



wwPDB EM Validation Summary Report ⓘ

Mar 20, 2026 – 07:06 AM UTC

PDB ID : 7EYD / pdb_00007eyd
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:

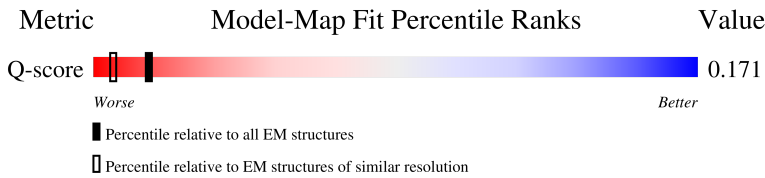
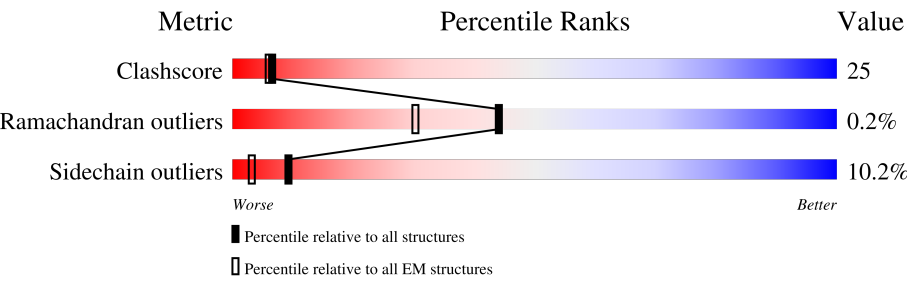
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8855 (3.40 - 4.40)

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% 44% 39% 14%
1	A4	247	78% 43% 41% 14%
2	B1	163	95% 68% 29% ..
2	B2	163	27% 64% 33% ..

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	B3	163	99% 64% 33% ..
2	B4	163	91% 66% 31% ..
2	B5	163	72% 74% 22% ..
2	B6	163	28% 66% 31% ..
2	B7	163	99% 64% 33% ..
2	BA	163	72% 74% 22% ..
2	D1	163	98% 71% 27% ..
2	D2	163	77% 69% 28% ..
2	D3	163	99% 68% 29% ..
2	D4	163	96% 69% 28% ..
2	D5	163	77% 73% 25% ..
2	D6	163	71% 70% 27% ..
2	D7	163	99% 69% 28% ..
2	DA	163	86% 73% 25% ..
2	F1	163	99% 72% 26% ..
2	F2	163	58% 72% 25% ..
2	F3	163	99% 72% 25% ..
2	F4	163	99% 69% 28% ..
2	F5	163	60% 70% 26% ..
2	F6	163	49% 72% 25% ..
2	F7	163	99% 71% 26% ..
2	FA	163	65% 69% 26% ..
2	H1	163	98% 74% 23% ..
2	H2	163	71% 71% 25% ..
2	H3	163	99% 68% 28% ..

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	H4	163	96% 73% 25% ..
2	H5	163	77% 72% 25% ..
2	H6	163	66% 69% 27% ..
2	H7	163	99% 69% 26% ..
2	HA	163	82% 74% 23% ..
2	J1	163	99% 67% 30% ..
2	J2	163	64% 71% 26% ..
2	J3	163	99% 69% 28% ..
2	J4	163	99% 68% 29% ..
2	J5	163	77% 74% 23% ..
2	J6	163	66% 73% 24% ..
2	J7	163	99% 72% 25% ..
2	JA	163	80% 77% 20% ..
2	L1	163	97% 69% 29% ..
2	L2	163	53% 66% 29% 5% .
2	L3	163	99% 65% 30% ..
2	L4	163	98% 69% 29% ..
2	L5	163	71% 75% 20% ..
2	L6	163	48% 64% 31% 5% .
2	L7	163	99% 66% 29% ..
2	LA	163	79% 72% 23% ..
2	O1	163	99% 74% 25% ..
2	O2	163	95% 73% 22% ..
2	O4	163	99% 75% 23% ..
2	O5	163	94% 75% 22% ..

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	O6	163	96% 71%25% ..
2	OA	163	97% 74%23% ..
2	Q1	163	99% 73%25% ..
2	Q2	163	92% 72%24% ..
2	Q4	163	99% 73%24% ..
2	Q5	163	95% 74%23% ..
2	Q6	163	84% 71%25% ..
2	QA	163	96% 74%22% ..
2	S1	163	99% 75%21% ..
2	S2	163	90% 68%27% ..
2	S4	163	99% 76%21% ..
2	S5	163	97% 74%22% ..
2	S6	163	90% 68%27% ..
2	SA	163	97% 76%20% ..
2	U1	163	99% 74%24% ..
2	U2	163	93% 69%28% ..
2	U4	163	99% 75%22% ..
2	U5	163	97% 75%23% ..
2	U6	163	94% 71%27% ..
2	UA	163	98% 74%24% ..
2	W1	163	99% 71%26% ..
2	W2	163	98% 71%26% ..
2	W4	163	99% 71%26% ..
2	W5	163	98% 75%21% ..
2	W6	163	95% 69%28% ..

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	WA	163	99% 75% 21% ..
2	Y1	163	99% 75% 23% ..
2	Y2	163	96% 72% 25% ..
2	Y4	163	99% 75% 23% ..
2	Y5	163	98% 75% 21% ..
2	Y6	163	94% 72% 25% ..
2	YA	163	99% 74% 23% ..
3	C1	173	96% 73% 24% ...
3	C2	173	47% 62% 32% 5% .
3	C3	173	98% 62% 33% . .
3	C4	173	95% 72% 24% ...
3	C5	173	69% 62% 32% . . .
3	C6	173	45% 62% 33% . .
3	C7	173	99% 61% 33% 5% .
3	CA	173	79% 62% 32% . . .
3	E1	173	99% 73% 23% . .
3	E2	173	74% 68% 25% 7%
3	E3	173	100% 68% 26% 6%
3	E4	173	95% 73% 23% . . .
3	E5	173	71% 63% 31% . . .
3	E6	173	60% 68% 25% 6%
3	E7	173	100% 68% 25% 6%
3	EA	173	77% 64% 31% . . .
3	G1	173	97% 72% 24% . . .
3	G2	173	44% 62% 33% 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	G3	173	
3	G4	173	
3	G5	173	
3	G6	173	
3	G7	173	
3	GA	173	
3	I1	173	
3	I2	173	
3	I3	173	
3	I4	173	
3	I5	173	
3	I6	173	
3	I7	173	
3	IA	173	
3	K1	173	
3	K2	173	
3	K3	173	
3	K4	173	
3	K5	173	
3	K6	173	
3	K7	173	
3	KA	173	
3	M1	173	
3	M2	173	
3	M3	173	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	M4	173	97% 75% 21% . .
3	M5	173	65% 61% 33% . .
3	M6	173	51% 68% 28% . .
3	M7	173	99% 68% 28% . .
3	MA	173	80% 62% 32% . .
3	P1	173	99% 76% 20% . .
3	P2	173	91% 65% 27% 7% .
3	P4	173	99% 76% 21% . .
3	P5	173	91% 65% 30% . .
3	P6	173	87% 64% 28% 7% .
3	PA	173	97% 64% 31% . .
3	R1	173	99% 72% 25% . .
3	R2	173	86% 64% 31% 5% .
3	R4	173	99% 74% 23% . .
3	R5	173	93% 65% 28% 5% .
3	R6	173	79% 64% 31% 5% .
3	RA	173	93% 65% 29% 5% .
3	T1	173	99% 72% 24% . .
3	T2	173	86% 66% 28% 5% .
3	T4	173	99% 73% 24% . .
3	T5	173	94% 61% 34% . .
3	T6	173	82% 65% 29% 5% .
3	TA	173	94% 63% 31% . .
3	V1	173	99% 77% 19% . .
3	V2	173	98% 68% 28% . .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	V4	173	99% 76% 20% ..
3	V5	173	98% 66% 29% ..
3	V6	173	97% 68% 28% ..
3	VA	173	99% 66% 28% ..
3	X1	173	99% 74% 23% ...
3	X2	173	94% 66% 28% 5% .
3	X4	173	99% 75% 23% ...
3	X5	173	99% 66% 27% 6% ..
3	X6	173	95% 66% 27% 6% .
3	XA	173	98% 64% 29% 5% ..
3	Z1	173	99% 76% 21% ..
3	Z2	173	95% 63% 32% ..
3	Z4	173	99% 77% 20% ..
3	Z5	173	97% 65% 29% ..
3	Z6	173	94% 64% 32% ..
3	ZA	173	99% 66% 28% 5% ..
4	N1	286	99% 69% 28% ..
4	N2	286	71% 64% 33% ..
4	N3	286	20% 9% 10% . 80%
4	N4	286	99% 69% 27% ..
4	N5	286	83% 71% 28% ..
4	N6	286	65% 66% 32% ..
4	N7	286	20% 9% 10% . 80%
4	NA	286	88% 70% 28% ..
5	A2	253	19% 62% 32% ..

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	A5	253	
5	A6	253	
5	AA	253	
6	A3	279	
6	A7	279	
7	A8	161	
7	A9	161	
7	C8	161	
7	C9	161	
7	E8	161	
7	E9	161	
7	G9	161	
7	H8	161	
7	I9	161	
7	J8	161	
7	K9	161	
7	L8	161	
7	N9	161	
7	O8	161	
7	P9	161	
7	Q8	161	
7	R9	161	
7	S8	161	
7	T9	161	
7	V8	161	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
7	X8	161	
7	X9	161	
7	Z8	161	
7	Z9	161	
7	b9	161	
7	c8	161	
7	d9	161	
7	e8	161	
7	f9	161	
7	g8	161	
7	i9	161	
7	j8	161	
7	k9	161	
7	l8	161	
7	n8	161	
7	o9	161	
7	p8	161	
7	q9	161	
7	r8	161	
7	s9	161	
7	t8	161	
7	u9	161	
7	w9	161	
7	y9	161	
8	B8	162	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	B9	162	
8	D8	162	
8	D9	162	
8	F8	162	
8	F9	162	
8	H9	162	
8	I8	162	
8	J9	162	
8	K8	162	
8	L9	162	
8	M8	162	
8	M9	162	
8	O9	162	
8	P8	162	
8	R8	162	
8	S9	162	
8	T8	162	
8	U9	162	
8	W8	162	
8	W9	162	
8	Y8	162	
8	Y9	162	
8	a8	162	
8	a9	162	
8	c9	162	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	d8	162	
8	e9	162	
8	f8	162	
8	h8	162	
8	h9	162	
8	j9	162	
8	k8	162	
8	l9	162	
8	m8	162	
8	n9	162	
8	o8	162	
8	p9	162	
8	q8	162	
8	r9	162	
8	s8	162	
8	t9	162	
8	u8	162	
8	v9	162	
8	x9	162	
8	z9	162	
9	29	68	
9	39	68	
9	49	68	
9	G8	68	
9	N8	68	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	U8	68	
9	b8	68	
9	i8	68	
10	09	1132	
10	19	1132	
11	Q9	169	
11	g9	169	
12	V9	161	
12	m9	161	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CYC	09	1201	-	-	X	-
13	CYC	19	1201	-	-	X	-
13	CYC	A3	301	-	-	X	-
13	CYC	A5	302	-	-	X	-
13	CYC	A5	303	-	-	X	-
13	CYC	A5	304	-	-	X	-
13	CYC	A7	301	-	-	X	-
13	CYC	AA	302	-	-	X	-
13	CYC	AA	303	-	-	X	-
13	CYC	AA	304	-	-	X	-
13	CYC	B2	1001	-	-	X	-
13	CYC	B3	1001	-	-	X	-
13	CYC	B6	1001	-	-	X	-
13	CYC	B7	1001	-	-	X	-
13	CYC	B8	1001	-	-	X	-
13	CYC	C1	302	-	-	X	-
13	CYC	C2	201	-	-	X	-
13	CYC	C2	202	-	-	X	-
13	CYC	C3	201	-	-	X	-
13	CYC	C4	302	-	-	X	-
13	CYC	C5	201	-	-	X	-
13	CYC	C6	201	-	-	X	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CYC	C6	202	-	-	X	-
13	CYC	C7	201	-	-	X	-
13	CYC	CA	201	-	-	X	-
13	CYC	D1	1001	-	-	X	-
13	CYC	D4	1001	-	-	X	-
13	CYC	D8	1001	-	-	X	-
13	CYC	D9	1001	-	-	X	-
13	CYC	E1	202	-	-	X	-
13	CYC	E2	201	-	-	X	-
13	CYC	E2	202	-	-	X	-
13	CYC	E3	201	-	-	X	-
13	CYC	E3	202	-	-	X	-
13	CYC	E4	202	-	-	X	-
13	CYC	E5	201	-	-	X	-
13	CYC	E6	201	-	-	X	-
13	CYC	E6	202	-	-	X	-
13	CYC	E7	201	-	-	X	-
13	CYC	E7	202	-	-	X	-
13	CYC	EA	201	-	-	X	-
13	CYC	F8	1001	-	-	X	-
13	CYC	G1	201	-	-	X	-
13	CYC	G1	202	-	-	X	-
13	CYC	G2	201	-	-	X	-
13	CYC	G3	202	-	-	X	-
13	CYC	G4	201	-	-	X	-
13	CYC	G4	202	-	-	X	-
13	CYC	G5	201	-	-	X	-
13	CYC	G6	201	-	-	X	-
13	CYC	G7	202	-	-	X	-
13	CYC	GA	1002	-	-	X	-
13	CYC	I1	202	-	-	X	-
13	CYC	I2	201	-	-	X	-
13	CYC	I2	202	-	-	X	-
13	CYC	I3	201	-	-	X	-
13	CYC	I3	202	-	-	X	-
13	CYC	I4	202	-	-	X	-
13	CYC	I5	202	-	-	X	-
13	CYC	I6	201	-	-	X	-
13	CYC	I6	202	-	-	X	-
13	CYC	I7	201	-	-	X	-
13	CYC	I7	202	-	-	X	-
13	CYC	I8	1001	-	-	X	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CYC	IA	202	-	-	X	-
13	CYC	J1	1001	-	-	X	-
13	CYC	J2	1001	-	-	X	-
13	CYC	J3	1001	-	-	X	-
13	CYC	J4	1001	-	-	X	-
13	CYC	J6	1001	-	-	X	-
13	CYC	J7	1001	-	-	X	-
13	CYC	K1	201	-	-	X	-
13	CYC	K1	202	-	-	X	-
13	CYC	K2	201	-	-	X	-
13	CYC	K2	202	-	-	X	-
13	CYC	K3	201	-	-	X	-
13	CYC	K3	202	-	-	X	-
13	CYC	K4	201	-	-	X	-
13	CYC	K4	202	-	-	X	-
13	CYC	K5	201	-	-	X	-
13	CYC	K6	201	-	-	X	-
13	CYC	K6	202	-	-	X	-
13	CYC	K7	201	-	-	X	-
13	CYC	K7	202	-	-	X	-
13	CYC	K8	1001	-	-	X	-
13	CYC	KA	201	-	-	X	-
13	CYC	M1	201	-	-	X	-
13	CYC	M1	202	-	-	X	-
13	CYC	M2	201	-	-	X	-
13	CYC	M3	201	-	-	X	-
13	CYC	M4	201	-	-	X	-
13	CYC	M4	202	-	-	X	-
13	CYC	M5	1002	-	-	X	-
13	CYC	M5	1003	-	-	X	-
13	CYC	M6	201	-	-	X	-
13	CYC	M7	201	-	-	X	-
13	CYC	M8	1001	-	-	X	-
13	CYC	MA	1002	-	-	X	-
13	CYC	MA	1003	-	-	X	-
13	CYC	N2	301	-	-	X	-
13	CYC	N3	301	-	-	X	-
13	CYC	N6	301	-	-	X	-
13	CYC	N7	301	-	-	X	-
13	CYC	O1	1001	-	-	X	-
13	CYC	O4	1001	-	-	X	-
13	CYC	P1	201	-	-	X	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CYC	P1	202	-	-	X	-
13	CYC	P2	201	-	-	X	-
13	CYC	P4	201	-	-	X	-
13	CYC	P4	202	-	-	X	-
13	CYC	P5	201	-	-	X	-
13	CYC	P5	202	-	-	X	-
13	CYC	P6	201	-	-	X	-
13	CYC	P8	1001	-	-	X	-
13	CYC	PA	201	-	-	X	-
13	CYC	PA	202	-	-	X	-
13	CYC	Q1	202	-	-	X	-
13	CYC	Q2	201	-	-	X	-
13	CYC	Q4	202	-	-	X	-
13	CYC	Q6	201	-	-	X	-
13	CYC	R2	1001	-	-	X	-
13	CYC	R5	201	-	-	X	-
13	CYC	R6	1001	-	-	X	-
13	CYC	R8	1001	-	-	X	-
13	CYC	RA	201	-	-	X	-
13	CYC	S2	1001	-	-	X	-
13	CYC	S4	1001	-	-	X	-
13	CYC	S6	1001	-	-	X	-
13	CYC	T1	201	-	-	X	-
13	CYC	T1	202	-	-	X	-
13	CYC	T2	201	-	-	X	-
13	CYC	T4	201	-	-	X	-
13	CYC	T4	202	-	-	X	-
13	CYC	T5	201	-	-	X	-
13	CYC	T5	202	-	-	X	-
13	CYC	T6	201	-	-	X	-
13	CYC	T8	1001	-	-	X	-
13	CYC	TA	201	-	-	X	-
13	CYC	TA	202	-	-	X	-
13	CYC	U2	201	-	-	X	-
13	CYC	U2	202	-	-	X	-
13	CYC	U6	201	-	-	X	-
13	CYC	U6	202	-	-	X	-
13	CYC	V1	201	-	-	X	-
13	CYC	V1	202	-	-	X	-
13	CYC	V2	201	-	-	X	-
13	CYC	V2	202	-	-	X	-
13	CYC	V4	201	-	-	X	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CYC	V4	202	-	-	X	-
13	CYC	V5	201	-	-	X	-
13	CYC	V5	202	-	-	X	-
13	CYC	V6	201	-	-	X	-
13	CYC	V6	202	-	-	X	-
13	CYC	VA	201	-	-	X	-
13	CYC	VA	202	-	-	X	-
13	CYC	W1	1001	-	-	X	-
13	CYC	W2	201	-	-	X	-
13	CYC	W2	202	-	-	X	-
13	CYC	W2	203	-	-	X	-
13	CYC	W4	1001	-	-	X	-
13	CYC	W6	201	-	-	X	-
13	CYC	W6	202	-	-	X	-
13	CYC	W8	1001	-	-	X	-
13	CYC	X1	201	-	-	X	-
13	CYC	X1	202	-	-	X	-
13	CYC	X4	202	-	-	X	-
13	CYC	X5	202	-	-	X	-
13	CYC	X6	202	-	-	X	-
13	CYC	XA	202	-	-	X	-
13	CYC	Y2	201	-	-	X	-
13	CYC	Y6	201	-	-	X	-
13	CYC	Y8	1001	-	-	X	-
13	CYC	Z1	201	-	-	X	-
13	CYC	Z2	201	-	-	X	-
13	CYC	Z2	202	-	-	X	-
13	CYC	Z4	201	-	-	X	-
13	CYC	Z5	202	-	-	X	-
13	CYC	Z6	201	-	-	X	-
13	CYC	Z6	202	-	-	X	-
13	CYC	ZA	202	-	-	X	-
13	CYC	b8	1001	-	-	X	-
13	CYC	d8	1001	-	-	X	-
13	CYC	f8	1001	-	-	X	-
13	CYC	h8	1001	-	-	X	-
13	CYC	k8	1001	-	-	X	-
13	CYC	o8	1001	-	-	X	-
13	CYC	q8	1001	-	-	X	-
13	CYC	s8	1001	-	-	X	-

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
1	A1	213	Total	C	N	O	0	0
			1774	1135	308	331		
1	A4	213	Total	C	N	O	0	0
			1774	1135	308	331		

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

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

Continued on next page...

Continued from previous page...

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		

Continued on next page...

Continued from previous page...

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		

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

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

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

Continued on next page...

Continued from previous page...

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		

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

- 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	C	N	O	0	0
			2265	1425	407	433		
4	N2	284	Total	C	N	O	0	0
			2265	1425	407	433		
4	N3	57	Total	C	N	O	0	0
			444	278	83	83		
4	N4	284	Total	C	N	O	0	0
			2265	1425	407	433		
4	N5	284	Total	C	N	O	0	0
			2265	1425	407	433		
4	N6	284	Total	C	N	O	0	0
			2265	1425	407	433		
4	N7	57	Total	C	N	O	0	0
			444	278	83	83		
4	NA	284	Total	C	N	O	0	0
			2265	1425	407	433		

- 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		

Continued on next page...

Continued from previous page...

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		

Continued on next page...

Continued from previous page...

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		

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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		

Continued on next page...

Continued from previous page...

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		

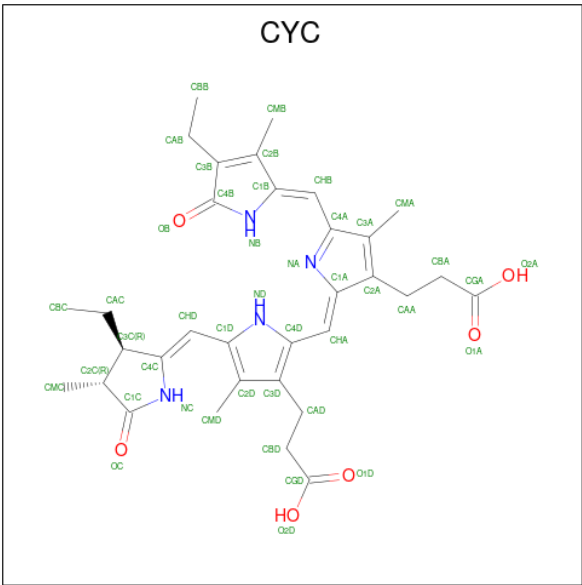
- Molecule 11 is a protein called Allophycocyanin subunit beta-18.

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 (CCD ID: CYC) (formula: C₃₃H₄₀N₄O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
13	B1	1	Total	C	N	O	0
			43	33	4	6	
13	C1	1	Total	C	N	O	0
			43	33	4	6	
13	C1	1	Total	C	N	O	0
			43	33	4	6	
13	D1	1	Total	C	N	O	0
			43	33	4	6	
13	E1	1	Total	C	N	O	0
			43	33	4	6	
13	E1	1	Total	C	N	O	0
			43	33	4	6	
13	F1	1	Total	C	N	O	0
			43	33	4	6	
13	G1	1	Total	C	N	O	0
			43	33	4	6	
13	G1	1	Total	C	N	O	0
			43	33	4	6	
13	H1	1	Total	C	N	O	0
			43	33	4	6	
13	I1	1	Total	C	N	O	0
			43	33	4	6	
13	I1	1	Total	C	N	O	0
			43	33	4	6	
13	J1	1	Total	C	N	O	0
			43	33	4	6	
13	K1	1	Total	C	N	O	0
			43	33	4	6	

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
13	V4	1	Total 43	C 33	N 4	O 6	0
13	W4	1	Total 43	C 33	N 4	O 6	0
13	X4	1	Total 43	C 33	N 4	O 6	0
13	X4	1	Total 43	C 33	N 4	O 6	0
13	Y4	1	Total 43	C 33	N 4	O 6	0
13	Z4	1	Total 43	C 33	N 4	O 6	0
13	Z4	1	Total 43	C 33	N 4	O 6	0
13	A5	1	Total 43	C 33	N 4	O 6	0
13	A5	1	Total 43	C 33	N 4	O 6	0
13	A5	1	Total 43	C 33	N 4	O 6	0
13	A5	1	Total 43	C 33	N 4	O 6	0
13	B5	1	Total 43	C 33	N 4	O 6	0
13	C5	1	Total 43	C 33	N 4	O 6	0
13	D5	1	Total 43	C 33	N 4	O 6	0
13	E5	1	Total 43	C 33	N 4	O 6	0
13	E5	1	Total 43	C 33	N 4	O 6	0
13	G5	1	Total 43	C 33	N 4	O 6	0
13	I5	1	Total 43	C 33	N 4	O 6	0
13	I5	1	Total 43	C 33	N 4	O 6	0
13	J5	1	Total 43	C 33	N 4	O 6	0
13	K5	1	Total 43	C 33	N 4	O 6	0

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
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 43	C 33	N 4	O 6	0
13	U6	1	Total 43	C 33	N 4	O 6	0
13	V6	1	Total 43	C 33	N 4	O 6	0
13	V6	1	Total 43	C 33	N 4	O 6	0
13	W6	1	Total 43	C 33	N 4	O 6	0
13	W6	1	Total 43	C 33	N 4	O 6	0
13	X6	1	Total 43	C 33	N 4	O 6	0
13	X6	1	Total 43	C 33	N 4	O 6	0
13	Y6	1	Total 43	C 33	N 4	O 6	0
13	Z6	1	Total 43	C 33	N 4	O 6	0
13	Z6	1	Total 43	C 33	N 4	O 6	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 43	C 33	N 4	O 6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
13	E7	1	Total 43	C 33	N 4	O 6	0
13	F7	1	Total 43	C 33	N 4	O 6	0
13	G7	1	Total 43	C 33	N 4	O 6	0
13	G7	1	Total 43	C 33	N 4	O 6	0
13	H7	1	Total 43	C 33	N 4	O 6	0
13	I7	1	Total 43	C 33	N 4	O 6	0
13	I7	1	Total 43	C 33	N 4	O 6	0
13	J7	1	Total 43	C 33	N 4	O 6	0
13	K7	1	Total 43	C 33	N 4	O 6	0
13	K7	1	Total 43	C 33	N 4	O 6	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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
13	h8	1	Total 43	C 33	N 4	O 6	0
13	j8	1	Total 43	C 33	N 4	O 6	0
13	k8	1	Total 43	C 33	N 4	O 6	0
13	l8	1	Total 43	C 33	N 4	O 6	0
13	n8	1	Total 43	C 33	N 4	O 6	0
13	o8	1	Total 43	C 33	N 4	O 6	0
13	p8	1	Total 43	C 33	N 4	O 6	0
13	q8	1	Total 43	C 33	N 4	O 6	0
13	r8	1	Total 43	C 33	N 4	O 6	0
13	s8	1	Total 43	C 33	N 4	O 6	0
13	t8	1	Total 43	C 33	N 4	O 6	0
13	09	1	Total 43	C 33	N 4	O 6	0
13	09	1	Total 43	C 33	N 4	O 6	0
13	09	1	Total 43	C 33	N 4	O 6	0
13	19	1	Total 43	C 33	N 4	O 6	0
13	19	1	Total 43	C 33	N 4	O 6	0
13	19	1	Total 43	C 33	N 4	O 6	0
13	19	1	Total 43	C 33	N 4	O 6	0
13	19	1	Total 43	C 33	N 4	O 6	0
13	29	1	Total 43	C 33	N 4	O 6	0
13	39	1	Total 43	C 33	N 4	O 6	0

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
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 43	C 33	N 4	O 6	0
13	AA	1	Total 43	C 33	N 4	O 6	0
13	AA	1	Total 43	C 33	N 4	O 6	0
13	AA	1	Total 43	C 33	N 4	O 6	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 43	C 33	N 4	O 6	0
13	EA	1	Total 43	C 33	N 4	O 6	0
13	GA	1	Total 43	C 33	N 4	O 6	0
13	GA	1	Total 43	C 33	N 4	O 6	0
13	IA	1	Total 43	C 33	N 4	O 6	0
13	IA	1	Total 43	C 33	N 4	O 6	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 43	C 33	N 4	O 6	0
13	MA	1	Total 43	C 33	N 4	O 6	0

Continued on next page...

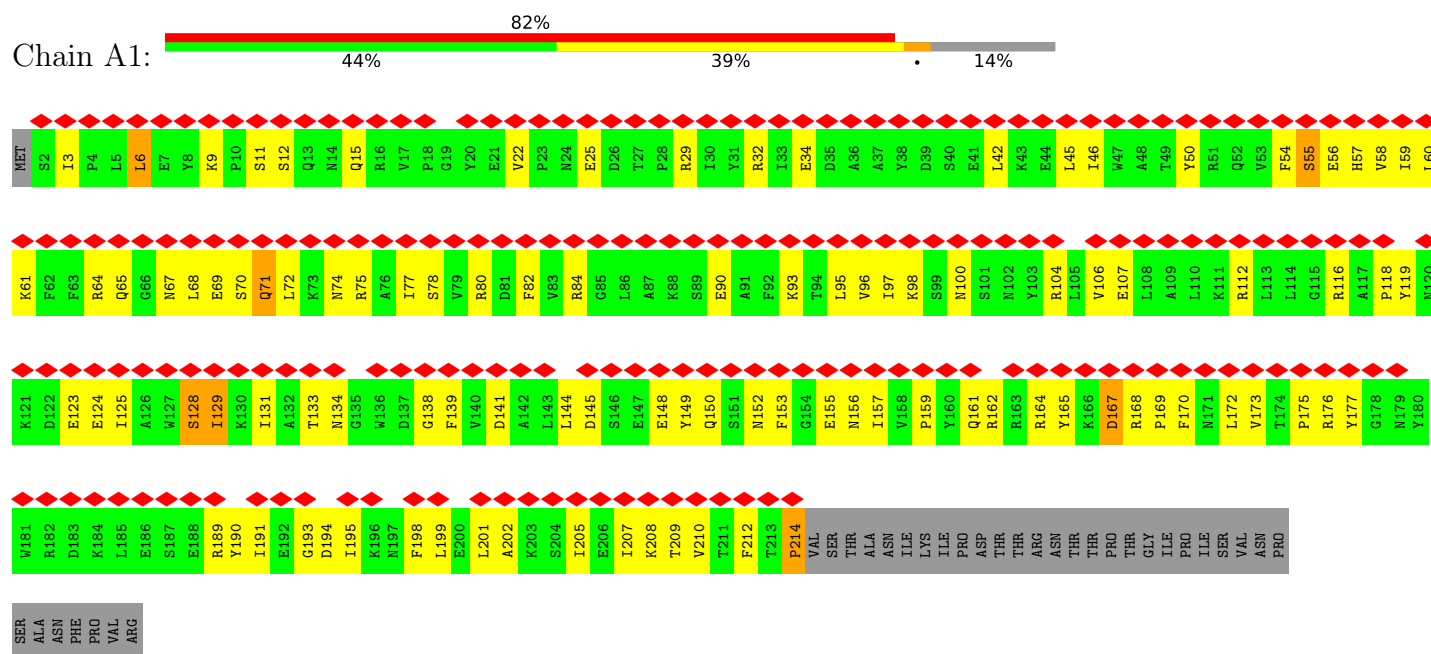
Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
13	MA	1	Total 43	C 33	N 4	O 6	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 43	C 33	N 4	O 6	0
13	PA	1	Total 43	C 33	N 4	O 6	0
13	PA	1	Total 43	C 33	N 4	O 6	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 43	C 33	N 4	O 6	0
13	TA	1	Total 43	C 33	N 4	O 6	0
13	UA	1	Total 43	C 33	N 4	O 6	0
13	VA	1	Total 43	C 33	N 4	O 6	0
13	VA	1	Total 43	C 33	N 4	O 6	0
13	WA	1	Total 43	C 33	N 4	O 6	0
13	XA	1	Total 43	C 33	N 4	O 6	0
13	XA	1	Total 43	C 33	N 4	O 6	0
13	YA	1	Total 43	C 33	N 4	O 6	0
13	ZA	1	Total 43	C 33	N 4	O 6	0
13	ZA	1	Total 43	C 33	N 4	O 6	0

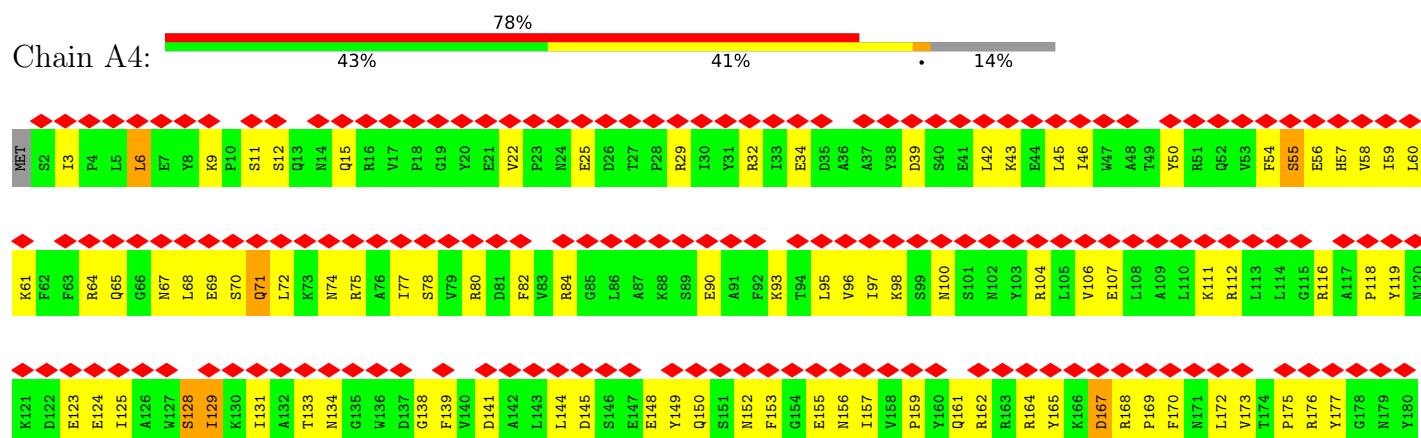
3 Residue-property plots [i](#)

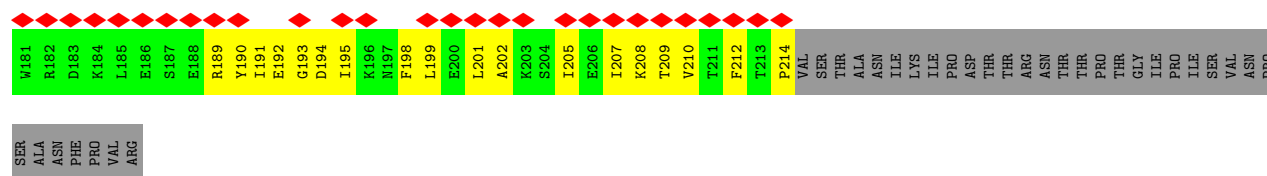
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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

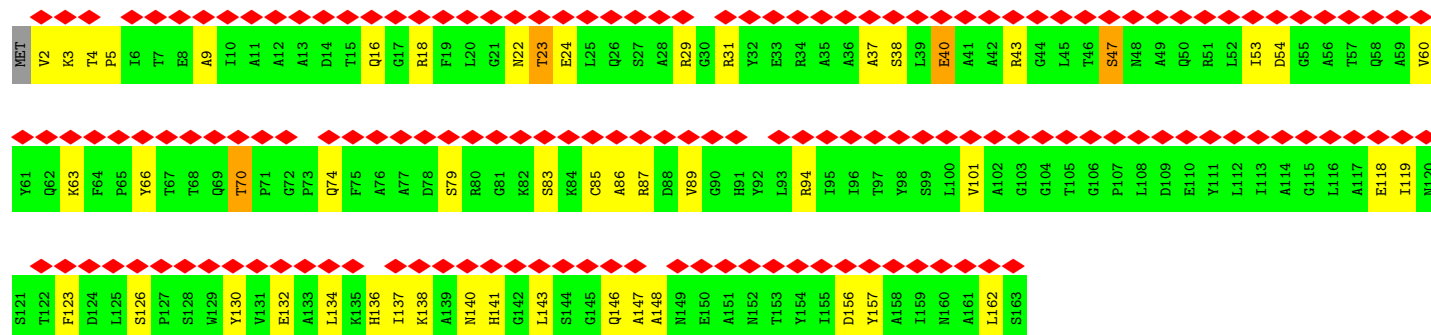


• Molecule 1: Phycobilisome rod-core linker polypeptide CpcG2

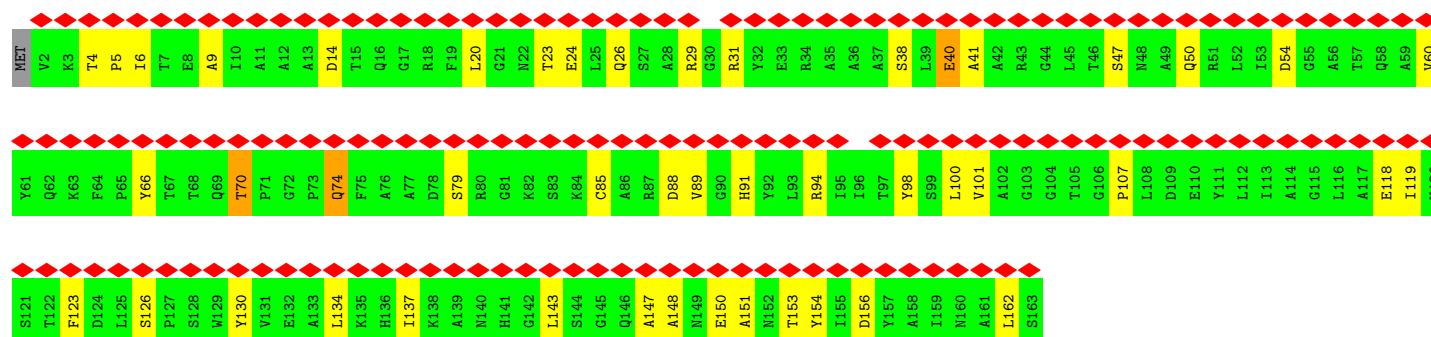




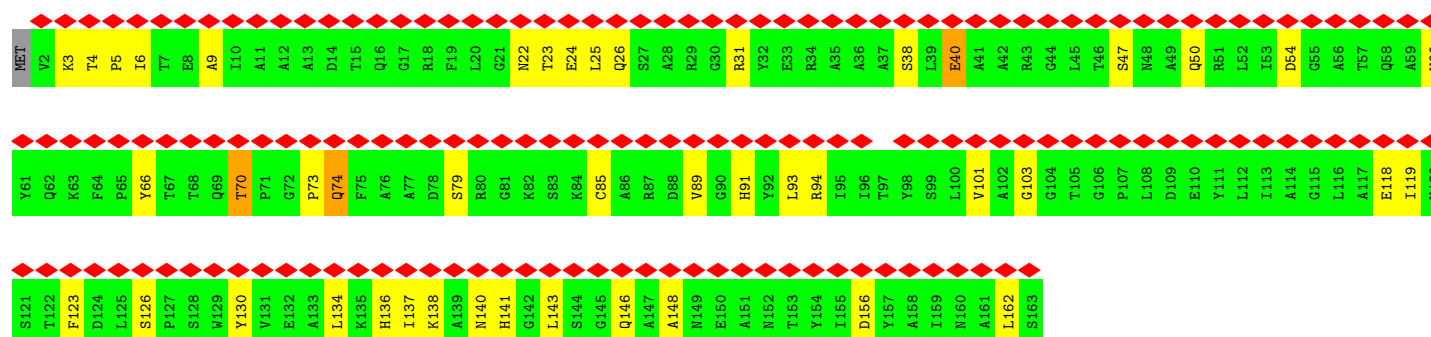
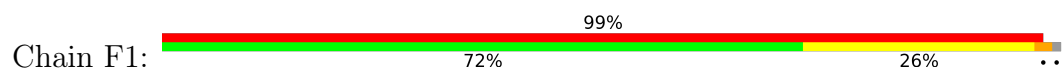
• Molecule 2: C-phycoerythrin alpha subunit



• Molecule 2: C-phycoerythrin alpha subunit

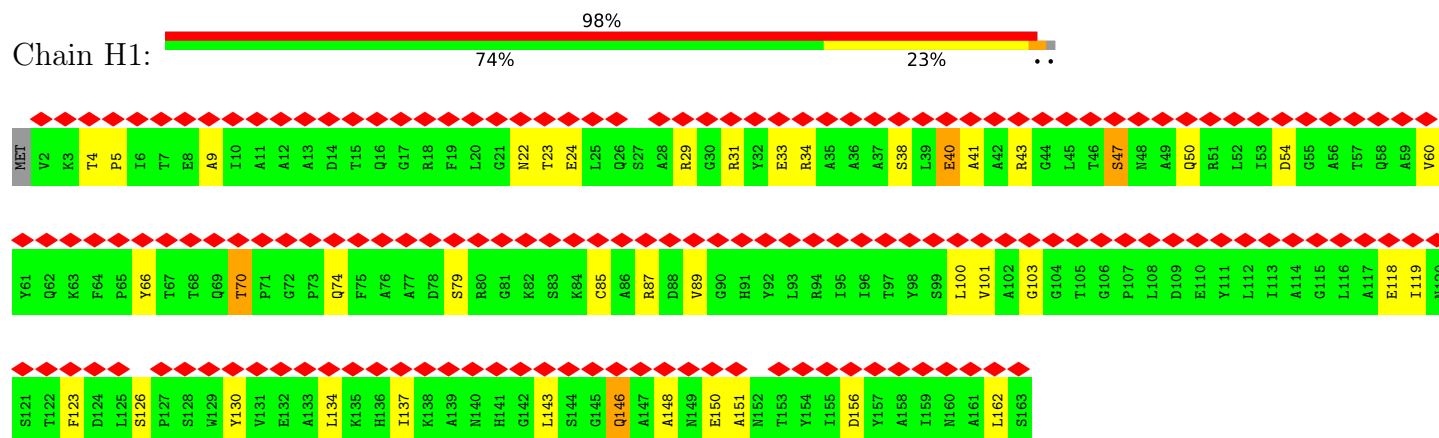


• Molecule 2: C-phycoerythrin alpha subunit



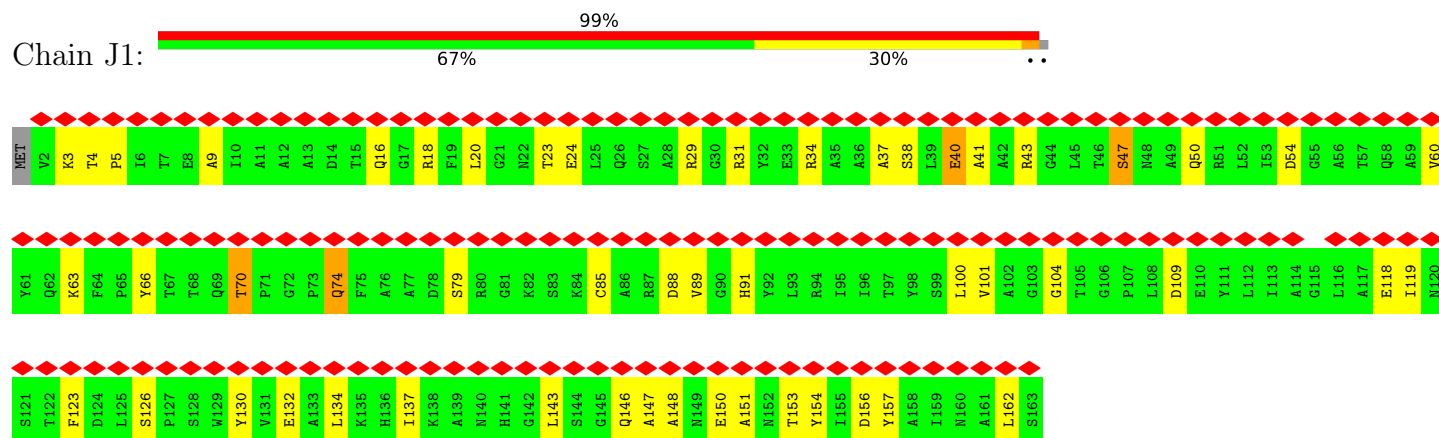
● Molecule 2: C-phycoerythrin alpha subunit

Chain H1:



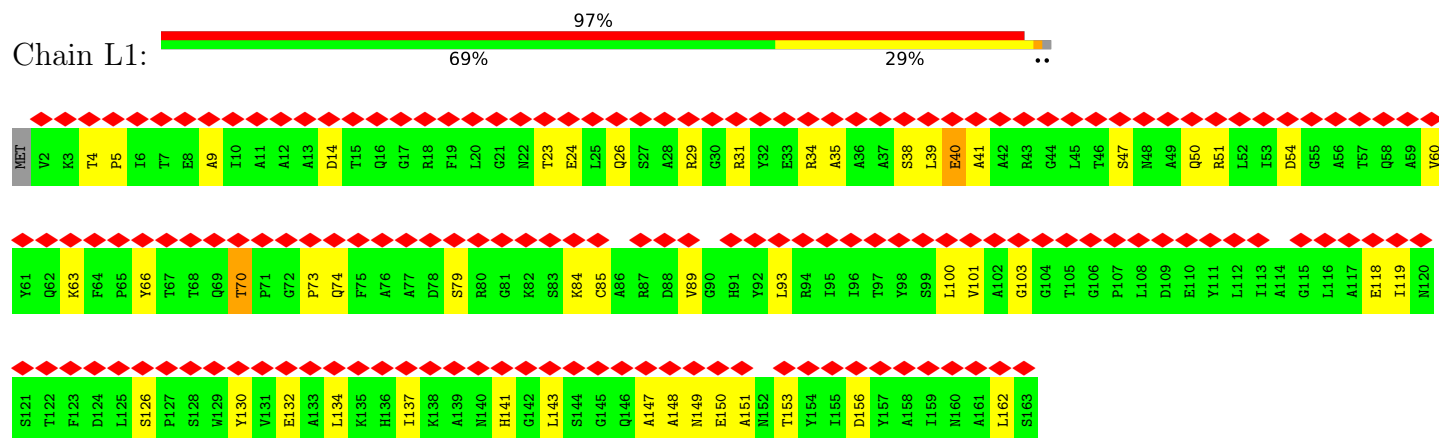
● Molecule 2: C-phycoerythrin alpha subunit

Chain J1:



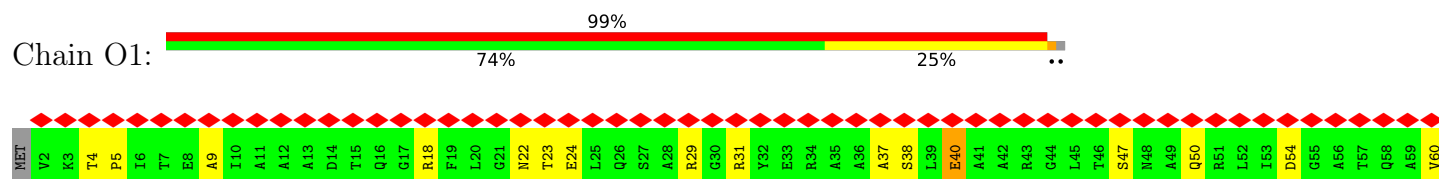
● Molecule 2: C-phycoerythrin alpha subunit

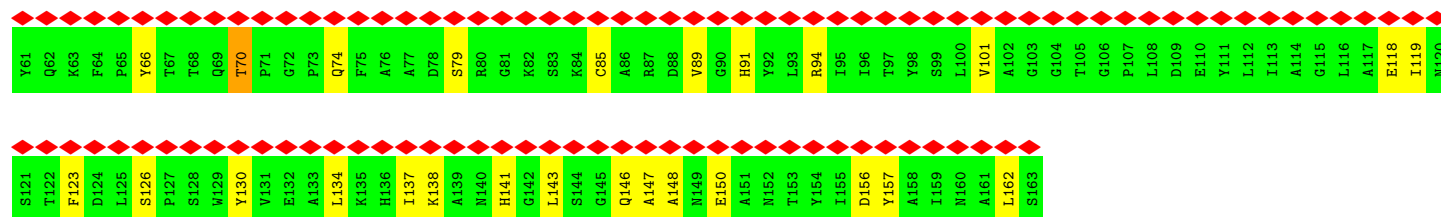
Chain L1:



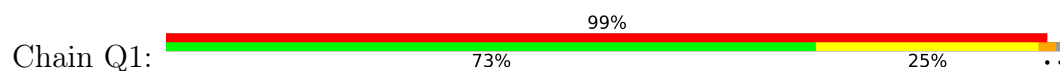
● Molecule 2: C-phycoerythrin alpha subunit

Chain O1:

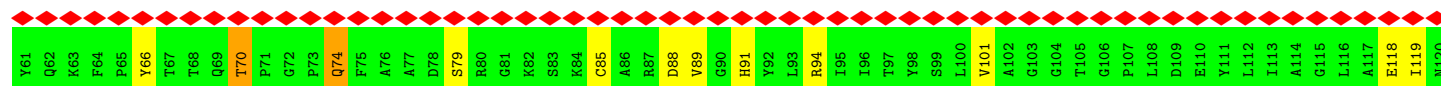
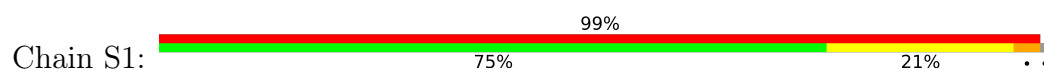




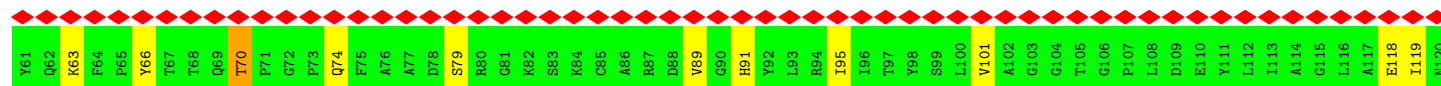
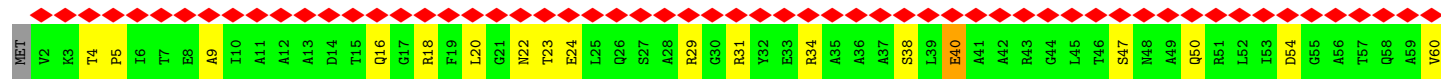
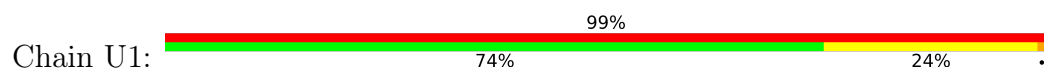
• Molecule 2: C-phycoerythrin alpha subunit



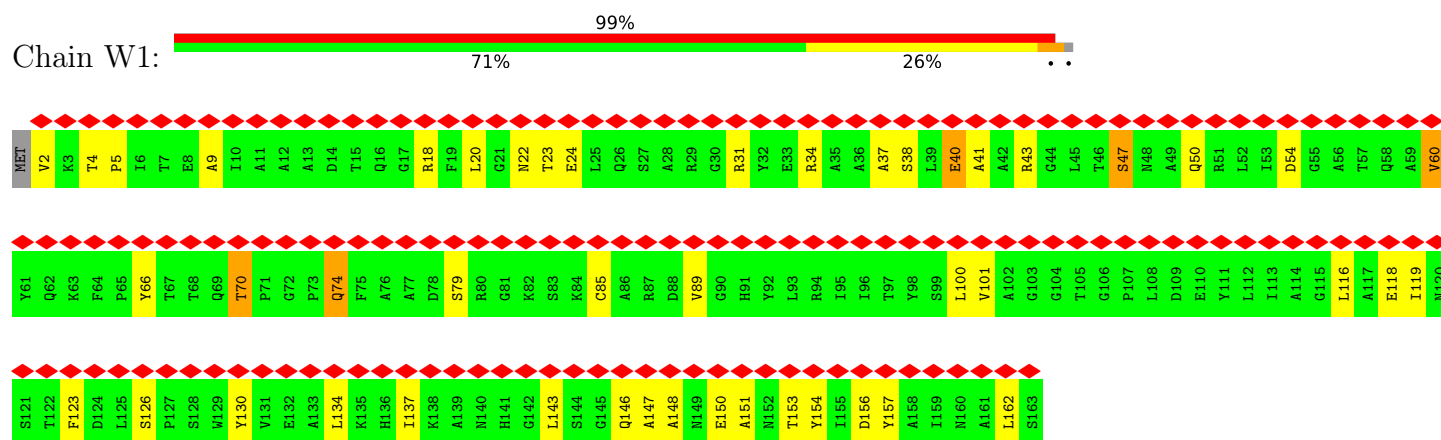
• Molecule 2: C-phycoerythrin alpha subunit



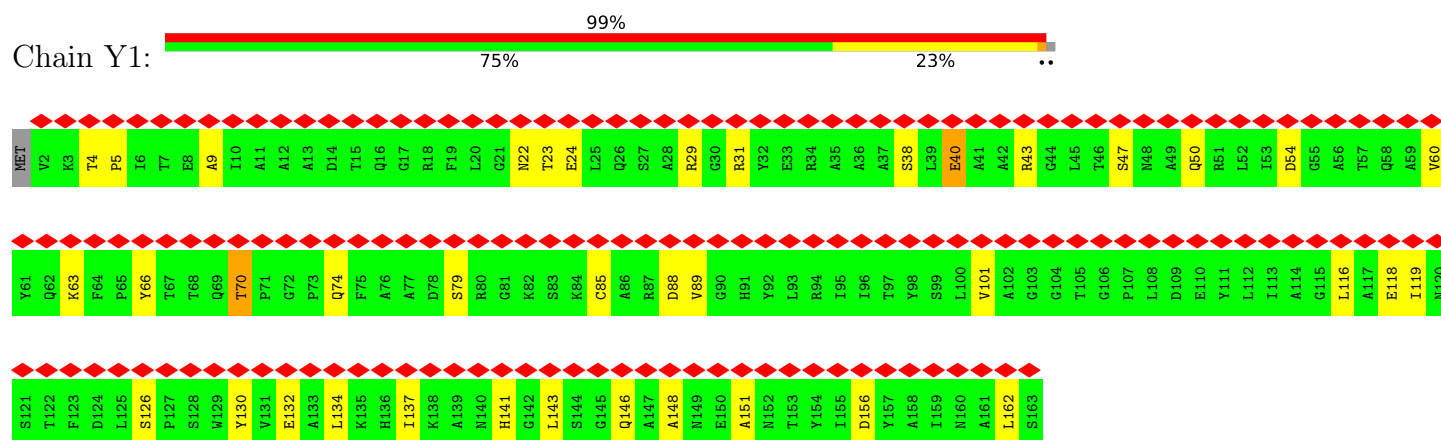
• Molecule 2: C-phycoerythrin alpha subunit



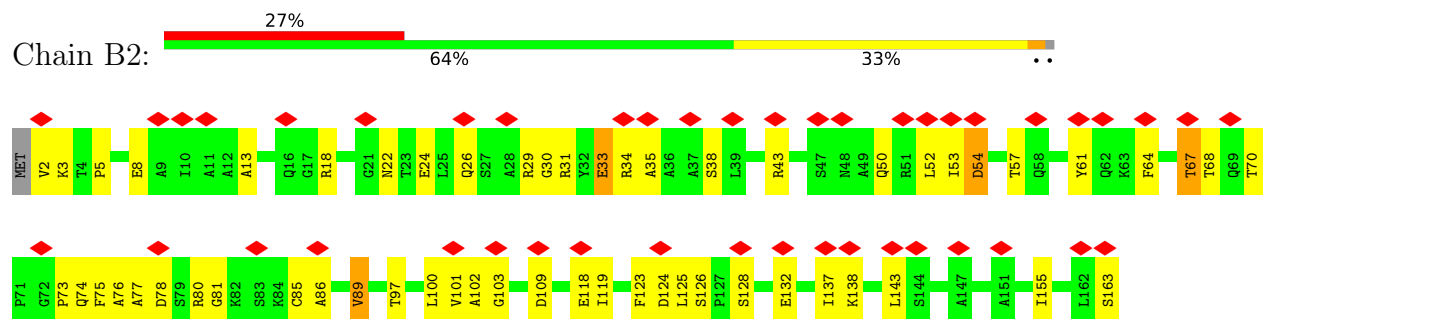
- Molecule 2: C-phycoerythrin alpha subunit



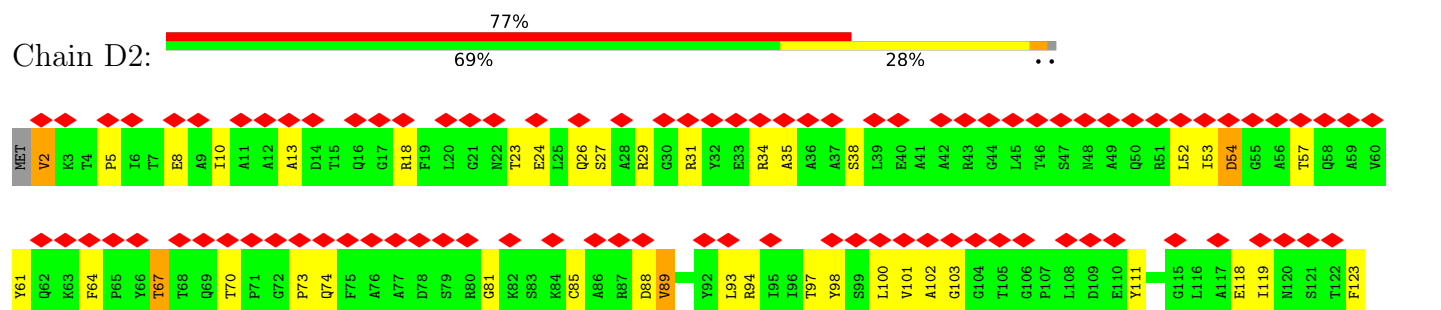
- Molecule 2: C-phycoerythrin alpha subunit

