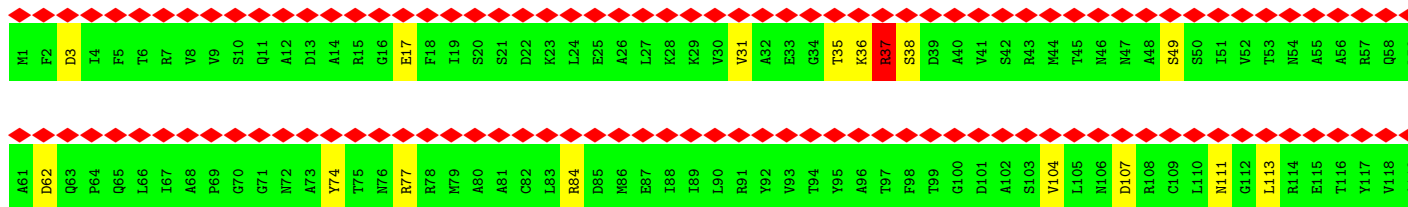
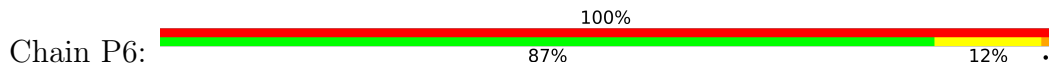
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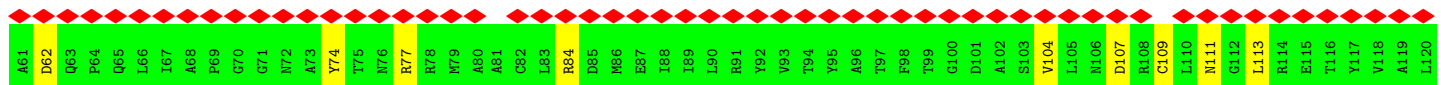
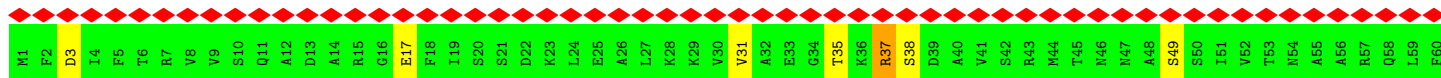
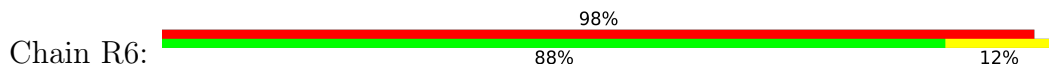


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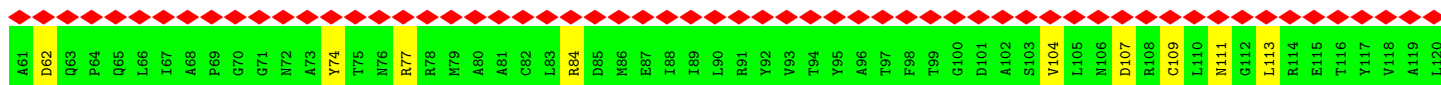
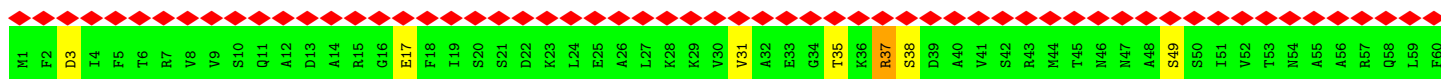
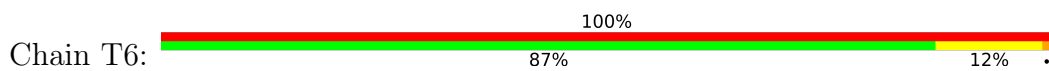




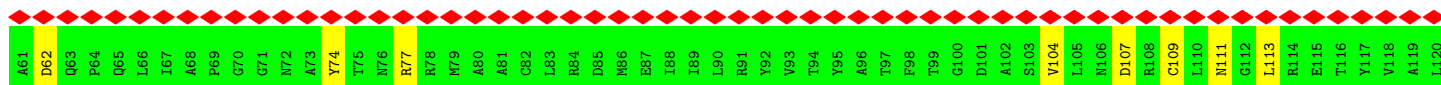
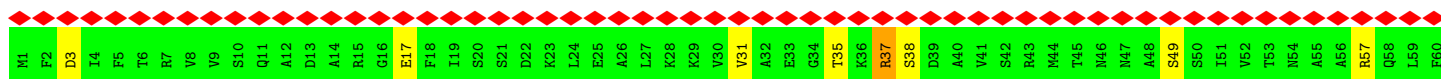
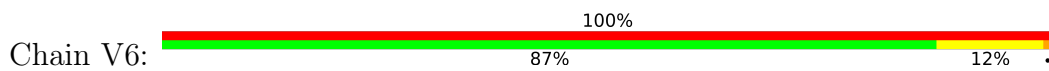
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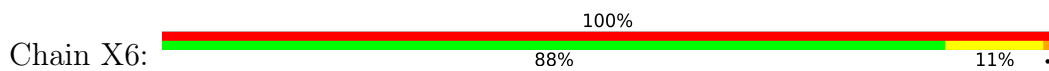
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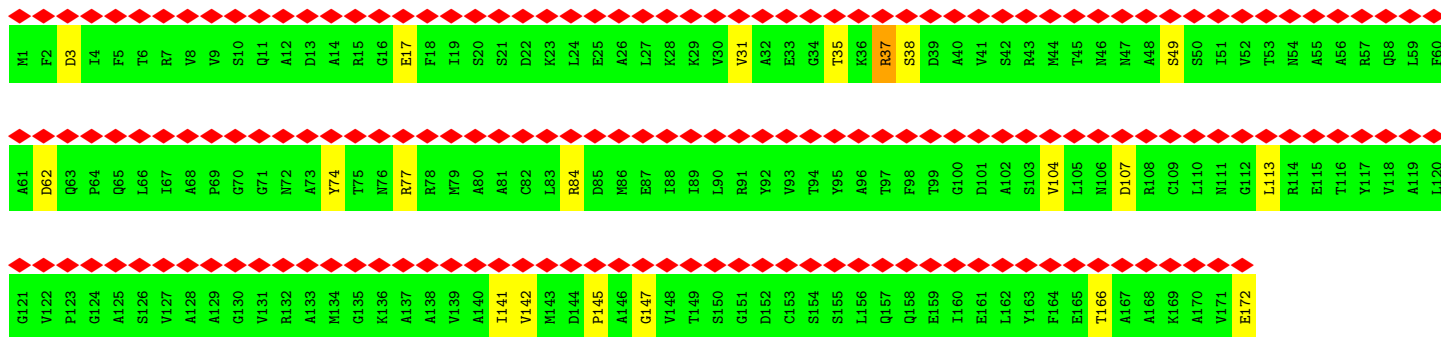


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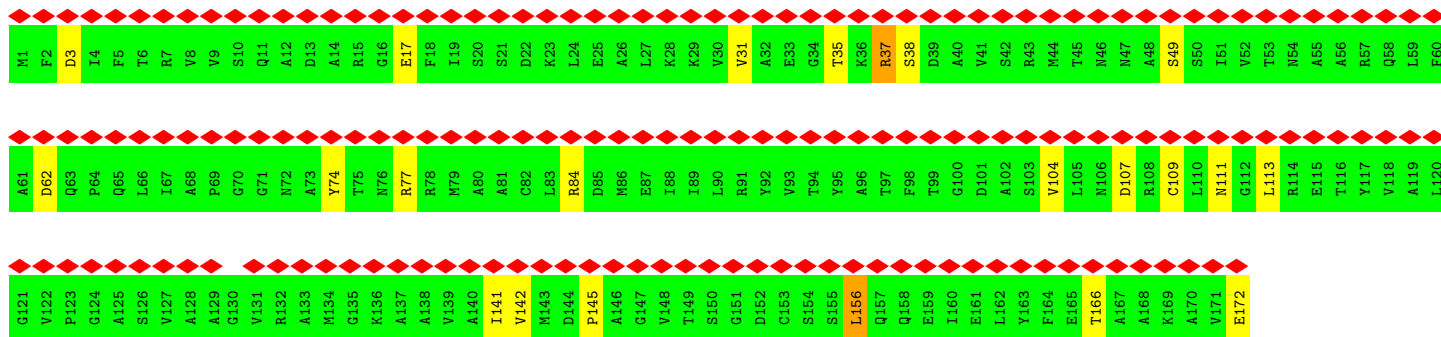
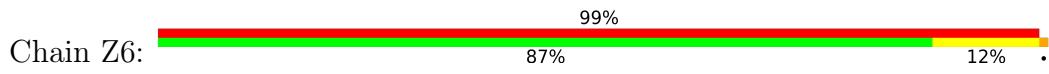


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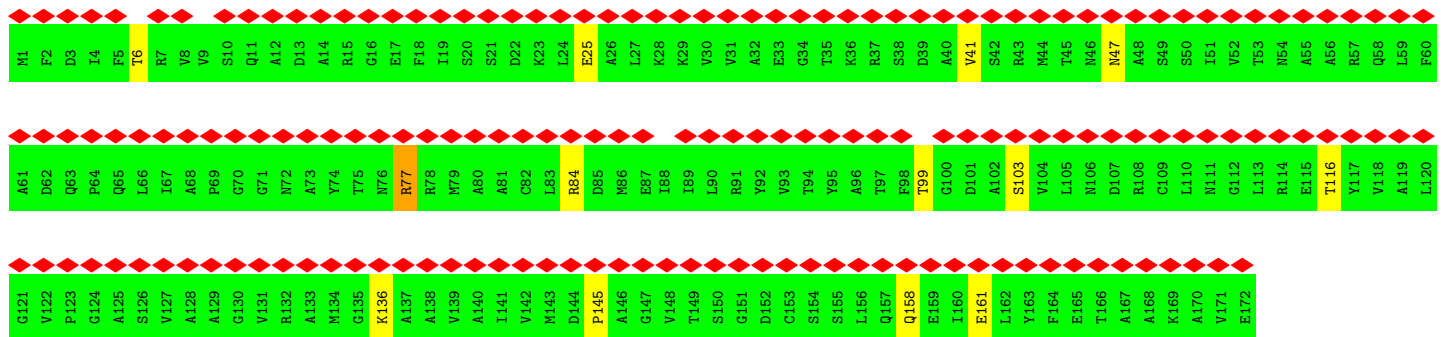
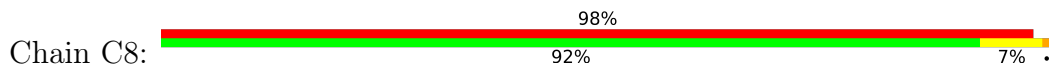




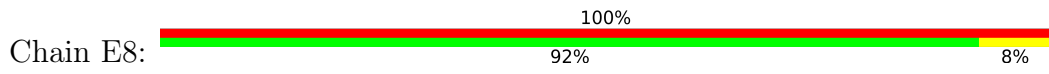
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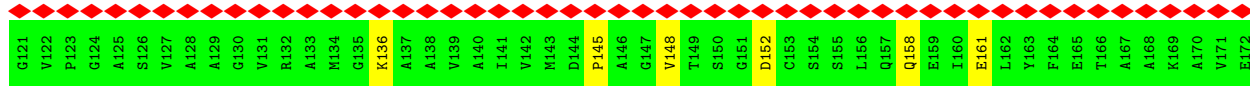


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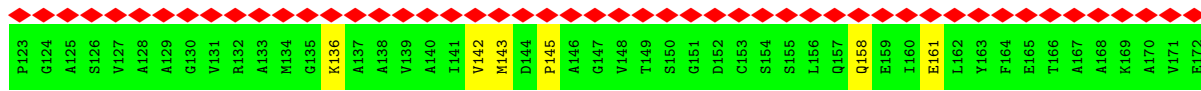
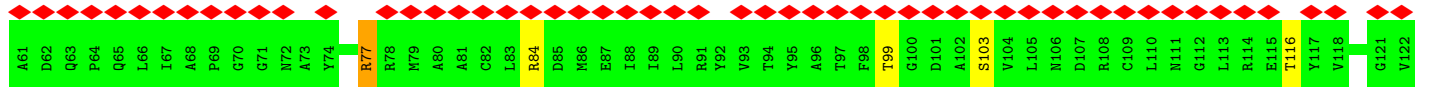
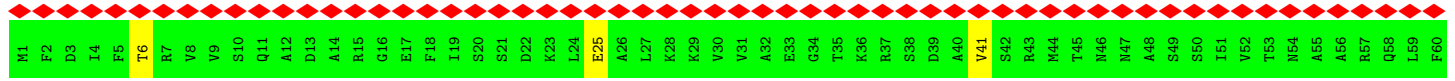


• Molecule 3: C-phycoerythrin subunit beta

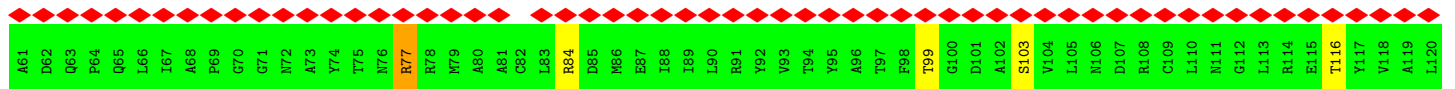
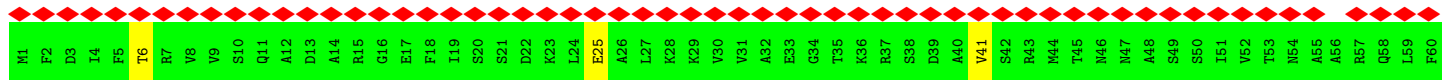
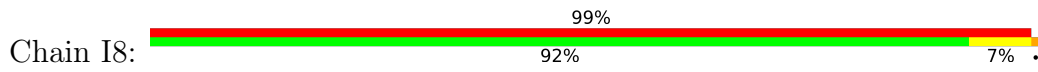




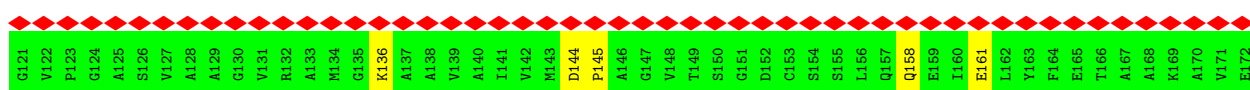
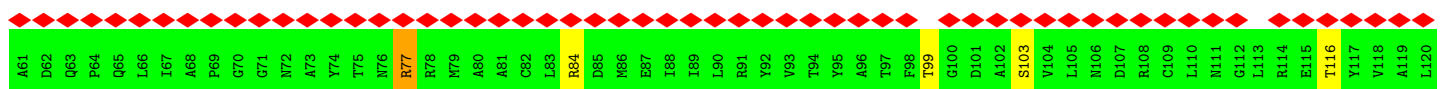
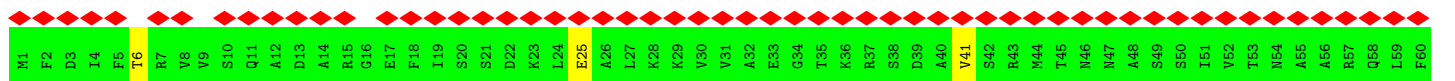
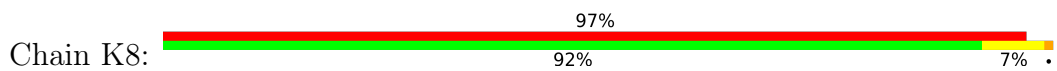
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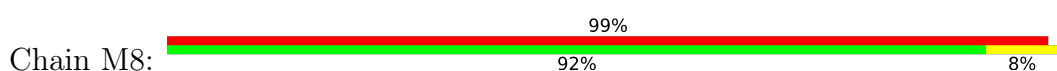
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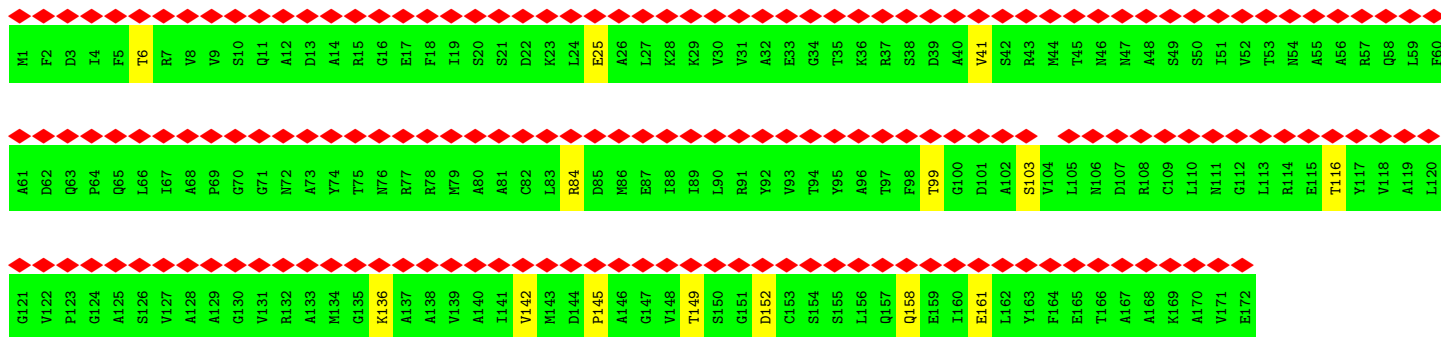


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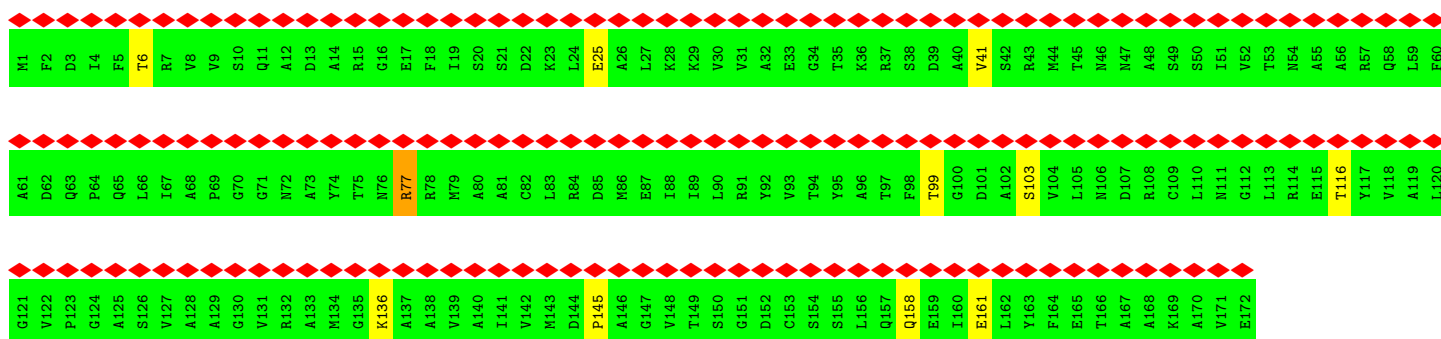


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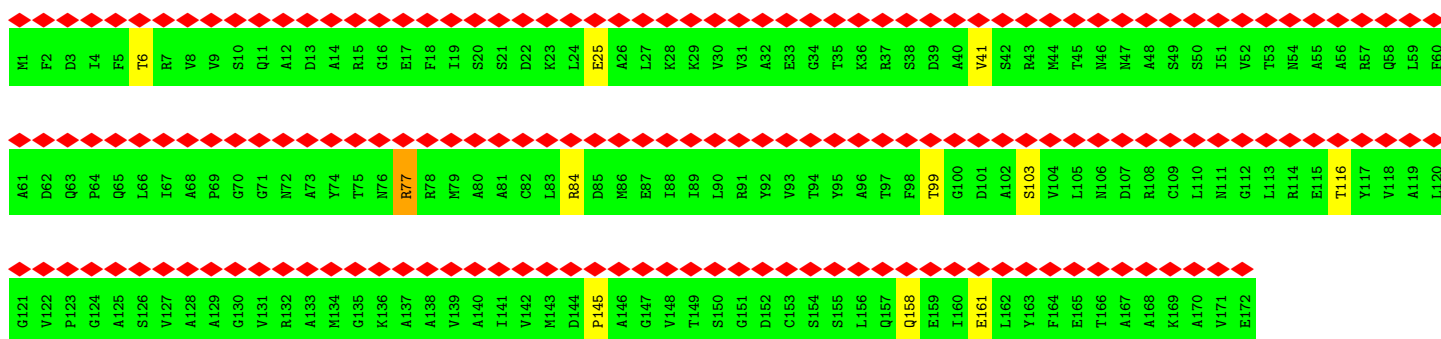




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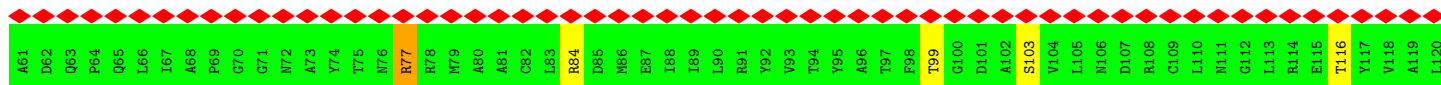
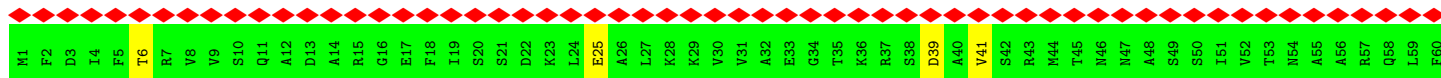
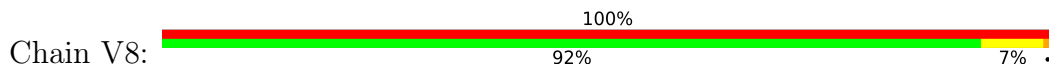


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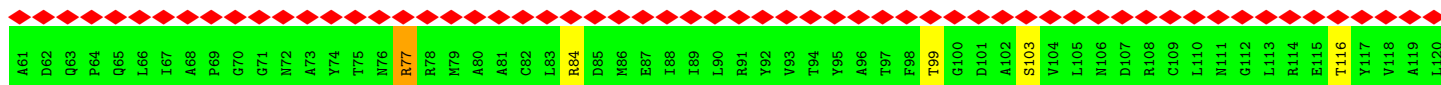
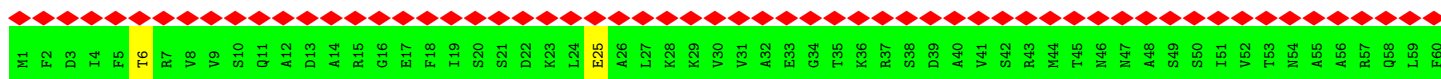




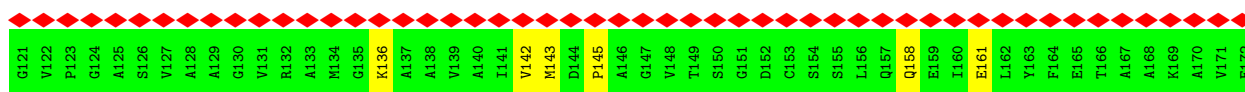
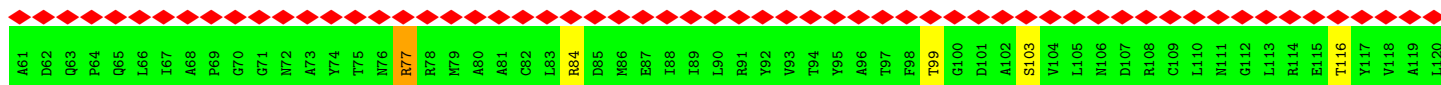
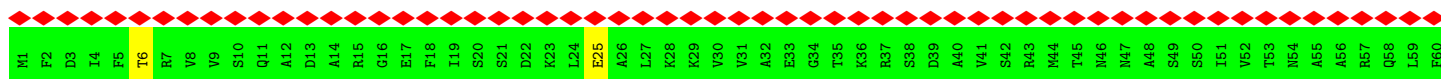
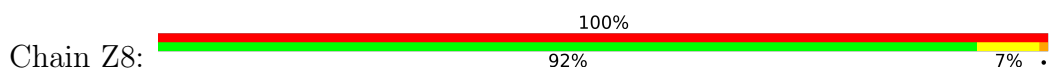
• Molecule 3: C-phycoyanin subunit beta



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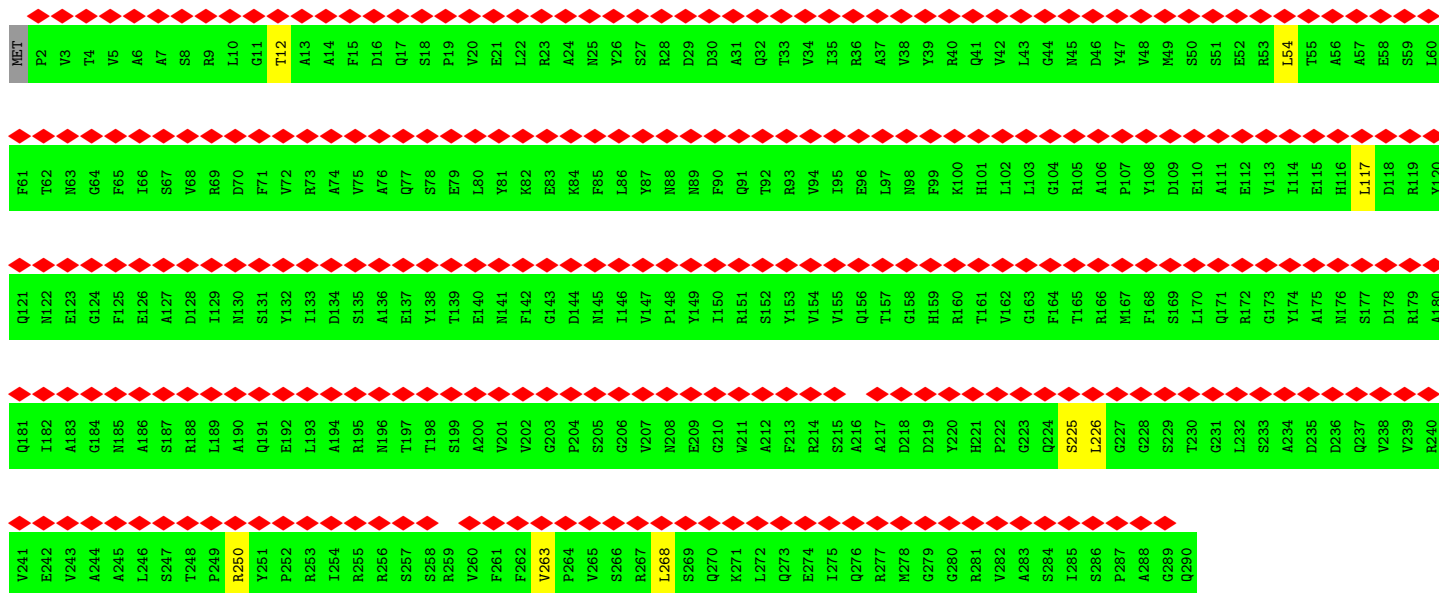


• Molecule 3: C-phycoyanin subunit beta

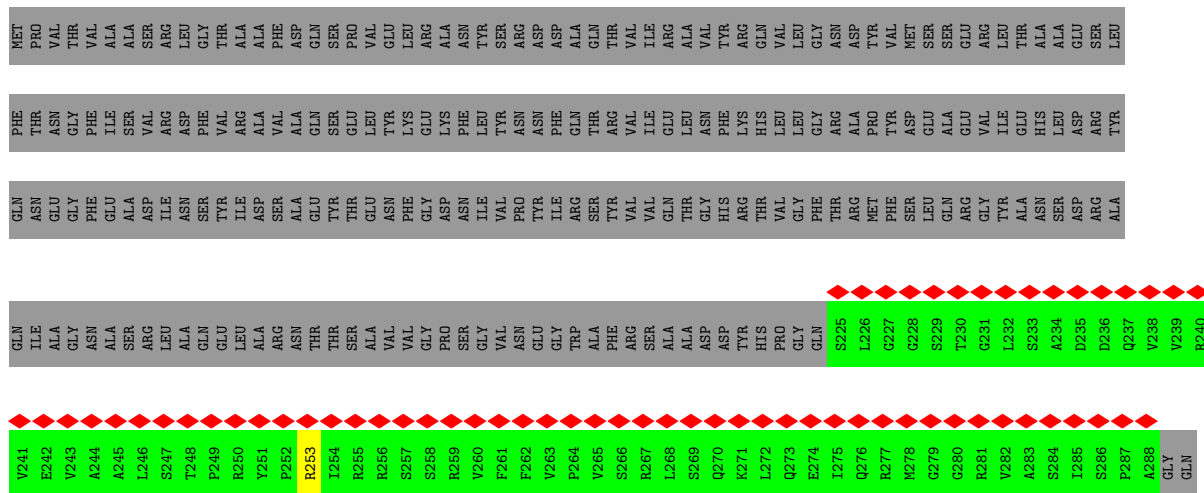


• Molecule 4: Phycobilisome 32.3 kDa linker polypeptide, phycocyanin-associated, rod

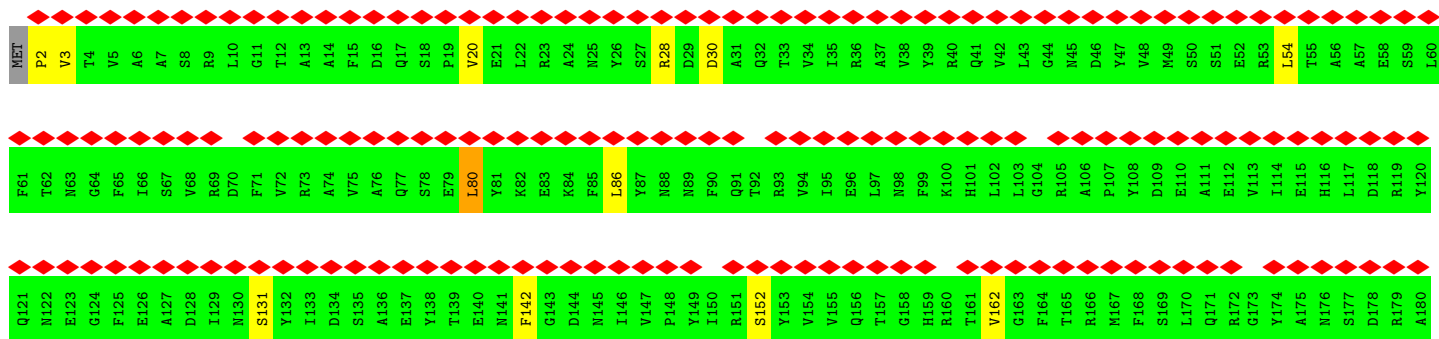


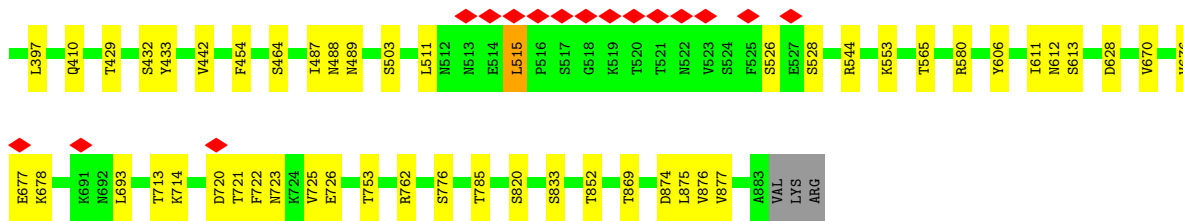


• Molecule 4: Phycobilisome 32.3 kDa linker polypeptide, phycocyanin-associated, rod

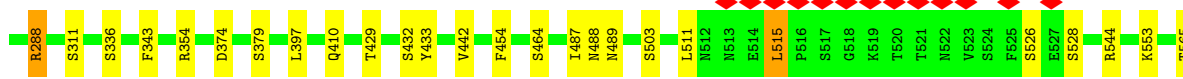
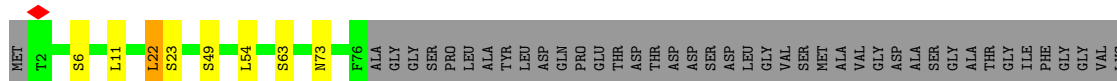
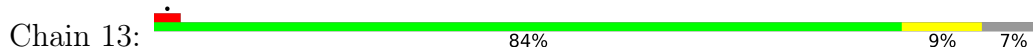


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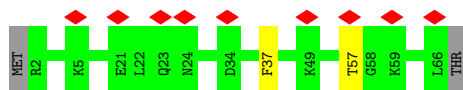




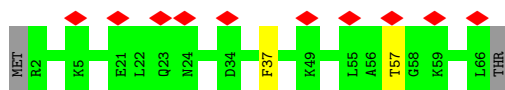
• Molecule 5: Phycobiliprotein ApcE



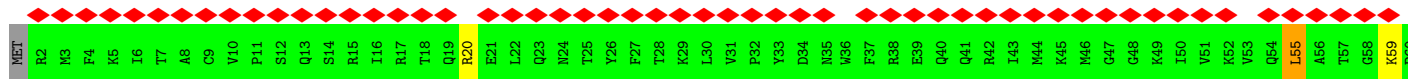
• Molecule 6: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core

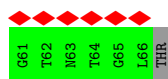


• Molecule 6: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core

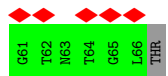
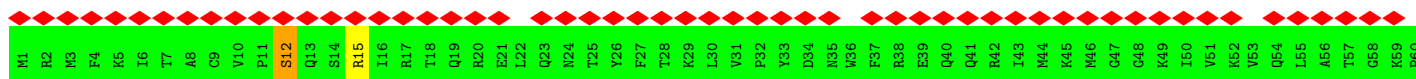


• Molecule 6: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core

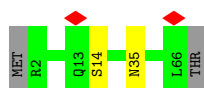




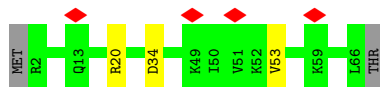
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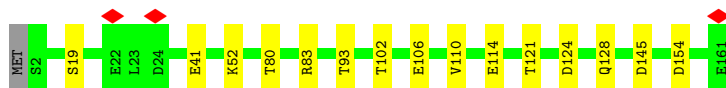
- Molecule 6: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core



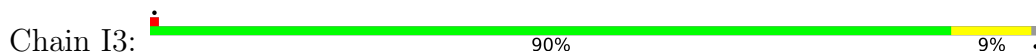
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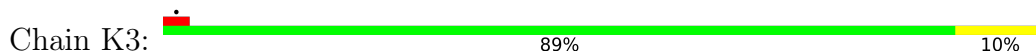
- Molecule 7: Allophycocyanin alpha subunit



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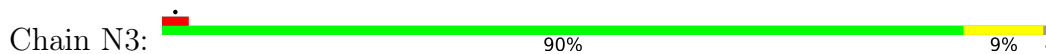


- Molecule 7: Allophycocyanin alpha subunit

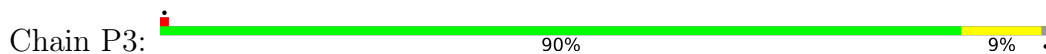




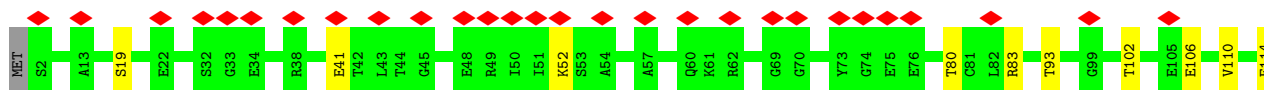
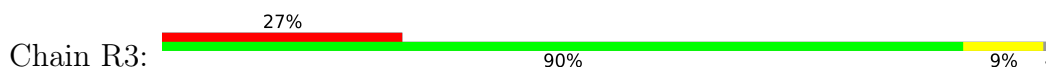
- Molecule 7: Allophycocyanin alpha subunit



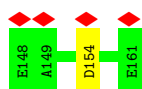
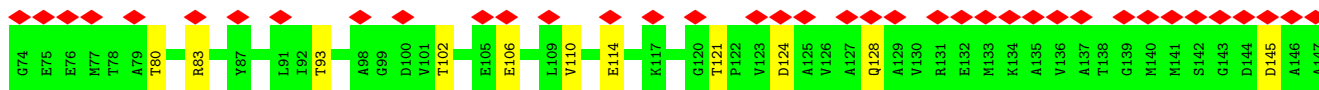
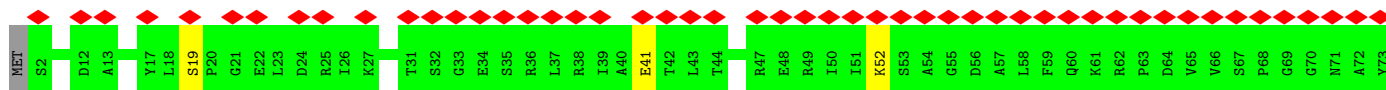
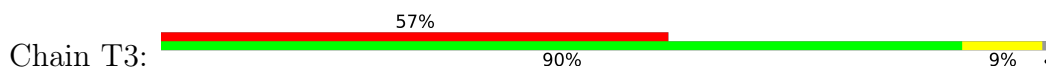
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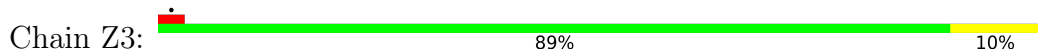


- Molecule 7: Allophycocyanin alpha subunit

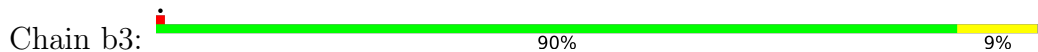




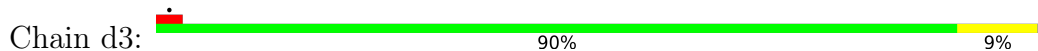
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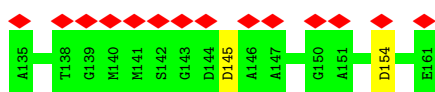
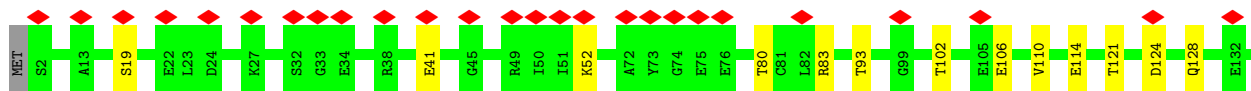
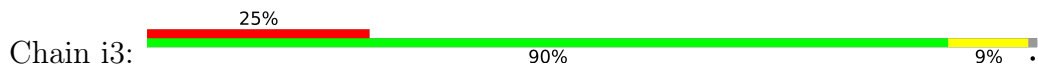
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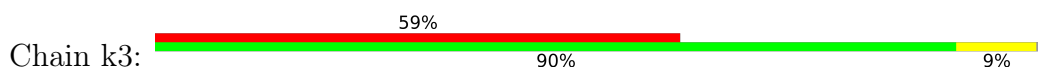
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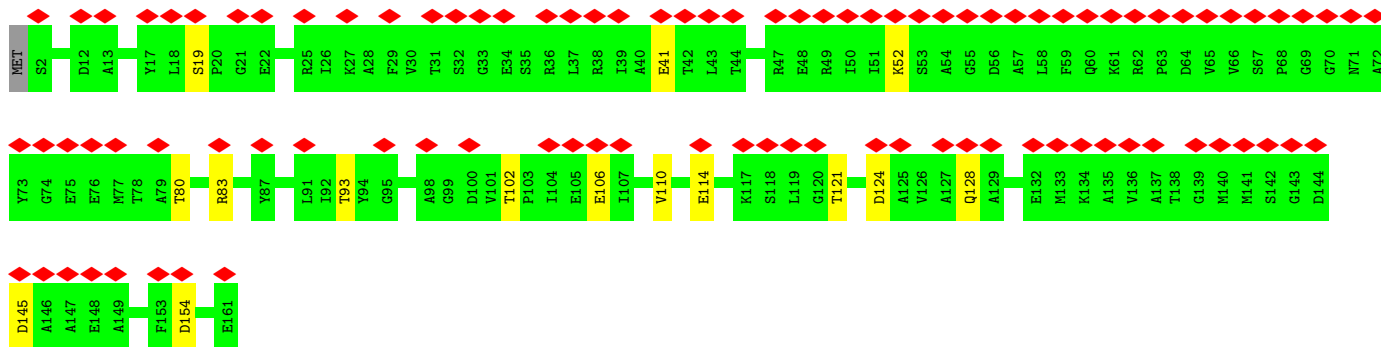


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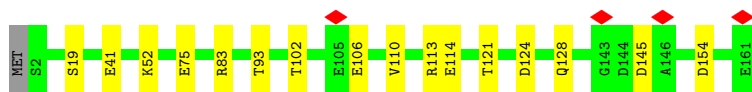
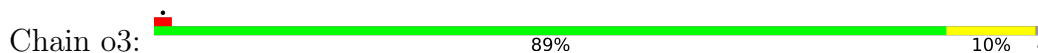


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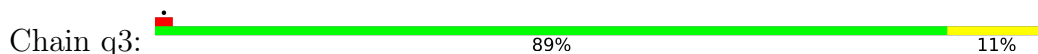




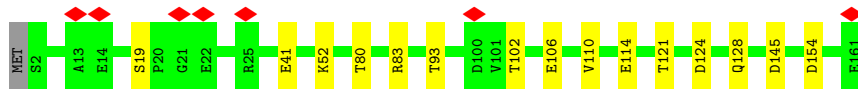
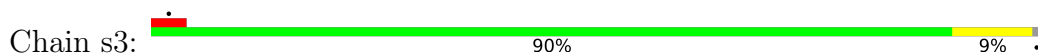
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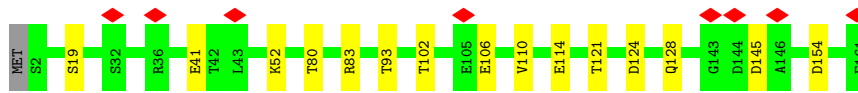
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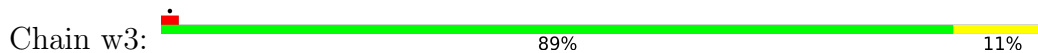
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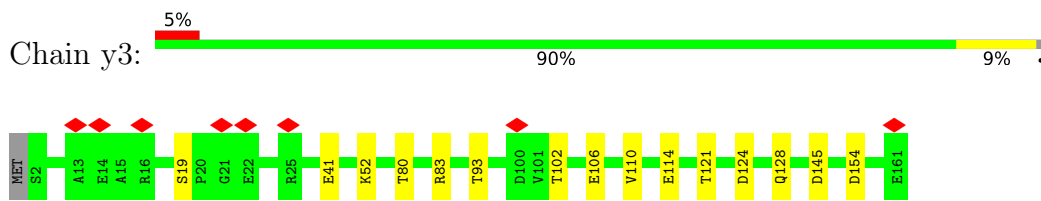
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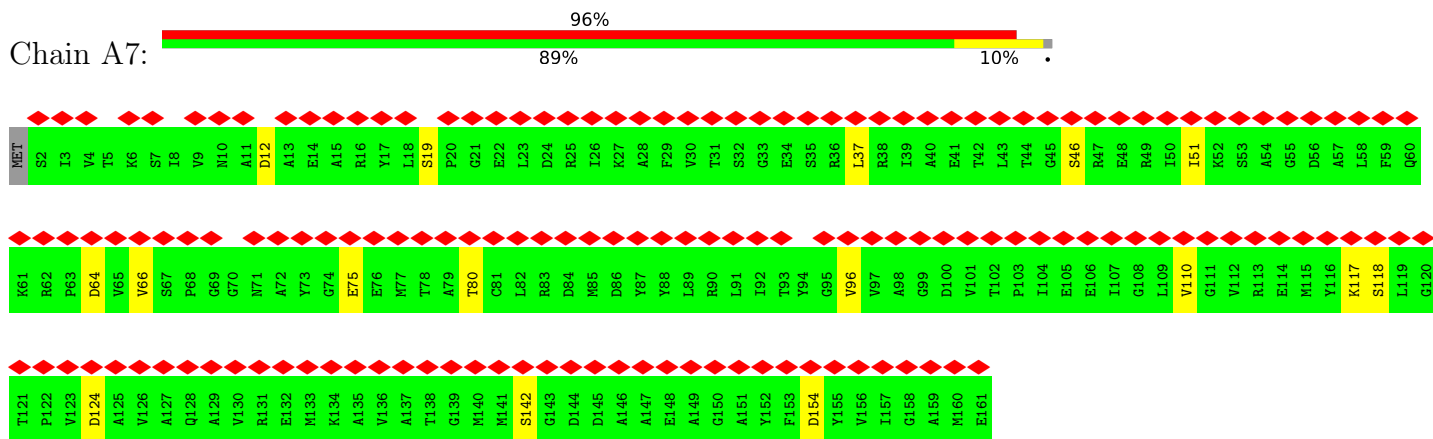
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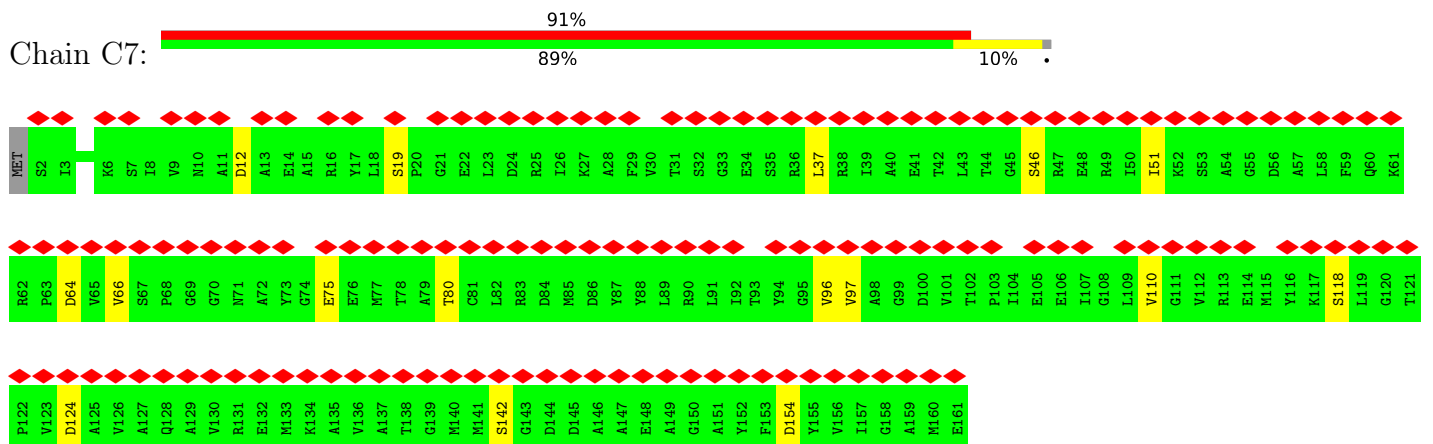
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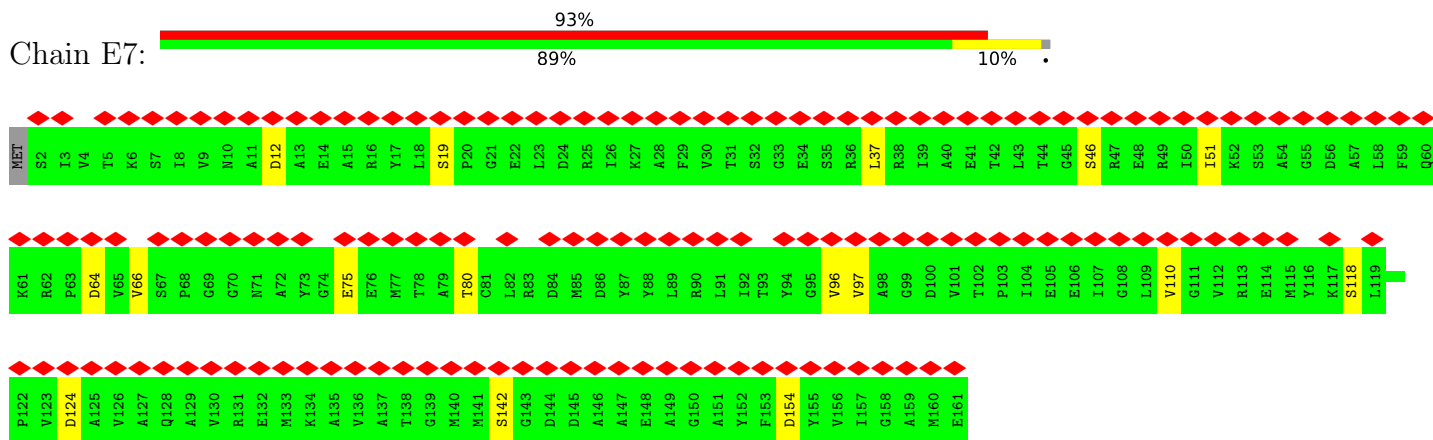
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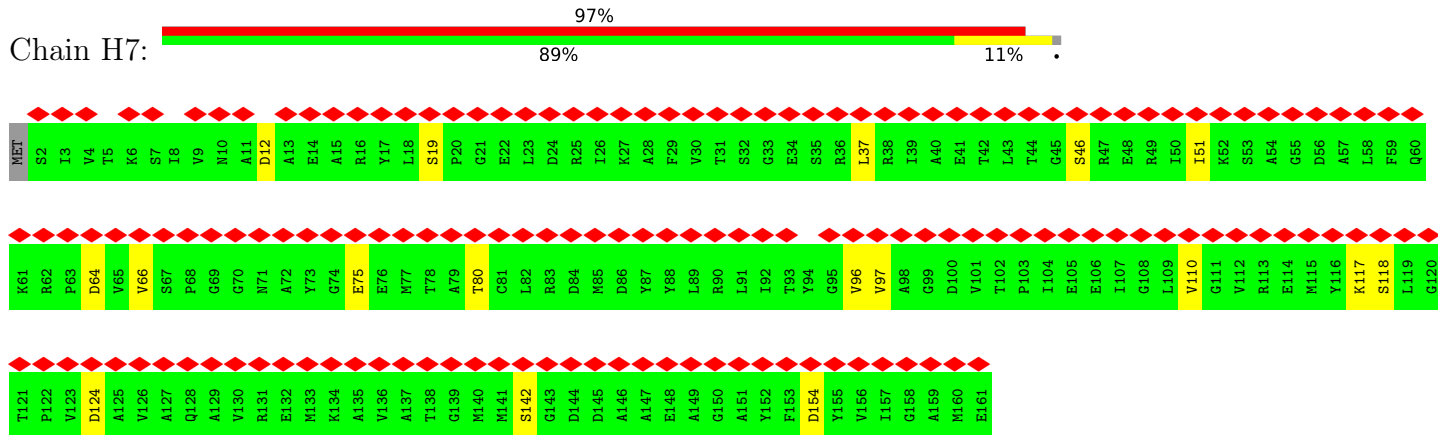
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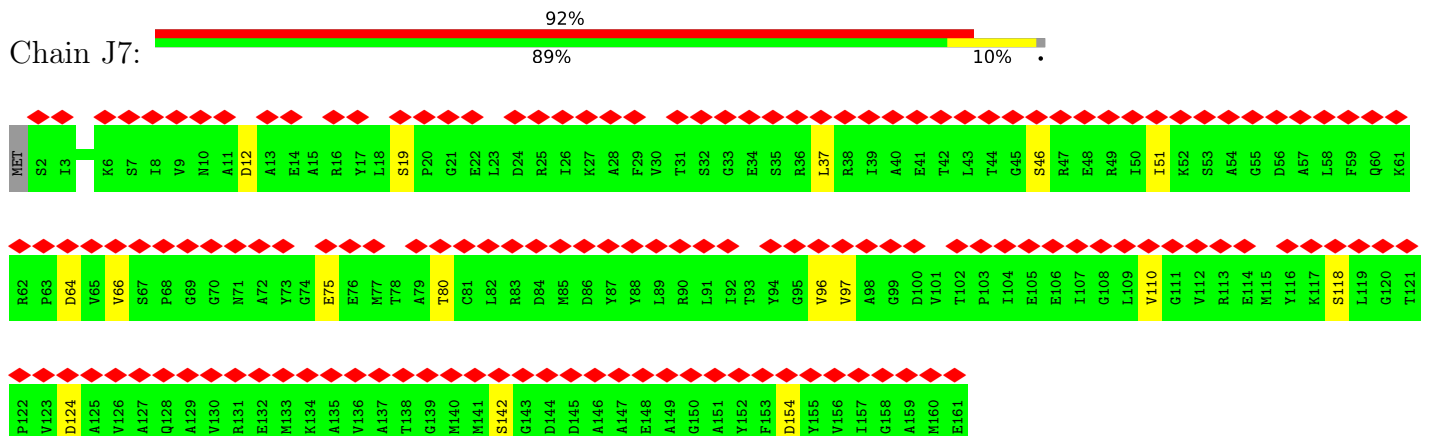
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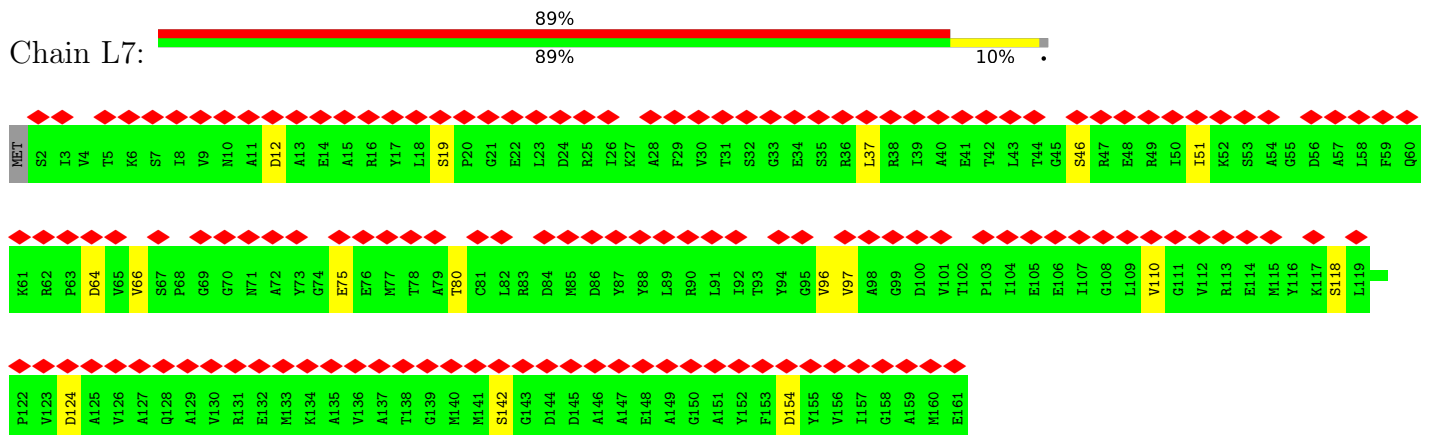
Molecule 7: Allophycocyanin alpha subunit



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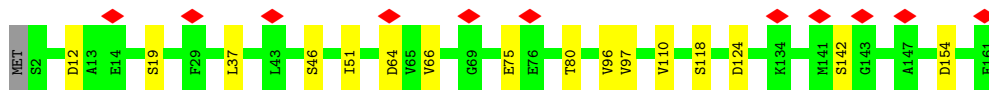


Molecule 7: Allophycocyanin alpha subunit

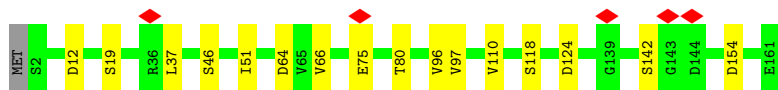
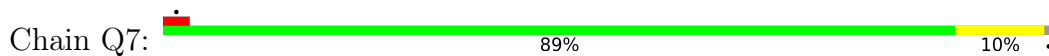


Molecule 7: Allophycocyanin alpha subunit

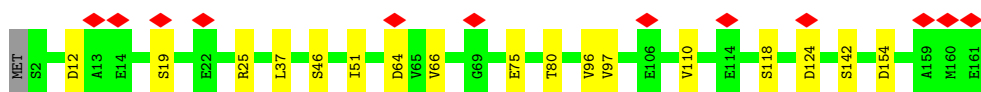
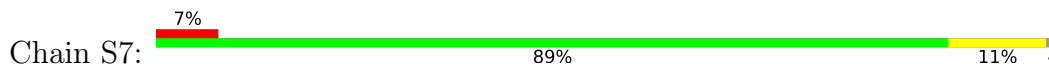




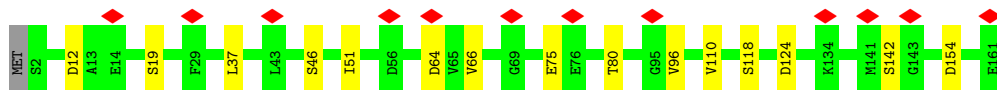
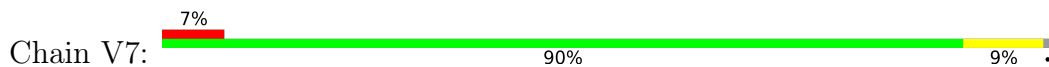
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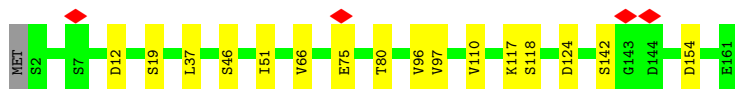
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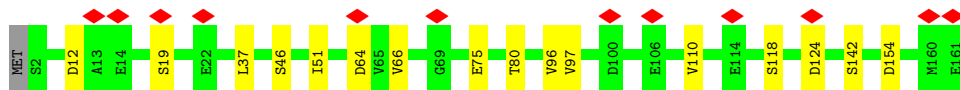
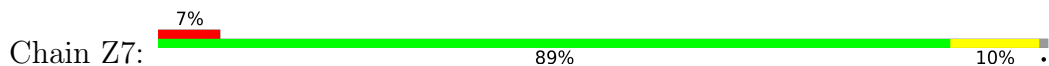
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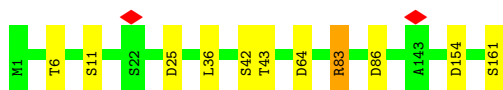
• Molecule 7: Allophycocyanin alpha subunit



• Molecule 7: Allophycocyanin alpha subunit



• Molecule 8: Allophycocyanin beta subunit



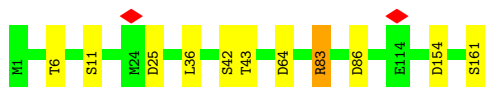
• Molecule 8: Allophycocyanin beta subunit



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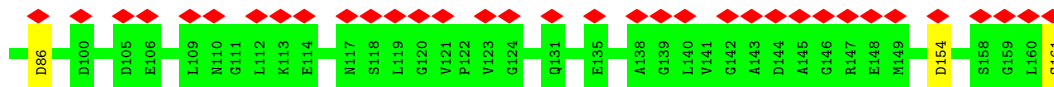
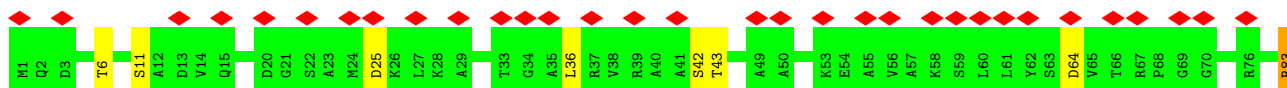
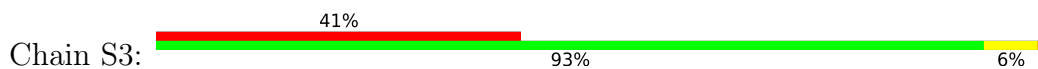
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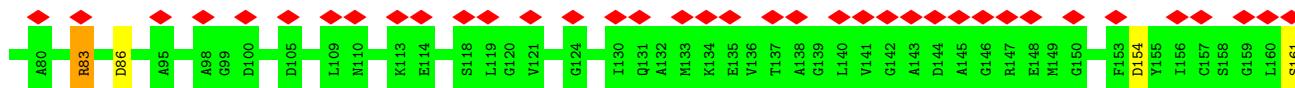
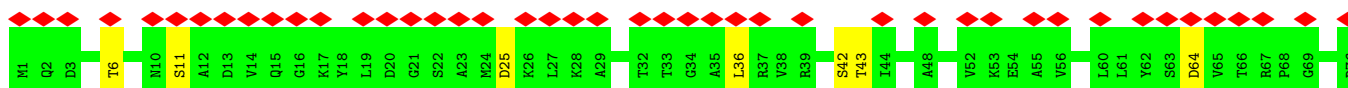
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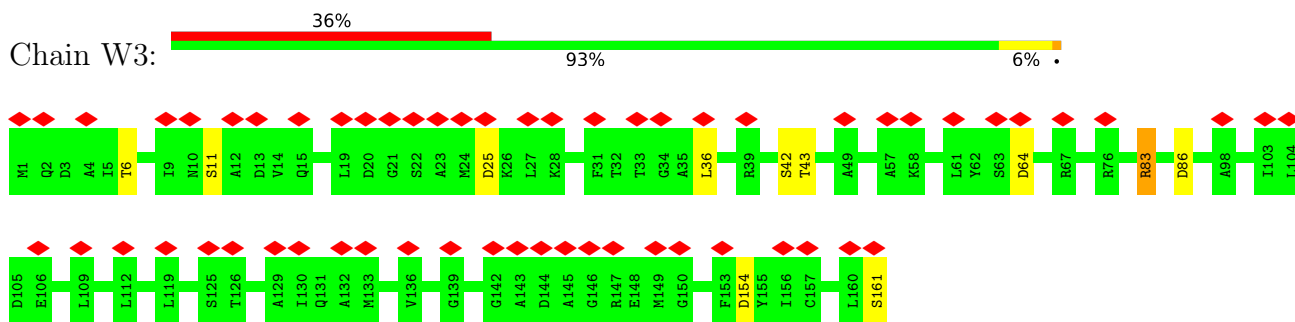
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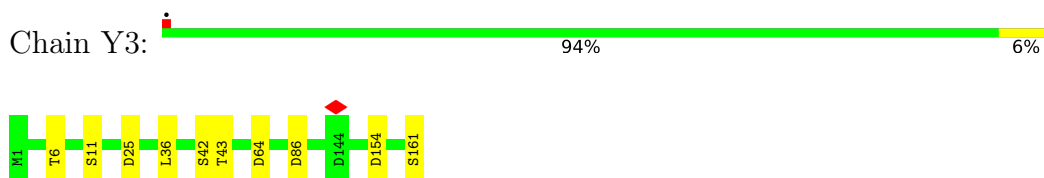
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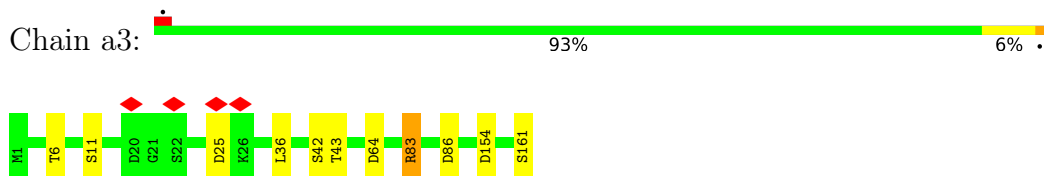
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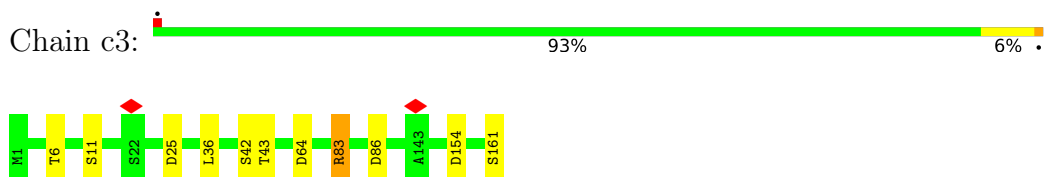
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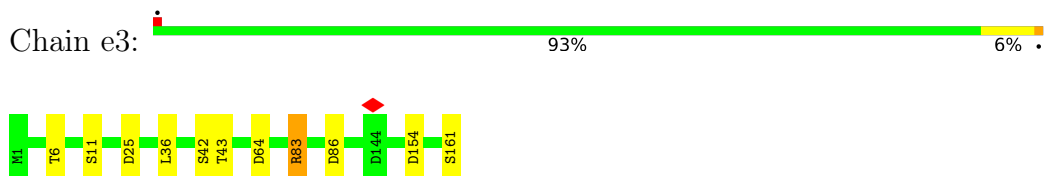
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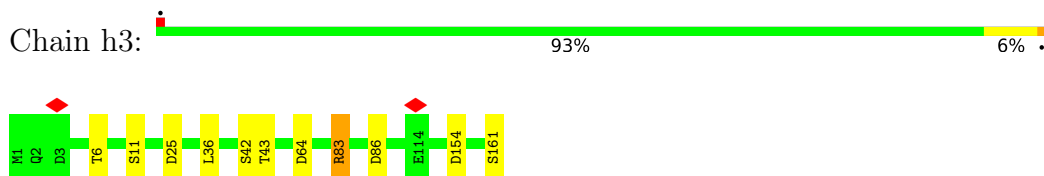
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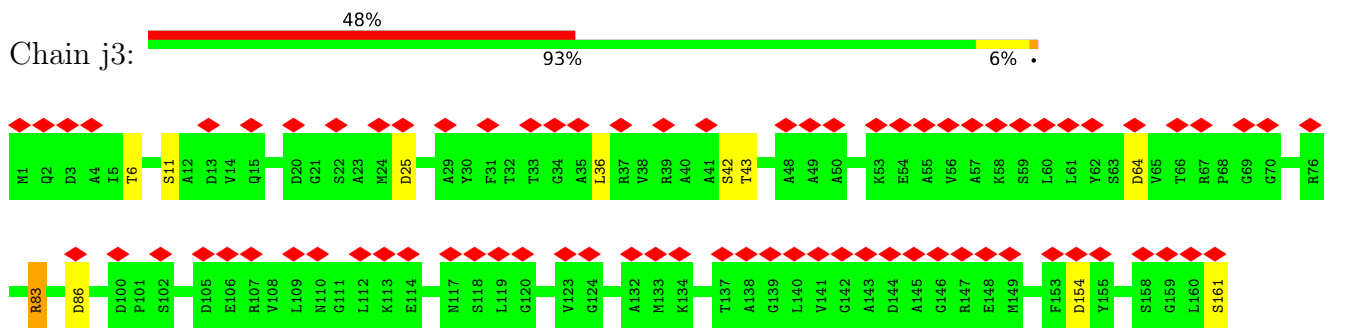
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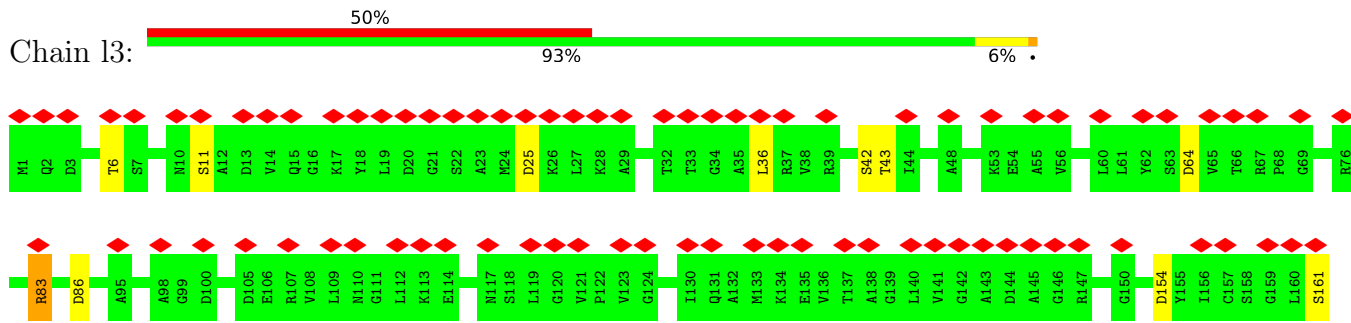
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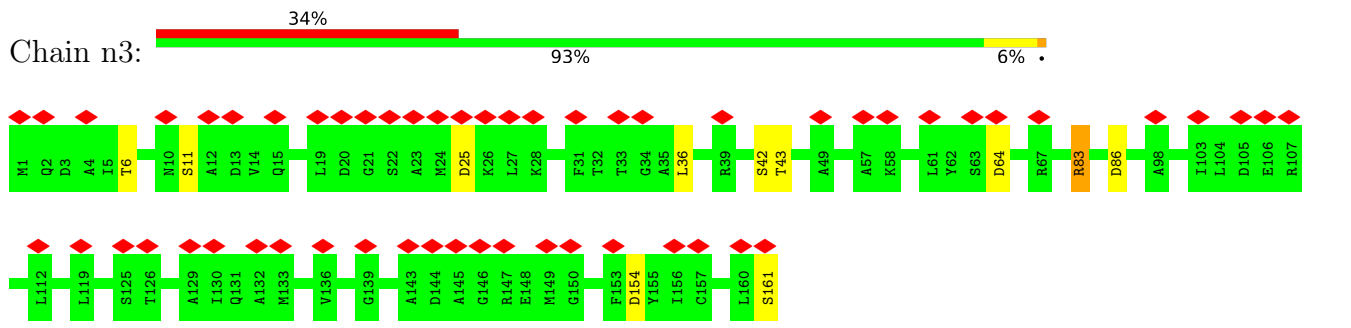
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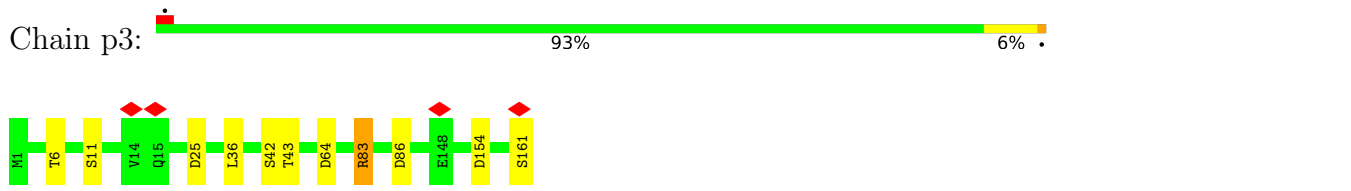
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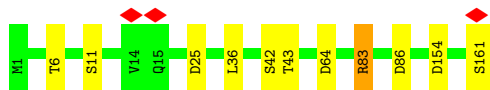


• Molecule 8: Allophycocyanin beta subunit

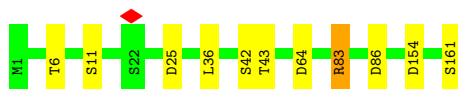




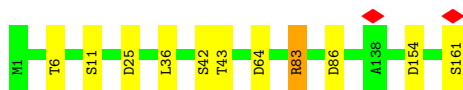
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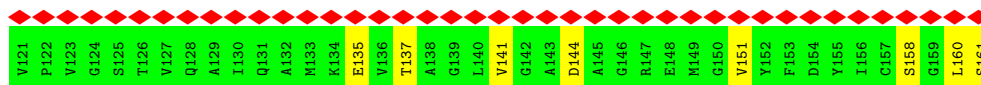
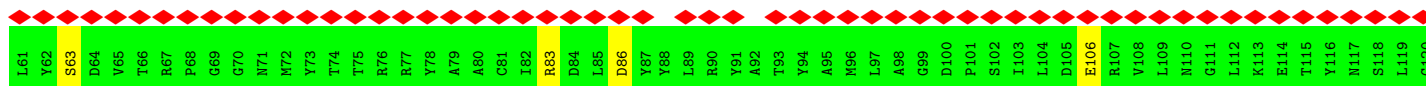
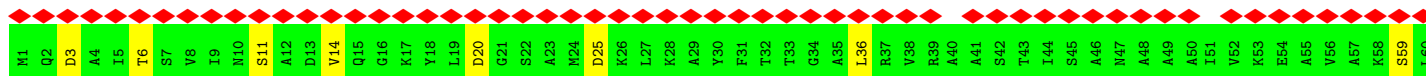
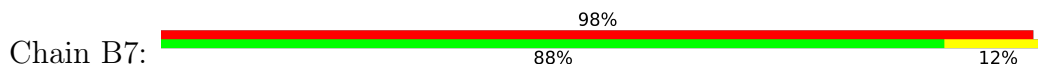
• Molecule 8: Allophycocyanin beta subunit



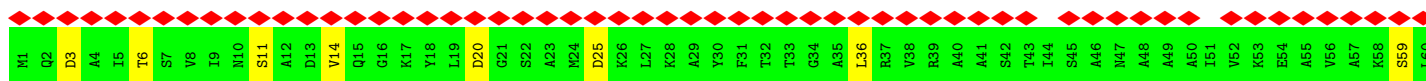
• Molecule 8: Allophycocyanin beta subunit

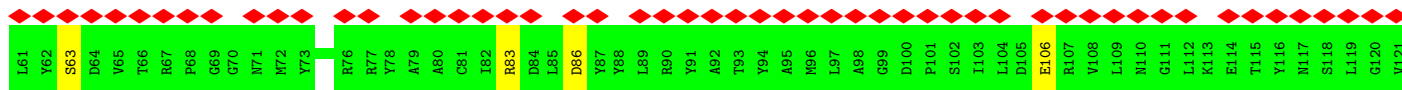


• Molecule 8: Allophycocyanin beta subunit

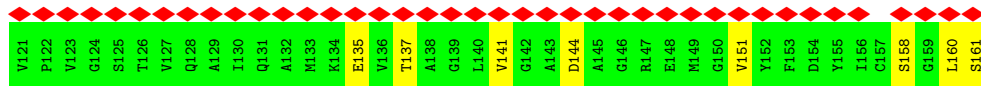
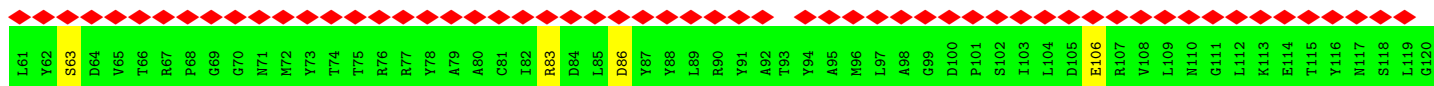
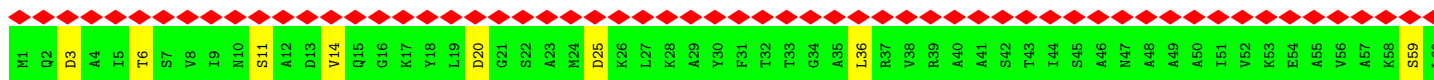
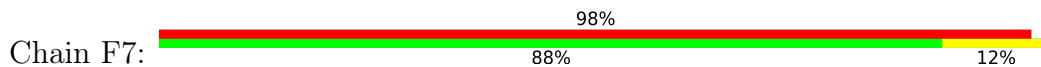


• Molecule 8: Allophycocyanin beta subunit

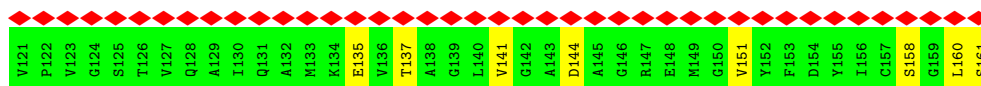
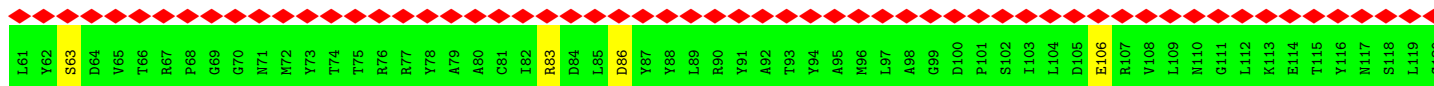
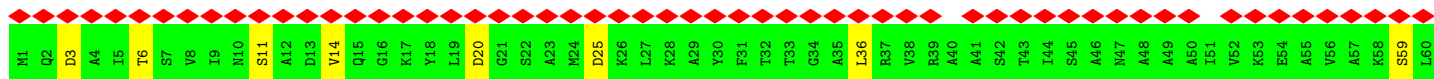
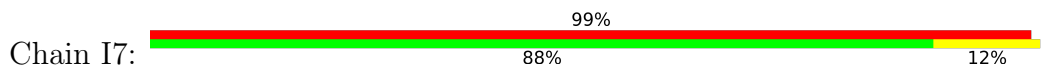




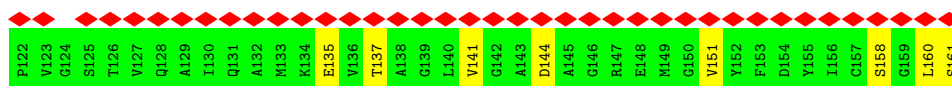
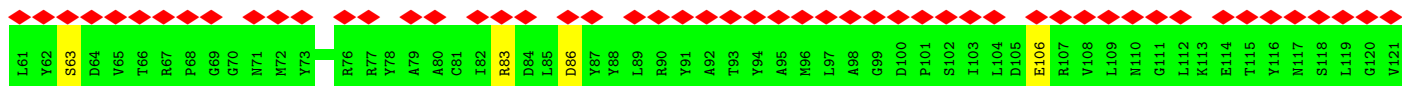
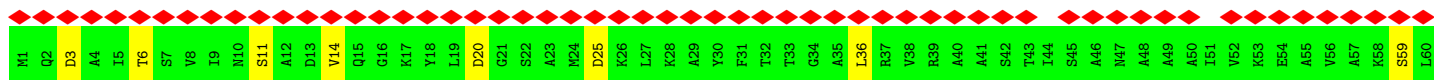
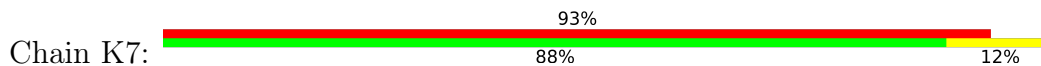
• Molecule 8: Allophycocyanin beta subunit



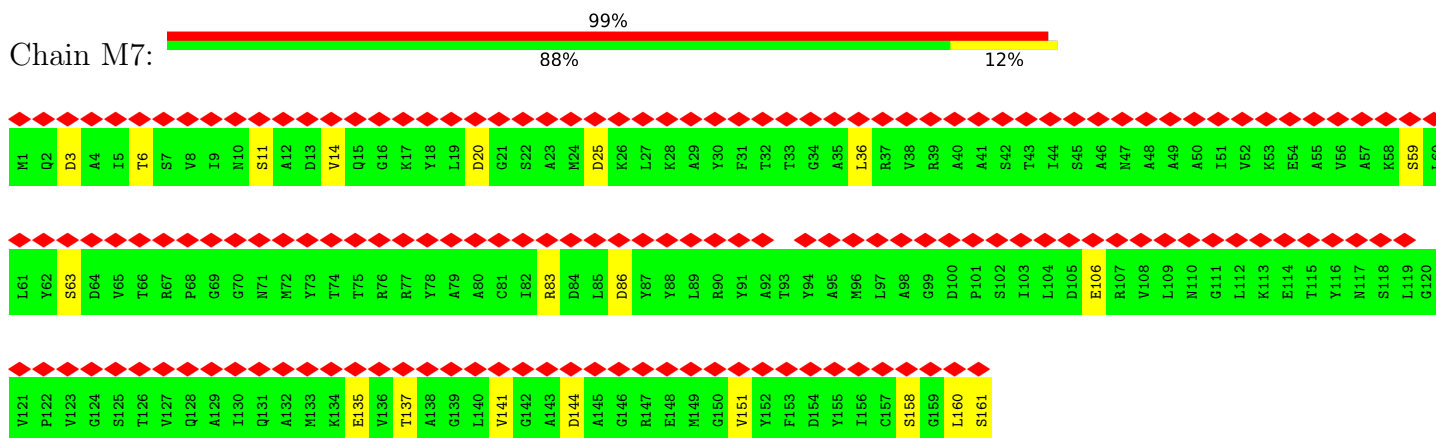
• Molecule 8: Allophycocyanin beta subunit



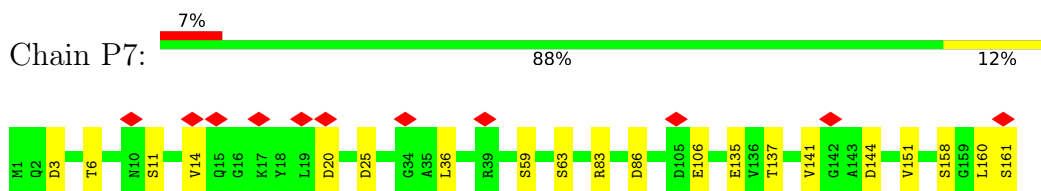
• Molecule 8: Allophycocyanin beta subunit



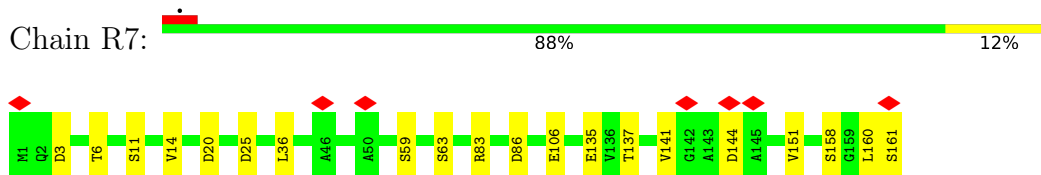
- Molecule 8: Allophycocyanin beta subunit



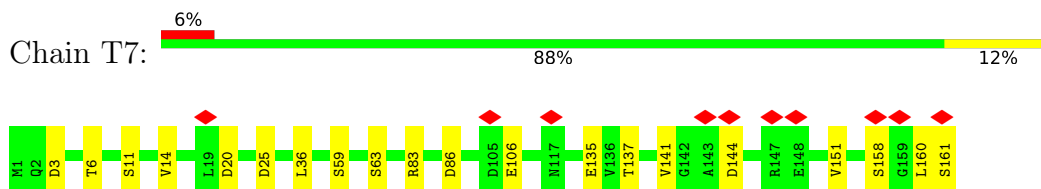
- Molecule 8: Allophycocyanin beta subunit



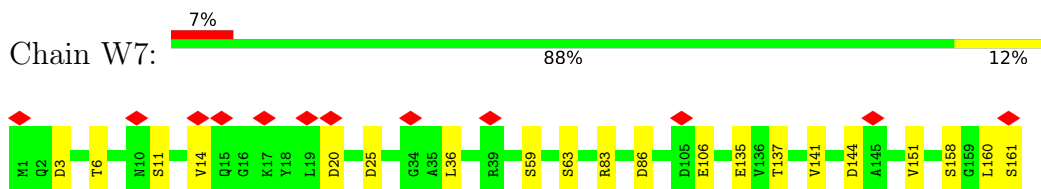
- Molecule 8: Allophycocyanin beta subunit



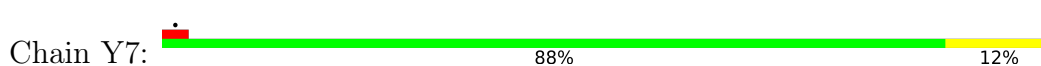
- Molecule 8: Allophycocyanin beta subunit



- Molecule 8: Allophycocyanin beta subunit

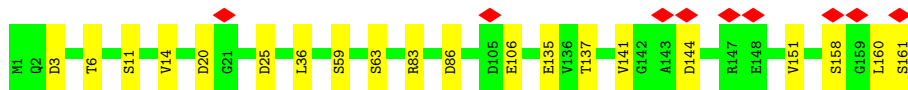
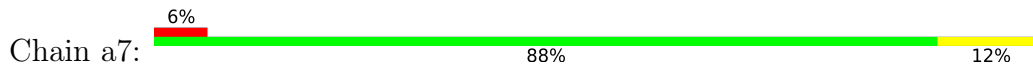


- Molecule 8: Allophycocyanin beta subunit





• Molecule 8: Allophycocyanin beta subunit



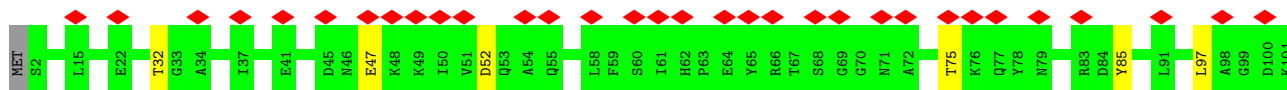
• Molecule 9: Allophycocyanin subunit beta-18



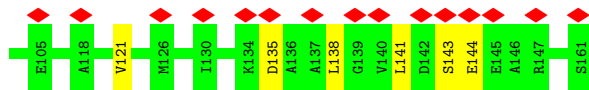
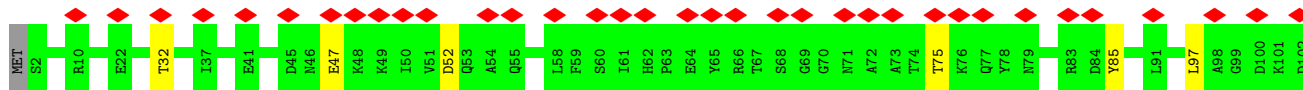
• Molecule 9: Allophycocyanin subunit beta-18



• Molecule 10: Allophycocyanin subunit alpha-B



• Molecule 10: Allophycocyanin subunit alpha-B



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	64268	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	64	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.082	Depositor
Minimum map value	-0.028	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0167	Depositor
Map size (Å)	527.5, 527.5, 527.5	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.055, 1.055, 1.055	Depositor

5 Model quality i

5.1 Standard geometry i

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

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	A1	0.62	2/1884 (0.1%)	0.81	7/2554 (0.3%)
1	A2	0.50	1/1909 (0.1%)	0.61	3/2588 (0.1%)
1	A4	0.64	4/1884 (0.2%)	0.73	4/2554 (0.2%)
1	A5	0.62	2/1884 (0.1%)	0.81	7/2554 (0.3%)
1	A6	0.50	1/1909 (0.1%)	0.60	3/2588 (0.1%)
1	A8	0.64	4/1884 (0.2%)	0.75	5/2554 (0.2%)
2	B1	0.40	0/1264	0.53	0/1718
2	B2	0.54	2/1264 (0.2%)	0.63	2/1718 (0.1%)
2	B4	0.64	4/1264 (0.3%)	0.99	8/1718 (0.5%)
2	B5	0.40	0/1264	0.53	0/1718
2	B6	0.54	2/1264 (0.2%)	0.63	2/1718 (0.1%)
2	B8	0.64	4/1264 (0.3%)	0.99	8/1718 (0.5%)
2	D1	0.40	0/1264	0.54	0/1718
2	D2	0.54	2/1264 (0.2%)	0.63	2/1718 (0.1%)
2	D4	0.64	4/1264 (0.3%)	0.99	8/1718 (0.5%)
2	D5	0.40	0/1264	0.54	0/1718
2	D6	0.54	2/1264 (0.2%)	0.63	2/1718 (0.1%)
2	D8	0.64	4/1264 (0.3%)	0.99	8/1718 (0.5%)
2	F1	0.41	0/1264	0.55	0/1718
2	F2	0.54	2/1264 (0.2%)	0.63	2/1718 (0.1%)
2	F4	0.65	4/1264 (0.3%)	1.00	8/1718 (0.5%)
2	F5	0.40	0/1264	0.55	0/1718
2	F6	0.54	2/1264 (0.2%)	0.63	2/1718 (0.1%)
2	F8	0.65	4/1264 (0.3%)	1.00	8/1718 (0.5%)
2	H1	0.40	0/1264	0.54	0/1718
2	H2	0.54	2/1264 (0.2%)	0.63	2/1718 (0.1%)
2	H4	0.64	4/1264 (0.3%)	0.99	8/1718 (0.5%)
2	H5	0.40	0/1264	0.54	0/1718
2	H6	0.54	2/1264 (0.2%)	0.63	2/1718 (0.1%)
2	H8	0.64	4/1264 (0.3%)	0.99	8/1718 (0.5%)
2	J1	0.40	0/1264	0.54	0/1718
2	J2	0.54	2/1264 (0.2%)	0.63	2/1718 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	J4	0.64	4/1264 (0.3%)	1.00	8/1718 (0.5%)
2	J5	0.40	0/1264	0.54	0/1718
2	J6	0.54	2/1264 (0.2%)	0.63	2/1718 (0.1%)
2	J8	0.65	4/1264 (0.3%)	1.00	8/1718 (0.5%)
2	L1	0.40	0/1264	0.54	0/1718
2	L2	0.54	2/1264 (0.2%)	0.63	2/1718 (0.1%)
2	L4	0.65	4/1264 (0.3%)	1.00	8/1718 (0.5%)
2	L5	0.40	0/1264	0.54	0/1718
2	L6	0.54	2/1264 (0.2%)	0.63	2/1718 (0.1%)
2	L8	0.64	4/1264 (0.3%)	1.00	8/1718 (0.5%)
2	O1	0.40	0/1256	0.54	0/1708
2	O2	0.54	2/1264 (0.2%)	0.63	2/1718 (0.1%)
2	O4	0.64	4/1264 (0.3%)	0.98	8/1718 (0.5%)
2	O5	0.40	0/1256	0.54	0/1708
2	O6	0.54	2/1264 (0.2%)	0.63	2/1718 (0.1%)
2	O8	0.64	4/1264 (0.3%)	0.98	8/1718 (0.5%)
2	Q1	0.40	0/1264	0.54	0/1718
2	Q2	0.54	2/1264 (0.2%)	0.63	2/1718 (0.1%)
2	Q4	0.64	4/1264 (0.3%)	0.99	8/1718 (0.5%)
2	Q5	0.40	0/1264	0.54	0/1718
2	Q6	0.54	2/1264 (0.2%)	0.63	2/1718 (0.1%)
2	Q8	0.64	4/1264 (0.3%)	0.99	8/1718 (0.5%)
2	S1	0.40	0/1264	0.54	0/1718
2	S2	0.54	2/1264 (0.2%)	0.63	2/1718 (0.1%)
2	S4	0.64	4/1264 (0.3%)	0.73	5/1718 (0.3%)
2	S5	0.40	0/1264	0.54	0/1718
2	S6	0.54	2/1264 (0.2%)	0.63	2/1718 (0.1%)
2	S8	0.64	4/1264 (0.3%)	0.73	5/1718 (0.3%)
2	U1	0.40	0/1264	0.55	0/1718
2	U2	0.54	2/1264 (0.2%)	0.63	2/1718 (0.1%)
2	U4	0.64	4/1264 (0.3%)	1.00	8/1718 (0.5%)
2	U5	0.40	0/1264	0.55	0/1718
2	U6	0.54	2/1264 (0.2%)	0.63	2/1718 (0.1%)
2	U8	0.64	4/1264 (0.3%)	1.00	8/1718 (0.5%)
2	W1	0.40	0/1264	0.55	0/1718
2	W2	0.54	2/1264 (0.2%)	0.63	2/1718 (0.1%)
2	W4	0.64	4/1264 (0.3%)	1.00	8/1718 (0.5%)
2	W5	0.40	0/1264	0.55	0/1718
2	W6	0.54	2/1264 (0.2%)	0.63	2/1718 (0.1%)
2	W8	0.64	4/1264 (0.3%)	1.00	8/1718 (0.5%)
2	Y1	0.40	0/1264	0.54	0/1718
2	Y2	0.54	2/1264 (0.2%)	0.63	2/1718 (0.1%)
2	Y4	0.64	4/1264 (0.3%)	1.00	8/1718 (0.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	Y5	0.40	0/1264	0.54	0/1718
2	Y6	0.54	2/1264 (0.2%)	0.63	2/1718 (0.1%)
2	Y8	0.64	4/1264 (0.3%)	1.00	8/1718 (0.5%)
3	C1	0.39	0/1295	1.20	11/1751 (0.6%)
3	C2	0.41	0/1295	1.06	8/1751 (0.5%)
3	C4	0.50	1/1295 (0.1%)	1.06	4/1751 (0.2%)
3	C5	0.39	0/1295	1.20	11/1751 (0.6%)
3	C6	0.41	0/1295	1.07	8/1751 (0.5%)
3	C8	0.50	1/1295 (0.1%)	1.06	4/1751 (0.2%)
3	E1	0.39	0/1295	1.20	11/1751 (0.6%)
3	E2	0.41	0/1295	1.05	7/1751 (0.4%)
3	E4	0.51	1/1295 (0.1%)	1.06	4/1751 (0.2%)
3	E5	0.39	0/1295	1.20	11/1751 (0.6%)
3	E6	0.41	0/1295	1.05	7/1751 (0.4%)
3	E8	0.51	1/1295 (0.1%)	1.07	4/1751 (0.2%)
3	G1	0.39	0/1295	1.00	8/1751 (0.5%)
3	G2	0.40	0/1295	1.04	7/1751 (0.4%)
3	G4	0.51	1/1295 (0.1%)	1.06	4/1751 (0.2%)
3	G5	0.39	0/1295	1.00	8/1751 (0.5%)
3	G6	0.41	0/1295	1.04	7/1751 (0.4%)
3	G8	0.51	1/1295 (0.1%)	1.06	4/1751 (0.2%)
3	I1	0.39	0/1295	1.20	11/1751 (0.6%)
3	I2	0.41	0/1295	1.06	8/1751 (0.5%)
3	I4	0.52	1/1295 (0.1%)	1.07	4/1751 (0.2%)
3	I5	0.39	0/1295	1.20	11/1751 (0.6%)
3	I6	0.41	0/1295	1.06	8/1751 (0.5%)
3	I8	0.52	1/1295 (0.1%)	1.07	4/1751 (0.2%)
3	K1	0.39	0/1295	1.20	11/1751 (0.6%)
3	K2	0.39	0/1295	0.98	5/1751 (0.3%)
3	K4	0.52	1/1295 (0.1%)	1.08	4/1751 (0.2%)
3	K5	0.39	0/1295	1.20	11/1751 (0.6%)
3	K6	0.39	0/1295	0.98	5/1751 (0.3%)
3	K8	0.51	1/1295 (0.1%)	1.08	4/1751 (0.2%)
3	M1	0.39	0/1295	1.20	11/1751 (0.6%)
3	M2	0.40	0/1295	1.02	6/1751 (0.3%)
3	M4	0.50	1/1295 (0.1%)	1.05	3/1751 (0.2%)
3	M5	0.39	0/1295	1.20	11/1751 (0.6%)
3	M6	0.40	0/1295	1.02	6/1751 (0.3%)
3	M8	0.50	1/1295 (0.1%)	1.05	3/1751 (0.2%)
3	P1	0.39	0/1295	1.20	11/1751 (0.6%)
3	P2	0.40	0/1295	1.06	7/1751 (0.4%)
3	P4	0.51	1/1295 (0.1%)	0.66	1/1751 (0.1%)
3	P5	0.39	0/1295	1.20	11/1751 (0.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	P6	0.40	0/1295	1.05	7/1751 (0.4%)
3	P8	0.51	1/1295 (0.1%)	0.66	1/1751 (0.1%)
3	R1	0.39	0/1295	1.20	11/1751 (0.6%)
3	R2	0.41	0/1295	1.03	6/1751 (0.3%)
3	R4	0.50	1/1295 (0.1%)	1.07	4/1751 (0.2%)
3	R5	0.39	0/1295	1.20	11/1751 (0.6%)
3	R6	0.41	0/1295	1.03	6/1751 (0.3%)
3	R8	0.50	1/1295 (0.1%)	1.07	4/1751 (0.2%)
3	T1	0.39	0/1295	1.20	11/1751 (0.6%)
3	T2	0.40	0/1295	1.01	6/1751 (0.3%)
3	T4	0.50	1/1295 (0.1%)	0.64	1/1751 (0.1%)
3	T5	0.39	0/1295	1.20	11/1751 (0.6%)
3	T6	0.40	0/1295	1.01	6/1751 (0.3%)
3	T8	0.50	1/1295 (0.1%)	0.64	1/1751 (0.1%)
3	V1	0.39	0/1295	1.20	11/1751 (0.6%)
3	V2	0.42	0/1295	0.69	5/1751 (0.3%)
3	V4	0.51	1/1295 (0.1%)	1.06	4/1751 (0.2%)
3	V5	0.39	0/1295	1.20	11/1751 (0.6%)
3	V6	0.42	0/1295	0.69	5/1751 (0.3%)
3	V8	0.51	1/1295 (0.1%)	1.06	4/1751 (0.2%)
3	X1	0.39	0/1295	1.20	11/1751 (0.6%)
3	X2	0.40	0/1295	1.03	6/1751 (0.3%)
3	X4	0.47	0/1295	1.04	4/1751 (0.2%)
3	X5	0.39	0/1295	1.20	11/1751 (0.6%)
3	X6	0.40	0/1295	1.03	6/1751 (0.3%)
3	X8	0.47	0/1295	1.04	4/1751 (0.2%)
3	Z1	0.39	0/1295	1.20	11/1751 (0.6%)
3	Z2	0.41	0/1295	1.05	7/1751 (0.4%)
3	Z4	0.47	0/1295	1.04	4/1751 (0.2%)
3	Z5	0.39	0/1295	1.20	11/1751 (0.6%)
3	Z6	0.41	0/1295	1.05	7/1751 (0.4%)
3	Z8	0.47	0/1295	1.04	4/1751 (0.2%)
4	N1	0.54	1/2313 (0.0%)	0.72	4/3133 (0.1%)
4	N2	0.56	1/2313 (0.0%)	0.77	6/3133 (0.2%)
4	N4	0.55	1/2313 (0.0%)	0.71	4/3133 (0.1%)
4	N5	0.54	1/2313 (0.0%)	0.72	4/3133 (0.1%)
4	N6	0.56	1/2313 (0.0%)	0.77	6/3133 (0.2%)
4	N8	0.55	1/2313 (0.0%)	0.71	4/3133 (0.1%)
4	a1	0.46	0/493	0.78	1/664 (0.2%)
4	a2	0.43	1/493 (0.2%)	0.61	0/664
4	a4	0.46	1/475 (0.2%)	0.72	0/640
4	a5	0.46	0/493	0.78	1/664 (0.2%)
4	a6	0.43	1/493 (0.2%)	0.61	0/664

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
4	a8	0.46	1/475 (0.2%)	0.72	0/640
5	03	0.46	1/6727 (0.0%)	0.64	5/9089 (0.1%)
5	13	0.47	2/6727 (0.0%)	0.64	6/9089 (0.1%)
6	23	0.56	1/538 (0.2%)	0.70	1/721 (0.1%)
6	33	0.56	1/538 (0.2%)	0.70	1/721 (0.1%)
6	G7	0.42	0/538	0.66	1/721 (0.1%)
6	N7	0.34	0/546	0.62	0/731
6	U7	0.38	0/538	0.57	0/721
6	b7	0.38	0/538	0.59	0/721
7	A7	0.39	0/1214	0.52	0/1640
7	C7	0.39	0/1214	0.52	0/1640
7	E7	0.39	0/1214	0.52	0/1640
7	G3	0.35	0/1214	0.99	3/1640 (0.2%)
7	H7	0.39	0/1214	0.53	0/1640
7	I3	0.35	0/1214	0.99	3/1640 (0.2%)
7	J7	0.39	0/1214	0.52	0/1640
7	K3	0.35	0/1214	0.99	3/1640 (0.2%)
7	L7	0.39	0/1214	0.52	0/1640
7	N3	0.35	0/1214	0.99	3/1640 (0.2%)
7	O7	0.39	0/1214	0.52	0/1640
7	P3	0.35	0/1214	0.99	3/1640 (0.2%)
7	Q7	0.39	0/1214	0.52	0/1640
7	R3	0.35	0/1214	0.99	3/1640 (0.2%)
7	S7	0.39	0/1214	0.52	0/1640
7	T3	0.35	0/1214	0.99	3/1640 (0.2%)
7	V7	0.39	0/1214	0.52	0/1640
7	X3	0.35	0/1214	0.99	3/1640 (0.2%)
7	X7	0.39	0/1214	0.52	0/1640
7	Z3	0.35	0/1214	0.99	3/1640 (0.2%)
7	Z7	0.39	0/1214	0.52	0/1640
7	b3	0.35	0/1214	0.99	3/1640 (0.2%)
7	d3	0.35	0/1214	0.99	3/1640 (0.2%)
7	f3	0.35	0/1214	0.99	3/1640 (0.2%)
7	i3	0.35	0/1214	0.99	3/1640 (0.2%)
7	k3	0.35	0/1214	0.99	3/1640 (0.2%)
7	o3	0.35	0/1214	1.00	3/1640 (0.2%)
7	q3	0.35	0/1214	0.99	3/1640 (0.2%)
7	s3	0.35	0/1214	0.99	3/1640 (0.2%)
7	u3	0.35	0/1214	0.99	3/1640 (0.2%)
7	w3	0.35	0/1214	1.00	3/1640 (0.2%)
7	y3	0.35	0/1214	0.99	3/1640 (0.2%)
8	B7	0.41	0/1221	0.96	3/1653 (0.2%)
8	D7	0.41	0/1221	0.96	3/1653 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
8	F7	0.41	0/1221	0.96	3/1653 (0.2%)
8	H3	0.40	0/1221	0.85	3/1653 (0.2%)
8	I7	0.41	0/1221	0.95	3/1653 (0.2%)
8	J3	0.40	0/1221	0.51	0/1653
8	K7	0.41	0/1221	0.96	3/1653 (0.2%)
8	L3	0.40	0/1221	0.85	3/1653 (0.2%)
8	M3	0.40	0/1221	0.85	3/1653 (0.2%)
8	M7	0.41	0/1221	0.96	3/1653 (0.2%)
8	O3	0.40	0/1221	0.85	3/1653 (0.2%)
8	P7	0.41	0/1221	0.96	3/1653 (0.2%)
8	R7	0.41	0/1221	0.96	3/1653 (0.2%)
8	S3	0.40	0/1221	0.85	3/1653 (0.2%)
8	T7	0.41	0/1221	0.95	3/1653 (0.2%)
8	U3	0.40	0/1221	0.85	3/1653 (0.2%)
8	W3	0.40	0/1221	0.85	3/1653 (0.2%)
8	W7	0.41	0/1221	0.96	3/1653 (0.2%)
8	Y3	0.40	0/1221	0.51	0/1653
8	Y7	0.41	0/1221	0.96	3/1653 (0.2%)
8	a3	0.40	0/1221	0.85	3/1653 (0.2%)
8	a7	0.41	0/1221	0.96	3/1653 (0.2%)
8	c3	0.40	0/1221	0.85	3/1653 (0.2%)
8	e3	0.40	0/1221	0.85	3/1653 (0.2%)
8	h3	0.40	0/1221	0.85	3/1653 (0.2%)
8	j3	0.40	0/1221	0.85	3/1653 (0.2%)
8	l3	0.40	0/1221	0.85	3/1653 (0.2%)
8	n3	0.40	0/1221	0.85	3/1653 (0.2%)
8	p3	0.40	0/1221	0.85	3/1653 (0.2%)
8	r3	0.40	0/1221	0.85	3/1653 (0.2%)
8	t3	0.40	0/1221	0.85	3/1653 (0.2%)
8	v3	0.40	0/1221	0.85	3/1653 (0.2%)
8	x3	0.40	0/1221	0.85	3/1653 (0.2%)
8	z3	0.40	0/1221	0.85	3/1653 (0.2%)
9	Q3	0.40	0/1334	0.59	0/1806
9	g3	0.40	0/1334	0.59	0/1806
10	V3	0.40	0/1255	0.59	0/1698
10	m3	0.40	0/1255	0.59	0/1698
All	All	0.47	193/314616 (0.1%)	0.87	959/426078 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A1	0	1
1	A2	0	1
1	A4	0	1
1	A5	0	1
1	A6	0	1
1	A8	0	1
2	W1	0	1
2	W5	0	1
3	C2	0	1
3	C6	0	1
3	E2	0	1
3	E6	0	1
3	G2	0	1
3	G6	0	1
3	K2	0	1
3	K6	0	1
3	R2	0	1
3	R6	0	1
3	T2	0	1
3	T6	0	1
3	V2	0	1
3	V6	0	1
3	Z2	0	1
3	Z6	0	1
4	N1	0	1
4	N5	0	1
4	a4	0	1
4	a8	0	1
5	03	0	1
5	13	0	2
6	N7	0	1
All	All	0	32

The worst 5 of 193 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H4	28	TYR	CB-CG	10.22	1.67	1.51
2	L4	28	TYR	CB-CG	10.21	1.67	1.51
2	B4	28	TYR	CZ-OH	10.21	1.55	1.37
2	H4	28	TYR	CZ-OH	10.20	1.55	1.37
2	O4	28	TYR	CB-CG	10.20	1.67	1.51

The worst 5 of 959 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I6	84	ARG	NE-CZ-NH2	24.22	132.41	120.30
3	I2	84	ARG	NE-CZ-NH2	24.21	132.41	120.30
3	X2	84	ARG	NE-CZ-NH2	24.21	132.40	120.30
3	R2	84	ARG	NE-CZ-NH2	24.19	132.40	120.30
3	Z2	84	ARG	NE-CZ-NH2	24.18	132.39	120.30

There are no chirality outliers.

5 of 32 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A1	24	GLY	Peptide
1	A2	54	PHE	Peptide
3	C2	109	CYS	Peptide
4	N1	225	SER	Peptide
2	W1	1	MET	Peptide

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	A1	223/248 (90%)	205 (92%)	17 (8%)	1 (0%)	34	72
1	A2	226/248 (91%)	216 (96%)	10 (4%)	0	100	100
1	A4	223/248 (90%)	210 (94%)	12 (5%)	1 (0%)	34	72
1	A5	223/248 (90%)	205 (92%)	17 (8%)	1 (0%)	34	72
1	A6	226/248 (91%)	217 (96%)	9 (4%)	0	100	100
1	A8	223/248 (90%)	210 (94%)	12 (5%)	1 (0%)	34	72
2	B1	160/162 (99%)	158 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B2	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
2	B4	160/162 (99%)	160 (100%)	0	0	100	100
2	B5	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
2	B6	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
2	B8	160/162 (99%)	160 (100%)	0	0	100	100
2	D1	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
2	D2	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
2	D4	160/162 (99%)	160 (100%)	0	0	100	100
2	D5	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
2	D6	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
2	D8	160/162 (99%)	160 (100%)	0	0	100	100
2	F1	160/162 (99%)	157 (98%)	3 (2%)	0	100	100
2	F2	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
2	F4	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
2	F5	160/162 (99%)	157 (98%)	3 (2%)	0	100	100
2	F6	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
2	F8	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
2	H1	160/162 (99%)	157 (98%)	3 (2%)	0	100	100
2	H2	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
2	H4	160/162 (99%)	160 (100%)	0	0	100	100
2	H5	160/162 (99%)	157 (98%)	3 (2%)	0	100	100
2	H6	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
2	H8	160/162 (99%)	160 (100%)	0	0	100	100
2	J1	160/162 (99%)	157 (98%)	3 (2%)	0	100	100
2	J2	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
2	J4	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
2	J5	160/162 (99%)	157 (98%)	3 (2%)	0	100	100
2	J6	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
2	J8	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
2	L1	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
2	L2	160/162 (99%)	159 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	L4	160/162 (99%)	160 (100%)	0	0	100	100
2	L5	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
2	L6	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
2	L8	160/162 (99%)	160 (100%)	0	0	100	100
2	O1	159/162 (98%)	157 (99%)	2 (1%)	0	100	100
2	O2	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
2	O4	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
2	O5	159/162 (98%)	157 (99%)	2 (1%)	0	100	100
2	O6	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
2	O8	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
2	Q1	160/162 (99%)	157 (98%)	3 (2%)	0	100	100
2	Q2	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
2	Q4	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
2	Q5	160/162 (99%)	157 (98%)	3 (2%)	0	100	100
2	Q6	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
2	Q8	160/162 (99%)	157 (98%)	3 (2%)	0	100	100
2	S1	160/162 (99%)	157 (98%)	3 (2%)	0	100	100
2	S2	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
2	S4	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
2	S5	160/162 (99%)	157 (98%)	3 (2%)	0	100	100
2	S6	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
2	S8	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
2	U1	160/162 (99%)	157 (98%)	3 (2%)	0	100	100
2	U2	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
2	U4	160/162 (99%)	160 (100%)	0	0	100	100
2	U5	160/162 (99%)	157 (98%)	3 (2%)	0	100	100
2	U6	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
2	U8	160/162 (99%)	160 (100%)	0	0	100	100
2	W1	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
2	W2	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
2	W4	160/162 (99%)	160 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	W5	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
2	W6	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
2	W8	160/162 (99%)	160 (100%)	0	0	100	100
2	Y1	160/162 (99%)	157 (98%)	3 (2%)	0	100	100
2	Y2	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
2	Y4	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
2	Y5	160/162 (99%)	157 (98%)	3 (2%)	0	100	100
2	Y6	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
2	Y8	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
3	C1	170/172 (99%)	168 (99%)	2 (1%)	0	100	100
3	C2	170/172 (99%)	163 (96%)	5 (3%)	2 (1%)	13	50
3	C4	170/172 (99%)	167 (98%)	2 (1%)	1 (1%)	25	64
3	C5	170/172 (99%)	168 (99%)	2 (1%)	0	100	100
3	C6	170/172 (99%)	165 (97%)	3 (2%)	2 (1%)	13	50
3	C8	170/172 (99%)	167 (98%)	2 (1%)	1 (1%)	25	64
3	E1	170/172 (99%)	168 (99%)	2 (1%)	0	100	100
3	E2	170/172 (99%)	168 (99%)	1 (1%)	1 (1%)	25	64
3	E4	170/172 (99%)	167 (98%)	2 (1%)	1 (1%)	25	64
3	E5	170/172 (99%)	168 (99%)	2 (1%)	0	100	100
3	E6	170/172 (99%)	168 (99%)	1 (1%)	1 (1%)	25	64
3	E8	170/172 (99%)	167 (98%)	2 (1%)	1 (1%)	25	64
3	G1	170/172 (99%)	168 (99%)	2 (1%)	0	100	100
3	G2	170/172 (99%)	167 (98%)	2 (1%)	1 (1%)	25	64
3	G4	170/172 (99%)	167 (98%)	2 (1%)	1 (1%)	25	64
3	G5	170/172 (99%)	168 (99%)	2 (1%)	0	100	100
3	G6	170/172 (99%)	169 (99%)	0	1 (1%)	25	64
3	G8	170/172 (99%)	167 (98%)	2 (1%)	1 (1%)	25	64
3	I1	170/172 (99%)	168 (99%)	2 (1%)	0	100	100
3	I2	170/172 (99%)	168 (99%)	1 (1%)	1 (1%)	25	64
3	I4	170/172 (99%)	166 (98%)	4 (2%)	0	100	100
3	I5	170/172 (99%)	168 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	I6	170/172 (99%)	168 (99%)	1 (1%)	1 (1%)	25	64
3	I8	170/172 (99%)	166 (98%)	4 (2%)	0	100	100
3	K1	170/172 (99%)	168 (99%)	2 (1%)	0	100	100
3	K2	170/172 (99%)	169 (99%)	0	1 (1%)	25	64
3	K4	170/172 (99%)	167 (98%)	2 (1%)	1 (1%)	25	64
3	K5	170/172 (99%)	168 (99%)	2 (1%)	0	100	100
3	K6	170/172 (99%)	169 (99%)	0	1 (1%)	25	64
3	K8	170/172 (99%)	167 (98%)	2 (1%)	1 (1%)	25	64
3	M1	170/172 (99%)	168 (99%)	2 (1%)	0	100	100
3	M2	170/172 (99%)	169 (99%)	0	1 (1%)	25	64
3	M4	170/172 (99%)	167 (98%)	2 (1%)	1 (1%)	25	64
3	M5	170/172 (99%)	168 (99%)	2 (1%)	0	100	100
3	M6	170/172 (99%)	169 (99%)	0	1 (1%)	25	64
3	M8	170/172 (99%)	167 (98%)	2 (1%)	1 (1%)	25	64
3	P1	170/172 (99%)	168 (99%)	2 (1%)	0	100	100
3	P2	170/172 (99%)	166 (98%)	2 (1%)	2 (1%)	13	50
3	P4	170/172 (99%)	167 (98%)	2 (1%)	1 (1%)	25	64
3	P5	170/172 (99%)	168 (99%)	2 (1%)	0	100	100
3	P6	170/172 (99%)	166 (98%)	2 (1%)	2 (1%)	13	50
3	P8	170/172 (99%)	167 (98%)	2 (1%)	1 (1%)	25	64
3	R1	170/172 (99%)	168 (99%)	2 (1%)	0	100	100
3	R2	170/172 (99%)	169 (99%)	0	1 (1%)	25	64
3	R4	170/172 (99%)	166 (98%)	3 (2%)	1 (1%)	25	64
3	R5	170/172 (99%)	168 (99%)	2 (1%)	0	100	100
3	R6	170/172 (99%)	169 (99%)	0	1 (1%)	25	64
3	R8	170/172 (99%)	166 (98%)	3 (2%)	1 (1%)	25	64
3	T1	170/172 (99%)	168 (99%)	2 (1%)	0	100	100
3	T2	170/172 (99%)	169 (99%)	0	1 (1%)	25	64
3	T4	170/172 (99%)	167 (98%)	2 (1%)	1 (1%)	25	64
3	T5	170/172 (99%)	168 (99%)	2 (1%)	0	100	100
3	T6	170/172 (99%)	169 (99%)	0	1 (1%)	25	64

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	T8	170/172 (99%)	167 (98%)	2 (1%)	1 (1%)	25	64
3	V1	170/172 (99%)	168 (99%)	2 (1%)	0	100	100
3	V2	170/172 (99%)	167 (98%)	2 (1%)	1 (1%)	25	64
3	V4	170/172 (99%)	167 (98%)	2 (1%)	1 (1%)	25	64
3	V5	170/172 (99%)	168 (99%)	2 (1%)	0	100	100
3	V6	170/172 (99%)	167 (98%)	2 (1%)	1 (1%)	25	64
3	V8	170/172 (99%)	167 (98%)	2 (1%)	1 (1%)	25	64
3	X1	170/172 (99%)	168 (99%)	2 (1%)	0	100	100
3	X2	170/172 (99%)	167 (98%)	1 (1%)	2 (1%)	13	50
3	X4	170/172 (99%)	167 (98%)	2 (1%)	1 (1%)	25	64
3	X5	170/172 (99%)	168 (99%)	2 (1%)	0	100	100
3	X6	170/172 (99%)	167 (98%)	1 (1%)	2 (1%)	13	50
3	X8	170/172 (99%)	167 (98%)	2 (1%)	1 (1%)	25	64
3	Z1	170/172 (99%)	168 (99%)	2 (1%)	0	100	100
3	Z2	170/172 (99%)	169 (99%)	0	1 (1%)	25	64
3	Z4	170/172 (99%)	167 (98%)	2 (1%)	1 (1%)	25	64
3	Z5	170/172 (99%)	168 (99%)	2 (1%)	0	100	100
3	Z6	170/172 (99%)	169 (99%)	0	1 (1%)	25	64
3	Z8	170/172 (99%)	167 (98%)	2 (1%)	1 (1%)	25	64
4	N1	287/290 (99%)	273 (95%)	13 (4%)	1 (0%)	41	75
4	N2	287/290 (99%)	276 (96%)	11 (4%)	0	100	100
4	N4	287/290 (99%)	272 (95%)	14 (5%)	1 (0%)	41	75
4	N5	287/290 (99%)	273 (95%)	13 (4%)	1 (0%)	41	75
4	N6	287/290 (99%)	276 (96%)	11 (4%)	0	100	100
4	N8	287/290 (99%)	272 (95%)	14 (5%)	1 (0%)	41	75
4	a1	62/290 (21%)	55 (89%)	7 (11%)	0	100	100
4	a2	62/290 (21%)	57 (92%)	4 (6%)	1 (2%)	9	43
4	a4	59/290 (20%)	54 (92%)	4 (7%)	1 (2%)	9	42
4	a5	62/290 (21%)	55 (89%)	7 (11%)	0	100	100
4	a6	62/290 (21%)	57 (92%)	4 (6%)	1 (2%)	9	43
4	a8	59/290 (20%)	54 (92%)	4 (7%)	1 (2%)	9	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	03	822/886 (93%)	773 (94%)	49 (6%)	0	100	100
5	13	822/886 (93%)	767 (93%)	54 (7%)	1 (0%)	51	84
6	23	63/67 (94%)	60 (95%)	3 (5%)	0	100	100
6	33	63/67 (94%)	60 (95%)	3 (5%)	0	100	100
6	G7	63/67 (94%)	60 (95%)	3 (5%)	0	100	100
6	N7	64/67 (96%)	59 (92%)	5 (8%)	0	100	100
6	U7	63/67 (94%)	61 (97%)	2 (3%)	0	100	100
6	b7	63/67 (94%)	61 (97%)	2 (3%)	0	100	100
7	A7	158/161 (98%)	152 (96%)	6 (4%)	0	100	100
7	C7	158/161 (98%)	152 (96%)	6 (4%)	0	100	100
7	E7	158/161 (98%)	152 (96%)	6 (4%)	0	100	100
7	G3	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
7	H7	158/161 (98%)	152 (96%)	6 (4%)	0	100	100
7	I3	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
7	J7	158/161 (98%)	152 (96%)	6 (4%)	0	100	100
7	K3	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
7	L7	158/161 (98%)	152 (96%)	6 (4%)	0	100	100
7	N3	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
7	O7	158/161 (98%)	152 (96%)	6 (4%)	0	100	100
7	P3	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
7	Q7	158/161 (98%)	152 (96%)	6 (4%)	0	100	100
7	R3	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
7	S7	158/161 (98%)	152 (96%)	6 (4%)	0	100	100
7	T3	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
7	V7	158/161 (98%)	152 (96%)	6 (4%)	0	100	100
7	X3	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
7	X7	158/161 (98%)	152 (96%)	6 (4%)	0	100	100
7	Z3	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
7	Z7	158/161 (98%)	152 (96%)	6 (4%)	0	100	100
7	b3	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
7	d3	158/161 (98%)	154 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	f3	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
7	i3	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
7	k3	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
7	o3	158/161 (98%)	152 (96%)	5 (3%)	1 (1%)	25	64
7	q3	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
7	s3	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
7	u3	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
7	w3	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
7	y3	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
8	B7	159/161 (99%)	155 (98%)	4 (2%)	0	100	100
8	D7	159/161 (99%)	155 (98%)	4 (2%)	0	100	100
8	F7	159/161 (99%)	155 (98%)	4 (2%)	0	100	100
8	H3	159/161 (99%)	151 (95%)	8 (5%)	0	100	100
8	I7	159/161 (99%)	155 (98%)	4 (2%)	0	100	100
8	J3	159/161 (99%)	151 (95%)	8 (5%)	0	100	100
8	K7	159/161 (99%)	155 (98%)	4 (2%)	0	100	100
8	L3	159/161 (99%)	152 (96%)	7 (4%)	0	100	100
8	M3	159/161 (99%)	151 (95%)	8 (5%)	0	100	100
8	M7	159/161 (99%)	155 (98%)	4 (2%)	0	100	100
8	O3	159/161 (99%)	151 (95%)	8 (5%)	0	100	100
8	P7	159/161 (99%)	155 (98%)	4 (2%)	0	100	100
8	R7	159/161 (99%)	155 (98%)	4 (2%)	0	100	100
8	S3	159/161 (99%)	152 (96%)	7 (4%)	0	100	100
8	T7	159/161 (99%)	155 (98%)	4 (2%)	0	100	100
8	U3	159/161 (99%)	151 (95%)	8 (5%)	0	100	100
8	W3	159/161 (99%)	151 (95%)	8 (5%)	0	100	100
8	W7	159/161 (99%)	155 (98%)	4 (2%)	0	100	100
8	Y3	159/161 (99%)	151 (95%)	8 (5%)	0	100	100
8	Y7	159/161 (99%)	155 (98%)	4 (2%)	0	100	100
8	a3	159/161 (99%)	151 (95%)	8 (5%)	0	100	100
8	a7	159/161 (99%)	155 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	c3	159/161 (99%)	151 (95%)	8 (5%)	0	100	100
8	e3	159/161 (99%)	151 (95%)	8 (5%)	0	100	100
8	h3	159/161 (99%)	151 (95%)	8 (5%)	0	100	100
8	j3	159/161 (99%)	151 (95%)	8 (5%)	0	100	100
8	l3	159/161 (99%)	151 (95%)	8 (5%)	0	100	100
8	n3	159/161 (99%)	151 (95%)	8 (5%)	0	100	100
8	p3	159/161 (99%)	152 (96%)	7 (4%)	0	100	100
8	r3	159/161 (99%)	152 (96%)	7 (4%)	0	100	100
8	t3	159/161 (99%)	151 (95%)	8 (5%)	0	100	100
8	v3	159/161 (99%)	152 (96%)	7 (4%)	0	100	100
8	x3	159/161 (99%)	151 (95%)	8 (5%)	0	100	100
8	z3	159/161 (99%)	151 (95%)	8 (5%)	0	100	100
9	Q3	167/169 (99%)	156 (93%)	11 (7%)	0	100	100
9	g3	167/169 (99%)	156 (93%)	11 (7%)	0	100	100
10	V3	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
10	m3	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
All	All	40325/42476 (95%)	39326 (98%)	933 (2%)	66 (0%)	50	81

5 of 66 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A1	210	PRO
3	C2	154	SER
7	o3	75	GLU
1	A4	37	ILE
1	A5	210	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A1	199/218 (91%)	197 (99%)	2 (1%)	76	88
1	A2	202/218 (93%)	193 (96%)	9 (4%)	27	61
1	A4	199/218 (91%)	197 (99%)	2 (1%)	76	88
1	A5	199/218 (91%)	195 (98%)	4 (2%)	55	79
1	A6	202/218 (93%)	192 (95%)	10 (5%)	24	58
1	A8	199/218 (91%)	196 (98%)	3 (2%)	65	84
2	B1	126/126 (100%)	116 (92%)	10 (8%)	12	41
2	B2	126/126 (100%)	111 (88%)	15 (12%)	5	25
2	B4	126/126 (100%)	110 (87%)	16 (13%)	4	22
2	B5	126/126 (100%)	116 (92%)	10 (8%)	12	41
2	B6	126/126 (100%)	111 (88%)	15 (12%)	5	25
2	B8	126/126 (100%)	111 (88%)	15 (12%)	5	25
2	D1	126/126 (100%)	117 (93%)	9 (7%)	14	46
2	D2	126/126 (100%)	111 (88%)	15 (12%)	5	25
2	D4	126/126 (100%)	110 (87%)	16 (13%)	4	22
2	D5	126/126 (100%)	117 (93%)	9 (7%)	14	46
2	D6	126/126 (100%)	111 (88%)	15 (12%)	5	25
2	D8	126/126 (100%)	111 (88%)	15 (12%)	5	25
2	F1	126/126 (100%)	117 (93%)	9 (7%)	14	46
2	F2	126/126 (100%)	111 (88%)	15 (12%)	5	25
2	F4	126/126 (100%)	110 (87%)	16 (13%)	4	22
2	F5	126/126 (100%)	117 (93%)	9 (7%)	14	46
2	F6	126/126 (100%)	111 (88%)	15 (12%)	5	25
2	F8	126/126 (100%)	110 (87%)	16 (13%)	4	22
2	H1	126/126 (100%)	117 (93%)	9 (7%)	14	46
2	H2	126/126 (100%)	111 (88%)	15 (12%)	5	25
2	H4	126/126 (100%)	109 (86%)	17 (14%)	4	21
2	H5	126/126 (100%)	117 (93%)	9 (7%)	14	46
2	H6	126/126 (100%)	111 (88%)	15 (12%)	5	25
2	H8	126/126 (100%)	109 (86%)	17 (14%)	4	21
2	J1	126/126 (100%)	117 (93%)	9 (7%)	14	46
2	J2	126/126 (100%)	111 (88%)	15 (12%)	5	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	J4	126/126 (100%)	110 (87%)	16 (13%)	4	22
2	J5	126/126 (100%)	116 (92%)	10 (8%)	12	41
2	J6	126/126 (100%)	111 (88%)	15 (12%)	5	25
2	J8	126/126 (100%)	110 (87%)	16 (13%)	4	22
2	L1	126/126 (100%)	117 (93%)	9 (7%)	14	46
2	L2	126/126 (100%)	111 (88%)	15 (12%)	5	25
2	L4	126/126 (100%)	113 (90%)	13 (10%)	7	32
2	L5	126/126 (100%)	117 (93%)	9 (7%)	14	46
2	L6	126/126 (100%)	111 (88%)	15 (12%)	5	25
2	L8	126/126 (100%)	112 (89%)	14 (11%)	6	28
2	O1	125/126 (99%)	116 (93%)	9 (7%)	14	45
2	O2	126/126 (100%)	111 (88%)	15 (12%)	5	25
2	O4	126/126 (100%)	110 (87%)	16 (13%)	4	22
2	O5	125/126 (99%)	116 (93%)	9 (7%)	14	45
2	O6	126/126 (100%)	111 (88%)	15 (12%)	5	25
2	O8	126/126 (100%)	110 (87%)	16 (13%)	4	22
2	Q1	126/126 (100%)	117 (93%)	9 (7%)	14	46
2	Q2	126/126 (100%)	111 (88%)	15 (12%)	5	25
2	Q4	126/126 (100%)	111 (88%)	15 (12%)	5	25
2	Q5	126/126 (100%)	117 (93%)	9 (7%)	14	46
2	Q6	126/126 (100%)	111 (88%)	15 (12%)	5	25
2	Q8	126/126 (100%)	111 (88%)	15 (12%)	5	25
2	S1	126/126 (100%)	117 (93%)	9 (7%)	14	46
2	S2	126/126 (100%)	111 (88%)	15 (12%)	5	25
2	S4	126/126 (100%)	112 (89%)	14 (11%)	6	28
2	S5	126/126 (100%)	117 (93%)	9 (7%)	14	46
2	S6	126/126 (100%)	111 (88%)	15 (12%)	5	25
2	S8	126/126 (100%)	112 (89%)	14 (11%)	6	28
2	U1	126/126 (100%)	117 (93%)	9 (7%)	14	46
2	U2	126/126 (100%)	111 (88%)	15 (12%)	5	25
2	U4	126/126 (100%)	112 (89%)	14 (11%)	6	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	U5	126/126 (100%)	117 (93%)	9 (7%)	14	46
2	U6	126/126 (100%)	111 (88%)	15 (12%)	5	25
2	U8	126/126 (100%)	112 (89%)	14 (11%)	6	28
2	W1	126/126 (100%)	117 (93%)	9 (7%)	14	46
2	W2	126/126 (100%)	111 (88%)	15 (12%)	5	25
2	W4	126/126 (100%)	112 (89%)	14 (11%)	6	28
2	W5	126/126 (100%)	117 (93%)	9 (7%)	14	46
2	W6	126/126 (100%)	111 (88%)	15 (12%)	5	25
2	W8	126/126 (100%)	112 (89%)	14 (11%)	6	28
2	Y1	126/126 (100%)	117 (93%)	9 (7%)	14	46
2	Y2	126/126 (100%)	111 (88%)	15 (12%)	5	25
2	Y4	126/126 (100%)	112 (89%)	14 (11%)	6	28
2	Y5	126/126 (100%)	117 (93%)	9 (7%)	14	46
2	Y6	126/126 (100%)	111 (88%)	15 (12%)	5	25
2	Y8	126/126 (100%)	112 (89%)	14 (11%)	6	28
3	C1	133/133 (100%)	123 (92%)	10 (8%)	13	43
3	C2	133/133 (100%)	113 (85%)	20 (15%)	3	17
3	C4	133/133 (100%)	122 (92%)	11 (8%)	11	40
3	C5	133/133 (100%)	123 (92%)	10 (8%)	13	43
3	C6	133/133 (100%)	112 (84%)	21 (16%)	2	15
3	C8	133/133 (100%)	123 (92%)	10 (8%)	13	43
3	E1	133/133 (100%)	123 (92%)	10 (8%)	13	43
3	E2	133/133 (100%)	115 (86%)	18 (14%)	4	21
3	E4	133/133 (100%)	122 (92%)	11 (8%)	11	40
3	E5	133/133 (100%)	123 (92%)	10 (8%)	13	43
3	E6	133/133 (100%)	115 (86%)	18 (14%)	4	21
3	E8	133/133 (100%)	122 (92%)	11 (8%)	11	40
3	G1	133/133 (100%)	123 (92%)	10 (8%)	13	43
3	G2	133/133 (100%)	115 (86%)	18 (14%)	4	21
3	G4	133/133 (100%)	122 (92%)	11 (8%)	11	40
3	G5	133/133 (100%)	123 (92%)	10 (8%)	13	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	G6	133/133 (100%)	116 (87%)	17 (13%)	4	22
3	G8	133/133 (100%)	122 (92%)	11 (8%)	11	40
3	I1	133/133 (100%)	123 (92%)	10 (8%)	13	43
3	I2	133/133 (100%)	116 (87%)	17 (13%)	4	22
3	I4	133/133 (100%)	122 (92%)	11 (8%)	11	40
3	I5	133/133 (100%)	123 (92%)	10 (8%)	13	43
3	I6	133/133 (100%)	116 (87%)	17 (13%)	4	22
3	I8	133/133 (100%)	122 (92%)	11 (8%)	11	40
3	K1	133/133 (100%)	123 (92%)	10 (8%)	13	43
3	K2	133/133 (100%)	118 (89%)	15 (11%)	6	27
3	K4	133/133 (100%)	123 (92%)	10 (8%)	13	43
3	K5	133/133 (100%)	123 (92%)	10 (8%)	13	43
3	K6	133/133 (100%)	118 (89%)	15 (11%)	6	27
3	K8	133/133 (100%)	123 (92%)	10 (8%)	13	43
3	M1	133/133 (100%)	123 (92%)	10 (8%)	13	43
3	M2	133/133 (100%)	117 (88%)	16 (12%)	5	24
3	M4	133/133 (100%)	122 (92%)	11 (8%)	11	40
3	M5	133/133 (100%)	123 (92%)	10 (8%)	13	43
3	M6	133/133 (100%)	117 (88%)	16 (12%)	5	24
3	M8	133/133 (100%)	122 (92%)	11 (8%)	11	40
3	P1	133/133 (100%)	123 (92%)	10 (8%)	13	43
3	P2	133/133 (100%)	113 (85%)	20 (15%)	3	17
3	P4	133/133 (100%)	124 (93%)	9 (7%)	16	48
3	P5	133/133 (100%)	123 (92%)	10 (8%)	13	43
3	P6	133/133 (100%)	113 (85%)	20 (15%)	3	17
3	P8	133/133 (100%)	124 (93%)	9 (7%)	16	48
3	R1	133/133 (100%)	123 (92%)	10 (8%)	13	43
3	R2	133/133 (100%)	116 (87%)	17 (13%)	4	22
3	R4	133/133 (100%)	125 (94%)	8 (6%)	19	52
3	R5	133/133 (100%)	123 (92%)	10 (8%)	13	43
3	R6	133/133 (100%)	116 (87%)	17 (13%)	4	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	R8	133/133 (100%)	125 (94%)	8 (6%)	19	52
3	T1	133/133 (100%)	123 (92%)	10 (8%)	13	43
3	T2	133/133 (100%)	115 (86%)	18 (14%)	4	21
3	T4	133/133 (100%)	124 (93%)	9 (7%)	16	48
3	T5	133/133 (100%)	123 (92%)	10 (8%)	13	43
3	T6	133/133 (100%)	115 (86%)	18 (14%)	4	21
3	T8	133/133 (100%)	124 (93%)	9 (7%)	16	48
3	V1	133/133 (100%)	123 (92%)	10 (8%)	13	43
3	V2	133/133 (100%)	115 (86%)	18 (14%)	4	21
3	V4	133/133 (100%)	123 (92%)	10 (8%)	13	43
3	V5	133/133 (100%)	123 (92%)	10 (8%)	13	43
3	V6	133/133 (100%)	115 (86%)	18 (14%)	4	21
3	V8	133/133 (100%)	123 (92%)	10 (8%)	13	43
3	X1	133/133 (100%)	123 (92%)	10 (8%)	13	43
3	X2	133/133 (100%)	116 (87%)	17 (13%)	4	22
3	X4	133/133 (100%)	124 (93%)	9 (7%)	16	48
3	X5	133/133 (100%)	123 (92%)	10 (8%)	13	43
3	X6	133/133 (100%)	117 (88%)	16 (12%)	5	24
3	X8	133/133 (100%)	124 (93%)	9 (7%)	16	48
3	Z1	133/133 (100%)	123 (92%)	10 (8%)	13	43
3	Z2	133/133 (100%)	115 (86%)	18 (14%)	4	21
3	Z4	133/133 (100%)	122 (92%)	11 (8%)	11	40
3	Z5	133/133 (100%)	123 (92%)	10 (8%)	13	43
3	Z6	133/133 (100%)	115 (86%)	18 (14%)	4	21
3	Z8	133/133 (100%)	122 (92%)	11 (8%)	11	40
4	N1	239/240 (100%)	238 (100%)	1 (0%)	91	96
4	N2	239/240 (100%)	227 (95%)	12 (5%)	24	58
4	N4	239/240 (100%)	237 (99%)	2 (1%)	81	91
4	N5	239/240 (100%)	238 (100%)	1 (0%)	91	96
4	N6	239/240 (100%)	227 (95%)	12 (5%)	24	58
4	N8	239/240 (100%)	237 (99%)	2 (1%)	81	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	a1	54/240 (22%)	54 (100%)	0	100	100
4	a2	54/240 (22%)	54 (100%)	0	100	100
4	a4	52/240 (22%)	52 (100%)	0	100	100
4	a5	54/240 (22%)	54 (100%)	0	100	100
4	a6	54/240 (22%)	54 (100%)	0	100	100
4	a8	52/240 (22%)	52 (100%)	0	100	100
5	03	704/745 (94%)	632 (90%)	72 (10%)	7	32
5	13	704/745 (94%)	628 (89%)	76 (11%)	6	30
6	23	58/60 (97%)	57 (98%)	1 (2%)	60	82
6	33	58/60 (97%)	57 (98%)	1 (2%)	60	82
6	G7	58/60 (97%)	55 (95%)	3 (5%)	23	56
6	N7	59/60 (98%)	57 (97%)	2 (3%)	37	68
6	U7	58/60 (97%)	56 (97%)	2 (3%)	37	68
6	b7	58/60 (97%)	55 (95%)	3 (5%)	23	56
7	A7	124/125 (99%)	108 (87%)	16 (13%)	4	22
7	C7	124/125 (99%)	108 (87%)	16 (13%)	4	22
7	E7	124/125 (99%)	108 (87%)	16 (13%)	4	22
7	G3	124/125 (99%)	110 (89%)	14 (11%)	6	27
7	H7	124/125 (99%)	107 (86%)	17 (14%)	3	20
7	I3	124/125 (99%)	110 (89%)	14 (11%)	6	27
7	J7	124/125 (99%)	108 (87%)	16 (13%)	4	22
7	K3	124/125 (99%)	109 (88%)	15 (12%)	5	24
7	L7	124/125 (99%)	108 (87%)	16 (13%)	4	22
7	N3	124/125 (99%)	110 (89%)	14 (11%)	6	27
7	O7	124/125 (99%)	108 (87%)	16 (13%)	4	22
7	P3	124/125 (99%)	110 (89%)	14 (11%)	6	27
7	Q7	124/125 (99%)	108 (87%)	16 (13%)	4	22
7	R3	124/125 (99%)	110 (89%)	14 (11%)	6	27
7	S7	124/125 (99%)	107 (86%)	17 (14%)	3	20
7	T3	124/125 (99%)	110 (89%)	14 (11%)	6	27
7	V7	124/125 (99%)	109 (88%)	15 (12%)	5	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	X3	124/125 (99%)	109 (88%)	15 (12%)	5	24
7	X7	124/125 (99%)	108 (87%)	16 (13%)	4	22
7	Z3	124/125 (99%)	109 (88%)	15 (12%)	5	24
7	Z7	124/125 (99%)	108 (87%)	16 (13%)	4	22
7	b3	124/125 (99%)	110 (89%)	14 (11%)	6	27
7	d3	124/125 (99%)	110 (89%)	14 (11%)	6	27
7	f3	124/125 (99%)	110 (89%)	14 (11%)	6	27
7	i3	124/125 (99%)	110 (89%)	14 (11%)	6	27
7	k3	124/125 (99%)	110 (89%)	14 (11%)	6	27
7	o3	124/125 (99%)	110 (89%)	14 (11%)	6	27
7	q3	124/125 (99%)	108 (87%)	16 (13%)	4	22
7	s3	124/125 (99%)	110 (89%)	14 (11%)	6	27
7	u3	124/125 (99%)	110 (89%)	14 (11%)	6	27
7	w3	124/125 (99%)	108 (87%)	16 (13%)	4	22
7	y3	124/125 (99%)	110 (89%)	14 (11%)	6	27
8	B7	124/124 (100%)	105 (85%)	19 (15%)	2	17
8	D7	124/124 (100%)	105 (85%)	19 (15%)	2	17
8	F7	124/124 (100%)	105 (85%)	19 (15%)	2	17
8	H3	124/124 (100%)	113 (91%)	11 (9%)	9	37
8	I7	124/124 (100%)	105 (85%)	19 (15%)	2	17
8	J3	124/124 (100%)	114 (92%)	10 (8%)	11	41
8	K7	124/124 (100%)	105 (85%)	19 (15%)	2	17
8	L3	124/124 (100%)	113 (91%)	11 (9%)	9	37
8	M3	124/124 (100%)	113 (91%)	11 (9%)	9	37
8	M7	124/124 (100%)	105 (85%)	19 (15%)	2	17
8	O3	124/124 (100%)	113 (91%)	11 (9%)	9	37
8	P7	124/124 (100%)	105 (85%)	19 (15%)	2	17
8	R7	124/124 (100%)	105 (85%)	19 (15%)	2	17
8	S3	124/124 (100%)	113 (91%)	11 (9%)	9	37
8	T7	124/124 (100%)	105 (85%)	19 (15%)	2	17
8	U3	124/124 (100%)	113 (91%)	11 (9%)	9	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	W3	124/124 (100%)	113 (91%)	11 (9%)	9	37
8	W7	124/124 (100%)	105 (85%)	19 (15%)	2	17
8	Y3	124/124 (100%)	114 (92%)	10 (8%)	11	41
8	Y7	124/124 (100%)	105 (85%)	19 (15%)	2	17
8	a3	124/124 (100%)	113 (91%)	11 (9%)	9	37
8	a7	124/124 (100%)	105 (85%)	19 (15%)	2	17
8	c3	124/124 (100%)	113 (91%)	11 (9%)	9	37
8	e3	124/124 (100%)	113 (91%)	11 (9%)	9	37
8	h3	124/124 (100%)	113 (91%)	11 (9%)	9	37
8	j3	124/124 (100%)	113 (91%)	11 (9%)	9	37
8	l3	124/124 (100%)	113 (91%)	11 (9%)	9	37
8	n3	124/124 (100%)	113 (91%)	11 (9%)	9	37
8	p3	124/124 (100%)	113 (91%)	11 (9%)	9	37
8	r3	124/124 (100%)	113 (91%)	11 (9%)	9	37
8	t3	124/124 (100%)	113 (91%)	11 (9%)	9	37
8	v3	124/124 (100%)	113 (91%)	11 (9%)	9	37
8	x3	124/124 (100%)	113 (91%)	11 (9%)	9	37
8	z3	124/124 (100%)	113 (91%)	11 (9%)	9	37
9	Q3	136/136 (100%)	130 (96%)	6 (4%)	28	62
9	g3	136/136 (100%)	130 (96%)	6 (4%)	28	62
10	V3	129/130 (99%)	117 (91%)	12 (9%)	9	35
10	m3	129/130 (99%)	117 (91%)	12 (9%)	9	35
All	All	32071/33434 (96%)	29023 (90%)	3048 (10%)	12	34

5 of 3048 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	V5	50	SER
2	Y6	143	THR
1	A6	191	PHE
2	U5	143	THR
2	L6	84	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 448 such sidechains are listed below:

Mol	Chain	Res	Type
2	Y4	15	GLN
2	Y8	139	ASN
2	Q5	21	ASN
2	W8	151	ASN
2	J8	53	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

