



wwPDB EM Validation Summary Report ⓘ

Nov 23, 2022 – 12:31 AM JST

PDB ID : 7EYD
EMDB ID : EMD-31381
Title : Cryo-EM structure of cyanobacterial phycobilisome from *Anabaena* sp. PCC 7120
Authors : Zheng, L.; Zheng, Z.; Li, X.; Wang, G.; Zhang, K.; Wei, P.; Zhao, J.; Gao, N.
Deposited on : 2021-05-30
Resolution : 3.90 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:

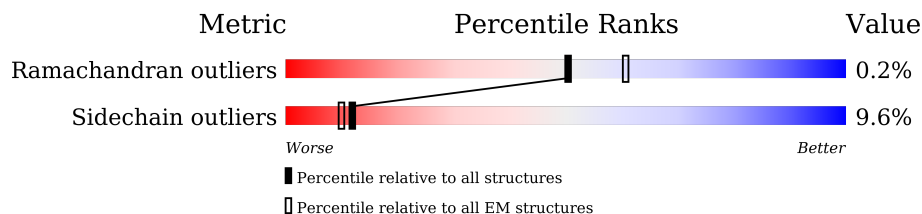
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (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 3.90 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	247	 82% 83% 14% 83% 14%
1	A4	247	 78% 83% 14%
2	B1	163	 95% 90% 10% .
2	B2	163	 27% 92% 7% .
2	B3	163	 99% 92% 7% .
2	B4	163	 91% 89% 10% .
2	B5	163	 72% 90% 10% .
2	B6	163	 28% 92% 7% .
2	B7	163	 99% 92% 7% .

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Mol	Chain	Length	Quality of chain
2	BA	163	72% 90% 10%
2	D1	163	98% 89% 10%
2	D2	163	77% 91% 9%
2	D3	163	99% 91% 9%
2	D4	163	96% 89% 10%
2	D5	163	77% 90% 9%
2	D6	163	71% 91% 9%
2	D7	163	99% 91% 9%
2	DA	163	86% 90% 9%
2	F1	163	99% 89% 10%
2	F2	163	58% 92% 7%
2	F3	163	99% 92% 7%
2	F4	163	99% 89% 10%
2	F5	163	60% 90% 9%
2	F6	163	49% 92% 7%
2	F7	163	99% 92% 7%
2	FA	163	65% 90% 9%
2	H1	163	98% 89% 10%
2	H2	163	71% 90% 9%
2	H3	163	99% 90% 9%
2	H4	163	96% 89% 10%
2	H5	163	77% 90% 9%
2	H6	163	66% 91% 9%
2	H7	163	99% 90% 9%
2	HA	163	82% 90% 9%

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Mol	Chain	Length	Quality of chain
2	J1	163	99% 89% 10%
2	J2	163	64% 91% 9%
2	J3	163	99% 91% 9%
2	J4	163	99% 89% 10%
2	J5	163	77% 90% 10%
2	J6	163	66% 91% 9%
2	J7	163	99% 91% 9%
2	JA	163	80% 90% 10%
2	L1	163	97% 90% 10%
2	L2	163	53% 91% 9%
2	L3	163	99% 91% 9%
2	L4	163	98% 90% 10%
2	L5	163	71% 90% 10%
2	L6	163	48% 91% 9%
2	L7	163	99% 91% 9%
2	LA	163	79% 90% 10%
2	O1	163	99% 89% 10%
2	O2	163	95% 91% 9%
2	O4	163	99% 89% 10%
2	O5	163	94% 90% 9%
2	O6	163	96% 91% 9%
2	OA	163	97% 90% 9%
2	Q1	163	99% 89% 10%
2	Q2	163	92% 90% 9%
2	Q4	163	99% 89% 10%

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Mol	Chain	Length	Quality of chain
2	Q5	163	95% 90% 10%
2	Q6	163	84% 90% 9%
2	QA	163	96% 90% 10%
2	S1	163	99% 89% 10%
2	S2	163	90% 91% 9%
2	S4	163	99% 89% 10%
2	S5	163	97% 90% 9%
2	S6	163	90% 91% 9%
2	SA	163	97% 90% 9%
2	U1	163	99% 88% 11%
2	U2	163	93% 92% 7%
2	U4	163	99% 88% 11%
2	U5	163	97% 90% 10%
2	U6	163	94% 92% 7%
2	UA	163	98% 90% 10%
2	W1	163	99% 89% 10%
2	W2	163	98% 90% 9%
2	W4	163	99% 89% 10%
2	W5	163	98% 90% 10%
2	W6	163	95% 91% 9%
2	WA	163	99% 90% 10%
2	Y1	163	99% 89% 10%
2	Y2	163	96% 91% 9%
2	Y4	163	99% 89% 10%
2	Y5	163	98% 90% 9%

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Mol	Chain	Length	Quality of chain
2	Y6	163	94% 91% 9%
2	YA	163	99% 90% 9%
3	C1	173	96% 92% 7%
3	C2	173	47% 87% 12%
3	C3	173	98% 87% 12%
3	C4	173	95% 92% 7%
3	C5	173	69% 87% 10%
3	C6	173	45% 87% 12%
3	C7	173	99% 87% 12%
3	CA	173	79% 87% 10%
3	E1	173	99% 93% 6%
3	E2	173	74% 88% 12%
3	E3	173	100% 88% 12%
3	E4	173	95% 93% 6%
3	E5	173	71% 88% 10%
3	E6	173	60% 88% 12%
3	E7	173	100% 88% 12%
3	EA	173	77% 88% 10%
3	G1	173	97% 92% 8%
3	G2	173	44% 89% 10%
3	G3	173	100% 89% 10%
3	G4	173	90% 92% 8%
3	G5	173	53% 87% 10%
3	G6	173	36% 89% 10%
3	G7	173	100% 89% 10%

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Mol	Chain	Length	Quality of chain
3	GA	173	56% 87% 10% ..
3	I1	173	98% 94% 6%
3	I2	173	77% 88% 11% .
3	I3	173	100% 88% 12%
3	I4	173	100% 93% 7%
3	I5	173	77% 88% 9% ..
3	I6	173	73% 88% 12% .
3	I7	173	100% 88% 12%
3	IA	173	82% 88% 9% ..
3	K1	173	99% 92% 8% .
3	K2	173	57% 87% 12% ..
3	K3	173	99% 87% 12% ..
3	K4	173	98% 92% 8% .
3	K5	173	83% 87% 10% ..
3	K6	173	49% 87% 12% ..
3	K7	173	99% 87% 12% ..
3	KA	173	83% 87% 10% ..
3	M1	173	98% 93% 6% .
3	M2	173	64% 90% 9% ..
3	M3	173	99% 90% 9% ..
3	M4	173	97% 93% 6% .
3	M5	173	65% 87% 10% ..
3	M6	173	51% 91% 8% ..
3	M7	173	99% 90% 9% ..
3	MA	173	80% 87% 10% ..

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Mol	Chain	Length	Quality of chain
3	P1	173	99% 94% 6% ..
3	P2	173	91% 87% 12% ..
3	P4	173	99% 94% 6% ..
3	P5	173	91% 87% 10% ..
3	P6	173	87% 87% 12% ..
3	PA	173	97% 87% 10% ..
3	R1	173	99% 94% 5% ..
3	R2	173	86% 87% 12% ..
3	R4	173	99% 94% 5% ..
3	R5	173	93% 88% 10% ..
3	R6	173	79% 87% 12% ..
3	RA	173	93% 88% 10% ..
3	T1	173	99% 94% 6% ..
3	T2	173	86% 88% 10% ..
3	T4	173	99% 94% 6% ..
3	T5	173	94% 87% 10% ..
3	T6	173	82% 88% 11% ..
3	TA	173	94% 87% 10% ..
3	V1	173	99% 93% 6% ..
3	V2	173	98% 89% 10% ..
3	V4	173	99% 93% 6% ..
3	V5	173	98% 87% 10% ..
3	V6	173	97% 88% 10% ..
3	VA	173	99% 87% 10% ..
3	X1	173	99% 95% 5% ..

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Mol	Chain	Length	Quality of chain
3	X2	173	94% 89% 10% ..
3	X4	173	99% 94% 5% .
3	X5	173	99% 87% 11% ..
3	X6	173	95% 88% 10% ..
3	XA	173	98% 87% 11% ..
3	Z1	173	99% 95% 5% .
3	Z2	173	95% 90% 9% ..
3	Z4	173	99% 94% 5% .
3	Z5	173	97% 88% 10% ..
3	Z6	173	94% 90% 9% ..
3	ZA	173	99% 88% 10% ..
4	N1	286	99% 97% ..
4	N2	286	71% 97% ..
4	N3	286	20% 20% 80%
4	N4	286	99% 97% ..
4	N5	286	83% 96%
4	N6	286	65% 97% ..
4	N7	286	20% 20% 80%
4	NA	286	88% 96%
5	A2	253	19% 95% ..
5	A5	253	42% 90% 6%
5	A6	253	17% 96% ..
5	AA	253	45% 91% 6%
6	A3	279	49% 47% 51%
6	A7	279	48% 47% 51%

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Mol	Chain	Length	Quality of chain
7	A8	161	21% 91% 7% ..
7	A9	161	29% 93% 6% .
7	C8	161	6% 91% 7% ..
7	C9	161	29% 92% 7% .
7	E8	161	30% 91% 7% ..
7	E9	161	13% 93% 6% .
7	G9	161	. 93% 6% .
7	H8	161	24% 91% 7% ..
7	I9	161	. 93% 6% .
7	J8	161	6% 91% 7% ..
7	K9	161	14% 93% 6% .
7	L8	161	28% 91% 7% ..
7	N9	161	6% 93% 6% .
7	O8	161	28% 91% 7% ..
7	P9	161	. 93% 6% .
7	Q8	161	22% 91% 7% ..
7	R9	161	42% 93% 6% .
7	S8	161	17% 91% 7% ..
7	T9	161	36% 93% 6% .
7	V8	161	54% 91% 7% ..
7	X8	161	22% 91% 7% ..
7	X9	161	6% 93% 6% .
7	Z8	161	11% 91% 7% ..
7	Z9	161	11% 93% 6% .
7	b9	161	7% 93% 6% .

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Mol	Chain	Length	Quality of chain
7	c8	161	55% 91% 7% ..
7	d9	161	7% 93% 6% .
7	e8	161	25% 91% 7% ..
7	f9	161	5% 93% 6% .
7	g8	161	9% 91% 7% ..
7	i9	161	54% 93% 6% .
7	j8	161	25% 91% 7% ..
7	k9	161	42% 93% 6% .
7	l8	161	32% 91% 7% ..
7	n8	161	9% 91% 7% ..
7	o9	161	15% 93% 6% .
7	p8	161	28% 91% 7% ..
7	q9	161	10% 93% 6% .
7	r8	161	37% 91% 7% ..
7	s9	161	7% 93% 6% .
7	t8	161	6% 91% 7% ..
7	u9	161	18% 93% 6% .
7	w9	161	7% 93% 6% .
7	y9	161	10% 93% 6% .
8	B8	162	16% 90% 9% .
8	B9	162	27% 93% 6% .
8	D8	162	12% 90% 9% .
8	D9	162	23% 93% 6% .
8	F8	162	18% 90% 9% .
8	F9	162	18% 94% 5% .

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Mol	Chain	Length	Quality of chain
8	H9	162	94% 5%
8	I8	162	19% 90% 9%
8	J9	162	5% 94% 5%
8	K8	162	13% 90% 9%
8	L9	162	9% 93% 6%
8	M8	162	20% 90% 9%
8	M9	162	12% 94% 5%
8	O9	162	94% 5%
8	P8	162	27% 90% 9%
8	R8	162	29% 90% 9%
8	S9	162	36% 93% 6%
8	T8	162	20% 90% 9%
8	U9	162	36% 93% 6%
8	W8	162	42% 90% 9%
8	W9	162	19% 94% 5%
8	Y8	162	9% 90% 9%
8	Y9	162	93% 6%
8	a8	162	21% 90% 9%
8	a9	162	8% 94% 5%
8	c9	162	93% 6%
8	d8	162	39% 91% 7%
8	e9	162	93% 6%
8	f8	162	16% 90% 9%
8	h8	162	24% 90% 9%
8	h9	162	8% 93% 6%

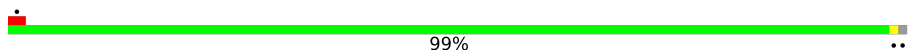
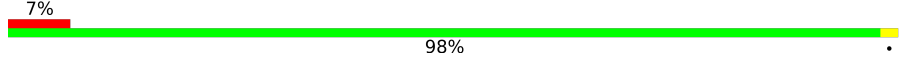
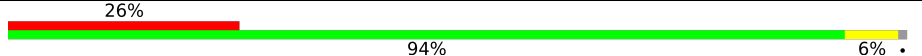
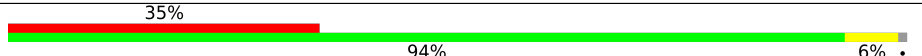
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Mol	Chain	Length	Quality of chain
8	j9	162	35% 93% 6%
8	k8	162	26% 90% 9%
8	l9	162	35% 93% 6%
8	m8	162	12% 90% 9%
8	n9	162	25% 93% 6%
8	o8	162	10% 90% 8%
8	p9	162	7% 93% 6%
8	q8	162	22% 90% 9%
8	r9	162	7% 94% 5%
8	s8	162	10% 90% 9%
8	t9	162	5% 93% 6%
8	u8	162	9% 90% 9%
8	v9	162	7% 94% 5%
8	x9	162	6% 94% 5%
8	z9	162	6% 93% 6%
9	29	68	15% 85% 9%
9	39	68	16% 85% 9%
9	49	68	18% 84% 12%
9	G8	68	15% 87% 7%
9	N8	68	15% 87% 7%
9	U8	68	18% 87% 7%
9	b8	68	26% 90% 6%
9	i8	68	29% 88% 7%
10	09	1132	7% 90% 7%
10	19	1132	6% 89% 8%

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Mol	Chain	Length	Quality of chain
11	Q9	169	 <p>99%</p>
11	g9	169	 <p>7% 98%</p>
12	V9	161	 <p>26% 94% 6%</p>
12	m9	161	 <p>35% 94% 6%</p>

2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 387586 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 CpcG2.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	A1	213	1774	1135	308	331	0	0
1	A4	213	1774	1135	308	331	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B1	162	1223	765	217	240	1	0	0
2	D1	162	1223	765	217	240	1	0	0
2	F1	162	1223	765	217	240	1	0	0
2	H1	162	1223	765	217	240	1	0	0
2	J1	162	1223	765	217	240	1	0	0
2	L1	162	1223	765	217	240	1	0	0
2	O1	162	1223	765	217	240	1	0	0
2	Q1	162	1223	765	217	240	1	0	0
2	S1	162	1223	765	217	240	1	0	0
2	U1	162	1223	765	217	240	1	0	0
2	W1	162	1223	765	217	240	1	0	0
2	Y1	162	1223	765	217	240	1	0	0
2	B2	162	1223	765	217	240	1	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	D2	162	Total	C	N	O	S	0	0
			1223	765	217	240	1		
2	F2	162	Total	C	N	O	S	0	0
			1223	765	217	240	1		
2	H2	162	Total	C	N	O	S	0	0
			1223	765	217	240	1		
2	J2	162	Total	C	N	O	S	0	0
			1223	765	217	240	1		
2	L2	162	Total	C	N	O	S	0	0
			1223	765	217	240	1		
2	O2	162	Total	C	N	O	S	0	0
			1223	765	217	240	1		
2	Q2	162	Total	C	N	O	S	0	0
			1223	765	217	240	1		
2	S2	162	Total	C	N	O	S	0	0
			1223	765	217	240	1		
2	U2	162	Total	C	N	O	S	0	0
			1223	765	217	240	1		
2	W2	162	Total	C	N	O	S	0	0
			1223	765	217	240	1		
2	Y2	162	Total	C	N	O	S	0	0
			1223	765	217	240	1		
2	B3	162	Total	C	N	O	S	0	0
			1223	765	217	240	1		
2	D3	162	Total	C	N	O	S	0	0
			1223	765	217	240	1		
2	F3	162	Total	C	N	O	S	0	0
			1223	765	217	240	1		
2	H3	162	Total	C	N	O	S	0	0
			1223	765	217	240	1		
2	J3	162	Total	C	N	O	S	0	0
			1223	765	217	240	1		
2	L3	162	Total	C	N	O	S	0	0
			1223	765	217	240	1		
2	B4	162	Total	C	N	O	S	0	0
			1223	765	217	240	1		
2	D4	162	Total	C	N	O	S	0	0
			1223	765	217	240	1		
2	F4	162	Total	C	N	O	S	0	0
			1223	765	217	240	1		
2	H4	162	Total	C	N	O	S	0	0
			1223	765	217	240	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	J4	162	Total	C	N	O	S	0	0
			1223	765	217	240	1		
2	L4	162	Total	C	N	O	S	0	0
			1223	765	217	240	1		
2	O4	162	Total	C	N	O	S	0	0
			1223	765	217	240	1		
2	Q4	162	Total	C	N	O	S	0	0
			1223	765	217	240	1		
2	S4	162	Total	C	N	O	S	0	0
			1223	765	217	240	1		
2	U4	162	Total	C	N	O	S	0	0
			1223	765	217	240	1		
2	W4	162	Total	C	N	O	S	0	0
			1223	765	217	240	1		
2	Y4	162	Total	C	N	O	S	0	0
			1223	765	217	240	1		
2	B5	162	Total	C	N	O	S	0	0
			1223	765	217	240	1		
2	D5	162	Total	C	N	O	S	0	0
			1223	765	217	240	1		
2	F5	162	Total	C	N	O	S	0	0
			1223	765	217	240	1		
2	H5	162	Total	C	N	O	S	0	0
			1223	765	217	240	1		
2	J5	162	Total	C	N	O	S	0	0
			1223	765	217	240	1		
2	L5	162	Total	C	N	O	S	0	0
			1223	765	217	240	1		
2	O5	162	Total	C	N	O	S	0	0
			1223	765	217	240	1		
2	Q5	162	Total	C	N	O	S	0	0
			1223	765	217	240	1		
2	S5	162	Total	C	N	O	S	0	0
			1223	765	217	240	1		
2	U5	162	Total	C	N	O	S	0	0
			1223	765	217	240	1		
2	W5	162	Total	C	N	O	S	0	0
			1223	765	217	240	1		
2	Y5	162	Total	C	N	O	S	0	0
			1223	765	217	240	1		
2	B6	162	Total	C	N	O	S	0	0
			1223	765	217	240	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	D6	162	Total	C	N	O	S	0	0
			1223	765	217	240	1		
2	F6	162	Total	C	N	O	S	0	0
			1223	765	217	240	1		
2	H6	162	Total	C	N	O	S	0	0
			1223	765	217	240	1		
2	J6	162	Total	C	N	O	S	0	0
			1223	765	217	240	1		
2	L6	162	Total	C	N	O	S	0	0
			1223	765	217	240	1		
2	O6	162	Total	C	N	O	S	0	0
			1223	765	217	240	1		
2	Q6	162	Total	C	N	O	S	0	0
			1223	765	217	240	1		
2	S6	162	Total	C	N	O	S	0	0
			1223	765	217	240	1		
2	U6	162	Total	C	N	O	S	0	0
			1223	765	217	240	1		
2	W6	162	Total	C	N	O	S	0	0
			1223	765	217	240	1		
2	Y6	162	Total	C	N	O	S	0	0
			1223	765	217	240	1		
2	B7	162	Total	C	N	O	S	0	0
			1223	765	217	240	1		
2	D7	162	Total	C	N	O	S	0	0
			1223	765	217	240	1		
2	F7	162	Total	C	N	O	S	0	0
			1223	765	217	240	1		
2	H7	162	Total	C	N	O	S	0	0
			1223	765	217	240	1		
2	J7	162	Total	C	N	O	S	0	0
			1223	765	217	240	1		
2	L7	162	Total	C	N	O	S	0	0
			1223	765	217	240	1		
2	BA	162	Total	C	N	O	S	0	0
			1223	765	217	240	1		
2	DA	162	Total	C	N	O	S	0	0
			1223	765	217	240	1		
2	FA	162	Total	C	N	O	S	0	0
			1223	765	217	240	1		
2	HA	162	Total	C	N	O	S	0	0
			1223	765	217	240	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	JA	162	1223	765	217	240	1	0	0
2	LA	162	1223	765	217	240	1	0	0
2	OA	162	1223	765	217	240	1	0	0
2	QA	162	1223	765	217	240	1	0	0
2	SA	162	1223	765	217	240	1	0	0
2	UA	162	1223	765	217	240	1	0	0
2	WA	162	1223	765	217	240	1	0	0
2	YA	162	1223	765	217	240	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C1	172	1278	788	229	255	6	0	0
3	E1	172	1278	788	229	255	6	0	0
3	G1	172	1278	788	229	255	6	0	0
3	I1	173	1286	793	230	256	7	0	0
3	K1	172	1278	788	229	255	6	0	0
3	M1	172	1278	788	229	255	6	0	0
3	P1	172	1278	788	229	255	6	0	0
3	R1	172	1278	788	229	255	6	0	0
3	T1	172	1278	788	229	255	6	0	0
3	V1	172	1278	788	229	255	6	0	0
3	X1	172	1278	788	229	255	6	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	Z1	172	Total	C	N	O	S	0	0
			1278	788	229	255	6		
3	C2	172	Total	C	N	O	S	0	0
			1278	788	229	255	6		
3	E2	173	Total	C	N	O	S	0	0
			1286	793	230	256	7		
3	G2	173	Total	C	N	O	S	0	0
			1286	793	230	256	7		
3	I2	173	Total	C	N	O	S	0	0
			1286	793	230	256	7		
3	K2	172	Total	C	N	O	S	0	0
			1278	788	229	255	6		
3	M2	172	Total	C	N	O	S	0	0
			1278	788	229	255	6		
3	P2	172	Total	C	N	O	S	0	0
			1278	788	229	255	6		
3	R2	172	Total	C	N	O	S	0	0
			1278	788	229	255	6		
3	T2	172	Total	C	N	O	S	0	0
			1278	788	229	255	6		
3	V2	172	Total	C	N	O	S	0	0
			1278	788	229	255	6		
3	X2	172	Total	C	N	O	S	0	0
			1278	788	229	255	6		
3	Z2	172	Total	C	N	O	S	0	0
			1278	788	229	255	6		
3	C3	172	Total	C	N	O	S	0	0
			1278	788	229	255	6		
3	E3	173	Total	C	N	O	S	0	0
			1286	793	230	256	7		
3	G3	173	Total	C	N	O	S	0	0
			1286	793	230	256	7		
3	I3	173	Total	C	N	O	S	0	0
			1286	793	230	256	7		
3	K3	172	Total	C	N	O	S	0	0
			1278	788	229	255	6		
3	M3	172	Total	C	N	O	S	0	0
			1278	788	229	255	6		
3	C4	172	Total	C	N	O	S	0	0
			1278	788	229	255	6		
3	E4	172	Total	C	N	O	S	0	0
			1278	788	229	255	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	G4	172	1278	788	229	255	6	0	0
3	I4	173	1286	793	230	256	7	0	0
3	K4	172	1278	788	229	255	6	0	0
3	M4	172	1278	788	229	255	6	0	0
3	P4	172	1278	788	229	255	6	0	0
3	R4	172	1278	788	229	255	6	0	0
3	T4	172	1278	788	229	255	6	0	0
3	V4	172	1278	788	229	255	6	0	0
3	X4	172	1278	788	229	255	6	0	0
3	Z4	172	1278	788	229	255	6	0	0
3	C5	172	1278	788	229	255	6	0	0
3	E5	172	1278	788	229	255	6	0	0
3	G5	172	1278	788	229	255	6	0	0
3	I5	172	1278	788	229	255	6	0	0
3	K5	172	1278	788	229	255	6	0	0
3	M5	172	1278	788	229	255	6	0	0
3	P5	172	1278	788	229	255	6	0	0
3	R5	172	1278	788	229	255	6	0	0
3	T5	172	1278	788	229	255	6	0	0
3	V5	172	1278	788	229	255	6	0	0
3	X5	172	1278	788	229	255	6	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	Z5	172	1278	788	229	255	6	0	0
3	C6	172	1278	788	229	255	6	0	0
3	E6	173	1286	793	230	256	7	0	0
3	G6	173	1286	793	230	256	7	0	0
3	I6	173	1286	793	230	256	7	0	0
3	K6	172	1278	788	229	255	6	0	0
3	M6	172	1278	788	229	255	6	0	0
3	P6	172	1278	788	229	255	6	0	0
3	R6	172	1278	788	229	255	6	0	0
3	T6	172	1278	788	229	255	6	0	0
3	V6	172	1278	788	229	255	6	0	0
3	X6	172	1278	788	229	255	6	0	0
3	Z6	172	1278	788	229	255	6	0	0
3	C7	172	1278	788	229	255	6	0	0
3	E7	173	1286	793	230	256	7	0	0
3	G7	173	1286	793	230	256	7	0	0
3	I7	173	1286	793	230	256	7	0	0
3	K7	172	1278	788	229	255	6	0	0
3	M7	172	1278	788	229	255	6	0	0
3	CA	172	1278	788	229	255	6	0	0
3	EA	172	1278	788	229	255	6	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace	
3	GA	172	Total 1278	C 788	N 229	O 255	S 6	0	0
3	IA	172	Total 1278	C 788	N 229	O 255	S 6	0	0
3	KA	172	Total 1278	C 788	N 229	O 255	S 6	0	0
3	MA	172	Total 1278	C 788	N 229	O 255	S 6	0	0
3	PA	172	Total 1278	C 788	N 229	O 255	S 6	0	0
3	RA	172	Total 1278	C 788	N 229	O 255	S 6	0	0
3	TA	172	Total 1278	C 788	N 229	O 255	S 6	0	0
3	VA	172	Total 1278	C 788	N 229	O 255	S 6	0	0
3	XA	172	Total 1278	C 788	N 229	O 255	S 6	0	0
3	ZA	172	Total 1278	C 788	N 229	O 255	S 6	0	0

- Molecule 4 is a protein called Phycobilisome 32.1 kDa linker polypeptide, phycocyanin-associated, rod.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	N1	284	Total 2265	C 1425	N 407	O 433	0	0
4	N2	284	Total 2265	C 1425	N 407	O 433	0	0
4	N3	57	Total 444	C 278	N 83	O 83	0	0
4	N4	284	Total 2265	C 1425	N 407	O 433	0	0
4	N5	284	Total 2265	C 1425	N 407	O 433	0	0
4	N6	284	Total 2265	C 1425	N 407	O 433	0	0
4	N7	57	Total 444	C 278	N 83	O 83	0	0
4	NA	284	Total 2265	C 1425	N 407	O 433	0	0

- Molecule 5 is a protein called Phycobilisome rod-core linker polypeptide CpcG4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A2	249	Total	C	N	O	S	0	0
			2038	1285	364	388	1		
5	A5	237	Total	C	N	O	S	0	0
			1944	1228	349	366	1		
5	A6	249	Total	C	N	O	S	0	0
			2038	1285	364	388	1		
5	AA	237	Total	C	N	O	S	0	0
			1944	1228	349	366	1		

- Molecule 6 is a protein called Phycobilisome rod-core linker polypeptide CpcG1.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	A3	138	Total	C	N	O	0	0
			1127	710	203	214		
6	A7	138	Total	C	N	O	0	0
			1127	710	203	214		

- Molecule 7 is a protein called Allophycocyanin subunit alpha 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A8	159	Total	C	N	O	S	0	0
			1204	754	210	237	3		
7	C8	159	Total	C	N	O	S	0	0
			1204	754	210	237	3		
7	E8	159	Total	C	N	O	S	0	0
			1204	754	210	237	3		
7	H8	159	Total	C	N	O	S	0	0
			1204	754	210	237	3		
7	J8	159	Total	C	N	O	S	0	0
			1204	754	210	237	3		
7	L8	159	Total	C	N	O	S	0	0
			1204	754	210	237	3		
7	O8	159	Total	C	N	O	S	0	0
			1204	754	210	237	3		
7	Q8	159	Total	C	N	O	S	0	0
			1204	754	210	237	3		
7	S8	159	Total	C	N	O	S	0	0
			1204	754	210	237	3		
7	V8	159	Total	C	N	O	S	0	0
			1204	754	210	237	3		
7	X8	159	Total	C	N	O	S	0	0
			1204	754	210	237	3		
7	Z8	159	Total	C	N	O	S	0	0
			1204	754	210	237	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
7	c8	159	Total	C	N	O	S	0	0
			1204	754	210	237	3		
7	e8	159	Total	C	N	O	S	0	0
			1204	754	210	237	3		
7	g8	159	Total	C	N	O	S	0	0
			1204	754	210	237	3		
7	j8	159	Total	C	N	O	S	0	0
			1204	754	210	237	3		
7	l8	159	Total	C	N	O	S	0	0
			1204	754	210	237	3		
7	n8	159	Total	C	N	O	S	0	0
			1204	754	210	237	3		
7	p8	159	Total	C	N	O	S	0	0
			1204	754	210	237	3		
7	r8	159	Total	C	N	O	S	0	0
			1204	754	210	237	3		
7	t8	159	Total	C	N	O	S	0	0
			1204	754	210	237	3		
7	A9	159	Total	C	N	O	S	0	0
			1204	754	210	237	3		
7	C9	159	Total	C	N	O	S	0	0
			1204	754	210	237	3		
7	E9	159	Total	C	N	O	S	0	0
			1204	754	210	237	3		
7	G9	159	Total	C	N	O	S	0	0
			1204	754	210	237	3		
7	I9	159	Total	C	N	O	S	0	0
			1204	754	210	237	3		
7	K9	159	Total	C	N	O	S	0	0
			1204	754	210	237	3		
7	N9	159	Total	C	N	O	S	0	0
			1204	754	210	237	3		
7	P9	159	Total	C	N	O	S	0	0
			1204	754	210	237	3		
7	R9	159	Total	C	N	O	S	0	0
			1204	754	210	237	3		
7	T9	159	Total	C	N	O	S	0	0
			1204	754	210	237	3		
7	X9	159	Total	C	N	O	S	0	0
			1204	754	210	237	3		
7	Z9	159	Total	C	N	O	S	0	0
			1204	754	210	237	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
7	b9	159	Total	C	N	O	S	0	0
			1204	754	210	237	3		
7	d9	159	Total	C	N	O	S	0	0
			1204	754	210	237	3		
7	f9	159	Total	C	N	O	S	0	0
			1204	754	210	237	3		
7	i9	159	Total	C	N	O	S	0	0
			1204	754	210	237	3		
7	k9	159	Total	C	N	O	S	0	0
			1204	754	210	237	3		
7	o9	159	Total	C	N	O	S	0	0
			1204	754	210	237	3		
7	q9	159	Total	C	N	O	S	0	0
			1204	754	210	237	3		
7	s9	159	Total	C	N	O	S	0	0
			1204	754	210	237	3		
7	u9	159	Total	C	N	O	S	0	0
			1204	754	210	237	3		
7	w9	159	Total	C	N	O	S	0	0
			1204	754	210	237	3		
7	y9	159	Total	C	N	O	S	0	0
			1204	754	210	237	3		

- Molecule 8 is a protein called Allophycocyanin subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B8	160	Total	C	N	O	S	0	0
			1201	758	201	238	4		
8	D8	160	Total	C	N	O	S	0	0
			1201	758	201	238	4		
8	F8	160	Total	C	N	O	S	0	0
			1201	758	201	238	4		
8	I8	160	Total	C	N	O	S	0	0
			1201	758	201	238	4		
8	K8	160	Total	C	N	O	S	0	0
			1201	758	201	238	4		
8	M8	160	Total	C	N	O	S	0	0
			1201	758	201	238	4		
8	P8	159	Total	C	N	O	S	0	0
			1192	753	199	236	4		
8	R8	160	Total	C	N	O	S	0	0
			1201	758	201	238	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
8	T8	160	Total 1201	C 758	N 201	O 238	S 4	0	0
8	W8	160	Total 1201	C 758	N 201	O 238	S 4	0	0
8	Y8	160	Total 1201	C 758	N 201	O 238	S 4	0	0
8	a8	160	Total 1201	C 758	N 201	O 238	S 4	0	0
8	d8	160	Total 1201	C 758	N 201	O 238	S 4	0	0
8	f8	160	Total 1201	C 758	N 201	O 238	S 4	0	0
8	h8	160	Total 1201	C 758	N 201	O 238	S 4	0	0
8	k8	160	Total 1201	C 758	N 201	O 238	S 4	0	0
8	m8	160	Total 1201	C 758	N 201	O 238	S 4	0	0
8	o8	159	Total 1192	C 753	N 199	O 236	S 4	0	0
8	q8	159	Total 1192	C 753	N 199	O 236	S 4	0	0
8	s8	160	Total 1201	C 758	N 201	O 238	S 4	0	0
8	u8	160	Total 1201	C 758	N 201	O 238	S 4	0	0
8	B9	160	Total 1201	C 758	N 201	O 238	S 4	0	0
8	D9	160	Total 1201	C 758	N 201	O 238	S 4	0	0
8	F9	160	Total 1201	C 758	N 201	O 238	S 4	0	0
8	H9	160	Total 1201	C 758	N 201	O 238	S 4	0	0
8	J9	160	Total 1201	C 758	N 201	O 238	S 4	0	0
8	L9	160	Total 1201	C 758	N 201	O 238	S 4	0	0
8	M9	160	Total 1201	C 758	N 201	O 238	S 4	0	0
8	O9	160	Total 1201	C 758	N 201	O 238	S 4	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
8	S9	160	Total	C	N	O	S	0	0
			1201	758	201	238	4		
8	U9	160	Total	C	N	O	S	0	0
			1201	758	201	238	4		
8	W9	160	Total	C	N	O	S	0	0
			1201	758	201	238	4		
8	Y9	160	Total	C	N	O	S	0	0
			1201	758	201	238	4		
8	a9	160	Total	C	N	O	S	0	0
			1201	758	201	238	4		
8	c9	160	Total	C	N	O	S	0	0
			1201	758	201	238	4		
8	e9	160	Total	C	N	O	S	0	0
			1201	758	201	238	4		
8	h9	160	Total	C	N	O	S	0	0
			1201	758	201	238	4		
8	j9	160	Total	C	N	O	S	0	0
			1201	758	201	238	4		
8	l9	160	Total	C	N	O	S	0	0
			1201	758	201	238	4		
8	n9	160	Total	C	N	O	S	0	0
			1201	758	201	238	4		
8	p9	160	Total	C	N	O	S	0	0
			1201	758	201	238	4		
8	r9	160	Total	C	N	O	S	0	0
			1201	758	201	238	4		
8	t9	160	Total	C	N	O	S	0	0
			1201	758	201	238	4		
8	v9	160	Total	C	N	O	S	0	0
			1201	758	201	238	4		
8	x9	160	Total	C	N	O	S	0	0
			1201	758	201	238	4		
8	z9	160	Total	C	N	O	S	0	0
			1201	758	201	238	4		

- Molecule 9 is a protein called Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	G8	65	Total	C	N	O	0	0
			529	337	99	93		
9	N8	65	Total	C	N	O	0	0
			529	337	99	93		

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Mol	Chain	Residues	Atoms				AltConf	Trace
9	U8	65	Total	C	N	O	0	0
			529	337	99	93		
9	b8	65	Total	C	N	O	0	0
			529	337	99	93		
9	i8	65	Total	C	N	O	0	0
			529	337	99	93		
9	29	65	Total	C	N	O	0	0
			529	337	99	93		
9	39	65	Total	C	N	O	0	0
			529	337	99	93		
9	49	65	Total	C	N	O	0	0
			529	337	99	93		

- Molecule 10 is a protein called Phycobiliprotein ApcE.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	09	1049	Total	C	N	O	S	0	0
			8352	5315	1471	1558	8		
10	19	1043	Total	C	N	O	S	0	0
			8299	5285	1459	1547	8		

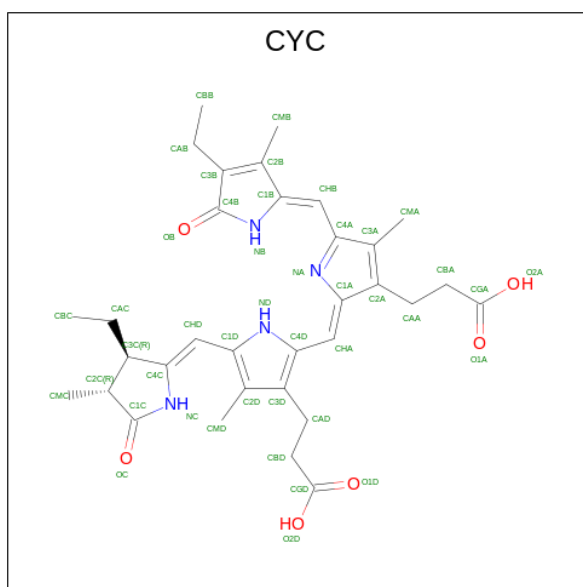
- Molecule 11 is a protein called Allophycocyanin subunit beta-18.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Q9	168	Total	C	N	O	S	0	0
			1304	817	232	253	2		
11	g9	169	Total	C	N	O	S	0	0
			1312	822	233	254	3		

- Molecule 12 is a protein called Allophycocyanin subunit alpha-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	V9	160	Total	C	N	O	S	0	0
			1244	793	210	237	4		
12	m9	160	Total	C	N	O	S	0	0
			1244	793	210	237	4		

- Molecule 13 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	
13	B1	1	Total	C	N	O	0
			43	33	4	6	
13	C1	1	Total	C	N	O	0
			86	66	8	12	
13	C1	1	Total	C	N	O	0
			86	66	8	12	
13	D1	1	Total	C	N	O	0
			43	33	4	6	
13	E1	1	Total	C	N	O	0
			86	66	8	12	
13	E1	1	Total	C	N	O	0
			86	66	8	12	
13	F1	1	Total	C	N	O	0
			43	33	4	6	
13	G1	1	Total	C	N	O	0
			86	66	8	12	
13	G1	1	Total	C	N	O	0
			86	66	8	12	
13	H1	1	Total	C	N	O	0
			43	33	4	6	
13	I1	1	Total	C	N	O	0
			86	66	8	12	
13	I1	1	Total	C	N	O	0
			86	66	8	12	
13	J1	1	Total	C	N	O	0
			43	33	4	6	
13	K1	1	Total	C	N	O	0
			86	66	8	12	

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
13	K1	1	Total 86	C 66	N 8	O 12	0
13	L1	1	Total 43	C 33	N 4	O 6	0
13	M1	1	Total 86	C 66	N 8	O 12	0
13	M1	1	Total 86	C 66	N 8	O 12	0
13	O1	1	Total 43	C 33	N 4	O 6	0
13	P1	1	Total 86	C 66	N 8	O 12	0
13	P1	1	Total 86	C 66	N 8	O 12	0
13	Q1	1	Total 86	C 66	N 8	O 12	0
13	Q1	1	Total 86	C 66	N 8	O 12	0
13	R1	1	Total 43	C 33	N 4	O 6	0
13	S1	1	Total 43	C 33	N 4	O 6	0
13	T1	1	Total 86	C 66	N 8	O 12	0
13	T1	1	Total 86	C 66	N 8	O 12	0
13	U1	1	Total 43	C 33	N 4	O 6	0
13	V1	1	Total 86	C 66	N 8	O 12	0
13	V1	1	Total 86	C 66	N 8	O 12	0
13	W1	1	Total 43	C 33	N 4	O 6	0
13	X1	1	Total 86	C 66	N 8	O 12	0
13	X1	1	Total 86	C 66	N 8	O 12	0
13	Y1	1	Total 43	C 33	N 4	O 6	0
13	Z1	1	Total 86	C 66	N 8	O 12	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
13	Z1	1	Total 86	C 66	N 8	O 12	0
13	B2	1	Total 43	C 33	N 4	O 6	0
13	C2	1	Total 86	C 66	N 8	O 12	0
13	C2	1	Total 86	C 66	N 8	O 12	0
13	D2	1	Total 43	C 33	N 4	O 6	0
13	E2	1	Total 86	C 66	N 8	O 12	0
13	E2	1	Total 86	C 66	N 8	O 12	0
13	F2	1	Total 43	C 33	N 4	O 6	0
13	G2	1	Total 86	C 66	N 8	O 12	0
13	G2	1	Total 86	C 66	N 8	O 12	0
13	H2	1	Total 43	C 33	N 4	O 6	0
13	I2	1	Total 86	C 66	N 8	O 12	0
13	I2	1	Total 86	C 66	N 8	O 12	0
13	J2	1	Total 43	C 33	N 4	O 6	0
13	K2	1	Total 86	C 66	N 8	O 12	0
13	K2	1	Total 86	C 66	N 8	O 12	0
13	L2	1	Total 43	C 33	N 4	O 6	0
13	M2	1	Total 43	C 33	N 4	O 6	0
13	N2	1	Total 86	C 66	N 8	O 12	0
13	N2	1	Total 86	C 66	N 8	O 12	0
13	O2	1	Total 43	C 33	N 4	O 6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
13	P2	1	43	33	4	6	0
13	Q2	1	43	33	4	6	0
13	R2	1	43	33	4	6	0
13	S2	1	43	33	4	6	0
13	T2	1	43	33	4	6	0
13	U2	1	86	66	8	12	0
13	U2	1	86	66	8	12	0
13	V2	1	86	66	8	12	0
13	V2	1	86	66	8	12	0
13	W2	1	129	99	12	18	0
13	W2	1	129	99	12	18	0
13	W2	1	129	99	12	18	0
13	X2	1	43	33	4	6	0
13	Y2	1	43	33	4	6	0
13	Z2	1	86	66	8	12	0
13	Z2	1	86	66	8	12	0
13	A3	1	43	33	4	6	0
13	B3	1	43	33	4	6	0
13	C3	1	43	33	4	6	0
13	D3	1	43	33	4	6	0
13	E3	1	86	66	8	12	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
13	E3	1	86	66	8	12	0
13	F3	1	43	33	4	6	0
13	G3	1	86	66	8	12	0
13	G3	1	86	66	8	12	0
13	H3	1	43	33	4	6	0
13	I3	1	86	66	8	12	0
13	I3	1	86	66	8	12	0
13	J3	1	43	33	4	6	0
13	K3	1	86	66	8	12	0
13	K3	1	86	66	8	12	0
13	L3	1	43	33	4	6	0
13	M3	1	43	33	4	6	0
13	N3	1	43	33	4	6	0
13	B4	1	43	33	4	6	0
13	C4	1	86	66	8	12	0
13	C4	1	86	66	8	12	0
13	D4	1	43	33	4	6	0
13	E4	1	86	66	8	12	0
13	E4	1	86	66	8	12	0
13	F4	1	43	33	4	6	0
13	G4	1	86	66	8	12	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
13	G4	1	Total 86	C 66	N 8	O 12	0
13	H4	1	Total 43	C 33	N 4	O 6	0
13	I4	1	Total 86	C 66	N 8	O 12	0
13	I4	1	Total 86	C 66	N 8	O 12	0
13	J4	1	Total 43	C 33	N 4	O 6	0
13	K4	1	Total 86	C 66	N 8	O 12	0
13	K4	1	Total 86	C 66	N 8	O 12	0
13	L4	1	Total 43	C 33	N 4	O 6	0
13	M4	1	Total 86	C 66	N 8	O 12	0
13	M4	1	Total 86	C 66	N 8	O 12	0
13	O4	1	Total 43	C 33	N 4	O 6	0
13	P4	1	Total 86	C 66	N 8	O 12	0
13	P4	1	Total 86	C 66	N 8	O 12	0
13	Q4	1	Total 86	C 66	N 8	O 12	0
13	Q4	1	Total 86	C 66	N 8	O 12	0
13	R4	1	Total 43	C 33	N 4	O 6	0
13	S4	1	Total 43	C 33	N 4	O 6	0
13	T4	1	Total 86	C 66	N 8	O 12	0
13	T4	1	Total 86	C 66	N 8	O 12	0
13	U4	1	Total 43	C 33	N 4	O 6	0
13	V4	1	Total 86	C 66	N 8	O 12	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
13	V4	1	86	66	8	12	0
13	W4	1	43	33	4	6	0
13	X4	1	86	66	8	12	0
13	X4	1	86	66	8	12	0
13	Y4	1	43	33	4	6	0
13	Z4	1	86	66	8	12	0
13	Z4	1	86	66	8	12	0
13	A5	1	172	132	16	24	0
13	A5	1	172	132	16	24	0
13	A5	1	172	132	16	24	0
13	A5	1	172	132	16	24	0
13	B5	1	43	33	4	6	0
13	C5	1	43	33	4	6	0
13	D5	1	43	33	4	6	0
13	E5	1	86	66	8	12	0
13	E5	1	86	66	8	12	0
13	G5	1	43	33	4	6	0
13	I5	1	86	66	8	12	0
13	I5	1	86	66	8	12	0
13	J5	1	43	33	4	6	0
13	K5	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
13	L5	1	43	33	4	6	0
13	M5	1	129	99	12	18	0
13	M5	1	129	99	12	18	0
13	M5	1	129	99	12	18	0
13	N5	1	43	33	4	6	0
13	O5	1	43	33	4	6	0
13	P5	1	129	99	12	18	0
13	P5	1	129	99	12	18	0
13	P5	1	129	99	12	18	0
13	R5	1	43	33	4	6	0
13	S5	1	43	33	4	6	0
13	T5	1	86	66	8	12	0
13	T5	1	86	66	8	12	0
13	U5	1	43	33	4	6	0
13	V5	1	86	66	8	12	0
13	V5	1	86	66	8	12	0
13	W5	1	43	33	4	6	0
13	X5	1	86	66	8	12	0
13	X5	1	86	66	8	12	0
13	Y5	1	43	33	4	6	0
13	Z5	1	86	66	8	12	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
13	Z5	1	Total 86	C 66	N 8	O 12	0
13	B6	1	Total 43	C 33	N 4	O 6	0
13	C6	1	Total 86	C 66	N 8	O 12	0
13	C6	1	Total 86	C 66	N 8	O 12	0
13	D6	1	Total 43	C 33	N 4	O 6	0
13	E6	1	Total 86	C 66	N 8	O 12	0
13	E6	1	Total 86	C 66	N 8	O 12	0
13	F6	1	Total 43	C 33	N 4	O 6	0
13	G6	1	Total 86	C 66	N 8	O 12	0
13	G6	1	Total 86	C 66	N 8	O 12	0
13	H6	1	Total 43	C 33	N 4	O 6	0
13	I6	1	Total 86	C 66	N 8	O 12	0
13	I6	1	Total 86	C 66	N 8	O 12	0
13	J6	1	Total 43	C 33	N 4	O 6	0
13	K6	1	Total 86	C 66	N 8	O 12	0
13	K6	1	Total 86	C 66	N 8	O 12	0
13	L6	1	Total 43	C 33	N 4	O 6	0
13	M6	1	Total 43	C 33	N 4	O 6	0
13	N6	1	Total 86	C 66	N 8	O 12	0
13	N6	1	Total 86	C 66	N 8	O 12	0
13	O6	1	Total 43	C 33	N 4	O 6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
13	P6	1	Total 43	C 33	N 4	O 6	0
13	Q6	1	Total 43	C 33	N 4	O 6	0
13	R6	1	Total 43	C 33	N 4	O 6	0
13	S6	1	Total 43	C 33	N 4	O 6	0
13	T6	1	Total 43	C 33	N 4	O 6	0
13	U6	1	Total 86	C 66	N 8	O 12	0
13	U6	1	Total 86	C 66	N 8	O 12	0
13	V6	1	Total 86	C 66	N 8	O 12	0
13	V6	1	Total 86	C 66	N 8	O 12	0
13	W6	1	Total 86	C 66	N 8	O 12	0
13	W6	1	Total 86	C 66	N 8	O 12	0
13	X6	1	Total 86	C 66	N 8	O 12	0
13	X6	1	Total 86	C 66	N 8	O 12	0
13	Y6	1	Total 43	C 33	N 4	O 6	0
13	Z6	1	Total 86	C 66	N 8	O 12	0
13	Z6	1	Total 86	C 66	N 8	O 12	0
13	A7	1	Total 43	C 33	N 4	O 6	0
13	B7	1	Total 43	C 33	N 4	O 6	0
13	C7	1	Total 43	C 33	N 4	O 6	0
13	D7	1	Total 43	C 33	N 4	O 6	0
13	E7	1	Total 86	C 66	N 8	O 12	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
13	E7	1	Total 86	C 66	N 8	O 12	0
13	F7	1	Total 43	C 33	N 4	O 6	0
13	G7	1	Total 86	C 66	N 8	O 12	0
13	G7	1	Total 86	C 66	N 8	O 12	0
13	H7	1	Total 43	C 33	N 4	O 6	0
13	I7	1	Total 86	C 66	N 8	O 12	0
13	I7	1	Total 86	C 66	N 8	O 12	0
13	J7	1	Total 43	C 33	N 4	O 6	0
13	K7	1	Total 86	C 66	N 8	O 12	0
13	K7	1	Total 86	C 66	N 8	O 12	0
13	L7	1	Total 43	C 33	N 4	O 6	0
13	M7	1	Total 43	C 33	N 4	O 6	0
13	N7	1	Total 43	C 33	N 4	O 6	0
13	A8	1	Total 43	C 33	N 4	O 6	0
13	B8	1	Total 43	C 33	N 4	O 6	0
13	C8	1	Total 43	C 33	N 4	O 6	0
13	D8	1	Total 43	C 33	N 4	O 6	0
13	E8	1	Total 43	C 33	N 4	O 6	0
13	F8	1	Total 43	C 33	N 4	O 6	0
13	H8	1	Total 43	C 33	N 4	O 6	0
13	I8	1	Total 43	C 33	N 4	O 6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
13	J8	1	43	33	4	6	0
13	K8	1	43	33	4	6	0
13	L8	1	43	33	4	6	0
13	M8	1	43	33	4	6	0
13	O8	1	43	33	4	6	0
13	P8	1	43	33	4	6	0
13	Q8	1	43	33	4	6	0
13	R8	1	43	33	4	6	0
13	S8	1	43	33	4	6	0
13	T8	1	43	33	4	6	0
13	V8	1	43	33	4	6	0
13	W8	1	43	33	4	6	0
13	X8	1	43	33	4	6	0
13	Y8	1	43	33	4	6	0
13	Z8	1	43	33	4	6	0
13	b8	1	43	33	4	6	0
13	c8	1	43	33	4	6	0
13	d8	1	43	33	4	6	0
13	e8	1	43	33	4	6	0
13	f8	1	43	33	4	6	0
13	g8	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
13	h8	1	43	33	4	6	0
13	j8	1	43	33	4	6	0
13	k8	1	43	33	4	6	0
13	l8	1	43	33	4	6	0
13	n8	1	43	33	4	6	0
13	o8	1	43	33	4	6	0
13	p8	1	43	33	4	6	0
13	q8	1	43	33	4	6	0
13	r8	1	43	33	4	6	0
13	s8	1	43	33	4	6	0
13	t8	1	43	33	4	6	0
13	09	1	129	99	12	18	0
13	09	1	129	99	12	18	0
13	09	1	129	99	12	18	0
13	19	1	215	165	20	30	0
13	19	1	215	165	20	30	0
13	19	1	215	165	20	30	0
13	19	1	215	165	20	30	0
13	19	1	215	165	20	30	0
13	29	1	43	33	4	6	0
13	39	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
13	A9	1	43	33	4	6	0
13	B9	1	43	33	4	6	0
13	C9	1	43	33	4	6	0
13	D9	1	43	33	4	6	0
13	E9	1	43	33	4	6	0
13	F9	1	43	33	4	6	0
13	G9	1	43	33	4	6	0
13	H9	1	43	33	4	6	0
13	I9	1	43	33	4	6	0
13	J9	1	43	33	4	6	0
13	K9	1	43	33	4	6	0
13	L9	1	43	33	4	6	0
13	N9	1	43	33	4	6	0
13	O9	1	43	33	4	6	0
13	P9	1	43	33	4	6	0
13	Q9	1	43	33	4	6	0
13	R9	1	43	33	4	6	0
13	S9	1	43	33	4	6	0
13	T9	1	43	33	4	6	0
13	U9	1	43	33	4	6	0
13	V9	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
13	X9	1	43	33	4	6	0
13	Z9	1	43	33	4	6	0
13	b9	1	43	33	4	6	0
13	c9	1	43	33	4	6	0
13	d9	1	43	33	4	6	0
13	e9	1	43	33	4	6	0
13	f9	1	43	33	4	6	0
13	g9	1	43	33	4	6	0
13	i9	1	43	33	4	6	0
13	j9	1	43	33	4	6	0
13	k9	1	43	33	4	6	0
13	l9	1	43	33	4	6	0
13	m9	1	43	33	4	6	0
13	o9	1	43	33	4	6	0
13	p9	1	43	33	4	6	0
13	q9	1	43	33	4	6	0
13	r9	1	43	33	4	6	0
13	s9	1	43	33	4	6	0
13	t9	1	43	33	4	6	0
13	u9	1	43	33	4	6	0
13	v9	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
13	w9	1	Total 43	C 33	N 4	O 6	0
13	x9	1	Total 43	C 33	N 4	O 6	0
13	y9	1	Total 43	C 33	N 4	O 6	0
13	z9	1	Total 43	C 33	N 4	O 6	0
13	AA	1	Total 172	C 132	N 16	O 24	0
13	AA	1	Total 172	C 132	N 16	O 24	0
13	AA	1	Total 172	C 132	N 16	O 24	0
13	AA	1	Total 172	C 132	N 16	O 24	0
13	CA	1	Total 43	C 33	N 4	O 6	0
13	DA	1	Total 43	C 33	N 4	O 6	0
13	EA	1	Total 86	C 66	N 8	O 12	0
13	EA	1	Total 86	C 66	N 8	O 12	0
13	GA	1	Total 86	C 66	N 8	O 12	0
13	GA	1	Total 86	C 66	N 8	O 12	0
13	IA	1	Total 86	C 66	N 8	O 12	0
13	IA	1	Total 86	C 66	N 8	O 12	0
13	JA	1	Total 43	C 33	N 4	O 6	0
13	KA	1	Total 43	C 33	N 4	O 6	0
13	LA	1	Total 43	C 33	N 4	O 6	0
13	MA	1	Total 129	C 99	N 12	O 18	0
13	MA	1	Total 129	C 99	N 12	O 18	0

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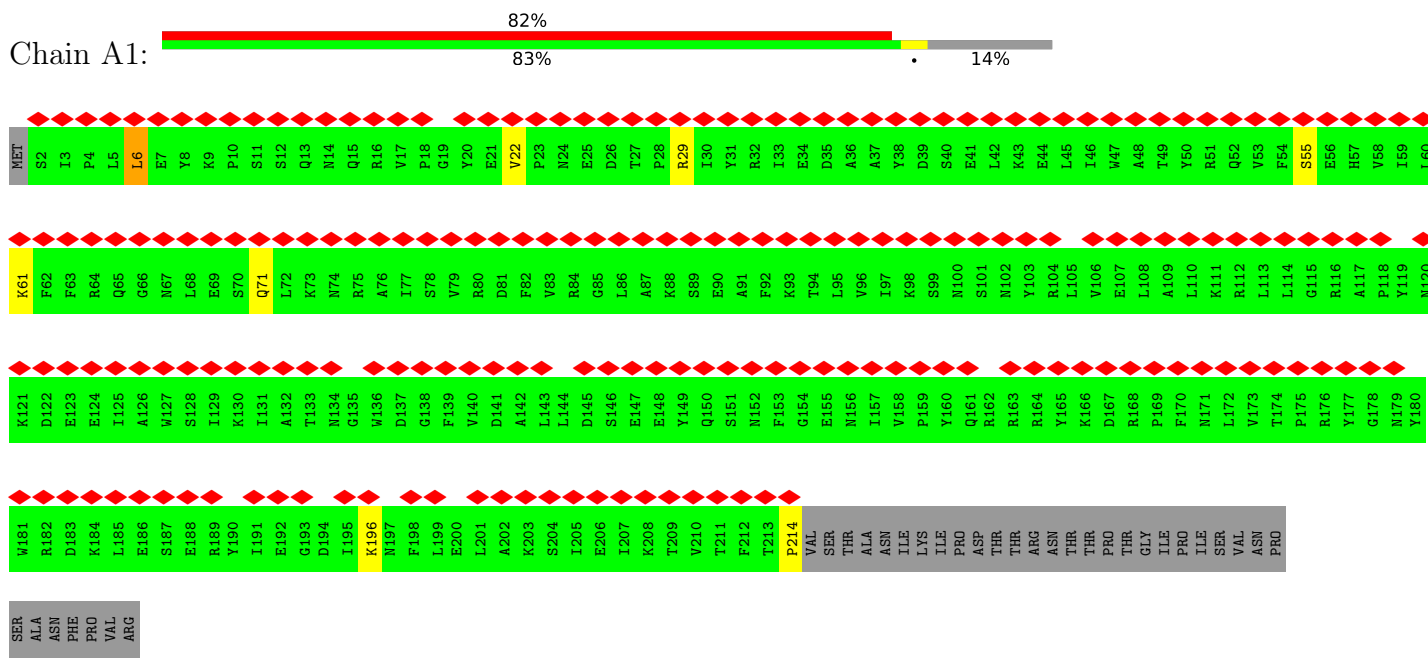
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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
13	MA	1	Total 129	C 99	N 12	O 18	0
13	NA	1	Total 43	C 33	N 4	O 6	0
13	OA	1	Total 43	C 33	N 4	O 6	0
13	PA	1	Total 129	C 99	N 12	O 18	0
13	PA	1	Total 129	C 99	N 12	O 18	0
13	PA	1	Total 129	C 99	N 12	O 18	0
13	RA	1	Total 43	C 33	N 4	O 6	0
13	SA	1	Total 43	C 33	N 4	O 6	0
13	TA	1	Total 86	C 66	N 8	O 12	0
13	TA	1	Total 86	C 66	N 8	O 12	0
13	UA	1	Total 43	C 33	N 4	O 6	0
13	VA	1	Total 86	C 66	N 8	O 12	0
13	VA	1	Total 86	C 66	N 8	O 12	0
13	WA	1	Total 43	C 33	N 4	O 6	0
13	XA	1	Total 86	C 66	N 8	O 12	0
13	XA	1	Total 86	C 66	N 8	O 12	0
13	YA	1	Total 43	C 33	N 4	O 6	0
13	ZA	1	Total 86	C 66	N 8	O 12	0
13	ZA	1	Total 86	C 66	N 8	O 12	0

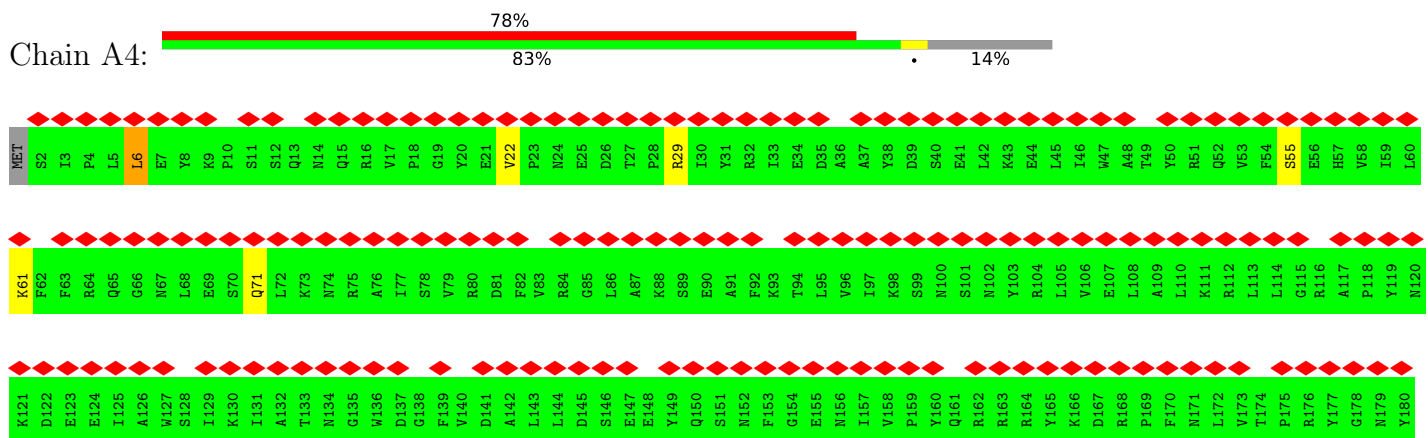
3 Residue-property plots [i](#)

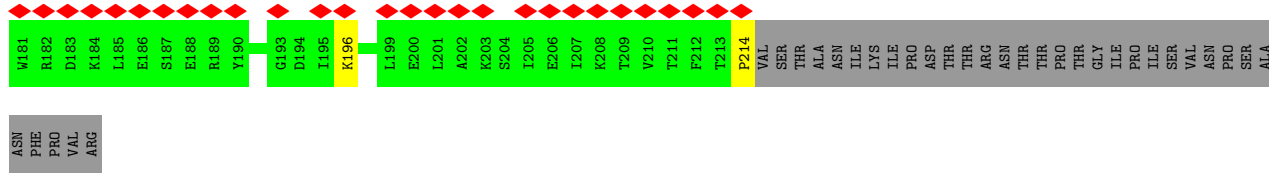
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Phycobilisome rod-core linker polypeptide CpcG2

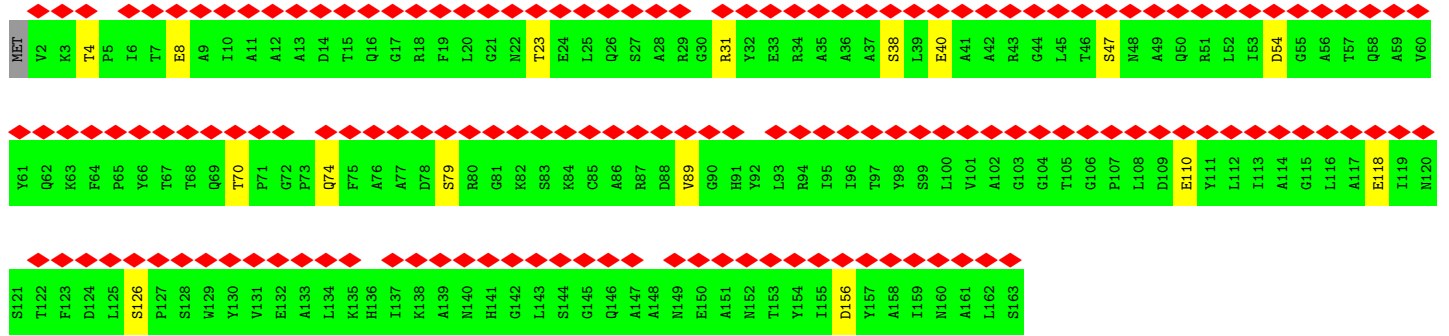
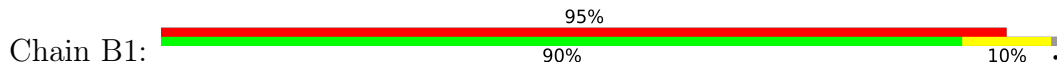


- Molecule 1: Phycobilisome rod-core linker polypeptide CpcG2

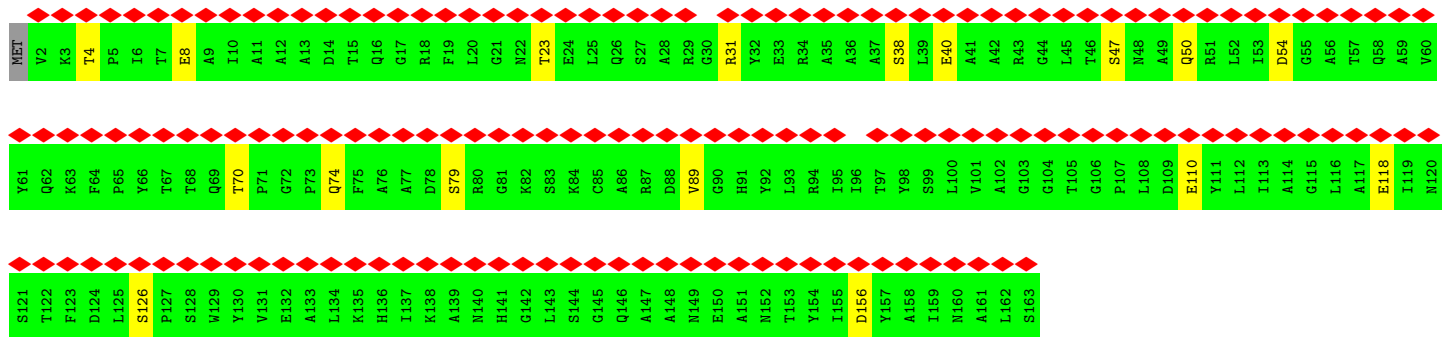
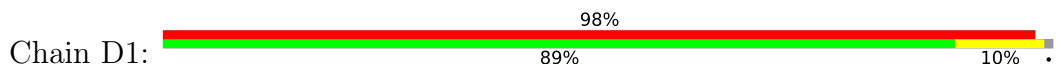




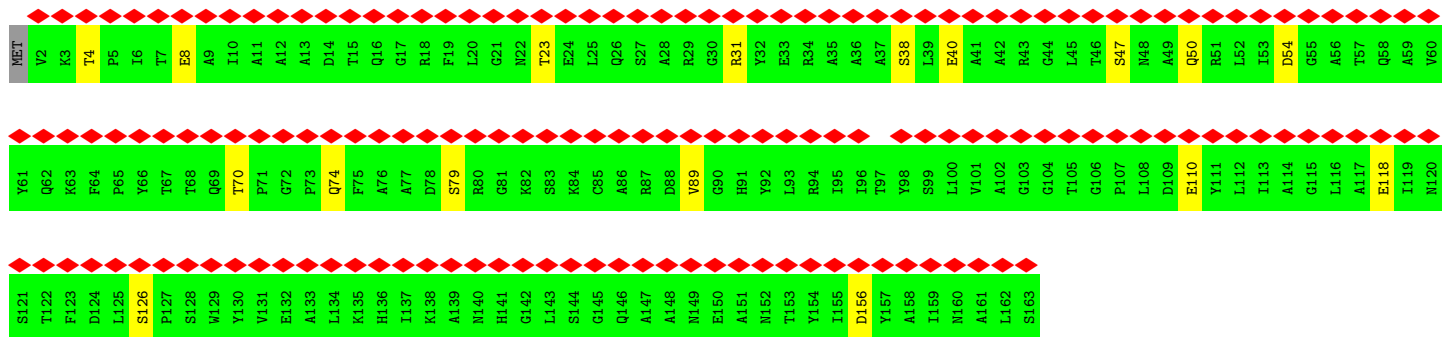
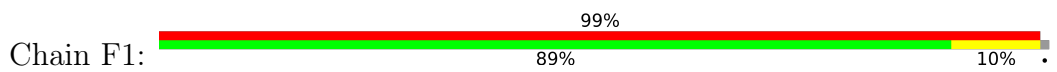
● Molecule 2: C-phycoerythrin alpha subunit



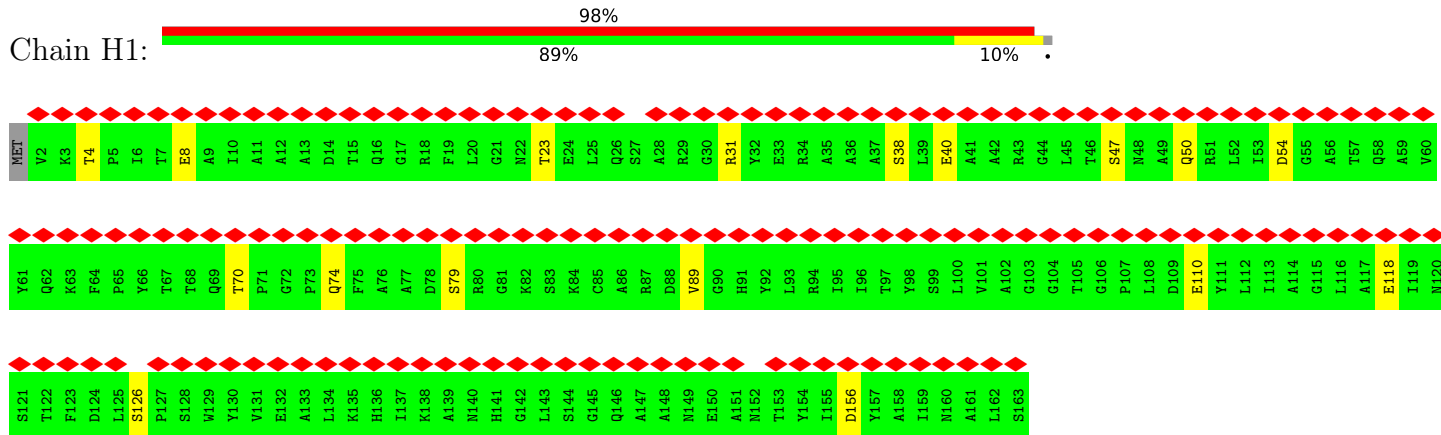
● Molecule 2: C-phycoerythrin alpha subunit



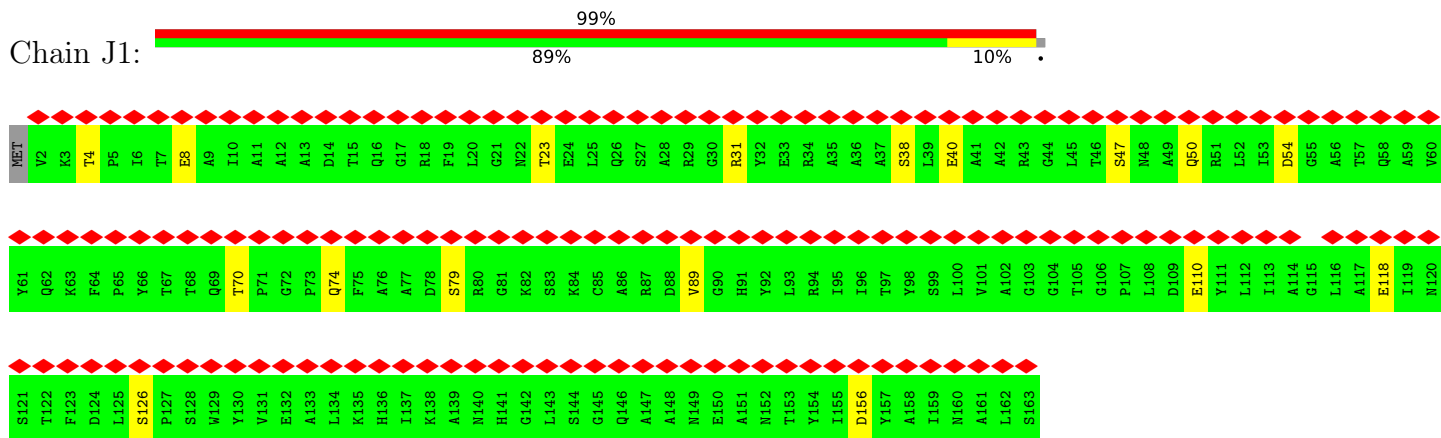
● Molecule 2: C-phycoerythrin alpha subunit



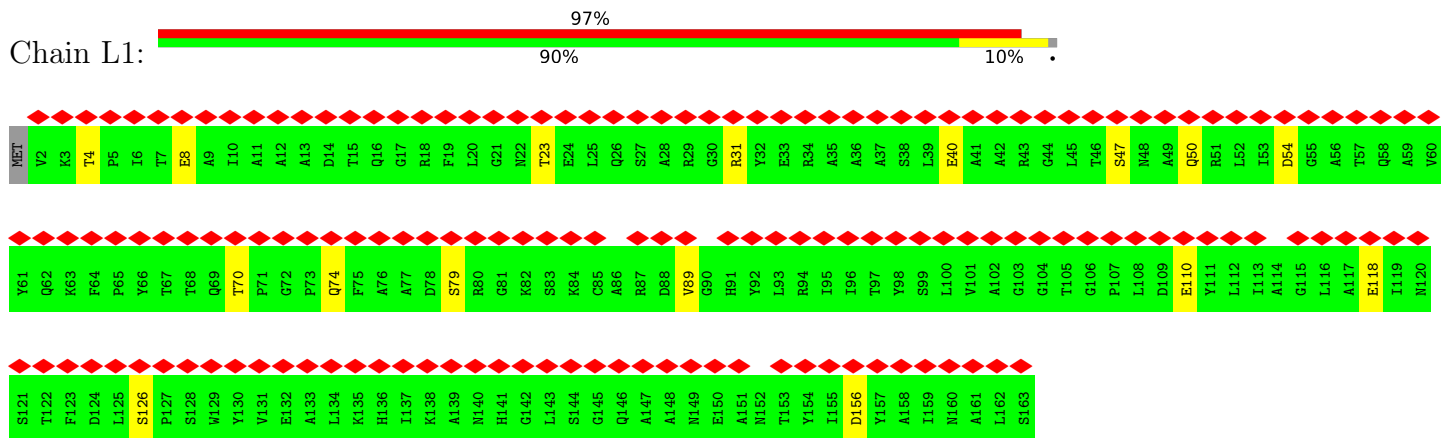
• Molecule 2: C-phycoerythrin alpha subunit



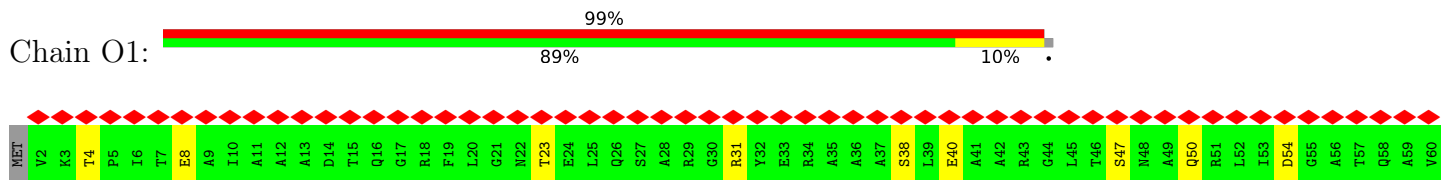
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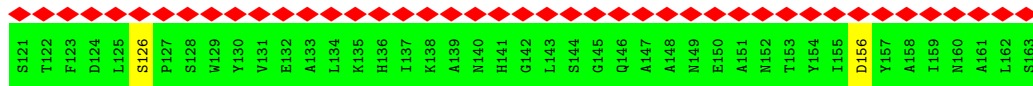
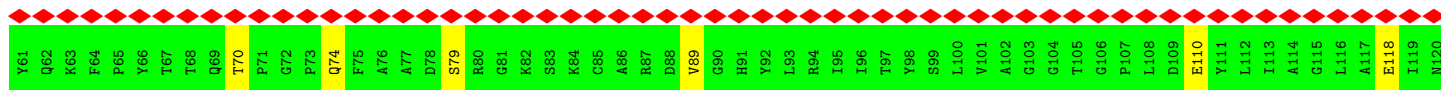


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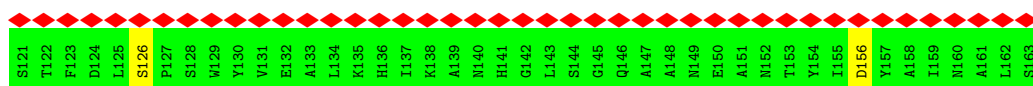
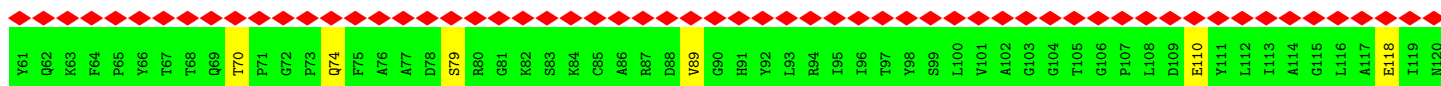
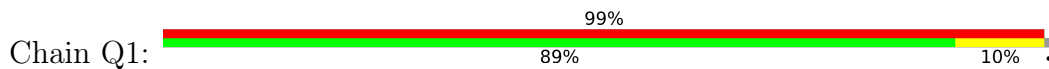


• Molecule 2: C-phycoerythrin alpha subunit

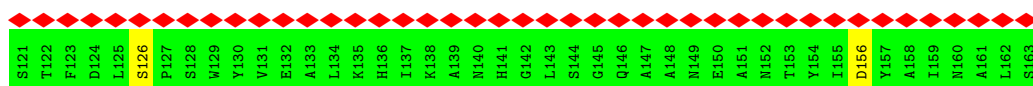
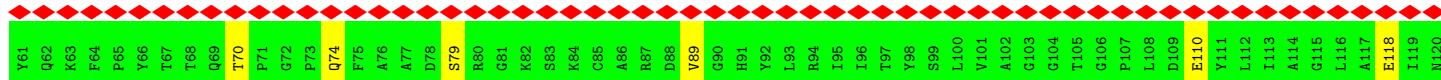
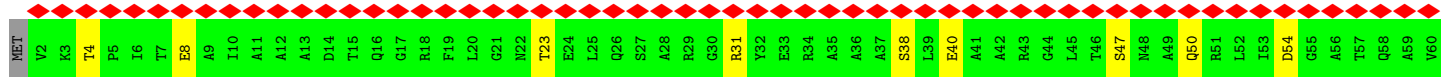
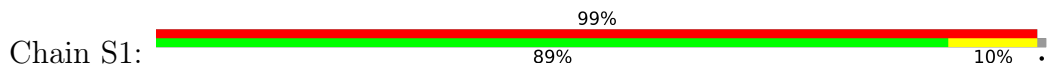




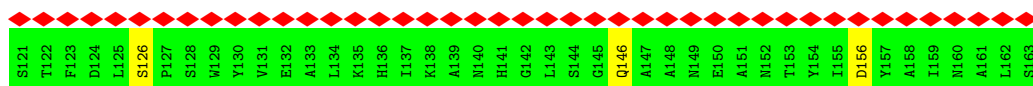
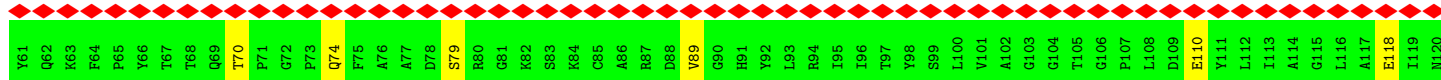
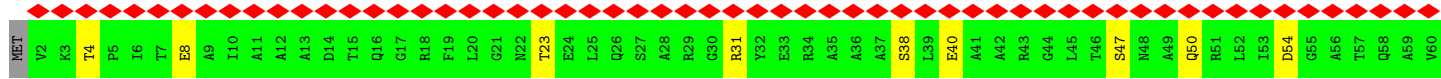
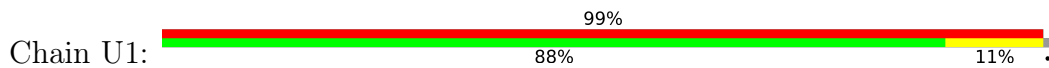
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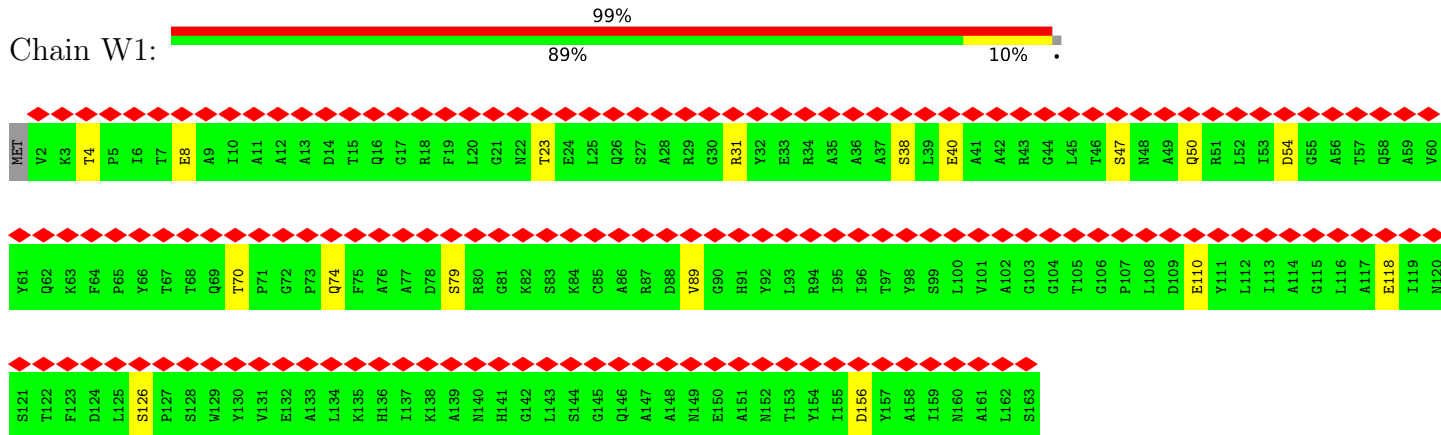
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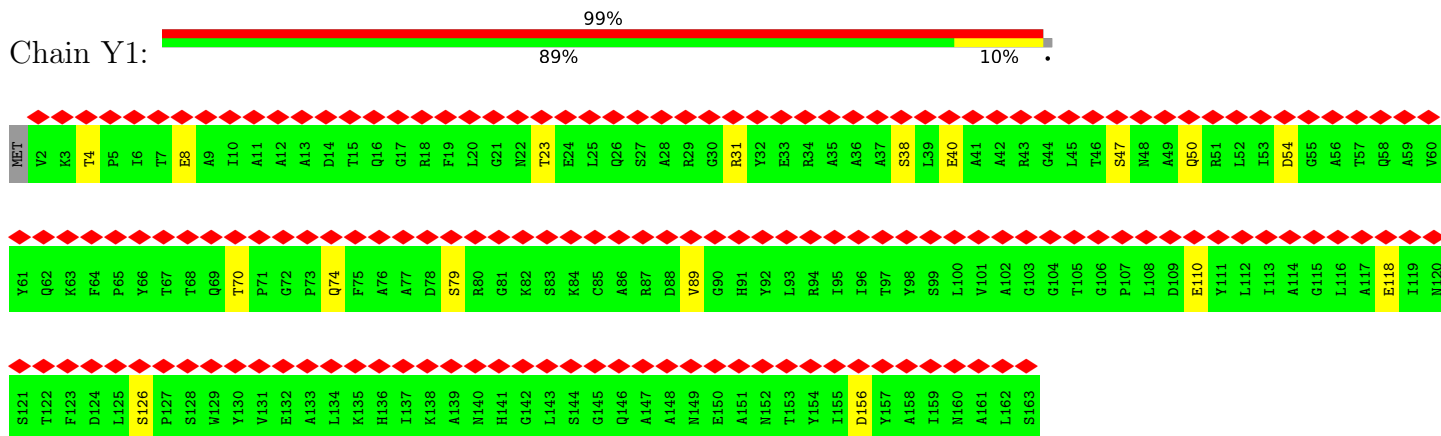
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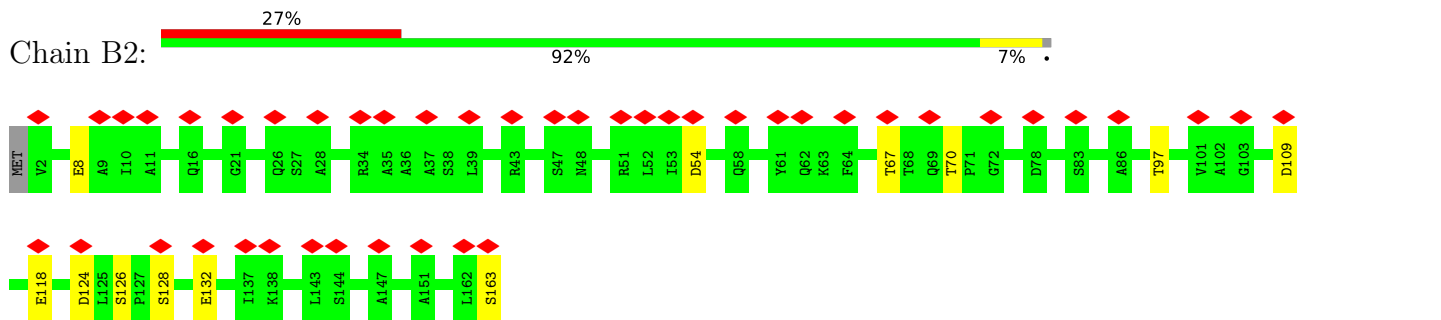
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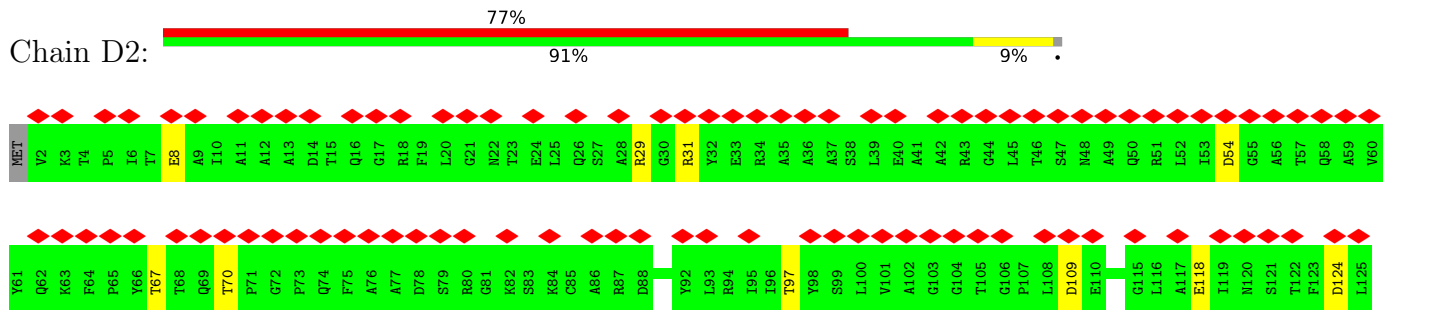
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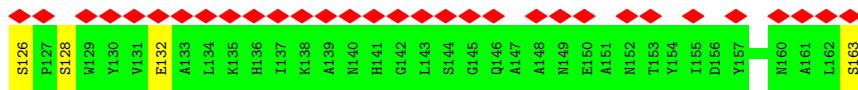


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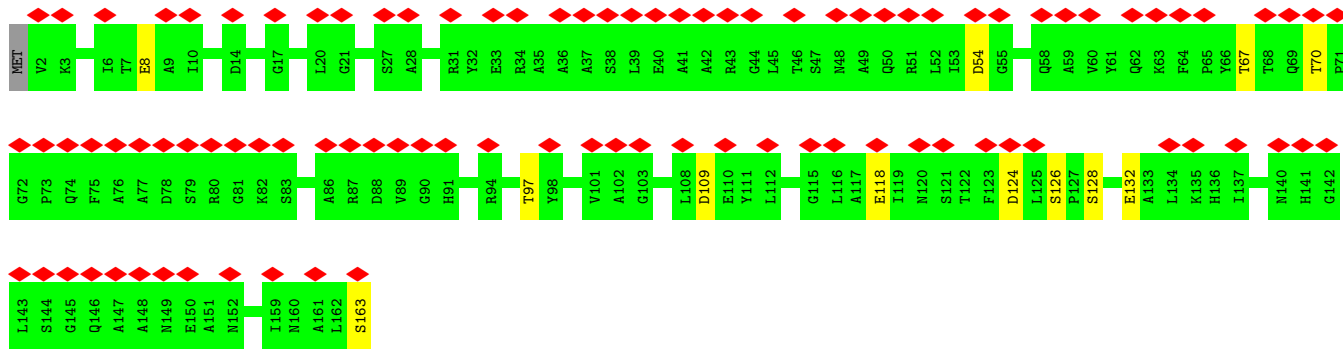
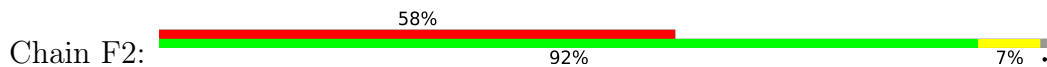


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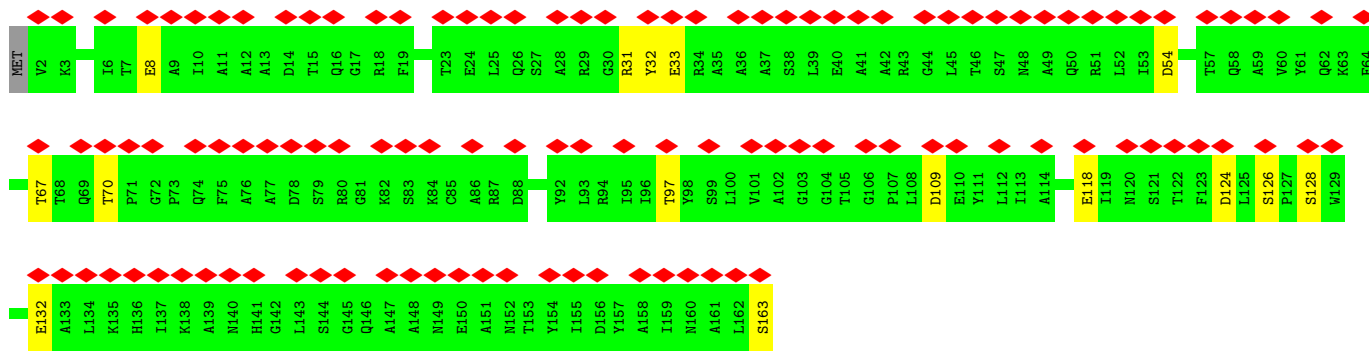
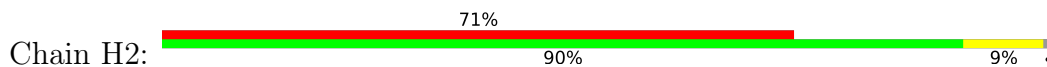




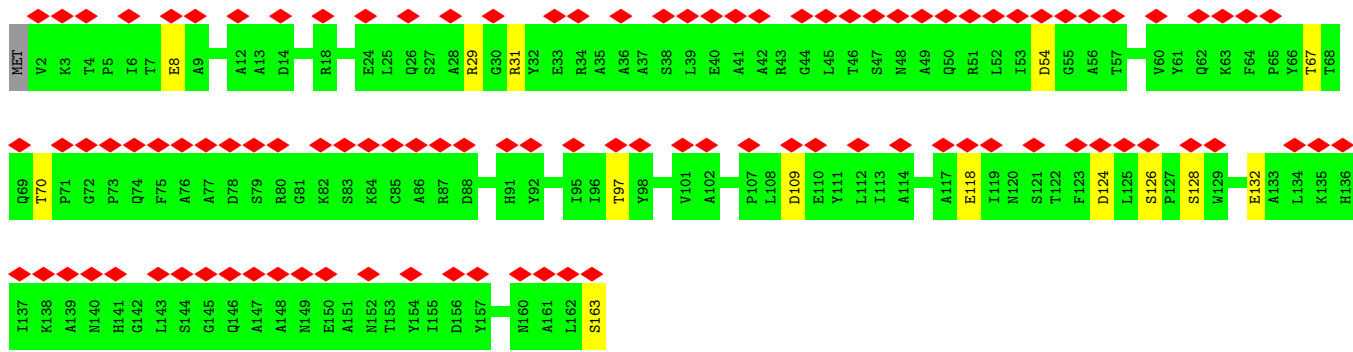
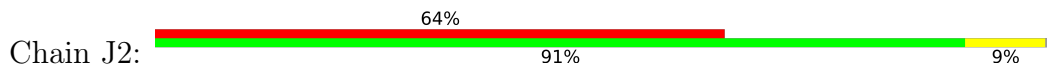
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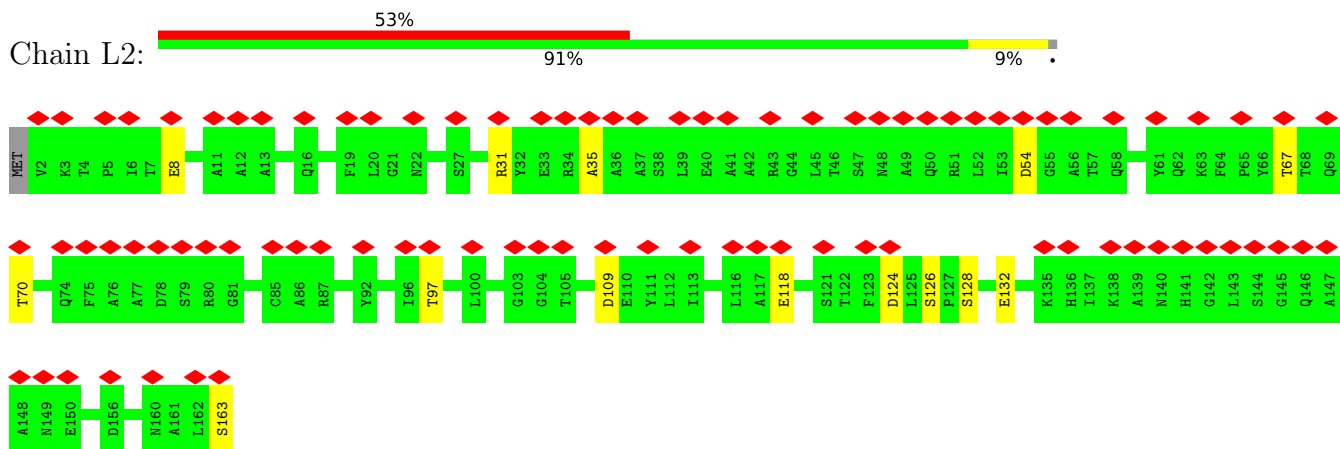
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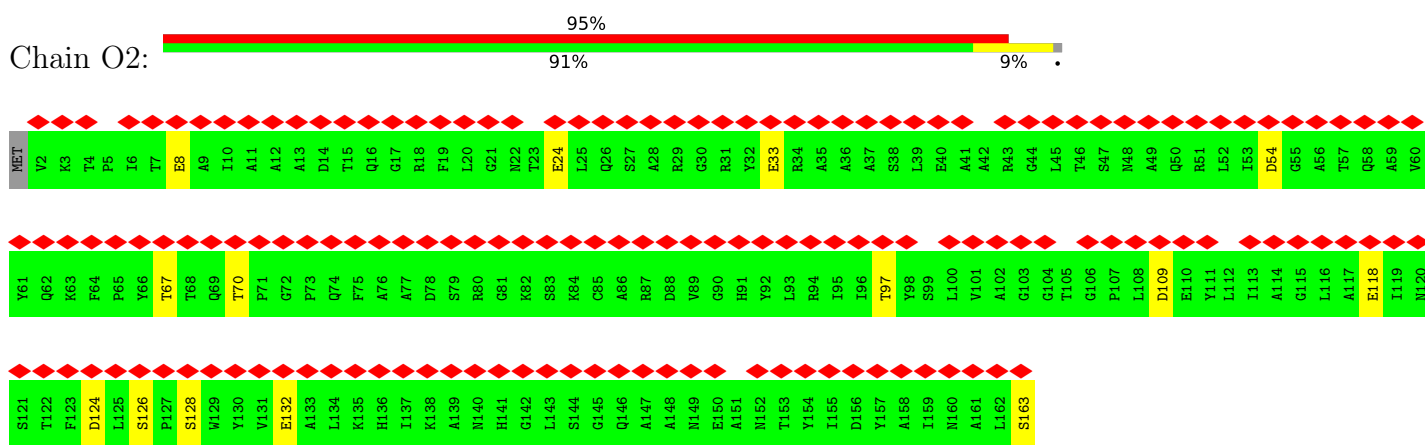
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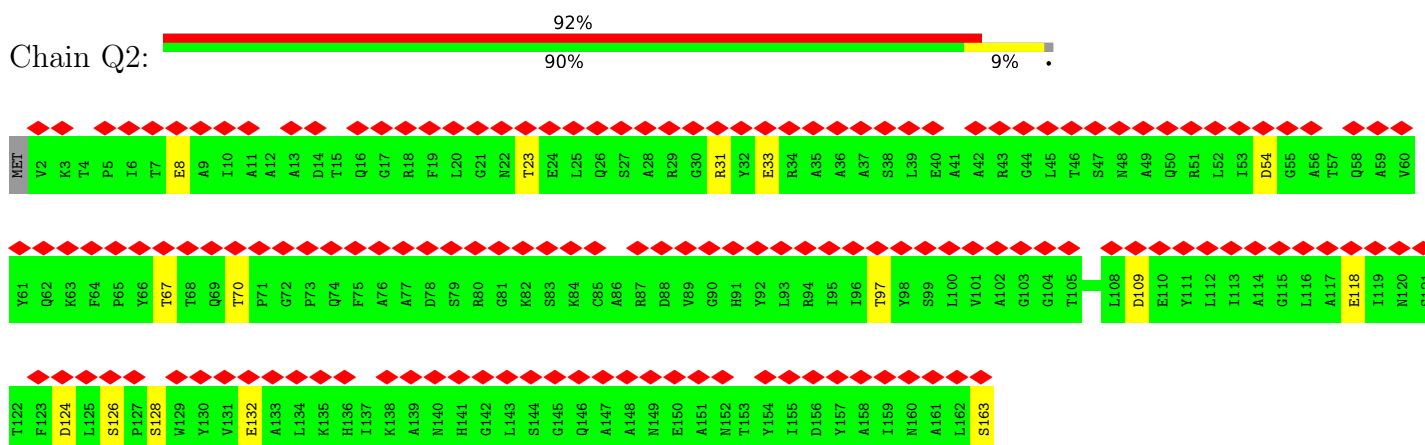
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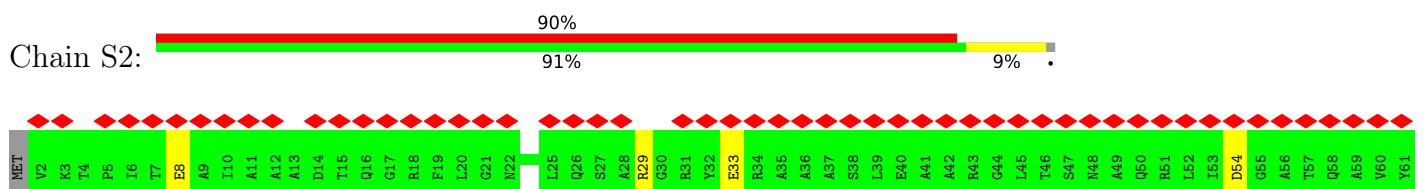
• Molecule 2: C-phyco cyanin alpha subunit



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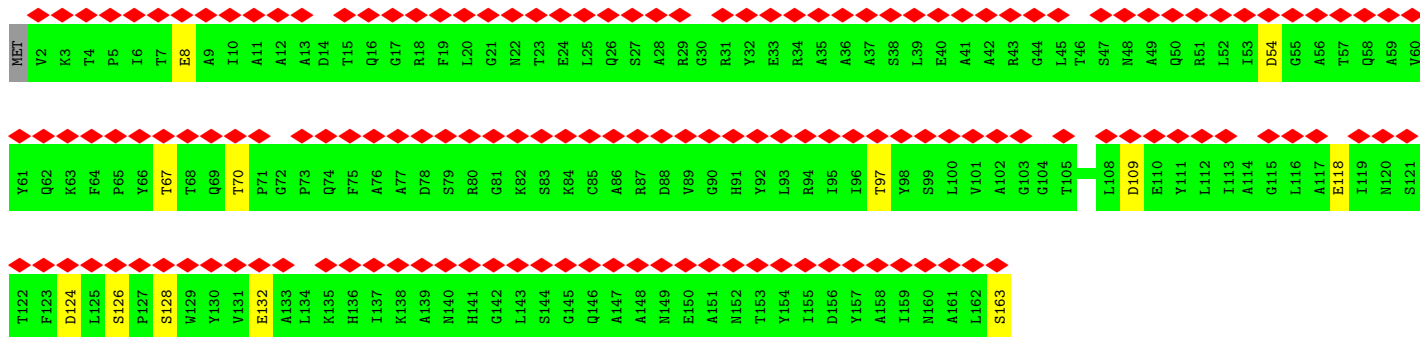
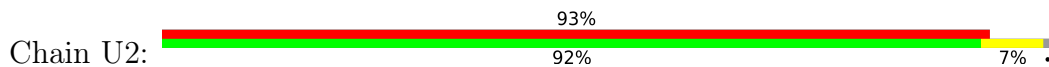


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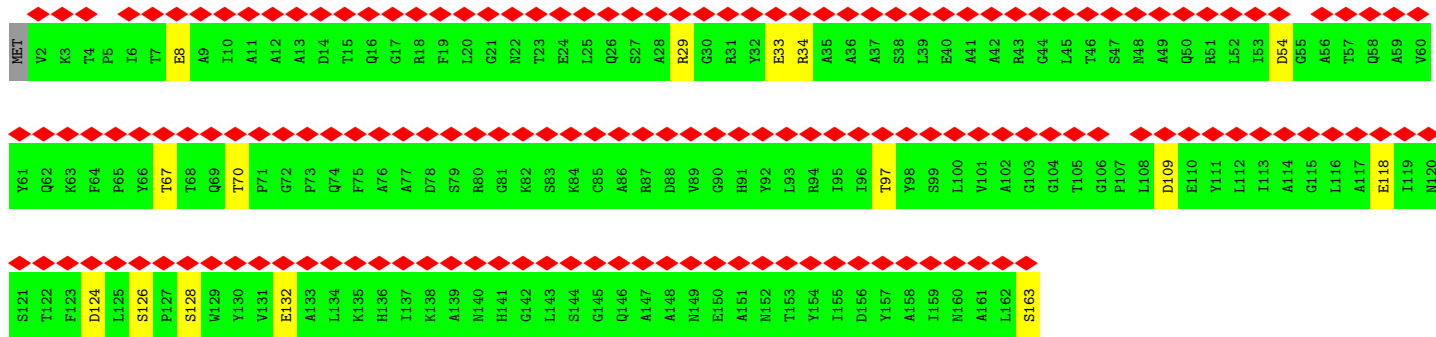
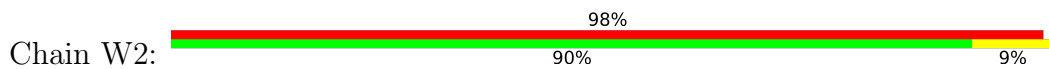




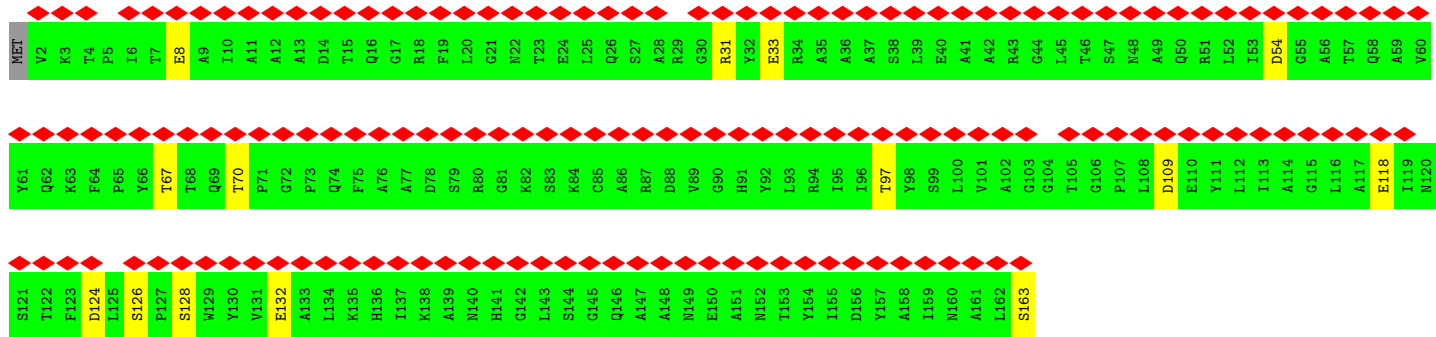
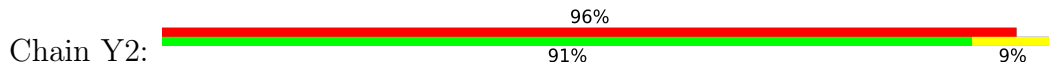
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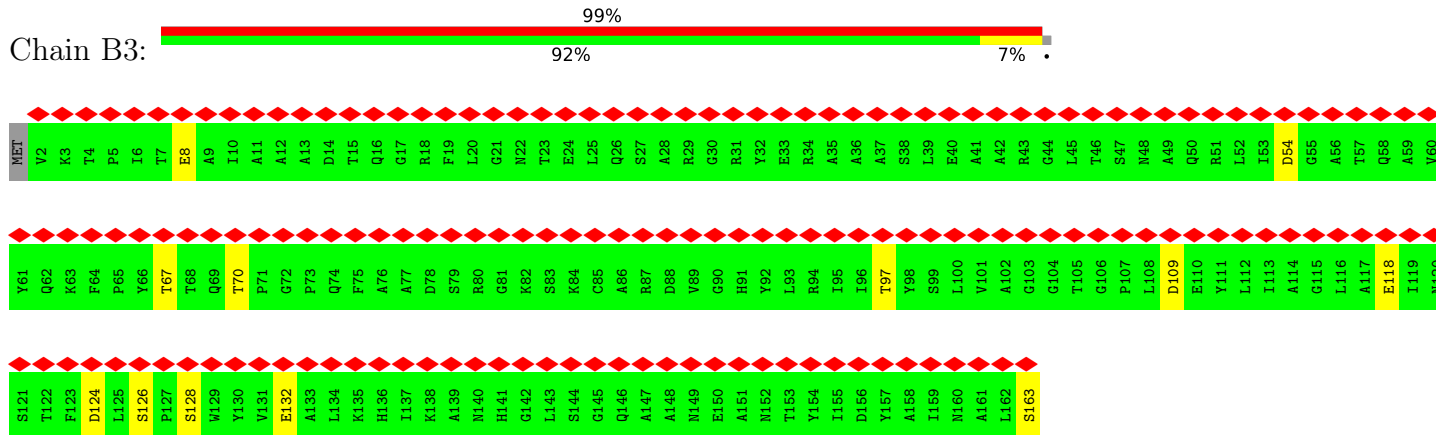
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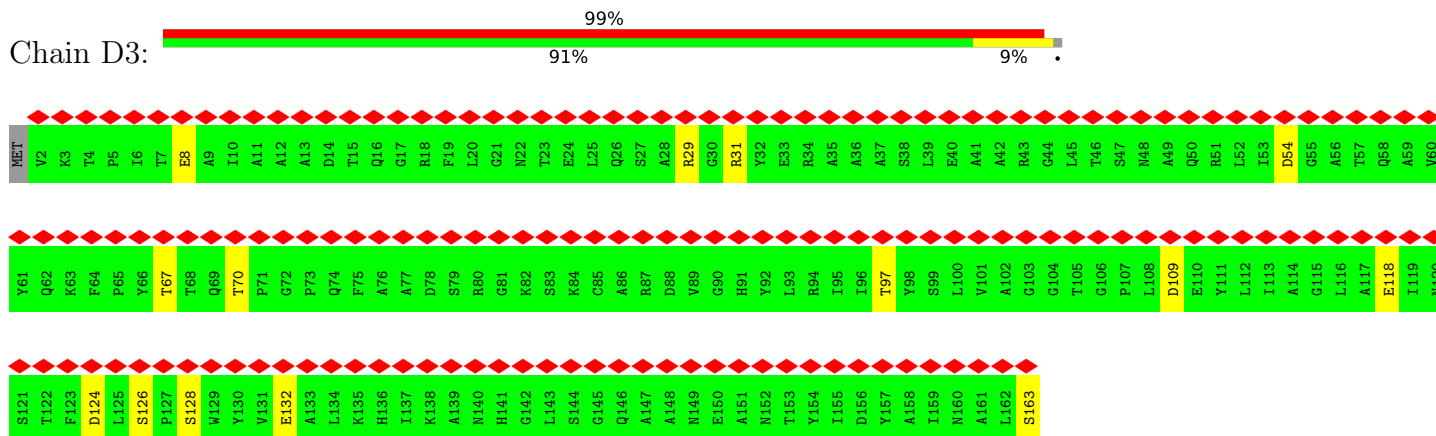
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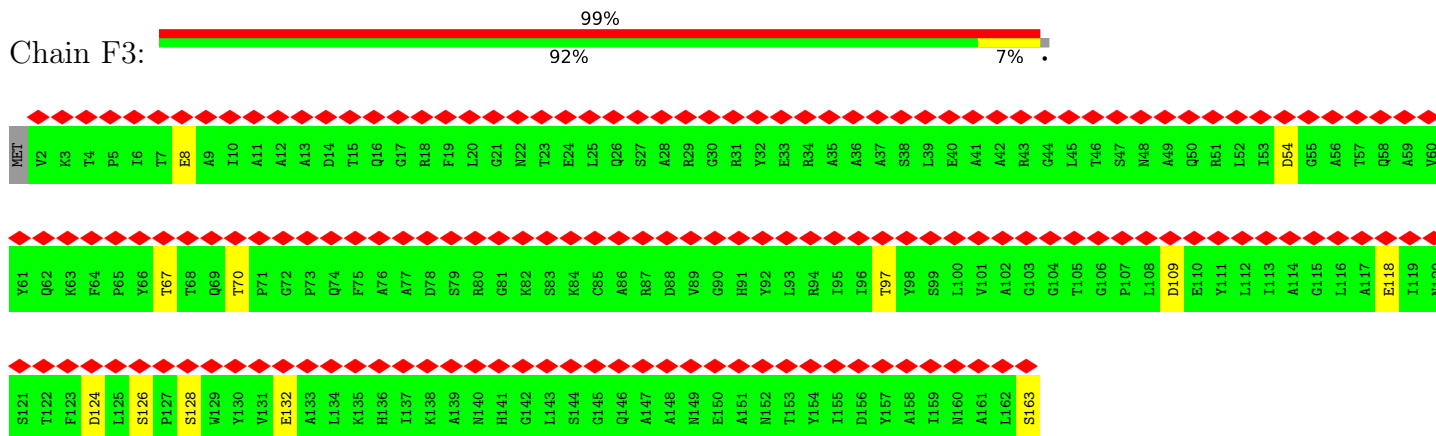
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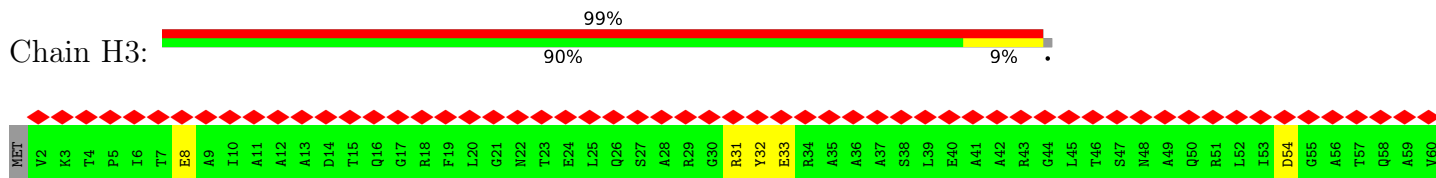
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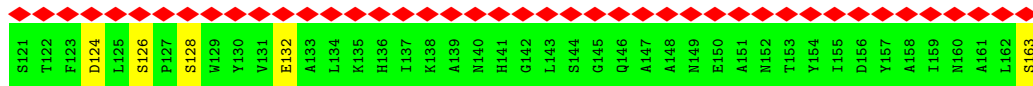
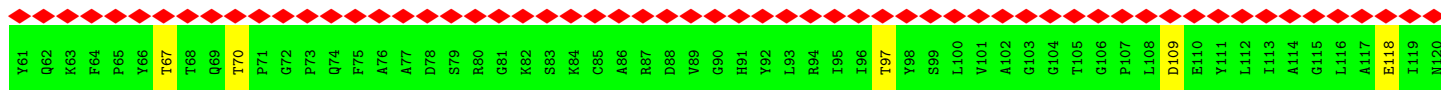


• Molecule 2: C-phycoerythrin alpha subunit

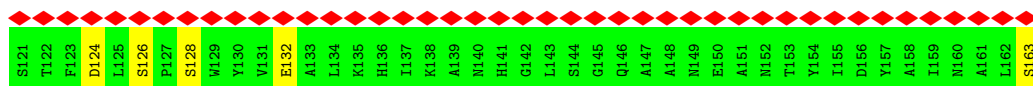
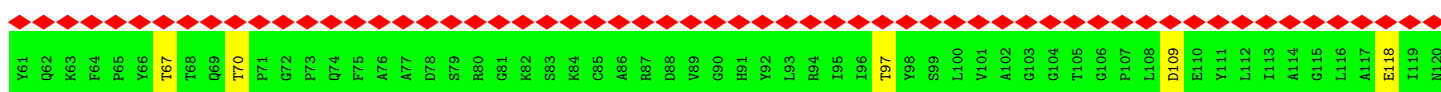
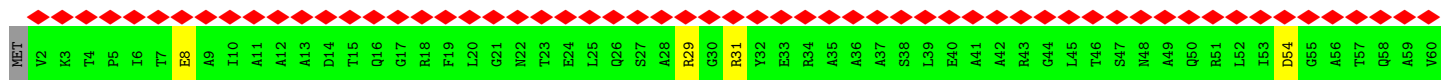
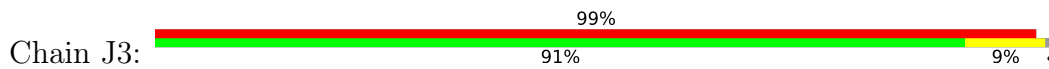


• Molecule 2: C-phycoerythrin alpha subunit

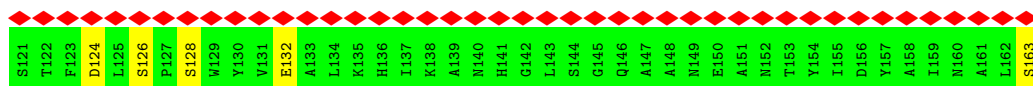
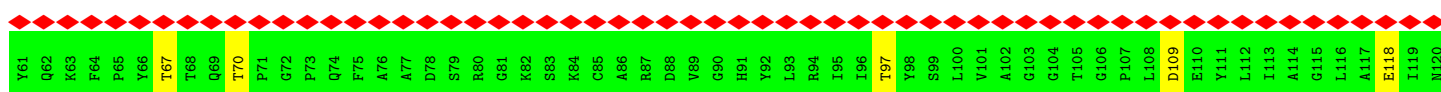
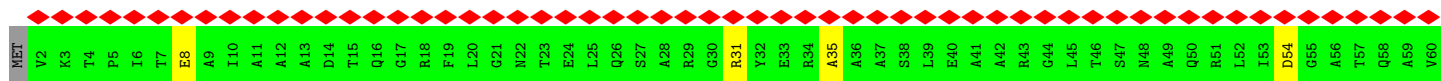
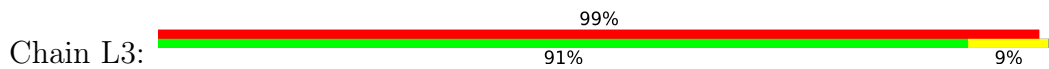




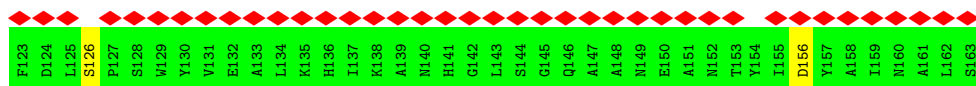
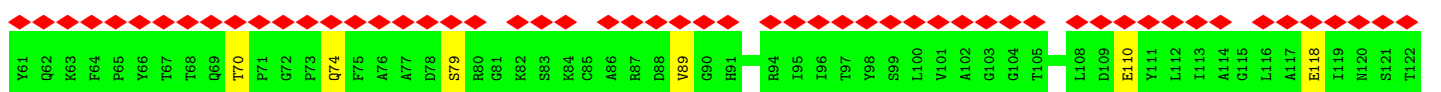
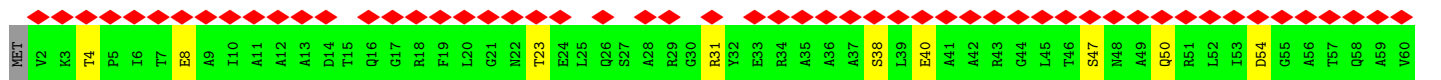
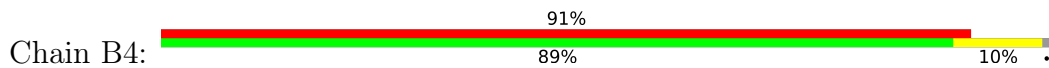
• Molecule 2: C-phycoerythrin alpha subunit



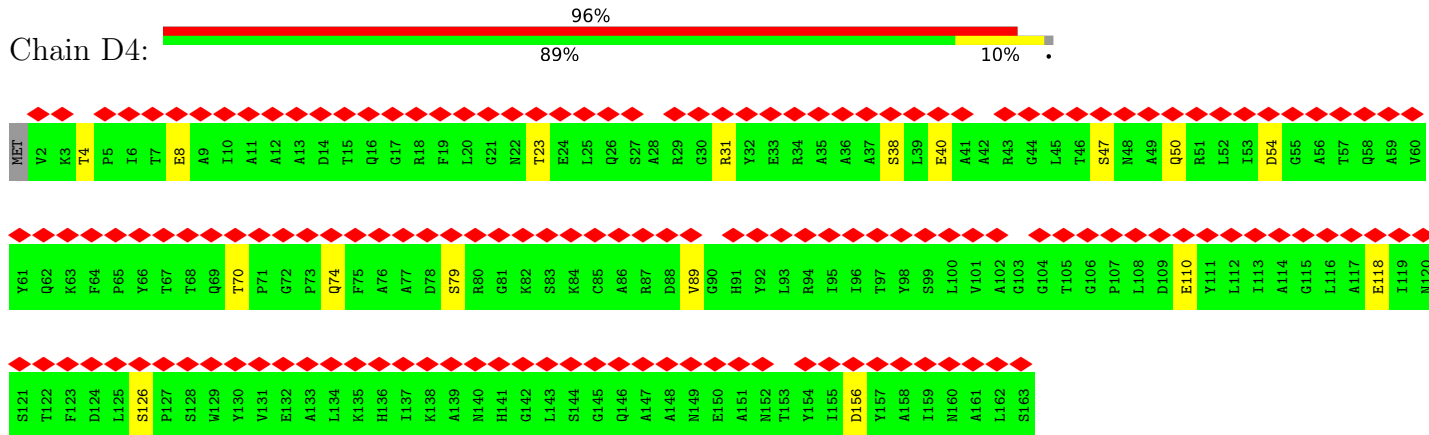
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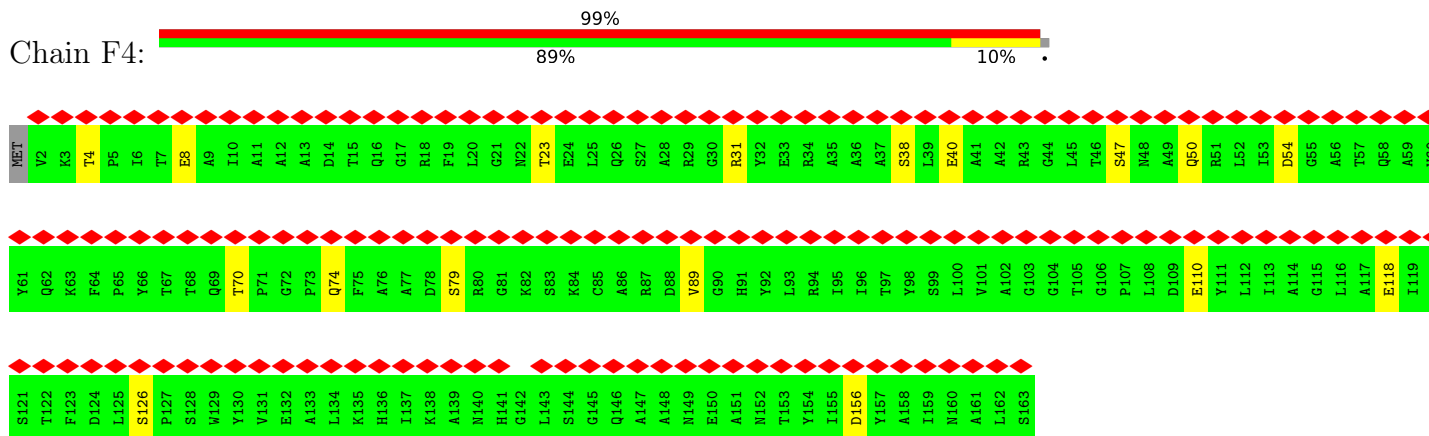
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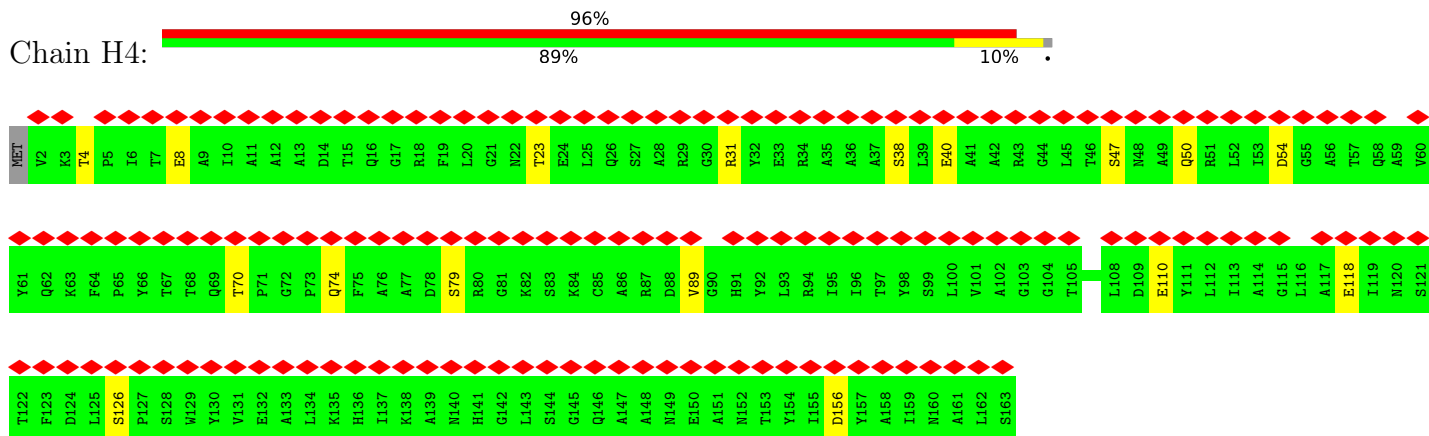
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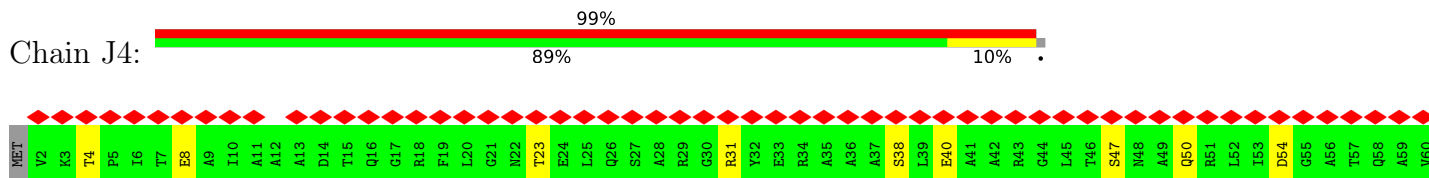
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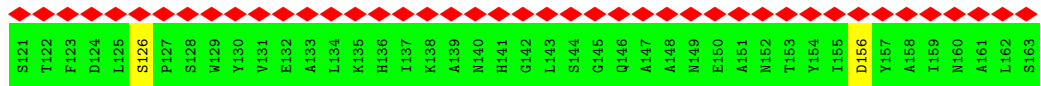
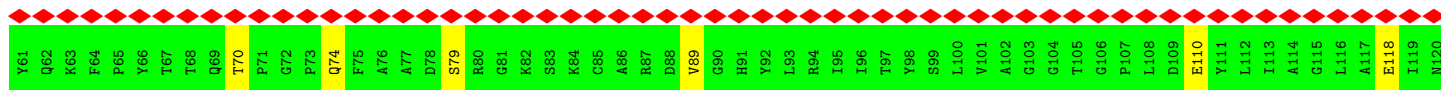


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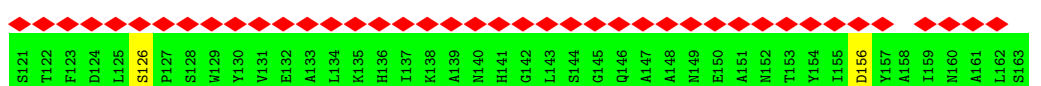
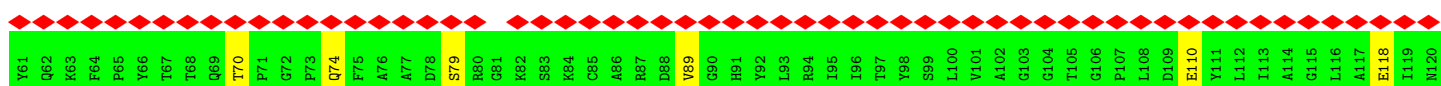
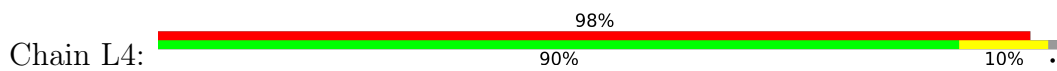


• Molecule 2: C-phycoerythrin alpha subunit

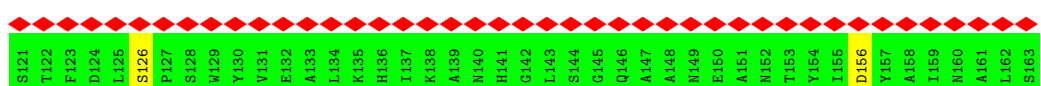
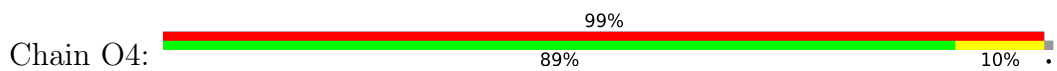




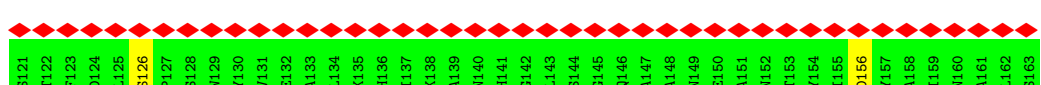
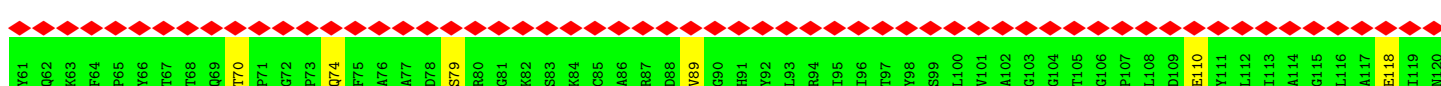
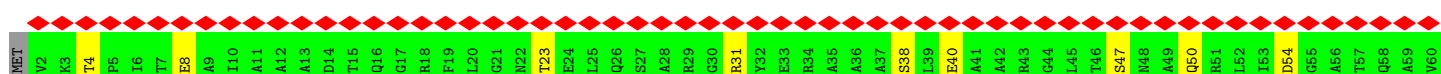
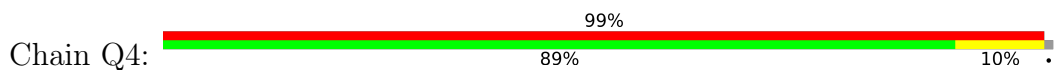
• Molecule 2: C-phycoerythrin alpha subunit



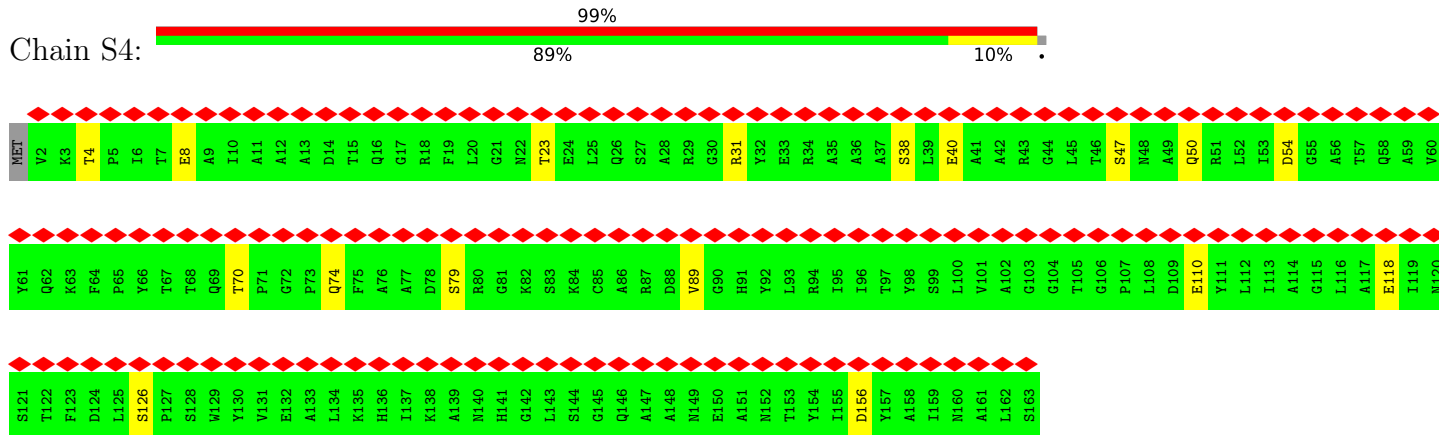
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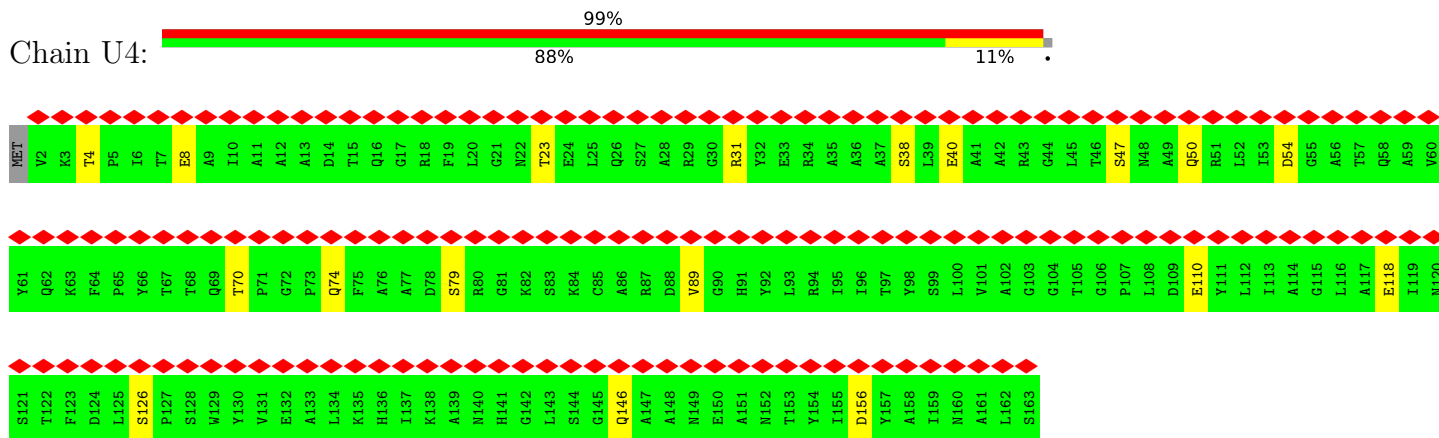
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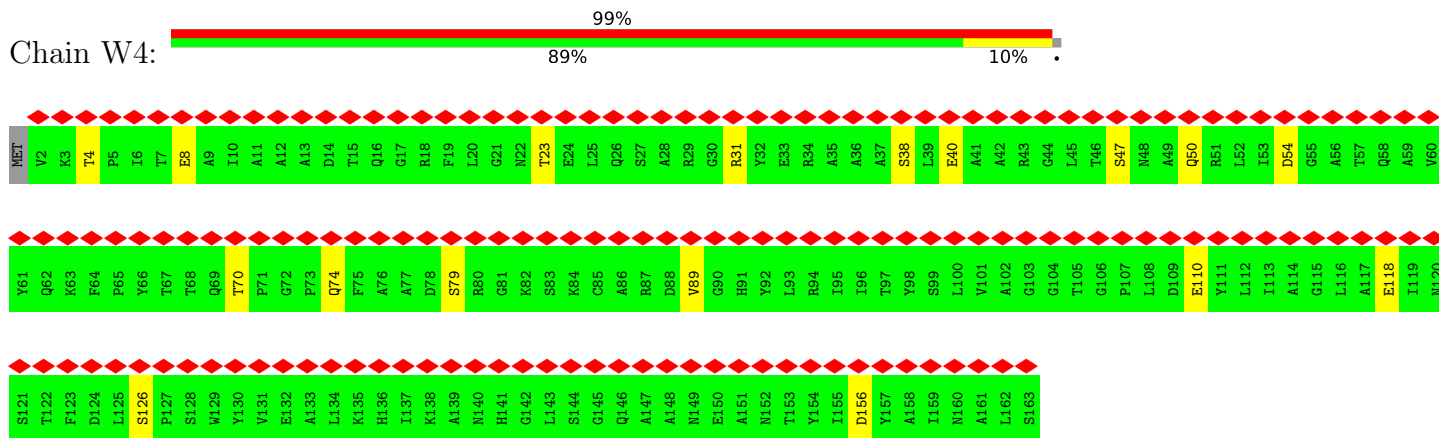
- Molecule 2: C-phycoerythrin alpha subunit



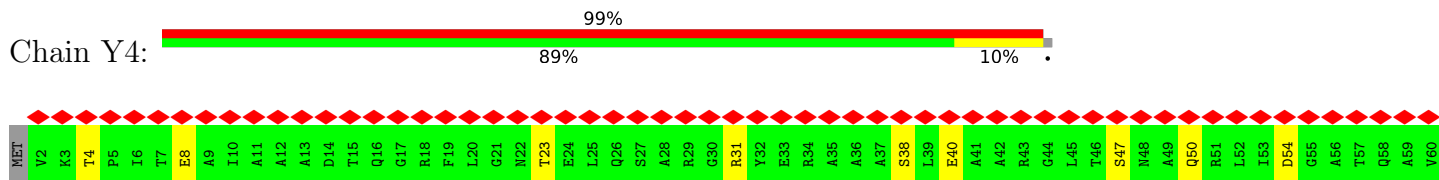
- Molecule 2: C-phycoerythrin alpha subunit

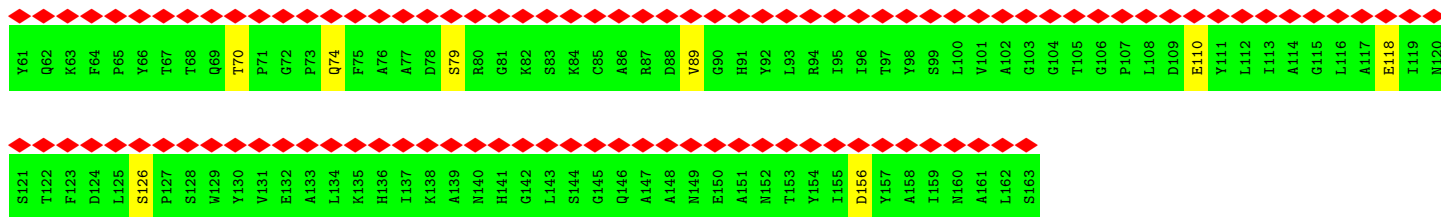


- Molecule 2: C-phycoerythrin alpha subunit

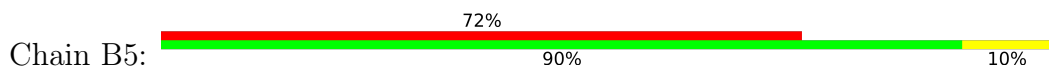


- Molecule 2: C-phycoerythrin alpha subunit

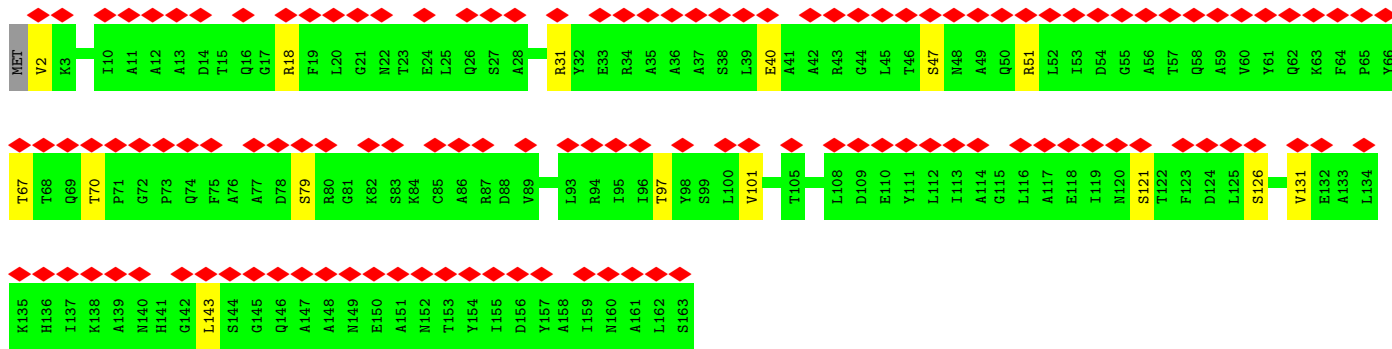
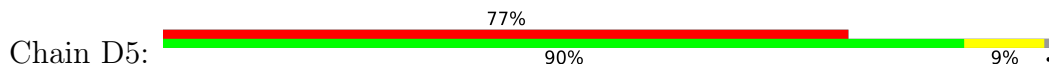




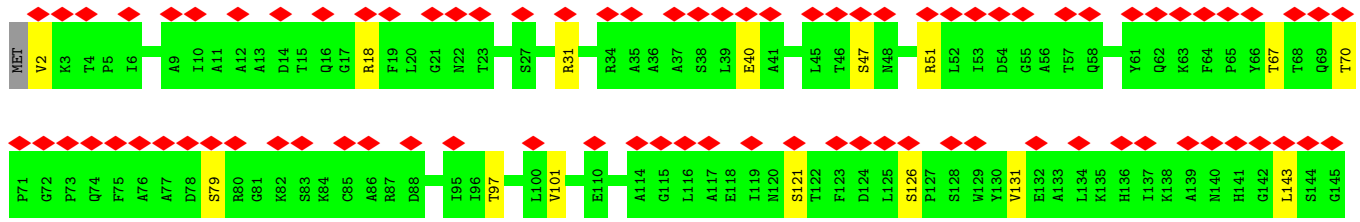
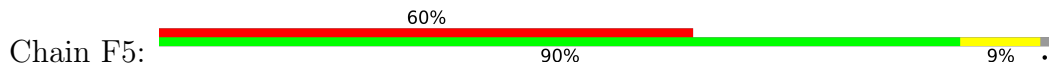
• Molecule 2: C-phycoerythrin alpha subunit

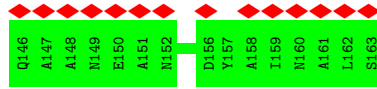


• Molecule 2: C-phycoerythrin alpha subunit

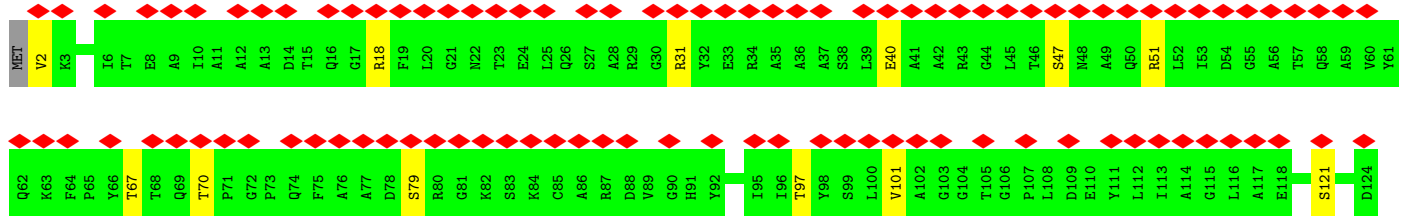
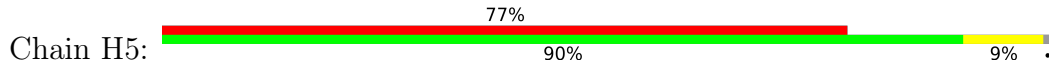


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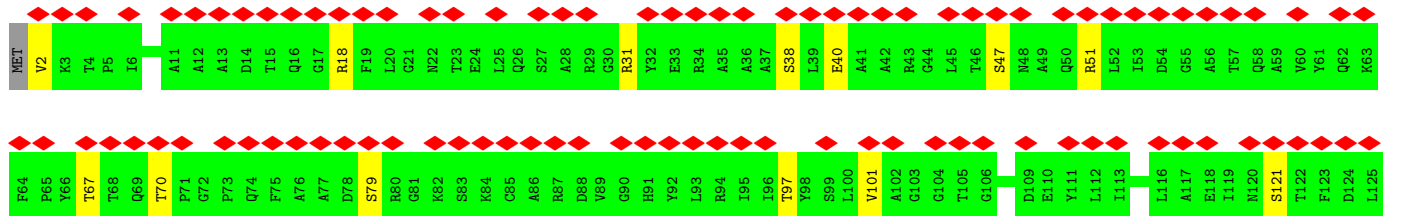
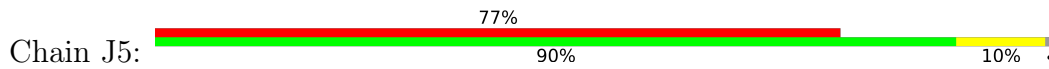




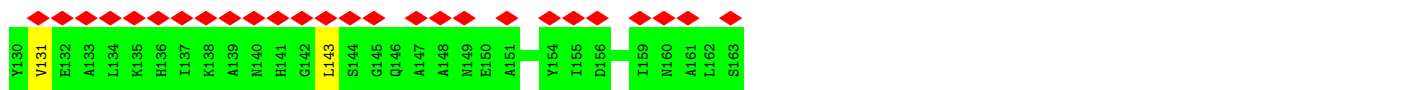
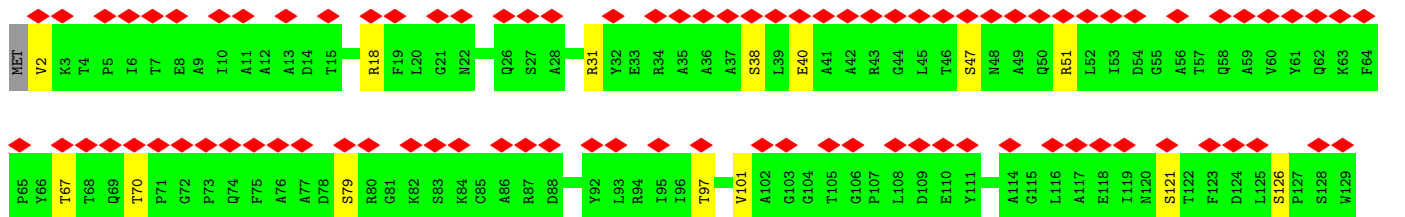
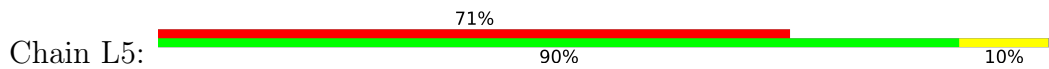
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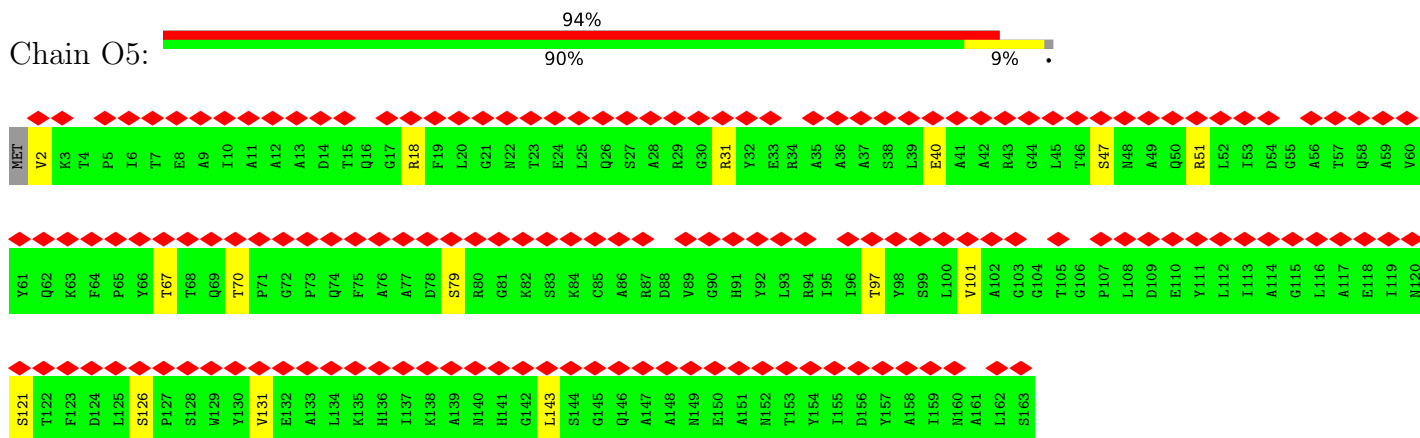
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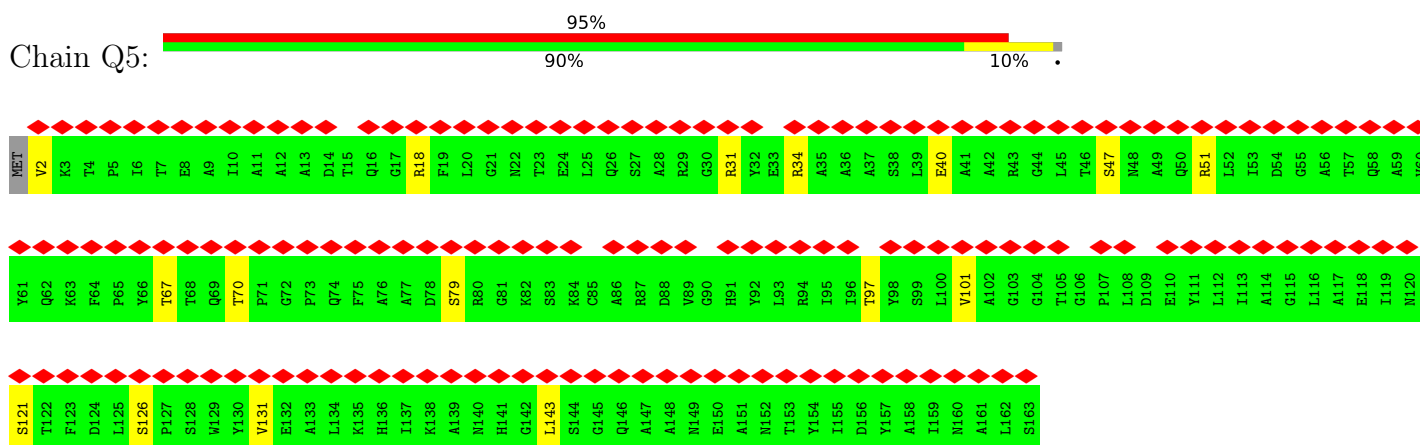
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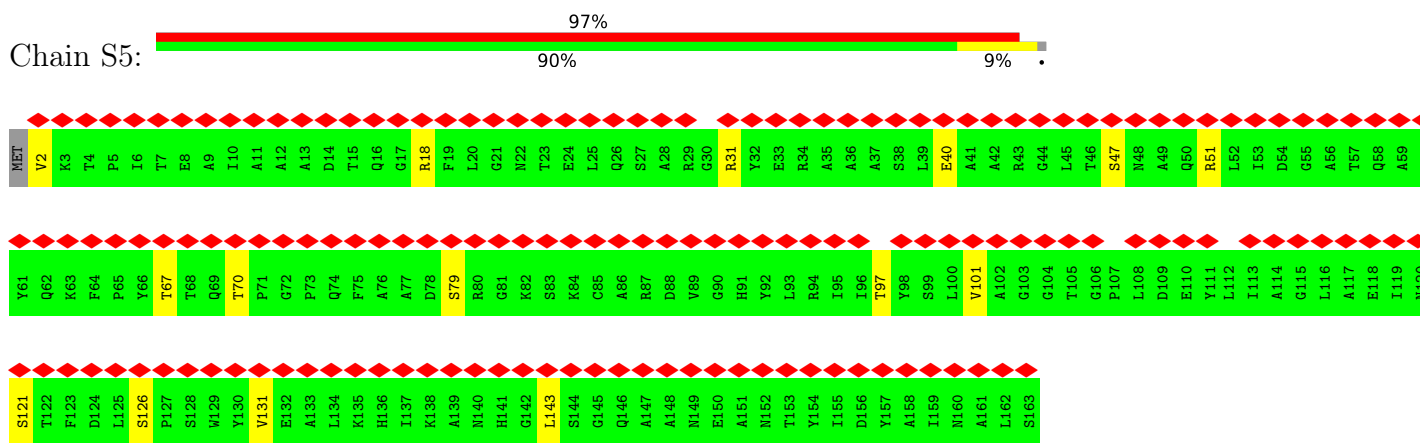
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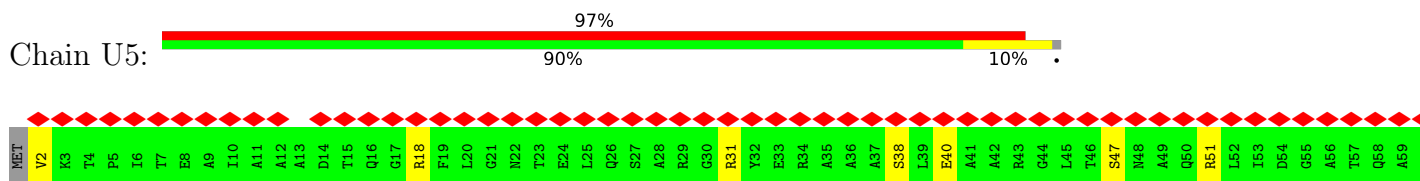
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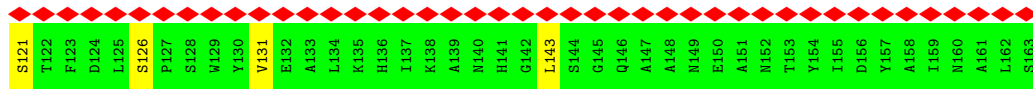
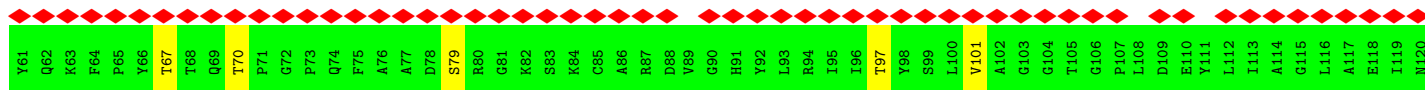


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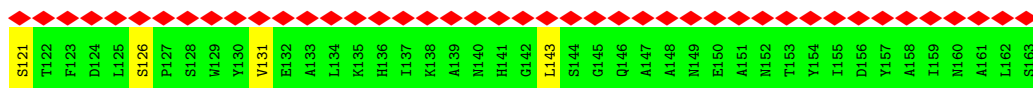
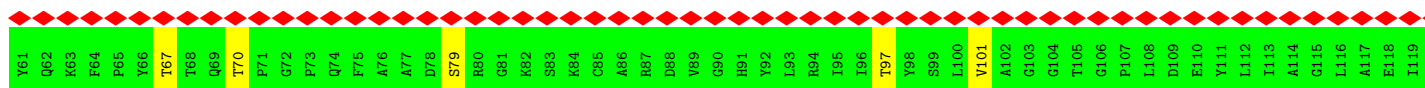
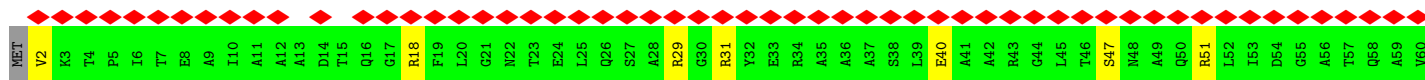
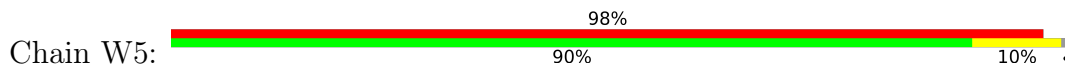


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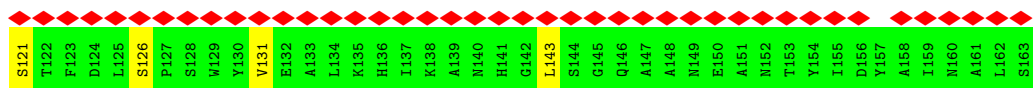
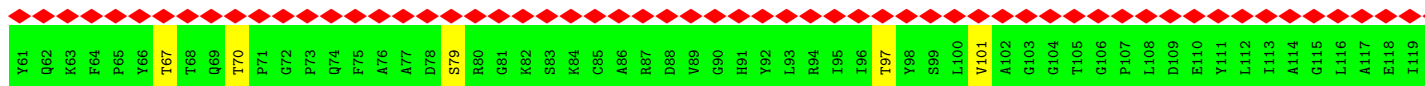
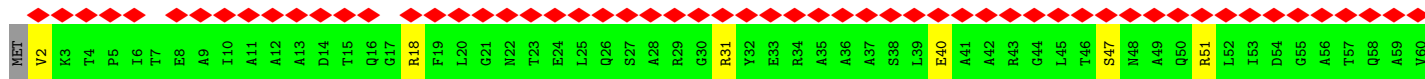
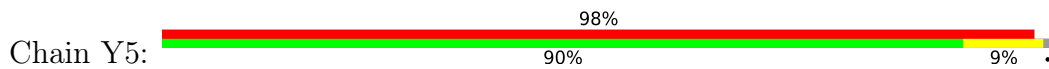




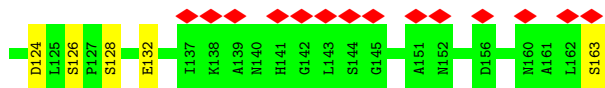
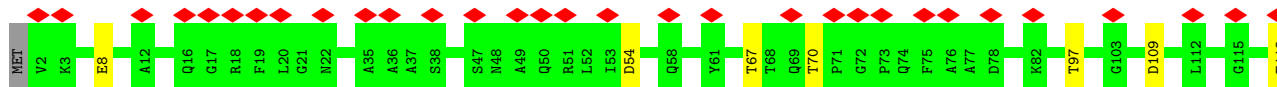
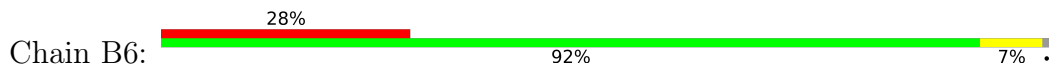
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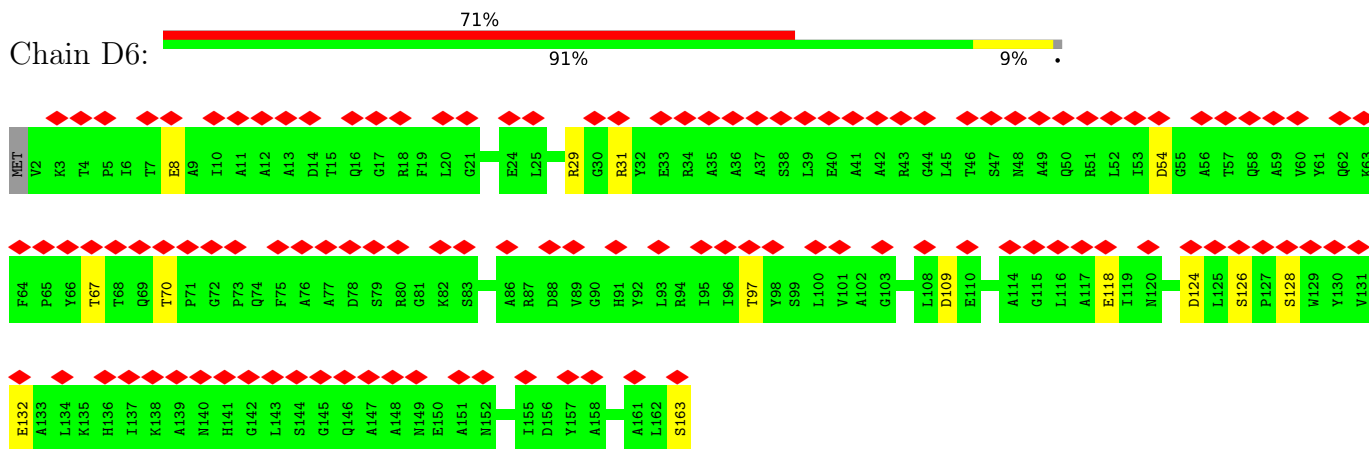
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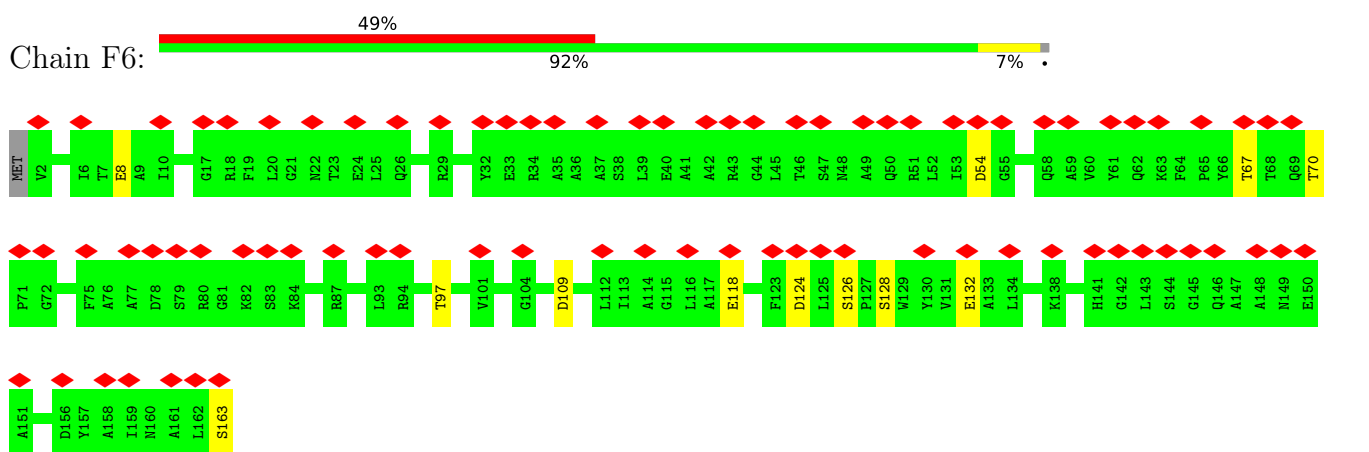
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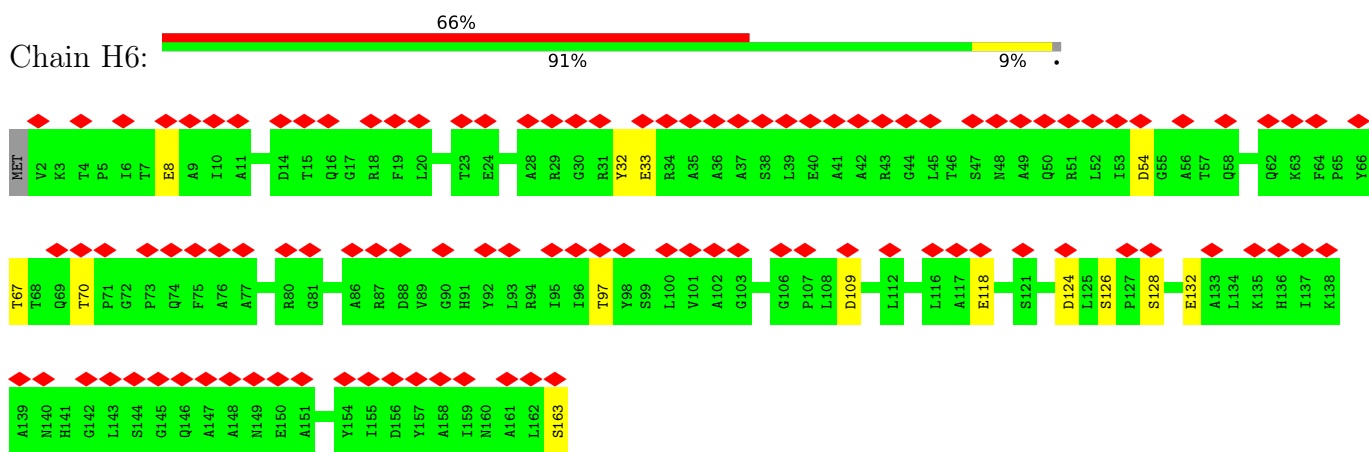
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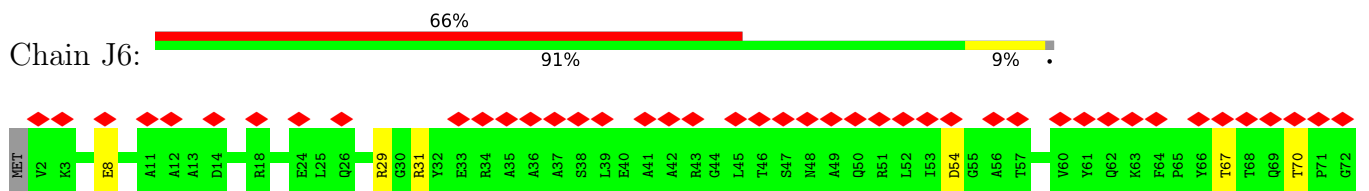
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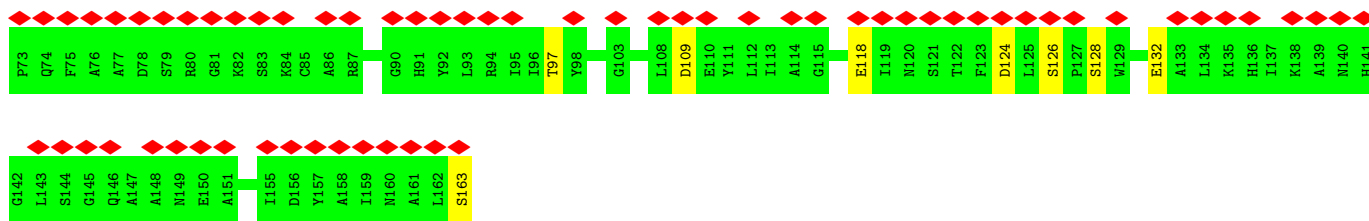


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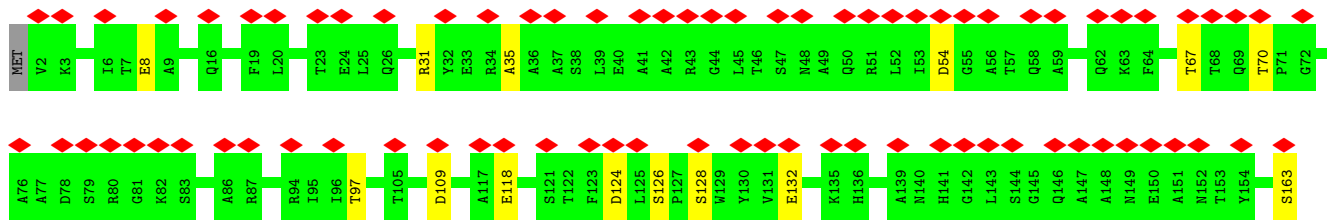
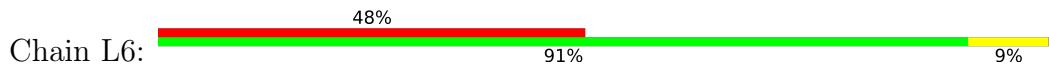


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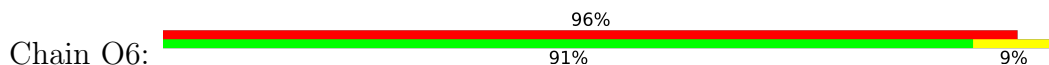




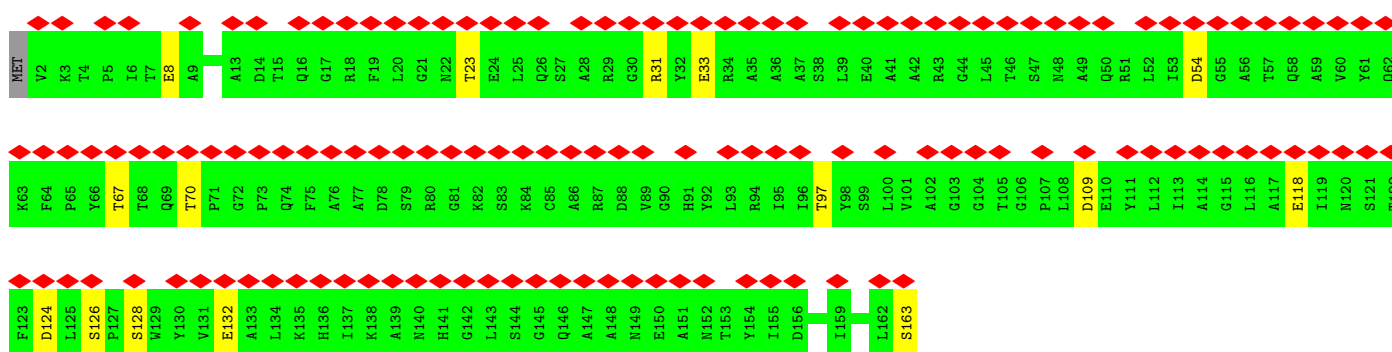
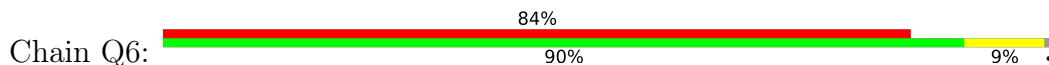
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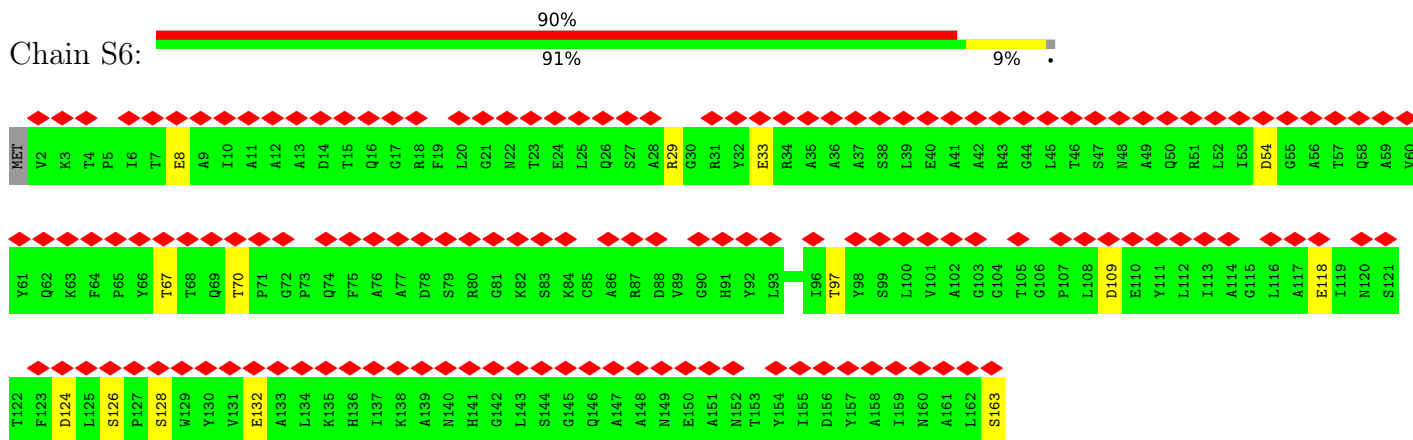
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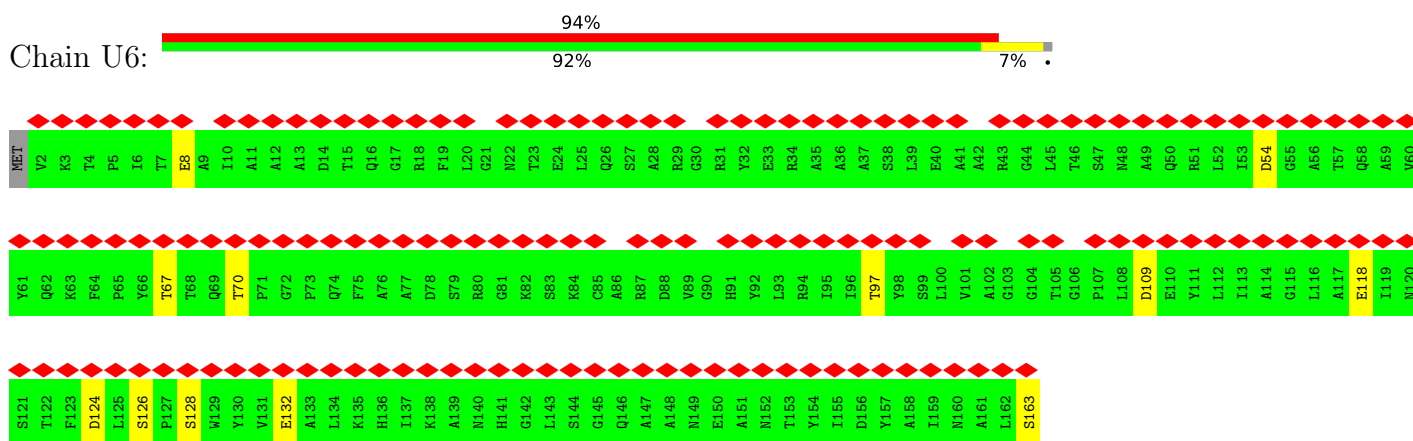
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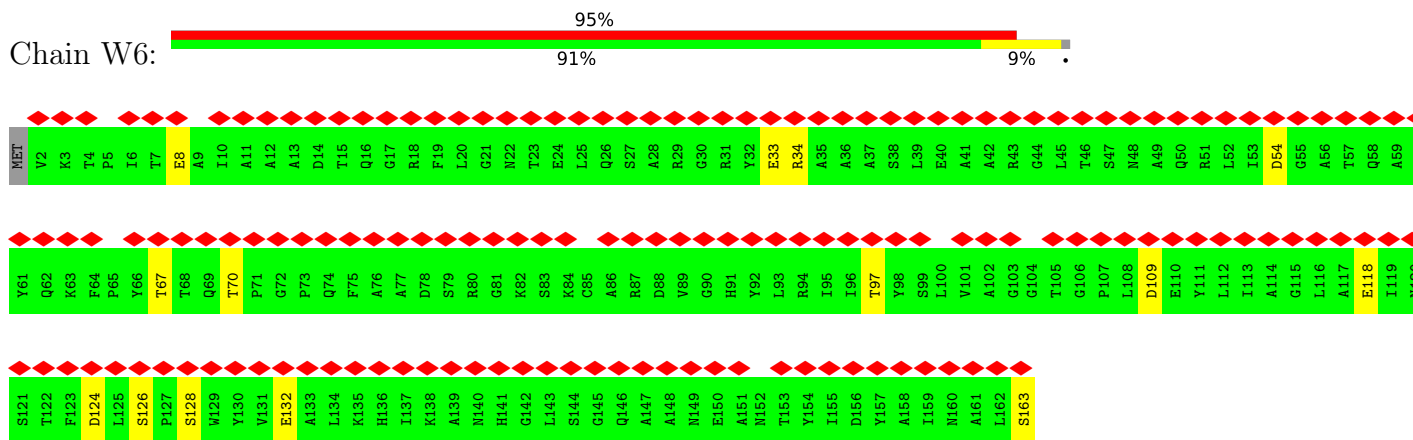
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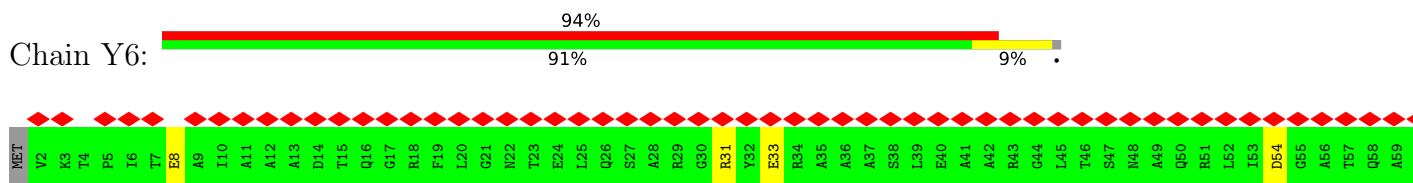
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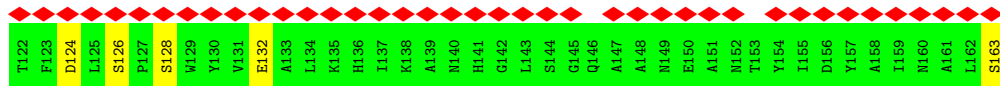
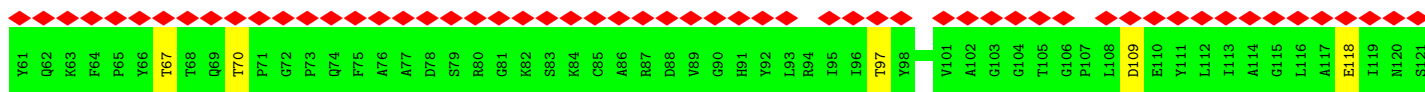


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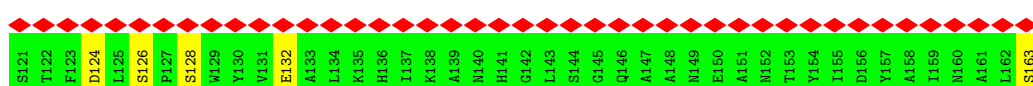
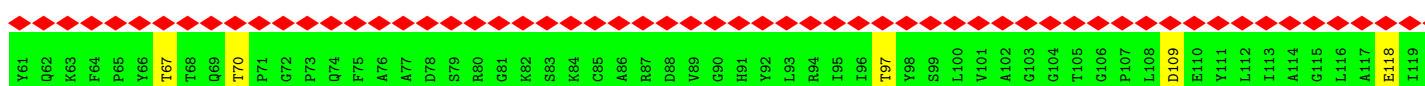
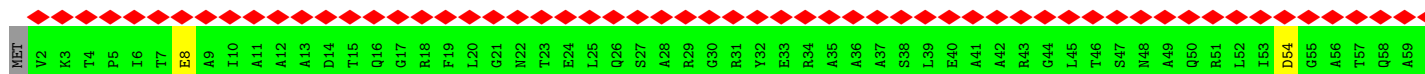
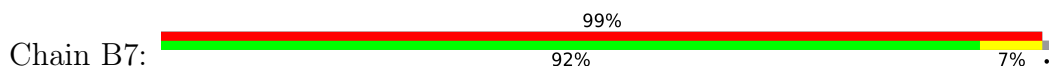


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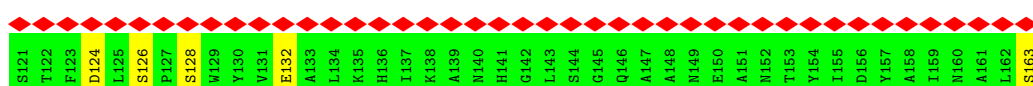
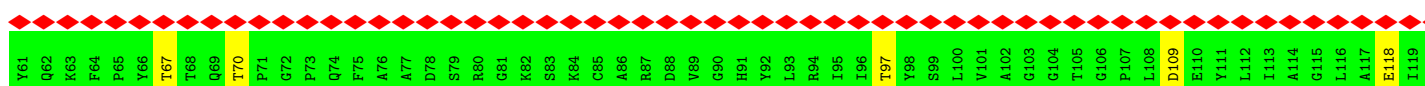
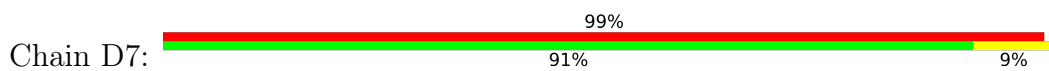




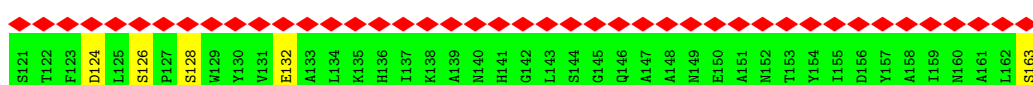
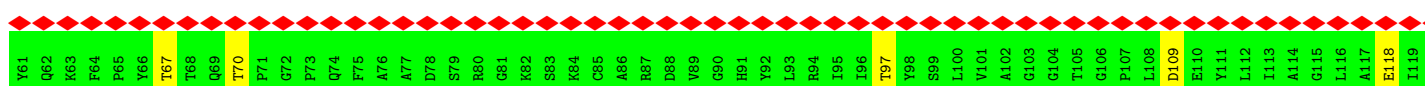
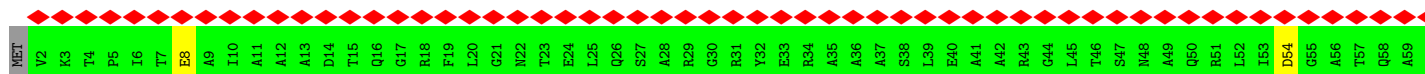
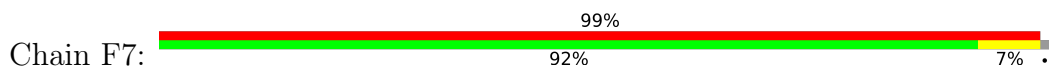
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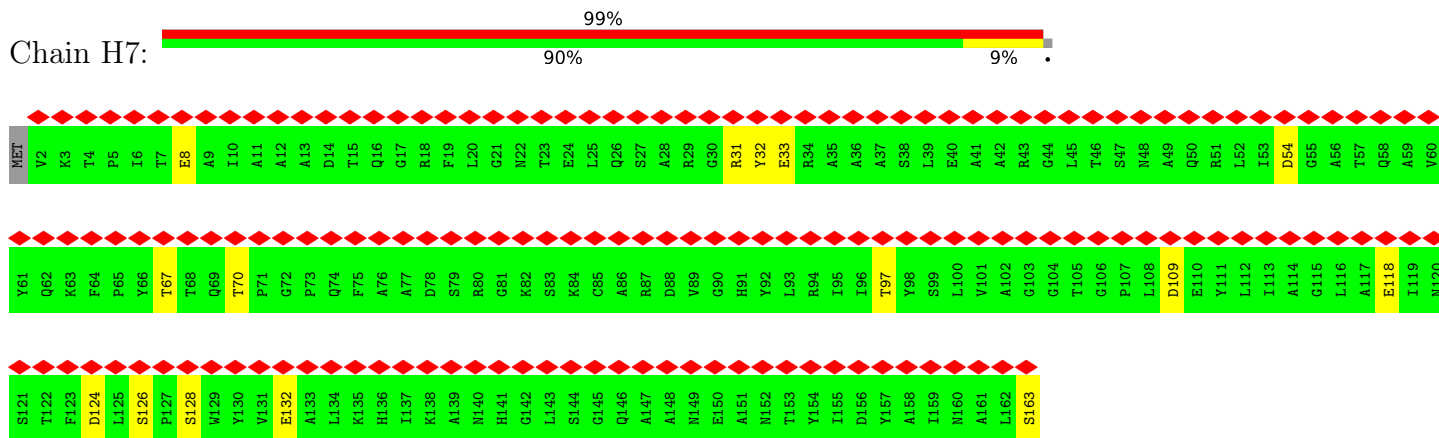
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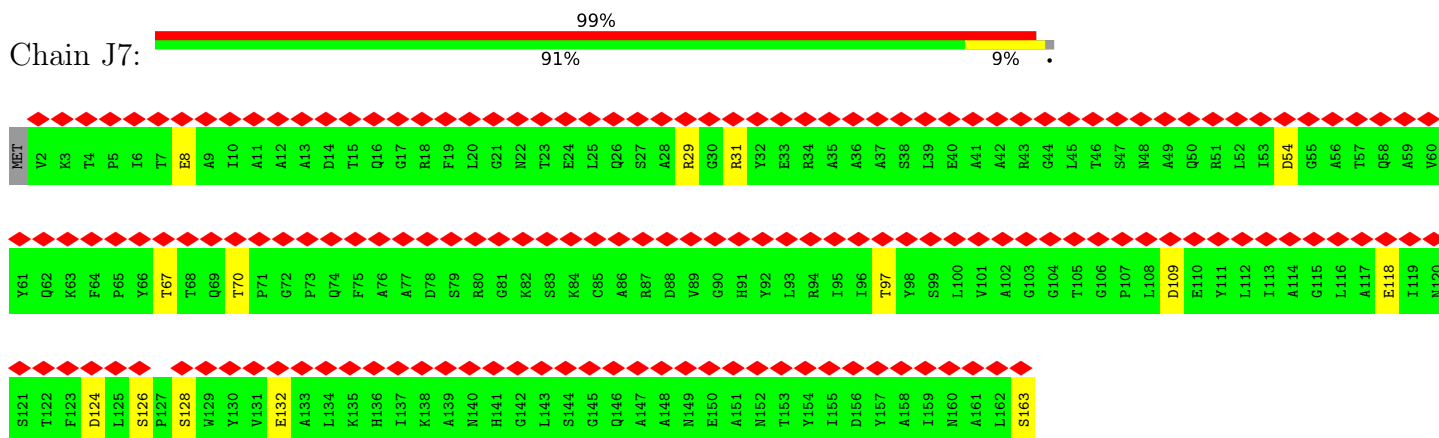
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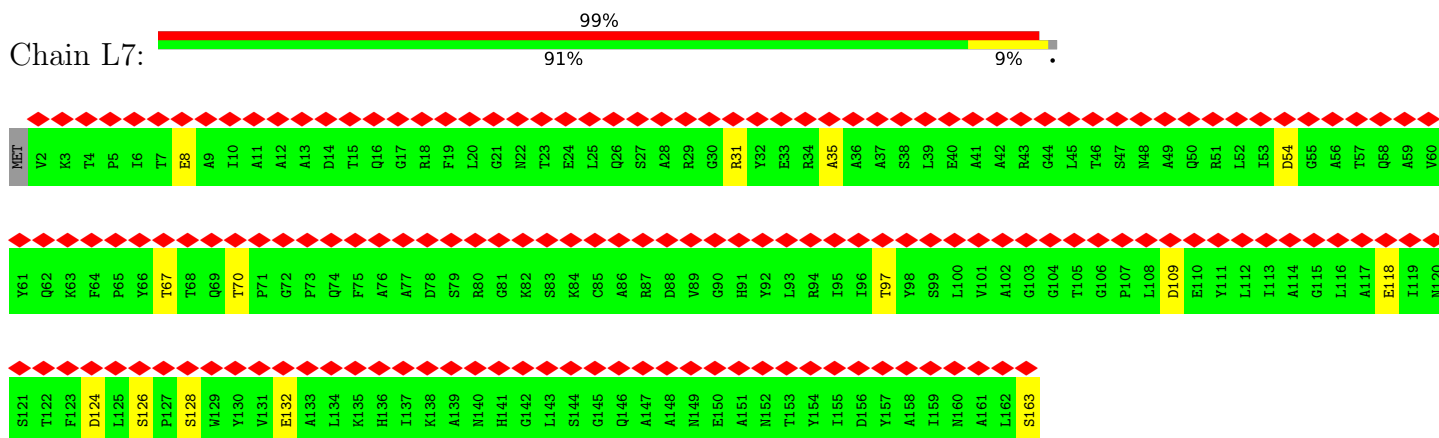
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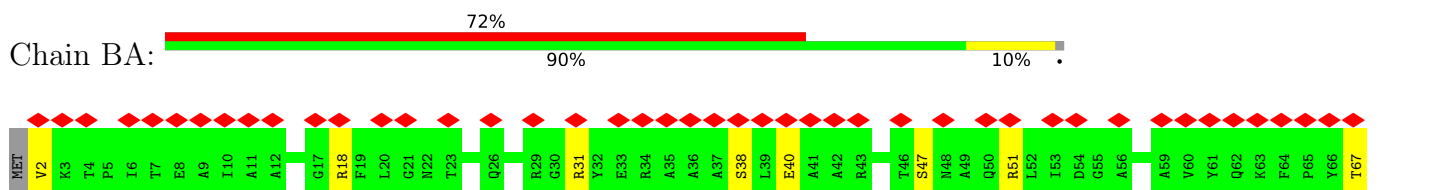
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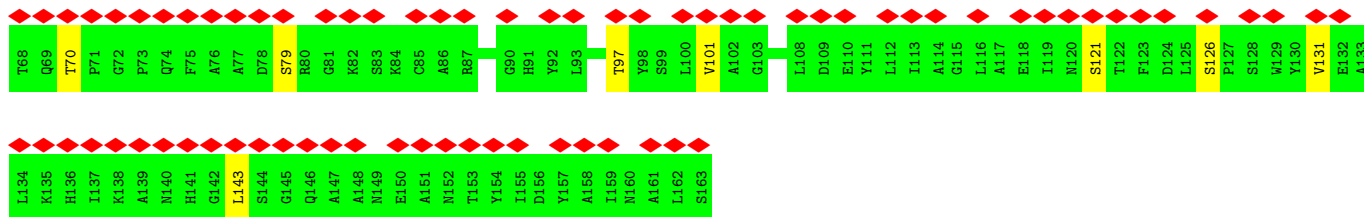


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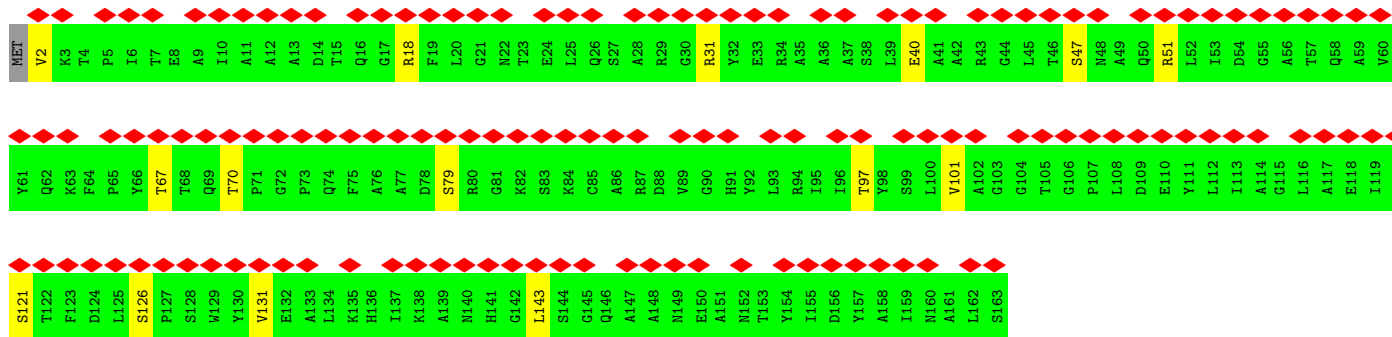
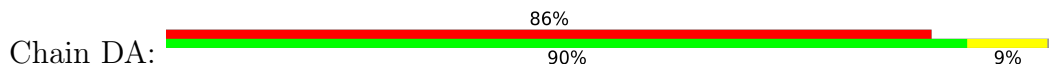


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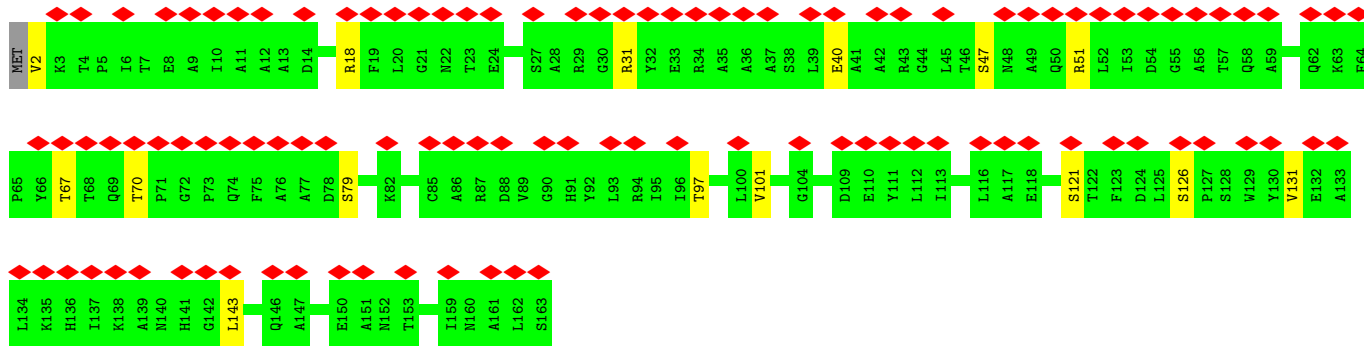
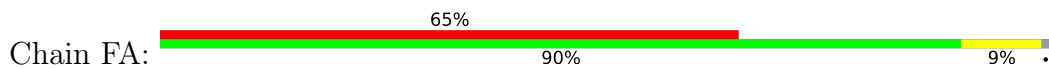




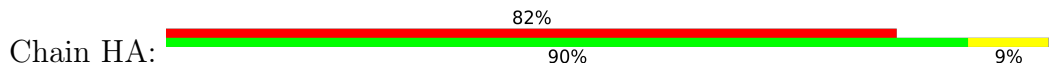
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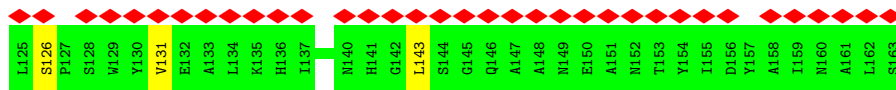


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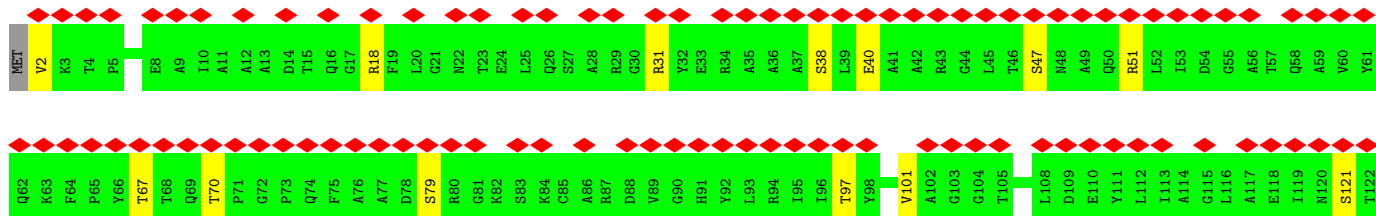
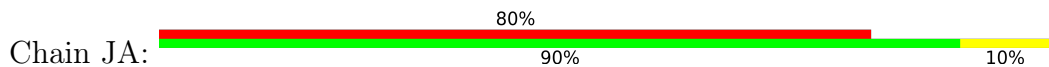


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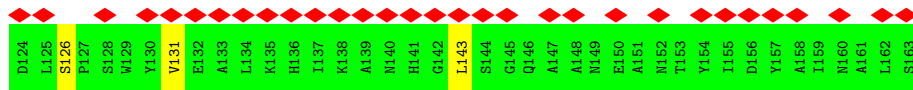
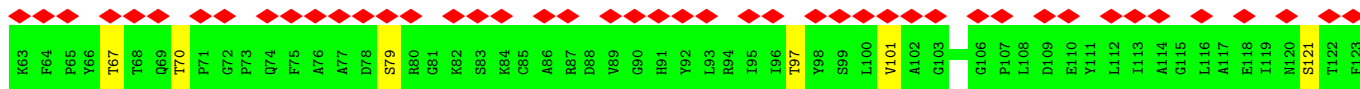
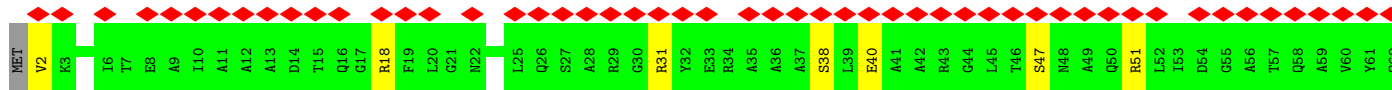
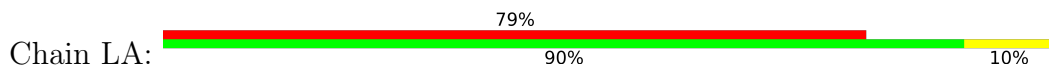




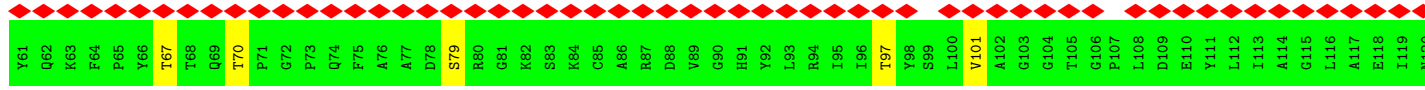
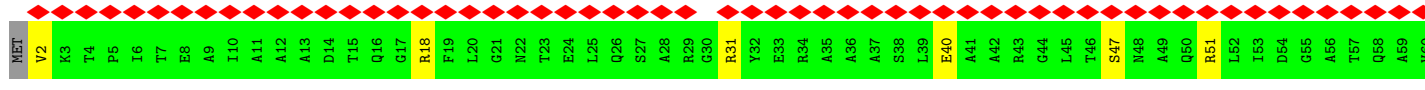
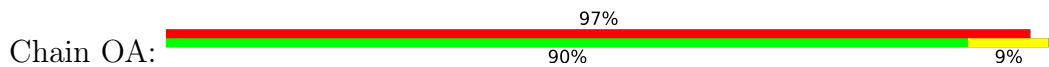
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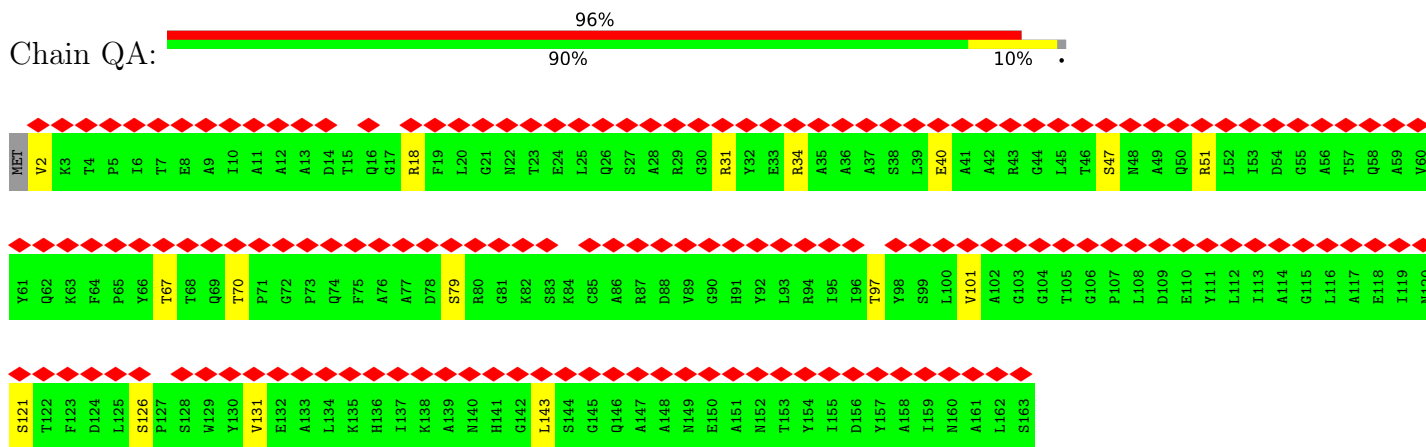
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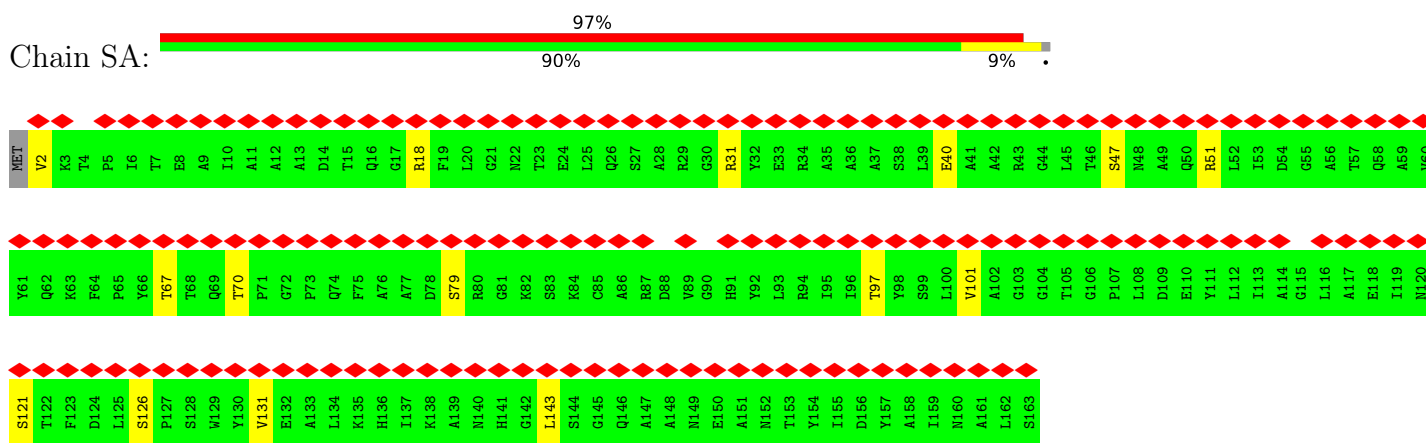
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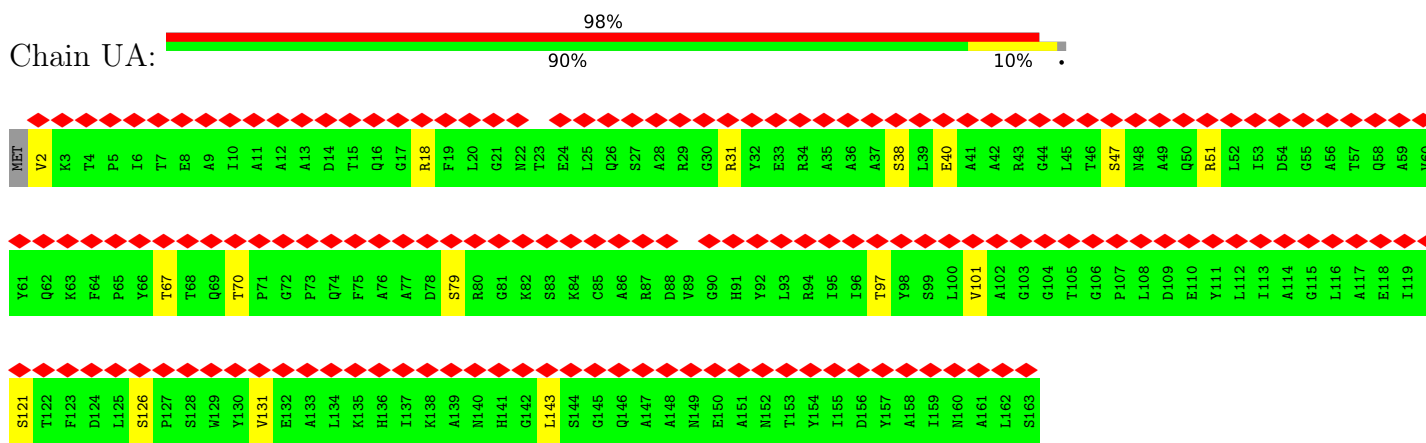
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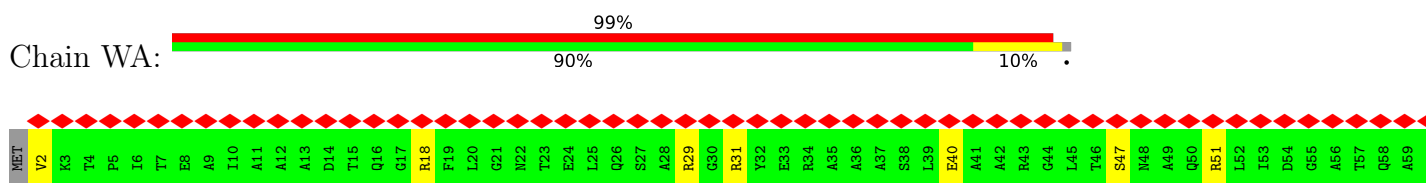
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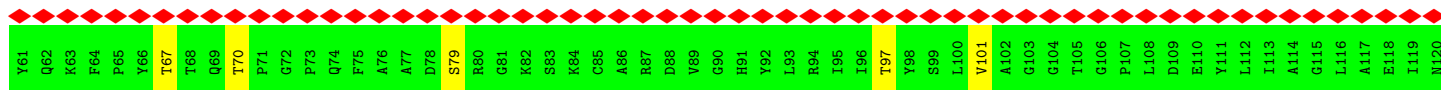


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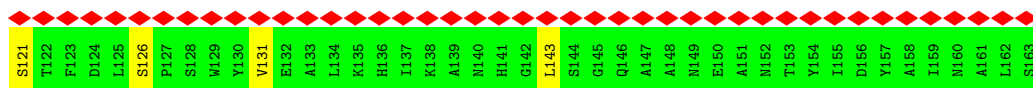
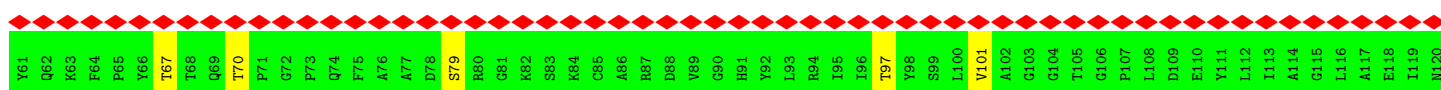
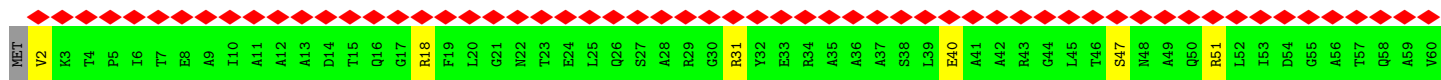
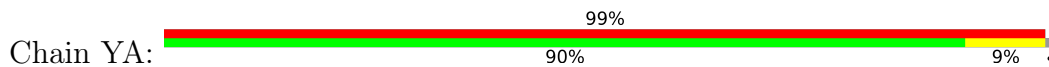


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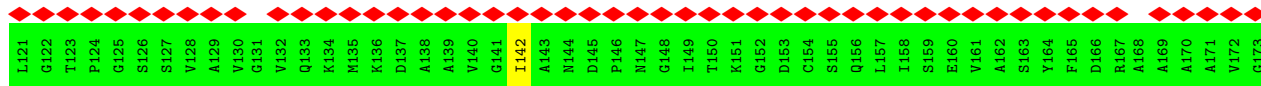
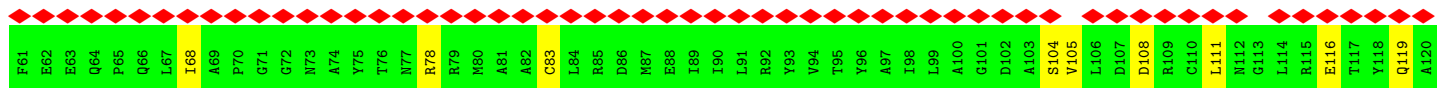
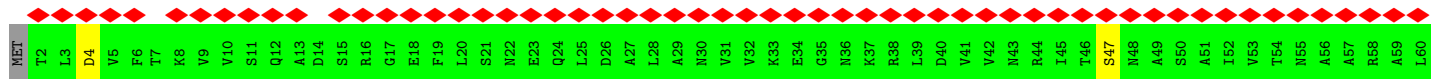
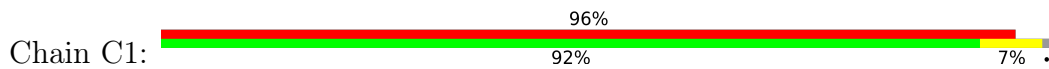




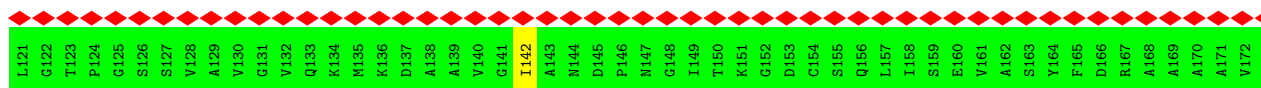
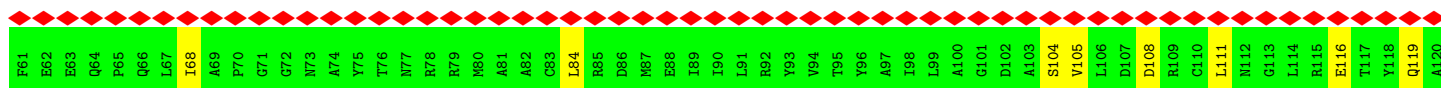
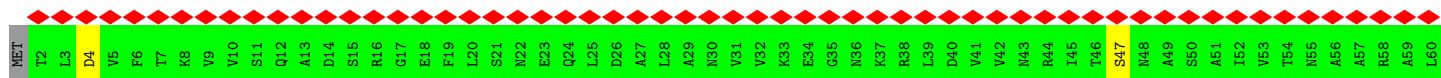
• Molecule 2: C-phycoerythrin alpha subunit



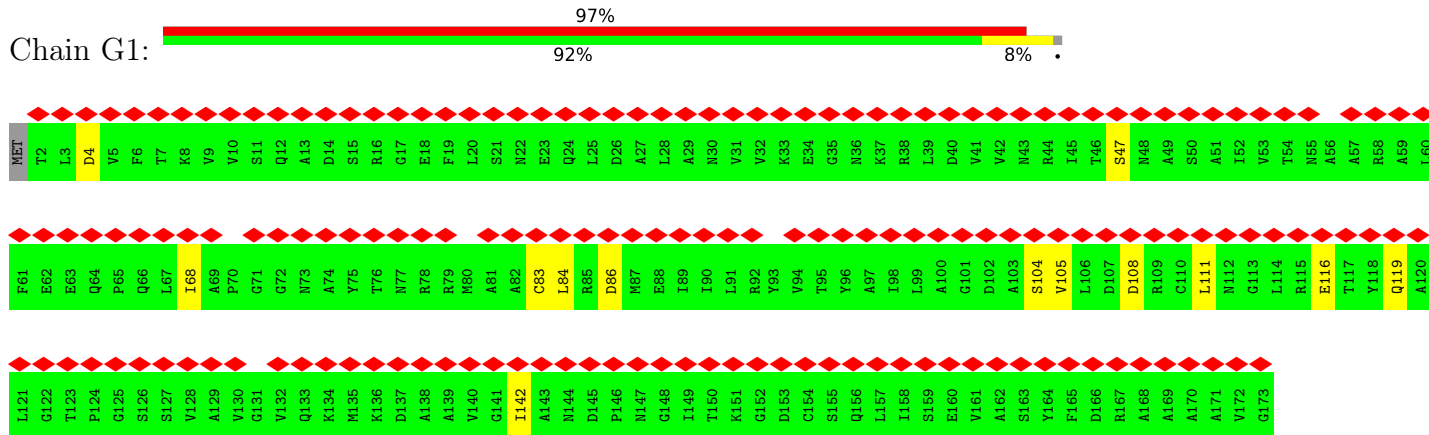
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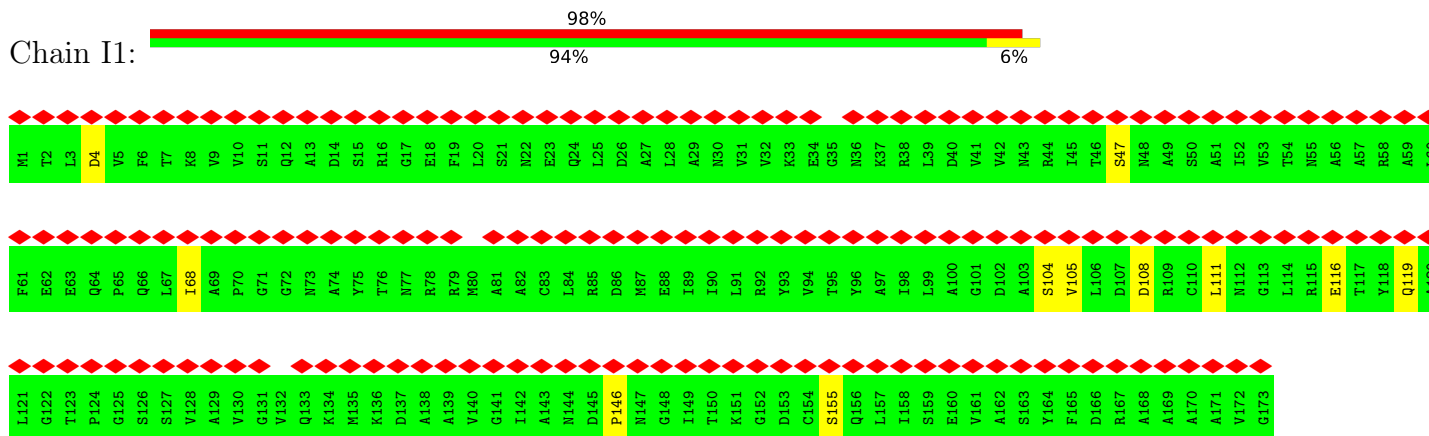
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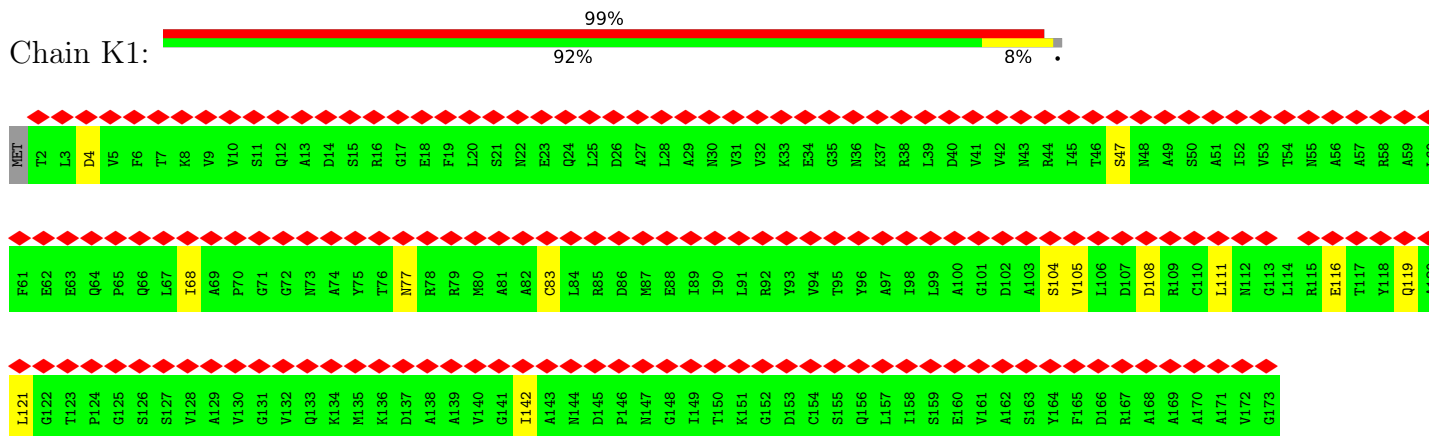
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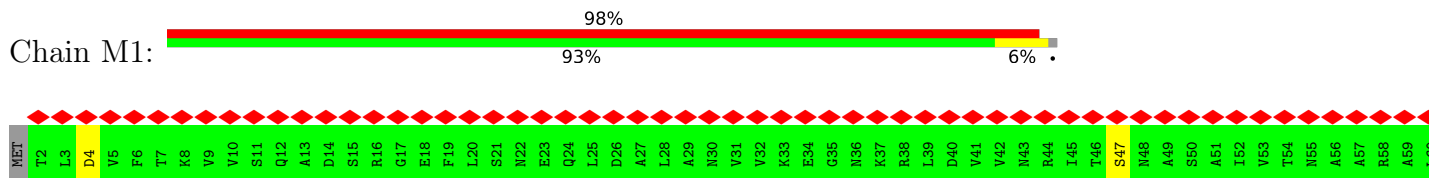
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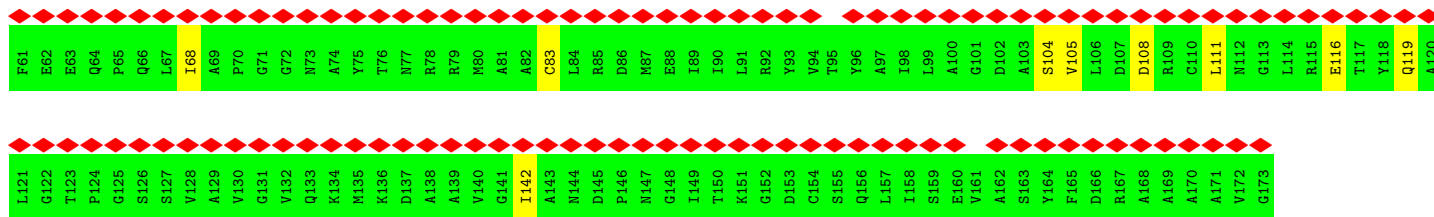


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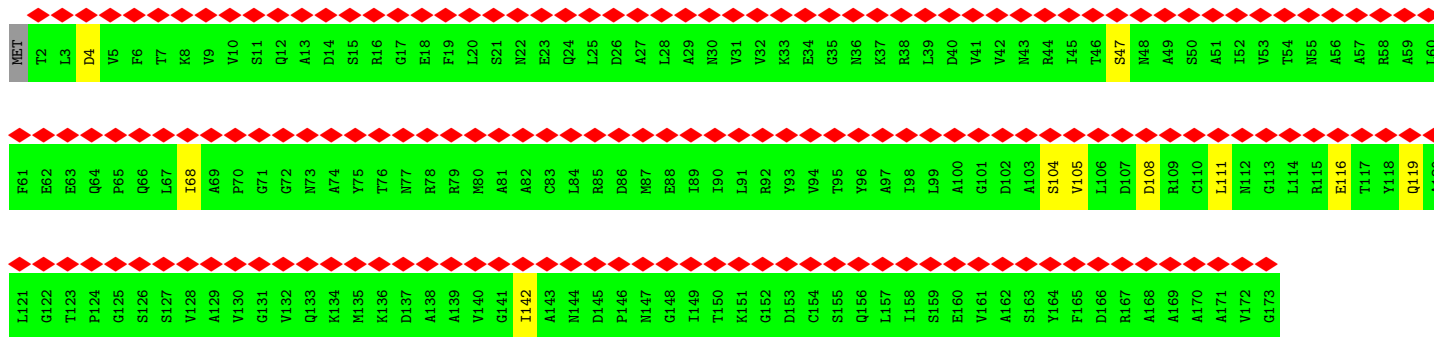


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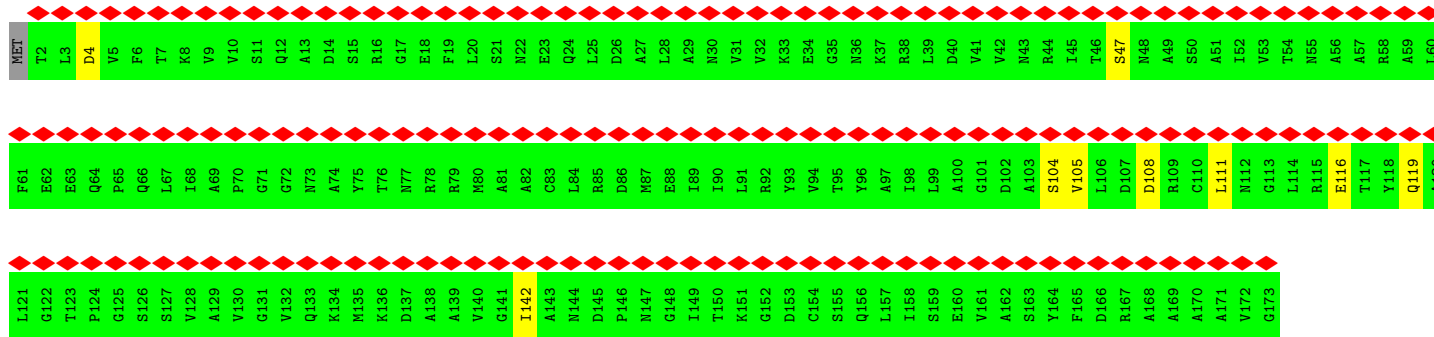




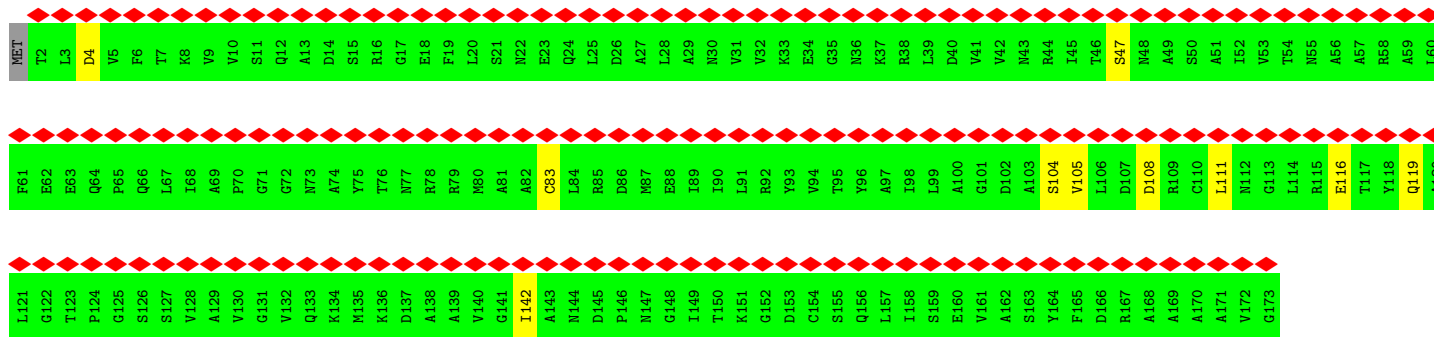
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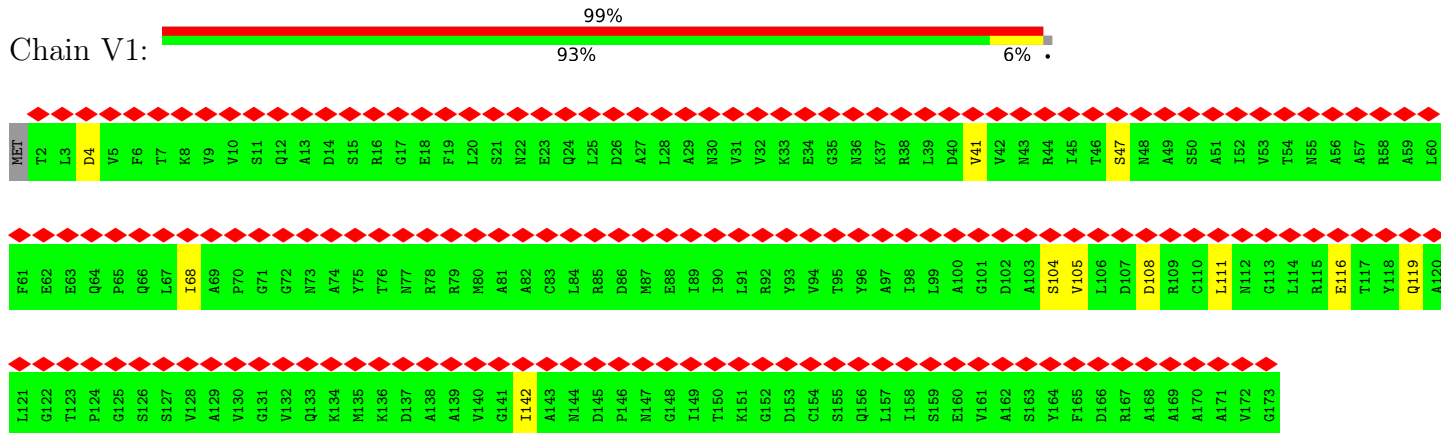
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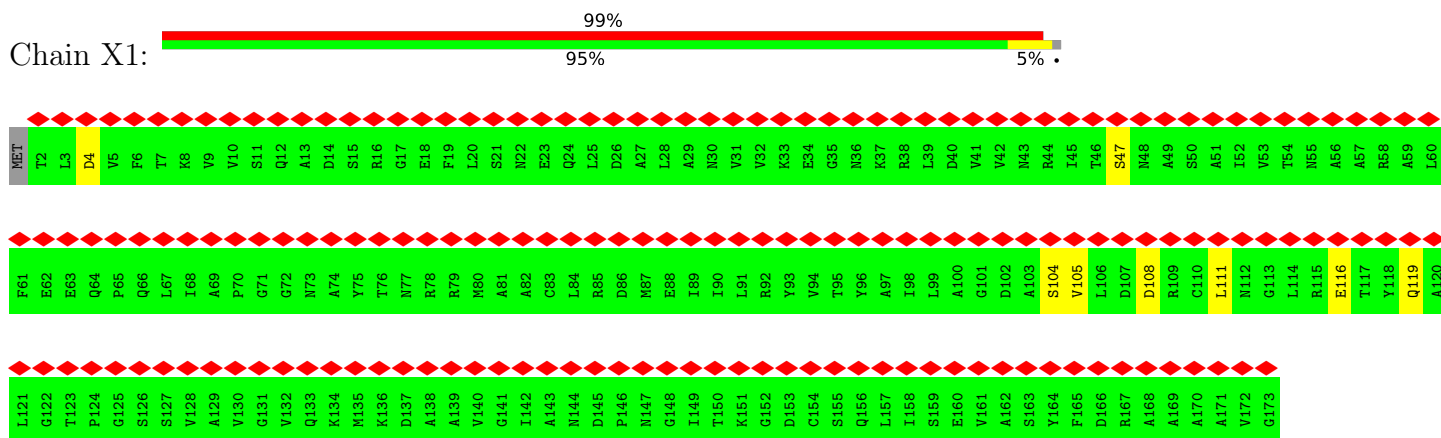
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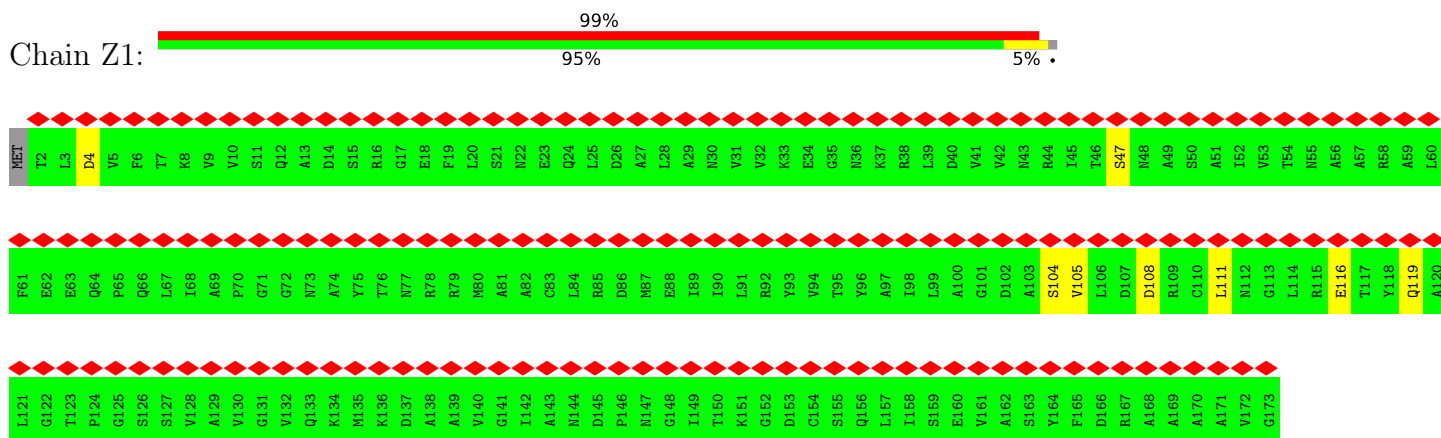
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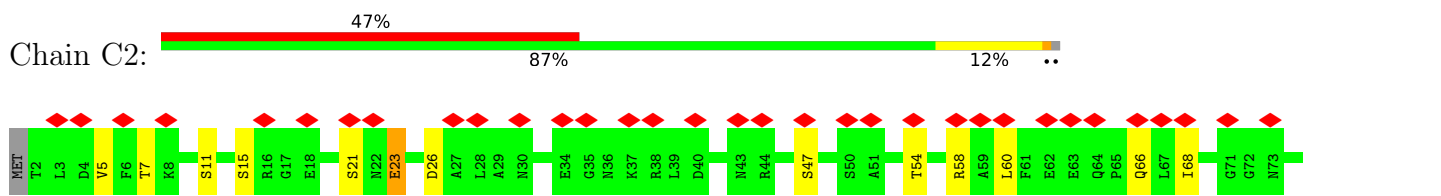
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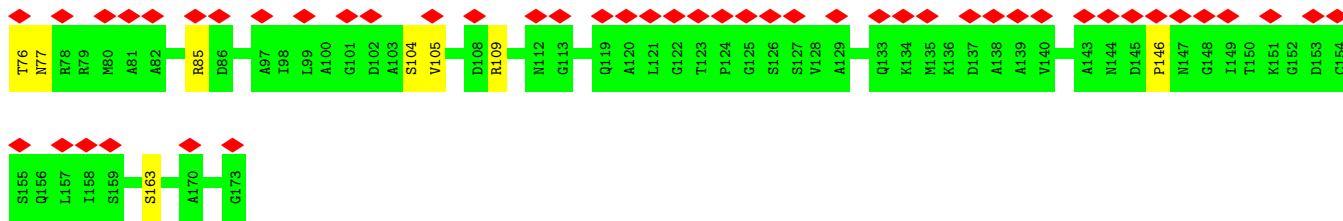