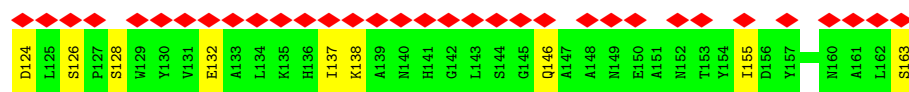


- Molecule 2: C-phycoerythrin alpha subunit

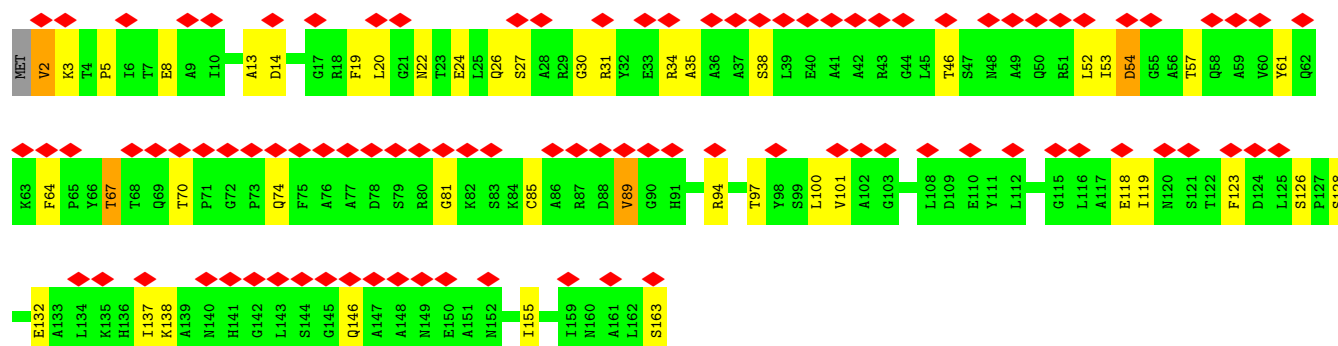
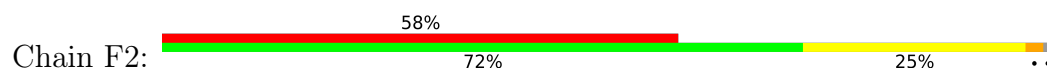


- Molecule 2: C-phycoerythrin alpha subunit

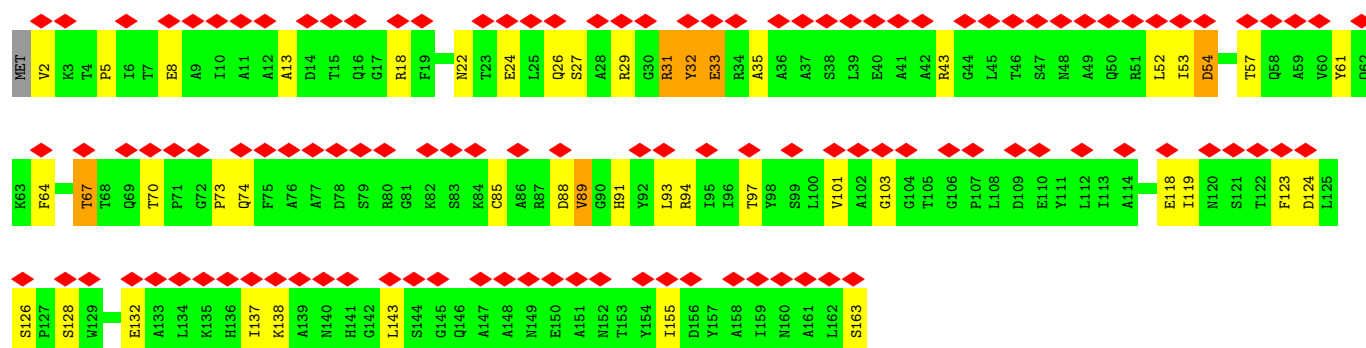
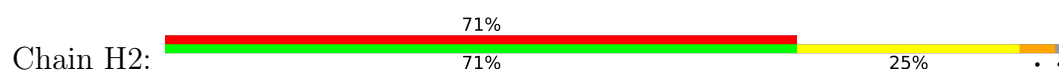




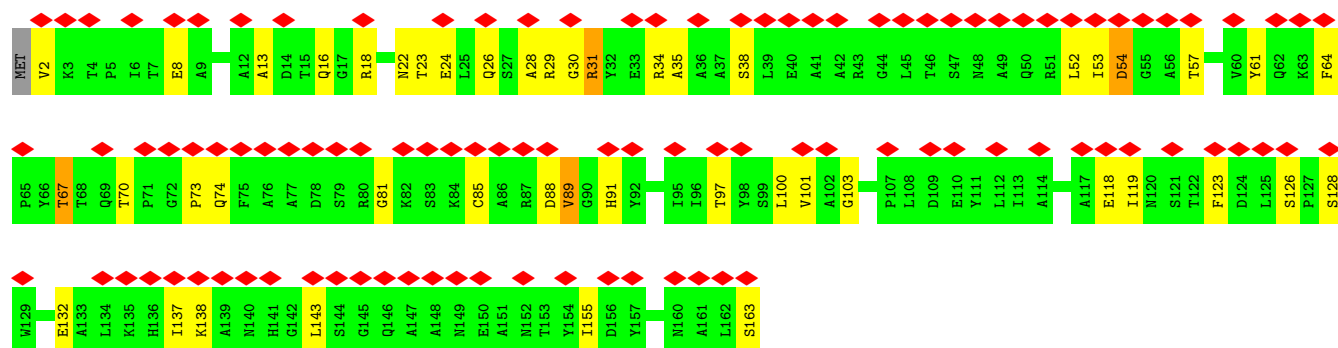
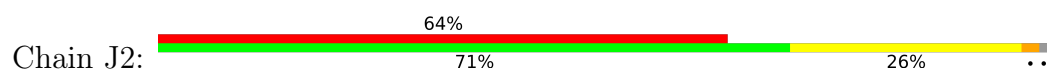
• Molecule 2: C-phycoerythrin alpha subunit



• Molecule 2: C-phycoerythrin alpha subunit

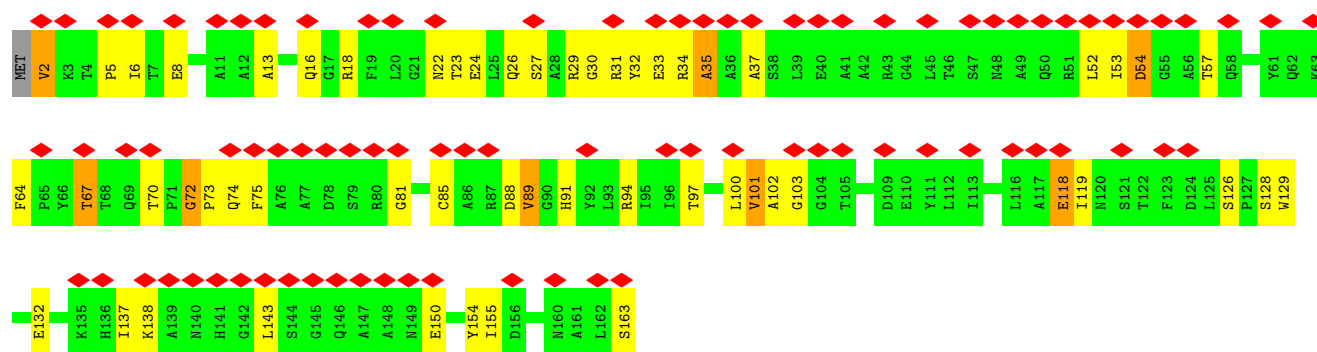


• Molecule 2: C-phycoerythrin alpha subunit

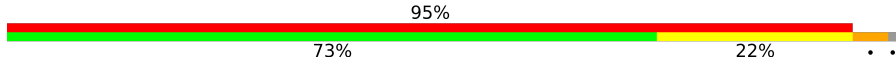


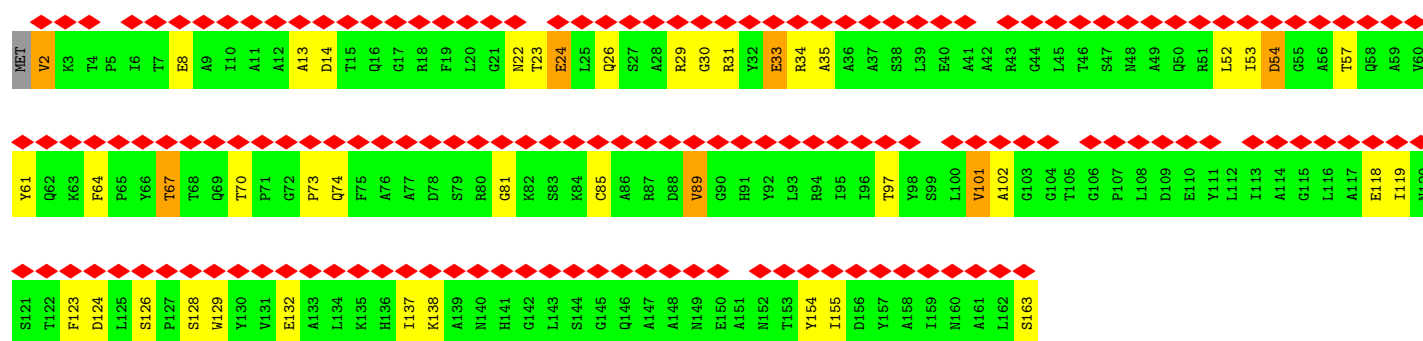
• Molecule 2: C-phycoerythrin alpha subunit

Chain L2: 

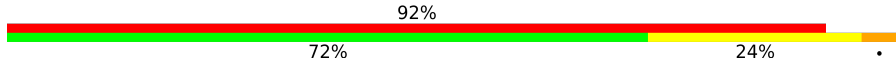


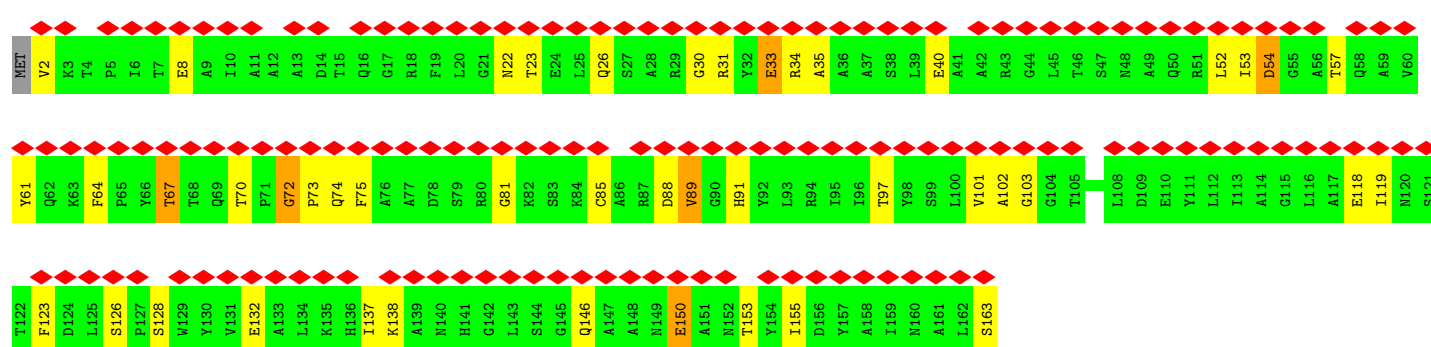
• Molecule 2: C-phycoerythrin alpha subunit

Chain O2: 



• Molecule 2: C-phycoerythrin alpha subunit

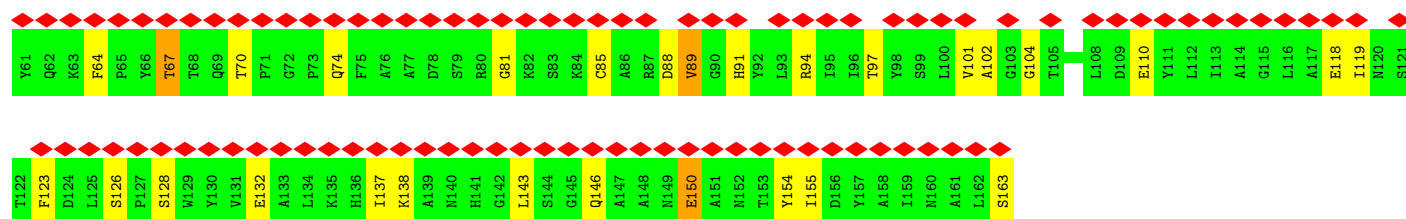
Chain Q2: 



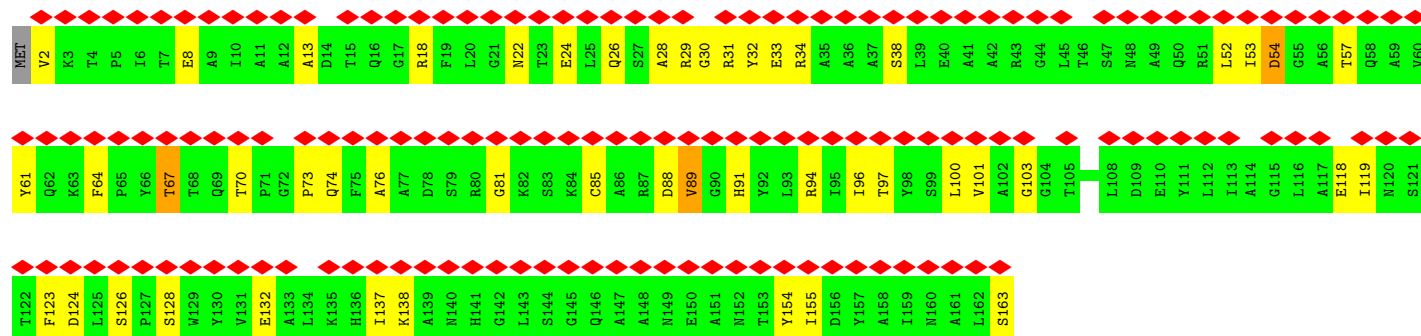
• Molecule 2: C-phycoerythrin alpha subunit

Chain S2: 

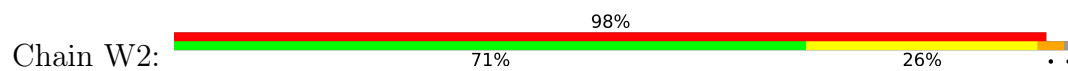




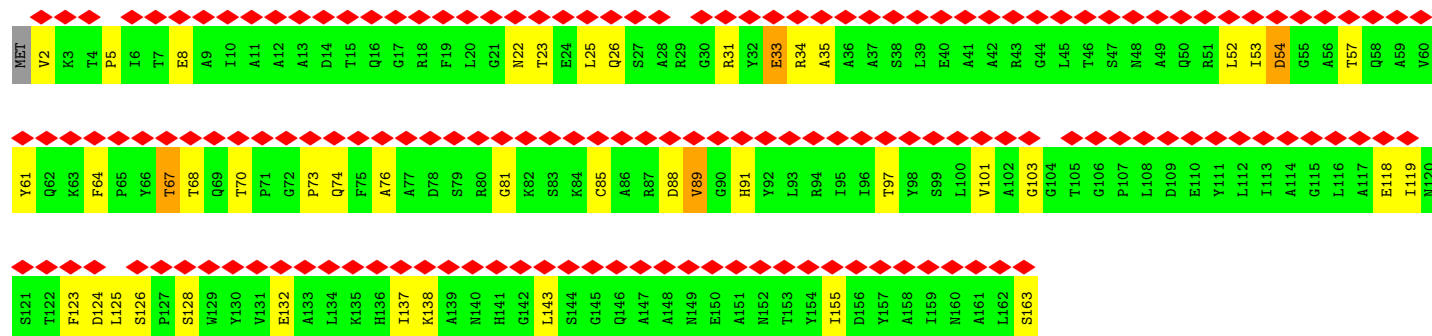
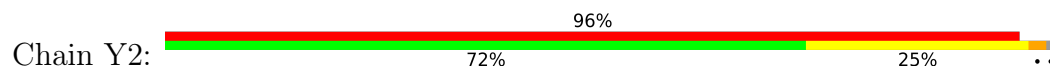
• Molecule 2: C-phycoerythrin alpha subunit



• Molecule 2: C-phycoerythrin alpha subunit

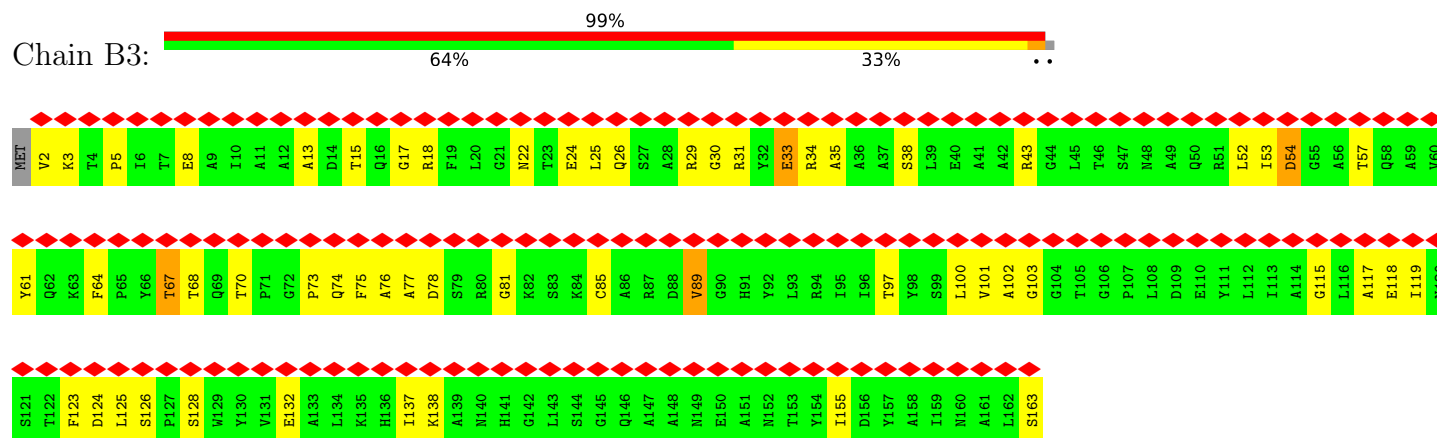


• Molecule 2: C-phycoerythrin alpha subunit



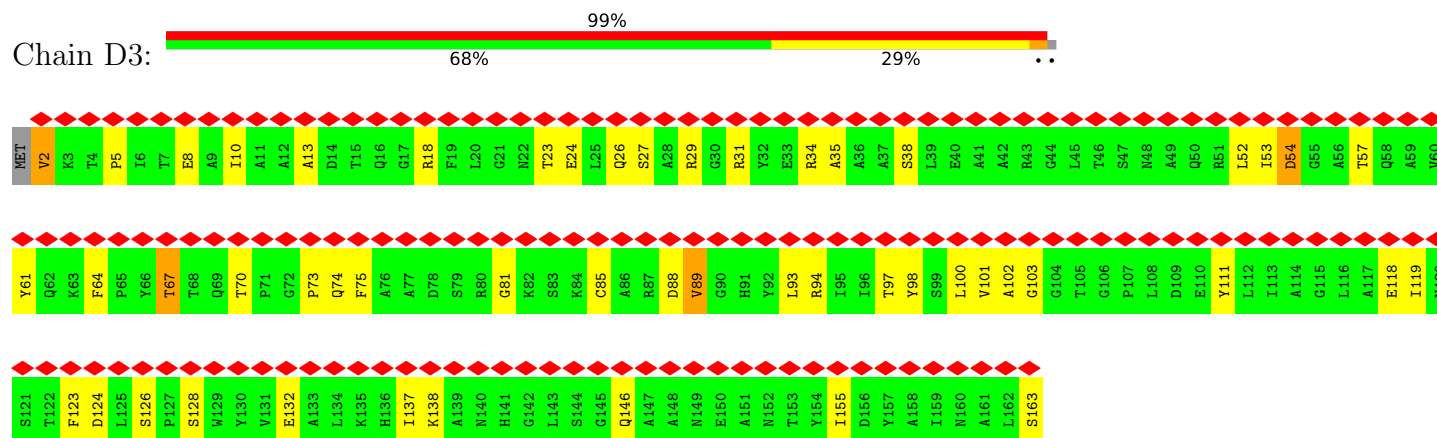
● Molecule 2: C-phycoerythrin alpha subunit

Chain B3:



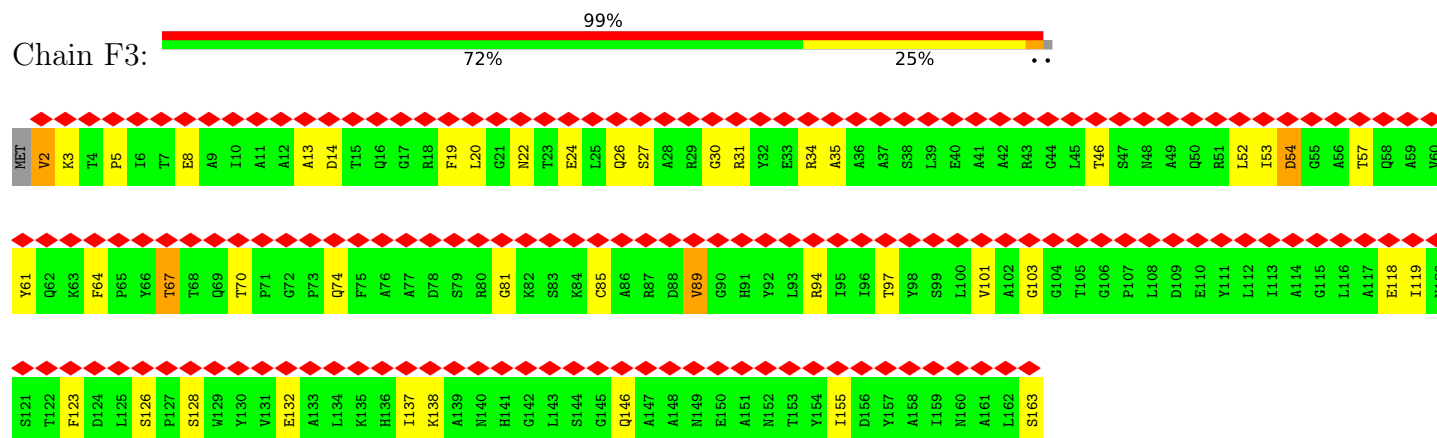
● Molecule 2: C-phycoerythrin alpha subunit

Chain D3:



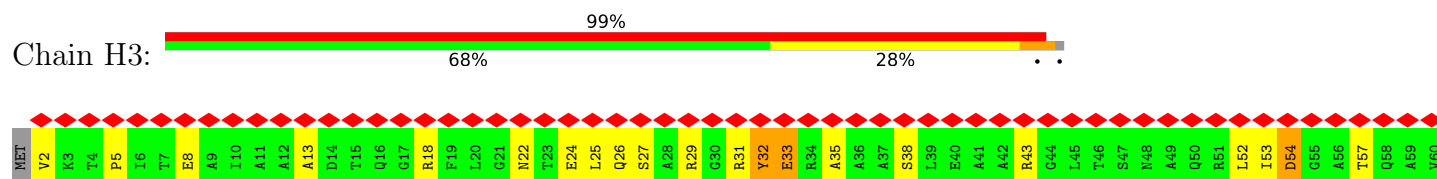
● Molecule 2: C-phycoerythrin alpha subunit

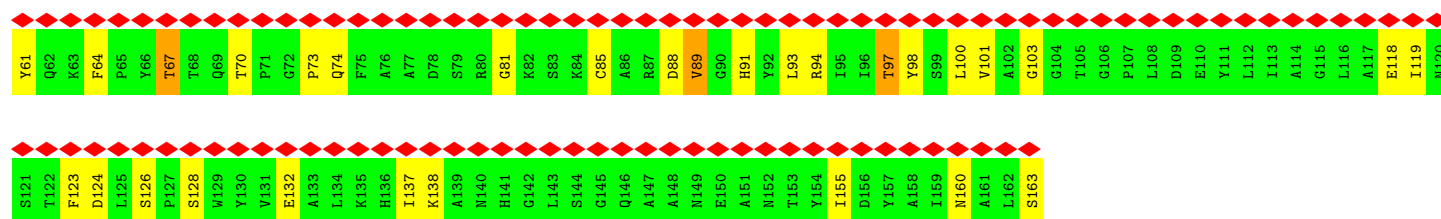
Chain F3:



● Molecule 2: C-phycoerythrin alpha subunit

Chain H3:





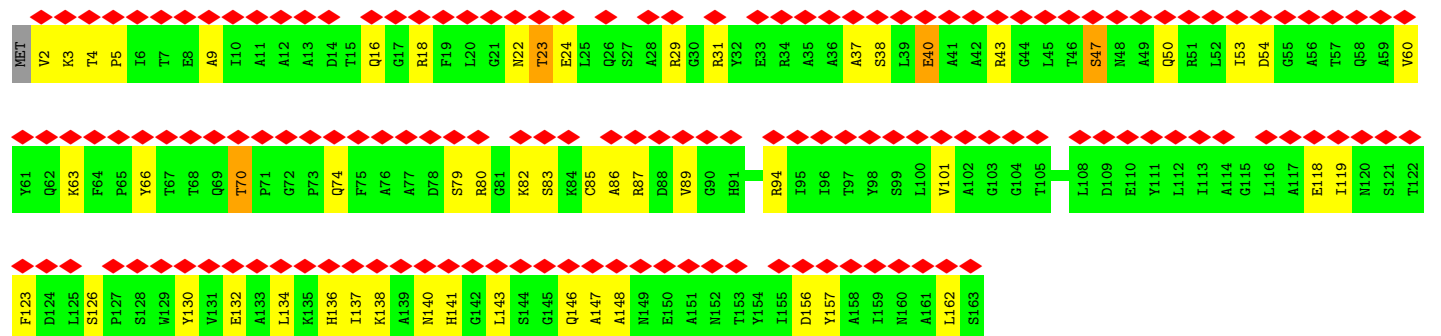
• Molecule 2: C-phycoerythrin alpha subunit



• Molecule 2: C-phycoerythrin alpha subunit

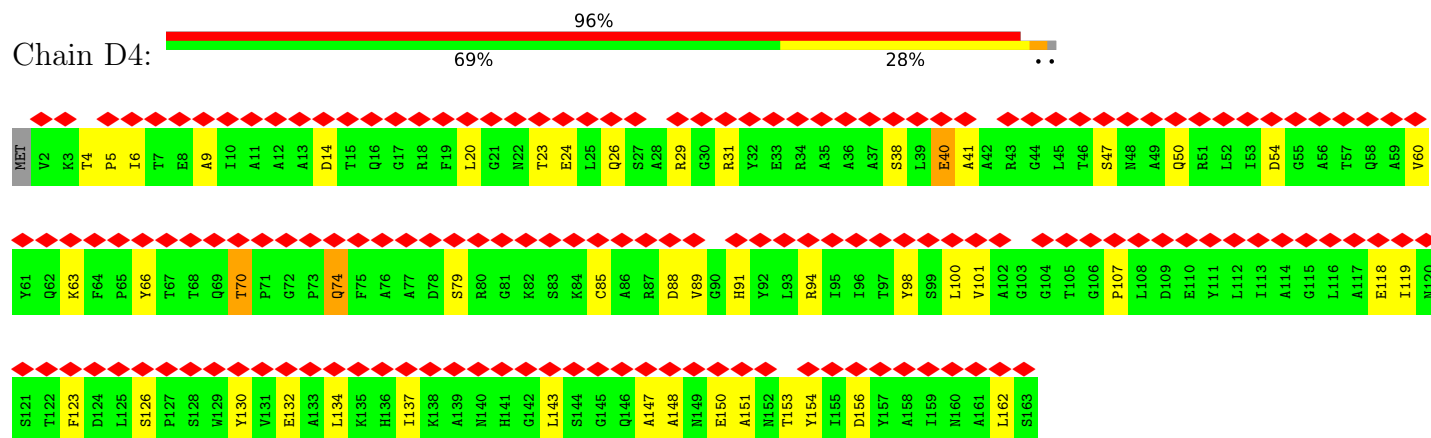


• Molecule 2: C-phycoerythrin alpha subunit



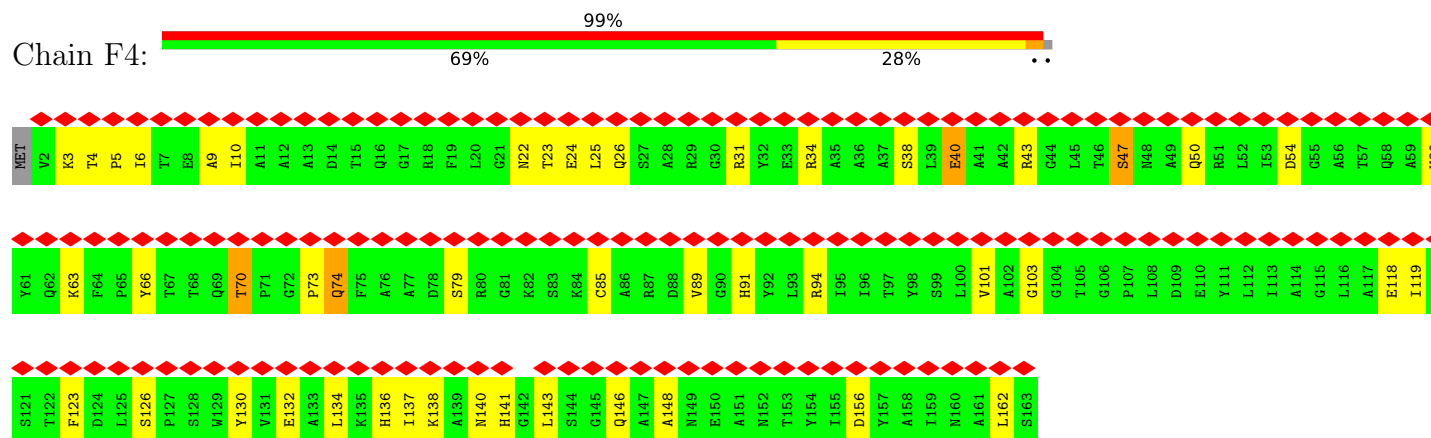
- Molecule 2: C-phycoerythrin alpha subunit

Chain D4:



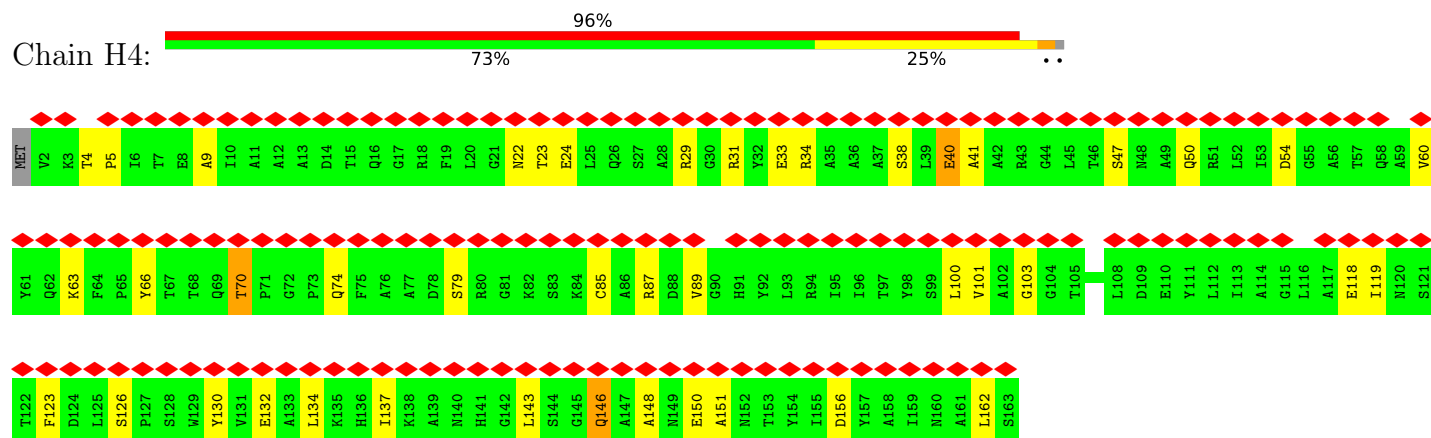
- Molecule 2: C-phycoerythrin alpha subunit

Chain F4:



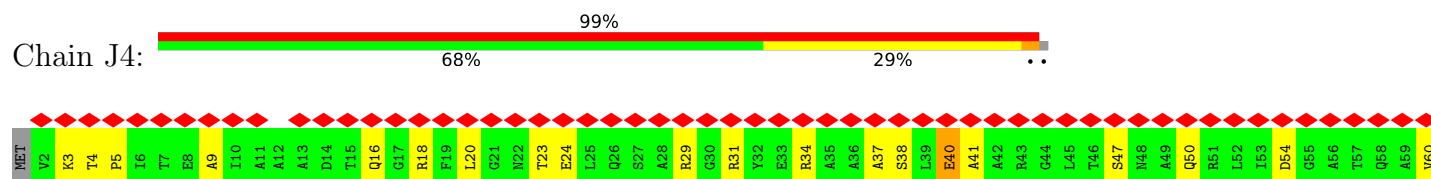
- Molecule 2: C-phycoerythrin alpha subunit

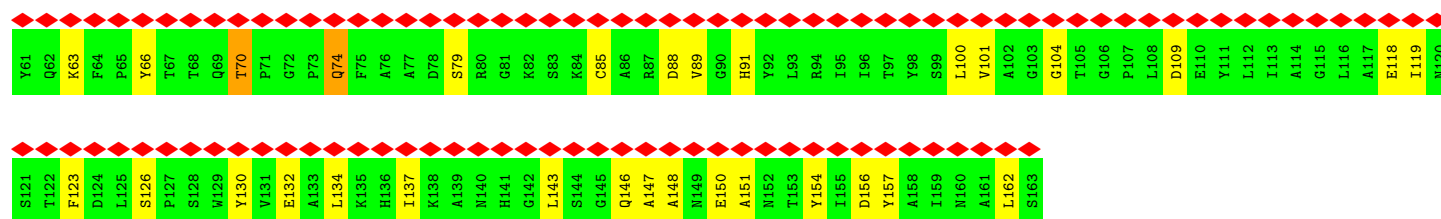
Chain H4:



- Molecule 2: C-phycoerythrin alpha subunit

Chain J4:





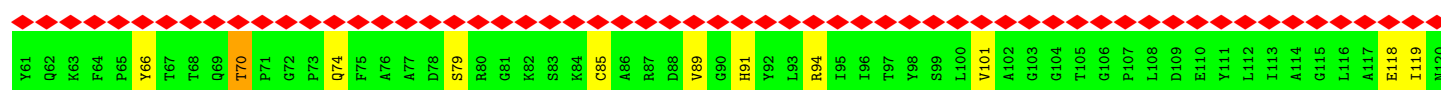
• Molecule 2: C-phycoerythrin alpha subunit

Chain L4: 98%
69% 29%



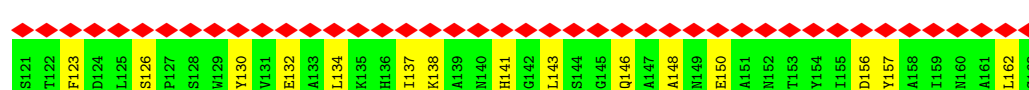
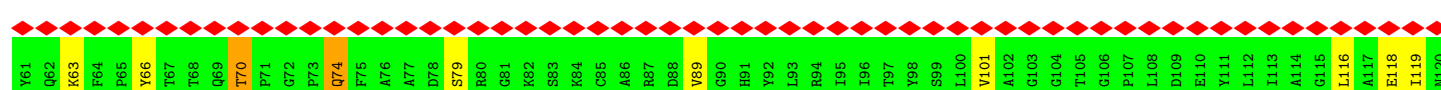
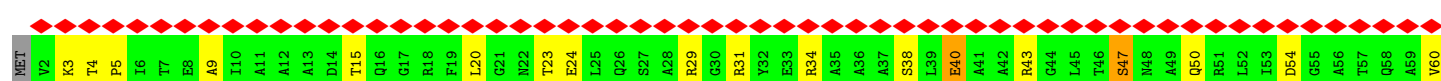
• Molecule 2: C-phycoerythrin alpha subunit

Chain O4: 99%
75% 23%



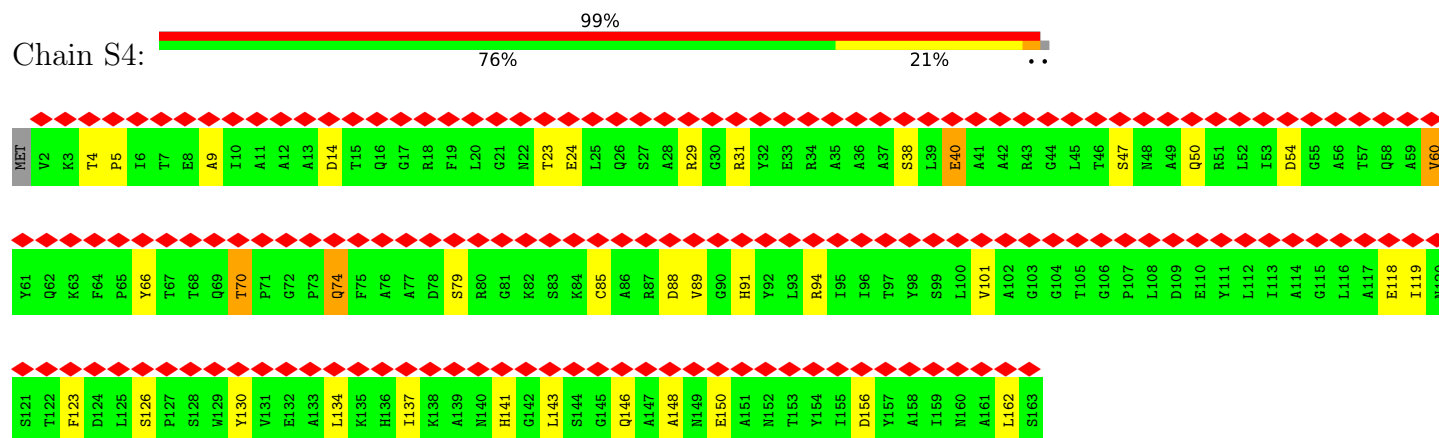
• Molecule 2: C-phycoerythrin alpha subunit

Chain Q4: 99%
73% 24%



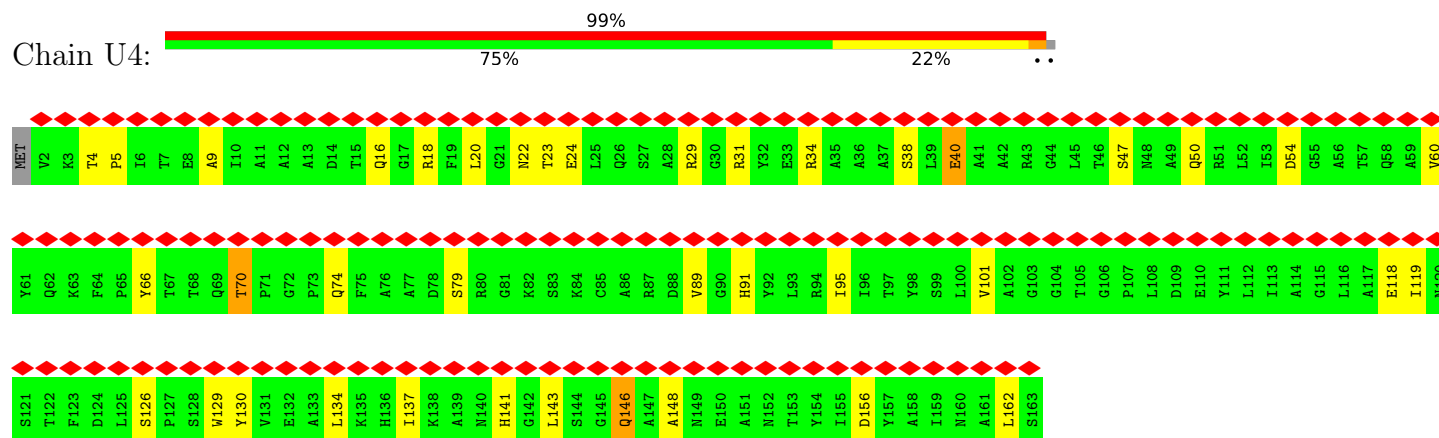
- Molecule 2: C-phycoerythrin alpha subunit

Chain S4:



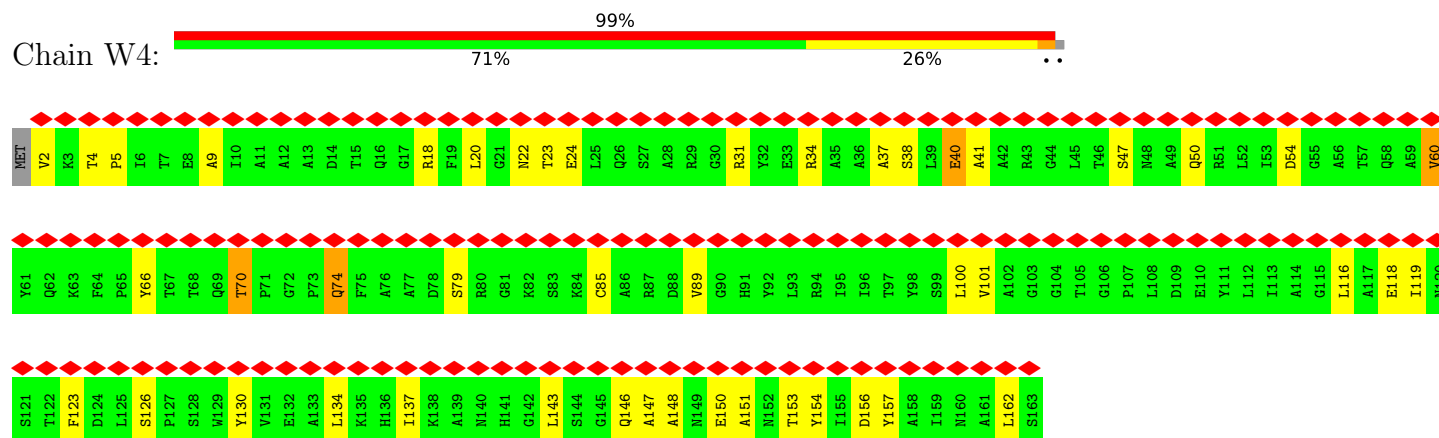
- Molecule 2: C-phycoerythrin alpha subunit

Chain U4:



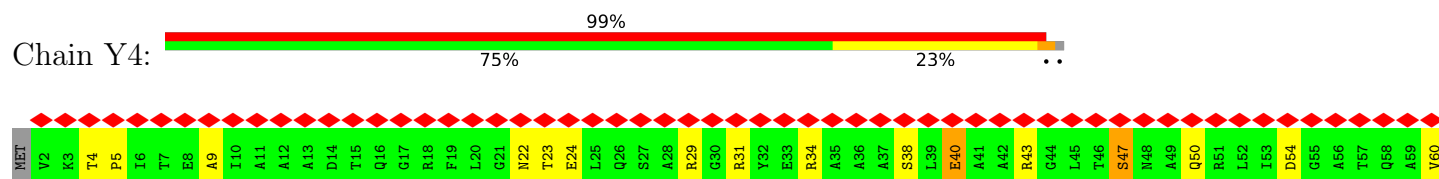
- Molecule 2: C-phycoerythrin alpha subunit

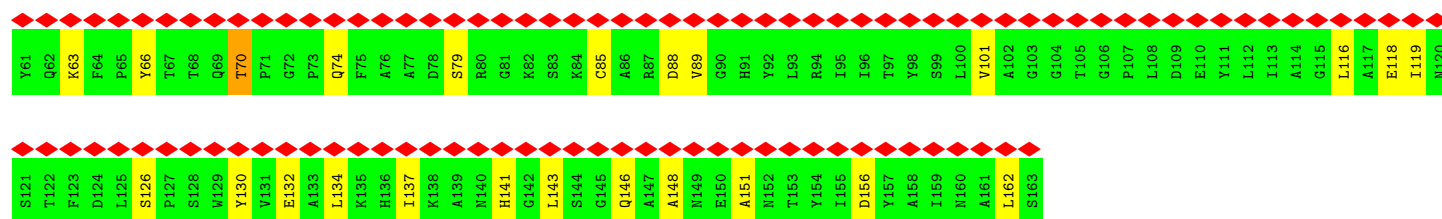
Chain W4:



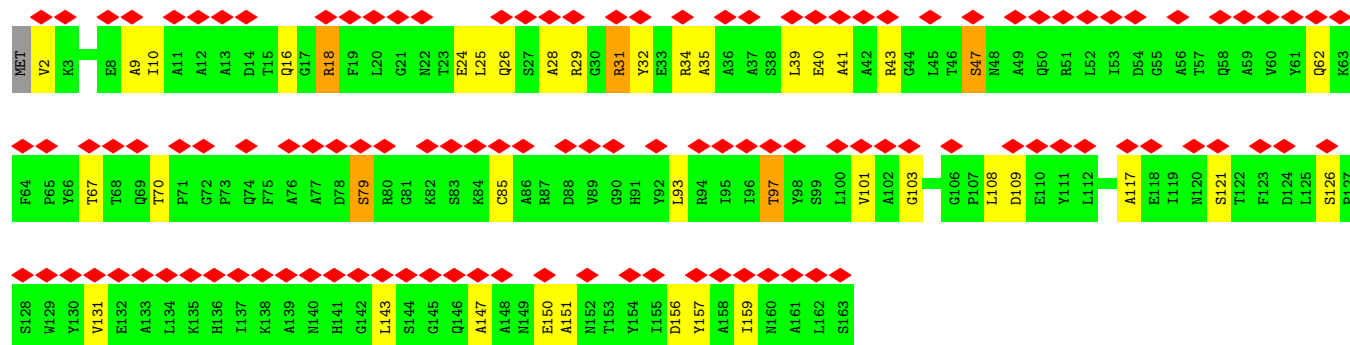
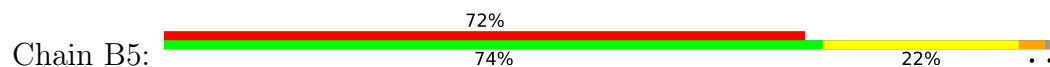
- Molecule 2: C-phycoerythrin alpha subunit

Chain Y4:

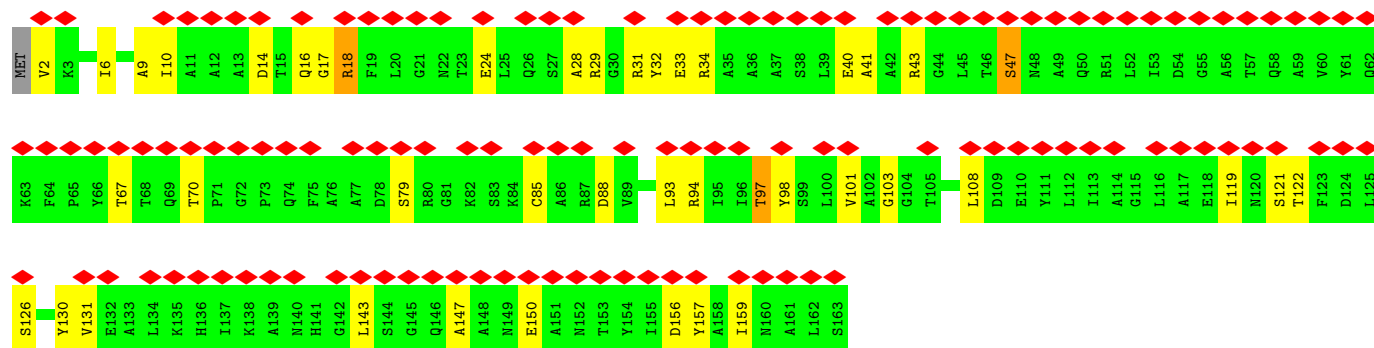
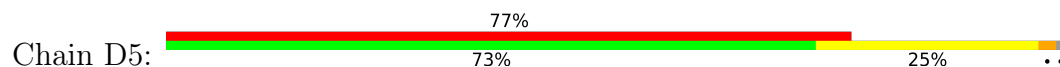




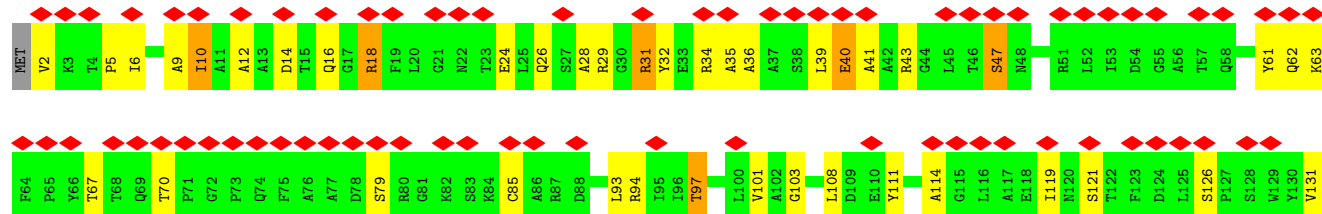
• Molecule 2: C-phycoerythrin alpha subunit

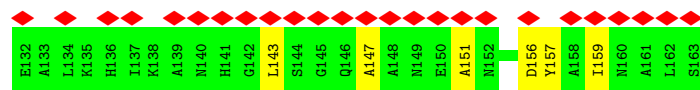


• Molecule 2: C-phycoerythrin alpha subunit

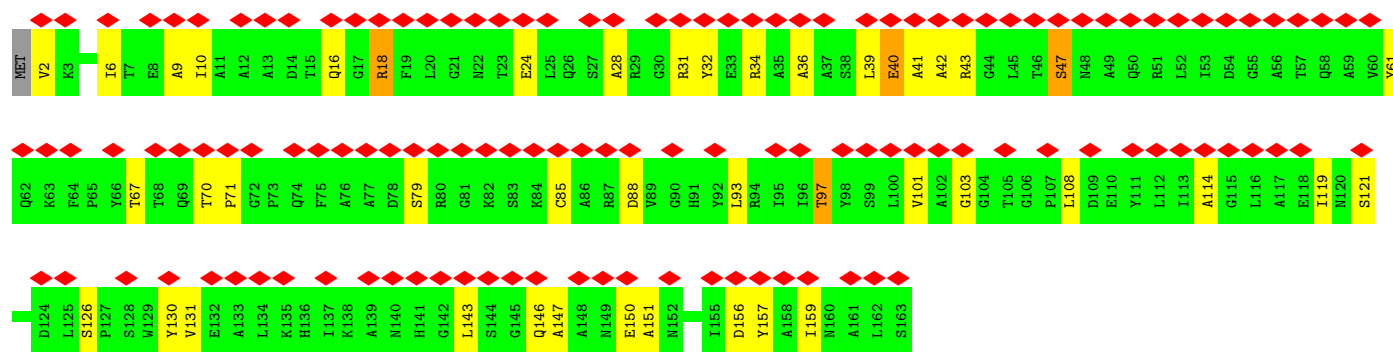
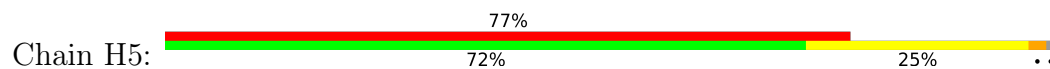


• Molecule 2: C-phycoerythrin alpha subunit

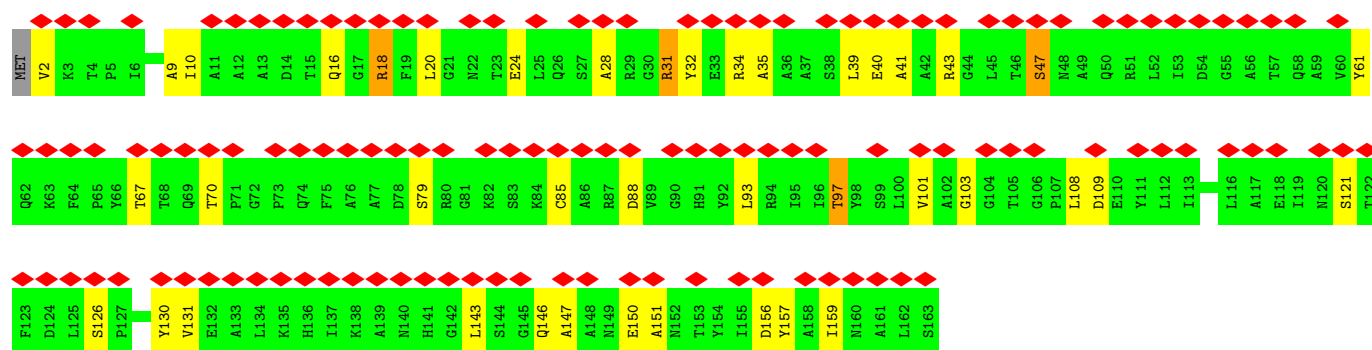
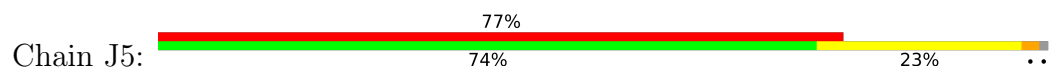




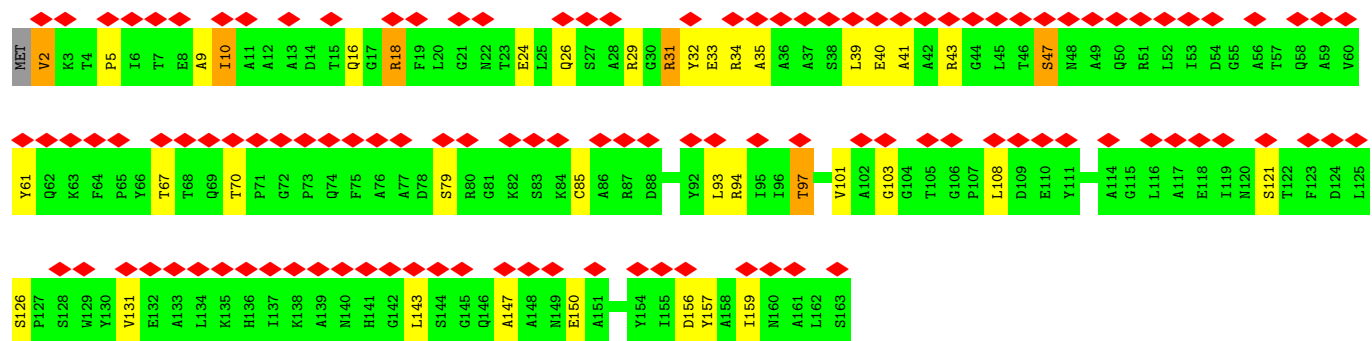
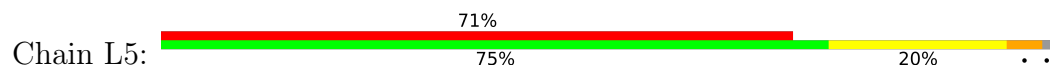
• Molecule 2: C-phycocyanin alpha subunit