288 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CYC	K1	201	-	42,46,46	3.08	14 (33%)	50,67,67	3.27	26 (52%)
11	CYC	Z6	202	-	42,46,46	1.08	1 (2%)	50,67,67	0.96	2 (4%)
11	CYC	I4	203	-	42,46,46	3.19	14 (33%)	50,67,67	2.95	20 (40%)
11	CYC	X4	202	-	42,46,46	1.04	1 (2%)	50,67,67	0.96	2 (4%)
11	CYC	R8	201	-	42,46,46	1.08	1 (2%)	50,67,67	0.95	2 (4%)
11	CYC	V3	201	-	42,46,46	3.18	15 (35%)	50,67,67	3.30	21 (42%)
11	CYC	V1	202	-	42,46,46	3.17	13 (30%)	50,67,67	4.44	29 (58%)
11	CYC	X5	203	-	42,46,46	3.17	13 (30%)	50,67,67	4.45	29 (58%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CYC	Q6	201	-	42,46,46	3.05	13 (30%)	50,67,67	3.56	25 (50%)
11	CYC	03	902	-	42,46,46	3.09	15 (35%)	50,67,67	3.76	22 (44%)
11	CYC	P2	202	-	42,46,46	1.07	1 (2%)	50,67,67	0.95	2 (4%)
11	CYC	T3	1001	-	42,46,46	3.25	13 (30%)	50,67,67	3.27	20 (40%)
11	CYC	N4	301	-	42,46,46	3.22	17 (40%)	50,67,67	3.36	24 (48%)
11	CYC	N5	301	-	42,46,46	3.09	14 (33%)	50,67,67	3.27	26 (52%)
11	CYC	Z3	1001	-	42,46,46	3.25	14 (33%)	50,67,67	3.28	20 (40%)
11	CYC	m3	201	-	42,46,46	3.17	14 (33%)	50,67,67	3.30	21 (42%)
11	CYC	K4	202	-	42,46,46	1.06	1 (2%)	50,67,67	0.97	2 (4%)
11	CYC	V6	202	-	42,46,46	1.09	1 (2%)	50,67,67	0.95	2 (4%)
11	CYC	d3	1001	-	42,46,46	3.25	14 (33%)	50,67,67	3.28	20 (40%)
11	CYC	L5	201	-	42,46,46	3.18	13 (30%)	50,67,67	4.44	29 (58%)
11	CYC	C2	202	-	42,46,46	1.11	1 (2%)	50,67,67	0.95	2 (4%)
11	CYC	O4	201	-	42,46,46	3.16	14 (33%)	50,67,67	2.93	20 (40%)
11	CYC	C4	201	-	42,46,46	1.12	1 (2%)	50,67,67	0.96	2 (4%)
11	CYC	P5	201	-	42,46,46	3.09	14 (33%)	50,67,67	3.26	25 (50%)
11	CYC	T6	201	-	42,46,46	1.09	1 (2%)	50,67,67	0.96	2 (4%)
11	CYC	C1	202	-	42,46,46	3.17	14 (33%)	50,67,67	4.45	29 (58%)
11	CYC	M2	201	-	42,46,46	3.02	13 (30%)	50,67,67	3.87	23 (46%)
11	CYC	r3	1001	-	42,46,46	3.10	15 (35%)	50,67,67	3.76	22 (44%)
11	CYC	D4	201	-	42,46,46	3.18	14 (33%)	50,67,67	2.95	20 (40%)
11	CYC	M6	202	-	42,46,46	1.09	1 (2%)	50,67,67	0.94	2 (4%)
11	CYC	I8	203	-	42,46,46	3.17	14 (33%)	50,67,67	2.94	20 (40%)
11	CYC	O1	201	-	42,46,46	3.17	13 (30%)	50,67,67	4.45	29 (58%)
11	CYC	M4	201	-	42,46,46	3.17	15 (35%)	50,67,67	2.94	20 (40%)
11	CYC	B6	201	-	42,46,46	3.06	13 (30%)	50,67,67	3.58	25 (50%)
11	CYC	v3	1001	-	42,46,46	3.09	14 (33%)	50,67,67	3.76	22 (44%)
11	CYC	E8	201	-	42,46,46	3.22	16 (38%)	50,67,67	3.36	25 (50%)
11	CYC	F6	201	-	42,46,46	3.07	13 (30%)	50,67,67	3.57	25 (50%)
11	CYC	U3	1001	-	42,46,46	3.10	15 (35%)	50,67,67	3.76	22 (44%)
11	CYC	R1	201	-	42,46,46	3.09	14 (33%)	50,67,67	3.27	26 (52%)
11	CYC	K2	201	-	42,46,46	3.02	13 (30%)	50,67,67	3.87	23 (46%)
11	CYC	A1	302	-	42,46,46	3.09	14 (33%)	50,67,67	3.28	26 (52%)
11	CYC	y3	1001	-	42,46,46	3.24	14 (33%)	50,67,67	3.27	20 (40%)
11	CYC	P5	202	-	42,46,46	3.24	13 (30%)	50,67,67	3.51	20 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CYC	M1	202	-	42,46,46	3.23	12 (28%)	50,67,67	3.52	20 (40%)
11	CYC	X5	202	-	42,46,46	3.22	12 (28%)	50,67,67	3.52	20 (40%)
11	CYC	K6	201	-	42,46,46	3.02	13 (30%)	50,67,67	3.87	23 (46%)
11	CYC	G6	201	-	42,46,46	1.08	1 (2%)	50,67,67	0.96	2 (4%)
11	CYC	X6	201	-	42,46,46	3.01	13 (30%)	50,67,67	3.88	23 (46%)
11	CYC	P4	202	-	42,46,46	1.07	1 (2%)	50,67,67	0.95	2 (4%)
11	CYC	J5	201	-	42,46,46	3.15	13 (30%)	50,67,67	4.44	29 (58%)
11	CYC	C7	1001	-	42,46,46	3.25	15 (35%)	50,67,67	2.78	21 (42%)
11	CYC	Z1	201	-	42,46,46	3.08	14 (33%)	50,67,67	3.27	26 (52%)
11	CYC	13	903	-	42,46,46	3.09	14 (33%)	50,67,67	3.76	22 (44%)
11	CYC	O5	201	-	42,46,46	3.18	13 (30%)	50,67,67	4.45	29 (58%)
11	CYC	M4	202	-	42,46,46	3.24	16 (38%)	50,67,67	3.36	25 (50%)
11	CYC	Q2	201	-	42,46,46	3.05	13 (30%)	50,67,67	3.57	25 (50%)
11	CYC	I3	1001	-	42,46,46	3.24	14 (33%)	50,67,67	3.27	20 (40%)
11	CYC	V5	201	-	42,46,46	3.08	15 (35%)	50,67,67	3.27	26 (52%)
11	CYC	U5	202	-	42,46,46	3.22	12 (28%)	50,67,67	3.53	20 (40%)
11	CYC	I2	201	-	42,46,46	3.03	13 (30%)	50,67,67	3.88	23 (46%)
11	CYC	V5	202	-	42,46,46	3.18	13 (30%)	50,67,67	4.44	29 (58%)
11	CYC	P8	201	-	42,46,46	3.23	16 (38%)	50,67,67	3.36	25 (50%)
11	CYC	K8	201	-	42,46,46	3.22	17 (40%)	50,67,67	3.36	24 (48%)
11	CYC	I2	202	-	42,46,46	1.12	1 (2%)	50,67,67	0.96	2 (4%)
11	CYC	R5	201	-	42,46,46	3.08	14 (33%)	50,67,67	3.27	26 (52%)
11	CYC	O7	1001	-	42,46,46	3.25	15 (35%)	50,67,67	2.78	21 (42%)
11	CYC	T8	201	-	42,46,46	3.22	16 (38%)	50,67,67	3.37	26 (52%)
11	CYC	T4	201	-	42,46,46	3.23	16 (38%)	50,67,67	3.37	26 (52%)
11	CYC	M2	202	-	42,46,46	1.08	1 (2%)	50,67,67	0.94	2 (4%)
11	CYC	B1	201	-	42,46,46	3.17	13 (30%)	50,67,67	4.45	29 (58%)
11	CYC	O6	201	-	42,46,46	3.04	13 (30%)	50,67,67	3.57	25 (50%)
11	CYC	C8	201	-	42,46,46	1.13	1 (2%)	50,67,67	0.95	2 (4%)
11	CYC	F8	201	-	42,46,46	1.08	1 (2%)	50,67,67	0.97	2 (4%)
11	CYC	O8	201	-	42,46,46	3.16	14 (33%)	50,67,67	2.94	20 (40%)
11	CYC	P4	203	-	42,46,46	3.15	14 (33%)	50,67,67	2.92	20 (40%)
11	CYC	A7	1001	-	42,46,46	3.25	15 (35%)	50,67,67	2.77	21 (42%)
11	CYC	C5	202	-	42,46,46	3.17	14 (33%)	50,67,67	4.45	29 (58%)
11	CYC	K1	202	-	42,46,46	3.22	13 (30%)	50,67,67	3.52	20 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CYC	Q3	1001	9	42,46,46	3.19	15 (35%)	50,67,67	2.99	17 (34%)
11	CYC	Z6	201	-	42,46,46	3.01	13 (30%)	50,67,67	3.88	23 (46%)
11	CYC	G4	202	-	42,46,46	3.22	17 (40%)	50,67,67	3.36	24 (48%)
11	CYC	U1	201	-	42,46,46	3.17	13 (30%)	50,67,67	4.45	29 (58%)
11	CYC	A4	301	-	42,46,46	3.23	16 (38%)	50,67,67	3.36	25 (50%)
11	CYC	D5	201	-	42,46,46	3.21	13 (30%)	50,67,67	3.50	20 (40%)
11	CYC	U8	201	-	42,46,46	3.17	14 (33%)	50,67,67	2.95	20 (40%)
11	CYC	M5	201	-	42,46,46	3.08	14 (33%)	50,67,67	3.27	26 (52%)
11	CYC	g3	1001	9	42,46,46	3.17	14 (33%)	50,67,67	2.99	17 (34%)
11	CYC	B2	201	-	42,46,46	3.06	13 (30%)	50,67,67	3.58	25 (50%)
11	CYC	Z5	201	-	42,46,46	3.08	14 (33%)	50,67,67	3.27	26 (52%)
11	CYC	L4	202	-	42,46,46	1.08	1 (2%)	50,67,67	0.94	2 (4%)
11	CYC	S2	201	-	42,46,46	3.06	13 (30%)	50,67,67	3.58	25 (50%)
11	CYC	P6	201	-	42,46,46	3.01	13 (30%)	50,67,67	3.88	23 (46%)
11	CYC	V8	201	-	42,46,46	3.22	17 (40%)	50,67,67	3.37	24 (48%)
11	CYC	L1	201	-	42,46,46	3.18	13 (30%)	50,67,67	4.45	29 (58%)
11	CYC	I2	203	-	42,46,46	3.06	13 (30%)	50,67,67	3.58	25 (50%)
11	CYC	T7	1001	-	42,46,46	3.14	12 (28%)	50,67,67	3.28	25 (50%)
11	CYC	X2	202	-	42,46,46	1.06	1 (2%)	50,67,67	0.96	2 (4%)
11	CYC	R3	1001	-	42,46,46	3.25	15 (35%)	50,67,67	3.27	19 (38%)
11	CYC	G5	202	-	42,46,46	3.22	13 (30%)	50,67,67	3.52	20 (40%)
11	CYC	X1	202	-	42,46,46	3.23	12 (28%)	50,67,67	3.52	20 (40%)
11	CYC	N2	301	4	42,46,46	3.00	13 (30%)	50,67,67	3.87	23 (46%)
11	CYC	R2	201	-	42,46,46	1.08	1 (2%)	50,67,67	0.95	2 (4%)
11	CYC	T2	201	-	42,46,46	3.05	13 (30%)	50,67,67	3.58	25 (50%)
11	CYC	q3	1001	-	42,46,46	3.24	14 (33%)	50,67,67	3.27	19 (38%)
11	CYC	D8	201	-	42,46,46	3.16	14 (33%)	50,67,67	2.95	20 (40%)
11	CYC	I5	201	-	42,46,46	3.08	14 (33%)	50,67,67	3.26	26 (52%)
11	CYC	R1	202	-	42,46,46	3.22	13 (30%)	50,67,67	3.52	21 (42%)
11	CYC	w3	1001	-	42,46,46	3.25	15 (35%)	50,67,67	3.27	20 (40%)
11	CYC	I8	201	-	42,46,46	3.22	15 (35%)	50,67,67	3.36	24 (48%)
11	CYC	I6	201	-	42,46,46	3.04	13 (30%)	50,67,67	3.89	23 (46%)
11	CYC	z3	1001	-	42,46,46	3.08	14 (33%)	50,67,67	3.75	22 (44%)
11	CYC	C2	201	-	42,46,46	3.02	13 (30%)	50,67,67	3.88	23 (46%)
11	CYC	N8	301	-	42,46,46	3.22	16 (38%)	50,67,67	3.36	25 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CYC	X5	201	-	42,46,46	3.08	14 (33%)	50,67,67	3.26	26 (52%)
11	CYC	j3	1001	-	42,46,46	3.09	15 (35%)	50,67,67	3.76	22 (44%)
11	CYC	X4	201	-	42,46,46	3.23	16 (38%)	50,67,67	3.36	24 (48%)
11	CYC	V4	202	-	42,46,46	1.09	1 (2%)	50,67,67	0.95	2 (4%)
11	CYC	c3	1001	-	42,46,46	3.08	14 (33%)	50,67,67	3.75	22 (44%)
11	CYC	H3	1001	-	42,46,46	3.09	14 (33%)	50,67,67	3.77	22 (44%)
11	CYC	G8	201	-	42,46,46	3.16	14 (33%)	50,67,67	2.95	20 (40%)
11	CYC	L6	201	-	42,46,46	3.07	13 (30%)	50,67,67	3.58	25 (50%)
11	CYC	l3	901	-	42,46,46	3.20	13 (30%)	50,67,67	3.14	19 (38%)
11	CYC	T1	201	-	42,46,46	3.23	12 (28%)	50,67,67	3.52	20 (40%)
11	CYC	Z8	201	-	42,46,46	3.23	16 (38%)	50,67,67	3.36	25 (50%)
11	CYC	K4	201	-	42,46,46	3.21	16 (38%)	50,67,67	3.37	24 (48%)
11	CYC	Z8	202	-	42,46,46	1.07	1 (2%)	50,67,67	0.96	2 (4%)
11	CYC	L8	201	-	42,46,46	3.17	14 (33%)	50,67,67	2.94	20 (40%)
11	CYC	K5	201	-	42,46,46	3.07	14 (33%)	50,67,67	3.27	25 (50%)
11	CYC	G8	202	-	42,46,46	3.22	17 (40%)	50,67,67	3.36	24 (48%)
11	CYC	U5	201	-	42,46,46	3.16	13 (30%)	50,67,67	4.44	29 (58%)
11	CYC	n3	1001	-	42,46,46	3.09	14 (33%)	50,67,67	3.76	22 (44%)
11	CYC	i3	1001	-	42,46,46	3.24	14 (33%)	50,67,67	3.26	20 (40%)
11	CYC	X7	1001	-	42,46,46	3.25	15 (35%)	50,67,67	2.77	22 (44%)
11	CYC	A5	302	-	42,46,46	3.10	14 (33%)	50,67,67	3.27	26 (52%)
11	CYC	C6	202	-	42,46,46	1.12	1 (2%)	50,67,67	0.95	2 (4%)
11	CYC	M6	201	-	42,46,46	3.02	13 (30%)	50,67,67	3.87	23 (46%)
11	CYC	S7	1001	-	42,46,46	3.26	14 (33%)	50,67,67	2.77	21 (42%)
11	CYC	B7	1001	-	42,46,46	3.14	12 (28%)	50,67,67	3.28	25 (50%)
11	CYC	I1	202	-	42,46,46	3.22	13 (30%)	50,67,67	3.53	20 (40%)
11	CYC	G3	1001	-	42,46,46	3.25	13 (30%)	50,67,67	3.27	20 (40%)
11	CYC	H5	201	-	42,46,46	3.17	13 (30%)	50,67,67	4.44	29 (58%)
11	CYC	F7	1001	-	42,46,46	3.14	12 (28%)	50,67,67	3.28	25 (50%)
11	CYC	F4	201	-	42,46,46	1.07	1 (2%)	50,67,67	0.97	2 (4%)
11	CYC	Q1	201	-	42,46,46	3.17	13 (30%)	50,67,67	4.45	29 (58%)
11	CYC	W2	201	-	42,46,46	3.06	13 (30%)	50,67,67	3.58	25 (50%)
11	CYC	E6	201	-	42,46,46	3.02	13 (30%)	50,67,67	3.88	23 (46%)
11	CYC	e3	1001	-	42,46,46	3.08	14 (33%)	50,67,67	3.76	22 (44%)
11	CYC	E7	1001	-	42,46,46	3.26	15 (35%)	50,67,67	2.78	21 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CYC	P1	201	-	42,46,46	3.08	14 (33%)	50,67,67	3.27	26 (52%)
11	CYC	Z2	202	-	42,46,46	3.02	13 (30%)	50,67,67	3.88	23 (46%)
11	CYC	G5	201	-	42,46,46	3.07	14 (33%)	50,67,67	3.27	25 (50%)
11	CYC	X1	203	-	42,46,46	3.17	14 (33%)	50,67,67	4.45	29 (58%)
11	CYC	X1	201	-	42,46,46	3.08	14 (33%)	50,67,67	3.27	25 (50%)
11	CYC	I6	202	-	42,46,46	1.12	1 (2%)	50,67,67	0.96	2 (4%)
11	CYC	E2	202	-	42,46,46	1.07	1 (2%)	50,67,67	0.95	2 (4%)
11	CYC	V2	201	-	42,46,46	3.01	13 (30%)	50,67,67	3.87	23 (46%)
11	CYC	P3	1001	-	42,46,46	3.25	14 (33%)	50,67,67	3.26	19 (38%)
11	CYC	X6	202	-	42,46,46	1.06	1 (2%)	50,67,67	0.96	2 (4%)
11	CYC	H7	1001	-	42,46,46	3.26	15 (35%)	50,67,67	2.77	21 (42%)
11	CYC	G1	201	-	42,46,46	3.07	14 (33%)	50,67,67	3.26	25 (50%)
11	CYC	o3	1001	7	42,46,46	3.24	15 (35%)	50,67,67	3.27	20 (40%)
11	CYC	T5	201	-	42,46,46	3.23	12 (28%)	50,67,67	3.52	21 (42%)
11	CYC	A8	301	-	42,46,46	3.23	16 (38%)	50,67,67	3.36	26 (52%)
11	CYC	Z5	202	-	42,46,46	3.23	12 (28%)	50,67,67	3.52	21 (42%)
11	CYC	G1	202	-	42,46,46	3.23	13 (30%)	50,67,67	3.52	20 (40%)
11	CYC	D1	201	-	42,46,46	3.21	13 (30%)	50,67,67	3.51	20 (40%)
11	CYC	N3	1001	-	42,46,46	3.24	14 (33%)	50,67,67	3.26	19 (38%)
11	CYC	p3	1001	-	42,46,46	3.09	15 (35%)	50,67,67	3.76	22 (44%)
11	CYC	Q5	201	-	42,46,46	3.18	13 (30%)	50,67,67	4.46	29 (58%)
11	CYC	P1	202	-	42,46,46	3.24	13 (30%)	50,67,67	3.52	20 (40%)
11	CYC	W3	1001	-	42,46,46	3.09	14 (33%)	50,67,67	3.75	22 (44%)
11	CYC	u3	1001	-	42,46,46	3.24	13 (30%)	50,67,67	3.27	19 (38%)
11	CYC	G4	201	-	42,46,46	3.16	14 (33%)	50,67,67	2.94	20 (40%)
11	CYC	B5	201	-	42,46,46	3.16	14 (33%)	50,67,67	4.45	29 (58%)
11	CYC	E2	203	-	42,46,46	3.06	13 (30%)	50,67,67	3.57	25 (50%)
11	CYC	X8	201	-	42,46,46	3.22	17 (40%)	50,67,67	3.36	24 (48%)
11	CYC	S1	201	-	42,46,46	3.17	13 (30%)	50,67,67	4.45	29 (58%)
11	CYC	S4	201	-	42,46,46	3.15	14 (33%)	50,67,67	2.94	20 (40%)
11	CYC	W4	201	-	42,46,46	3.16	14 (33%)	50,67,67	2.94	20 (40%)
11	CYC	F5	201	-	42,46,46	3.16	14 (33%)	50,67,67	4.45	29 (58%)
11	CYC	E6	202	-	42,46,46	1.07	1 (2%)	50,67,67	0.95	2 (4%)
11	CYC	13	904	-	42,46,46	3.09	13 (30%)	50,67,67	3.76	22 (44%)
11	CYC	C1	201	-	42,46,46	3.22	13 (30%)	50,67,67	3.51	20 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CYC	R6	201	-	42,46,46	1.09	1 (2%)	50,67,67	0.95	2 (4%)
11	CYC	K7	1001	-	42,46,46	3.13	12 (28%)	50,67,67	3.29	25 (50%)
11	CYC	W7	1001	-	42,46,46	3.14	12 (28%)	50,67,67	3.28	25 (50%)
11	CYC	K8	202	-	42,46,46	1.05	1 (2%)	50,67,67	0.97	2 (4%)
11	CYC	M8	201	-	42,46,46	3.16	15 (35%)	50,67,67	2.94	20 (40%)
11	CYC	Q7	1001	-	42,46,46	3.27	16 (38%)	50,67,67	2.77	21 (42%)
11	CYC	M8	202	-	42,46,46	3.23	16 (38%)	50,67,67	3.36	25 (50%)
11	CYC	P8	202	-	42,46,46	1.08	1 (2%)	50,67,67	0.95	2 (4%)
11	CYC	X2	201	-	42,46,46	3.00	13 (30%)	50,67,67	3.87	23 (46%)
11	CYC	I5	202	-	42,46,46	3.23	12 (28%)	50,67,67	3.53	20 (40%)
11	CYC	Y7	1001	-	42,46,46	3.14	12 (28%)	50,67,67	3.28	25 (50%)
11	CYC	I3	1001	-	42,46,46	3.09	14 (33%)	50,67,67	3.76	22 (44%)
11	CYC	C6	203	-	42,46,46	3.06	13 (30%)	50,67,67	3.58	25 (50%)
11	CYC	a7	1001	-	42,46,46	3.14	12 (28%)	50,67,67	3.29	25 (50%)
11	CYC	M7	1001	-	42,46,46	3.15	12 (28%)	50,67,67	3.29	25 (50%)
11	CYC	Z1	202	-	42,46,46	3.23	12 (28%)	50,67,67	3.52	21 (42%)
11	CYC	E8	203	-	42,46,46	3.16	14 (33%)	50,67,67	2.94	20 (40%)
11	CYC	C5	201	-	42,46,46	3.22	13 (30%)	50,67,67	3.52	20 (40%)
11	CYC	C6	201	-	42,46,46	3.02	13 (30%)	50,67,67	3.87	23 (46%)
11	CYC	s3	1001	-	42,46,46	3.25	15 (35%)	50,67,67	3.27	19 (38%)
11	CYC	N6	302	-	42,46,46	3.00	13 (30%)	50,67,67	3.88	23 (46%)
11	CYC	H1	201	-	42,46,46	3.17	13 (30%)	50,67,67	4.45	29 (58%)
11	CYC	O3	1001	-	42,46,46	3.09	14 (33%)	50,67,67	3.76	22 (44%)
11	CYC	G2	201	-	42,46,46	1.07	1 (2%)	50,67,67	0.97	2 (4%)
11	CYC	V8	202	-	42,46,46	1.10	1 (2%)	50,67,67	0.95	2 (4%)
11	CYC	L8	202	-	42,46,46	1.08	1 (2%)	50,67,67	0.94	2 (4%)
11	CYC	Z2	203	-	42,46,46	1.08	1 (2%)	50,67,67	0.96	2 (4%)
11	CYC	k3	1001	-	42,46,46	3.25	14 (33%)	50,67,67	3.27	20 (40%)
11	CYC	V7	1001	-	42,46,46	3.25	15 (35%)	50,67,67	2.78	21 (42%)
11	CYC	T4	202	-	42,46,46	1.06	1 (2%)	50,67,67	0.96	2 (4%)
11	CYC	E4	203	-	42,46,46	3.16	14 (33%)	50,67,67	2.94	20 (40%)
11	CYC	V6	201	-	42,46,46	3.01	13 (30%)	50,67,67	3.87	23 (46%)
11	CYC	T8	202	-	42,46,46	1.07	1 (2%)	50,67,67	0.96	2 (4%)
11	CYC	J6	201	-	42,46,46	3.06	13 (30%)	50,67,67	3.58	25 (50%)
11	CYC	Y8	201	-	42,46,46	3.16	14 (33%)	50,67,67	2.94	20 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CYC	P7	1001	-	42,46,46	3.15	12 (28%)	50,67,67	3.29	25 (50%)
11	CYC	P8	203	-	42,46,46	3.15	14 (33%)	50,67,67	2.94	20 (40%)
11	CYC	M5	202	-	42,46,46	3.22	12 (28%)	50,67,67	3.53	20 (40%)
11	CYC	K5	202	-	42,46,46	3.21	13 (30%)	50,67,67	3.52	20 (40%)
11	CYC	E8	202	-	42,46,46	1.07	1 (2%)	50,67,67	0.94	2 (4%)
11	CYC	K2	202	-	42,46,46	1.06	1 (2%)	50,67,67	0.96	2 (4%)
11	CYC	S8	201	-	42,46,46	3.16	14 (33%)	50,67,67	2.94	20 (40%)
11	CYC	J3	201	-	42,46,46	3.08	14 (33%)	50,67,67	3.76	22 (44%)
11	CYC	W6	201	-	42,46,46	3.07	13 (30%)	50,67,67	3.58	25 (50%)
11	CYC	Y6	201	-	42,46,46	3.06	13 (30%)	50,67,67	3.58	25 (50%)
11	CYC	D7	1001	-	42,46,46	3.15	12 (28%)	50,67,67	3.28	25 (50%)
11	CYC	V4	201	-	42,46,46	3.22	17 (40%)	50,67,67	3.36	24 (48%)
11	CYC	F1	201	-	42,46,46	3.16	13 (30%)	50,67,67	4.45	29 (58%)
11	CYC	X2	203	-	42,46,46	3.05	13 (30%)	50,67,67	3.58	25 (50%)
11	CYC	Z4	201	-	42,46,46	3.24	16 (38%)	50,67,67	3.36	24 (48%)
11	CYC	N1	301	-	42,46,46	3.09	15 (35%)	50,67,67	3.27	26 (52%)
11	CYC	E4	201	-	42,46,46	3.21	16 (38%)	50,67,67	3.37	25 (50%)
11	CYC	S5	201	-	42,46,46	3.17	13 (30%)	50,67,67	4.45	29 (58%)
11	CYC	R4	201	-	42,46,46	1.09	1 (2%)	50,67,67	0.95	2 (4%)
11	CYC	Z4	202	-	42,46,46	1.07	1 (2%)	50,67,67	0.95	2 (4%)
11	CYC	M1	201	-	42,46,46	3.08	14 (33%)	50,67,67	3.27	26 (52%)
11	CYC	Z7	1001	-	42,46,46	3.26	15 (35%)	50,67,67	2.77	22 (44%)
11	CYC	D2	201	-	42,46,46	3.06	13 (30%)	50,67,67	3.57	25 (50%)
11	CYC	A5	301	-	42,46,46	3.08	14 (33%)	50,67,67	3.27	25 (50%)
11	CYC	I4	201	-	42,46,46	3.22	17 (40%)	50,67,67	3.36	23 (46%)
11	CYC	P4	201	-	42,46,46	3.22	16 (38%)	50,67,67	3.36	26 (52%)
11	CYC	L7	1001	-	42,46,46	3.27	15 (35%)	50,67,67	2.78	22 (44%)
11	CYC	U1	202	-	42,46,46	3.22	12 (28%)	50,67,67	3.52	21 (42%)
11	CYC	T2	202	-	42,46,46	1.07	1 (2%)	50,67,67	0.96	2 (4%)
11	CYC	V2	202	-	42,46,46	1.09	1 (2%)	50,67,67	0.95	2 (4%)
11	CYC	E4	202	-	42,46,46	1.08	1 (2%)	50,67,67	0.95	2 (4%)
11	CYC	I4	202	-	42,46,46	1.11	1 (2%)	50,67,67	0.96	2 (4%)
11	CYC	L4	201	-	42,46,46	3.17	14 (33%)	50,67,67	2.94	20 (40%)
11	CYC	R5	202	-	42,46,46	3.23	13 (30%)	50,67,67	3.53	21 (42%)
11	CYC	N6	301	4	42,46,46	3.01	13 (30%)	50,67,67	3.87	23 (46%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CYC	Z2	201	-	42,46,46	3.05	13 (30%)	50,67,67	3.57	25 (50%)
11	CYC	N2	302	-	42,46,46	3.01	13 (30%)	50,67,67	3.87	23 (46%)
11	CYC	t3	1001	-	42,46,46	3.08	14 (33%)	50,67,67	3.76	22 (44%)
11	CYC	x3	1001	-	42,46,46	3.08	14 (33%)	50,67,67	3.76	22 (44%)
11	CYC	P6	202	-	42,46,46	1.08	1 (2%)	50,67,67	0.96	2 (4%)
11	CYC	I7	1001	-	42,46,46	3.14	12 (28%)	50,67,67	3.29	25 (50%)
11	CYC	H2	201	-	42,46,46	3.05	13 (30%)	50,67,67	3.58	25 (50%)
11	CYC	b3	1001	-	42,46,46	3.24	14 (33%)	50,67,67	3.27	20 (40%)
11	CYC	f3	1001	-	42,46,46	3.25	14 (33%)	50,67,67	3.27	19 (38%)
11	CYC	J7	1001	-	42,46,46	3.26	15 (35%)	50,67,67	2.77	21 (42%)
11	CYC	I1	201	-	42,46,46	3.08	14 (33%)	50,67,67	3.26	26 (52%)
11	CYC	K2	203	-	42,46,46	3.06	13 (30%)	50,67,67	3.58	25 (50%)
11	CYC	X8	202	-	42,46,46	1.05	1 (2%)	50,67,67	0.96	2 (4%)
11	CYC	E2	201	-	42,46,46	3.02	13 (30%)	50,67,67	3.88	23 (46%)
11	CYC	S3	1001	-	42,46,46	3.09	14 (33%)	50,67,67	3.76	22 (44%)
11	CYC	K6	202	-	42,46,46	1.06	1 (2%)	50,67,67	0.96	2 (4%)
11	CYC	R6	202	-	42,46,46	3.05	13 (30%)	50,67,67	3.58	25 (50%)
11	CYC	W8	201	-	42,46,46	3.16	14 (33%)	50,67,67	2.94	20 (40%)
11	CYC	A2	301	-	42,46,46	3.02	13 (30%)	50,67,67	3.88	23 (46%)
11	CYC	U4	201	-	42,46,46	3.18	14 (33%)	50,67,67	2.95	20 (40%)
11	CYC	U6	201	-	42,46,46	3.05	13 (30%)	50,67,67	3.57	25 (50%)
11	CYC	R7	1001	-	42,46,46	3.14	12 (28%)	50,67,67	3.29	25 (50%)
11	CYC	03	901	-	42,46,46	3.20	13 (30%)	50,67,67	3.15	19 (38%)
11	CYC	P2	201	-	42,46,46	3.02	13 (30%)	50,67,67	3.88	23 (46%)
11	CYC	K3	1001	-	42,46,46	3.25	15 (35%)	50,67,67	3.26	20 (40%)
11	CYC	X3	1001	-	42,46,46	3.26	14 (33%)	50,67,67	3.27	20 (40%)
11	CYC	V1	201	-	42,46,46	3.08	15 (35%)	50,67,67	3.27	26 (52%)
11	CYC	A6	301	-	42,46,46	3.02	13 (30%)	50,67,67	3.89	23 (46%)
11	CYC	13	902	-	42,46,46	3.10	14 (33%)	50,67,67	3.77	22 (44%)
11	CYC	M3	201	-	42,46,46	3.09	14 (33%)	50,67,67	3.76	22 (44%)
11	CYC	A1	301	-	42,46,46	3.08	14 (33%)	50,67,67	3.27	26 (52%)
11	CYC	I8	202	-	42,46,46	1.11	1 (2%)	50,67,67	0.96	2 (4%)
11	CYC	H6	201	-	42,46,46	3.06	13 (30%)	50,67,67	3.58	25 (50%)
11	CYC	Y4	201	-	42,46,46	3.15	14 (33%)	50,67,67	2.94	20 (40%)
11	CYC	J1	201	-	42,46,46	3.16	13 (30%)	50,67,67	4.44	29 (58%)

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
11	CYC	K1	201	-	-	10/25/74/74	0/4/4/4
11	CYC	Z6	202	-	-	12/25/74/74	0/4/4/4
11	CYC	I4	203	-	-	11/25/74/74	0/4/4/4
11	CYC	X4	202	-	-	12/25/74/74	0/4/4/4
11	CYC	R8	201	-	-	12/25/74/74	0/4/4/4
11	CYC	V3	201	-	-	11/25/74/74	0/4/4/4
11	CYC	V1	202	-	-	12/25/74/74	0/4/4/4
11	CYC	X5	203	-	-	12/25/74/74	0/4/4/4
11	CYC	Q6	201	-	-	12/25/74/74	0/4/4/4
11	CYC	03	902	-	-	4/25/74/74	0/4/4/4
11	CYC	P2	202	-	-	12/25/74/74	0/4/4/4
11	CYC	T3	1001	-	-	7/25/74/74	0/4/4/4
11	CYC	N4	301	-	-	10/25/74/74	0/4/4/4
11	CYC	N5	301	-	-	10/25/74/74	0/4/4/4
11	CYC	Z3	1001	-	-	7/25/74/74	0/4/4/4
11	CYC	m3	201	-	-	11/25/74/74	0/4/4/4
11	CYC	K4	202	-	-	12/25/74/74	0/4/4/4
11	CYC	V6	202	-	-	12/25/74/74	0/4/4/4
11	CYC	d3	1001	-	-	7/25/74/74	0/4/4/4
11	CYC	L5	201	-	-	12/25/74/74	0/4/4/4
11	CYC	C2	202	-	-	12/25/74/74	0/4/4/4
11	CYC	O4	201	-	-	11/25/74/74	0/4/4/4
11	CYC	C4	201	-	-	12/25/74/74	0/4/4/4
11	CYC	P5	201	-	-	10/25/74/74	0/4/4/4
11	CYC	T6	201	-	-	12/25/74/74	0/4/4/4
11	CYC	C1	202	-	-	12/25/74/74	0/4/4/4
11	CYC	M2	201	-	-	6/25/74/74	0/4/4/4
11	CYC	r3	1001	-	-	4/25/74/74	0/4/4/4
11	CYC	D4	201	-	-	11/25/74/74	0/4/4/4
11	CYC	M6	202	-	-	12/25/74/74	0/4/4/4
11	CYC	I8	203	-	-	11/25/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CYC	O1	201	-	-	12/25/74/74	0/4/4/4
11	CYC	M4	201	-	-	11/25/74/74	0/4/4/4
11	CYC	B6	201	-	-	12/25/74/74	0/4/4/4
11	CYC	v3	1001	-	-	4/25/74/74	0/4/4/4
11	CYC	E8	201	-	-	10/25/74/74	0/4/4/4
11	CYC	F6	201	-	-	12/25/74/74	0/4/4/4
11	CYC	U3	1001	-	-	4/25/74/74	0/4/4/4
11	CYC	R1	201	-	-	10/25/74/74	0/4/4/4
11	CYC	K2	201	-	-	6/25/74/74	0/4/4/4
11	CYC	A1	302	-	-	10/25/74/74	0/4/4/4
11	CYC	y3	1001	-	-	7/25/74/74	0/4/4/4
11	CYC	P5	202	-	-	11/25/74/74	0/4/4/4
11	CYC	M1	202	-	-	11/25/74/74	0/4/4/4
11	CYC	X5	202	-	-	11/25/74/74	0/4/4/4
11	CYC	K6	201	-	-	6/25/74/74	0/4/4/4
11	CYC	G6	201	-	-	12/25/74/74	0/4/4/4
11	CYC	X6	201	-	-	6/25/74/74	0/4/4/4
11	CYC	P4	202	-	-	12/25/74/74	0/4/4/4
11	CYC	J5	201	-	-	12/25/74/74	0/4/4/4
11	CYC	C7	1001	-	-	8/25/74/74	0/4/4/4
11	CYC	Z1	201	-	-	10/25/74/74	0/4/4/4
11	CYC	13	903	-	-	4/25/74/74	0/4/4/4
11	CYC	O5	201	-	-	12/25/74/74	0/4/4/4
11	CYC	M4	202	-	-	10/25/74/74	0/4/4/4
11	CYC	Q2	201	-	-	12/25/74/74	0/4/4/4
11	CYC	I3	1001	-	-	7/25/74/74	0/4/4/4
11	CYC	V5	201	-	-	10/25/74/74	0/4/4/4
11	CYC	U5	202	-	-	11/25/74/74	0/4/4/4
11	CYC	I2	201	-	-	6/25/74/74	0/4/4/4
11	CYC	V5	202	-	-	12/25/74/74	0/4/4/4
11	CYC	P8	201	-	-	10/25/74/74	0/4/4/4
11	CYC	K8	201	-	-	10/25/74/74	0/4/4/4
11	CYC	I2	202	-	-	12/25/74/74	0/4/4/4
11	CYC	R5	201	-	-	10/25/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CYC	O7	1001	-	-	8/25/74/74	0/4/4/4
11	CYC	T8	201	-	-	10/25/74/74	0/4/4/4
11	CYC	T4	201	-	-	10/25/74/74	0/4/4/4
11	CYC	M2	202	-	-	12/25/74/74	0/4/4/4
11	CYC	B1	201	-	-	12/25/74/74	0/4/4/4
11	CYC	O6	201	-	-	12/25/74/74	0/4/4/4
11	CYC	C8	201	-	-	12/25/74/74	0/4/4/4
11	CYC	F8	201	-	-	12/25/74/74	0/4/4/4
11	CYC	O8	201	-	-	11/25/74/74	0/4/4/4
11	CYC	P4	203	-	-	11/25/74/74	0/4/4/4
11	CYC	A7	1001	-	-	8/25/74/74	0/4/4/4
11	CYC	C5	202	-	-	12/25/74/74	0/4/4/4
11	CYC	K1	202	-	-	11/25/74/74	0/4/4/4
11	CYC	Q3	1001	9	-	7/25/74/74	0/4/4/4
11	CYC	Z6	201	-	-	6/25/74/74	0/4/4/4
11	CYC	G4	202	-	-	10/25/74/74	0/4/4/4
11	CYC	U1	201	-	-	12/25/74/74	0/4/4/4
11	CYC	A4	301	-	-	10/25/74/74	0/4/4/4
11	CYC	D5	201	-	-	11/25/74/74	0/4/4/4
11	CYC	U8	201	-	-	11/25/74/74	0/4/4/4
11	CYC	M5	201	-	-	10/25/74/74	0/4/4/4
11	CYC	g3	1001	9	-	7/25/74/74	0/4/4/4
11	CYC	B2	201	-	-	12/25/74/74	0/4/4/4
11	CYC	Z5	201	-	-	10/25/74/74	0/4/4/4
11	CYC	L4	202	-	-	12/25/74/74	0/4/4/4
11	CYC	S2	201	-	-	12/25/74/74	0/4/4/4
11	CYC	P6	201	-	-	6/25/74/74	0/4/4/4
11	CYC	V8	201	-	-	10/25/74/74	0/4/4/4
11	CYC	L1	201	-	-	12/25/74/74	0/4/4/4
11	CYC	I2	203	-	-	12/25/74/74	0/4/4/4
11	CYC	T7	1001	-	-	11/25/74/74	0/4/4/4
11	CYC	X2	202	-	-	12/25/74/74	0/4/4/4
11	CYC	R3	1001	-	-	7/25/74/74	0/4/4/4
11	CYC	G5	202	-	-	11/25/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CYC	X1	202	-	-	11/25/74/74	0/4/4/4
11	CYC	N2	301	4	-	6/25/74/74	0/4/4/4
11	CYC	R2	201	-	-	12/25/74/74	0/4/4/4
11	CYC	T2	201	-	-	12/25/74/74	0/4/4/4
11	CYC	q3	1001	-	-	7/25/74/74	0/4/4/4
11	CYC	D8	201	-	-	11/25/74/74	0/4/4/4
11	CYC	I5	201	-	-	10/25/74/74	0/4/4/4
11	CYC	R1	202	-	-	11/25/74/74	0/4/4/4
11	CYC	w3	1001	-	-	7/25/74/74	0/4/4/4
11	CYC	I8	201	-	-	10/25/74/74	0/4/4/4
11	CYC	I6	201	-	-	6/25/74/74	0/4/4/4
11	CYC	z3	1001	-	-	4/25/74/74	0/4/4/4
11	CYC	C2	201	-	-	6/25/74/74	0/4/4/4
11	CYC	N8	301	-	-	10/25/74/74	0/4/4/4
11	CYC	X5	201	-	-	10/25/74/74	0/4/4/4
11	CYC	j3	1001	-	-	4/25/74/74	0/4/4/4
11	CYC	X4	201	-	-	10/25/74/74	0/4/4/4
11	CYC	V4	202	-	-	12/25/74/74	0/4/4/4
11	CYC	c3	1001	-	-	4/25/74/74	0/4/4/4
11	CYC	H3	1001	-	-	4/25/74/74	0/4/4/4
11	CYC	G8	201	-	-	11/25/74/74	0/4/4/4
11	CYC	L6	201	-	-	12/25/74/74	0/4/4/4
11	CYC	I3	901	-	-	9/25/74/74	0/4/4/4
11	CYC	T1	201	-	-	11/25/74/74	0/4/4/4
11	CYC	Z8	201	-	-	10/25/74/74	0/4/4/4
11	CYC	K4	201	-	-	10/25/74/74	0/4/4/4
11	CYC	Z8	202	-	-	12/25/74/74	0/4/4/4
11	CYC	L8	201	-	-	11/25/74/74	0/4/4/4
11	CYC	K5	201	-	-	10/25/74/74	0/4/4/4
11	CYC	G8	202	-	-	10/25/74/74	0/4/4/4
11	CYC	U5	201	-	-	12/25/74/74	0/4/4/4
11	CYC	n3	1001	-	-	4/25/74/74	0/4/4/4
11	CYC	i3	1001	-	-	7/25/74/74	0/4/4/4
11	CYC	X7	1001	-	-	8/25/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CYC	A5	302	-	-	10/25/74/74	0/4/4/4
11	CYC	C6	202	-	-	12/25/74/74	0/4/4/4
11	CYC	M6	201	-	-	6/25/74/74	0/4/4/4
11	CYC	S7	1001	-	-	8/25/74/74	0/4/4/4
11	CYC	B7	1001	-	-	11/25/74/74	0/4/4/4
11	CYC	I1	202	-	-	11/25/74/74	0/4/4/4
11	CYC	G3	1001	-	-	7/25/74/74	0/4/4/4
11	CYC	H5	201	-	-	12/25/74/74	0/4/4/4
11	CYC	F7	1001	-	-	11/25/74/74	0/4/4/4
11	CYC	F4	201	-	-	12/25/74/74	0/4/4/4
11	CYC	Q1	201	-	-	12/25/74/74	0/4/4/4
11	CYC	W2	201	-	-	12/25/74/74	0/4/4/4
11	CYC	E6	201	-	-	6/25/74/74	0/4/4/4
11	CYC	e3	1001	-	-	4/25/74/74	0/4/4/4
11	CYC	E7	1001	-	-	8/25/74/74	0/4/4/4
11	CYC	P1	201	-	-	10/25/74/74	0/4/4/4
11	CYC	Z2	202	-	-	6/25/74/74	0/4/4/4
11	CYC	G5	201	-	-	10/25/74/74	0/4/4/4
11	CYC	X1	203	-	-	12/25/74/74	0/4/4/4
11	CYC	X1	201	-	-	10/25/74/74	0/4/4/4
11	CYC	I6	202	-	-	12/25/74/74	0/4/4/4
11	CYC	E2	202	-	-	12/25/74/74	0/4/4/4
11	CYC	V2	201	-	-	6/25/74/74	0/4/4/4
11	CYC	P3	1001	-	-	7/25/74/74	0/4/4/4
11	CYC	X6	202	-	-	12/25/74/74	0/4/4/4
11	CYC	H7	1001	-	-	8/25/74/74	0/4/4/4
11	CYC	G1	201	-	-	10/25/74/74	0/4/4/4
11	CYC	o3	1001	7	-	7/25/74/74	0/4/4/4
11	CYC	T5	201	-	-	11/25/74/74	0/4/4/4
11	CYC	A8	301	-	-	10/25/74/74	0/4/4/4
11	CYC	Z5	202	-	-	11/25/74/74	0/4/4/4
11	CYC	G1	202	-	-	11/25/74/74	0/4/4/4
11	CYC	D1	201	-	-	11/25/74/74	0/4/4/4
11	CYC	N3	1001	-	-	7/25/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CYC	p3	1001	-	-	4/25/74/74	0/4/4/4
11	CYC	Q5	201	-	-	12/25/74/74	0/4/4/4
11	CYC	P1	202	-	-	11/25/74/74	0/4/4/4
11	CYC	W3	1001	-	-	4/25/74/74	0/4/4/4
11	CYC	u3	1001	-	-	7/25/74/74	0/4/4/4
11	CYC	G4	201	-	-	11/25/74/74	0/4/4/4
11	CYC	B5	201	-	-	12/25/74/74	0/4/4/4
11	CYC	E2	203	-	-	12/25/74/74	0/4/4/4
11	CYC	X8	201	-	-	10/25/74/74	0/4/4/4
11	CYC	S1	201	-	-	12/25/74/74	0/4/4/4
11	CYC	S4	201	-	-	11/25/74/74	0/4/4/4
11	CYC	W4	201	-	-	11/25/74/74	0/4/4/4
11	CYC	F5	201	-	-	12/25/74/74	0/4/4/4
11	CYC	E6	202	-	-	12/25/74/74	0/4/4/4
11	CYC	l3	904	-	-	4/25/74/74	0/4/4/4
11	CYC	C1	201	-	-	11/25/74/74	0/4/4/4
11	CYC	R6	201	-	-	12/25/74/74	0/4/4/4
11	CYC	K7	1001	-	-	11/25/74/74	0/4/4/4
11	CYC	W7	1001	-	-	11/25/74/74	0/4/4/4
11	CYC	K8	202	-	-	12/25/74/74	0/4/4/4
11	CYC	M8	201	-	-	11/25/74/74	0/4/4/4
11	CYC	Q7	1001	-	-	8/25/74/74	0/4/4/4
11	CYC	M8	202	-	-	10/25/74/74	0/4/4/4
11	CYC	P8	202	-	-	12/25/74/74	0/4/4/4
11	CYC	X2	201	-	-	6/25/74/74	0/4/4/4
11	CYC	I5	202	-	-	11/25/74/74	0/4/4/4
11	CYC	Y7	1001	-	-	11/25/74/74	0/4/4/4
11	CYC	l3	1001	-	-	4/25/74/74	0/4/4/4
11	CYC	C6	203	-	-	12/25/74/74	0/4/4/4
11	CYC	a7	1001	-	-	11/25/74/74	0/4/4/4
11	CYC	M7	1001	-	-	11/25/74/74	0/4/4/4
11	CYC	Z1	202	-	-	11/25/74/74	0/4/4/4
11	CYC	E8	203	-	-	11/25/74/74	0/4/4/4
11	CYC	C5	201	-	-	11/25/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CYC	C6	201	-	-	6/25/74/74	0/4/4/4
11	CYC	s3	1001	-	-	7/25/74/74	0/4/4/4
11	CYC	N6	302	-	-	6/25/74/74	0/4/4/4
11	CYC	H1	201	-	-	12/25/74/74	0/4/4/4
11	CYC	O3	1001	-	-	4/25/74/74	0/4/4/4
11	CYC	G2	201	-	-	12/25/74/74	0/4/4/4
11	CYC	V8	202	-	-	12/25/74/74	0/4/4/4
11	CYC	L8	202	-	-	12/25/74/74	0/4/4/4
11	CYC	Z2	203	-	-	12/25/74/74	0/4/4/4
11	CYC	k3	1001	-	-	7/25/74/74	0/4/4/4
11	CYC	V7	1001	-	-	8/25/74/74	0/4/4/4
11	CYC	T4	202	-	-	12/25/74/74	0/4/4/4
11	CYC	E4	203	-	-	11/25/74/74	0/4/4/4
11	CYC	V6	201	-	-	6/25/74/74	0/4/4/4
11	CYC	T8	202	-	-	12/25/74/74	0/4/4/4
11	CYC	J6	201	-	-	12/25/74/74	0/4/4/4
11	CYC	Y8	201	-	-	11/25/74/74	0/4/4/4
11	CYC	P7	1001	-	-	11/25/74/74	0/4/4/4
11	CYC	P8	203	-	-	11/25/74/74	0/4/4/4
11	CYC	M5	202	-	-	11/25/74/74	0/4/4/4
11	CYC	K5	202	-	-	11/25/74/74	0/4/4/4
11	CYC	E8	202	-	-	12/25/74/74	0/4/4/4
11	CYC	K2	202	-	-	12/25/74/74	0/4/4/4
11	CYC	S8	201	-	-	11/25/74/74	0/4/4/4
11	CYC	J3	201	-	-	4/25/74/74	0/4/4/4
11	CYC	W6	201	-	-	12/25/74/74	0/4/4/4
11	CYC	Y6	201	-	-	12/25/74/74	0/4/4/4
11	CYC	D7	1001	-	-	11/25/74/74	0/4/4/4
11	CYC	V4	201	-	-	10/25/74/74	0/4/4/4
11	CYC	F1	201	-	-	12/25/74/74	0/4/4/4
11	CYC	X2	203	-	-	12/25/74/74	0/4/4/4
11	CYC	Z4	201	-	-	10/25/74/74	0/4/4/4
11	CYC	N1	301	-	-	10/25/74/74	0/4/4/4
11	CYC	E4	201	-	-	10/25/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CYC	S5	201	-	-	12/25/74/74	0/4/4/4
11	CYC	R4	201	-	-	12/25/74/74	0/4/4/4
11	CYC	Z4	202	-	-	12/25/74/74	0/4/4/4
11	CYC	M1	201	-	-	10/25/74/74	0/4/4/4
11	CYC	Z7	1001	-	-	8/25/74/74	0/4/4/4
11	CYC	D2	201	-	-	12/25/74/74	0/4/4/4
11	CYC	A5	301	-	-	10/25/74/74	0/4/4/4
11	CYC	I4	201	-	-	10/25/74/74	0/4/4/4
11	CYC	P4	201	-	-	10/25/74/74	0/4/4/4
11	CYC	L7	1001	-	-	8/25/74/74	0/4/4/4
11	CYC	U1	202	-	-	11/25/74/74	0/4/4/4
11	CYC	T2	202	-	-	12/25/74/74	0/4/4/4
11	CYC	V2	202	-	-	12/25/74/74	0/4/4/4
11	CYC	E4	202	-	-	12/25/74/74	0/4/4/4
11	CYC	I4	202	-	-	12/25/74/74	0/4/4/4
11	CYC	L4	201	-	-	11/25/74/74	0/4/4/4
11	CYC	R5	202	-	-	11/25/74/74	0/4/4/4
11	CYC	N6	301	4	-	6/25/74/74	0/4/4/4
11	CYC	Z2	201	-	-	12/25/74/74	0/4/4/4
11	CYC	N2	302	-	-	6/25/74/74	0/4/4/4
11	CYC	t3	1001	-	-	4/25/74/74	0/4/4/4
11	CYC	x3	1001	-	-	4/25/74/74	0/4/4/4
11	CYC	P6	202	-	-	12/25/74/74	0/4/4/4
11	CYC	I7	1001	-	-	11/25/74/74	0/4/4/4
11	CYC	H2	201	-	-	12/25/74/74	0/4/4/4
11	CYC	b3	1001	-	-	7/25/74/74	0/4/4/4
11	CYC	f3	1001	-	-	7/25/74/74	0/4/4/4
11	CYC	J7	1001	-	-	8/25/74/74	0/4/4/4
11	CYC	I1	201	-	-	10/25/74/74	0/4/4/4
11	CYC	K2	203	-	-	12/25/74/74	0/4/4/4
11	CYC	X8	202	-	-	12/25/74/74	0/4/4/4
11	CYC	E2	201	-	-	6/25/74/74	0/4/4/4
11	CYC	S3	1001	-	-	4/25/74/74	0/4/4/4
11	CYC	K6	202	-	-	12/25/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CYC	R6	202	-	-	12/25/74/74	0/4/4/4
11	CYC	W8	201	-	-	11/25/74/74	0/4/4/4
11	CYC	A2	301	-	-	6/25/74/74	0/4/4/4
11	CYC	U4	201	-	-	11/25/74/74	0/4/4/4
11	CYC	U6	201	-	-	12/25/74/74	0/4/4/4
11	CYC	R7	1001	-	-	11/25/74/74	0/4/4/4
11	CYC	03	901	-	-	9/25/74/74	0/4/4/4
11	CYC	P2	201	-	-	6/25/74/74	0/4/4/4
11	CYC	K3	1001	-	-	7/25/74/74	0/4/4/4
11	CYC	X3	1001	-	-	7/25/74/74	0/4/4/4
11	CYC	V1	201	-	-	10/25/74/74	0/4/4/4
11	CYC	A6	301	-	-	6/25/74/74	0/4/4/4
11	CYC	13	902	-	-	4/25/74/74	0/4/4/4
11	CYC	M3	201	-	-	4/25/74/74	0/4/4/4
11	CYC	A1	301	-	-	10/25/74/74	0/4/4/4
11	CYC	I8	202	-	-	12/25/74/74	0/4/4/4
11	CYC	H6	201	-	-	12/25/74/74	0/4/4/4
11	CYC	Y4	201	-	-	11/25/74/74	0/4/4/4
11	CYC	J1	201	-	-	12/25/74/74	0/4/4/4

The worst 5 of 3360 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	P5	202	CYC	CHA-C1A	16.58	1.49	1.35
11	P1	202	CYC	CHA-C1A	16.54	1.48	1.35
11	Z5	202	CYC	CHA-C1A	16.53	1.48	1.35
11	T5	201	CYC	CHA-C1A	16.49	1.48	1.35
11	Z1	202	CYC	CHA-C1A	16.46	1.48	1.35

The worst 5 of 5665 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	Z6	201	CYC	O2A-CGA-O1A	-15.39	84.93	123.30
11	I2	201	CYC	O2A-CGA-O1A	-15.39	84.94	123.30
11	S5	201	CYC	O2A-CGA-O1A	-15.39	84.94	123.30
11	F1	201	CYC	O2A-CGA-O1A	-15.38	84.95	123.30
11	I6	201	CYC	O2A-CGA-O1A	-15.38	84.96	123.30

There are no chirality outliers.

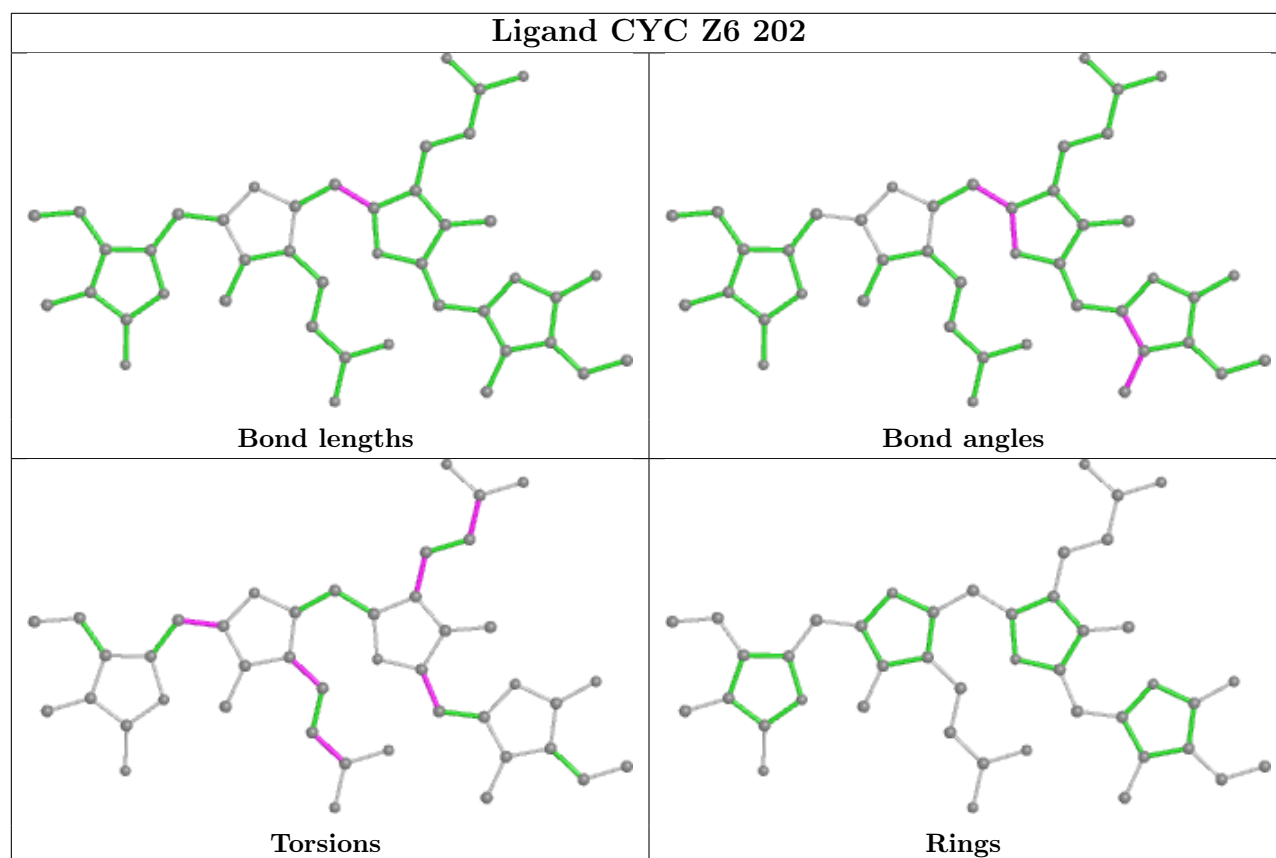
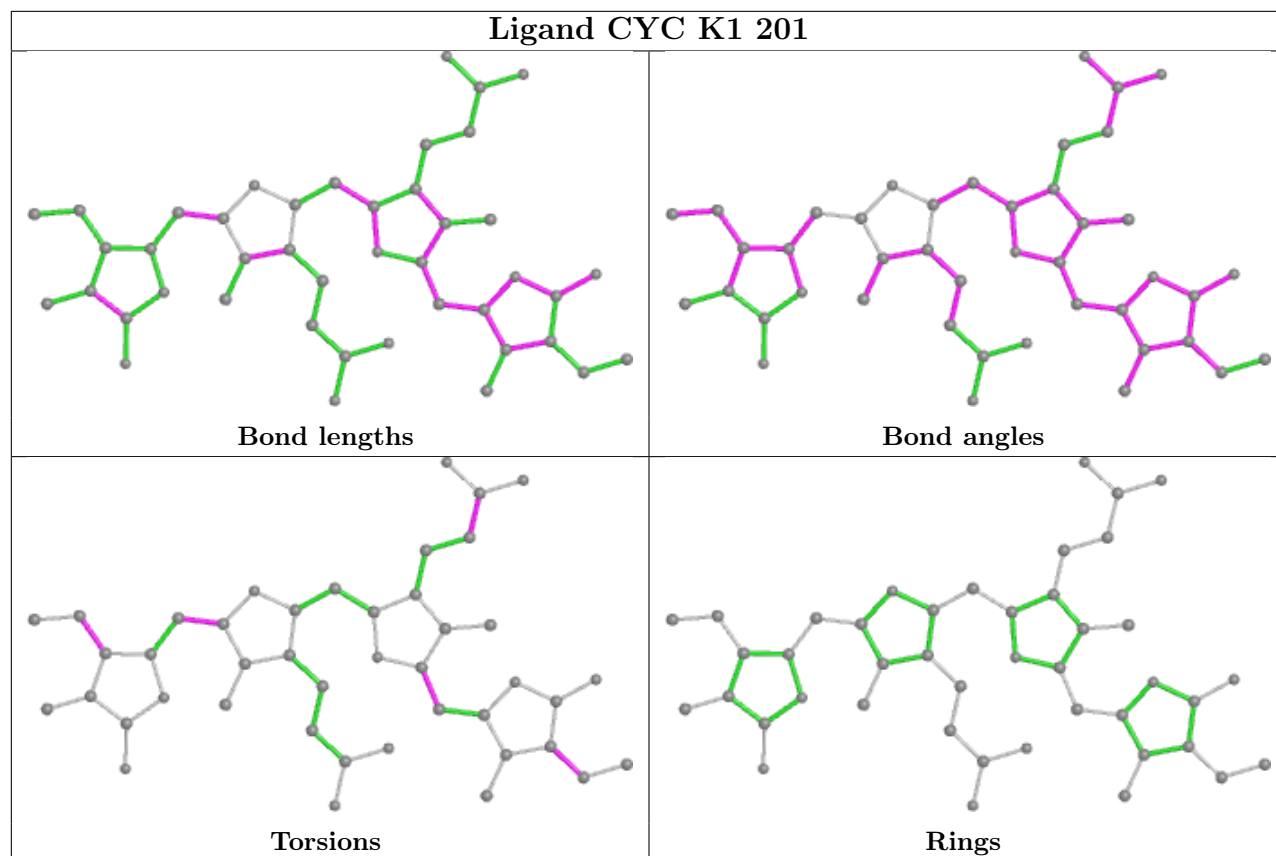
5 of 2814 torsion outliers are listed below:

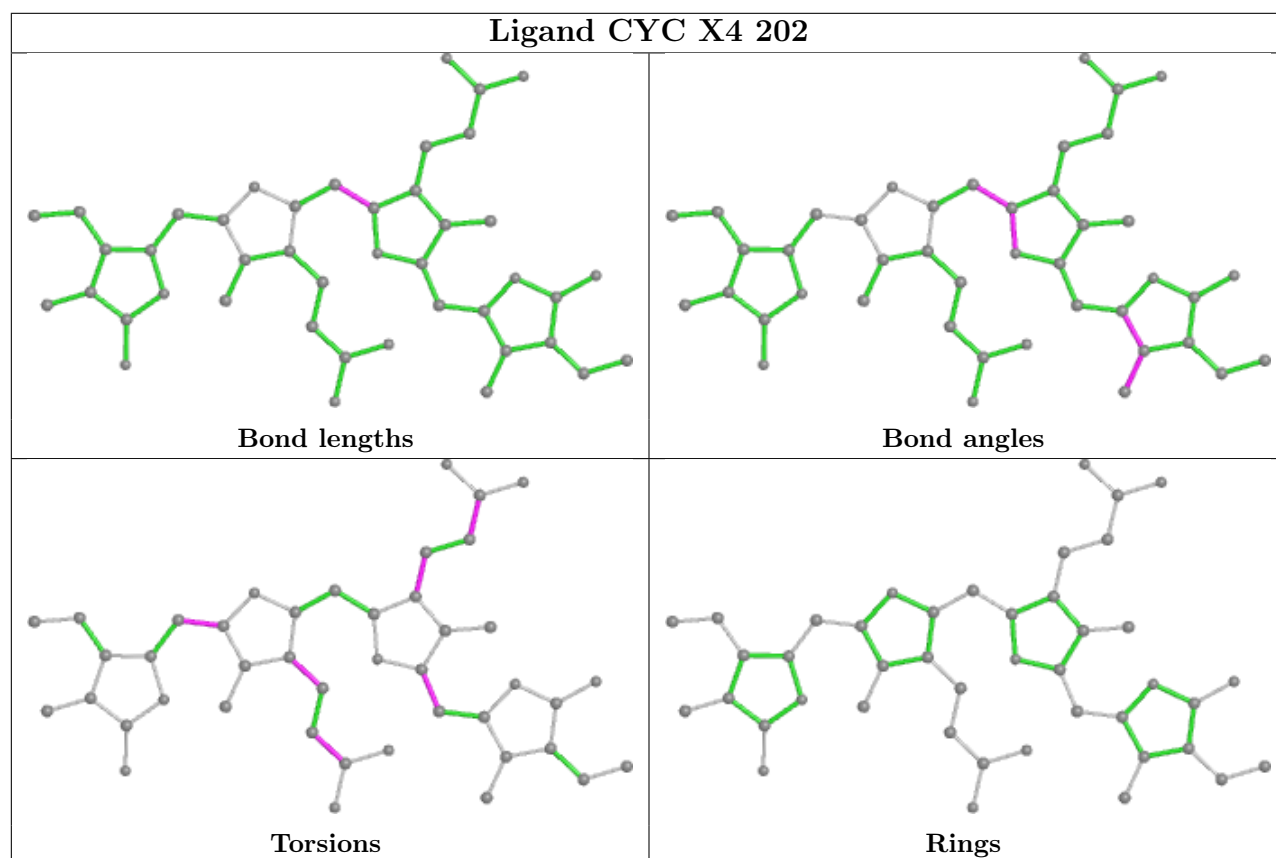
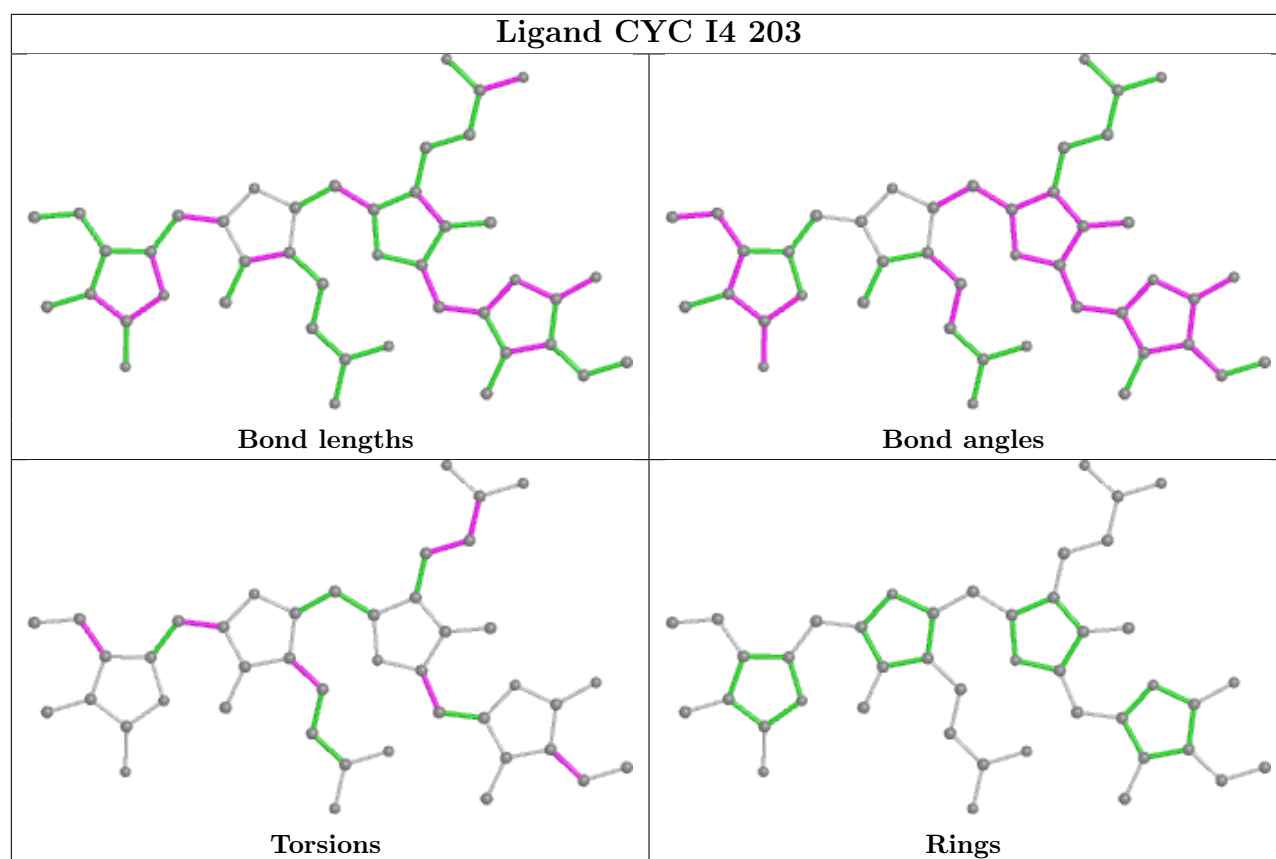
Mol	Chain	Res	Type	Atoms
11	A1	301	CYC	C2C-C3C-CAC-CBC
11	A1	301	CYC	C4C-C3C-CAC-CBC
11	A1	301	CYC	ND-C1D-CHD-C4C
11	A1	301	CYC	C2D-C1D-CHD-C4C
11	A1	302	CYC	C2C-C3C-CAC-CBC

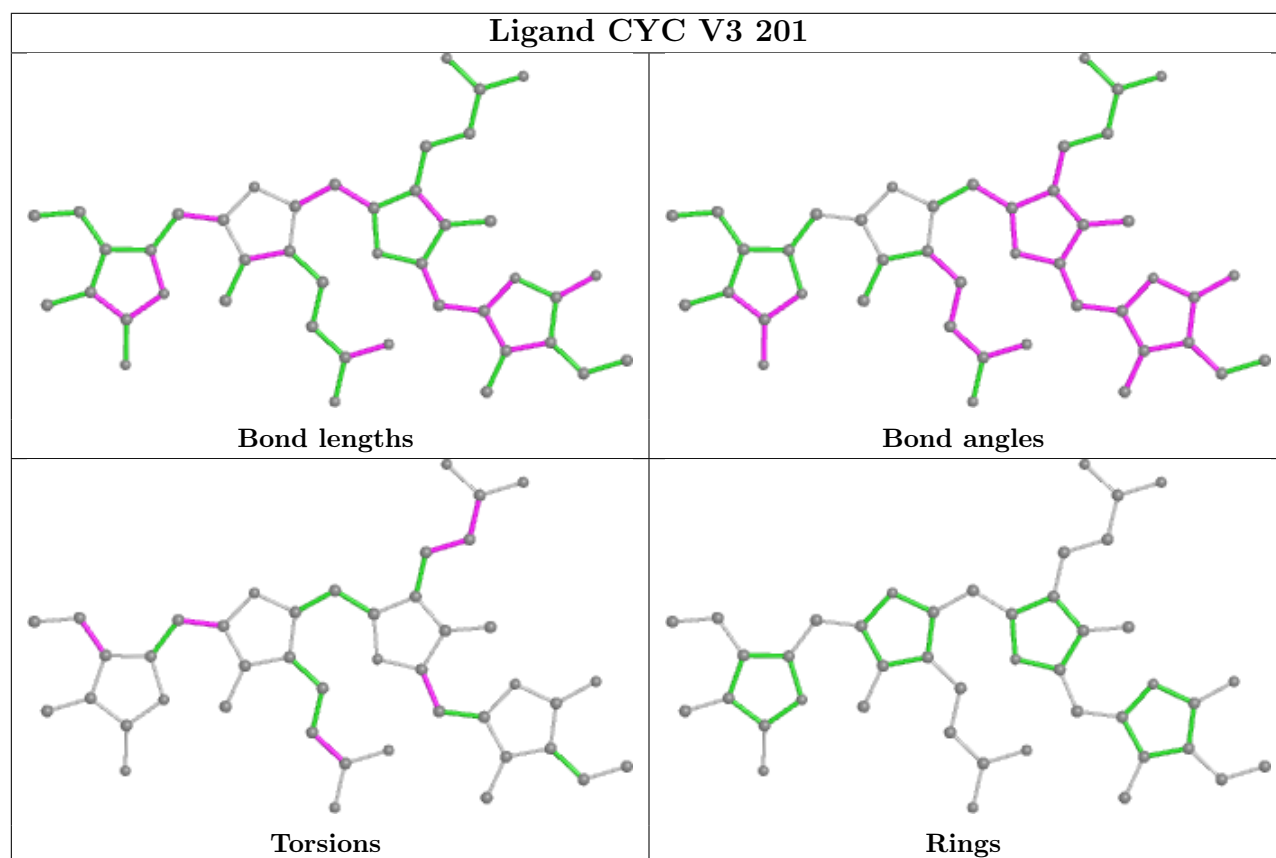
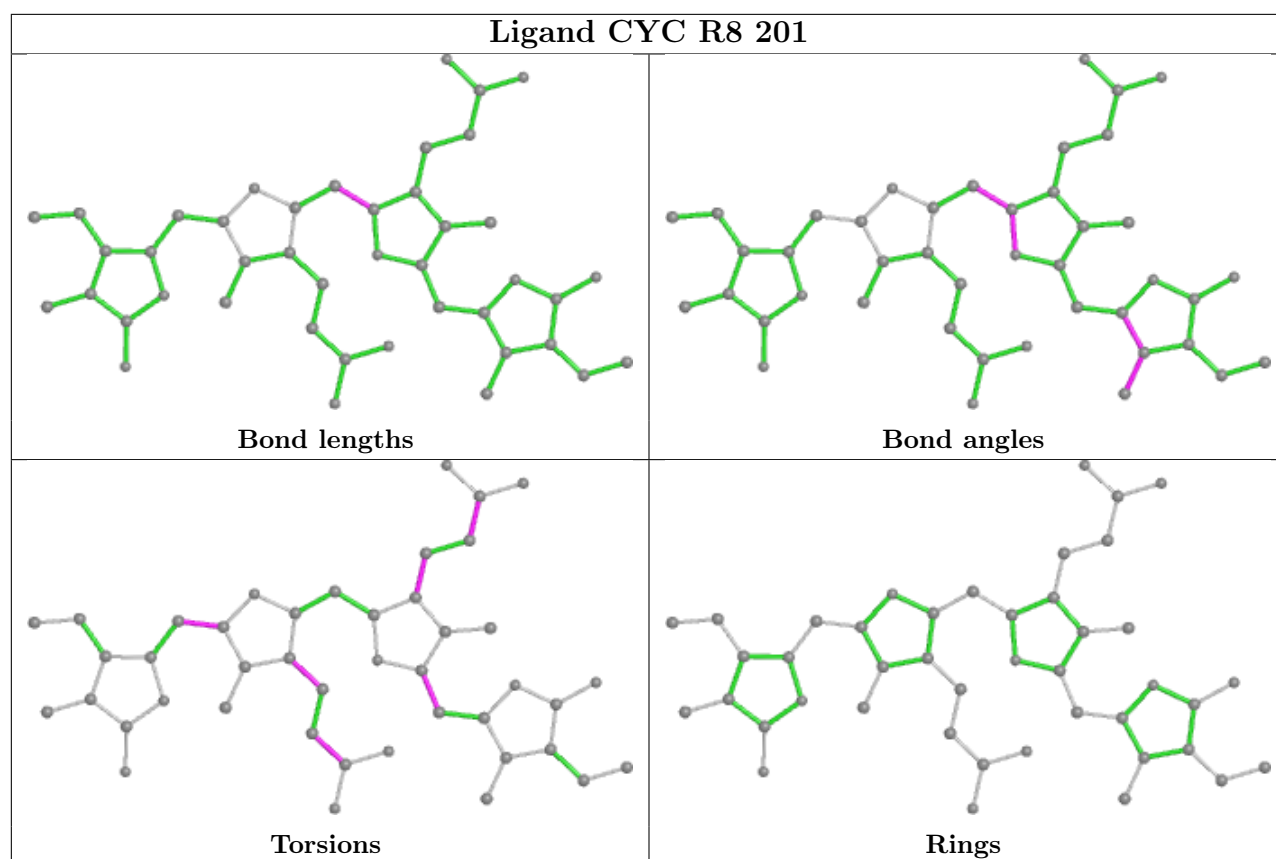
There are no ring outliers.

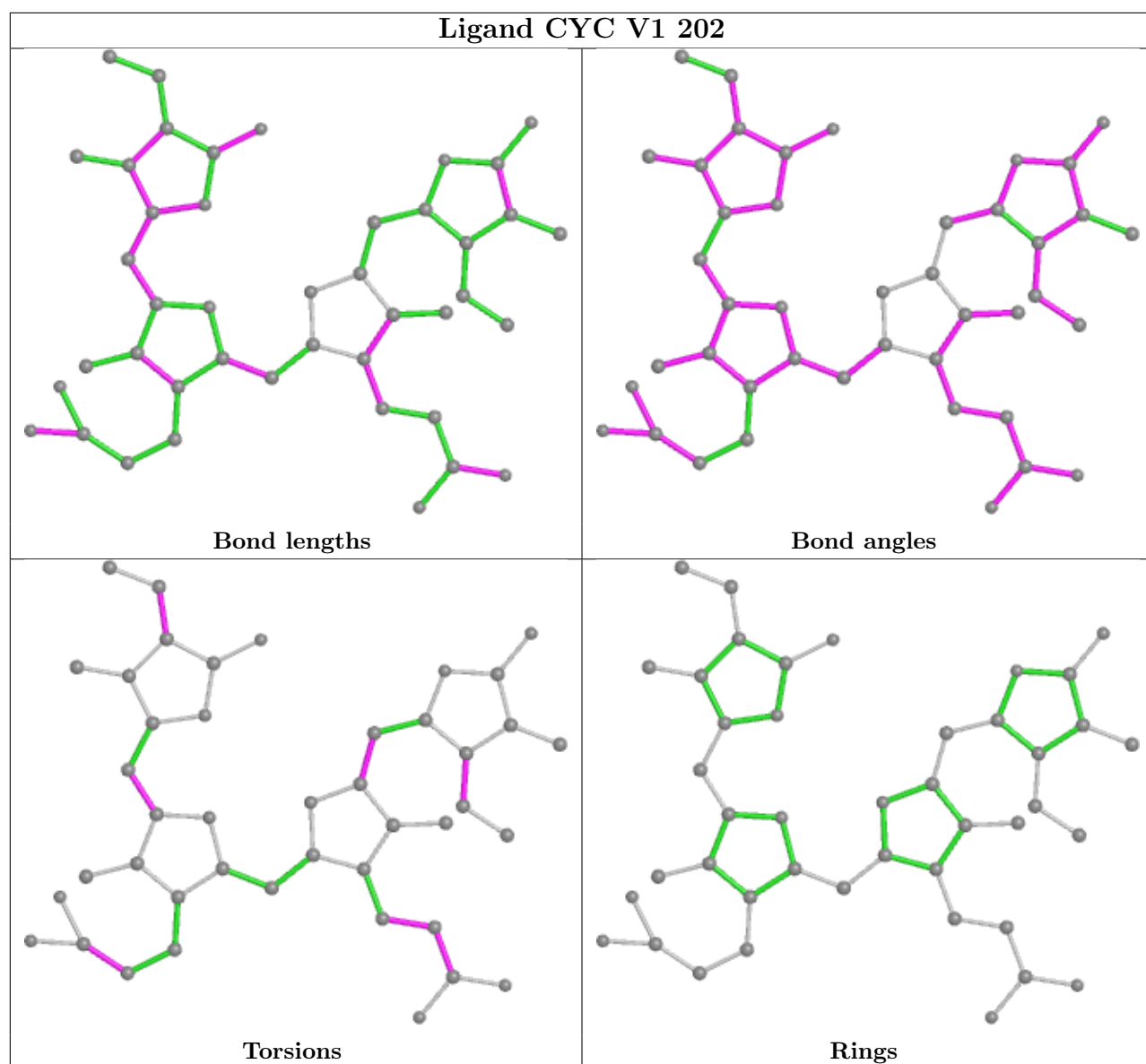
No monomer is involved in short contacts.

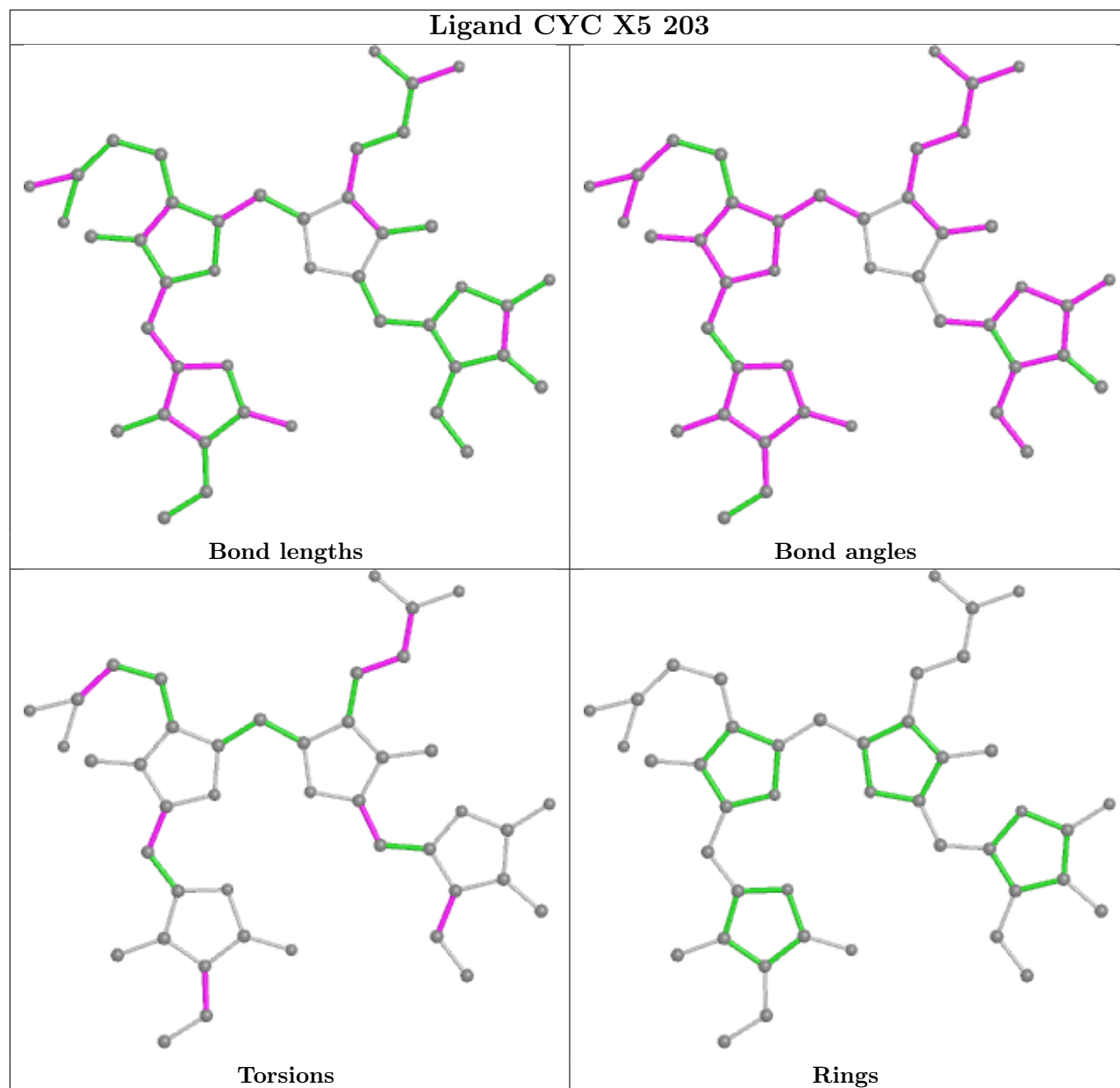
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

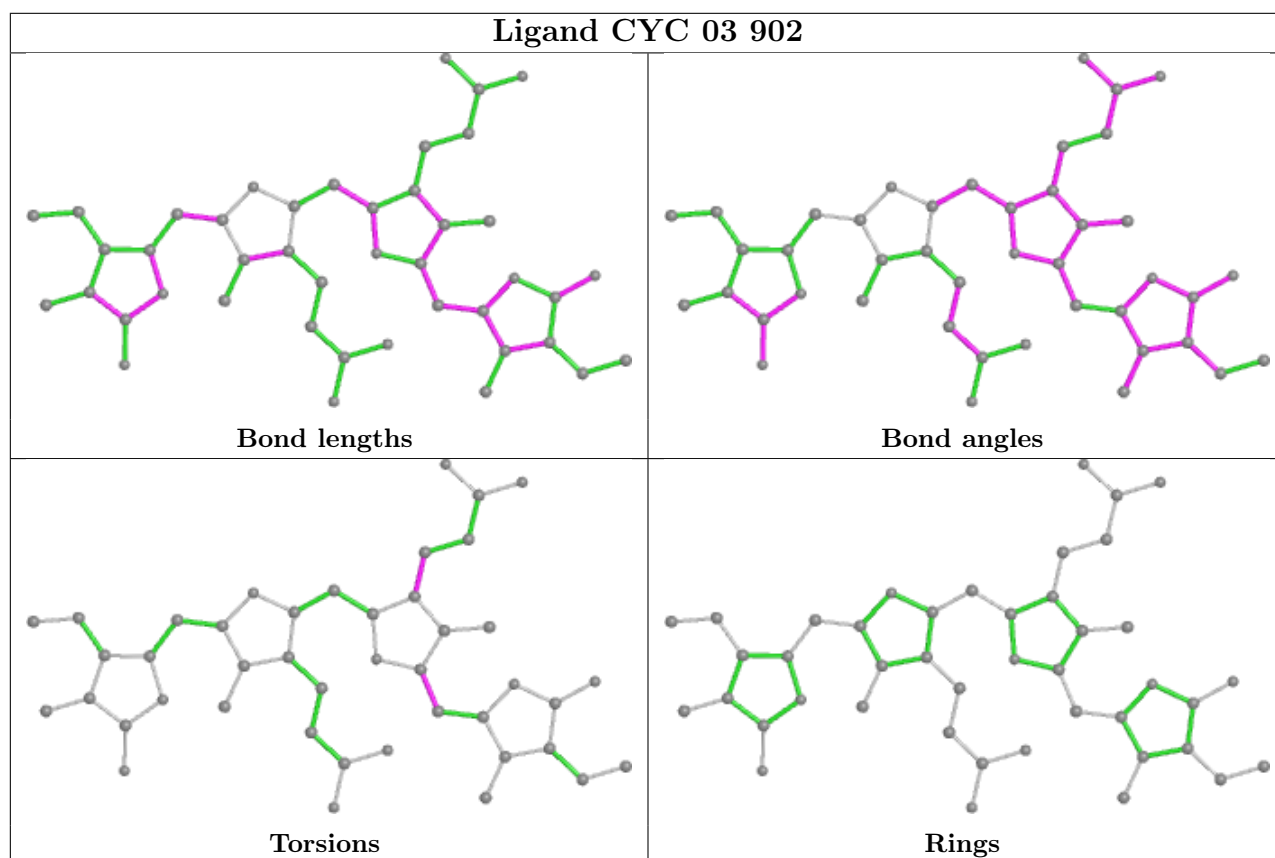
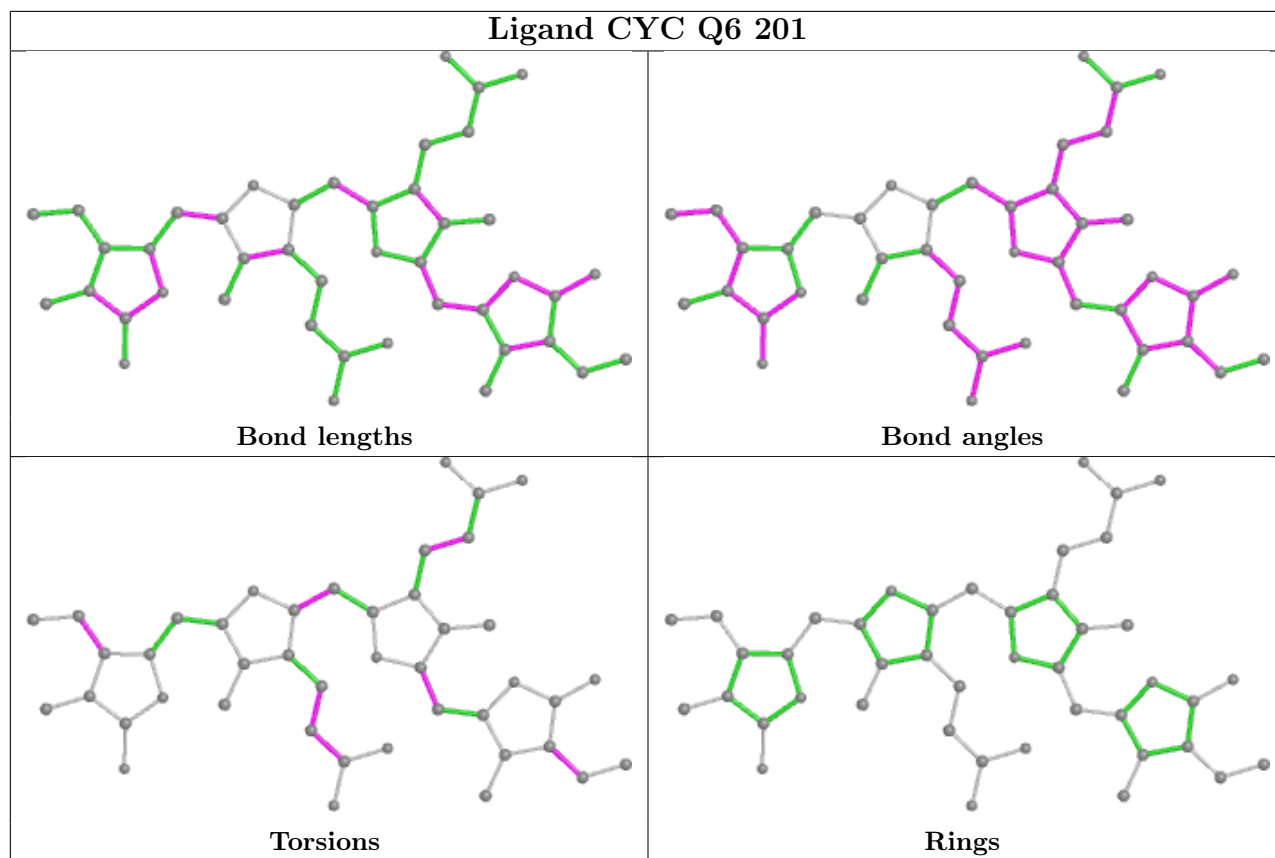


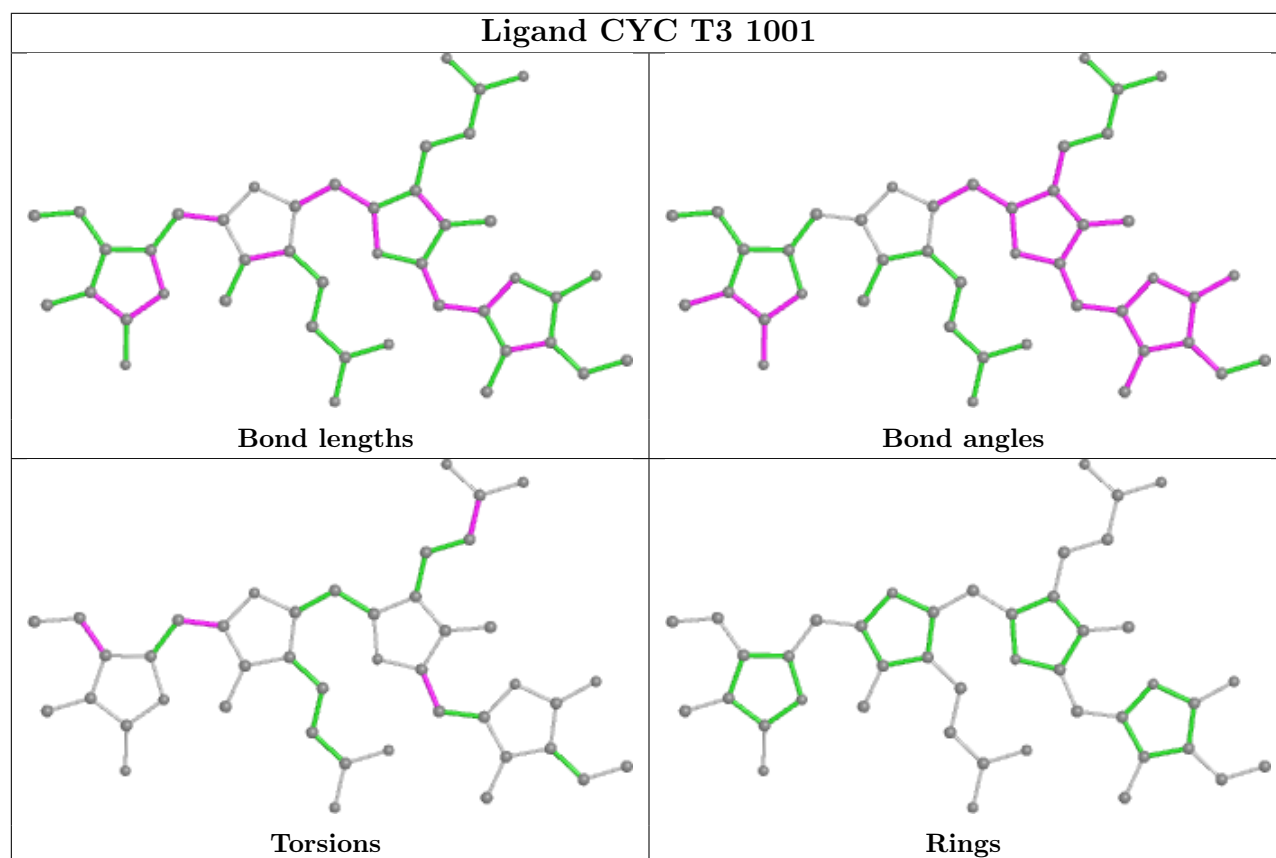
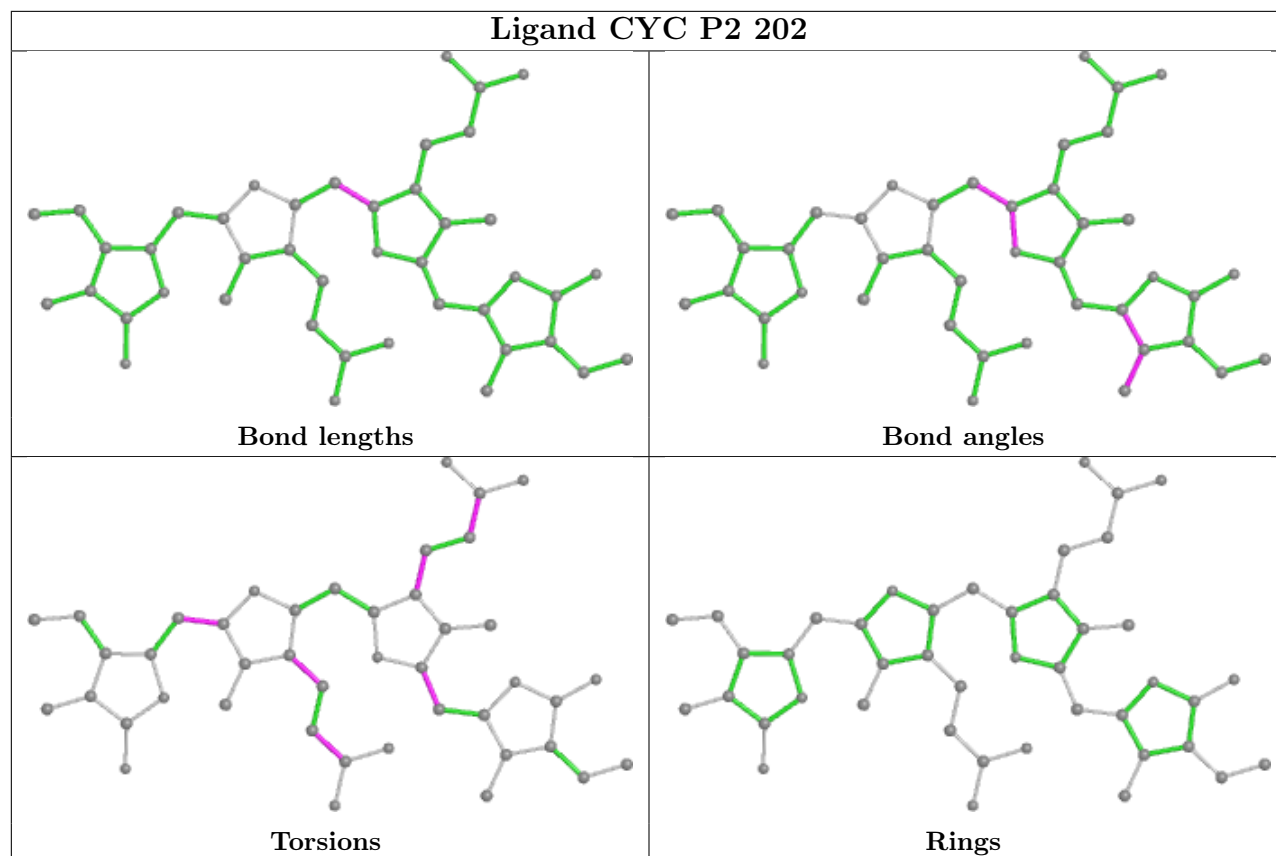


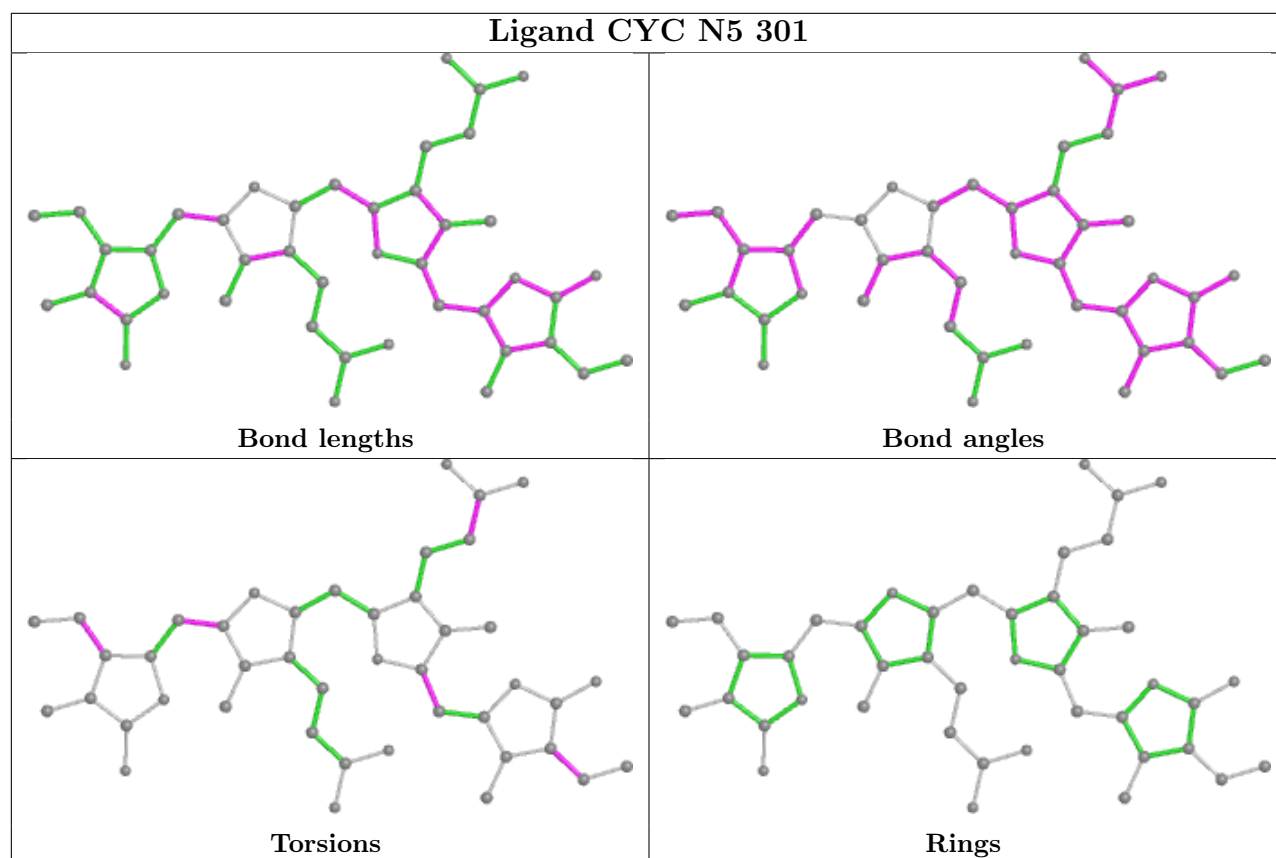
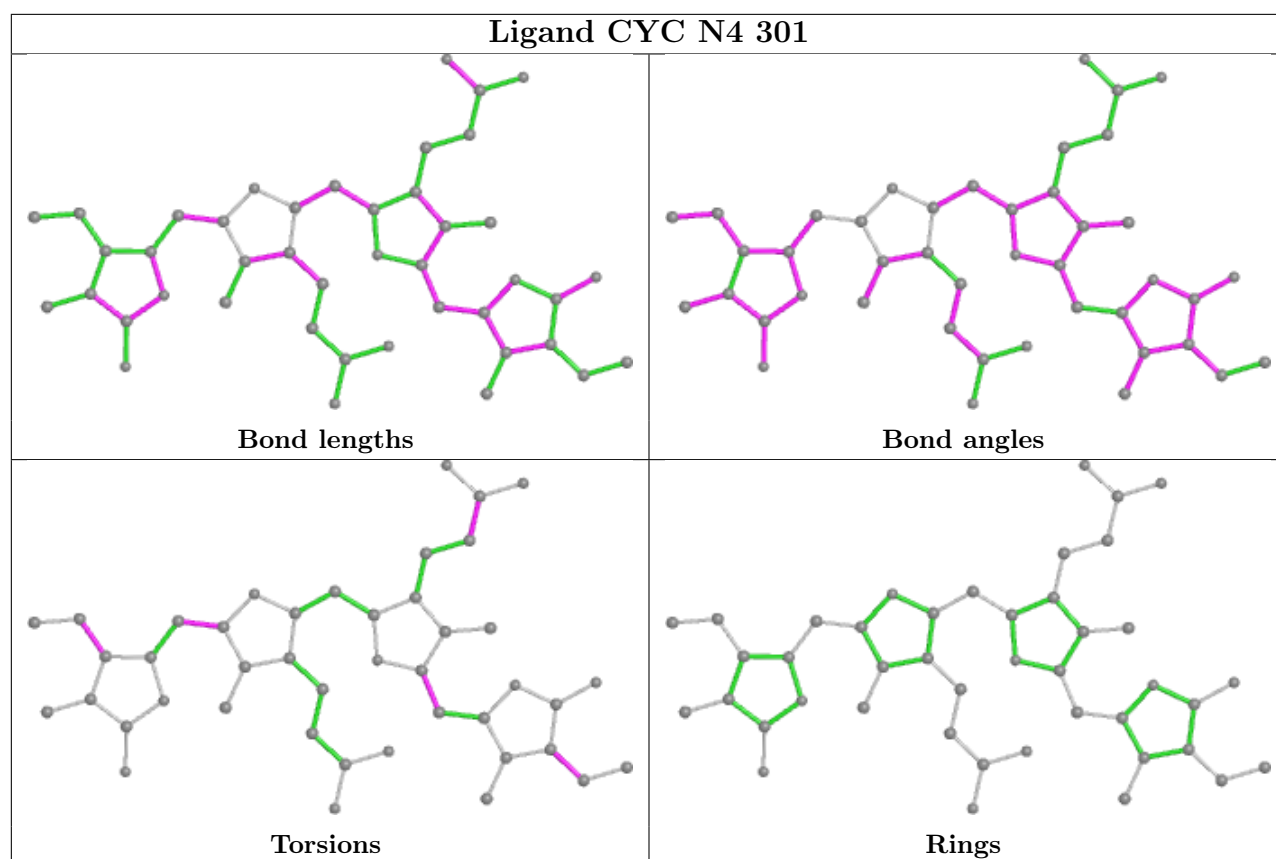


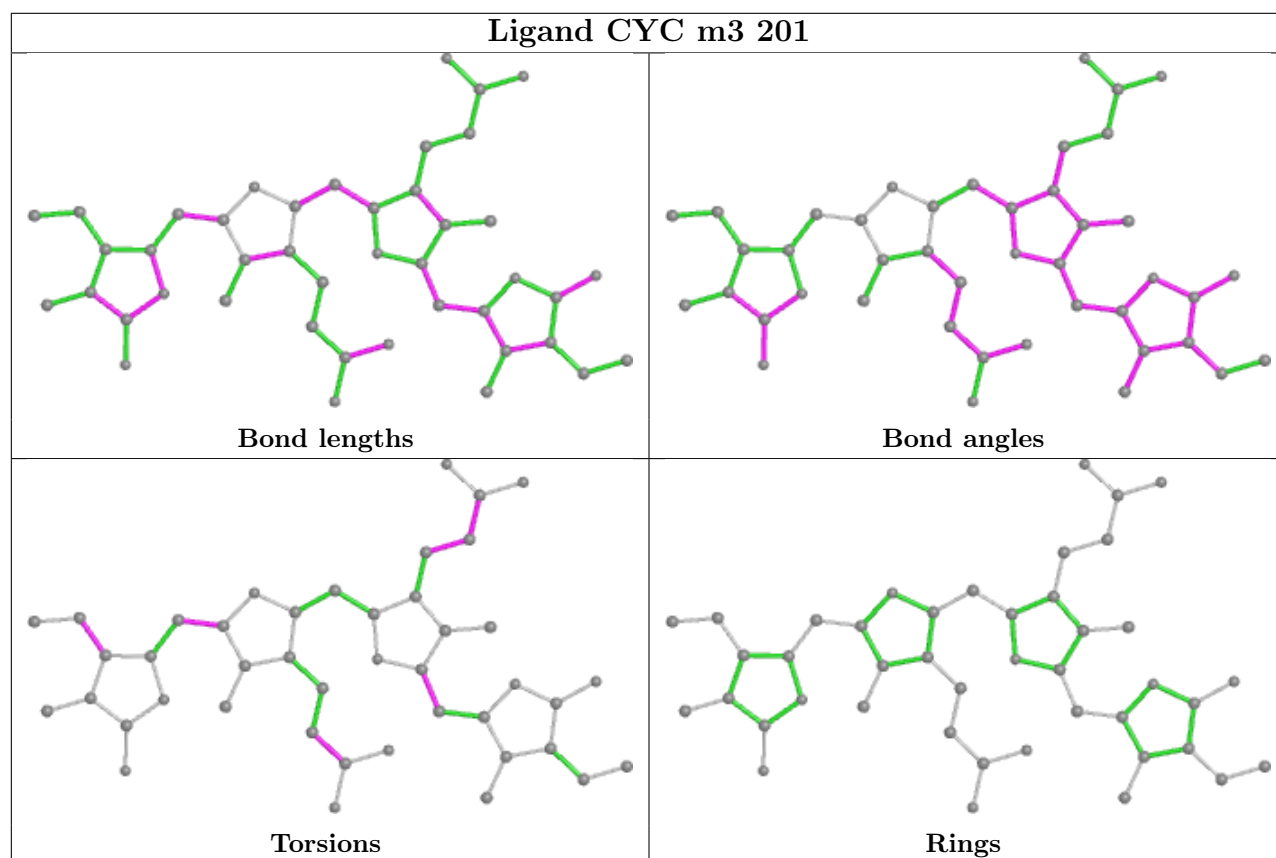
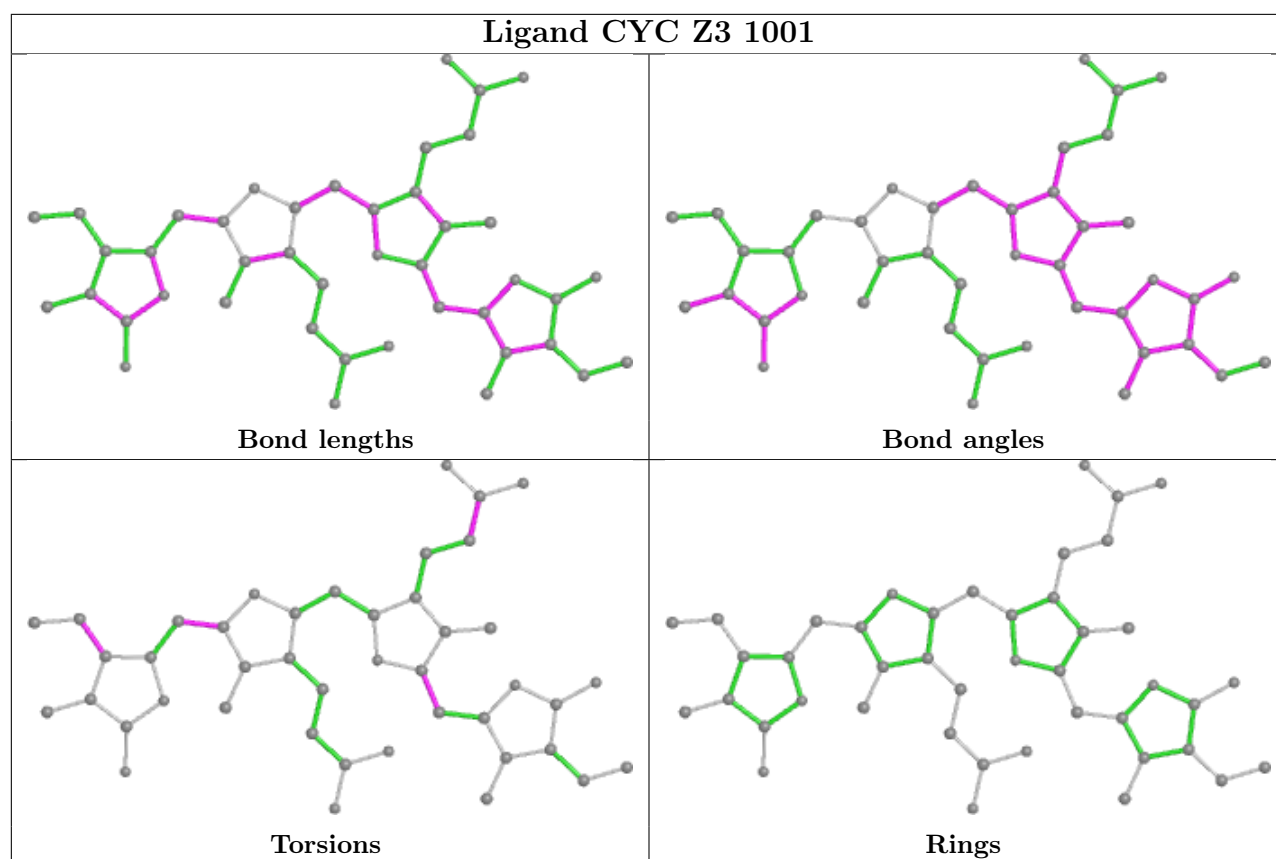


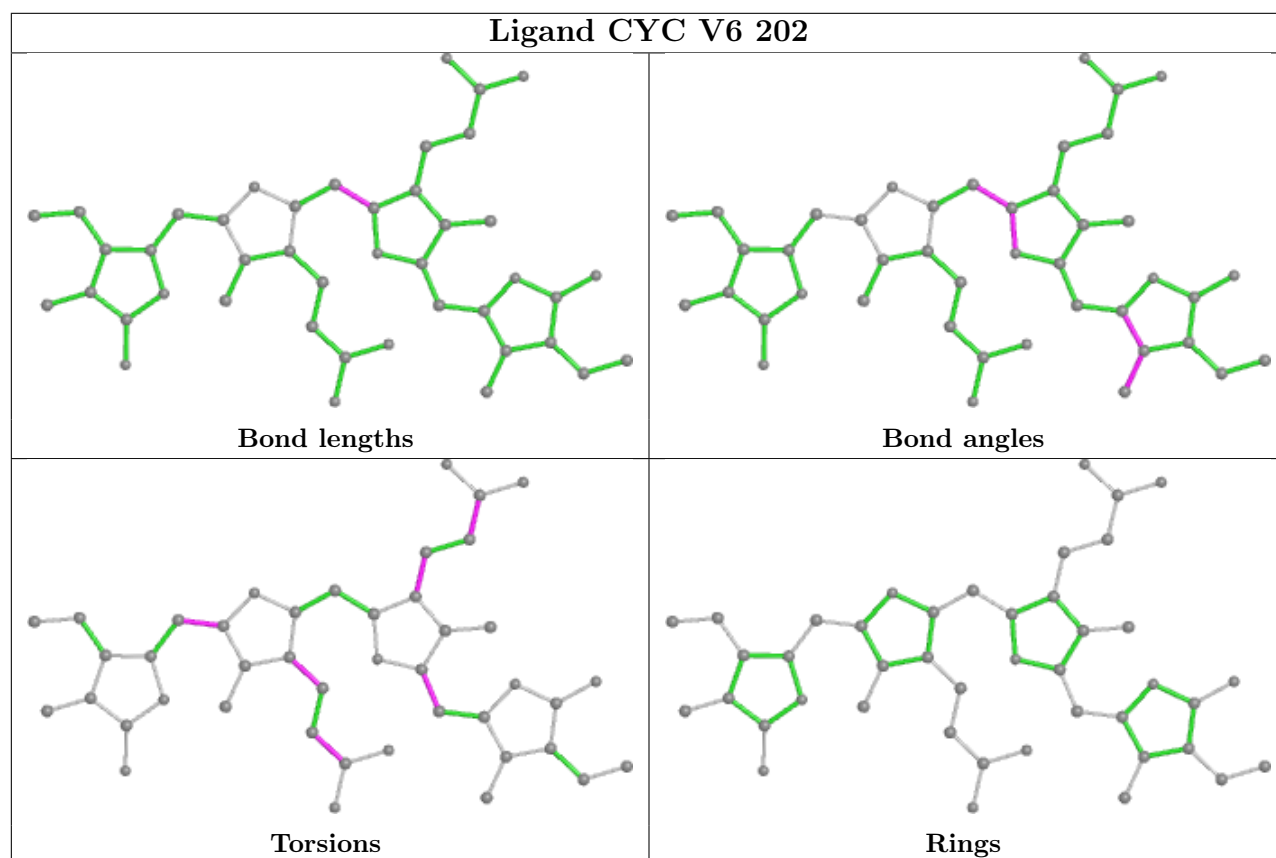
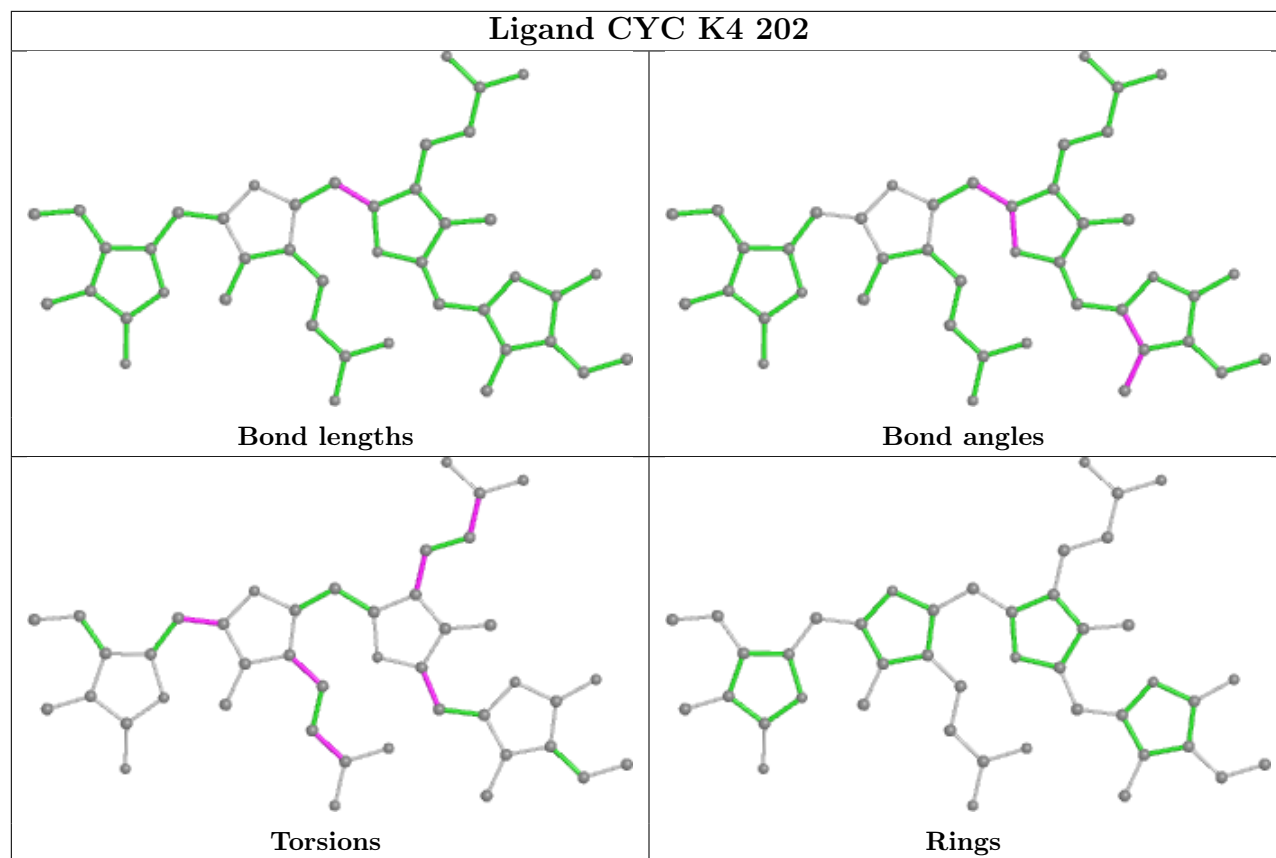


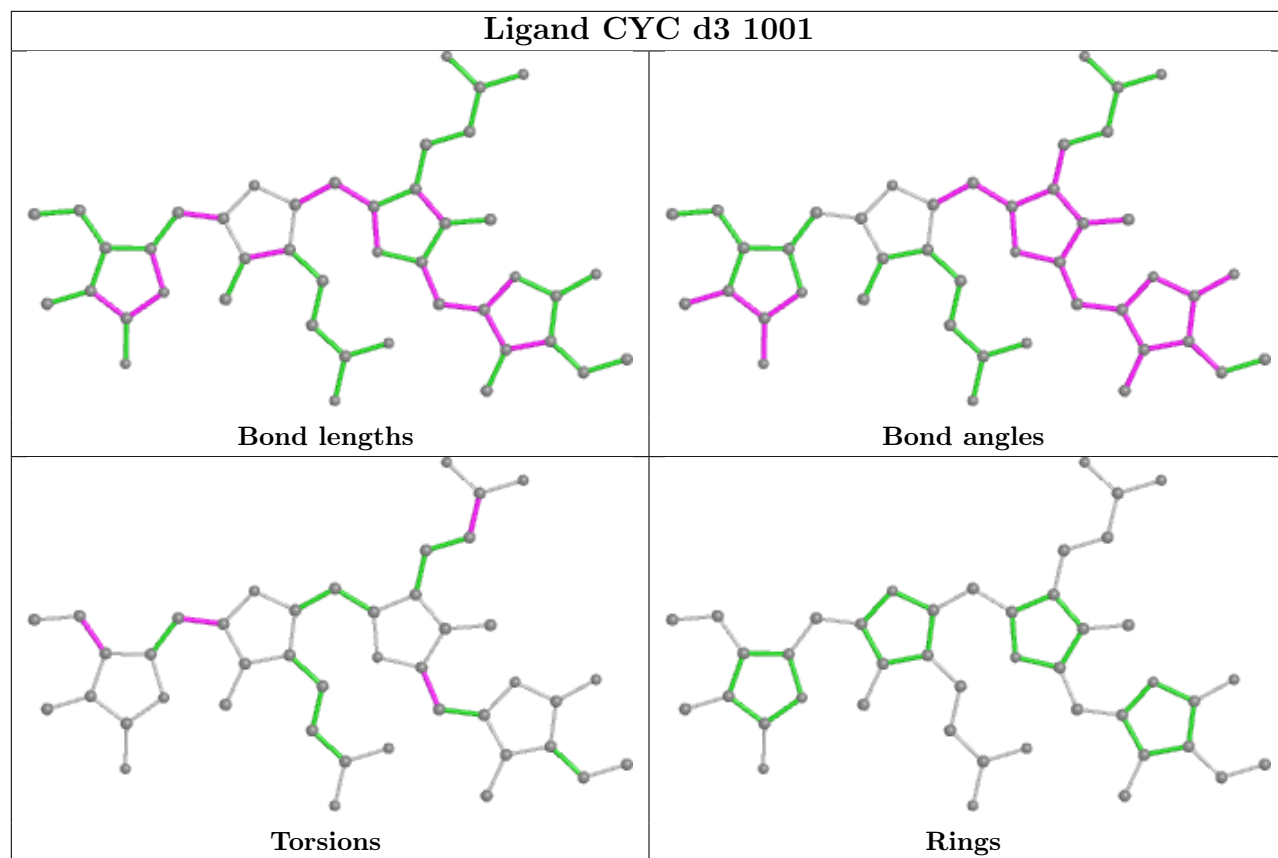


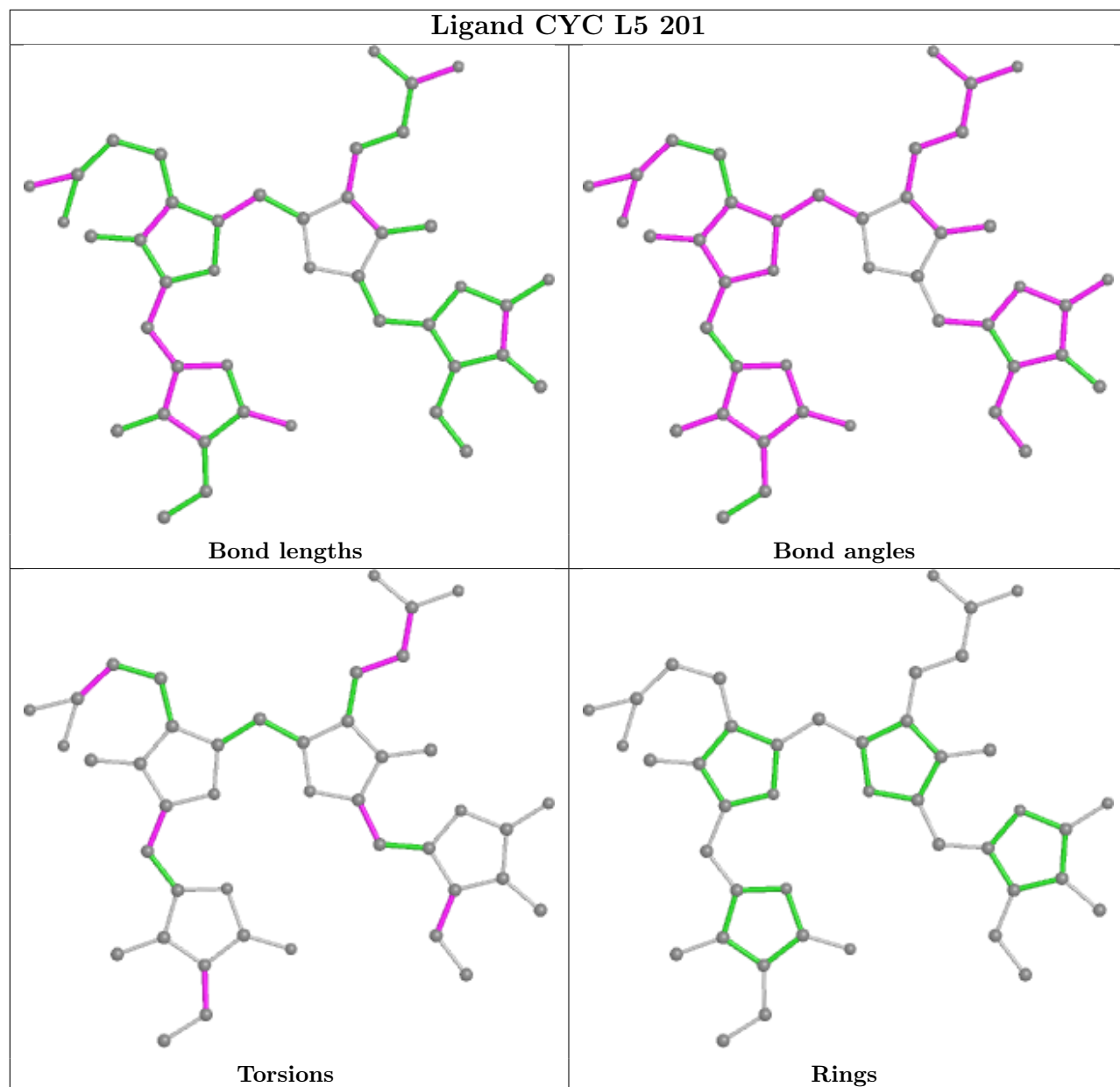


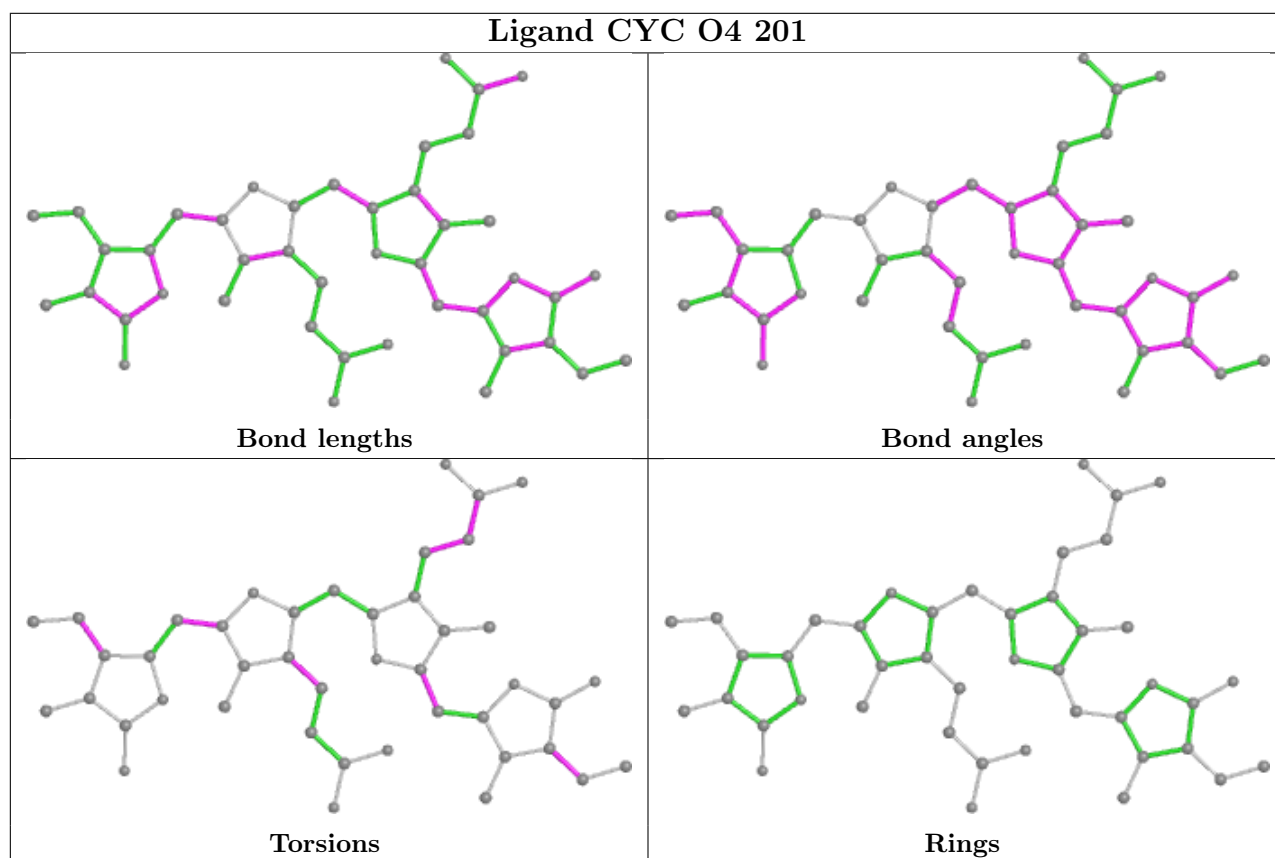
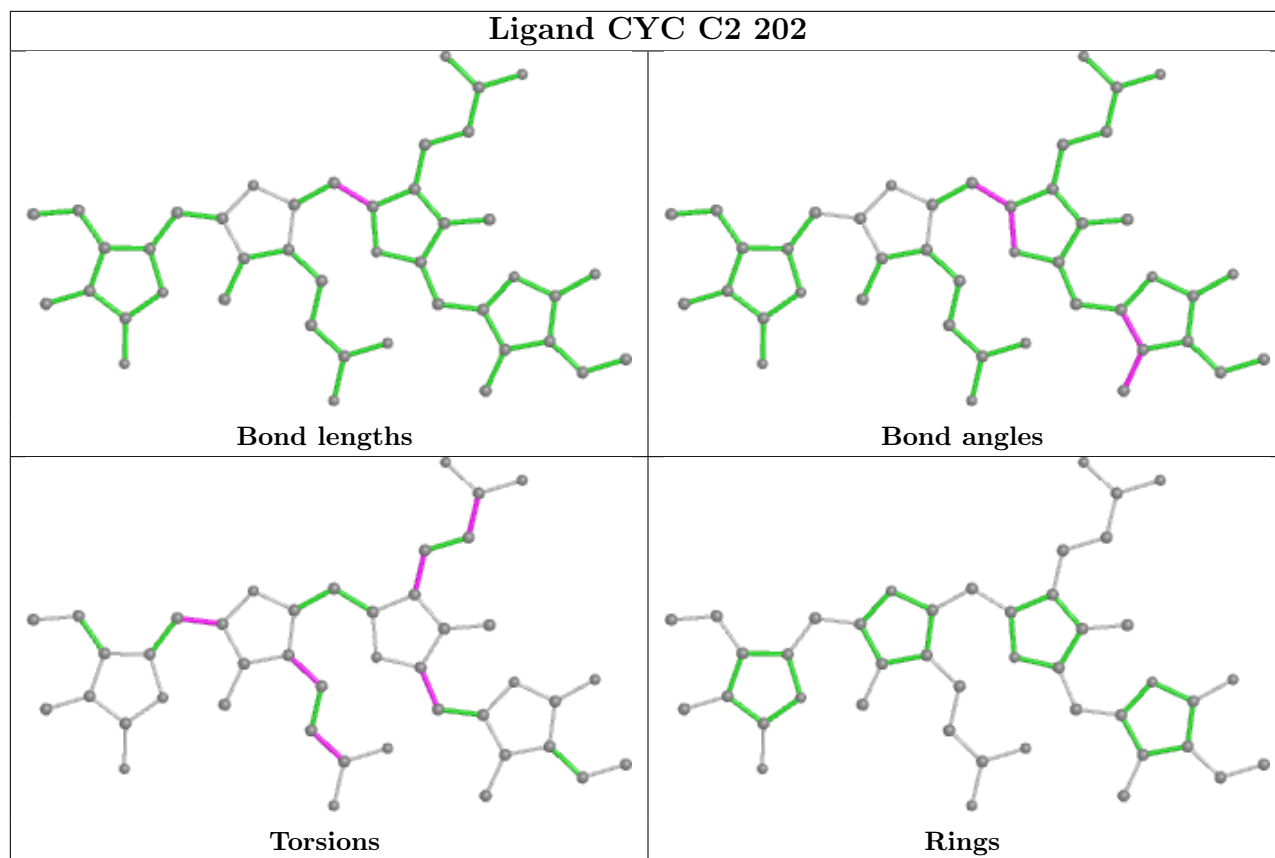


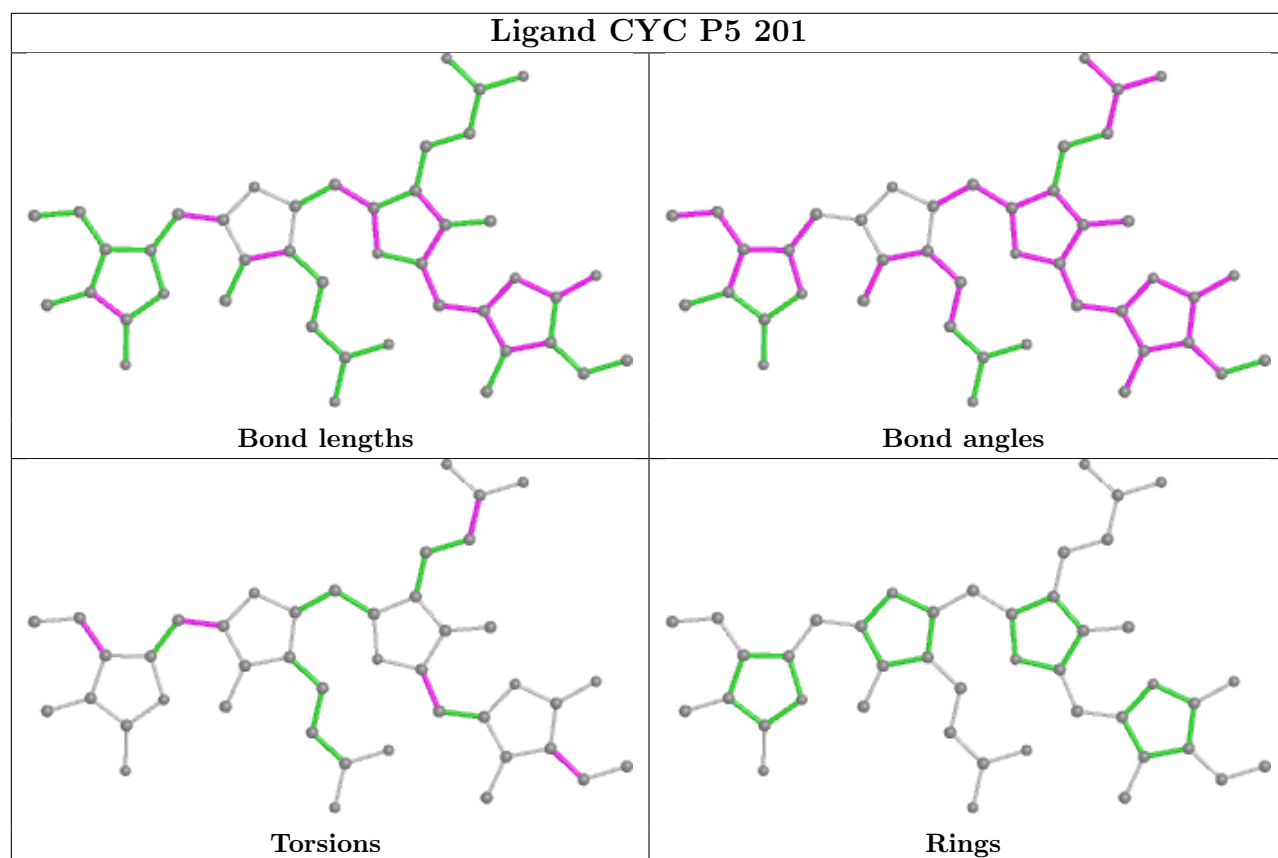
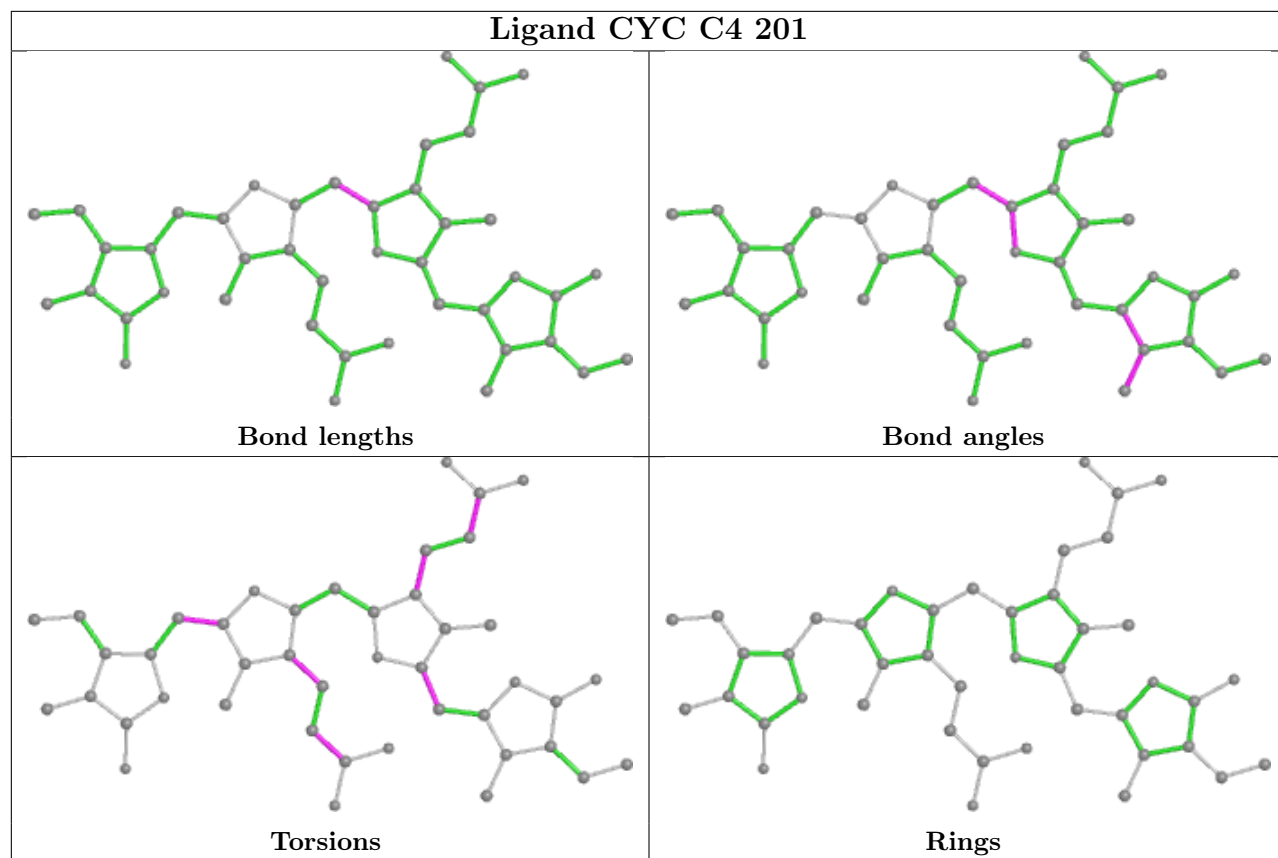


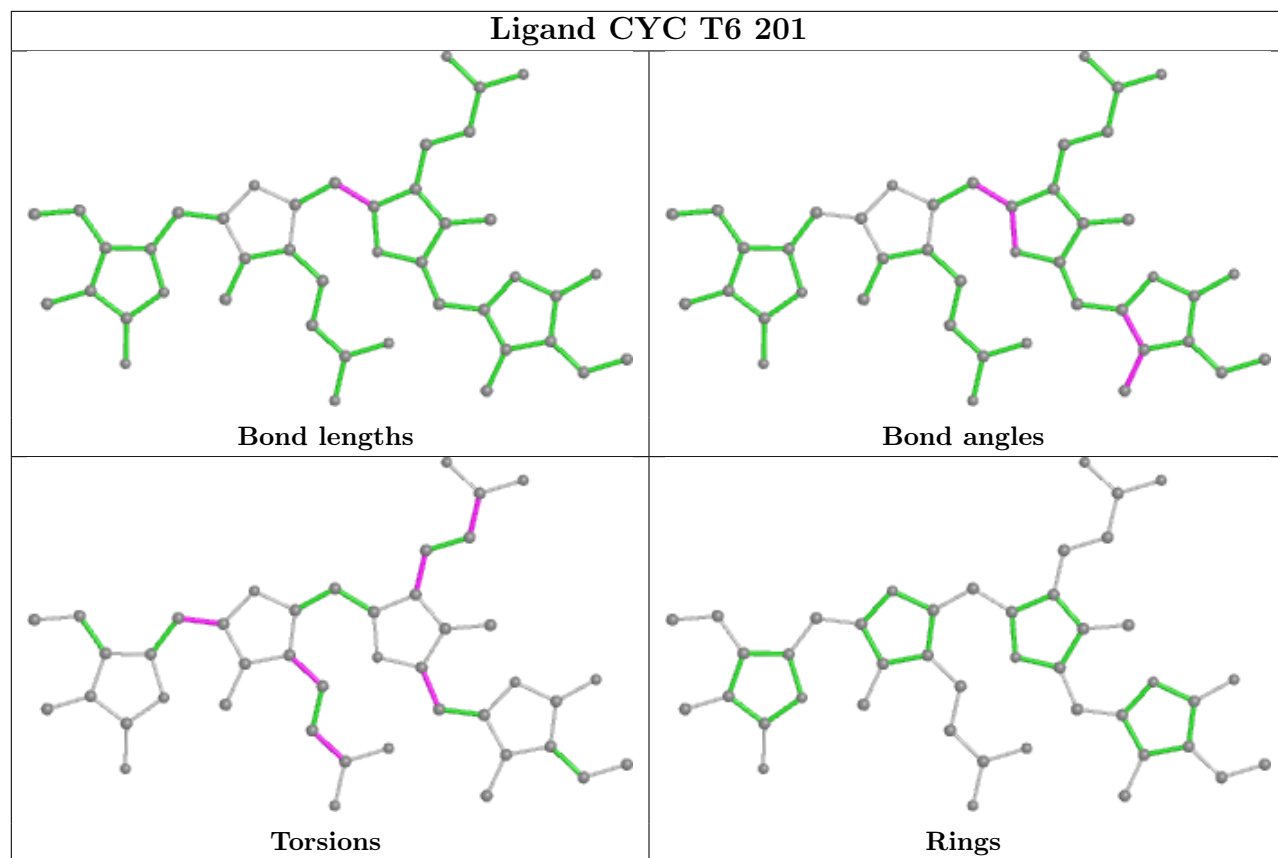


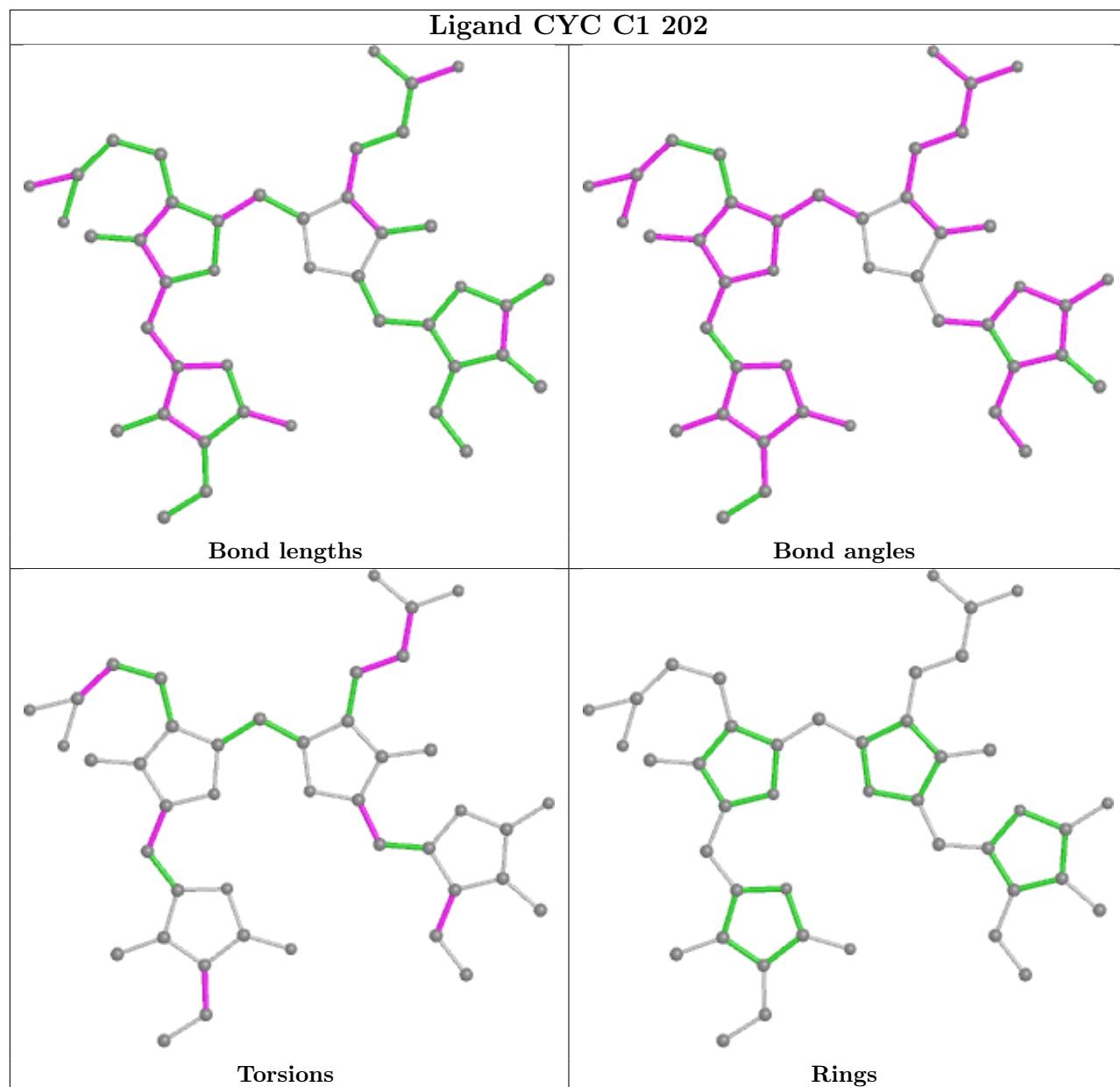


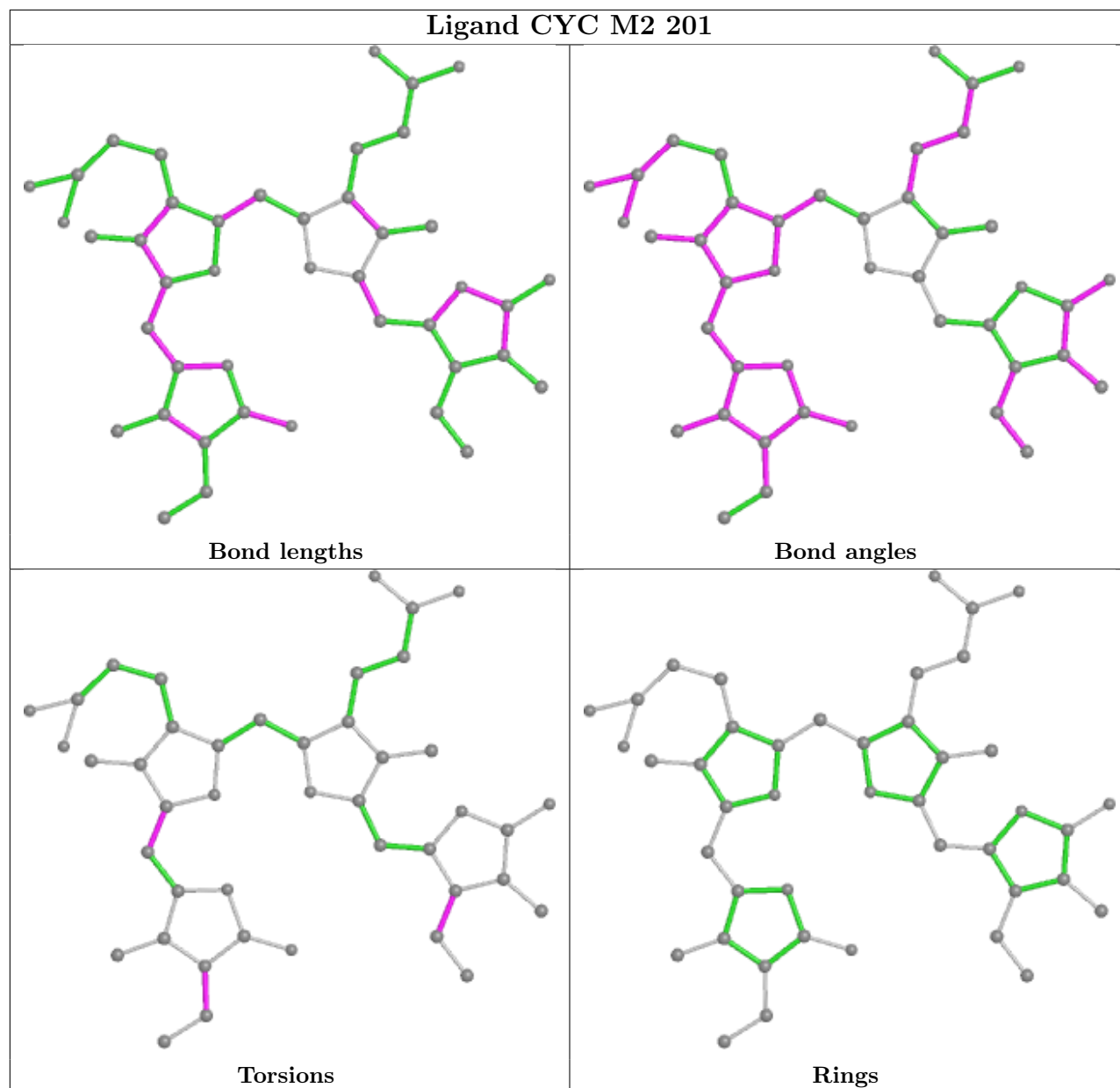


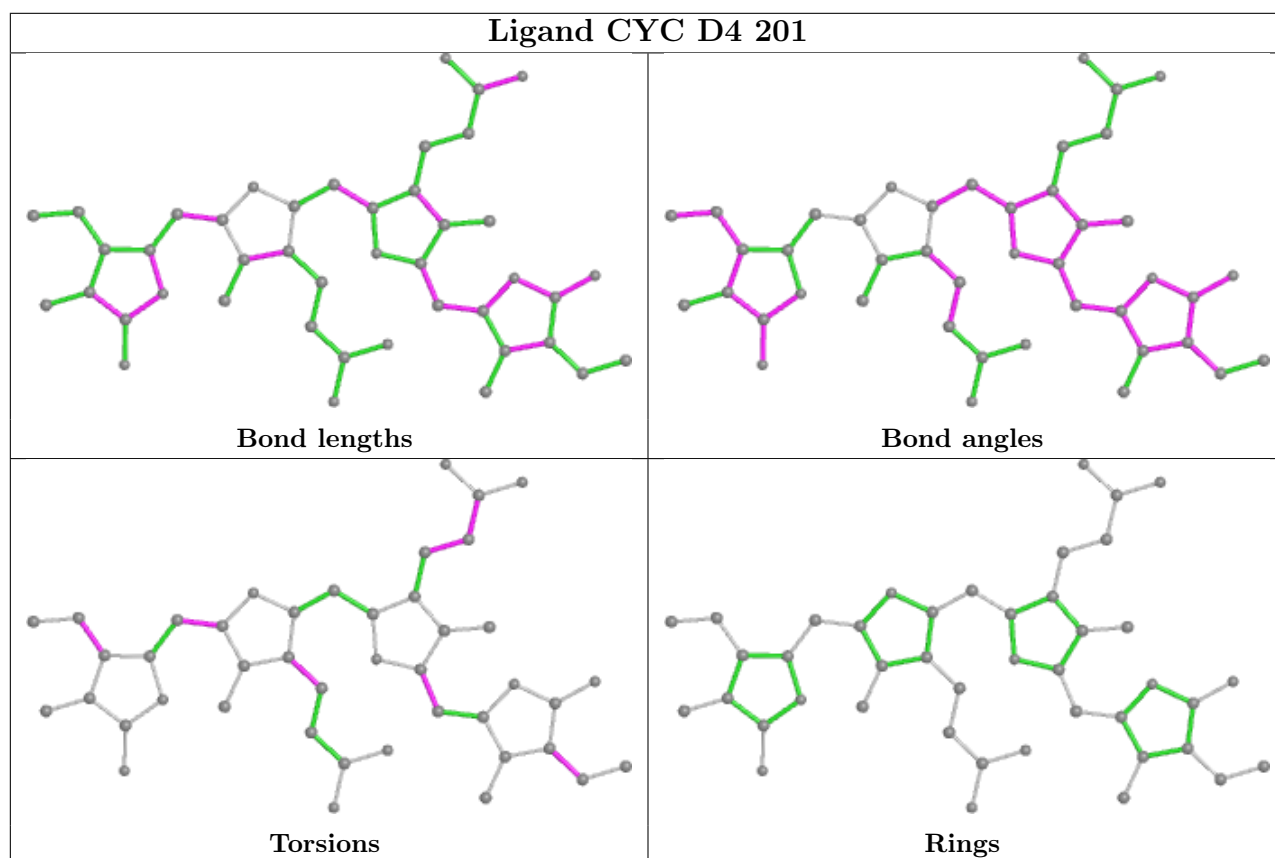
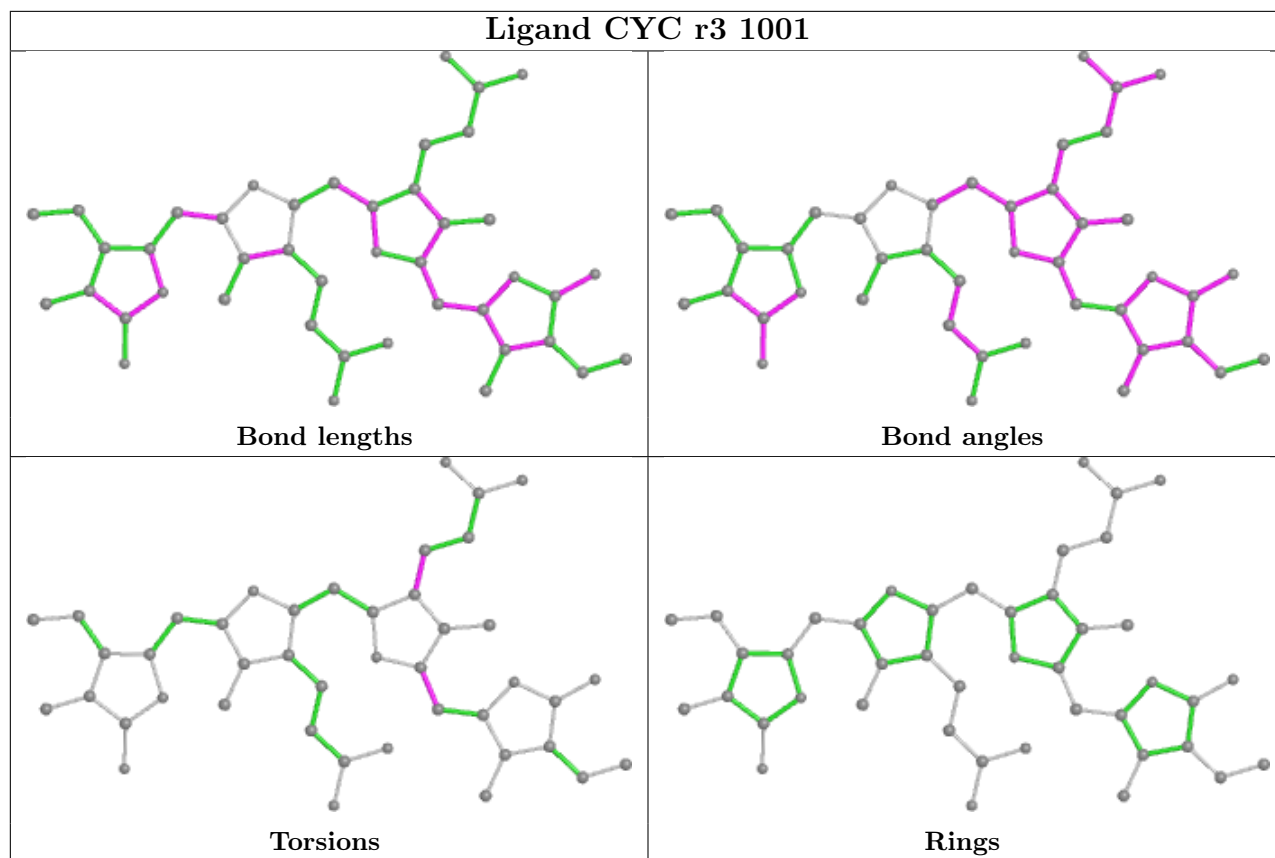


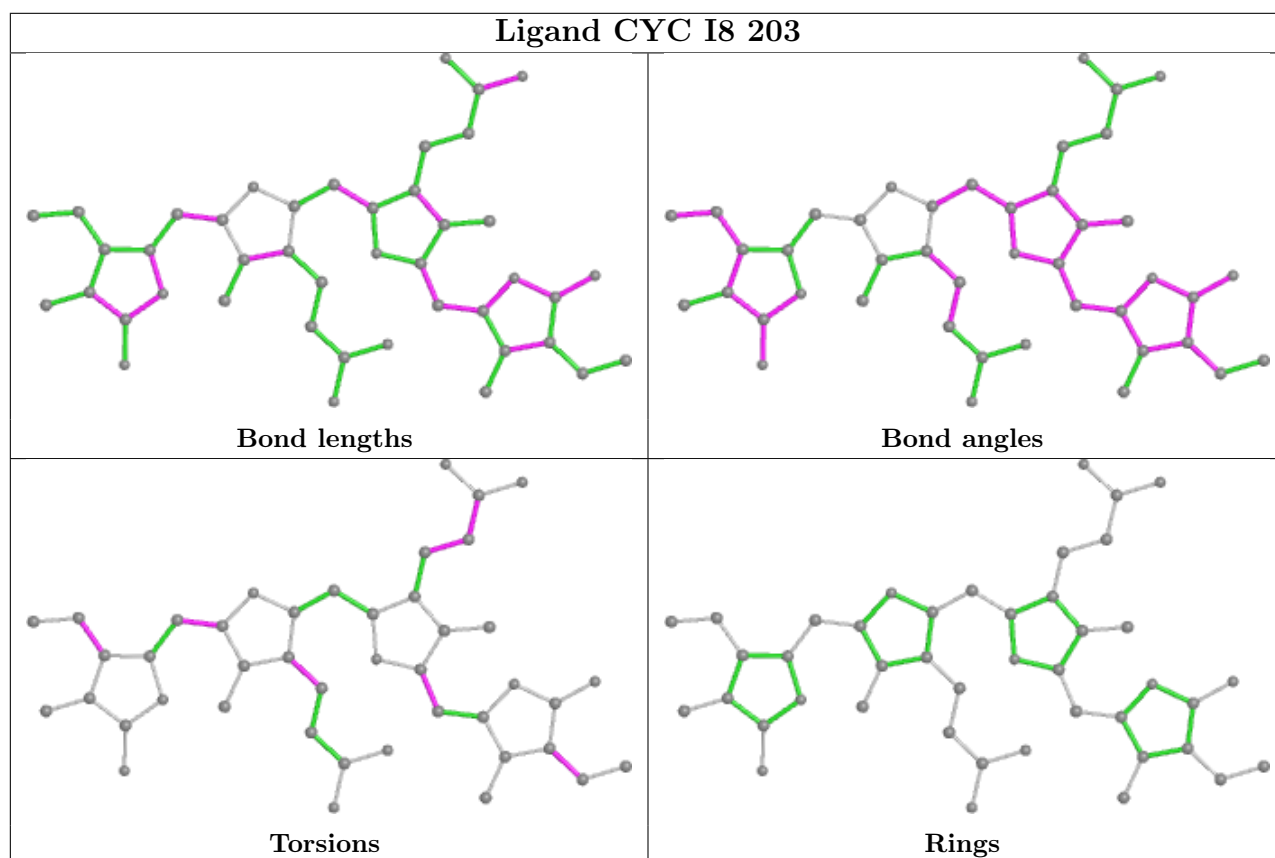
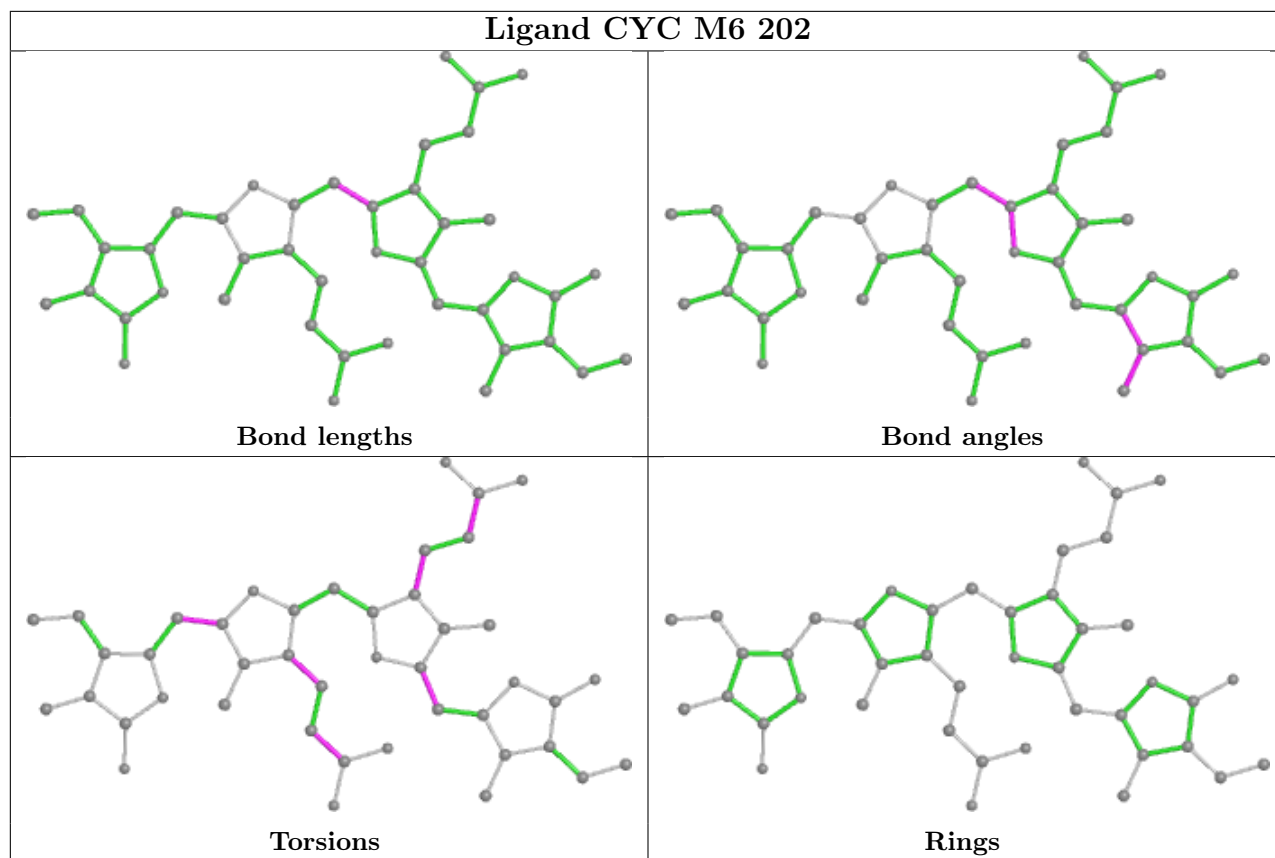