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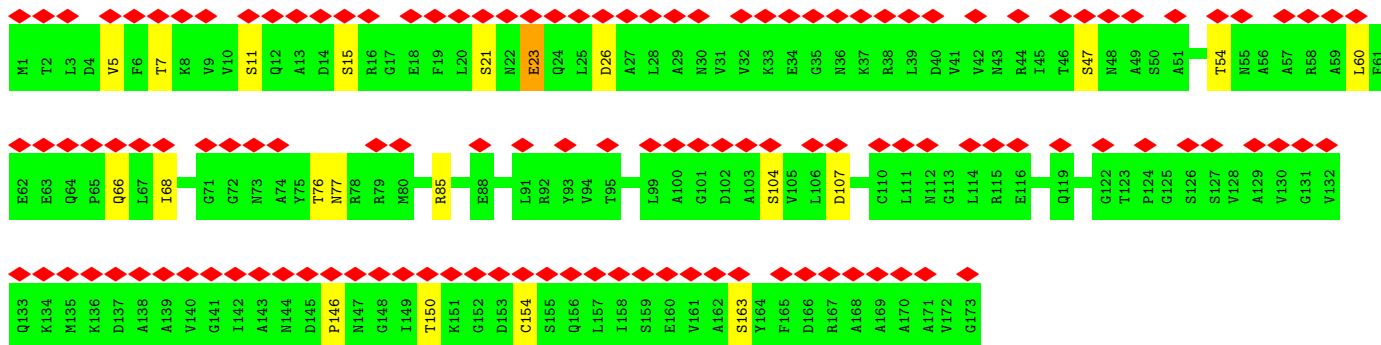
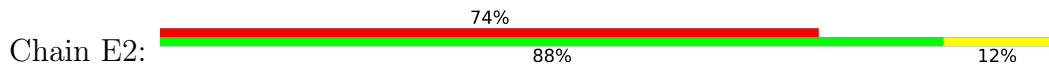


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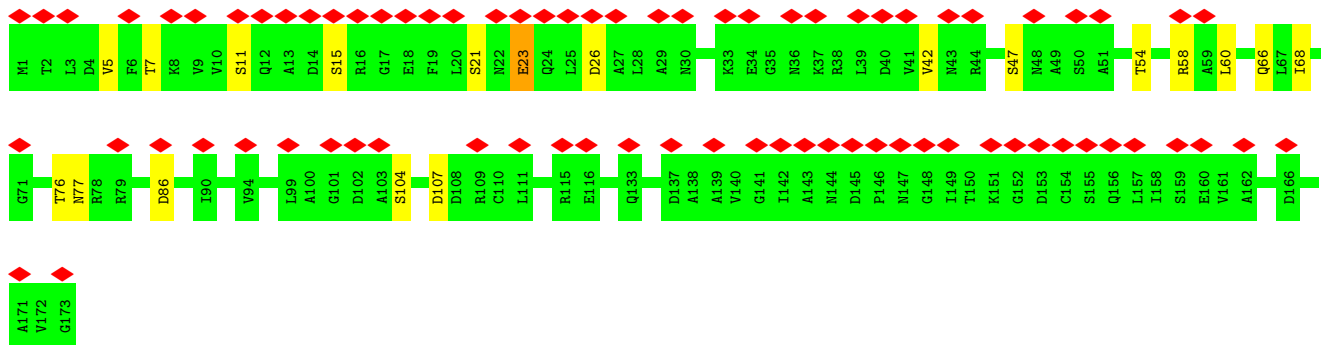
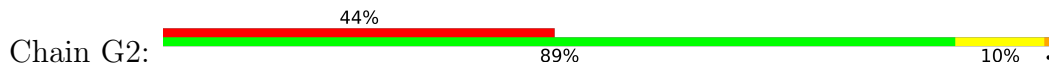




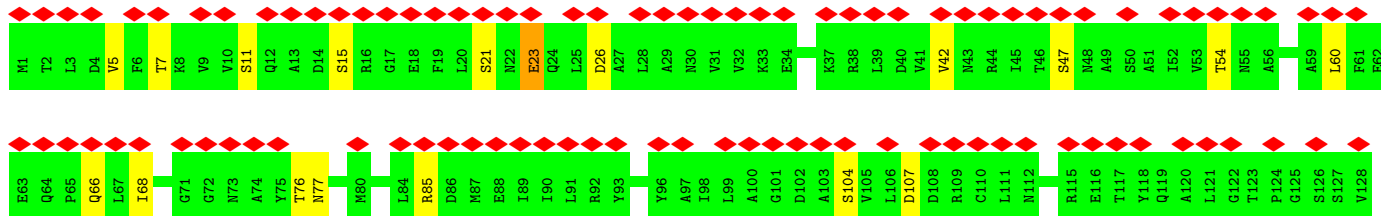
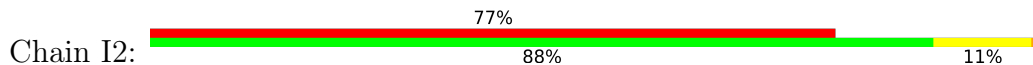
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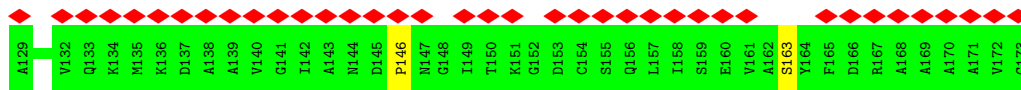


• Molecule 3: C-phycoerythrin beta subunit

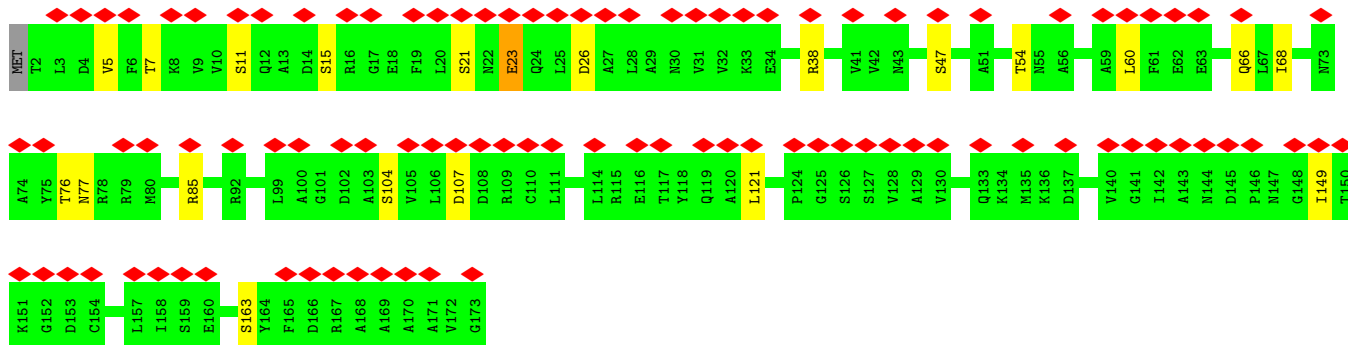
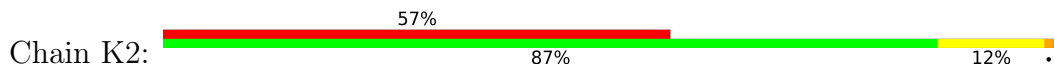


• Molecule 3: C-phycoerythrin beta subunit

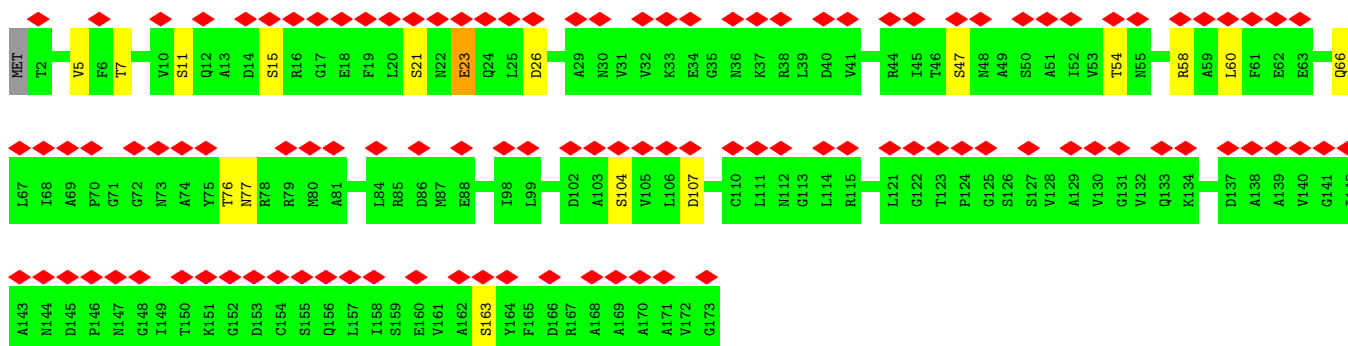
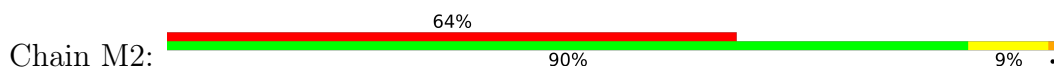




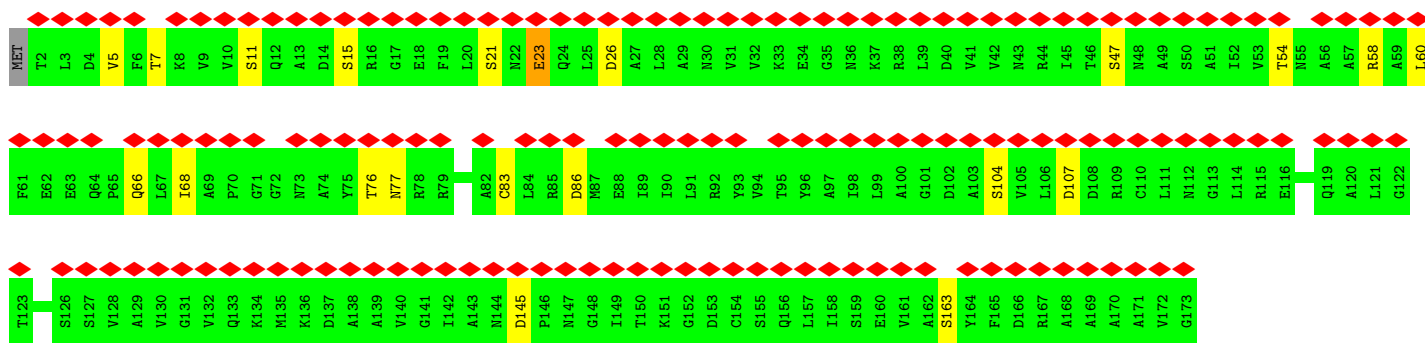
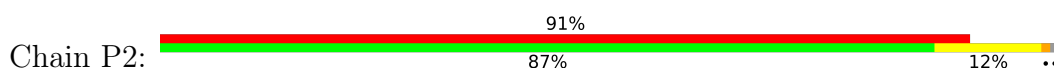
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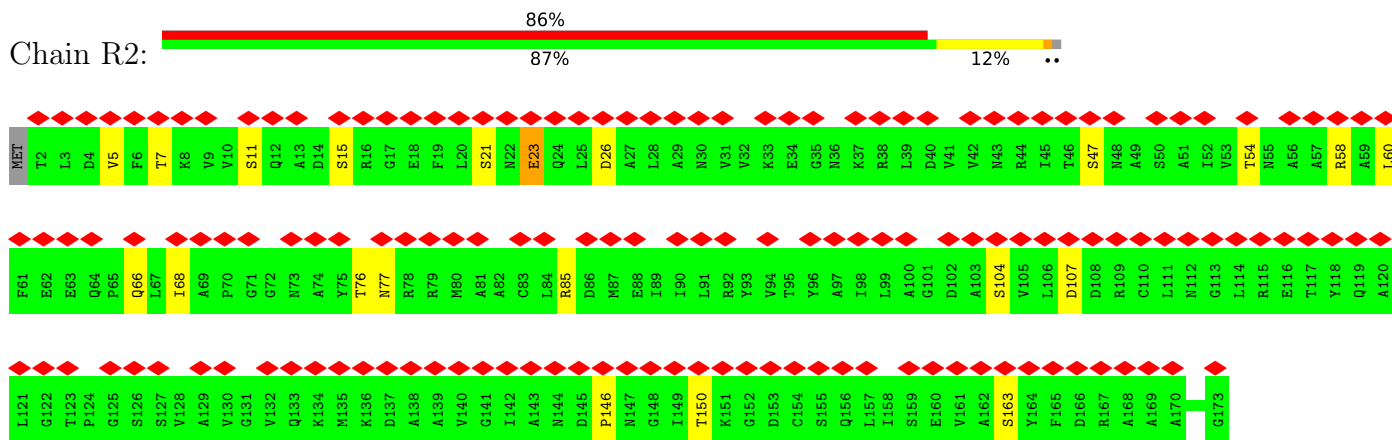
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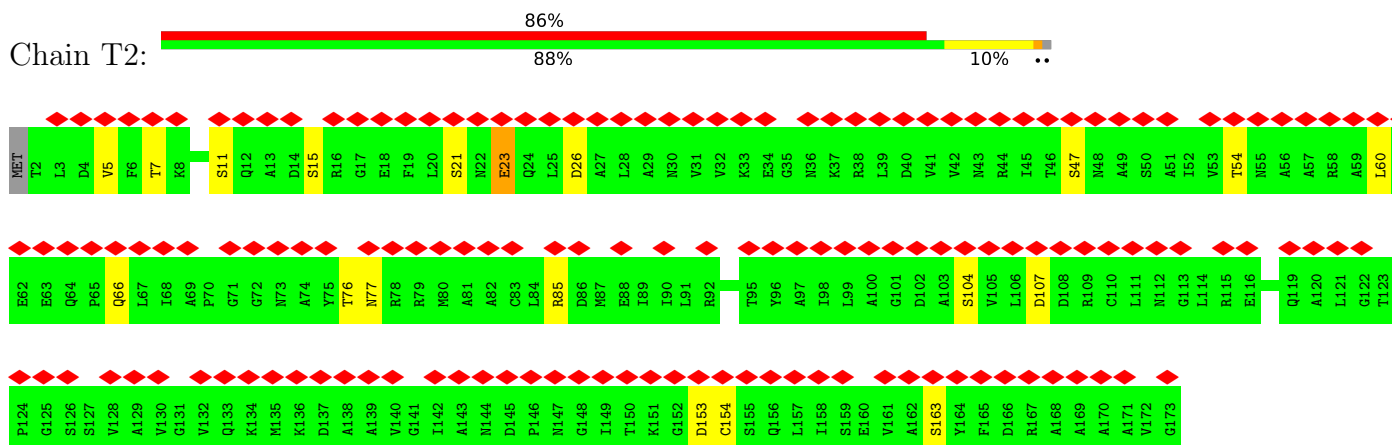
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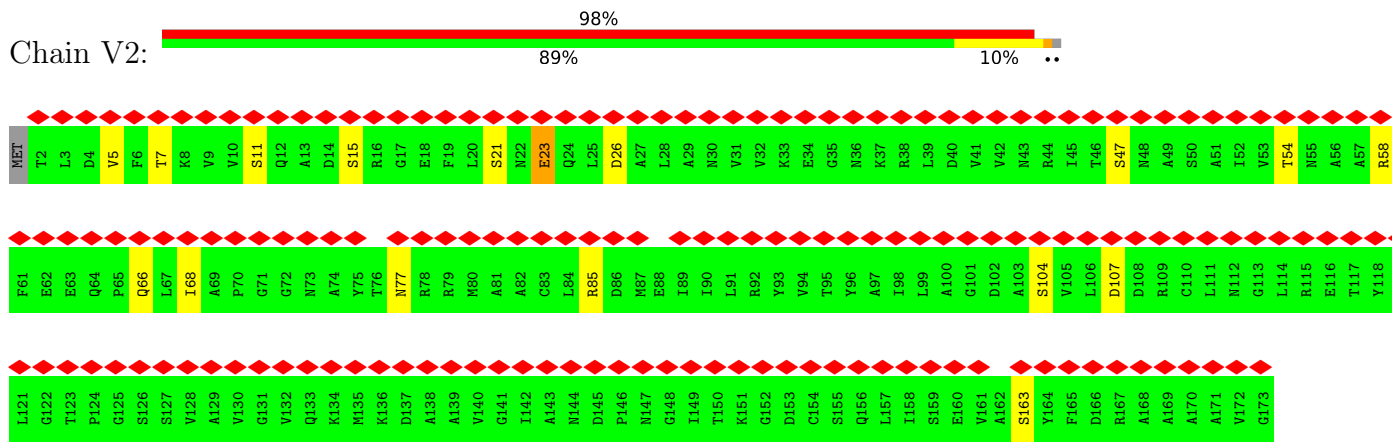
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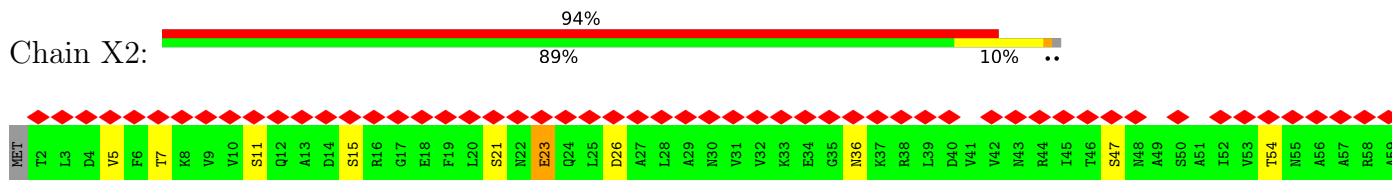
• Molecule 3: C-phycoyanin beta subunit



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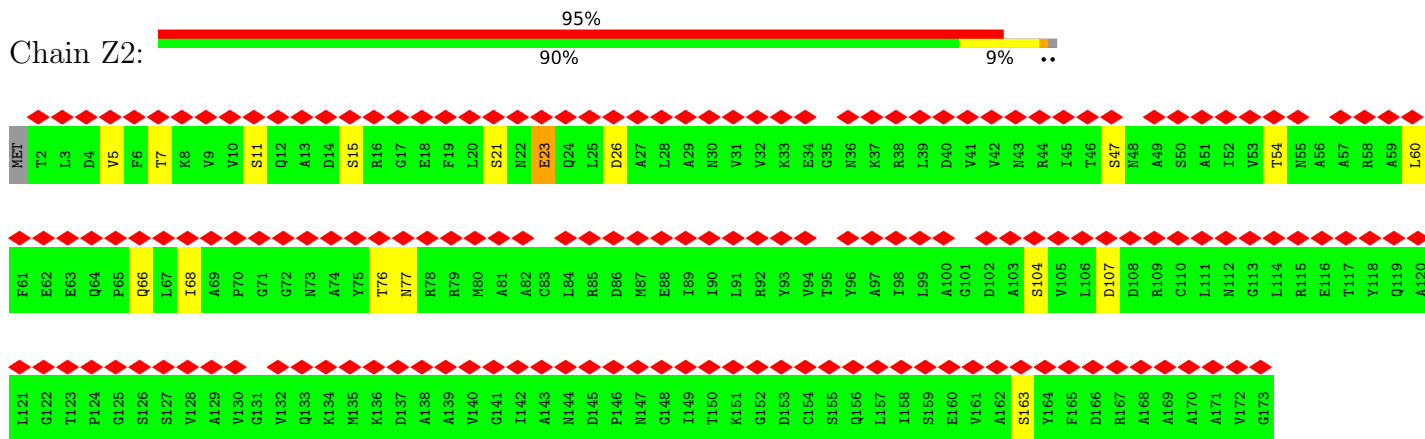


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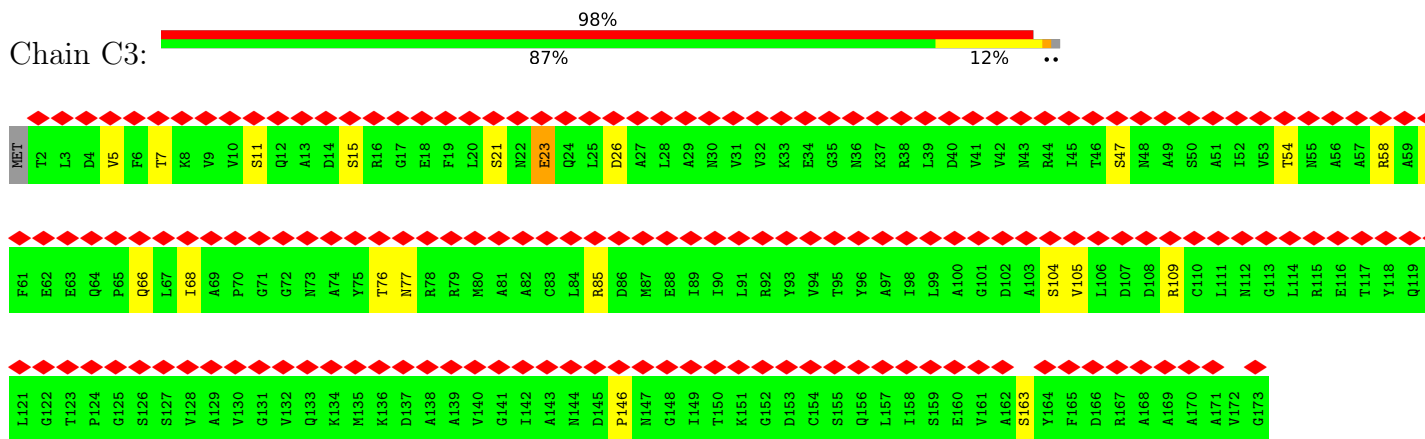




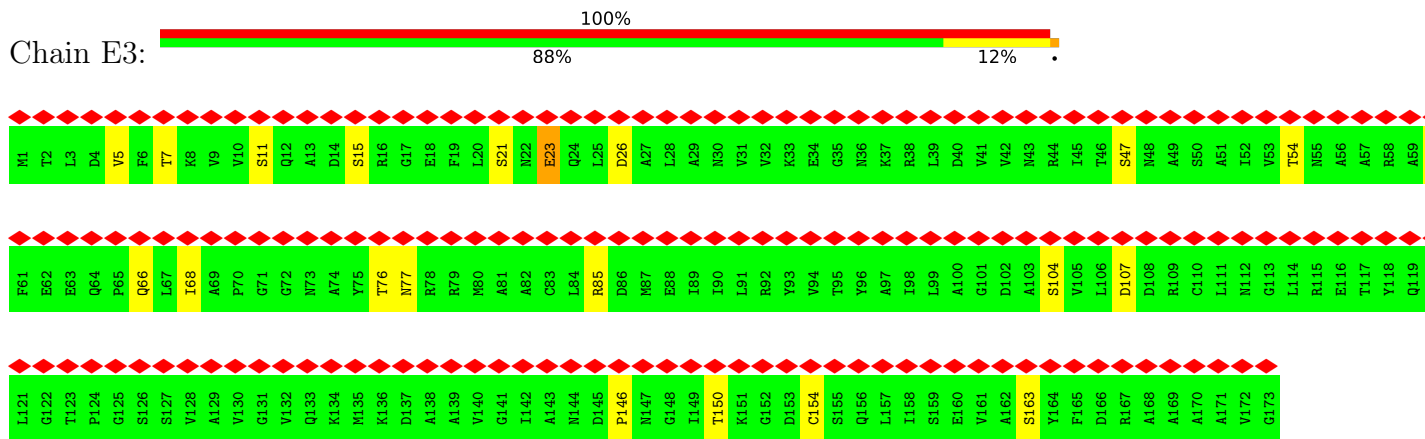
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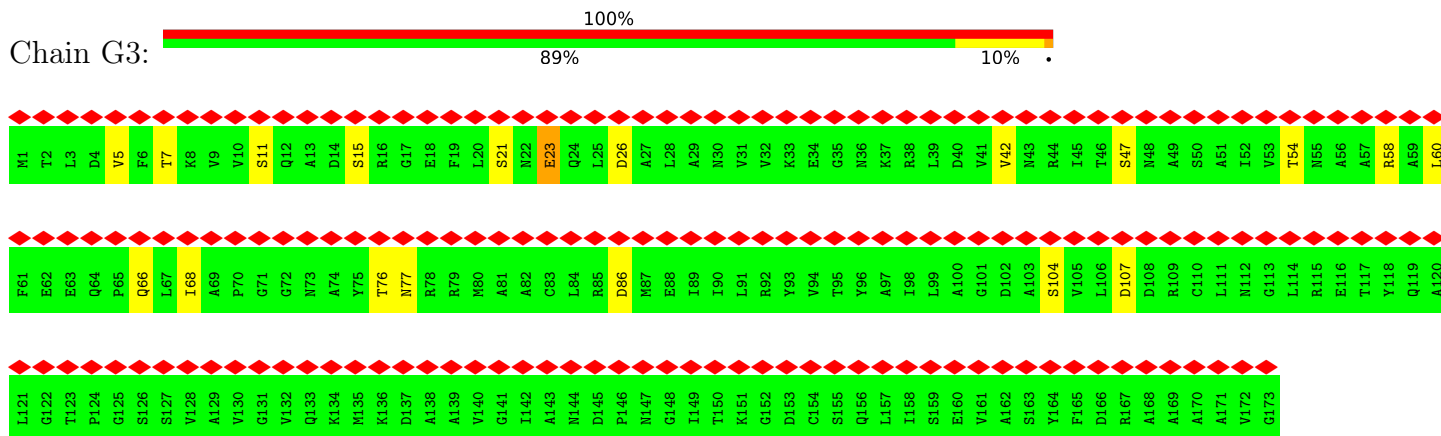
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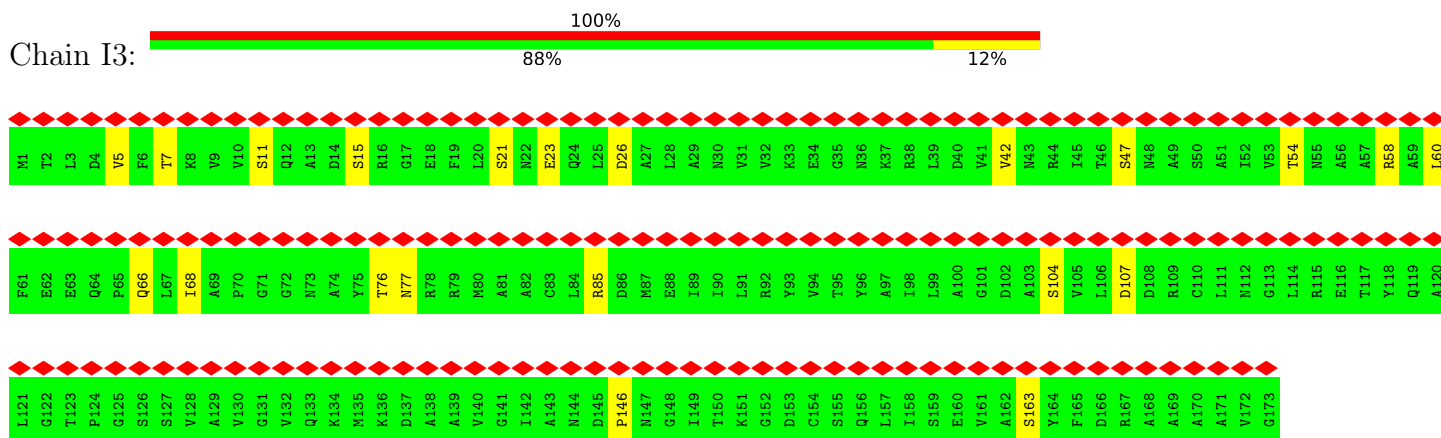
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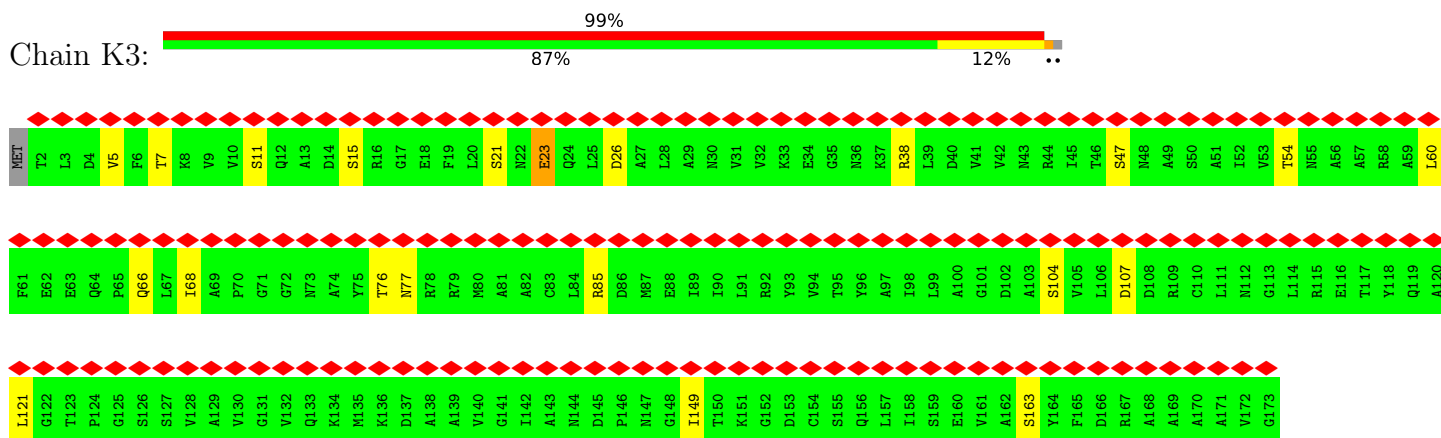
• Molecule 3: C-phycoerythrin beta subunit



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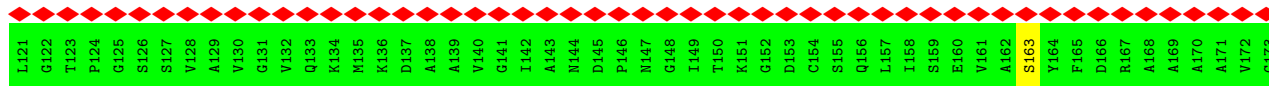
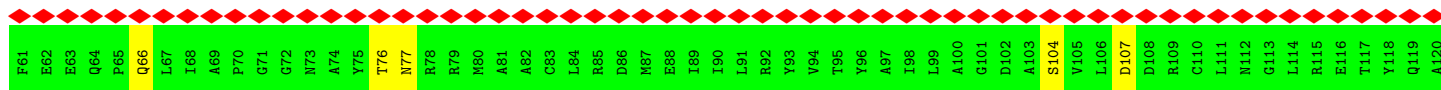


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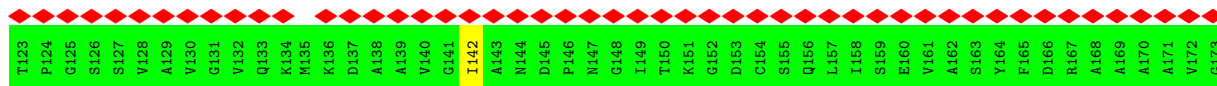
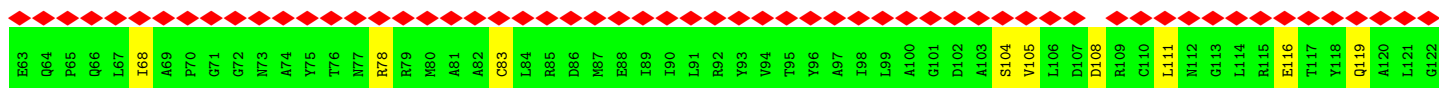
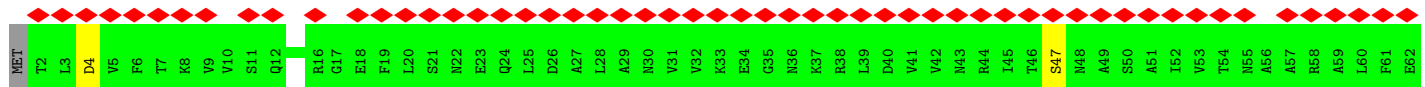
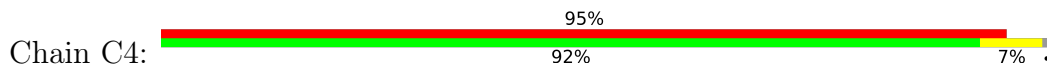


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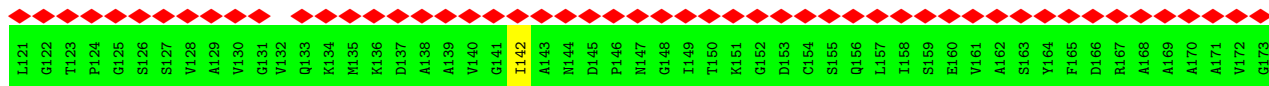
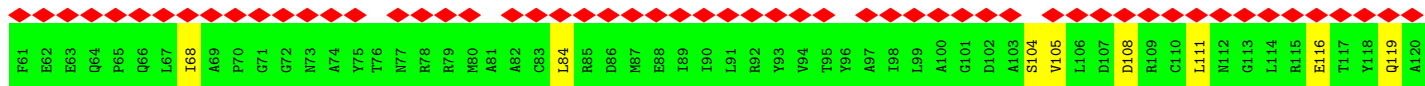
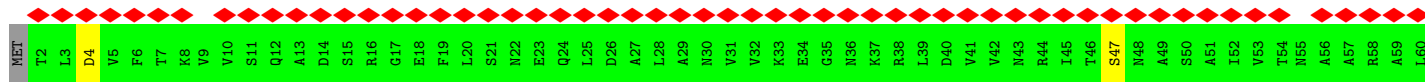




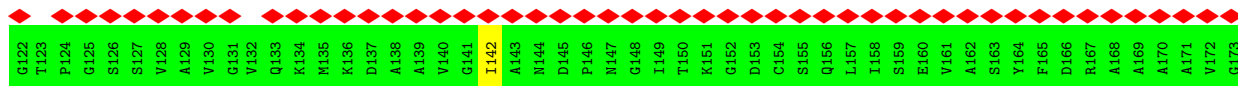
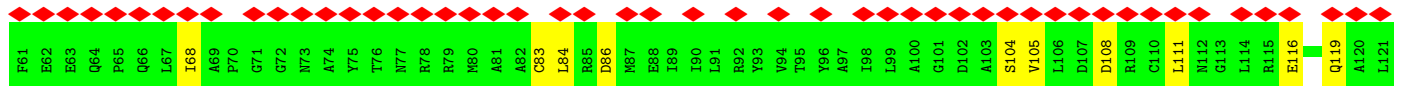
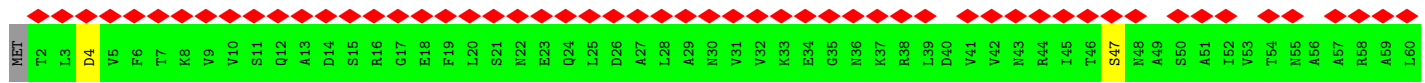
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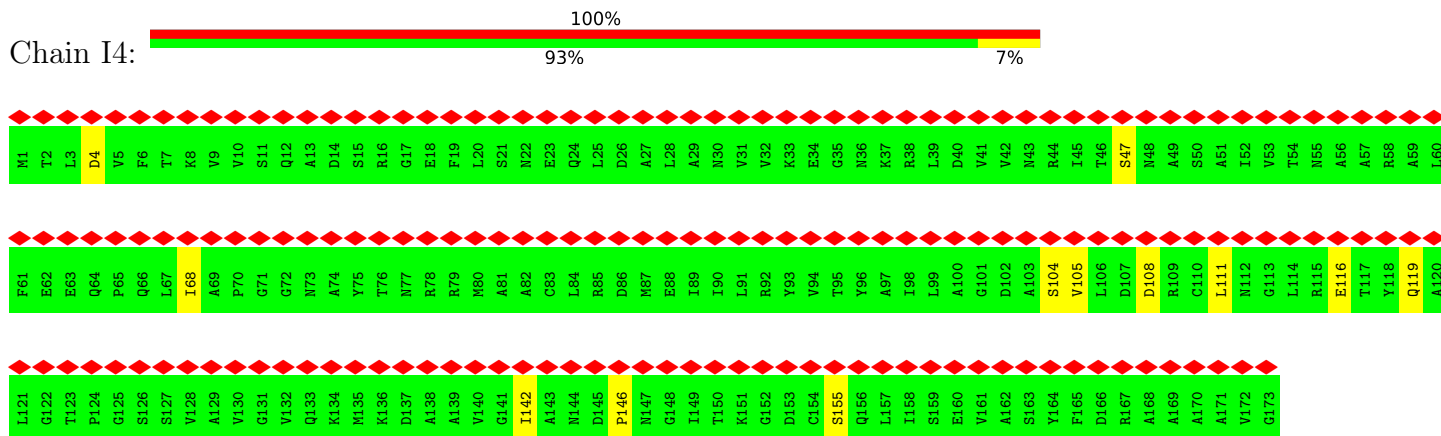
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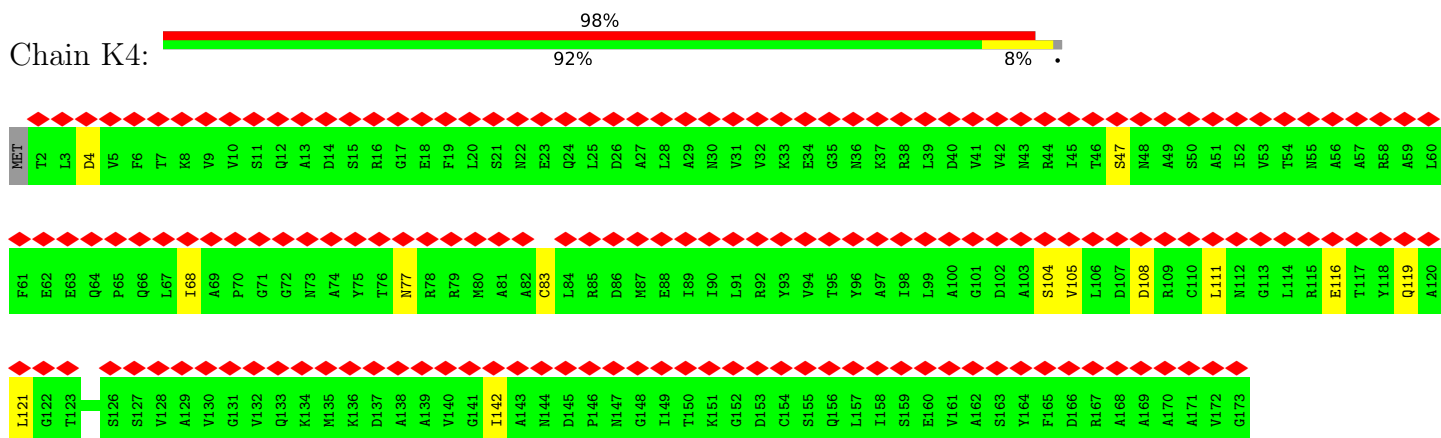
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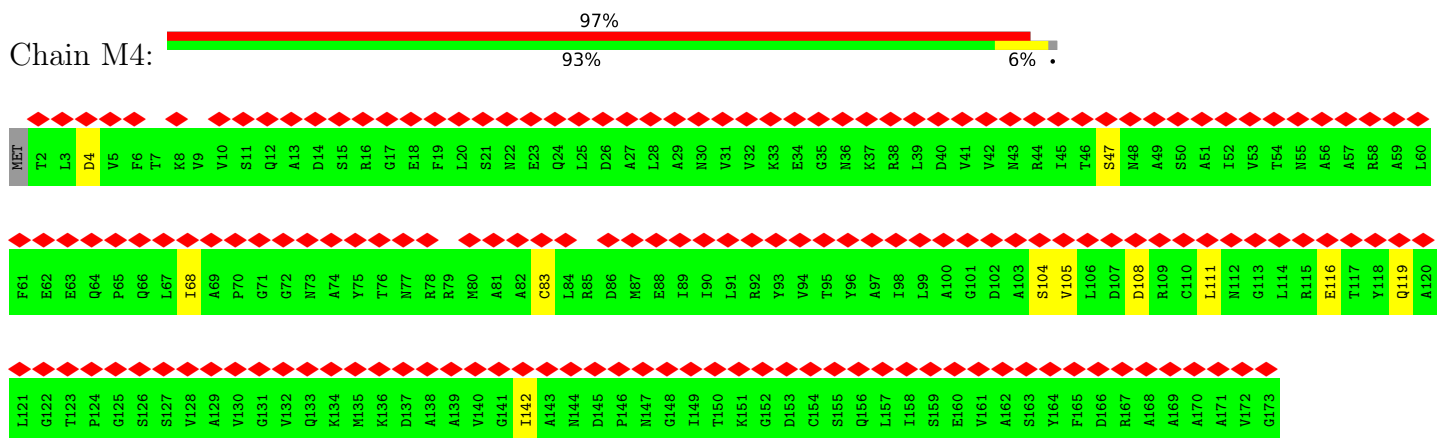
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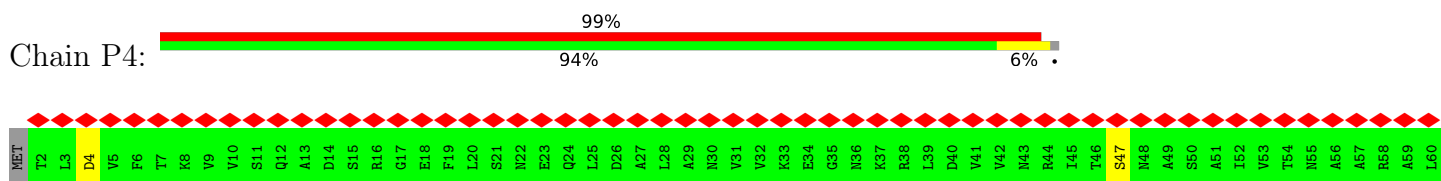
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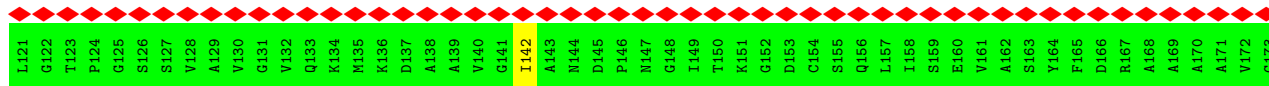
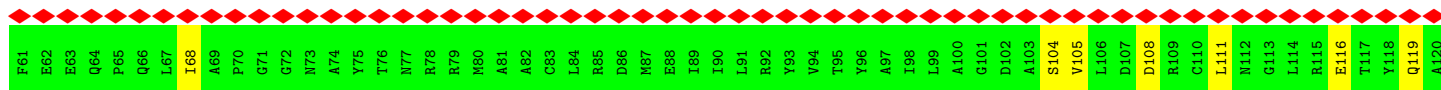


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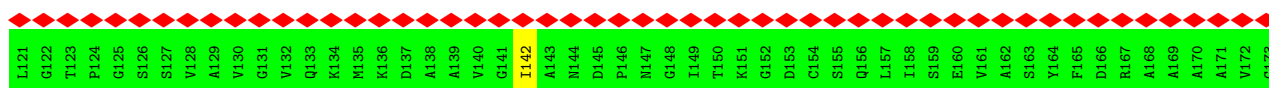
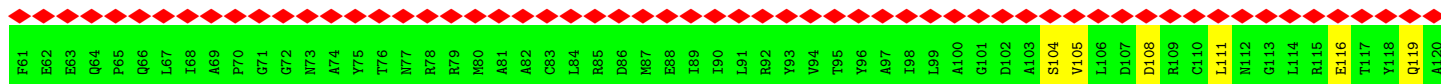
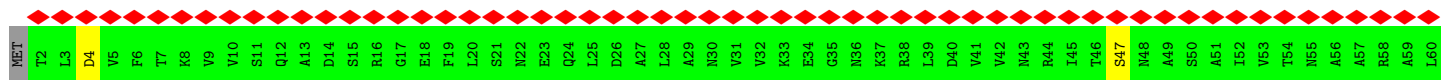


• Molecule 3: C-phycoerythrin beta subunit

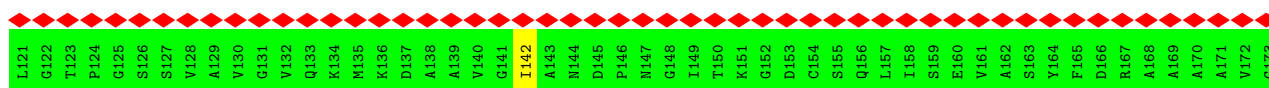
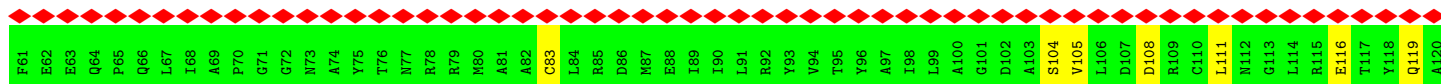
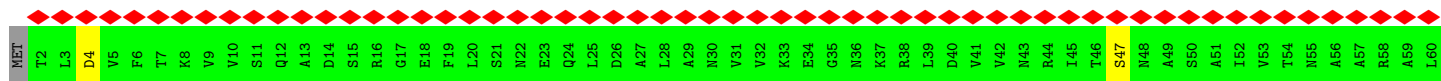




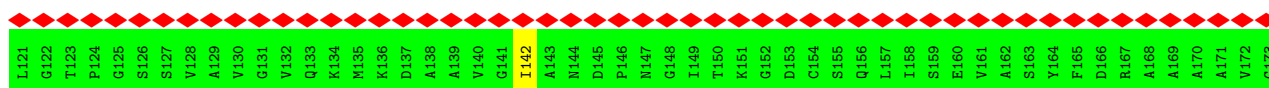
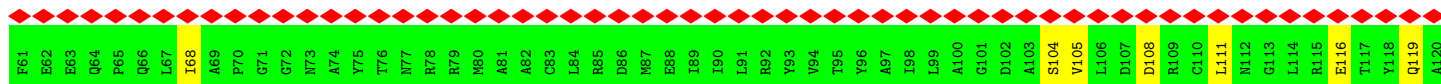
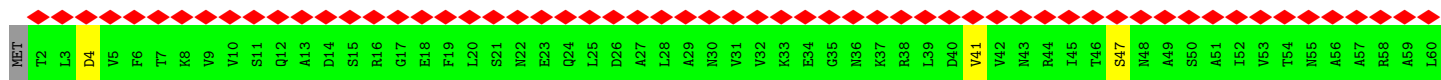
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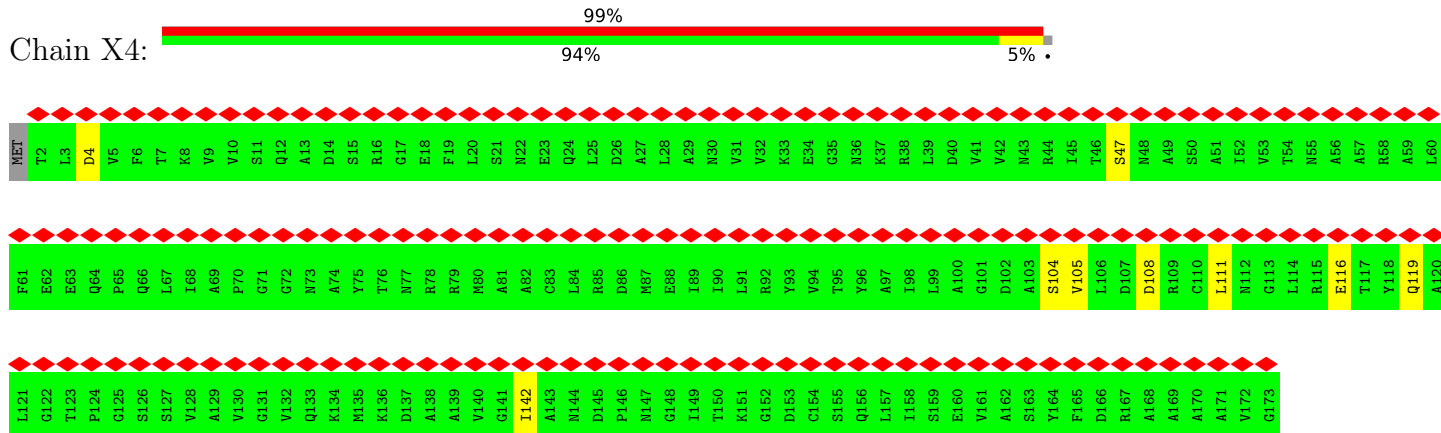
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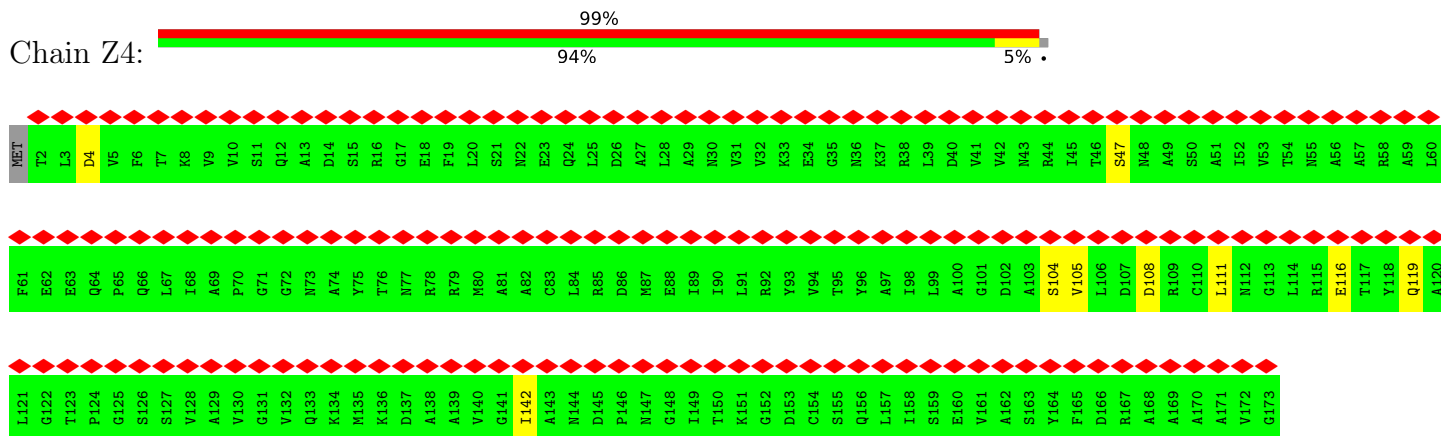
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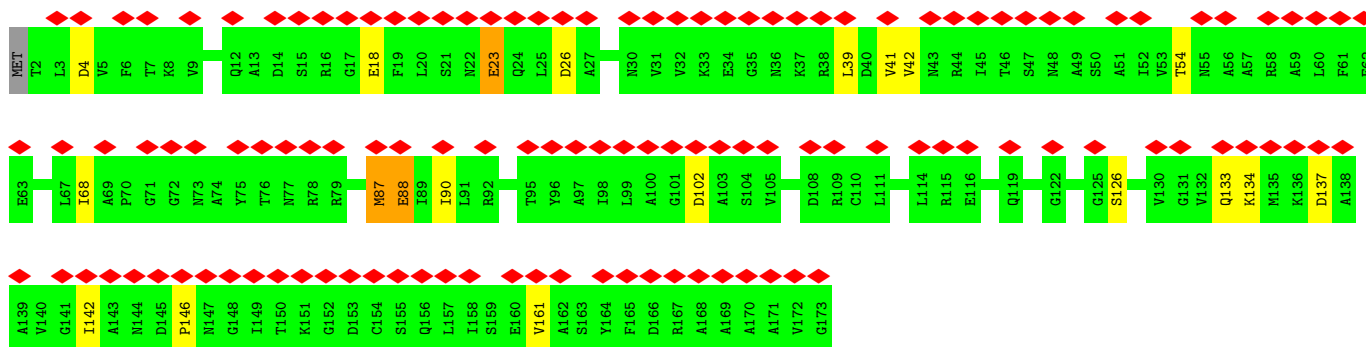


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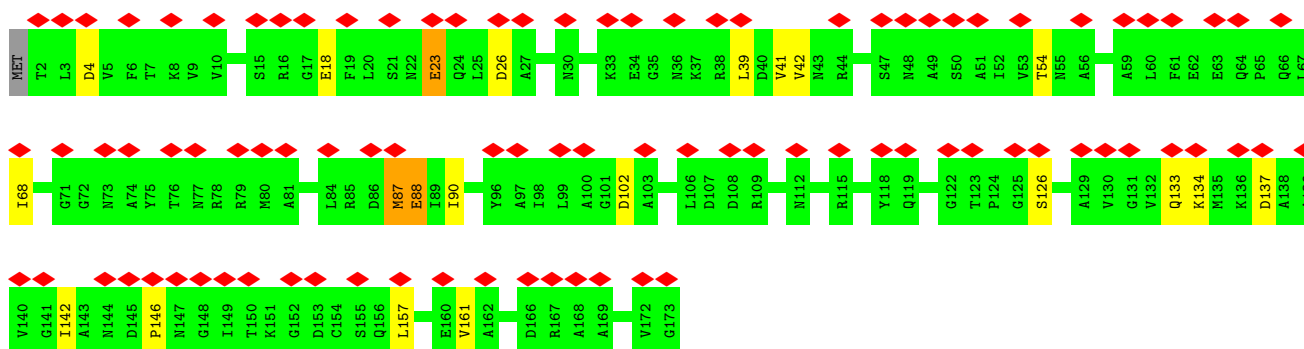


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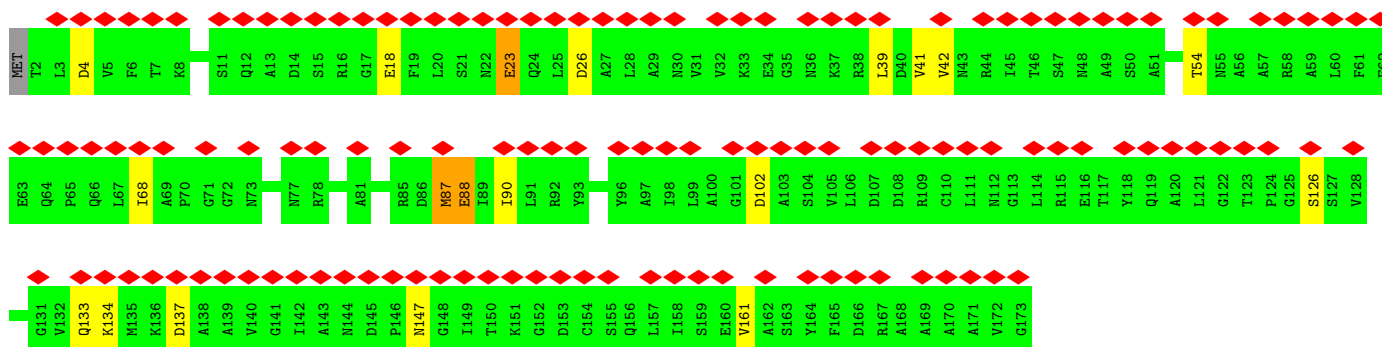
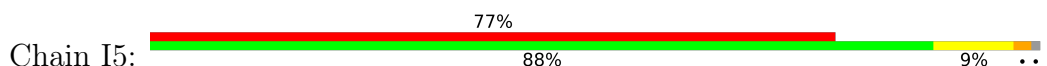




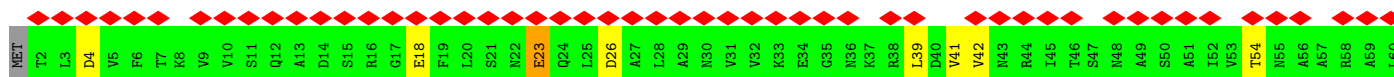
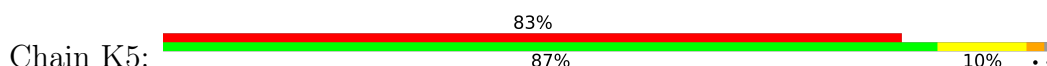
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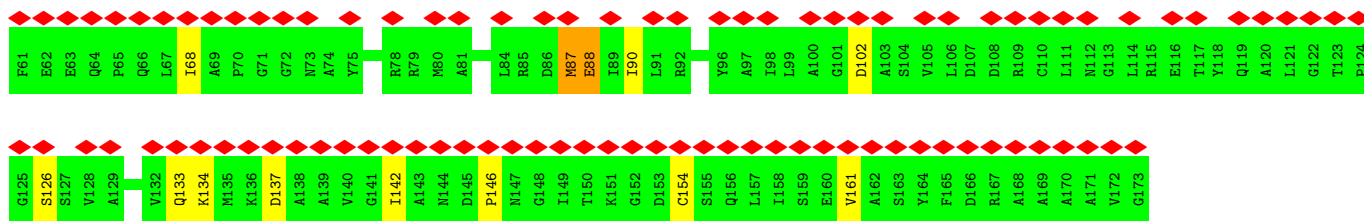


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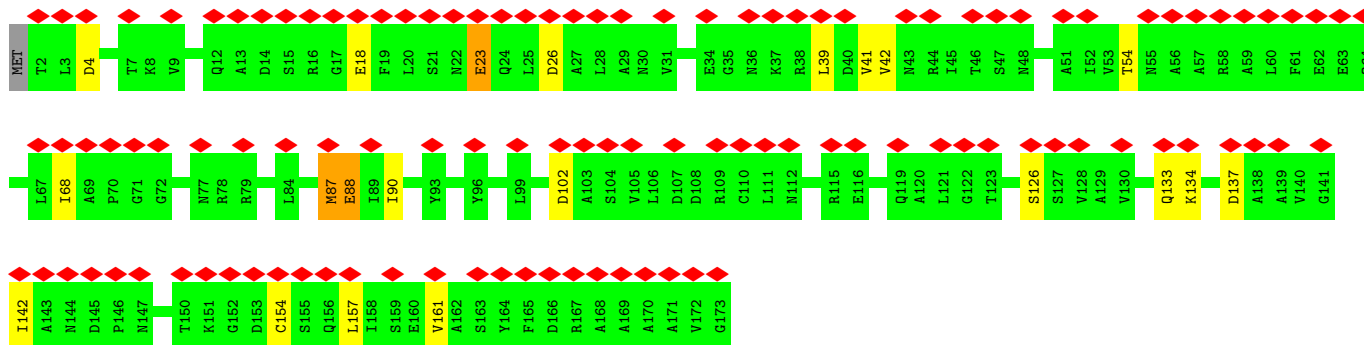
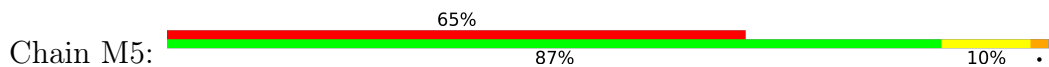


• Molecule 3: C-phycoerythrin beta subunit

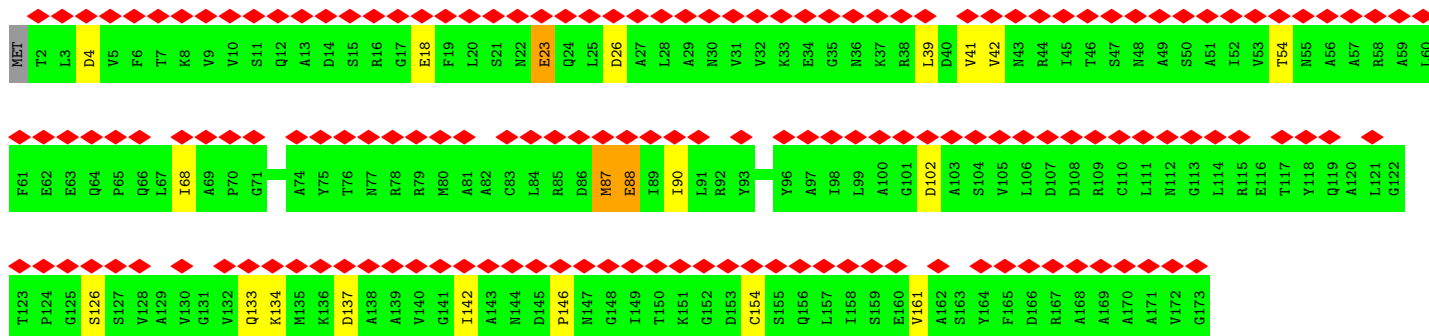
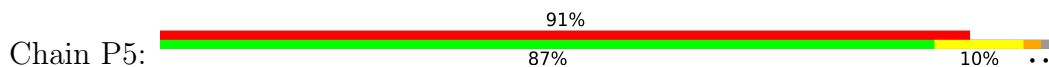




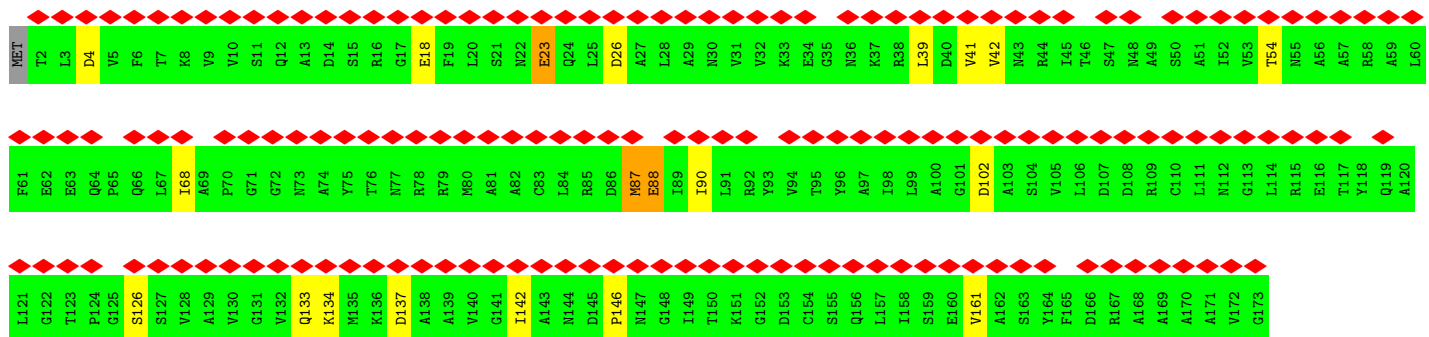
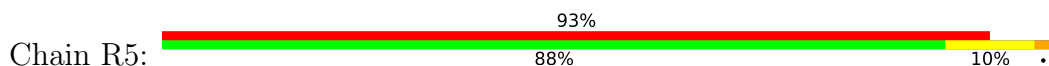
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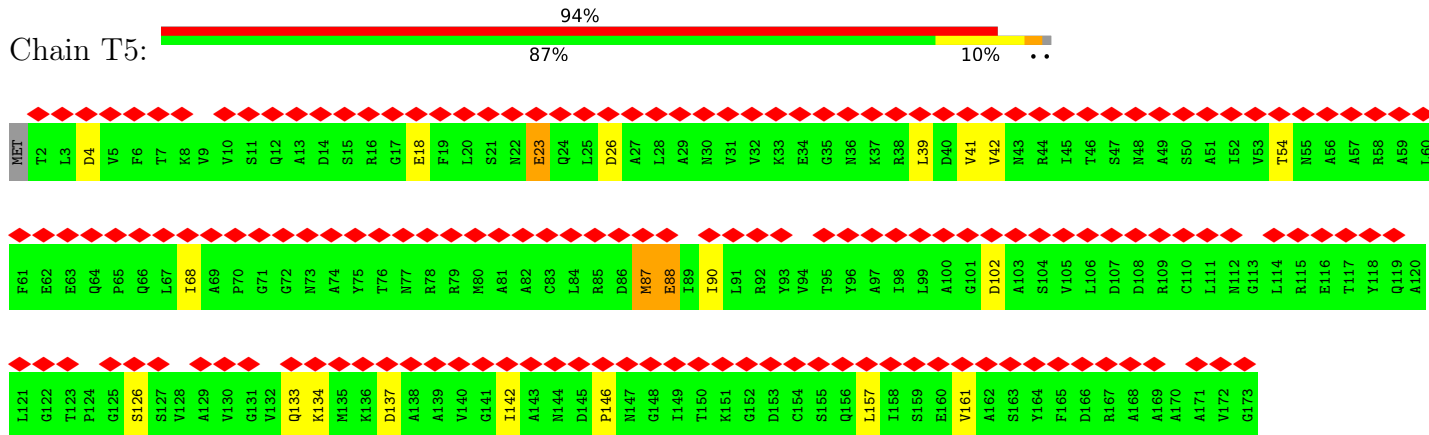
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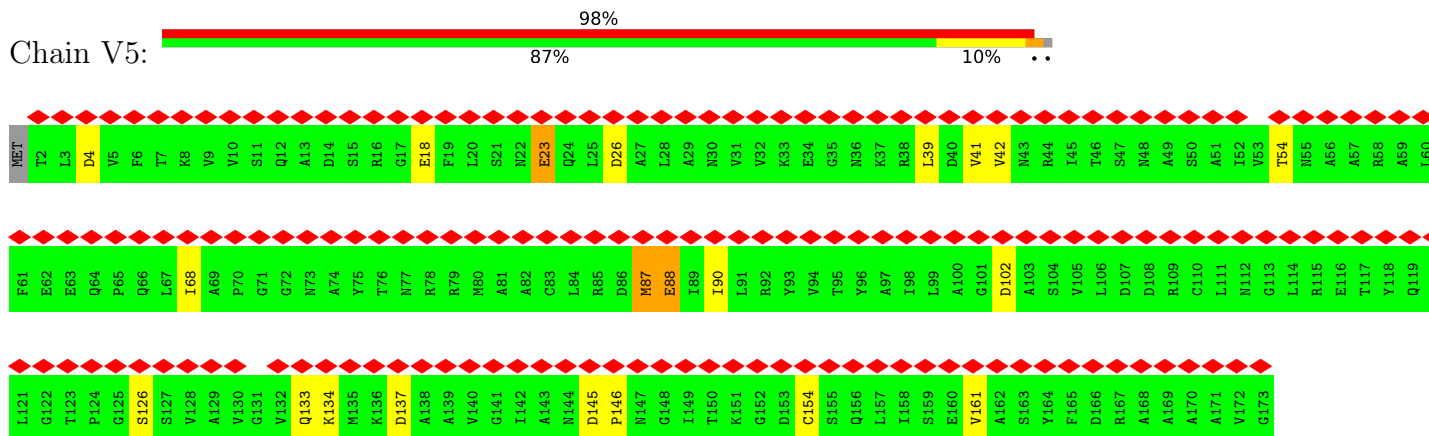
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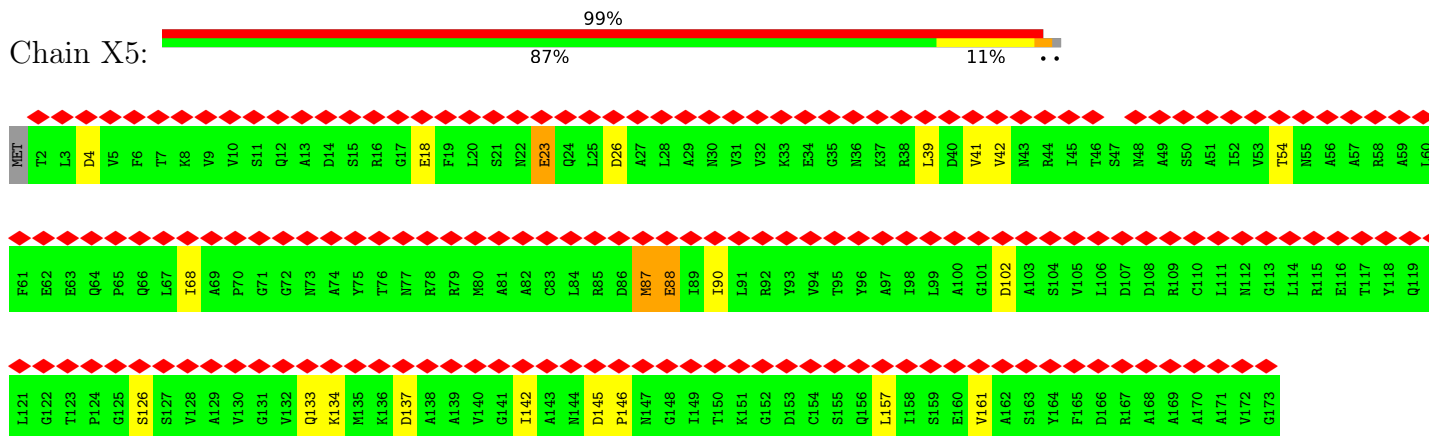
• Molecule 3: C-phycoerythrin beta subunit



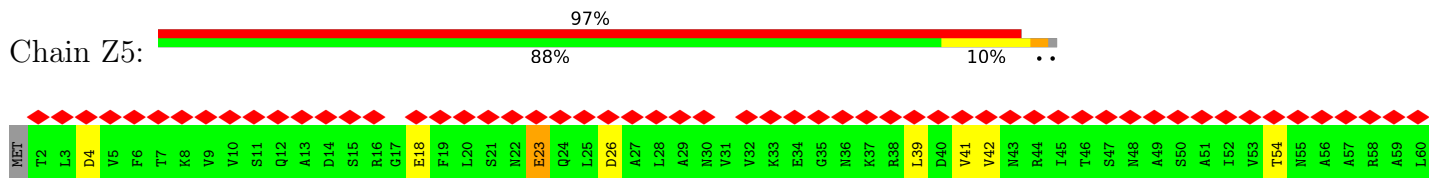
• Molecule 3: C-phycoerythrin beta subunit

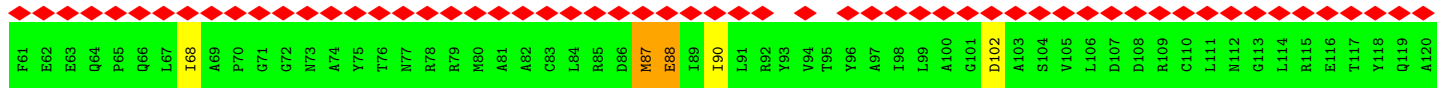


• Molecule 3: C-phycoerythrin beta subunit

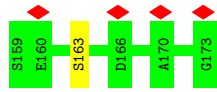
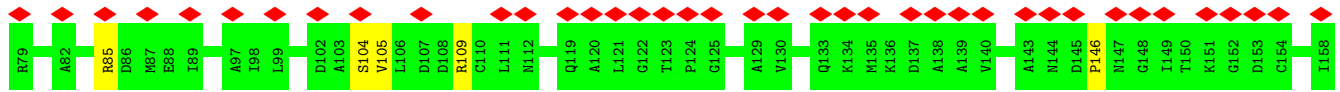
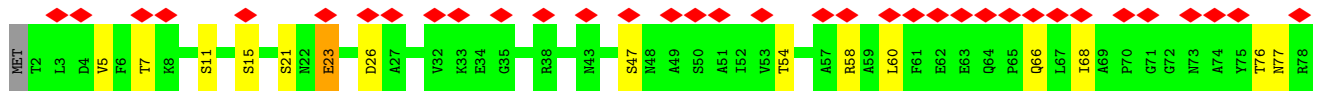
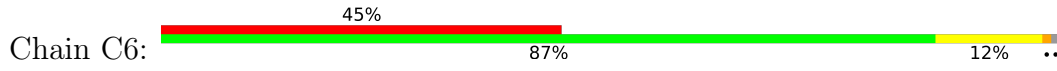


• Molecule 3: C-phycoerythrin beta subunit

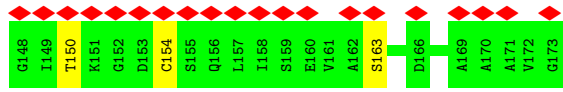
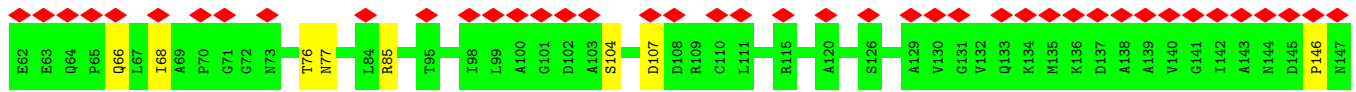
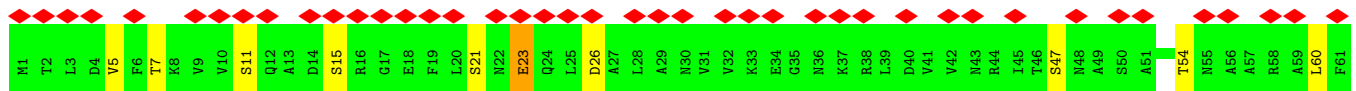
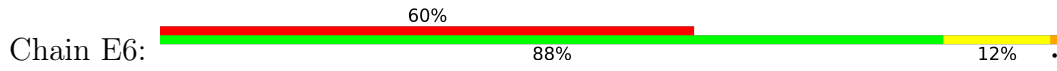




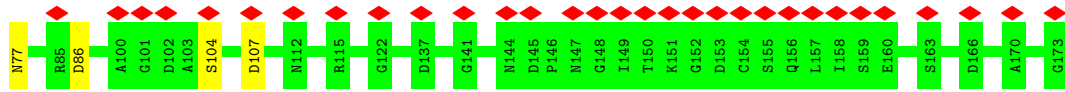
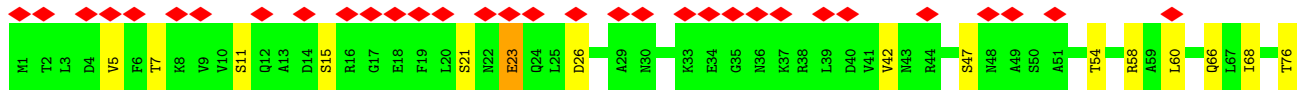
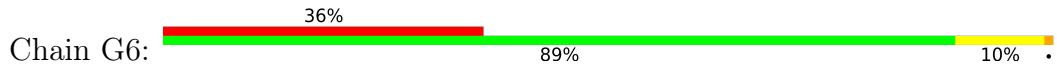
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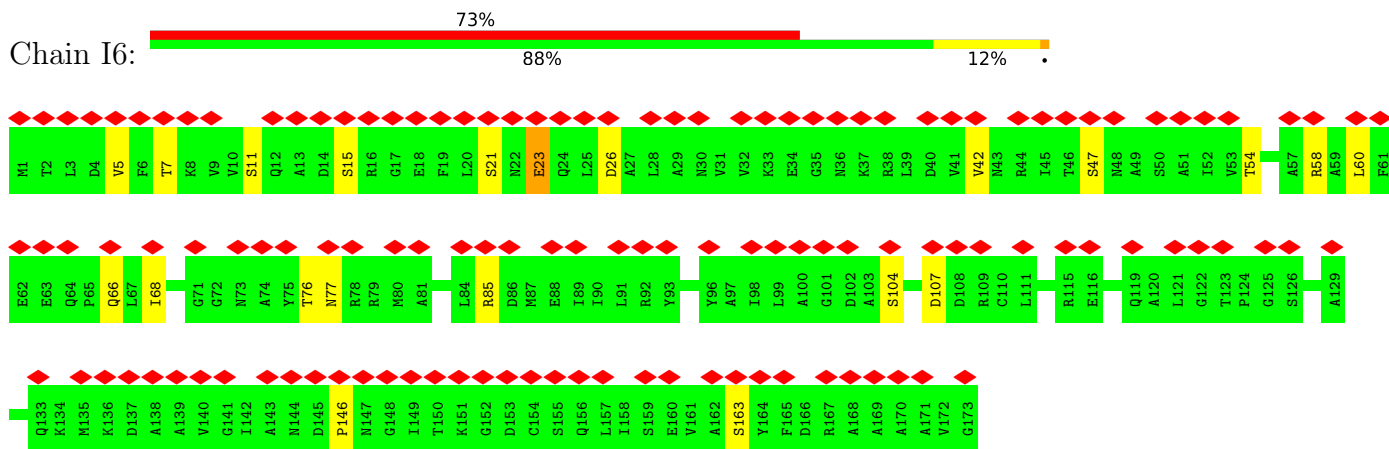
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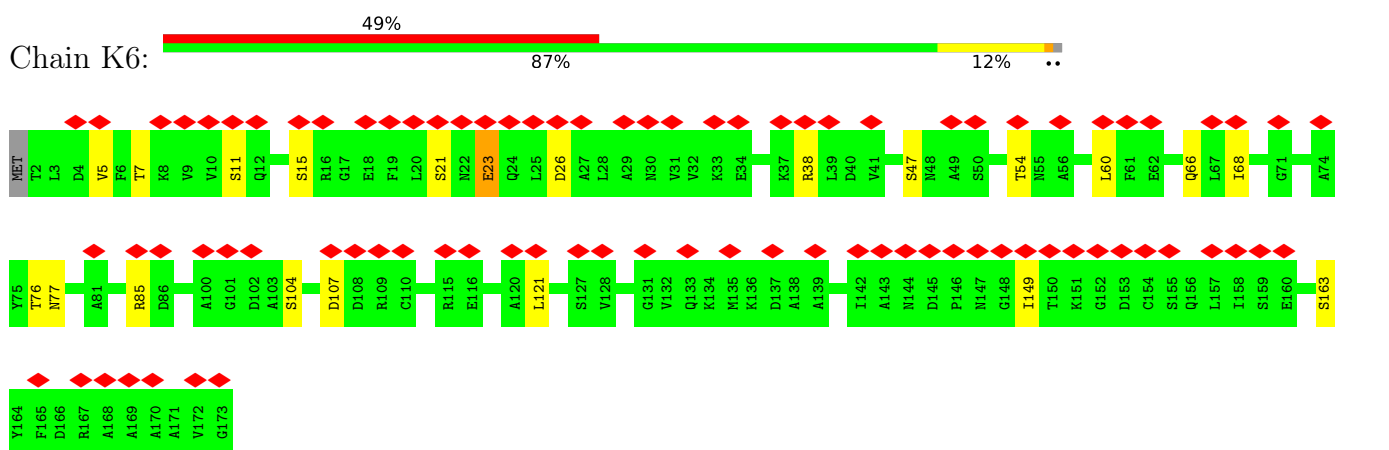
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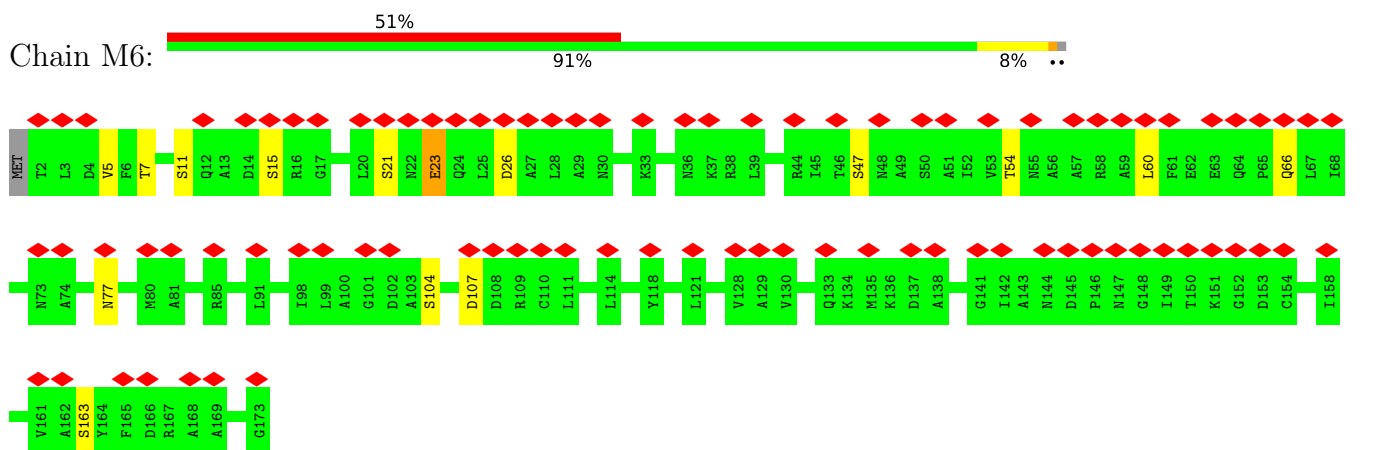
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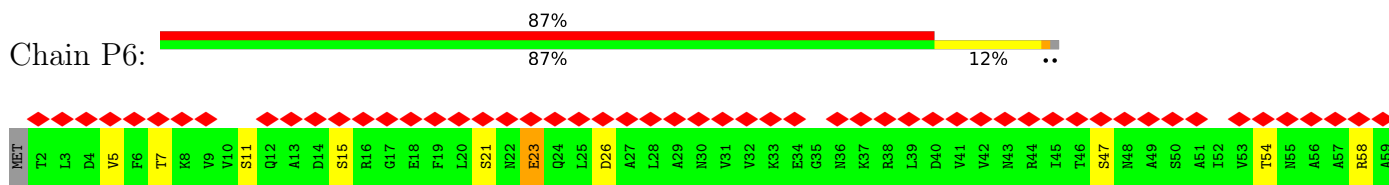
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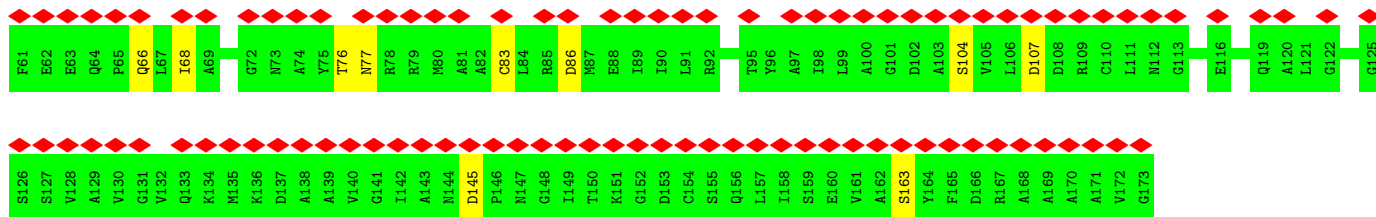


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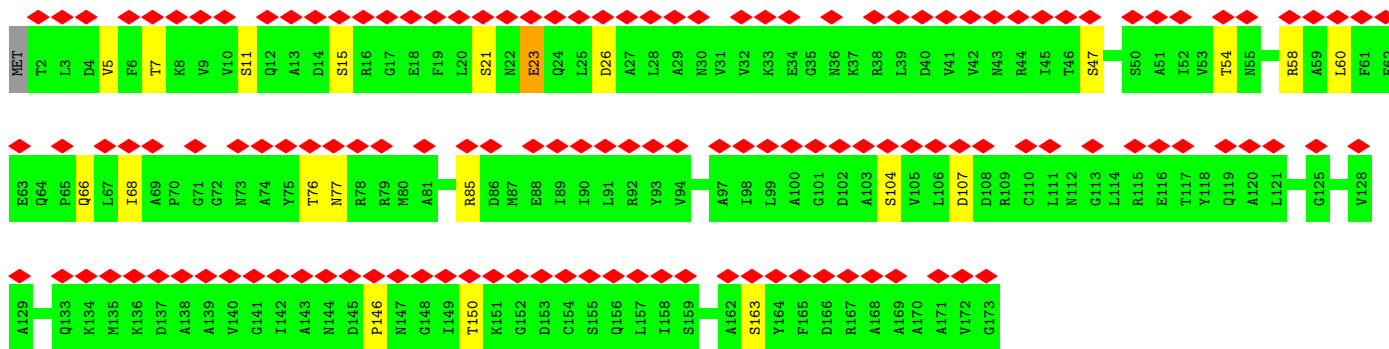
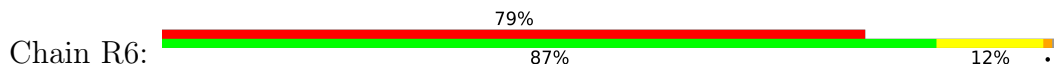


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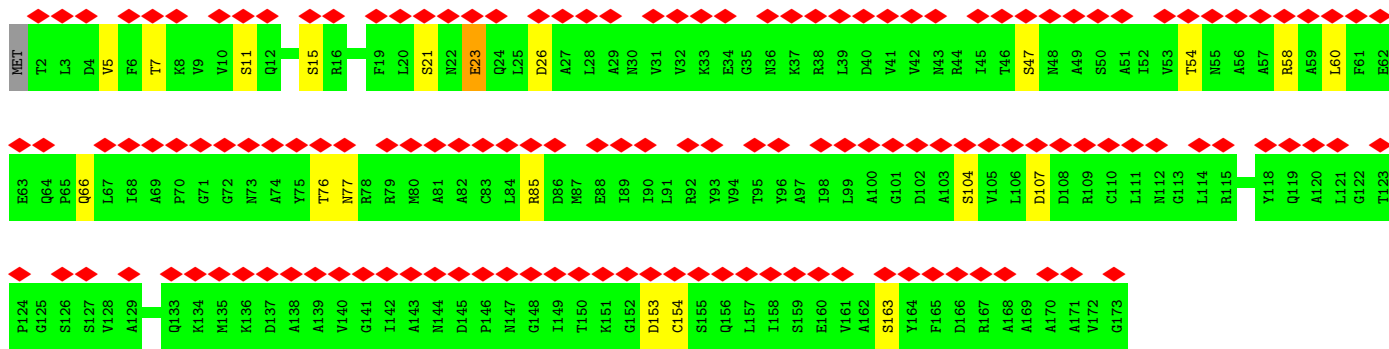
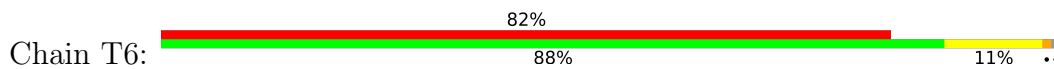




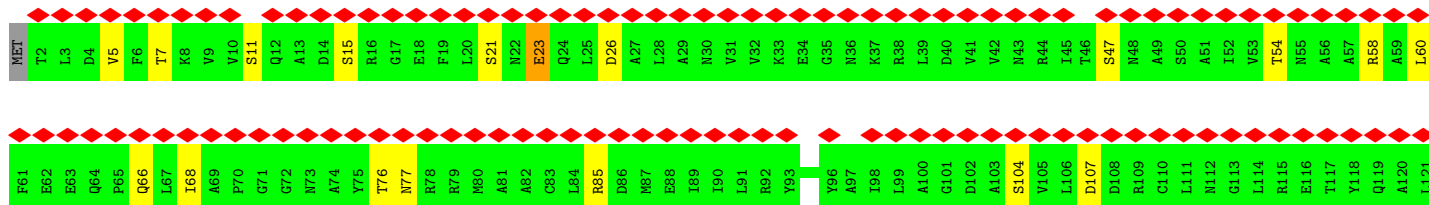
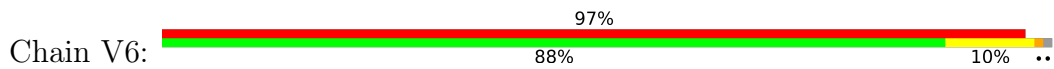
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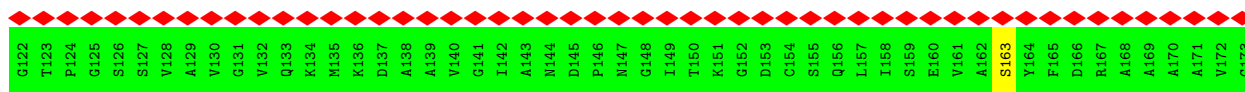


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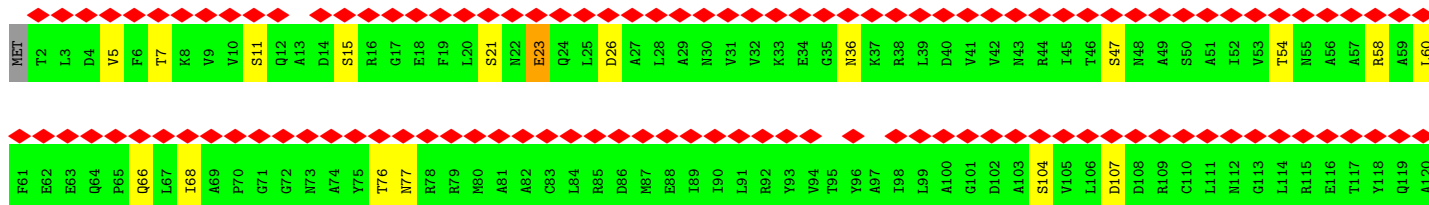
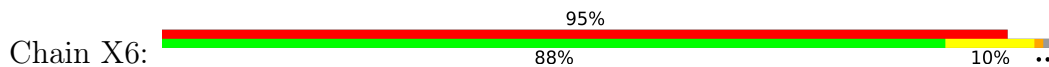


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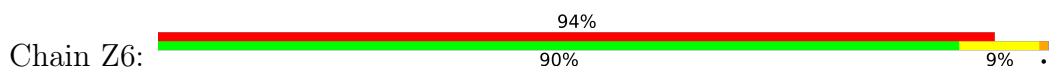




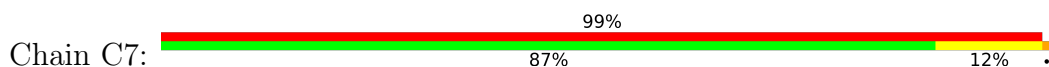
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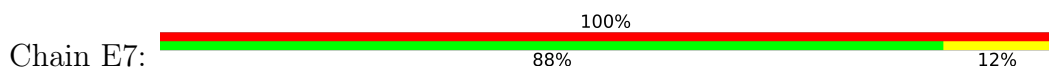
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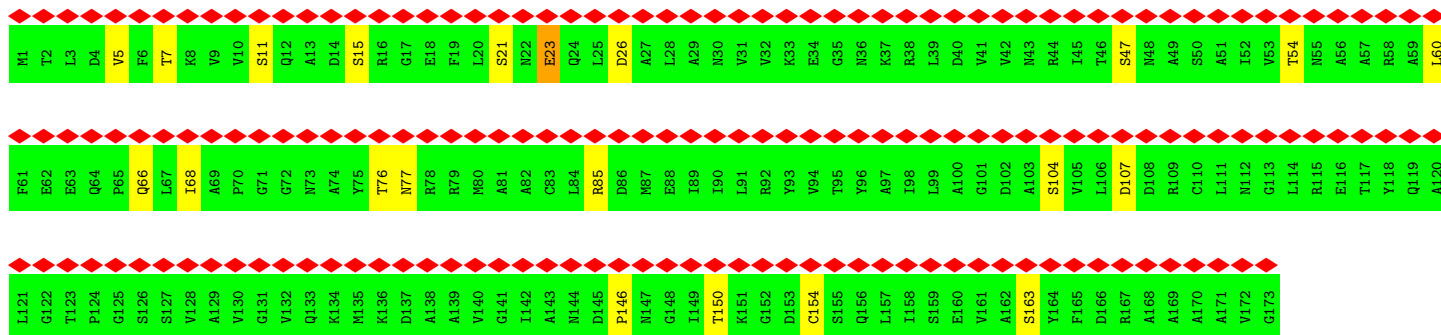


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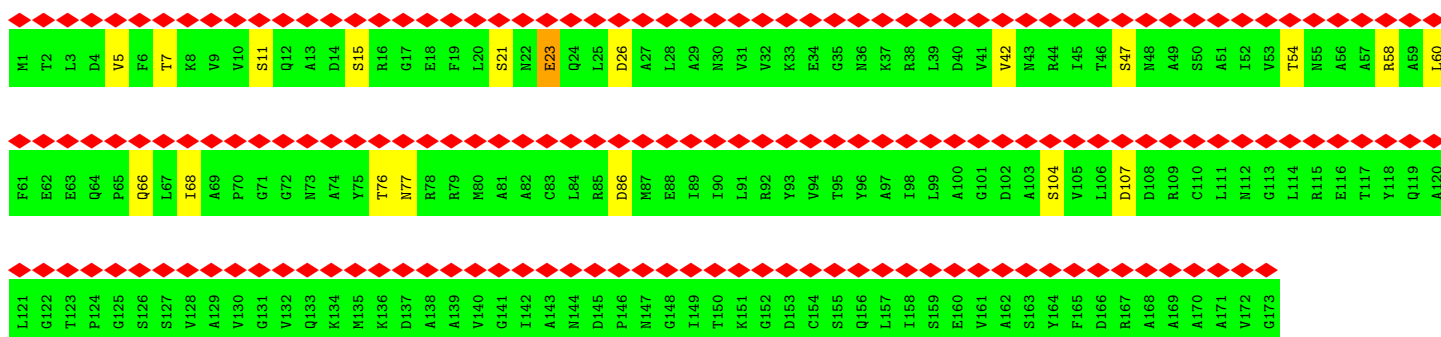
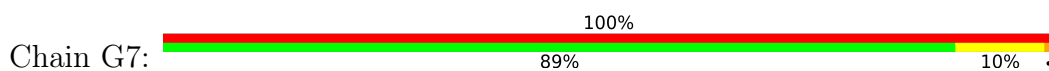


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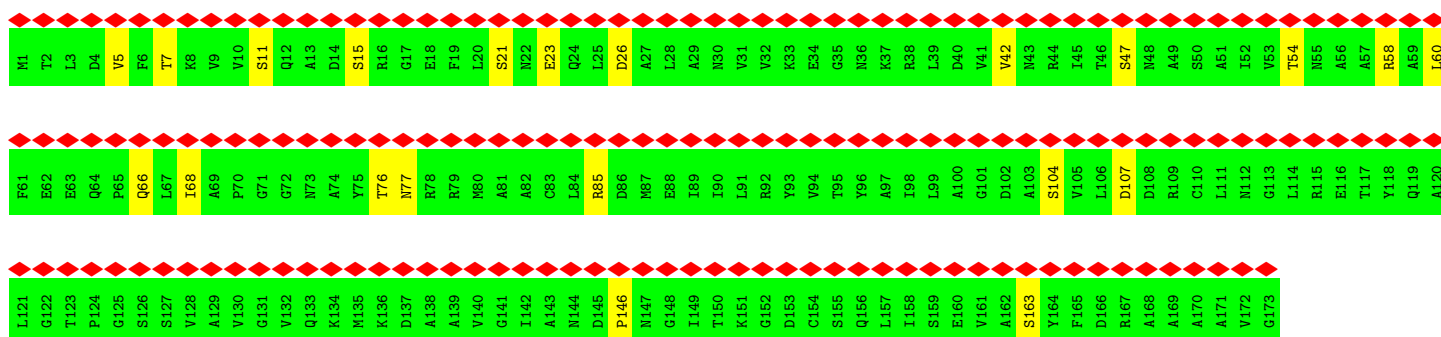
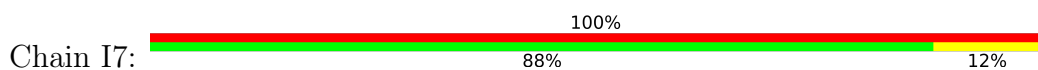




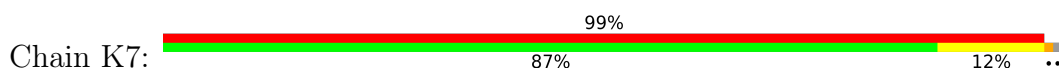
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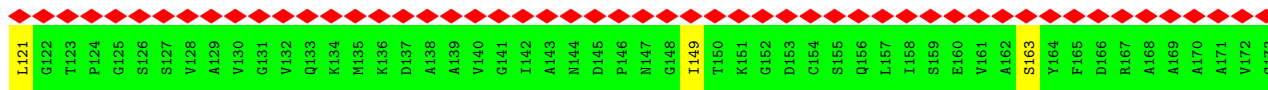


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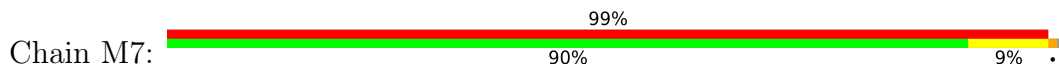


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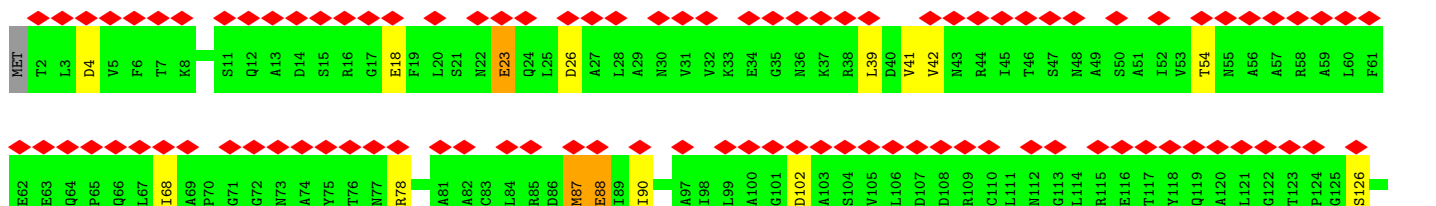
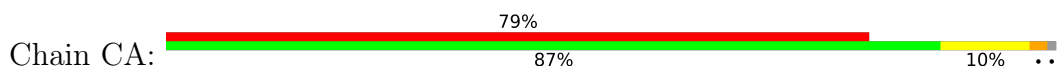




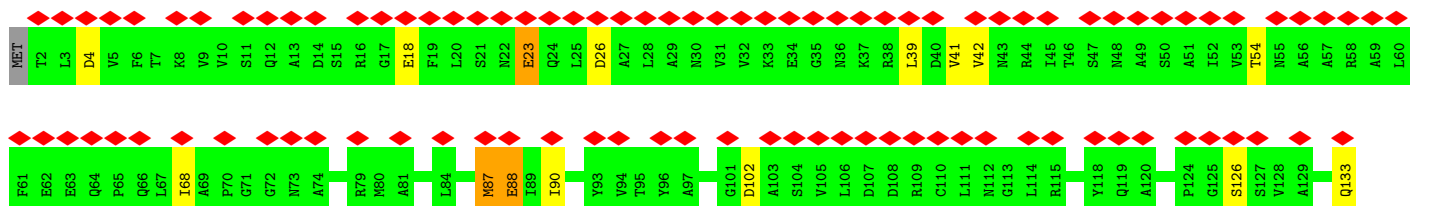
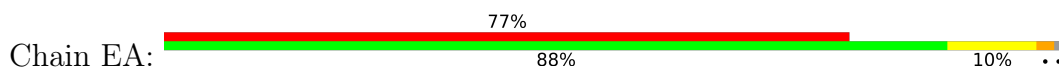
• Molecule 3: C-phycoerythrin beta subunit



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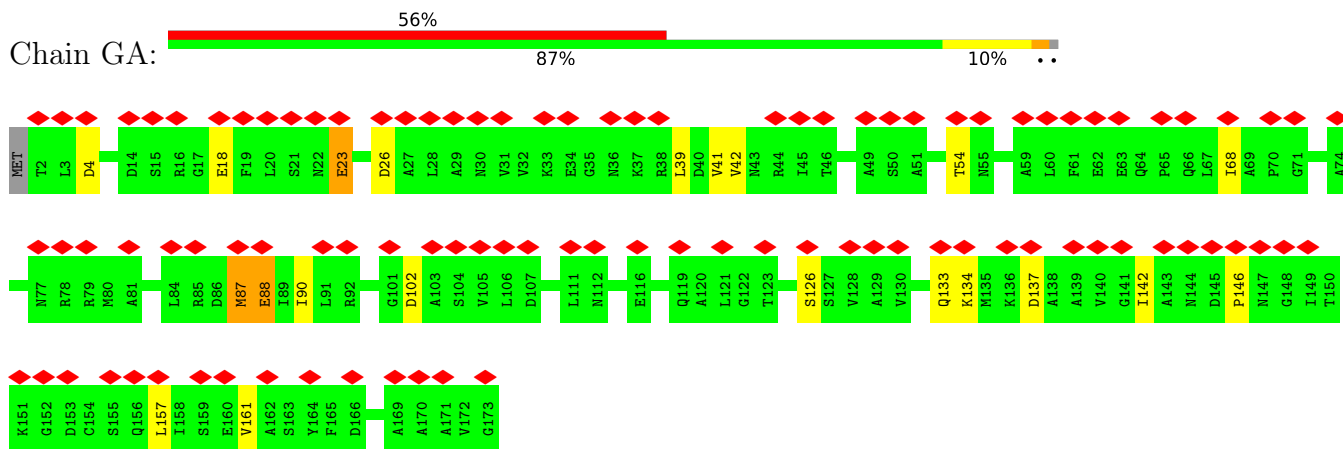


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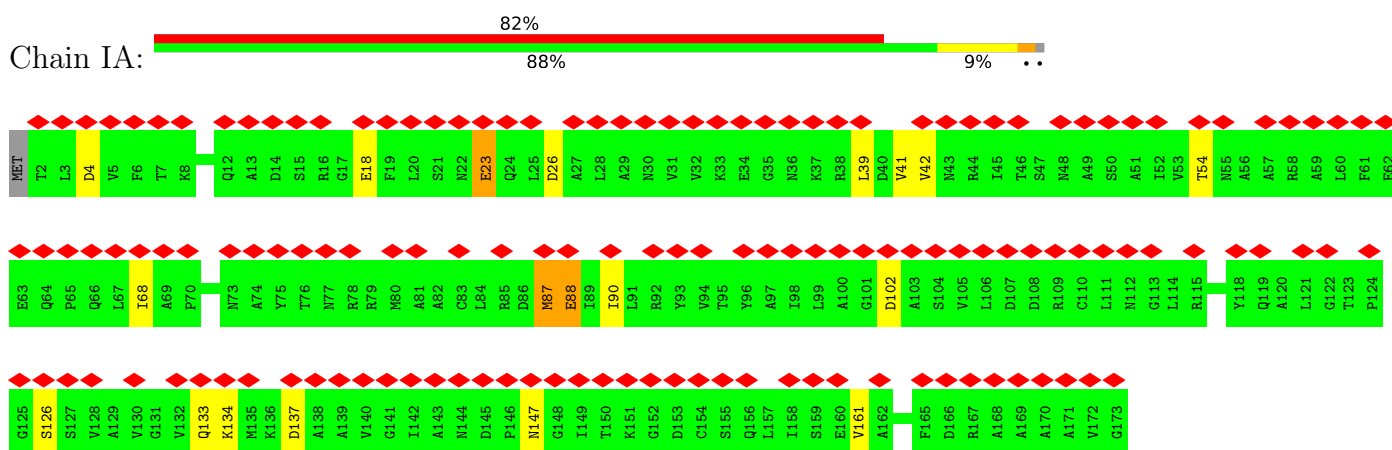


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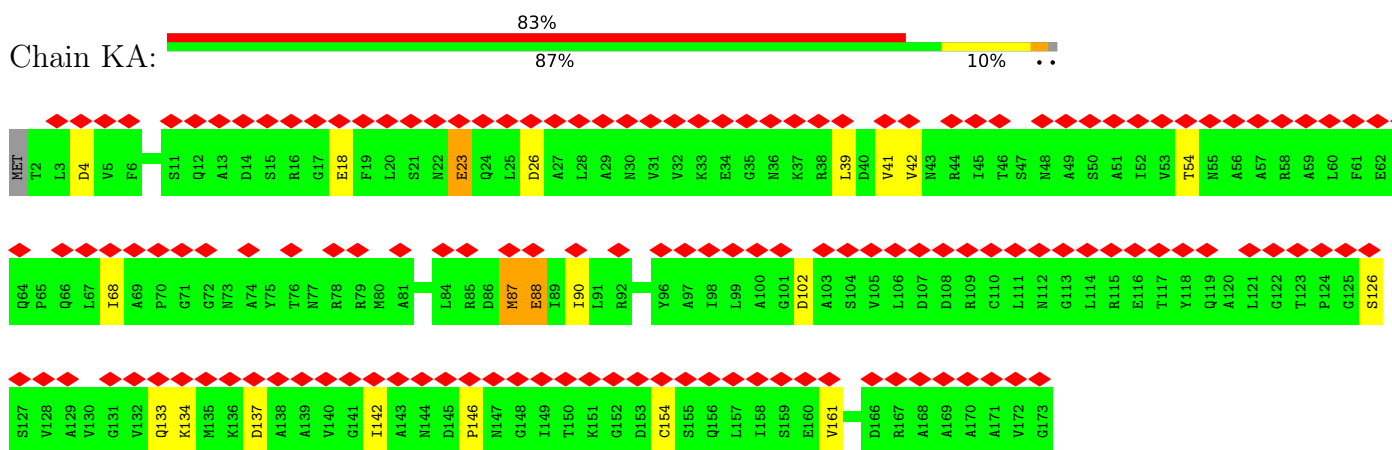




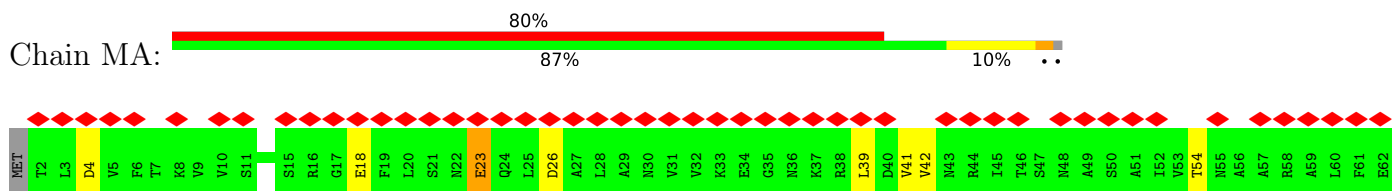
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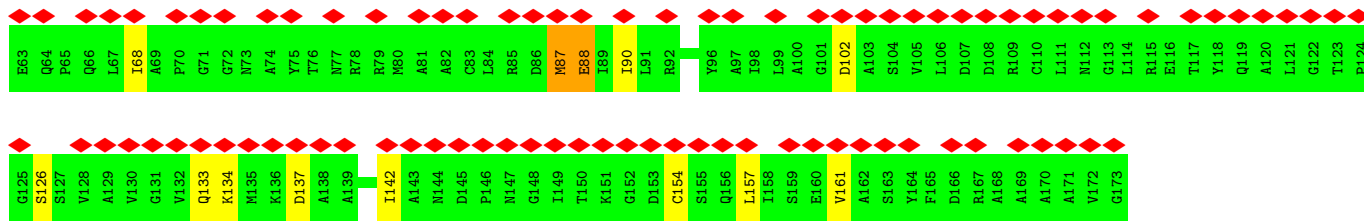


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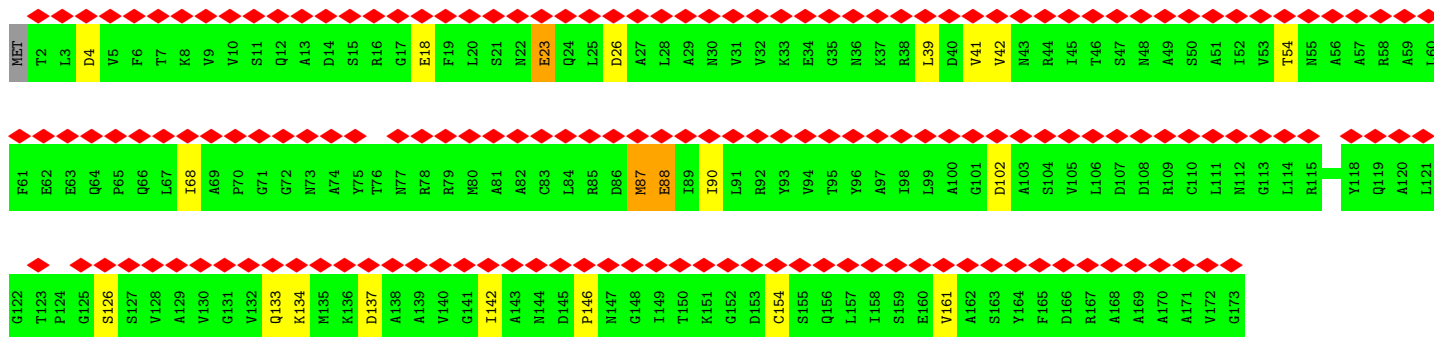
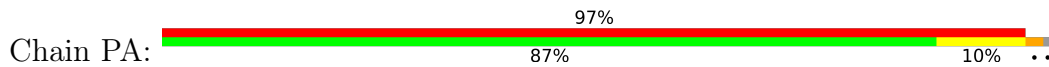


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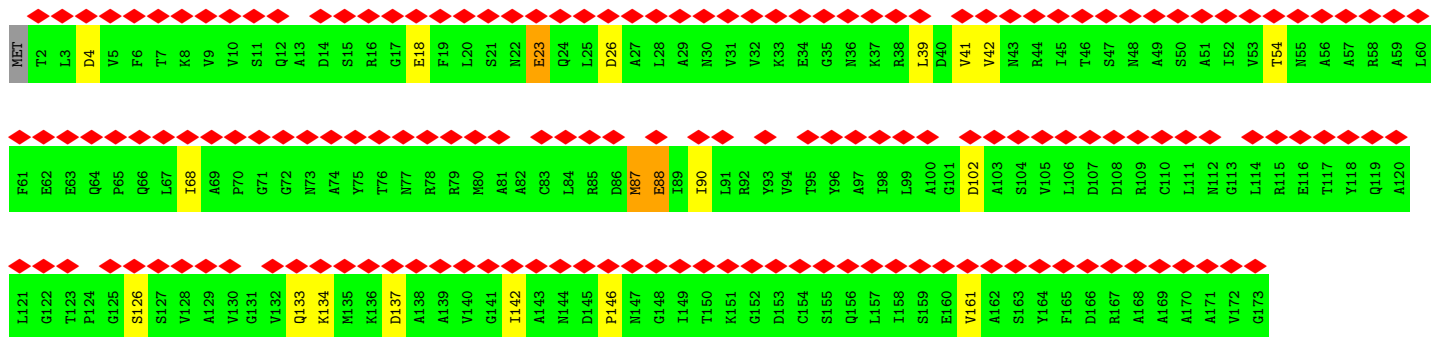
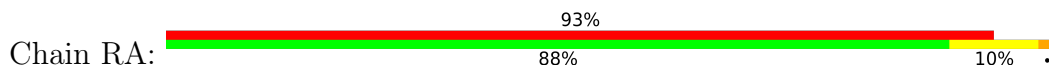




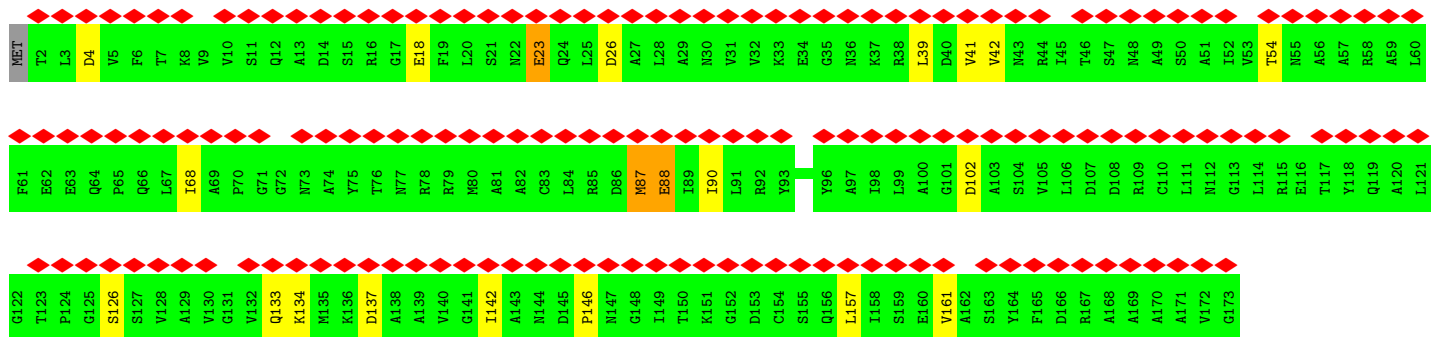
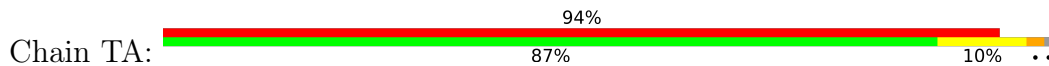
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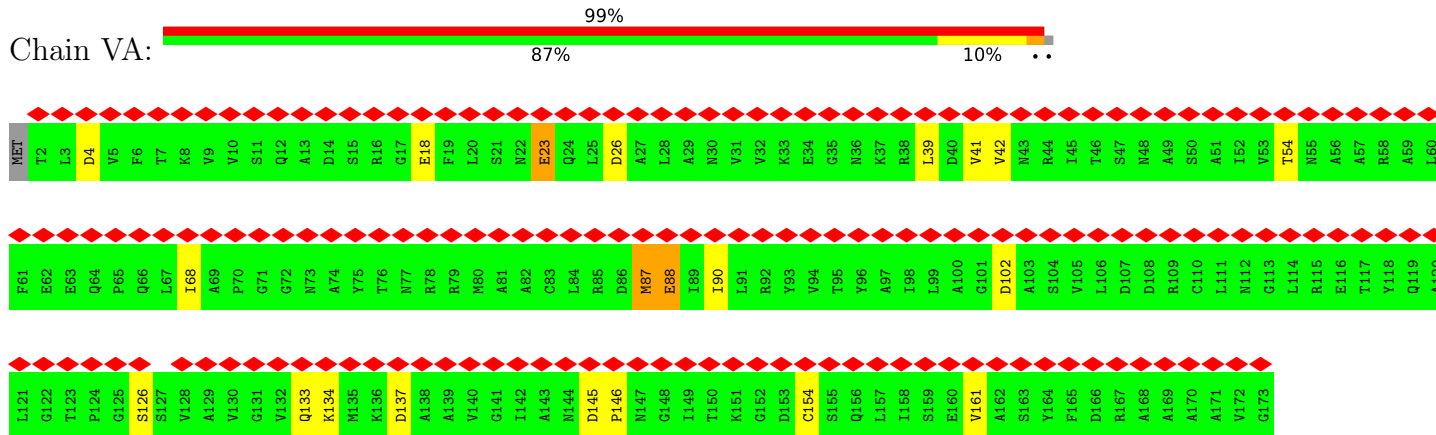
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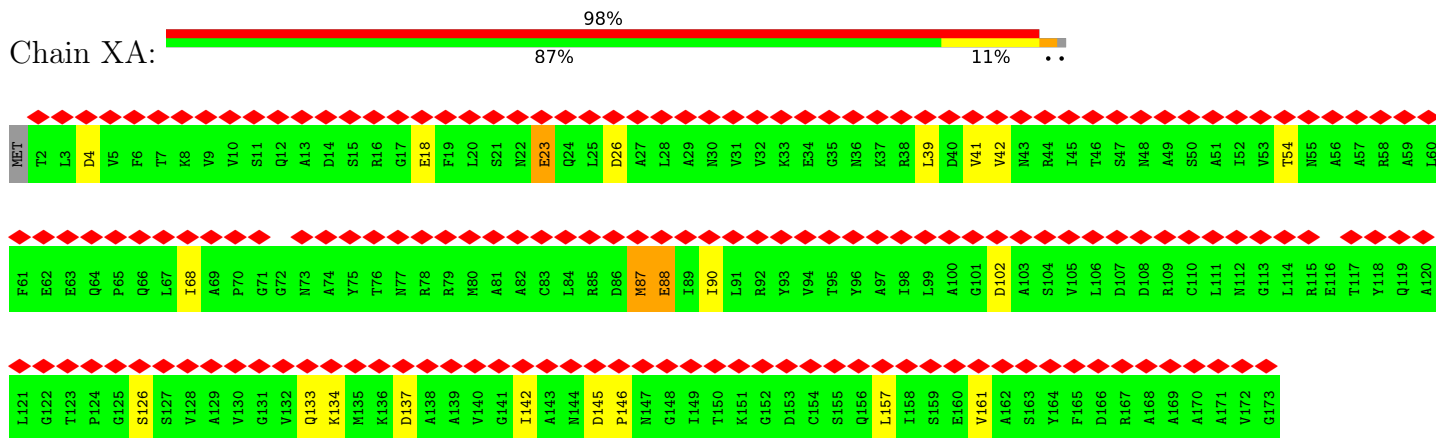
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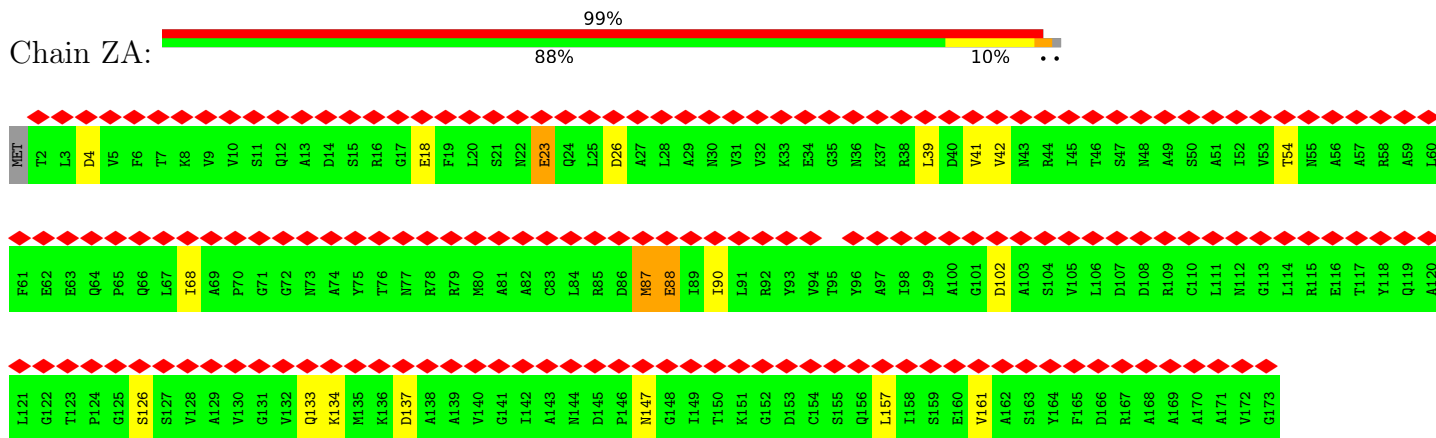
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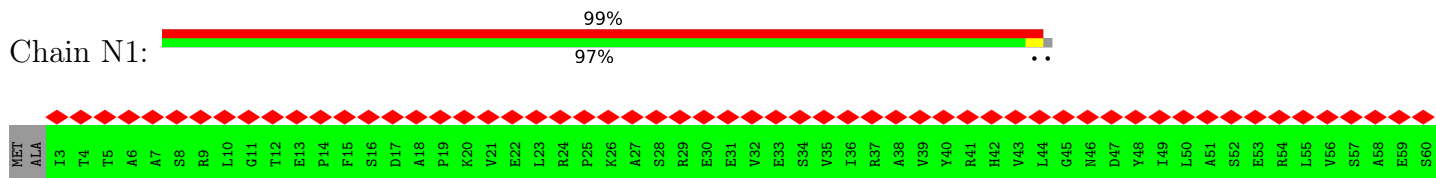
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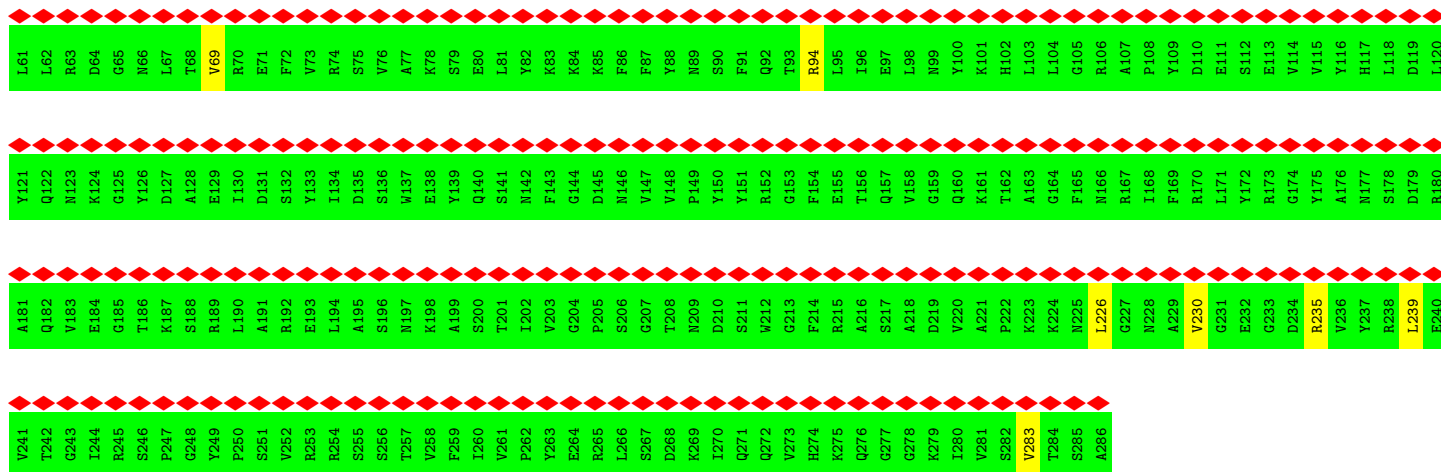


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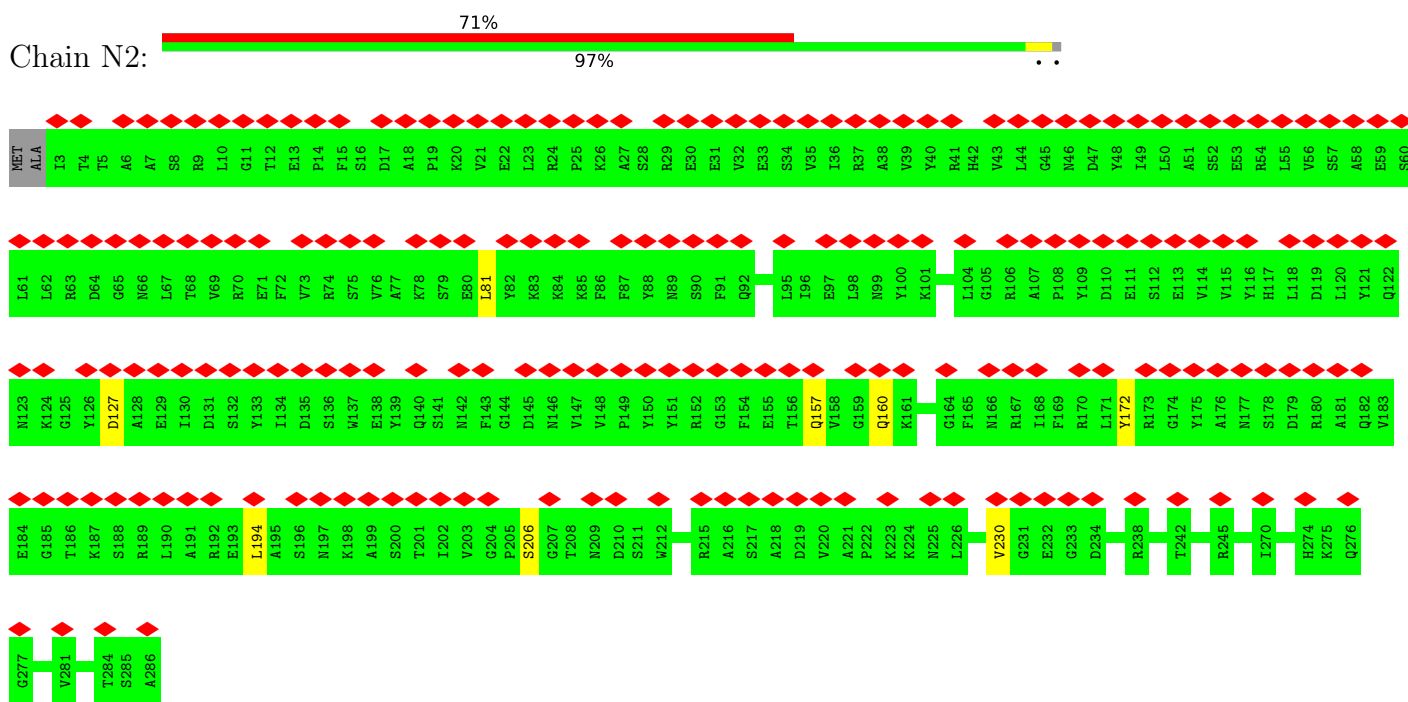


• Molecule 4: Phycobilisome 32.1 kDa linker polypeptide, phycocyanin-associated, rod

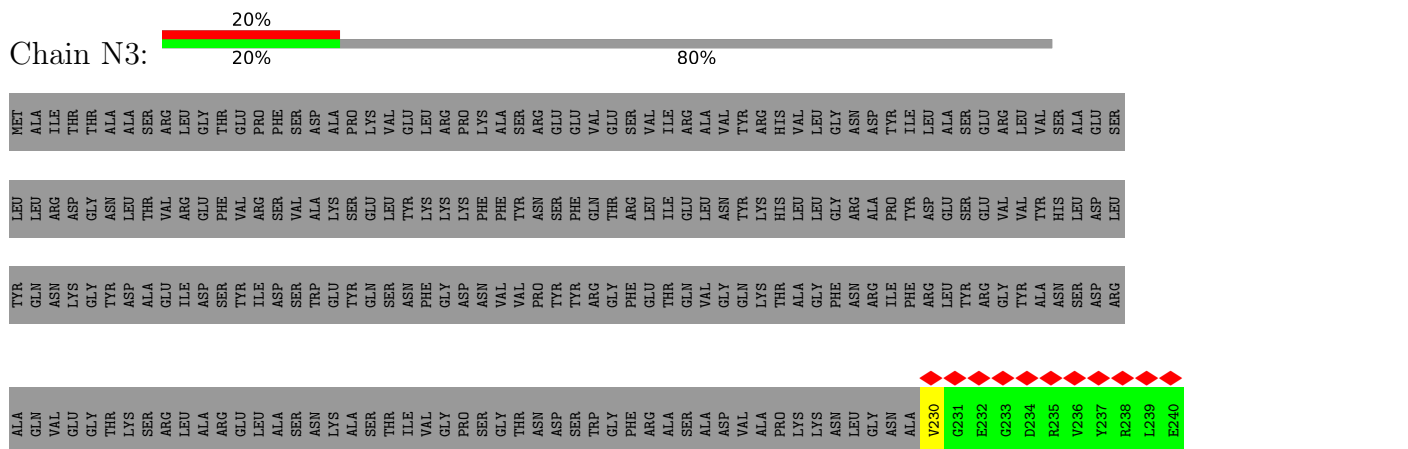


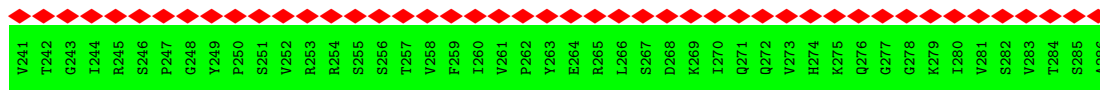


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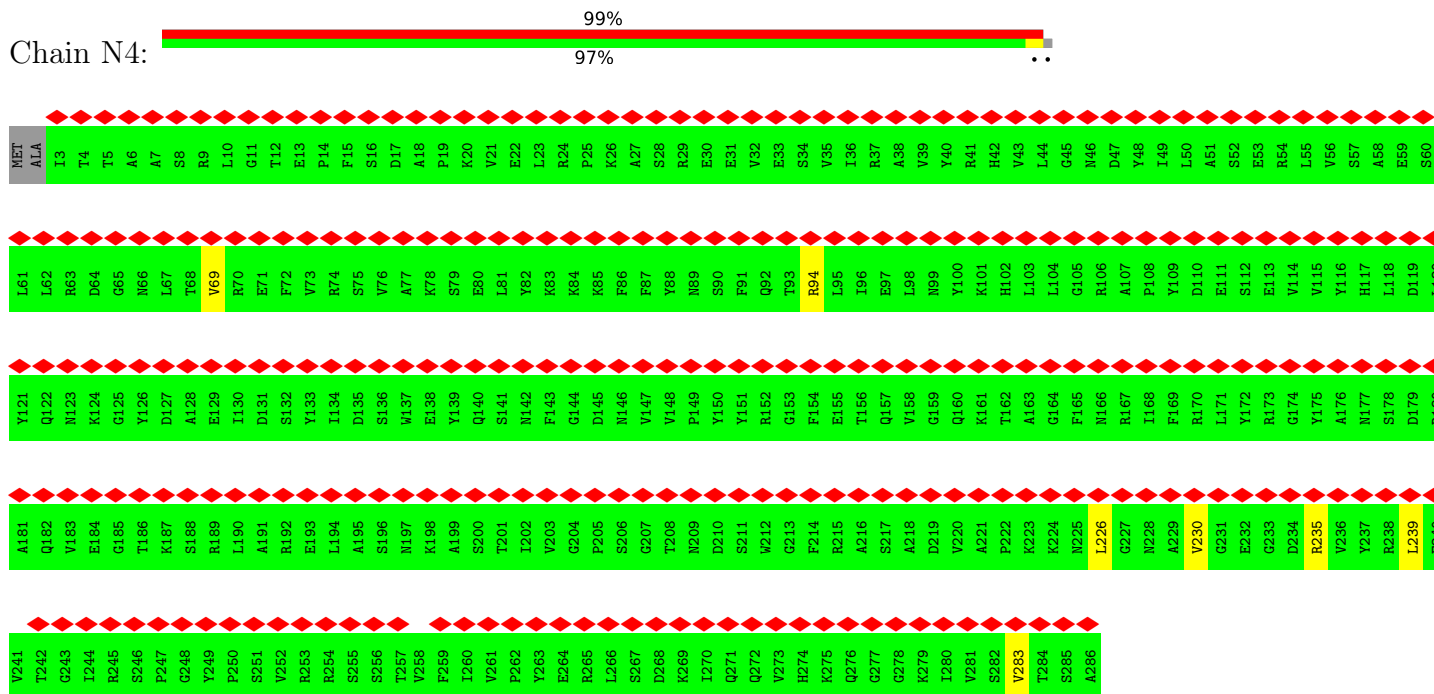


• Molecule 4: Phycobilisome 32.1 kDa linker polypeptide, phycocyanin-associated, rod

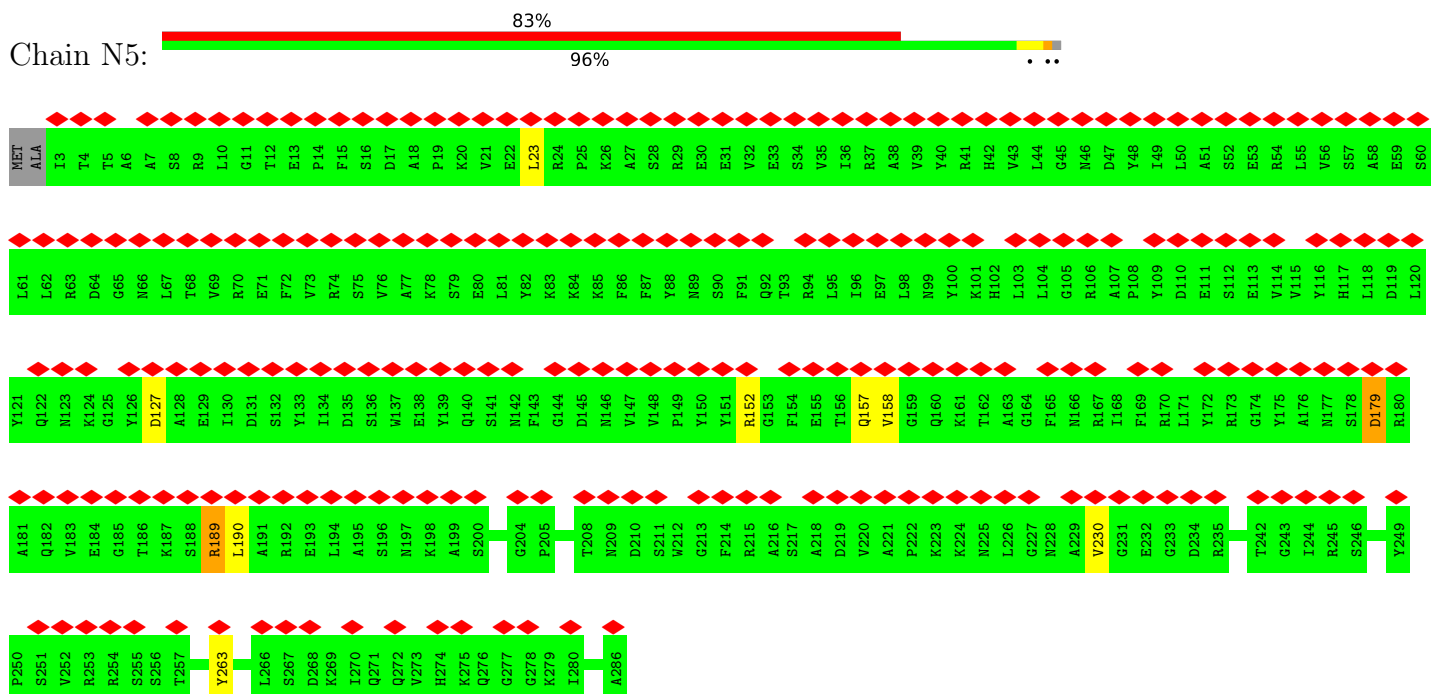




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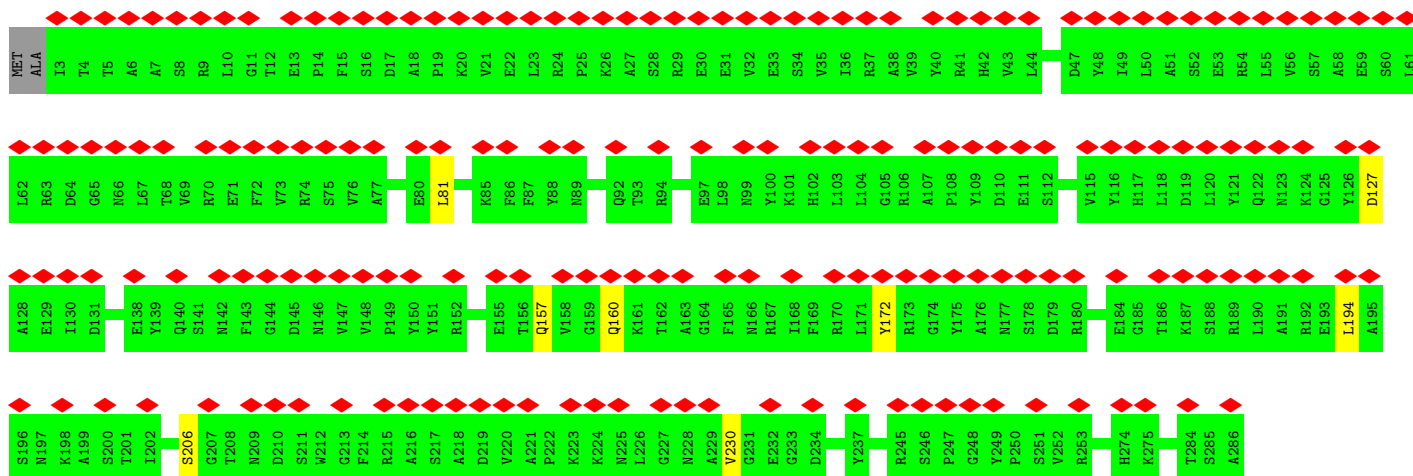


• Molecule 4: Phycobilisome 32.1 kDa linker polypeptide, phycocyanin-associated, rod

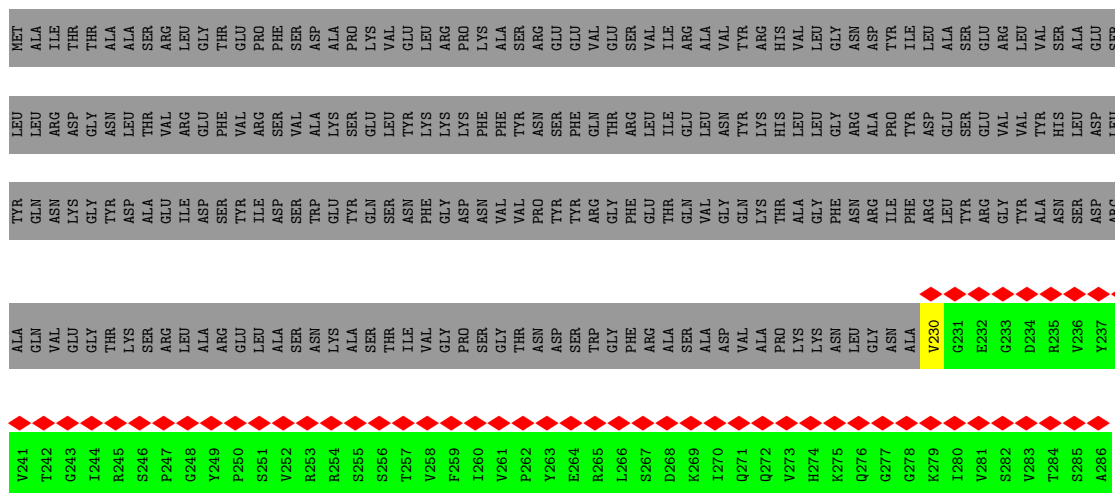


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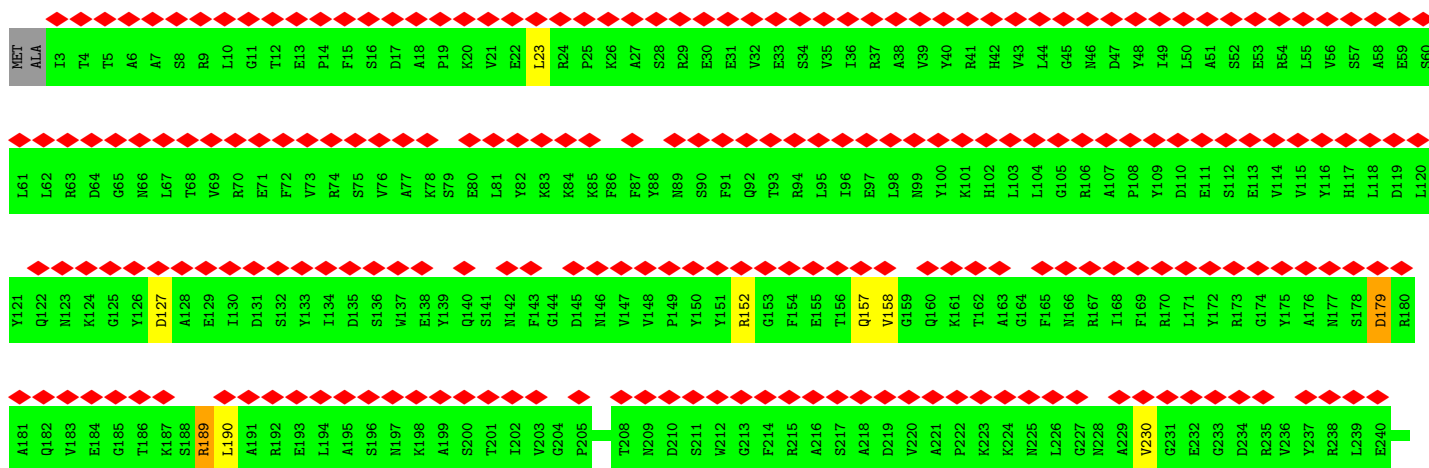
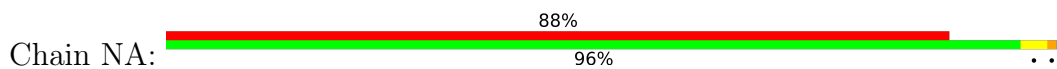


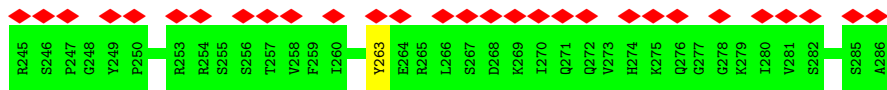


• Molecule 4: Phycobilisome 32.1 kDa linker polypeptide, phycocyanin-associated, rod

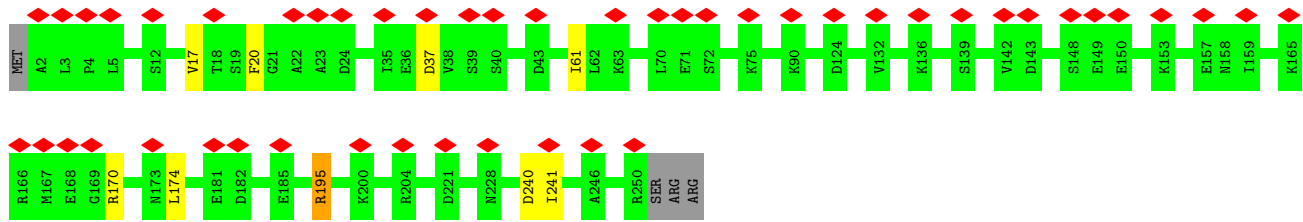


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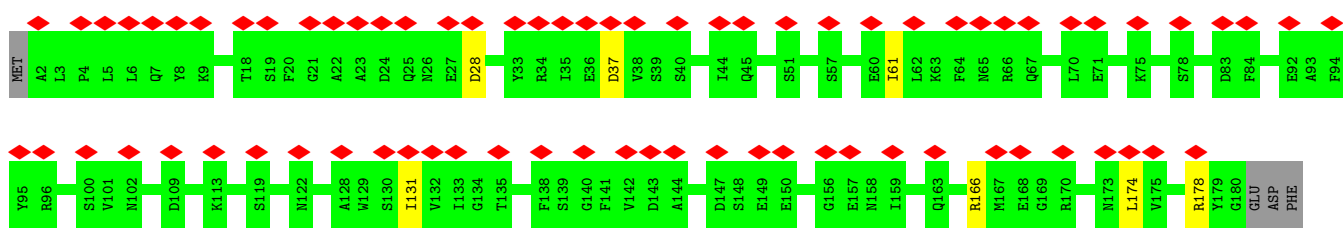
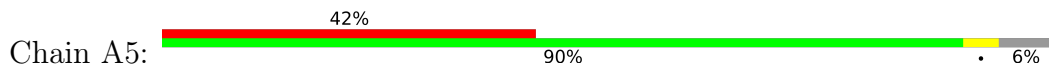




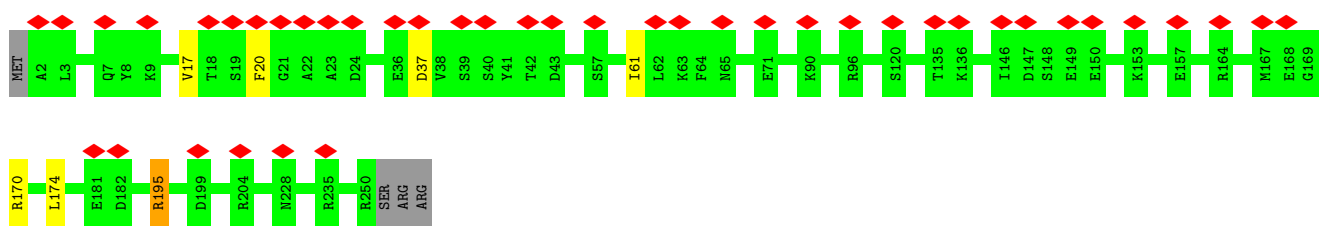
● Molecule 5: Phycobilisome rod-core linker polypeptide CpcG4



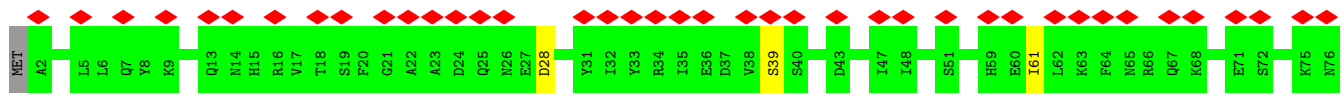
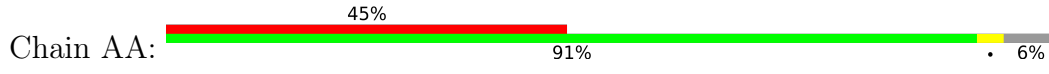
● Molecule 5: Phycobilisome rod-core linker polypeptide CpcG4

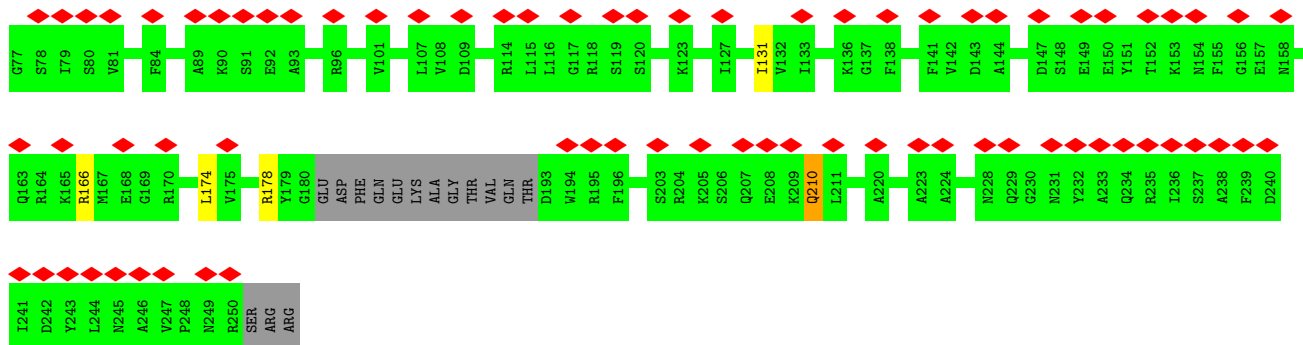


● Molecule 5: Phycobilisome rod-core linker polypeptide CpcG4

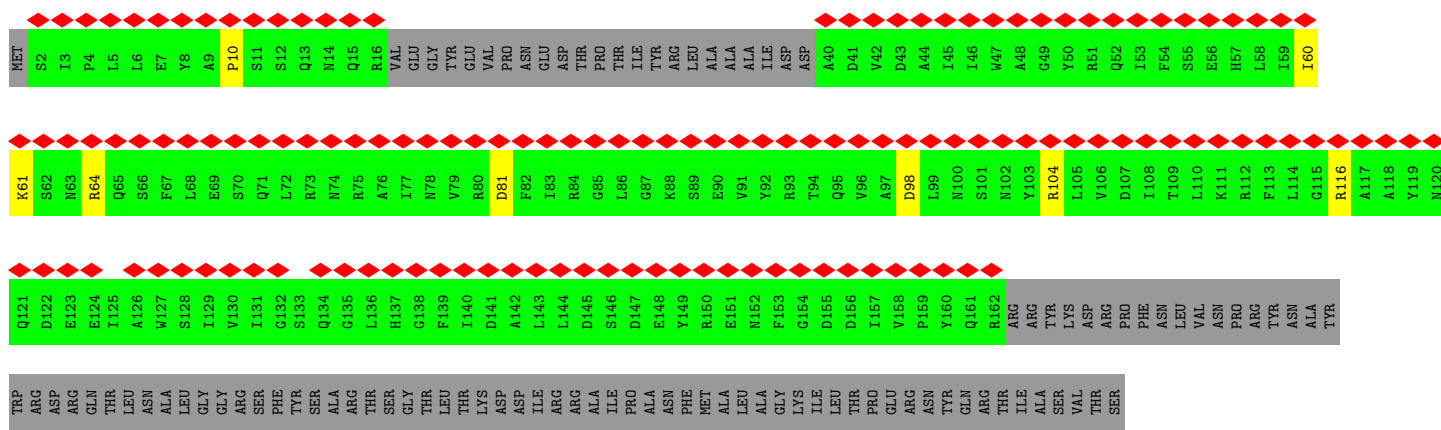


● Molecule 5: Phycobilisome rod-core linker polypeptide CpcG4

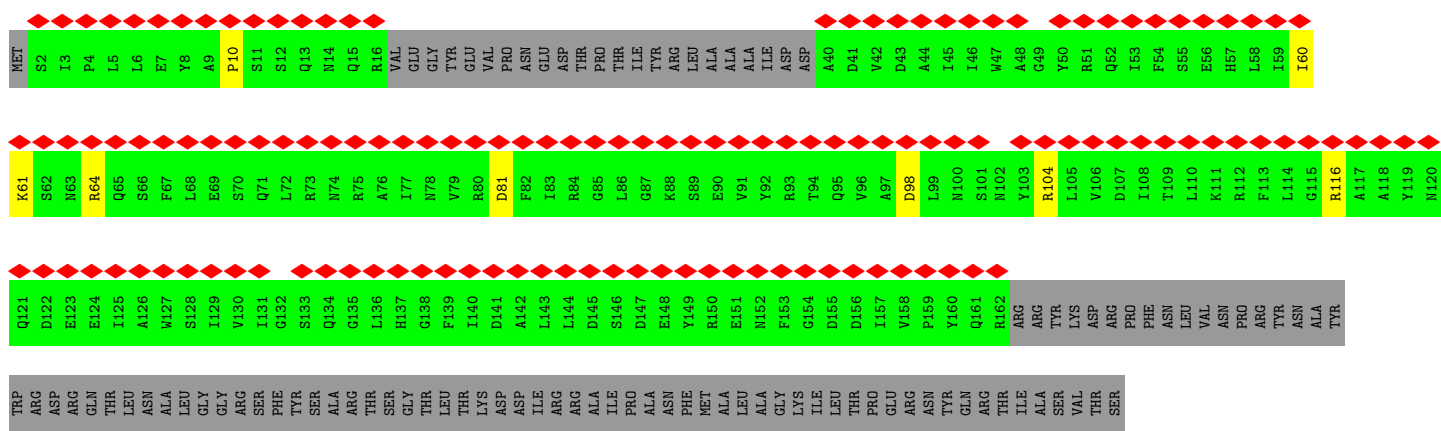




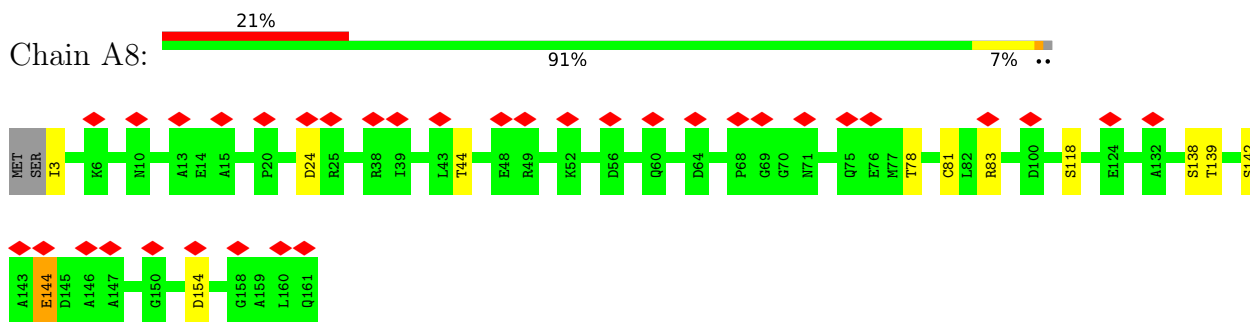
• Molecule 6: Phycobilisome rod-core linker polypeptide CpcG1



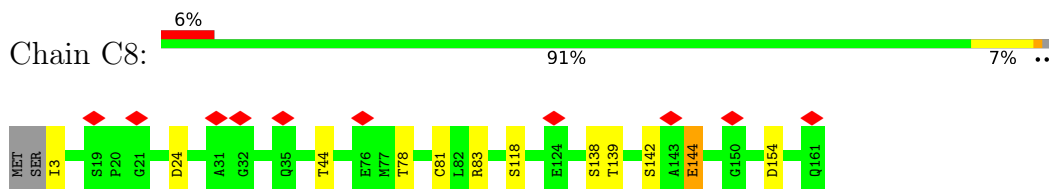
• Molecule 6: Phycobilisome rod-core linker polypeptide CpcG1



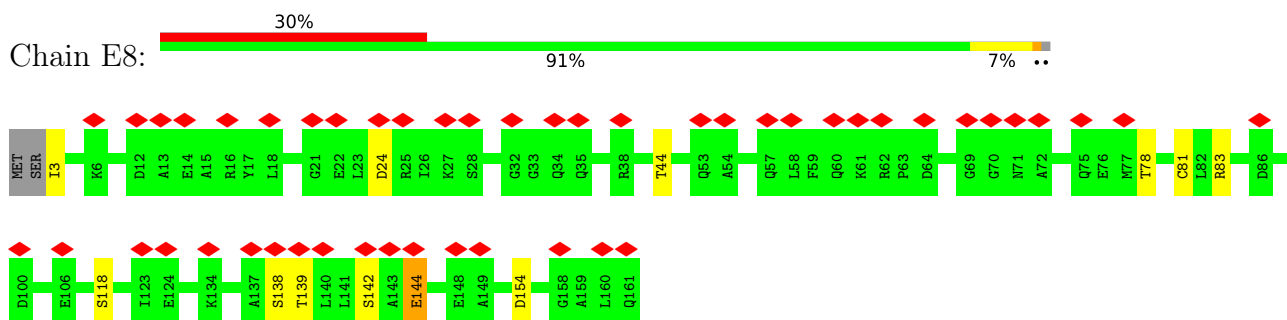
- Molecule 7: Allophycocyanin subunit alpha 1



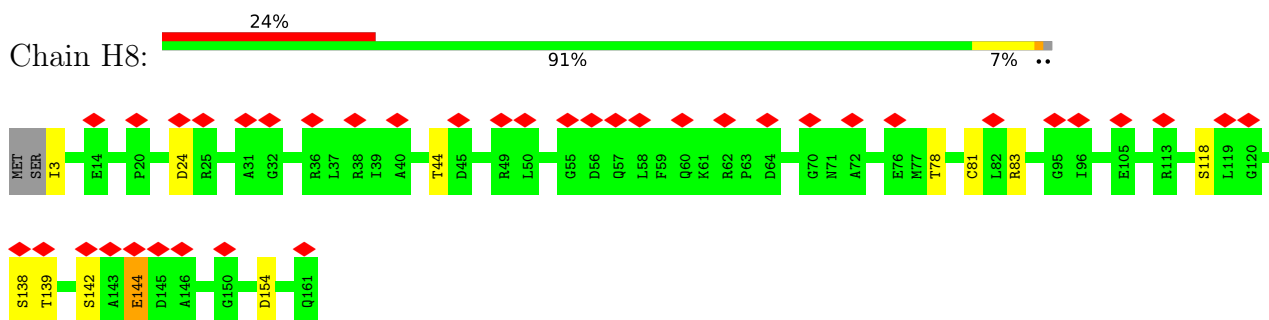
- Molecule 7: Allophycocyanin subunit alpha 1



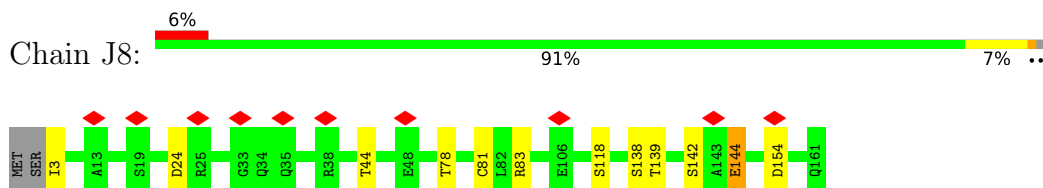
- Molecule 7: Allophycocyanin subunit alpha 1



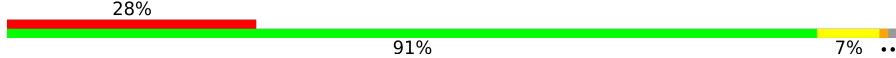
- Molecule 7: Allophycocyanin subunit alpha 1

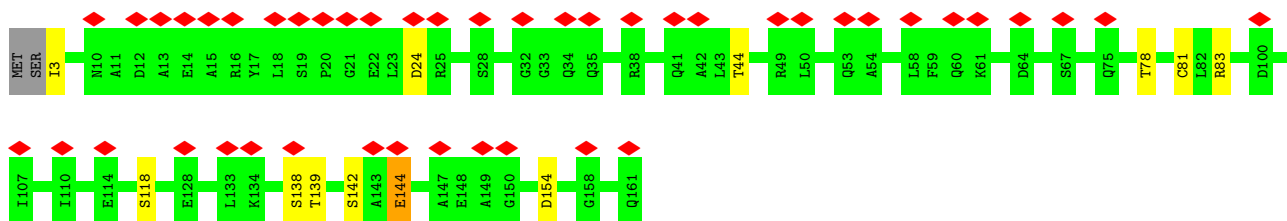


- Molecule 7: Allophycocyanin subunit alpha 1



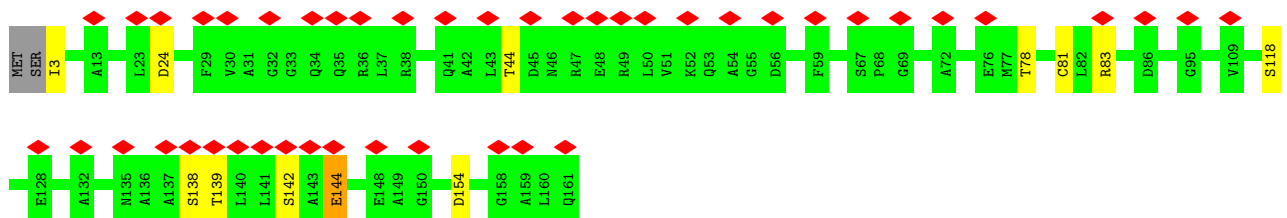
- Molecule 7: Allophycocyanin subunit alpha 1

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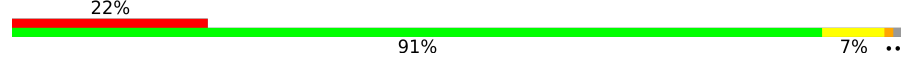


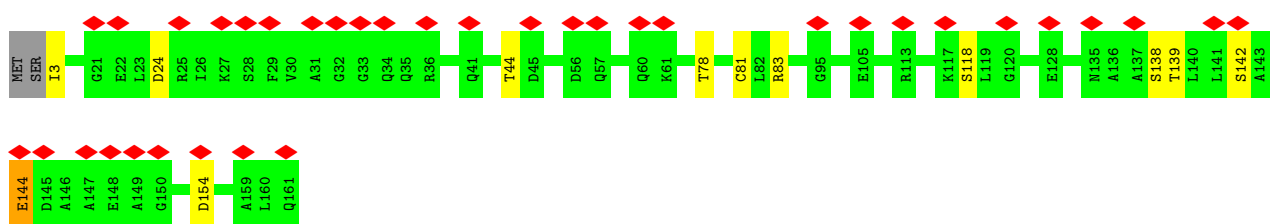
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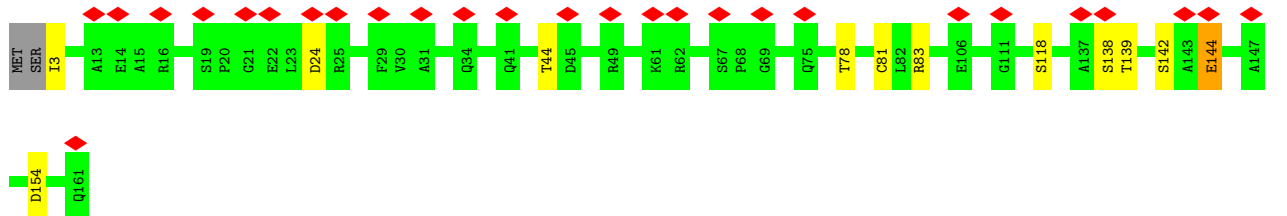
- Molecule 7: Allophycocyanin subunit alpha 1

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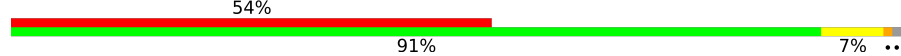


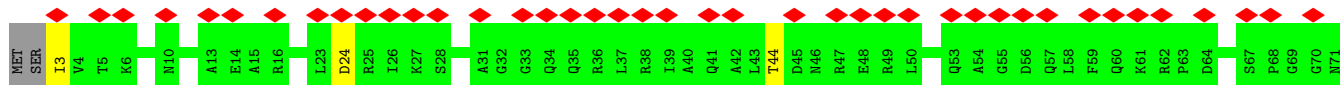
- Molecule 7: Allophycocyanin subunit alpha 1

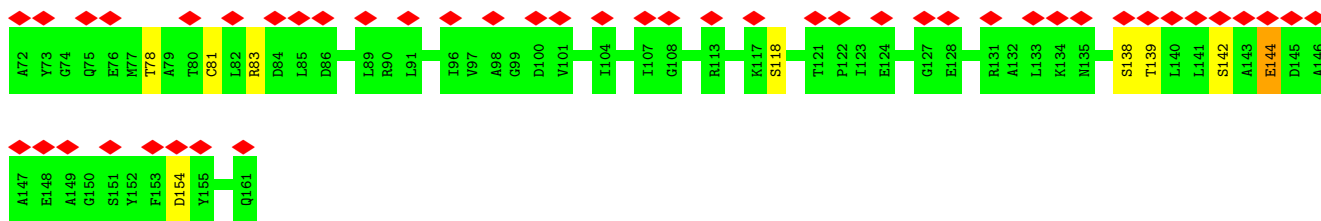
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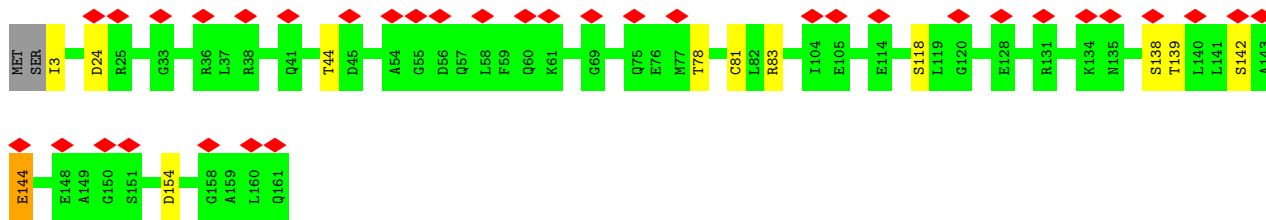
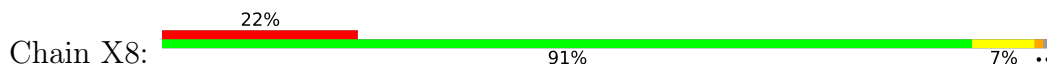
- Molecule 7: Allophycocyanin subunit alpha 1

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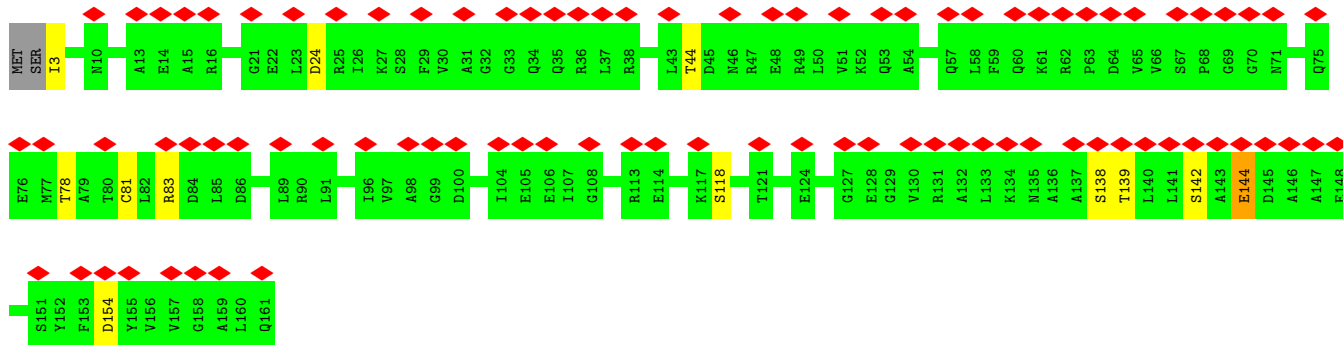
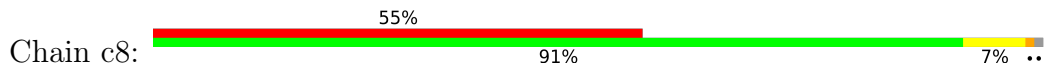
• Molecule 7: Allophycocyanin subunit alpha 1



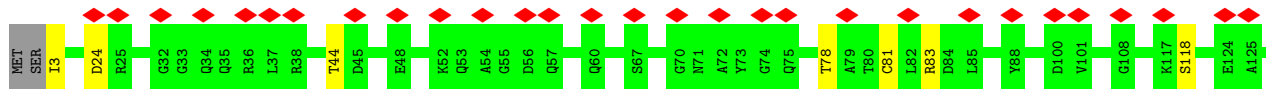
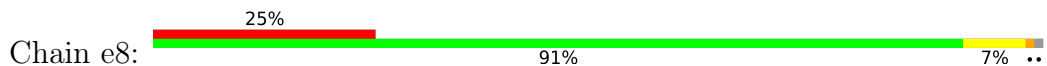
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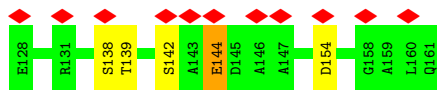


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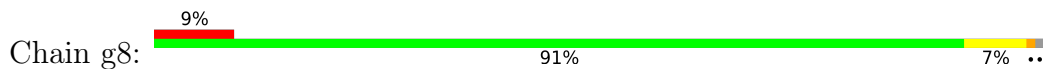


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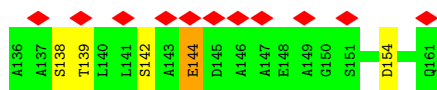
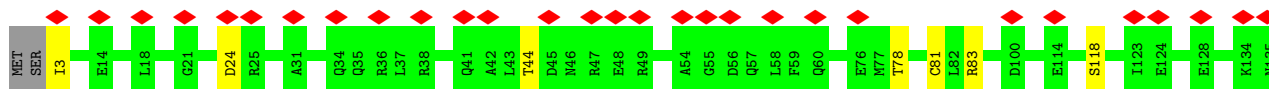
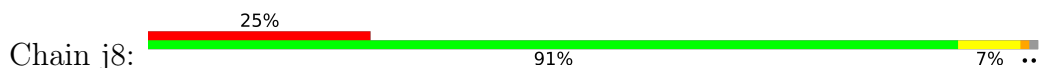




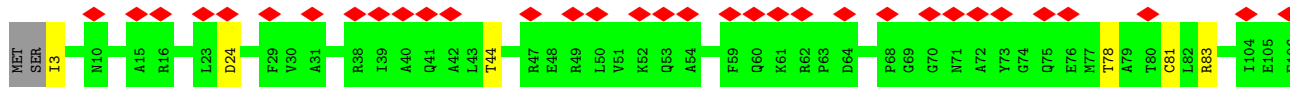
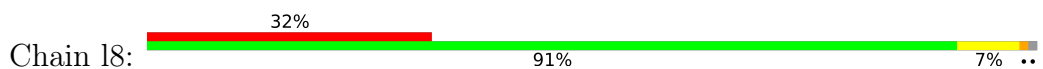
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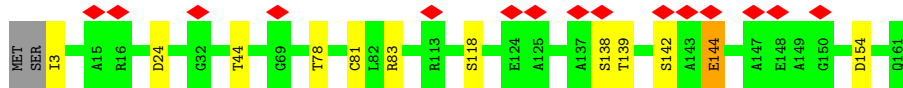
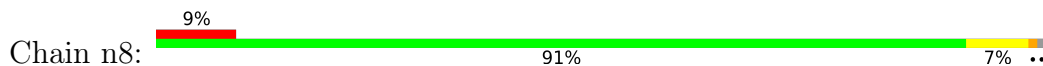
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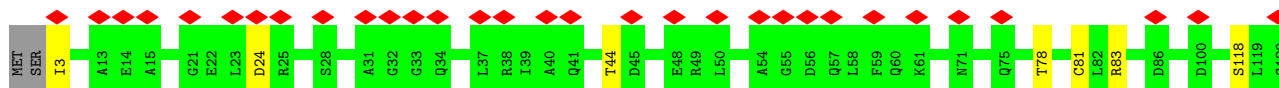
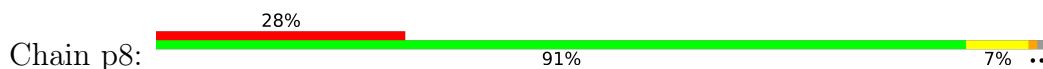
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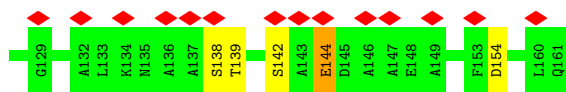


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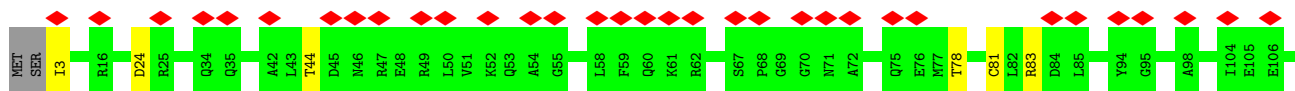
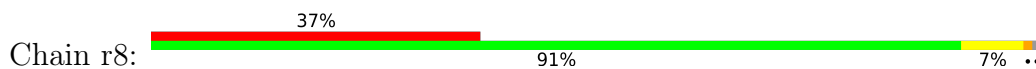


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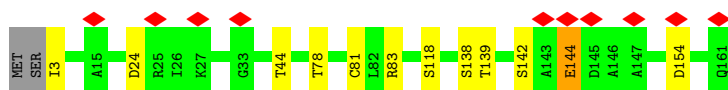
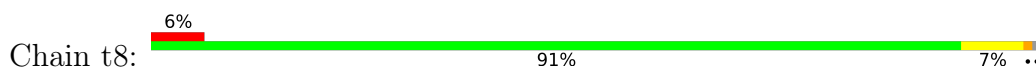




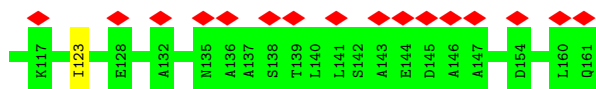
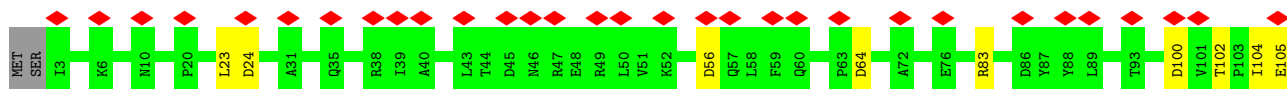
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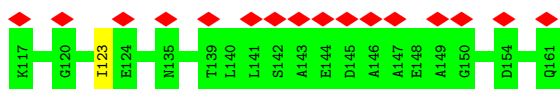
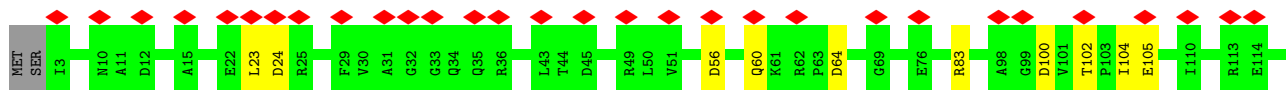
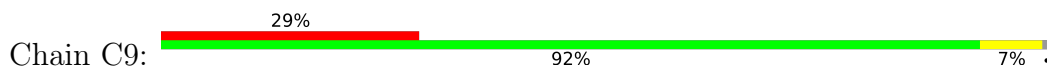
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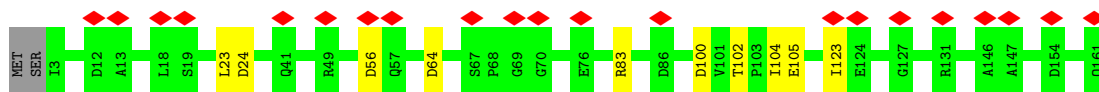


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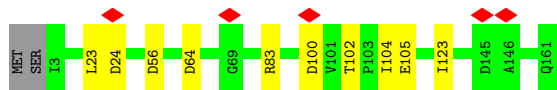


- Molecule 7: Allophycocyanin subunit alpha 1

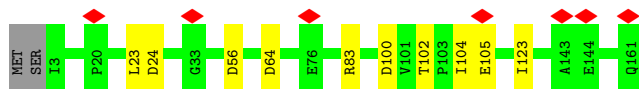




• Molecule 7: Allophycocyanin subunit alpha 1



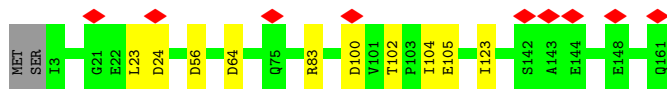
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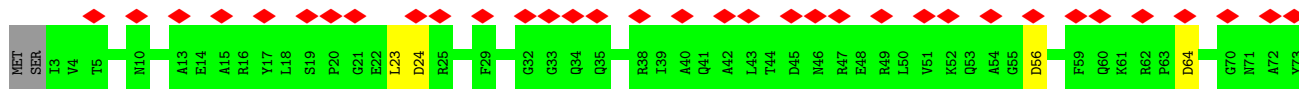
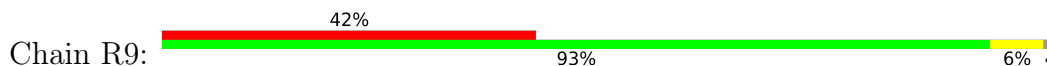
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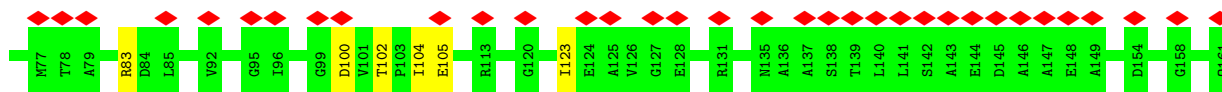


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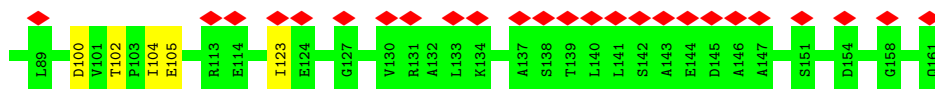
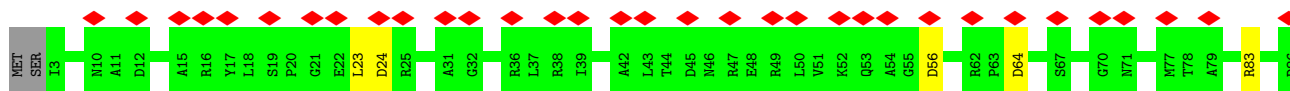


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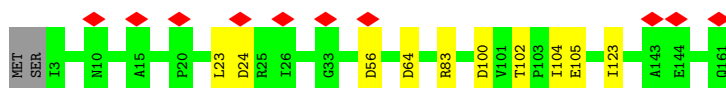




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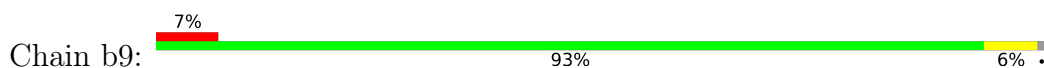
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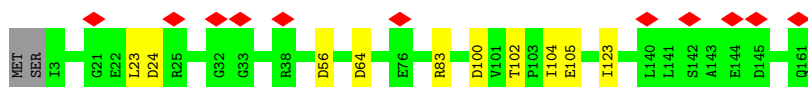
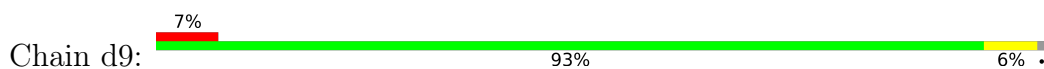
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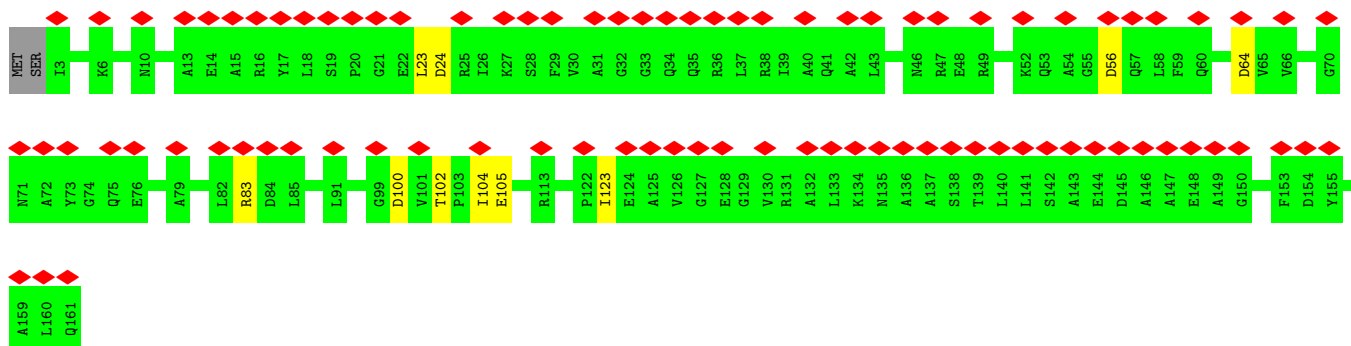
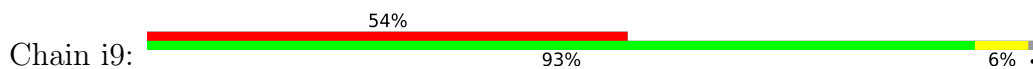


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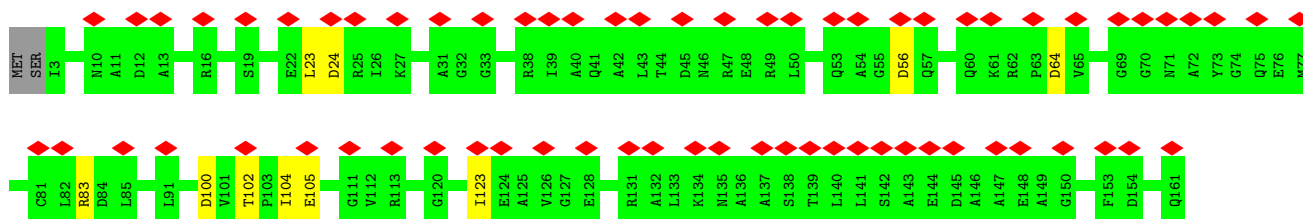
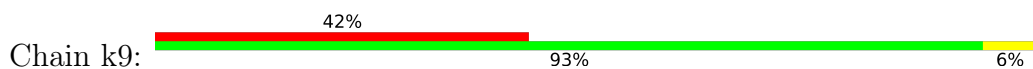




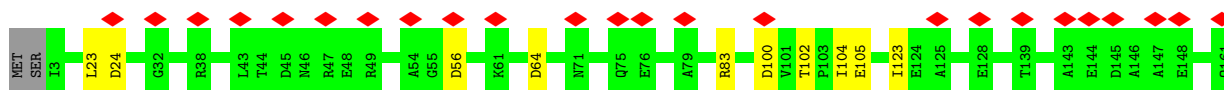
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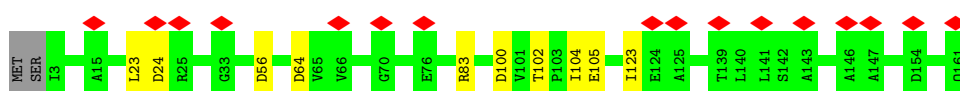
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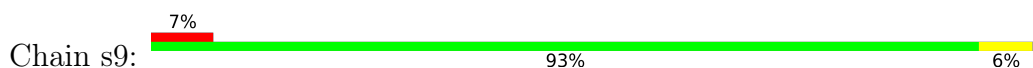
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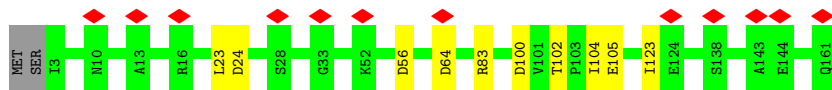


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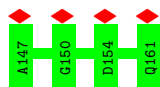
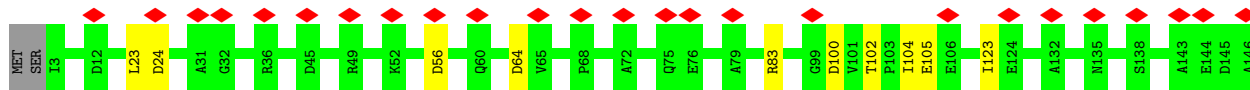
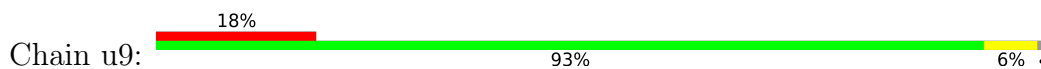


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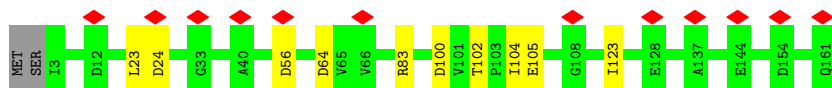




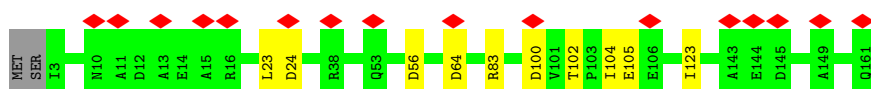
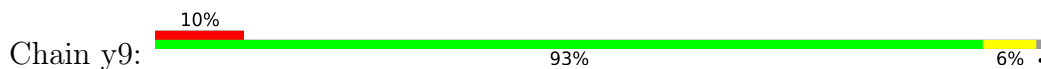
• Molecule 7: Allophycocyanin subunit alpha 1



• Molecule 7: Allophycocyanin subunit alpha 1



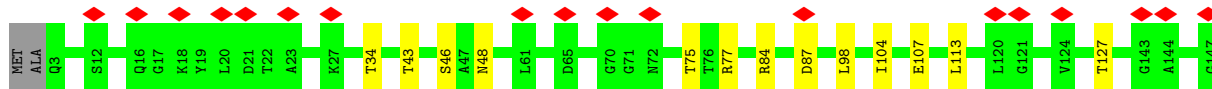
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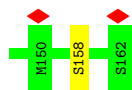


• Molecule 8: Allophycocyanin subunit beta

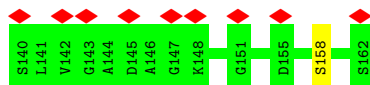
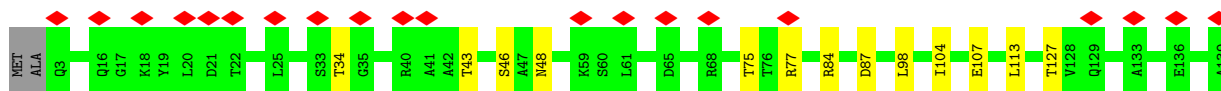
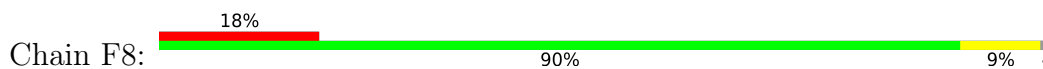


• Molecule 8: Allophycocyanin subunit beta

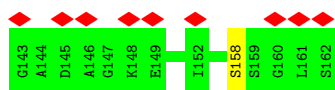
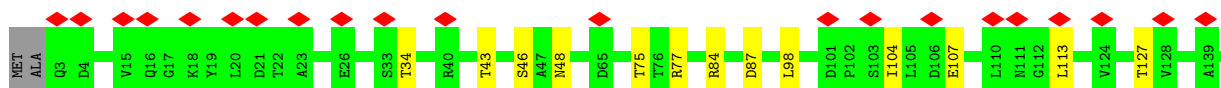
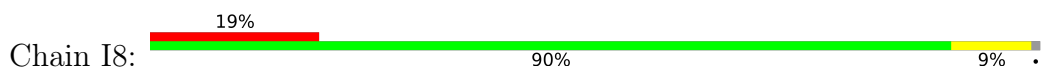




- Molecule 8: Allophycocyanin subunit beta



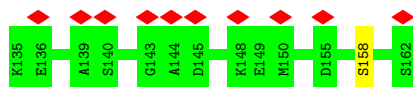
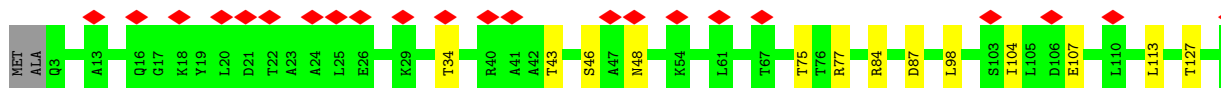
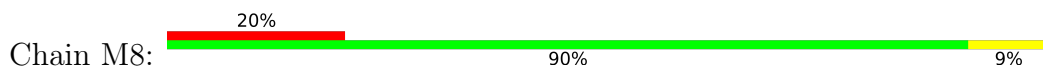
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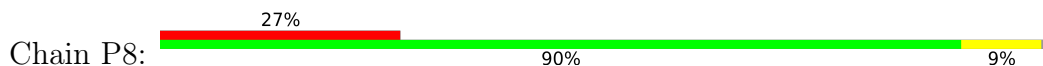
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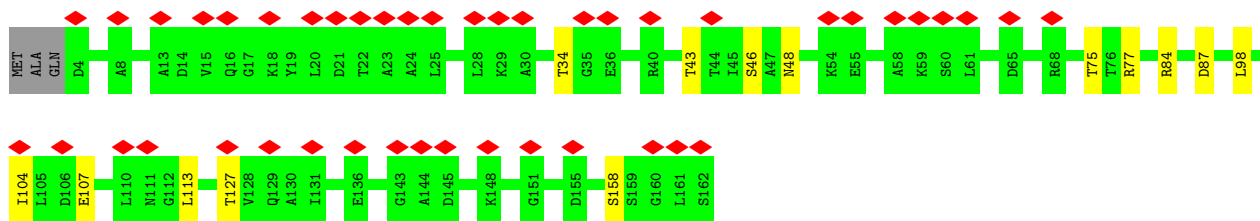


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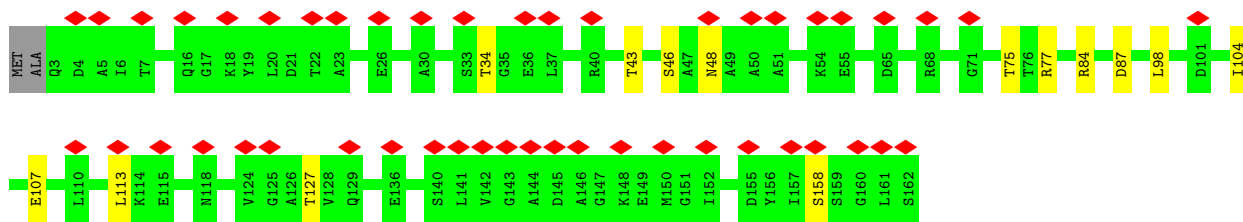
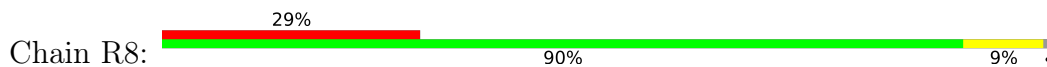


- Molecule 8: Allophycocyanin subunit beta

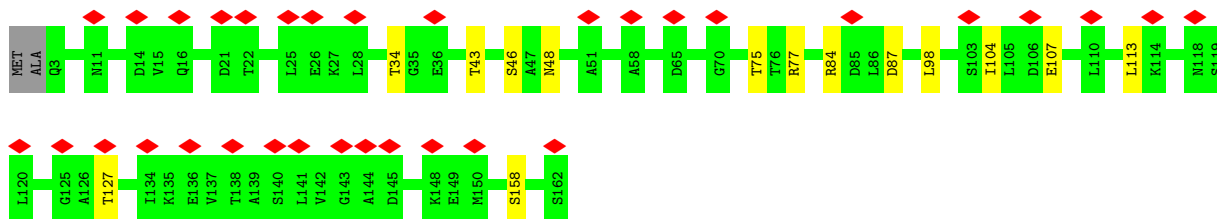
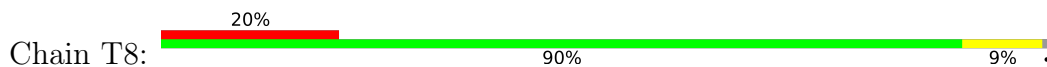




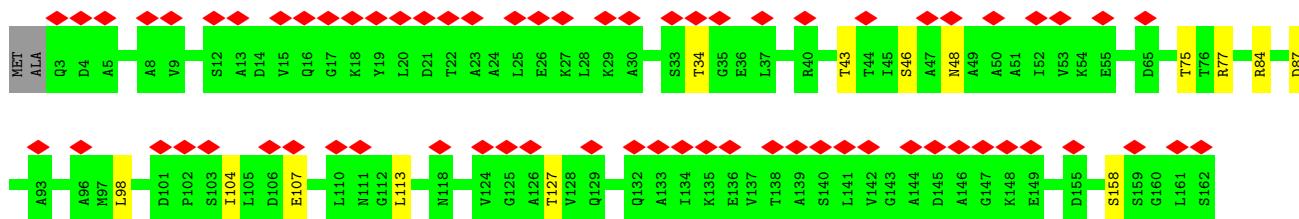
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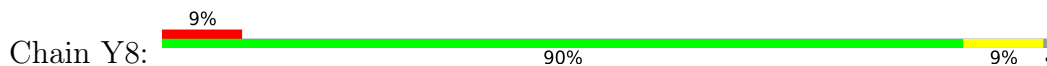
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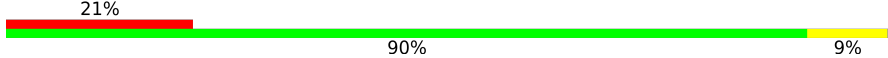
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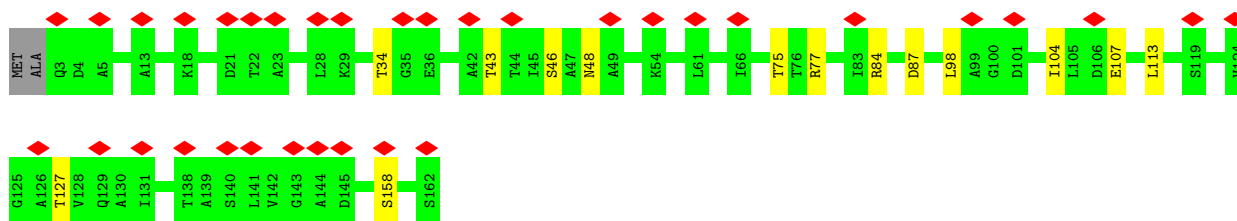


- Molecule 8: Allophycocyanin subunit beta

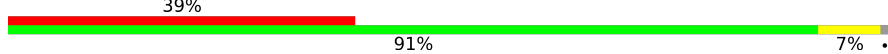


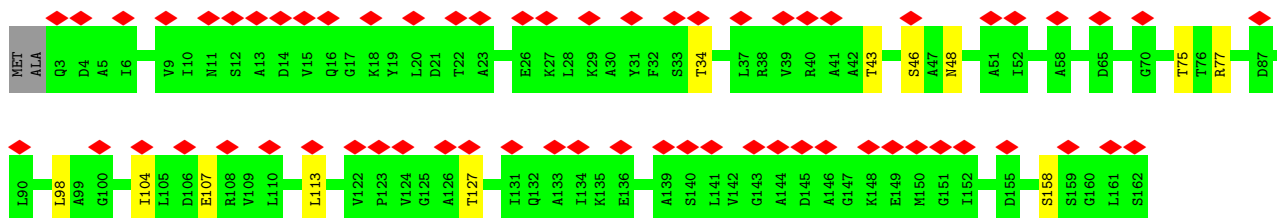
- Molecule 8: Allophycocyanin subunit beta

Chain a8: 




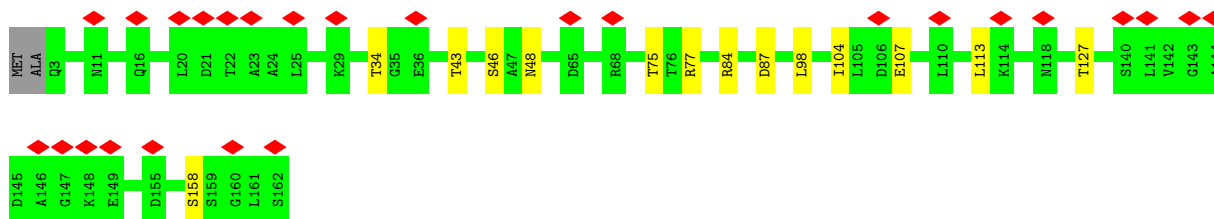
• Molecule 8: Allophycocyanin subunit beta

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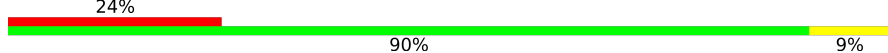


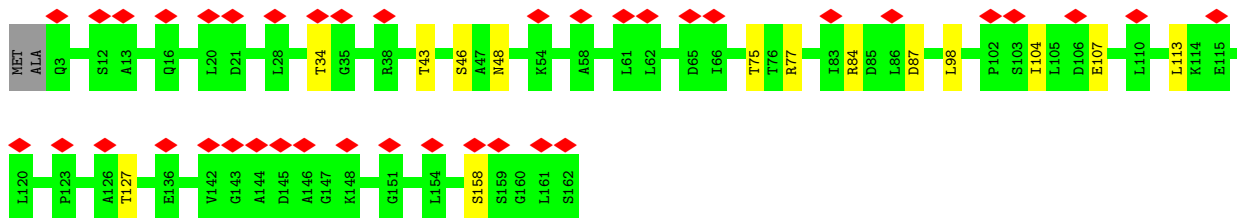
• Molecule 8: Allophycocyanin subunit beta

Chain f8: 

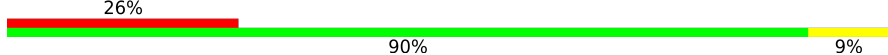


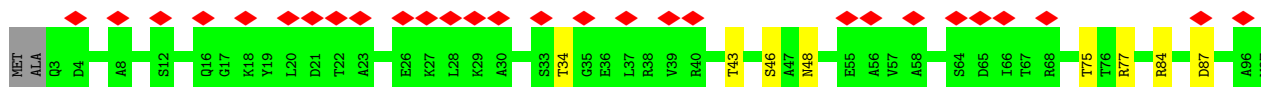
• Molecule 8: Allophycocyanin subunit beta

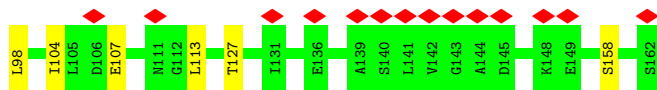
Chain h8: 



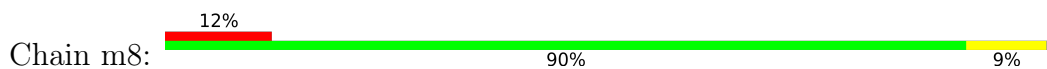
• Molecule 8: Allophycocyanin subunit beta

Chain k8: 

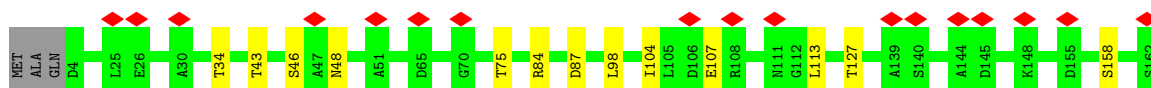
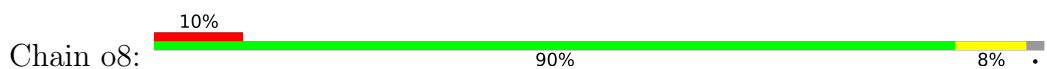




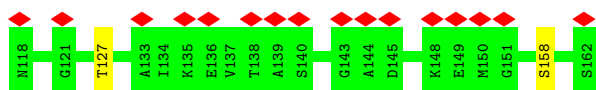
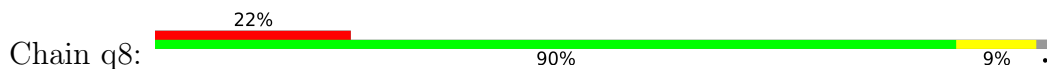
- Molecule 8: Allophycocyanin subunit beta



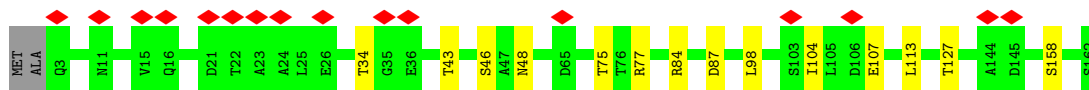
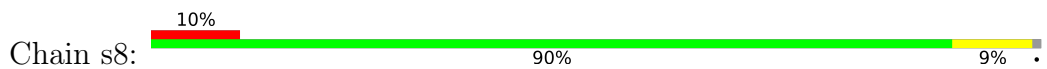
- Molecule 8: Allophycocyanin subunit beta



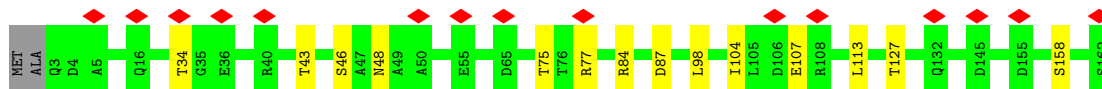
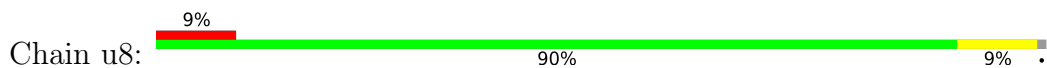
- Molecule 8: Allophycocyanin subunit beta



- Molecule 8: Allophycocyanin subunit beta

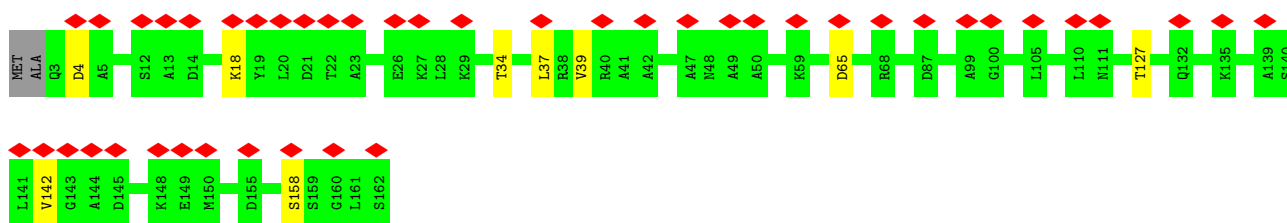


- Molecule 8: Allophycocyanin subunit beta



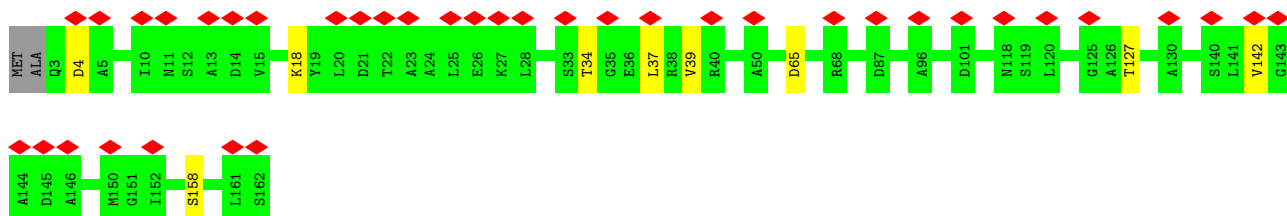
- Molecule 8: Allophycocyanin subunit beta

Chain B9: 



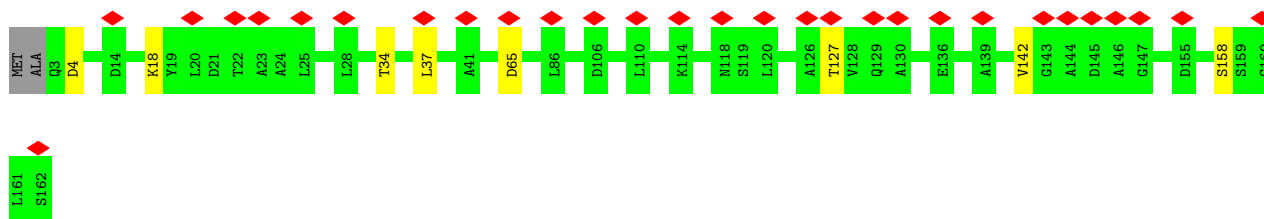
- Molecule 8: Allophycocyanin subunit beta

Chain D9: 



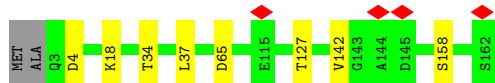
- Molecule 8: Allophycocyanin subunit beta

Chain F9: 



- Molecule 8: Allophycocyanin subunit beta

Chain H9: 



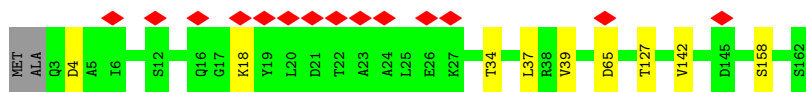
- Molecule 8: Allophycocyanin subunit beta

Chain J9: 

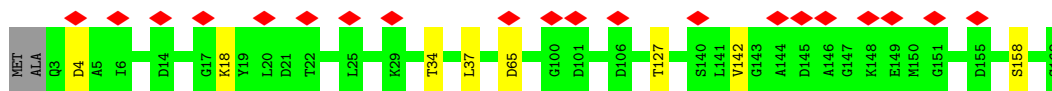


- Molecule 8: Allophycocyanin subunit beta

Chain L9: 



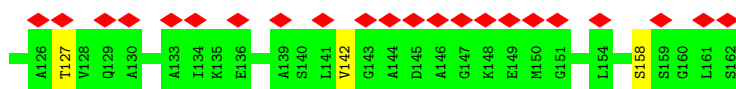
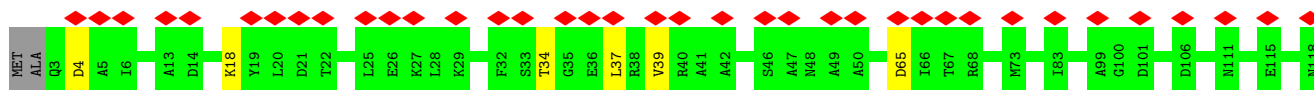
- Molecule 8: Allophycocyanin subunit beta



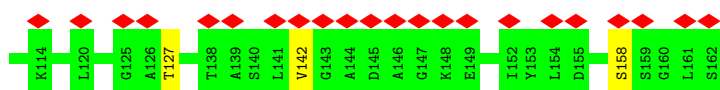
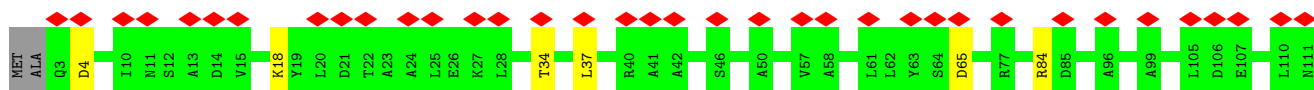
- Molecule 8: Allophycocyanin subunit beta



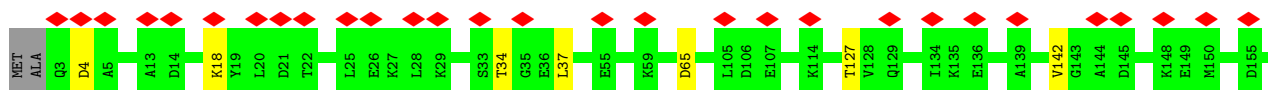
- Molecule 8: Allophycocyanin subunit beta



- Molecule 8: Allophycocyanin subunit beta

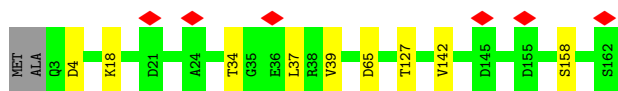


- Molecule 8: Allophycocyanin subunit beta

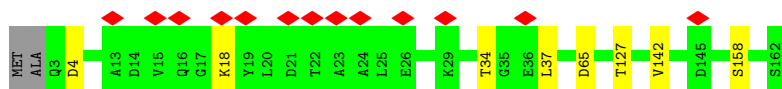




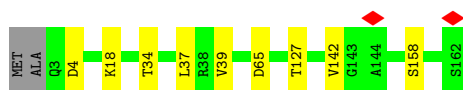
- Molecule 8: Allophycocyanin subunit beta



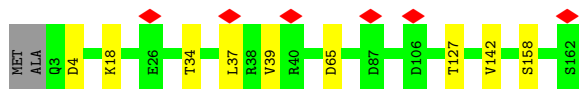
- Molecule 8: Allophycocyanin subunit beta



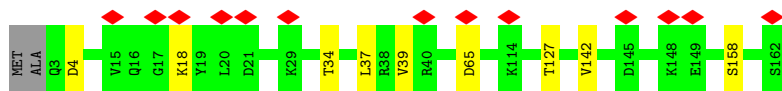
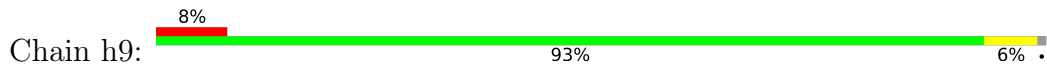
- Molecule 8: Allophycocyanin subunit beta



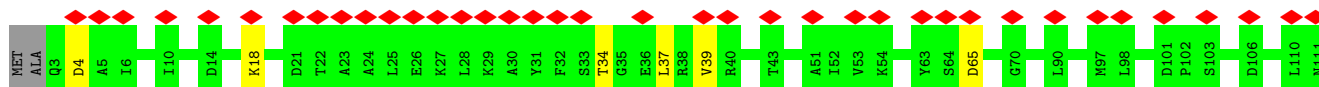
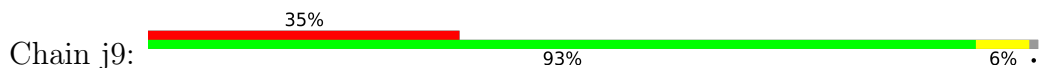
- Molecule 8: Allophycocyanin subunit beta

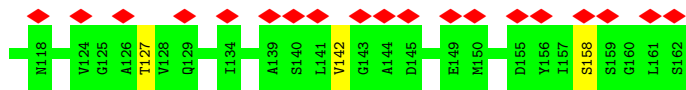


- Molecule 8: Allophycocyanin subunit beta

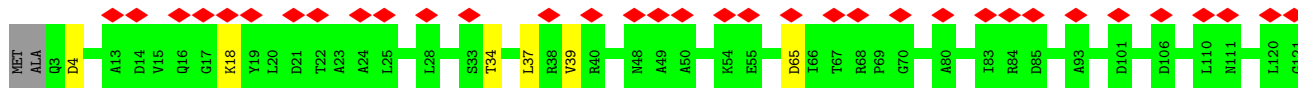
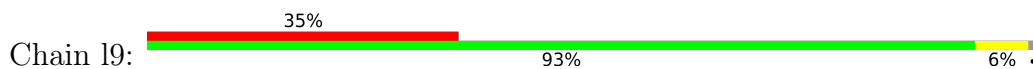


- Molecule 8: Allophycocyanin subunit beta

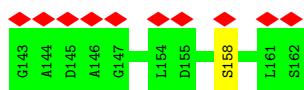
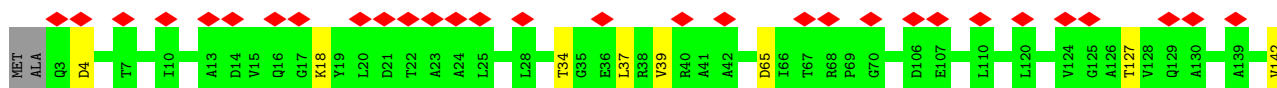
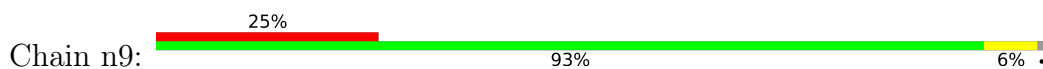




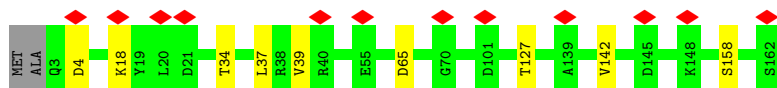
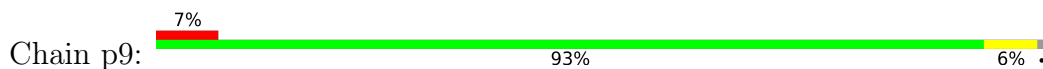
- Molecule 8: Allophycocyanin subunit beta



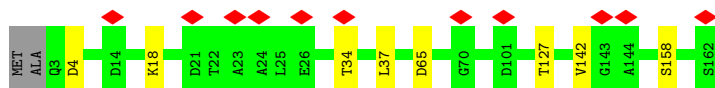
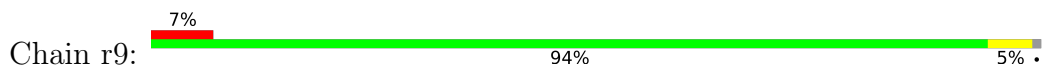
- Molecule 8: Allophycocyanin subunit beta



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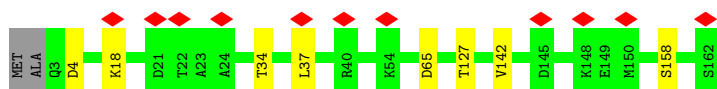
- Molecule 8: Allophycocyanin subunit beta



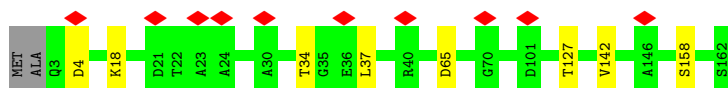
- Molecule 8: Allophycocyanin subunit beta



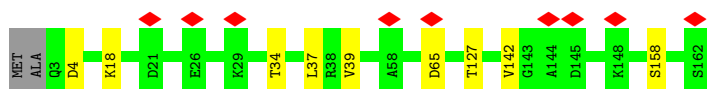
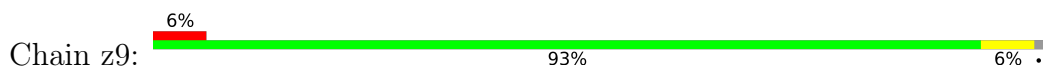
- Molecule 8: Allophycocyanin subunit beta



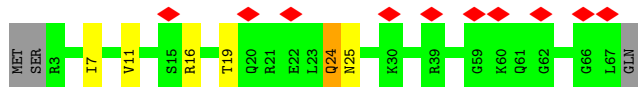
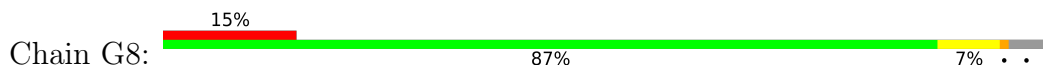
- Molecule 8: Allophycocyanin subunit beta



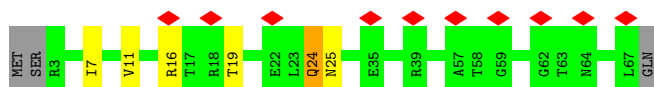
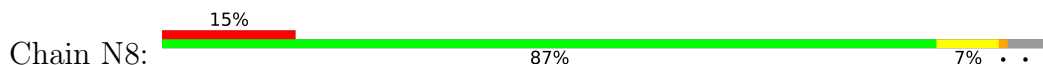
- Molecule 8: Allophycocyanin subunit beta



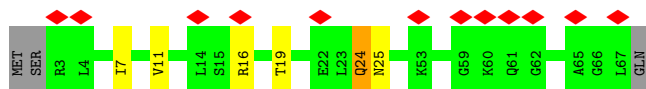
- Molecule 9: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core



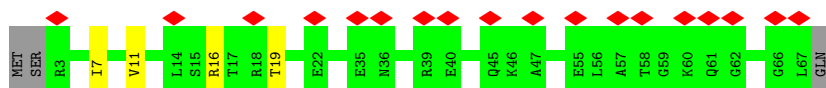
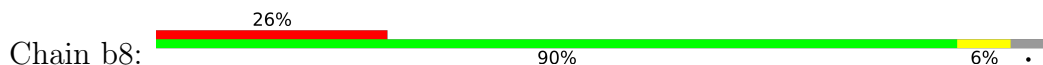
- Molecule 9: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core



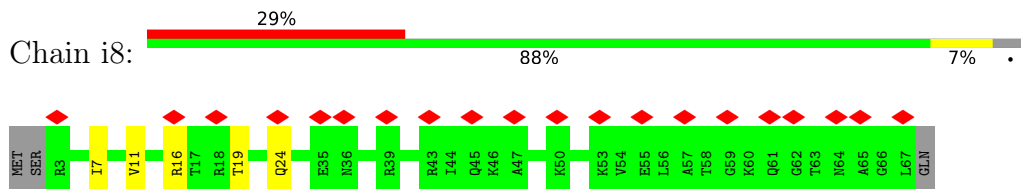
- Molecule 9: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core



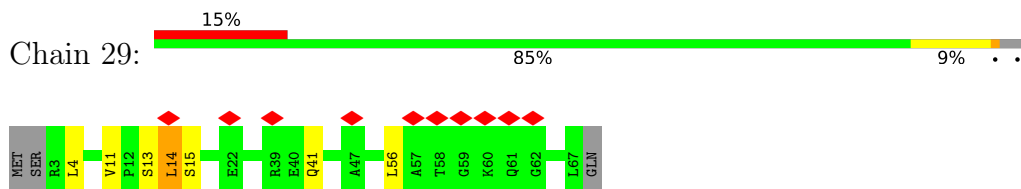
- Molecule 9: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core



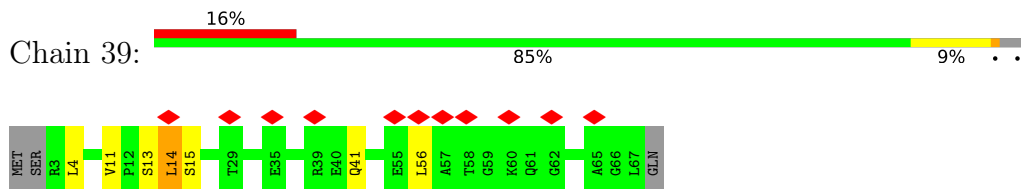
- Molecule 9: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core



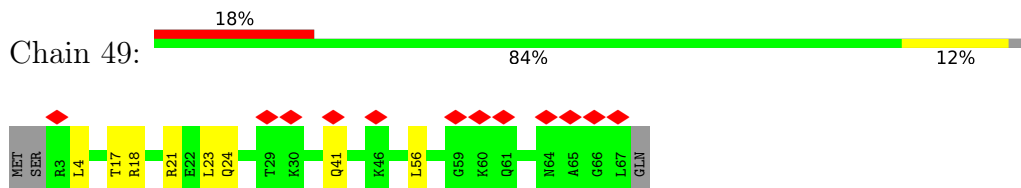
- Molecule 9: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core



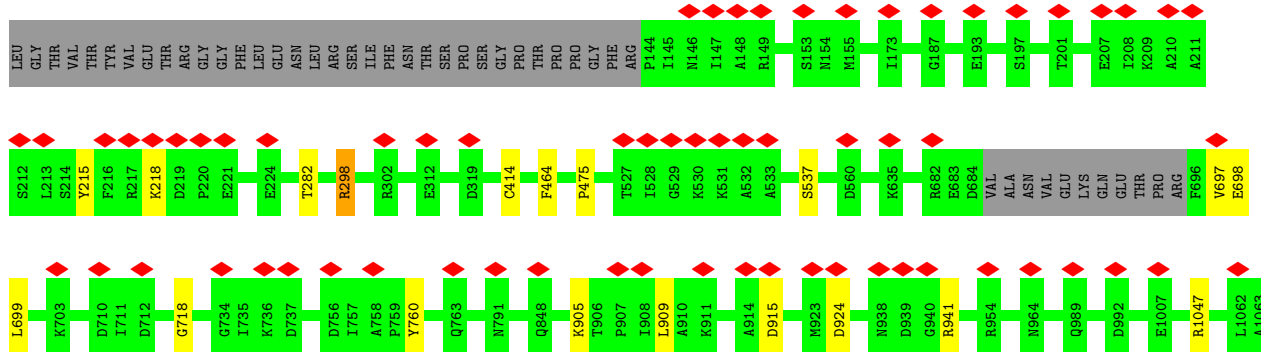
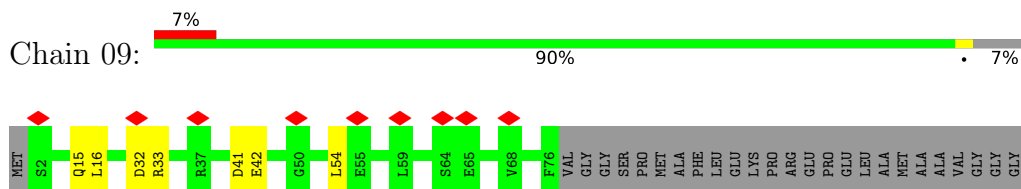
- Molecule 9: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core

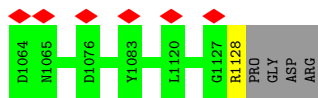


- Molecule 9: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core

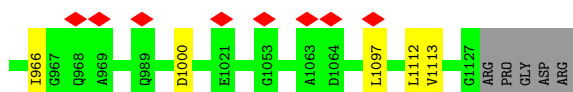
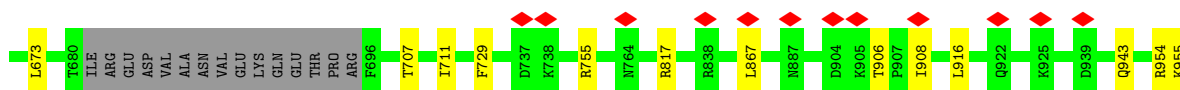
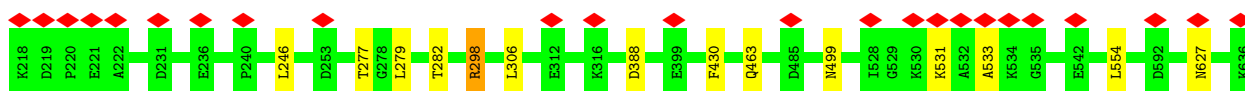
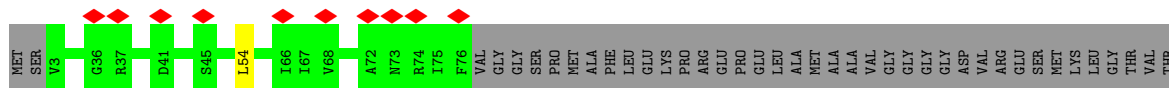
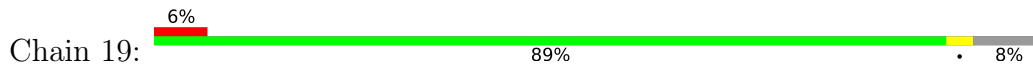


- Molecule 10: Phycobiliprotein ApcE

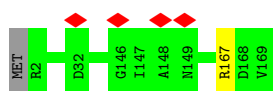




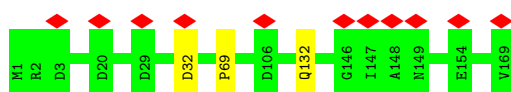
• Molecule 10: Phycobiliprotein ApcE



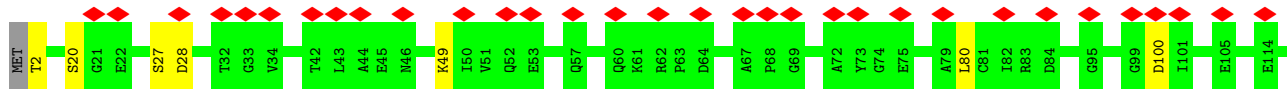
• Molecule 11: Allophycocyanin subunit beta-18

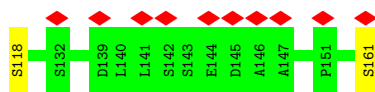


• Molecule 11: Allophycocyanin subunit beta-18



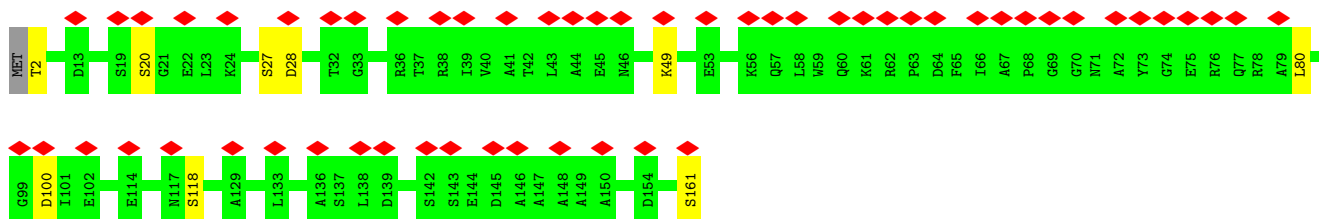
• Molecule 12: Allophycocyanin subunit alpha-B





- Molecule 12: Allophycocyanin subunit alpha-B

Chain m9: 35% 94% 6%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	62439	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	0.083	Depositor
Minimum map value	-0.035	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0195	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	0.45	0/1814	0.67	2/2452 (0.1%)
1	A4	0.45	0/1814	0.67	2/2452 (0.1%)
2	B1	0.31	0/1246	0.48	0/1693
2	B2	0.36	0/1246	0.47	0/1693
2	B3	0.36	0/1246	0.47	0/1693
2	B4	0.31	0/1246	0.49	0/1693
2	B5	0.35	0/1246	0.48	0/1693
2	B6	0.36	0/1246	0.47	0/1693
2	B7	0.36	0/1246	0.47	0/1693
2	BA	0.35	0/1246	0.48	0/1693
2	D1	0.31	0/1246	0.49	0/1693
2	D2	0.36	0/1246	0.47	0/1693
2	D3	0.36	0/1246	0.48	0/1693
2	D4	0.31	0/1246	0.49	0/1693
2	D5	0.35	0/1246	0.48	0/1693
2	D6	0.36	0/1246	0.47	0/1693
2	D7	0.36	0/1246	0.47	0/1693
2	DA	0.36	0/1246	0.48	0/1693
2	F1	0.31	0/1246	0.49	0/1693
2	F2	0.36	0/1246	0.47	0/1693
2	F3	0.36	0/1246	0.47	0/1693
2	F4	0.31	0/1246	0.49	0/1693
2	F5	0.35	0/1246	0.48	0/1693
2	F6	0.35	0/1246	0.47	0/1693
2	F7	0.36	0/1246	0.47	0/1693
2	FA	0.35	0/1246	0.48	0/1693
2	H1	0.31	0/1246	0.49	0/1693
2	H2	0.36	0/1246	0.48	0/1693
2	H3	0.36	0/1246	0.48	0/1693
2	H4	0.31	0/1246	0.49	0/1693
2	H5	0.35	0/1246	0.48	0/1693
2	H6	0.36	0/1246	0.48	0/1693

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	H7	0.36	0/1246	0.48	0/1693
2	HA	0.35	0/1246	0.48	0/1693
2	J1	0.31	0/1246	0.49	0/1693
2	J2	0.36	0/1246	0.48	0/1693
2	J3	0.36	0/1246	0.48	0/1693
2	J4	0.31	0/1246	0.49	0/1693
2	J5	0.35	0/1246	0.48	0/1693
2	J6	0.36	0/1246	0.48	0/1693
2	J7	0.36	0/1246	0.48	0/1693
2	JA	0.35	0/1246	0.48	0/1693
2	L1	0.30	0/1246	0.49	0/1693
2	L2	0.35	0/1246	0.48	0/1693
2	L3	0.35	0/1246	0.48	0/1693
2	L4	0.30	0/1246	0.49	0/1693
2	L5	0.35	0/1246	0.48	0/1693
2	L6	0.35	0/1246	0.48	0/1693
2	L7	0.35	0/1246	0.48	0/1693
2	LA	0.35	0/1246	0.48	0/1693
2	O1	0.31	0/1246	0.49	0/1693
2	O2	0.36	0/1246	0.48	0/1693
2	O4	0.31	0/1246	0.49	0/1693
2	O5	0.35	0/1246	0.48	0/1693
2	O6	0.36	0/1246	0.48	0/1693
2	OA	0.35	0/1246	0.48	0/1693
2	Q1	0.31	0/1246	0.49	0/1693
2	Q2	0.35	0/1246	0.47	0/1693
2	Q4	0.31	0/1246	0.49	0/1693
2	Q5	0.35	0/1246	0.48	0/1693
2	Q6	0.35	0/1246	0.47	0/1693
2	QA	0.35	0/1246	0.48	0/1693
2	S1	0.31	0/1246	0.49	0/1693
2	S2	0.35	0/1246	0.49	0/1693
2	S4	0.31	0/1246	0.49	0/1693
2	S5	0.35	0/1246	0.48	0/1693
2	S6	0.35	0/1246	0.49	0/1693
2	SA	0.35	0/1246	0.48	0/1693
2	U1	0.31	0/1246	0.50	0/1693
2	U2	0.35	0/1246	0.47	0/1693
2	U4	0.31	0/1246	0.49	0/1693
2	U5	0.35	0/1246	0.48	0/1693
2	U6	0.35	0/1246	0.47	0/1693
2	UA	0.35	0/1246	0.48	0/1693
2	W1	0.31	0/1246	0.49	0/1693

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	W2	0.35	0/1246	0.47	0/1693
2	W4	0.31	0/1246	0.49	0/1693
2	W5	0.35	0/1246	0.48	0/1693
2	W6	0.35	0/1246	0.47	0/1693
2	WA	0.35	0/1246	0.48	0/1693
2	Y1	0.31	0/1246	0.49	0/1693
2	Y2	0.35	0/1246	0.47	0/1693
2	Y4	0.31	0/1246	0.49	0/1693
2	Y5	0.35	0/1246	0.48	0/1693
2	Y6	0.35	0/1246	0.47	0/1693
2	YA	0.35	0/1246	0.48	0/1693
3	C1	0.33	0/1290	0.53	0/1748
3	C2	0.43	1/1290 (0.1%)	0.63	2/1748 (0.1%)
3	C3	0.44	1/1290 (0.1%)	0.63	2/1748 (0.1%)
3	C4	0.33	0/1290	0.53	0/1748
3	C5	0.44	0/1290	0.71	5/1748 (0.3%)
3	C6	0.43	0/1290	0.63	2/1748 (0.1%)
3	C7	0.43	1/1290 (0.1%)	0.63	2/1748 (0.1%)
3	CA	0.44	0/1290	0.71	5/1748 (0.3%)
3	E1	0.33	0/1290	0.53	0/1748
3	E2	0.42	0/1298	0.59	1/1758 (0.1%)
3	E3	0.43	0/1298	0.59	1/1758 (0.1%)
3	E4	0.33	0/1290	0.53	0/1748
3	E5	0.44	0/1290	0.71	5/1748 (0.3%)
3	E6	0.42	0/1298	0.59	1/1758 (0.1%)
3	E7	0.43	0/1298	0.59	1/1758 (0.1%)
3	EA	0.44	0/1290	0.71	5/1748 (0.3%)
3	G1	0.33	0/1290	0.52	0/1748
3	G2	0.44	1/1298 (0.1%)	0.62	2/1758 (0.1%)
3	G3	0.44	0/1298	0.62	2/1758 (0.1%)
3	G4	0.33	0/1290	0.52	0/1748
3	G5	0.43	0/1290	0.70	5/1748 (0.3%)
3	G6	0.44	1/1298 (0.1%)	0.62	2/1758 (0.1%)
3	G7	0.44	1/1298 (0.1%)	0.62	2/1758 (0.1%)
3	GA	0.44	0/1290	0.70	5/1748 (0.3%)
3	I1	0.33	0/1298	0.54	0/1758
3	I2	0.46	0/1298	0.63	1/1758 (0.1%)
3	I3	0.47	0/1298	0.63	1/1758 (0.1%)
3	I4	0.33	0/1298	0.54	0/1758
3	I5	0.44	0/1290	0.71	5/1748 (0.3%)
3	I6	0.47	1/1298 (0.1%)	0.63	2/1758 (0.1%)
3	I7	0.47	0/1298	0.63	1/1758 (0.1%)
3	IA	0.44	0/1290	0.71	5/1748 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	K1	0.33	0/1290	0.54	0/1748
3	K2	0.43	0/1290	0.60	1/1748 (0.1%)
3	K3	0.43	0/1290	0.60	1/1748 (0.1%)
3	K4	0.33	0/1290	0.54	0/1748
3	K5	0.45	0/1290	0.72	5/1748 (0.3%)
3	K6	0.43	0/1290	0.60	1/1748 (0.1%)
3	K7	0.43	0/1290	0.60	1/1748 (0.1%)
3	KA	0.45	0/1290	0.72	5/1748 (0.3%)
3	M1	0.32	0/1290	0.52	0/1748
3	M2	0.45	1/1290 (0.1%)	0.63	1/1748 (0.1%)
3	M3	0.45	1/1290 (0.1%)	0.63	1/1748 (0.1%)
3	M4	0.32	0/1290	0.52	0/1748
3	M5	0.44	0/1290	0.72	5/1748 (0.3%)
3	M6	0.45	0/1290	0.63	1/1748 (0.1%)
3	M7	0.45	1/1290 (0.1%)	0.63	1/1748 (0.1%)
3	MA	0.44	0/1290	0.72	5/1748 (0.3%)
3	P1	0.33	0/1290	0.54	0/1748
3	P2	0.41	0/1290	0.59	2/1748 (0.1%)
3	P4	0.33	0/1290	0.54	0/1748
3	P5	0.45	0/1290	0.72	5/1748 (0.3%)
3	P6	0.41	0/1290	0.59	2/1748 (0.1%)
3	PA	0.44	0/1290	0.72	5/1748 (0.3%)
3	R1	0.33	0/1290	0.52	0/1748
3	R2	0.43	0/1290	0.58	1/1748 (0.1%)
3	R4	0.33	0/1290	0.52	0/1748
3	R5	0.44	0/1290	0.71	5/1748 (0.3%)
3	R6	0.43	0/1290	0.58	1/1748 (0.1%)
3	RA	0.44	0/1290	0.71	5/1748 (0.3%)
3	T1	0.32	0/1290	0.53	0/1748
3	T2	0.45	0/1290	0.63	1/1748 (0.1%)
3	T4	0.32	0/1290	0.53	0/1748
3	T5	0.44	0/1290	0.71	5/1748 (0.3%)
3	T6	0.45	1/1290 (0.1%)	0.63	1/1748 (0.1%)
3	TA	0.44	0/1290	0.71	5/1748 (0.3%)
3	V1	0.33	0/1290	0.52	0/1748
3	V2	0.46	1/1290 (0.1%)	0.64	1/1748 (0.1%)
3	V4	0.33	0/1290	0.52	0/1748
3	V5	0.44	0/1290	0.71	5/1748 (0.3%)
3	V6	0.45	1/1290 (0.1%)	0.64	2/1748 (0.1%)
3	VA	0.45	0/1290	0.71	5/1748 (0.3%)
3	X1	0.33	0/1290	0.52	0/1748
3	X2	0.45	0/1290	0.64	1/1748 (0.1%)
3	X4	0.33	0/1290	0.52	0/1748

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	X5	0.44	0/1290	0.71	5/1748 (0.3%)
3	X6	0.45	0/1290	0.64	2/1748 (0.1%)
3	XA	0.44	0/1290	0.71	5/1748 (0.3%)
3	Z1	0.32	0/1290	0.52	0/1748
3	Z2	0.42	0/1290	0.59	1/1748 (0.1%)
3	Z4	0.32	0/1290	0.52	0/1748
3	Z5	0.44	0/1290	0.71	5/1748 (0.3%)
3	Z6	0.42	0/1290	0.59	1/1748 (0.1%)
3	ZA	0.44	0/1290	0.71	5/1748 (0.3%)
4	N1	0.46	0/2311	0.70	2/3123 (0.1%)
4	N2	0.55	1/2311 (0.0%)	0.71	4/3123 (0.1%)
4	N3	0.57	0/451	0.77	0/608
4	N4	0.46	0/2311	0.70	2/3123 (0.1%)
4	N5	0.50	1/2311 (0.0%)	0.76	4/3123 (0.1%)
4	N6	0.55	1/2311 (0.0%)	0.71	4/3123 (0.1%)
4	N7	0.57	0/451	0.77	0/608
4	NA	0.50	1/2311 (0.0%)	0.76	4/3123 (0.1%)
5	A2	0.46	1/2081 (0.0%)	0.72	3/2810 (0.1%)
5	A5	0.40	0/1985	0.64	2/2679 (0.1%)
5	A6	0.46	1/2081 (0.0%)	0.71	3/2810 (0.1%)
5	AA	0.40	0/1985	0.65	2/2679 (0.1%)
6	A3	0.22	0/1147	0.52	1/1549 (0.1%)
6	A7	0.22	0/1147	0.51	1/1549 (0.1%)
7	A8	0.41	0/1219	1.05	4/1650 (0.2%)
7	A9	0.39	0/1219	1.02	3/1650 (0.2%)
7	C8	0.41	0/1219	1.05	4/1650 (0.2%)
7	C9	0.39	0/1219	1.02	3/1650 (0.2%)
7	E8	0.41	0/1219	1.05	4/1650 (0.2%)
7	E9	0.39	0/1219	1.01	3/1650 (0.2%)
7	G9	0.39	0/1219	1.01	3/1650 (0.2%)
7	H8	0.41	0/1219	1.05	4/1650 (0.2%)
7	I9	0.39	0/1219	1.01	3/1650 (0.2%)
7	J8	0.41	0/1219	1.05	4/1650 (0.2%)
7	K9	0.39	0/1219	1.02	3/1650 (0.2%)
7	L8	0.41	0/1219	1.05	4/1650 (0.2%)
7	N9	0.39	0/1219	1.02	3/1650 (0.2%)
7	O8	0.41	0/1219	1.05	4/1650 (0.2%)
7	P9	0.39	0/1219	1.02	3/1650 (0.2%)
7	Q8	0.41	0/1219	1.05	4/1650 (0.2%)
7	R9	0.39	0/1219	1.02	3/1650 (0.2%)
7	S8	0.41	0/1219	1.05	4/1650 (0.2%)
7	T9	0.39	0/1219	1.02	3/1650 (0.2%)
7	V8	0.41	0/1219	1.05	4/1650 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
7	X8	0.41	0/1219	1.05	4/1650 (0.2%)
7	X9	0.39	0/1219	1.01	3/1650 (0.2%)
7	Z8	0.41	0/1219	1.05	4/1650 (0.2%)
7	Z9	0.39	0/1219	1.02	3/1650 (0.2%)
7	b9	0.39	0/1219	1.02	3/1650 (0.2%)
7	c8	0.41	0/1219	1.05	4/1650 (0.2%)
7	d9	0.39	0/1219	1.02	3/1650 (0.2%)
7	e8	0.41	0/1219	1.05	4/1650 (0.2%)
7	f9	0.39	0/1219	1.02	3/1650 (0.2%)
7	g8	0.41	0/1219	1.05	4/1650 (0.2%)
7	i9	0.39	0/1219	1.02	3/1650 (0.2%)
7	j8	0.41	0/1219	1.05	4/1650 (0.2%)
7	k9	0.39	0/1219	1.02	3/1650 (0.2%)
7	l8	0.41	0/1219	1.05	4/1650 (0.2%)
7	n8	0.41	0/1219	1.05	4/1650 (0.2%)
7	o9	0.39	0/1219	1.02	3/1650 (0.2%)
7	p8	0.41	0/1219	1.05	4/1650 (0.2%)
7	q9	0.39	0/1219	1.01	3/1650 (0.2%)
7	r8	0.41	0/1219	1.05	4/1650 (0.2%)
7	s9	0.39	0/1219	1.02	3/1650 (0.2%)
7	t8	0.41	0/1219	1.05	4/1650 (0.2%)
7	u9	0.39	0/1219	1.02	3/1650 (0.2%)
7	w9	0.39	0/1219	1.01	3/1650 (0.2%)
7	y9	0.39	0/1219	1.02	3/1650 (0.2%)
8	B8	0.41	0/1216	1.18	6/1650 (0.4%)
8	B9	0.41	0/1216	0.52	0/1650
8	D8	0.41	0/1216	1.18	6/1650 (0.4%)
8	D9	0.41	0/1216	0.52	0/1650
8	F8	0.41	0/1216	1.18	6/1650 (0.4%)
8	F9	0.41	0/1216	0.52	0/1650
8	H9	0.41	0/1216	0.52	0/1650
8	I8	0.41	0/1216	1.18	6/1650 (0.4%)
8	J9	0.41	0/1216	0.52	0/1650
8	K8	0.41	0/1216	1.18	6/1650 (0.4%)
8	L9	0.41	0/1216	0.52	0/1650
8	M8	0.41	0/1216	1.18	6/1650 (0.4%)
8	M9	0.41	0/1216	0.52	0/1650
8	O9	0.41	0/1216	0.52	0/1650
8	P8	0.41	0/1207	1.18	6/1638 (0.4%)
8	R8	0.41	0/1216	1.18	6/1650 (0.4%)
8	S9	0.41	0/1216	0.52	0/1650
8	T8	0.41	0/1216	1.18	6/1650 (0.4%)
8	U9	0.41	0/1216	0.52	0/1650

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
8	W8	0.38	0/1216	1.18	6/1650 (0.4%)
8	W9	0.41	0/1216	0.52	0/1650
8	Y8	0.41	0/1216	1.18	6/1650 (0.4%)
8	Y9	0.41	0/1216	0.52	0/1650
8	a8	0.41	0/1216	1.18	6/1650 (0.4%)
8	a9	0.41	0/1216	0.52	0/1650
8	c9	0.41	0/1216	0.52	0/1650
8	d8	0.37	0/1216	0.91	3/1650 (0.2%)
8	e9	0.41	0/1216	0.52	0/1650
8	f8	0.41	0/1216	1.18	6/1650 (0.4%)
8	h8	0.41	0/1216	1.18	6/1650 (0.4%)
8	h9	0.41	0/1216	0.52	0/1650
8	j9	0.41	0/1216	0.52	0/1650
8	k8	0.41	0/1216	1.18	6/1650 (0.4%)
8	l9	0.41	0/1216	0.51	0/1650
8	m8	0.41	0/1216	1.18	6/1650 (0.4%)
8	n9	0.41	0/1216	0.52	0/1650
8	o8	0.37	0/1207	0.91	3/1638 (0.2%)
8	p9	0.41	0/1216	0.52	0/1650
8	q8	0.41	0/1207	1.18	6/1638 (0.4%)
8	r9	0.41	0/1216	0.52	0/1650
8	s8	0.41	0/1216	1.18	6/1650 (0.4%)
8	t9	0.41	0/1216	0.52	0/1650
8	u8	0.41	0/1216	1.18	6/1650 (0.4%)
8	v9	0.41	0/1216	0.52	0/1650
8	x9	0.41	0/1216	0.52	0/1650
8	z9	0.41	0/1216	0.52	0/1650
9	29	0.57	1/537 (0.2%)	0.94	5/721 (0.7%)
9	39	0.57	1/537 (0.2%)	0.94	5/721 (0.7%)
9	49	0.56	1/537 (0.2%)	0.81	3/721 (0.4%)
9	G8	0.51	0/537	0.68	1/721 (0.1%)
9	N8	0.51	0/537	0.68	1/721 (0.1%)
9	U8	0.51	0/537	0.68	1/721 (0.1%)
9	b8	0.48	0/537	0.61	0/721
9	i8	0.44	0/537	0.55	0/721
10	09	0.53	6/8528 (0.1%)	0.67	8/11537 (0.1%)
10	19	0.52	4/8475 (0.0%)	0.72	16/11467 (0.1%)
11	Q9	0.53	0/1323	0.65	0/1795
11	g9	0.52	0/1331	0.68	2/1805 (0.1%)
12	V9	0.45	0/1265	0.73	1/1713 (0.1%)
12	m9	0.45	0/1265	0.73	1/1713 (0.1%)
All	All	0.40	32/377986 (0.0%)	0.71	522/512380 (0.1%)

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	2
1	A4	0	2
4	N1	0	1
4	N2	0	1
4	N4	0	1
4	N5	0	2
4	N6	0	1
4	NA	0	2
5	A2	0	1
5	A6	0	1
10	09	0	4
10	19	0	5
All	All	0	23

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	09	760	TYR	CD1-CE1	-11.77	1.21	1.39
10	09	42	GLU	CG-CD	-8.41	1.39	1.51
4	N6	172	TYR	CD1-CE1	-7.85	1.27	1.39
4	N2	172	TYR	CD1-CE1	-7.79	1.27	1.39
10	19	282	THR	CB-CG2	-5.95	1.32	1.52

The worst 5 of 522 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	L8	83	ARG	NE-CZ-NH2	22.76	131.68	120.30
7	Q8	83	ARG	NE-CZ-NH2	22.75	131.68	120.30
7	n8	83	ARG	NE-CZ-NH2	22.72	131.66	120.30
7	r8	83	ARG	NE-CZ-NH2	22.72	131.66	120.30
7	t8	83	ARG	NE-CZ-NH2	22.70	131.65	120.30

There are no chirality outliers.