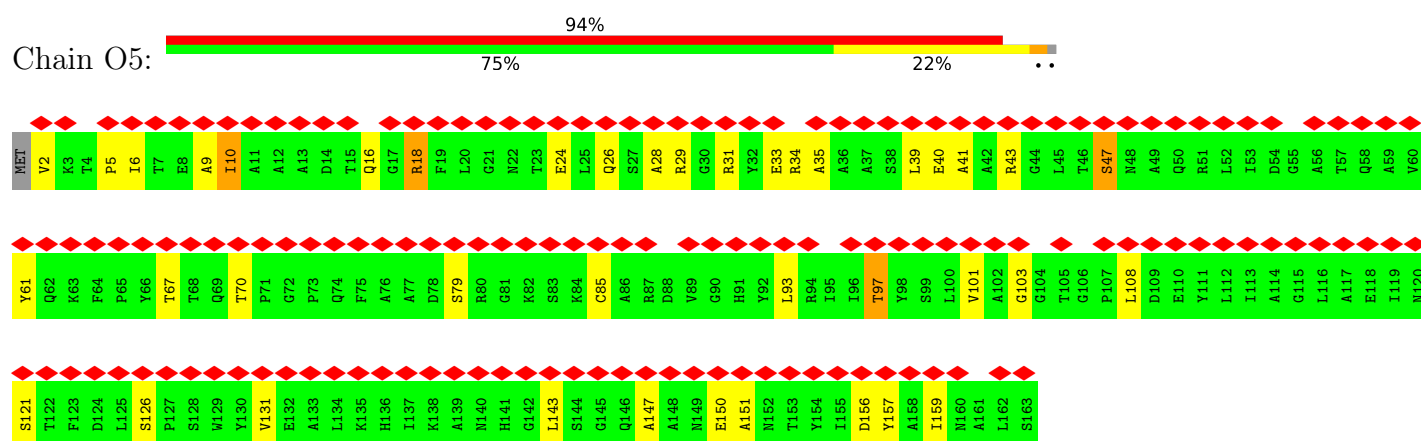
• Molecule 2: C-phycocyanin alpha subunit



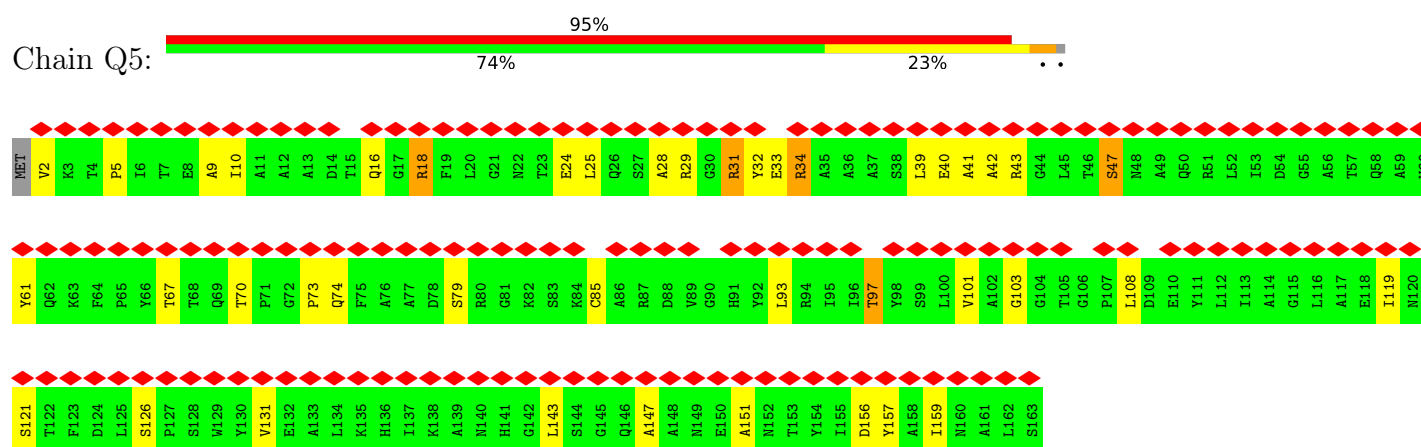
• Molecule 2: C-phycocyanin alpha subunit



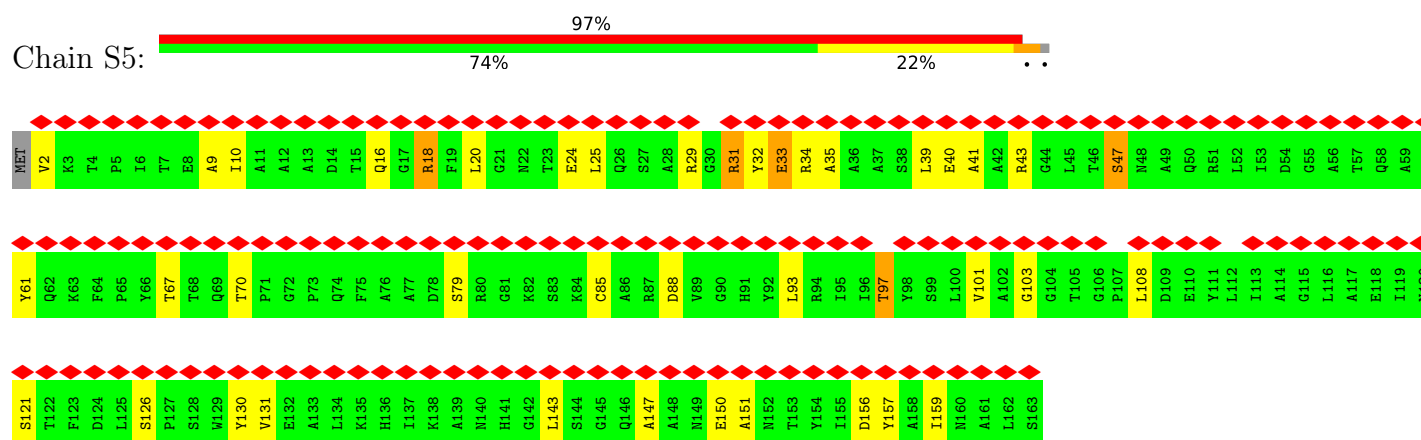
• Molecule 2: C-phycocyanin alpha subunit



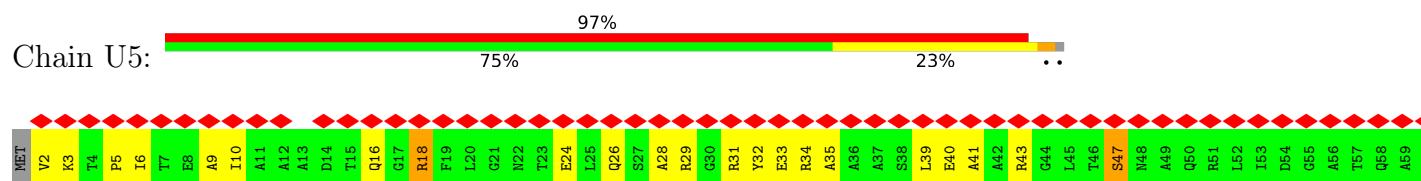
- Molecule 2: C-phycocyanin alpha subunit

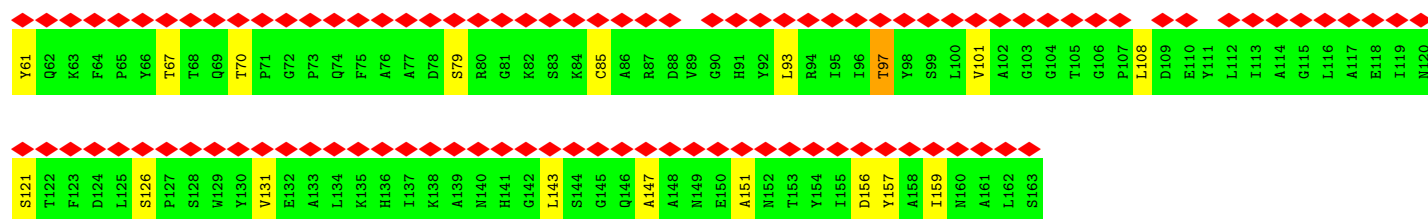


- Molecule 2: C-phycocyanin alpha subunit

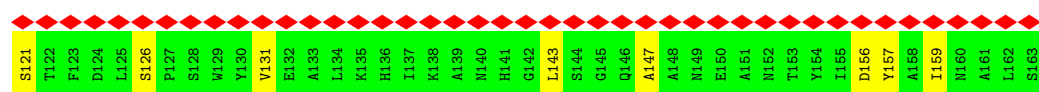
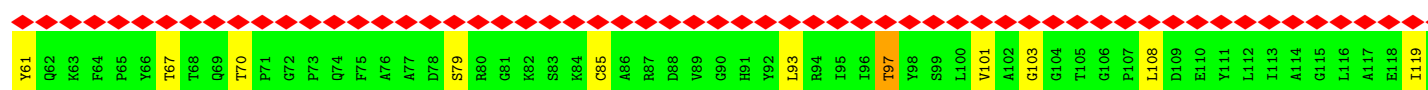
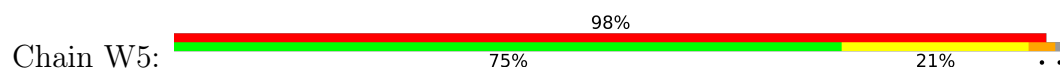


- Molecule 2: C-phycocyanin alpha subunit

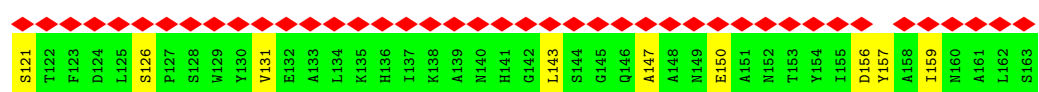
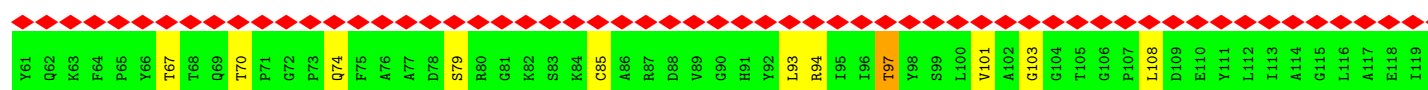
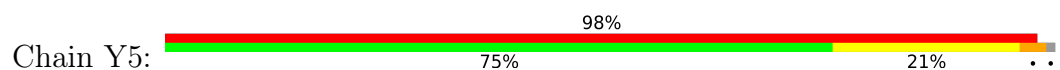




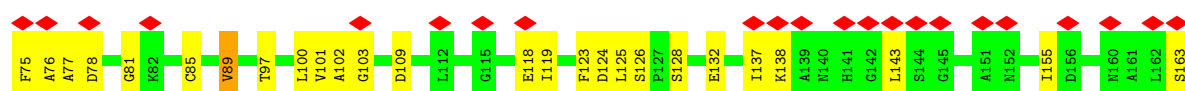
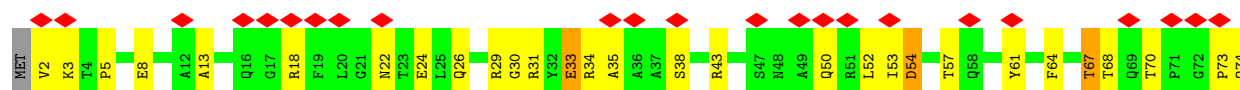
• Molecule 2: C-phycoerythrin alpha subunit



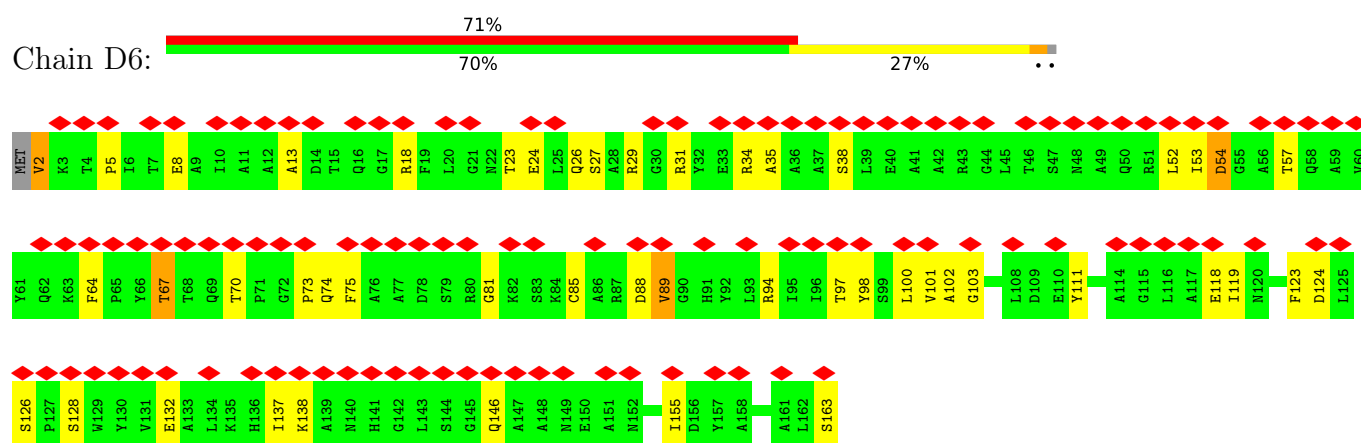
• Molecule 2: C-phycoerythrin alpha subunit



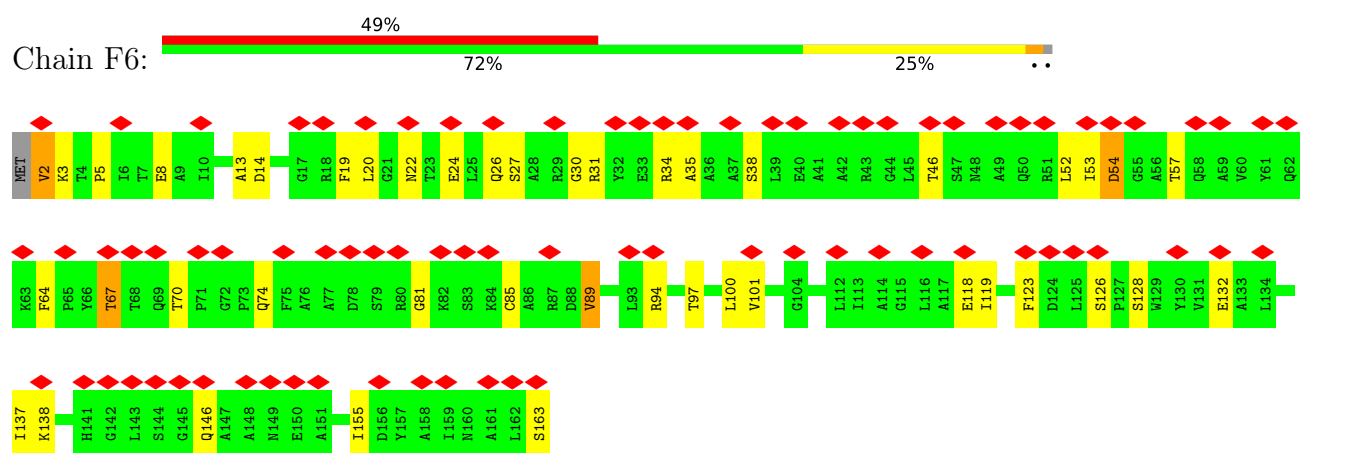
• Molecule 2: C-phycoerythrin alpha subunit



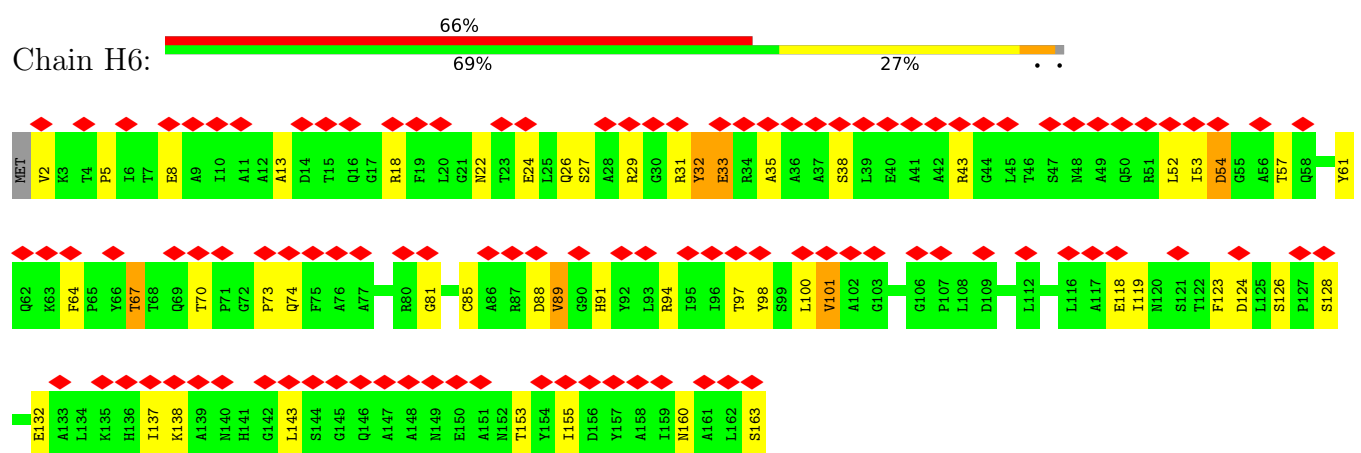
• Molecule 2: C-phycoerythrin alpha subunit



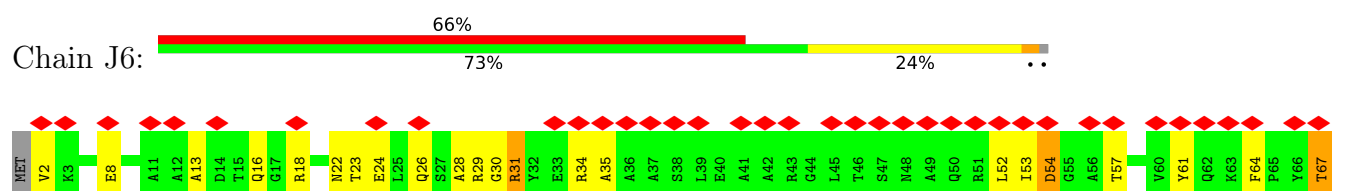
- Molecule 2: C-phycoerythrin alpha subunit

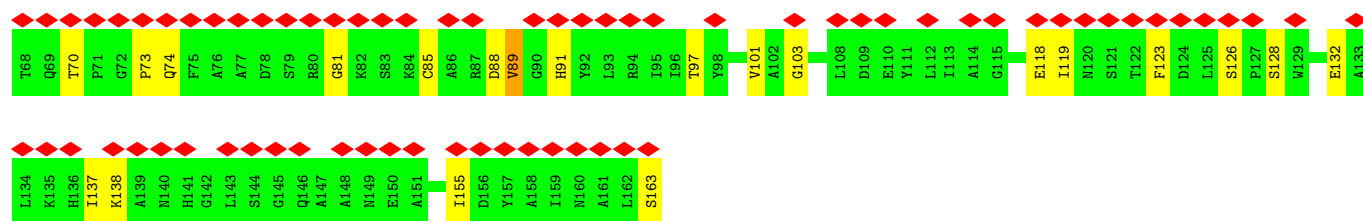


- Molecule 2: C-phycoerythrin alpha subunit

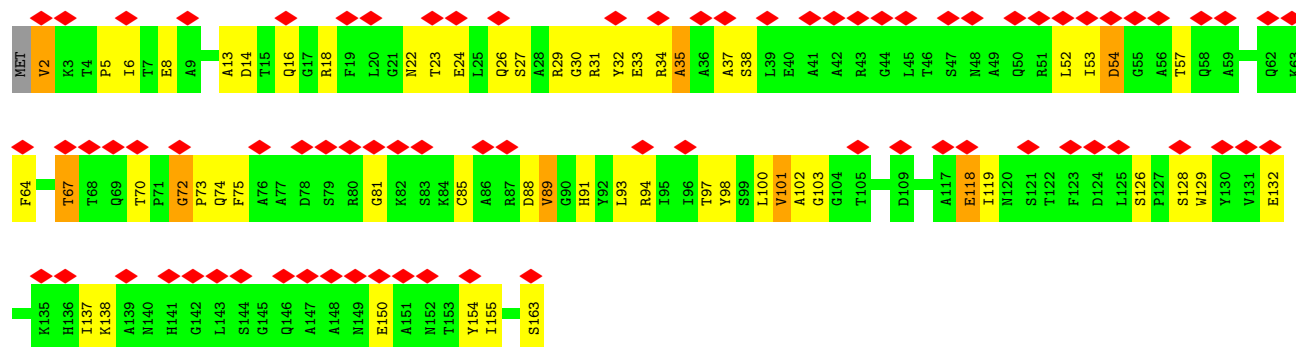


- Molecule 2: C-phycoerythrin alpha subunit

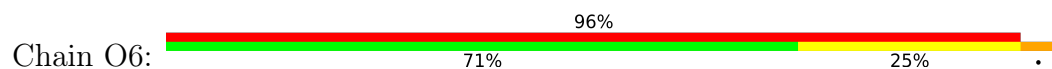




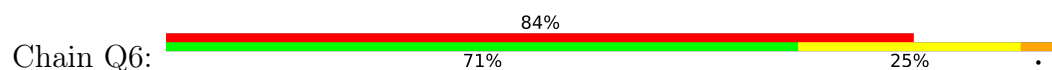
• Molecule 2: C-phycocyanin alpha subunit

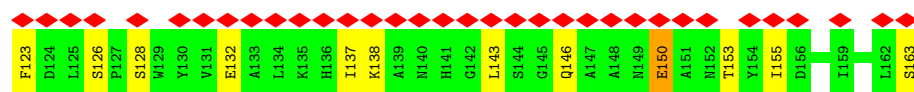


• Molecule 2: C-phycocyanin alpha subunit

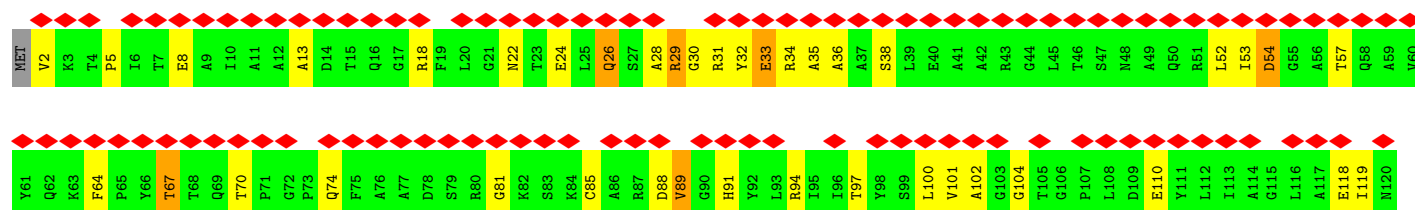


• Molecule 2: C-phycocyanin alpha subunit

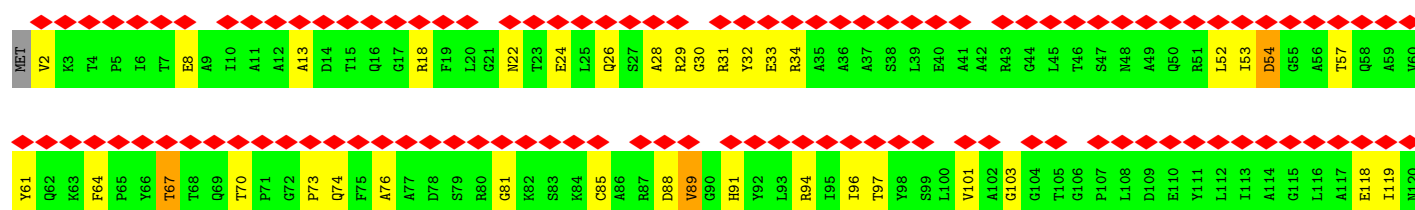
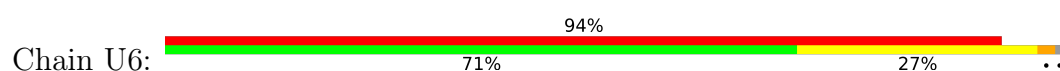




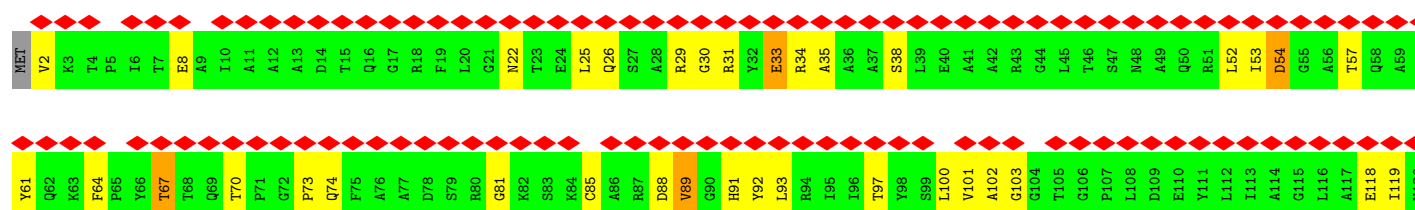
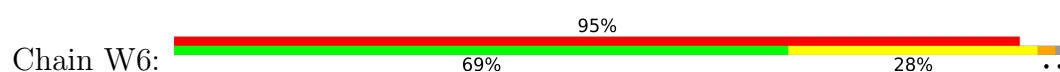
• Molecule 2: C-phycoerythrin alpha subunit



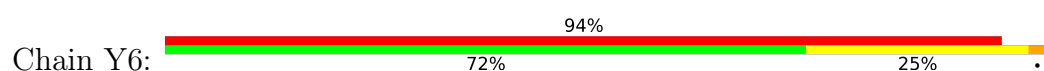
• Molecule 2: C-phycoerythrin alpha subunit

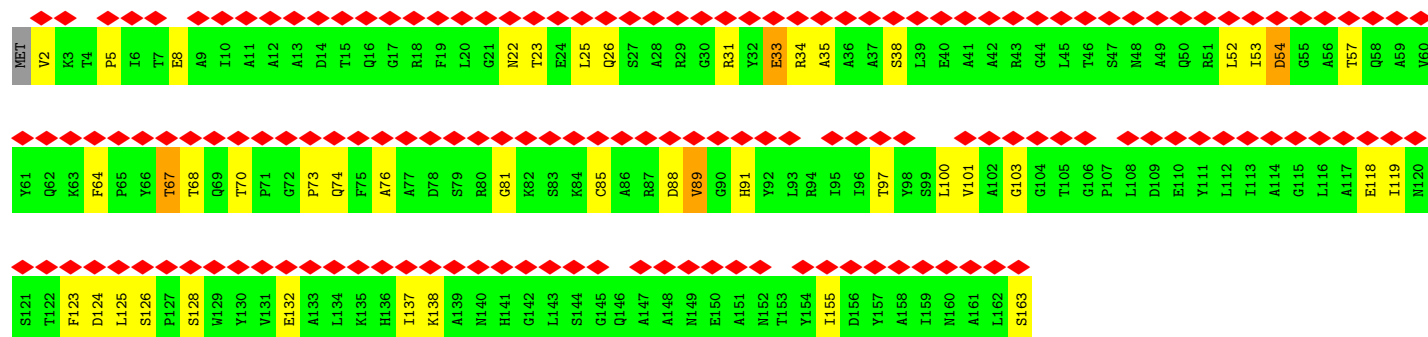


• Molecule 2: C-phycoerythrin alpha subunit

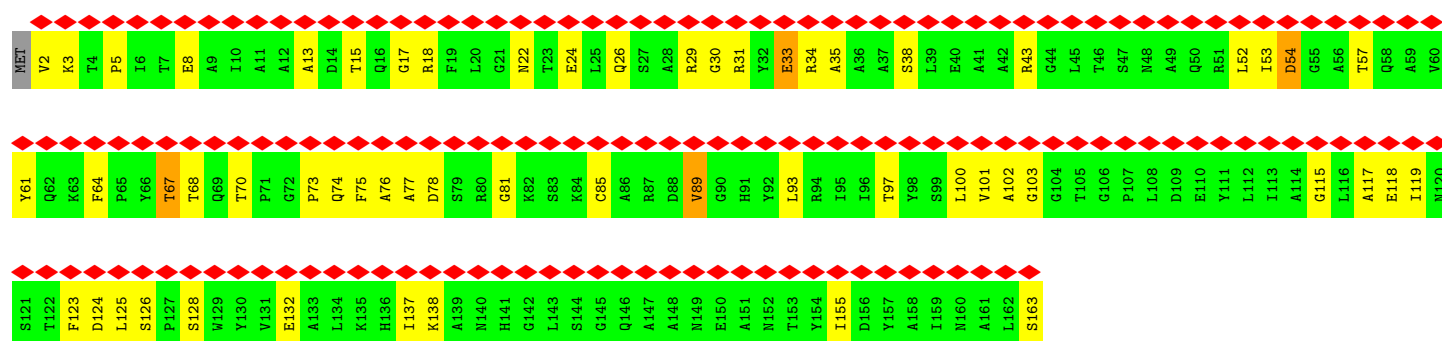


• Molecule 2: C-phycoerythrin alpha subunit

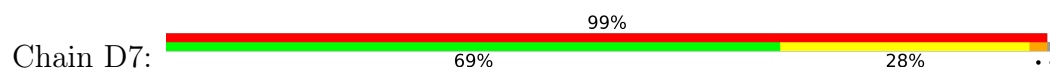




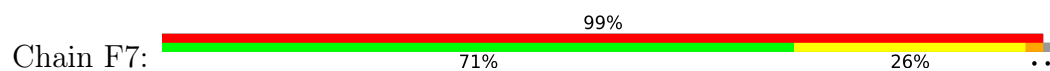
• Molecule 2: C-phycoerythrin alpha subunit



• Molecule 2: C-phycoerythrin alpha subunit

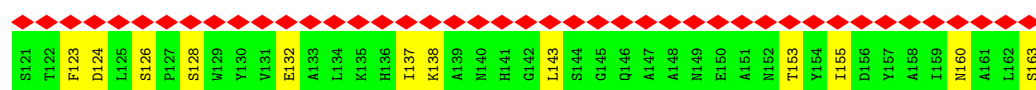
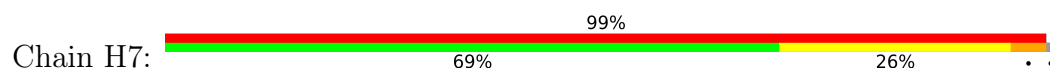


• Molecule 2: C-phycoerythrin alpha subunit

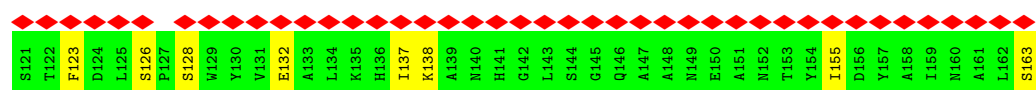
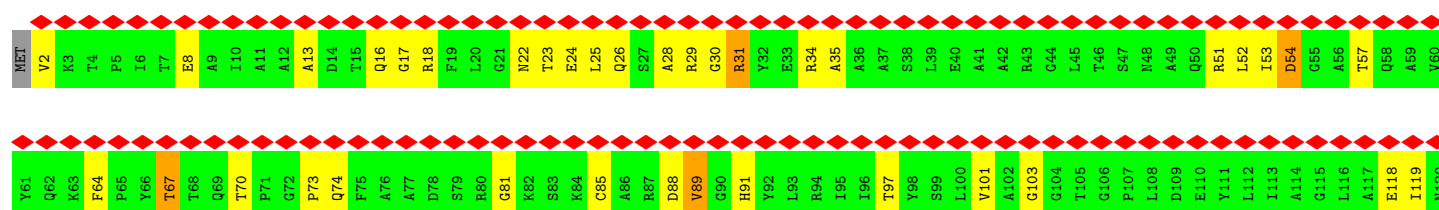
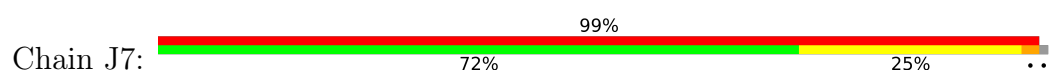




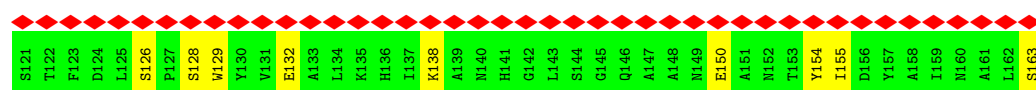
- Molecule 2: C-phycoerythrin alpha subunit



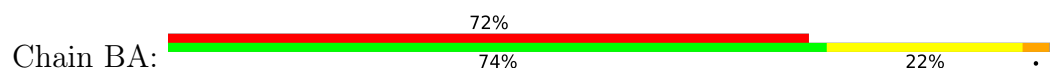
- Molecule 2: C-phycoerythrin alpha subunit

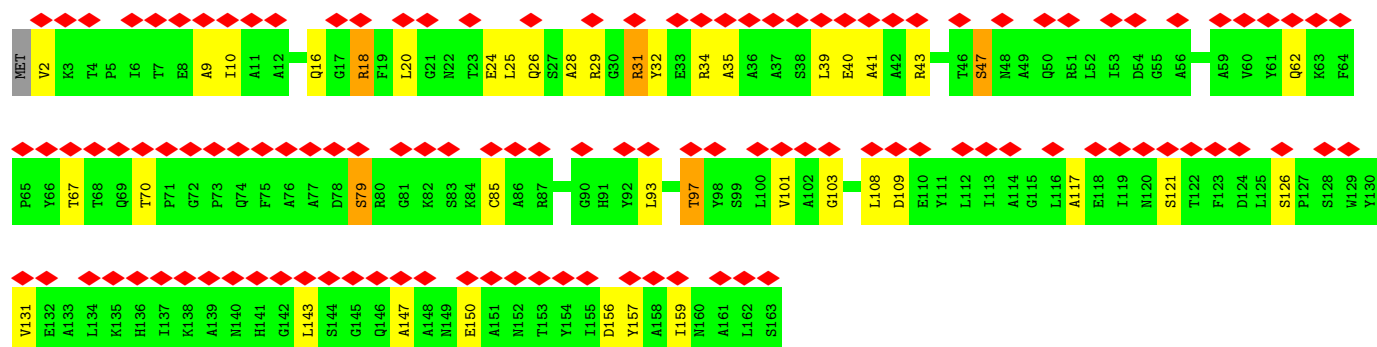


- Molecule 2: C-phycoerythrin alpha subunit

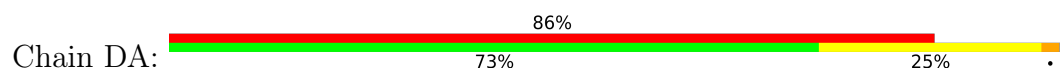


- Molecule 2: C-phycoerythrin alpha subunit

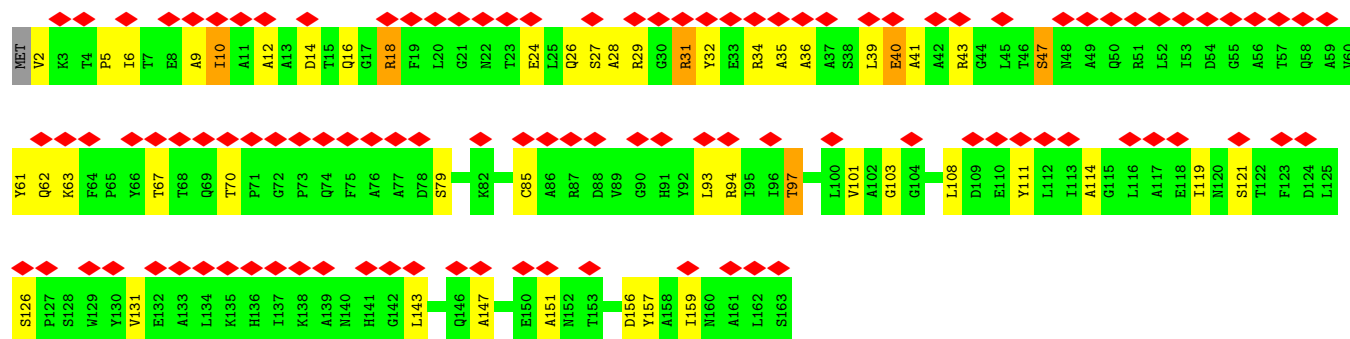




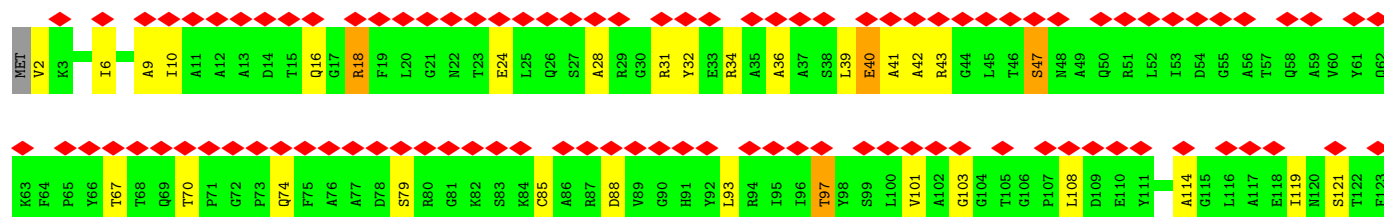
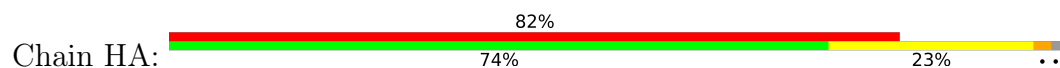
• Molecule 2: C-phycoerythrin alpha subunit

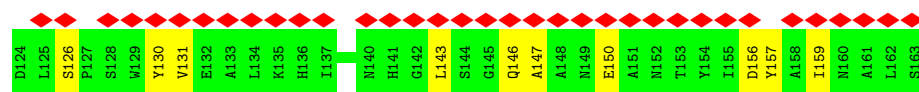


• Molecule 2: C-phycoerythrin alpha subunit

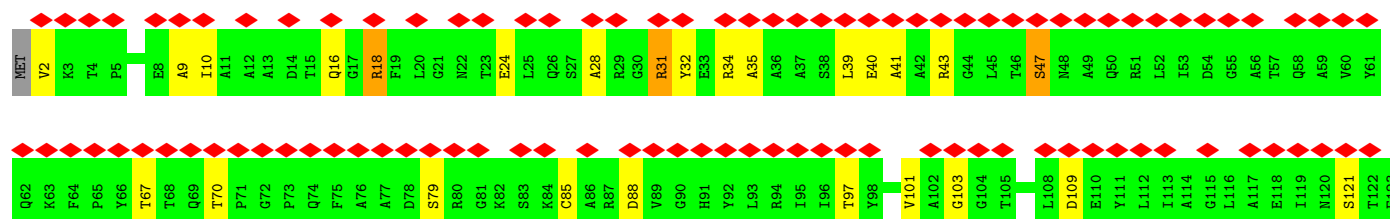
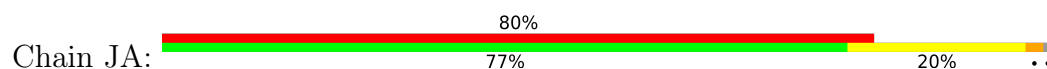


• Molecule 2: C-phycoerythrin alpha subunit

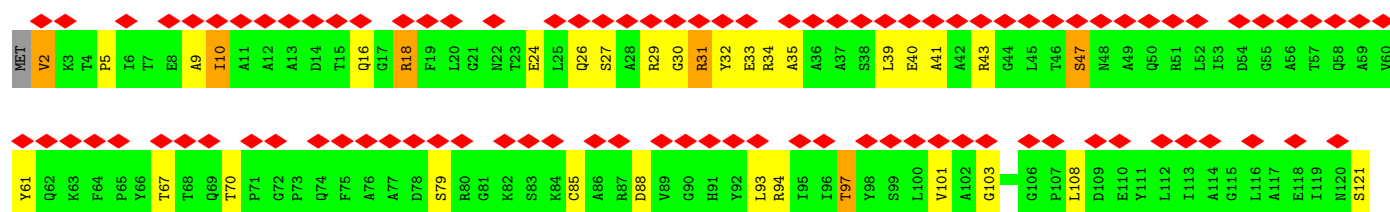
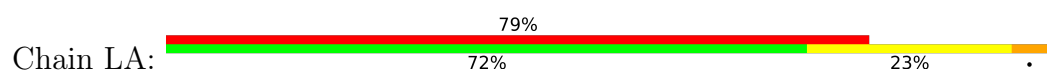




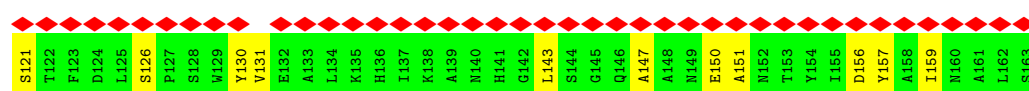
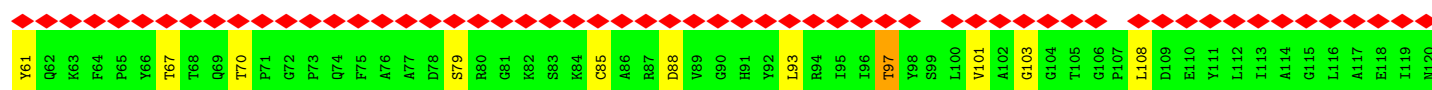
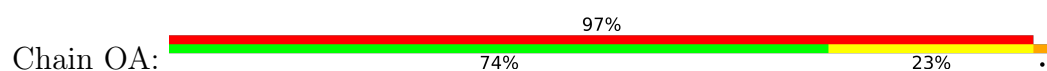
• Molecule 2: C-phycocyanin alpha subunit



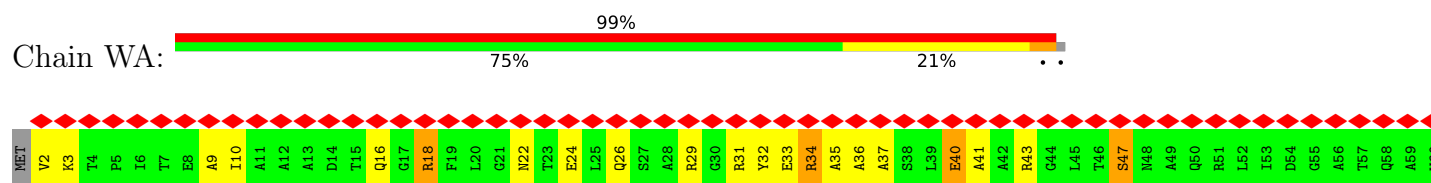
• Molecule 2: C-phycocyanin alpha subunit



• Molecule 2: C-phycocyanin alpha subunit

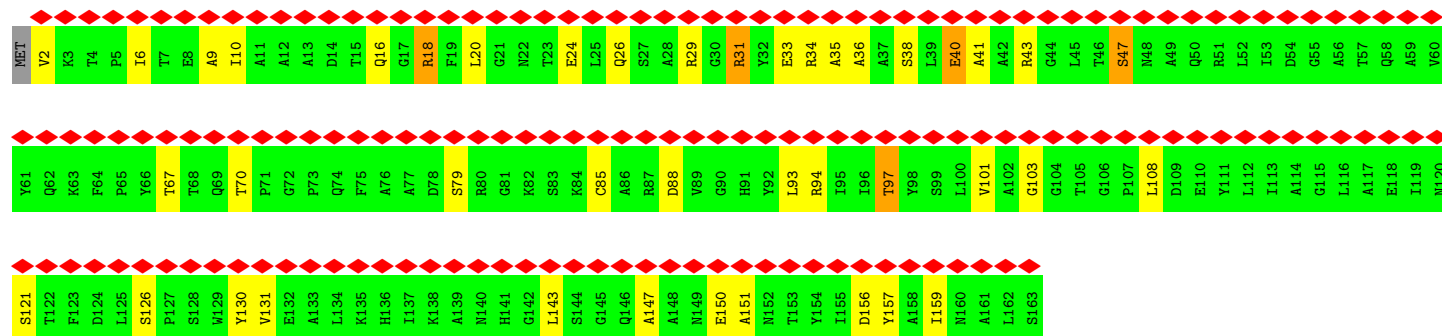
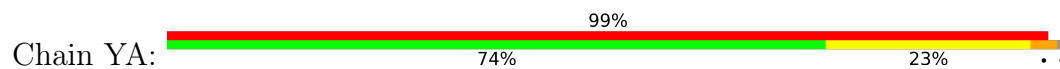


• Molecule 2: C-phycocyanin alpha subunit

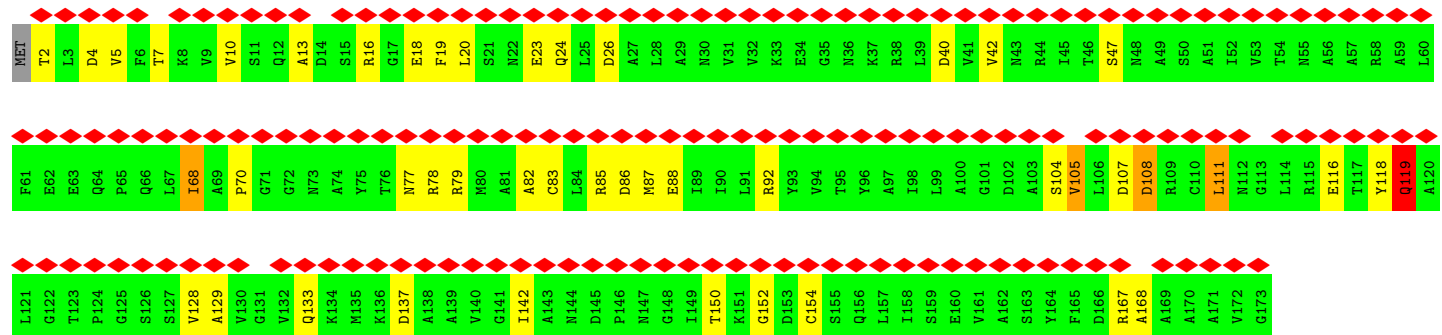
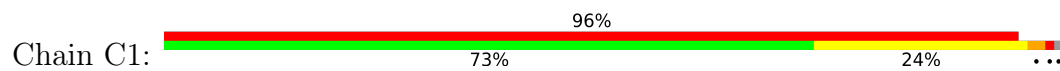




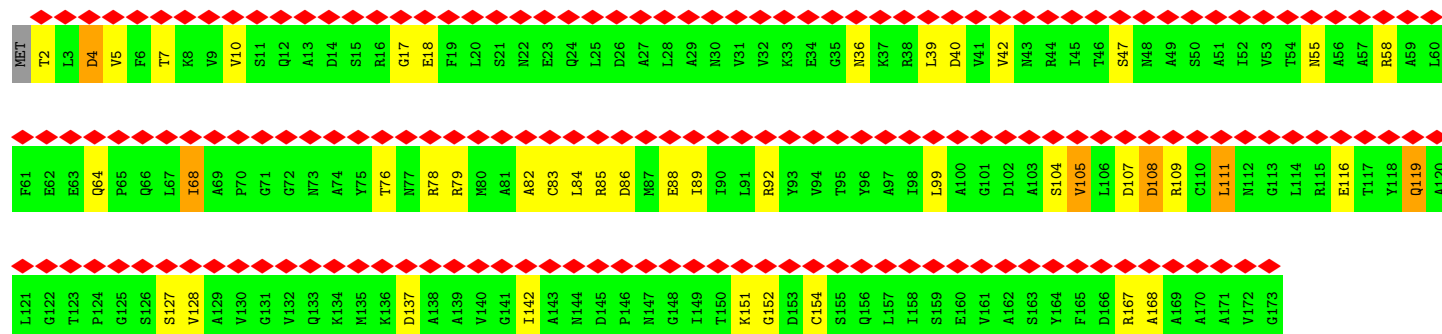
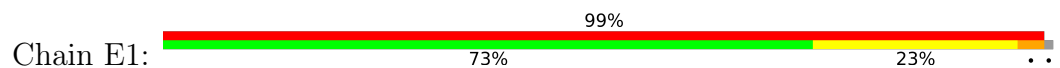
• Molecule 2: C-phycoerythrin alpha subunit



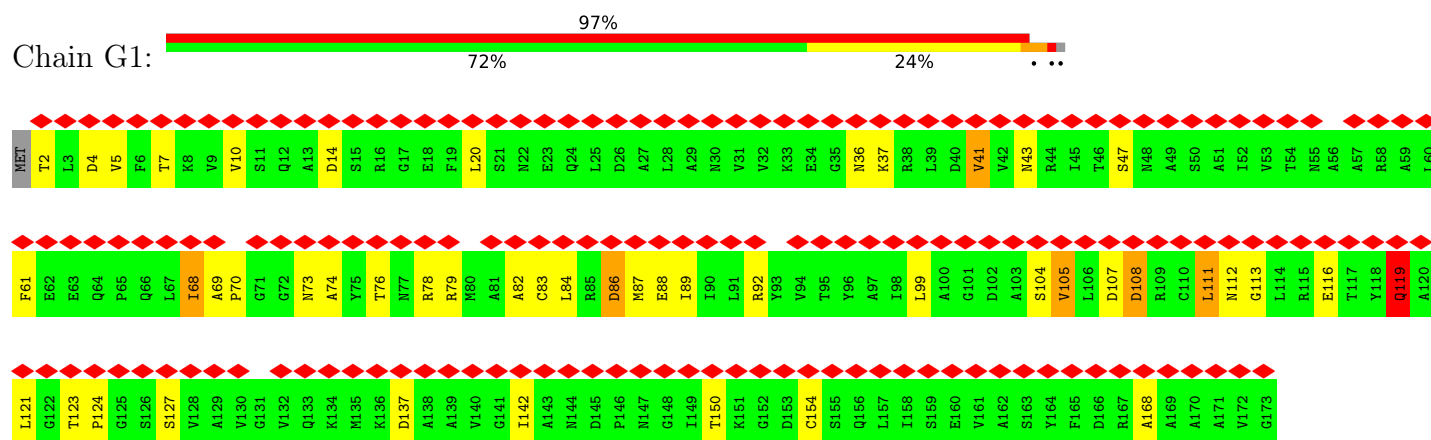
• Molecule 3: C-phycoerythrin beta subunit



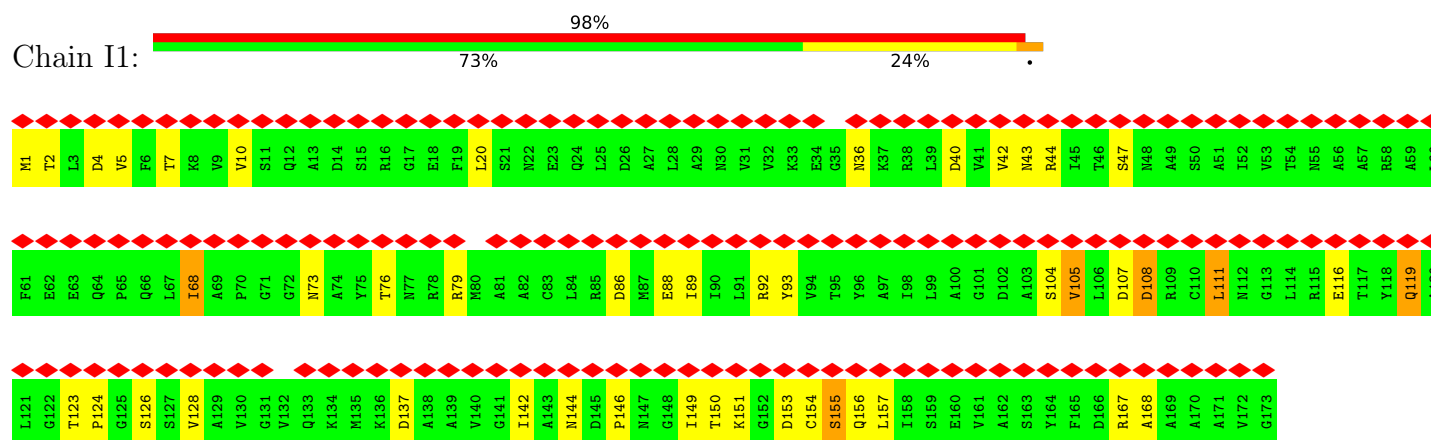
• Molecule 3: C-phycoerythrin beta subunit



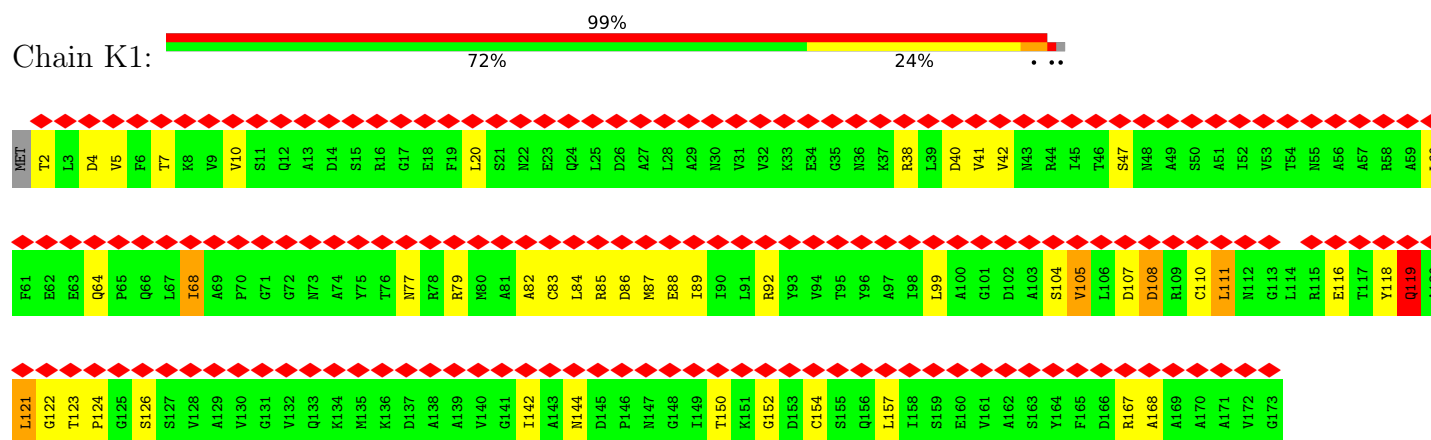
- Molecule 3: C-phyco cyanin beta subunit



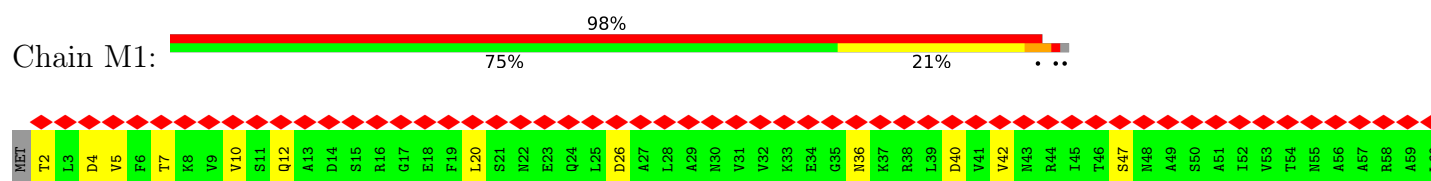
- Molecule 3: C-phyco cyanin beta subunit

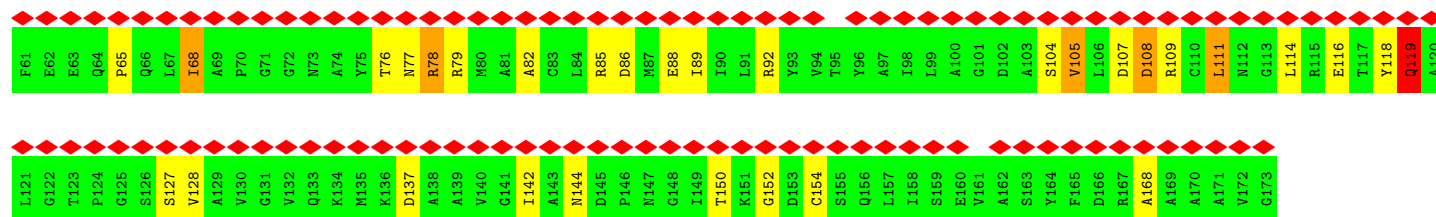


- Molecule 3: C-phyco cyanin beta subunit



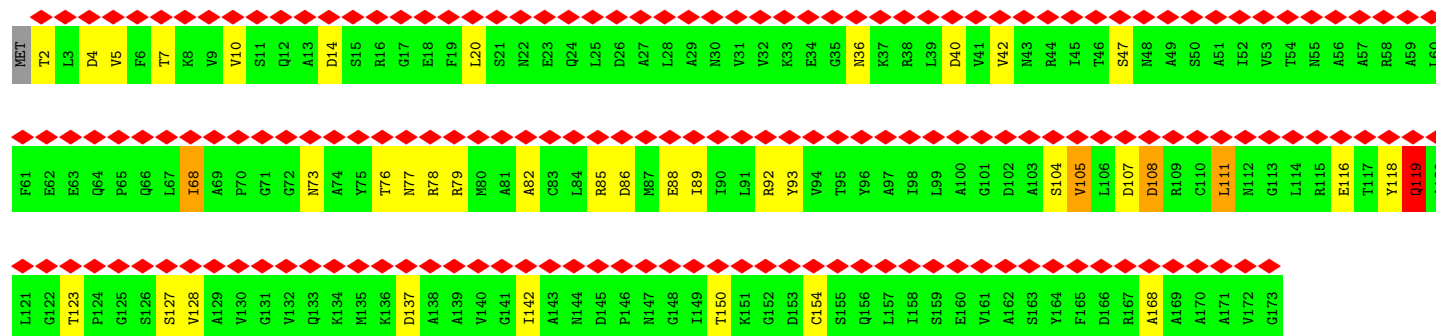
- Molecule 3: C-phyco cyanin beta subunit





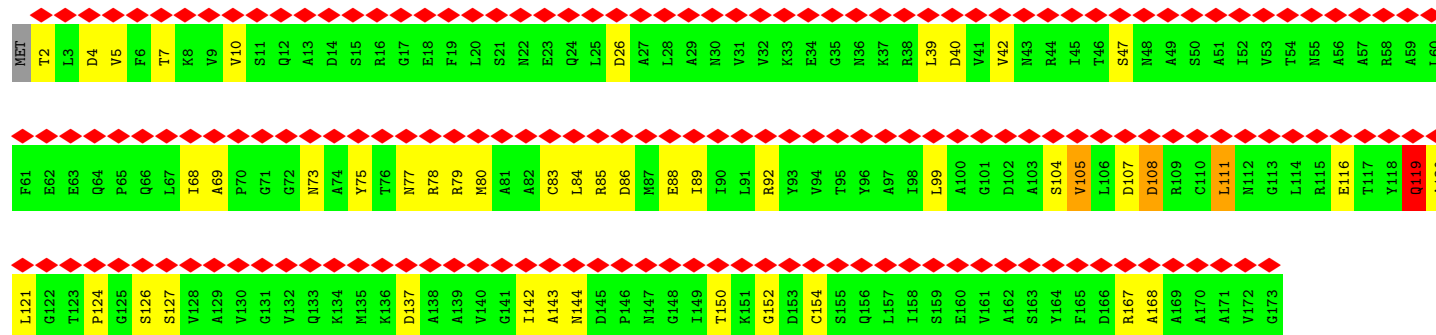
• Molecule 3: C-phycoerythrin beta subunit

Chain P1: 99% 76% 20% ...