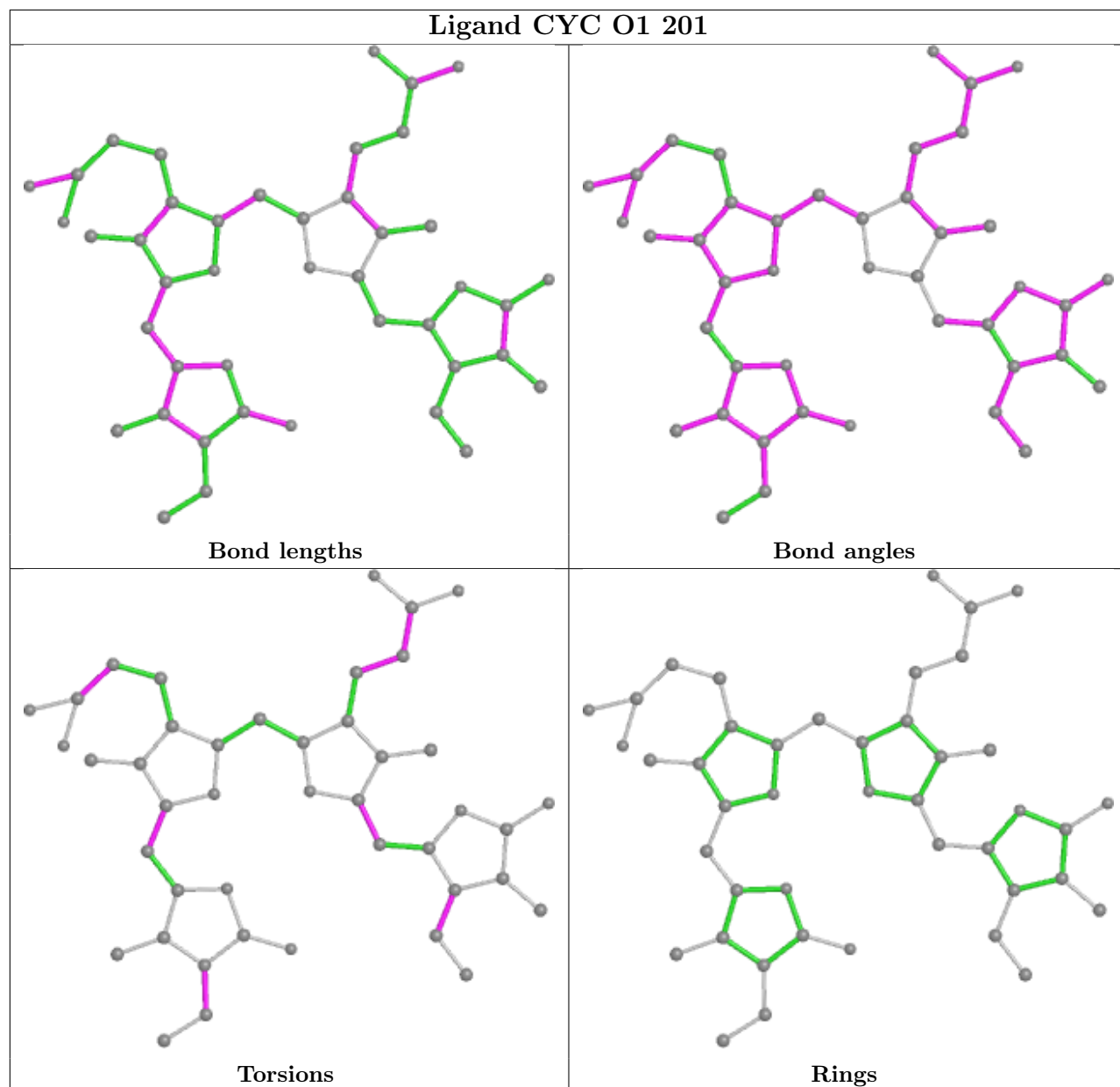


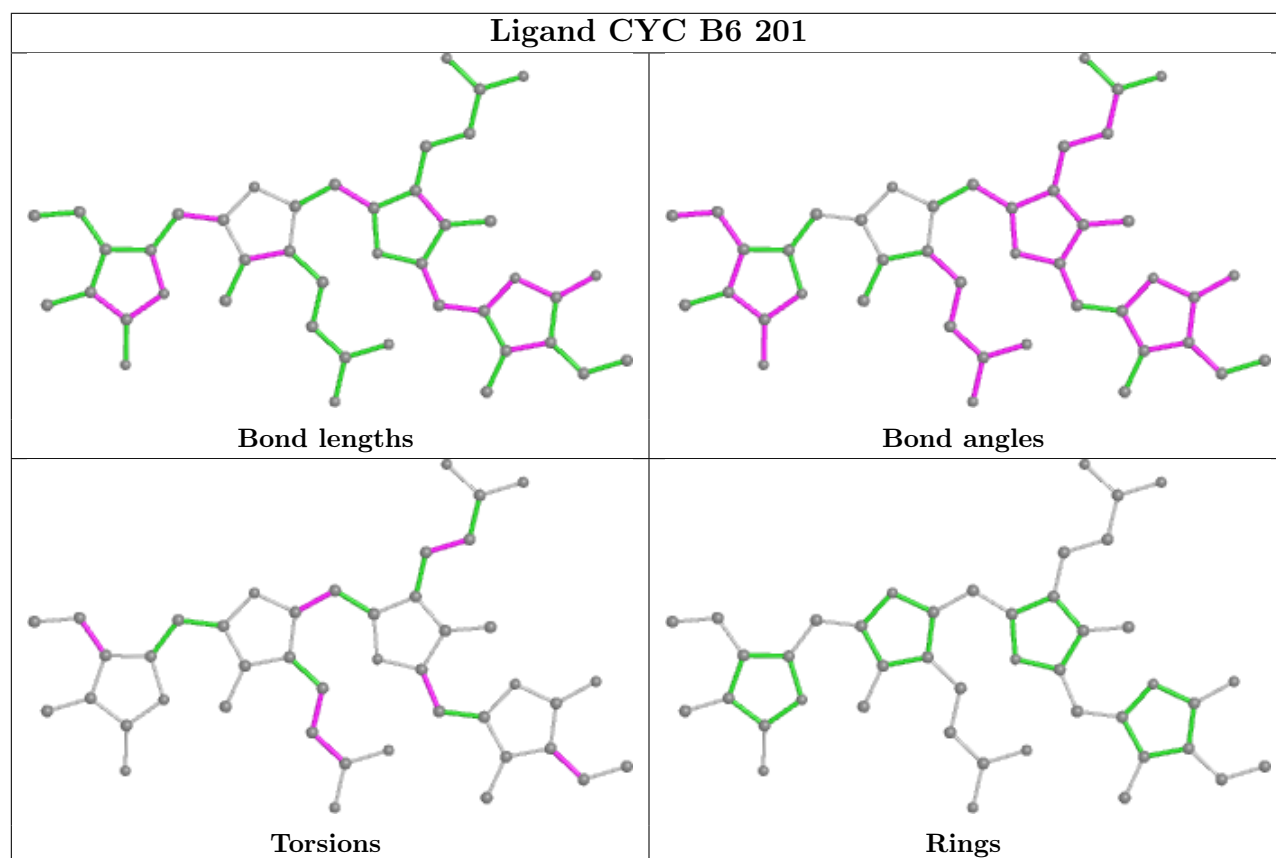
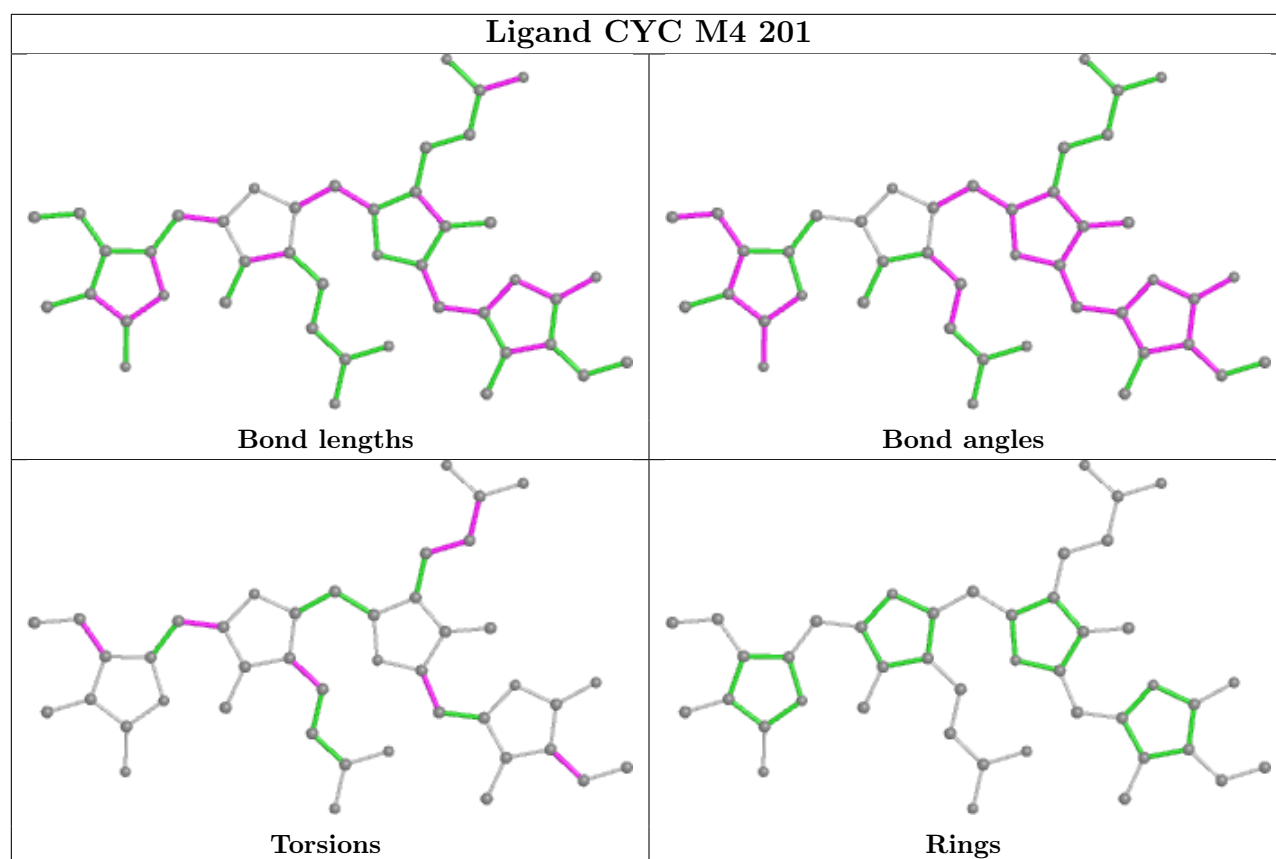


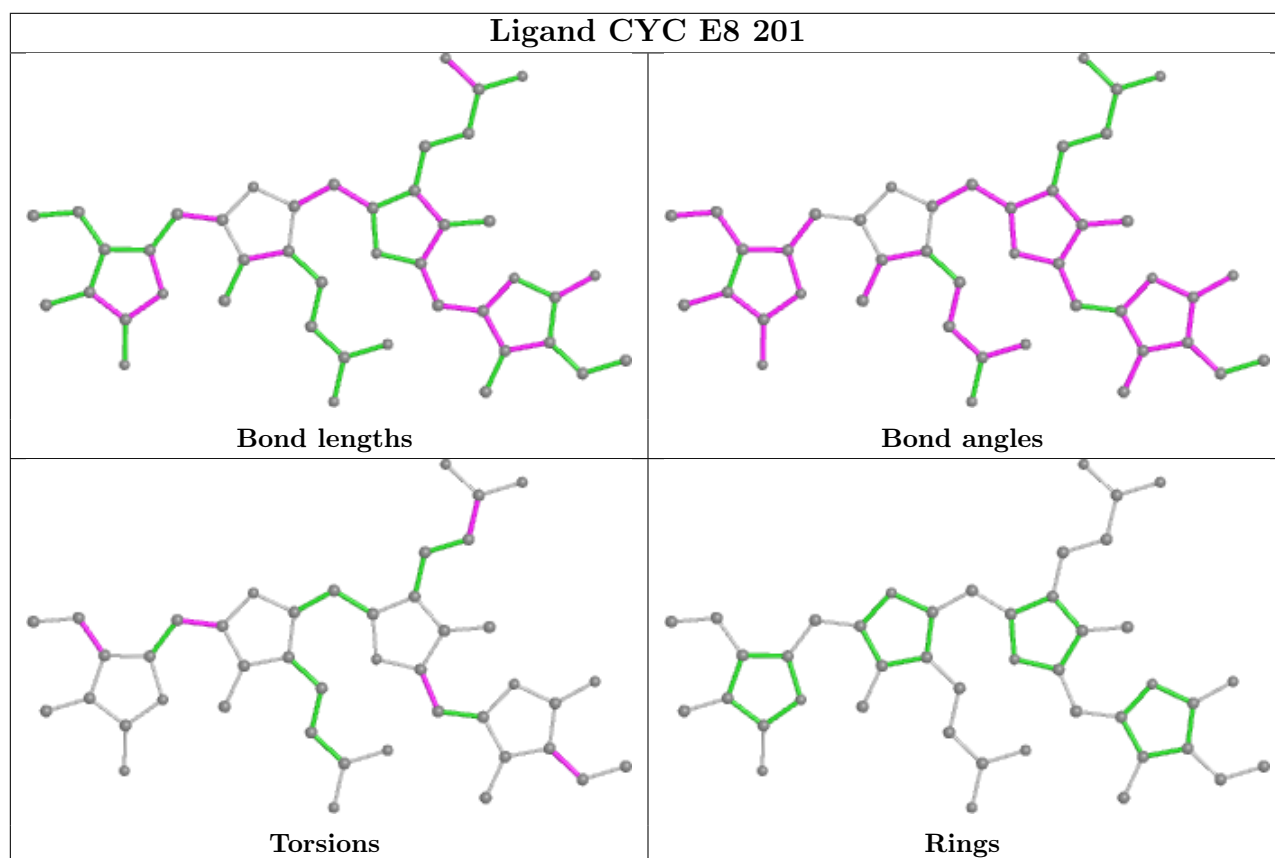
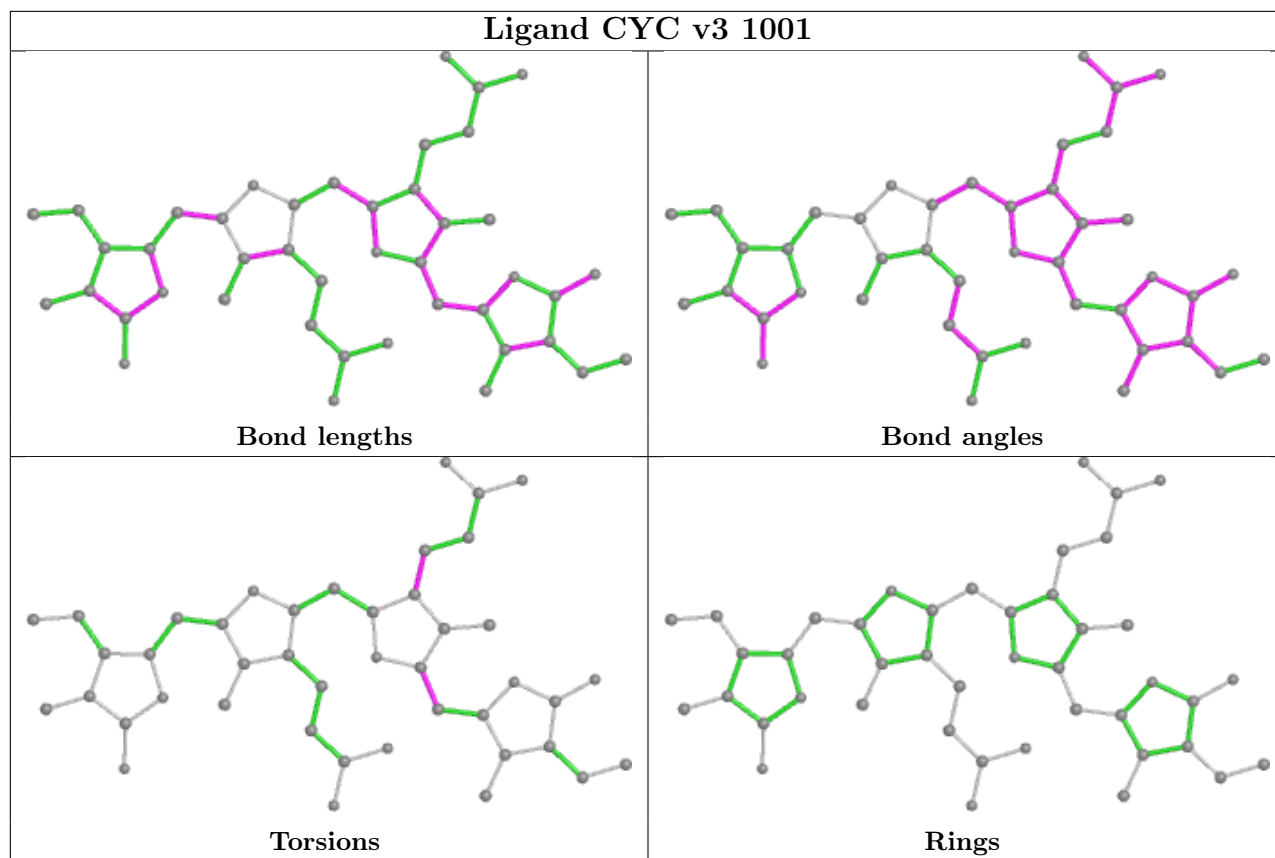


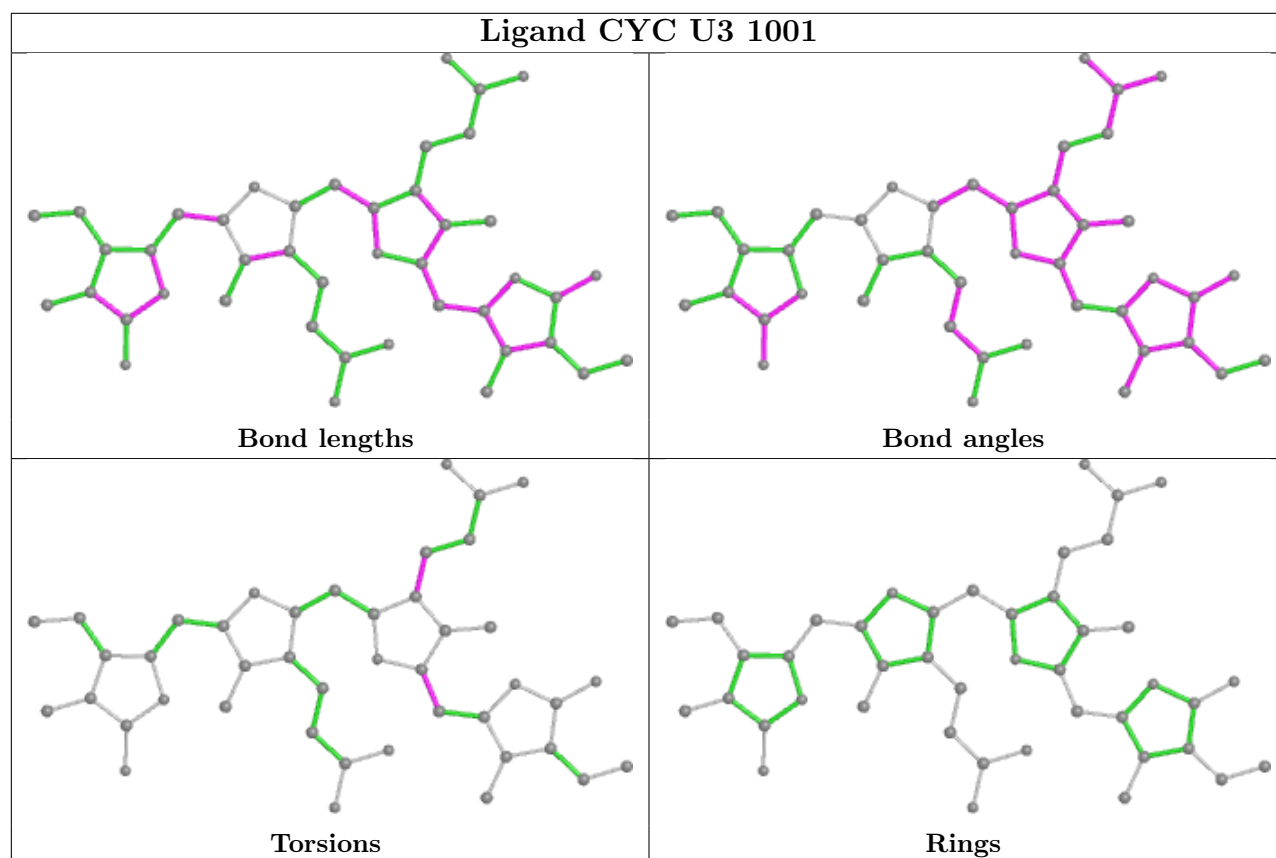
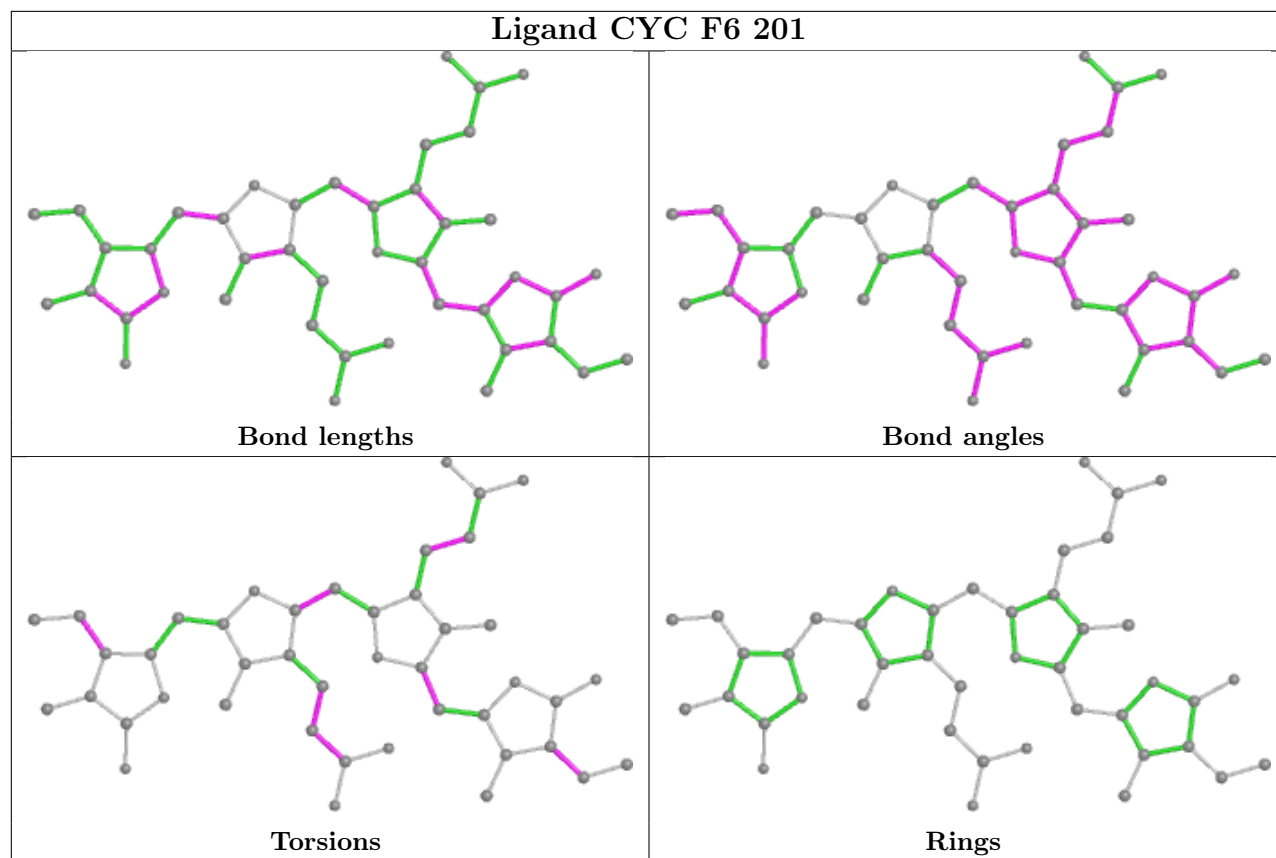


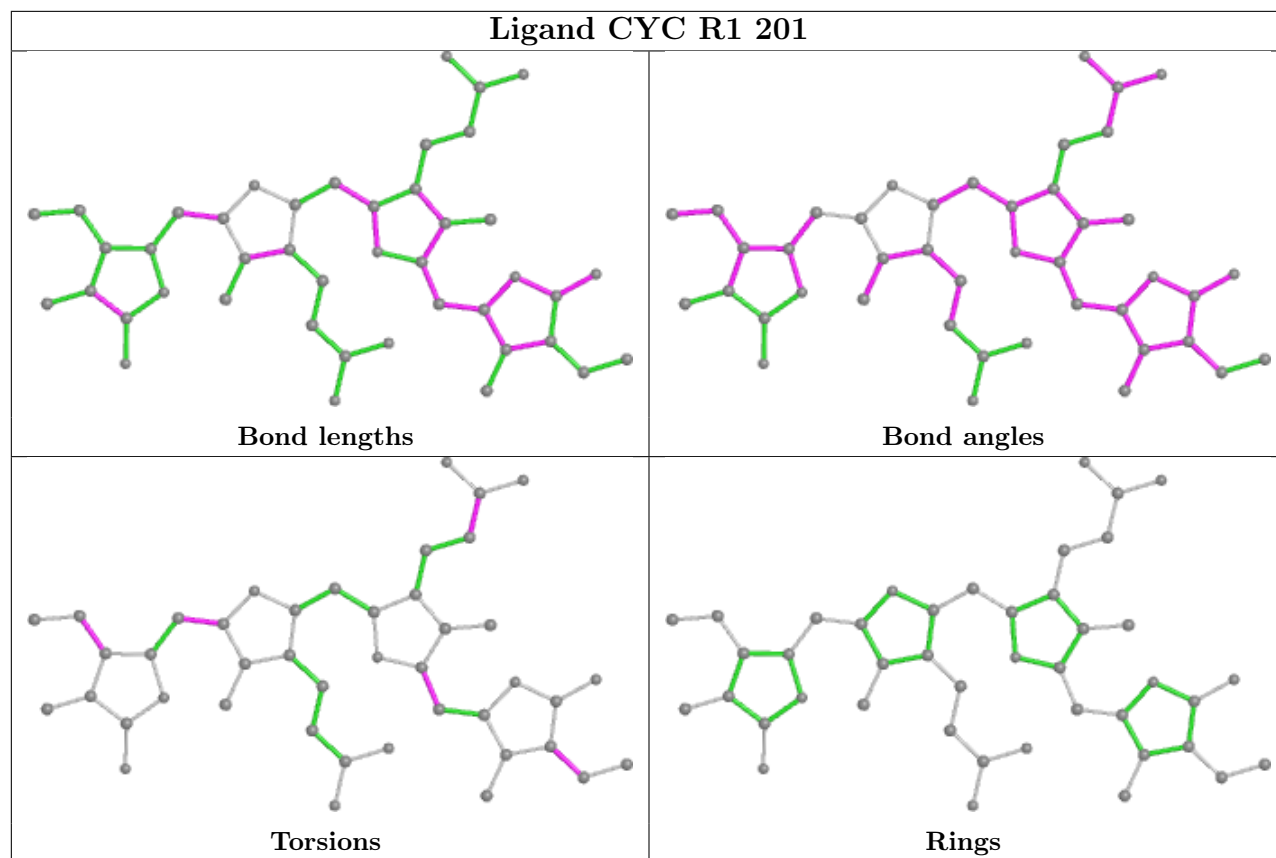


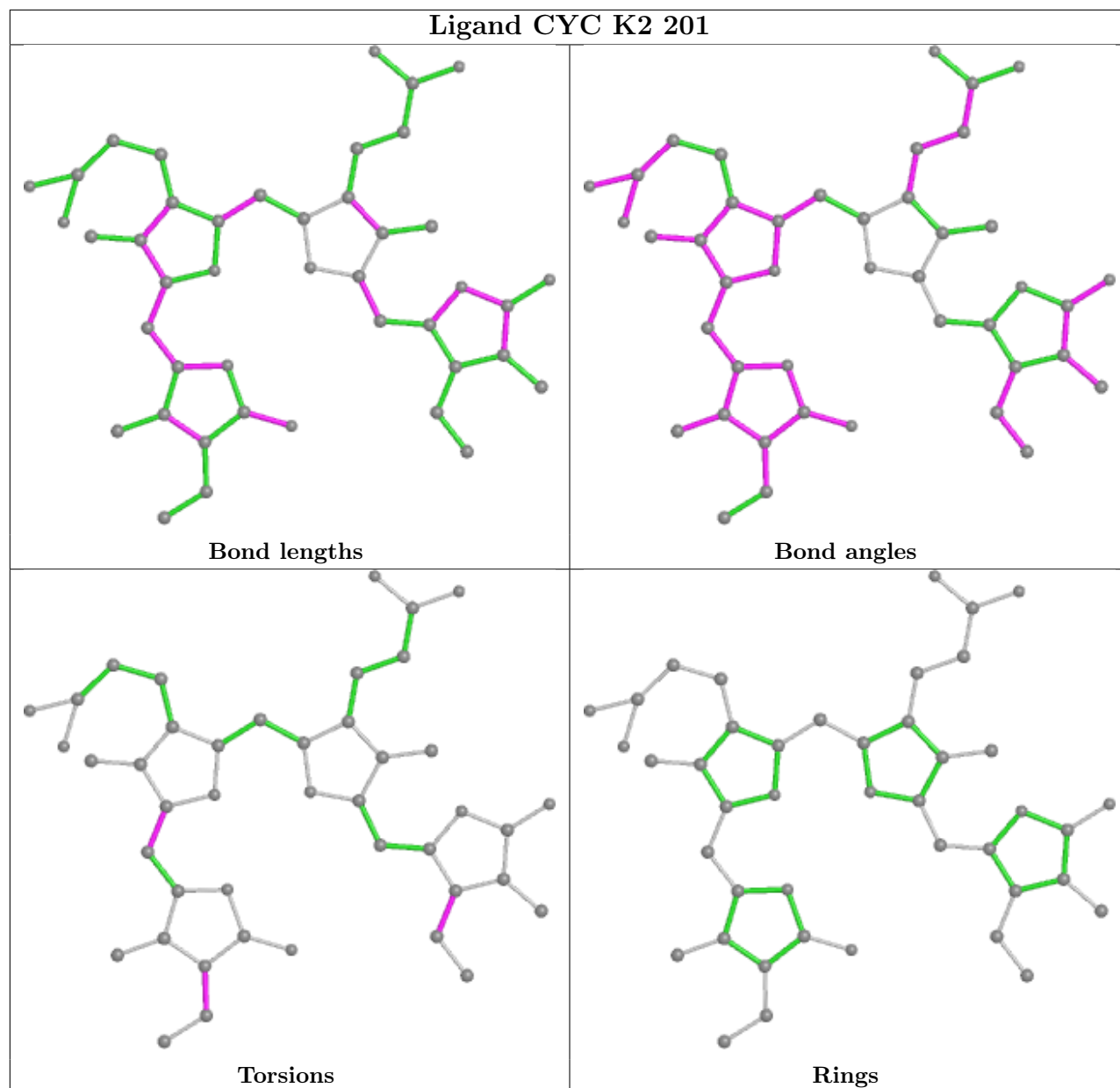


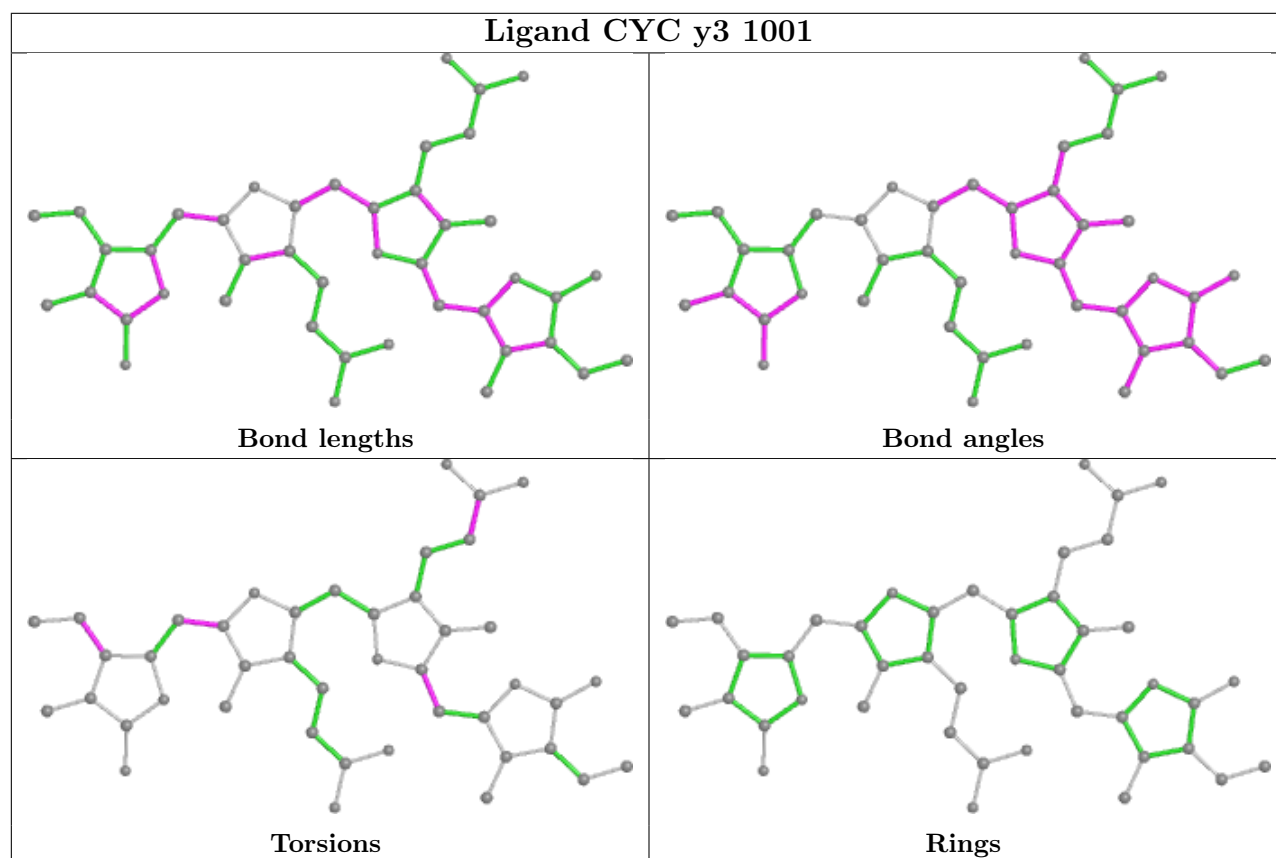
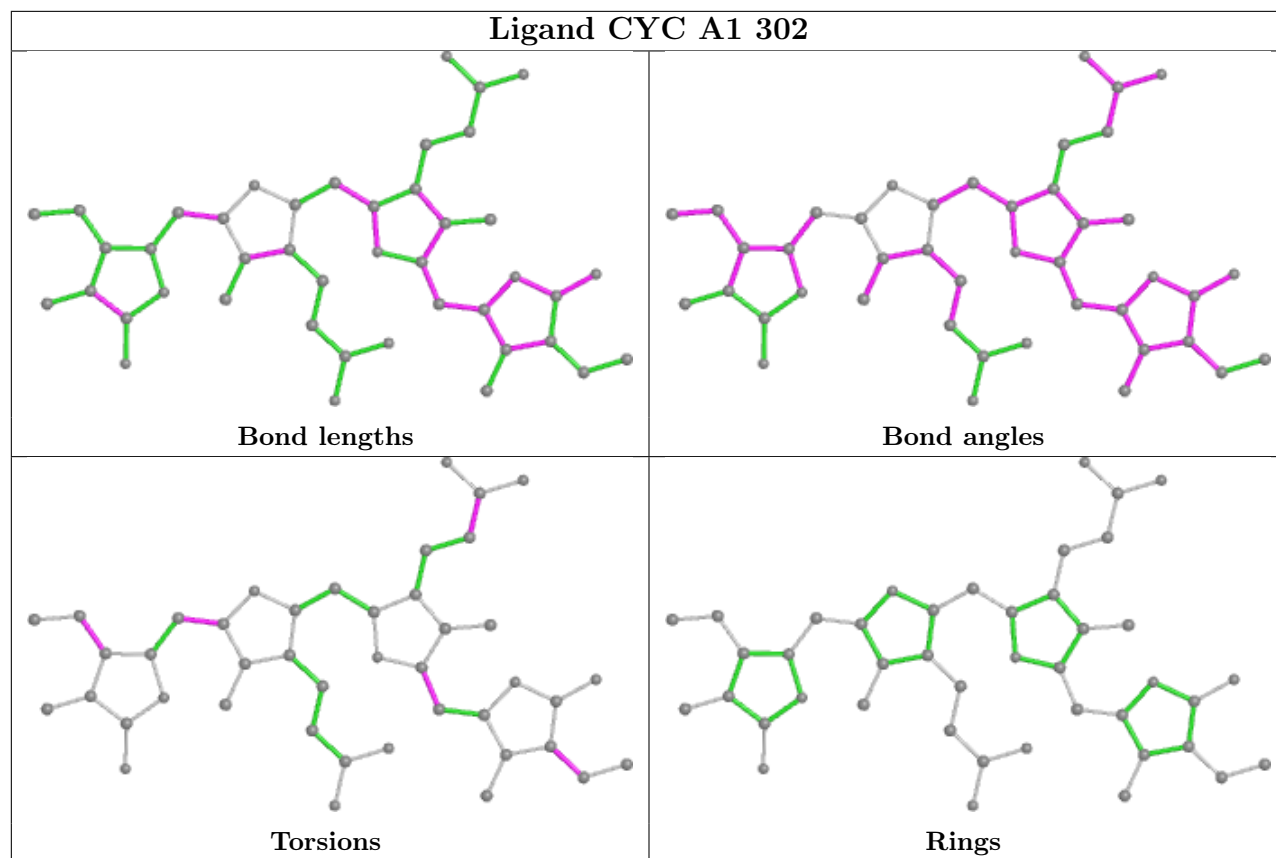


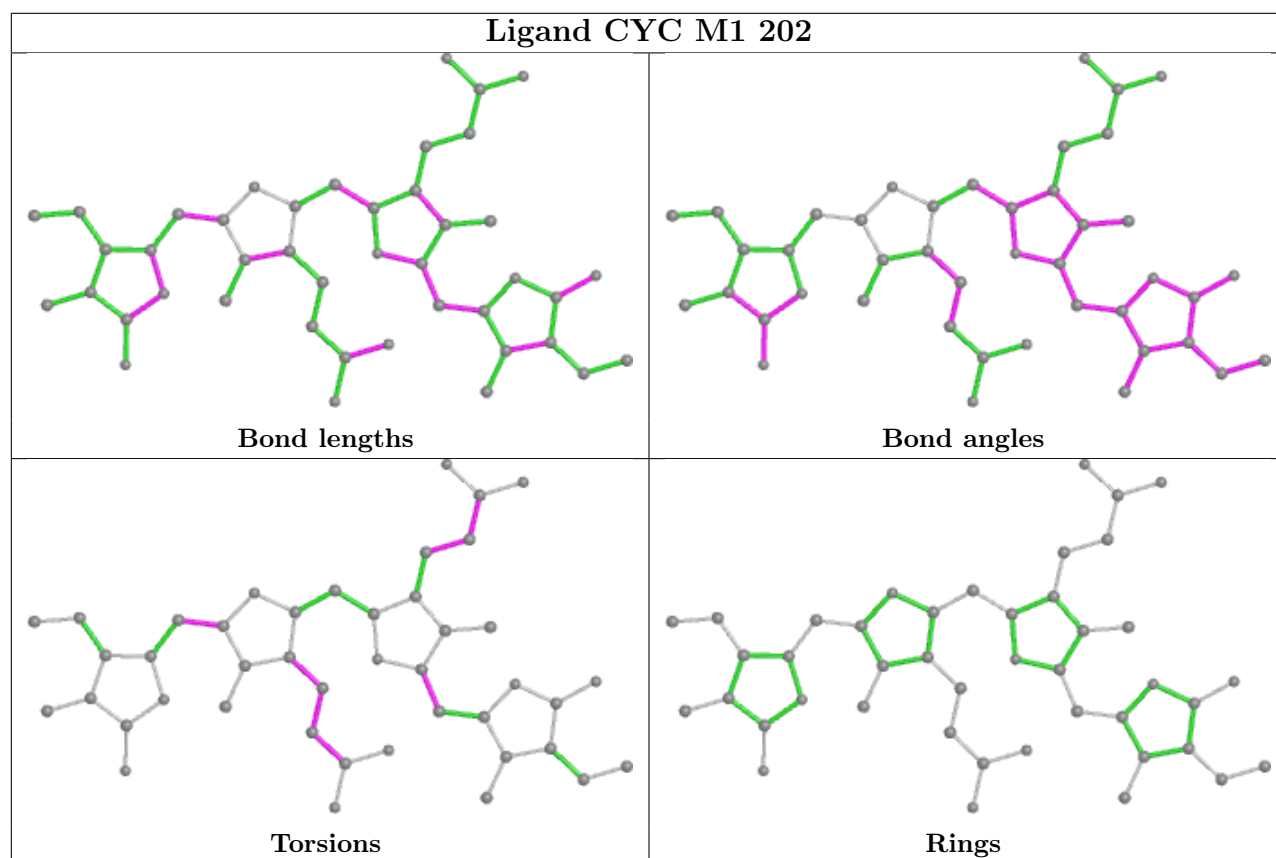
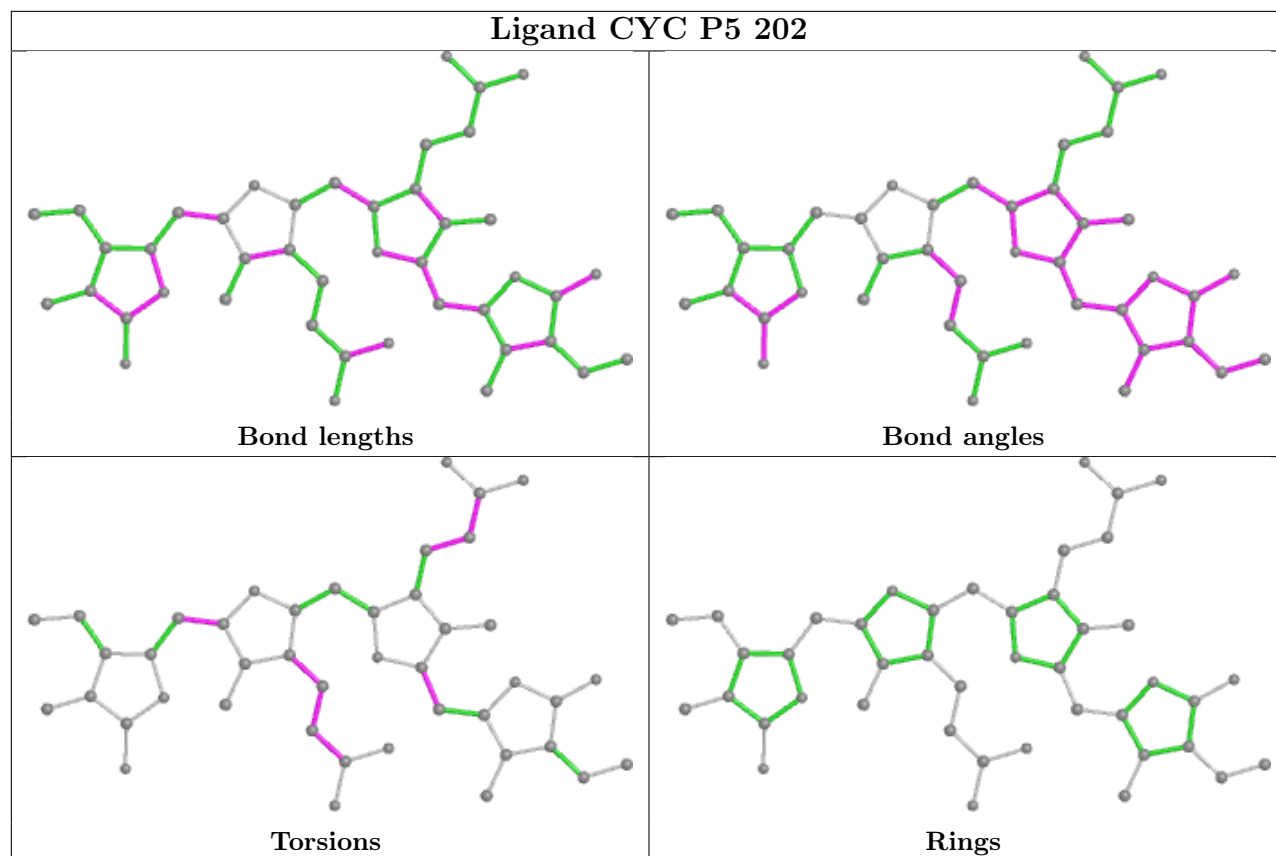


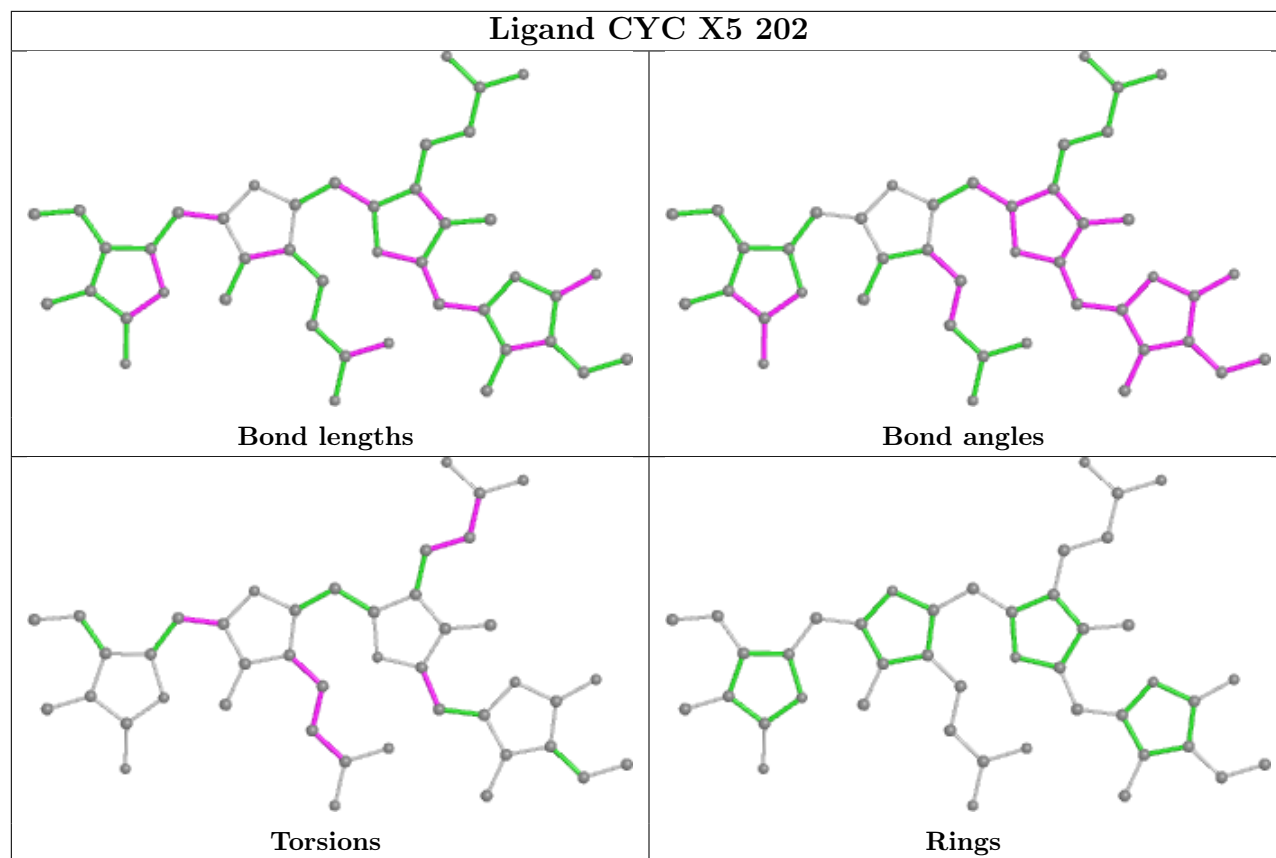


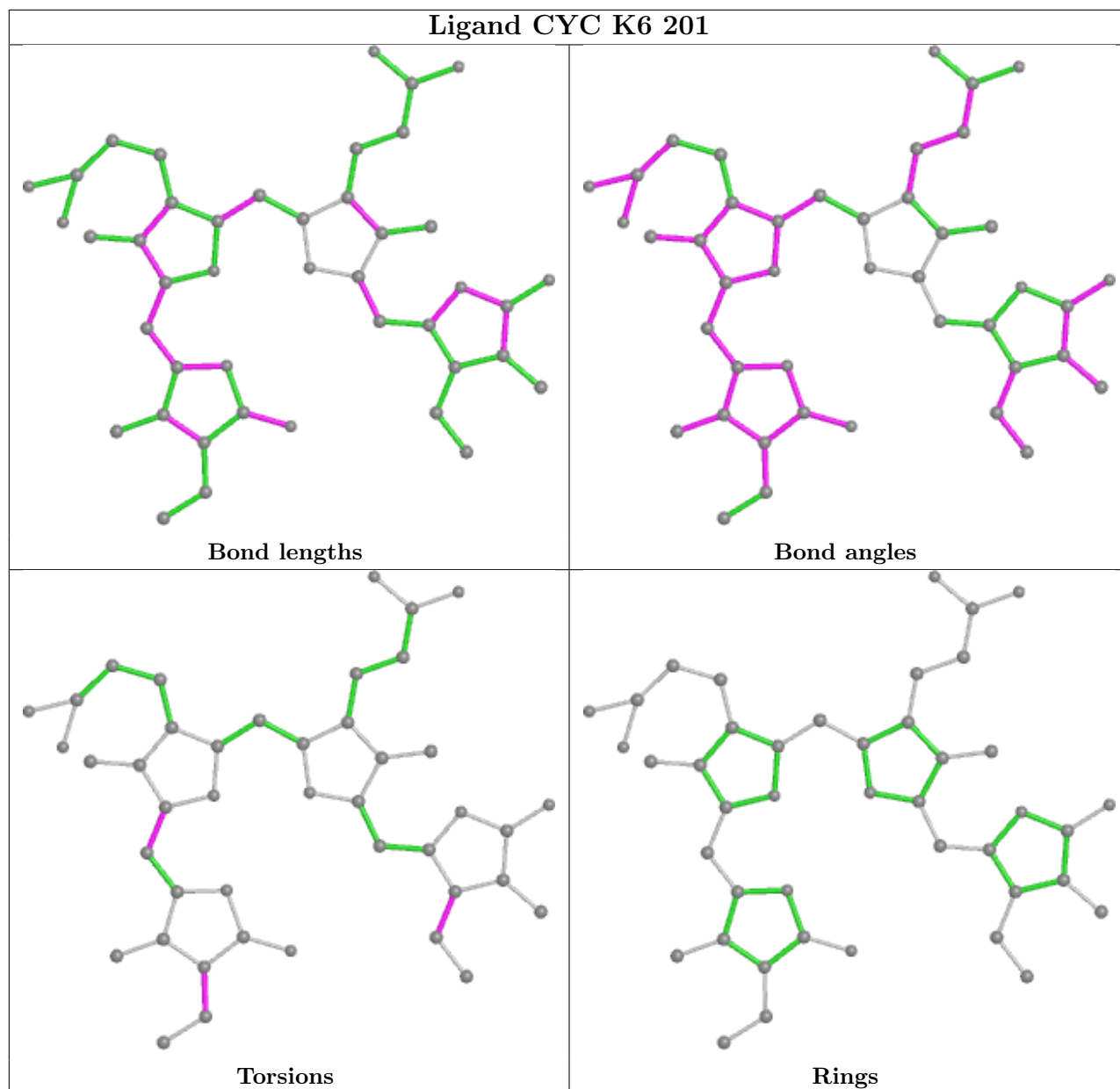


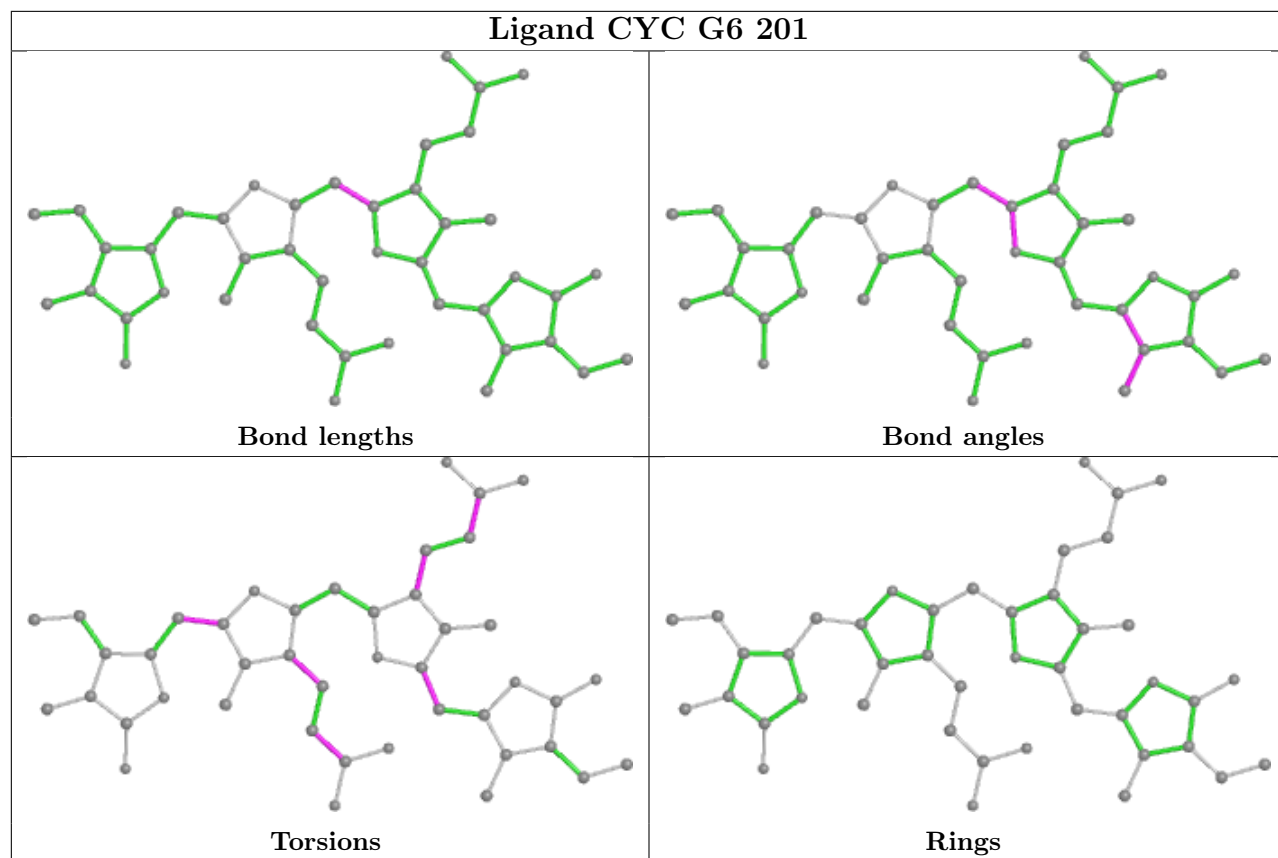


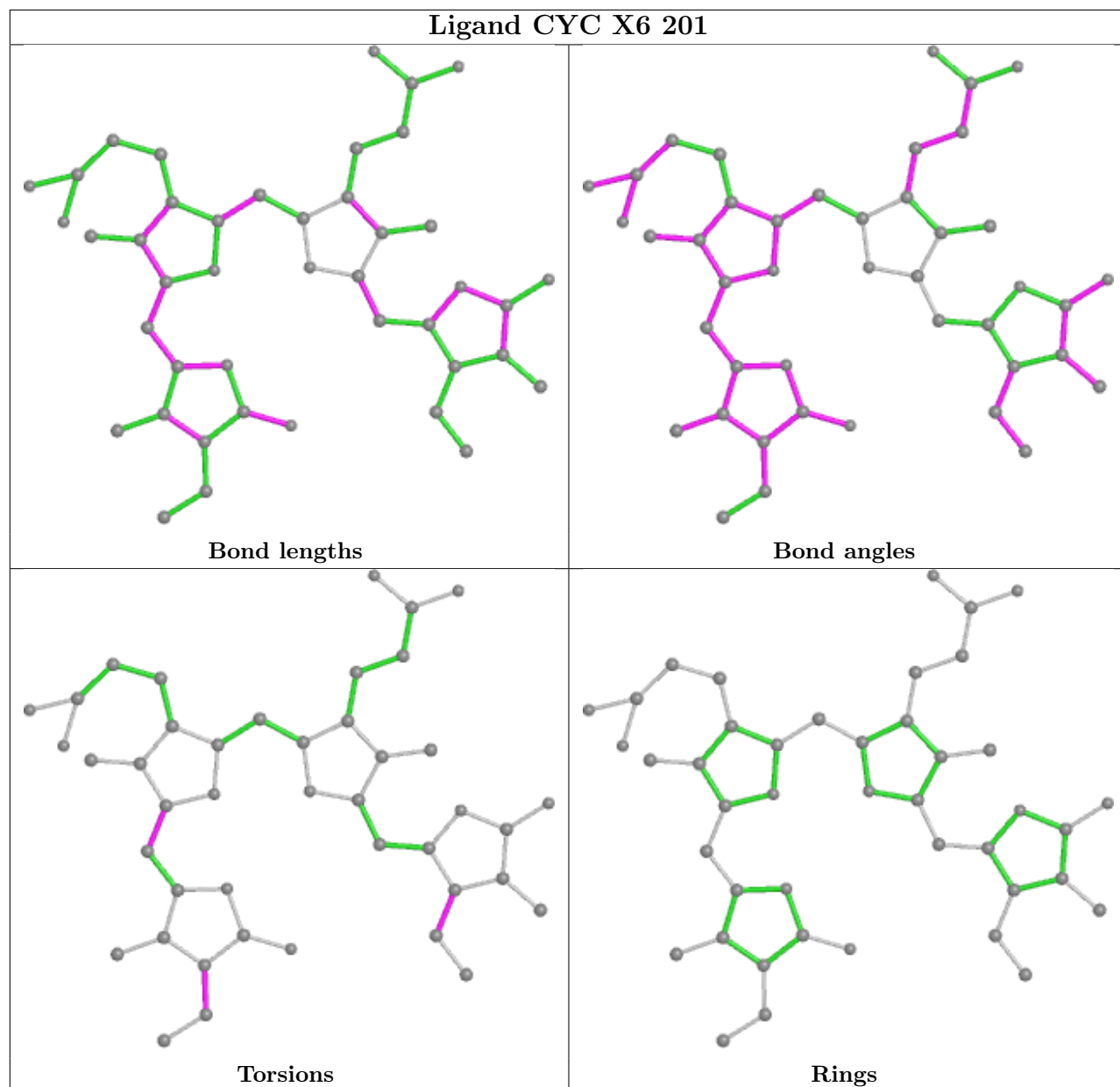


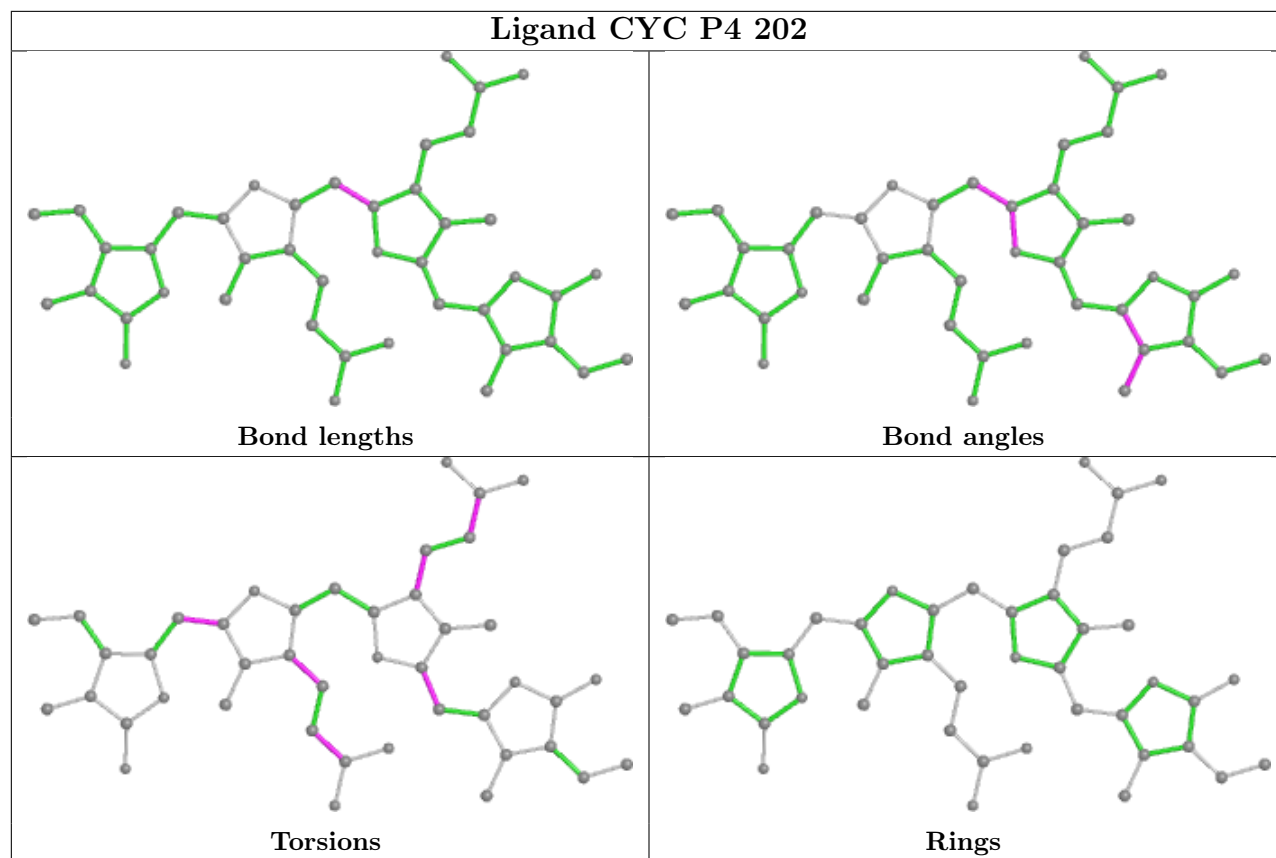


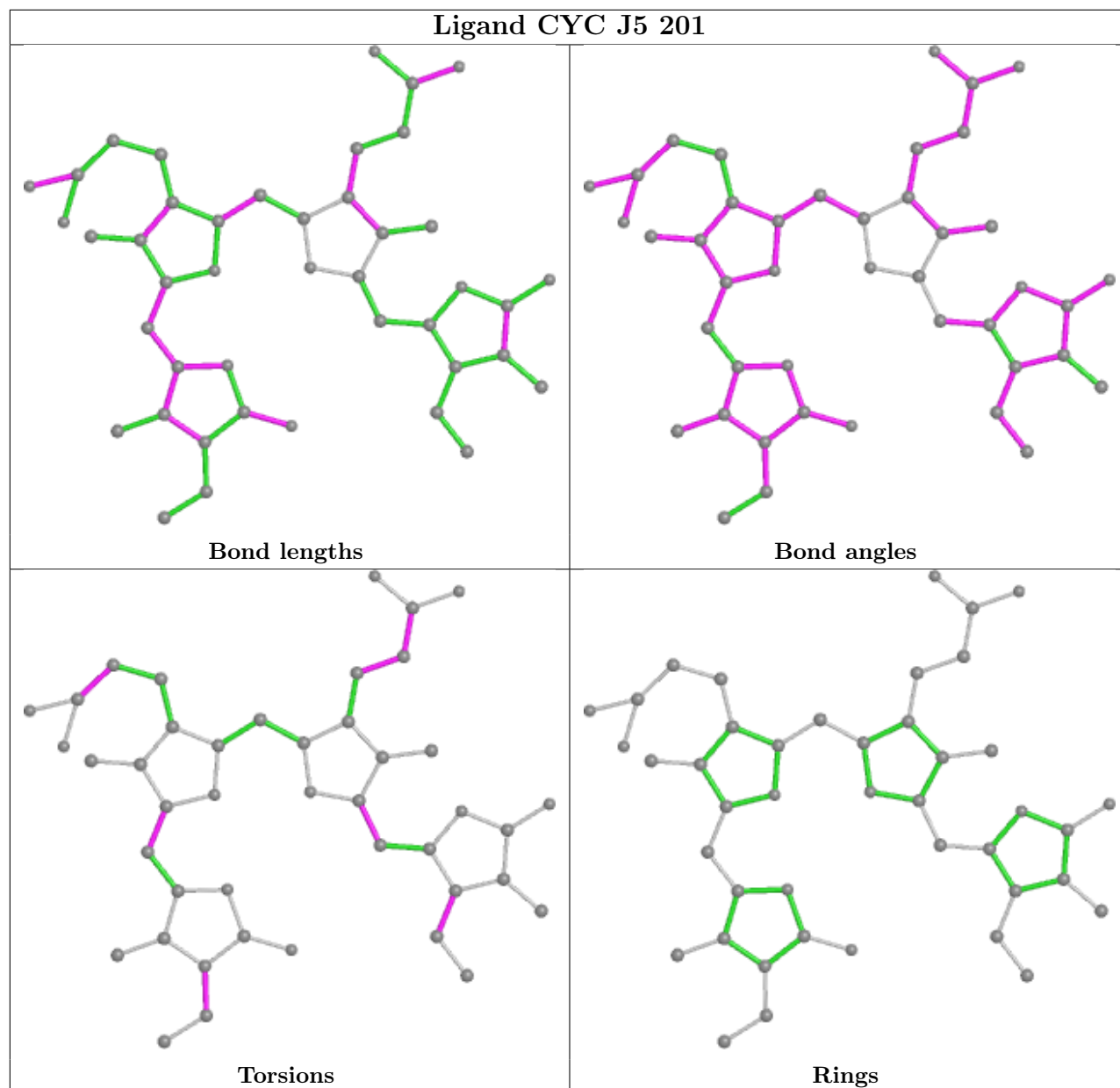


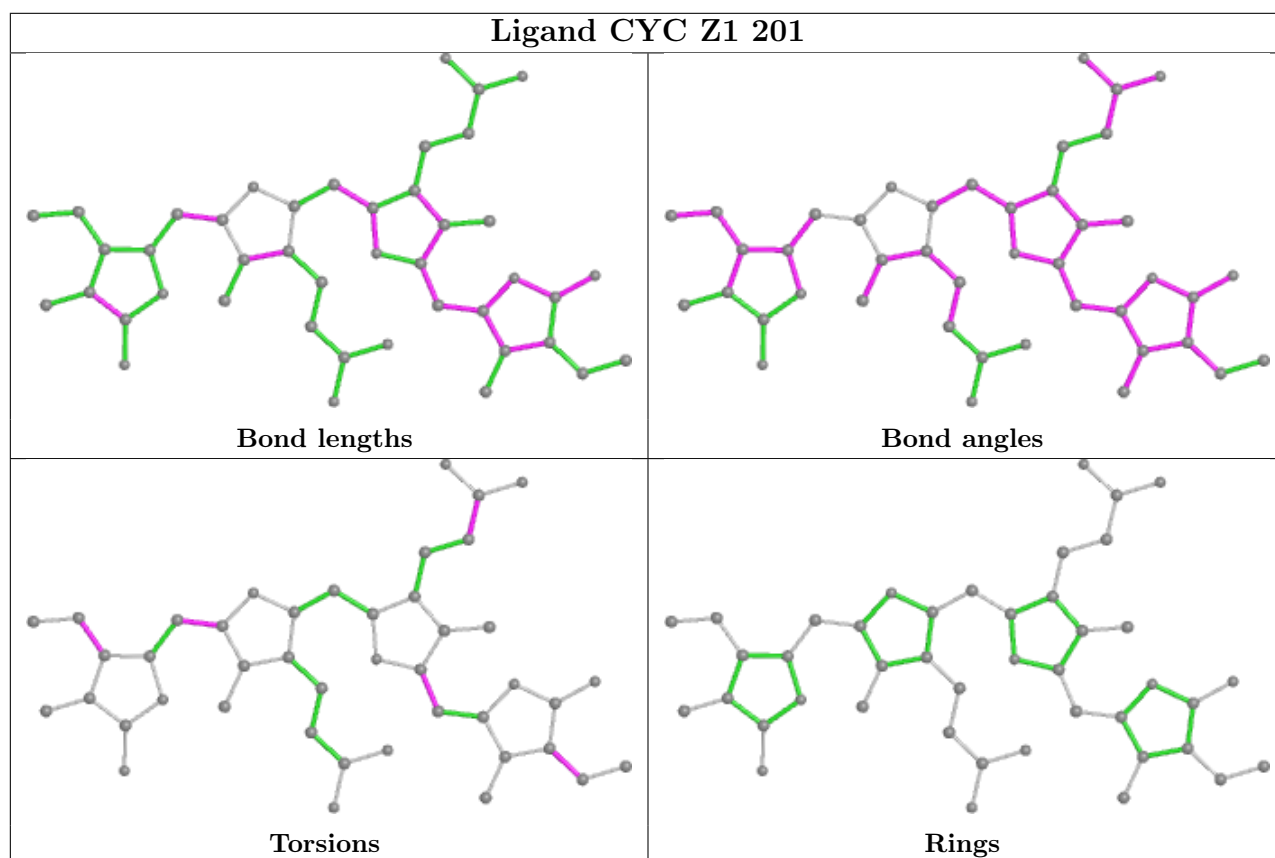
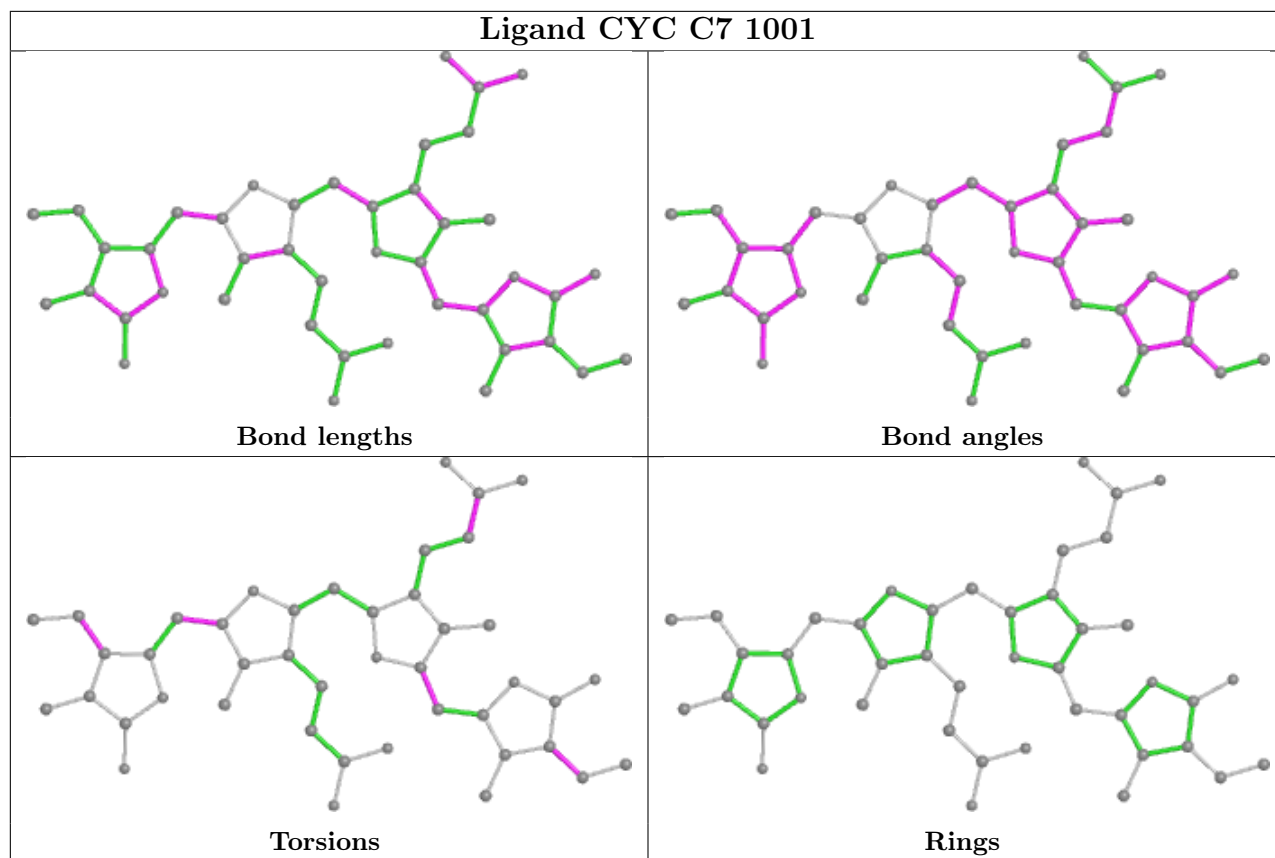


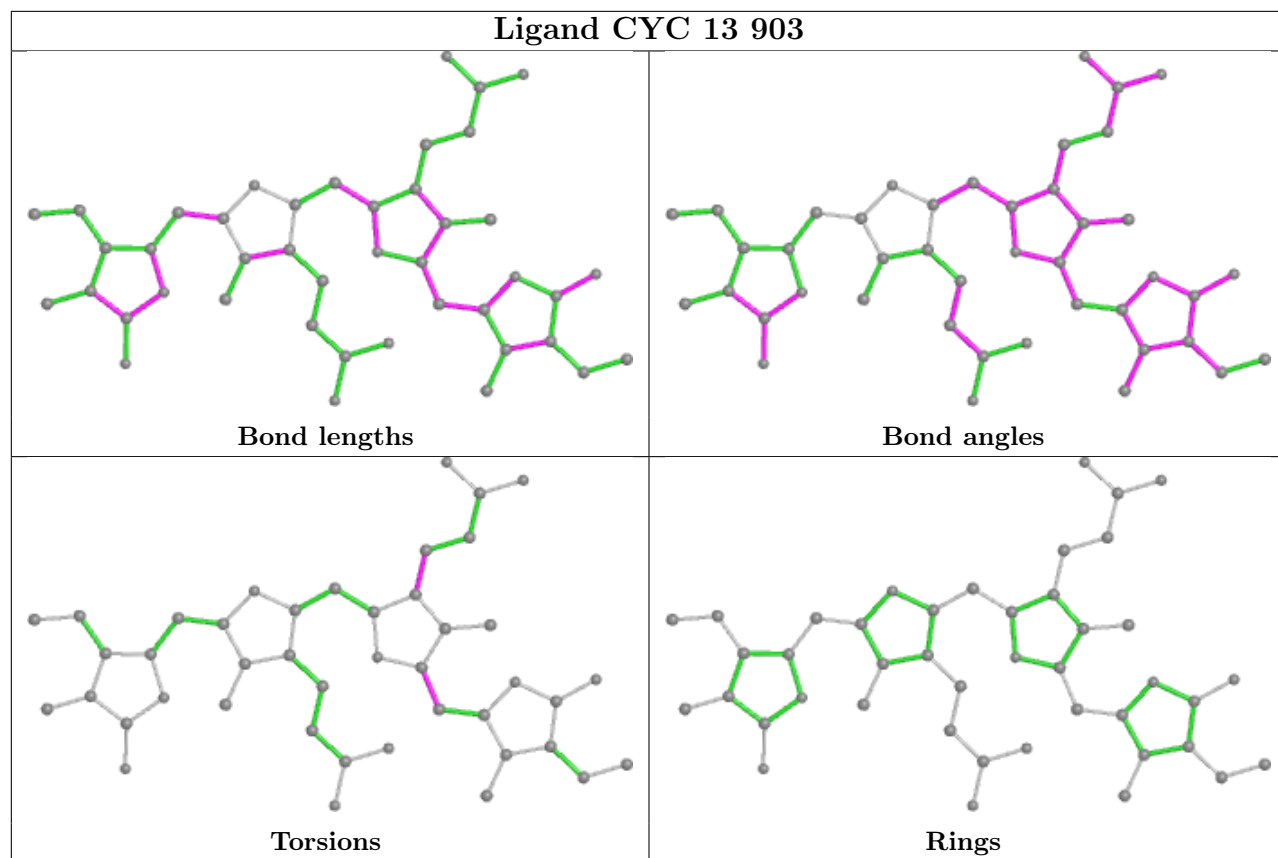


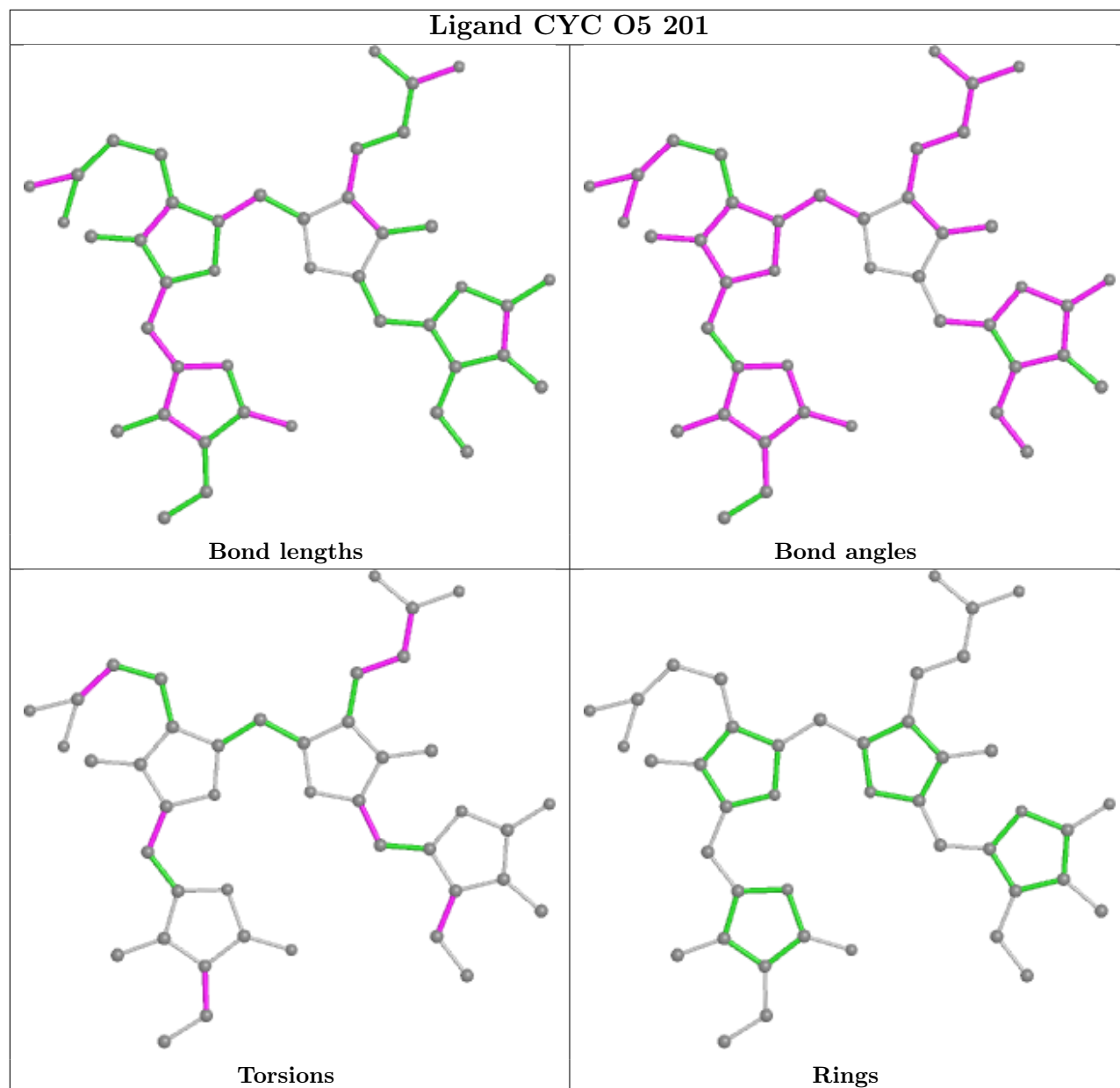


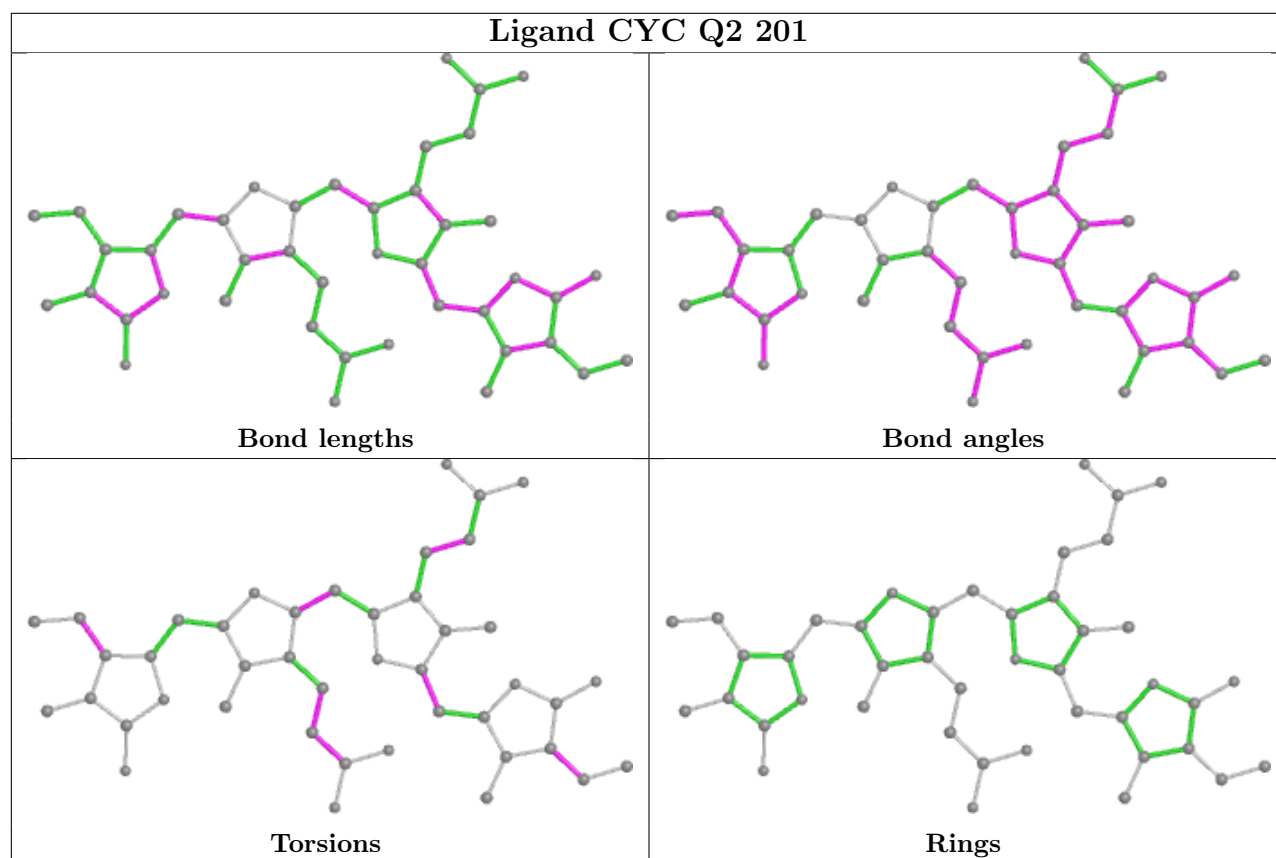
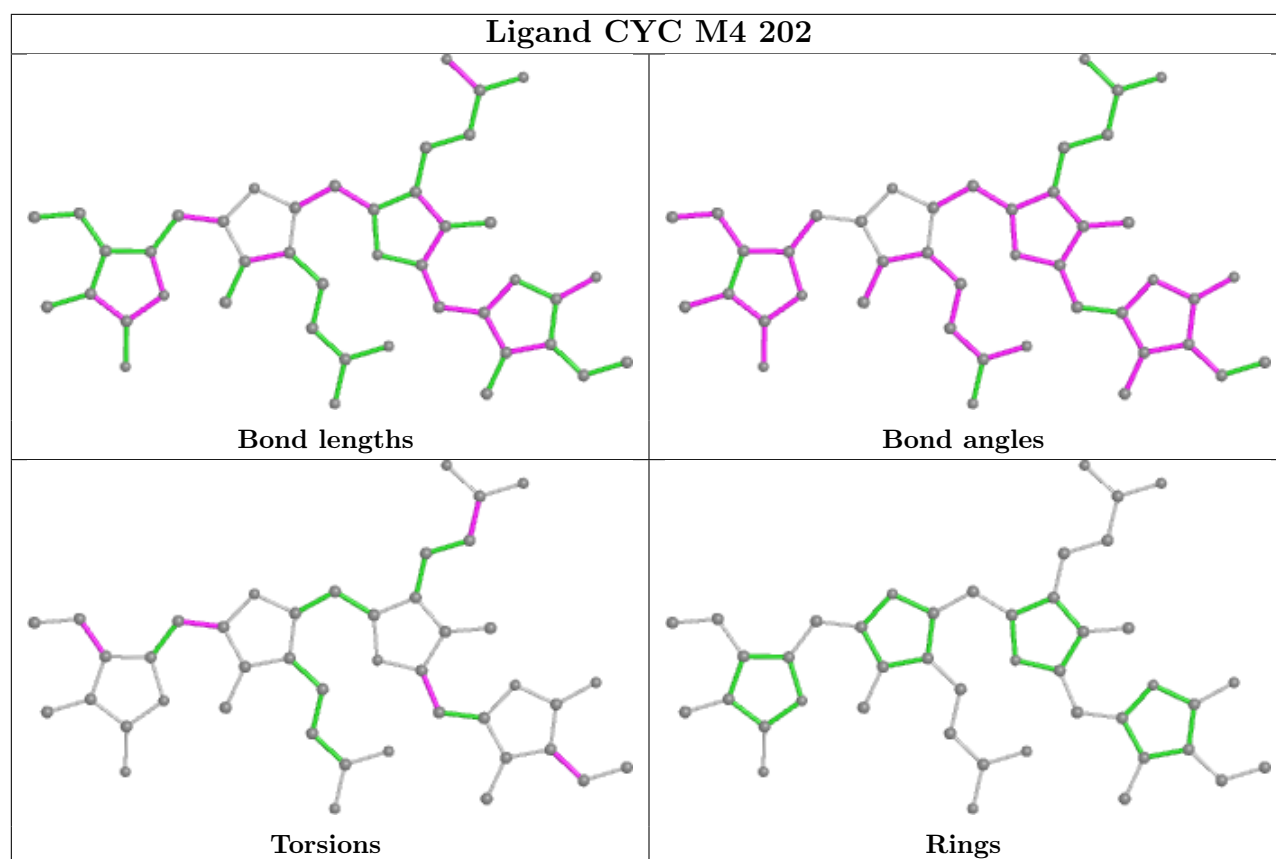


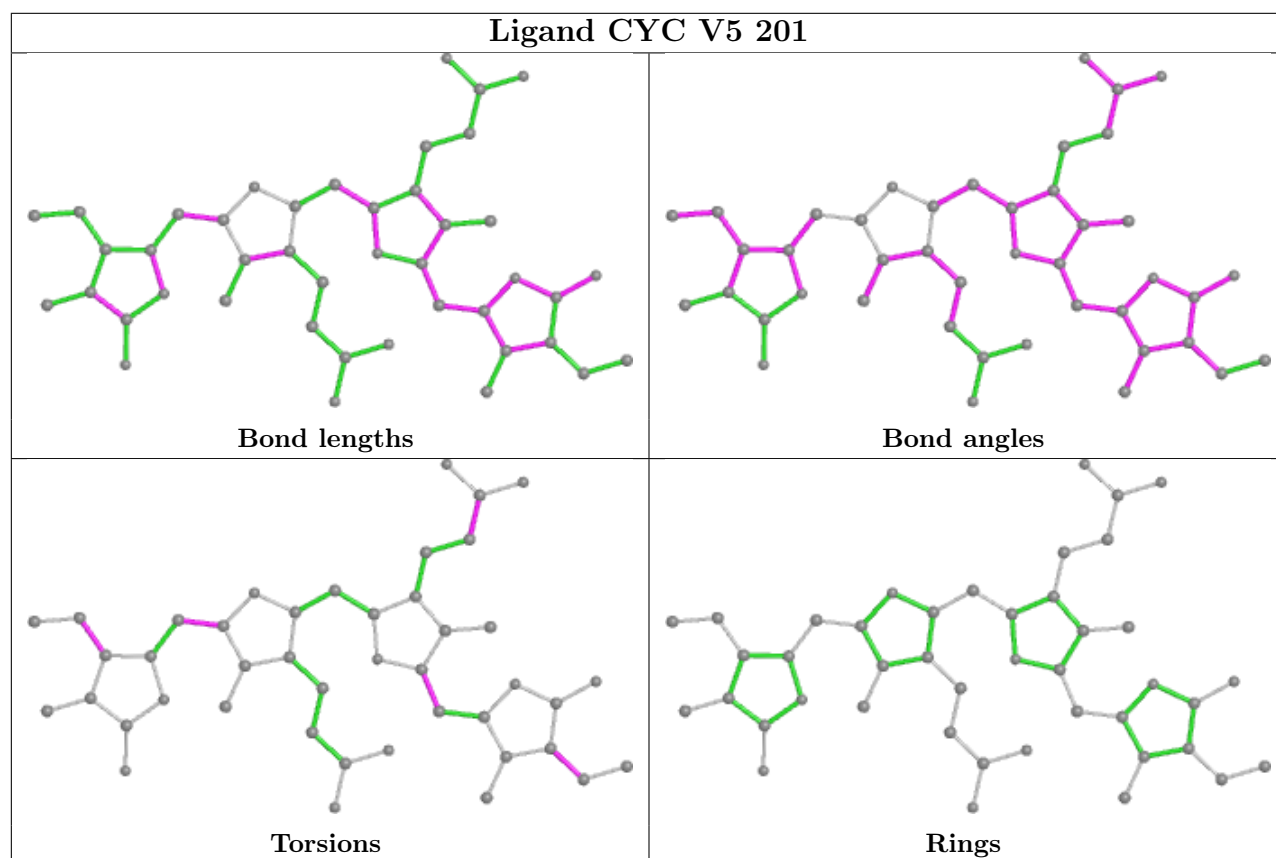
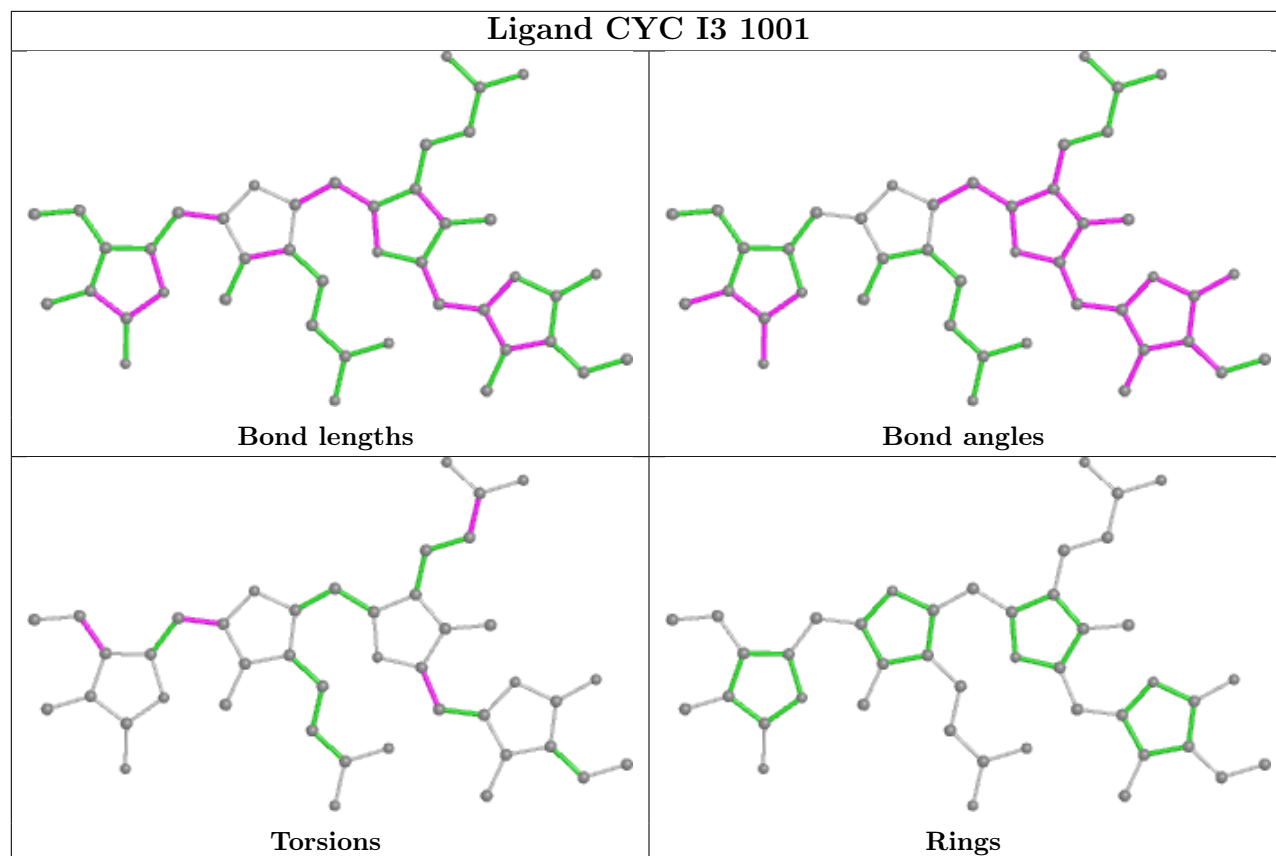


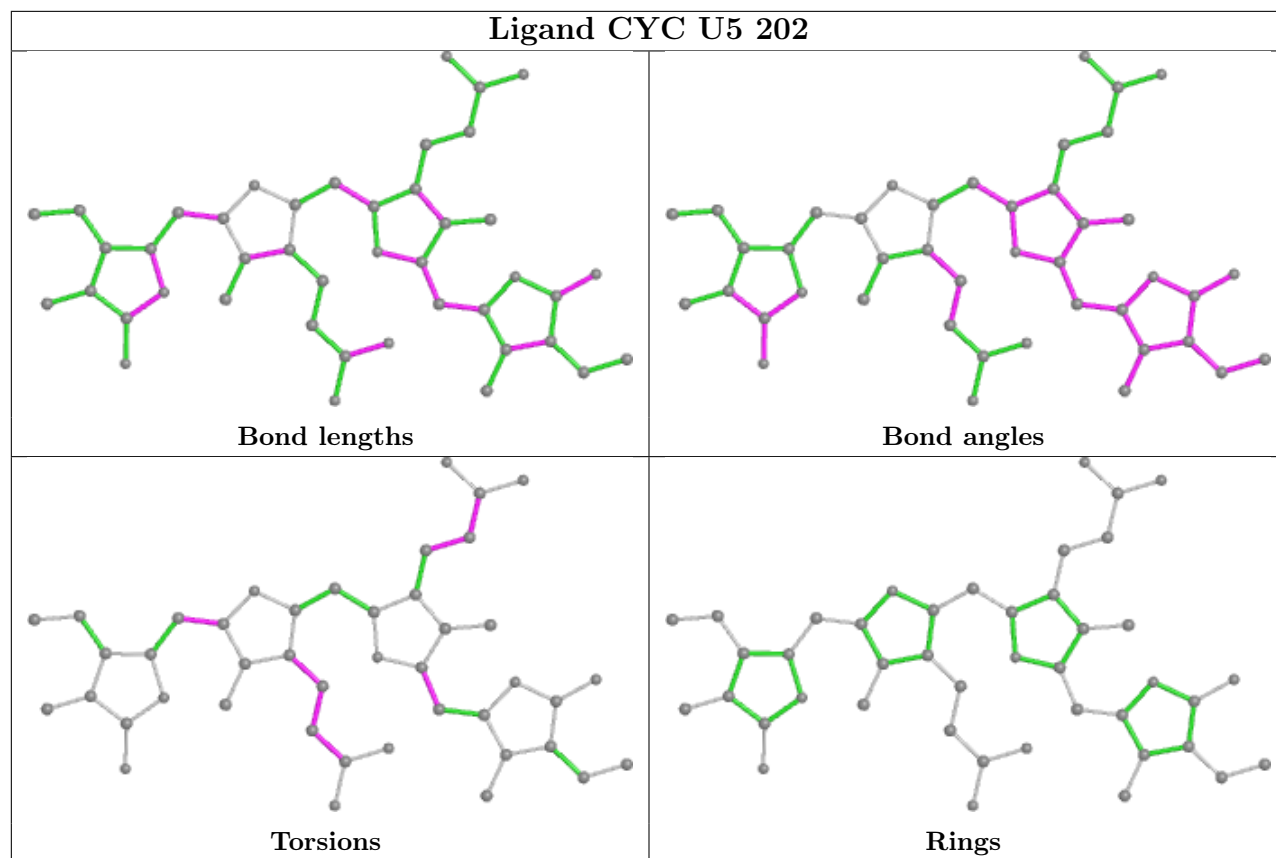


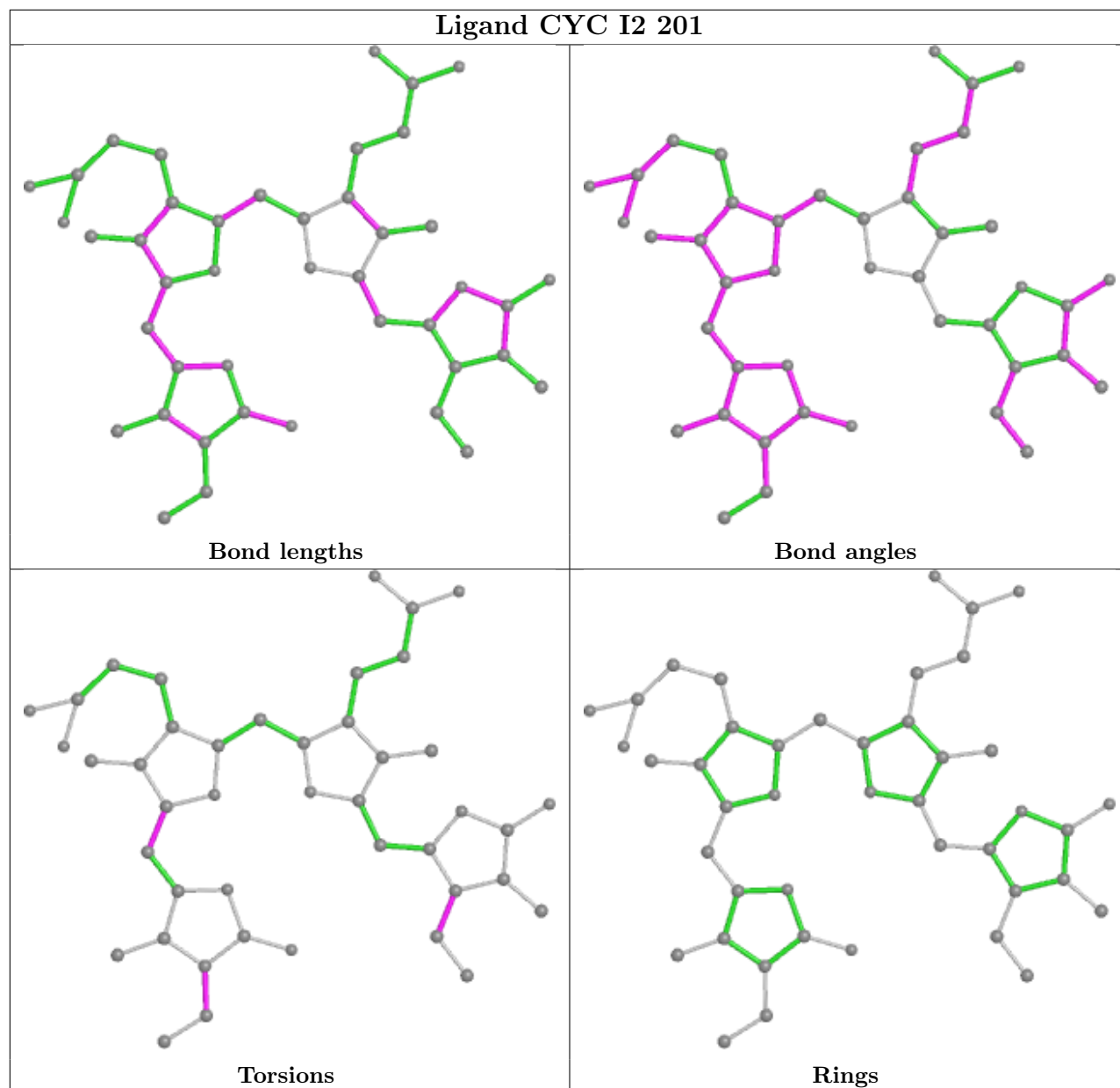


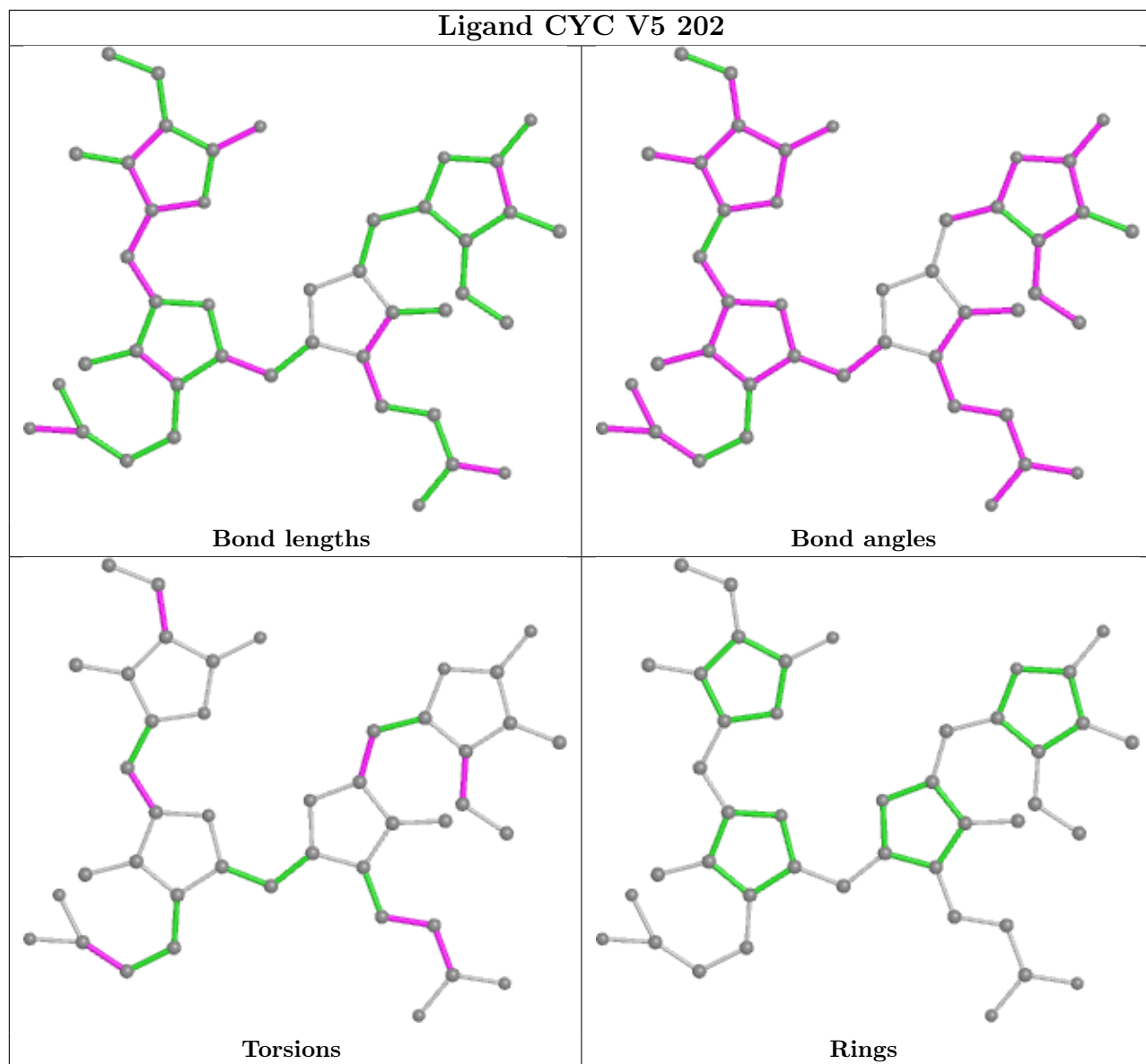


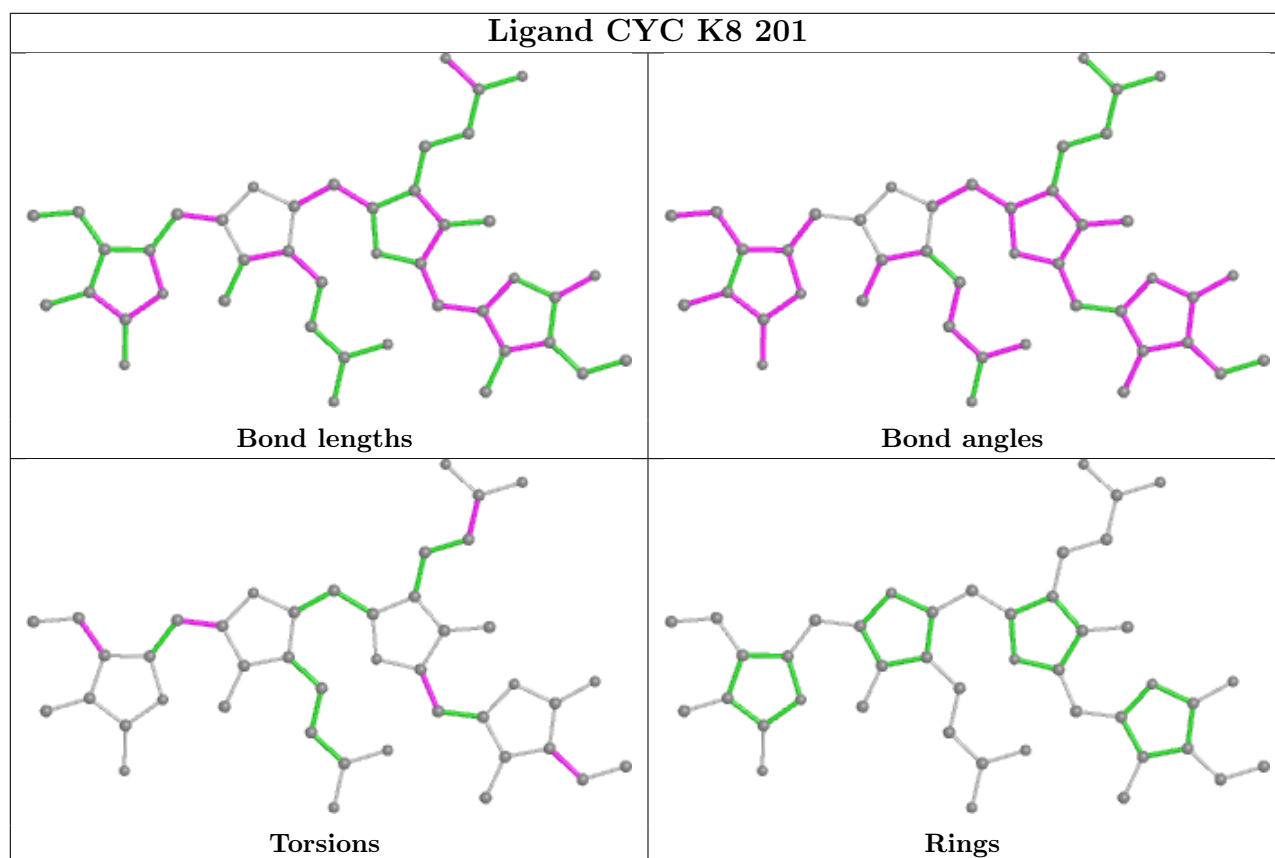
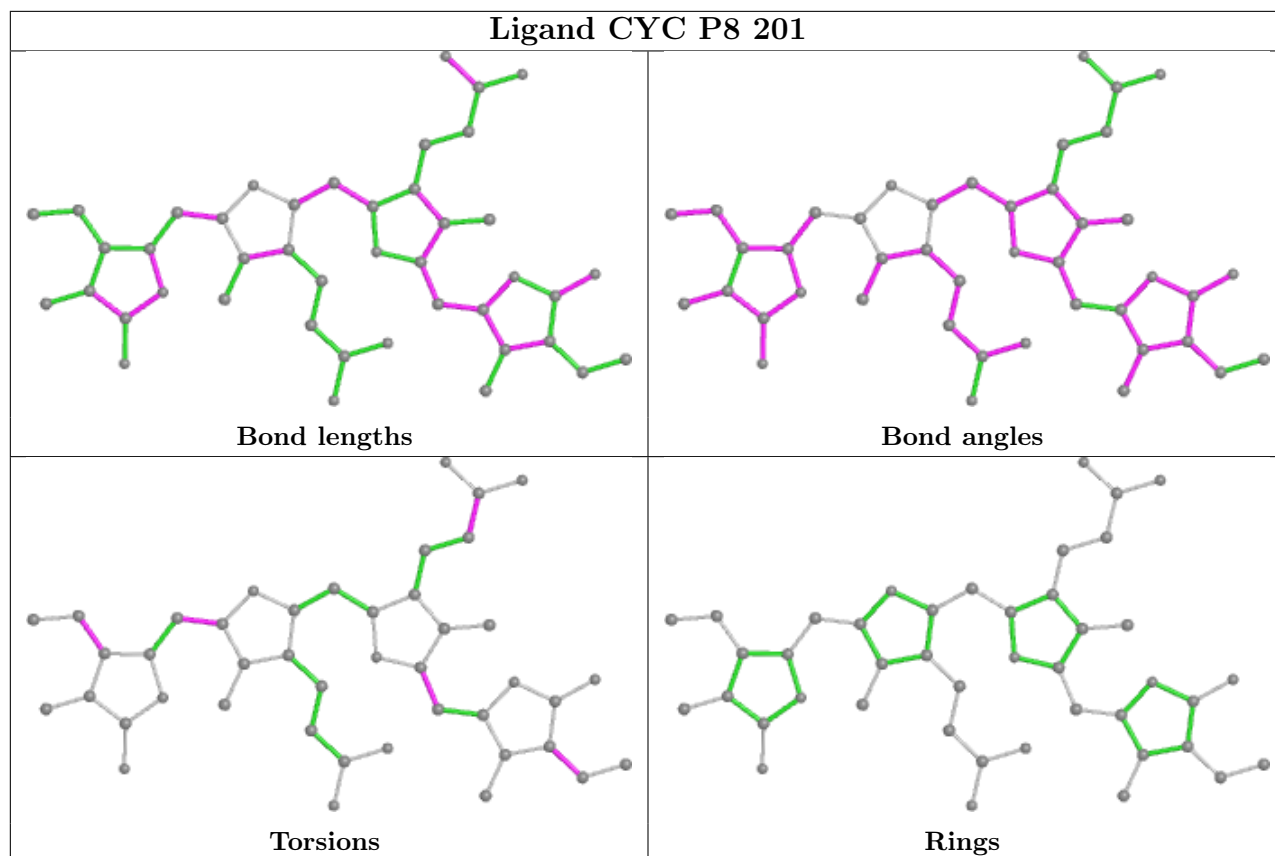


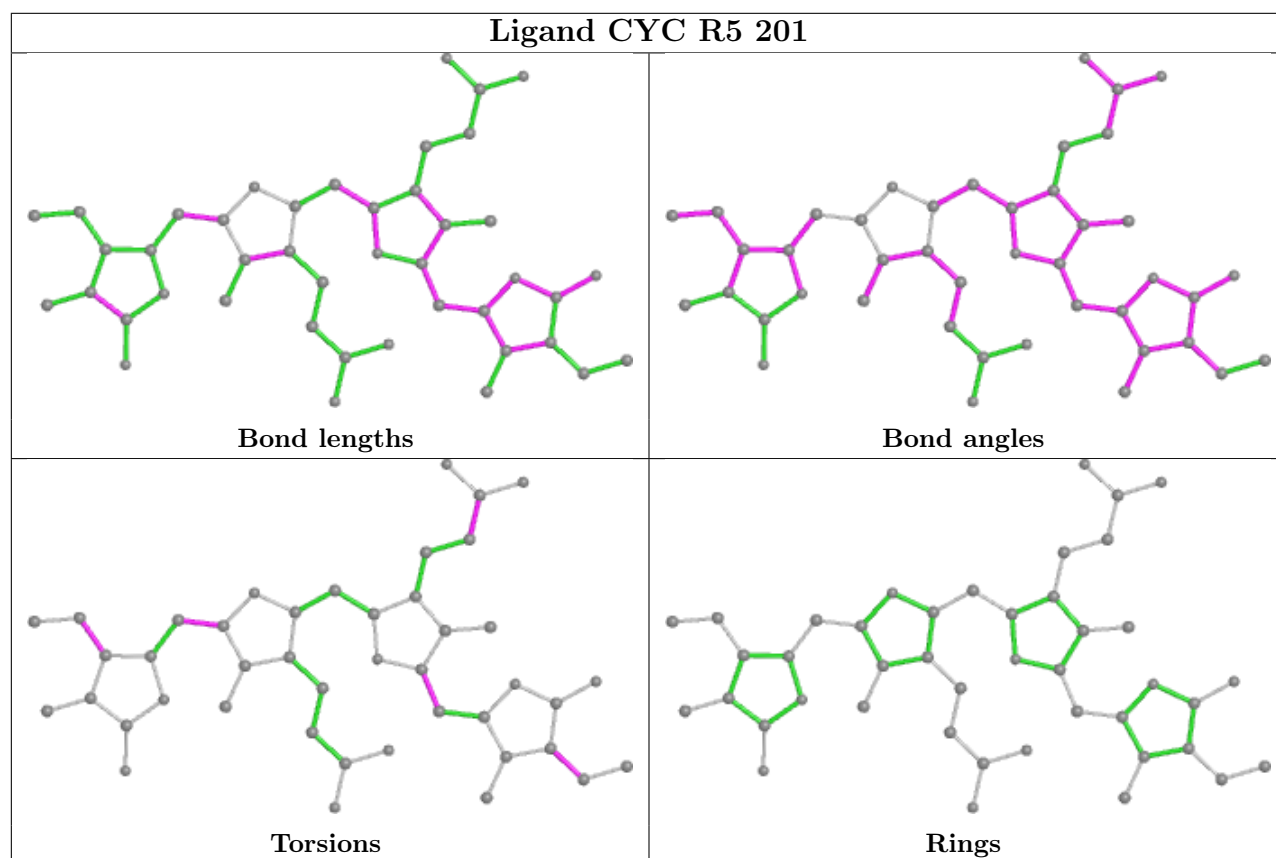
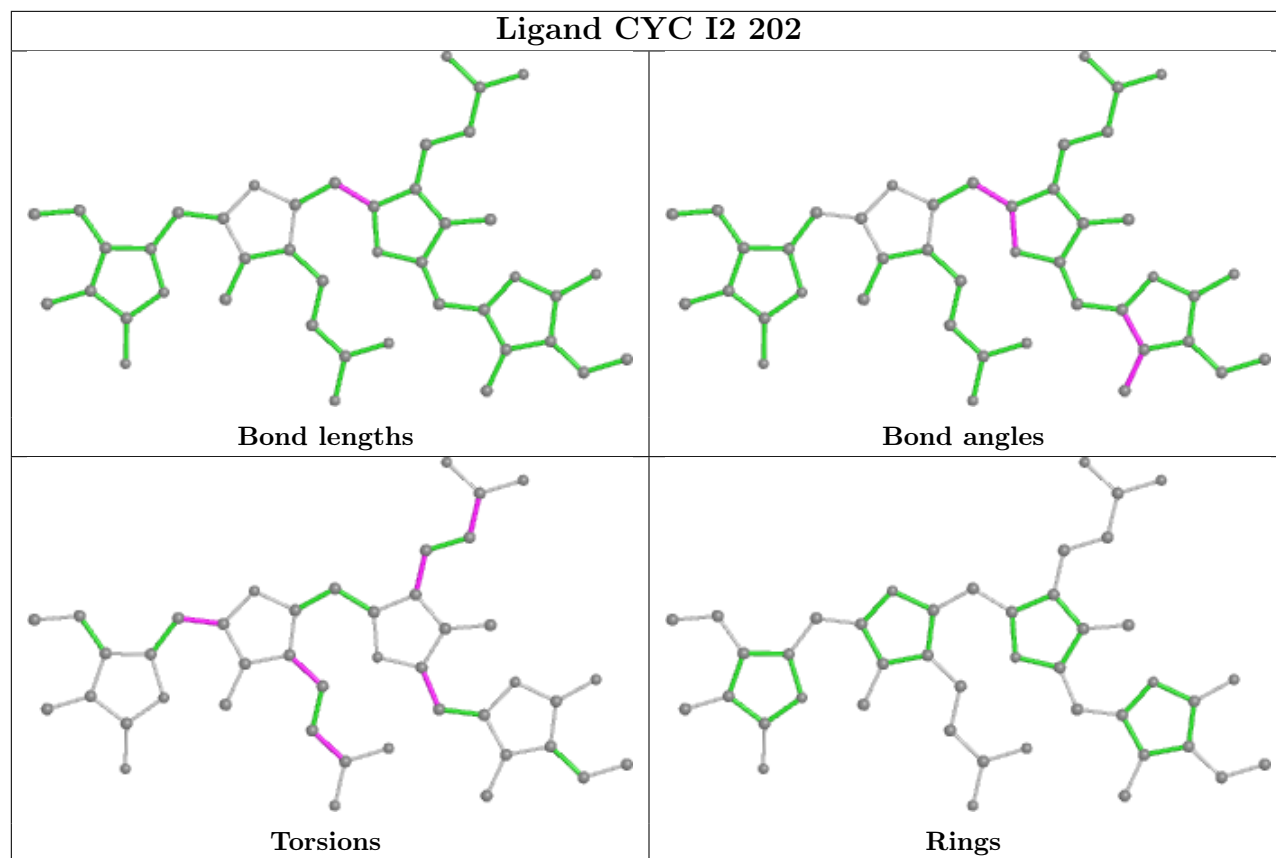


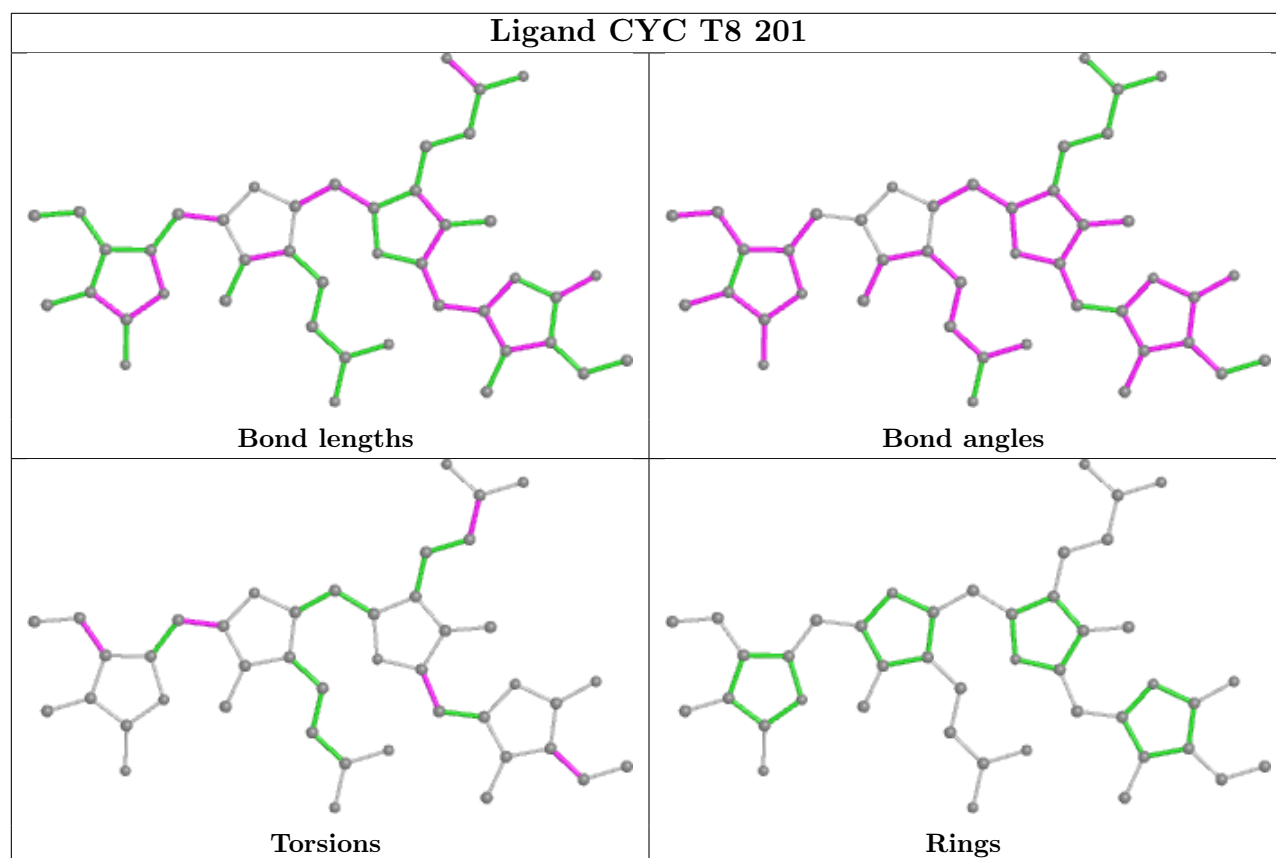
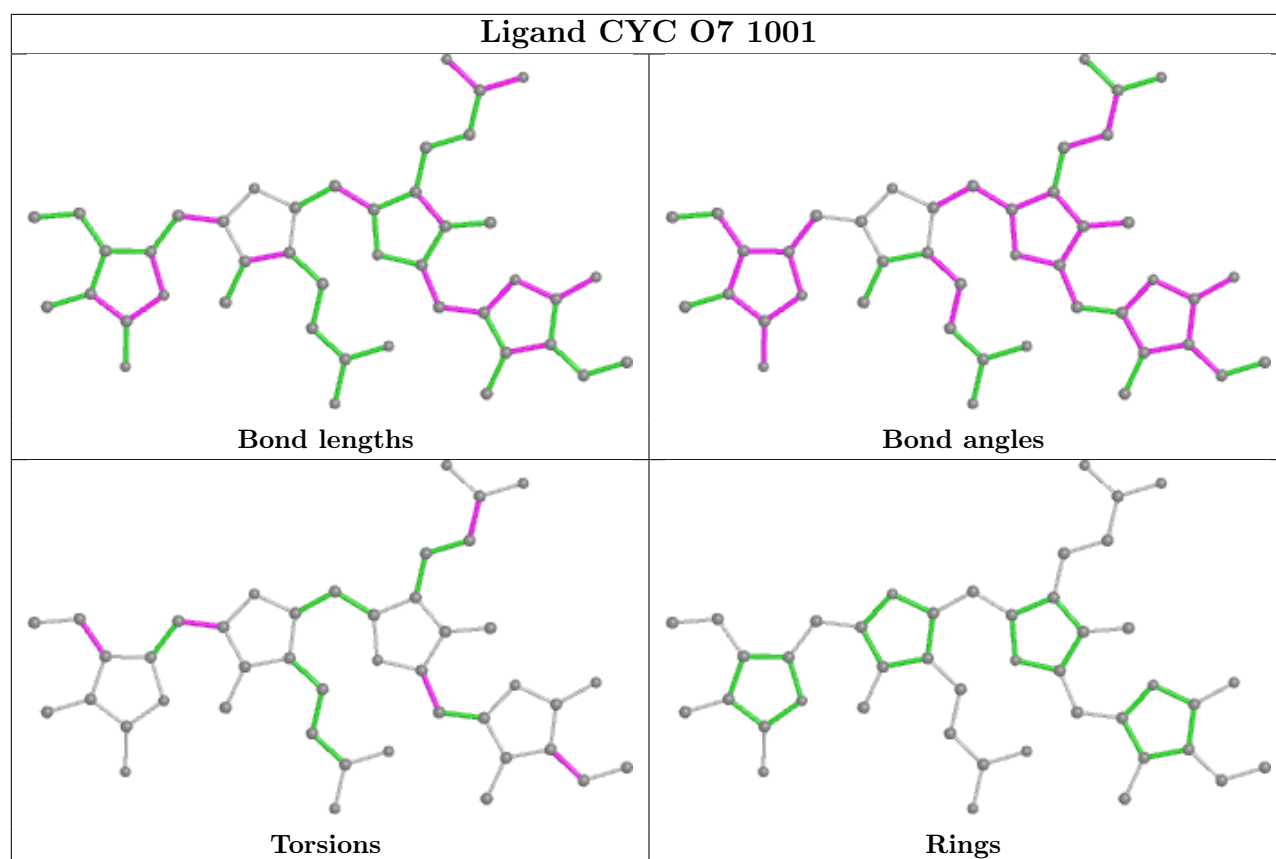


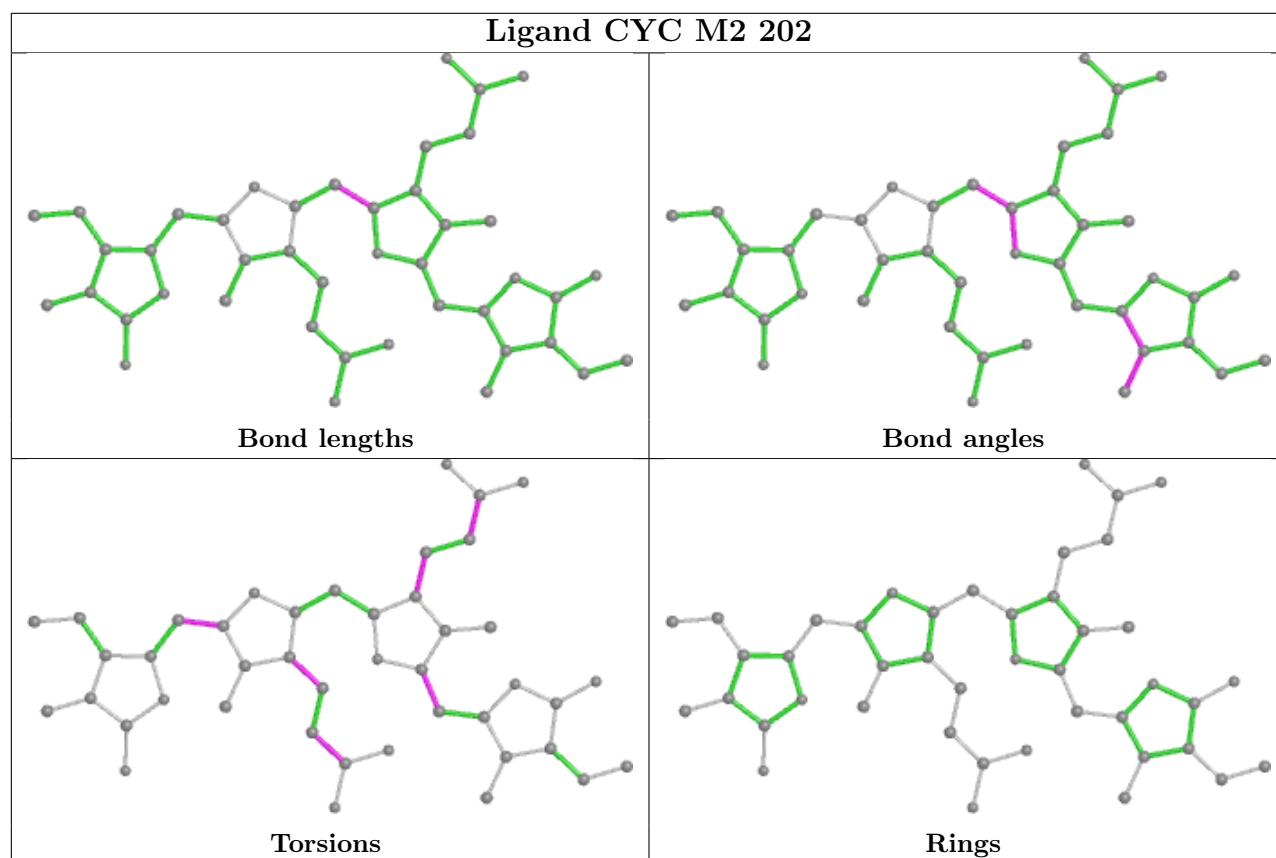
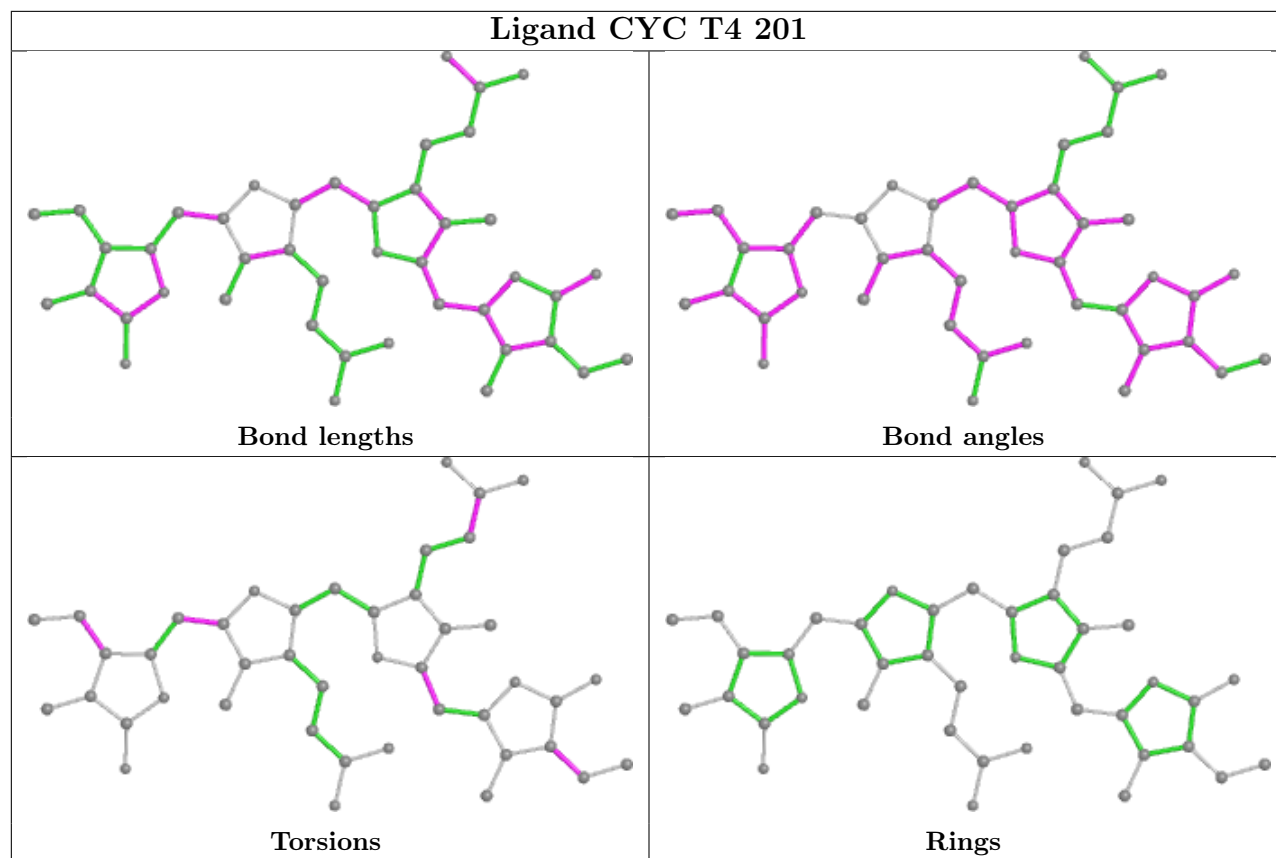


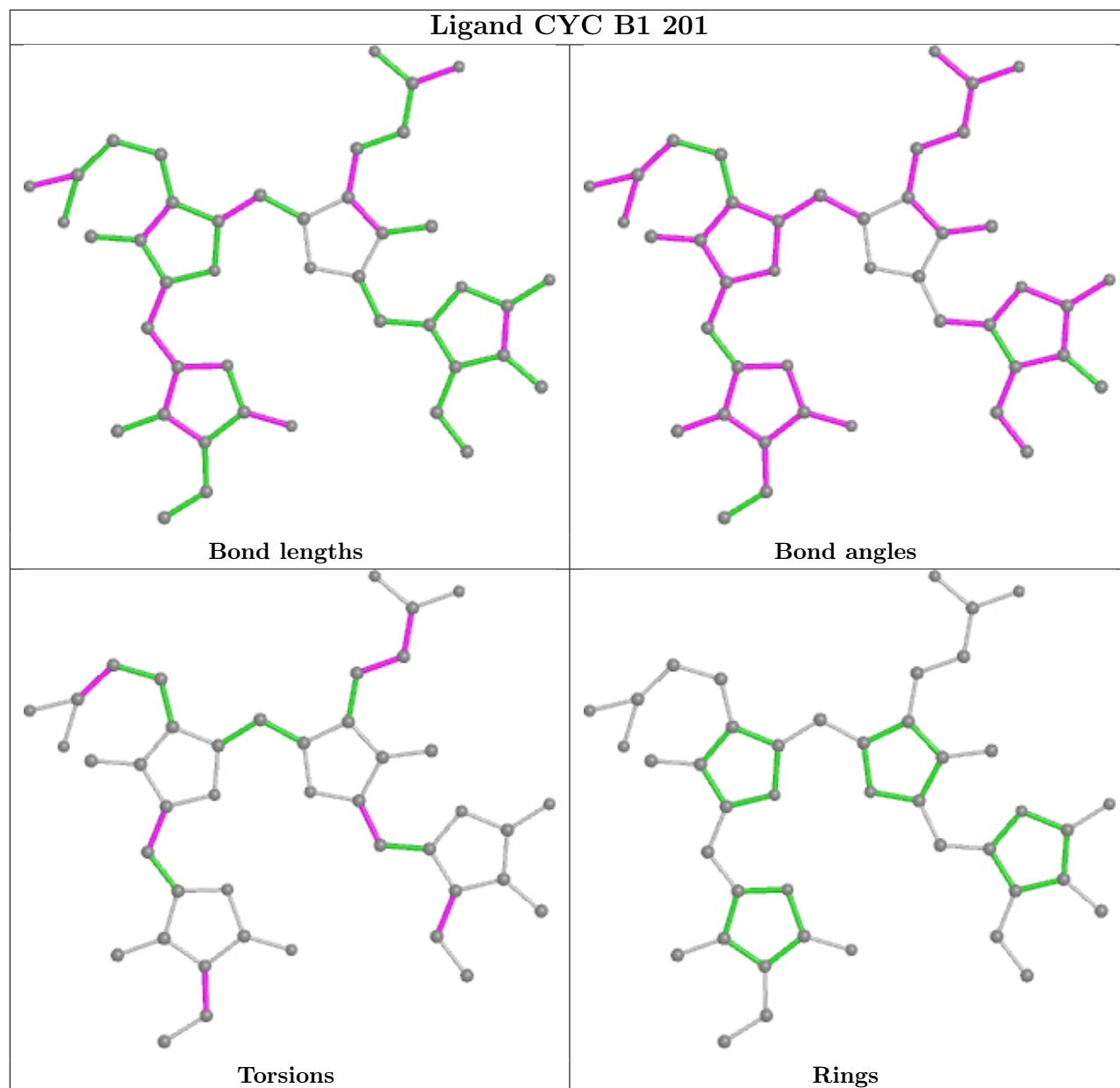


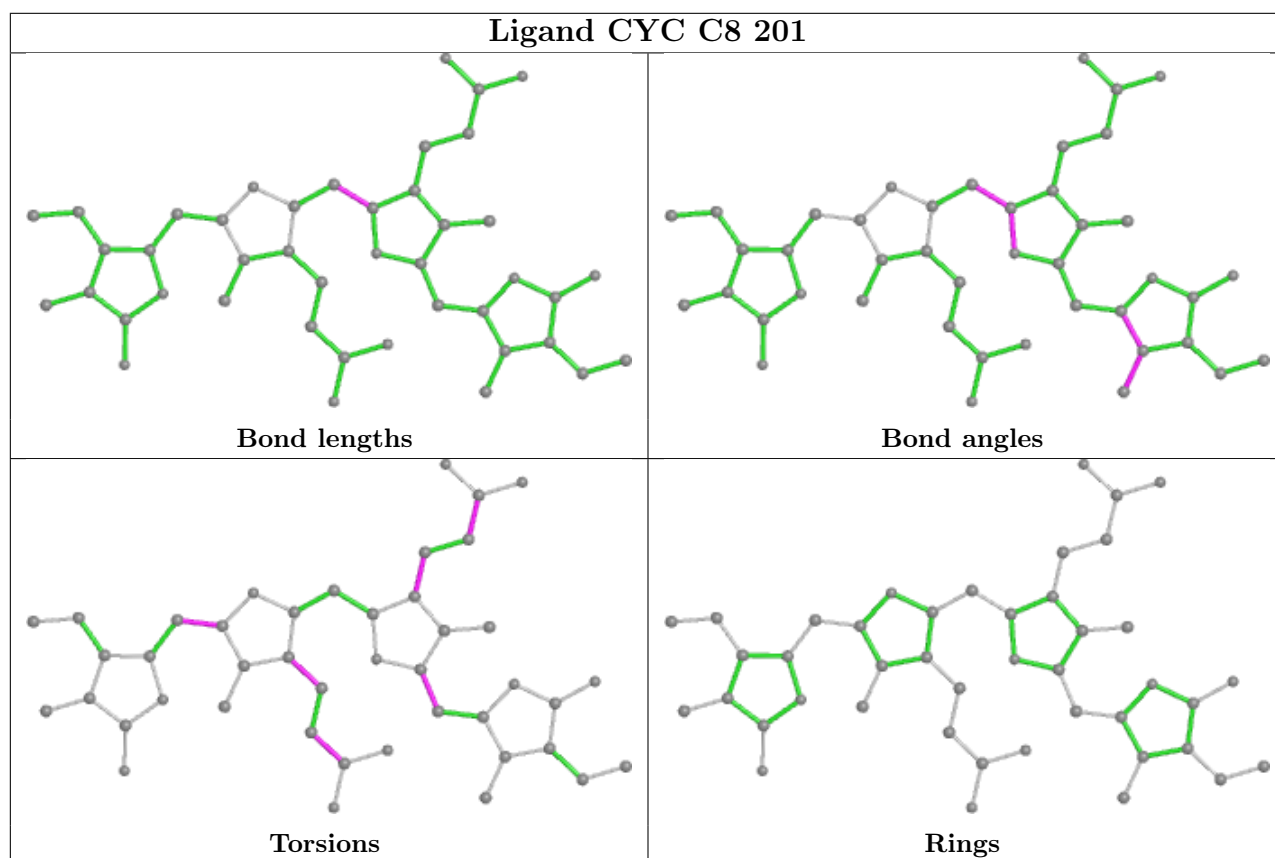
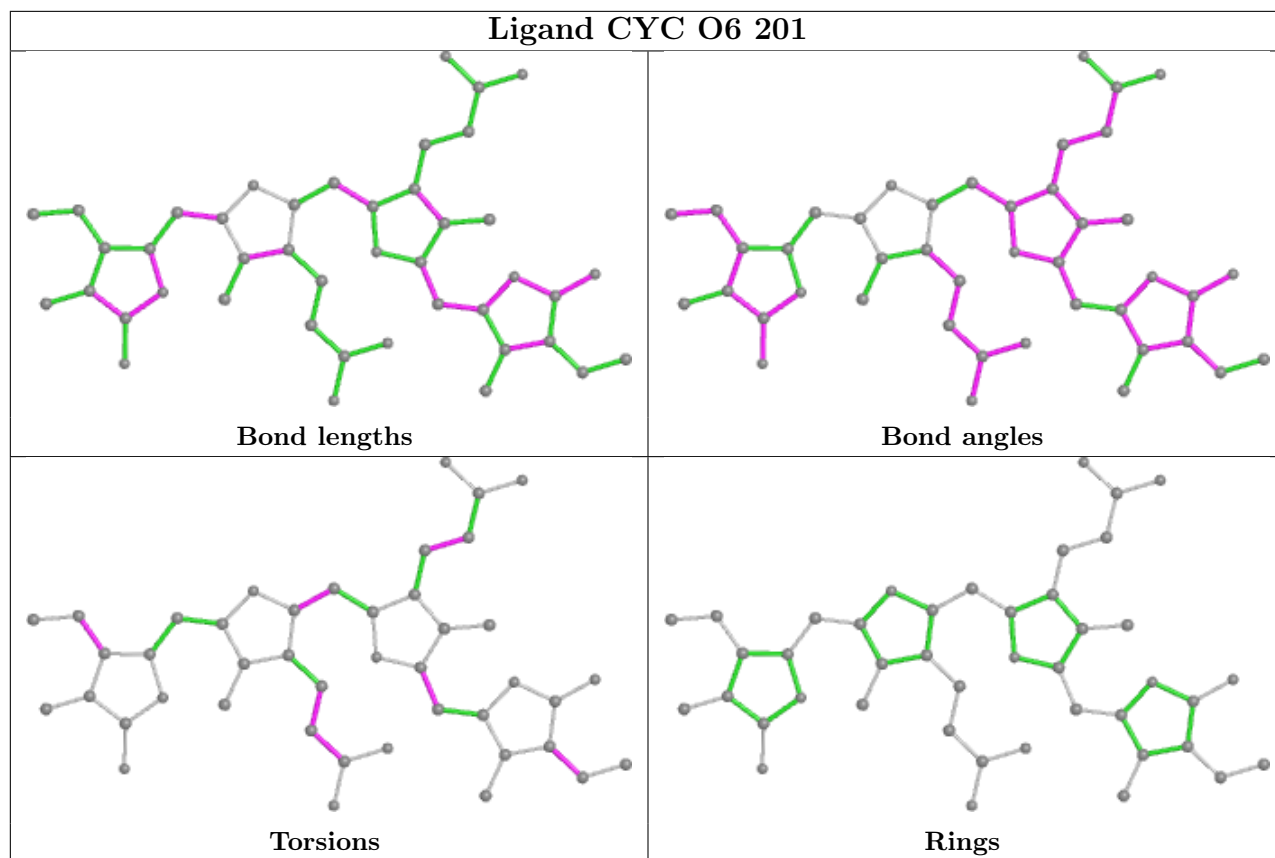


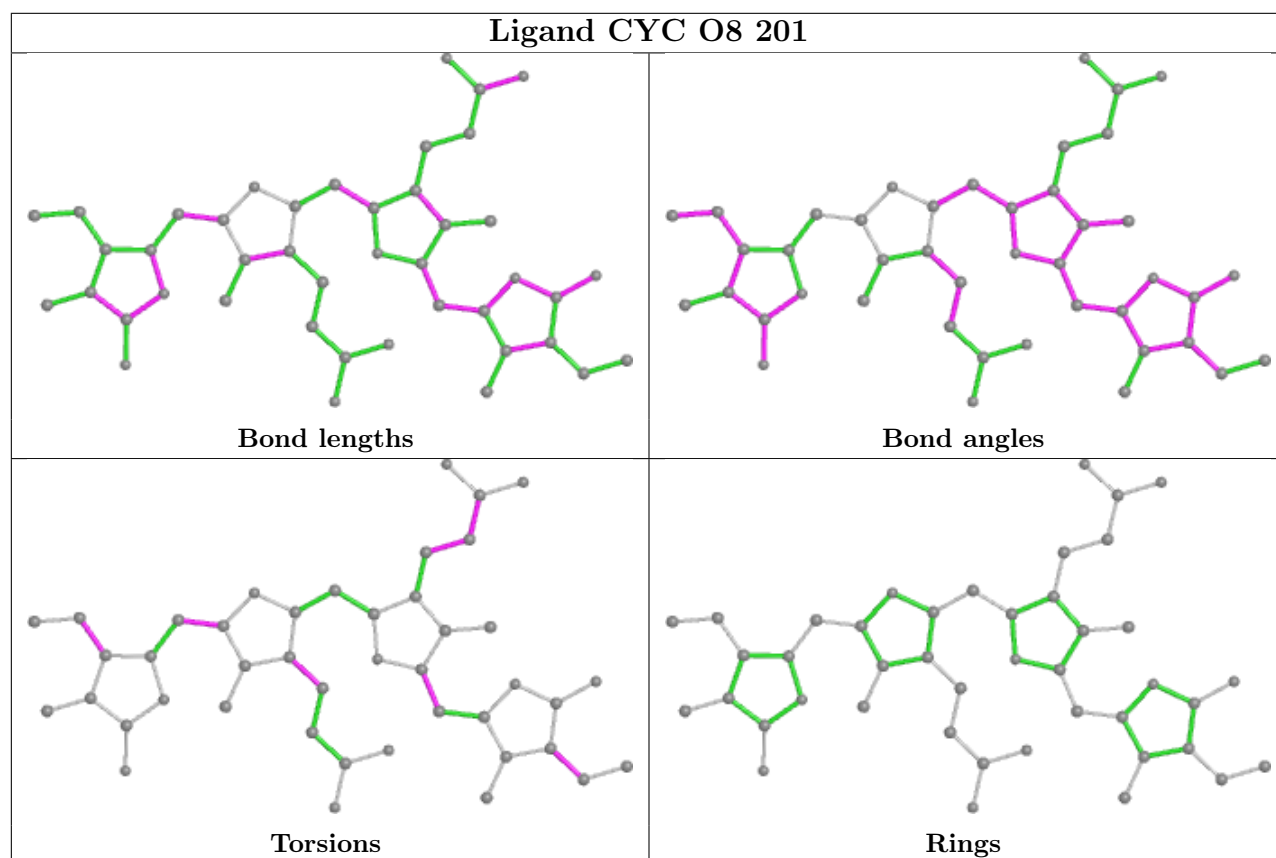
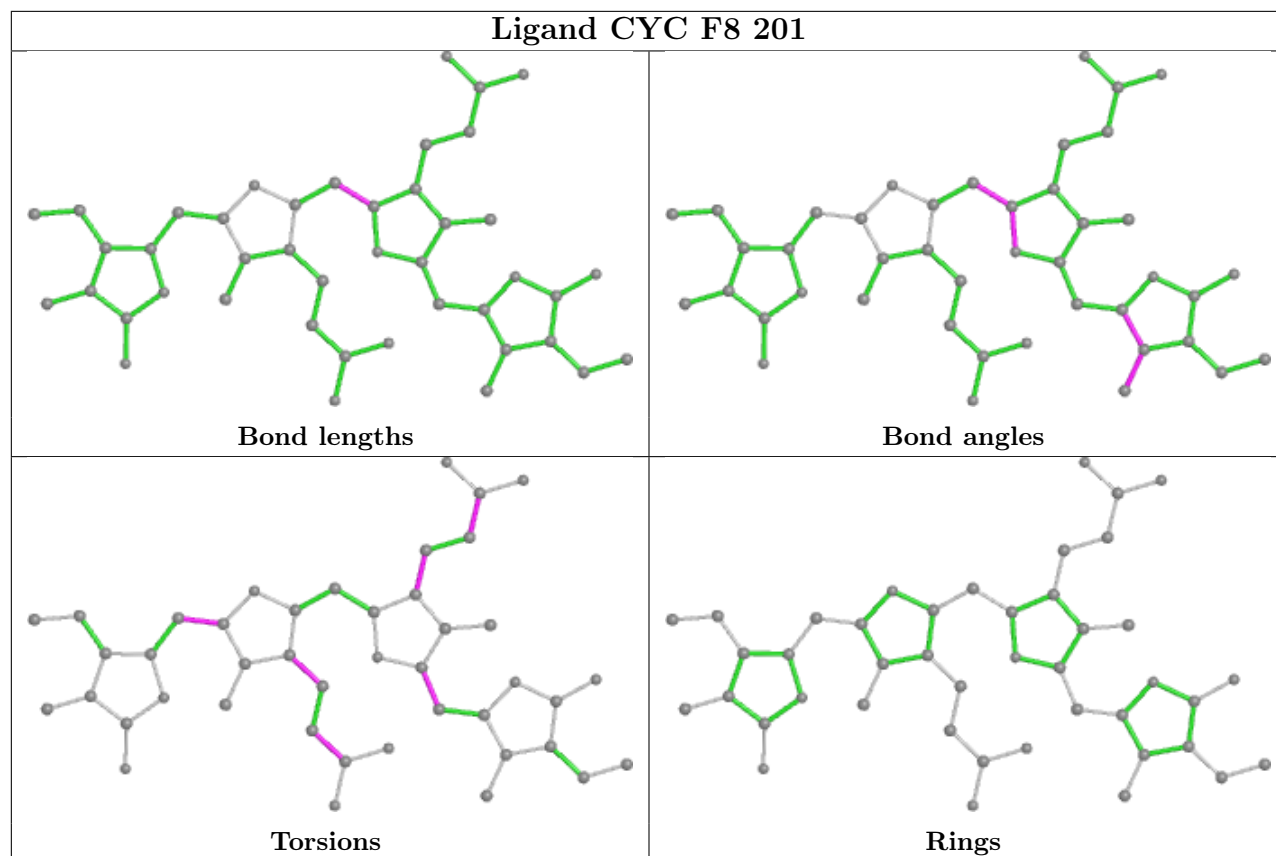


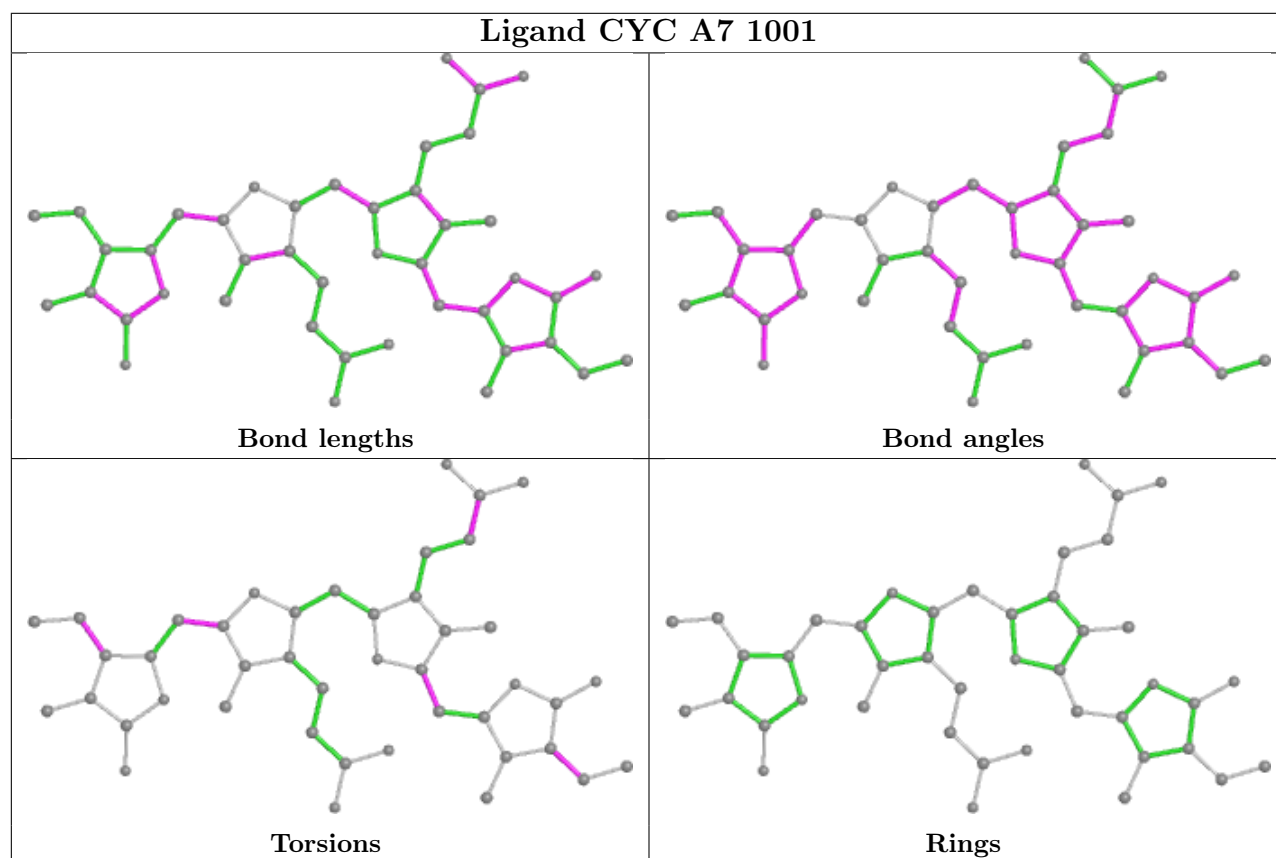
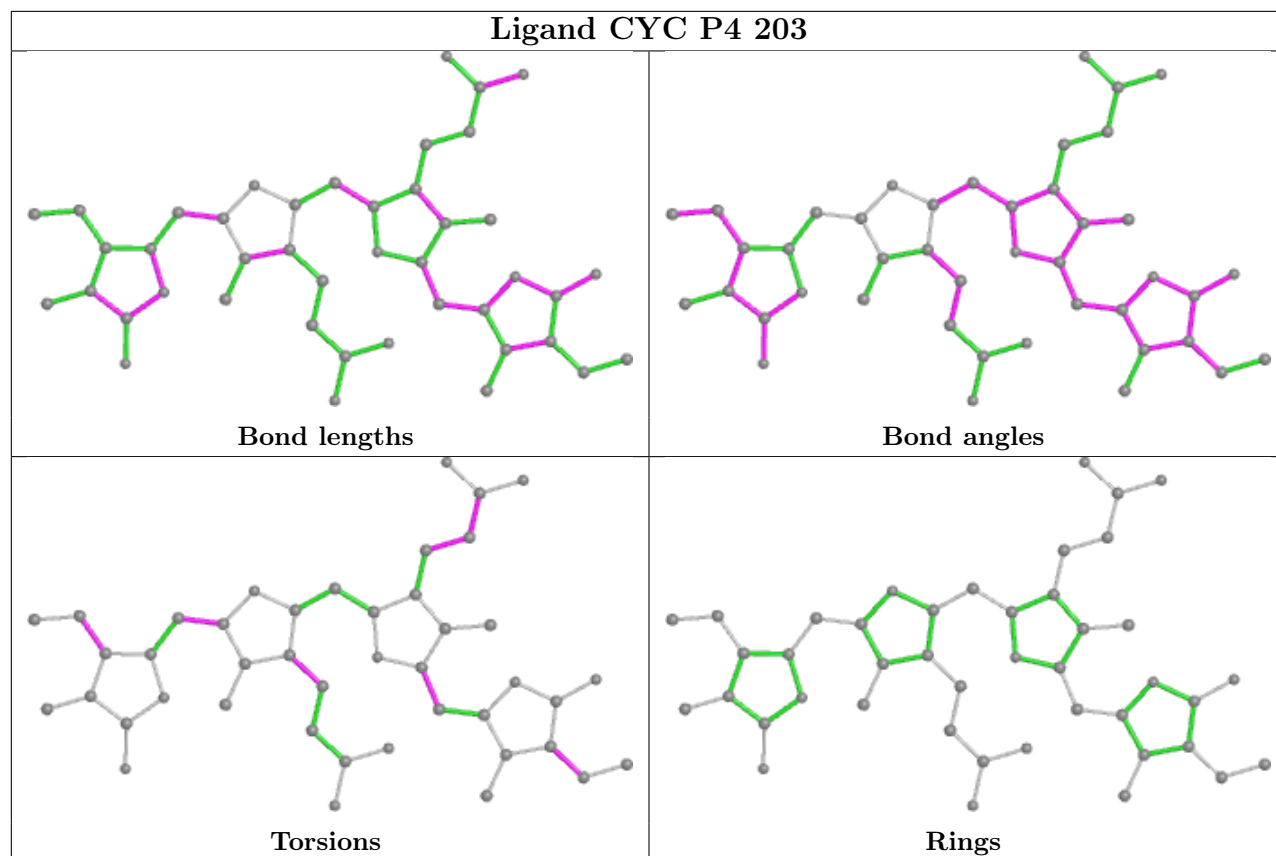