5 of 23 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A1	22	VAL	Peptide
1	A1	29	ARG	Peptide

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Mol	Chain	Res	Type	Group
5	A2	37	ASP	Peptide
4	N1	235	ARG	Peptide
4	N2	206	SER	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	211/247 (85%)	189 (90%)	21 (10%)	1 (0%)	29	67
1	A4	211/247 (85%)	189 (90%)	21 (10%)	1 (0%)	29	67
2	B1	160/163 (98%)	156 (98%)	4 (2%)	0	100	100
2	B2	160/163 (98%)	159 (99%)	1 (1%)	0	100	100
2	B3	160/163 (98%)	159 (99%)	1 (1%)	0	100	100
2	B4	160/163 (98%)	156 (98%)	4 (2%)	0	100	100
2	B5	160/163 (98%)	159 (99%)	1 (1%)	0	100	100
2	B6	160/163 (98%)	159 (99%)	1 (1%)	0	100	100
2	B7	160/163 (98%)	159 (99%)	1 (1%)	0	100	100
2	BA	160/163 (98%)	159 (99%)	1 (1%)	0	100	100
2	D1	160/163 (98%)	156 (98%)	4 (2%)	0	100	100
2	D2	160/163 (98%)	158 (99%)	2 (1%)	0	100	100
2	D3	160/163 (98%)	158 (99%)	2 (1%)	0	100	100
2	D4	160/163 (98%)	156 (98%)	4 (2%)	0	100	100
2	D5	160/163 (98%)	159 (99%)	1 (1%)	0	100	100
2	D6	160/163 (98%)	158 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D7	160/163 (98%)	158 (99%)	2 (1%)	0	100	100
2	DA	160/163 (98%)	159 (99%)	1 (1%)	0	100	100
2	F1	160/163 (98%)	156 (98%)	4 (2%)	0	100	100
2	F2	160/163 (98%)	159 (99%)	1 (1%)	0	100	100
2	F3	160/163 (98%)	159 (99%)	1 (1%)	0	100	100
2	F4	160/163 (98%)	156 (98%)	4 (2%)	0	100	100
2	F5	160/163 (98%)	159 (99%)	1 (1%)	0	100	100
2	F6	160/163 (98%)	159 (99%)	1 (1%)	0	100	100
2	F7	160/163 (98%)	159 (99%)	1 (1%)	0	100	100
2	FA	160/163 (98%)	159 (99%)	1 (1%)	0	100	100
2	H1	160/163 (98%)	156 (98%)	4 (2%)	0	100	100
2	H2	160/163 (98%)	158 (99%)	2 (1%)	0	100	100
2	H3	160/163 (98%)	158 (99%)	2 (1%)	0	100	100
2	H4	160/163 (98%)	156 (98%)	4 (2%)	0	100	100
2	H5	160/163 (98%)	159 (99%)	1 (1%)	0	100	100
2	H6	160/163 (98%)	158 (99%)	2 (1%)	0	100	100
2	H7	160/163 (98%)	158 (99%)	2 (1%)	0	100	100
2	HA	160/163 (98%)	159 (99%)	1 (1%)	0	100	100
2	J1	160/163 (98%)	156 (98%)	4 (2%)	0	100	100
2	J2	160/163 (98%)	158 (99%)	2 (1%)	0	100	100
2	J3	160/163 (98%)	158 (99%)	2 (1%)	0	100	100
2	J4	160/163 (98%)	156 (98%)	4 (2%)	0	100	100
2	J5	160/163 (98%)	159 (99%)	1 (1%)	0	100	100
2	J6	160/163 (98%)	158 (99%)	2 (1%)	0	100	100
2	J7	160/163 (98%)	158 (99%)	2 (1%)	0	100	100
2	JA	160/163 (98%)	159 (99%)	1 (1%)	0	100	100
2	L1	160/163 (98%)	156 (98%)	4 (2%)	0	100	100
2	L2	160/163 (98%)	157 (98%)	2 (1%)	1 (1%)	25	63
2	L3	160/163 (98%)	157 (98%)	2 (1%)	1 (1%)	25	63
2	L4	160/163 (98%)	156 (98%)	4 (2%)	0	100	100
2	L5	160/163 (98%)	159 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	L6	160/163 (98%)	157 (98%)	2 (1%)	1 (1%)	25	63
2	L7	160/163 (98%)	157 (98%)	2 (1%)	1 (1%)	25	63
2	LA	160/163 (98%)	159 (99%)	1 (1%)	0	100	100
2	O1	160/163 (98%)	156 (98%)	4 (2%)	0	100	100
2	O2	160/163 (98%)	158 (99%)	2 (1%)	0	100	100
2	O4	160/163 (98%)	156 (98%)	4 (2%)	0	100	100
2	O5	160/163 (98%)	159 (99%)	1 (1%)	0	100	100
2	O6	160/163 (98%)	158 (99%)	2 (1%)	0	100	100
2	OA	160/163 (98%)	159 (99%)	1 (1%)	0	100	100
2	Q1	160/163 (98%)	156 (98%)	4 (2%)	0	100	100
2	Q2	160/163 (98%)	158 (99%)	2 (1%)	0	100	100
2	Q4	160/163 (98%)	156 (98%)	4 (2%)	0	100	100
2	Q5	160/163 (98%)	159 (99%)	1 (1%)	0	100	100
2	Q6	160/163 (98%)	158 (99%)	2 (1%)	0	100	100
2	QA	160/163 (98%)	159 (99%)	1 (1%)	0	100	100
2	S1	160/163 (98%)	156 (98%)	4 (2%)	0	100	100
2	S2	160/163 (98%)	159 (99%)	1 (1%)	0	100	100
2	S4	160/163 (98%)	156 (98%)	4 (2%)	0	100	100
2	S5	160/163 (98%)	159 (99%)	1 (1%)	0	100	100
2	S6	160/163 (98%)	159 (99%)	1 (1%)	0	100	100
2	SA	160/163 (98%)	159 (99%)	1 (1%)	0	100	100
2	U1	160/163 (98%)	156 (98%)	4 (2%)	0	100	100
2	U2	160/163 (98%)	159 (99%)	1 (1%)	0	100	100
2	U4	160/163 (98%)	156 (98%)	4 (2%)	0	100	100
2	U5	160/163 (98%)	159 (99%)	1 (1%)	0	100	100
2	U6	160/163 (98%)	159 (99%)	1 (1%)	0	100	100
2	UA	160/163 (98%)	159 (99%)	1 (1%)	0	100	100
2	W1	160/163 (98%)	156 (98%)	4 (2%)	0	100	100
2	W2	160/163 (98%)	159 (99%)	1 (1%)	0	100	100
2	W4	160/163 (98%)	156 (98%)	4 (2%)	0	100	100
2	W5	160/163 (98%)	159 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	W6	160/163 (98%)	159 (99%)	1 (1%)	0	100	100
2	WA	160/163 (98%)	159 (99%)	1 (1%)	0	100	100
2	Y1	160/163 (98%)	156 (98%)	4 (2%)	0	100	100
2	Y2	160/163 (98%)	159 (99%)	1 (1%)	0	100	100
2	Y4	160/163 (98%)	156 (98%)	4 (2%)	0	100	100
2	Y5	160/163 (98%)	159 (99%)	1 (1%)	0	100	100
2	Y6	160/163 (98%)	159 (99%)	1 (1%)	0	100	100
2	YA	160/163 (98%)	159 (99%)	1 (1%)	0	100	100
3	C1	170/173 (98%)	165 (97%)	5 (3%)	0	100	100
3	C2	170/173 (98%)	167 (98%)	2 (1%)	1 (1%)	25	63
3	C3	170/173 (98%)	167 (98%)	2 (1%)	1 (1%)	25	63
3	C4	170/173 (98%)	166 (98%)	4 (2%)	0	100	100
3	C5	170/173 (98%)	168 (99%)	2 (1%)	0	100	100
3	C6	170/173 (98%)	167 (98%)	2 (1%)	1 (1%)	25	63
3	C7	170/173 (98%)	167 (98%)	2 (1%)	1 (1%)	25	63
3	CA	170/173 (98%)	168 (99%)	2 (1%)	0	100	100
3	E1	170/173 (98%)	166 (98%)	4 (2%)	0	100	100
3	E2	171/173 (99%)	166 (97%)	4 (2%)	1 (1%)	25	63
3	E3	171/173 (99%)	166 (97%)	4 (2%)	1 (1%)	25	63
3	E4	170/173 (98%)	166 (98%)	4 (2%)	0	100	100
3	E5	170/173 (98%)	169 (99%)	0	1 (1%)	25	63
3	E6	171/173 (99%)	166 (97%)	4 (2%)	1 (1%)	25	63
3	E7	171/173 (99%)	166 (97%)	4 (2%)	1 (1%)	25	63
3	EA	170/173 (98%)	169 (99%)	0	1 (1%)	25	63
3	G1	170/173 (98%)	166 (98%)	4 (2%)	0	100	100
3	G2	171/173 (99%)	168 (98%)	3 (2%)	0	100	100
3	G3	171/173 (99%)	168 (98%)	3 (2%)	0	100	100
3	G4	170/173 (98%)	166 (98%)	4 (2%)	0	100	100
3	G5	170/173 (98%)	168 (99%)	1 (1%)	1 (1%)	25	63
3	G6	171/173 (99%)	168 (98%)	3 (2%)	0	100	100
3	G7	171/173 (99%)	168 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	GA	170/173 (98%)	168 (99%)	1 (1%)	1 (1%)	25	63
3	I1	171/173 (99%)	165 (96%)	4 (2%)	2 (1%)	13	49
3	I2	171/173 (99%)	167 (98%)	3 (2%)	1 (1%)	25	63
3	I3	171/173 (99%)	167 (98%)	3 (2%)	1 (1%)	25	63
3	I4	171/173 (99%)	165 (96%)	4 (2%)	2 (1%)	13	49
3	I5	170/173 (98%)	169 (99%)	1 (1%)	0	100	100
3	I6	171/173 (99%)	167 (98%)	3 (2%)	1 (1%)	25	63
3	I7	171/173 (99%)	167 (98%)	3 (2%)	1 (1%)	25	63
3	IA	170/173 (98%)	169 (99%)	1 (1%)	0	100	100
3	K1	170/173 (98%)	166 (98%)	4 (2%)	0	100	100
3	K2	170/173 (98%)	166 (98%)	3 (2%)	1 (1%)	25	63
3	K3	170/173 (98%)	166 (98%)	3 (2%)	1 (1%)	25	63
3	K4	170/173 (98%)	166 (98%)	4 (2%)	0	100	100
3	K5	170/173 (98%)	169 (99%)	0	1 (1%)	25	63
3	K6	170/173 (98%)	166 (98%)	3 (2%)	1 (1%)	25	63
3	K7	170/173 (98%)	166 (98%)	3 (2%)	1 (1%)	25	63
3	KA	170/173 (98%)	169 (99%)	0	1 (1%)	25	63
3	M1	170/173 (98%)	166 (98%)	4 (2%)	0	100	100
3	M2	170/173 (98%)	167 (98%)	3 (2%)	0	100	100
3	M3	170/173 (98%)	167 (98%)	3 (2%)	0	100	100
3	M4	170/173 (98%)	166 (98%)	4 (2%)	0	100	100
3	M5	170/173 (98%)	169 (99%)	1 (1%)	0	100	100
3	M6	170/173 (98%)	167 (98%)	3 (2%)	0	100	100
3	M7	170/173 (98%)	167 (98%)	3 (2%)	0	100	100
3	MA	170/173 (98%)	169 (99%)	1 (1%)	0	100	100
3	P1	170/173 (98%)	166 (98%)	4 (2%)	0	100	100
3	P2	170/173 (98%)	166 (98%)	4 (2%)	0	100	100
3	P4	170/173 (98%)	166 (98%)	4 (2%)	0	100	100
3	P5	170/173 (98%)	169 (99%)	0	1 (1%)	25	63
3	P6	170/173 (98%)	166 (98%)	4 (2%)	0	100	100
3	PA	170/173 (98%)	169 (99%)	0	1 (1%)	25	63

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	R1	170/173 (98%)	166 (98%)	4 (2%)	0	100	100
3	R2	170/173 (98%)	165 (97%)	4 (2%)	1 (1%)	25	63
3	R4	170/173 (98%)	166 (98%)	4 (2%)	0	100	100
3	R5	170/173 (98%)	168 (99%)	1 (1%)	1 (1%)	25	63
3	R6	170/173 (98%)	165 (97%)	4 (2%)	1 (1%)	25	63
3	RA	170/173 (98%)	168 (99%)	1 (1%)	1 (1%)	25	63
3	T1	170/173 (98%)	166 (98%)	4 (2%)	0	100	100
3	T2	170/173 (98%)	166 (98%)	4 (2%)	0	100	100
3	T4	170/173 (98%)	166 (98%)	4 (2%)	0	100	100
3	T5	170/173 (98%)	169 (99%)	0	1 (1%)	25	63
3	T6	170/173 (98%)	166 (98%)	4 (2%)	0	100	100
3	TA	170/173 (98%)	169 (99%)	0	1 (1%)	25	63
3	V1	170/173 (98%)	166 (98%)	4 (2%)	0	100	100
3	V2	170/173 (98%)	166 (98%)	4 (2%)	0	100	100
3	V4	170/173 (98%)	166 (98%)	4 (2%)	0	100	100
3	V5	170/173 (98%)	169 (99%)	0	1 (1%)	25	63
3	V6	170/173 (98%)	166 (98%)	4 (2%)	0	100	100
3	VA	170/173 (98%)	169 (99%)	0	1 (1%)	25	63
3	X1	170/173 (98%)	166 (98%)	4 (2%)	0	100	100
3	X2	170/173 (98%)	166 (98%)	4 (2%)	0	100	100
3	X4	170/173 (98%)	165 (97%)	5 (3%)	0	100	100
3	X5	170/173 (98%)	169 (99%)	0	1 (1%)	25	63
3	X6	170/173 (98%)	166 (98%)	4 (2%)	0	100	100
3	XA	170/173 (98%)	169 (99%)	0	1 (1%)	25	63
3	Z1	170/173 (98%)	166 (98%)	4 (2%)	0	100	100
3	Z2	170/173 (98%)	166 (98%)	4 (2%)	0	100	100
3	Z4	170/173 (98%)	166 (98%)	4 (2%)	0	100	100
3	Z5	170/173 (98%)	170 (100%)	0	0	100	100
3	Z6	170/173 (98%)	166 (98%)	4 (2%)	0	100	100
3	ZA	170/173 (98%)	170 (100%)	0	0	100	100
4	N1	282/286 (99%)	257 (91%)	23 (8%)	2 (1%)	22	60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	N2	282/286 (99%)	259 (92%)	23 (8%)	0	100	100
4	N3	55/286 (19%)	46 (84%)	9 (16%)	0	100	100
4	N4	282/286 (99%)	257 (91%)	23 (8%)	2 (1%)	22	60
4	N5	282/286 (99%)	257 (91%)	23 (8%)	2 (1%)	22	60
4	N6	282/286 (99%)	259 (92%)	23 (8%)	0	100	100
4	N7	55/286 (19%)	46 (84%)	9 (16%)	0	100	100
4	NA	282/286 (99%)	257 (91%)	23 (8%)	2 (1%)	22	60
5	A2	247/253 (98%)	226 (92%)	18 (7%)	3 (1%)	13	49
5	A5	233/253 (92%)	218 (94%)	13 (6%)	2 (1%)	17	54
5	A6	247/253 (98%)	227 (92%)	18 (7%)	2 (1%)	19	57
5	AA	233/253 (92%)	218 (94%)	12 (5%)	3 (1%)	12	48
6	A3	134/279 (48%)	131 (98%)	1 (1%)	2 (2%)	10	45
6	A7	134/279 (48%)	131 (98%)	1 (1%)	2 (2%)	10	45
7	A8	157/161 (98%)	155 (99%)	2 (1%)	0	100	100
7	A9	157/161 (98%)	153 (98%)	4 (2%)	0	100	100
7	C8	157/161 (98%)	155 (99%)	2 (1%)	0	100	100
7	C9	157/161 (98%)	153 (98%)	4 (2%)	0	100	100
7	E8	157/161 (98%)	155 (99%)	2 (1%)	0	100	100
7	E9	157/161 (98%)	153 (98%)	4 (2%)	0	100	100
7	G9	157/161 (98%)	153 (98%)	4 (2%)	0	100	100
7	H8	157/161 (98%)	155 (99%)	2 (1%)	0	100	100
7	I9	157/161 (98%)	153 (98%)	4 (2%)	0	100	100
7	J8	157/161 (98%)	155 (99%)	2 (1%)	0	100	100
7	K9	157/161 (98%)	153 (98%)	4 (2%)	0	100	100
7	L8	157/161 (98%)	155 (99%)	2 (1%)	0	100	100
7	N9	157/161 (98%)	153 (98%)	4 (2%)	0	100	100
7	O8	157/161 (98%)	155 (99%)	2 (1%)	0	100	100
7	P9	157/161 (98%)	153 (98%)	4 (2%)	0	100	100
7	Q8	157/161 (98%)	155 (99%)	2 (1%)	0	100	100
7	R9	157/161 (98%)	153 (98%)	4 (2%)	0	100	100
7	S8	157/161 (98%)	155 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	T9	157/161 (98%)	153 (98%)	4 (2%)	0	100	100
7	V8	157/161 (98%)	155 (99%)	2 (1%)	0	100	100
7	X8	157/161 (98%)	155 (99%)	2 (1%)	0	100	100
7	X9	157/161 (98%)	153 (98%)	4 (2%)	0	100	100
7	Z8	157/161 (98%)	155 (99%)	2 (1%)	0	100	100
7	Z9	157/161 (98%)	153 (98%)	4 (2%)	0	100	100
7	b9	157/161 (98%)	153 (98%)	4 (2%)	0	100	100
7	c8	157/161 (98%)	155 (99%)	2 (1%)	0	100	100
7	d9	157/161 (98%)	154 (98%)	3 (2%)	0	100	100
7	e8	157/161 (98%)	155 (99%)	2 (1%)	0	100	100
7	f9	157/161 (98%)	153 (98%)	4 (2%)	0	100	100
7	g8	157/161 (98%)	155 (99%)	2 (1%)	0	100	100
7	i9	157/161 (98%)	153 (98%)	4 (2%)	0	100	100
7	j8	157/161 (98%)	155 (99%)	2 (1%)	0	100	100
7	k9	157/161 (98%)	153 (98%)	4 (2%)	0	100	100
7	l8	157/161 (98%)	155 (99%)	2 (1%)	0	100	100
7	n8	157/161 (98%)	155 (99%)	2 (1%)	0	100	100
7	o9	157/161 (98%)	153 (98%)	4 (2%)	0	100	100
7	p8	157/161 (98%)	154 (98%)	3 (2%)	0	100	100
7	q9	157/161 (98%)	153 (98%)	4 (2%)	0	100	100
7	r8	157/161 (98%)	155 (99%)	2 (1%)	0	100	100
7	s9	157/161 (98%)	153 (98%)	4 (2%)	0	100	100
7	t8	157/161 (98%)	155 (99%)	2 (1%)	0	100	100
7	u9	157/161 (98%)	153 (98%)	4 (2%)	0	100	100
7	w9	157/161 (98%)	153 (98%)	4 (2%)	0	100	100
7	y9	157/161 (98%)	153 (98%)	4 (2%)	0	100	100
8	B8	158/162 (98%)	154 (98%)	4 (2%)	0	100	100
8	B9	158/162 (98%)	154 (98%)	4 (2%)	0	100	100
8	D8	158/162 (98%)	155 (98%)	3 (2%)	0	100	100
8	D9	158/162 (98%)	154 (98%)	4 (2%)	0	100	100
8	F8	158/162 (98%)	154 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	F9	158/162 (98%)	154 (98%)	4 (2%)	0	100	100
8	H9	158/162 (98%)	154 (98%)	4 (2%)	0	100	100
8	I8	158/162 (98%)	155 (98%)	3 (2%)	0	100	100
8	J9	158/162 (98%)	154 (98%)	4 (2%)	0	100	100
8	K8	158/162 (98%)	154 (98%)	4 (2%)	0	100	100
8	L9	158/162 (98%)	154 (98%)	4 (2%)	0	100	100
8	M8	158/162 (98%)	154 (98%)	4 (2%)	0	100	100
8	M9	158/162 (98%)	154 (98%)	4 (2%)	0	100	100
8	O9	158/162 (98%)	154 (98%)	4 (2%)	0	100	100
8	P8	157/162 (97%)	154 (98%)	3 (2%)	0	100	100
8	R8	158/162 (98%)	155 (98%)	3 (2%)	0	100	100
8	S9	158/162 (98%)	154 (98%)	4 (2%)	0	100	100
8	T8	158/162 (98%)	155 (98%)	3 (2%)	0	100	100
8	U9	158/162 (98%)	154 (98%)	4 (2%)	0	100	100
8	W8	158/162 (98%)	154 (98%)	4 (2%)	0	100	100
8	W9	158/162 (98%)	154 (98%)	4 (2%)	0	100	100
8	Y8	158/162 (98%)	155 (98%)	3 (2%)	0	100	100
8	Y9	158/162 (98%)	154 (98%)	4 (2%)	0	100	100
8	a8	158/162 (98%)	155 (98%)	3 (2%)	0	100	100
8	a9	158/162 (98%)	154 (98%)	4 (2%)	0	100	100
8	c9	158/162 (98%)	154 (98%)	4 (2%)	0	100	100
8	d8	158/162 (98%)	155 (98%)	3 (2%)	0	100	100
8	e9	158/162 (98%)	154 (98%)	4 (2%)	0	100	100
8	f8	158/162 (98%)	154 (98%)	4 (2%)	0	100	100
8	h8	158/162 (98%)	154 (98%)	4 (2%)	0	100	100
8	h9	158/162 (98%)	154 (98%)	4 (2%)	0	100	100
8	j9	158/162 (98%)	154 (98%)	4 (2%)	0	100	100
8	k8	158/162 (98%)	155 (98%)	3 (2%)	0	100	100
8	l9	158/162 (98%)	154 (98%)	4 (2%)	0	100	100
8	m8	158/162 (98%)	155 (98%)	3 (2%)	0	100	100
8	n9	158/162 (98%)	154 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	o8	157/162 (97%)	154 (98%)	3 (2%)	0	100	100
8	p9	158/162 (98%)	154 (98%)	4 (2%)	0	100	100
8	q8	157/162 (97%)	154 (98%)	3 (2%)	0	100	100
8	r9	158/162 (98%)	154 (98%)	4 (2%)	0	100	100
8	s8	158/162 (98%)	155 (98%)	3 (2%)	0	100	100
8	t9	158/162 (98%)	154 (98%)	4 (2%)	0	100	100
8	u8	158/162 (98%)	154 (98%)	4 (2%)	0	100	100
8	v9	158/162 (98%)	154 (98%)	4 (2%)	0	100	100
8	x9	158/162 (98%)	154 (98%)	4 (2%)	0	100	100
8	z9	158/162 (98%)	154 (98%)	4 (2%)	0	100	100
9	29	63/68 (93%)	57 (90%)	6 (10%)	0	100	100
9	39	63/68 (93%)	57 (90%)	6 (10%)	0	100	100
9	49	63/68 (93%)	57 (90%)	6 (10%)	0	100	100
9	G8	63/68 (93%)	59 (94%)	4 (6%)	0	100	100
9	N8	63/68 (93%)	59 (94%)	4 (6%)	0	100	100
9	U8	63/68 (93%)	59 (94%)	4 (6%)	0	100	100
9	b8	63/68 (93%)	59 (94%)	4 (6%)	0	100	100
9	i8	63/68 (93%)	62 (98%)	1 (2%)	0	100	100
10	09	1043/1132 (92%)	989 (95%)	51 (5%)	3 (0%)	41	75
10	19	1037/1132 (92%)	939 (90%)	93 (9%)	5 (0%)	29	67
11	Q9	166/169 (98%)	160 (96%)	6 (4%)	0	100	100
11	g9	167/169 (99%)	160 (96%)	7 (4%)	0	100	100
12	V9	158/161 (98%)	150 (95%)	8 (5%)	0	100	100
12	m9	158/161 (98%)	150 (95%)	8 (5%)	0	100	100
All	All	48592/50580 (96%)	47338 (97%)	1180 (2%)	74 (0%)	50	79

5 of 74 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A1	55	SER
3	I1	155	SER
4	N1	230	VAL
5	A2	20	PHE
5	A2	241	ILE

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	191/223 (86%)	187 (98%)	4 (2%)	53	73
1	A4	191/223 (86%)	187 (98%)	4 (2%)	53	73
2	B1	122/123 (99%)	106 (87%)	16 (13%)	4	22
2	B2	122/123 (99%)	110 (90%)	12 (10%)	8	31
2	B3	122/123 (99%)	110 (90%)	12 (10%)	8	31
2	B4	122/123 (99%)	105 (86%)	17 (14%)	3	21
2	B5	122/123 (99%)	106 (87%)	16 (13%)	4	22
2	B6	122/123 (99%)	110 (90%)	12 (10%)	8	31
2	B7	122/123 (99%)	110 (90%)	12 (10%)	8	31
2	BA	122/123 (99%)	106 (87%)	16 (13%)	4	22
2	D1	122/123 (99%)	105 (86%)	17 (14%)	3	21
2	D2	122/123 (99%)	108 (88%)	14 (12%)	5	26
2	D3	122/123 (99%)	108 (88%)	14 (12%)	5	26
2	D4	122/123 (99%)	105 (86%)	17 (14%)	3	21
2	D5	122/123 (99%)	107 (88%)	15 (12%)	4	24
2	D6	122/123 (99%)	108 (88%)	14 (12%)	5	26
2	D7	122/123 (99%)	108 (88%)	14 (12%)	5	26
2	DA	122/123 (99%)	107 (88%)	15 (12%)	4	24
2	F1	122/123 (99%)	105 (86%)	17 (14%)	3	21
2	F2	122/123 (99%)	110 (90%)	12 (10%)	8	31
2	F3	122/123 (99%)	110 (90%)	12 (10%)	8	31
2	F4	122/123 (99%)	105 (86%)	17 (14%)	3	21
2	F5	122/123 (99%)	107 (88%)	15 (12%)	4	24
2	F6	122/123 (99%)	110 (90%)	12 (10%)	8	31
2	F7	122/123 (99%)	110 (90%)	12 (10%)	8	31
2	FA	122/123 (99%)	107 (88%)	15 (12%)	4	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H1	122/123 (99%)	105 (86%)	17 (14%)	3	21
2	H2	122/123 (99%)	107 (88%)	15 (12%)	4	24
2	H3	122/123 (99%)	107 (88%)	15 (12%)	4	24
2	H4	122/123 (99%)	105 (86%)	17 (14%)	3	21
2	H5	122/123 (99%)	107 (88%)	15 (12%)	4	24
2	H6	122/123 (99%)	108 (88%)	14 (12%)	5	26
2	H7	122/123 (99%)	107 (88%)	15 (12%)	4	24
2	HA	122/123 (99%)	107 (88%)	15 (12%)	4	24
2	J1	122/123 (99%)	105 (86%)	17 (14%)	3	21
2	J2	122/123 (99%)	108 (88%)	14 (12%)	5	26
2	J3	122/123 (99%)	108 (88%)	14 (12%)	5	26
2	J4	122/123 (99%)	105 (86%)	17 (14%)	3	21
2	J5	122/123 (99%)	106 (87%)	16 (13%)	4	22
2	J6	122/123 (99%)	108 (88%)	14 (12%)	5	26
2	J7	122/123 (99%)	108 (88%)	14 (12%)	5	26
2	JA	122/123 (99%)	106 (87%)	16 (13%)	4	22
2	L1	122/123 (99%)	106 (87%)	16 (13%)	4	22
2	L2	122/123 (99%)	109 (89%)	13 (11%)	6	29
2	L3	122/123 (99%)	109 (89%)	13 (11%)	6	29
2	L4	122/123 (99%)	106 (87%)	16 (13%)	4	22
2	L5	122/123 (99%)	106 (87%)	16 (13%)	4	22
2	L6	122/123 (99%)	109 (89%)	13 (11%)	6	29
2	L7	122/123 (99%)	109 (89%)	13 (11%)	6	29
2	LA	122/123 (99%)	106 (87%)	16 (13%)	4	22
2	O1	122/123 (99%)	105 (86%)	17 (14%)	3	21
2	O2	122/123 (99%)	108 (88%)	14 (12%)	5	26
2	O4	122/123 (99%)	105 (86%)	17 (14%)	3	21
2	O5	122/123 (99%)	107 (88%)	15 (12%)	4	24
2	O6	122/123 (99%)	108 (88%)	14 (12%)	5	26
2	OA	122/123 (99%)	107 (88%)	15 (12%)	4	24
2	Q1	122/123 (99%)	105 (86%)	17 (14%)	3	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	Q2	122/123 (99%)	107 (88%)	15 (12%)	4	24
2	Q4	122/123 (99%)	105 (86%)	17 (14%)	3	21
2	Q5	122/123 (99%)	106 (87%)	16 (13%)	4	22
2	Q6	122/123 (99%)	107 (88%)	15 (12%)	4	24
2	QA	122/123 (99%)	106 (87%)	16 (13%)	4	22
2	S1	122/123 (99%)	105 (86%)	17 (14%)	3	21
2	S2	122/123 (99%)	108 (88%)	14 (12%)	5	26
2	S4	122/123 (99%)	105 (86%)	17 (14%)	3	21
2	S5	122/123 (99%)	107 (88%)	15 (12%)	4	24
2	S6	122/123 (99%)	108 (88%)	14 (12%)	5	26
2	SA	122/123 (99%)	107 (88%)	15 (12%)	4	24
2	U1	122/123 (99%)	104 (85%)	18 (15%)	3	18
2	U2	122/123 (99%)	110 (90%)	12 (10%)	8	31
2	U4	122/123 (99%)	104 (85%)	18 (15%)	3	18
2	U5	122/123 (99%)	106 (87%)	16 (13%)	4	22
2	U6	122/123 (99%)	110 (90%)	12 (10%)	8	31
2	UA	122/123 (99%)	106 (87%)	16 (13%)	4	22
2	W1	122/123 (99%)	105 (86%)	17 (14%)	3	21
2	W2	122/123 (99%)	107 (88%)	15 (12%)	4	24
2	W4	122/123 (99%)	105 (86%)	17 (14%)	3	21
2	W5	122/123 (99%)	106 (87%)	16 (13%)	4	22
2	W6	122/123 (99%)	108 (88%)	14 (12%)	5	26
2	WA	122/123 (99%)	106 (87%)	16 (13%)	4	22
2	Y1	122/123 (99%)	105 (86%)	17 (14%)	3	21
2	Y2	122/123 (99%)	108 (88%)	14 (12%)	5	26
2	Y4	122/123 (99%)	105 (86%)	17 (14%)	3	21
2	Y5	122/123 (99%)	107 (88%)	15 (12%)	4	24
2	Y6	122/123 (99%)	108 (88%)	14 (12%)	5	26
2	YA	122/123 (99%)	107 (88%)	15 (12%)	4	24
3	C1	134/135 (99%)	122 (91%)	12 (9%)	9	36
3	C2	134/135 (99%)	115 (86%)	19 (14%)	3	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C3	134/135 (99%)	115 (86%)	19 (14%)	3	20
3	C4	134/135 (99%)	122 (91%)	12 (9%)	9	36
3	C5	134/135 (99%)	114 (85%)	20 (15%)	3	18
3	C6	134/135 (99%)	115 (86%)	19 (14%)	3	20
3	C7	134/135 (99%)	115 (86%)	19 (14%)	3	20
3	CA	134/135 (99%)	114 (85%)	20 (15%)	3	18
3	E1	134/135 (99%)	123 (92%)	11 (8%)	11	40
3	E2	135/135 (100%)	115 (85%)	20 (15%)	3	18
3	E3	135/135 (100%)	115 (85%)	20 (15%)	3	18
3	E4	134/135 (99%)	123 (92%)	11 (8%)	11	40
3	E5	134/135 (99%)	116 (87%)	18 (13%)	4	22
3	E6	135/135 (100%)	115 (85%)	20 (15%)	3	18
3	E7	135/135 (100%)	115 (85%)	20 (15%)	3	18
3	EA	134/135 (99%)	116 (87%)	18 (13%)	4	22
3	G1	134/135 (99%)	121 (90%)	13 (10%)	8	32
3	G2	135/135 (100%)	117 (87%)	18 (13%)	4	22
3	G3	135/135 (100%)	117 (87%)	18 (13%)	4	22
3	G4	134/135 (99%)	121 (90%)	13 (10%)	8	32
3	G5	134/135 (99%)	115 (86%)	19 (14%)	3	20
3	G6	135/135 (100%)	117 (87%)	18 (13%)	4	22
3	G7	135/135 (100%)	117 (87%)	18 (13%)	4	22
3	GA	134/135 (99%)	115 (86%)	19 (14%)	3	20
3	I1	135/135 (100%)	126 (93%)	9 (7%)	16	46
3	I2	135/135 (100%)	116 (86%)	19 (14%)	3	21
3	I3	135/135 (100%)	116 (86%)	19 (14%)	3	21
3	I4	135/135 (100%)	125 (93%)	10 (7%)	13	43
3	I5	134/135 (99%)	116 (87%)	18 (13%)	4	22
3	I6	135/135 (100%)	116 (86%)	19 (14%)	3	21
3	I7	135/135 (100%)	116 (86%)	19 (14%)	3	21
3	IA	134/135 (99%)	116 (87%)	18 (13%)	4	22
3	K1	134/135 (99%)	121 (90%)	13 (10%)	8	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	K2	134/135 (99%)	114 (85%)	20 (15%)	3	18
3	K3	134/135 (99%)	114 (85%)	20 (15%)	3	18
3	K4	134/135 (99%)	121 (90%)	13 (10%)	8	32
3	K5	134/135 (99%)	115 (86%)	19 (14%)	3	20
3	K6	134/135 (99%)	114 (85%)	20 (15%)	3	18
3	K7	134/135 (99%)	114 (85%)	20 (15%)	3	18
3	KA	134/135 (99%)	115 (86%)	19 (14%)	3	20
3	M1	134/135 (99%)	123 (92%)	11 (8%)	11	40
3	M2	134/135 (99%)	118 (88%)	16 (12%)	5	25
3	M3	134/135 (99%)	118 (88%)	16 (12%)	5	25
3	M4	134/135 (99%)	123 (92%)	11 (8%)	11	40
3	M5	134/135 (99%)	114 (85%)	20 (15%)	3	18
3	M6	134/135 (99%)	119 (89%)	15 (11%)	6	27
3	M7	134/135 (99%)	118 (88%)	16 (12%)	5	25
3	MA	134/135 (99%)	114 (85%)	20 (15%)	3	18
3	P1	134/135 (99%)	124 (92%)	10 (8%)	13	42
3	P2	134/135 (99%)	114 (85%)	20 (15%)	3	18
3	P4	134/135 (99%)	124 (92%)	10 (8%)	13	42
3	P5	134/135 (99%)	115 (86%)	19 (14%)	3	20
3	P6	134/135 (99%)	114 (85%)	20 (15%)	3	18
3	PA	134/135 (99%)	115 (86%)	19 (14%)	3	20
3	R1	134/135 (99%)	125 (93%)	9 (7%)	16	46
3	R2	134/135 (99%)	114 (85%)	20 (15%)	3	18
3	R4	134/135 (99%)	125 (93%)	9 (7%)	16	46
3	R5	134/135 (99%)	116 (87%)	18 (13%)	4	22
3	R6	134/135 (99%)	114 (85%)	20 (15%)	3	18
3	RA	134/135 (99%)	116 (87%)	18 (13%)	4	22
3	T1	134/135 (99%)	124 (92%)	10 (8%)	13	42
3	T2	134/135 (99%)	115 (86%)	19 (14%)	3	20
3	T4	134/135 (99%)	124 (92%)	10 (8%)	13	42
3	T5	134/135 (99%)	115 (86%)	19 (14%)	3	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	T6	134/135 (99%)	115 (86%)	19 (14%)	3	20
3	TA	134/135 (99%)	115 (86%)	19 (14%)	3	20
3	V1	134/135 (99%)	123 (92%)	11 (8%)	11	40
3	V2	134/135 (99%)	117 (87%)	17 (13%)	4	23
3	V4	134/135 (99%)	123 (92%)	11 (8%)	11	40
3	V5	134/135 (99%)	115 (86%)	19 (14%)	3	20
3	V6	134/135 (99%)	116 (87%)	18 (13%)	4	22
3	VA	134/135 (99%)	115 (86%)	19 (14%)	3	20
3	X1	134/135 (99%)	126 (94%)	8 (6%)	19	49
3	X2	134/135 (99%)	116 (87%)	18 (13%)	4	22
3	X4	134/135 (99%)	125 (93%)	9 (7%)	16	46
3	X5	134/135 (99%)	114 (85%)	20 (15%)	3	18
3	X6	134/135 (99%)	116 (87%)	18 (13%)	4	22
3	XA	134/135 (99%)	114 (85%)	20 (15%)	3	18
3	Z1	134/135 (99%)	126 (94%)	8 (6%)	19	49
3	Z2	134/135 (99%)	117 (87%)	17 (13%)	4	23
3	Z4	134/135 (99%)	125 (93%)	9 (7%)	16	46
3	Z5	134/135 (99%)	115 (86%)	19 (14%)	3	20
3	Z6	134/135 (99%)	117 (87%)	17 (13%)	4	23
3	ZA	134/135 (99%)	115 (86%)	19 (14%)	3	20
4	N1	242/243 (100%)	240 (99%)	2 (1%)	81	89
4	N2	242/243 (100%)	239 (99%)	3 (1%)	71	83
4	N3	50/243 (21%)	49 (98%)	1 (2%)	55	74
4	N4	242/243 (100%)	240 (99%)	2 (1%)	81	89
4	N5	242/243 (100%)	239 (99%)	3 (1%)	71	83
4	N6	242/243 (100%)	239 (99%)	3 (1%)	71	83
4	N7	50/243 (21%)	49 (98%)	1 (2%)	55	74
4	NA	242/243 (100%)	239 (99%)	3 (1%)	71	83
5	A2	220/224 (98%)	217 (99%)	3 (1%)	67	81
5	A5	210/224 (94%)	205 (98%)	5 (2%)	49	69
5	A6	220/224 (98%)	218 (99%)	2 (1%)	78	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	AA	210/224 (94%)	206 (98%)	4 (2%)	57	75
6	A3	120/242 (50%)	115 (96%)	5 (4%)	30	57
6	A7	120/242 (50%)	115 (96%)	5 (4%)	30	57
7	A8	124/126 (98%)	113 (91%)	11 (9%)	9	36
7	A9	124/126 (98%)	115 (93%)	9 (7%)	14	43
7	C8	124/126 (98%)	113 (91%)	11 (9%)	9	36
7	C9	124/126 (98%)	114 (92%)	10 (8%)	11	40
7	E8	124/126 (98%)	113 (91%)	11 (9%)	9	36
7	E9	124/126 (98%)	115 (93%)	9 (7%)	14	43
7	G9	124/126 (98%)	115 (93%)	9 (7%)	14	43
7	H8	124/126 (98%)	113 (91%)	11 (9%)	9	36
7	I9	124/126 (98%)	115 (93%)	9 (7%)	14	43
7	J8	124/126 (98%)	113 (91%)	11 (9%)	9	36
7	K9	124/126 (98%)	115 (93%)	9 (7%)	14	43
7	L8	124/126 (98%)	113 (91%)	11 (9%)	9	36
7	N9	124/126 (98%)	115 (93%)	9 (7%)	14	43
7	O8	124/126 (98%)	113 (91%)	11 (9%)	9	36
7	P9	124/126 (98%)	115 (93%)	9 (7%)	14	43
7	Q8	124/126 (98%)	113 (91%)	11 (9%)	9	36
7	R9	124/126 (98%)	115 (93%)	9 (7%)	14	43
7	S8	124/126 (98%)	113 (91%)	11 (9%)	9	36
7	T9	124/126 (98%)	115 (93%)	9 (7%)	14	43
7	V8	124/126 (98%)	113 (91%)	11 (9%)	9	36
7	X8	124/126 (98%)	113 (91%)	11 (9%)	9	36
7	X9	124/126 (98%)	115 (93%)	9 (7%)	14	43
7	Z8	124/126 (98%)	113 (91%)	11 (9%)	9	36
7	Z9	124/126 (98%)	115 (93%)	9 (7%)	14	43
7	b9	124/126 (98%)	115 (93%)	9 (7%)	14	43
7	c8	124/126 (98%)	113 (91%)	11 (9%)	9	36
7	d9	124/126 (98%)	115 (93%)	9 (7%)	14	43
7	e8	124/126 (98%)	113 (91%)	11 (9%)	9	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	f9	124/126 (98%)	115 (93%)	9 (7%)	14	43
7	g8	124/126 (98%)	113 (91%)	11 (9%)	9	36
7	i9	124/126 (98%)	115 (93%)	9 (7%)	14	43
7	j8	124/126 (98%)	113 (91%)	11 (9%)	9	36
7	k9	124/126 (98%)	115 (93%)	9 (7%)	14	43
7	l8	124/126 (98%)	113 (91%)	11 (9%)	9	36
7	n8	124/126 (98%)	113 (91%)	11 (9%)	9	36
7	o9	124/126 (98%)	115 (93%)	9 (7%)	14	43
7	p8	124/126 (98%)	113 (91%)	11 (9%)	9	36
7	q9	124/126 (98%)	115 (93%)	9 (7%)	14	43
7	r8	124/126 (98%)	113 (91%)	11 (9%)	9	36
7	s9	124/126 (98%)	115 (93%)	9 (7%)	14	43
7	t8	124/126 (98%)	113 (91%)	11 (9%)	9	36
7	u9	124/126 (98%)	115 (93%)	9 (7%)	14	43
7	w9	124/126 (98%)	115 (93%)	9 (7%)	14	43
7	y9	124/126 (98%)	115 (93%)	9 (7%)	14	43
8	B8	123/124 (99%)	111 (90%)	12 (10%)	8	31
8	B9	123/124 (99%)	114 (93%)	9 (7%)	14	43
8	D8	123/124 (99%)	111 (90%)	12 (10%)	8	31
8	D9	123/124 (99%)	114 (93%)	9 (7%)	14	43
8	F8	123/124 (99%)	111 (90%)	12 (10%)	8	31
8	F9	123/124 (99%)	115 (94%)	8 (6%)	17	46
8	H9	123/124 (99%)	115 (94%)	8 (6%)	17	46
8	I8	123/124 (99%)	111 (90%)	12 (10%)	8	31
8	J9	123/124 (99%)	115 (94%)	8 (6%)	17	46
8	K8	123/124 (99%)	111 (90%)	12 (10%)	8	31
8	L9	123/124 (99%)	114 (93%)	9 (7%)	14	43
8	M8	123/124 (99%)	111 (90%)	12 (10%)	8	31
8	M9	123/124 (99%)	115 (94%)	8 (6%)	17	46
8	O9	123/124 (99%)	115 (94%)	8 (6%)	17	46
8	P8	122/124 (98%)	110 (90%)	12 (10%)	8	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	R8	123/124 (99%)	111 (90%)	12 (10%)	8	31
8	S9	123/124 (99%)	114 (93%)	9 (7%)	14	43
8	T8	123/124 (99%)	111 (90%)	12 (10%)	8	31
8	U9	123/124 (99%)	114 (93%)	9 (7%)	14	43
8	W8	123/124 (99%)	111 (90%)	12 (10%)	8	31
8	W9	123/124 (99%)	115 (94%)	8 (6%)	17	46
8	Y8	123/124 (99%)	111 (90%)	12 (10%)	8	31
8	Y9	123/124 (99%)	114 (93%)	9 (7%)	14	43
8	a8	123/124 (99%)	111 (90%)	12 (10%)	8	31
8	a9	123/124 (99%)	115 (94%)	8 (6%)	17	46
8	c9	123/124 (99%)	114 (93%)	9 (7%)	14	43
8	d8	123/124 (99%)	112 (91%)	11 (9%)	9	36
8	e9	123/124 (99%)	114 (93%)	9 (7%)	14	43
8	f8	123/124 (99%)	111 (90%)	12 (10%)	8	31
8	h8	123/124 (99%)	111 (90%)	12 (10%)	8	31
8	h9	123/124 (99%)	114 (93%)	9 (7%)	14	43
8	j9	123/124 (99%)	114 (93%)	9 (7%)	14	43
8	k8	123/124 (99%)	111 (90%)	12 (10%)	8	31
8	l9	123/124 (99%)	114 (93%)	9 (7%)	14	43
8	m8	123/124 (99%)	111 (90%)	12 (10%)	8	31
8	n9	123/124 (99%)	114 (93%)	9 (7%)	14	43
8	o8	122/124 (98%)	110 (90%)	12 (10%)	8	31
8	p9	123/124 (99%)	114 (93%)	9 (7%)	14	43
8	q8	122/124 (98%)	110 (90%)	12 (10%)	8	31
8	r9	123/124 (99%)	115 (94%)	8 (6%)	17	46
8	s8	123/124 (99%)	111 (90%)	12 (10%)	8	31
8	t9	123/124 (99%)	114 (93%)	9 (7%)	14	43
8	u8	123/124 (99%)	111 (90%)	12 (10%)	8	31
8	v9	123/124 (99%)	115 (94%)	8 (6%)	17	46
8	x9	123/124 (99%)	115 (94%)	8 (6%)	17	46
8	z9	123/124 (99%)	114 (93%)	9 (7%)	14	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	29	56/59 (95%)	52 (93%)	4 (7%)	14	44
9	39	56/59 (95%)	52 (93%)	4 (7%)	14	44
9	49	56/59 (95%)	50 (89%)	6 (11%)	6	29
9	G8	56/59 (95%)	50 (89%)	6 (11%)	6	29
9	N8	56/59 (95%)	50 (89%)	6 (11%)	6	29
9	U8	56/59 (95%)	50 (89%)	6 (11%)	6	29
9	b8	56/59 (95%)	52 (93%)	4 (7%)	14	44
9	i8	56/59 (95%)	51 (91%)	5 (9%)	9	36
10	09	888/954 (93%)	880 (99%)	8 (1%)	78	87
10	19	882/954 (92%)	876 (99%)	6 (1%)	84	90
11	Q9	135/136 (99%)	134 (99%)	1 (1%)	84	90
11	g9	136/136 (100%)	135 (99%)	1 (1%)	84	90
12	V9	132/133 (99%)	124 (94%)	8 (6%)	18	48
12	m9	132/133 (99%)	124 (94%)	8 (6%)	18	48
All	All	38416/39608 (97%)	34744 (90%)	3672 (10%)	12	32

5 of 3672 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L6	67	THR
2	SA	131	VAL
8	B8	107	GLU
2	QA	97	THR
7	u9	23	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 504 such sidechains are listed below:

Mol	Chain	Res	Type
7	C8	53	GLN
7	u9	46	ASN
7	g8	57	GLN
8	r9	132	GLN
2	JA	26	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

348 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
13	CYC	UA	1001	-	42,46,46	3.26	15 (35%)	50,67,67	3.12	21 (42%)
13	CYC	R4	1001	3	42,46,46	3.25	15 (35%)	50,67,67	3.13	21 (42%)
13	CYC	T4	201	-	42,46,46	1.08	1 (2%)	50,67,67	0.96	2 (4%)
13	CYC	P8	1001	-	42,46,46	3.44	14 (33%)	50,67,67	2.94	21 (42%)
13	CYC	R1	1001	3	42,46,46	3.26	15 (35%)	50,67,67	3.13	21 (42%)
13	CYC	P1	202	-	42,46,46	1.01	1 (2%)	50,67,67	0.98	2 (4%)
13	CYC	u9	1001	-	42,46,46	3.25	13 (30%)	50,67,67	3.33	21 (42%)
13	CYC	X6	202	-	42,46,46	1.07	1 (2%)	50,67,67	0.98	2 (4%)
13	CYC	U6	202	-	42,46,46	3.25	15 (35%)	50,67,67	3.10	21 (42%)
13	CYC	W5	1001	-	42,46,46	3.24	15 (35%)	50,67,67	3.11	21 (42%)
13	CYC	E3	202	3	42,46,46	1.08	1 (2%)	50,67,67	1.01	2 (4%)
13	CYC	C1	302	-	42,46,46	1.09	1 (2%)	50,67,67	0.96	2 (4%)
13	CYC	EA	202	-	42,46,46	3.24	15 (35%)	50,67,67	3.11	21 (42%)
13	CYC	K7	202	-	42,46,46	1.06	1 (2%)	50,67,67	0.97	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CYC	I5	202	-	42,46,46	1.03	1 (2%)	50,67,67	0.97	2 (4%)
13	CYC	V2	202	-	42,46,46	3.25	15 (35%)	50,67,67	3.12	21 (42%)
13	CYC	W4	1001	-	42,46,46	3.25	15 (35%)	50,67,67	3.12	21 (42%)
13	CYC	I4	201	3	42,46,46	3.46	14 (33%)	50,67,67	3.14	24 (48%)
13	CYC	T4	202	-	42,46,46	3.27	15 (35%)	50,67,67	3.12	21 (42%)
13	CYC	R2	1001	-	42,46,46	3.27	15 (35%)	50,67,67	3.13	21 (42%)
13	CYC	n8	1001	-	42,46,46	3.21	12 (28%)	50,67,67	3.08	22 (44%)
13	CYC	W1	1001	-	42,46,46	3.25	15 (35%)	50,67,67	3.12	21 (42%)
13	CYC	H2	1001	-	42,46,46	3.25	14 (33%)	50,67,67	3.09	21 (42%)
13	CYC	B8	1001	-	42,46,46	3.44	14 (33%)	50,67,67	2.95	21 (42%)
13	CYC	B5	1001	-	42,46,46	3.24	15 (35%)	50,67,67	3.11	21 (42%)
13	CYC	C1	301	3	42,46,46	3.25	15 (35%)	50,67,67	3.12	21 (42%)
13	CYC	K4	201	-	42,46,46	1.07	1 (2%)	50,67,67	0.97	2 (4%)
13	CYC	K7	201	-	42,46,46	1.09	1 (2%)	50,67,67	0.97	2 (4%)
13	CYC	X4	201	-	42,46,46	3.43	14 (33%)	50,67,67	3.16	24 (48%)
13	CYC	Z5	201	-	42,46,46	3.40	15 (35%)	50,67,67	3.14	24 (48%)
13	CYC	TA	202	-	42,46,46	1.07	1 (2%)	50,67,67	0.96	2 (4%)
13	CYC	P5	201	-	42,46,46	1.07	1 (2%)	50,67,67	1.06	3 (6%)
13	CYC	KA	201	-	42,46,46	1.07	1 (2%)	50,67,67	0.96	2 (4%)
13	CYC	C6	202	-	42,46,46	1.08	1 (2%)	50,67,67	0.96	2 (4%)
13	CYC	V6	201	-	42,46,46	1.06	1 (2%)	50,67,67	0.97	2 (4%)
13	CYC	Z5	202	-	42,46,46	1.08	1 (2%)	50,67,67	0.98	2 (4%)
13	CYC	Z2	202	-	42,46,46	3.26	15 (35%)	50,67,67	3.12	21 (42%)
13	CYC	T9	1001	-	42,46,46	3.24	13 (30%)	50,67,67	3.32	21 (42%)
13	CYC	SA	1001	-	42,46,46	3.24	15 (35%)	50,67,67	3.11	21 (42%)
13	CYC	x9	1001	-	42,46,46	3.21	12 (28%)	50,67,67	4.05	24 (48%)
13	CYC	M6	201	-	42,46,46	1.10	1 (2%)	50,67,67	0.98	2 (4%)
13	CYC	Y4	201	-	42,46,46	3.24	15 (35%)	50,67,67	3.10	21 (42%)
13	CYC	r8	1001	-	42,46,46	3.20	12 (28%)	50,67,67	3.08	22 (44%)
13	CYC	Q4	201	-	42,46,46	3.24	15 (35%)	50,67,67	3.12	21 (42%)
13	CYC	I3	201	-	42,46,46	3.47	14 (33%)	50,67,67	3.13	24 (48%)
13	CYC	X8	1001	-	42,46,46	3.21	12 (28%)	50,67,67	3.09	22 (44%)
13	CYC	O1	1001	-	42,46,46	3.24	14 (33%)	50,67,67	3.11	21 (42%)
13	CYC	Y8	1001	-	42,46,46	3.44	14 (33%)	50,67,67	2.95	21 (42%)
13	CYC	U1	1001	-	42,46,46	3.25	15 (35%)	50,67,67	3.10	21 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CYC	S6	1001	-	42,46,46	3.24	15 (35%)	50,67,67	3.10	21 (42%)
13	CYC	D2	1001	-	42,46,46	3.23	15 (35%)	50,67,67	3.12	21 (42%)
13	CYC	TA	201	-	42,46,46	3.42	14 (33%)	50,67,67	3.14	24 (48%)
13	CYC	MA	1001	-	42,46,46	3.24	15 (35%)	50,67,67	3.11	21 (42%)
13	CYC	V5	202	-	42,46,46	1.05	1 (2%)	50,67,67	0.97	2 (4%)
13	CYC	z9	1001	-	42,46,46	3.22	12 (28%)	50,67,67	4.06	24 (48%)
13	CYC	V2	201	-	42,46,46	1.05	1 (2%)	50,67,67	0.97	2 (4%)
13	CYC	D7	1001	-	42,46,46	3.23	15 (35%)	50,67,67	3.11	21 (42%)
13	CYC	V9	201	-	42,46,46	3.21	14 (33%)	50,67,67	3.00	19 (38%)
13	CYC	S8	1001	-	42,46,46	3.20	12 (28%)	50,67,67	3.08	22 (44%)
13	CYC	GA	1002	-	42,46,46	1.06	1 (2%)	50,67,67	0.96	2 (4%)
13	CYC	g8	1001	-	42,46,46	3.20	12 (28%)	50,67,67	3.08	22 (44%)
13	CYC	N3	301	-	42,46,46	1.04	1 (2%)	50,67,67	1.08	4 (8%)
13	CYC	U2	202	-	42,46,46	3.27	15 (35%)	50,67,67	3.11	21 (42%)
13	CYC	L3	201	-	42,46,46	3.22	15 (35%)	50,67,67	3.12	20 (40%)
13	CYC	K6	201	-	42,46,46	1.10	1 (2%)	50,67,67	0.98	2 (4%)
13	CYC	M4	202	-	42,46,46	1.09	1 (2%)	50,67,67	0.96	2 (4%)
13	CYC	T6	201	-	42,46,46	1.07	1 (2%)	50,67,67	0.97	2 (4%)
13	CYC	U5	1001	-	42,46,46	3.25	15 (35%)	50,67,67	3.12	21 (42%)
13	CYC	k9	1001	-	42,46,46	3.25	13 (30%)	50,67,67	3.33	21 (42%)
13	CYC	Y5	201	-	42,46,46	3.24	15 (35%)	50,67,67	3.11	21 (42%)
13	CYC	Z6	202	-	42,46,46	3.26	15 (35%)	50,67,67	3.13	21 (42%)
13	CYC	JA	1001	-	42,46,46	3.23	15 (35%)	50,67,67	3.11	21 (42%)
13	CYC	P5	202	-	42,46,46	1.00	1 (2%)	50,67,67	0.97	2 (4%)
13	CYC	F7	1001	-	42,46,46	3.25	15 (35%)	50,67,67	3.13	21 (42%)
13	CYC	G4	201	-	42,46,46	1.06	1 (2%)	50,67,67	0.96	2 (4%)
13	CYC	DA	1001	-	42,46,46	3.23	15 (35%)	50,67,67	3.11	21 (42%)
13	CYC	C2	201	-	42,46,46	3.25	15 (35%)	50,67,67	3.12	21 (42%)
13	CYC	E7	201	-	42,46,46	3.31	15 (35%)	50,67,67	2.97	22 (44%)
13	CYC	M5	1001	-	42,46,46	3.25	15 (35%)	50,67,67	3.11	21 (42%)
13	CYC	B3	1001	-	42,46,46	3.21	15 (35%)	50,67,67	3.13	20 (40%)
13	CYC	H8	1001	-	42,46,46	3.20	12 (28%)	50,67,67	3.08	22 (44%)
13	CYC	I1	201	3	42,46,46	3.46	14 (33%)	50,67,67	3.14	24 (48%)
13	CYC	O8	1001	-	42,46,46	3.20	12 (28%)	50,67,67	3.08	22 (44%)
13	CYC	A5	304	-	42,46,46	3.43	14 (33%)	50,67,67	3.13	24 (48%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CYC	G2	202	3	42,46,46	3.25	15 (35%)	50,67,67	3.12	21 (42%)
13	CYC	Z4	202	-	42,46,46	3.25	15 (35%)	50,67,67	3.11	21 (42%)
13	CYC	Q8	1001	-	42,46,46	3.21	12 (28%)	50,67,67	3.07	22 (44%)
13	CYC	PA	202	-	42,46,46	1.00	1 (2%)	50,67,67	0.98	2 (4%)
13	CYC	H7	1001	-	42,46,46	3.25	14 (33%)	50,67,67	3.09	21 (42%)
13	CYC	VA	202	-	42,46,46	1.06	1 (2%)	50,67,67	0.96	2 (4%)
13	CYC	C4	302	-	42,46,46	1.09	1 (2%)	50,67,67	0.96	2 (4%)
13	CYC	L7	201	-	42,46,46	3.23	15 (35%)	50,67,67	3.12	20 (40%)
13	CYC	q9	1001	-	42,46,46	3.25	13 (30%)	50,67,67	3.33	21 (42%)
13	CYC	M7	201	-	42,46,46	1.10	1 (2%)	50,67,67	0.98	2 (4%)
13	CYC	MA	1003	-	42,46,46	1.06	1 (2%)	50,67,67	0.97	2 (4%)
13	CYC	F1	1001	-	42,46,46	3.23	15 (35%)	50,67,67	3.10	20 (40%)
13	CYC	Q2	201	-	42,46,46	3.25	15 (35%)	50,67,67	3.12	21 (42%)
13	CYC	M3	201	-	42,46,46	1.09	1 (2%)	50,67,67	0.98	2 (4%)
13	CYC	L2	201	-	42,46,46	3.24	15 (35%)	50,67,67	3.12	21 (42%)
13	CYC	I6	202	-	42,46,46	1.02	1 (2%)	50,67,67	0.97	2 (4%)
13	CYC	R9	1001	-	42,46,46	3.24	13 (30%)	50,67,67	3.33	21 (42%)
13	CYC	D5	1001	-	42,46,46	3.24	15 (35%)	50,67,67	3.11	21 (42%)
13	CYC	T5	202	-	42,46,46	1.07	1 (2%)	50,67,67	0.97	2 (4%)
13	CYC	Y1	201	-	42,46,46	3.23	15 (35%)	50,67,67	3.10	21 (42%)
13	CYC	G5	201	-	42,46,46	1.05	1 (2%)	50,67,67	0.97	2 (4%)
13	CYC	N6	301	-	42,46,46	1.04	1 (2%)	50,67,67	1.08	4 (8%)
13	CYC	U2	201	-	42,46,46	1.05	1 (2%)	50,67,67	0.98	2 (4%)
13	CYC	I6	201	-	42,46,46	3.46	14 (33%)	50,67,67	3.14	24 (48%)
13	CYC	PA	203	-	42,46,46	3.25	15 (35%)	50,67,67	3.12	21 (42%)
13	CYC	L4	201	-	42,46,46	3.24	15 (35%)	50,67,67	3.12	21 (42%)
13	CYC	G4	202	-	42,46,46	3.24	15 (35%)	50,67,67	3.12	21 (42%)
13	CYC	09	1201	10	42,46,46	3.44	14 (33%)	50,67,67	2.95	21 (42%)
13	CYC	C4	301	3	42,46,46	3.25	15 (35%)	50,67,67	3.12	21 (42%)
13	CYC	M4	201	3	42,46,46	1.04	1 (2%)	50,67,67	1.09	4 (8%)
13	CYC	E1	202	-	42,46,46	1.06	1 (2%)	50,67,67	1.00	2 (4%)
13	CYC	X1	201	-	42,46,46	3.44	14 (33%)	50,67,67	3.17	24 (48%)
13	CYC	X4	202	-	42,46,46	1.07	1 (2%)	50,67,67	0.96	2 (4%)
13	CYC	AA	301	-	42,46,46	3.32	15 (35%)	50,67,67	2.99	22 (44%)
13	CYC	O9	1001	-	42,46,46	3.22	12 (28%)	50,67,67	4.05	24 (48%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CYC	N6	302	-	42,46,46	3.28	15 (35%)	50,67,67	3.13	21 (42%)
13	CYC	b8	1001	-	42,46,46	3.45	14 (33%)	50,67,67	2.95	21 (42%)
13	CYC	Q1	202	-	42,46,46	1.06	1 (2%)	50,67,67	0.98	2 (4%)
13	CYC	W8	1001	-	42,46,46	3.45	14 (33%)	50,67,67	2.95	21 (42%)
13	CYC	E9	1001	-	42,46,46	3.25	13 (30%)	50,67,67	3.33	21 (42%)
13	CYC	AA	302	-	42,46,46	3.34	15 (35%)	50,67,67	2.97	22 (44%)
13	CYC	E4	201	3	42,46,46	3.32	15 (35%)	50,67,67	2.97	22 (44%)
13	CYC	M8	1001	-	42,46,46	3.45	14 (33%)	50,67,67	2.95	21 (42%)
13	CYC	O6	1001	-	42,46,46	3.23	15 (35%)	50,67,67	3.11	21 (42%)
13	CYC	l8	1001	-	42,46,46	3.20	12 (28%)	50,67,67	3.07	22 (44%)
13	CYC	P9	1001	-	42,46,46	3.24	13 (30%)	50,67,67	3.32	21 (42%)
13	CYC	IA	201	-	42,46,46	3.44	14 (33%)	50,67,67	3.15	24 (48%)
13	CYC	J1	1001	-	42,46,46	3.24	15 (35%)	50,67,67	3.11	21 (42%)
13	CYC	Q9	201	11	42,46,46	3.22	14 (33%)	50,67,67	2.91	20 (40%)
13	CYC	K1	201	-	42,46,46	1.05	1 (2%)	50,67,67	0.97	2 (4%)
13	CYC	Q1	201	-	42,46,46	3.24	15 (35%)	50,67,67	3.11	21 (42%)
13	CYC	G1	202	-	42,46,46	3.25	15 (35%)	50,67,67	3.12	21 (42%)
13	CYC	Q4	202	-	42,46,46	1.06	1 (2%)	50,67,67	0.97	2 (4%)
13	CYC	V4	201	-	42,46,46	1.04	1 (2%)	50,67,67	0.97	2 (4%)
13	CYC	EA	201	-	42,46,46	1.07	1 (2%)	50,67,67	1.00	2 (4%)
13	CYC	Z4	201	-	42,46,46	1.08	1 (2%)	50,67,67	0.98	2 (4%)
13	CYC	e9	1001	-	42,46,46	3.20	12 (28%)	50,67,67	4.04	24 (48%)
13	CYC	B9	1001	-	42,46,46	3.21	12 (28%)	50,67,67	4.05	24 (48%)
13	CYC	O4	1001	-	42,46,46	3.23	15 (35%)	50,67,67	3.12	21 (42%)
13	CYC	C2	202	-	42,46,46	1.08	1 (2%)	50,67,67	0.96	2 (4%)
13	CYC	t8	1001	-	42,46,46	3.20	12 (28%)	50,67,67	3.08	22 (44%)
13	CYC	19	1203	-	42,46,46	3.21	12 (28%)	50,67,67	4.05	24 (48%)
13	CYC	L6	201	-	42,46,46	3.23	15 (35%)	50,67,67	3.12	21 (42%)
13	CYC	I5	201	-	42,46,46	3.43	14 (33%)	50,67,67	3.15	24 (48%)
13	CYC	09	1203	-	42,46,46	3.21	12 (28%)	50,67,67	4.06	24 (48%)
13	CYC	IA	202	-	42,46,46	1.03	1 (2%)	50,67,67	0.97	2 (4%)
13	CYC	I8	1001	-	42,46,46	3.45	14 (33%)	50,67,67	2.95	21 (42%)
13	CYC	RA	201	-	42,46,46	1.06	1 (2%)	50,67,67	0.97	2 (4%)
13	CYC	Z1	201	-	42,46,46	1.08	1 (2%)	50,67,67	0.98	2 (4%)
13	CYC	V8	1001	-	42,46,46	3.21	12 (28%)	50,67,67	3.08	22 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CYC	B6	1001	-	42,46,46	3.22	15 (35%)	50,67,67	3.12	21 (42%)
13	CYC	F2	1001	-	42,46,46	3.25	15 (35%)	50,67,67	3.12	20 (40%)
13	CYC	m9	201	-	42,46,46	3.21	14 (33%)	50,67,67	2.99	19 (38%)
13	CYC	K8	1001	-	42,46,46	3.44	14 (33%)	50,67,67	2.95	21 (42%)
13	CYC	I3	202	-	42,46,46	1.04	1 (2%)	50,67,67	0.97	2 (4%)
13	CYC	c8	1001	-	42,46,46	3.19	12 (28%)	50,67,67	3.08	22 (44%)
13	CYC	GA	1001	-	42,46,46	3.24	15 (35%)	50,67,67	3.12	21 (42%)
13	CYC	P2	201	-	42,46,46	1.06	1 (2%)	50,67,67	1.06	3 (6%)
13	CYC	S1	1001	-	42,46,46	3.25	15 (35%)	50,67,67	3.10	21 (42%)
13	CYC	W6	201	-	42,46,46	0.99	1 (2%)	50,67,67	0.98	2 (4%)
13	CYC	i9	1001	-	42,46,46	3.24	13 (30%)	50,67,67	3.32	21 (42%)
13	CYC	X1	202	-	42,46,46	1.07	1 (2%)	50,67,67	0.96	2 (4%)
13	CYC	O2	1001	-	42,46,46	3.23	15 (35%)	50,67,67	3.11	21 (42%)
13	CYC	X9	1001	-	42,46,46	3.24	13 (30%)	50,67,67	3.32	21 (42%)
13	CYC	ZA	201	-	42,46,46	3.40	15 (35%)	50,67,67	3.14	24 (48%)
13	CYC	F3	1001	-	42,46,46	3.25	15 (35%)	50,67,67	3.13	21 (42%)
13	CYC	I9	1001	-	42,46,46	3.25	13 (30%)	50,67,67	3.32	21 (42%)
13	CYC	XA	201	-	42,46,46	3.42	14 (33%)	50,67,67	3.16	24 (48%)
13	CYC	B4	1001	-	42,46,46	3.24	15 (35%)	50,67,67	3.12	21 (42%)
13	CYC	U9	1001	-	42,46,46	3.20	12 (28%)	50,67,67	4.04	24 (48%)
13	CYC	K2	201	-	42,46,46	1.08	1 (2%)	50,67,67	0.98	2 (4%)
13	CYC	Z1	202	-	42,46,46	3.25	15 (35%)	50,67,67	3.10	21 (42%)
13	CYC	d9	1001	-	42,46,46	3.24	13 (30%)	50,67,67	3.32	21 (42%)
13	CYC	F6	1001	-	42,46,46	3.26	15 (35%)	50,67,67	3.11	21 (42%)
13	CYC	F9	1001	-	42,46,46	3.23	12 (28%)	50,67,67	4.05	24 (48%)
13	CYC	X2	201	-	42,46,46	3.44	14 (33%)	50,67,67	3.16	24 (48%)
13	CYC	M2	201	-	42,46,46	1.10	1 (2%)	50,67,67	0.97	2 (4%)
13	CYC	MA	1002	-	42,46,46	1.03	1 (2%)	50,67,67	1.08	4 (8%)
13	CYC	K2	202	-	42,46,46	1.07	1 (2%)	50,67,67	0.97	2 (4%)
13	CYC	H4	1001	-	42,46,46	3.25	14 (33%)	50,67,67	3.10	21 (42%)
13	CYC	R8	1001	-	42,46,46	3.44	14 (33%)	50,67,67	2.95	21 (42%)
13	CYC	R6	1001	-	42,46,46	3.25	15 (35%)	50,67,67	3.12	21 (42%)
13	CYC	C8	1001	-	42,46,46	3.20	12 (28%)	50,67,67	3.08	22 (44%)
13	CYC	K6	202	-	42,46,46	1.08	1 (2%)	50,67,67	0.97	2 (4%)
13	CYC	G9	1001	-	42,46,46	3.25	13 (30%)	50,67,67	3.33	21 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CYC	y9	1001	-	42,46,46	3.24	13 (30%)	50,67,67	3.33	21 (42%)
13	CYC	E5	201	-	42,46,46	1.07	1 (2%)	50,67,67	1.00	2 (4%)
13	CYC	j8	1001	-	42,46,46	3.20	12 (28%)	50,67,67	3.08	22 (44%)
13	CYC	19	1204	-	42,46,46	3.21	12 (28%)	50,67,67	4.05	24 (48%)
13	CYC	E2	201	-	42,46,46	3.31	15 (35%)	50,67,67	2.96	22 (44%)
13	CYC	PA	201	-	42,46,46	1.07	1 (2%)	50,67,67	1.07	3 (6%)
13	CYC	c9	1001	-	42,46,46	3.23	12 (28%)	50,67,67	4.06	25 (50%)
13	CYC	V4	202	-	42,46,46	3.26	15 (35%)	50,67,67	3.12	21 (42%)
13	CYC	D9	1001	-	42,46,46	3.20	12 (28%)	50,67,67	4.04	24 (48%)
13	CYC	J3	1001	-	42,46,46	3.24	15 (35%)	50,67,67	3.11	21 (42%)
13	CYC	J9	1001	-	42,46,46	3.21	13 (30%)	50,67,67	4.05	24 (48%)
13	CYC	M5	1002	-	42,46,46	1.04	1 (2%)	50,67,67	1.08	4 (8%)
13	CYC	b9	1001	-	42,46,46	3.26	13 (30%)	50,67,67	3.32	21 (42%)
13	CYC	NA	301	-	42,46,46	3.44	15 (35%)	50,67,67	3.16	24 (48%)
13	CYC	O5	1001	-	42,46,46	3.25	15 (35%)	50,67,67	3.12	21 (42%)
13	CYC	C7	201	-	42,46,46	1.09	1 (2%)	50,67,67	0.96	2 (4%)
13	CYC	E8	1001	-	42,46,46	3.20	12 (28%)	50,67,67	3.08	22 (44%)
13	CYC	J6	1001	-	42,46,46	3.24	15 (35%)	50,67,67	3.11	21 (42%)
13	CYC	q8	1001	-	42,46,46	3.45	14 (33%)	50,67,67	2.95	21 (42%)
13	CYC	ZA	202	-	42,46,46	1.08	1 (2%)	50,67,67	0.98	2 (4%)
13	CYC	E3	201	-	42,46,46	3.30	15 (35%)	50,67,67	2.97	22 (44%)
13	CYC	T2	201	-	42,46,46	1.08	1 (2%)	50,67,67	0.96	2 (4%)
13	CYC	Q6	201	-	42,46,46	3.26	15 (35%)	50,67,67	3.13	21 (42%)
13	CYC	B7	1001	-	42,46,46	3.22	14 (33%)	50,67,67	3.13	20 (40%)
13	CYC	X5	201	-	42,46,46	3.43	14 (33%)	50,67,67	3.16	24 (48%)
13	CYC	K3	201	-	42,46,46	1.09	1 (2%)	50,67,67	0.97	2 (4%)
13	CYC	Z8	1001	-	42,46,46	3.20	12 (28%)	50,67,67	3.08	22 (44%)
13	CYC	I1	202	-	42,46,46	1.01	1 (2%)	50,67,67	0.97	2 (4%)
13	CYC	T1	201	-	42,46,46	1.08	1 (2%)	50,67,67	0.96	2 (4%)
13	CYC	LA	201	-	42,46,46	3.23	15 (35%)	50,67,67	3.12	21 (42%)
13	CYC	M1	202	-	42,46,46	1.07	1 (2%)	50,67,67	0.97	2 (4%)
13	CYC	N7	301	-	42,46,46	1.04	1 (2%)	50,67,67	1.08	3 (6%)
13	CYC	19	1201	-	42,46,46	3.44	14 (33%)	50,67,67	2.95	21 (42%)
13	CYC	D6	1001	-	42,46,46	3.22	15 (35%)	50,67,67	3.12	21 (42%)
13	CYC	I2	202	-	42,46,46	1.03	1 (2%)	50,67,67	0.98	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CYC	e8	1001	-	42,46,46	3.21	12 (28%)	50,67,67	3.08	22 (44%)
13	CYC	29	1001	-	42,46,46	3.21	12 (28%)	50,67,67	4.04	24 (48%)
13	CYC	K3	202	-	42,46,46	1.06	1 (2%)	50,67,67	0.97	2 (4%)
13	CYC	j9	1001	-	42,46,46	3.20	12 (28%)	50,67,67	4.05	24 (48%)
13	CYC	o8	1001	-	42,46,46	3.44	14 (33%)	50,67,67	2.95	21 (42%)
13	CYC	P5	203	-	42,46,46	3.25	14 (33%)	50,67,67	3.12	21 (42%)
13	CYC	I2	201	-	42,46,46	3.47	14 (33%)	50,67,67	3.14	24 (48%)
13	CYC	S9	1001	-	42,46,46	3.22	12 (28%)	50,67,67	4.05	24 (48%)
13	CYC	G6	202	3	42,46,46	3.27	15 (35%)	50,67,67	3.13	21 (42%)
13	CYC	A8	1001	-	42,46,46	3.20	12 (28%)	50,67,67	3.08	22 (44%)
13	CYC	W6	202	-	42,46,46	3.25	15 (35%)	50,67,67	3.13	21 (42%)
13	CYC	X5	202	-	42,46,46	1.07	1 (2%)	50,67,67	0.96	2 (4%)
13	CYC	G3	201	3	42,46,46	3.26	15 (35%)	50,67,67	3.13	21 (42%)
13	CYC	U6	201	-	42,46,46	1.05	1 (2%)	50,67,67	0.98	2 (4%)
13	CYC	k8	1001	-	42,46,46	3.46	14 (33%)	50,67,67	2.95	21 (42%)
13	CYC	Y6	201	-	42,46,46	3.23	15 (35%)	50,67,67	3.12	21 (42%)
13	CYC	K9	1001	-	42,46,46	3.25	13 (30%)	50,67,67	3.32	21 (42%)
13	CYC	I4	202	-	42,46,46	1.00	1 (2%)	50,67,67	0.96	2 (4%)
13	CYC	V5	201	-	42,46,46	3.42	14 (33%)	50,67,67	3.13	24 (48%)
13	CYC	Z6	201	-	42,46,46	1.07	1 (2%)	50,67,67	0.99	2 (4%)
13	CYC	Z9	1001	-	42,46,46	3.25	13 (30%)	50,67,67	3.32	21 (42%)
13	CYC	H1	1001	-	42,46,46	3.24	16 (38%)	50,67,67	3.11	21 (42%)
13	CYC	F4	1001	-	42,46,46	3.24	15 (35%)	50,67,67	3.10	21 (42%)
13	CYC	s9	1001	-	42,46,46	3.24	13 (30%)	50,67,67	3.33	21 (42%)
13	CYC	G3	202	-	42,46,46	1.06	1 (2%)	50,67,67	0.97	2 (4%)
13	CYC	L5	201	-	42,46,46	3.24	15 (35%)	50,67,67	3.12	21 (42%)
13	CYC	P6	201	-	42,46,46	1.08	1 (2%)	50,67,67	1.06	3 (6%)
13	CYC	J8	1001	-	42,46,46	3.20	12 (28%)	50,67,67	3.07	22 (44%)
13	CYC	OA	1001	-	42,46,46	3.25	15 (35%)	50,67,67	3.10	21 (42%)
13	CYC	G1	201	-	42,46,46	1.05	1 (2%)	50,67,67	0.96	2 (4%)
13	CYC	Z2	201	-	42,46,46	1.06	1 (2%)	50,67,67	0.98	2 (4%)
13	CYC	T1	202	-	42,46,46	3.27	15 (35%)	50,67,67	3.12	21 (42%)
13	CYC	T5	201	-	42,46,46	3.43	14 (33%)	50,67,67	3.15	24 (48%)
13	CYC	d8	1001	-	42,46,46	3.45	14 (33%)	50,67,67	2.95	21 (42%)
13	CYC	K5	201	-	42,46,46	1.06	1 (2%)	50,67,67	0.96	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CYC	A7	301	-	42,46,46	3.23	14 (33%)	50,67,67	3.10	21 (42%)
13	CYC	v9	1001	-	42,46,46	3.21	12 (28%)	50,67,67	4.05	24 (48%)
13	CYC	G6	201	-	42,46,46	1.06	1 (2%)	50,67,67	0.96	2 (4%)
13	CYC	H3	1001	-	42,46,46	3.25	14 (33%)	50,67,67	3.09	21 (42%)
13	CYC	19	1202	10	42,46,46	3.21	13 (30%)	50,67,67	3.53	23 (46%)
13	CYC	R5	201	-	42,46,46	1.06	1 (2%)	50,67,67	0.97	2 (4%)
13	CYC	YA	201	-	42,46,46	3.25	15 (35%)	50,67,67	3.10	21 (42%)
13	CYC	39	1001	-	42,46,46	3.21	12 (28%)	50,67,67	4.06	24 (48%)
13	CYC	E6	202	3	42,46,46	1.07	1 (2%)	50,67,67	1.00	2 (4%)
13	CYC	N2	301	-	42,46,46	1.04	1 (2%)	50,67,67	1.09	3 (6%)
13	CYC	f9	1001	-	42,46,46	3.25	13 (30%)	50,67,67	3.33	21 (42%)
13	CYC	E6	201	-	42,46,46	3.30	15 (35%)	50,67,67	2.97	22 (44%)
13	CYC	S2	1001	-	42,46,46	3.23	15 (35%)	50,67,67	3.11	21 (42%)
13	CYC	E2	202	3	42,46,46	1.06	1 (2%)	50,67,67	1.00	2 (4%)
13	CYC	U4	1001	-	42,46,46	3.26	15 (35%)	50,67,67	3.11	21 (42%)
13	CYC	J5	1001	-	42,46,46	3.24	15 (35%)	50,67,67	3.12	21 (42%)
13	CYC	W2	201	-	42,46,46	0.98	1 (2%)	50,67,67	0.99	2 (4%)
13	CYC	19	1205	-	42,46,46	3.21	12 (28%)	50,67,67	4.06	24 (48%)
13	CYC	w9	1001	-	42,46,46	3.26	13 (30%)	50,67,67	3.32	21 (42%)
13	CYC	19	1001	-	42,46,46	3.22	12 (28%)	50,67,67	4.05	24 (48%)
13	CYC	I7	201	-	42,46,46	3.47	14 (33%)	50,67,67	3.13	24 (48%)
13	CYC	V6	202	-	42,46,46	3.26	15 (35%)	50,67,67	3.12	21 (42%)
13	CYC	S5	1001	-	42,46,46	3.25	14 (33%)	50,67,67	3.10	21 (42%)
13	CYC	Y2	201	-	42,46,46	3.24	15 (35%)	50,67,67	3.12	21 (42%)
13	CYC	X6	201	-	42,46,46	3.43	14 (33%)	50,67,67	3.16	24 (48%)
13	CYC	J7	1001	-	42,46,46	3.23	15 (35%)	50,67,67	3.11	21 (42%)
13	CYC	D4	1001	-	42,46,46	3.22	15 (35%)	50,67,67	3.11	21 (42%)
13	CYC	N2	302	-	42,46,46	3.27	15 (35%)	50,67,67	3.13	21 (42%)
13	CYC	M5	1003	-	42,46,46	1.08	1 (2%)	50,67,67	0.96	2 (4%)
13	CYC	G7	201	3	42,46,46	3.26	15 (35%)	50,67,67	3.12	21 (42%)
13	CYC	XA	202	-	42,46,46	1.08	1 (2%)	50,67,67	0.96	2 (4%)
13	CYC	P1	201	-	42,46,46	1.06	1 (2%)	50,67,67	1.07	3 (6%)
13	CYC	L8	1001	-	42,46,46	3.21	12 (28%)	50,67,67	3.08	22 (44%)
13	CYC	E5	202	-	42,46,46	3.25	15 (35%)	50,67,67	3.11	21 (42%)
13	CYC	V1	201	-	42,46,46	1.04	1 (2%)	50,67,67	0.97	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CYC	E7	202	3	42,46,46	1.07	1 (2%)	50,67,67	1.00	2 (4%)
13	CYC	I7	202	-	42,46,46	1.04	1 (2%)	50,67,67	0.97	2 (4%)
13	CYC	AA	303	-	42,46,46	3.41	15 (35%)	50,67,67	3.10	23 (46%)
13	CYC	C5	201	-	42,46,46	1.07	1 (2%)	50,67,67	0.95	2 (4%)
13	CYC	W2	202	-	42,46,46	3.25	15 (35%)	50,67,67	3.13	21 (42%)
13	CYC	J2	1001	-	42,46,46	3.24	15 (35%)	50,67,67	3.12	21 (42%)
13	CYC	AA	304	-	42,46,46	3.43	14 (33%)	50,67,67	3.14	24 (48%)
13	CYC	F8	1001	-	42,46,46	3.45	14 (33%)	50,67,67	2.95	21 (42%)
13	CYC	WA	1001	-	42,46,46	3.25	15 (35%)	50,67,67	3.12	21 (42%)
13	CYC	K1	202	-	42,46,46	1.06	1 (2%)	50,67,67	0.97	2 (4%)
13	CYC	A5	301	-	42,46,46	3.31	15 (35%)	50,67,67	2.98	22 (44%)
13	CYC	G7	202	-	42,46,46	1.06	1 (2%)	50,67,67	0.97	2 (4%)
13	CYC	B2	1001	-	42,46,46	3.21	14 (33%)	50,67,67	3.12	21 (42%)
13	CYC	J4	1001	-	42,46,46	3.24	15 (35%)	50,67,67	3.11	21 (42%)
13	CYC	VA	201	-	42,46,46	3.42	14 (33%)	50,67,67	3.13	24 (48%)
13	CYC	s8	1001	-	42,46,46	3.46	14 (33%)	50,67,67	2.96	21 (42%)
13	CYC	N9	1001	-	42,46,46	3.25	13 (30%)	50,67,67	3.32	21 (42%)
13	CYC	o9	1001	-	42,46,46	3.25	13 (30%)	50,67,67	3.33	21 (42%)
13	CYC	W2	203	-	42,46,46	1.09	1 (2%)	50,67,67	0.97	2 (4%)
13	CYC	p8	1001	-	42,46,46	3.19	12 (28%)	50,67,67	3.07	22 (44%)
13	CYC	g9	1001	11	42,46,46	3.22	14 (33%)	50,67,67	2.99	22 (44%)
13	CYC	D3	1001	-	42,46,46	3.23	15 (35%)	50,67,67	3.12	21 (42%)
13	CYC	CA	201	-	42,46,46	1.08	1 (2%)	50,67,67	0.95	2 (4%)
13	CYC	A5	302	-	42,46,46	3.33	15 (35%)	50,67,67	2.96	22 (44%)
13	CYC	H9	1001	-	42,46,46	3.22	13 (30%)	50,67,67	4.05	24 (48%)
13	CYC	H6	1001	-	42,46,46	3.24	14 (33%)	50,67,67	3.09	21 (42%)
13	CYC	S4	1001	-	42,46,46	3.25	15 (35%)	50,67,67	3.11	21 (42%)
13	CYC	L9	1001	-	42,46,46	3.22	12 (28%)	50,67,67	4.05	24 (48%)
13	CYC	P4	201	-	42,46,46	1.06	1 (2%)	50,67,67	1.07	3 (6%)
13	CYC	K4	202	-	42,46,46	1.07	1 (2%)	50,67,67	0.97	2 (4%)
13	CYC	C6	201	-	42,46,46	3.25	15 (35%)	50,67,67	3.12	21 (42%)
13	CYC	E4	202	-	42,46,46	1.05	1 (2%)	50,67,67	1.00	2 (4%)
13	CYC	r9	1001	-	42,46,46	3.21	12 (28%)	50,67,67	4.05	24 (48%)
13	CYC	h8	1001	-	42,46,46	3.45	14 (33%)	50,67,67	2.96	21 (42%)
13	CYC	V1	202	-	42,46,46	3.26	15 (35%)	50,67,67	3.11	21 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CYC	09	1202	-	42,46,46	3.12	13 (30%)	50,67,67	3.16	21 (42%)
13	CYC	G2	201	-	42,46,46	1.06	1 (2%)	50,67,67	0.96	2 (4%)
13	CYC	C3	201	-	42,46,46	1.08	1 (2%)	50,67,67	0.96	2 (4%)
13	CYC	E1	201	3	42,46,46	3.31	15 (35%)	50,67,67	2.98	22 (44%)
13	CYC	N5	301	-	42,46,46	3.44	15 (35%)	50,67,67	3.15	24 (48%)
13	CYC	t9	1001	-	42,46,46	3.20	12 (28%)	50,67,67	4.04	24 (48%)
13	CYC	L1	201	-	42,46,46	3.23	15 (35%)	50,67,67	3.12	21 (42%)
13	CYC	p9	1001	-	42,46,46	3.21	12 (28%)	50,67,67	4.05	24 (48%)
13	CYC	A3	301	-	42,46,46	3.22	14 (33%)	50,67,67	3.11	21 (42%)
13	CYC	P4	202	-	42,46,46	1.00	1 (2%)	50,67,67	0.98	2 (4%)
13	CYC	D8	1001	-	42,46,46	3.45	14 (33%)	50,67,67	2.95	21 (42%)
13	CYC	B1	1001	-	42,46,46	3.23	15 (35%)	50,67,67	3.12	21 (42%)
13	CYC	C9	1001	-	42,46,46	3.25	13 (30%)	50,67,67	3.33	21 (42%)
13	CYC	M1	201	3	42,46,46	1.03	1 (2%)	50,67,67	1.09	5 (10%)
13	CYC	A9	1001	-	42,46,46	3.25	13 (30%)	50,67,67	3.32	21 (42%)
13	CYC	f8	1001	-	42,46,46	3.45	14 (33%)	50,67,67	2.95	21 (42%)
13	CYC	A5	303	-	42,46,46	3.41	15 (35%)	50,67,67	3.11	24 (48%)
13	CYC	T8	1001	-	42,46,46	3.45	14 (33%)	50,67,67	2.95	21 (42%)
13	CYC	D1	1001	-	42,46,46	3.22	15 (35%)	50,67,67	3.12	21 (42%)

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
13	CYC	UA	1001	-	-	10/25/74/74	0/4/4/4
13	CYC	R4	1001	3	-	10/25/74/74	0/4/4/4
13	CYC	T4	201	-	-	12/25/74/74	0/4/4/4
13	CYC	P8	1001	-	-	9/25/74/74	0/4/4/4
13	CYC	R1	1001	3	-	10/25/74/74	0/4/4/4
13	CYC	P1	202	-	-	12/25/74/74	0/4/4/4
13	CYC	u9	1001	-	-	9/25/74/74	0/4/4/4
13	CYC	X6	202	-	-	12/25/74/74	0/4/4/4
13	CYC	U6	202	-	-	10/25/74/74	0/4/4/4
13	CYC	W5	1001	-	-	10/25/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CYC	E3	202	3	-	12/25/74/74	0/4/4/4
13	CYC	C1	302	-	-	12/25/74/74	0/4/4/4
13	CYC	EA	202	-	-	10/25/74/74	0/4/4/4
13	CYC	K7	202	-	-	12/25/74/74	0/4/4/4
13	CYC	I5	202	-	-	12/25/74/74	0/4/4/4
13	CYC	V2	202	-	-	10/25/74/74	0/4/4/4
13	CYC	W4	1001	-	-	10/25/74/74	0/4/4/4
13	CYC	I4	201	3	-	9/25/74/74	0/4/4/4
13	CYC	T4	202	-	-	10/25/74/74	0/4/4/4
13	CYC	R2	1001	-	-	10/25/74/74	0/4/4/4
13	CYC	n8	1001	-	-	9/25/74/74	0/4/4/4
13	CYC	W1	1001	-	-	10/25/74/74	0/4/4/4
13	CYC	H2	1001	-	-	10/25/74/74	0/4/4/4
13	CYC	B8	1001	-	-	9/25/74/74	0/4/4/4
13	CYC	B5	1001	-	-	10/25/74/74	0/4/4/4
13	CYC	C1	301	3	-	10/25/74/74	0/4/4/4
13	CYC	K4	201	-	-	12/25/74/74	0/4/4/4
13	CYC	K7	201	-	-	12/25/74/74	0/4/4/4
13	CYC	X4	201	-	-	9/25/74/74	0/4/4/4
13	CYC	Z5	201	-	-	9/25/74/74	0/4/4/4
13	CYC	TA	202	-	-	12/25/74/74	0/4/4/4
13	CYC	P5	201	-	-	8/25/74/74	0/4/4/4
13	CYC	KA	201	-	-	12/25/74/74	0/4/4/4
13	CYC	C6	202	-	-	12/25/74/74	0/4/4/4
13	CYC	V6	201	-	-	12/25/74/74	0/4/4/4
13	CYC	Z5	202	-	-	12/25/74/74	0/4/4/4
13	CYC	Z2	202	-	-	10/25/74/74	0/4/4/4
13	CYC	T9	1001	-	-	9/25/74/74	0/4/4/4
13	CYC	SA	1001	-	-	10/25/74/74	0/4/4/4
13	CYC	x9	1001	-	-	7/25/74/74	0/4/4/4
13	CYC	M6	201	-	-	12/25/74/74	0/4/4/4
13	CYC	Y4	201	-	-	10/25/74/74	0/4/4/4
13	CYC	r8	1001	-	-	9/25/74/74	0/4/4/4
13	CYC	Q4	201	-	-	10/25/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CYC	I3	201	-	-	9/25/74/74	0/4/4/4
13	CYC	X8	1001	-	-	9/25/74/74	0/4/4/4
13	CYC	O1	1001	-	-	10/25/74/74	0/4/4/4
13	CYC	Y8	1001	-	-	9/25/74/74	0/4/4/4
13	CYC	U1	1001	-	-	10/25/74/74	0/4/4/4
13	CYC	S6	1001	-	-	10/25/74/74	0/4/4/4
13	CYC	D2	1001	-	-	10/25/74/74	0/4/4/4
13	CYC	TA	201	-	-	9/25/74/74	0/4/4/4
13	CYC	MA	1001	-	-	10/25/74/74	0/4/4/4
13	CYC	V5	202	-	-	12/25/74/74	0/4/4/4
13	CYC	z9	1001	-	-	7/25/74/74	0/4/4/4
13	CYC	V2	201	-	-	12/25/74/74	0/4/4/4
13	CYC	D7	1001	-	-	10/25/74/74	0/4/4/4
13	CYC	V9	201	-	-	8/25/74/74	0/4/4/4
13	CYC	S8	1001	-	-	9/25/74/74	0/4/4/4
13	CYC	GA	1002	-	-	12/25/74/74	0/4/4/4
13	CYC	g8	1001	-	-	9/25/74/74	0/4/4/4
13	CYC	N3	301	-	-	10/25/74/74	0/4/4/4
13	CYC	U2	202	-	-	10/25/74/74	0/4/4/4
13	CYC	L3	201	-	-	10/25/74/74	0/4/4/4
13	CYC	K6	201	-	-	12/25/74/74	0/4/4/4
13	CYC	M4	202	-	-	12/25/74/74	0/4/4/4
13	CYC	T6	201	-	-	12/25/74/74	0/4/4/4
13	CYC	U5	1001	-	-	10/25/74/74	0/4/4/4
13	CYC	k9	1001	-	-	9/25/74/74	0/4/4/4
13	CYC	Y5	201	-	-	10/25/74/74	0/4/4/4
13	CYC	Z6	202	-	-	10/25/74/74	0/4/4/4
13	CYC	JA	1001	-	-	10/25/74/74	0/4/4/4
13	CYC	P5	202	-	-	12/25/74/74	0/4/4/4
13	CYC	F7	1001	-	-	10/25/74/74	0/4/4/4
13	CYC	G4	201	-	-	12/25/74/74	0/4/4/4
13	CYC	DA	1001	-	-	10/25/74/74	0/4/4/4
13	CYC	C2	201	-	-	10/25/74/74	0/4/4/4
13	CYC	E7	201	-	-	8/25/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CYC	M5	1001	-	-	10/25/74/74	0/4/4/4
13	CYC	B3	1001	-	-	10/25/74/74	0/4/4/4
13	CYC	H8	1001	-	-	9/25/74/74	0/4/4/4
13	CYC	I1	201	3	-	9/25/74/74	0/4/4/4
13	CYC	O8	1001	-	-	9/25/74/74	0/4/4/4
13	CYC	A5	304	-	-	9/25/74/74	0/4/4/4
13	CYC	G2	202	3	-	10/25/74/74	0/4/4/4
13	CYC	Z4	202	-	-	10/25/74/74	0/4/4/4
13	CYC	Q8	1001	-	-	9/25/74/74	0/4/4/4
13	CYC	PA	202	-	-	12/25/74/74	0/4/4/4
13	CYC	H7	1001	-	-	10/25/74/74	0/4/4/4
13	CYC	VA	202	-	-	12/25/74/74	0/4/4/4
13	CYC	C4	302	-	-	12/25/74/74	0/4/4/4
13	CYC	L7	201	-	-	10/25/74/74	0/4/4/4
13	CYC	q9	1001	-	-	9/25/74/74	0/4/4/4
13	CYC	M7	201	-	-	12/25/74/74	0/4/4/4
13	CYC	MA	1003	-	-	12/25/74/74	0/4/4/4
13	CYC	F1	1001	-	-	10/25/74/74	0/4/4/4
13	CYC	Q2	201	-	-	10/25/74/74	0/4/4/4
13	CYC	M3	201	-	-	12/25/74/74	0/4/4/4
13	CYC	L2	201	-	-	10/25/74/74	0/4/4/4
13	CYC	I6	202	-	-	12/25/74/74	0/4/4/4
13	CYC	R9	1001	-	-	9/25/74/74	0/4/4/4
13	CYC	D5	1001	-	-	10/25/74/74	0/4/4/4
13	CYC	T5	202	-	-	12/25/74/74	0/4/4/4
13	CYC	Y1	201	-	-	10/25/74/74	0/4/4/4
13	CYC	G5	201	-	-	12/25/74/74	0/4/4/4
13	CYC	N6	301	-	-	10/25/74/74	0/4/4/4
13	CYC	U2	201	-	-	12/25/74/74	0/4/4/4
13	CYC	I6	201	-	-	9/25/74/74	0/4/4/4
13	CYC	PA	203	-	-	10/25/74/74	0/4/4/4
13	CYC	L4	201	-	-	10/25/74/74	0/4/4/4
13	CYC	G4	202	-	-	10/25/74/74	0/4/4/4
13	CYC	09	1201	10	-	9/25/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CYC	C4	301	3	-	10/25/74/74	0/4/4/4
13	CYC	M4	201	3	-	10/25/74/74	0/4/4/4
13	CYC	E1	202	-	-	12/25/74/74	0/4/4/4
13	CYC	X1	201	-	-	9/25/74/74	0/4/4/4
13	CYC	X4	202	-	-	12/25/74/74	0/4/4/4
13	CYC	AA	301	-	-	8/25/74/74	0/4/4/4
13	CYC	O9	1001	-	-	7/25/74/74	0/4/4/4
13	CYC	N6	302	-	-	10/25/74/74	0/4/4/4
13	CYC	b8	1001	-	-	9/25/74/74	0/4/4/4
13	CYC	Q1	202	-	-	12/25/74/74	0/4/4/4
13	CYC	W8	1001	-	-	9/25/74/74	0/4/4/4
13	CYC	E9	1001	-	-	9/25/74/74	0/4/4/4
13	CYC	AA	302	-	-	8/25/74/74	0/4/4/4
13	CYC	E4	201	3	-	8/25/74/74	0/4/4/4
13	CYC	M8	1001	-	-	9/25/74/74	0/4/4/4
13	CYC	O6	1001	-	-	10/25/74/74	0/4/4/4
13	CYC	l8	1001	-	-	9/25/74/74	0/4/4/4
13	CYC	P9	1001	-	-	9/25/74/74	0/4/4/4
13	CYC	IA	201	-	-	9/25/74/74	0/4/4/4
13	CYC	J1	1001	-	-	10/25/74/74	0/4/4/4
13	CYC	Q9	201	11	-	11/25/74/74	0/4/4/4
13	CYC	K1	201	-	-	12/25/74/74	0/4/4/4
13	CYC	Q1	201	-	-	10/25/74/74	0/4/4/4
13	CYC	G1	202	-	-	10/25/74/74	0/4/4/4
13	CYC	Q4	202	-	-	12/25/74/74	0/4/4/4
13	CYC	V4	201	-	-	12/25/74/74	0/4/4/4
13	CYC	EA	201	-	-	12/25/74/74	0/4/4/4
13	CYC	Z4	201	-	-	12/25/74/74	0/4/4/4
13	CYC	e9	1001	-	-	7/25/74/74	0/4/4/4
13	CYC	B9	1001	-	-	7/25/74/74	0/4/4/4
13	CYC	O4	1001	-	-	10/25/74/74	0/4/4/4
13	CYC	C2	202	-	-	12/25/74/74	0/4/4/4
13	CYC	t8	1001	-	-	9/25/74/74	0/4/4/4
13	CYC	19	1203	-	-	7/25/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CYC	L6	201	-	-	10/25/74/74	0/4/4/4
13	CYC	I5	201	-	-	9/25/74/74	0/4/4/4
13	CYC	09	1203	-	-	7/25/74/74	0/4/4/4
13	CYC	IA	202	-	-	12/25/74/74	0/4/4/4
13	CYC	I8	1001	-	-	9/25/74/74	0/4/4/4
13	CYC	RA	201	-	-	12/25/74/74	0/4/4/4
13	CYC	Z1	201	-	-	12/25/74/74	0/4/4/4
13	CYC	V8	1001	-	-	9/25/74/74	0/4/4/4
13	CYC	B6	1001	-	-	10/25/74/74	0/4/4/4
13	CYC	F2	1001	-	-	10/25/74/74	0/4/4/4
13	CYC	m9	201	-	-	8/25/74/74	0/4/4/4
13	CYC	K8	1001	-	-	9/25/74/74	0/4/4/4
13	CYC	I3	202	-	-	12/25/74/74	0/4/4/4
13	CYC	c8	1001	-	-	9/25/74/74	0/4/4/4
13	CYC	GA	1001	-	-	10/25/74/74	0/4/4/4
13	CYC	P2	201	-	-	8/25/74/74	0/4/4/4
13	CYC	S1	1001	-	-	10/25/74/74	0/4/4/4
13	CYC	W6	201	-	-	12/25/74/74	0/4/4/4
13	CYC	i9	1001	-	-	9/25/74/74	0/4/4/4
13	CYC	X1	202	-	-	12/25/74/74	0/4/4/4
13	CYC	O2	1001	-	-	10/25/74/74	0/4/4/4
13	CYC	X9	1001	-	-	9/25/74/74	0/4/4/4
13	CYC	ZA	201	-	-	9/25/74/74	0/4/4/4
13	CYC	F3	1001	-	-	10/25/74/74	0/4/4/4
13	CYC	I9	1001	-	-	9/25/74/74	0/4/4/4
13	CYC	XA	201	-	-	9/25/74/74	0/4/4/4
13	CYC	B4	1001	-	-	10/25/74/74	0/4/4/4
13	CYC	U9	1001	-	-	7/25/74/74	0/4/4/4
13	CYC	K2	201	-	-	12/25/74/74	0/4/4/4
13	CYC	Z1	202	-	-	10/25/74/74	0/4/4/4
13	CYC	d9	1001	-	-	9/25/74/74	0/4/4/4
13	CYC	F6	1001	-	-	10/25/74/74	0/4/4/4
13	CYC	F9	1001	-	-	7/25/74/74	0/4/4/4
13	CYC	X2	201	-	-	9/25/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CYC	M2	201	-	-	12/25/74/74	0/4/4/4
13	CYC	MA	1002	-	-	10/25/74/74	0/4/4/4
13	CYC	K2	202	-	-	12/25/74/74	0/4/4/4
13	CYC	H4	1001	-	-	10/25/74/74	0/4/4/4
13	CYC	R8	1001	-	-	9/25/74/74	0/4/4/4
13	CYC	R6	1001	-	-	10/25/74/74	0/4/4/4
13	CYC	C8	1001	-	-	9/25/74/74	0/4/4/4
13	CYC	K6	202	-	-	12/25/74/74	0/4/4/4
13	CYC	G9	1001	-	-	9/25/74/74	0/4/4/4
13	CYC	y9	1001	-	-	9/25/74/74	0/4/4/4
13	CYC	E5	201	-	-	12/25/74/74	0/4/4/4
13	CYC	j8	1001	-	-	9/25/74/74	0/4/4/4
13	CYC	19	1204	-	-	7/25/74/74	0/4/4/4
13	CYC	E2	201	-	-	8/25/74/74	0/4/4/4
13	CYC	PA	201	-	-	8/25/74/74	0/4/4/4
13	CYC	c9	1001	-	-	7/25/74/74	0/4/4/4
13	CYC	V4	202	-	-	10/25/74/74	0/4/4/4
13	CYC	D9	1001	-	-	7/25/74/74	0/4/4/4
13	CYC	J3	1001	-	-	10/25/74/74	0/4/4/4
13	CYC	J9	1001	-	-	7/25/74/74	0/4/4/4
13	CYC	M5	1002	-	-	10/25/74/74	0/4/4/4
13	CYC	b9	1001	-	-	9/25/74/74	0/4/4/4
13	CYC	NA	301	-	-	9/25/74/74	0/4/4/4
13	CYC	O5	1001	-	-	10/25/74/74	0/4/4/4
13	CYC	C7	201	-	-	12/25/74/74	0/4/4/4
13	CYC	E8	1001	-	-	9/25/74/74	0/4/4/4
13	CYC	J6	1001	-	-	10/25/74/74	0/4/4/4
13	CYC	q8	1001	-	-	9/25/74/74	0/4/4/4
13	CYC	ZA	202	-	-	12/25/74/74	0/4/4/4
13	CYC	E3	201	-	-	8/25/74/74	0/4/4/4
13	CYC	T2	201	-	-	12/25/74/74	0/4/4/4
13	CYC	Q6	201	-	-	10/25/74/74	0/4/4/4
13	CYC	B7	1001	-	-	10/25/74/74	0/4/4/4
13	CYC	X5	201	-	-	9/25/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CYC	K3	201	-	-	12/25/74/74	0/4/4/4
13	CYC	Z8	1001	-	-	9/25/74/74	0/4/4/4
13	CYC	I1	202	-	-	12/25/74/74	0/4/4/4
13	CYC	T1	201	-	-	12/25/74/74	0/4/4/4
13	CYC	LA	201	-	-	10/25/74/74	0/4/4/4
13	CYC	M1	202	-	-	12/25/74/74	0/4/4/4
13	CYC	N7	301	-	-	10/25/74/74	0/4/4/4
13	CYC	19	1201	-	-	9/25/74/74	0/4/4/4
13	CYC	D6	1001	-	-	10/25/74/74	0/4/4/4
13	CYC	I2	202	-	-	12/25/74/74	0/4/4/4
13	CYC	e8	1001	-	-	9/25/74/74	0/4/4/4
13	CYC	29	1001	-	-	7/25/74/74	0/4/4/4
13	CYC	K3	202	-	-	12/25/74/74	0/4/4/4
13	CYC	j9	1001	-	-	7/25/74/74	0/4/4/4
13	CYC	o8	1001	-	-	9/25/74/74	0/4/4/4
13	CYC	P5	203	-	-	10/25/74/74	0/4/4/4
13	CYC	I2	201	-	-	9/25/74/74	0/4/4/4
13	CYC	S9	1001	-	-	7/25/74/74	0/4/4/4
13	CYC	G6	202	3	-	10/25/74/74	0/4/4/4
13	CYC	A8	1001	-	-	9/25/74/74	0/4/4/4
13	CYC	W6	202	-	-	10/25/74/74	0/4/4/4
13	CYC	X5	202	-	-	12/25/74/74	0/4/4/4
13	CYC	G3	201	3	-	10/25/74/74	0/4/4/4
13	CYC	U6	201	-	-	12/25/74/74	0/4/4/4
13	CYC	k8	1001	-	-	9/25/74/74	0/4/4/4
13	CYC	Y6	201	-	-	10/25/74/74	0/4/4/4
13	CYC	K9	1001	-	-	9/25/74/74	0/4/4/4
13	CYC	I4	202	-	-	12/25/74/74	0/4/4/4
13	CYC	V5	201	-	-	9/25/74/74	0/4/4/4
13	CYC	Z6	201	-	-	12/25/74/74	0/4/4/4
13	CYC	Z9	1001	-	-	9/25/74/74	0/4/4/4
13	CYC	H1	1001	-	-	10/25/74/74	0/4/4/4
13	CYC	F4	1001	-	-	10/25/74/74	0/4/4/4
13	CYC	s9	1001	-	-	9/25/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CYC	G3	202	-	-	12/25/74/74	0/4/4/4
13	CYC	L5	201	-	-	10/25/74/74	0/4/4/4
13	CYC	P6	201	-	-	8/25/74/74	0/4/4/4
13	CYC	J8	1001	-	-	9/25/74/74	0/4/4/4
13	CYC	OA	1001	-	-	10/25/74/74	0/4/4/4
13	CYC	G1	201	-	-	12/25/74/74	0/4/4/4
13	CYC	Z2	201	-	-	12/25/74/74	0/4/4/4
13	CYC	T1	202	-	-	10/25/74/74	0/4/4/4
13	CYC	T5	201	-	-	9/25/74/74	0/4/4/4
13	CYC	d8	1001	-	-	9/25/74/74	0/4/4/4
13	CYC	K5	201	-	-	12/25/74/74	0/4/4/4
13	CYC	A7	301	-	-	10/25/74/74	0/4/4/4
13	CYC	v9	1001	-	-	7/25/74/74	0/4/4/4
13	CYC	G6	201	-	-	12/25/74/74	0/4/4/4
13	CYC	H3	1001	-	-	10/25/74/74	0/4/4/4
13	CYC	19	1202	10	-	8/25/74/74	0/4/4/4
13	CYC	R5	201	-	-	12/25/74/74	0/4/4/4
13	CYC	YA	201	-	-	10/25/74/74	0/4/4/4
13	CYC	39	1001	-	-	7/25/74/74	0/4/4/4
13	CYC	E6	202	3	-	12/25/74/74	0/4/4/4
13	CYC	N2	301	-	-	10/25/74/74	0/4/4/4
13	CYC	f9	1001	-	-	9/25/74/74	0/4/4/4
13	CYC	E6	201	-	-	8/25/74/74	0/4/4/4
13	CYC	S2	1001	-	-	10/25/74/74	0/4/4/4
13	CYC	E2	202	3	-	12/25/74/74	0/4/4/4
13	CYC	U4	1001	-	-	10/25/74/74	0/4/4/4
13	CYC	J5	1001	-	-	10/25/74/74	0/4/4/4
13	CYC	W2	201	-	-	12/25/74/74	0/4/4/4
13	CYC	19	1205	-	-	7/25/74/74	0/4/4/4
13	CYC	w9	1001	-	-	9/25/74/74	0/4/4/4
13	CYC	19	1001	-	-	7/25/74/74	0/4/4/4
13	CYC	I7	201	-	-	9/25/74/74	0/4/4/4
13	CYC	V6	202	-	-	10/25/74/74	0/4/4/4
13	CYC	S5	1001	-	-	10/25/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CYC	Y2	201	-	-	10/25/74/74	0/4/4/4
13	CYC	X6	201	-	-	9/25/74/74	0/4/4/4
13	CYC	J7	1001	-	-	10/25/74/74	0/4/4/4
13	CYC	D4	1001	-	-	10/25/74/74	0/4/4/4
13	CYC	N2	302	-	-	10/25/74/74	0/4/4/4
13	CYC	M5	1003	-	-	12/25/74/74	0/4/4/4
13	CYC	G7	201	3	-	10/25/74/74	0/4/4/4
13	CYC	XA	202	-	-	12/25/74/74	0/4/4/4
13	CYC	P1	201	-	-	8/25/74/74	0/4/4/4
13	CYC	L8	1001	-	-	9/25/74/74	0/4/4/4
13	CYC	E5	202	-	-	10/25/74/74	0/4/4/4
13	CYC	V1	201	-	-	12/25/74/74	0/4/4/4
13	CYC	E7	202	3	-	12/25/74/74	0/4/4/4
13	CYC	I7	202	-	-	12/25/74/74	0/4/4/4
13	CYC	AA	303	-	-	9/25/74/74	0/4/4/4
13	CYC	C5	201	-	-	12/25/74/74	0/4/4/4
13	CYC	W2	202	-	-	10/25/74/74	0/4/4/4
13	CYC	J2	1001	-	-	10/25/74/74	0/4/4/4
13	CYC	AA	304	-	-	9/25/74/74	0/4/4/4
13	CYC	F8	1001	-	-	9/25/74/74	0/4/4/4
13	CYC	WA	1001	-	-	10/25/74/74	0/4/4/4
13	CYC	K1	202	-	-	12/25/74/74	0/4/4/4
13	CYC	A5	301	-	-	8/25/74/74	0/4/4/4
13	CYC	G7	202	-	-	12/25/74/74	0/4/4/4
13	CYC	B2	1001	-	-	10/25/74/74	0/4/4/4
13	CYC	J4	1001	-	-	10/25/74/74	0/4/4/4
13	CYC	VA	201	-	-	9/25/74/74	0/4/4/4
13	CYC	s8	1001	-	-	9/25/74/74	0/4/4/4
13	CYC	N9	1001	-	-	9/25/74/74	0/4/4/4
13	CYC	o9	1001	-	-	9/25/74/74	0/4/4/4
13	CYC	W2	203	-	-	12/25/74/74	0/4/4/4
13	CYC	p8	1001	-	-	9/25/74/74	0/4/4/4
13	CYC	g9	1001	11	-	9/25/74/74	0/4/4/4
13	CYC	D3	1001	-	-	10/25/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CYC	CA	201	-	-	12/25/74/74	0/4/4/4
13	CYC	A5	302	-	-	8/25/74/74	0/4/4/4
13	CYC	H9	1001	-	-	7/25/74/74	0/4/4/4
13	CYC	H6	1001	-	-	10/25/74/74	0/4/4/4
13	CYC	S4	1001	-	-	10/25/74/74	0/4/4/4
13	CYC	L9	1001	-	-	7/25/74/74	0/4/4/4
13	CYC	P4	201	-	-	8/25/74/74	0/4/4/4
13	CYC	K4	202	-	-	12/25/74/74	0/4/4/4
13	CYC	C6	201	-	-	10/25/74/74	0/4/4/4
13	CYC	E4	202	-	-	12/25/74/74	0/4/4/4
13	CYC	r9	1001	-	-	7/25/74/74	0/4/4/4
13	CYC	h8	1001	-	-	9/25/74/74	0/4/4/4
13	CYC	V1	202	-	-	10/25/74/74	0/4/4/4
13	CYC	09	1202	-	-	6/25/74/74	0/4/4/4
13	CYC	G2	201	-	-	12/25/74/74	0/4/4/4
13	CYC	C3	201	-	-	12/25/74/74	0/4/4/4
13	CYC	E1	201	3	-	8/25/74/74	0/4/4/4
13	CYC	N5	301	-	-	9/25/74/74	0/4/4/4
13	CYC	t9	1001	-	-	7/25/74/74	0/4/4/4
13	CYC	L1	201	-	-	10/25/74/74	0/4/4/4
13	CYC	p9	1001	-	-	7/25/74/74	0/4/4/4
13	CYC	A3	301	-	-	10/25/74/74	0/4/4/4
13	CYC	P4	202	-	-	12/25/74/74	0/4/4/4
13	CYC	D8	1001	-	-	9/25/74/74	0/4/4/4
13	CYC	B1	1001	-	-	10/25/74/74	0/4/4/4
13	CYC	C9	1001	-	-	9/25/74/74	0/4/4/4
13	CYC	M1	201	3	-	10/25/74/74	0/4/4/4
13	CYC	A9	1001	-	-	9/25/74/74	0/4/4/4
13	CYC	f8	1001	-	-	9/25/74/74	0/4/4/4
13	CYC	A5	303	-	-	9/25/74/74	0/4/4/4
13	CYC	T8	1001	-	-	9/25/74/74	0/4/4/4
13	CYC	D1	1001	-	-	10/25/74/74	0/4/4/4

The worst 5 of 3522 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	k8	1001	CYC	CHA-C1A	17.08	1.49	1.35
13	s8	1001	CYC	CHA-C1A	17.06	1.49	1.35
13	I8	1001	CYC	CHA-C1A	17.05	1.49	1.35
13	T8	1001	CYC	CHA-C1A	17.05	1.49	1.35
13	f8	1001	CYC	CHA-C1A	17.05	1.49	1.35

The worst 5 of 5529 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	39	1001	CYC	C3B-C4B-NB	16.45	120.07	106.78
13	c9	1001	CYC	C3B-C4B-NB	16.43	120.05	106.78
13	z9	1001	CYC	C3B-C4B-NB	16.42	120.05	106.78
13	09	1203	CYC	C3B-C4B-NB	16.42	120.05	106.78
13	19	1205	CYC	C3B-C4B-NB	16.42	120.05	106.78

There are no chirality outliers.

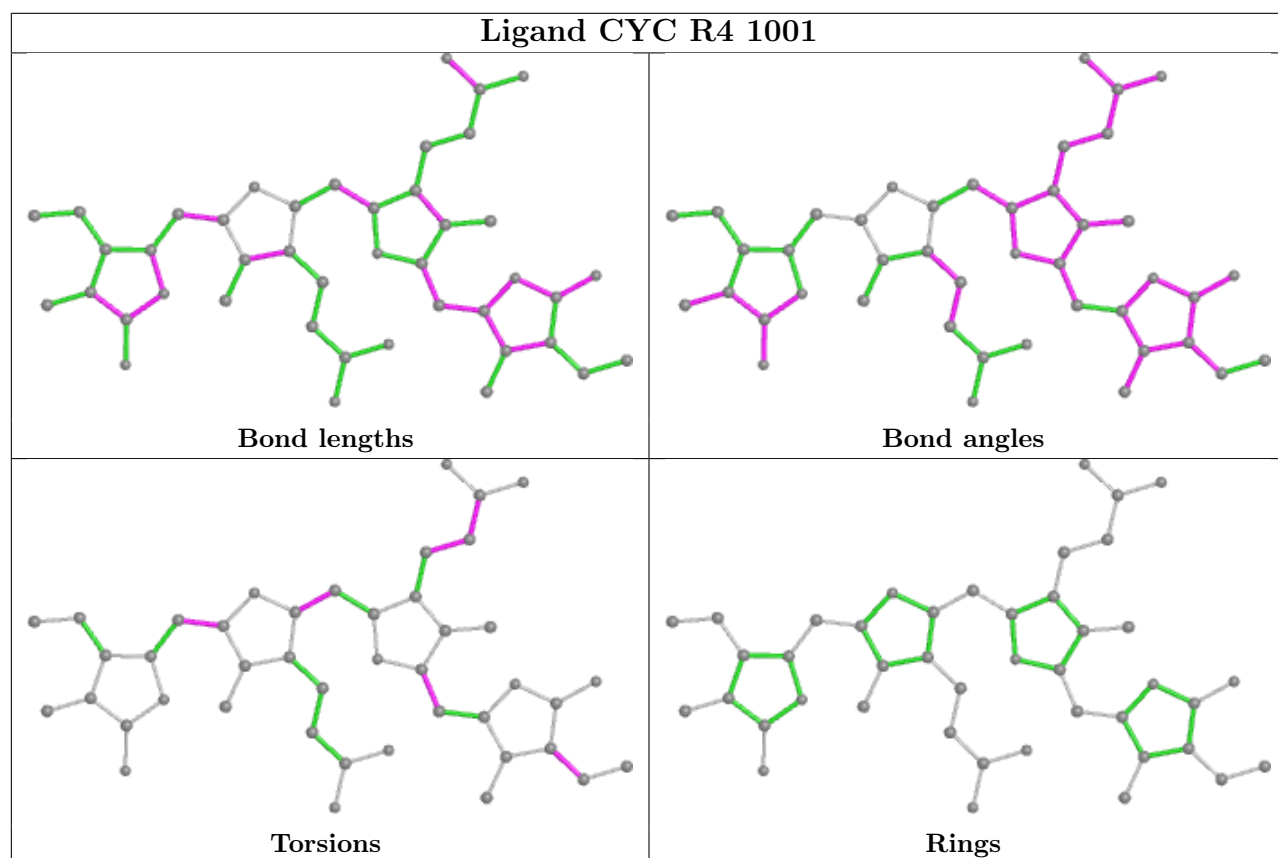
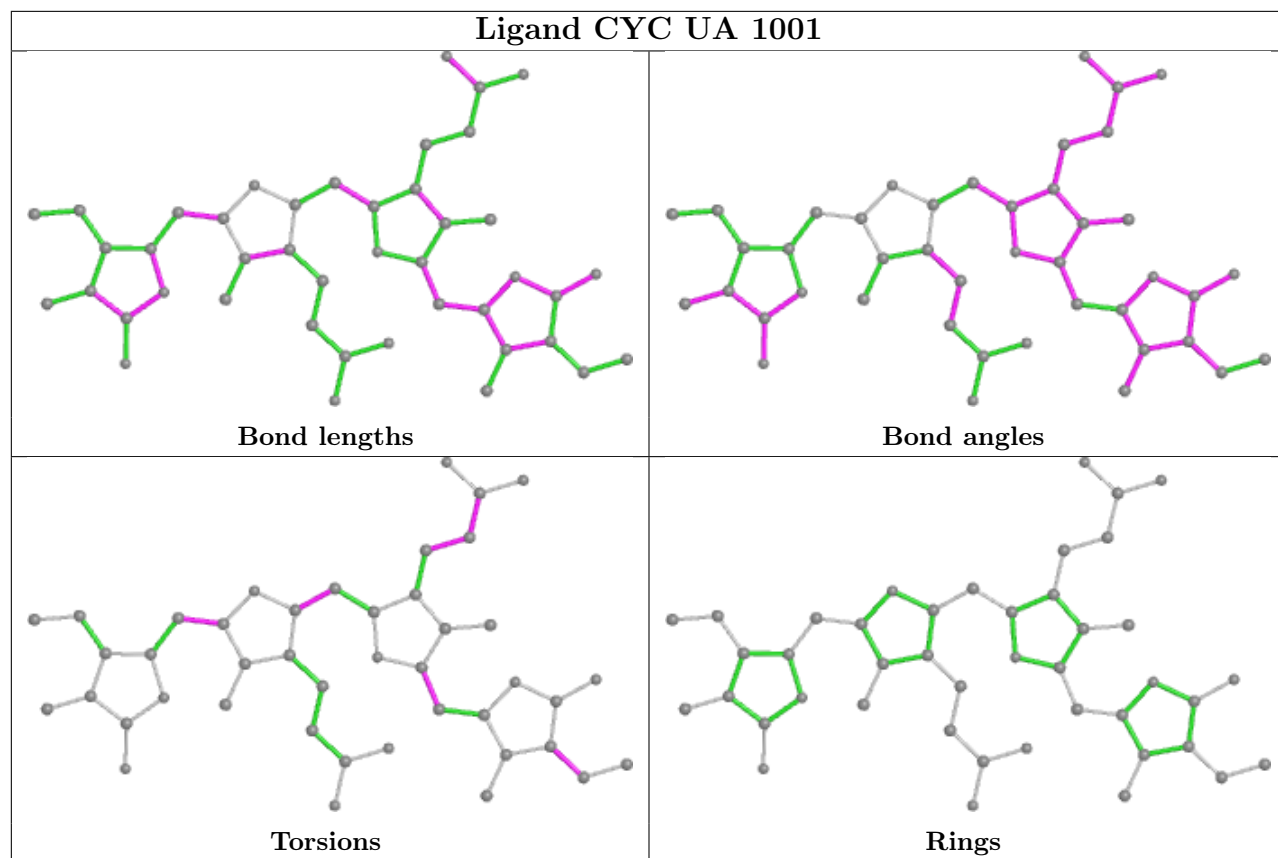
5 of 3452 torsion outliers are listed below:

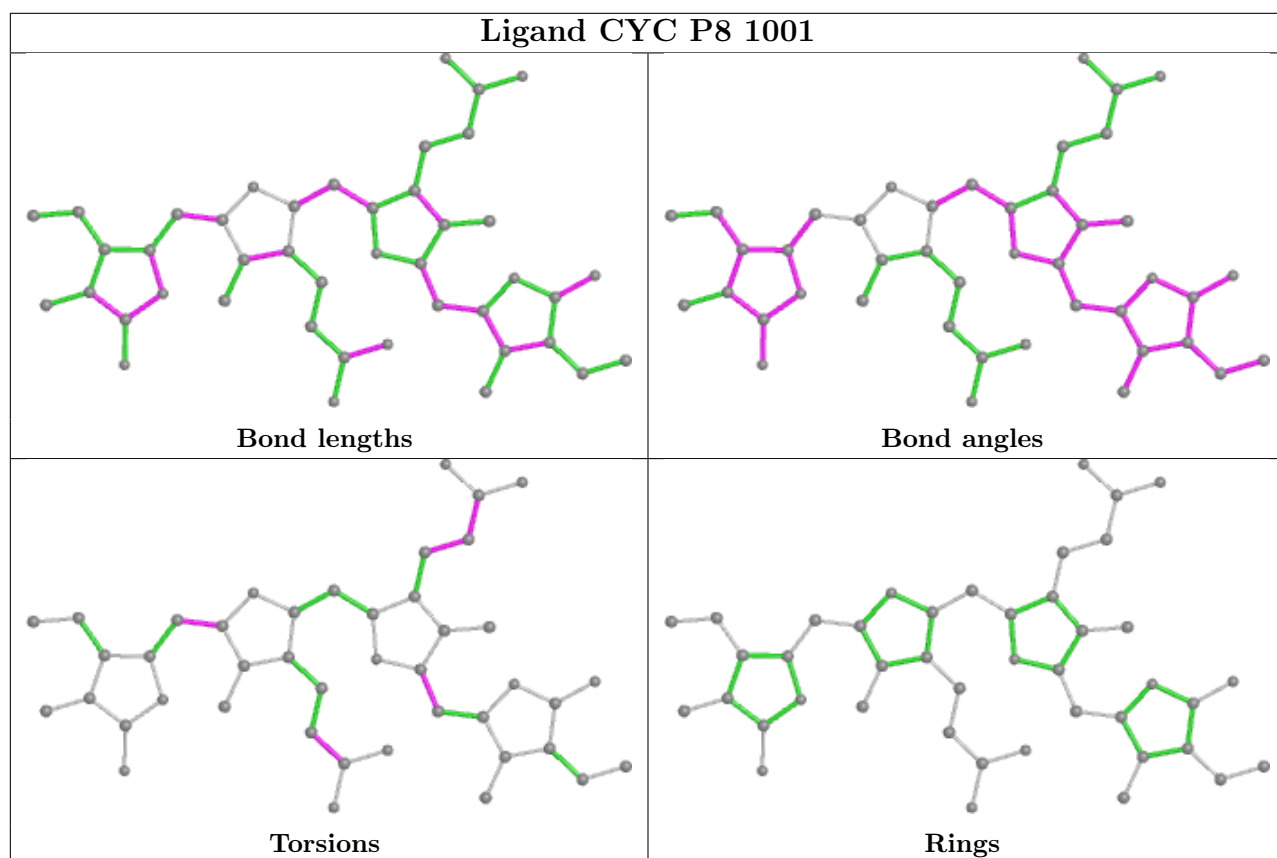
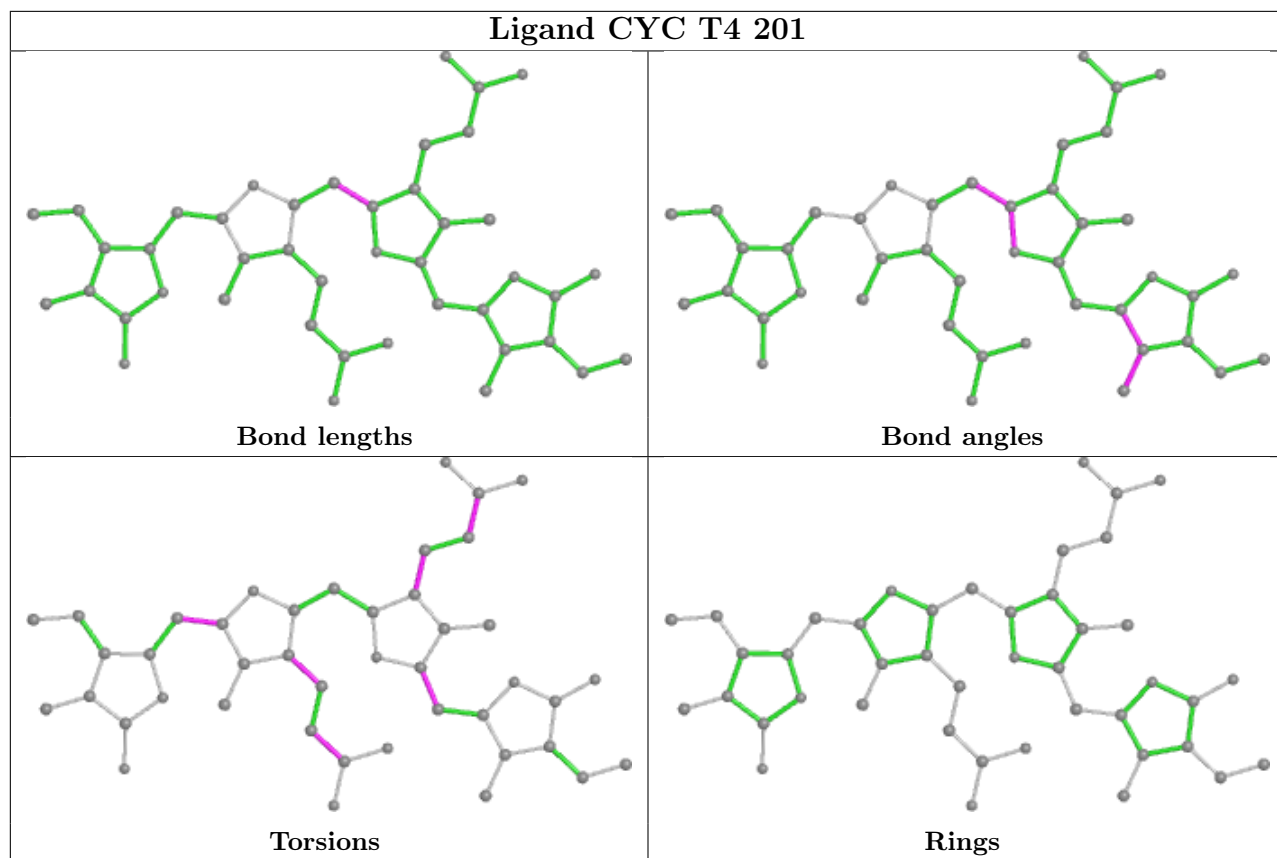
Mol	Chain	Res	Type	Atoms
13	B1	1001	CYC	ND-C4D-CHA-C1A
13	B1	1001	CYC	C3D-C4D-CHA-C1A
13	B1	1001	CYC	NA-C4A-CHB-C1B
13	B1	1001	CYC	ND-C1D-CHD-C4C
13	B1	1001	CYC	C2D-C1D-CHD-C4C

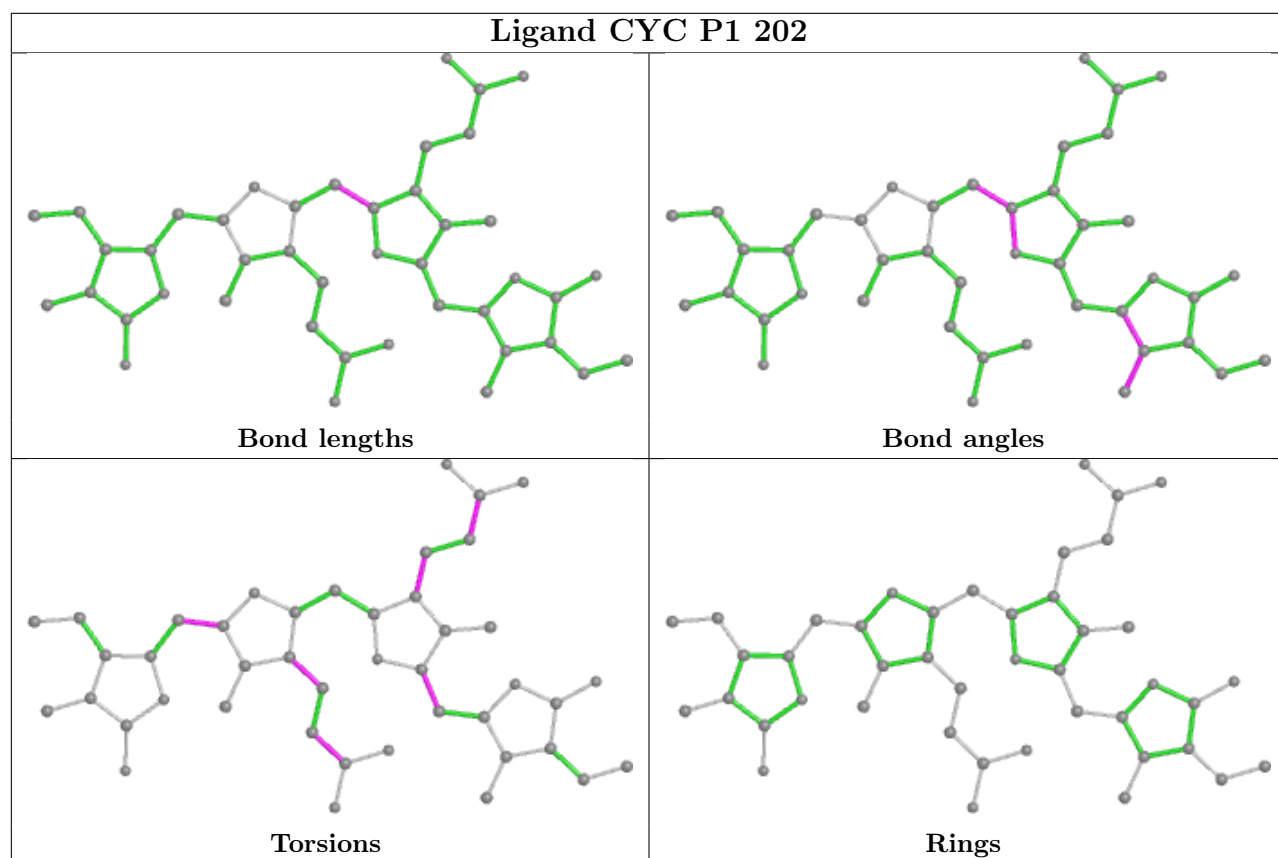
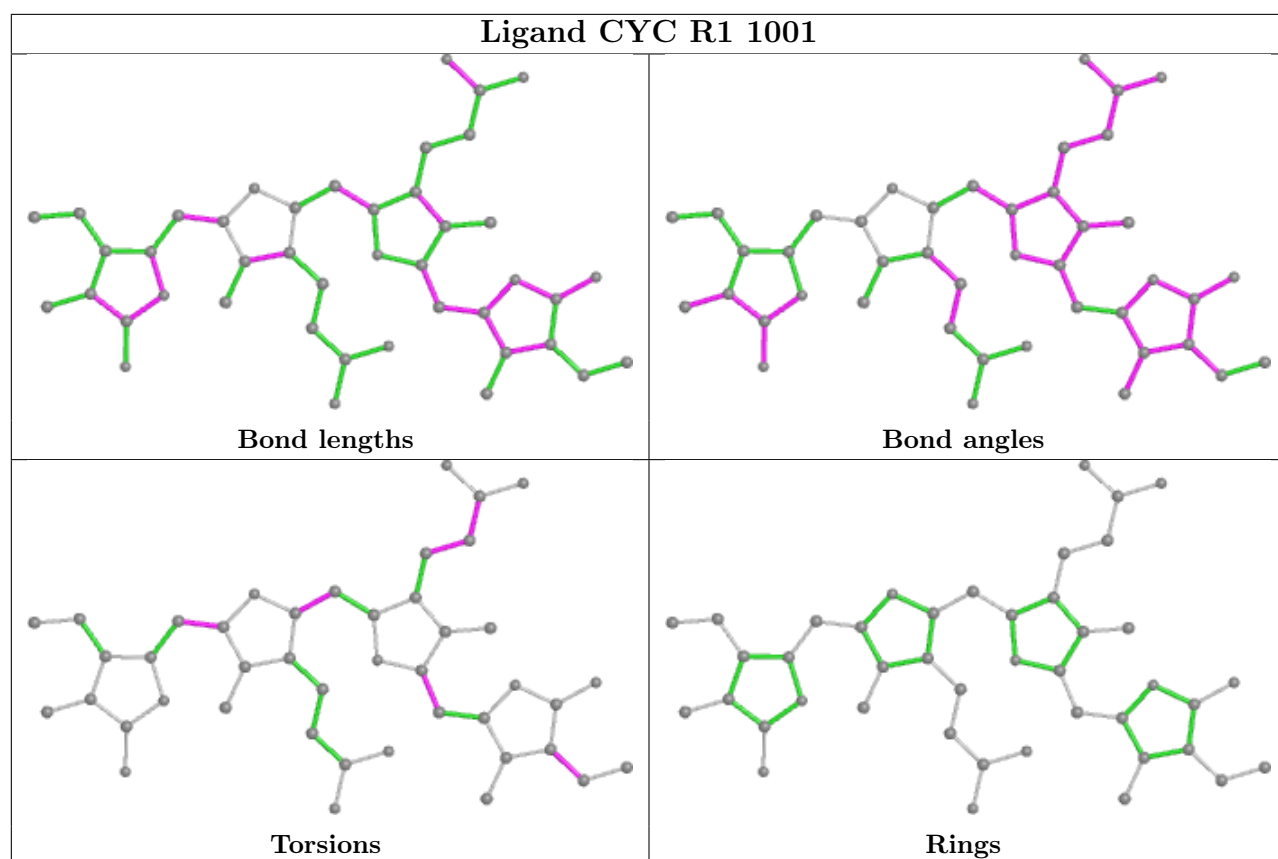
There are no ring outliers.

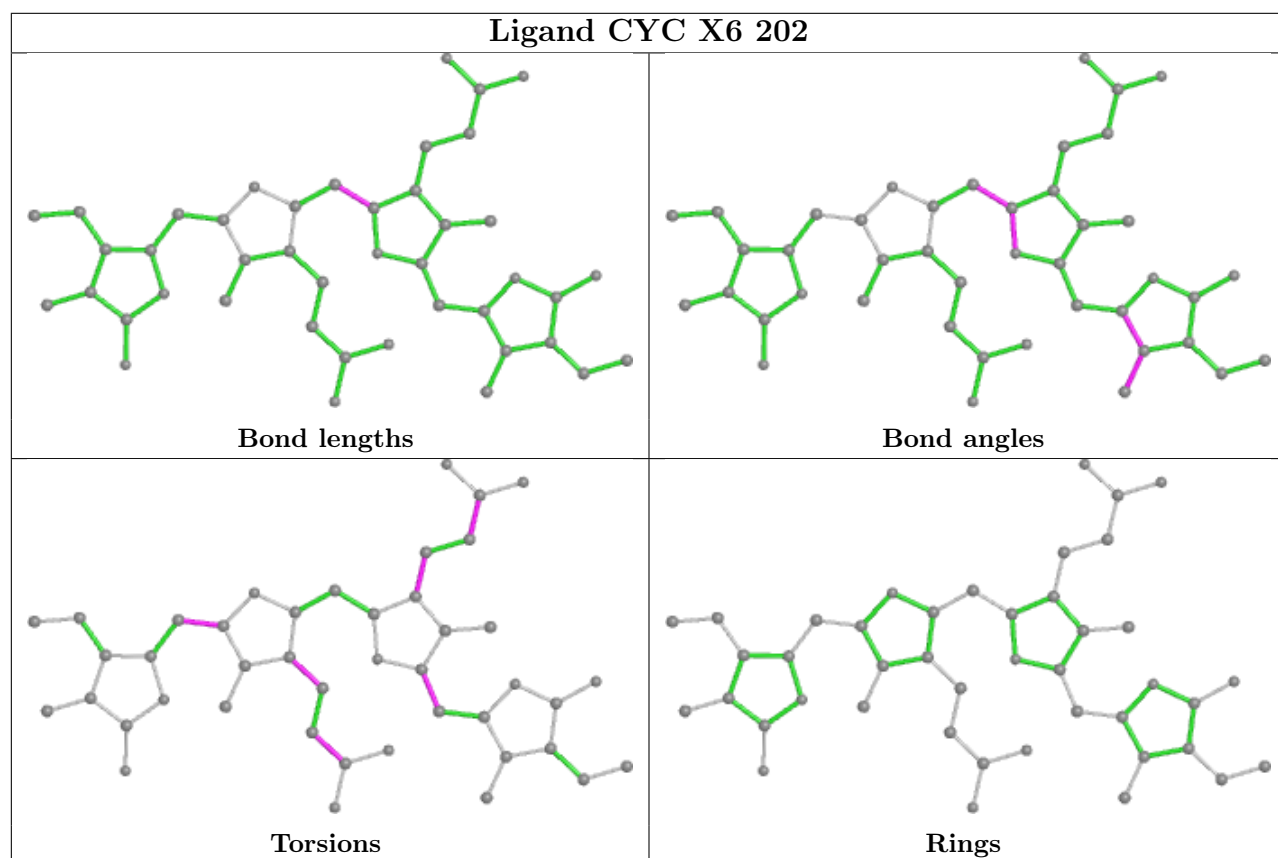
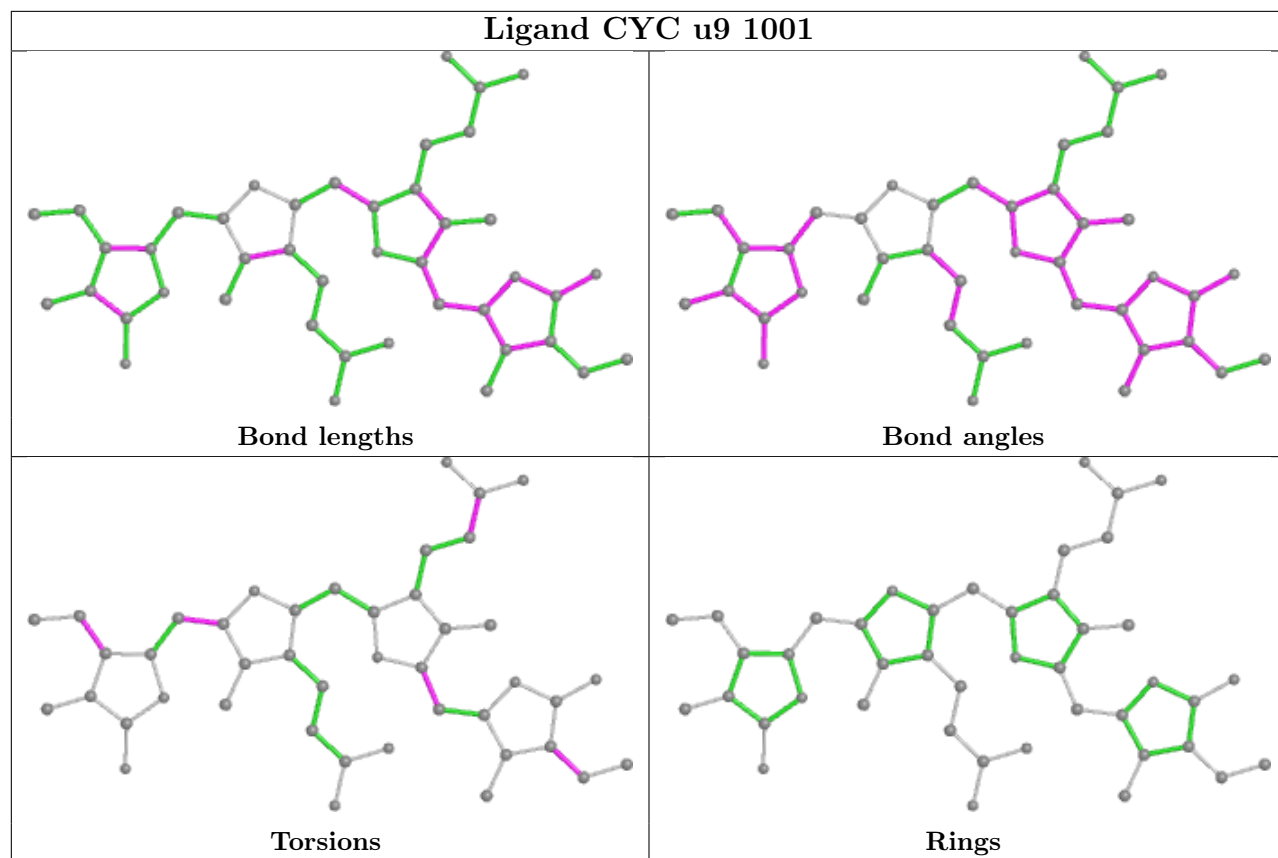
No monomer is involved in short contacts.

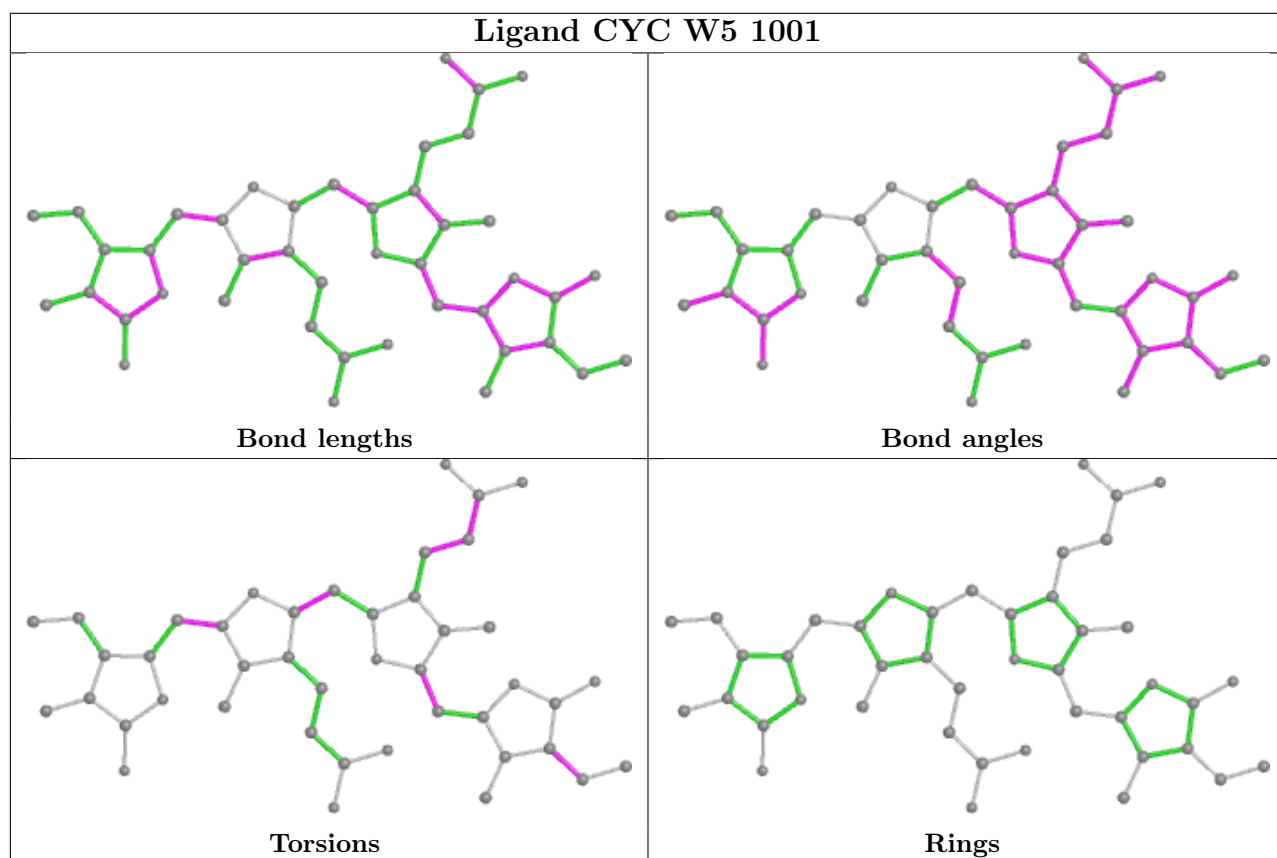
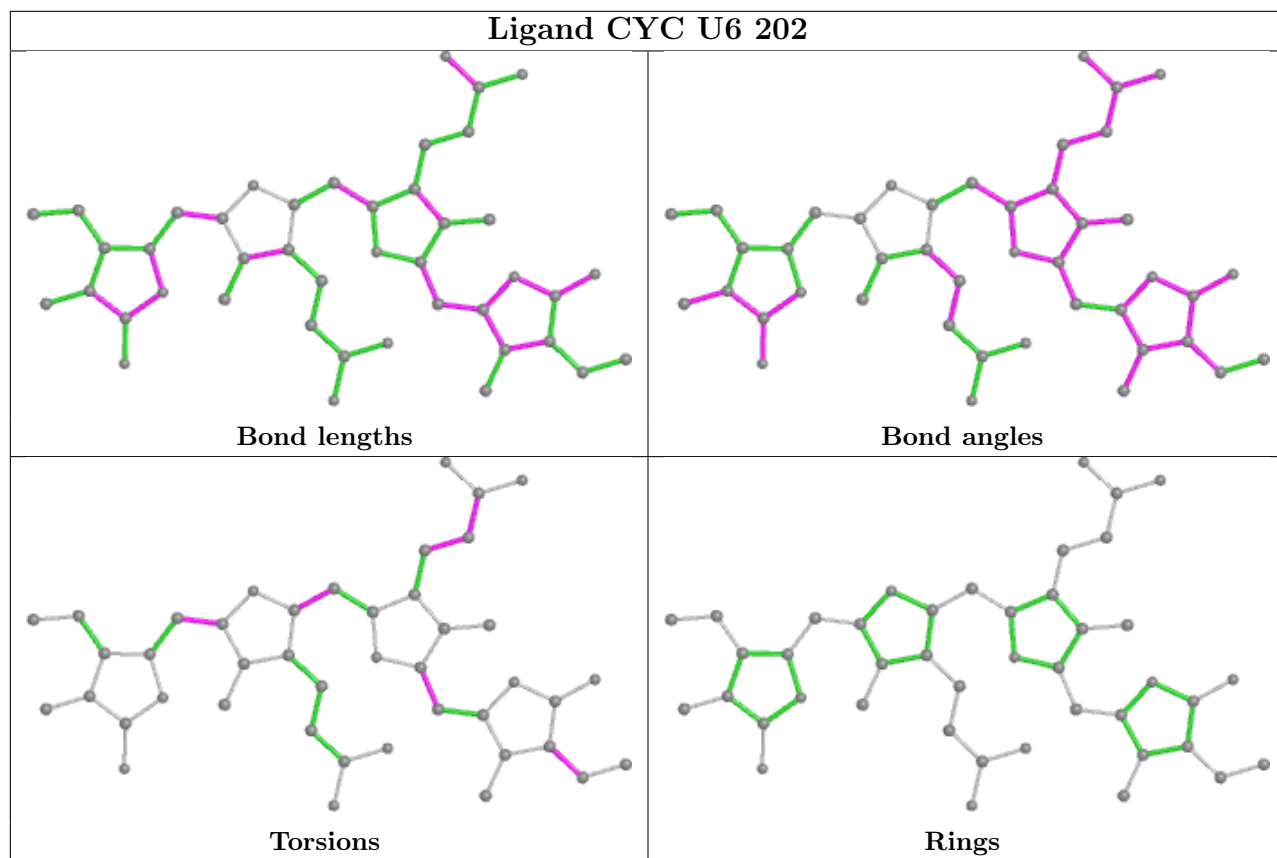
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

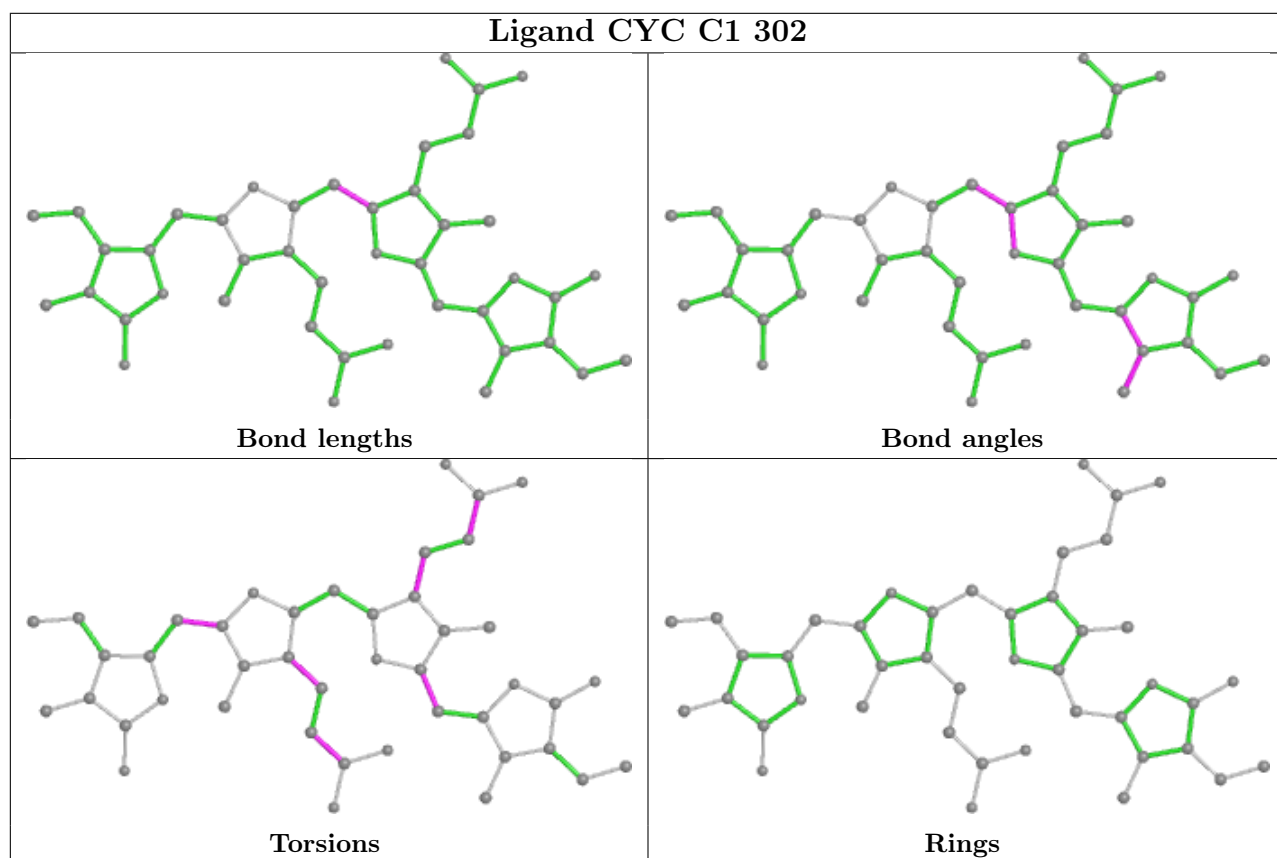
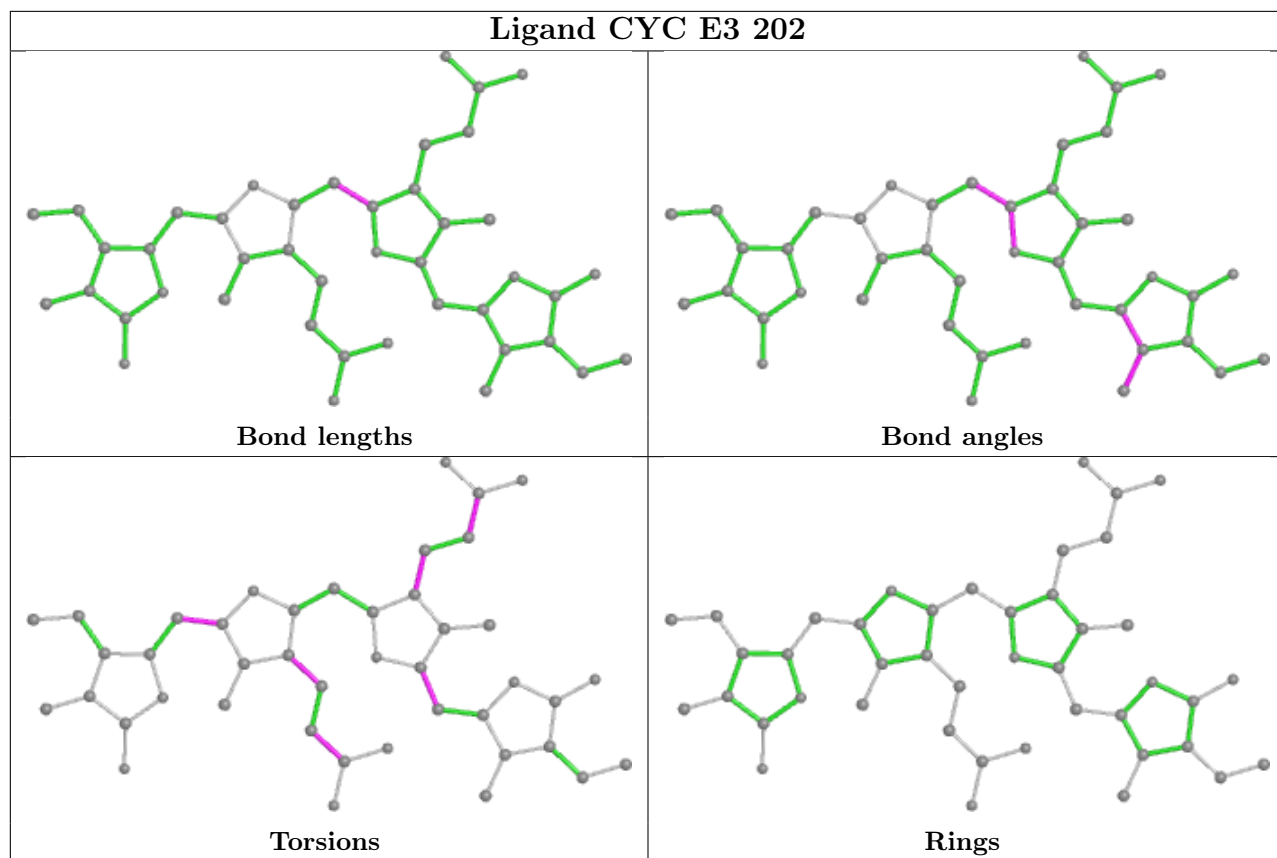


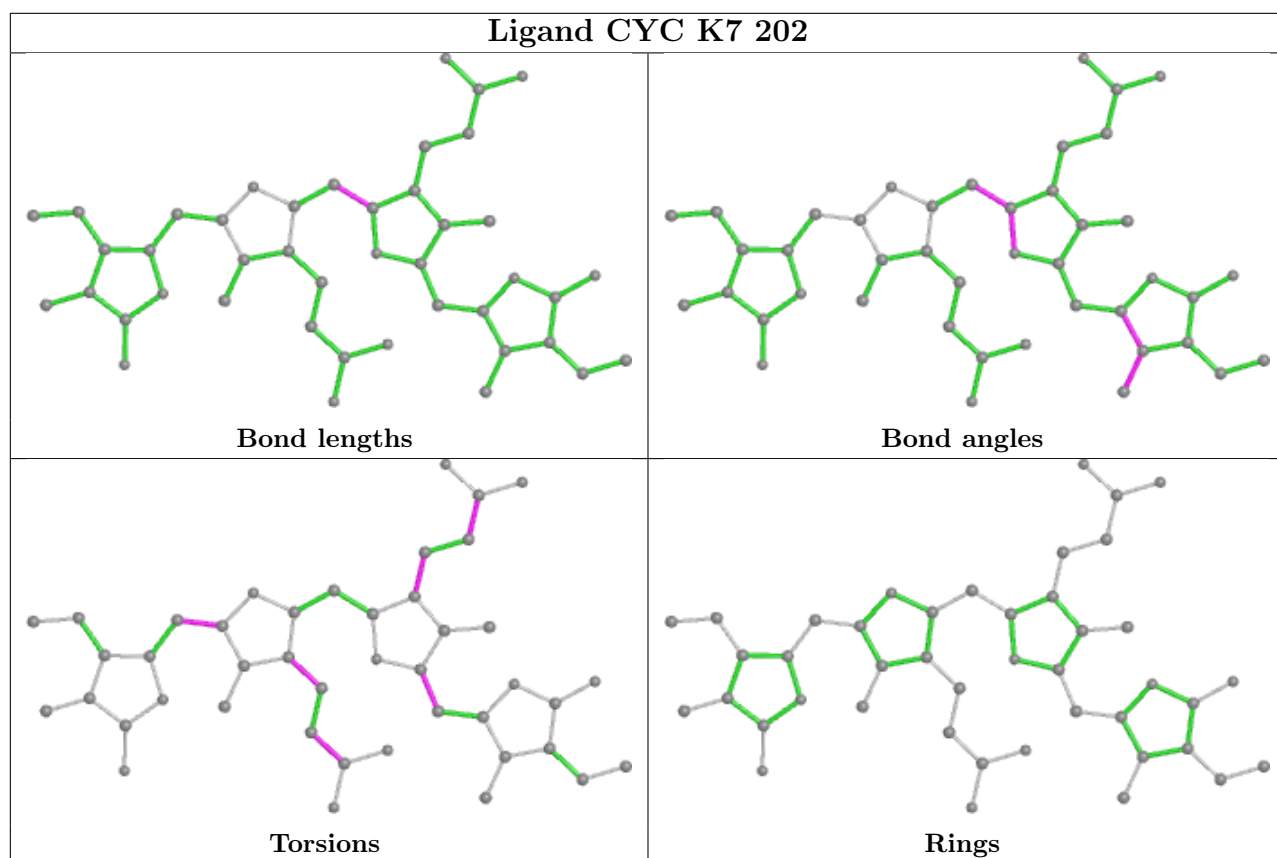
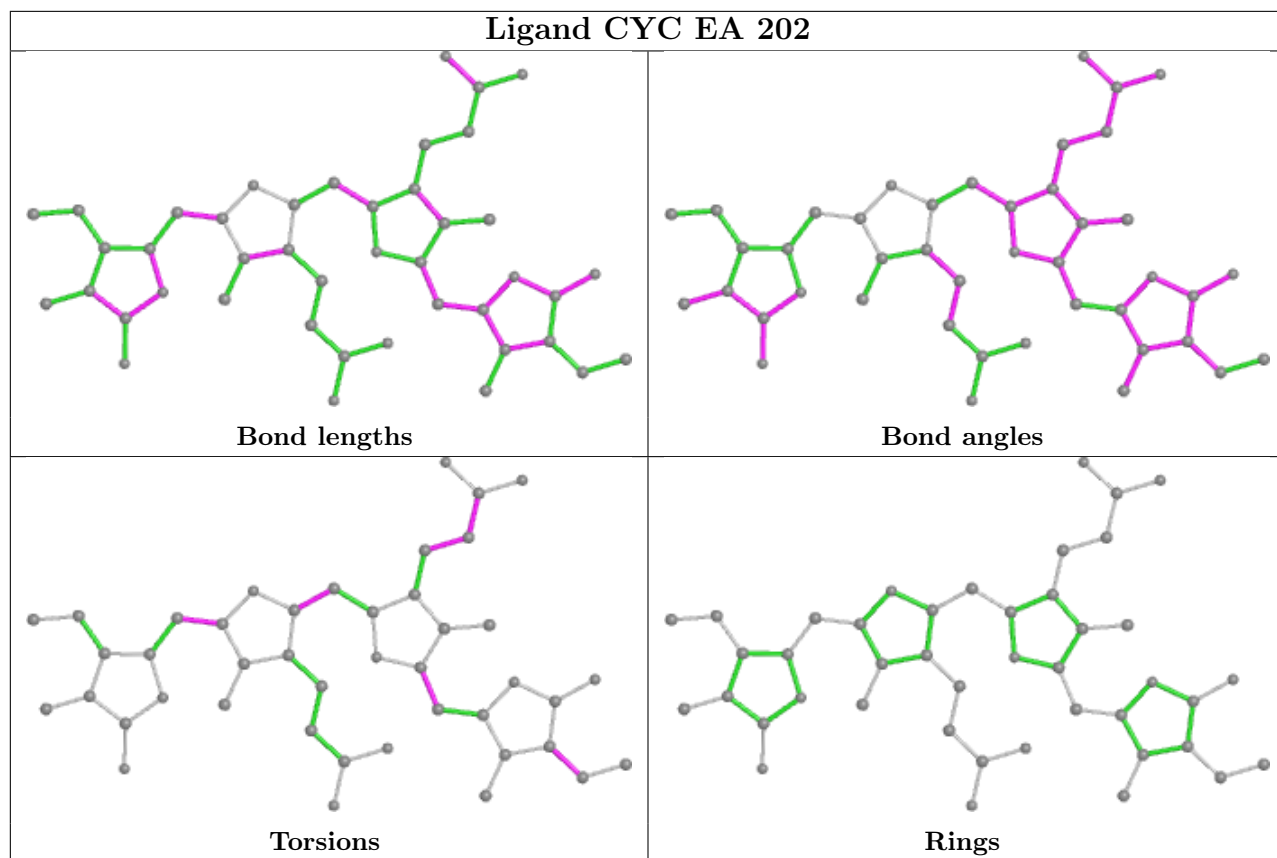


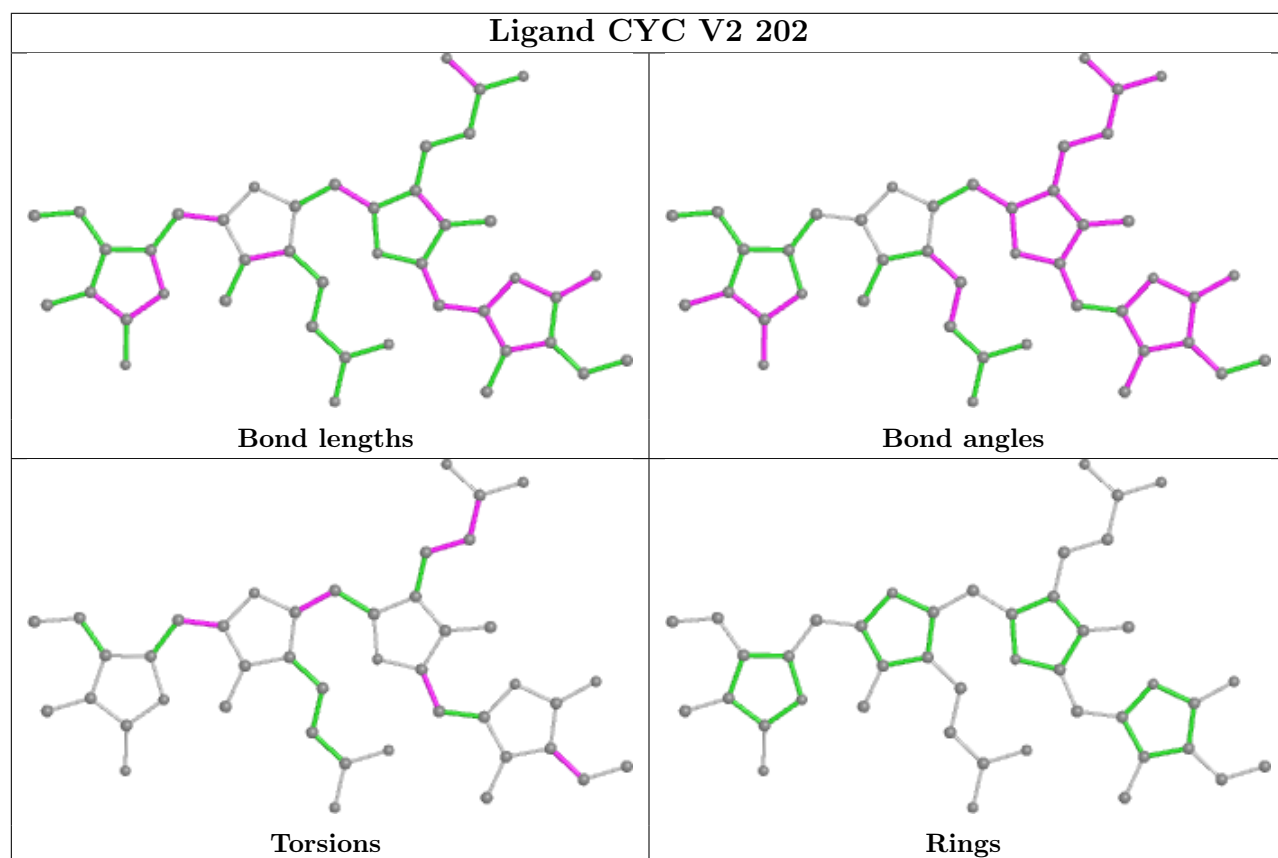
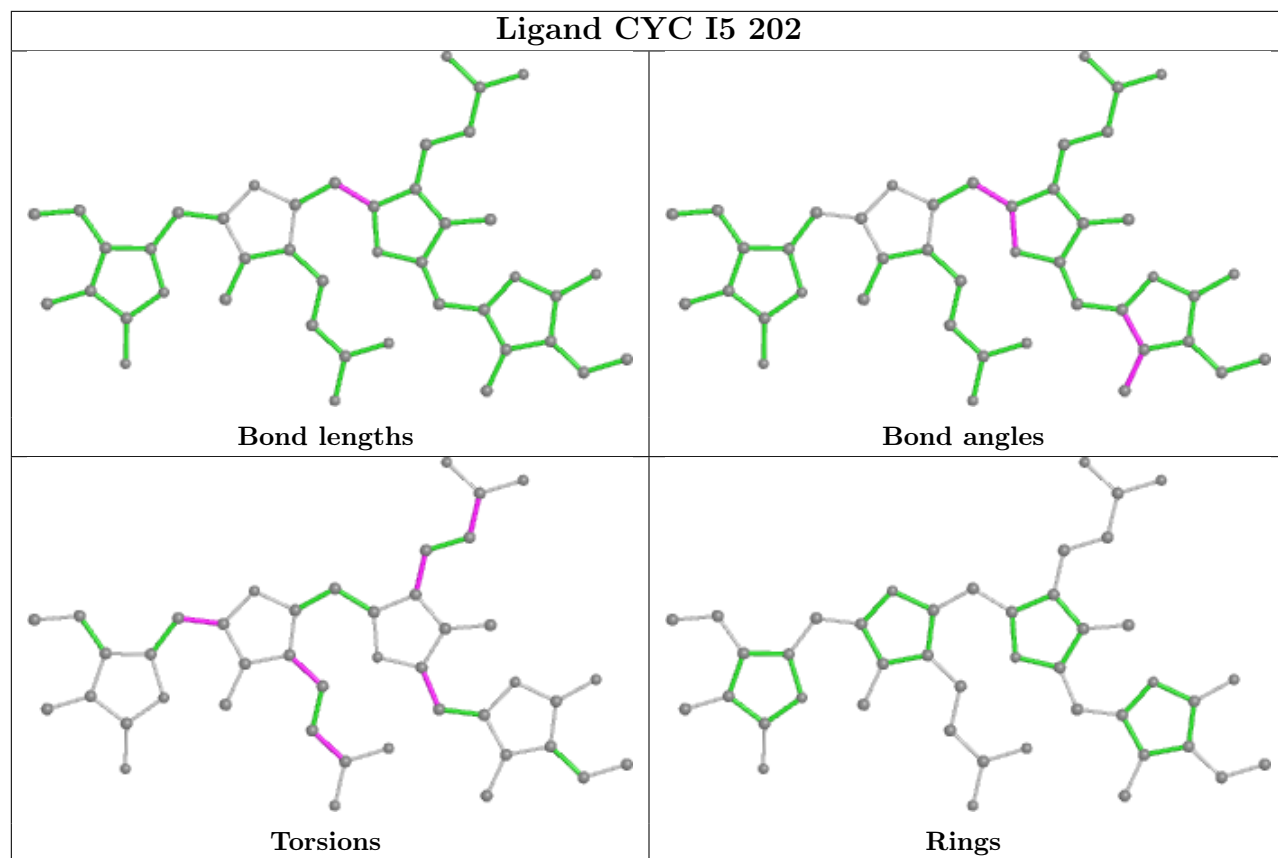


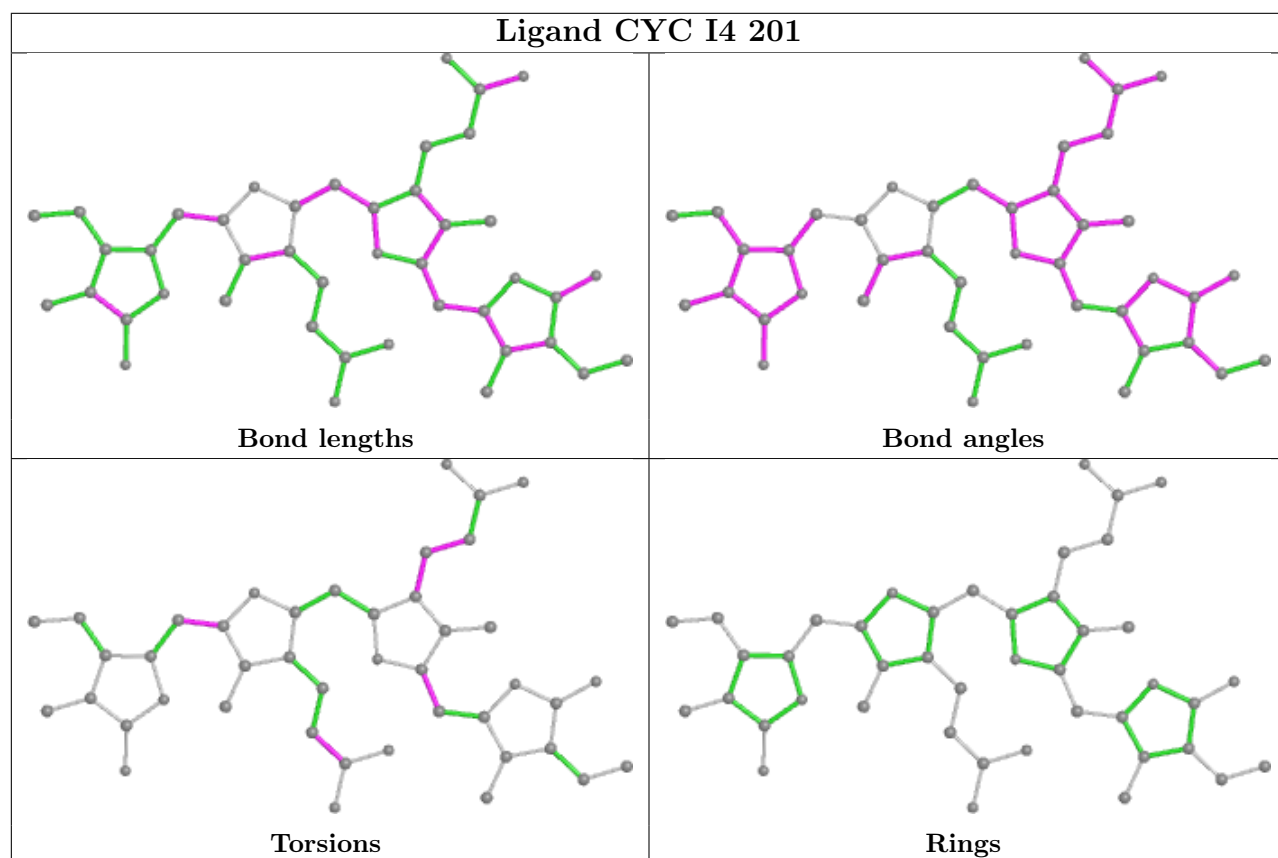
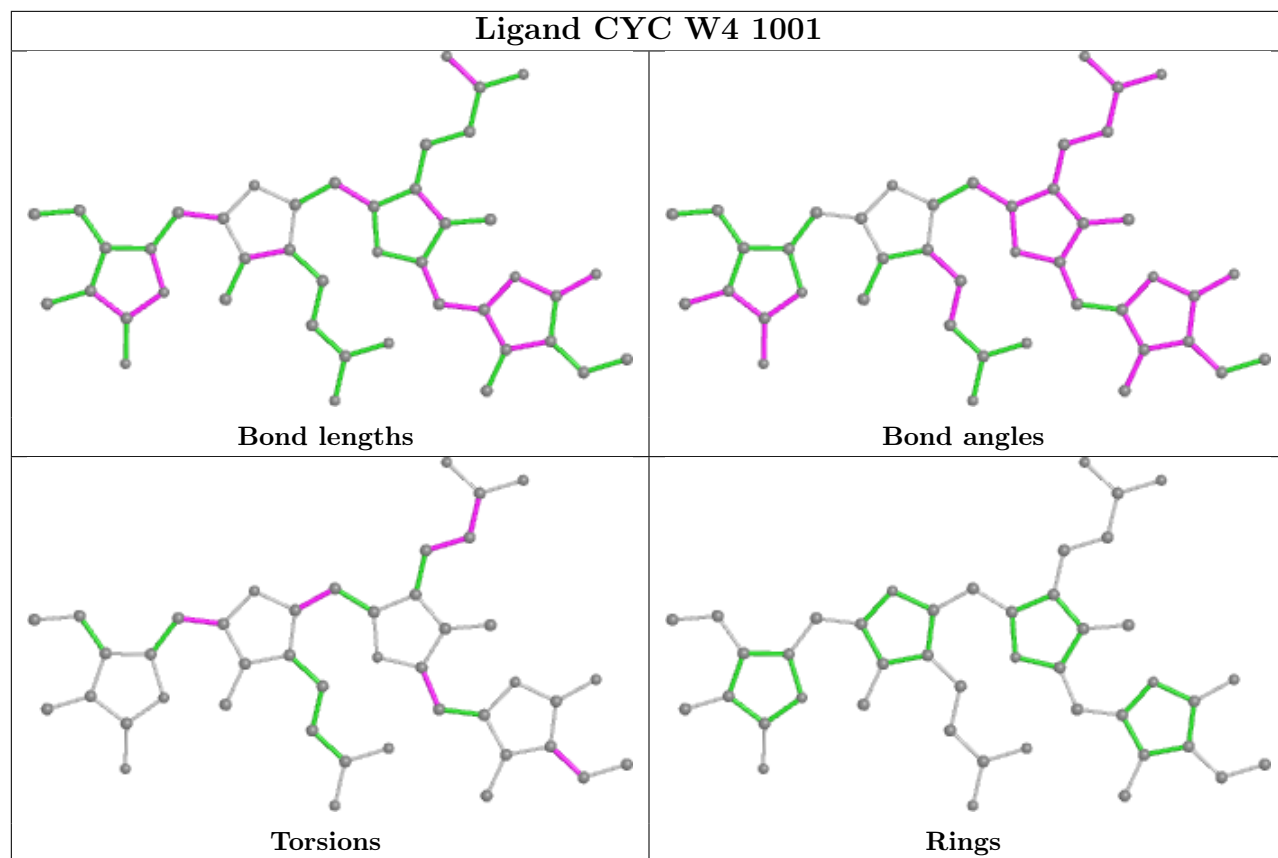


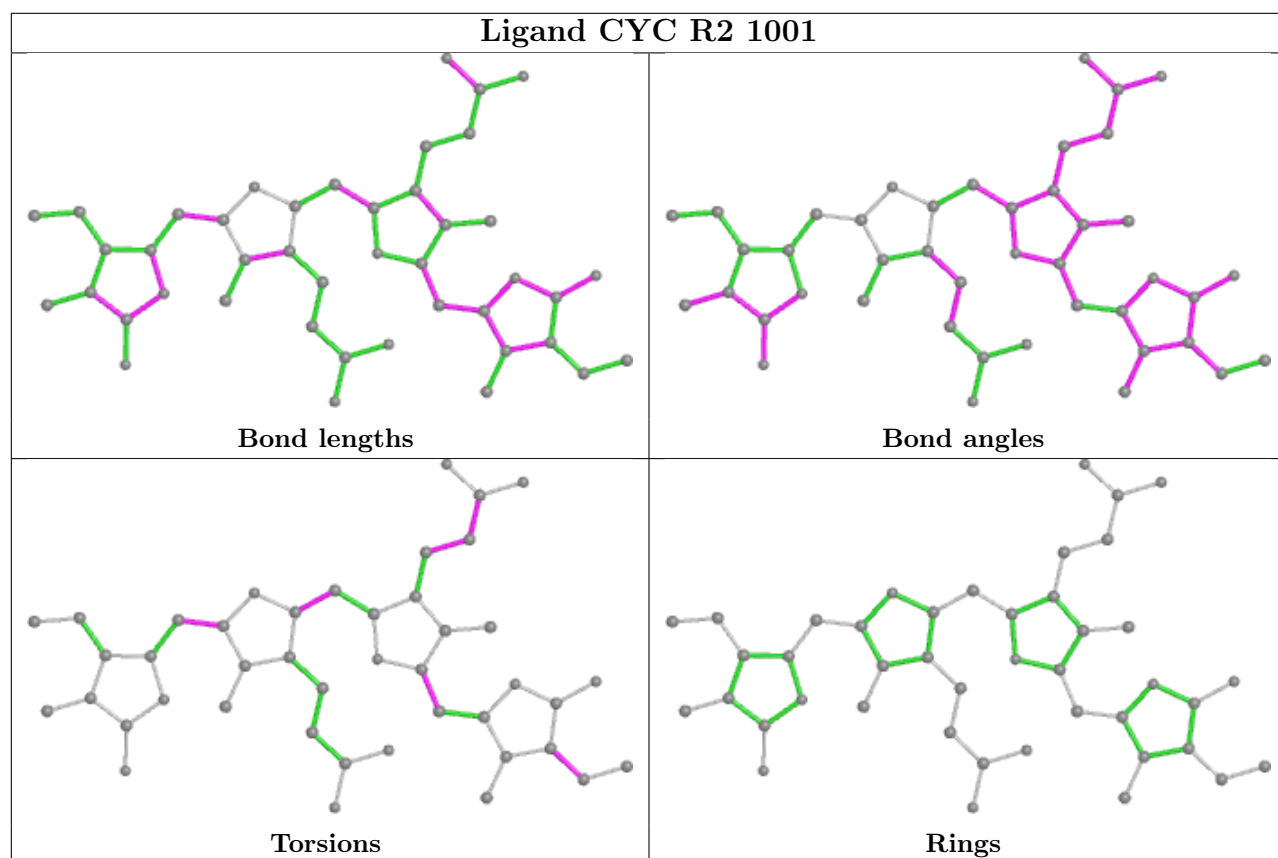
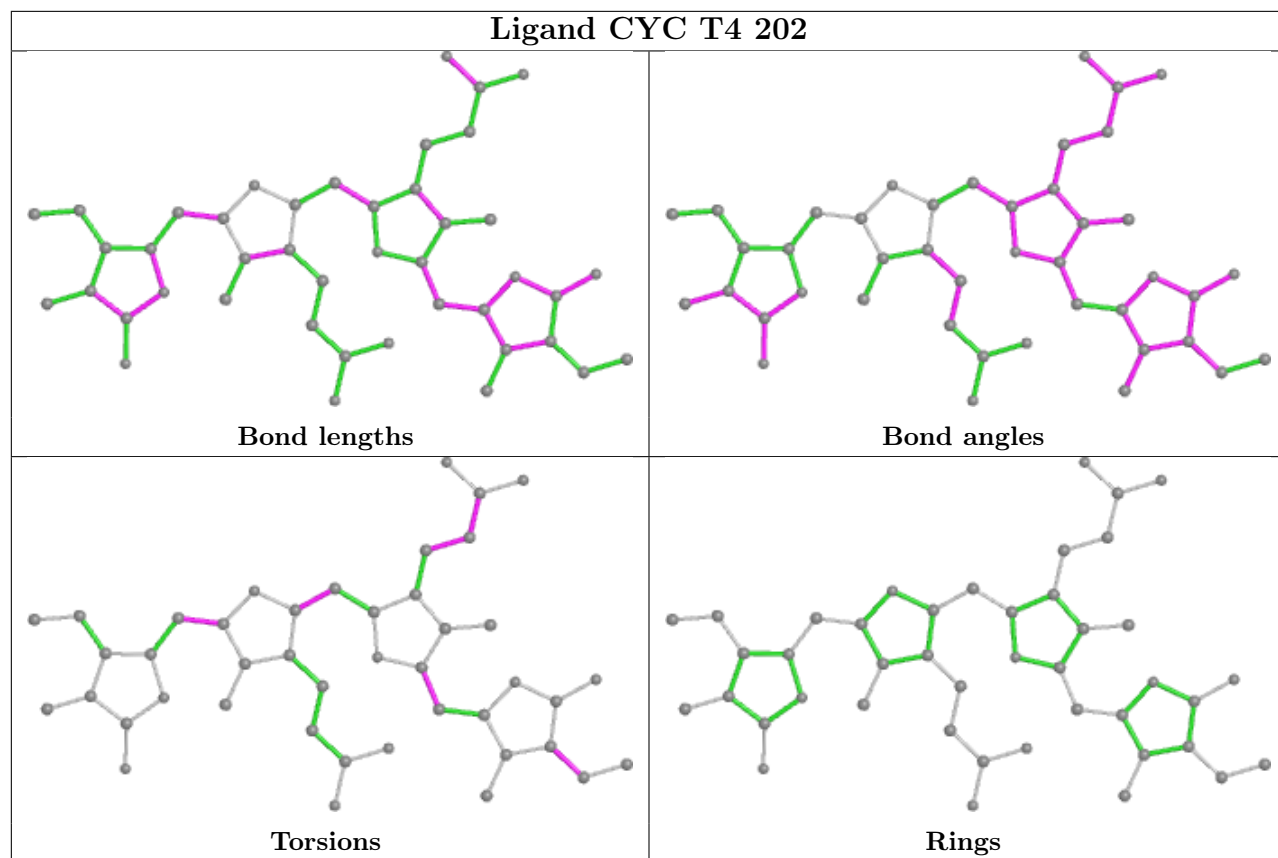


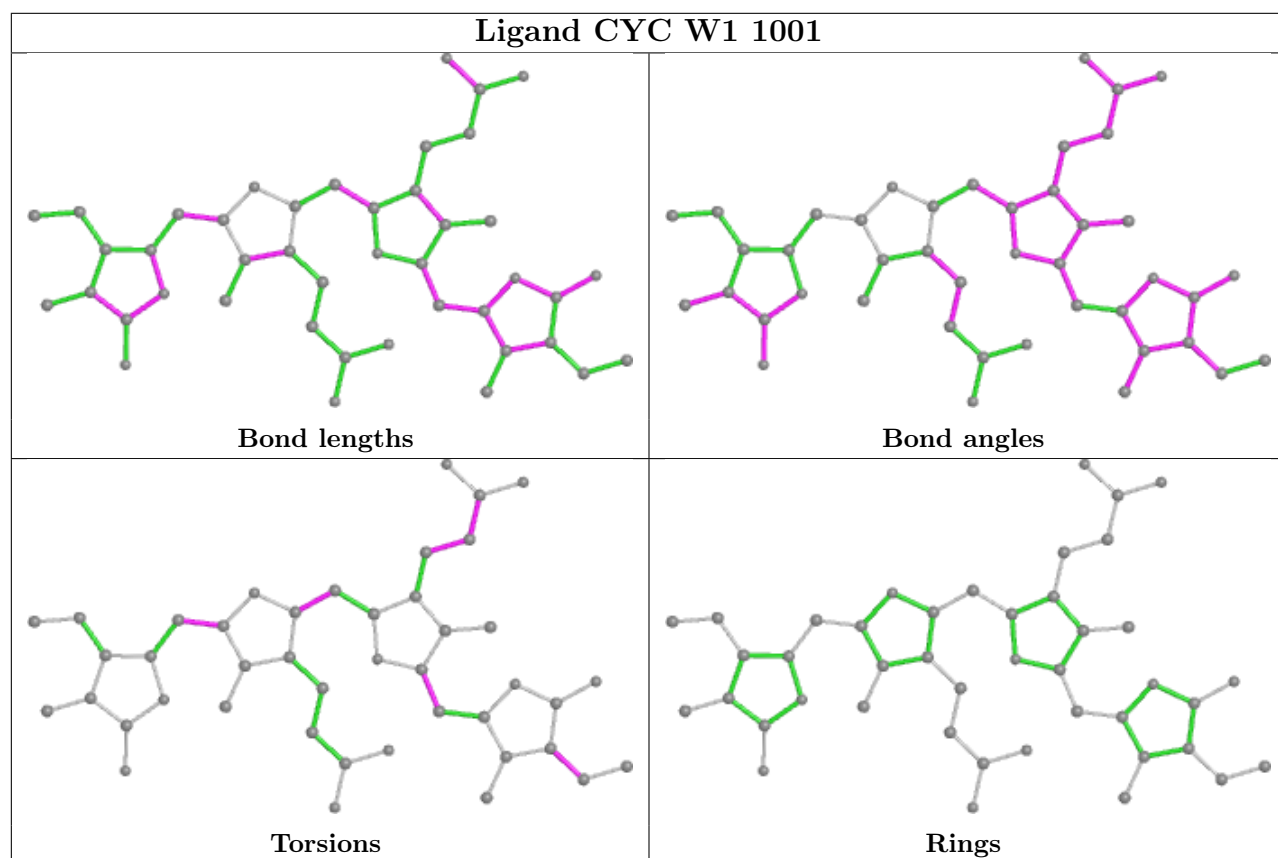
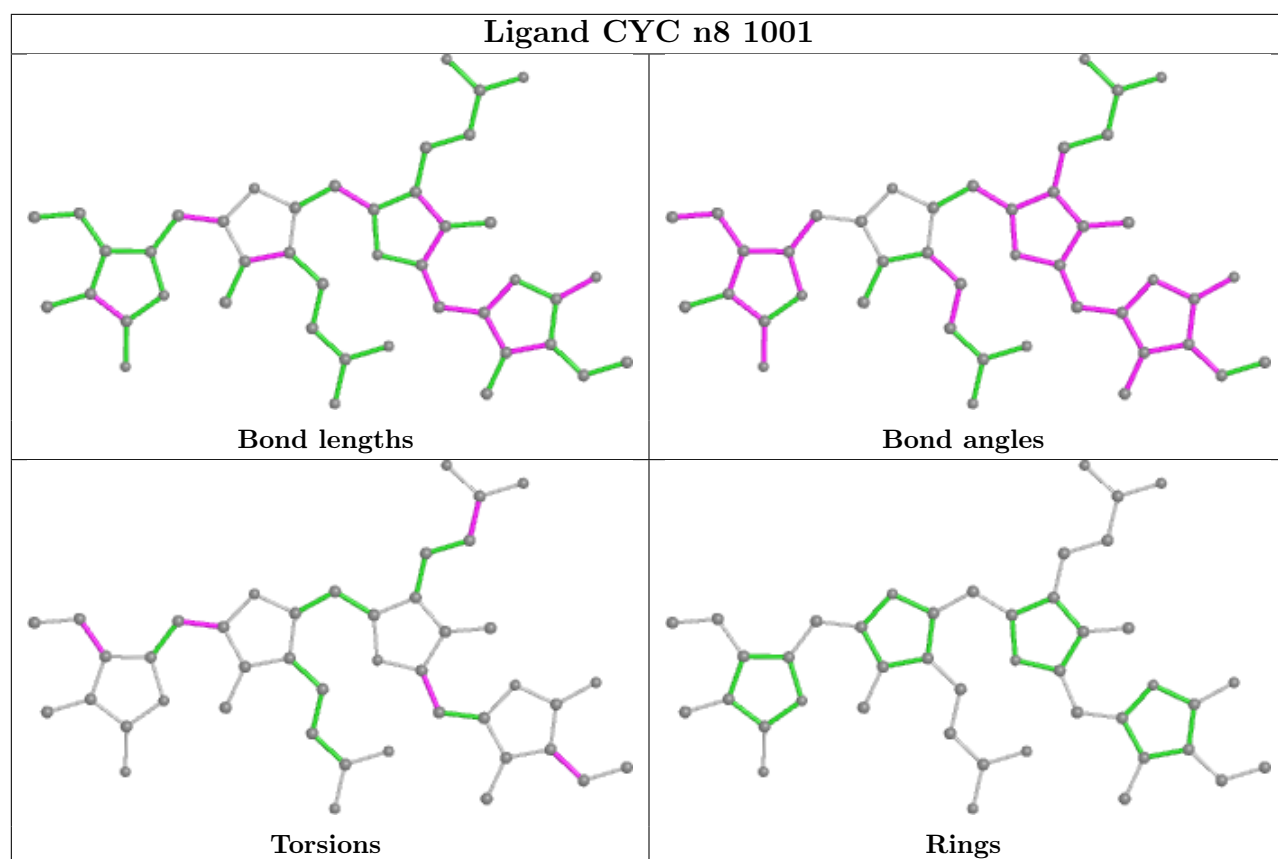


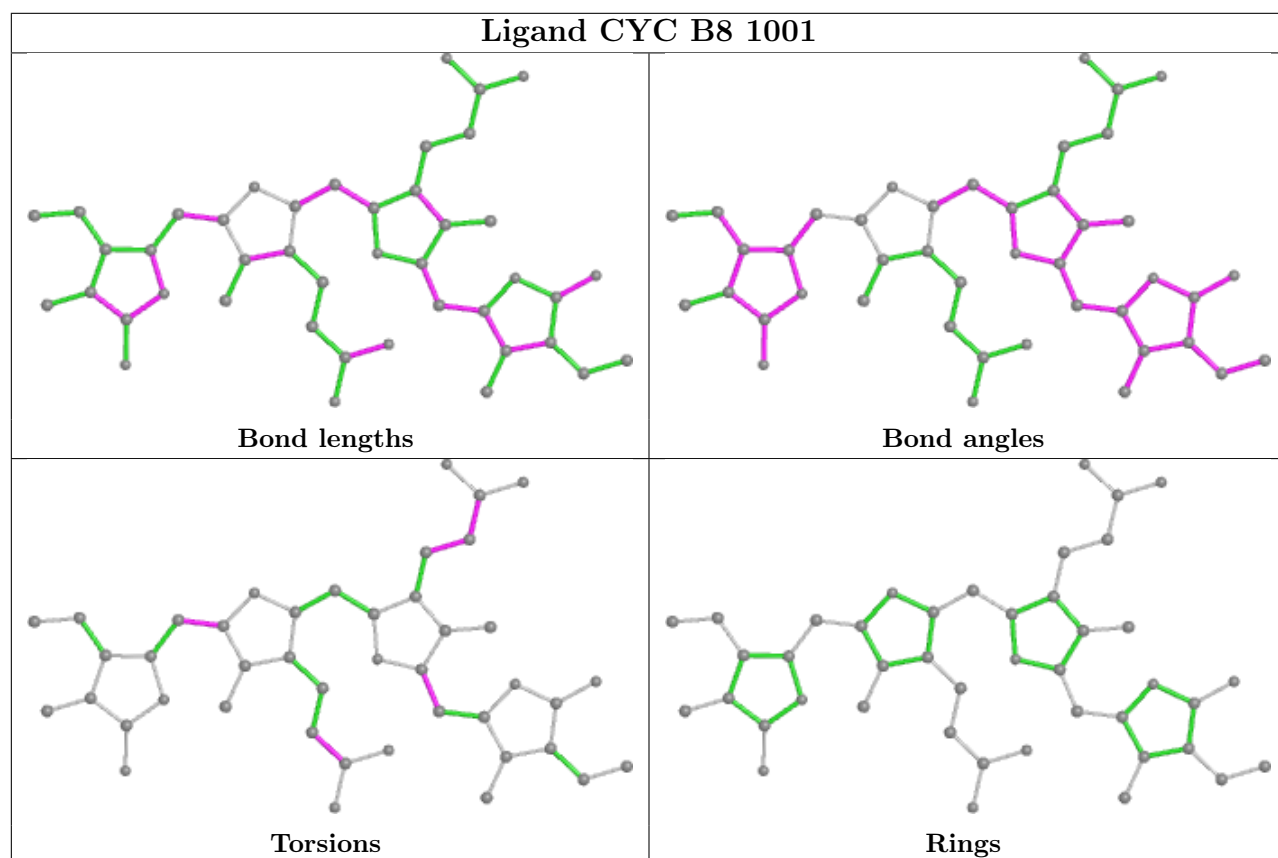
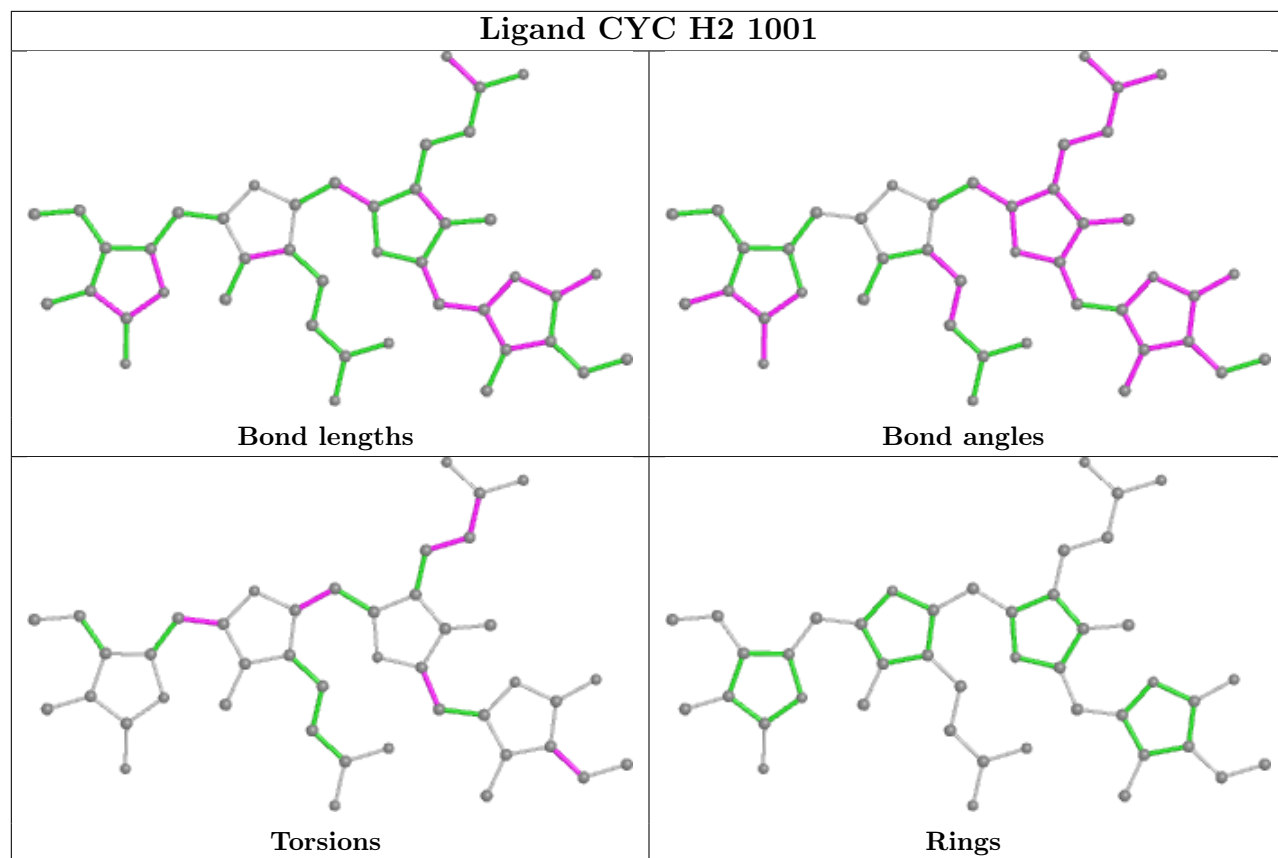


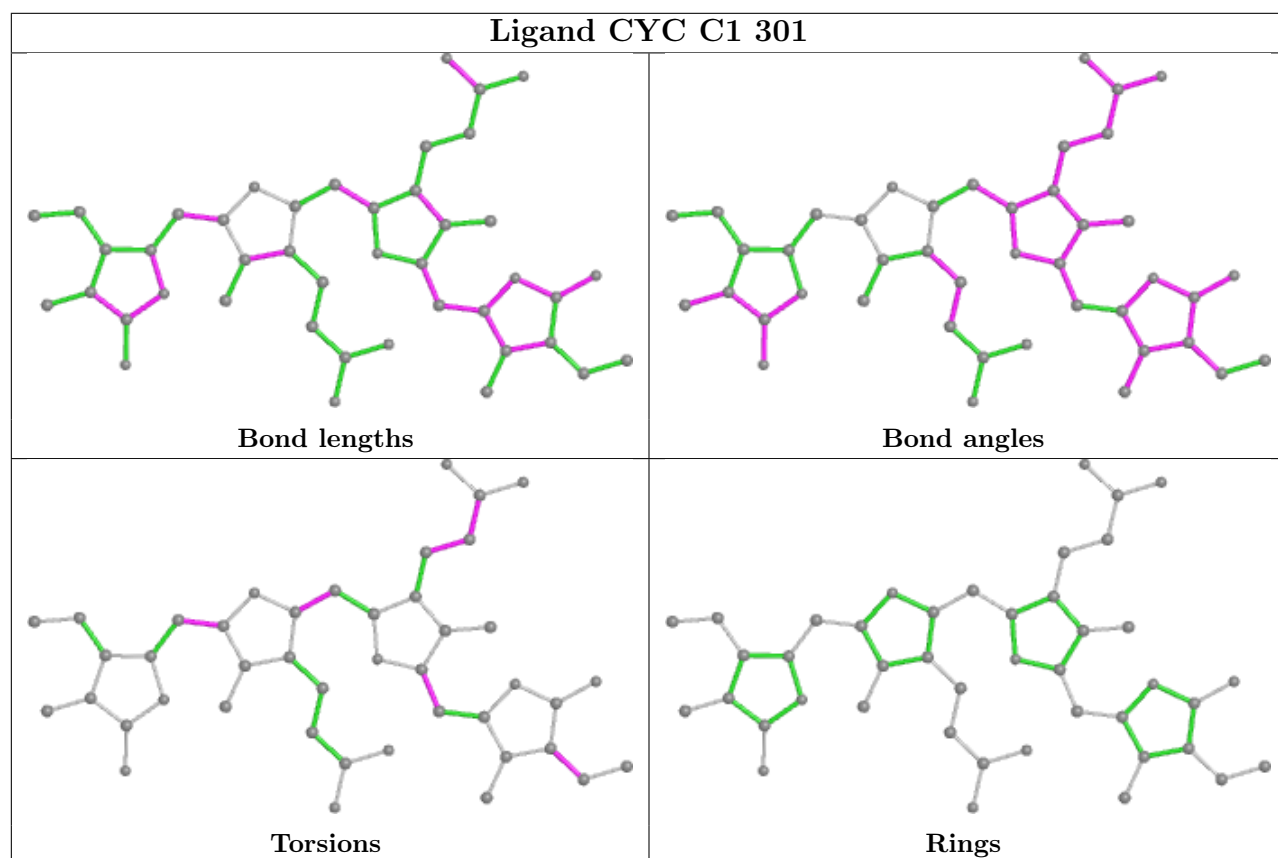
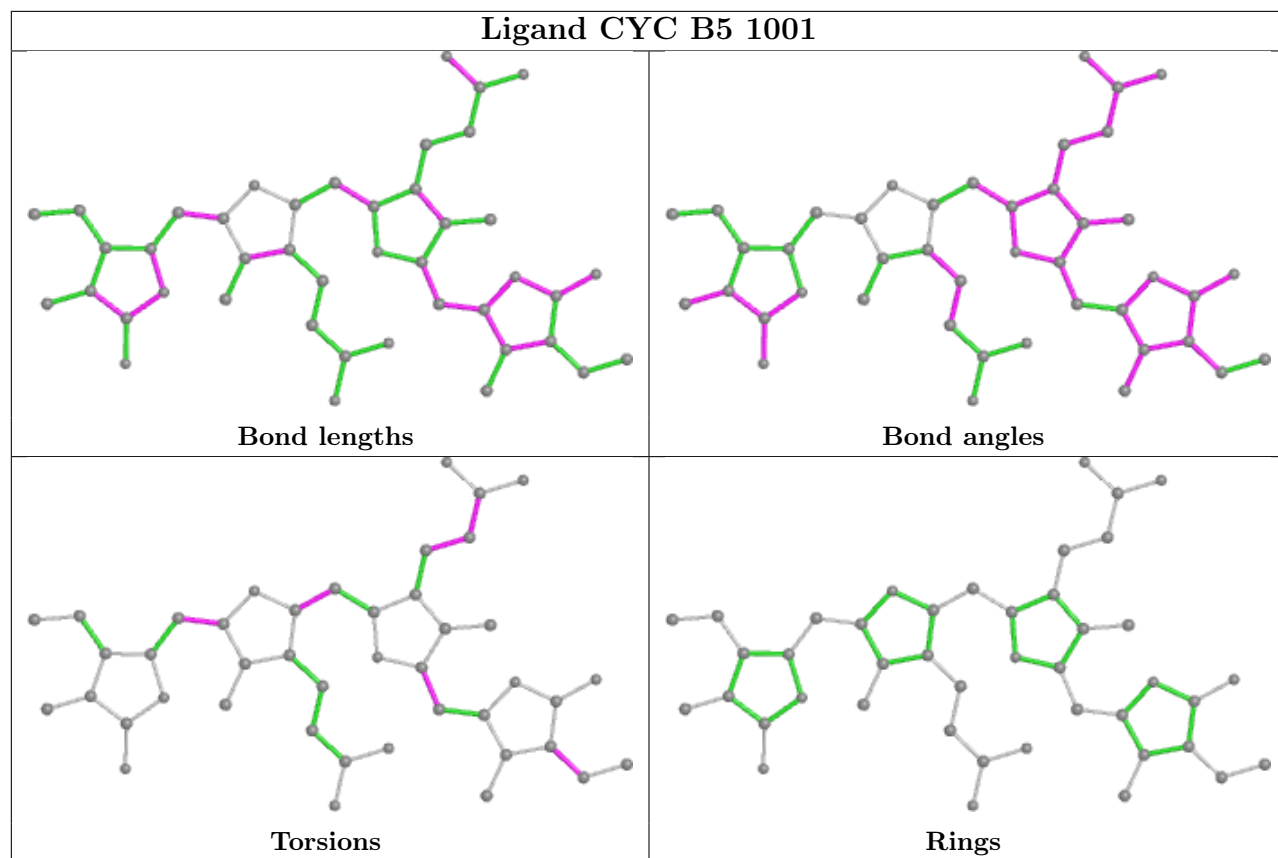


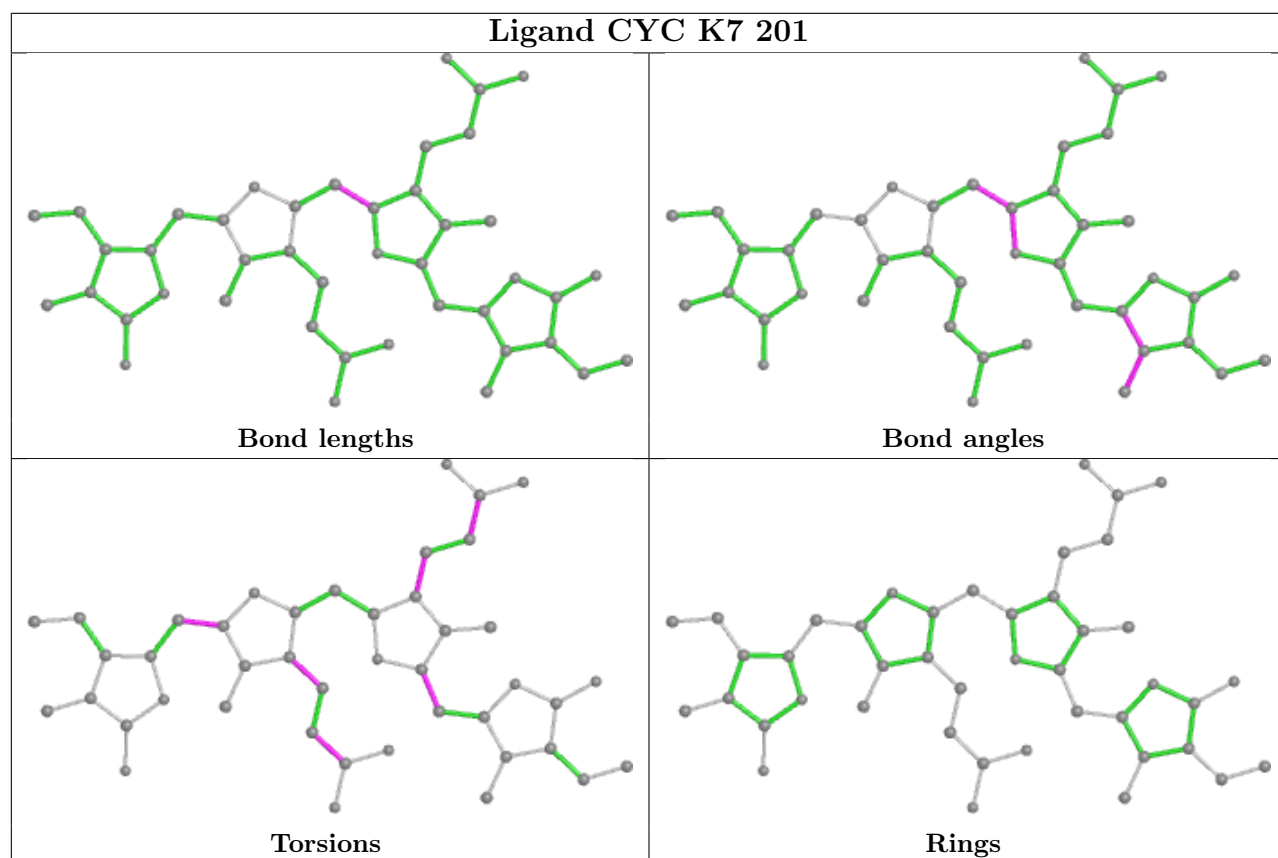
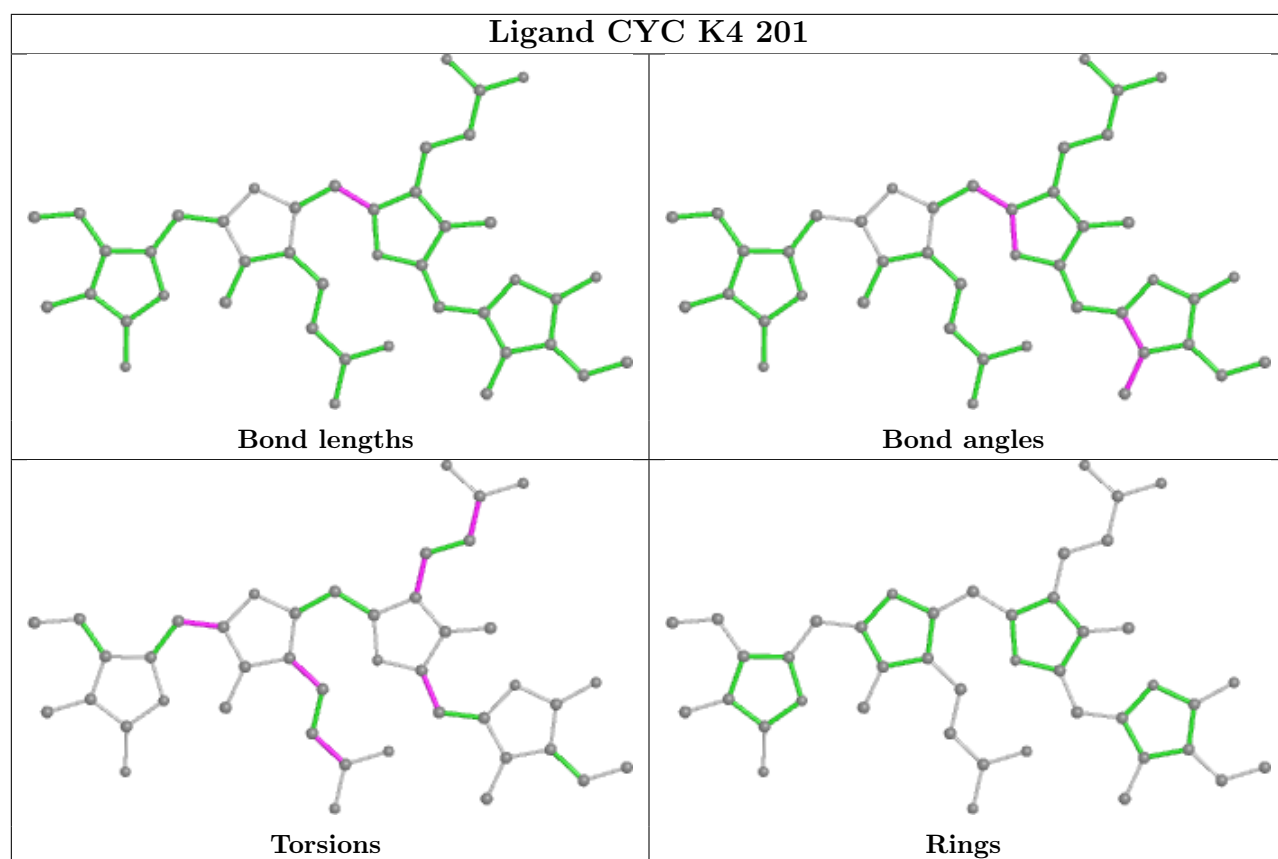