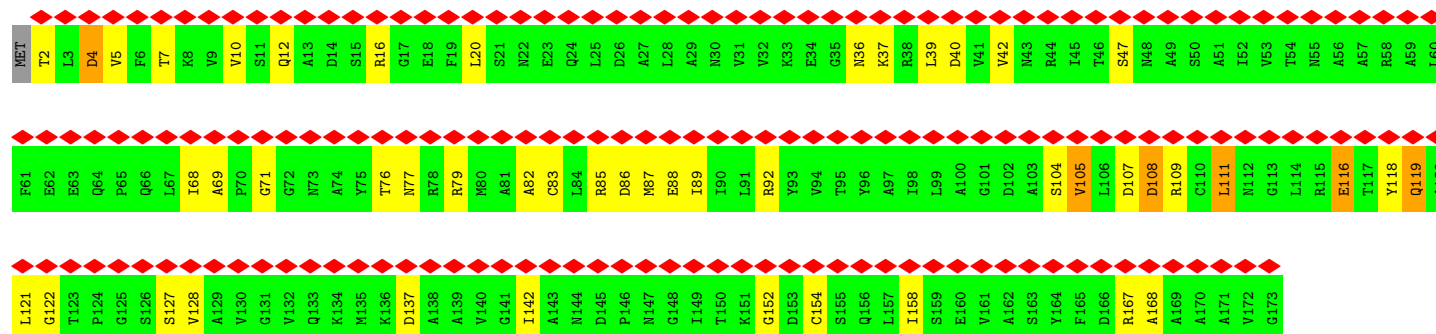
• Molecule 3: C-phycoerythrin beta subunit

Chain R1: 99% 72% 25% ...



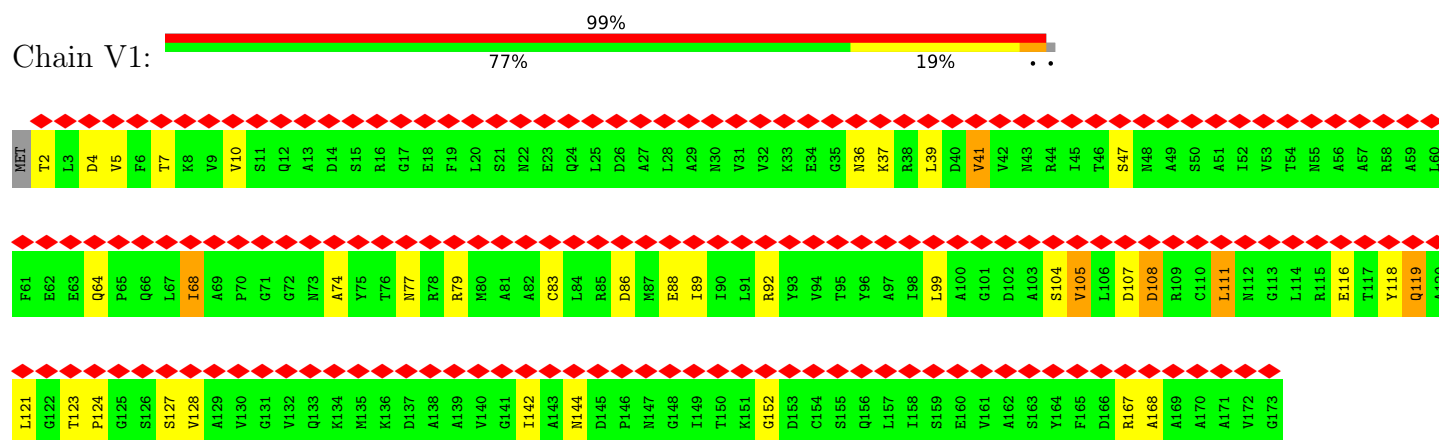
• Molecule 3: C-phycoerythrin beta subunit

Chain T1: 99% 72% 24% ...



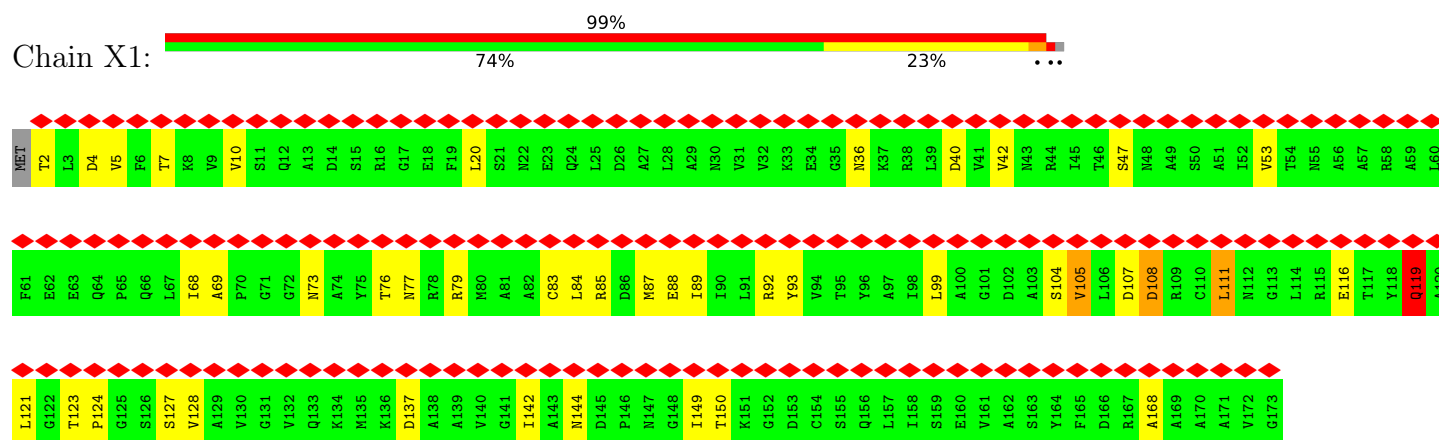
- Molecule 3: C-phycoerythrin beta subunit

Chain V1:



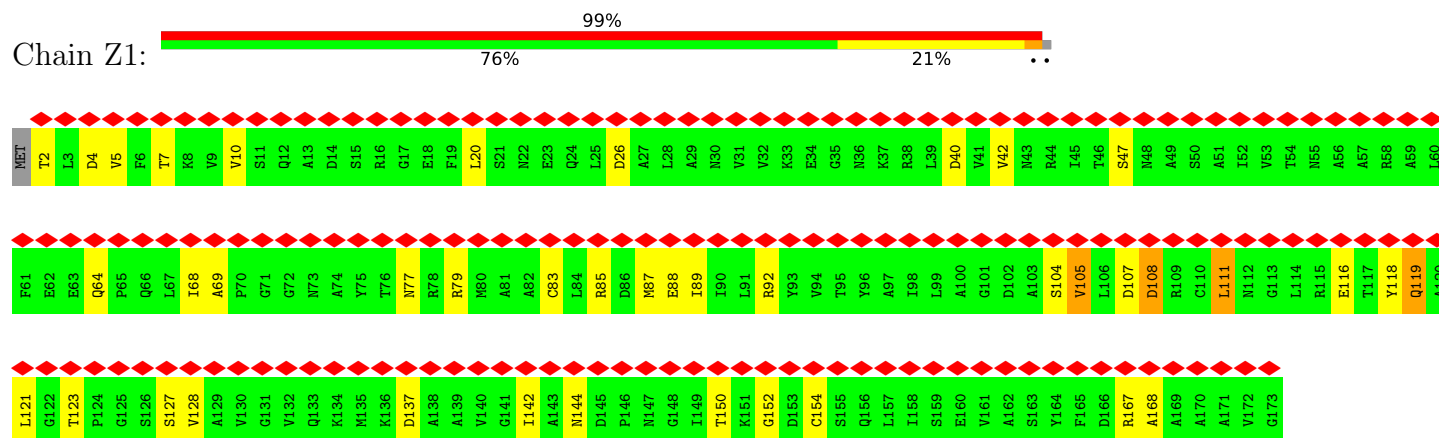
- Molecule 3: C-phycoerythrin beta subunit

Chain X1:



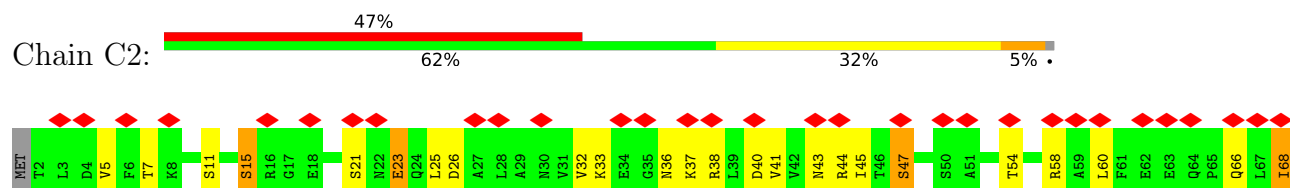
- Molecule 3: C-phycoerythrin beta subunit

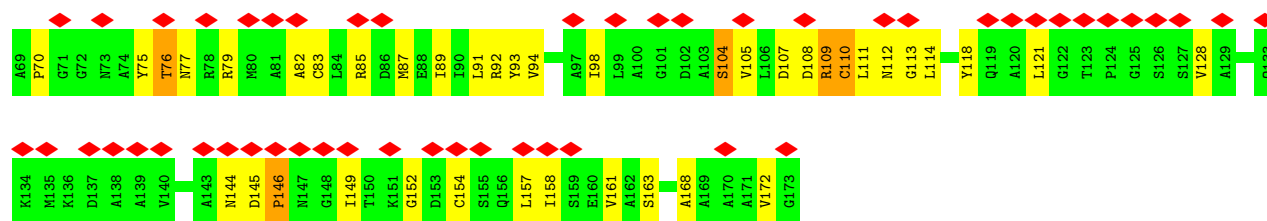
Chain Z1:



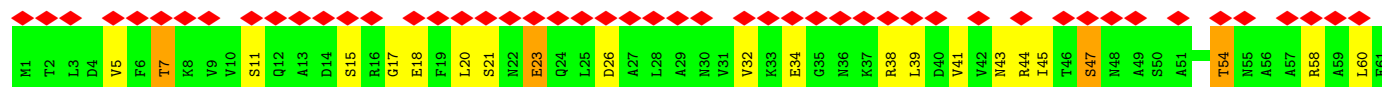
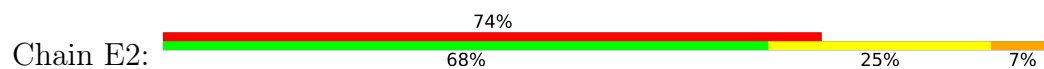
- Molecule 3: C-phycoerythrin beta subunit

Chain C2:

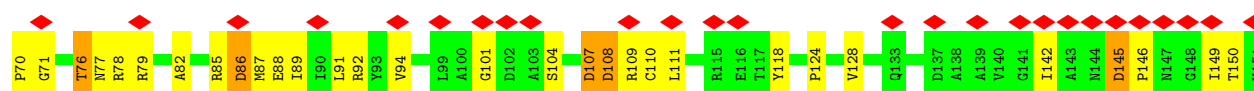
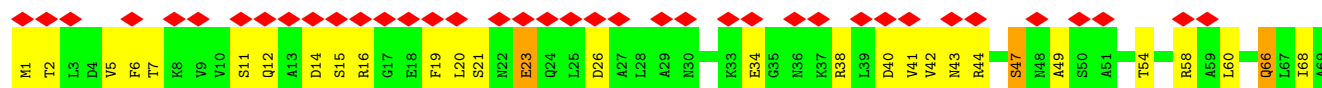




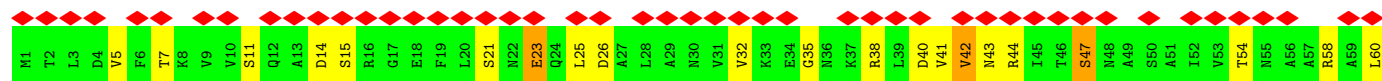
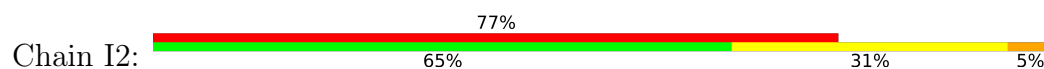
• Molecule 3: C-phycoerythrin beta subunit



• Molecule 3: C-phycoerythrin beta subunit

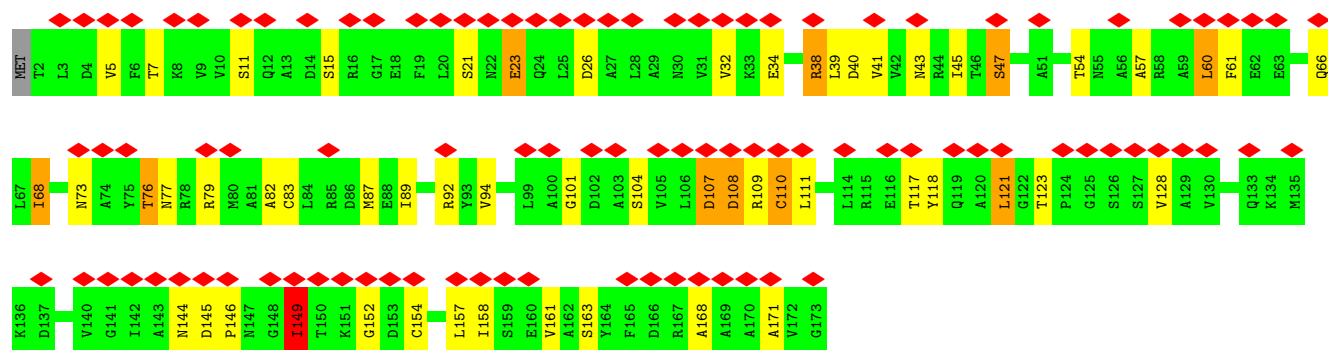


• Molecule 3: C-phycoerythrin beta subunit

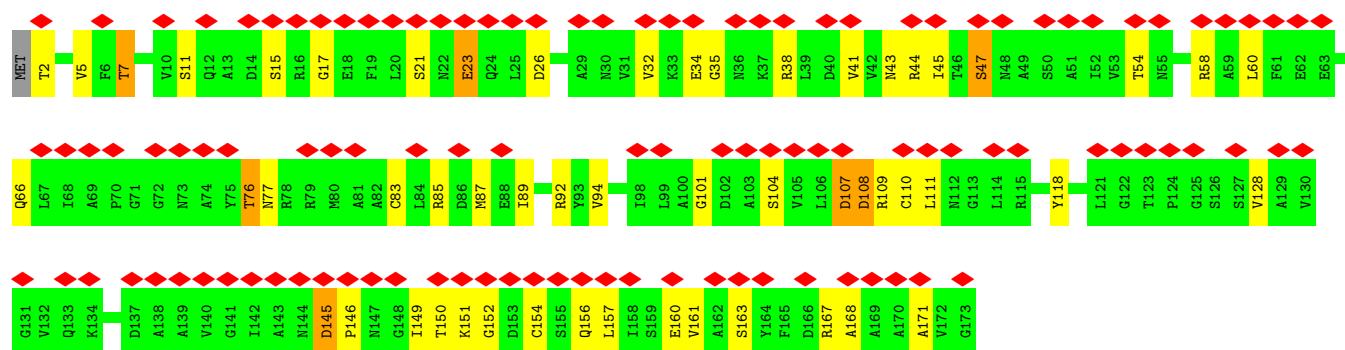




• Molecule 3: C-phycoerythrin beta subunit



• Molecule 3: C-phycoerythrin beta subunit

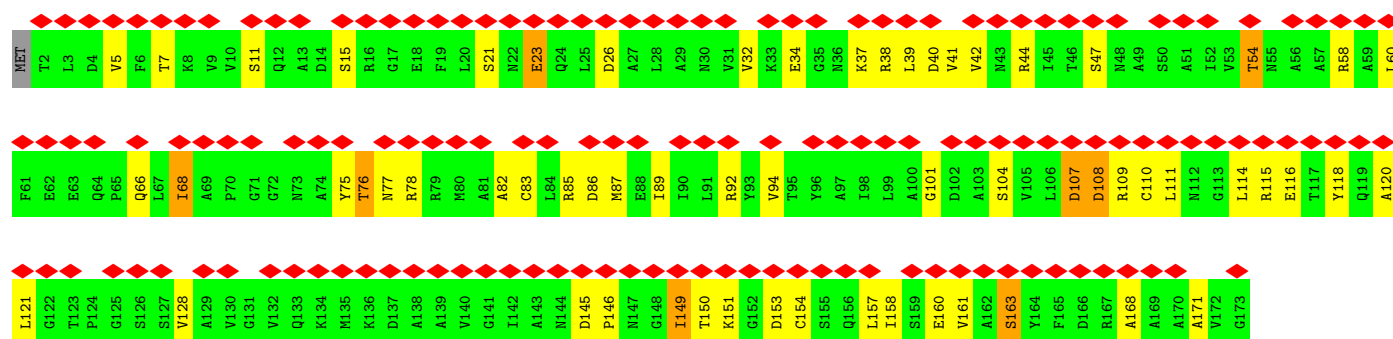


• Molecule 3: C-phycoerythrin beta subunit



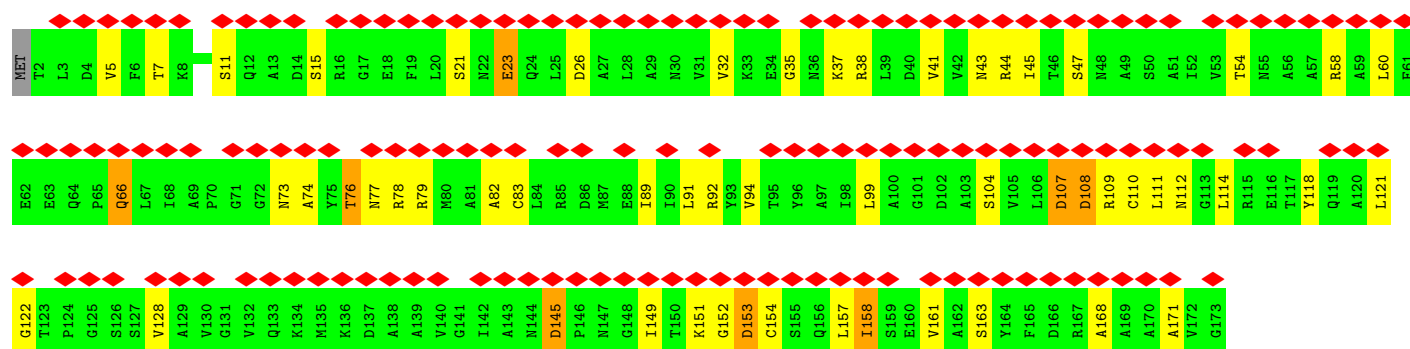
• Molecule 3: C-phycoerythrin beta subunit

Chain R2: 



• Molecule 3: C-phycoerythrin beta subunit

Chain T2: 

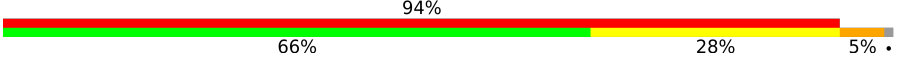


• Molecule 3: C-phycoerythrin beta subunit

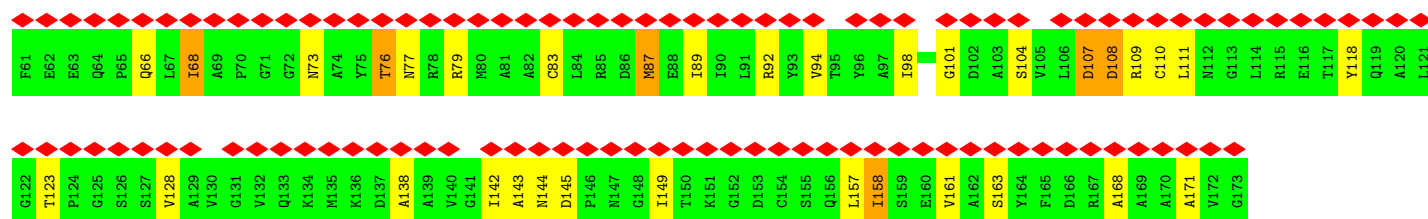
Chain V2: 



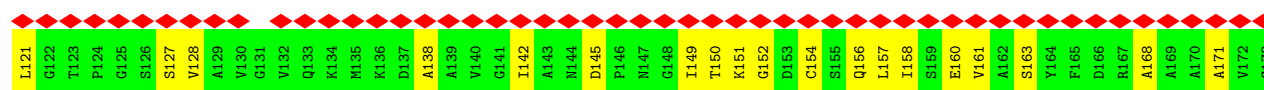
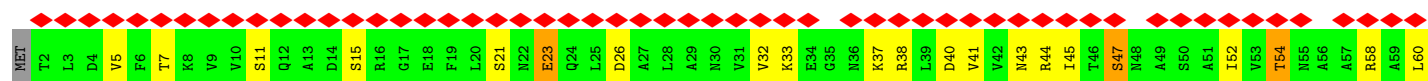
• Molecule 3: C-phycoerythrin beta subunit

Chain X2: 





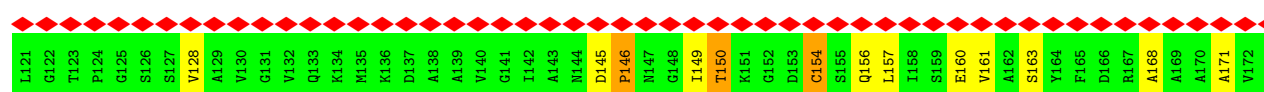
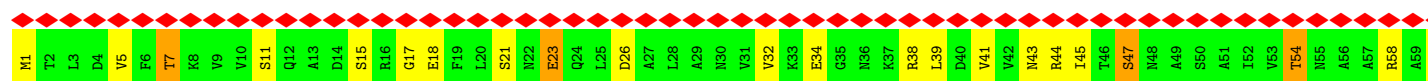
• Molecule 3: C-phycoerythrin beta subunit



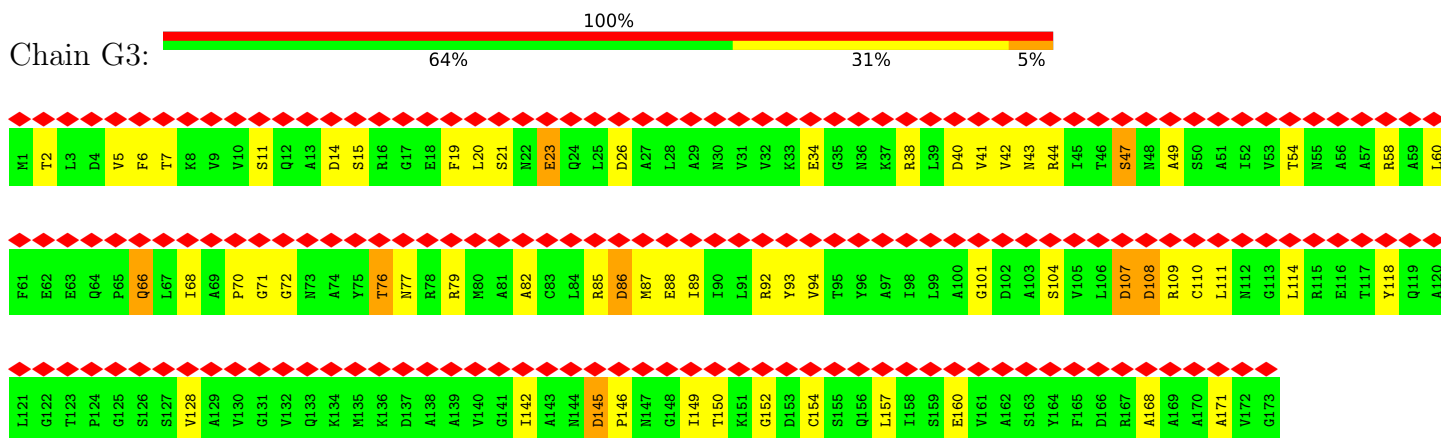
• Molecule 3: C-phycoerythrin beta subunit



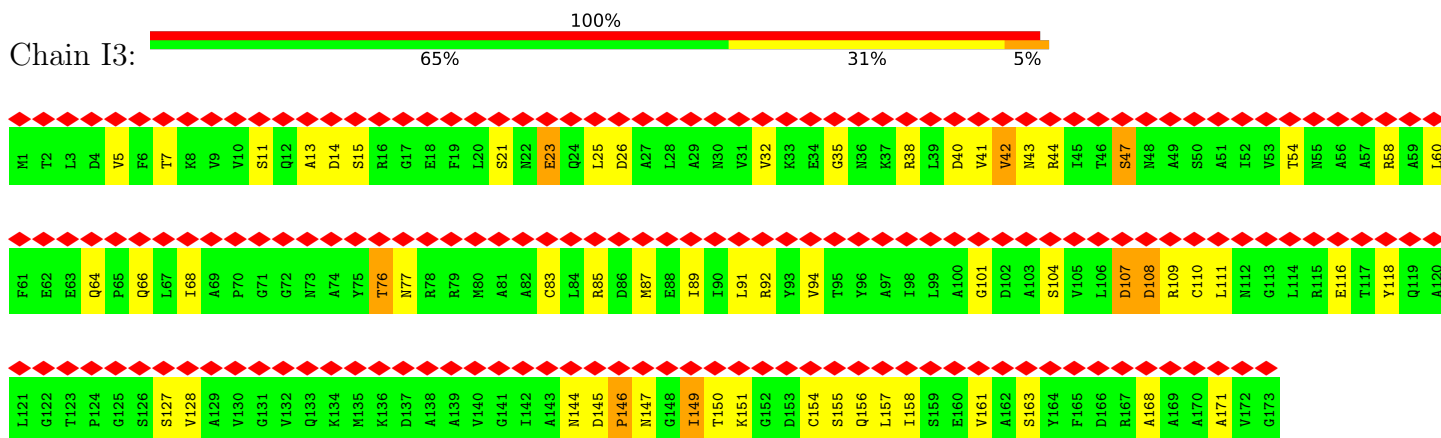
• Molecule 3: C-phycoerythrin beta subunit



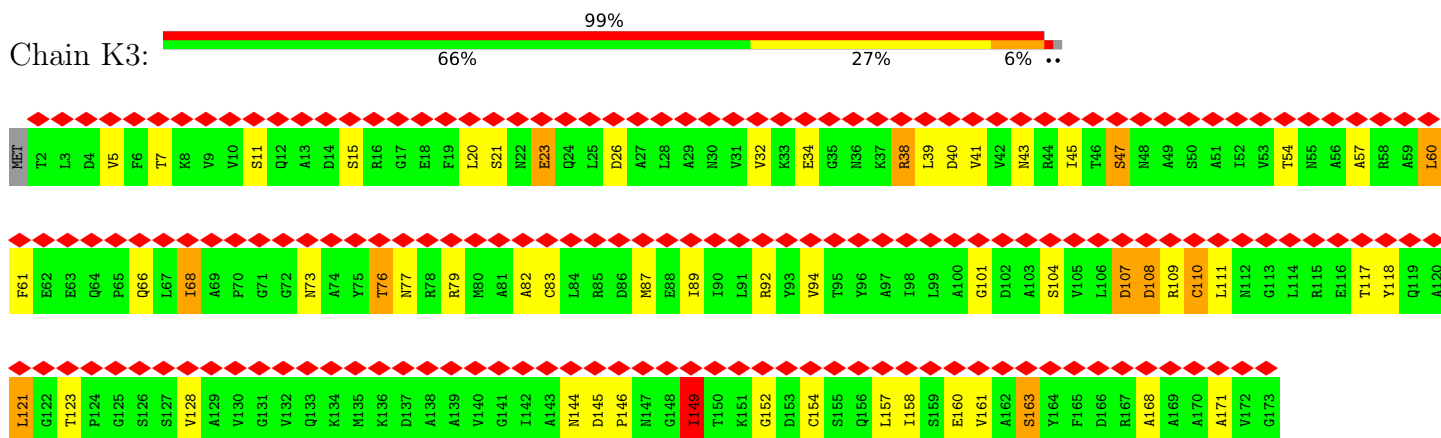
- Molecule 3: C-phycoerythrin beta subunit



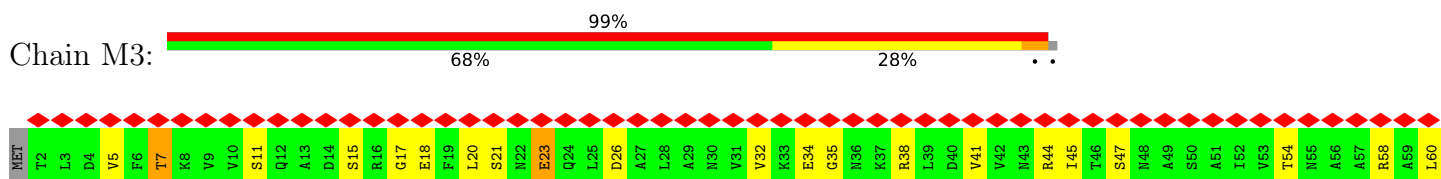
- Molecule 3: C-phycoerythrin beta subunit

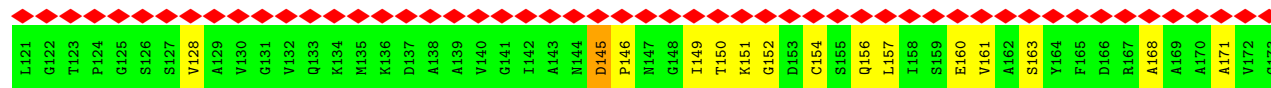


- Molecule 3: C-phycoerythrin beta subunit

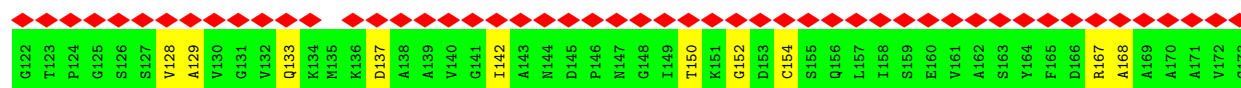
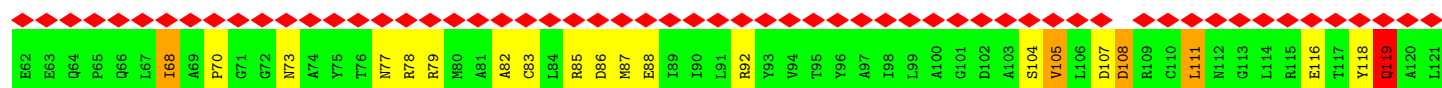
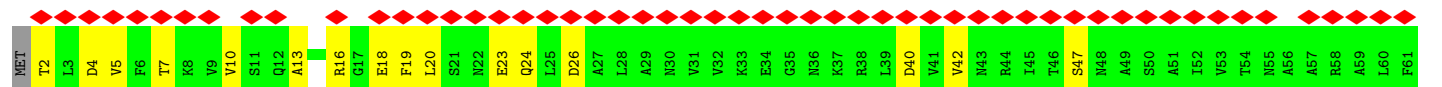
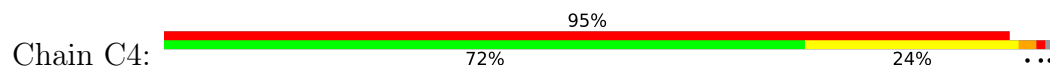


- Molecule 3: C-phycoerythrin beta subunit

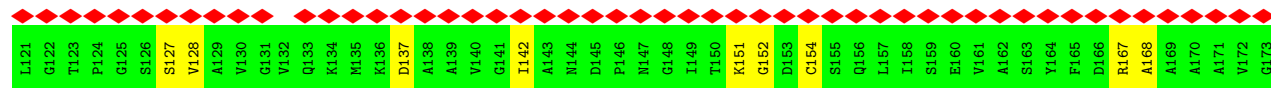
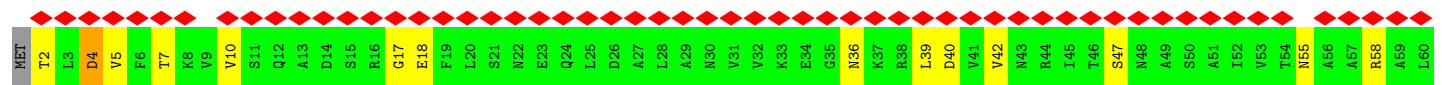
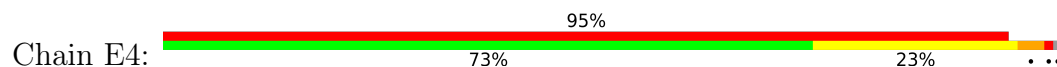




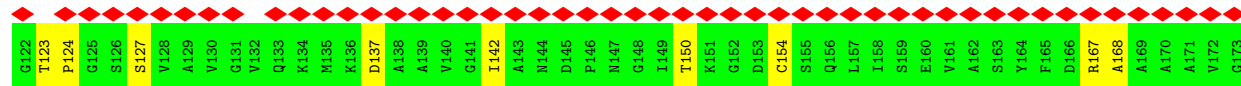
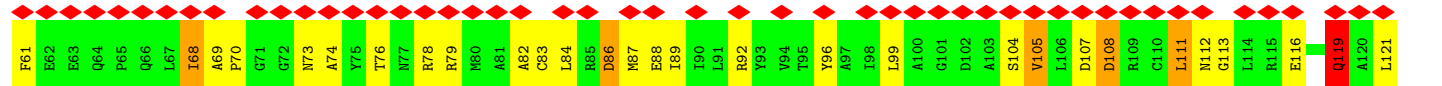
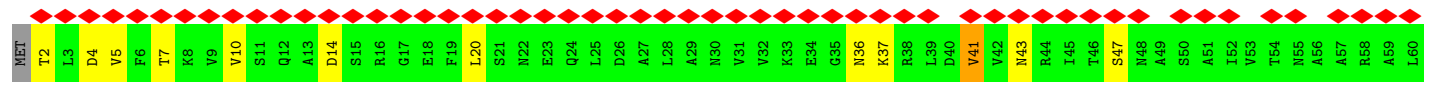
• Molecule 3: C-phycocyanin beta subunit



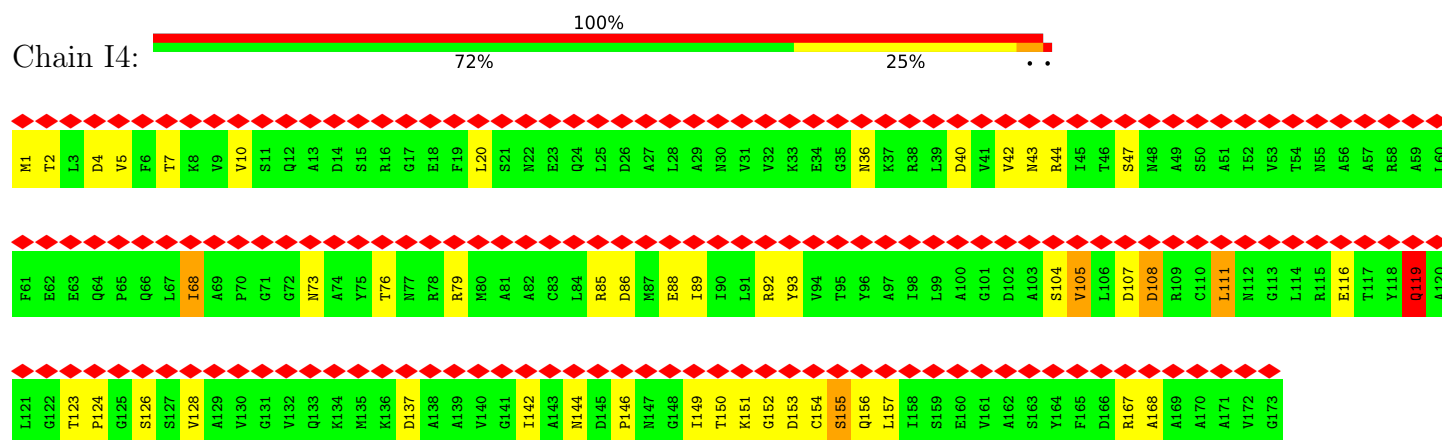
• Molecule 3: C-phycocyanin beta subunit



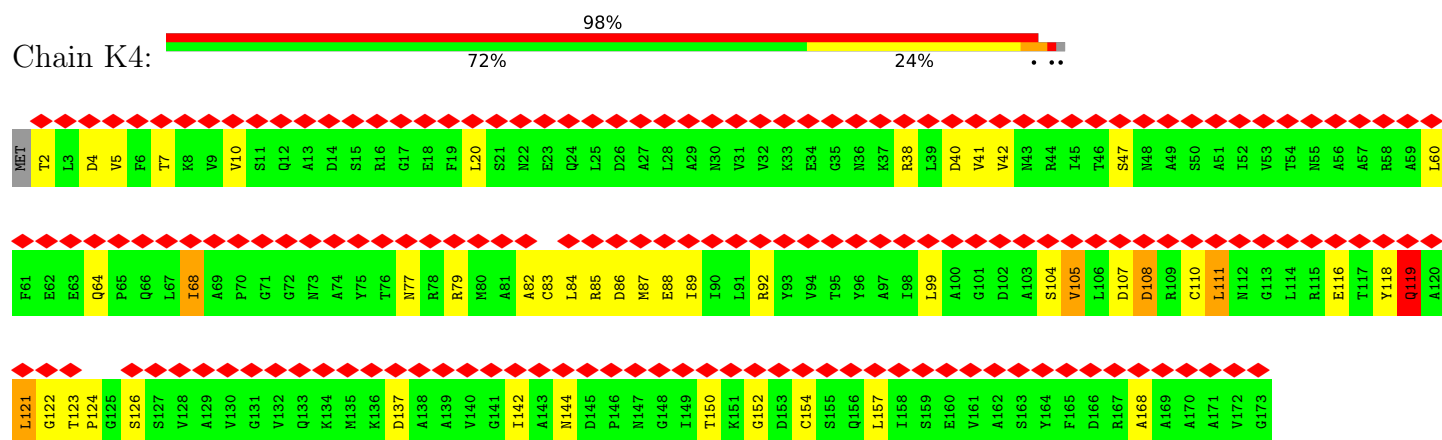
• Molecule 3: C-phycocyanin beta subunit



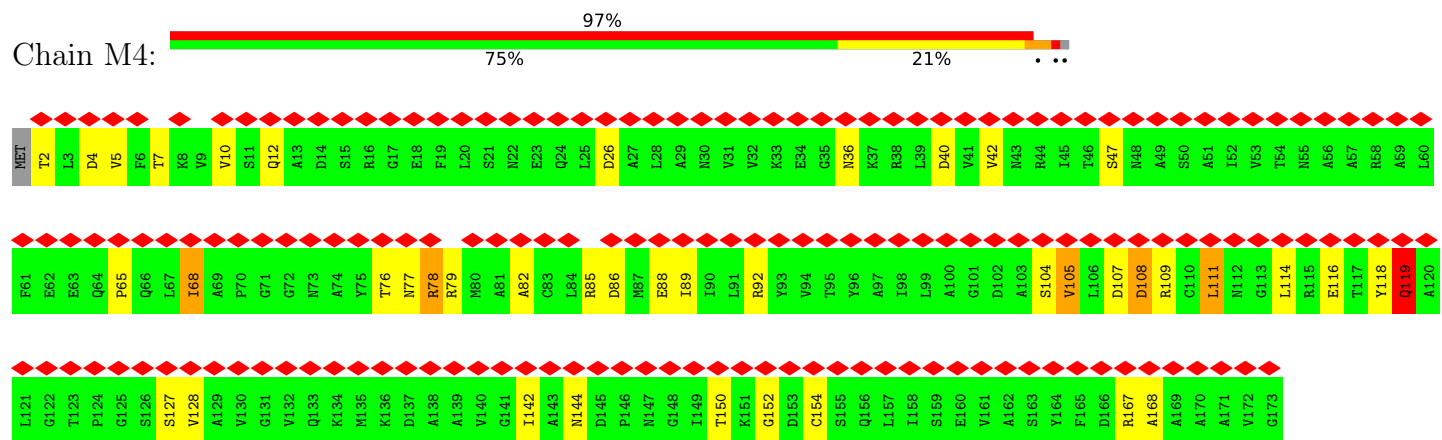
- Molecule 3: C-phycocyanin beta subunit



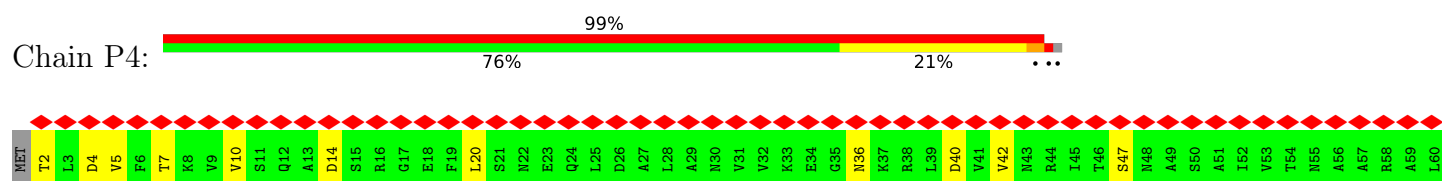
- Molecule 3: C-phycocyanin beta subunit



- Molecule 3: C-phycocyanin beta subunit

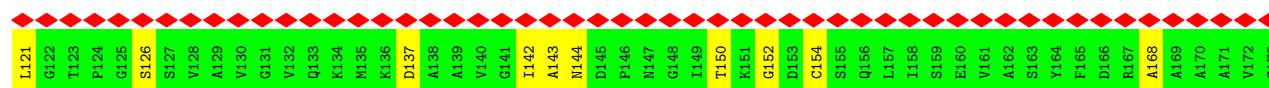
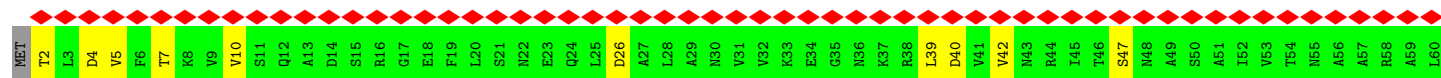
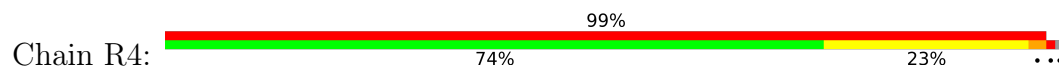


- Molecule 3: C-phycocyanin beta subunit

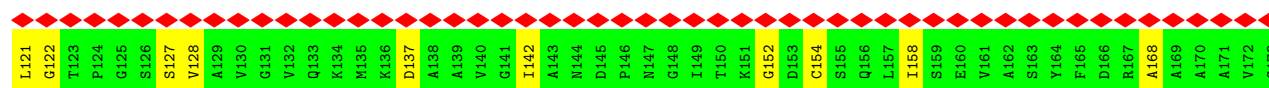
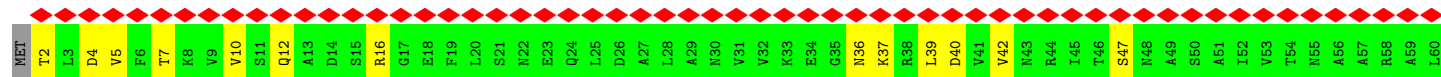




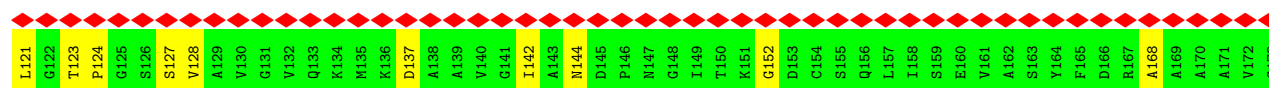
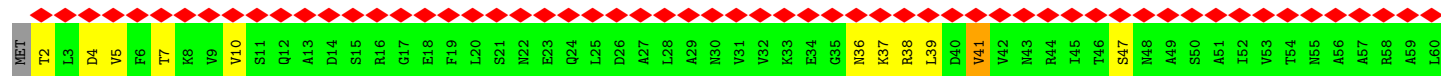
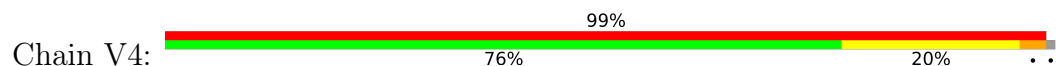
• Molecule 3: C-phycoerythrin beta subunit



• Molecule 3: C-phycoerythrin beta subunit

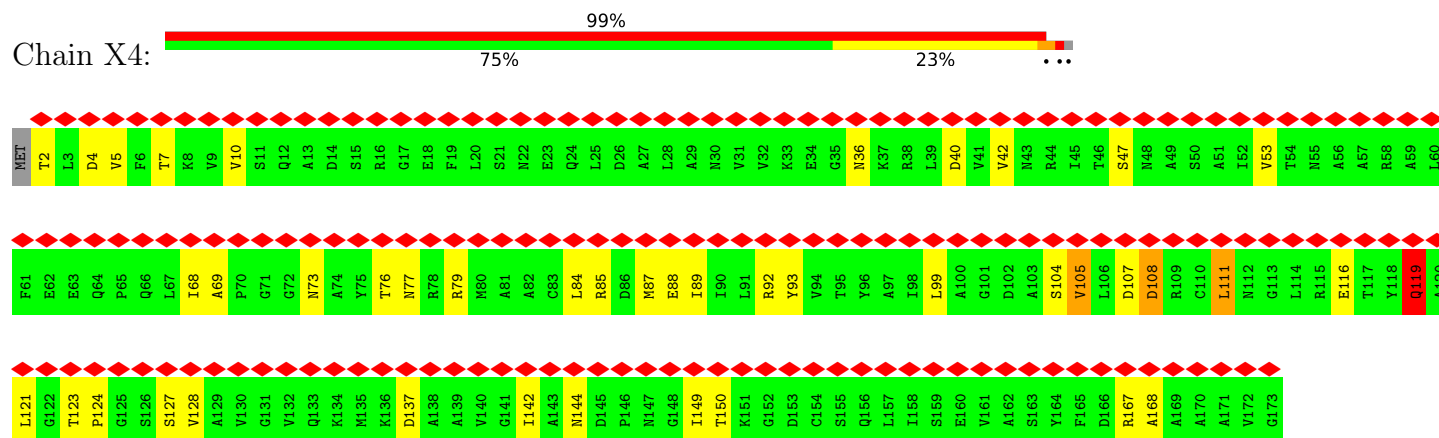


• Molecule 3: C-phycoerythrin beta subunit



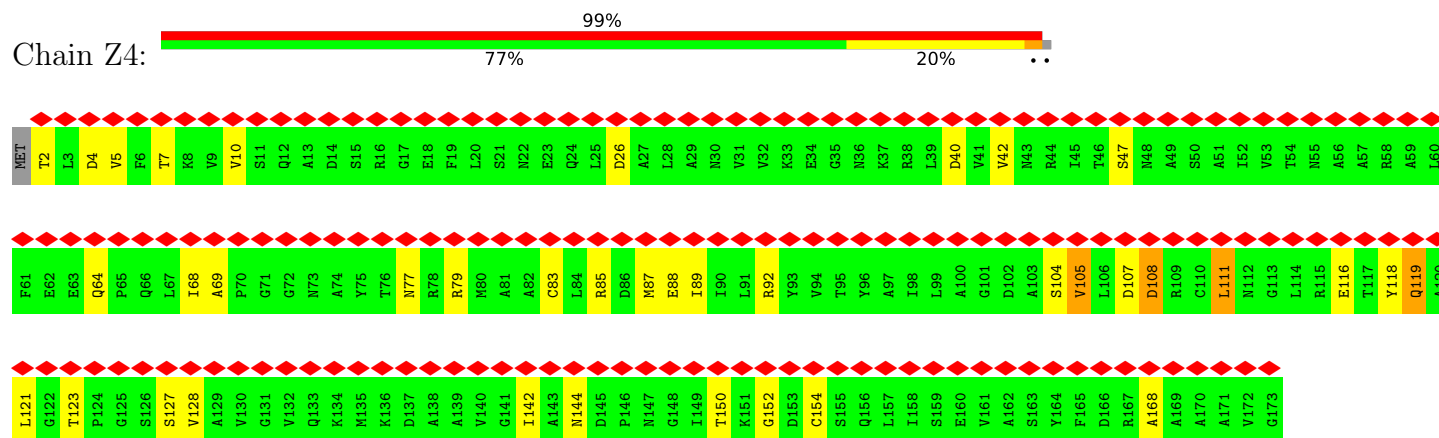
- Molecule 3: C-phycoerythrin beta subunit

Chain X4:



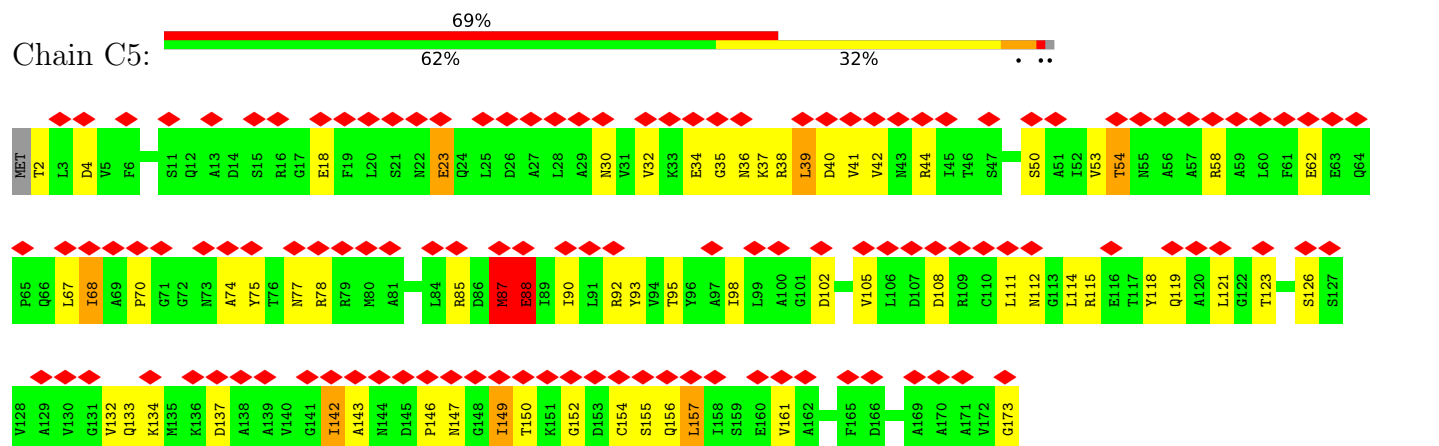
- Molecule 3: C-phycoerythrin beta subunit

Chain Z4:



- Molecule 3: C-phycoerythrin beta subunit

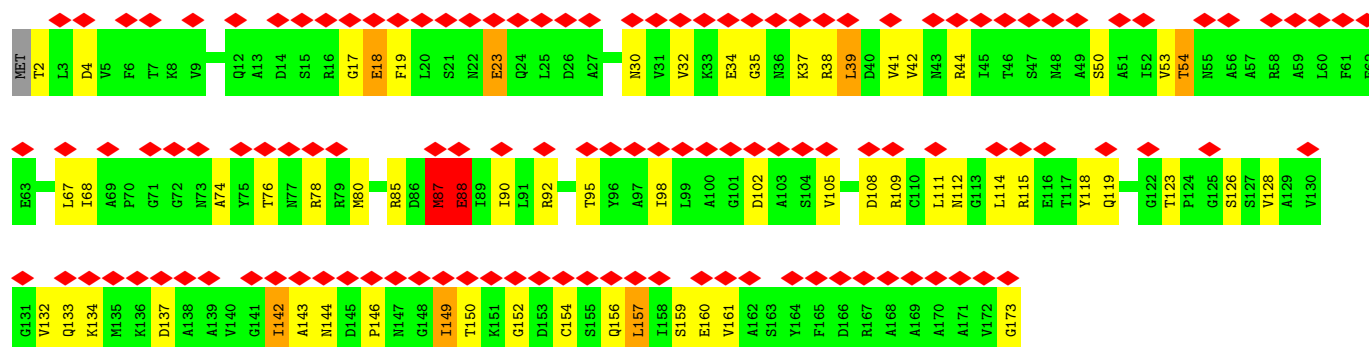
Chain C5:



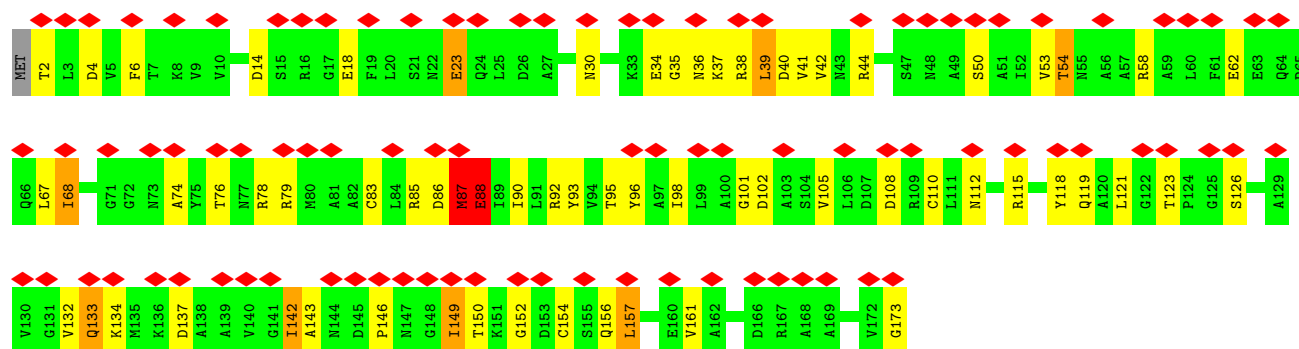
- Molecule 3: C-phycoerythrin beta subunit

Chain E5:

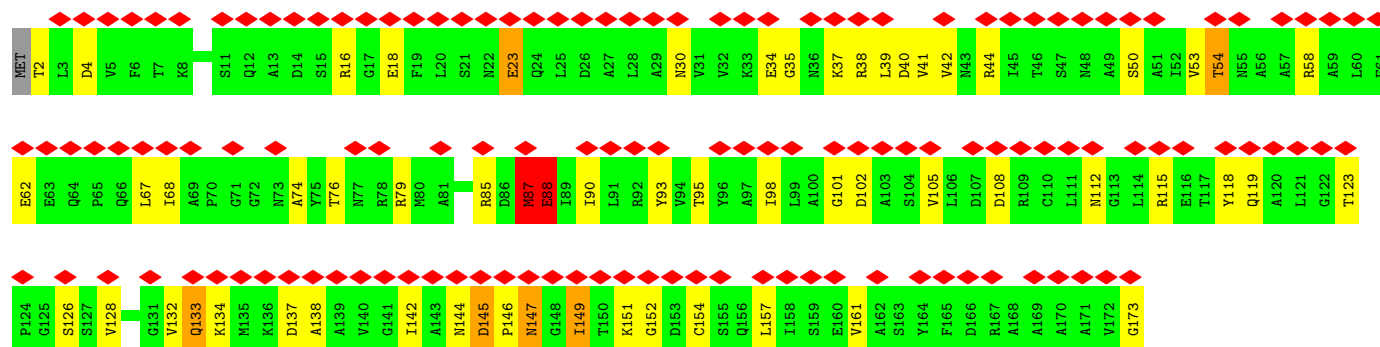
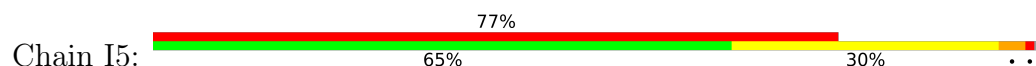




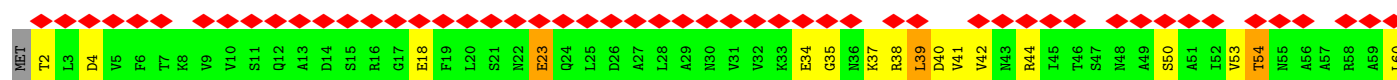
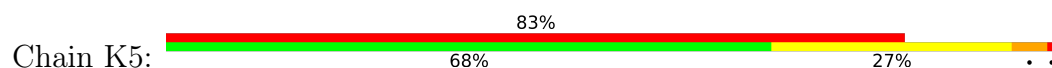
• Molecule 3: C-phycoerythrin beta subunit

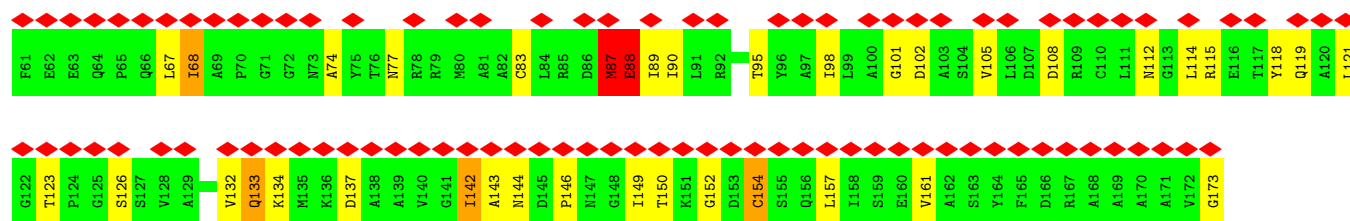


• Molecule 3: C-phycoerythrin beta subunit

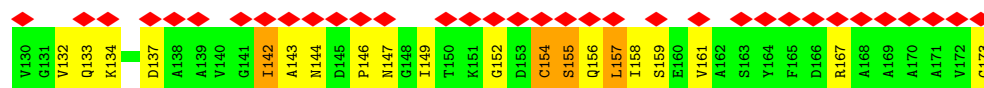
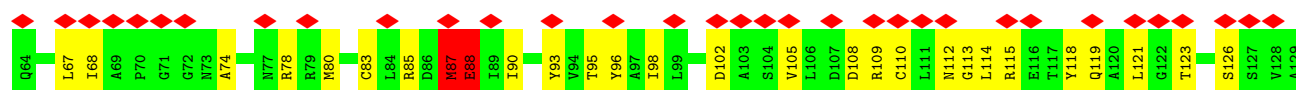
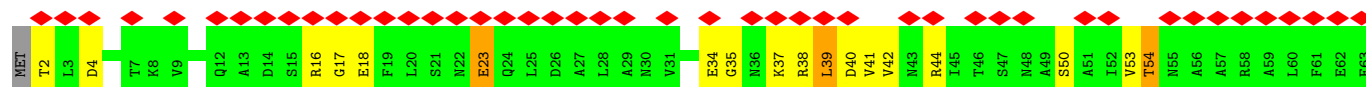


• Molecule 3: C-phycoerythrin beta subunit

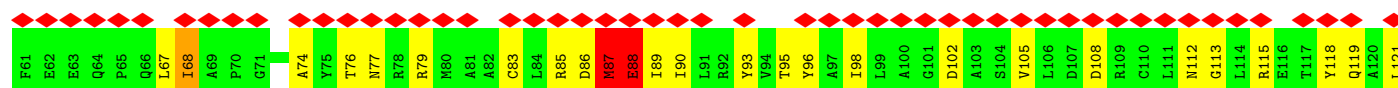
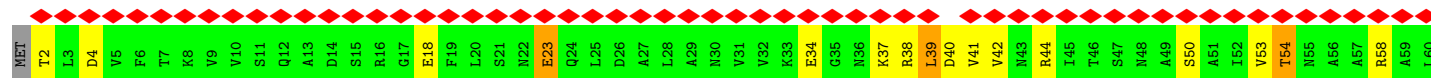




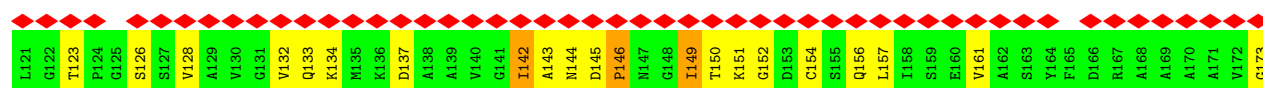
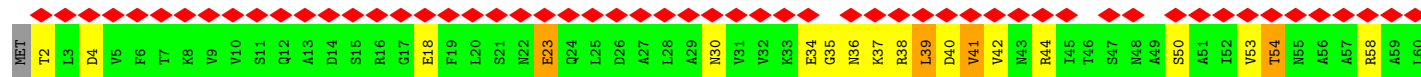
• Molecule 3: C-phycocyanin beta subunit



• Molecule 3: C-phycocyanin beta subunit

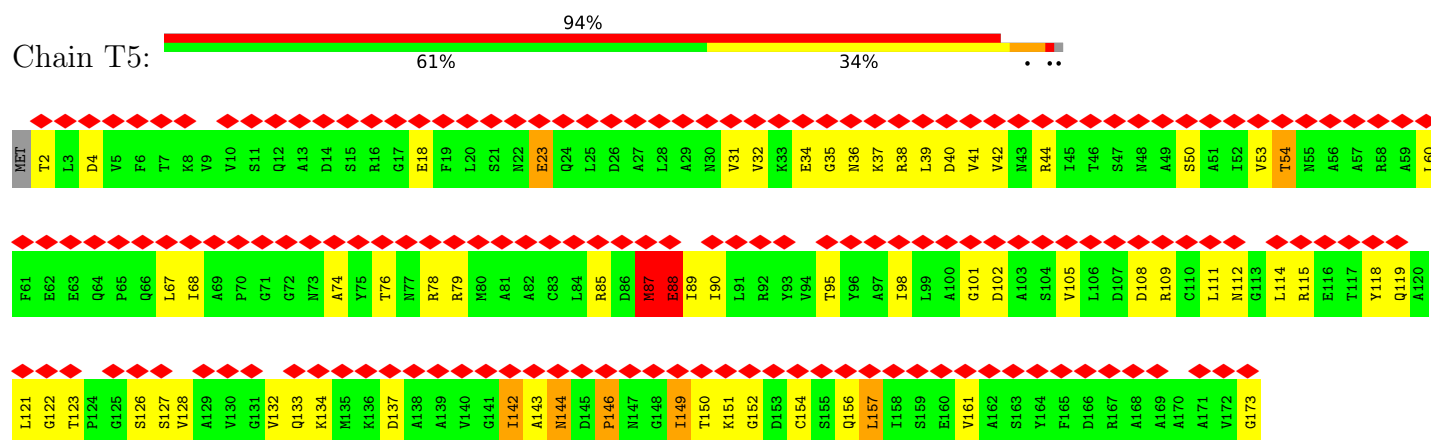


• Molecule 3: C-phycocyanin beta subunit



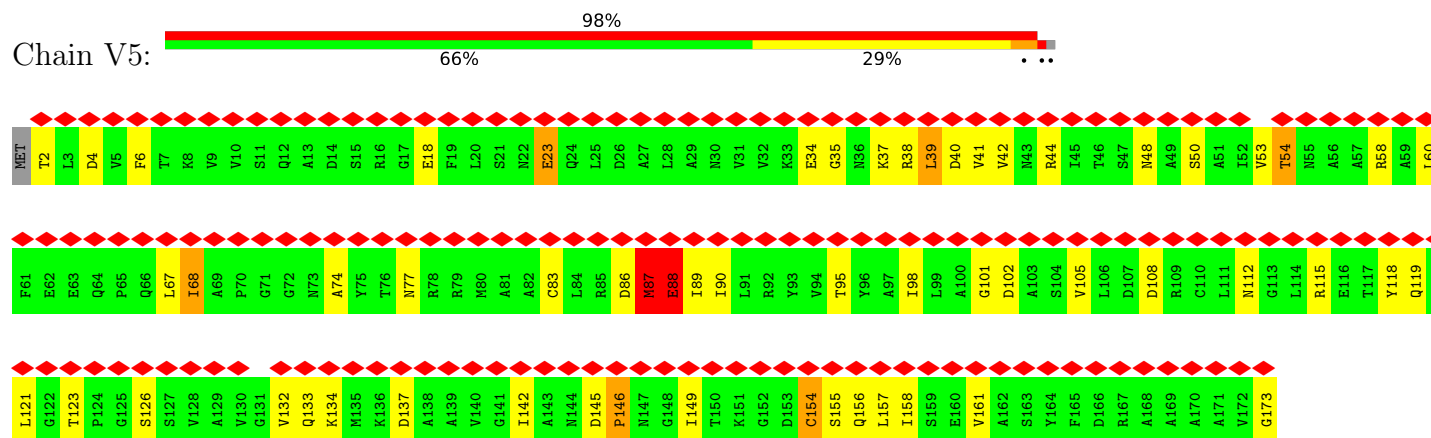
- Molecule 3: C-phycoerythrin beta subunit

Chain T5:



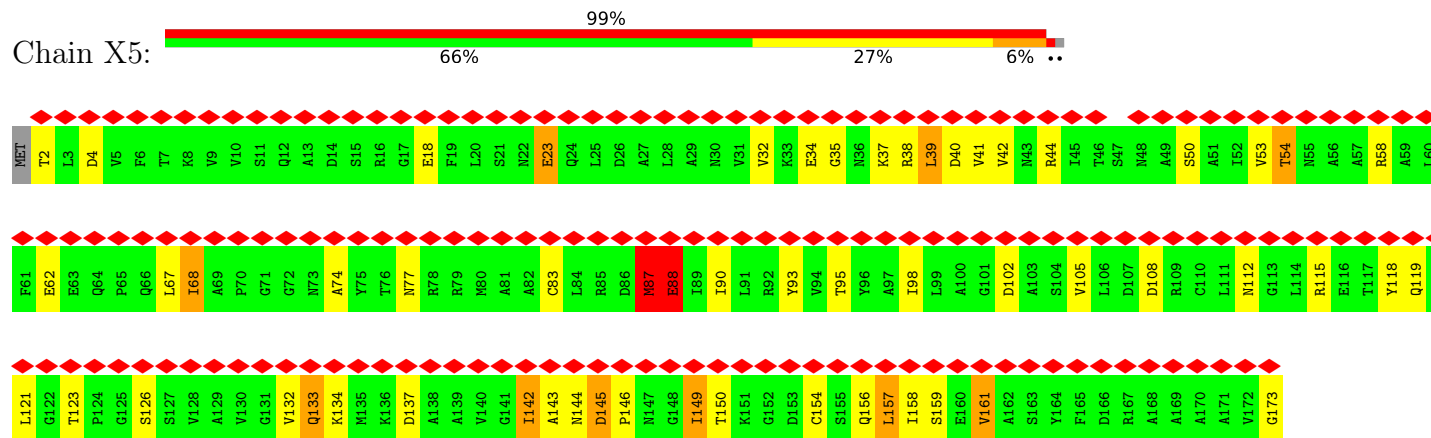
- Molecule 3: C-phycoerythrin beta subunit

Chain V5:



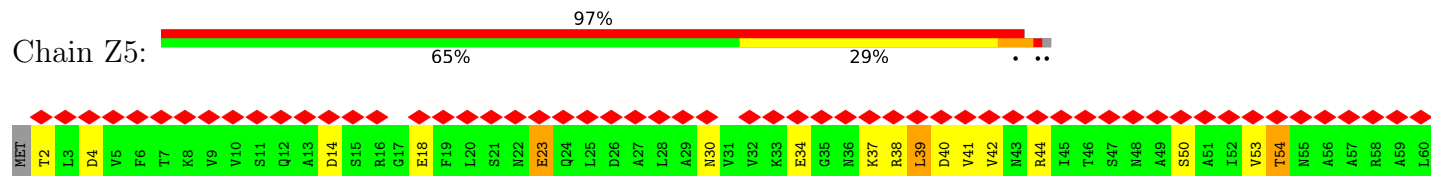
- Molecule 3: C-phycoerythrin beta subunit

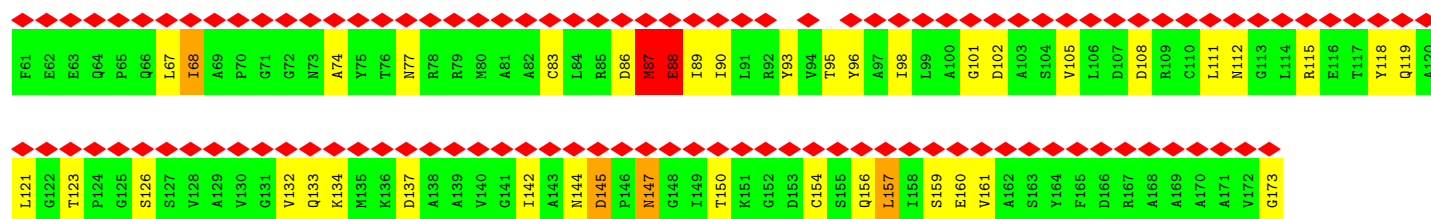
Chain X5:



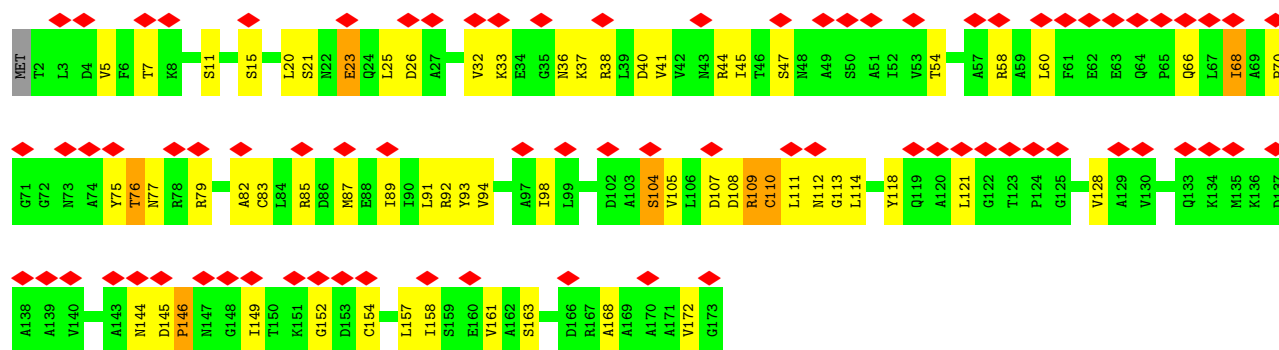
- Molecule 3: C-phycoerythrin beta subunit

Chain Z5:

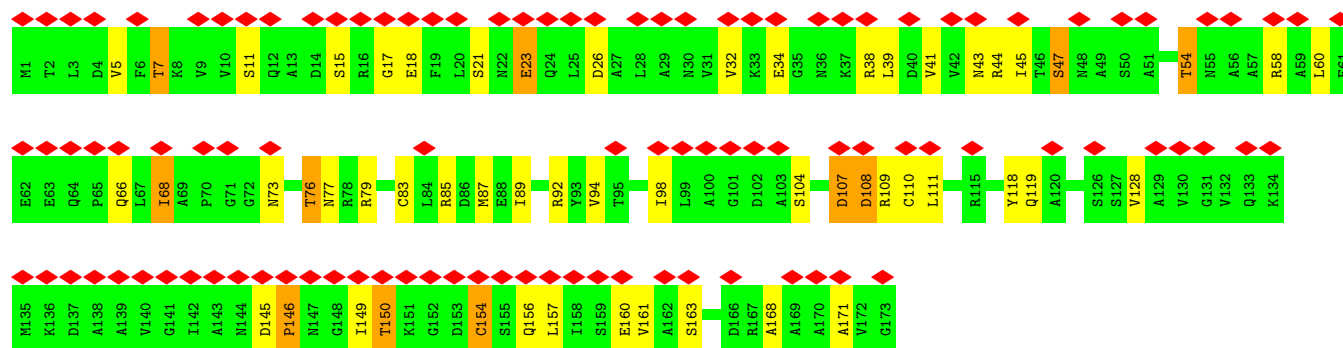




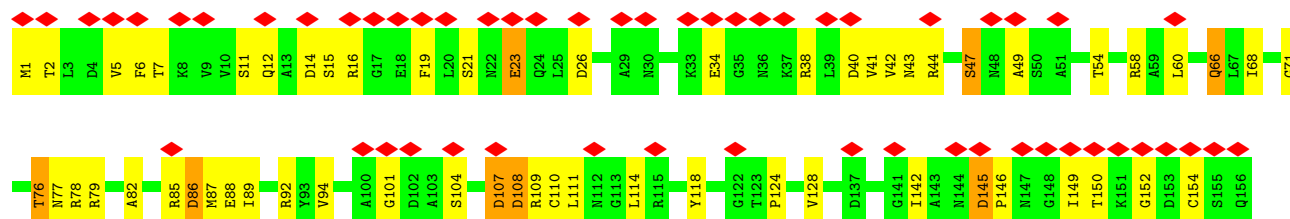
• Molecule 3: C-phycocyanin beta subunit

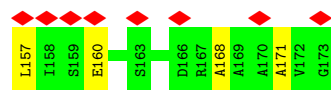


• Molecule 3: C-phycocyanin beta subunit

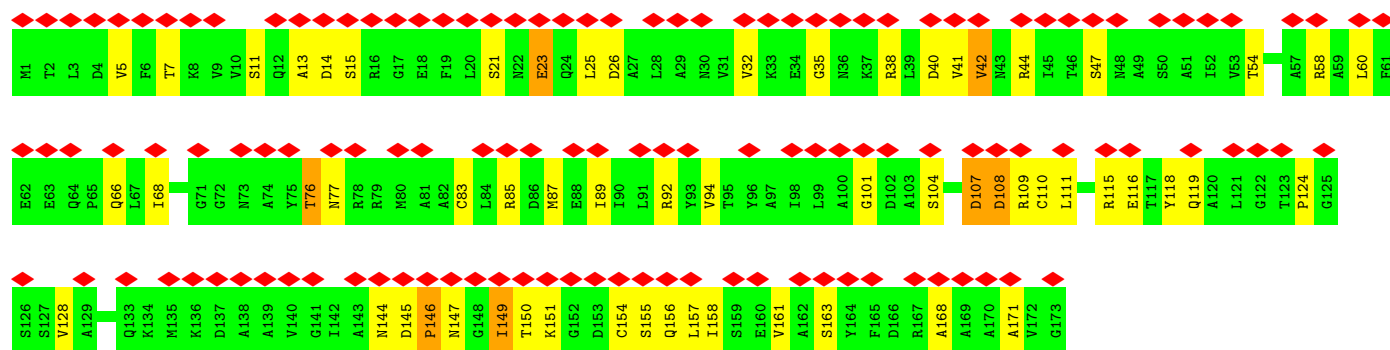
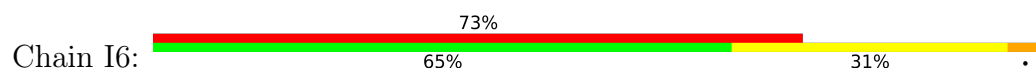


• Molecule 3: C-phycocyanin beta subunit

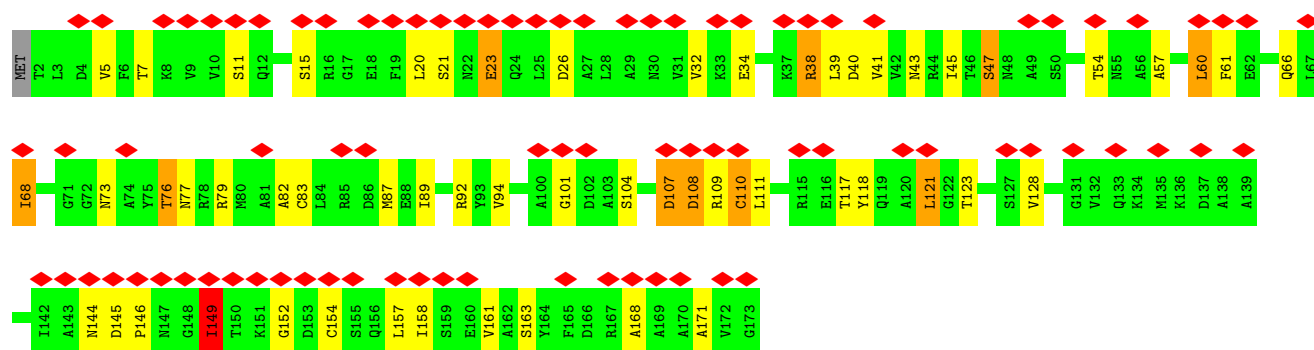




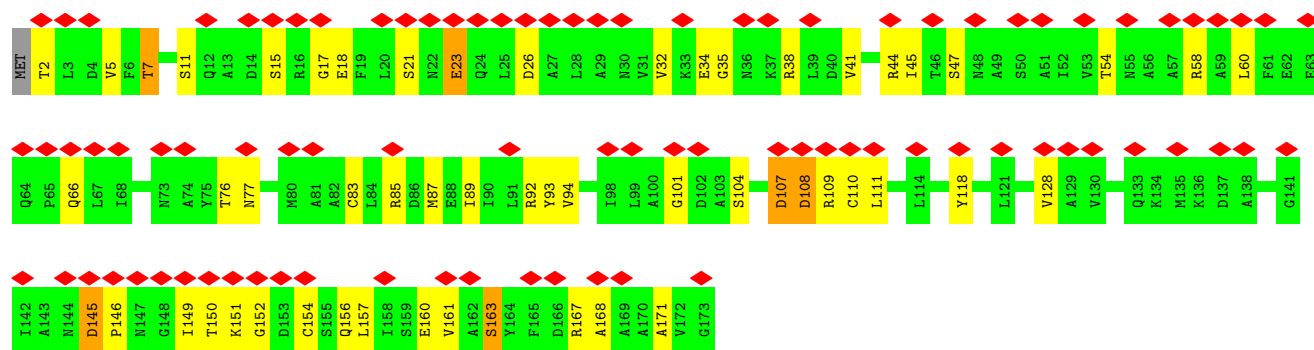
• Molecule 3: C-phycoerythrin beta subunit



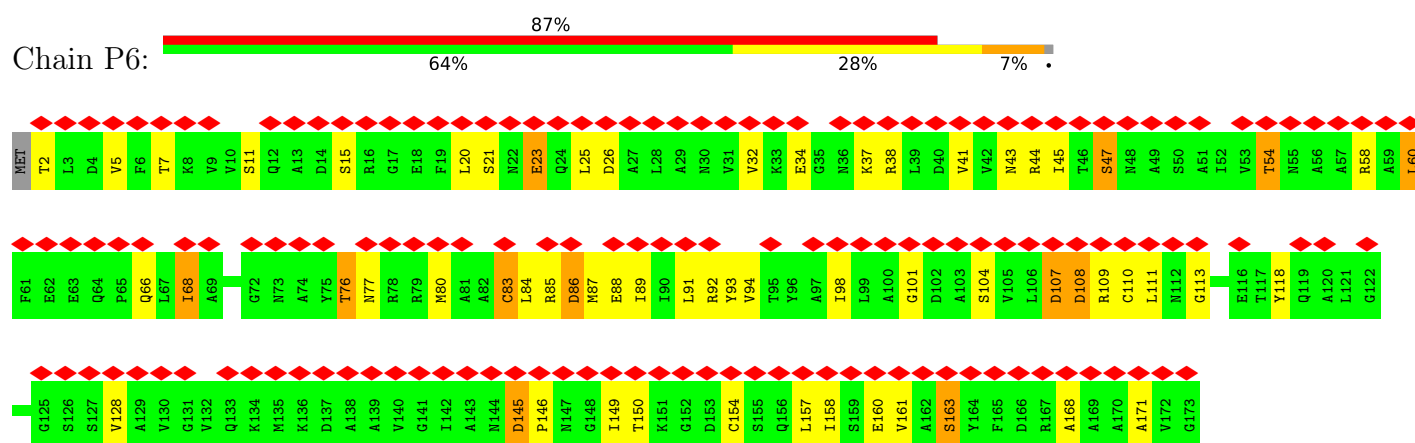
• Molecule 3: C-phycoerythrin beta subunit



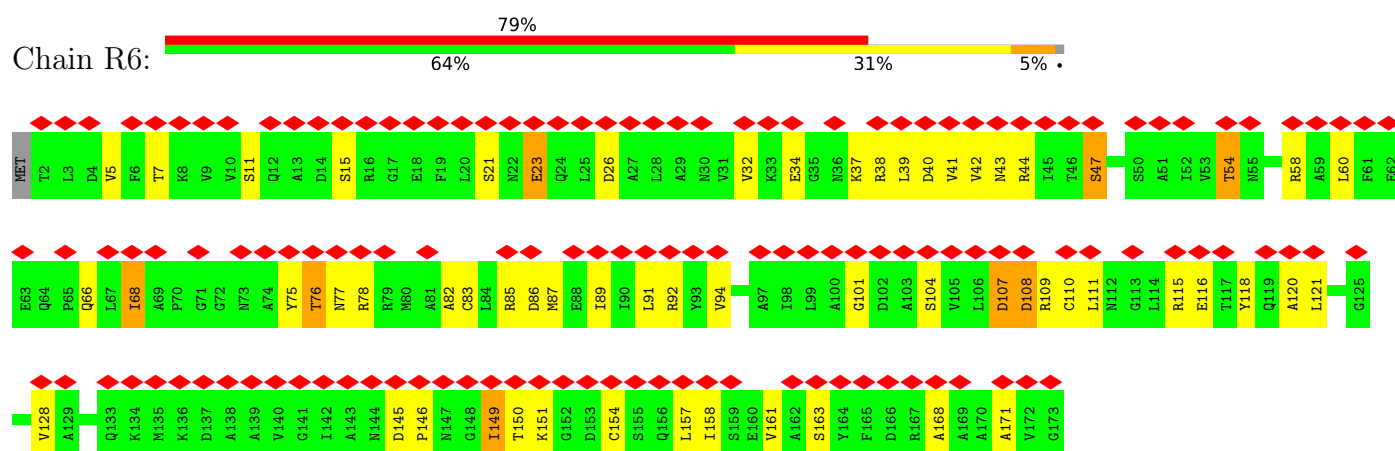
• Molecule 3: C-phycoerythrin beta subunit



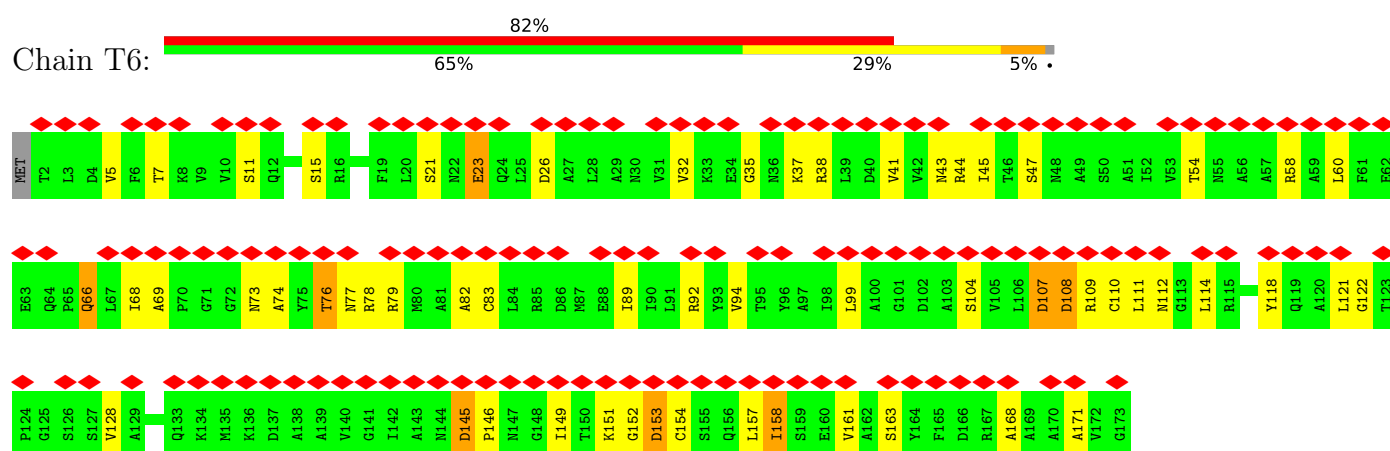
• Molecule 3: C-phycoerythrin beta subunit



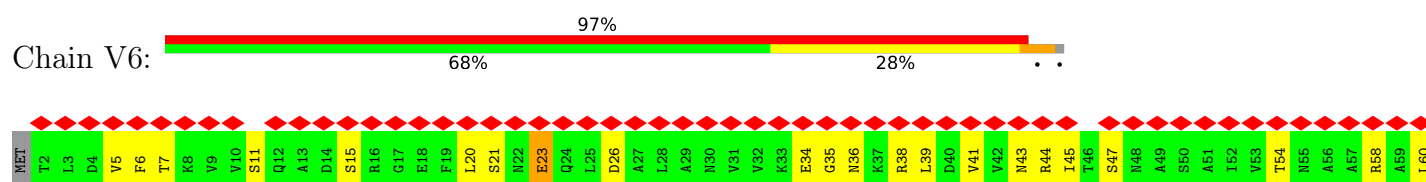
• Molecule 3: C-phycoerythrin beta subunit

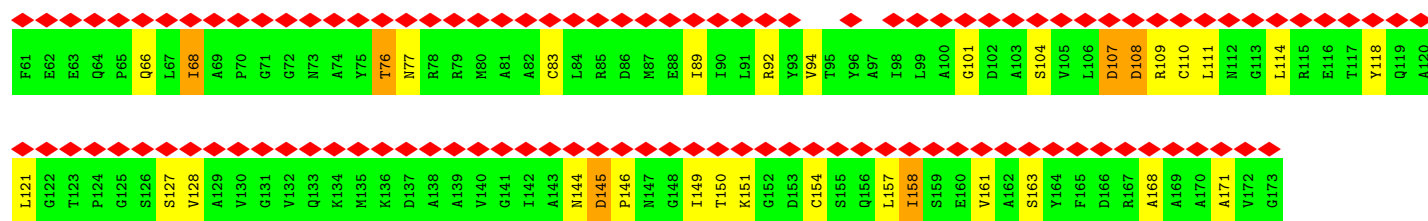


• Molecule 3: C-phycoerythrin beta subunit

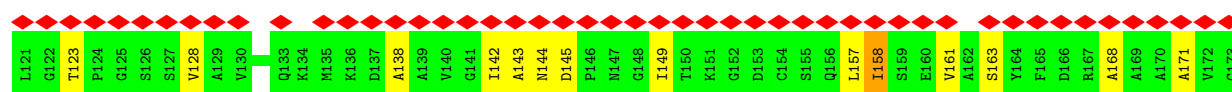


• Molecule 3: C-phycoerythrin beta subunit





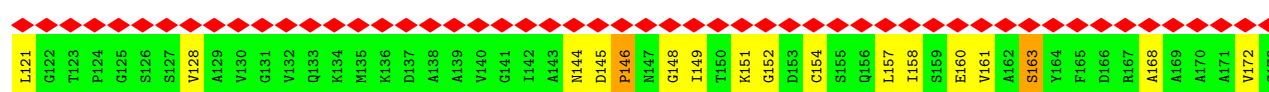
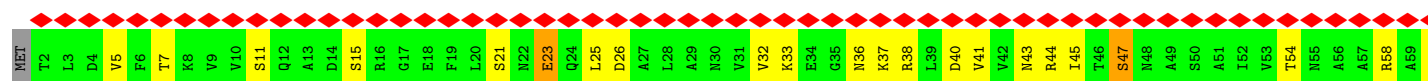
• Molecule 3: C-phycoerythrin beta subunit



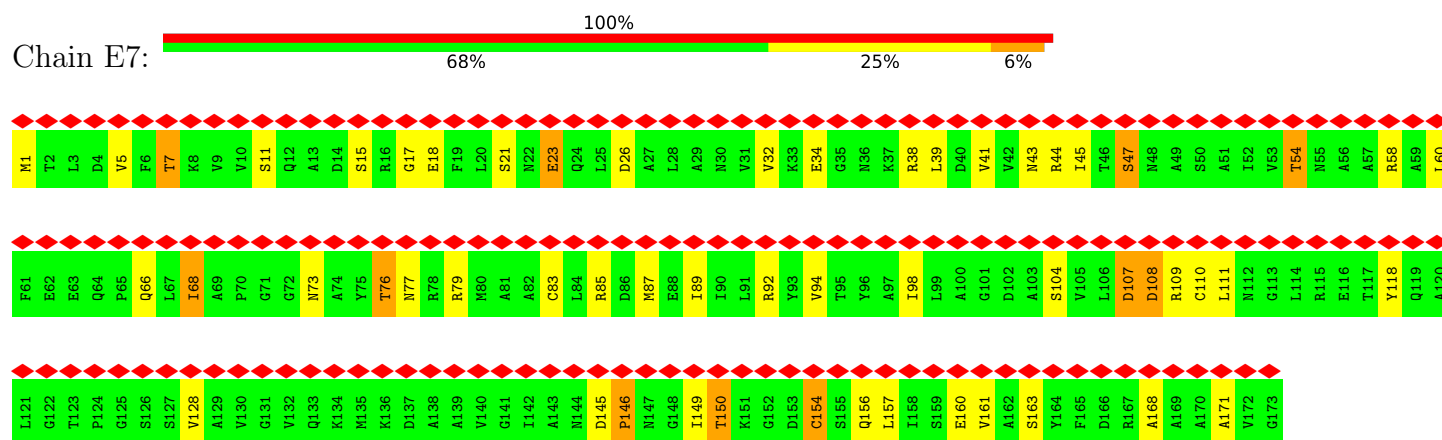
• Molecule 3: C-phycoerythrin beta subunit



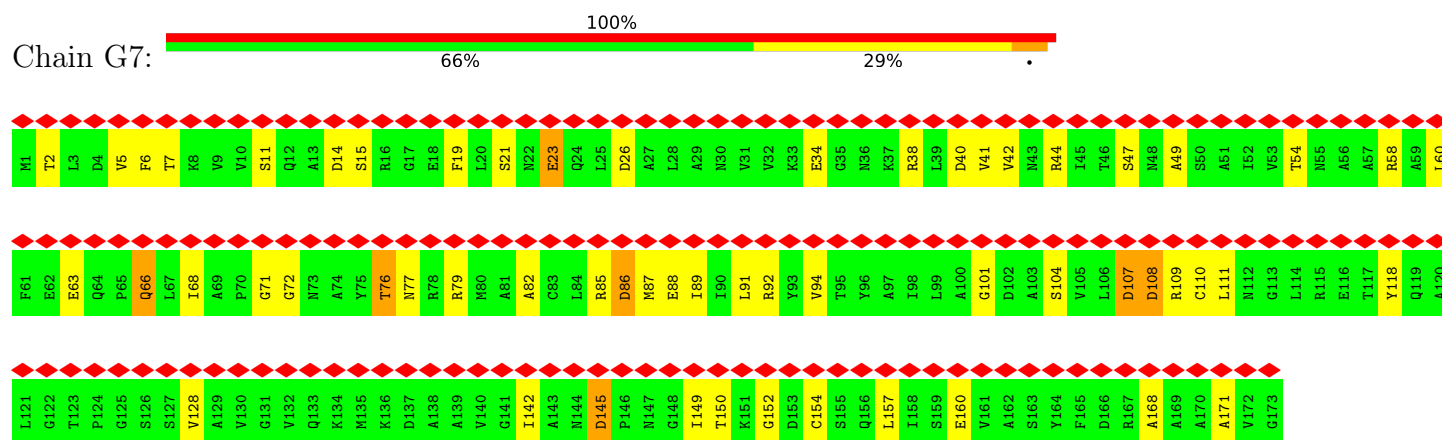
• Molecule 3: C-phycoerythrin beta subunit



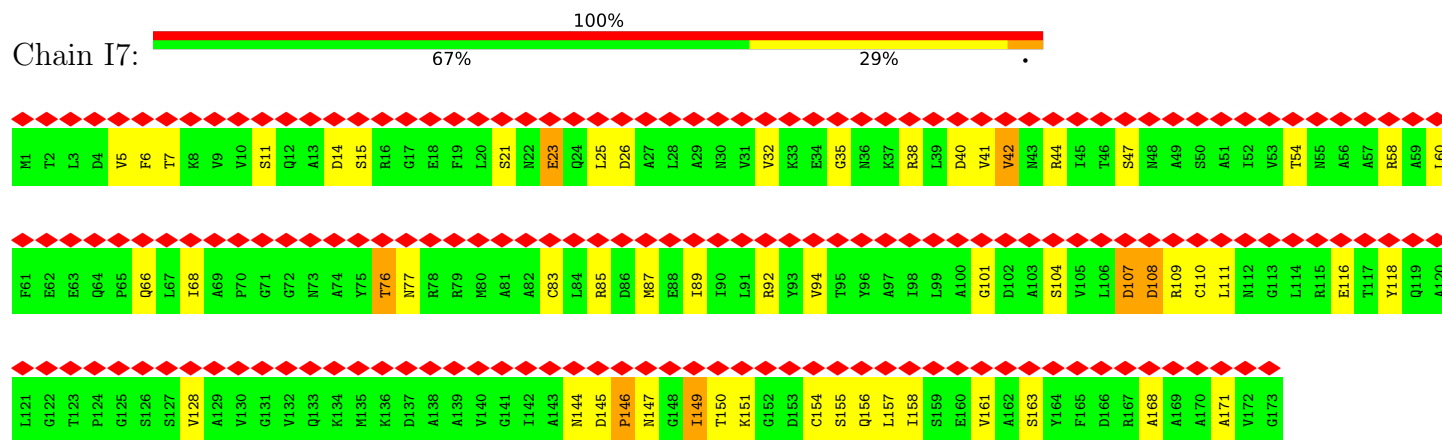
- Molecule 3: C-phyco cyanin beta subunit



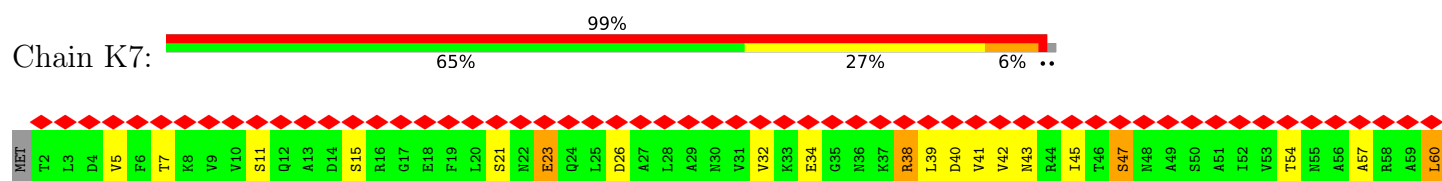
- Molecule 3: C-phyco cyanin beta subunit

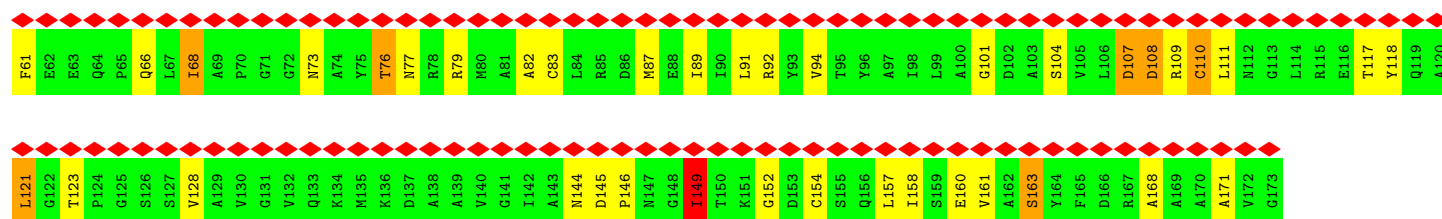


- Molecule 3: C-phyco cyanin beta subunit



- Molecule 3: C-phyco cyanin beta subunit

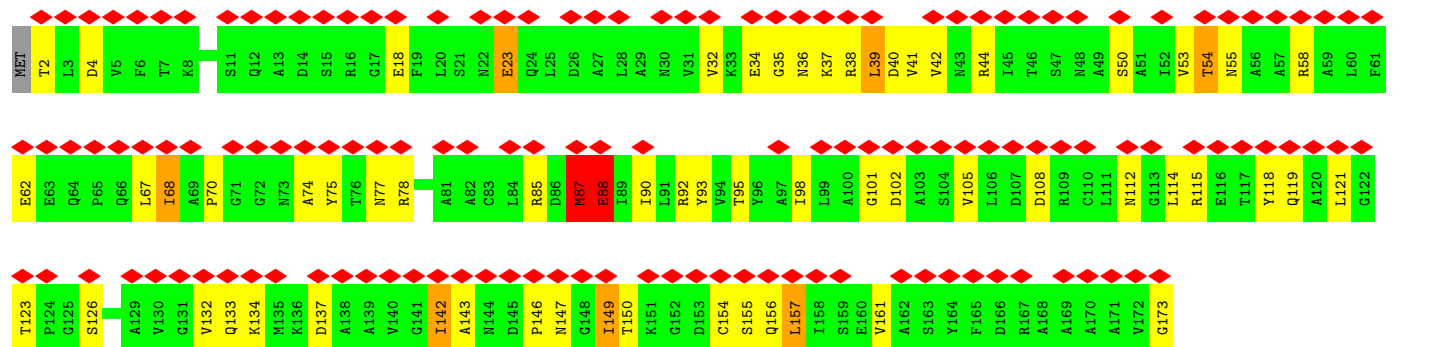
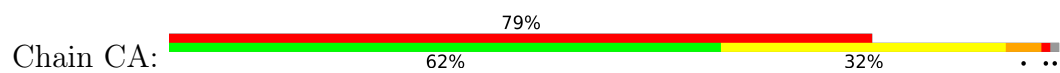




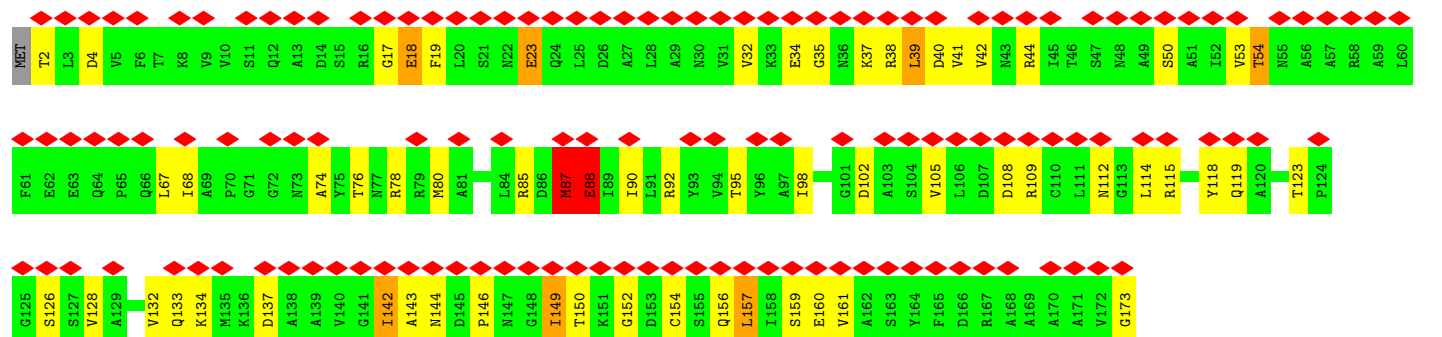
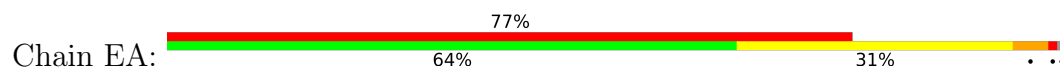
• Molecule 3: C-phycocyanin beta subunit



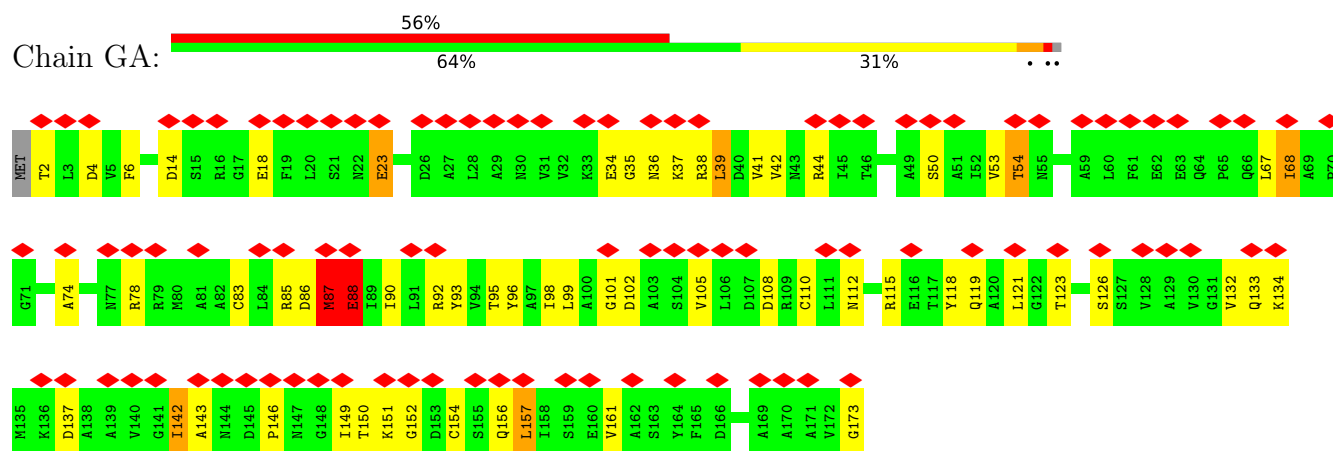
• Molecule 3: C-phycocyanin beta subunit



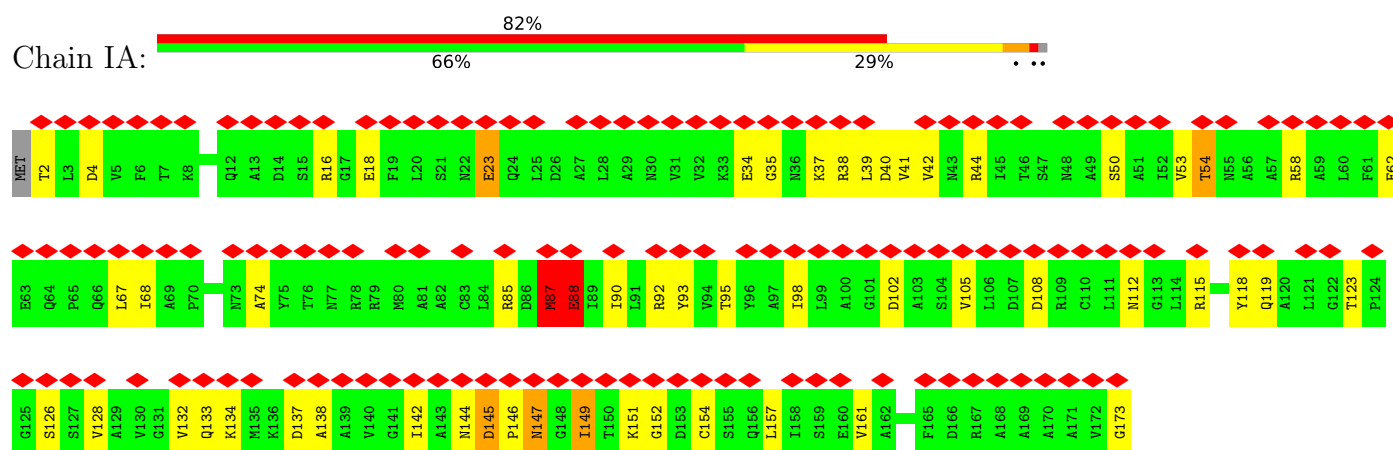
• Molecule 3: C-phycocyanin beta subunit



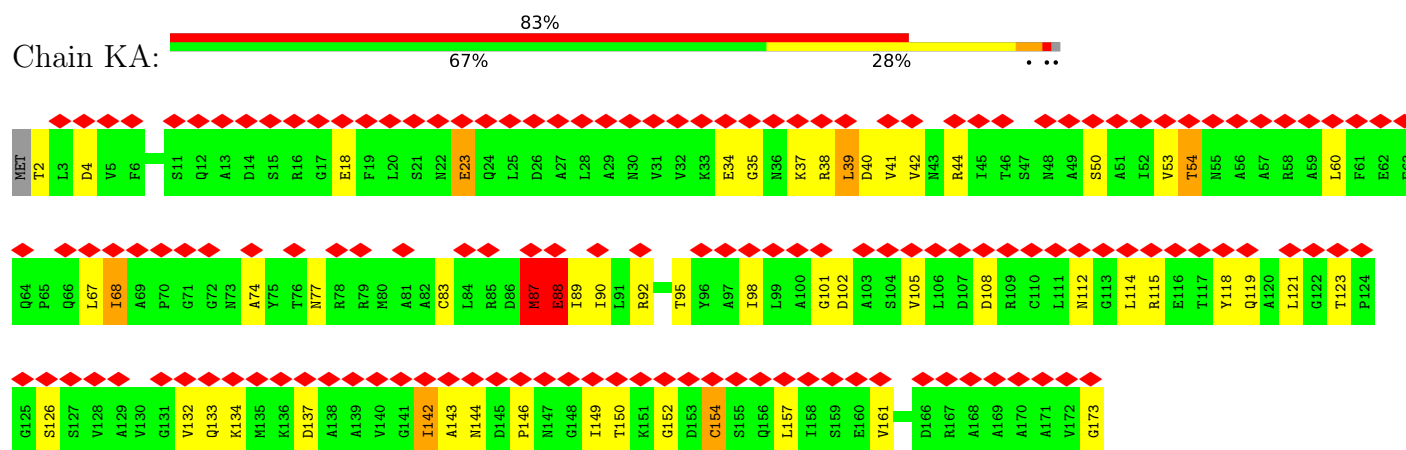
- Molecule 3: C-phyco cyanin beta subunit



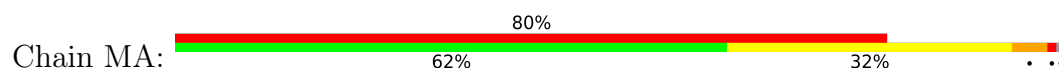
- Molecule 3: C-phyco cyanin beta subunit

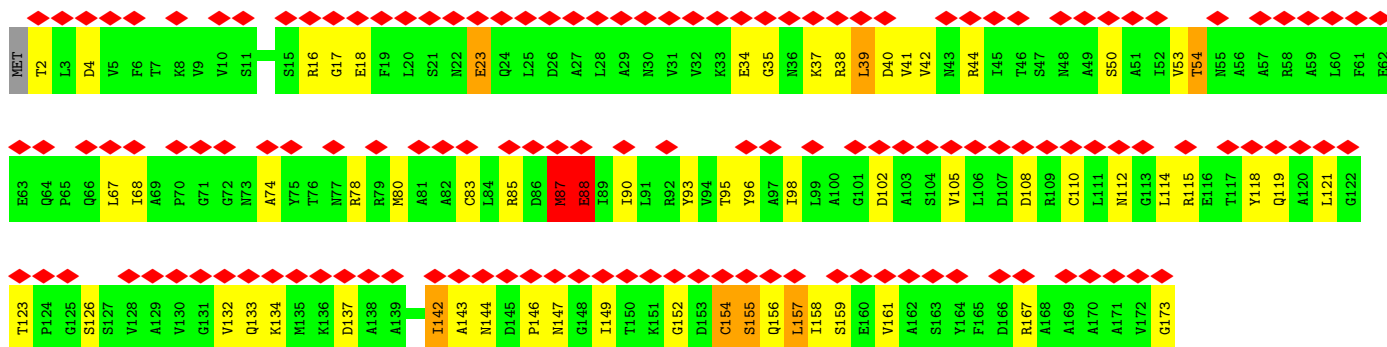


- Molecule 3: C-phyco cyanin beta subunit

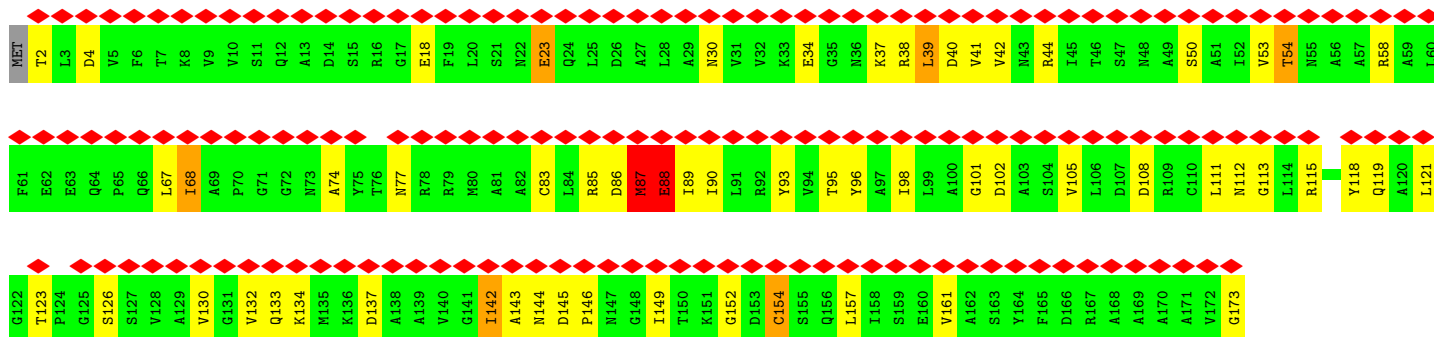


- Molecule 3: C-phyco cyanin beta subunit





• Molecule 3: C-phycoerythrin beta subunit

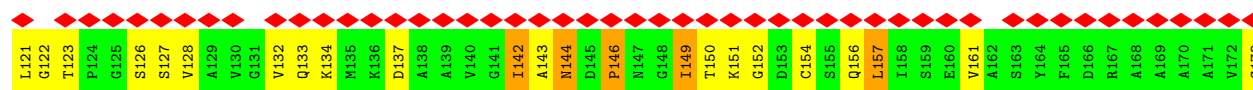


• Molecule 3: C-phycoerythrin beta subunit

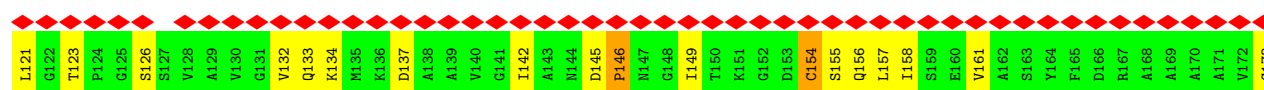


• Molecule 3: C-phycoerythrin beta subunit

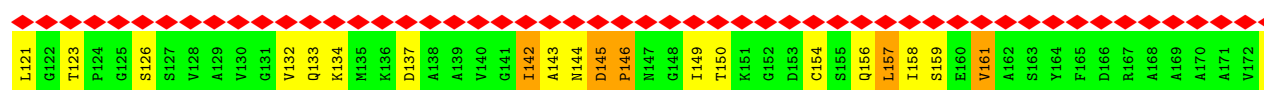
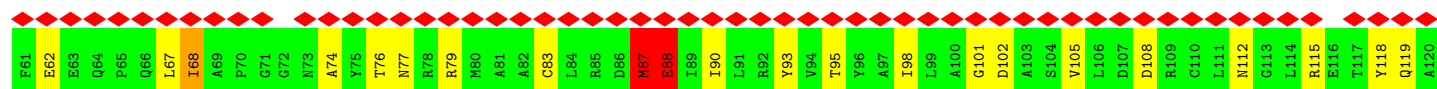