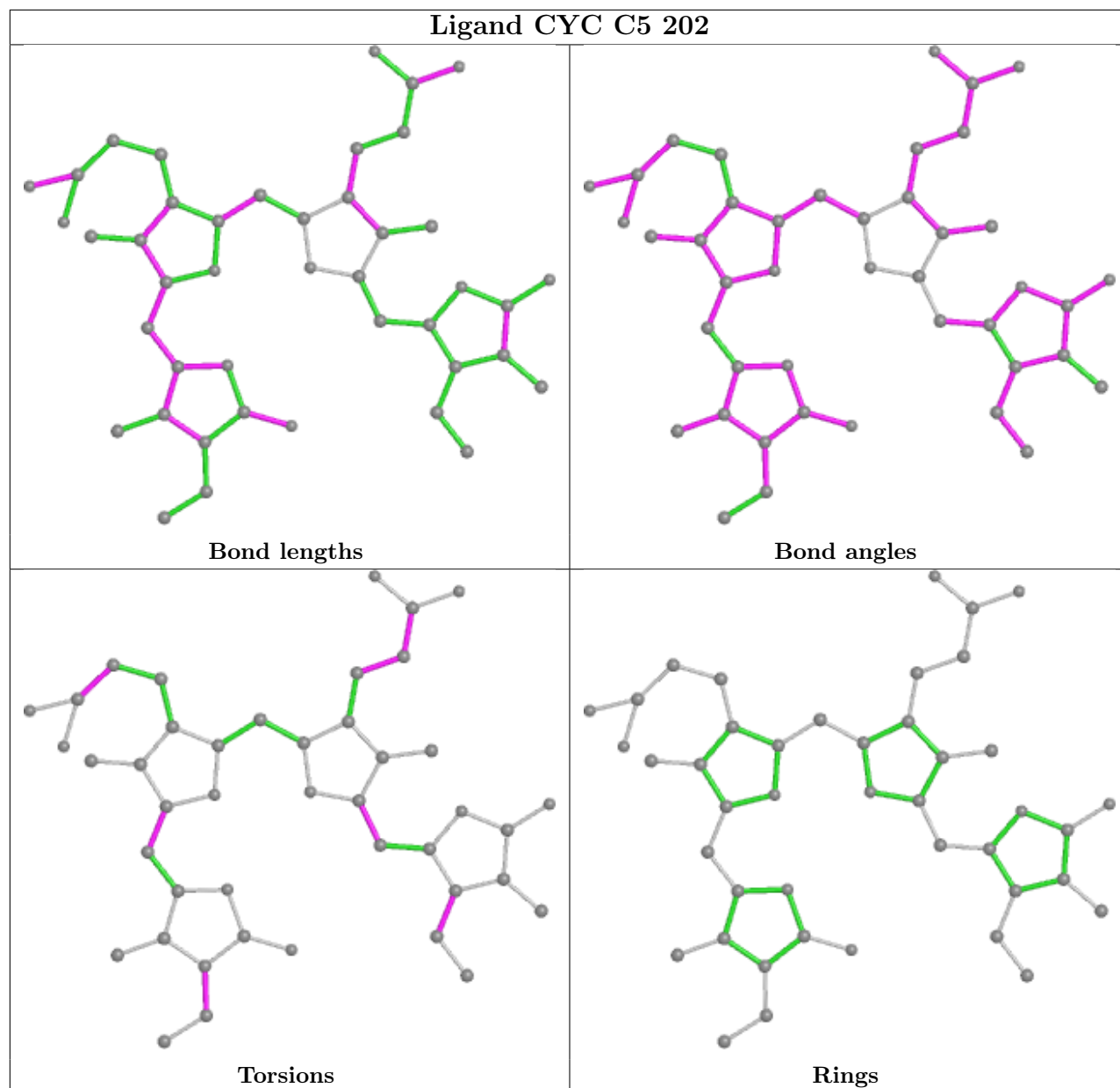


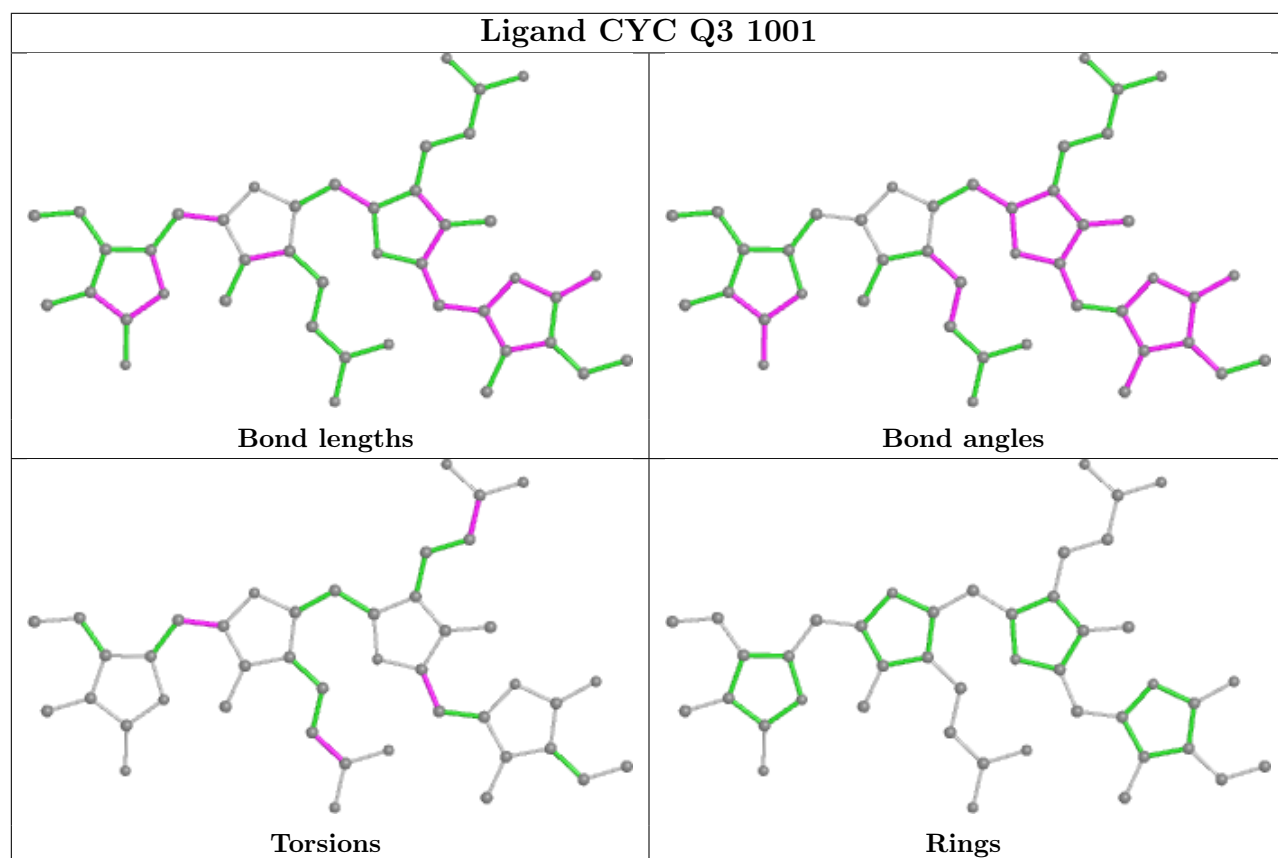
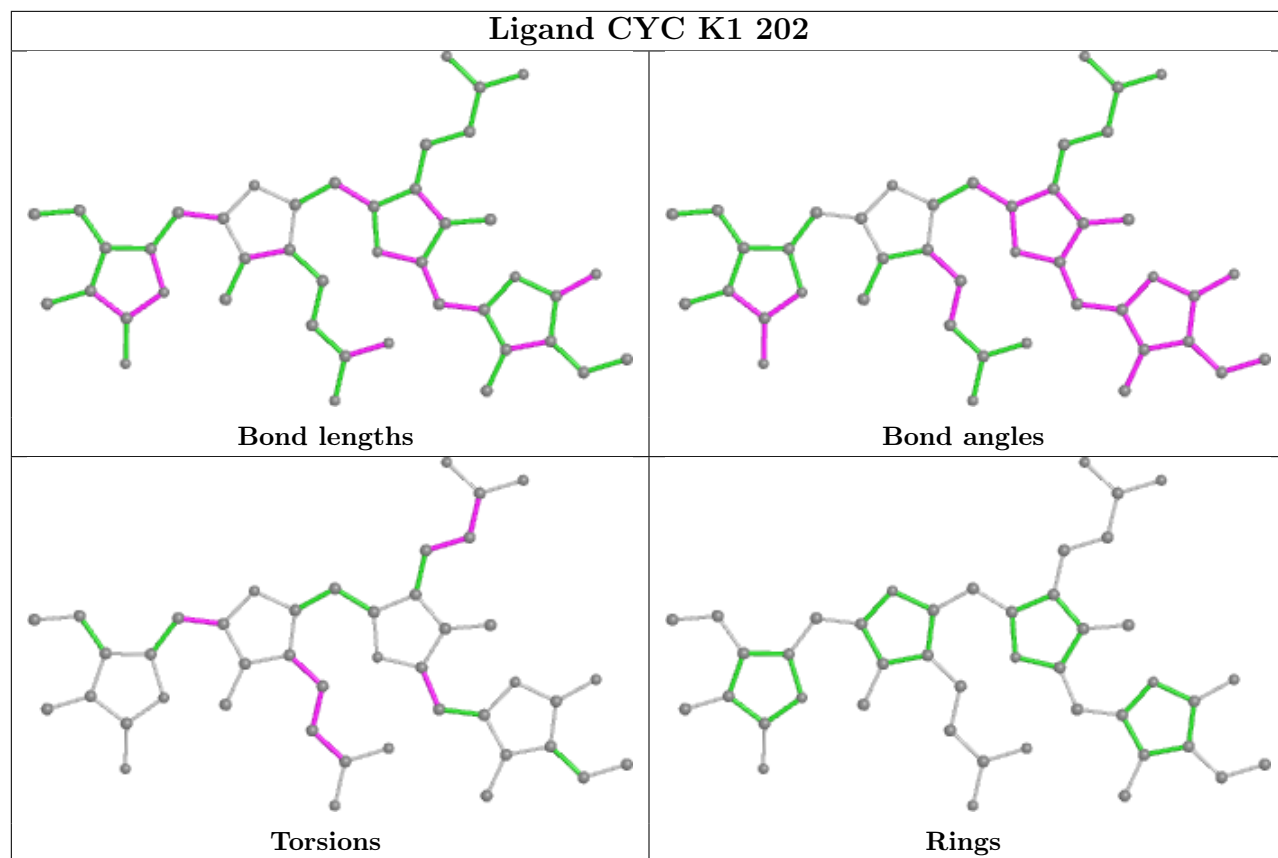


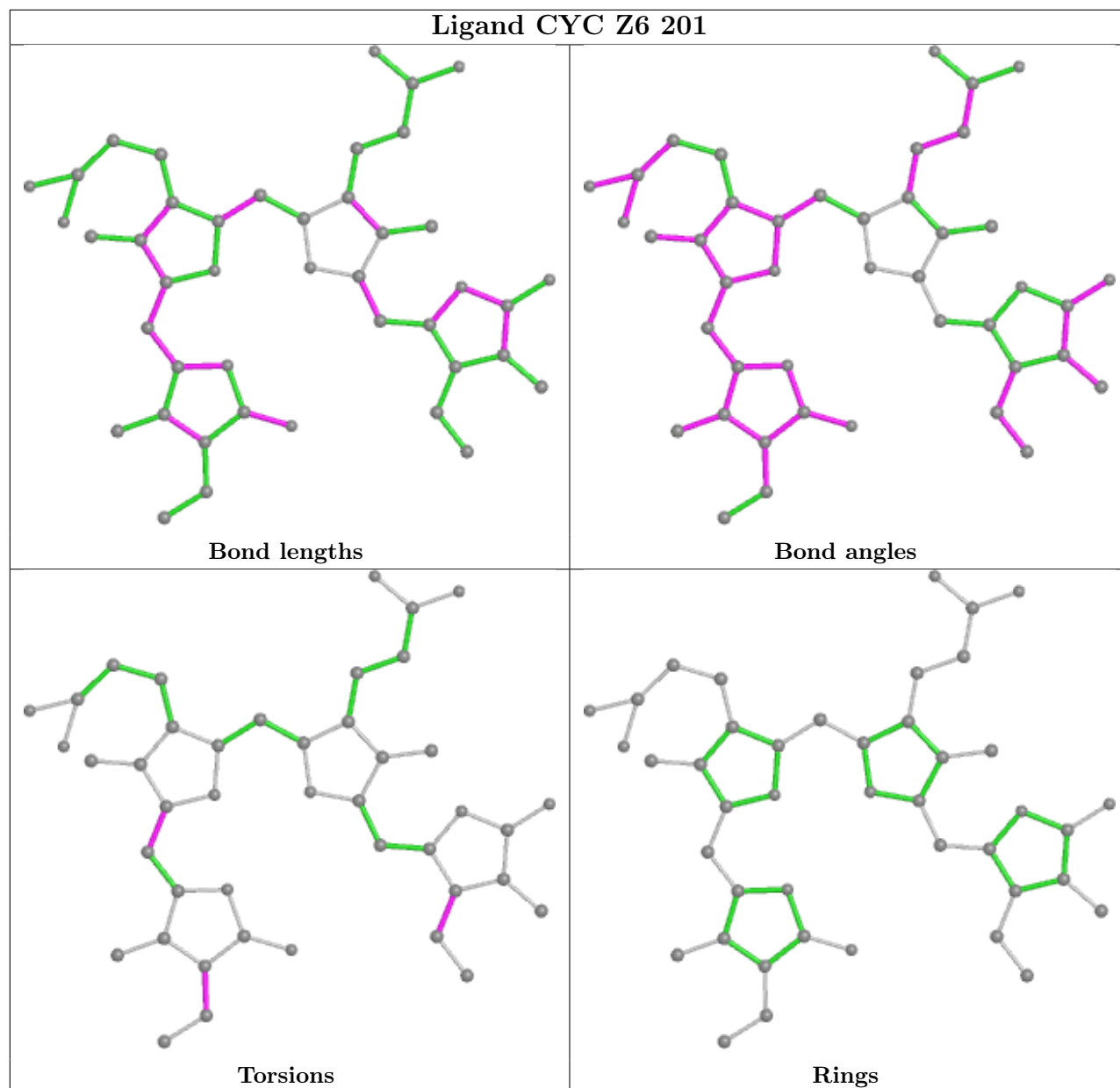


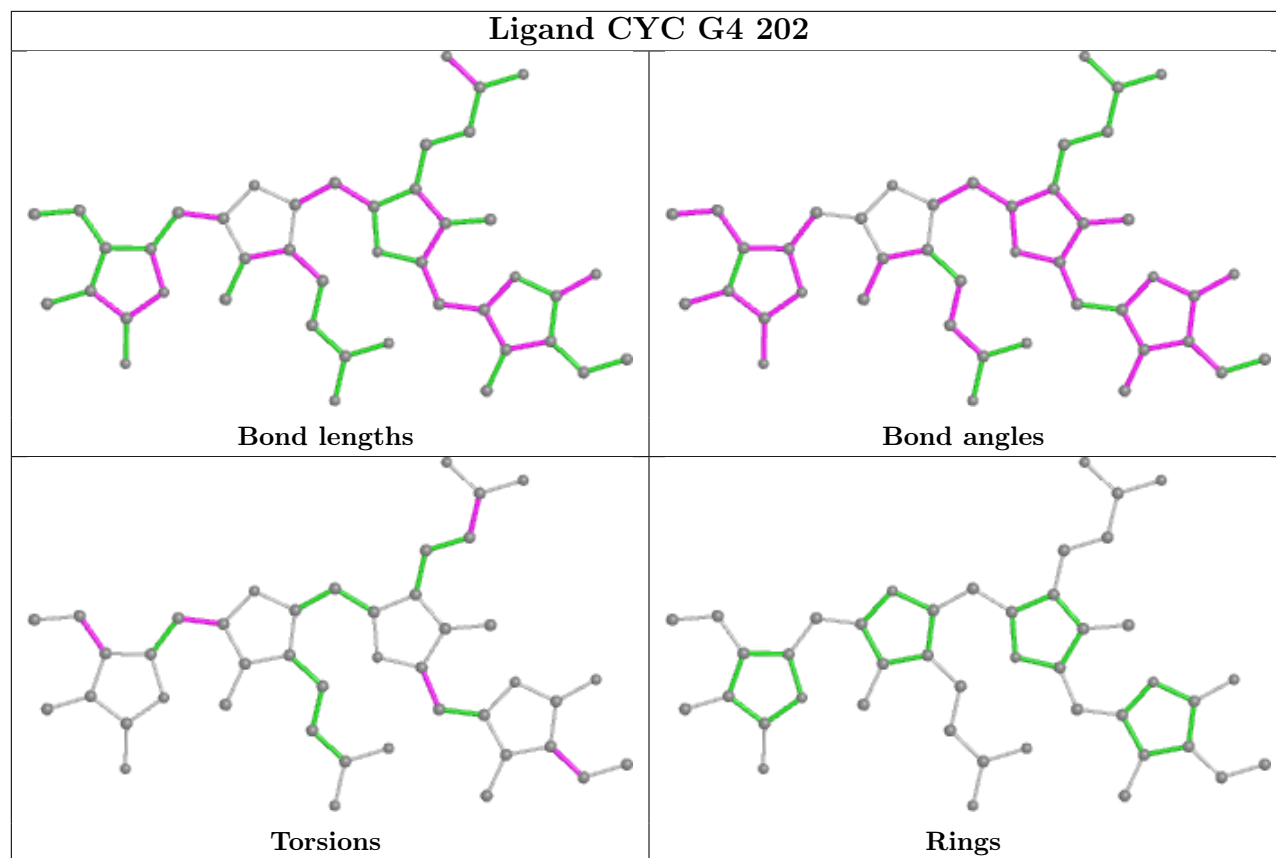


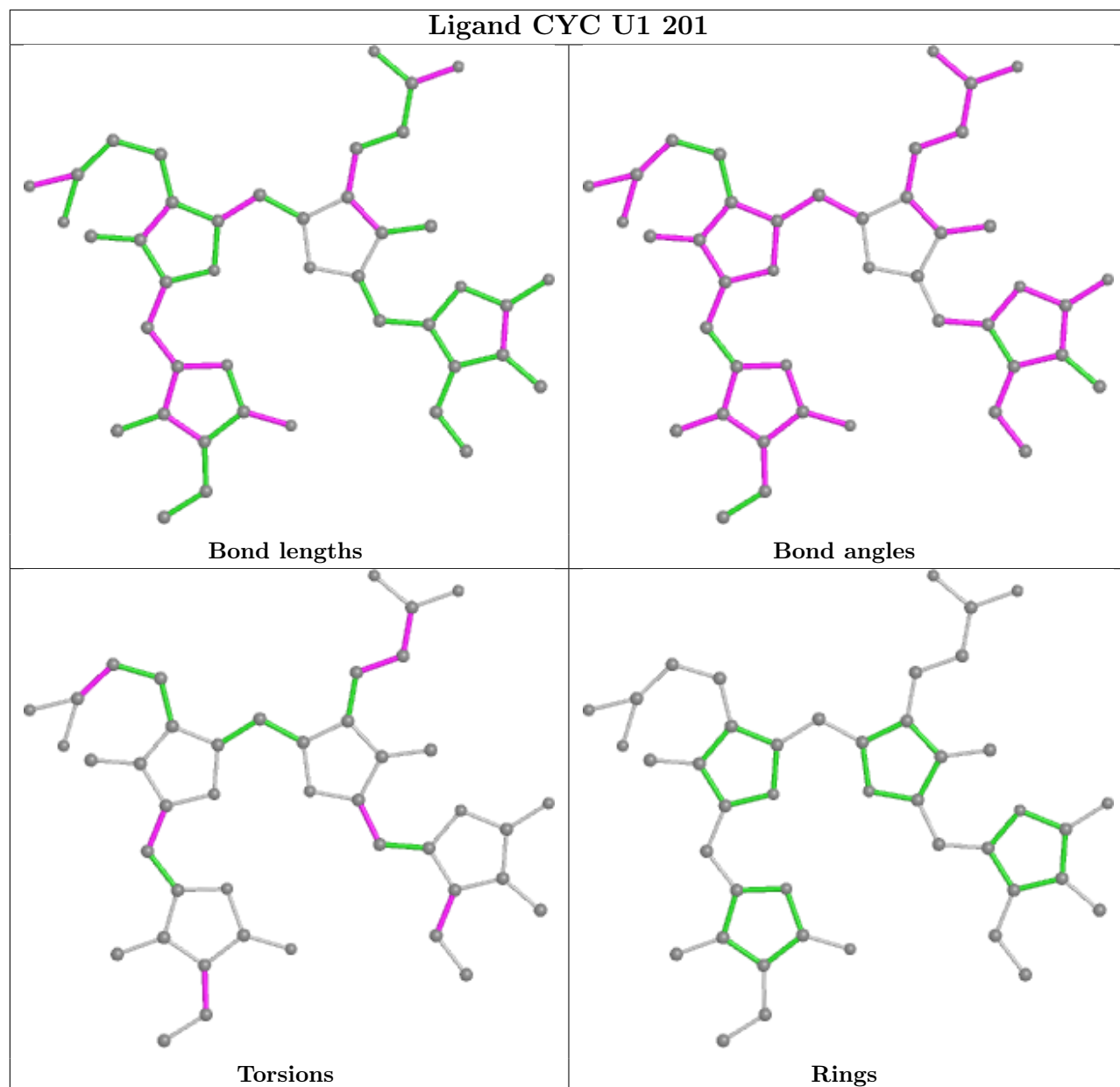


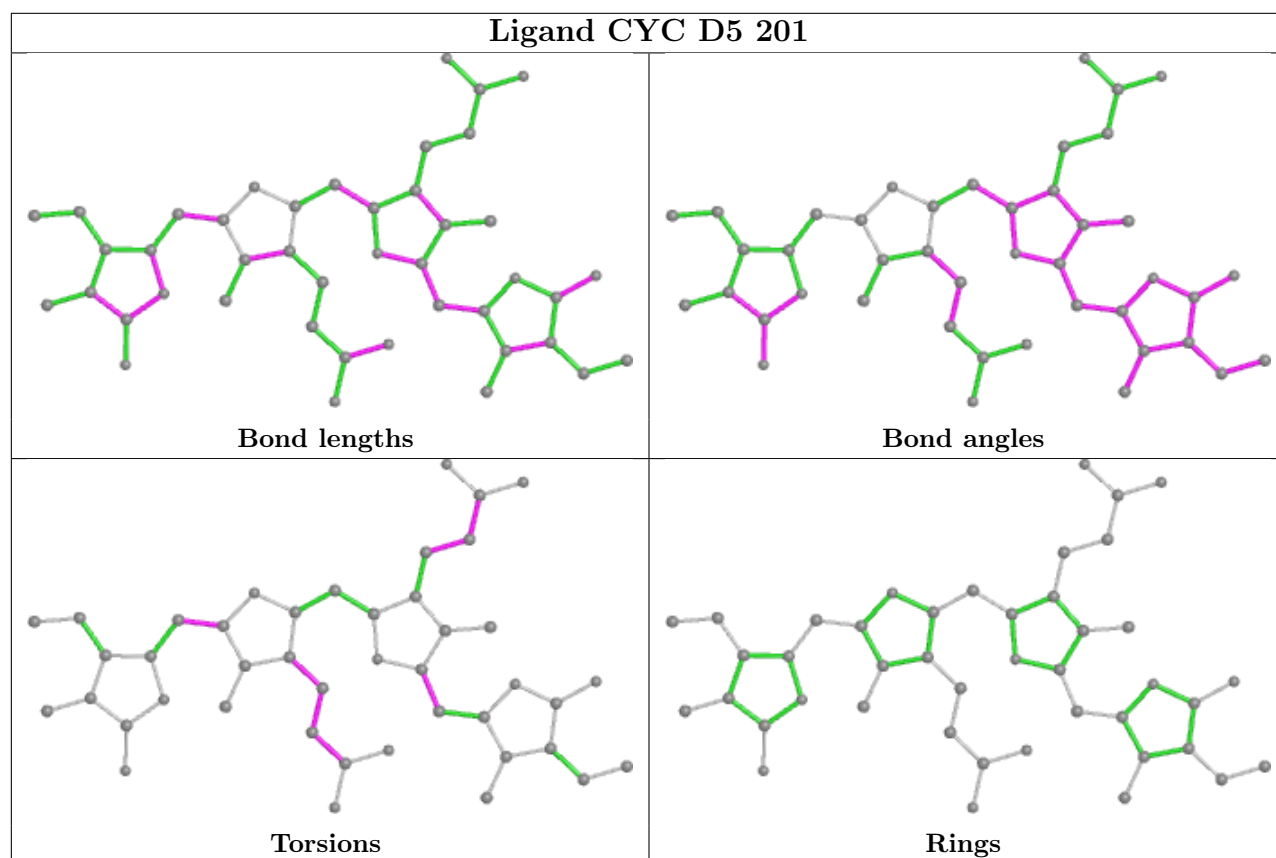
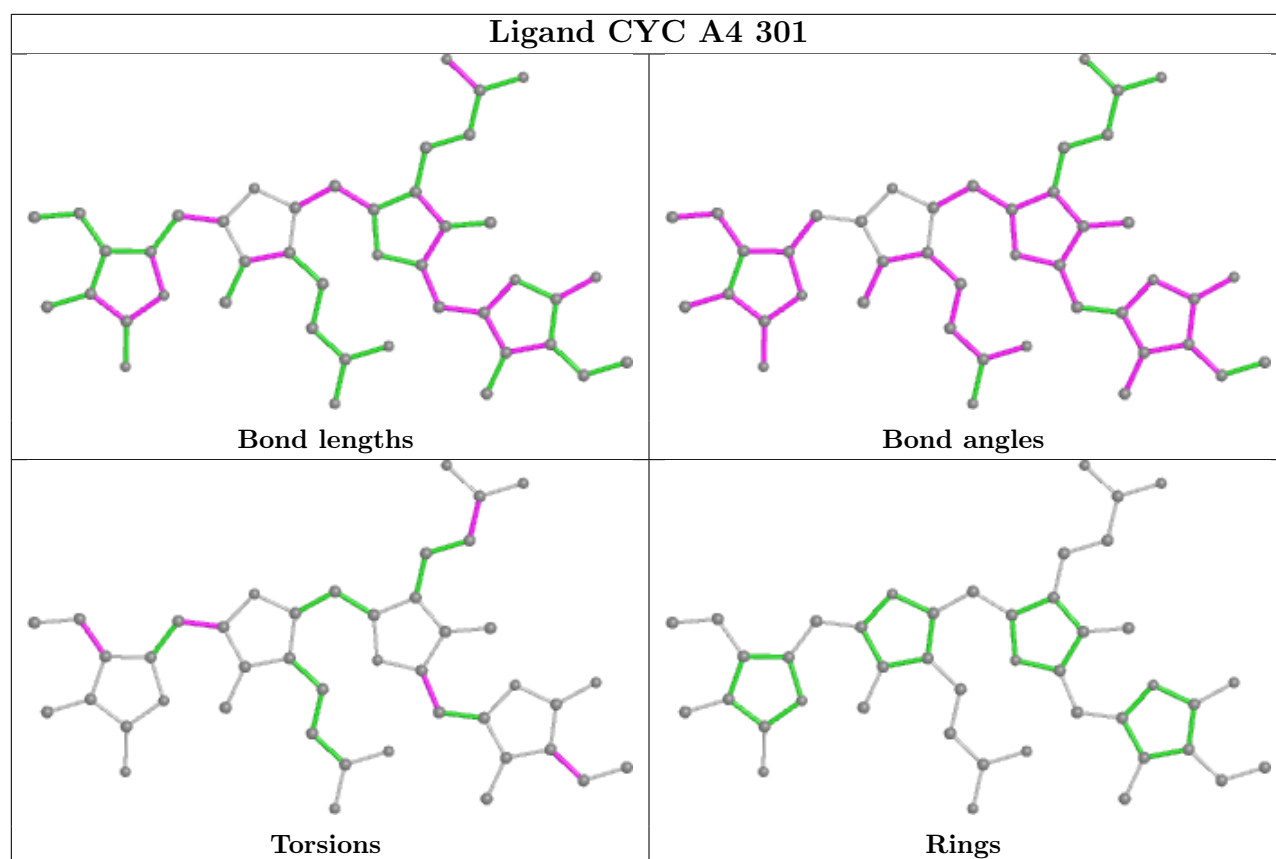


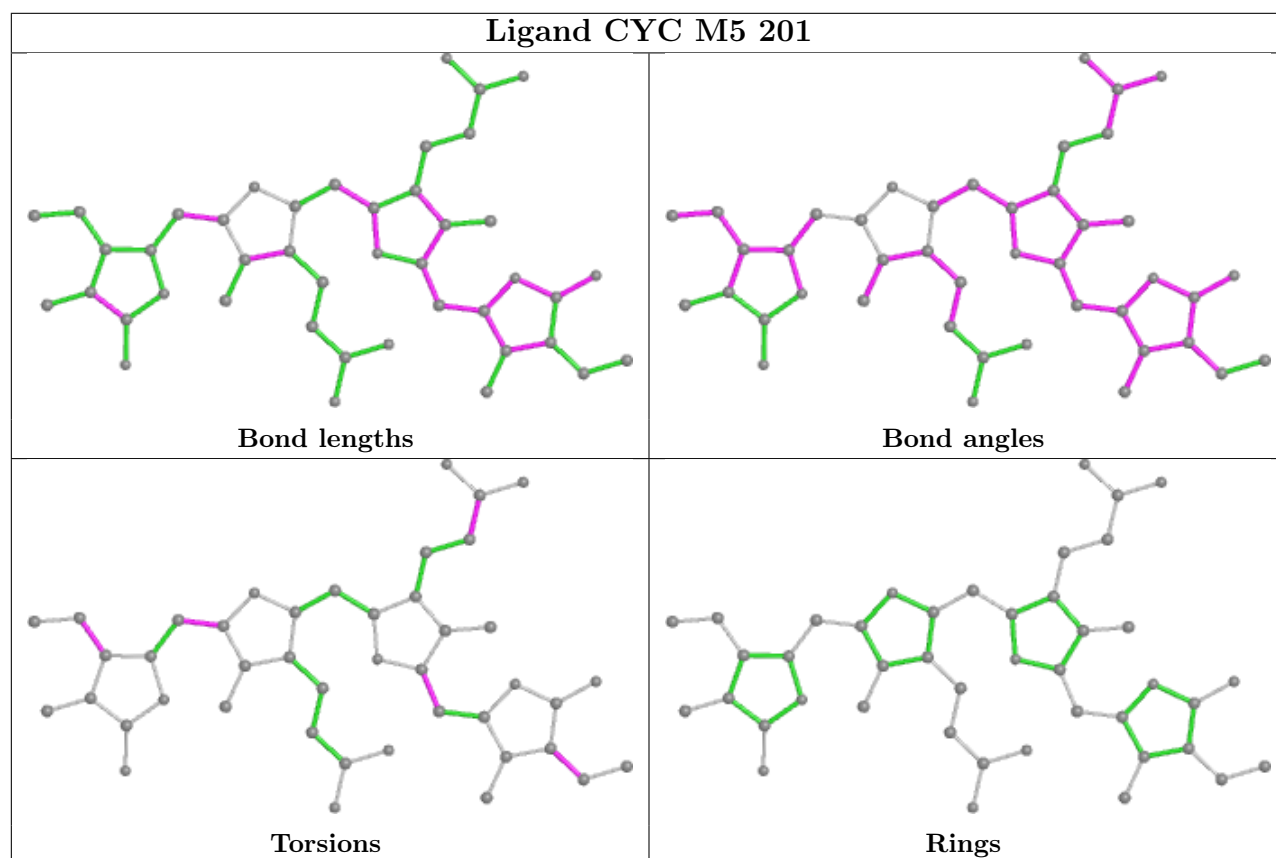
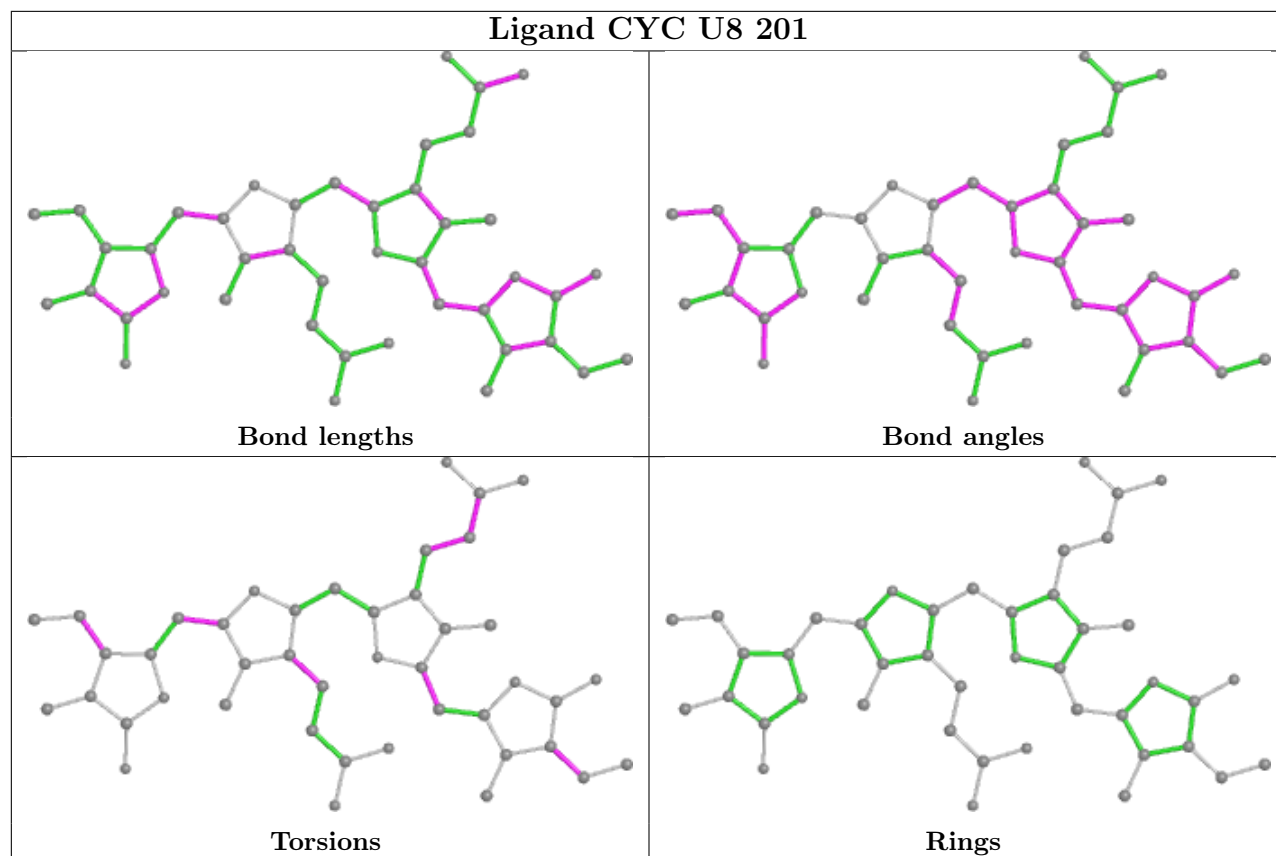


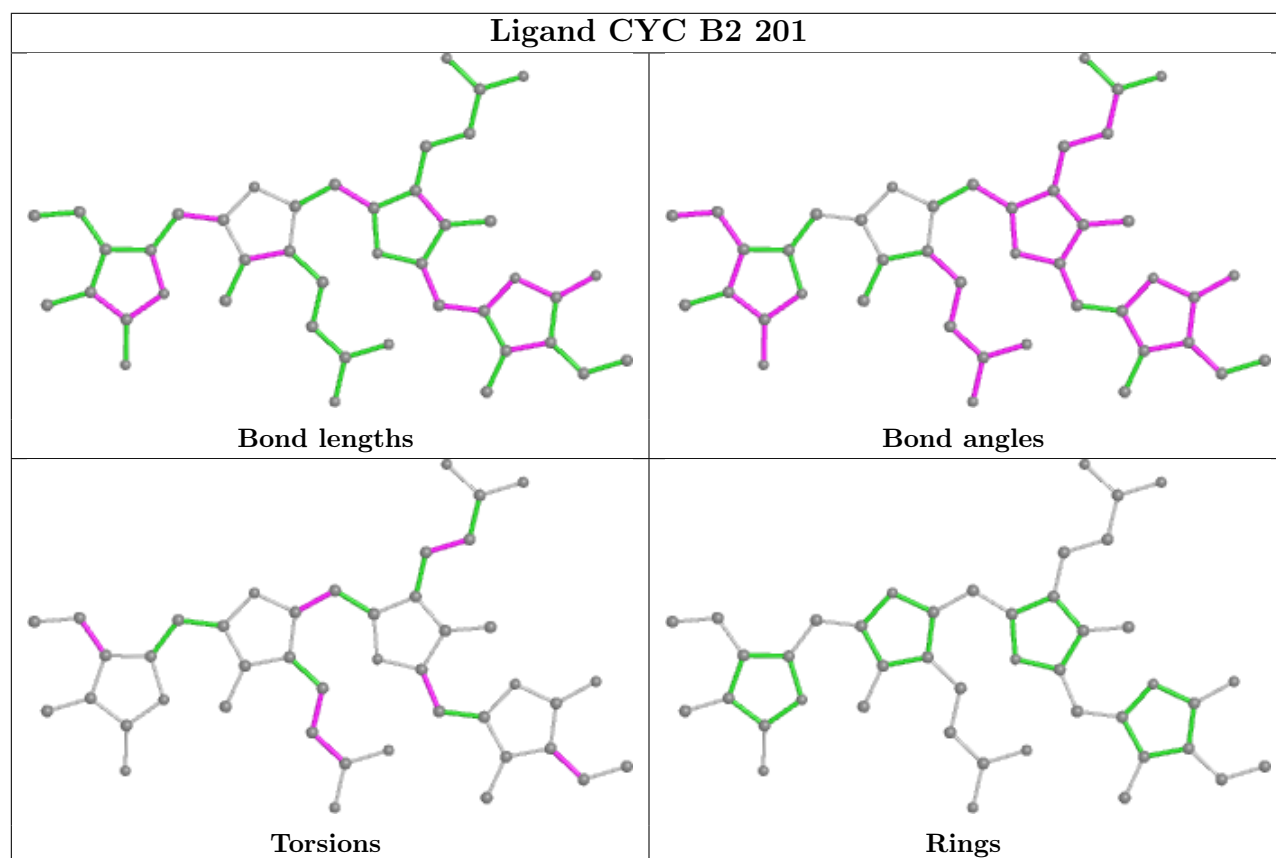
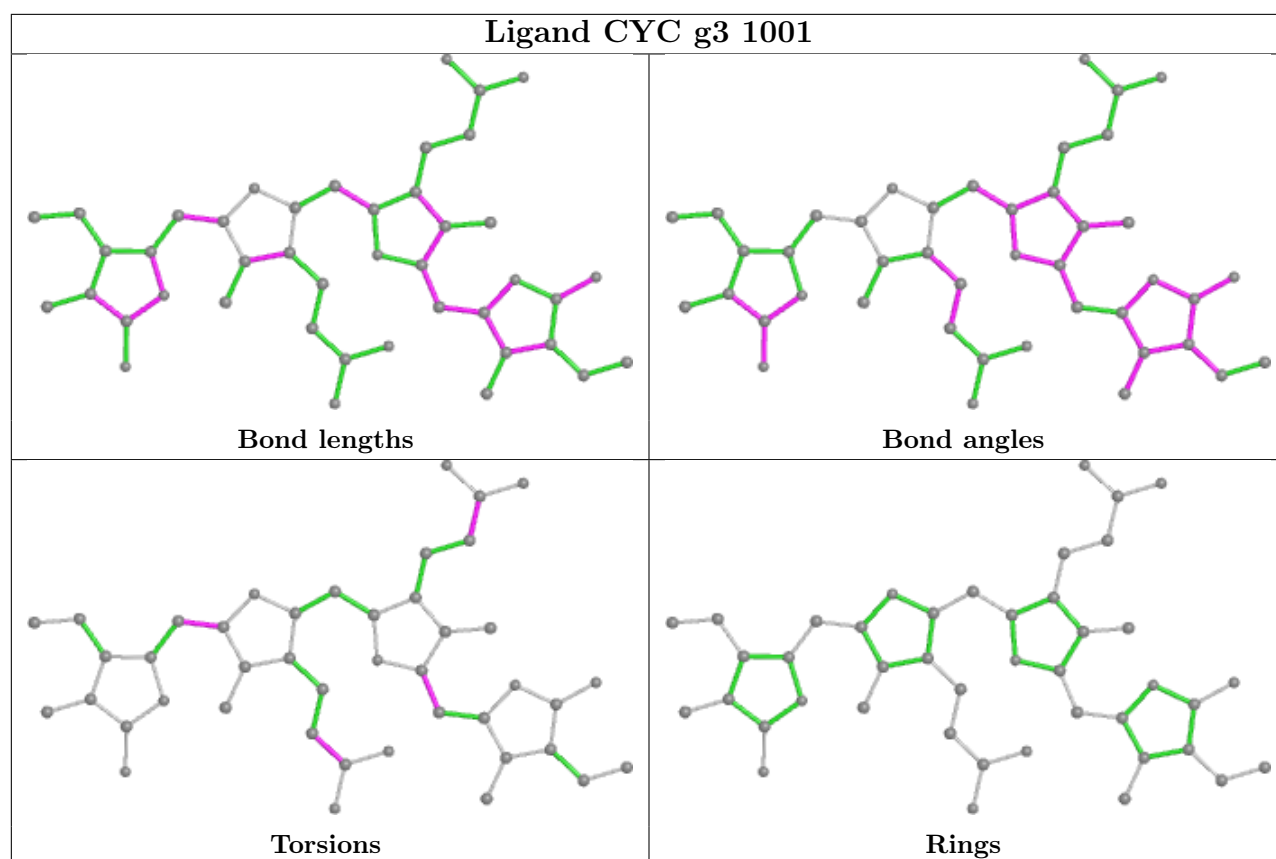


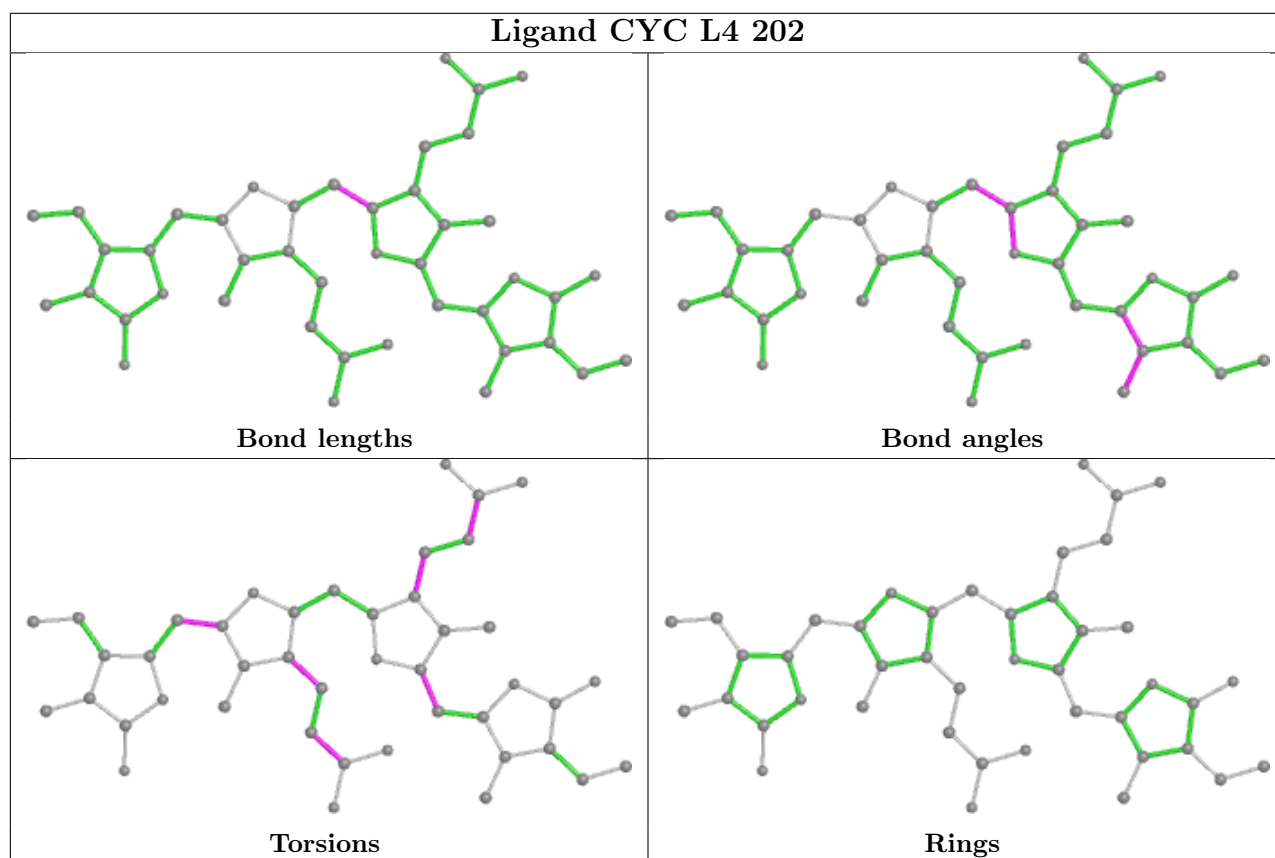
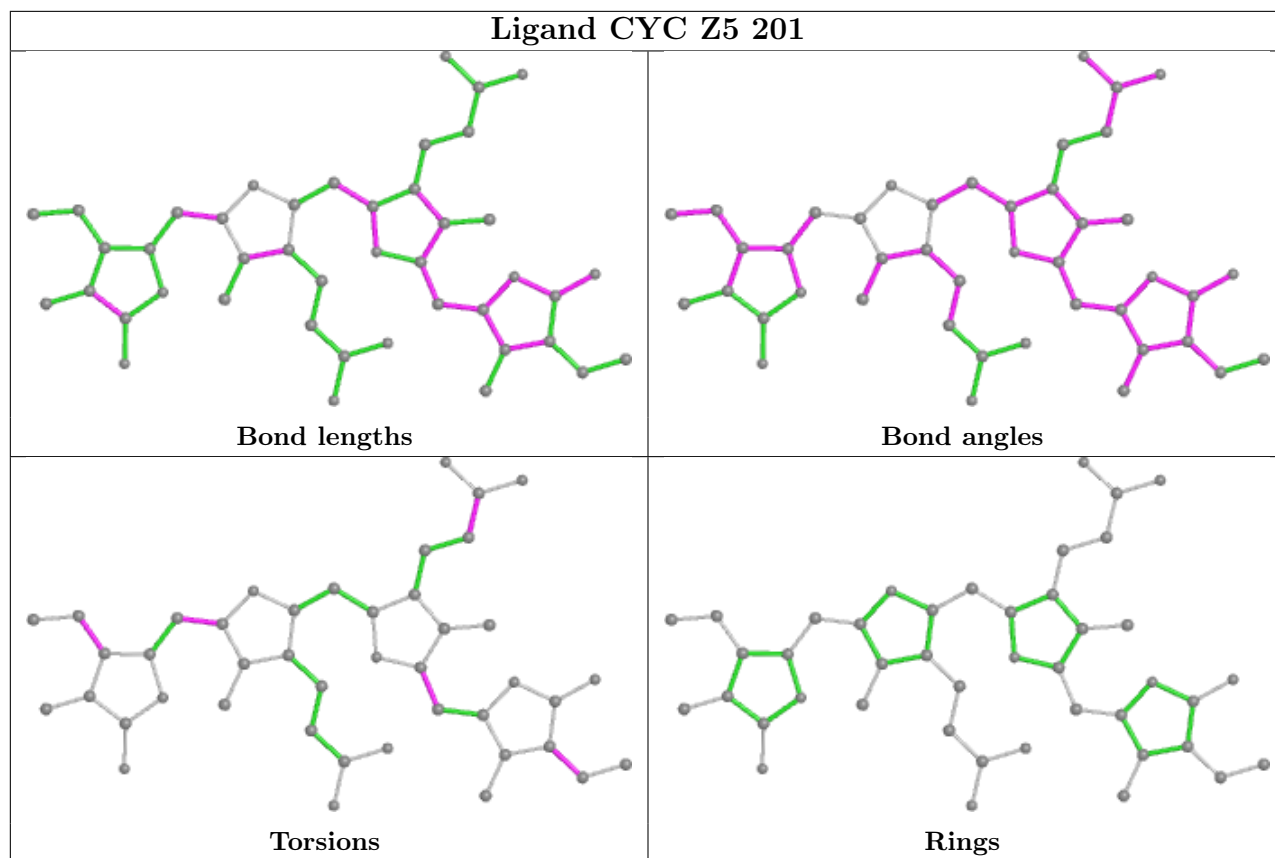


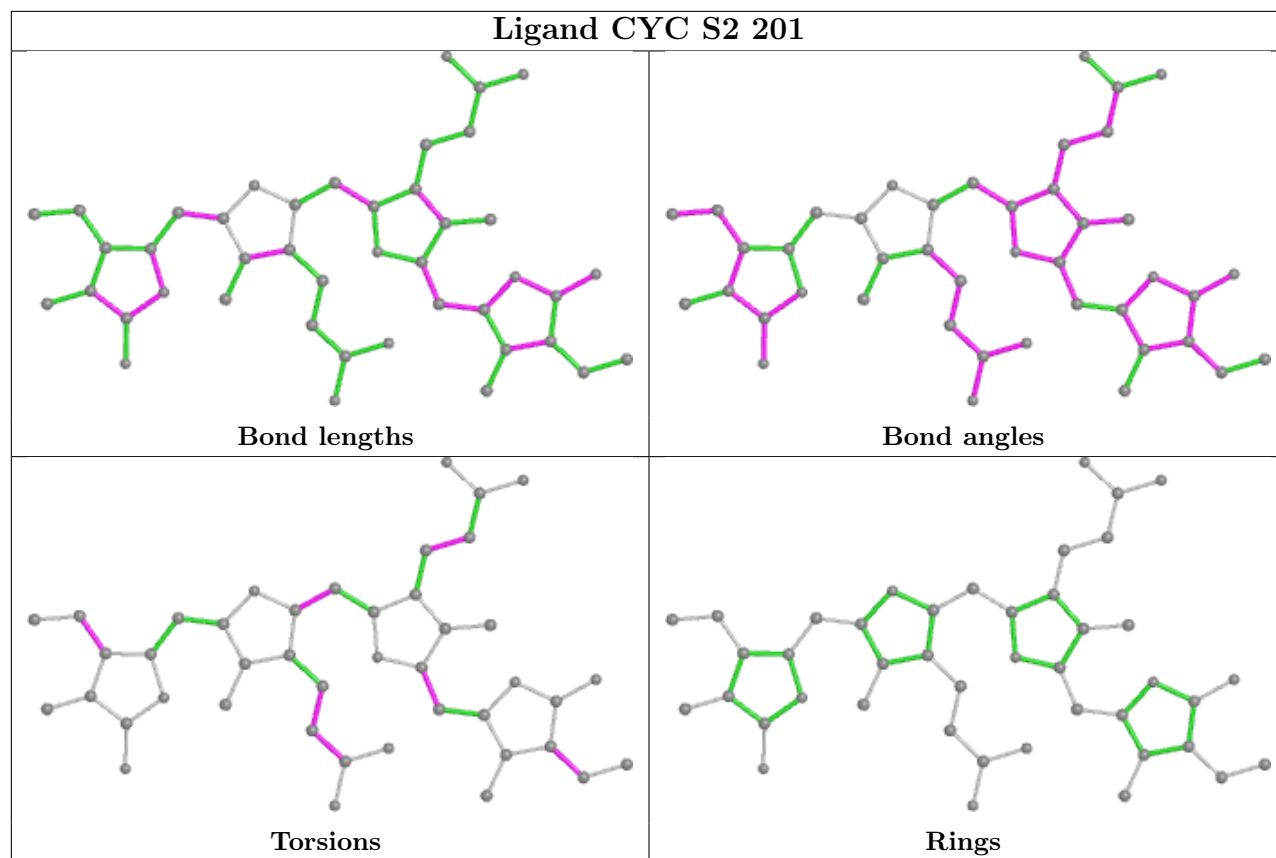


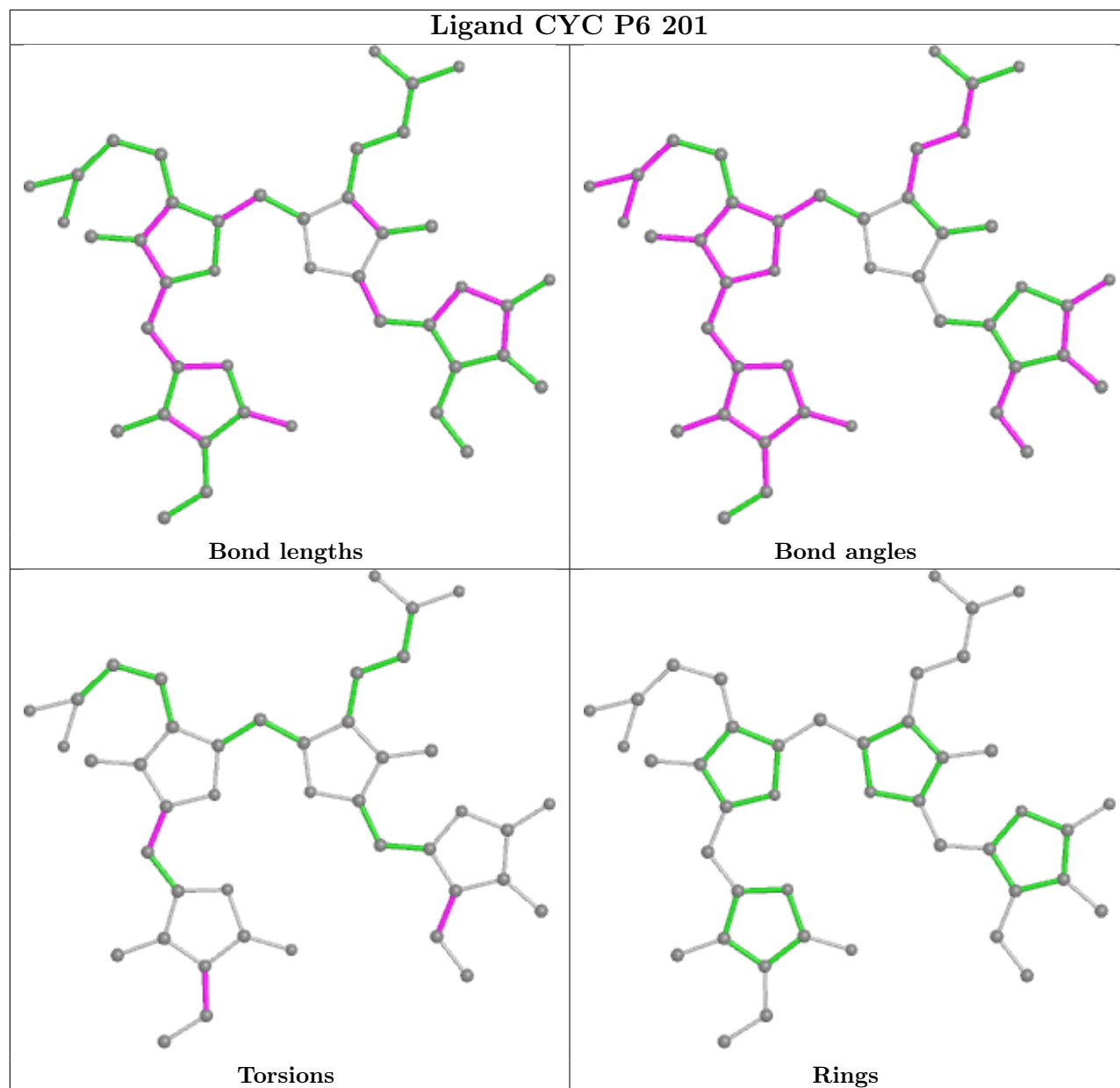


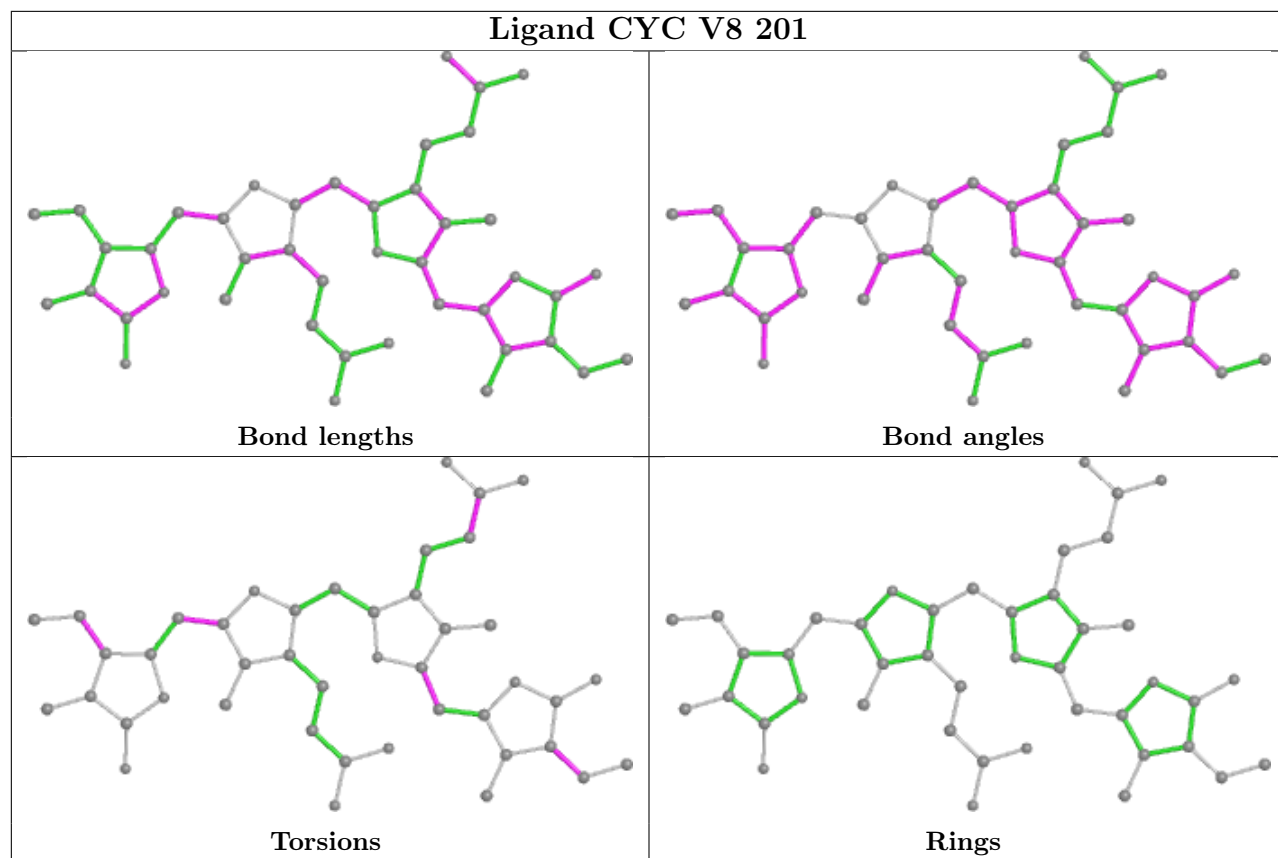


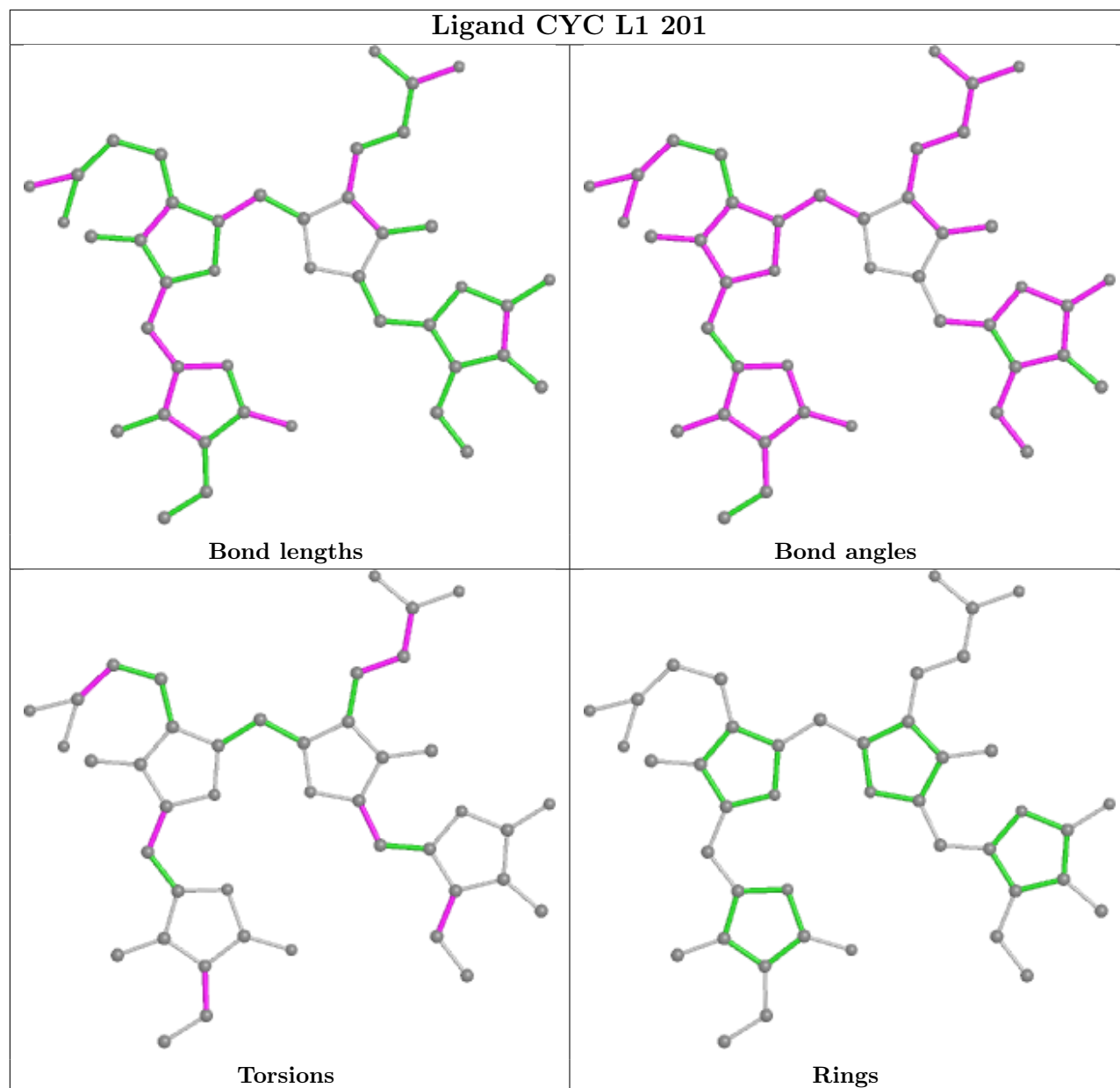


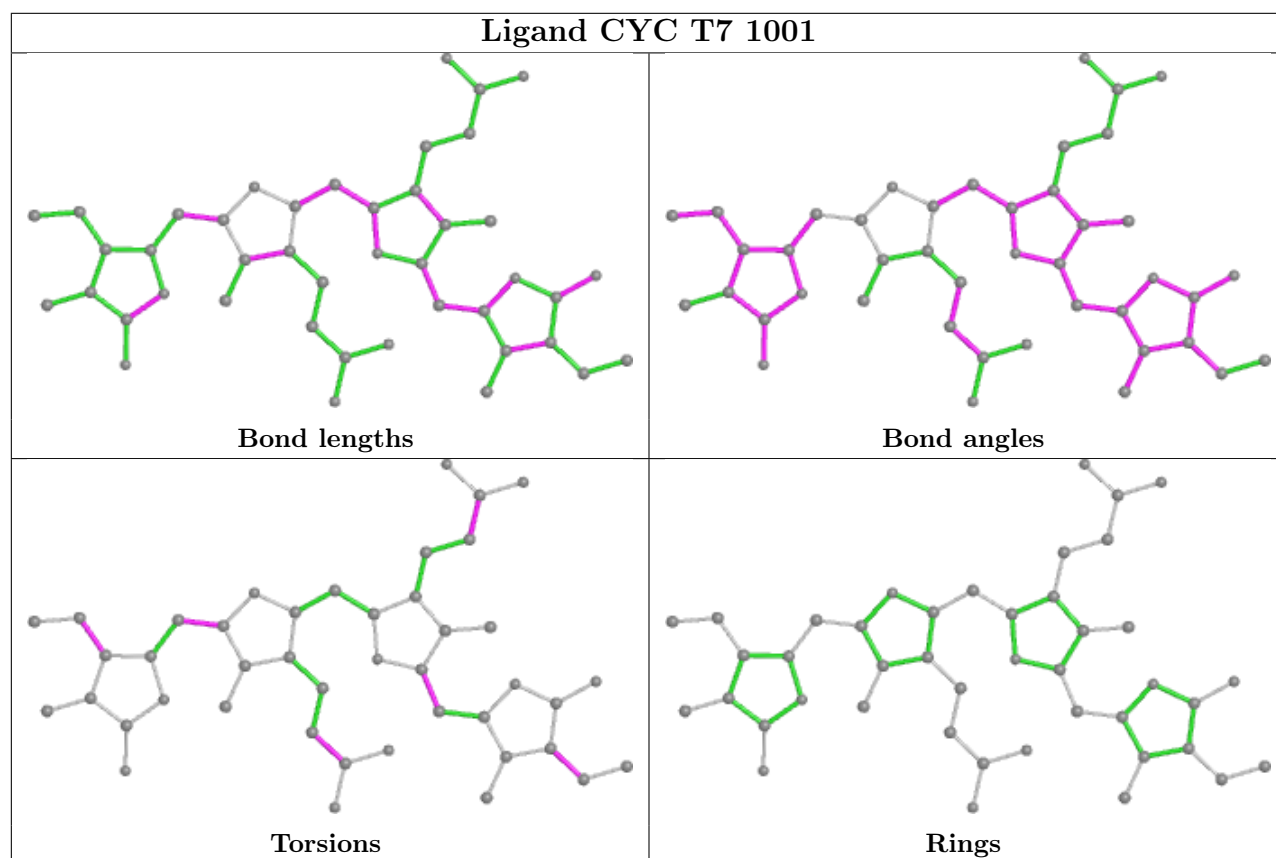
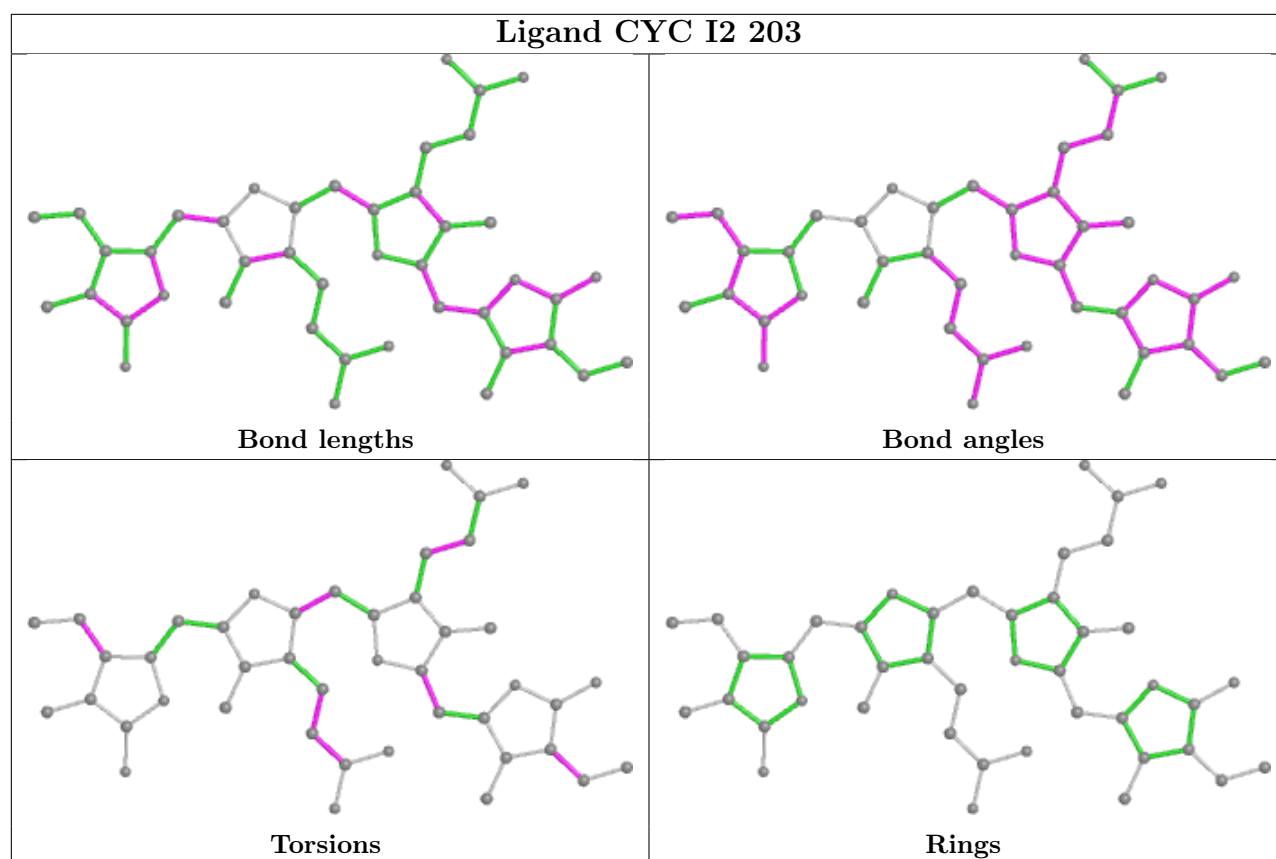


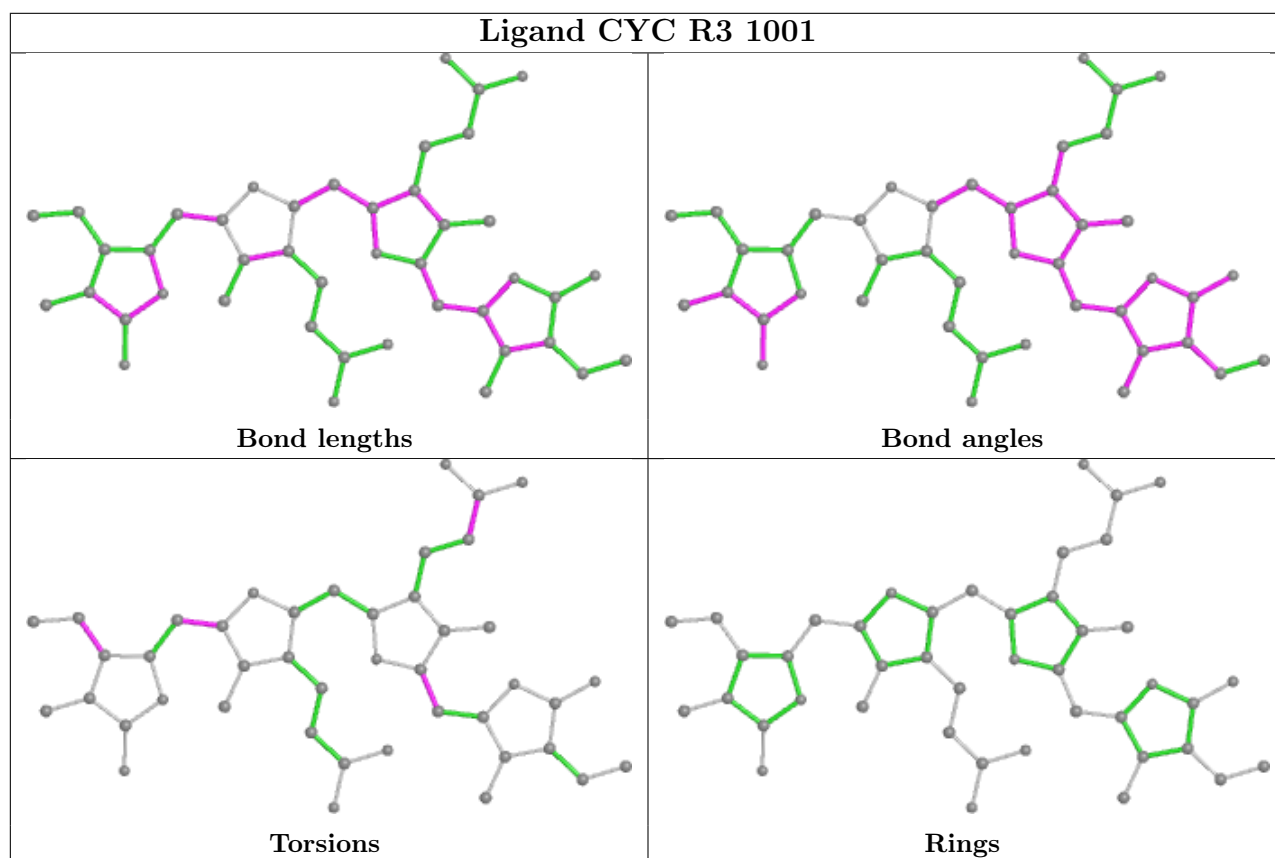
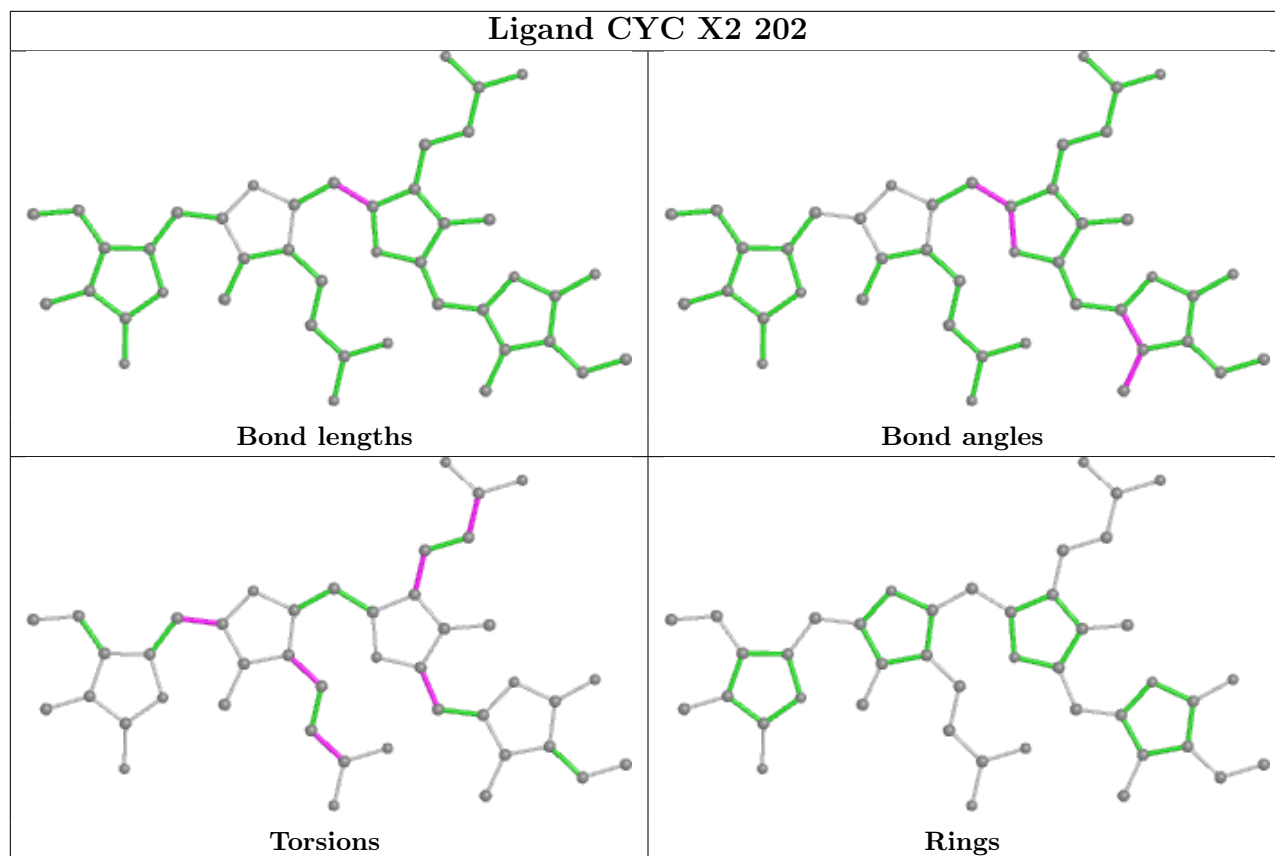


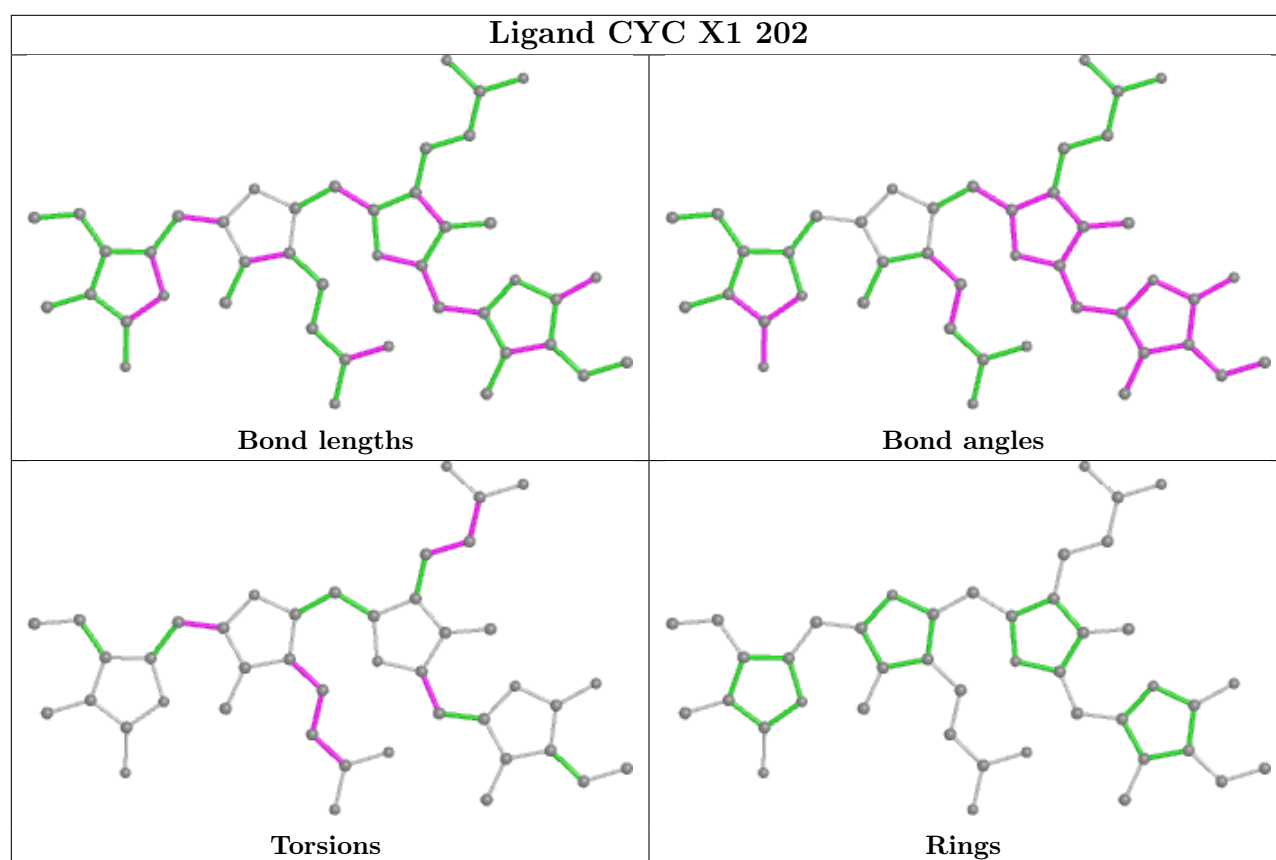
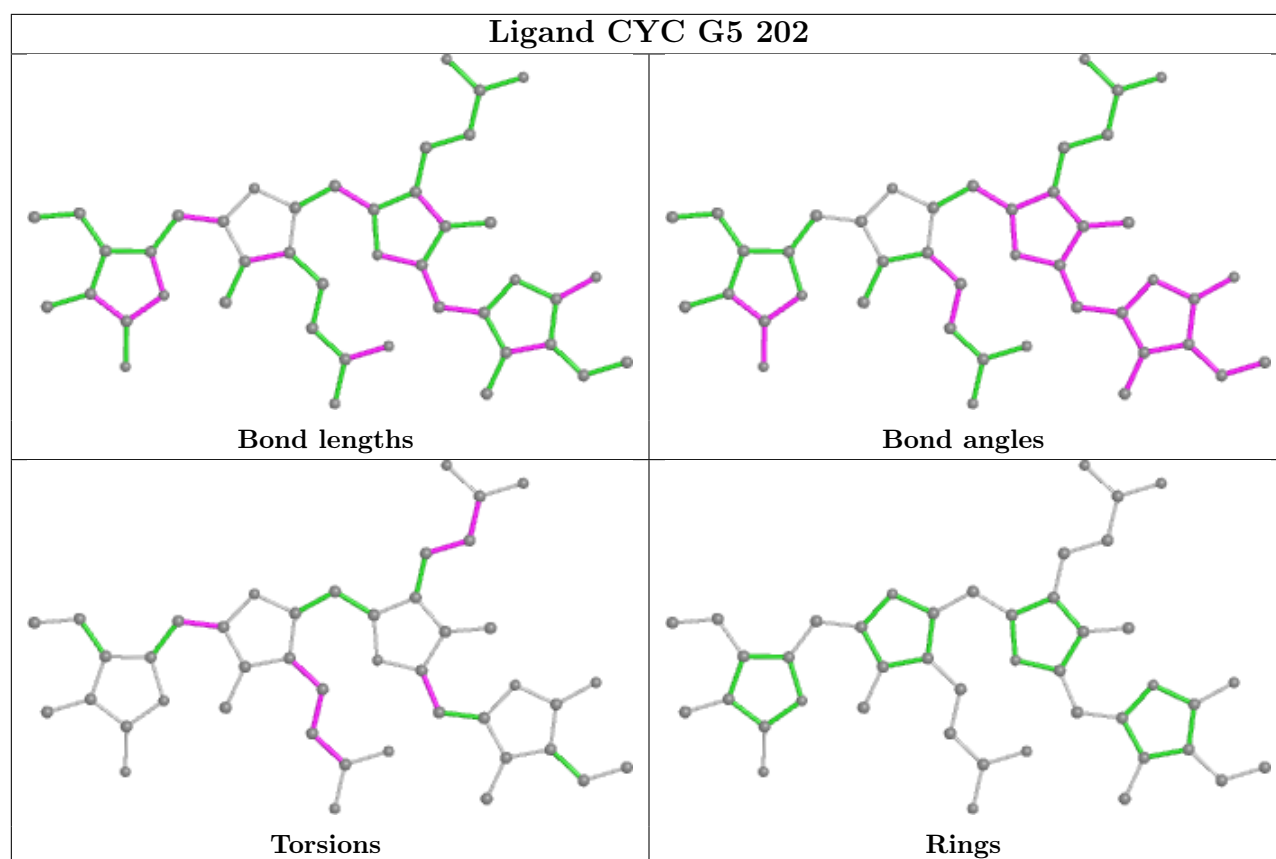


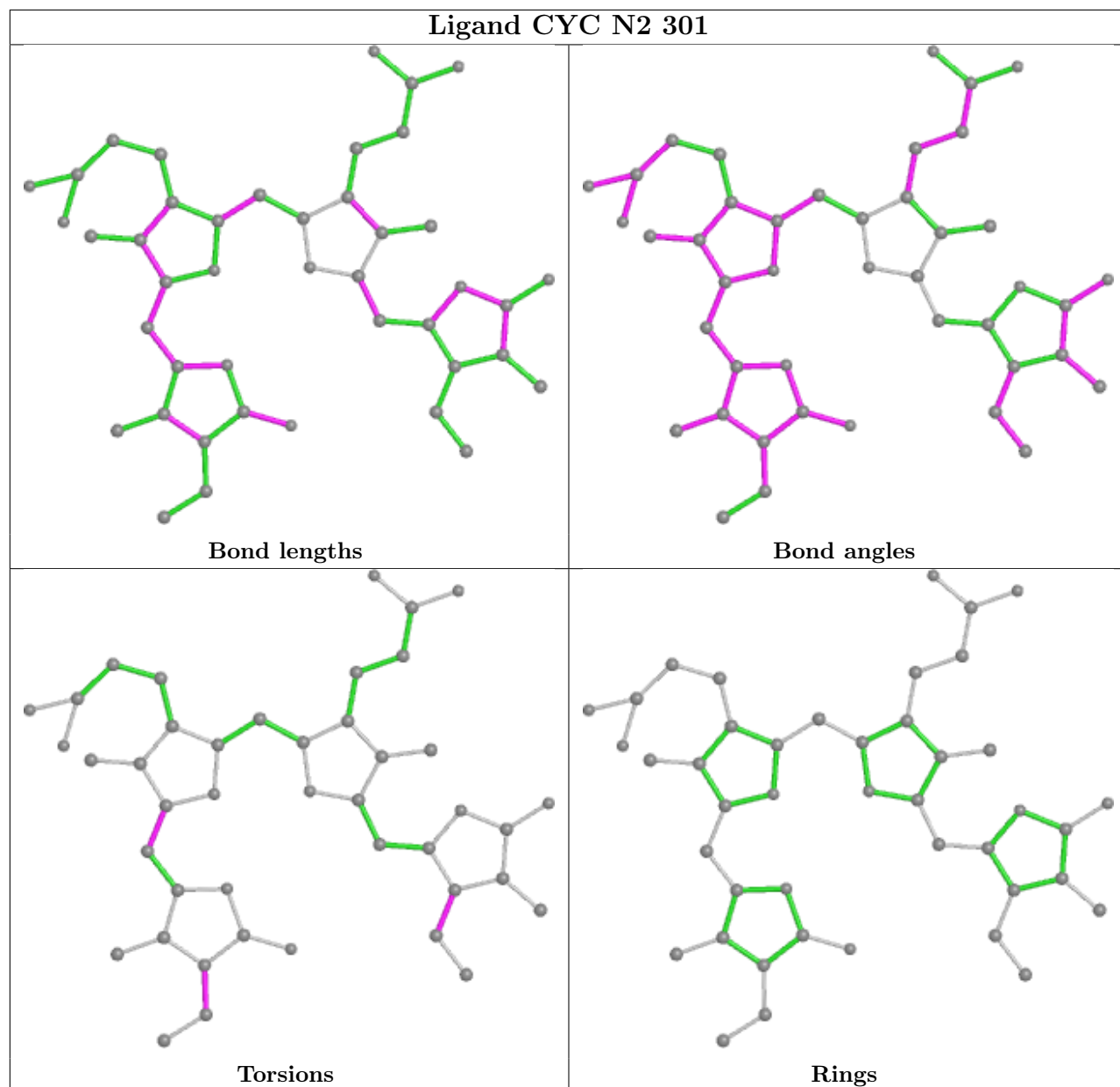


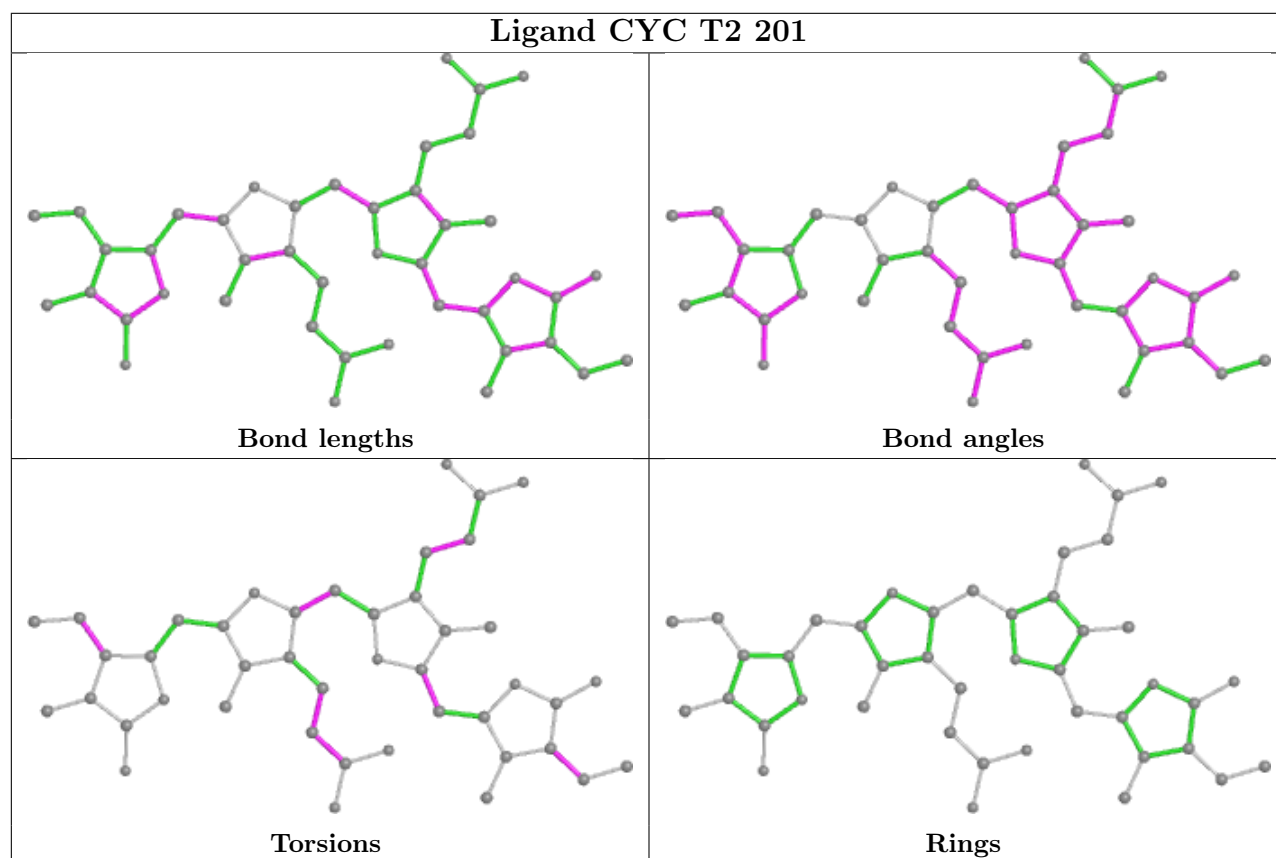
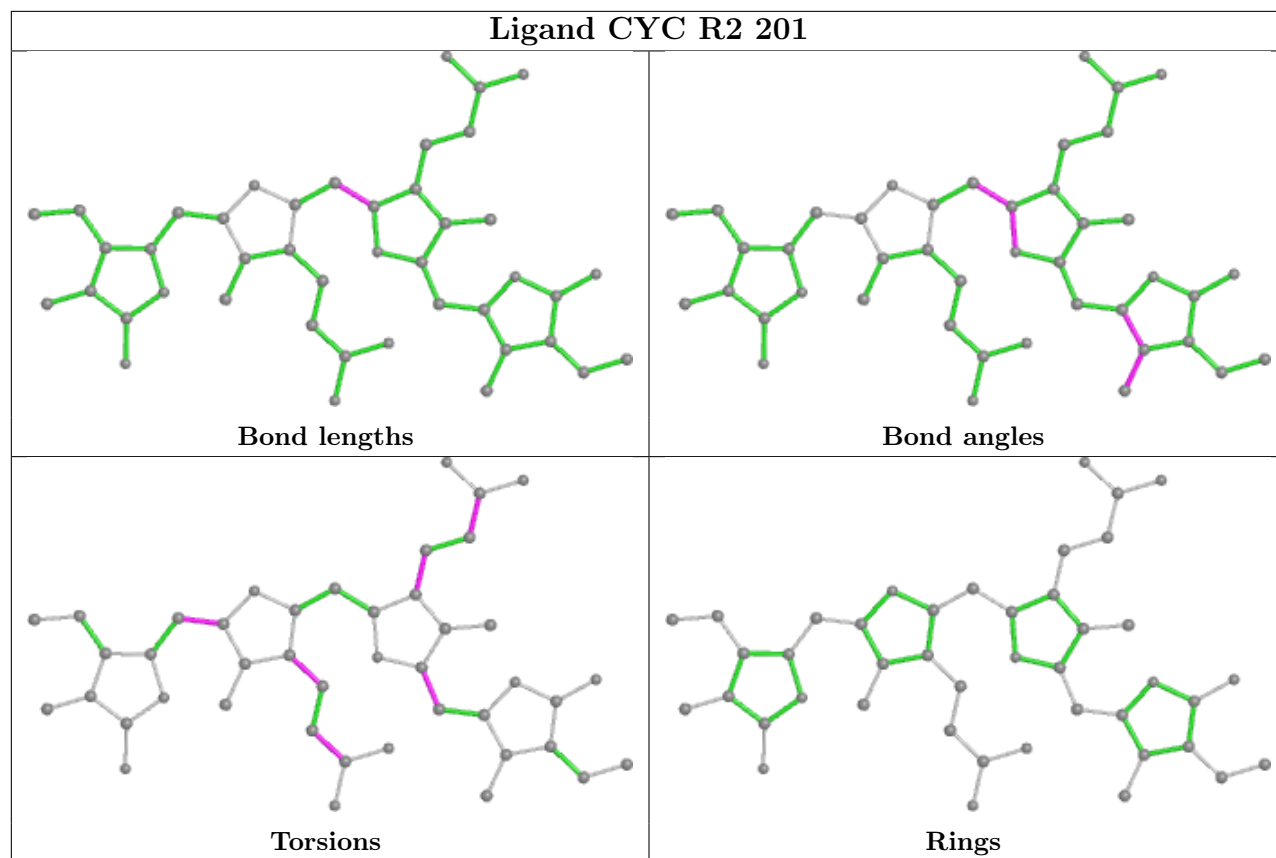


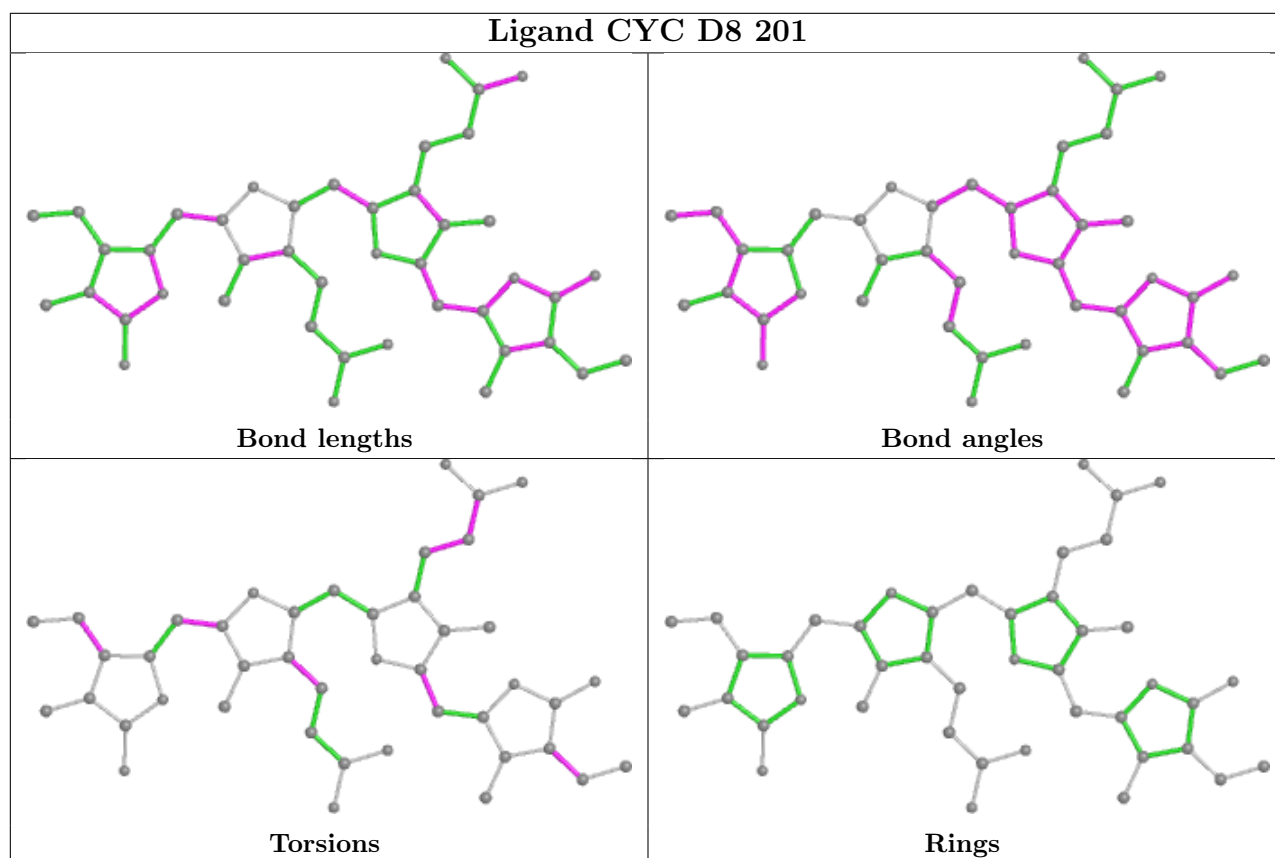
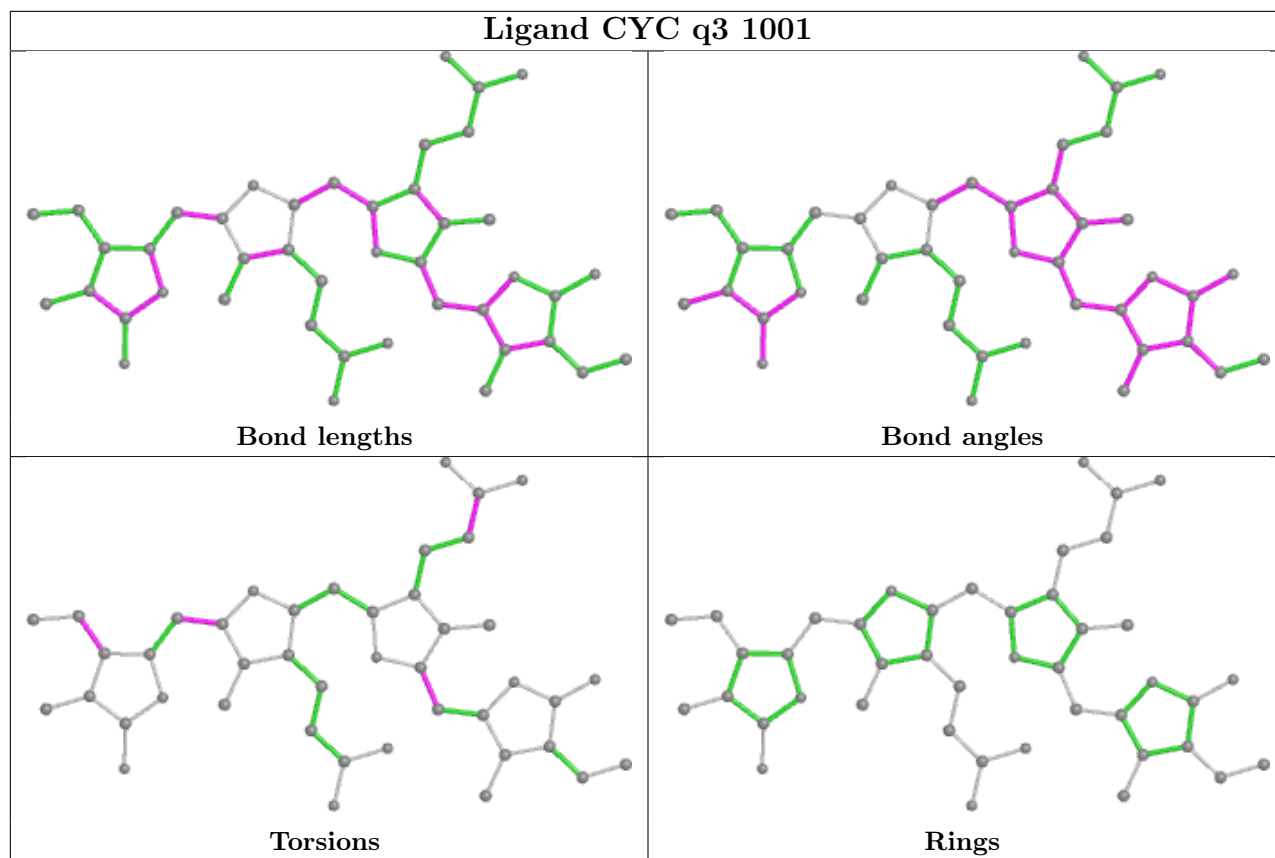


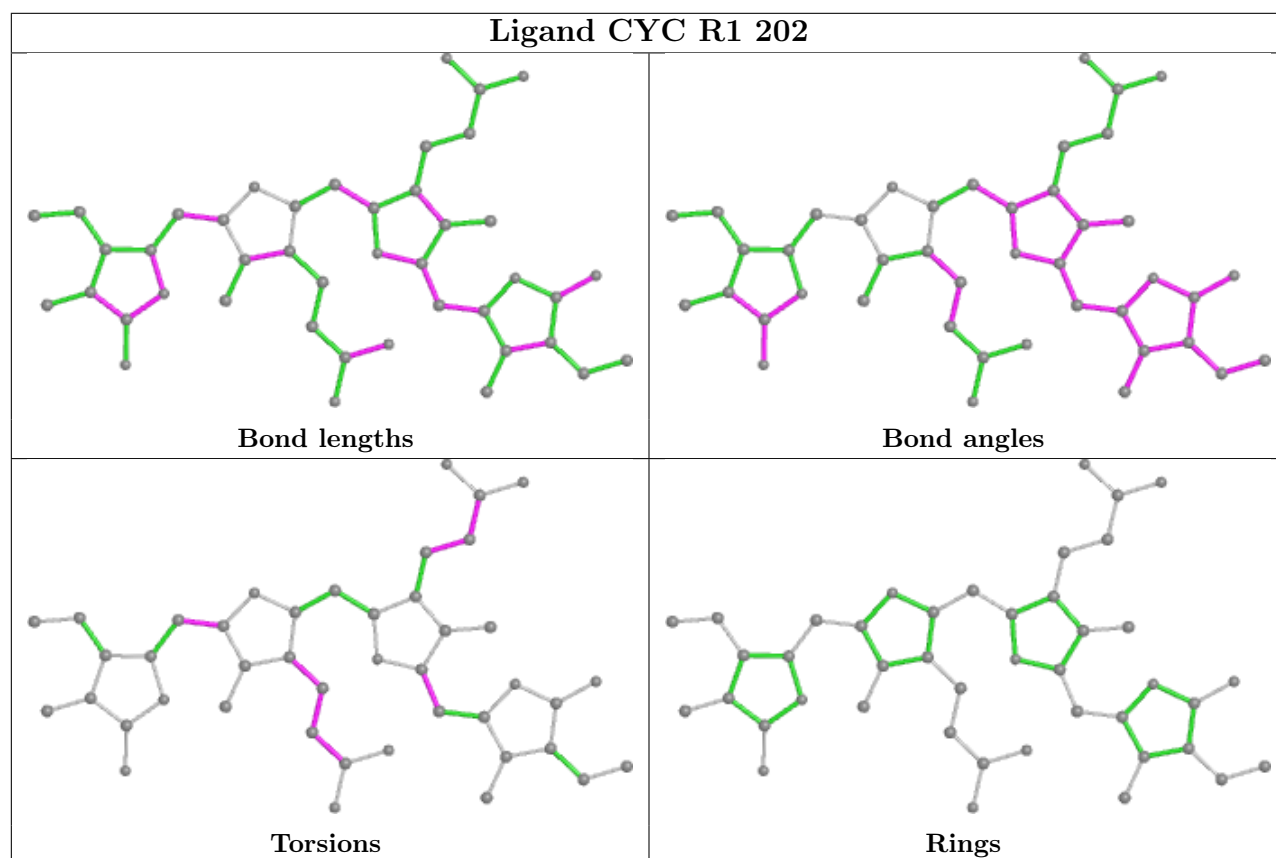
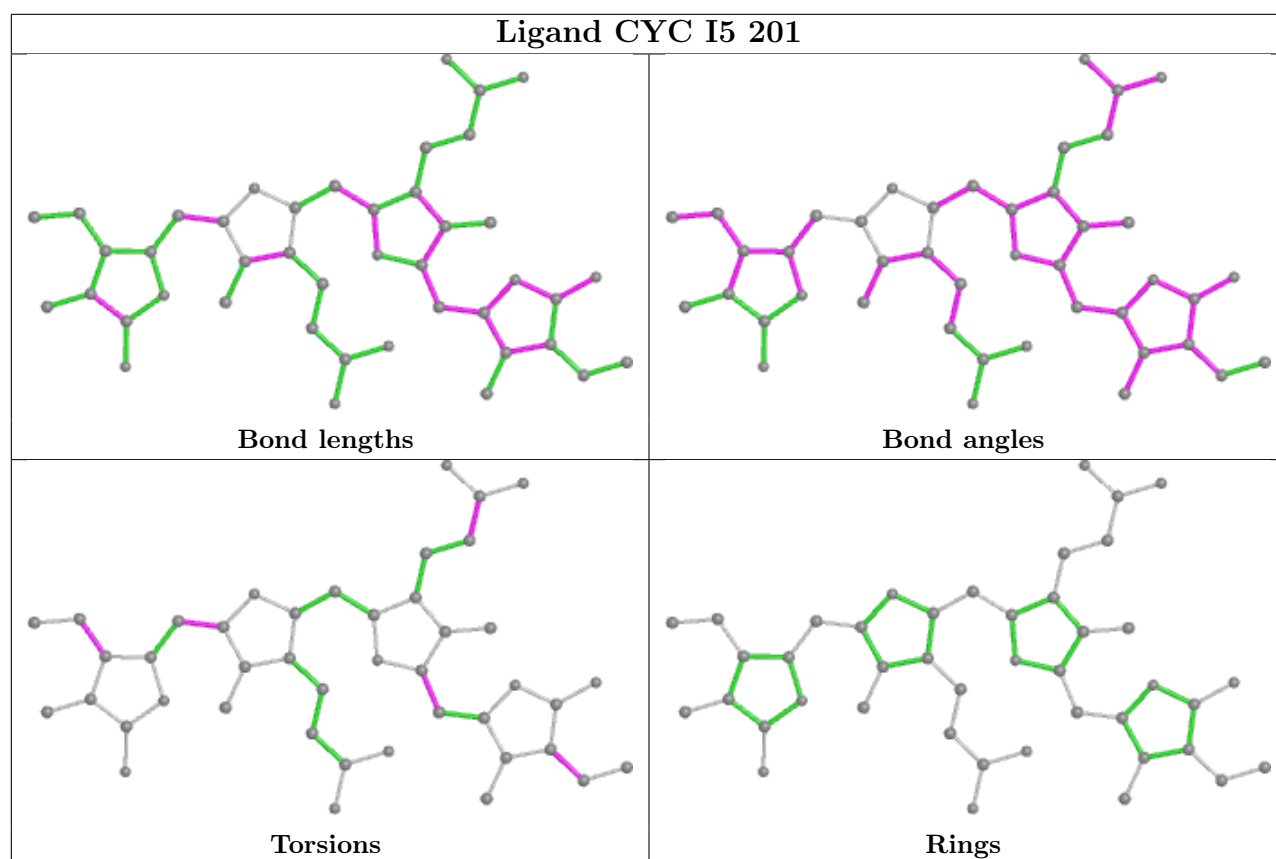


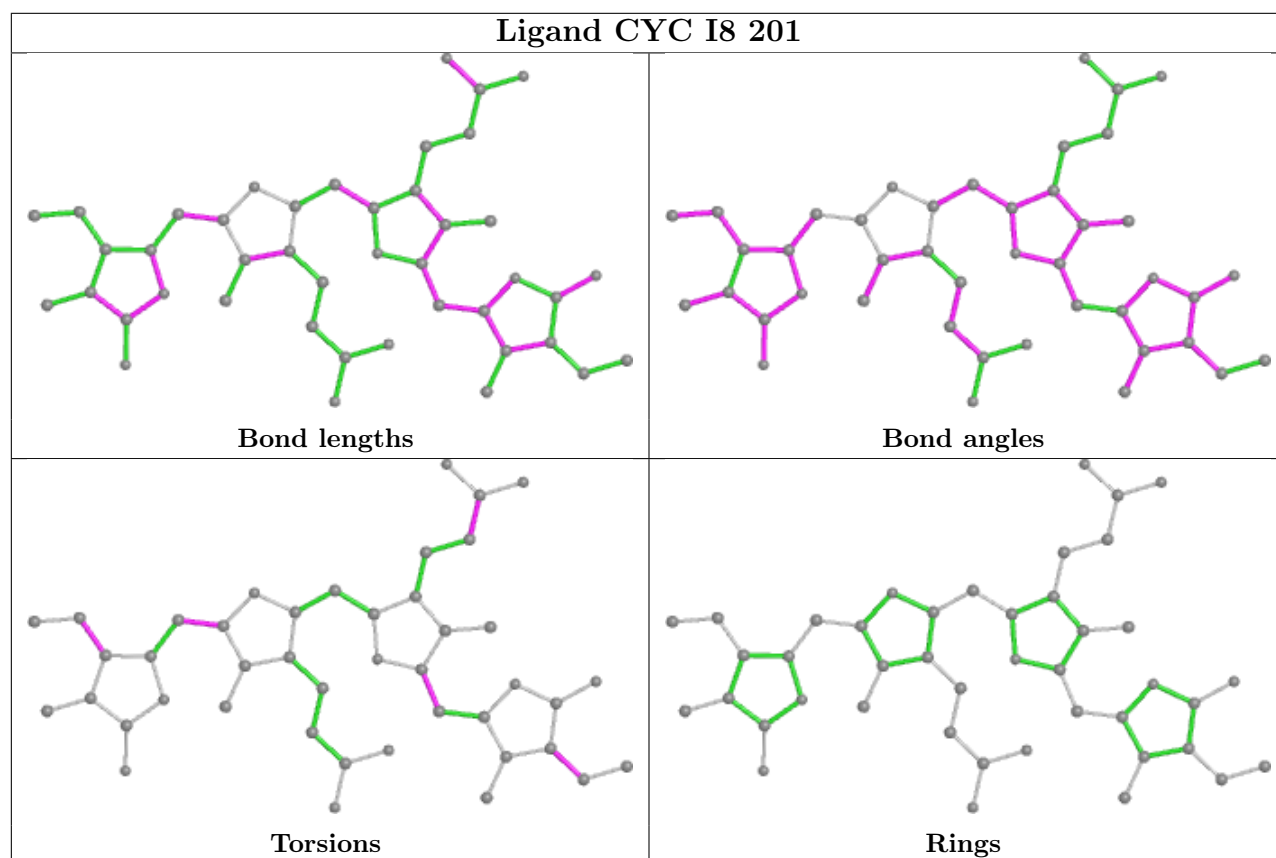
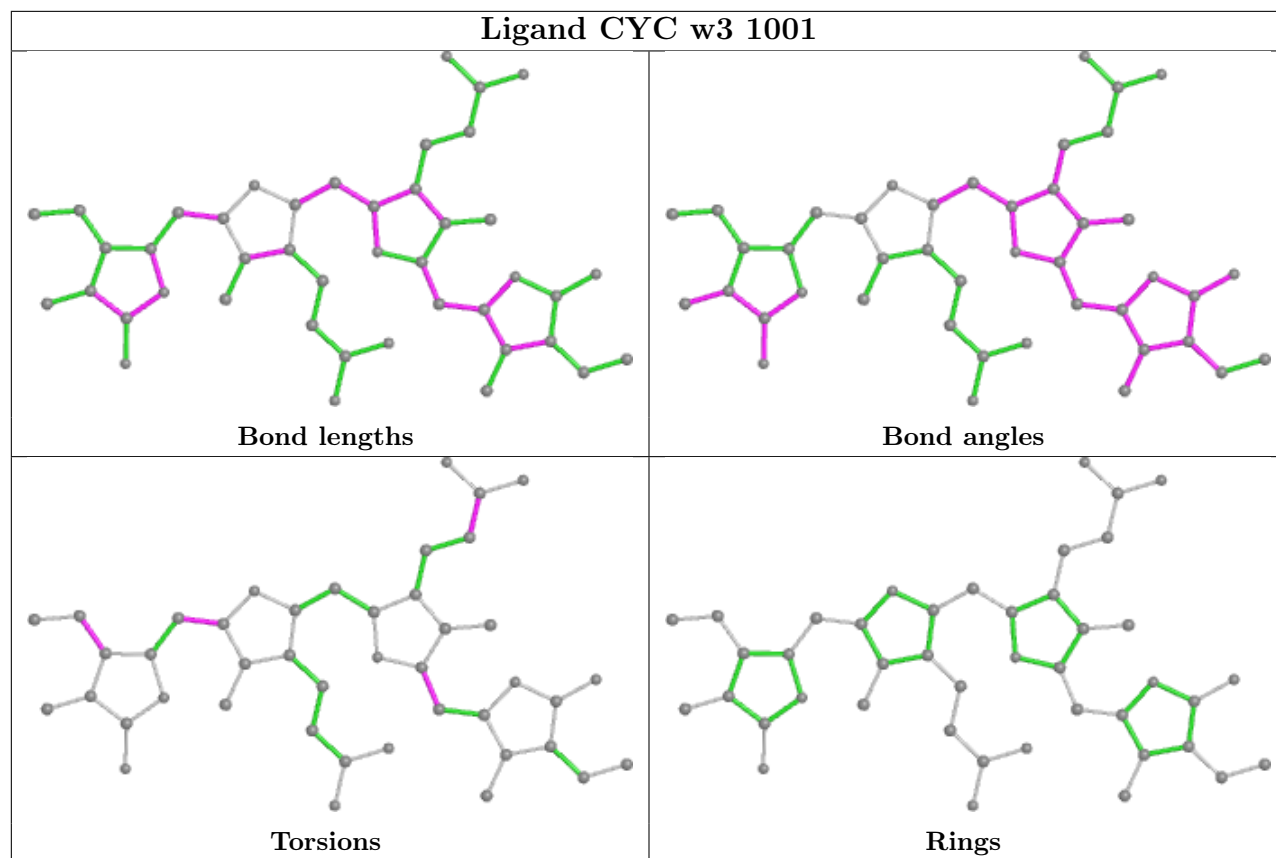


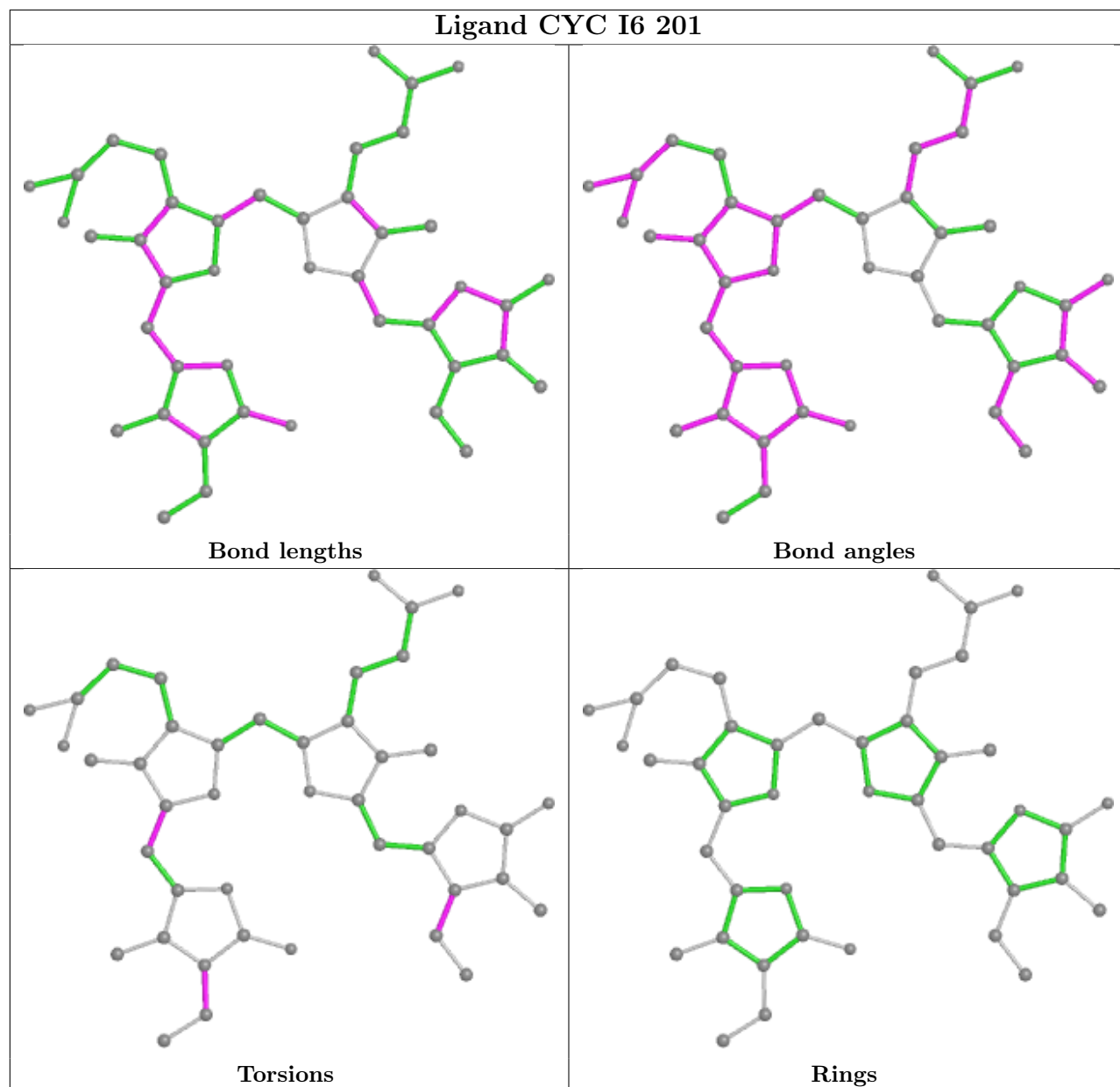


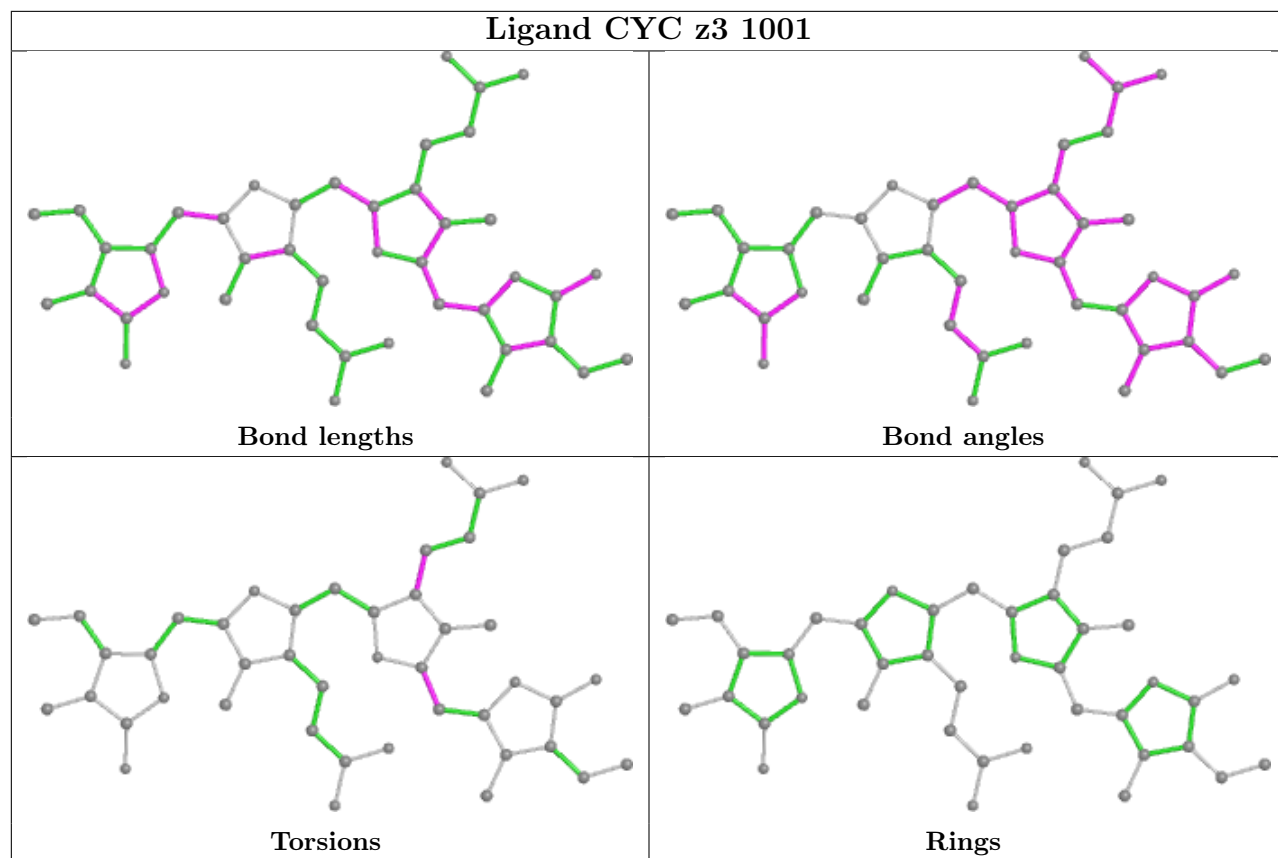


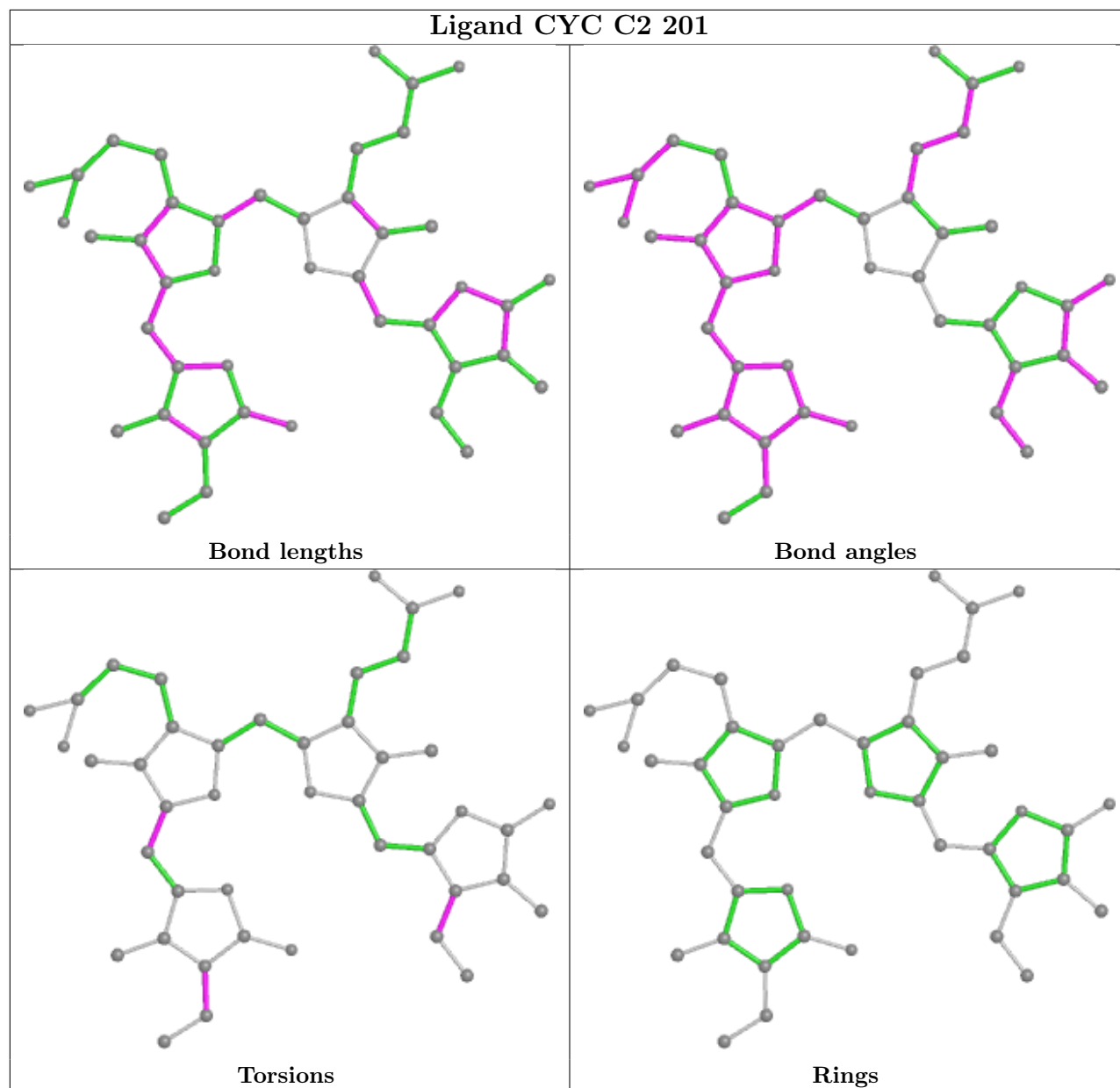


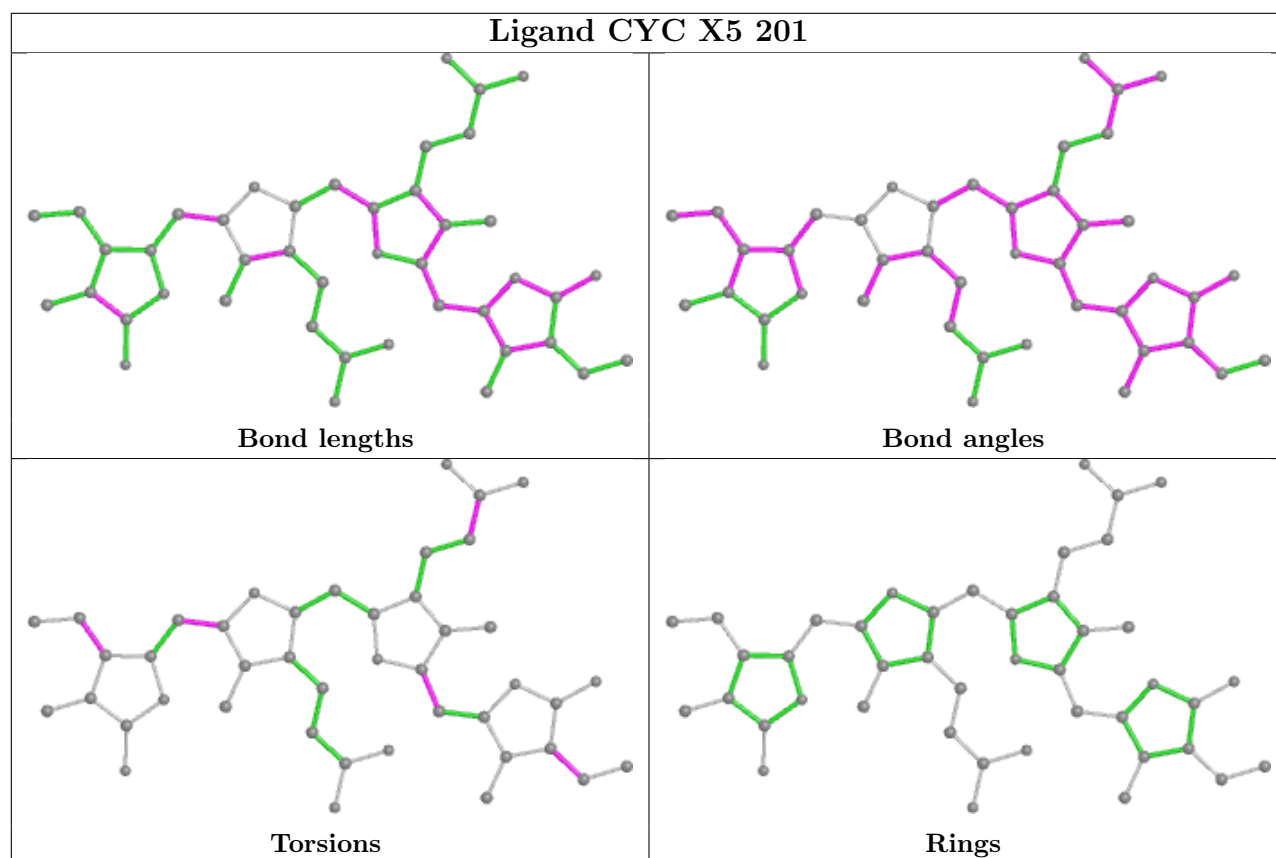
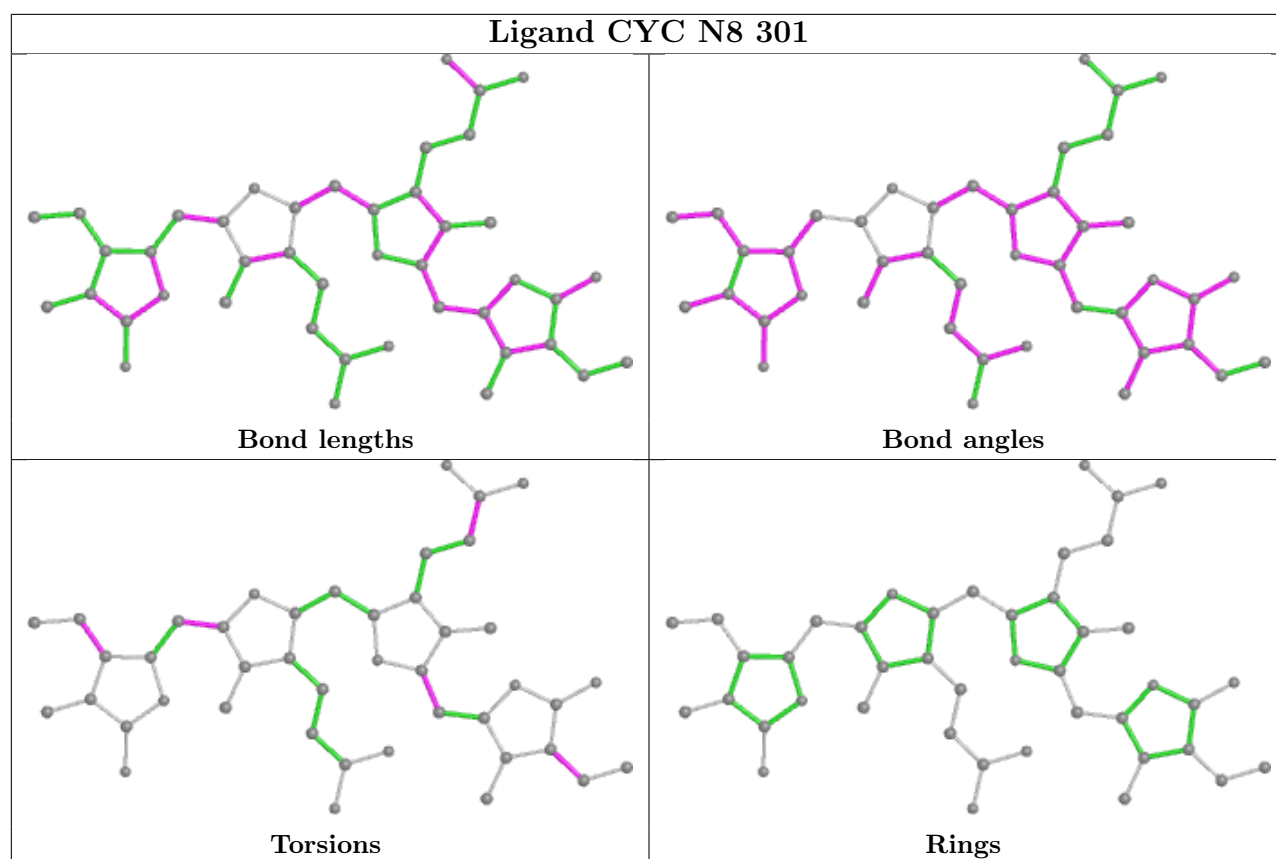


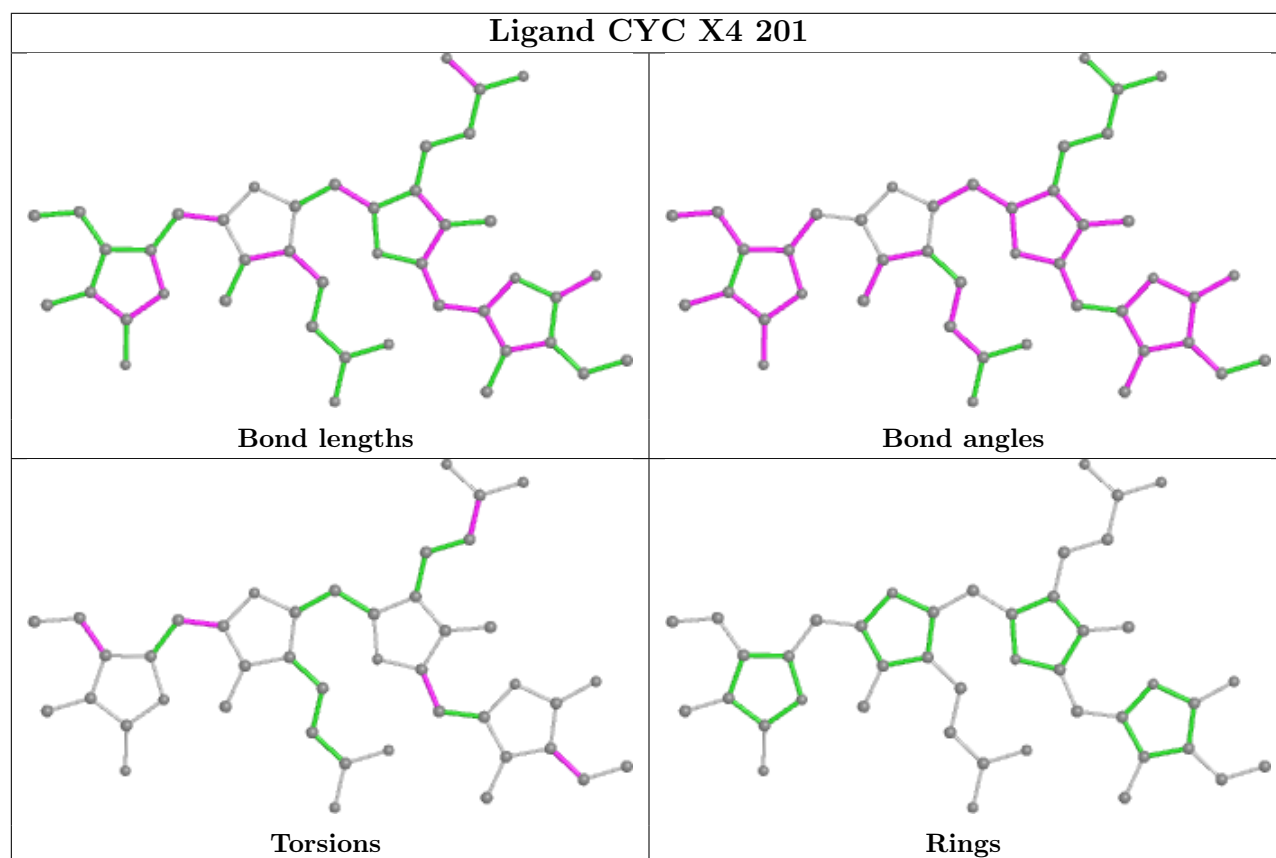
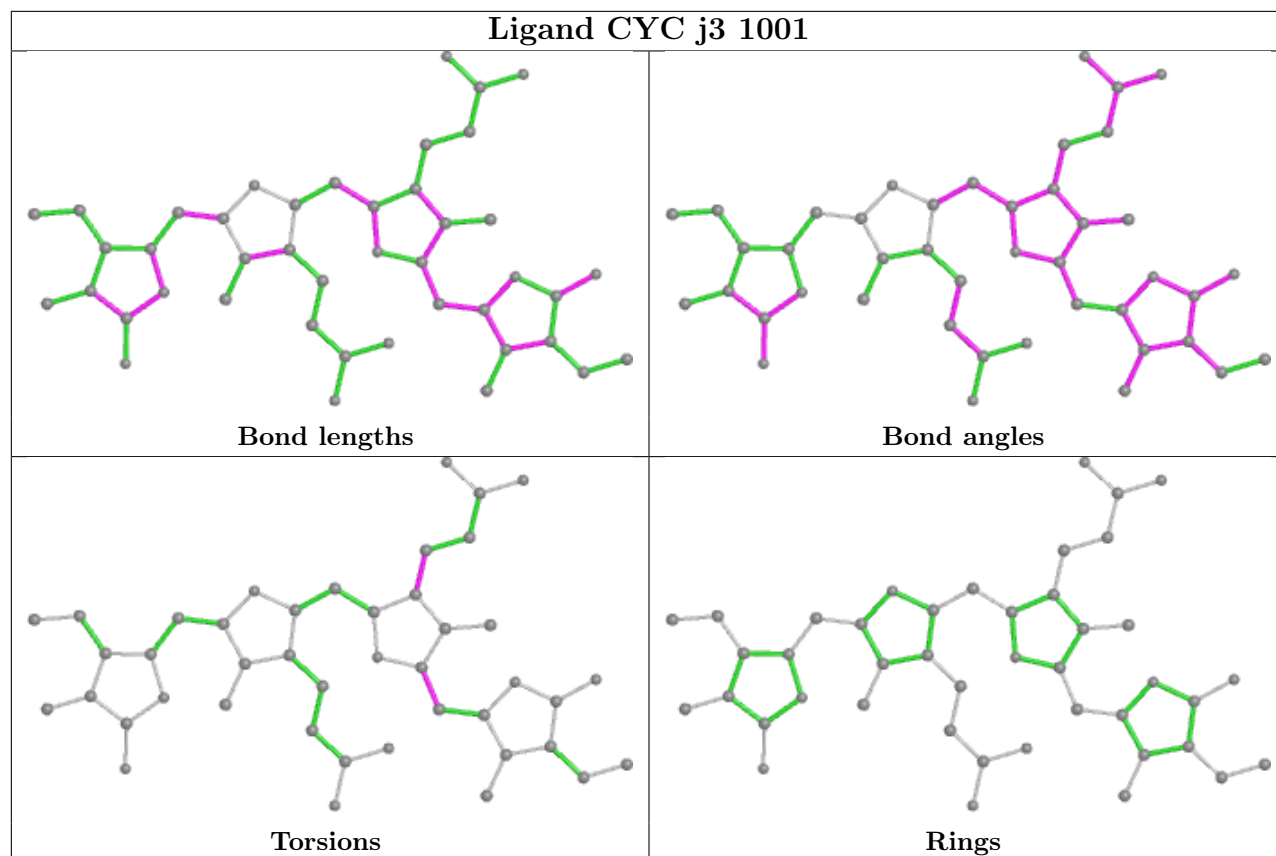


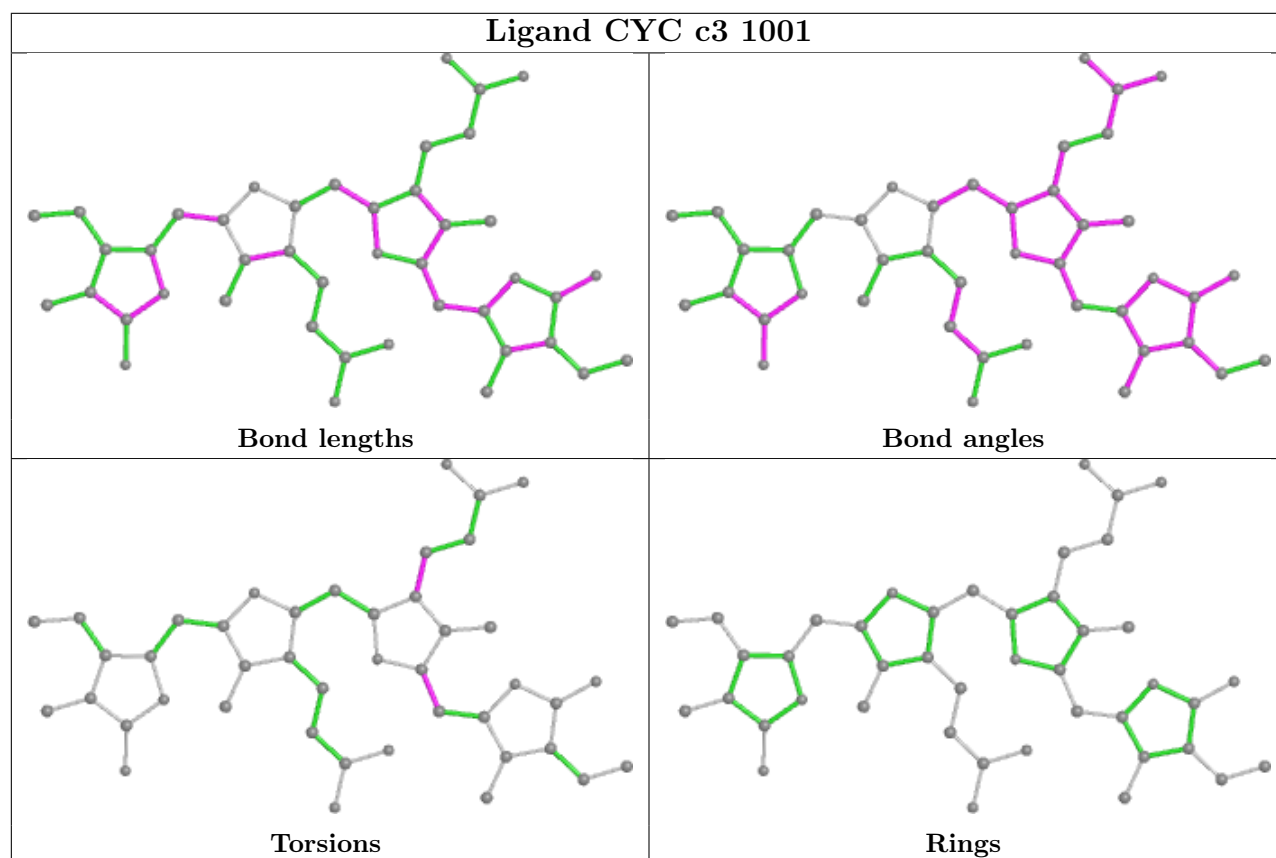
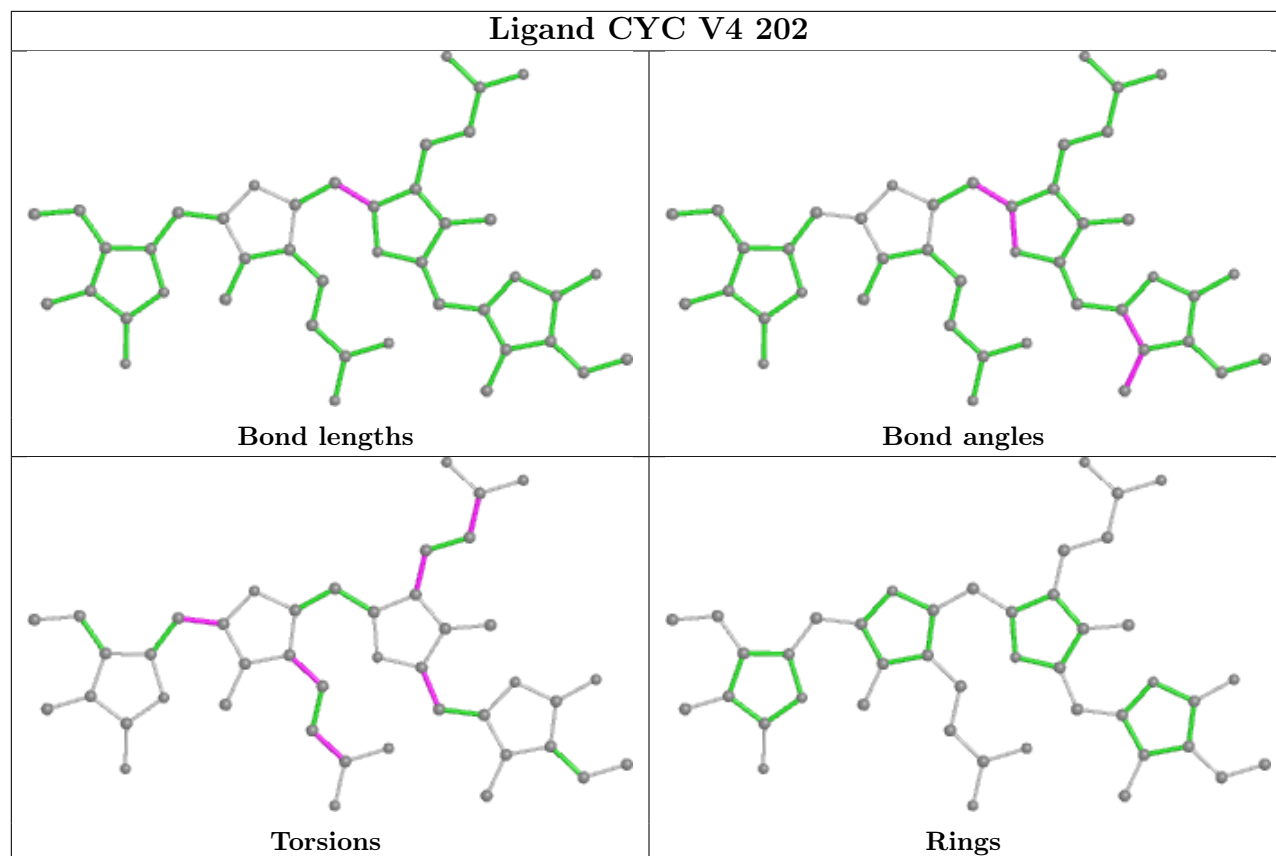


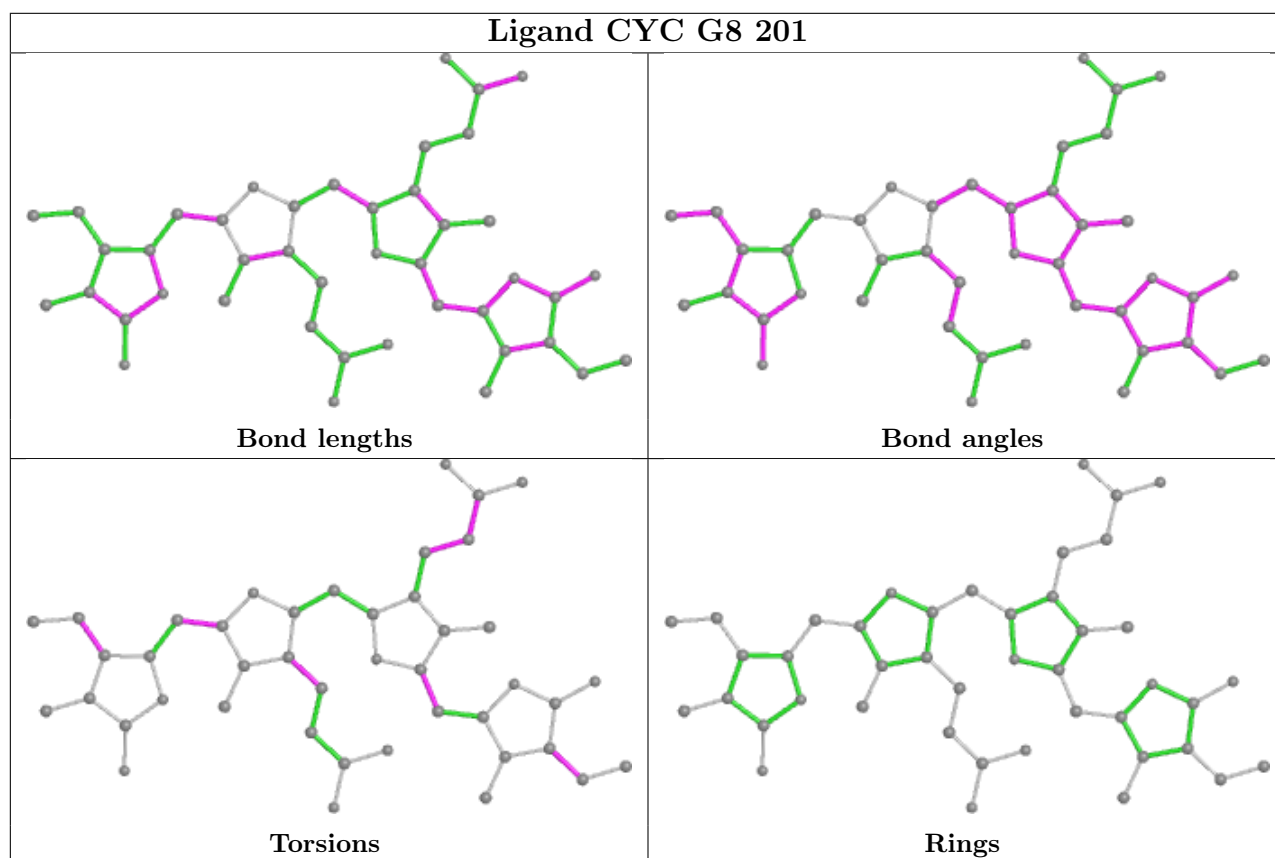
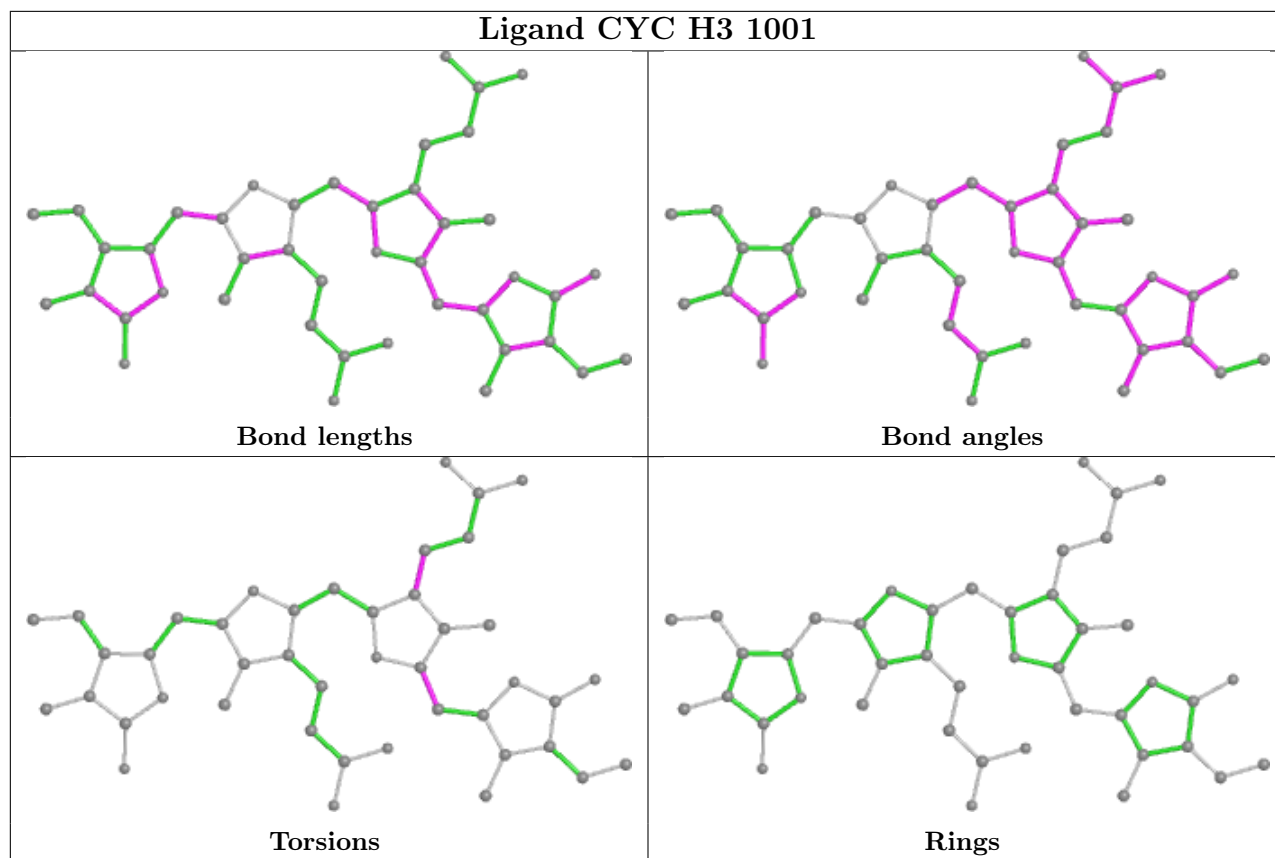