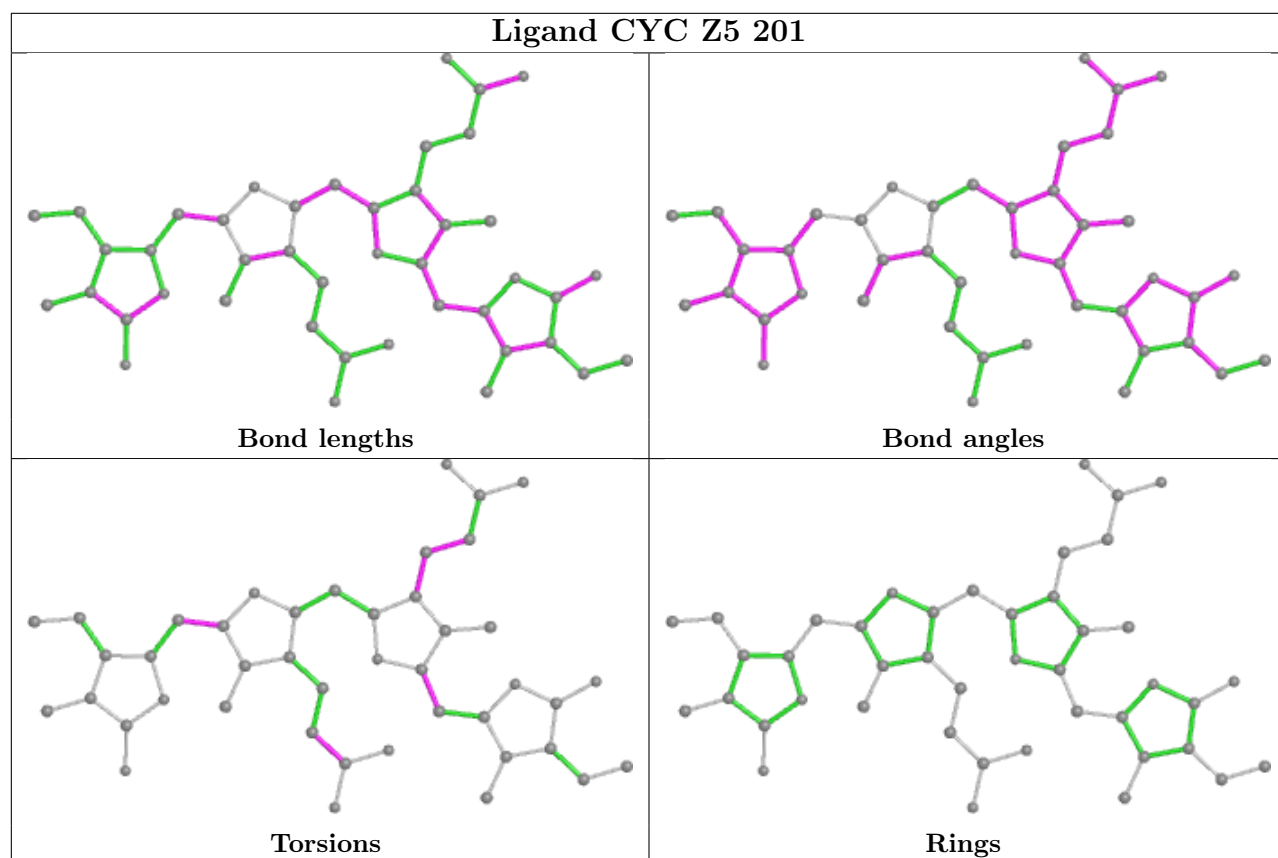
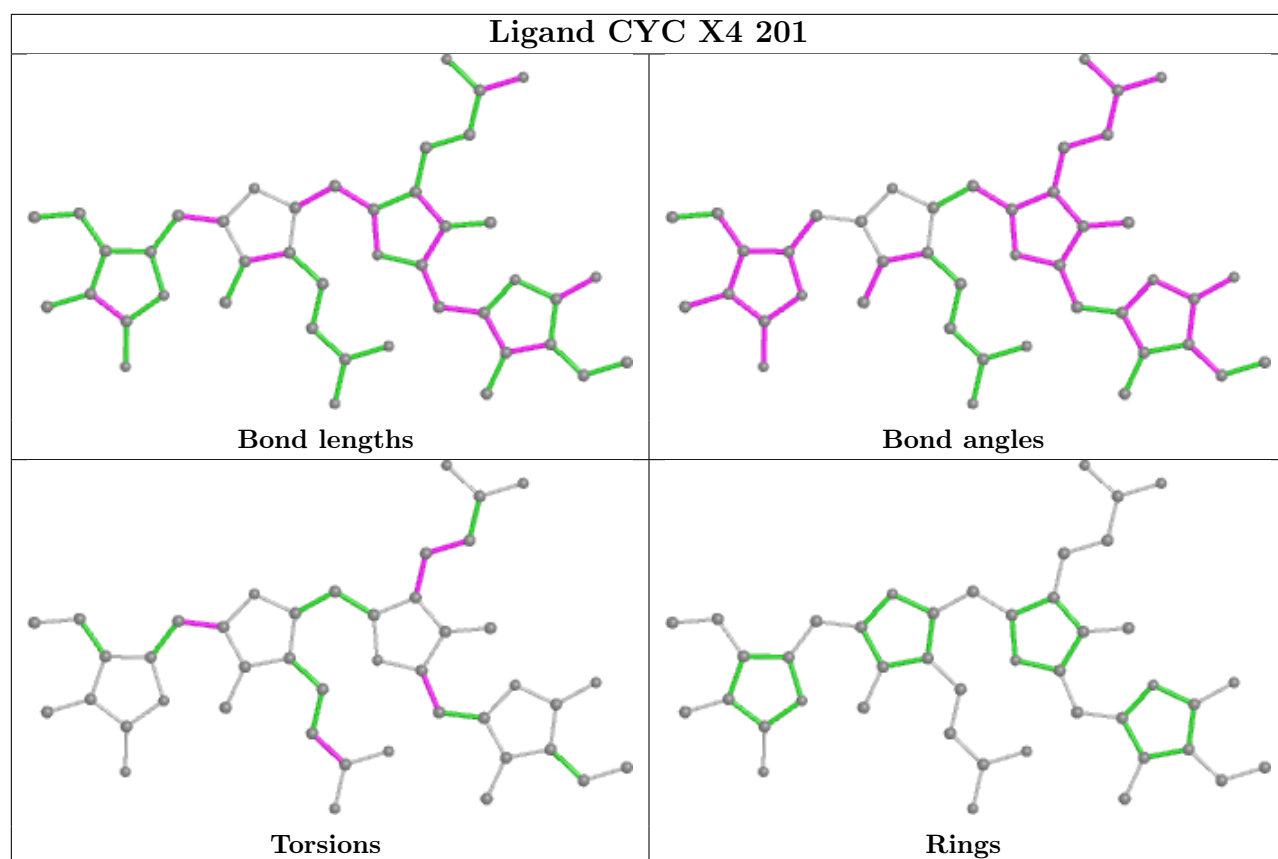


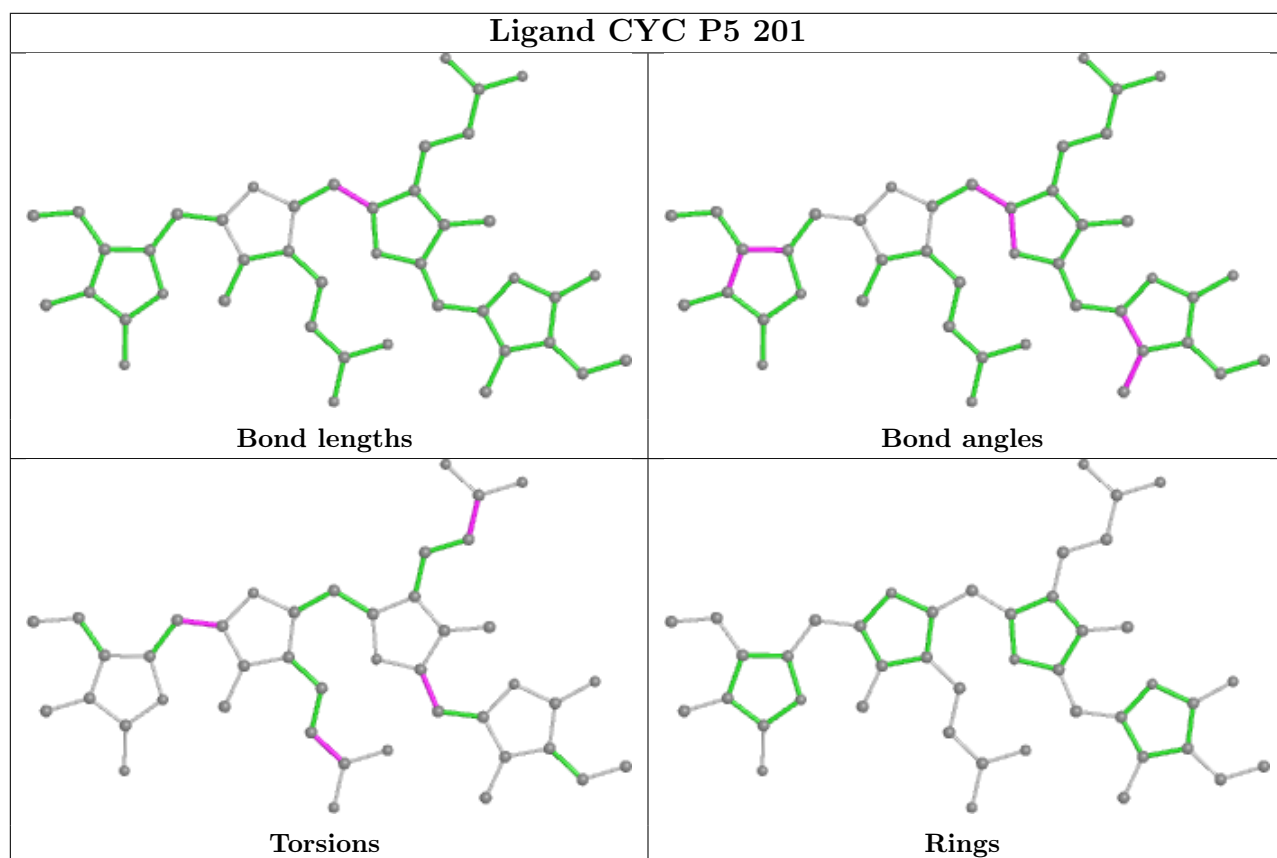
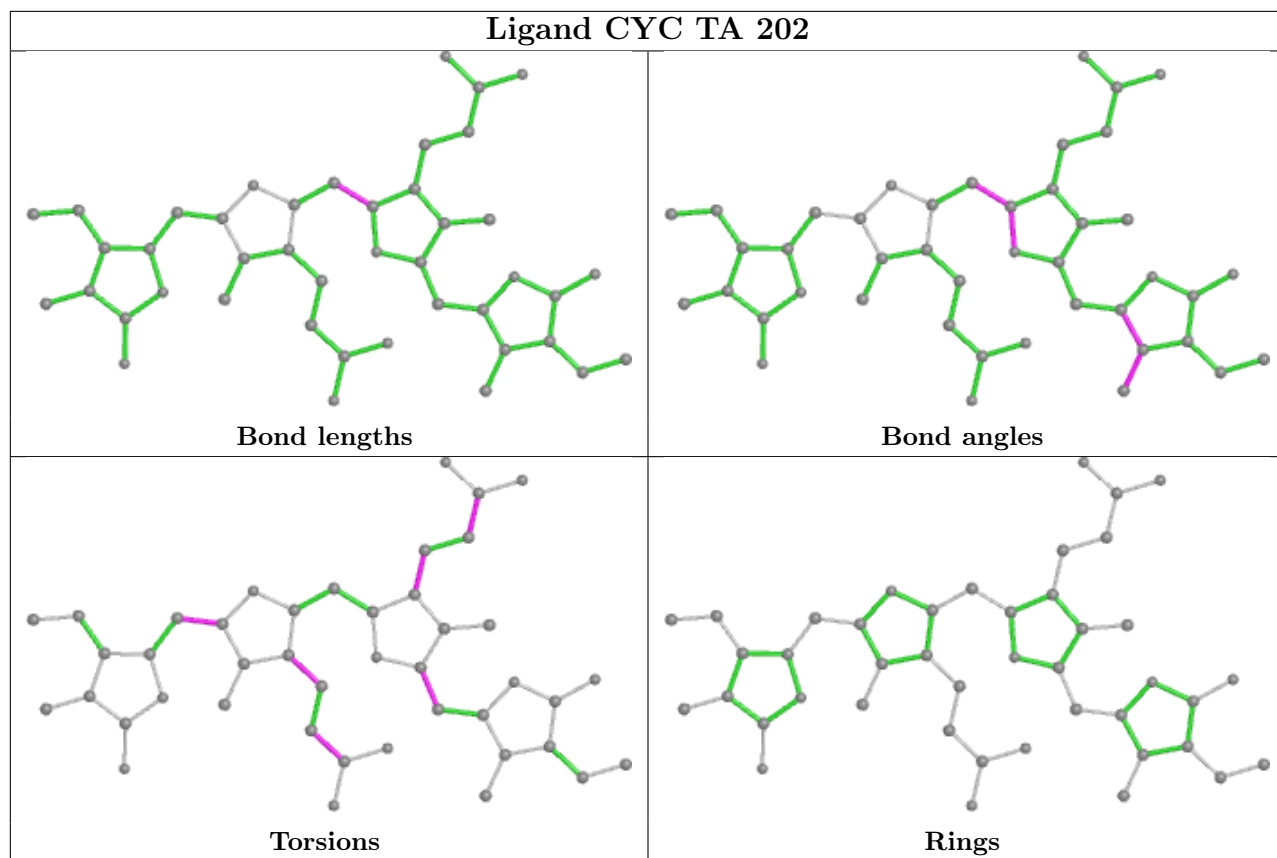


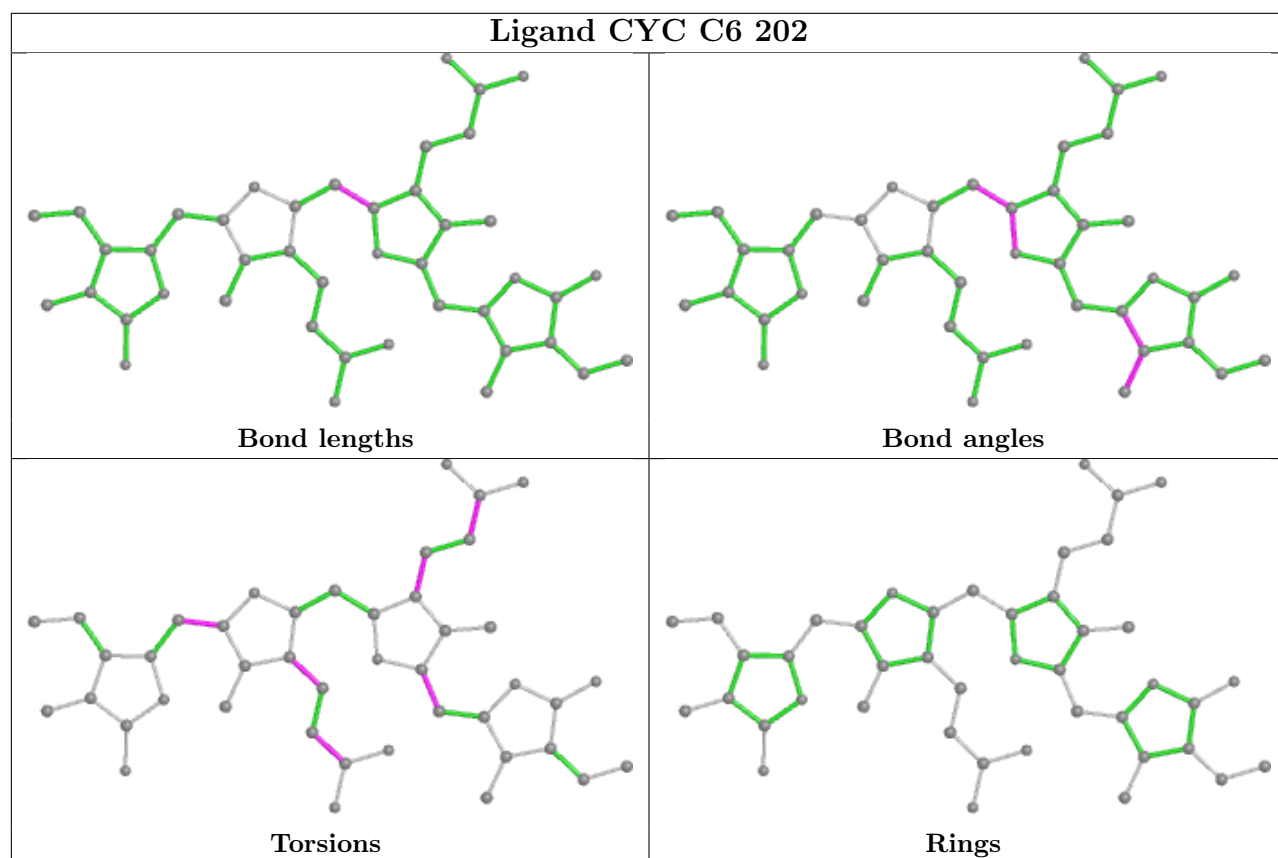
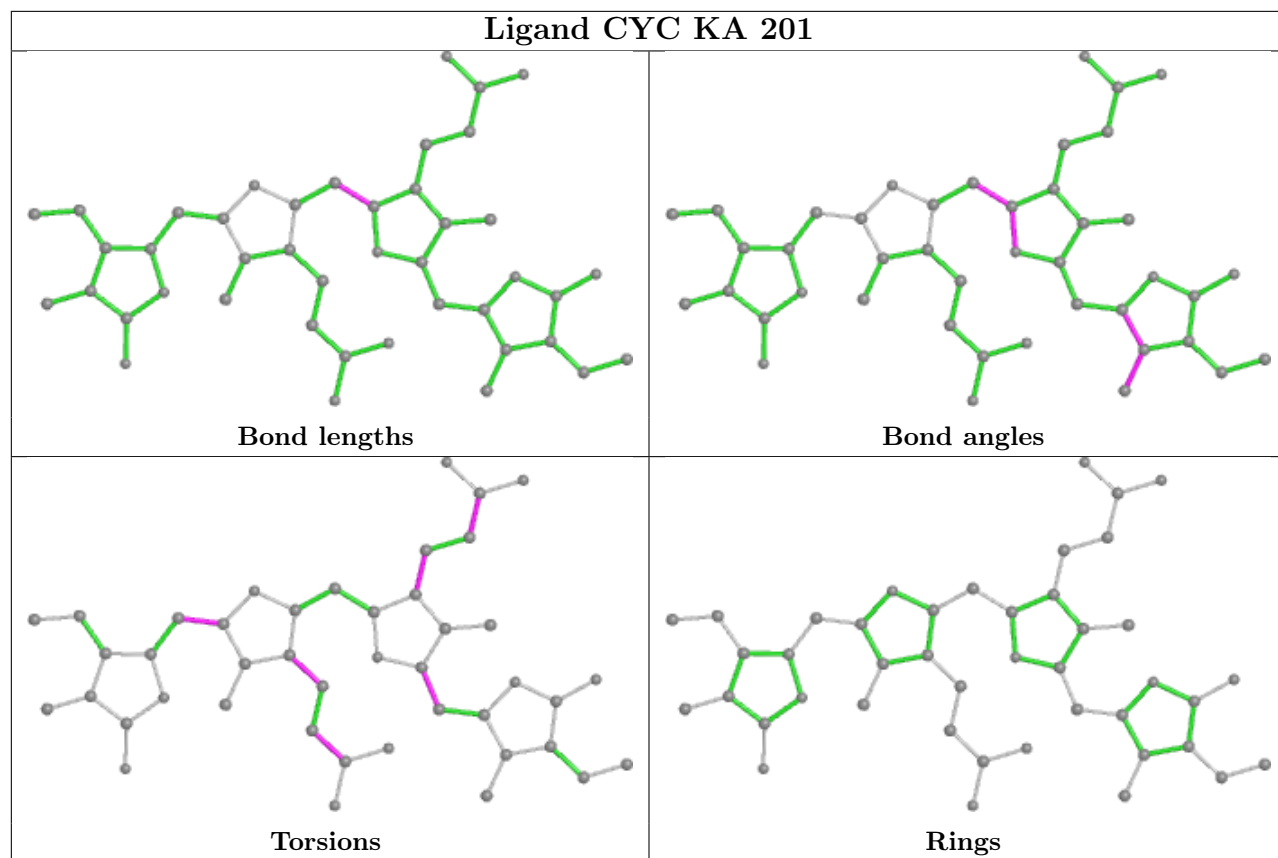


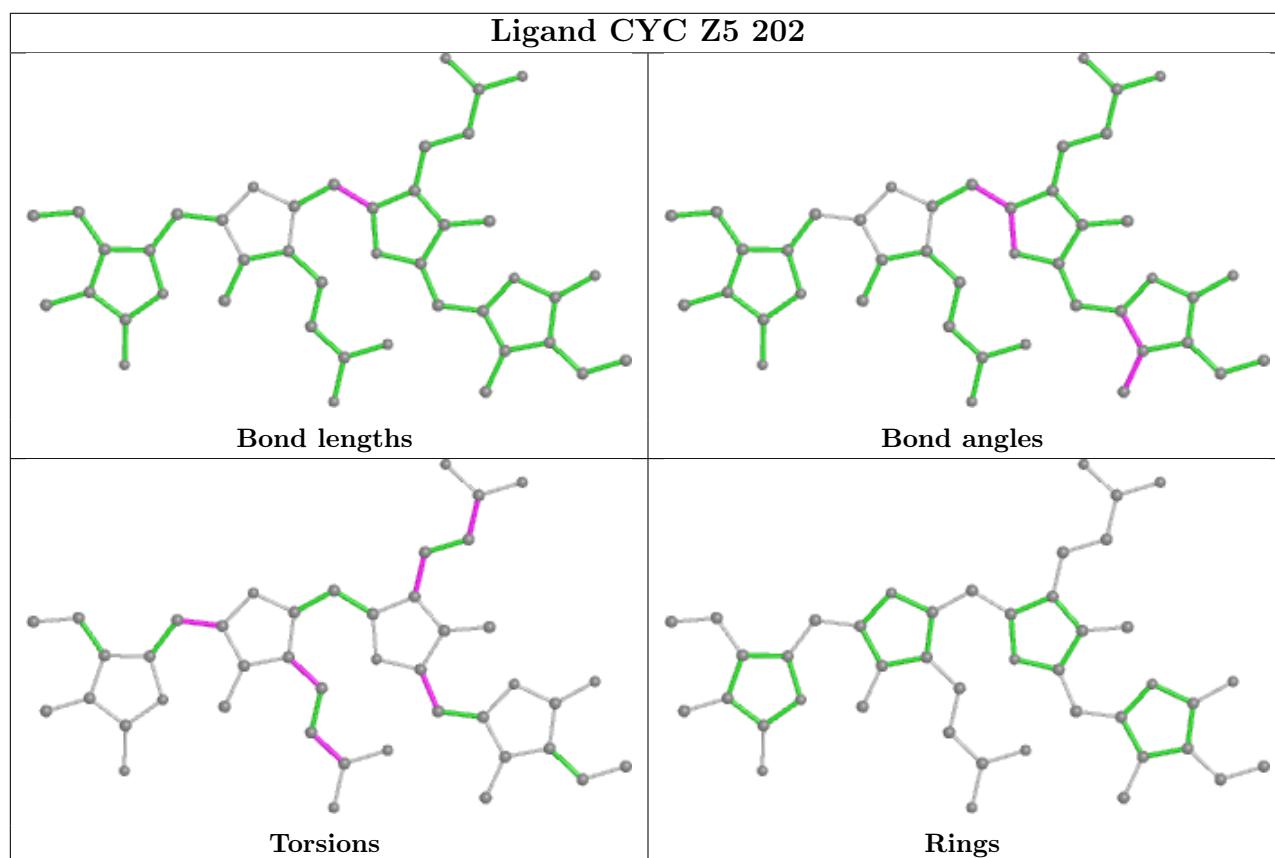
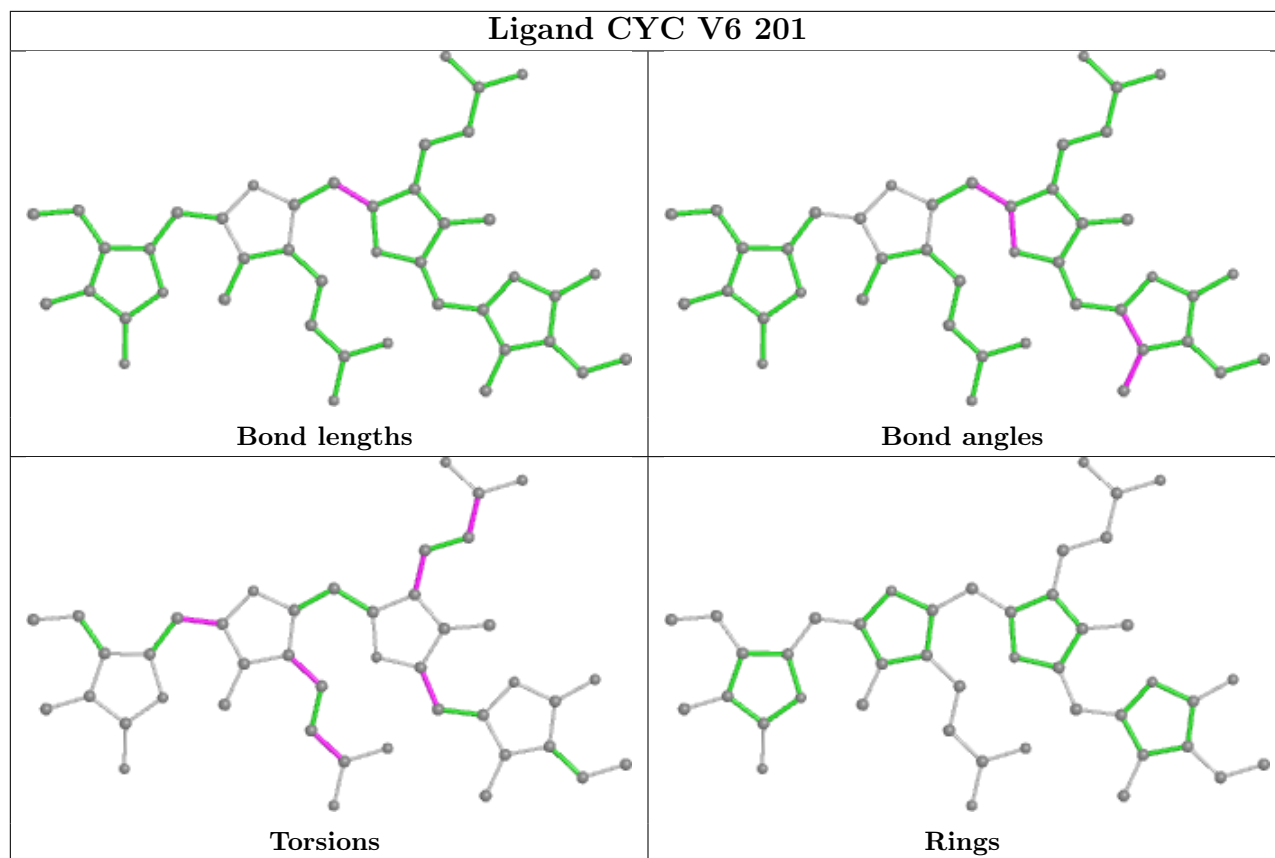


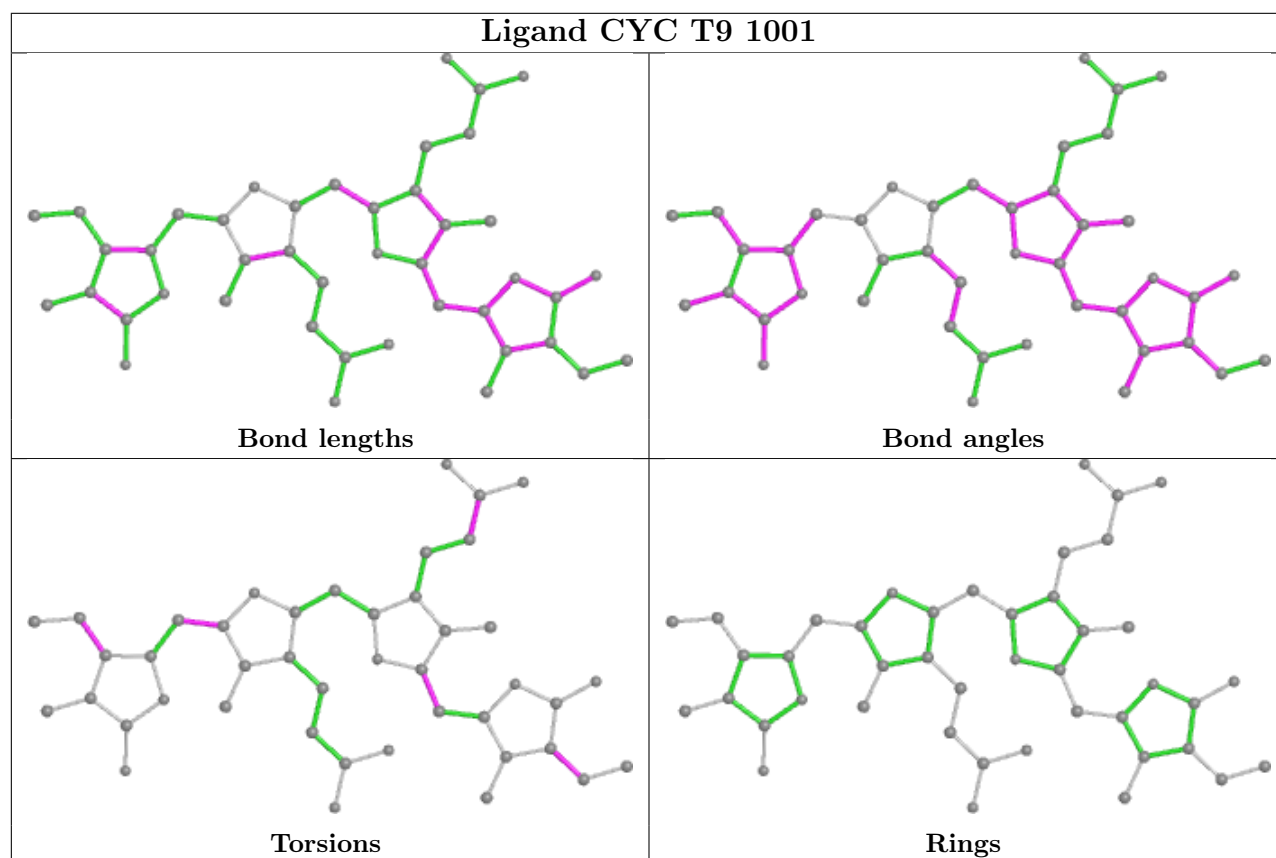
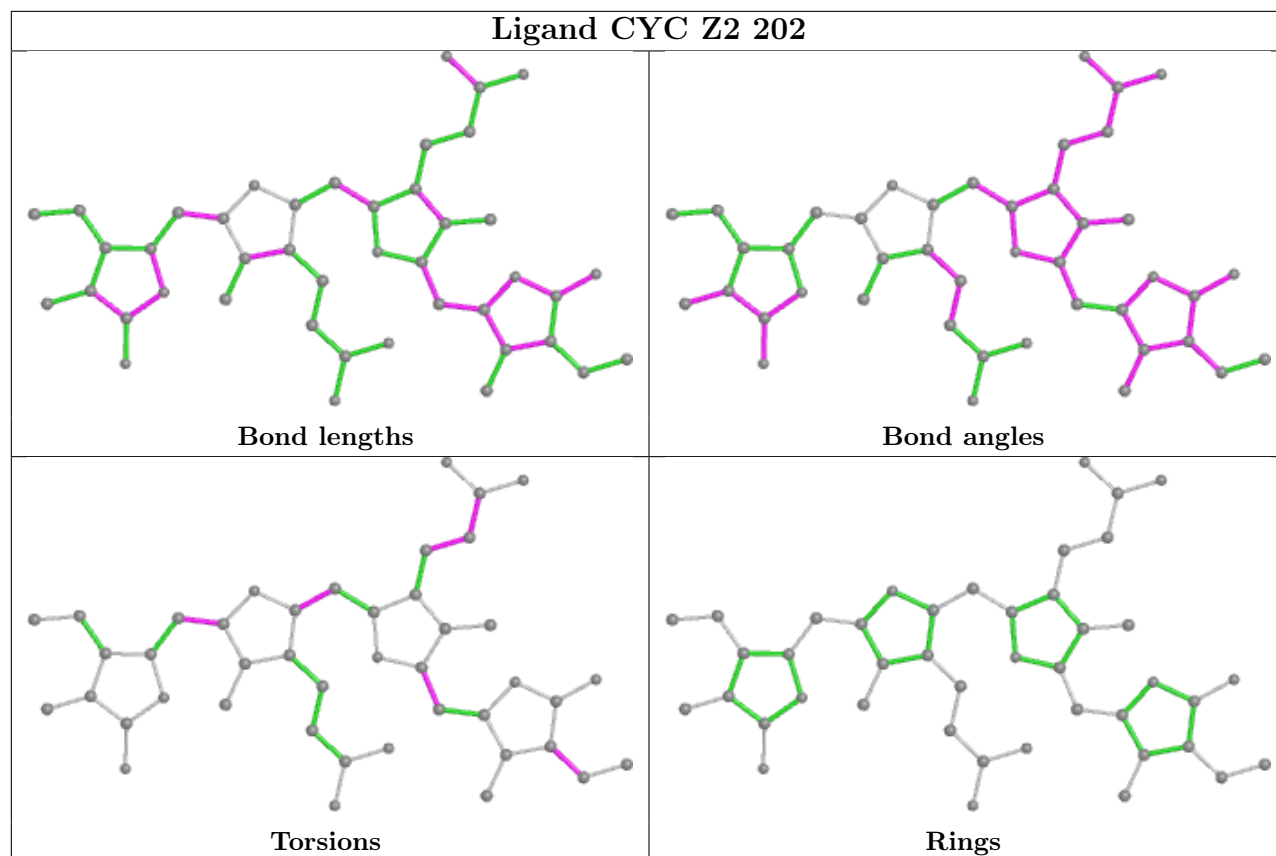


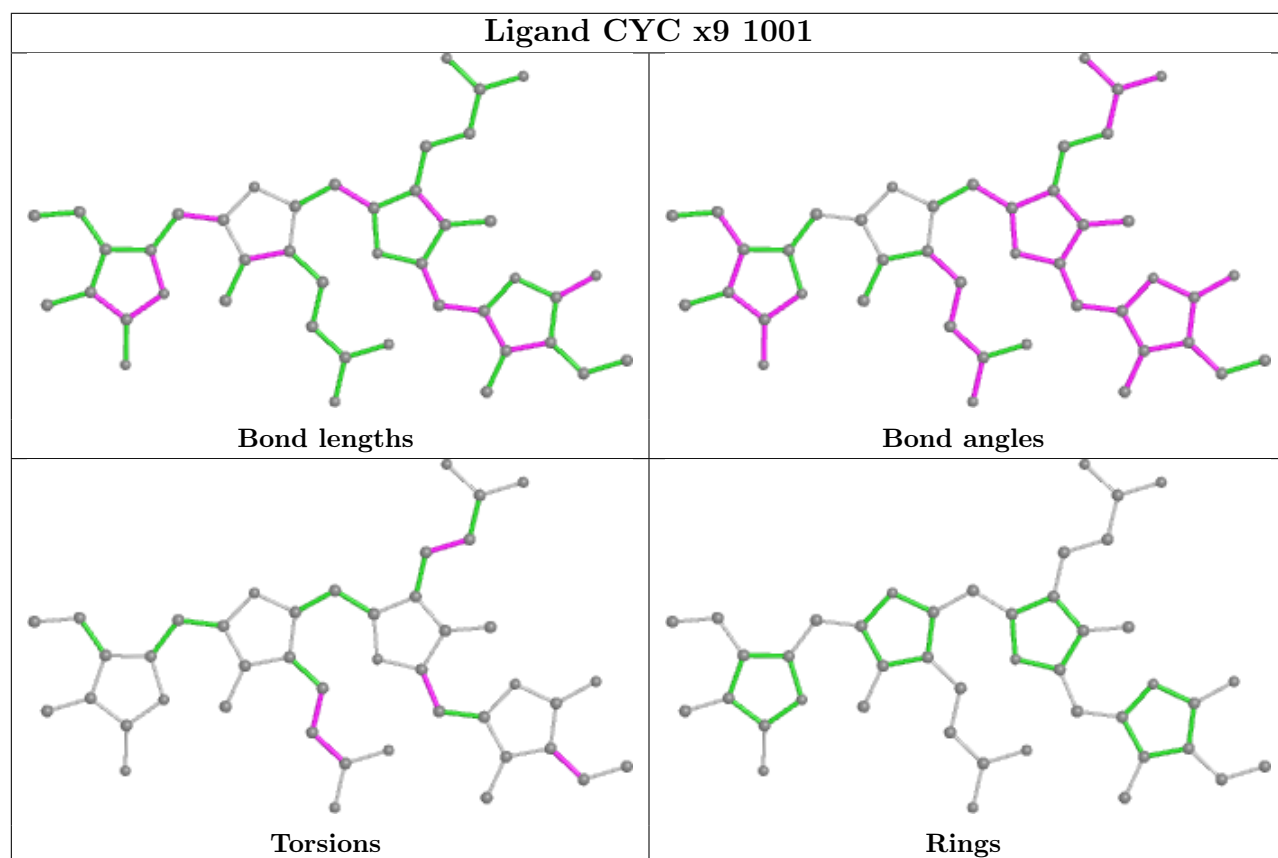
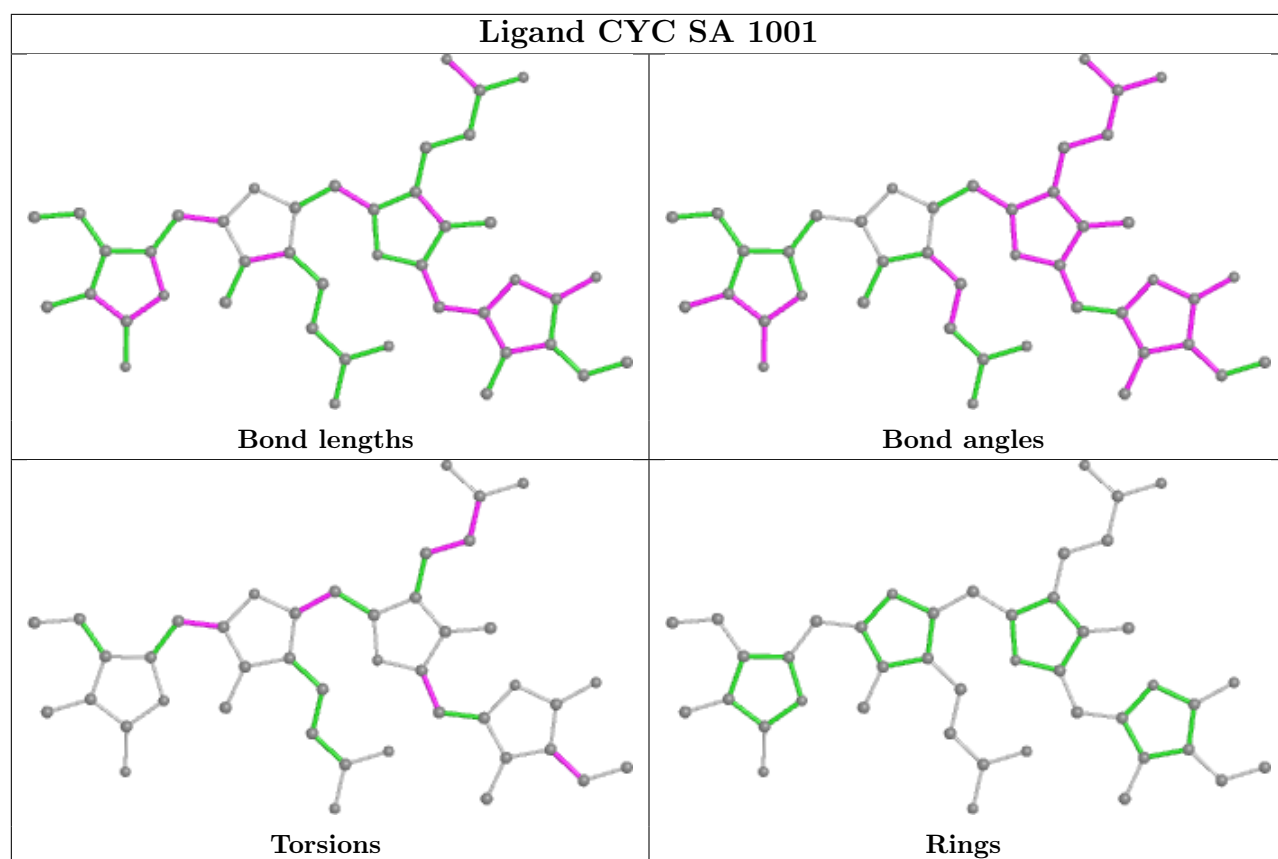


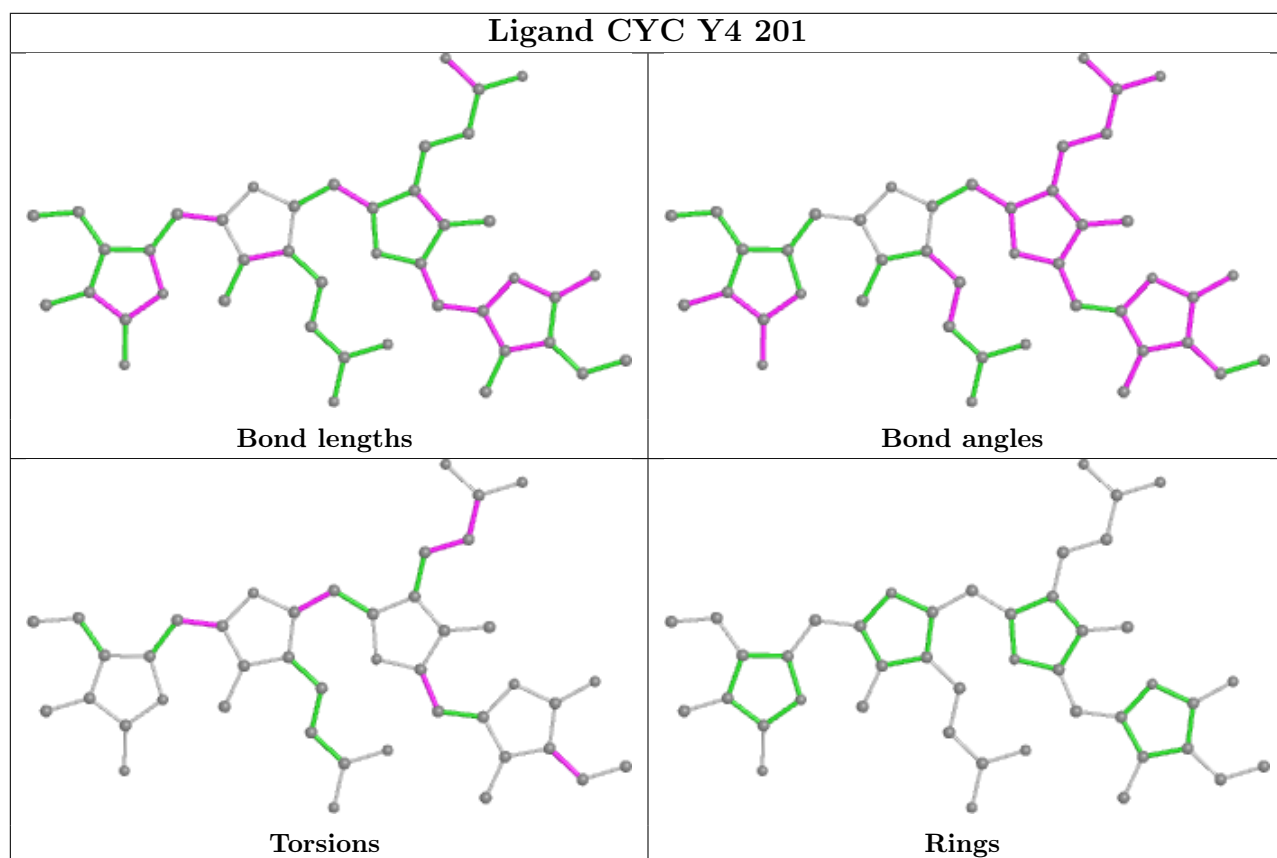
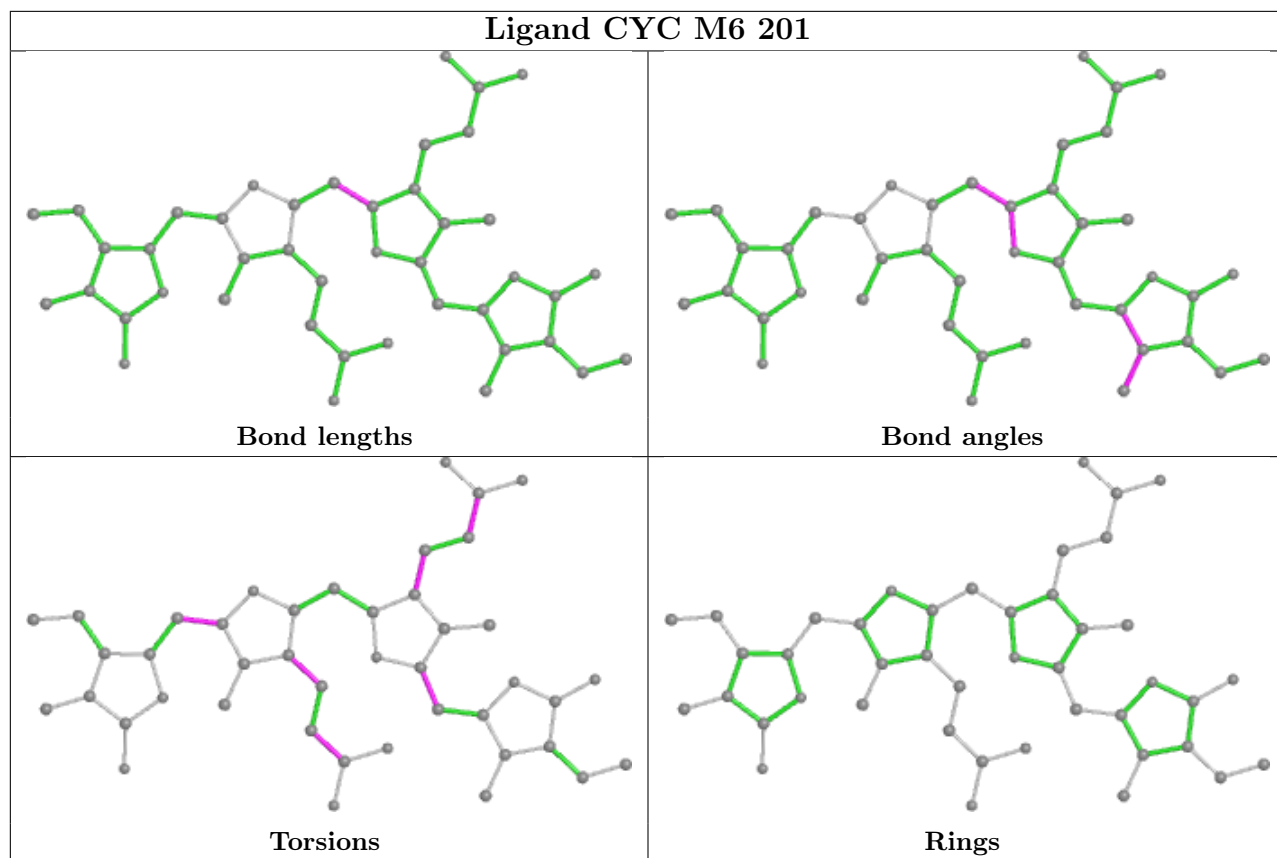


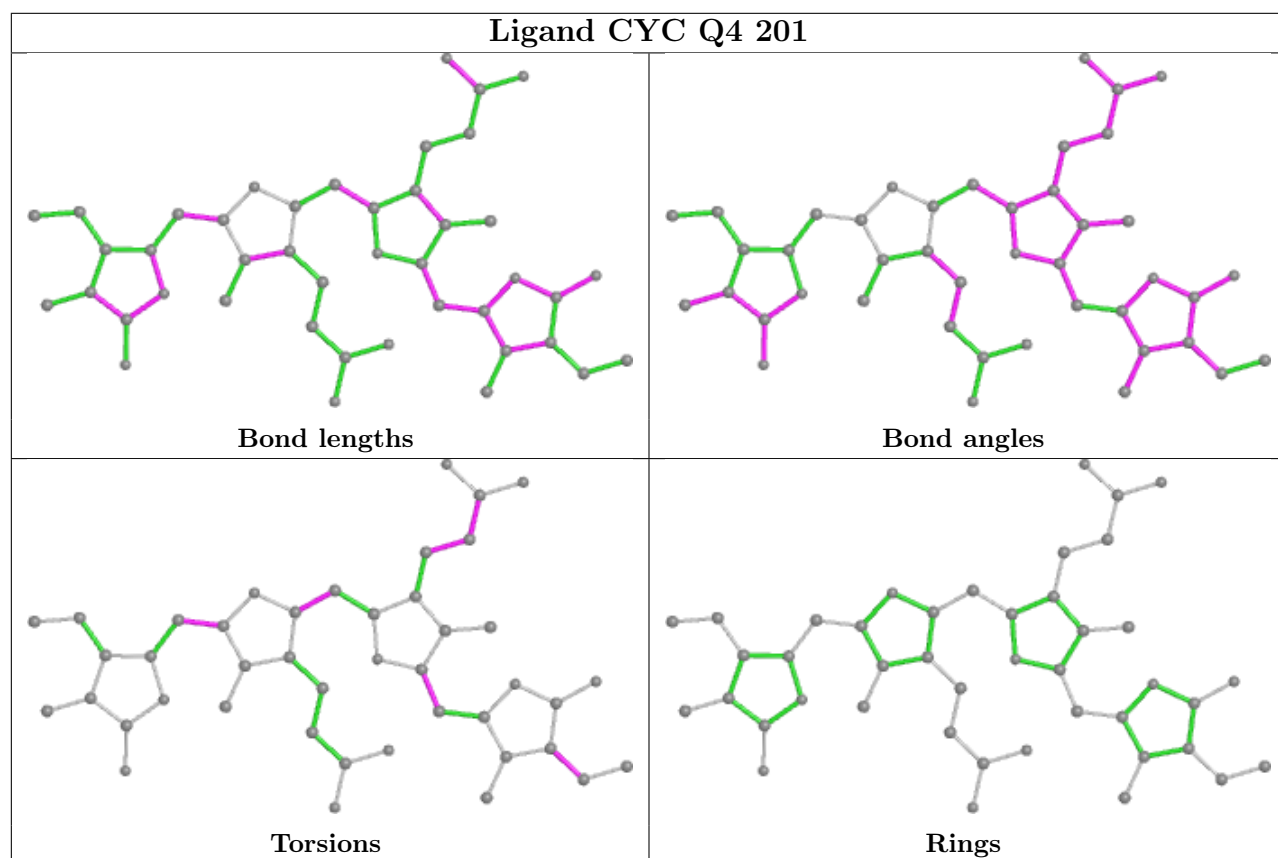
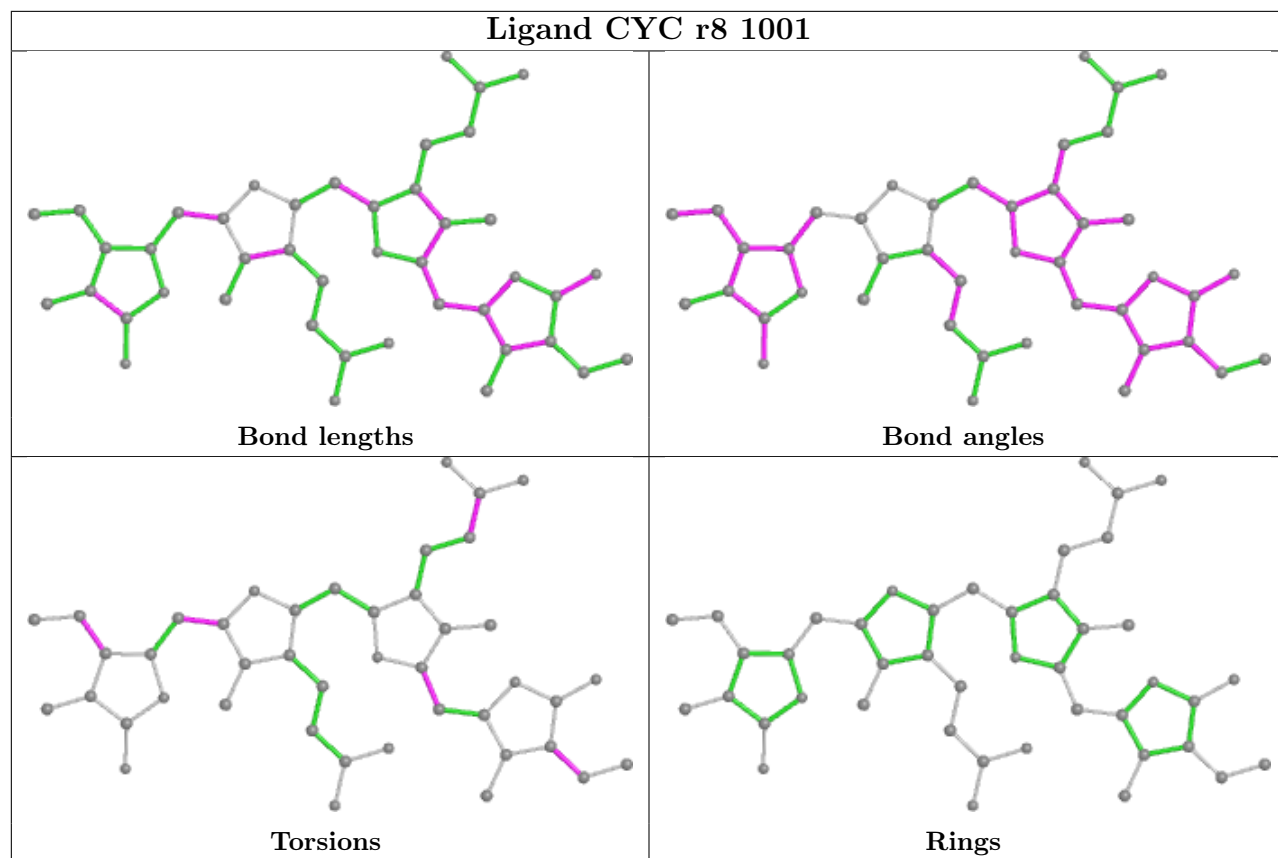


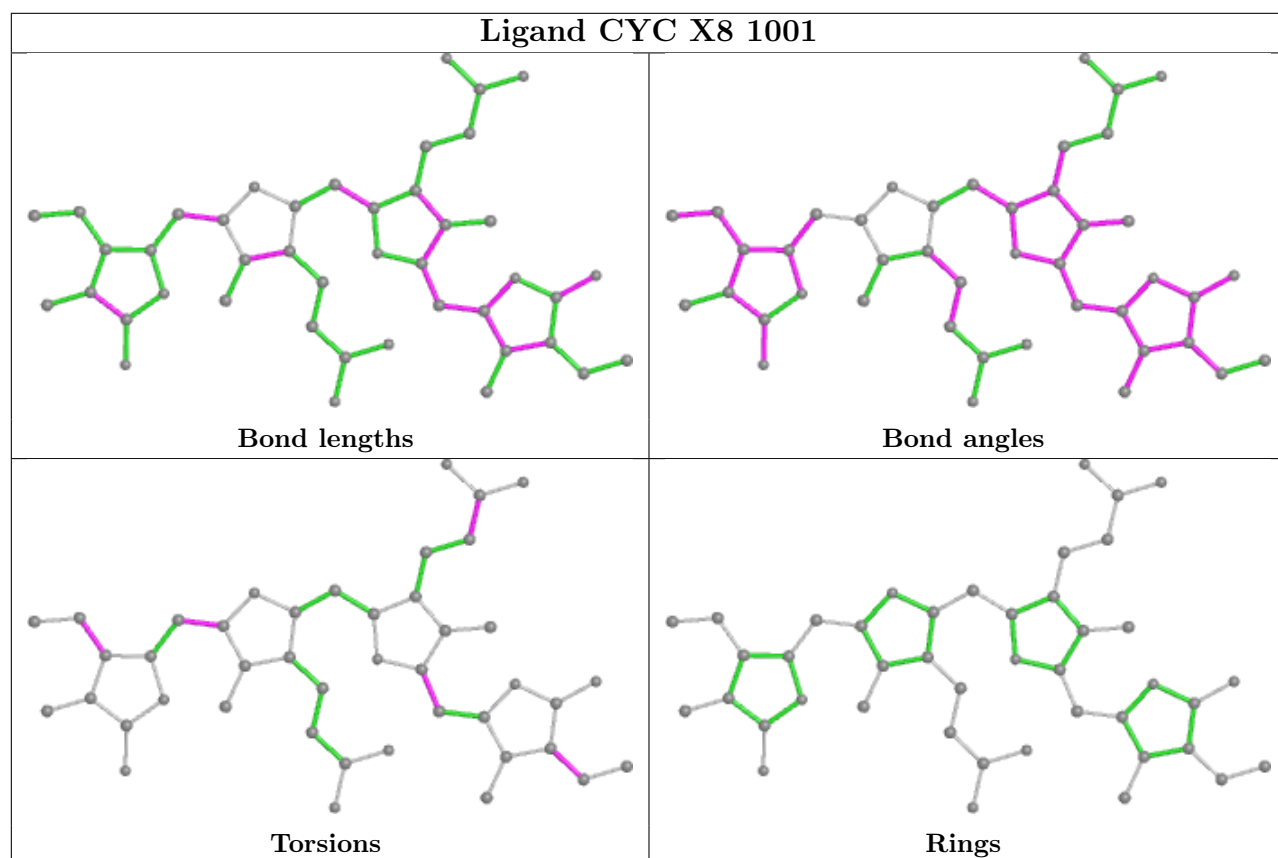
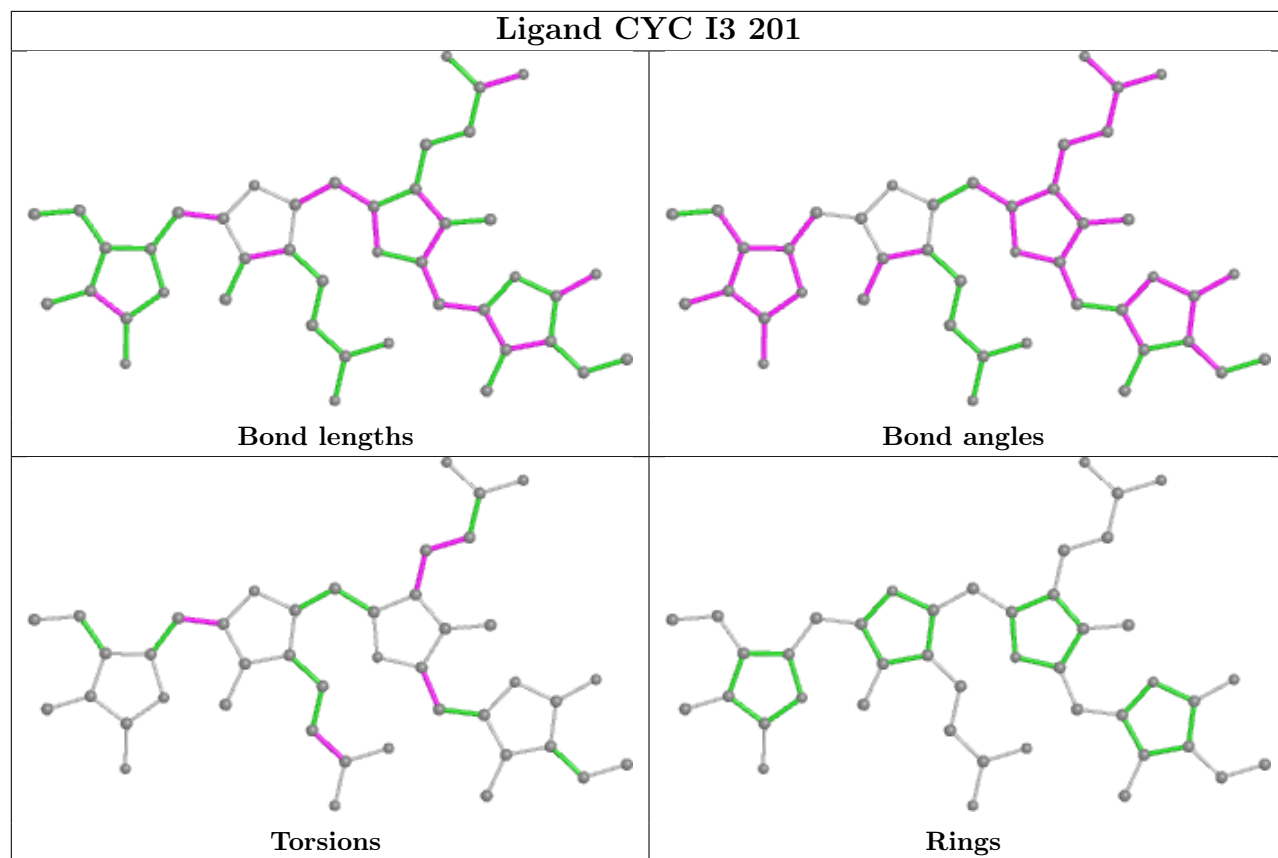


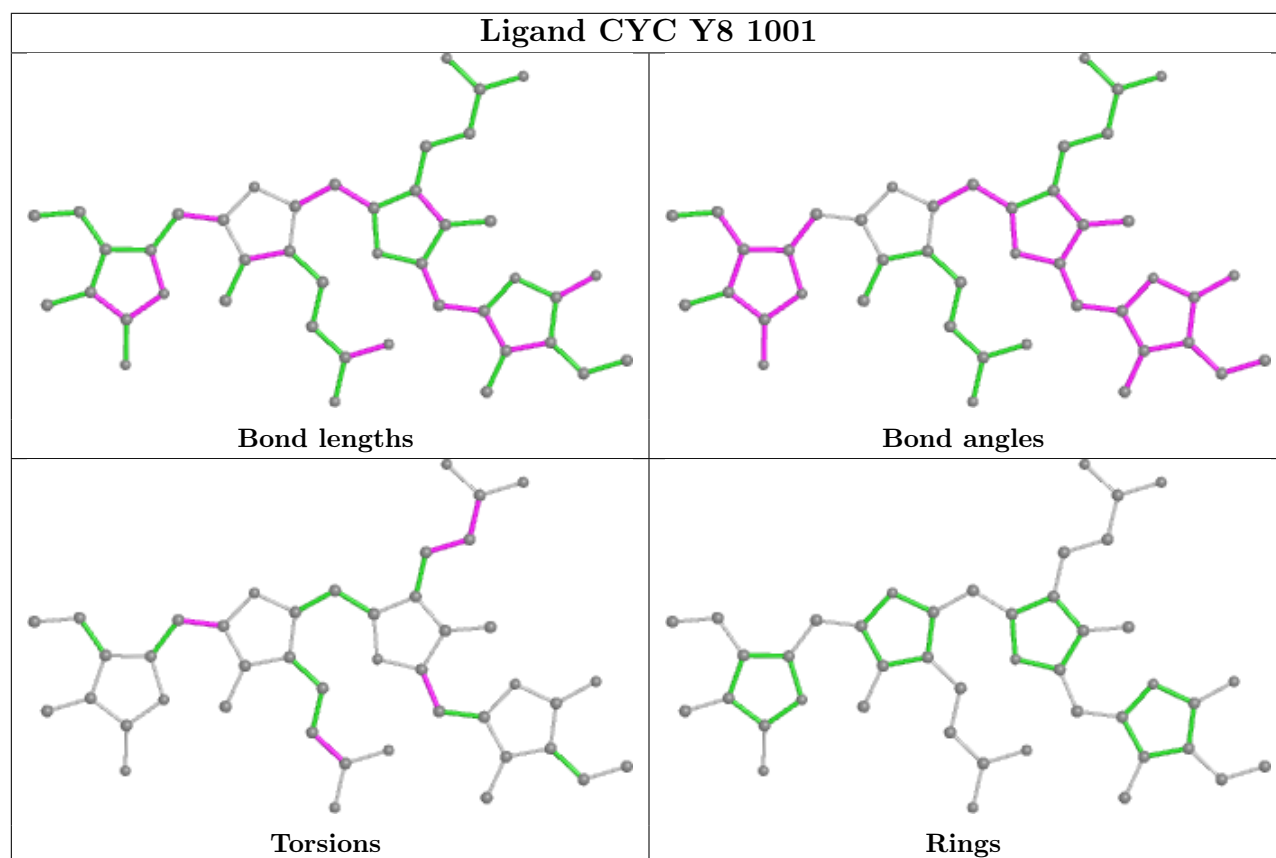
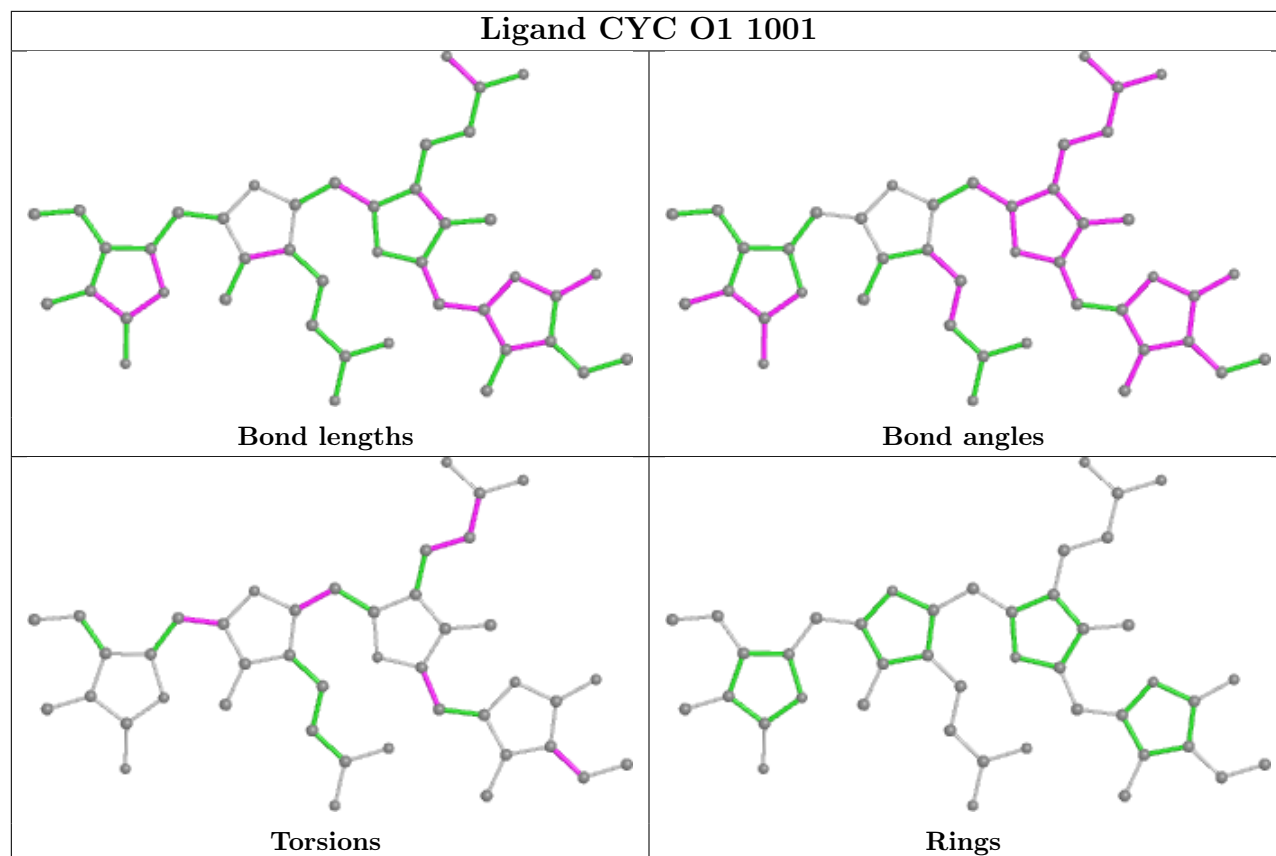


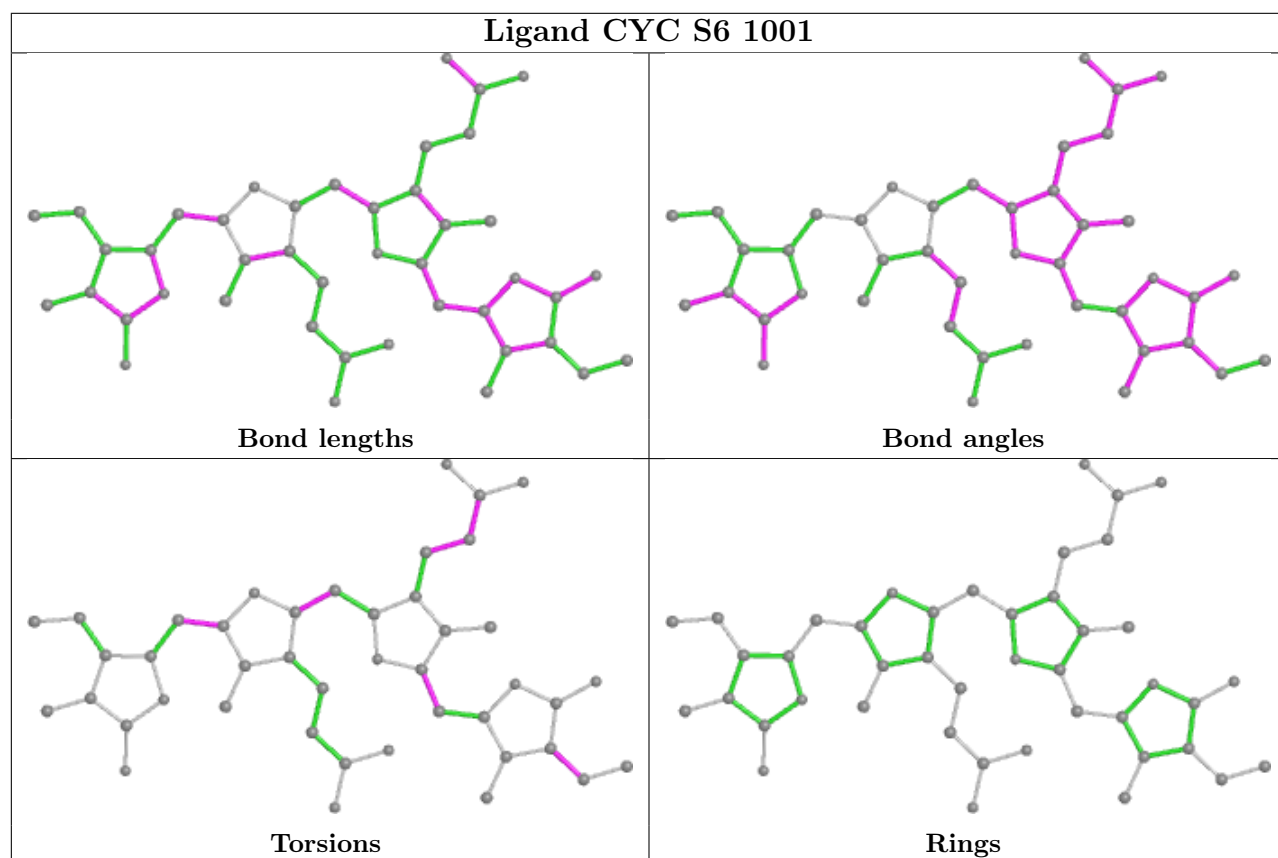
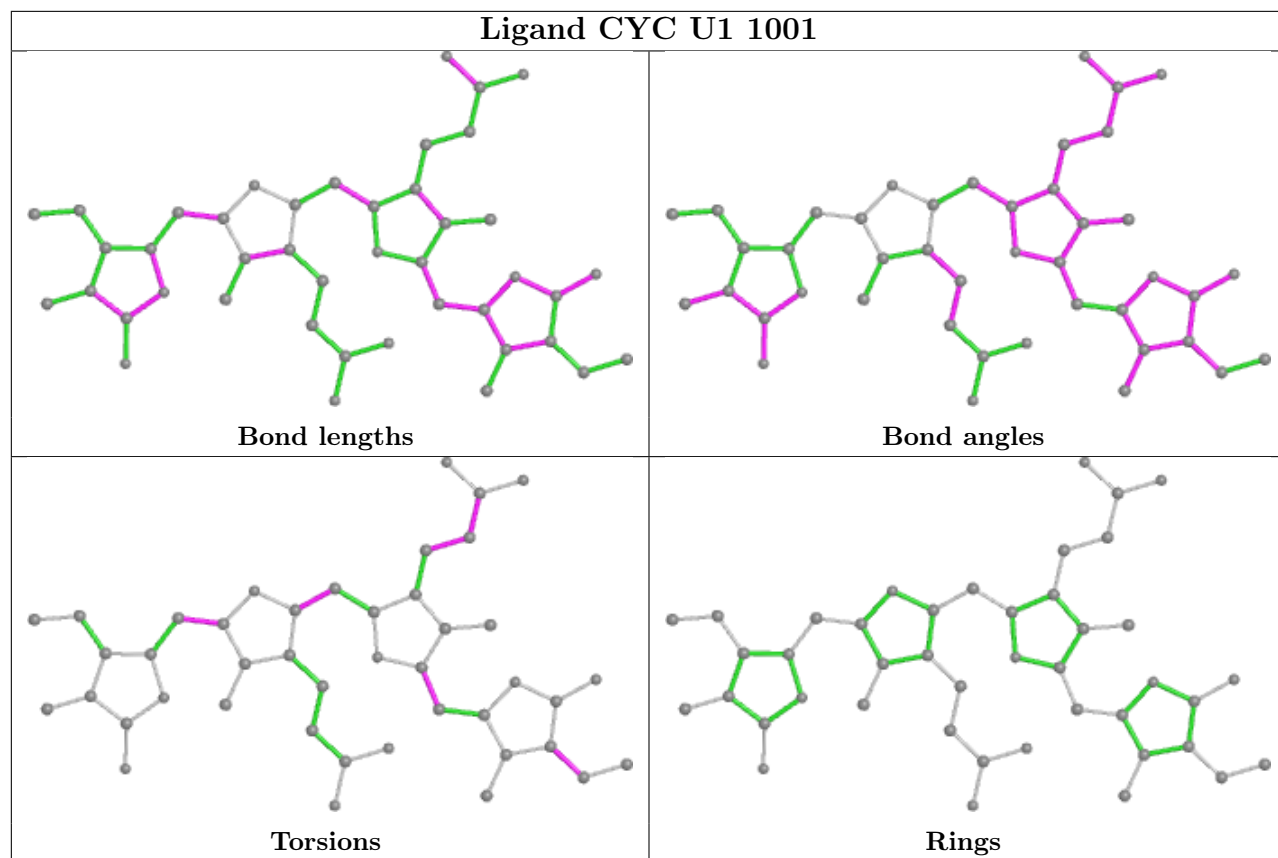


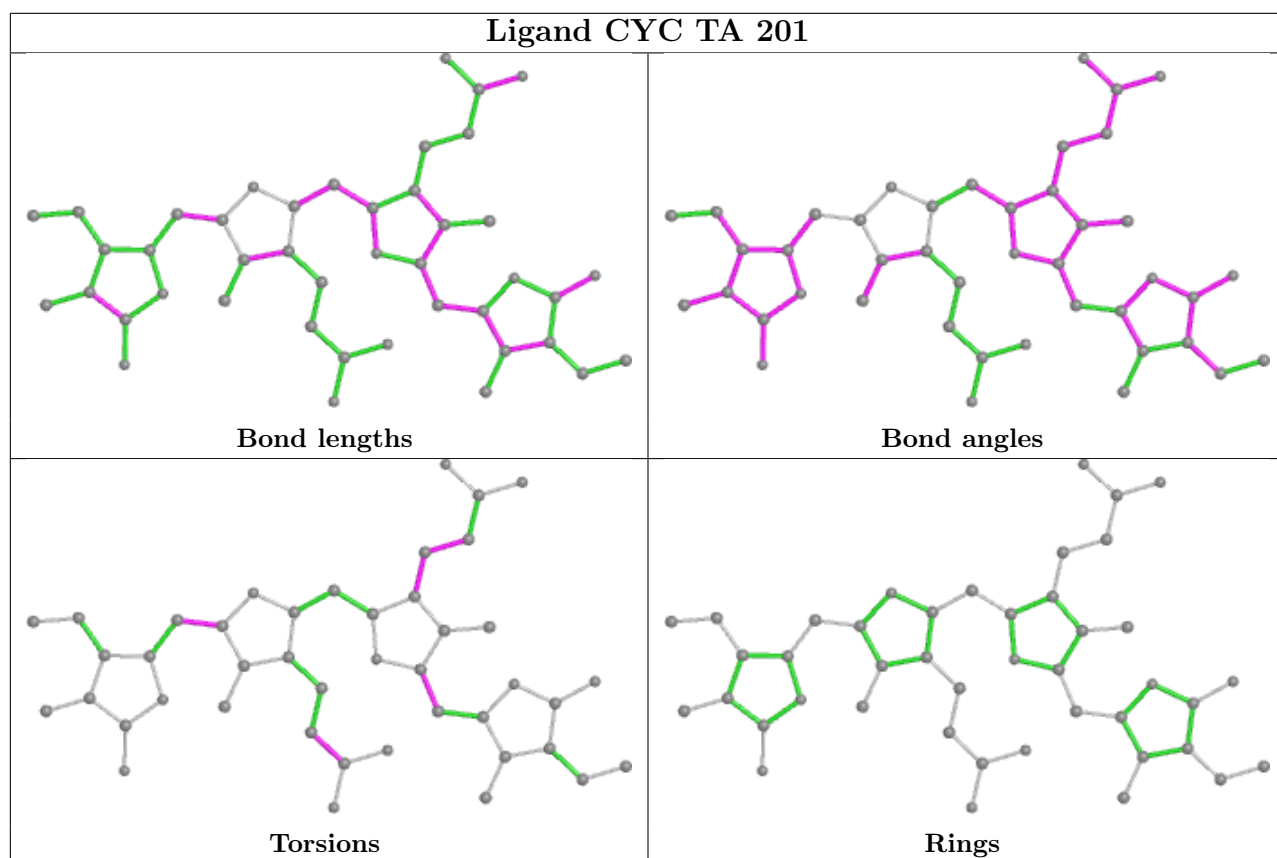
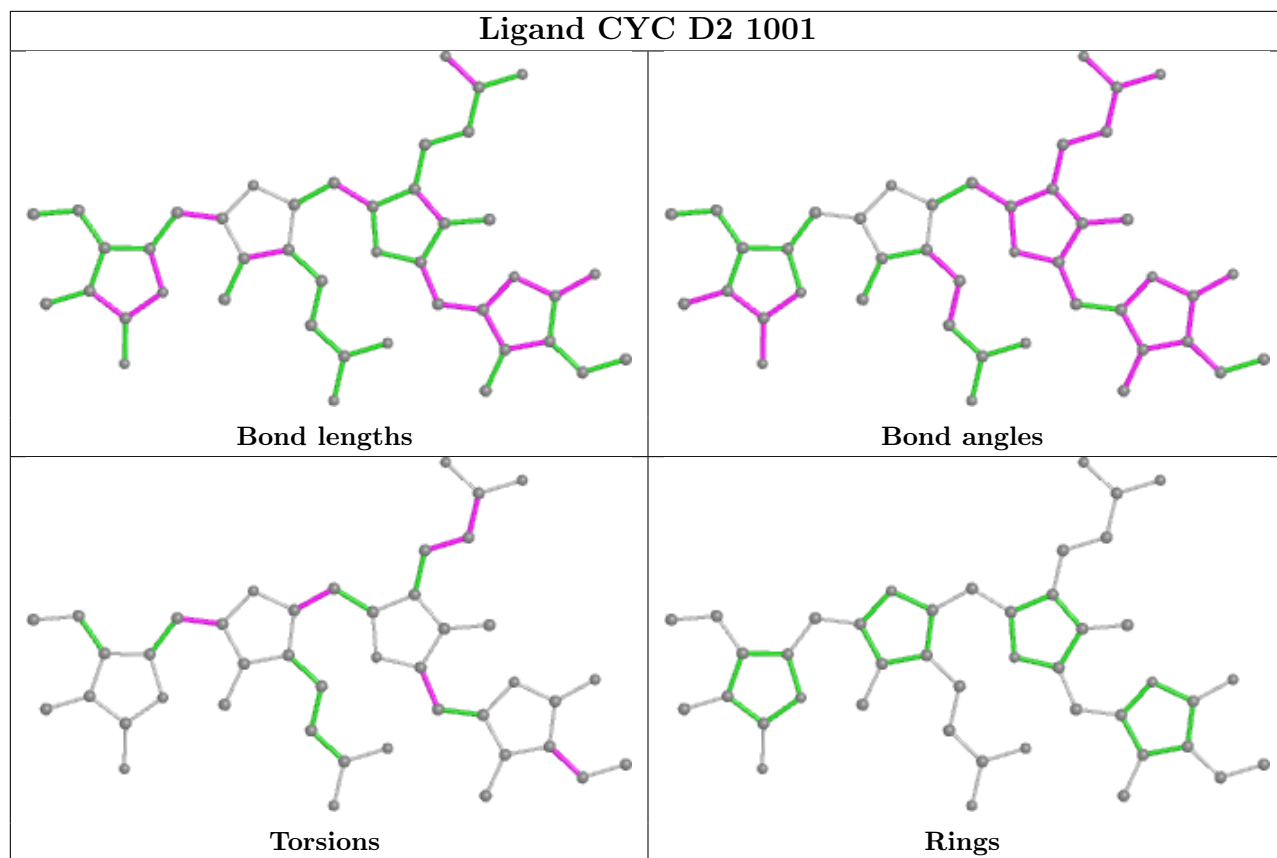


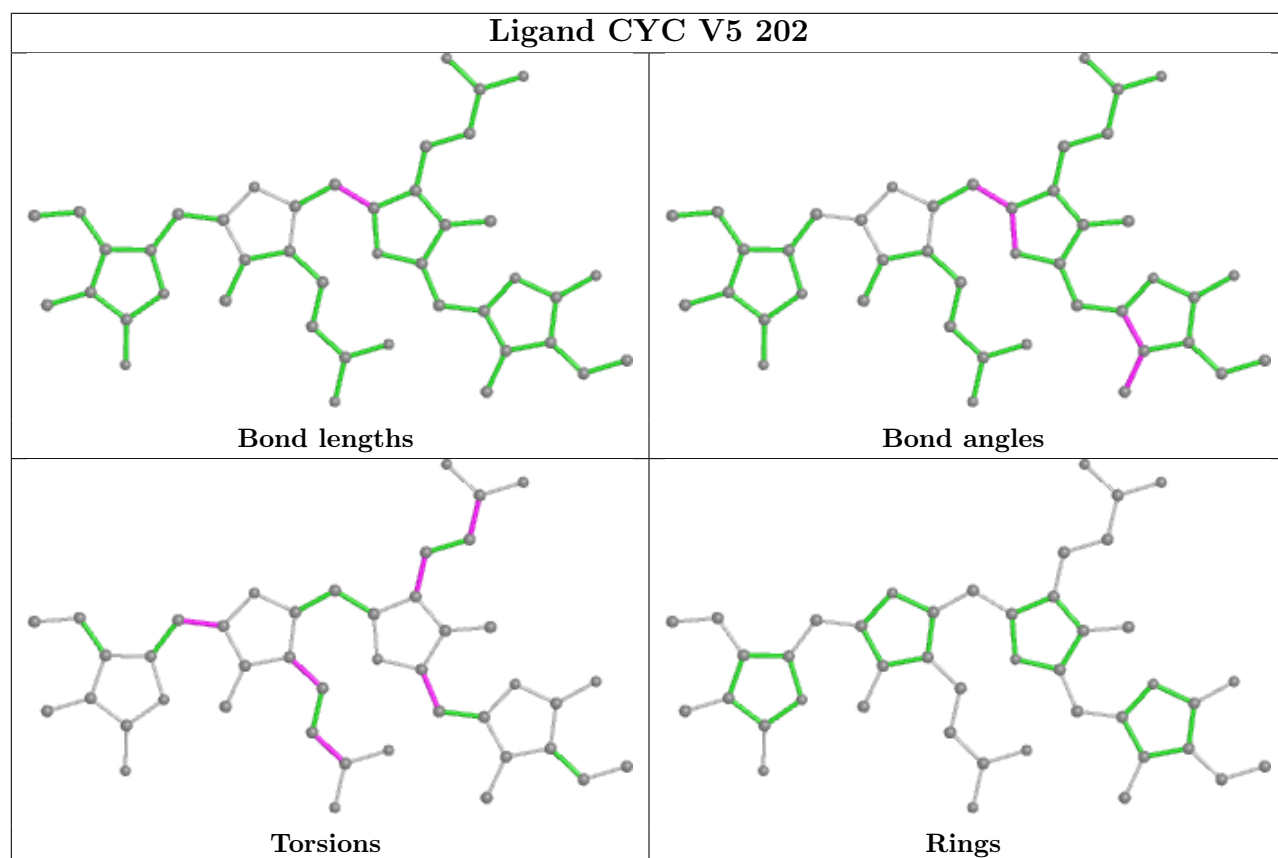
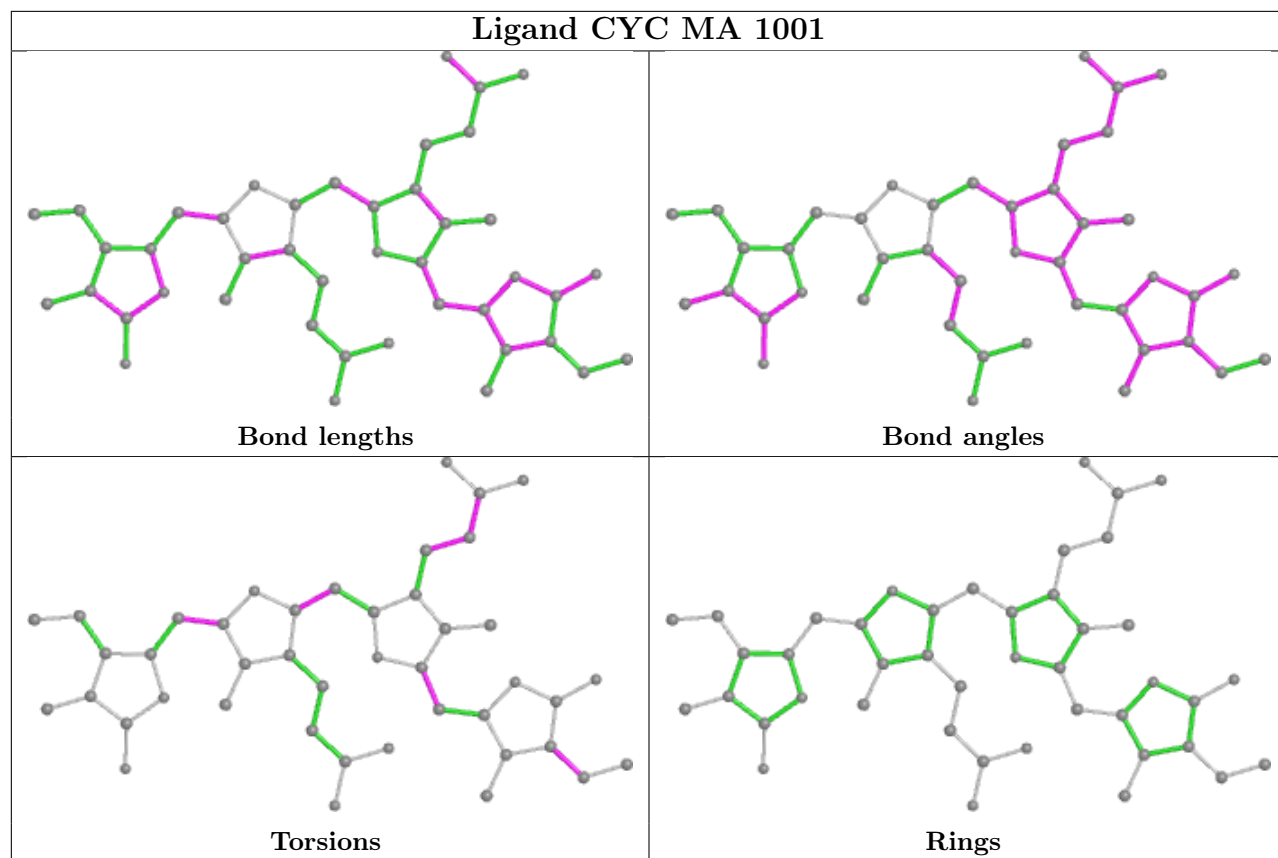


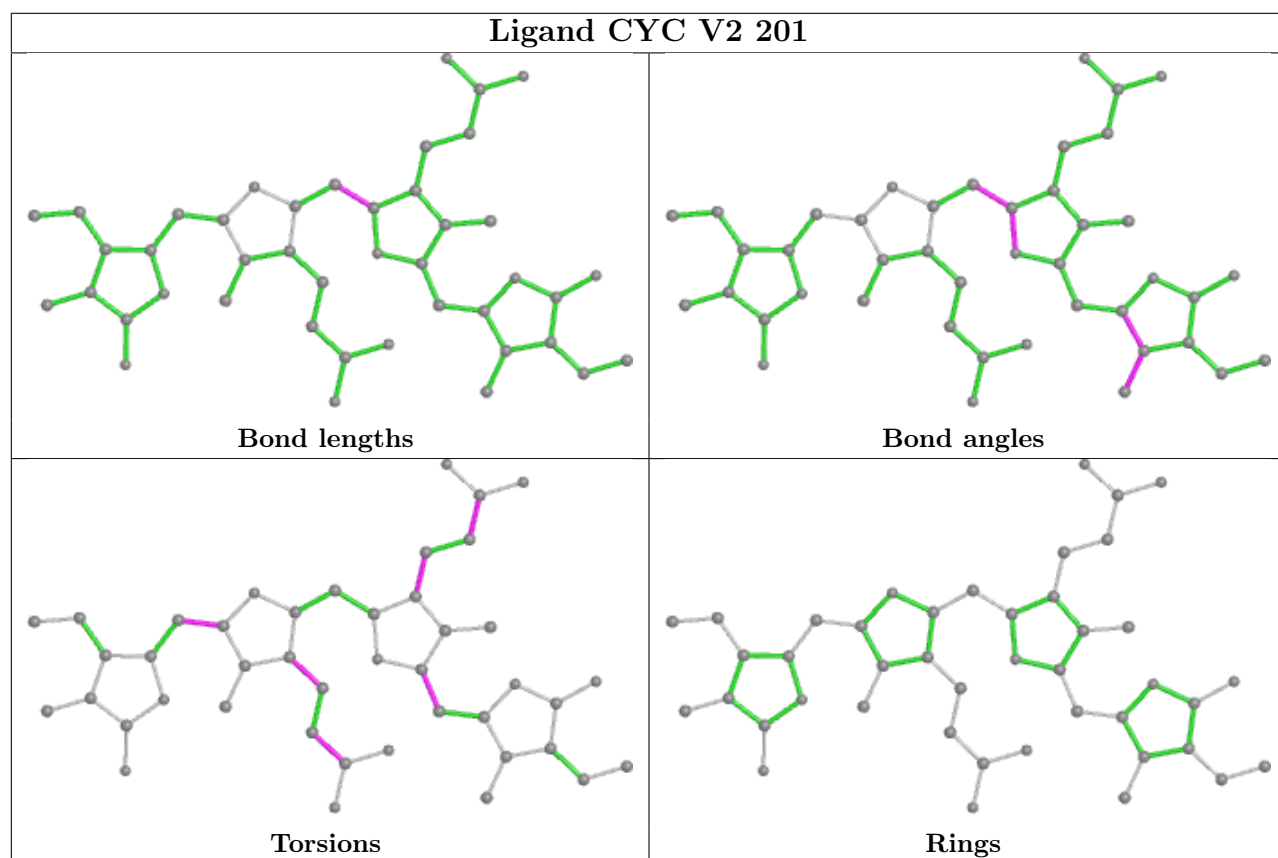
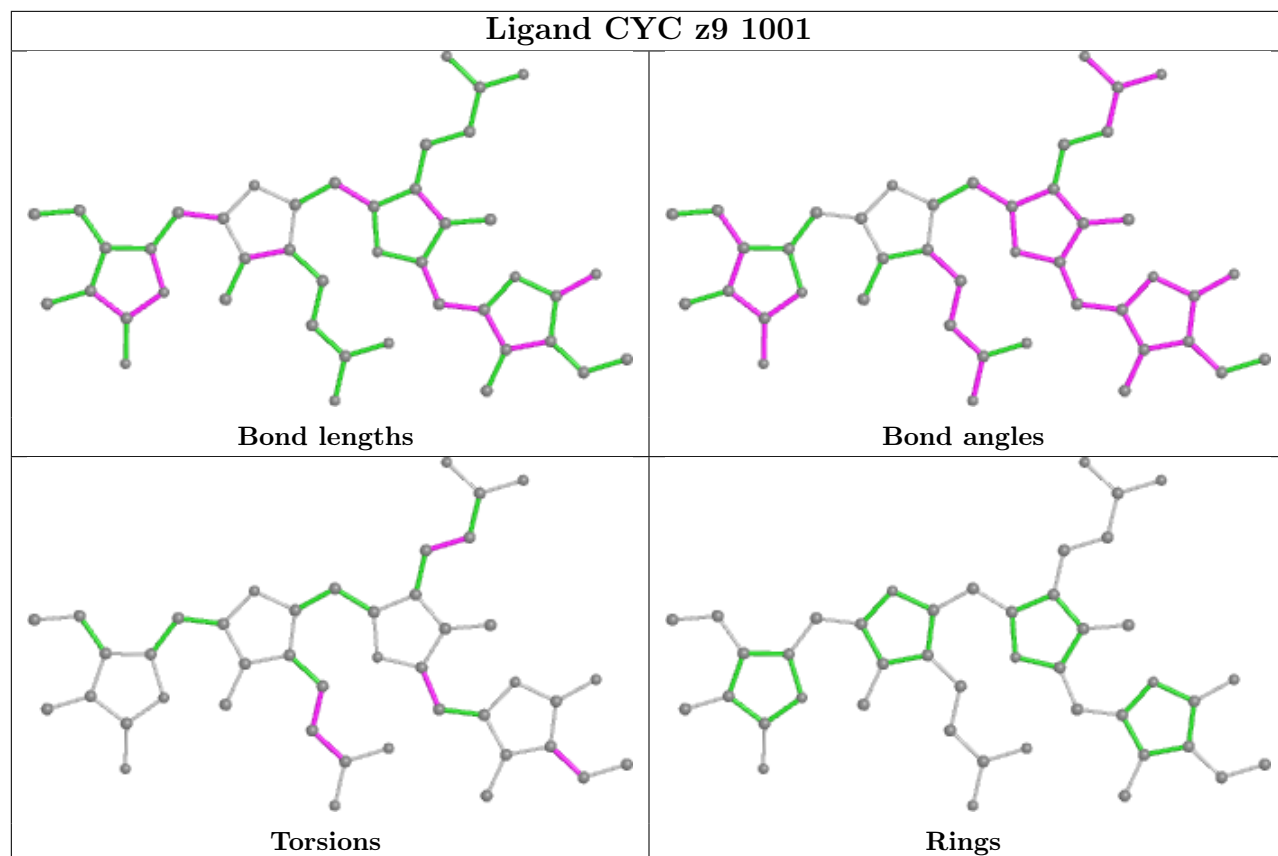


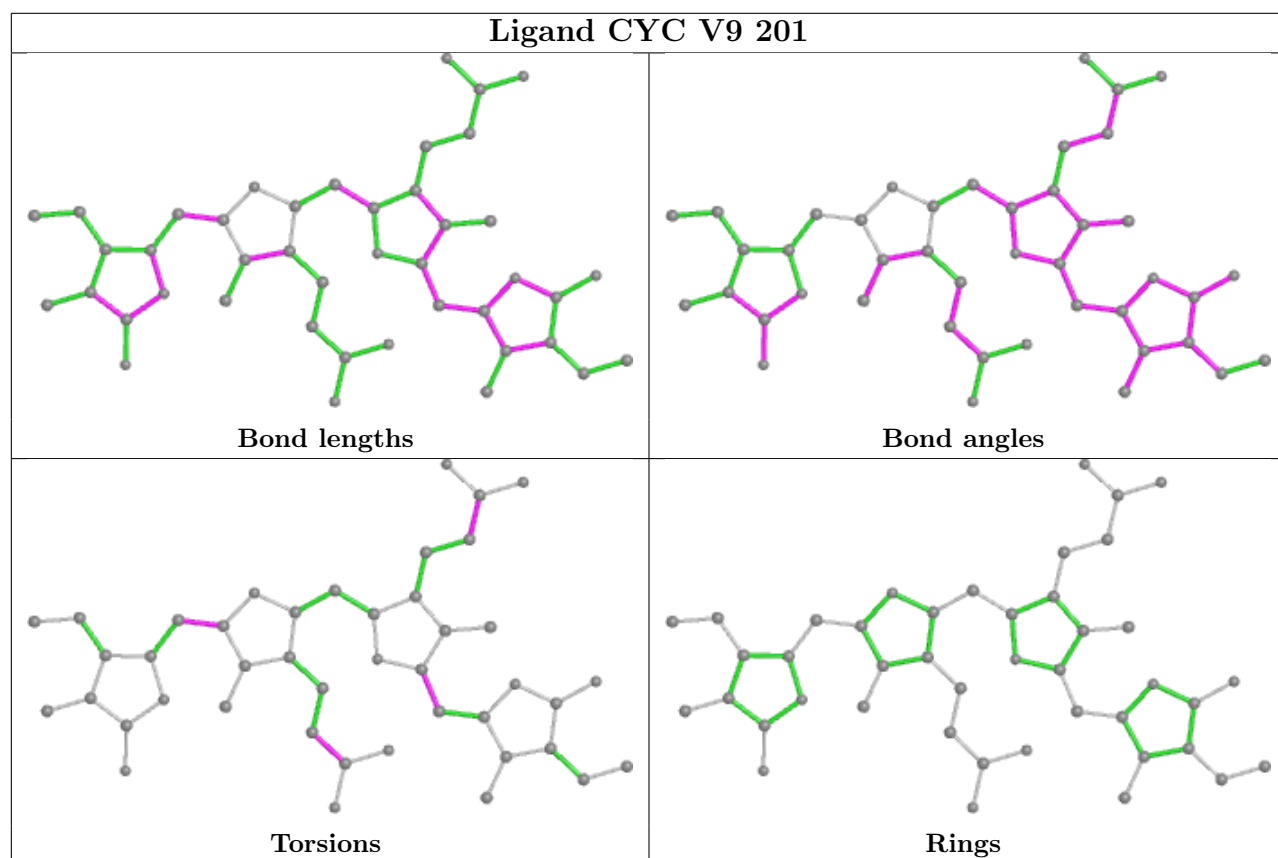
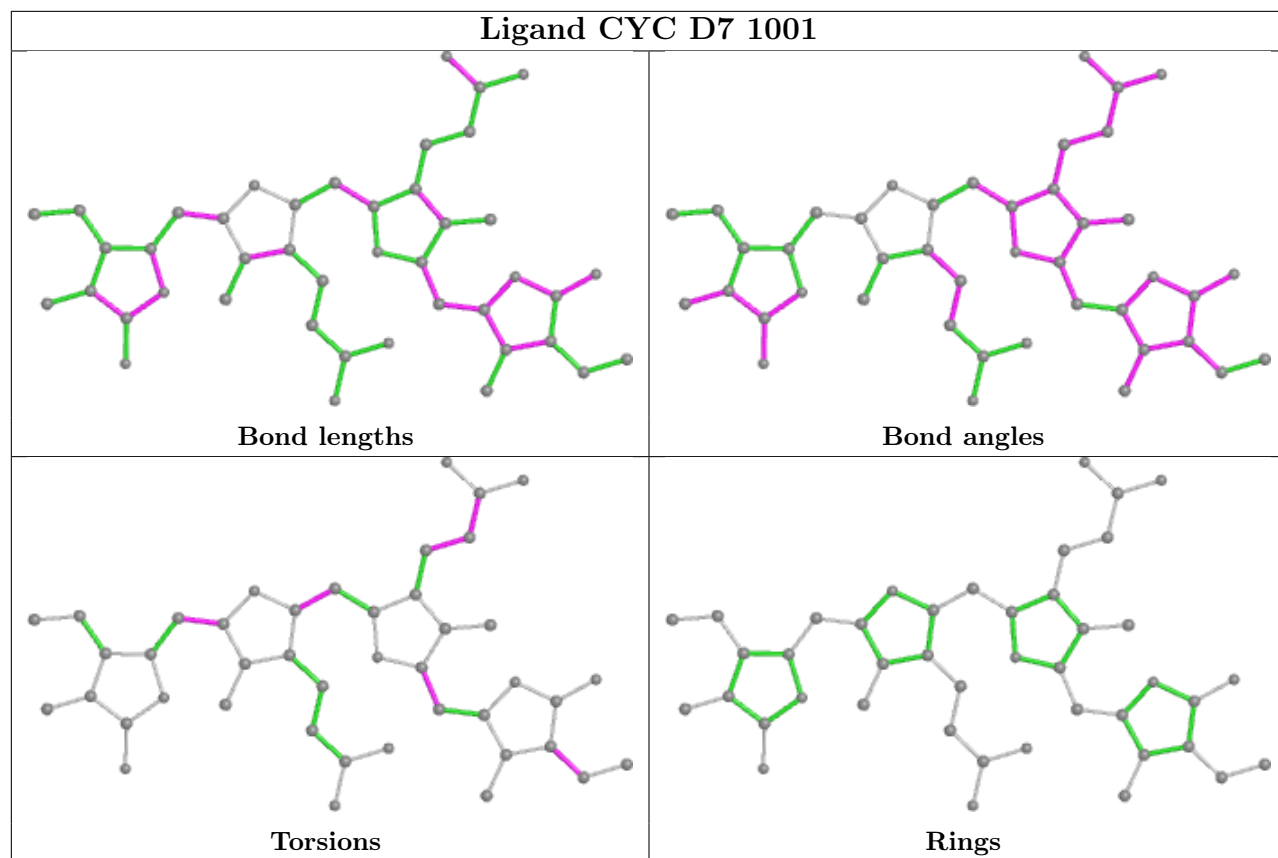


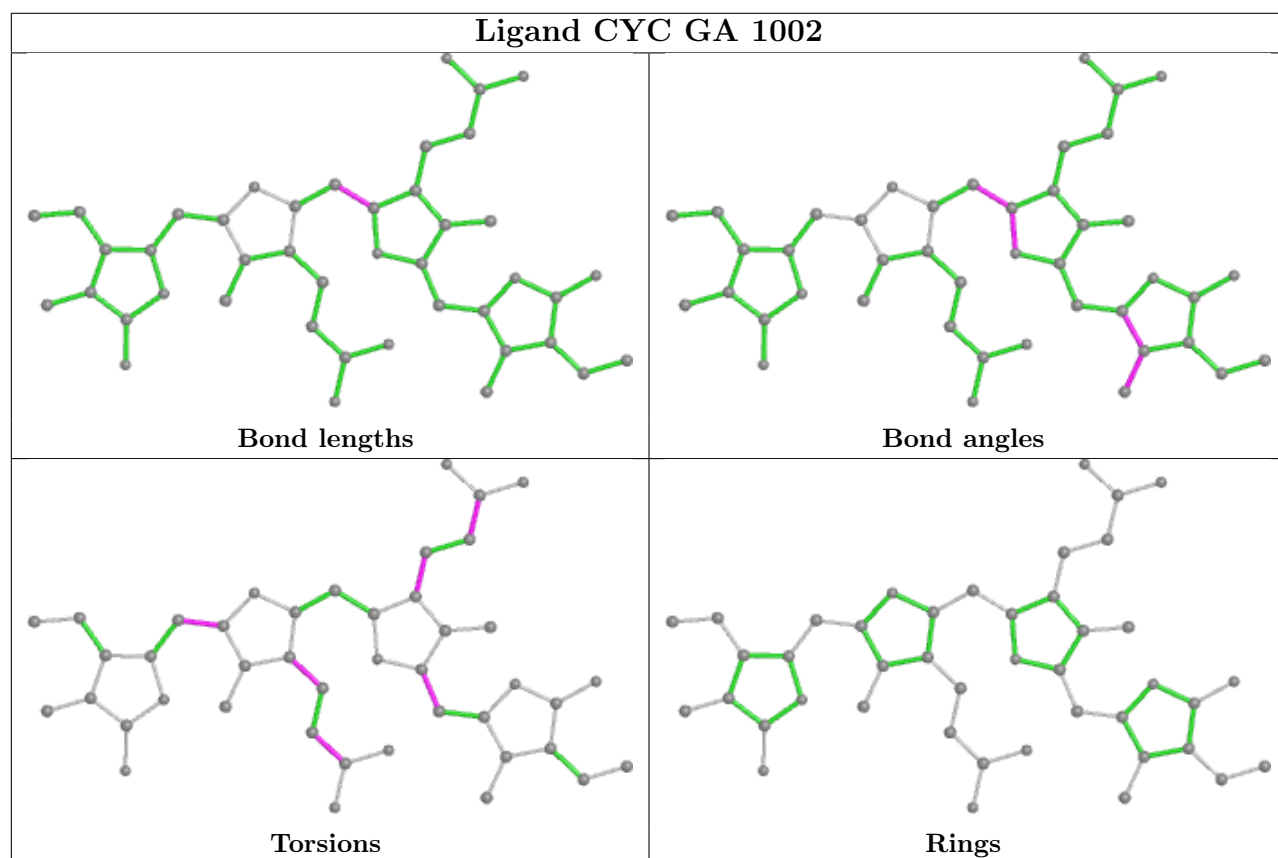
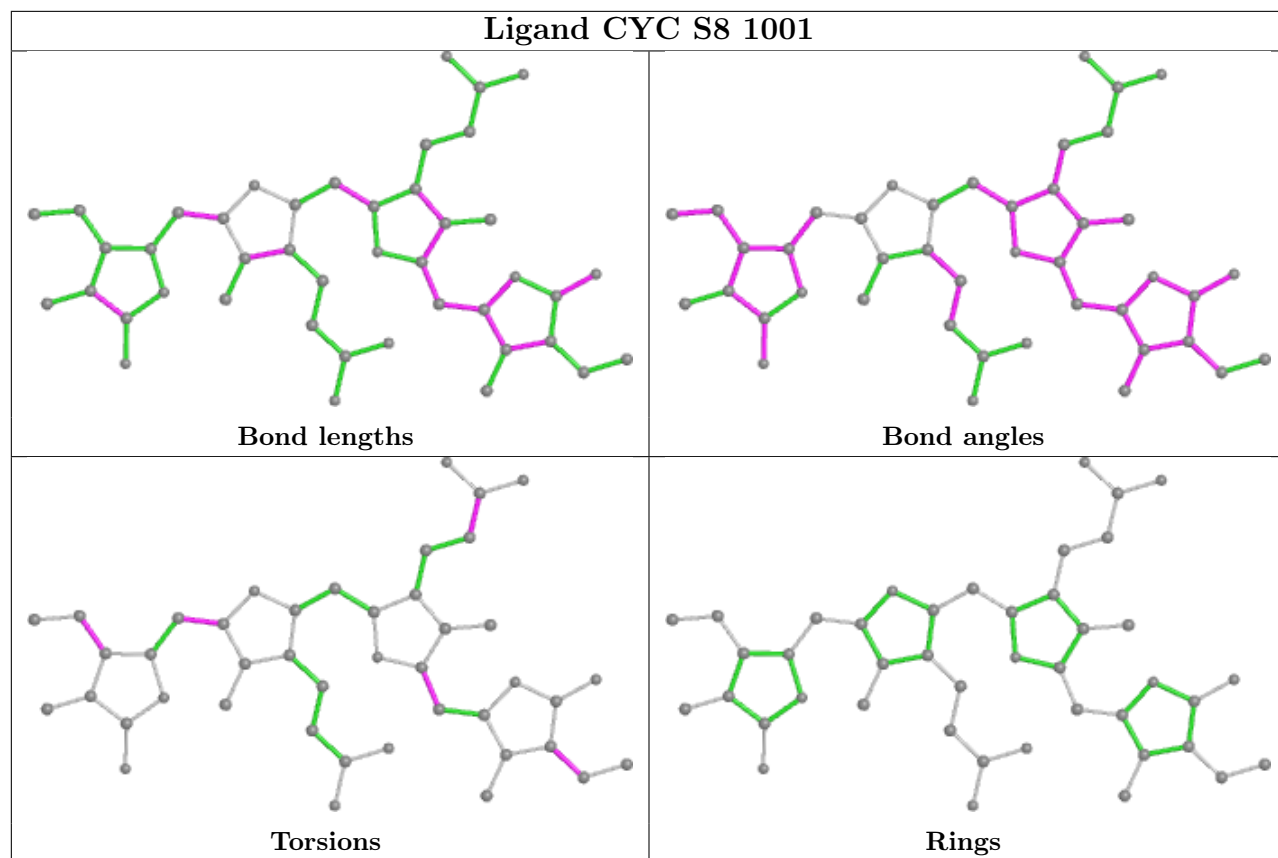


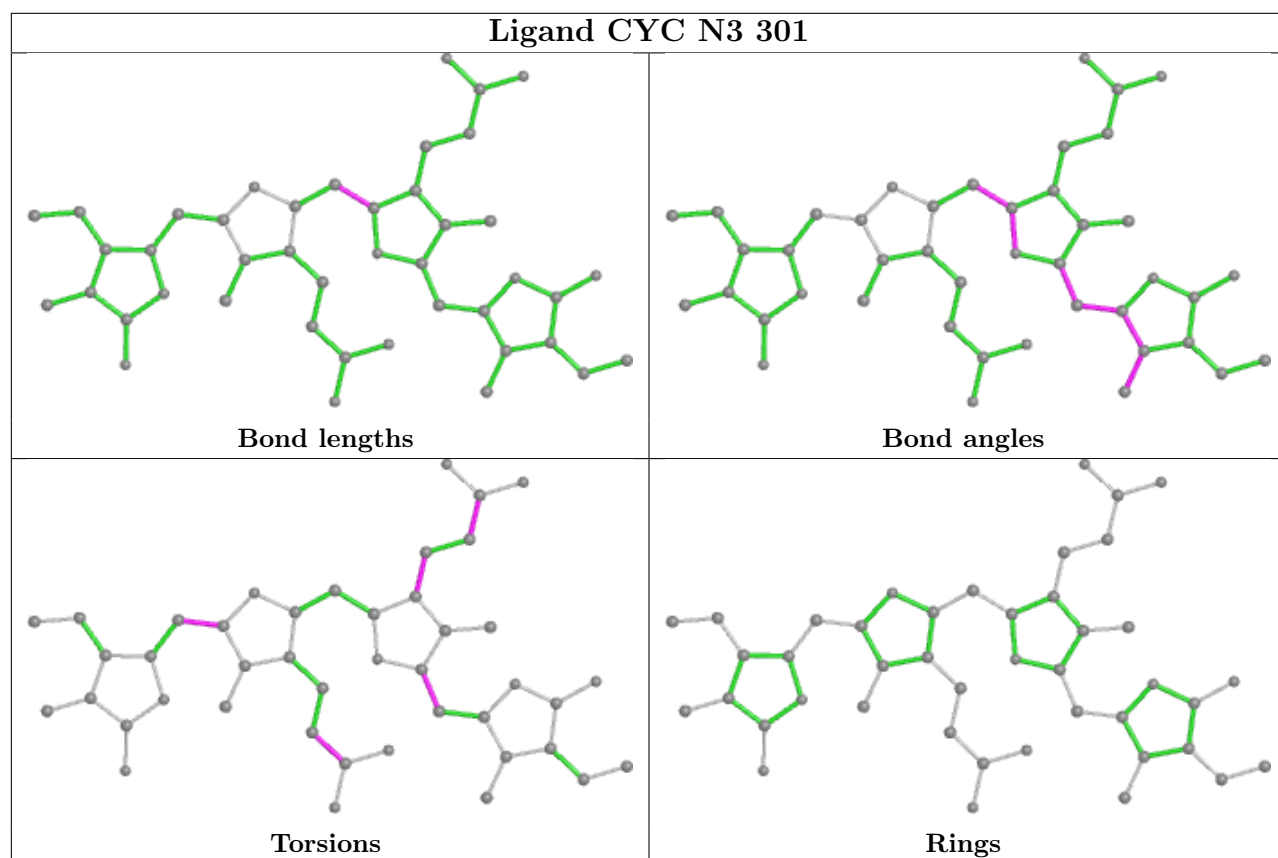
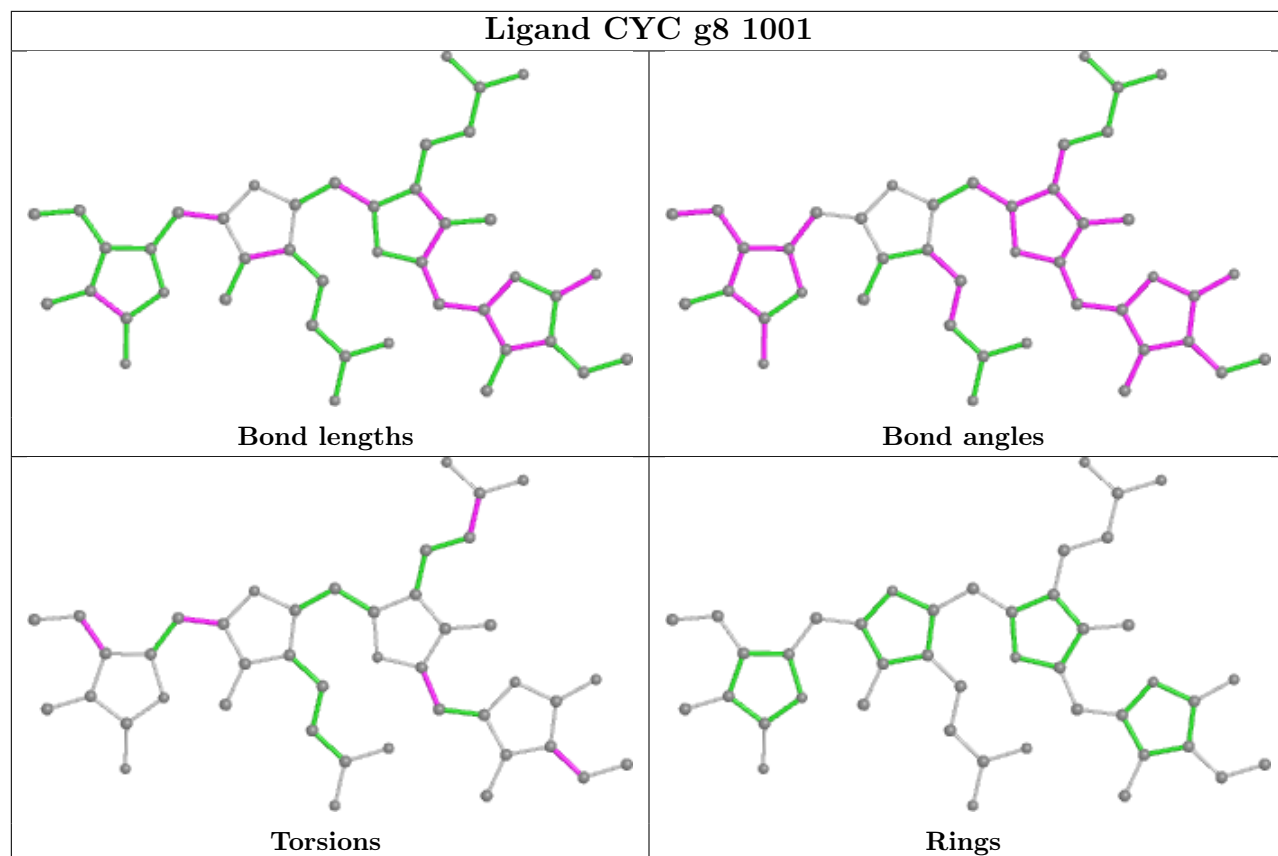


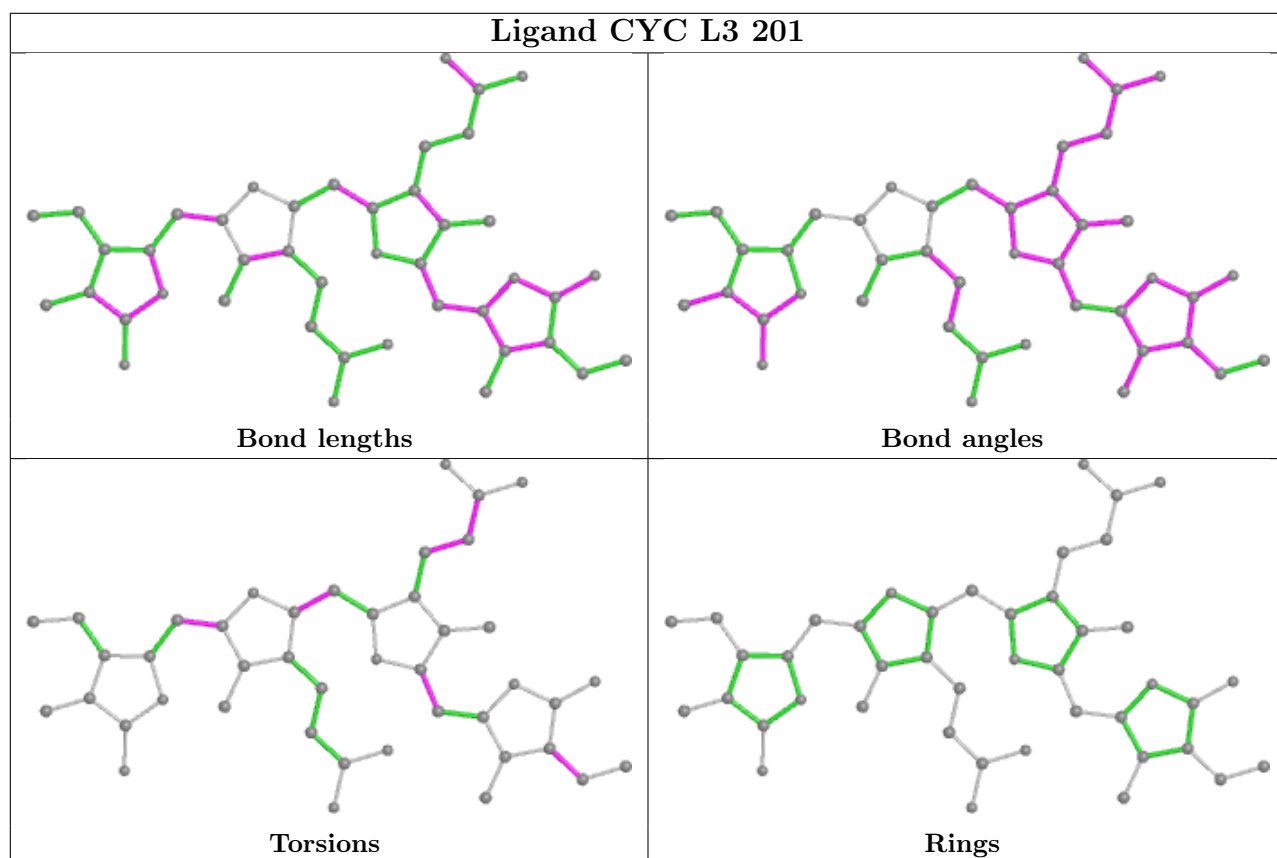
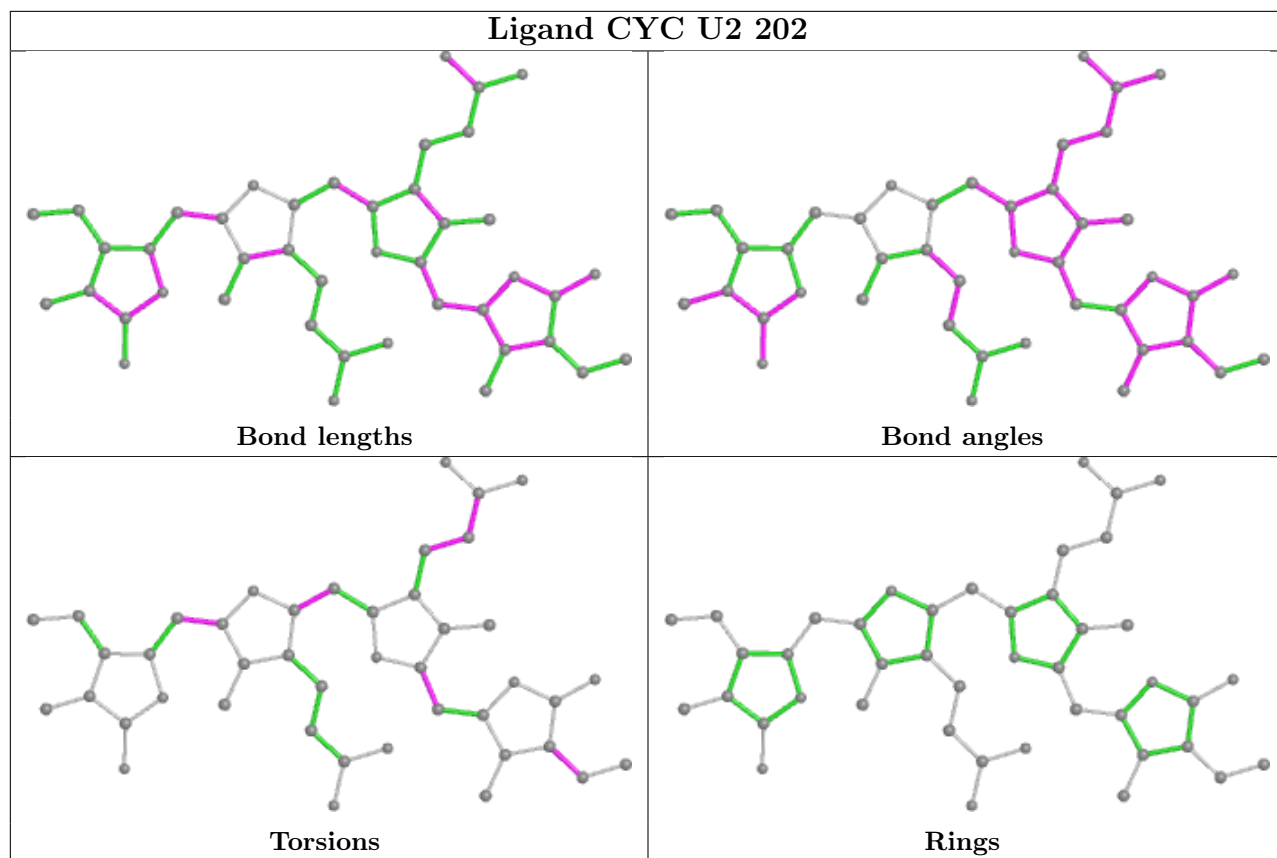


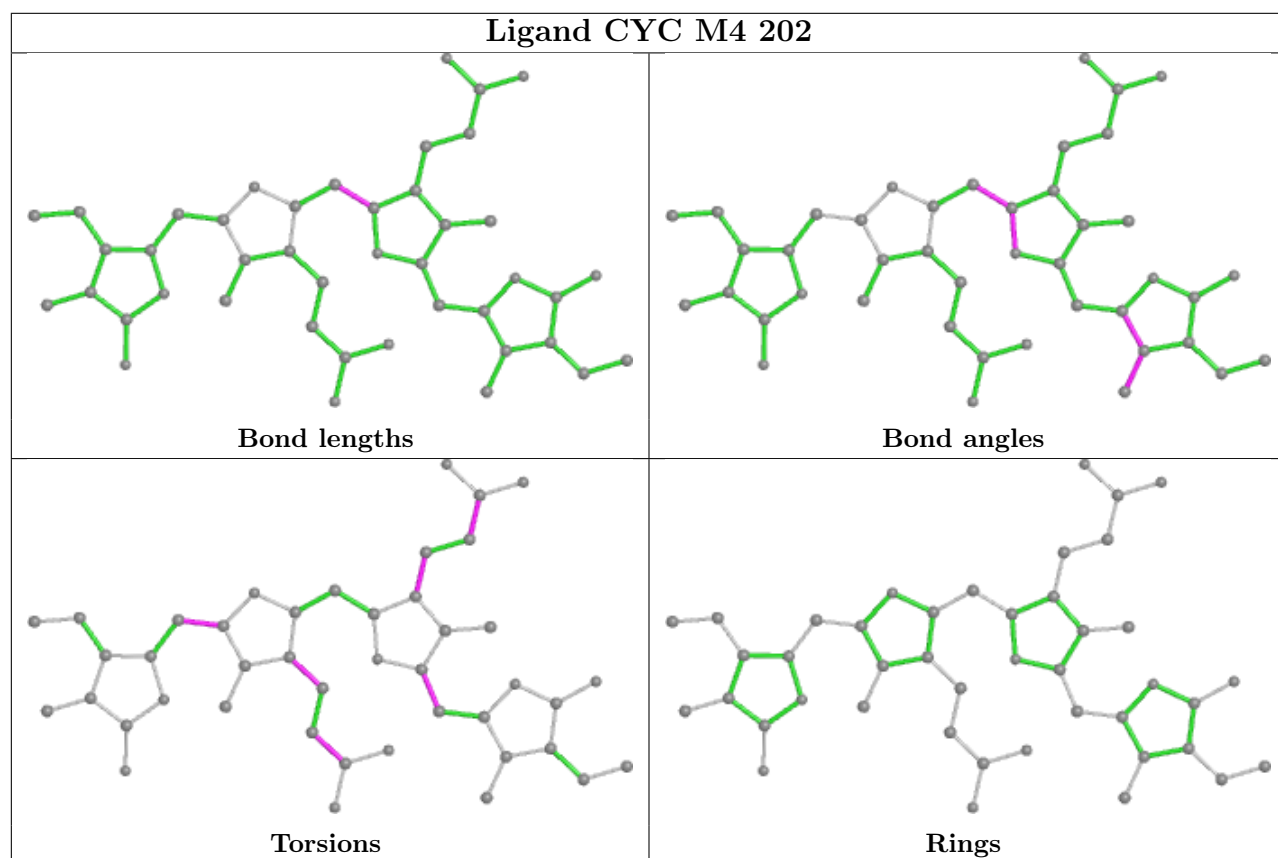
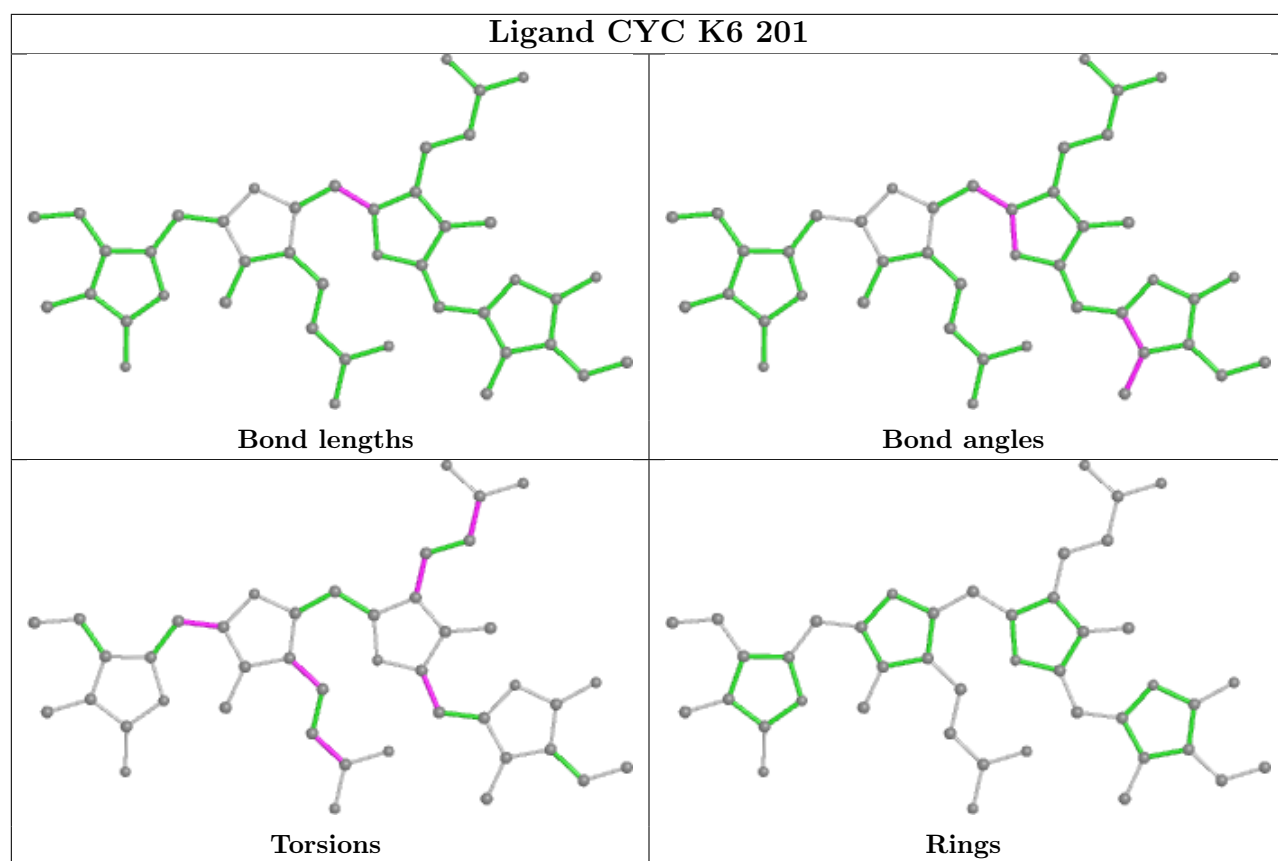


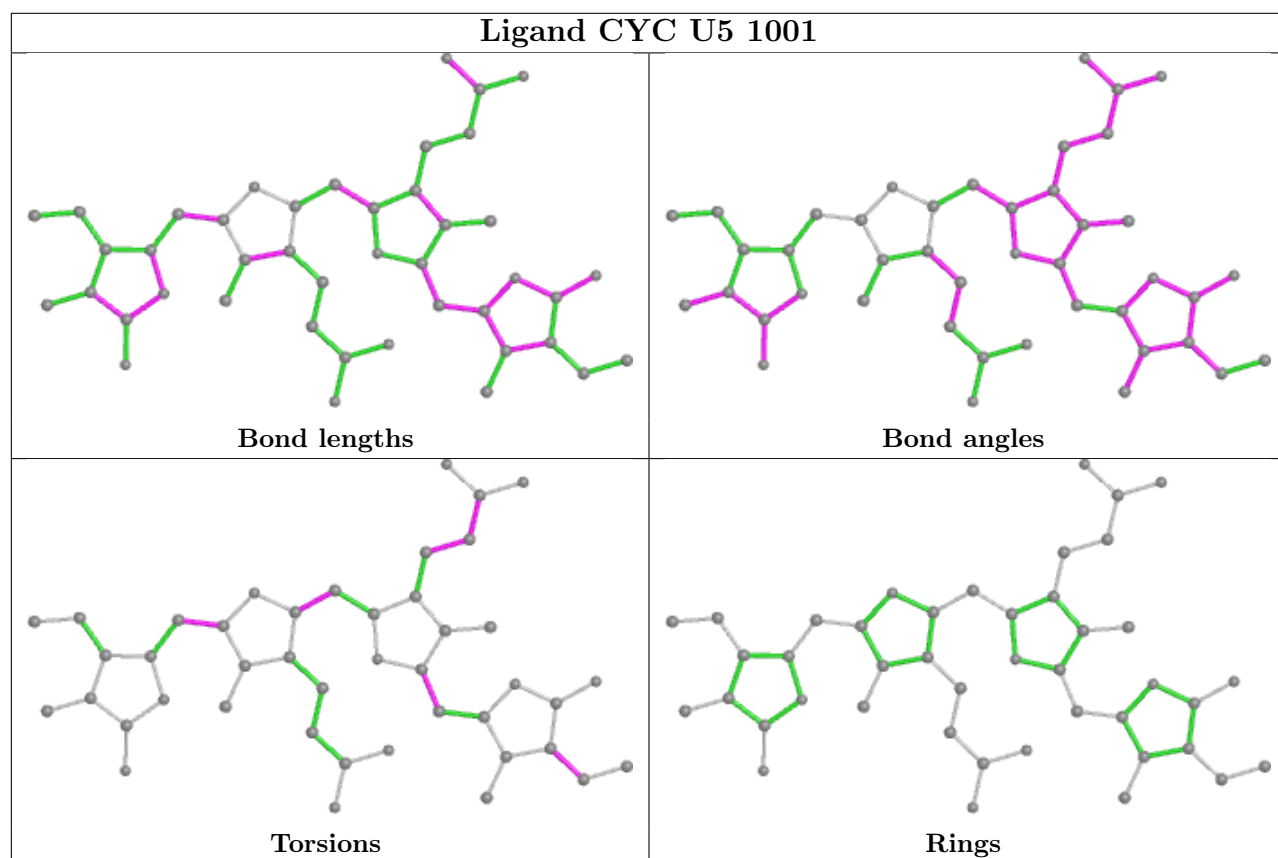
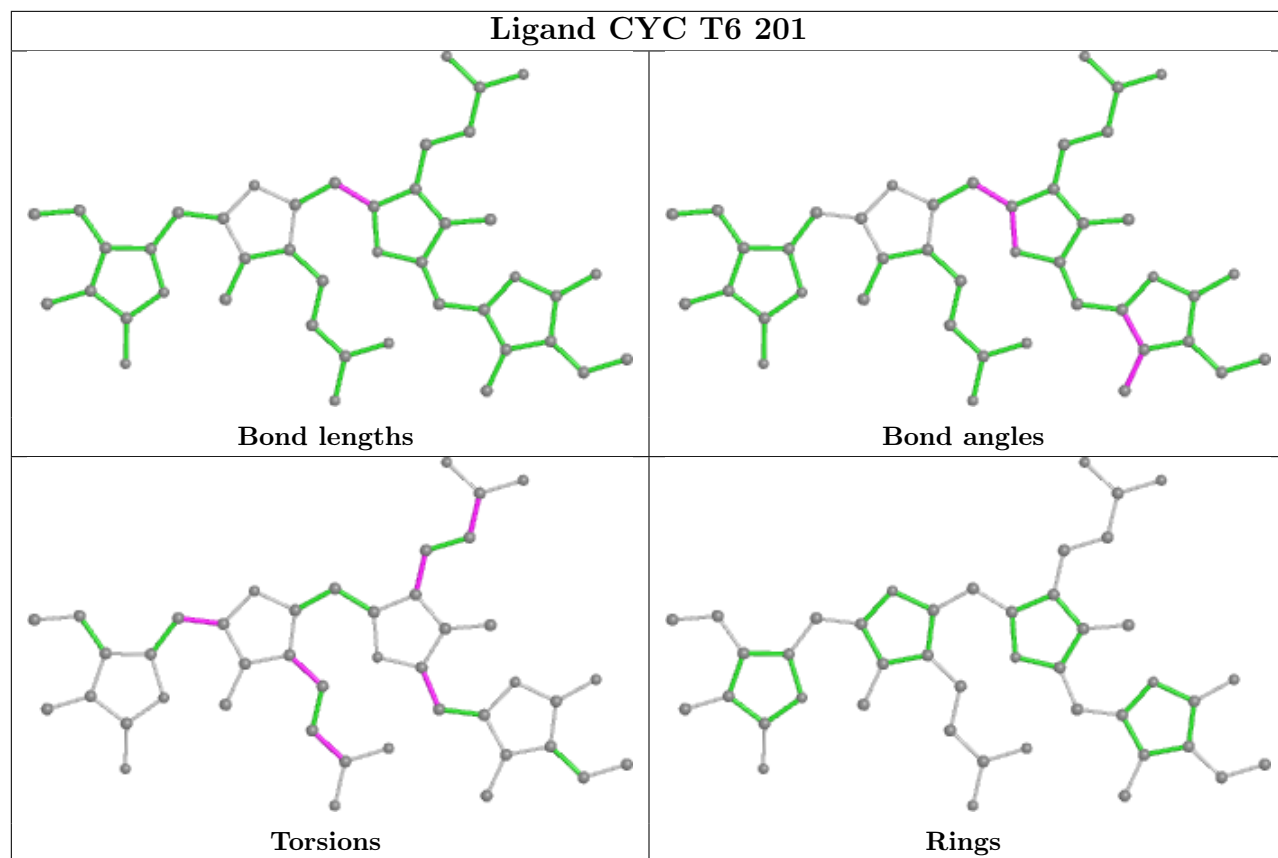


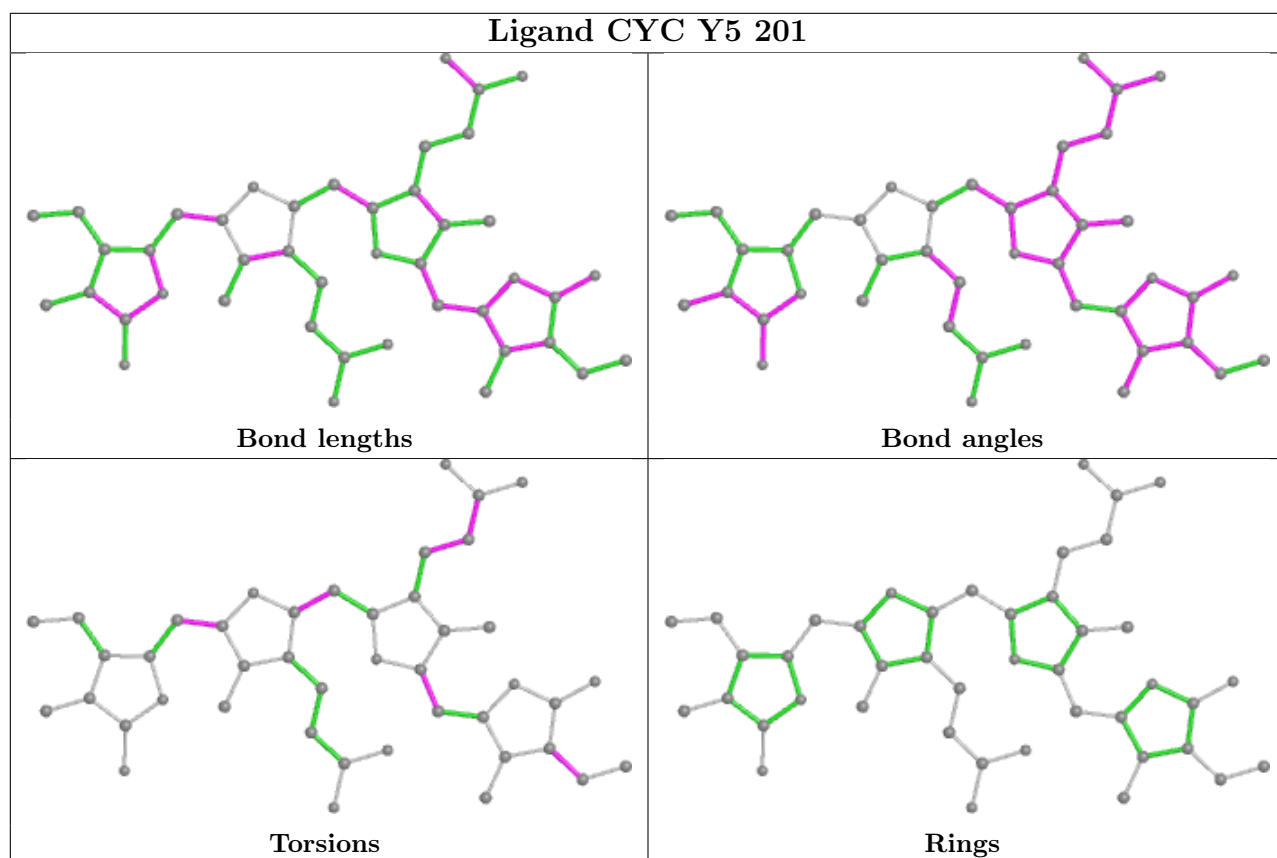
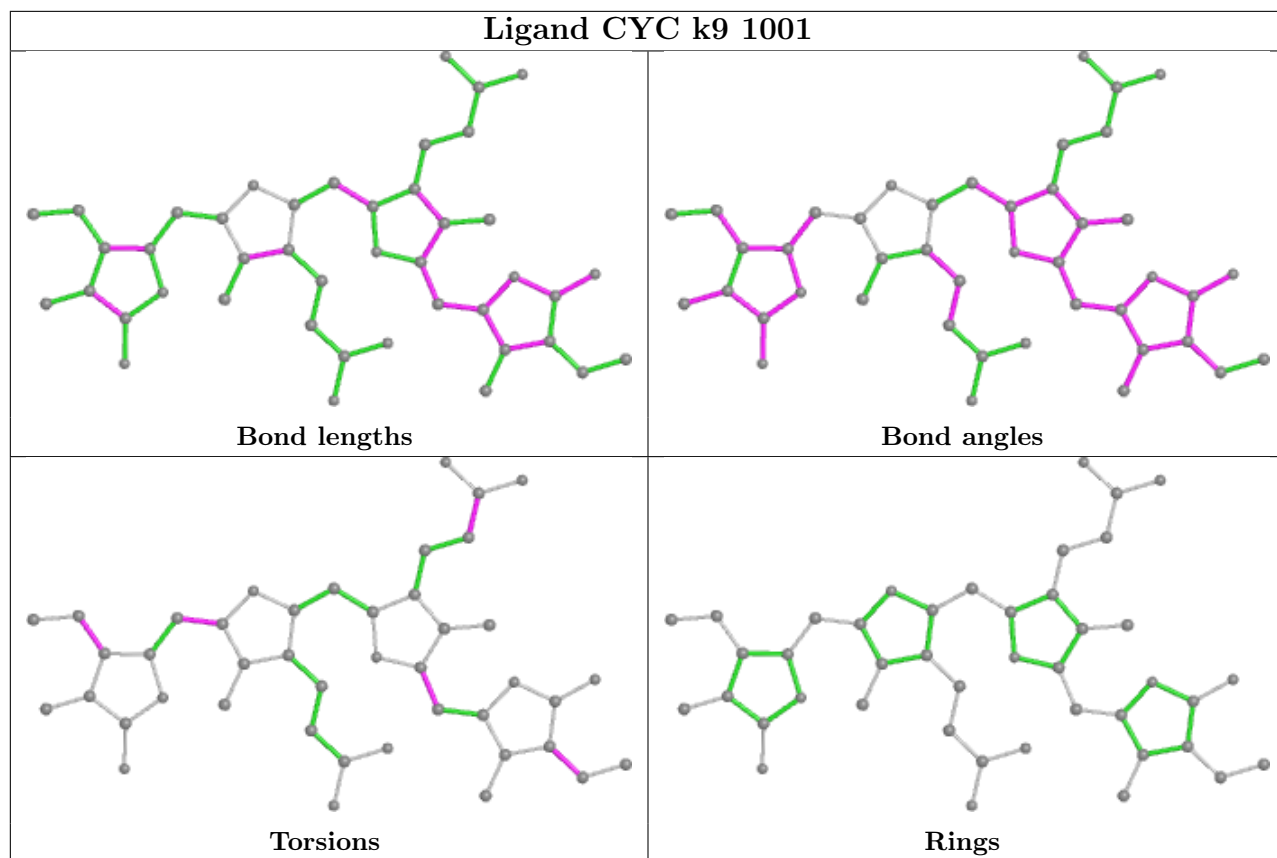


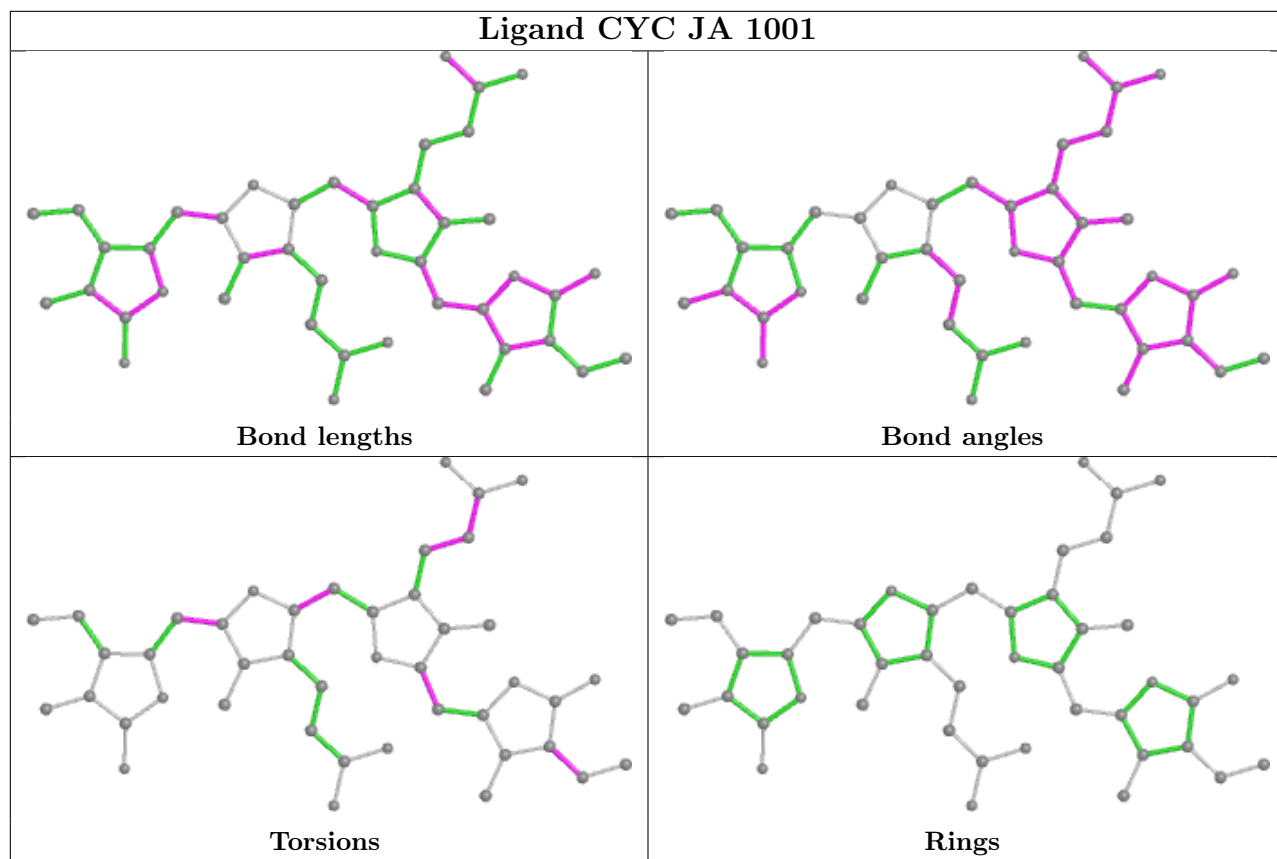
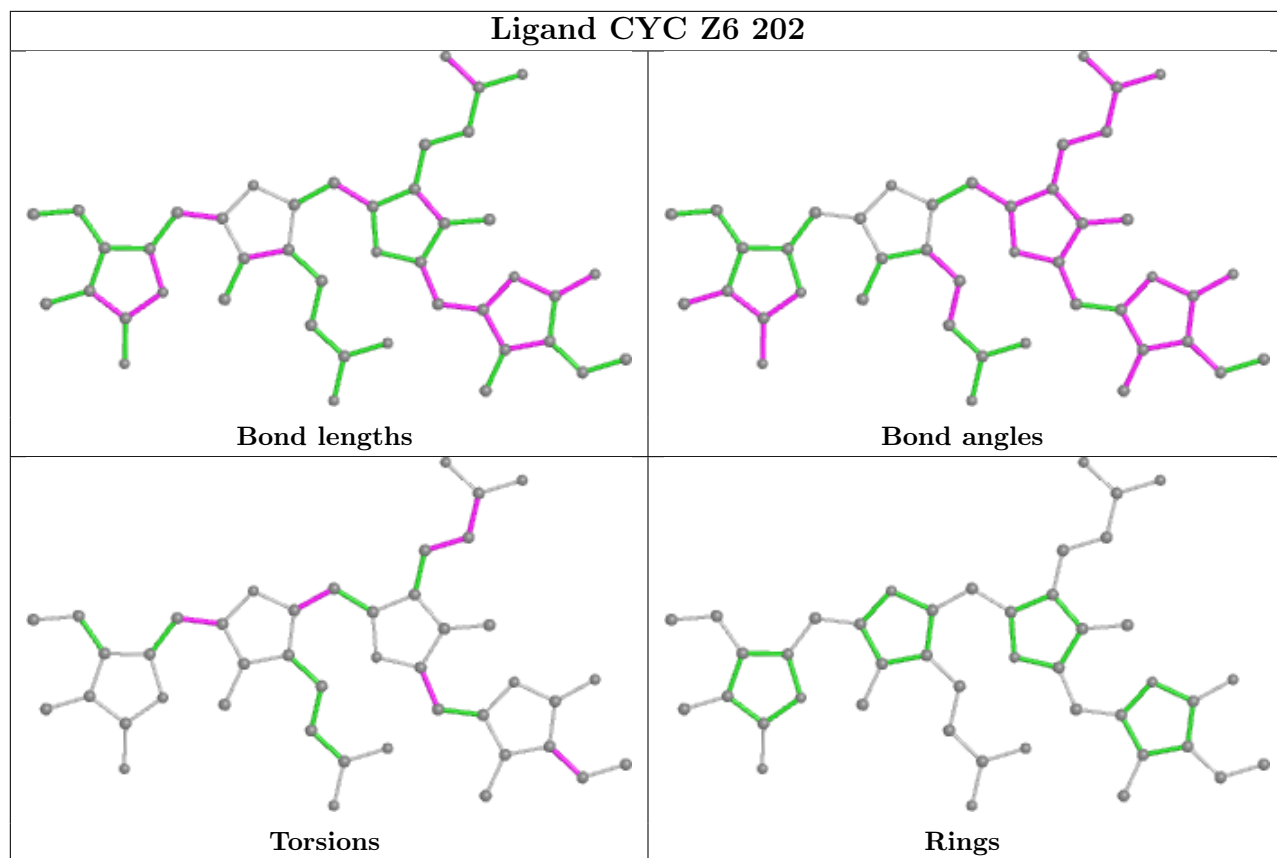


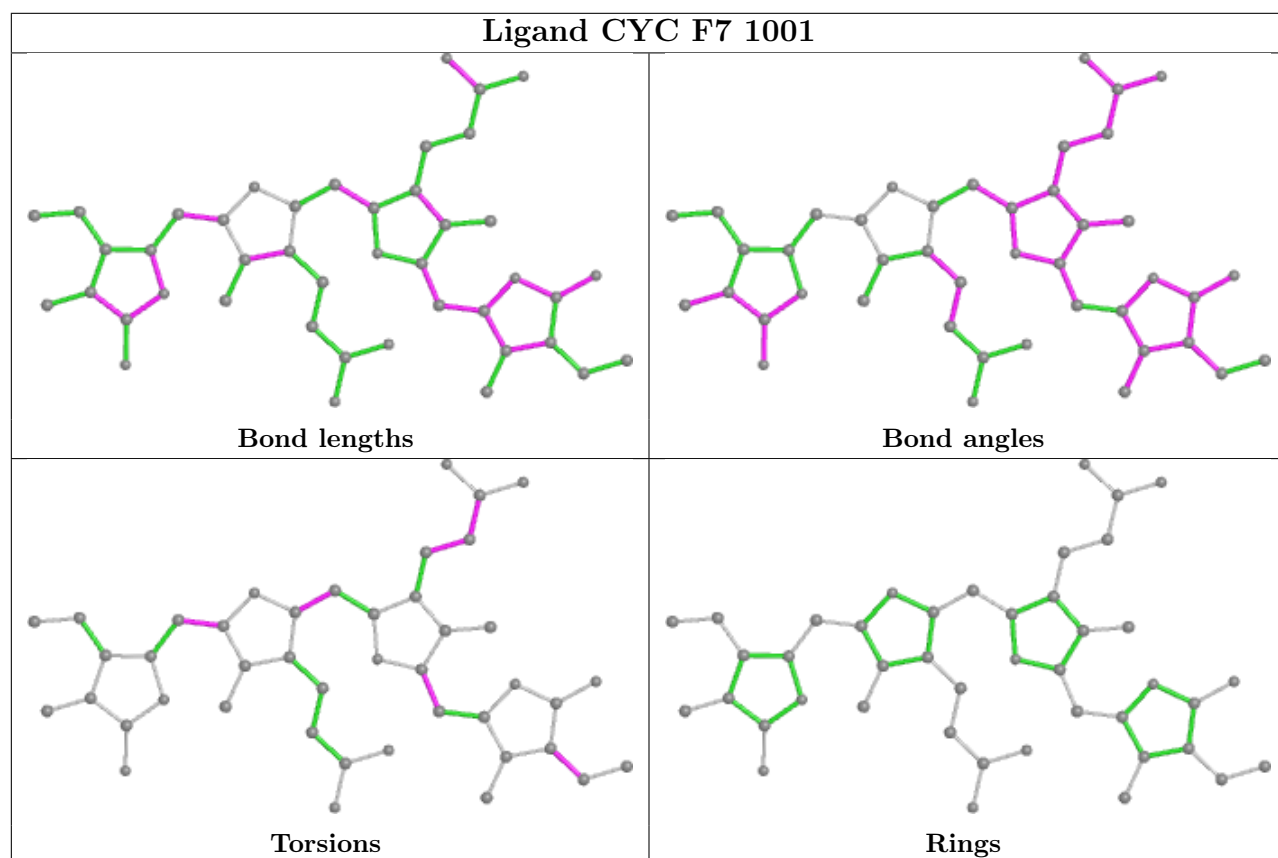
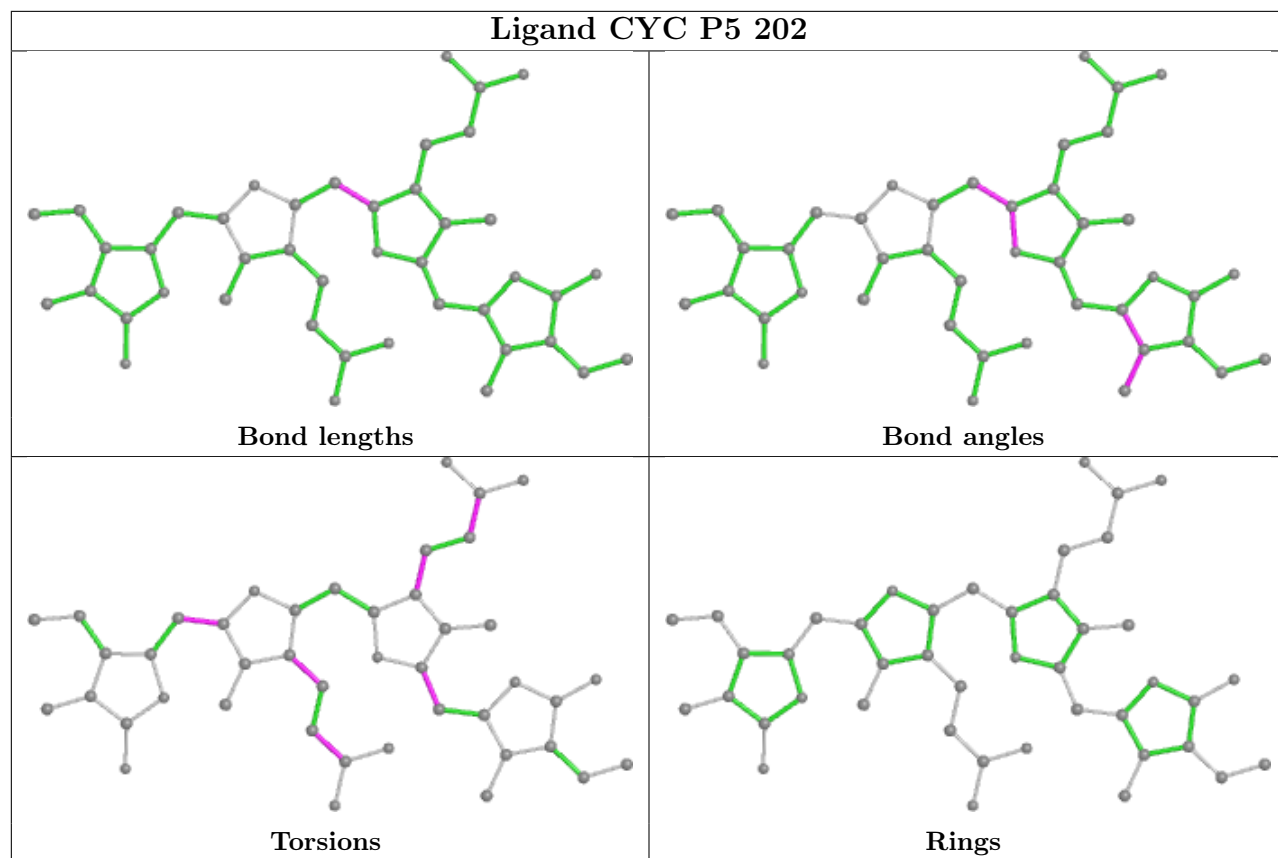


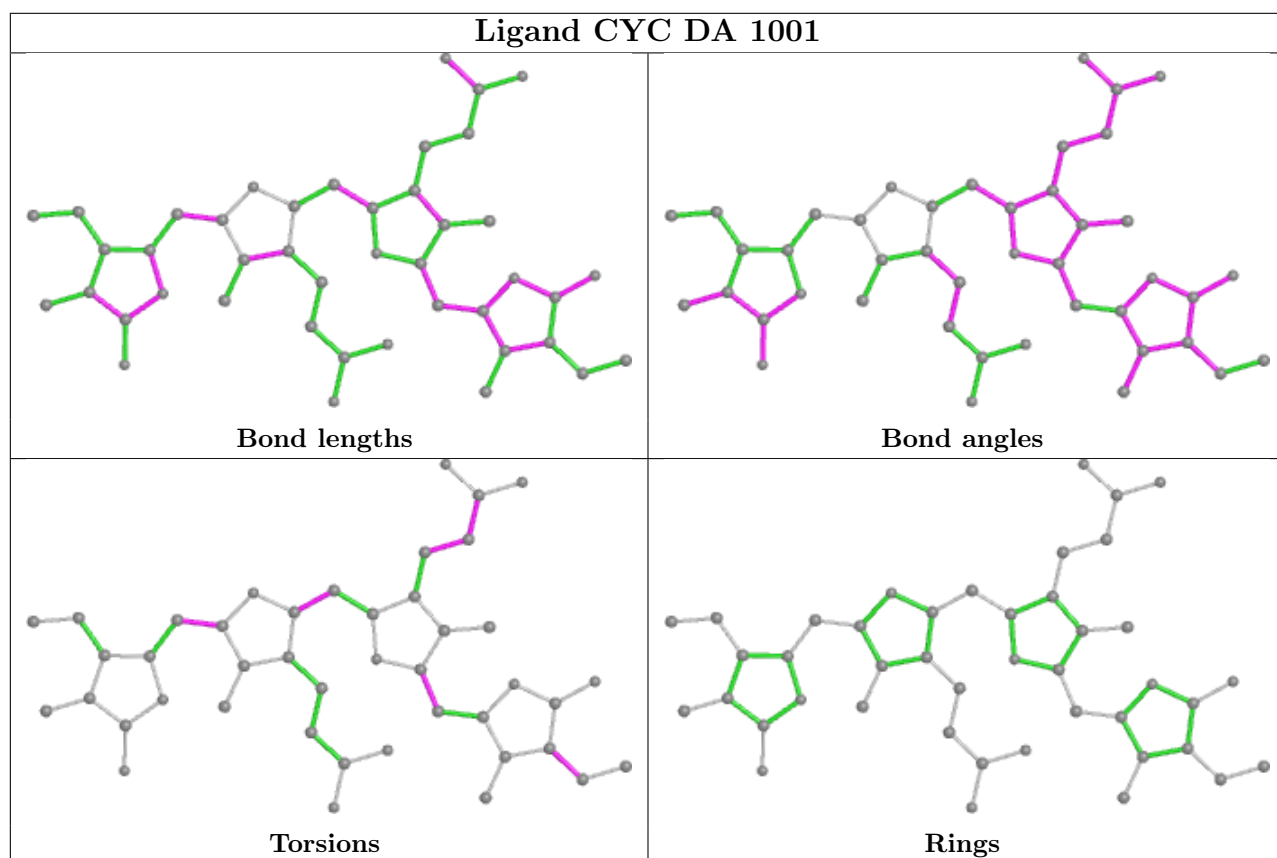
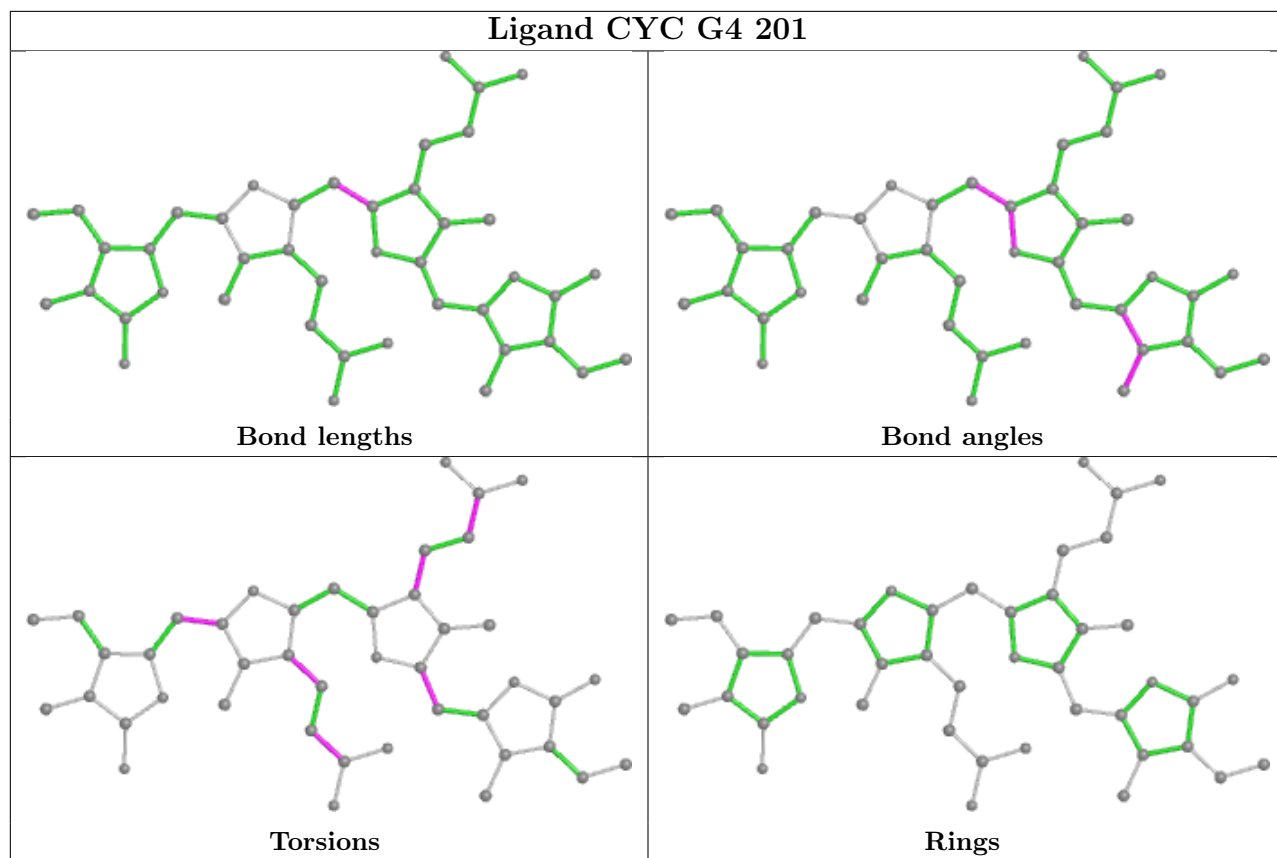


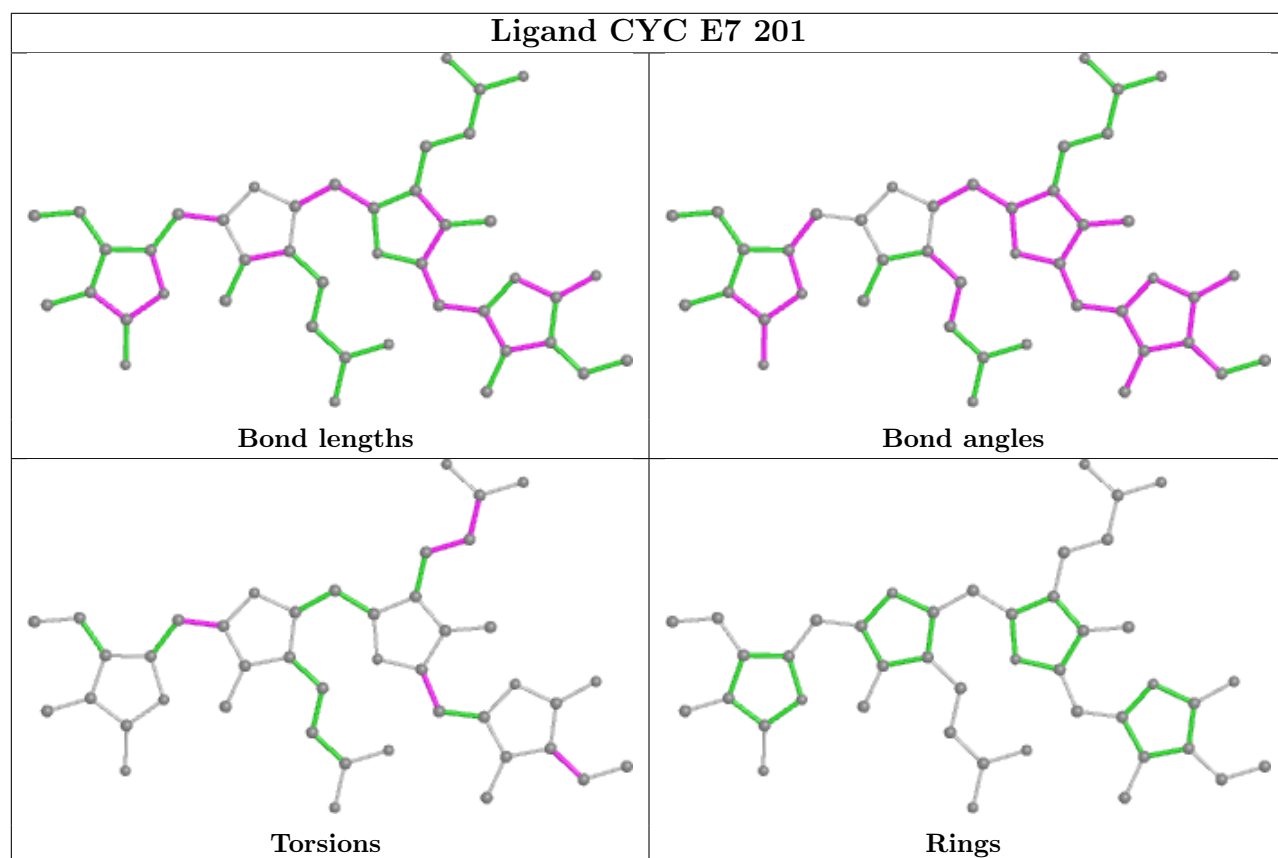
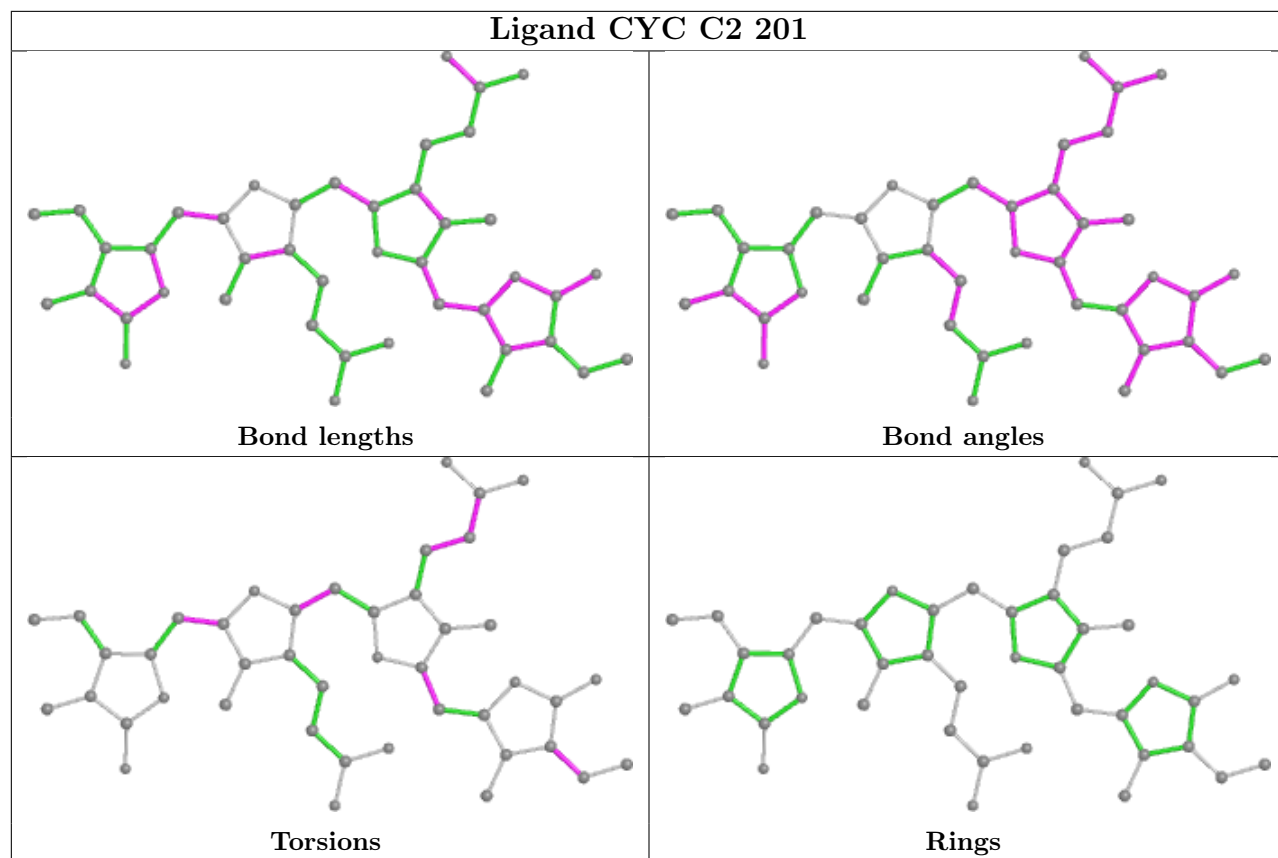


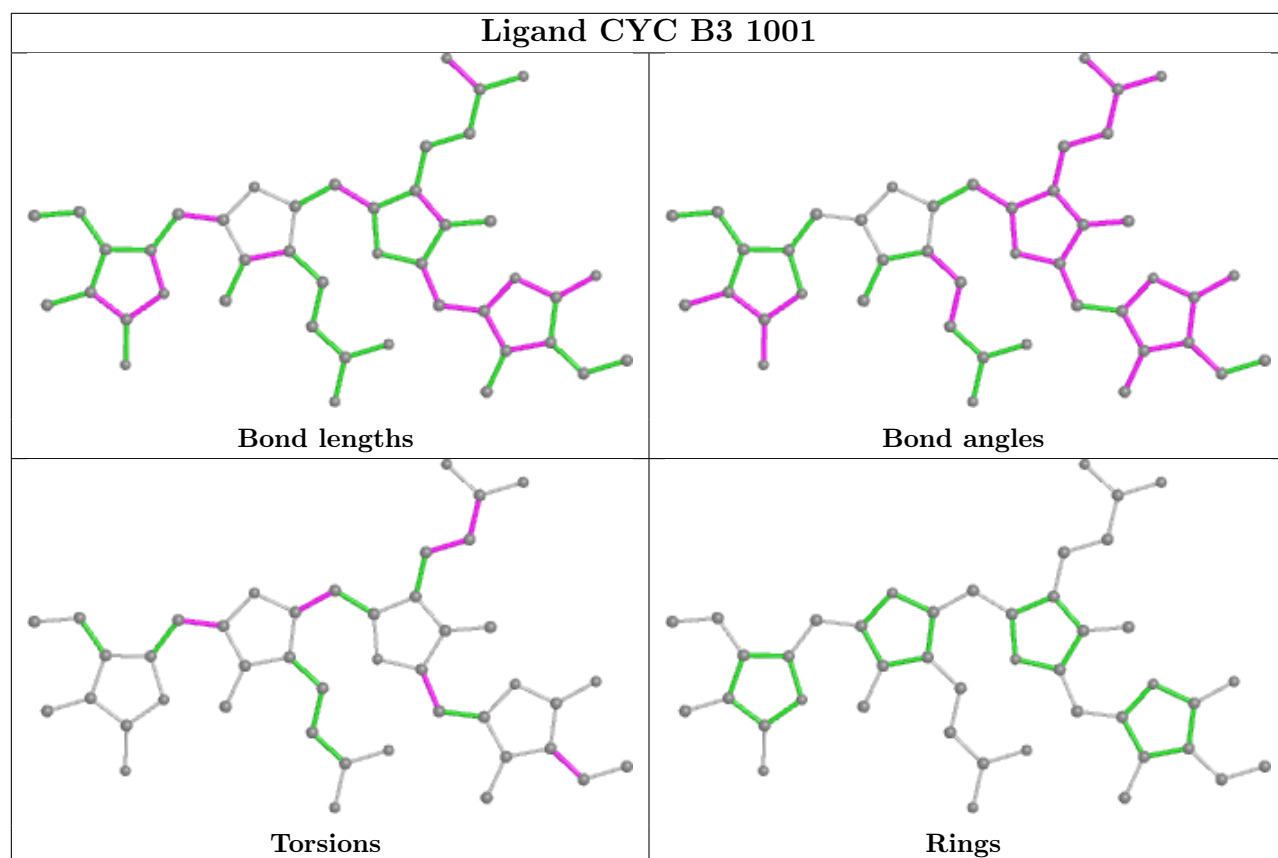
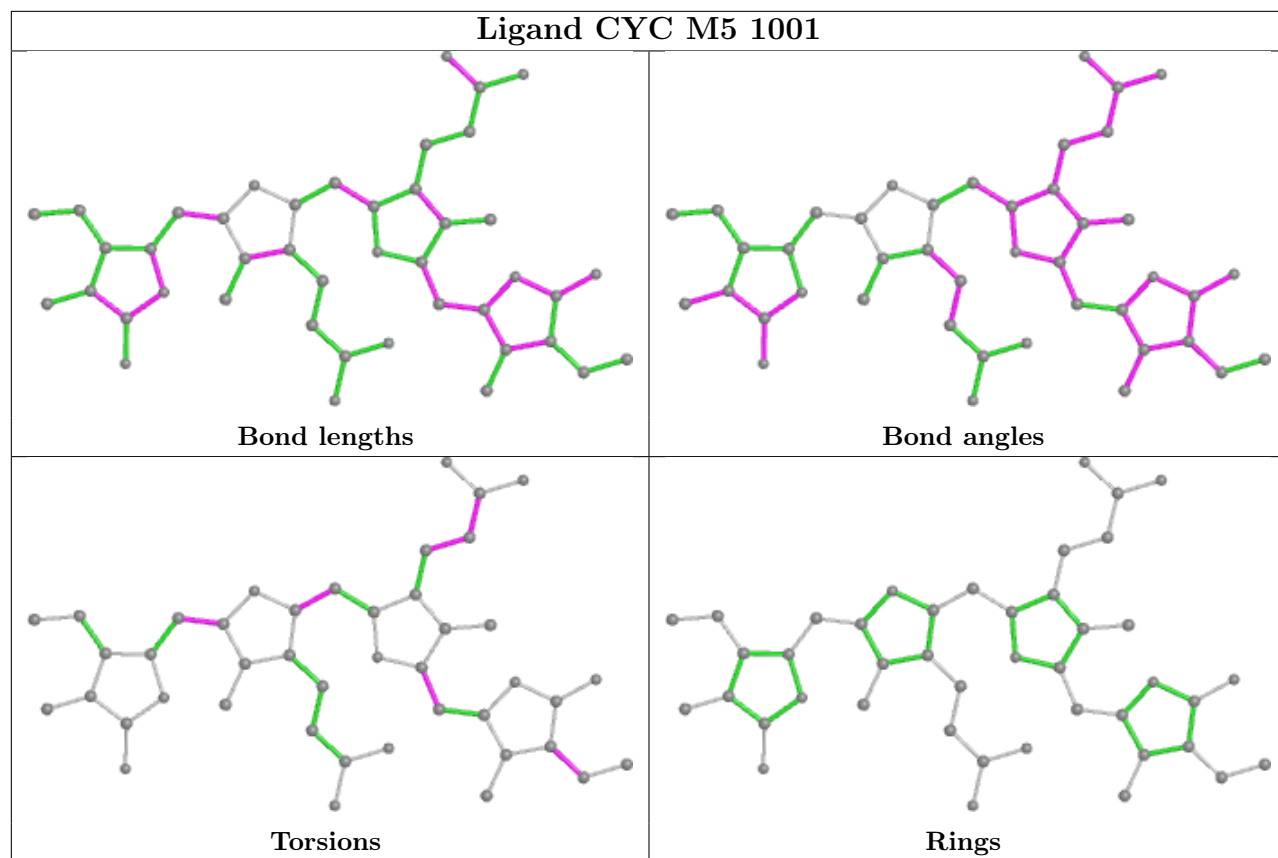


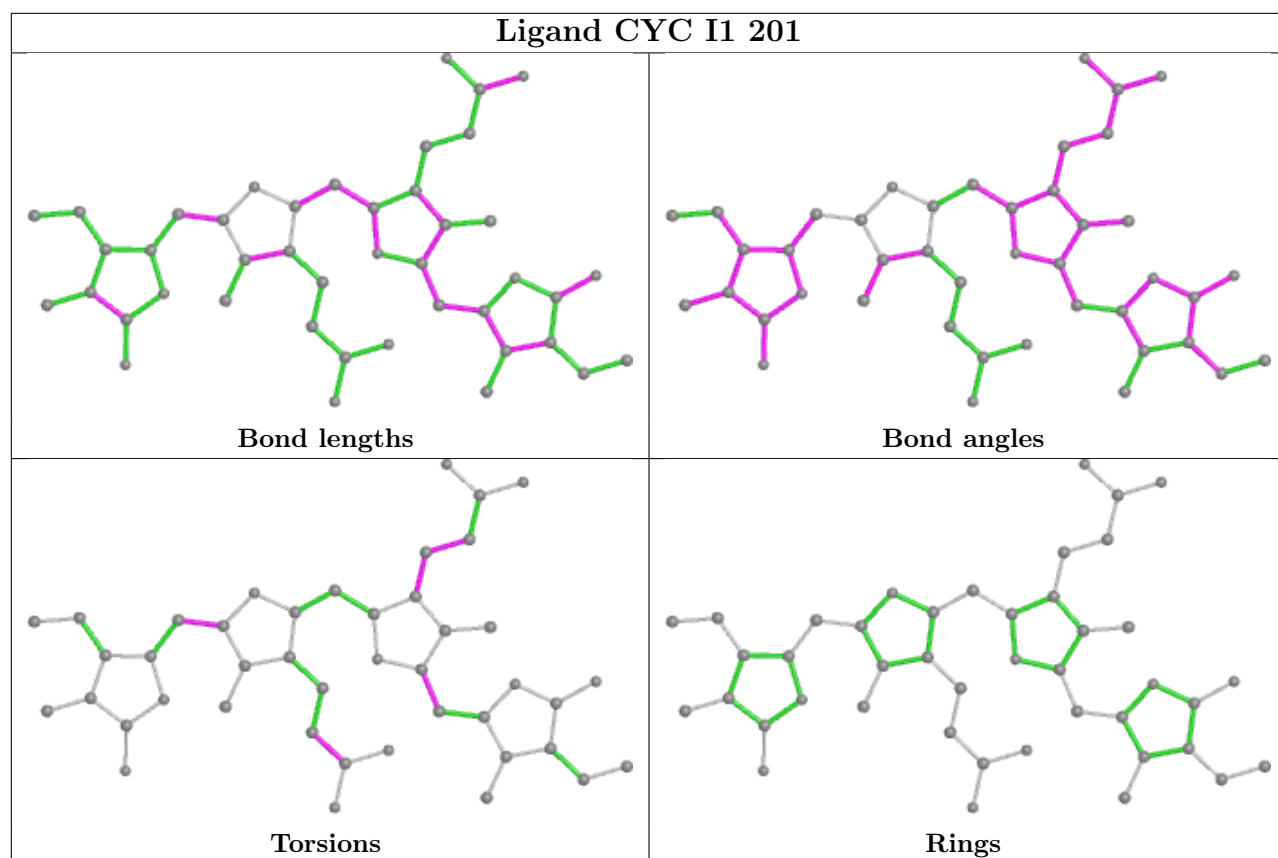
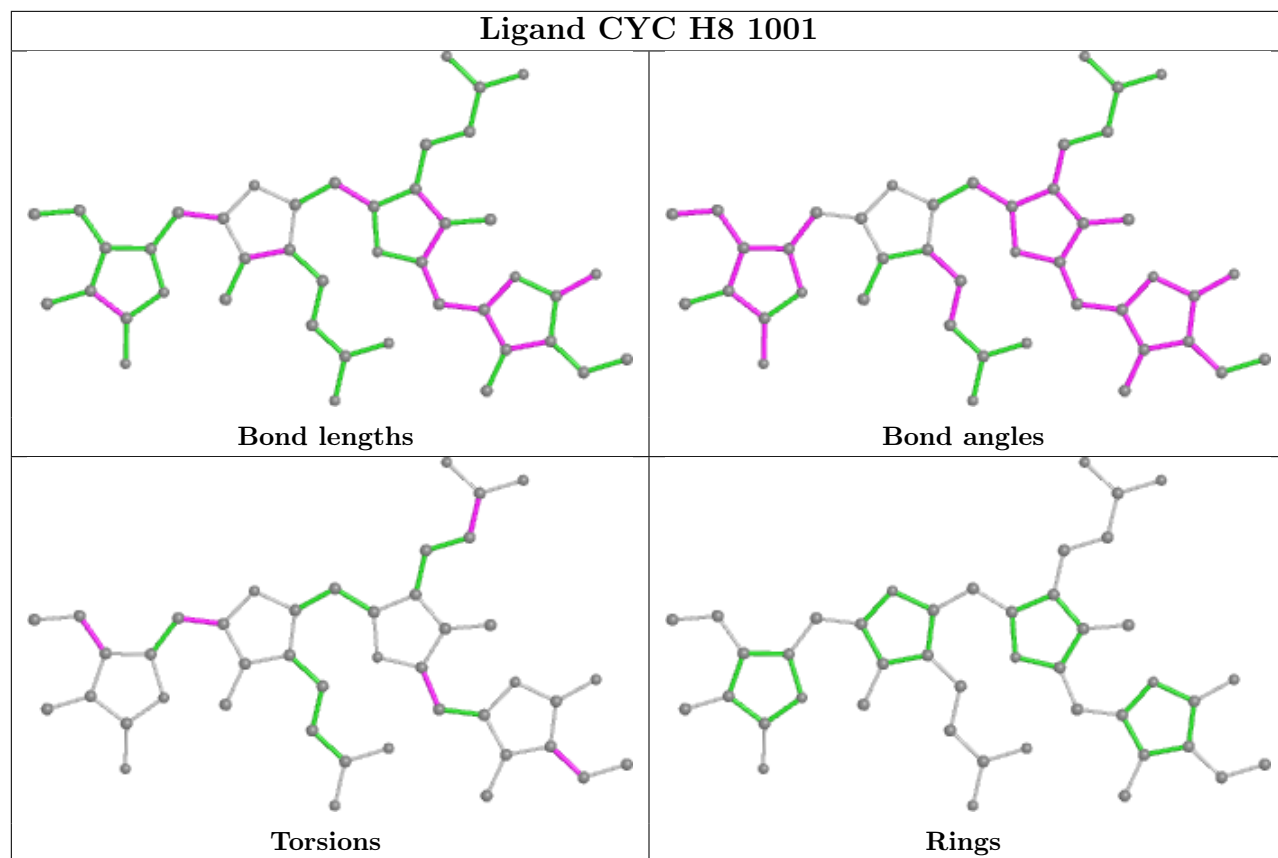


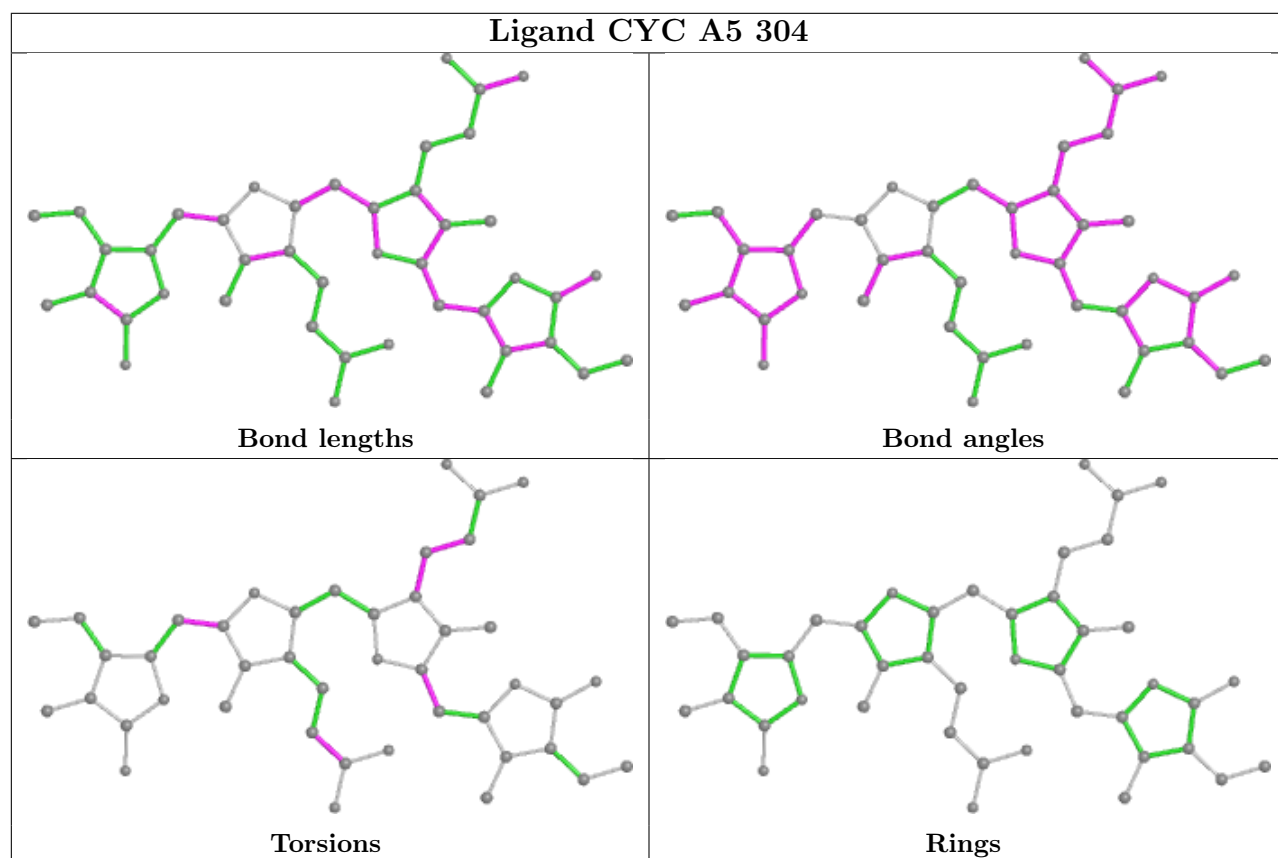
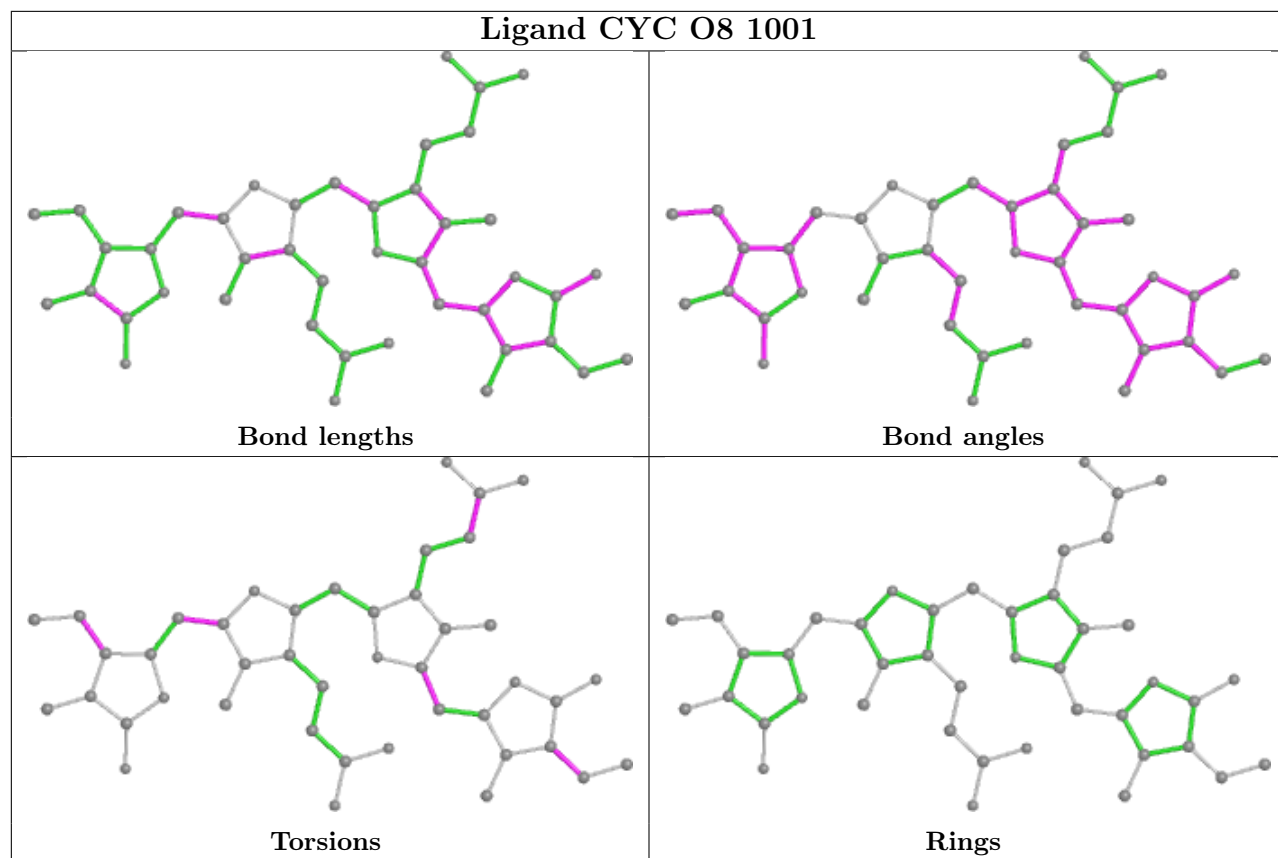


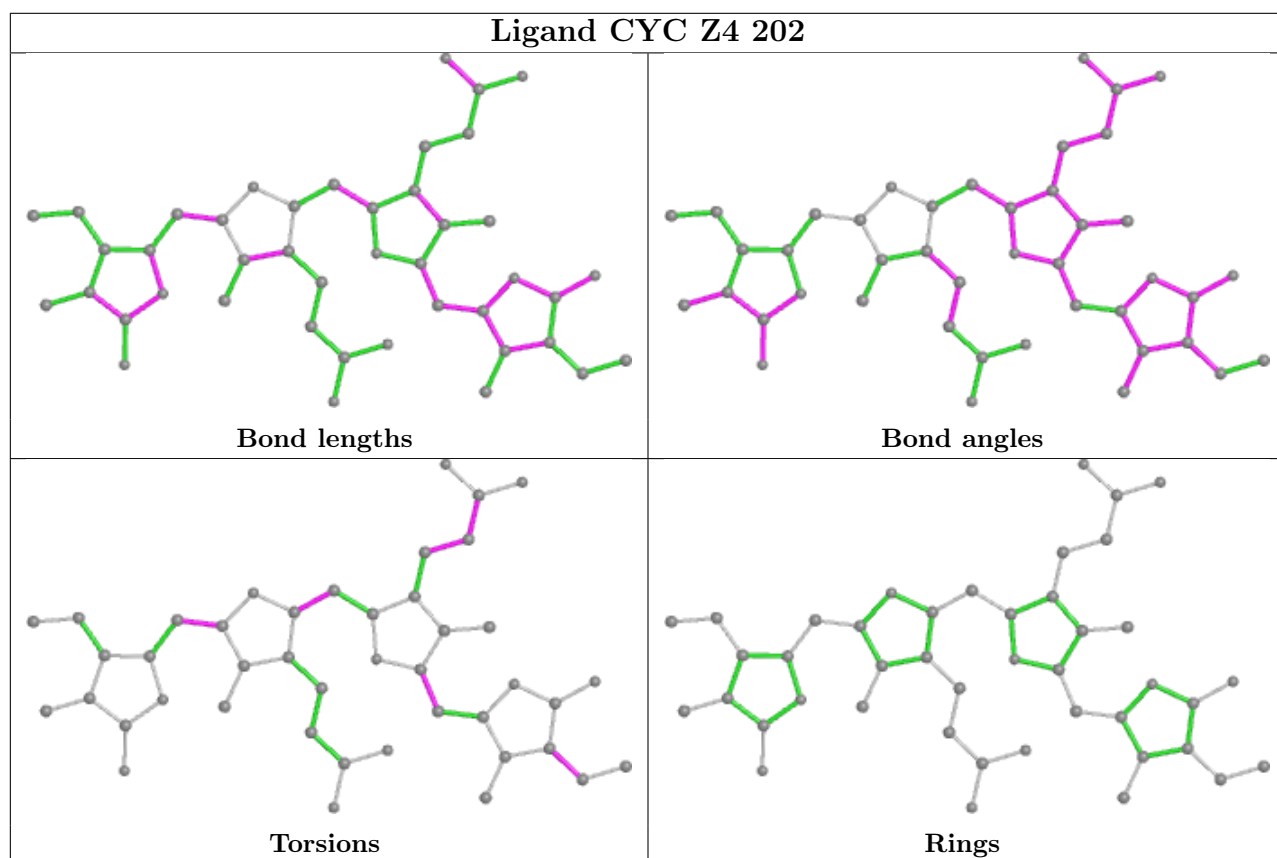
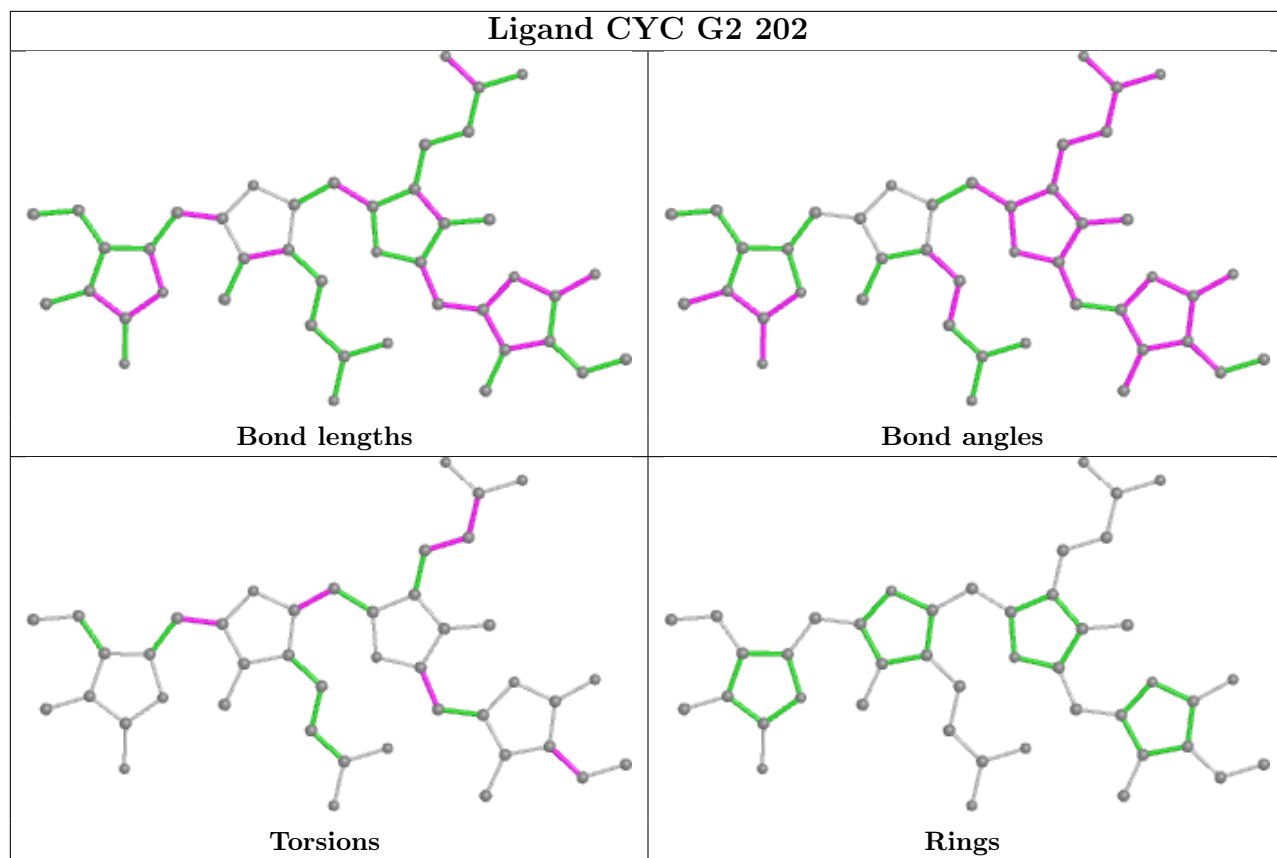


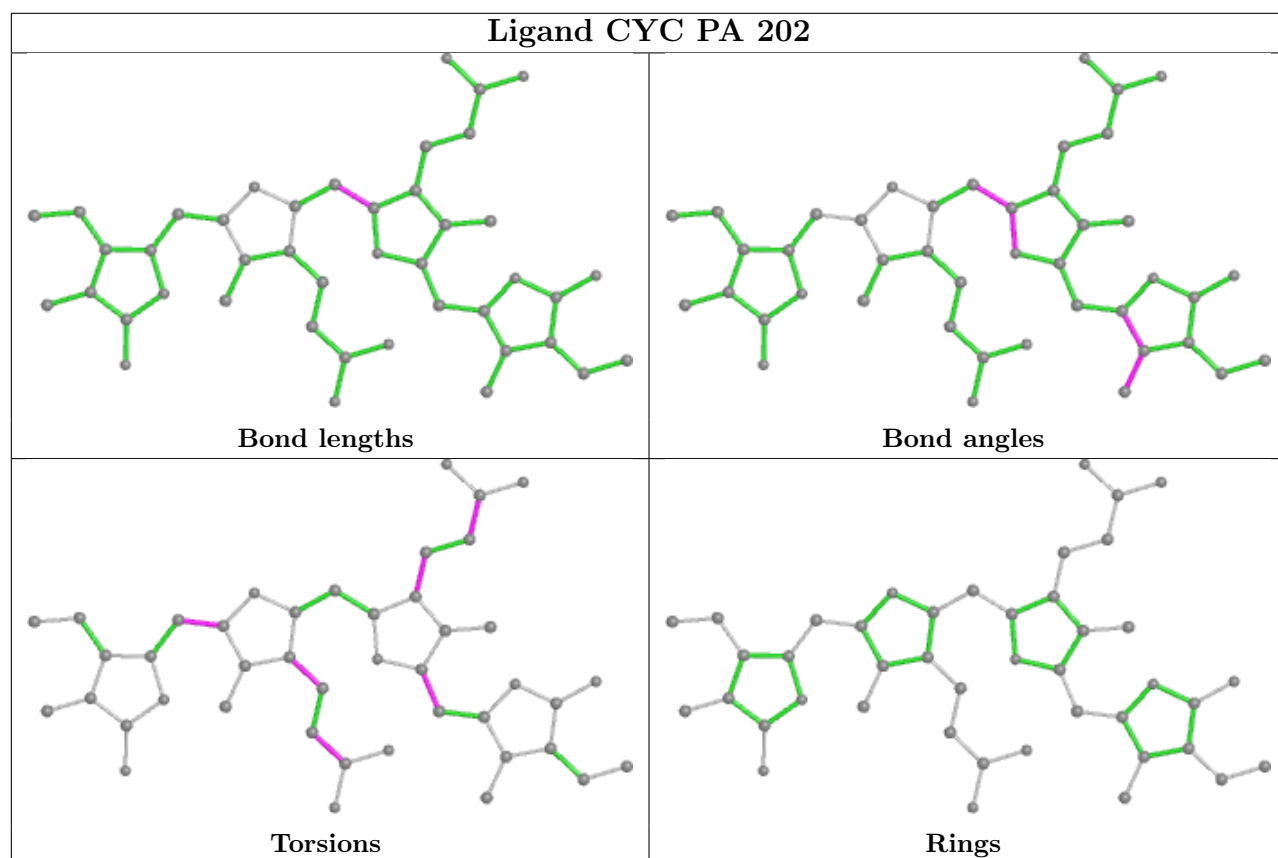
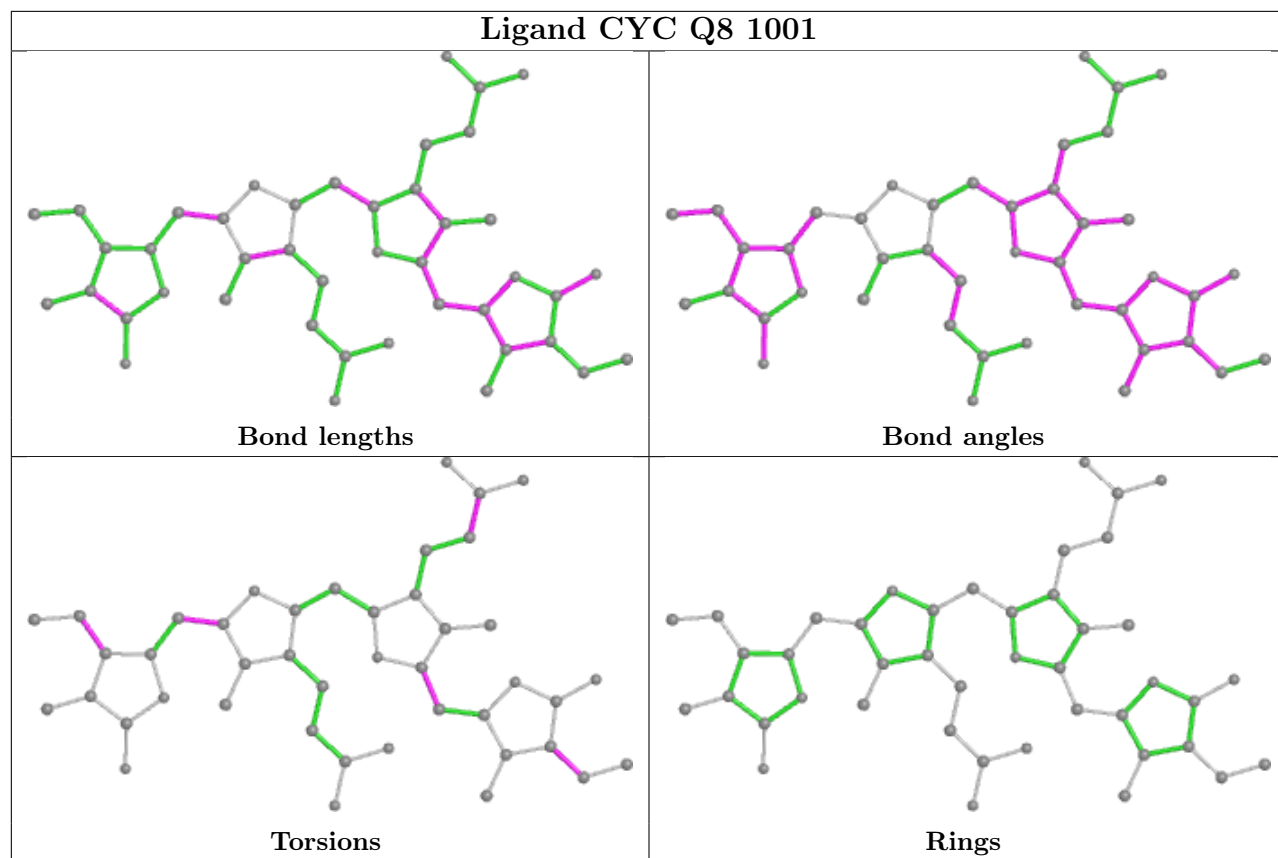


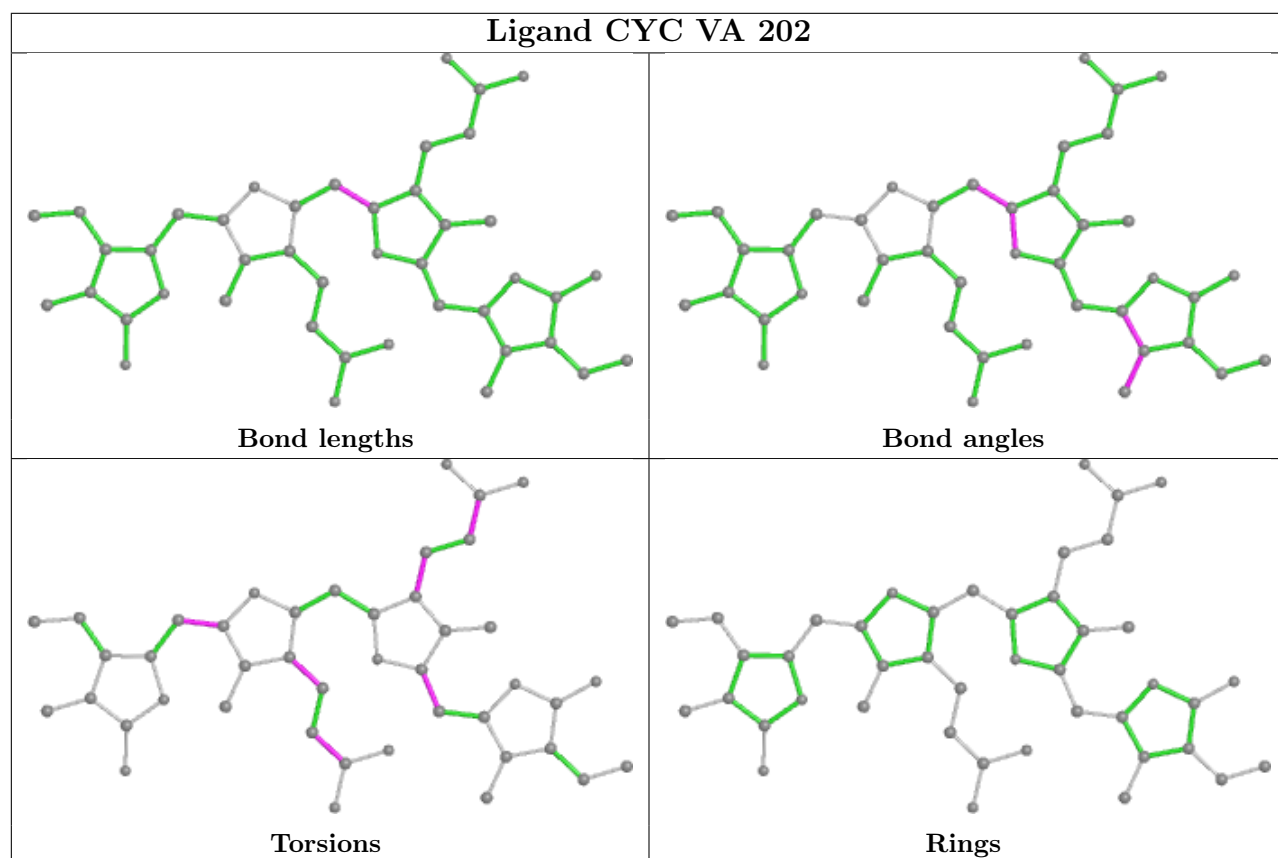
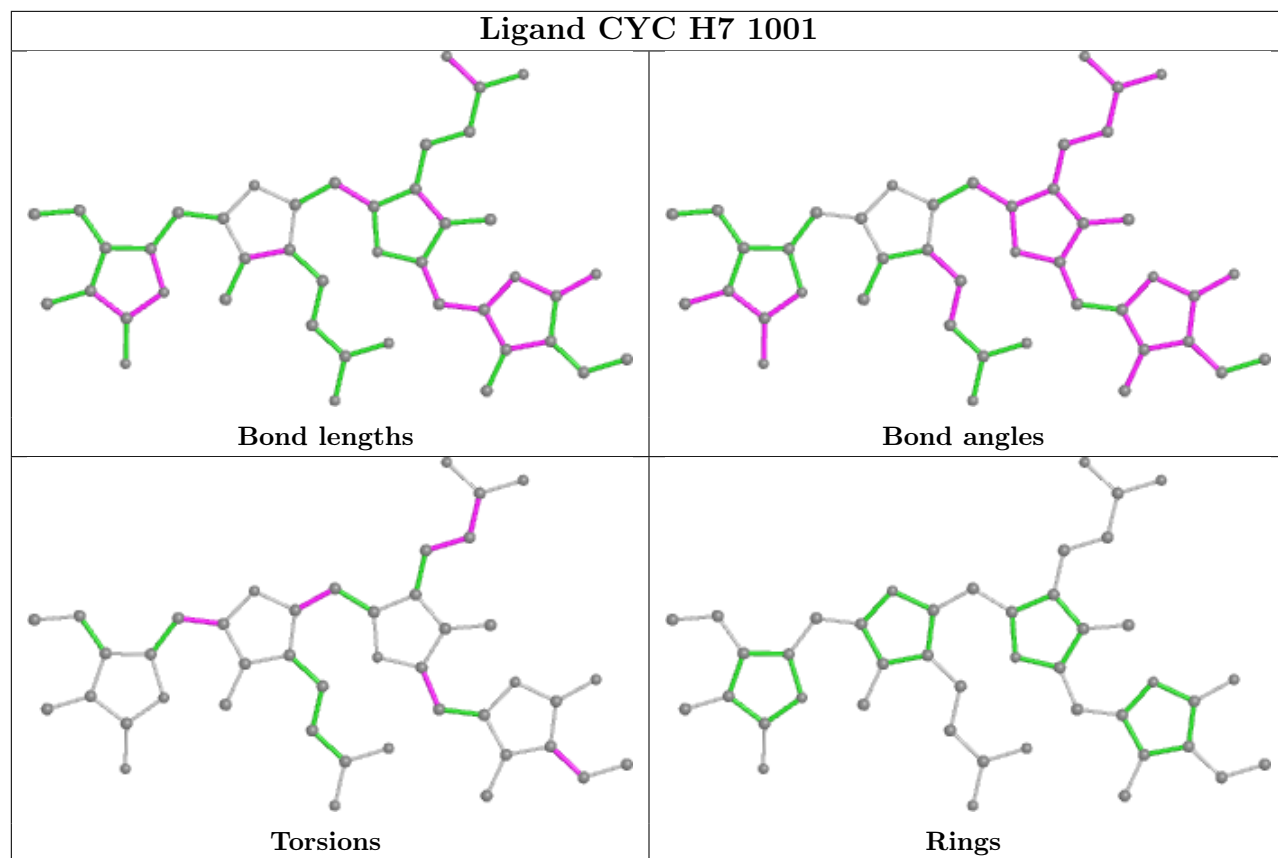


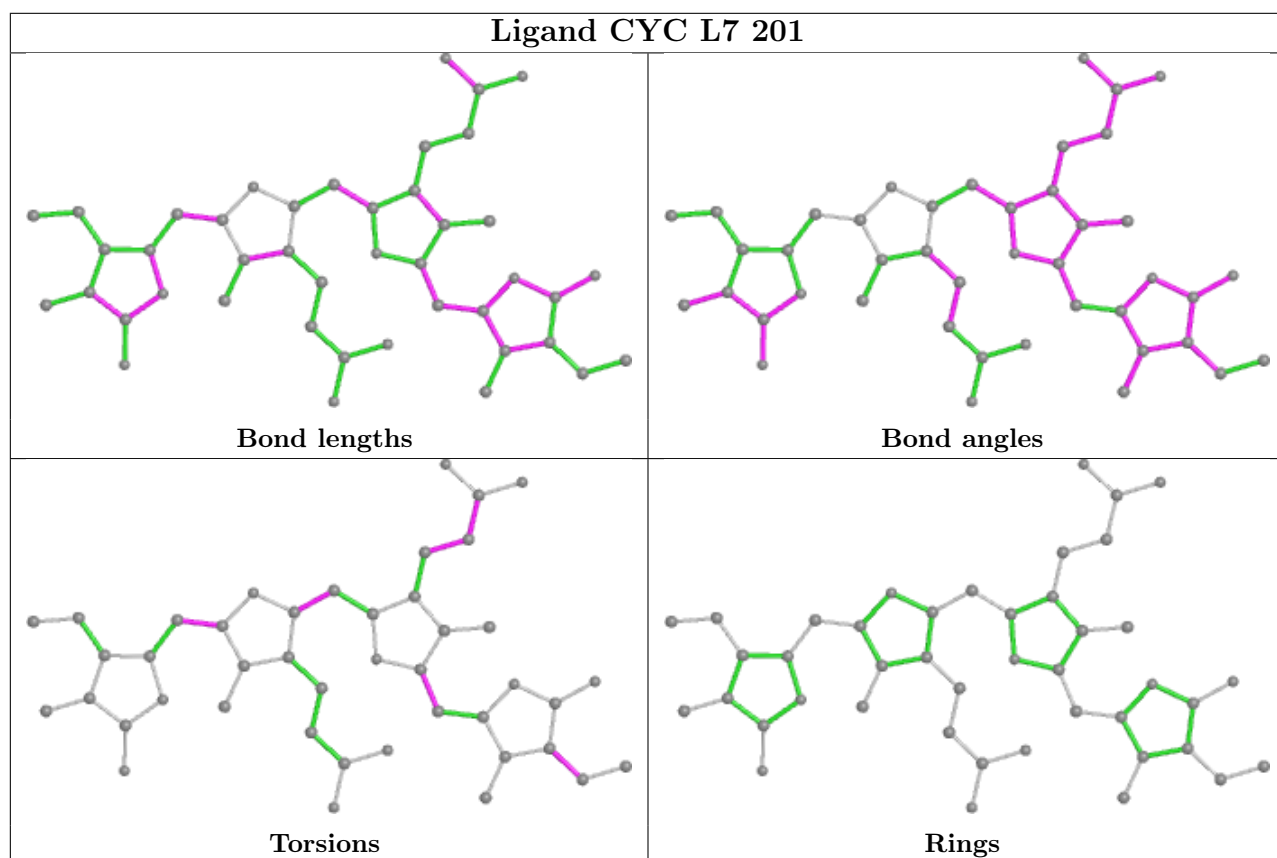
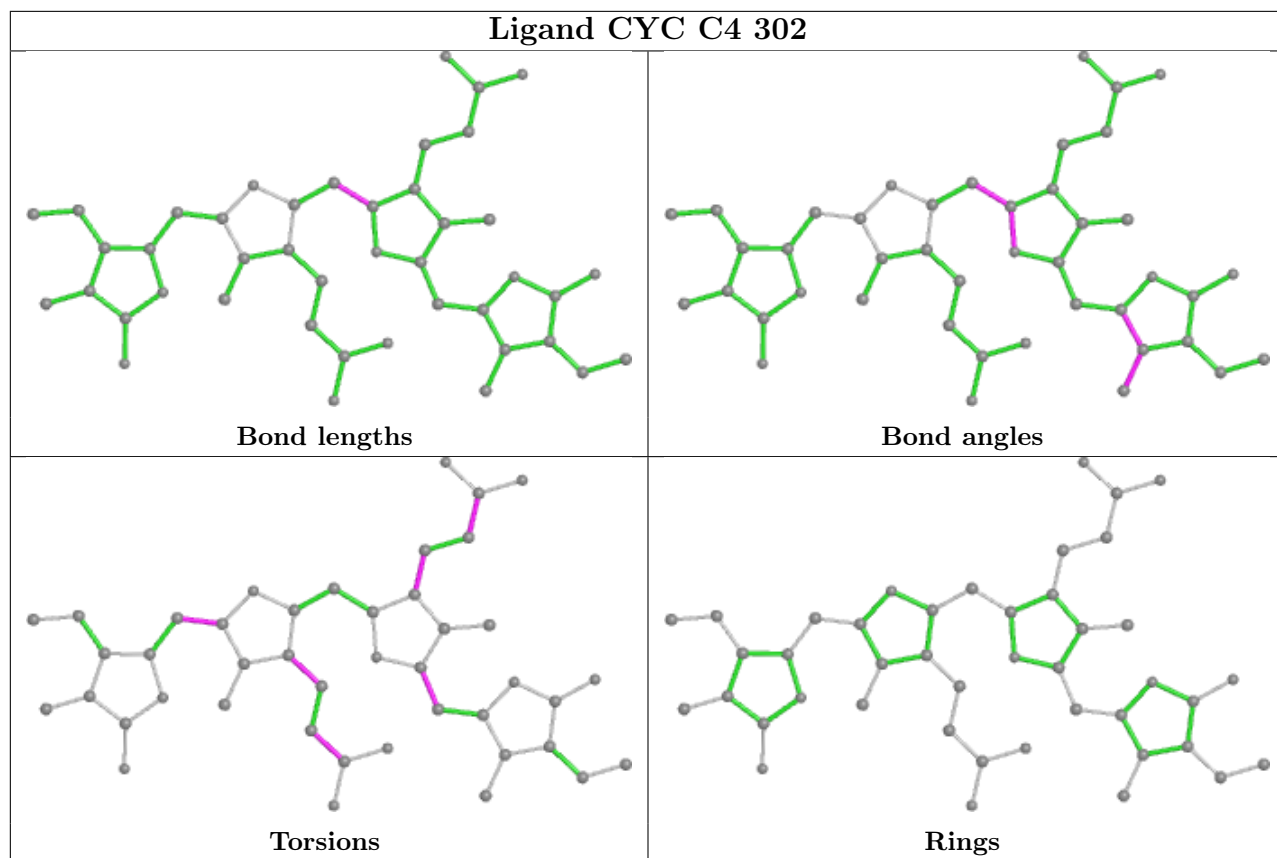


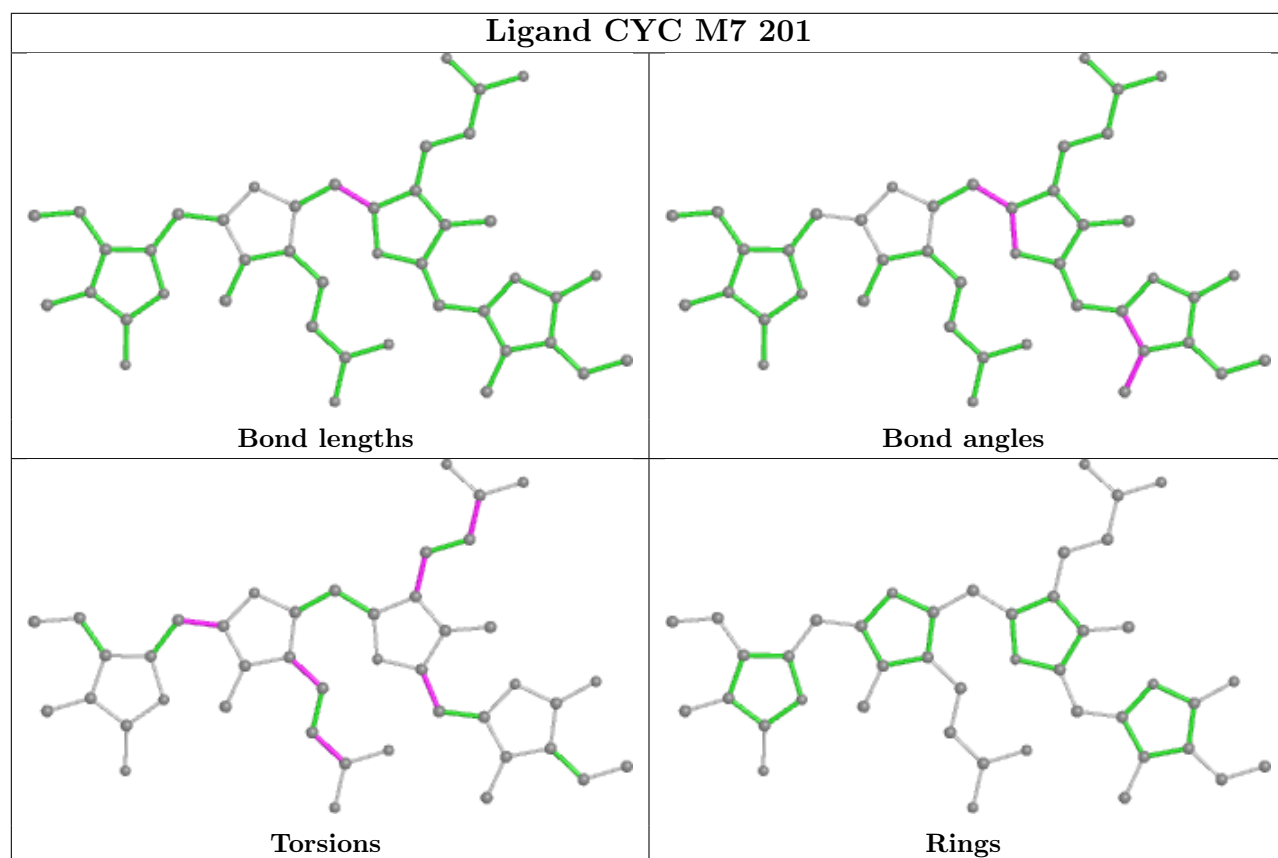
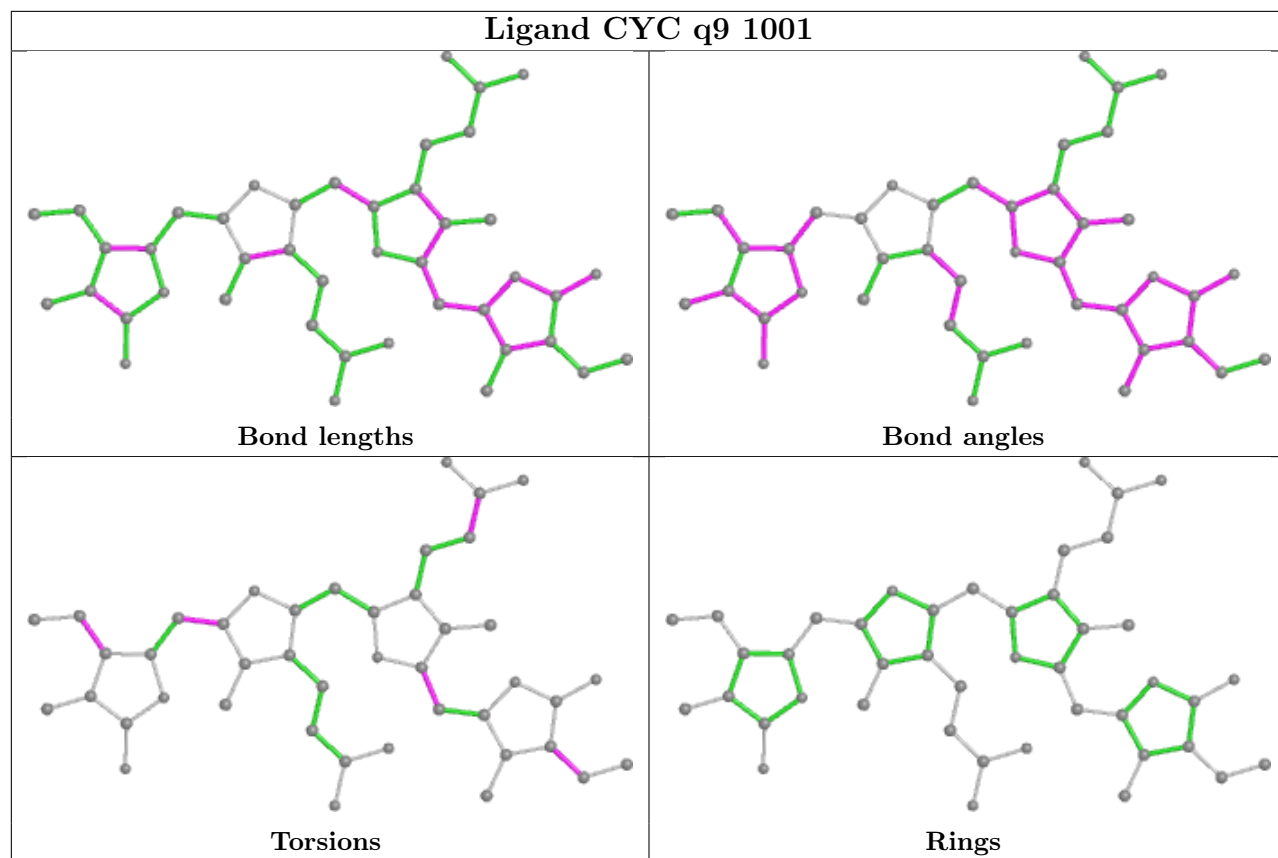