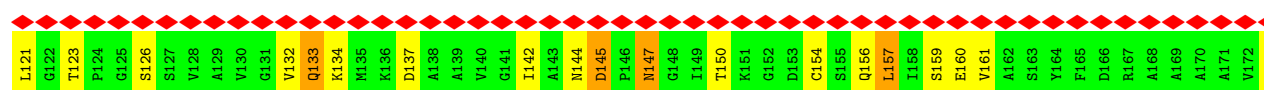
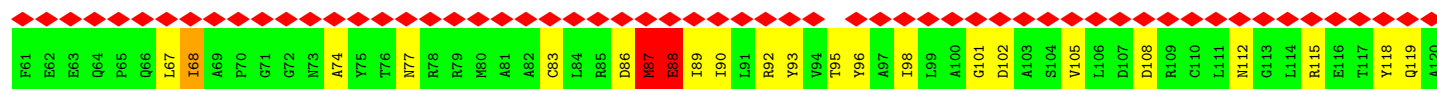
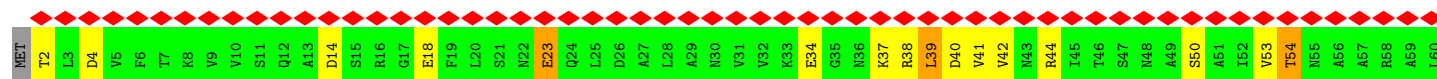
• Molecule 3: C-phycoerythrin beta subunit



• Molecule 3: C-phycoerythrin beta subunit

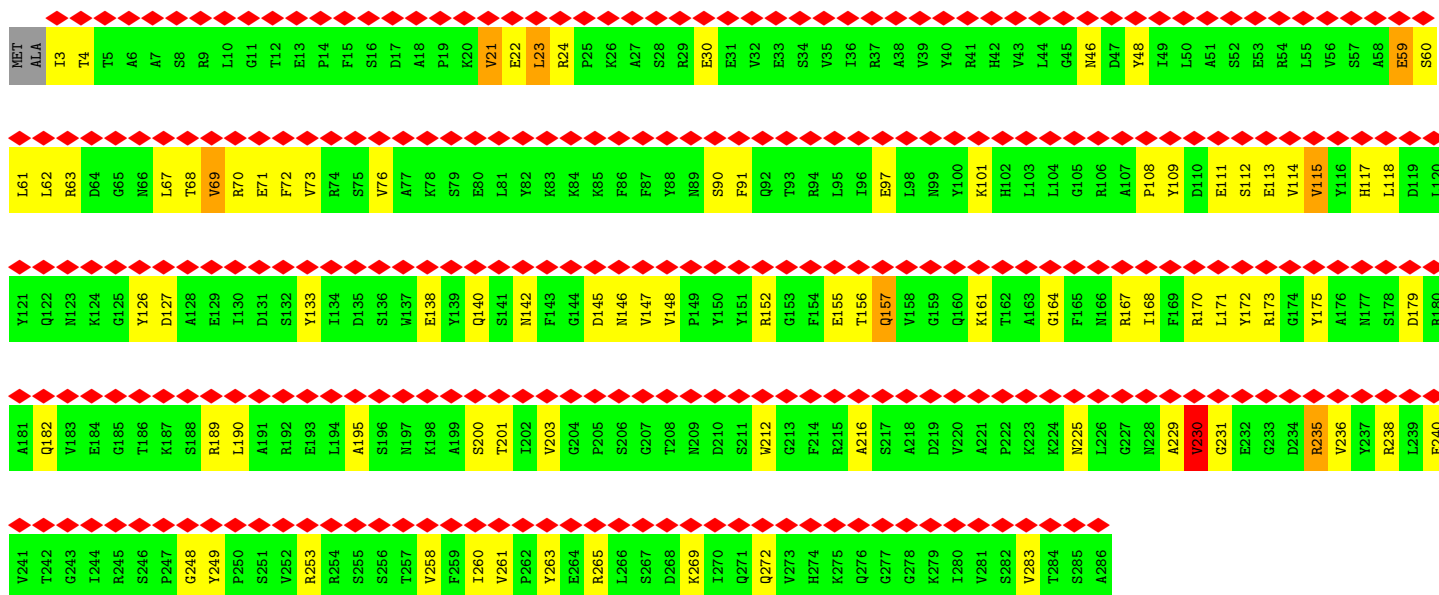


• Molecule 3: C-phycoerythrin beta subunit

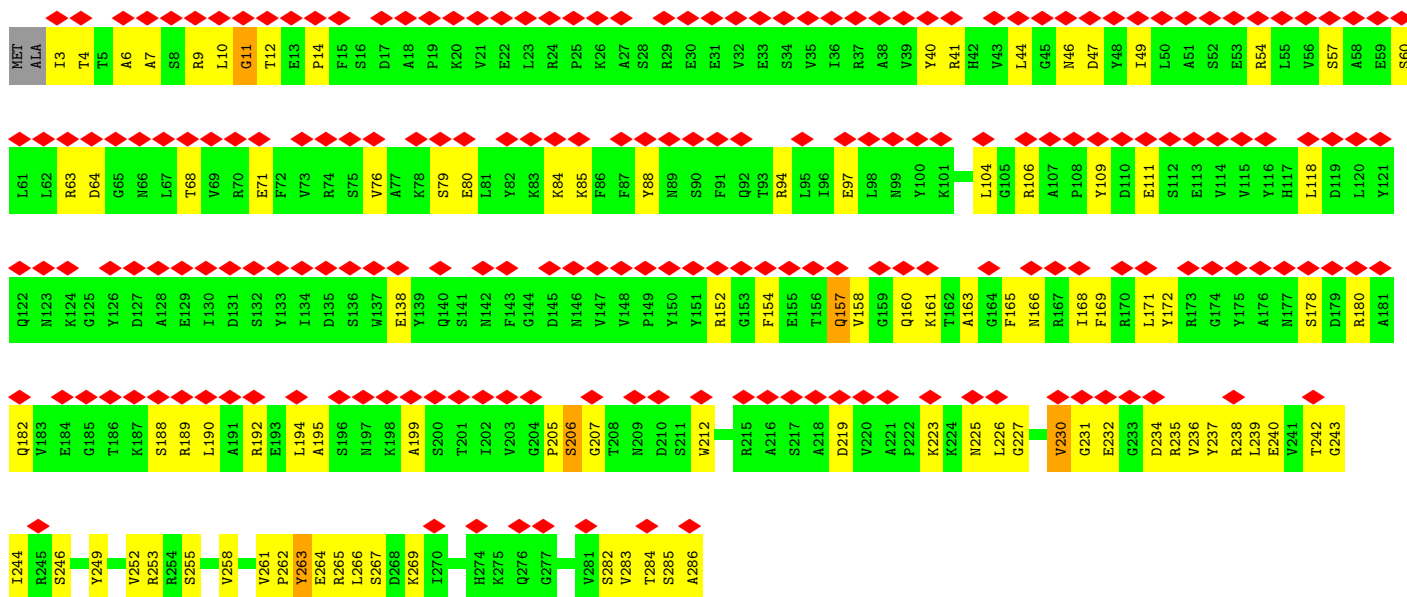


• Molecule 4: Phycobilisome 32.1 kDa linker polypeptide, phycoerythrin-associated, rod

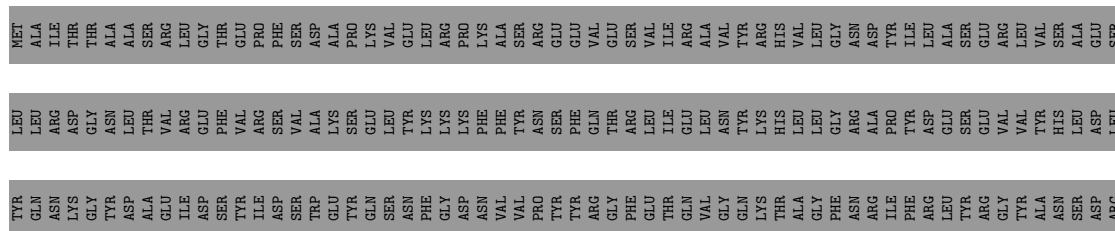


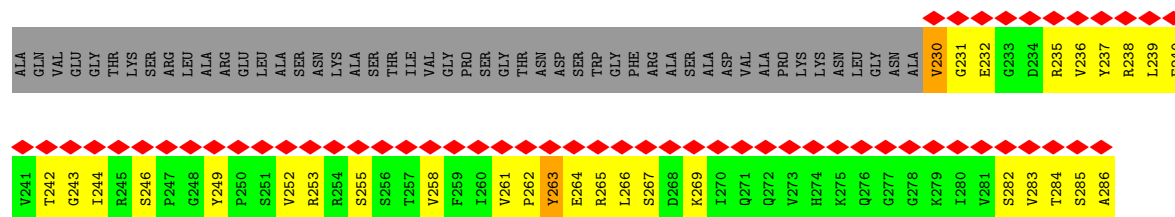


- Molecule 4: Phycobilisome 32.1 kDa linker polypeptide, phycocyanin-associated, rod

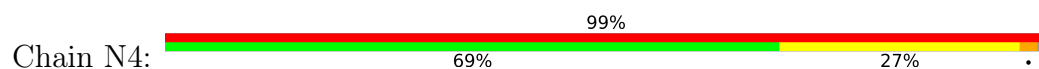


- Molecule 4: Phycobilisome 32.1 kDa linker polypeptide, phycocyanin-associated, rod

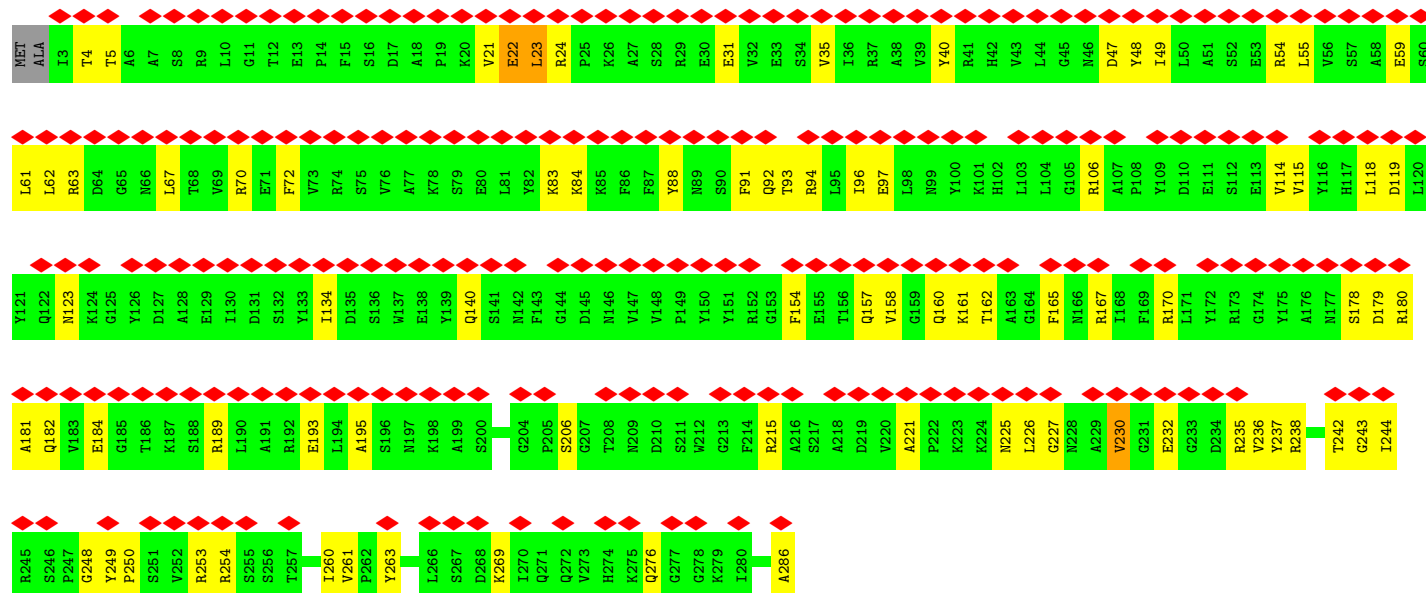
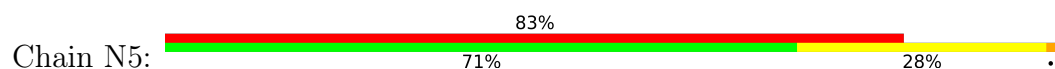




- Molecule 4: Phycobilisome 32.1 kDa linker polypeptide, phycocyanin-associated, rod



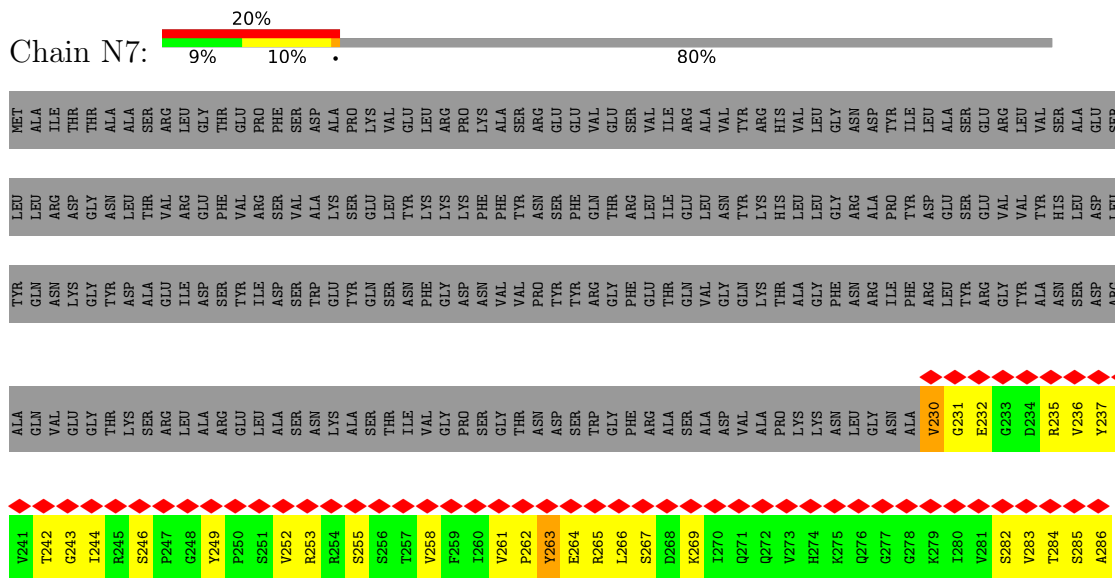
- Molecule 4: Phycobilisome 32.1 kDa linker polypeptide, phycocyanin-associated, rod



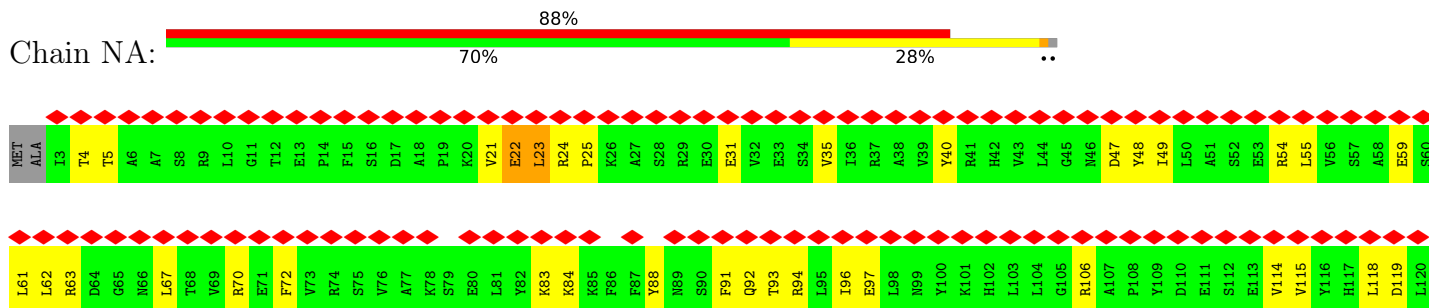
- Chain N6:

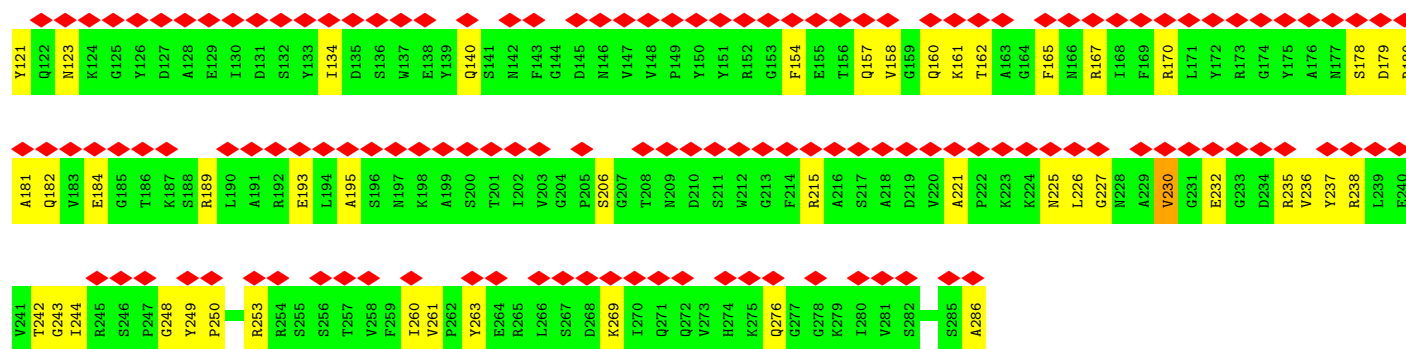


Chain N7:

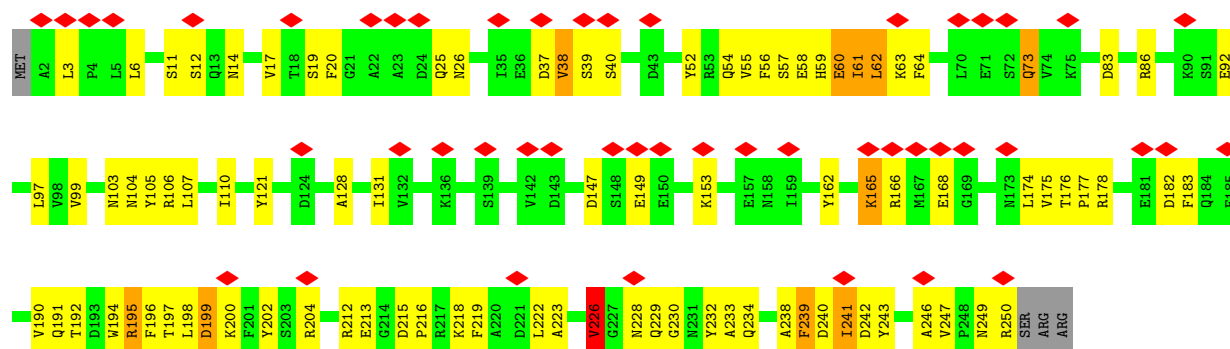


- Chain NA:

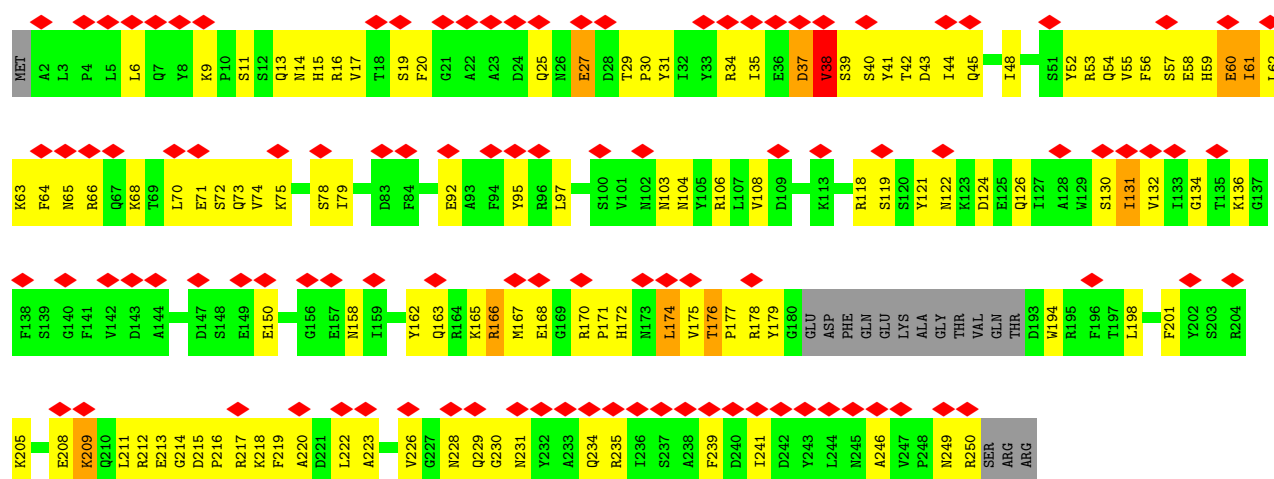
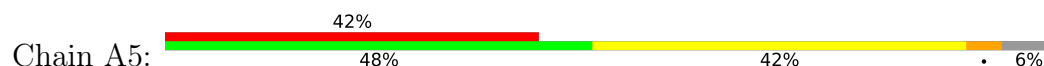




• Molecule 5: Phycobilisome rod-core linker polypeptide CpcG4



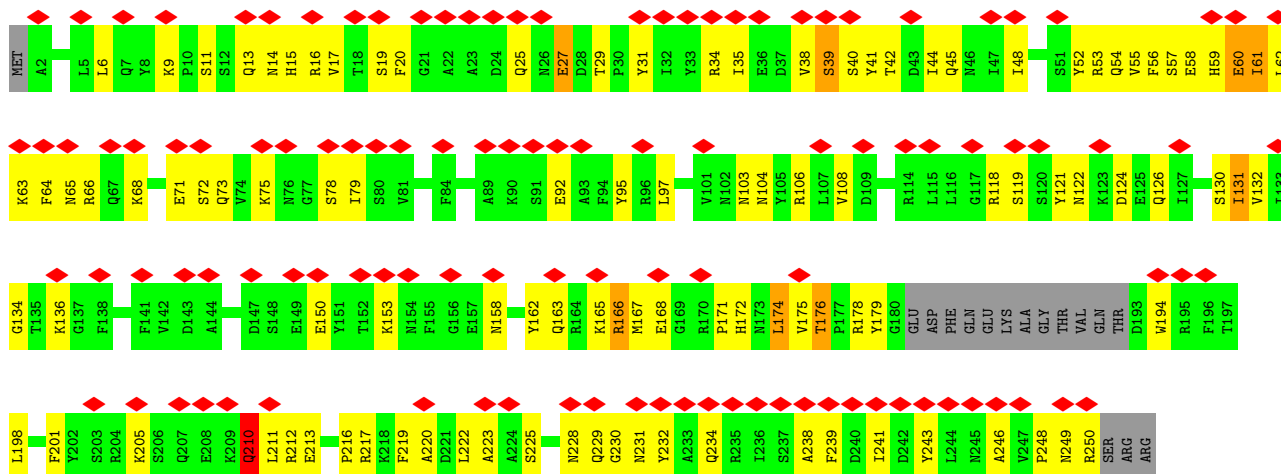
• Molecule 5: Phycobilisome rod-core linker polypeptide CpcG4



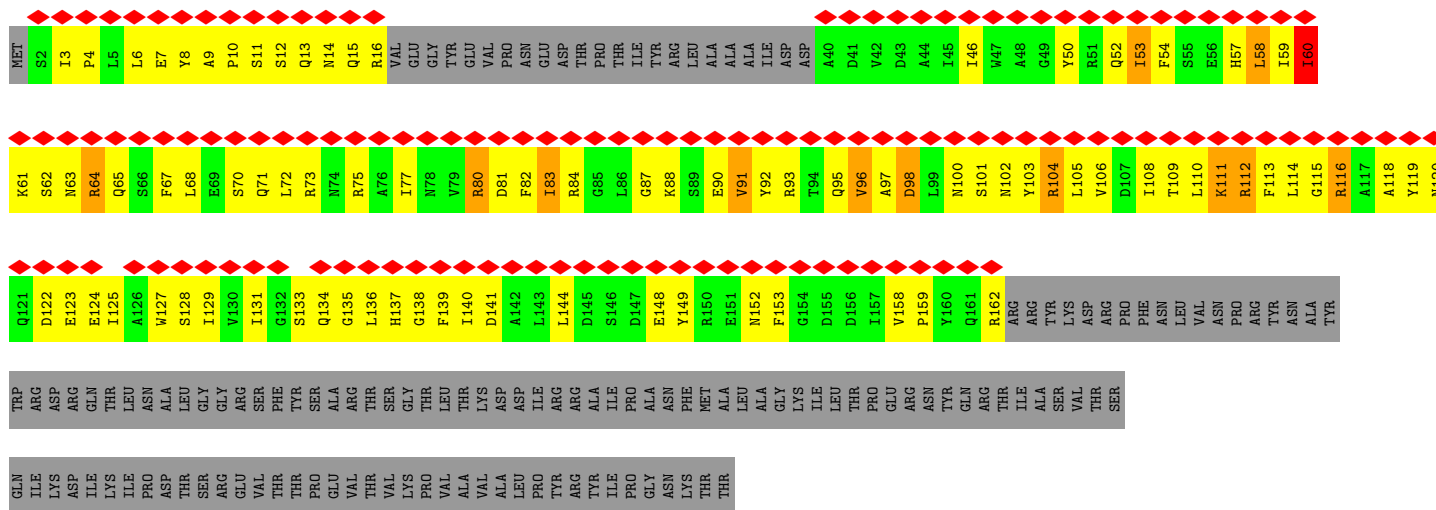
• Molecule 5: Phycobilisome rod-core linker polypeptide CpcG4



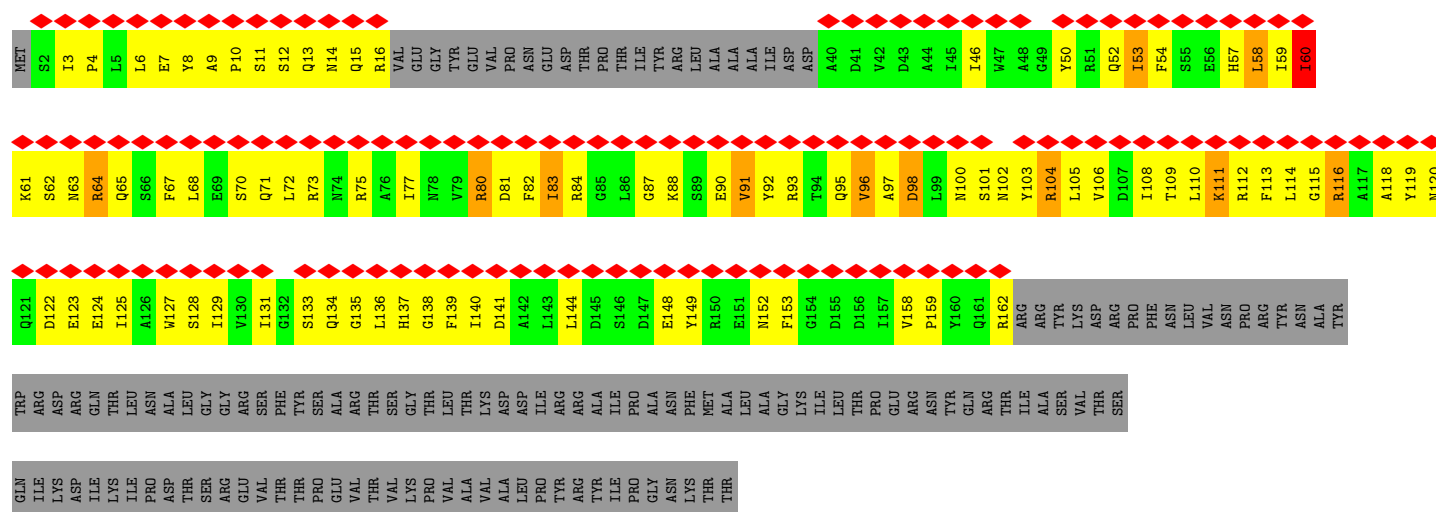
- Molecule 5: Phycobilisome rod-core linker polypeptide CpcG4



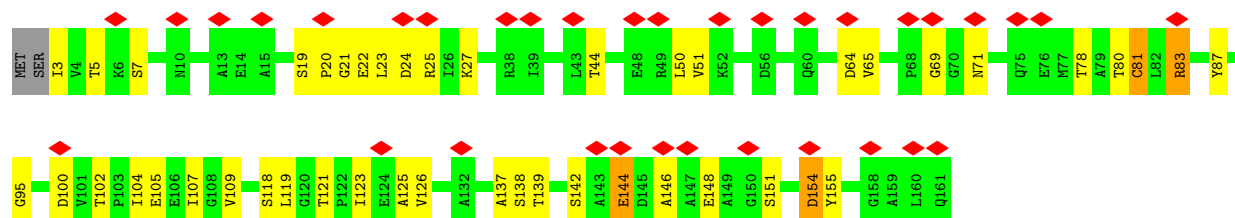
- Molecule 6: Phycobilisome rod-core linker polypeptide CpcG1



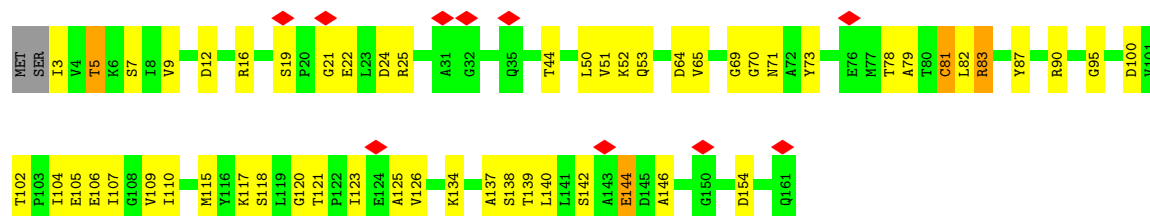
- Molecule 6: Phycobilisome rod-core linker polypeptide CpcG1



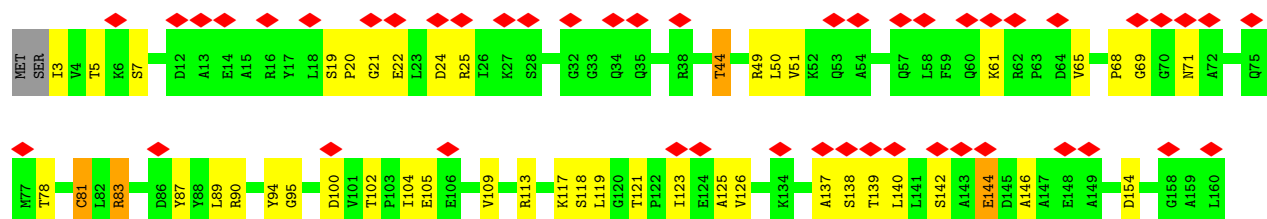
• Molecule 7: Allophycocyanin subunit alpha 1



• Molecule 7: Allophycocyanin subunit alpha 1



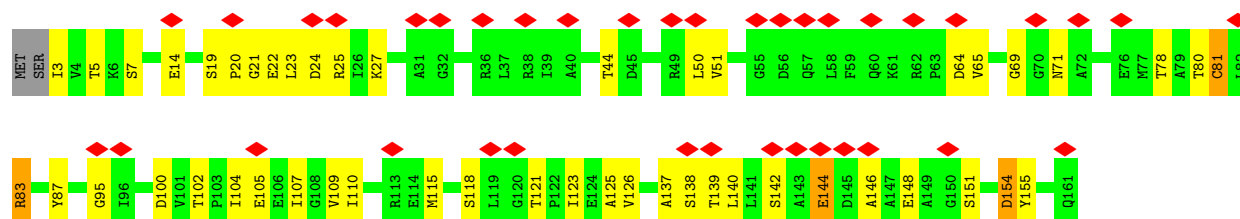
• Molecule 7: Allophycocyanin subunit alpha 1





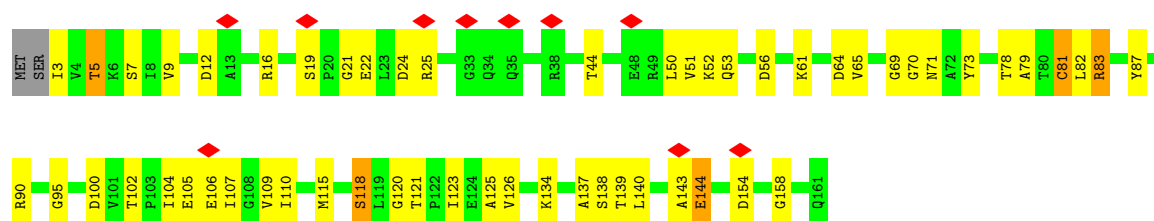
• Molecule 7: Allophycocyanin subunit alpha 1

Chain H8: 24% 68% 28% ..



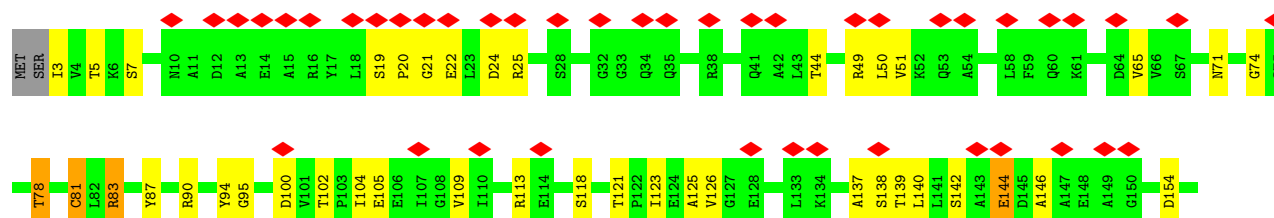
• Molecule 7: Allophycocyanin subunit alpha 1

Chain J8: 6% 64% 32% ..



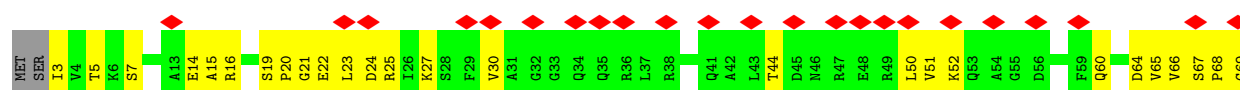
• Molecule 7: Allophycocyanin subunit alpha 1

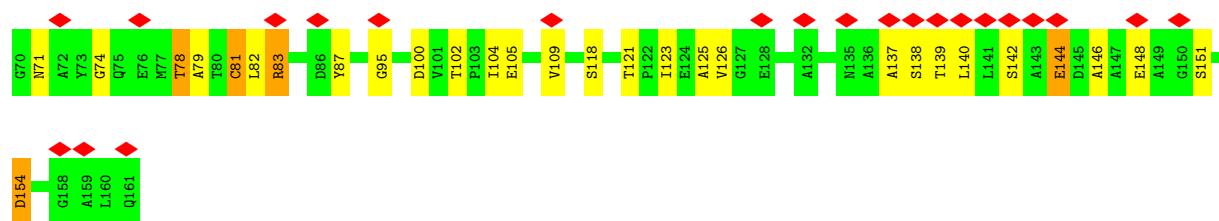
Chain L8: 28% 73% 24% ..



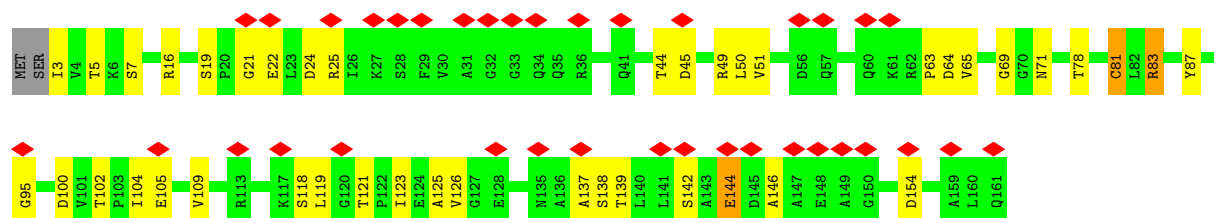
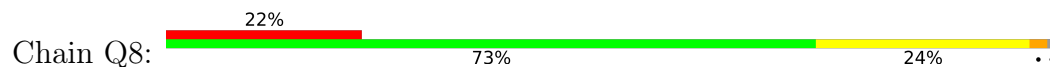
• Molecule 7: Allophycocyanin subunit alpha 1

Chain O8: 28% 65% 31% ..

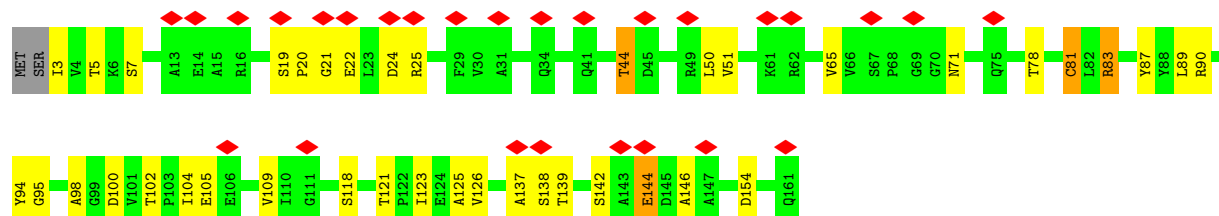
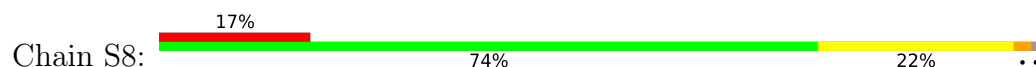




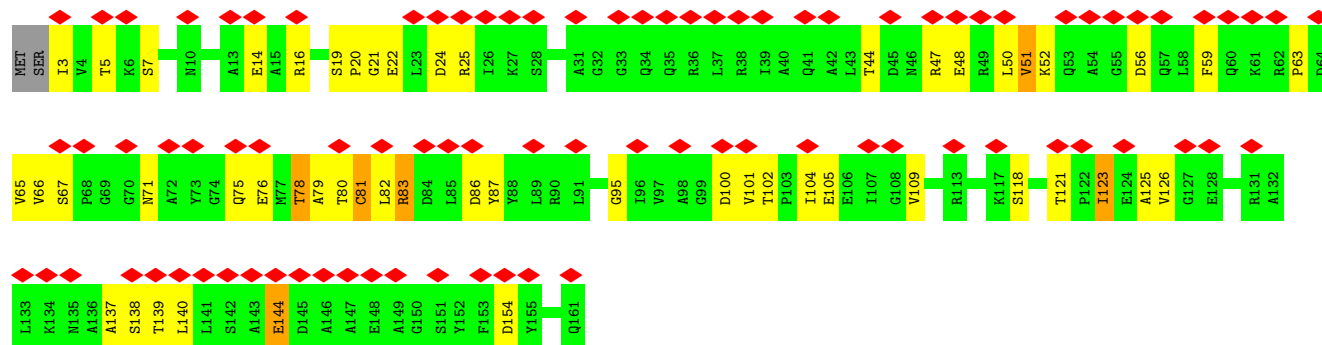
• Molecule 7: Allophycocyanin subunit alpha 1



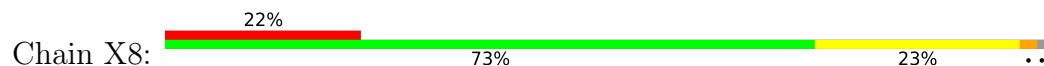
• Molecule 7: Allophycocyanin subunit alpha 1

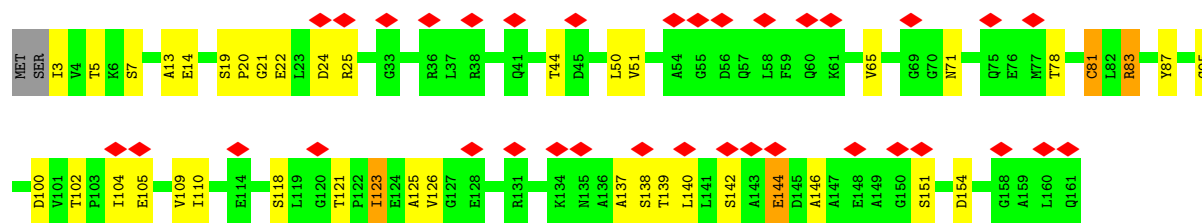


• Molecule 7: Allophycocyanin subunit alpha 1



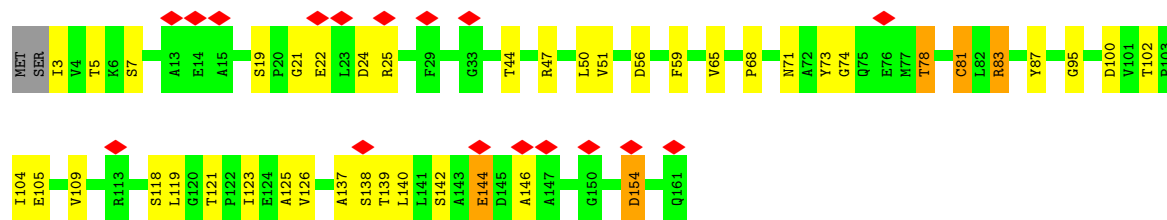
• Molecule 7: Allophycocyanin subunit alpha 1





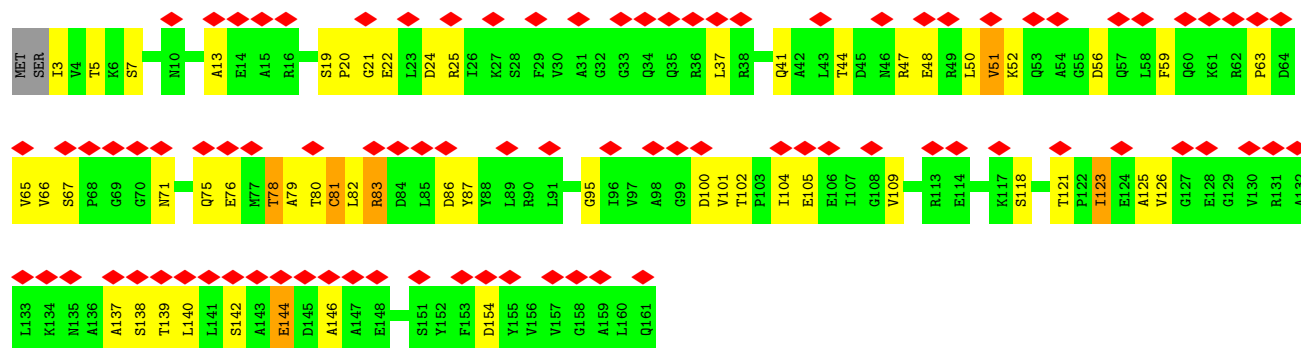
• Molecule 7: Allophycocyanin subunit alpha 1

Chain Z8: 11% 72% 24% ..



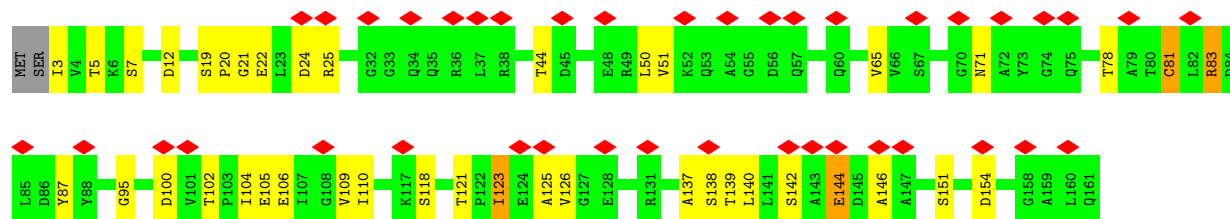
• Molecule 7: Allophycocyanin subunit alpha 1

Chain c8: 55% 65% 30% ..



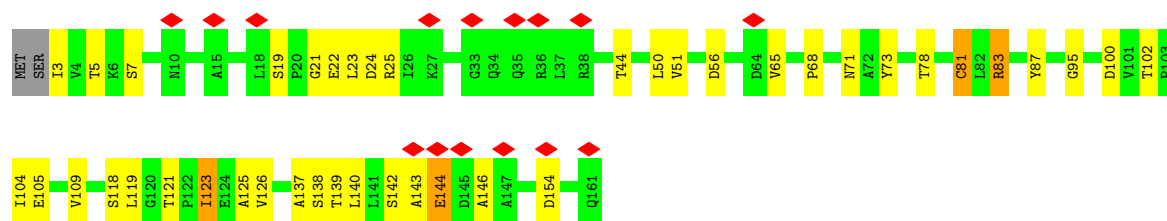
• Molecule 7: Allophycocyanin subunit alpha 1

Chain e8: 25% 73% 23% ..

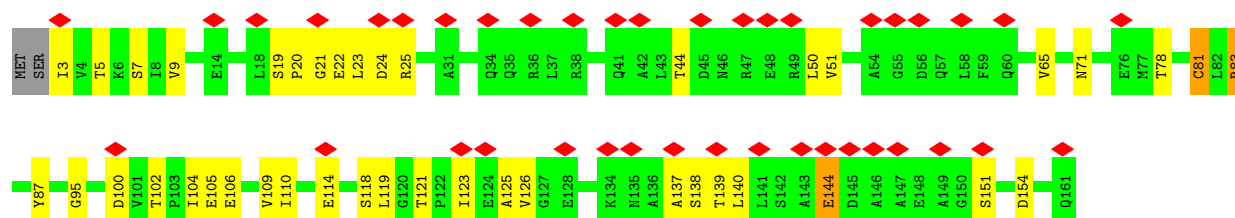
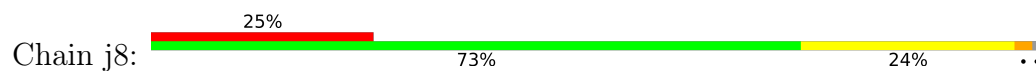


• Molecule 7: Allophycocyanin subunit alpha 1

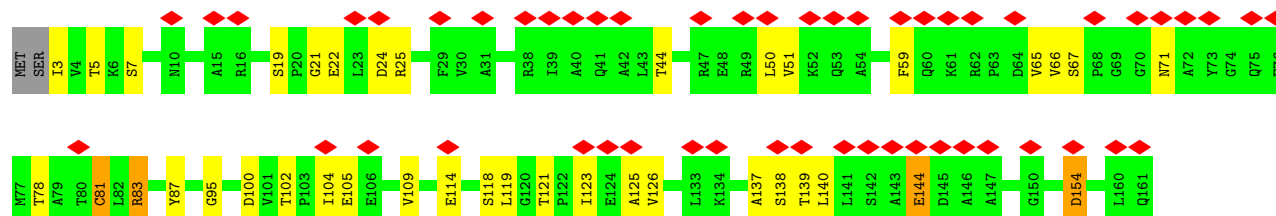
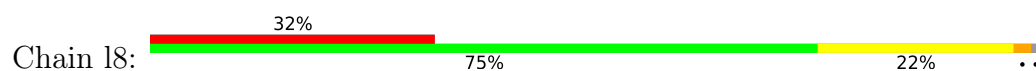
Chain g8: 9% 73% 24% ..



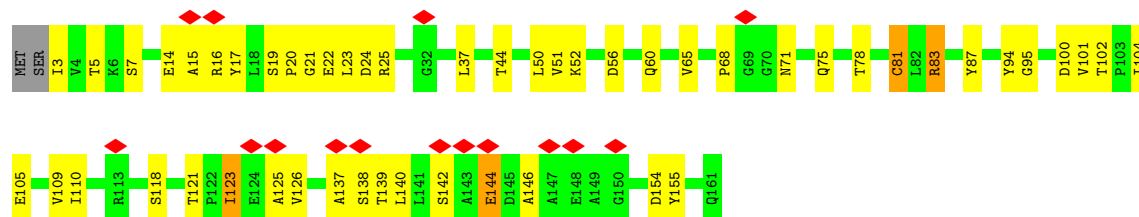
• Molecule 7: Allophycocyanin subunit alpha 1



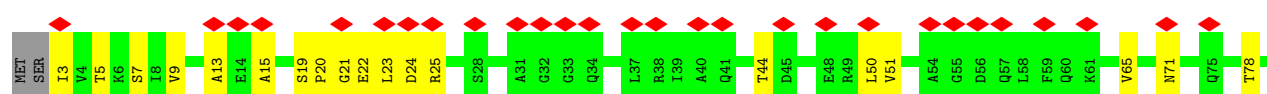
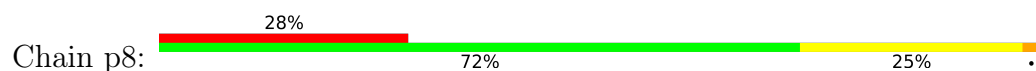
• Molecule 7: Allophycocyanin subunit alpha 1

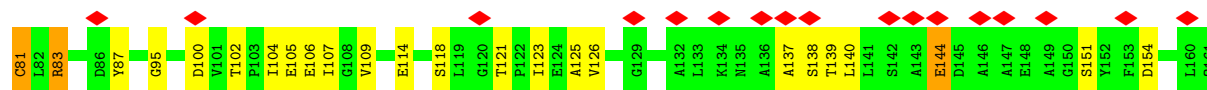


• Molecule 7: Allophycocyanin subunit alpha 1

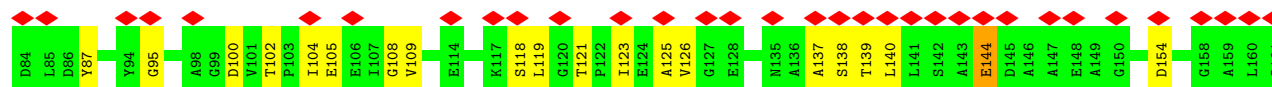
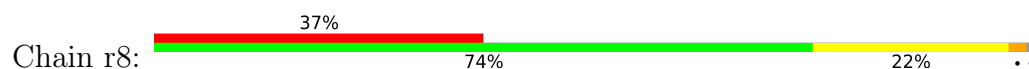


• Molecule 7: Allophycocyanin subunit alpha 1

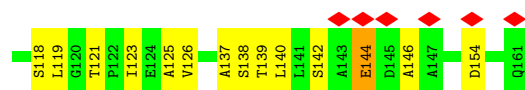




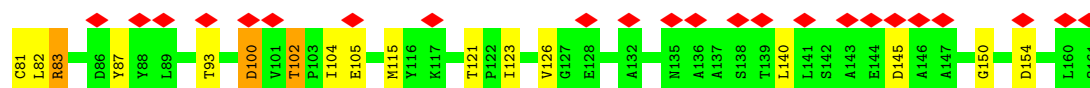
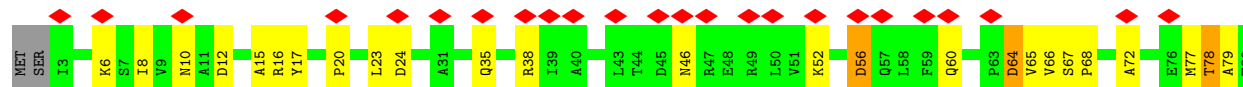
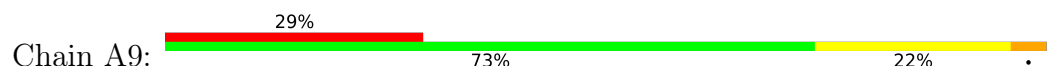
• Molecule 7: Allophycocyanin subunit alpha 1



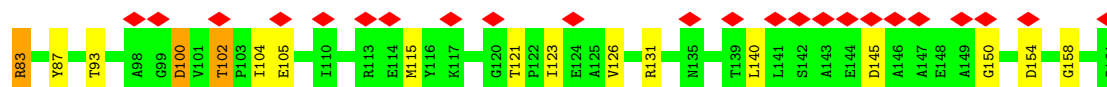
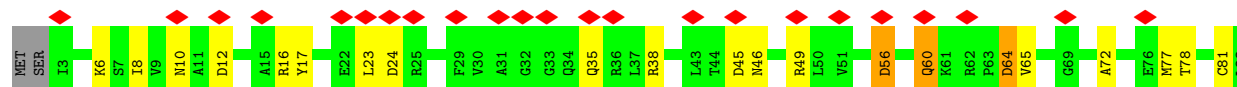
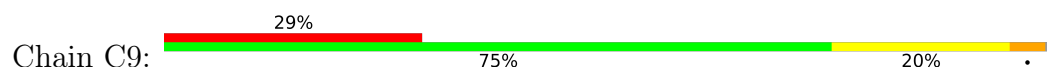
• Molecule 7: Allophycocyanin subunit alpha 1



• Molecule 7: Allophycocyanin subunit alpha 1

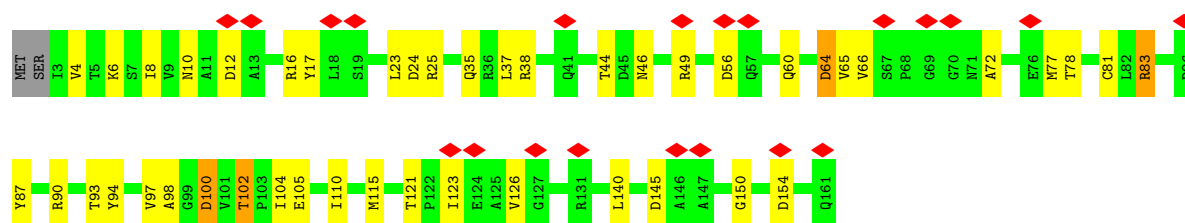


• Molecule 7: Allophycocyanin subunit alpha 1



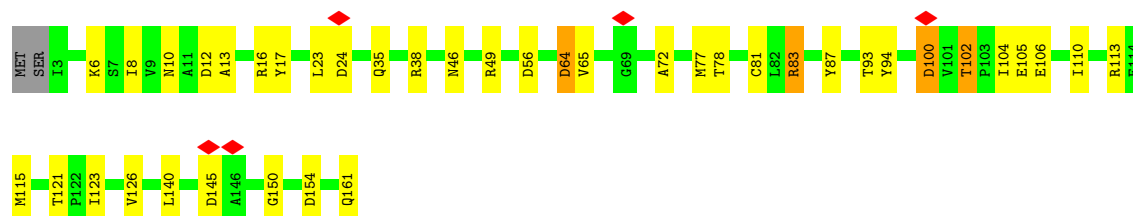
• Molecule 7: Allophycocyanin subunit alpha 1

Chain E9: 



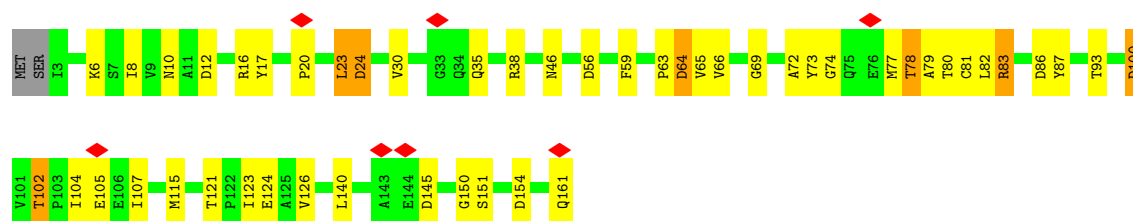
• Molecule 7: Allophycocyanin subunit alpha 1

Chain G9: 



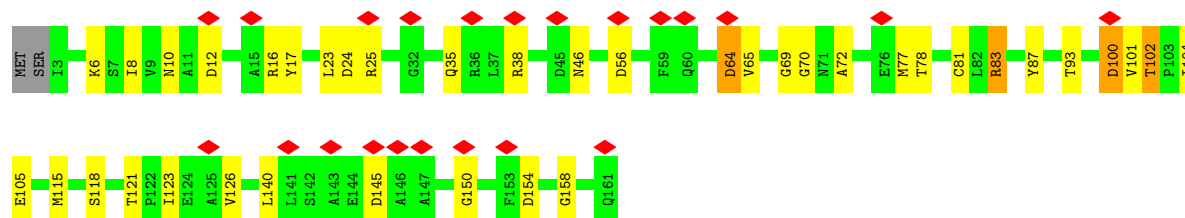
• Molecule 7: Allophycocyanin subunit alpha 1

Chain I9: 



• Molecule 7: Allophycocyanin subunit alpha 1

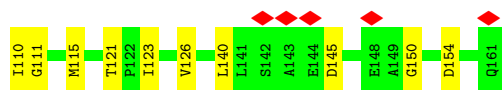
Chain K9: 



• Molecule 7: Allophycocyanin subunit alpha 1

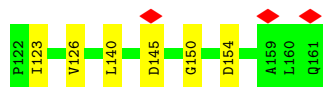
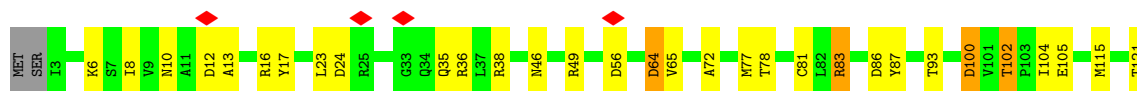
Chain N9: 





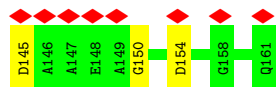
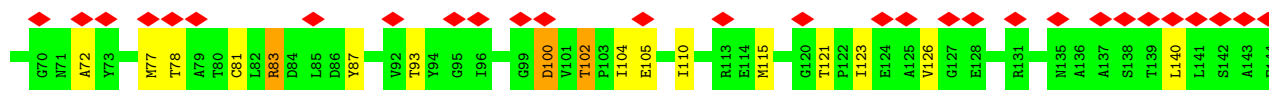
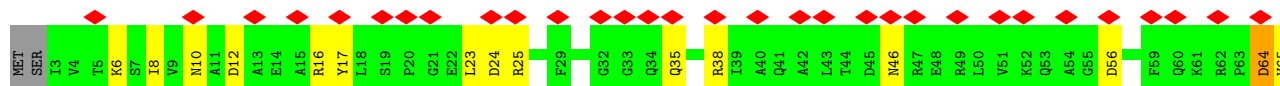
- Molecule 7: Allophycocyanin subunit alpha 1

Chain P9: 76% 20% ..