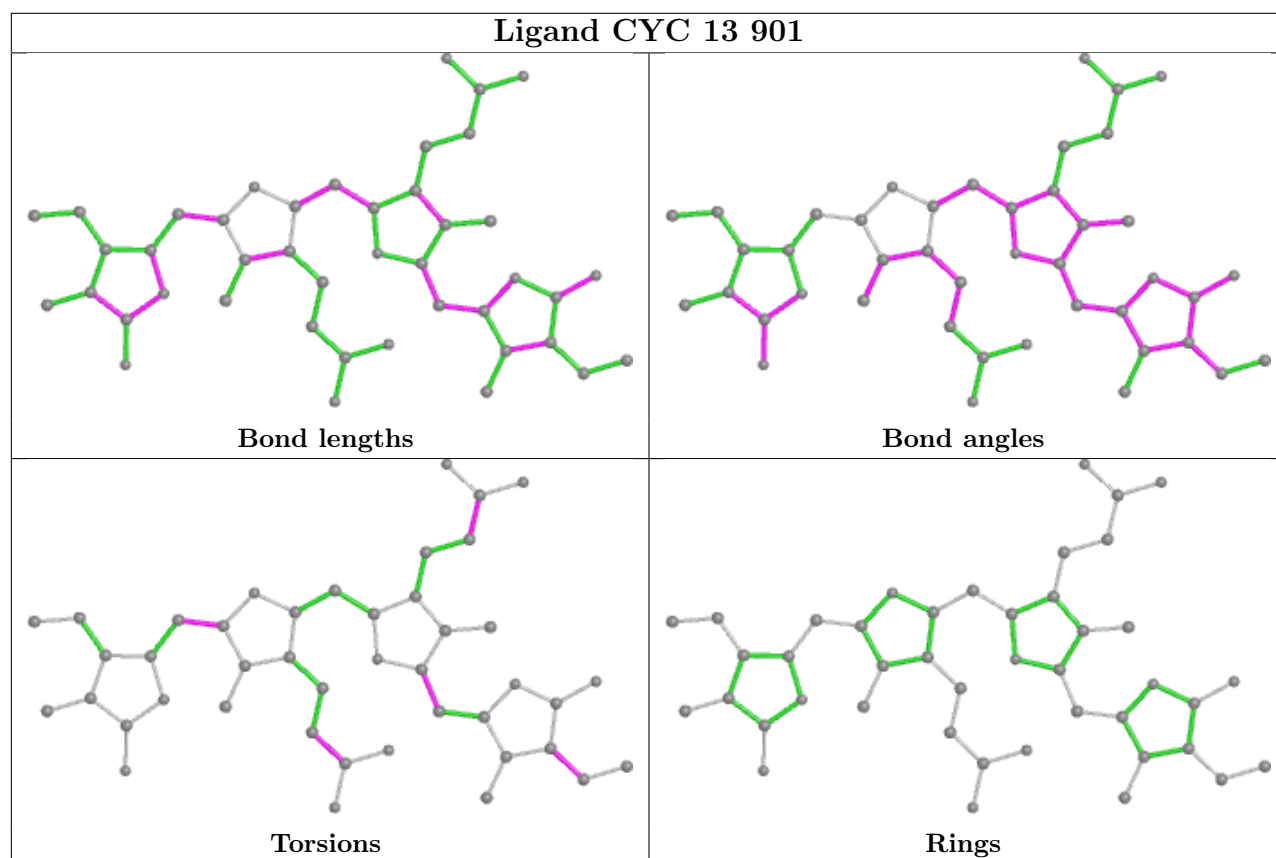
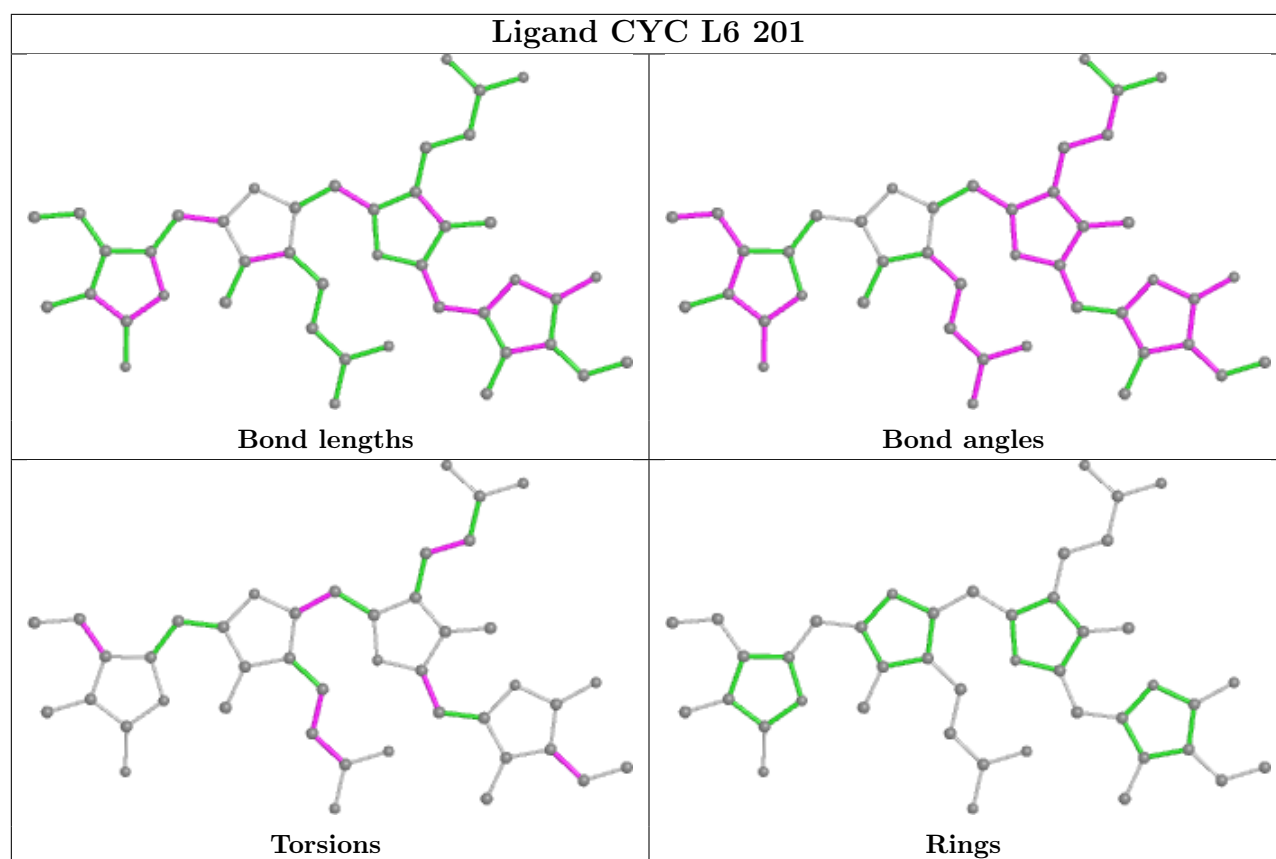


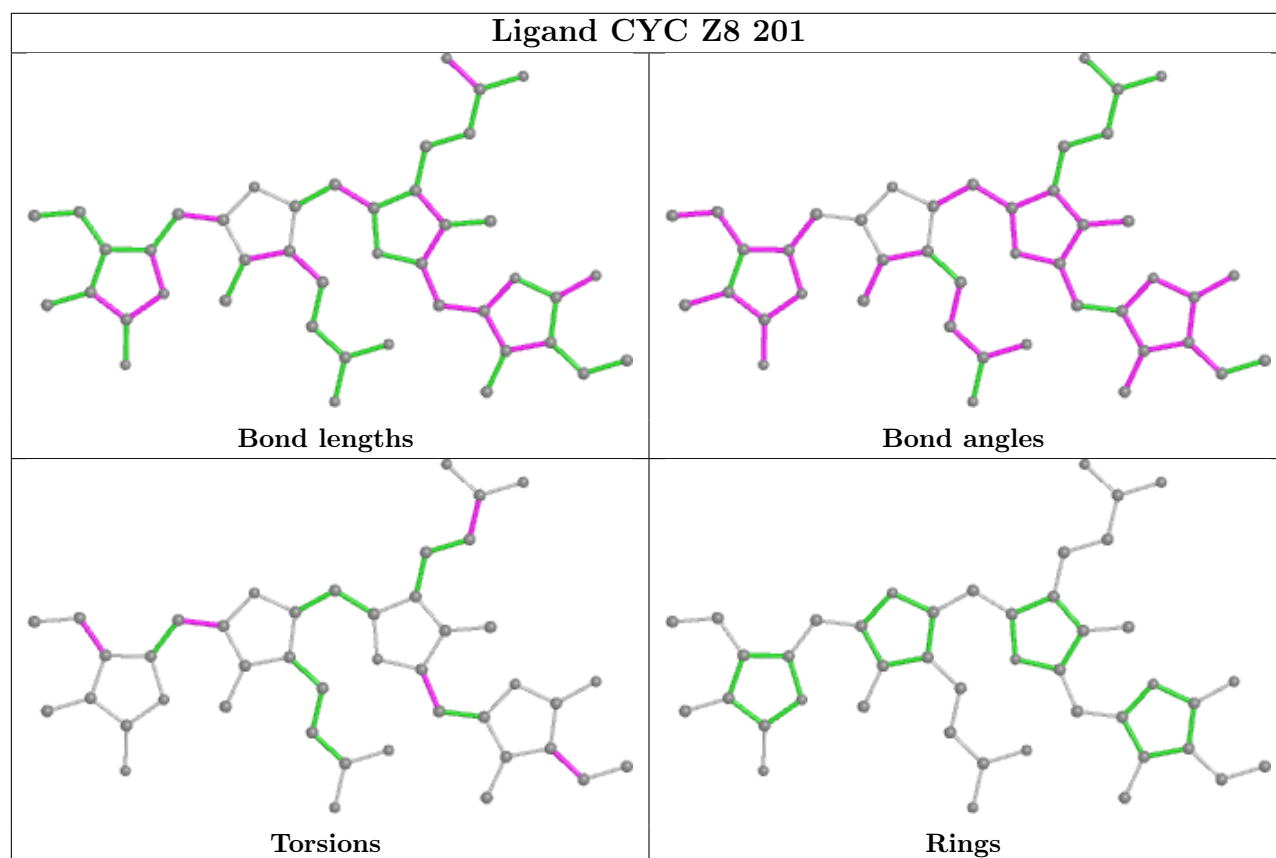
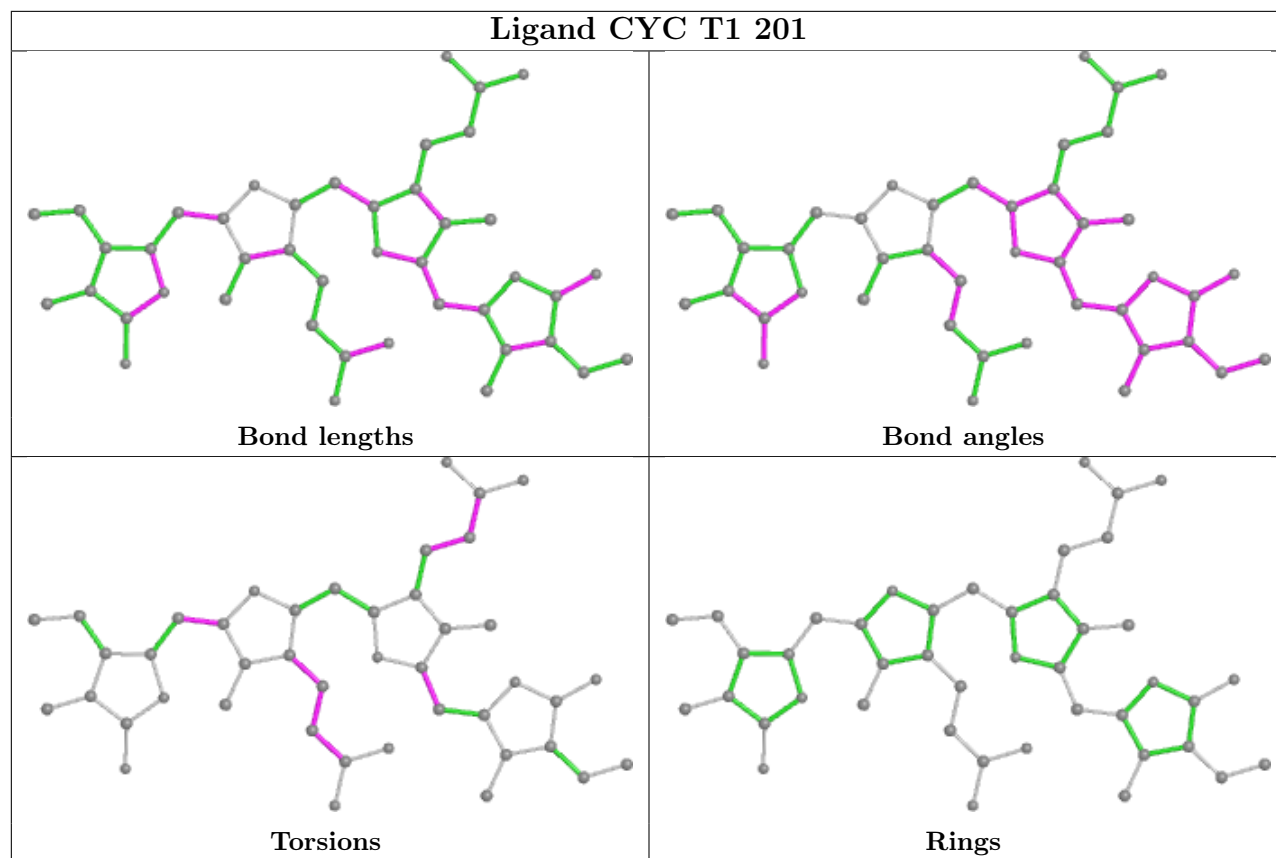


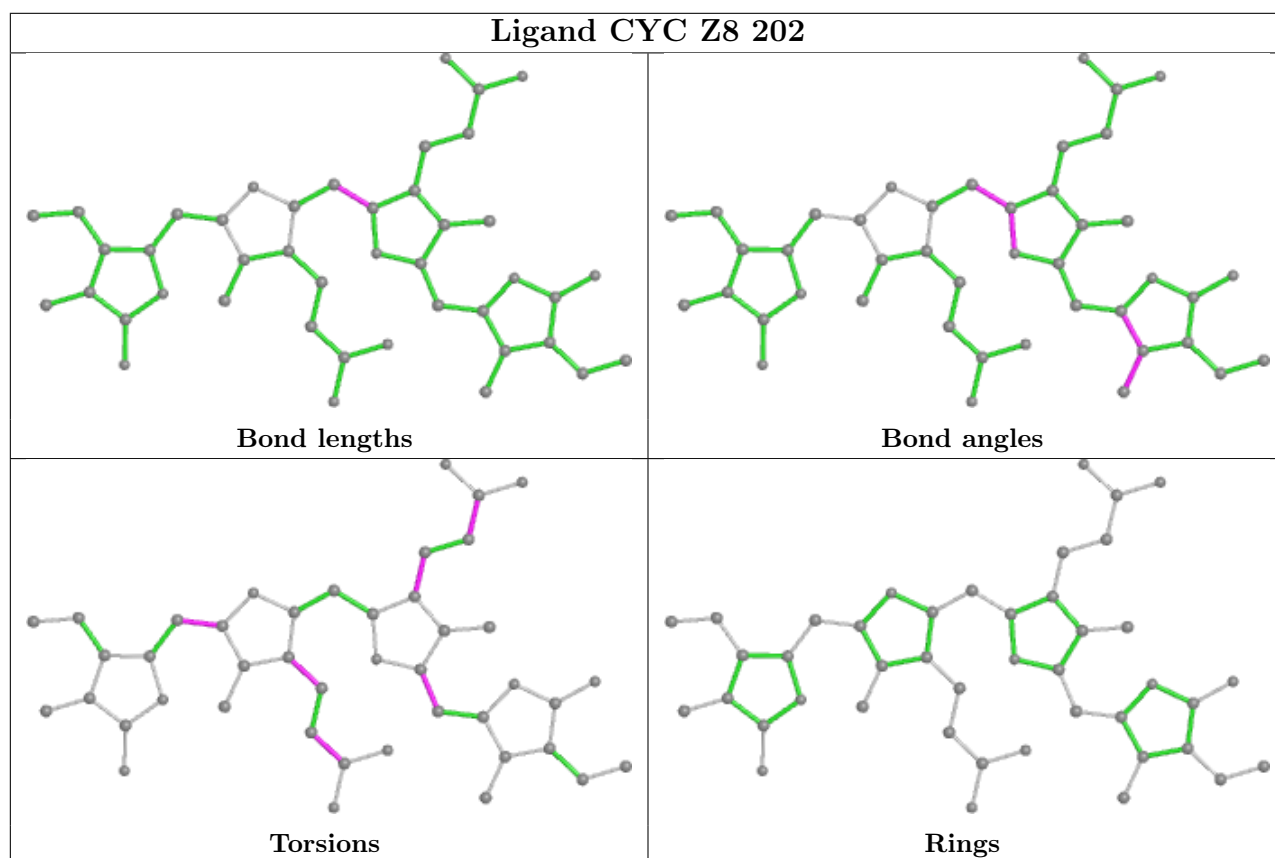
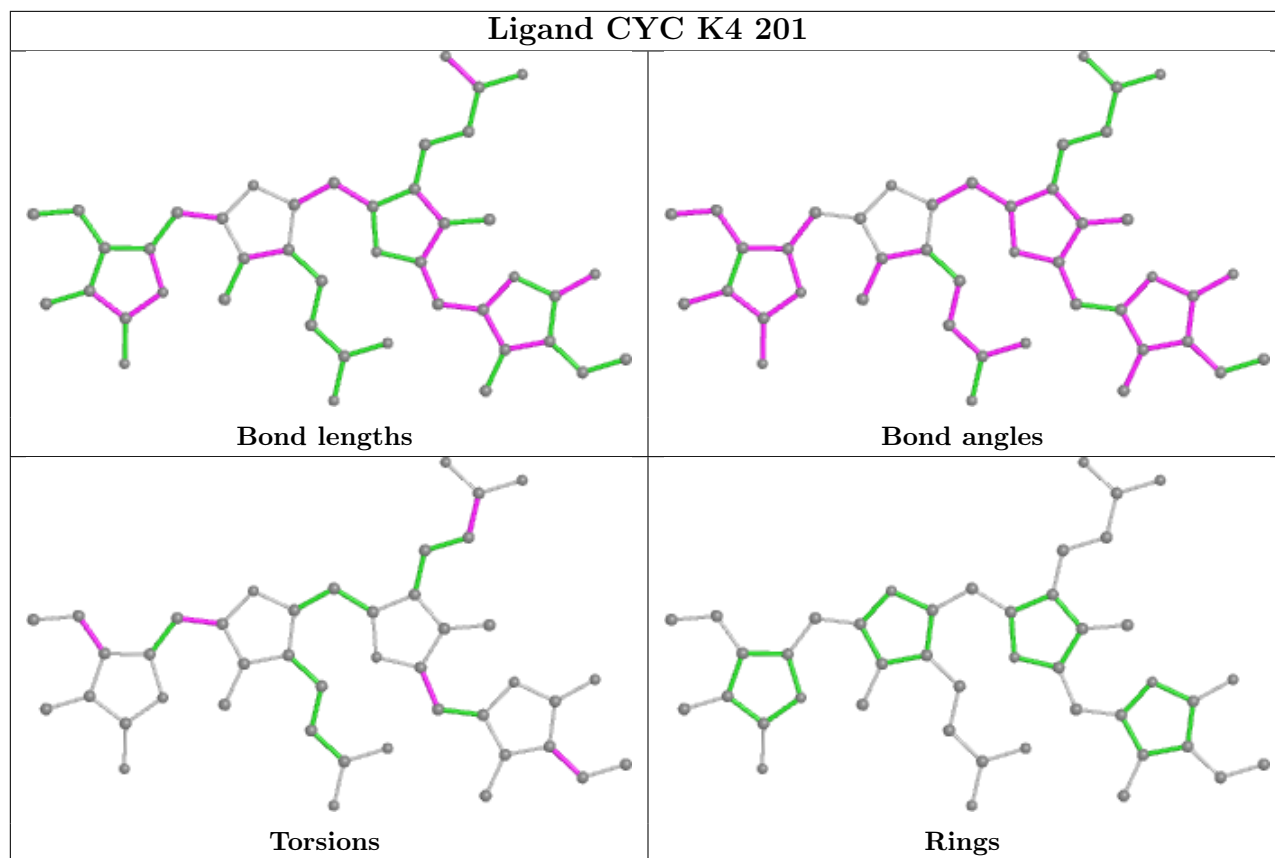


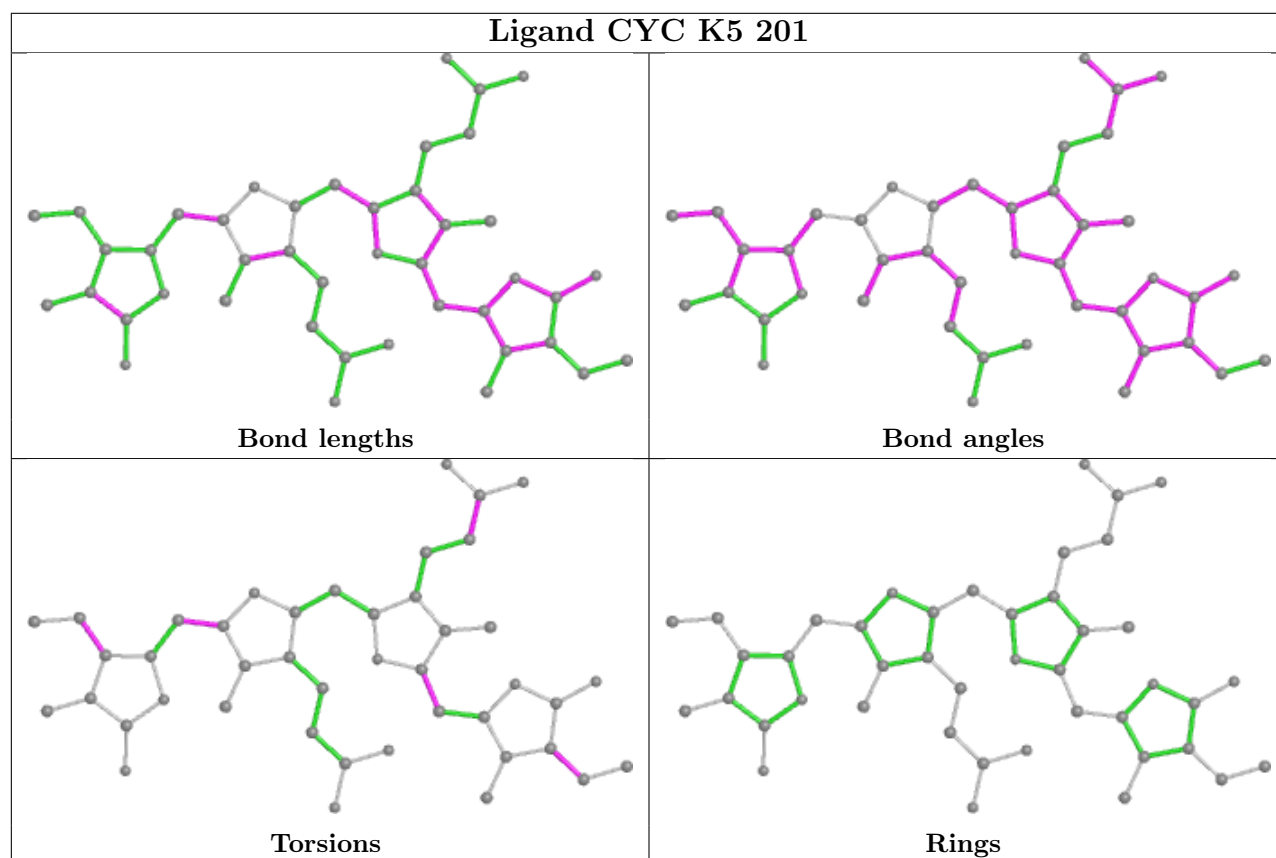
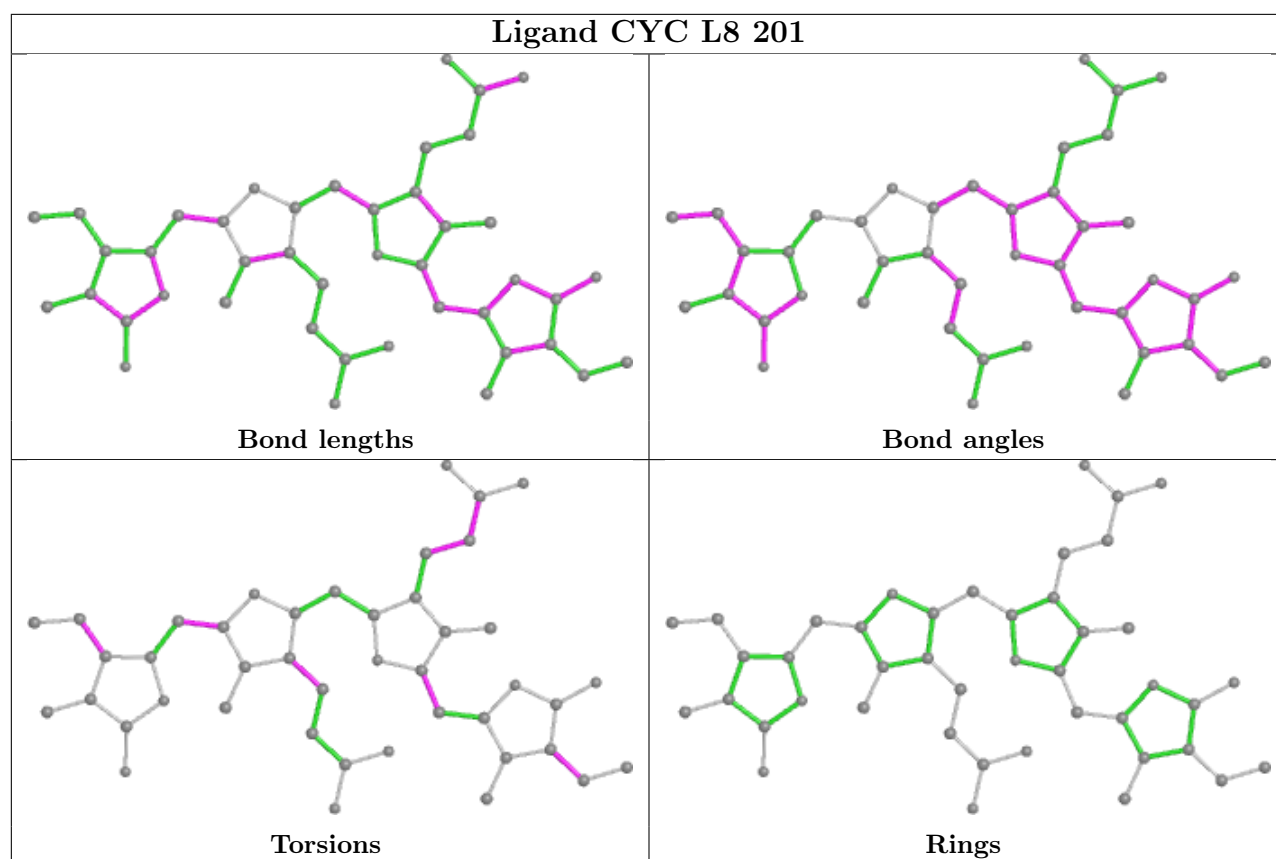


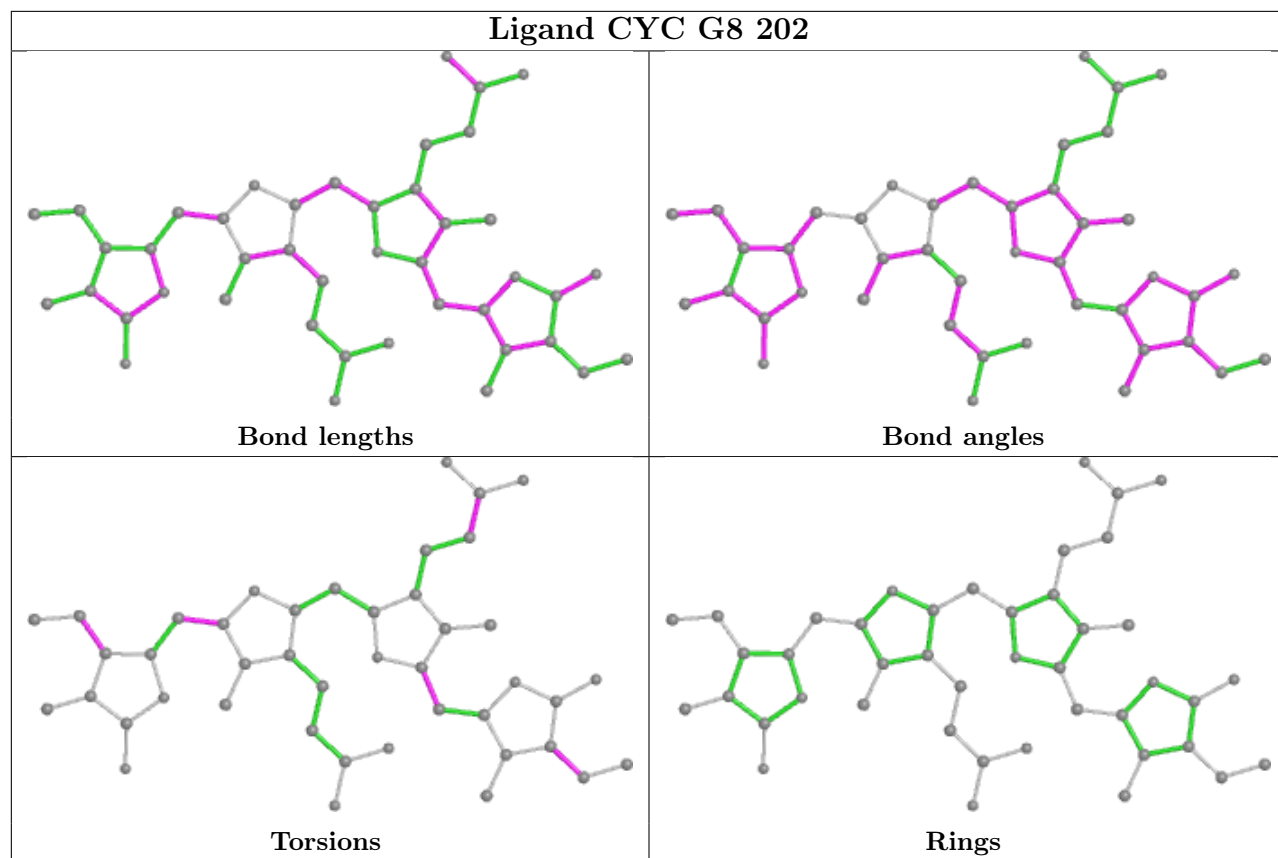


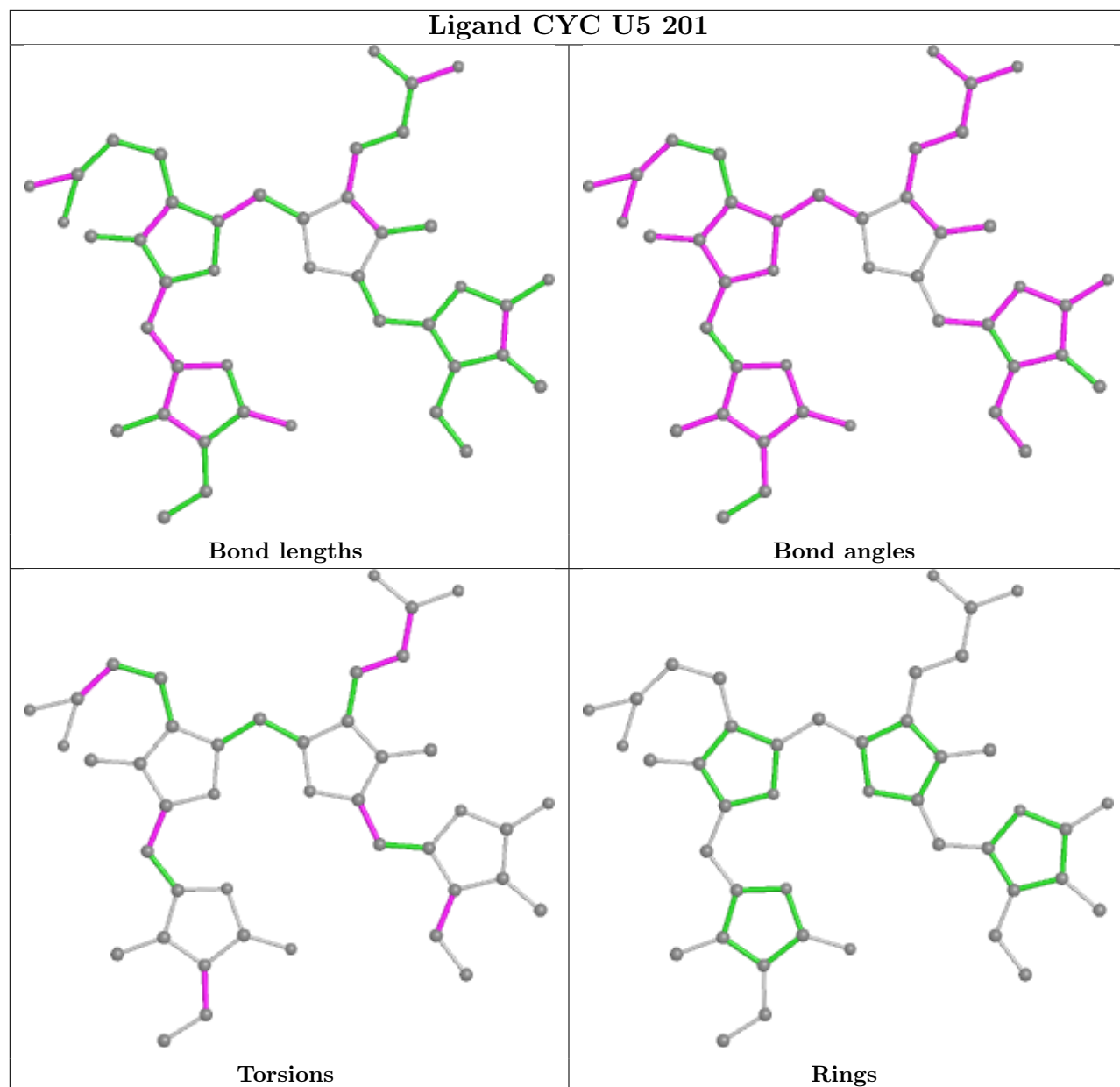


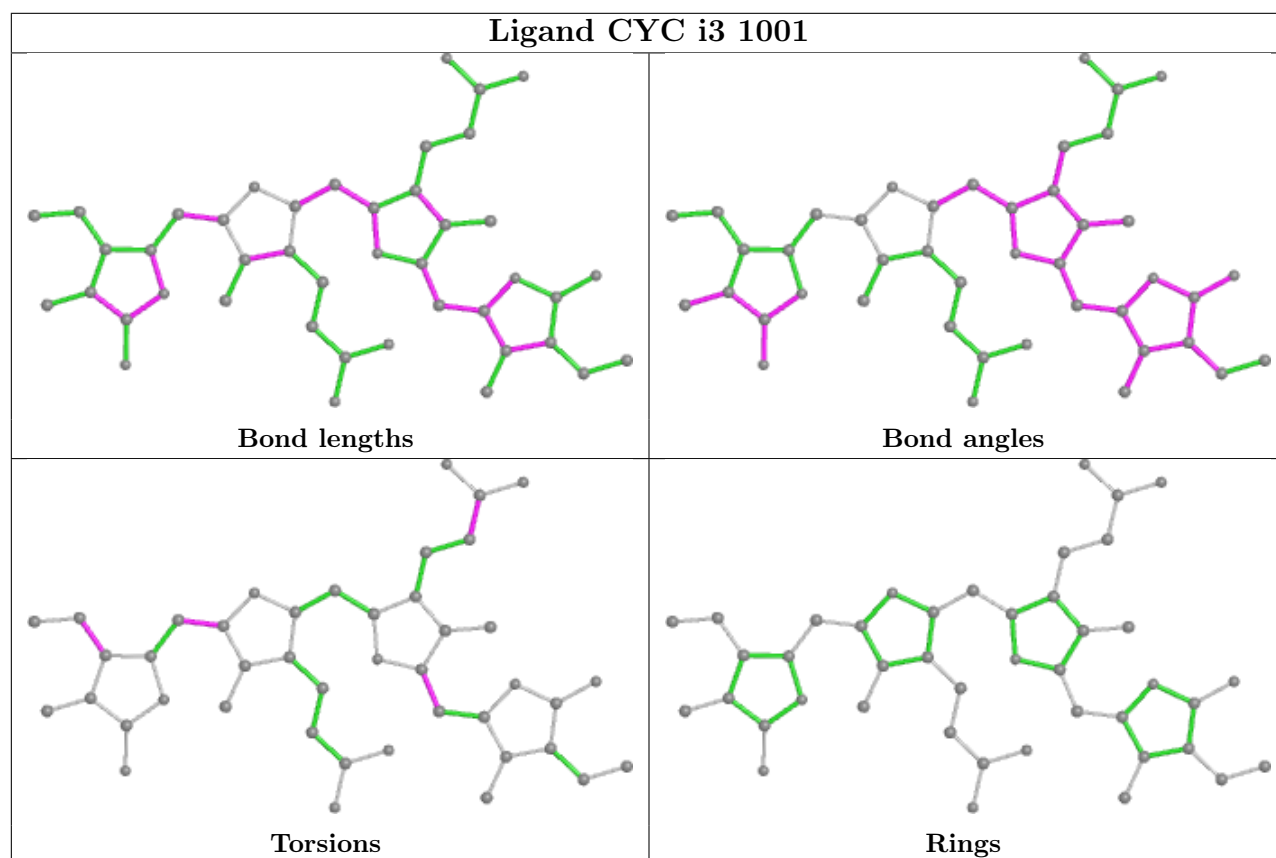
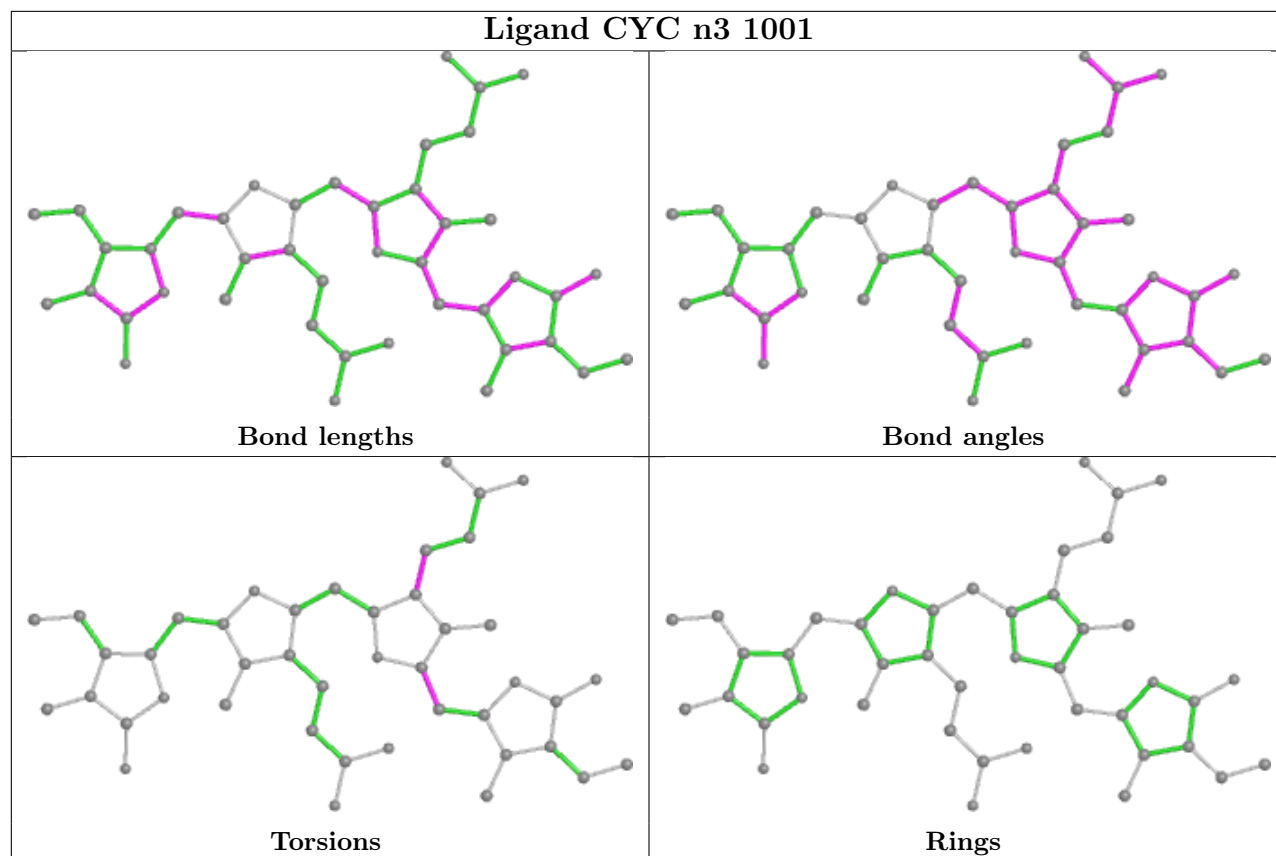


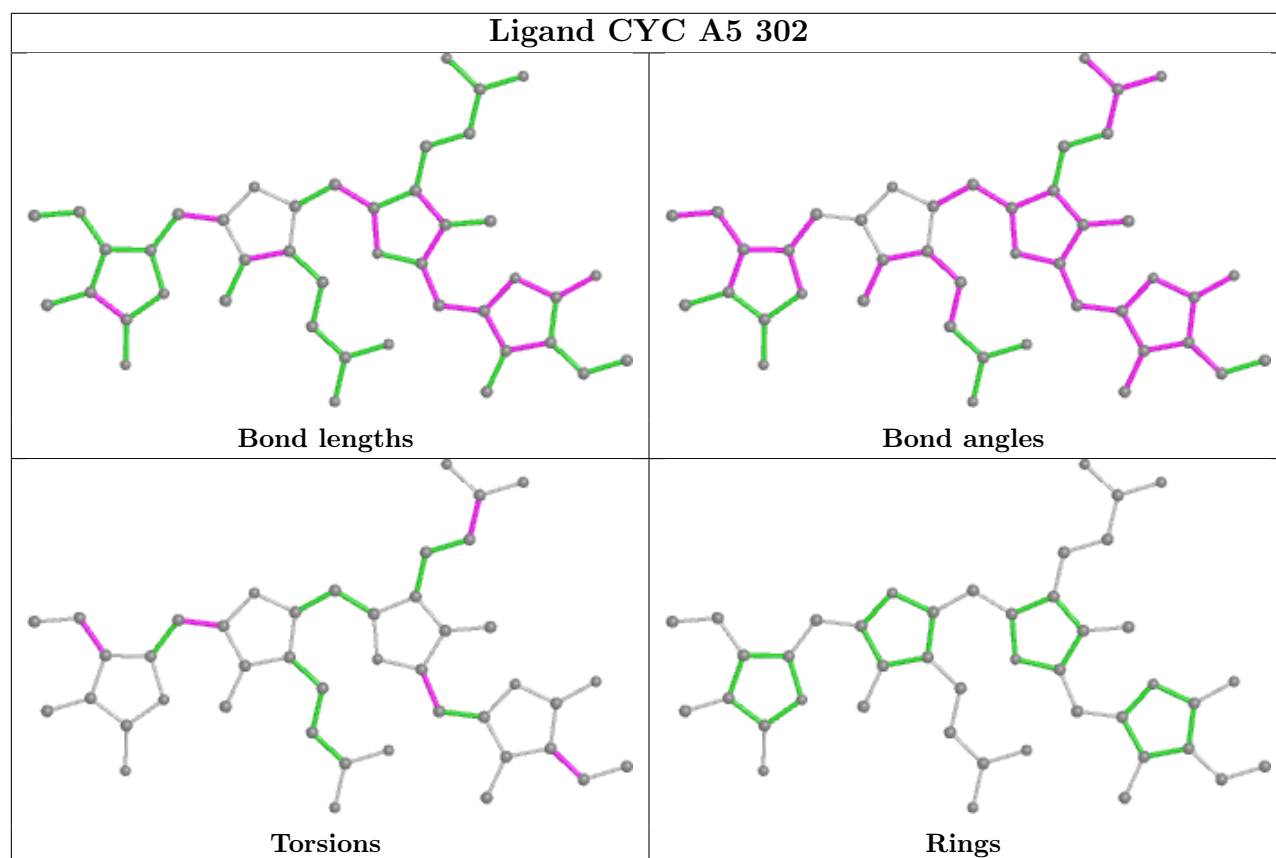
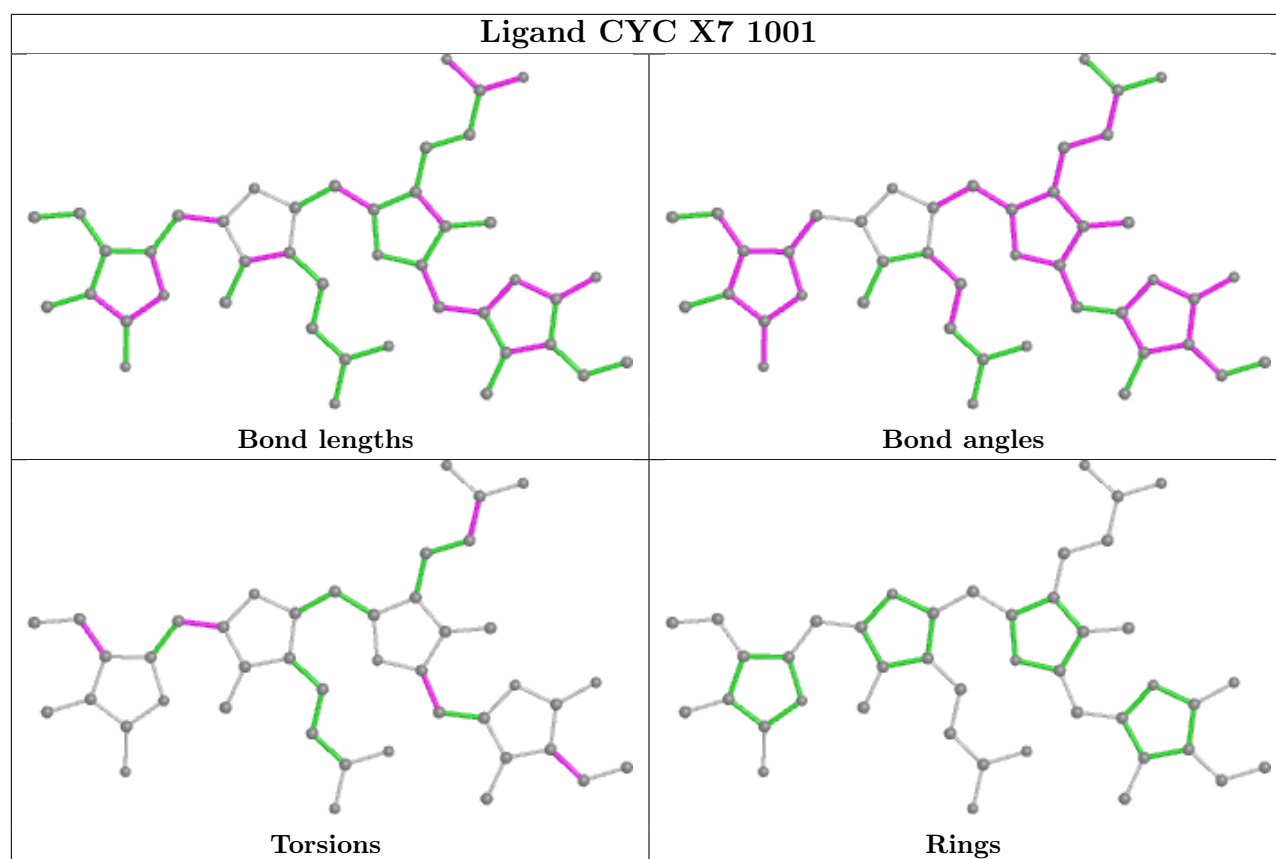


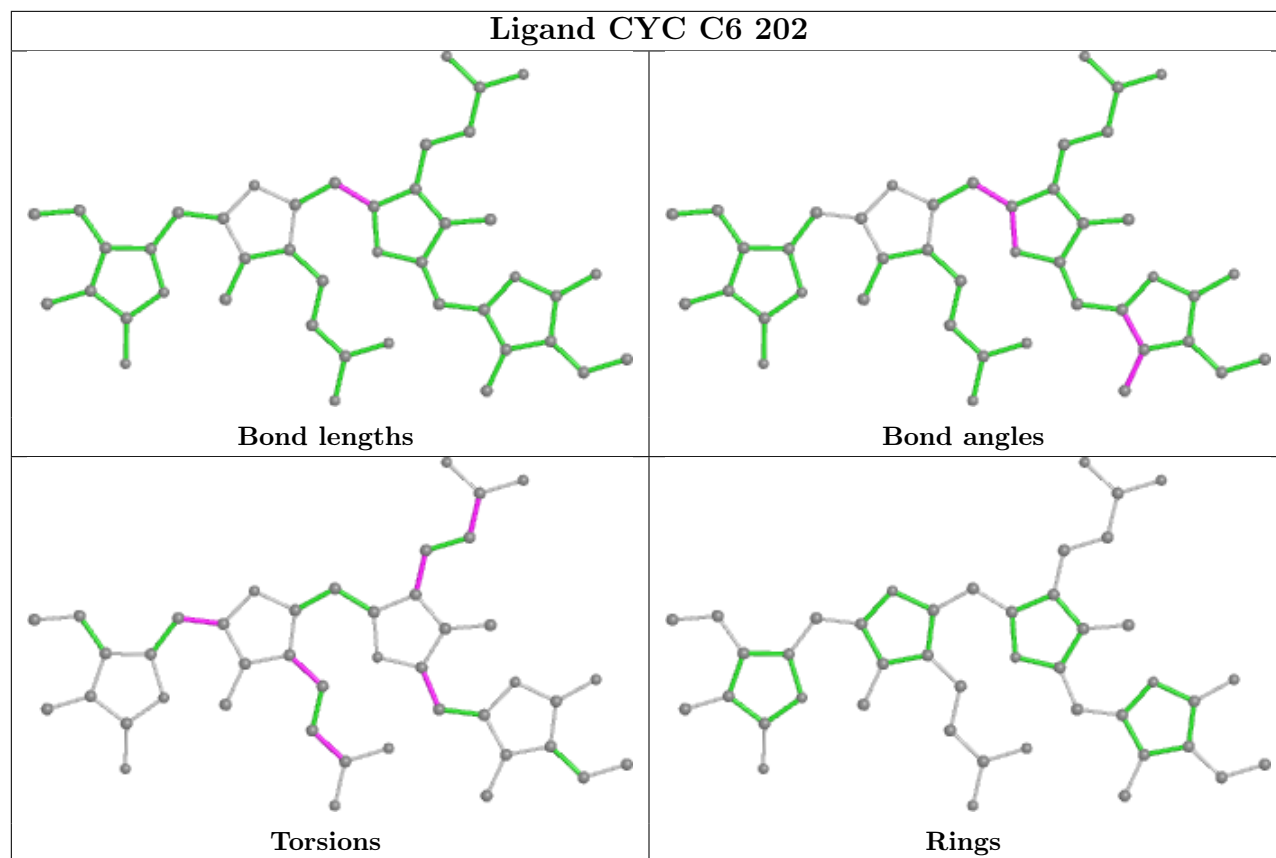


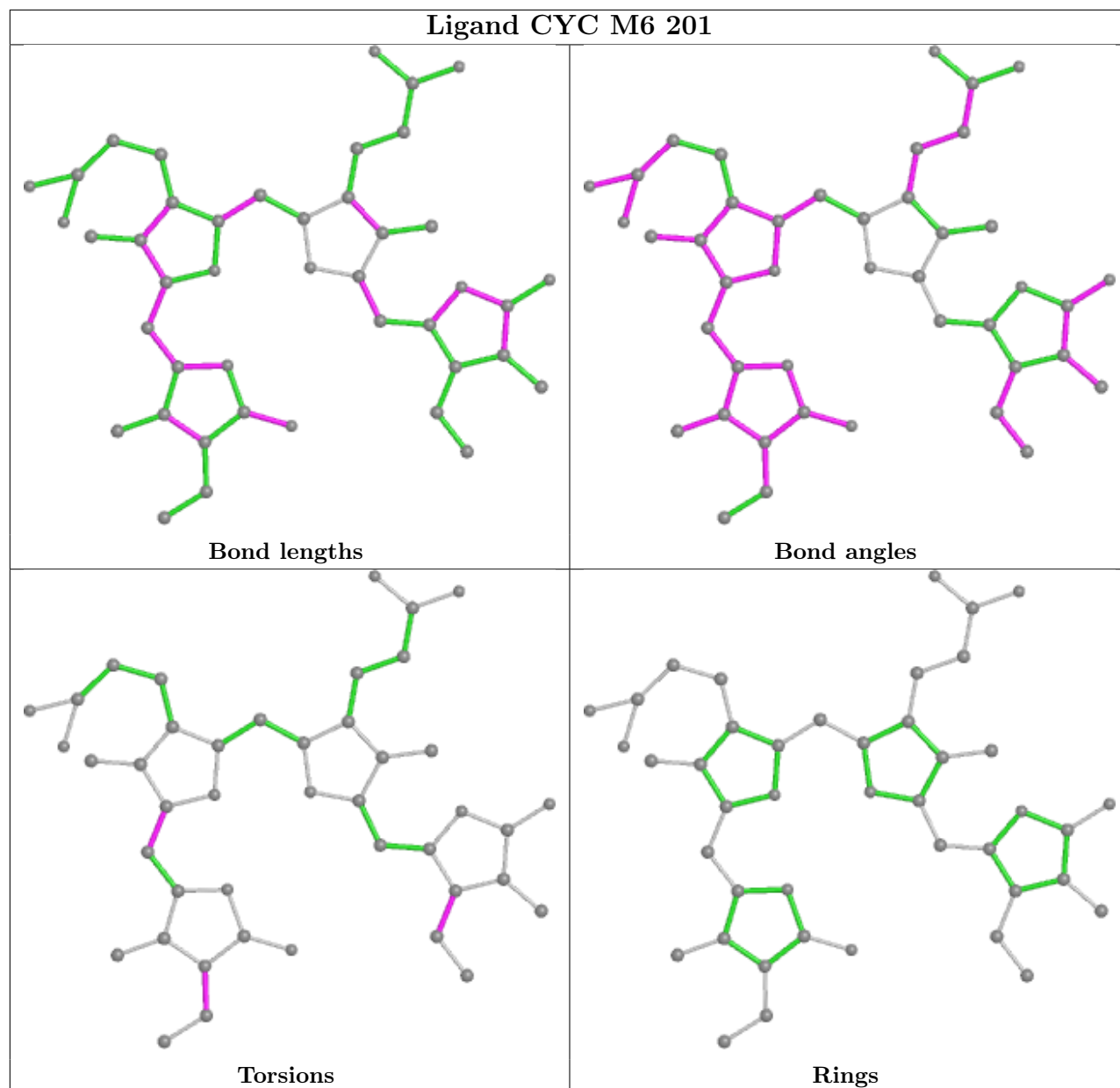


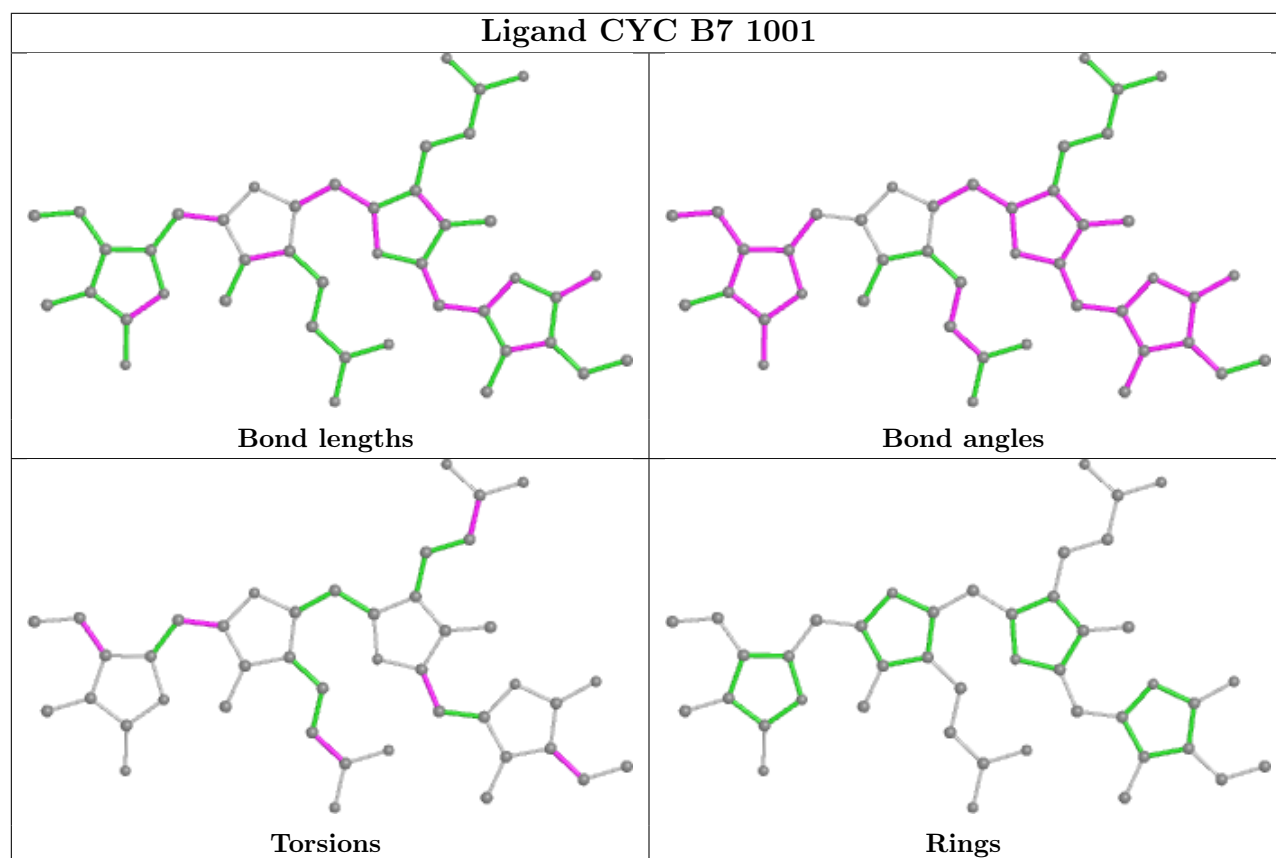
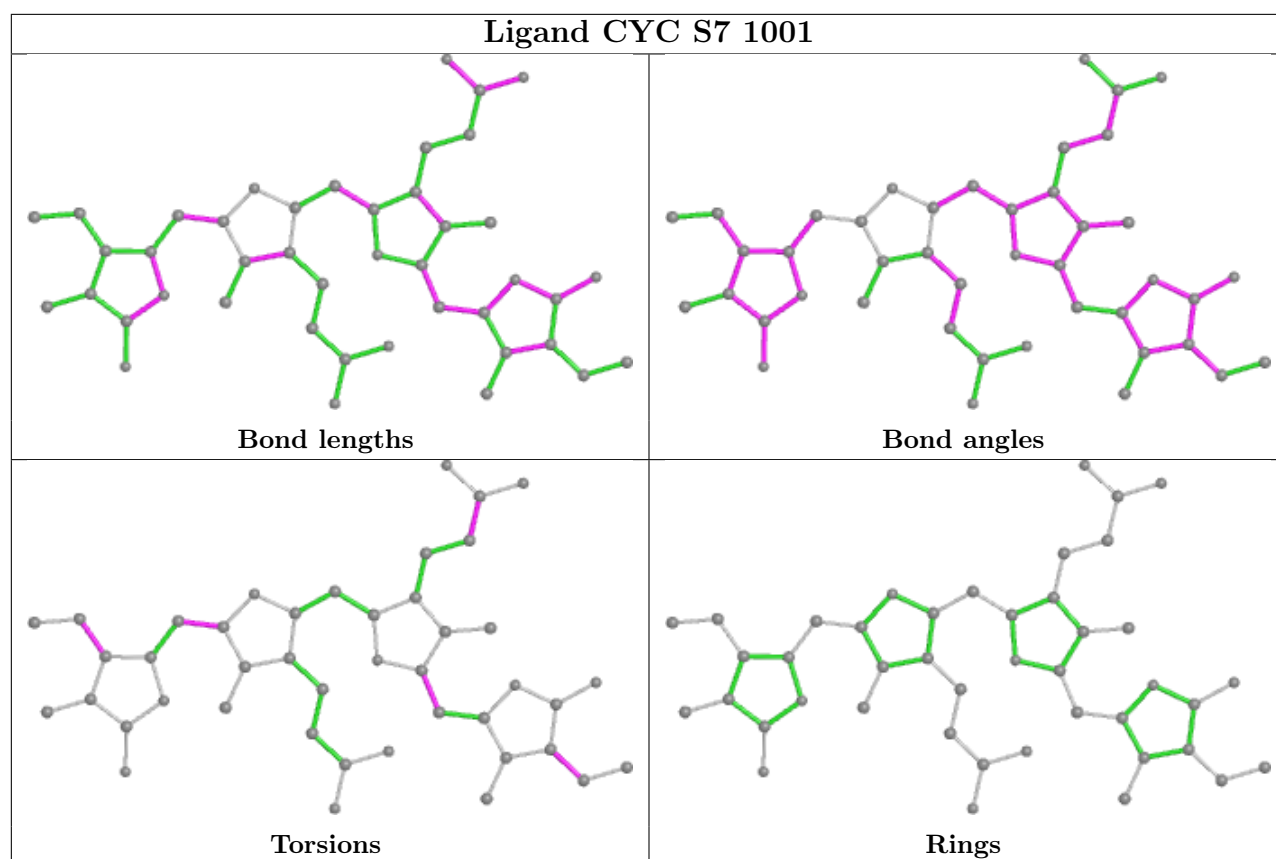


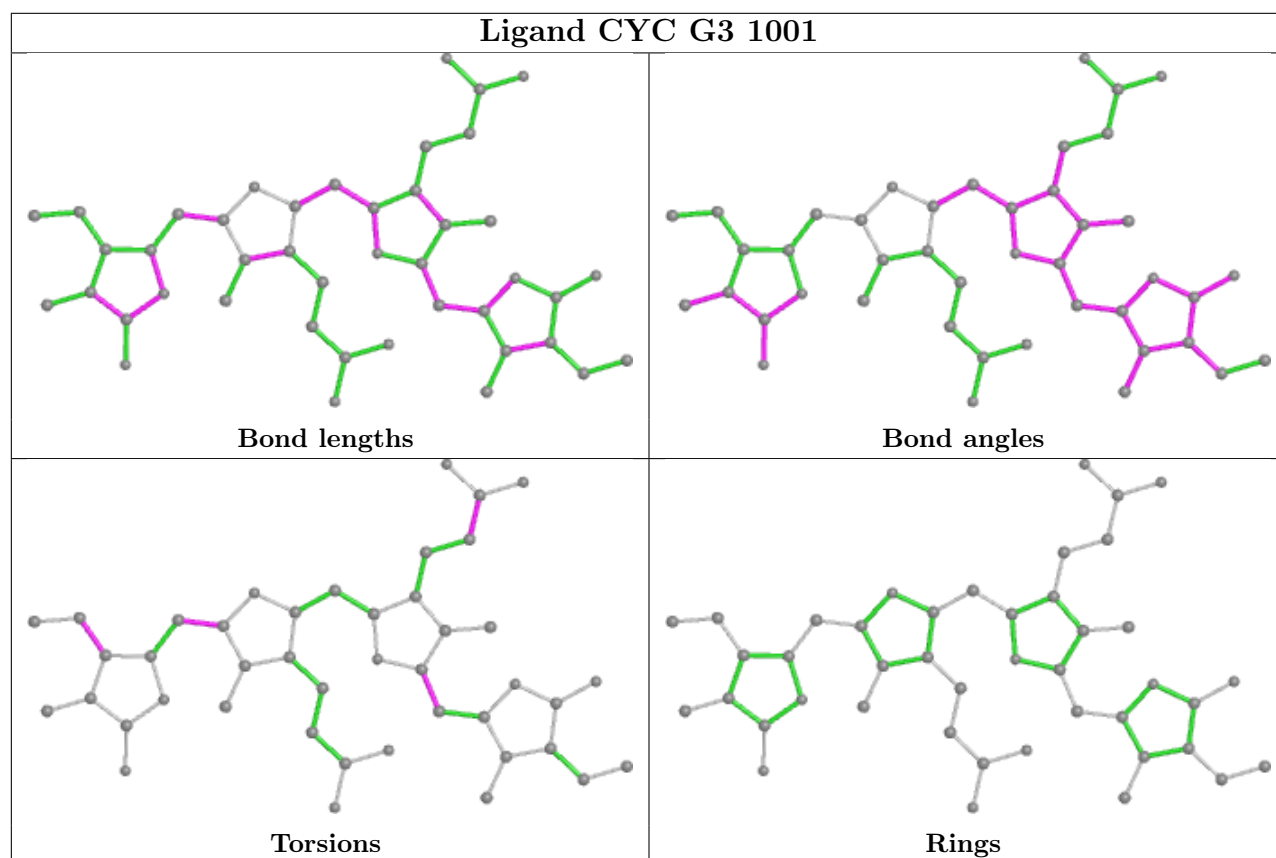
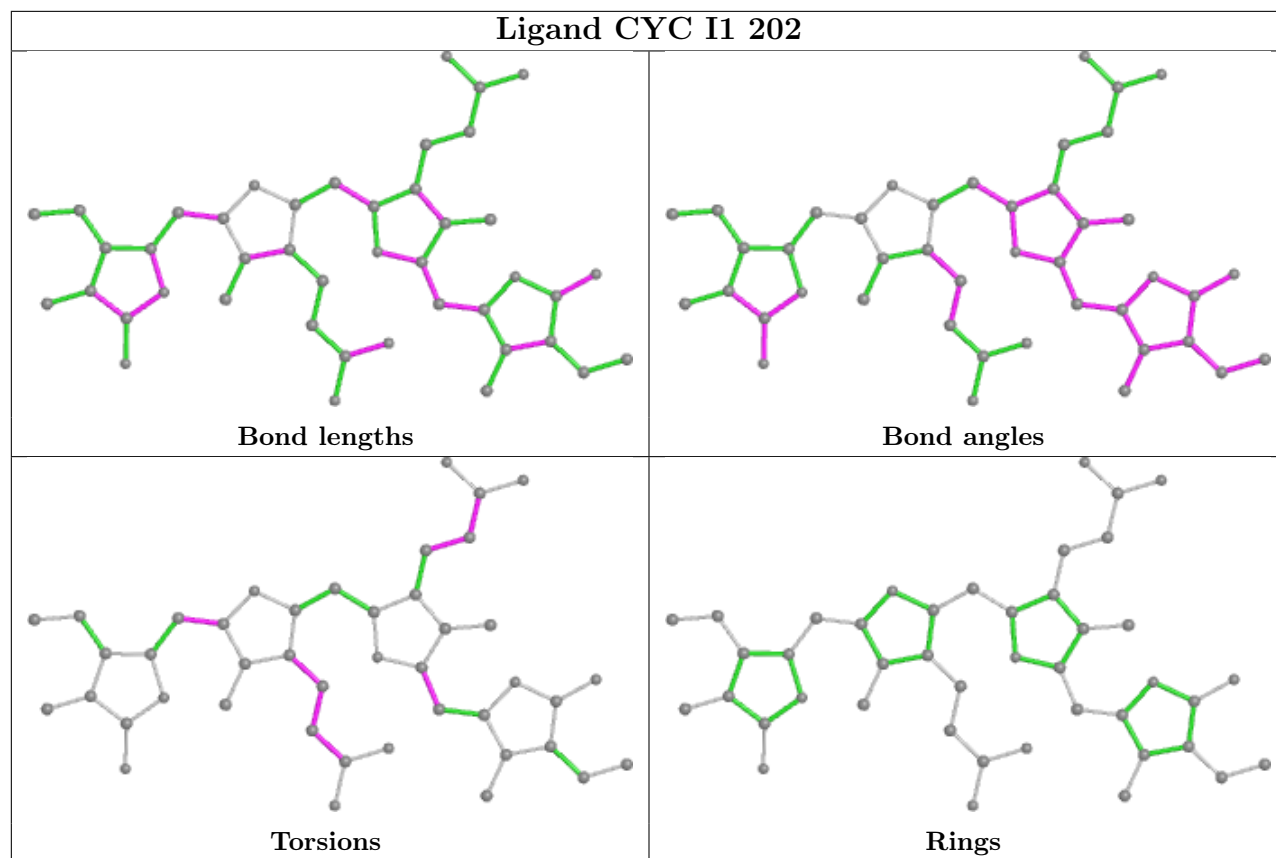


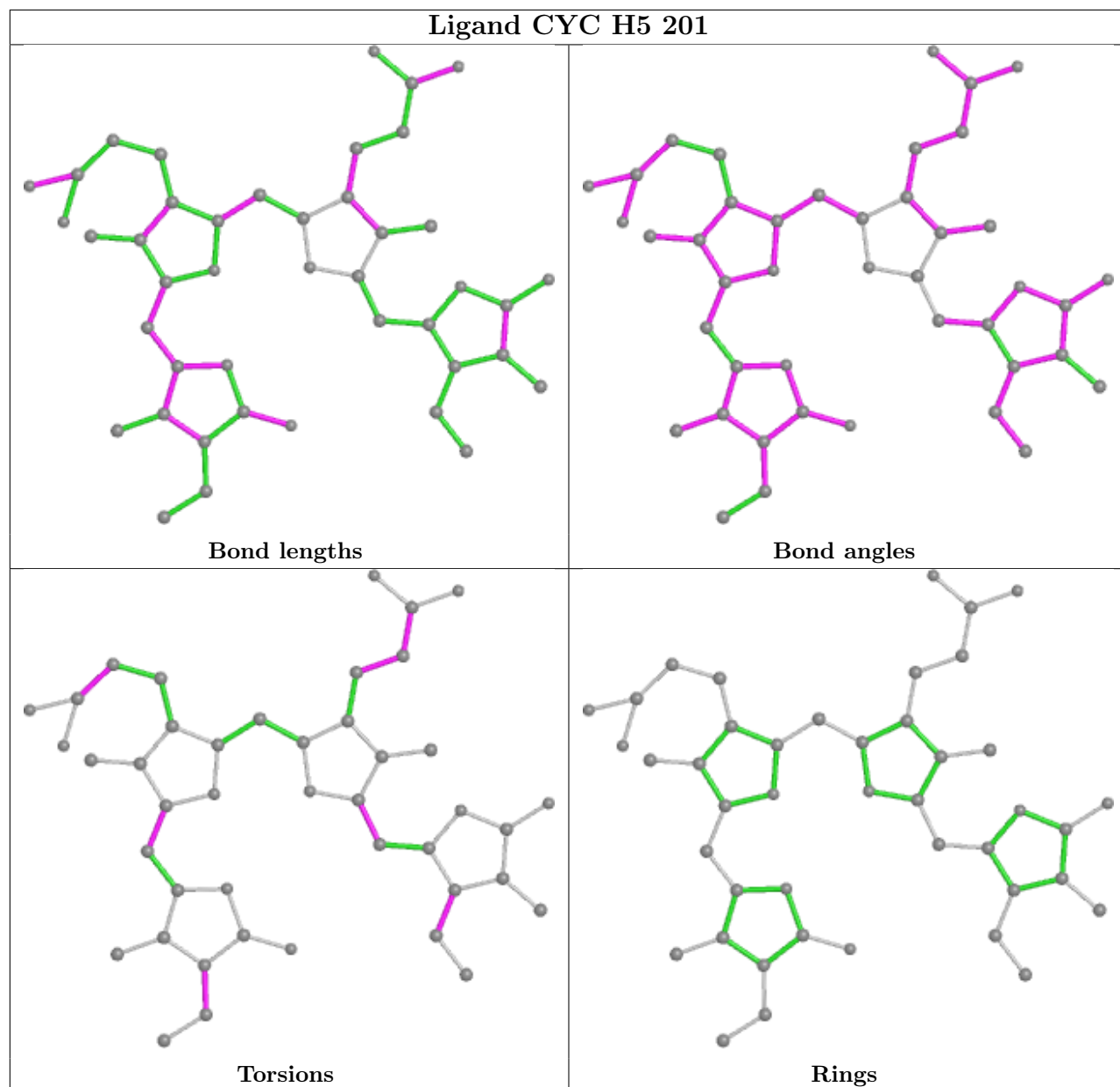


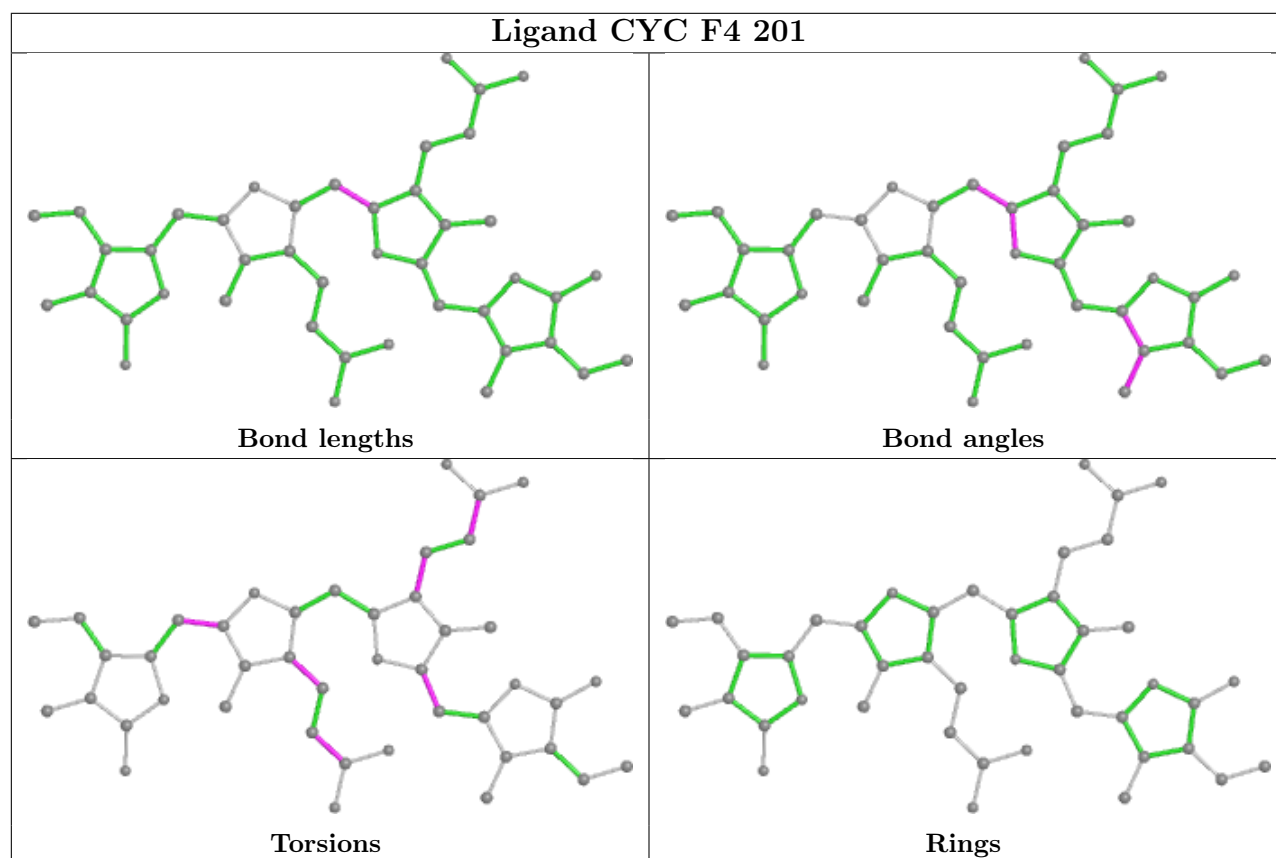
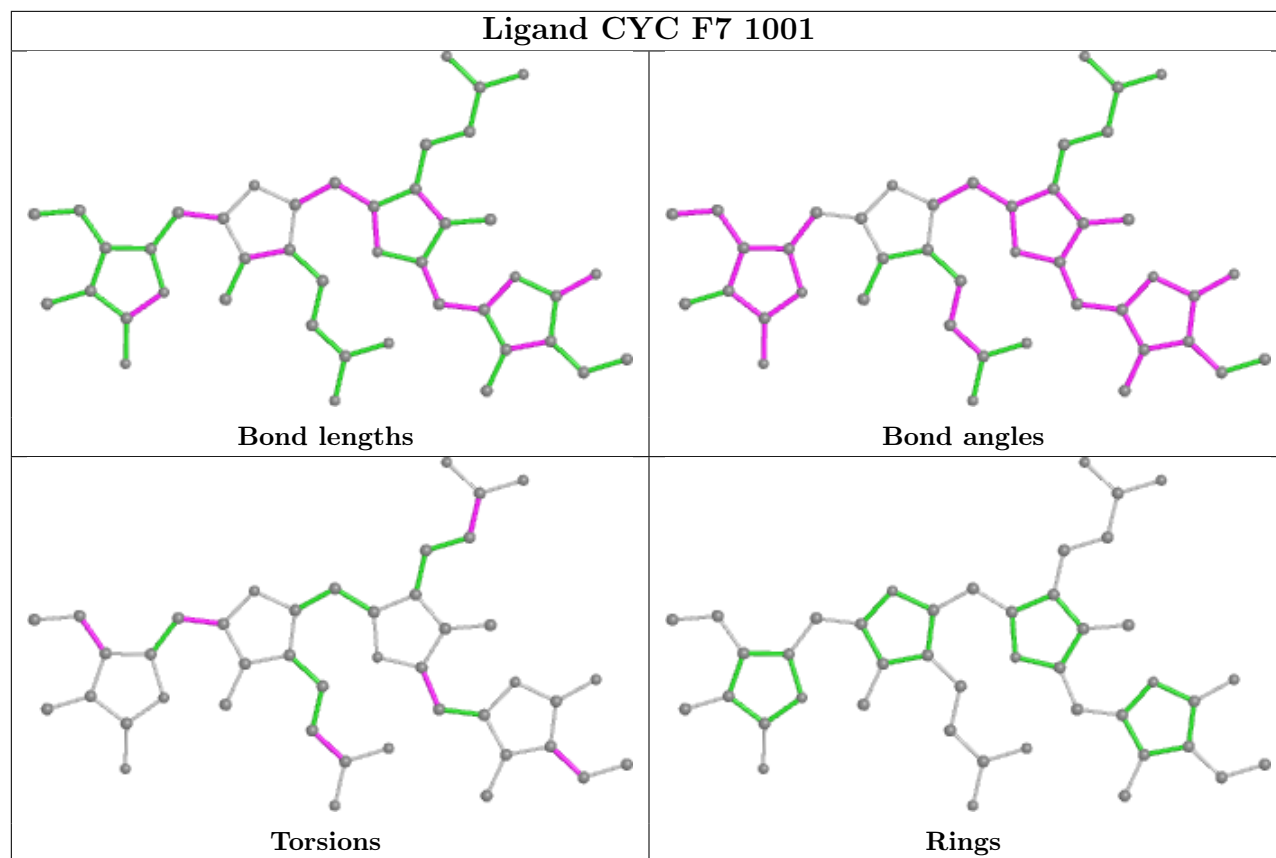


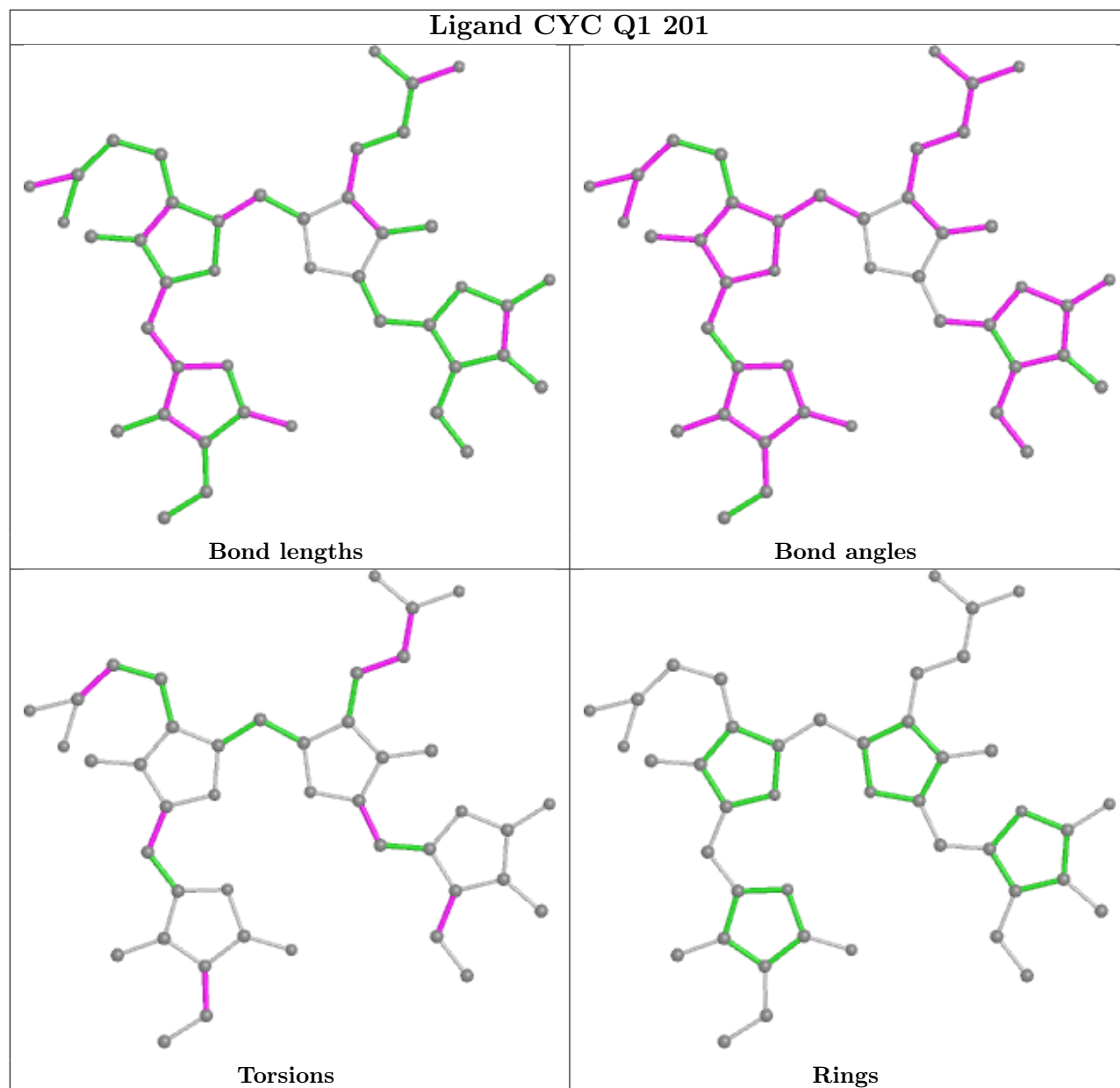


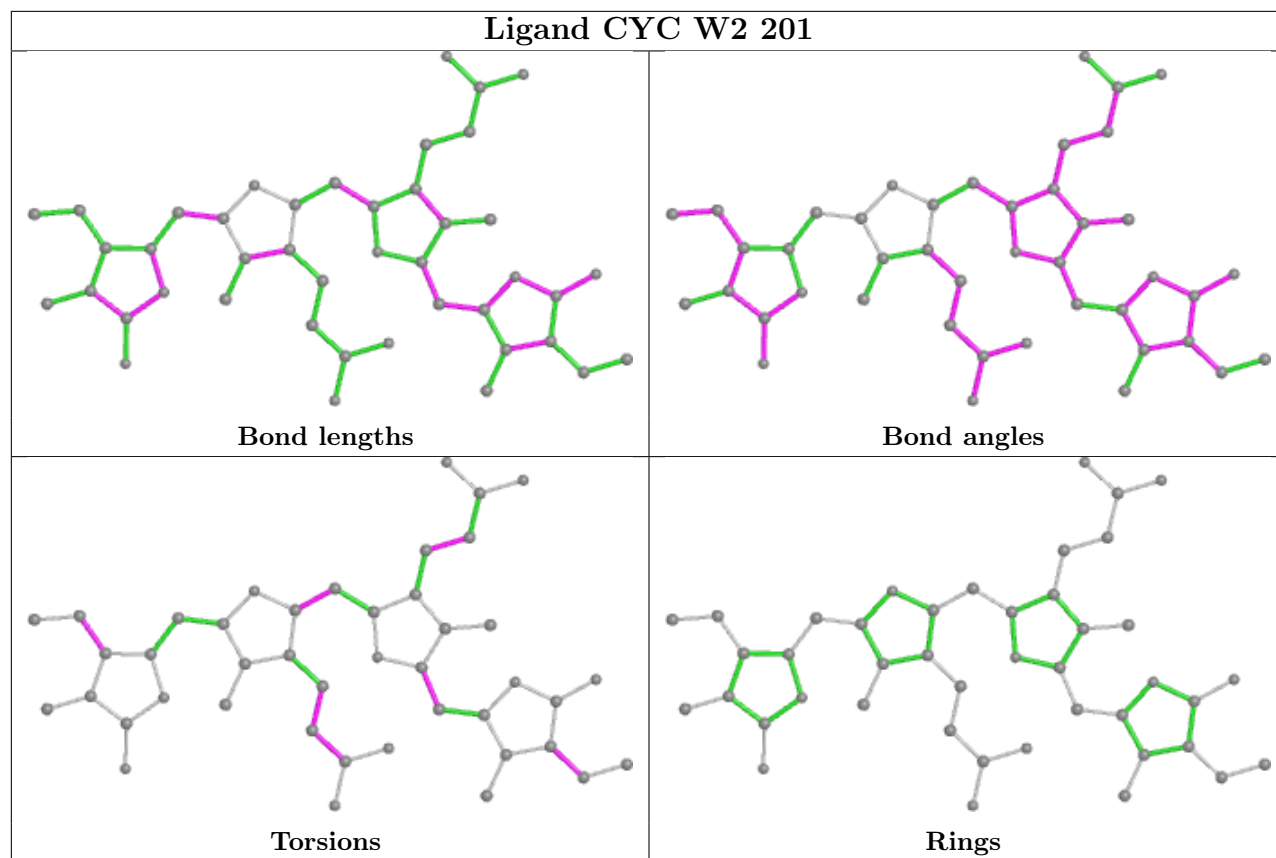


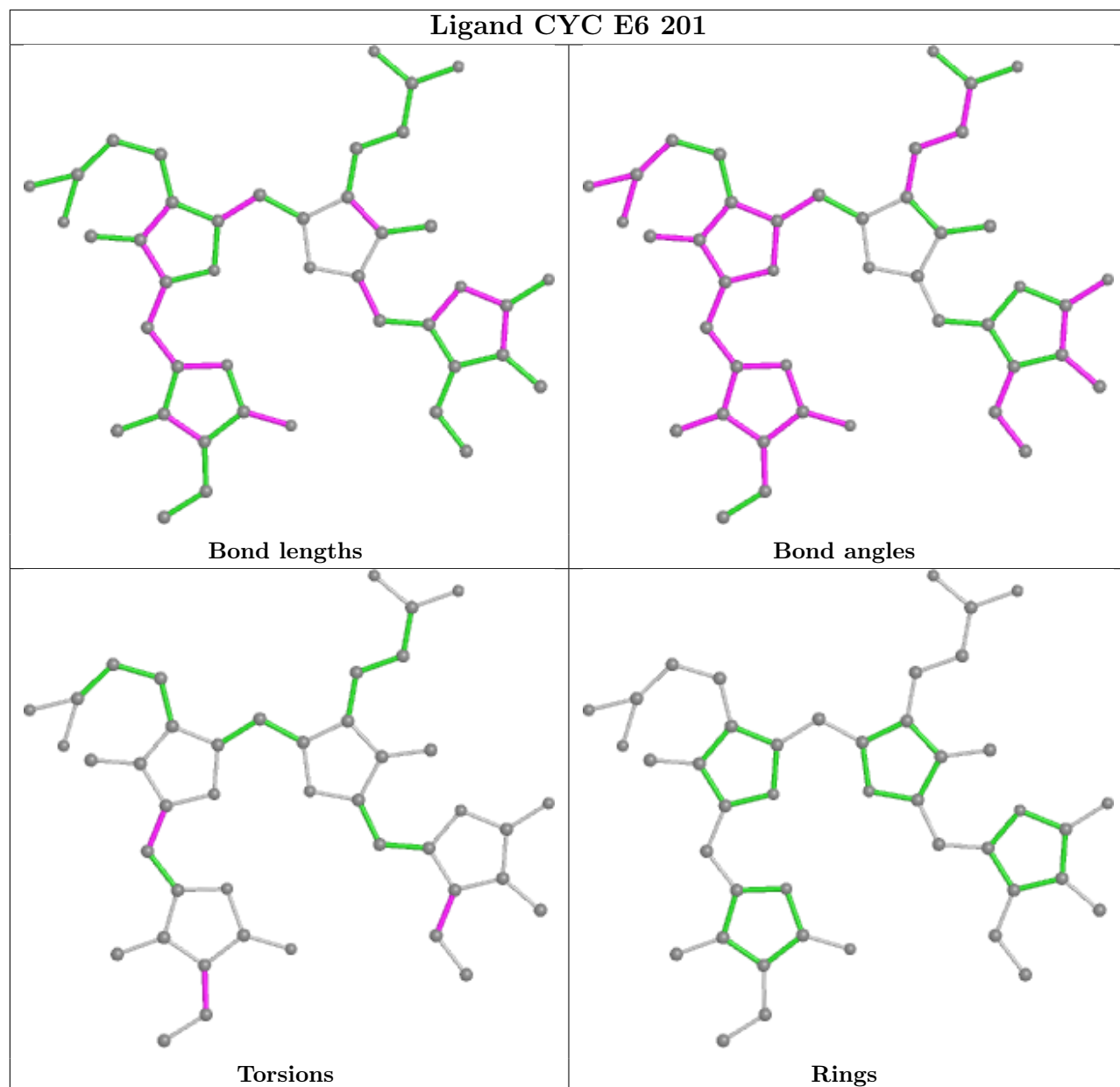


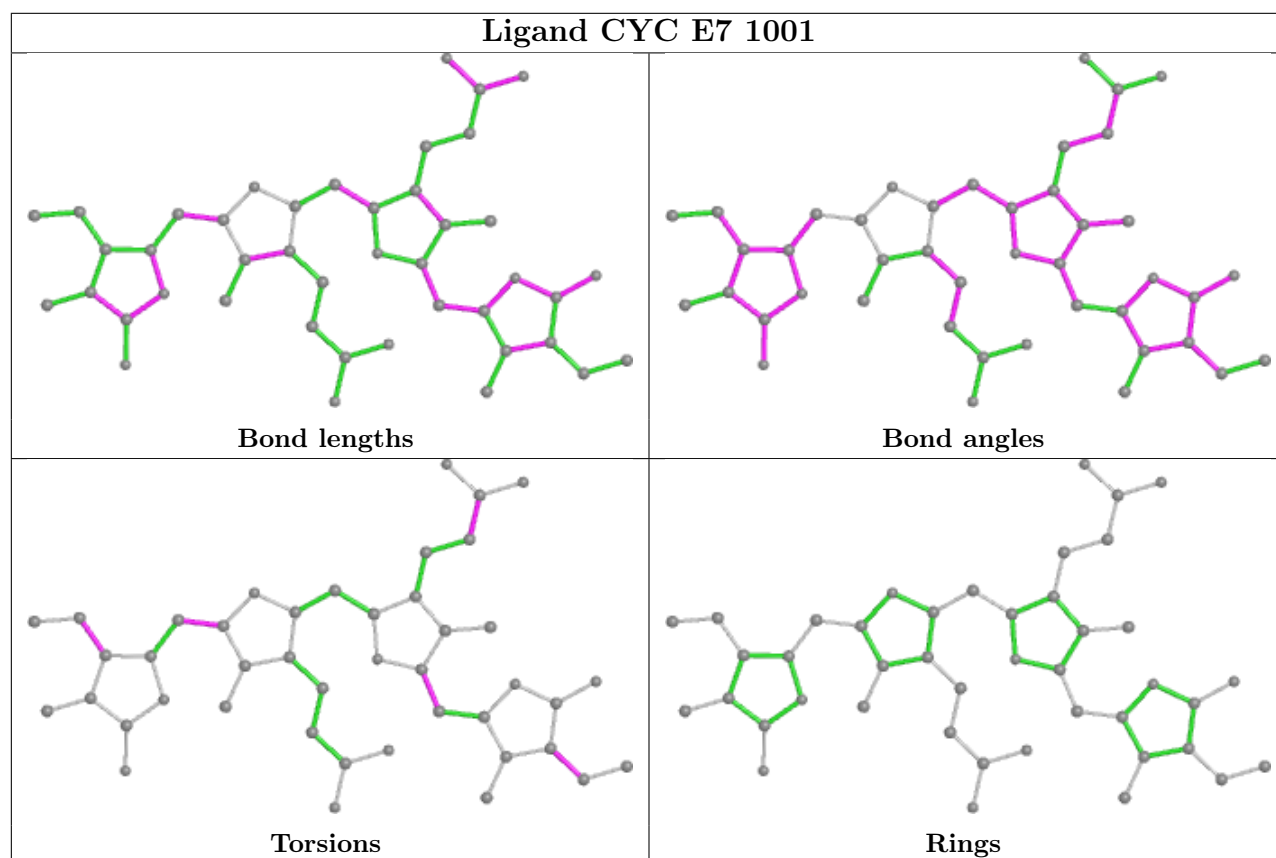
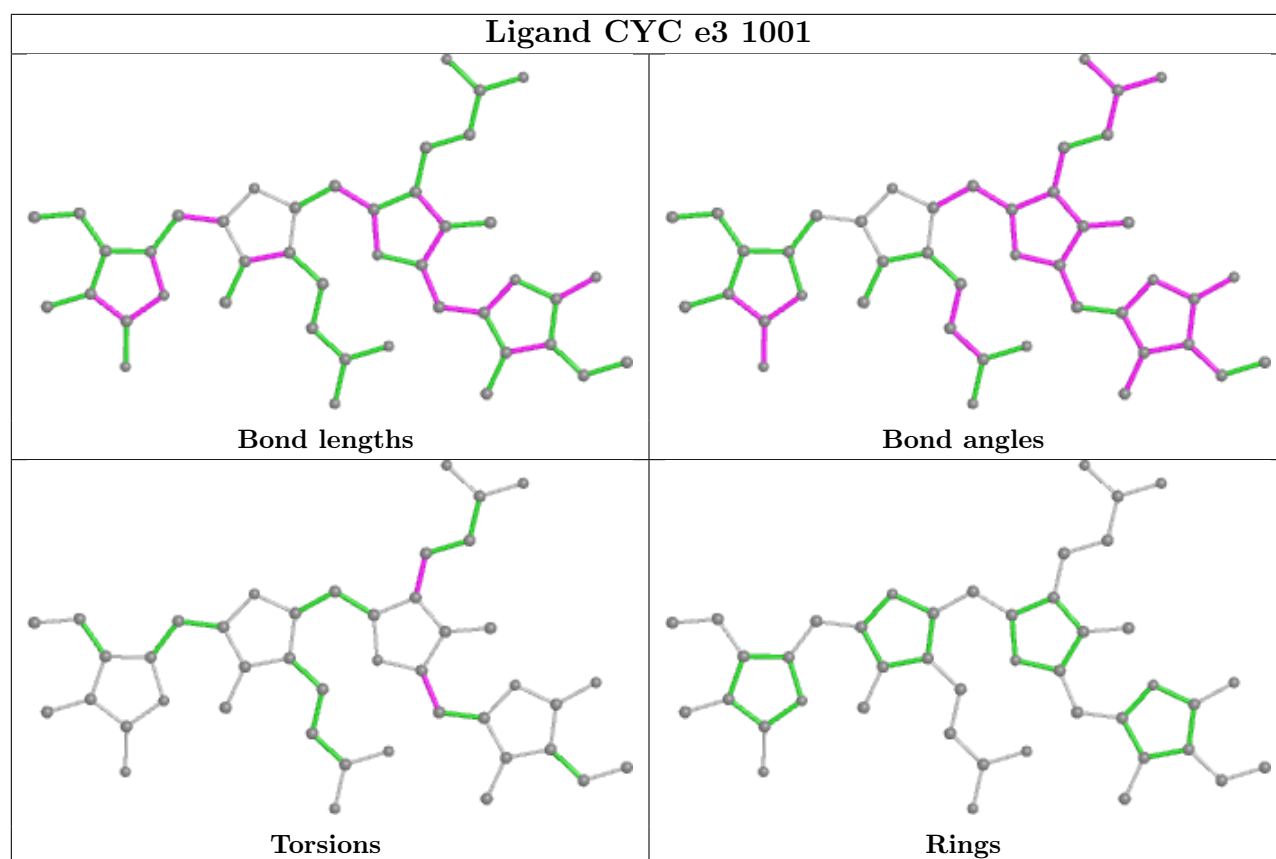


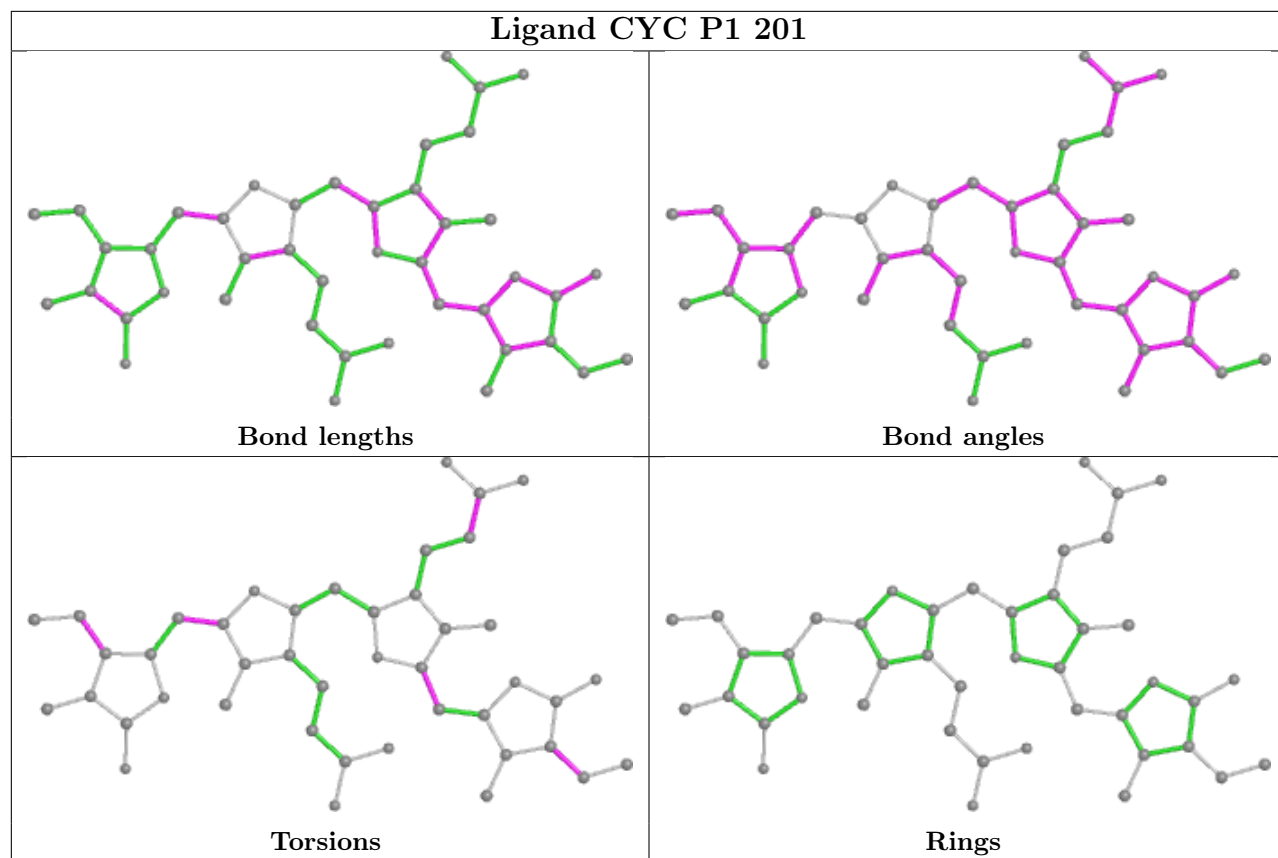


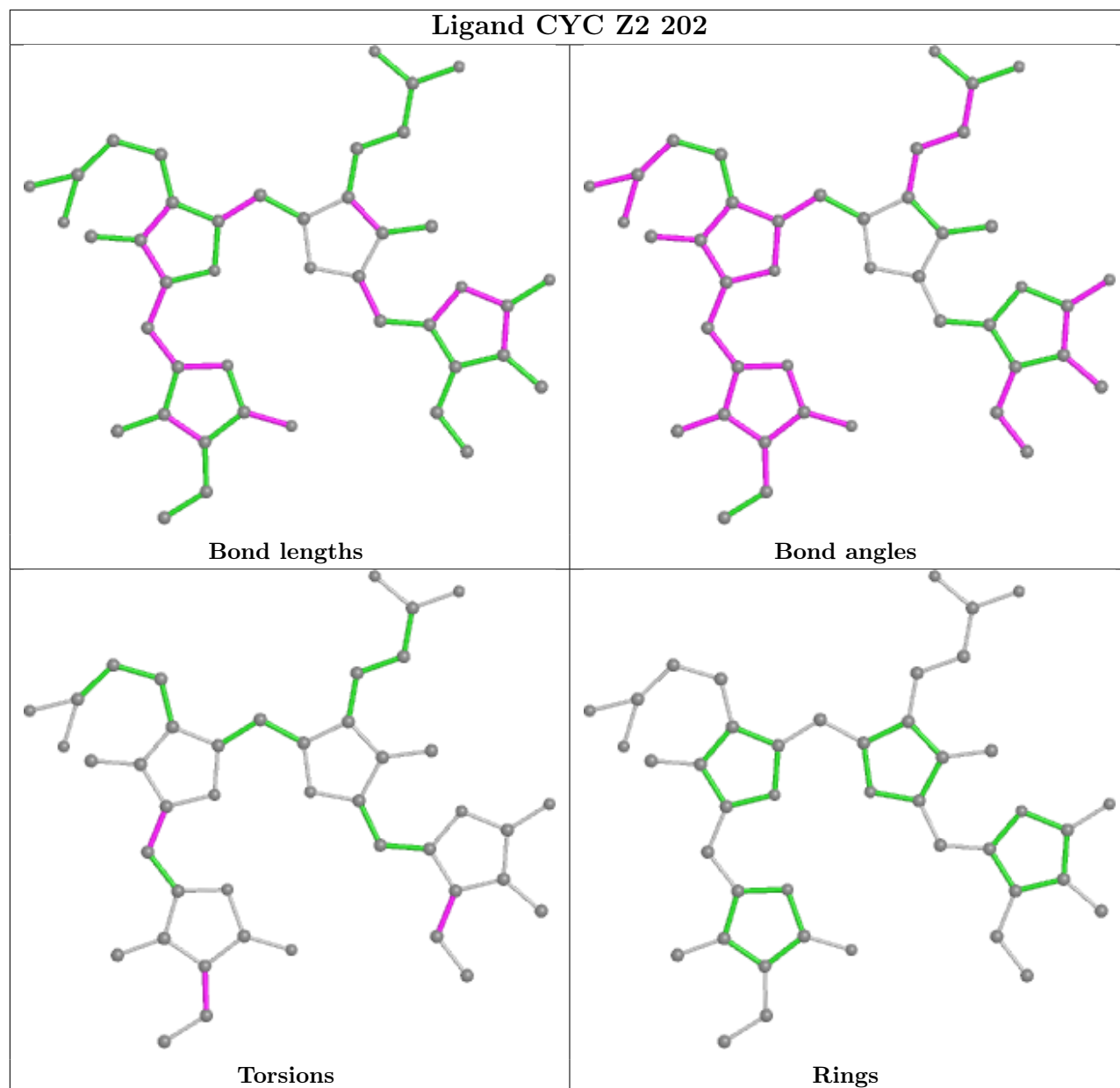


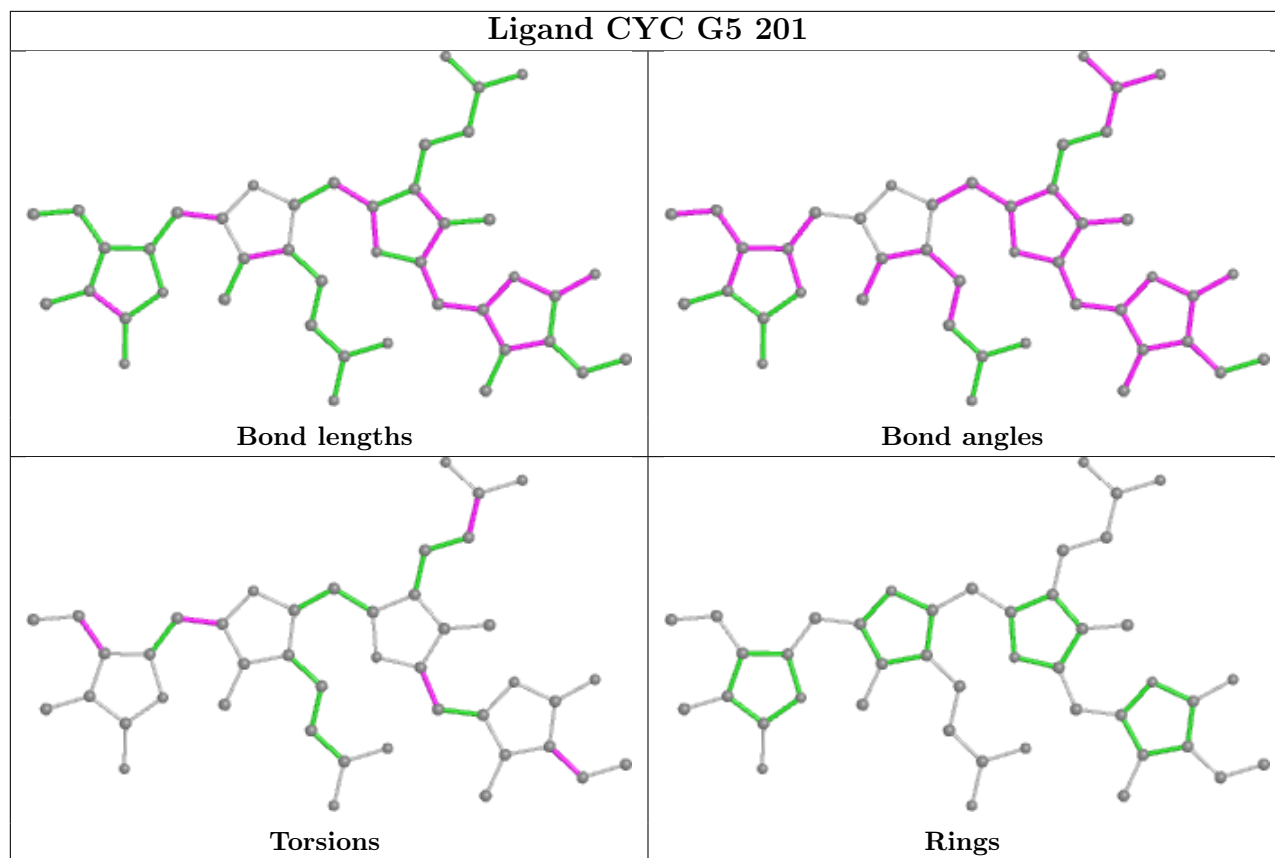


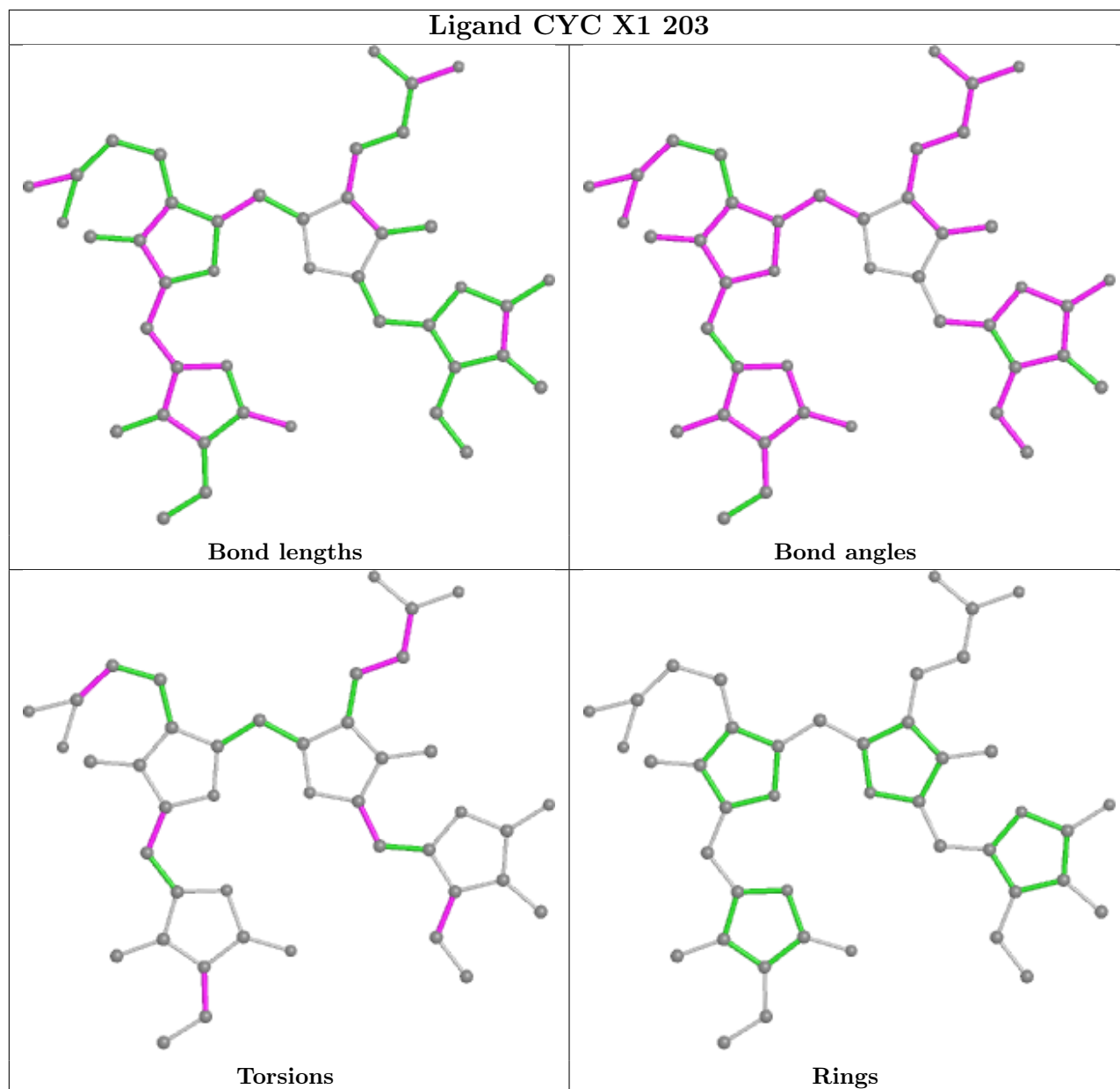


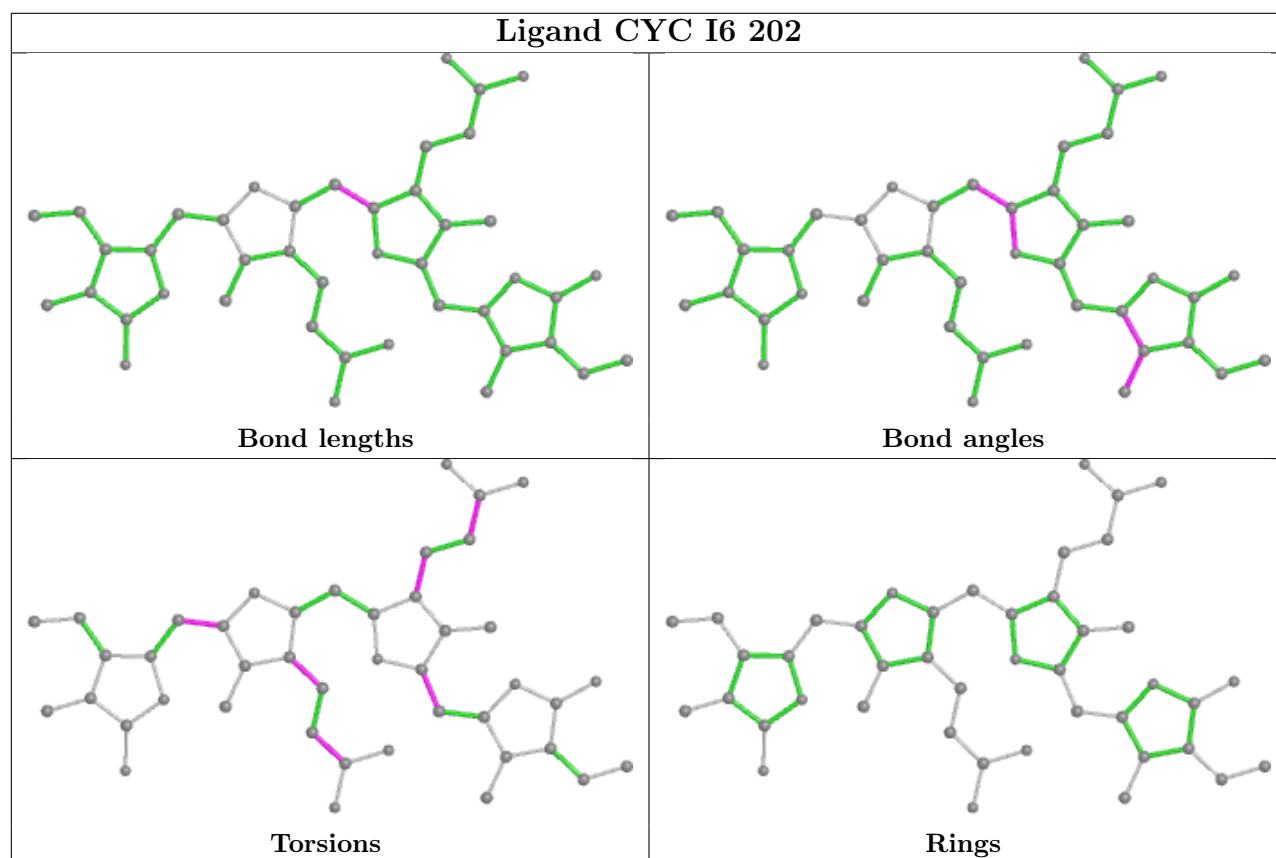
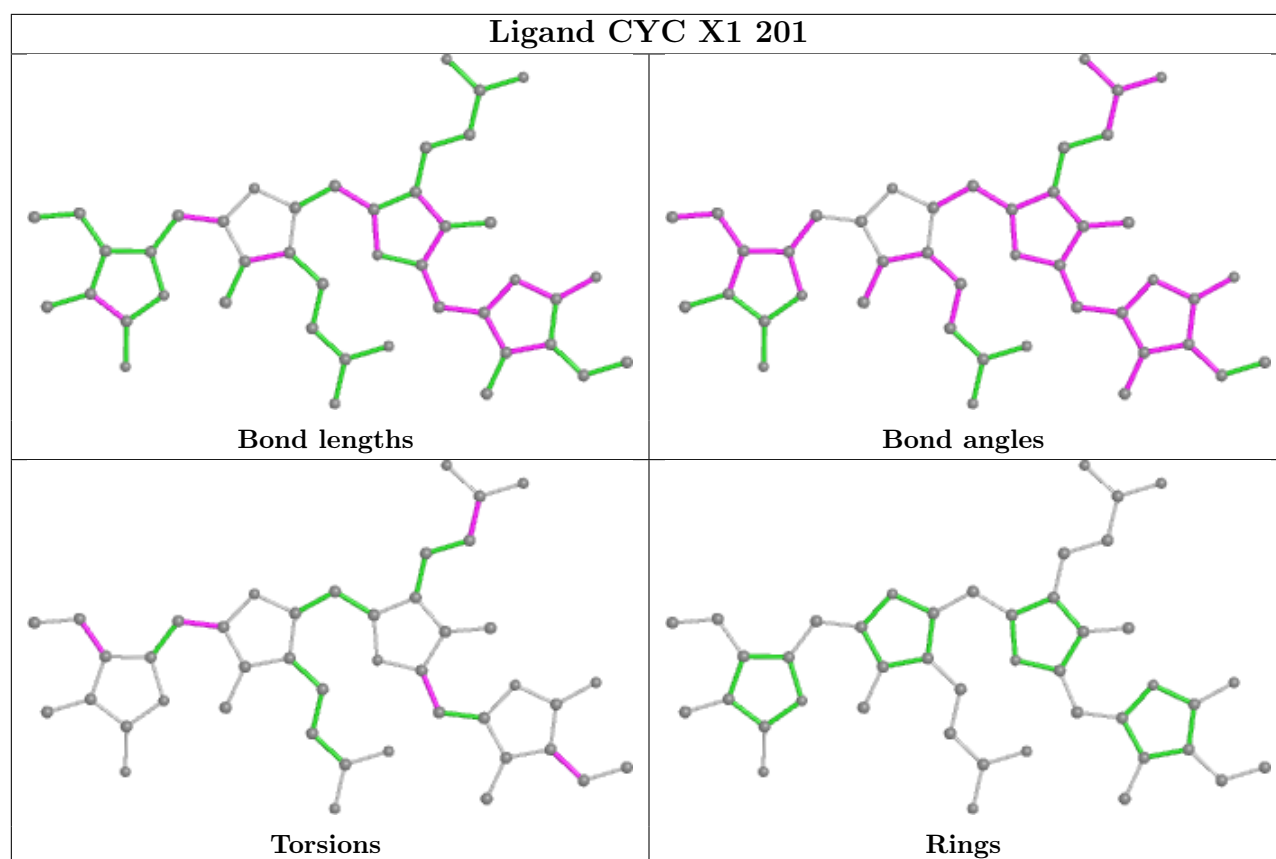


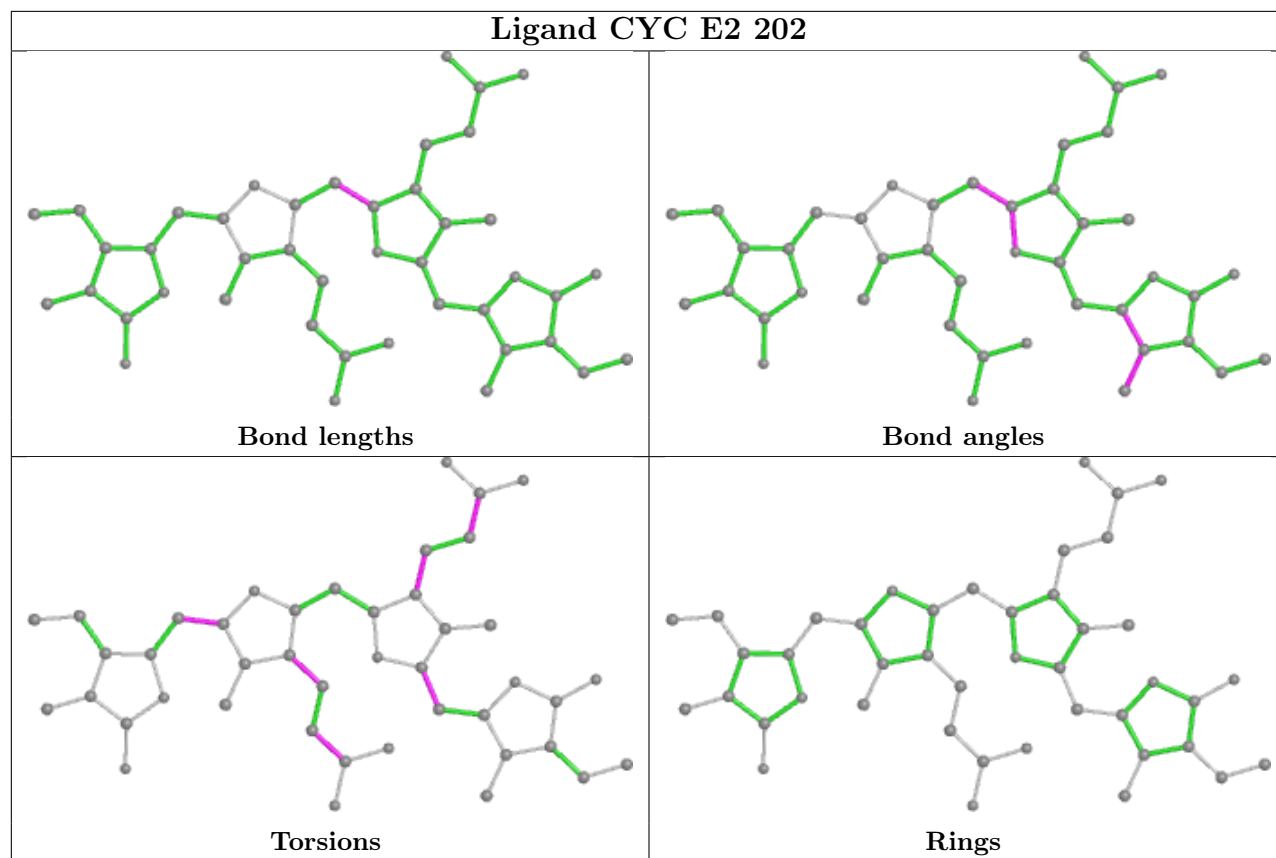


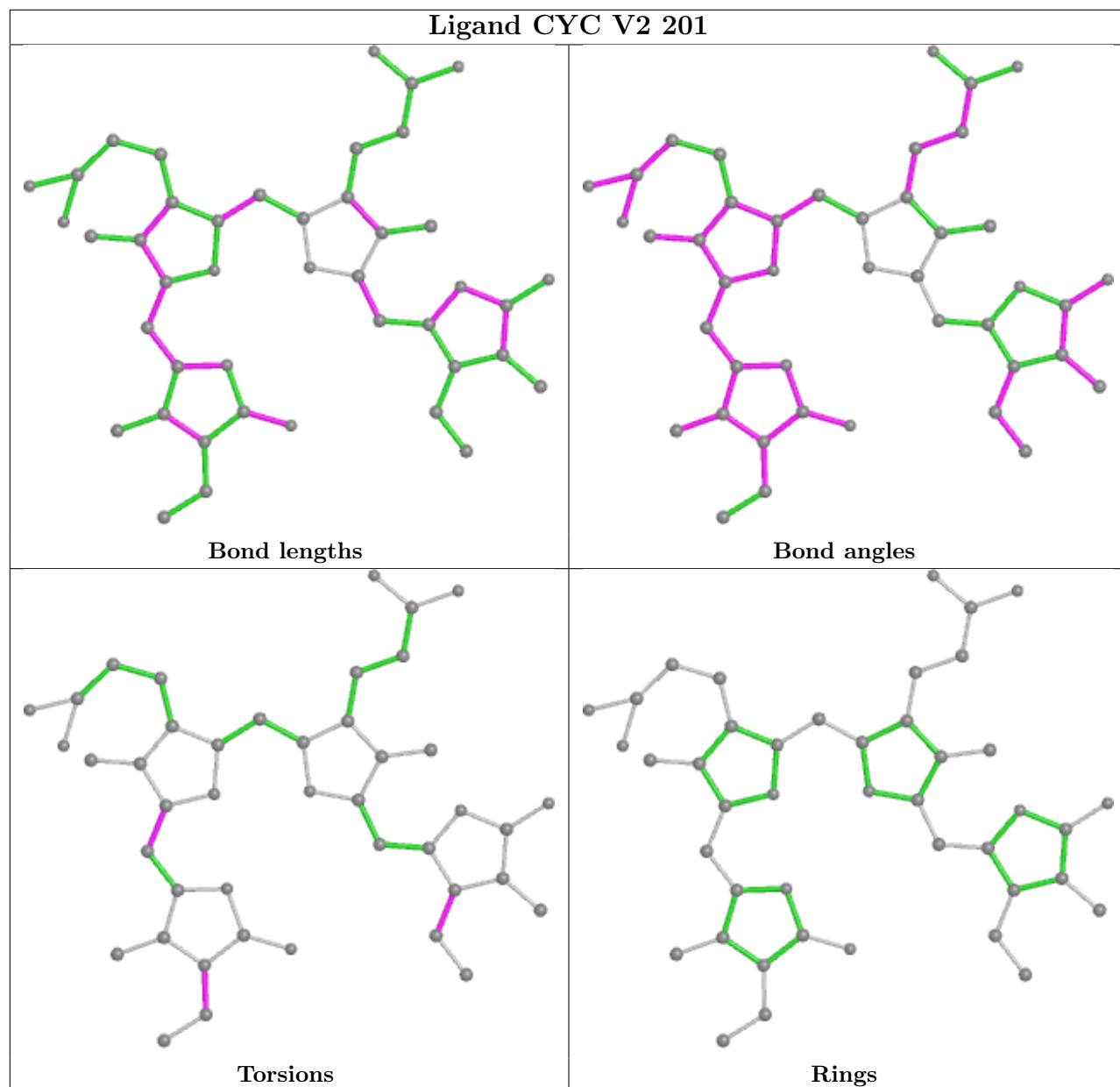


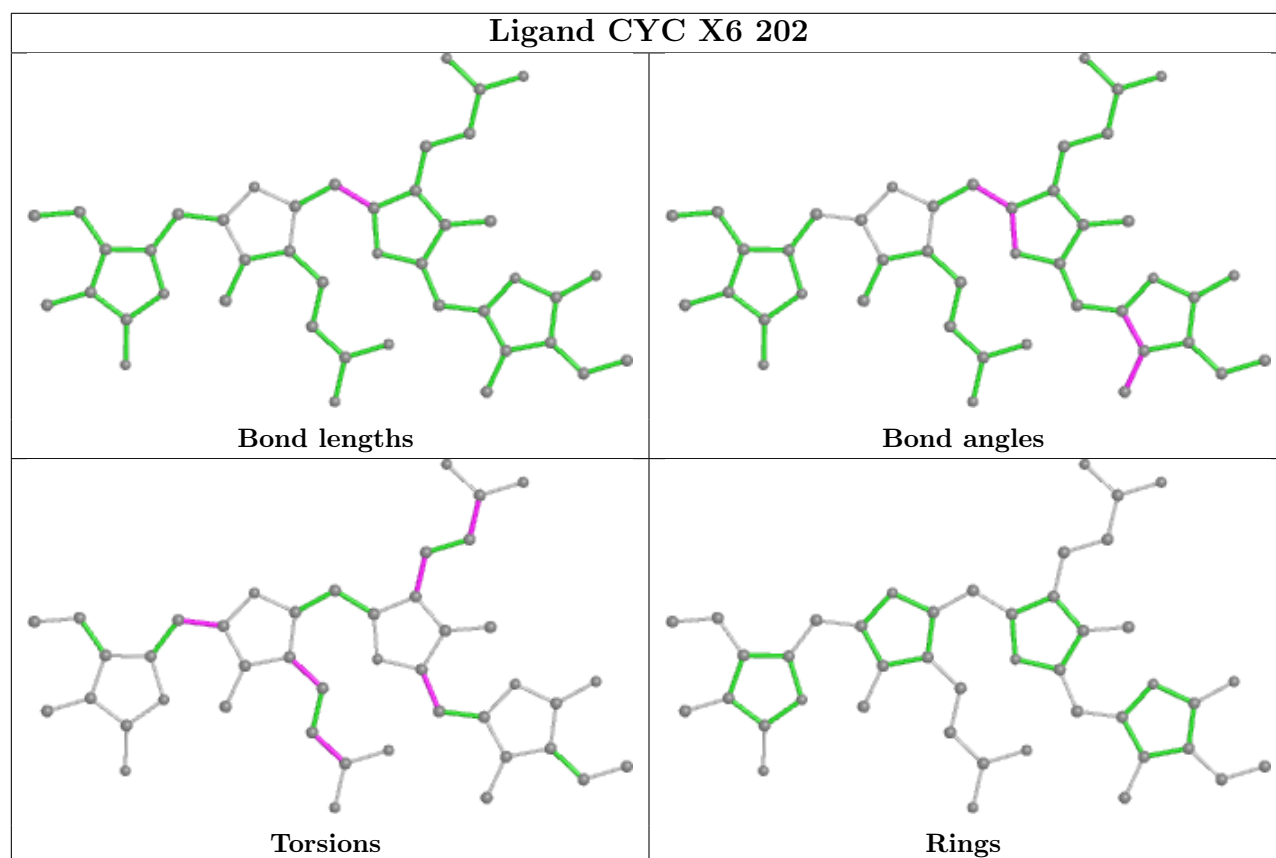
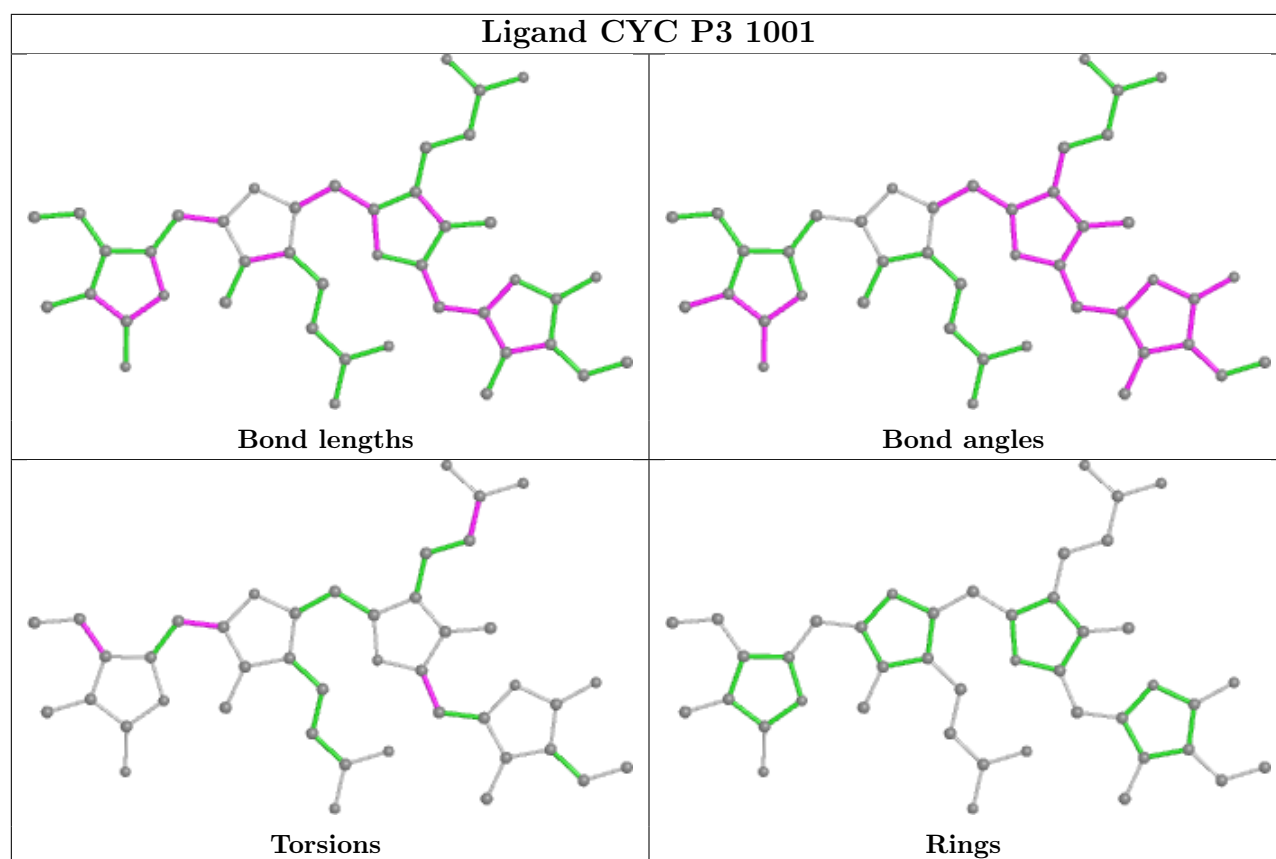


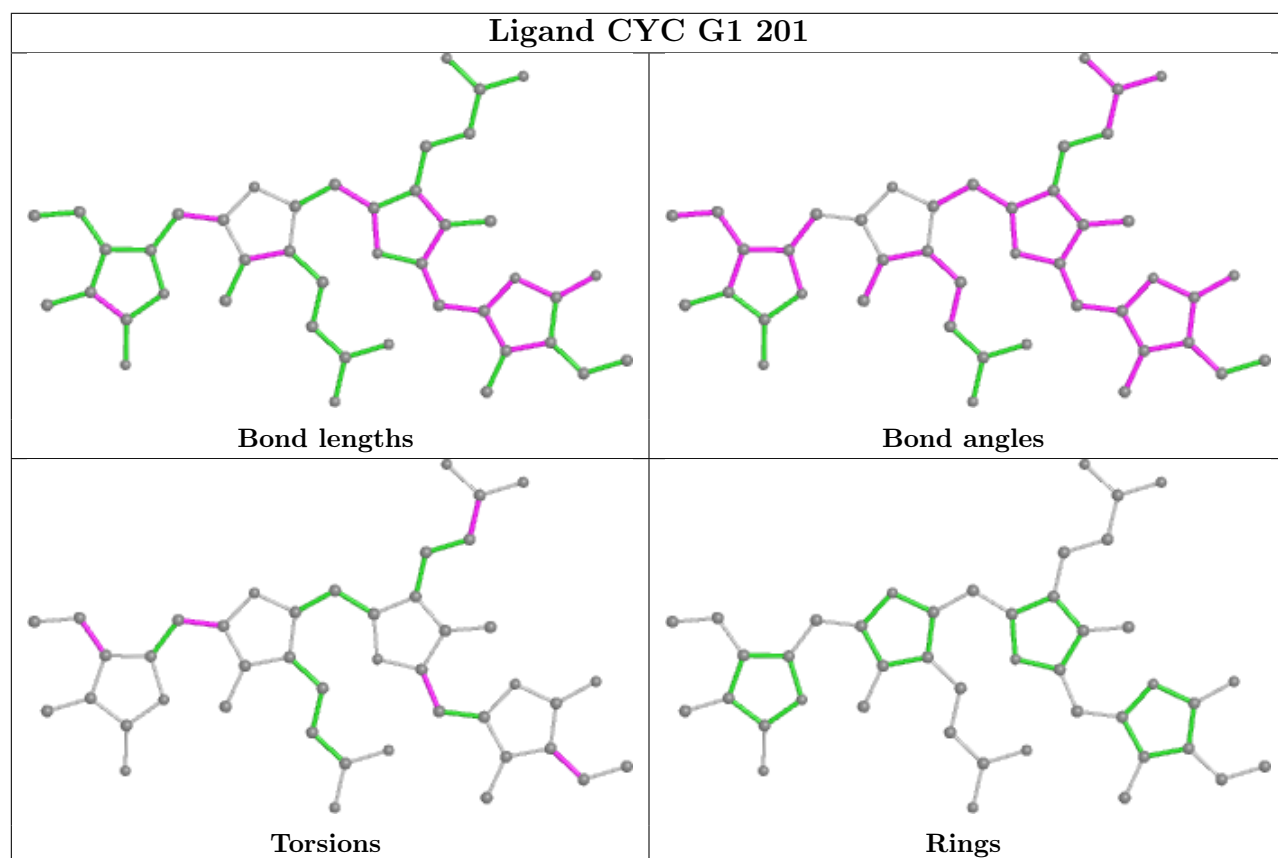
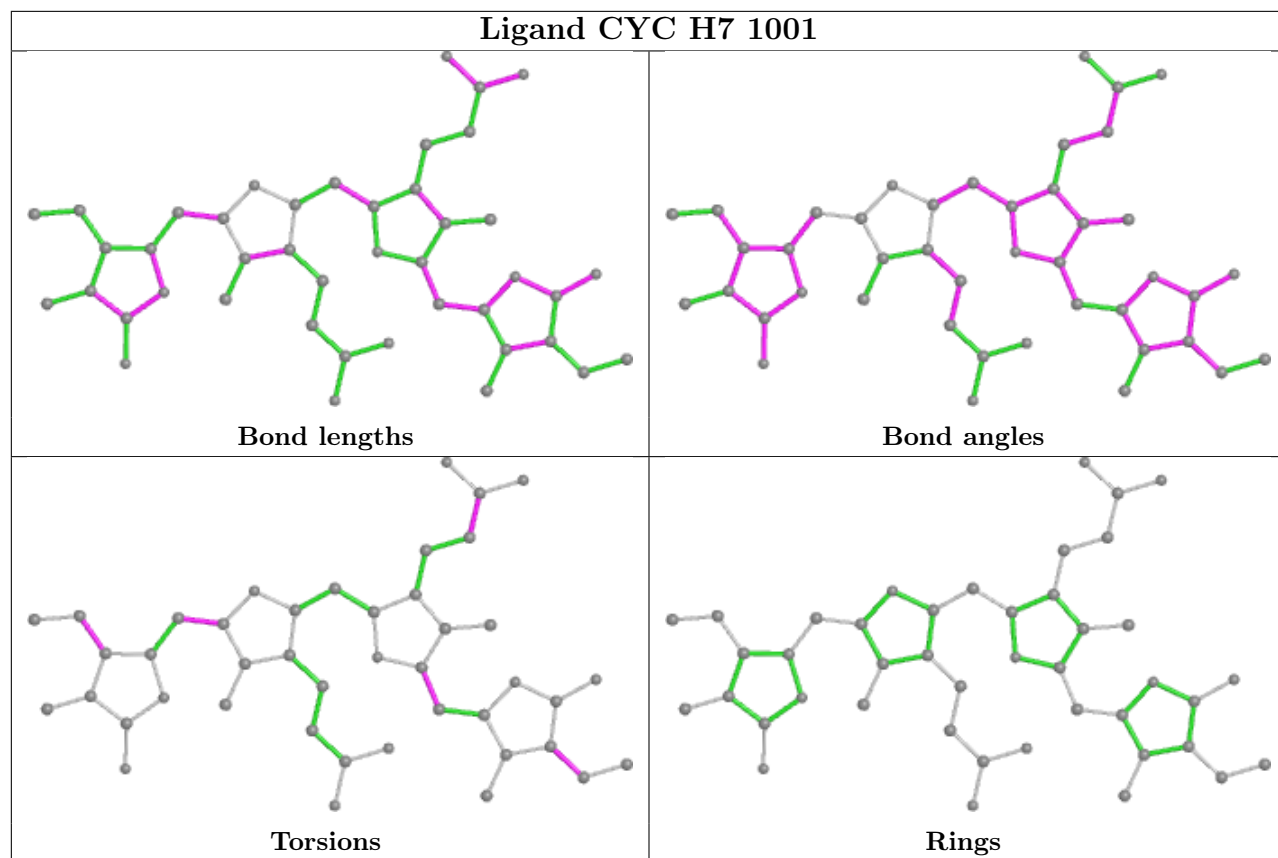


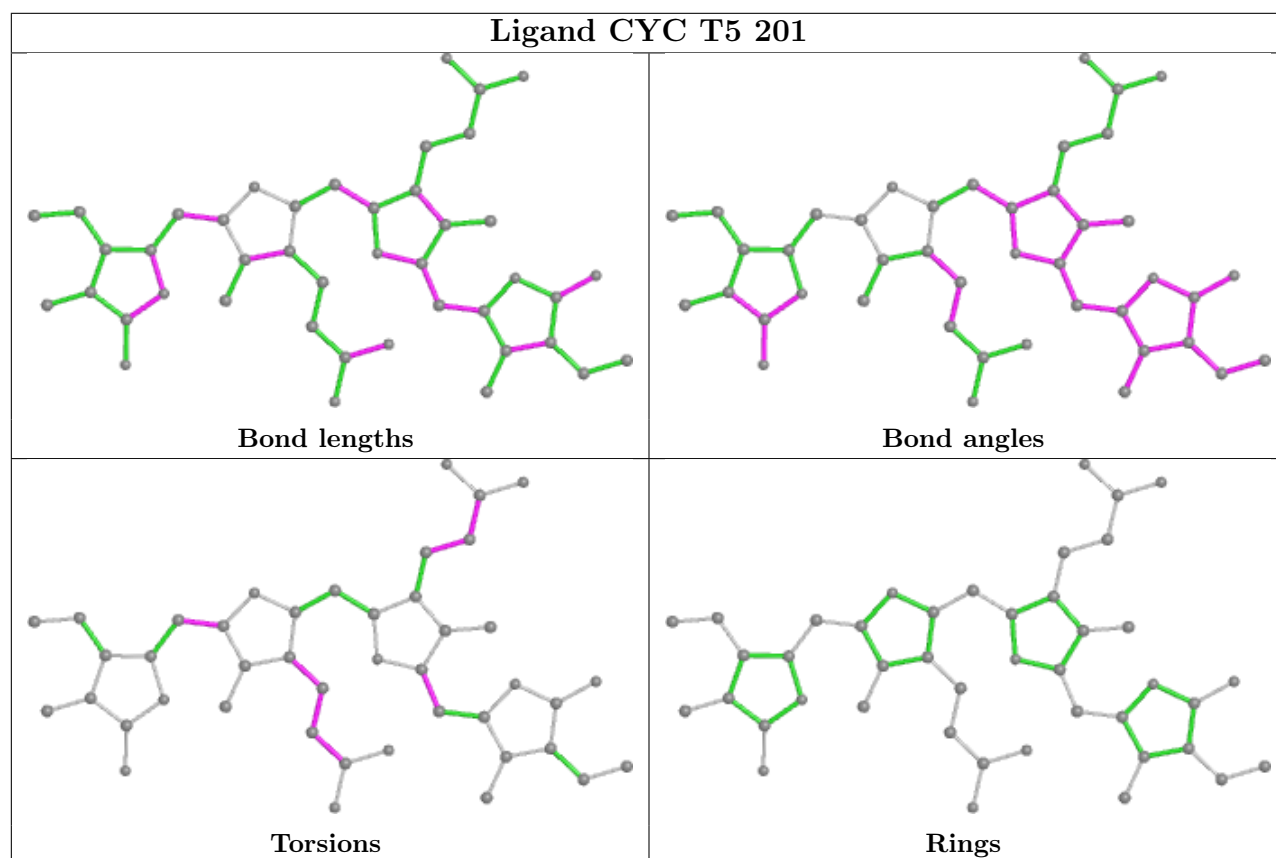
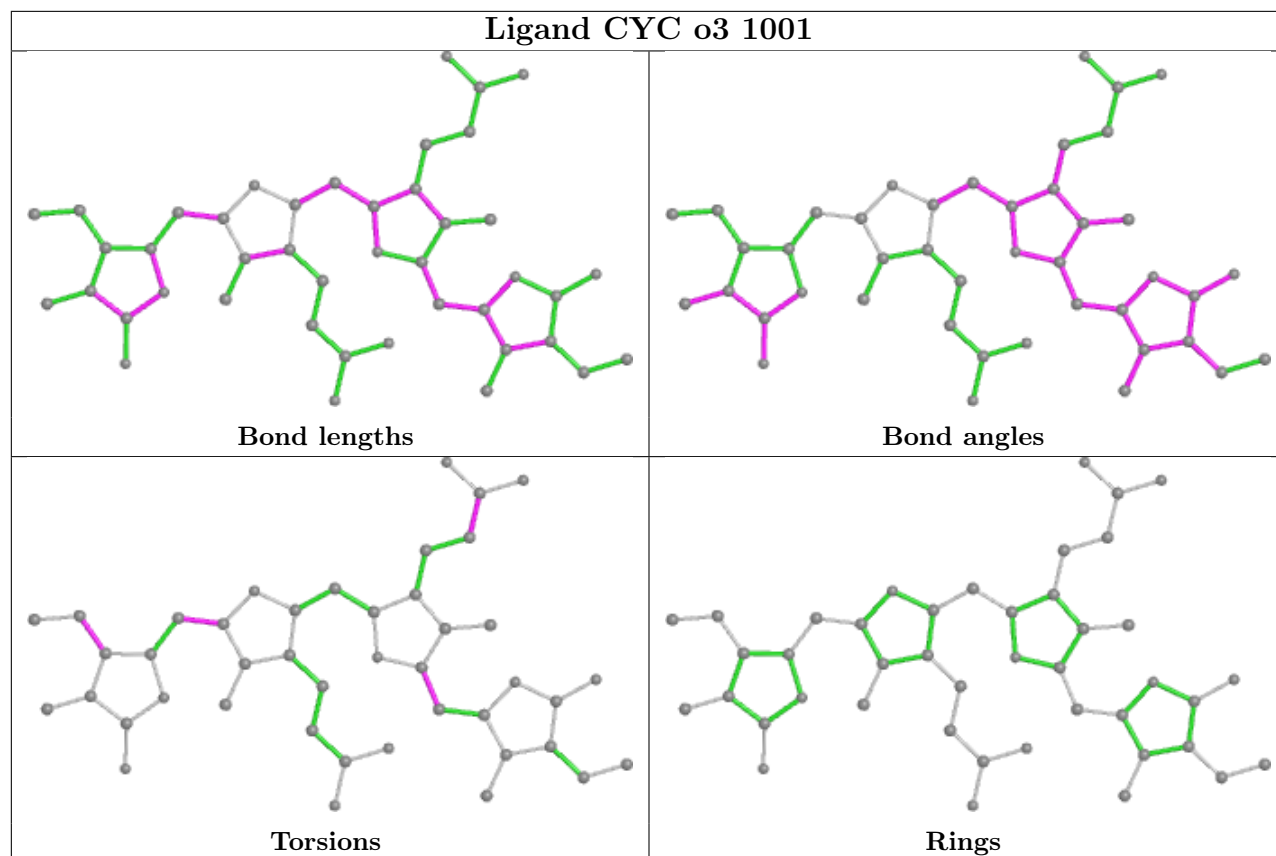


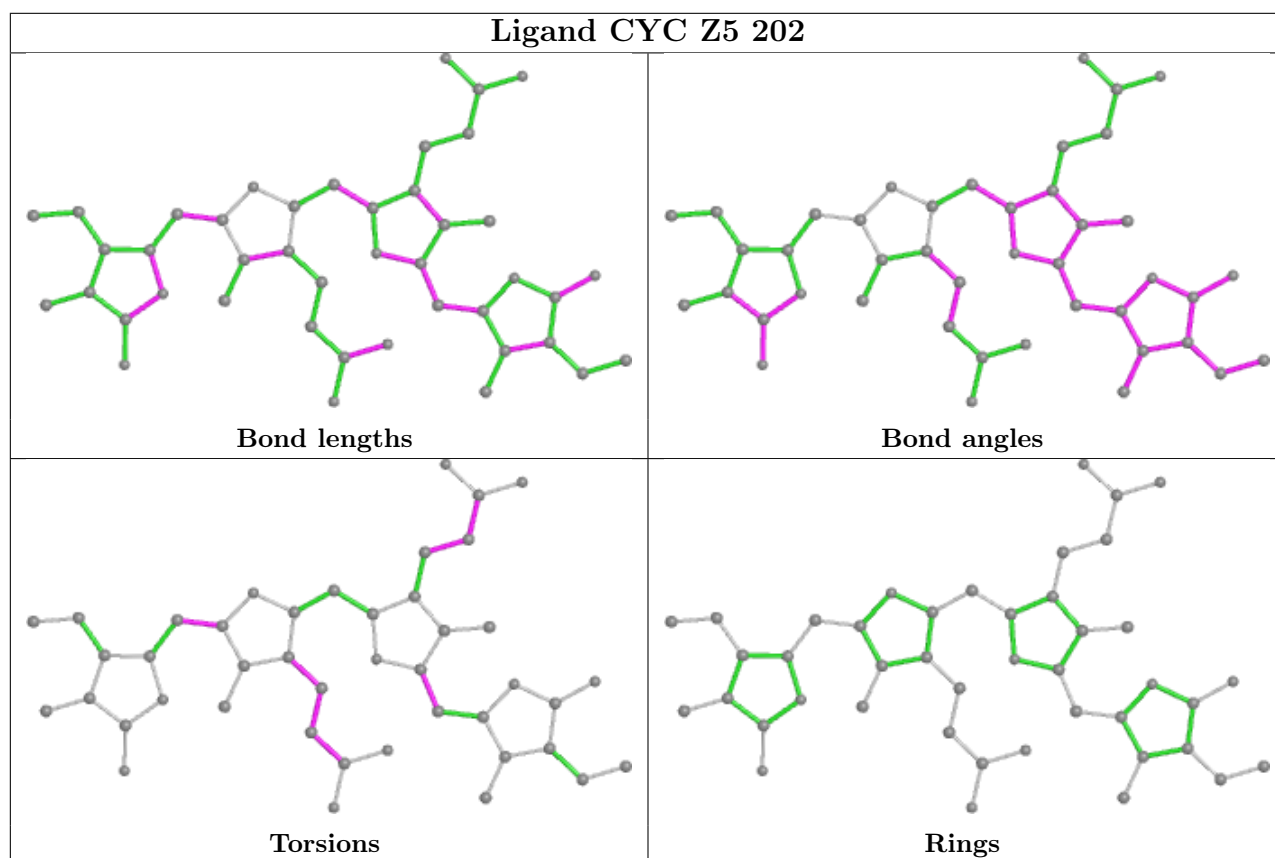
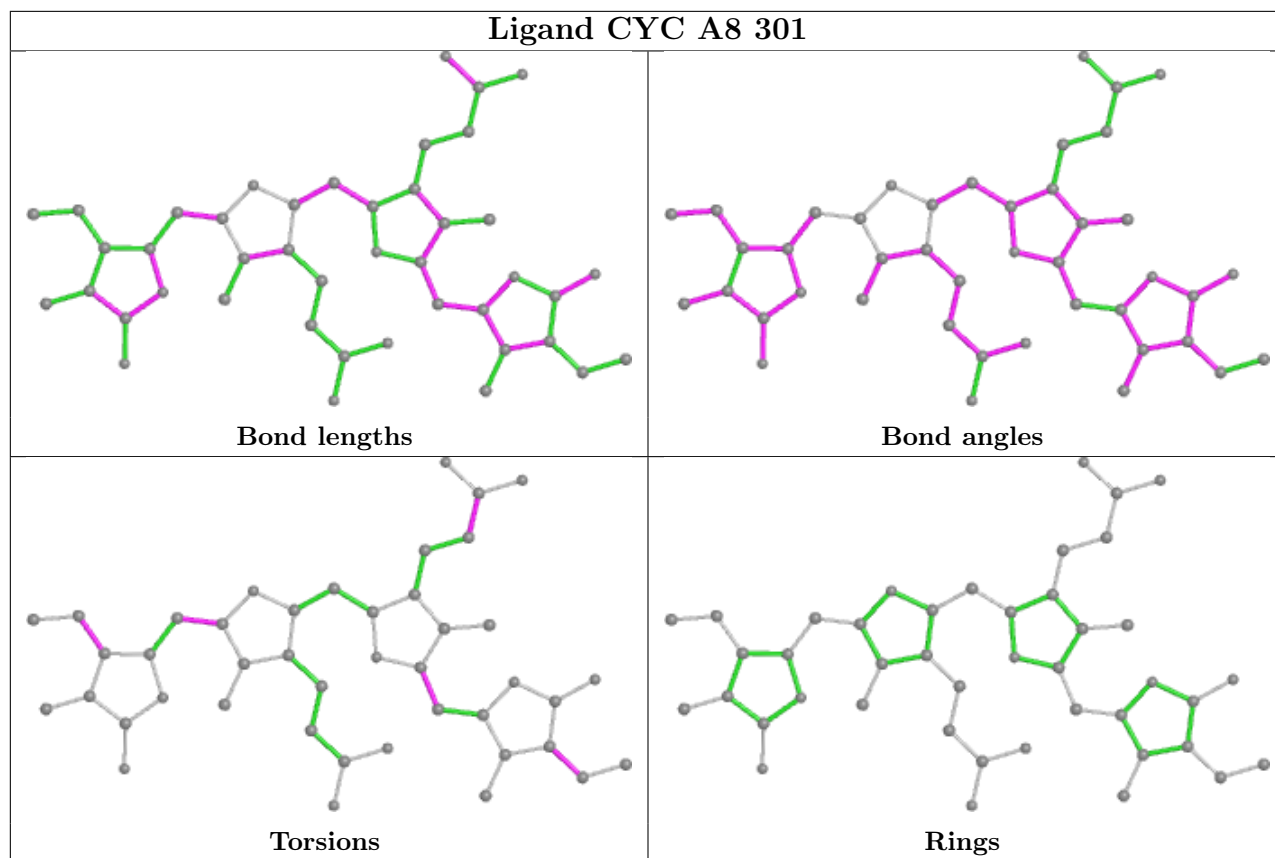