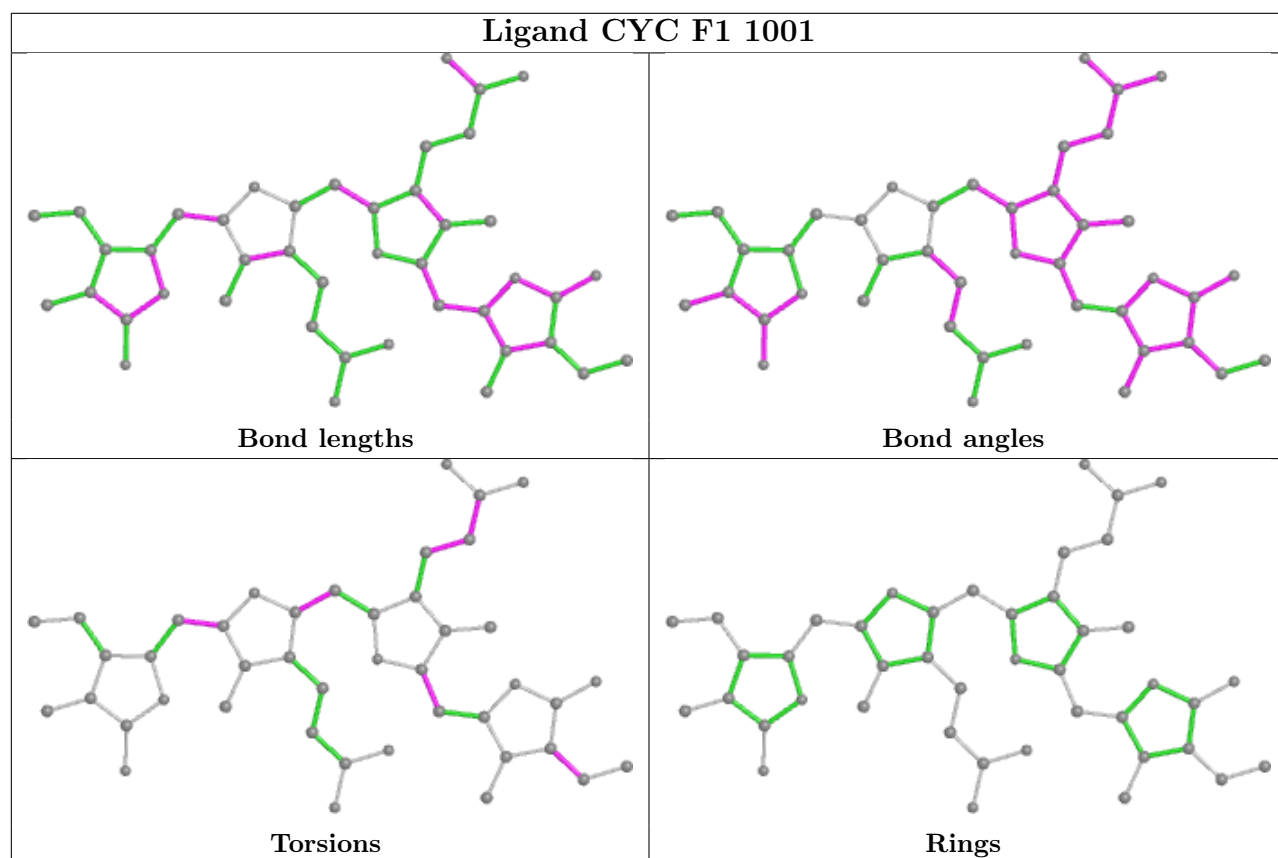
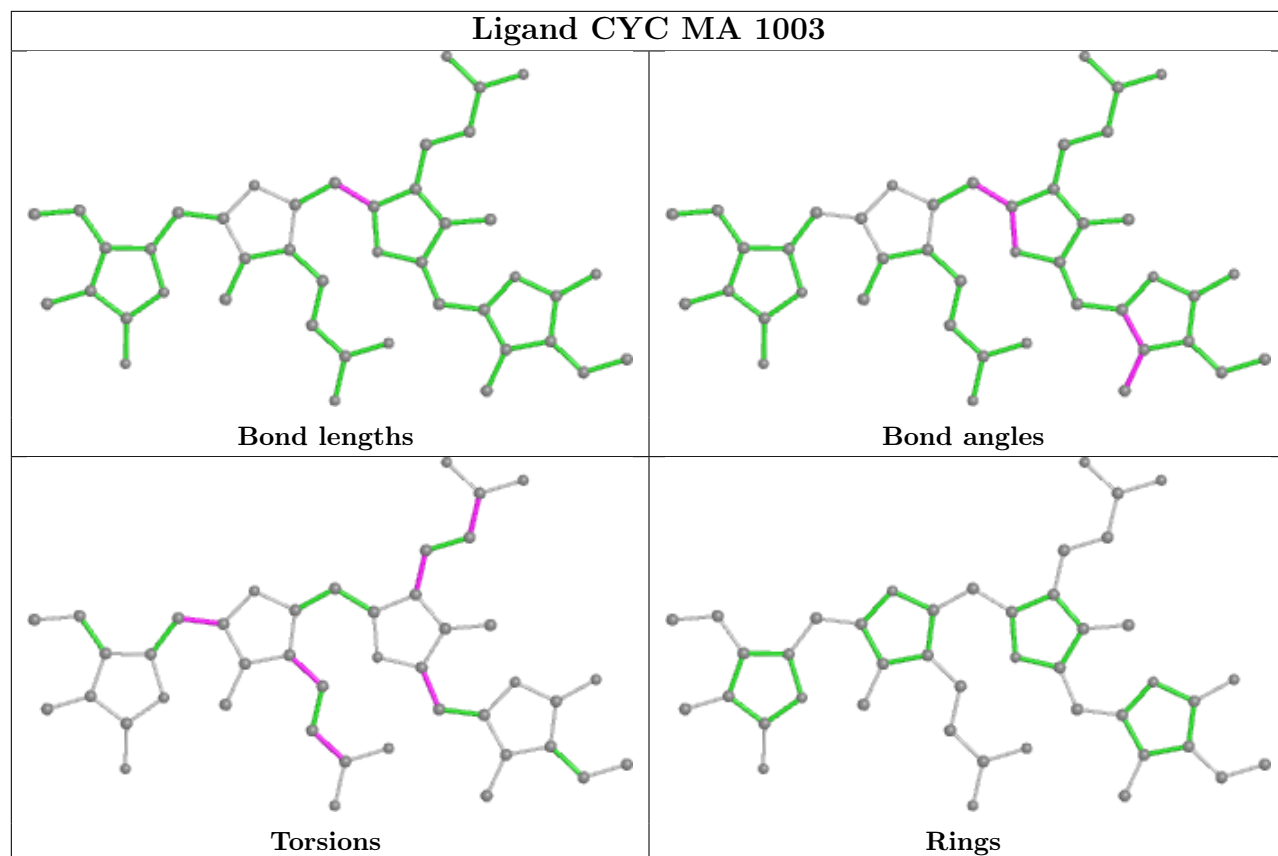


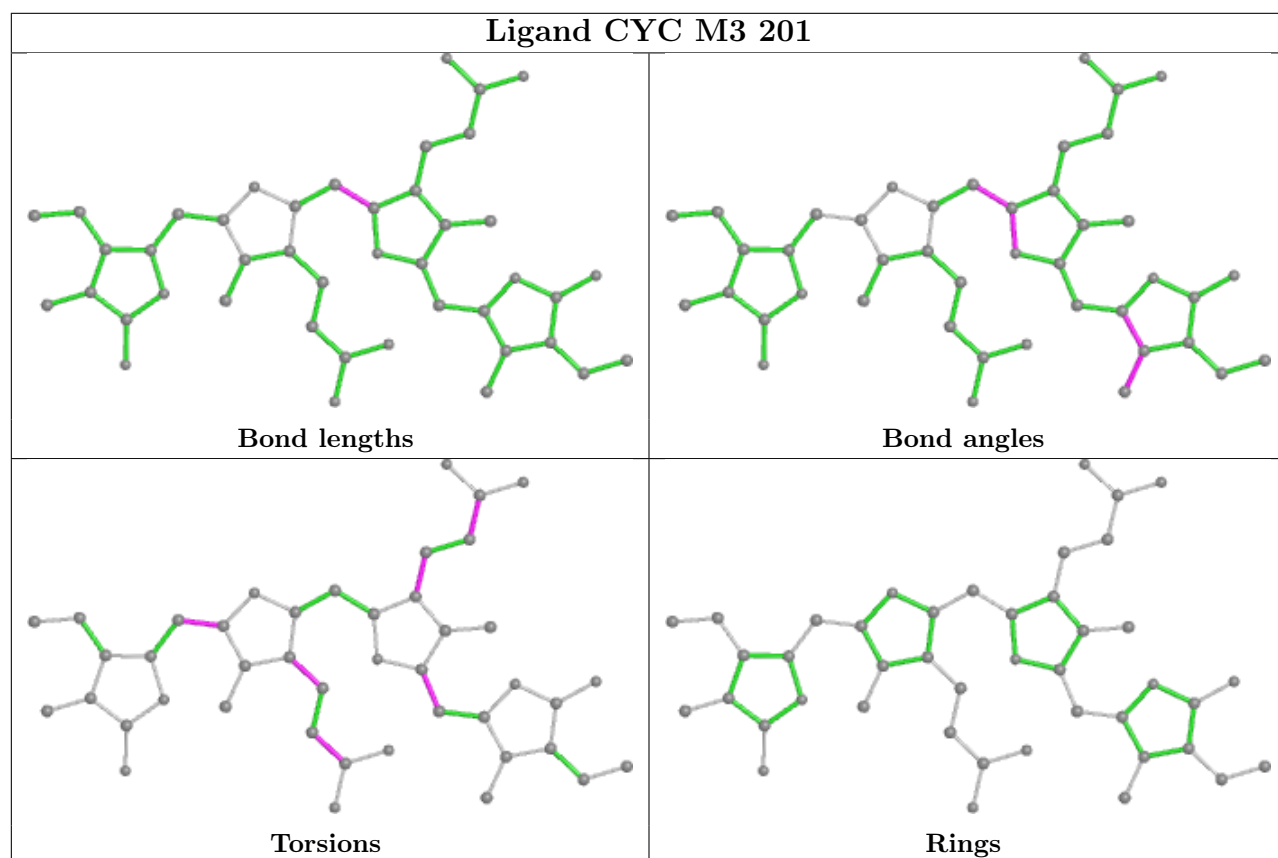
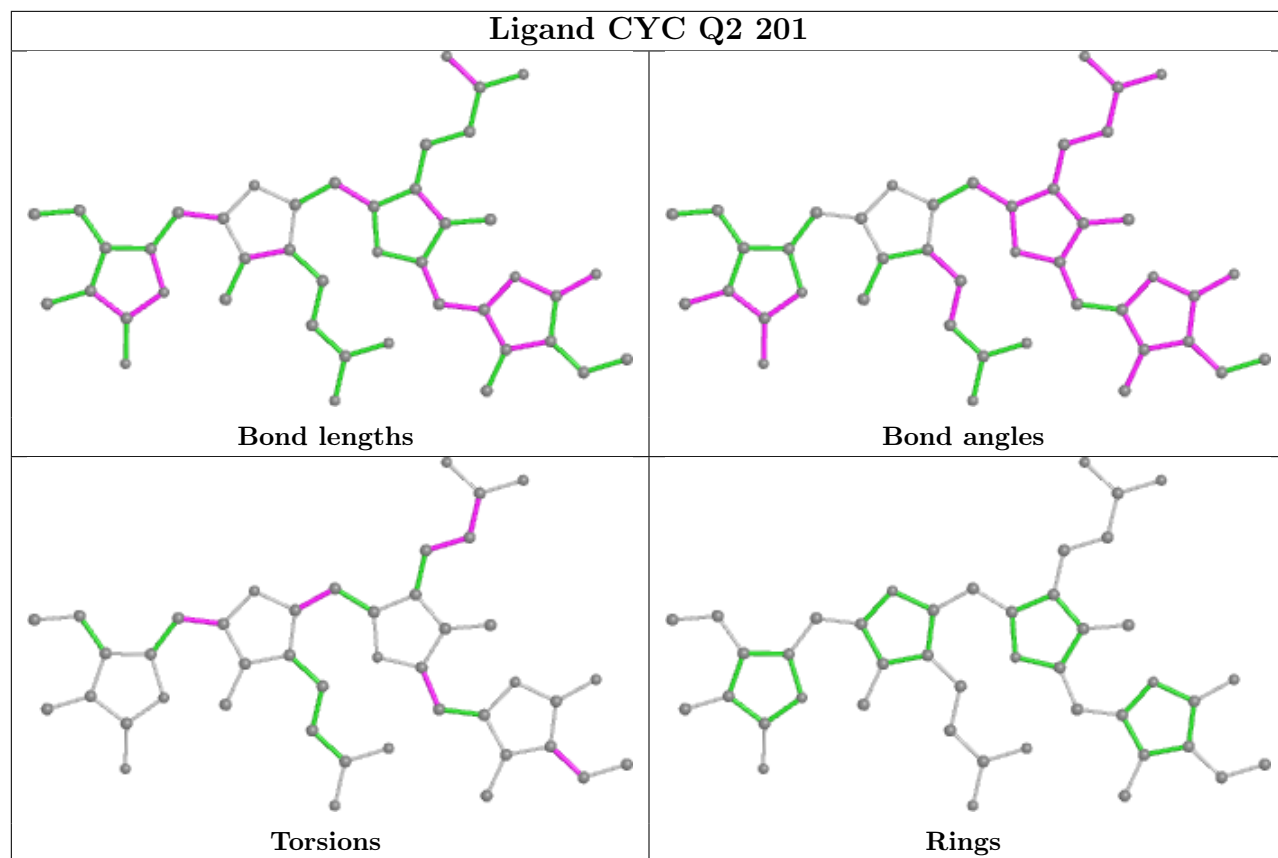


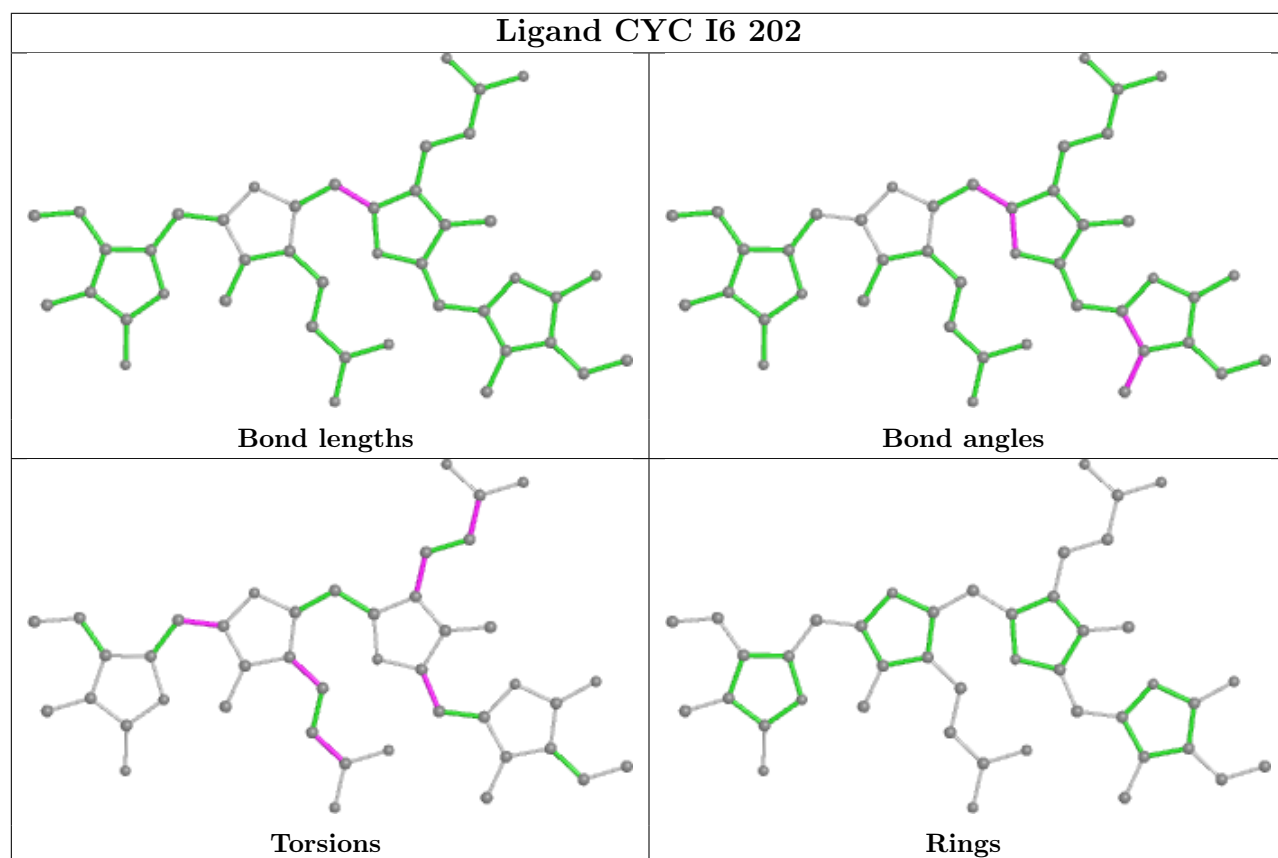
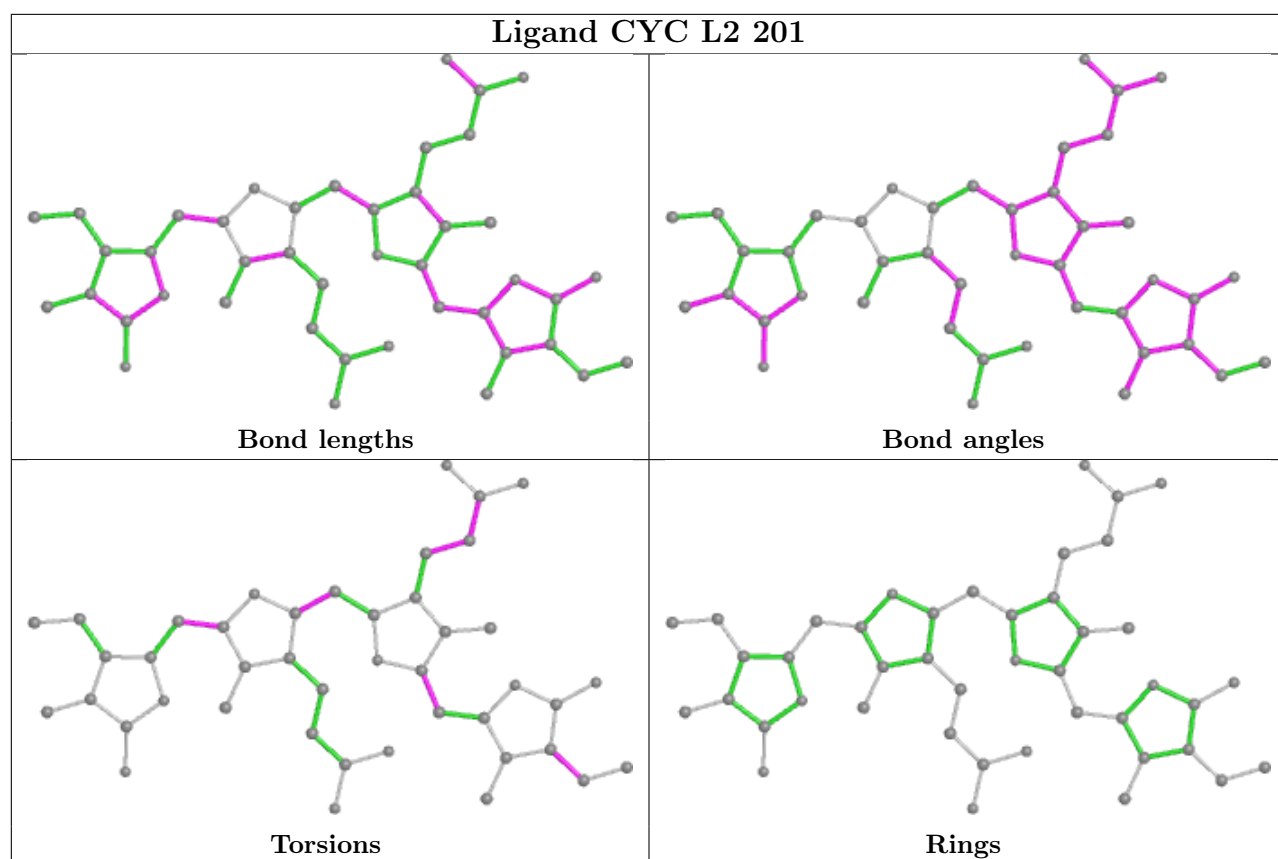


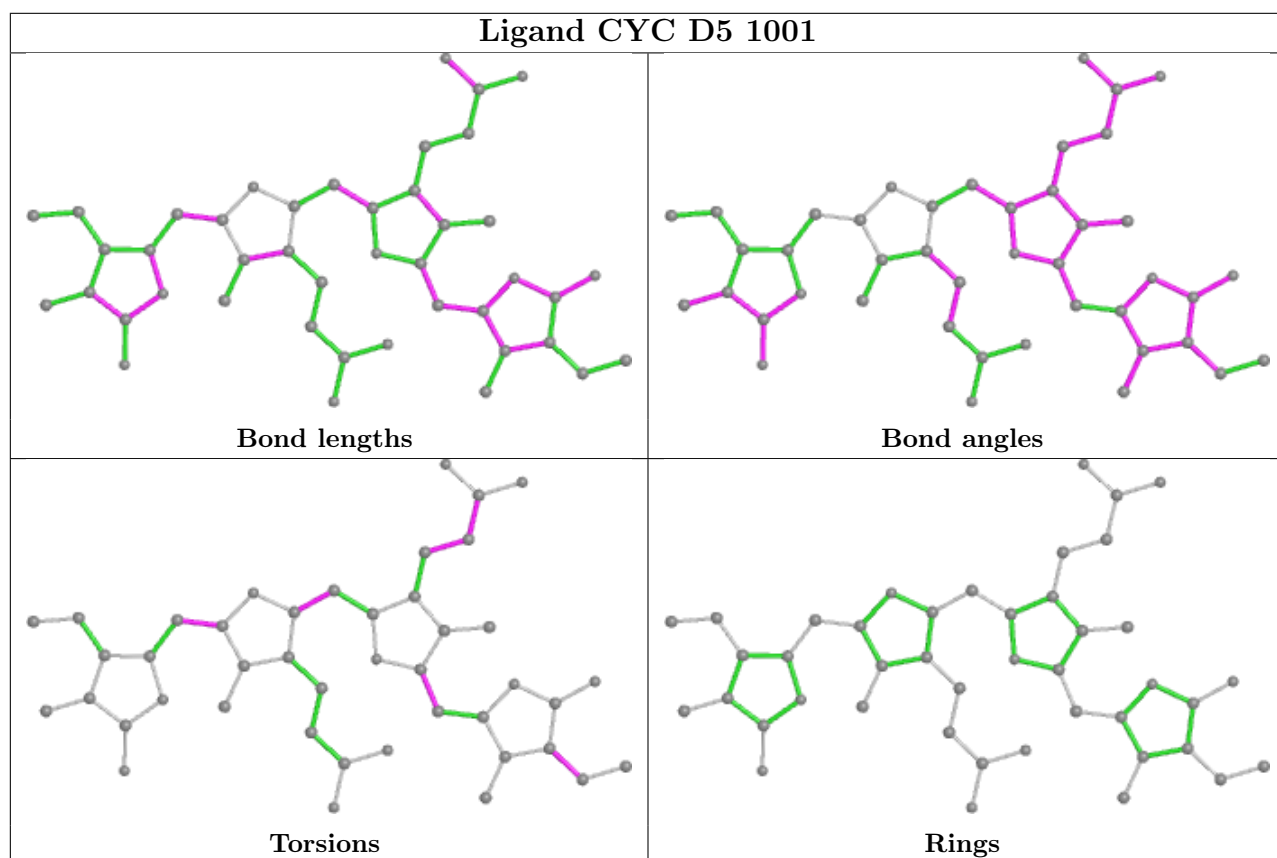
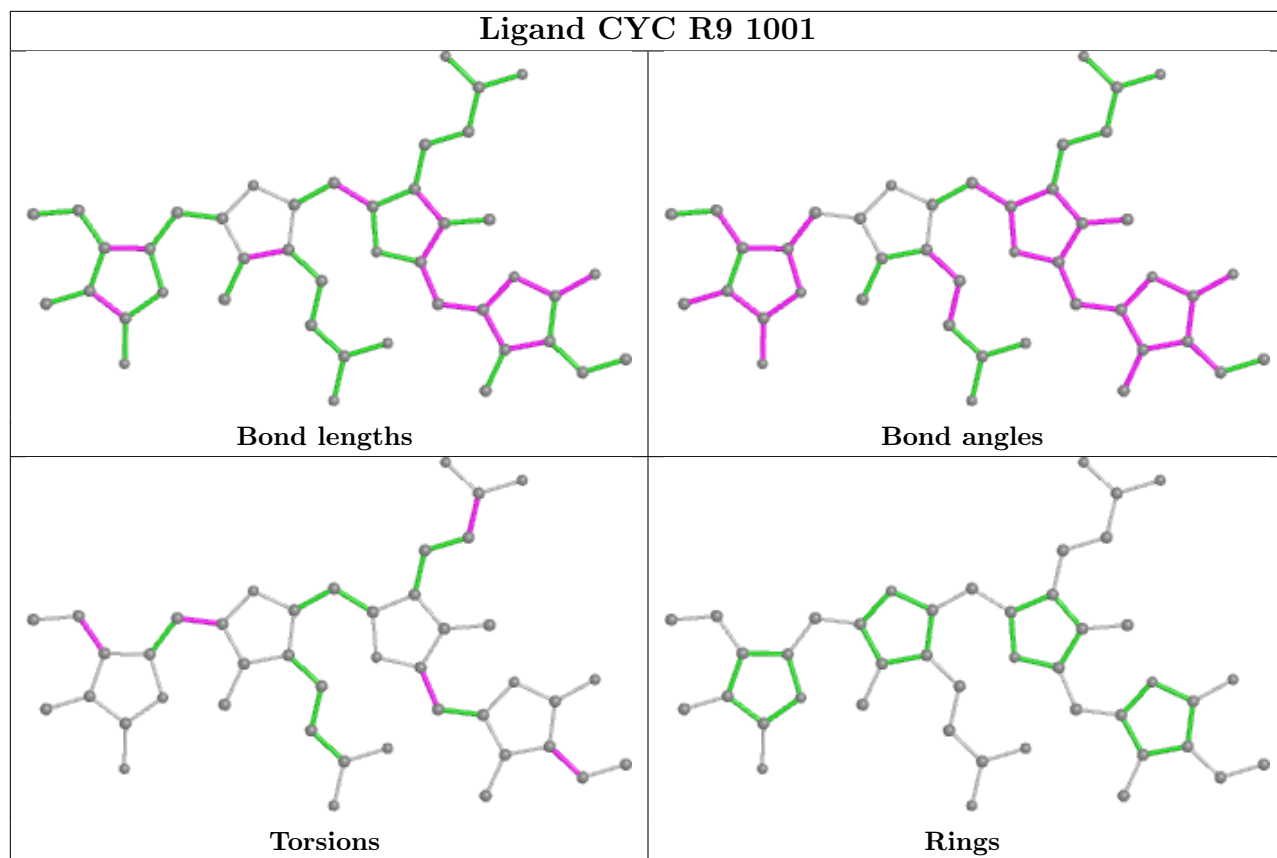


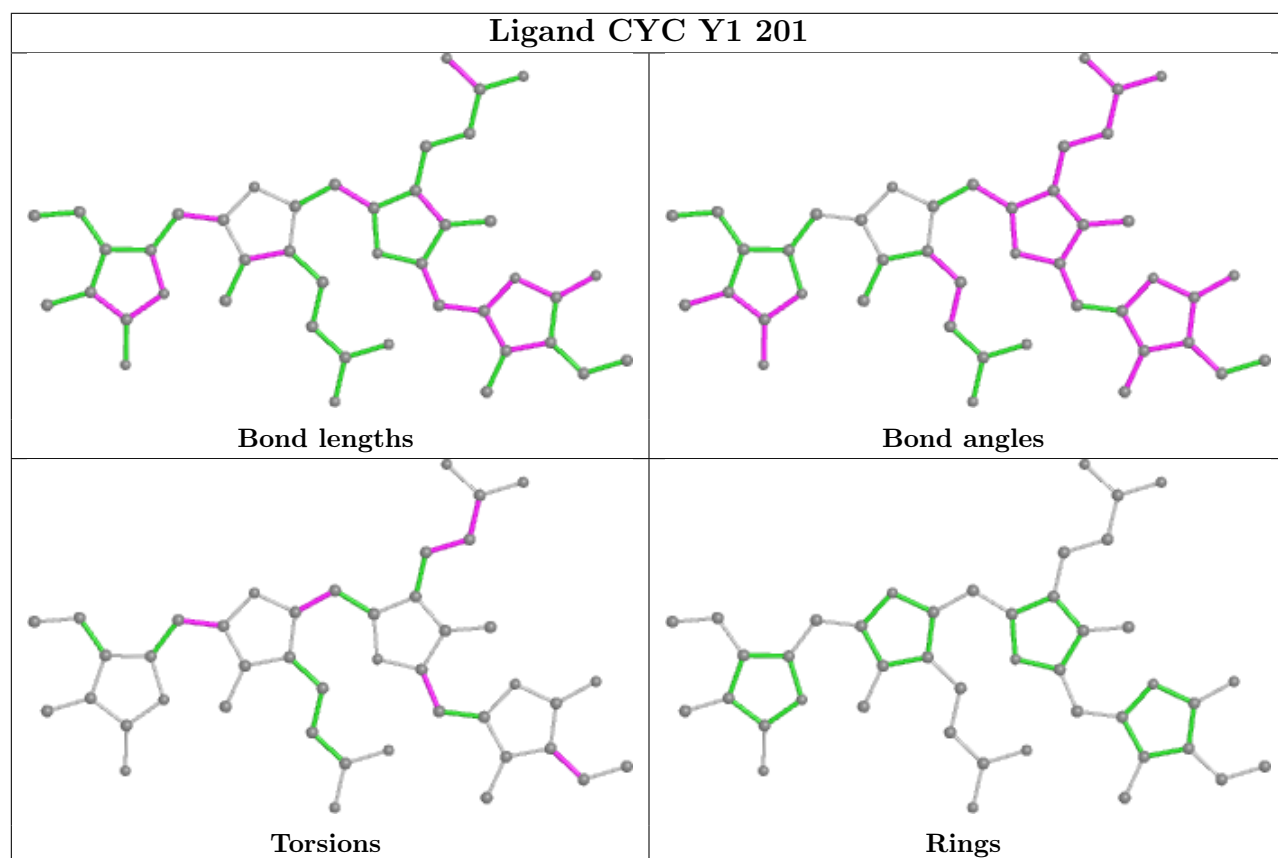
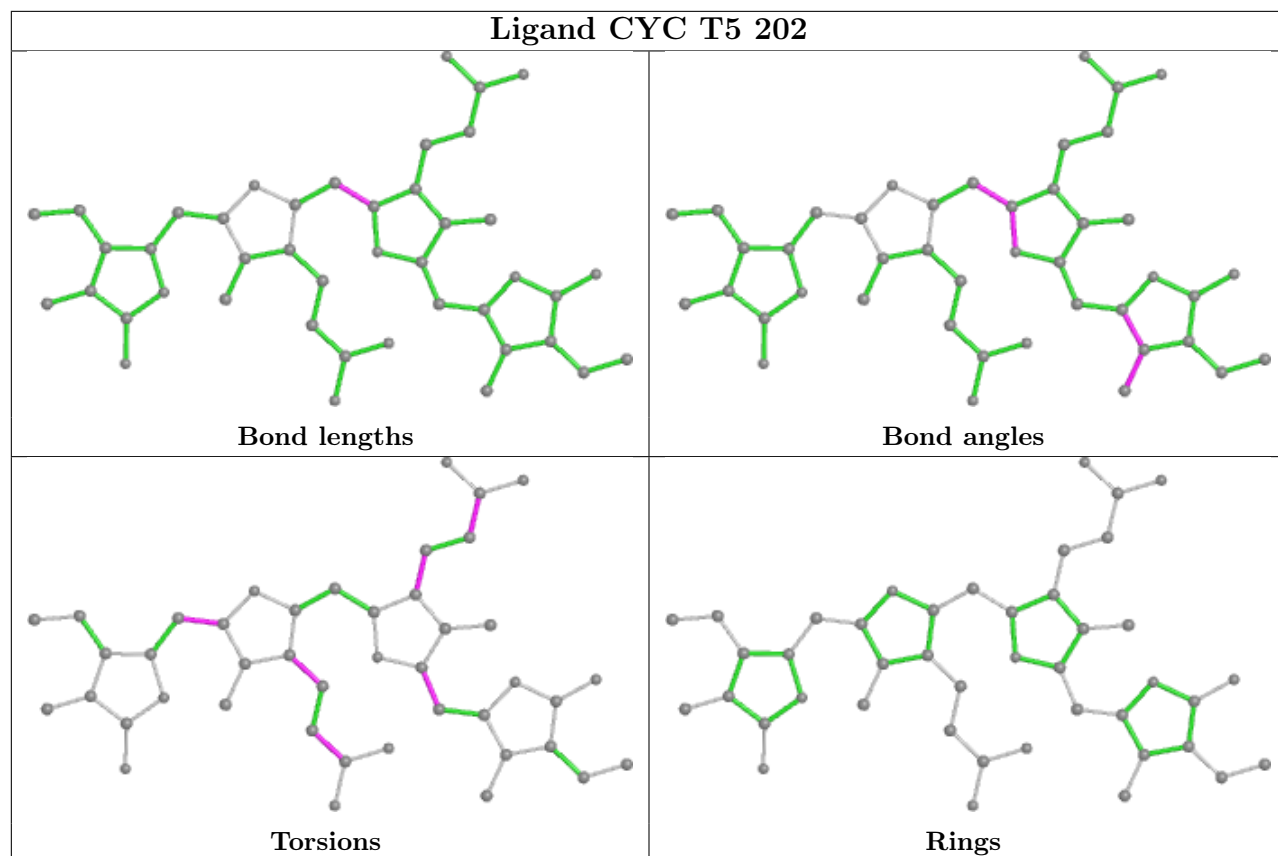


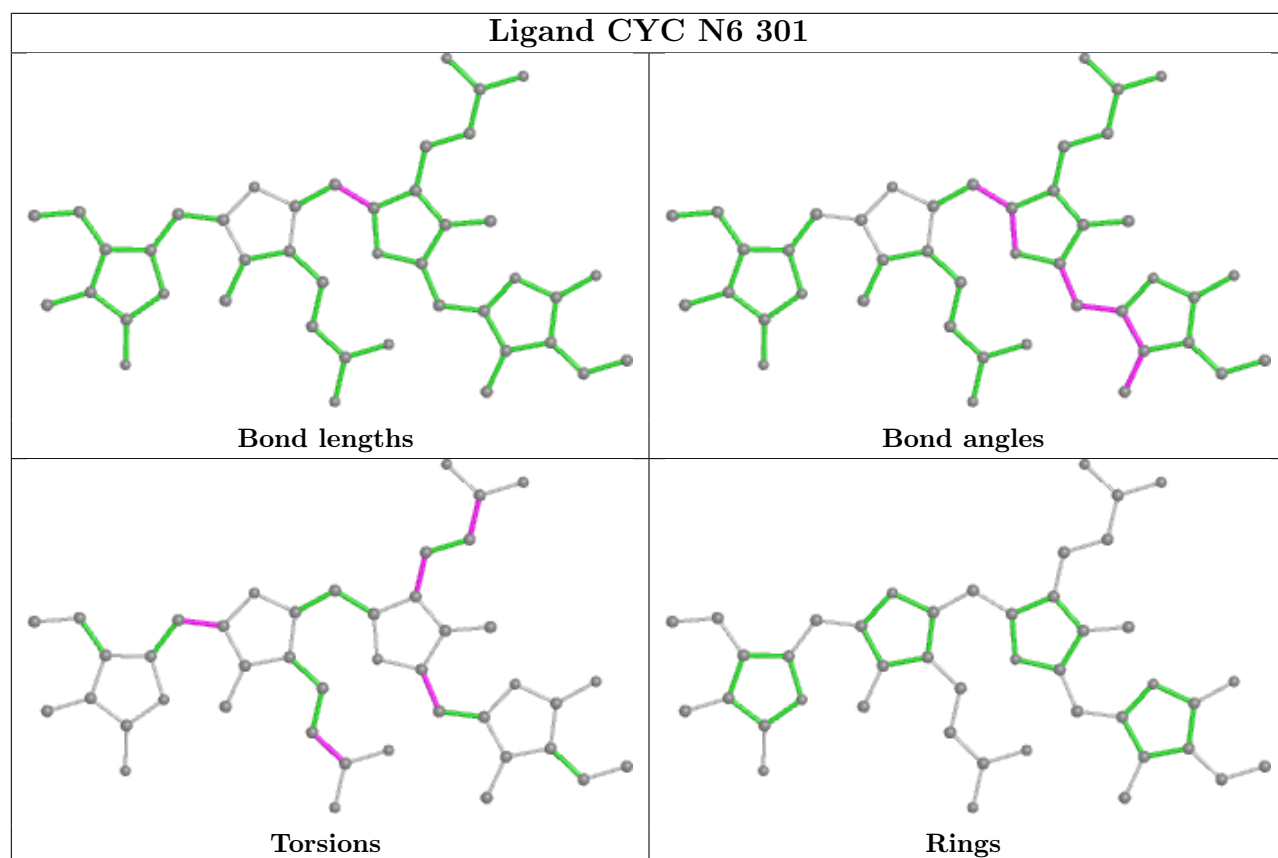
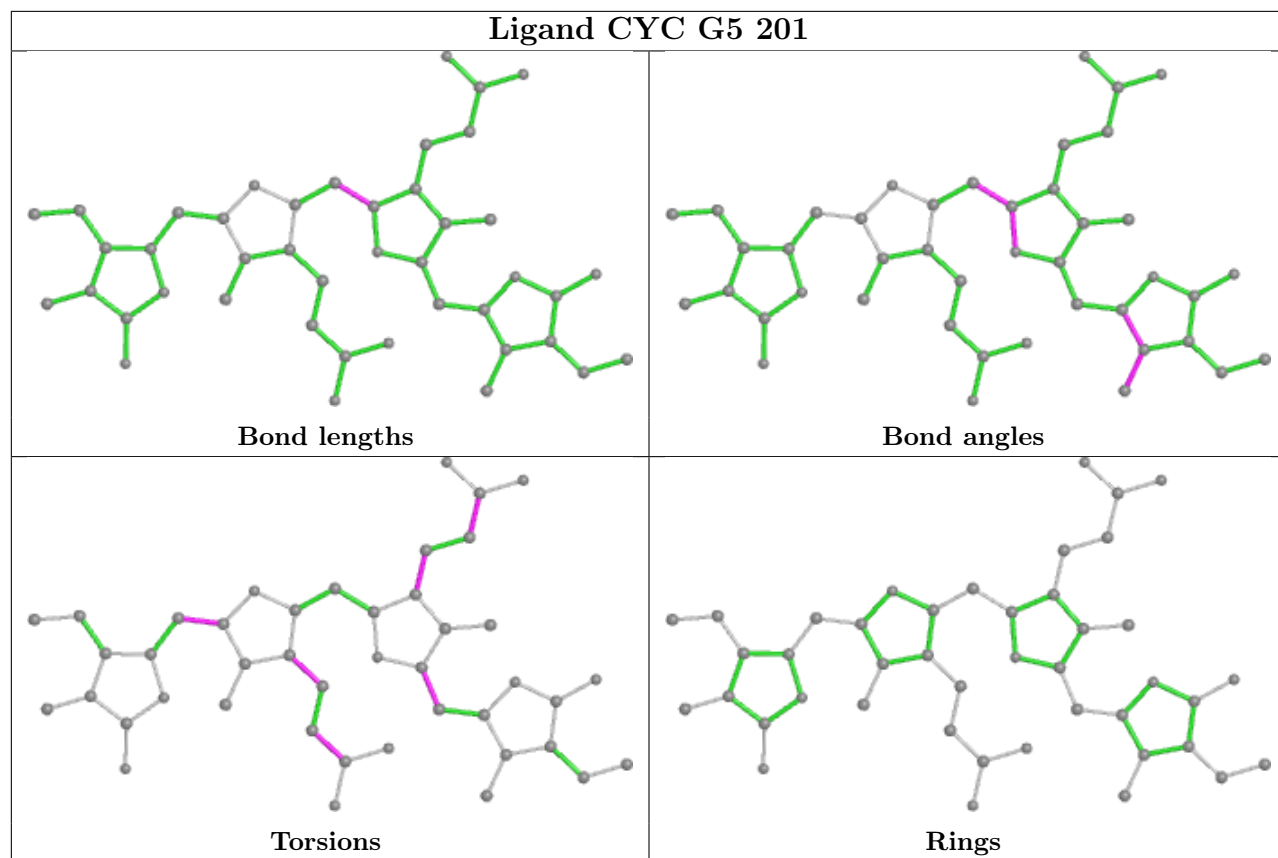


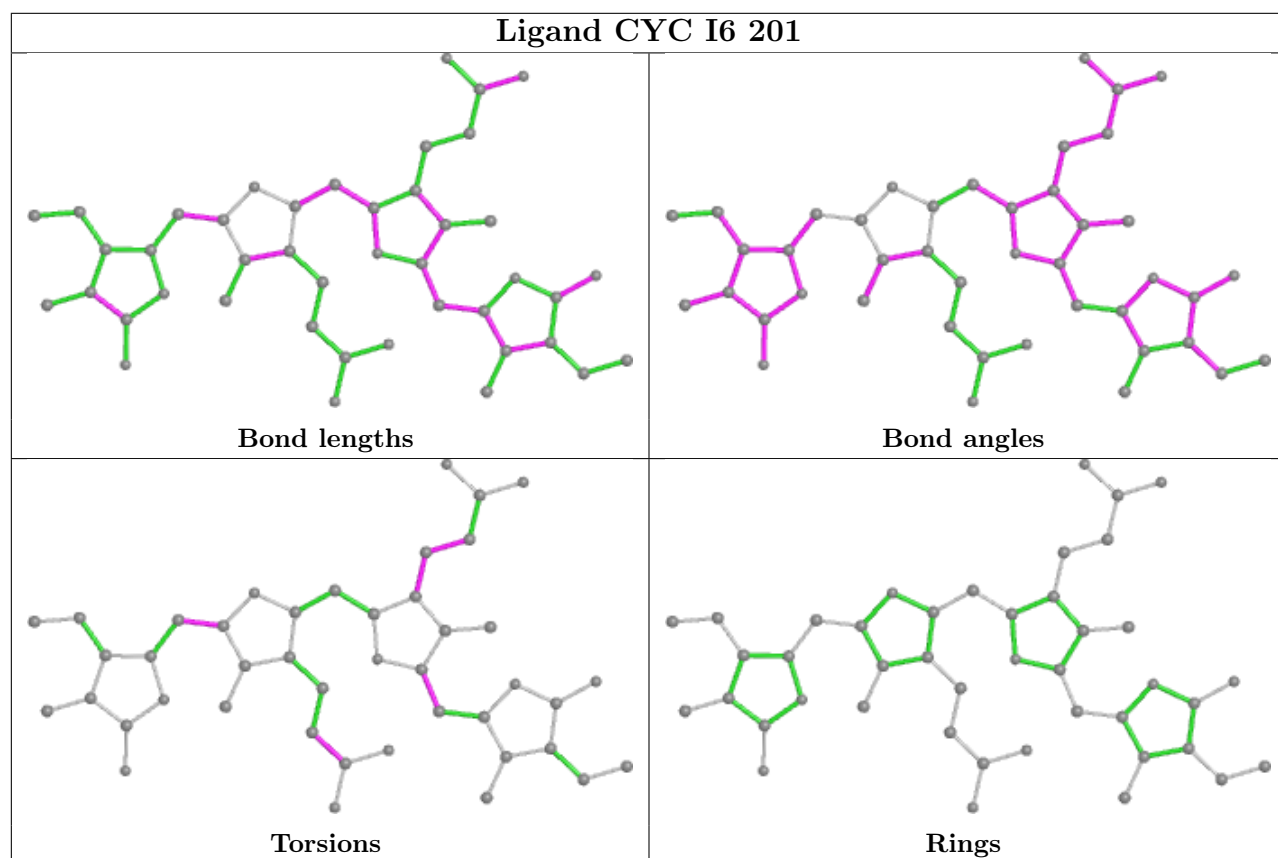
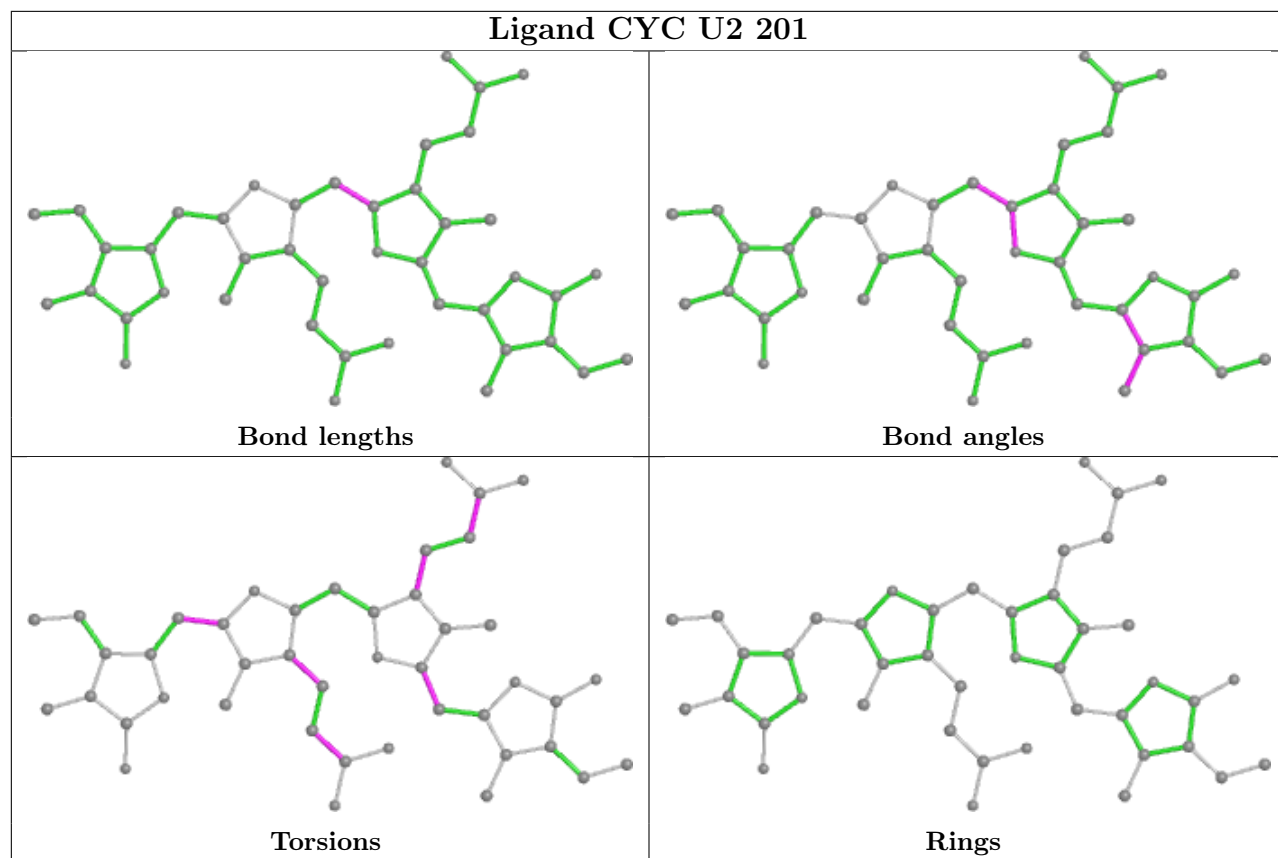


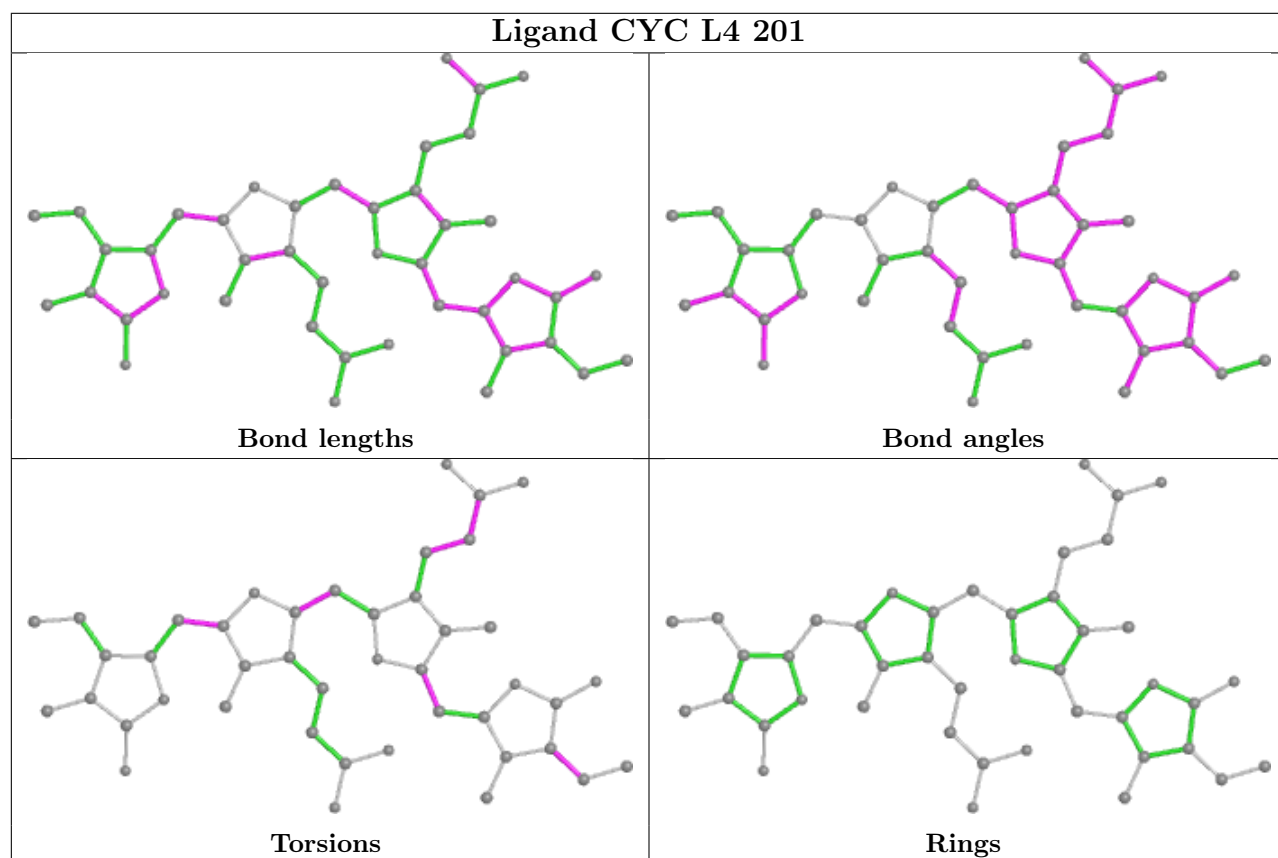
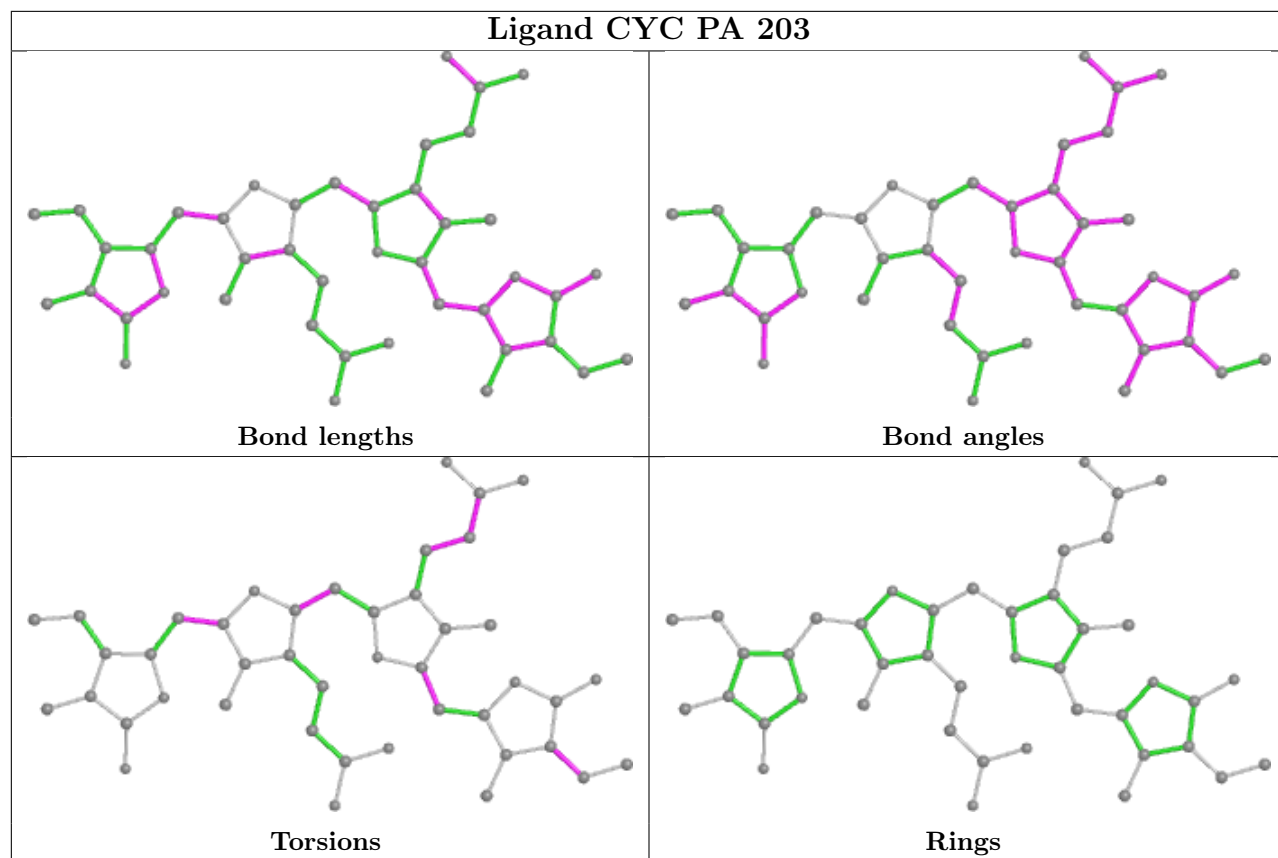


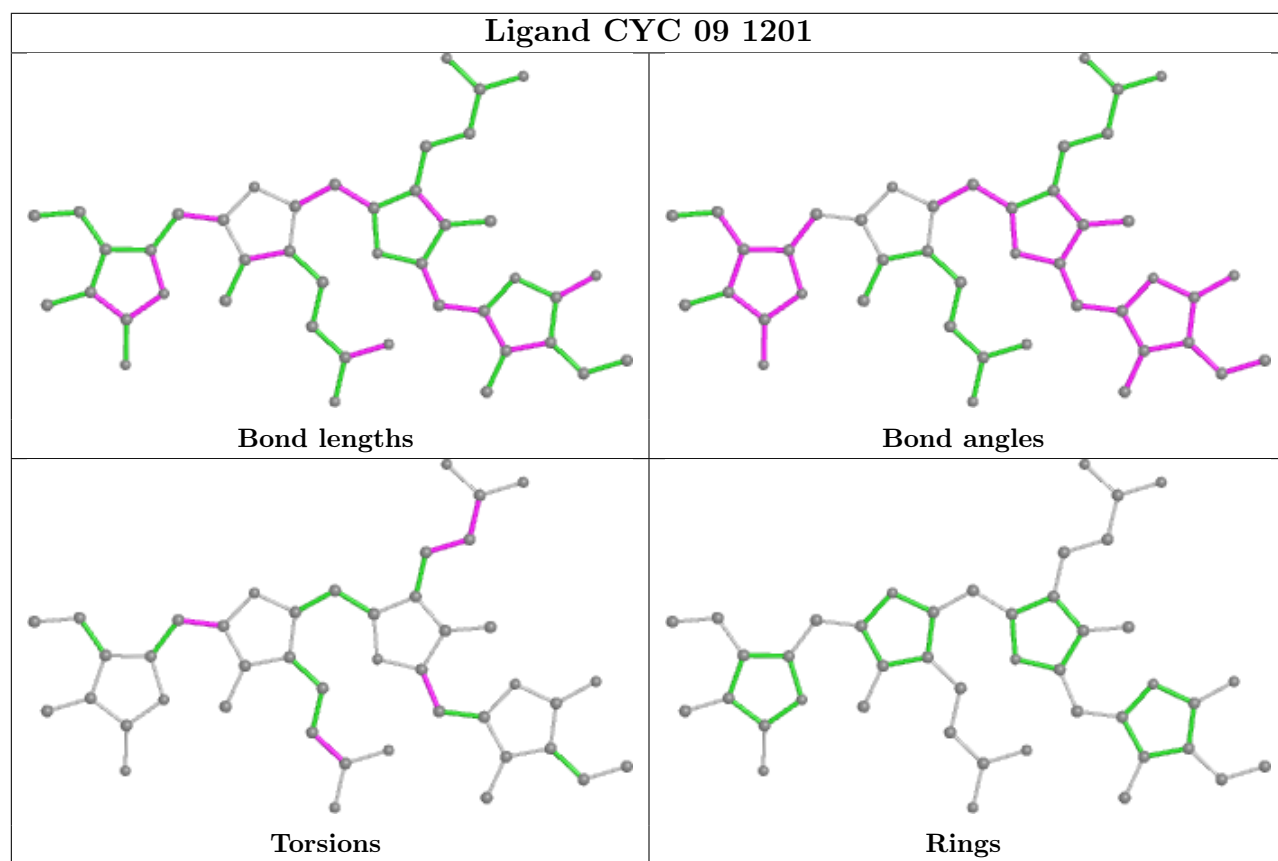
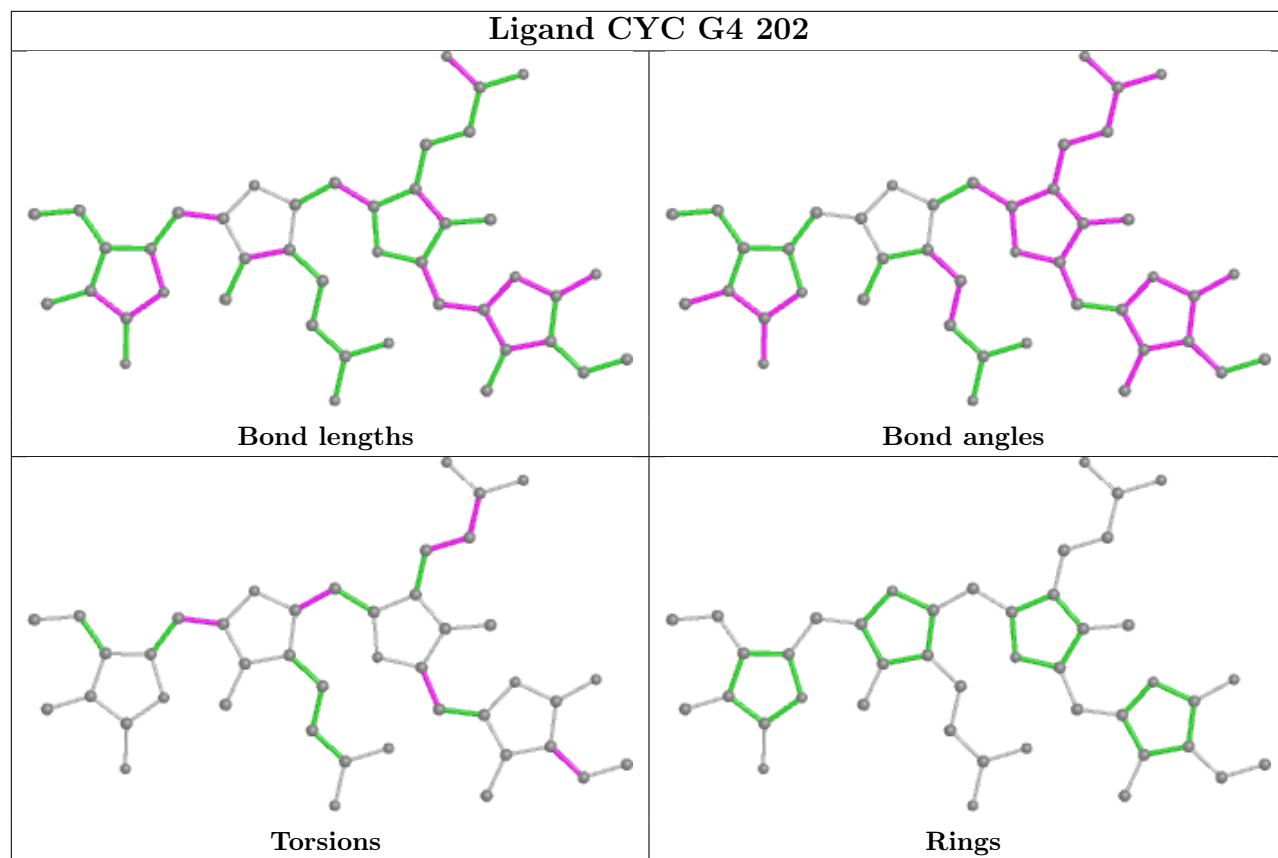


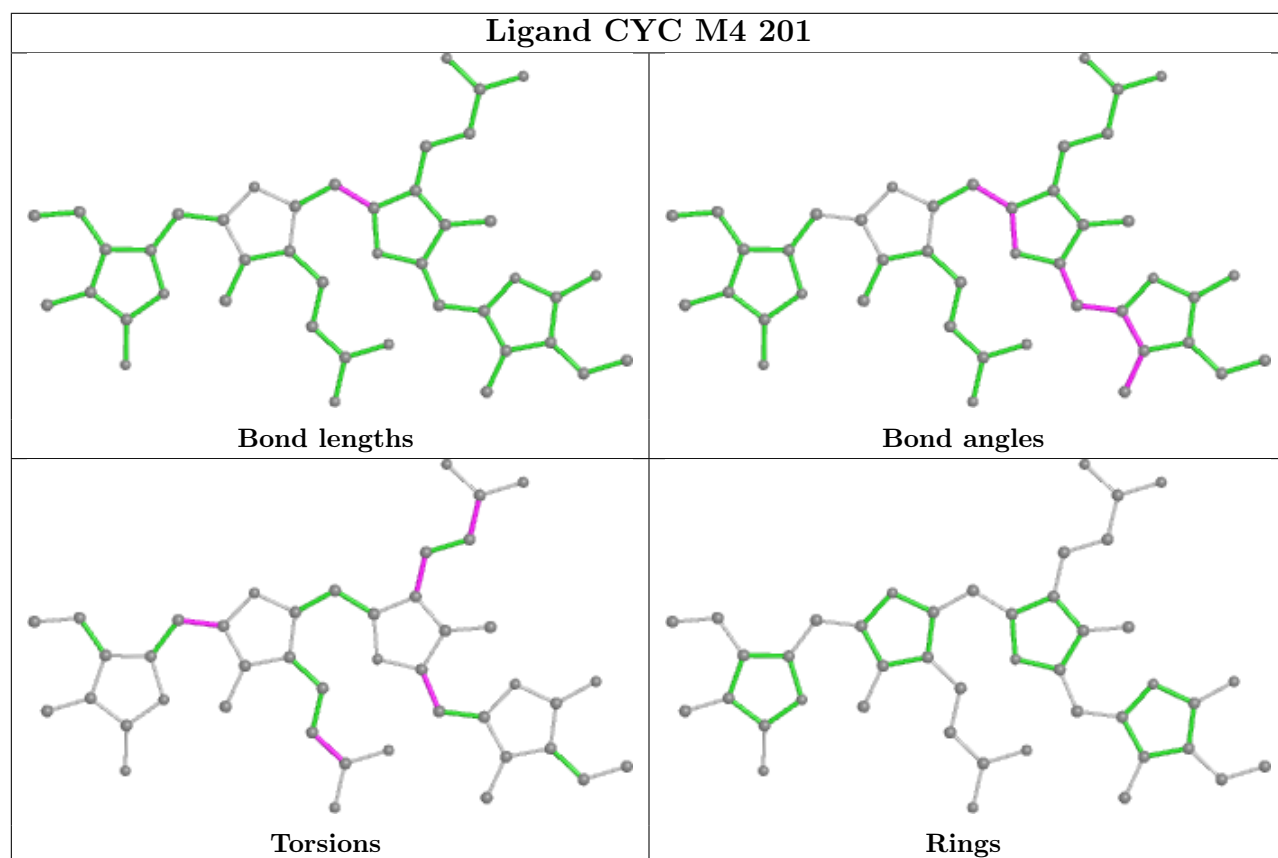
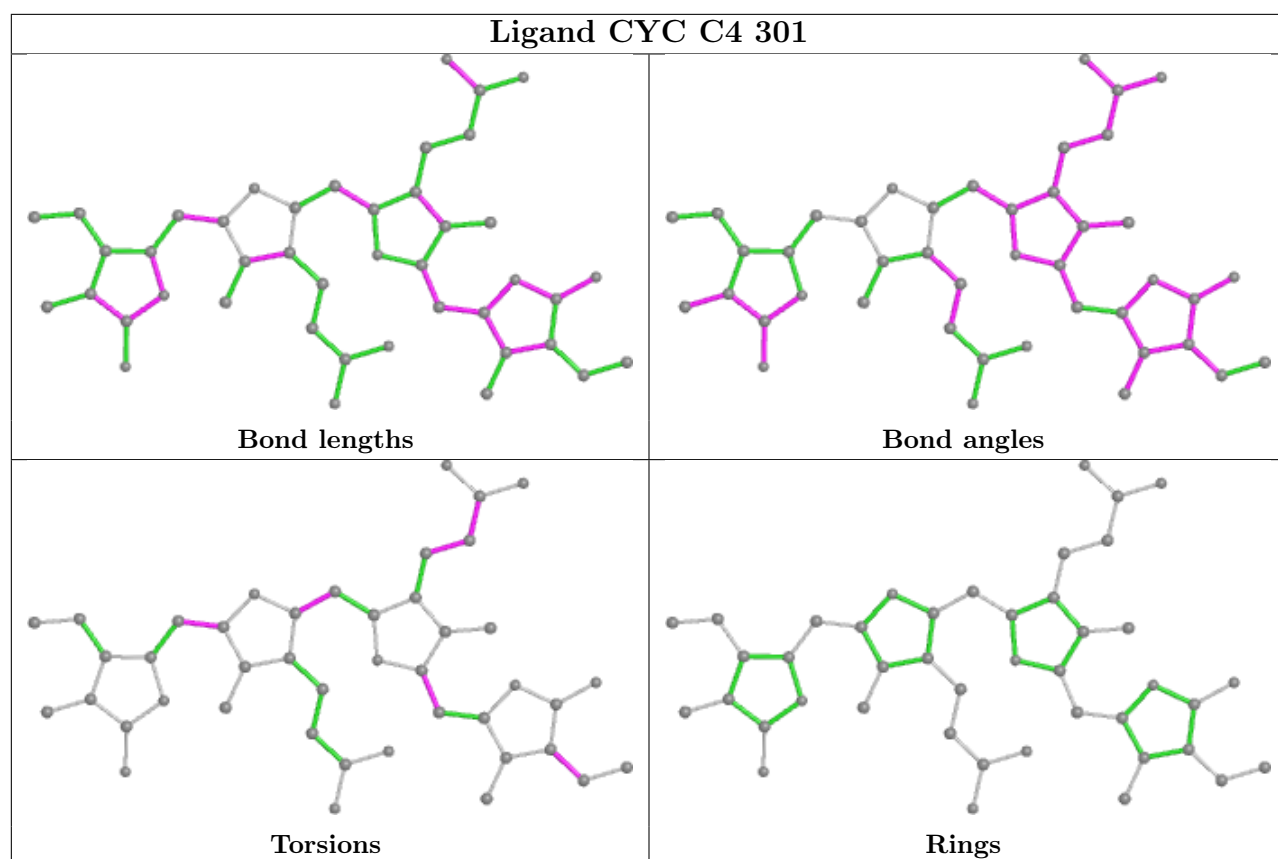


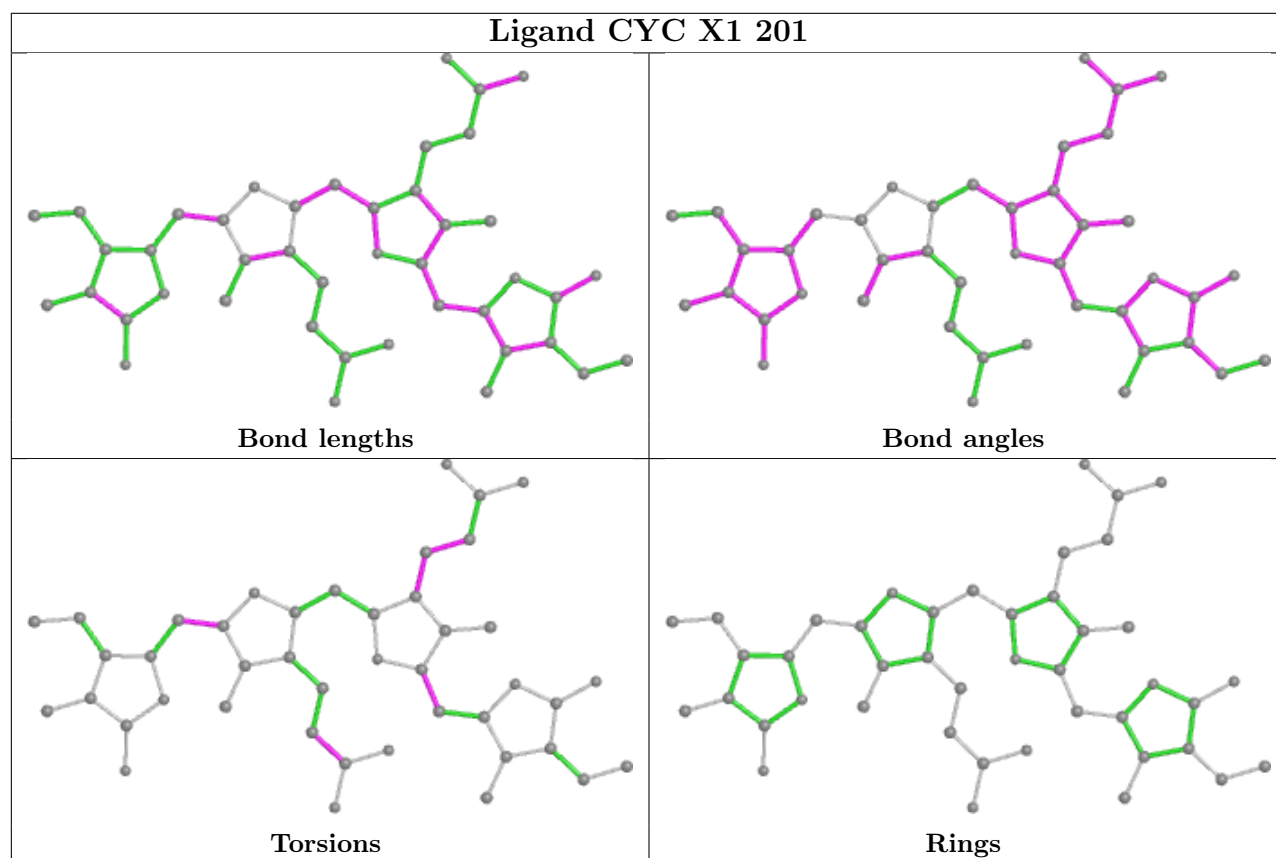
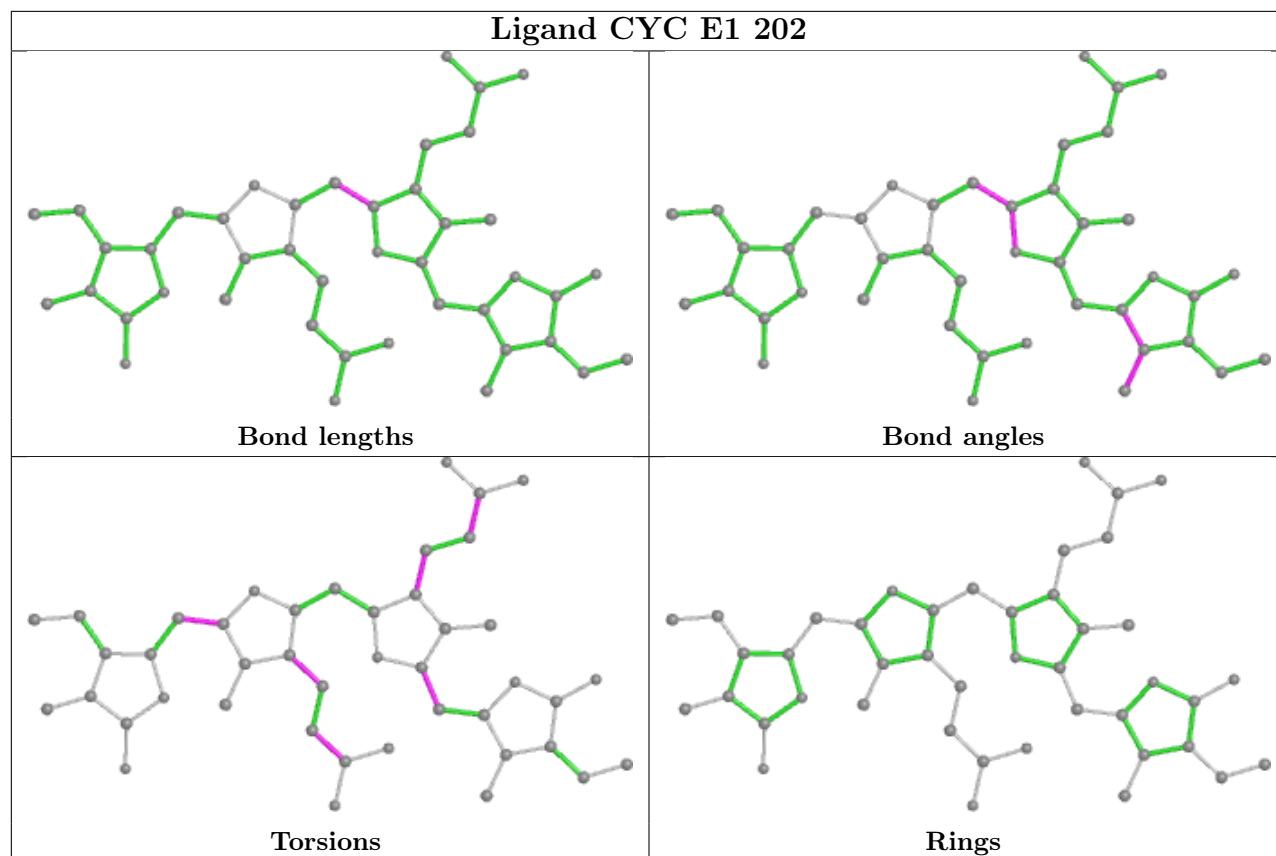


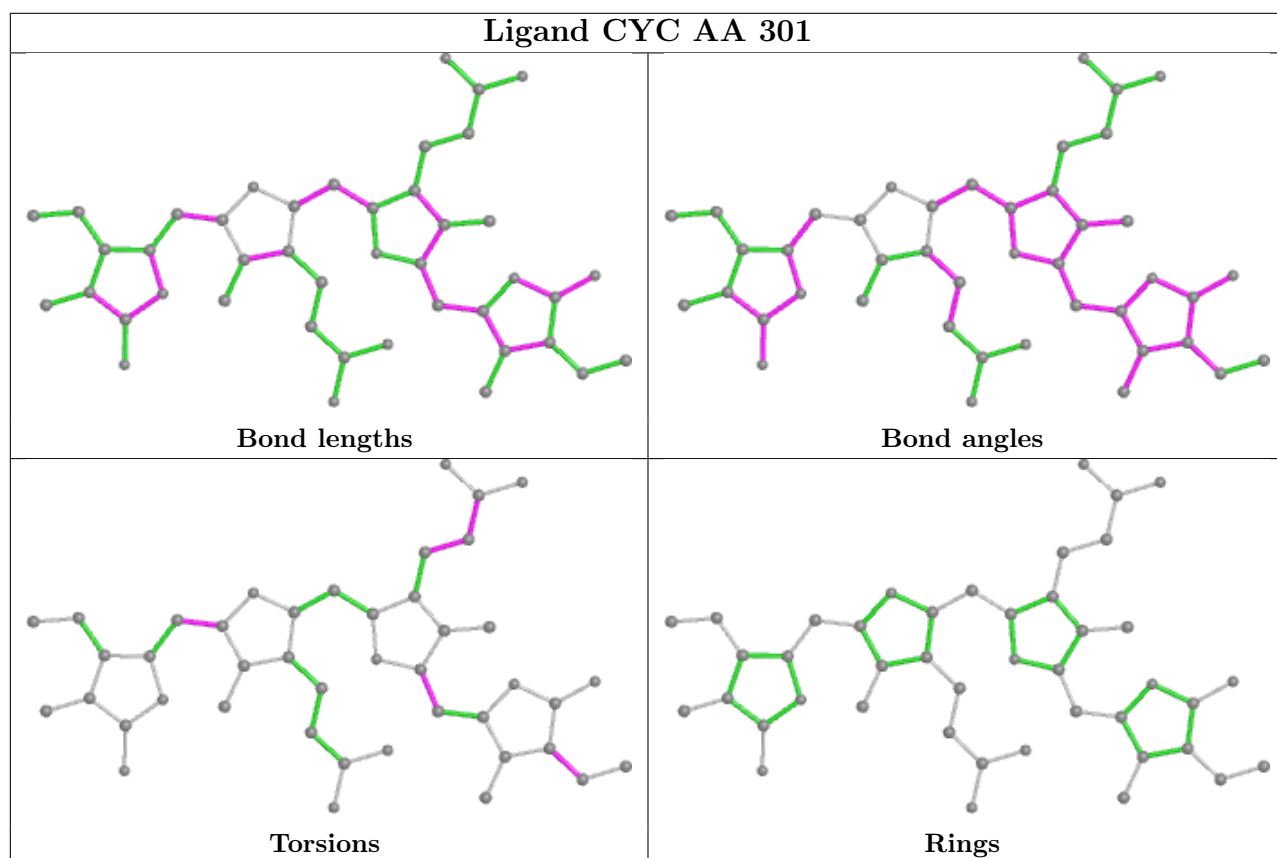
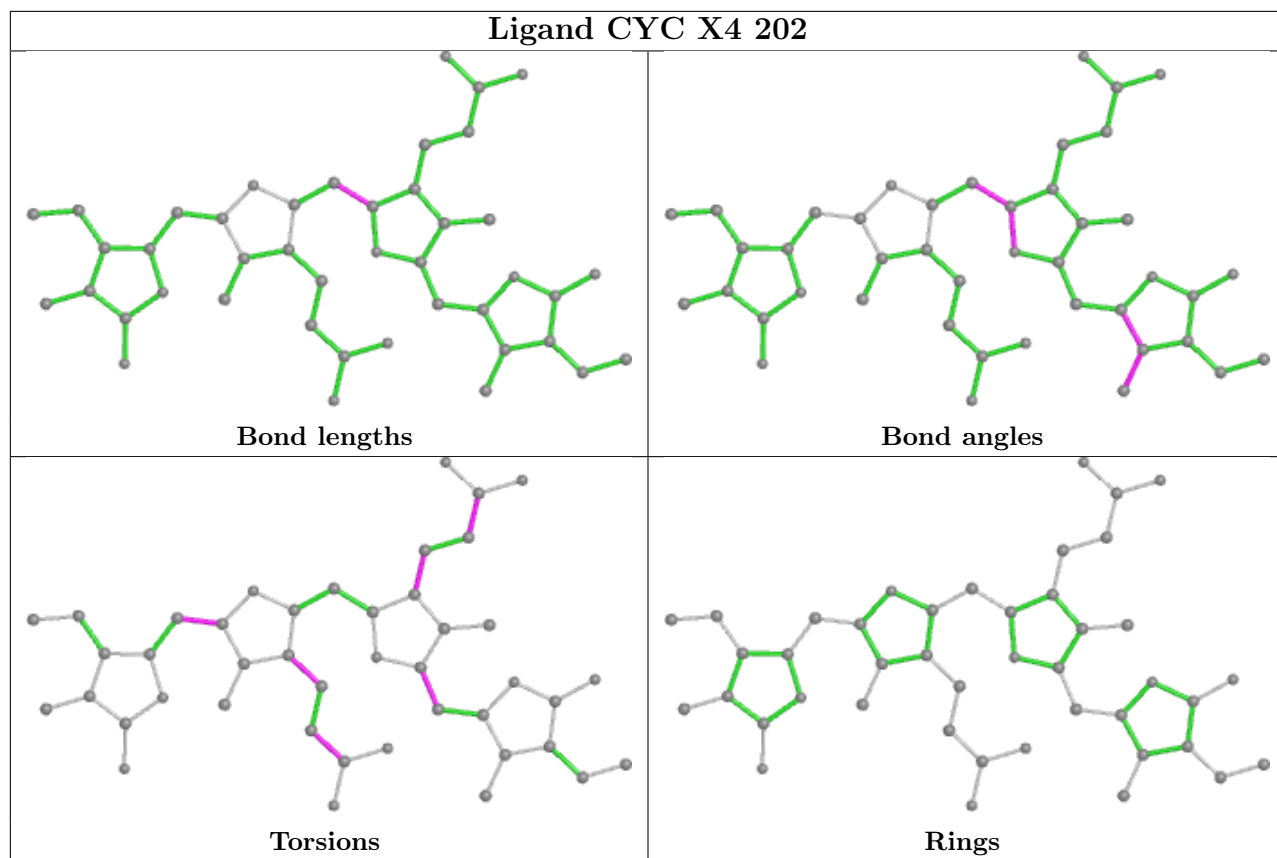


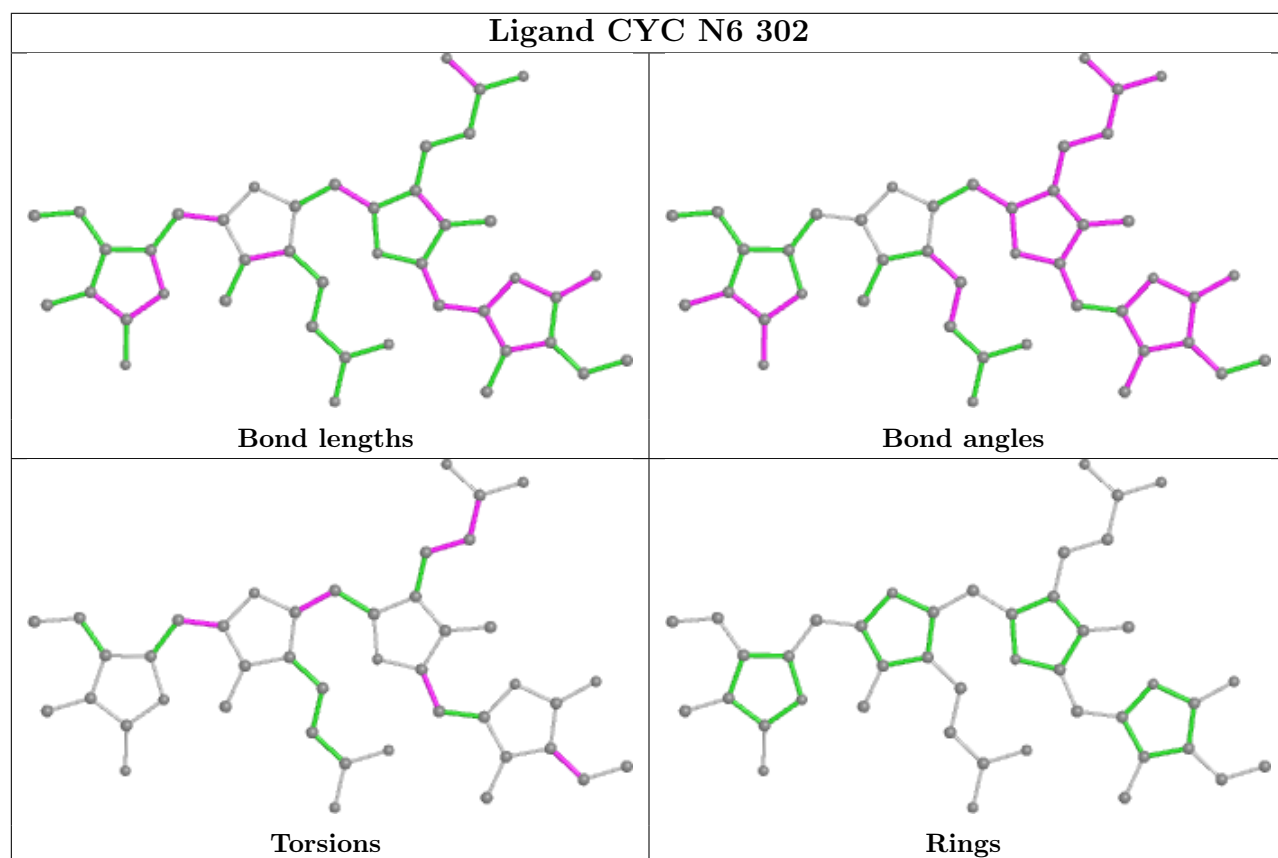
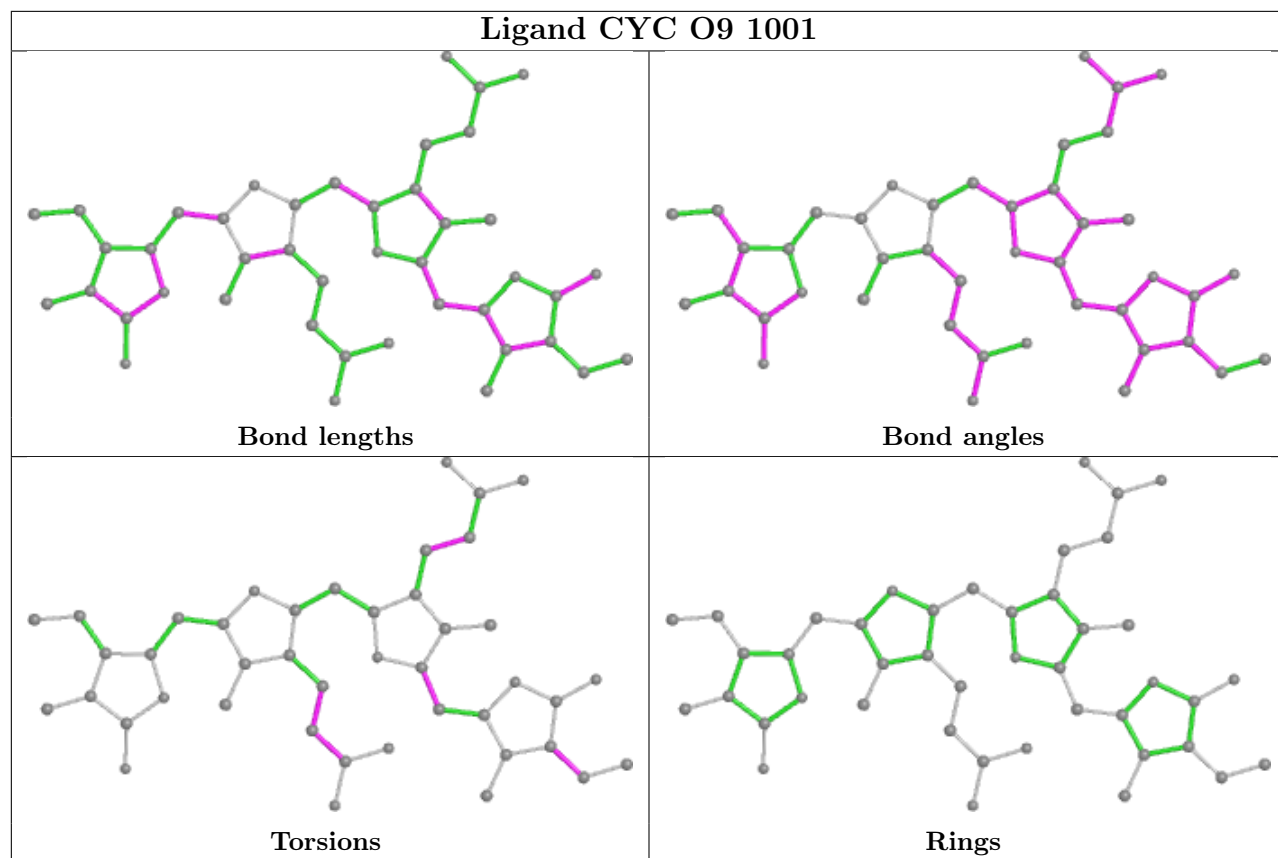


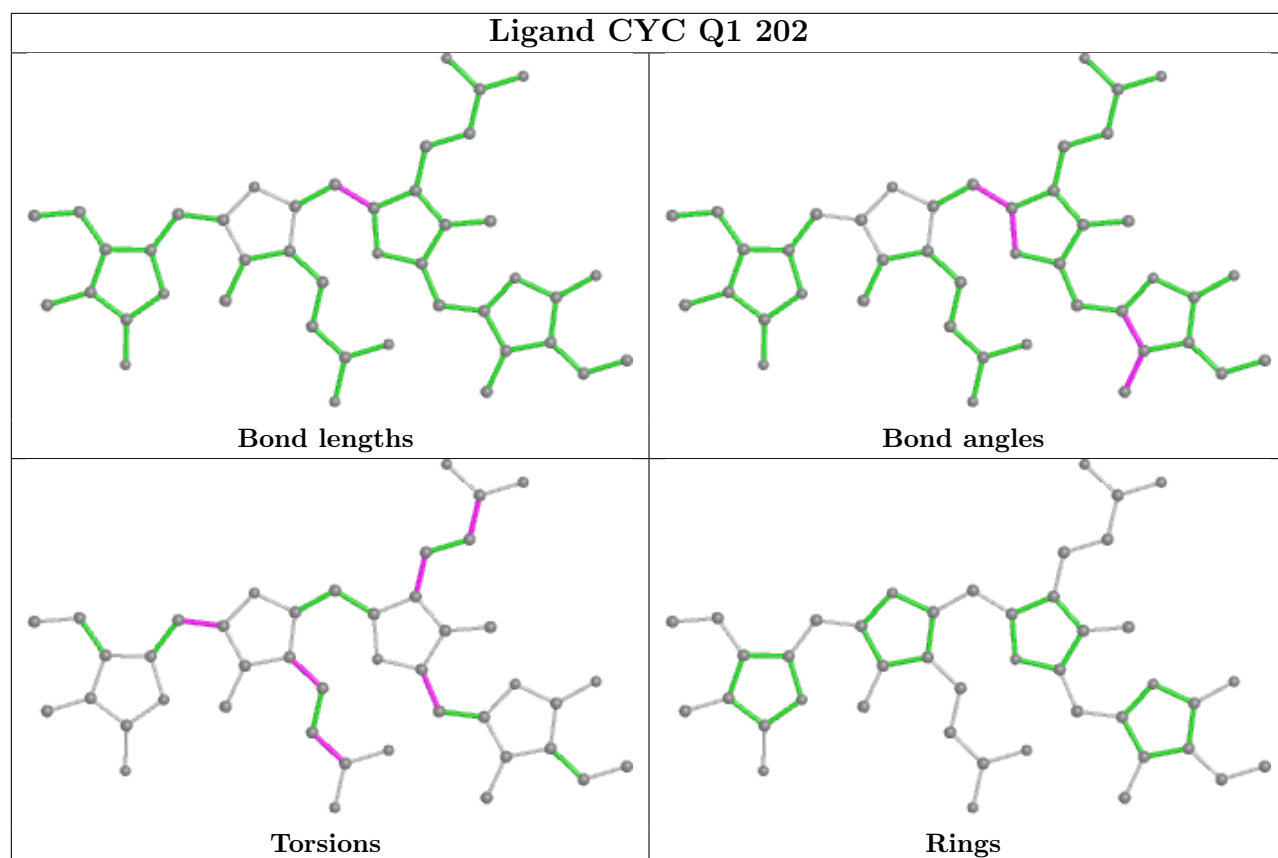
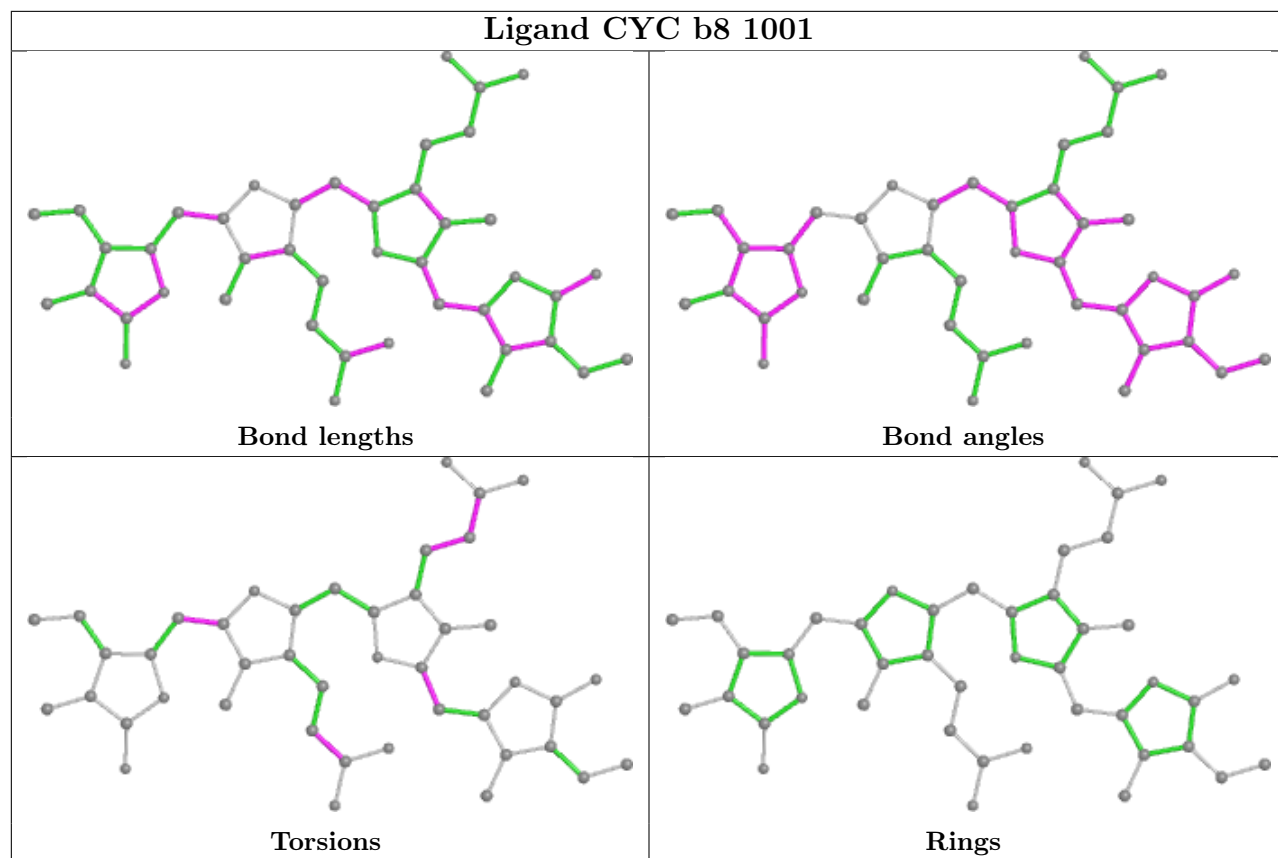


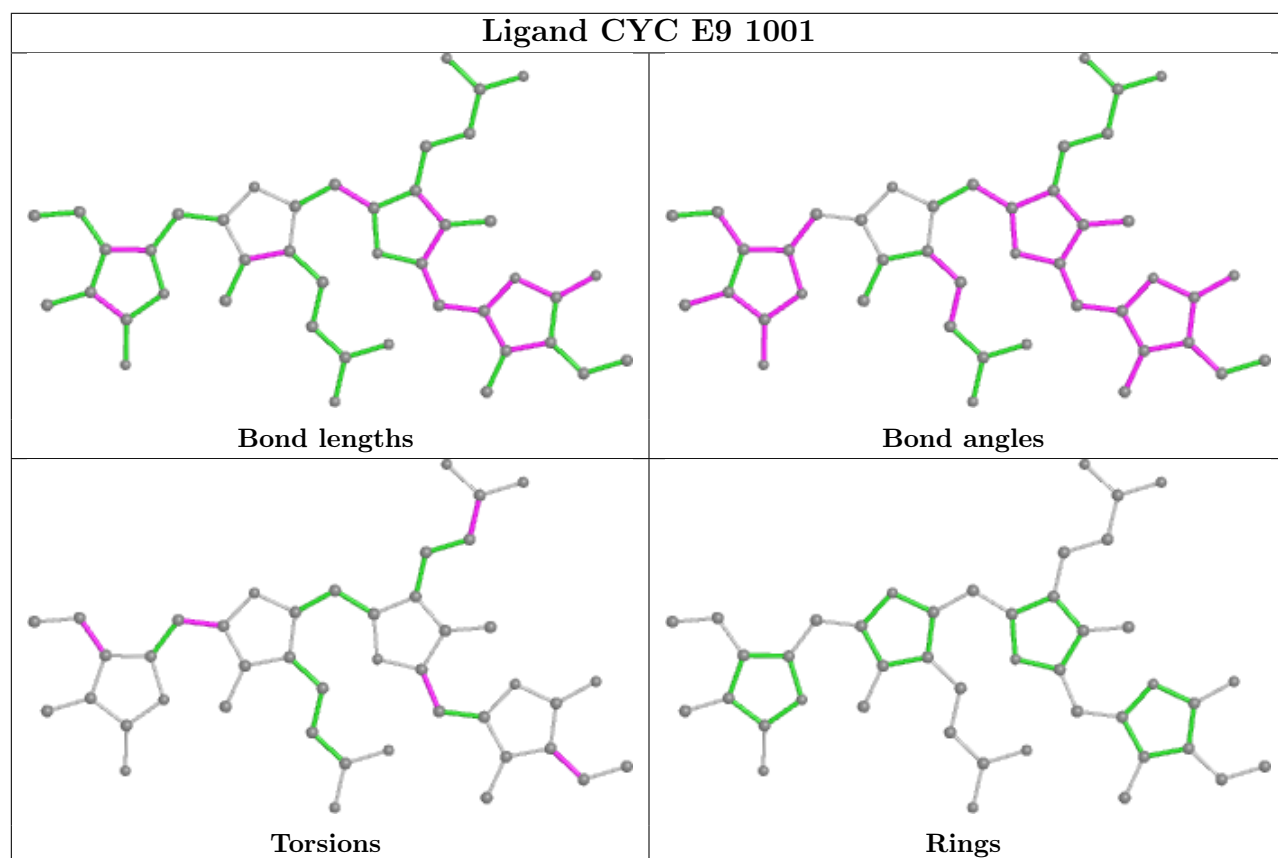
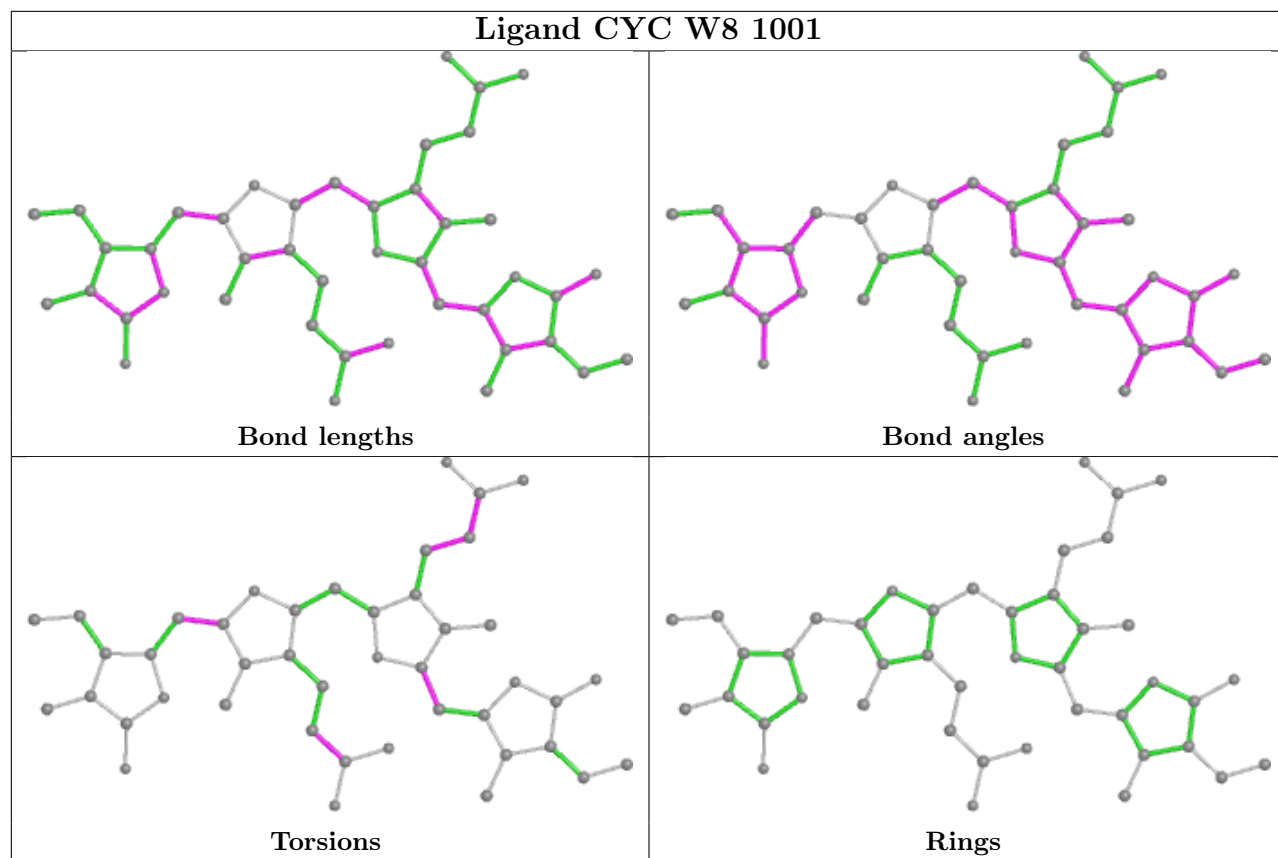


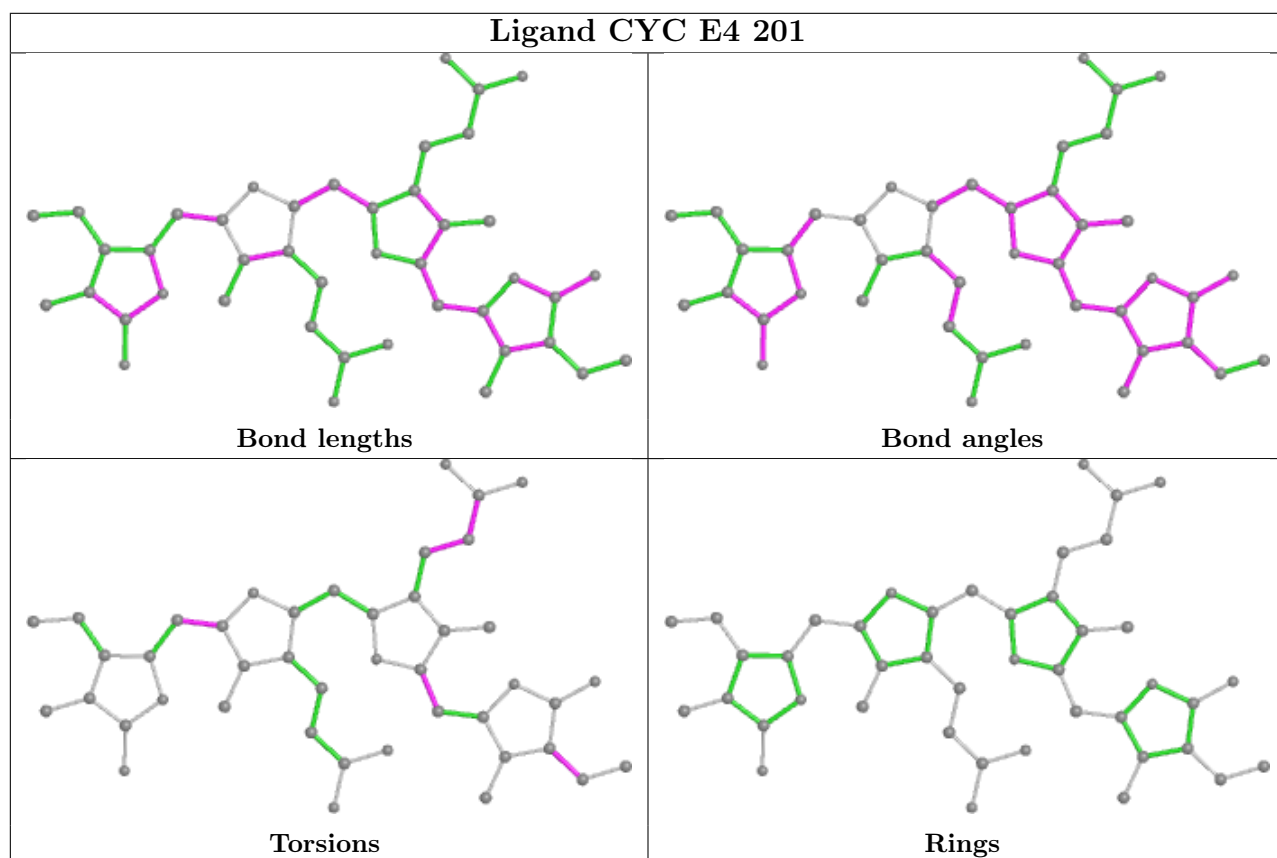
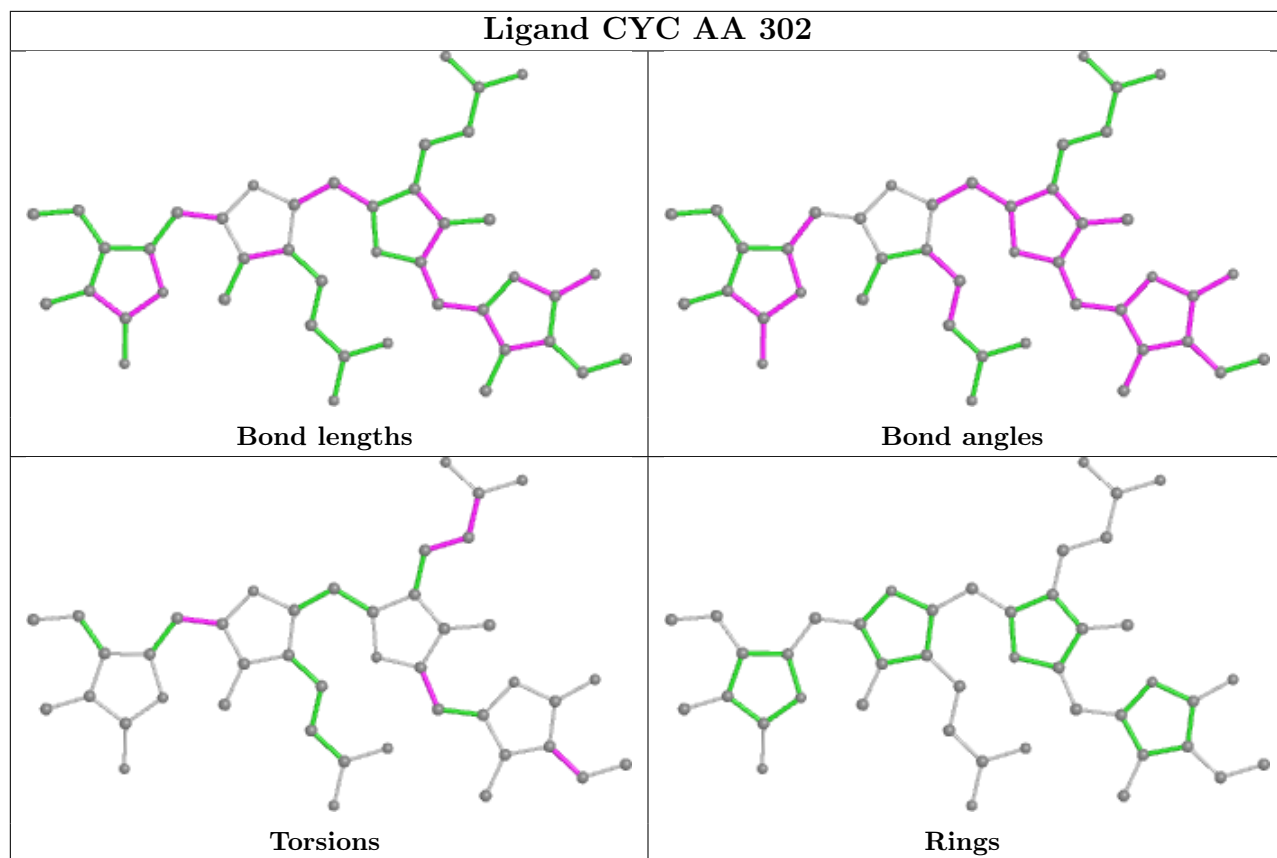


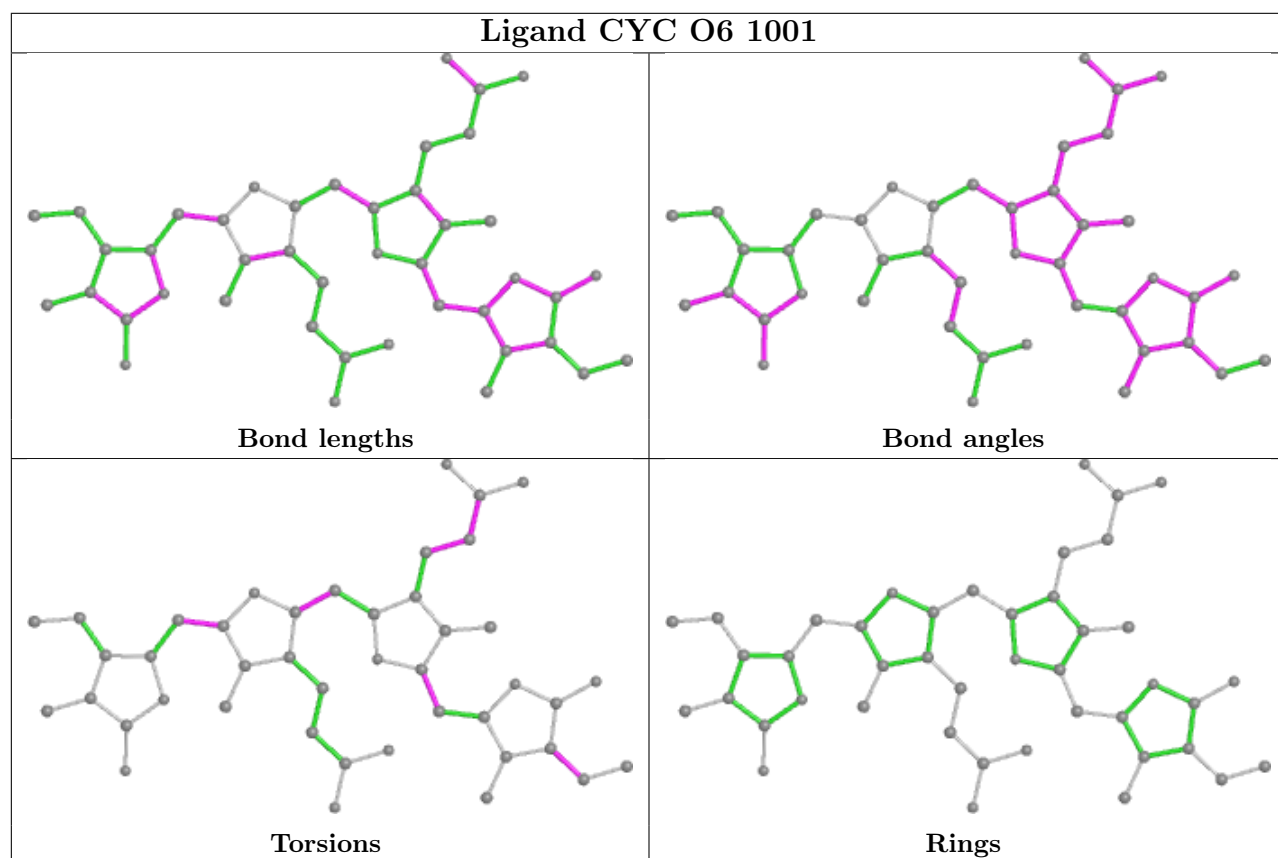
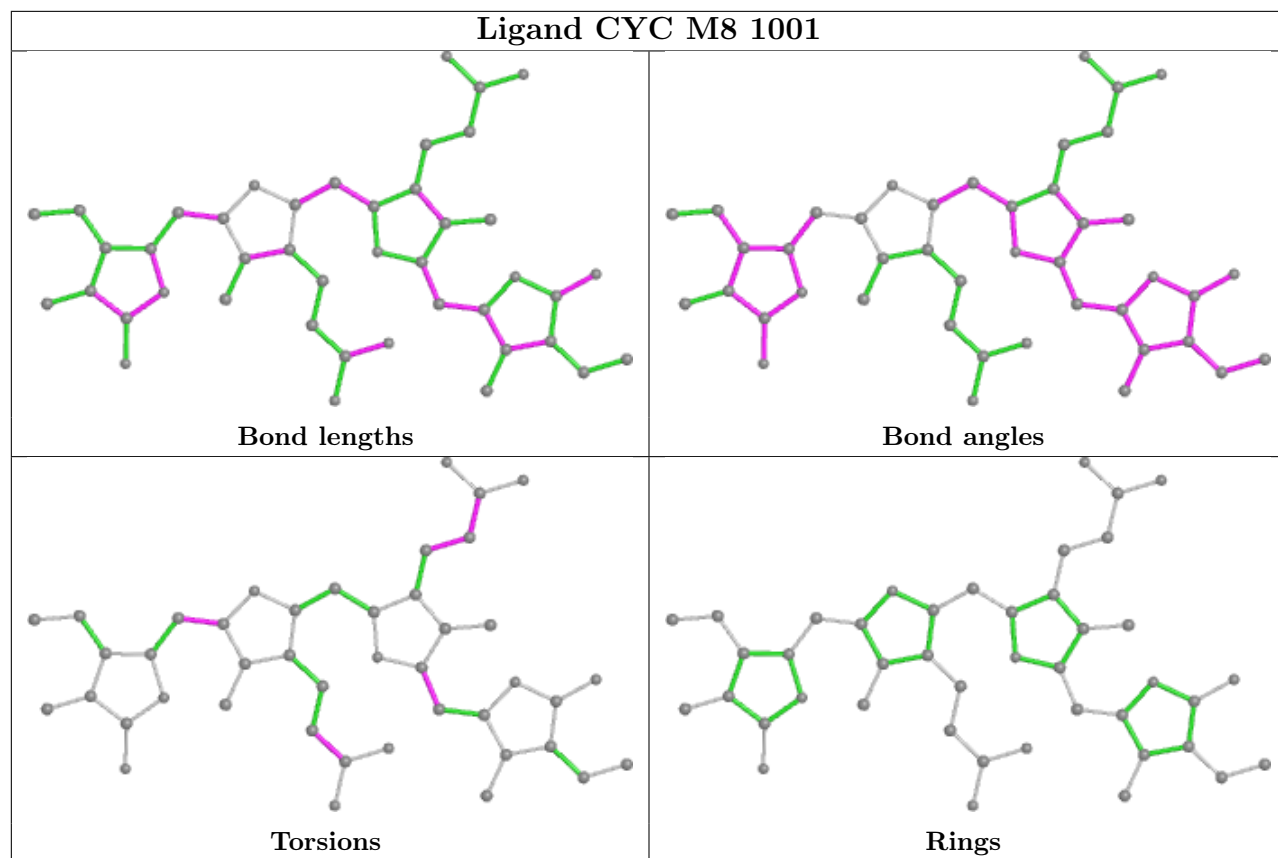


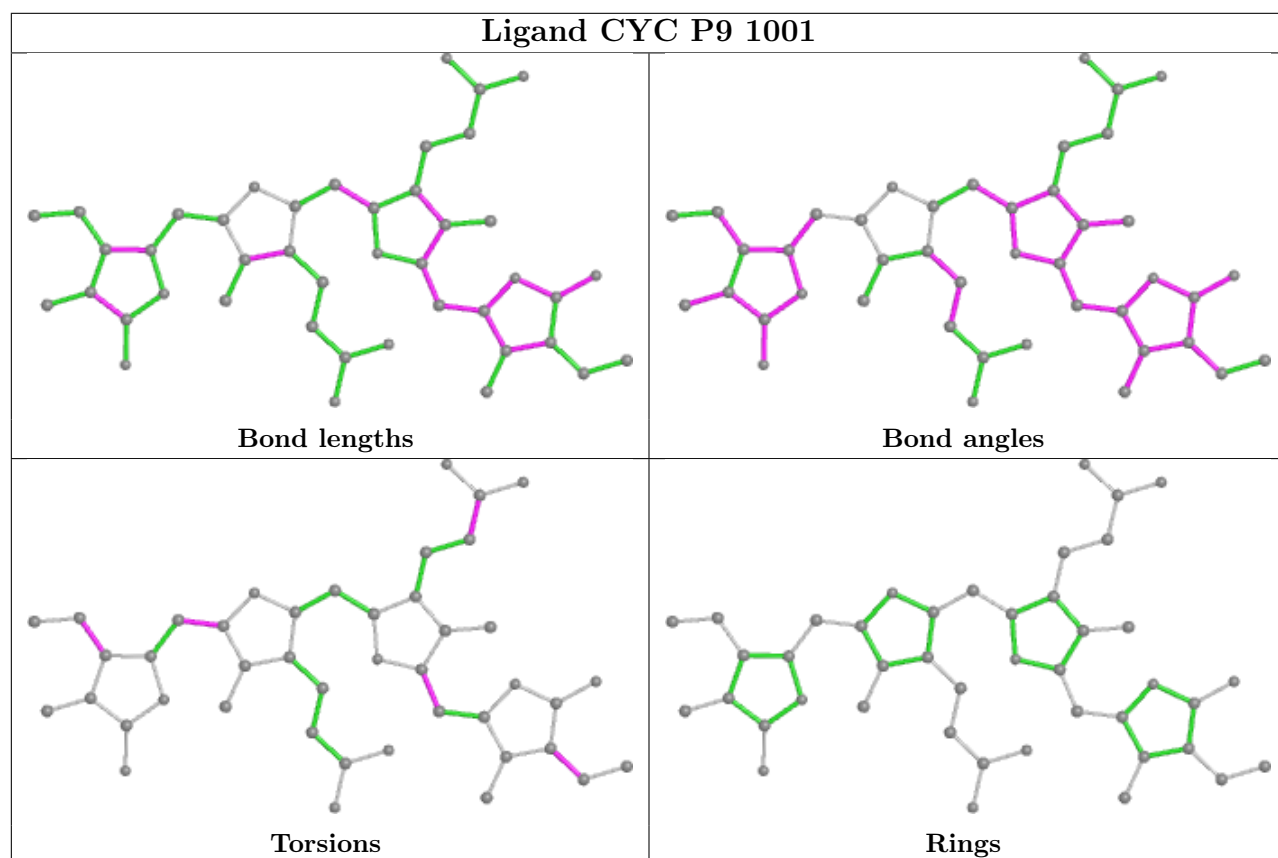
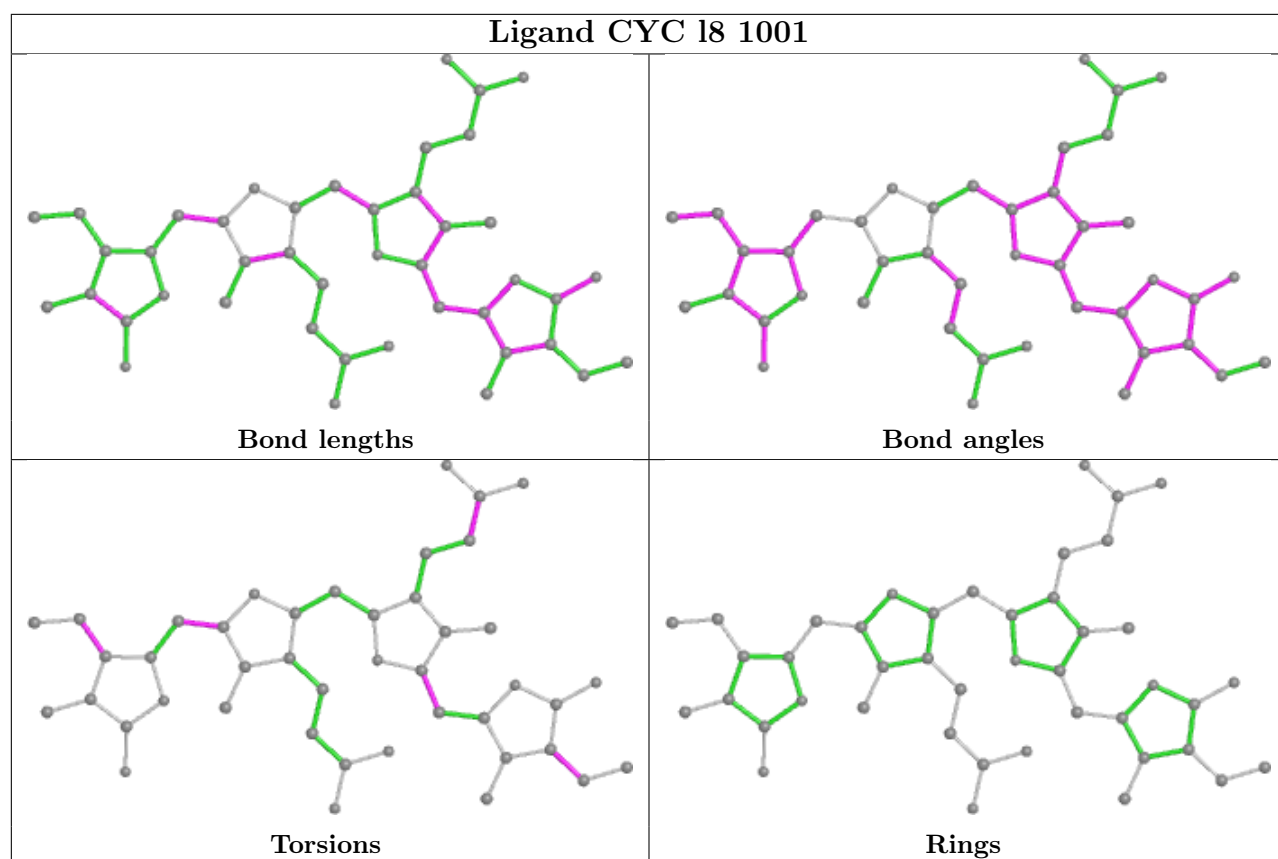


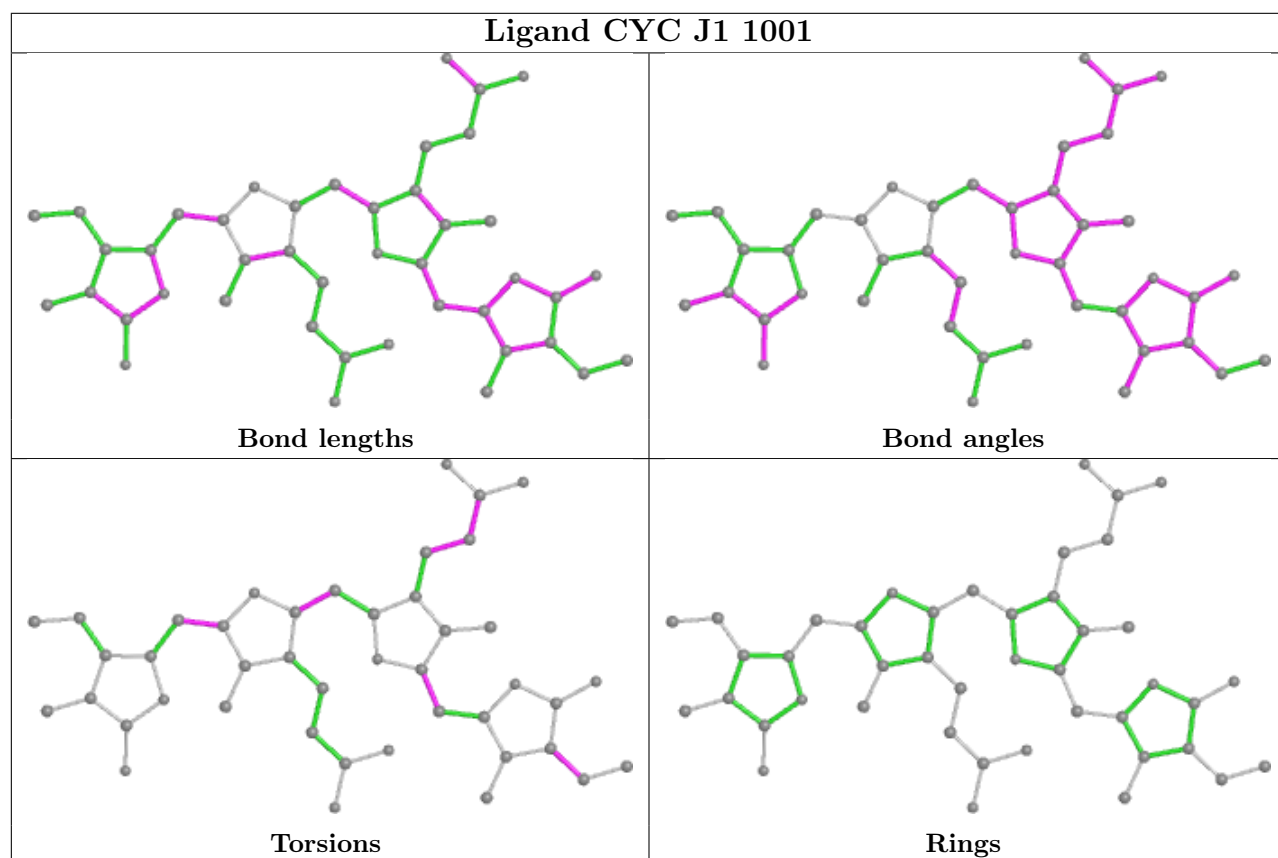
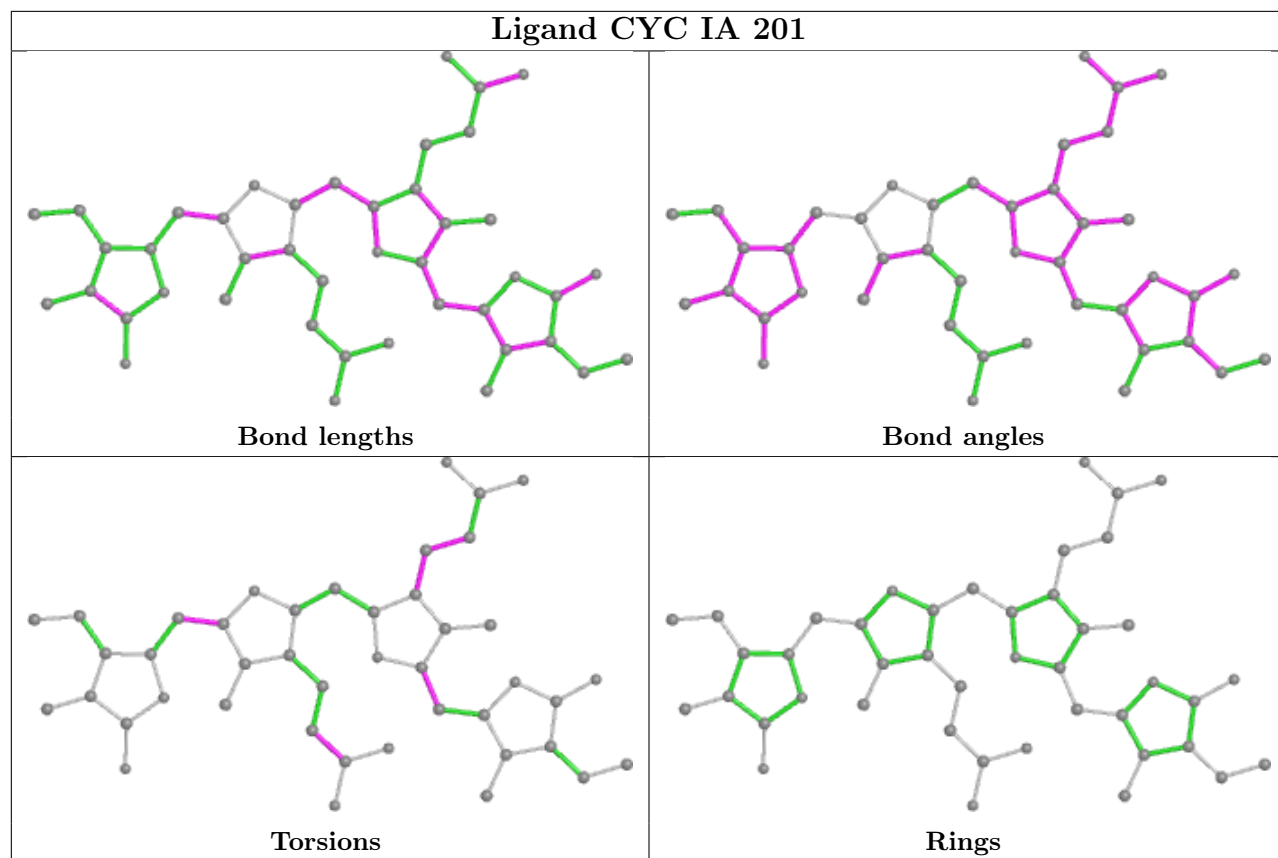


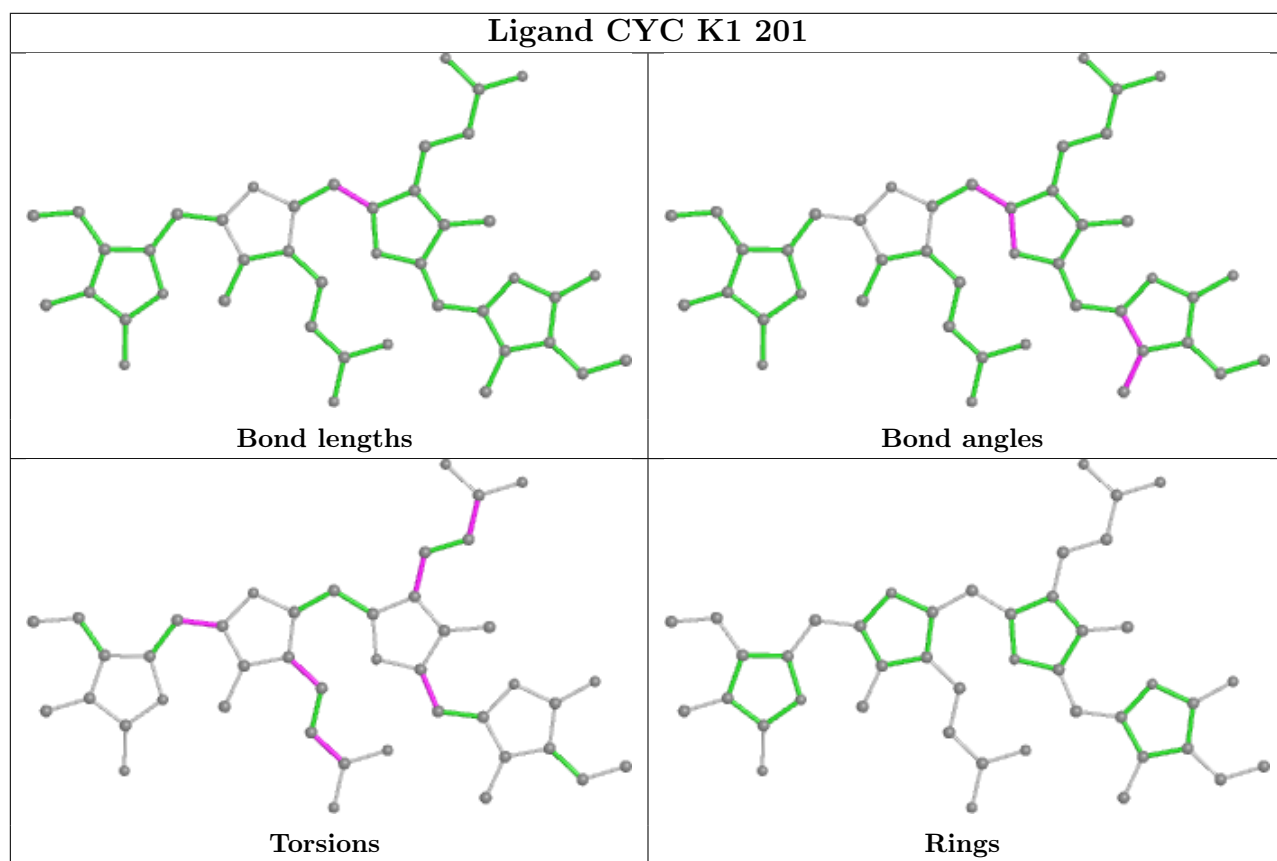
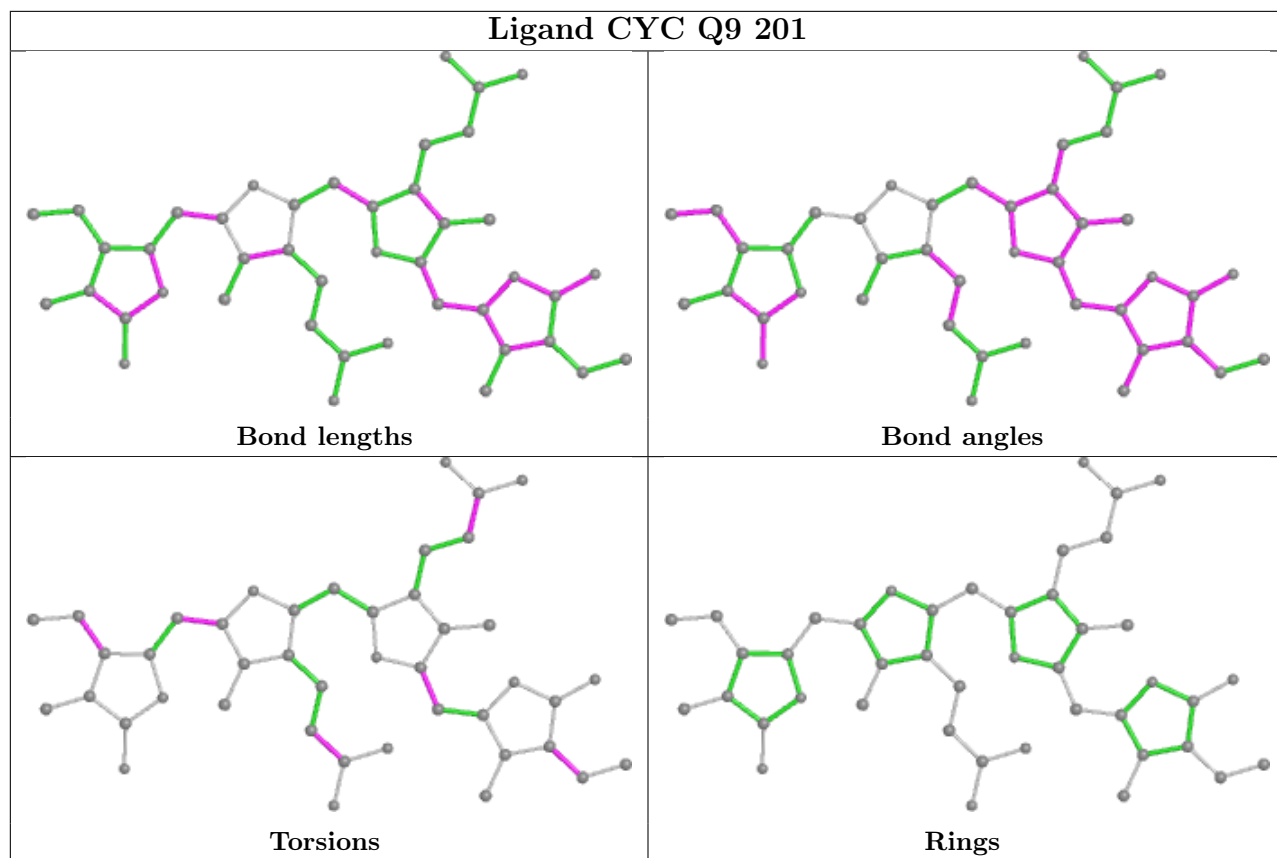


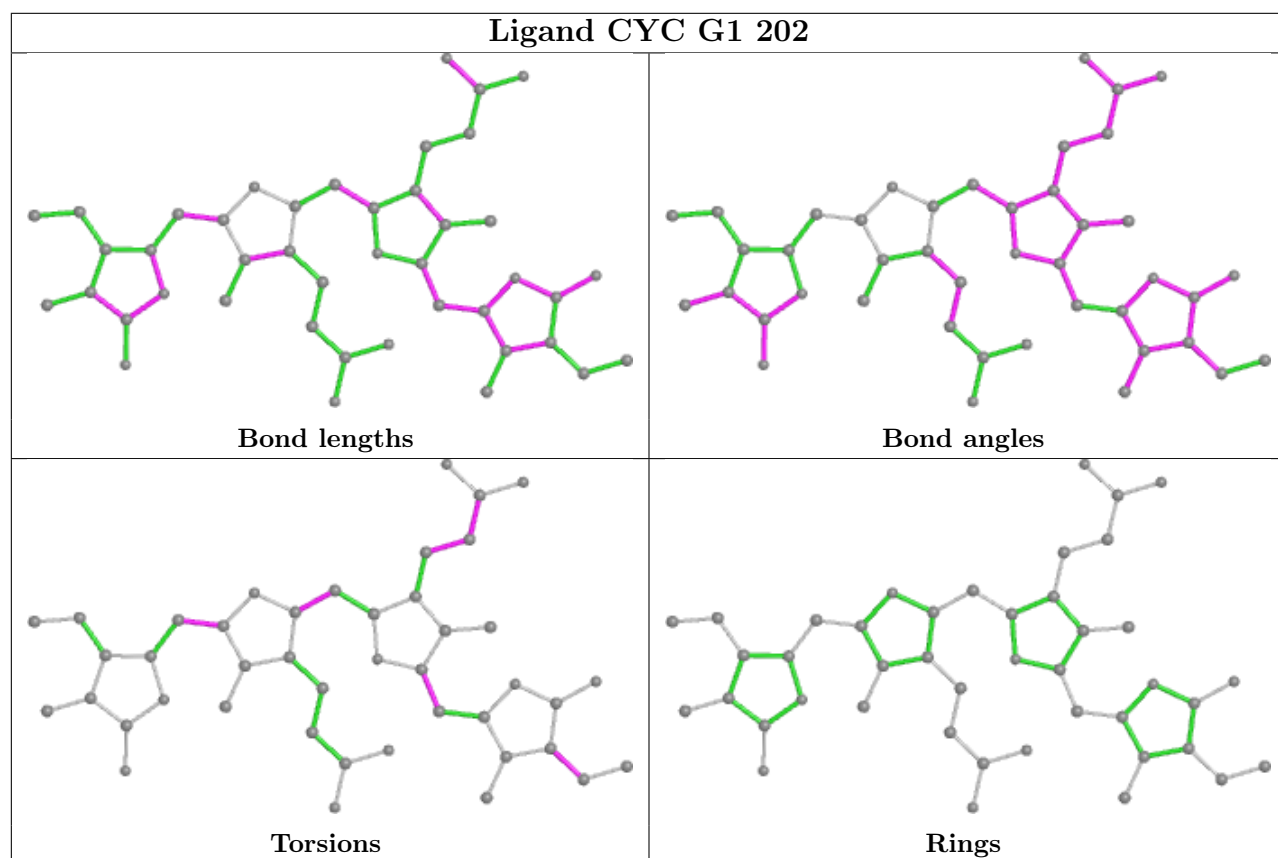
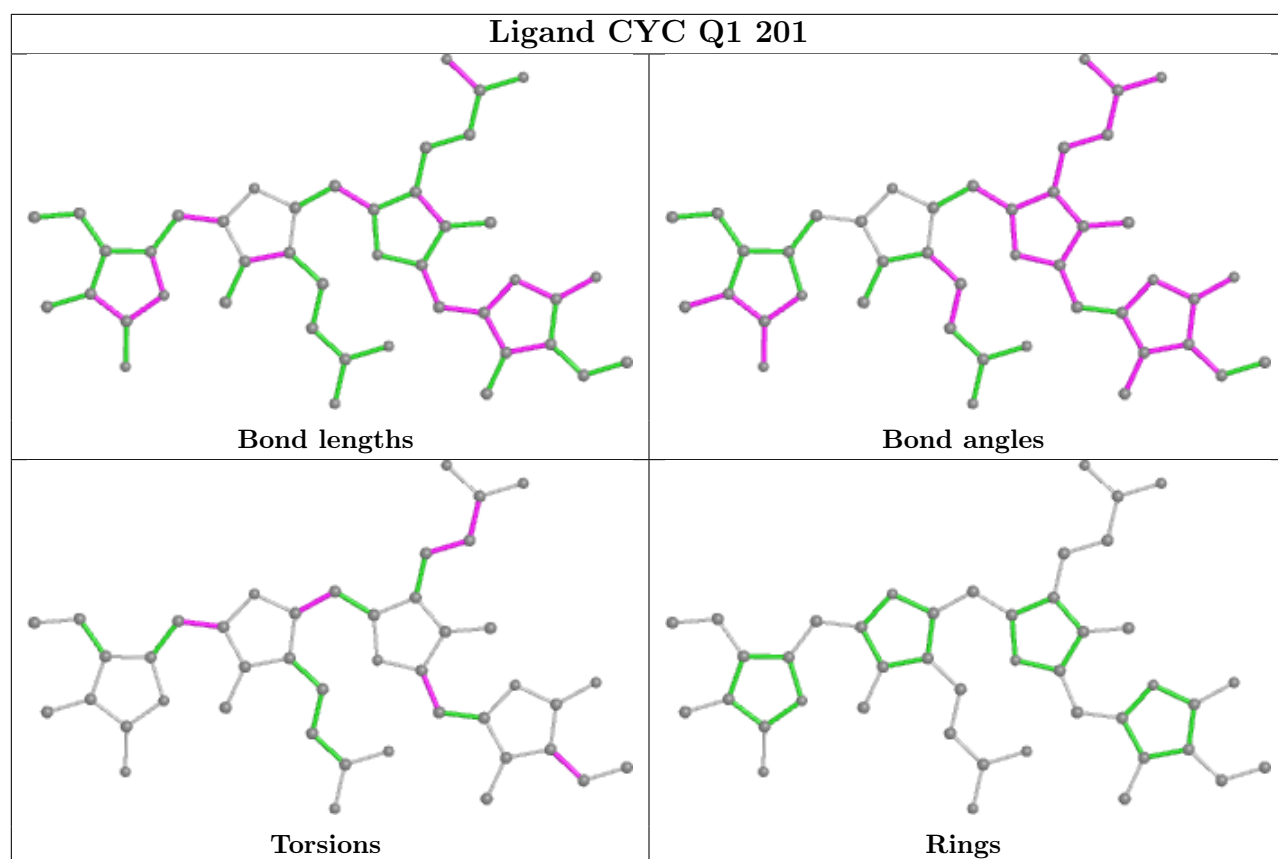


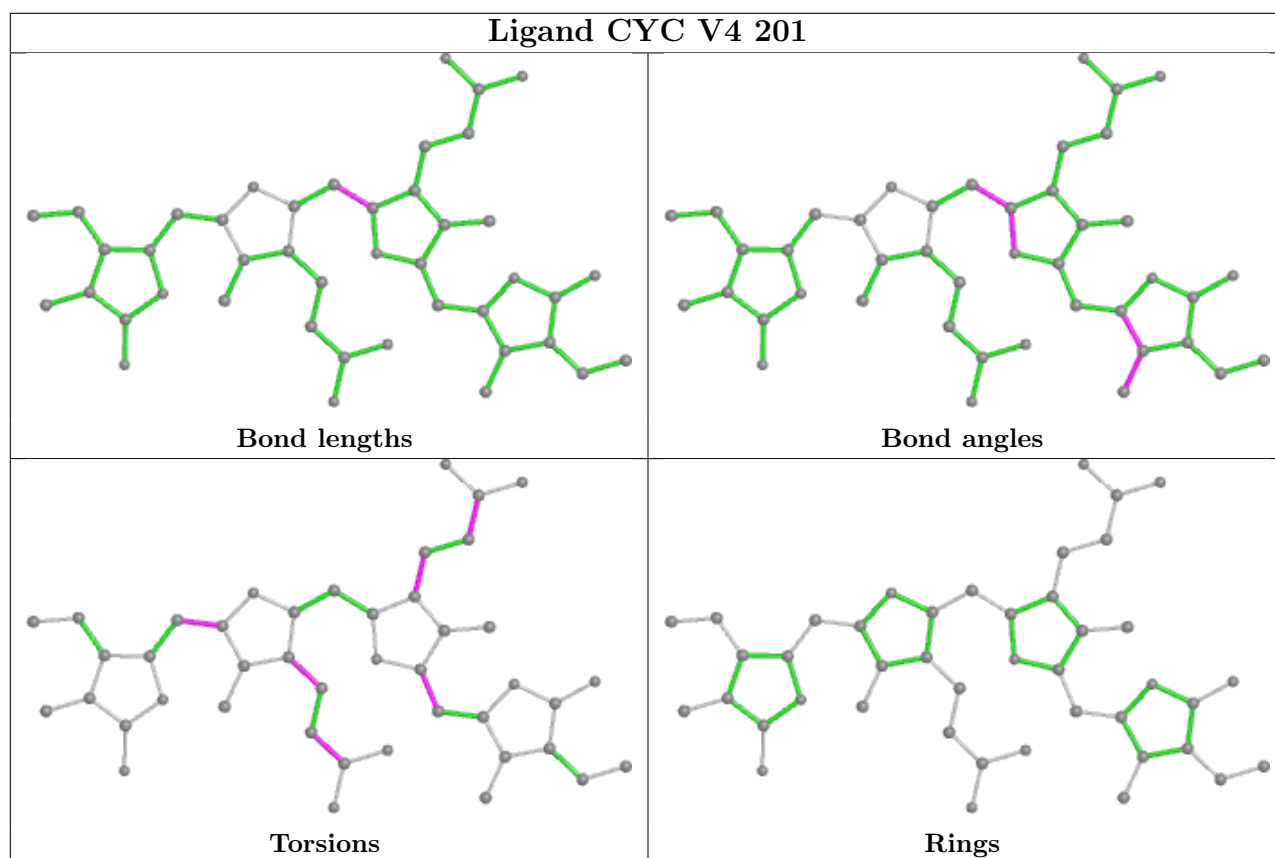
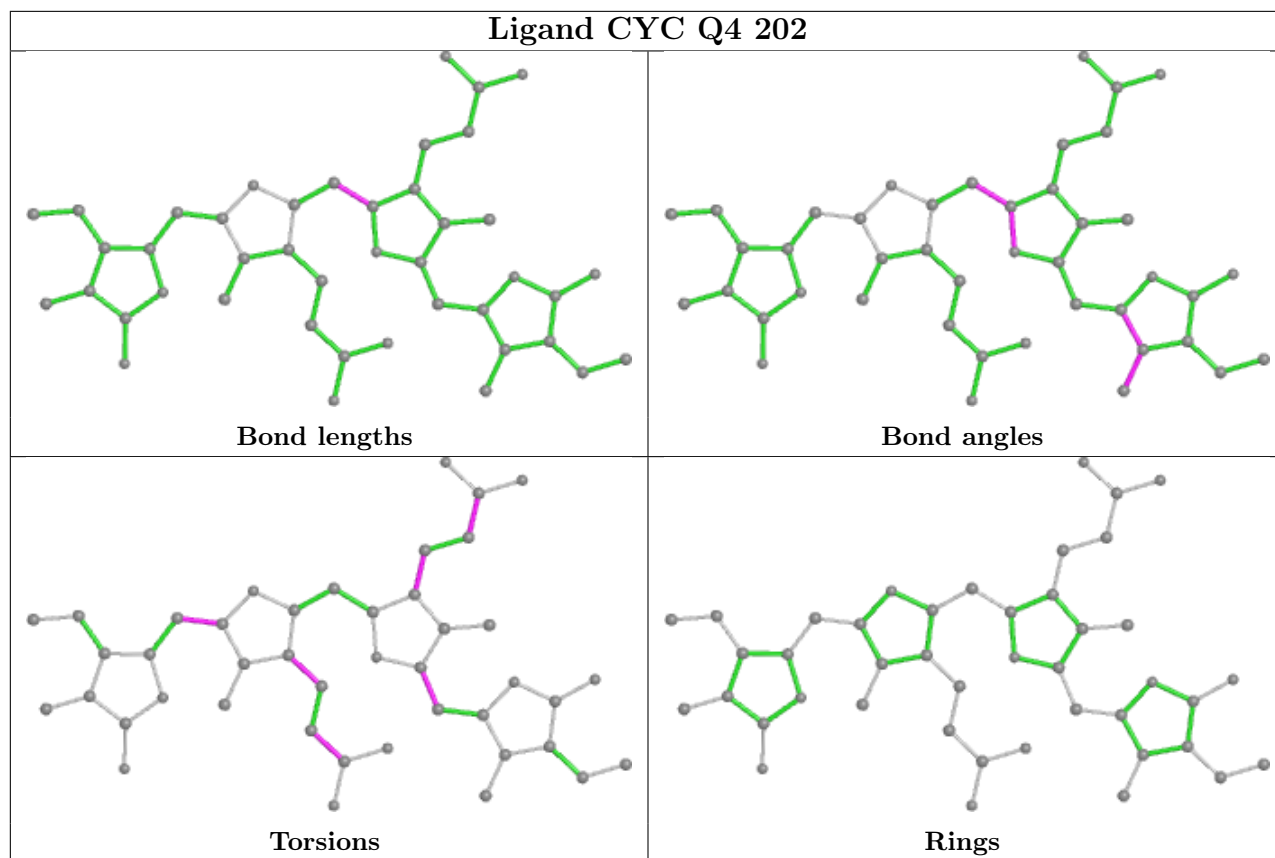


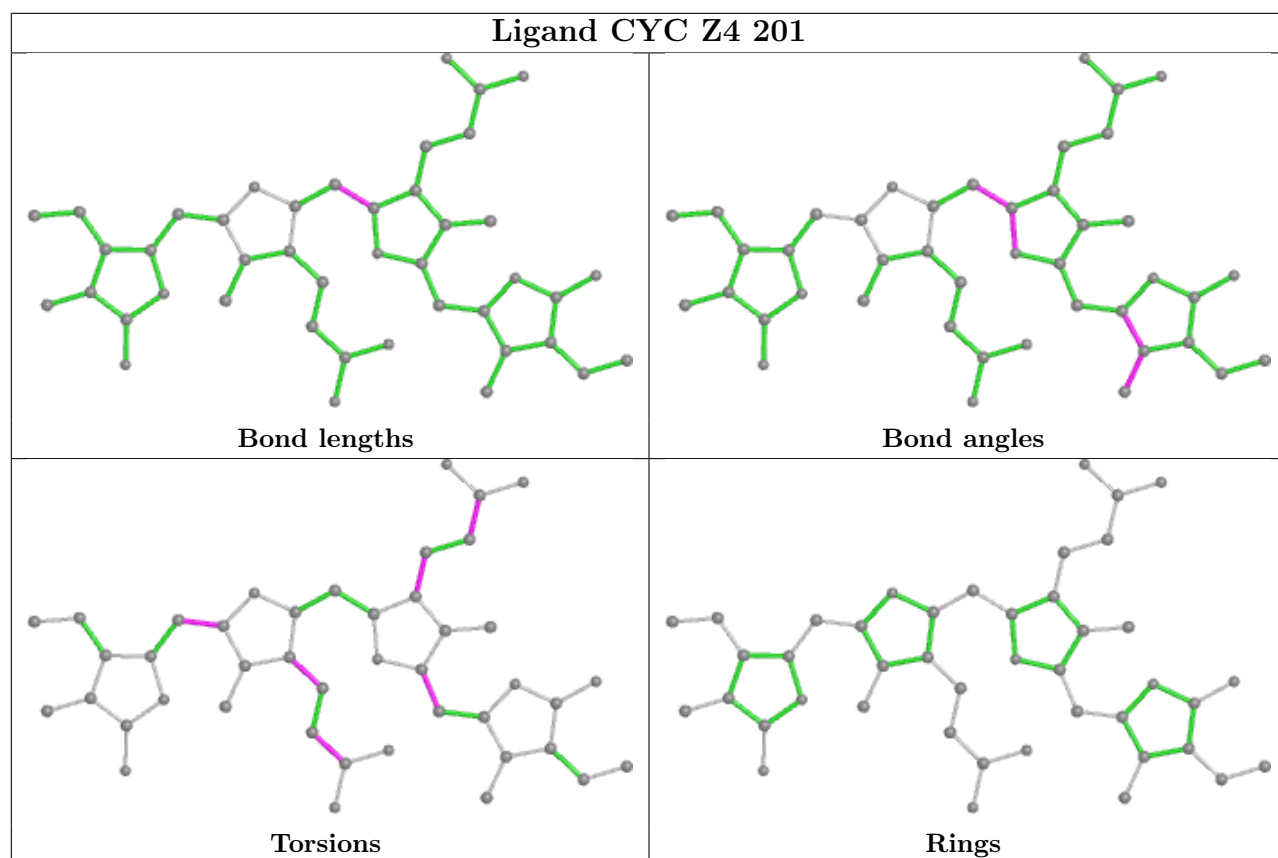
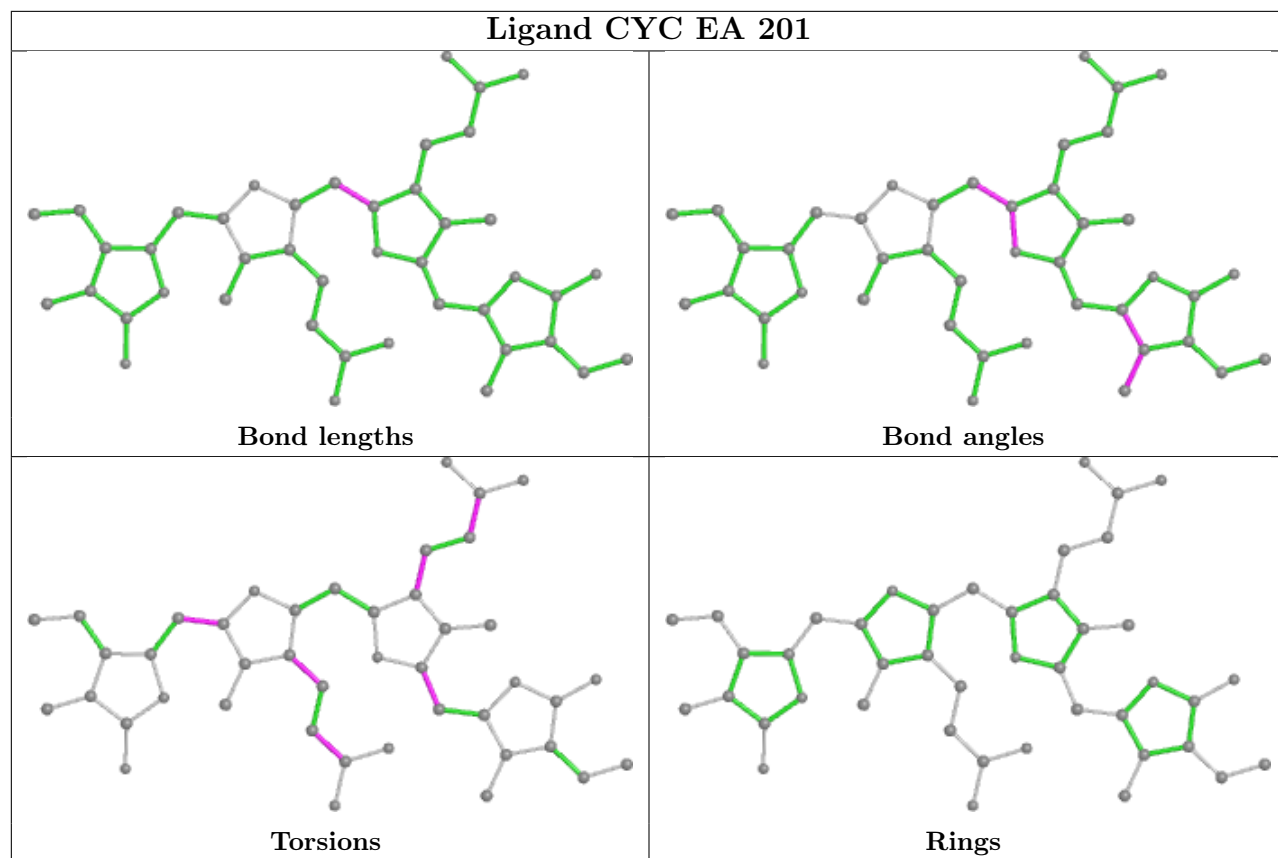


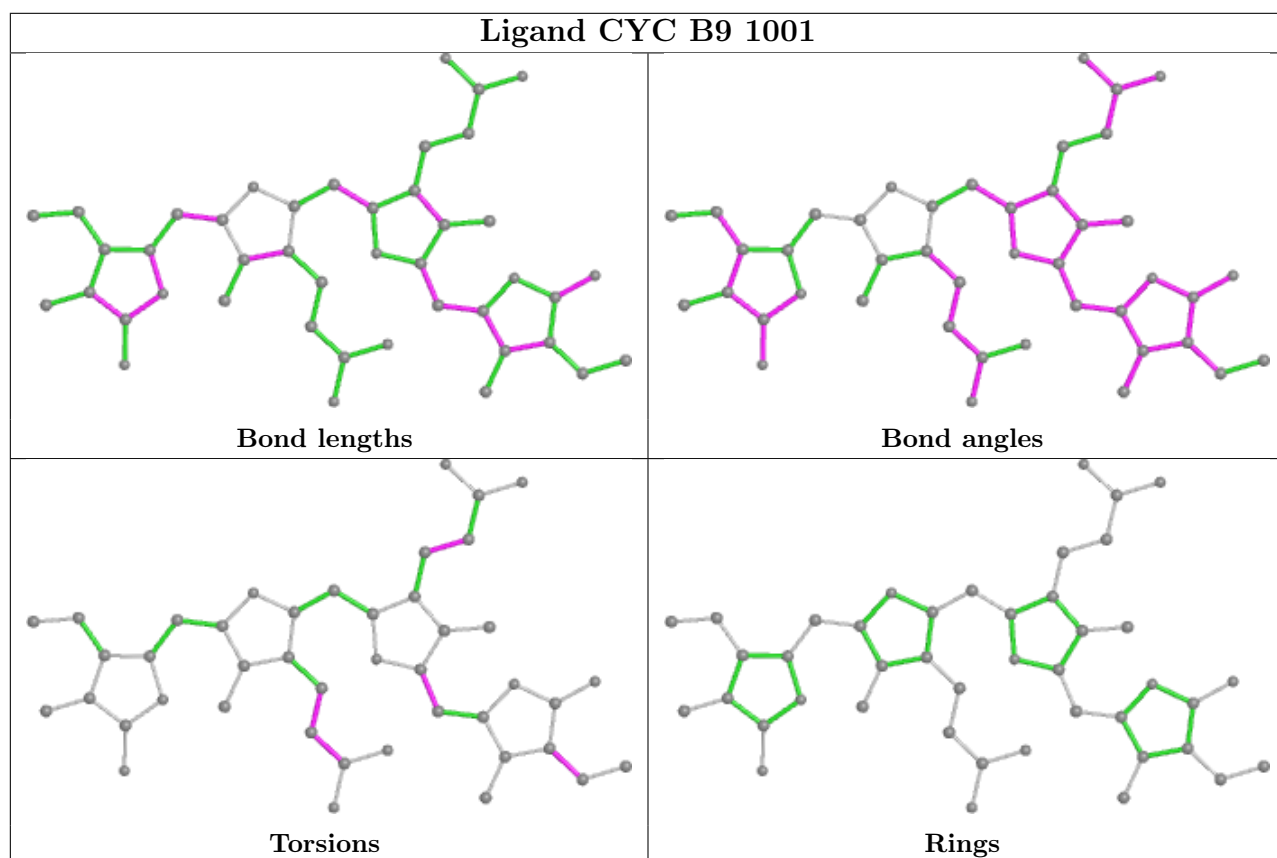
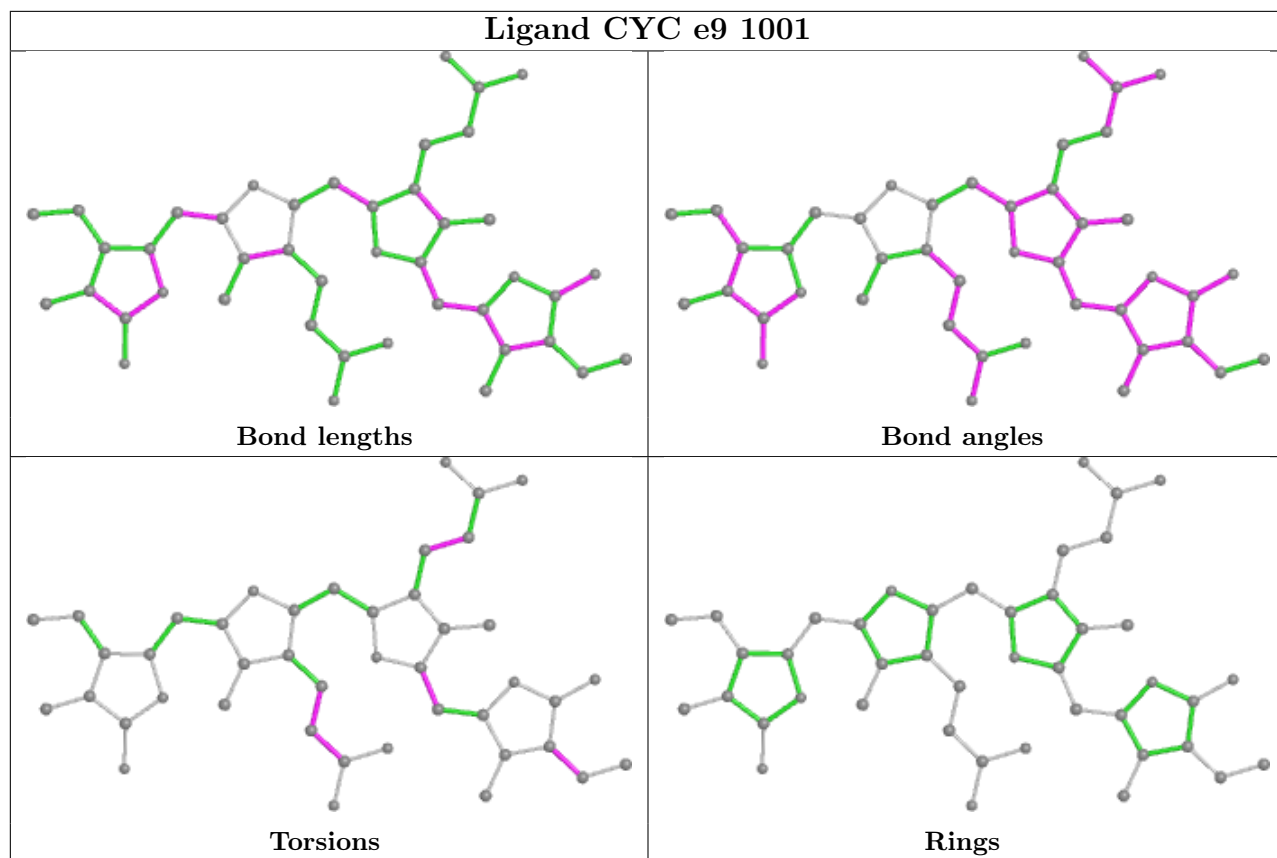


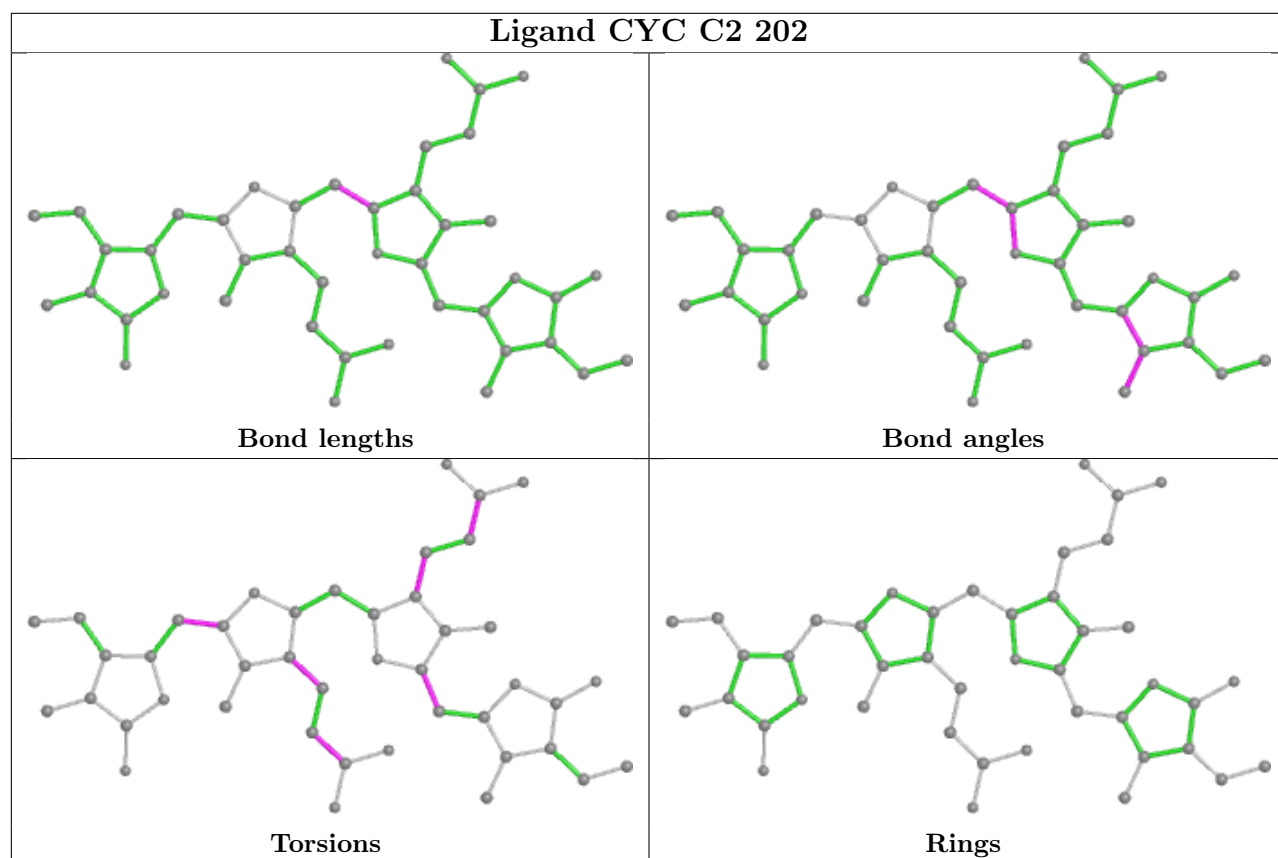
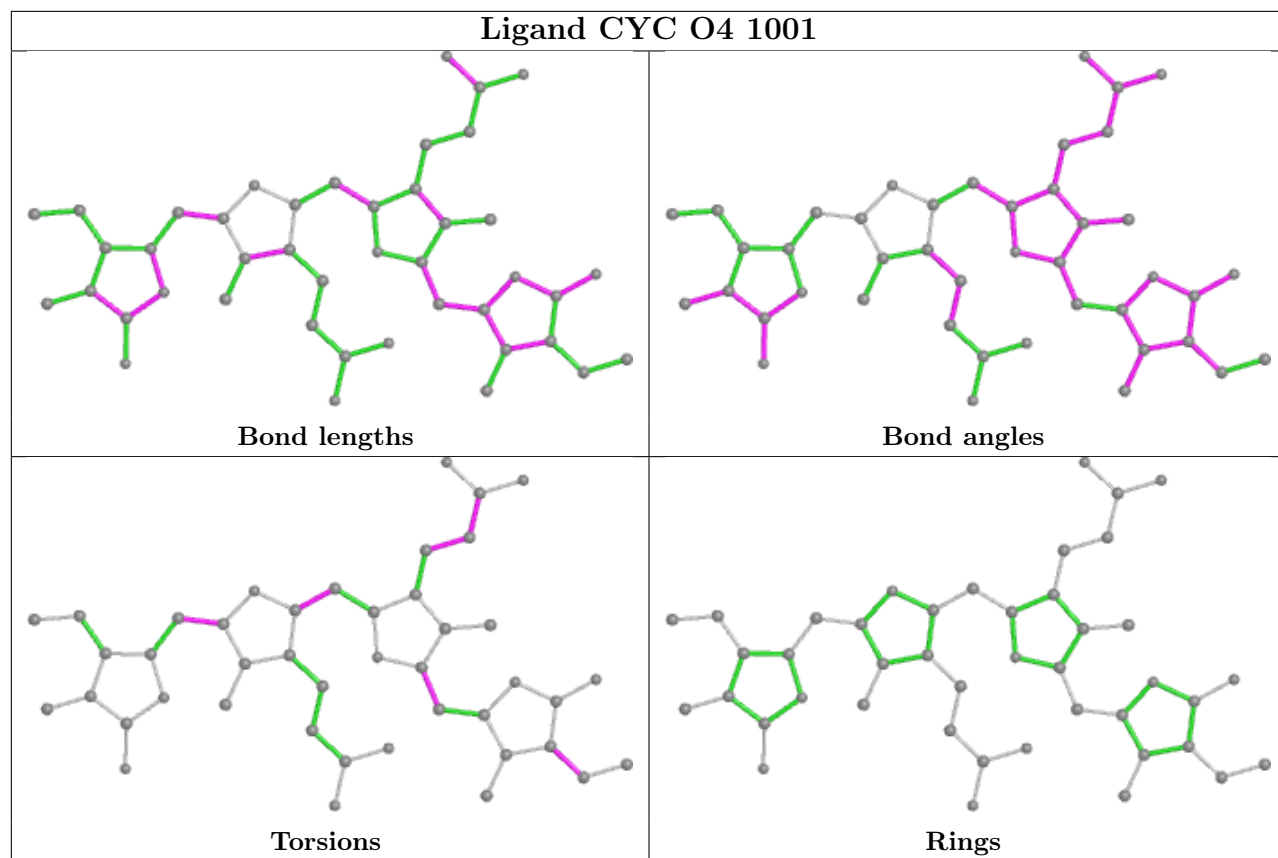


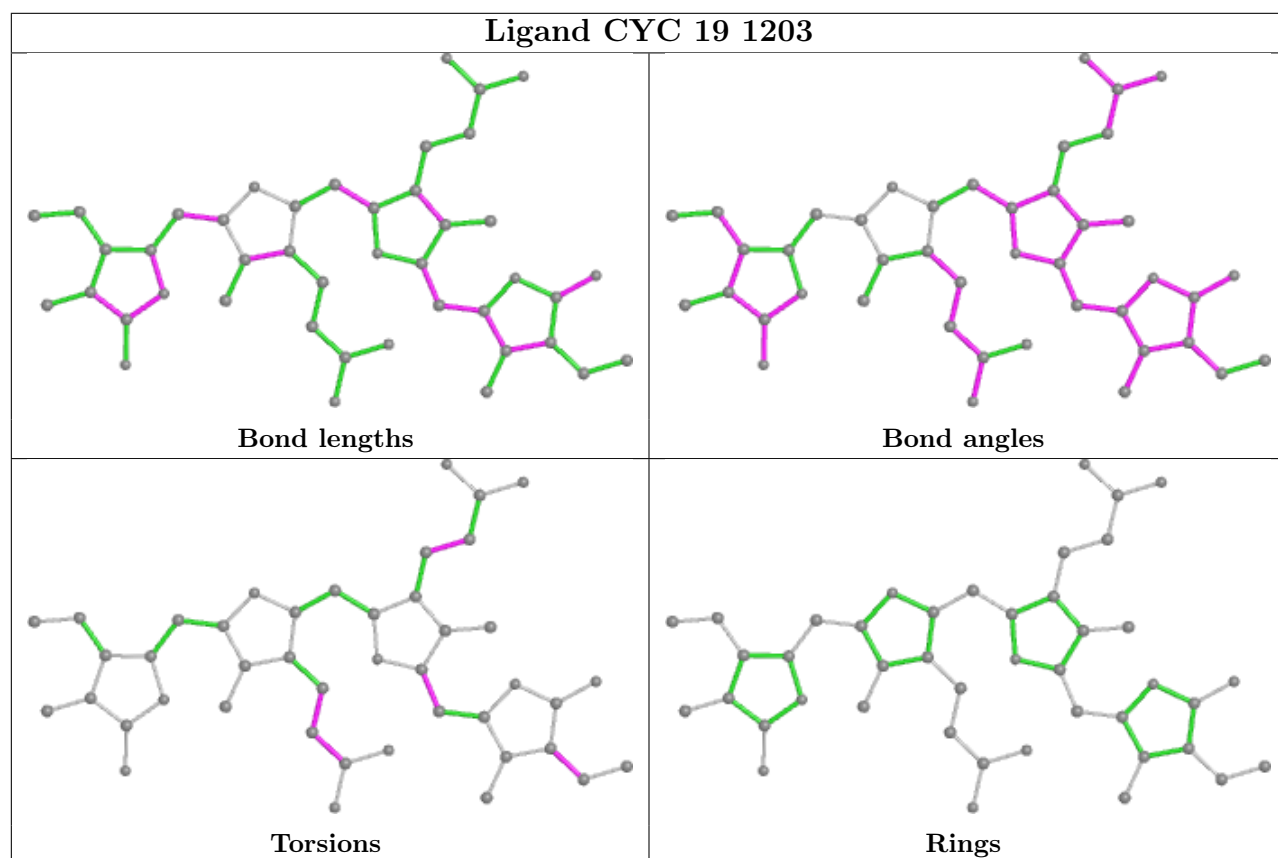
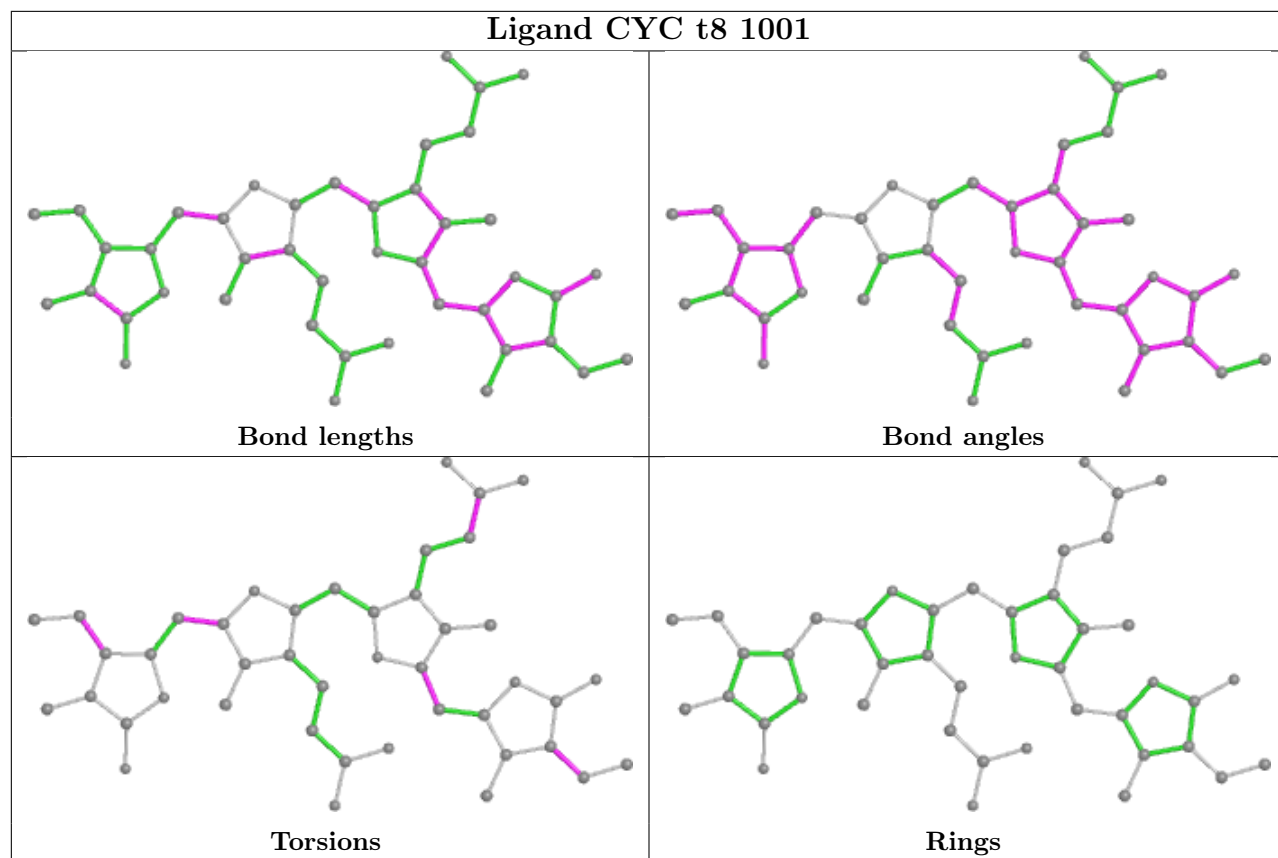


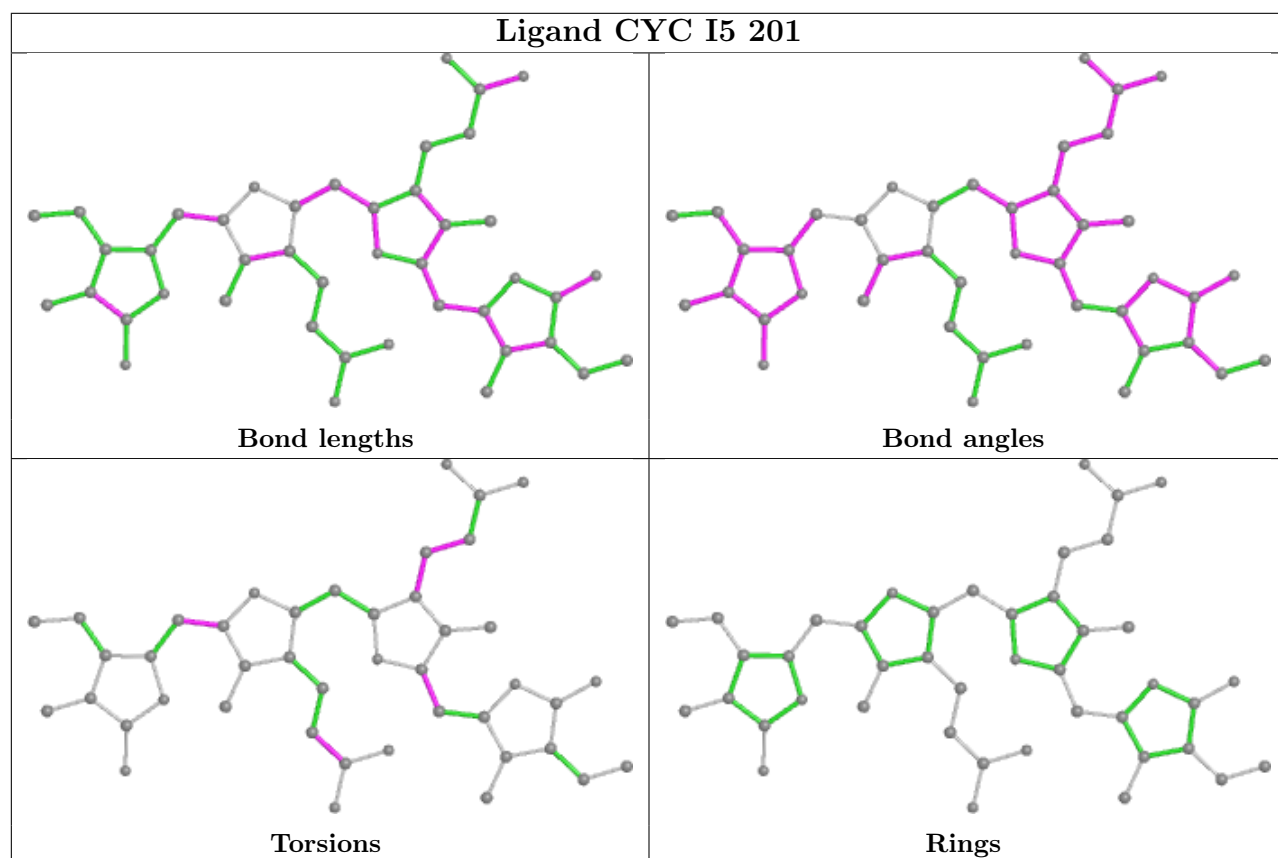
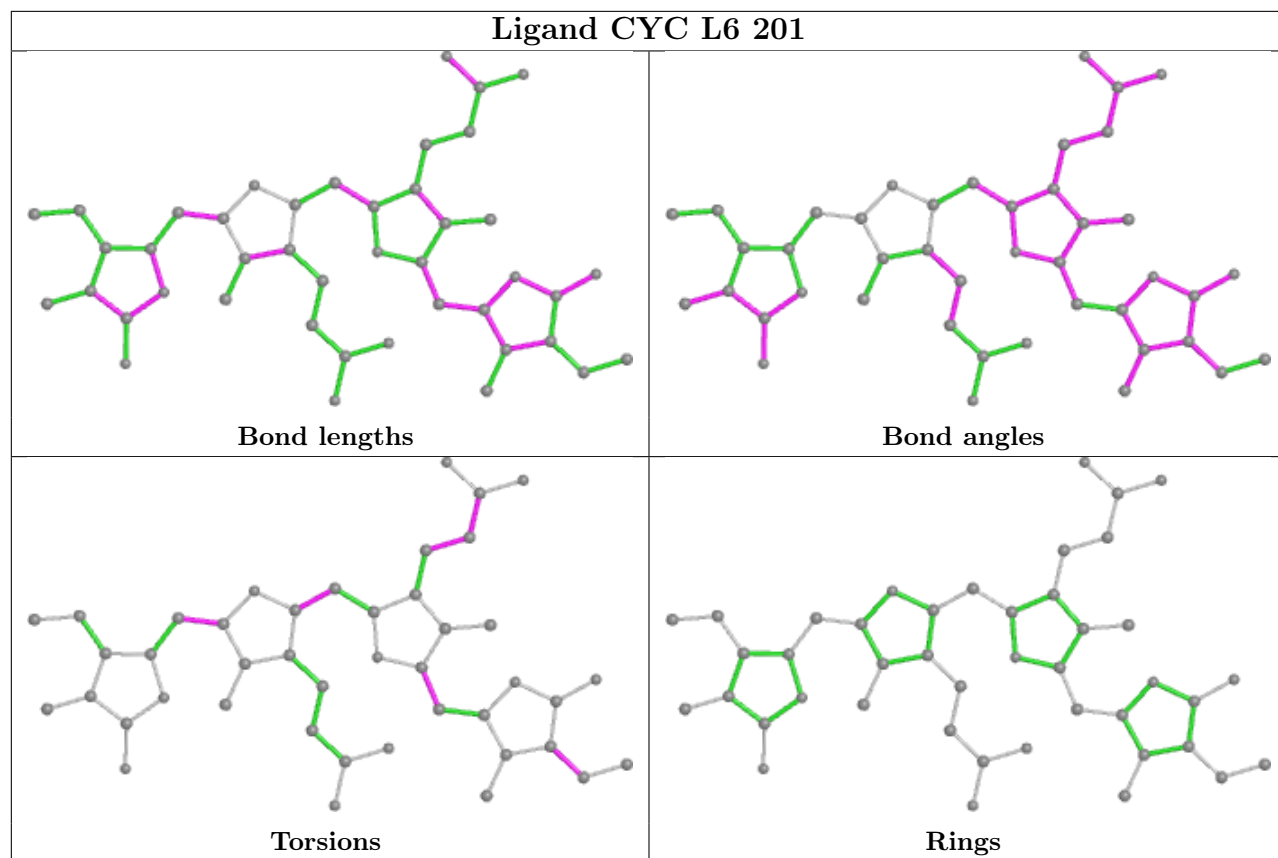


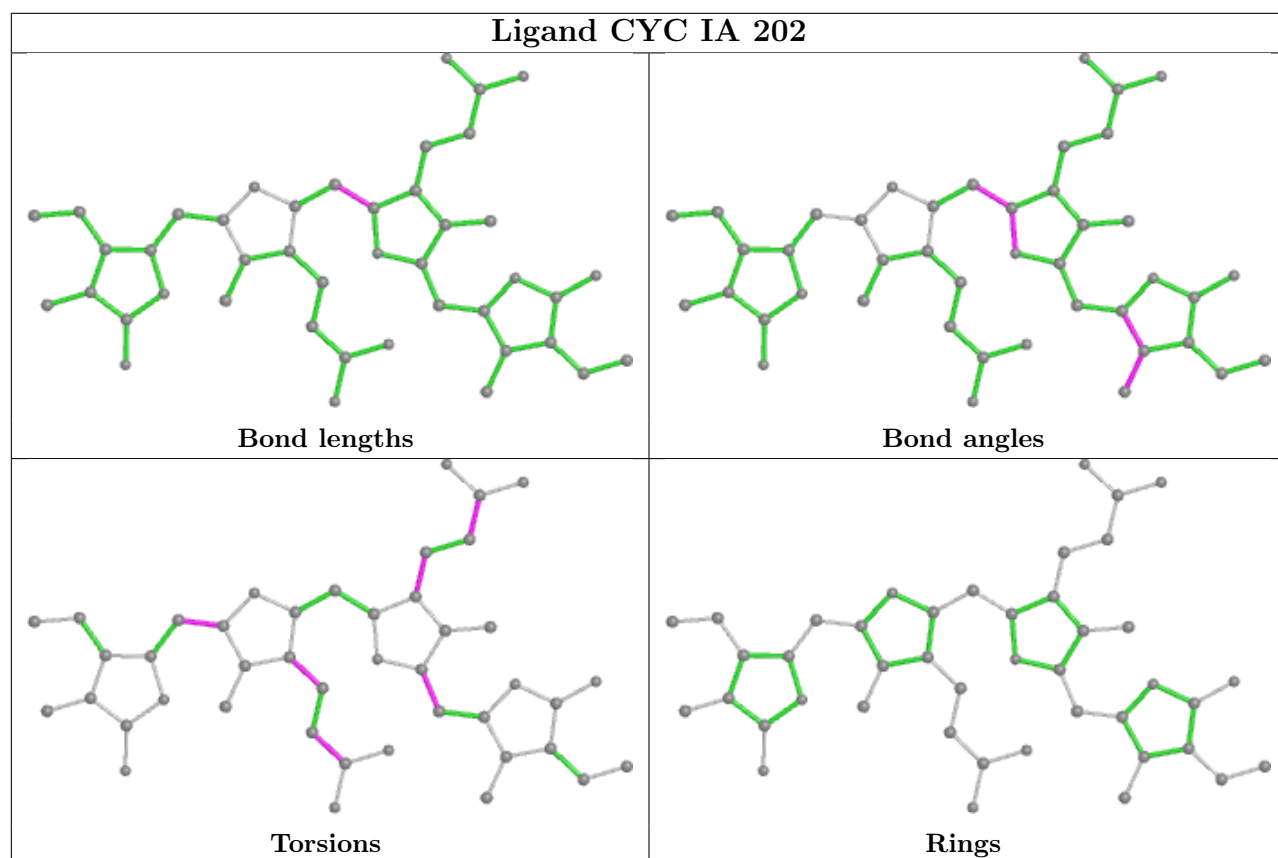
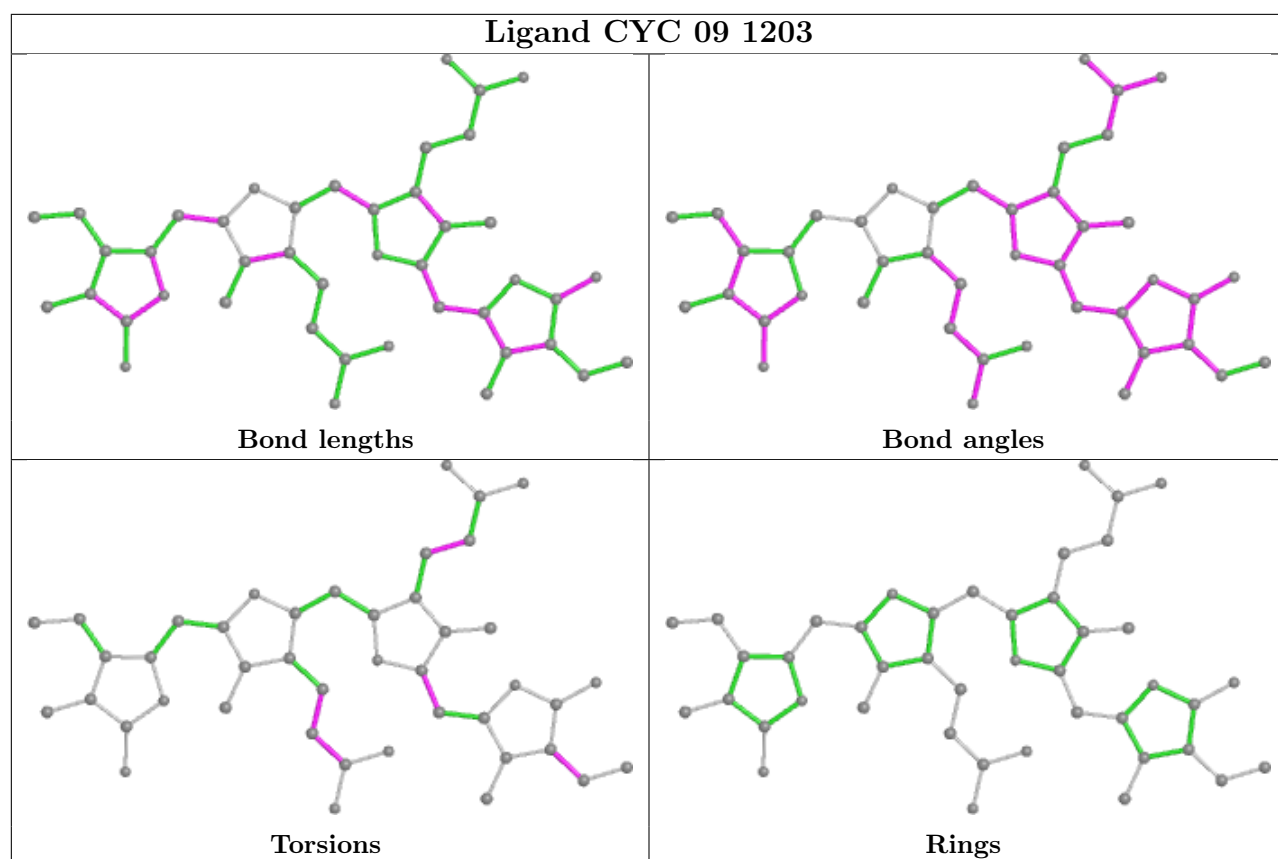


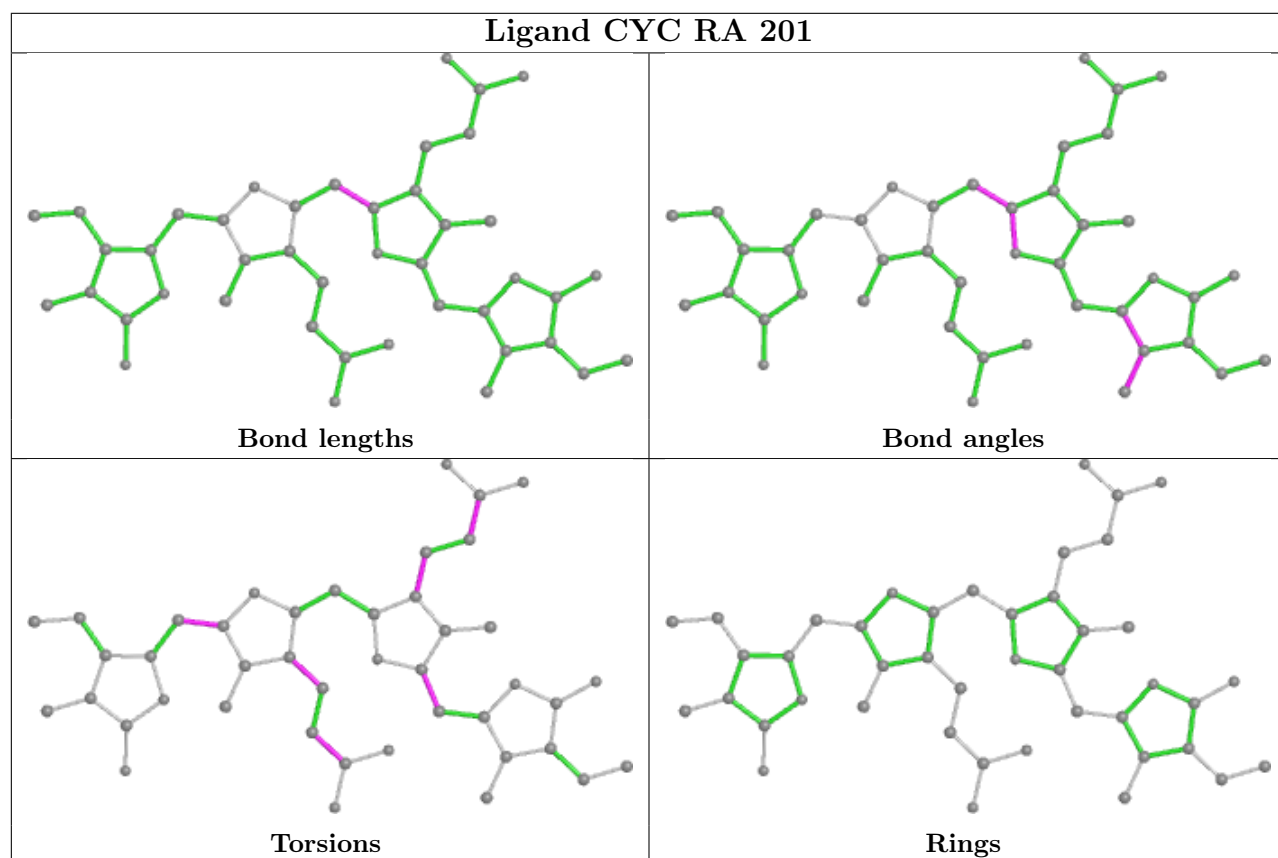
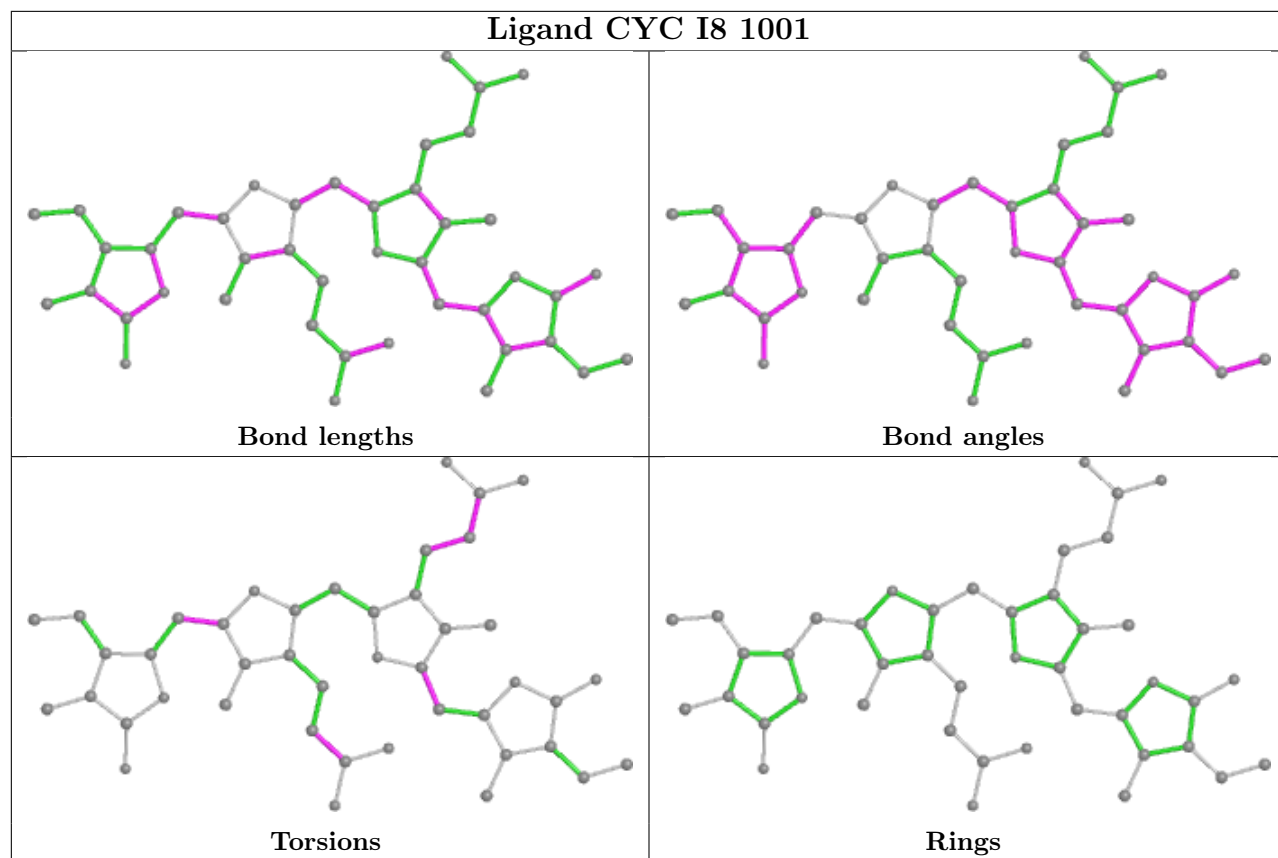


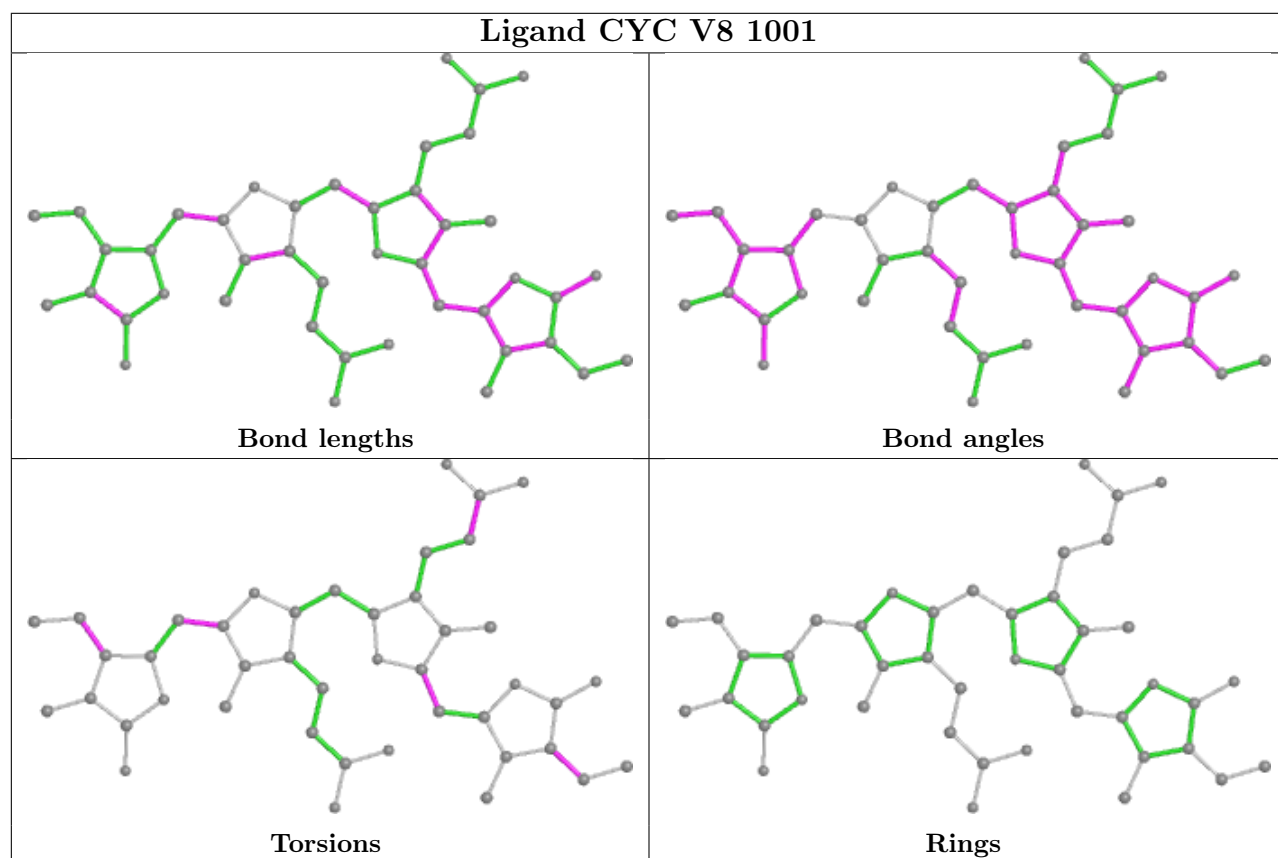
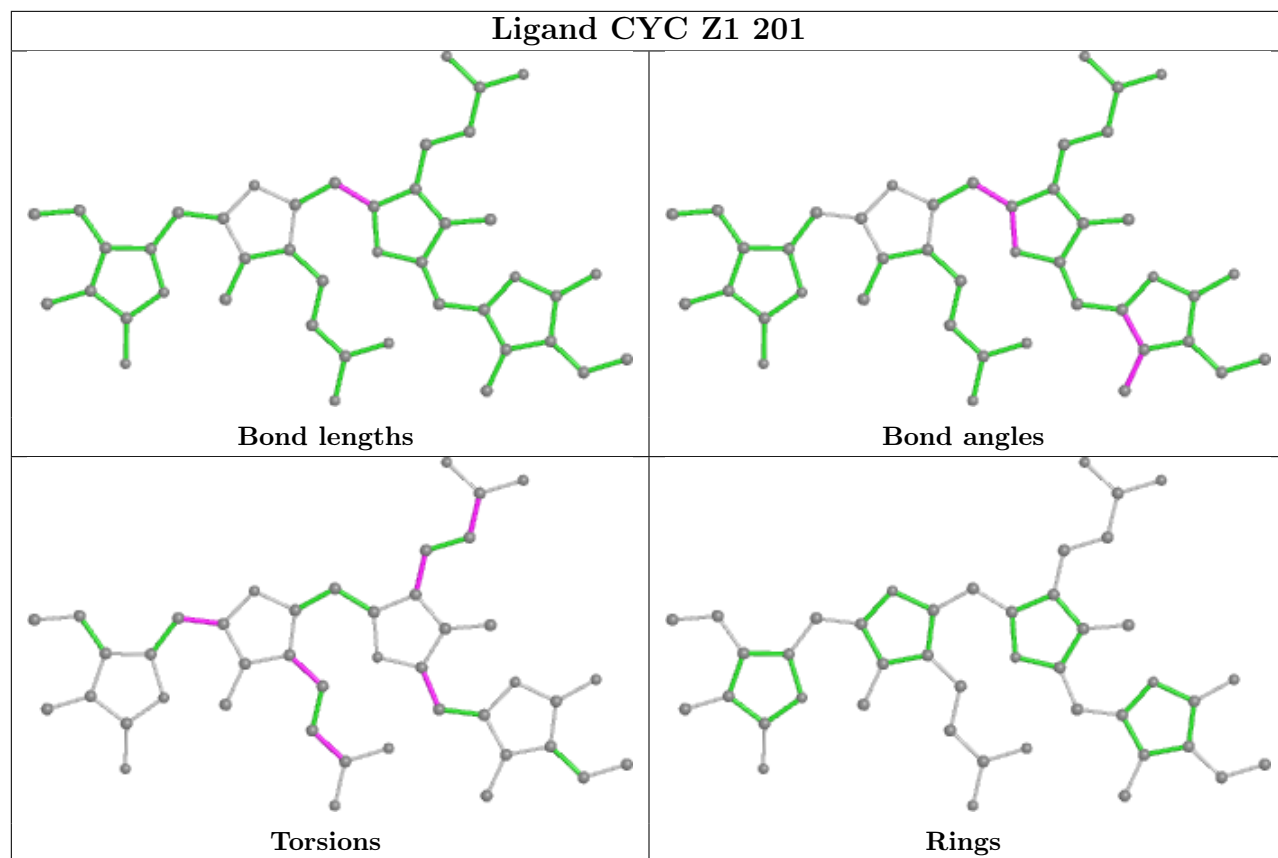


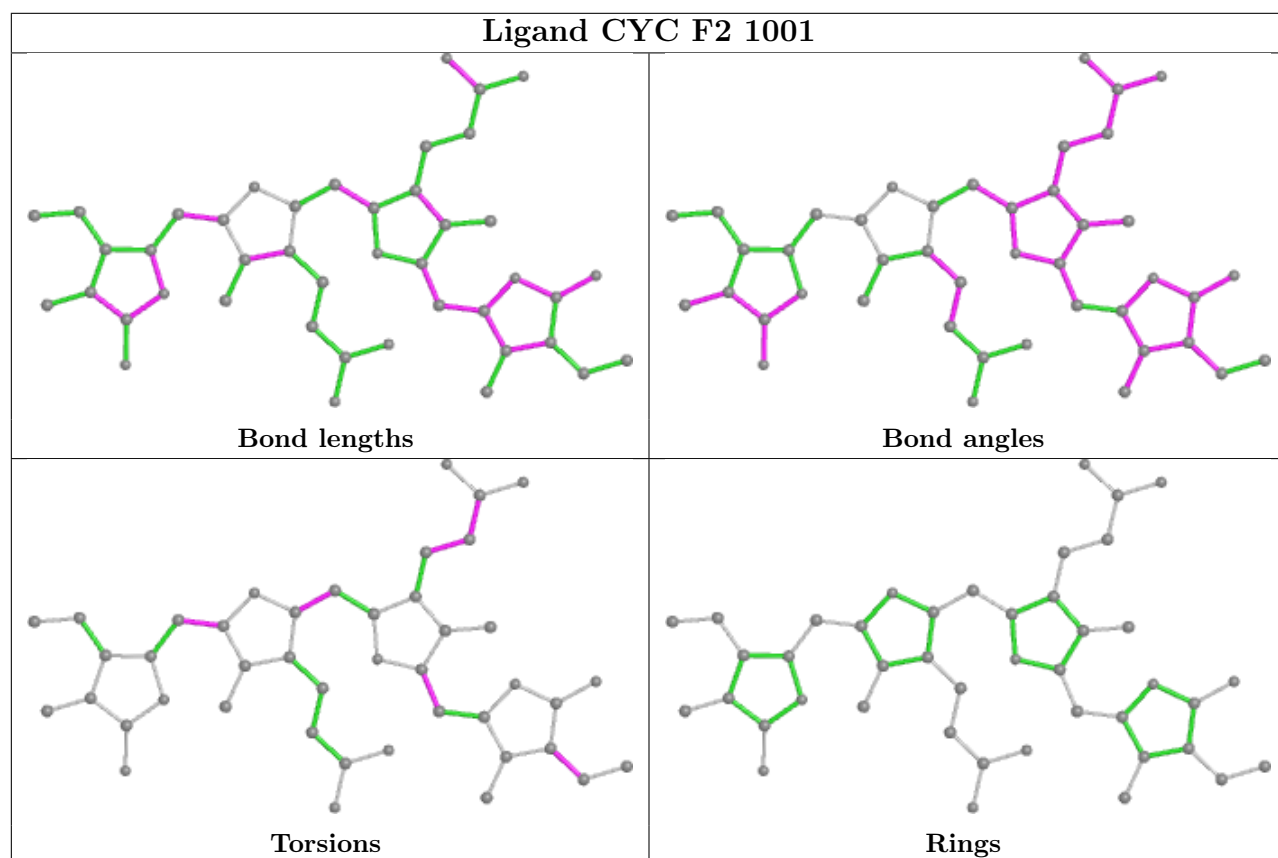
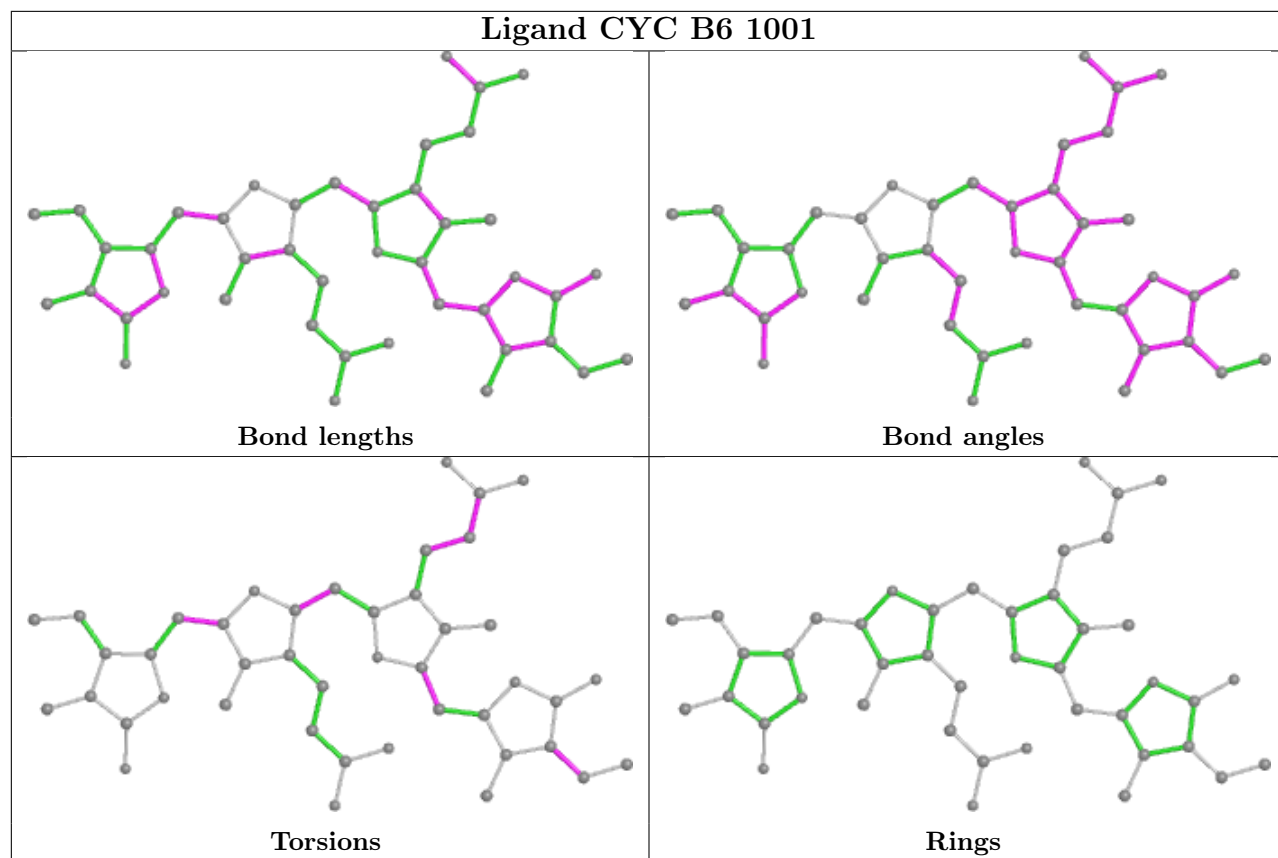


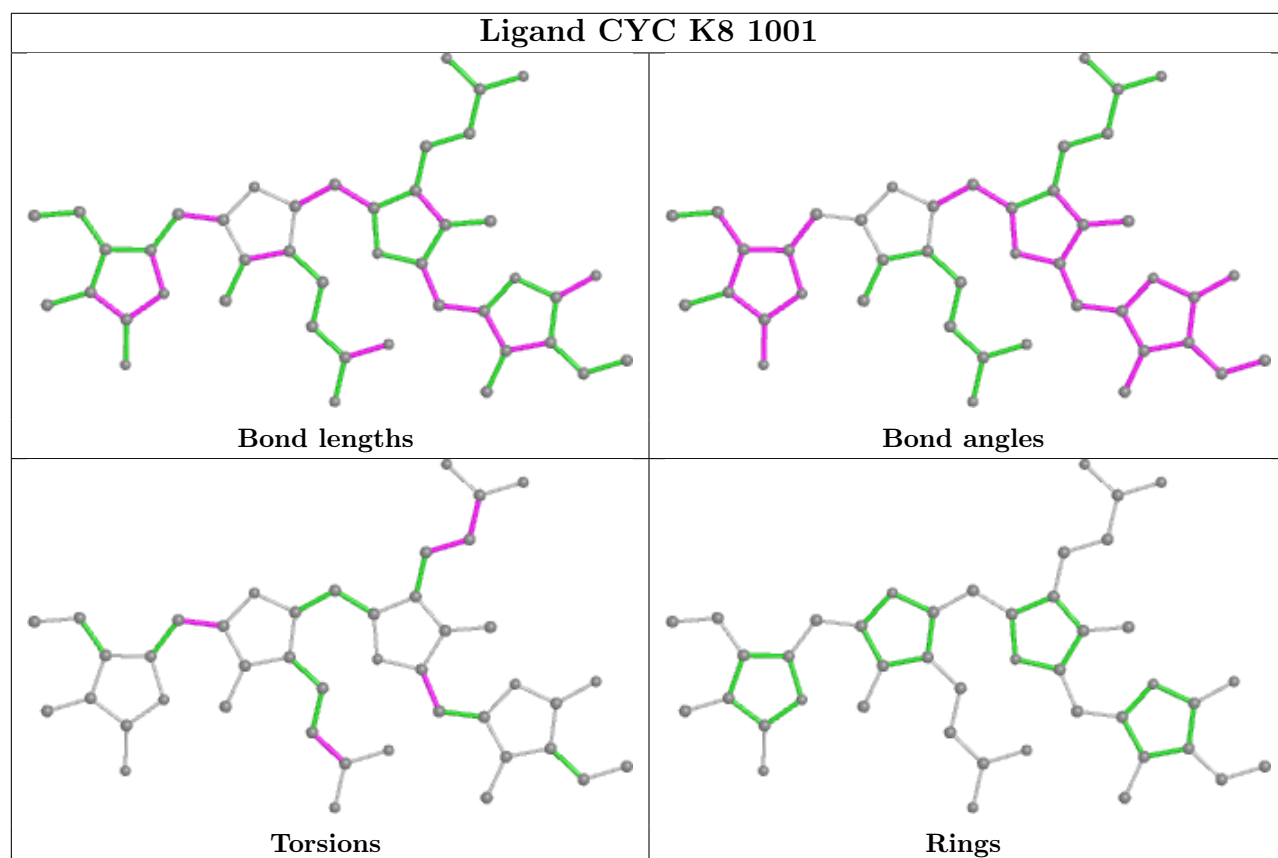
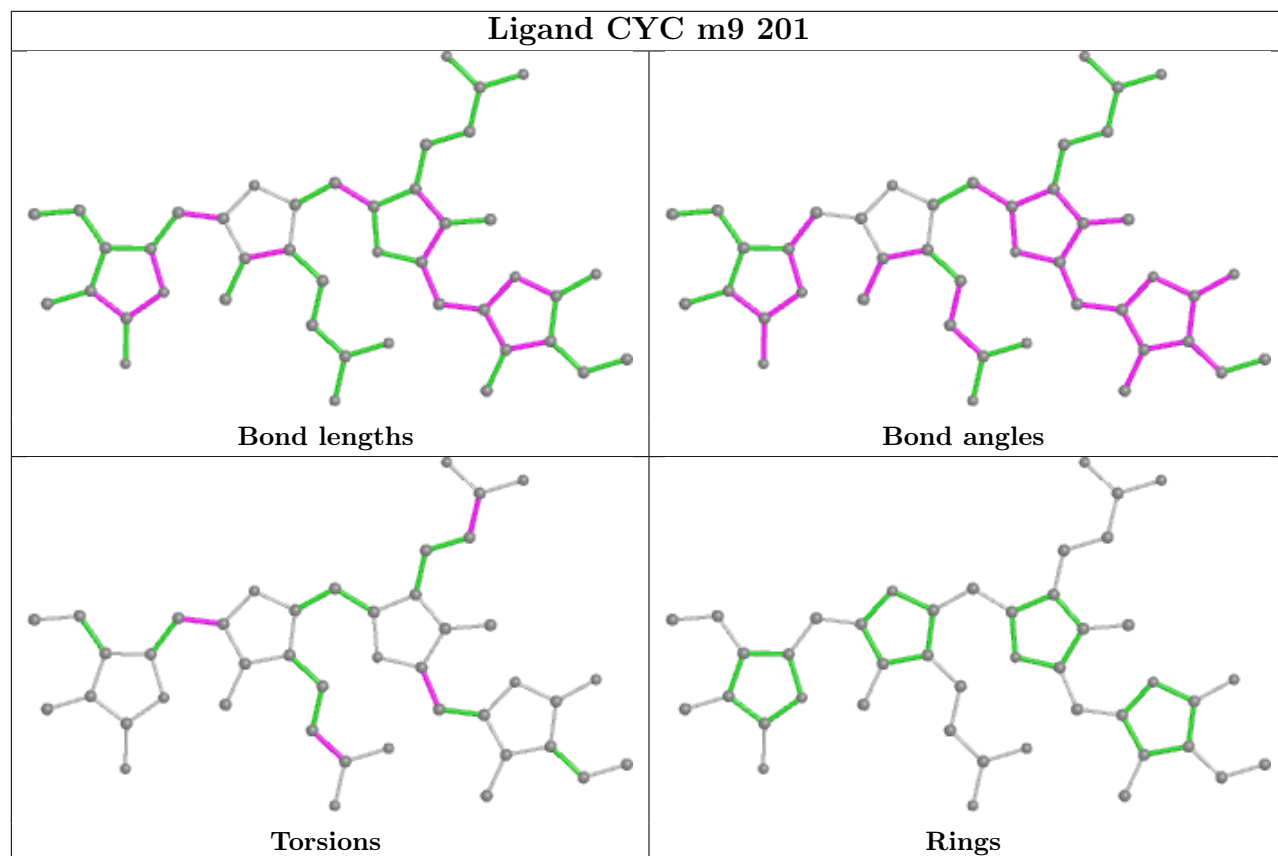


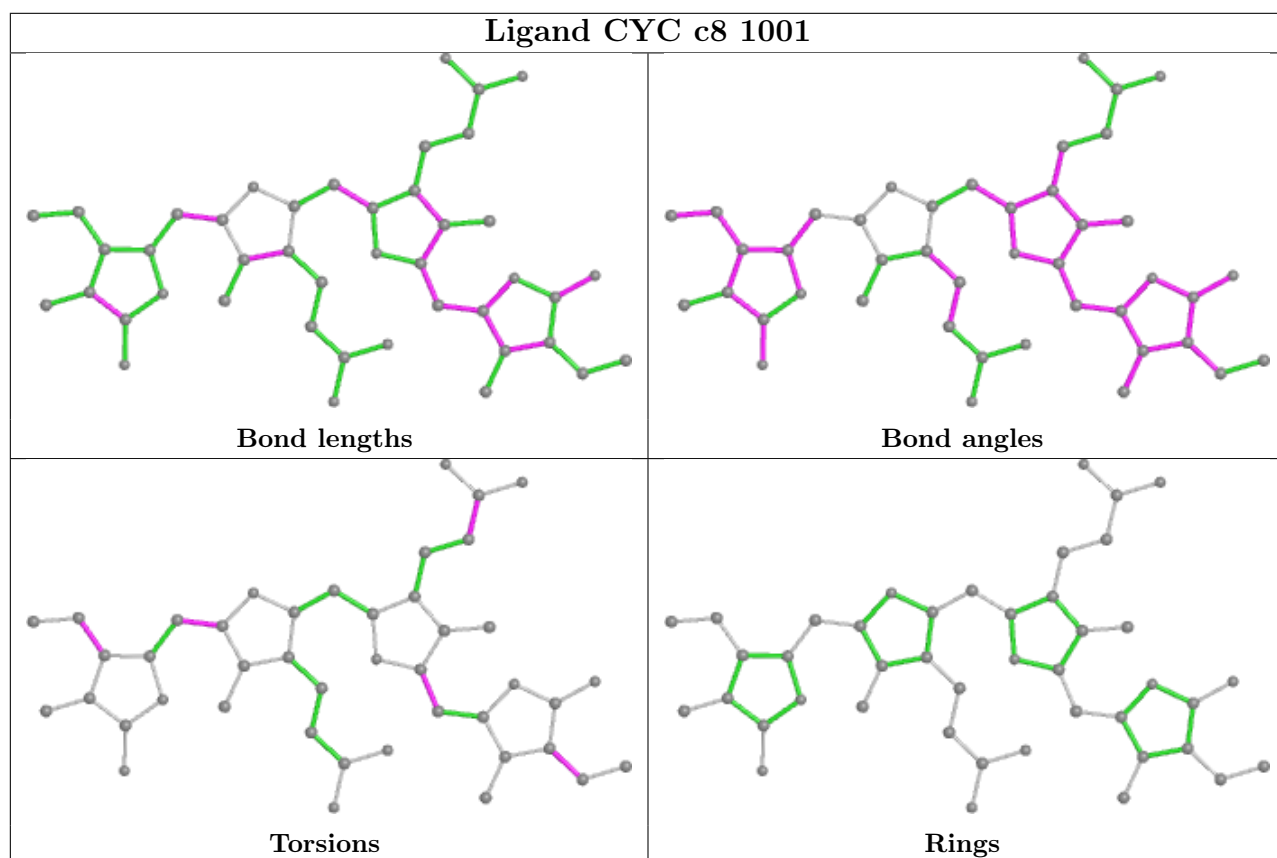
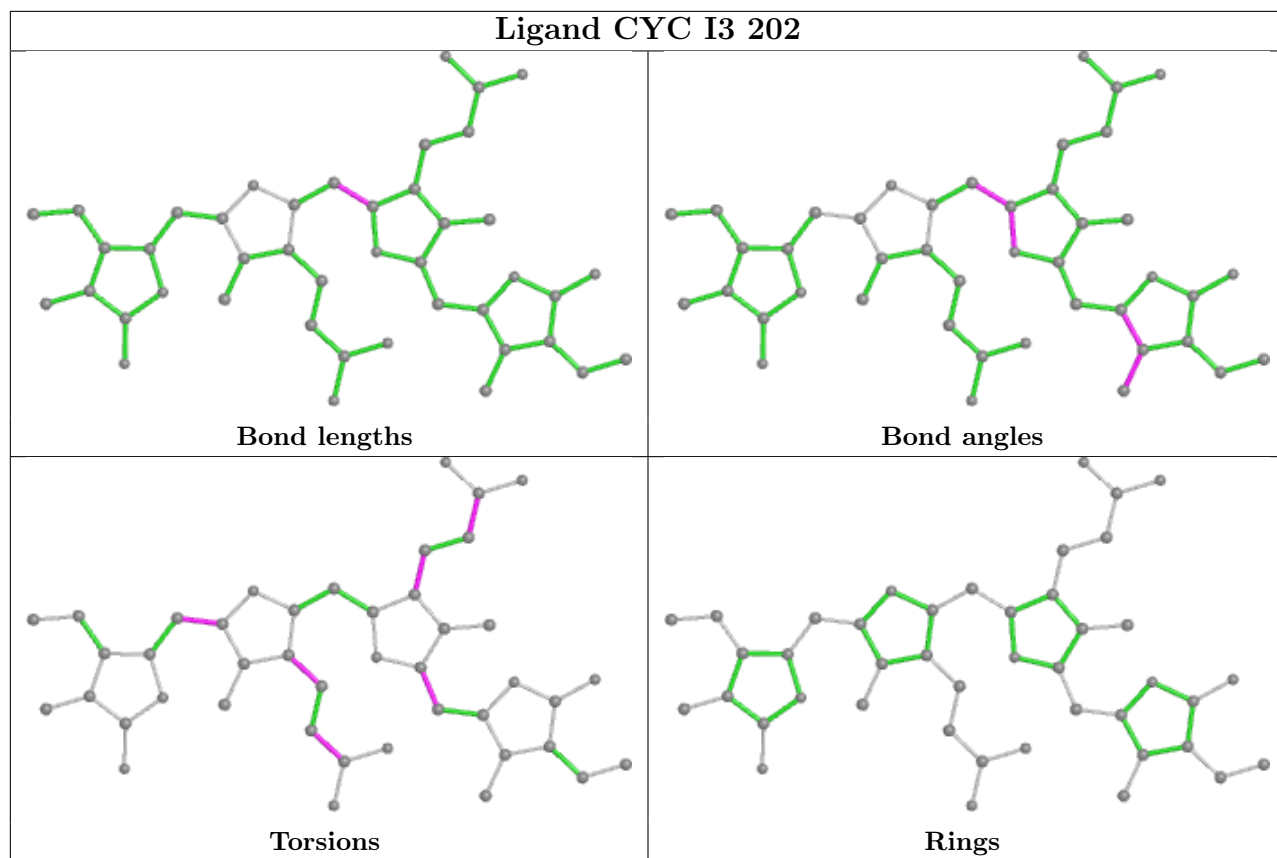