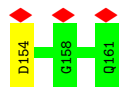
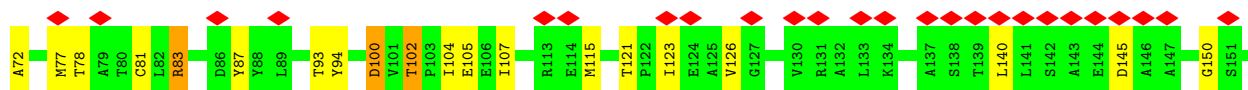
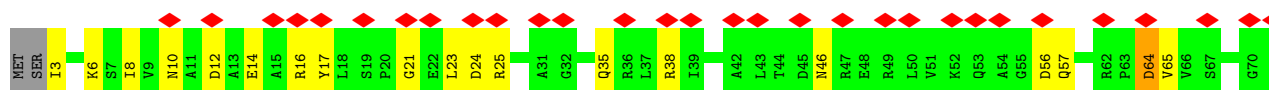
- Molecule 7: Allophycocyanin subunit alpha 1

Chain R9: 42% 77% 19% ..



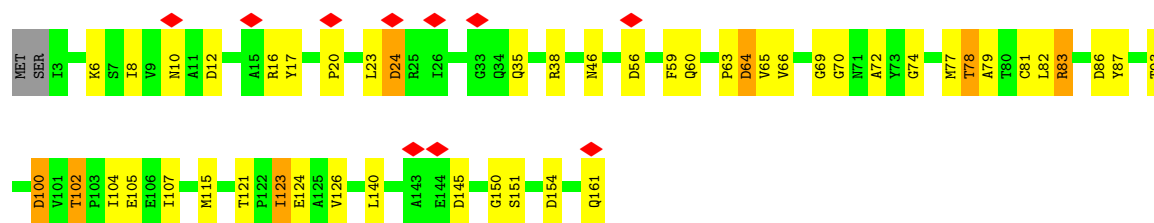
- Molecule 7: Allophycocyanin subunit alpha 1

Chain T9: 36% 74% 22% ..

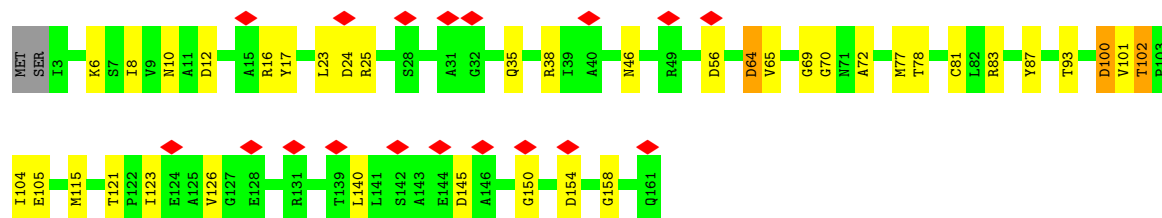
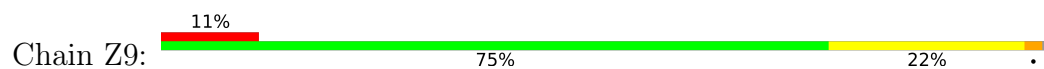


- Molecule 7: Allophycocyanin subunit alpha 1

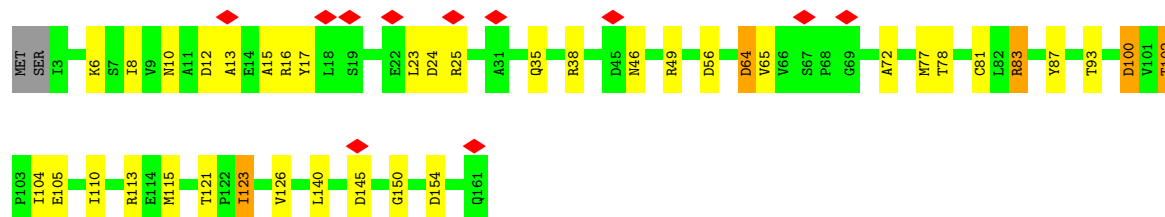
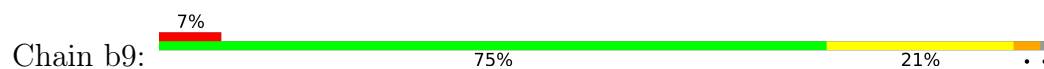
Chain X9: 6% 69% 25% ..



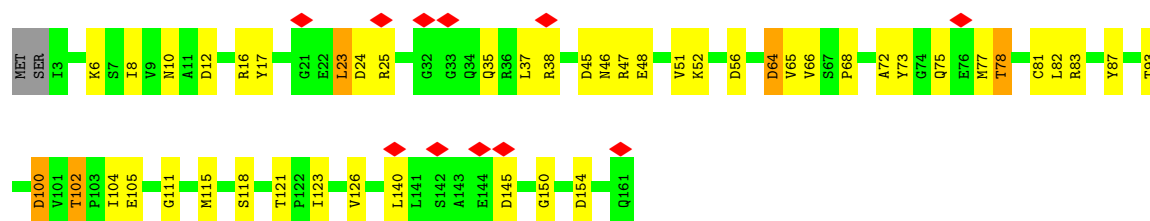
• Molecule 7: Allophycocyanin subunit alpha 1



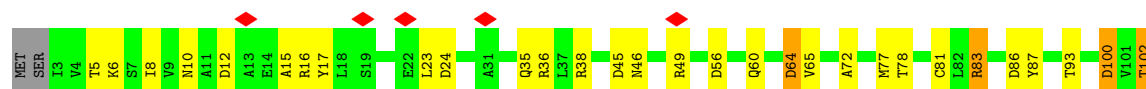
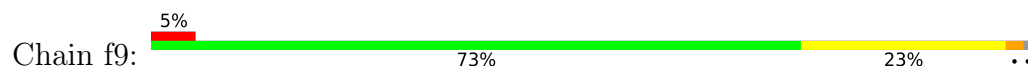
• Molecule 7: Allophycocyanin subunit alpha 1



• Molecule 7: Allophycocyanin subunit alpha 1

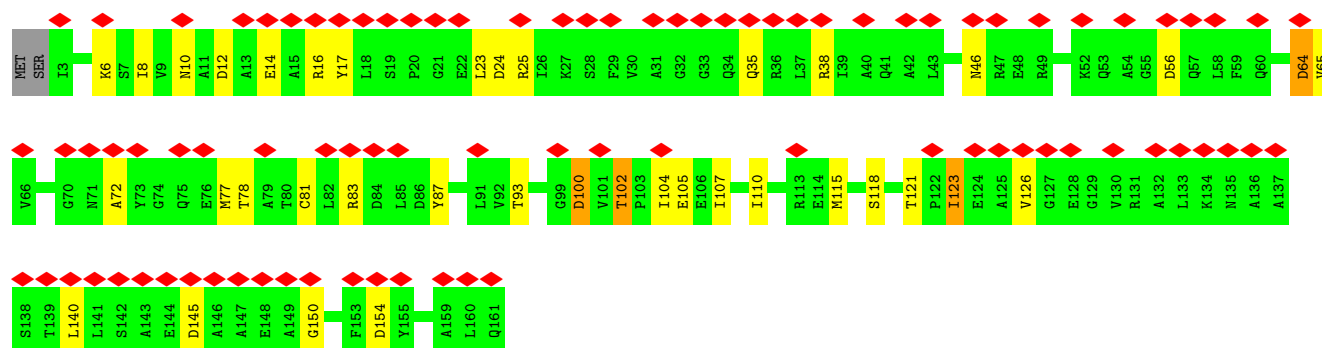
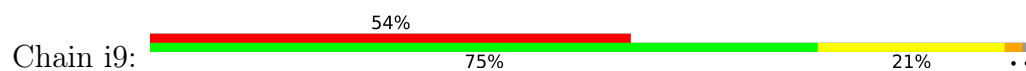


• Molecule 7: Allophycocyanin subunit alpha 1

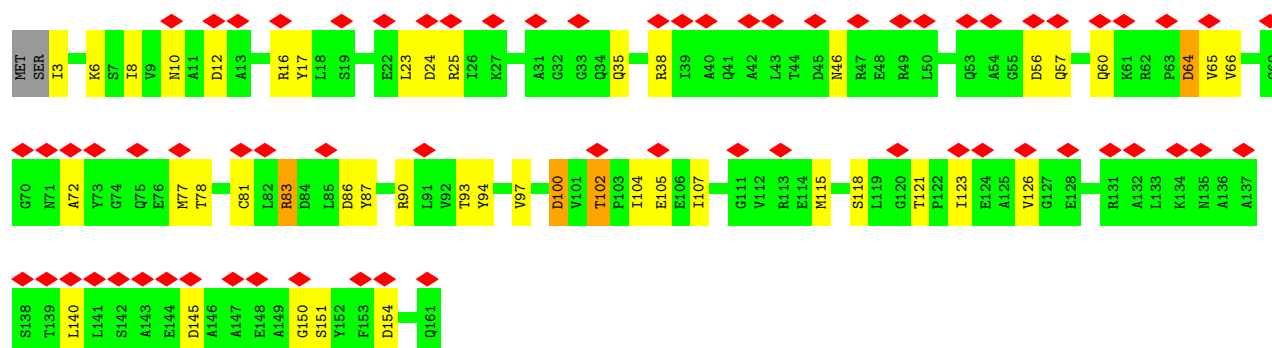
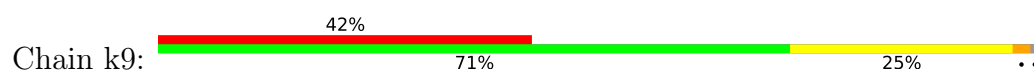




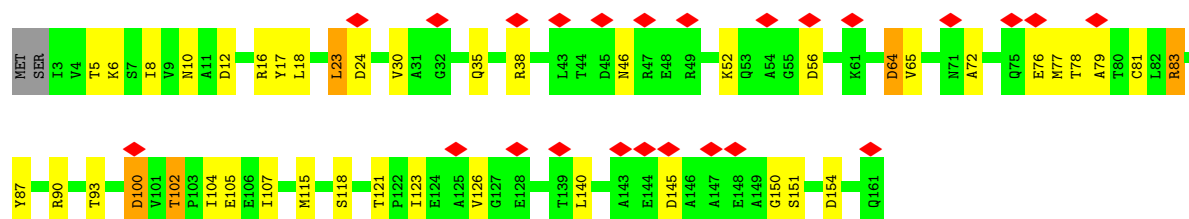
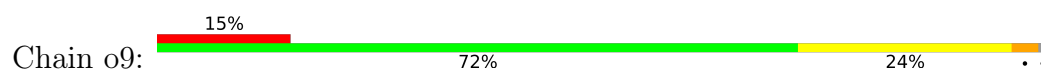
• Molecule 7: Allophycocyanin subunit alpha 1



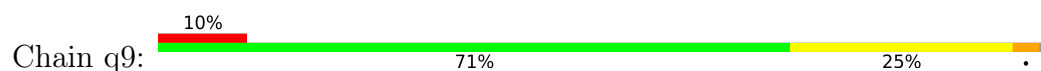
• Molecule 7: Allophycocyanin subunit alpha 1

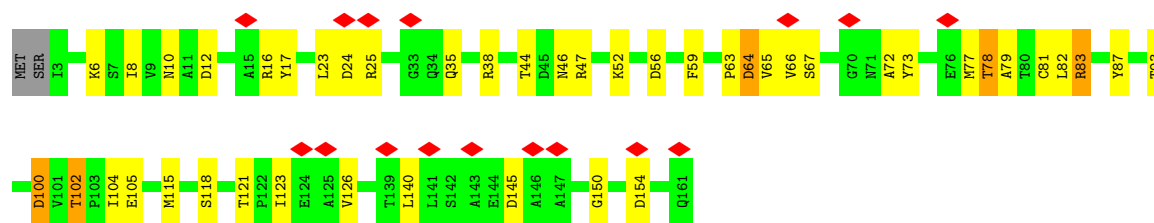


• Molecule 7: Allophycocyanin subunit alpha 1

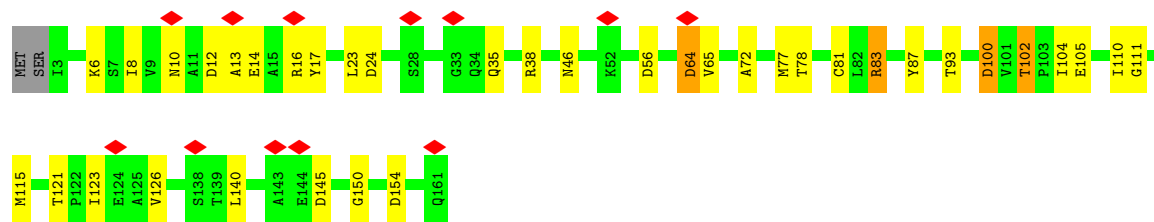
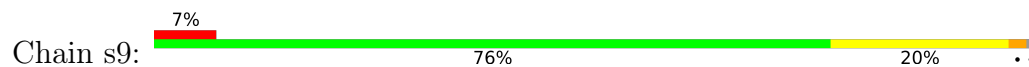


• Molecule 7: Allophycocyanin subunit alpha 1

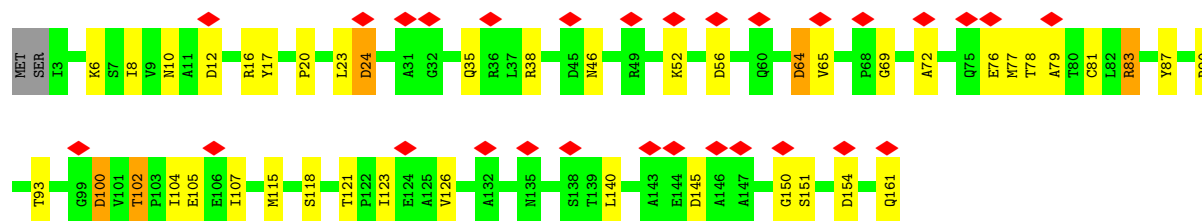
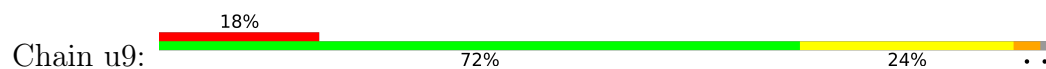




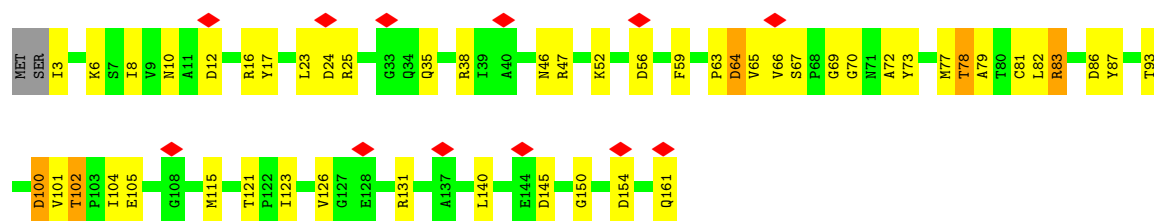
• Molecule 7: Allophycocyanin subunit alpha 1



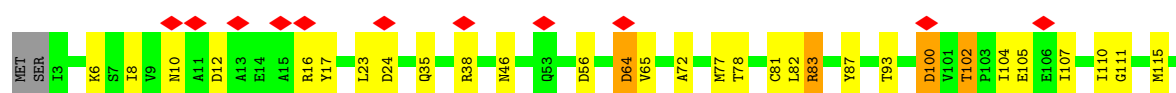
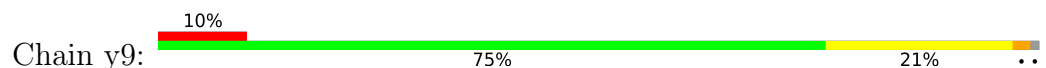
• Molecule 7: Allophycocyanin subunit alpha 1

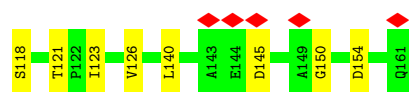


• Molecule 7: Allophycocyanin subunit alpha 1

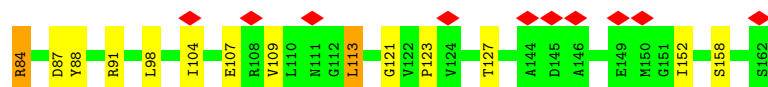
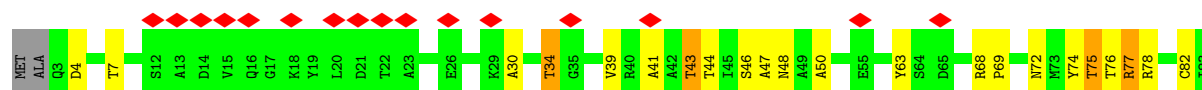
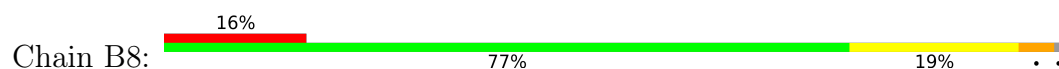


• Molecule 7: Allophycocyanin subunit alpha 1

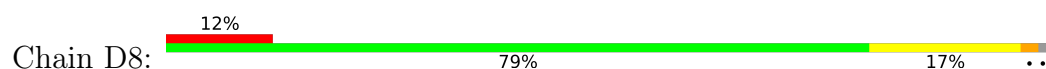




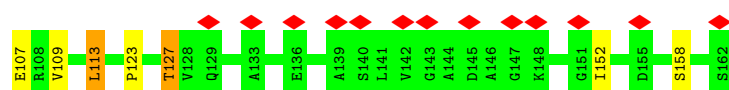
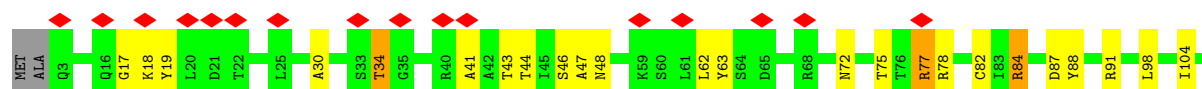
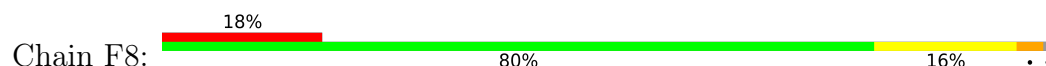
- Molecule 8: Allophycocyanin subunit beta



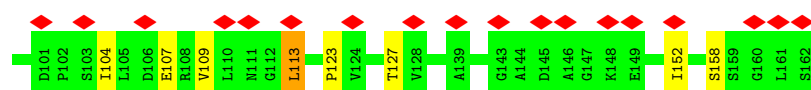
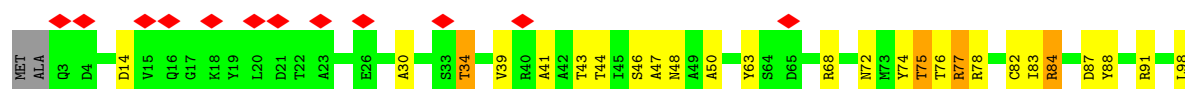
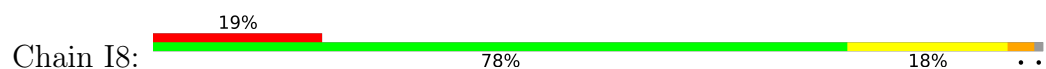
- Molecule 8: Allophycocyanin subunit beta



- Molecule 8: Allophycocyanin subunit beta

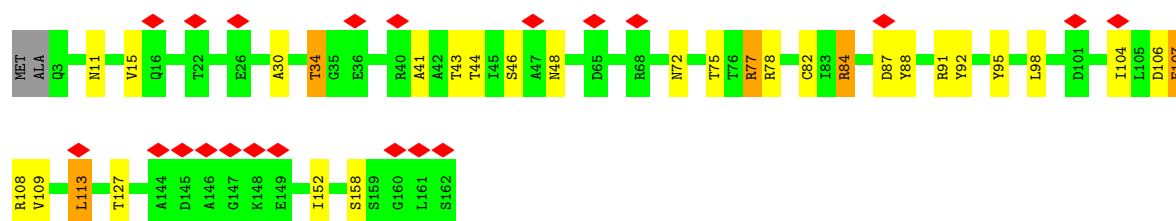


- Molecule 8: Allophycocyanin subunit beta



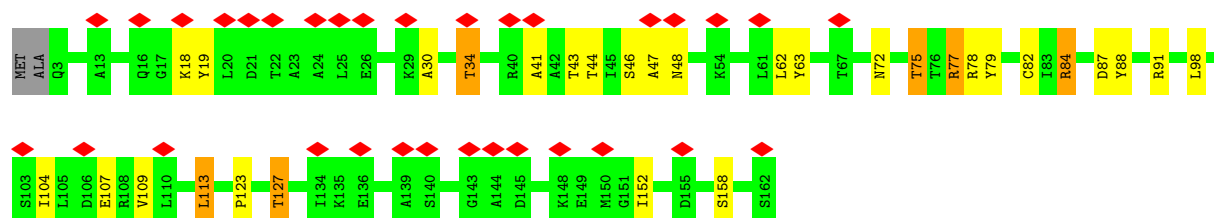
- Molecule 8: Allophycocyanin subunit beta

Chain K8: 



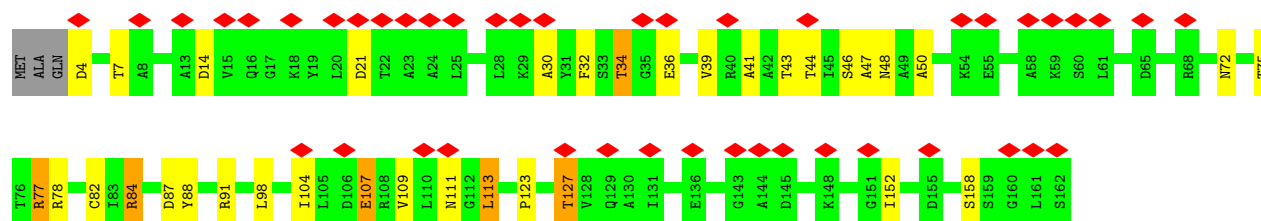
• Molecule 8: Allophycocyanin subunit beta

Chain M8: 



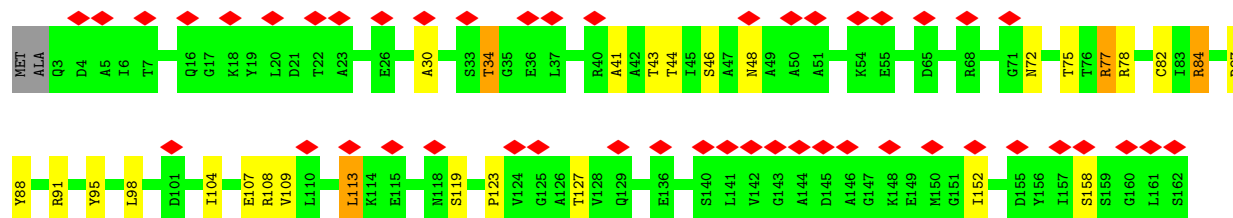
• Molecule 8: Allophycocyanin subunit beta

Chain P8: 



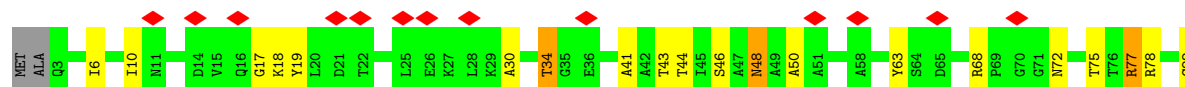
• Molecule 8: Allophycocyanin subunit beta

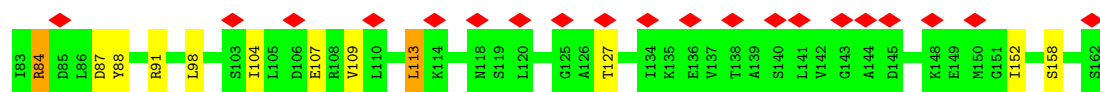
Chain R8: 



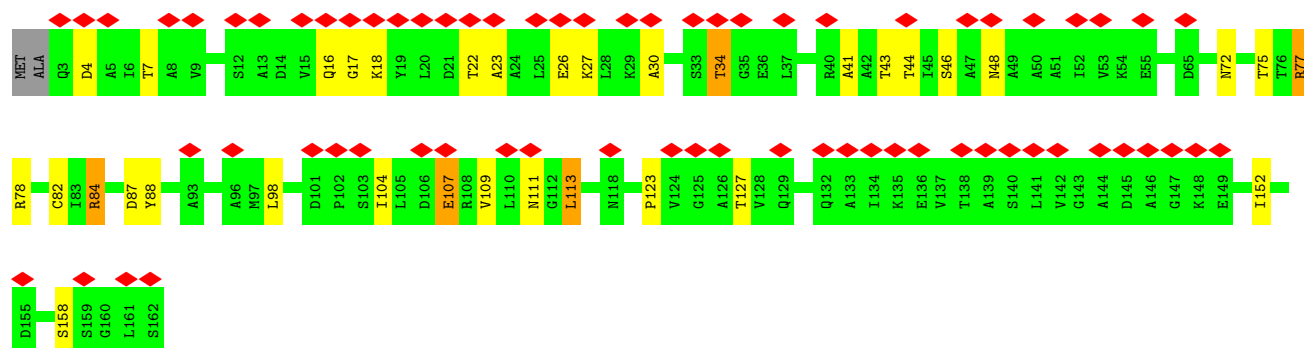
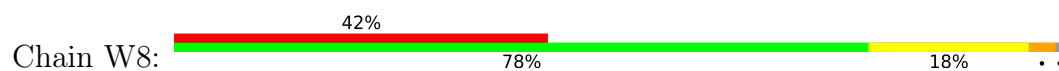
• Molecule 8: Allophycocyanin subunit beta

Chain T8: 

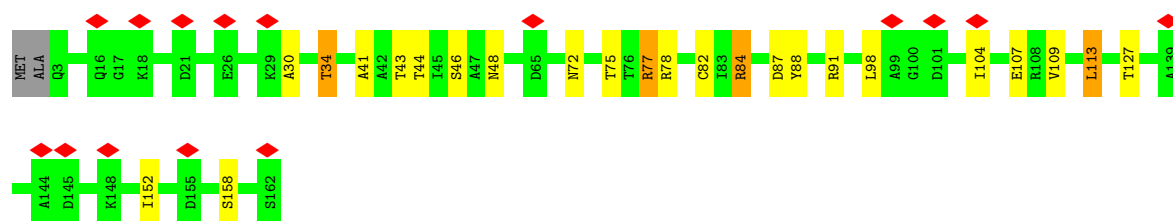
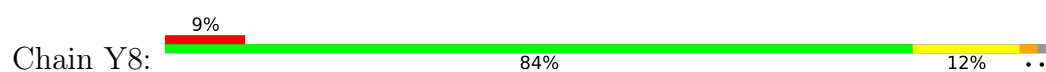




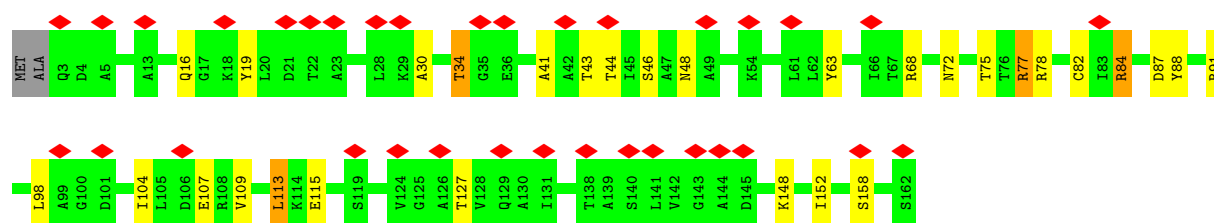
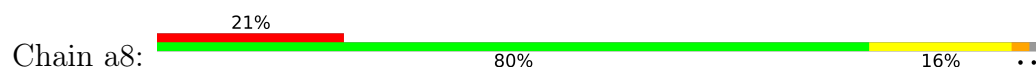
• Molecule 8: Allophycocyanin subunit beta



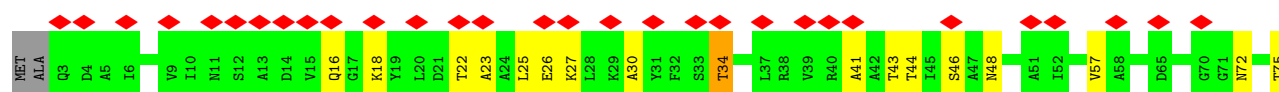
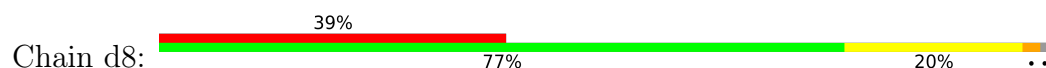
• Molecule 8: Allophycocyanin subunit beta

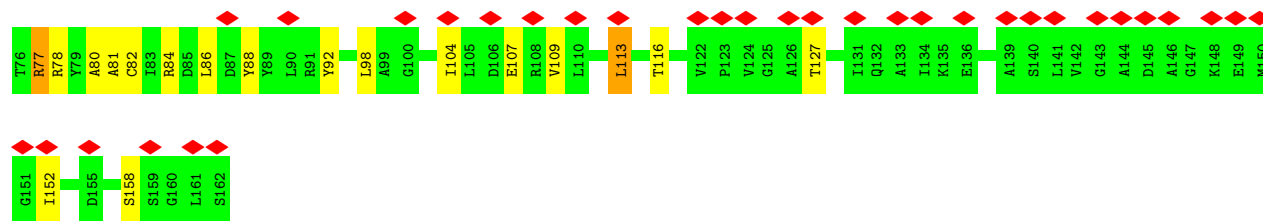


• Molecule 8: Allophycocyanin subunit beta

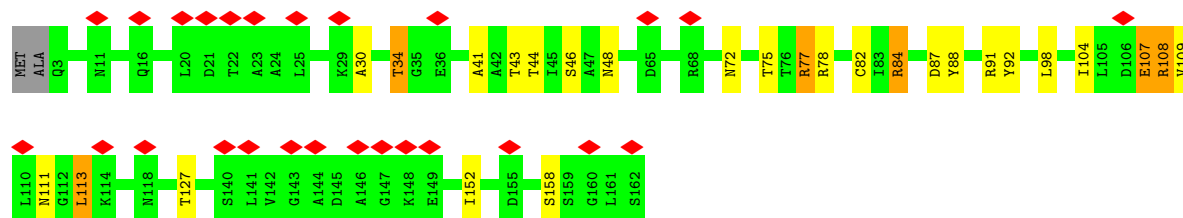
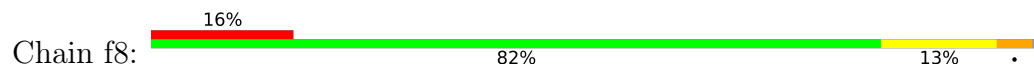


• Molecule 8: Allophycocyanin subunit beta

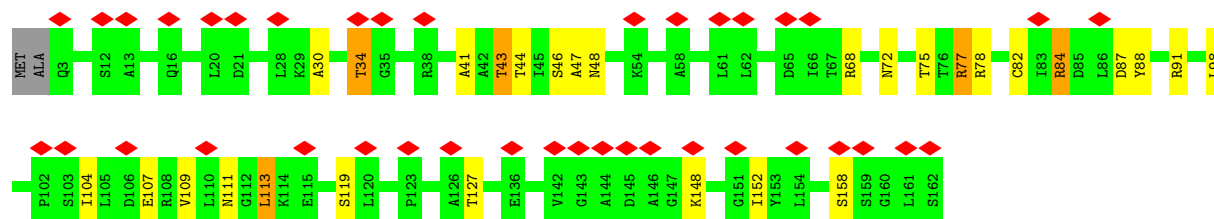
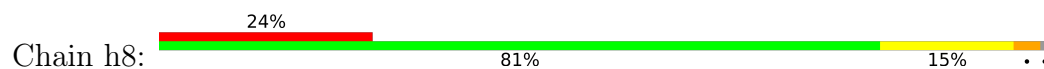




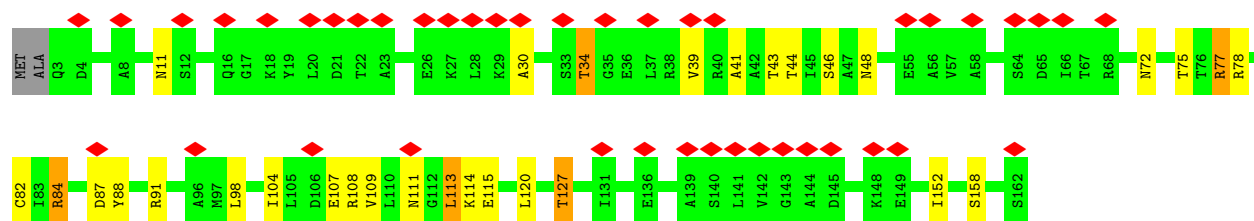
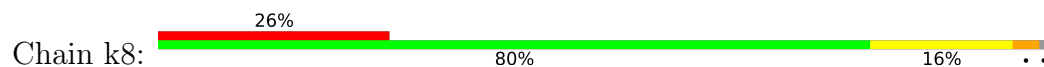
• Molecule 8: Allophycocyanin subunit beta



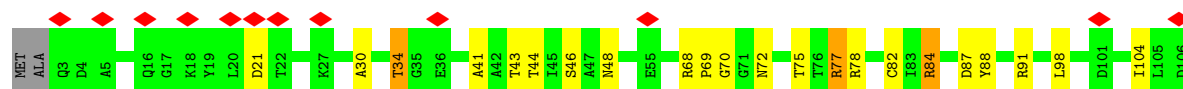
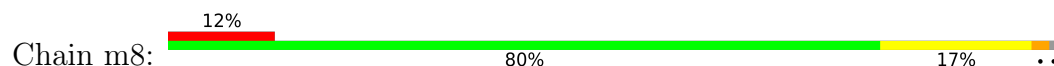
• Molecule 8: Allophycocyanin subunit beta

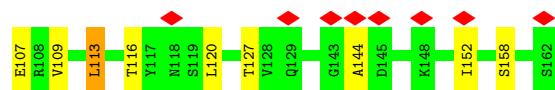


• Molecule 8: Allophycocyanin subunit beta

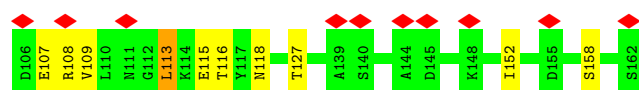
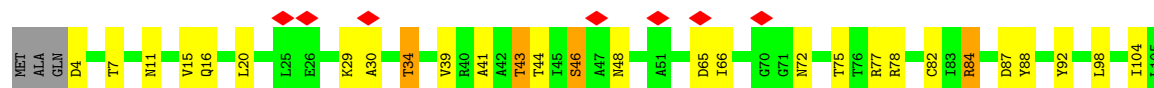
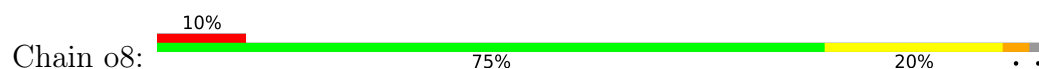


• Molecule 8: Allophycocyanin subunit beta

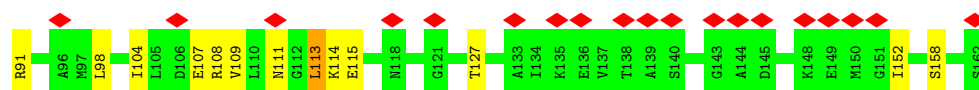
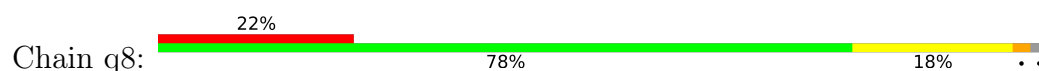




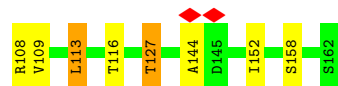
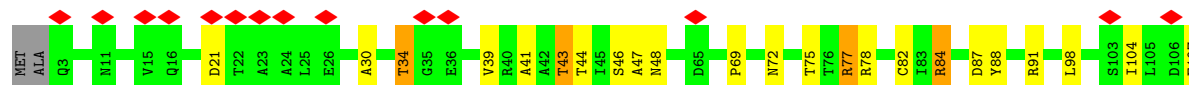
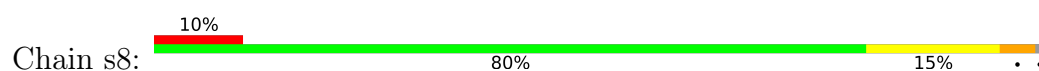
- Molecule 8: Allophycocyanin subunit beta



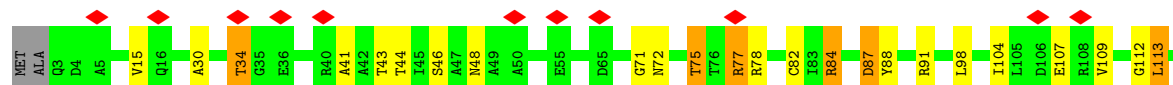
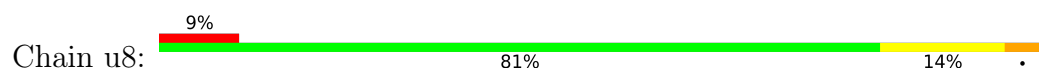
- Molecule 8: Allophycocyanin subunit beta



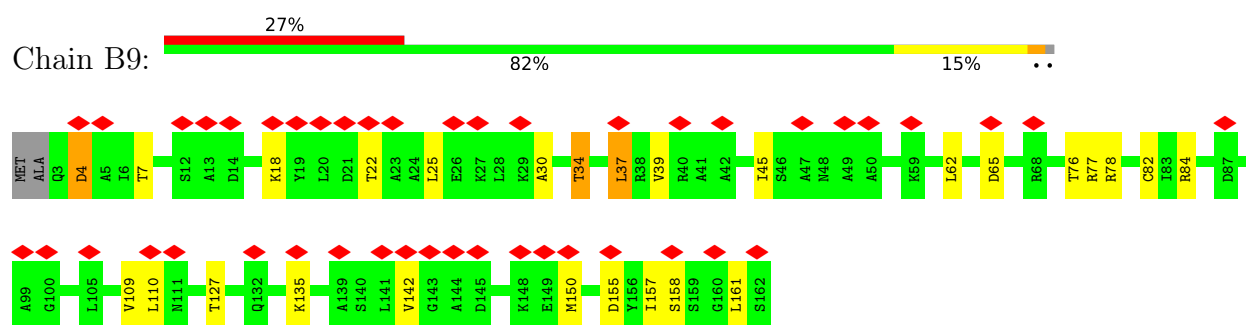
- Molecule 8: Allophycocyanin subunit beta



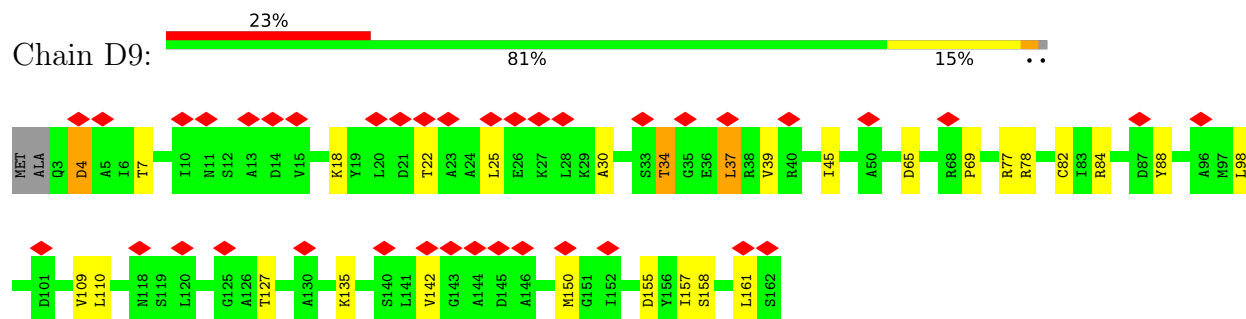
- Molecule 8: Allophycocyanin subunit beta



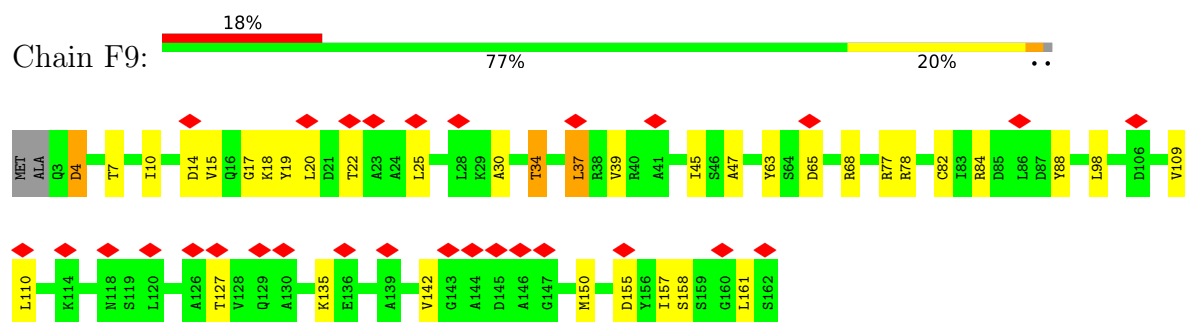
- Molecule 8: Allophycocyanin subunit beta



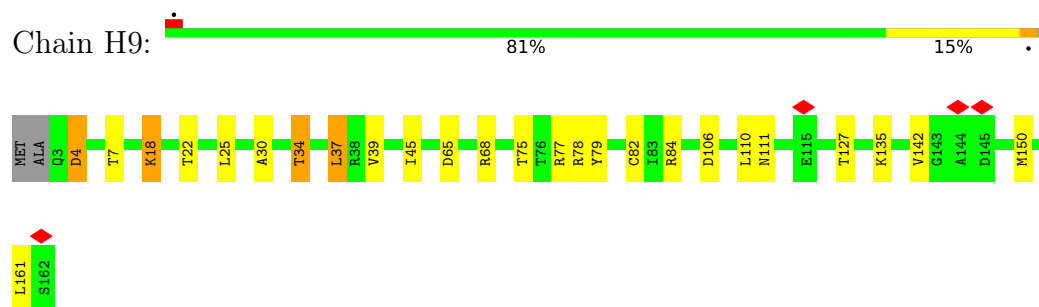
- Molecule 8: Allophycocyanin subunit beta



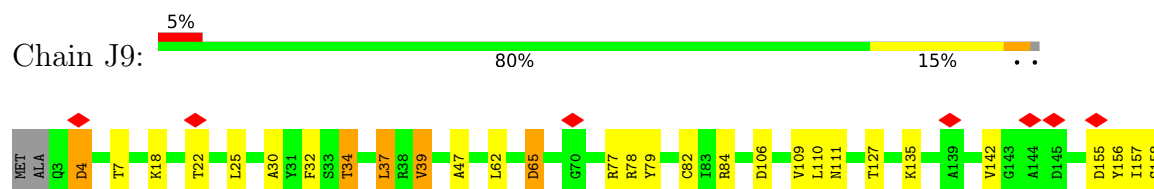
- Molecule 8: Allophycocyanin subunit beta



- Molecule 8: Allophycocyanin subunit beta

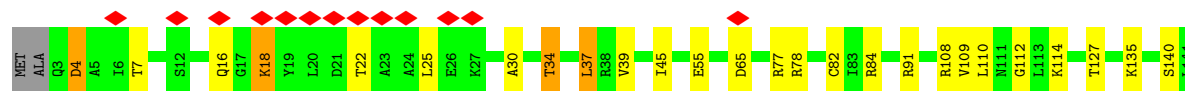
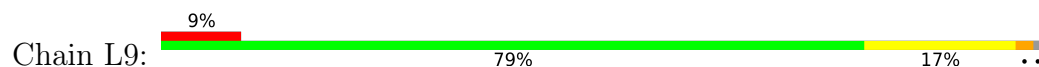


- Molecule 8: Allophycocyanin subunit beta

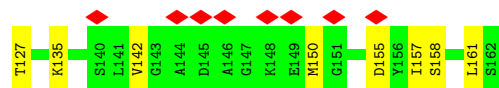
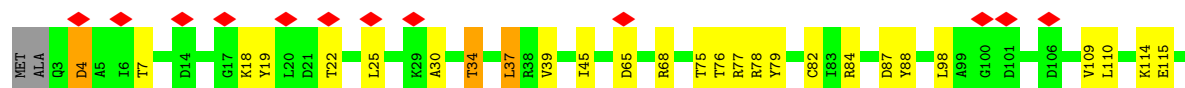
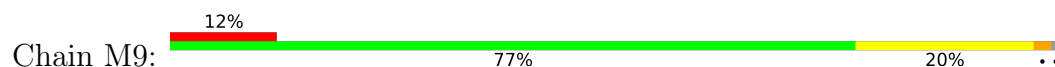




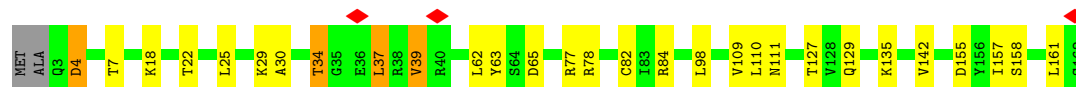
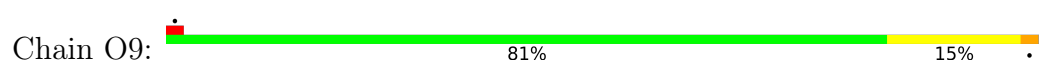
- Molecule 8: Allophycocyanin subunit beta



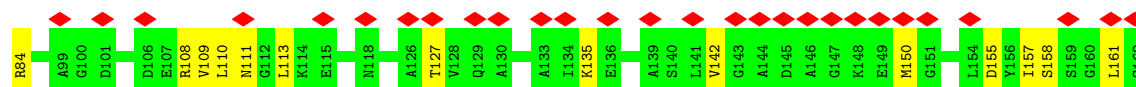
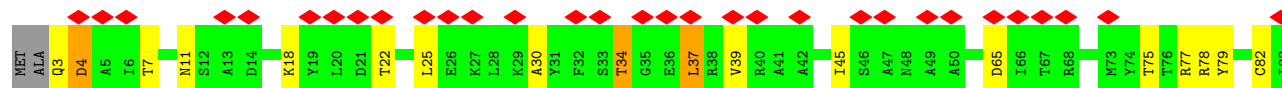
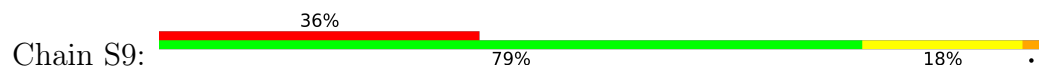
- Molecule 8: Allophycocyanin subunit beta



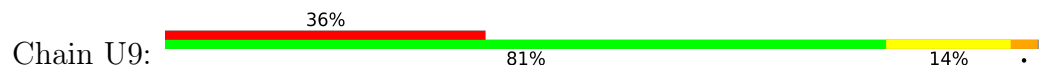
- Molecule 8: Allophycocyanin subunit beta

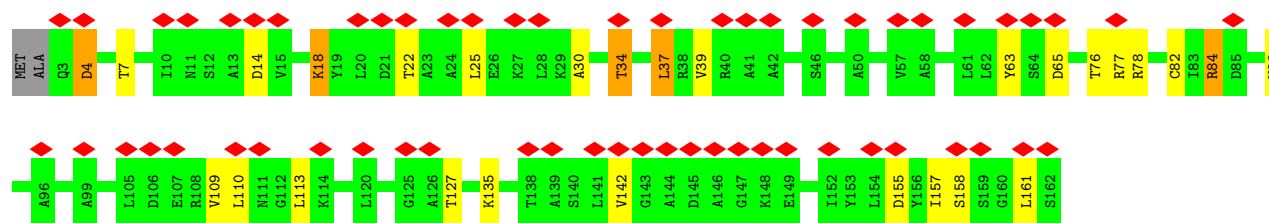


- Molecule 8: Allophycocyanin subunit beta

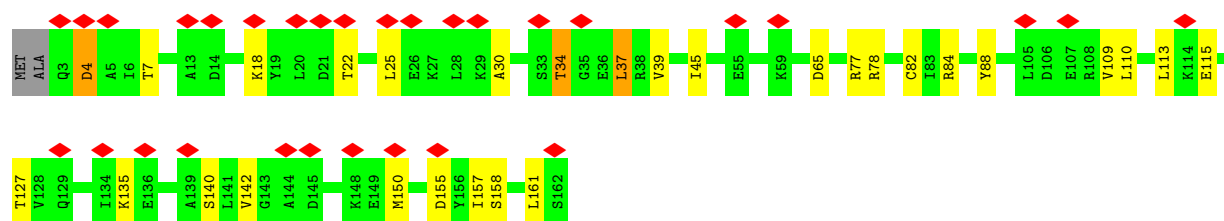
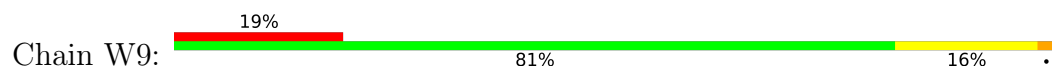


- Molecule 8: Allophycocyanin subunit beta

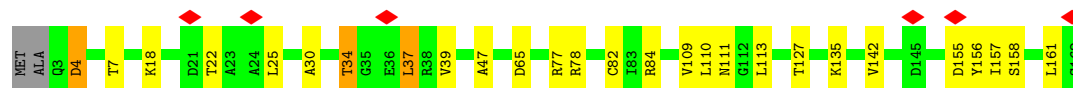
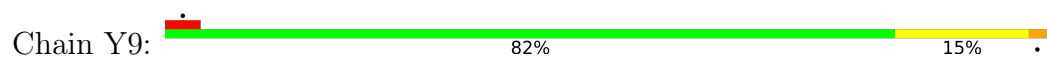




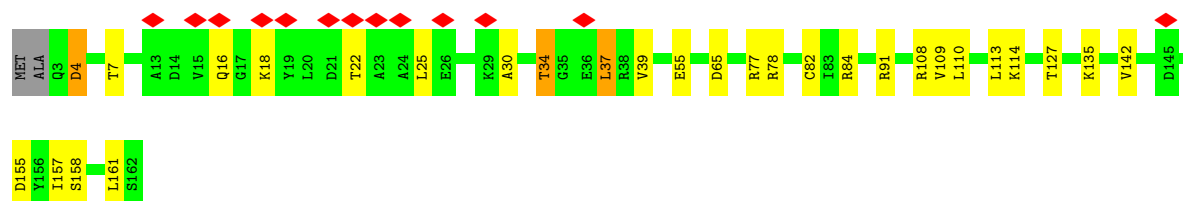
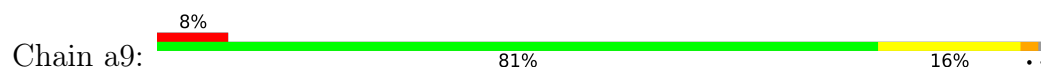
• Molecule 8: Allophycocyanin subunit beta



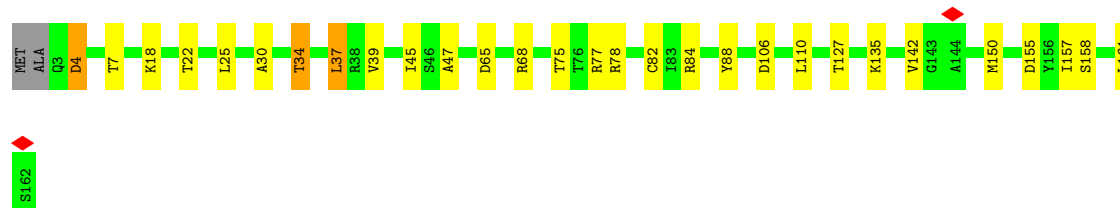
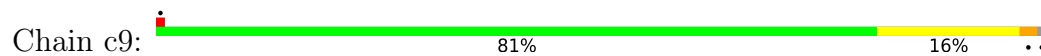
• Molecule 8: Allophycocyanin subunit beta



• Molecule 8: Allophycocyanin subunit beta



• Molecule 8: Allophycocyanin subunit beta



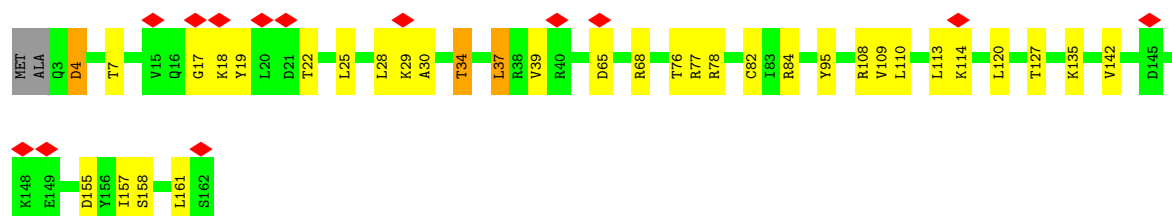
• Molecule 8: Allophycocyanin subunit beta

Chain e9:  80% 17% ..



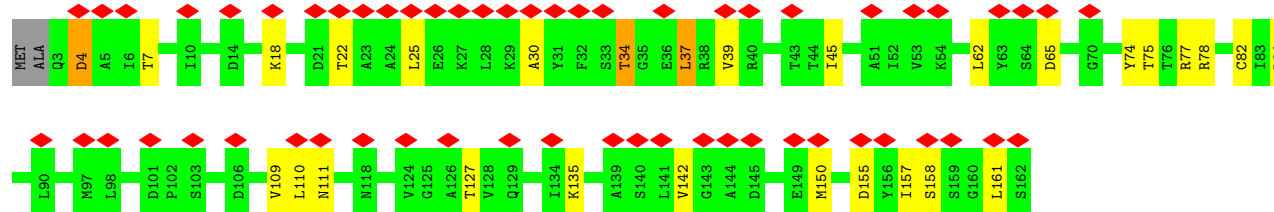
- Molecule 8: Allophycocyanin subunit beta

Chain h9:  8% 78% 19% ..



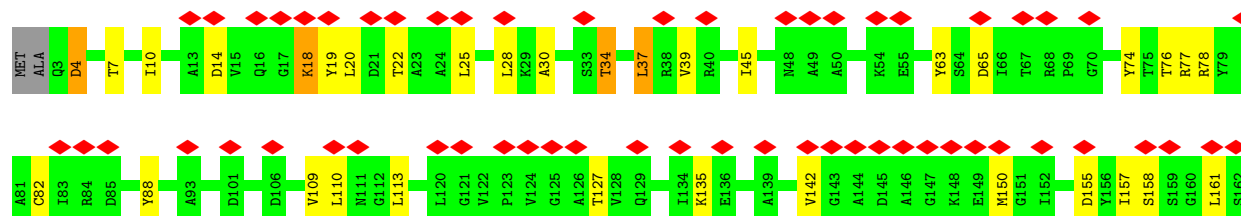
- Molecule 8: Allophycocyanin subunit beta

Chain j9:  35% 81% 16% ..