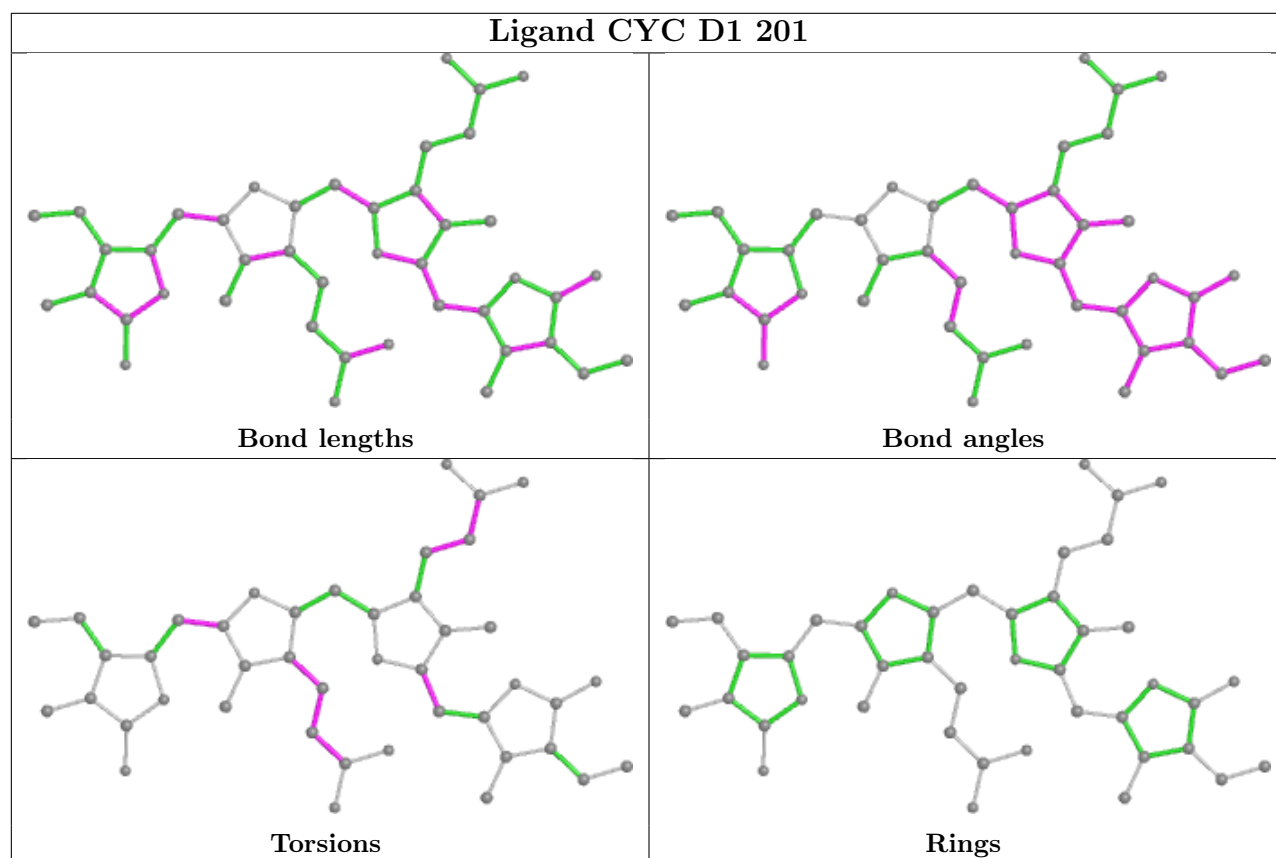
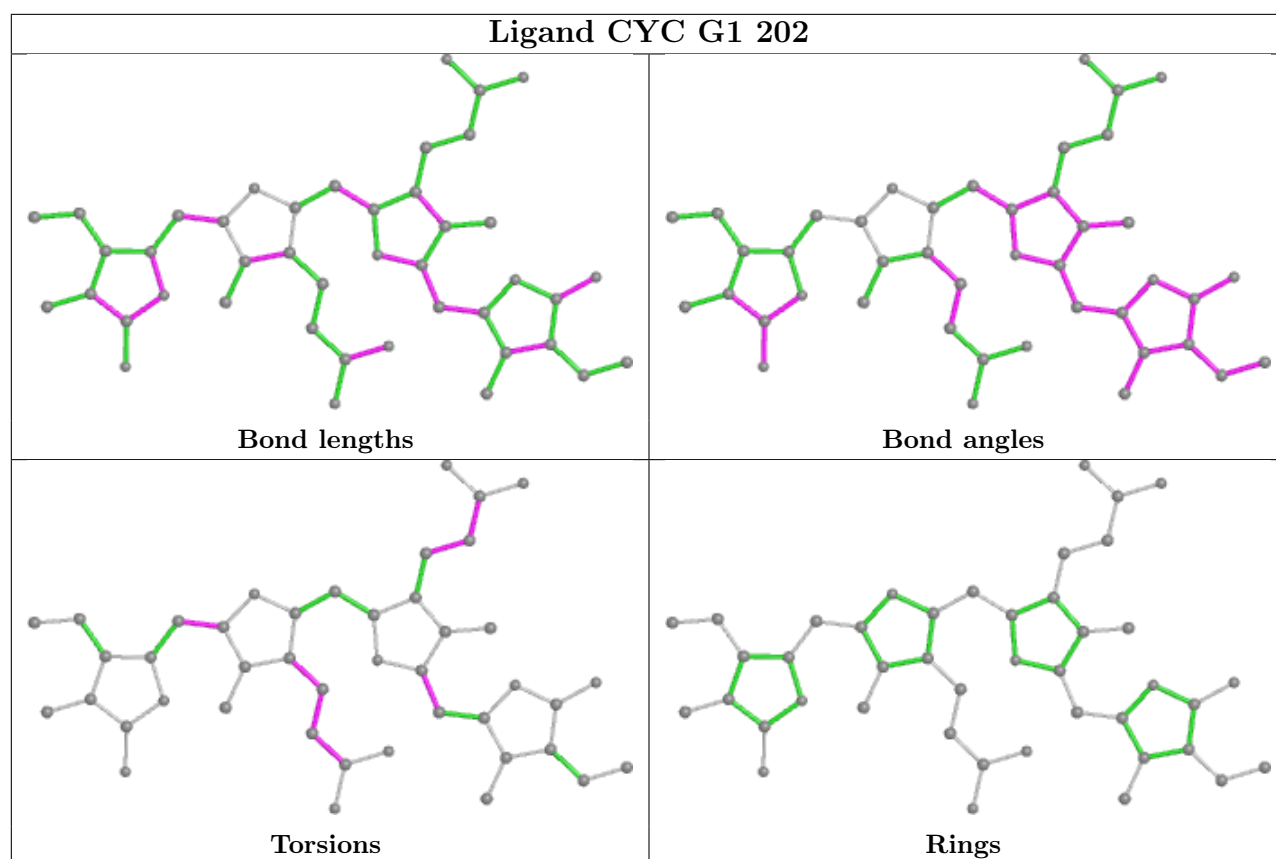


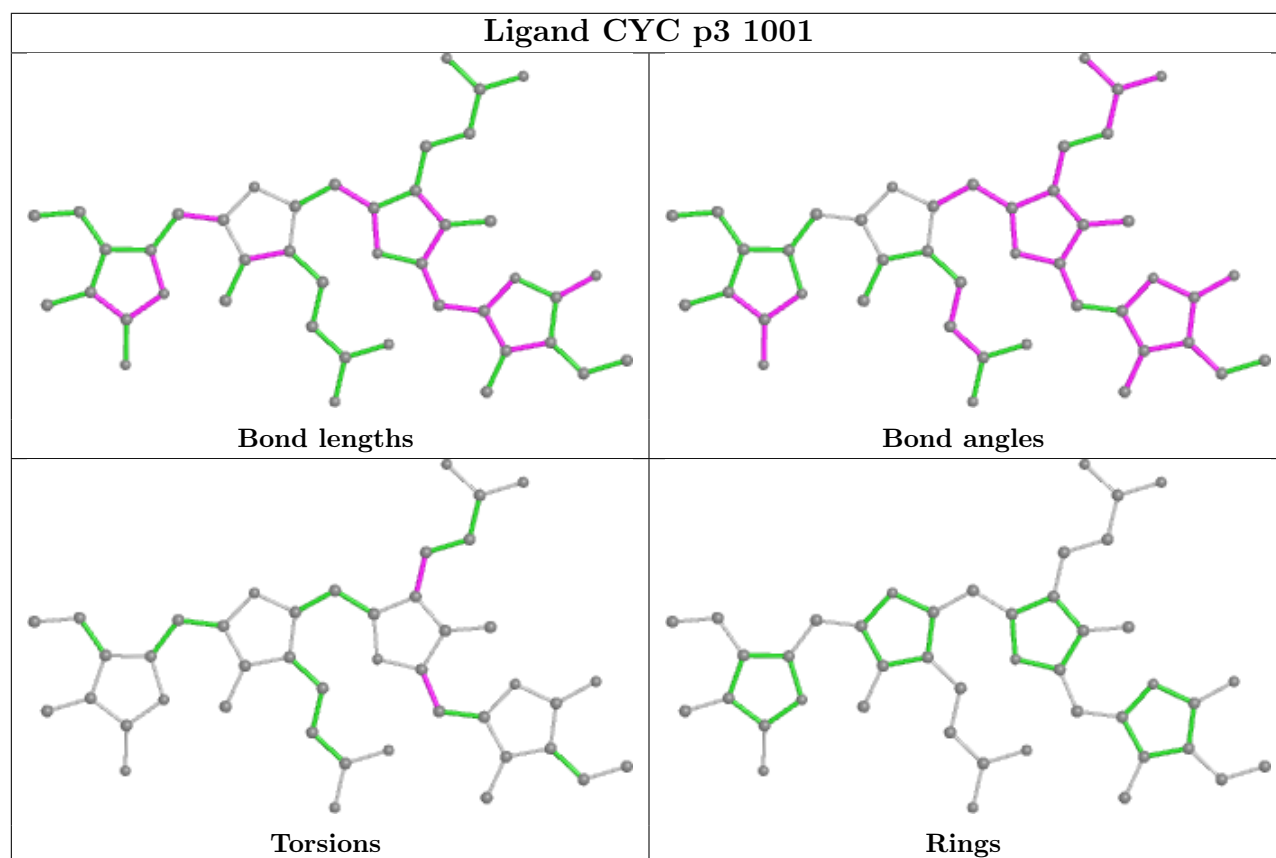
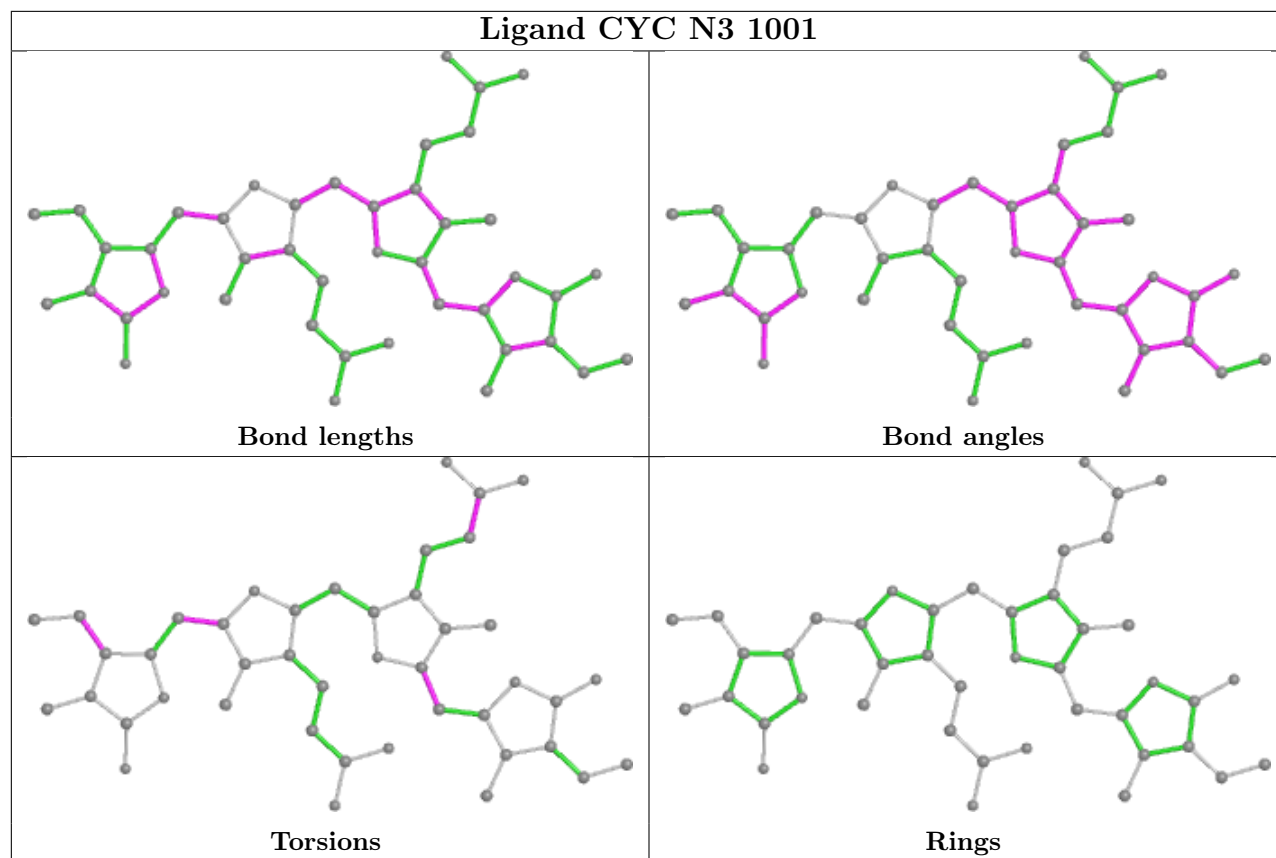


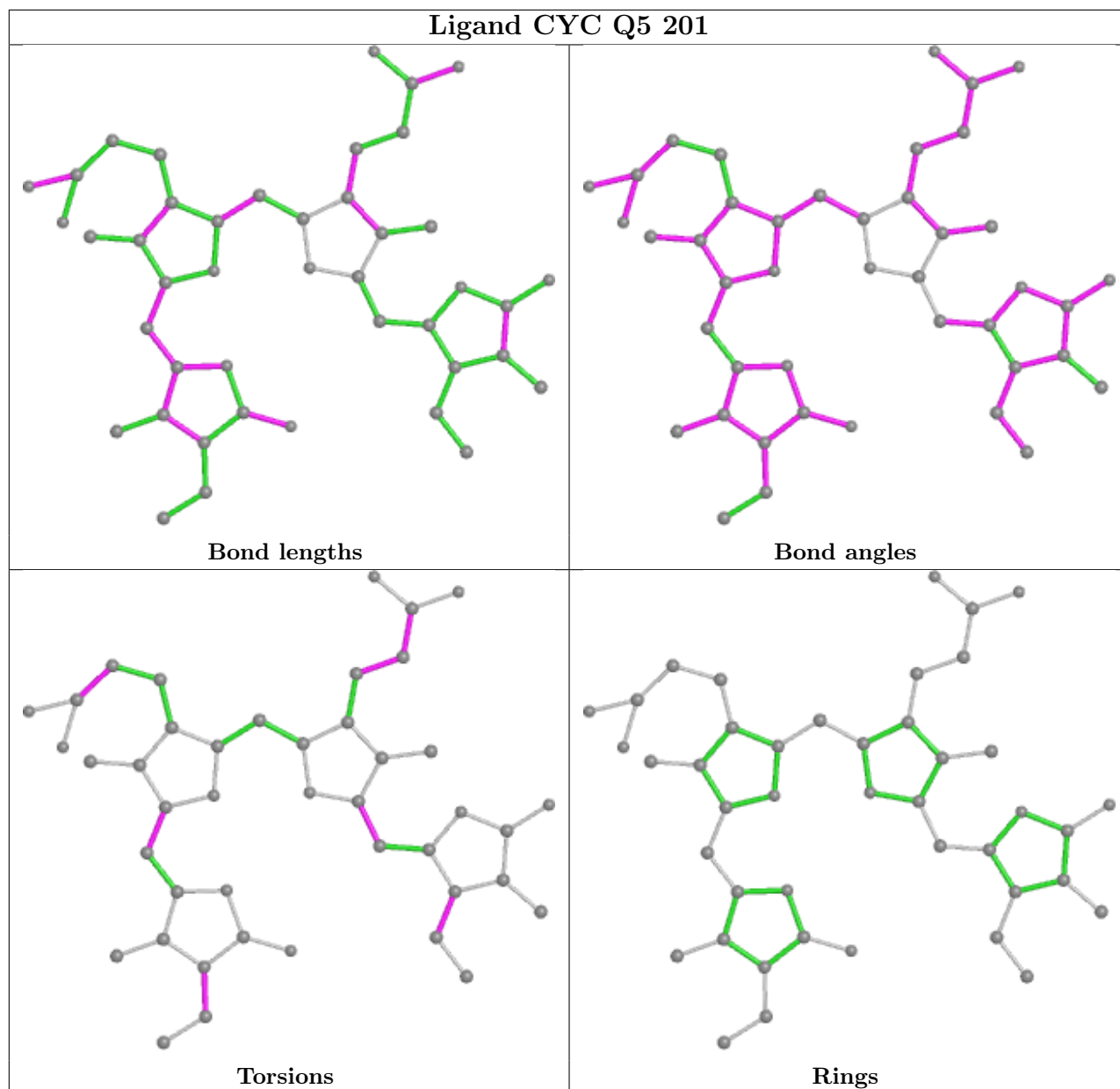


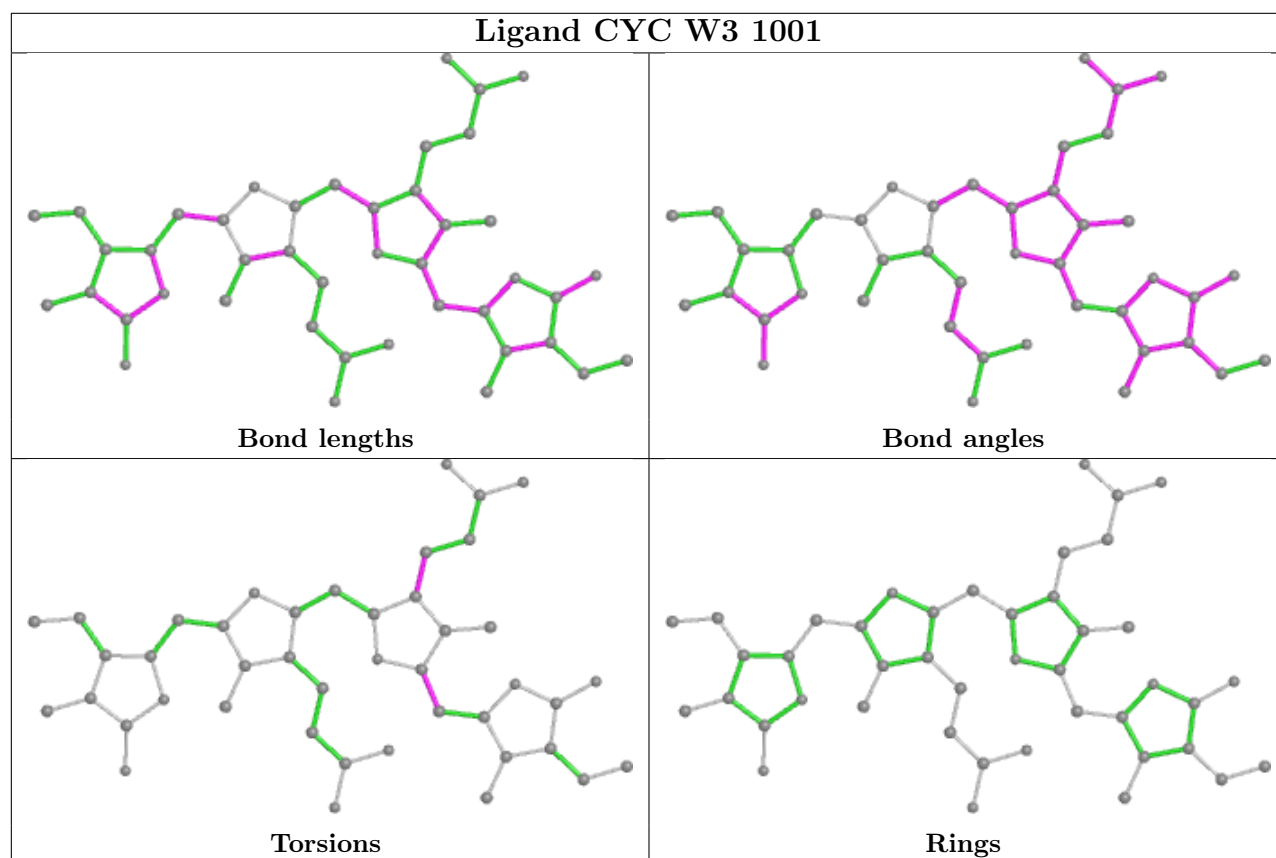
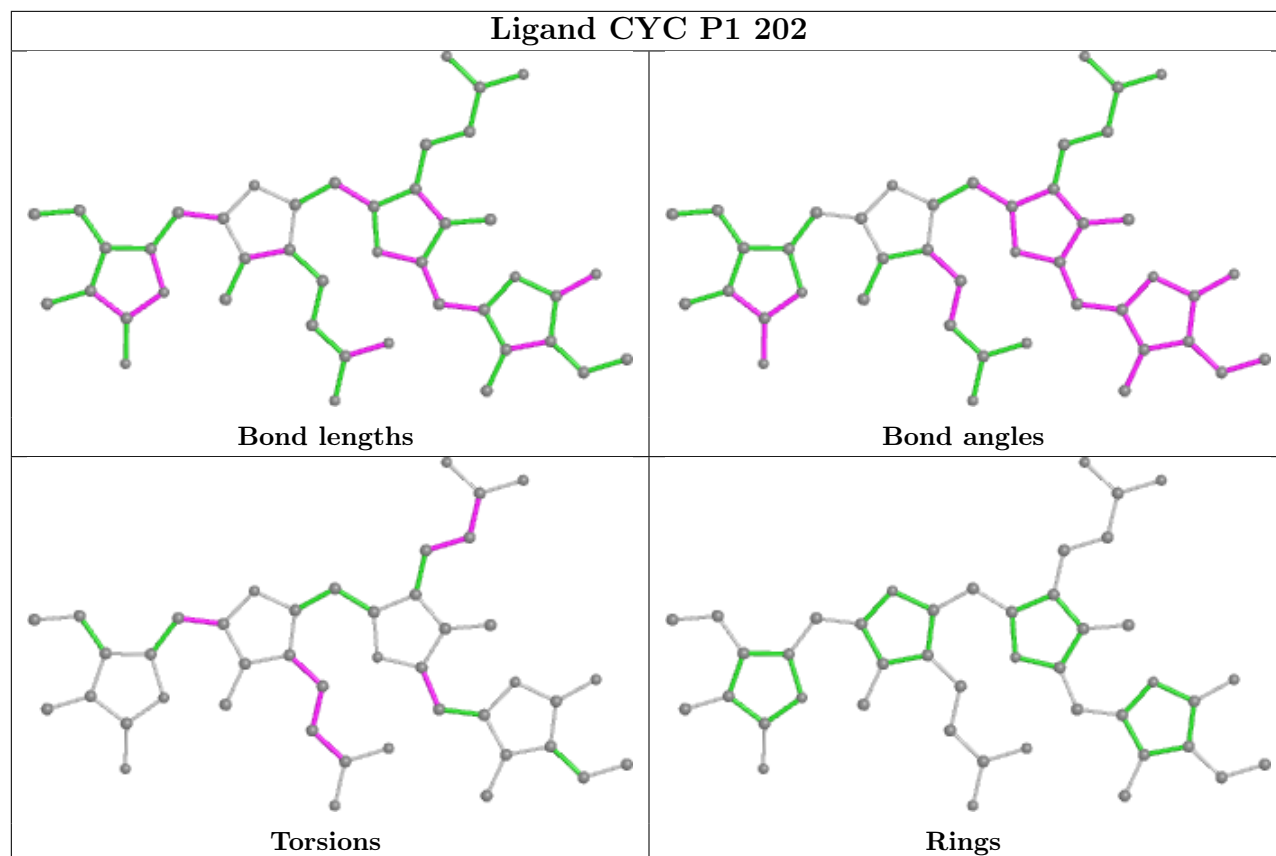


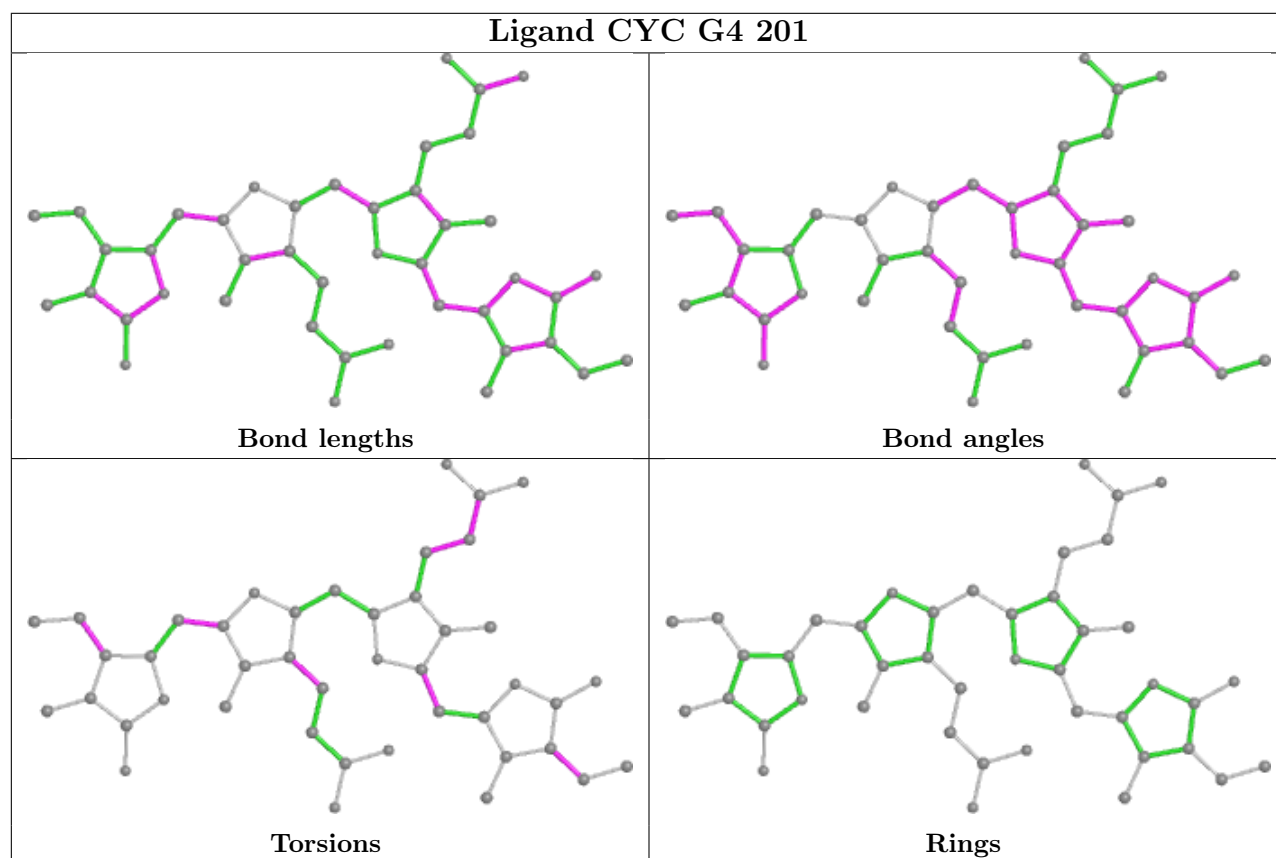
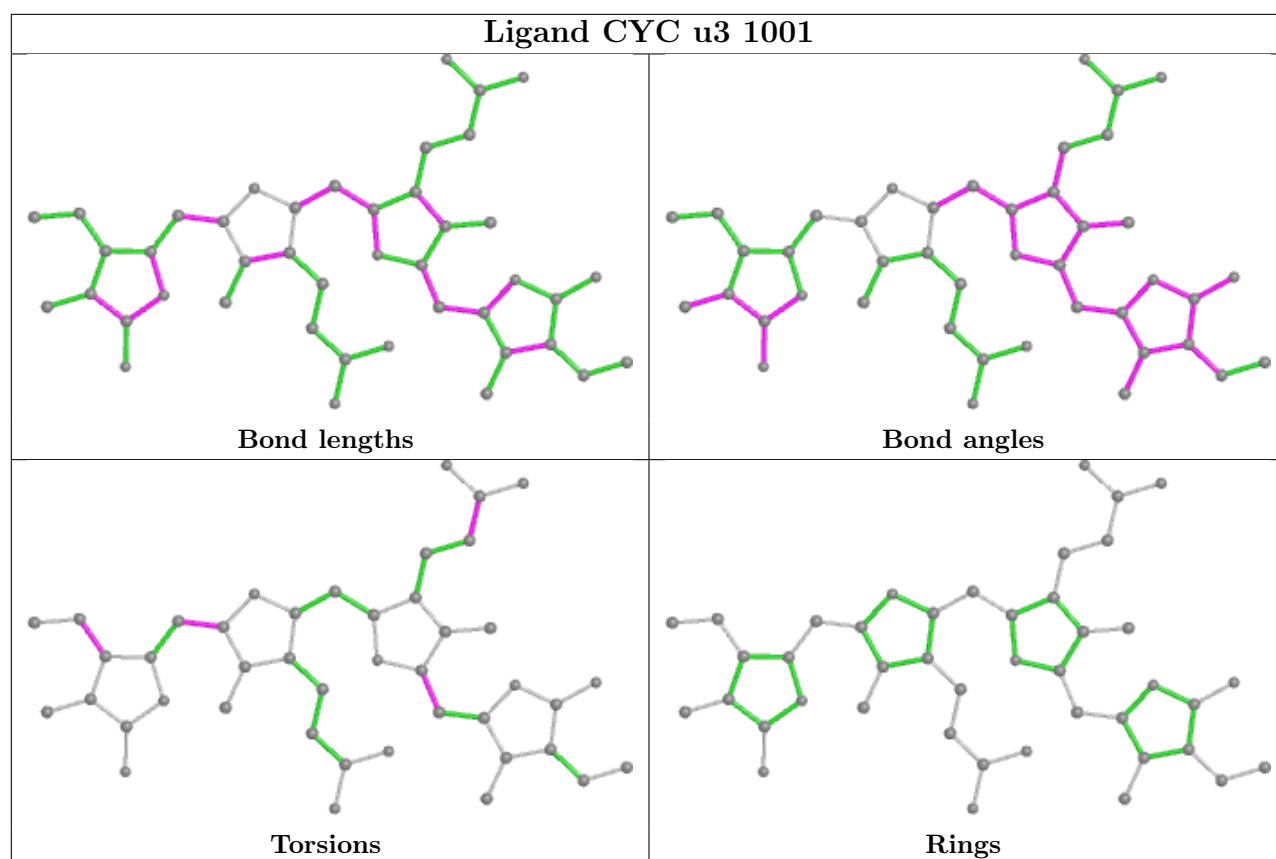


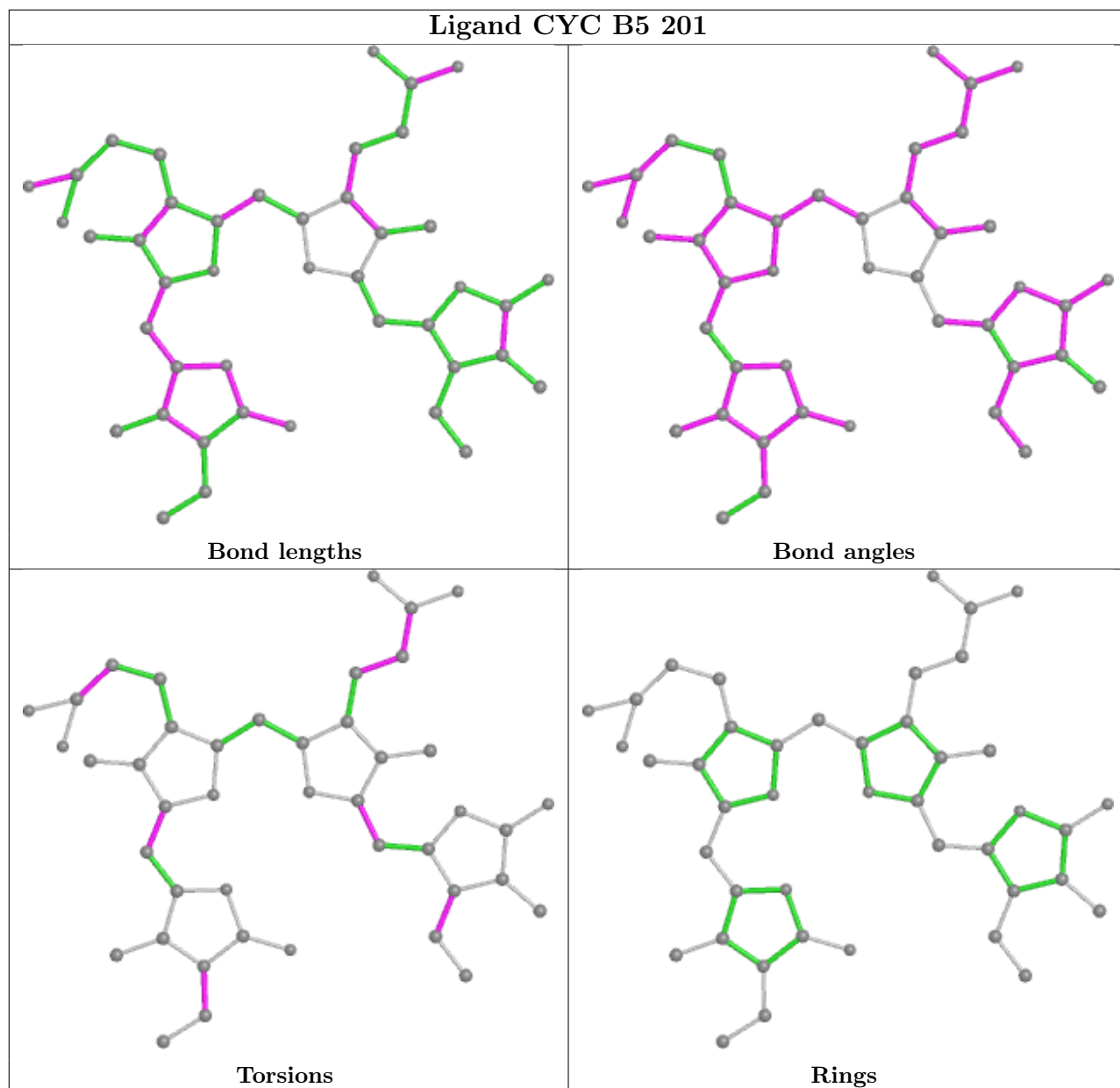


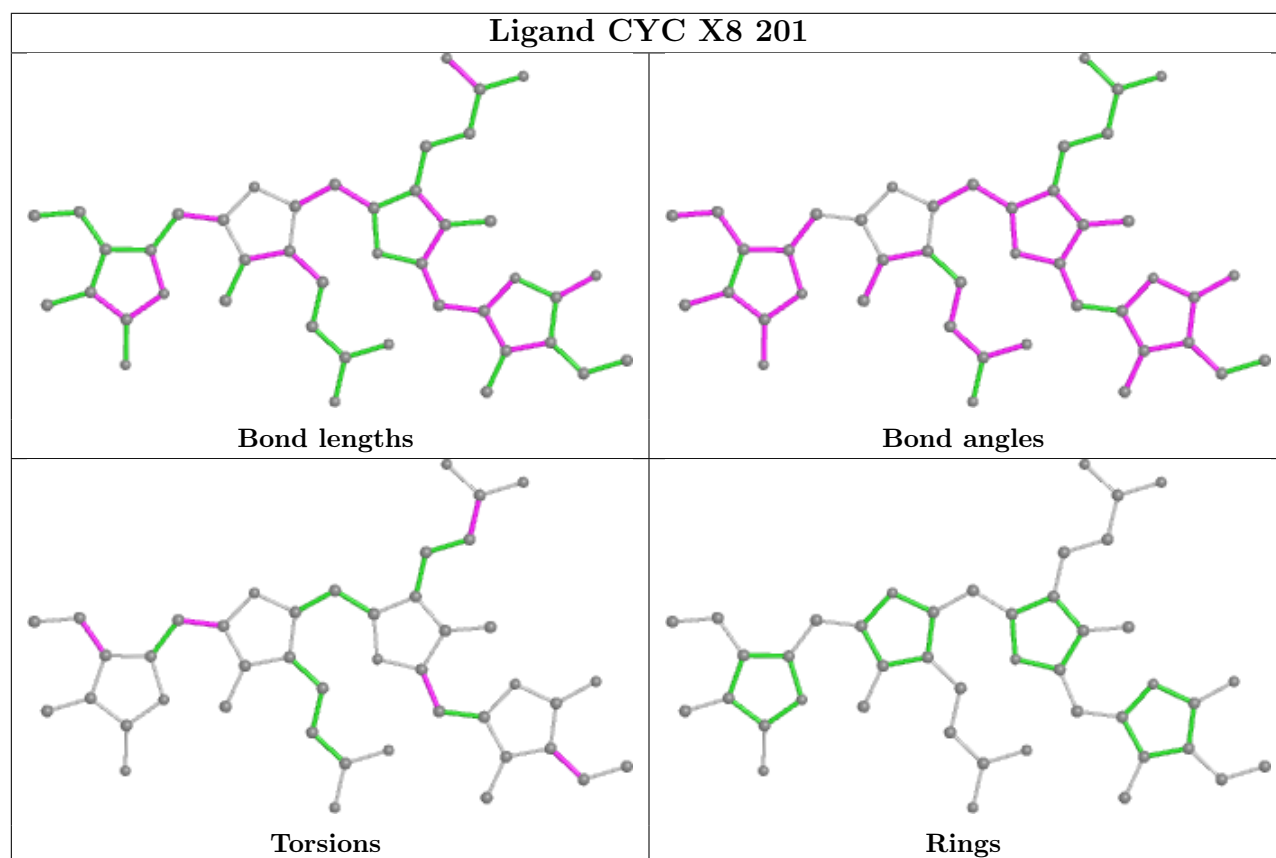
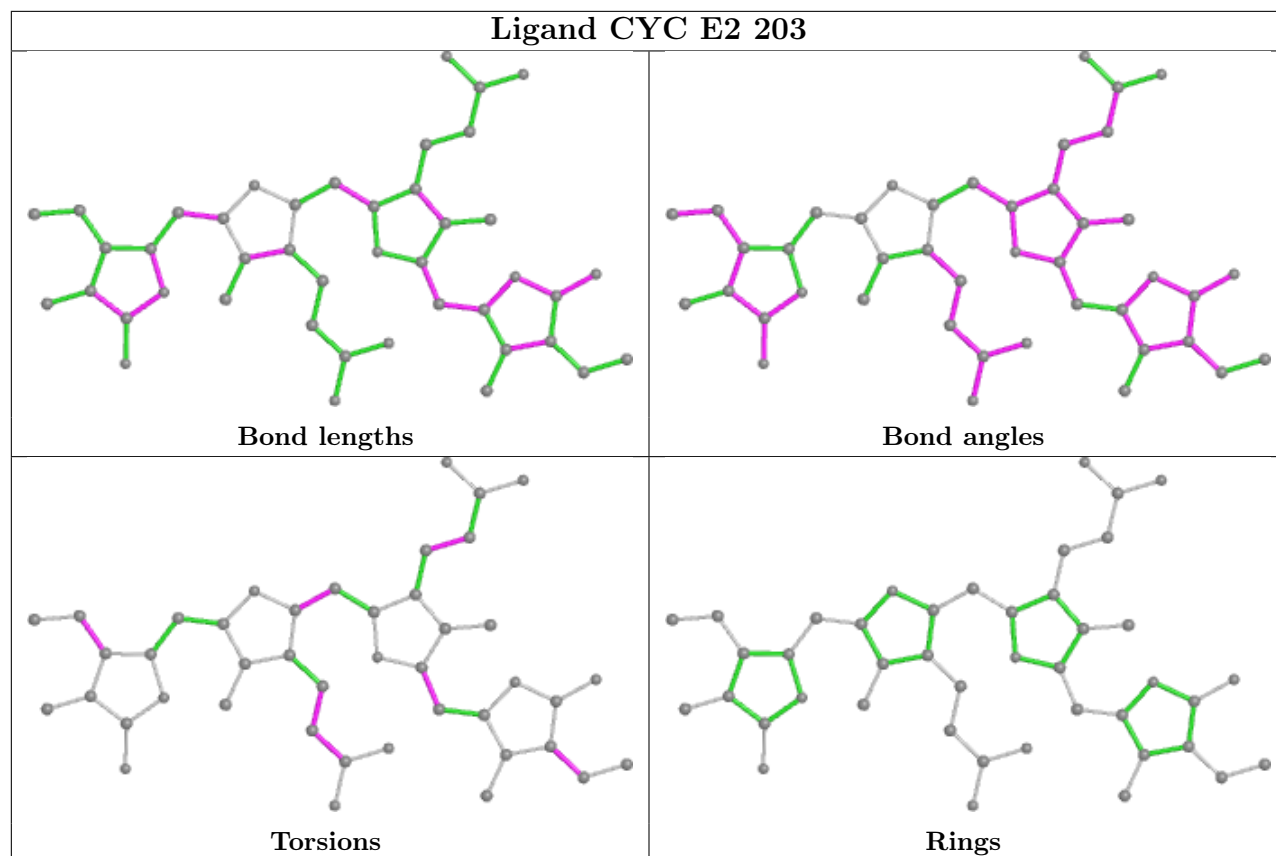


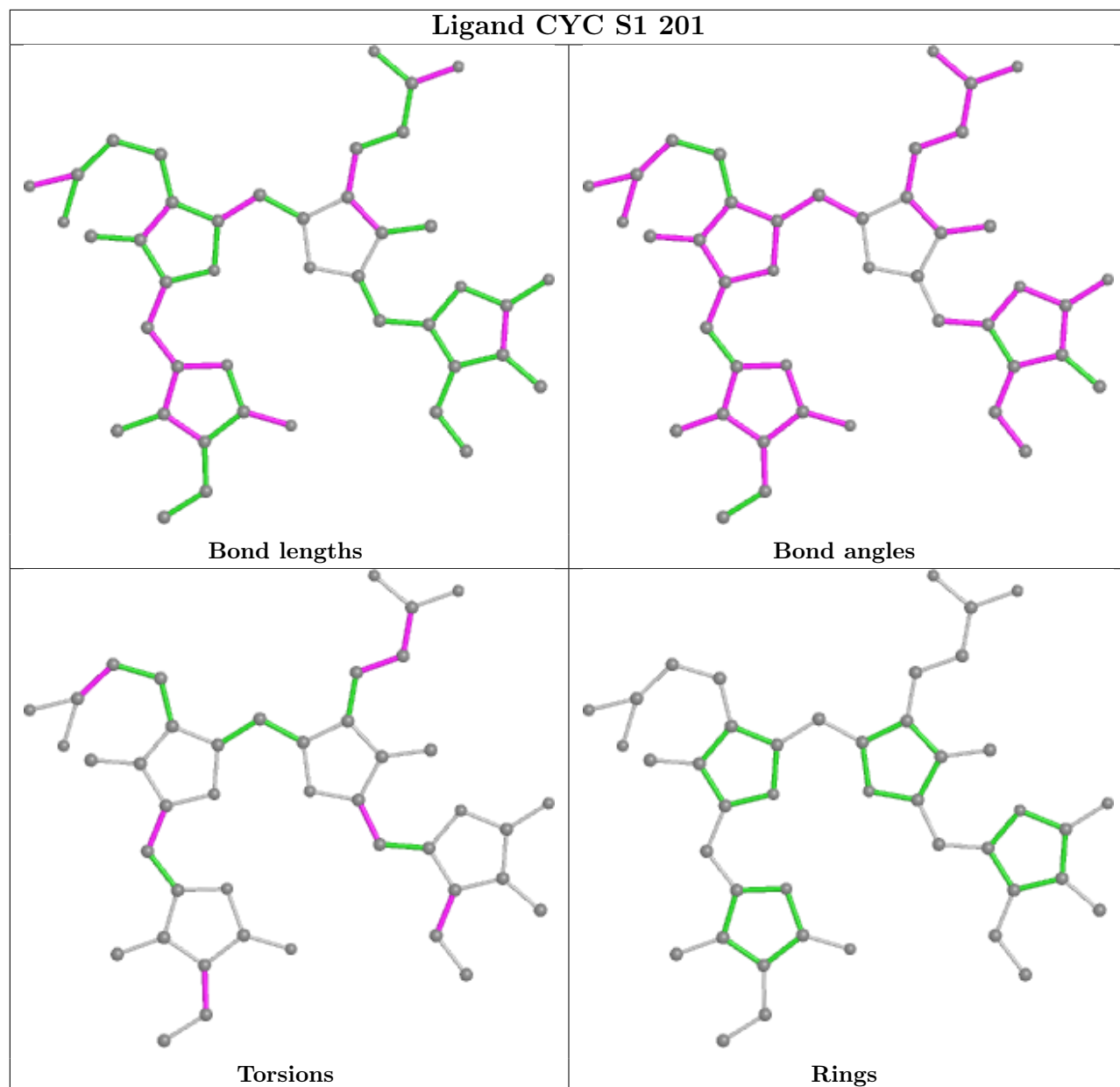


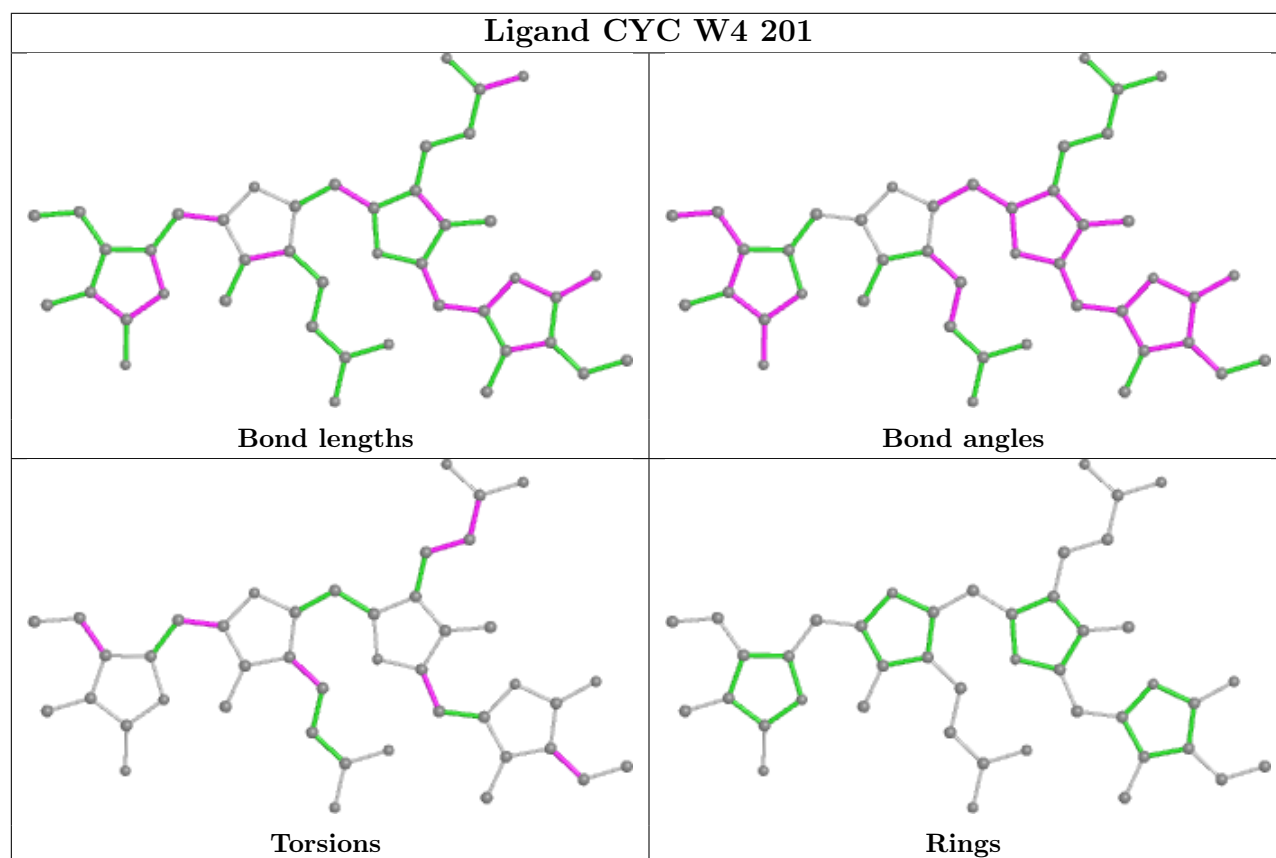
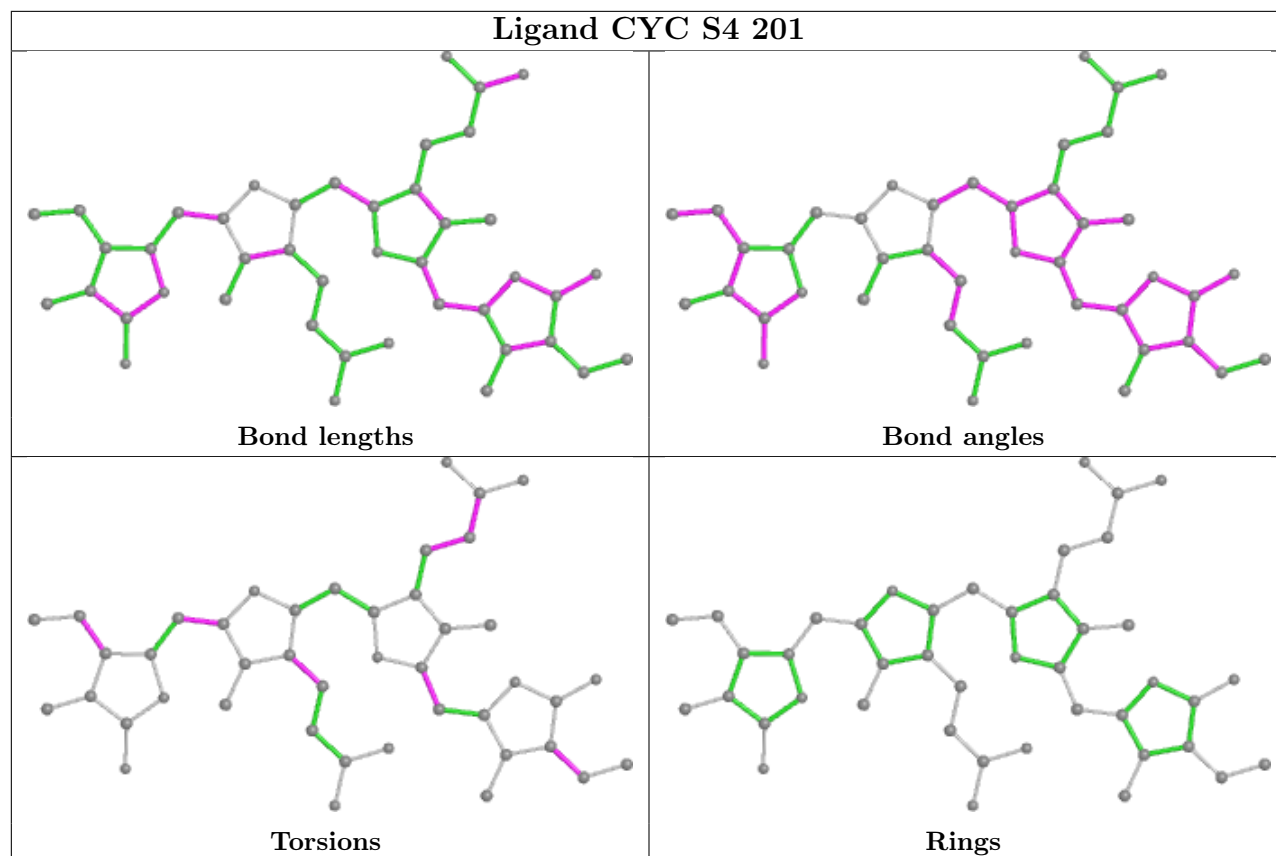


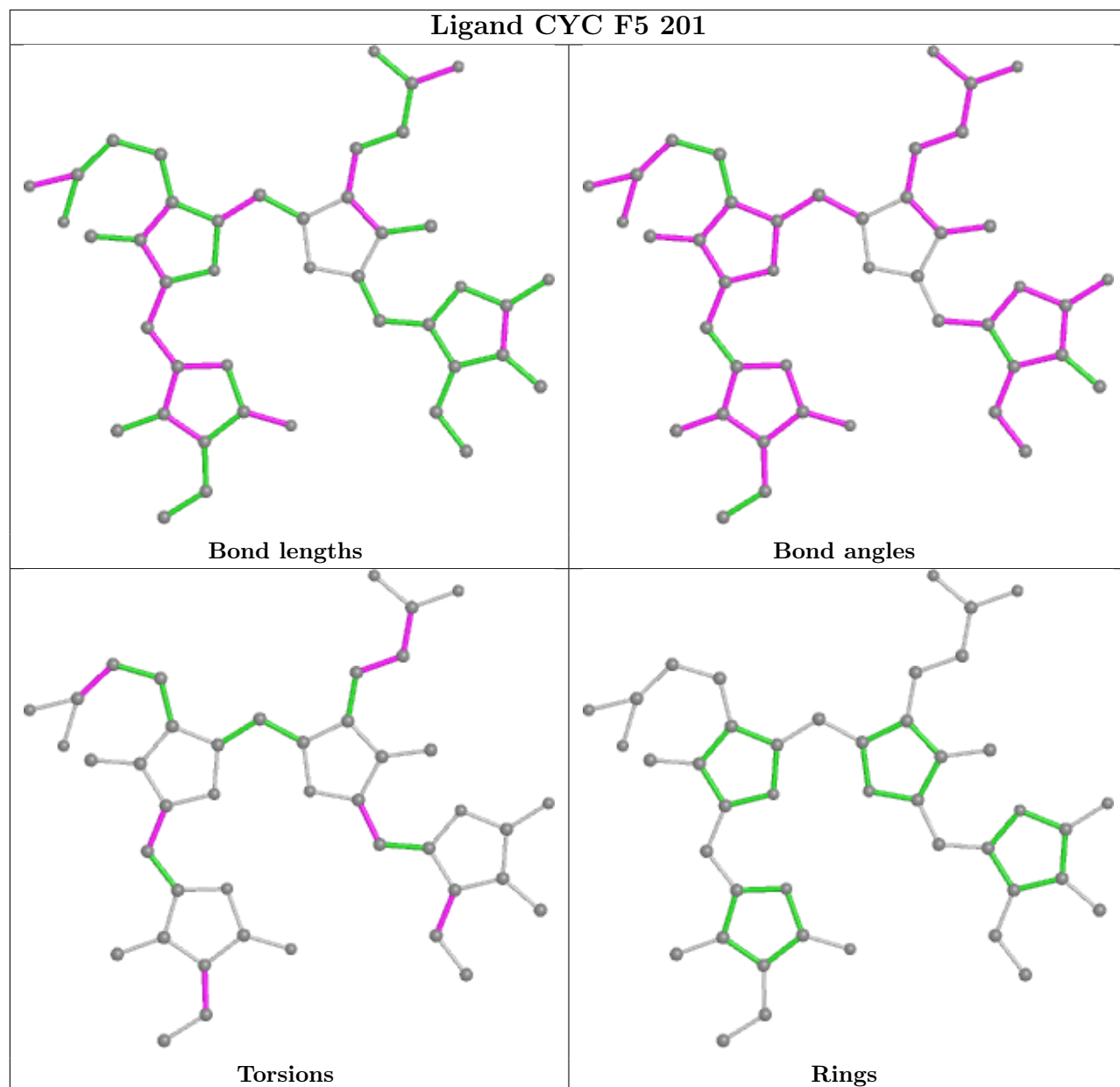


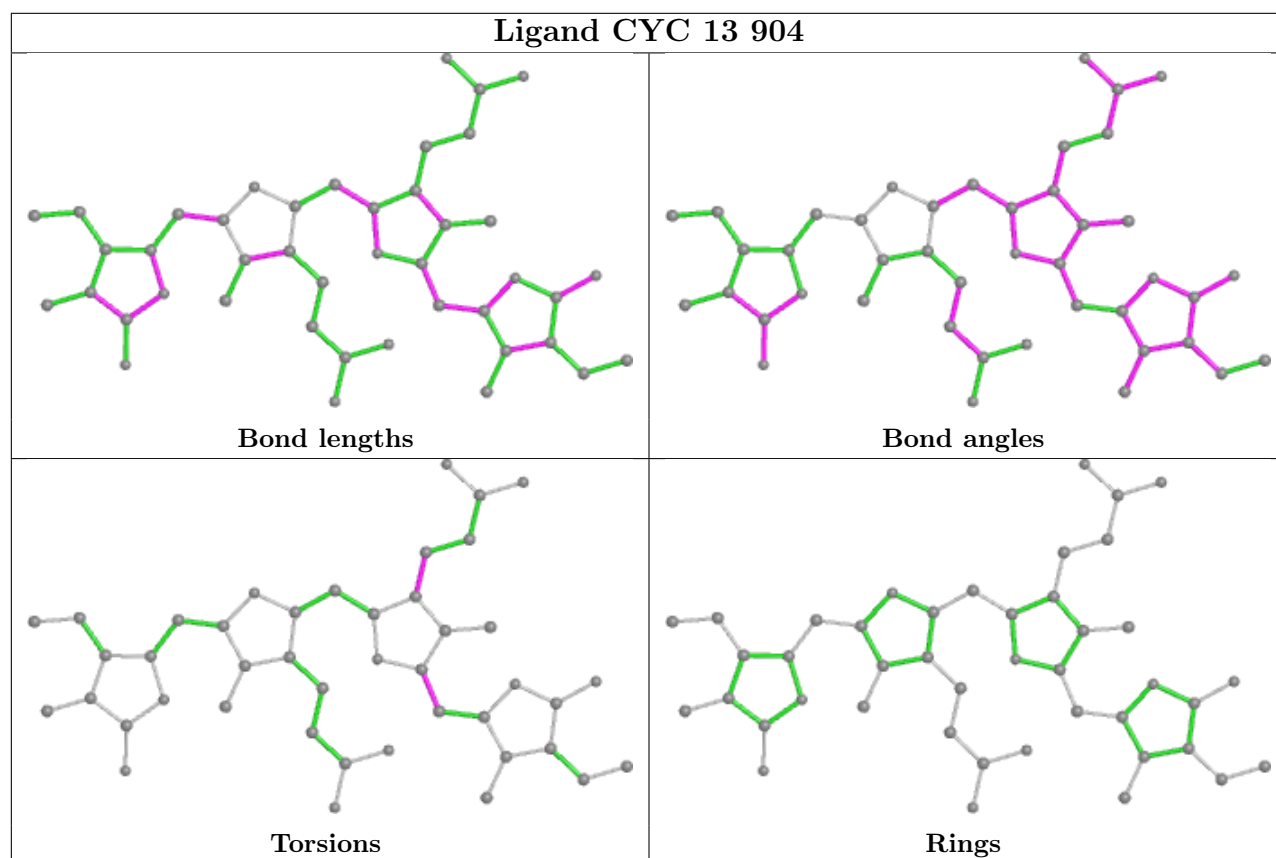
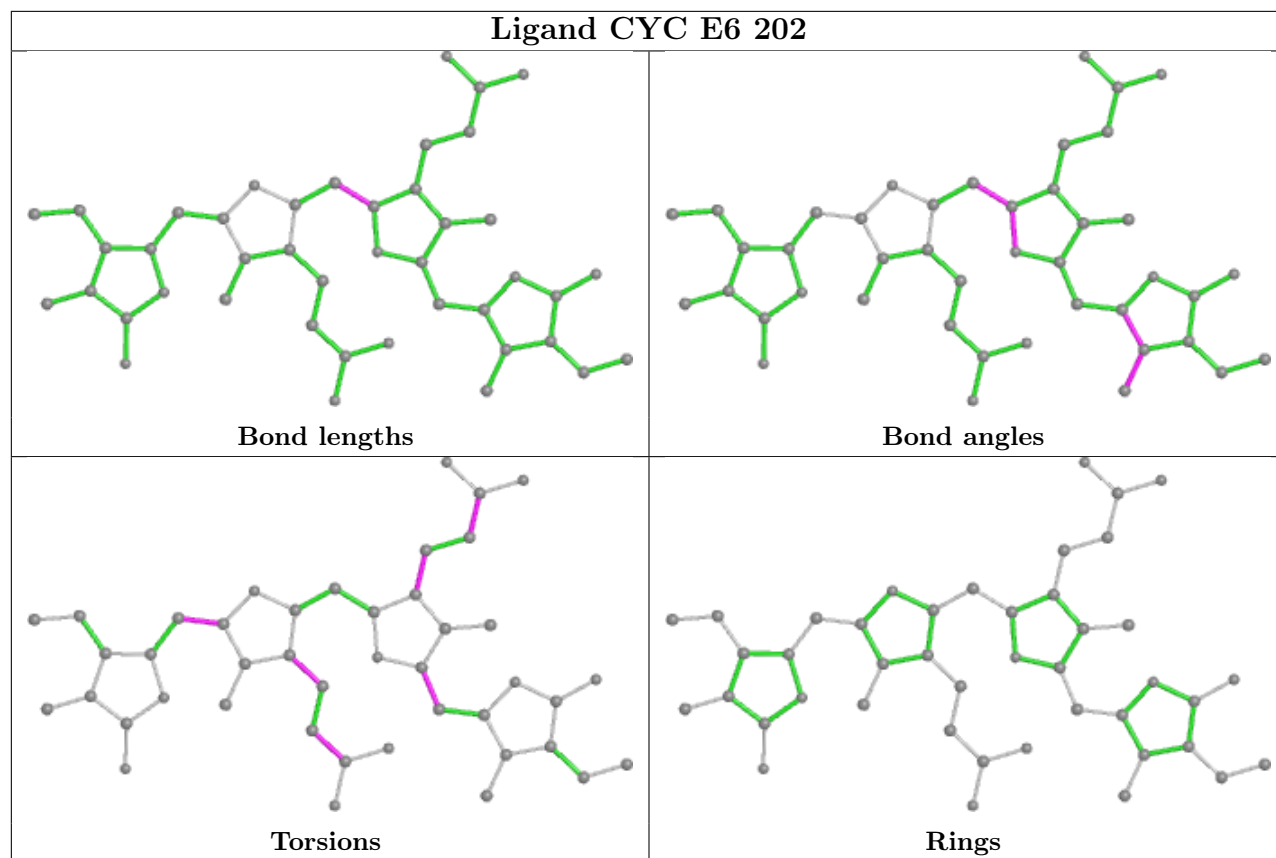


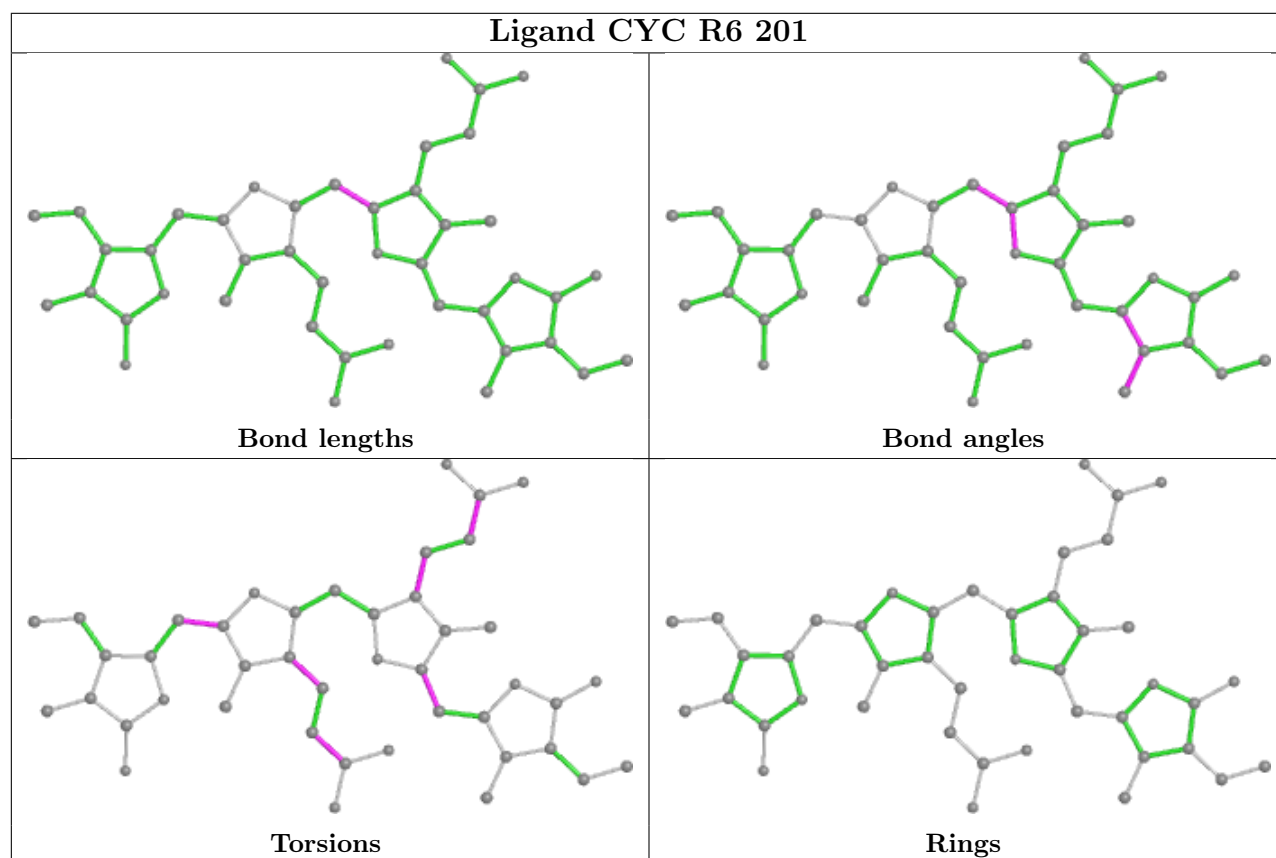
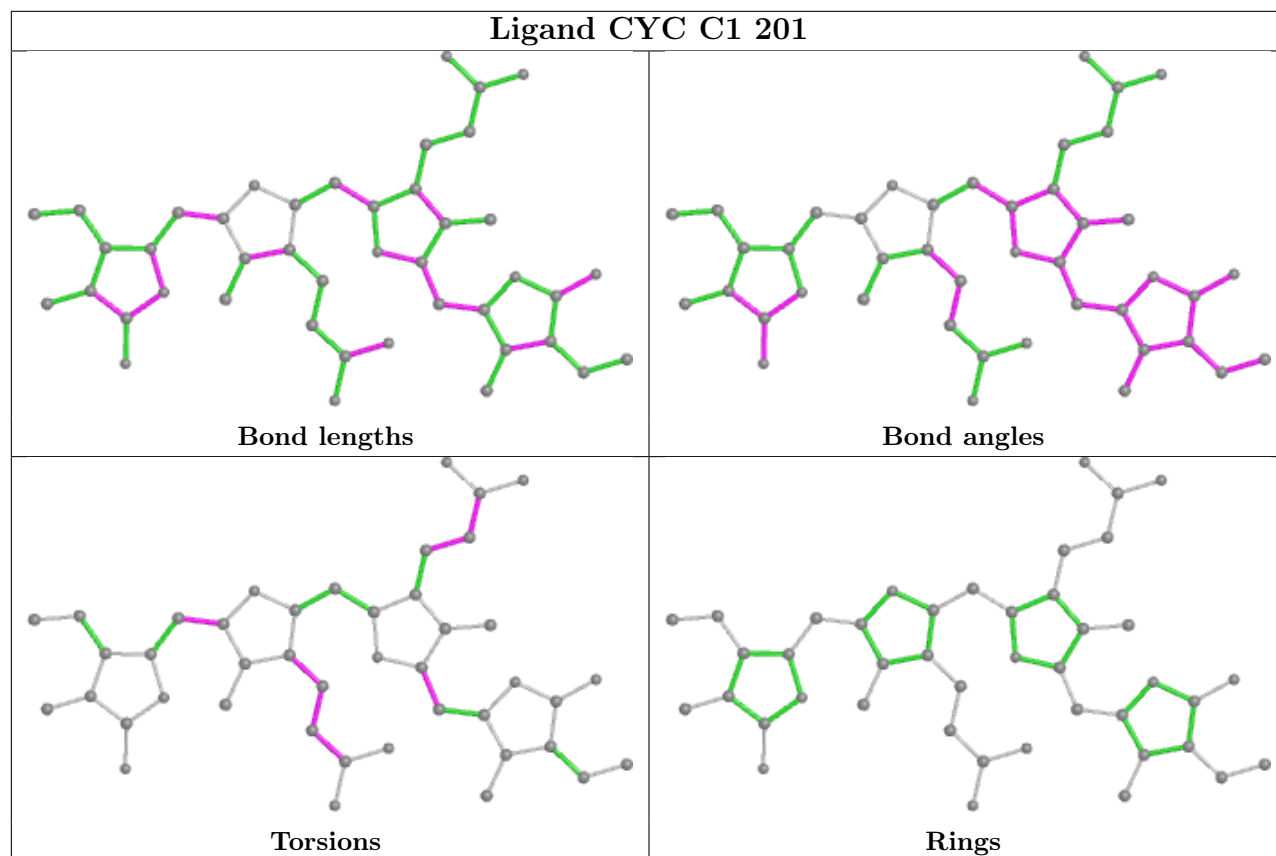


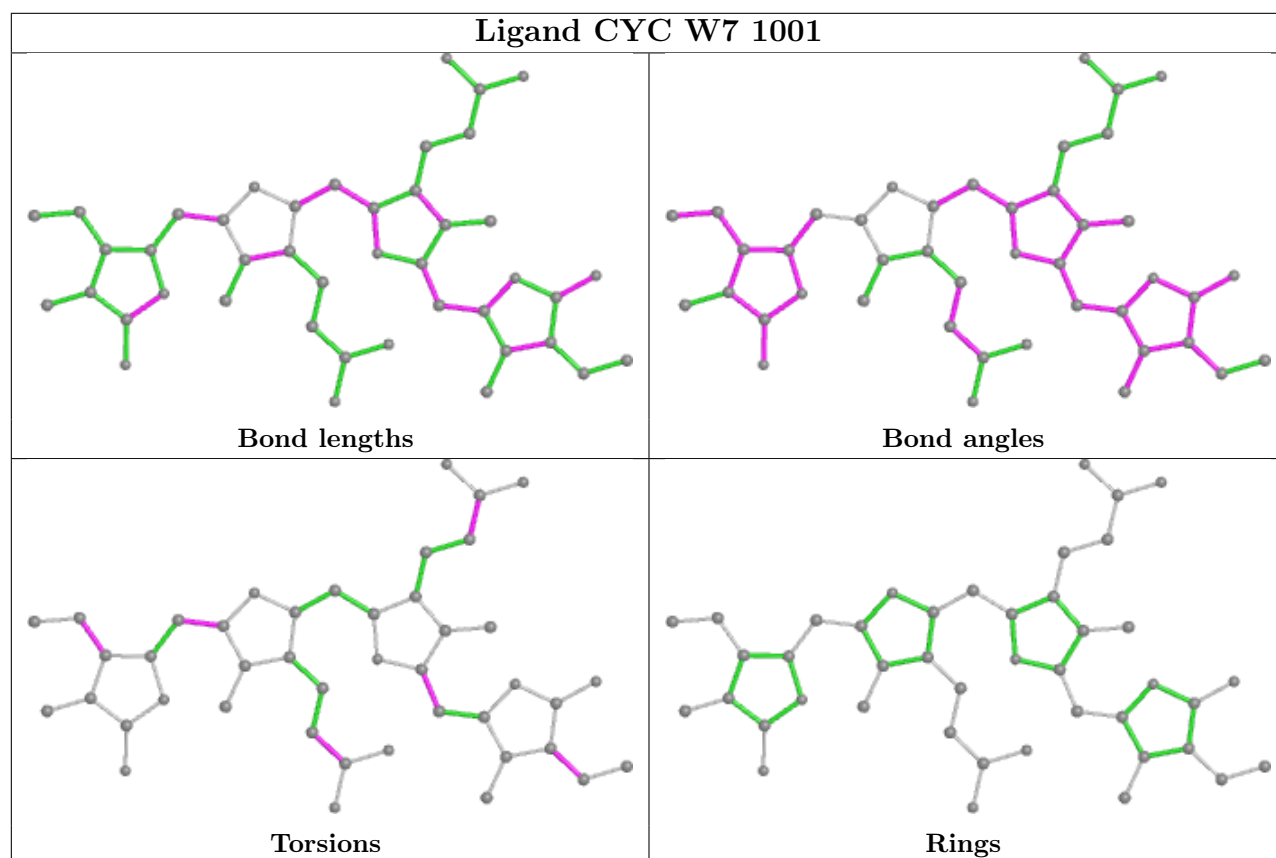
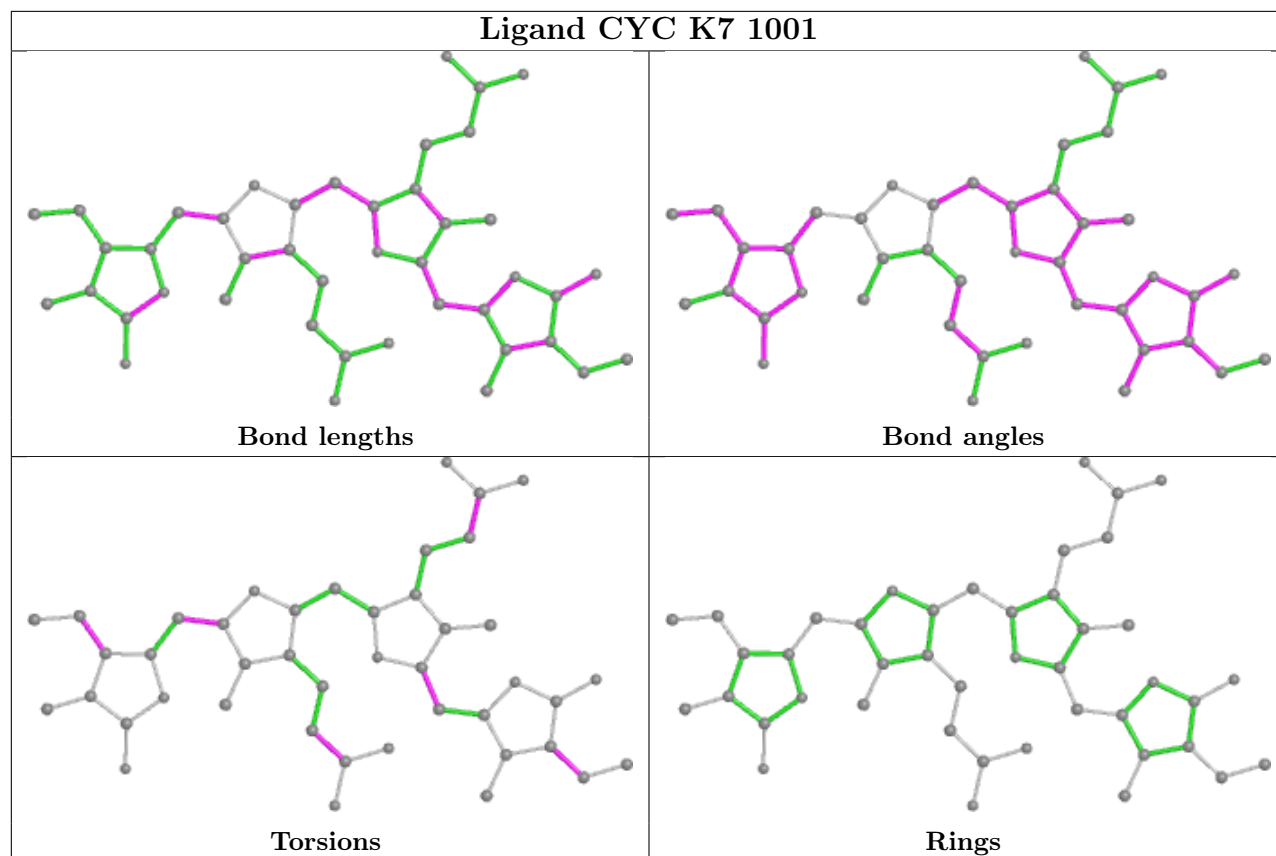


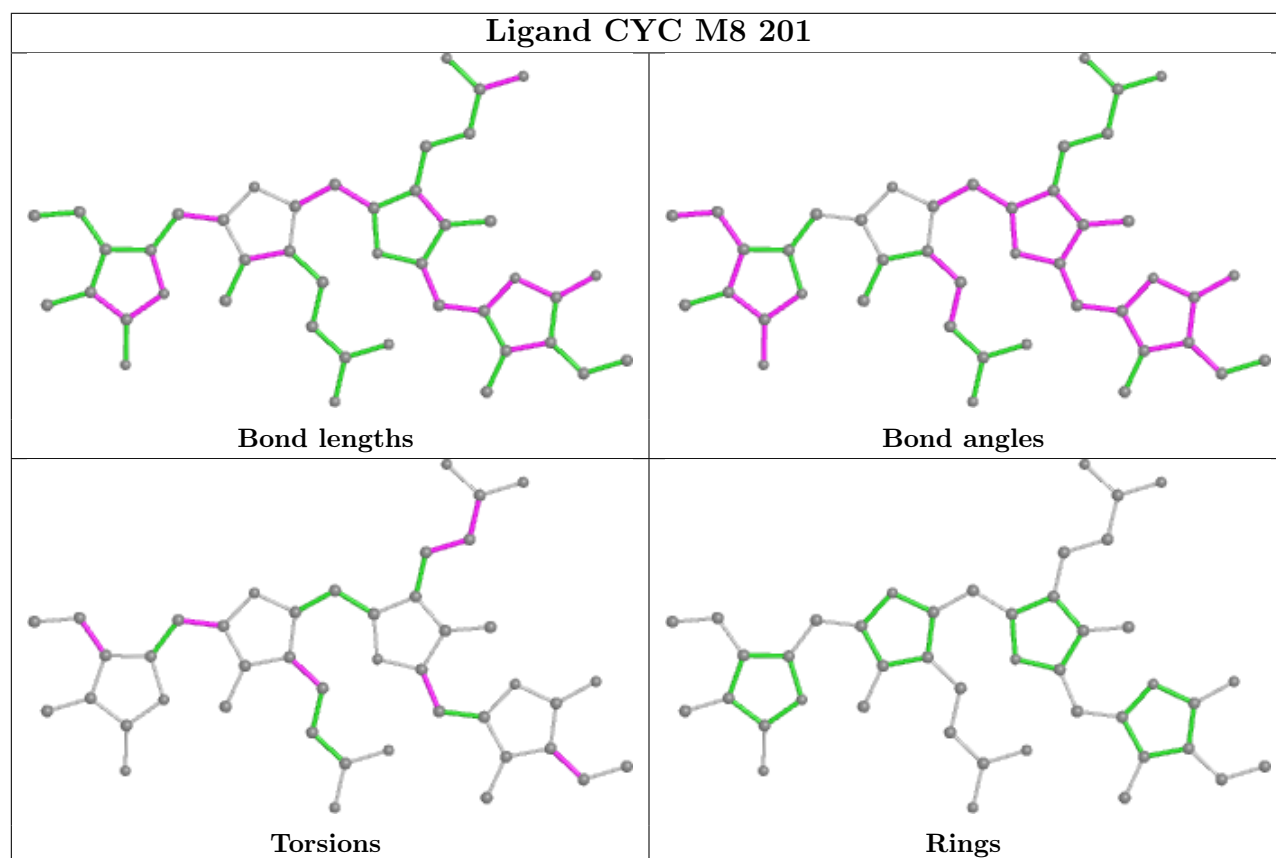
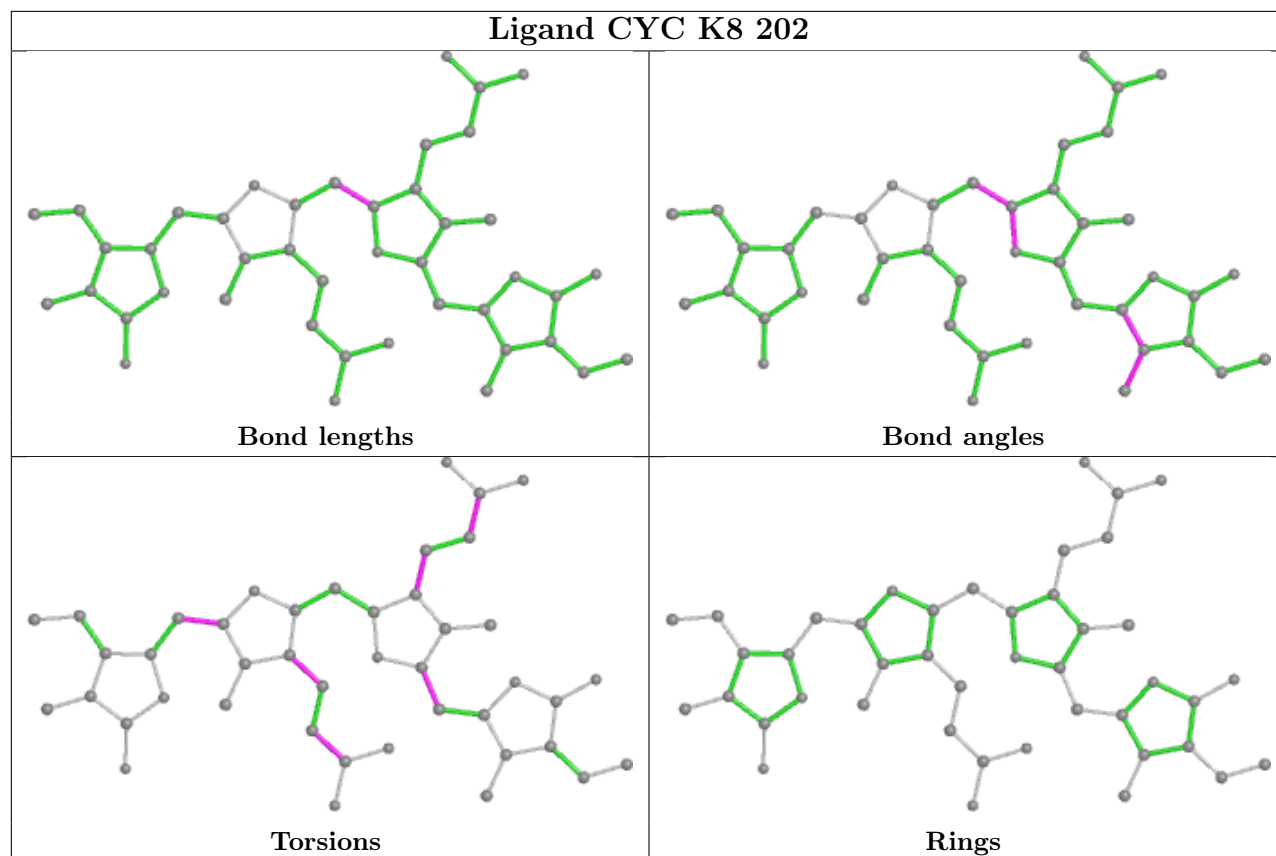


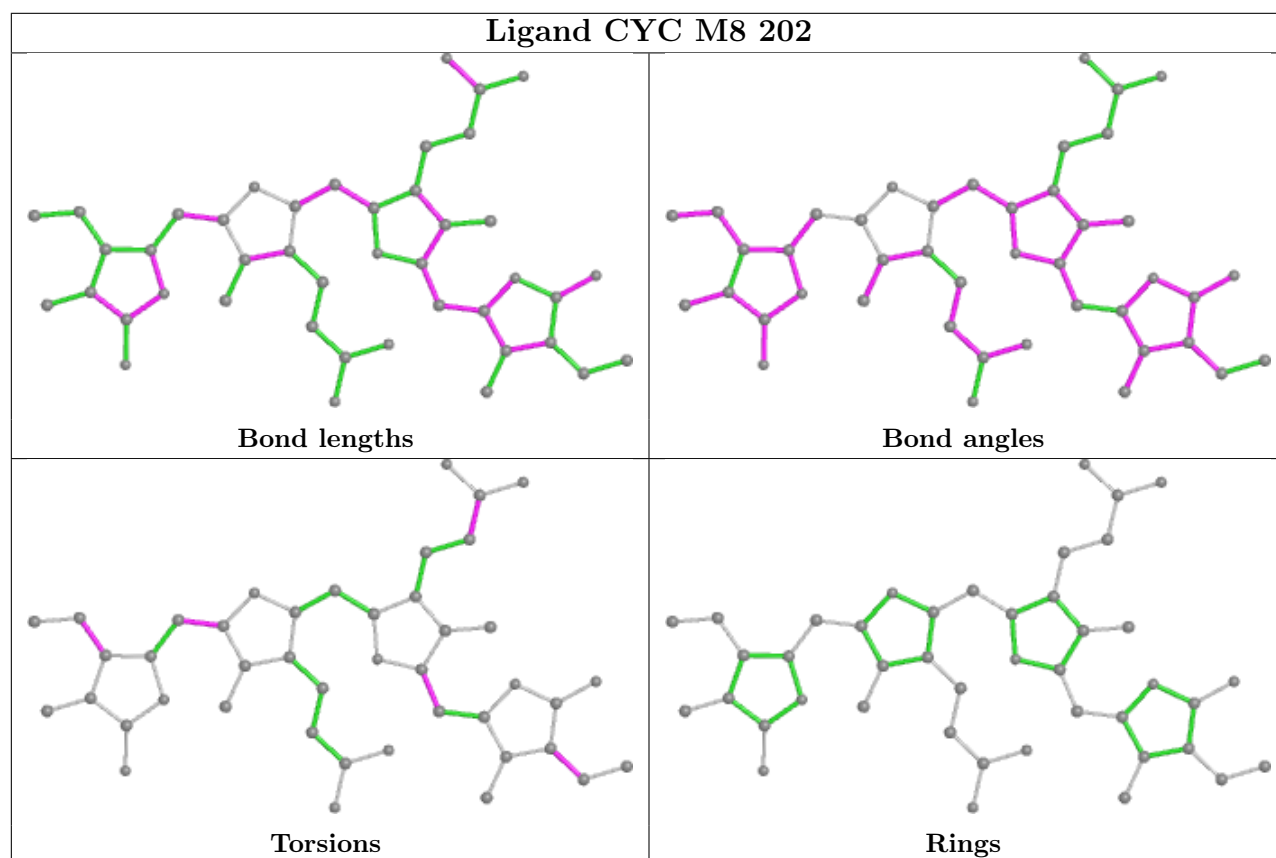
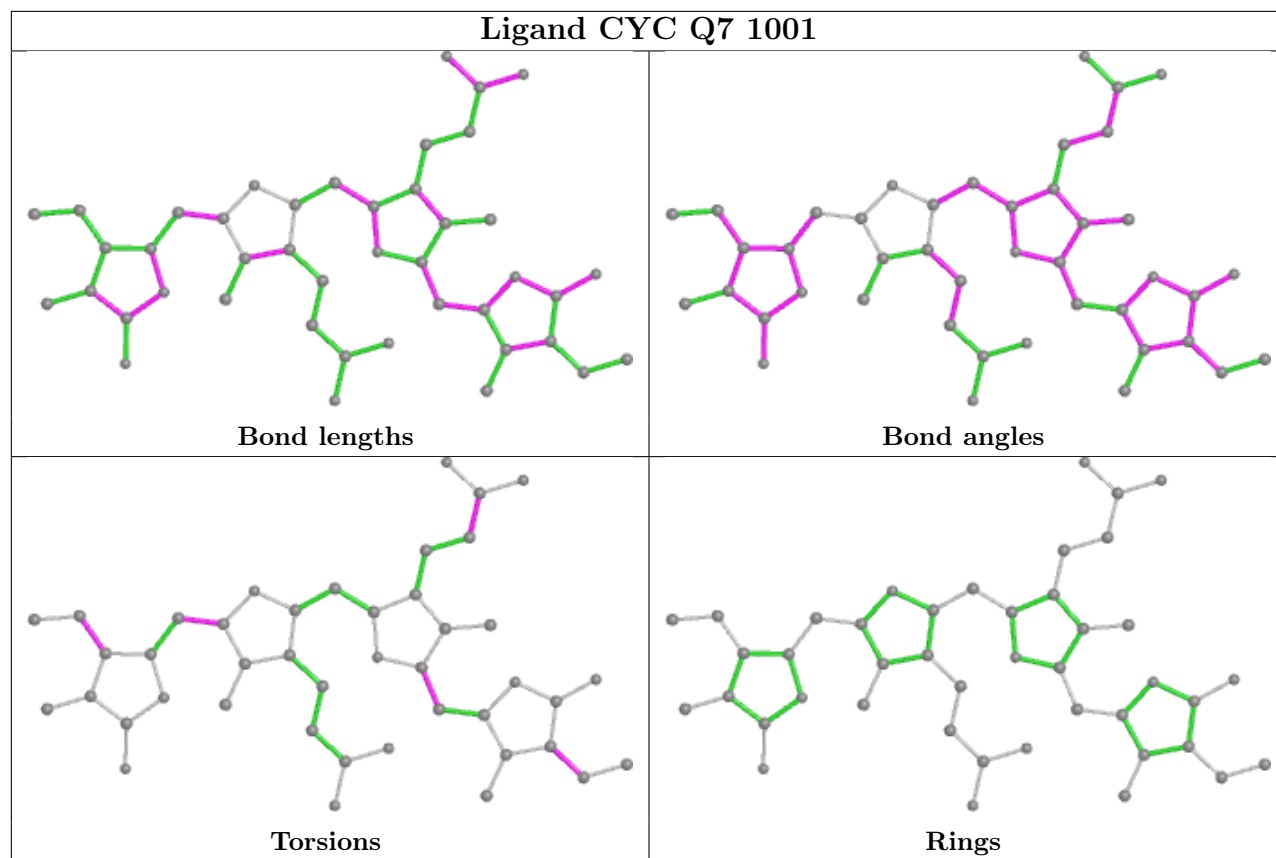


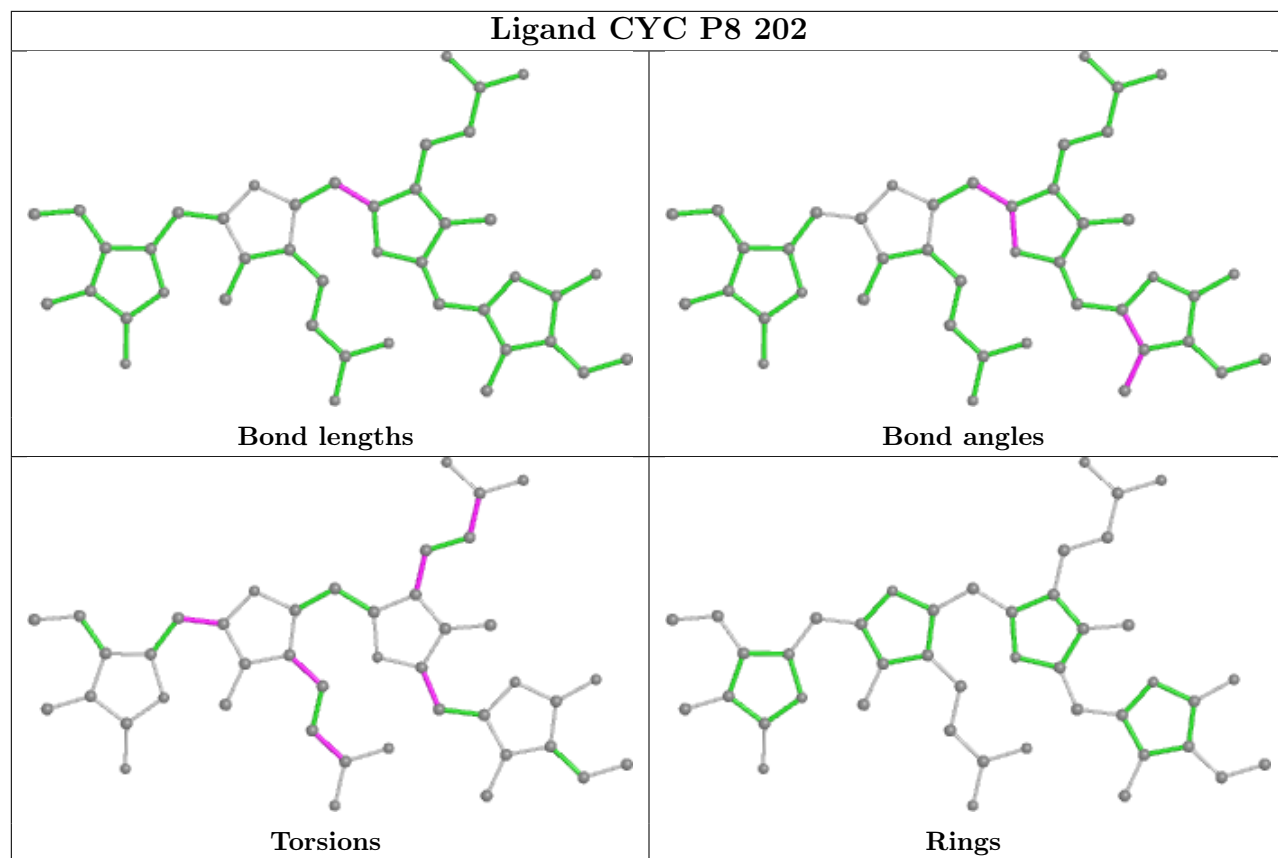


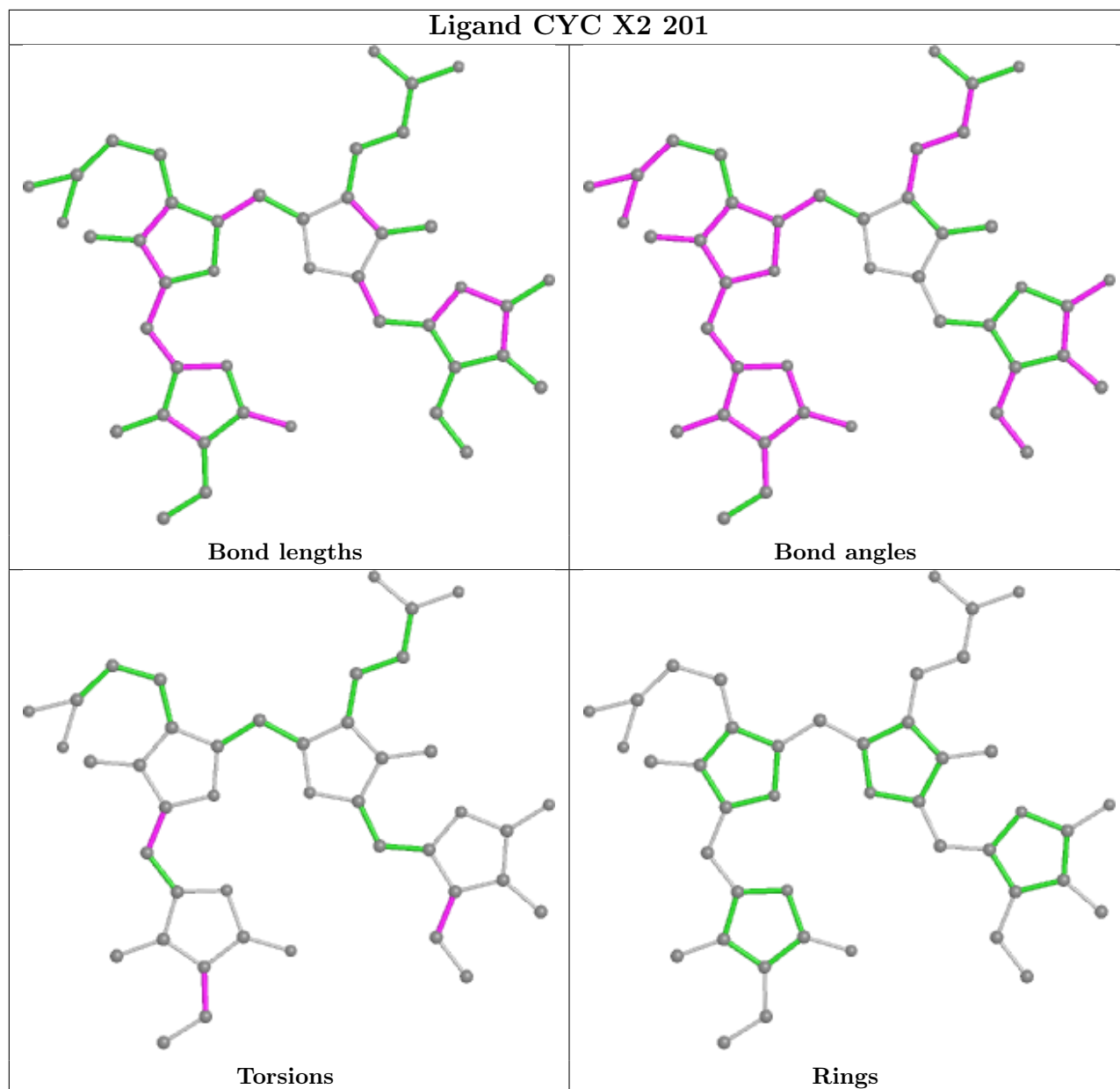


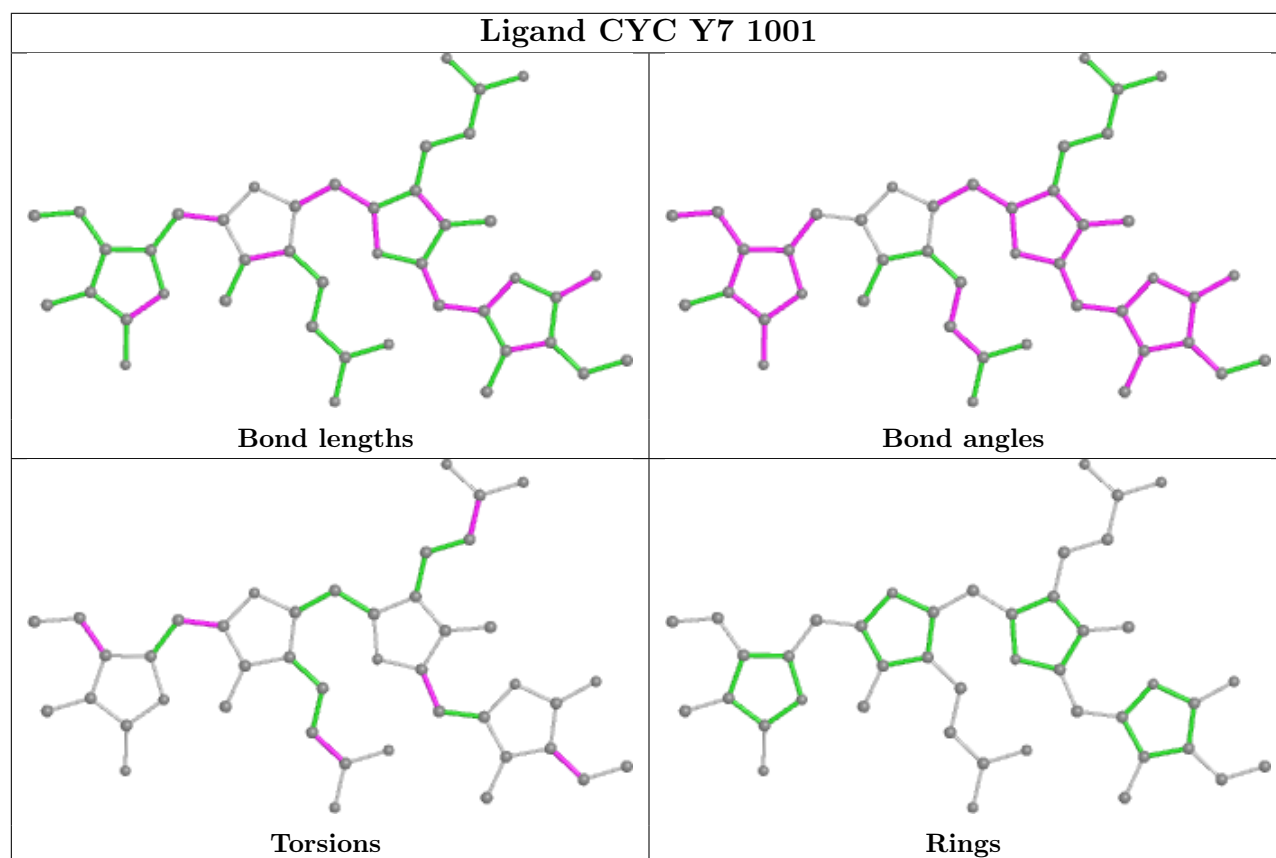
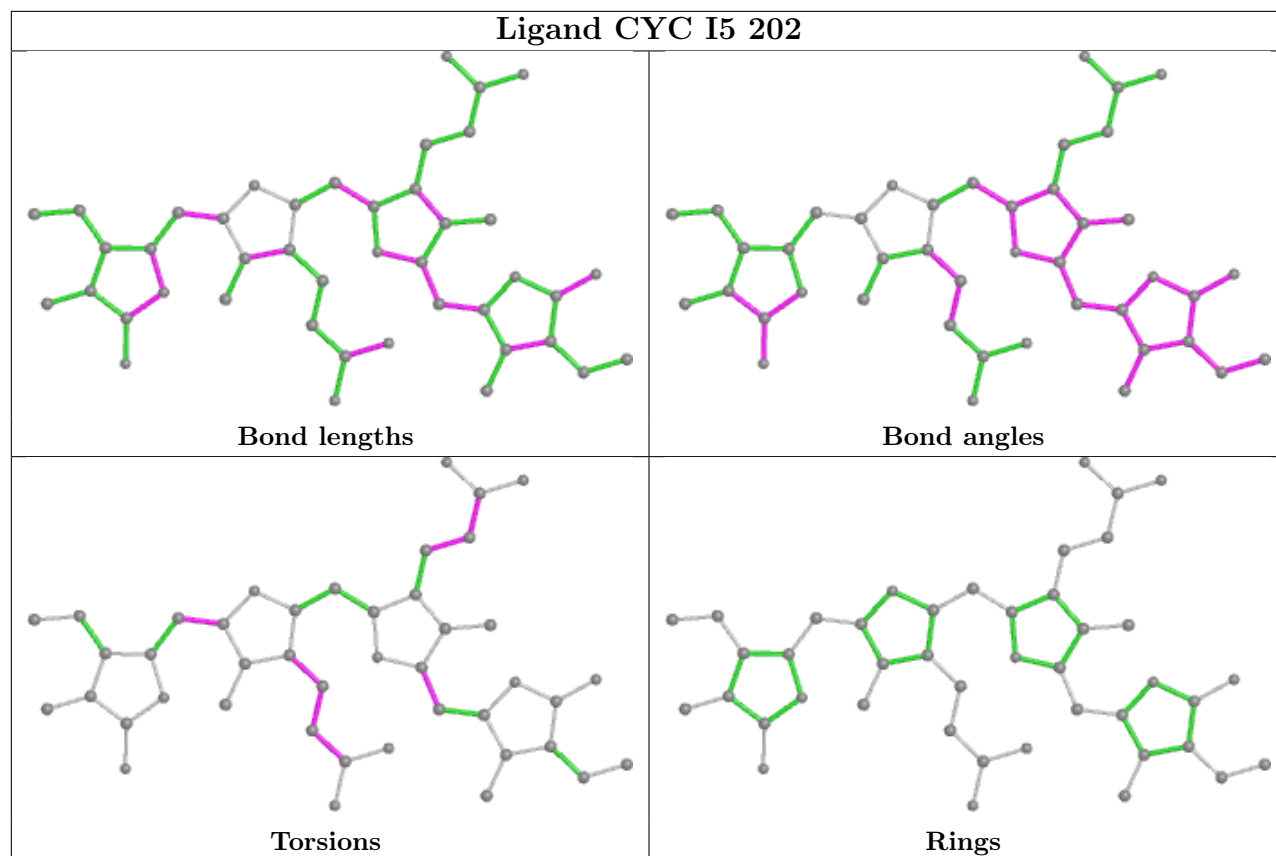


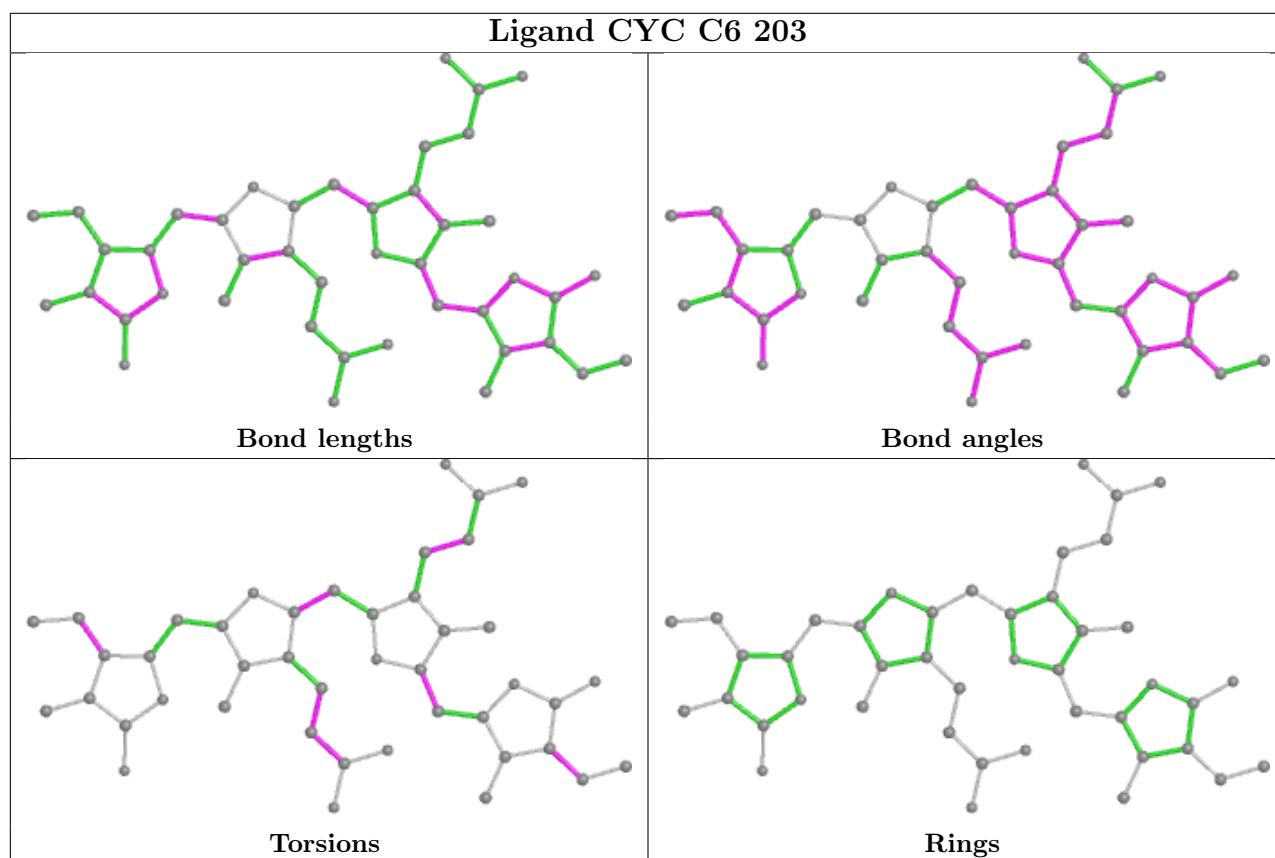
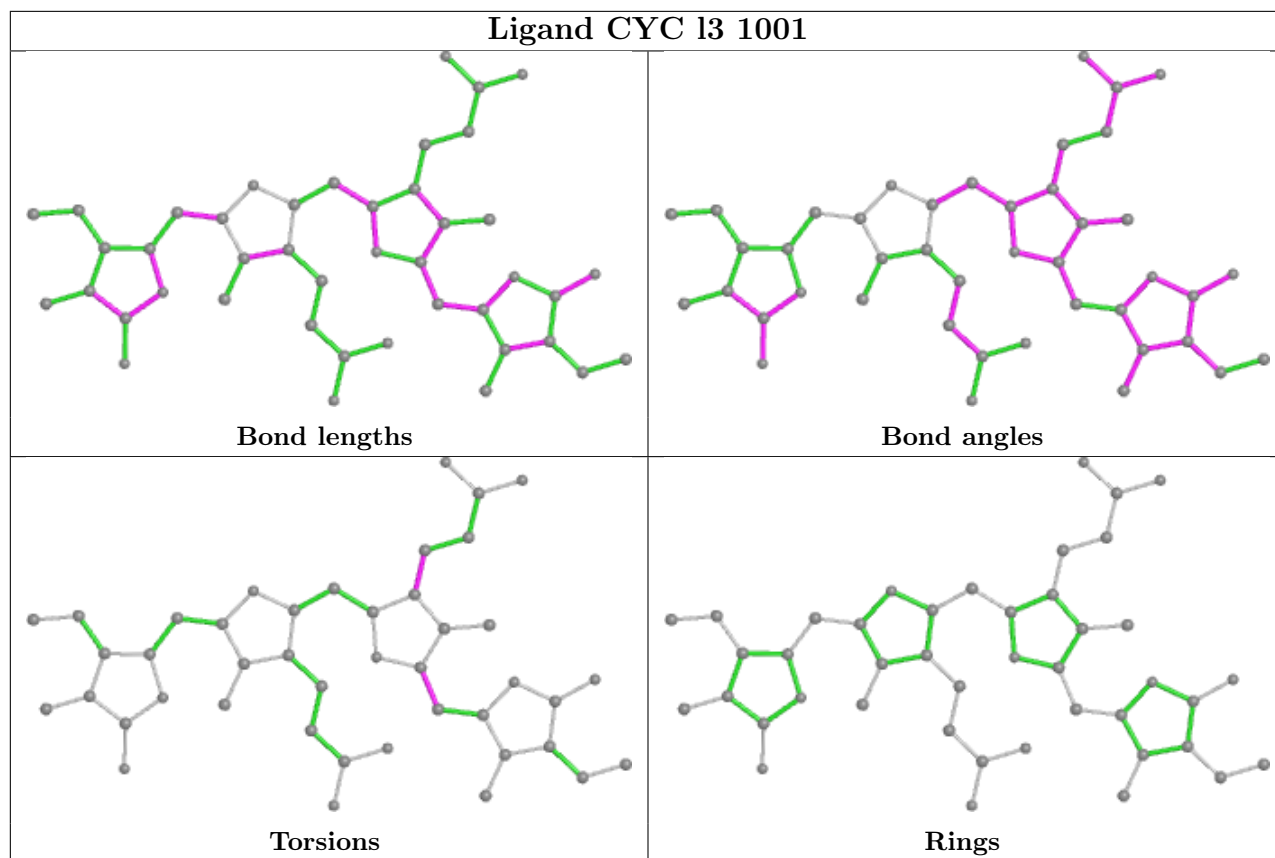


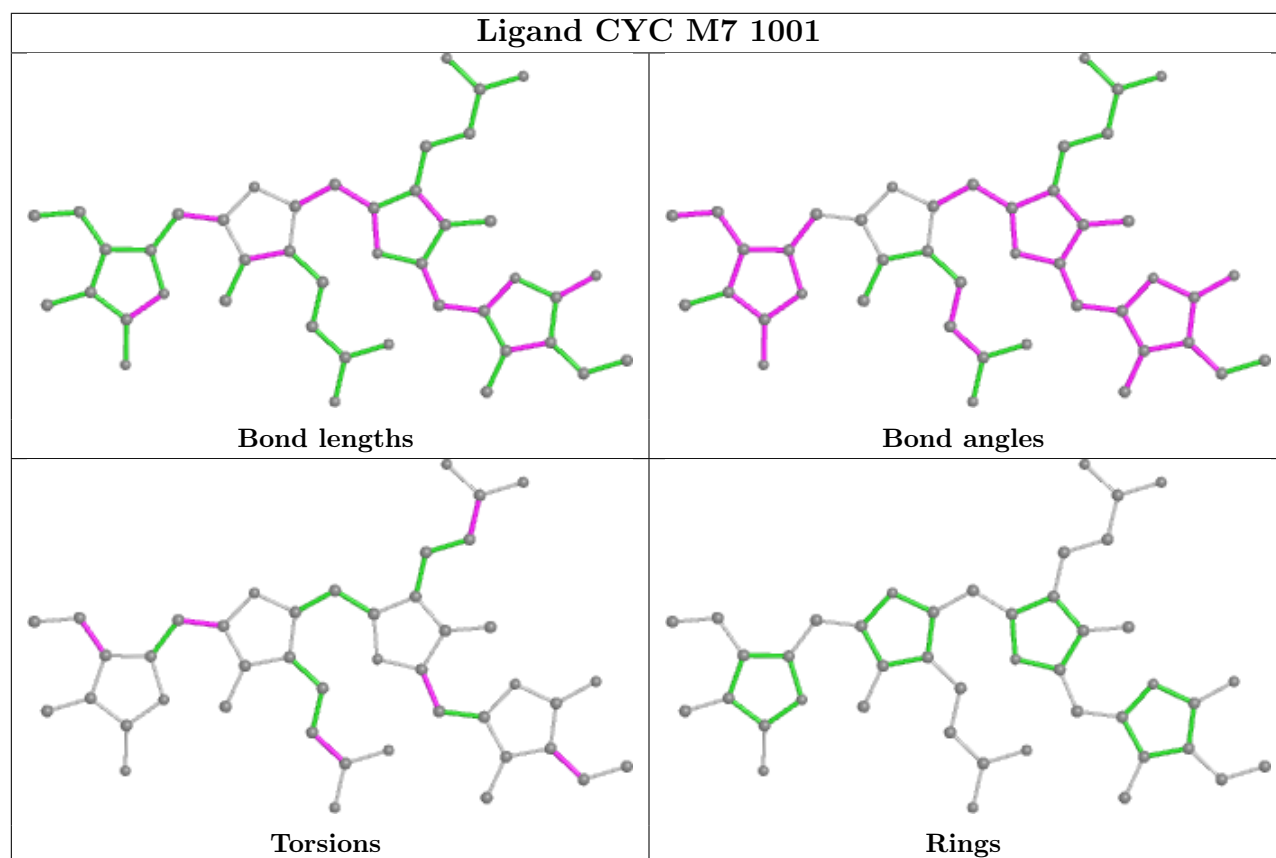
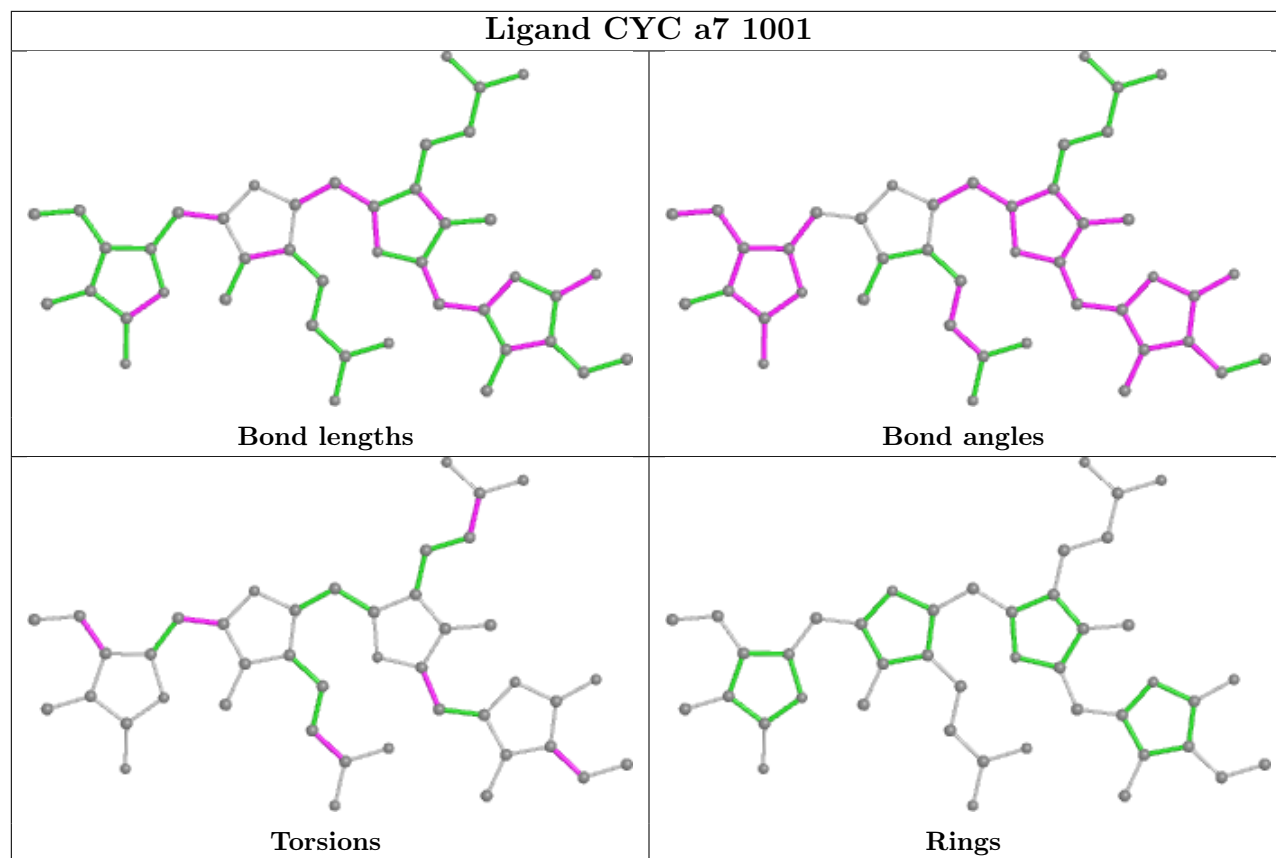


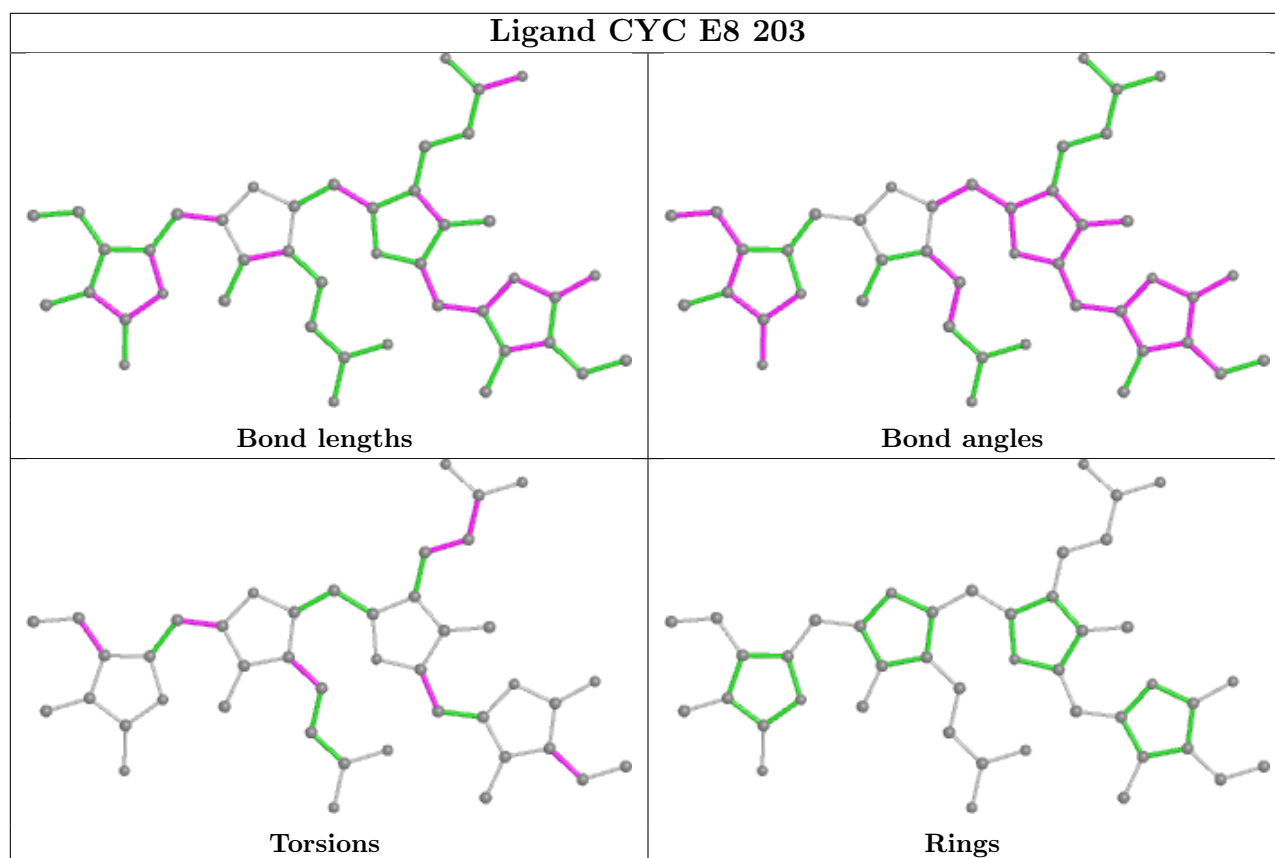
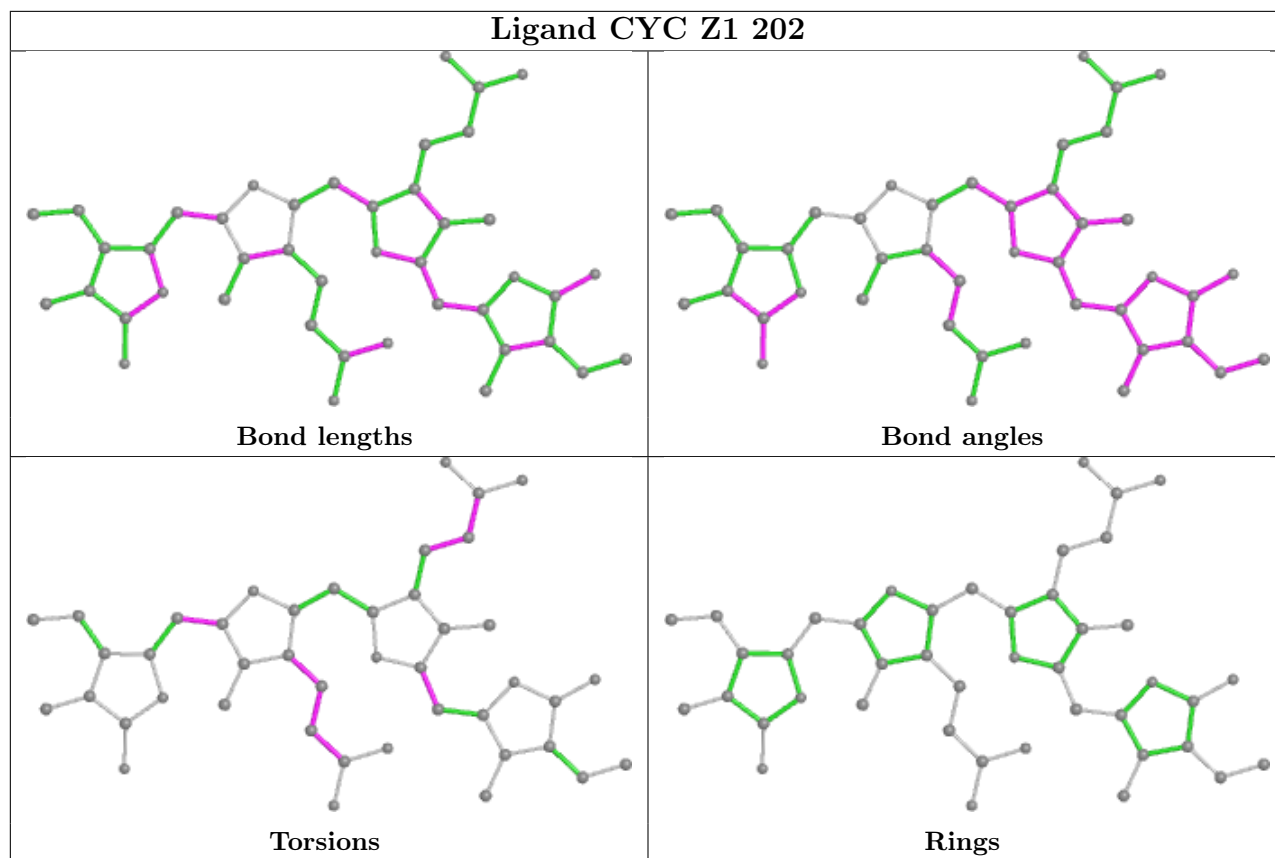


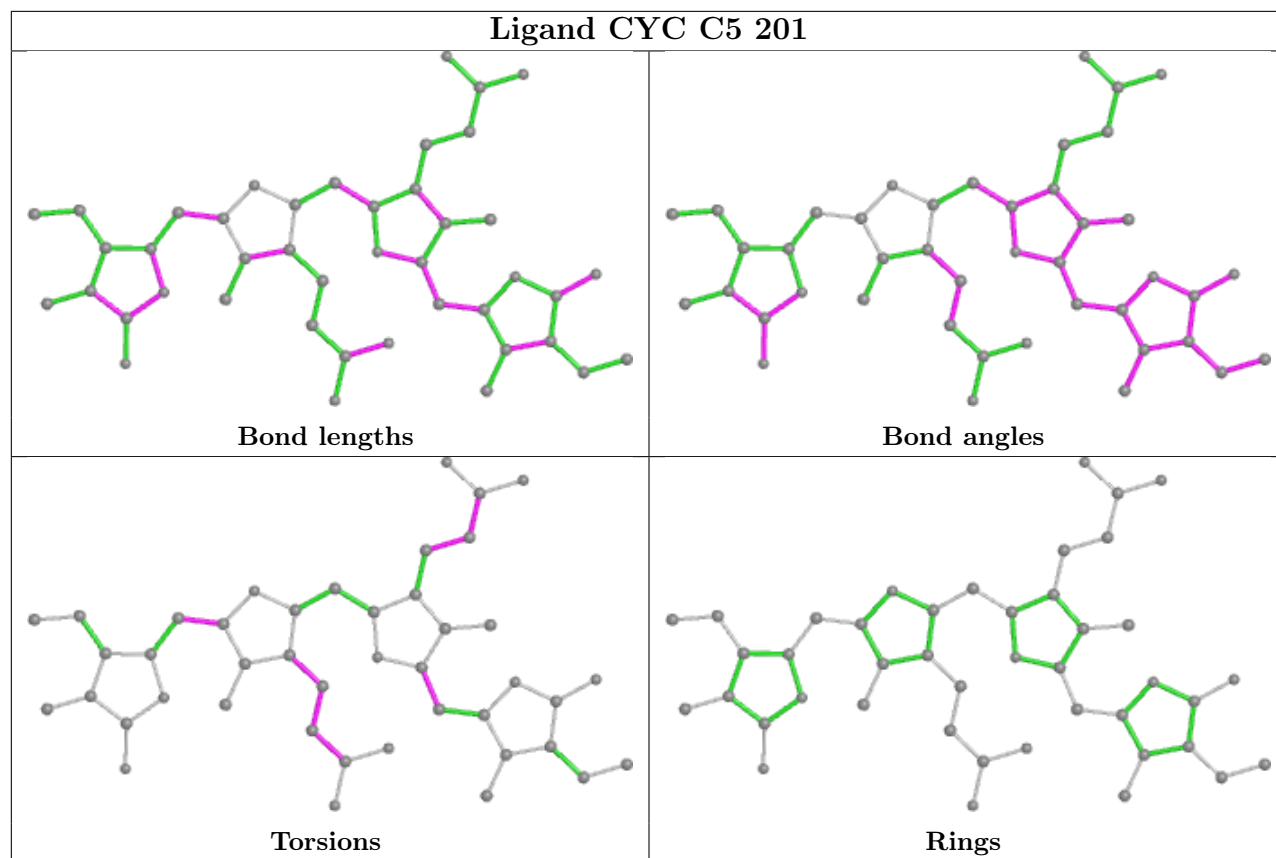


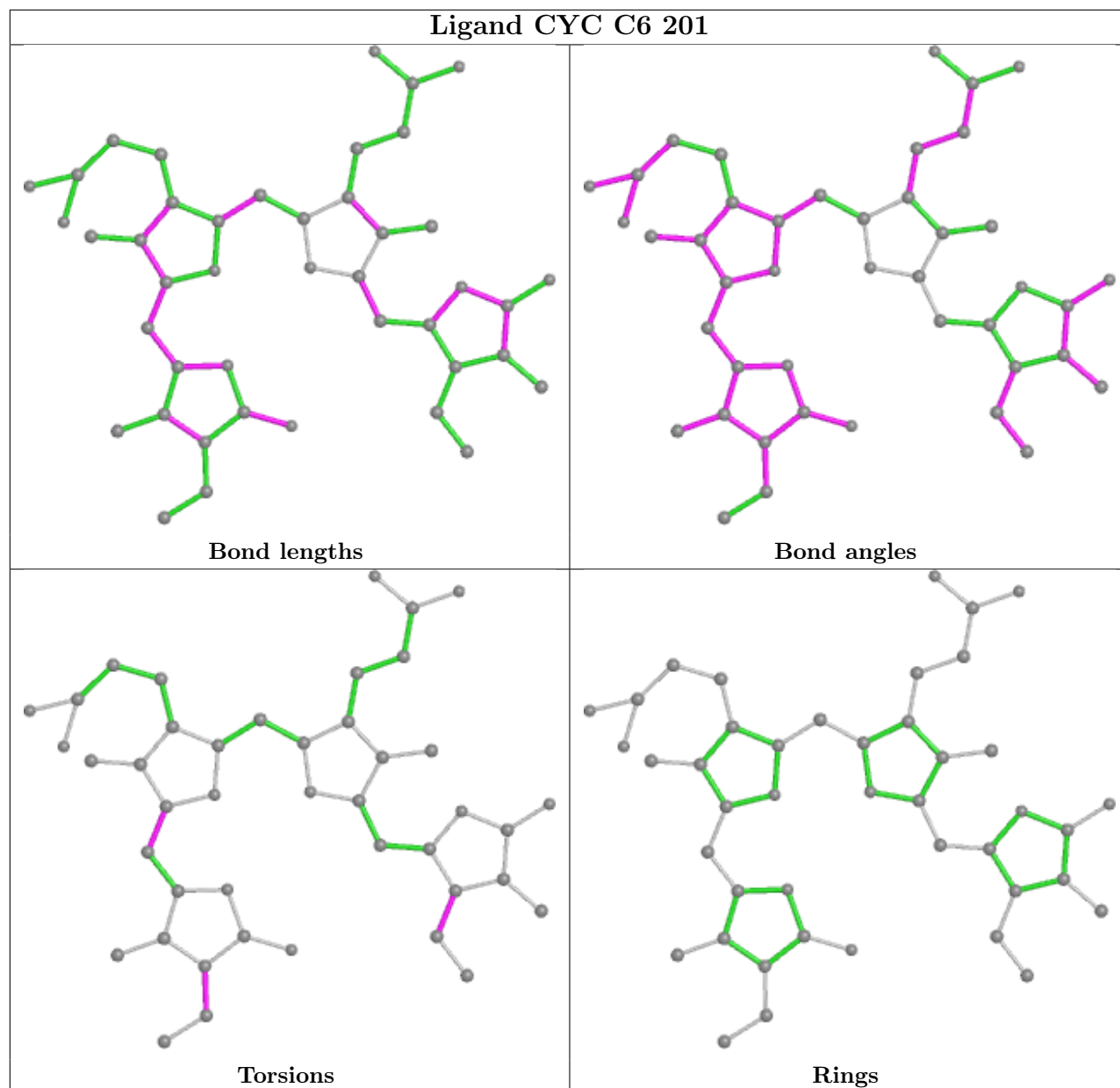


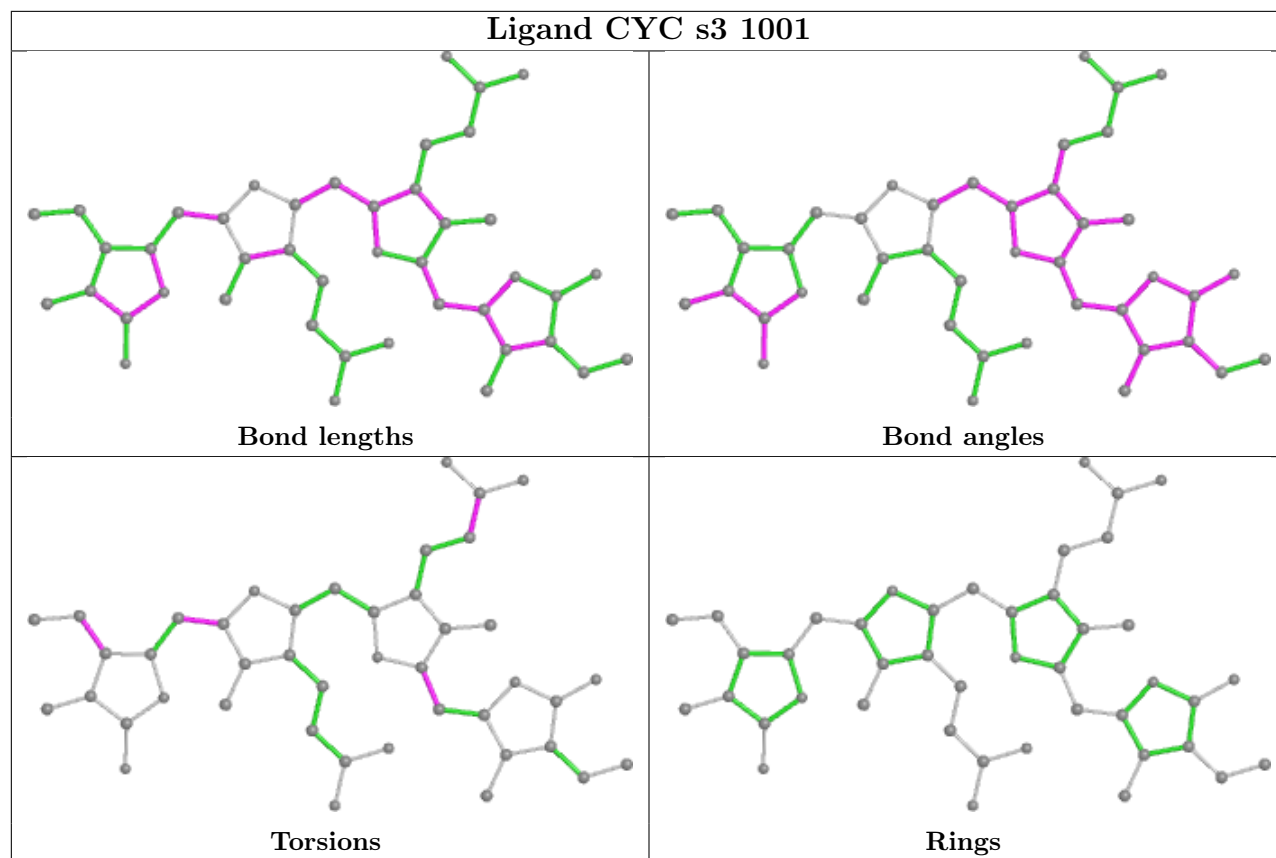


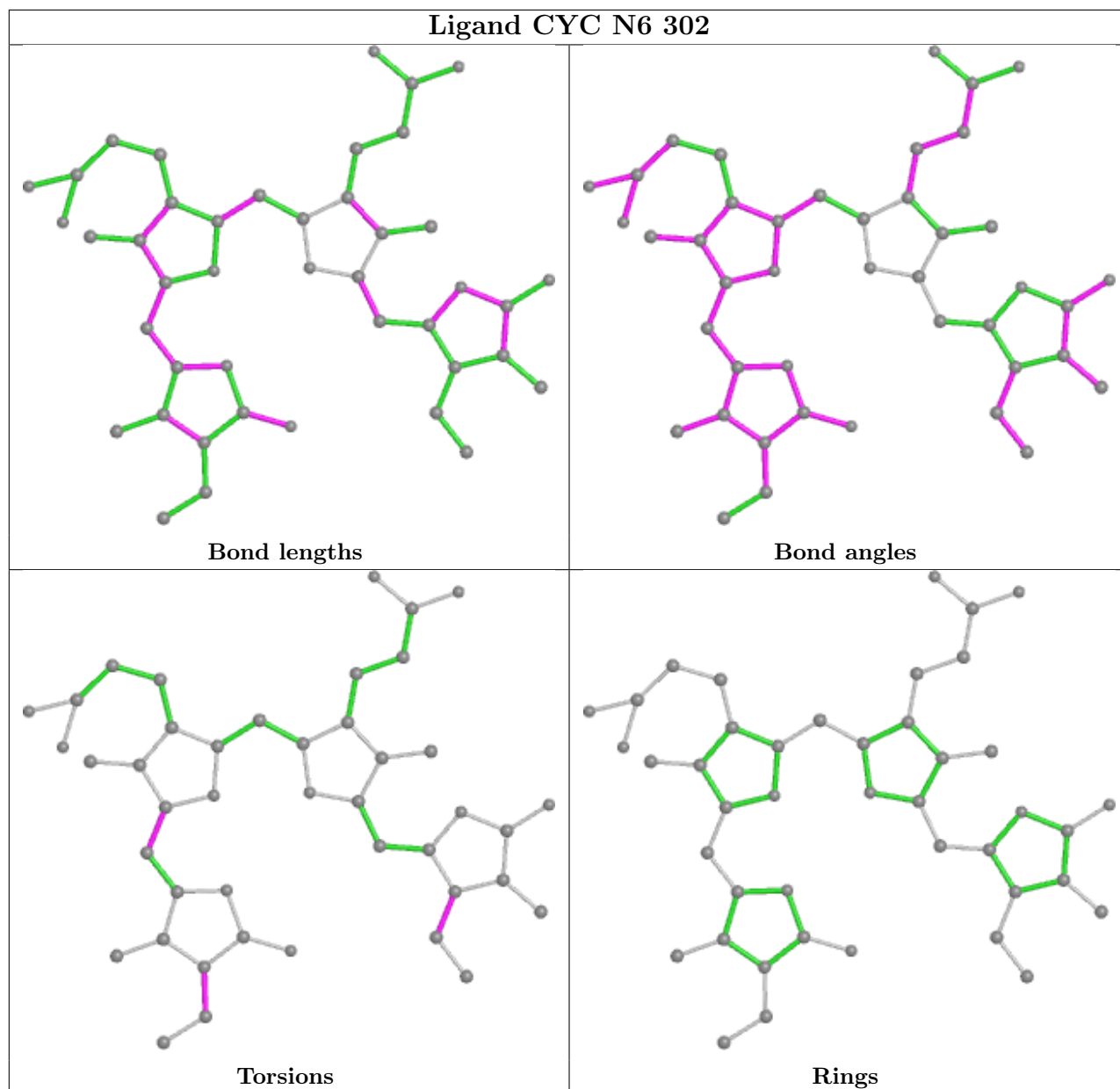


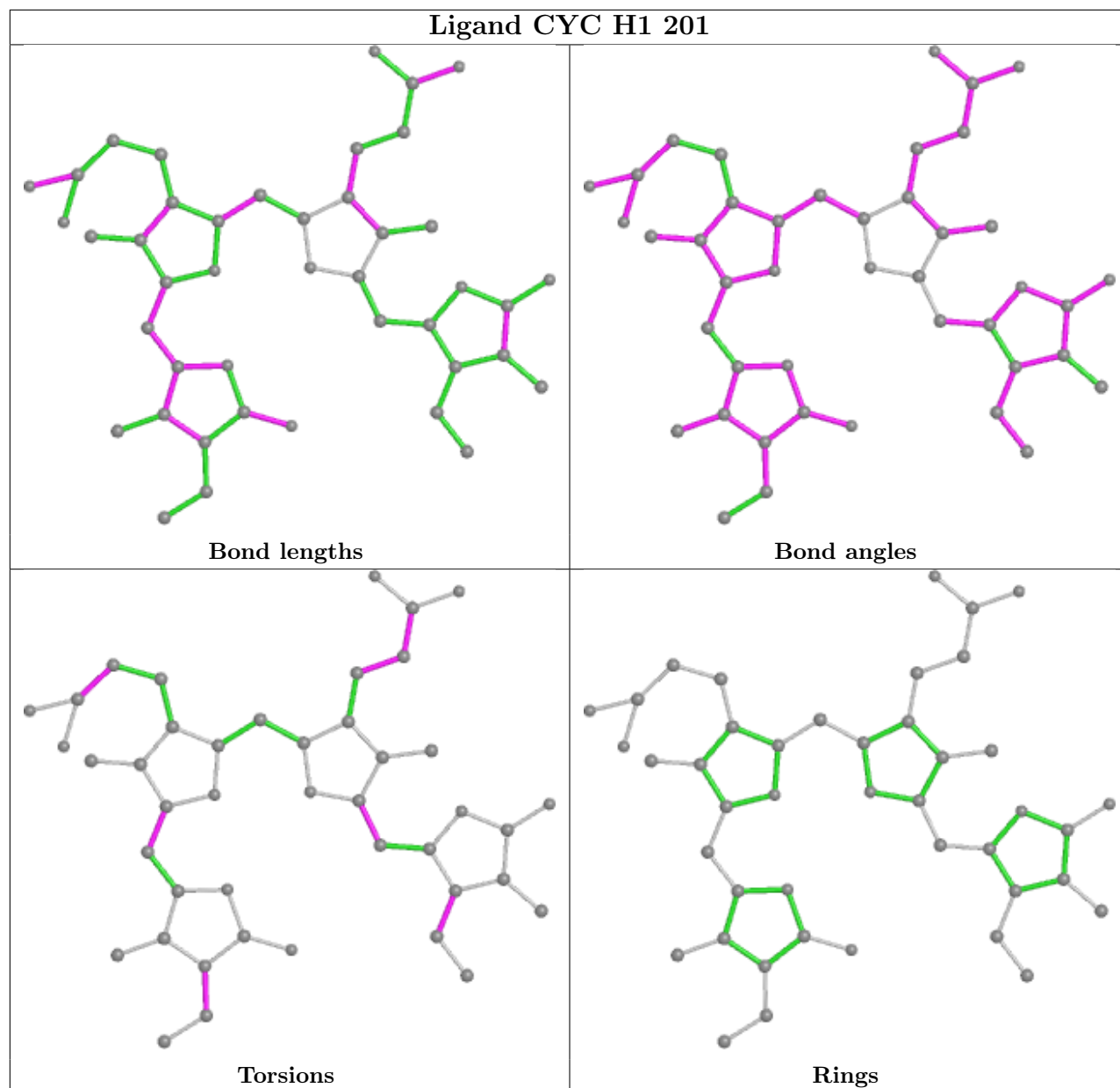


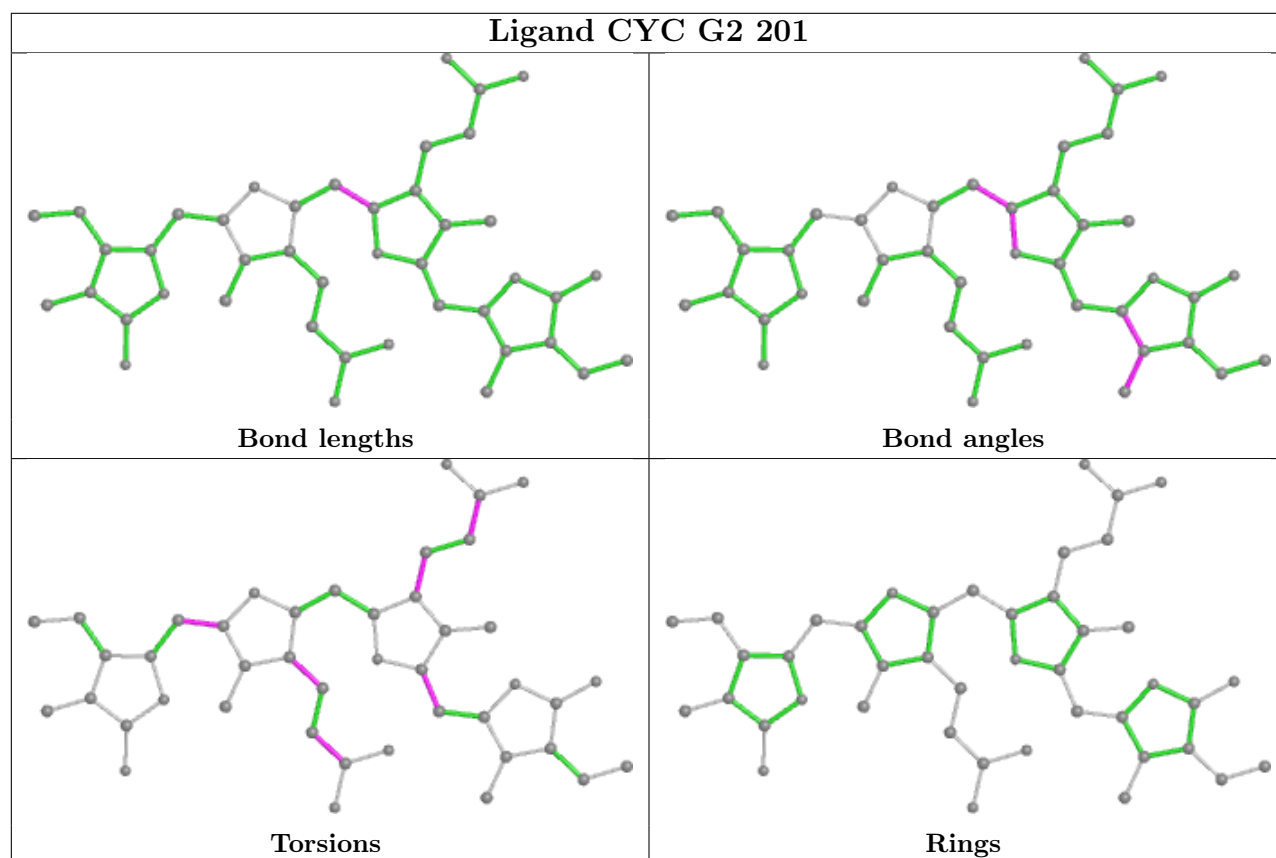
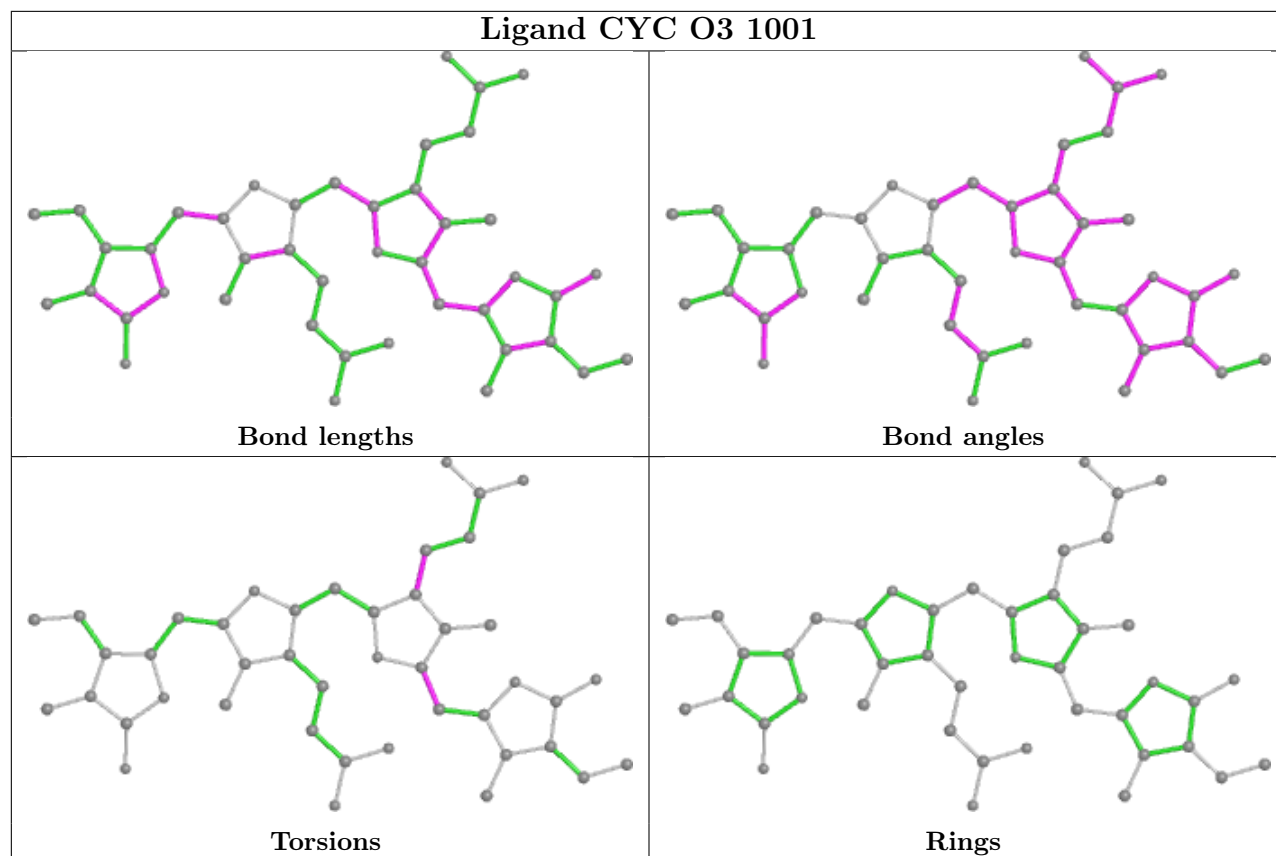


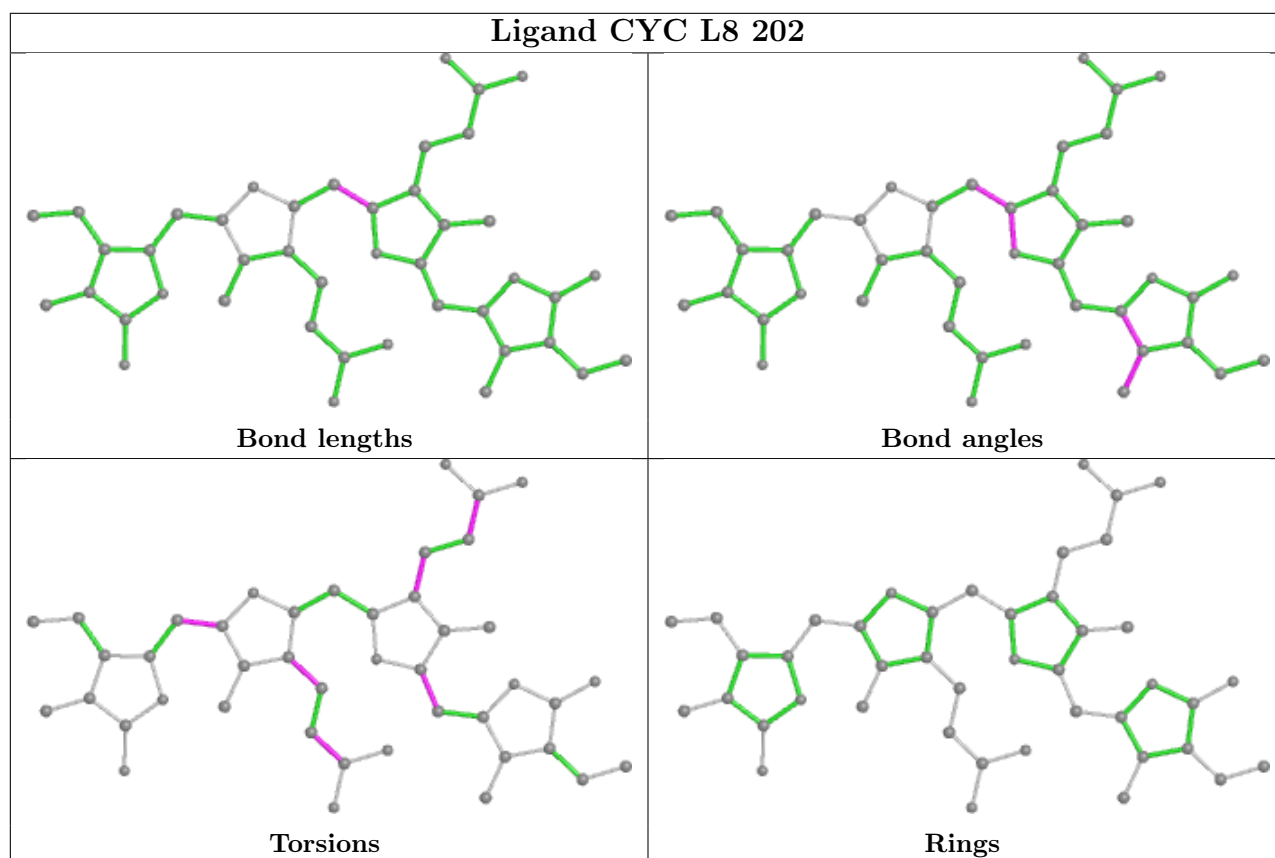
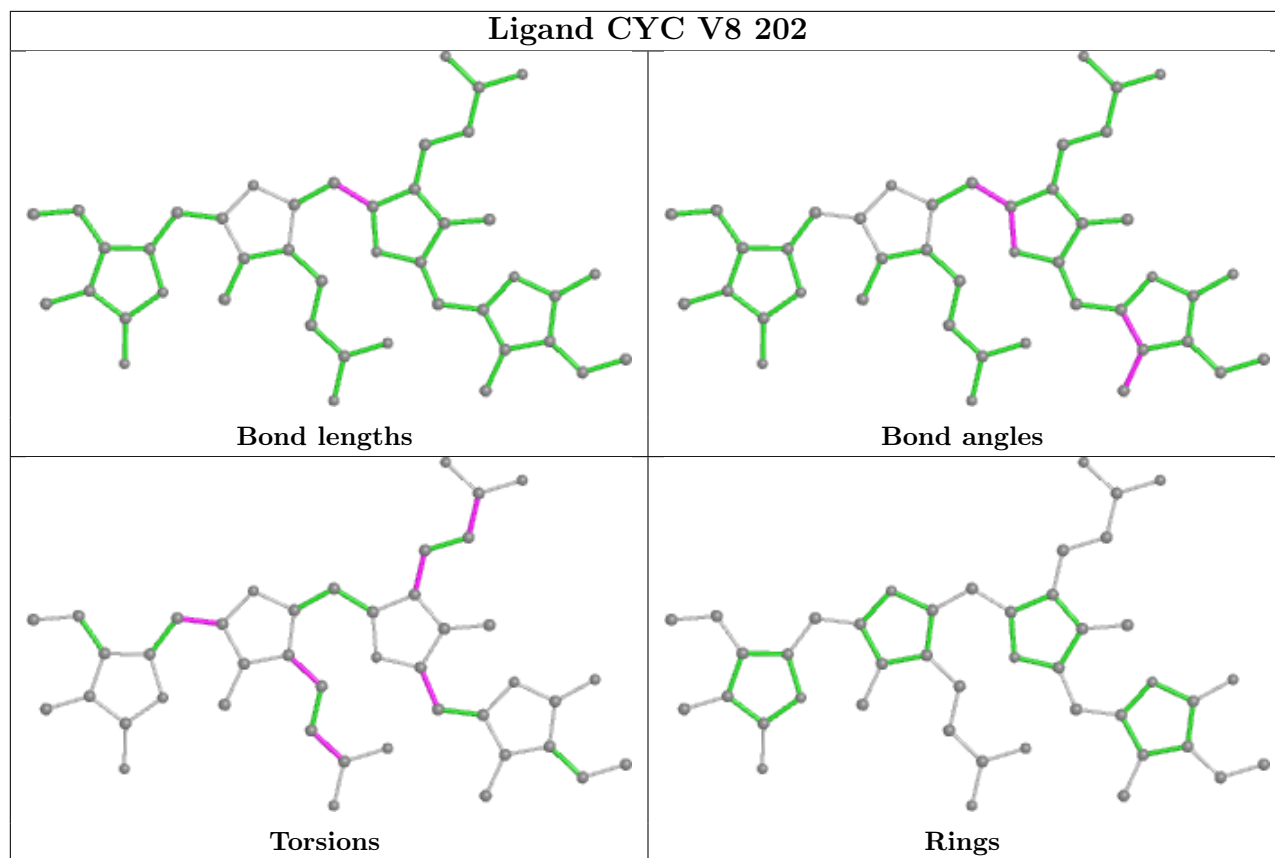