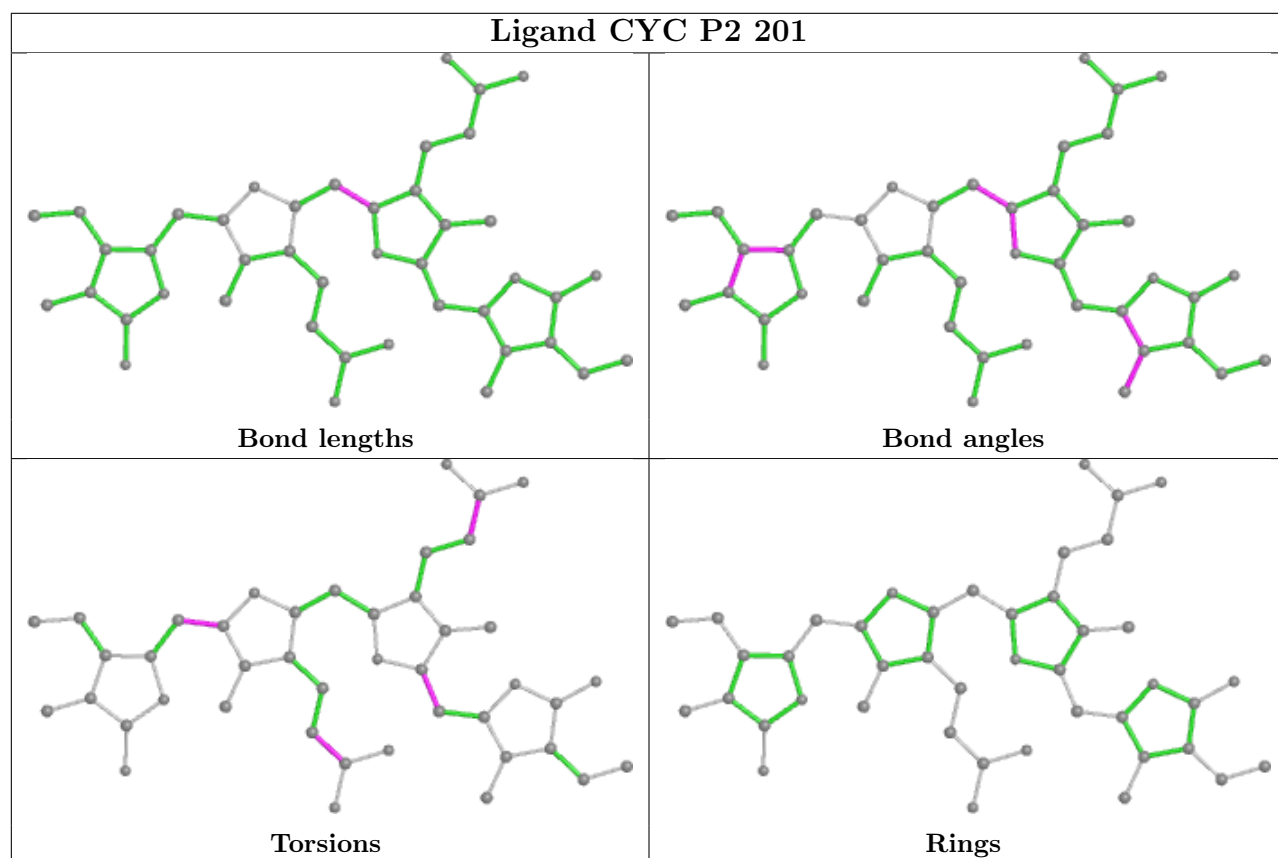
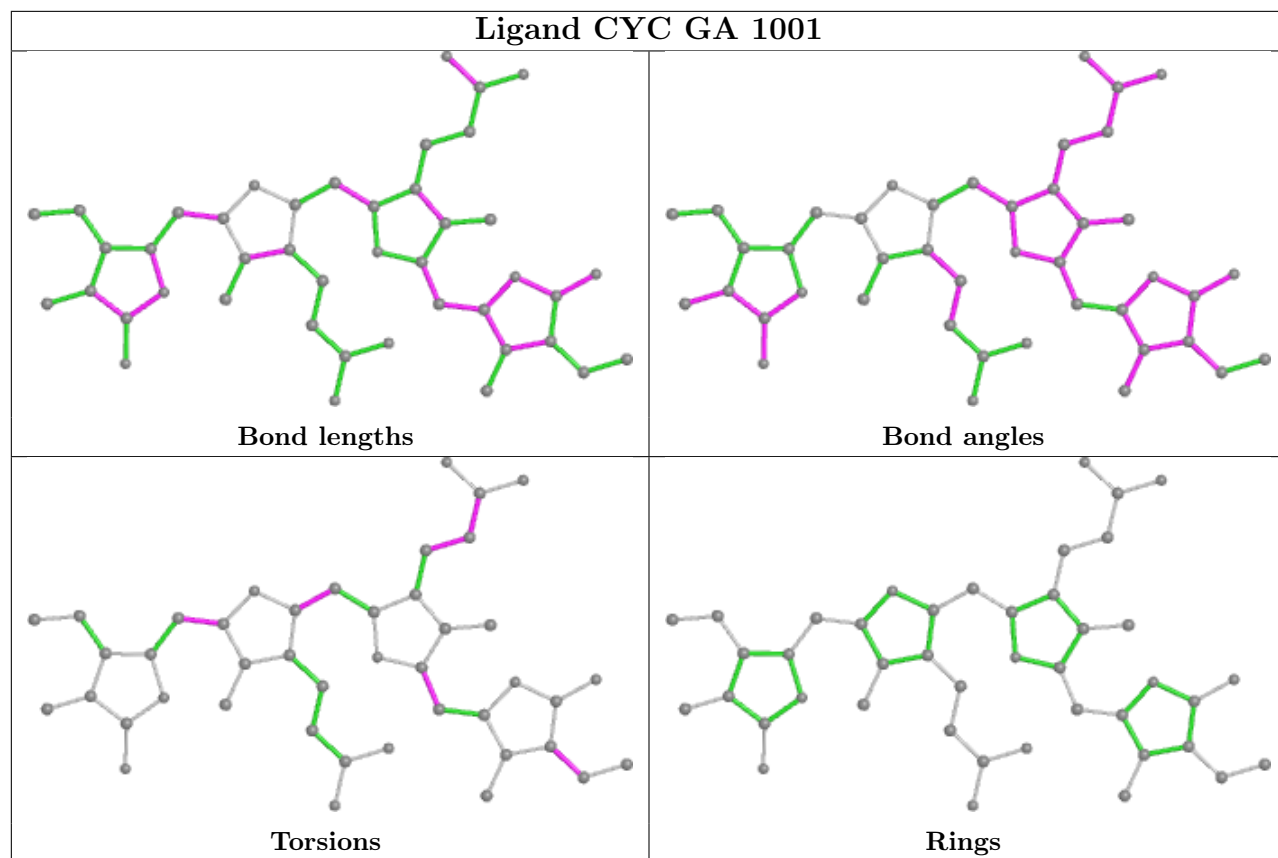


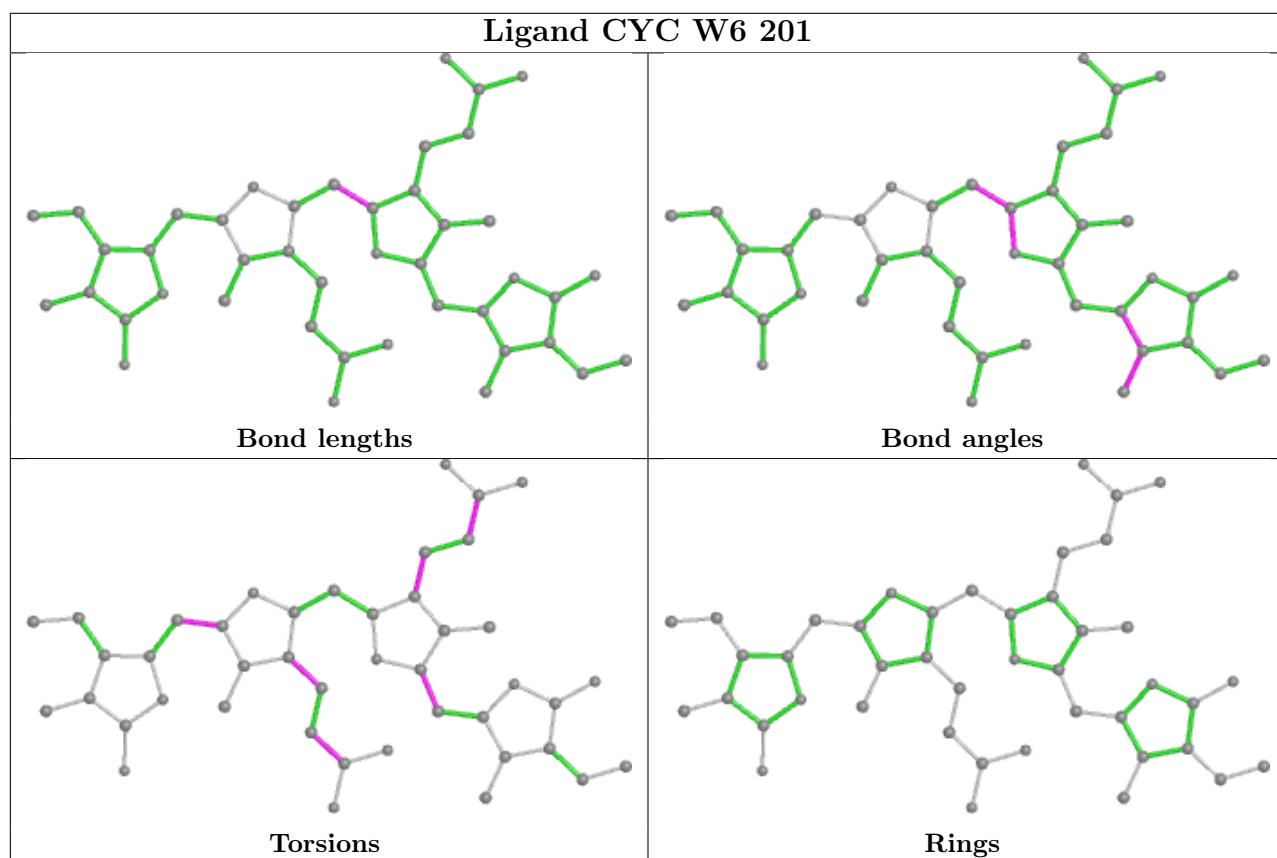
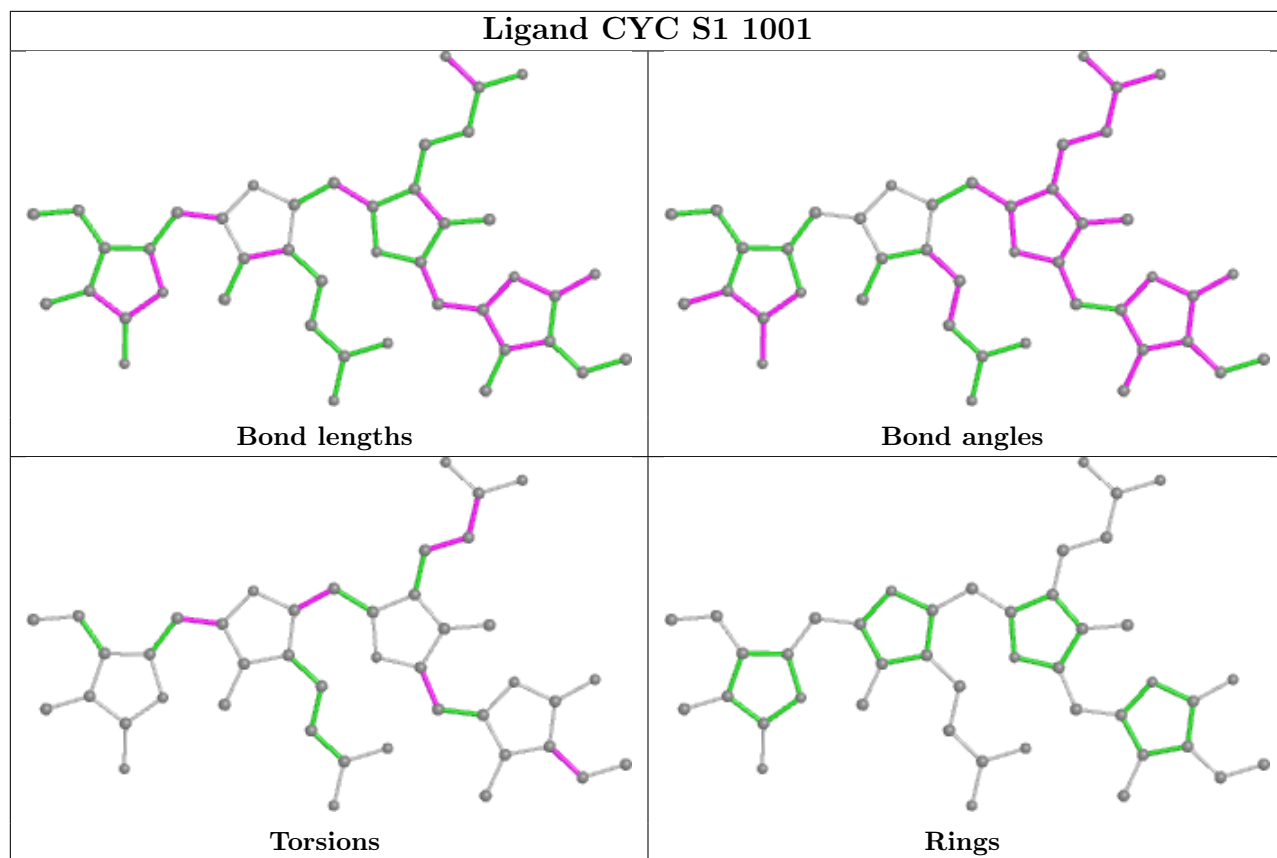


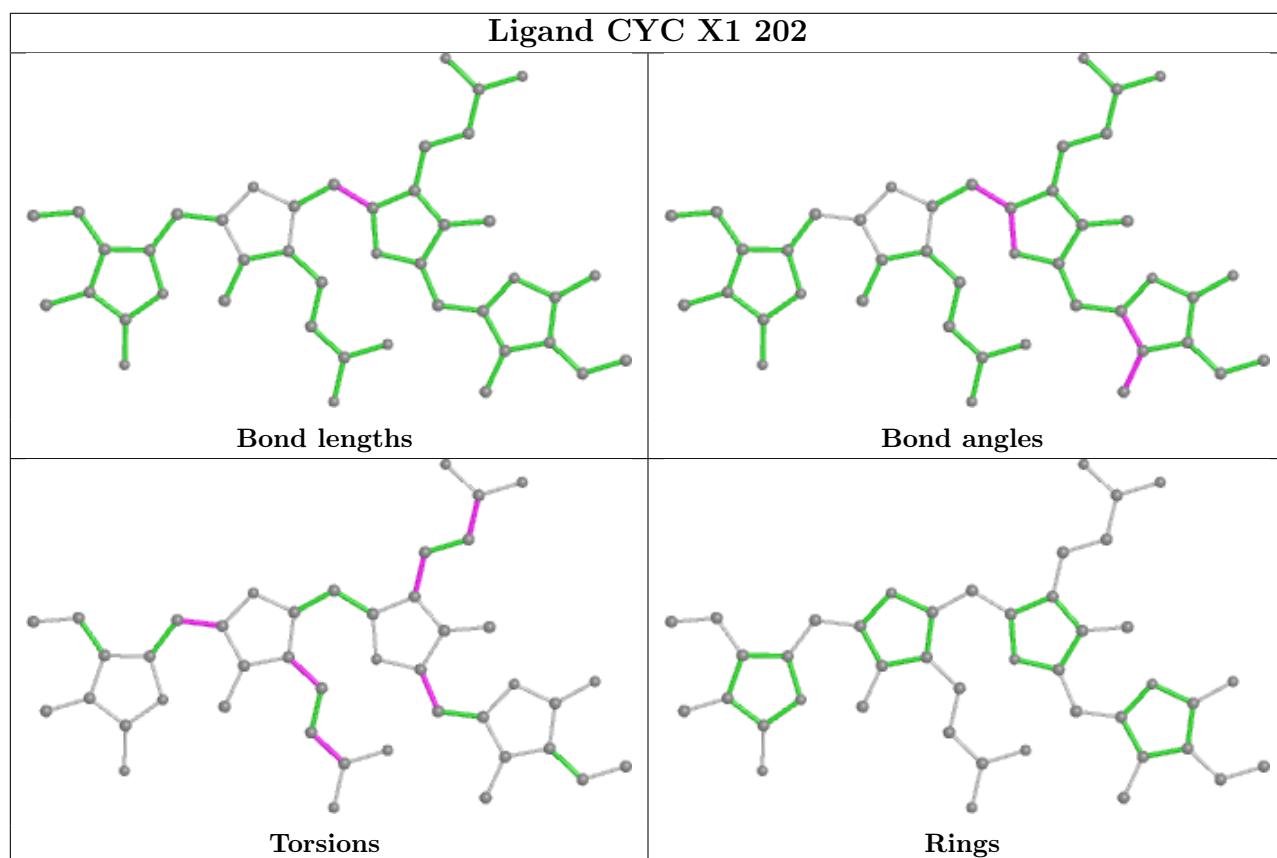
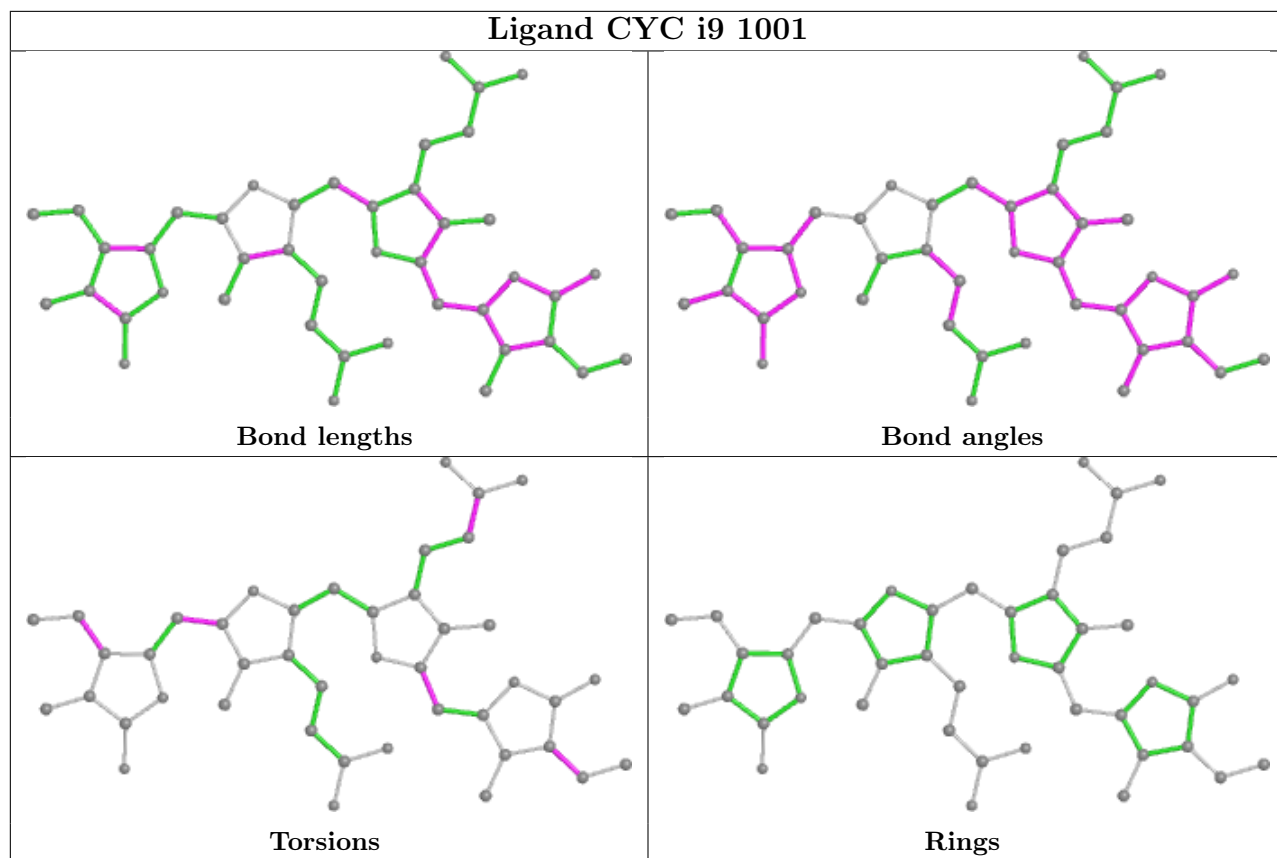


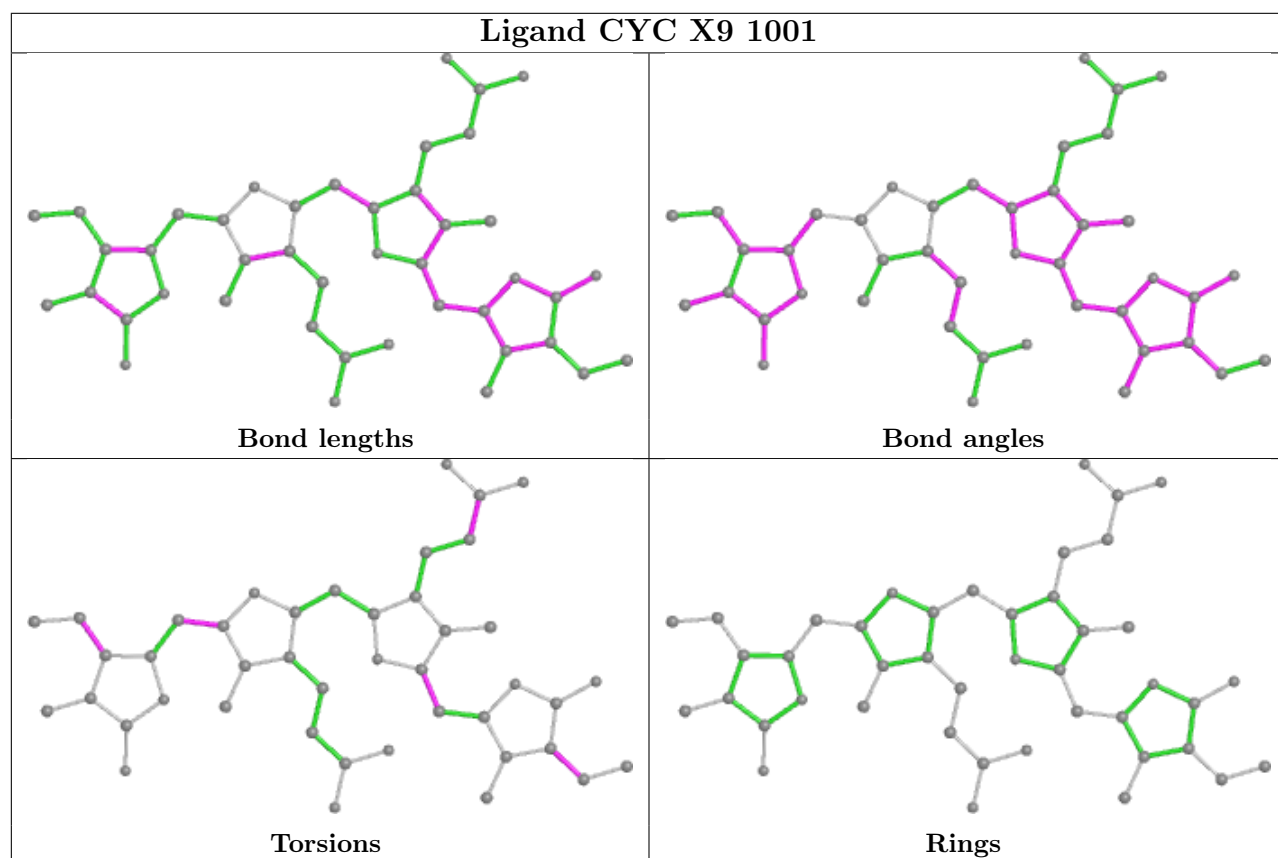
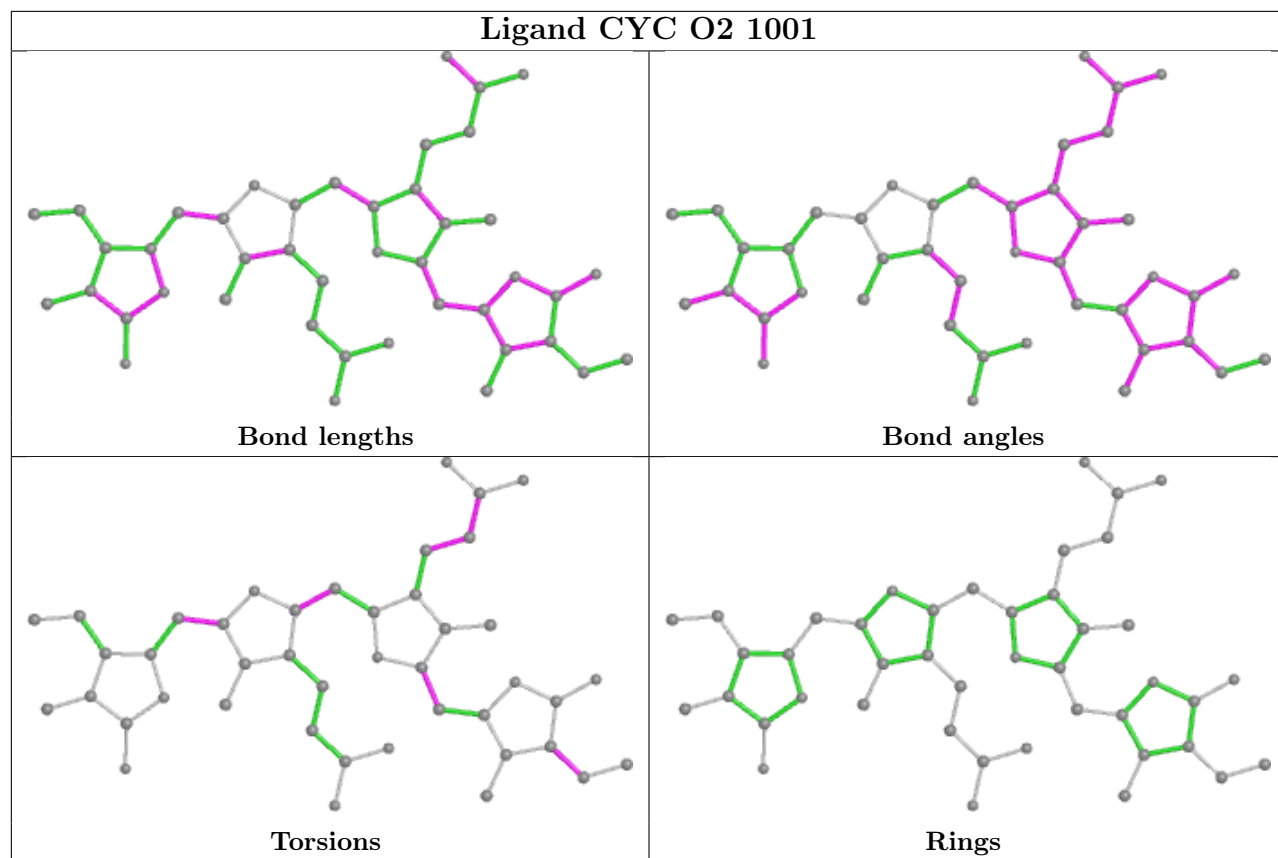


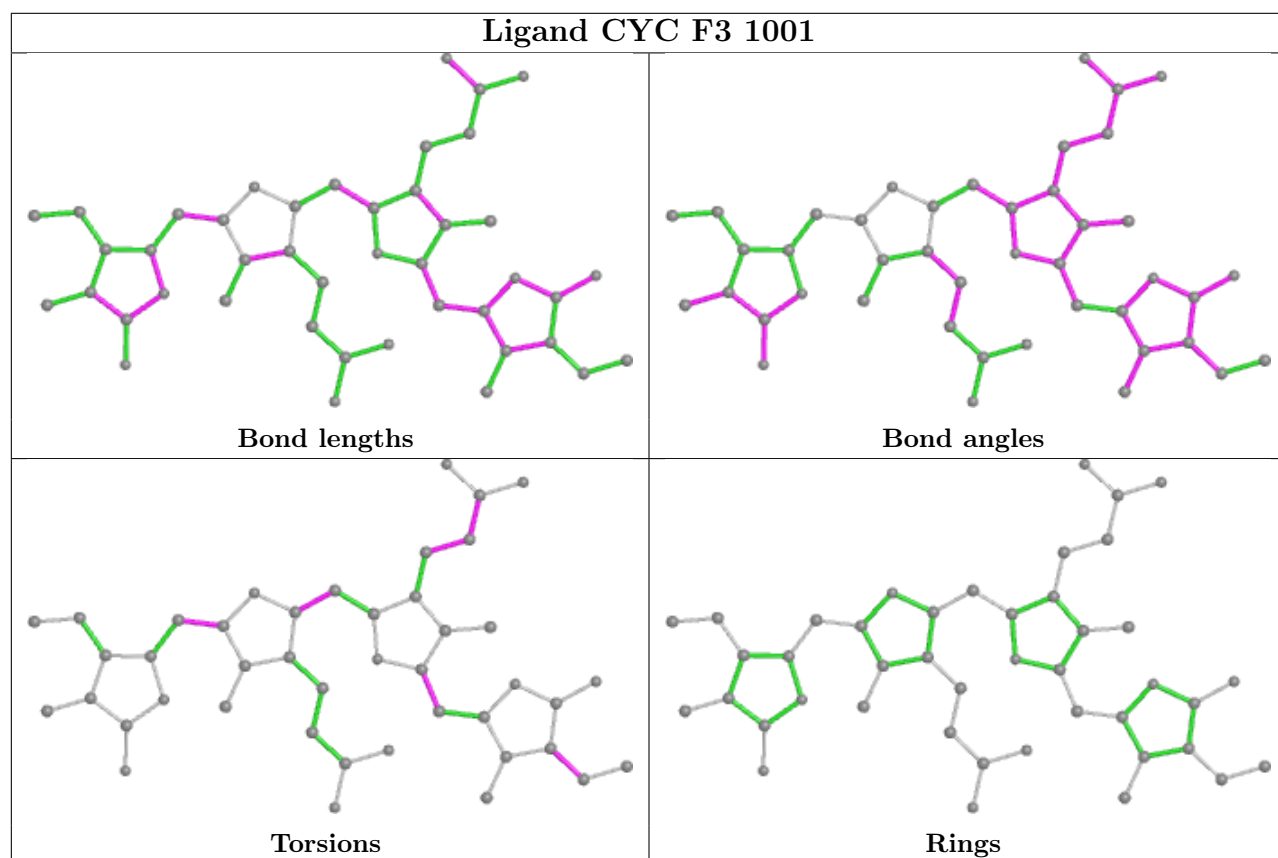
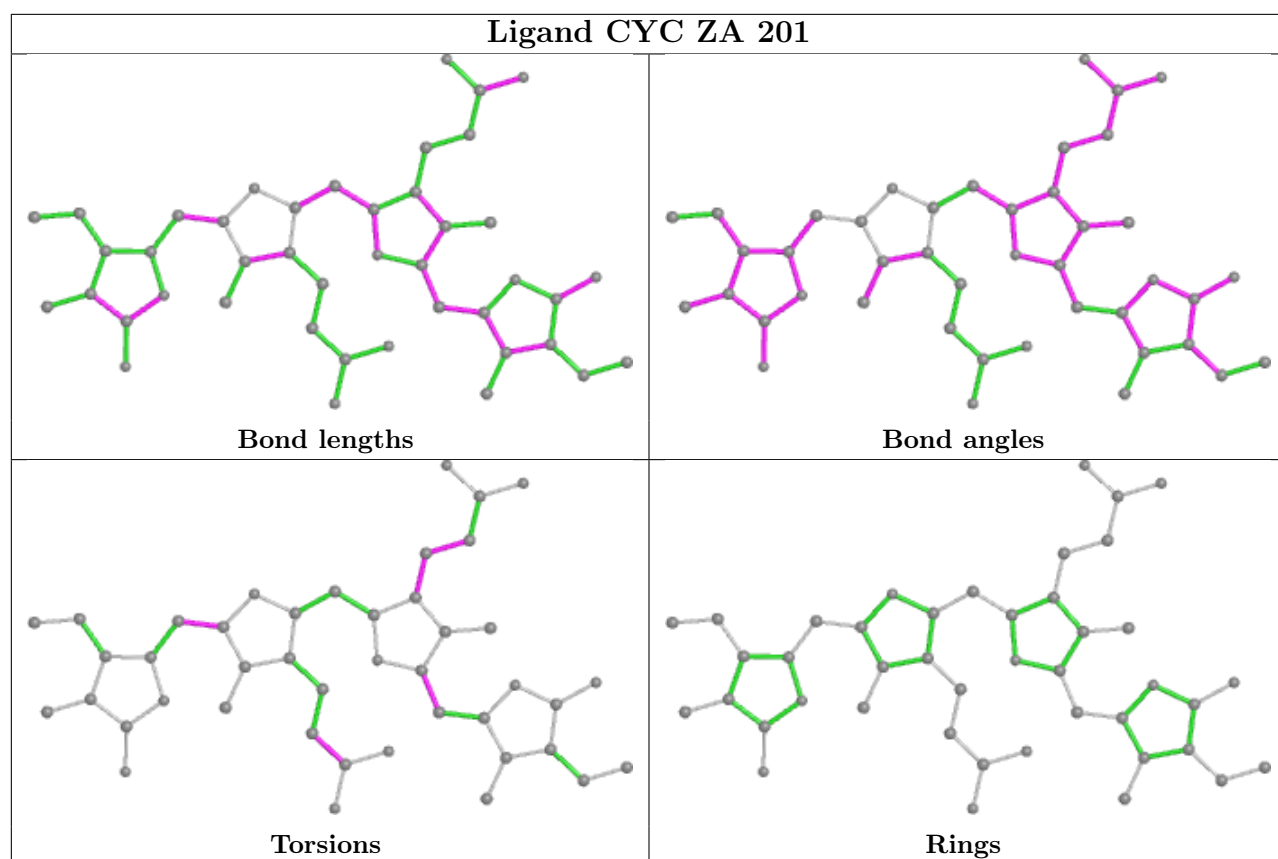


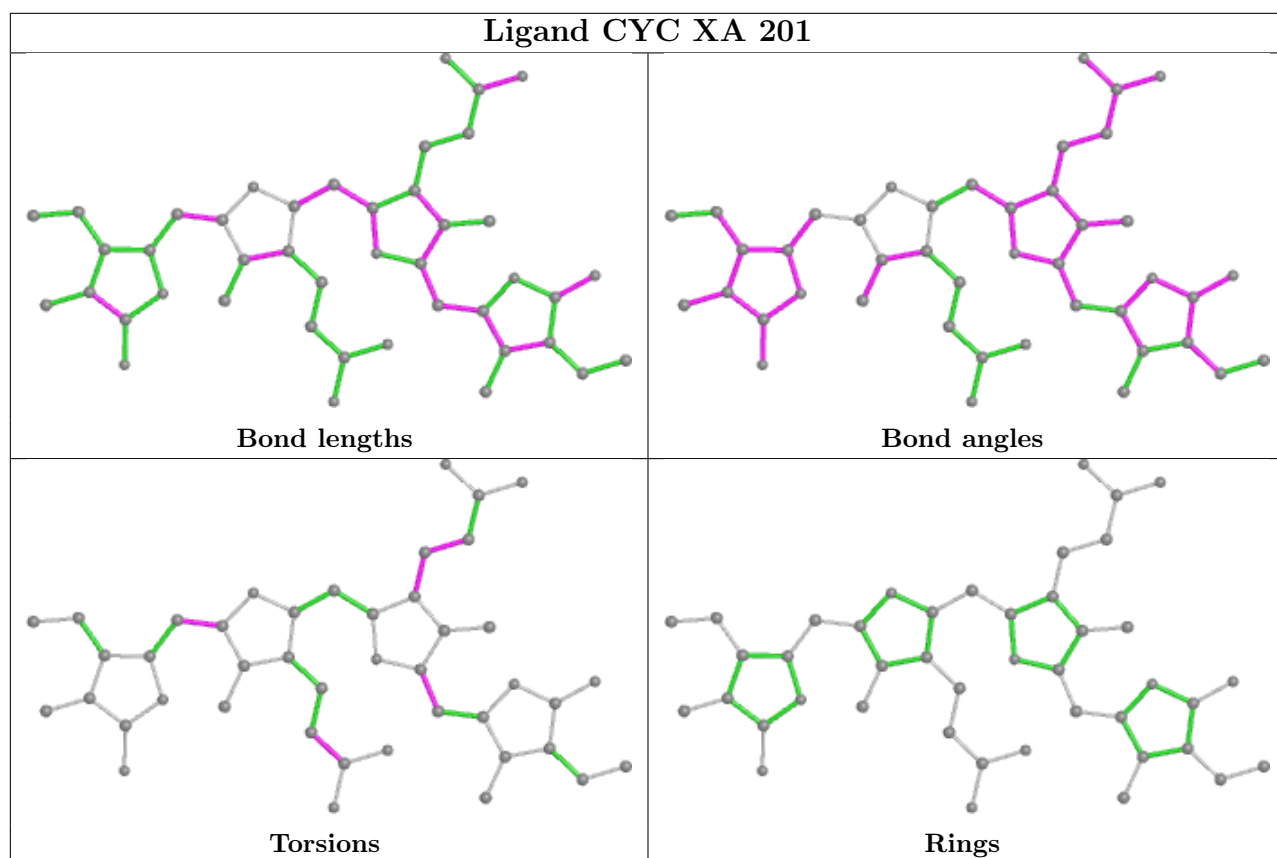
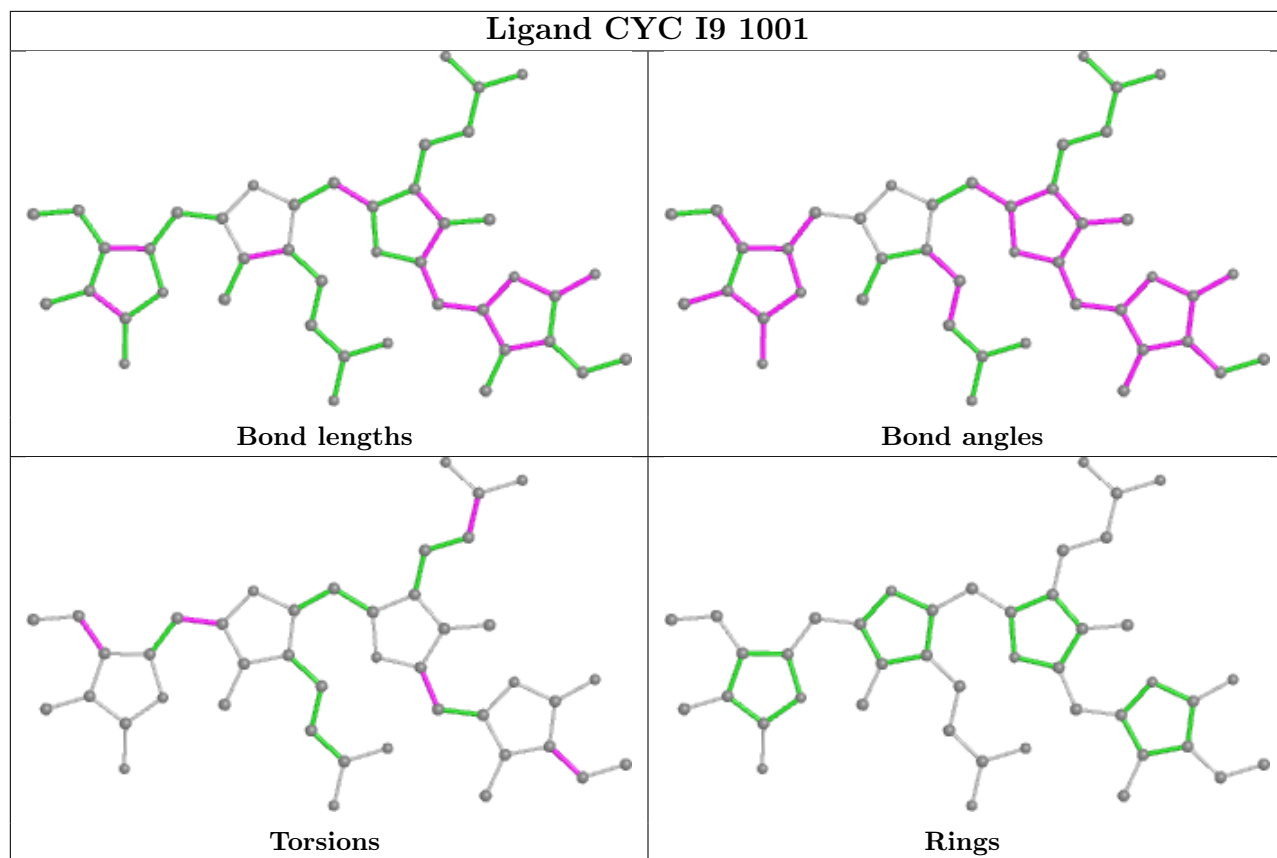


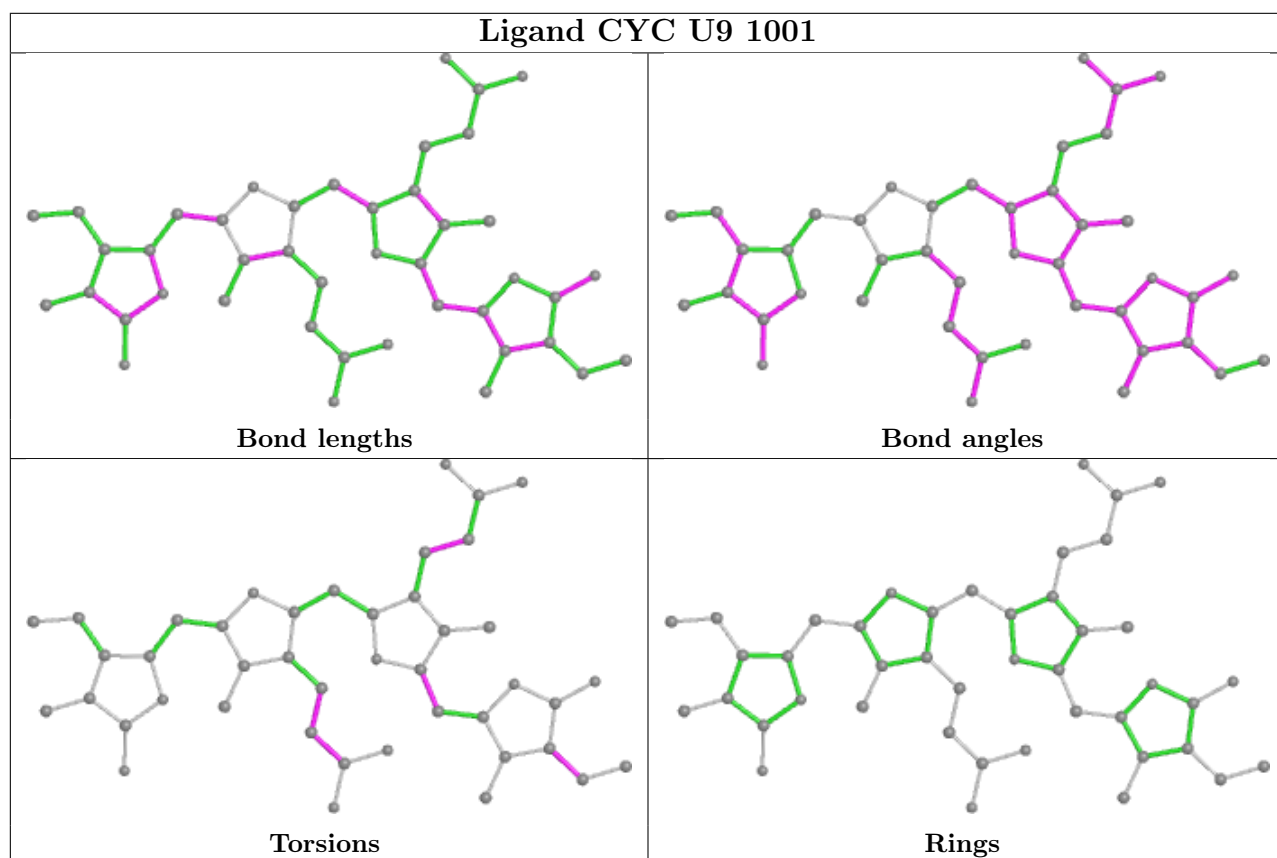
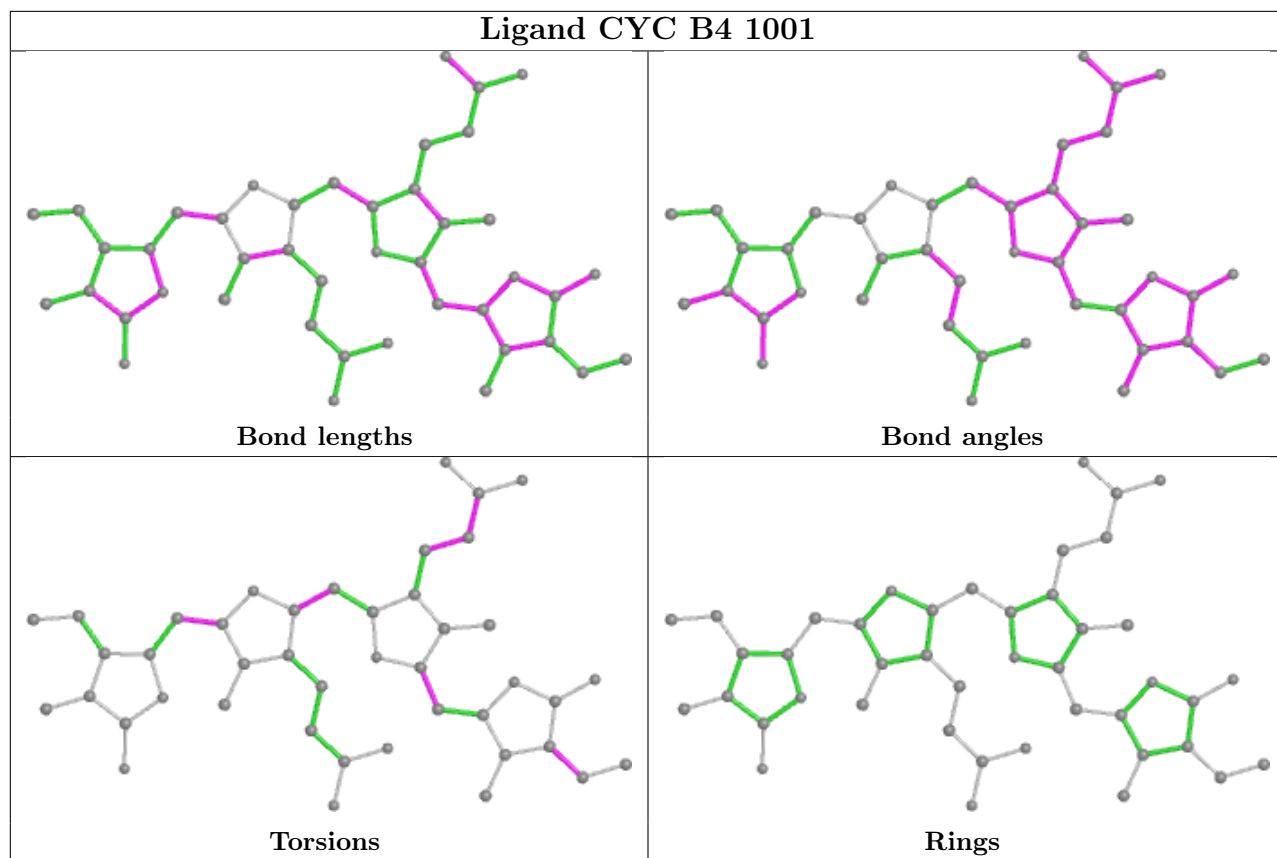


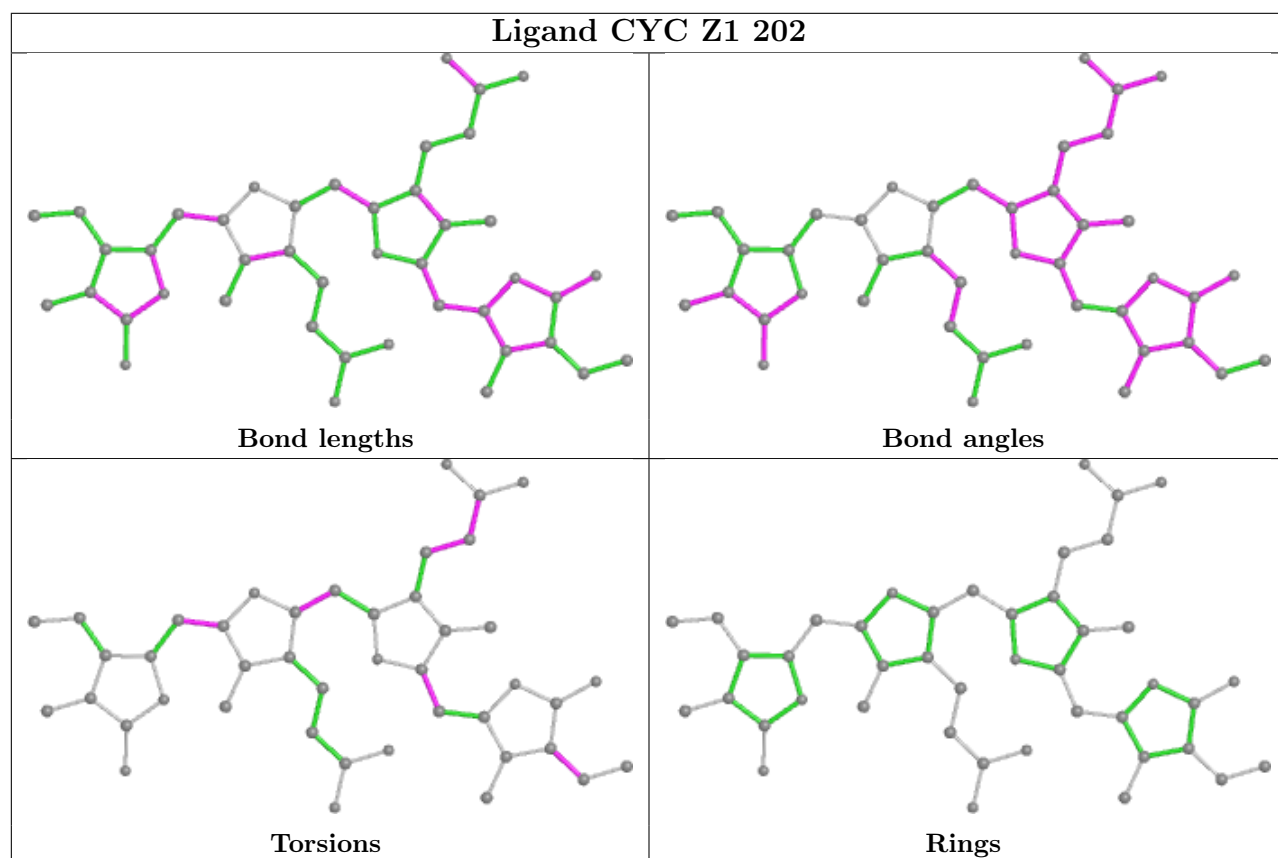
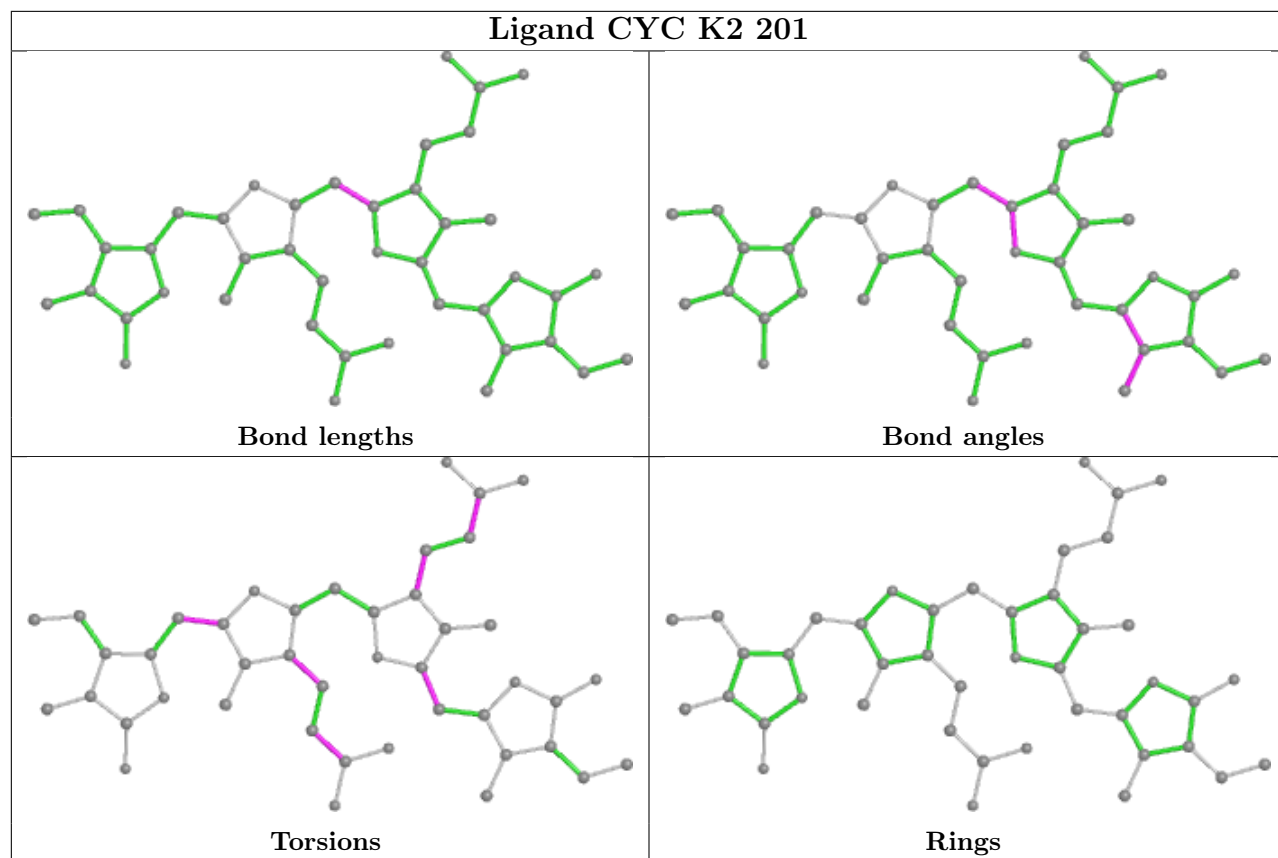


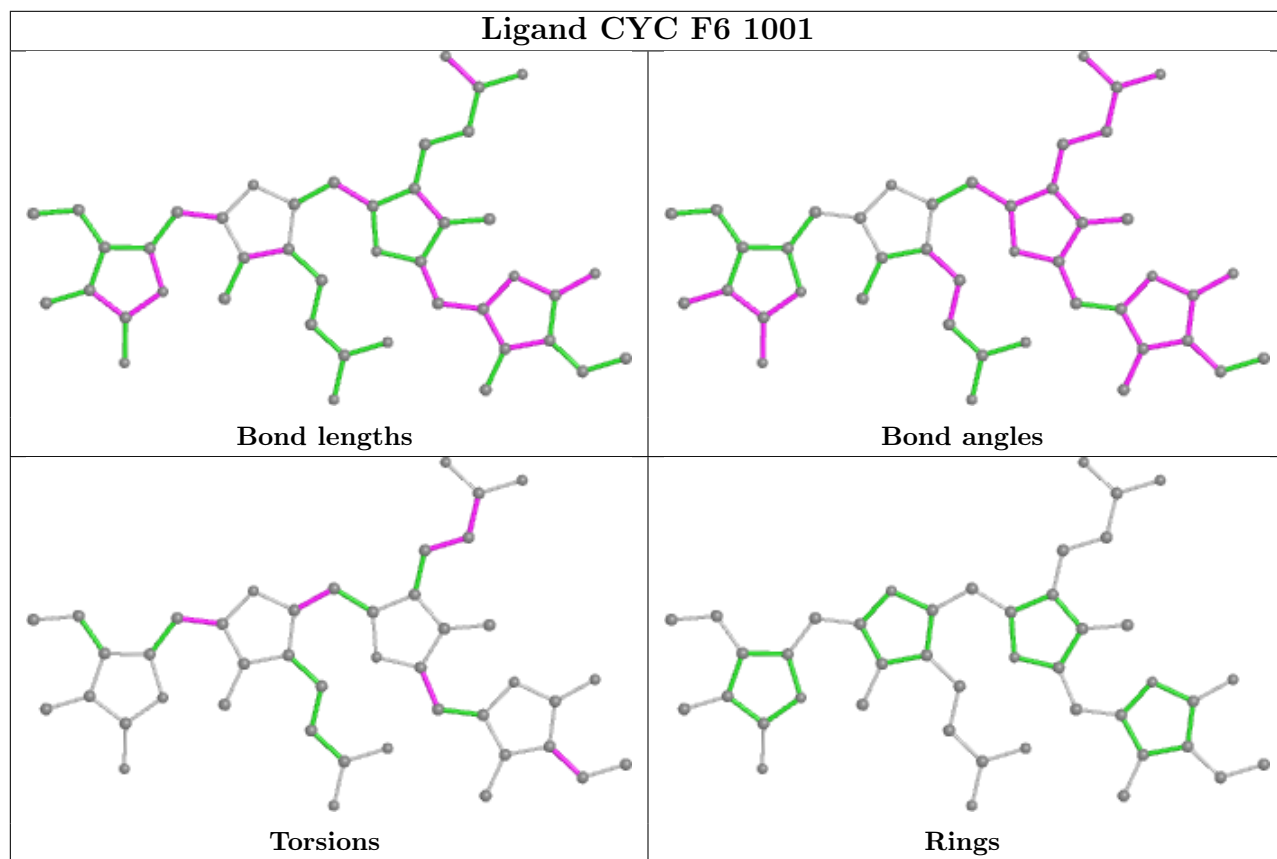
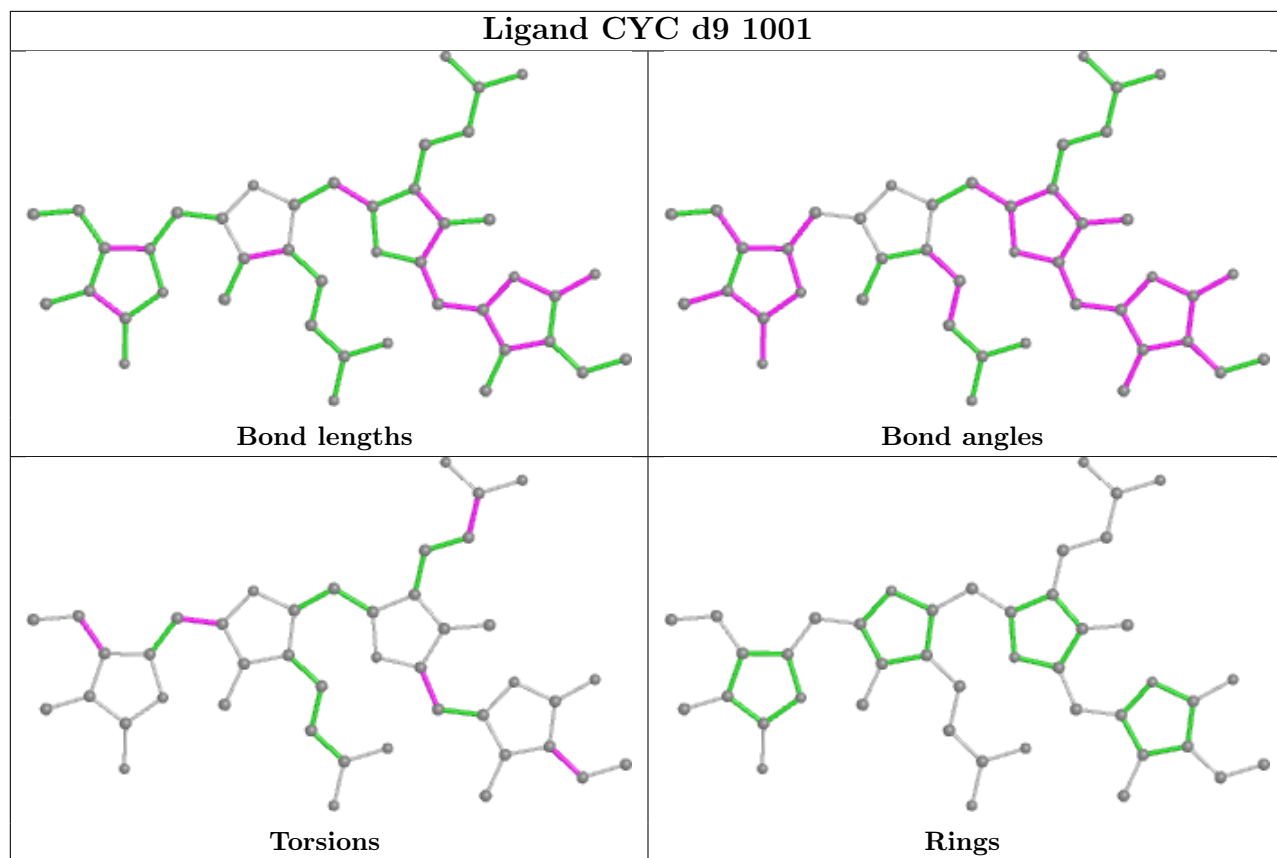


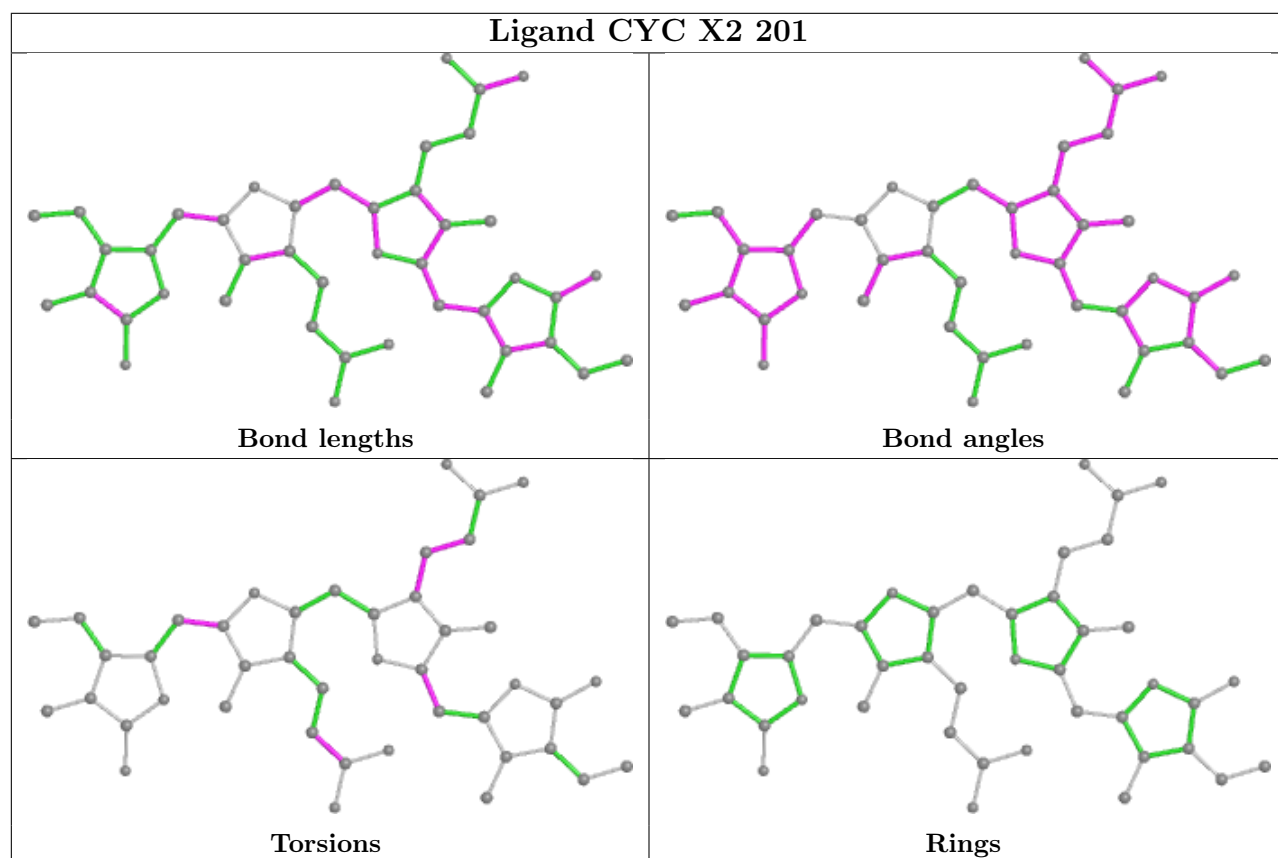
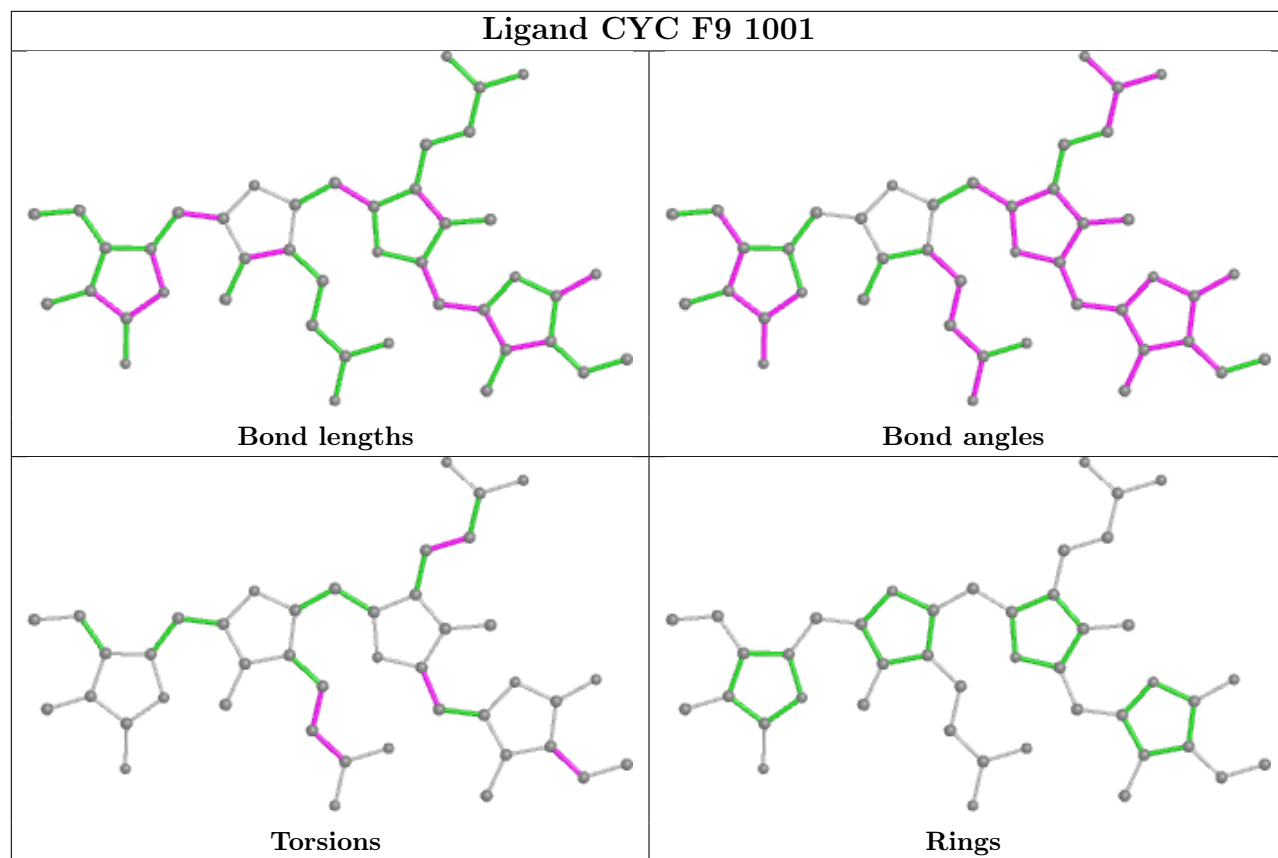


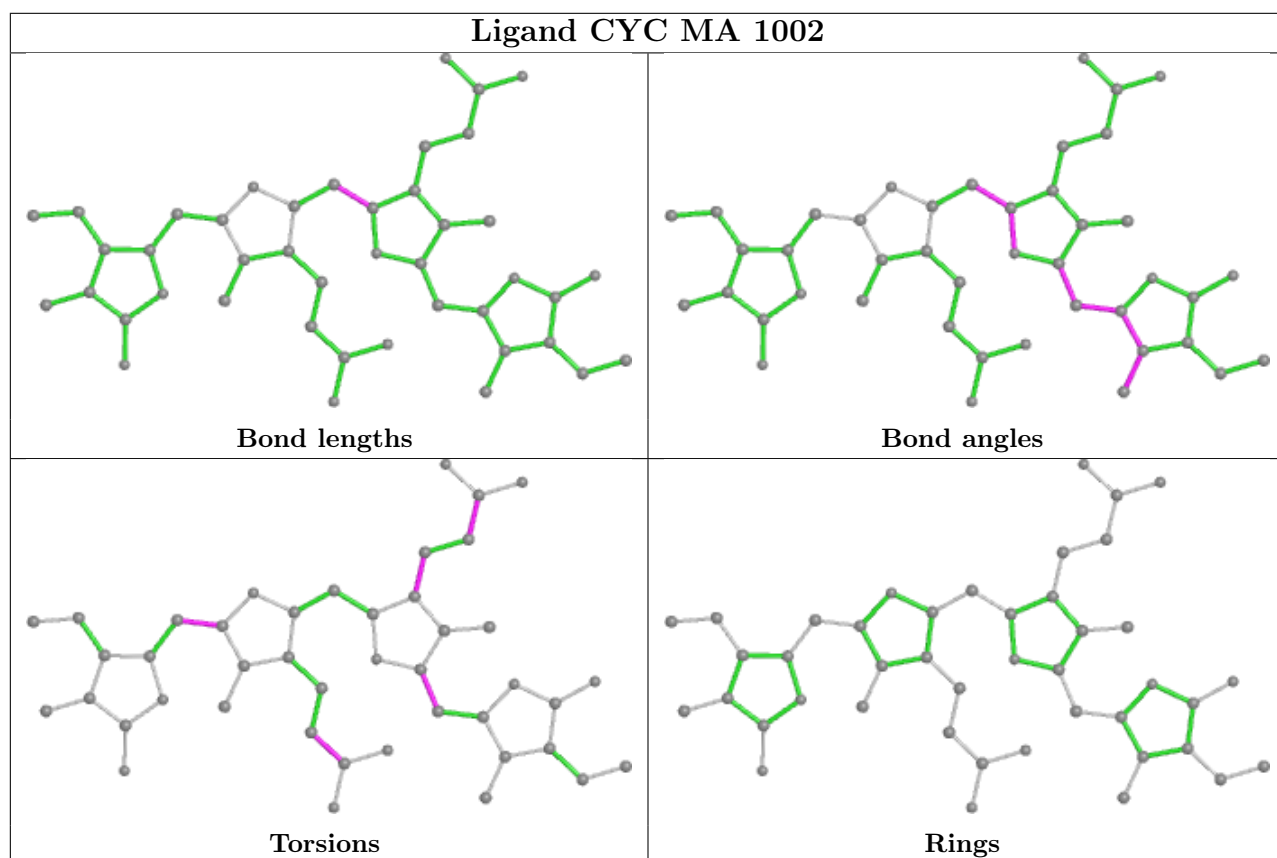
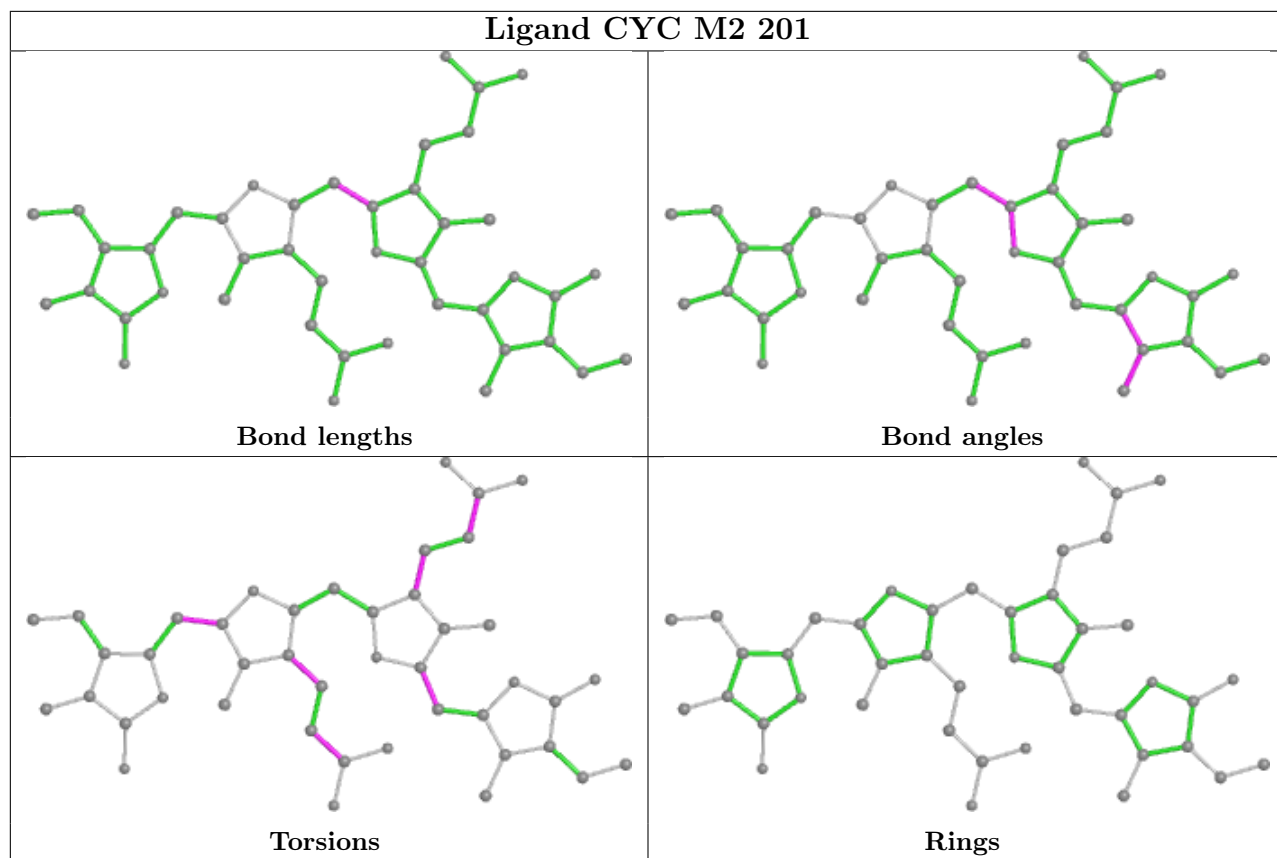


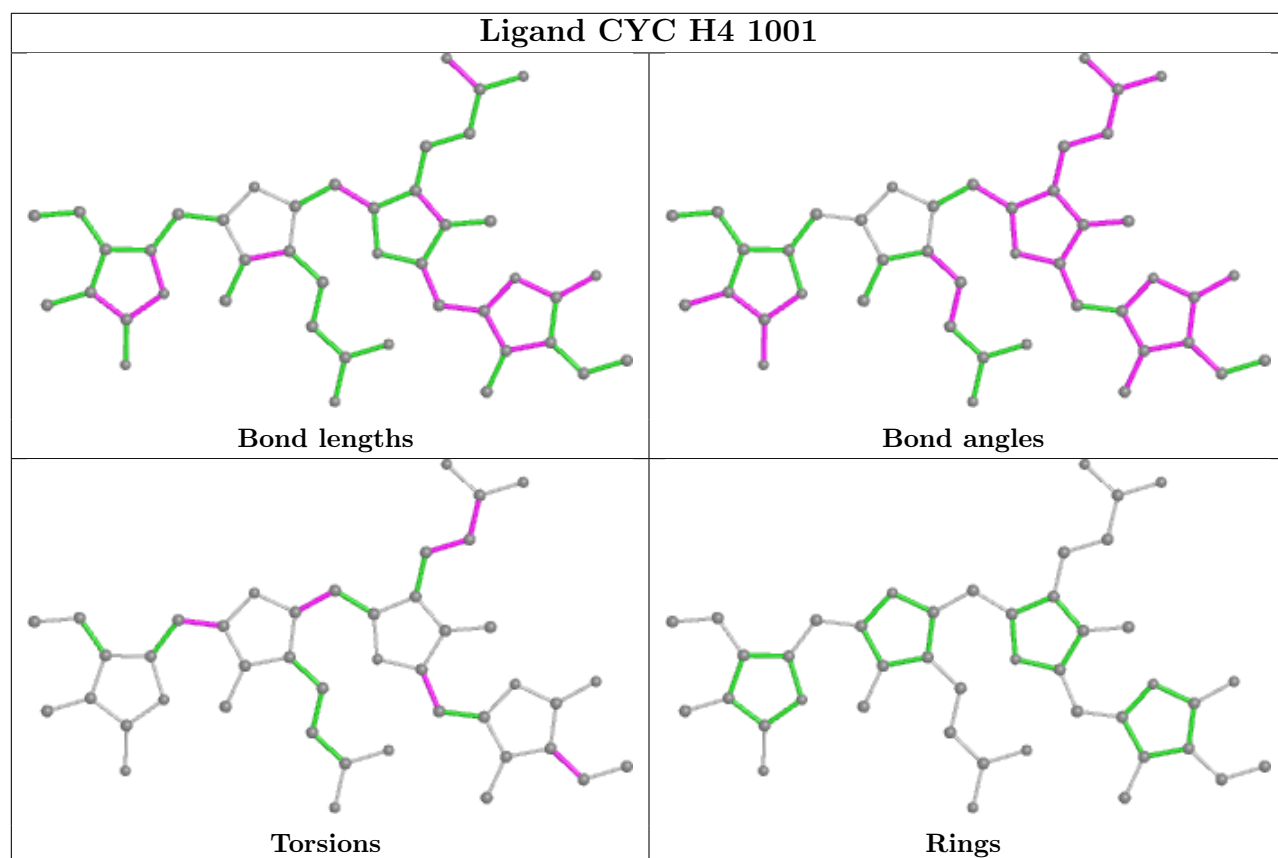
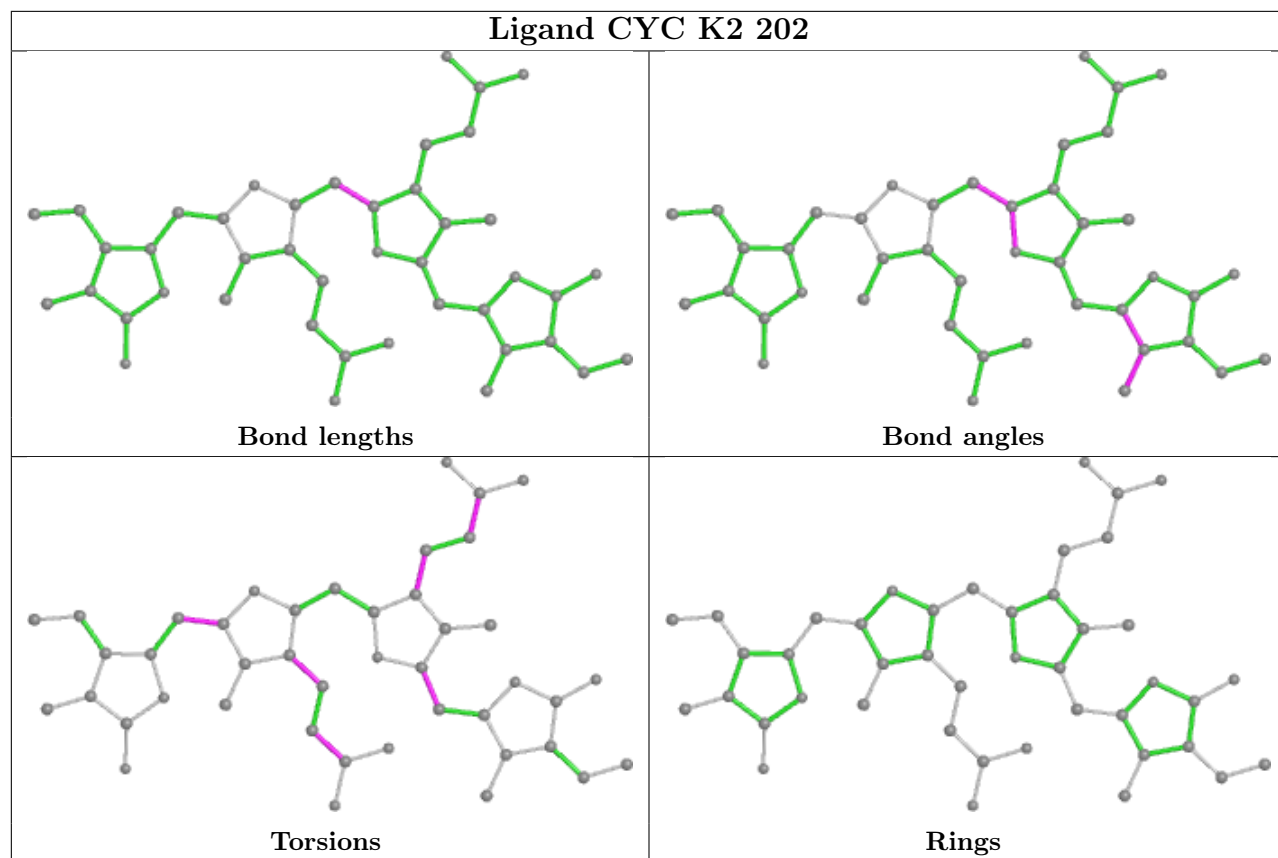


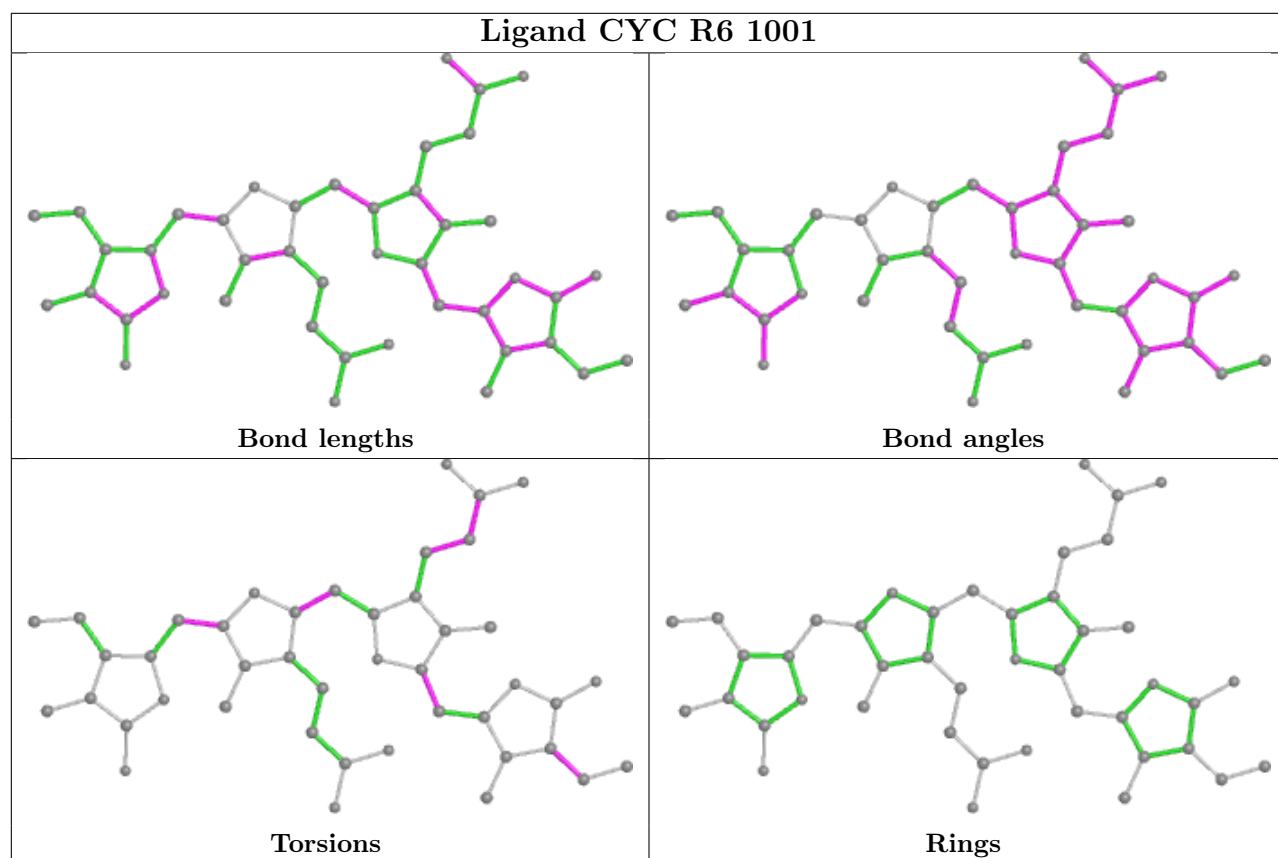
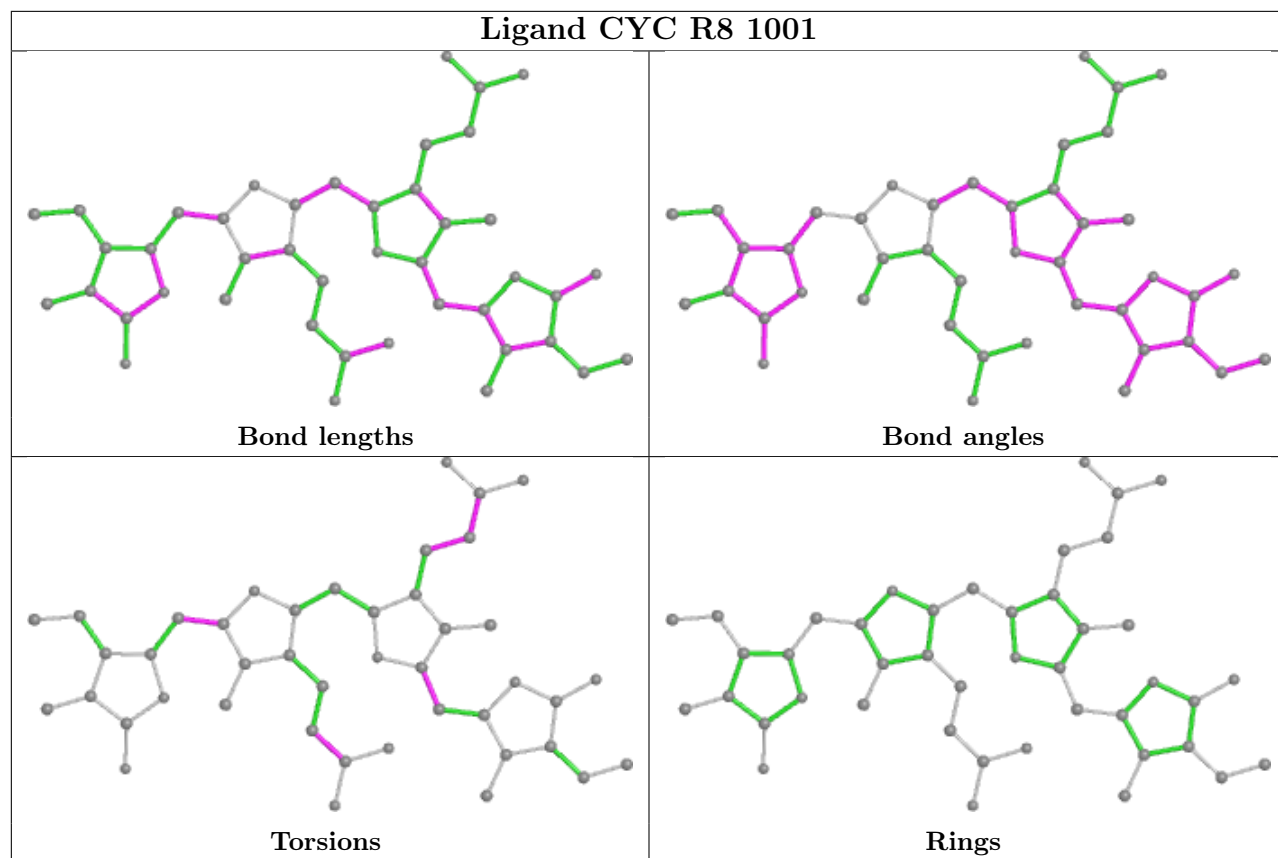


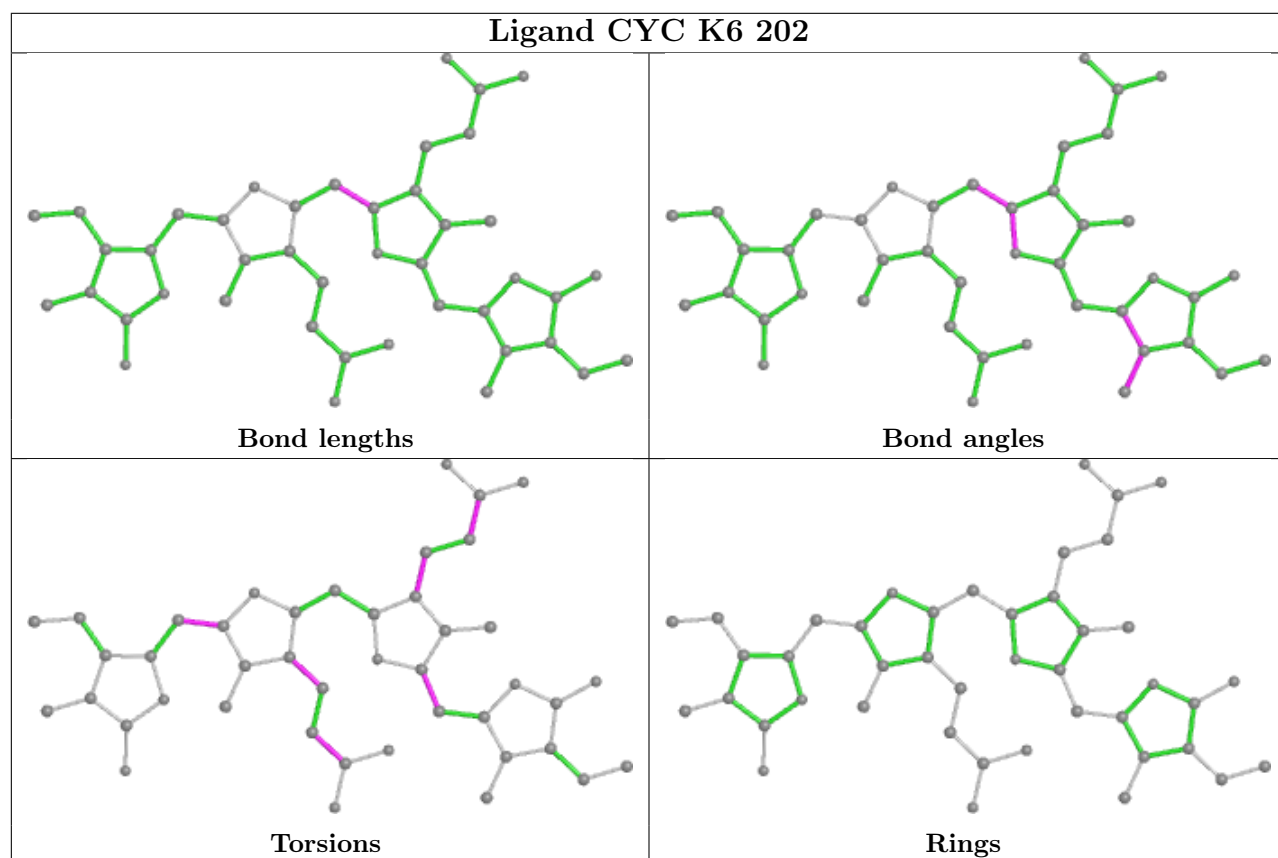
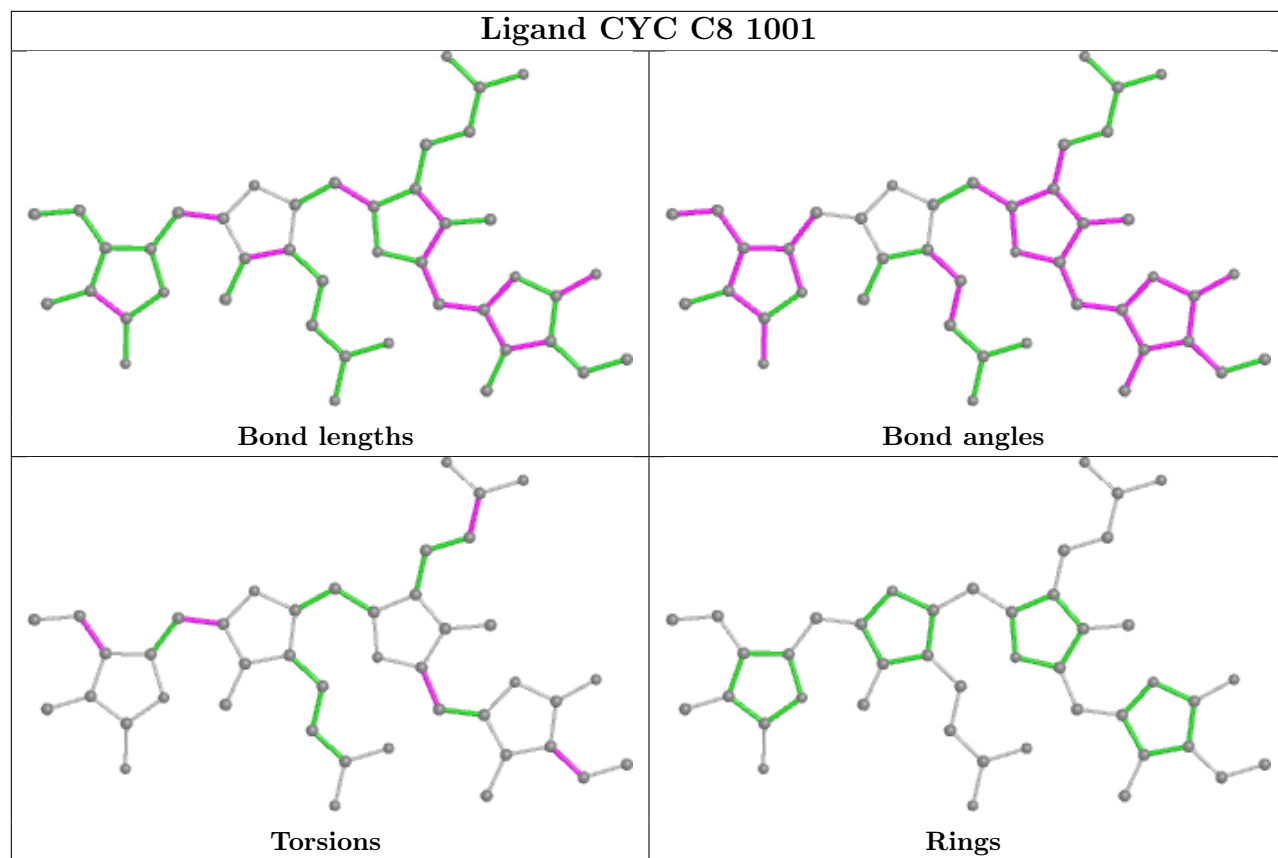


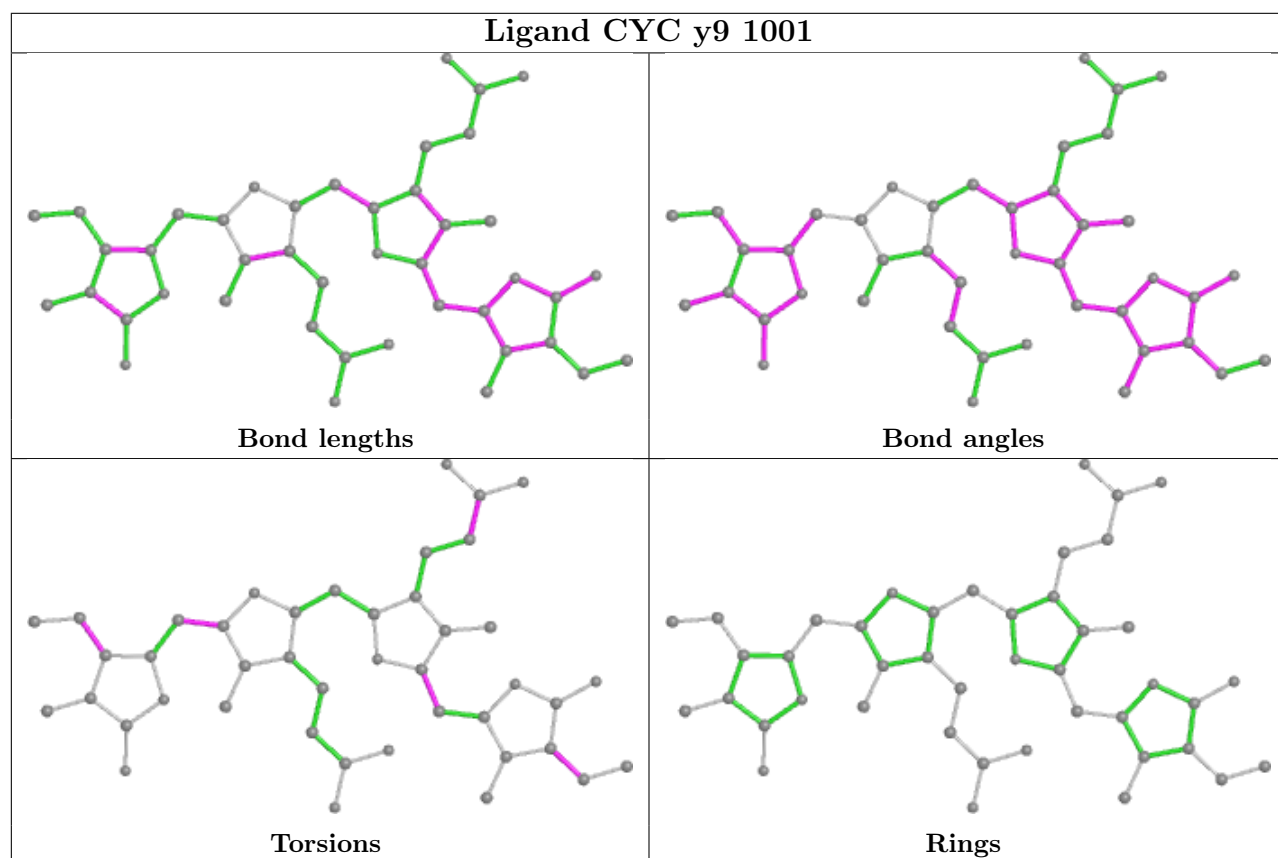
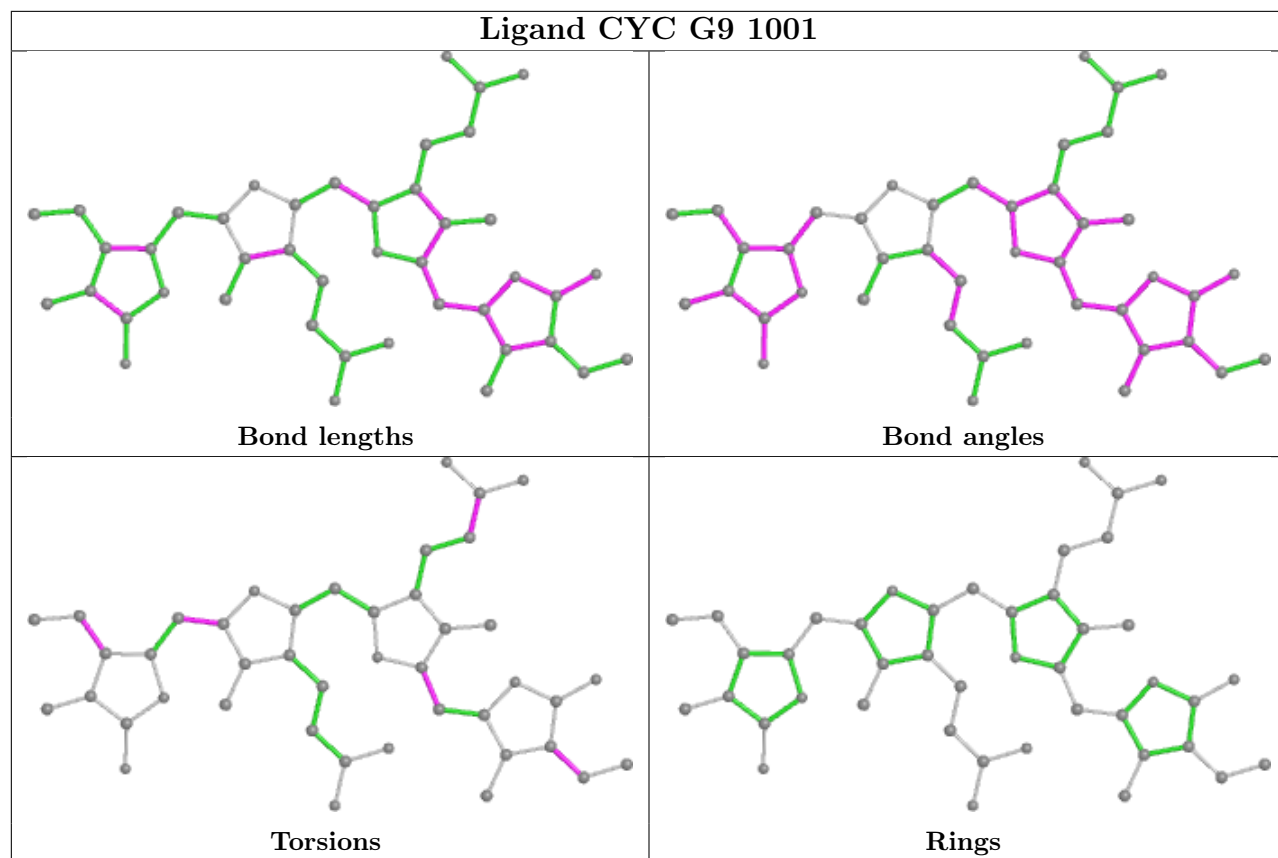


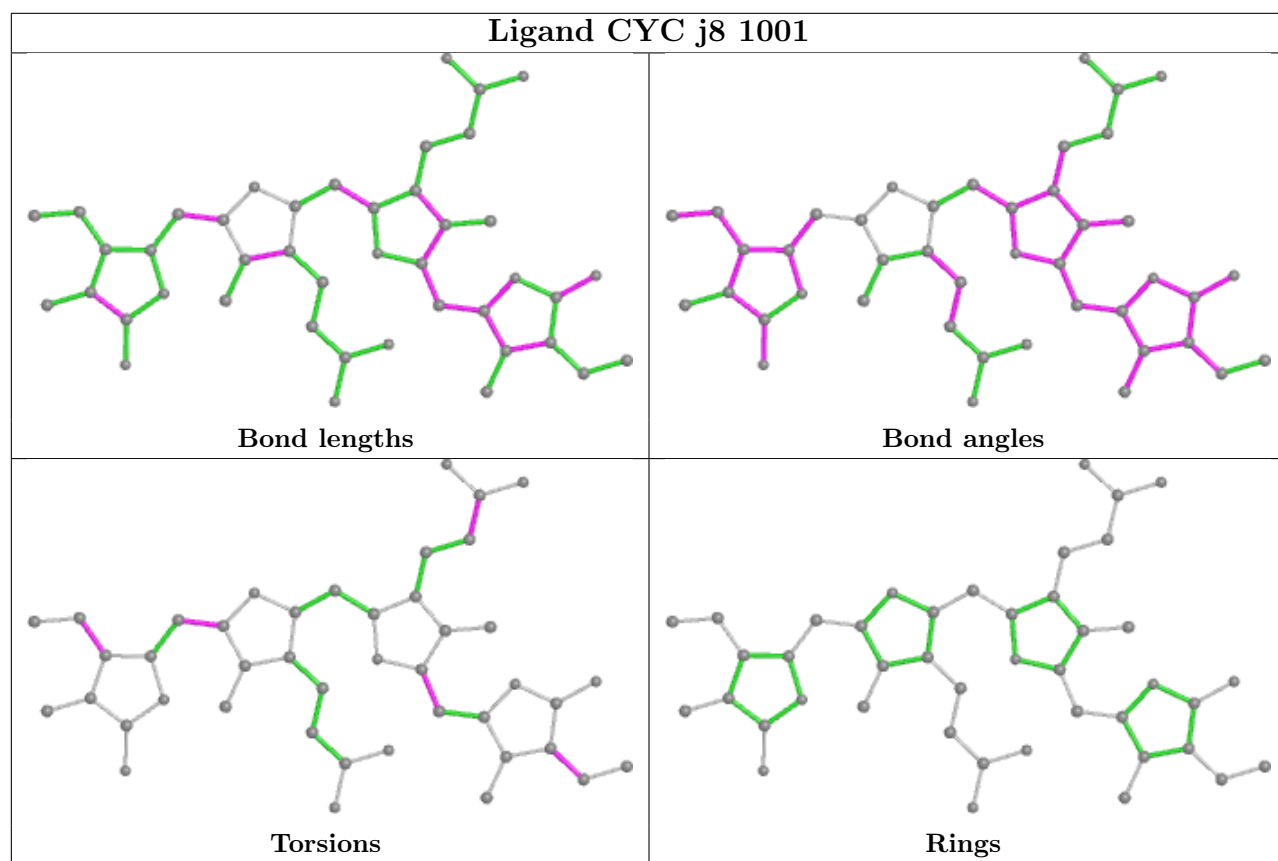
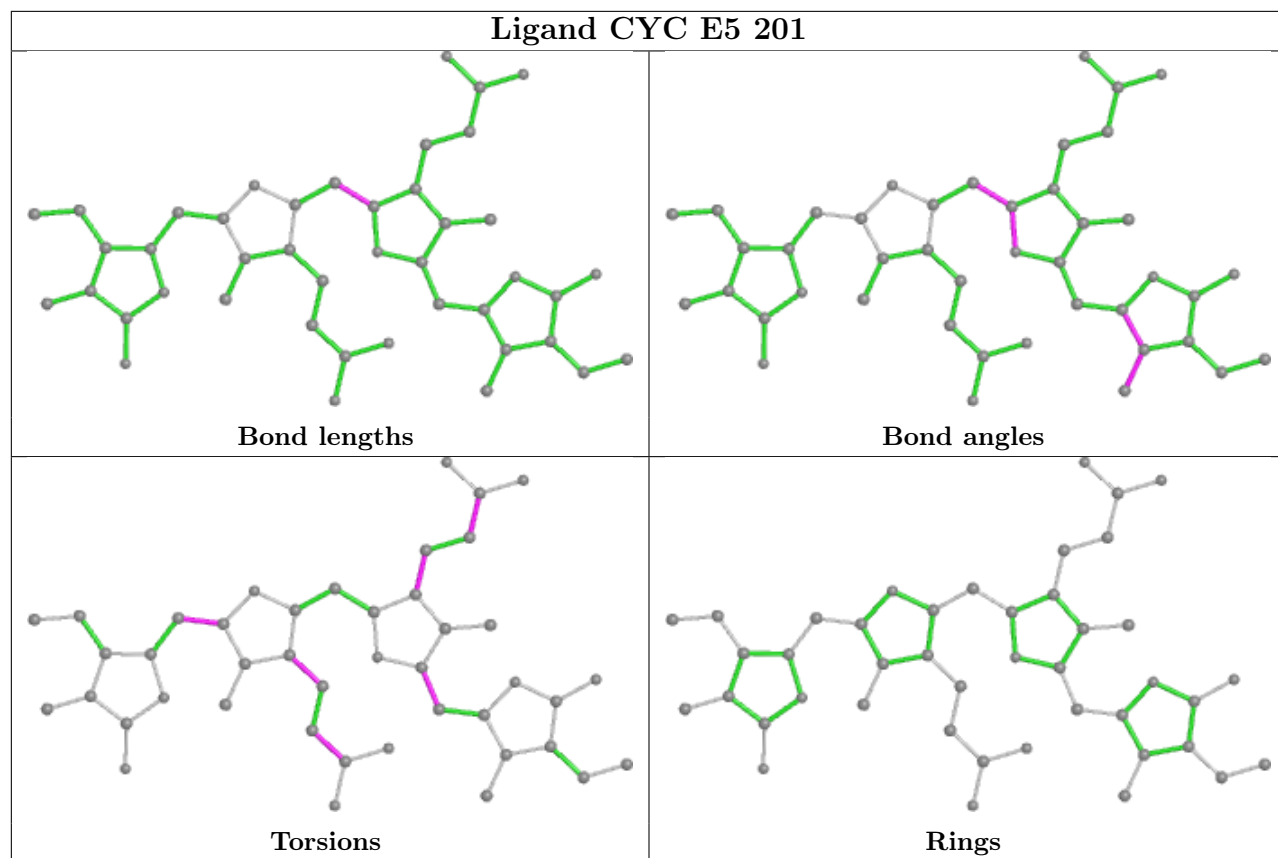


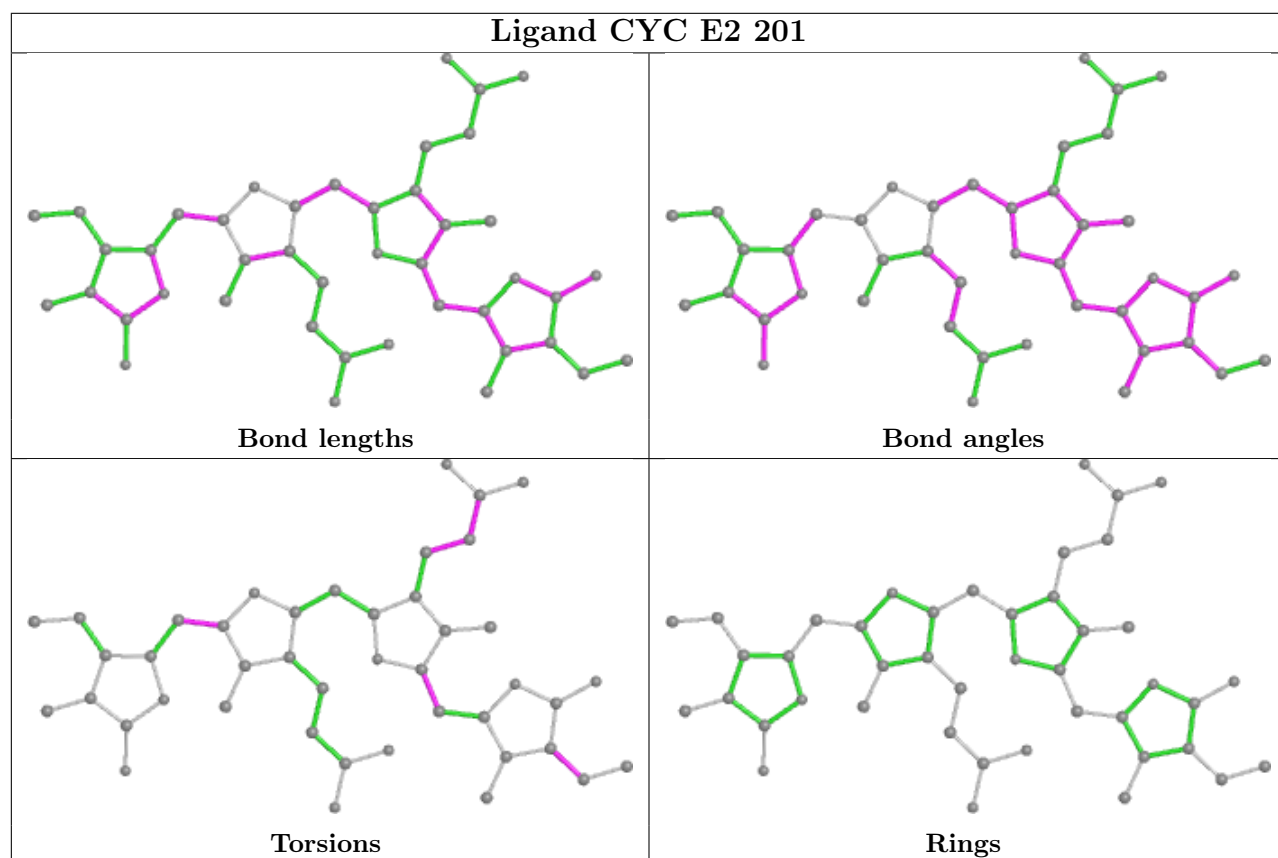
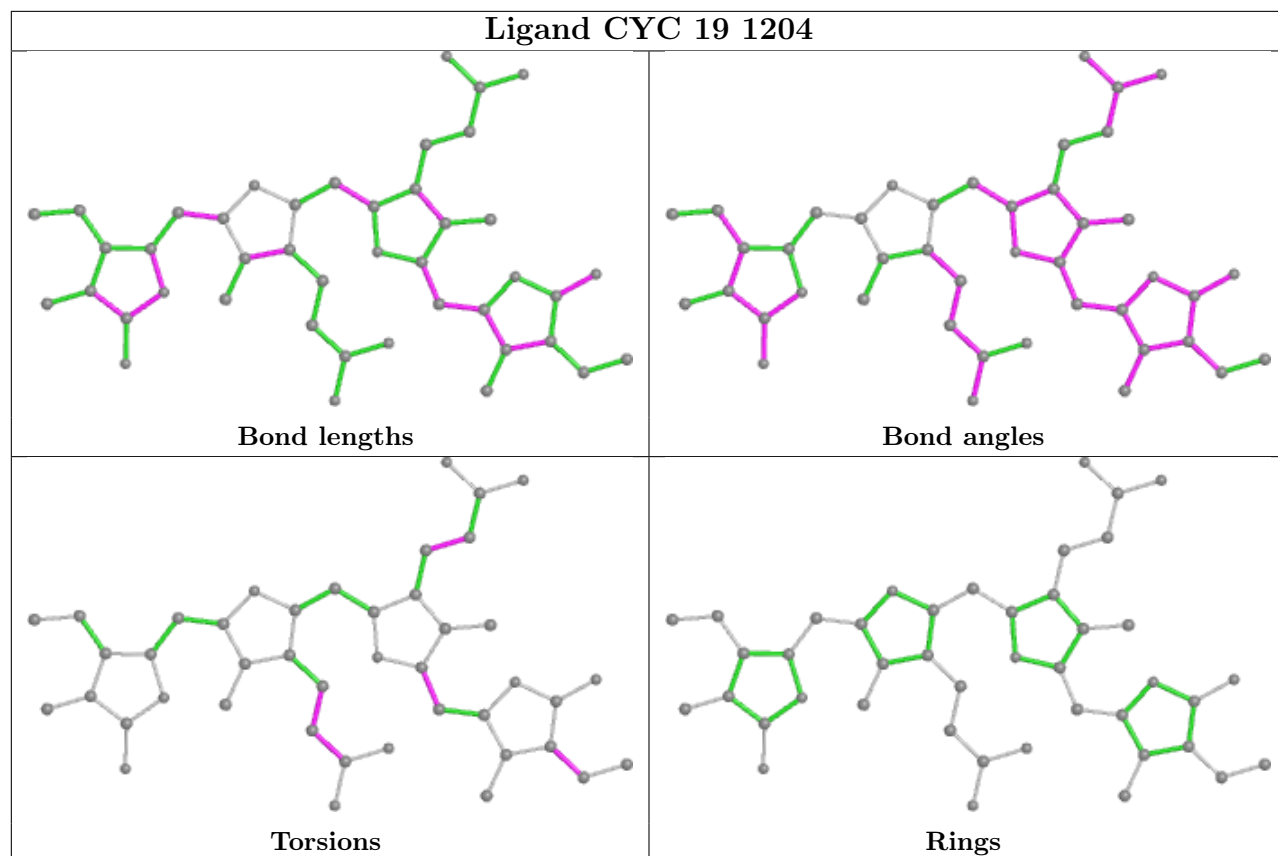


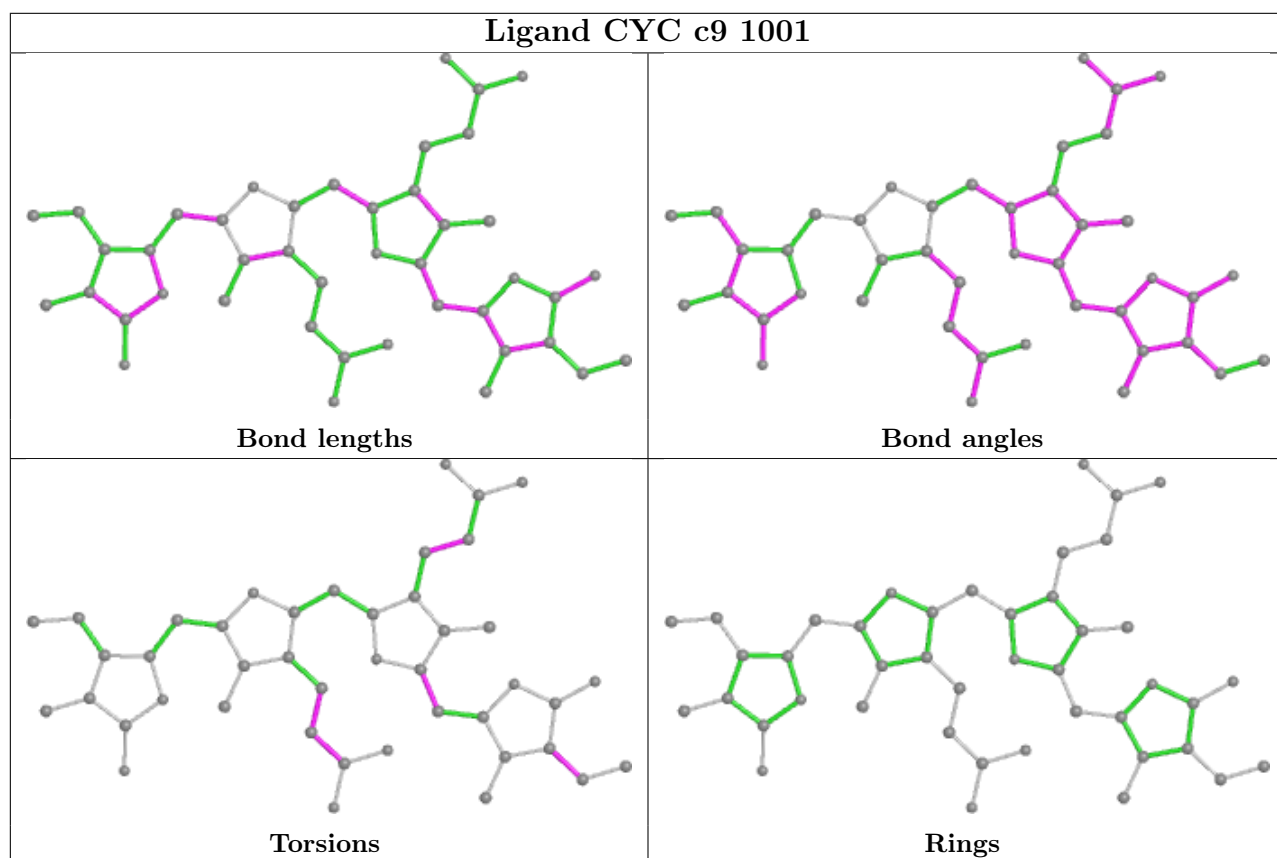
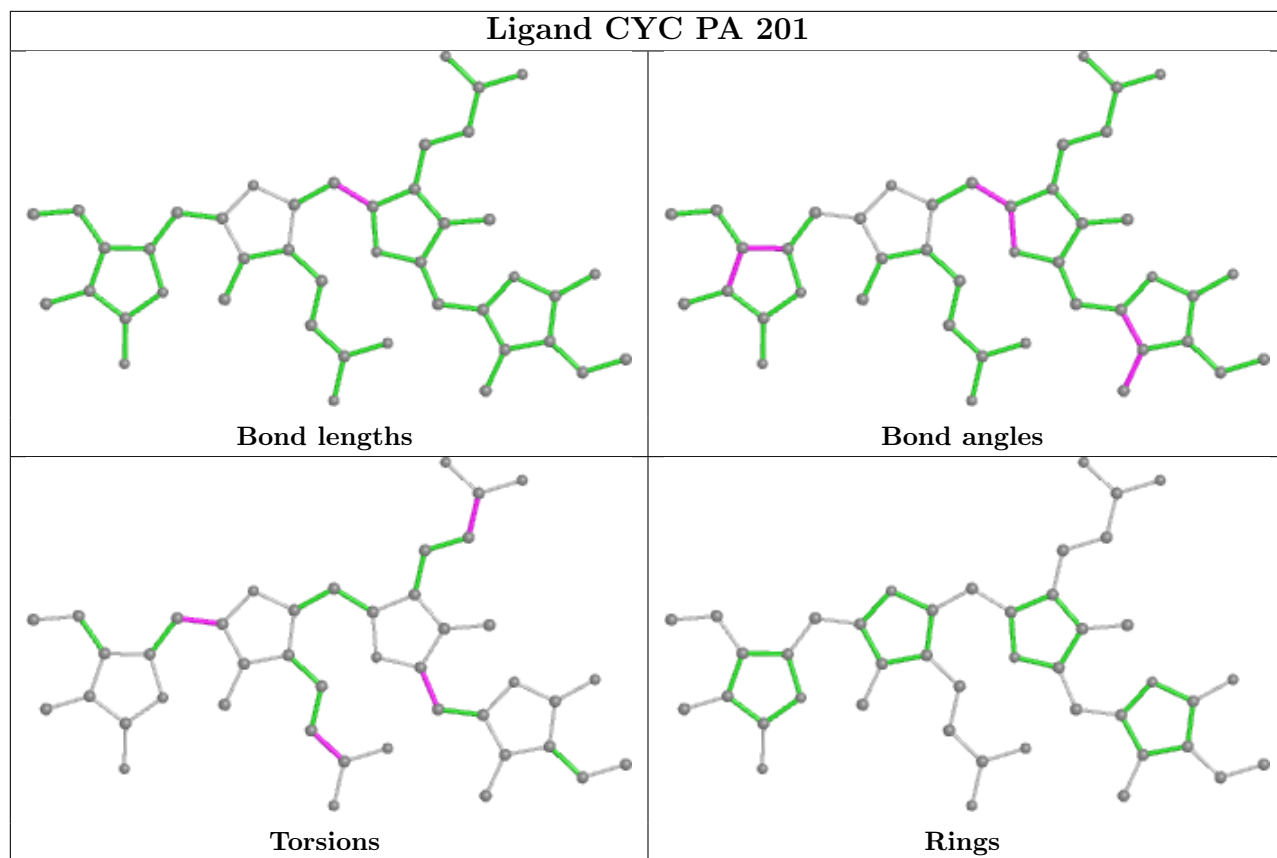


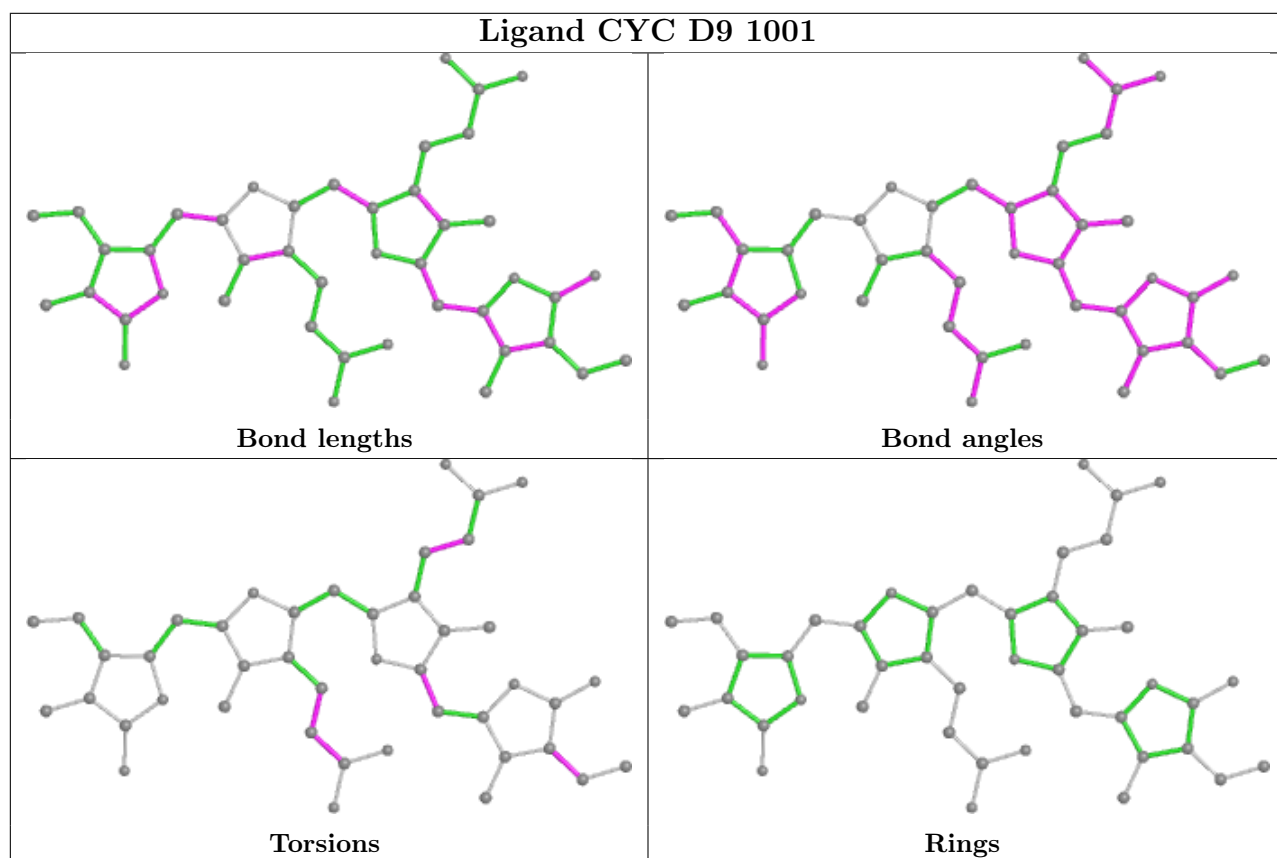
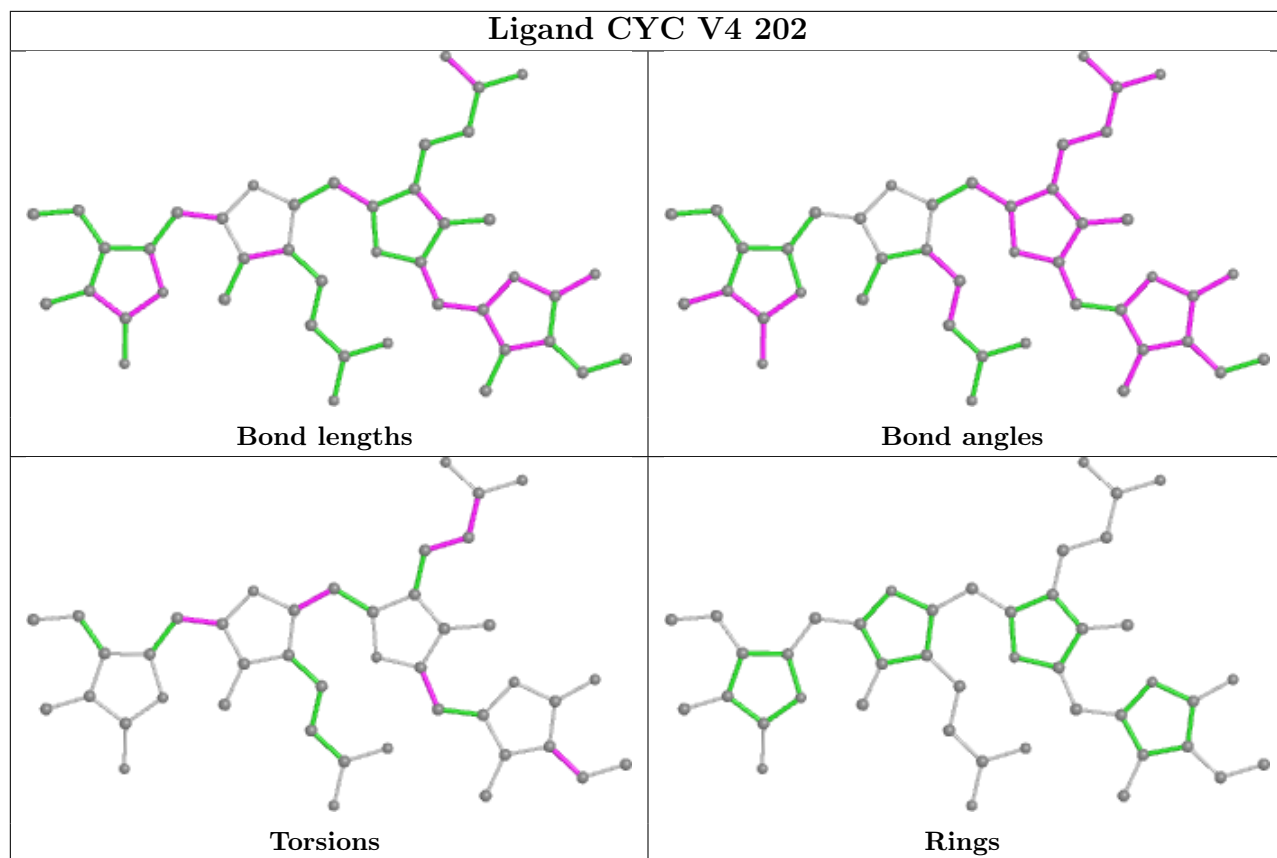


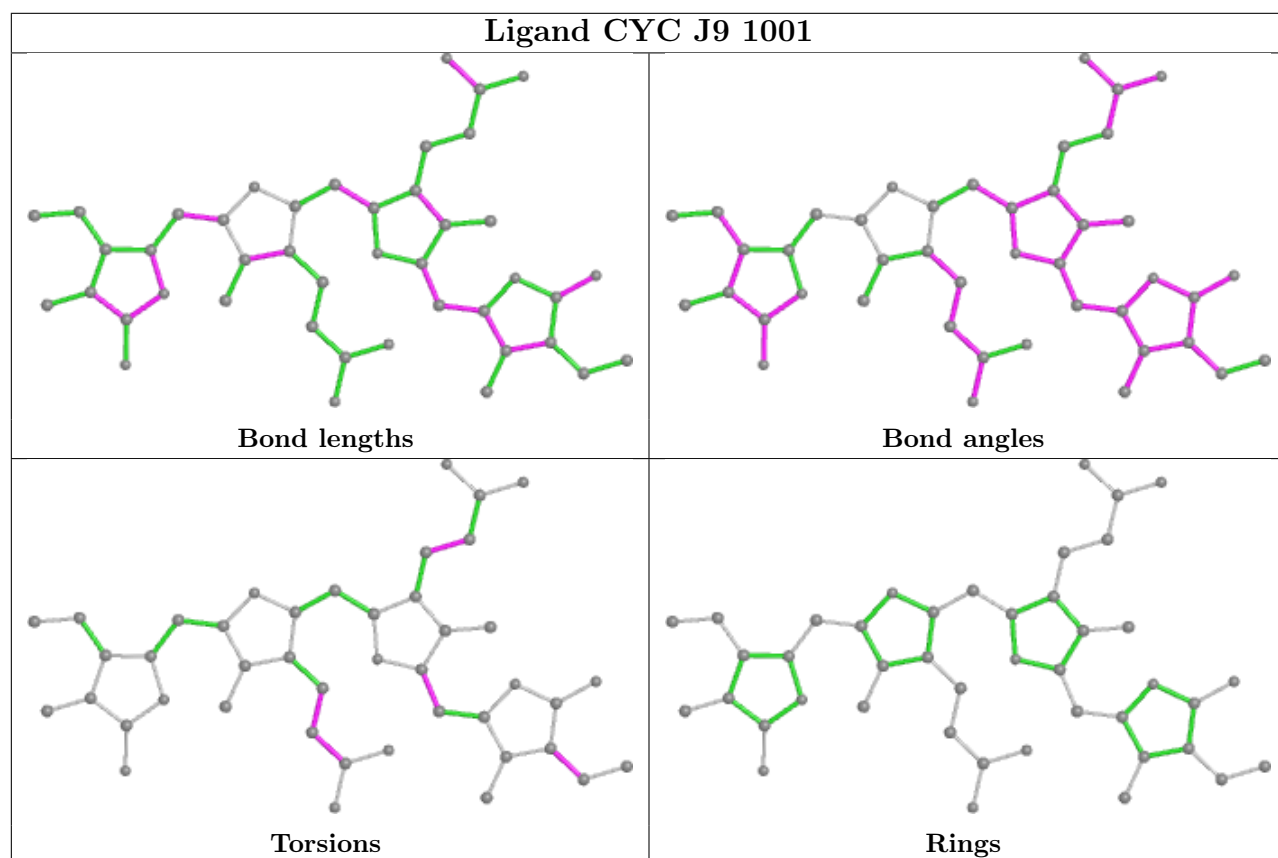
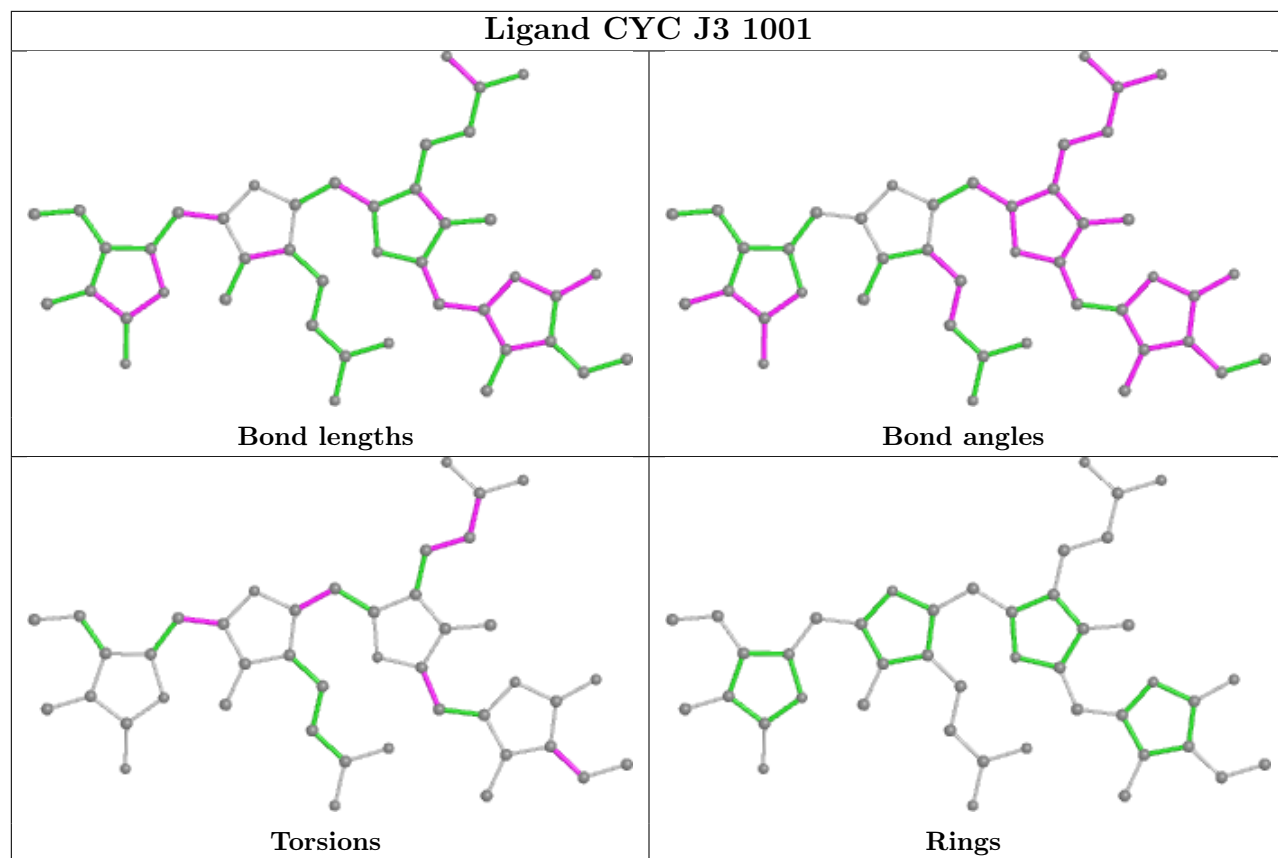


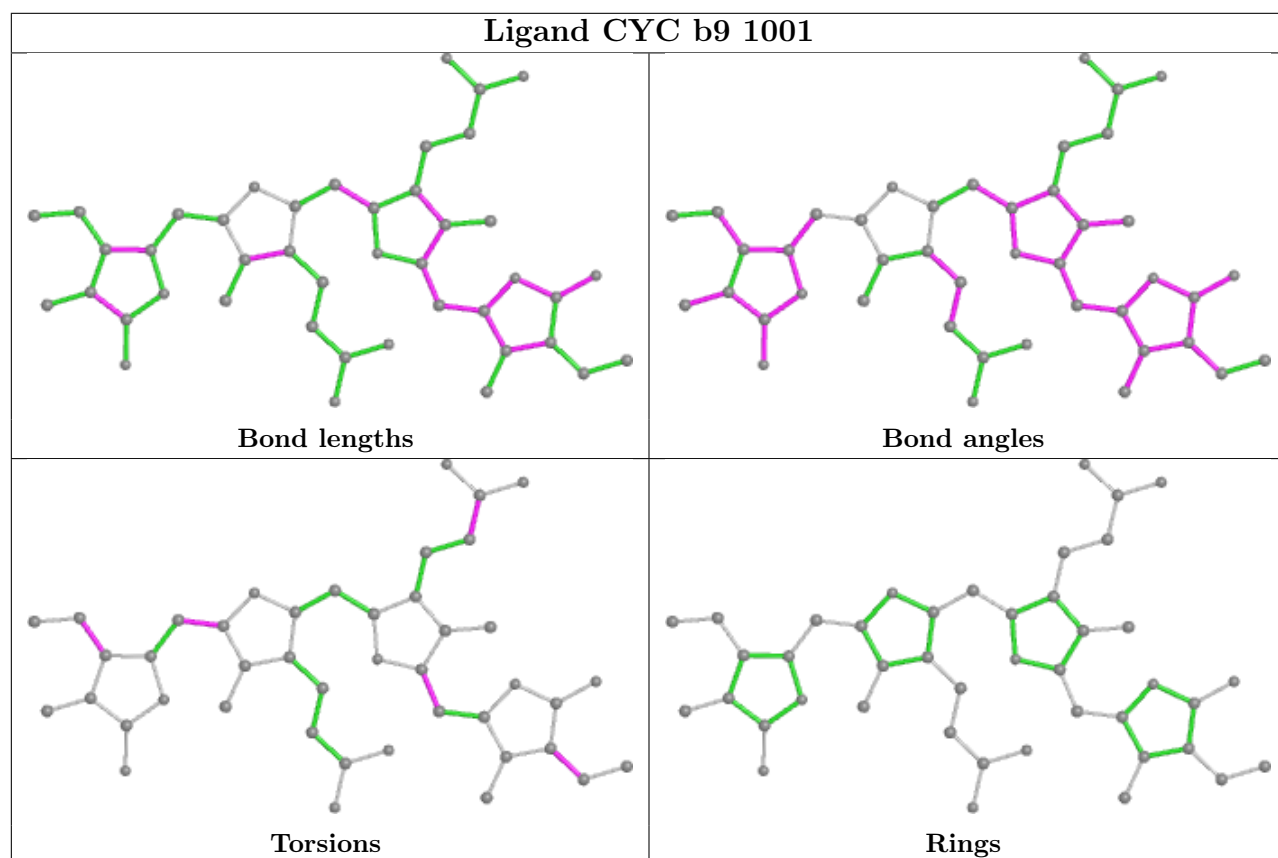
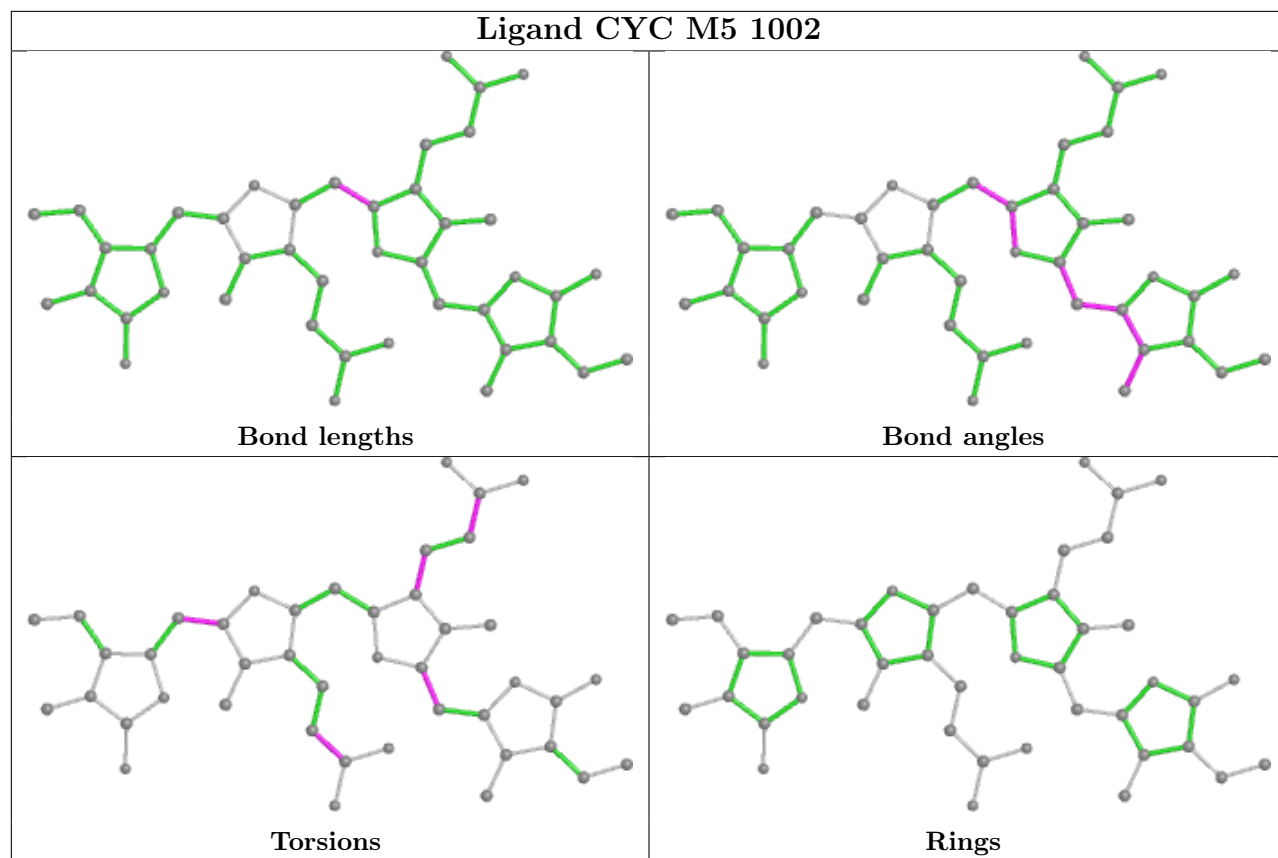


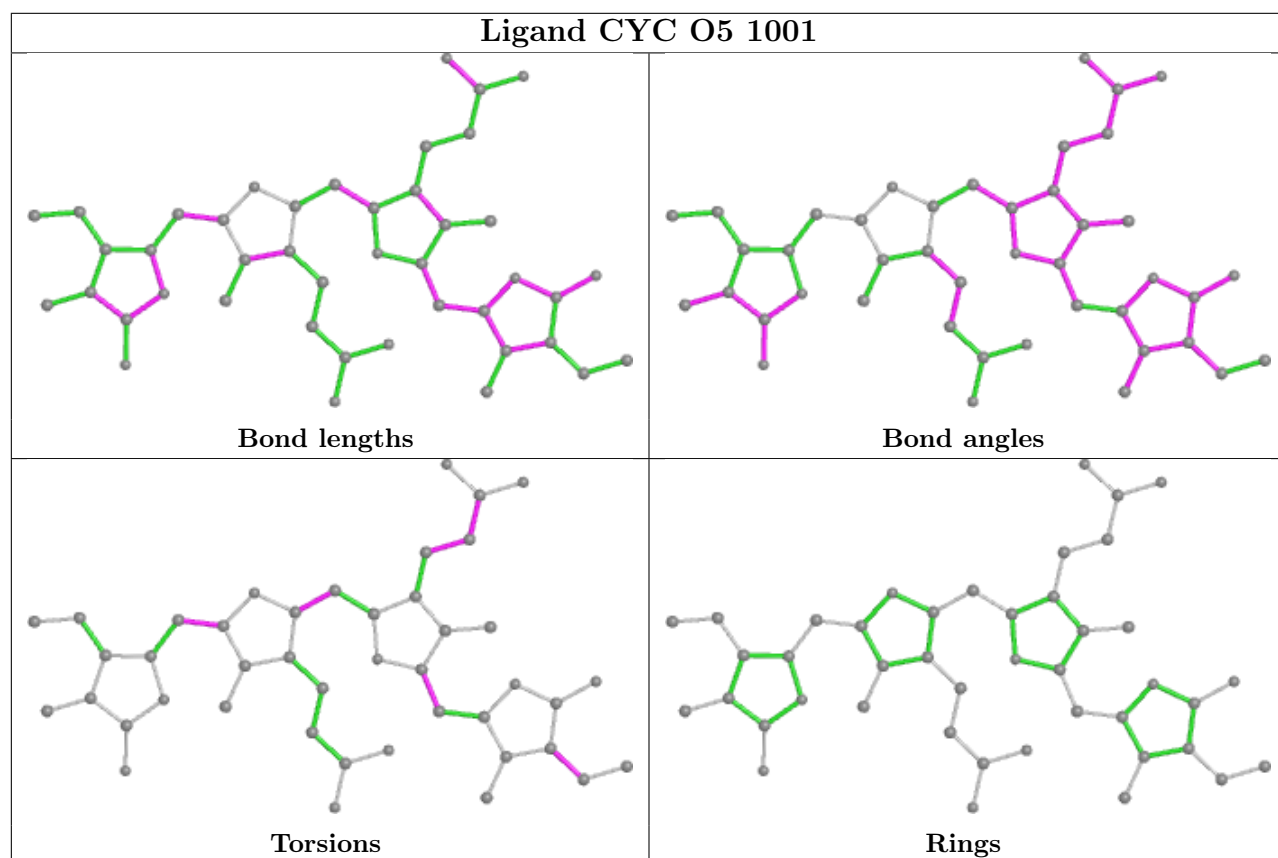
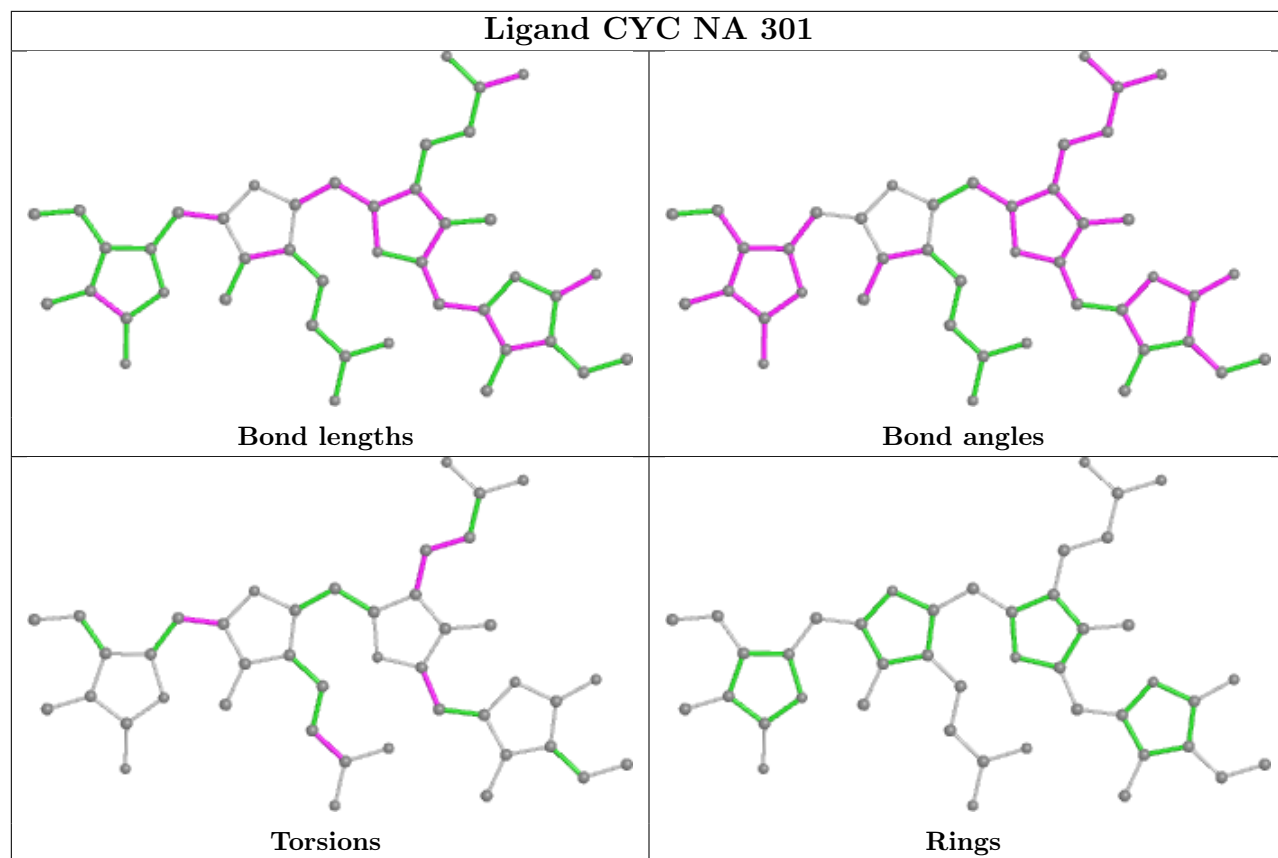


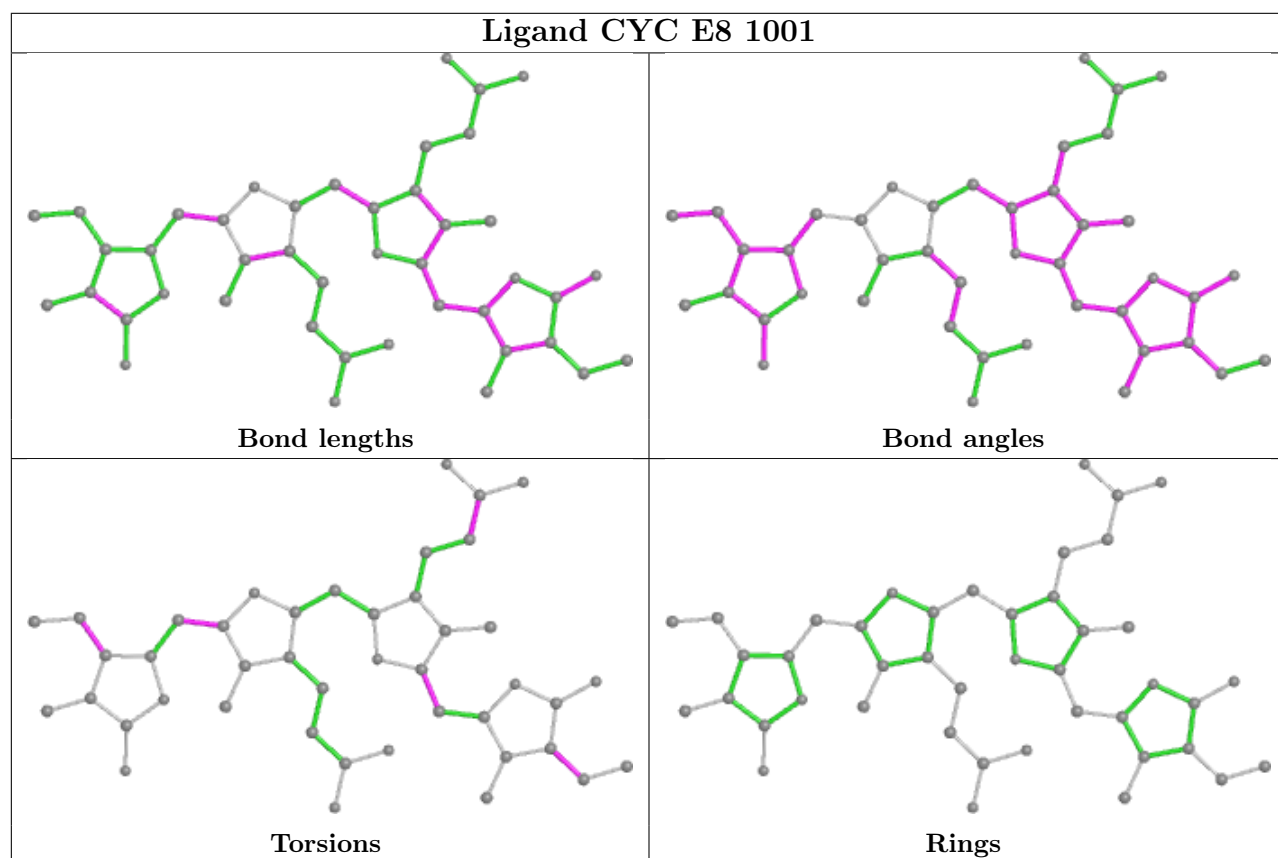
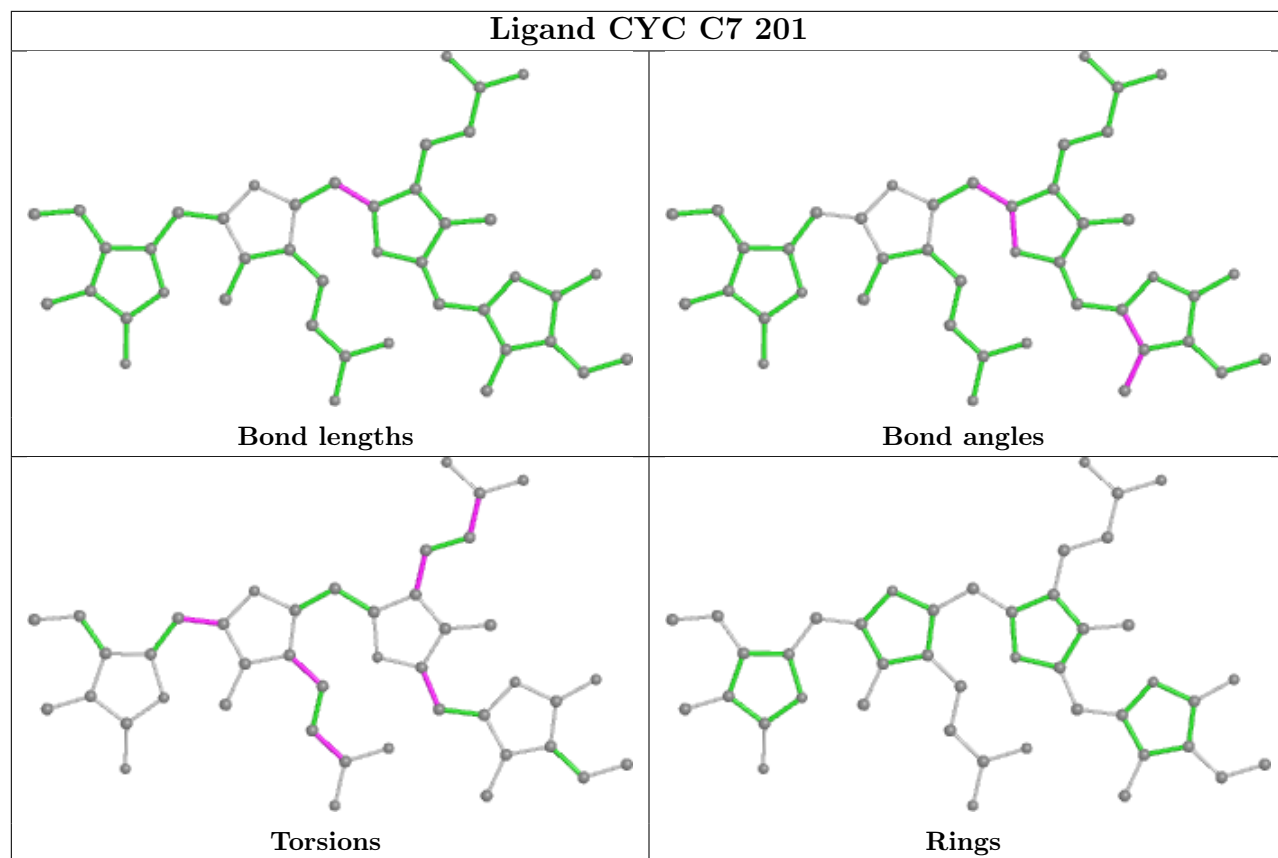


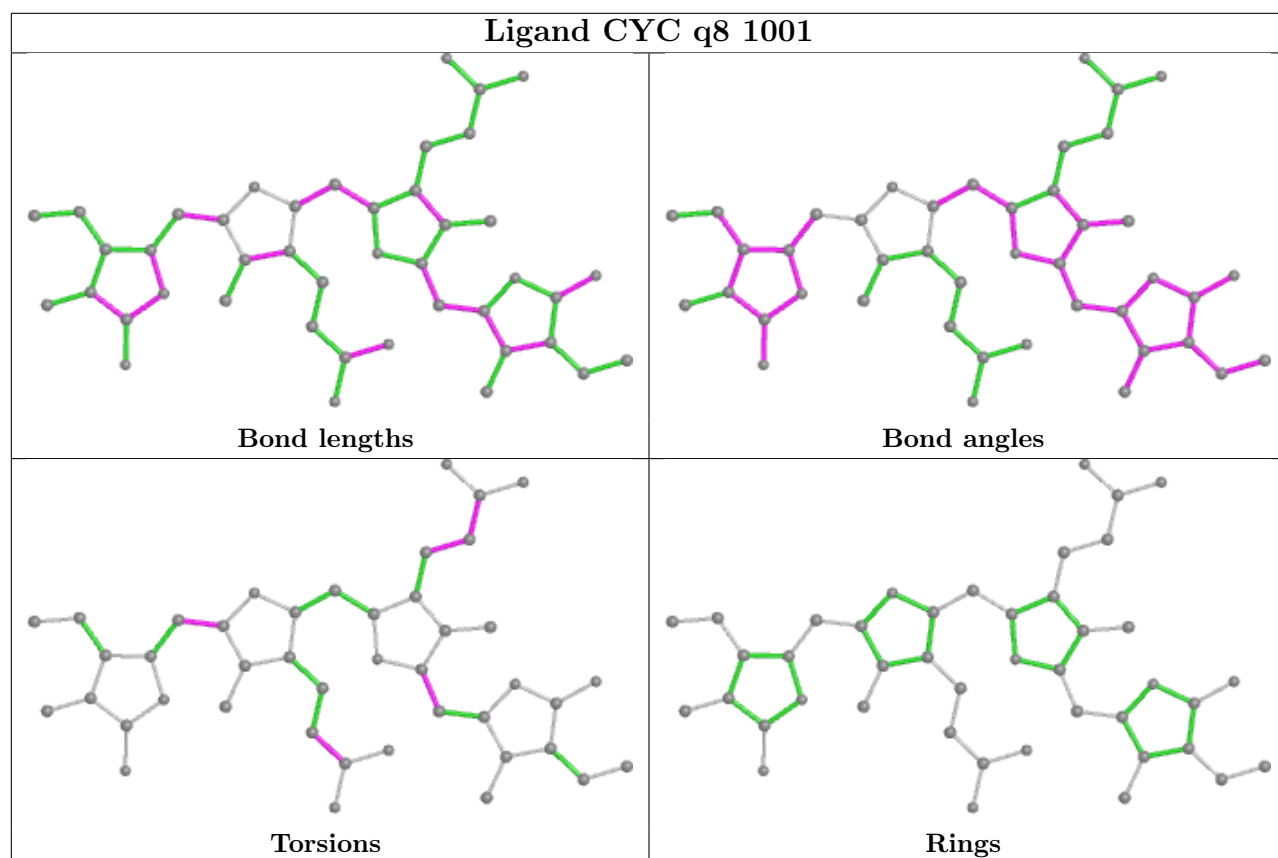
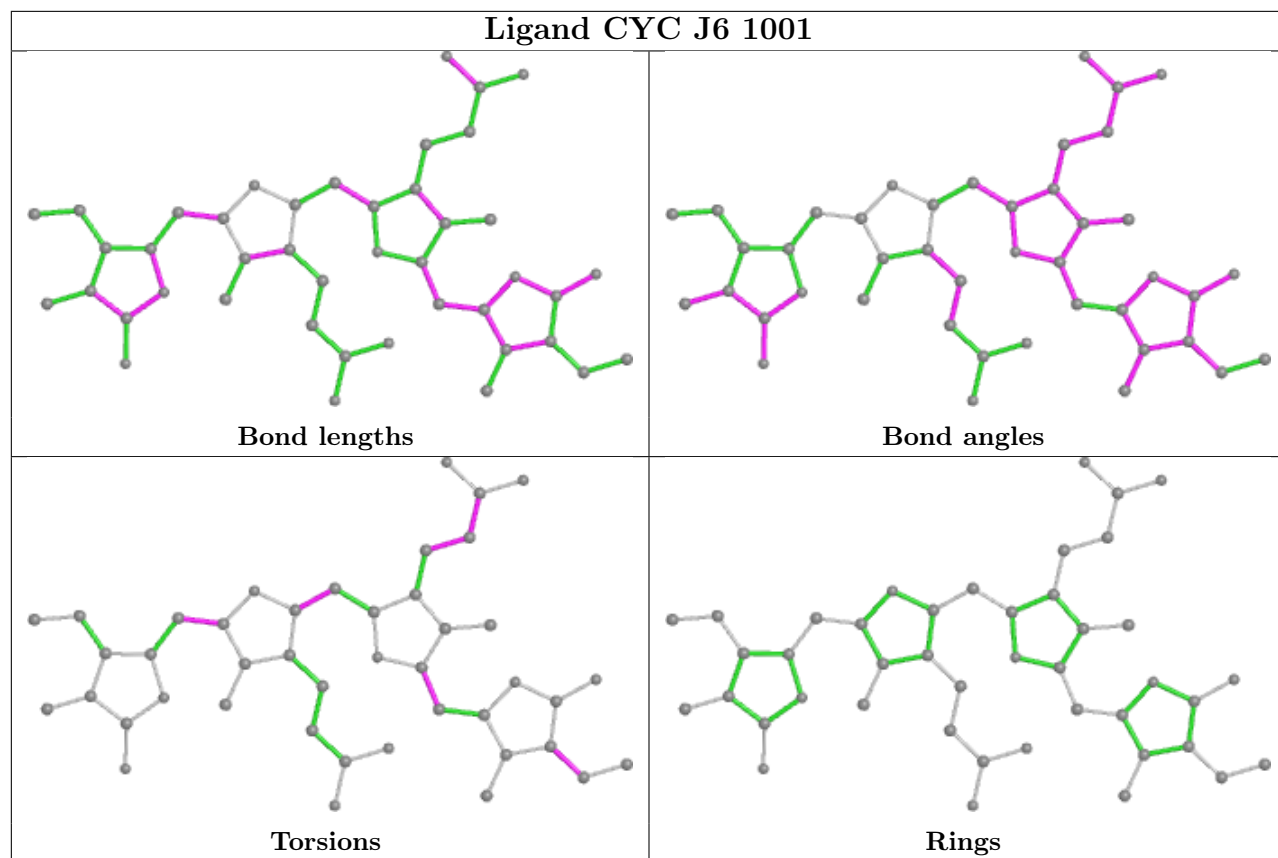


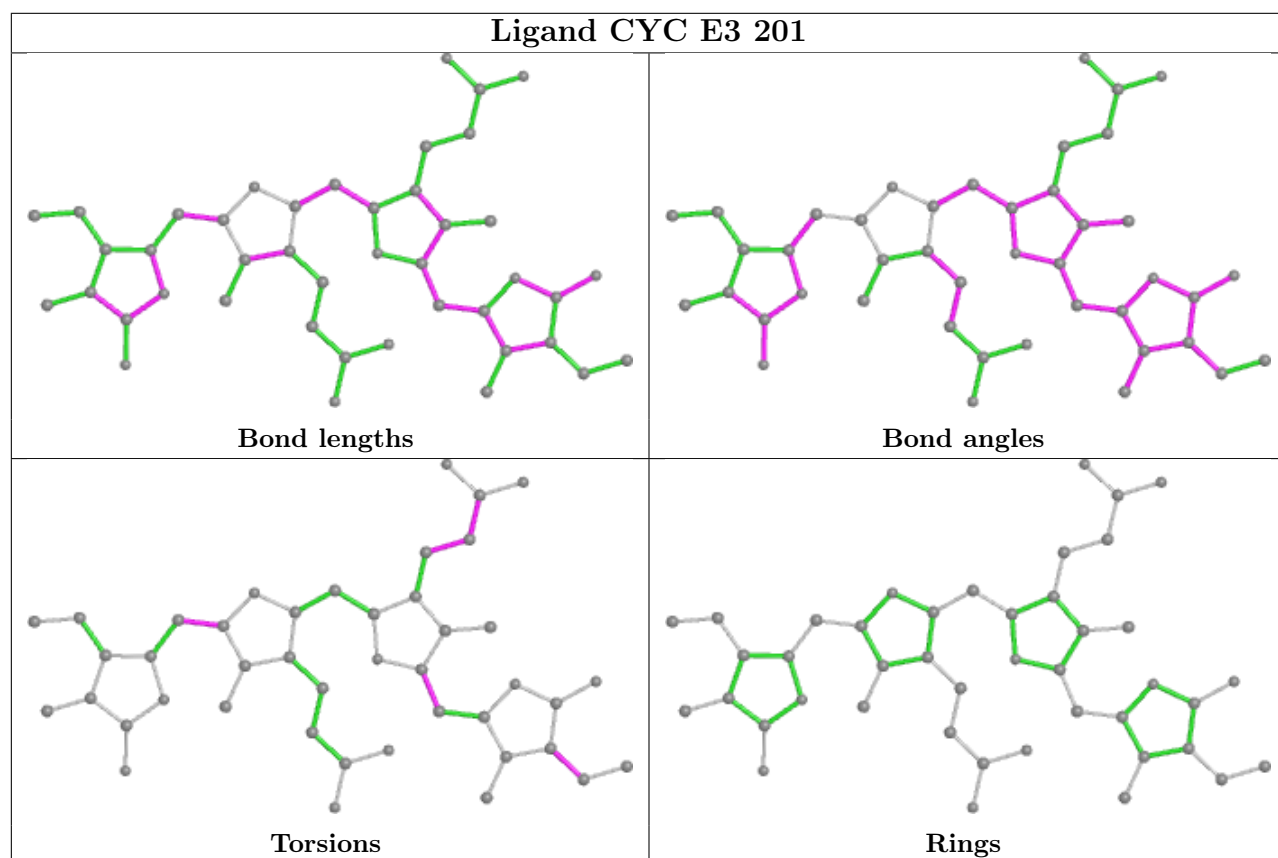
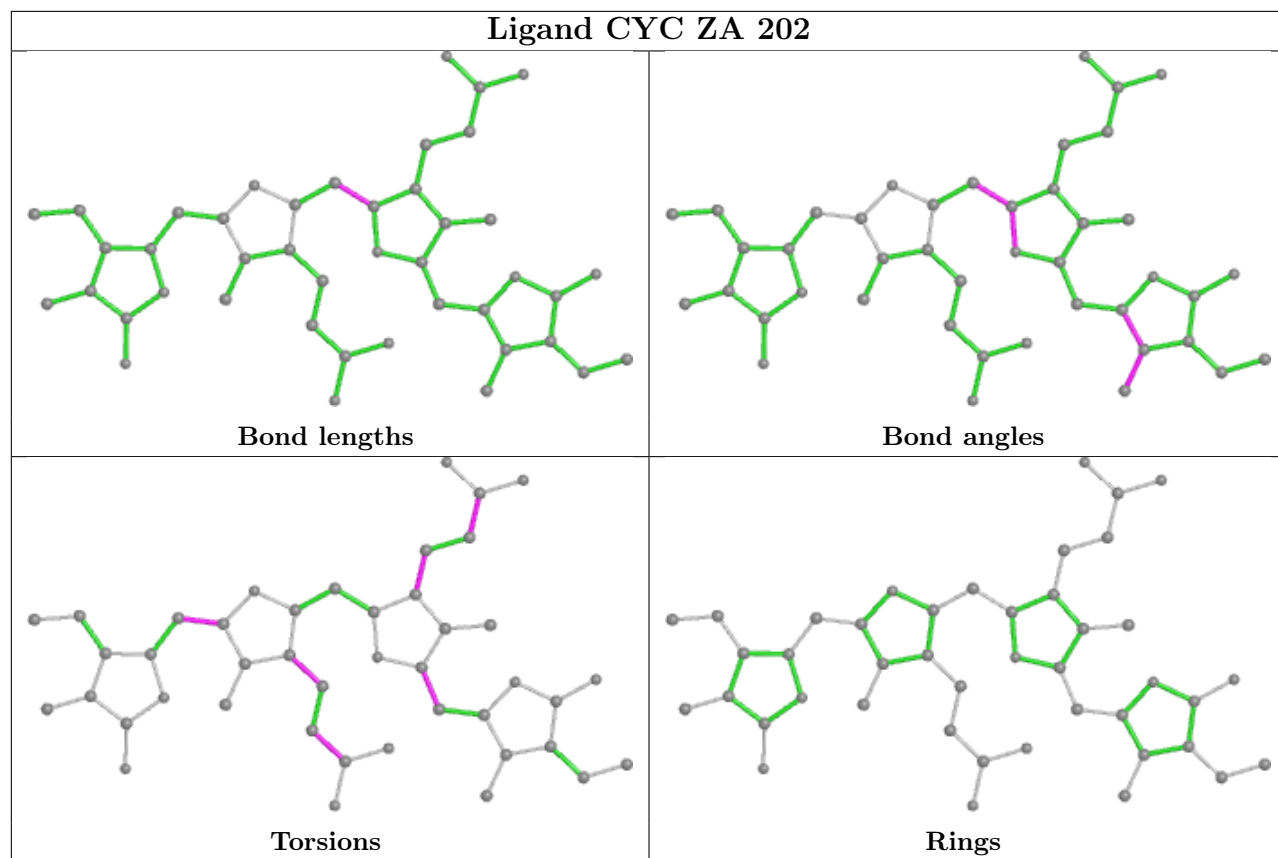


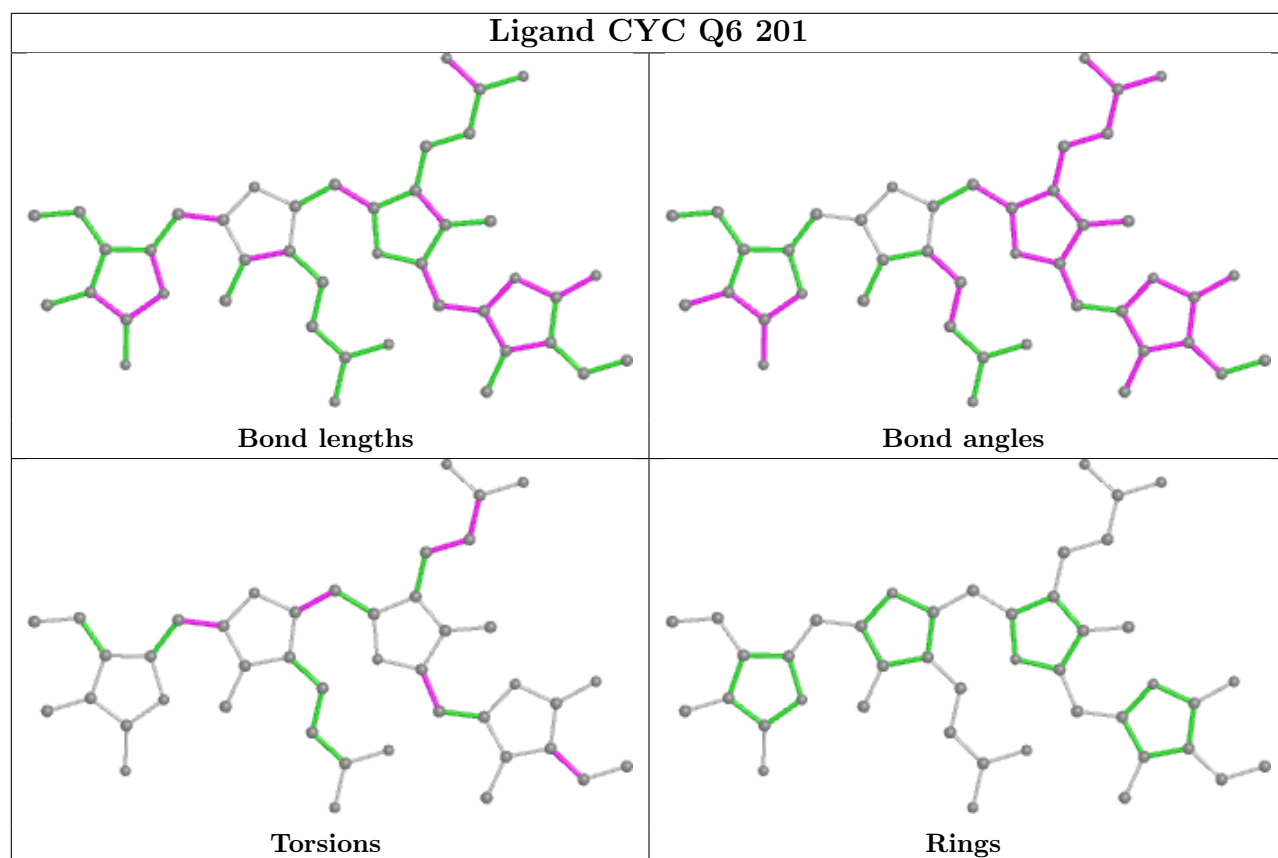
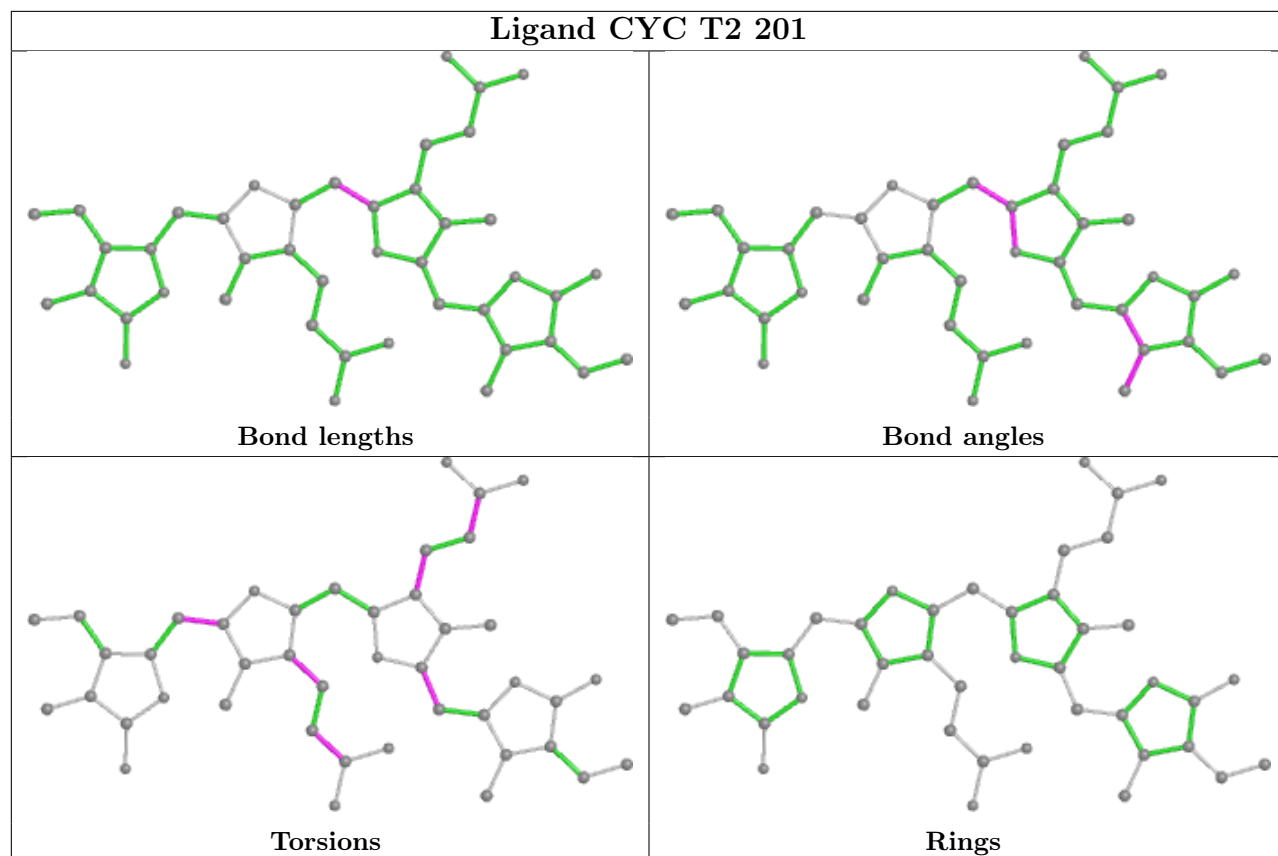


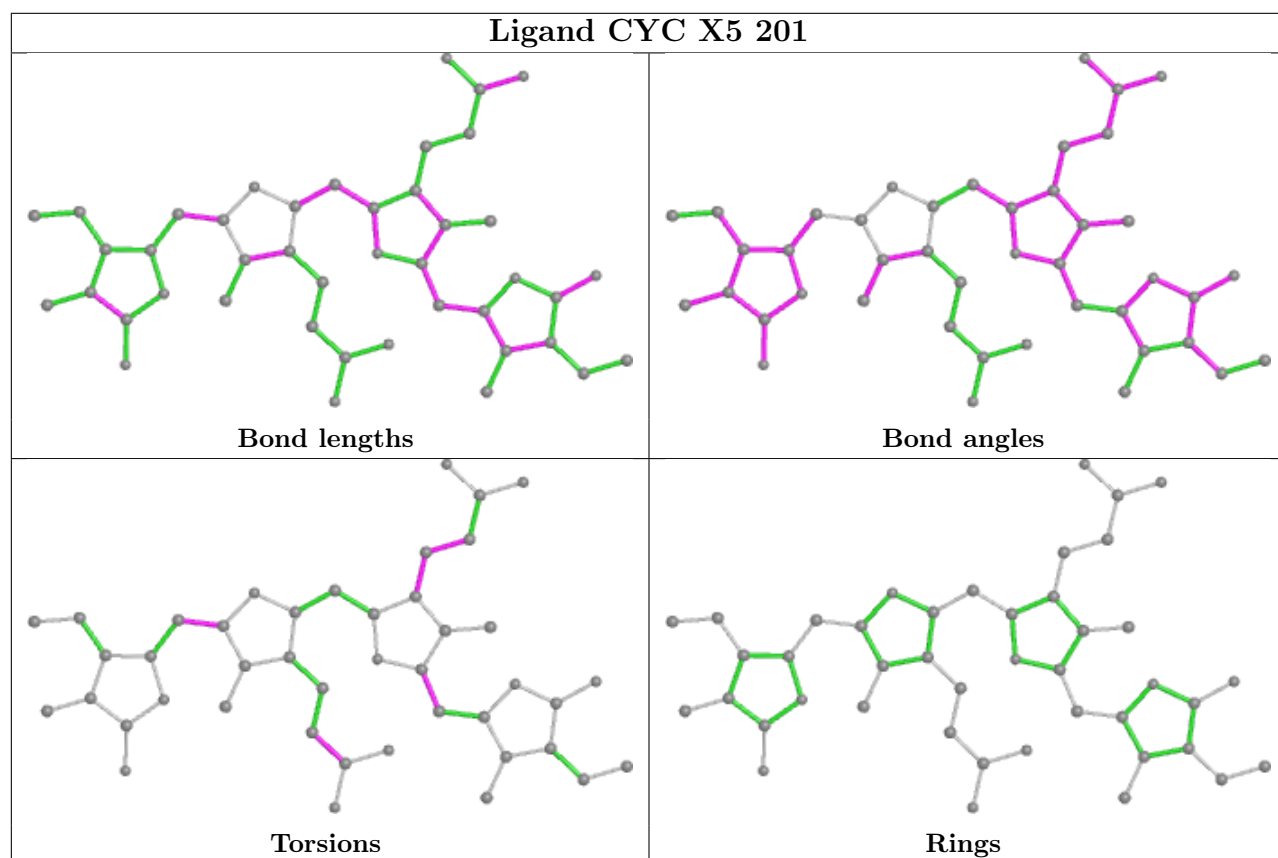
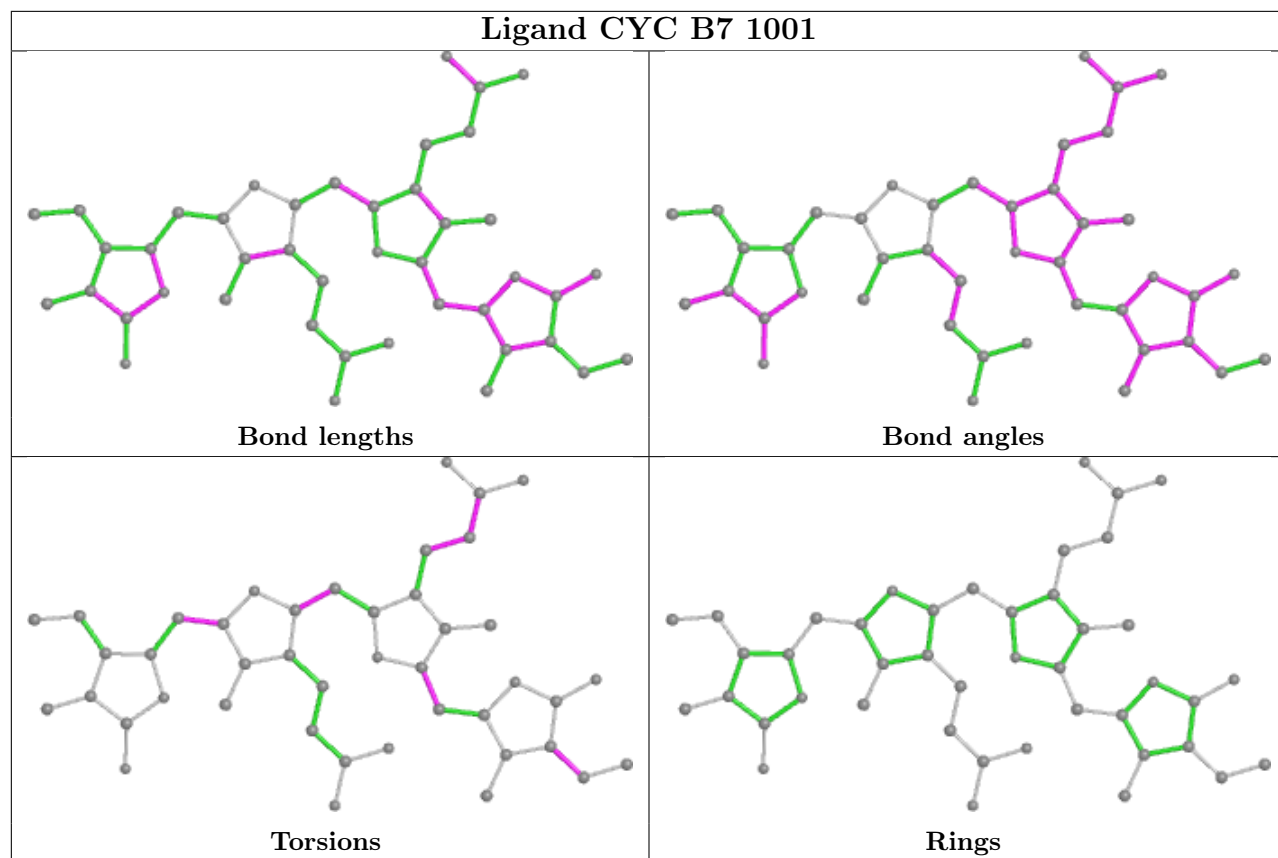


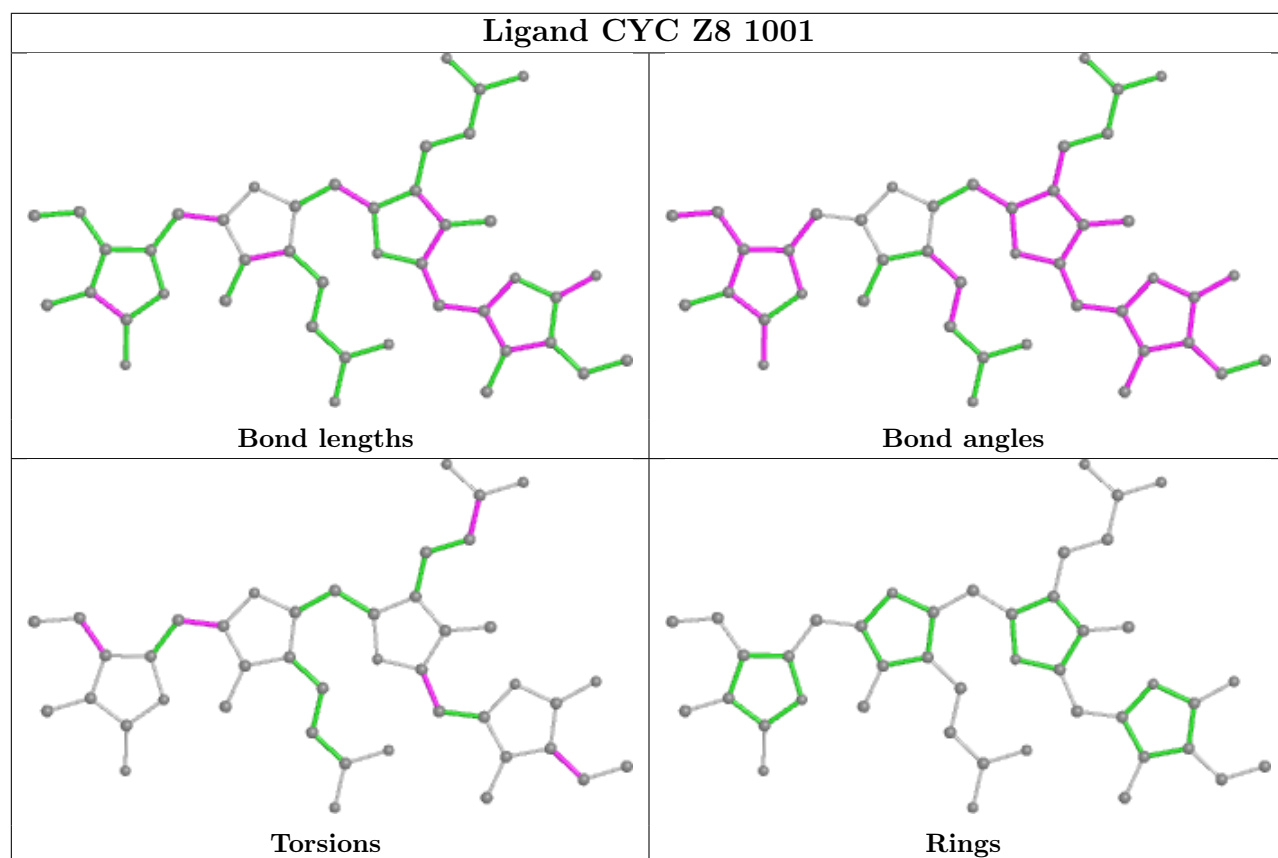
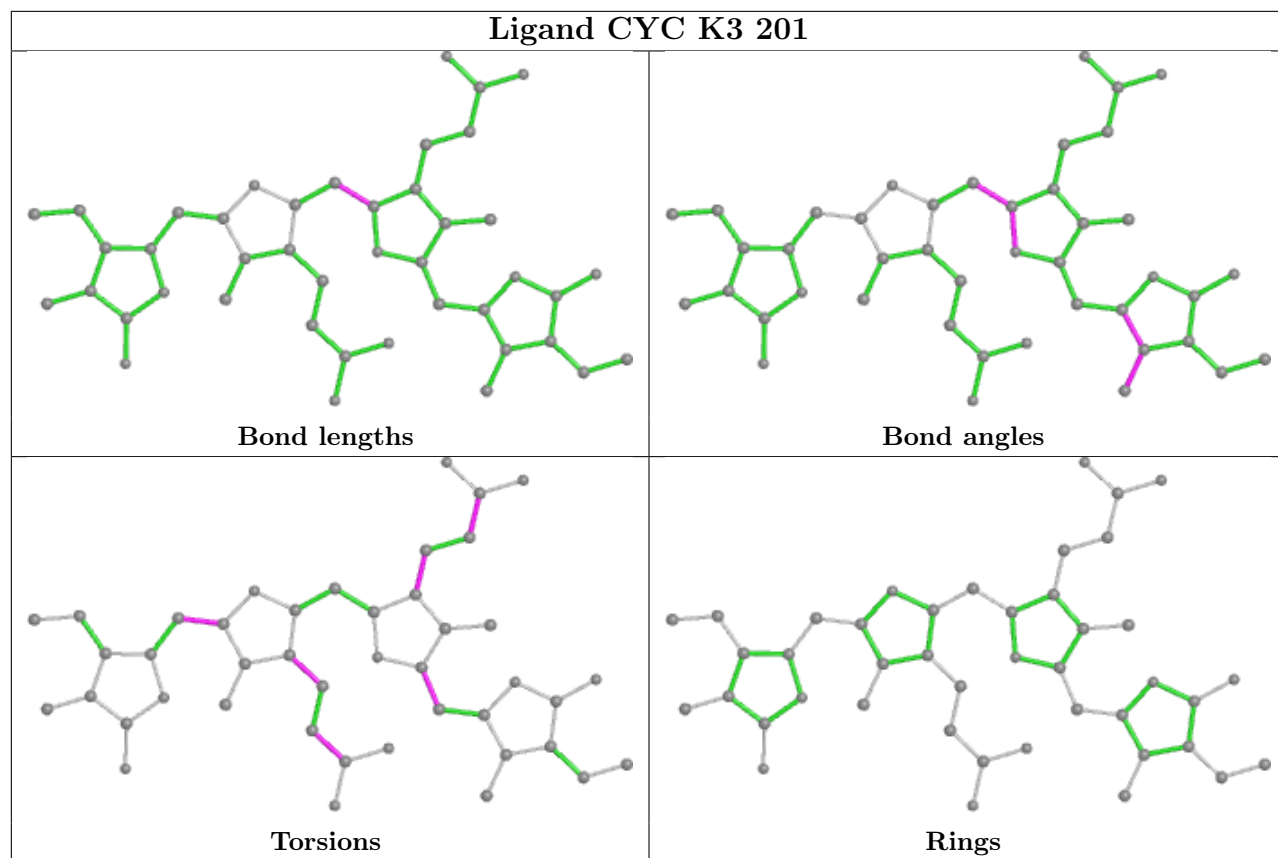


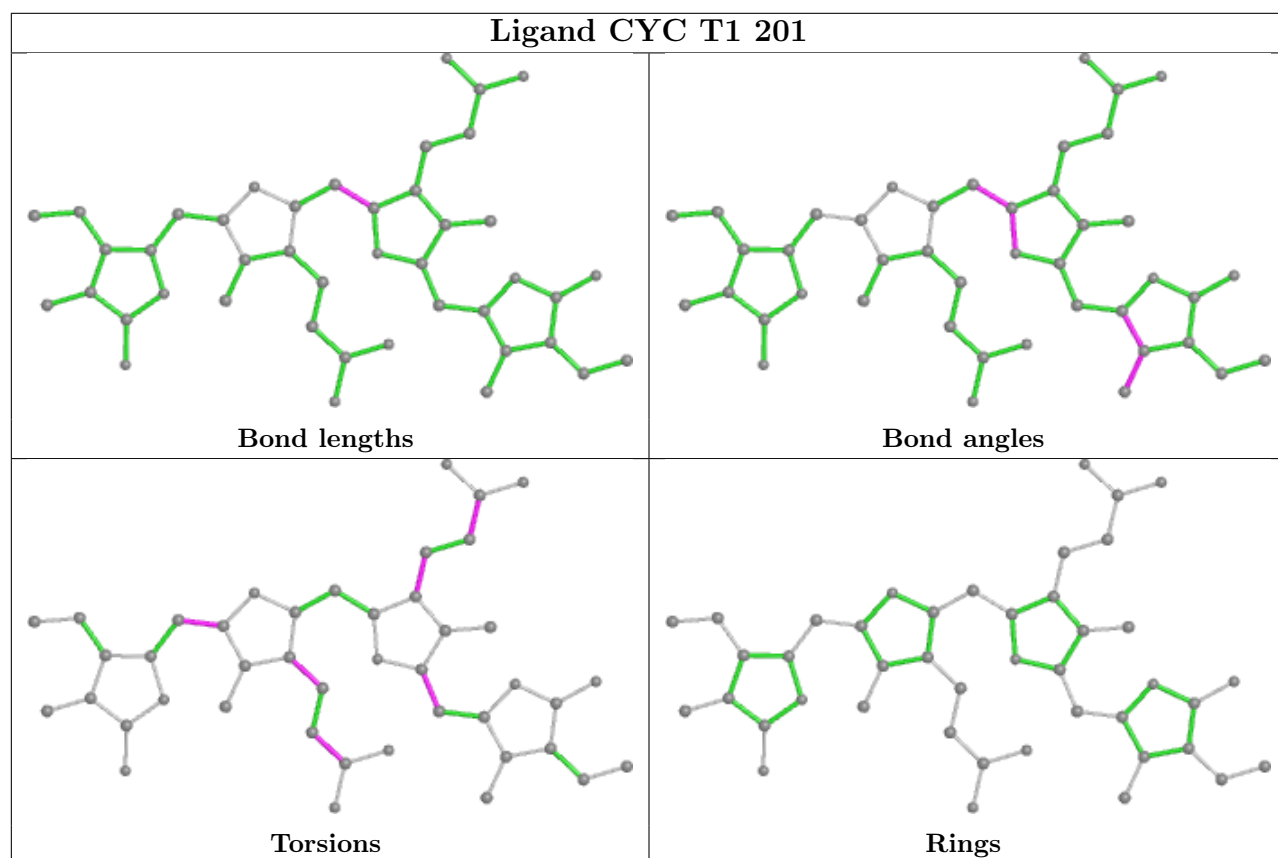
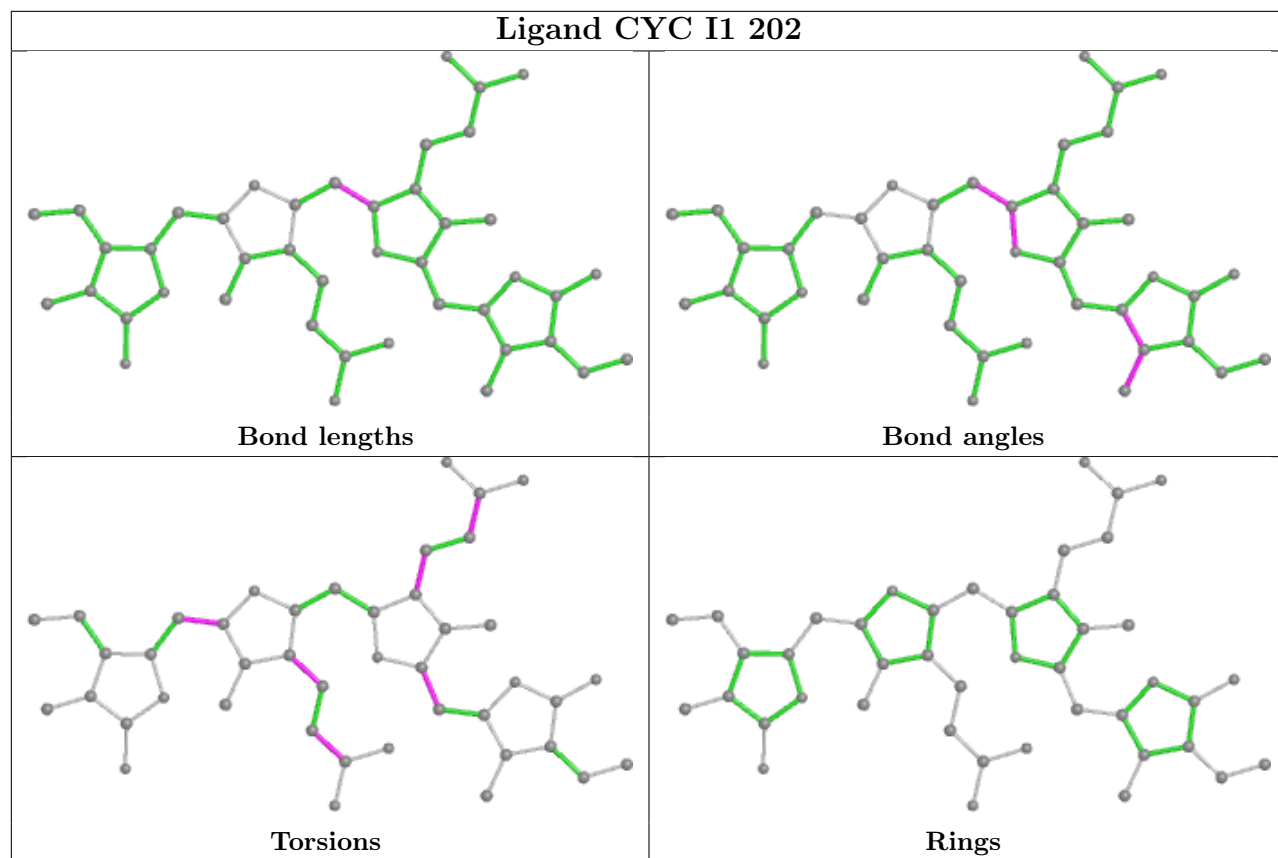


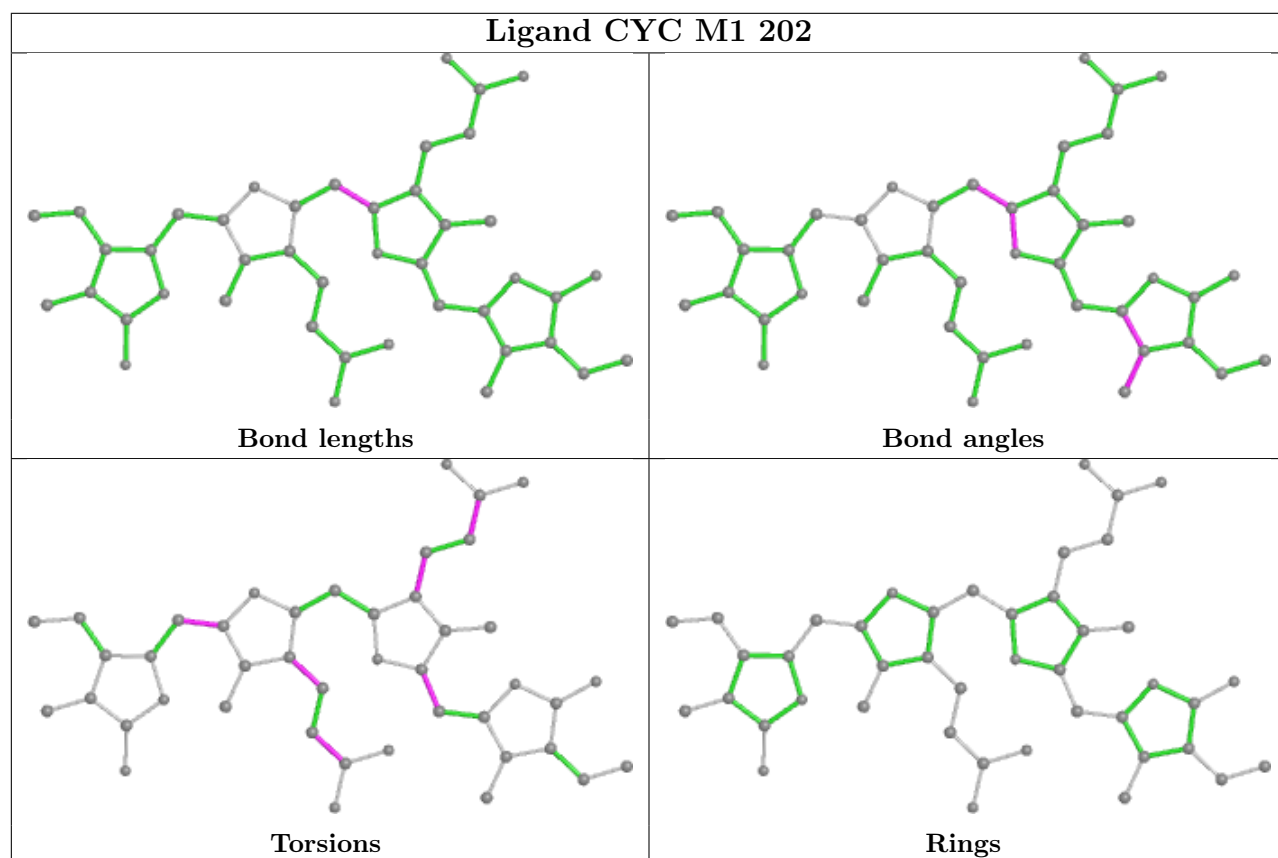
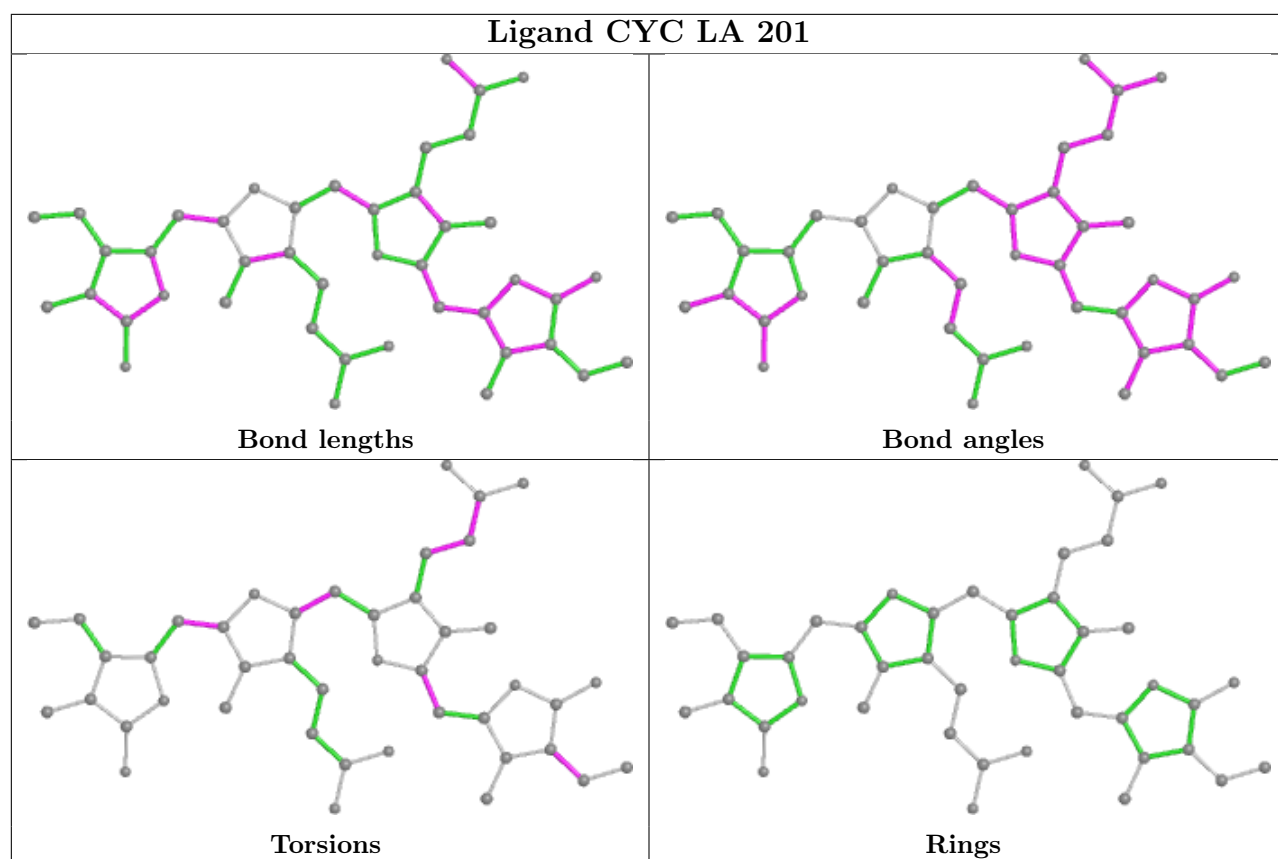


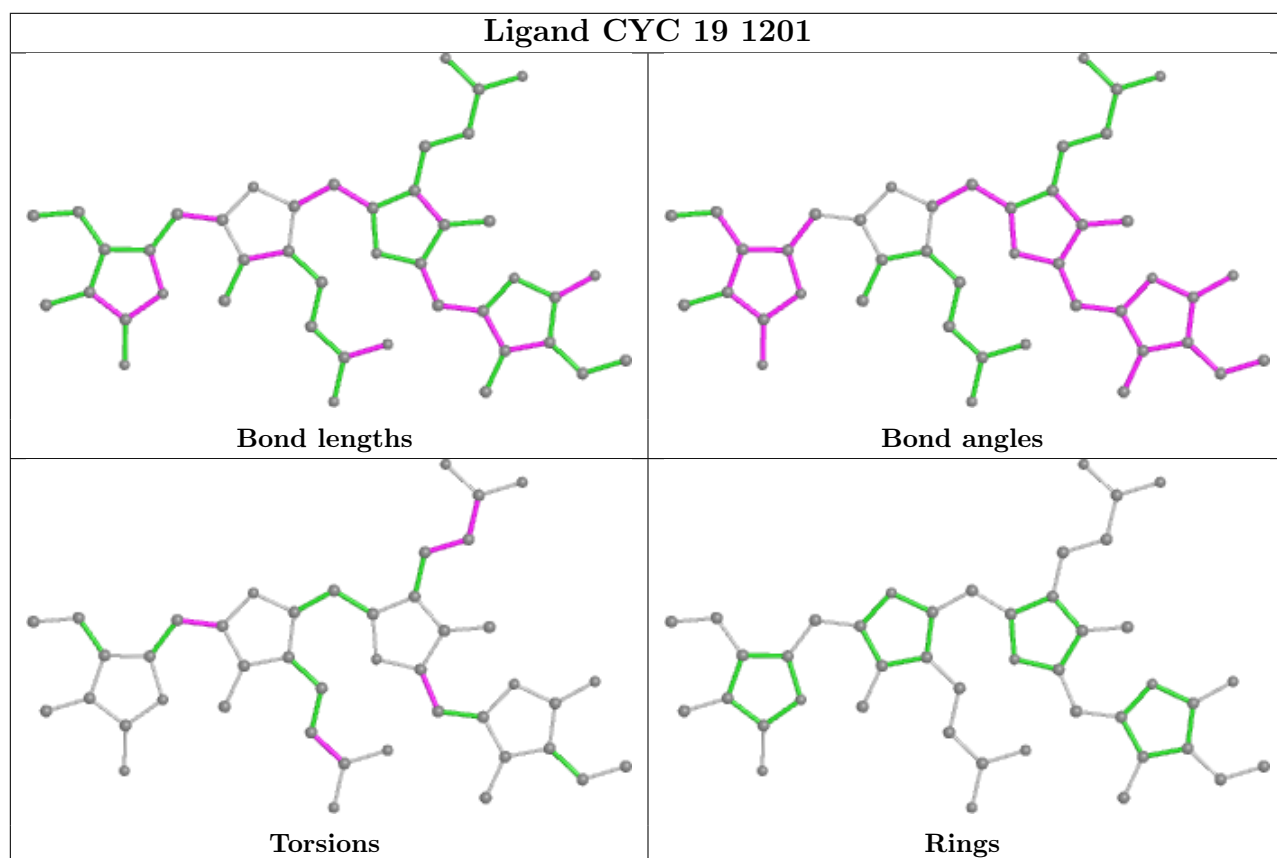
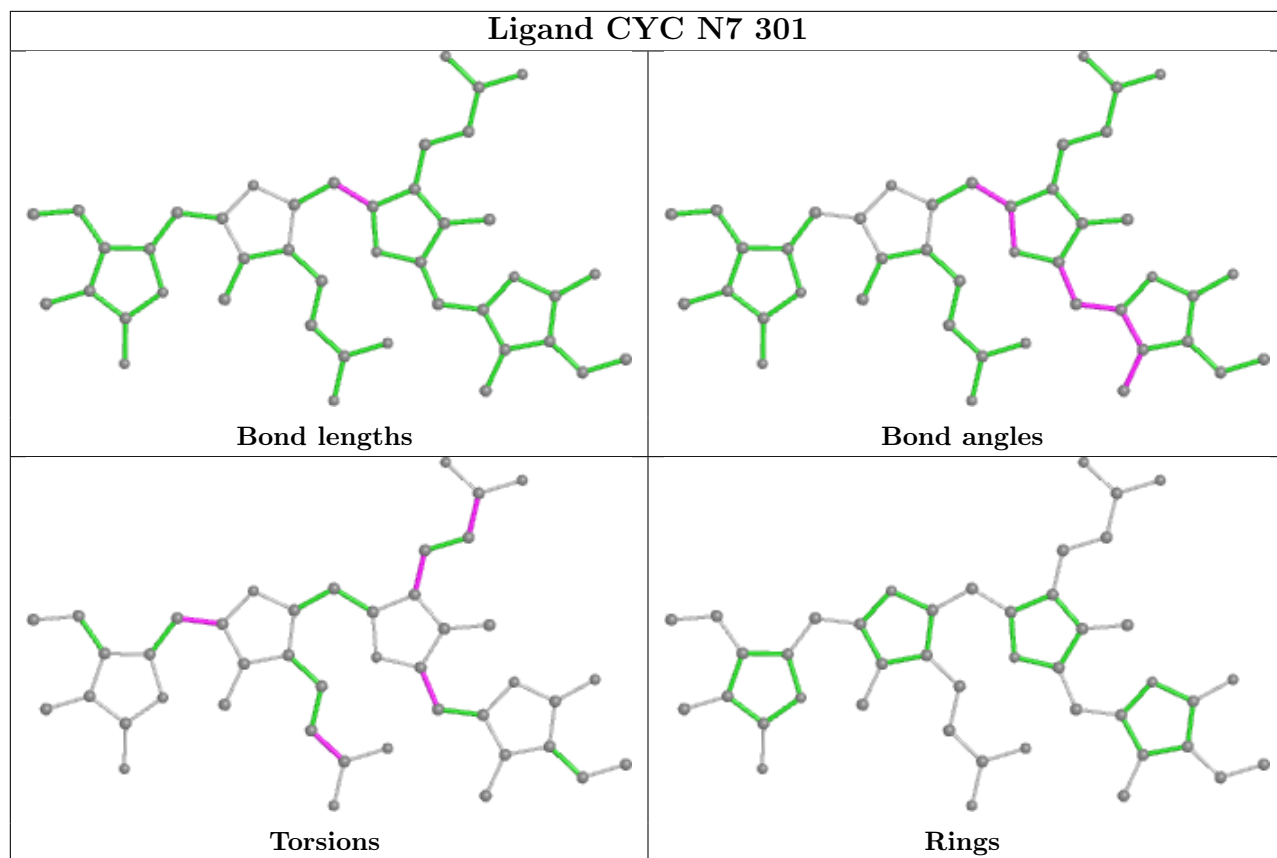


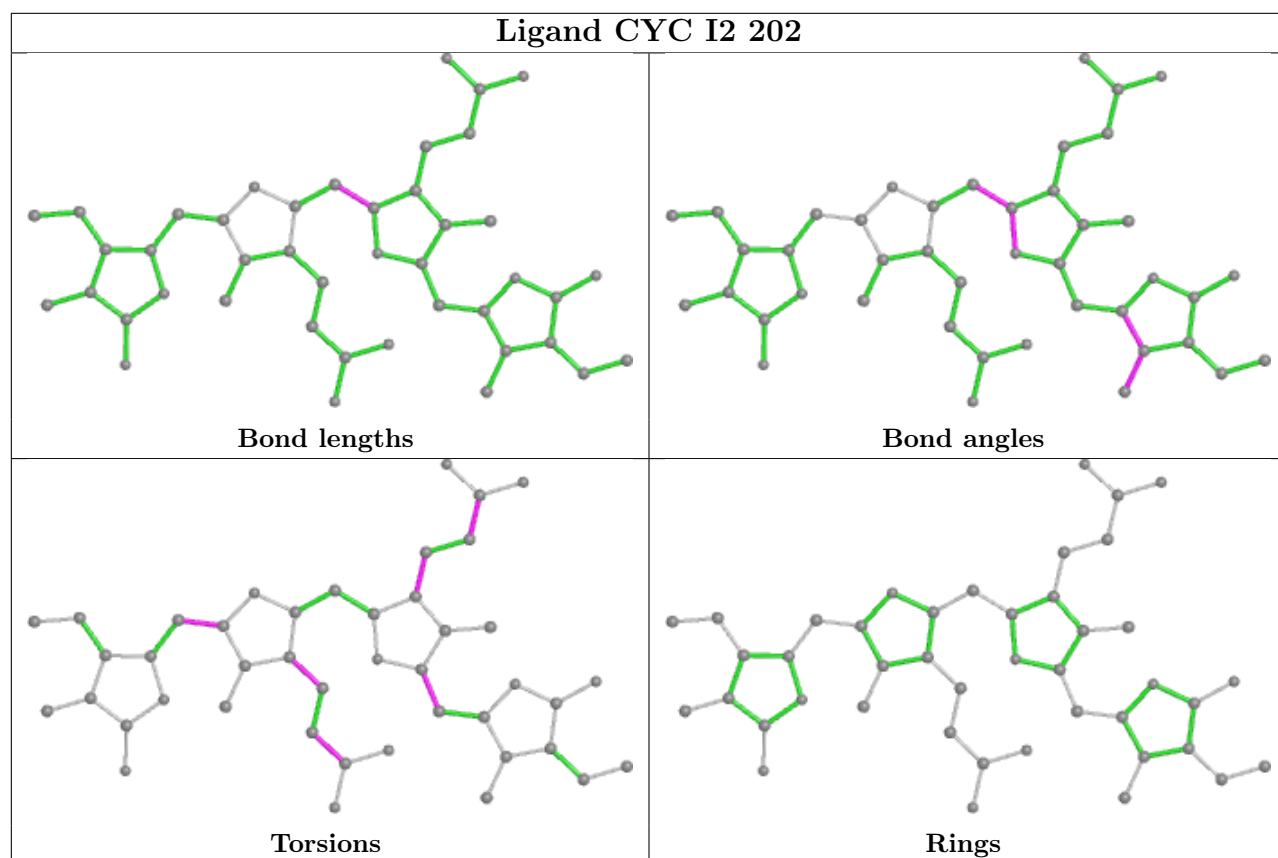
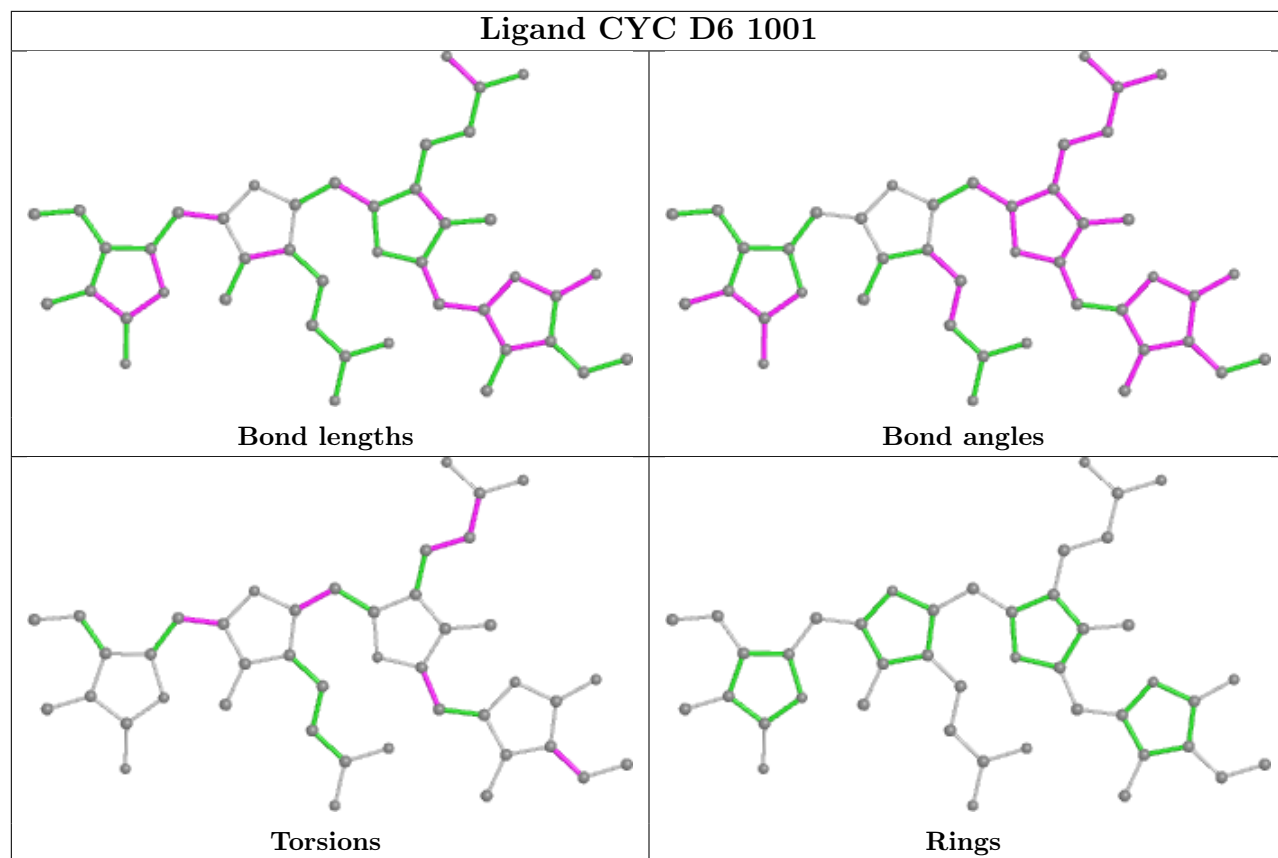


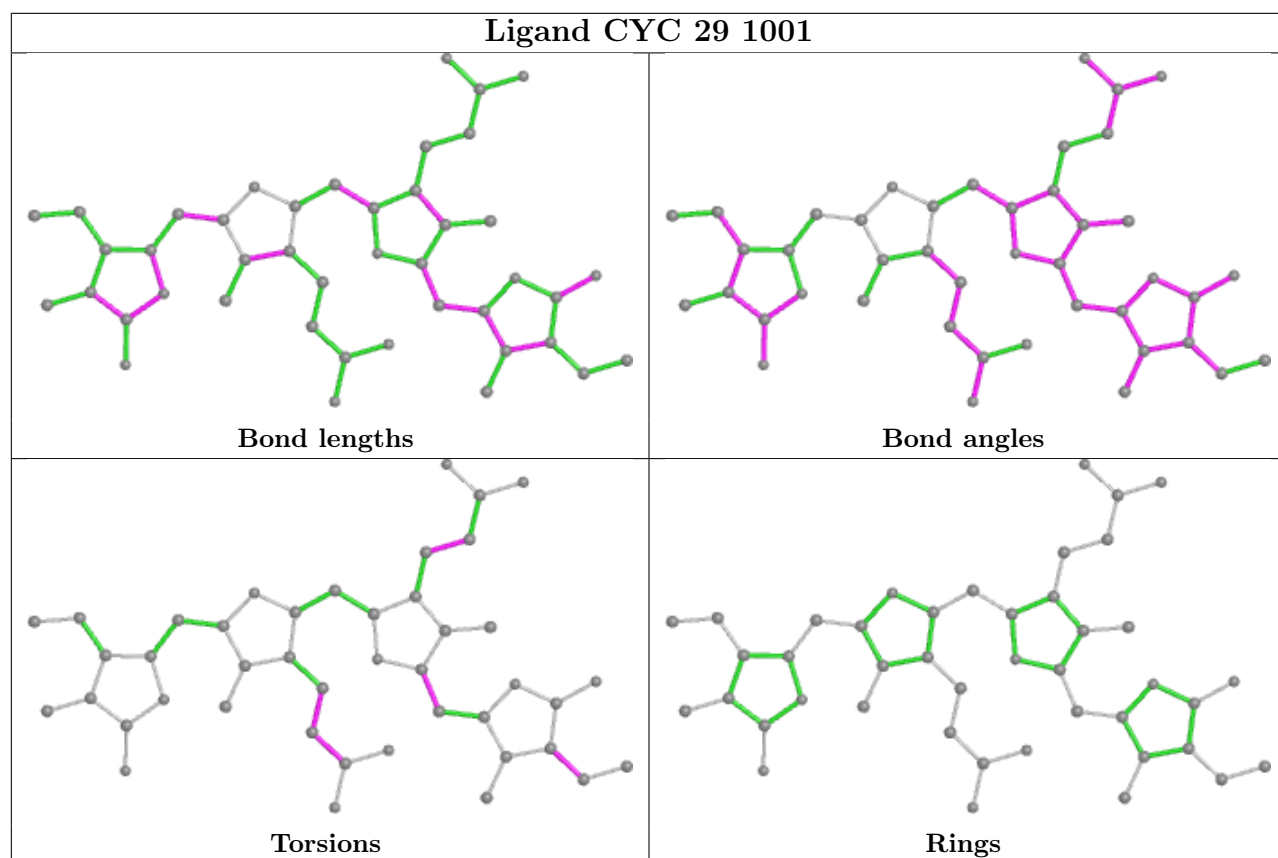
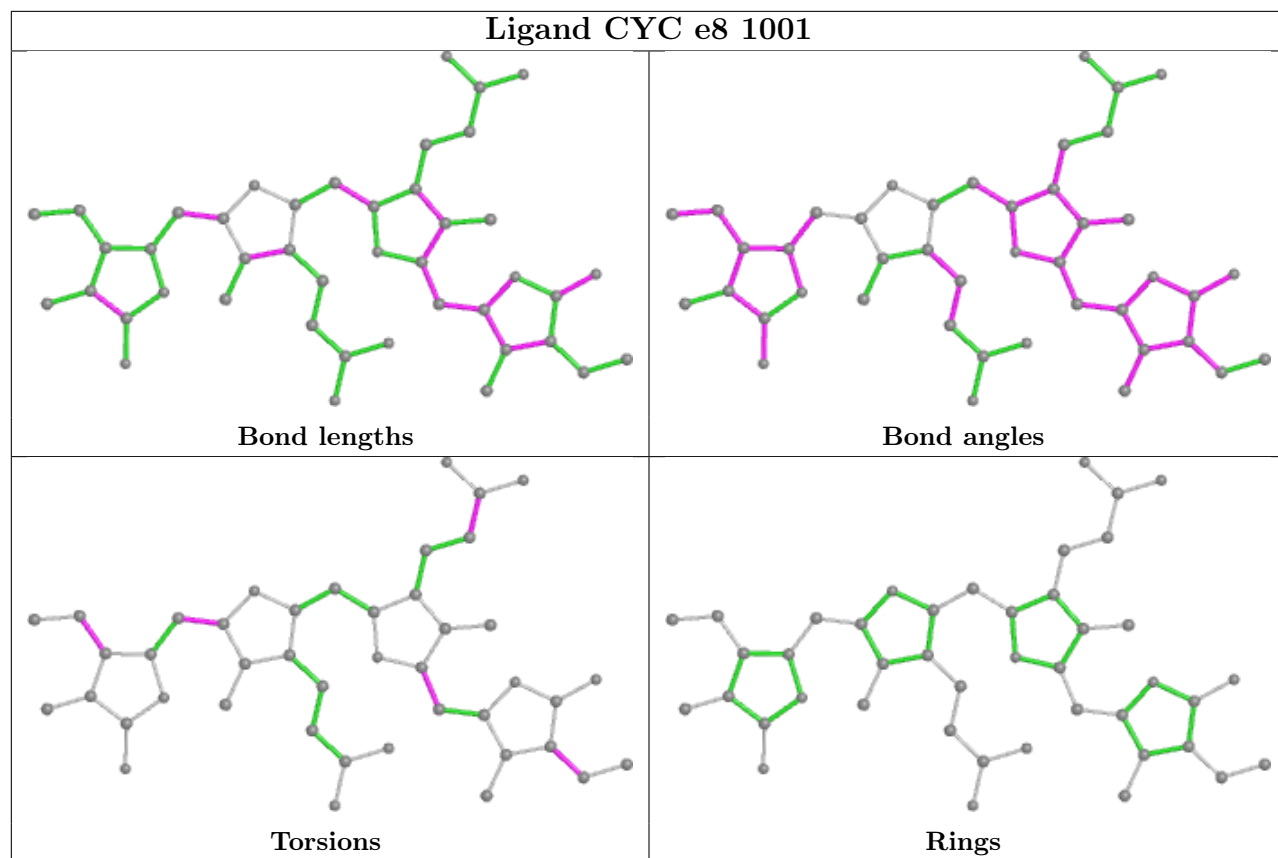