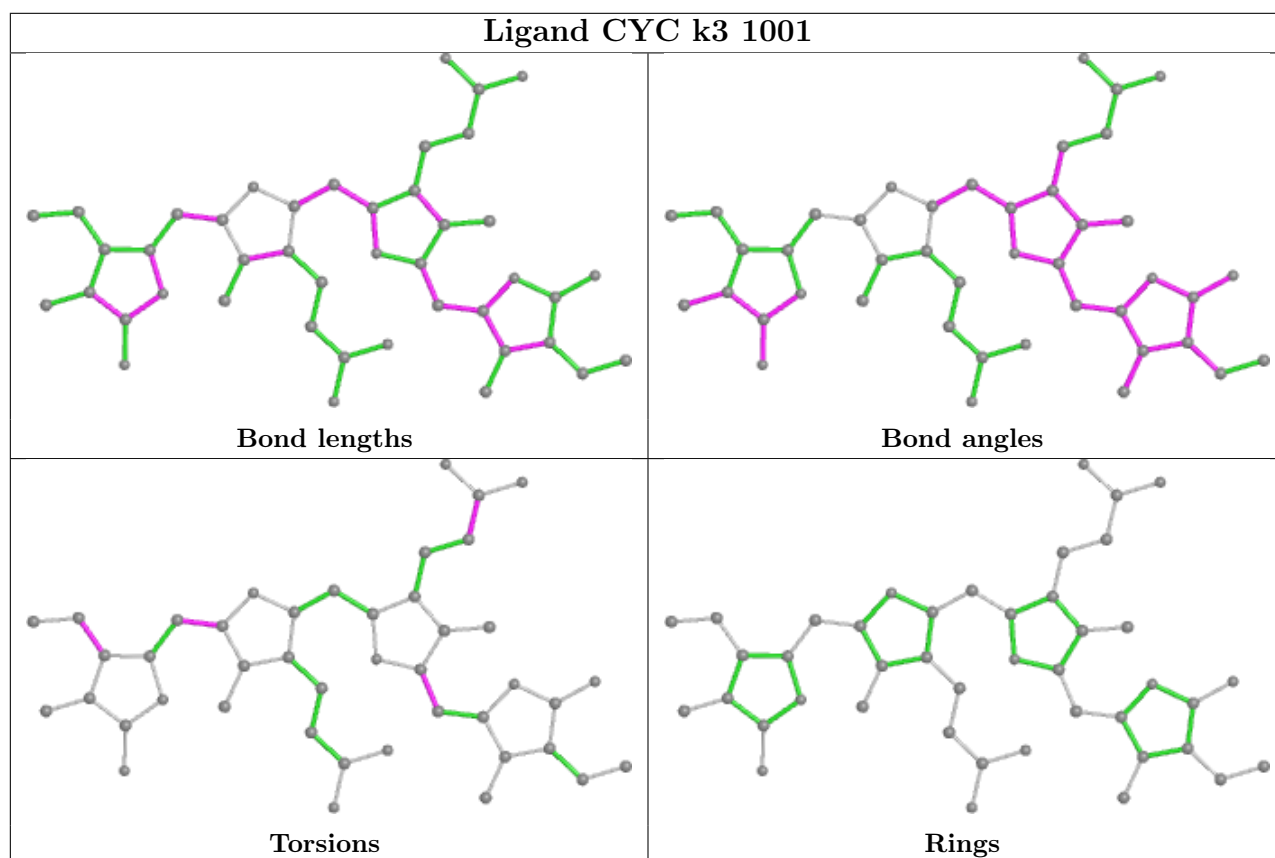
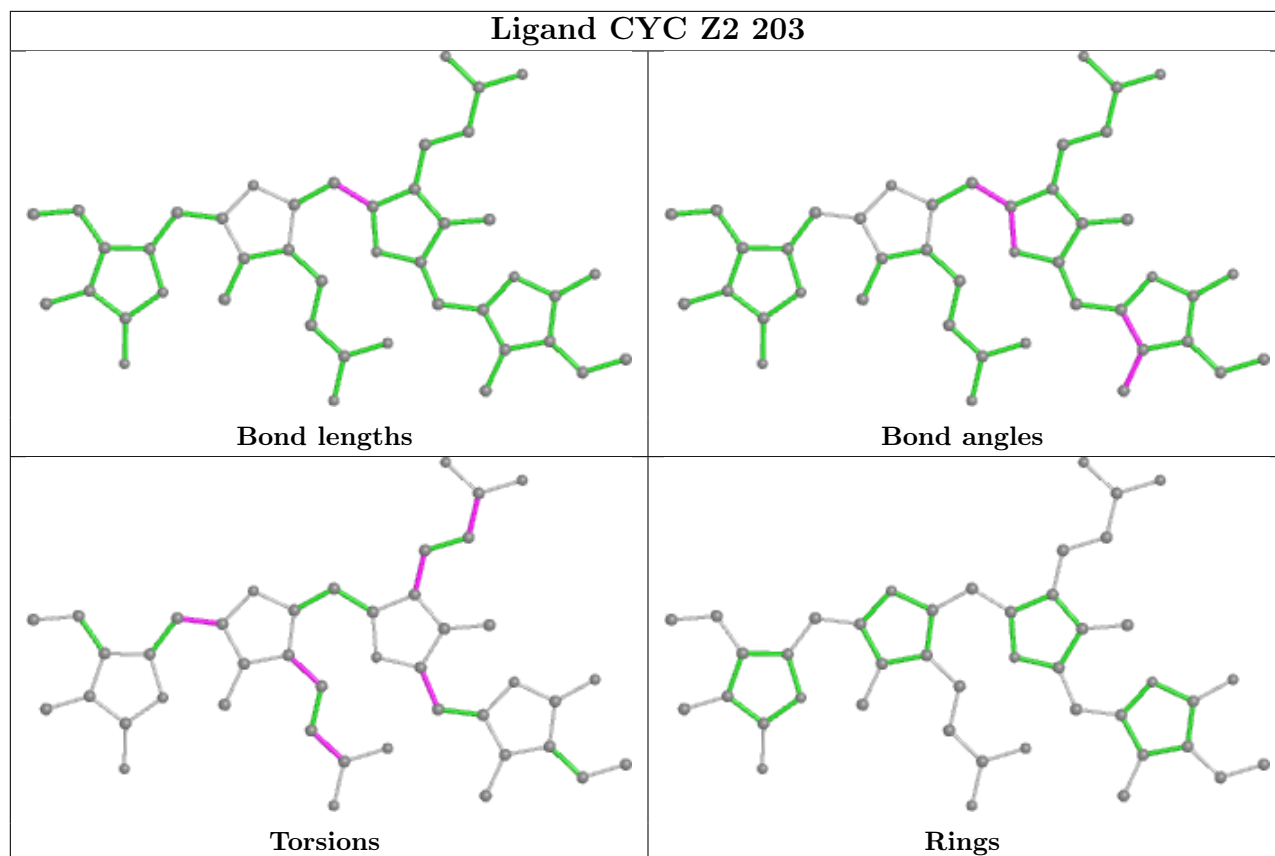


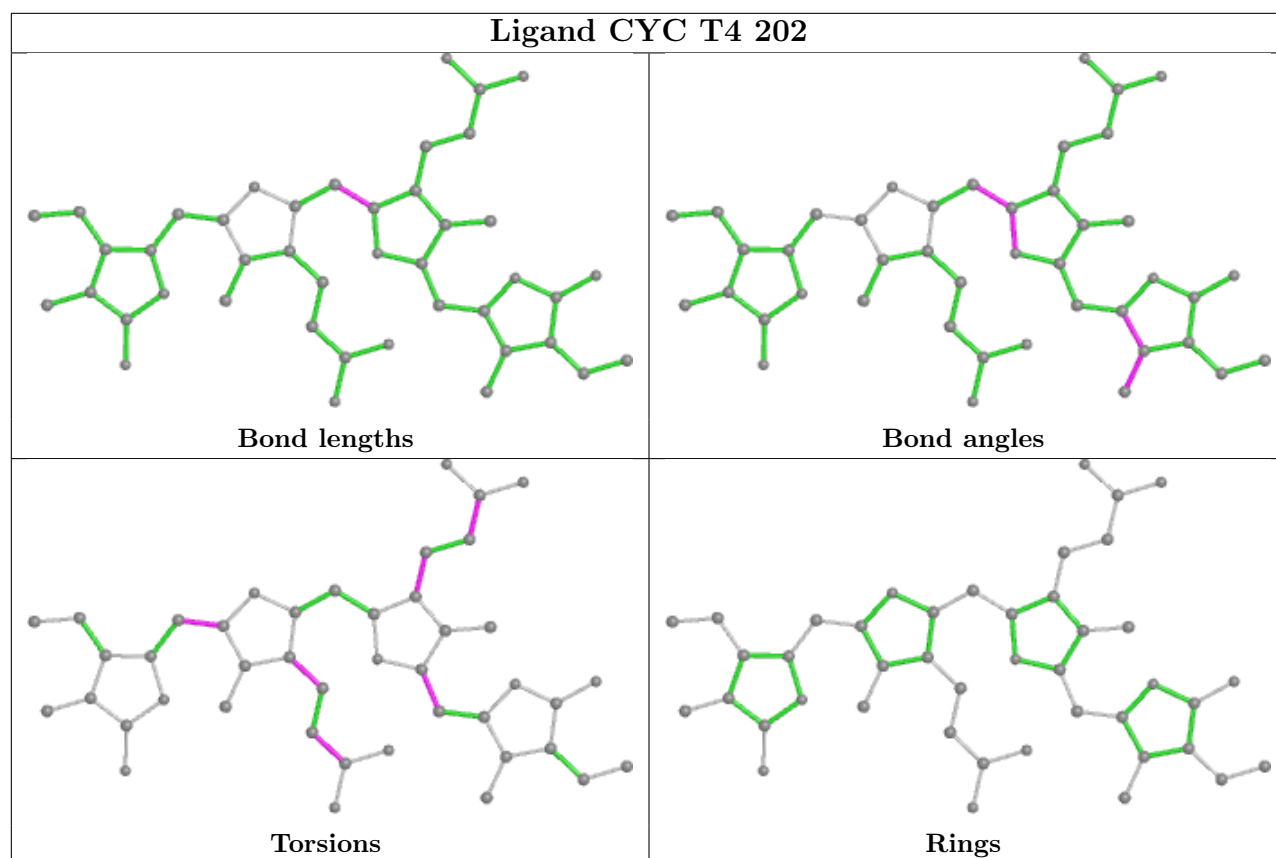
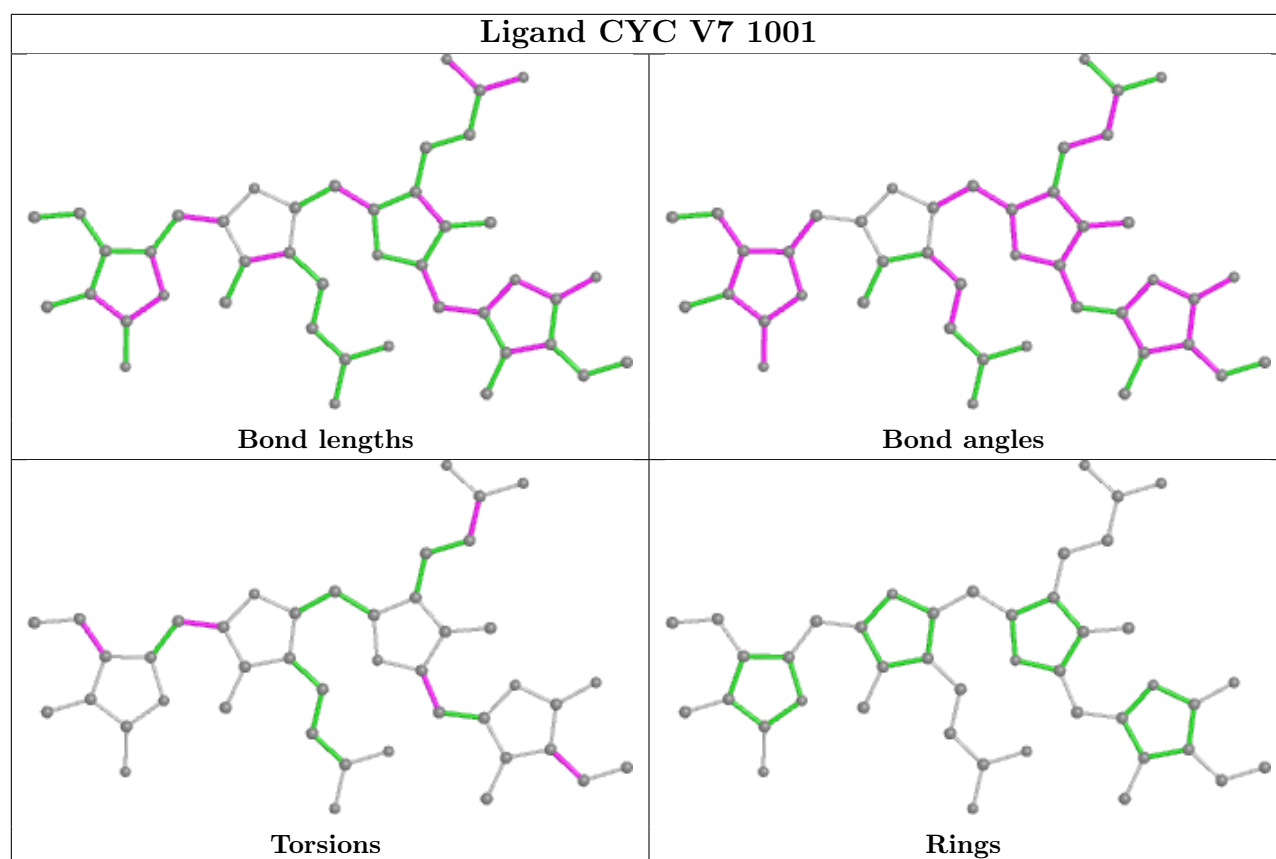


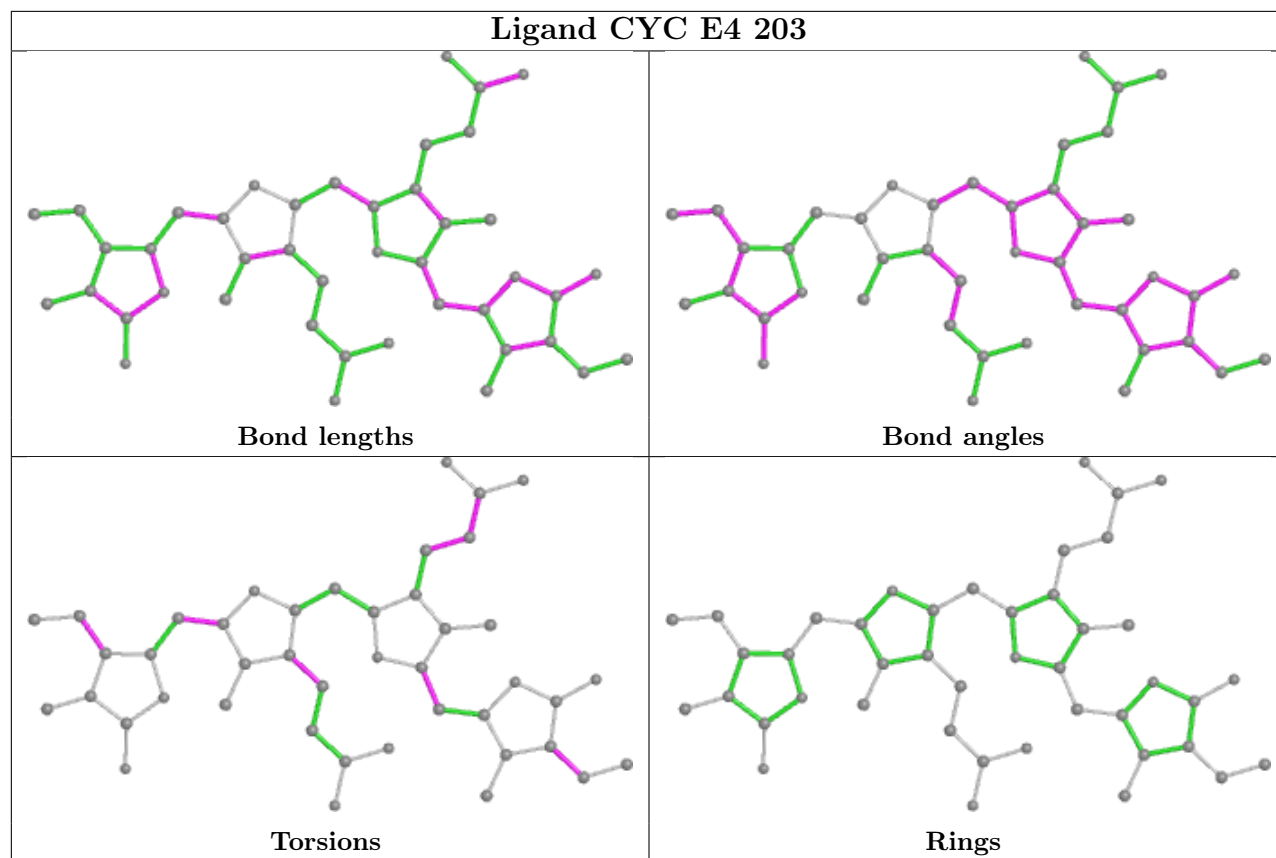


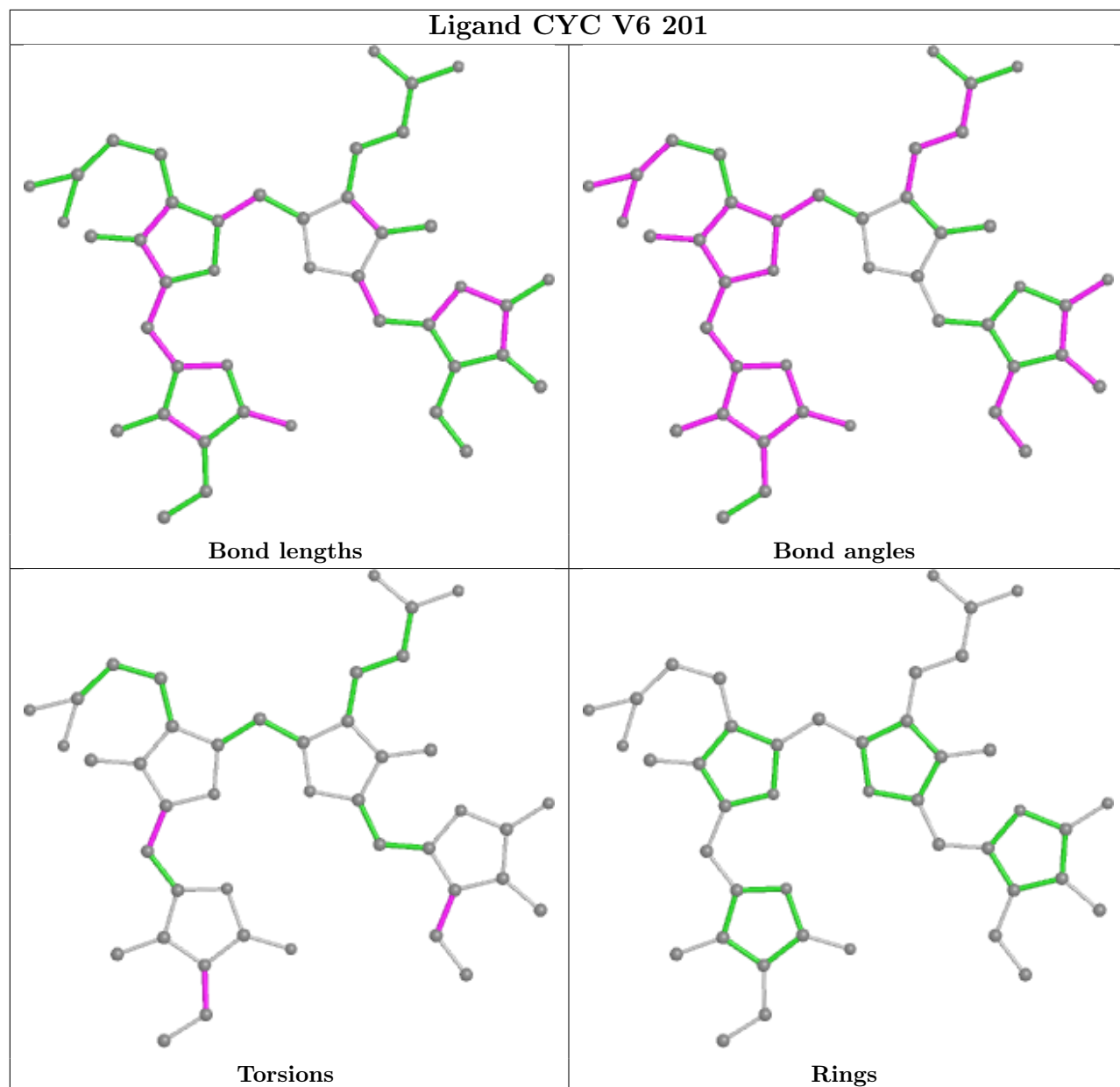


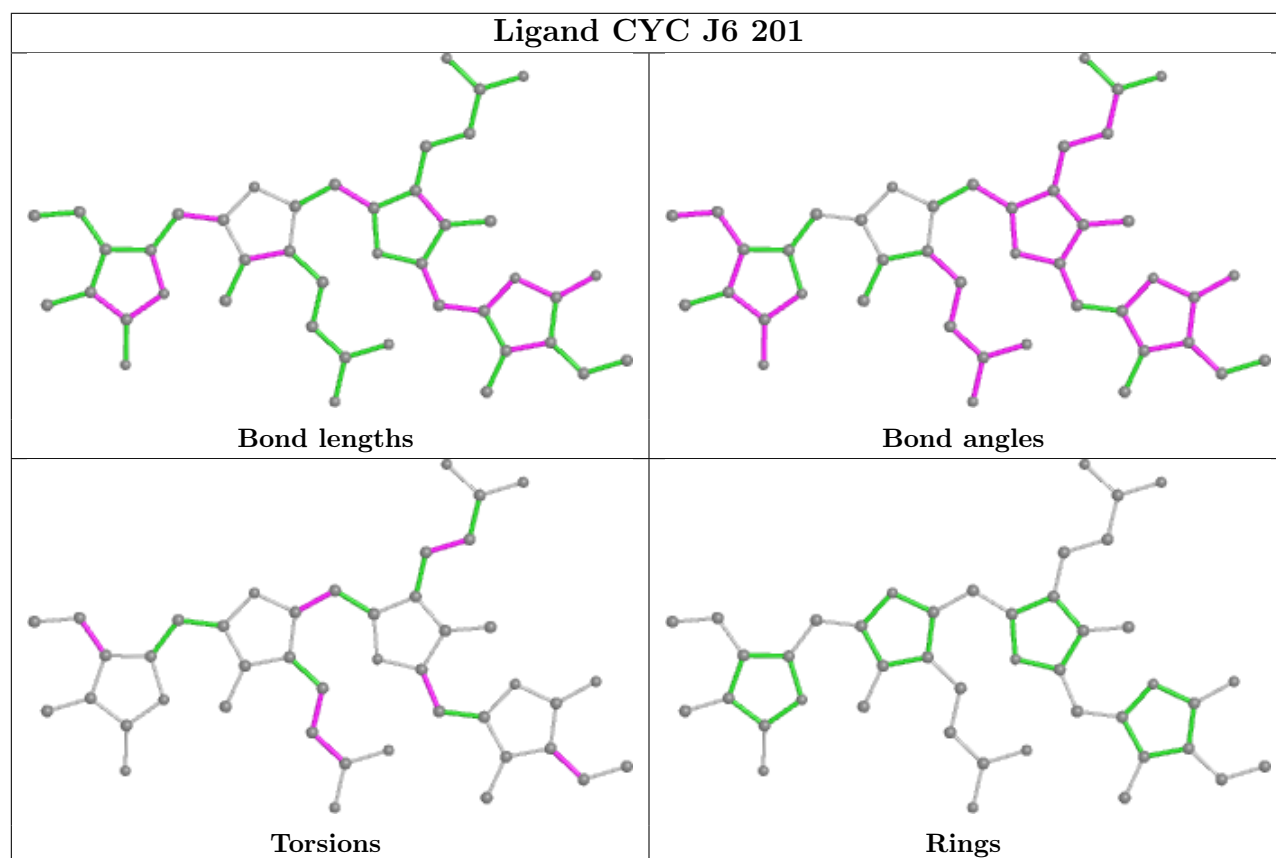
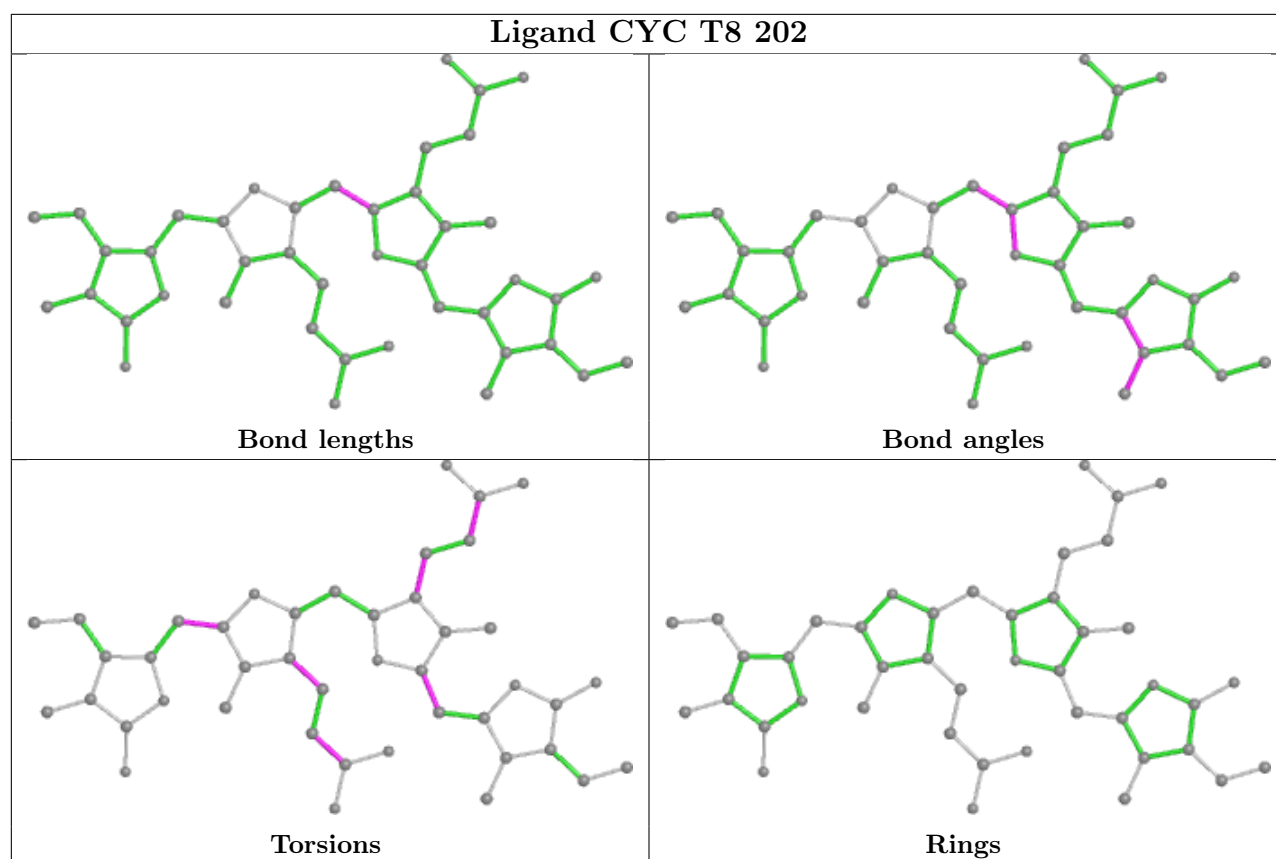


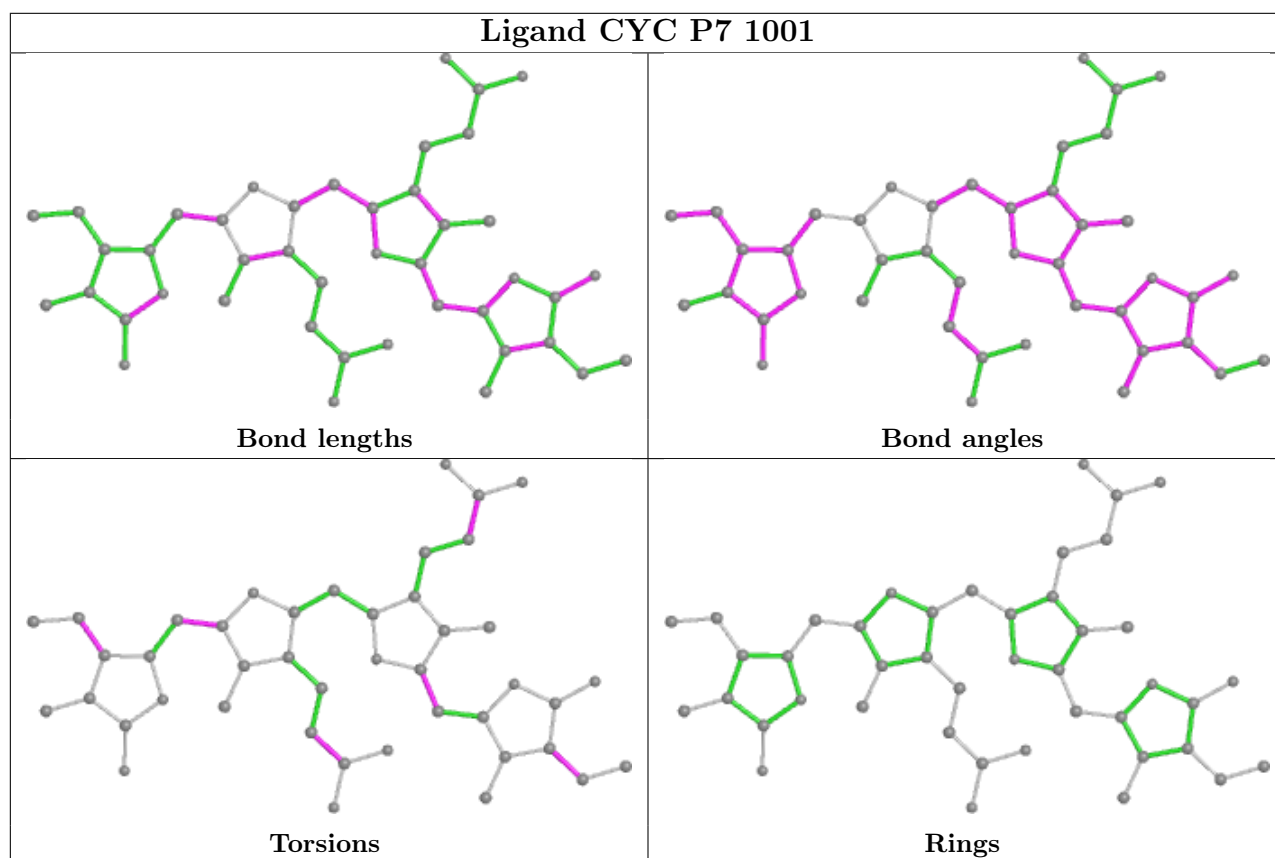
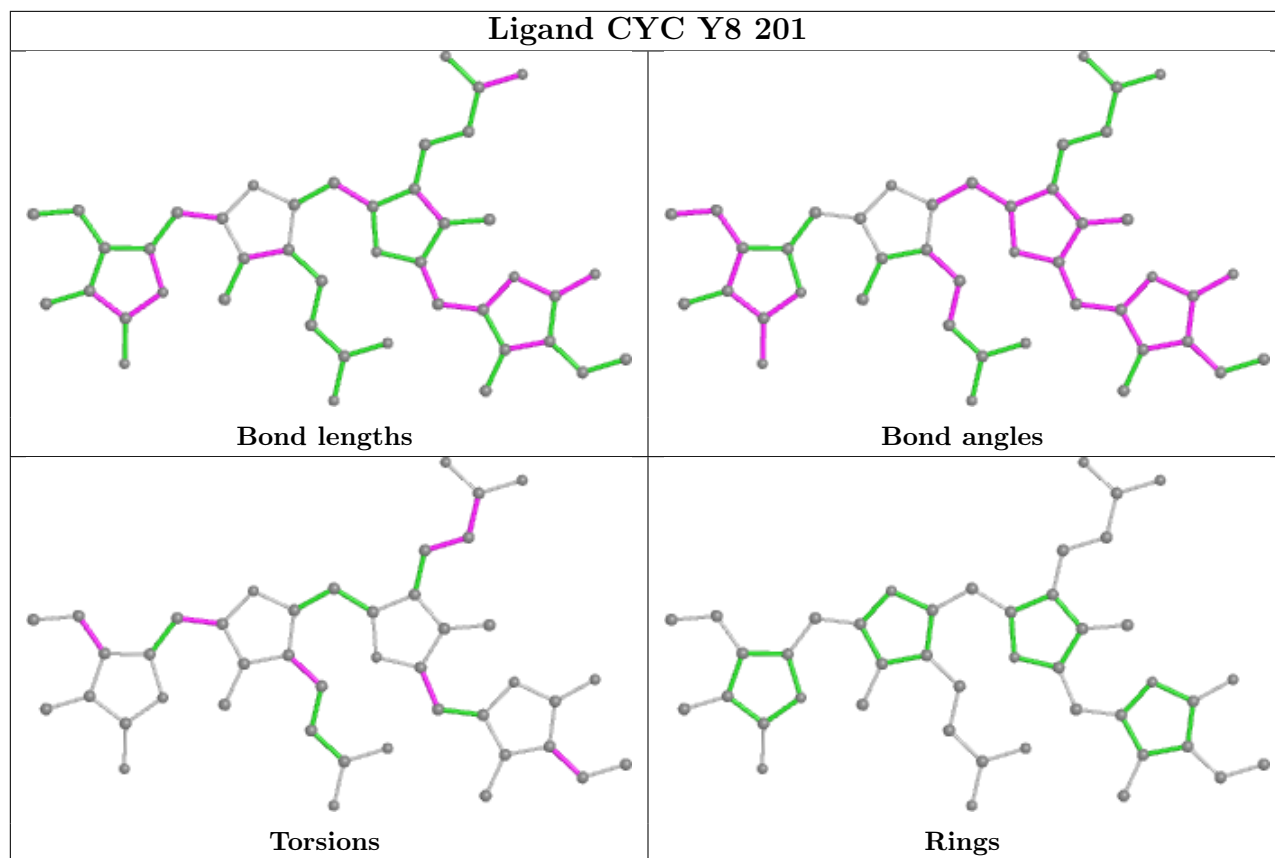


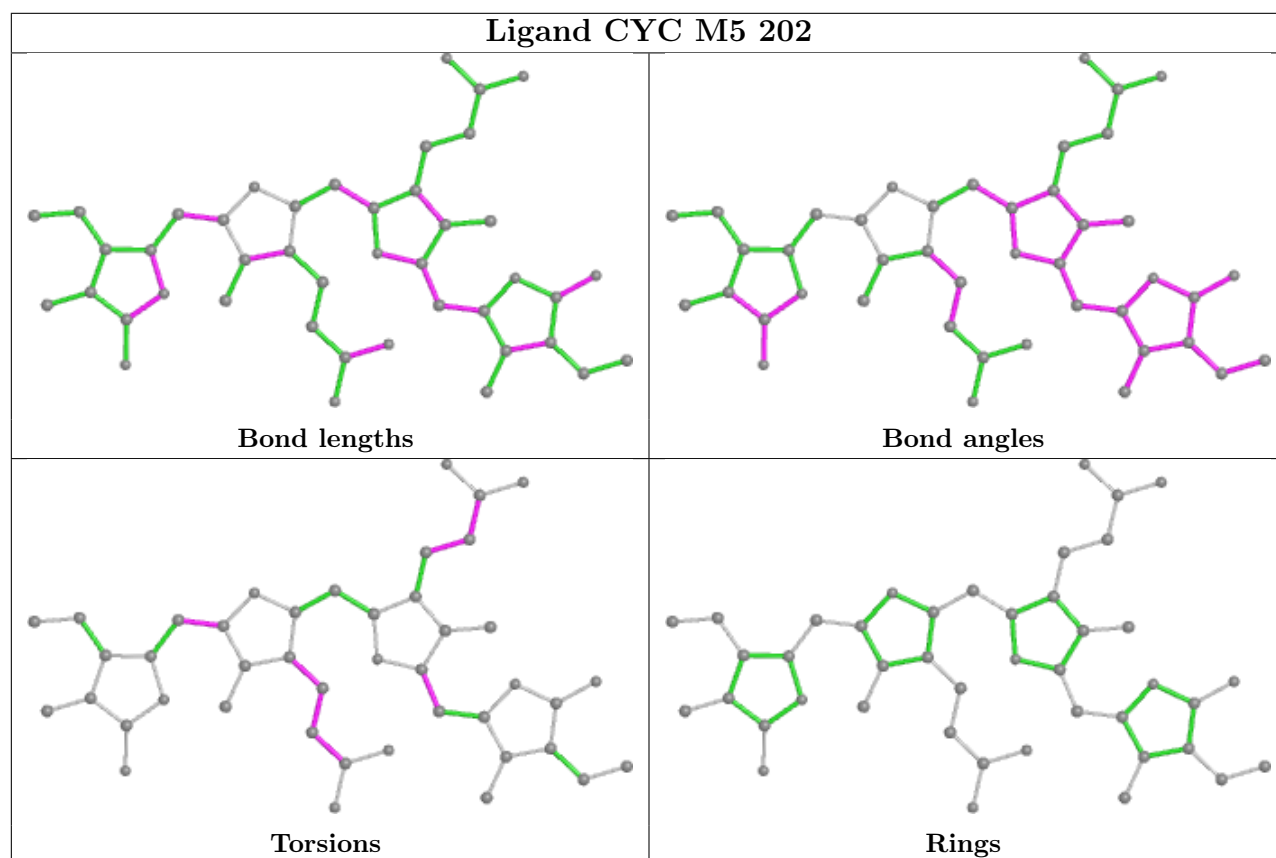
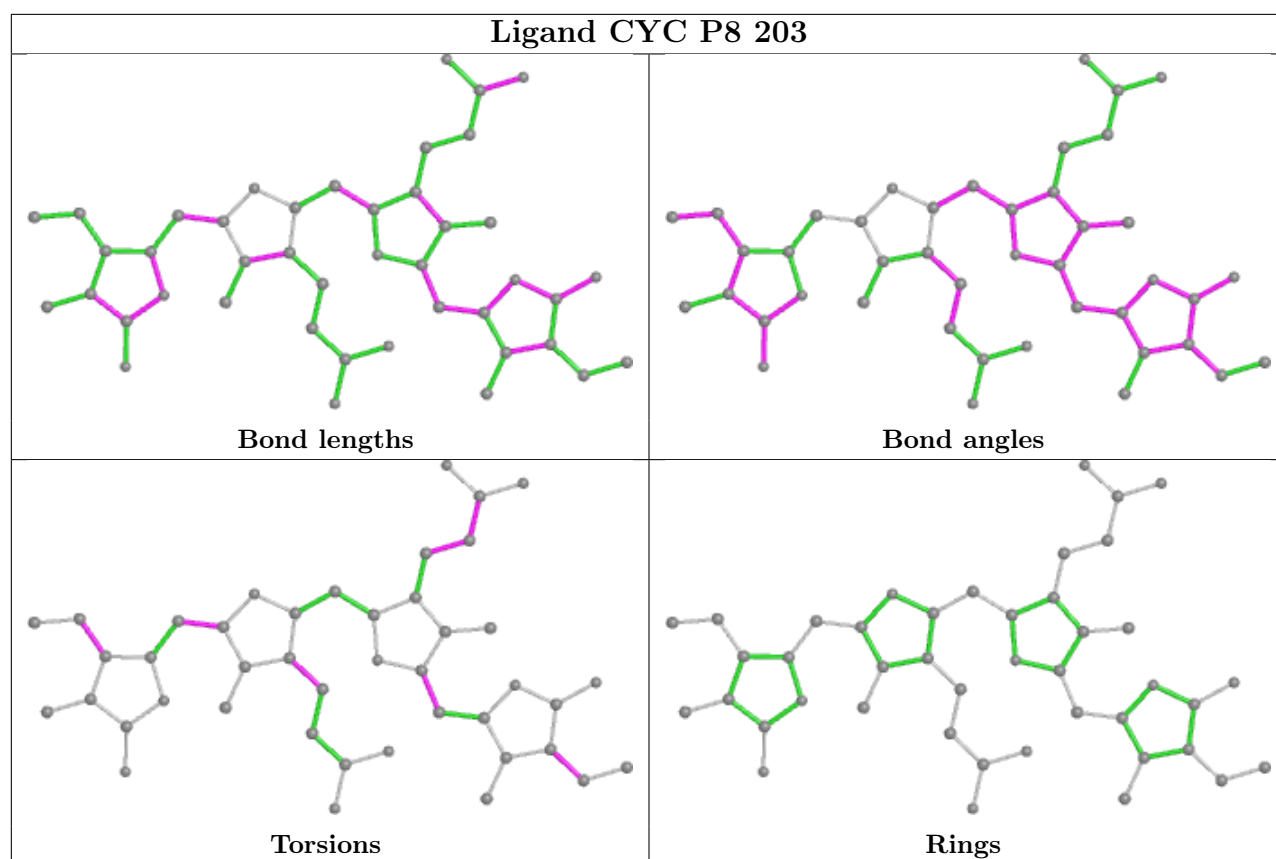


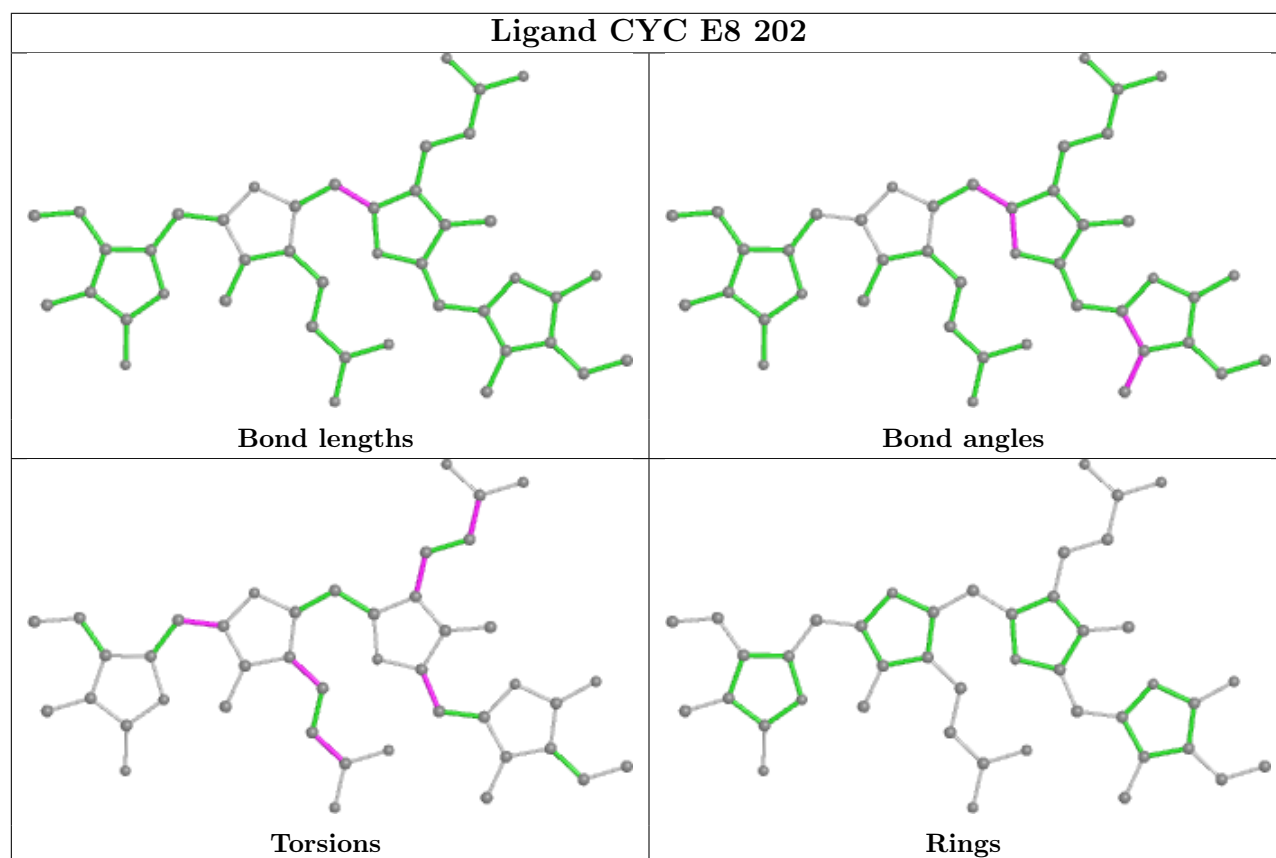
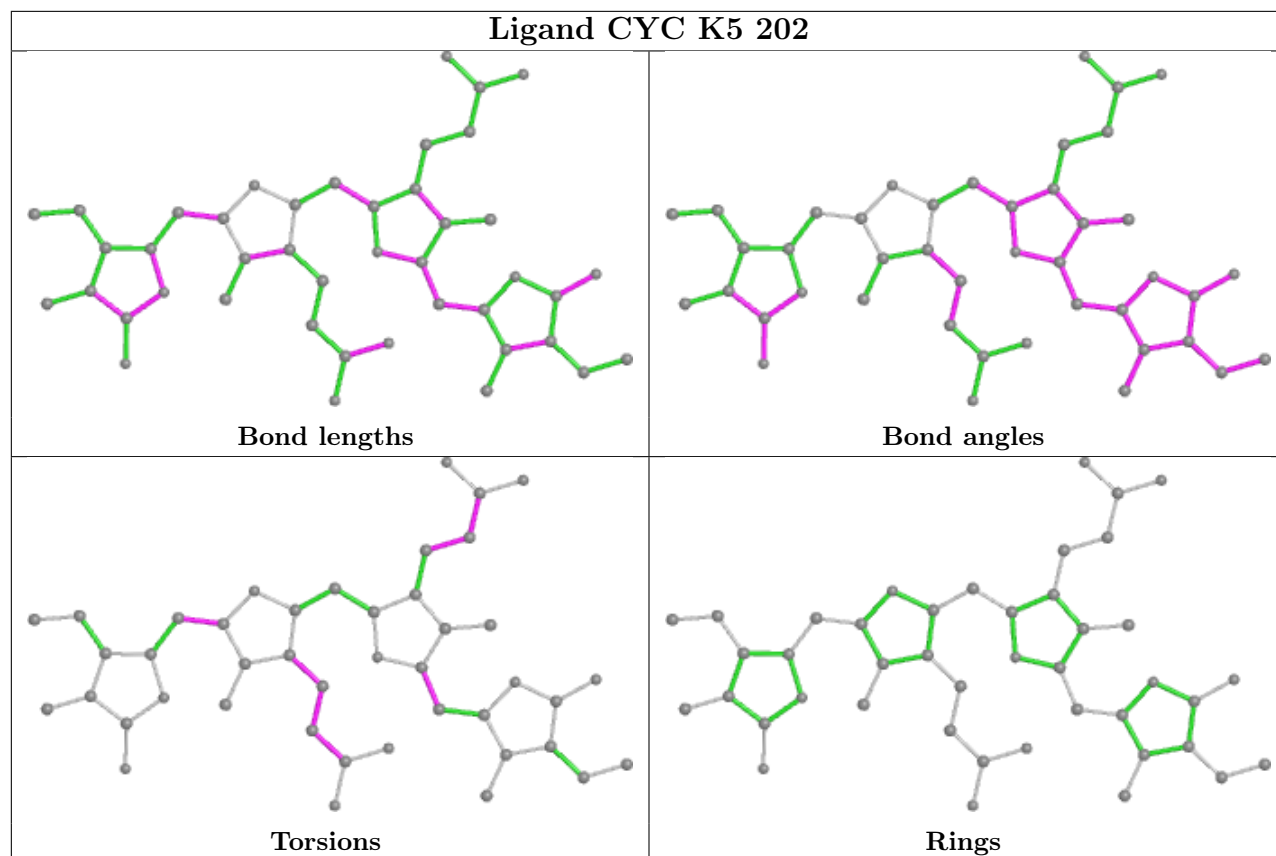


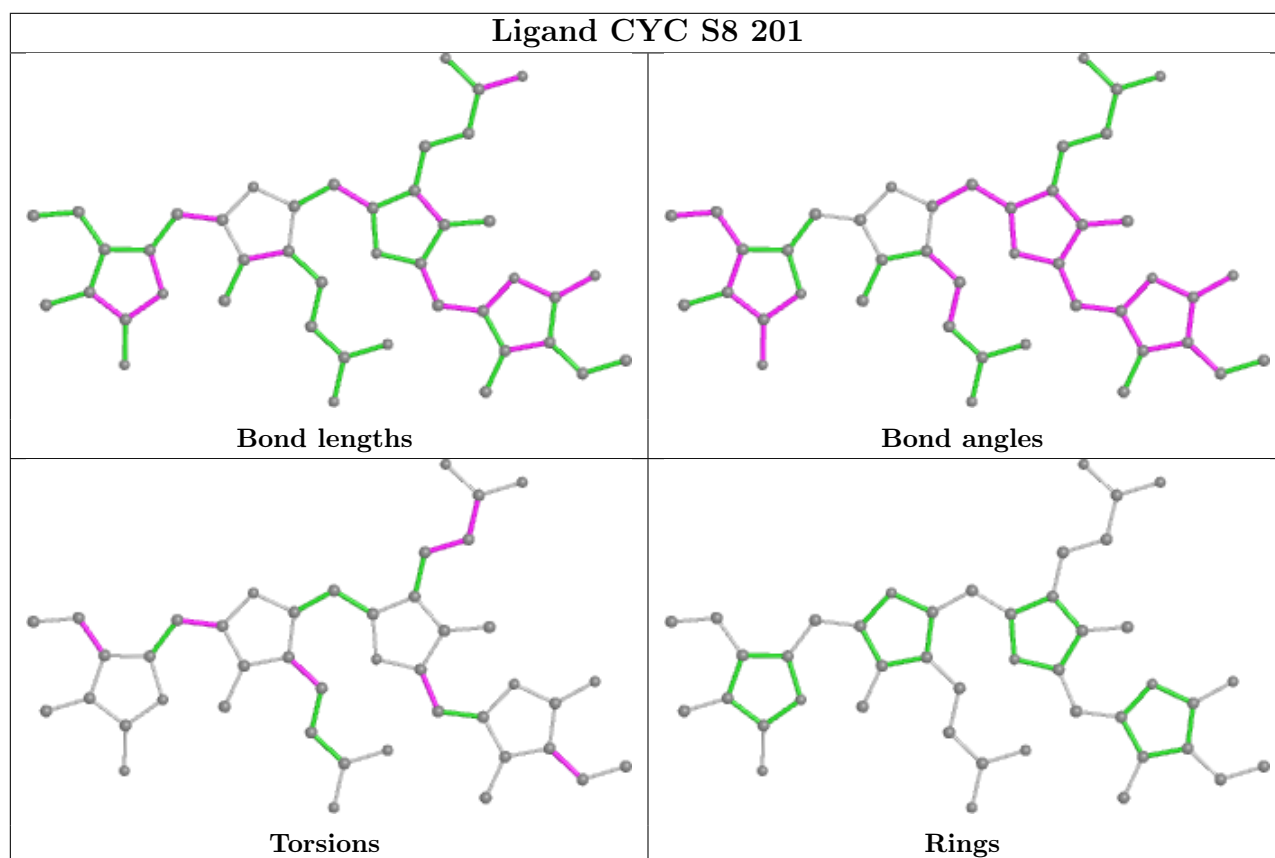
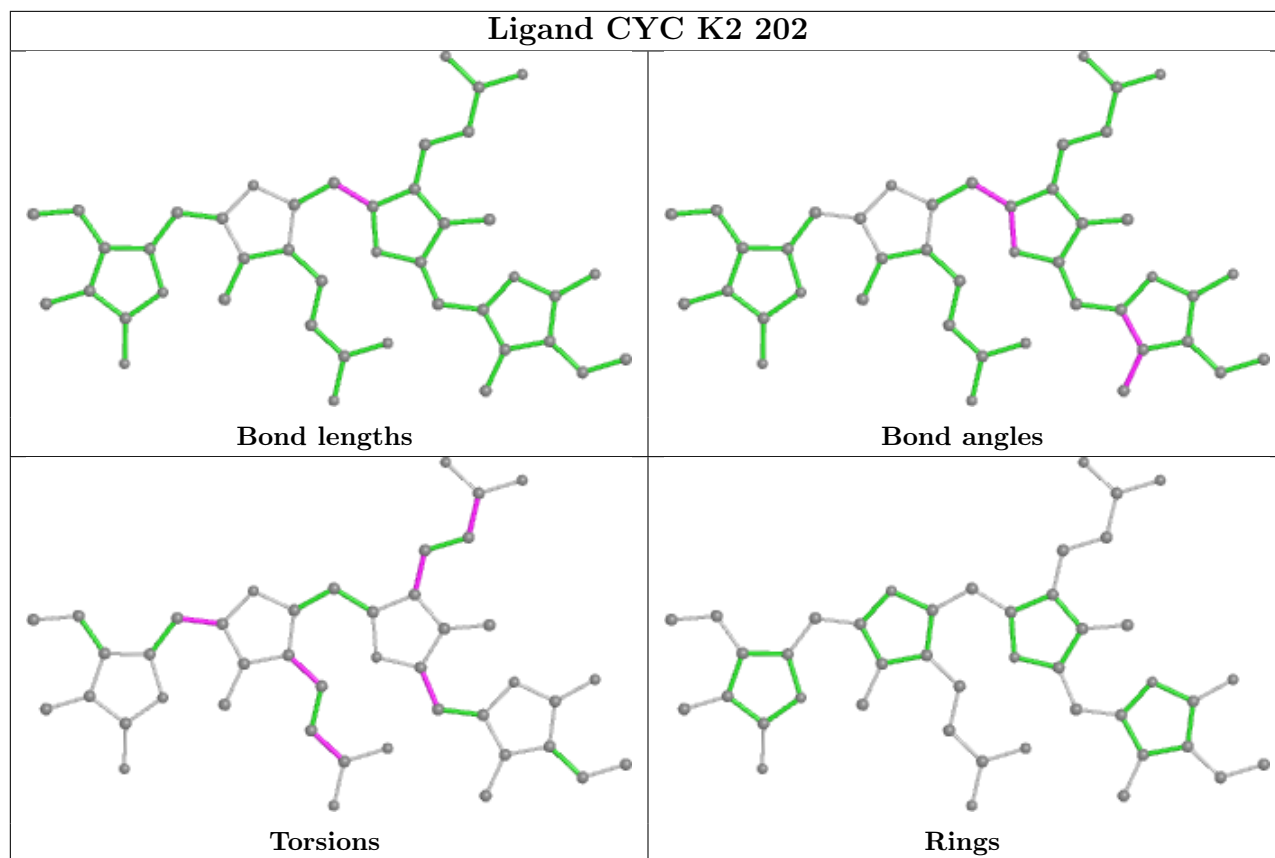


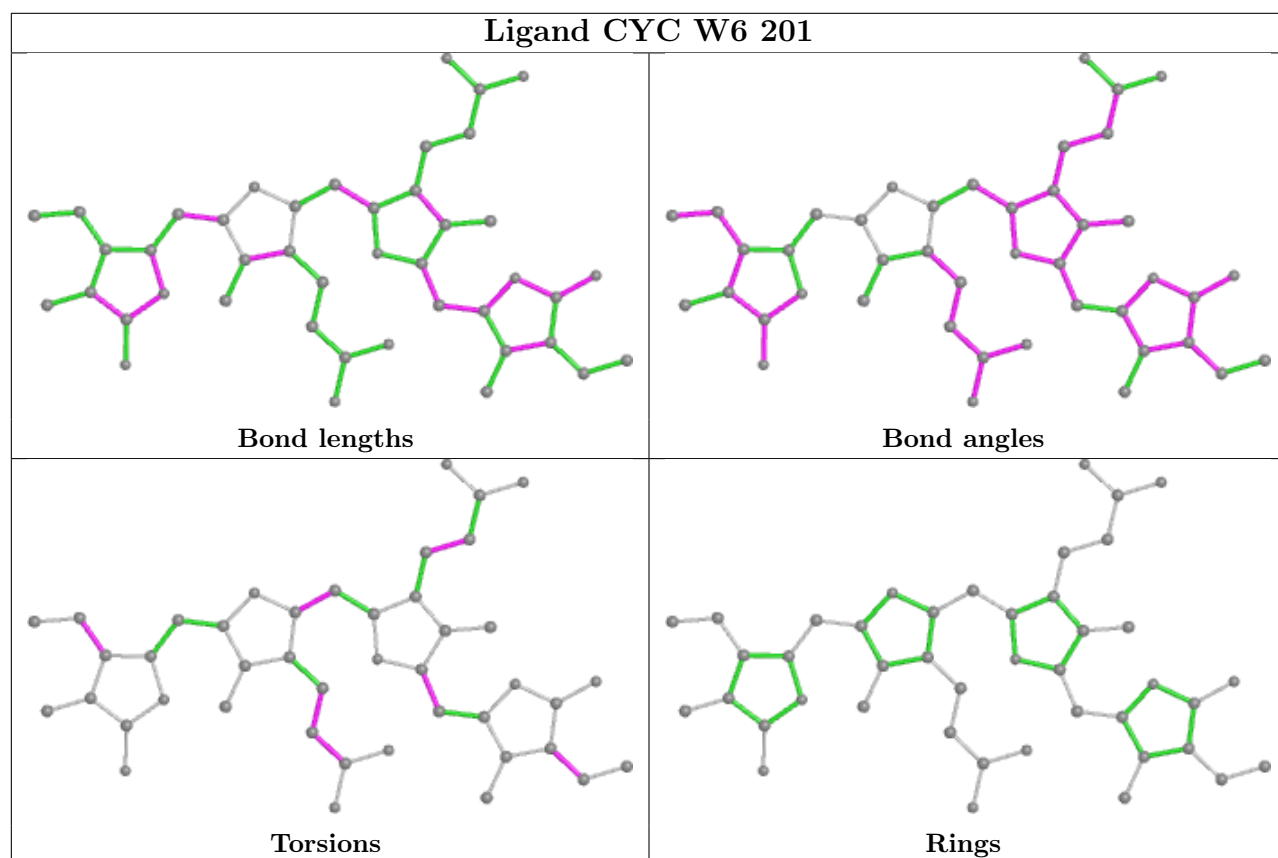
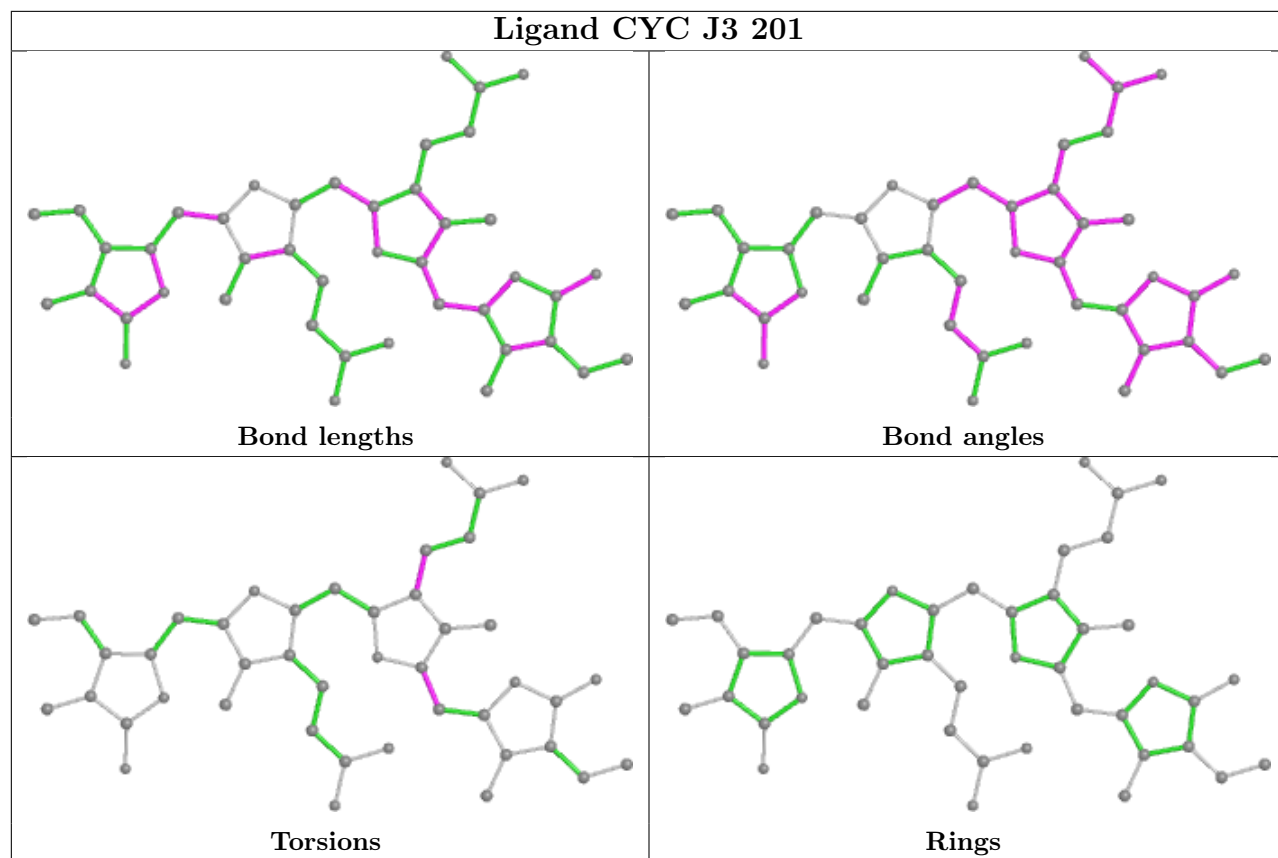


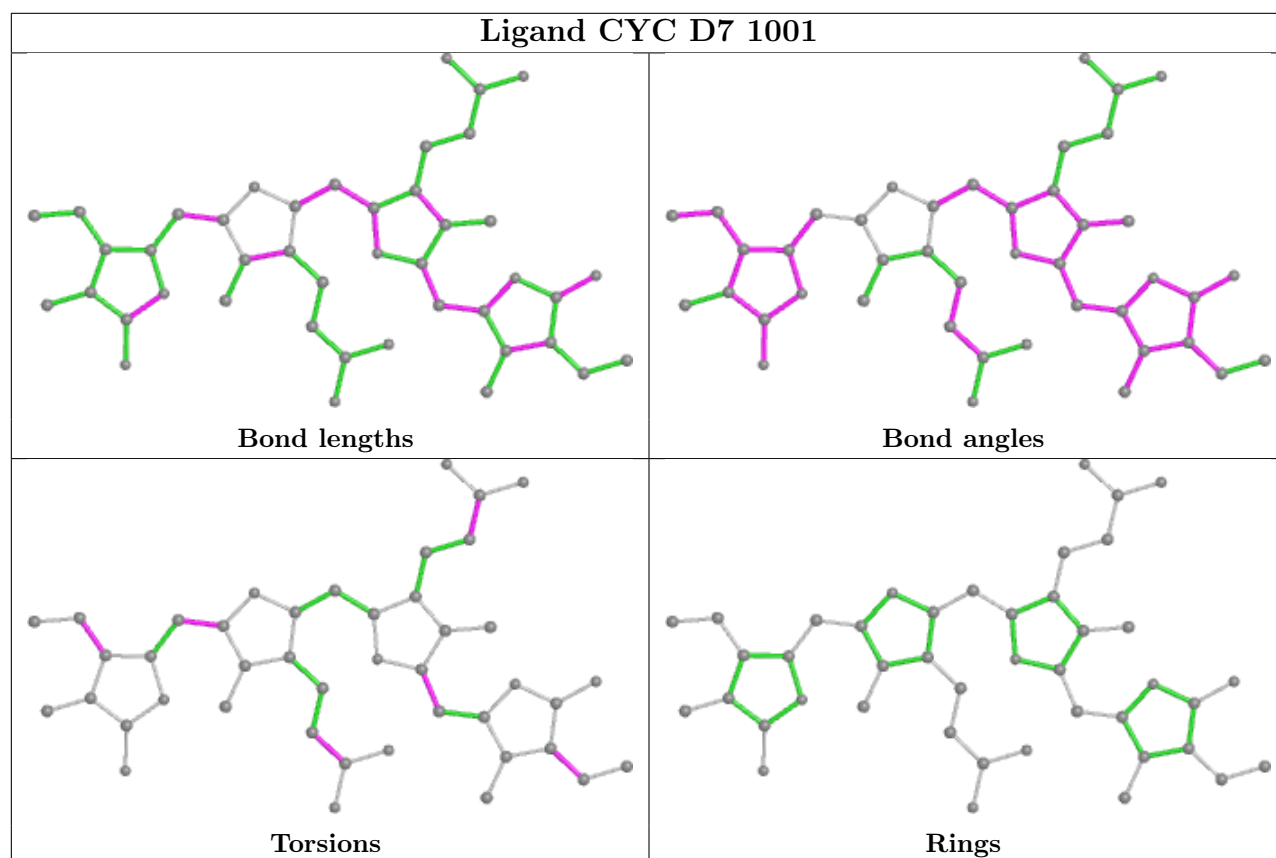
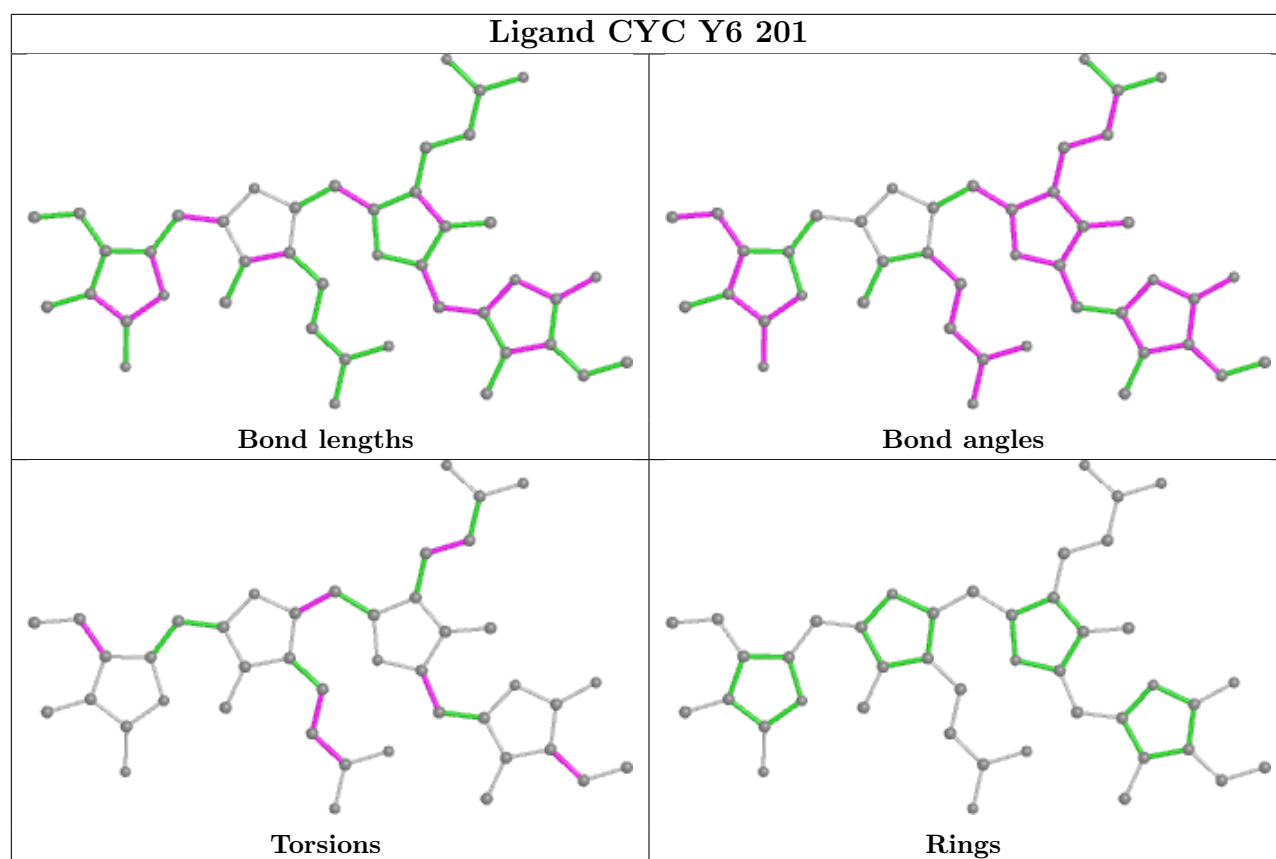


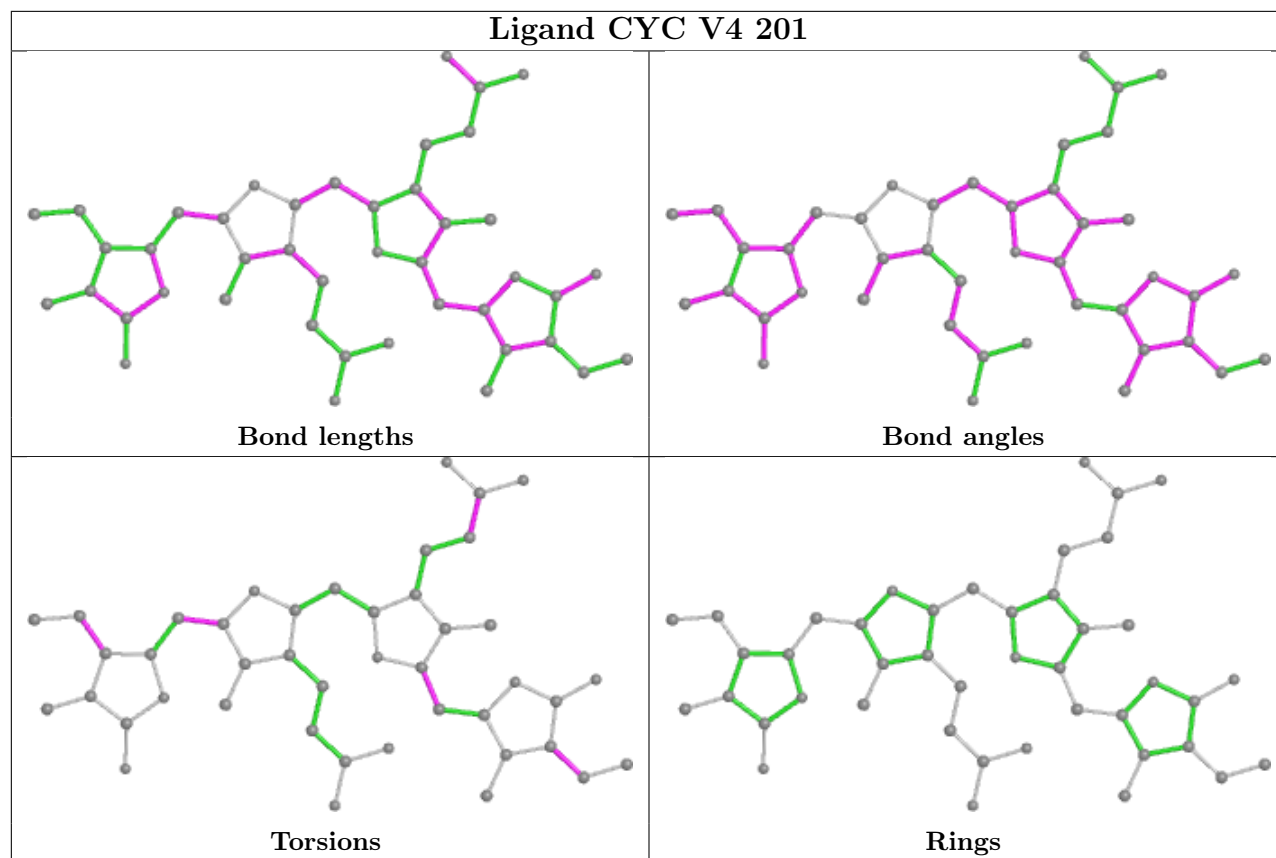


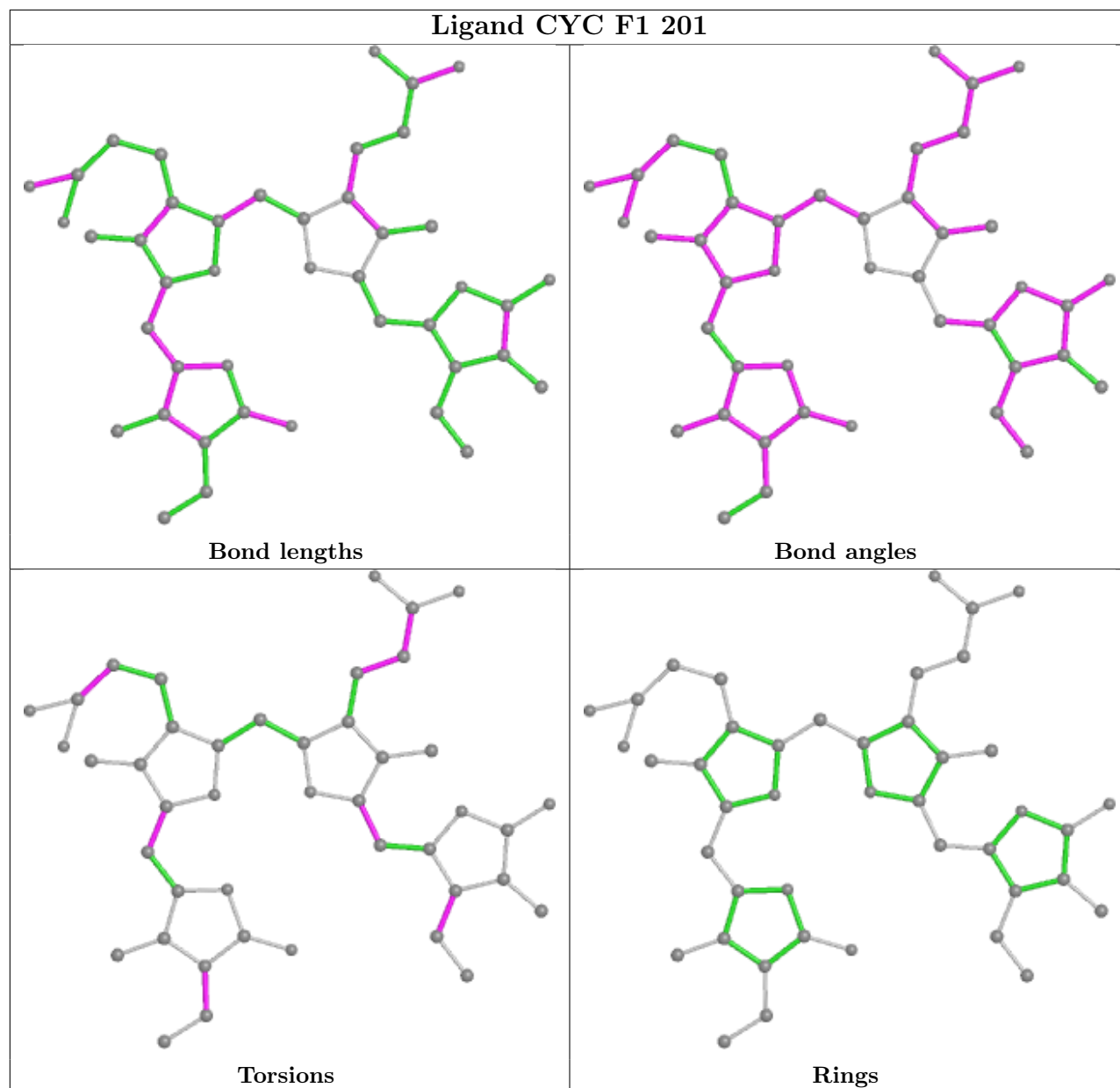


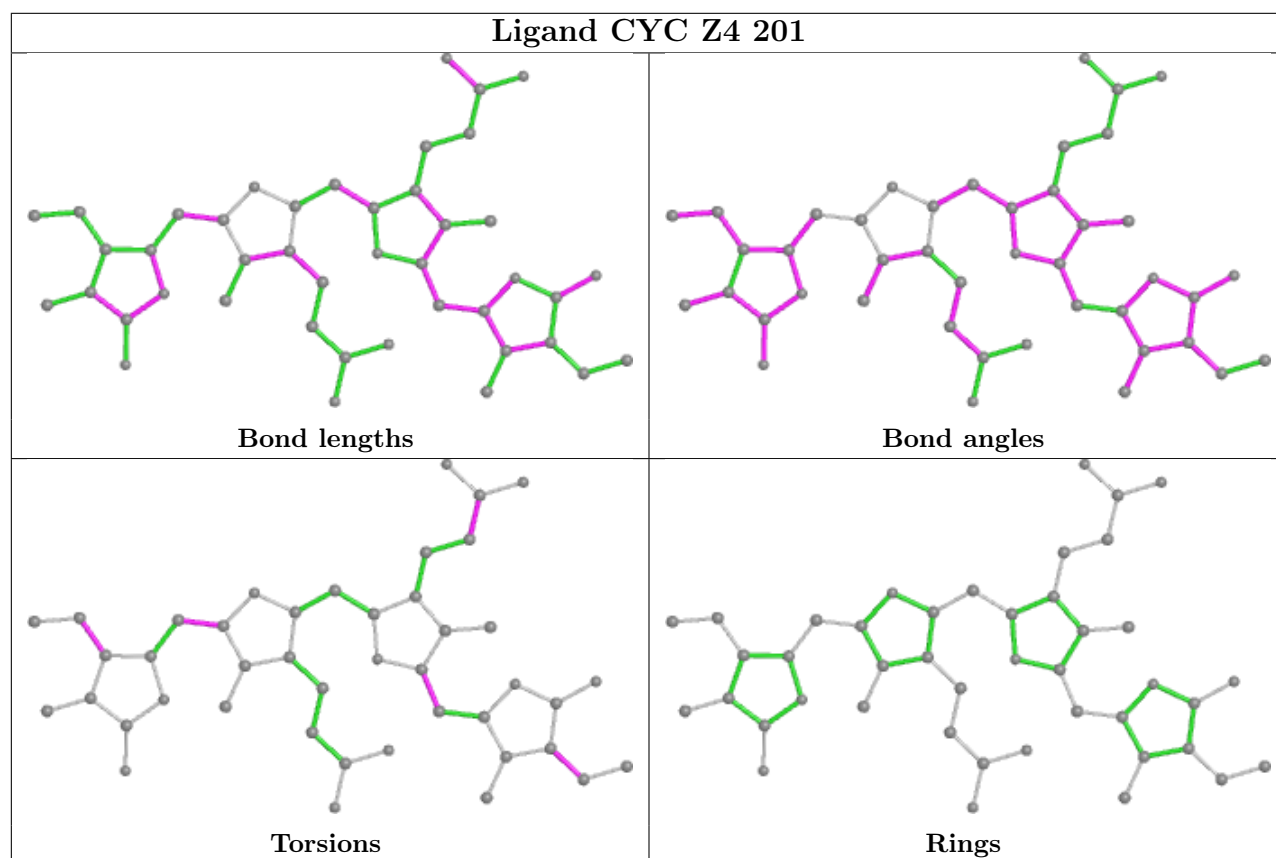
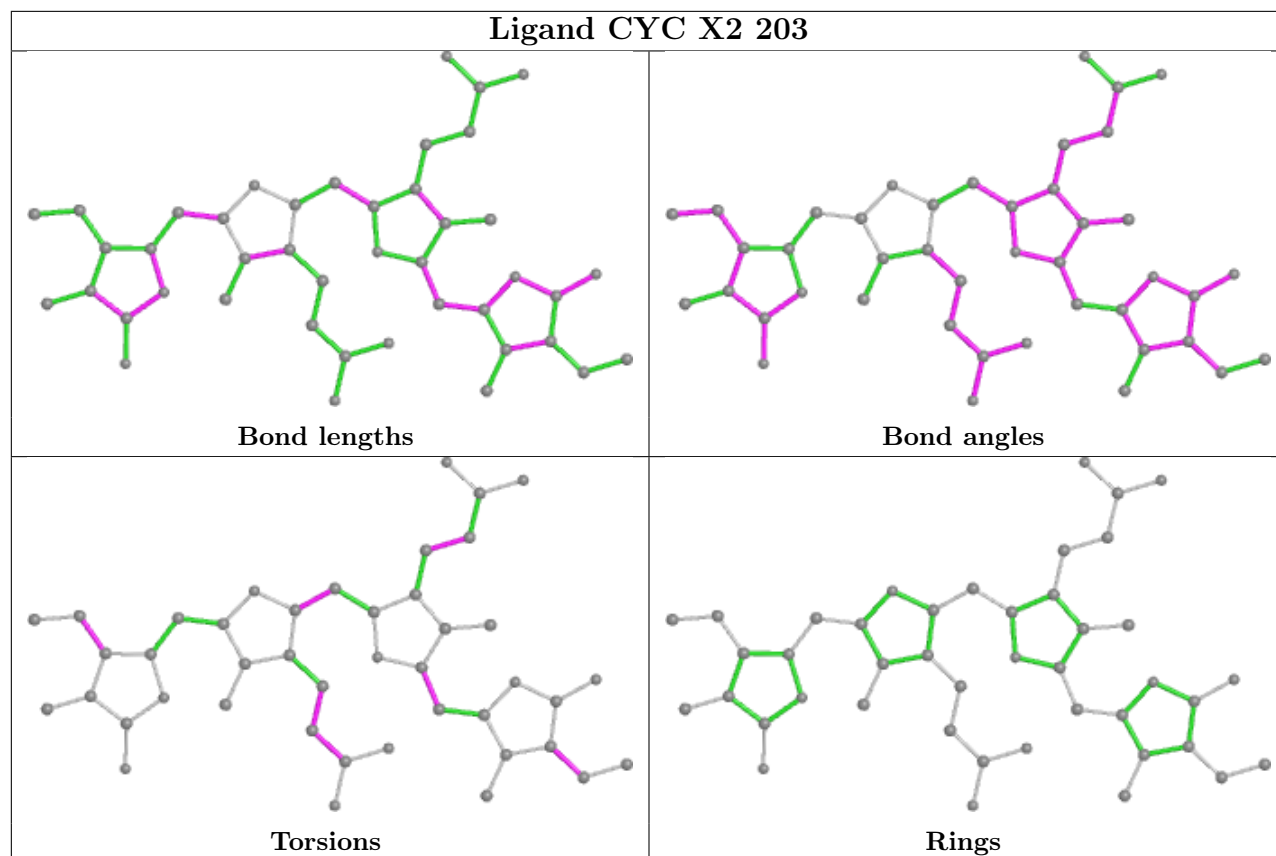


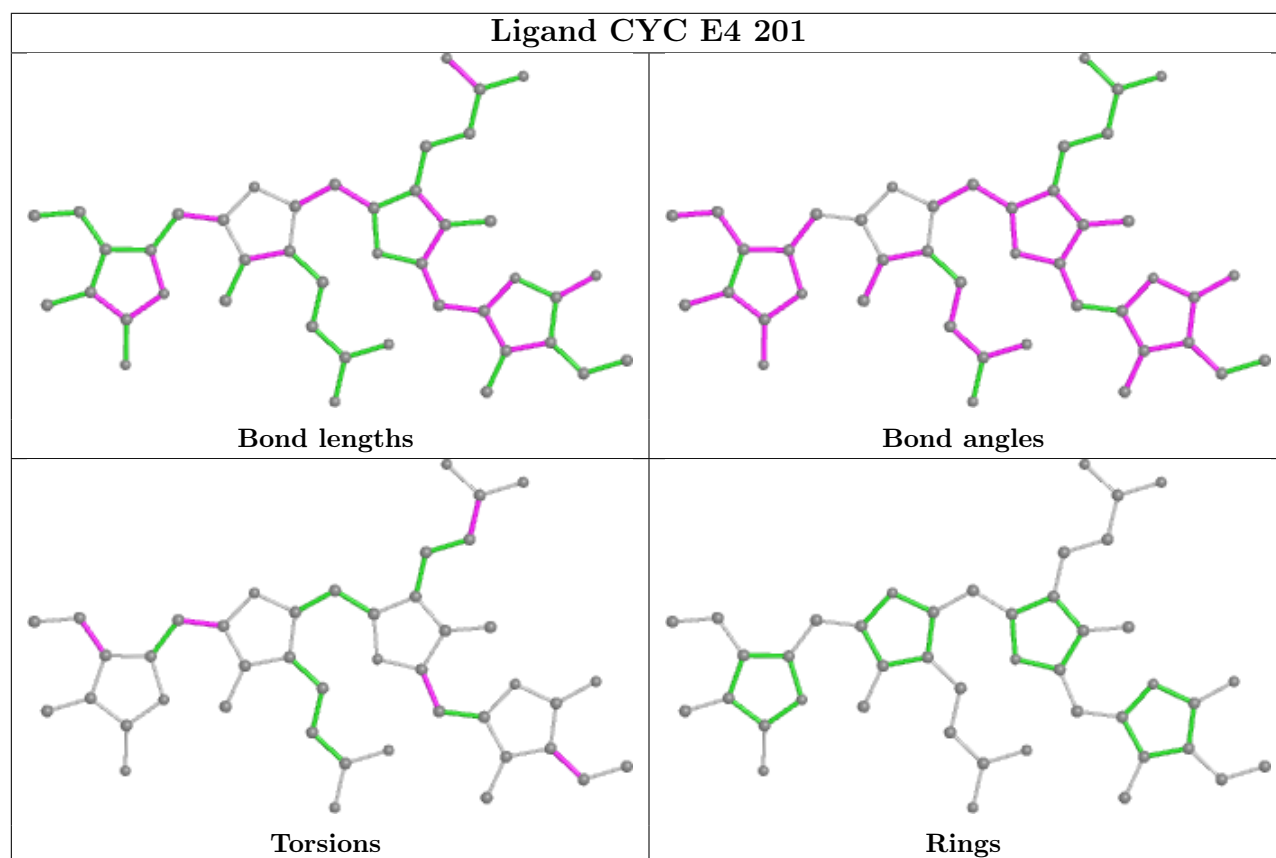
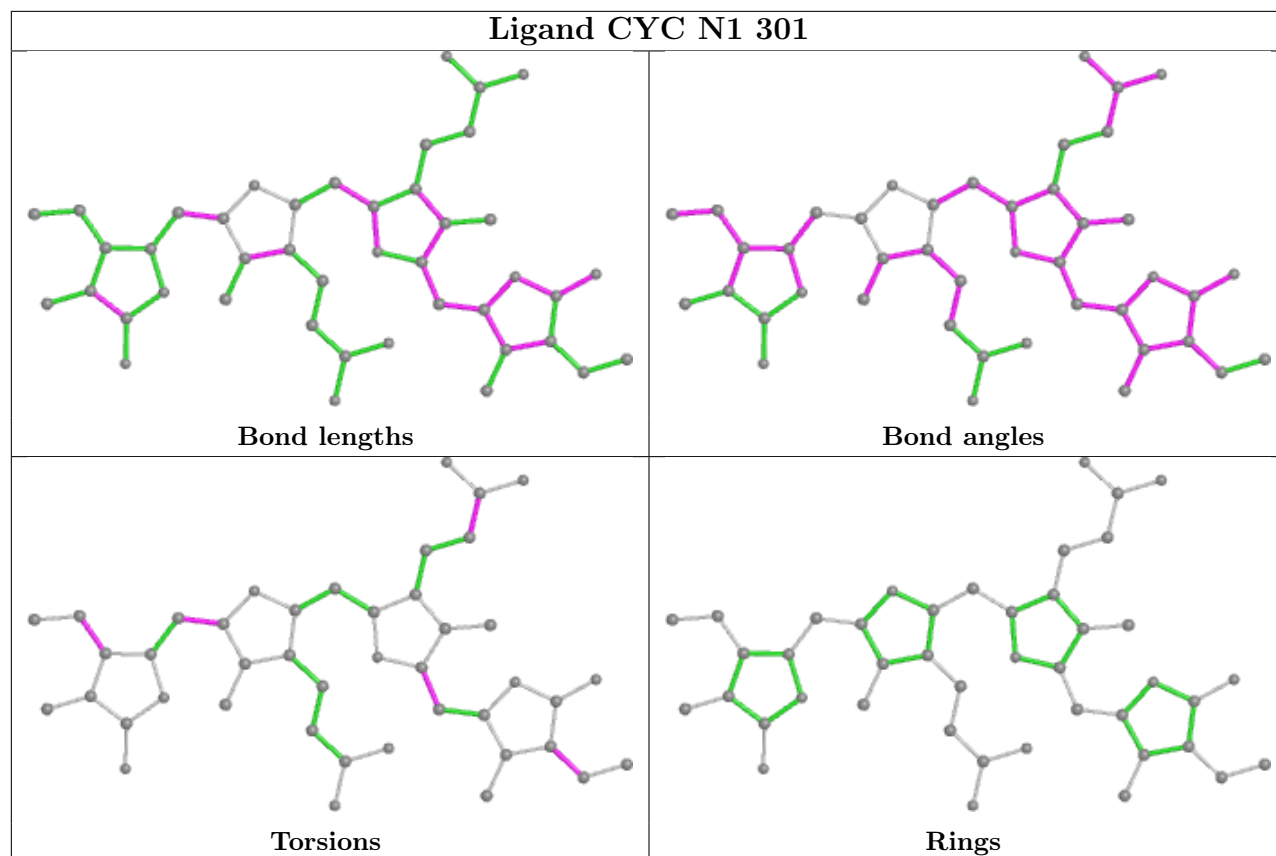


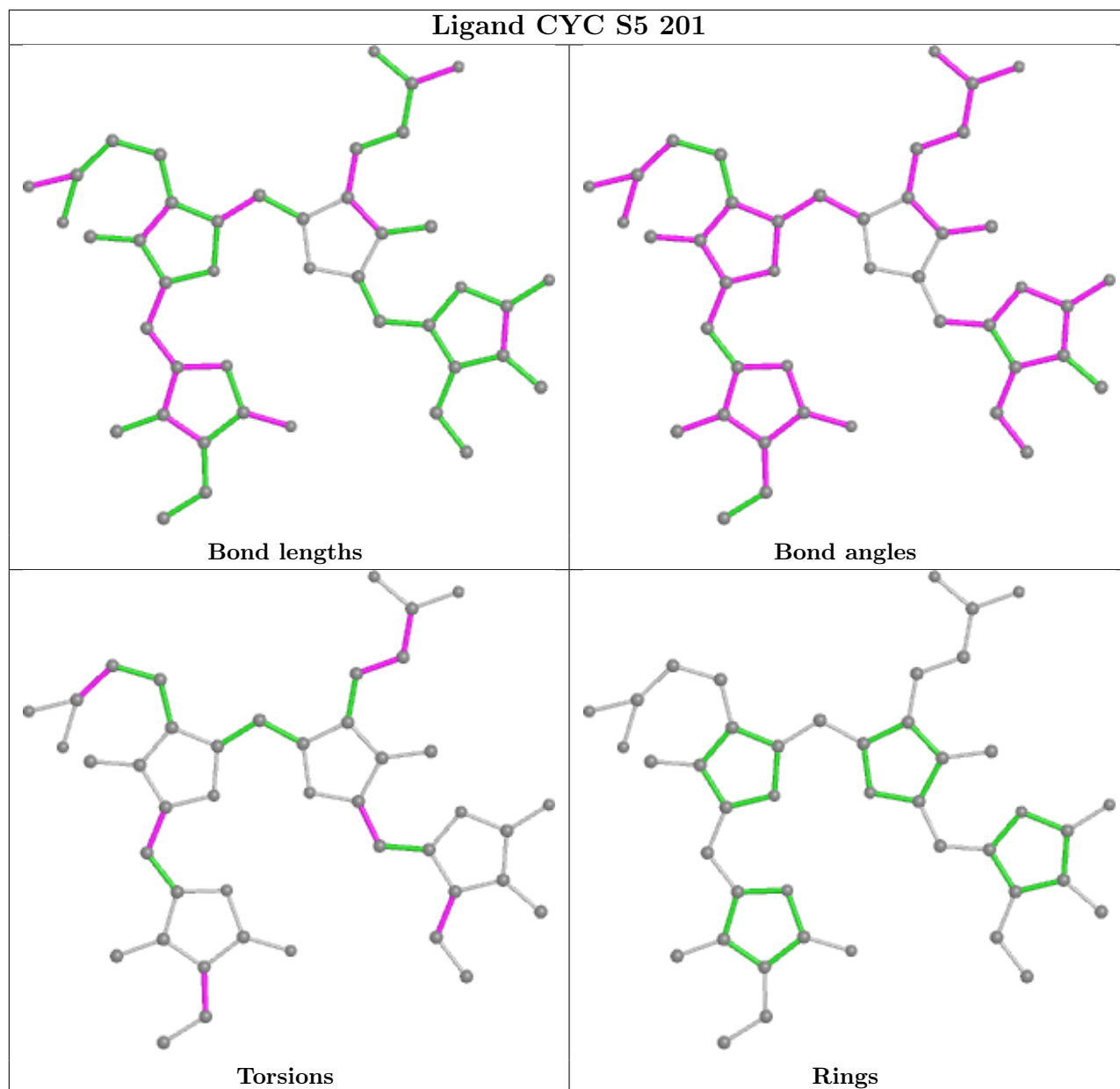


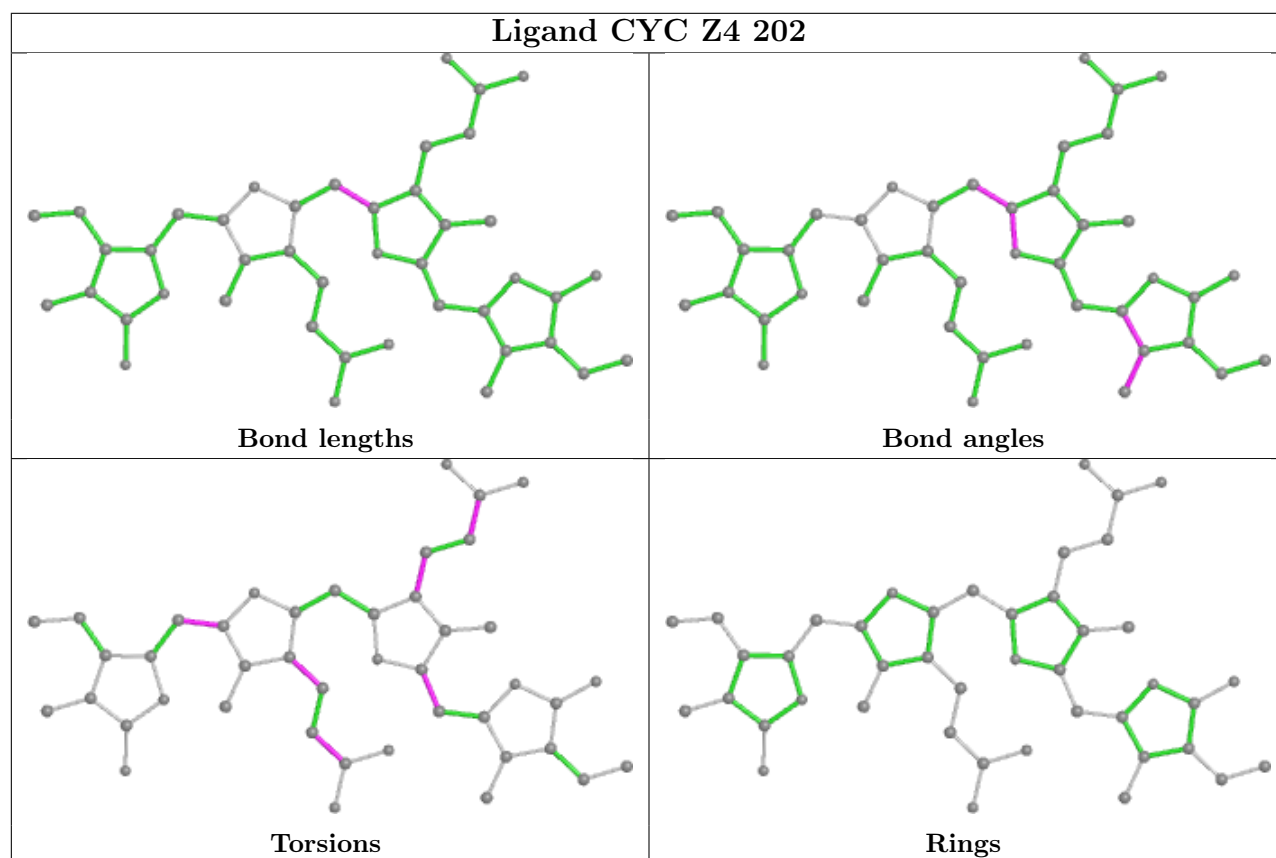
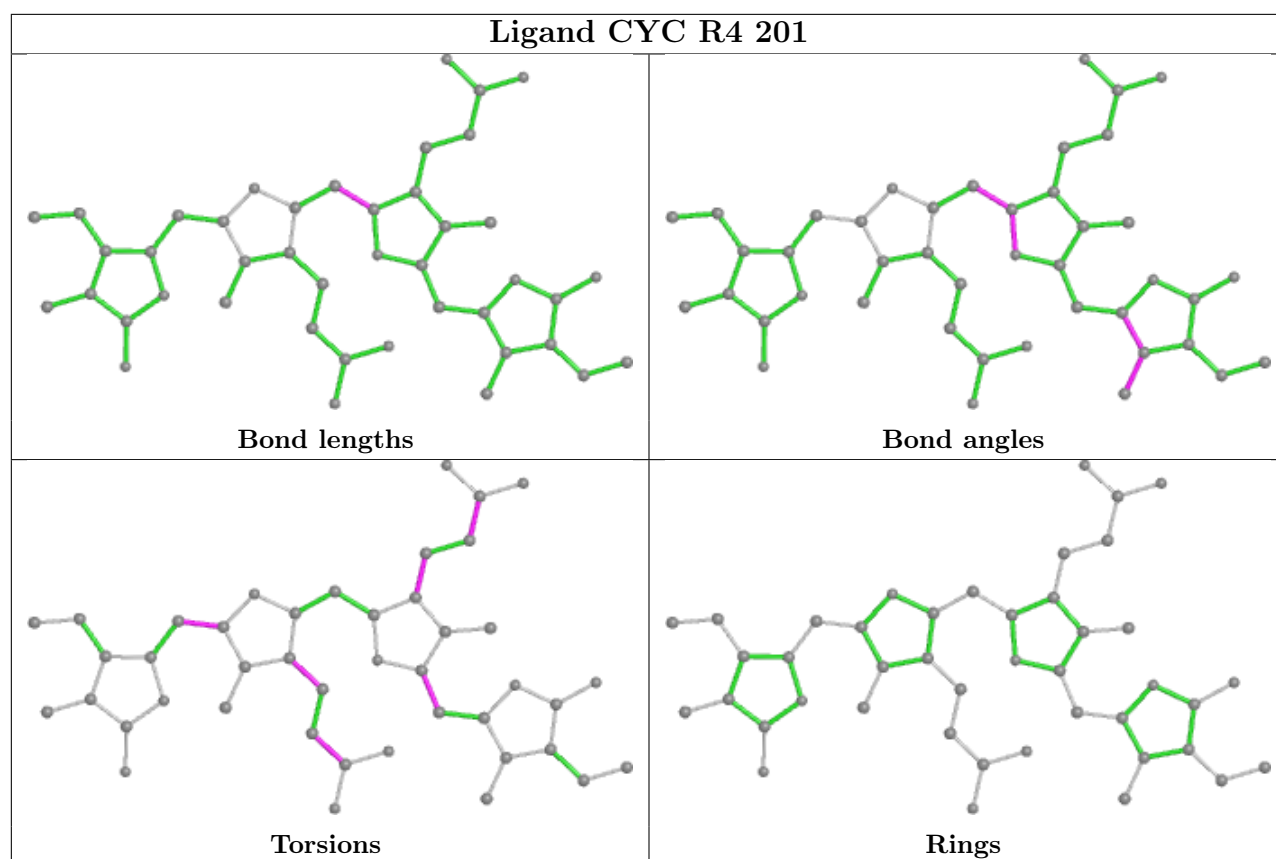


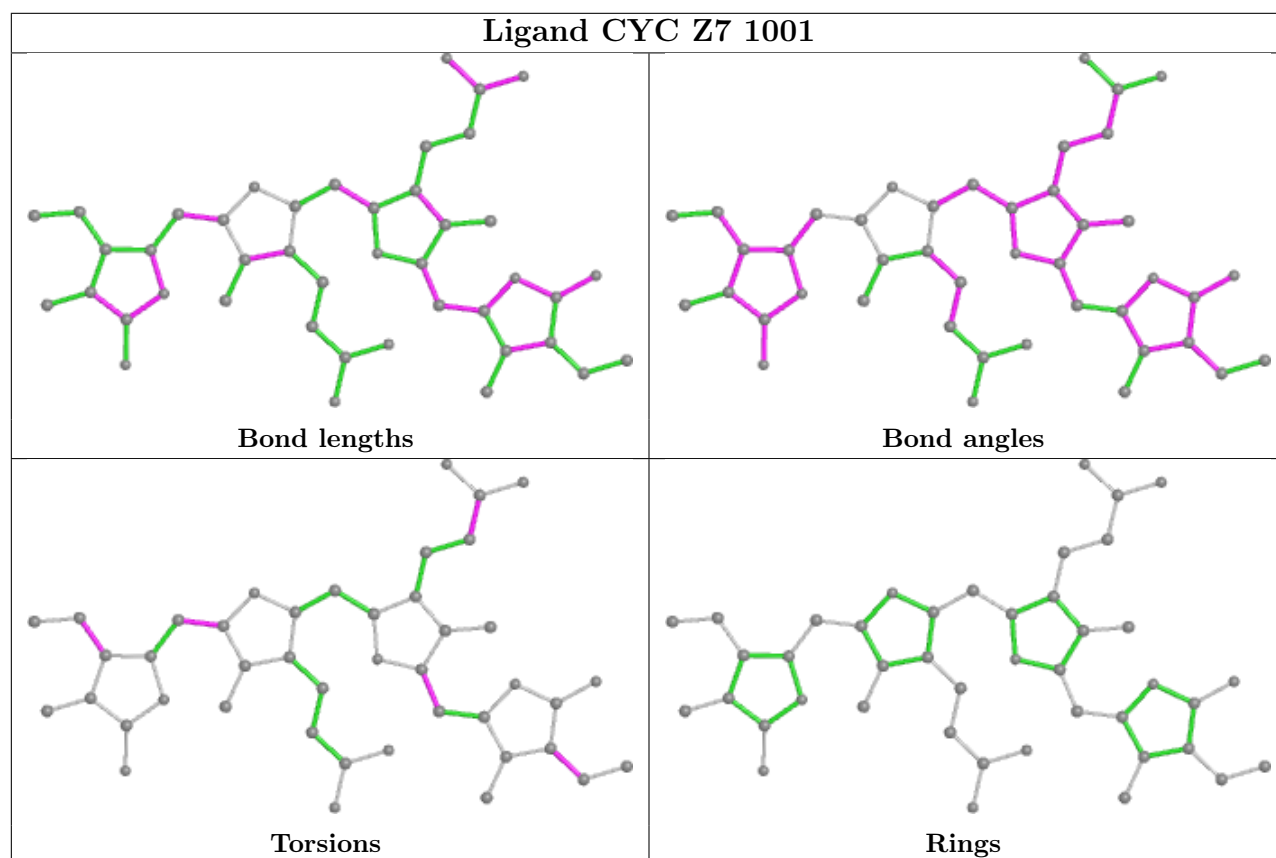
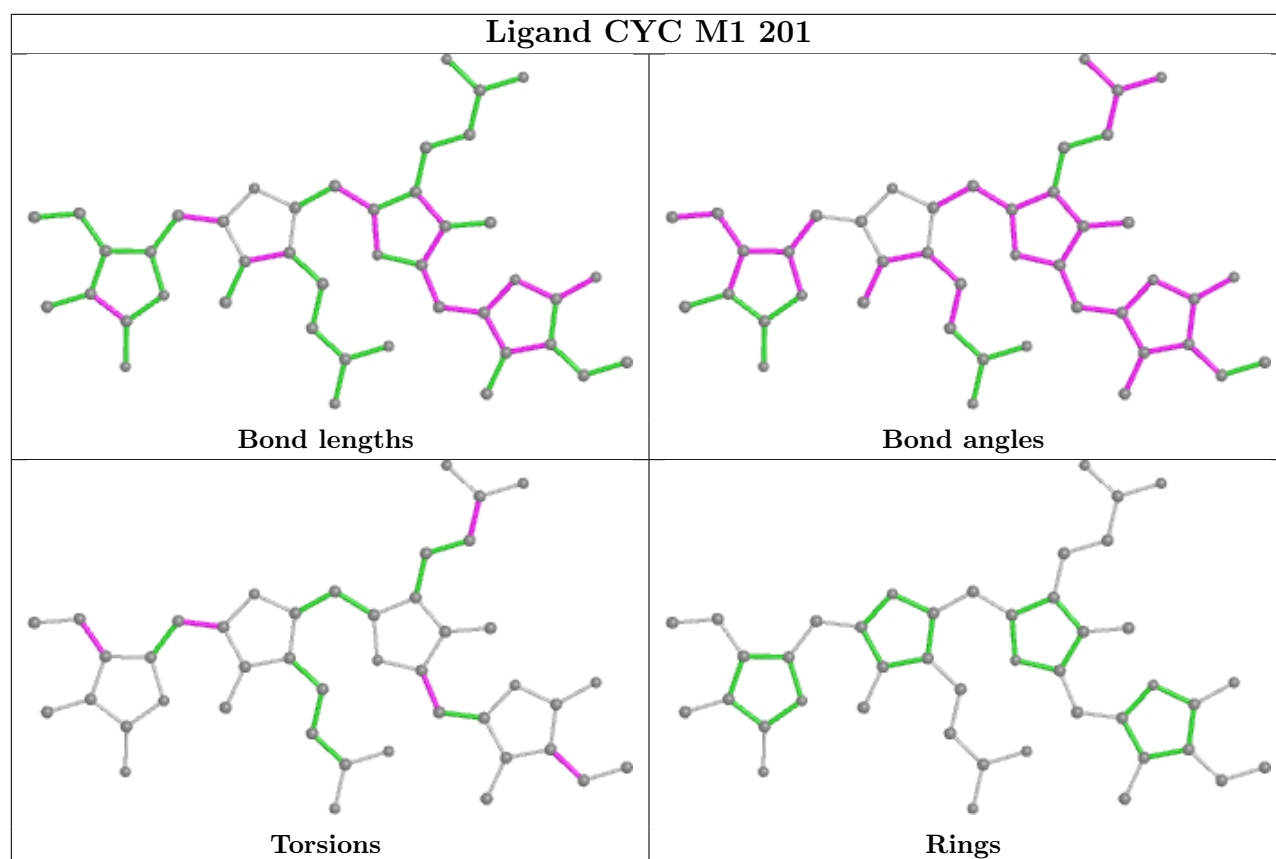


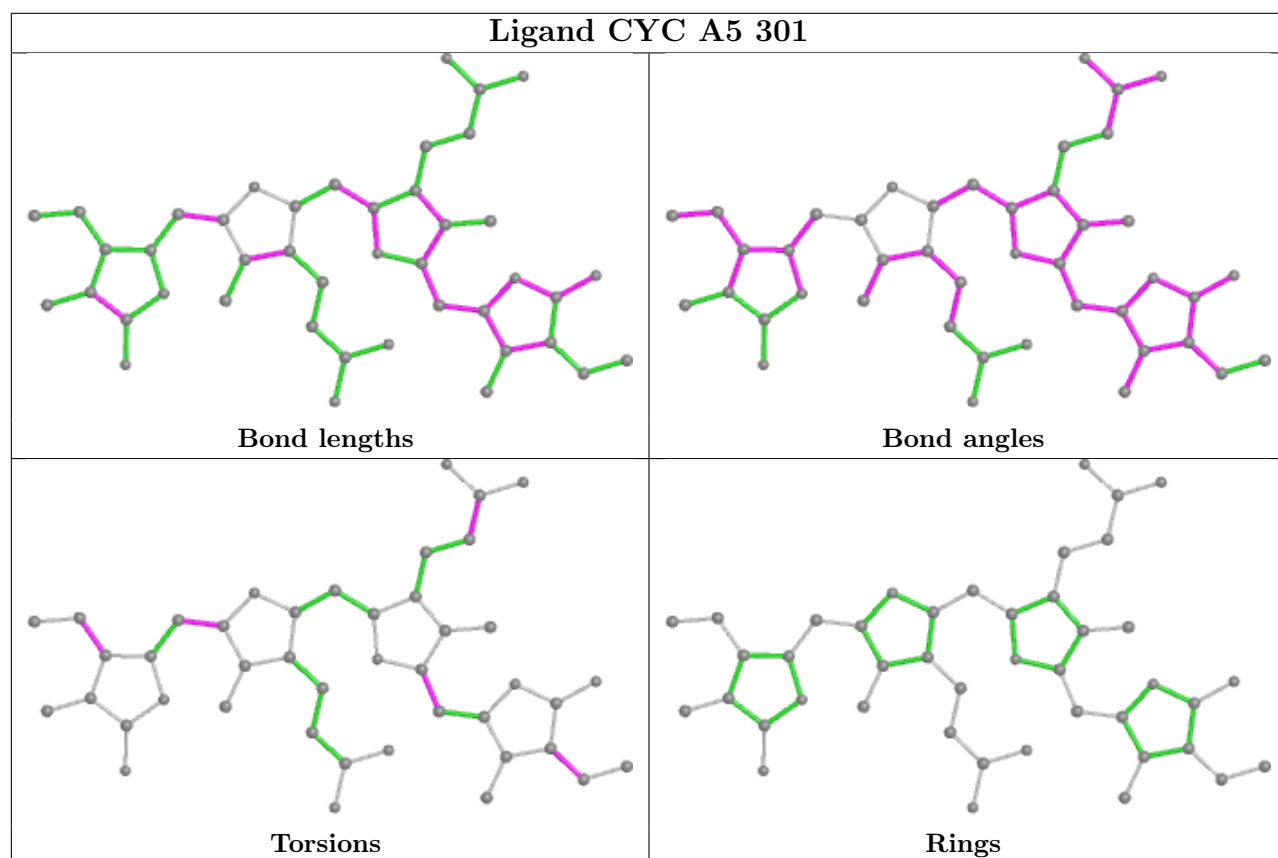
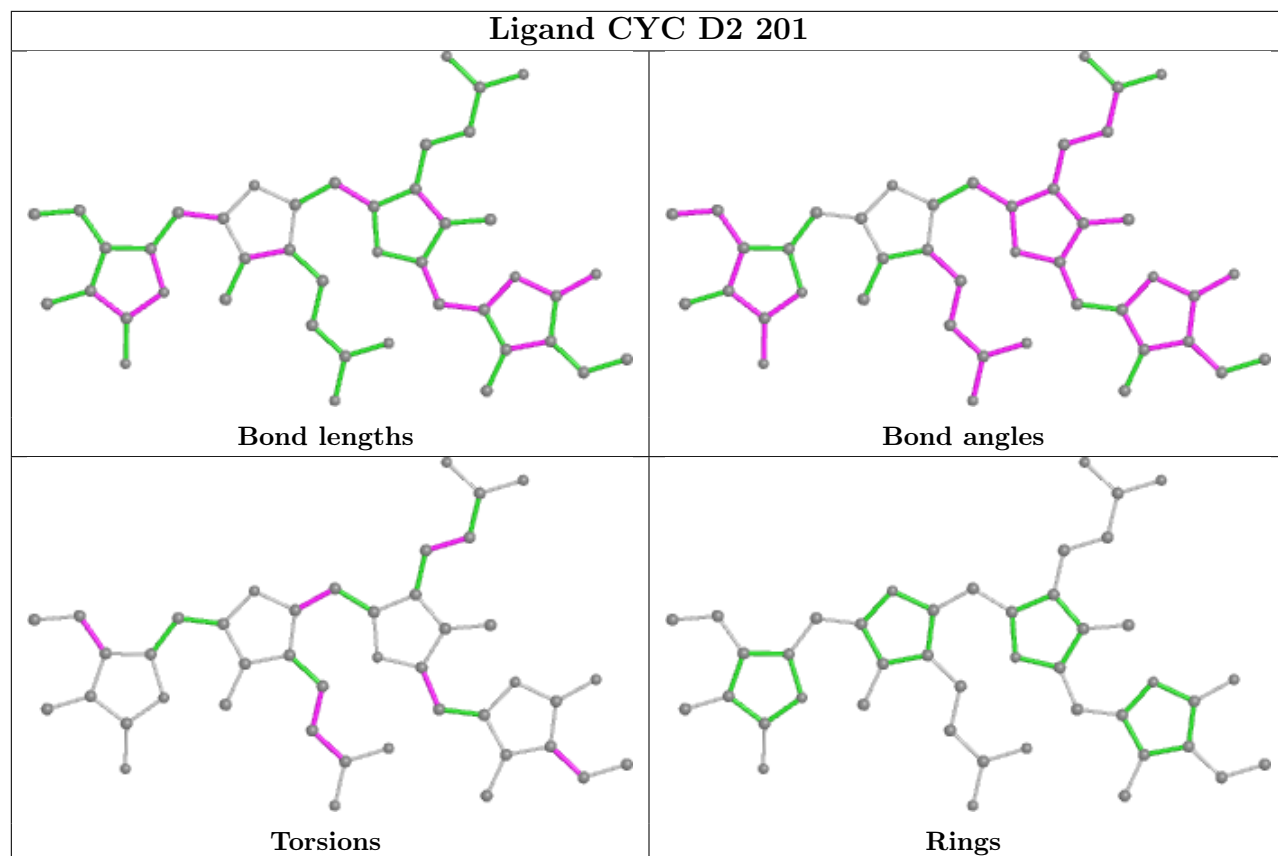


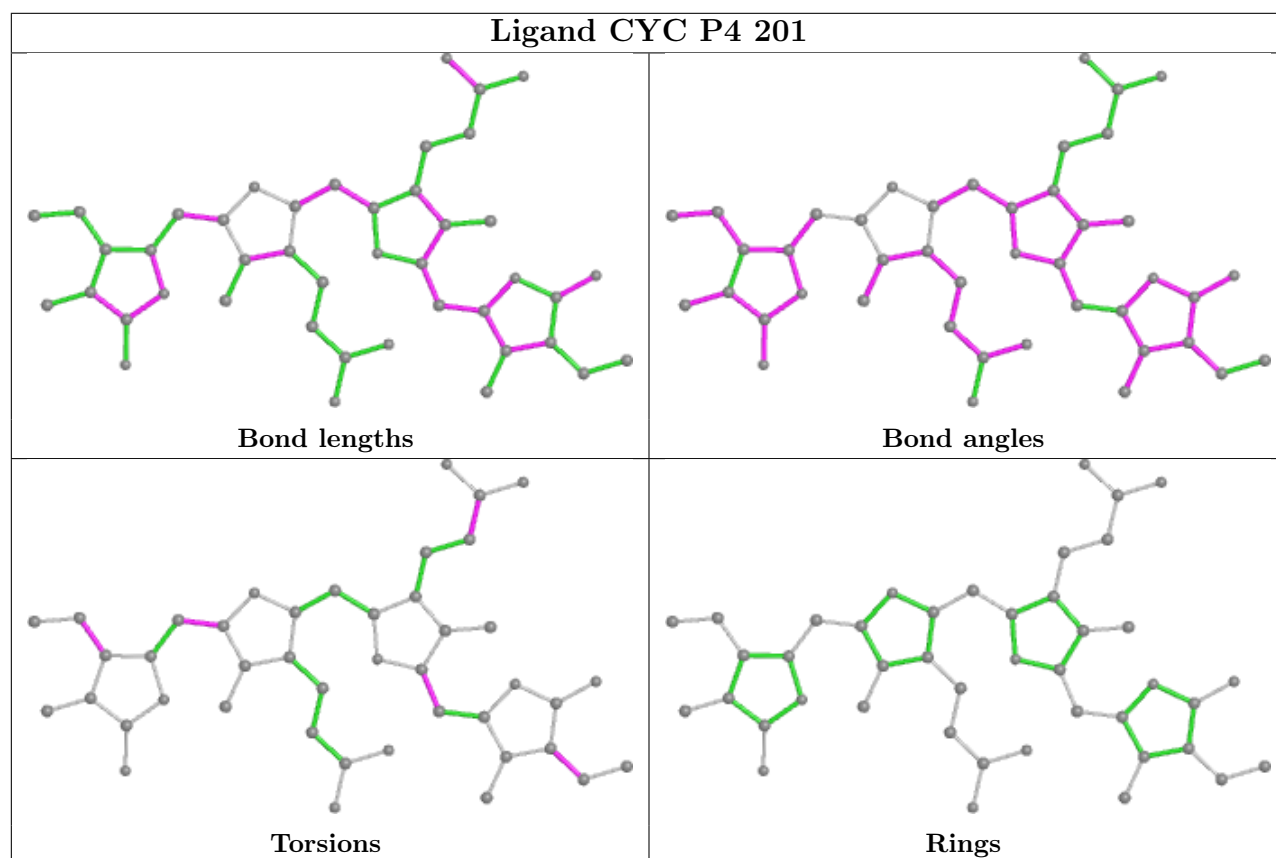
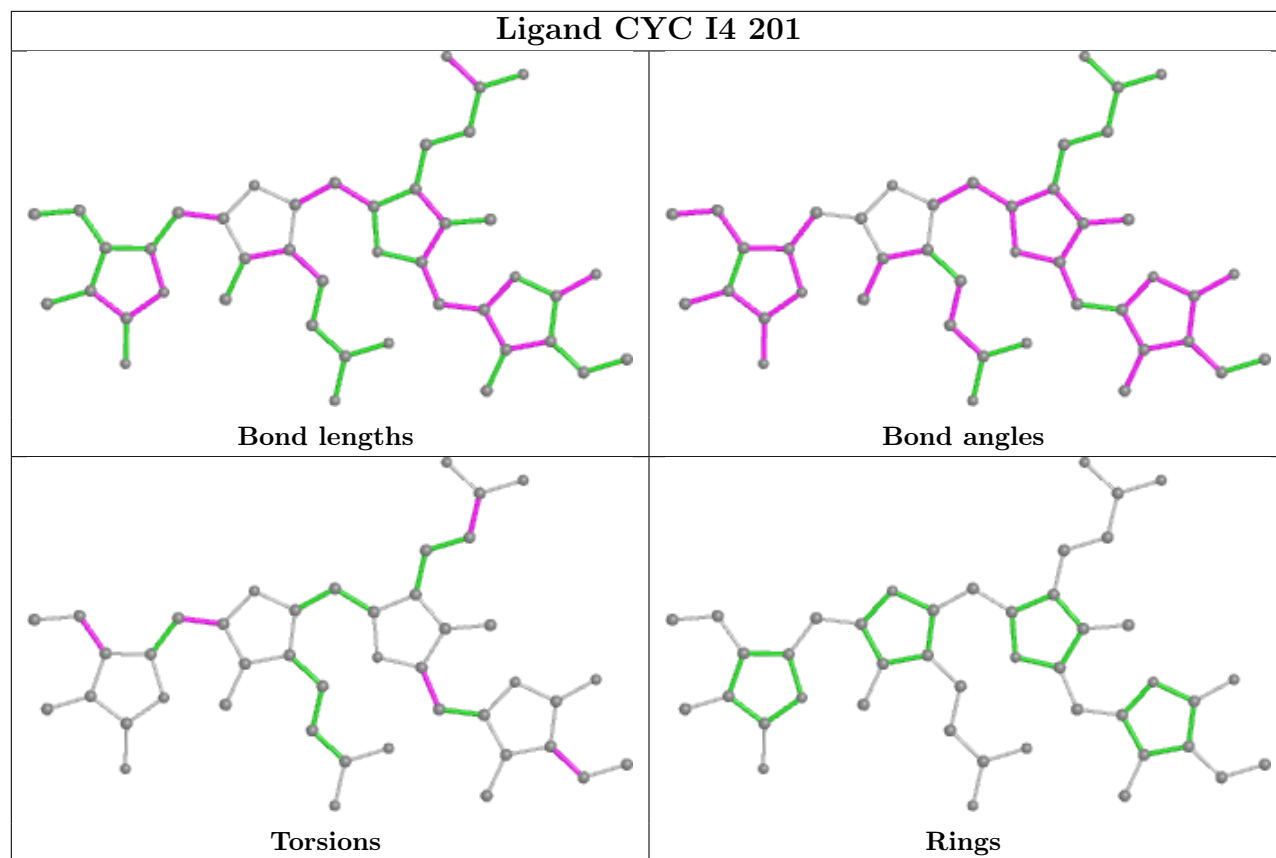


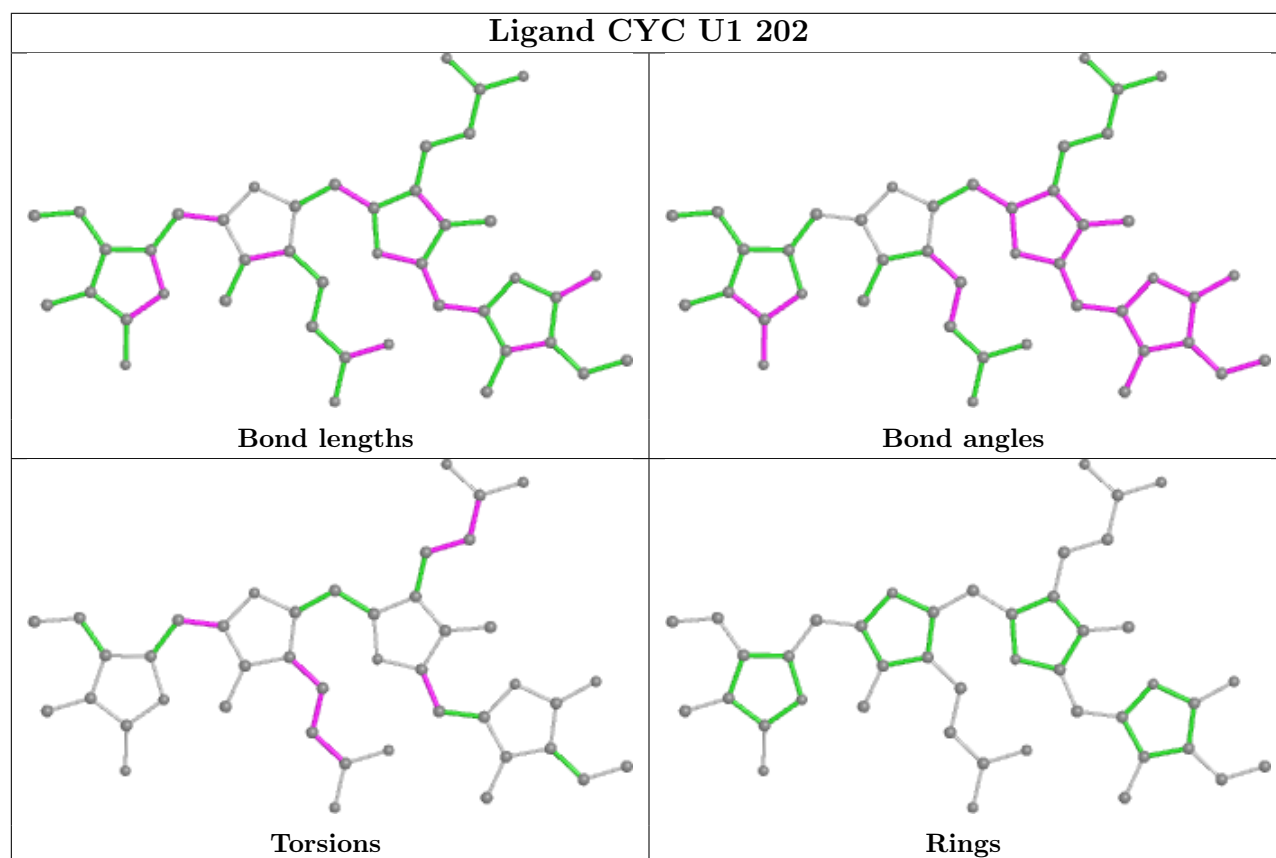
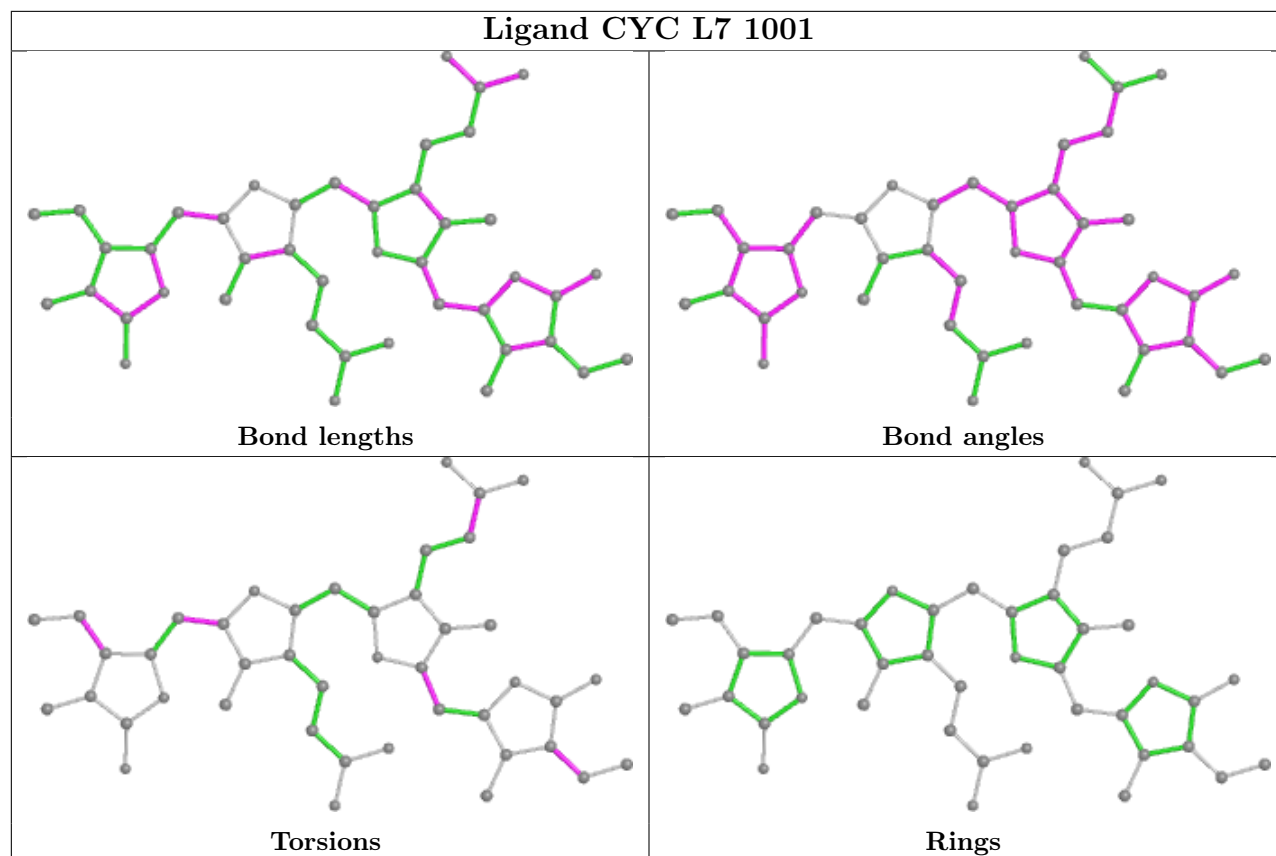


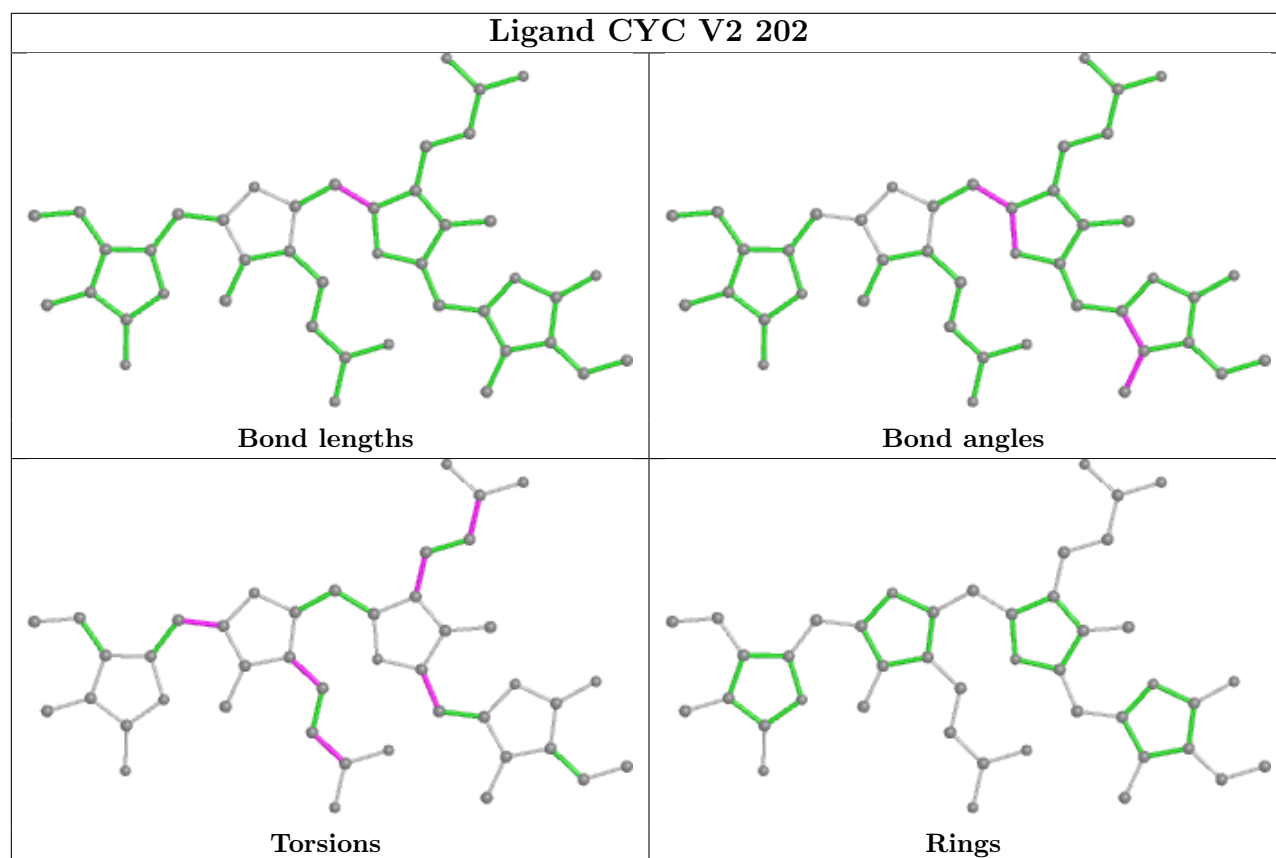
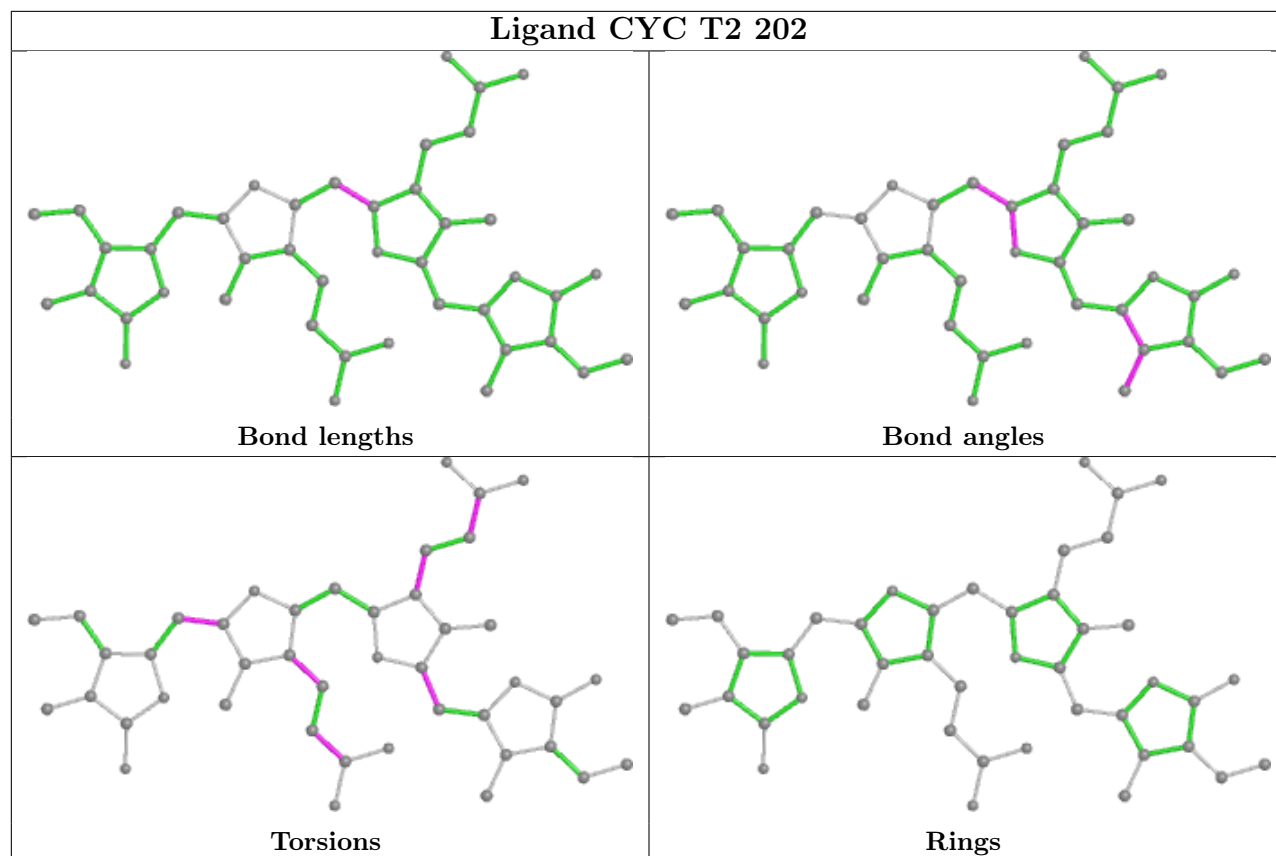


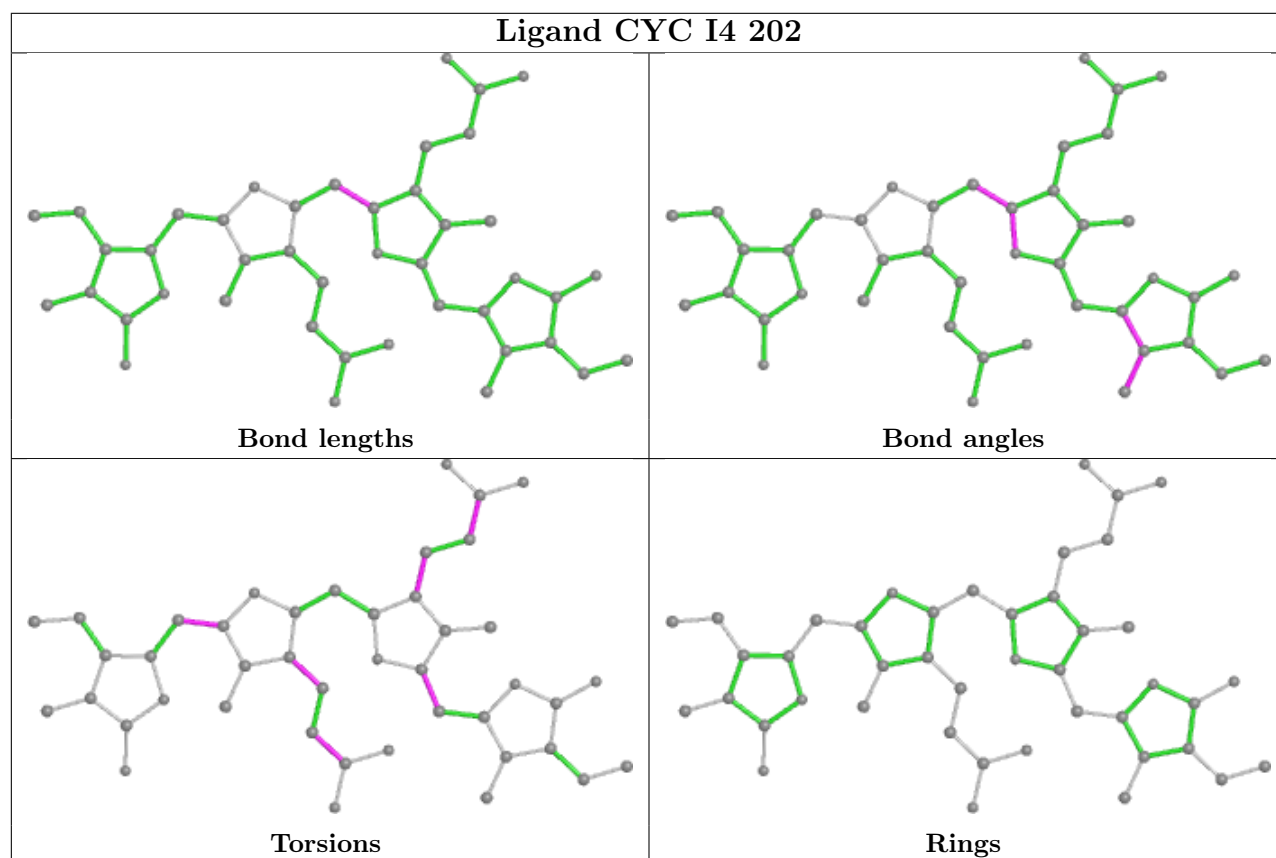
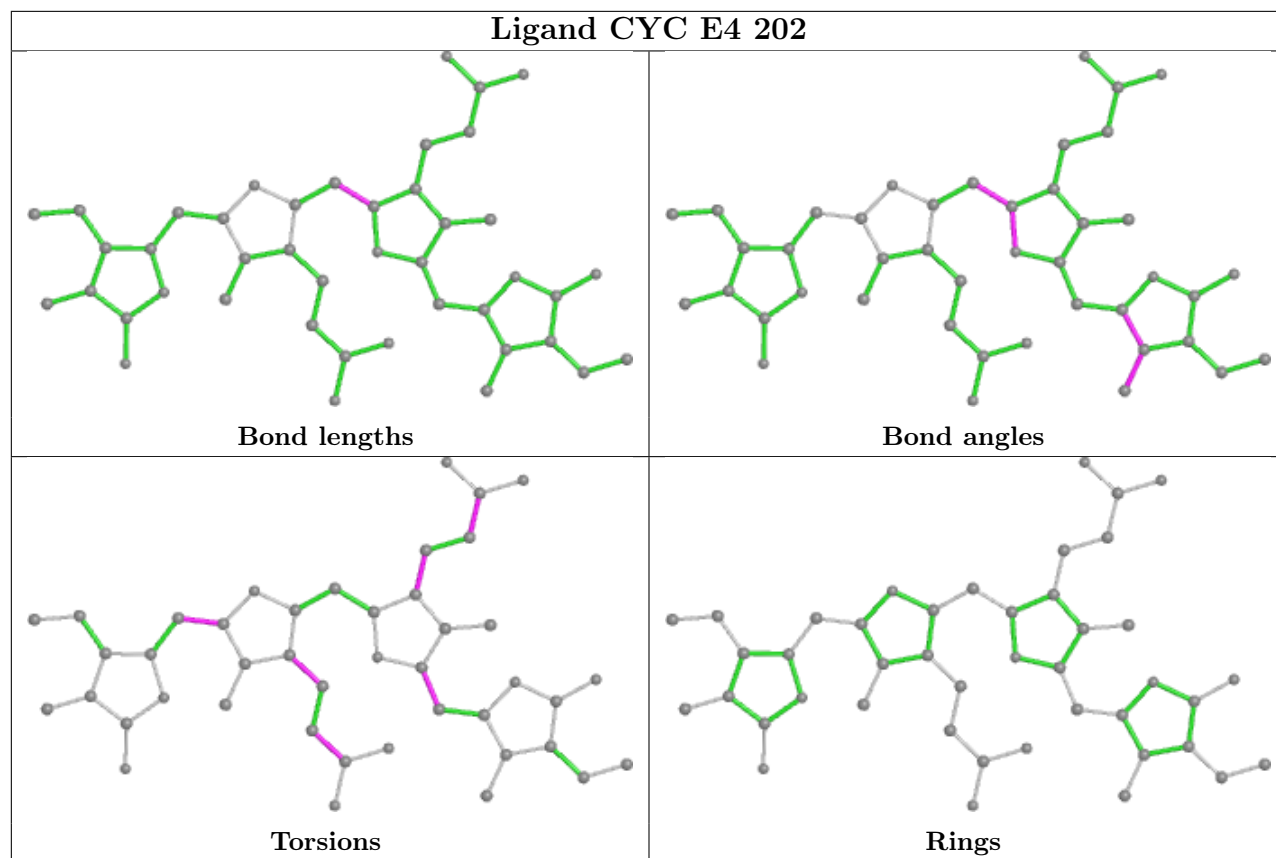


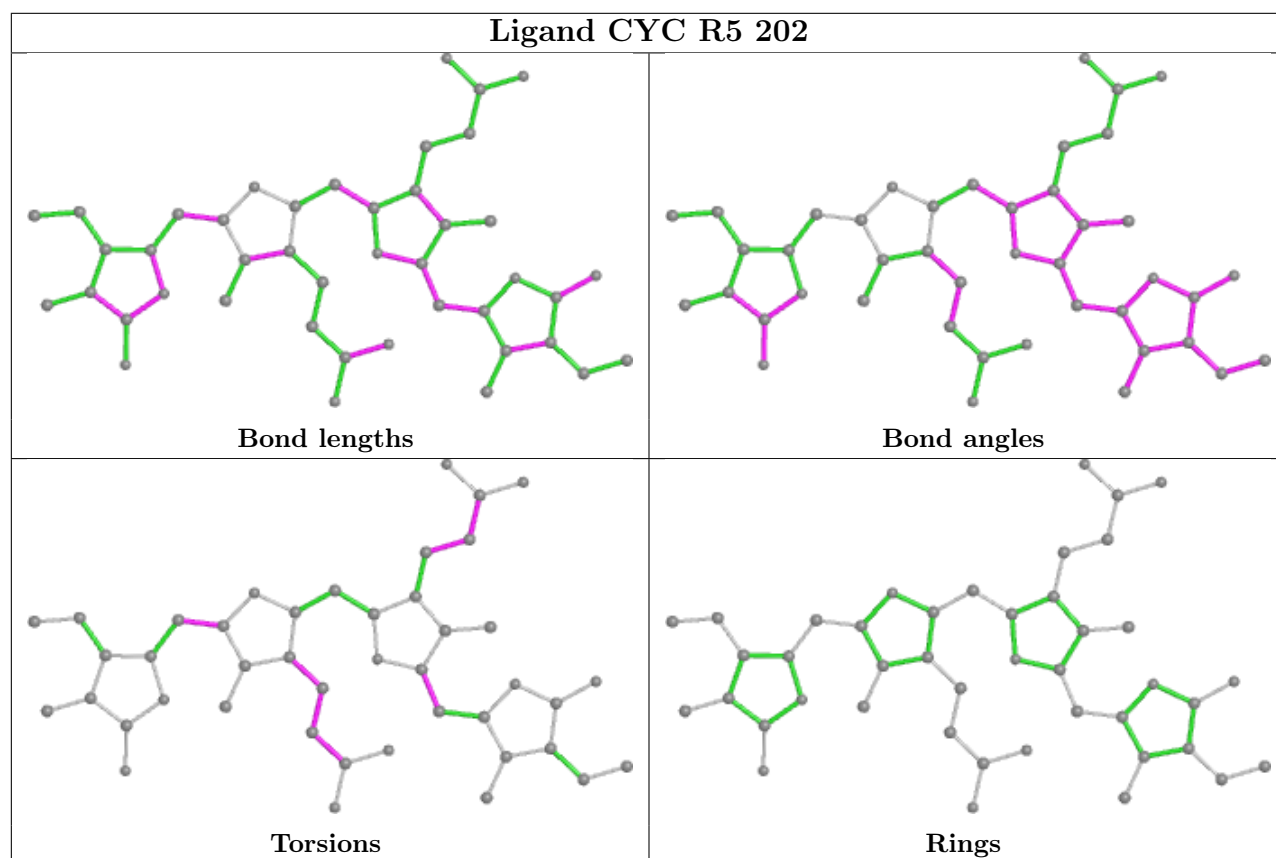
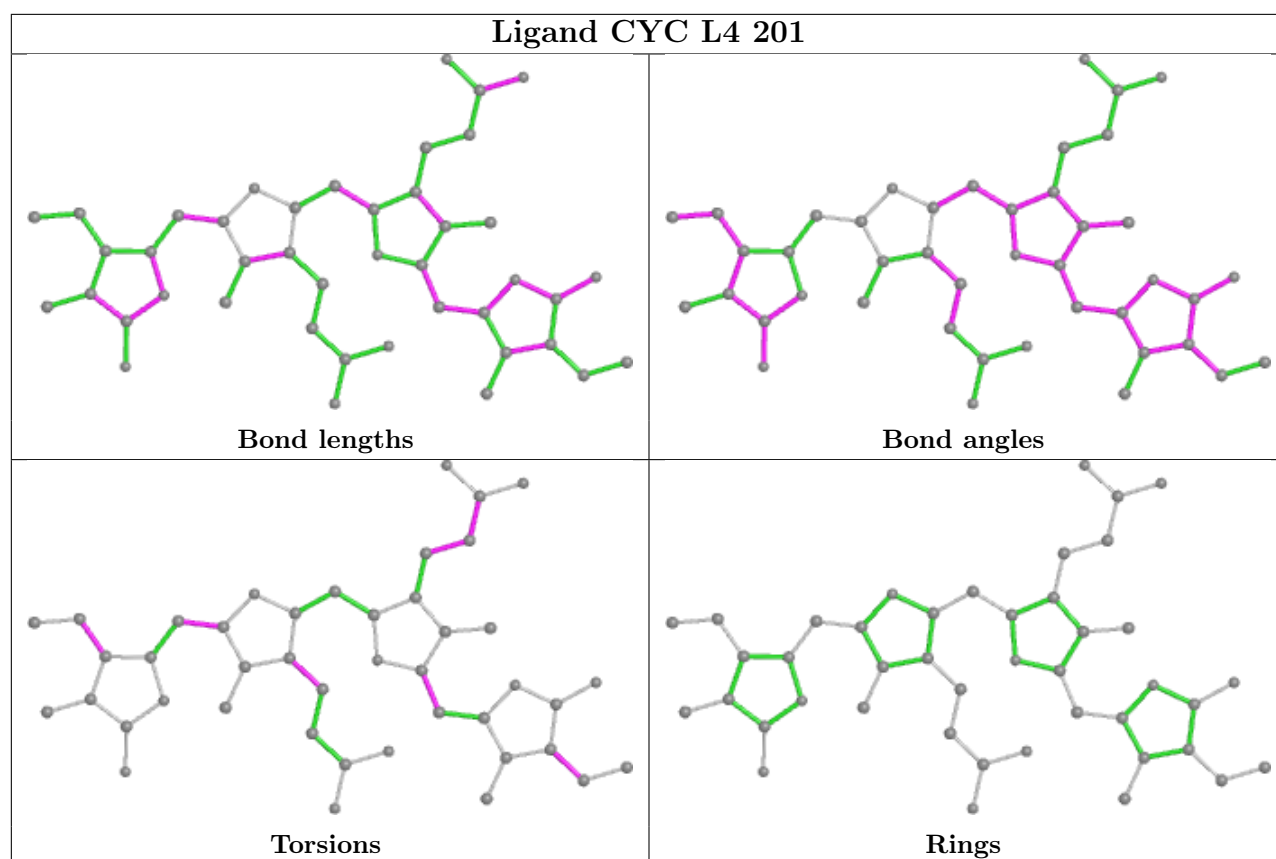


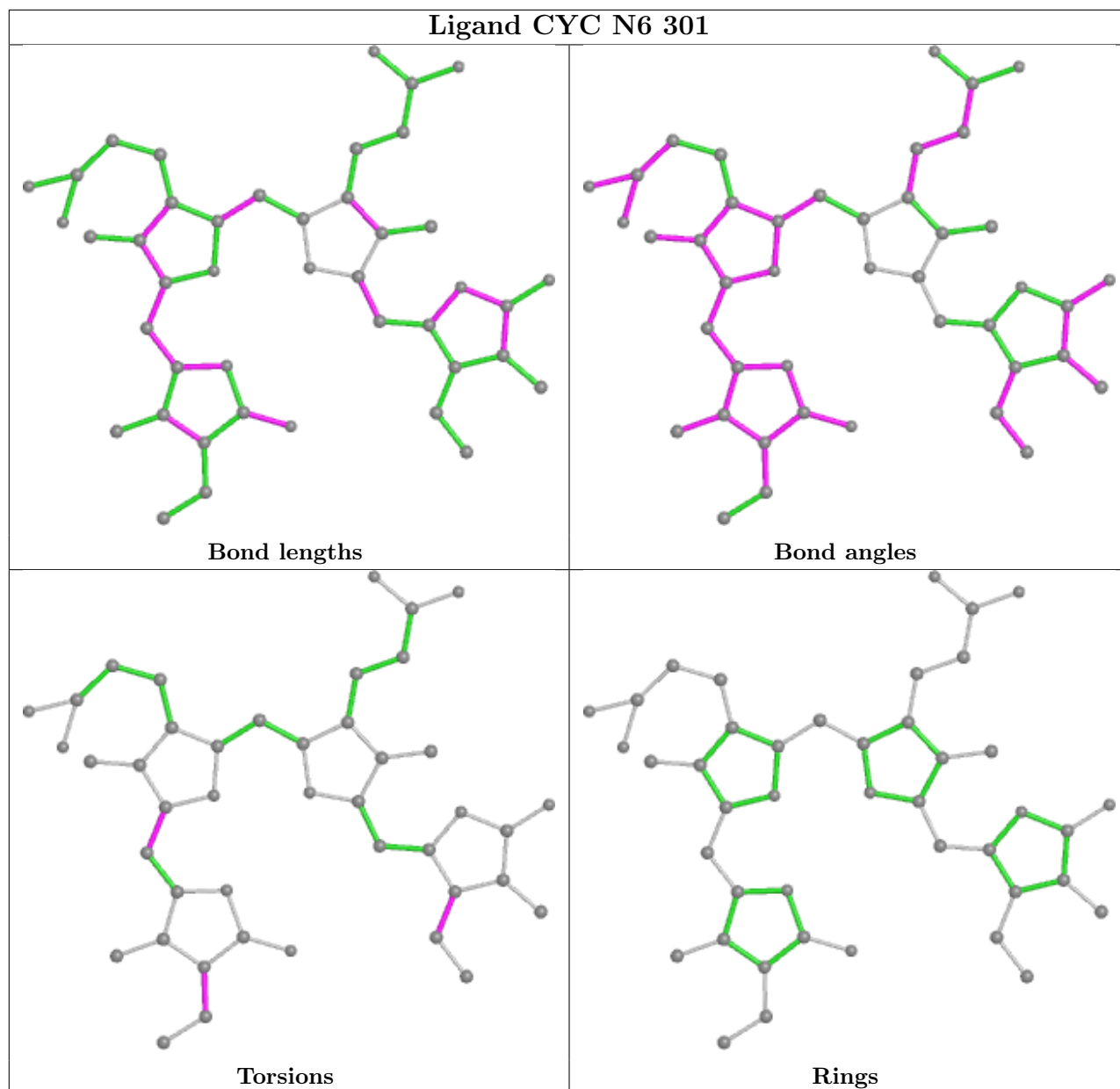


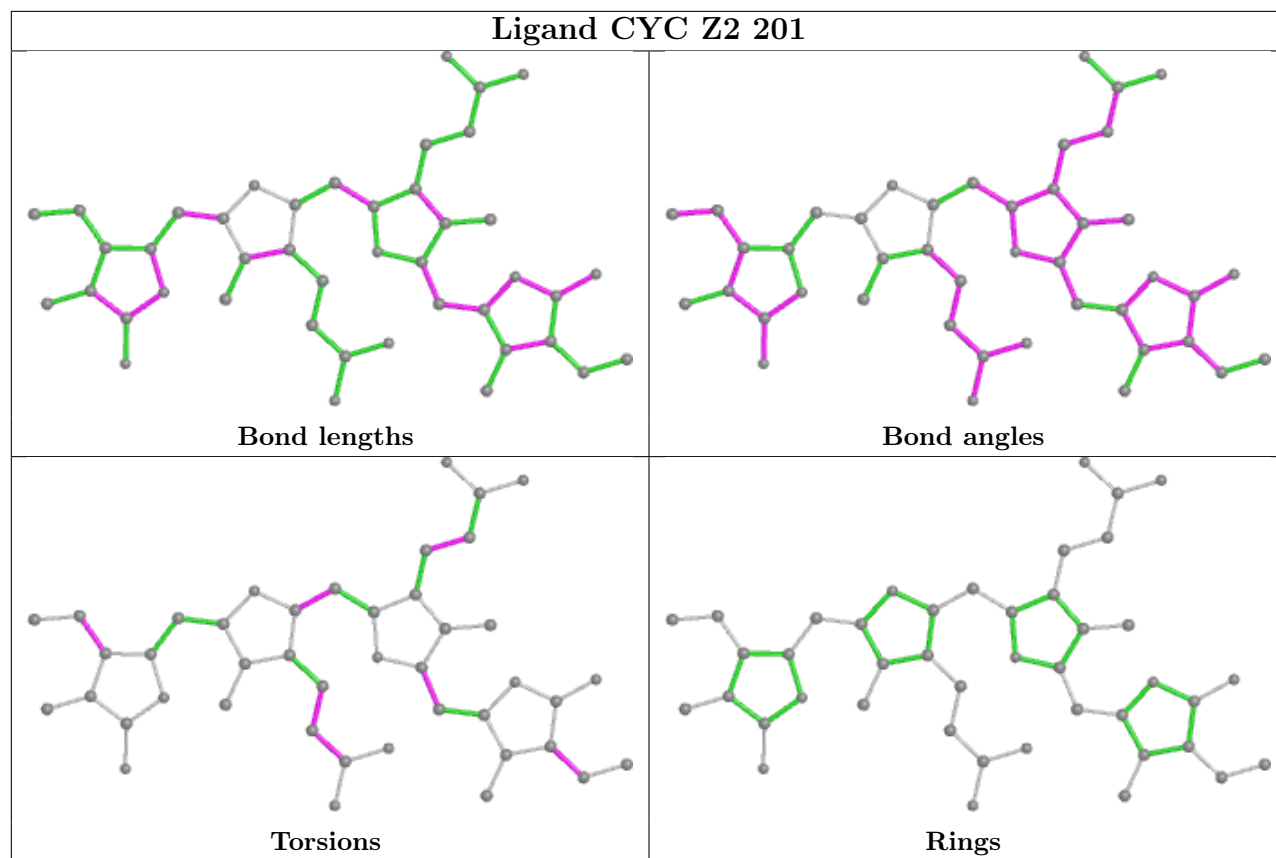


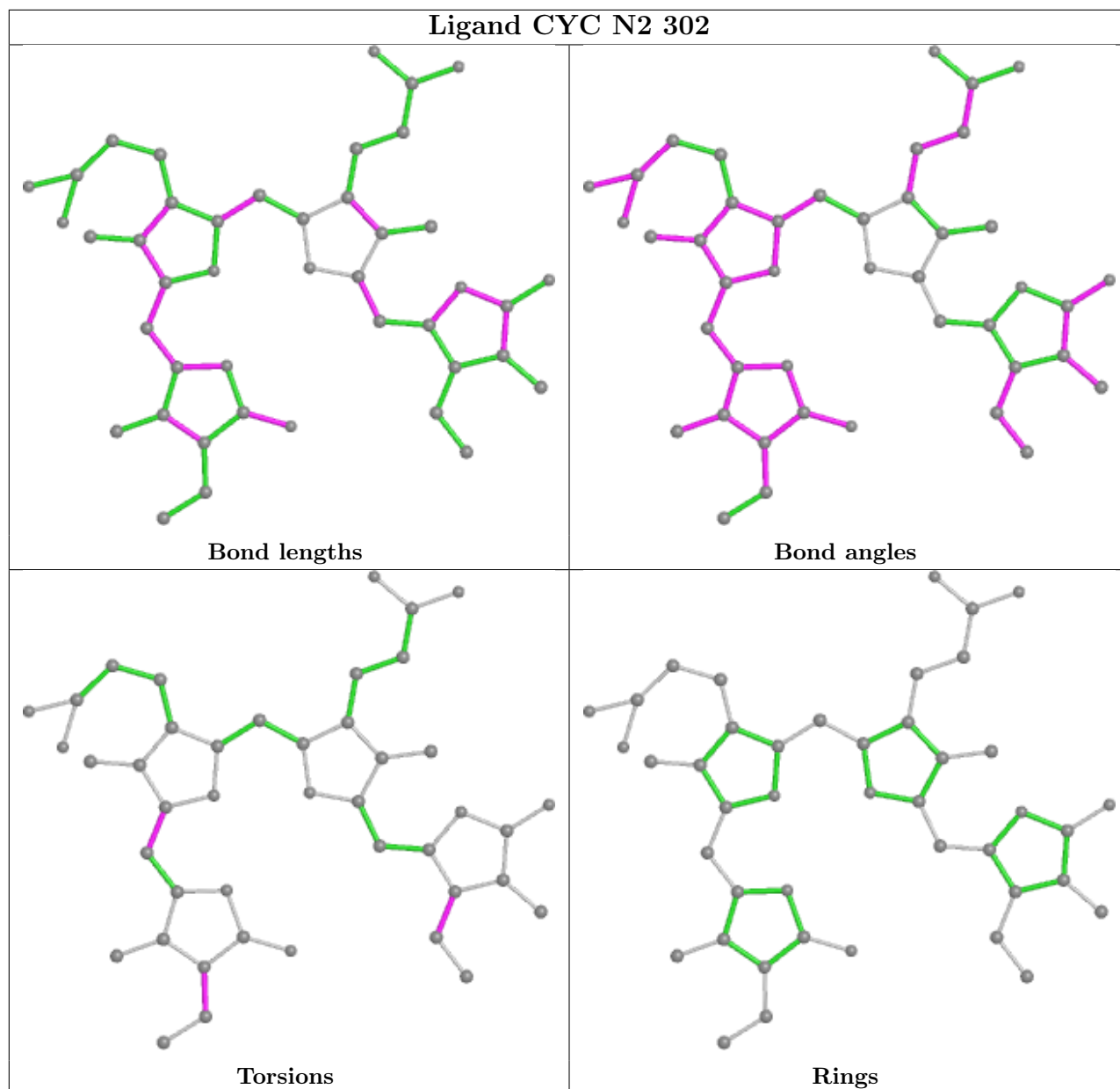


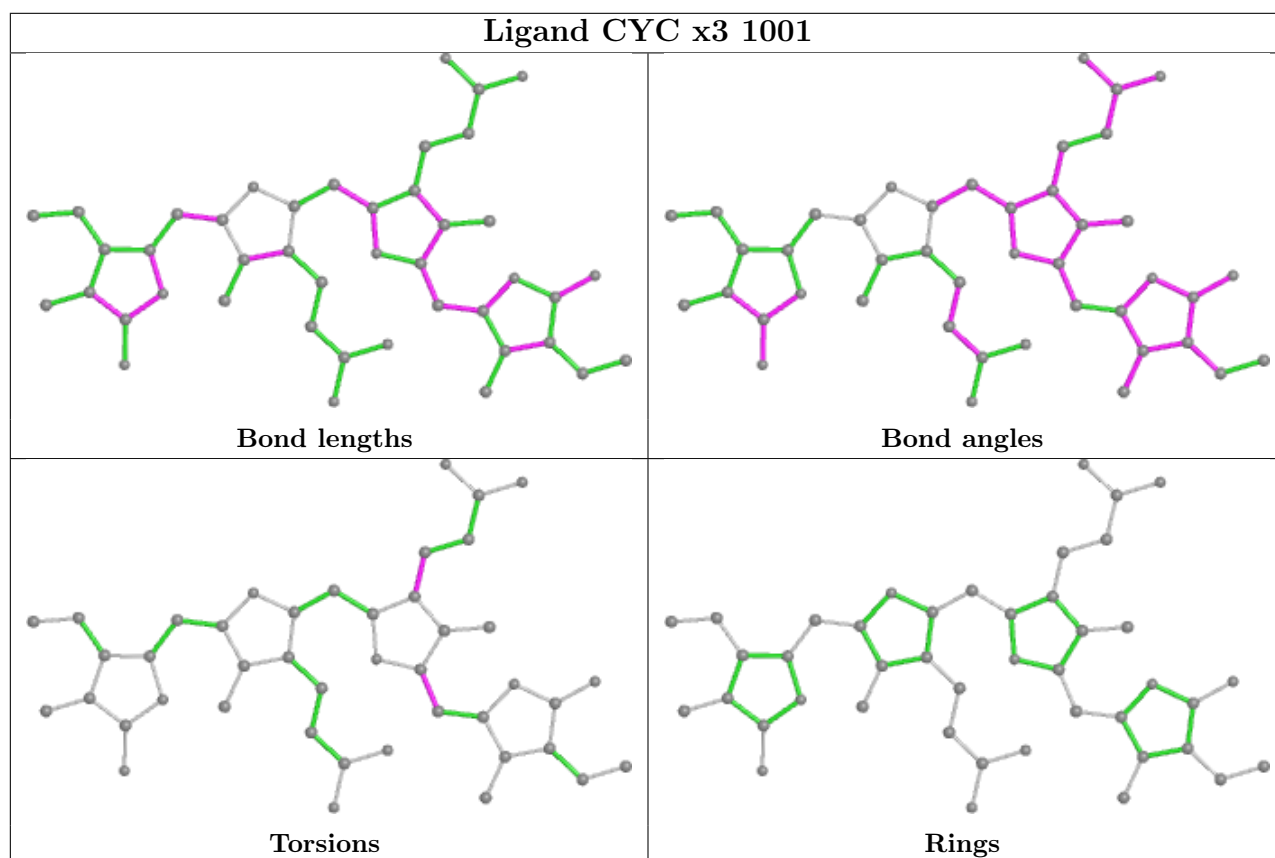
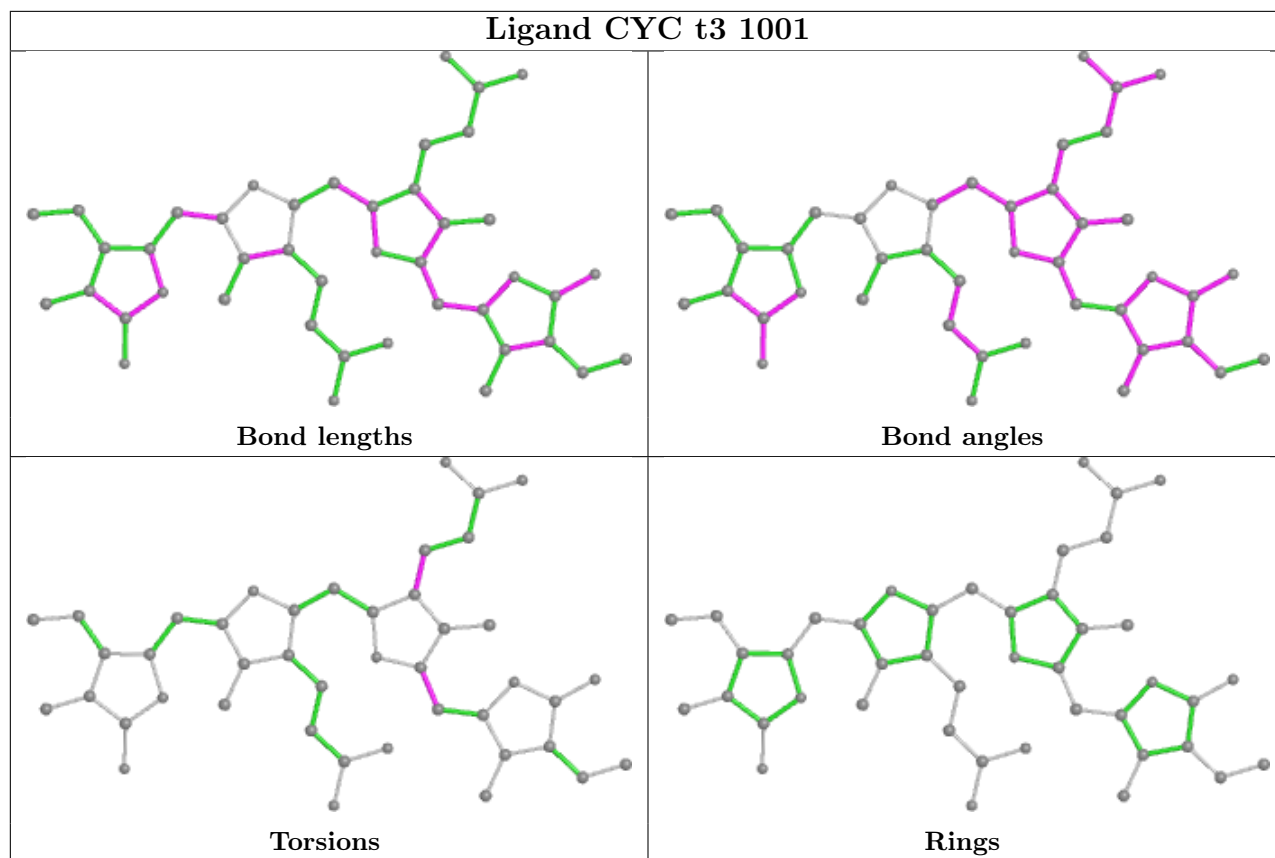


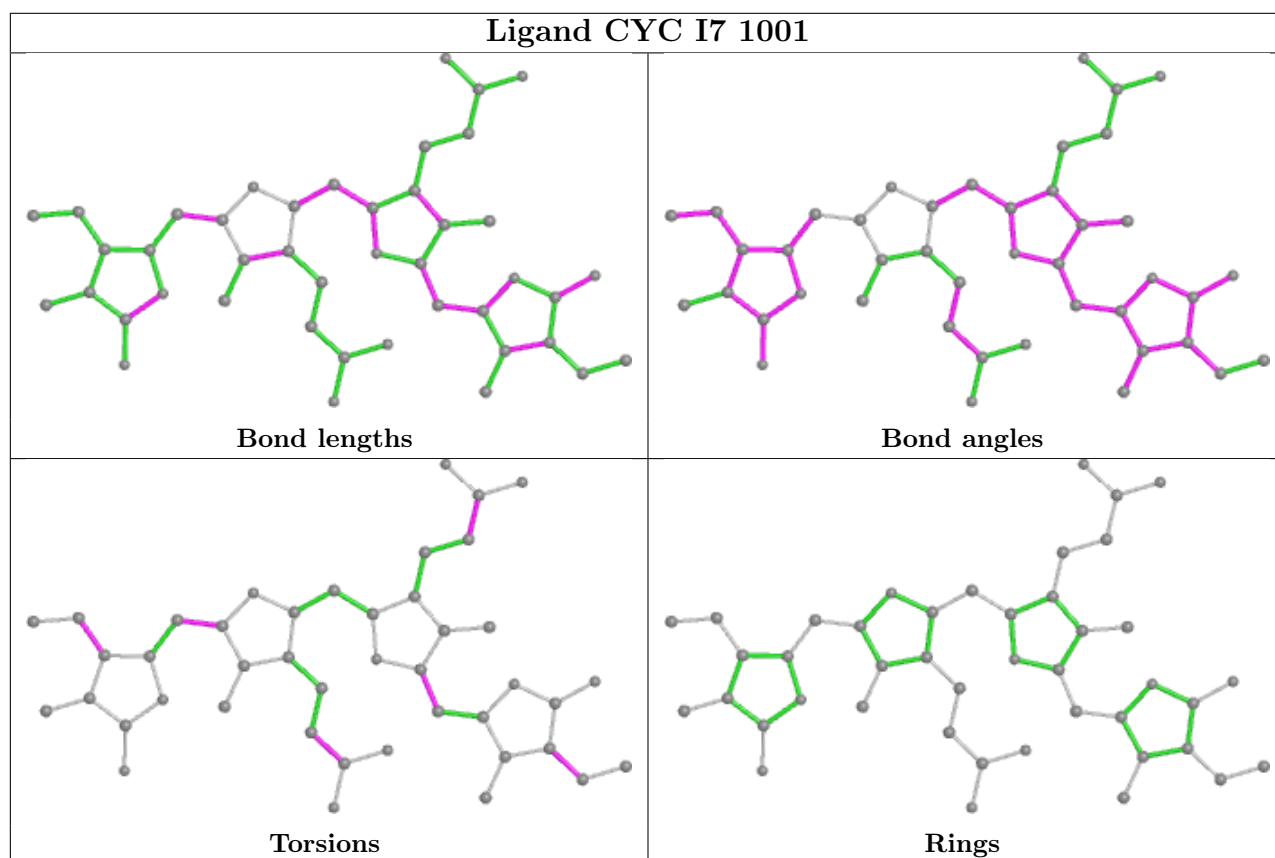
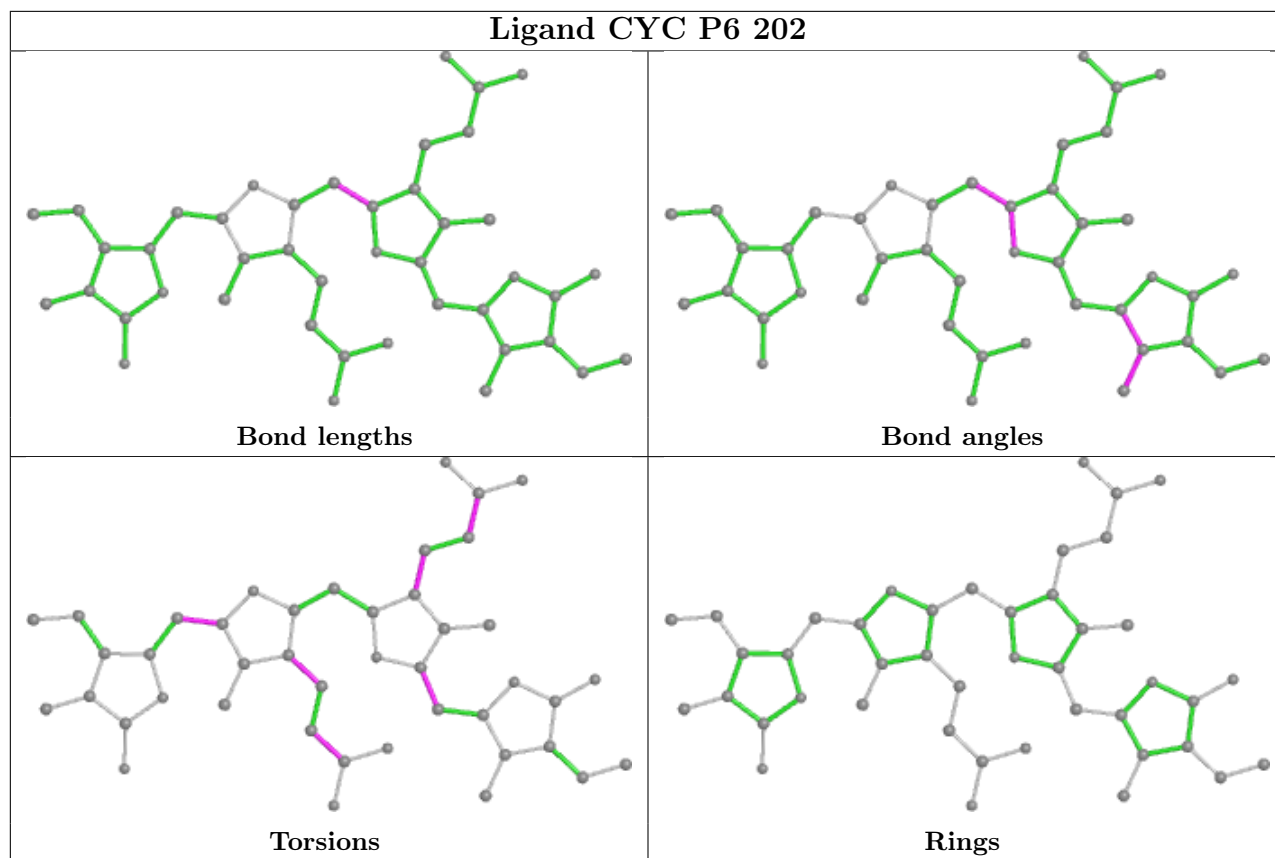


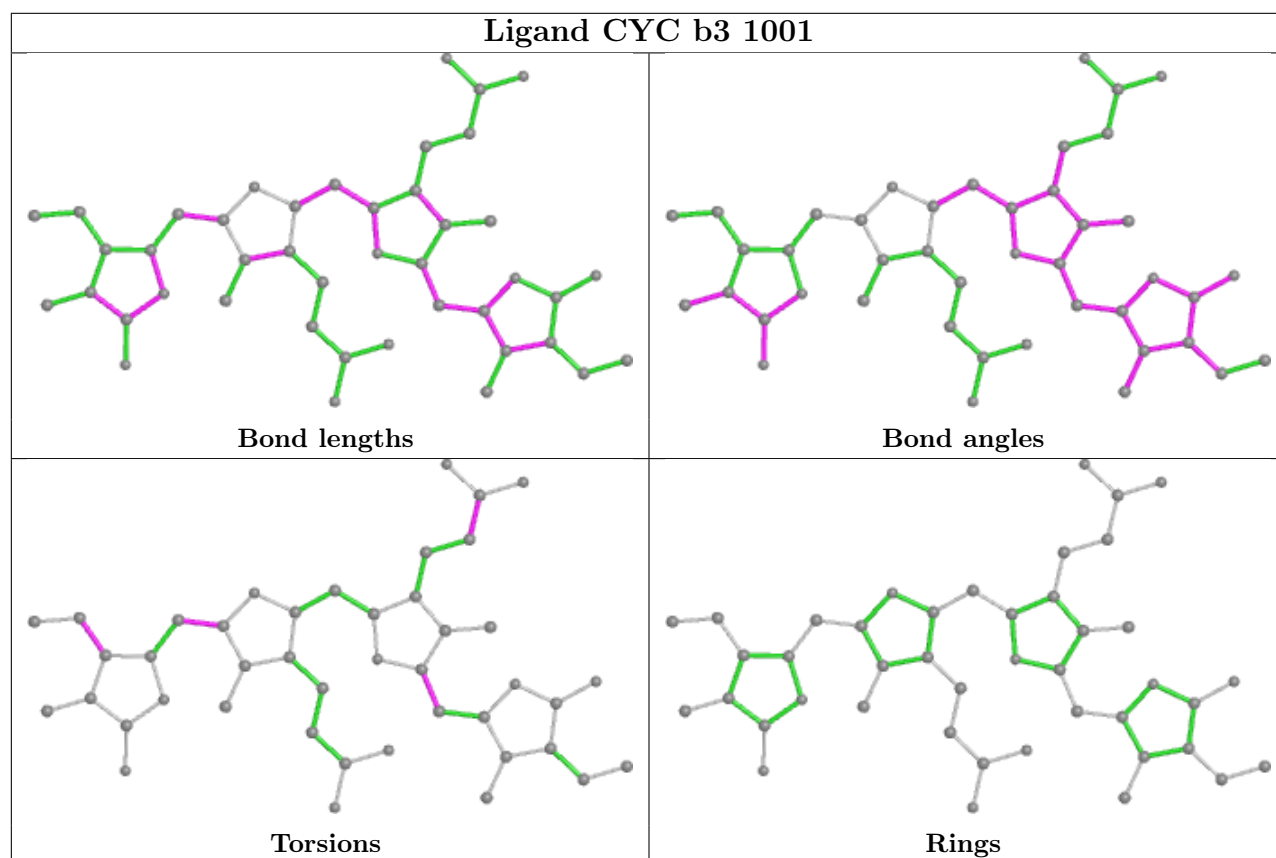
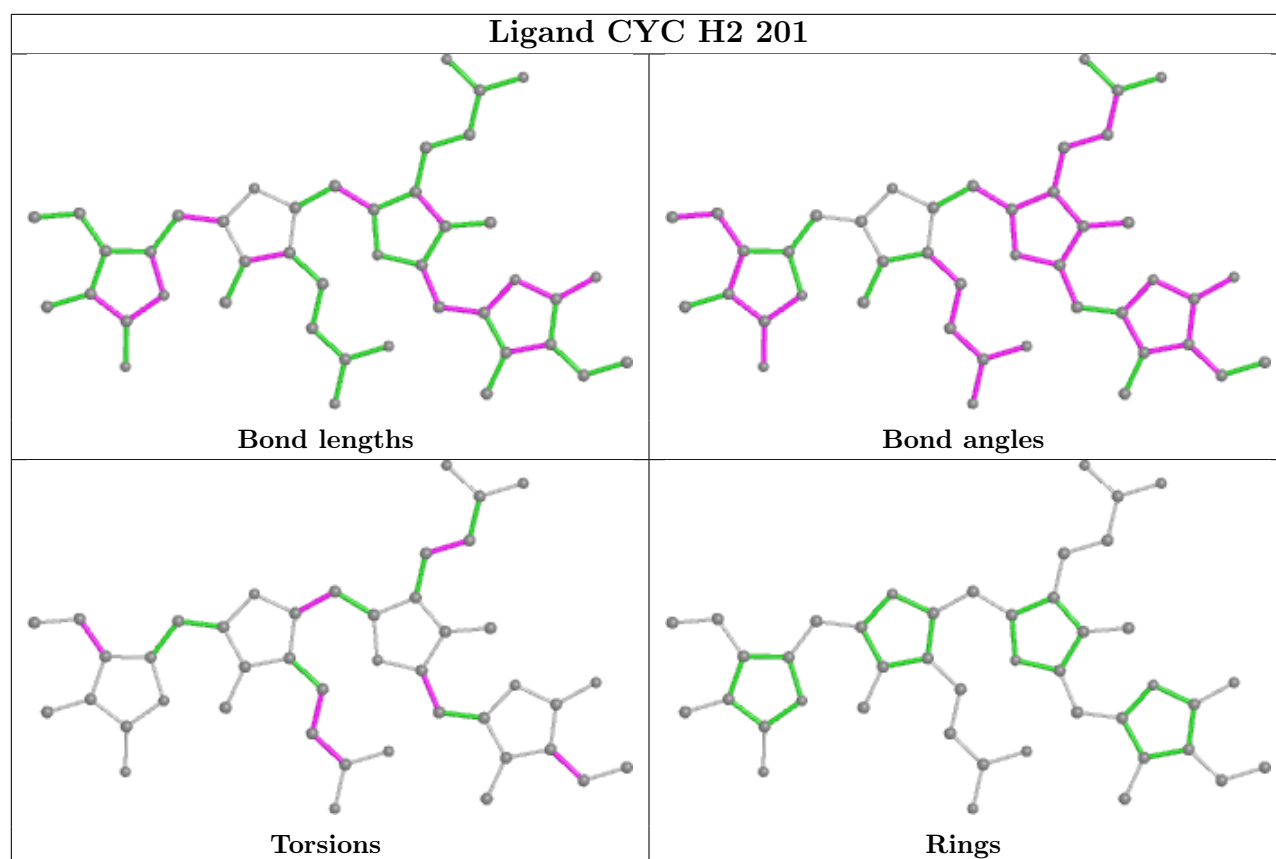


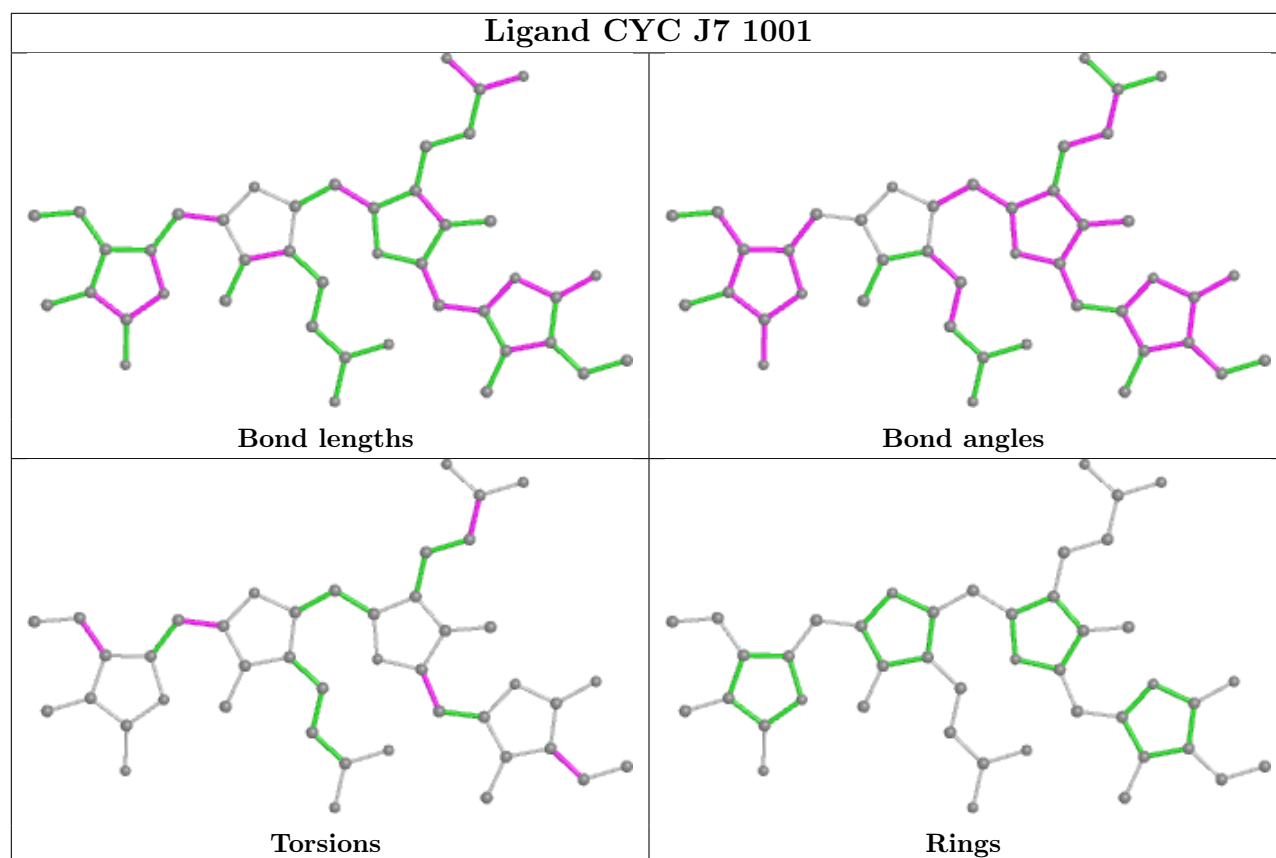
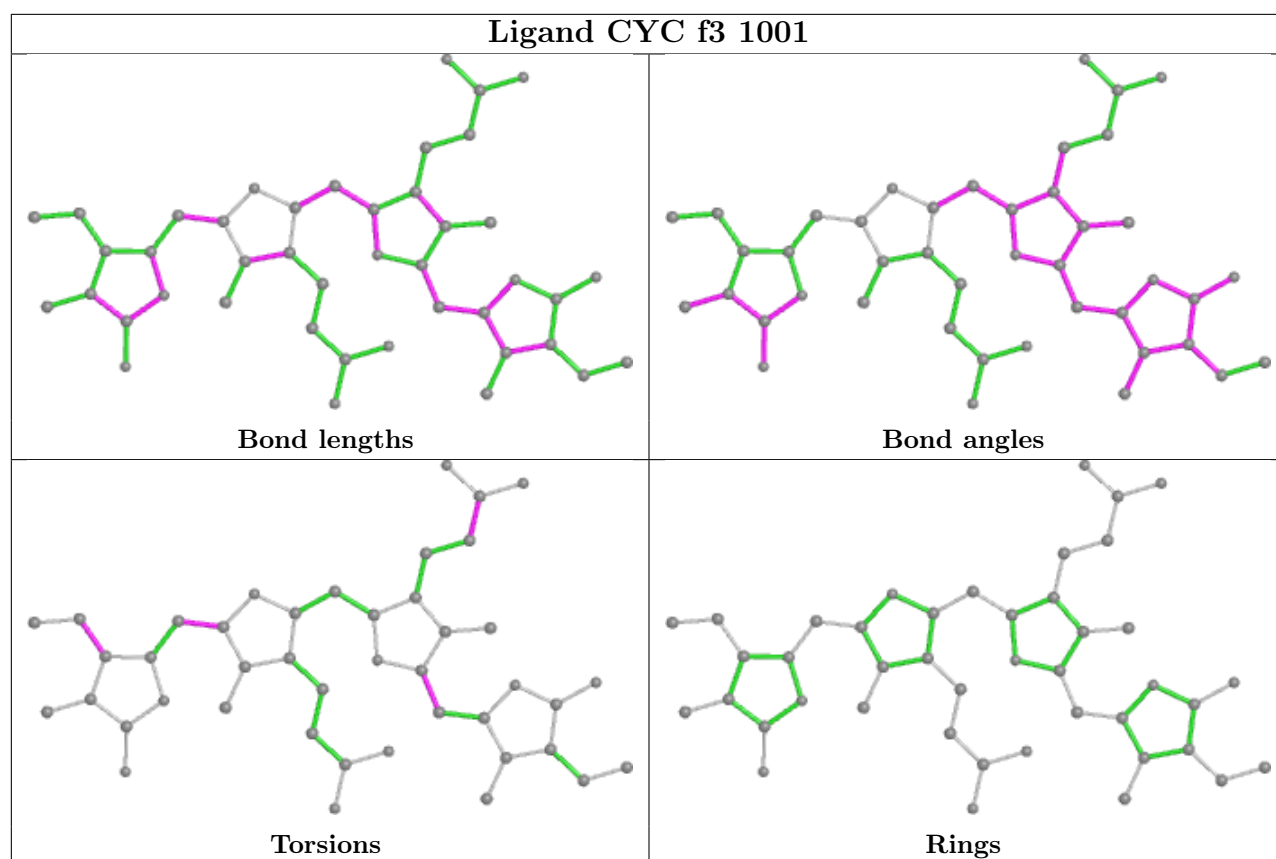


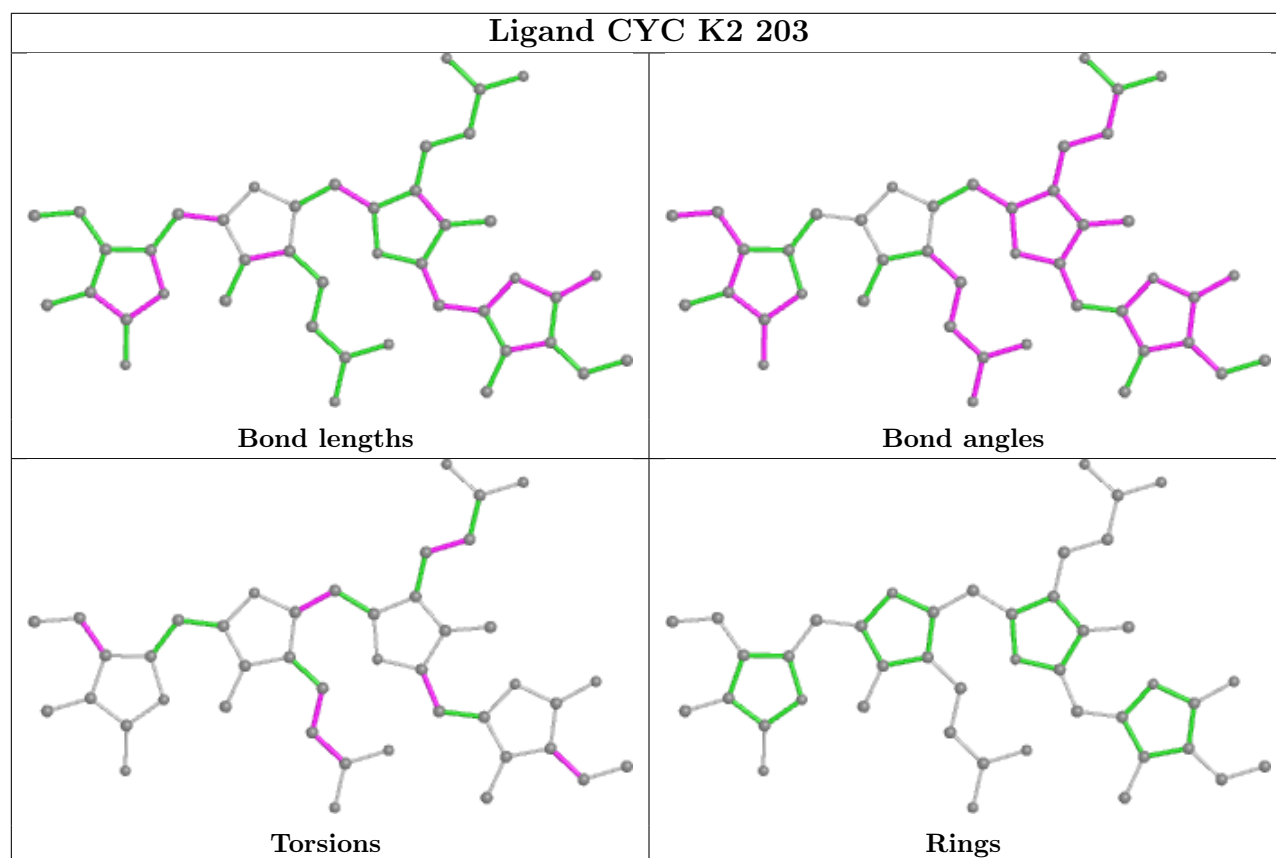
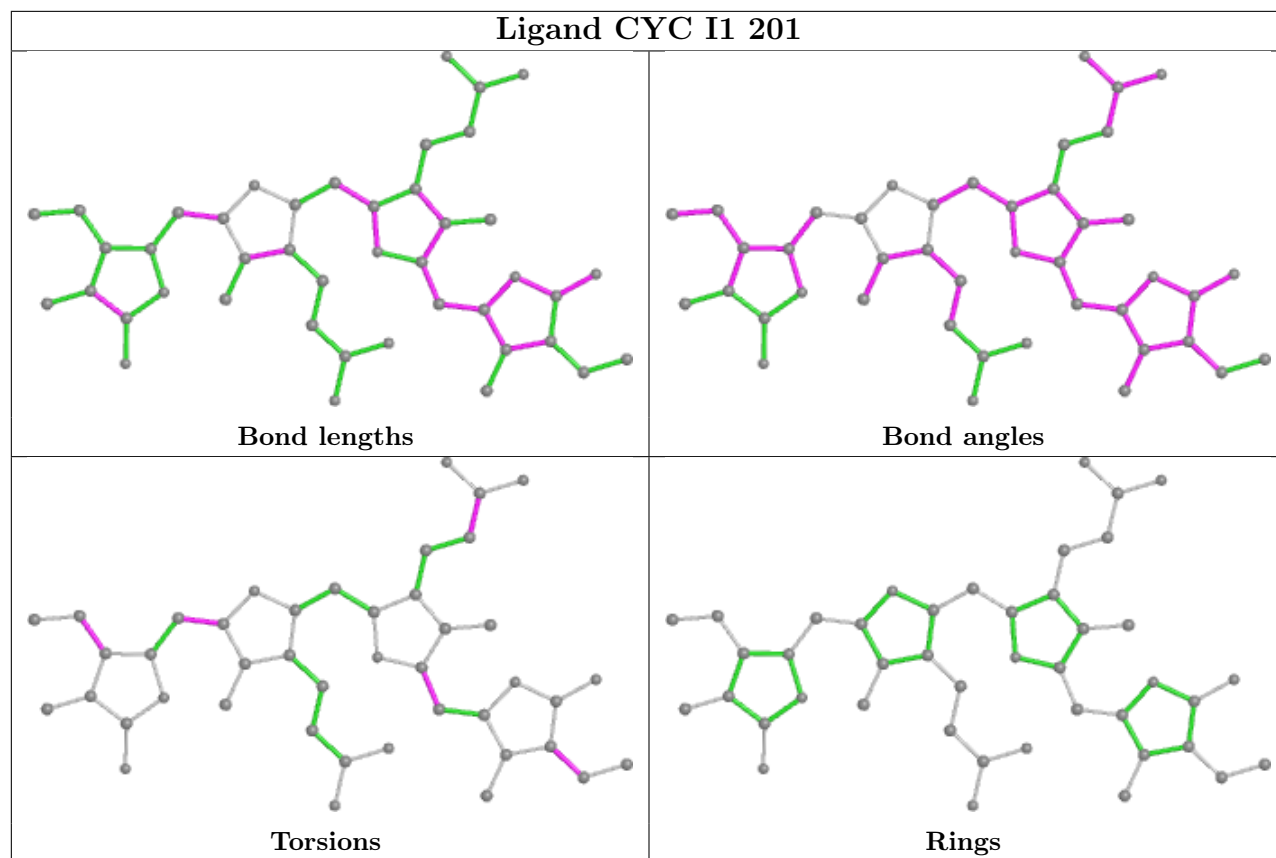


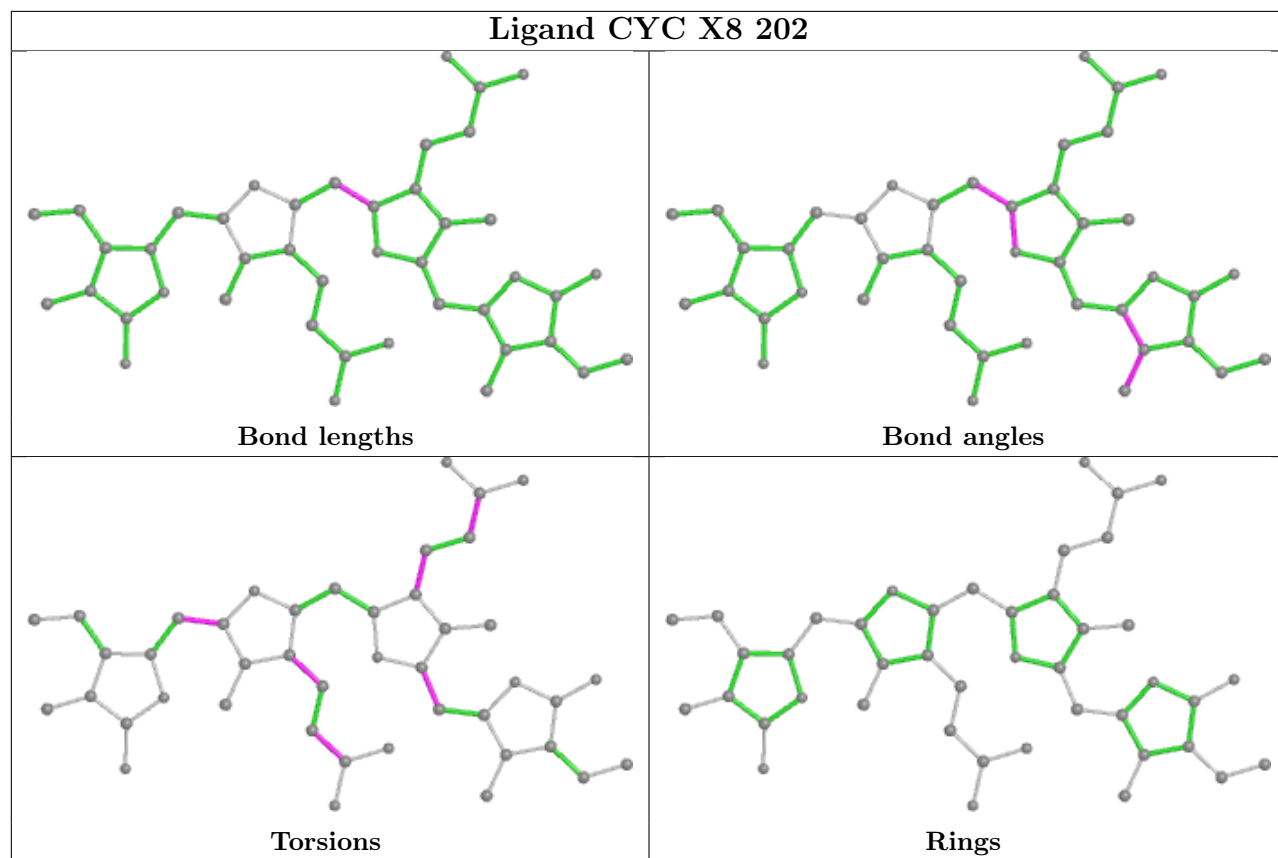


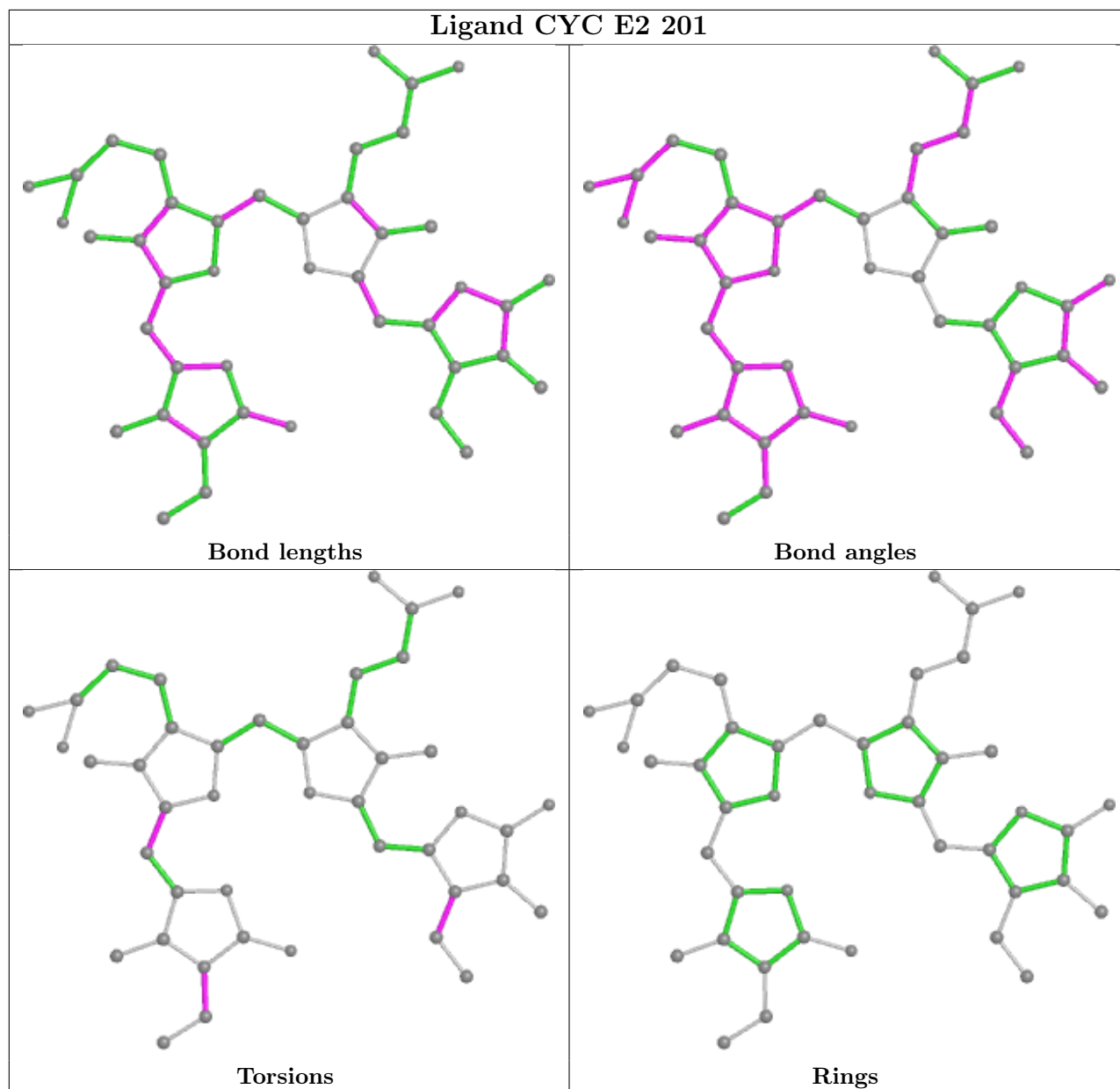


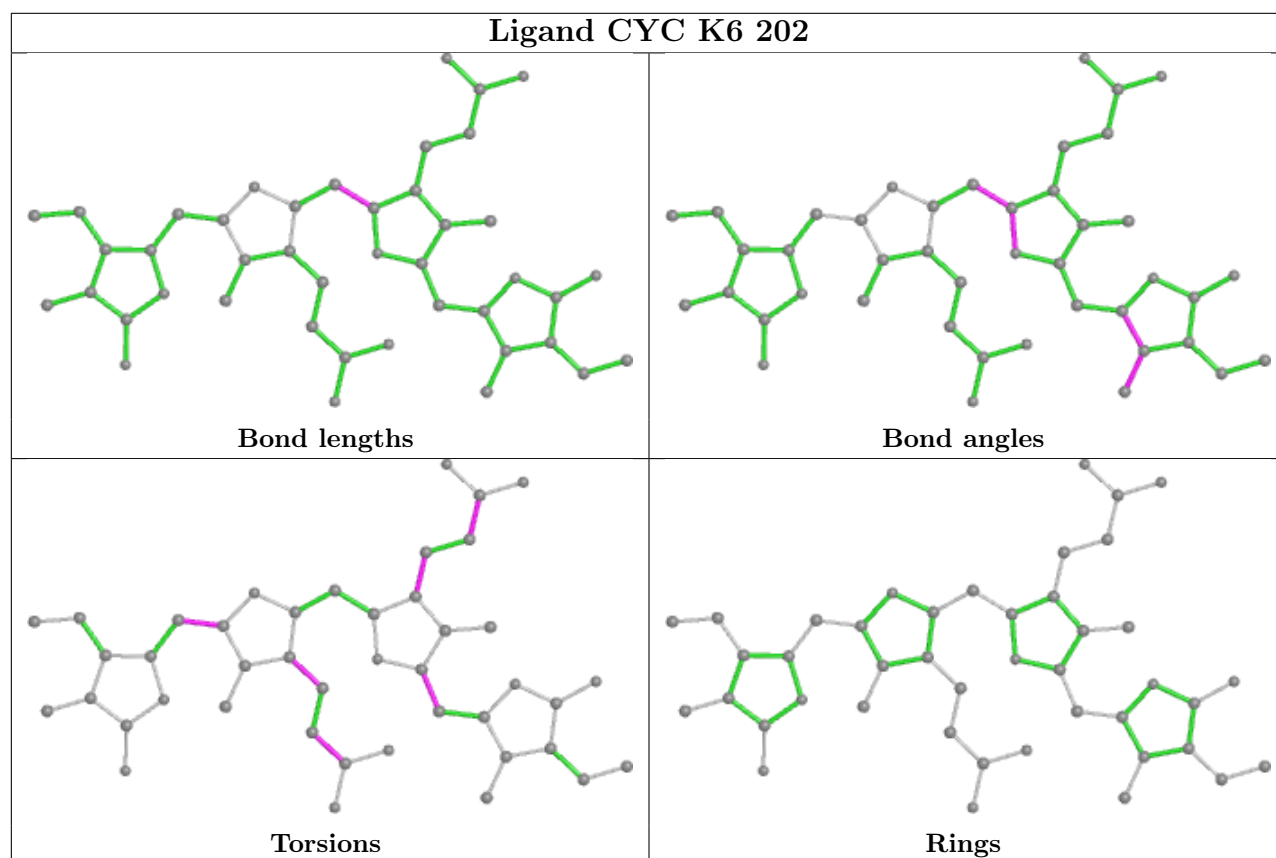
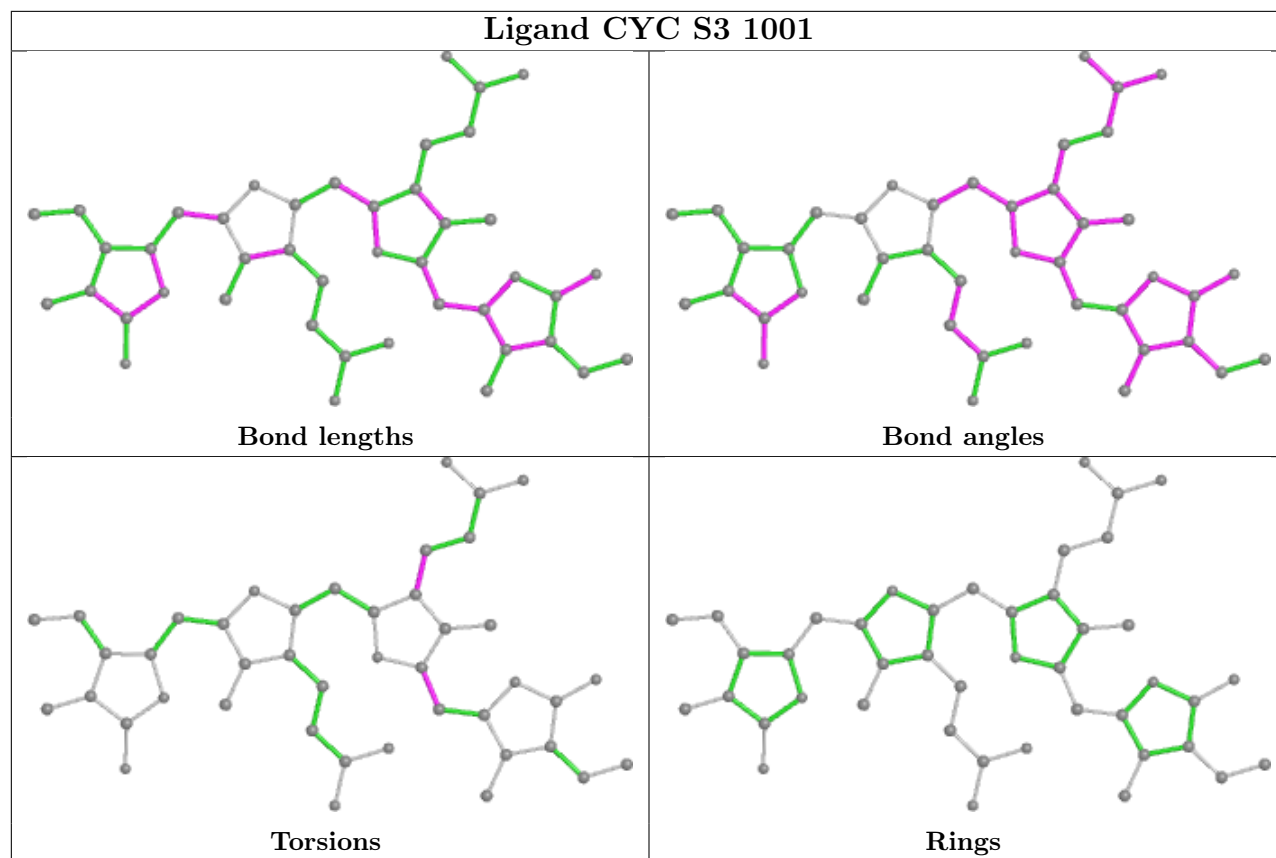


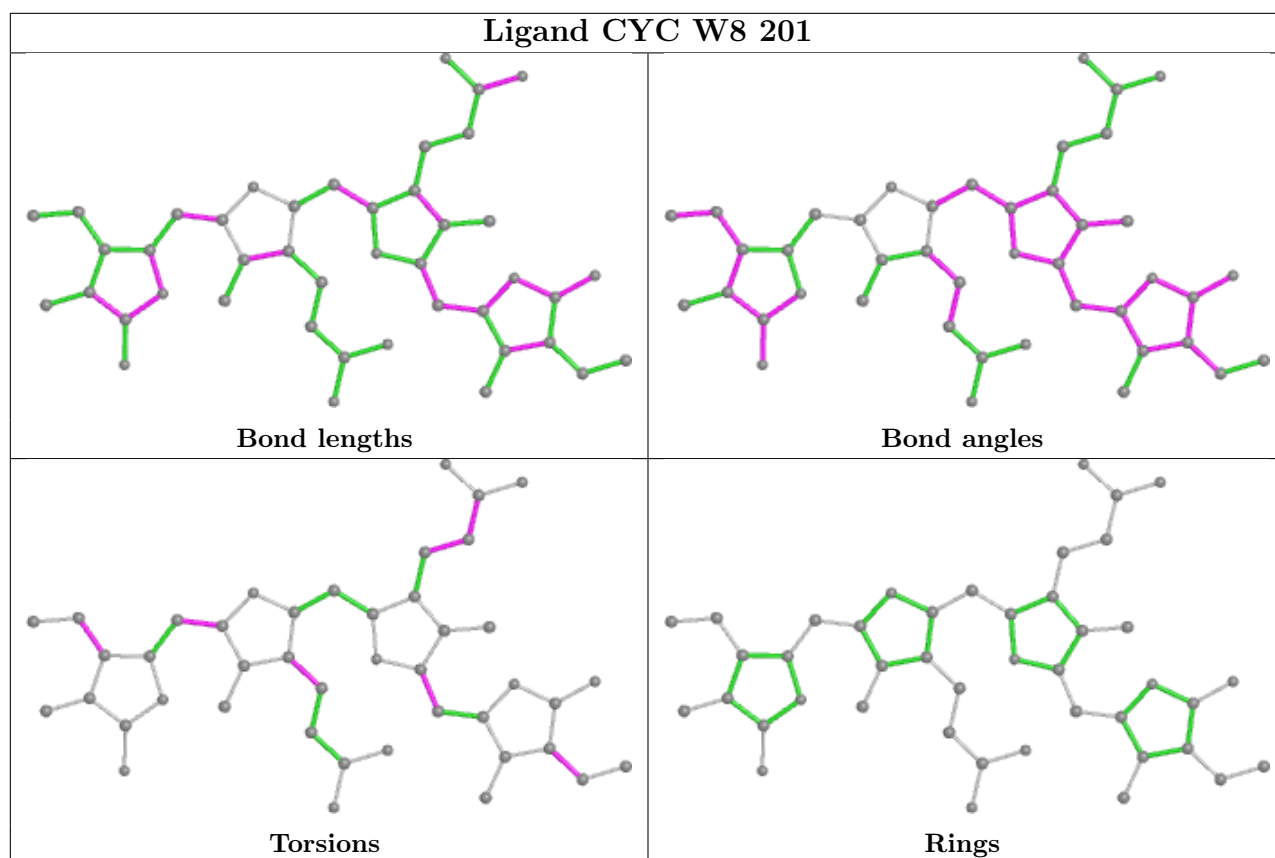
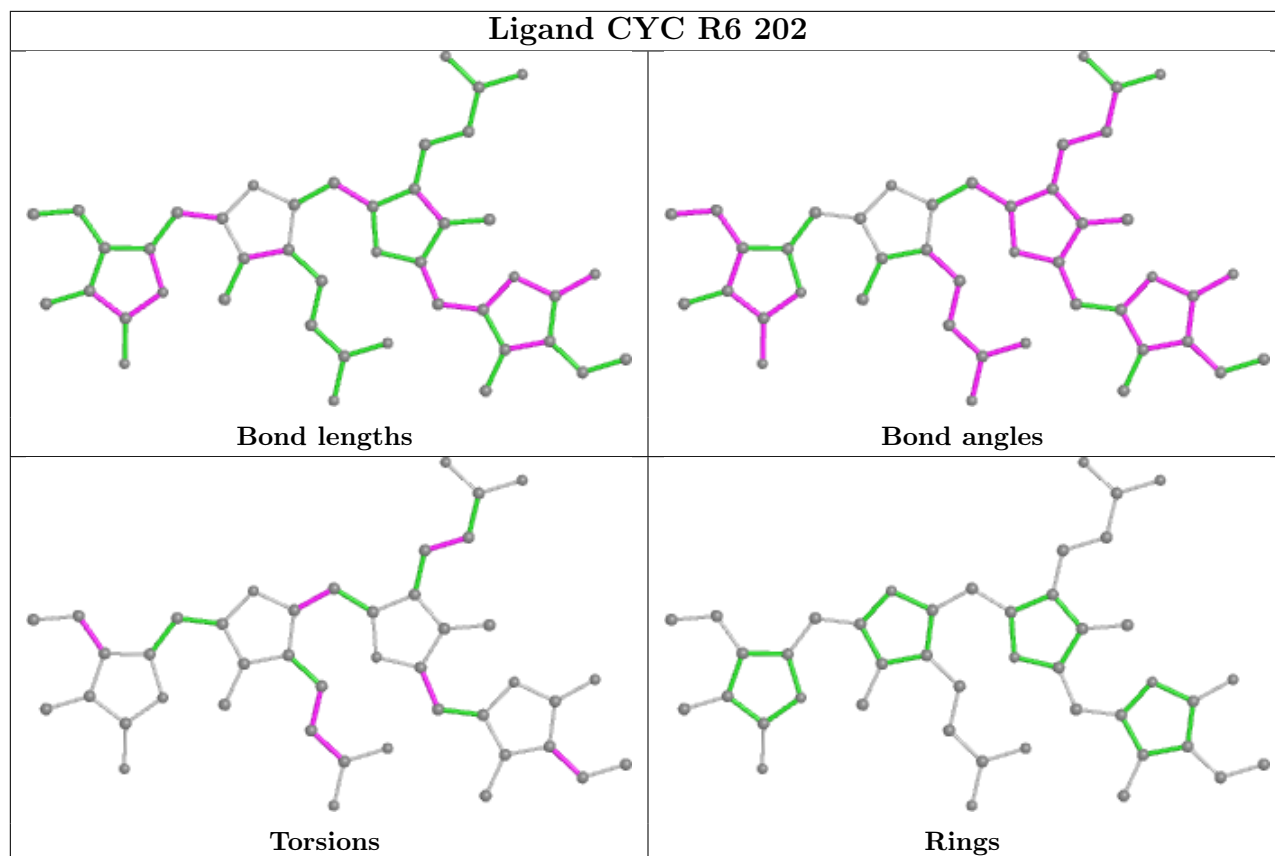


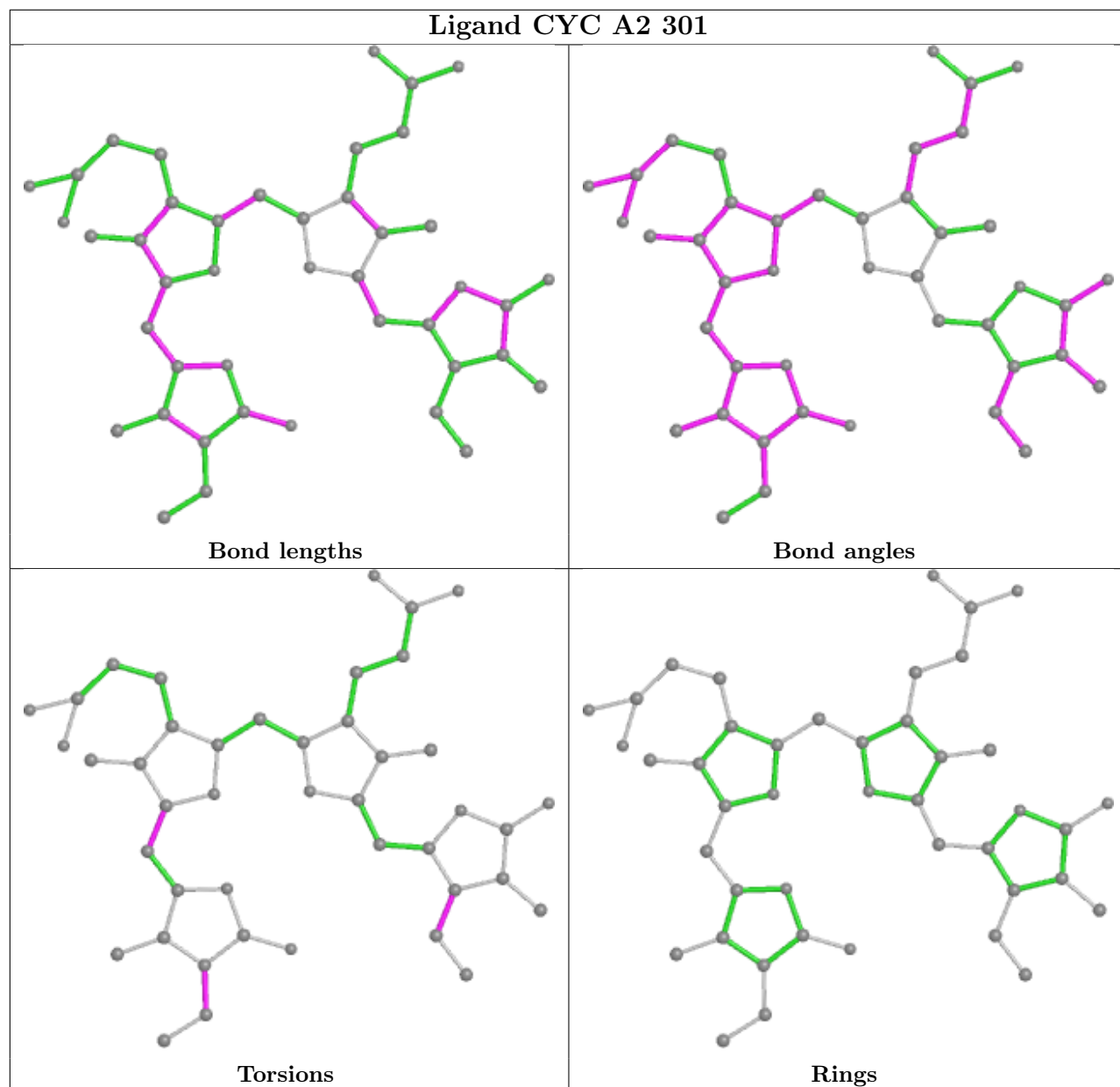


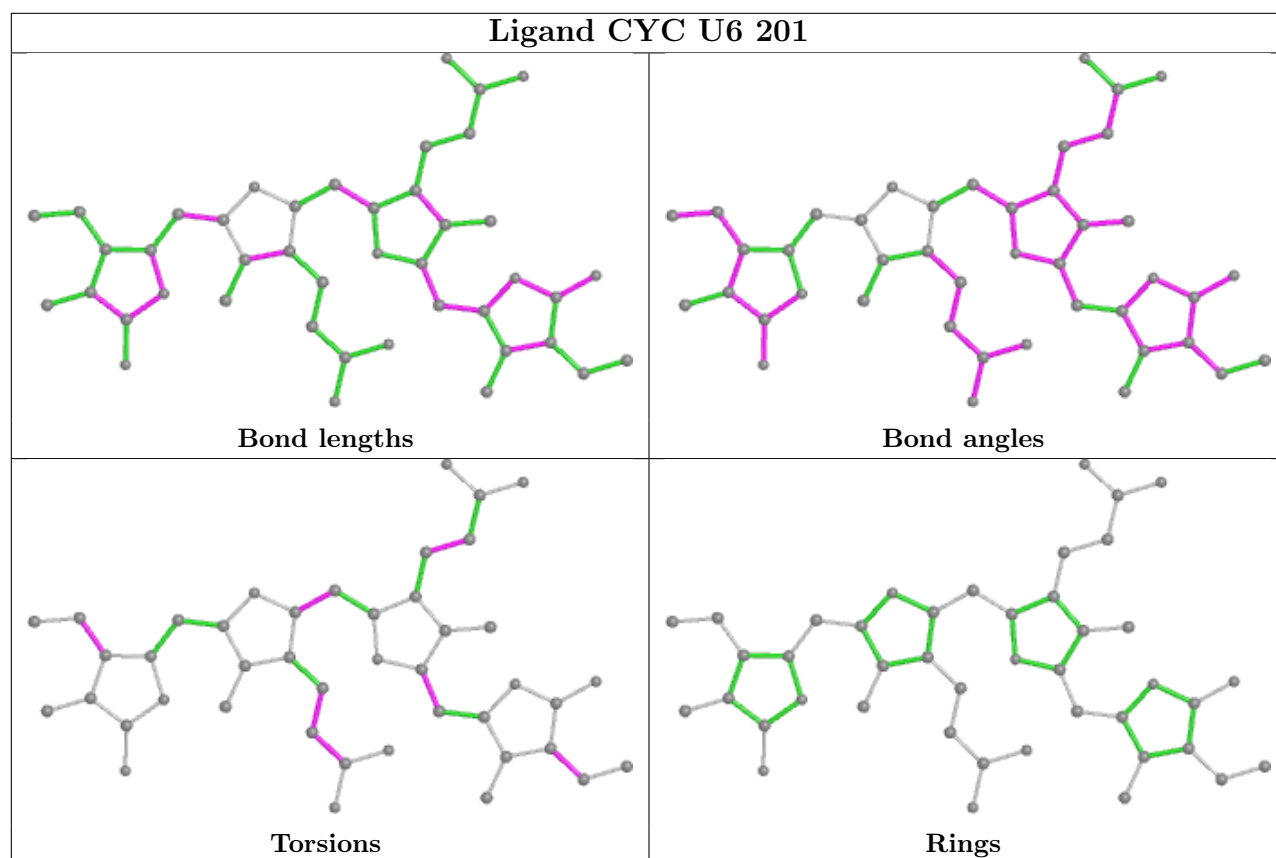
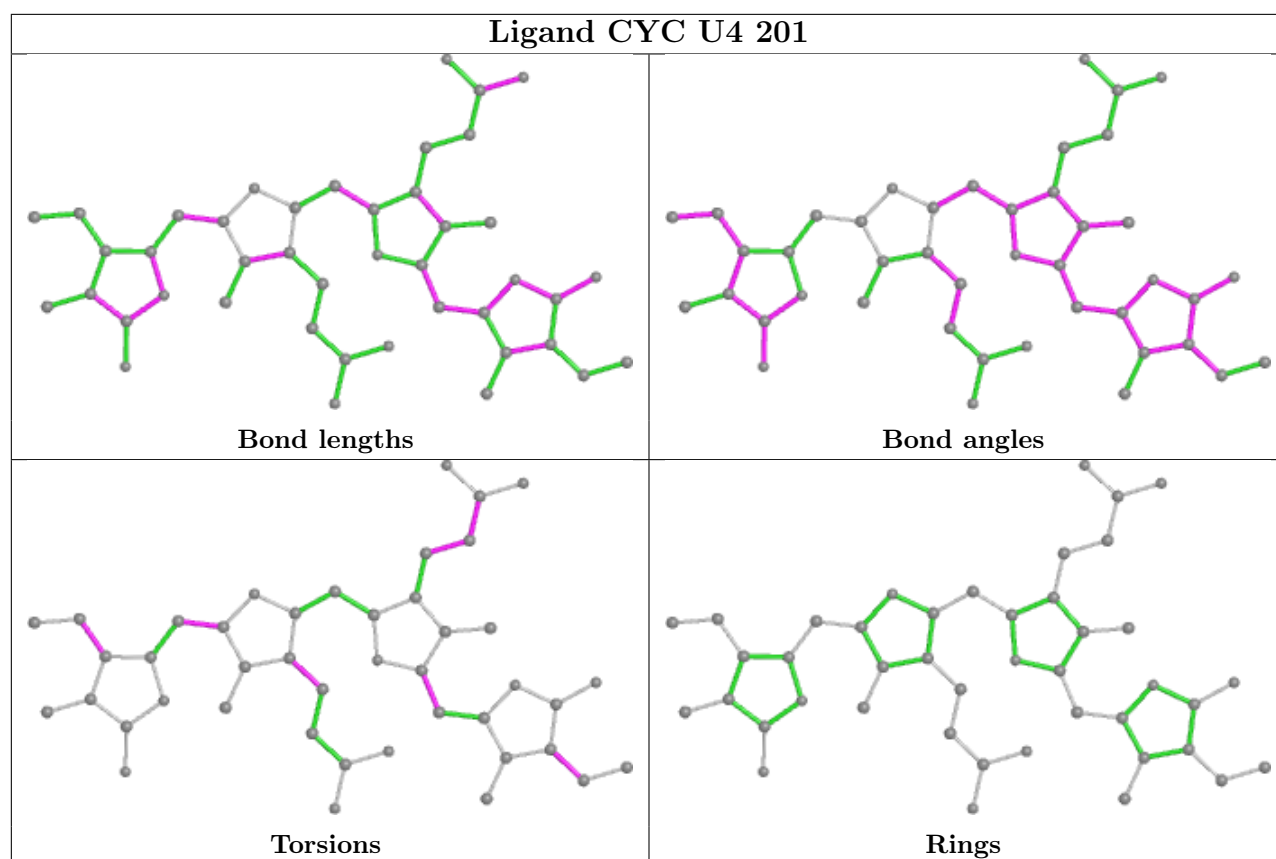


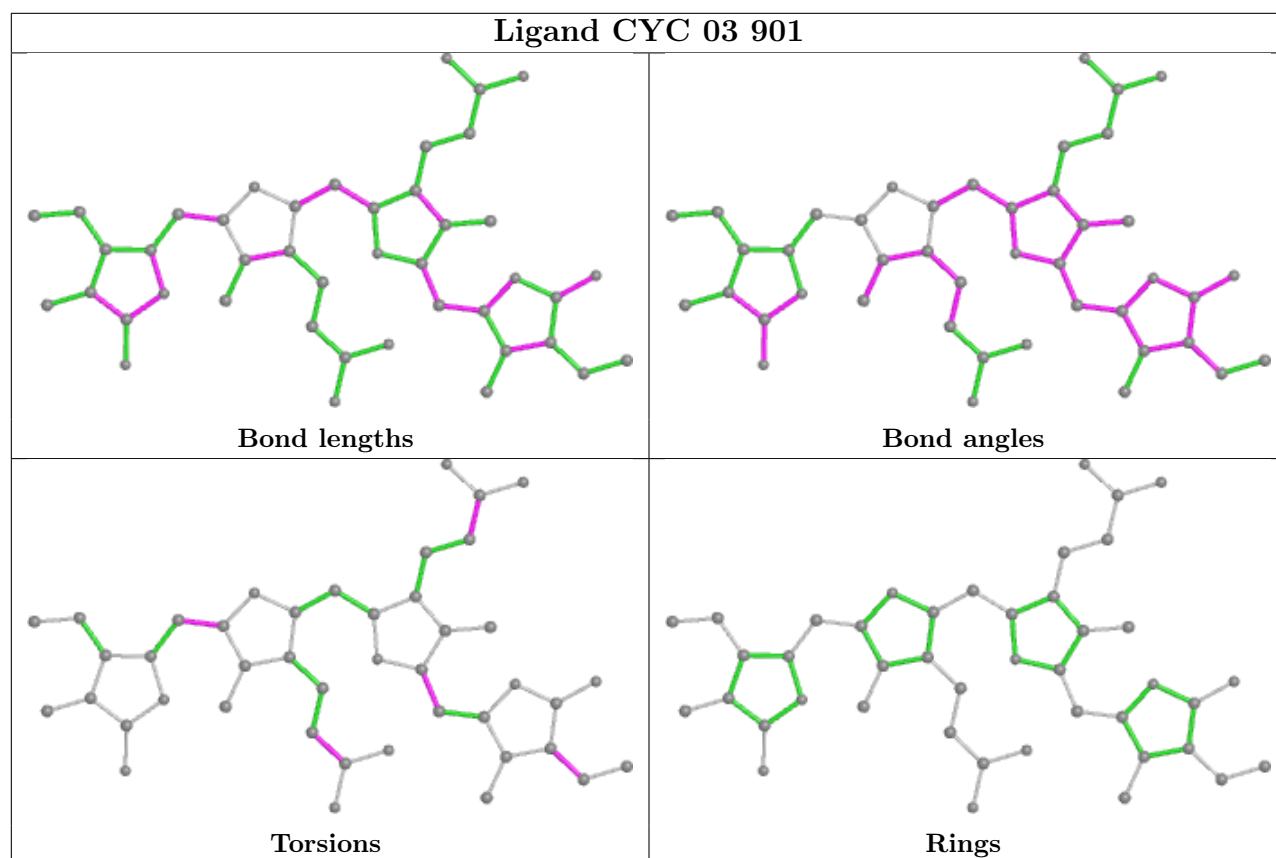
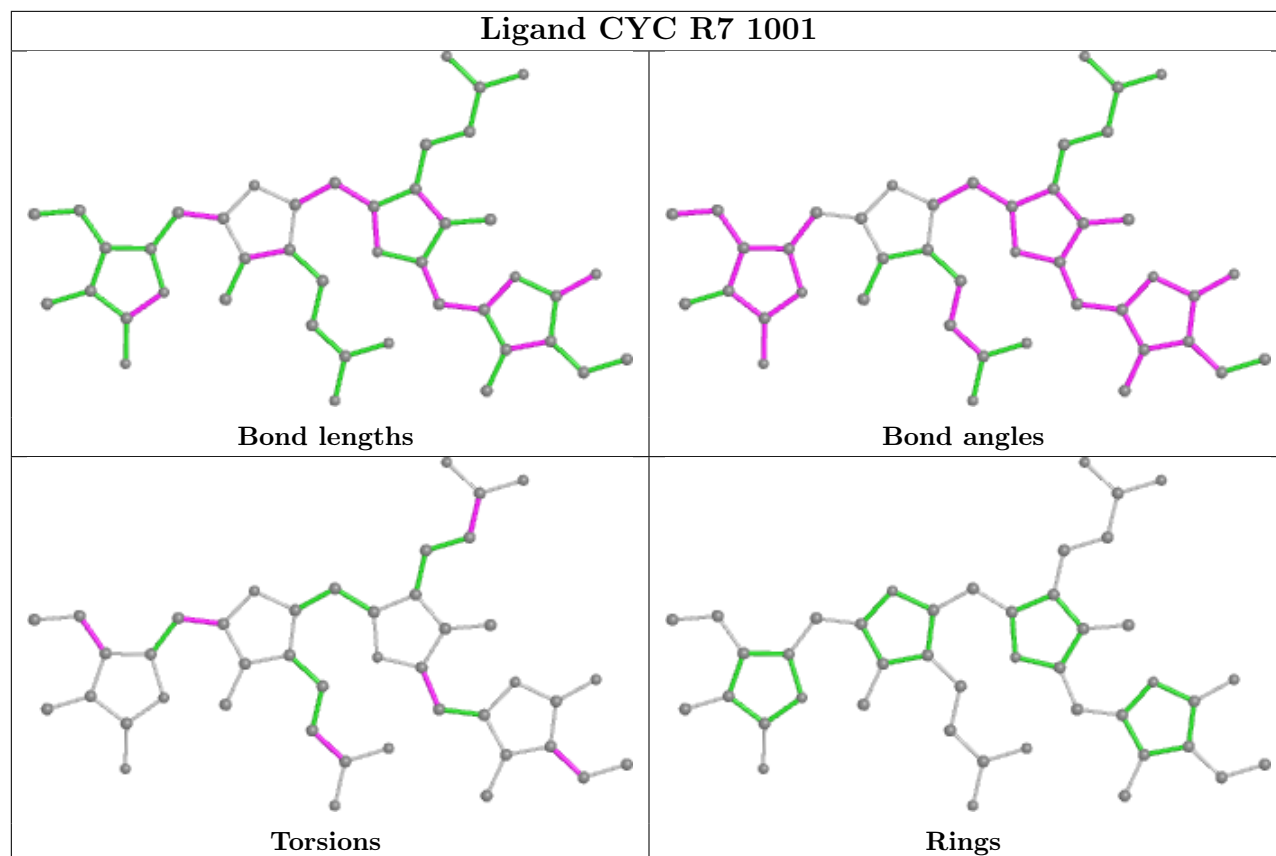


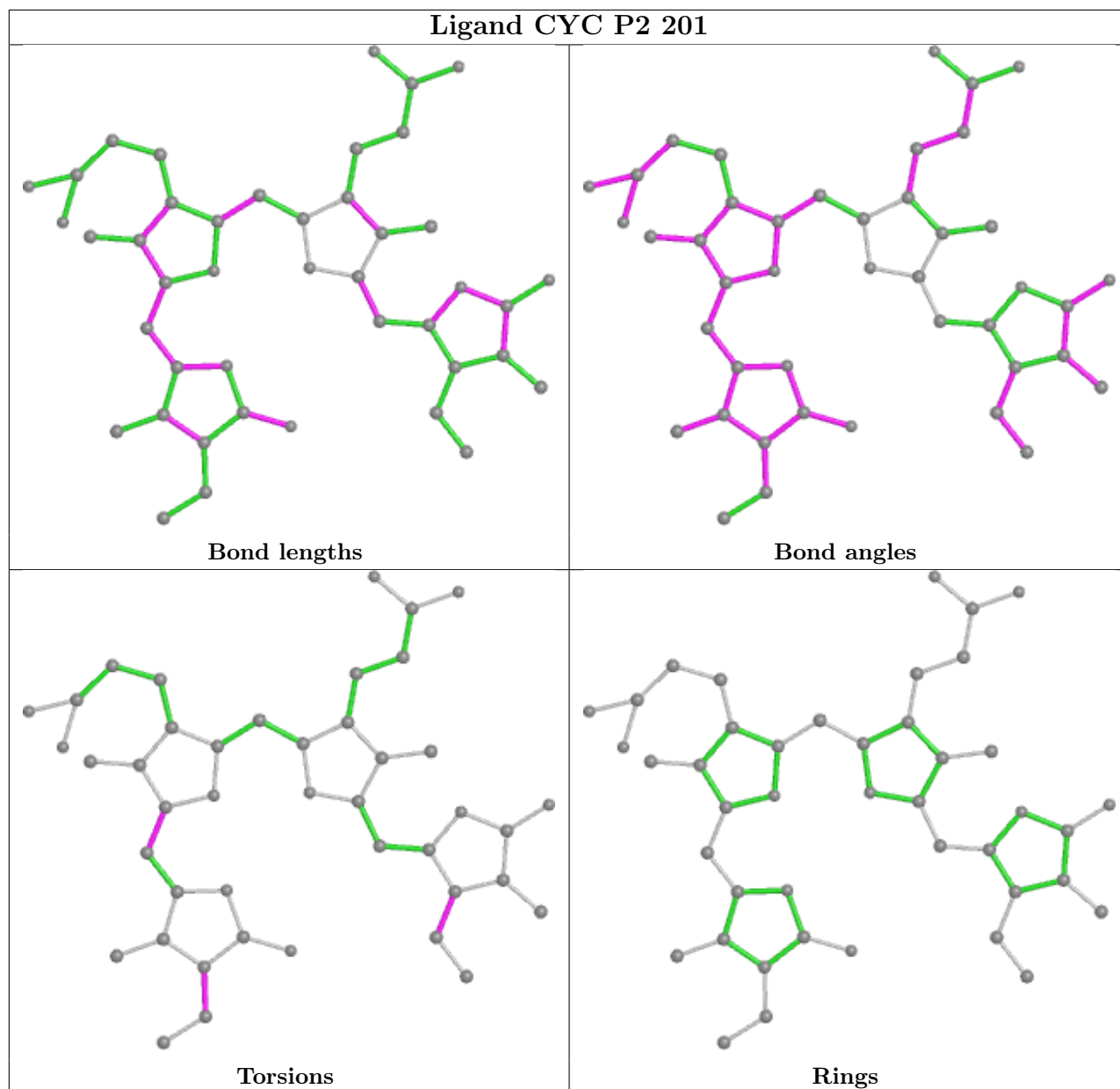


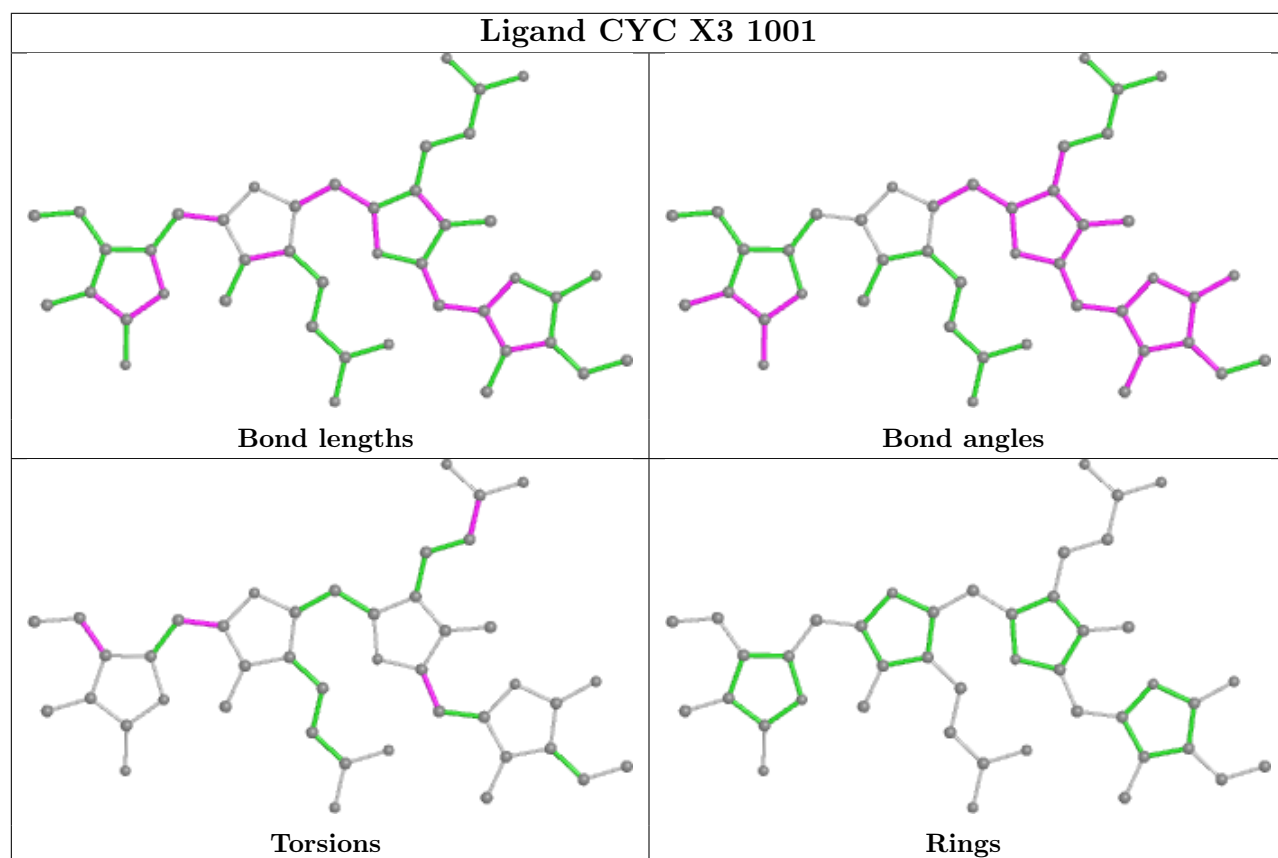
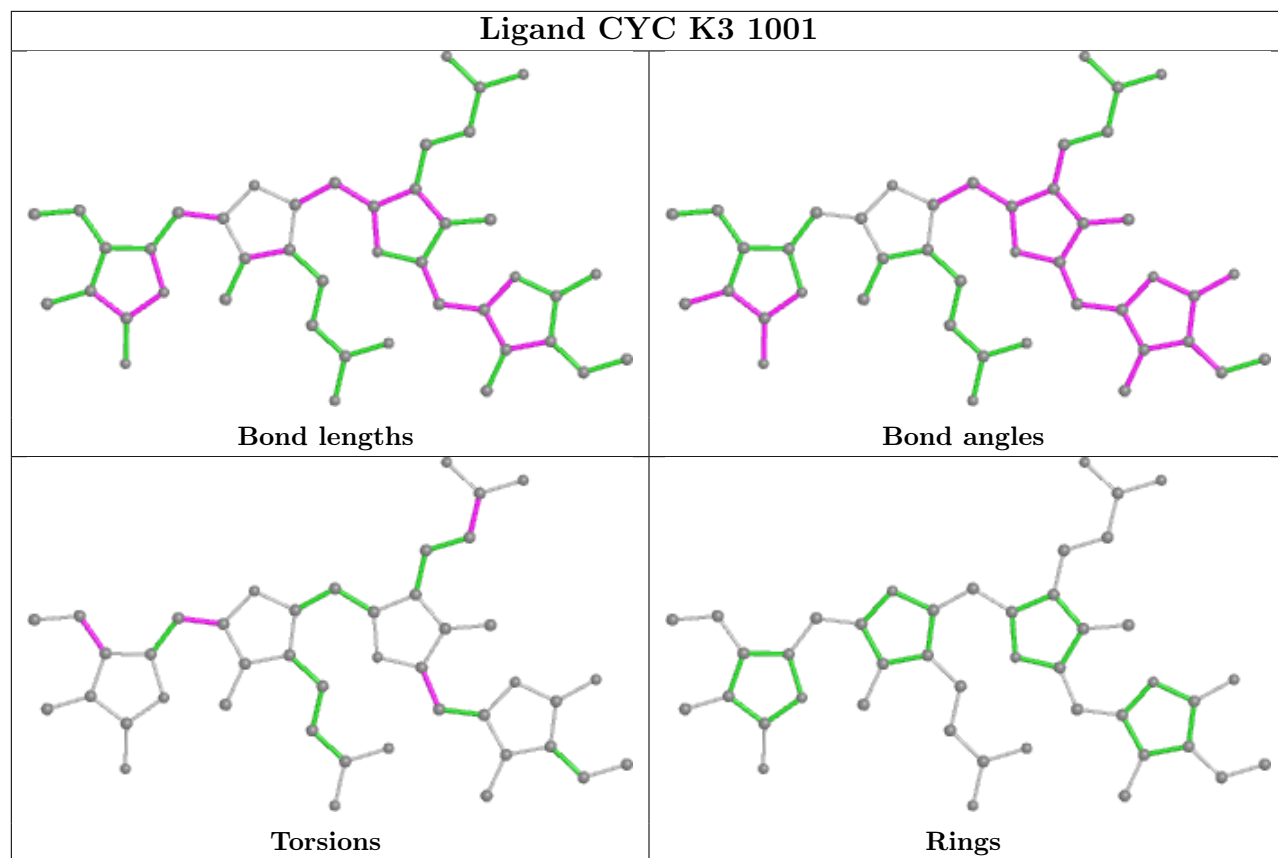


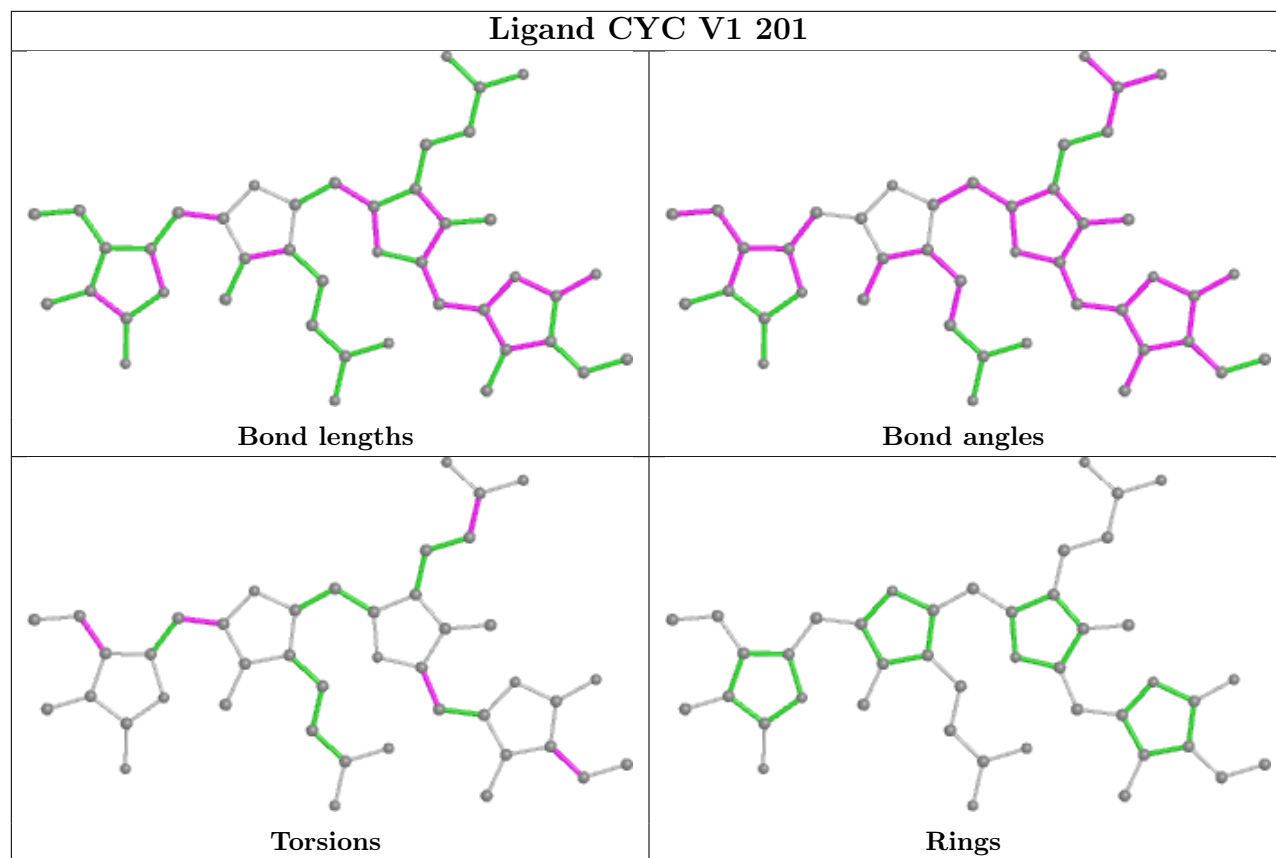


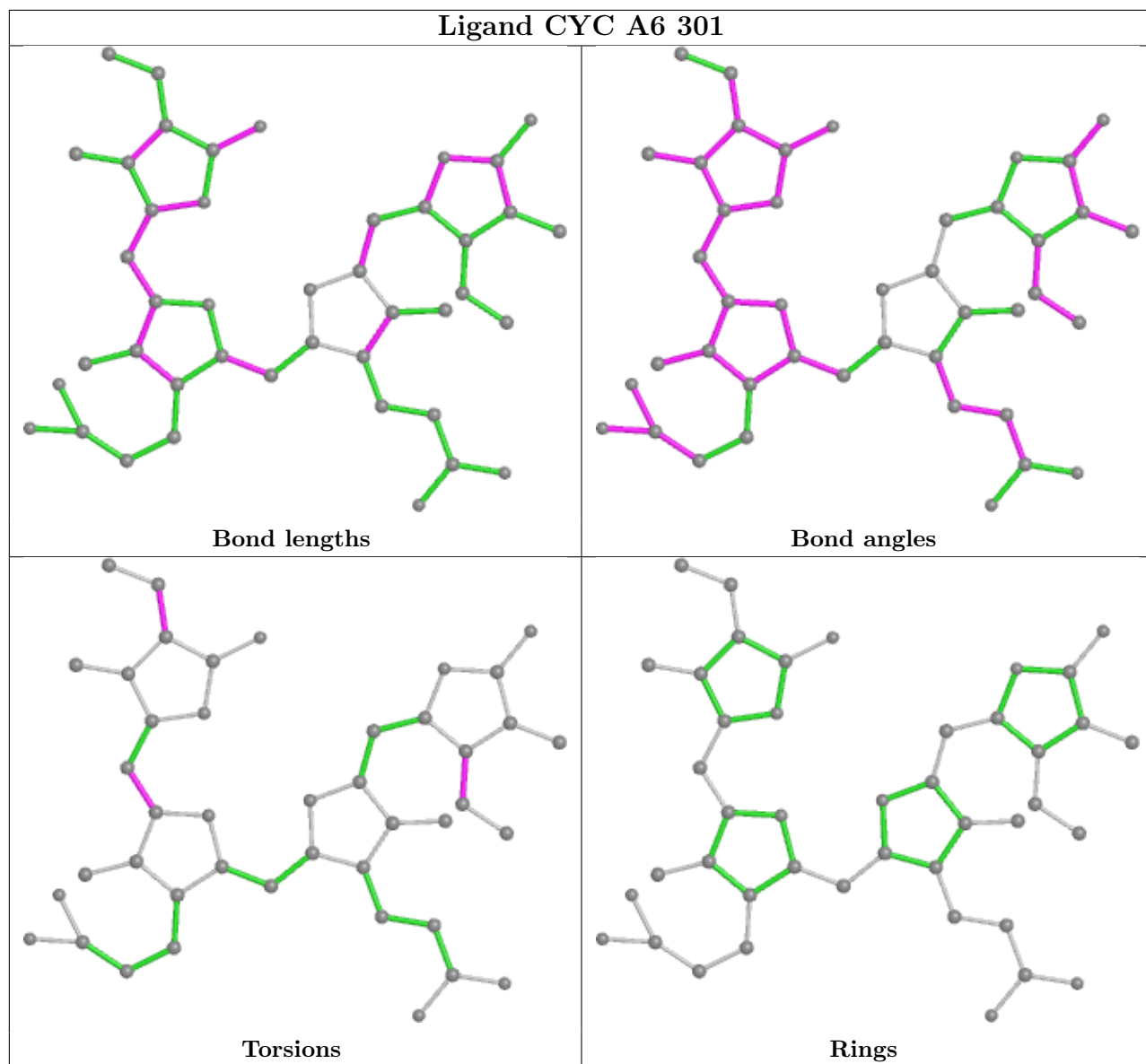


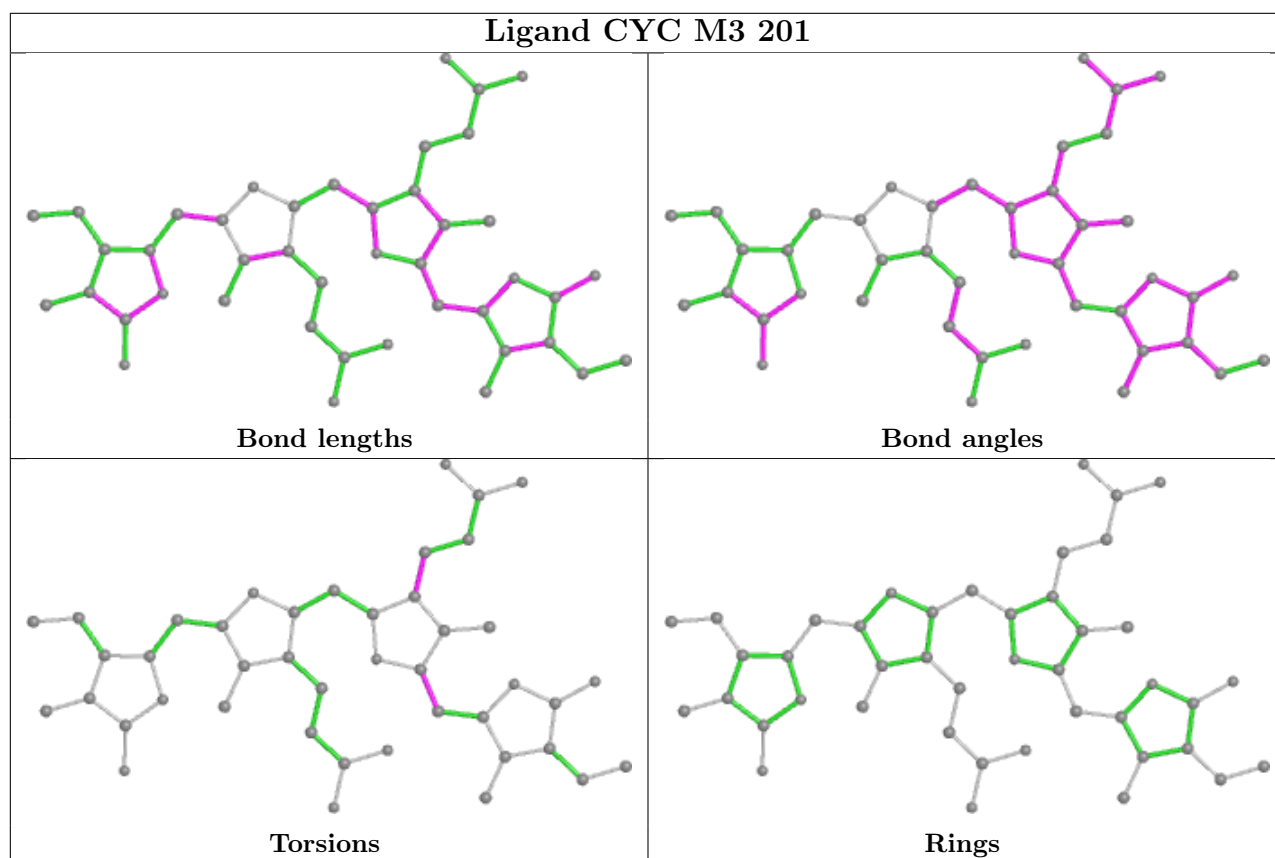
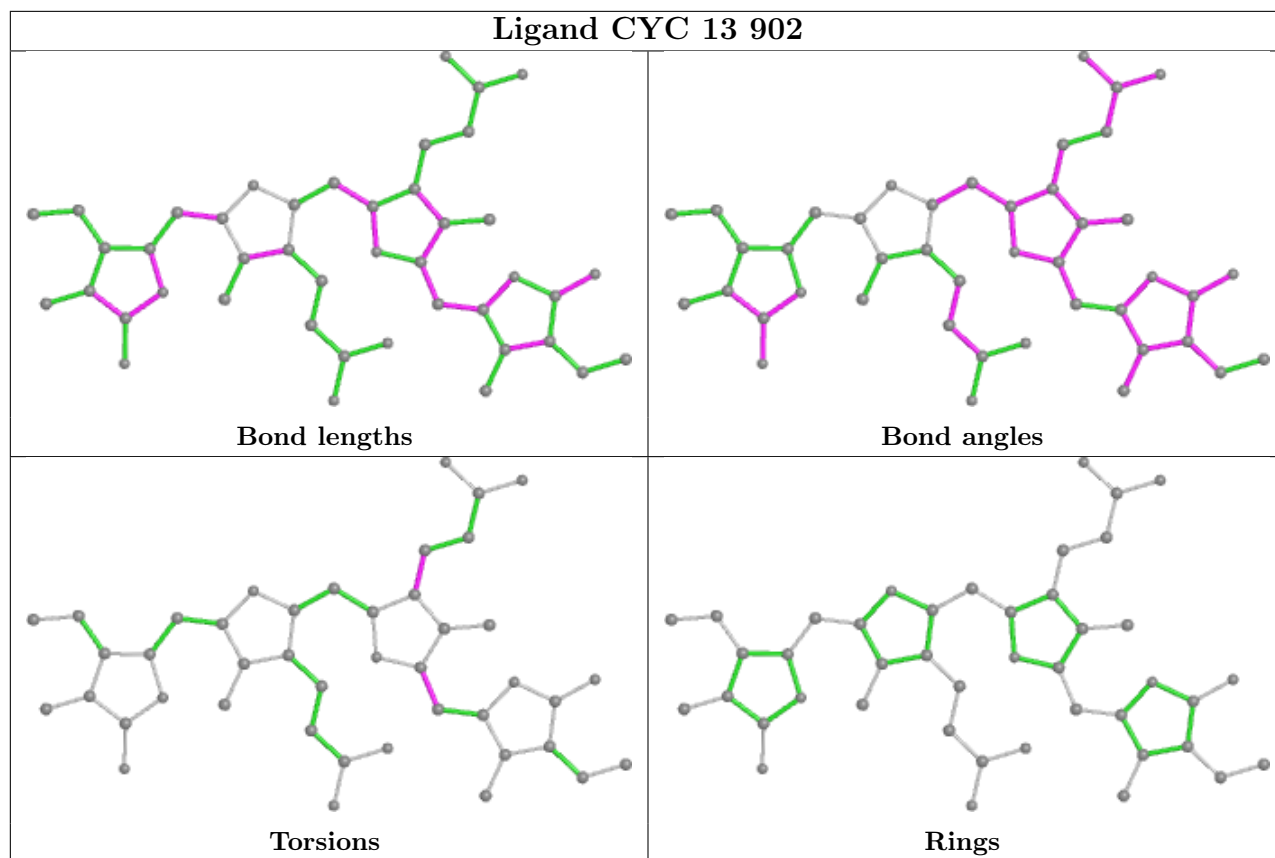


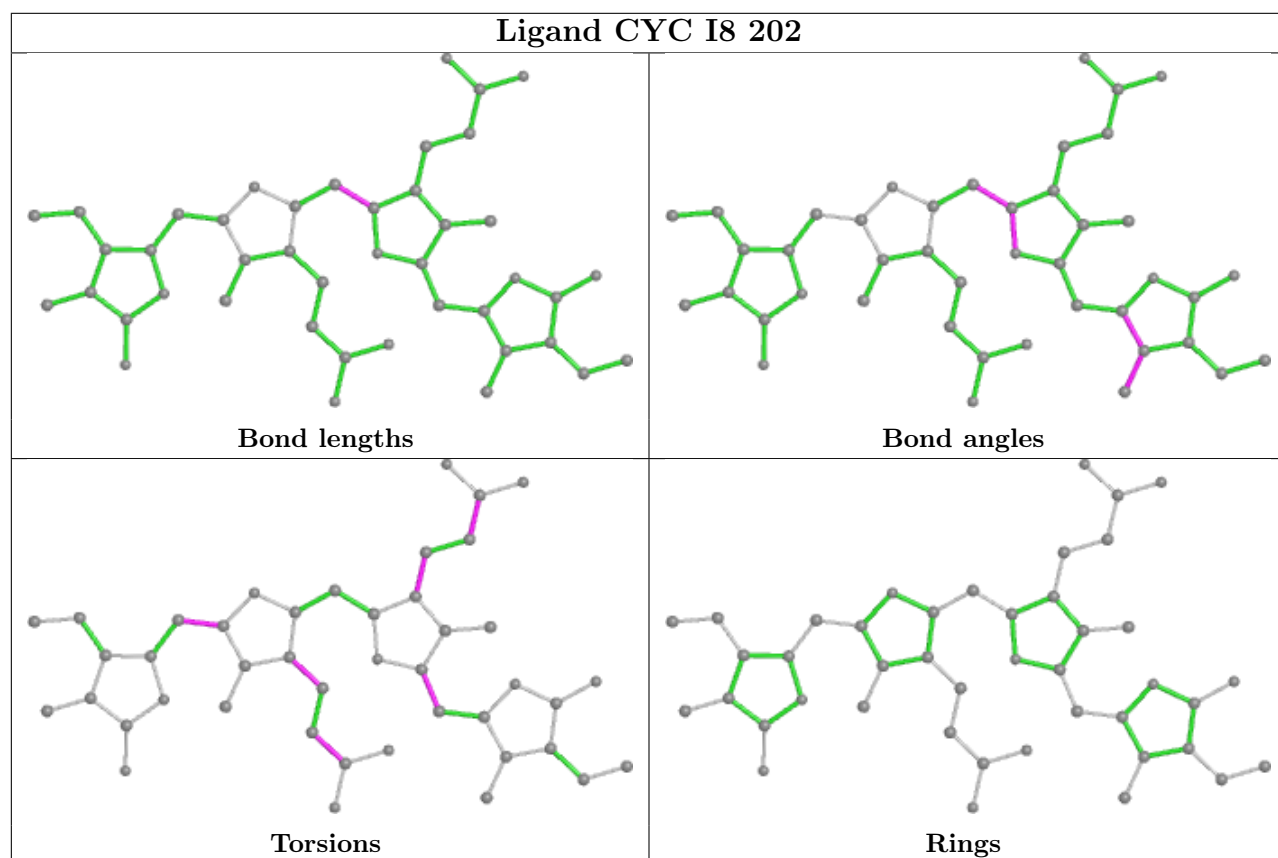
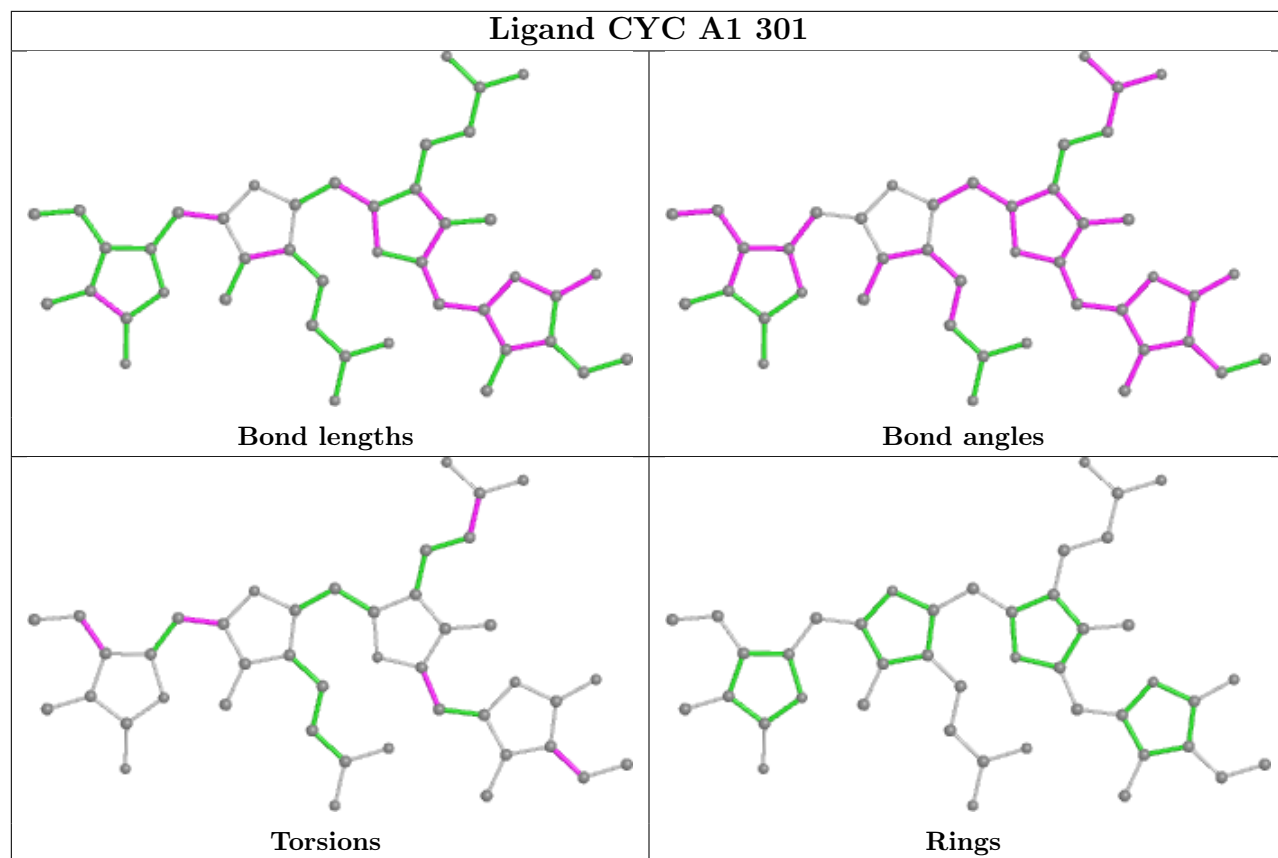


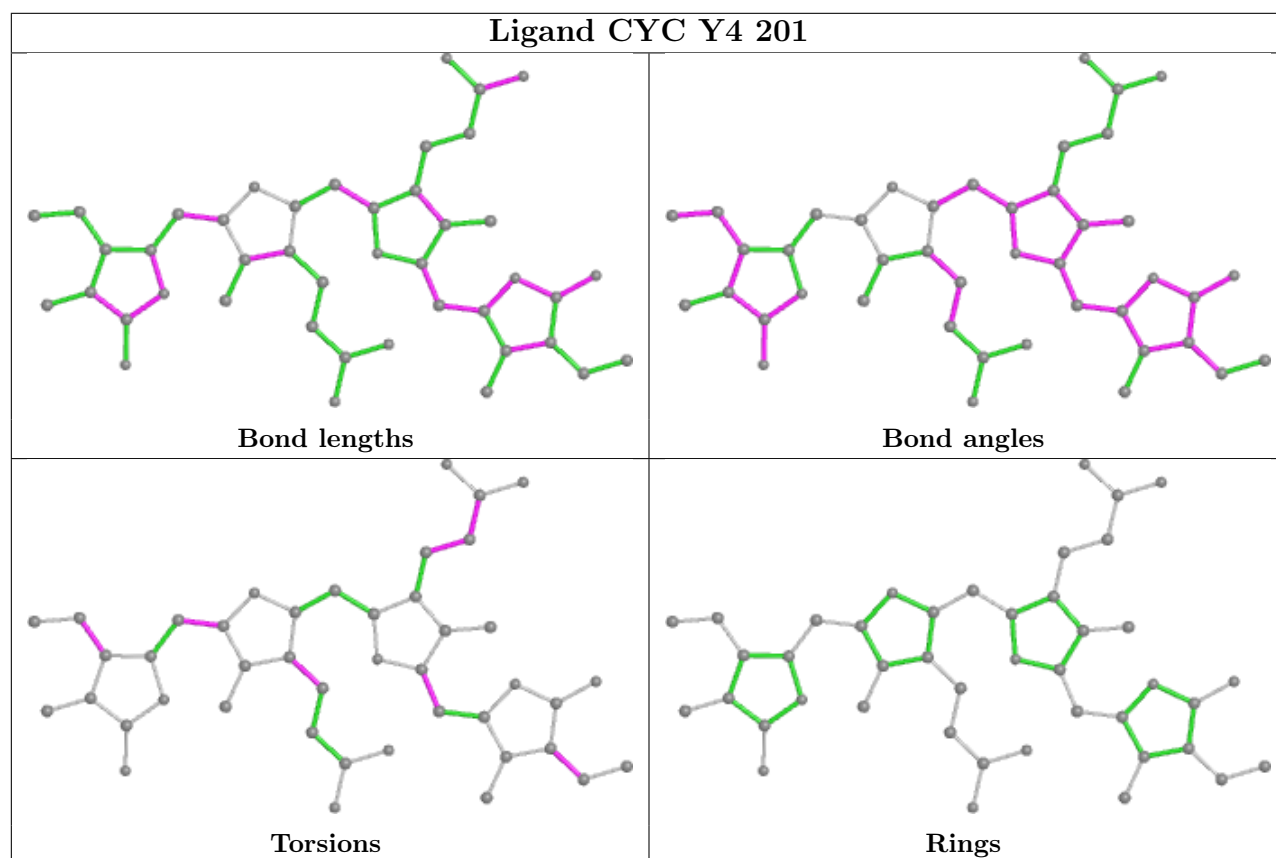
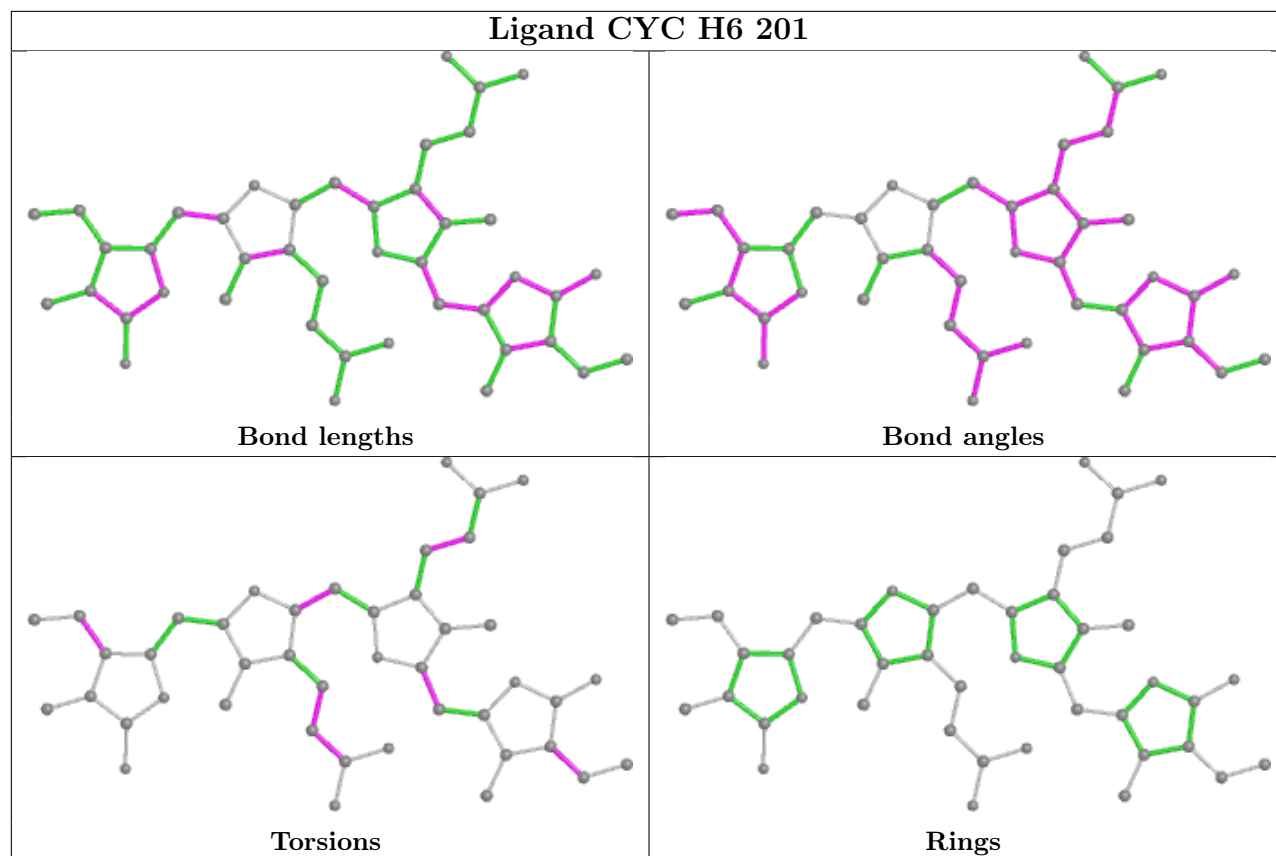


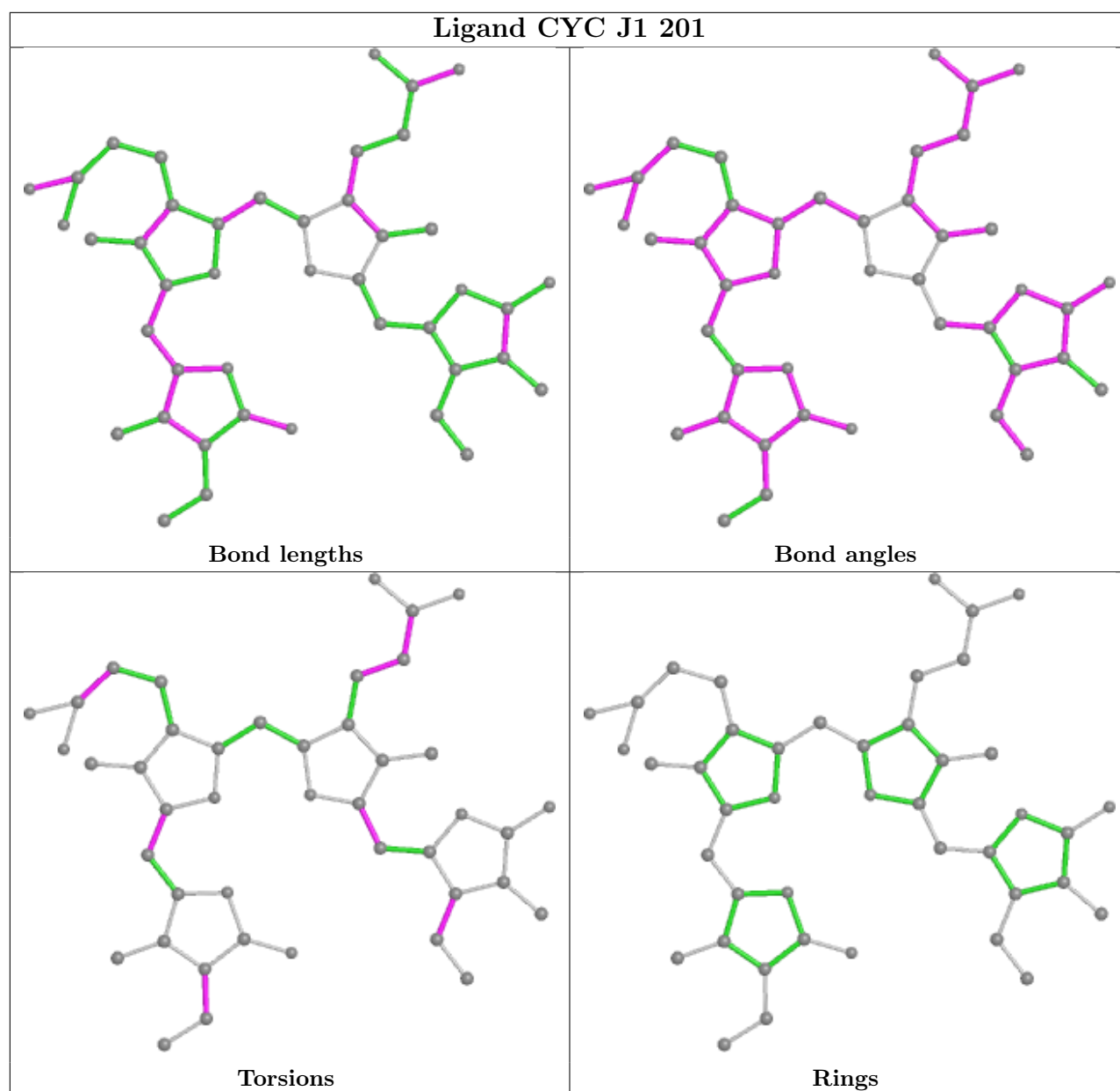












5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

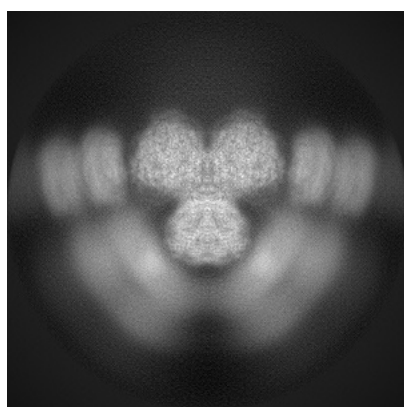
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31373. These allow visual inspection of the internal detail of the map and identification of artifacts.

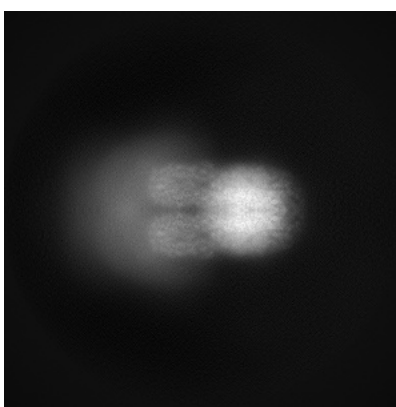
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

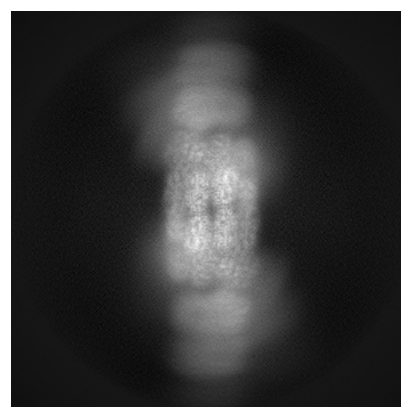
6.1.1 Primary map



X



Y

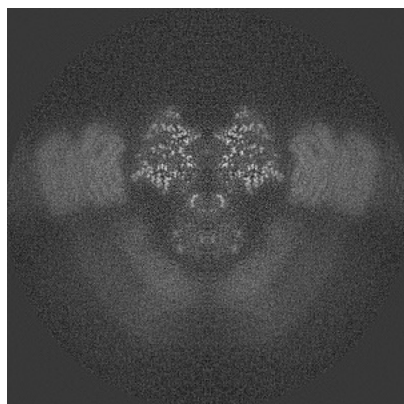


Z

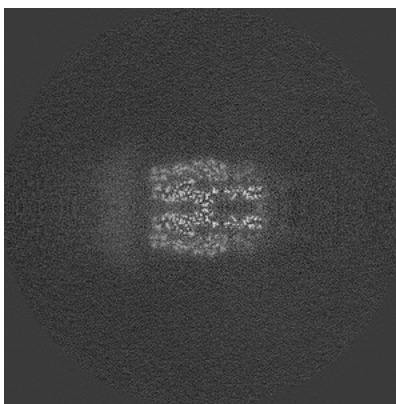
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

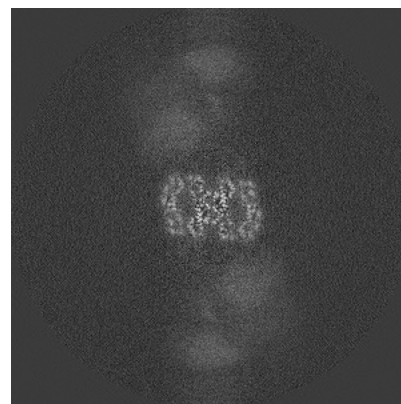
6.2.1 Primary map



X Index: 250



Y Index: 250

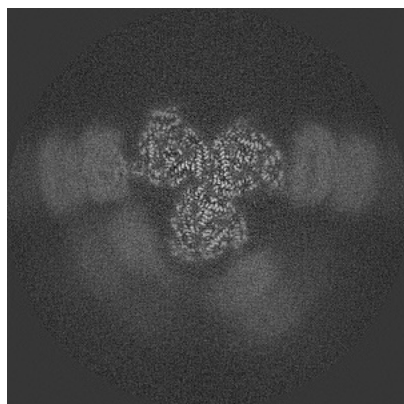


Z Index: 250

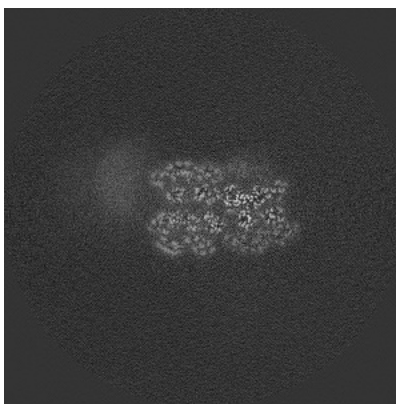
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

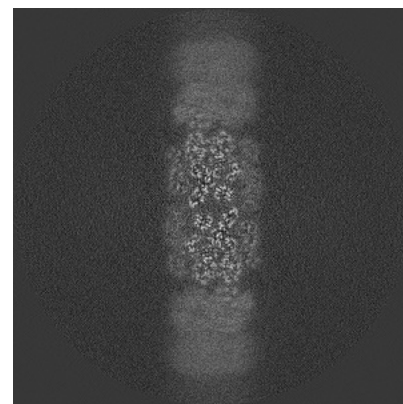
6.3.1 Primary map



X Index: 265



Y Index: 272

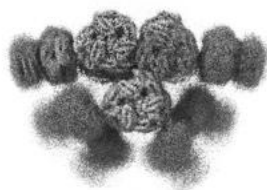


Z Index: 294

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0167. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

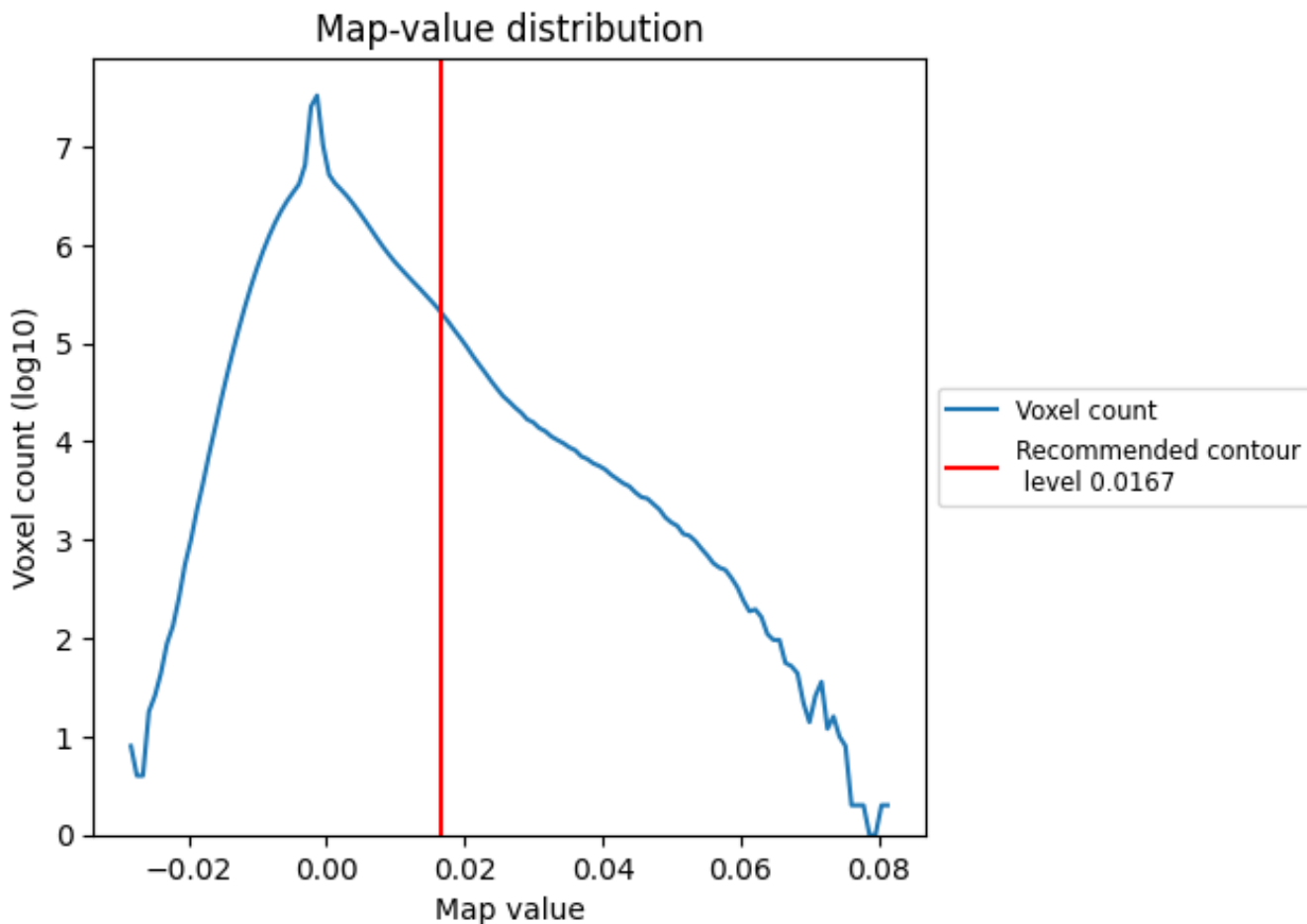
6.5 Mask visualisation

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

7 Map analysis [i](#)

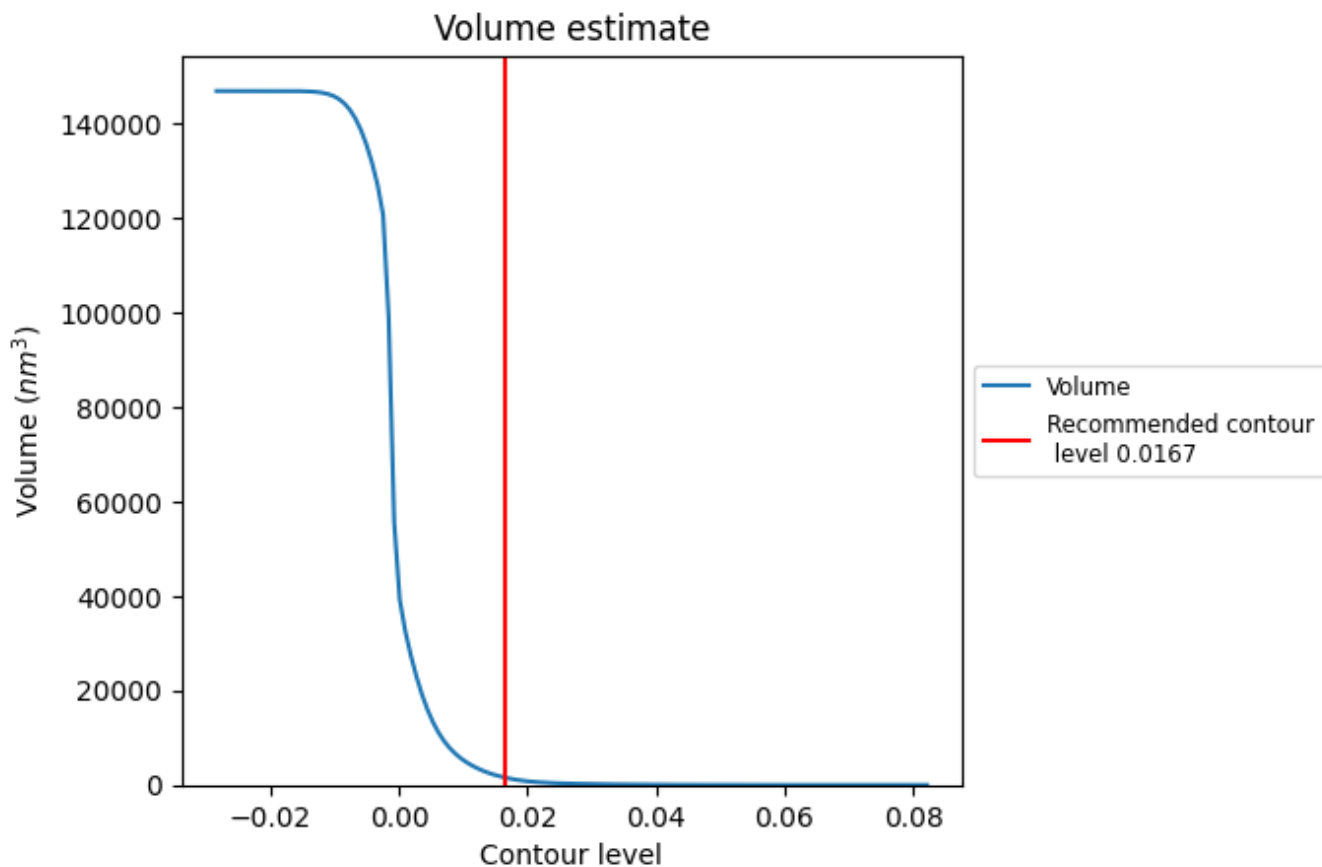
This section contains the results of statistical analysis of the map.

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.

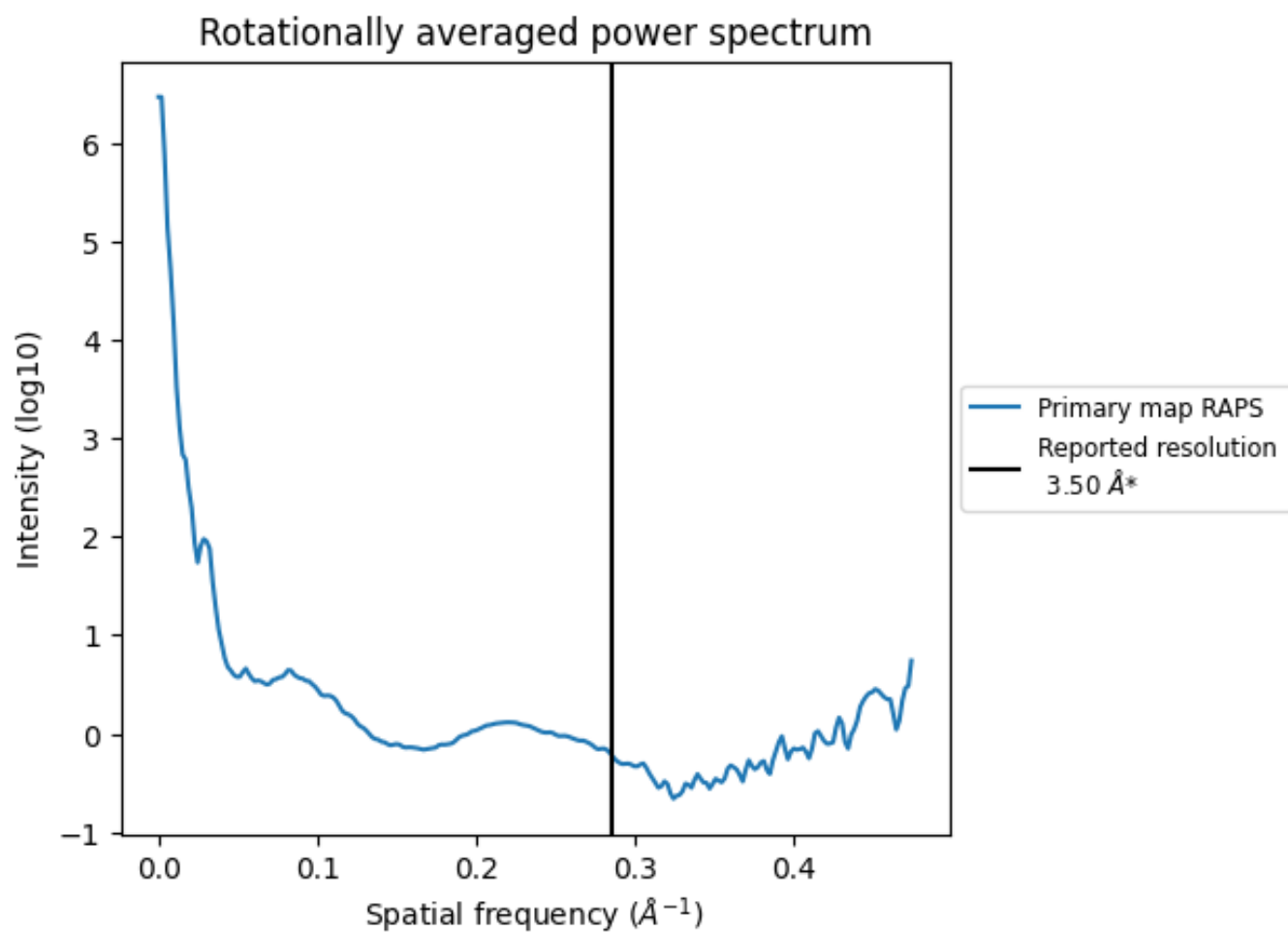
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 1508 nm^3 ; this corresponds to an approximate mass of 1362 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)



*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

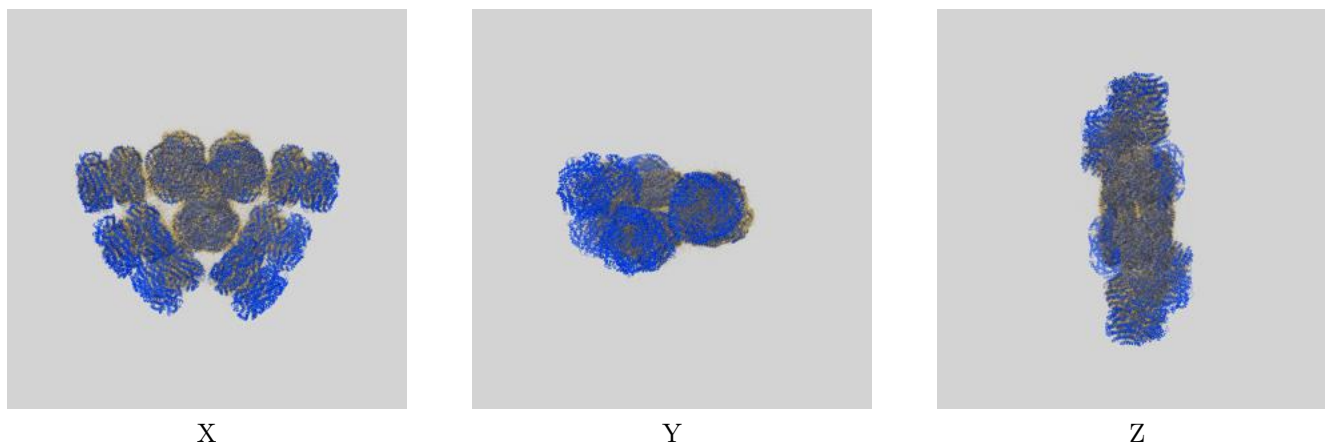
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

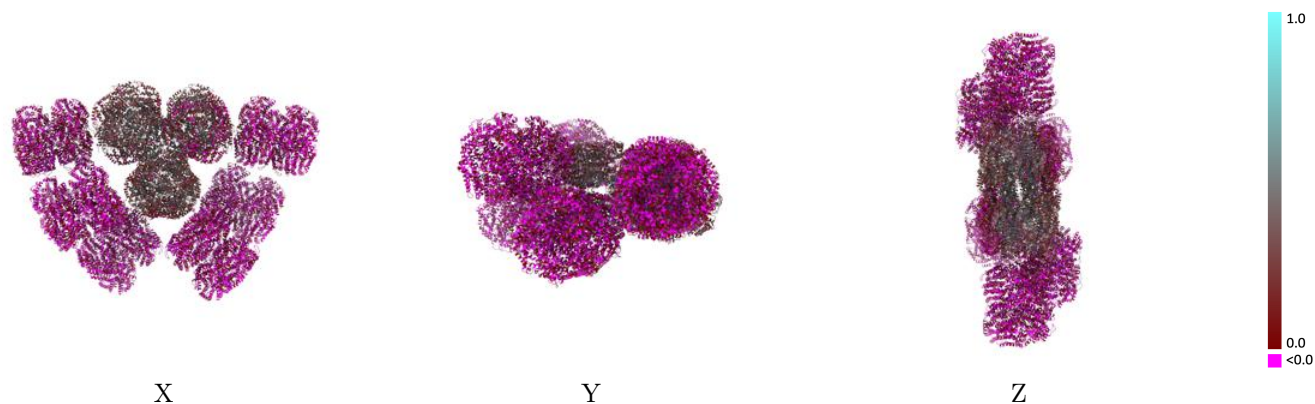
This section contains information regarding the fit between EMDB map EMD-31373 and PDB model 7EXT. Per-residue inclusion information can be found in section 3 on page 40.

9.1 Map-model overlay [i](#)



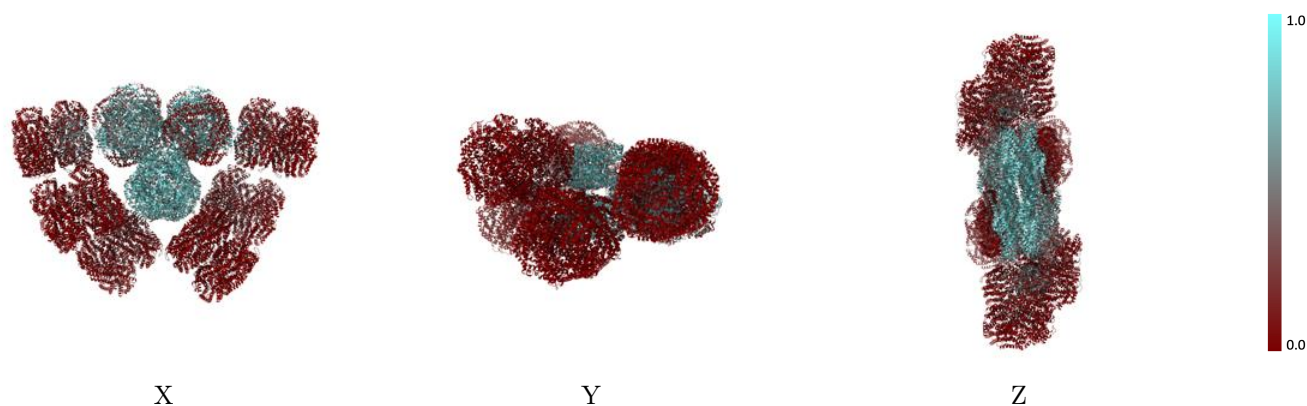
The images above show the 3D surface view of the map at the recommended contour level 0.0167 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



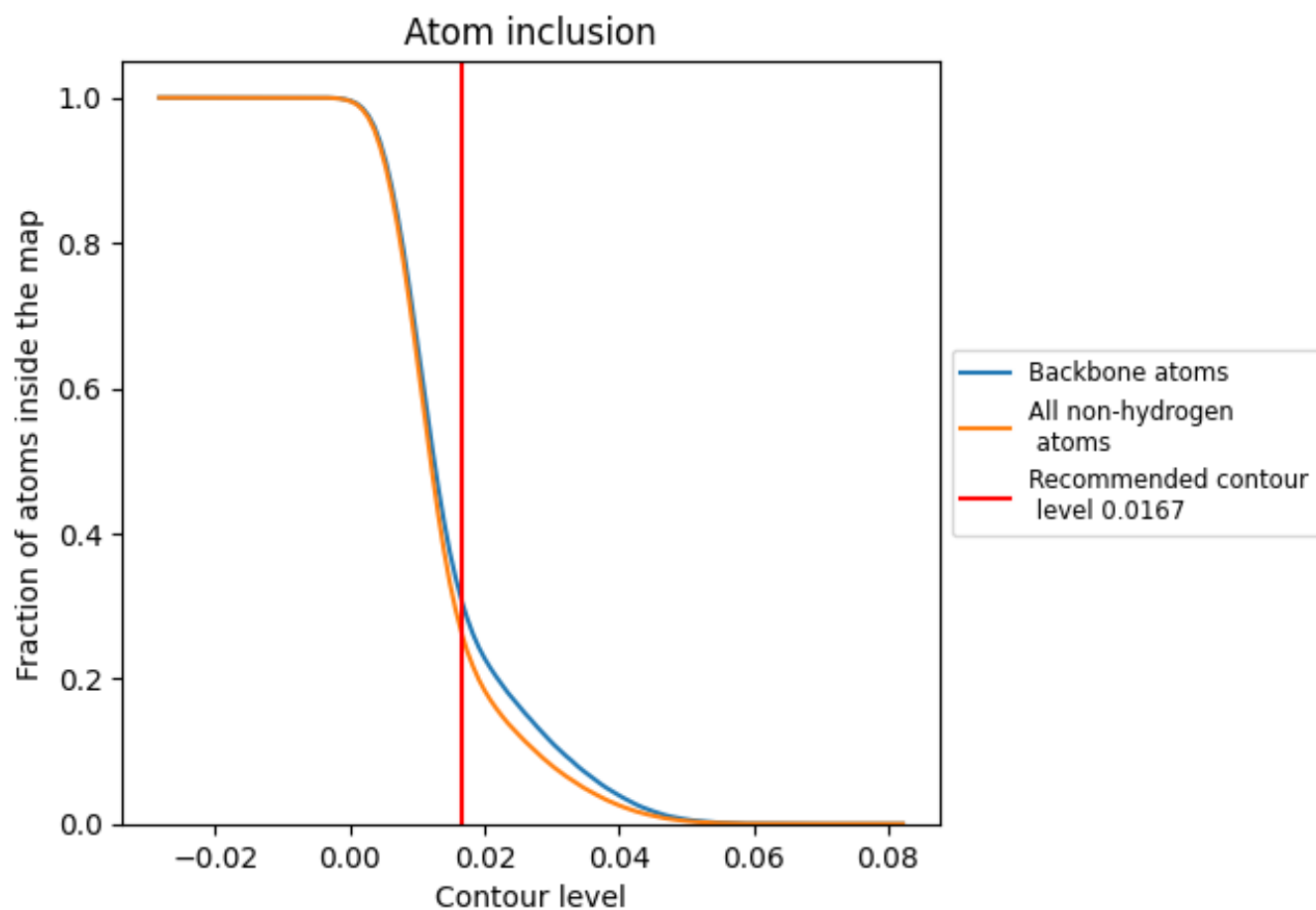
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0167).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 30% of all backbone atoms, 26% 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 (0.0167) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.2596	 0.1100
03	 0.8287	 0.4180
13	 0.8280	 0.4130
23	 0.5856	 0.3410
33	 0.5934	 0.3370
A1	 0.2034	 0.0530
A2	 0.4644	 0.0740
A4	 0.2741	 0.0400
A5	 0.1965	 0.0240
A6	 0.4546	 0.0680
A7	 0.1001	 0.1420
A8	 0.2927	 0.0510
B1	 0.0630	 0.0210
B2	 0.3780	 0.0530
B4	 0.1359	 -0.0000
B5	 0.0670	 0.0120
B6	 0.3429	 0.0570
B7	 0.0708	 0.0470
B8	 0.1450	 0.0020
C1	 0.0120	 0.0280
C2	 0.2357	 0.0370
C4	 0.0333	 0.0120
C5	 0.0180	 0.0310
C6	 0.2157	 0.0310
C7	 0.1257	 0.1330
C8	 0.0596	 0.0200
D1	 0.0048	 0.0120
D2	 0.1404	 0.0310
D4	 0.0247	 0.0100
D5	 0.0056	 0.0070
D6	 0.1318	 0.0350
D7	 0.1556	 0.0820
D8	 0.0335	 0.0080
E1	 0.0136	 -0.0120
E2	 0.1363	 0.0220



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Chain	Atom inclusion	Q-score
E4	0.0219	0.0170
E5	0.0088	-0.0000
E6	0.1411	0.0160
E7	0.1514	0.1480
E8	0.0343	-0.0070
F1	0.0463	0.0050
F2	0.1647	0.0310
F4	0.0797	0.0000
F5	0.0367	0.0050
F6	0.1699	0.0300
F7	0.0947	0.1230
F8	0.0869	0.0120
G1	0.0781	0.0120
G2	0.3661	0.0780
G3	0.8577	0.4280
G4	0.1029	0.0010
G5	0.0736	0.0200
G6	0.3615	0.0770
G7	0.1342	0.1370
G8	0.1081	-0.0040
H1	0.0287	0.0040
H2	0.1611	0.0130
H3	0.8510	0.4160
H4	0.0338	-0.0180
H5	0.0311	0.0140
H6	0.1523	0.0110
H7	0.0959	0.1410
H8	0.0321	-0.0160
I1	0.0473	0.0040
I2	0.2442	0.0240
I3	0.7998	0.3320
I4	0.0816	-0.0090
I5	0.0495	-0.0020
I6	0.2260	0.0250
I7	0.0733	0.0510
I8	0.0722	0.0030
J1	0.0821	-0.0050
J2	0.2710	0.0280
J3	0.8362	0.3990
J4	0.1277	0.0240
J5	0.0853	0.0070
J6	0.2751	0.0290





















































































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Chain	Atom inclusion	Q-score
J7	0.1166	0.1390
J8	0.1244	0.0160
K1	0.0390	0.0080
K2	0.1691	0.0200
K3	0.7585	0.3380
K4	0.1029	-0.0130
K5	0.0428	0.0100
K6	0.1637	0.0140
K7	0.1506	0.0750
K8	0.0908	-0.0080
L1	0.0215	0.0040
L2	0.1005	0.0270
L3	0.8587	0.4260
L4	0.0572	0.0150
L5	0.0231	0.0050
L6	0.0941	0.0400
L7	0.1663	0.1510
L8	0.0657	-0.0000
M1	0.0240	0.0010
M2	0.1502	0.0290
M3	0.8379	0.3830
M4	0.0706	0.0240
M5	0.0315	0.0210
M6	0.1419	0.0190
M7	0.0938	0.1250
M8	0.0601	-0.0050
N1	0.0447	-0.0070
N2	0.1470	0.0050
N3	0.7866	0.3530
N4	0.0925	0.0200
N5	0.0424	-0.0020
N6	0.1514	0.0090
N7	0.1322	0.1070
N8	0.0835	-0.0000
O1	0.0024	-0.0050
O2	0.0140	0.0120
O3	0.8741	0.4480
O4	0.0056	-0.0020
O5	0.0048	-0.0050
O6	0.0199	0.0060
O7	0.7213	0.2670
O8	0.0048	0.0010





















































































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Chain	Atom inclusion	Q-score
P1	 0.0075	 -0.0190
P2	 0.0450	 0.0060
P3	 0.8503	 0.4310
P4	 0.0131	 0.0110
P5	 0.0038	 0.0020
P6	 0.0465	 0.0160
P7	 0.7103	 0.2800
P8	 0.0124	 0.0100
Q1	 0.0040	 0.0090
Q2	 0.0407	 0.0220
Q3	 0.8438	 0.4240
Q4	 0.0033	 0.0140
Q5	 0.0024	 0.0060
Q6	 0.0478	 0.0280
Q7	 0.7428	 0.2860
Q8	 0.0074	 0.0210
R1	 0.0068	 0.0080
R2	 0.0735	 0.0260
R3	 0.5476	 0.3000
R4	 0.0132	 0.0060
R5	 0.0113	 0.0270
R6	 0.0608	 0.0110
R7	 0.7136	 0.2820
R8	 0.0085	 -0.0040
S1	 0.0016	 0.0130
S2	 0.0199	 -0.0030
S3	 0.4724	 0.3130
S4	 0.0016	 0.0030
S5	 0.0008	 -0.0170
S6	 0.0140	 0.0010
S7	 0.7196	 0.2700
S8	 0.0064	 0.0010
T1	 0.0085	 0.0130
T2	 0.0345	 0.0110
T3	 0.3714	 0.2400
T4	 0.0255	 0.0230
T5	 0.0046	 -0.0020
T6	 0.0310	 -0.0120
T7	 0.7465	 0.3090
T8	 0.0203	 0.0260
U1	 0.0015	 0.0110
U2	 0.0173	 0.0130













































































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Chain	Atom inclusion	Q-score
U3	 0.4239	 0.2870
U4	 0.0016	 -0.0010
U5	 0.0008	 0.0060
U6	 0.0159	 0.0010
U7	 0.7743	 0.3040
U8	 0.0000	 0.0130
V1	 0.0000	 0.0040
V2	 0.0270	 0.0130
V3	 0.5072	 0.2930
V4	 0.0015	 -0.0030
V5	 0.0008	 0.0180
V6	 0.0255	 0.0100
V7	 0.7055	 0.2510
V8	 0.0008	 -0.0160
W1	 0.0016	 0.0040
W2	 0.0144	 0.0000
W3	 0.5029	 0.3090
W4	 0.0072	 0.0070
W5	 0.0025	 -0.0010
W6	 0.0231	 -0.0060
W7	 0.7045	 0.2790
W8	 0.0040	 -0.0020
X1	 0.0007	 -0.0070
X2	 0.0168	 0.0150
X3	 0.7965	 0.3300
X4	 0.0098	 0.0260
X5	 0.0022	 0.0140
X6	 0.0090	 0.0010
X7	 0.7577	 0.2900
X8	 0.0068	 0.0060
Y1	 0.0008	 -0.0160
Y2	 0.0140	 0.0130
Y3	 0.8349	 0.3850
Y4	 0.0032	 0.0200
Y5	 0.0000	 0.0140
Y6	 0.0144	 0.0080
Y7	 0.7292	 0.2950
Y8	 0.0024	 0.0020
Z1	 0.0000	 -0.0050
Z2	 0.0197	 0.0060
Z3	 0.7568	 0.3380
Z4	 0.0030	 0.0160

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Chain	Atom inclusion	Q-score
Z5	 0.0030	 -0.0180
Z6	 0.0225	 0.0240
Z7	 0.7122	 0.2690
Z8	 0.0023	 -0.0090
a1	 0.0043	 0.0060
a2	 0.1004	 0.0430
a3	 0.8596	 0.4250
a4	 0.0178	 -0.0140
a5	 0.0043	 -0.0130
a6	 0.0919	 0.0450
a7	 0.7350	 0.2850
a8	 0.0133	 0.0300
b3	 0.8627	 0.4340
b7	 0.7568	 0.3150
c3	 0.8477	 0.4080
d3	 0.7734	 0.3240
e3	 0.8790	 0.4410
f3	 0.8503	 0.4340
g3	 0.8446	 0.4210
h3	 0.8255	 0.3660
i3	 0.5509	 0.2960
j3	 0.4494	 0.3000
k3	 0.3656	 0.2390
l3	 0.4321	 0.2890
m3	 0.5144	 0.3000
n3	 0.5078	 0.3090
o3	 0.7767	 0.3080
p3	 0.8247	 0.3610
q3	 0.7998	 0.3400
r3	 0.8675	 0.4220
s3	 0.8213	 0.3740
t3	 0.8510	 0.3880
u3	 0.7560	 0.2810
v3	 0.8230	 0.3520
w3	 0.8015	 0.3340
x3	 0.8782	 0.4330
y3	 0.8180	 0.3710
z3	 0.8502	 0.3870