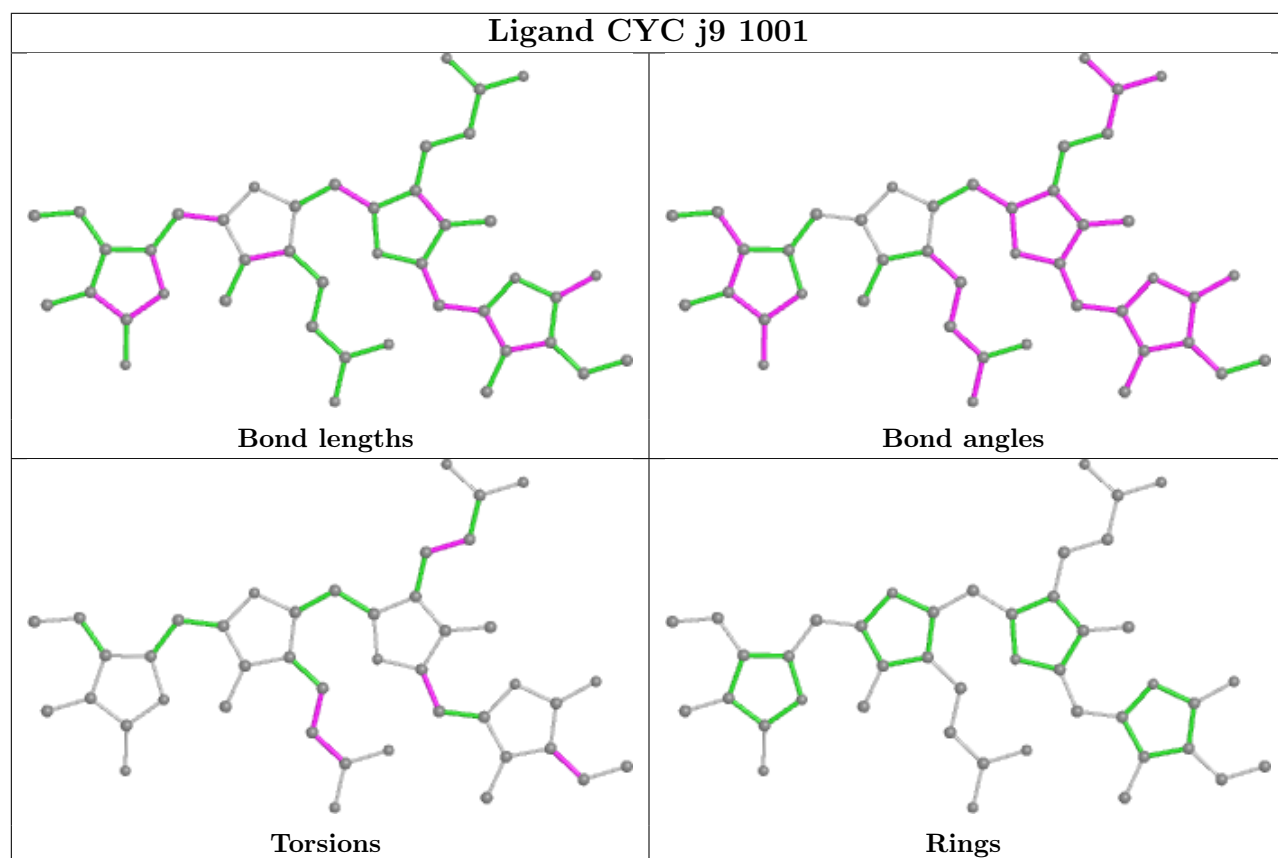
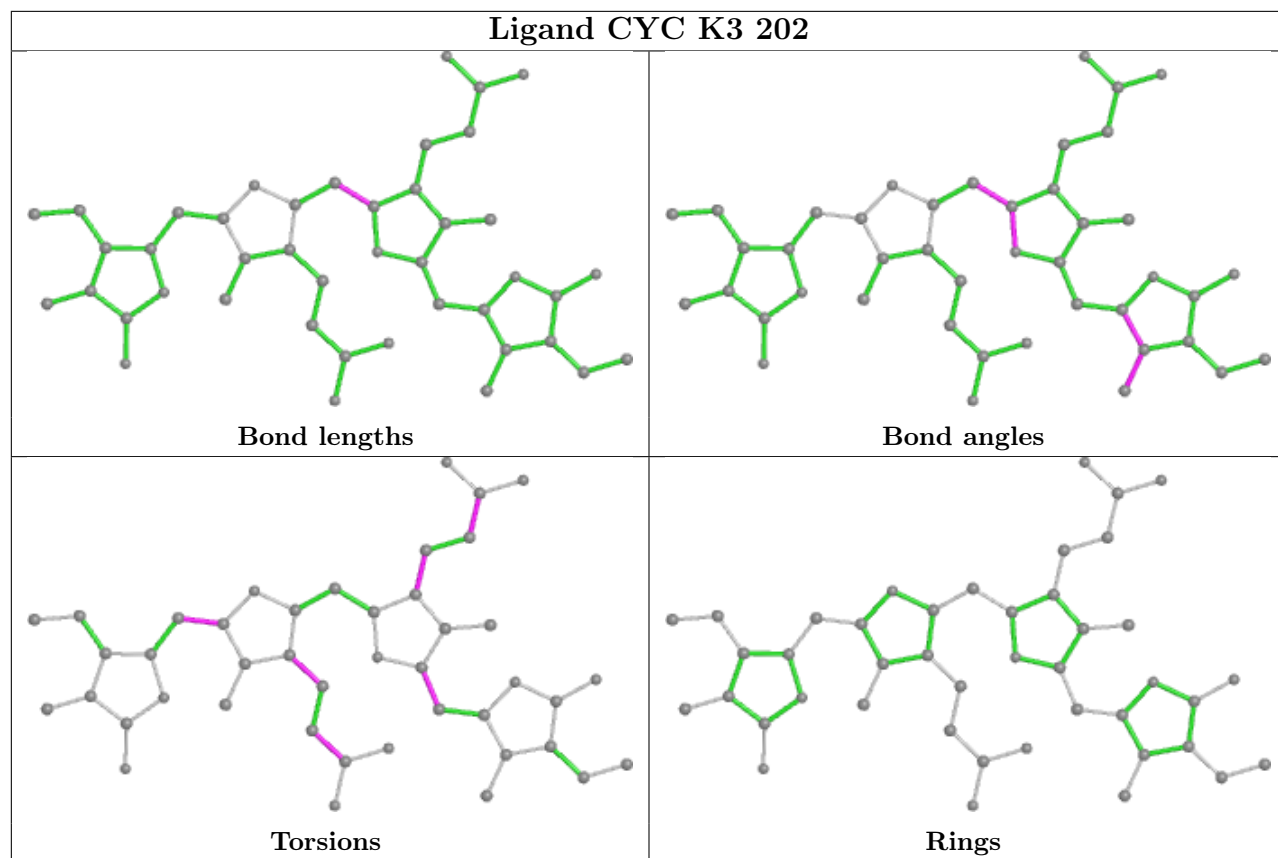


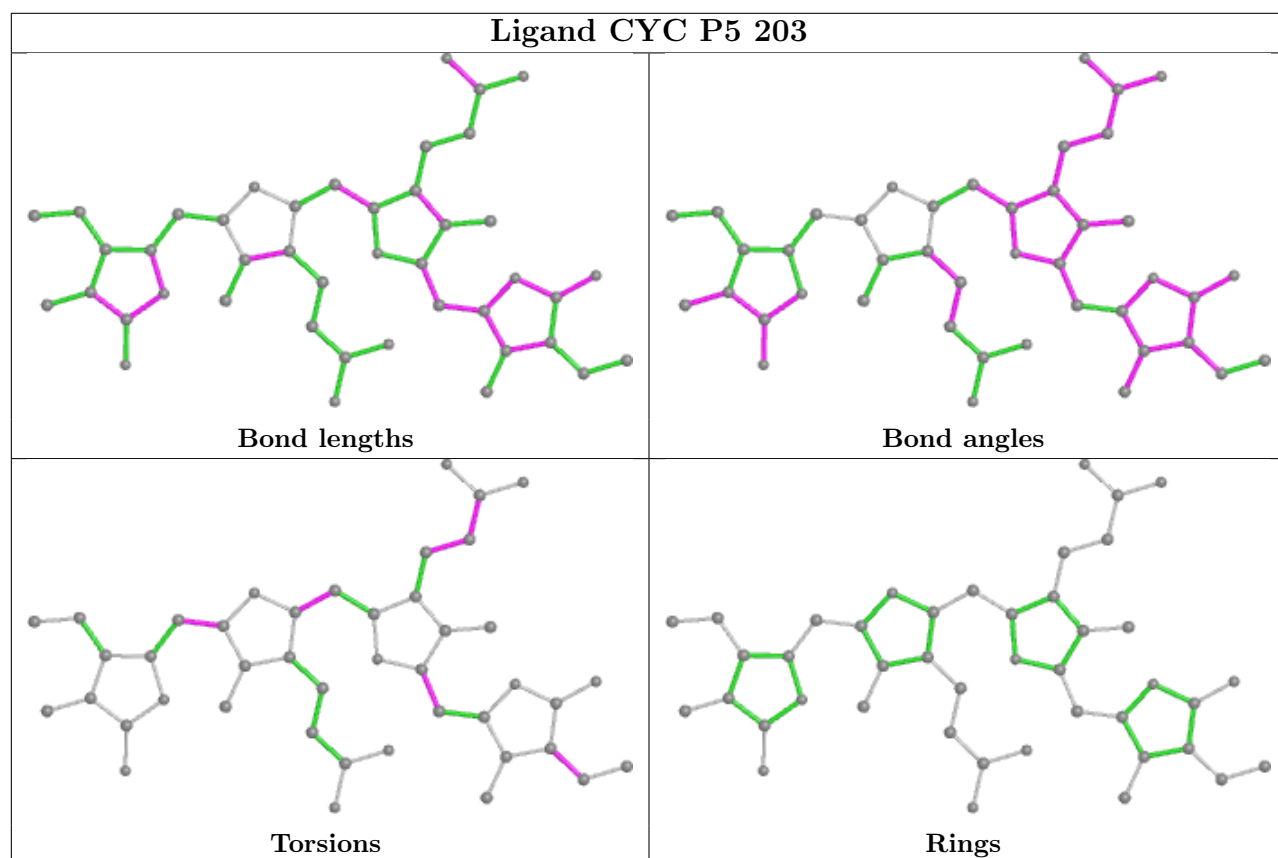
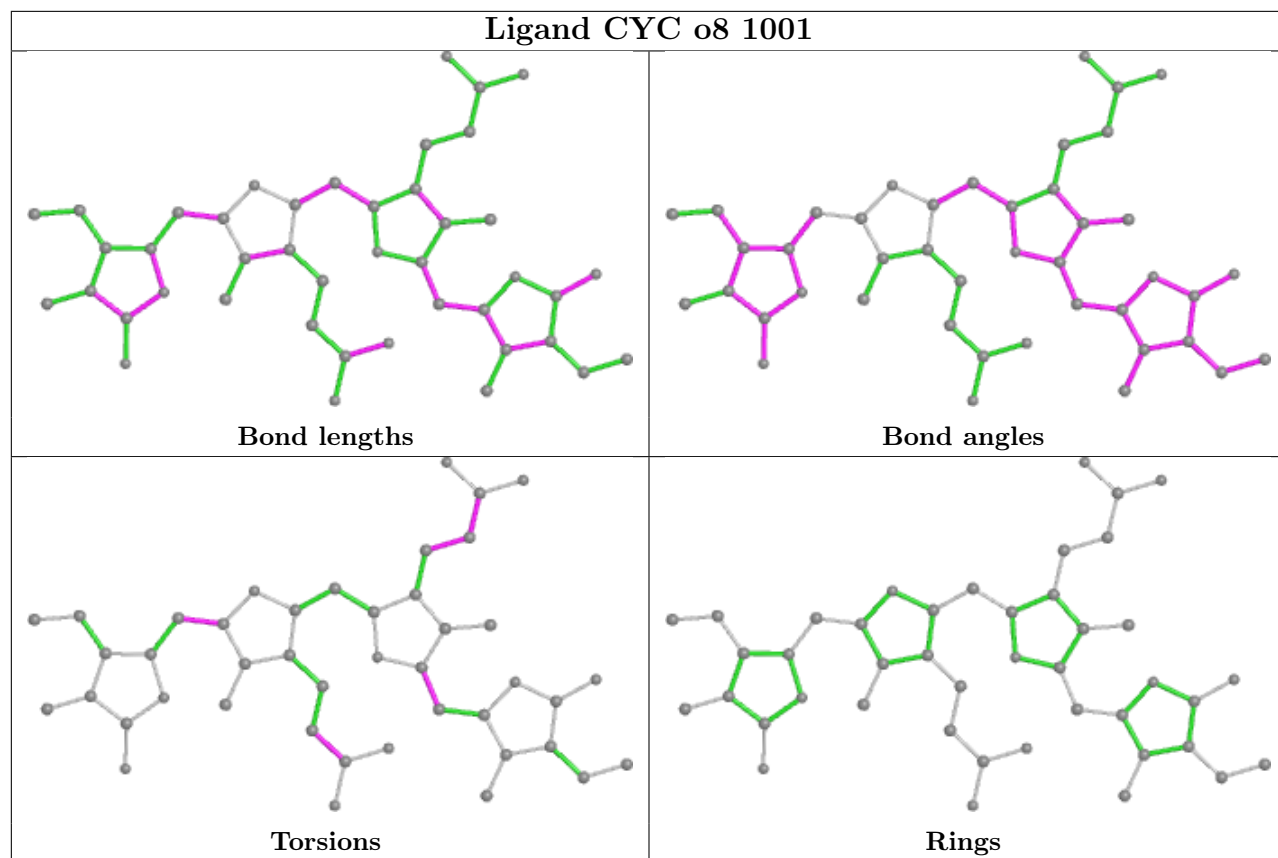


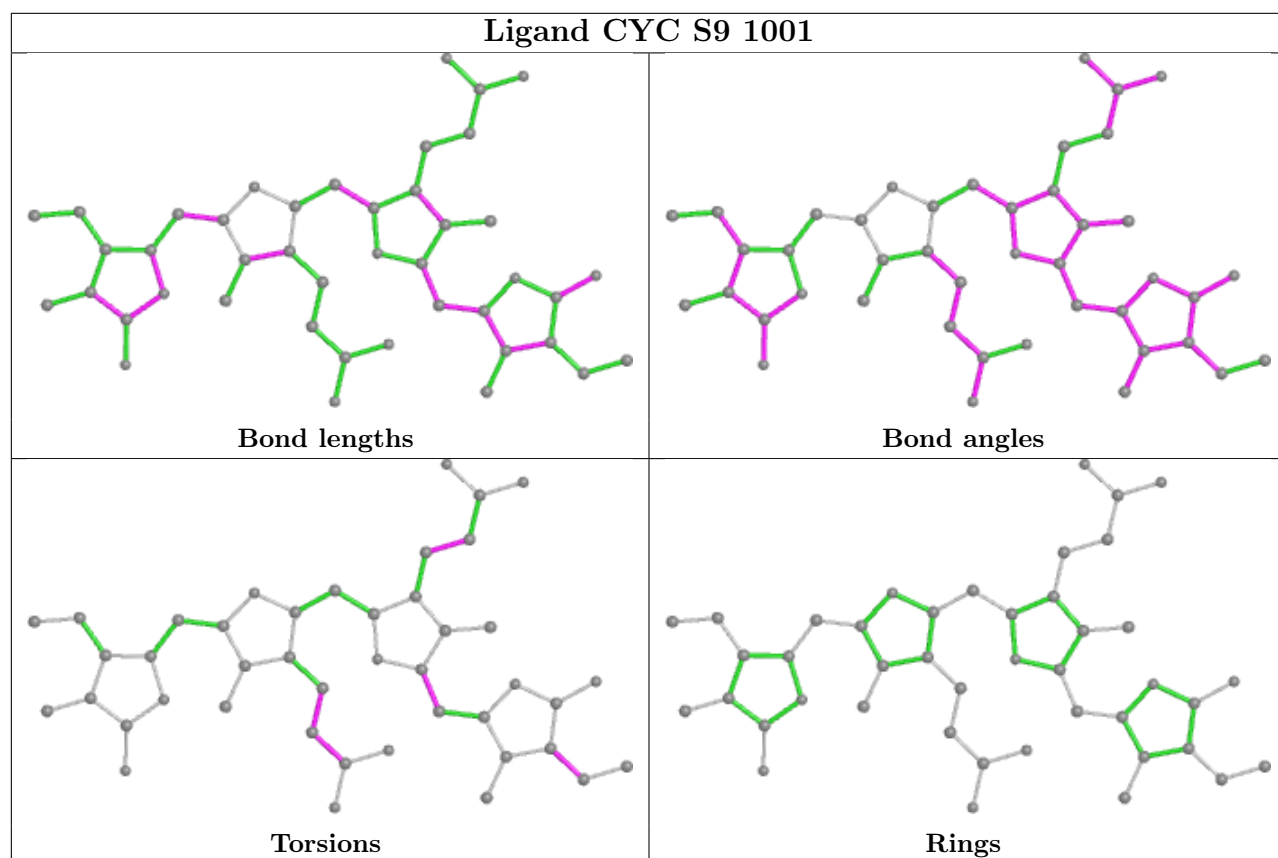
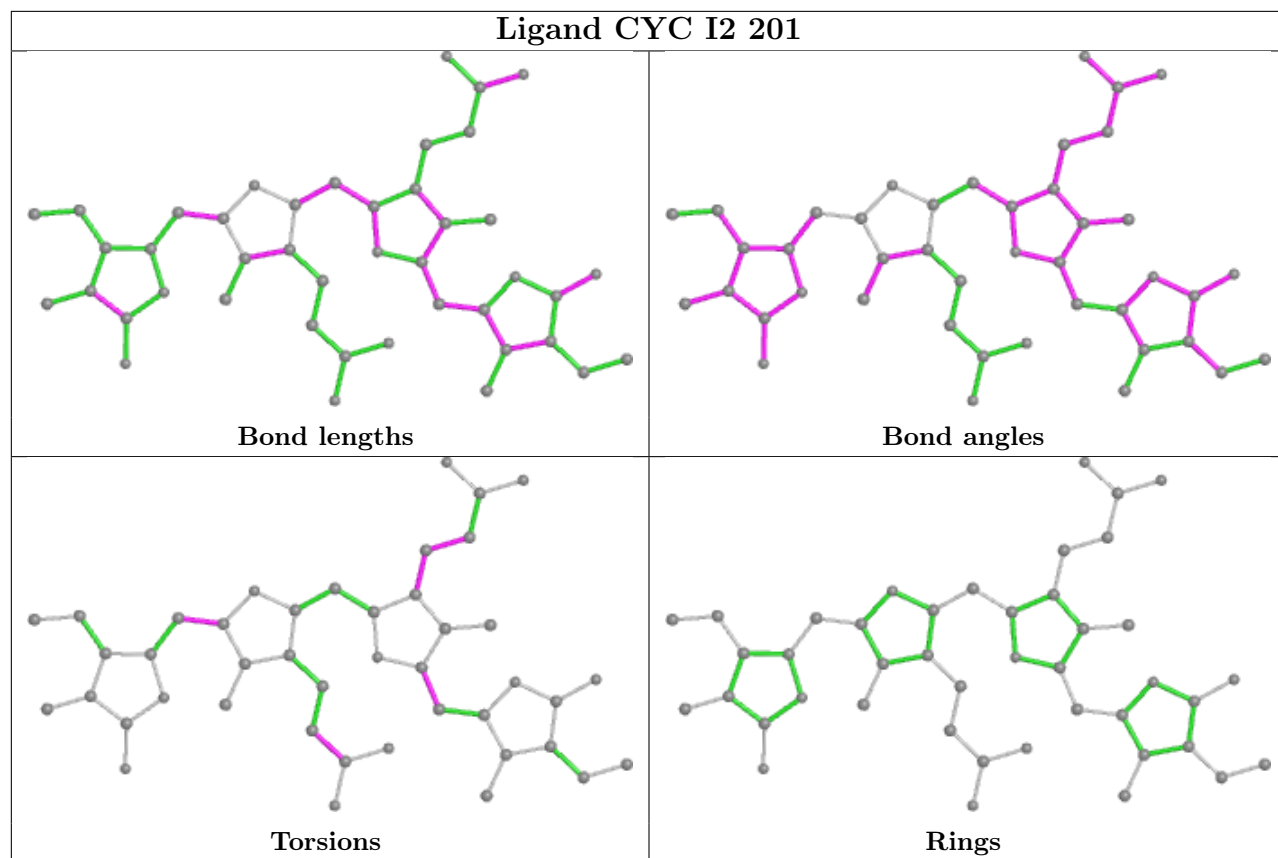


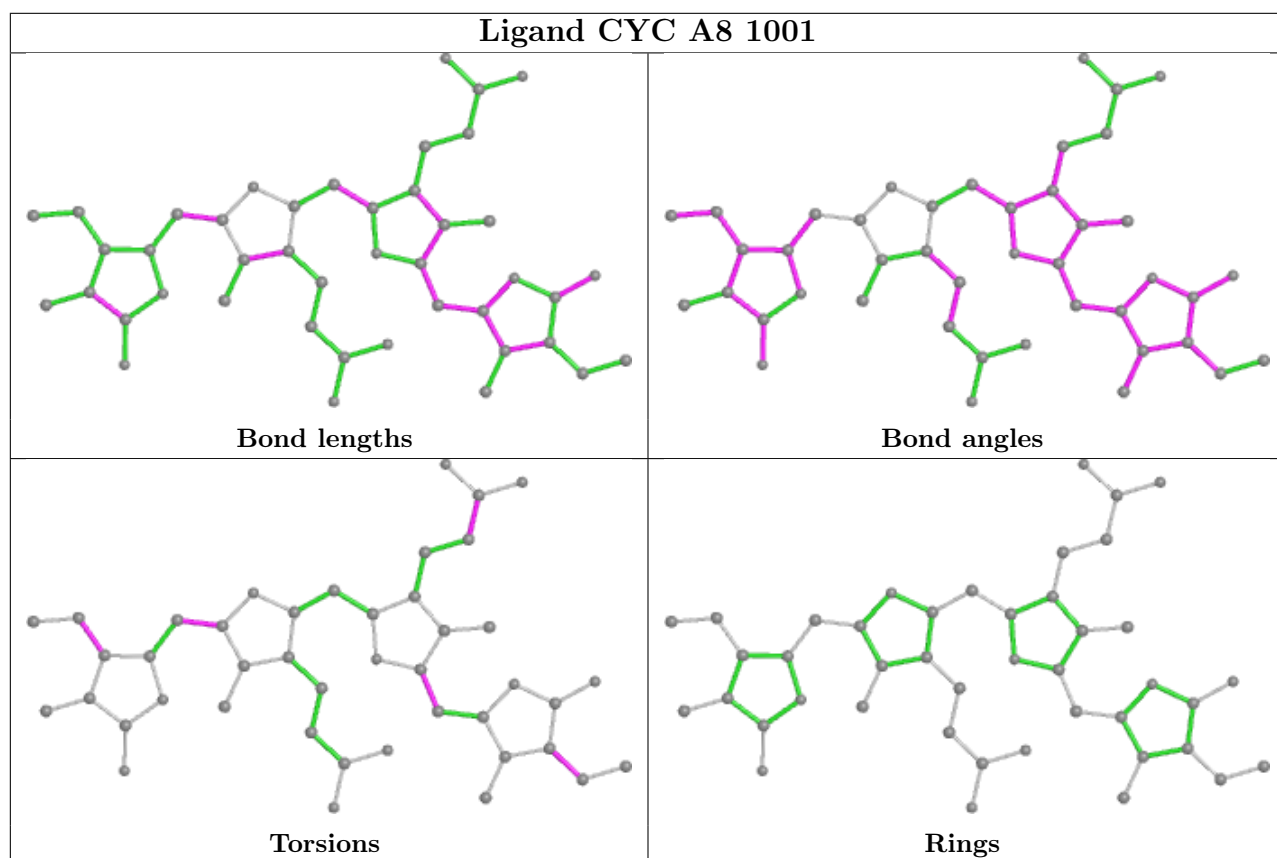
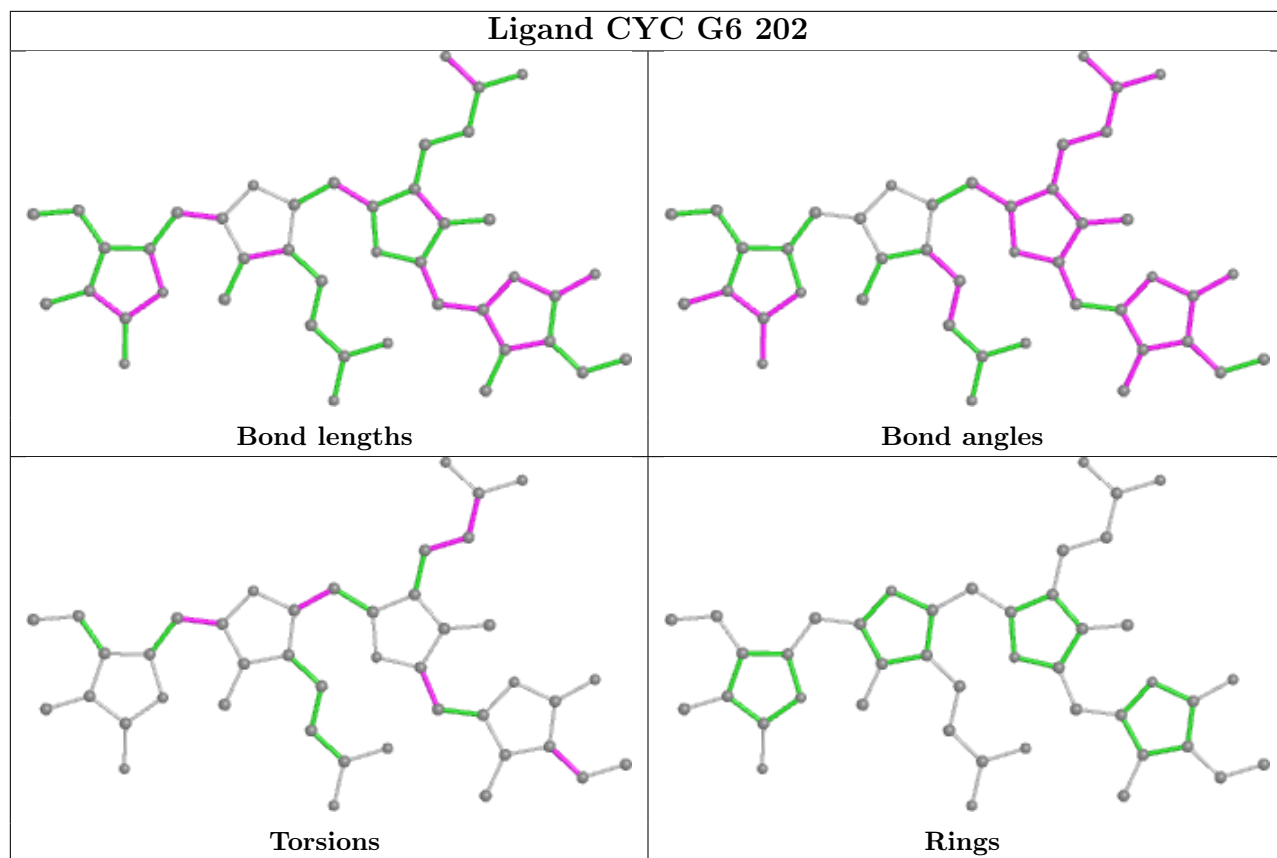


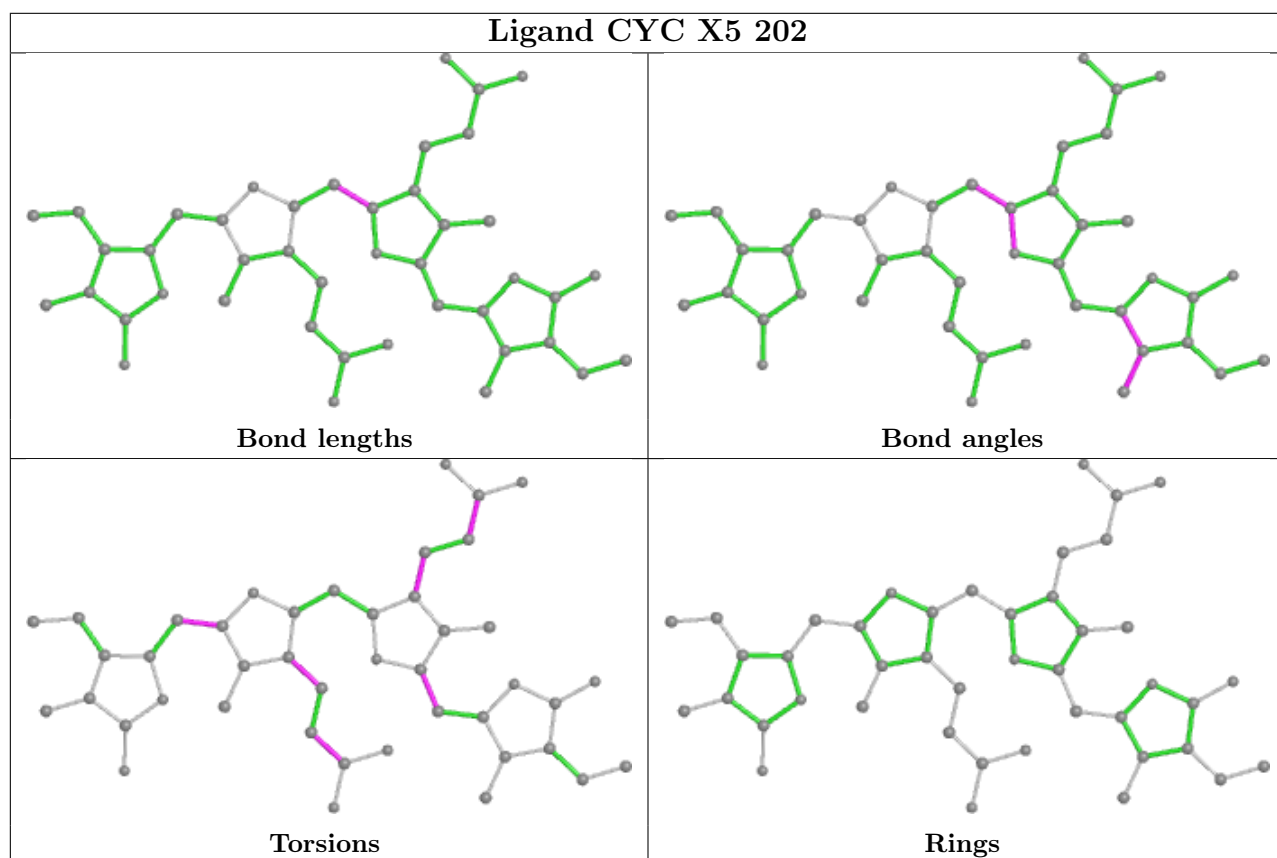
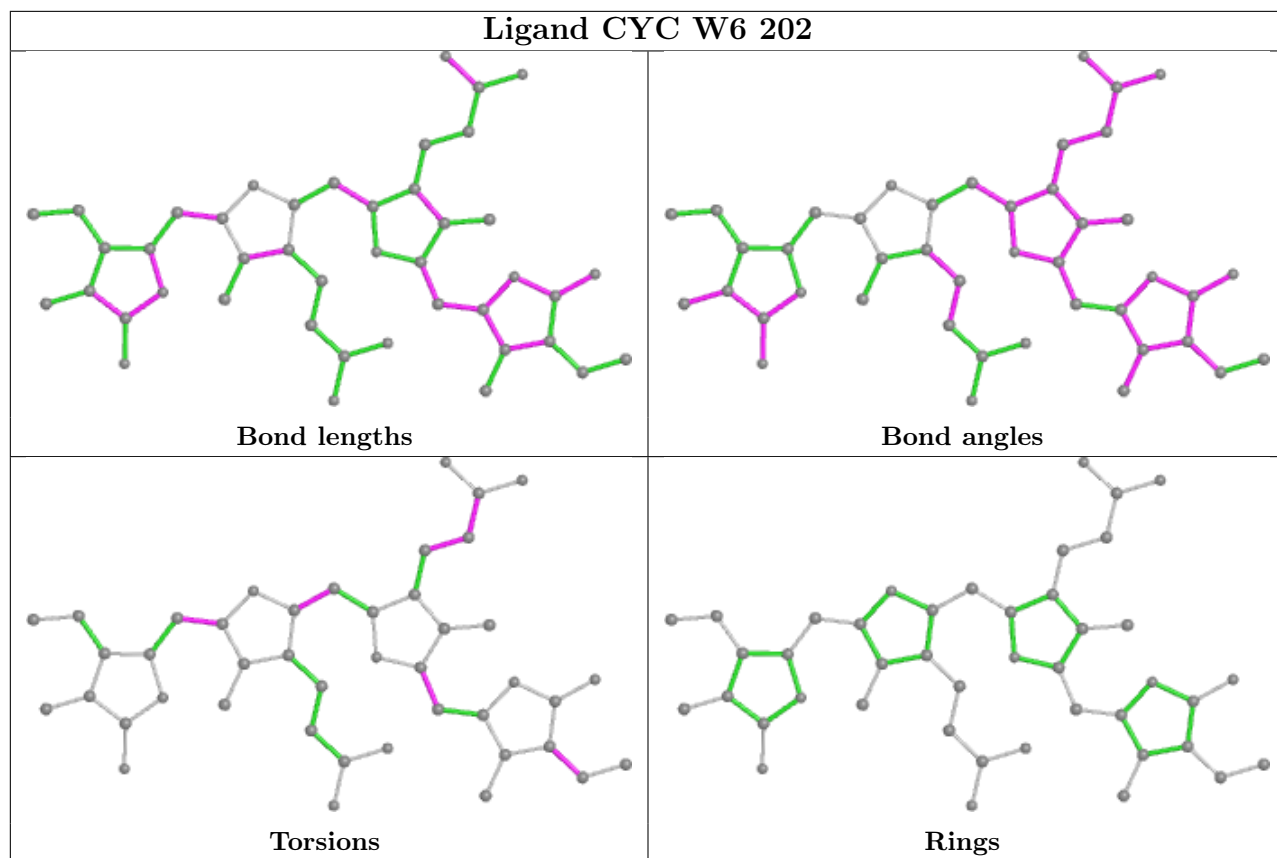


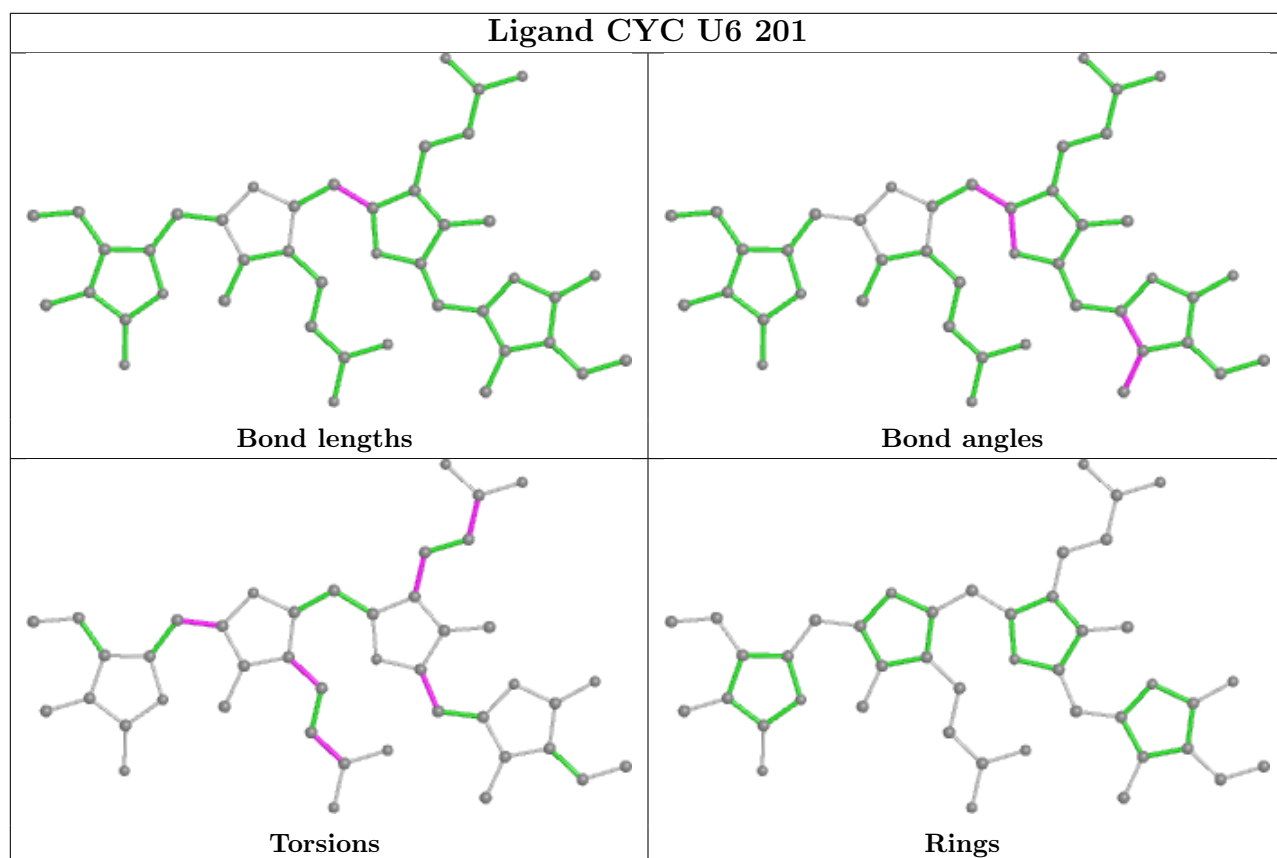
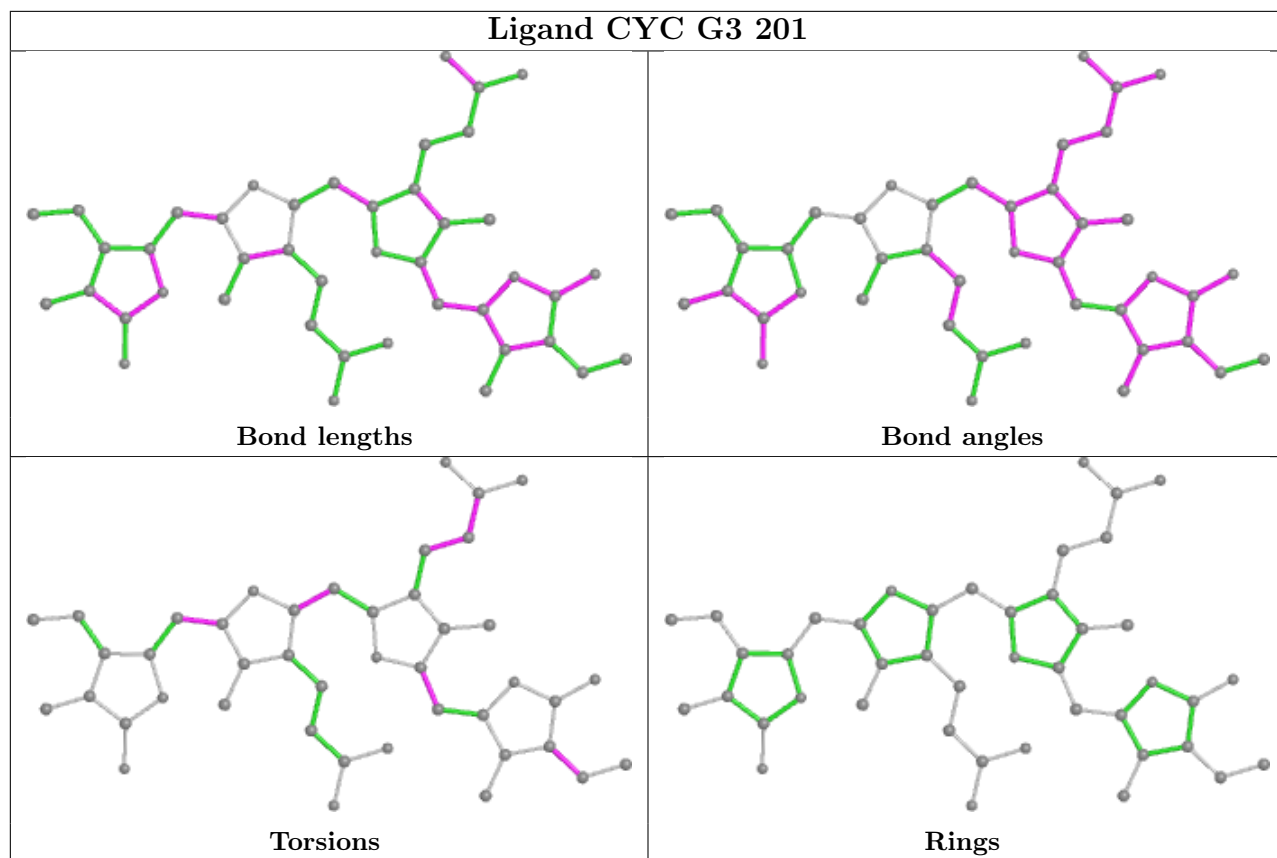


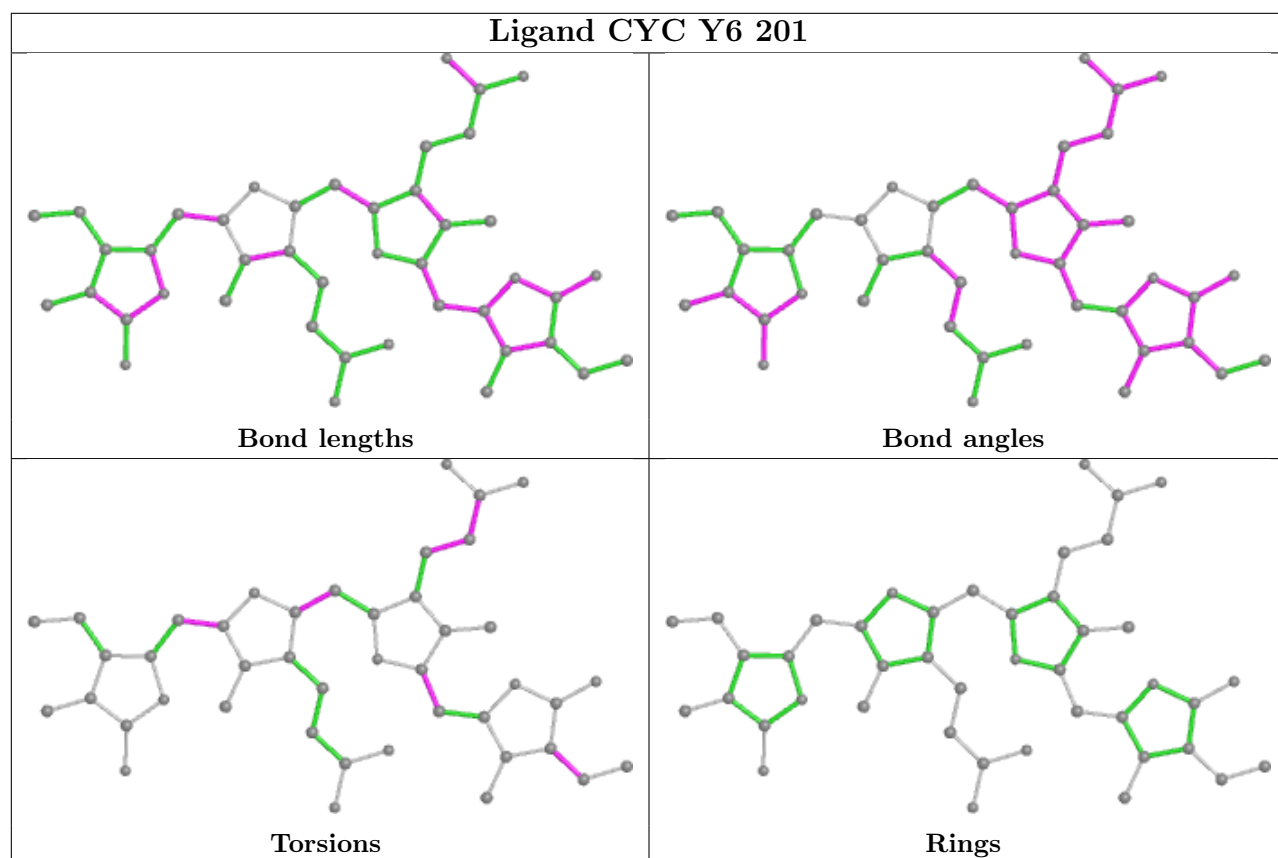
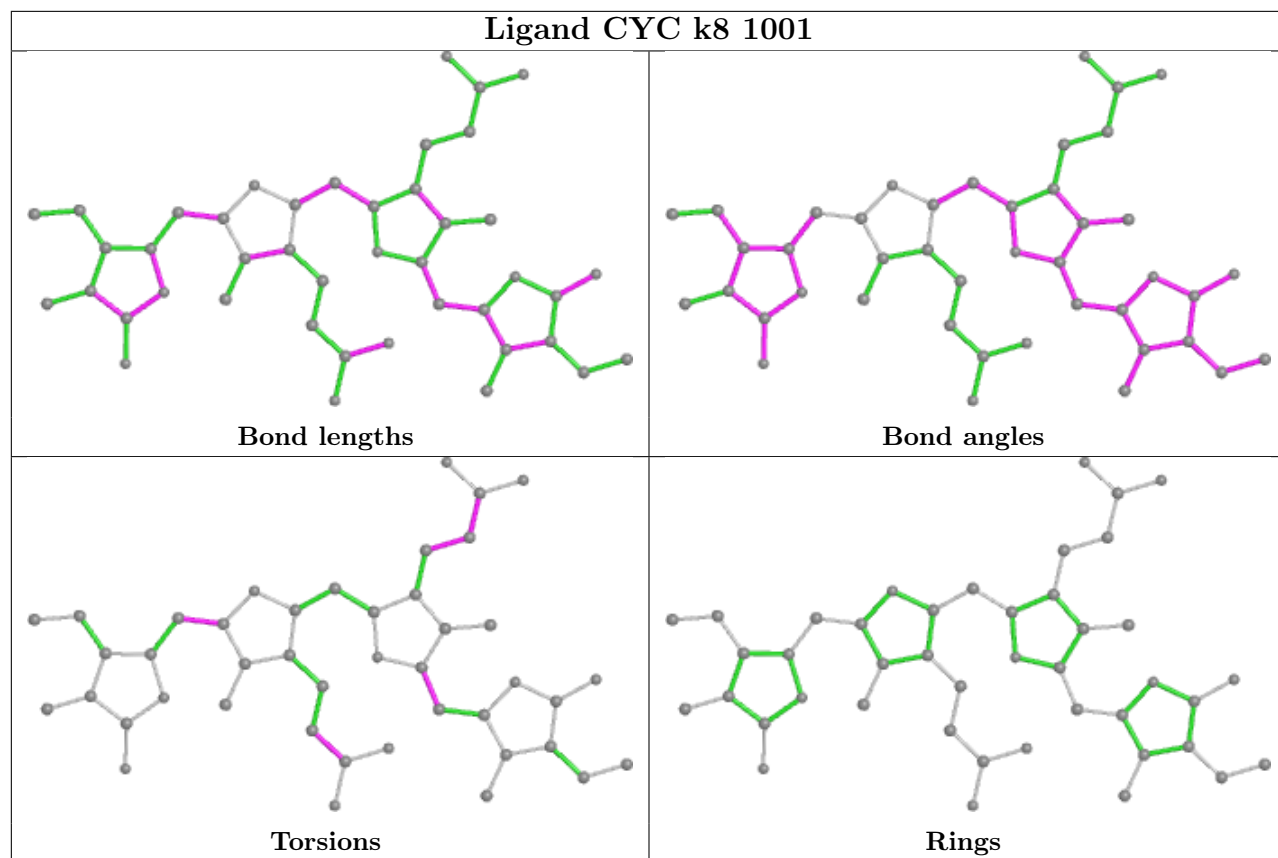


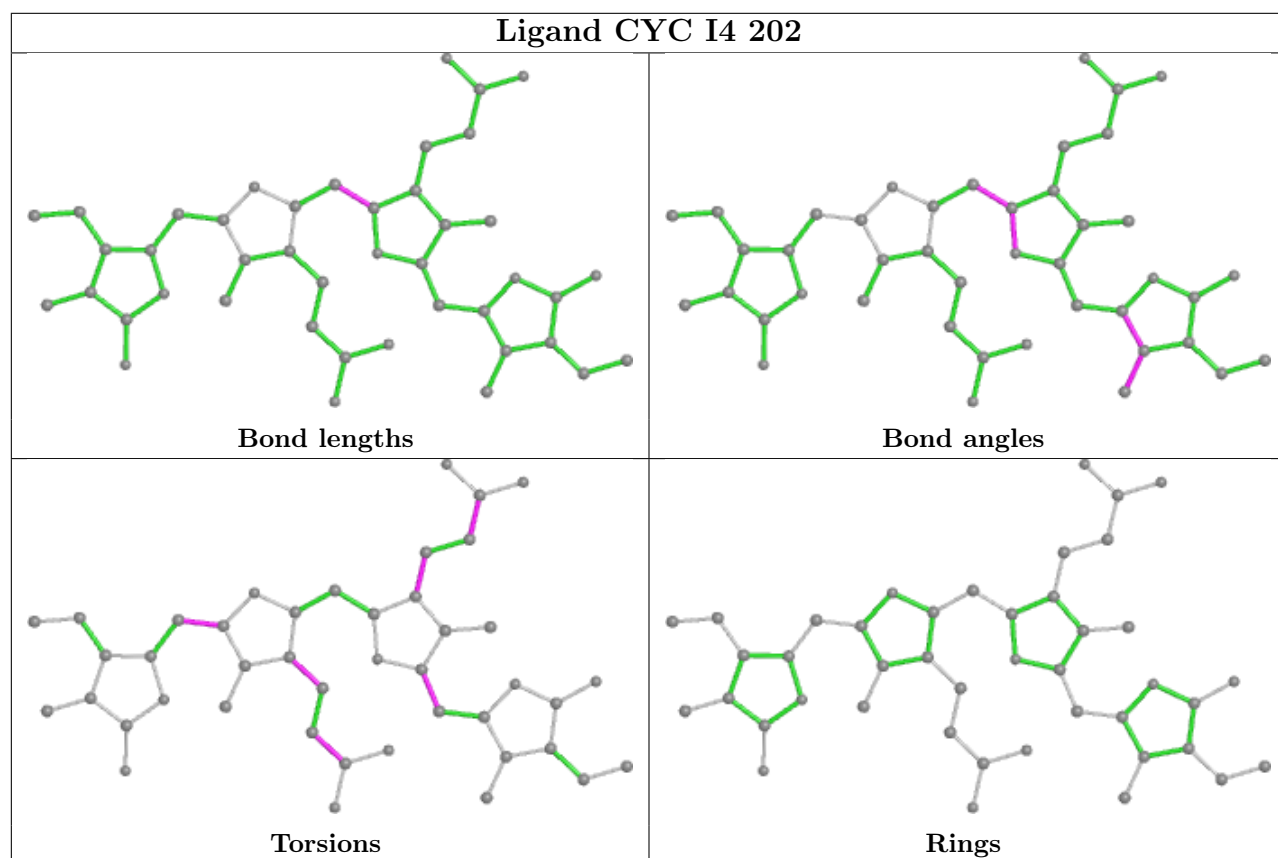
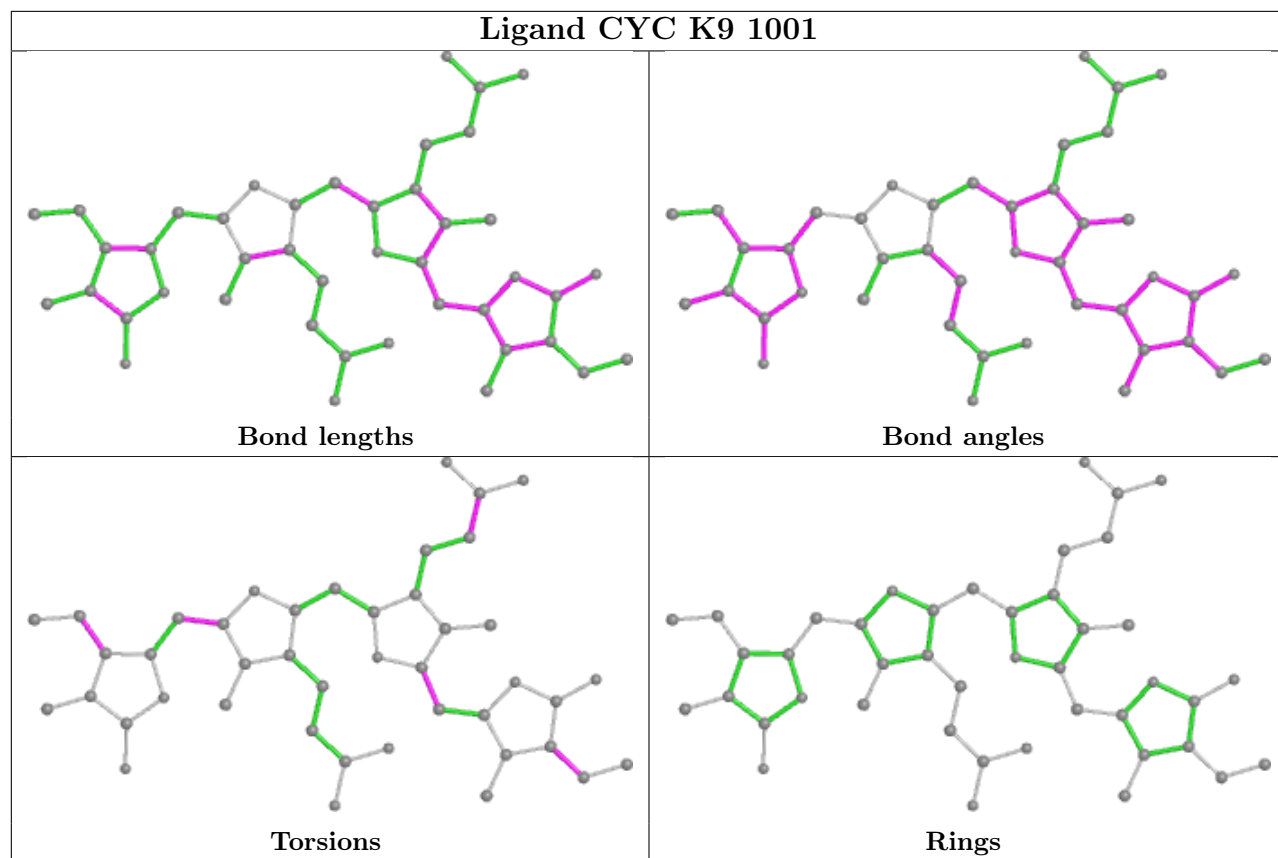


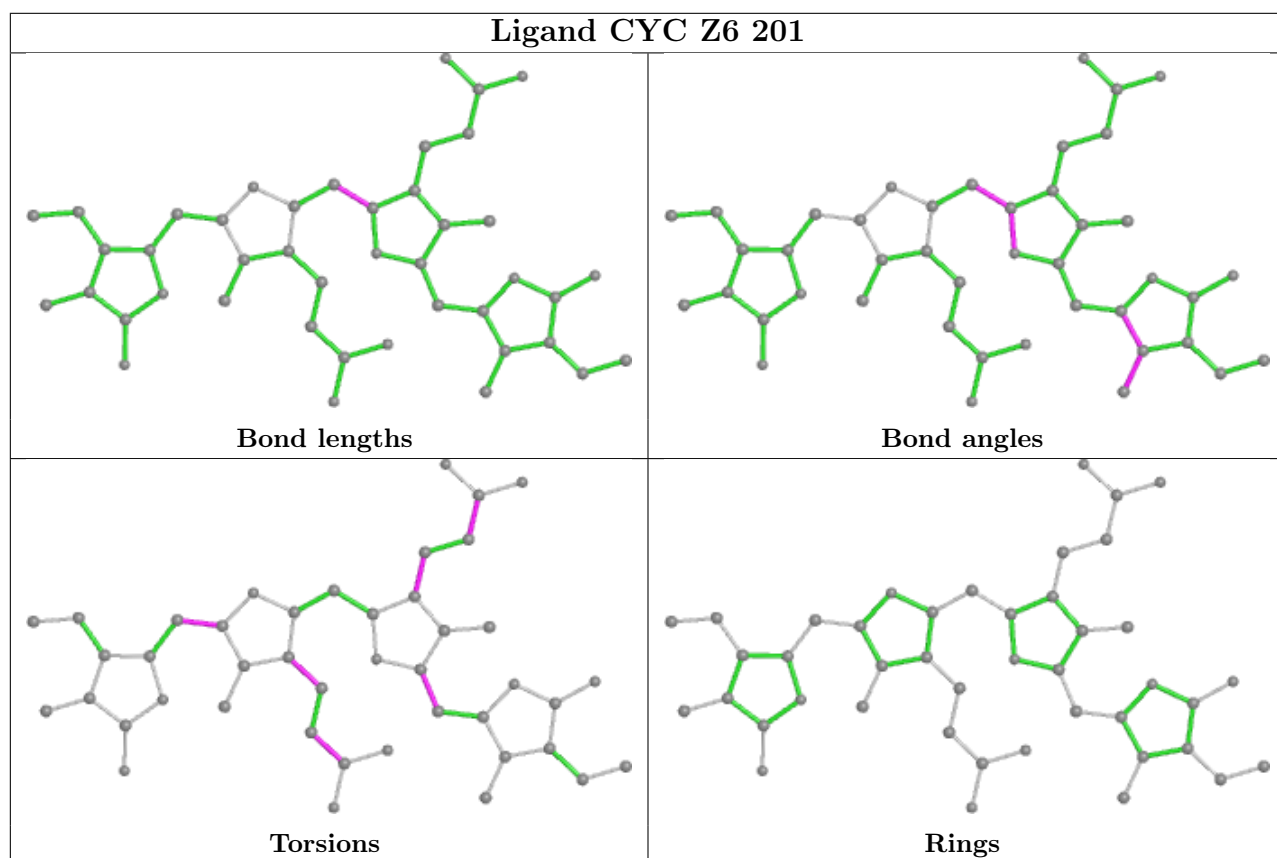
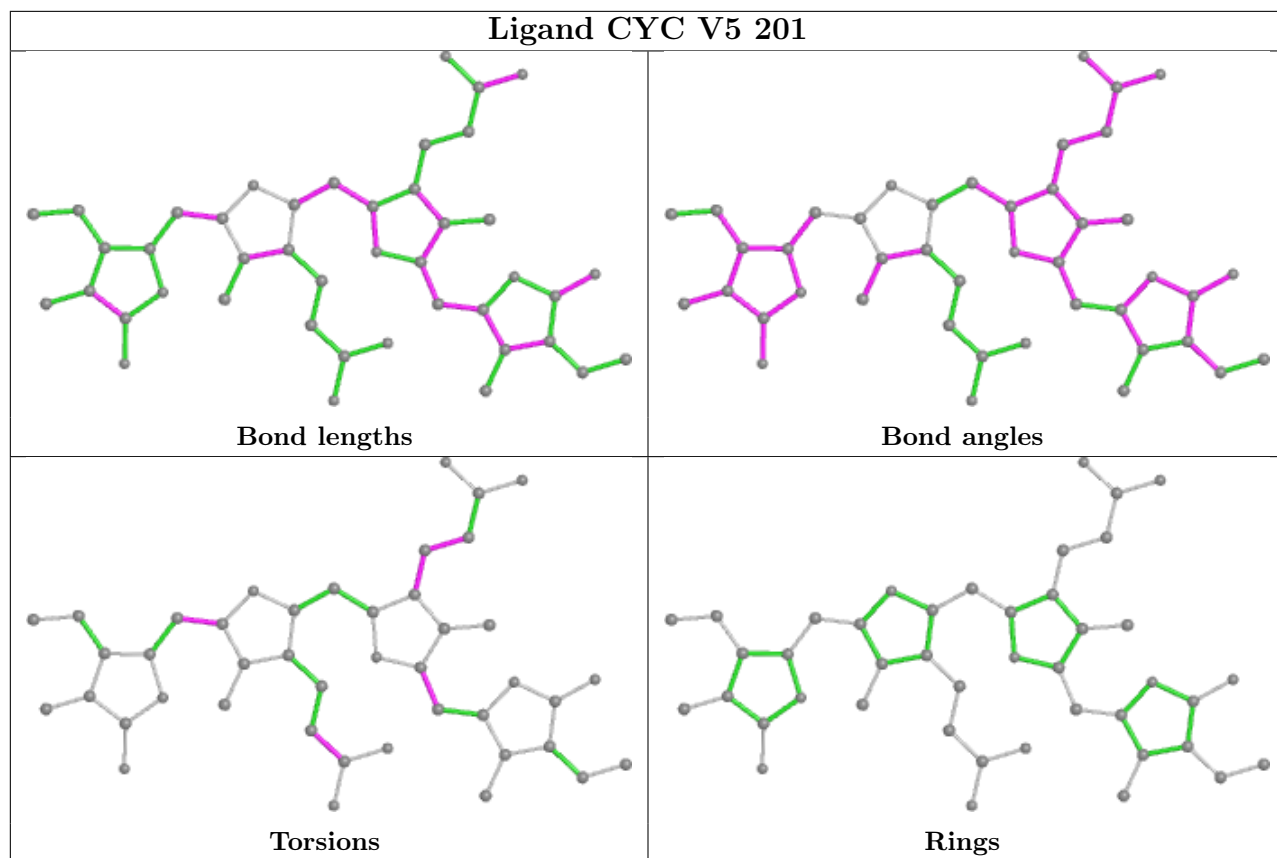


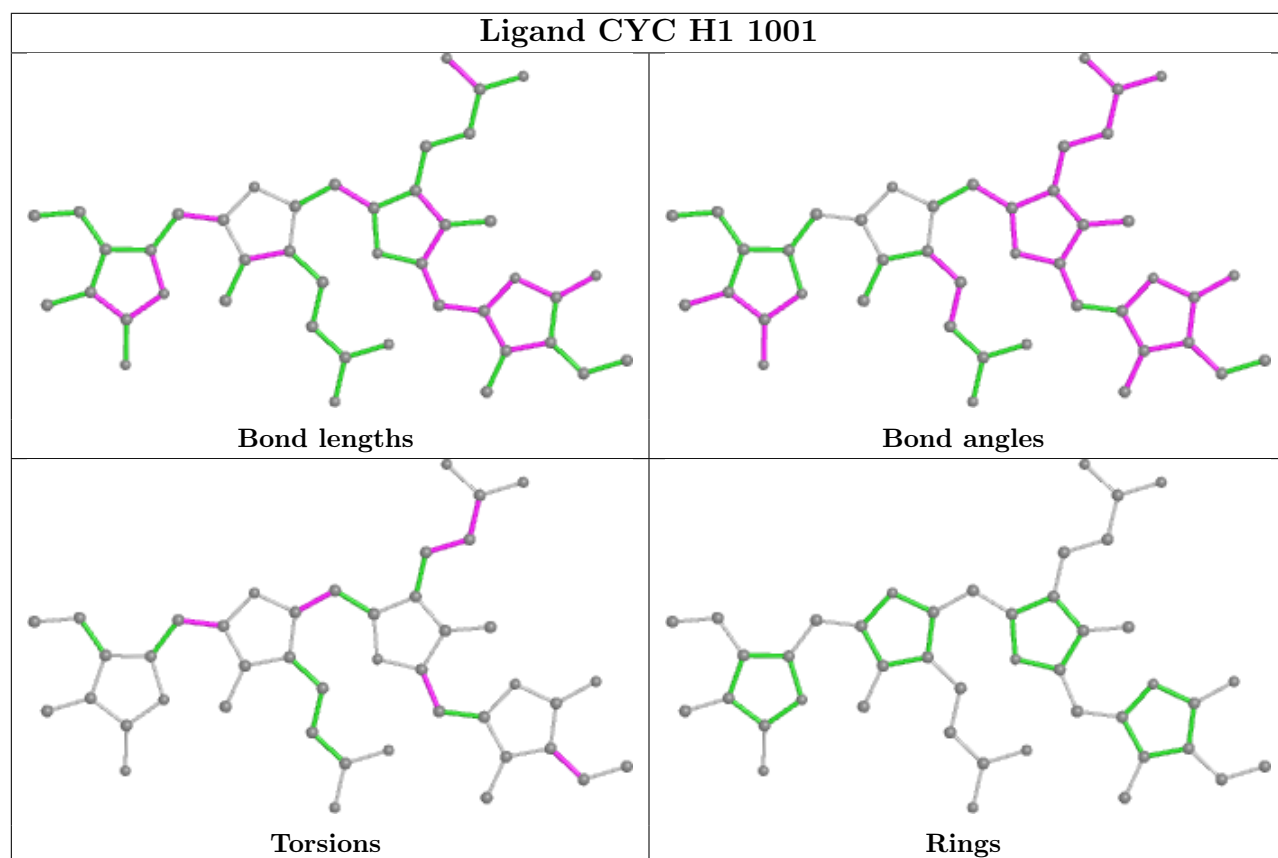
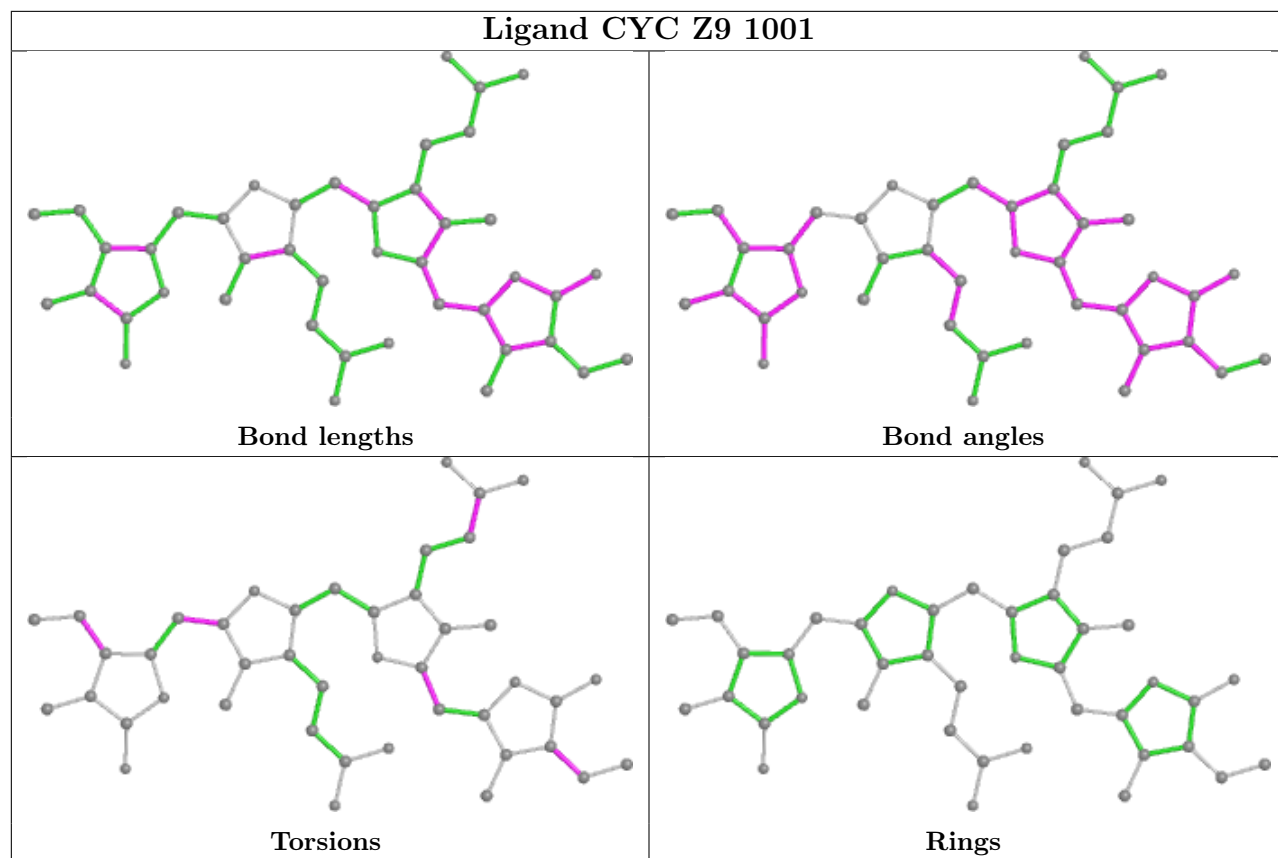


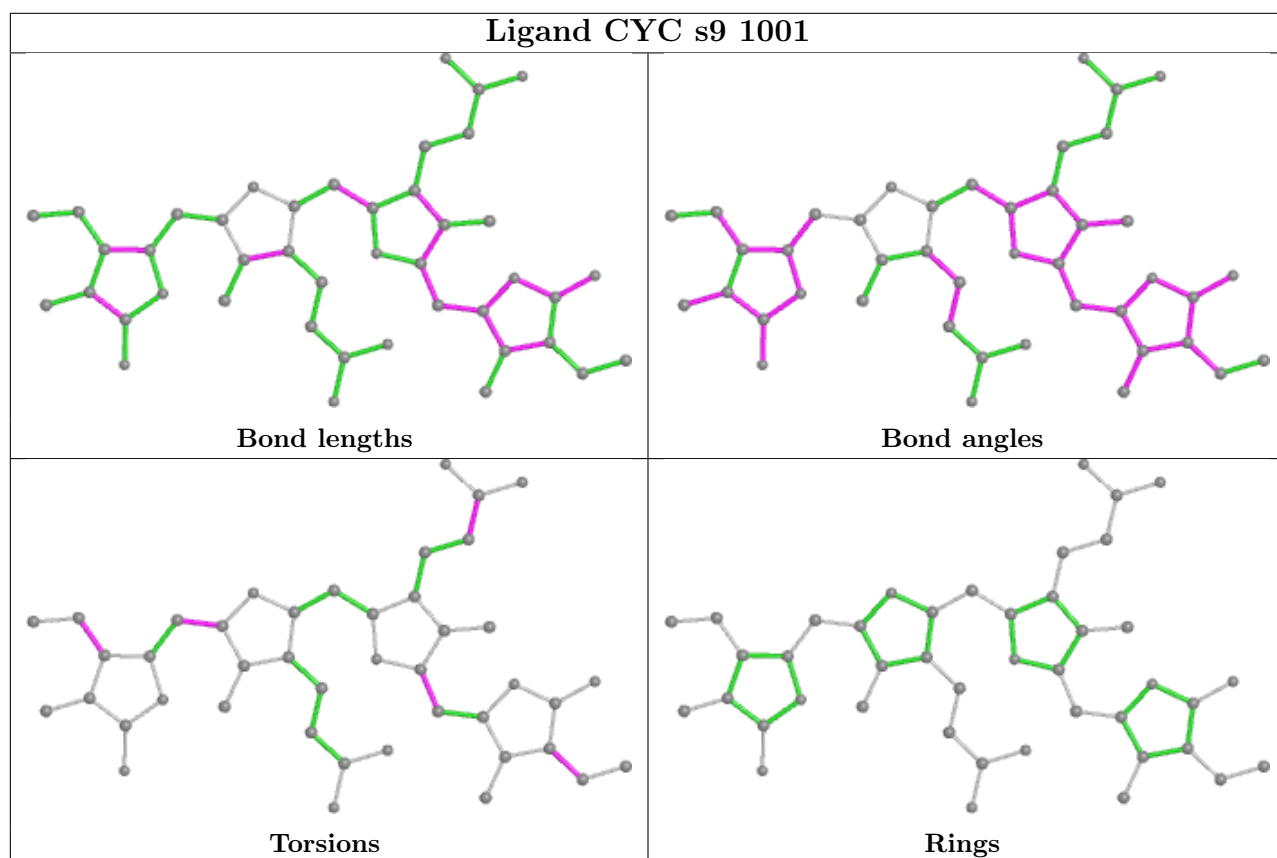
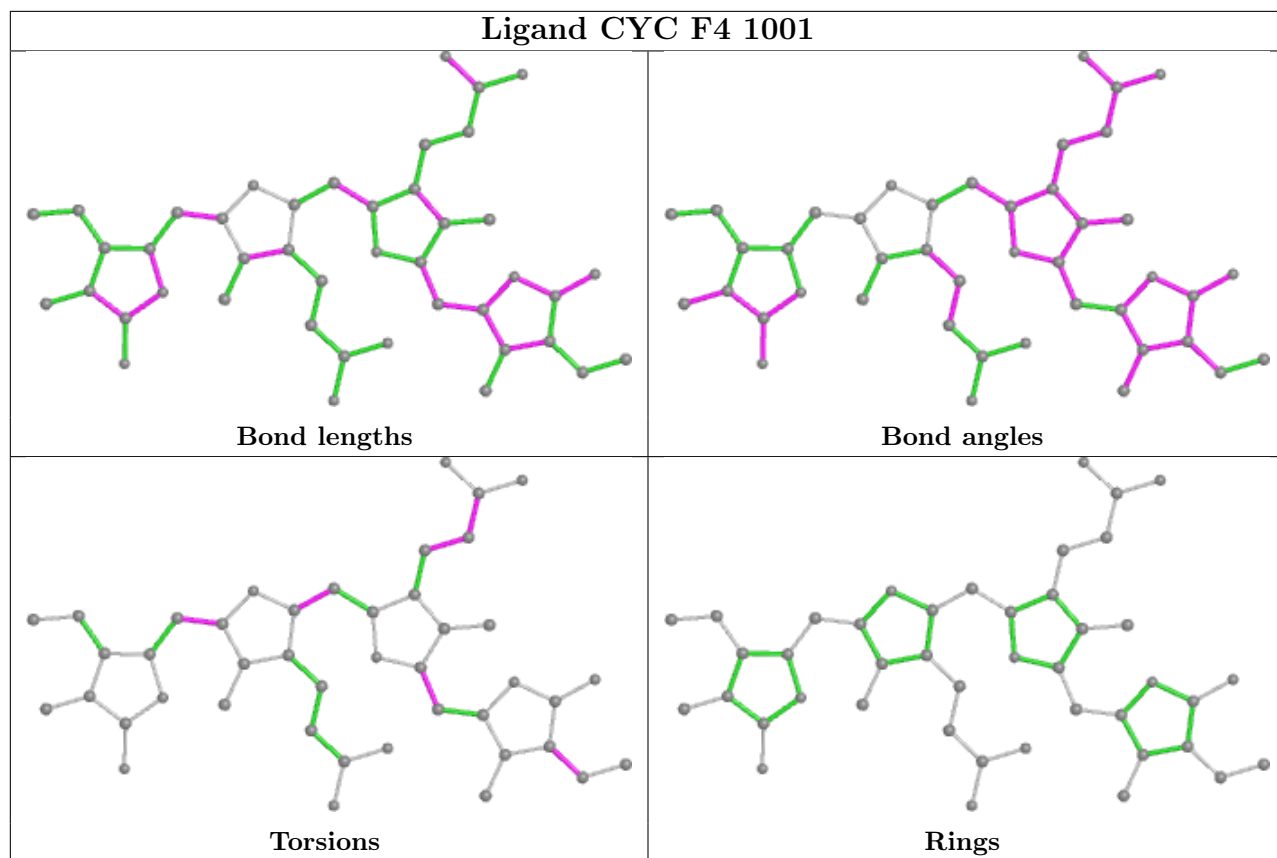


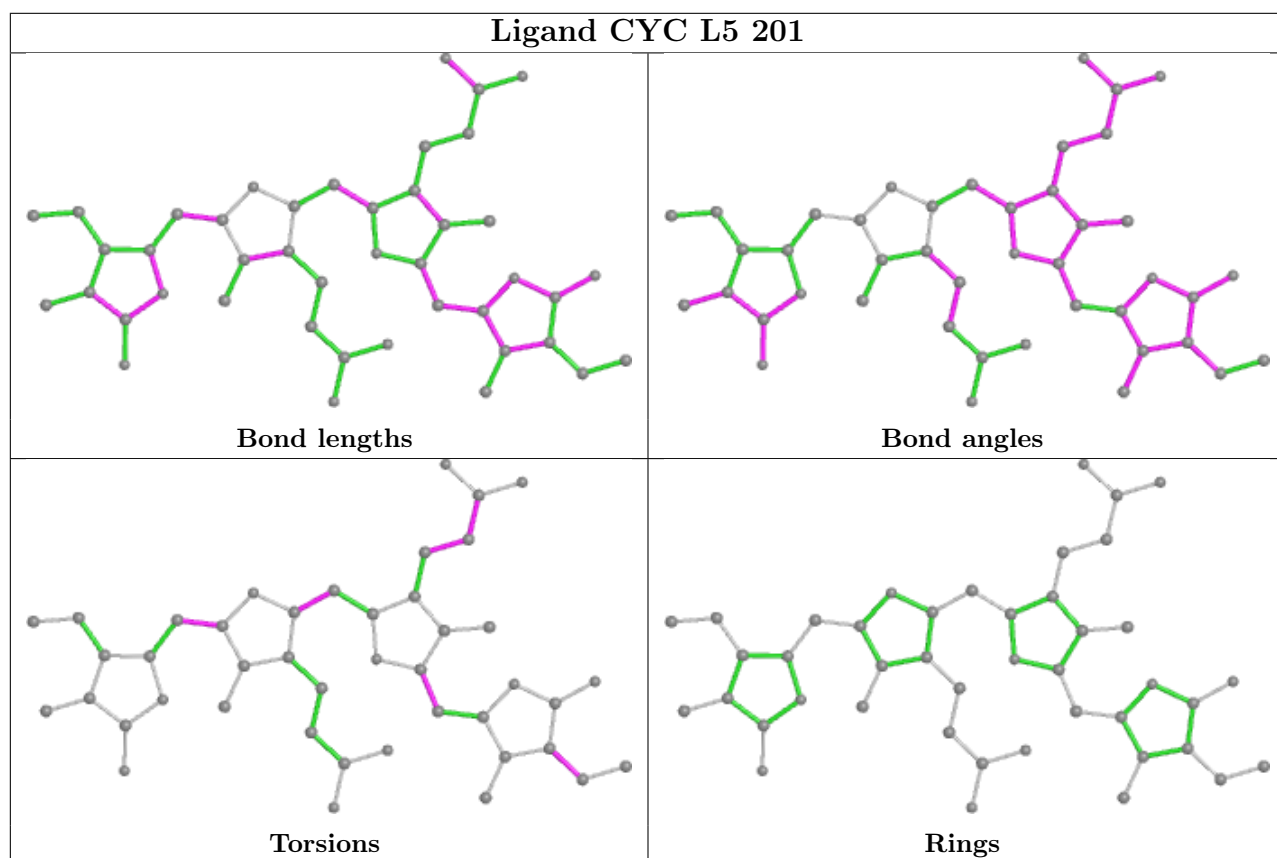
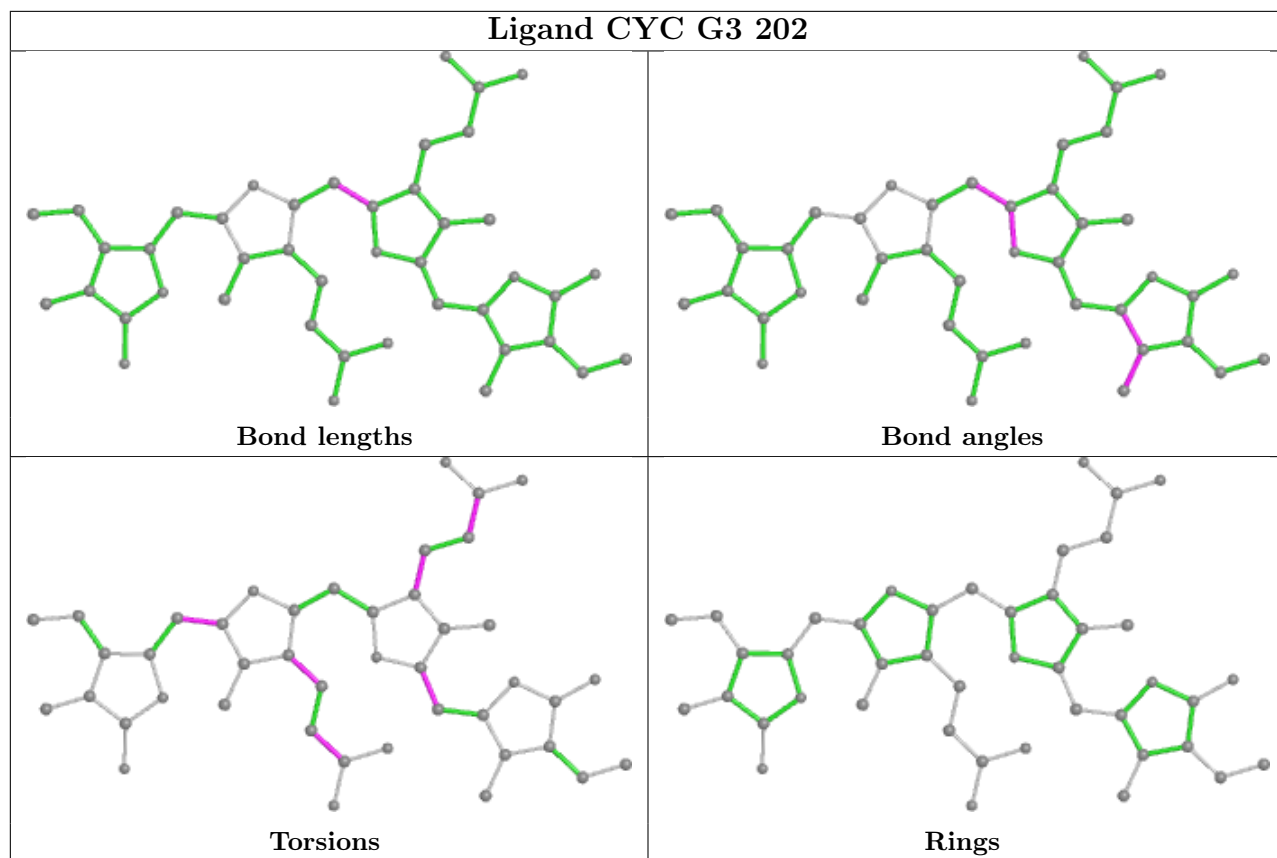


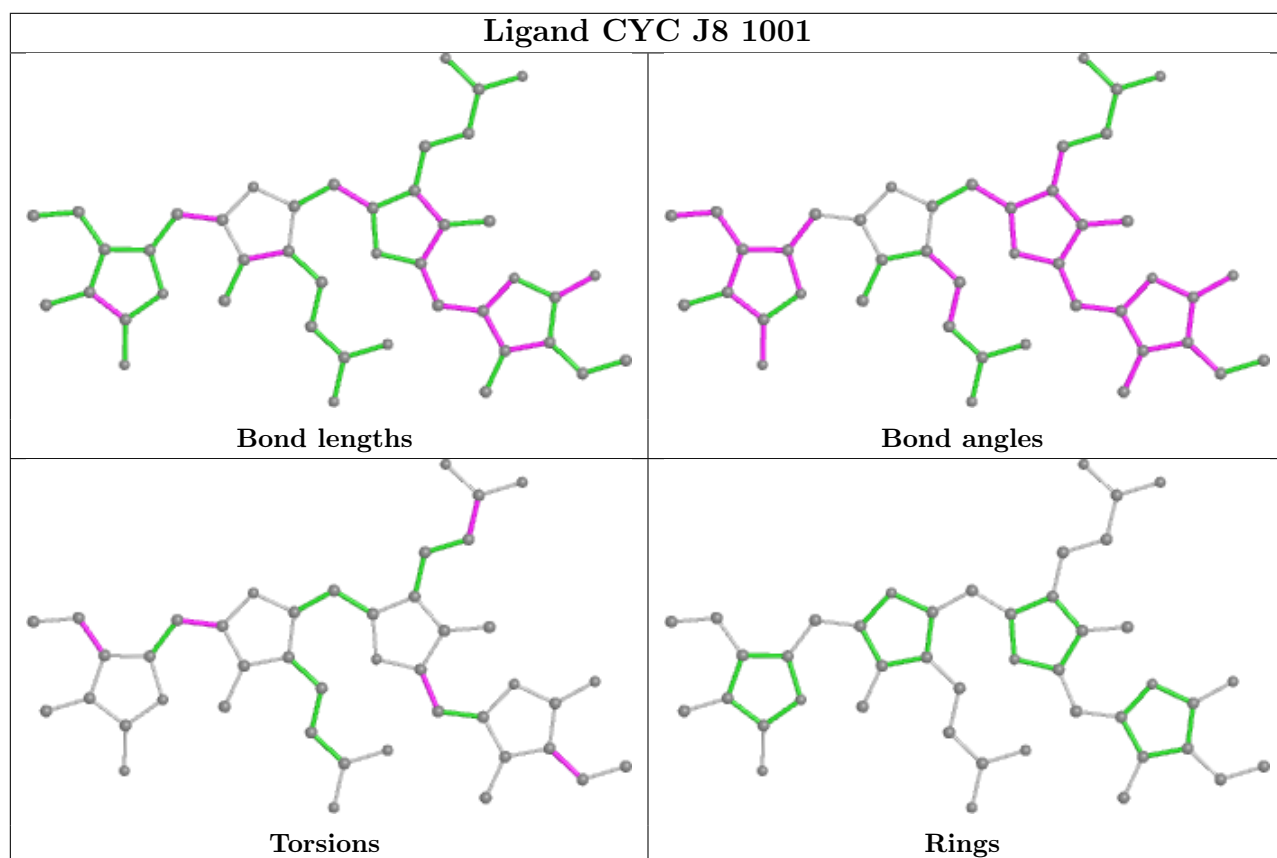
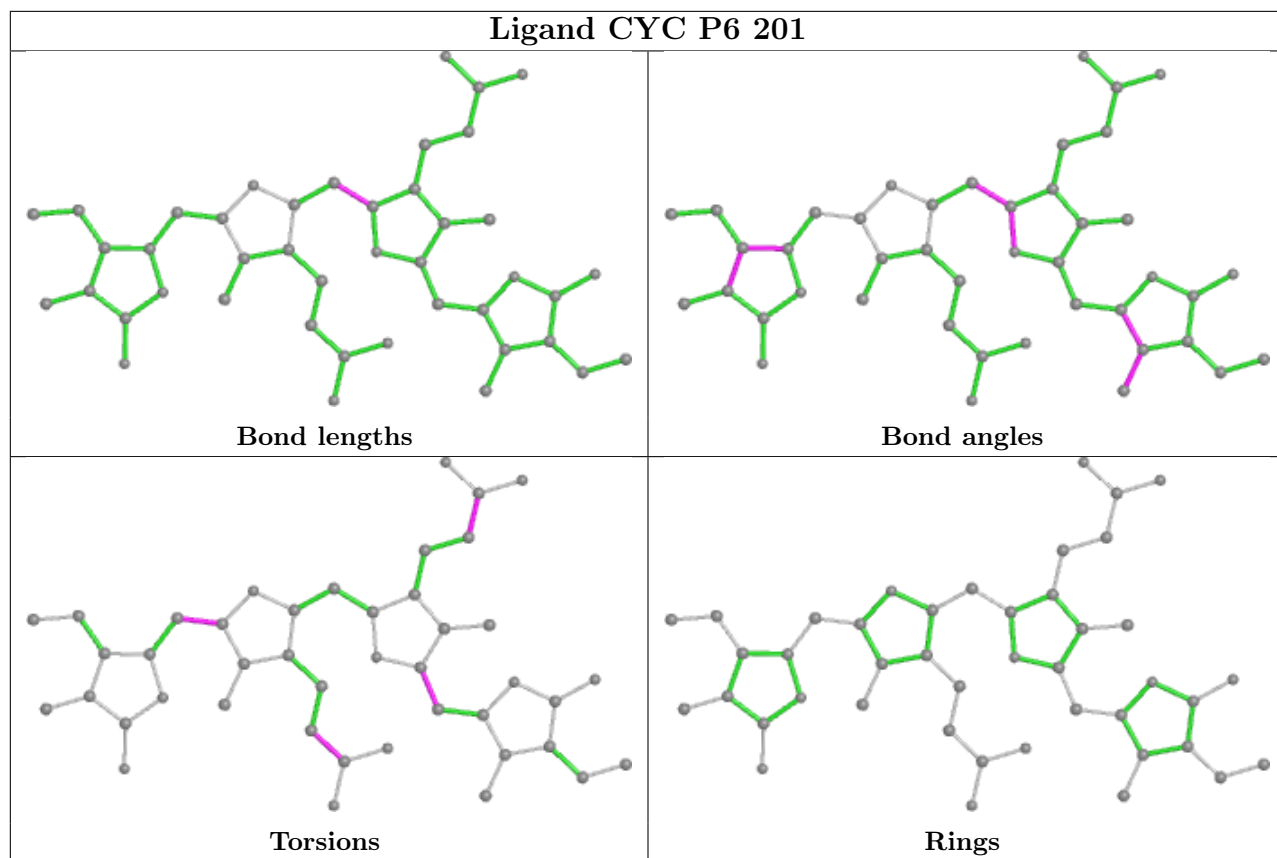


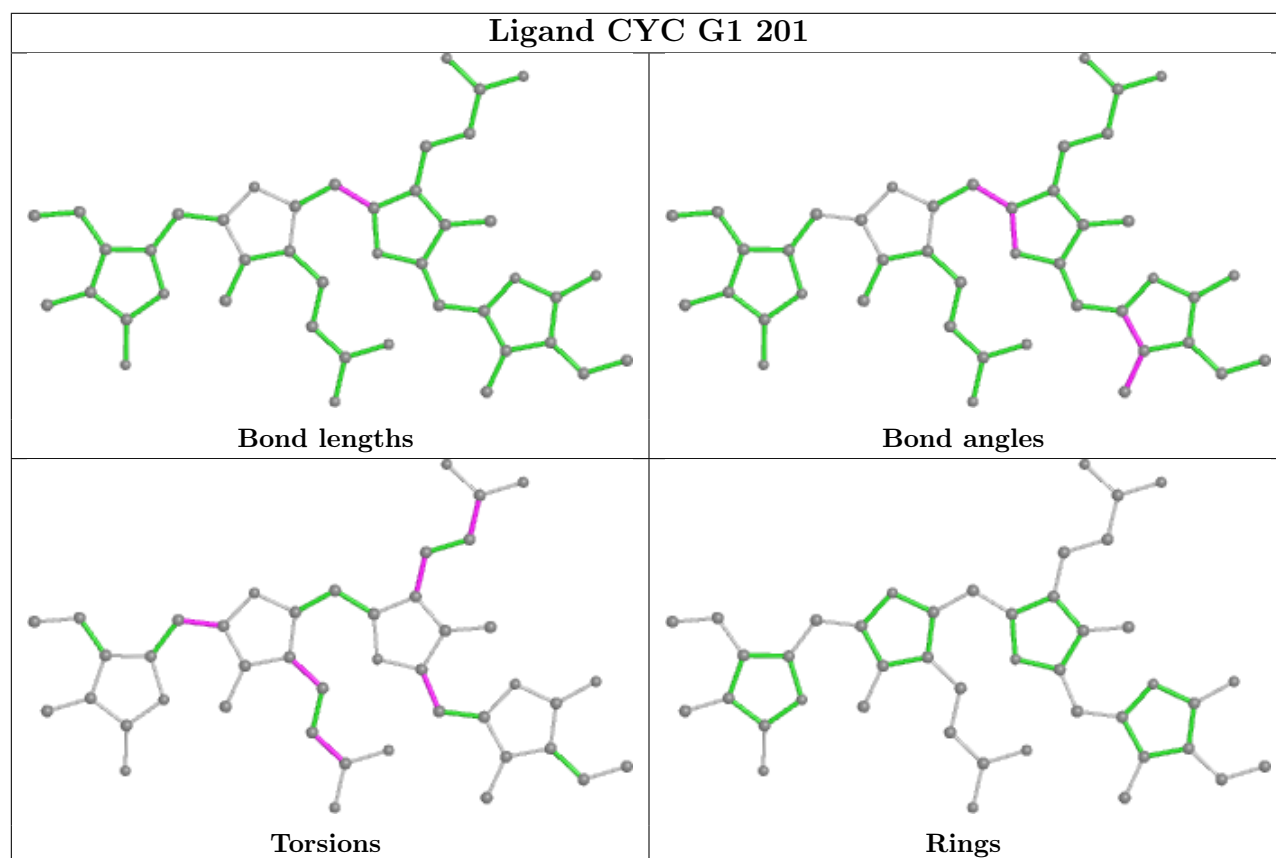
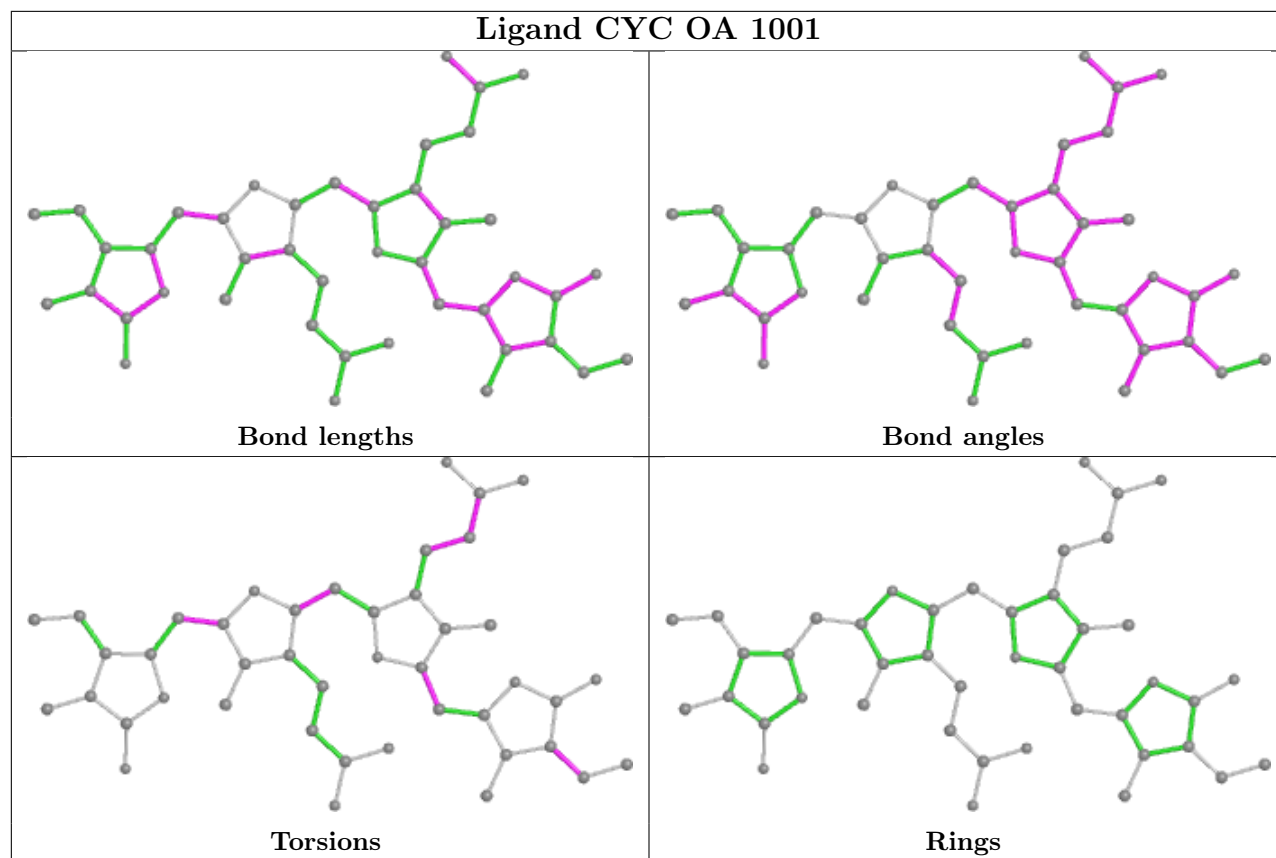


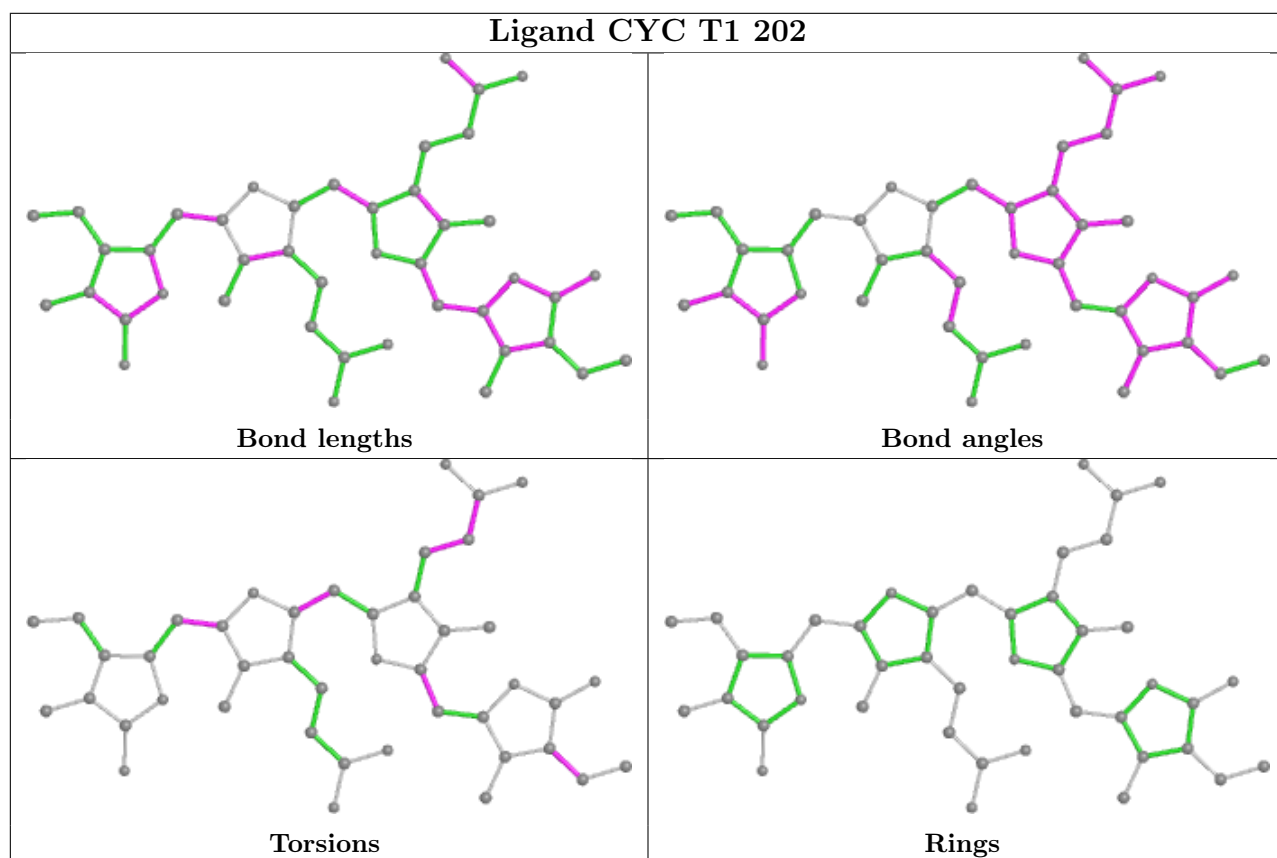
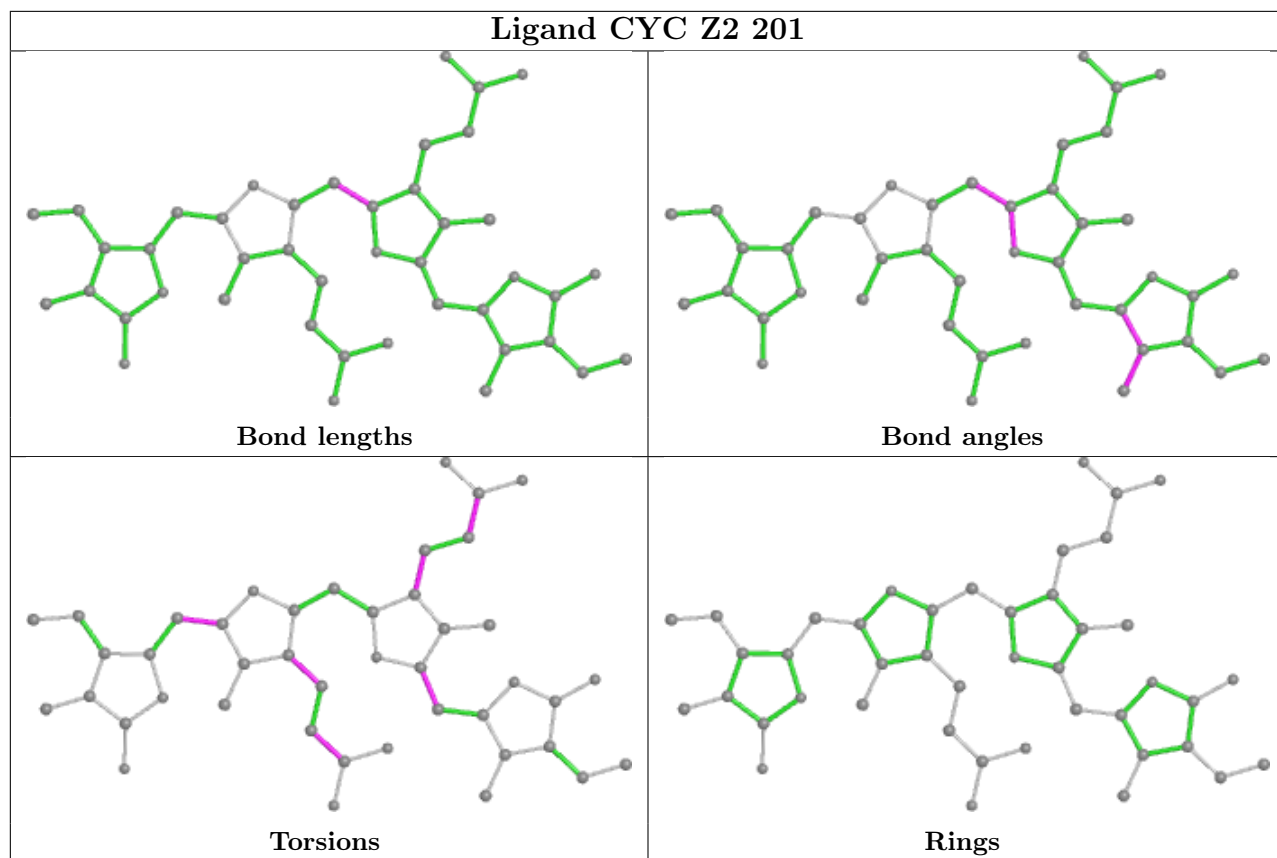


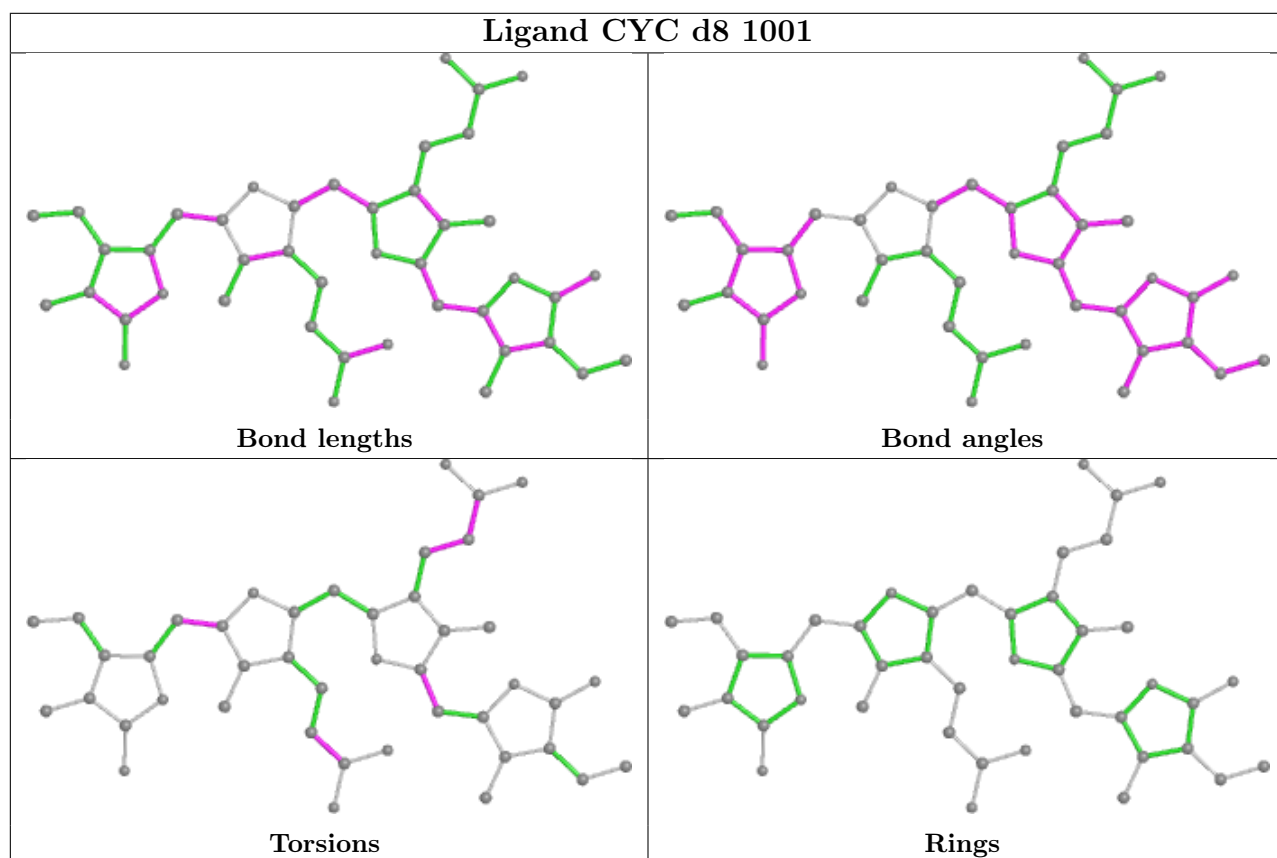
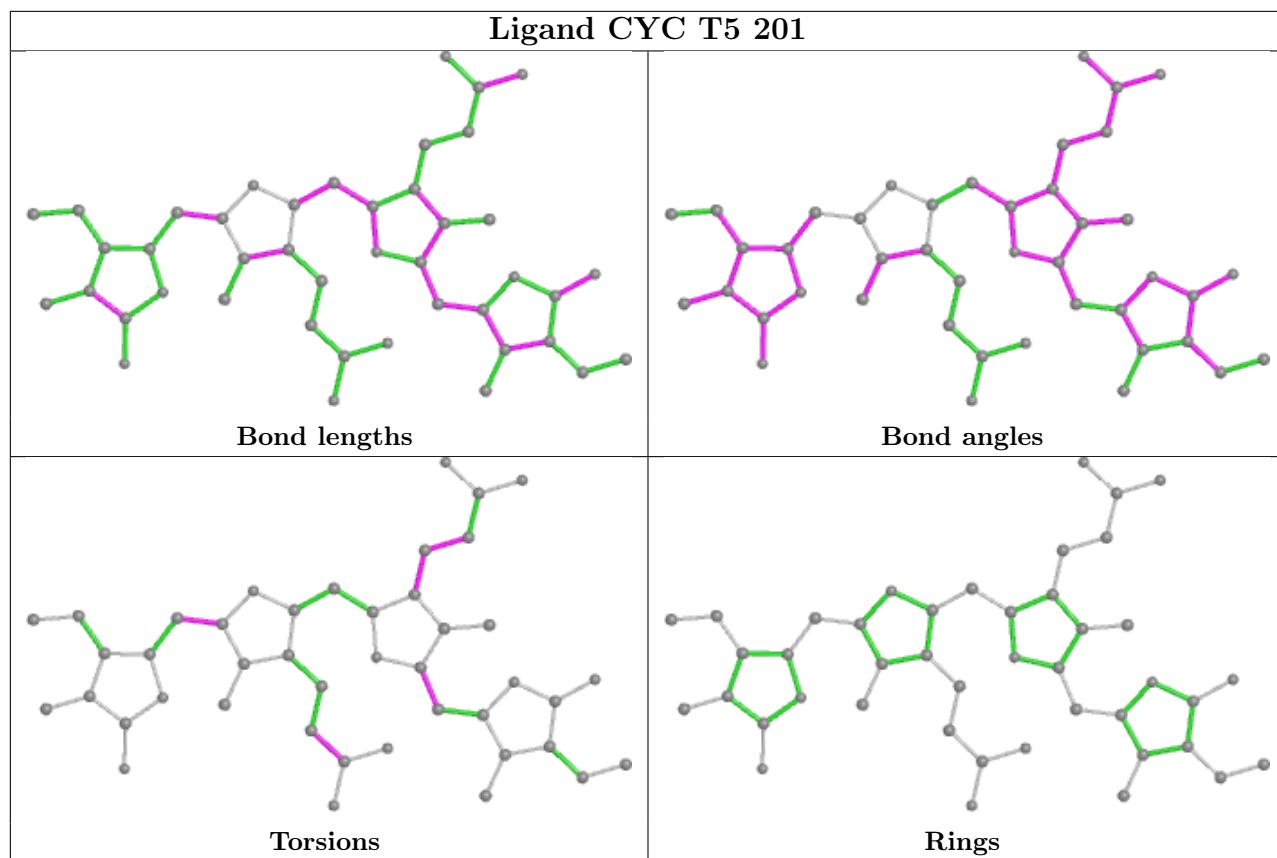


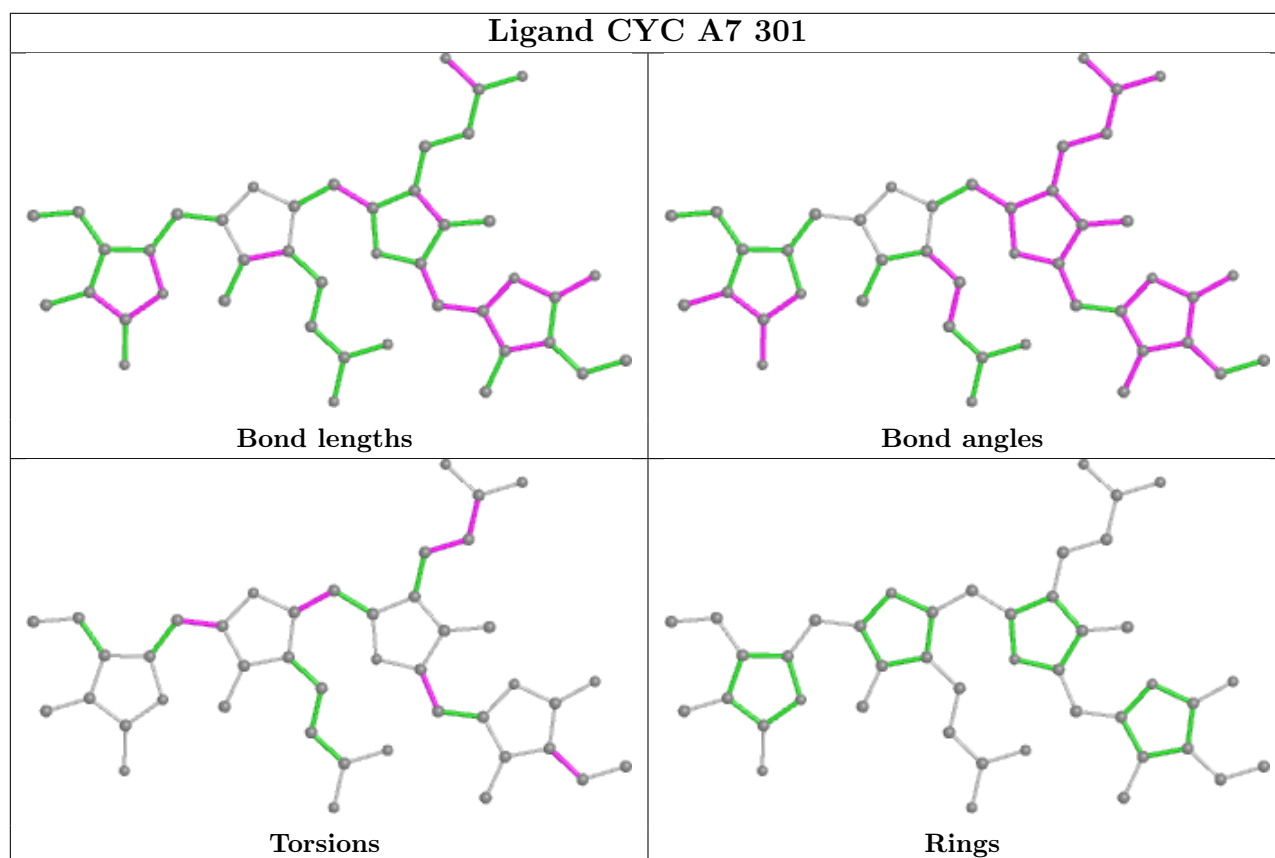
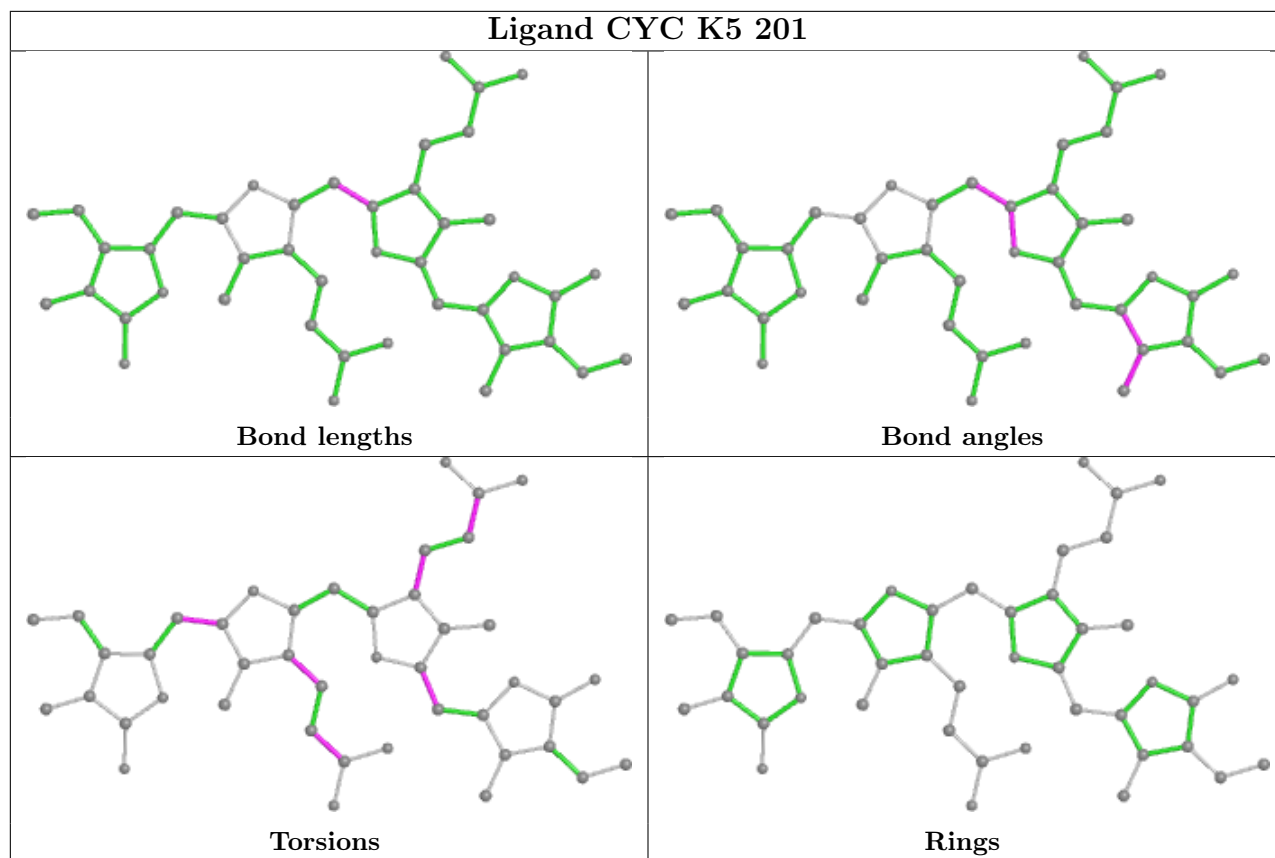


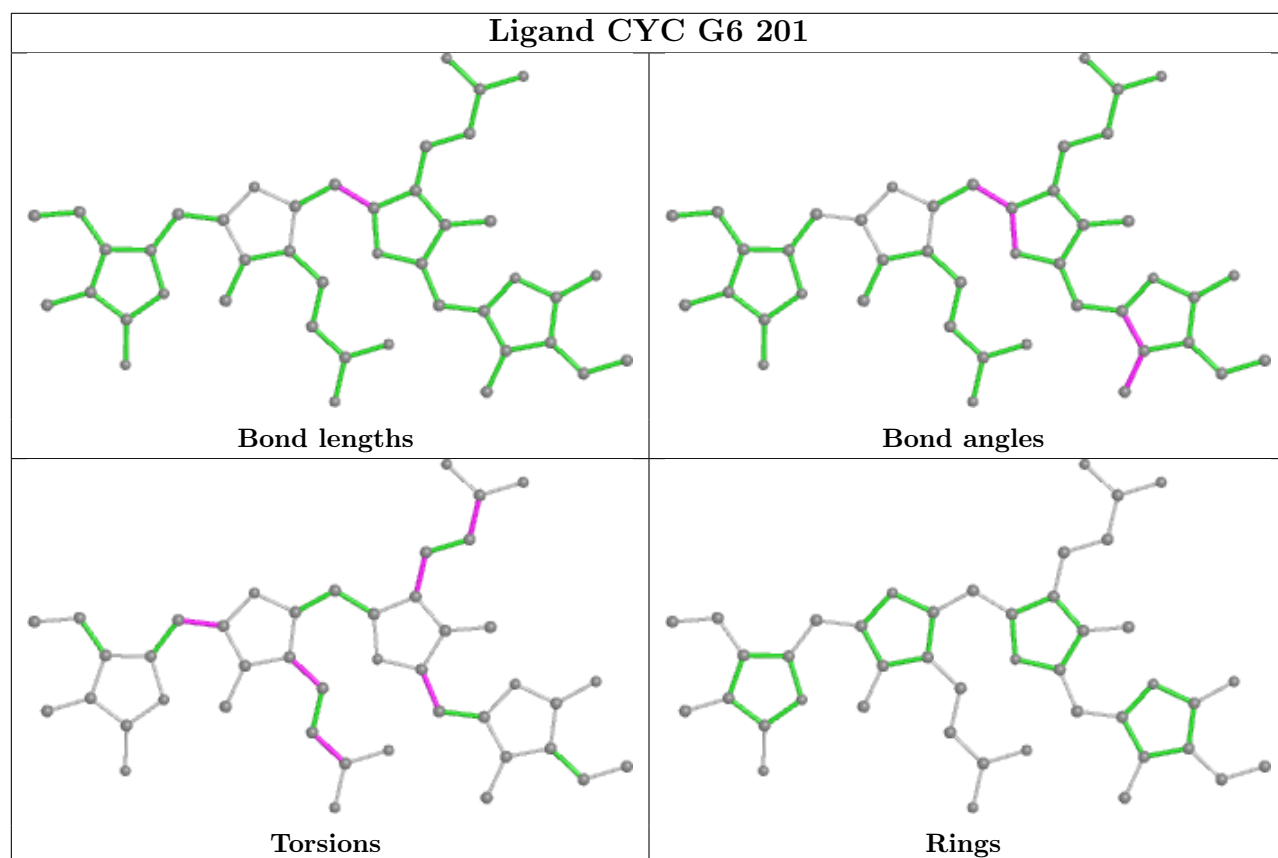
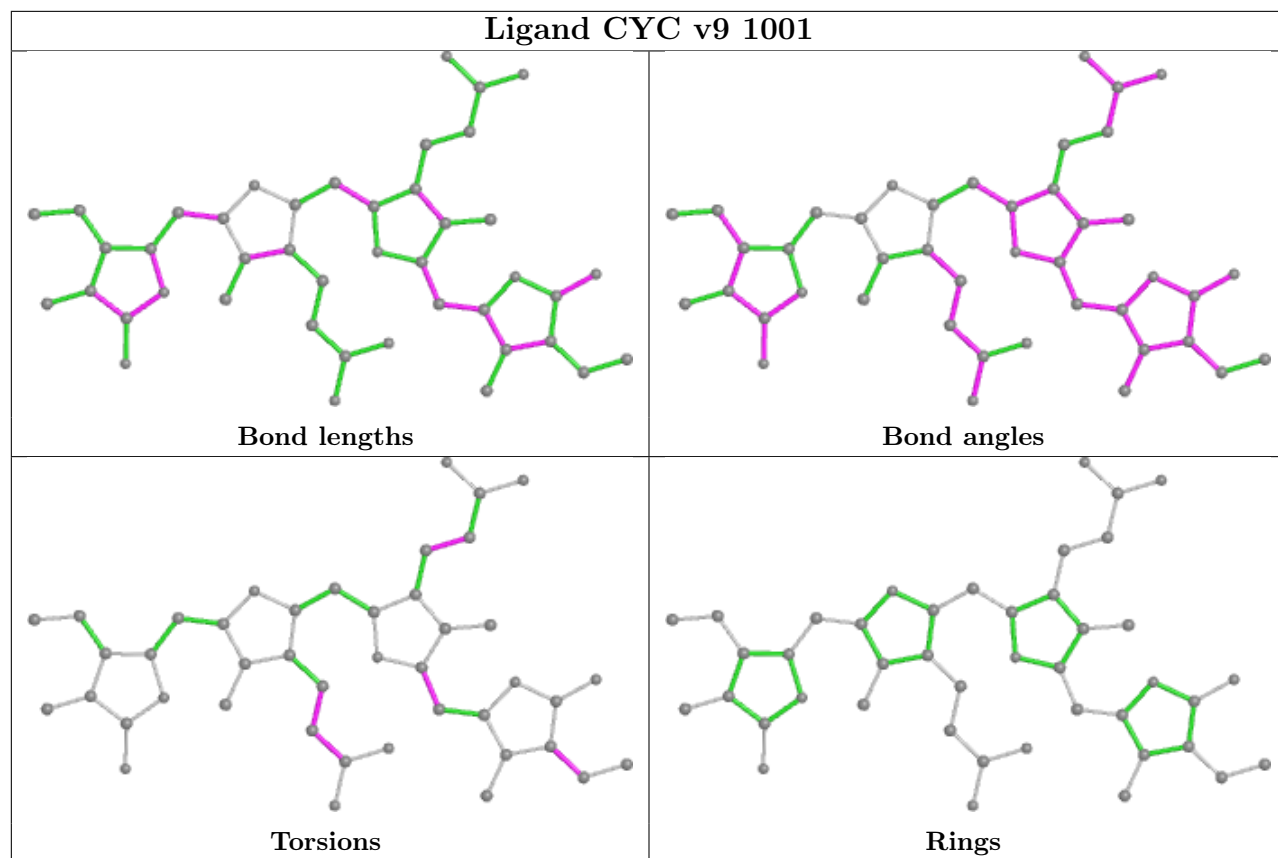


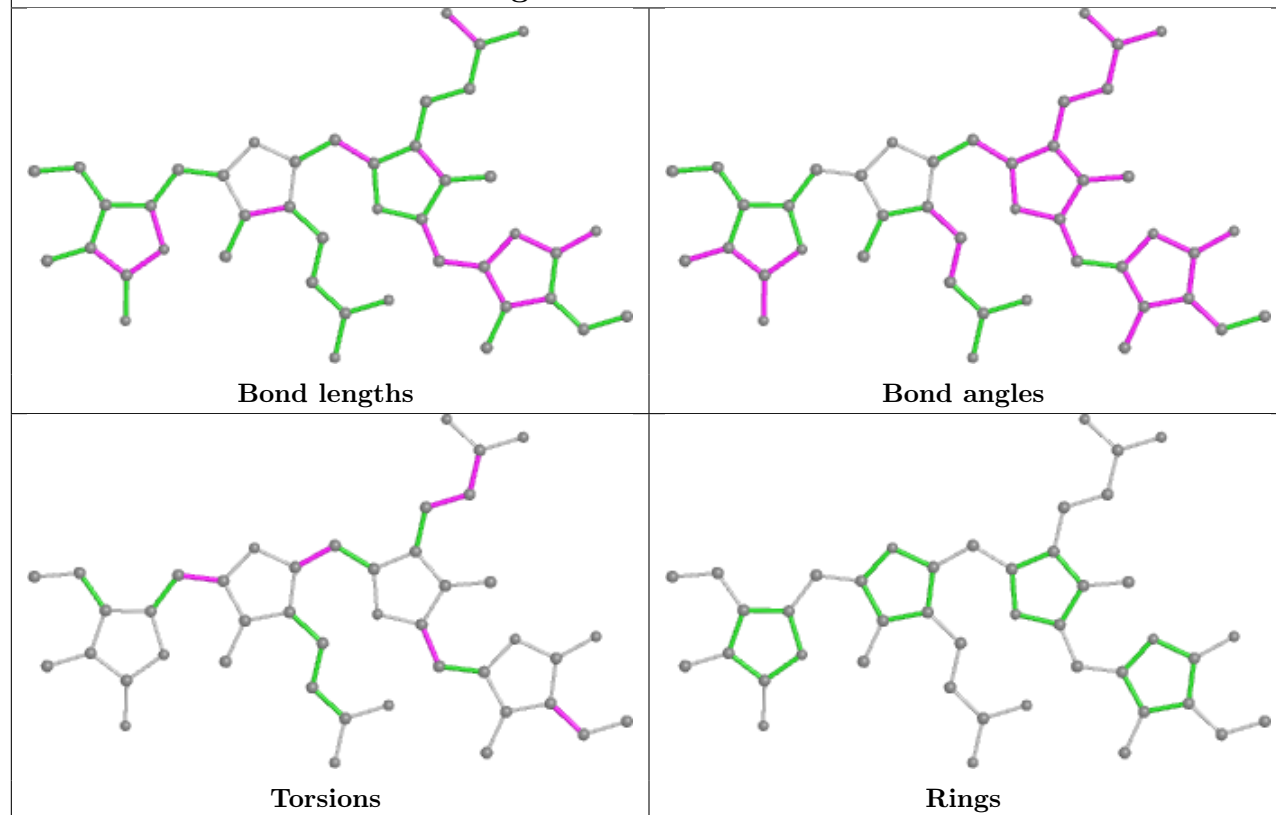
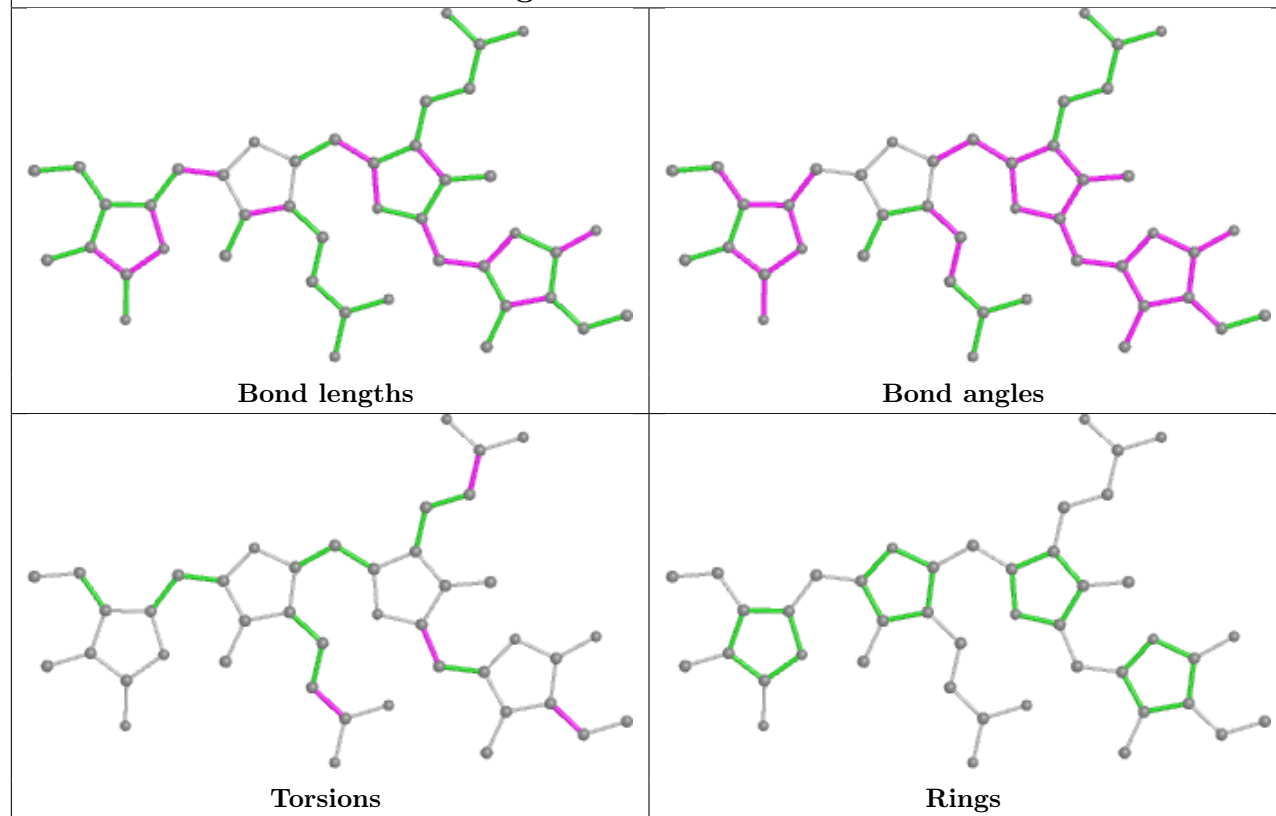


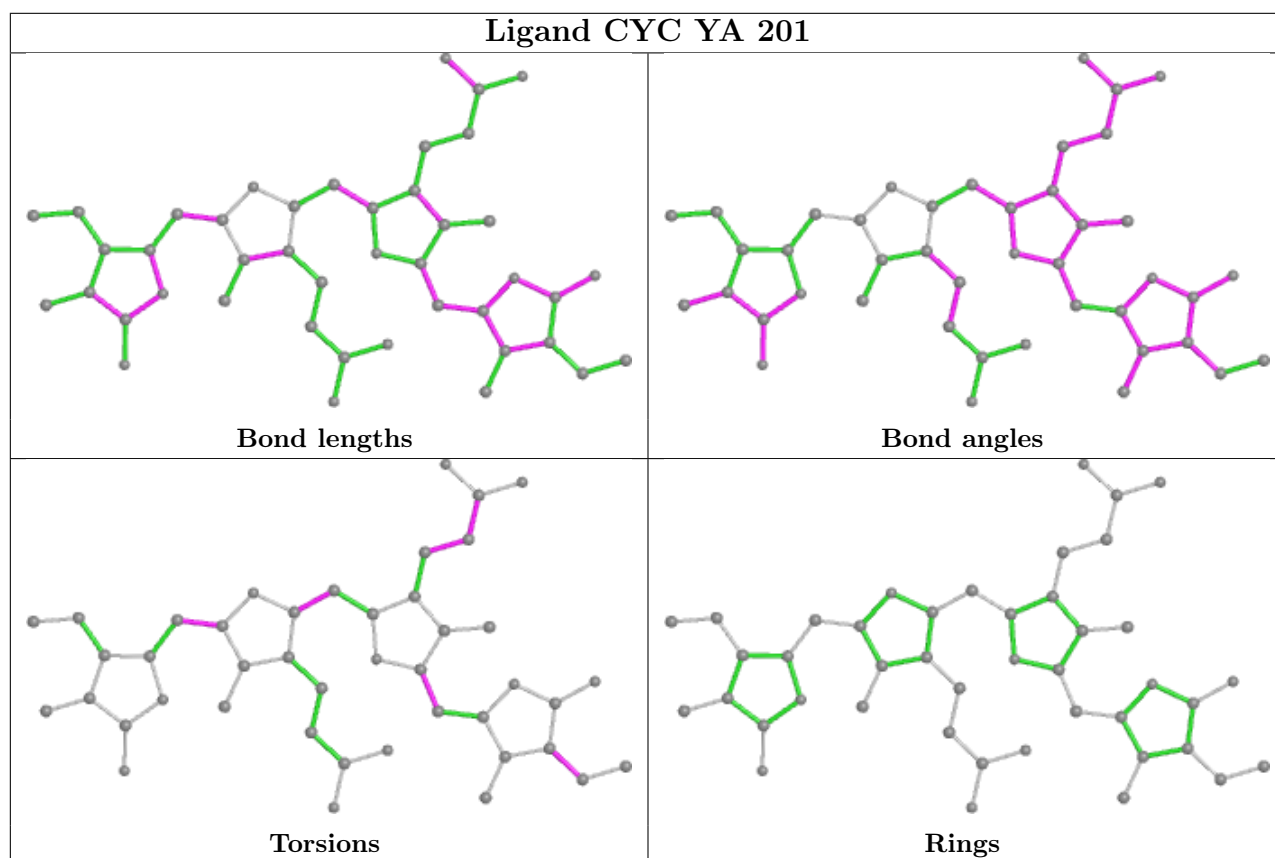
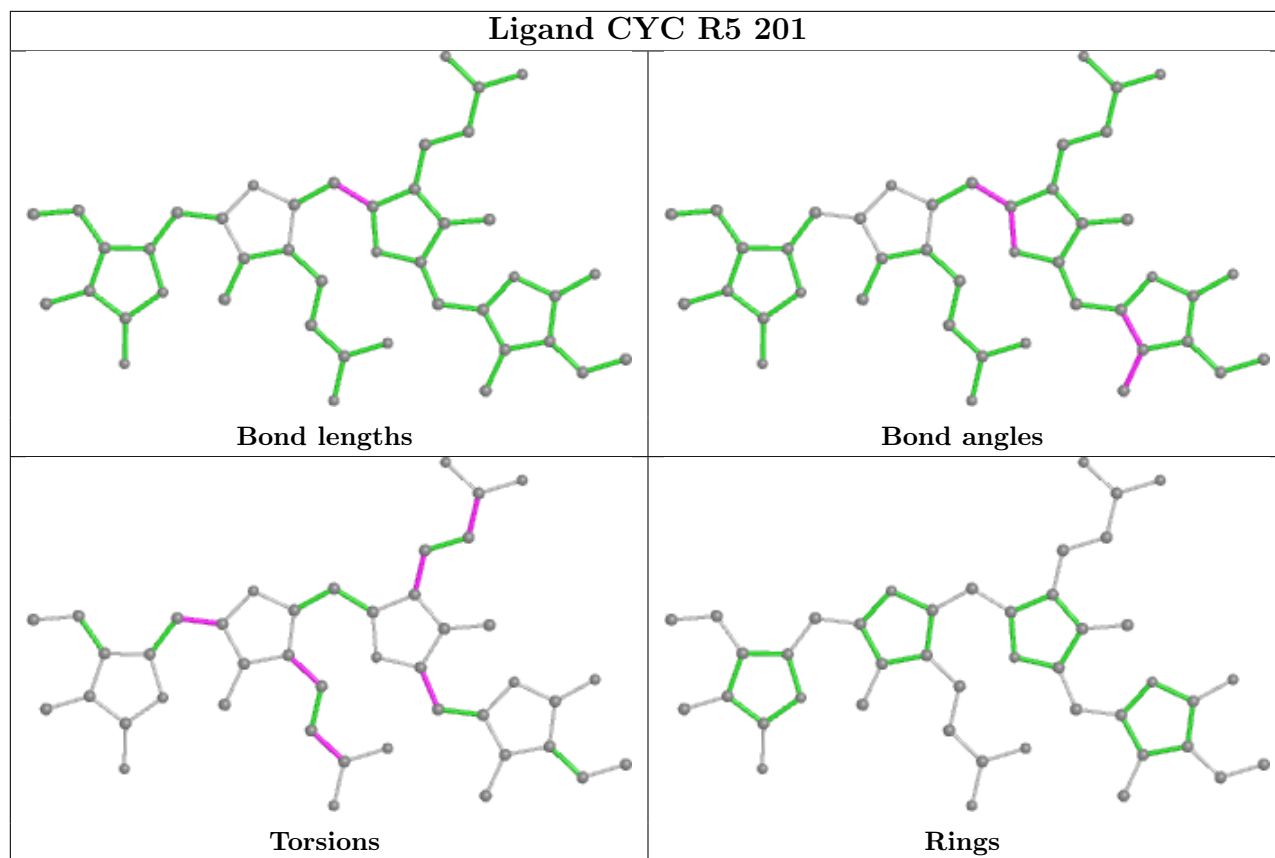


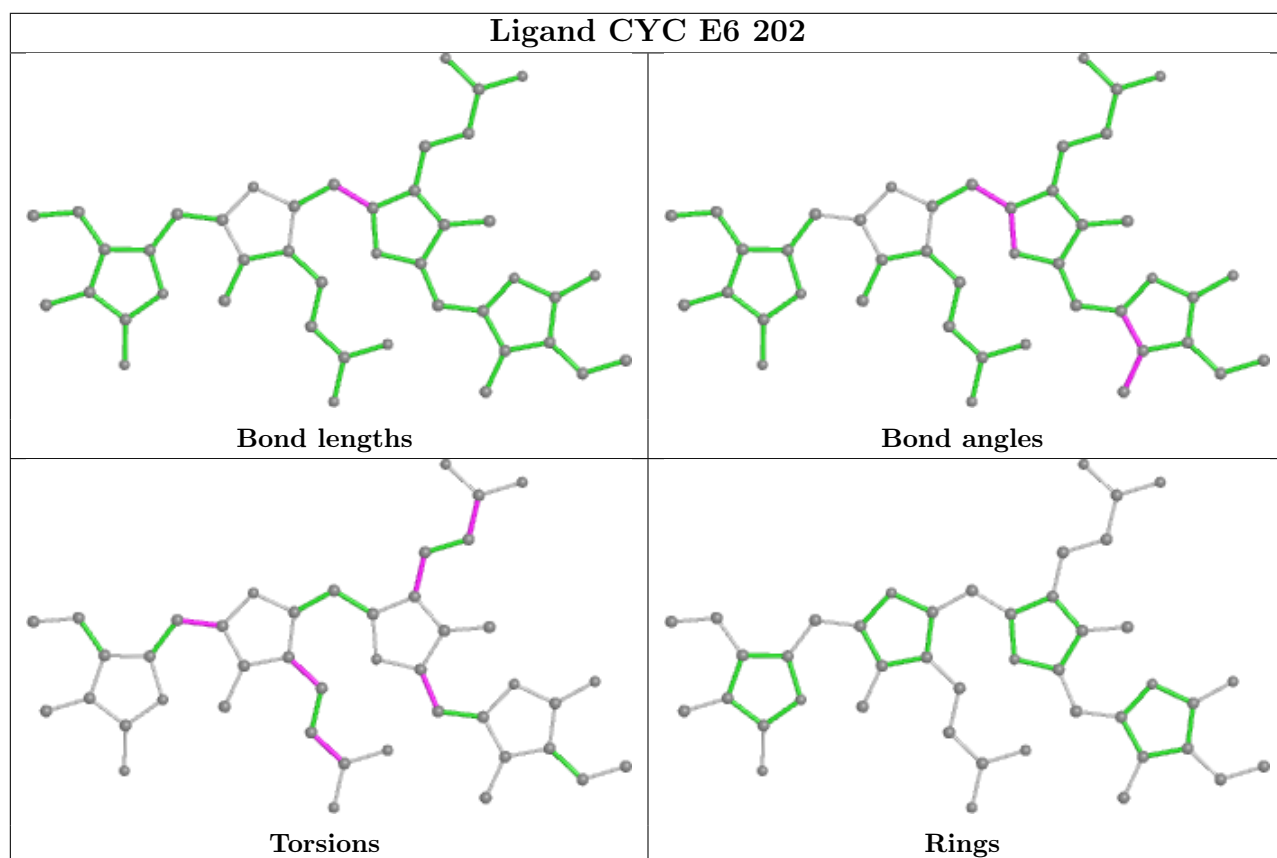
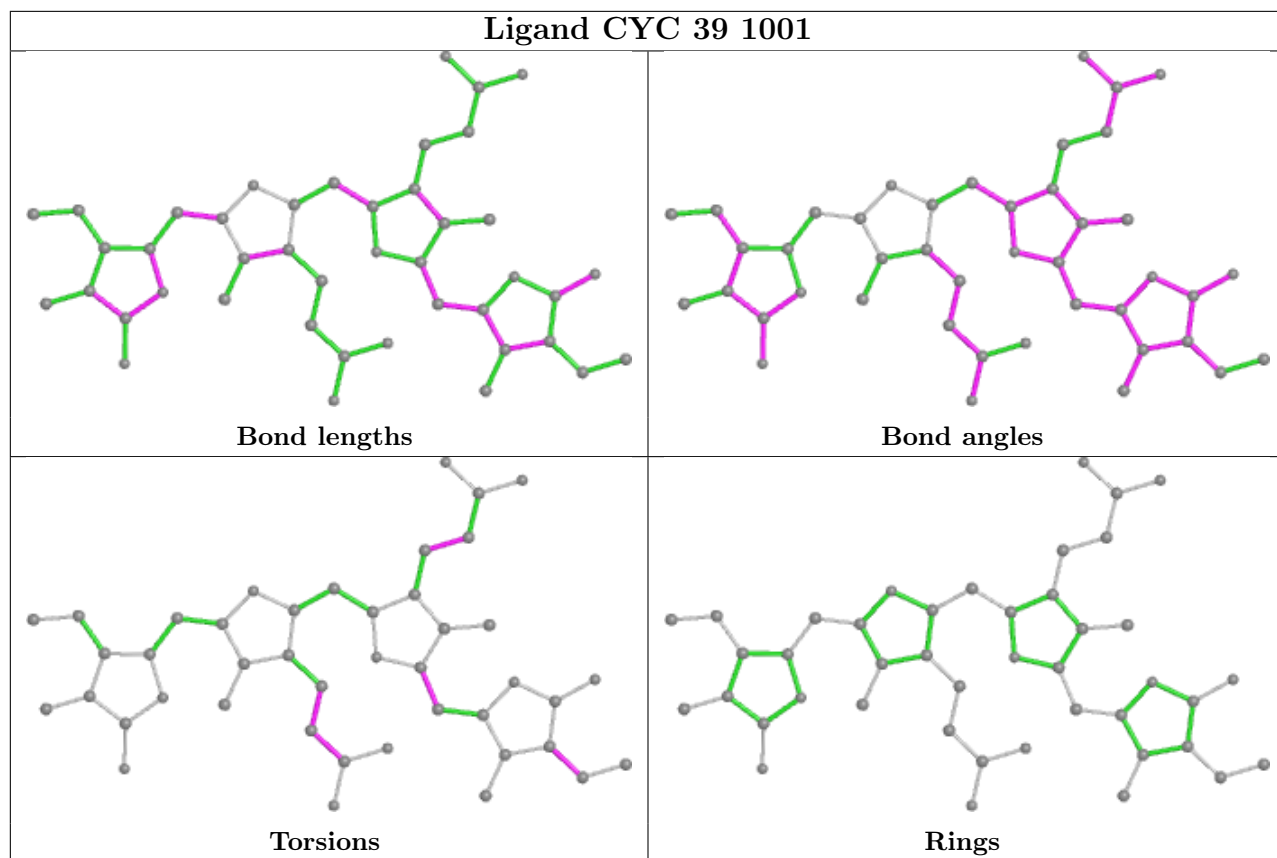


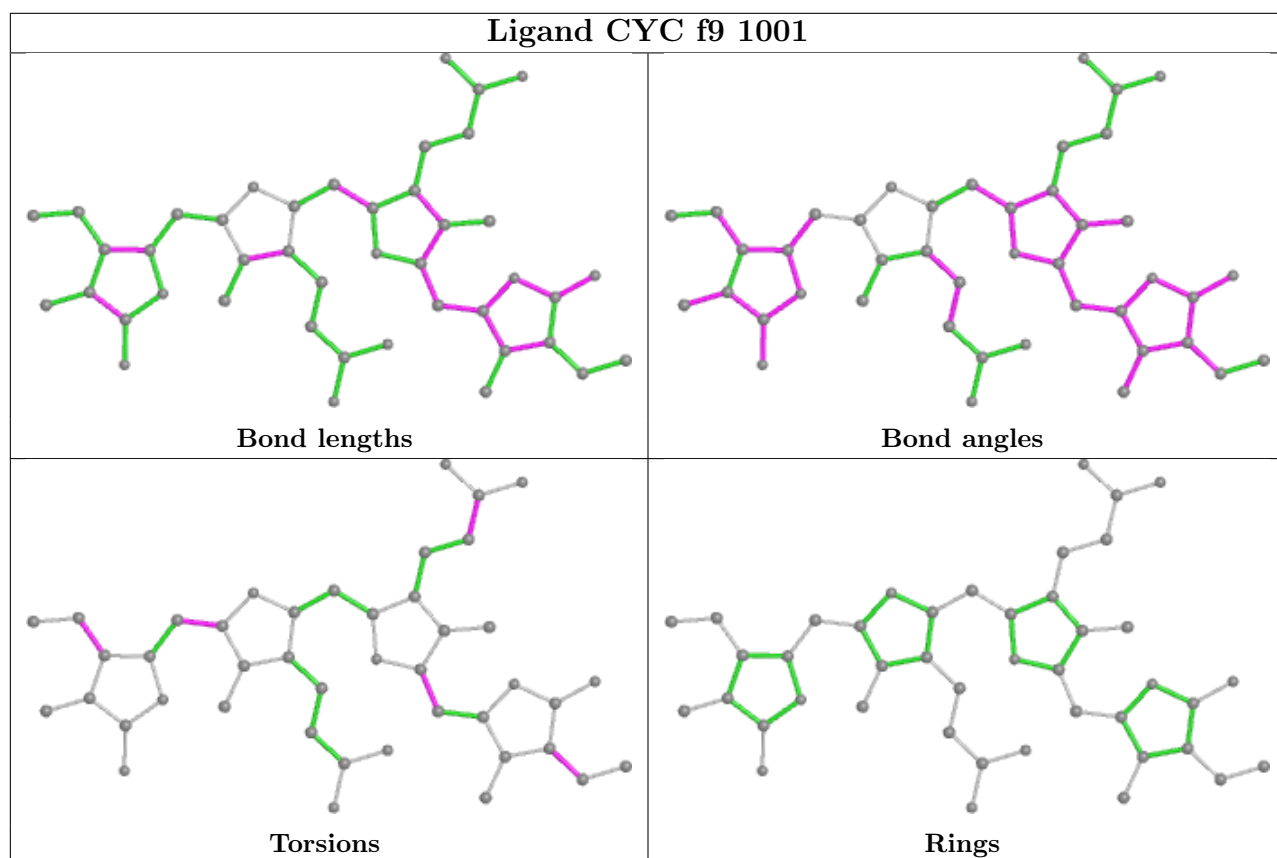
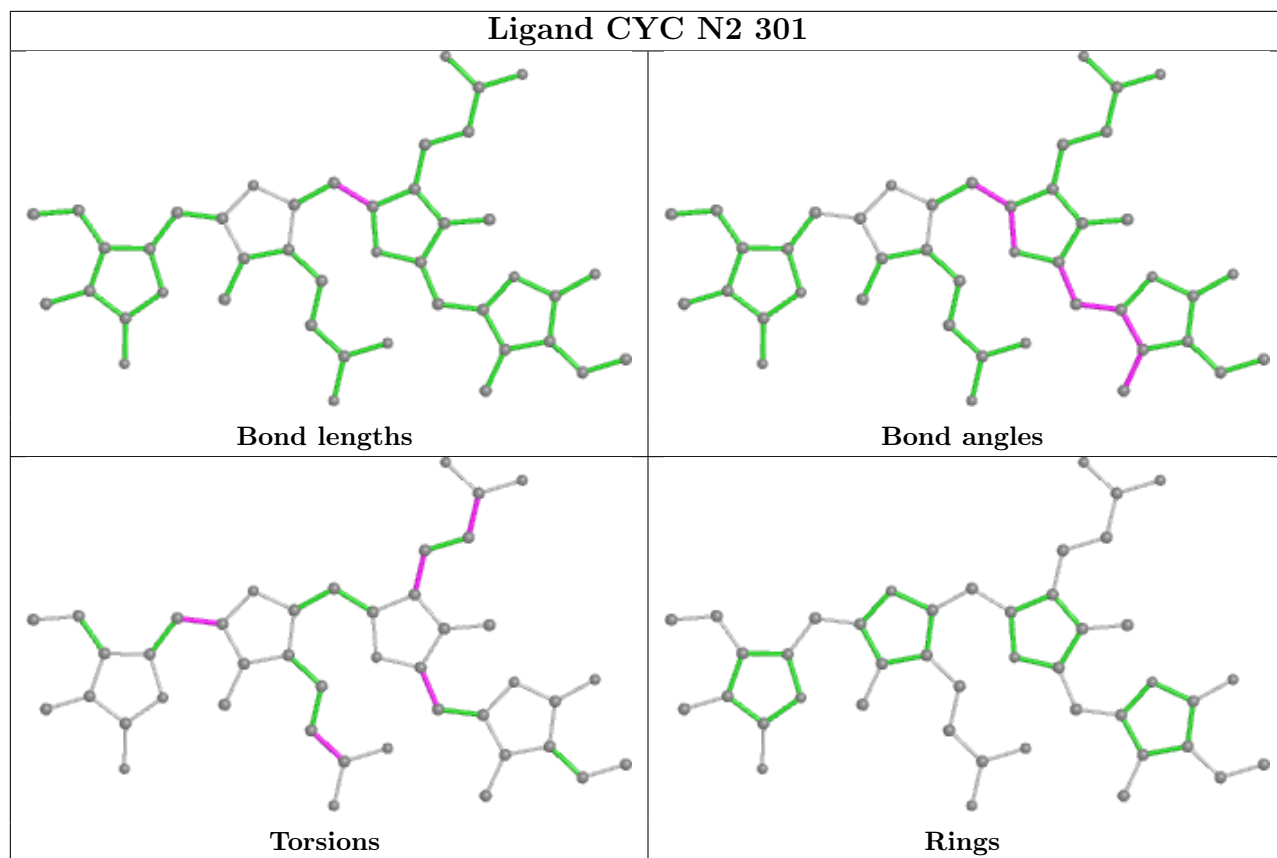


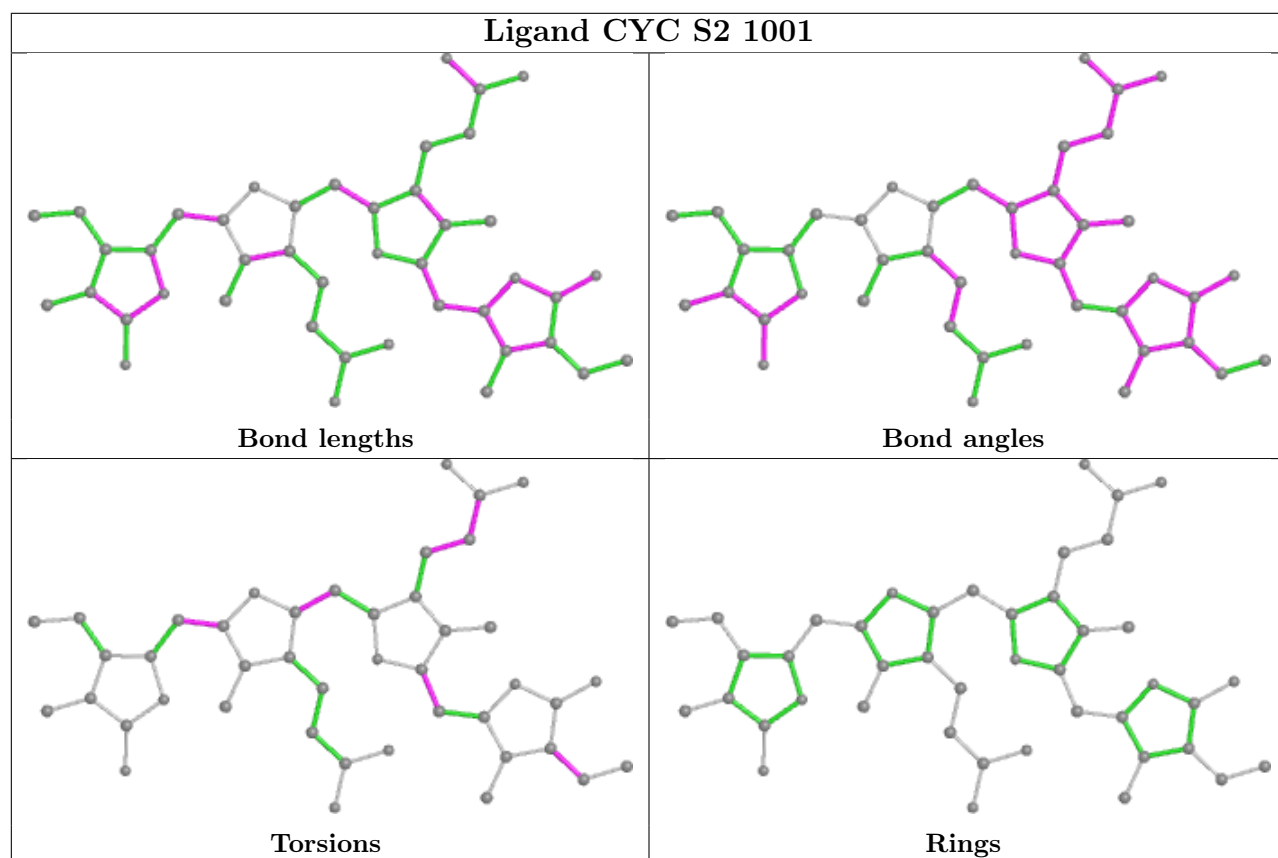
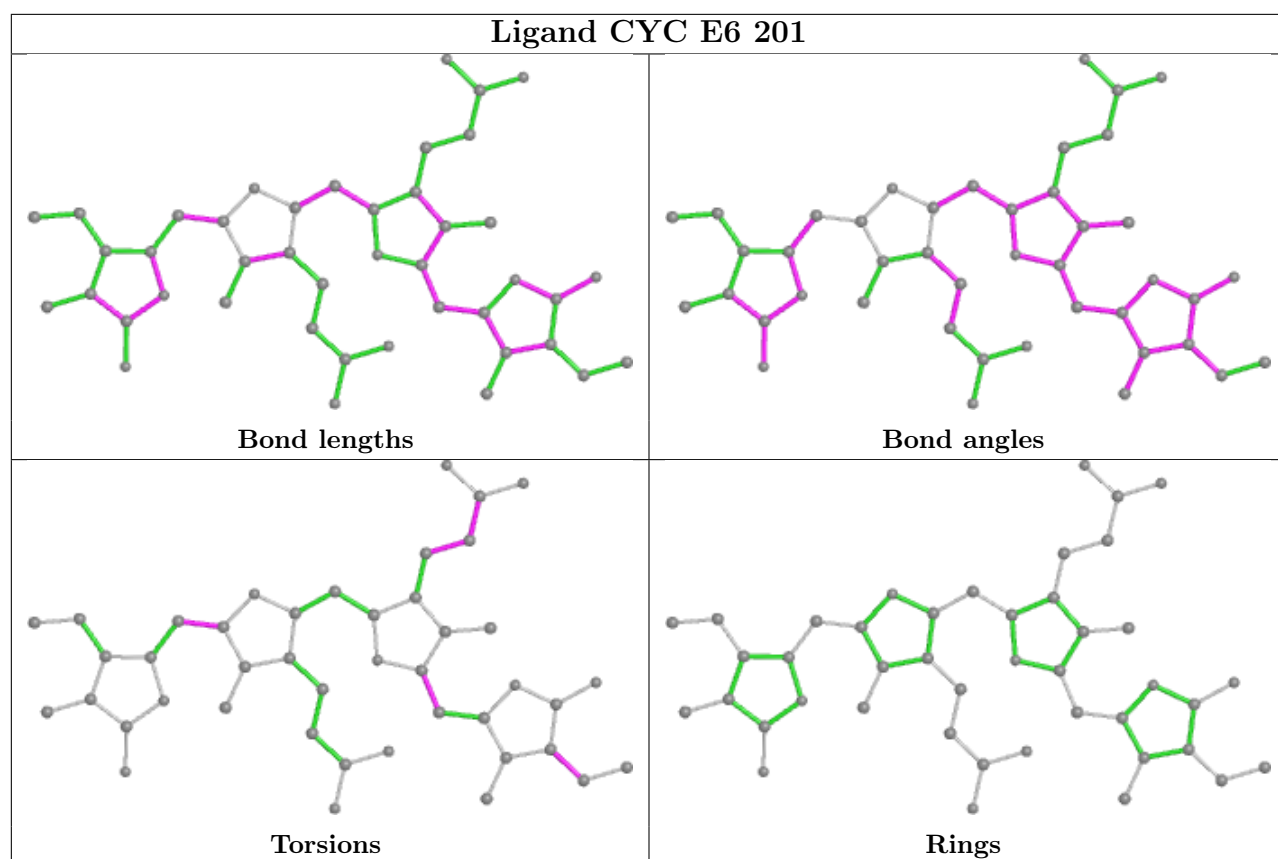


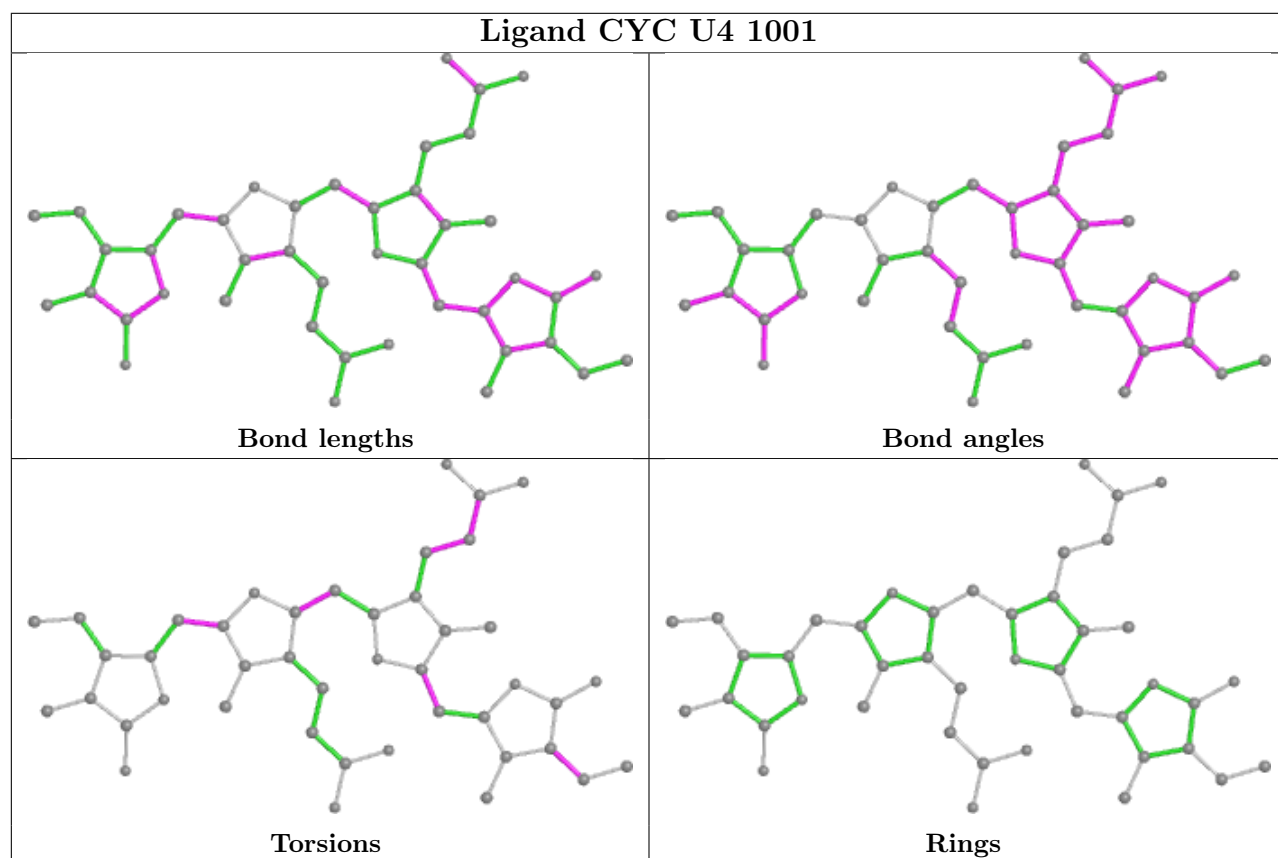
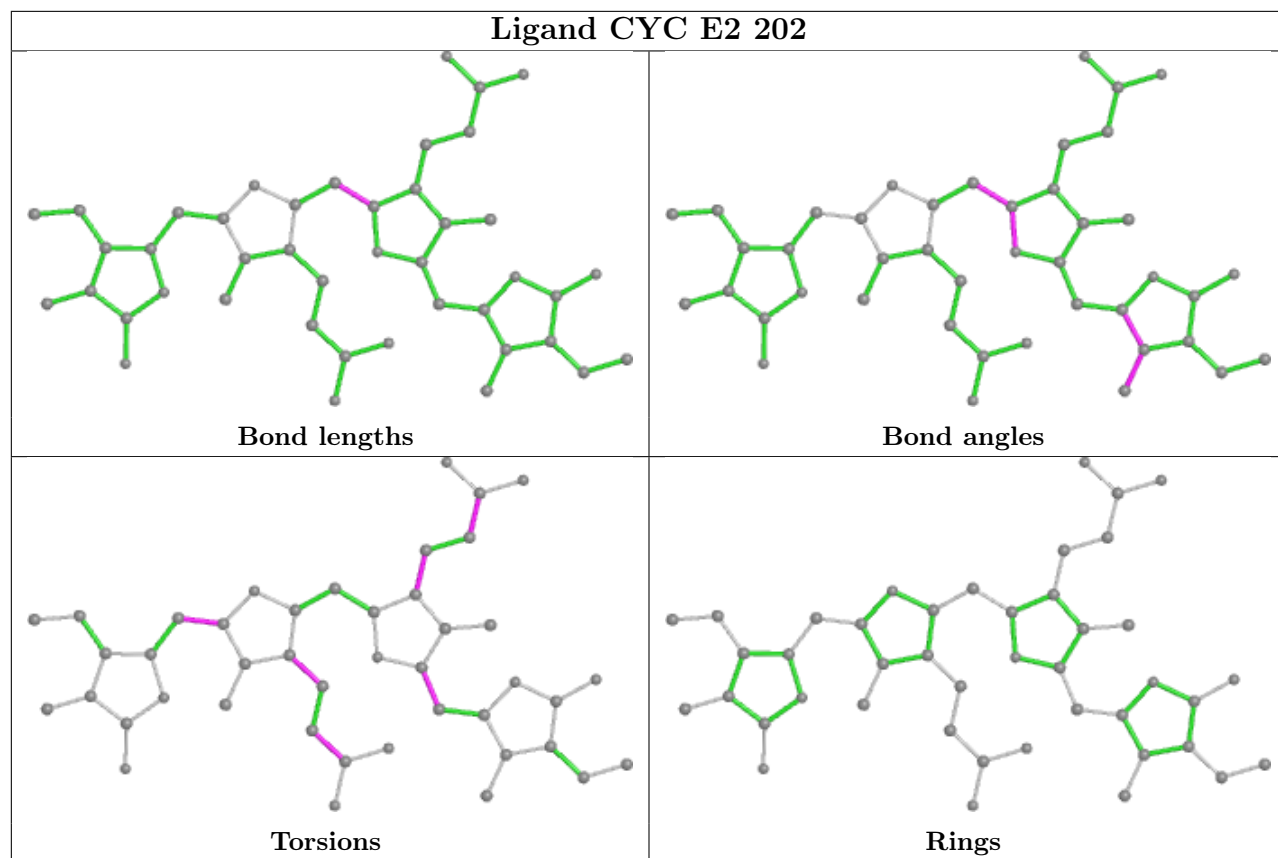
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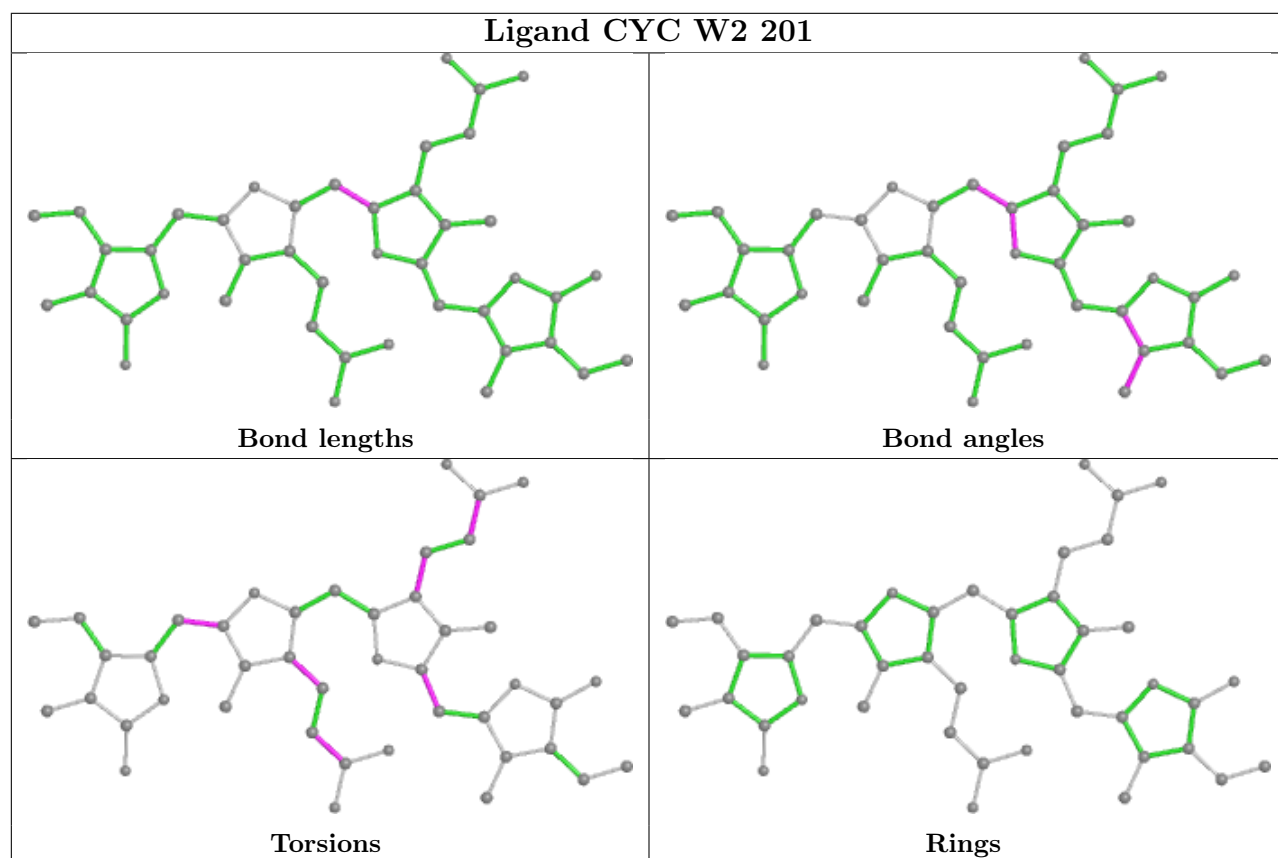
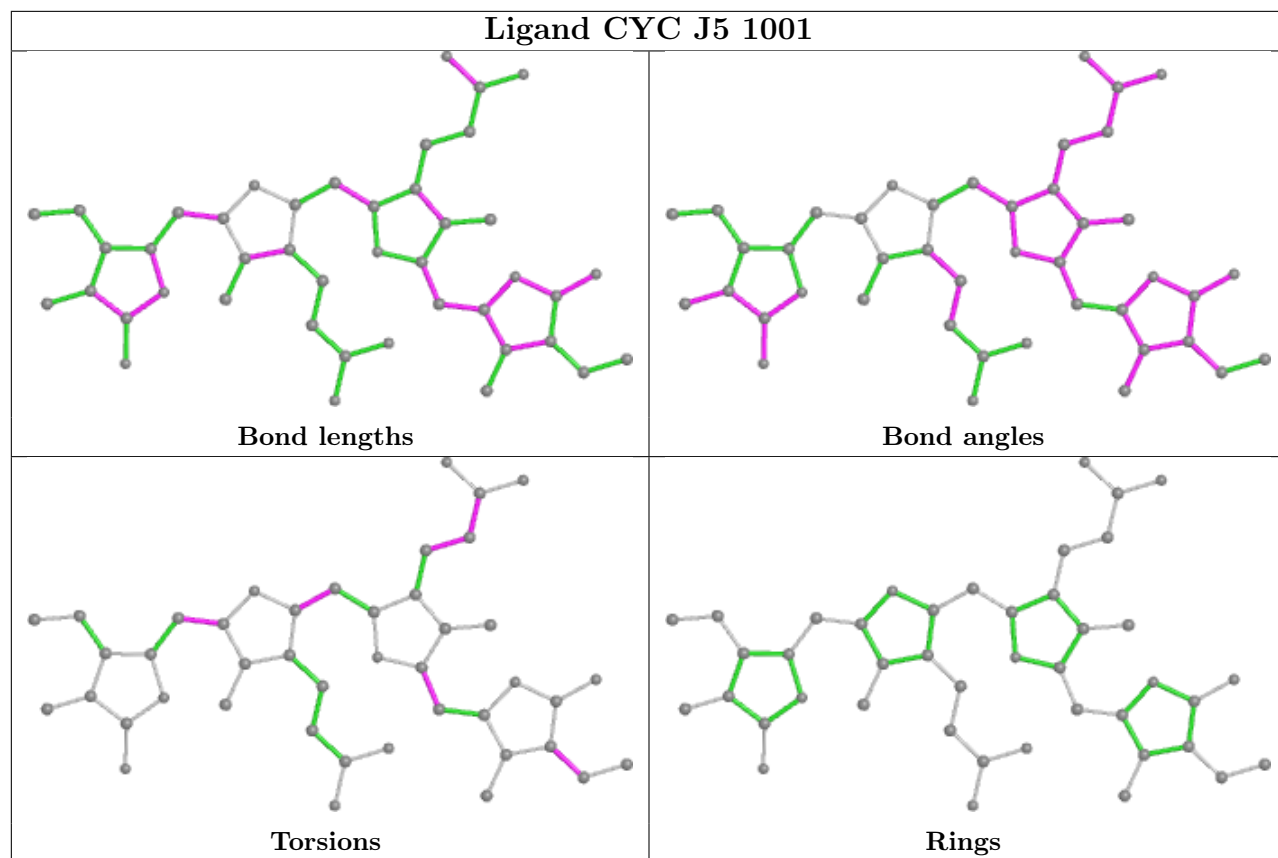


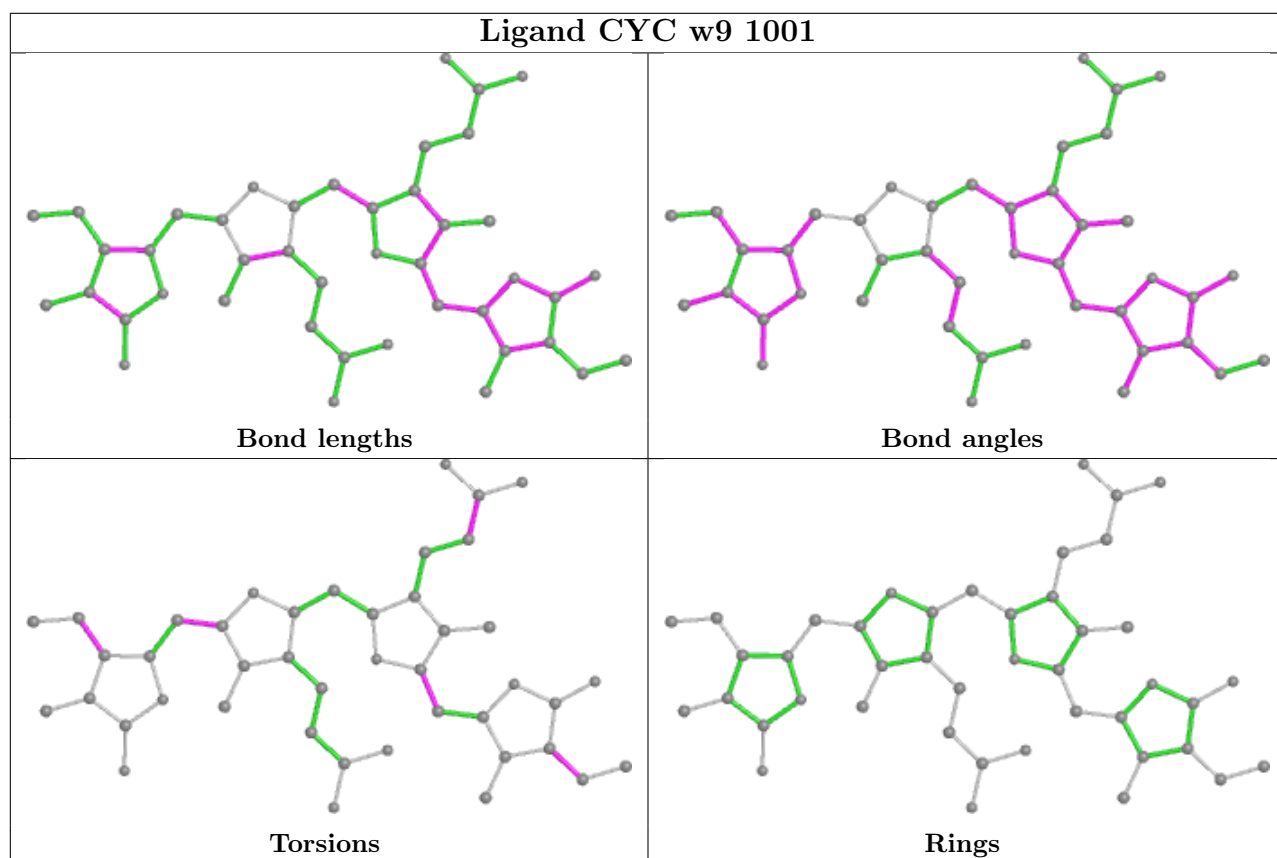
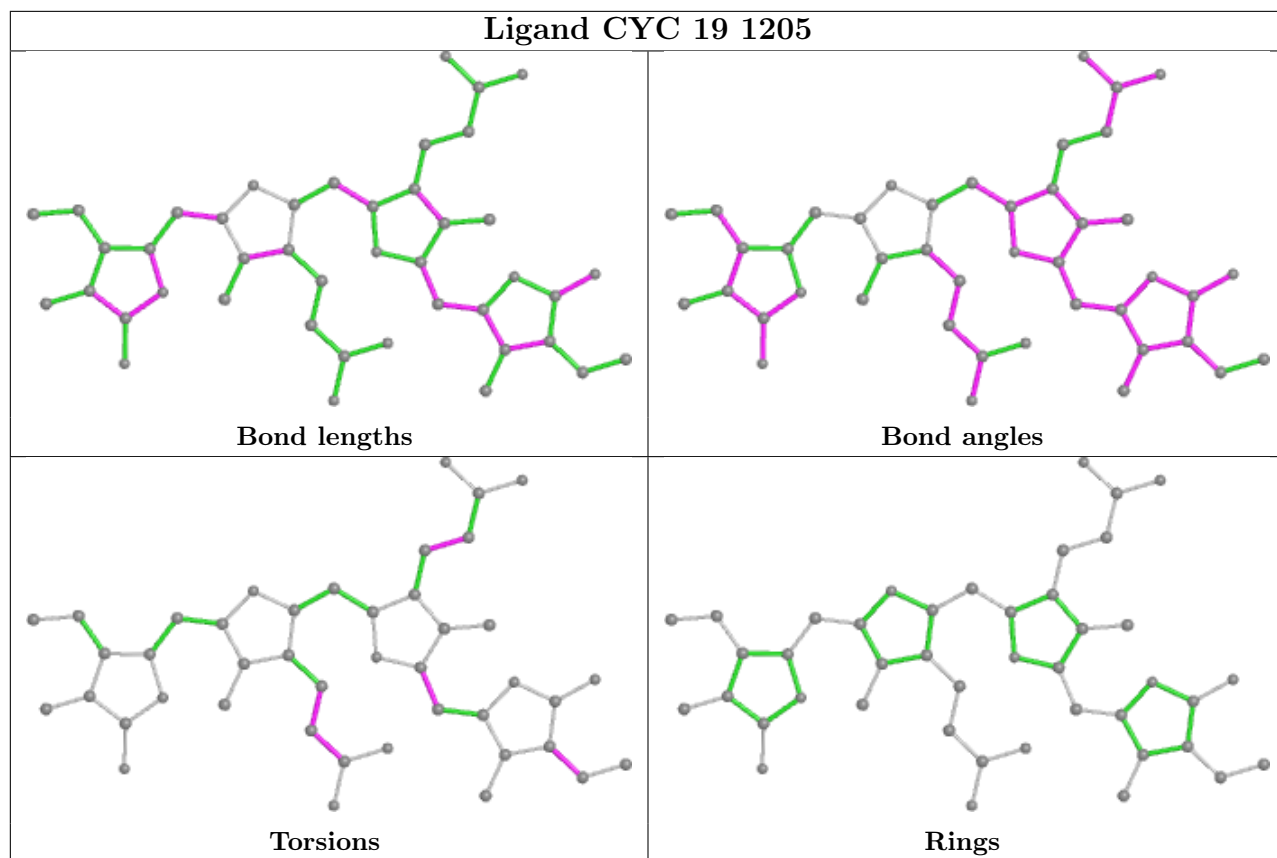


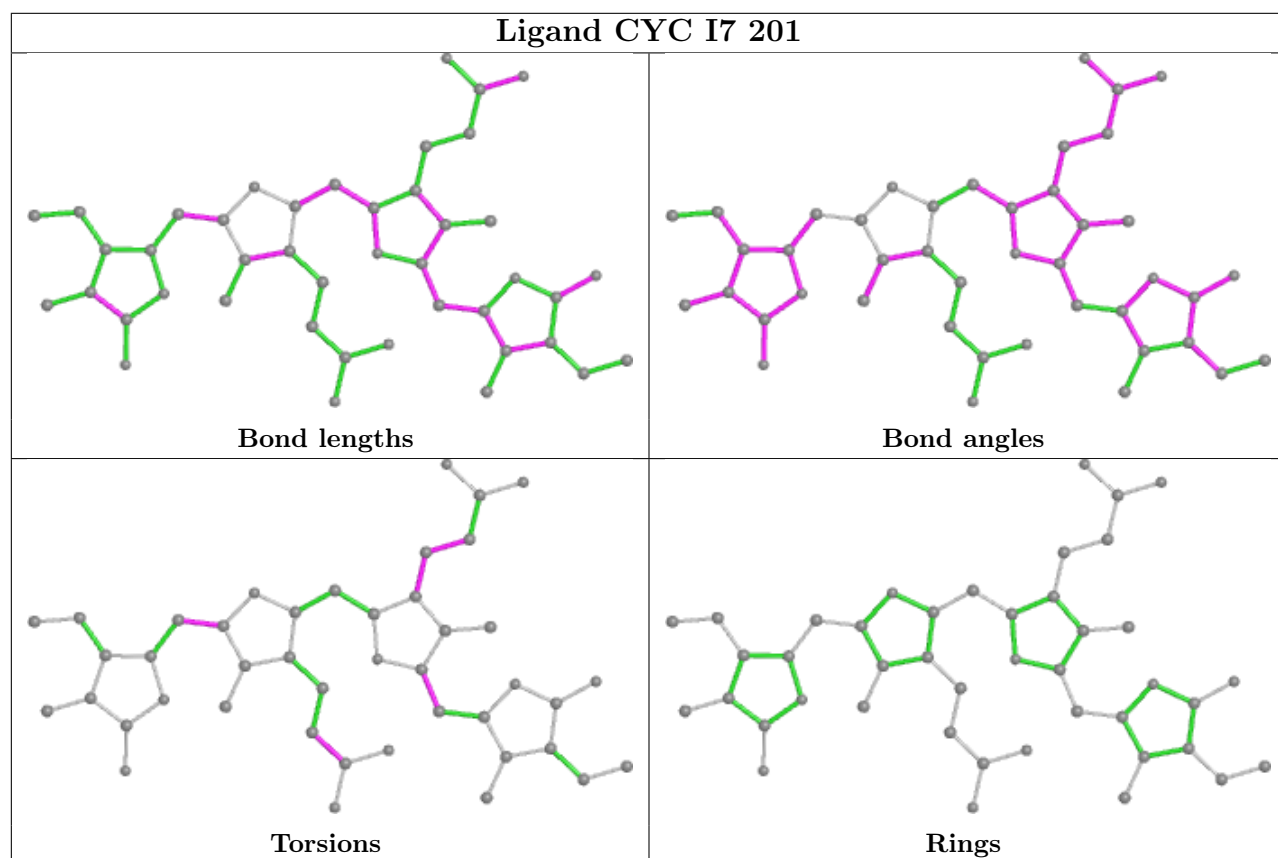
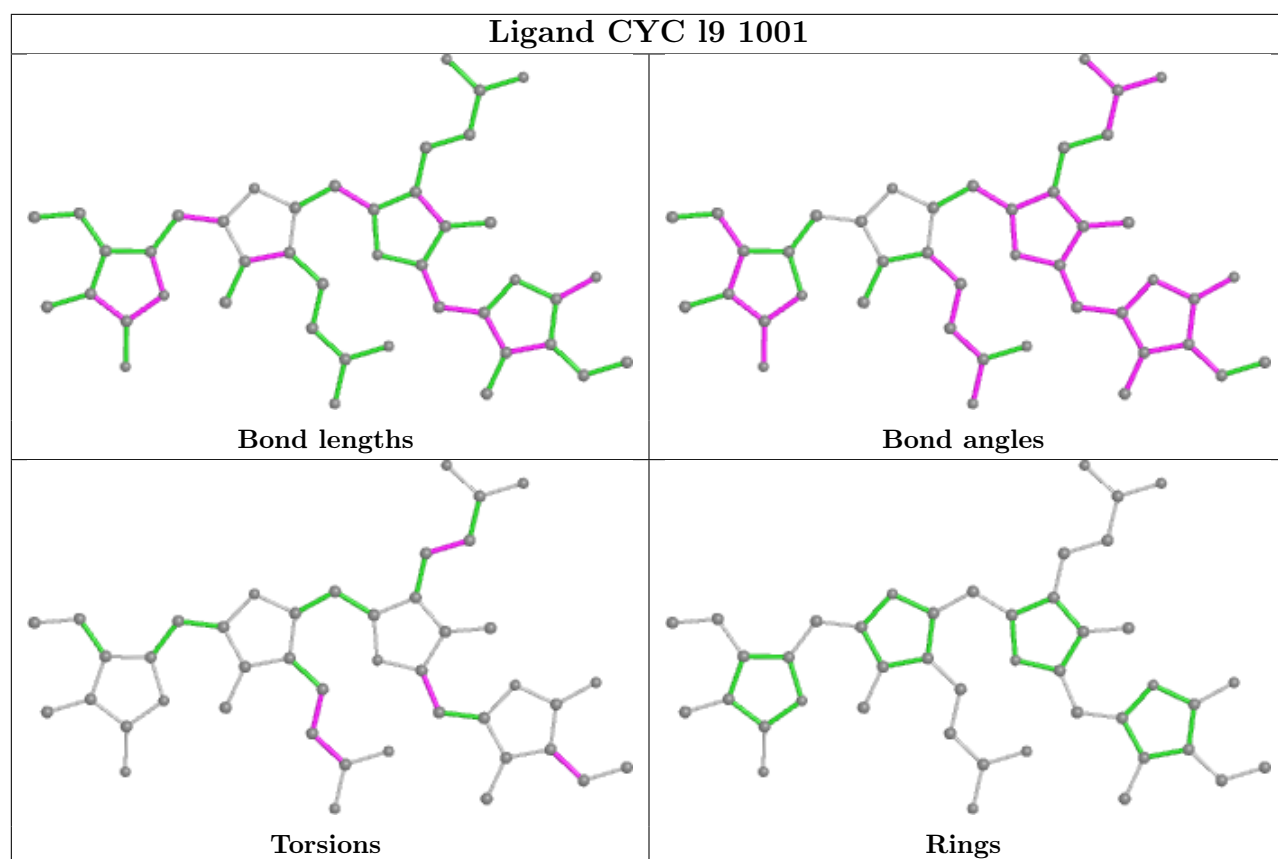


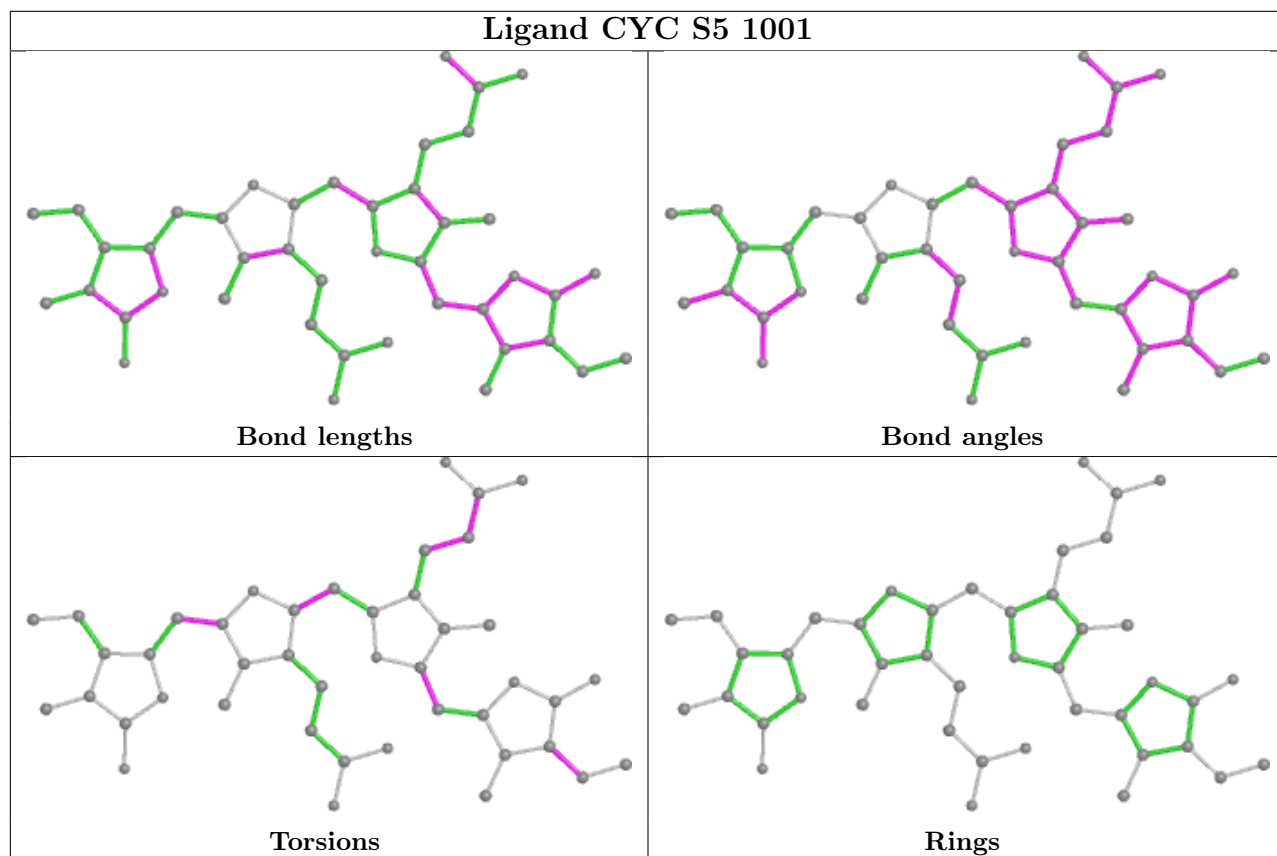
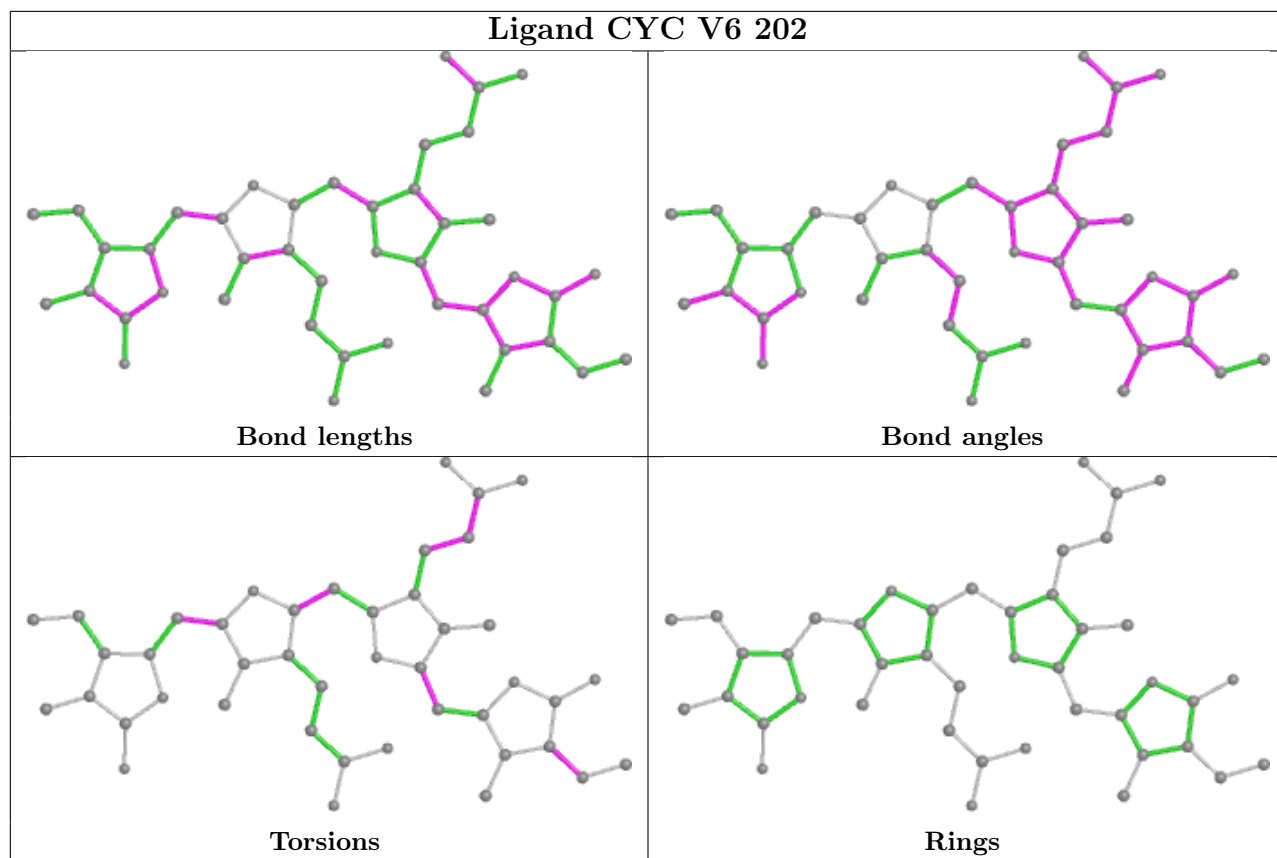


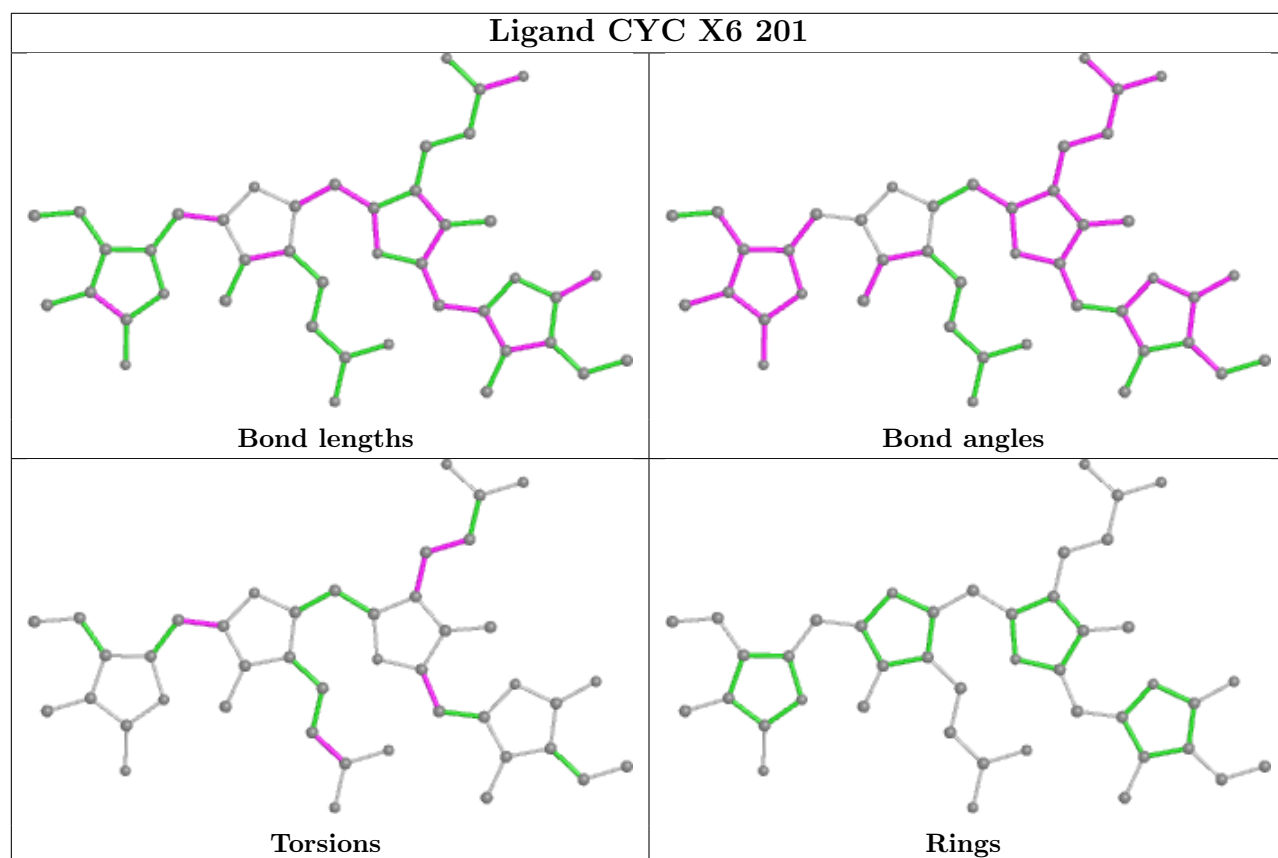
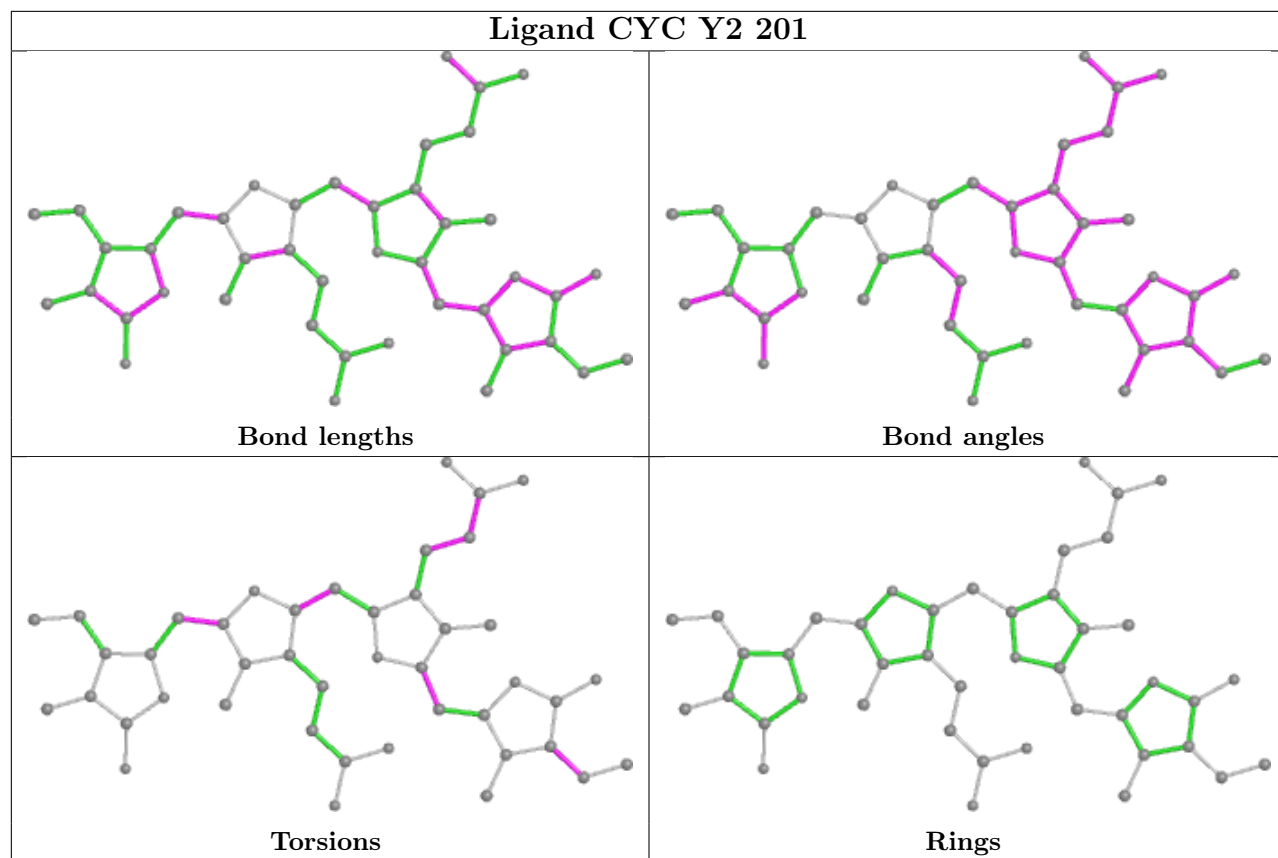


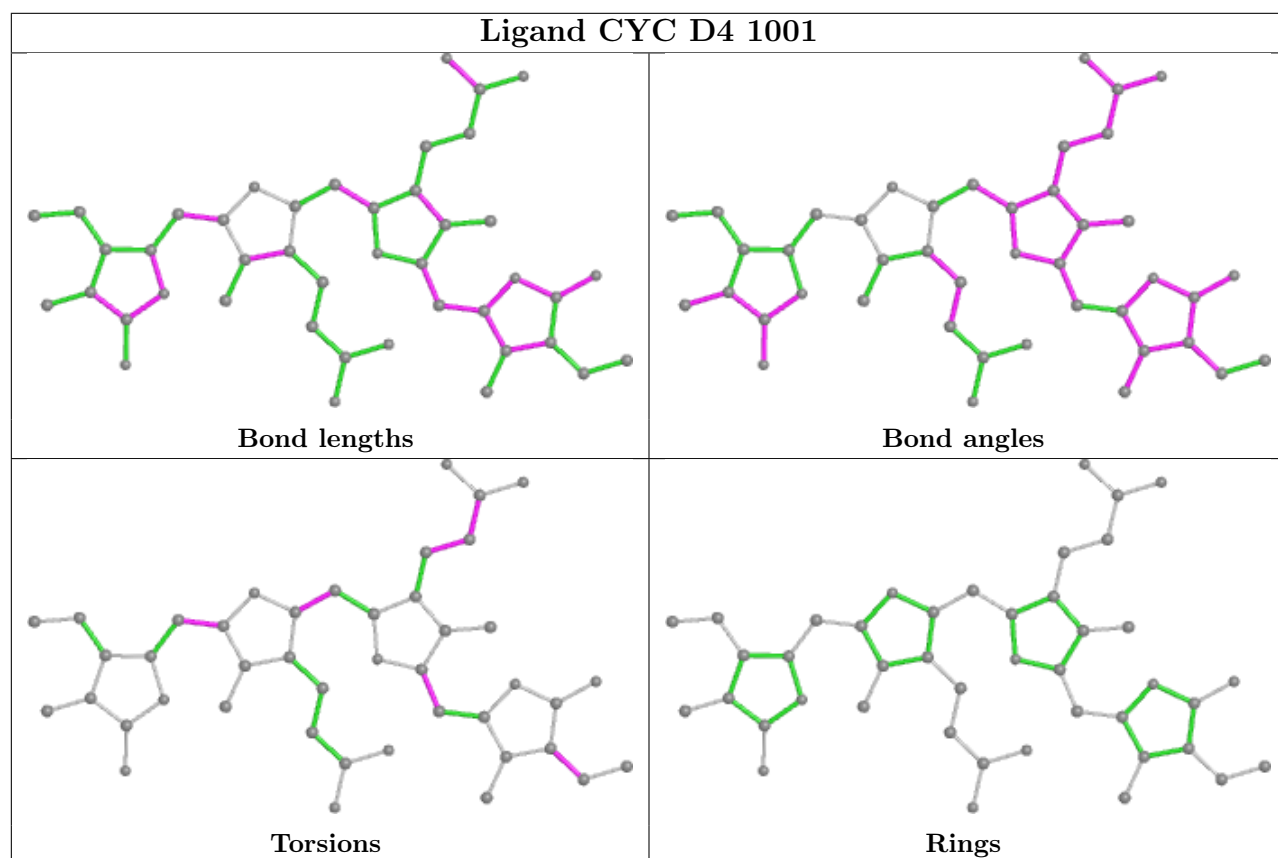
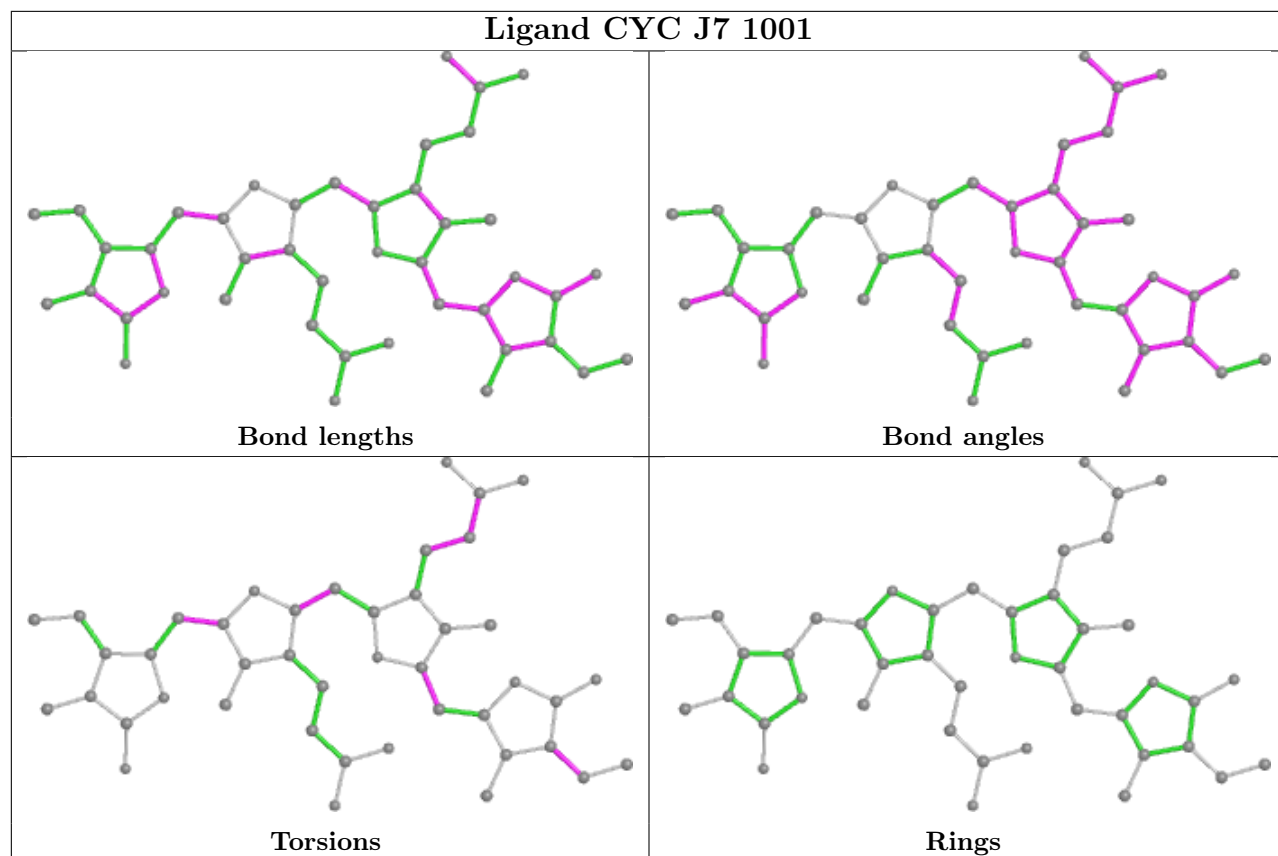


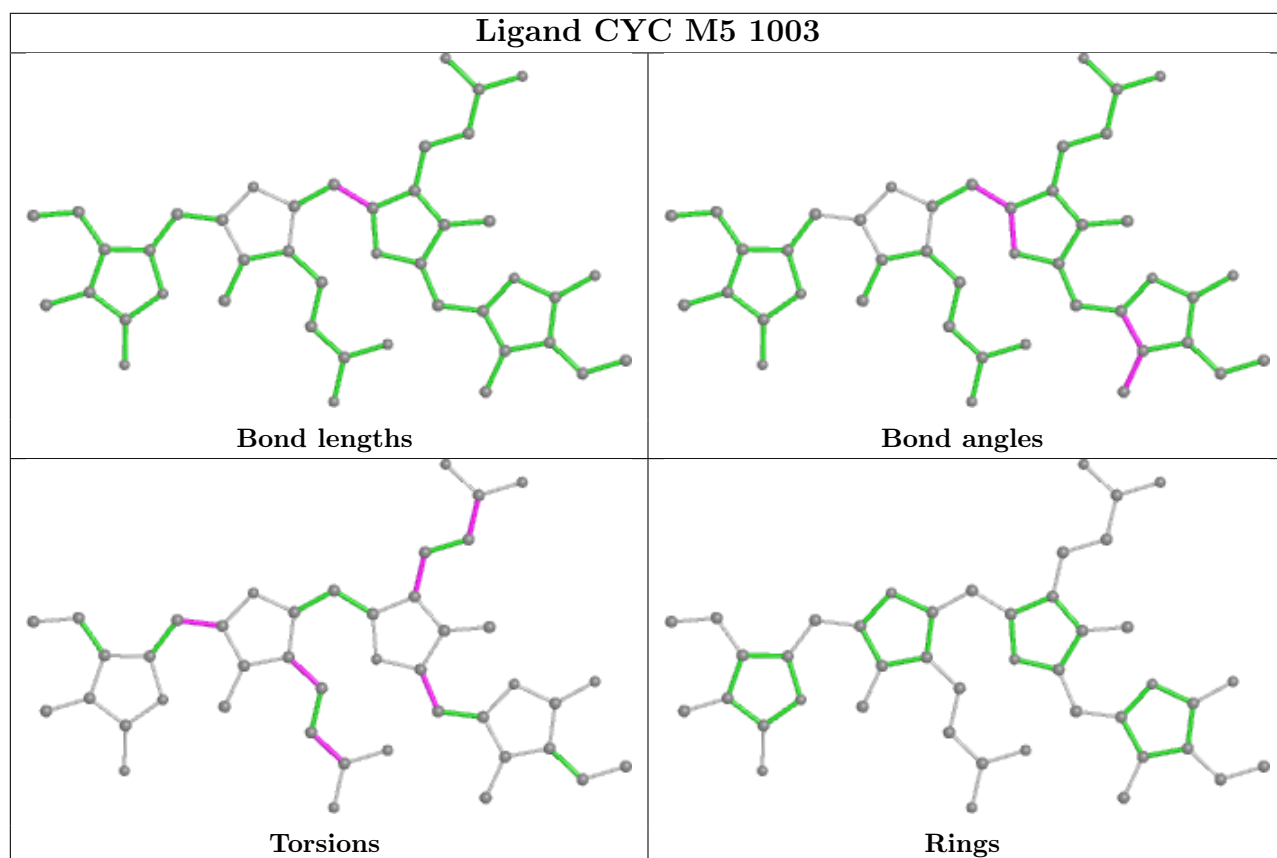
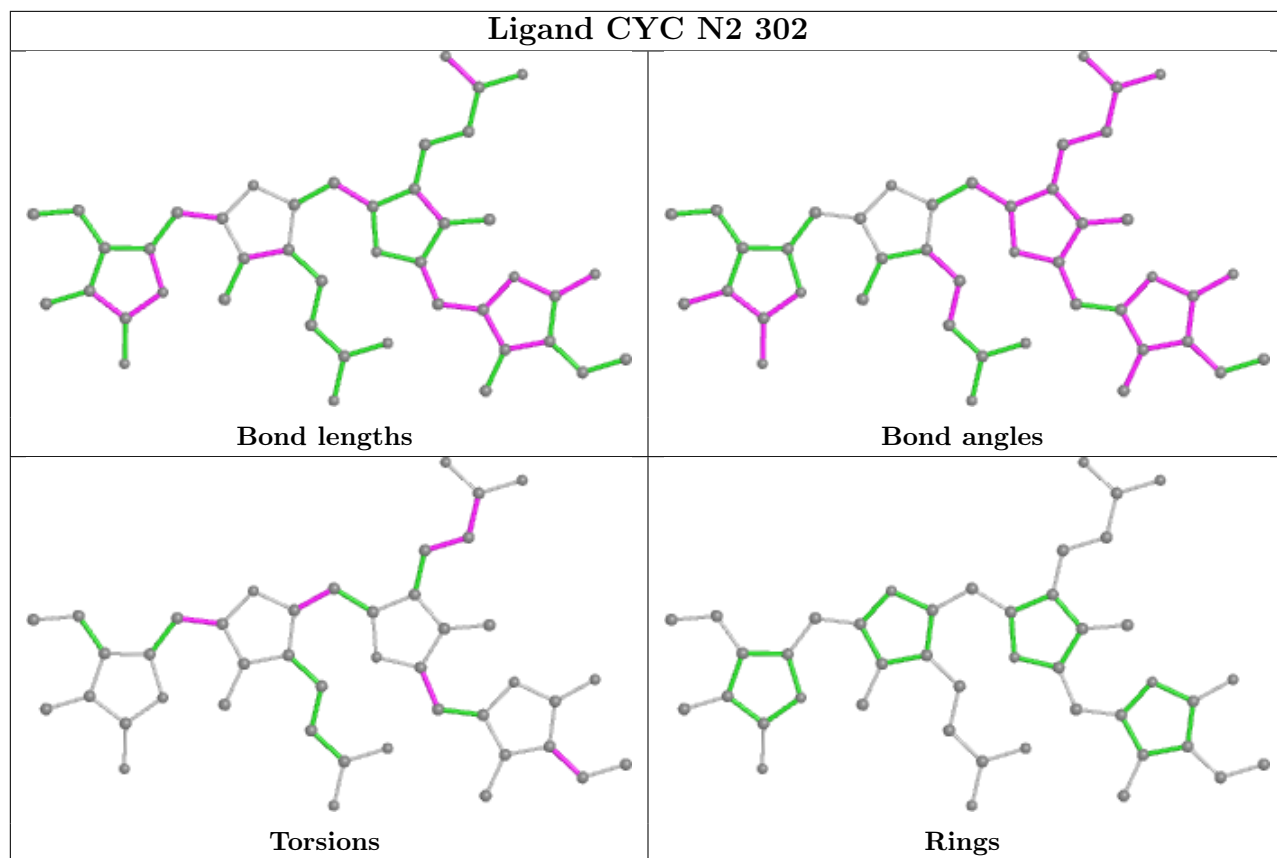


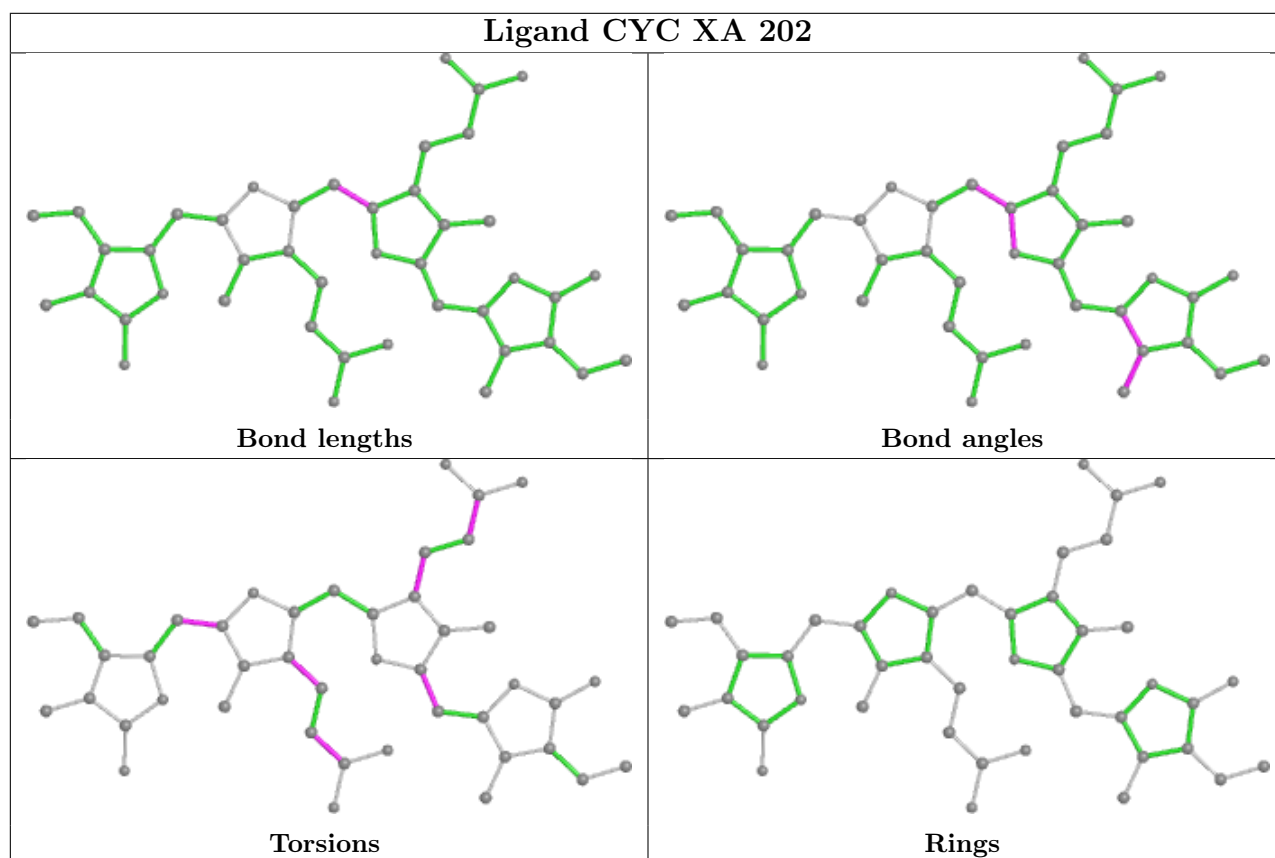
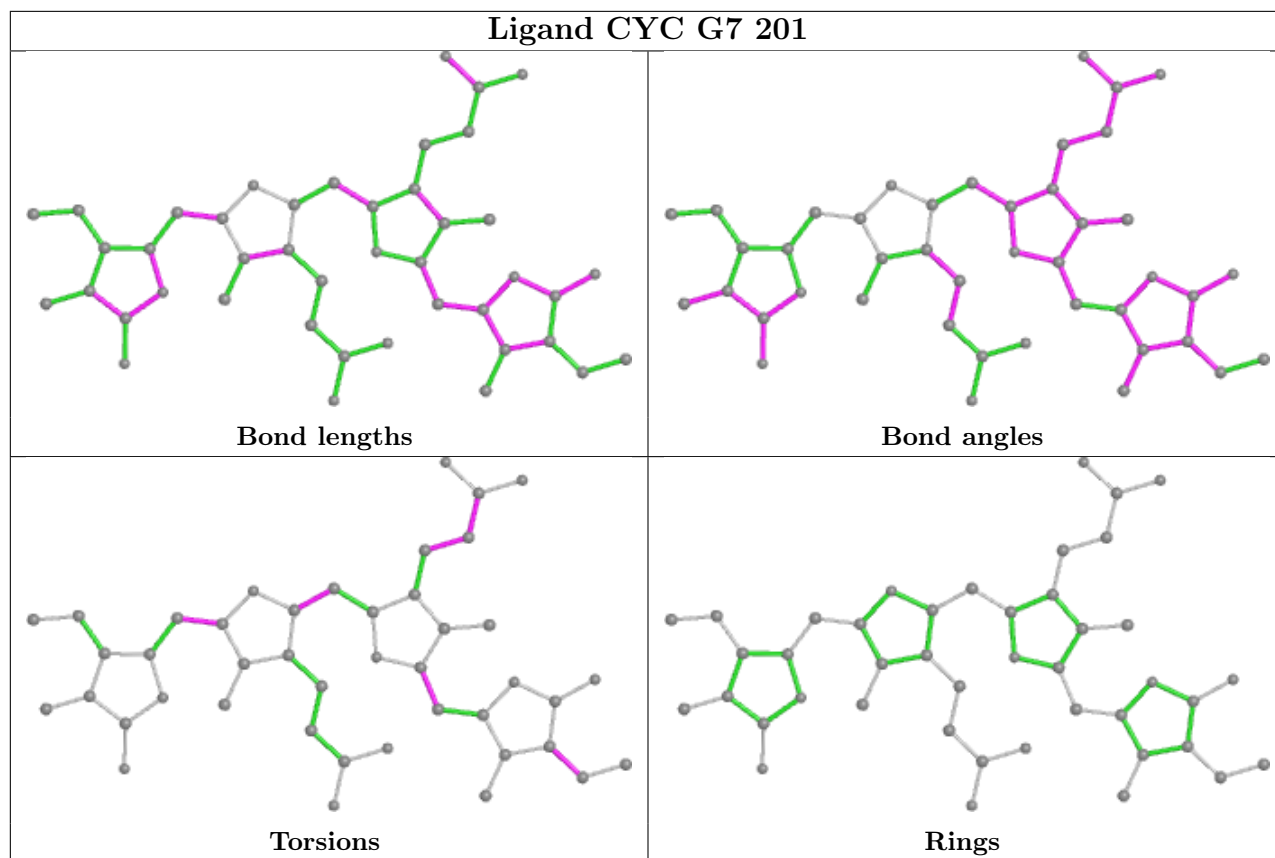


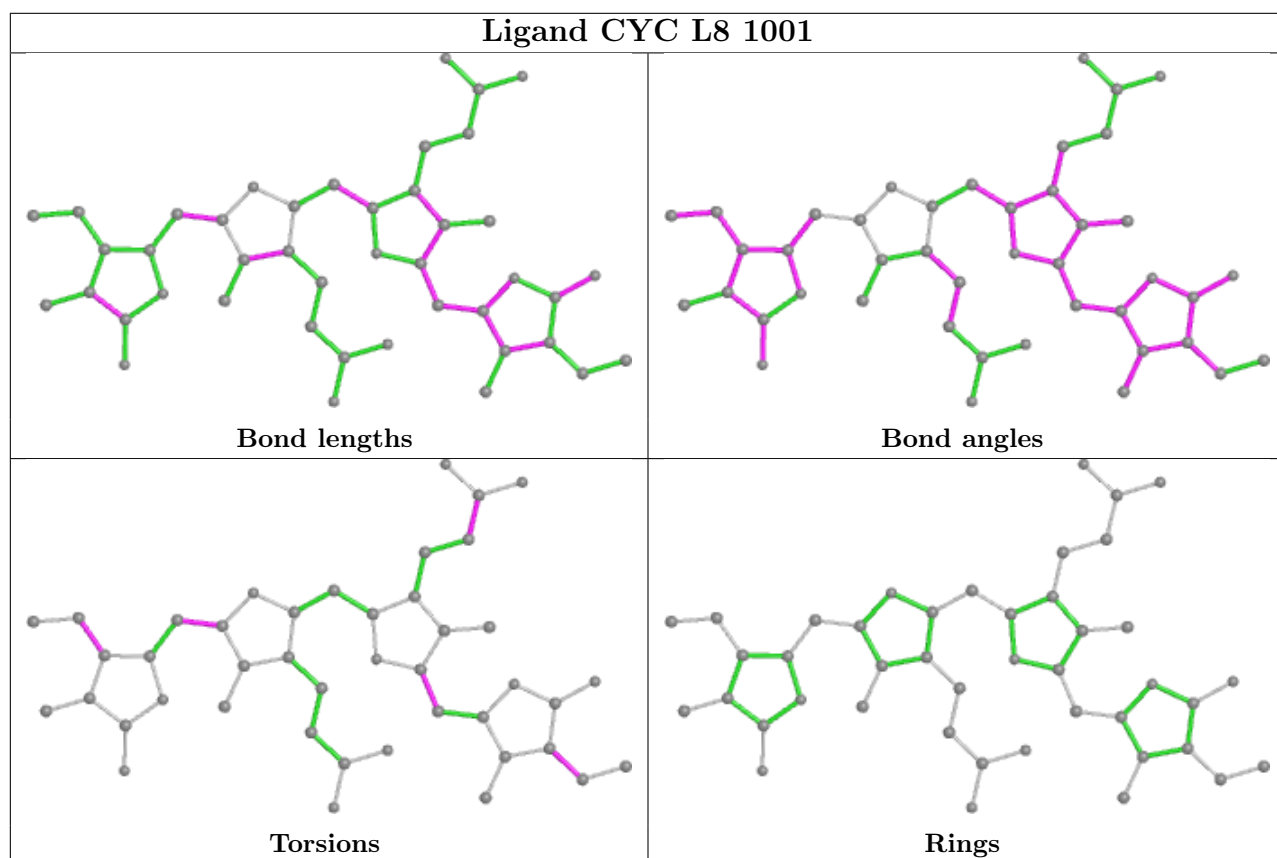
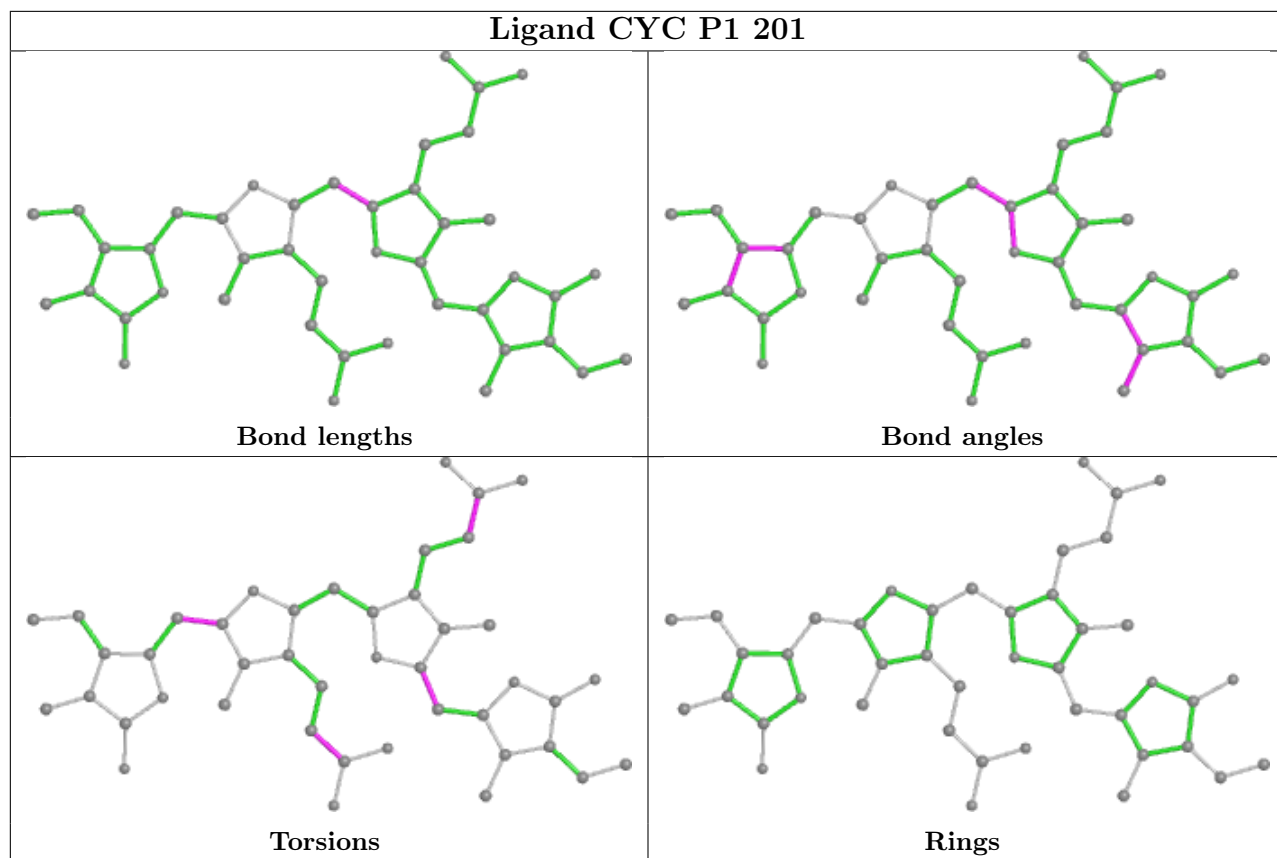


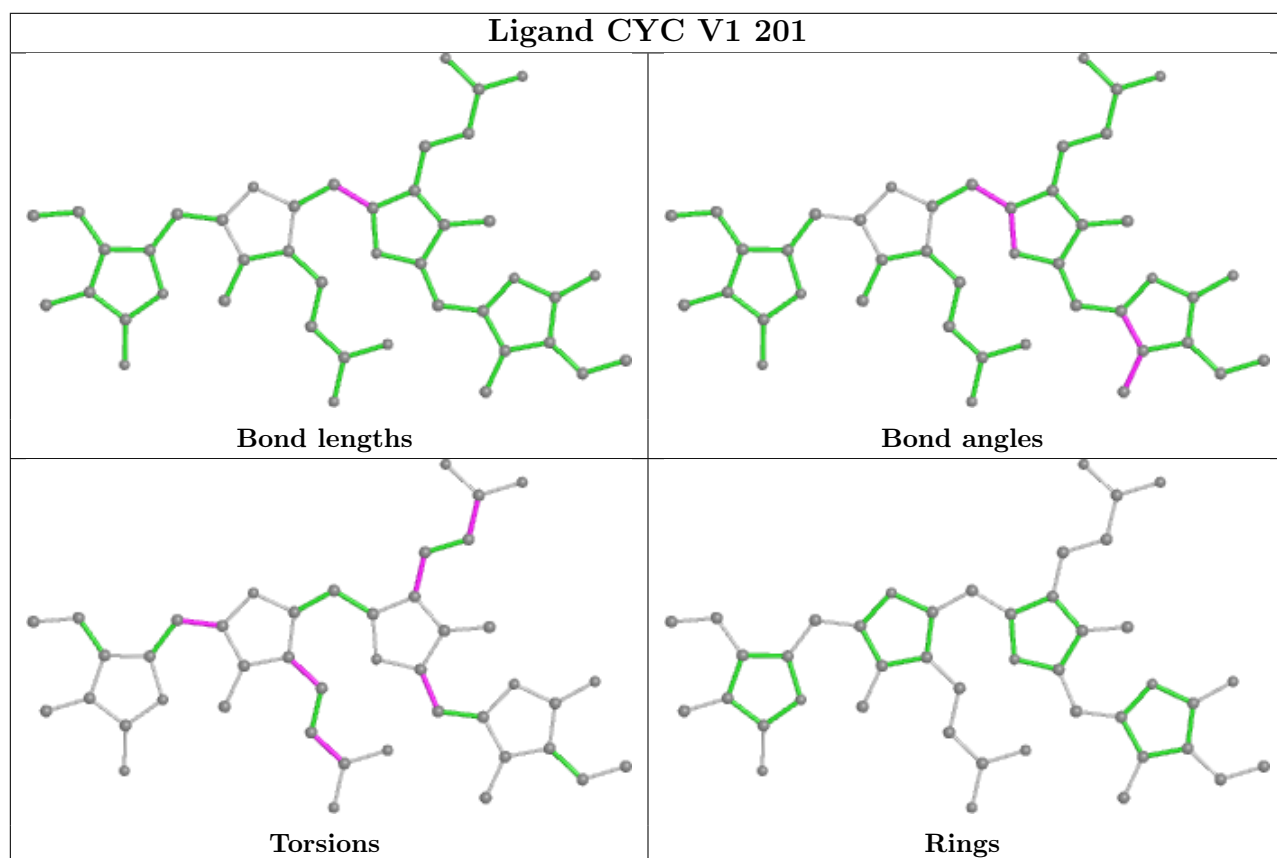
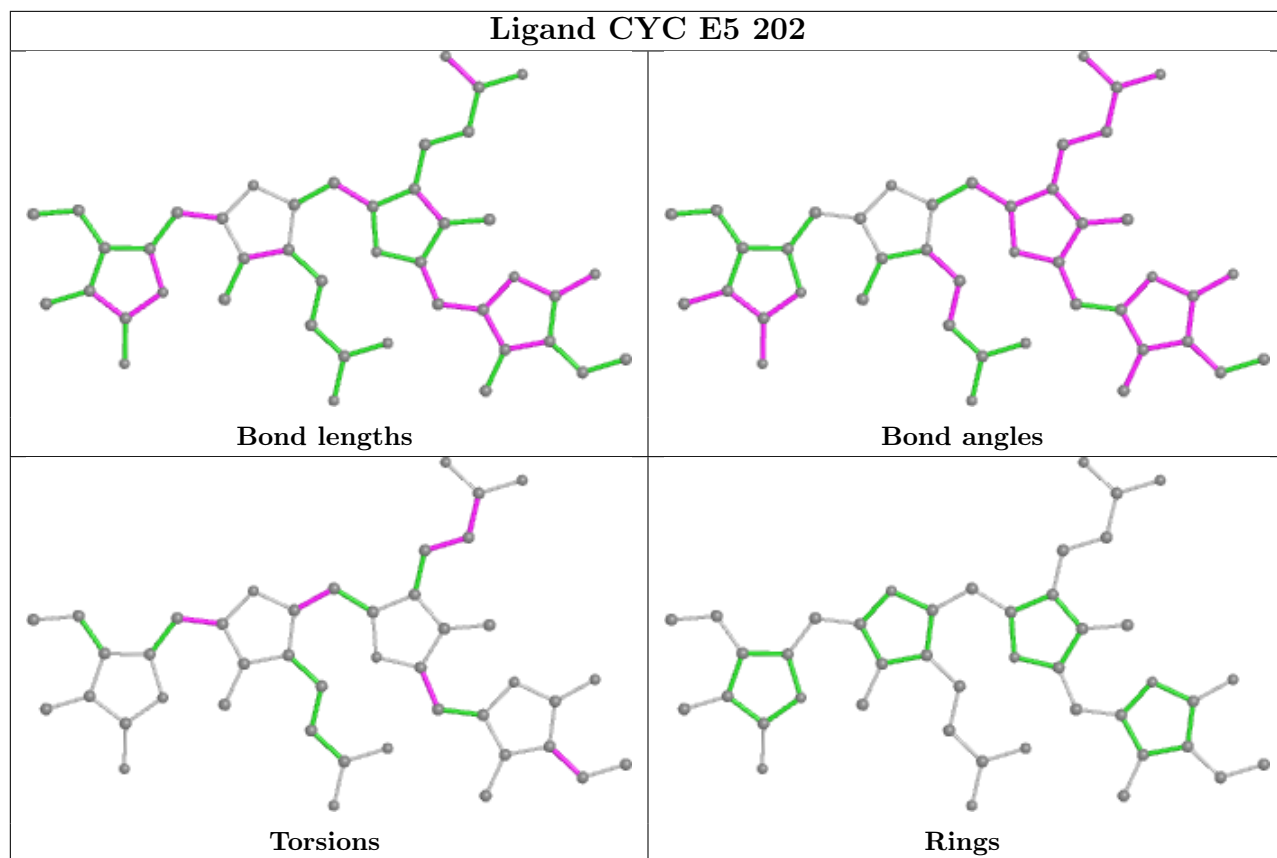


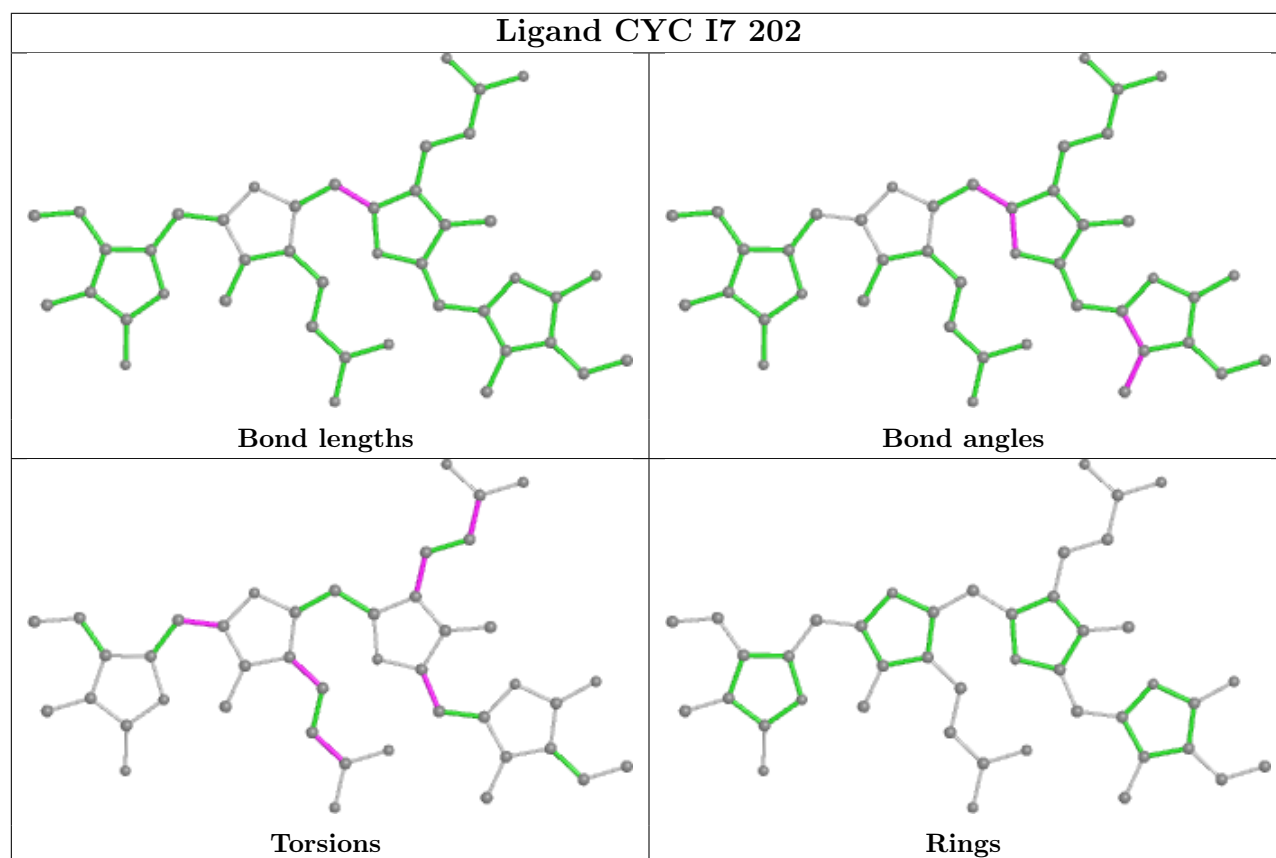
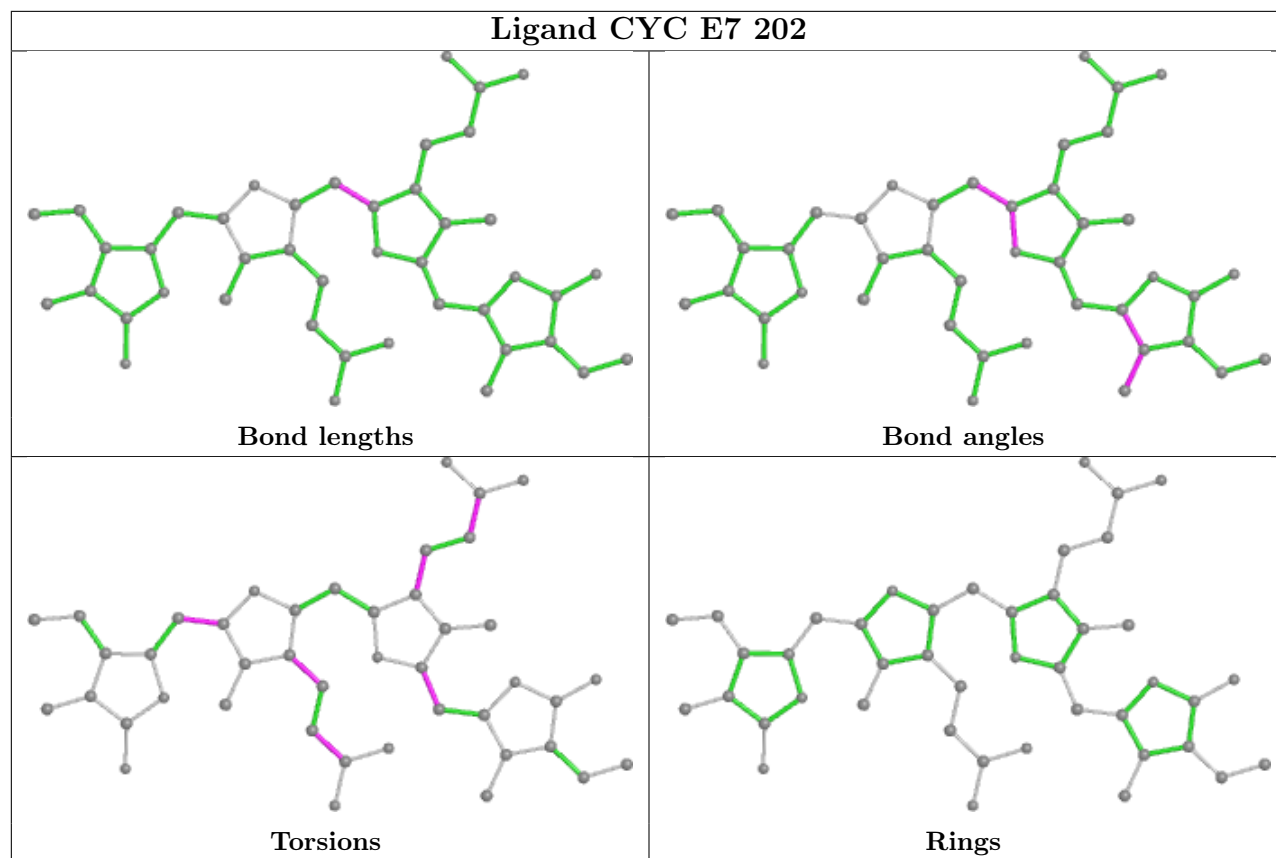


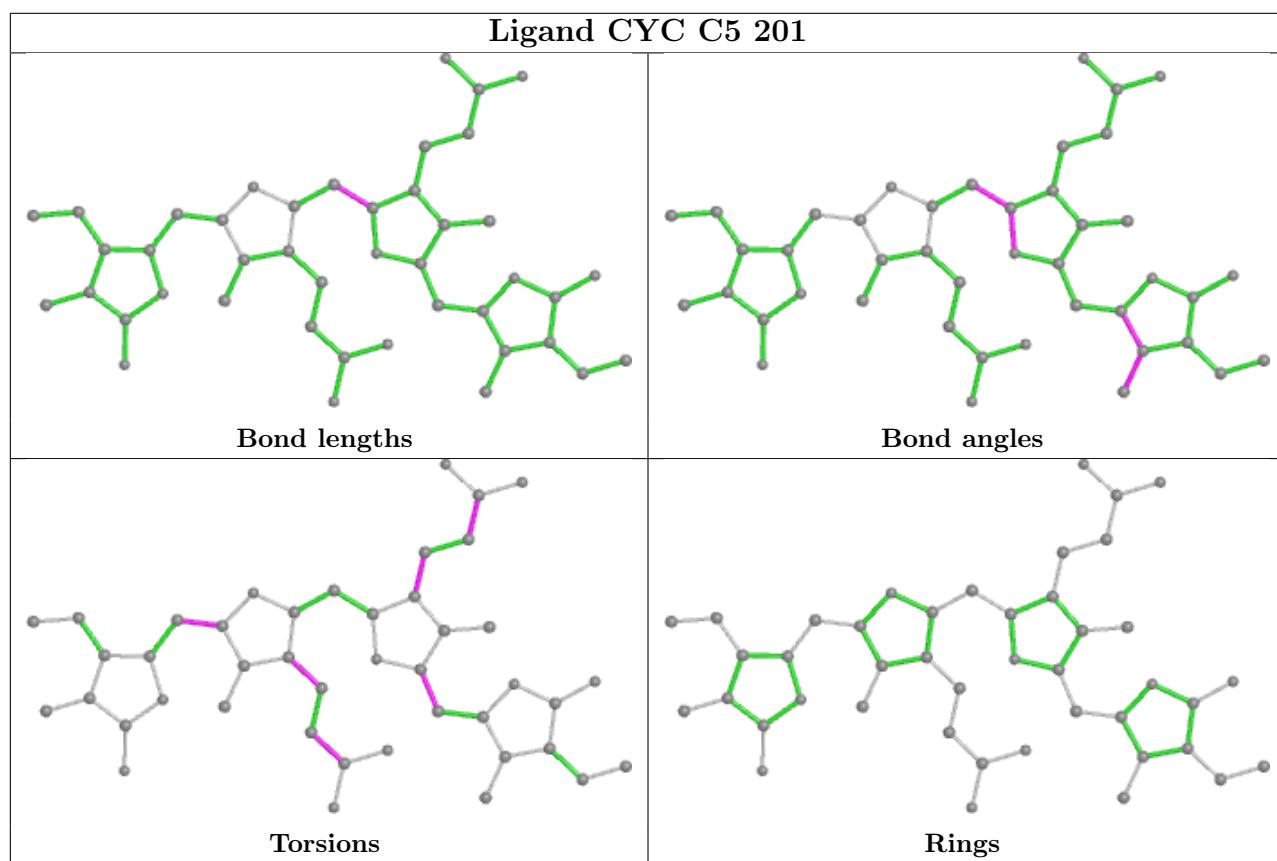
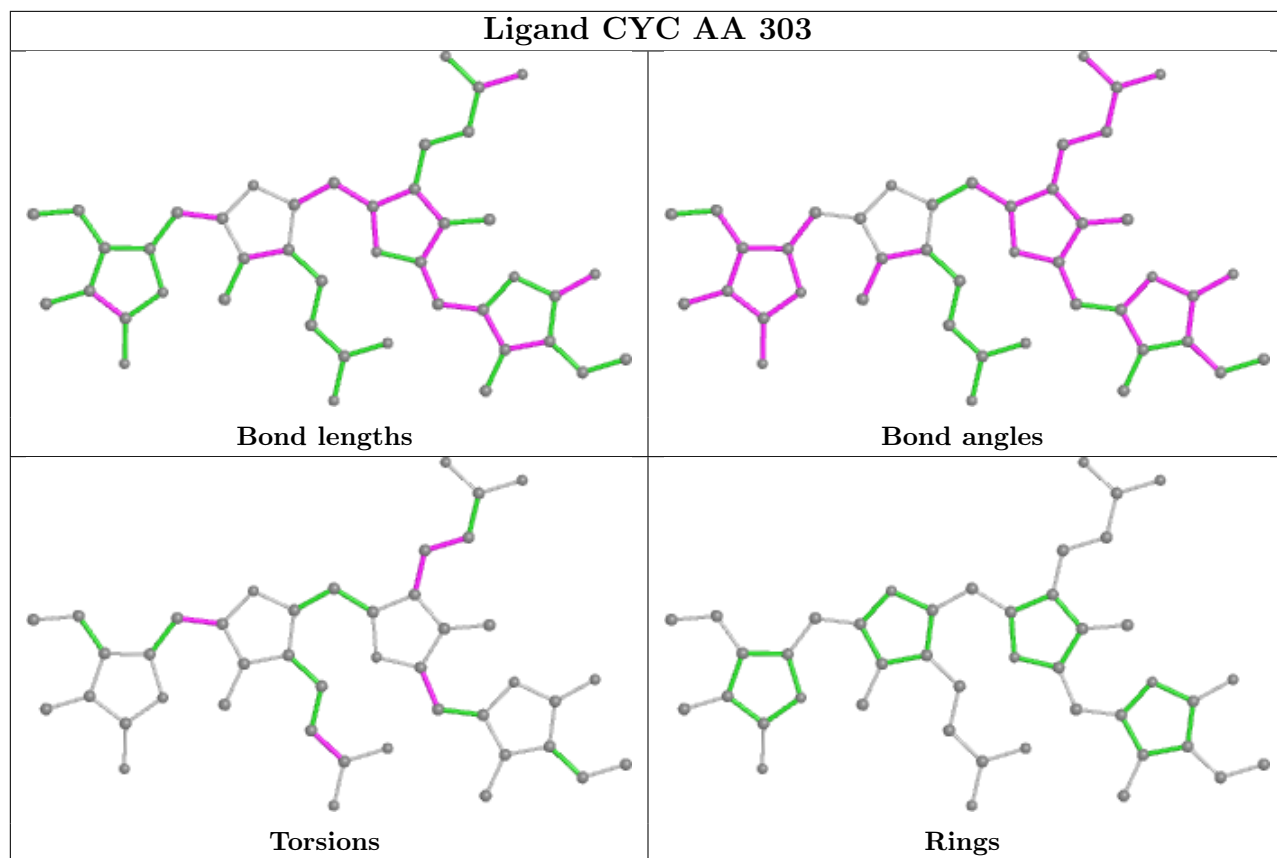


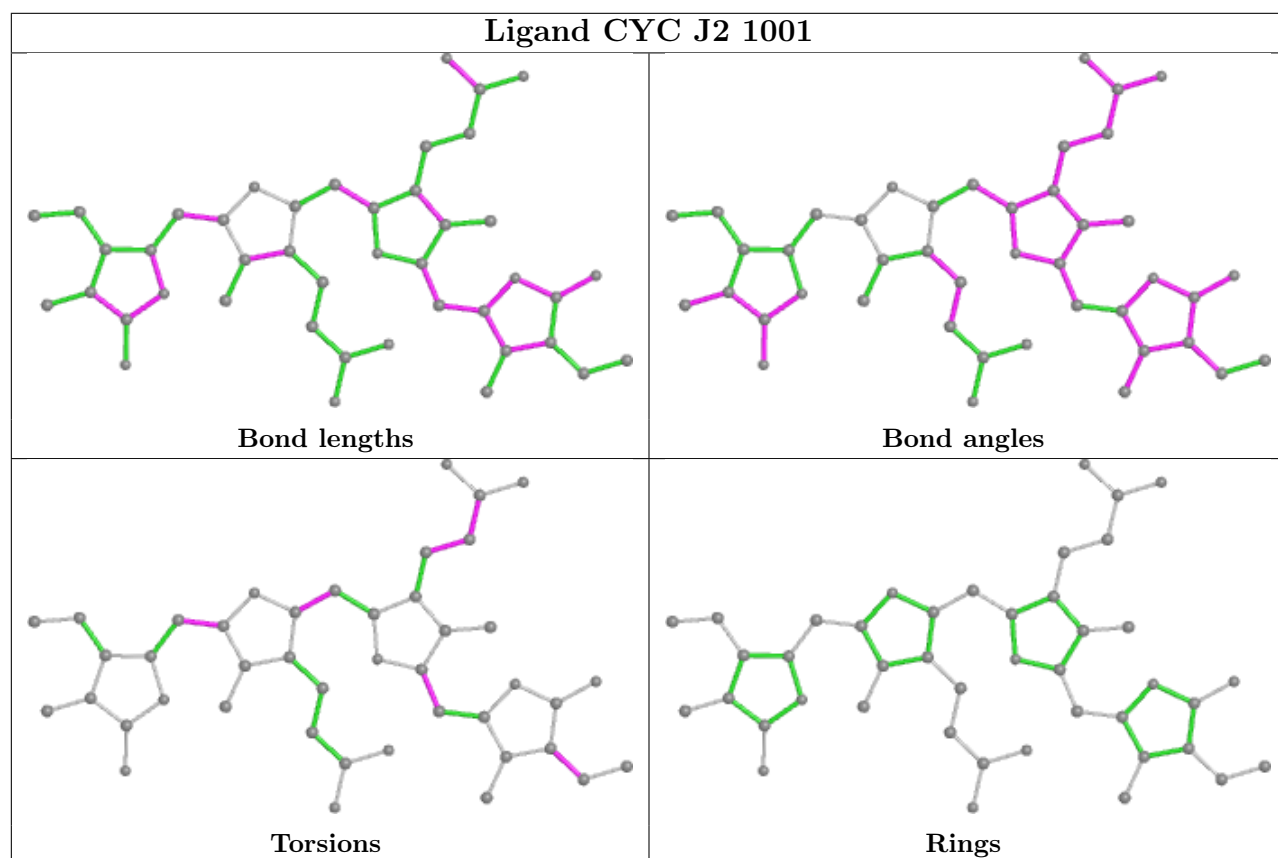
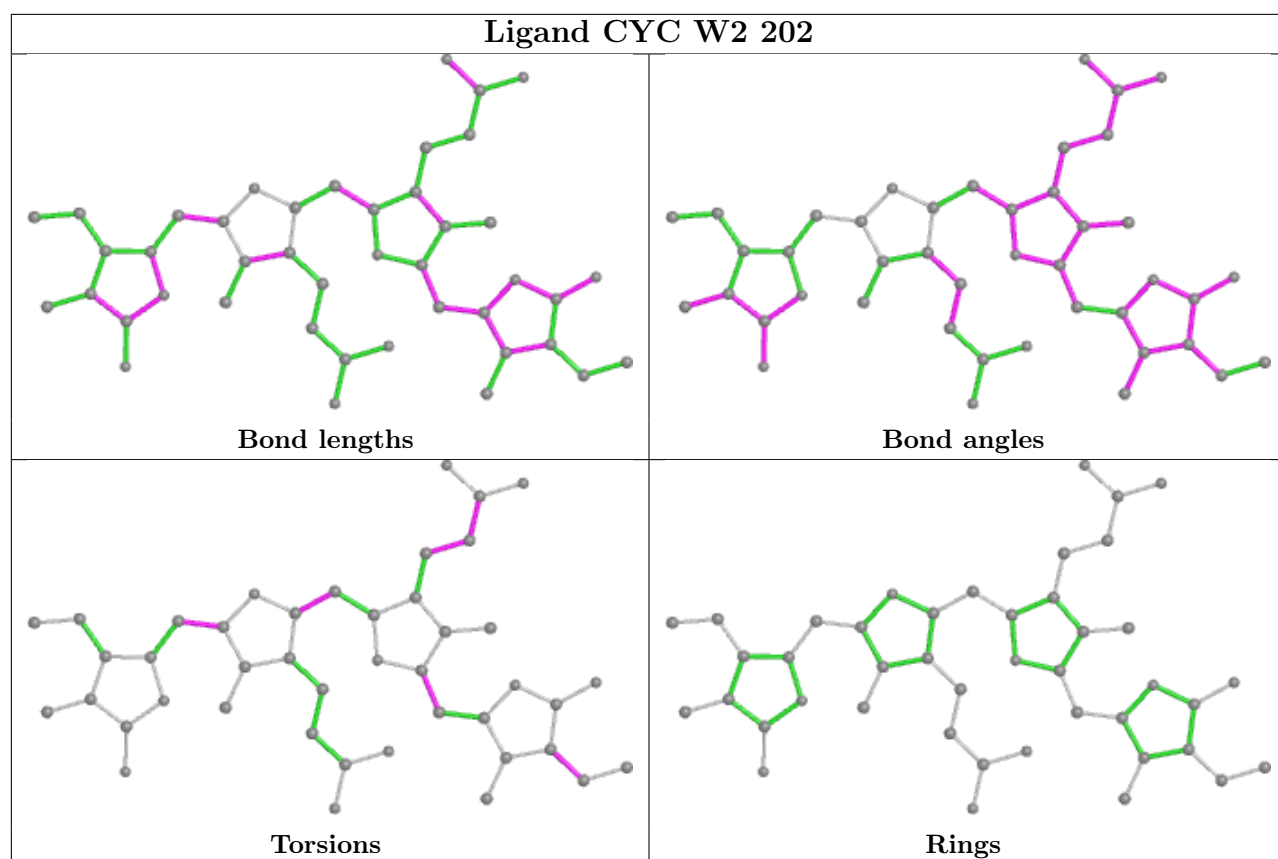


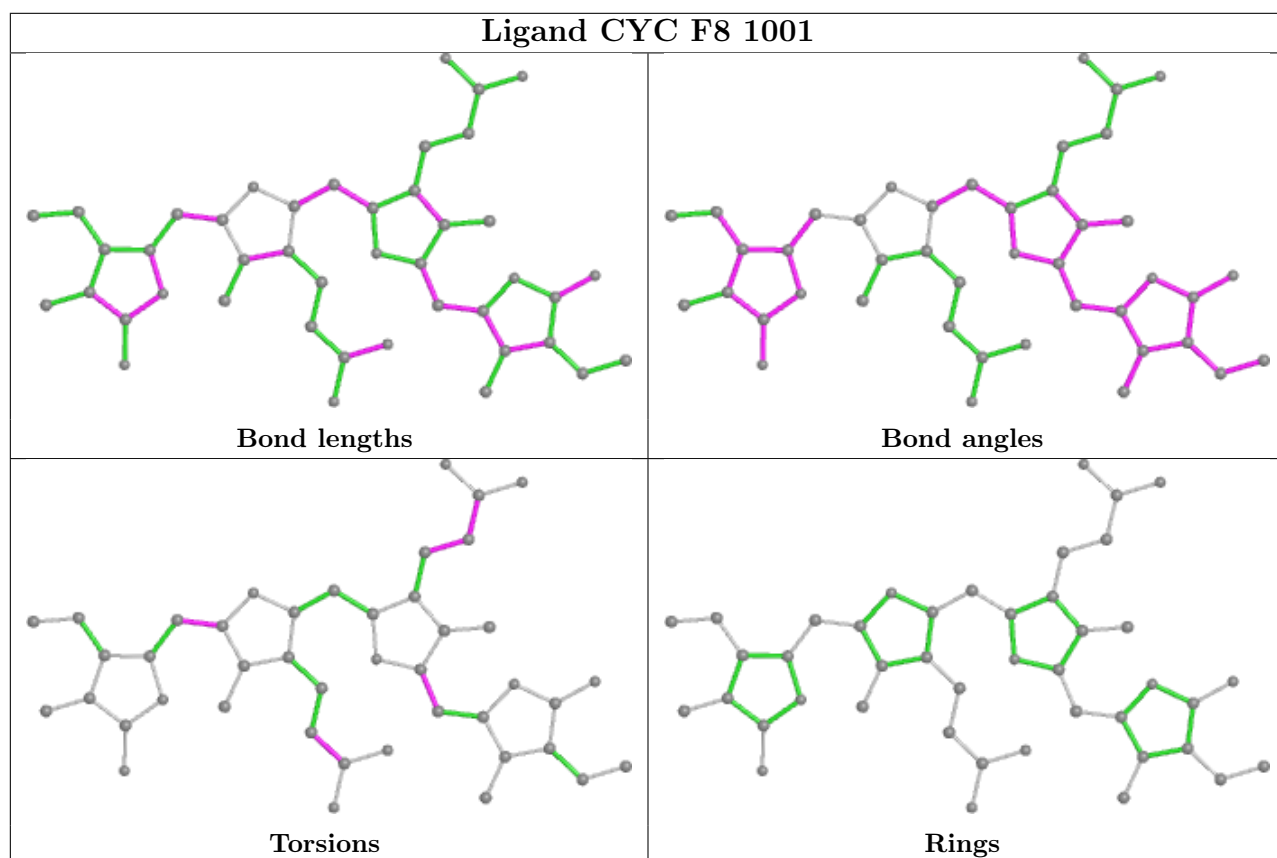
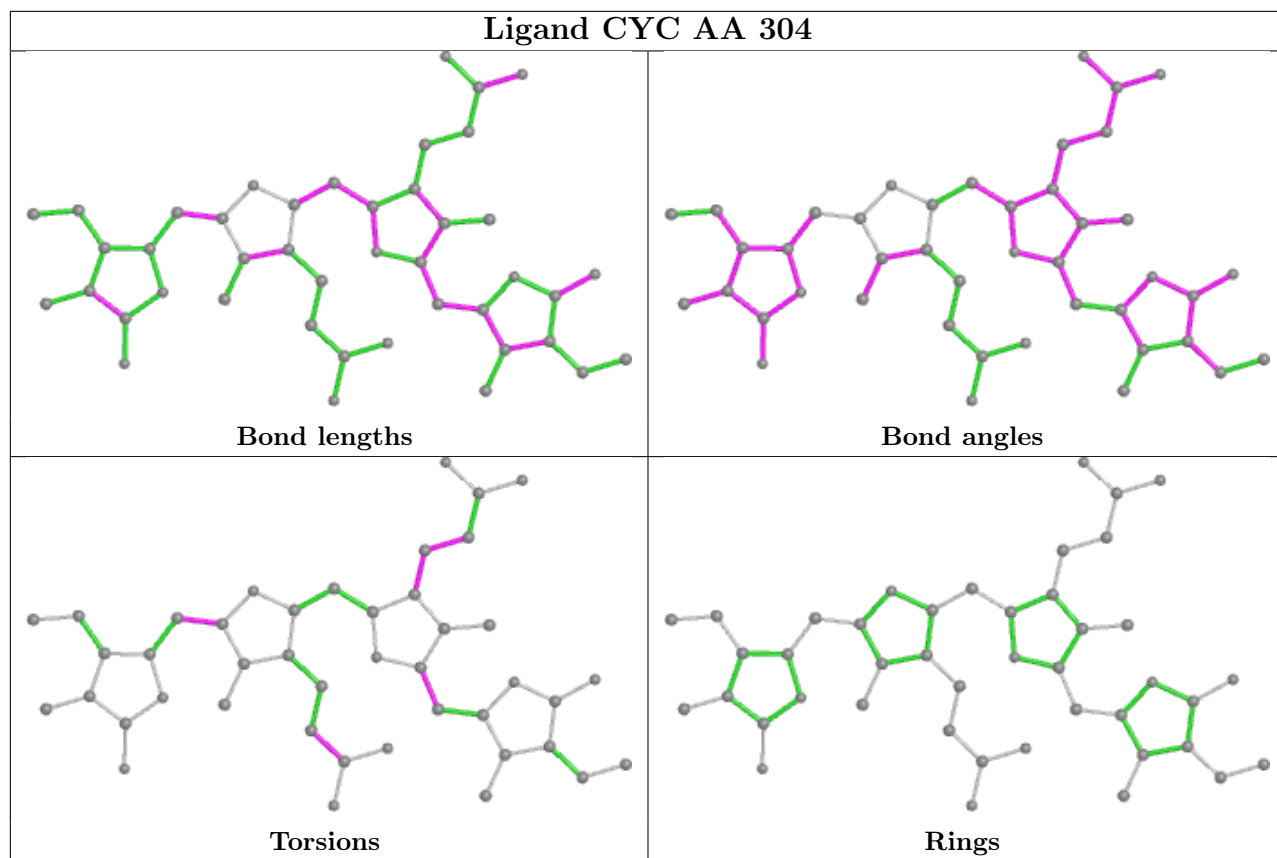


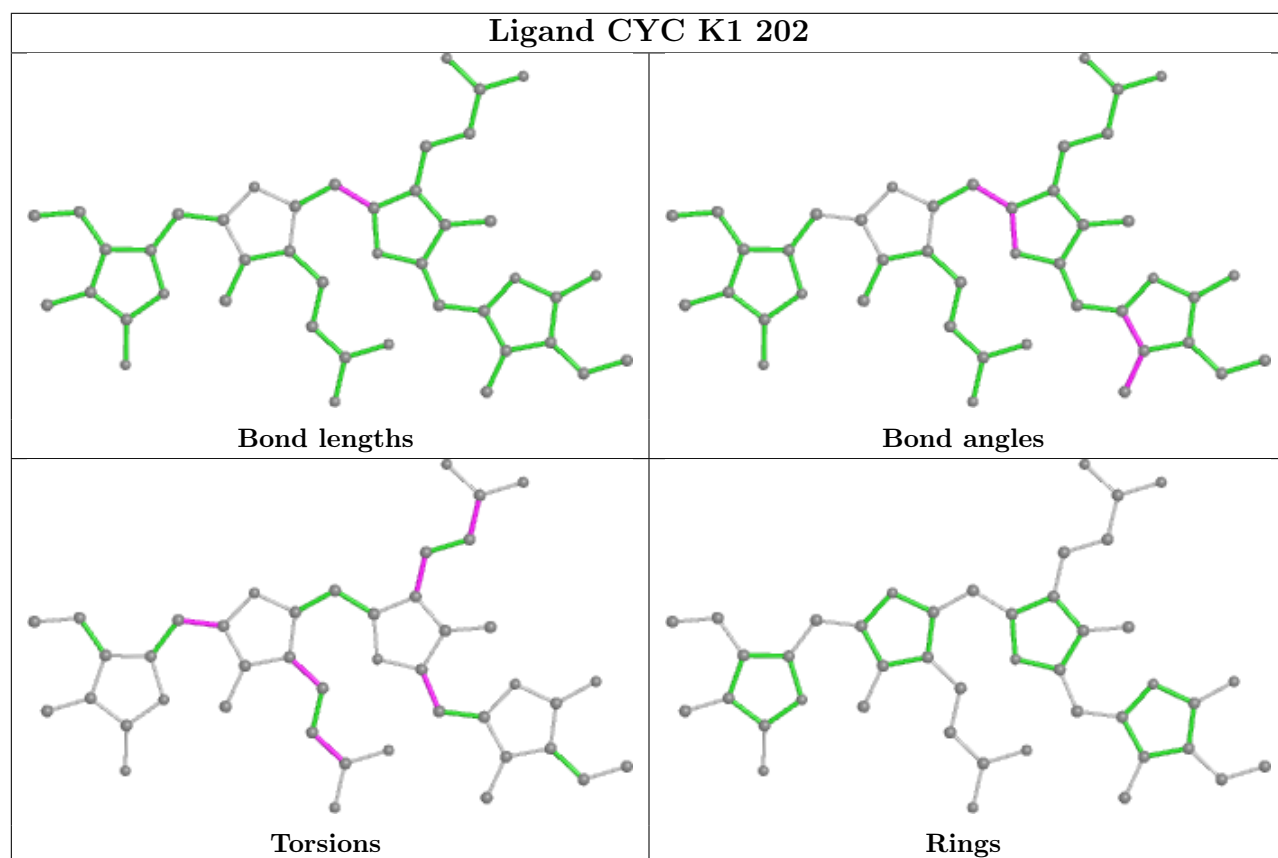
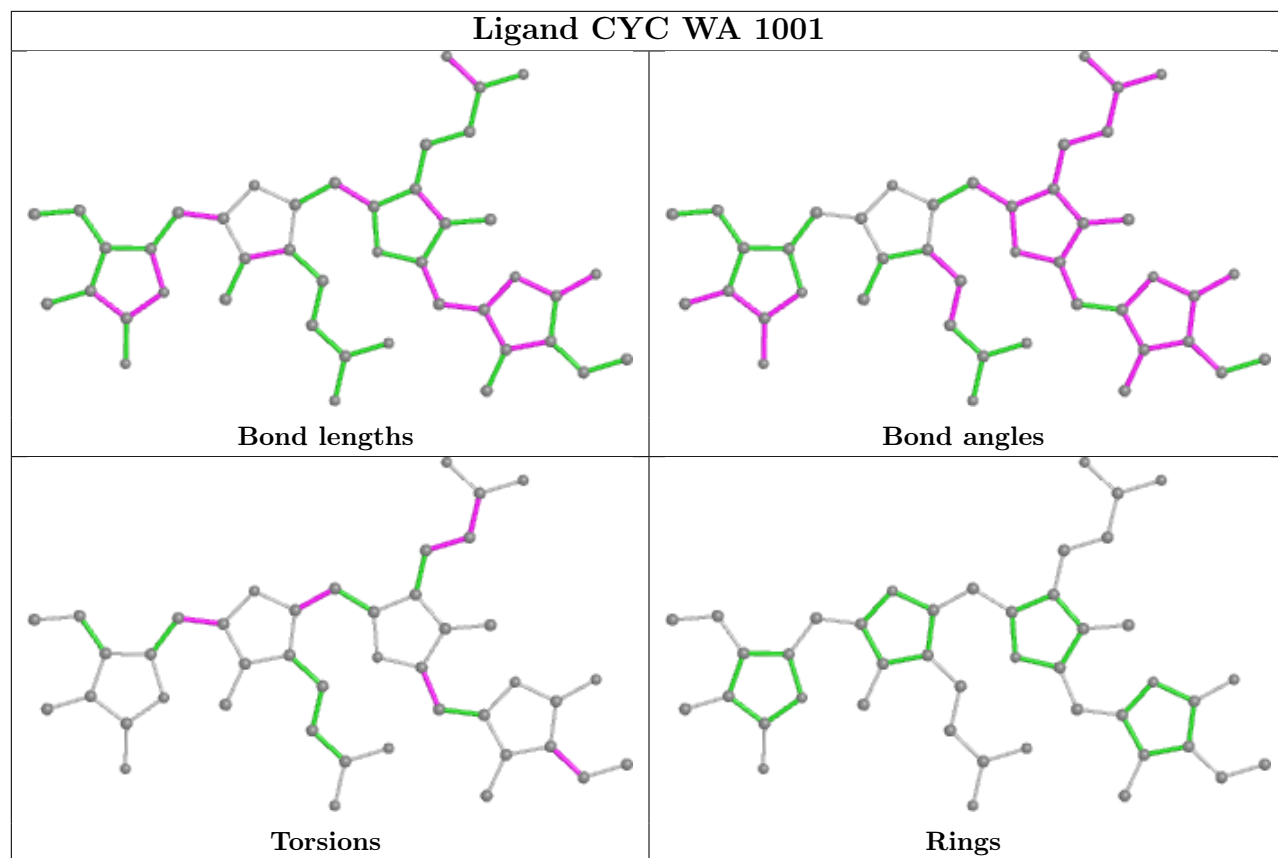


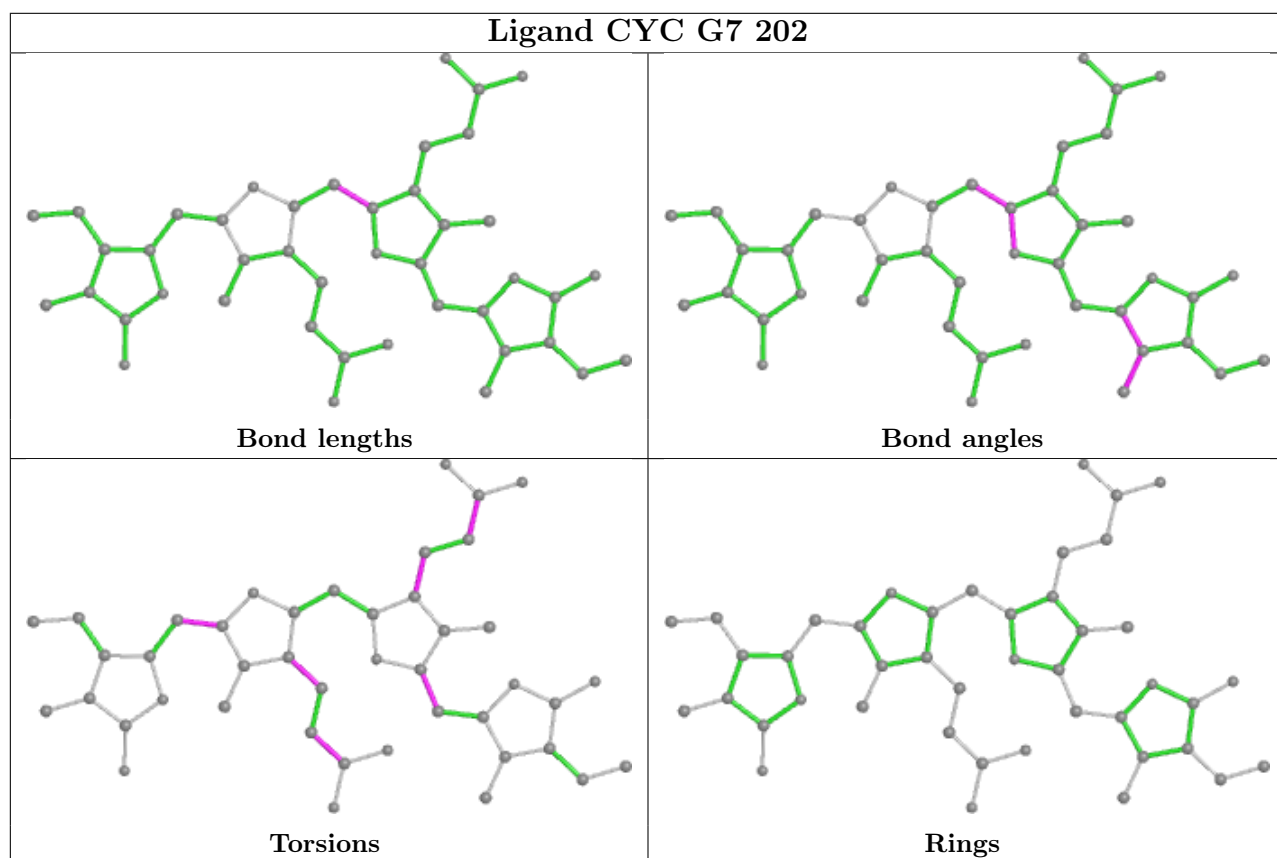
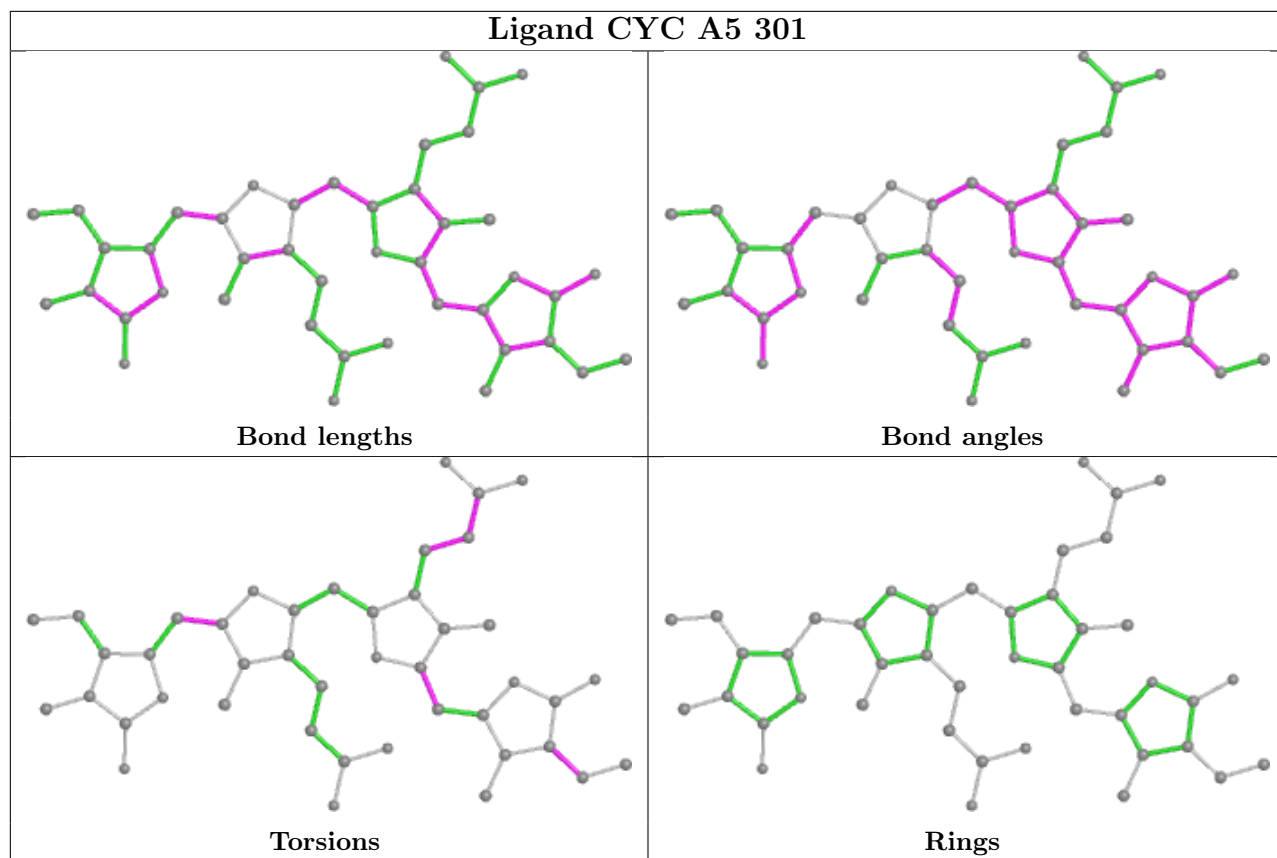


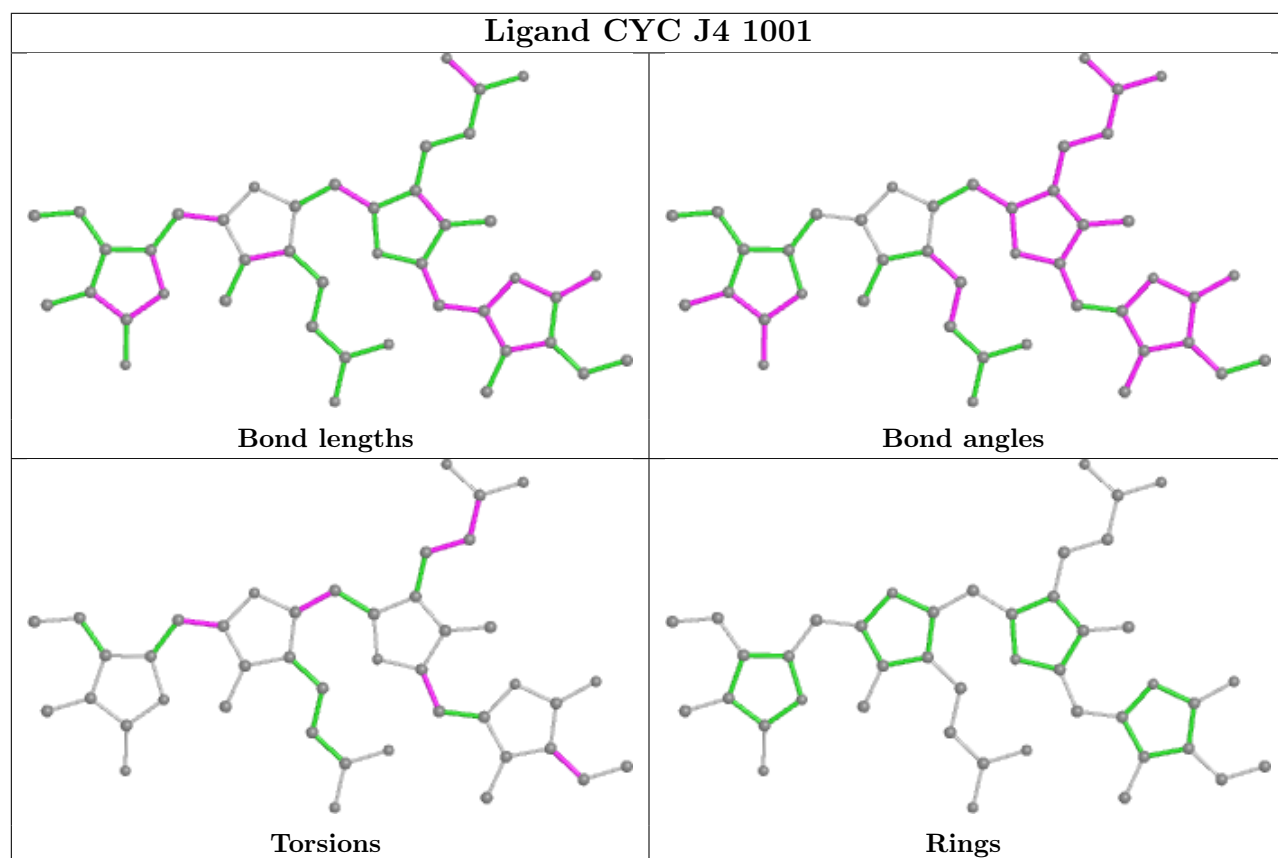
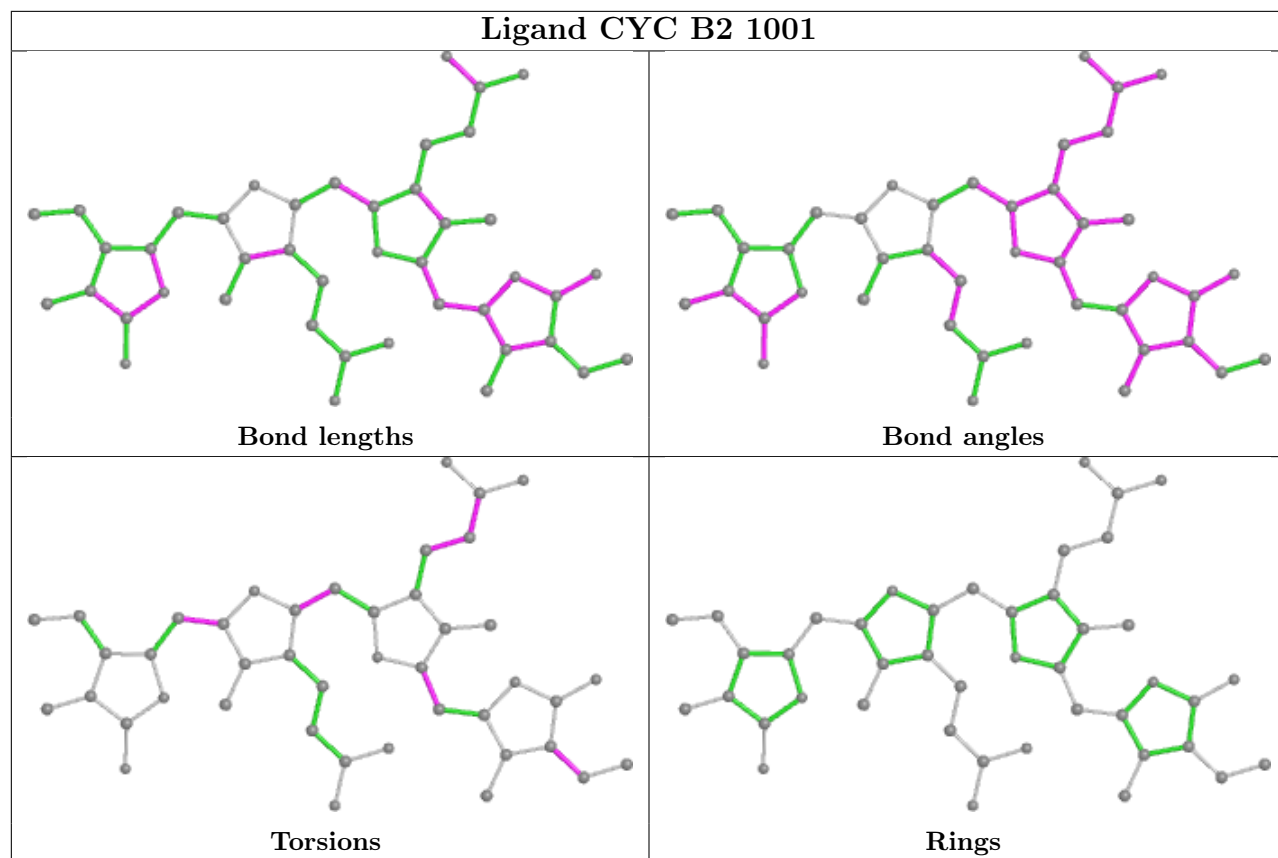


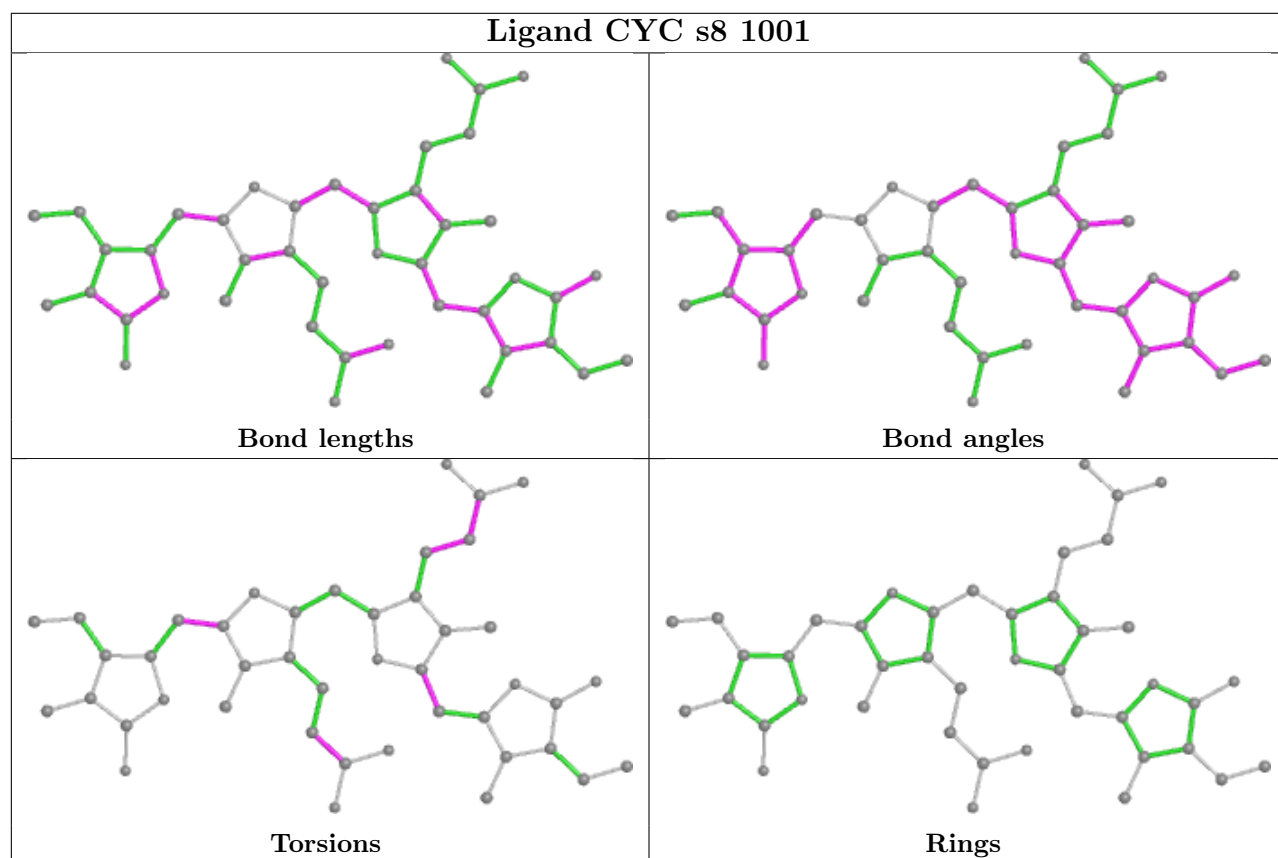
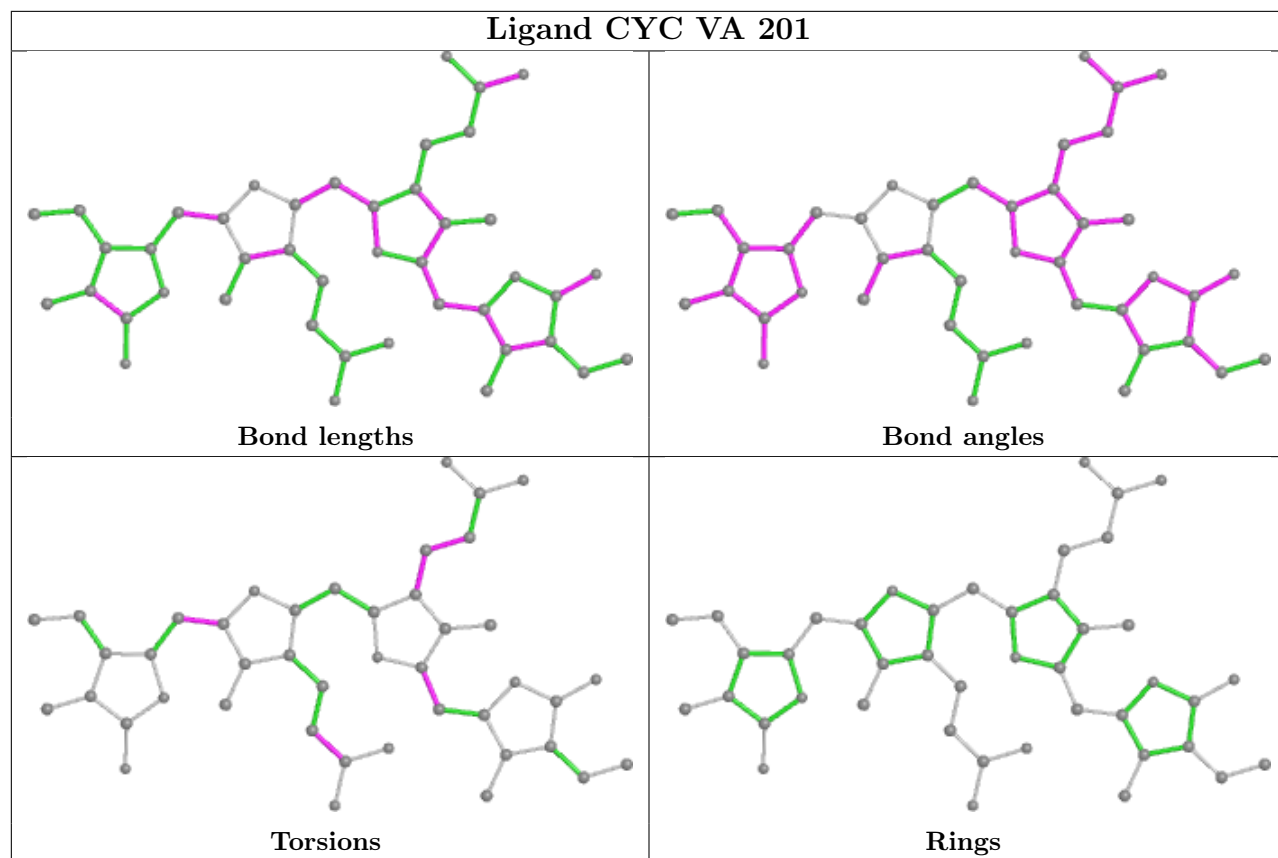


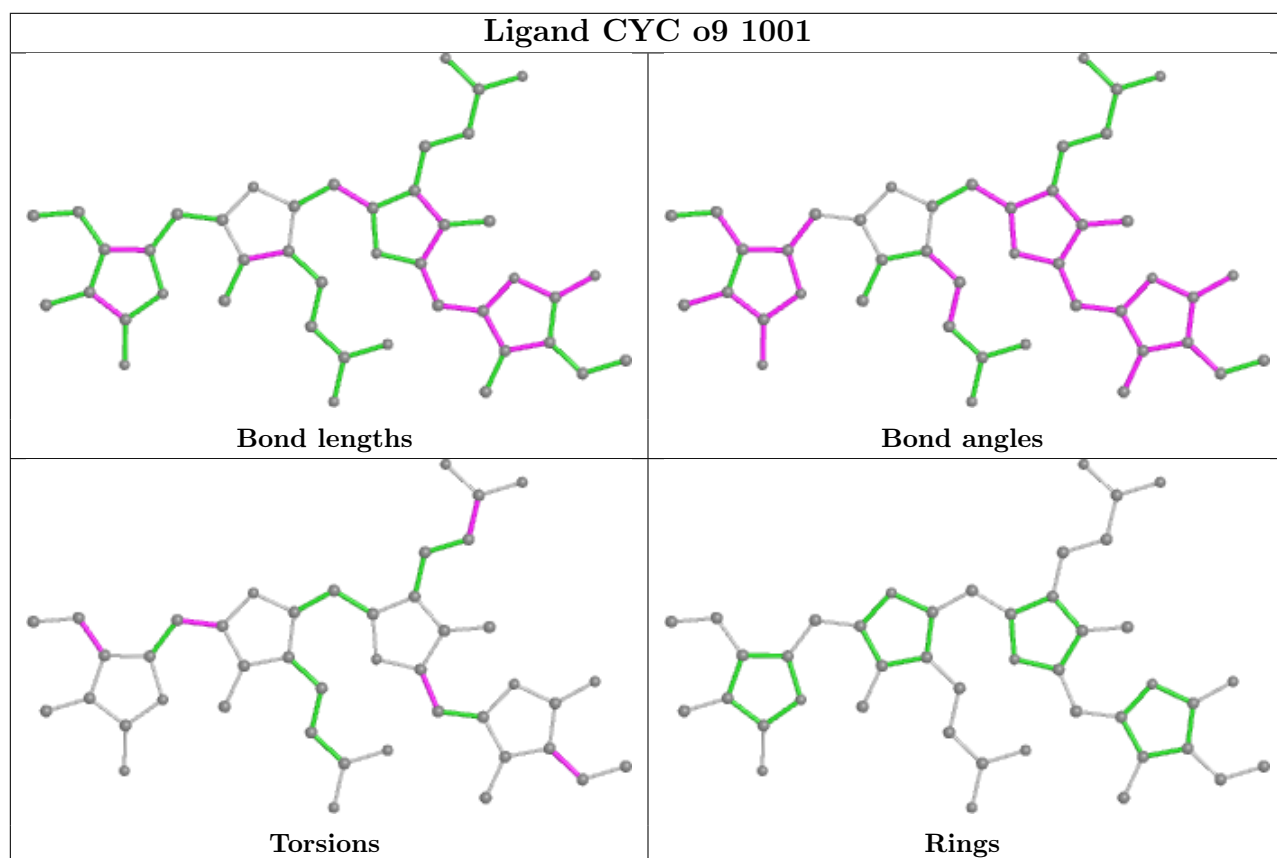
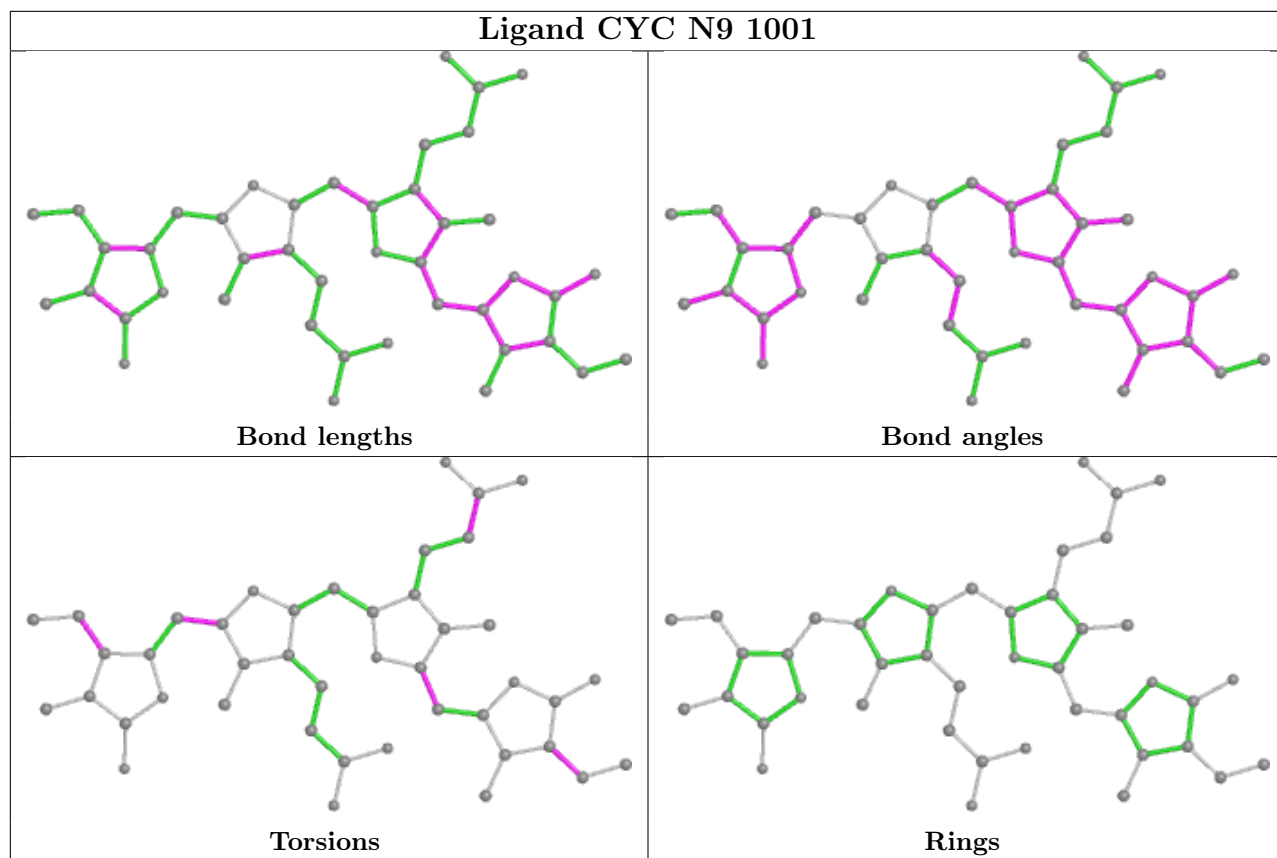


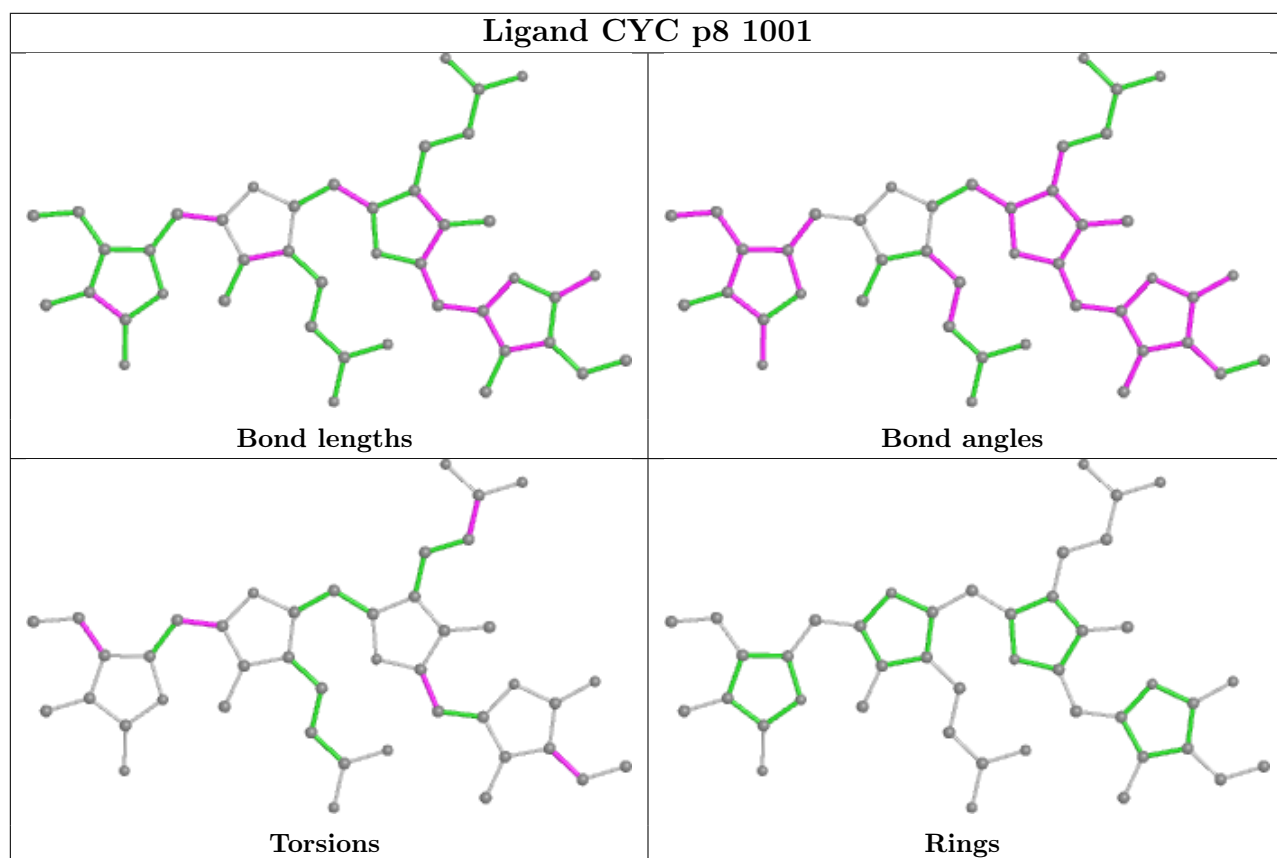
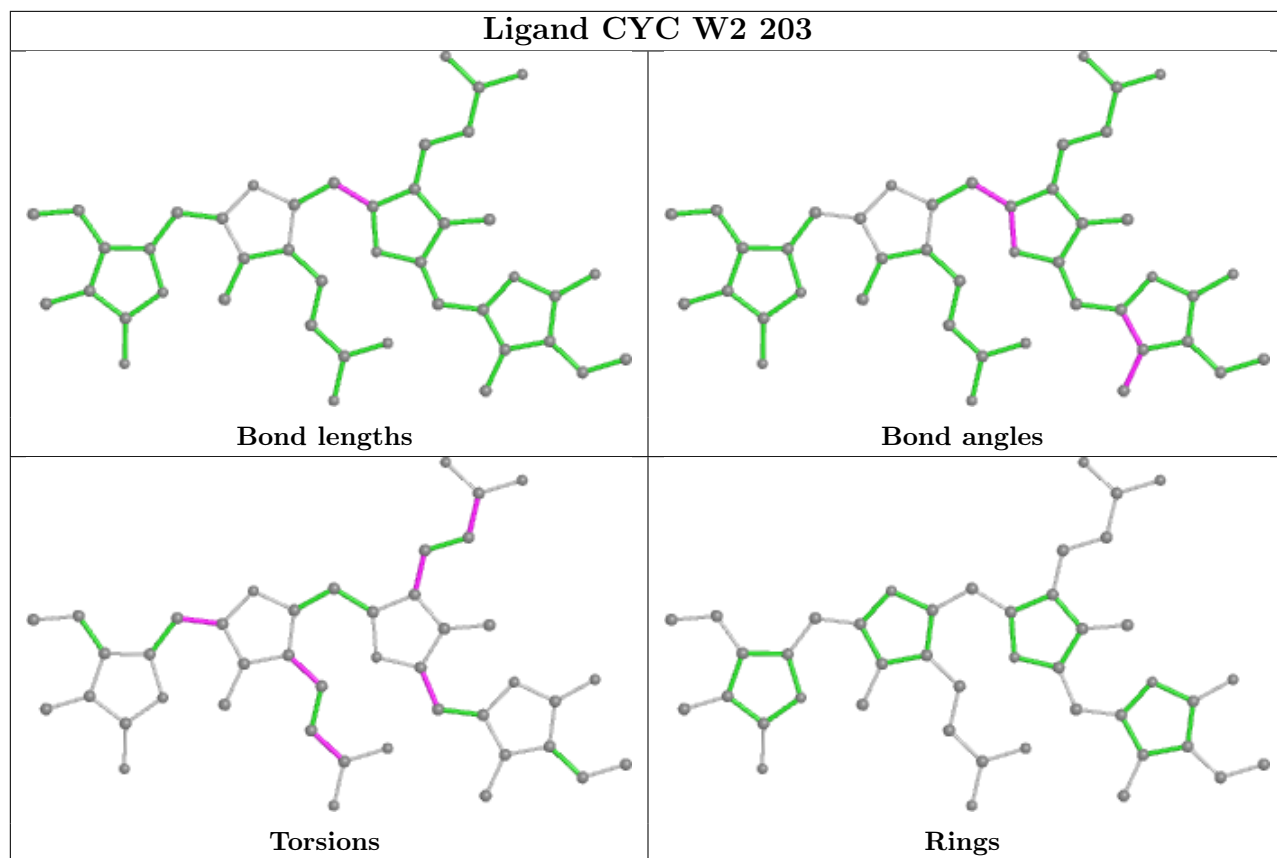


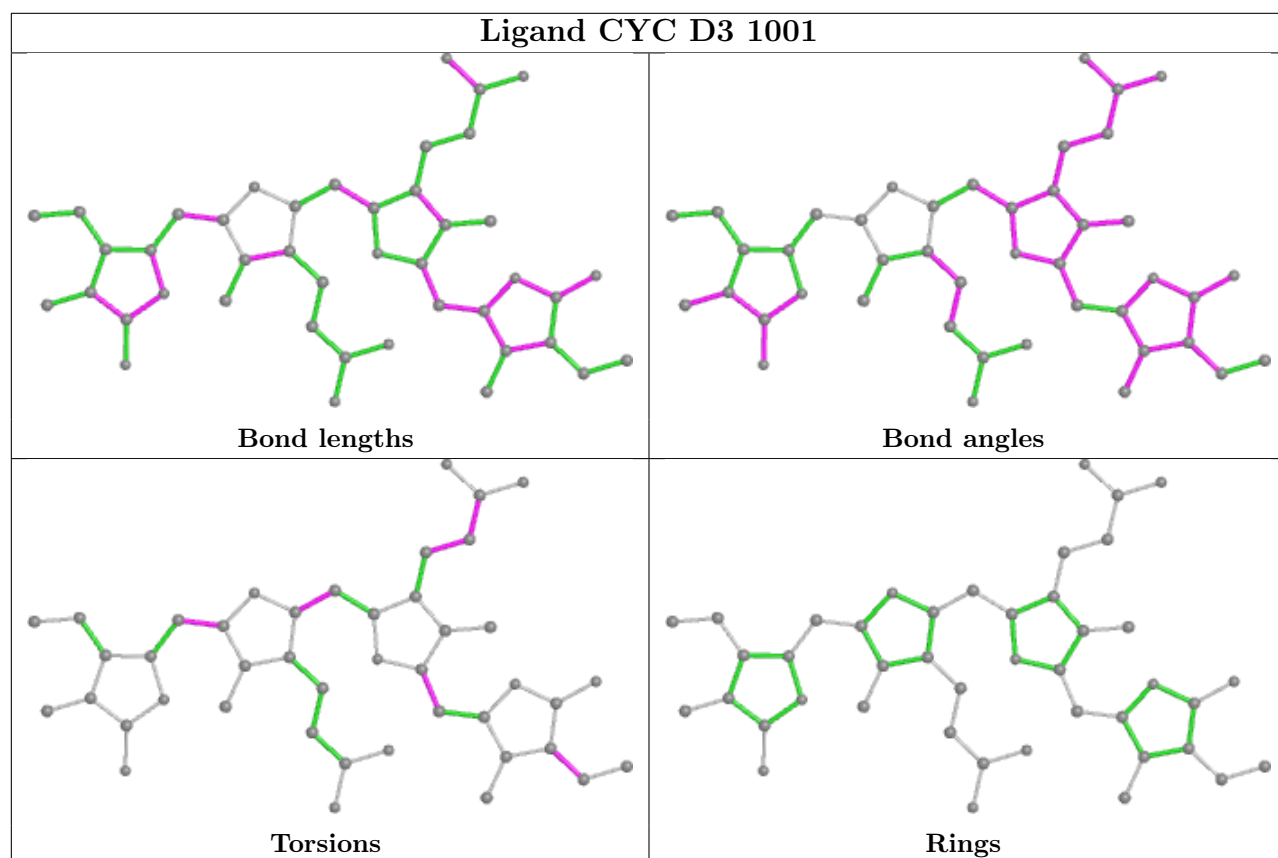
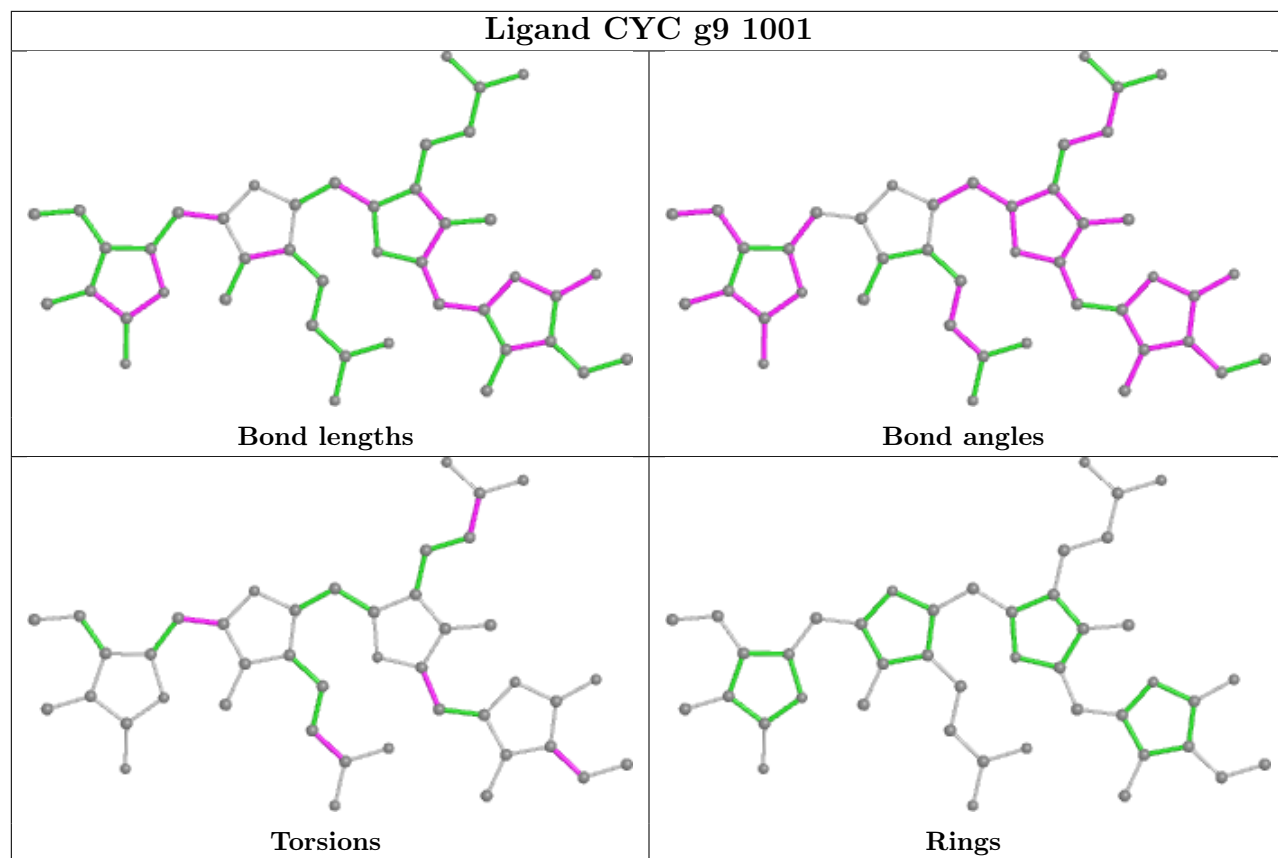


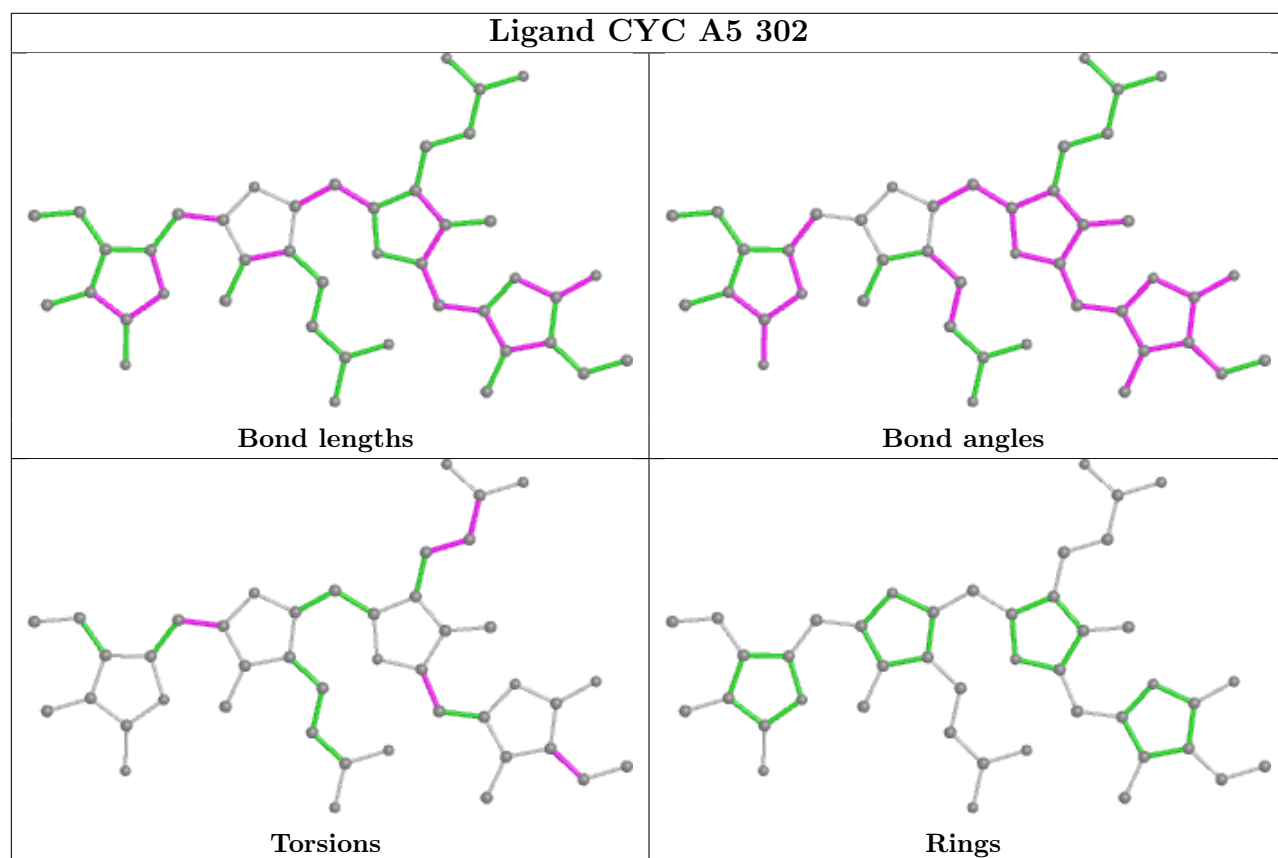
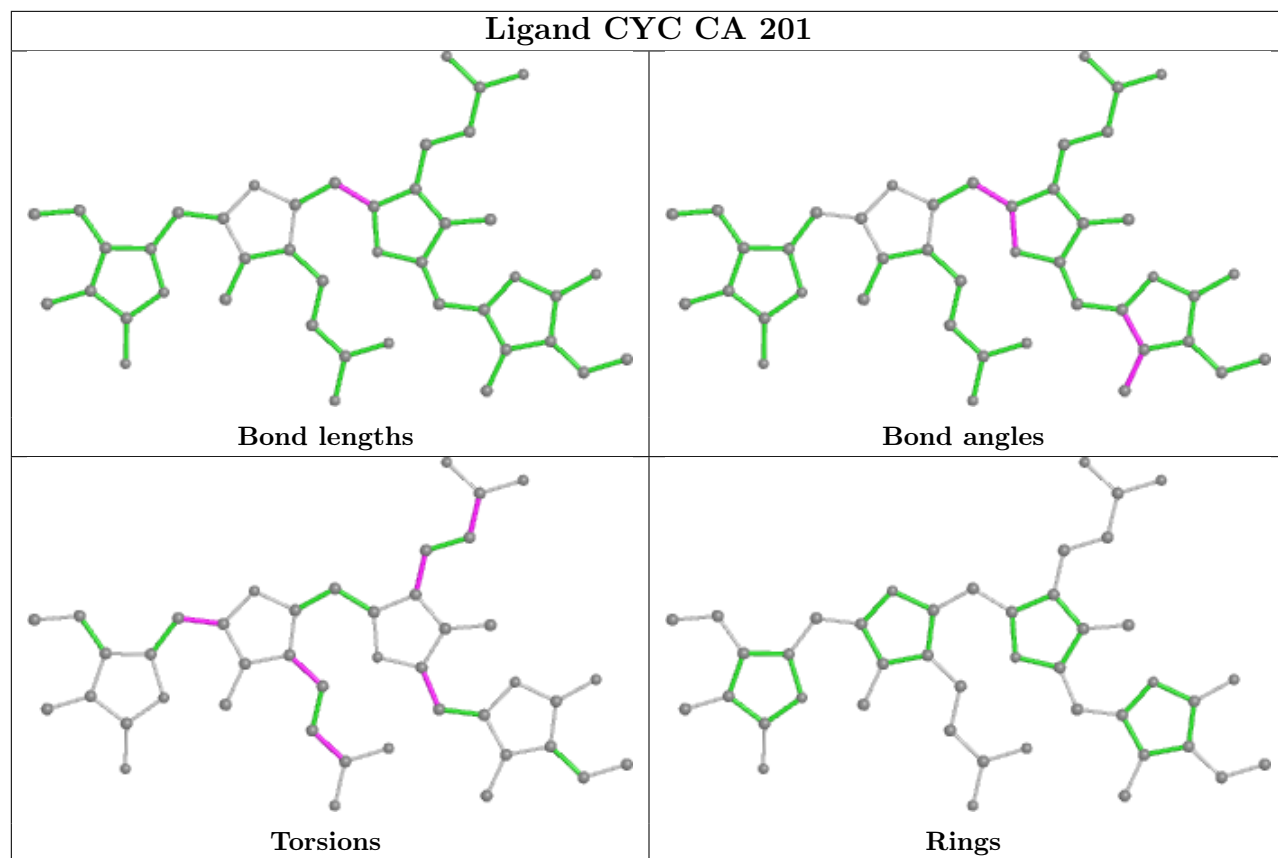


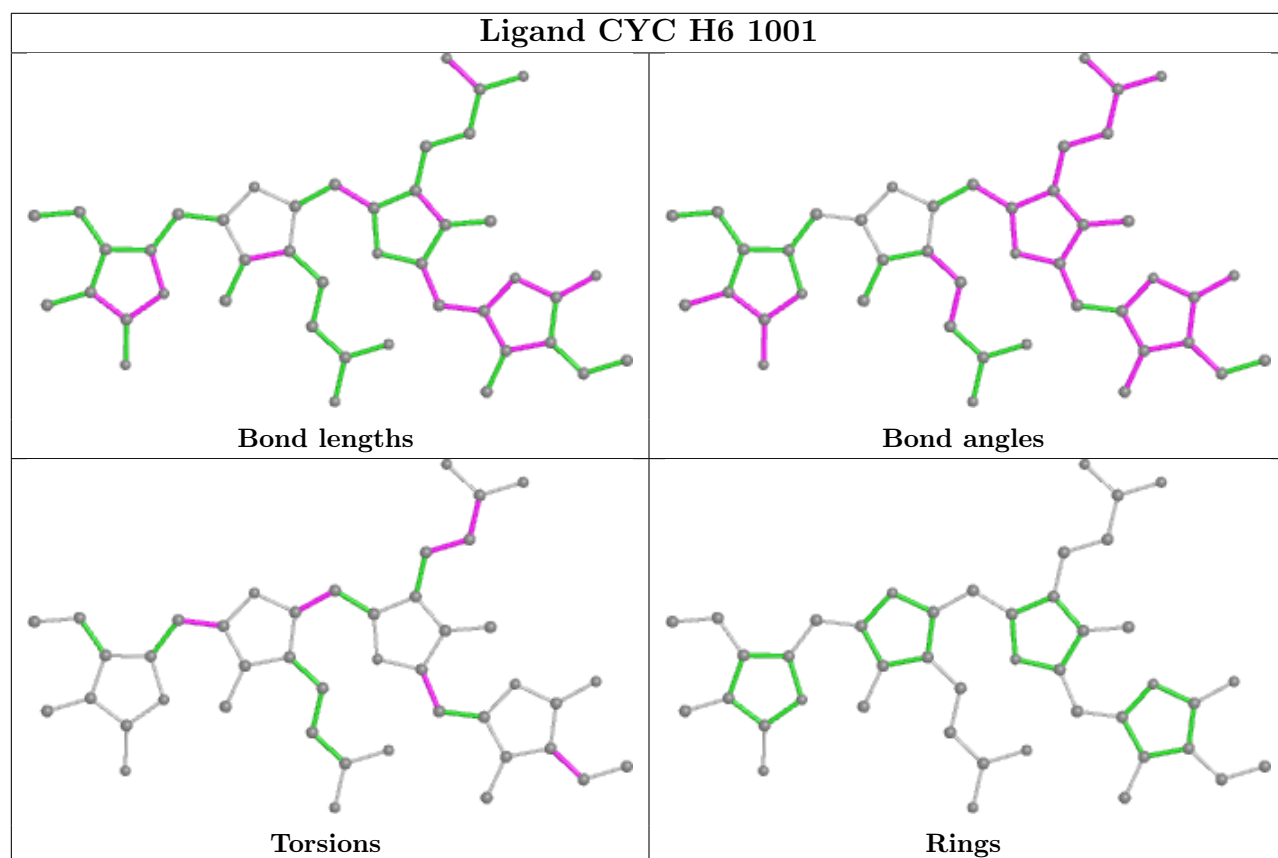
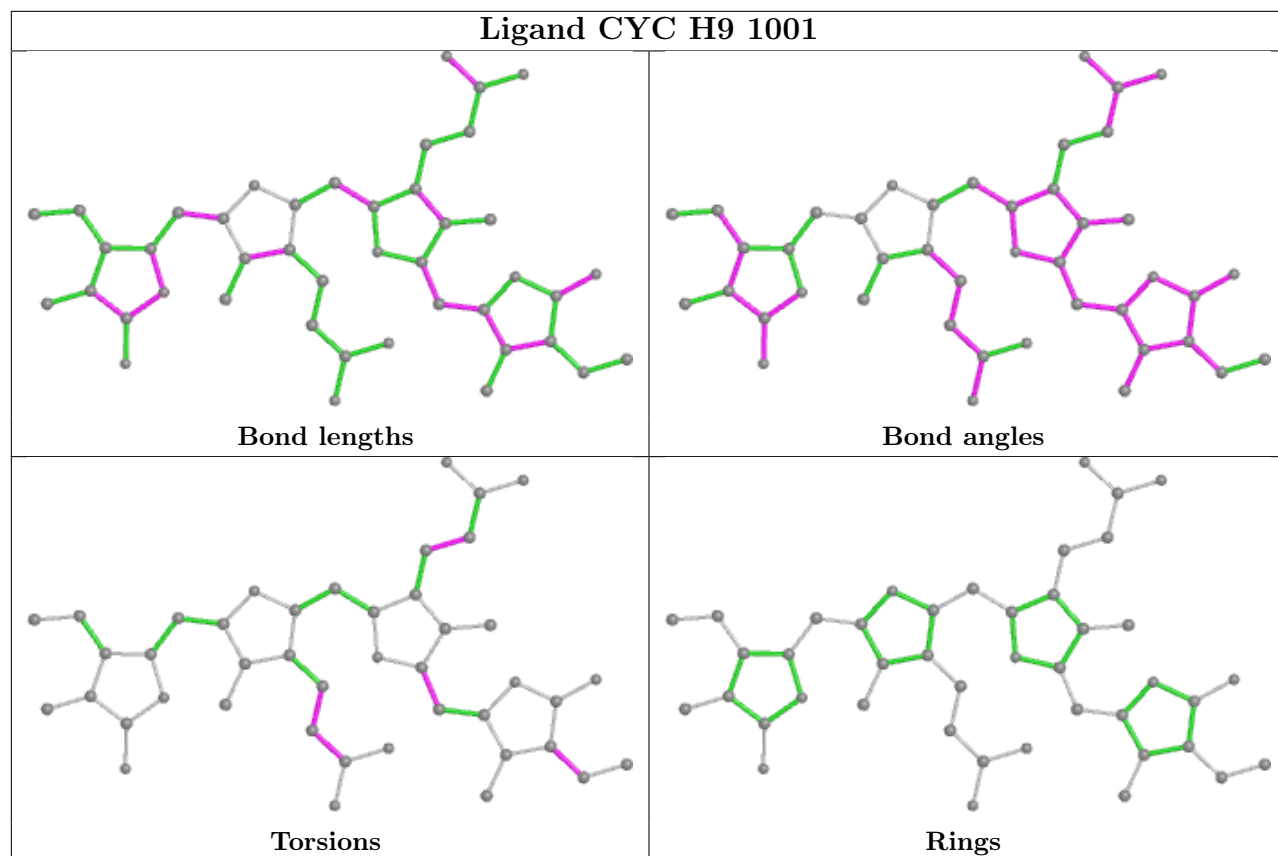


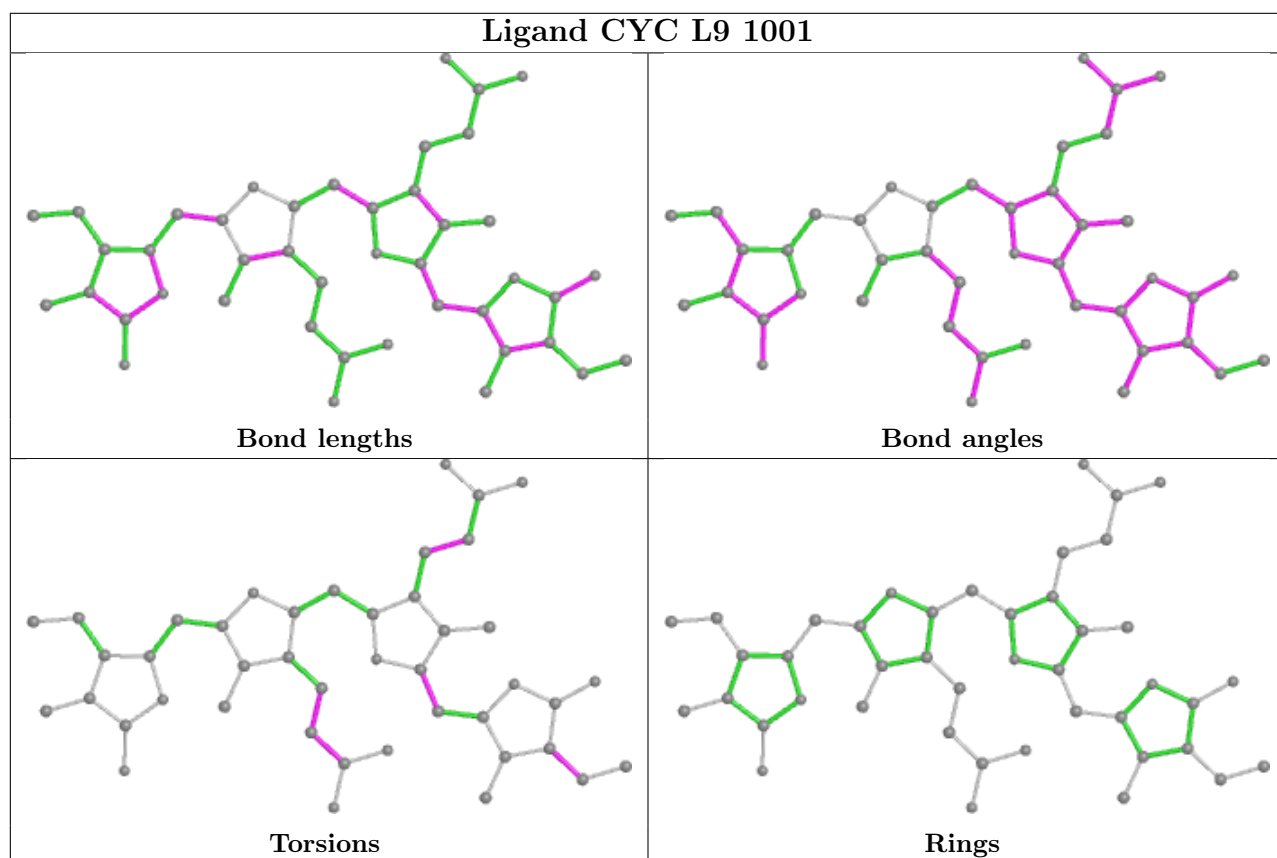
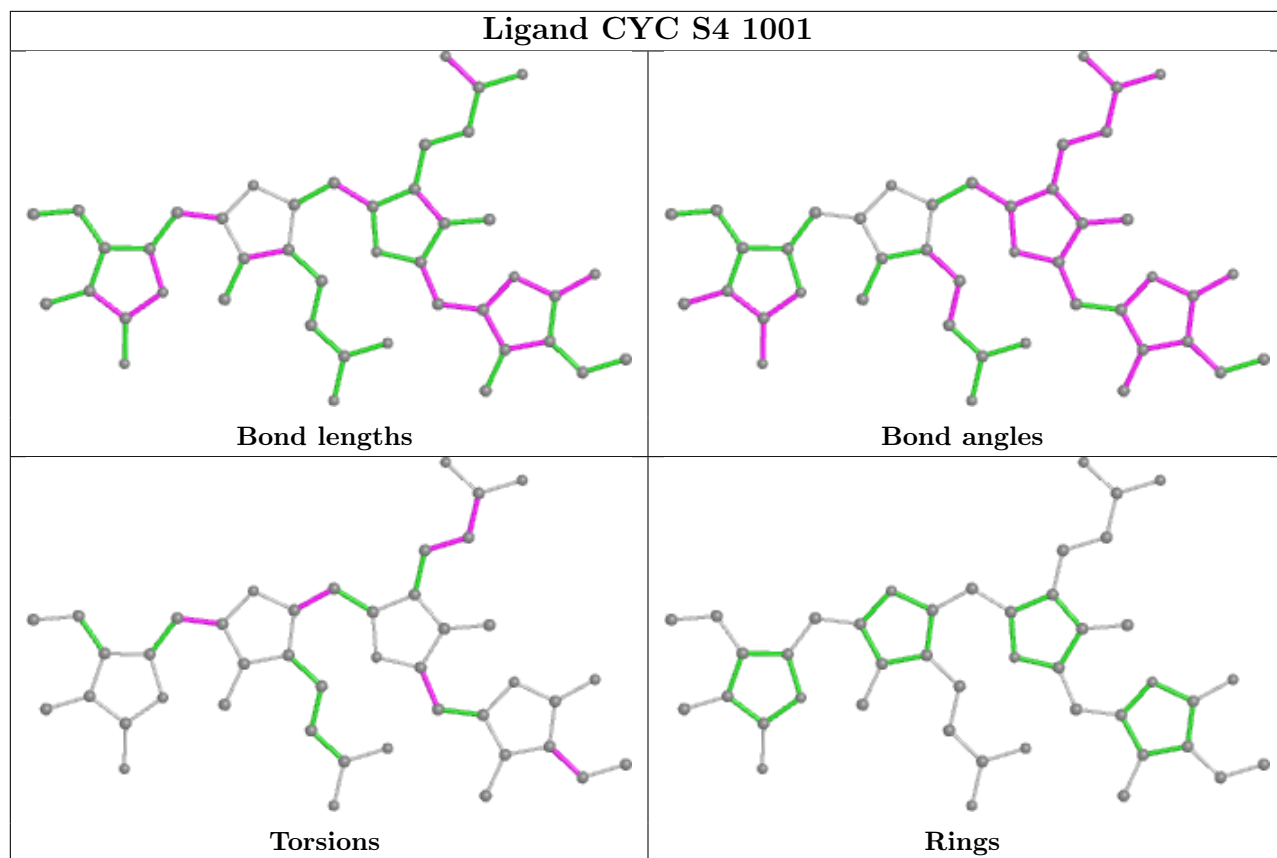


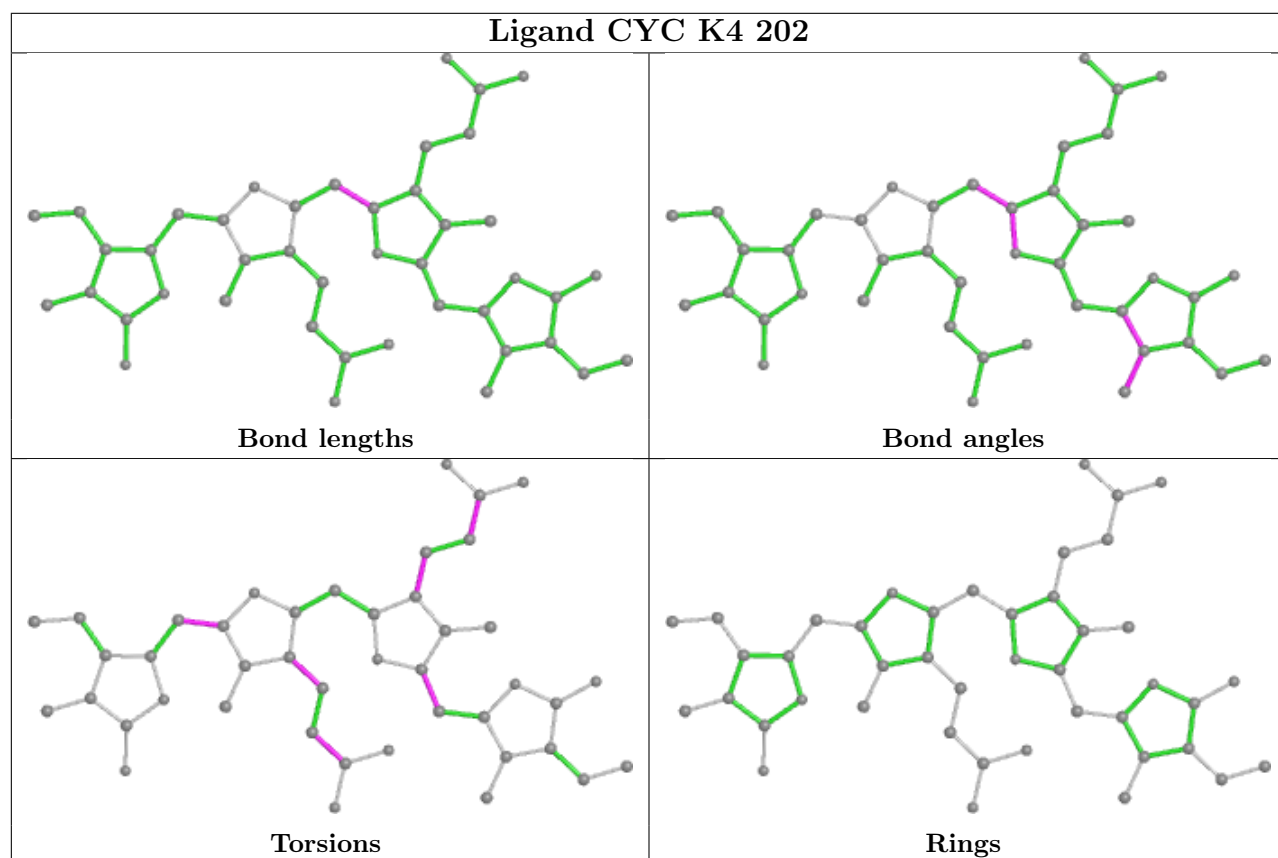
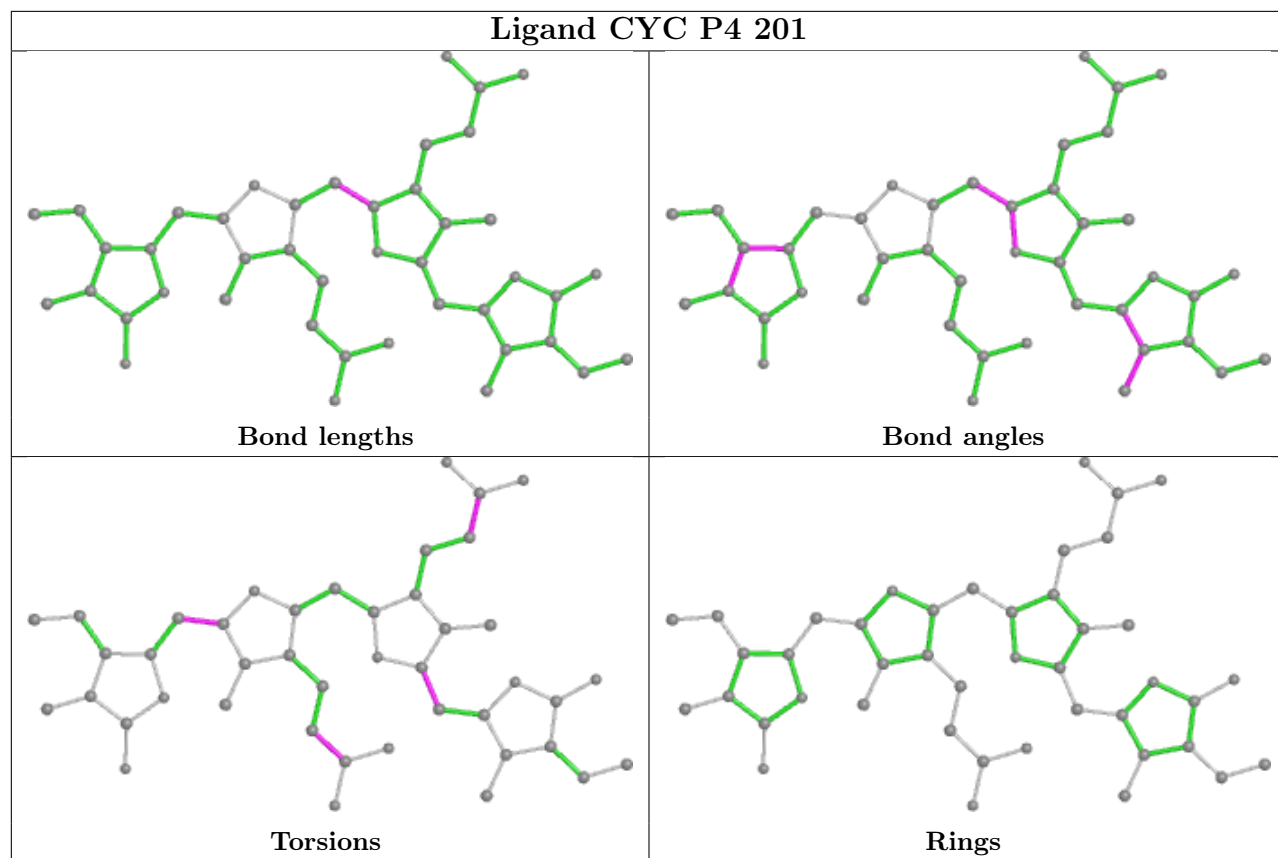


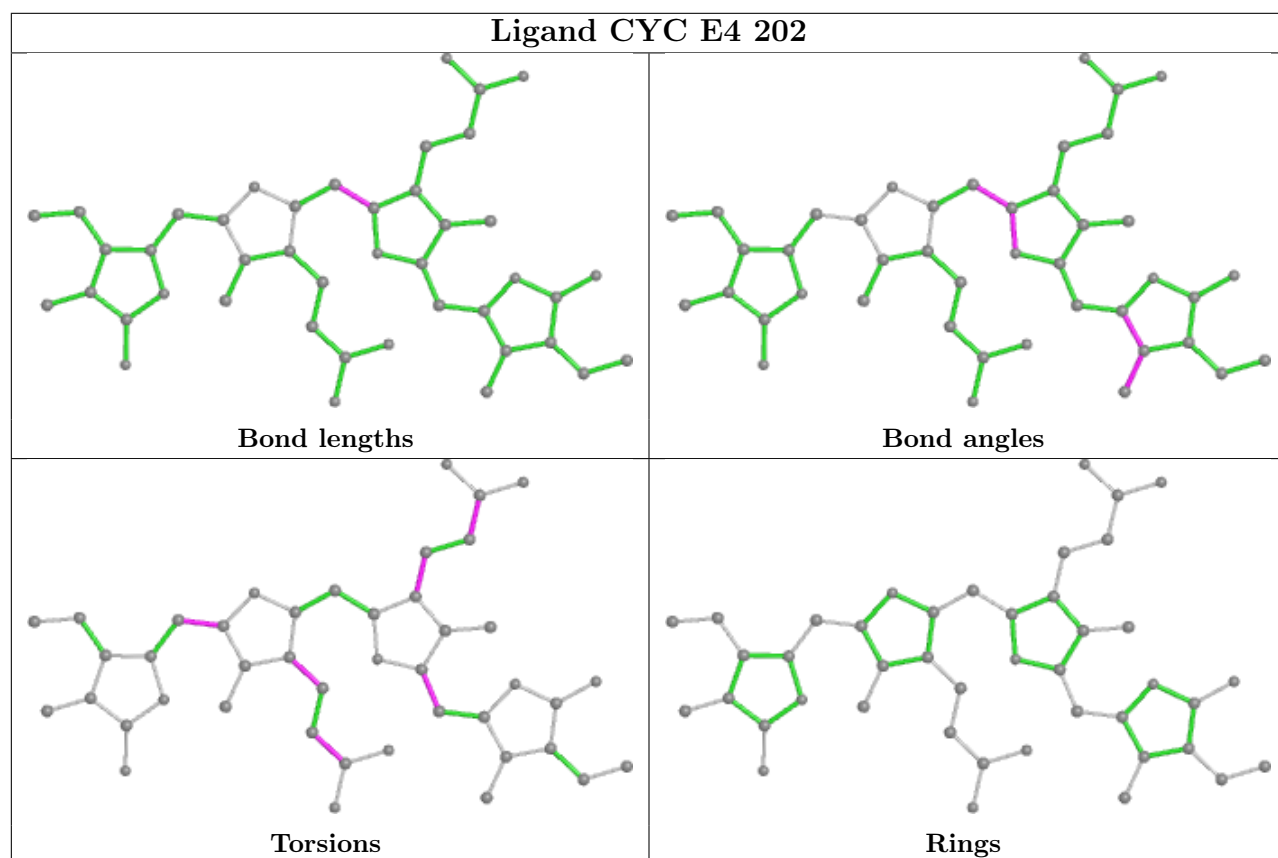
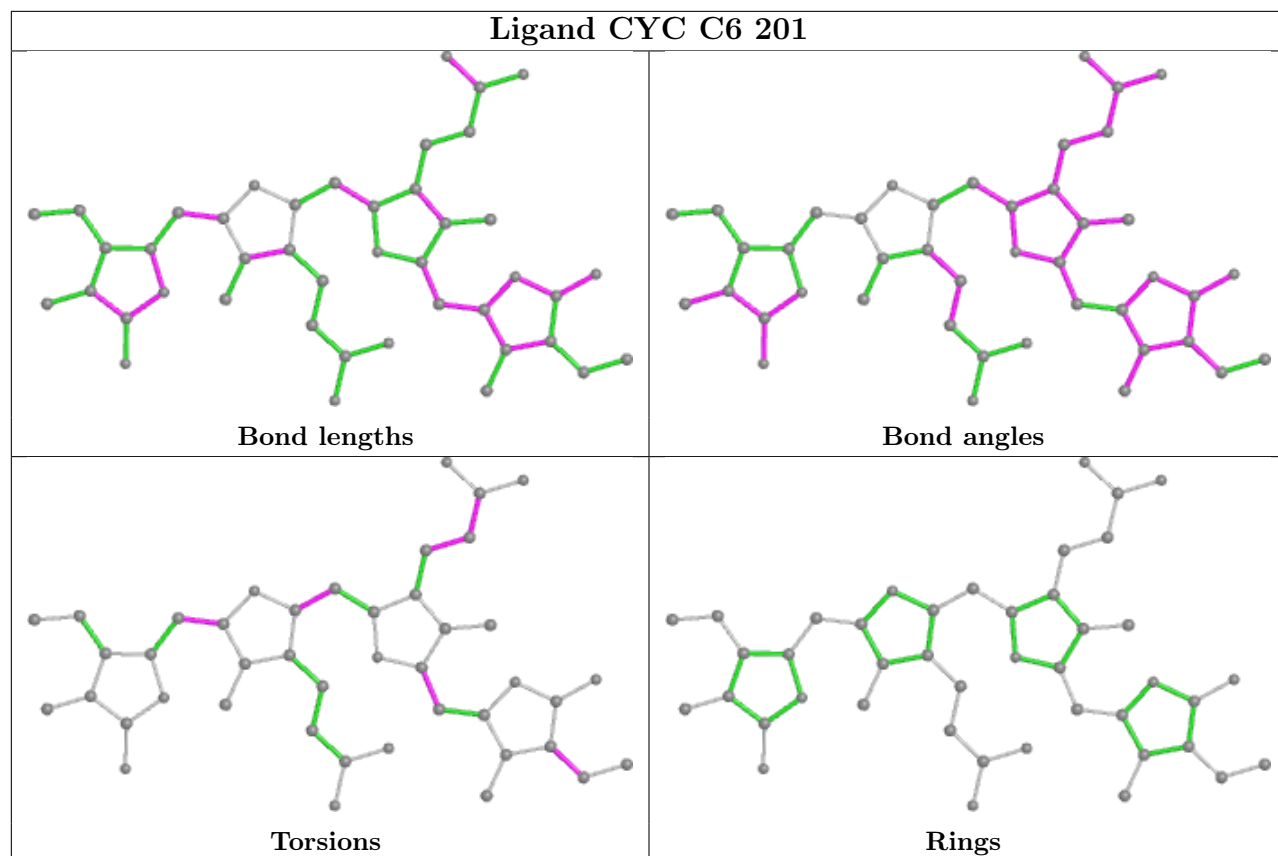


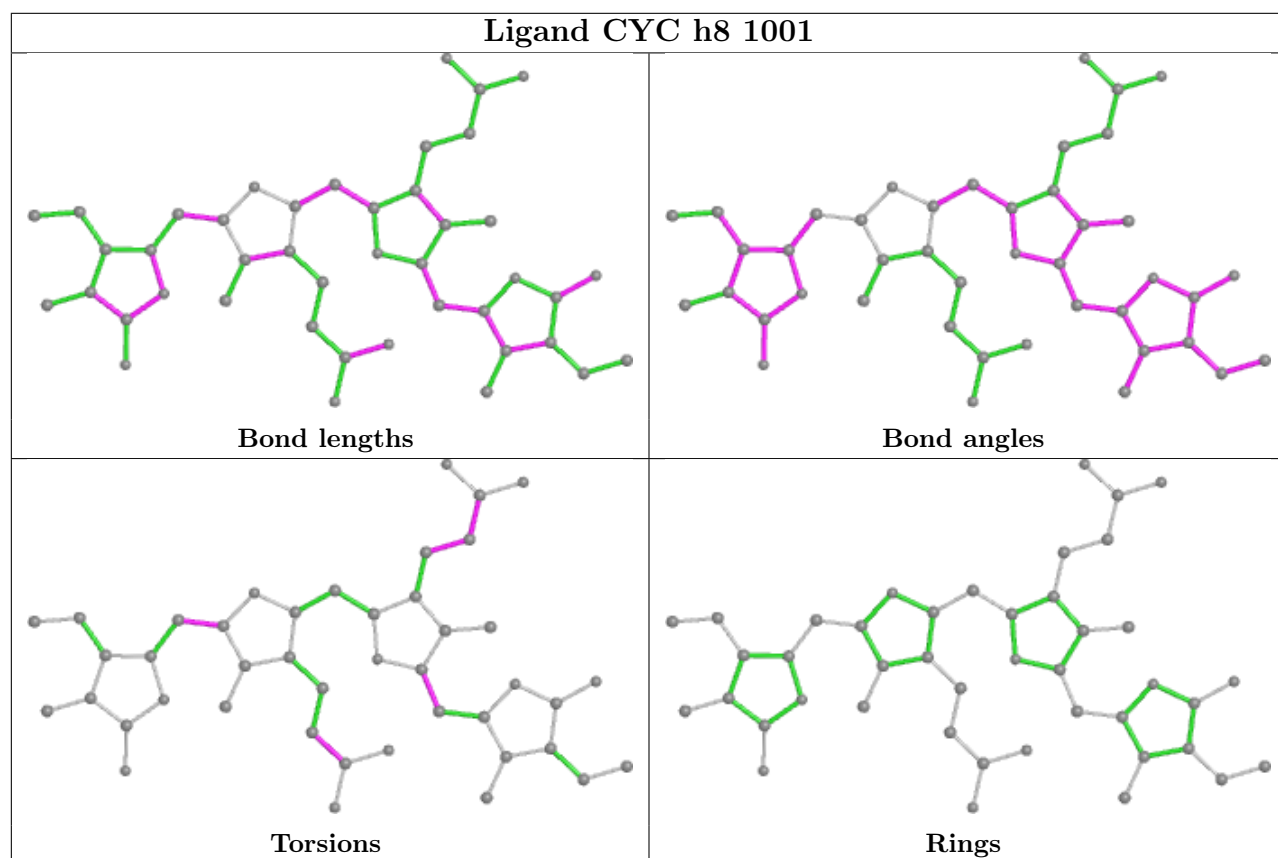
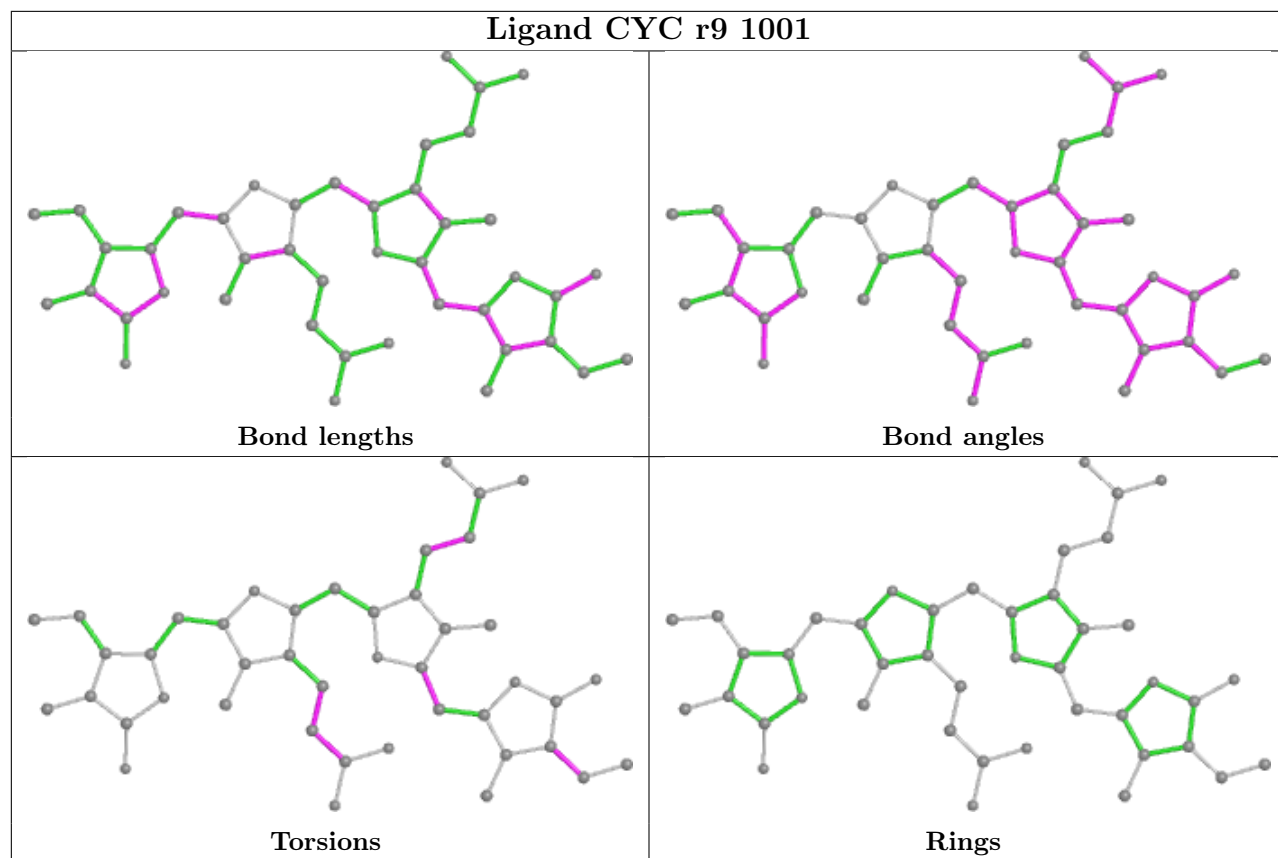


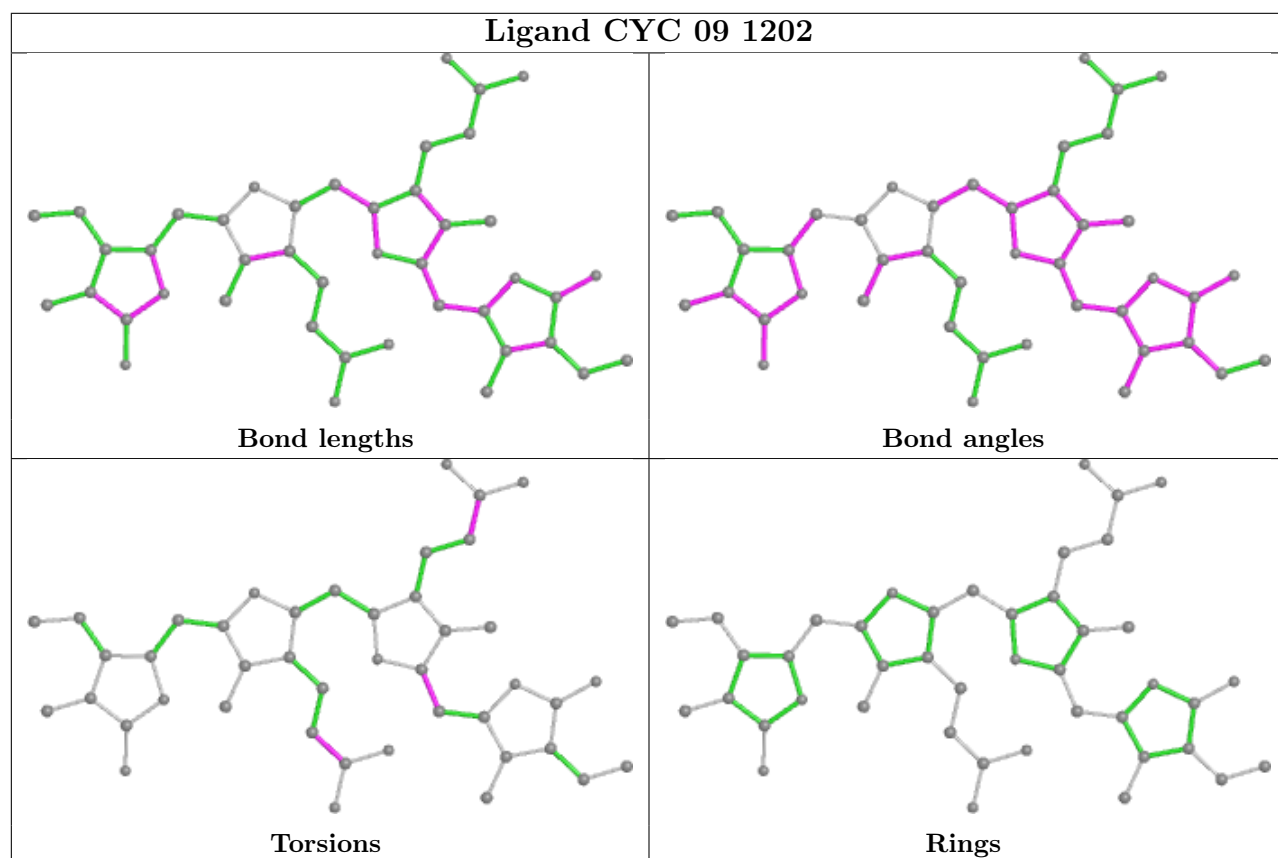
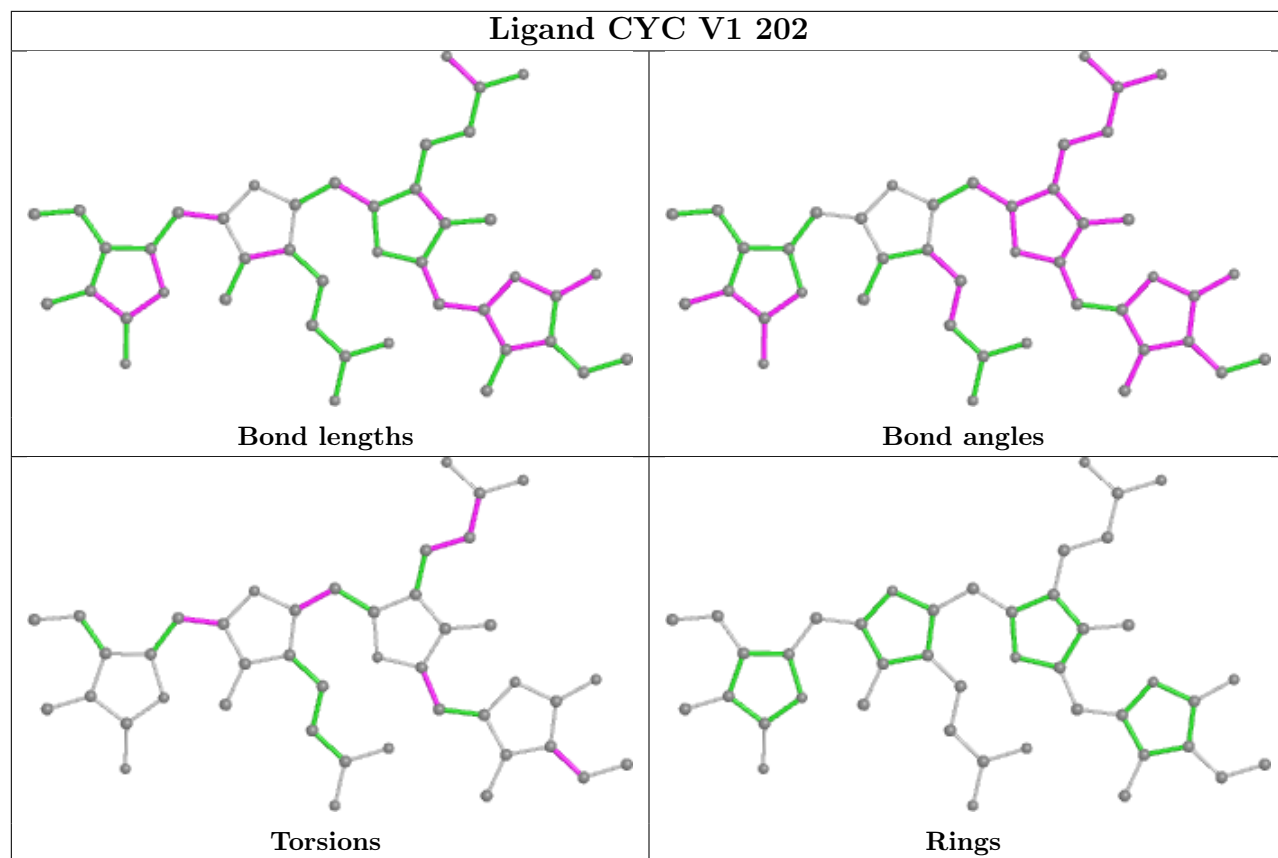


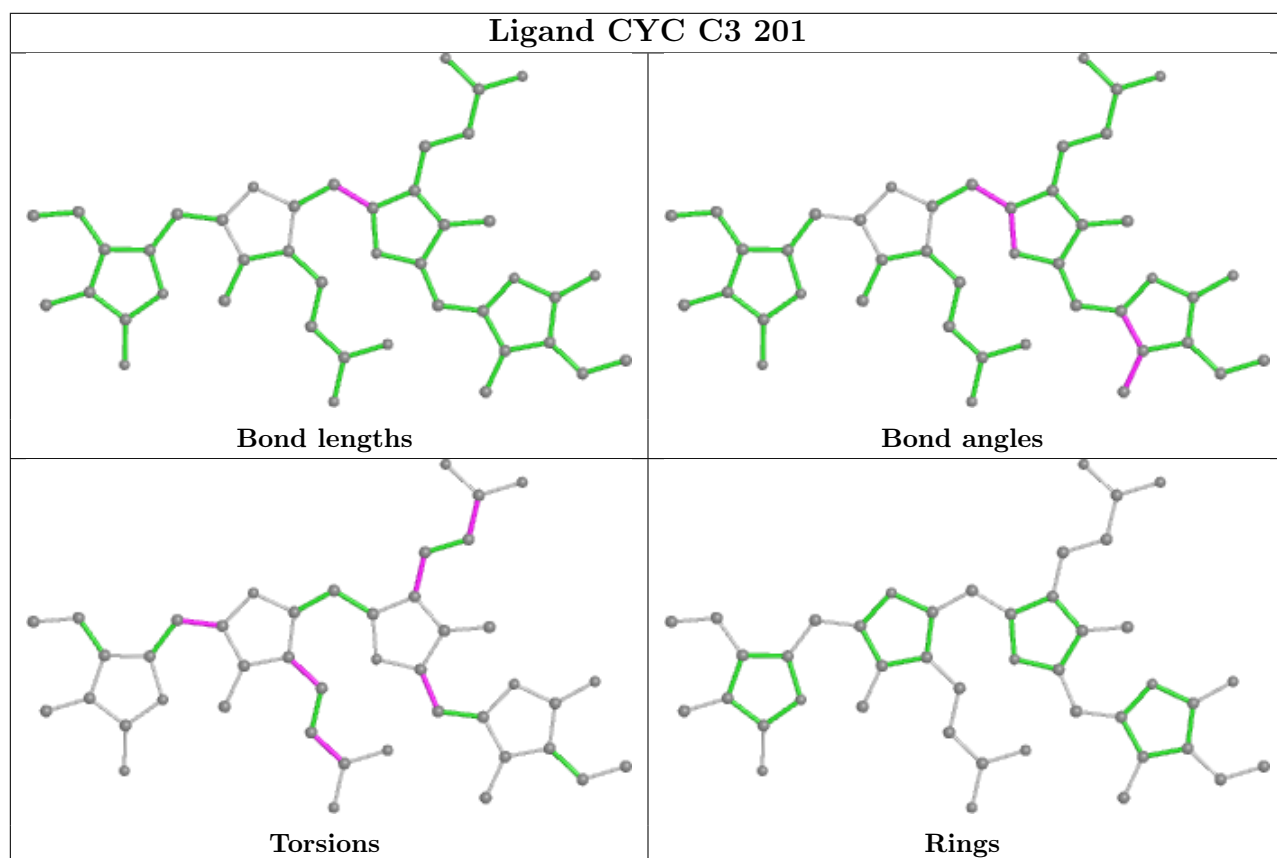
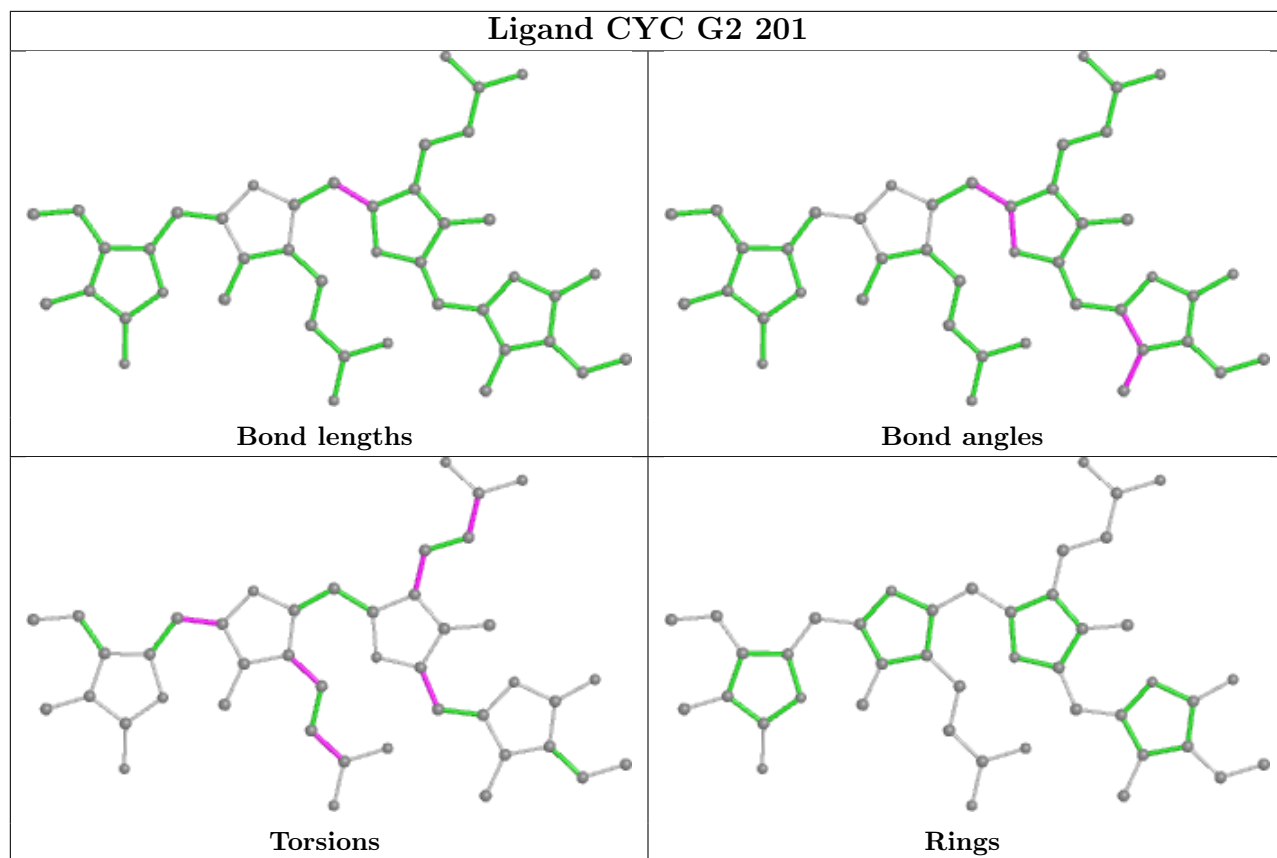


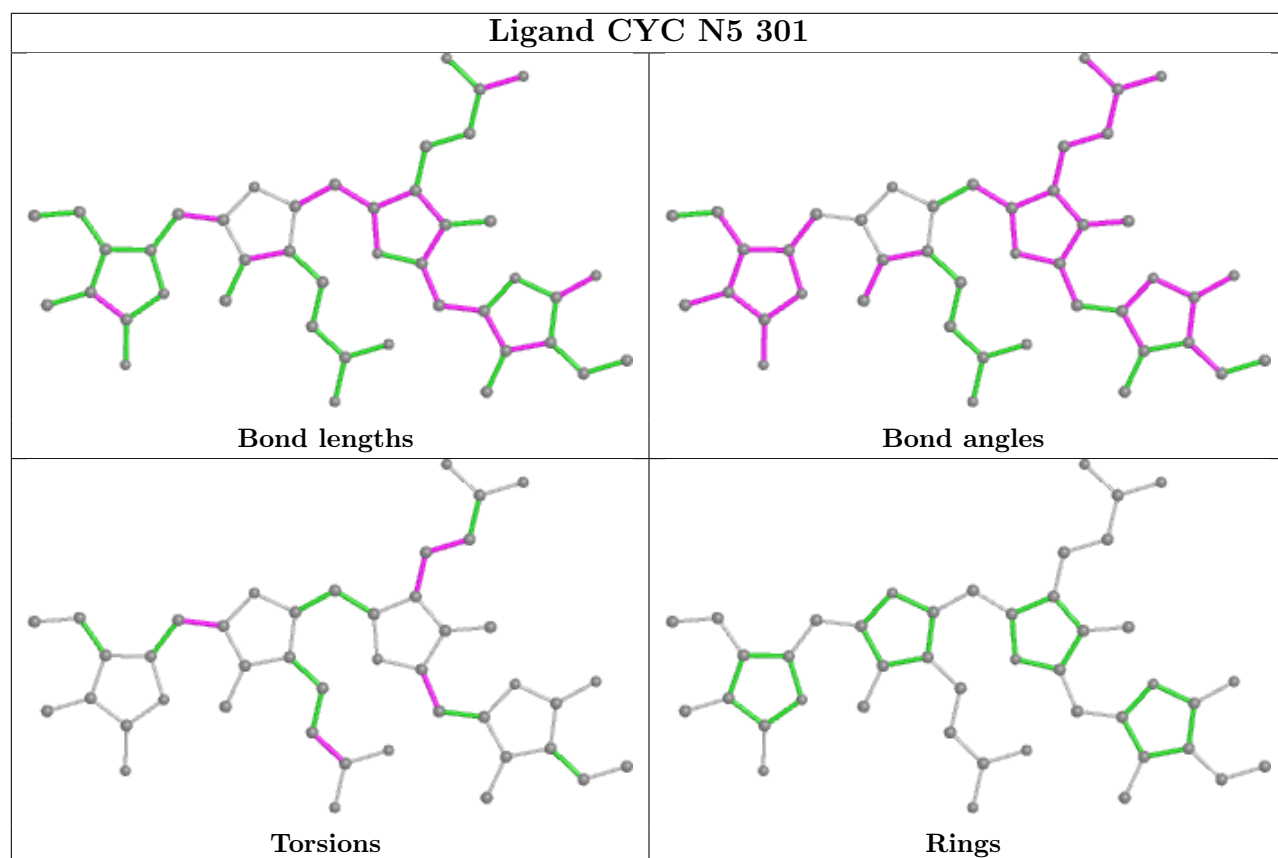
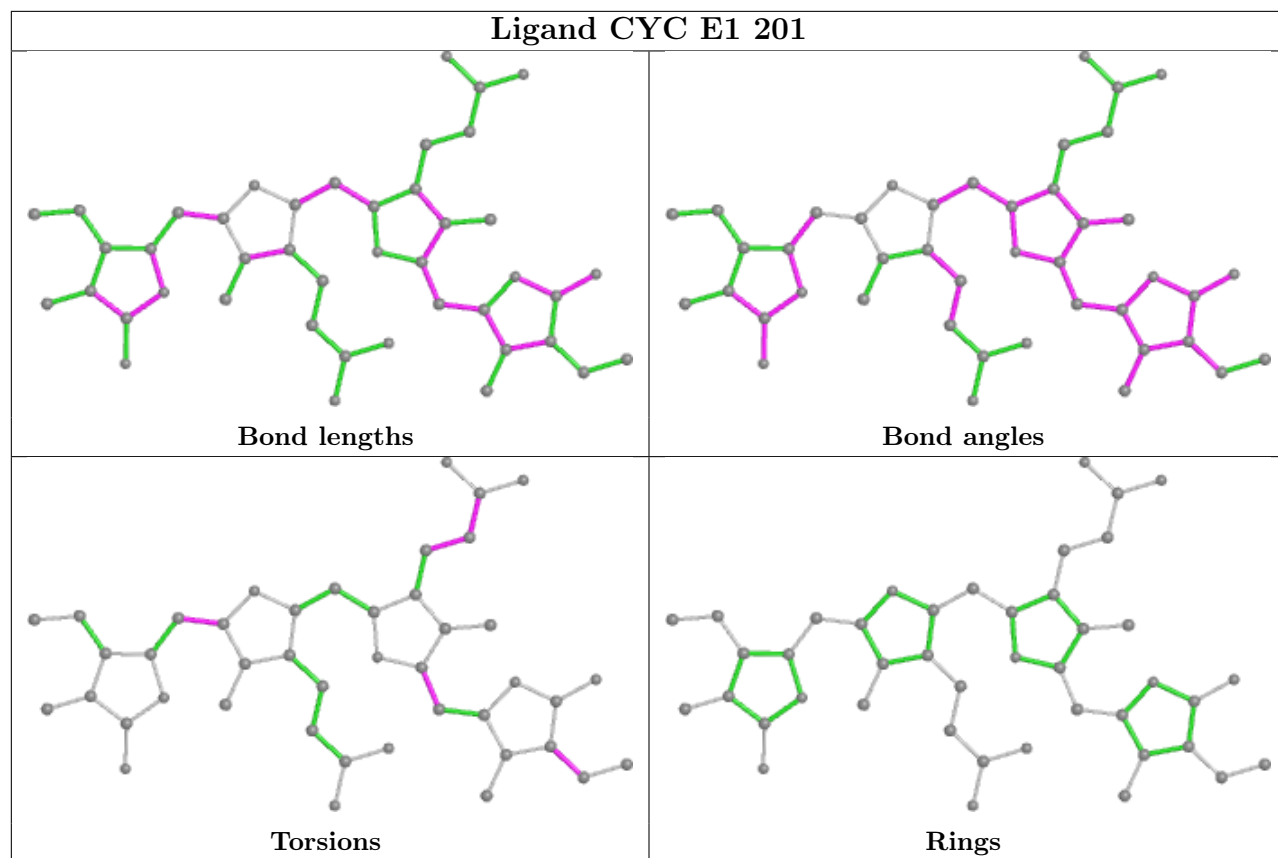


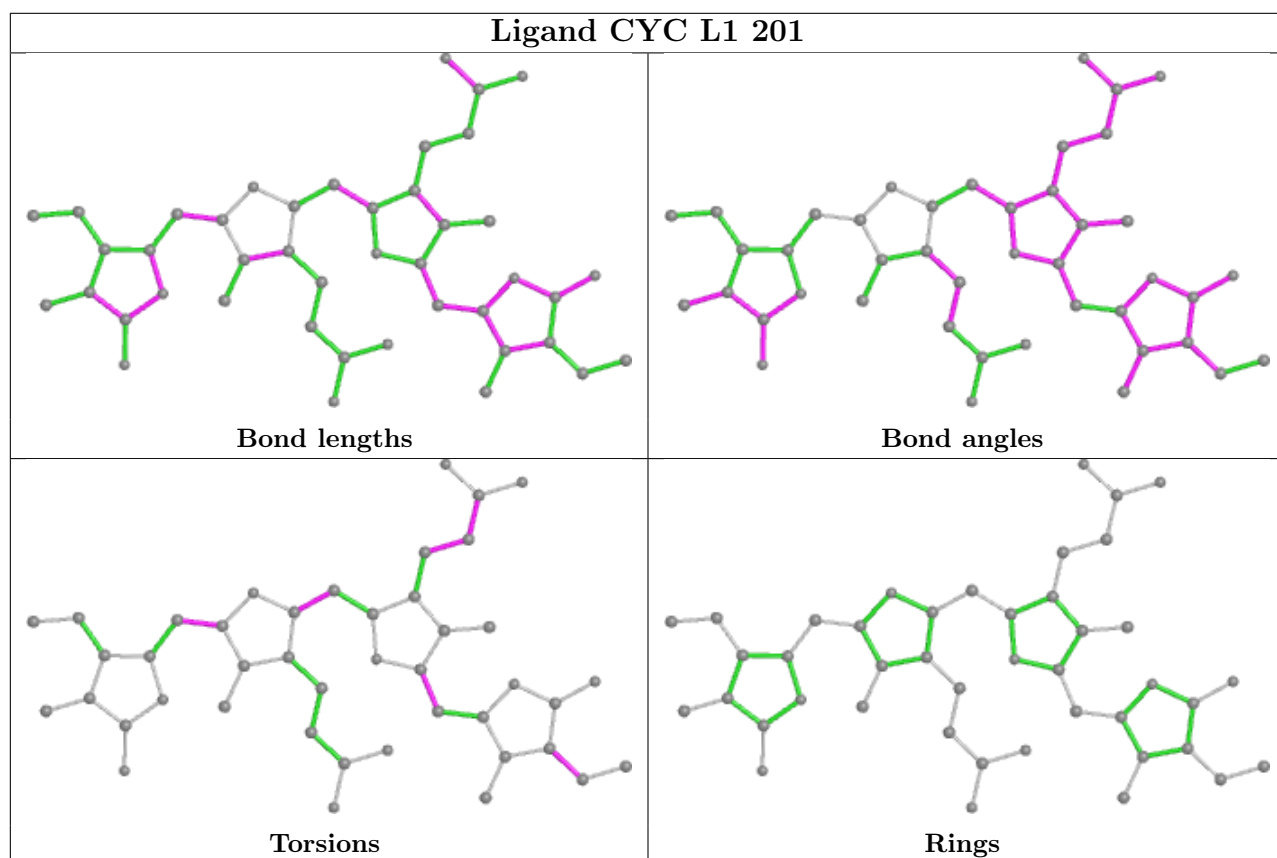
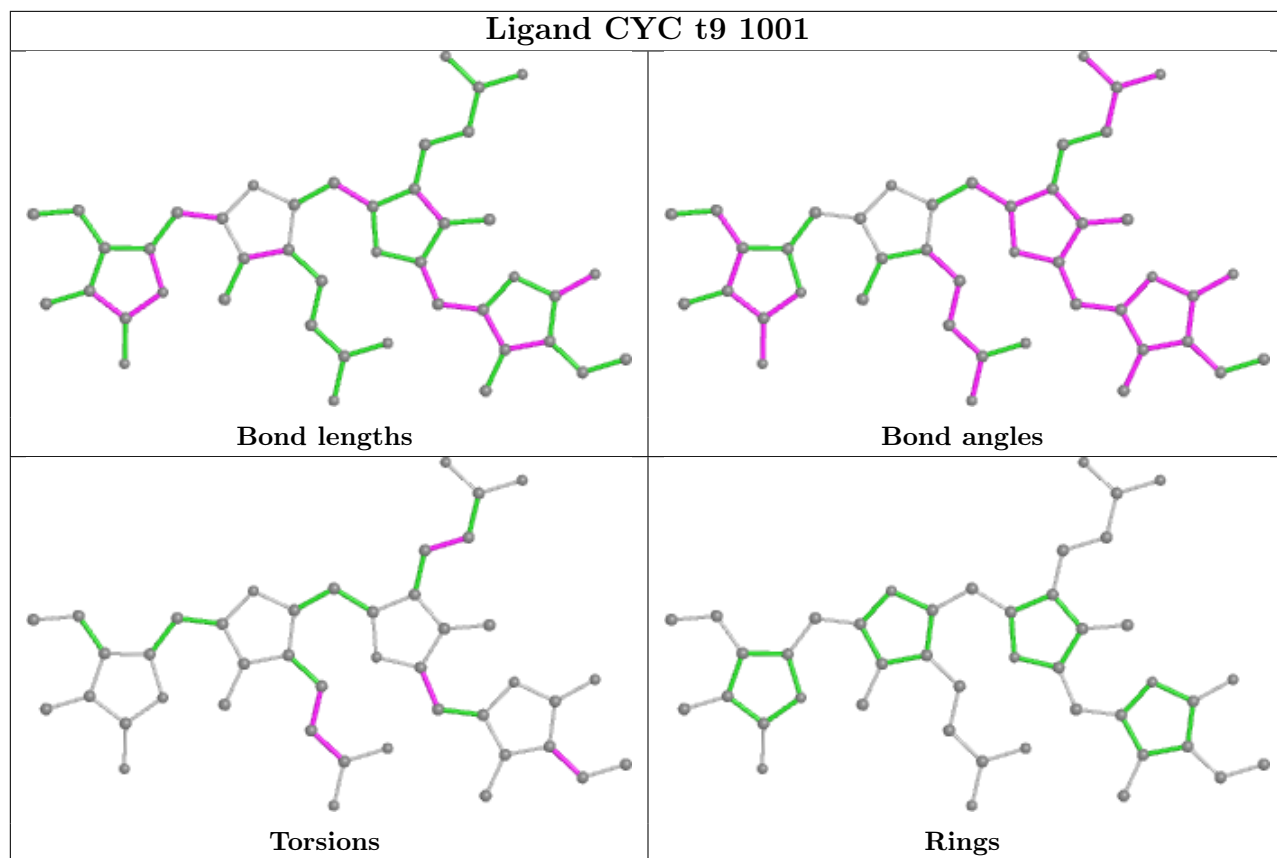


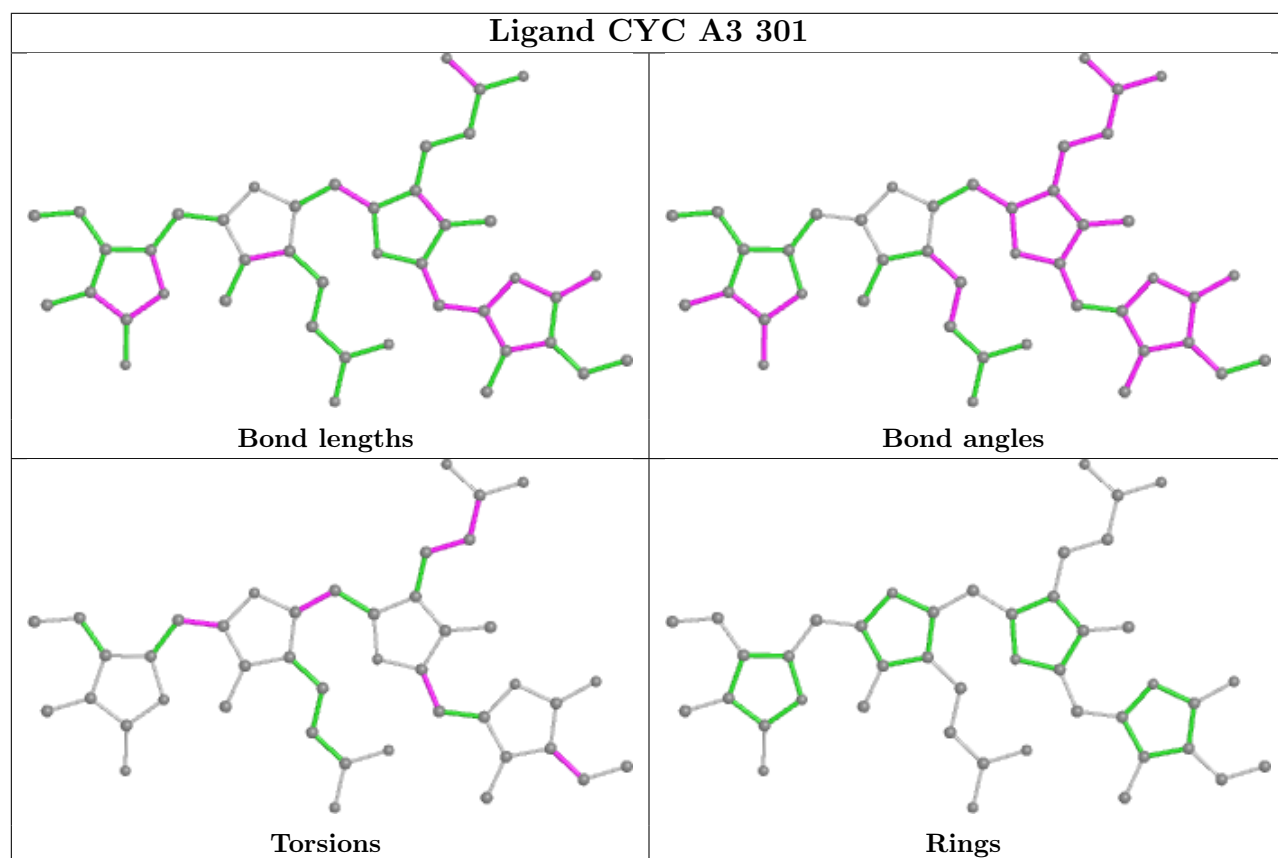
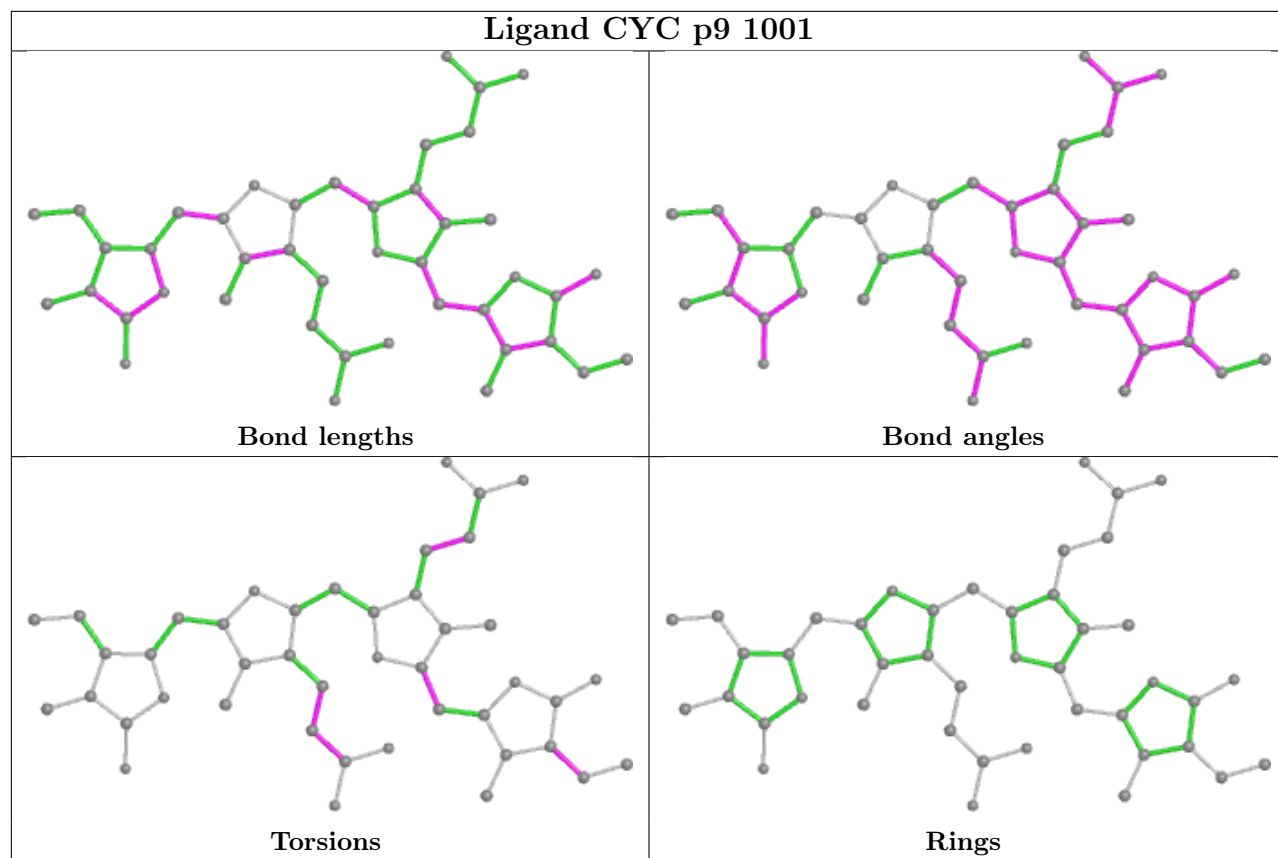


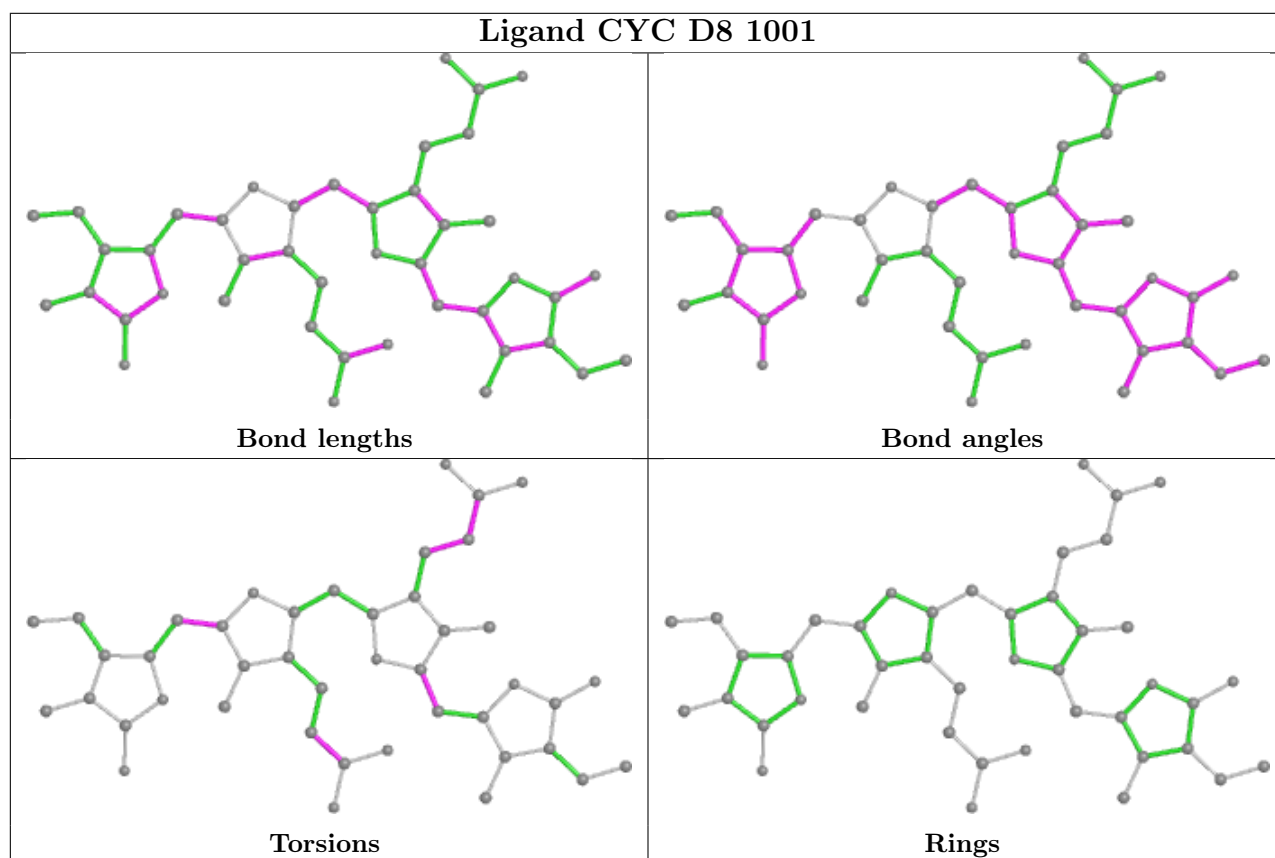
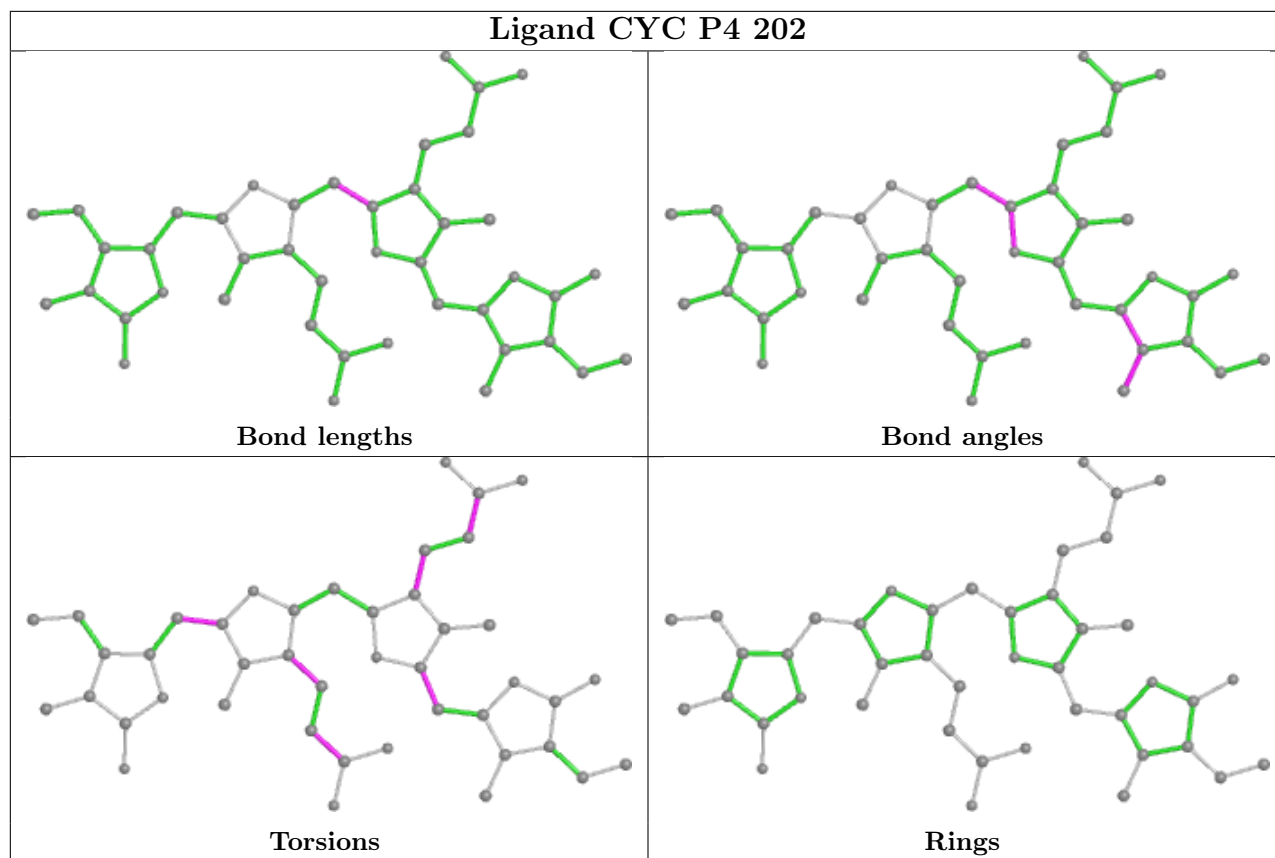


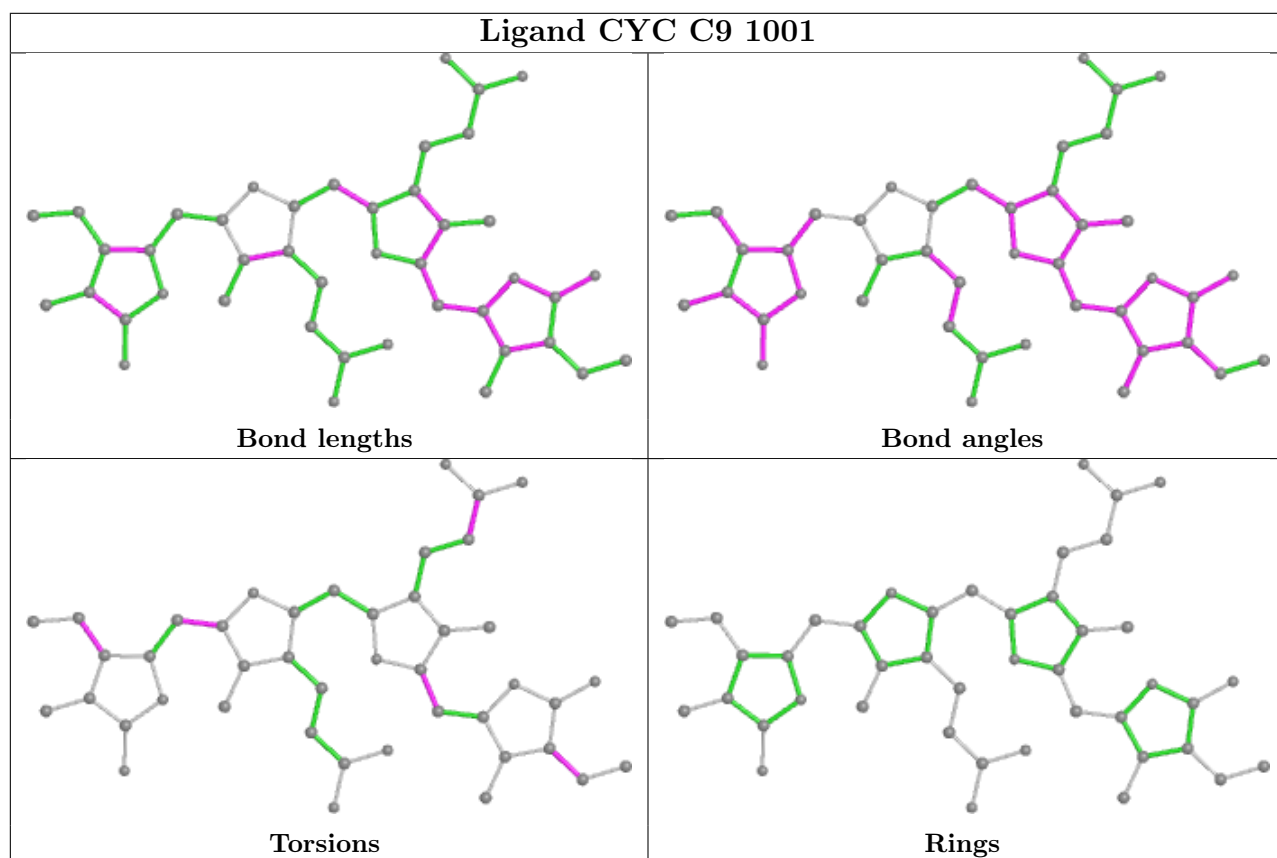
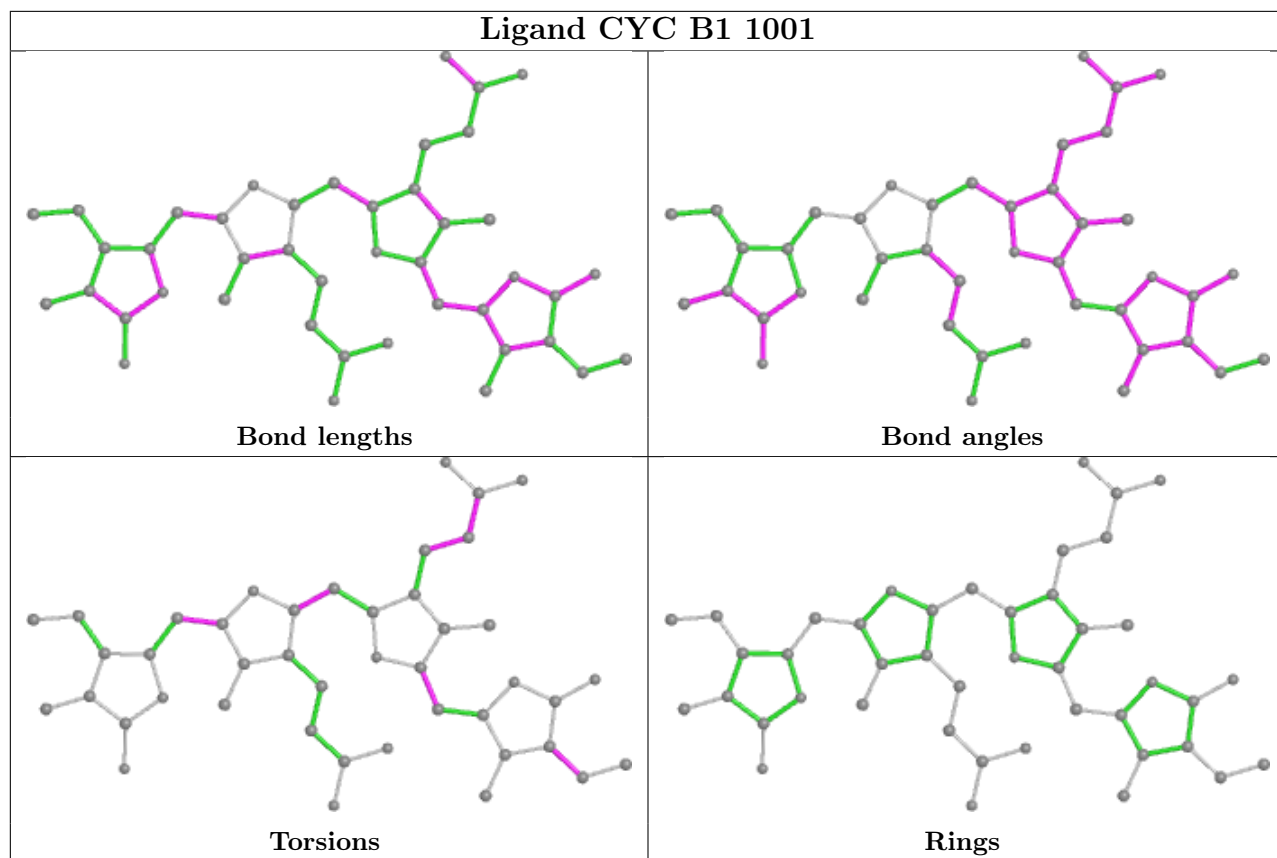


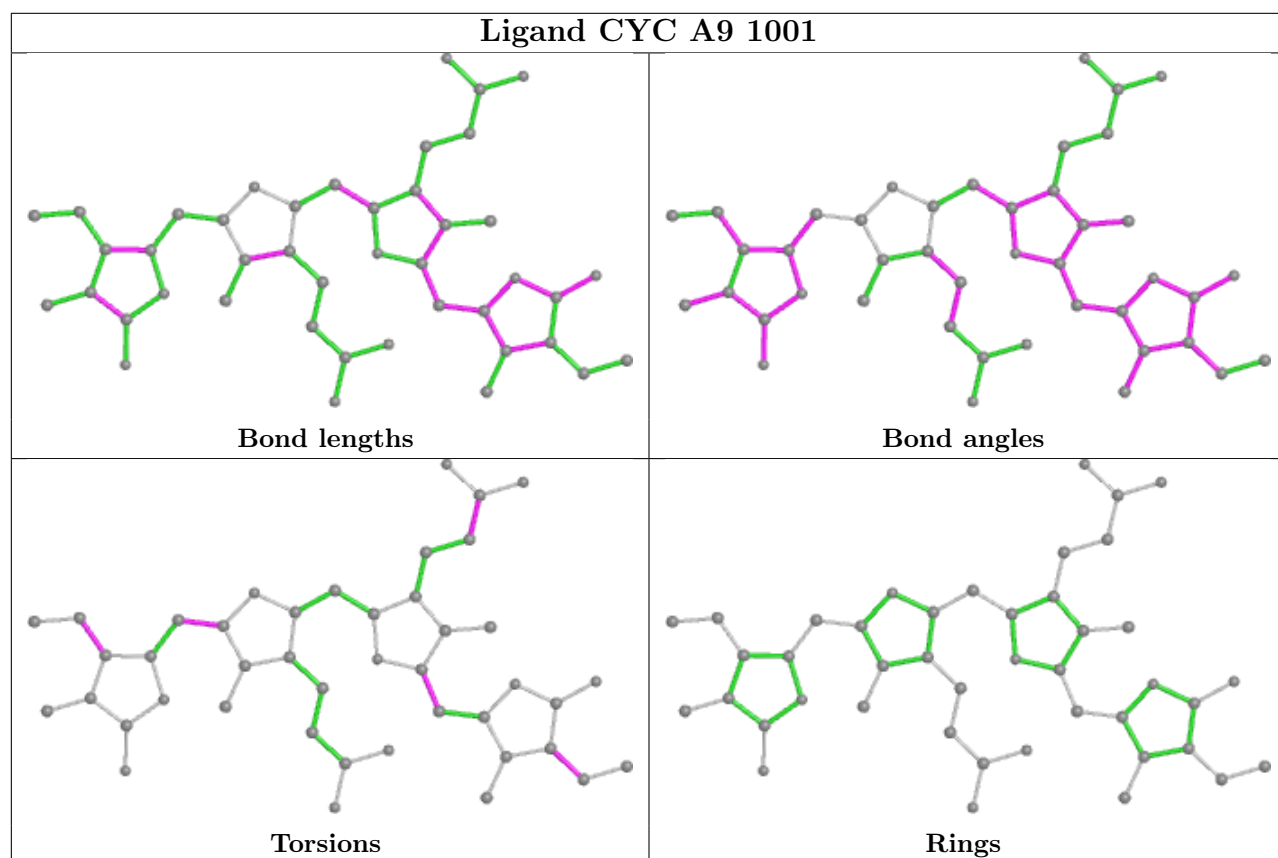
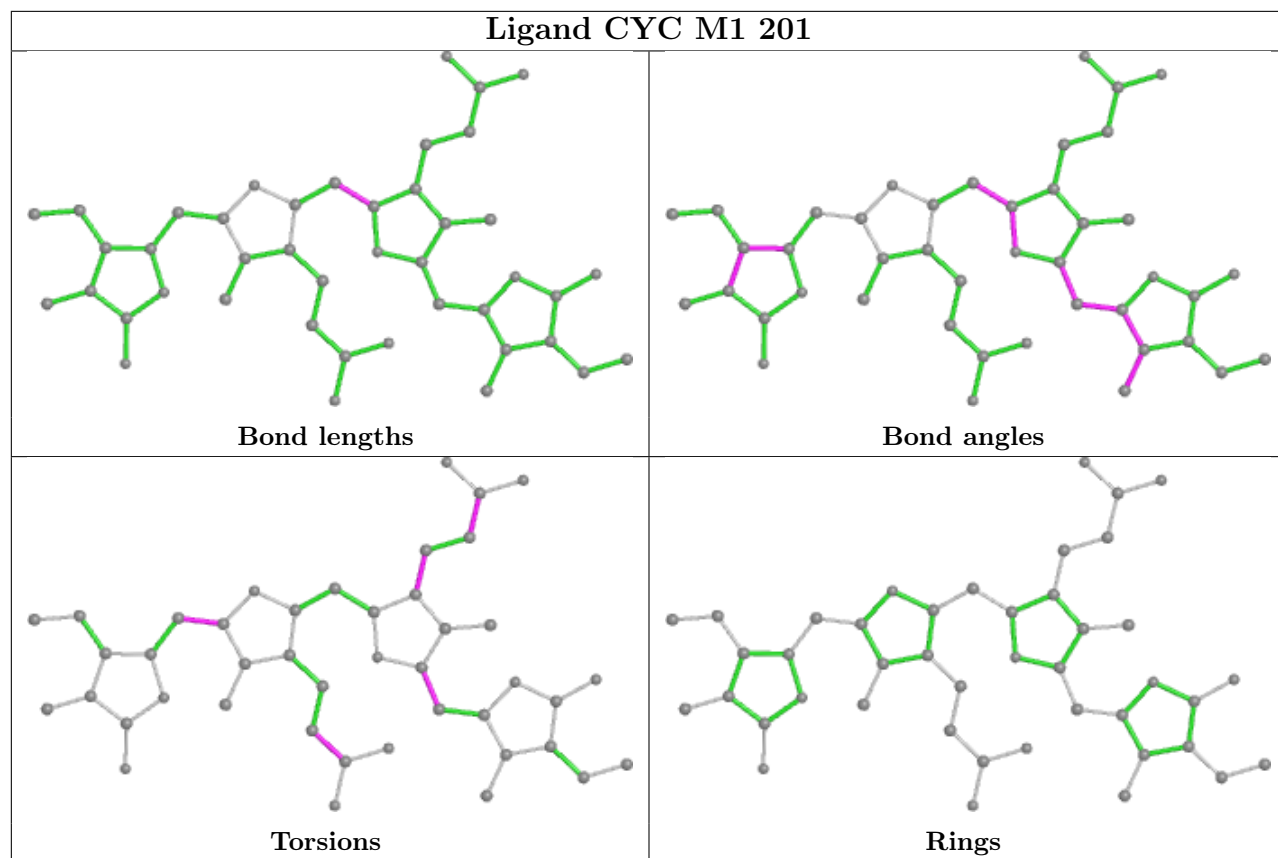


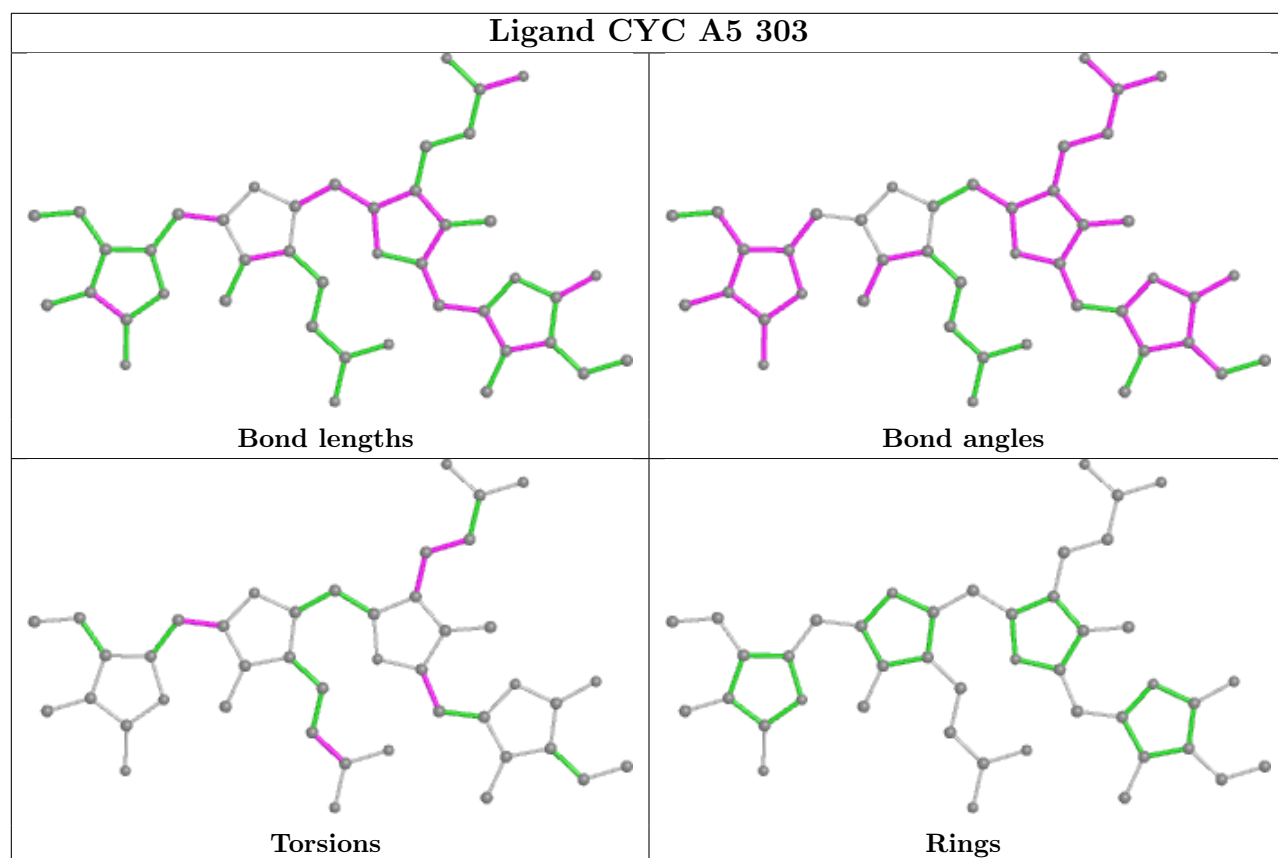
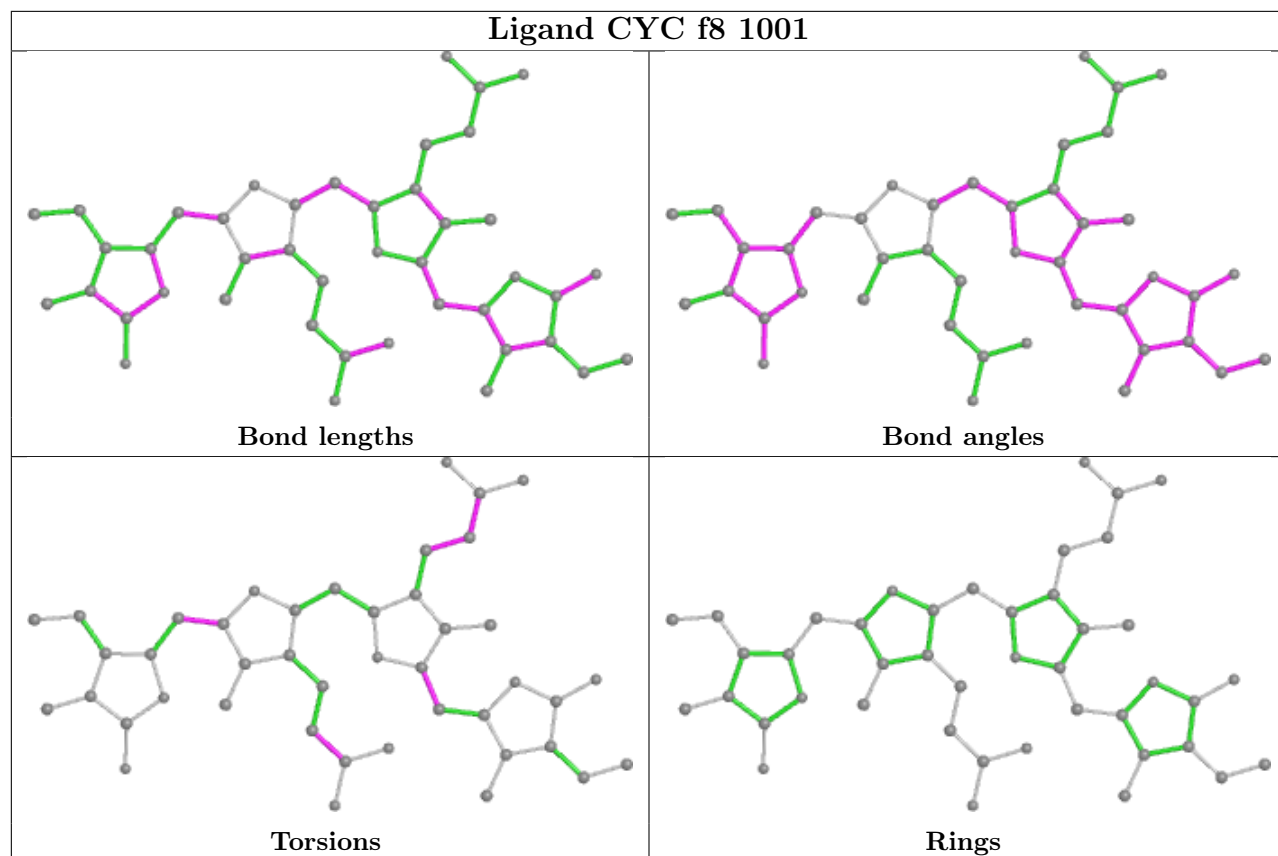


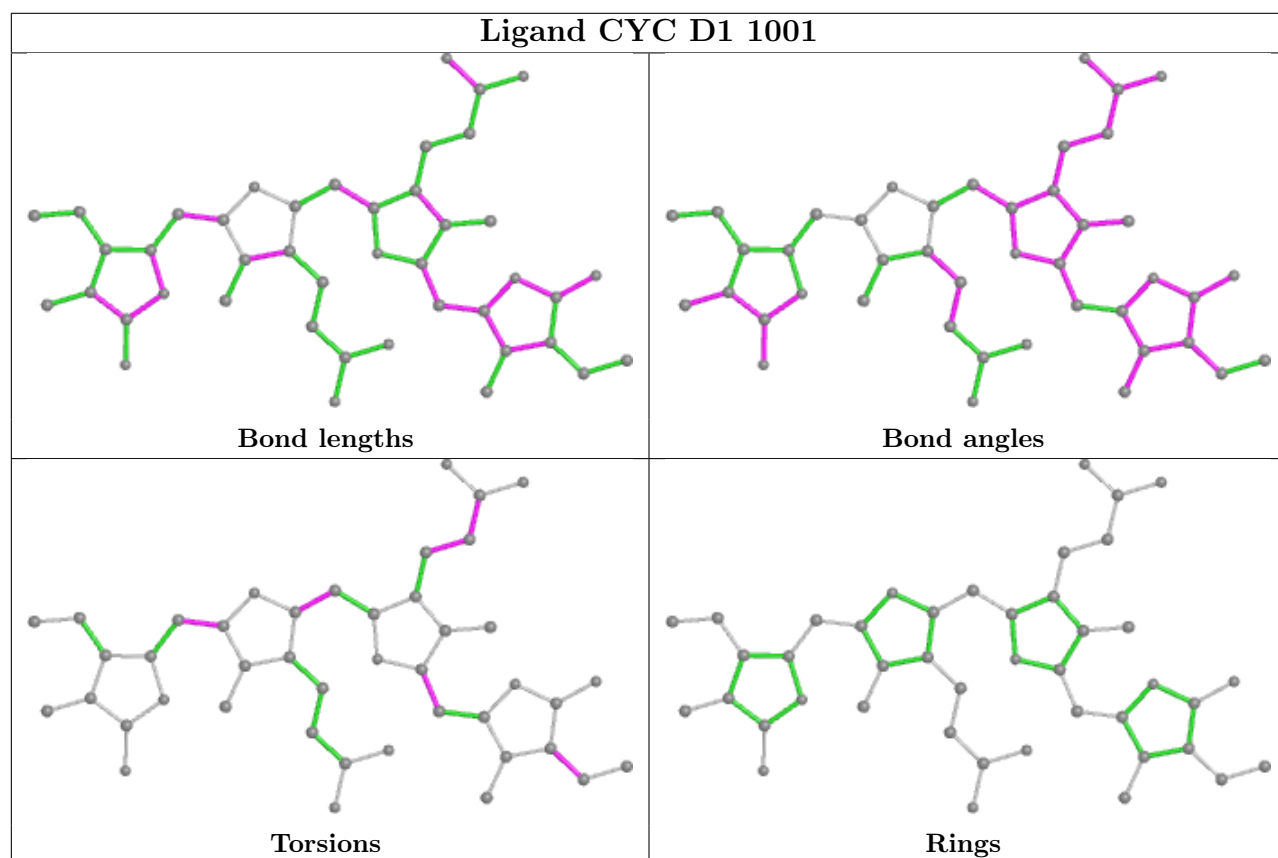
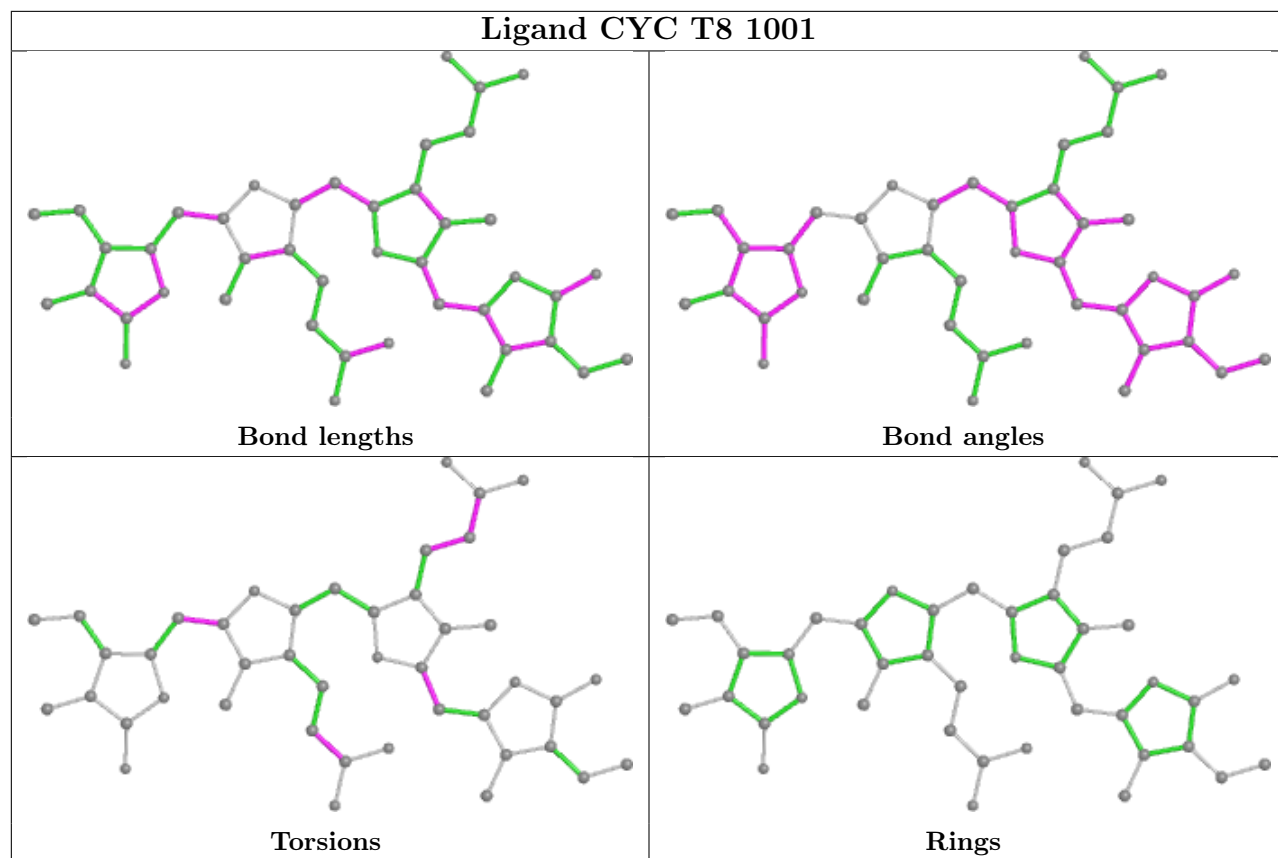












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

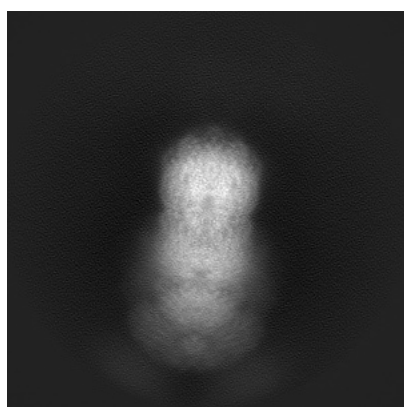
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31381. These allow visual inspection of the internal detail of the map and identification of artifacts.

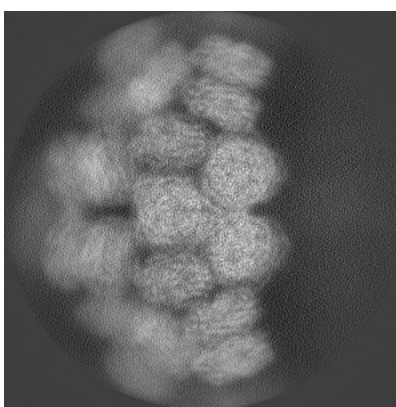
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

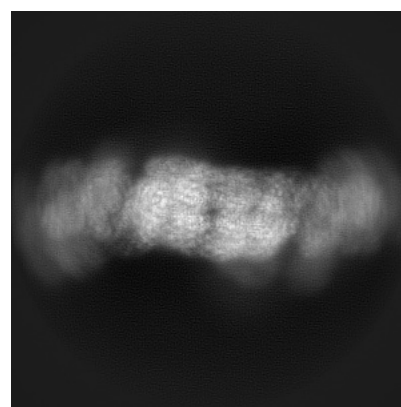
6.1.1 Primary map



X



Y

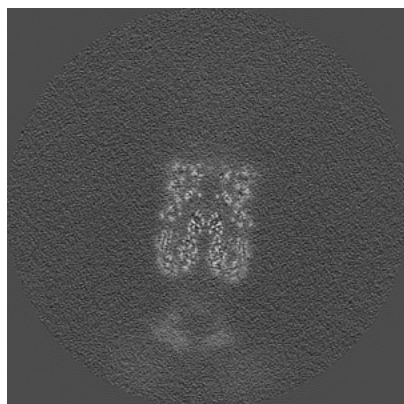


Z

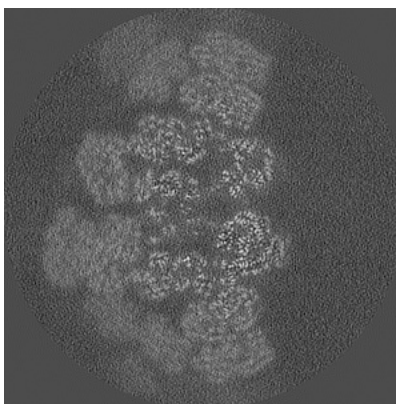
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

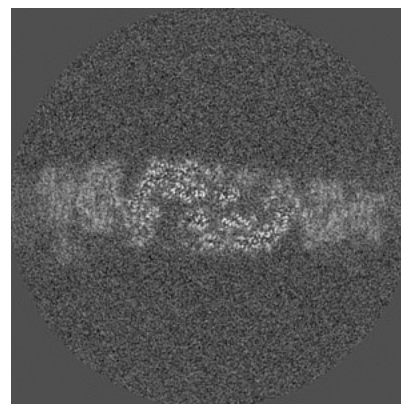
6.2.1 Primary map



X Index: 250



Y Index: 250

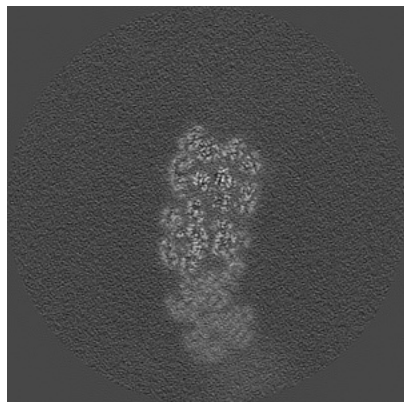


Z Index: 250

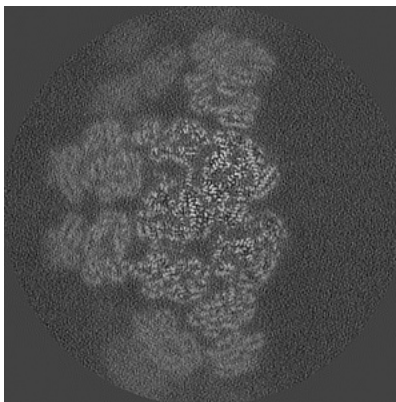
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

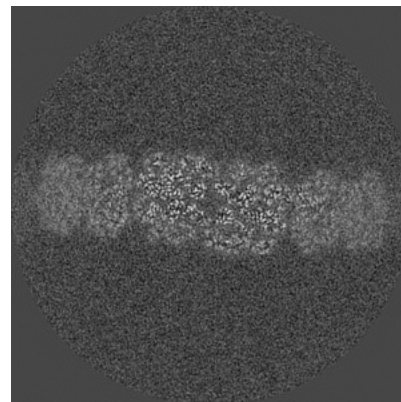
6.3.1 Primary map



X Index: 223



Y Index: 232

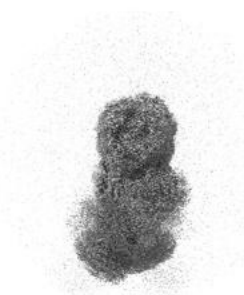


Z Index: 275

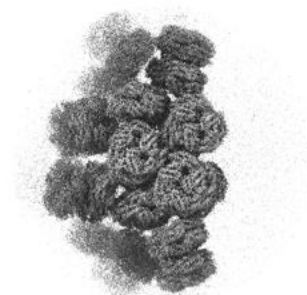
The images above show the largest variance slices of the map in three orthogonal directions.

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 0.0195. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

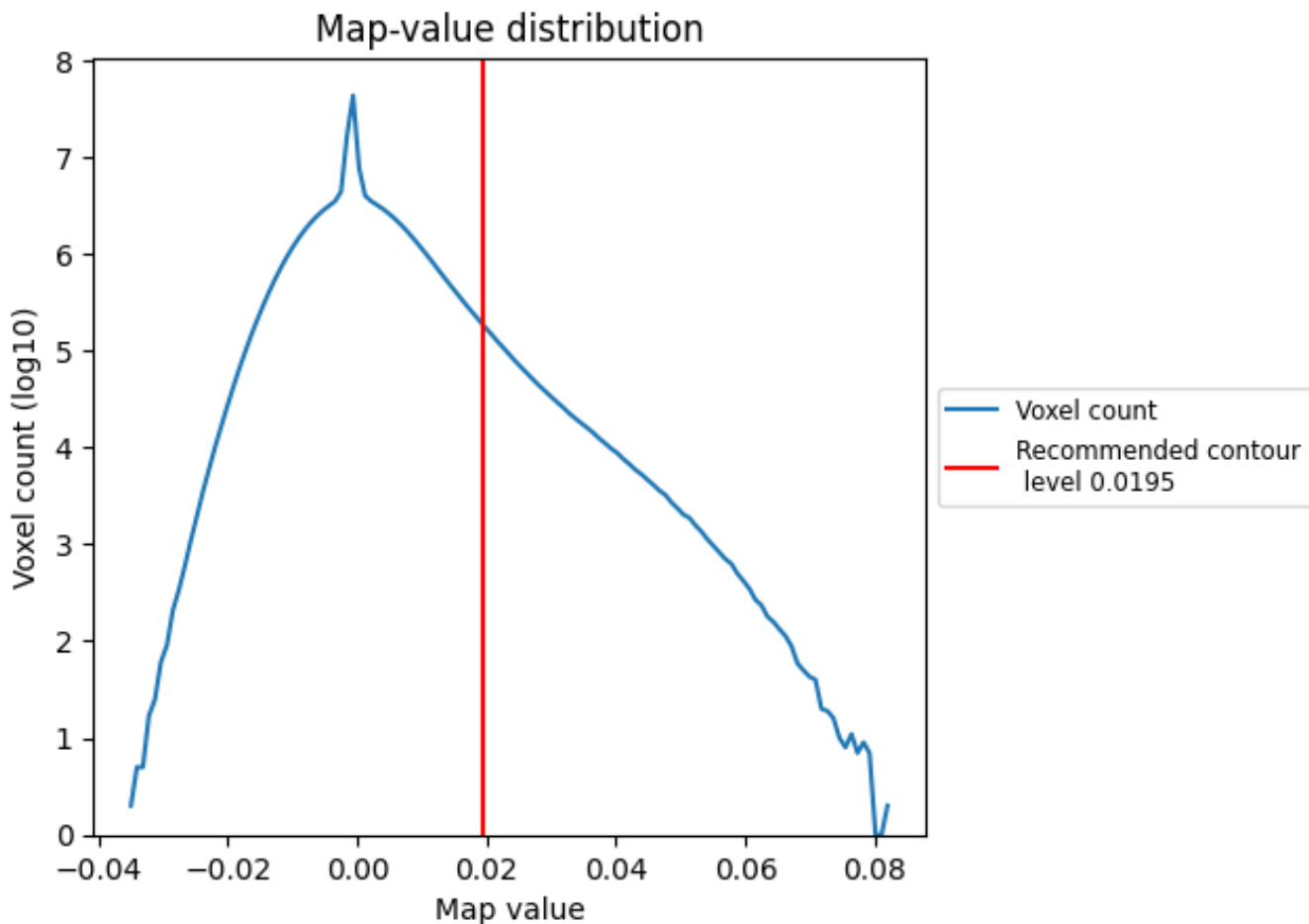
6.5 Mask visualisation

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

7 Map analysis [i](#)

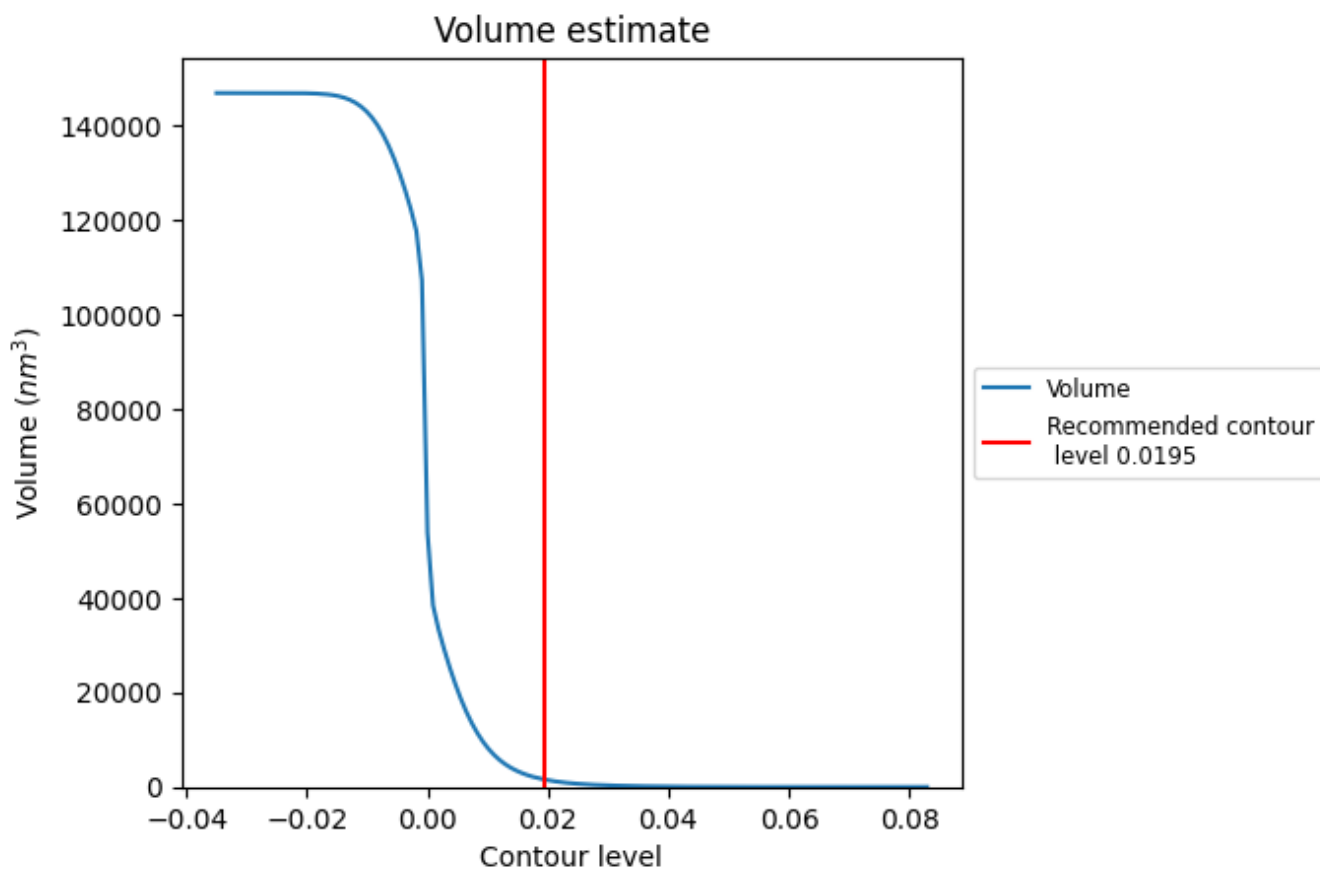
This section contains the results of statistical analysis of the map.

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.

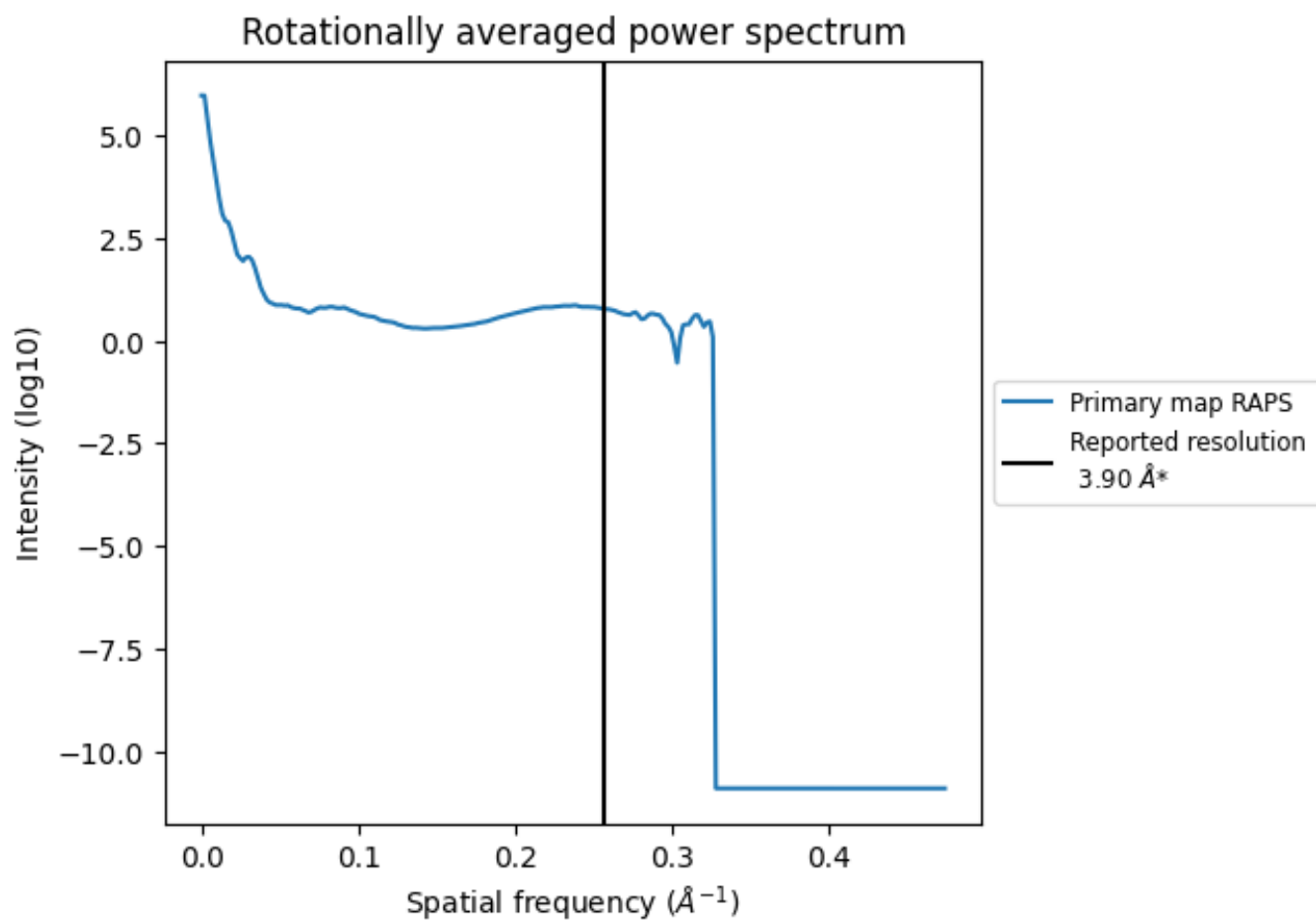
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 1555 nm³; this corresponds to an approximate mass of 1405 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 0.256 Å⁻¹

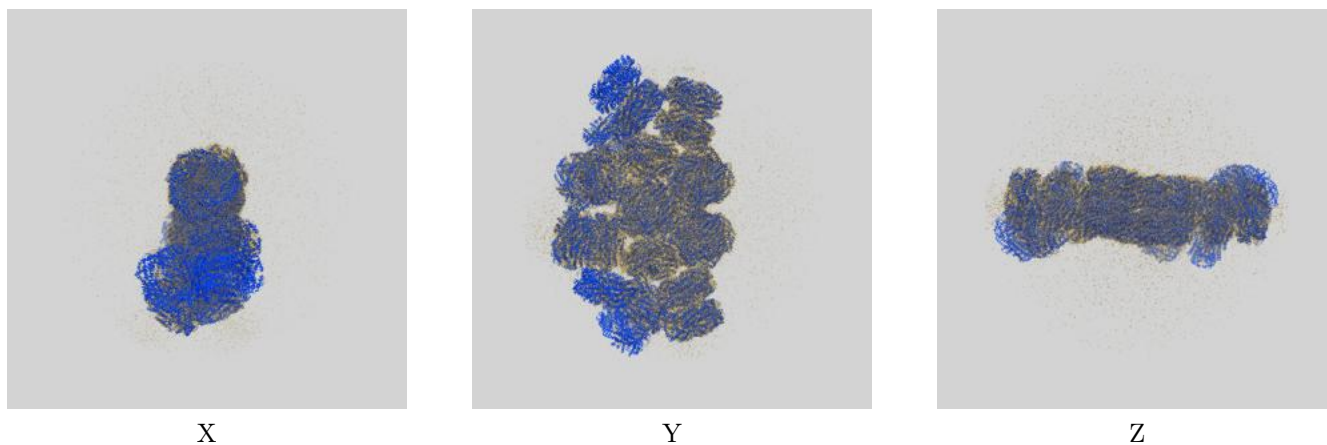
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

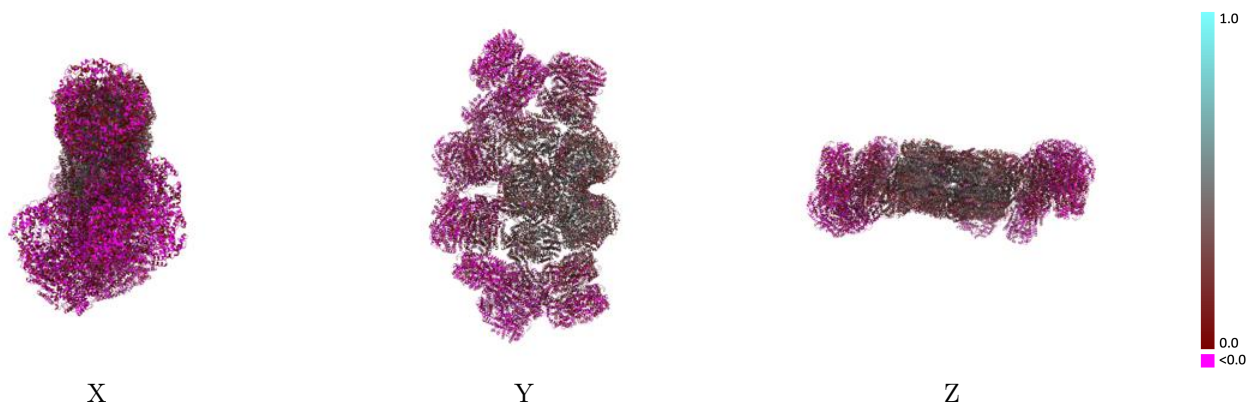
This section contains information regarding the fit between EMDB map EMD-31381 and PDB model 7EYD. Per-residue inclusion information can be found in section 3 on page 47.

9.1 Map-model overlay [i](#)



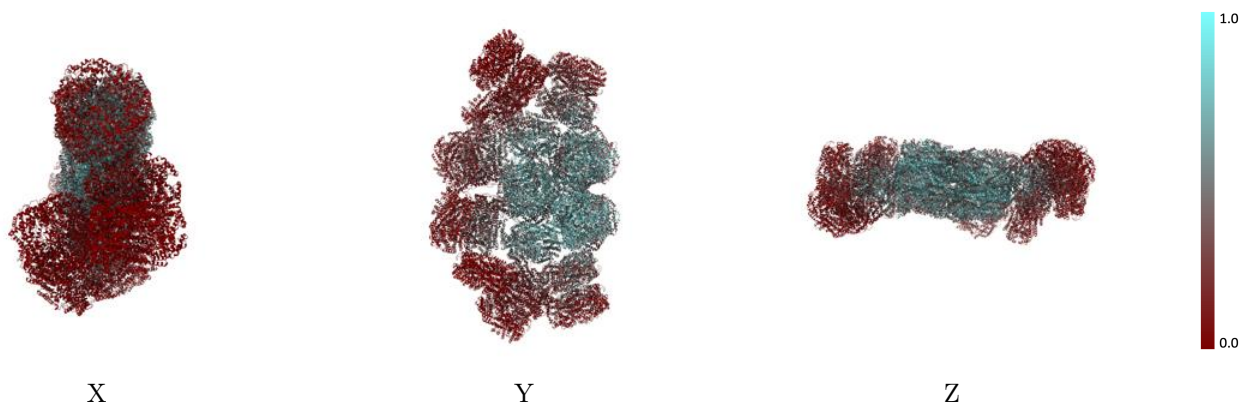
The images above show the 3D surface view of the map at the recommended contour level 0.0195 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



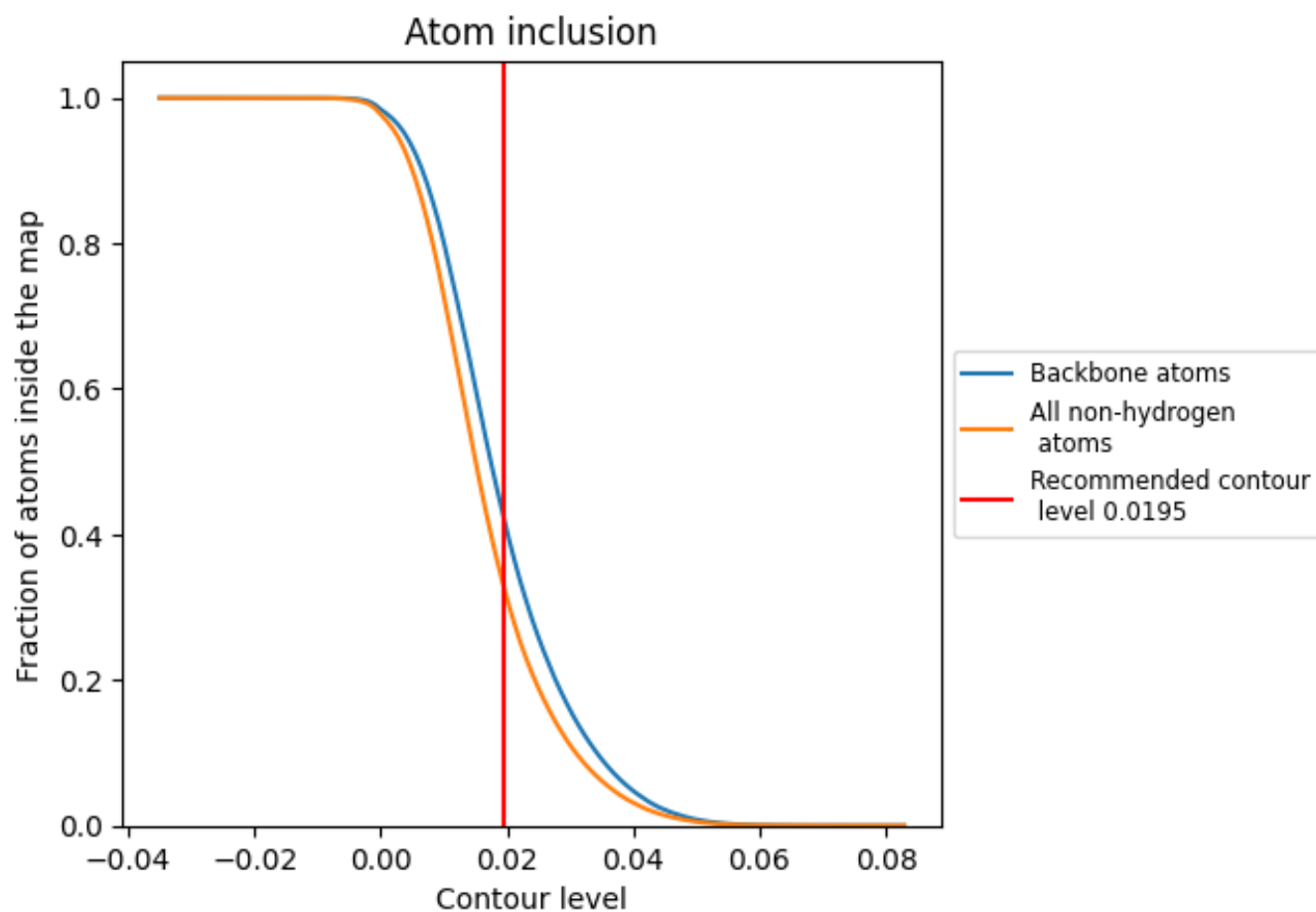
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0195).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 42% of all backbone atoms, 33% 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 (0.0195) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3285	 0.1710
09	 0.7180	 0.4170
19	 0.7211	 0.4210
29	 0.5993	 0.3650
39	 0.6011	 0.3640
49	 0.6012	 0.3620
A1	 0.1482	 0.0850
A2	 0.5906	 0.2960
A3	 0.0477	 0.0430
A4	 0.1801	 0.0850
A5	 0.4509	 0.2120
A6	 0.6189	 0.3240
A7	 0.0654	 0.0430
A8	 0.5750	 0.3230
A9	 0.5387	 0.2580
AA	 0.4118	 0.1900
B1	 0.1312	 0.0820
B2	 0.5077	 0.2620
B3	 0.0170	 0.0290
B4	 0.1700	 0.1020
B5	 0.3093	 0.1060
B6	 0.5320	 0.2630
B7	 0.0267	 0.0450
B8	 0.6265	 0.3170
B9	 0.5425	 0.2620
BA	 0.2987	 0.0940
C1	 0.0774	 0.0520
C2	 0.4455	 0.2230
C3	 0.0426	 0.0570
C4	 0.1150	 0.0860
C5	 0.2912	 0.1280
C6	 0.4673	 0.2260
C7	 0.0426	 0.0560
C8	 0.7018	 0.3800
C9	 0.5684	 0.2990



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Chain	Atom inclusion	Q-score
CA	0.2641	0.1300
D1	0.0680	0.0370
D2	0.2688	0.1200
D3	0.0356	0.0310
D4	0.0996	0.0510
D5	0.2583	0.1100
D6	0.3126	0.1240
D7	0.0543	0.0580
D8	0.6554	0.3540
D9	0.5647	0.3090
DA	0.2372	0.1320
E1	0.0706	0.0500
E2	0.2972	0.1490
E3	0.0164	0.0020
E4	0.1134	0.0690
E5	0.3043	0.1270
E6	0.3585	0.1630
E7	0.0291	-0.0060
E8	0.5568	0.2740
E9	0.6137	0.3120
EA	0.2727	0.1400
F1	0.0591	0.0330
F2	0.3862	0.1720
F3	0.0113	0.0110
F4	0.0704	0.0440
F5	0.3523	0.1490
F6	0.4089	0.1890
F7	0.0130	0.0300
F8	0.5952	0.3160
F9	0.5862	0.2890
FA	0.3197	0.1400
G1	0.0917	0.0680
G2	0.4578	0.2460
G3	0.0112	0.0480
G4	0.1375	0.0990
G5	0.4098	0.1700
G6	0.4929	0.2600
G7	0.0172	0.0410
G8	0.6284	0.3440
G9	0.7446	0.4030
GA	0.3711	0.1660
H1	0.0818	0.0300

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Chain	Atom inclusion	Q-score
H2	0.3166	0.1240
H3	0.0121	0.0170
H4	0.1085	0.0620
H5	0.2636	0.1390
H6	0.3247	0.1270
H7	0.0130	-0.0010
H8	0.5568	0.2990
H9	0.7642	0.4470
HA	0.2569	0.1320
I1	0.0605	0.0160
I2	0.2562	0.0900
I3	0.0209	0.0390
I4	0.0836	0.0270
I5	0.2592	0.1110
I6	0.3025	0.1360
I7	0.0276	0.0460
I8	0.6035	0.3360
I9	0.7273	0.3750
IA	0.2509	0.0920
J1	0.0559	0.0470
J2	0.3287	0.1580
J3	0.0283	0.0130
J4	0.0810	0.0260
J5	0.2729	0.1470
J6	0.3482	0.1670
J7	0.0405	0.0470
J8	0.7191	0.3850
J9	0.7255	0.4090
JA	0.2397	0.1120
K1	0.0819	0.0480
K2	0.3666	0.1610
K3	0.0135	0.0040
K4	0.0947	0.0270
K5	0.2262	0.0730
K6	0.4050	0.1650
K7	0.0248	0.0160
K8	0.6669	0.3480
K9	0.6516	0.3410
KA	0.2200	0.0840
L1	0.0947	0.0680
L2	0.4081	0.2010
L3	0.0113	0.0190

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Chain	Atom inclusion	Q-score
L4	0.1061	0.0650
L5	0.3312	0.1370
L6	0.4413	0.2000
L7	0.0113	0.0160
L8	0.5535	0.2600
L9	0.7312	0.3890
LA	0.2640	0.0790
M1	0.0661	0.0260
M2	0.3346	0.1500
M3	0.0046	0.0260
M4	0.0744	0.0230
M5	0.3129	0.1240
M6	0.3734	0.1670
M7	0.0116	0.0300
M8	0.5919	0.3240
M9	0.6752	0.3630
MA	0.2757	0.0890
N1	0.0264	0.0130
N2	0.2919	0.1380
N3	0.0213	0.0050
N4	0.0428	0.0210
N5	0.2166	0.0930
N6	0.3292	0.1530
N7	0.0597	0.0210
N8	0.6323	0.3730
N9	0.7158	0.3840
NA	0.1723	0.0660
O1	0.0032	-0.0190
O2	0.1312	0.0460
O4	0.0081	0.0080
O5	0.1231	0.0590
O6	0.1336	0.0550
O8	0.5321	0.2600
O9	0.7486	0.4320
OA	0.0947	0.0440
P1	0.0120	0.0400
P2	0.1634	0.0820
P4	0.0158	0.0210
P5	0.1386	0.0580
P6	0.1936	0.0750
P8	0.5507	0.2850
P9	0.7175	0.4090

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Chain	Atom inclusion	Q-score
PA	0.1298	0.0600
Q1	0.0055	0.0140
Q2	0.1636	0.0570
Q4	0.0039	0.0120
Q5	0.1180	0.0710
Q6	0.2162	0.0740
Q8	0.5898	0.3140
Q9	0.7460	0.4380
QA	0.0979	0.0480
R1	0.0124	0.0010
R2	0.2099	0.1000
R4	0.0132	0.0070
R5	0.1526	0.0710
R6	0.2595	0.1410
R8	0.5499	0.2960
R9	0.4621	0.2610
RA	0.1208	0.0550
S1	0.0057	0.0200
S2	0.1733	0.0780
S4	0.0081	0.0250
S5	0.1190	0.0450
S6	0.1725	0.0800
S8	0.5956	0.2850
S9	0.4955	0.2790
SA	0.0899	0.0200
T1	0.0105	0.0090
T2	0.2293	0.1000
T4	0.0105	0.0210
T5	0.1450	0.0750
T6	0.2262	0.1020
T8	0.5993	0.2940
T9	0.5041	0.2570
TA	0.1262	0.0810
U1	0.0049	0.0090
U2	0.1373	0.0630
U4	0.0040	-0.0010
U5	0.0988	0.0550
U6	0.1333	0.0540
U8	0.5798	0.3130
U9	0.5194	0.2760
UA	0.0688	0.0180
V1	0.0023	-0.0020





















































































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Chain	Atom inclusion	Q-score
V2	0.1029	0.0470
V4	0.0015	-0.0070
V5	0.0856	0.0150
V6	0.1157	0.0290
V8	0.4036	0.2150
V9	0.5601	0.3370
VA	0.0654	0.0370
W1	0.0016	0.0110
W2	0.0996	0.0610
W4	0.0024	-0.0350
W5	0.0648	0.0490
W6	0.1263	0.0430
W8	0.4806	0.2280
W9	0.5865	0.3180
WA	0.0648	0.0450
X1	0.0038	-0.0070
X2	0.1053	0.0670
X4	0.0030	-0.0050
X5	0.0834	0.0560
X6	0.1097	0.0550
X8	0.5980	0.2810
X9	0.7002	0.3700
XA	0.0548	0.0260
Y1	0.0040	0.0040
Y2	0.1263	0.0700
Y4	0.0049	0.0160
Y5	0.1028	0.0820
Y6	0.1368	0.0640
Y8	0.6554	0.3410
Y9	0.7101	0.3960
YA	0.0518	0.0450
Z1	0.0023	0.0270
Z2	0.0984	0.0300
Z4	0.0090	0.0150
Z5	0.0969	0.0380
Z6	0.1382	0.0750
Z8	0.6540	0.3560
Z9	0.6433	0.3330
ZA	0.0601	0.0230
a8	0.5601	0.2760
a9	0.7212	0.3780
b8	0.6047	0.3240





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Chain	Atom inclusion	Q-score
b9	 0.7158	 0.3840
c8	 0.4020	 0.1980
c9	 0.7791	 0.4430
d8	 0.4749	 0.2400
d9	 0.6730	 0.3610
e8	 0.5675	 0.2770
e9	 0.7535	 0.4400
f8	 0.6142	 0.3180
f9	 0.7035	 0.4060
g8	 0.6582	 0.3480
g9	 0.7156	 0.4280
h8	 0.5408	 0.2740
h9	 0.6888	 0.3730
i8	 0.5545	 0.2840
i9	 0.4102	 0.2230
j8	 0.5420	 0.2600
j9	 0.4996	 0.2670
k8	 0.5416	 0.2930
k9	 0.4563	 0.2150
l8	 0.4951	 0.2390
l9	 0.4773	 0.2580
m8	 0.6556	 0.3590
m9	 0.5203	 0.3020
n8	 0.6837	 0.3590
n9	 0.5516	 0.3010
o8	 0.6586	 0.3450
o9	 0.6203	 0.3040
p8	 0.5544	 0.2540
p9	 0.6974	 0.3700
q8	 0.5648	 0.2940
q9	 0.6656	 0.3330
r8	 0.4835	 0.2340
r9	 0.7444	 0.4080
s8	 0.6752	 0.3660
s9	 0.6829	 0.3710
t8	 0.7125	 0.3760
t9	 0.7172	 0.3990
u8	 0.6760	 0.3280
u9	 0.6096	 0.3020
v9	 0.6859	 0.3530
w9	 0.6606	 0.3310
x9	 0.7312	 0.3870

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Chain	Atom inclusion	Q-score
y9	 0.6928	 0.3650
z9	 0.7214	 0.3950