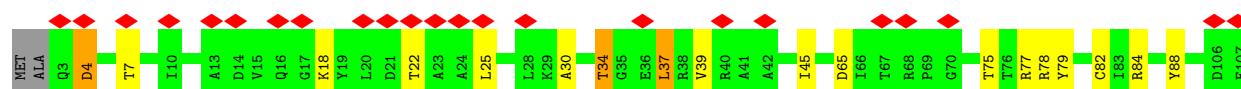
- Molecule 8: Allophycocyanin subunit beta

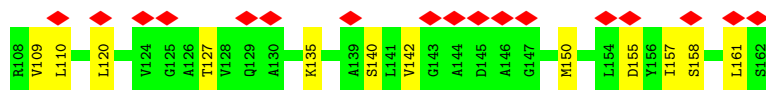
Chain i9:  35% 78% 19% ..



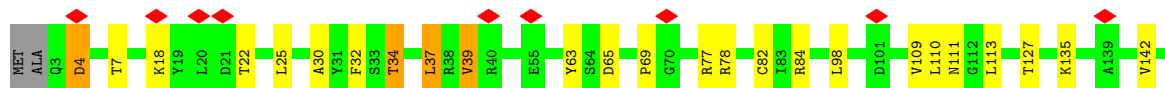
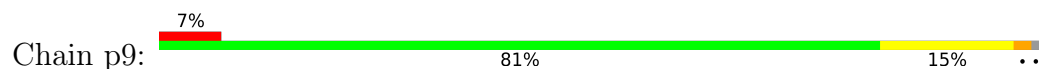
- Molecule 8: Allophycocyanin subunit beta

Chain n9:  25% 80% 17% ..

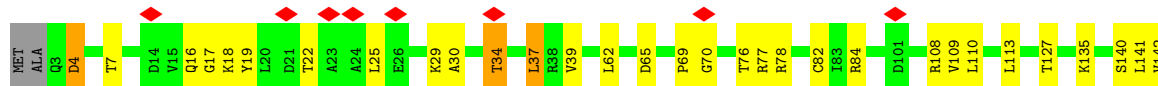
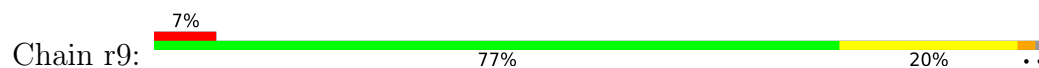




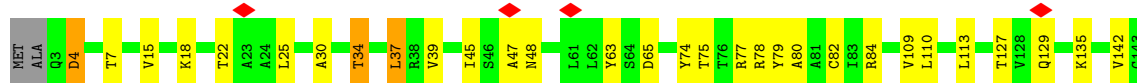
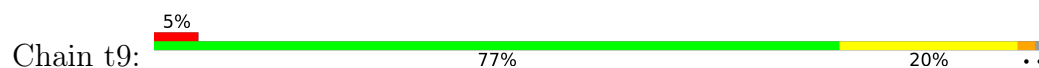
- Molecule 8: Allophycocyanin subunit beta



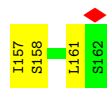
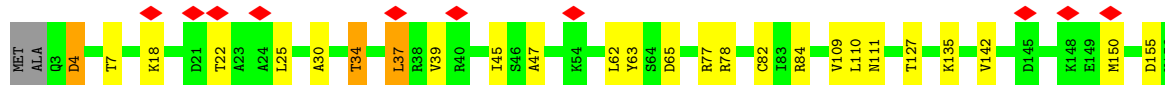
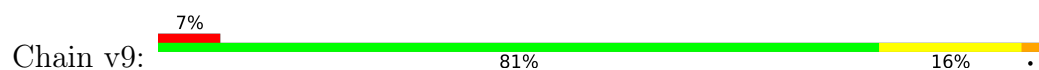
- Molecule 8: Allophycocyanin subunit beta



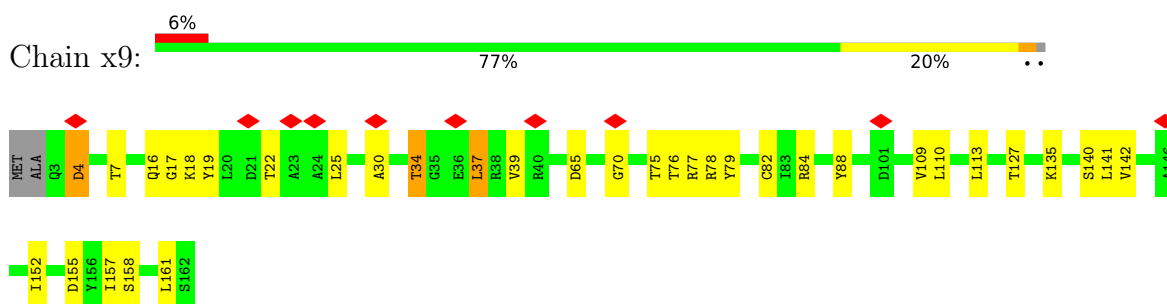
- Molecule 8: Allophycocyanin subunit beta



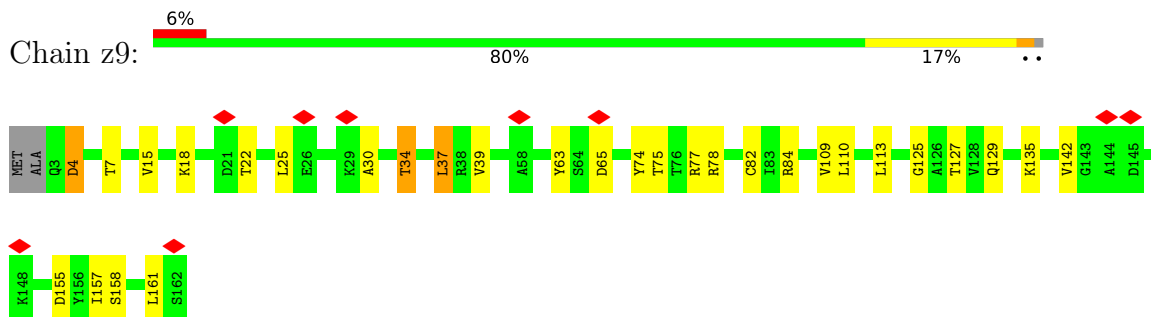
- Molecule 8: Allophycocyanin subunit beta



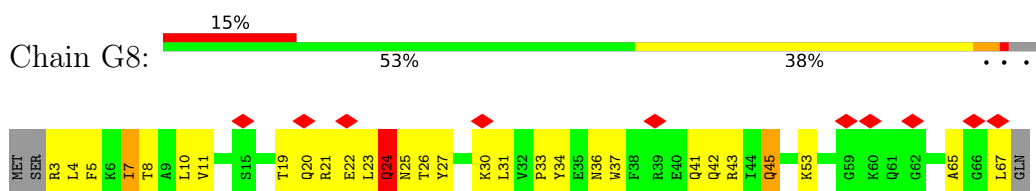
- Molecule 8: Allophycocyanin subunit beta



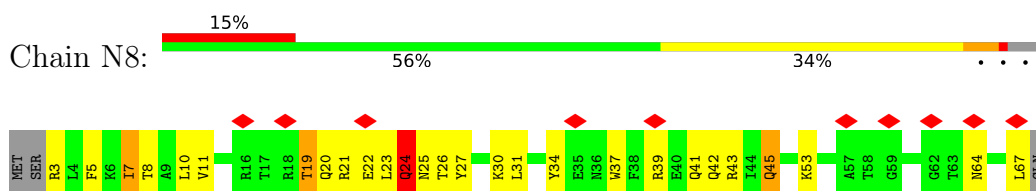
- Molecule 8: Allophycocyanin subunit beta



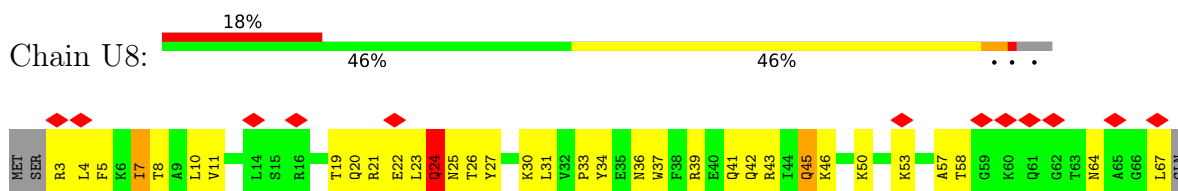
- Molecule 9: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core



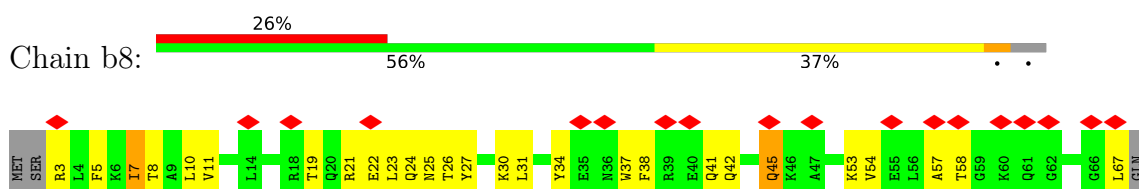
- Molecule 9: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core



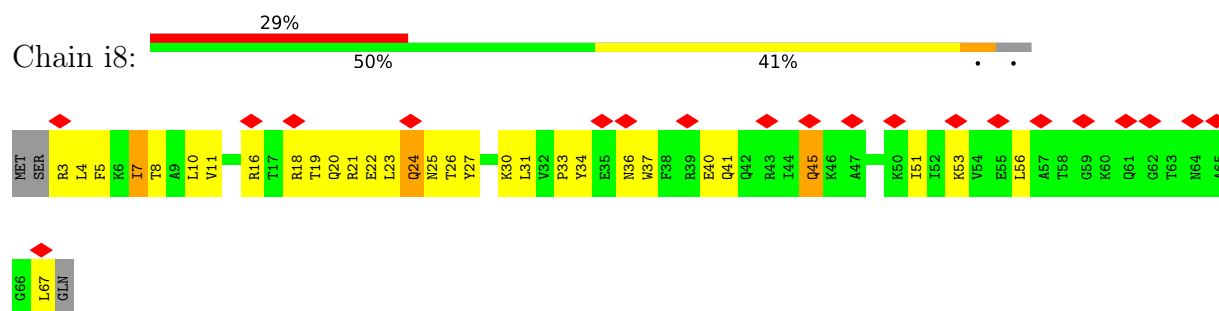
- Molecule 9: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core



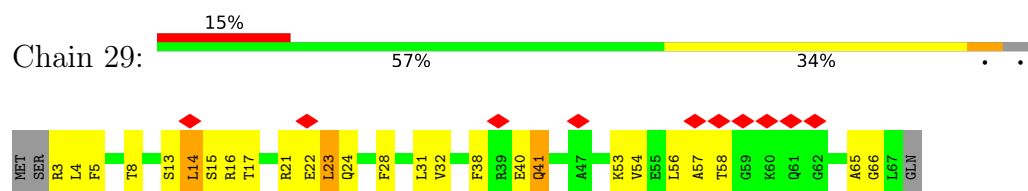
- Molecule 9: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core



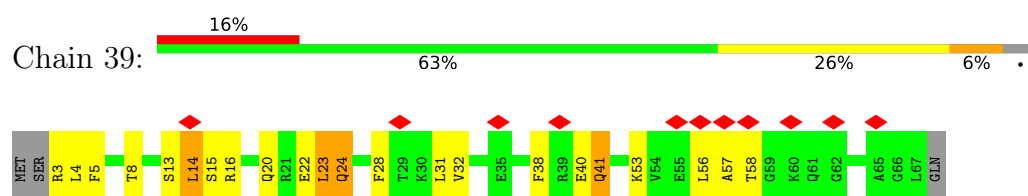
- Molecule 9: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core



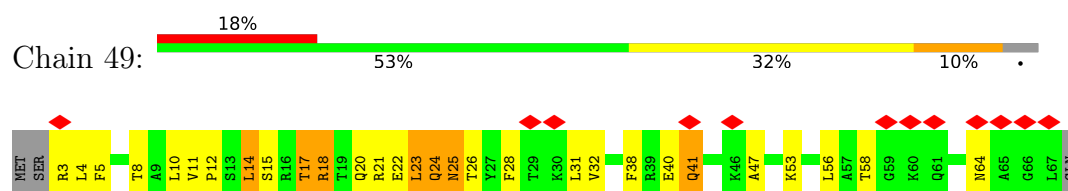
- Molecule 9: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core



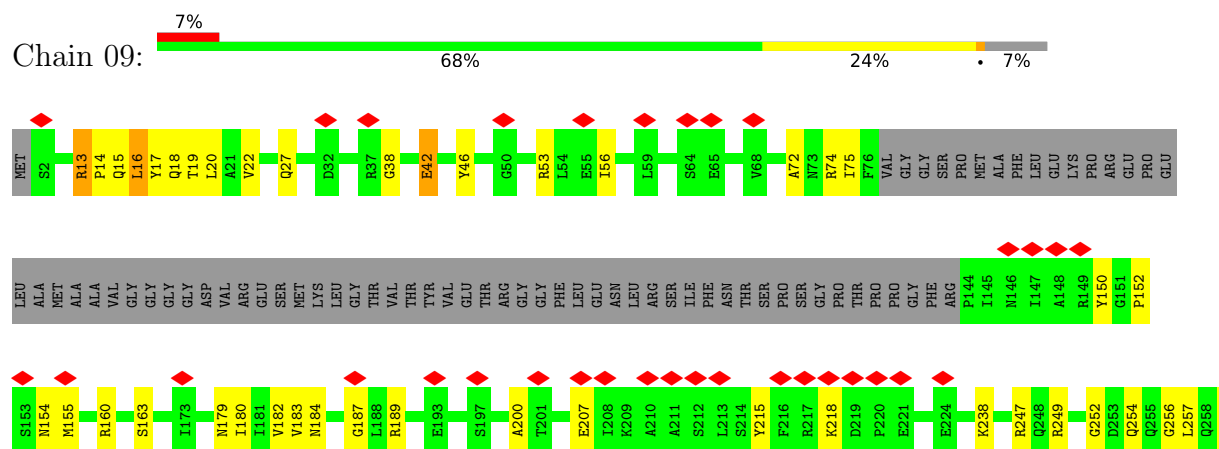
- Molecule 9: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core

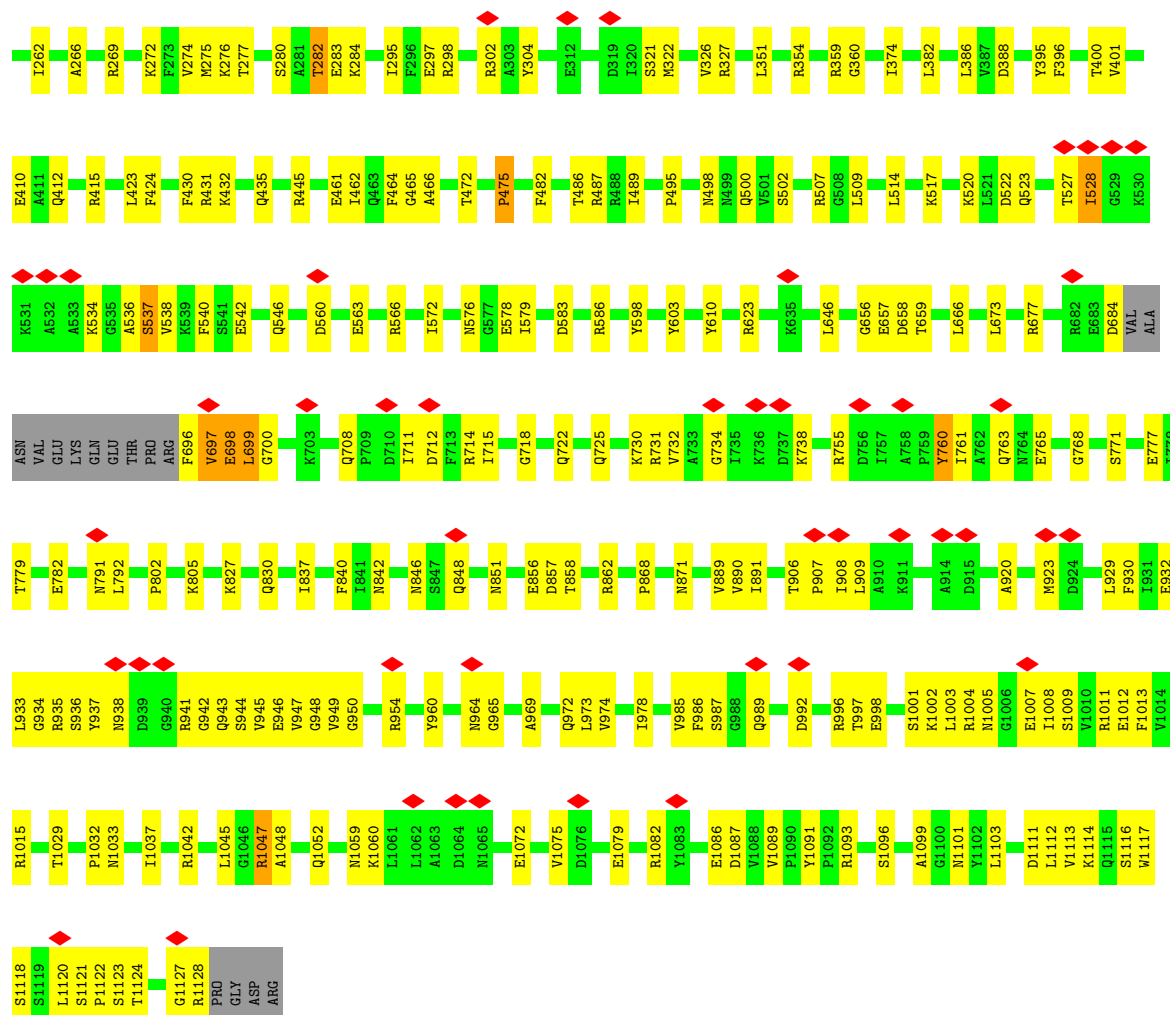


- Molecule 9: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core

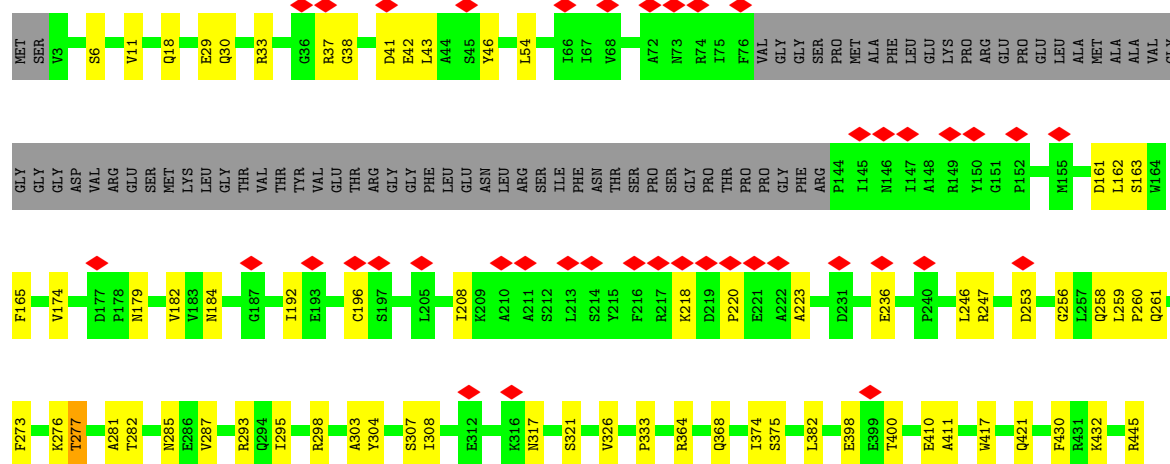


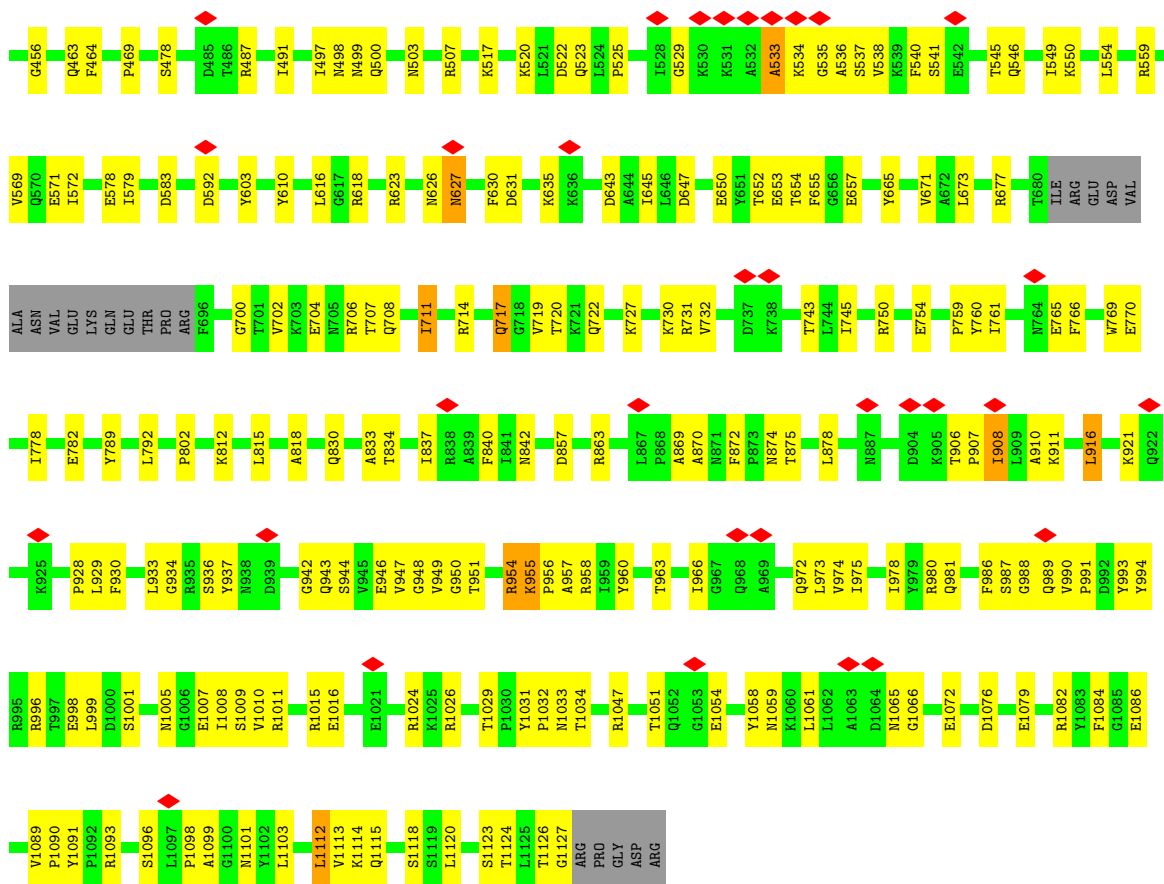
- Molecule 10: Phycobiliprotein ApcE



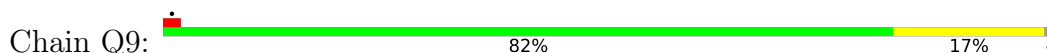


• Molecule 10: Phycobiliprotein ApcE

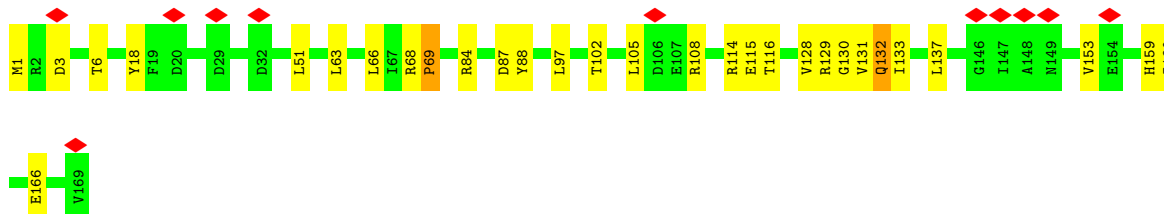
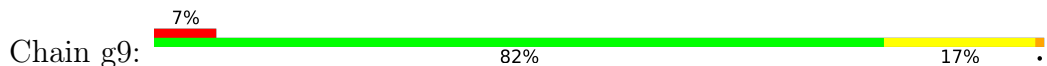




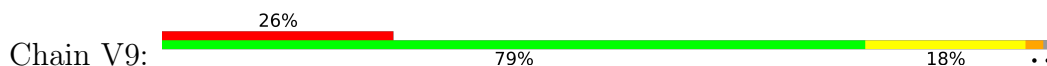
• Molecule 11: Allophycocyanin subunit beta-18

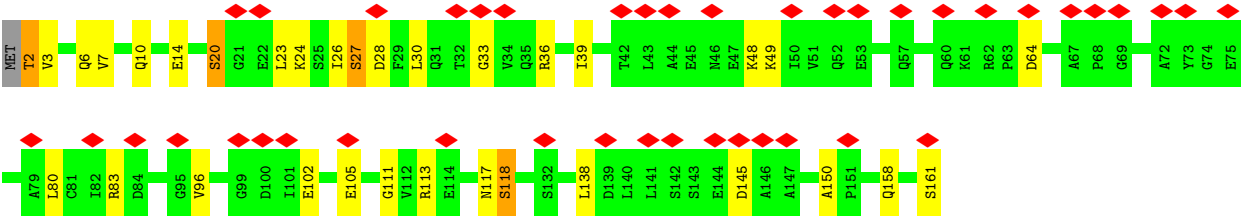


• Molecule 11: Allophycocyanin subunit beta-18

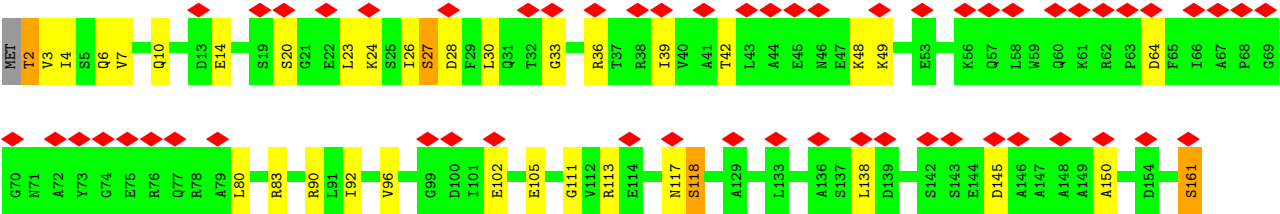
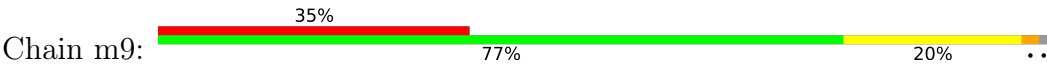


• Molecule 12: Allophycocyanin subunit alpha-B





• Molecule 12: Allophycocyanin subunit alpha-B



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

5.1 Standard geometry

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	0.39	0/1814	0.80	4/2452 (0.2%)
1	A4	0.39	0/1814	0.80	4/2452 (0.2%)
2	B1	0.25	0/1246	0.52	0/1693
2	B2	0.31	0/1246	0.54	0/1693
2	B3	0.32	0/1246	0.54	0/1693
2	B4	0.25	0/1246	0.52	0/1693
2	B5	0.30	0/1246	0.49	0/1693
2	B6	0.31	0/1246	0.54	0/1693
2	B7	0.32	0/1246	0.54	0/1693
2	BA	0.30	0/1246	0.49	0/1693
2	D1	0.25	0/1246	0.52	0/1693
2	D2	0.31	0/1246	0.56	0/1693
2	D3	0.32	0/1246	0.56	0/1693
2	D4	0.25	0/1246	0.52	0/1693
2	D5	0.30	0/1246	0.50	0/1693
2	D6	0.31	0/1246	0.56	0/1693
2	D7	0.32	0/1246	0.56	0/1693
2	DA	0.30	0/1246	0.50	0/1693
2	F1	0.25	0/1246	0.51	0/1693
2	F2	0.31	0/1246	0.55	0/1693
2	F3	0.32	0/1246	0.55	0/1693
2	F4	0.25	0/1246	0.51	0/1693
2	F5	0.30	0/1246	0.50	0/1693
2	F6	0.31	0/1246	0.55	0/1693
2	F7	0.32	0/1246	0.55	0/1693
2	FA	0.30	0/1246	0.50	0/1693
2	H1	0.25	0/1246	0.53	0/1693
2	H2	0.31	0/1246	0.54	0/1693
2	H3	0.32	0/1246	0.54	0/1693
2	H4	0.25	0/1246	0.53	0/1693
2	H5	0.30	0/1246	0.52	0/1693
2	H6	0.31	0/1246	0.54	0/1693

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	H7	0.32	0/1246	0.54	0/1693
2	HA	0.30	0/1246	0.52	0/1693
2	J1	0.25	0/1246	0.51	0/1693
2	J2	0.32	0/1246	0.54	0/1693
2	J3	0.32	0/1246	0.55	0/1693
2	J4	0.25	0/1246	0.51	0/1693
2	J5	0.30	0/1246	0.50	0/1693
2	J6	0.32	0/1246	0.54	0/1693
2	J7	0.32	0/1246	0.55	0/1693
2	JA	0.30	0/1246	0.50	0/1693
2	L1	0.26	0/1246	0.56	0/1693
2	L2	0.31	0/1246	0.60	2/1693 (0.1%)
2	L3	0.31	0/1246	0.60	2/1693 (0.1%)
2	L4	0.26	0/1246	0.56	0/1693
2	L5	0.30	0/1246	0.51	0/1693
2	L6	0.31	0/1246	0.60	2/1693 (0.1%)
2	L7	0.31	0/1246	0.60	2/1693 (0.1%)
2	LA	0.30	0/1246	0.51	0/1693
2	O1	0.25	0/1246	0.52	0/1693
2	O2	0.31	0/1246	0.55	0/1693
2	O4	0.25	0/1246	0.52	0/1693
2	O5	0.30	0/1246	0.51	0/1693
2	O6	0.31	0/1246	0.55	0/1693
2	OA	0.30	0/1246	0.51	0/1693
2	Q1	0.25	0/1246	0.52	0/1693
2	Q2	0.31	0/1246	0.60	2/1693 (0.1%)
2	Q4	0.25	0/1246	0.52	0/1693
2	Q5	0.30	0/1246	0.52	0/1693
2	Q6	0.31	0/1246	0.61	2/1693 (0.1%)
2	QA	0.30	0/1246	0.52	0/1693
2	S1	0.25	0/1246	0.51	0/1693
2	S2	0.32	0/1246	0.64	3/1693 (0.2%)
2	S4	0.25	0/1246	0.51	0/1693
2	S5	0.30	0/1246	0.50	0/1693
2	S6	0.32	0/1246	0.64	3/1693 (0.2%)
2	SA	0.30	0/1246	0.50	0/1693
2	U1	0.25	0/1246	0.53	0/1693
2	U2	0.31	0/1246	0.53	0/1693
2	U4	0.25	0/1246	0.53	0/1693
2	U5	0.30	0/1246	0.50	0/1693
2	U6	0.31	0/1246	0.53	0/1693
2	UA	0.30	0/1246	0.50	0/1693
2	W1	0.25	0/1246	0.52	0/1693

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	W2	0.31	0/1246	0.53	0/1693
2	W4	0.25	0/1246	0.52	0/1693
2	W5	0.30	0/1246	0.51	0/1693
2	W6	0.31	0/1246	0.53	0/1693
2	WA	0.30	0/1246	0.51	0/1693
2	Y1	0.25	0/1246	0.51	0/1693
2	Y2	0.31	0/1246	0.54	0/1693
2	Y4	0.25	0/1246	0.51	0/1693
2	Y5	0.30	0/1246	0.51	0/1693
2	Y6	0.31	0/1246	0.54	0/1693
2	YA	0.30	0/1246	0.51	0/1693
3	C1	0.30	0/1290	0.65	1/1748 (0.1%)
3	C2	0.41	0/1290	0.77	2/1748 (0.1%)
3	C3	0.41	0/1290	0.77	2/1748 (0.1%)
3	C4	0.29	0/1290	0.65	1/1748 (0.1%)
3	C5	0.40	0/1290	0.79	4/1748 (0.2%)
3	C6	0.41	0/1290	0.77	2/1748 (0.1%)
3	C7	0.41	0/1290	0.77	2/1748 (0.1%)
3	CA	0.40	0/1290	0.80	4/1748 (0.2%)
3	E1	0.29	0/1290	0.61	0/1748
3	E2	0.39	0/1298	0.75	1/1758 (0.1%)
3	E3	0.40	0/1298	0.76	1/1758 (0.1%)
3	E4	0.29	0/1290	0.61	1/1748 (0.1%)
3	E5	0.41	0/1290	0.79	4/1748 (0.2%)
3	E6	0.39	0/1298	0.76	1/1758 (0.1%)
3	E7	0.39	0/1298	0.76	1/1758 (0.1%)
3	EA	0.41	0/1290	0.78	4/1748 (0.2%)
3	G1	0.29	0/1290	0.61	1/1748 (0.1%)
3	G2	0.42	0/1298	0.79	3/1758 (0.2%)
3	G3	0.42	0/1298	0.79	3/1758 (0.2%)
3	G4	0.29	0/1290	0.60	1/1748 (0.1%)
3	G5	0.40	0/1290	0.79	4/1748 (0.2%)
3	G6	0.42	0/1298	0.79	3/1758 (0.2%)
3	G7	0.42	0/1298	0.79	3/1758 (0.2%)
3	GA	0.41	0/1290	0.79	4/1748 (0.2%)
3	I1	0.29	0/1298	0.65	0/1758
3	I2	0.43	0/1298	0.77	2/1758 (0.1%)
3	I3	0.44	0/1298	0.77	2/1758 (0.1%)
3	I4	0.29	0/1298	0.65	1/1758 (0.1%)
3	I5	0.40	0/1290	0.83	7/1748 (0.4%)
3	I6	0.43	0/1298	0.77	2/1758 (0.1%)
3	I7	0.44	0/1298	0.77	2/1758 (0.1%)
3	IA	0.40	0/1290	0.83	7/1748 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	K1	0.30	0/1290	0.64	1/1748 (0.1%)
3	K2	0.42	0/1290	0.78	1/1748 (0.1%)
3	K3	0.42	0/1290	0.78	1/1748 (0.1%)
3	K4	0.30	0/1290	0.64	1/1748 (0.1%)
3	K5	0.41	0/1290	0.81	4/1748 (0.2%)
3	K6	0.42	0/1290	0.78	1/1748 (0.1%)
3	K7	0.42	0/1290	0.78	1/1748 (0.1%)
3	KA	0.41	0/1290	0.81	4/1748 (0.2%)
3	M1	0.27	0/1290	0.63	2/1748 (0.1%)
3	M2	0.42	0/1290	0.89	3/1748 (0.2%)
3	M3	0.43	0/1290	0.89	3/1748 (0.2%)
3	M4	0.27	0/1290	0.63	2/1748 (0.1%)
3	M5	0.41	0/1290	0.82	6/1748 (0.3%)
3	M6	0.42	0/1290	0.89	3/1748 (0.2%)
3	M7	0.42	0/1290	0.89	3/1748 (0.2%)
3	MA	0.41	0/1290	0.82	6/1748 (0.3%)
3	P1	0.29	0/1290	0.62	1/1748 (0.1%)
3	P2	0.39	0/1290	0.90	4/1748 (0.2%)
3	P4	0.29	0/1290	0.62	1/1748 (0.1%)
3	P5	0.41	0/1290	0.81	6/1748 (0.3%)
3	P6	0.39	0/1290	0.90	4/1748 (0.2%)
3	PA	0.41	0/1290	0.81	6/1748 (0.3%)
3	R1	0.26	0/1290	0.58	1/1748 (0.1%)
3	R2	0.40	0/1290	0.77	3/1748 (0.2%)
3	R4	0.26	0/1290	0.58	1/1748 (0.1%)
3	R5	0.41	0/1290	0.78	4/1748 (0.2%)
3	R6	0.40	0/1290	0.77	3/1748 (0.2%)
3	RA	0.41	0/1290	0.78	4/1748 (0.2%)
3	T1	0.27	0/1290	0.63	0/1748
3	T2	0.43	0/1290	0.84	4/1748 (0.2%)
3	T4	0.27	0/1290	0.63	0/1748
3	T5	0.41	0/1290	0.80	5/1748 (0.3%)
3	T6	0.43	0/1290	0.84	4/1748 (0.2%)
3	TA	0.41	0/1290	0.80	5/1748 (0.3%)
3	V1	0.29	0/1290	0.61	0/1748
3	V2	0.44	0/1290	0.83	6/1748 (0.3%)
3	V4	0.29	0/1290	0.61	0/1748
3	V5	0.41	0/1290	0.79	4/1748 (0.2%)
3	V6	0.44	0/1290	0.83	6/1748 (0.3%)
3	VA	0.41	0/1290	0.79	4/1748 (0.2%)
3	X1	0.27	0/1290	0.59	1/1748 (0.1%)
3	X2	0.43	0/1290	0.87	4/1748 (0.2%)
3	X4	0.27	0/1290	0.59	1/1748 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	X5	0.40	0/1290	0.80	4/1748 (0.2%)
3	X6	0.43	0/1290	0.87	4/1748 (0.2%)
3	XA	0.40	0/1290	0.79	4/1748 (0.2%)
3	Z1	0.26	0/1290	0.60	0/1748
3	Z2	0.39	0/1290	0.79	2/1748 (0.1%)
3	Z4	0.26	0/1290	0.60	0/1748
3	Z5	0.41	0/1290	0.87	7/1748 (0.4%)
3	Z6	0.39	0/1290	0.79	2/1748 (0.1%)
3	ZA	0.41	0/1290	0.87	7/1748 (0.4%)
4	N1	0.41	0/2311	0.83	10/3123 (0.3%)
4	N2	0.47	0/2311	0.79	3/3123 (0.1%)
4	N3	0.52	0/451	0.94	1/608 (0.2%)
4	N4	0.40	0/2311	0.83	10/3123 (0.3%)
4	N5	0.45	0/2311	0.80	1/3123 (0.0%)
4	N6	0.47	0/2311	0.79	3/3123 (0.1%)
4	N7	0.52	0/451	0.95	1/608 (0.2%)
4	NA	0.45	0/2311	0.80	1/3123 (0.0%)
5	A2	0.41	0/2081	0.81	9/2810 (0.3%)
5	A5	0.40	0/1985	0.82	7/2679 (0.3%)
5	A6	0.40	0/2081	0.78	9/2810 (0.3%)
5	AA	0.39	0/1985	0.82	6/2679 (0.2%)
6	A3	0.31	0/1147	0.99	8/1549 (0.5%)
6	A7	0.31	0/1147	0.97	7/1549 (0.5%)
7	A8	0.33	0/1219	0.88	4/1650 (0.2%)
7	A9	0.30	0/1219	0.78	3/1650 (0.2%)
7	C8	0.33	0/1219	0.88	4/1650 (0.2%)
7	C9	0.31	0/1219	0.79	3/1650 (0.2%)
7	E8	0.33	0/1219	0.88	4/1650 (0.2%)
7	E9	0.30	0/1219	0.78	3/1650 (0.2%)
7	G9	0.30	0/1219	0.78	3/1650 (0.2%)
7	H8	0.33	0/1219	0.88	4/1650 (0.2%)
7	I9	0.30	0/1219	0.78	3/1650 (0.2%)
7	J8	0.33	0/1219	0.88	4/1650 (0.2%)
7	K9	0.30	0/1219	0.78	3/1650 (0.2%)
7	L8	0.33	0/1219	0.88	4/1650 (0.2%)
7	N9	0.30	0/1219	0.78	3/1650 (0.2%)
7	O8	0.33	0/1219	0.87	4/1650 (0.2%)
7	P9	0.30	0/1219	0.78	3/1650 (0.2%)
7	Q8	0.33	0/1219	0.88	4/1650 (0.2%)
7	R9	0.30	0/1219	0.78	3/1650 (0.2%)
7	S8	0.33	0/1219	0.87	4/1650 (0.2%)
7	T9	0.30	0/1219	0.78	3/1650 (0.2%)
7	V8	0.33	0/1219	0.88	4/1650 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
7	X8	0.33	0/1219	0.88	4/1650 (0.2%)
7	X9	0.30	0/1219	0.78	3/1650 (0.2%)
7	Z8	0.33	0/1219	0.88	4/1650 (0.2%)
7	Z9	0.30	0/1219	0.78	3/1650 (0.2%)
7	b9	0.30	0/1219	0.78	3/1650 (0.2%)
7	c8	0.33	0/1219	0.88	4/1650 (0.2%)
7	d9	0.30	0/1219	0.79	3/1650 (0.2%)
7	e8	0.33	0/1219	0.88	4/1650 (0.2%)
7	f9	0.30	0/1219	0.78	3/1650 (0.2%)
7	g8	0.33	0/1219	0.87	4/1650 (0.2%)
7	i9	0.30	0/1219	0.78	3/1650 (0.2%)
7	j8	0.33	0/1219	0.88	4/1650 (0.2%)
7	k9	0.30	0/1219	0.78	3/1650 (0.2%)
7	l8	0.33	0/1219	0.88	4/1650 (0.2%)
7	n8	0.33	0/1219	0.88	4/1650 (0.2%)
7	o9	0.30	0/1219	0.78	3/1650 (0.2%)
7	p8	0.33	0/1219	0.86	4/1650 (0.2%)
7	q9	0.30	0/1219	0.78	3/1650 (0.2%)
7	r8	0.33	0/1219	0.88	4/1650 (0.2%)
7	s9	0.30	0/1219	0.78	3/1650 (0.2%)
7	t8	0.33	0/1219	0.88	4/1650 (0.2%)
7	u9	0.30	0/1219	0.78	3/1650 (0.2%)
7	w9	0.30	0/1219	0.78	3/1650 (0.2%)
7	y9	0.30	0/1219	0.78	3/1650 (0.2%)
8	B8	0.32	0/1216	0.89	6/1650 (0.4%)
8	B9	0.31	0/1216	0.55	0/1650
8	D8	0.32	0/1216	0.89	6/1650 (0.4%)
8	D9	0.31	0/1216	0.55	0/1650
8	F8	0.32	0/1216	0.89	6/1650 (0.4%)
8	F9	0.31	0/1216	0.55	0/1650
8	H9	0.31	0/1216	0.55	0/1650
8	I8	0.32	0/1216	0.89	6/1650 (0.4%)
8	J9	0.31	0/1216	0.55	0/1650
8	K8	0.32	0/1216	0.89	6/1650 (0.4%)
8	L9	0.31	0/1216	0.55	0/1650
8	M8	0.32	0/1216	0.89	6/1650 (0.4%)
8	M9	0.31	0/1216	0.55	0/1650
8	O9	0.31	0/1216	0.55	0/1650
8	P8	0.32	0/1207	0.89	6/1638 (0.4%)
8	R8	0.32	0/1216	0.89	6/1650 (0.4%)
8	S9	0.31	0/1216	0.55	0/1650
8	T8	0.32	0/1216	0.89	6/1650 (0.4%)
8	U9	0.31	0/1216	0.55	0/1650

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
8	W8	0.31	0/1216	0.89	6/1650 (0.4%)
8	W9	0.31	0/1216	0.55	0/1650
8	Y8	0.32	0/1216	0.89	6/1650 (0.4%)
8	Y9	0.31	0/1216	0.55	0/1650
8	a8	0.32	0/1216	0.89	6/1650 (0.4%)
8	a9	0.31	0/1216	0.55	0/1650
8	c9	0.31	0/1216	0.55	0/1650
8	d8	0.29	0/1216	0.75	3/1650 (0.2%)
8	e9	0.31	0/1216	0.55	0/1650
8	f8	0.33	0/1216	0.91	7/1650 (0.4%)
8	h8	0.32	0/1216	0.89	6/1650 (0.4%)
8	h9	0.31	0/1216	0.55	0/1650
8	j9	0.31	0/1216	0.55	0/1650
8	k8	0.32	0/1216	0.89	6/1650 (0.4%)
8	l9	0.31	0/1216	0.55	0/1650
8	m8	0.32	0/1216	0.89	6/1650 (0.4%)
8	n9	0.31	0/1216	0.55	0/1650
8	o8	0.31	0/1207	0.76	3/1638 (0.2%)
8	p9	0.31	0/1216	0.55	0/1650
8	q8	0.32	0/1207	0.89	6/1638 (0.4%)
8	r9	0.31	0/1216	0.55	0/1650
8	s8	0.32	0/1216	0.89	6/1650 (0.4%)
8	t9	0.31	0/1216	0.55	0/1650
8	u8	0.32	0/1216	0.89	6/1650 (0.4%)
8	v9	0.31	0/1216	0.55	0/1650
8	x9	0.31	0/1216	0.55	0/1650
8	z9	0.31	0/1216	0.55	0/1650
9	29	0.51	1/537 (0.2%)	0.97	4/721 (0.6%)
9	39	0.52	1/537 (0.2%)	0.98	4/721 (0.6%)
9	49	0.52	1/537 (0.2%)	1.09	7/721 (1.0%)
9	G8	0.47	1/537 (0.2%)	0.74	2/721 (0.3%)
9	N8	0.47	1/537 (0.2%)	0.75	2/721 (0.3%)
9	U8	0.47	1/537 (0.2%)	0.74	2/721 (0.3%)
9	b8	0.46	1/537 (0.2%)	0.68	0/721
9	i8	0.41	1/537 (0.2%)	0.61	0/721
10	09	0.44	3/8528 (0.0%)	0.72	7/11537 (0.1%)
10	19	0.46	2/8475 (0.0%)	0.77	7/11467 (0.1%)
11	Q9	0.46	0/1323	0.70	0/1795
11	g9	0.45	0/1331	0.72	1/1805 (0.1%)
12	V9	0.39	0/1265	0.79	0/1713
12	m9	0.39	0/1265	0.79	0/1713
All	All	0.35	13/377986 (0.0%)	0.71	642/512380 (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	O9	0	4
10	19	0	5
All	All	0	23

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	19	627	ASN	CA-CB	7.05	1.65	1.53
9	39	41	GLN	CD-NE2	6.29	1.46	1.33
9	49	41	GLN	CD-NE2	6.29	1.46	1.33
9	29	41	GLN	CD-NE2	6.26	1.46	1.33
10	19	282	THR	CB-CG2	-6.01	1.32	1.52

The worst 5 of 642 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	Q8	83	ARG	NH1-CZ-NH2	-16.34	98.06	119.30
7	A8	83	ARG	NH1-CZ-NH2	-16.33	98.07	119.30
7	L8	83	ARG	NH1-CZ-NH2	-16.32	98.08	119.30
7	e8	83	ARG	NH1-CZ-NH2	-16.32	98.08	119.30
7	r8	83	ARG	NH1-CZ-NH2	-16.32	98.09	119.30

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

Continued on next page...

Continued from previous page...

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A1	1774	0	1753	295	0
1	A4	1774	0	1753	279	0
2	B1	1223	0	1198	83	0
2	B2	1223	0	1198	114	0
2	B3	1223	0	1197	106	0
2	B4	1223	0	1198	83	0
2	B5	1223	0	1197	48	0
2	B6	1223	0	1198	104	0
2	B7	1223	0	1197	106	0
2	BA	1223	0	1197	47	0
2	D1	1223	0	1198	53	0
2	D2	1223	0	1198	90	0
2	D3	1223	0	1198	91	0
2	D4	1223	0	1198	53	0
2	D5	1223	0	1197	41	0
2	D6	1223	0	1198	87	0
2	D7	1223	0	1198	87	0
2	DA	1223	0	1197	41	0
2	F1	1223	0	1198	51	0
2	F2	1223	0	1198	64	0
2	F3	1223	0	1198	66	0
2	F4	1223	0	1198	56	0
2	F5	1223	0	1197	70	0
2	F6	1223	0	1198	64	0
2	F7	1223	0	1198	70	0
2	FA	1223	0	1197	78	0
2	H1	1223	0	1198	34	0
2	H2	1223	0	1198	79	0
2	H3	1223	0	1198	86	0
2	H4	1223	0	1198	35	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H5	1223	0	1197	30	0
2	H6	1223	0	1197	77	0
2	H7	1223	0	1198	78	0
2	HA	1223	0	1197	26	0
2	J1	1223	0	1198	66	0
2	J2	1223	0	1198	74	0
2	J3	1223	0	1198	97	0
2	J4	1223	0	1198	61	0
2	J5	1223	0	1197	45	0
2	J6	1223	0	1198	69	0
2	J7	1223	0	1196	80	0
2	JA	1223	0	1197	40	0
2	L1	1223	0	1198	57	0
2	L2	1223	0	1198	88	0
2	L3	1223	0	1198	90	0
2	L4	1223	0	1198	62	0
2	L5	1223	0	1197	38	0
2	L6	1223	0	1198	95	0
2	L7	1223	0	1198	87	0
2	LA	1223	0	1197	43	0
2	O1	1223	0	1198	49	0
2	O2	1223	0	1198	84	0
2	O4	1223	0	1198	49	0
2	O5	1223	0	1197	42	0
2	O6	1223	0	1198	86	0
2	OA	1223	0	1197	43	0
2	Q1	1223	0	1197	34	0
2	Q2	1223	0	1198	94	0
2	Q4	1223	0	1197	34	0
2	Q5	1223	0	1197	44	0
2	Q6	1223	0	1198	96	0
2	QA	1223	0	1197	42	0
2	S1	1223	0	1198	43	0
2	S2	1223	0	1198	83	0
2	S4	1223	0	1198	42	0
2	S5	1223	0	1197	30	0
2	S6	1223	0	1198	79	0
2	SA	1223	0	1197	27	0
2	U1	1223	0	1198	22	0
2	U2	1223	0	1196	74	0
2	U4	1223	0	1198	22	0
2	U5	1223	0	1197	35	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	U6	1223	0	1196	76	0
2	UA	1223	0	1197	36	0
2	W1	1223	0	1198	45	0
2	W2	1223	0	1198	98	0
2	W4	1223	0	1198	44	0
2	W5	1223	0	1197	42	0
2	W6	1223	0	1198	94	0
2	WA	1223	0	1197	43	0
2	Y1	1223	0	1198	28	0
2	Y2	1223	0	1198	102	0
2	Y4	1223	0	1198	30	0
2	Y5	1223	0	1197	35	0
2	Y6	1223	0	1198	99	0
2	YA	1223	0	1197	36	0
3	C1	1278	0	1277	77	0
3	C2	1278	0	1279	107	0
3	C3	1278	0	1279	128	0
3	C4	1278	0	1277	77	0
3	C5	1278	0	1278	77	0
3	C6	1278	0	1279	104	0
3	C7	1278	0	1279	135	0
3	CA	1278	0	1278	77	0
3	E1	1278	0	1278	59	0
3	E2	1286	0	1290	66	0
3	E3	1286	0	1290	64	0
3	E4	1278	0	1278	59	0
3	E5	1278	0	1278	101	0
3	E6	1286	0	1290	70	0
3	E7	1286	0	1290	65	0
3	EA	1278	0	1278	103	0
3	G1	1278	0	1279	77	0
3	G2	1286	0	1290	143	0
3	G3	1286	0	1290	145	0
3	G4	1278	0	1279	86	0
3	G5	1278	0	1279	106	0
3	G6	1286	0	1290	137	0
3	G7	1286	0	1290	144	0
3	GA	1278	0	1278	99	0
3	I1	1286	0	1290	73	0
3	I2	1286	0	1291	85	0
3	I3	1286	0	1291	75	0
3	I4	1286	0	1290	77	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	I5	1278	0	1279	54	0
3	I6	1286	0	1291	83	0
3	I7	1286	0	1291	76	0
3	IA	1278	0	1279	51	0
3	K1	1278	0	1279	100	0
3	K2	1278	0	1279	83	0
3	K3	1278	0	1279	84	0
3	K4	1278	0	1279	101	0
3	K5	1278	0	1278	74	0
3	K6	1278	0	1279	84	0
3	K7	1278	0	1279	86	0
3	KA	1278	0	1278	74	0
3	M1	1278	0	1278	63	0
3	M2	1278	0	1279	70	0
3	M3	1278	0	1279	69	0
3	M4	1278	0	1278	52	0
3	M5	1278	0	1278	75	0
3	M6	1278	0	1279	73	0
3	M7	1278	0	1279	67	0
3	MA	1278	0	1278	73	0
3	P1	1278	0	1278	77	0
3	P2	1278	0	1279	75	0
3	P4	1278	0	1278	76	0
3	P5	1278	0	1278	72	0
3	P6	1278	0	1279	84	0
3	PA	1278	0	1278	73	0
3	R1	1278	0	1278	52	0
3	R2	1278	0	1279	83	0
3	R4	1278	0	1278	49	0
3	R5	1278	0	1279	95	0
3	R6	1278	0	1279	85	0
3	RA	1278	0	1279	94	0
3	T1	1278	0	1279	121	0
3	T2	1278	0	1279	82	0
3	T4	1278	0	1279	119	0
3	T5	1278	0	1277	85	0
3	T6	1278	0	1279	81	0
3	TA	1278	0	1277	83	0
3	V1	1278	0	1279	74	0
3	V2	1278	0	1279	92	0
3	V4	1278	0	1279	74	0
3	V5	1278	0	1278	81	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	V6	1278	0	1279	95	0
3	VA	1278	0	1278	79	0
3	X1	1278	0	1279	57	0
3	X2	1278	0	1279	87	0
3	X4	1278	0	1278	46	0
3	X5	1278	0	1279	75	0
3	X6	1278	0	1279	95	0
3	XA	1278	0	1279	70	0
3	Z1	1278	0	1279	44	0
3	Z2	1278	0	1279	93	0
3	Z4	1278	0	1279	40	0
3	Z5	1278	0	1278	74	0
3	Z6	1278	0	1279	98	0
3	ZA	1278	0	1278	74	0
4	N1	2265	0	2233	111	0
4	N2	2265	0	2233	146	0
4	N3	444	0	456	40	0
4	N4	2265	0	2233	112	0
4	N5	2265	0	2233	136	0
4	N6	2265	0	2233	143	0
4	N7	444	0	456	41	0
4	NA	2265	0	2233	133	0
5	A2	2038	0	1988	226	0
5	A5	1944	0	1903	360	0
5	A6	2038	0	1988	223	0
5	AA	1944	0	1902	307	0
6	A3	1127	0	1097	294	0
6	A7	1127	0	1097	281	0
7	A8	1204	0	1209	46	0
7	A9	1204	0	1208	107	0
7	C8	1204	0	1209	88	0
7	C9	1204	0	1207	45	0
7	E8	1204	0	1209	63	0
7	E9	1204	0	1208	57	0
7	G9	1204	0	1208	43	0
7	H8	1204	0	1209	58	0
7	I9	1204	0	1208	110	0
7	J8	1204	0	1209	86	0
7	K9	1204	0	1208	50	0
7	L8	1204	0	1209	59	0
7	N9	1204	0	1208	74	0
7	O8	1204	0	1209	96	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	P9	1204	0	1208	37	0
7	Q8	1204	0	1209	38	0
7	R9	1204	0	1208	37	0
7	S8	1204	0	1209	53	0
7	T9	1204	0	1207	46	0
7	V8	1204	0	1208	148	0
7	X8	1204	0	1209	36	0
7	X9	1204	0	1208	102	0
7	Z8	1204	0	1208	45	0
7	Z9	1204	0	1208	55	0
7	b9	1204	0	1208	43	0
7	c8	1204	0	1209	161	0
7	d9	1204	0	1208	78	0
7	e8	1204	0	1209	38	0
7	f9	1204	0	1208	41	0
7	g8	1204	0	1208	39	0
7	i9	1204	0	1208	34	0
7	j8	1204	0	1209	48	0
7	k9	1204	0	1208	71	0
7	l8	1204	0	1209	53	0
7	n8	1204	0	1209	82	0
7	o9	1204	0	1208	58	0
7	p8	1204	0	1209	51	0
7	q9	1204	0	1208	92	0
7	r8	1204	0	1209	39	0
7	s9	1204	0	1208	36	0
7	t8	1204	0	1209	67	0
7	u9	1204	0	1208	58	0
7	w9	1204	0	1208	116	0
7	y9	1204	0	1208	37	0
8	B8	1201	0	1216	72	0
8	B9	1201	0	1217	19	0
8	D8	1201	0	1217	52	0
8	D9	1201	0	1216	34	0
8	F8	1201	0	1217	37	0
8	F9	1201	0	1217	39	0
8	H9	1201	0	1217	25	0
8	I8	1201	0	1215	50	0
8	J9	1201	0	1217	29	0
8	K8	1201	0	1217	45	0
8	L9	1201	0	1217	27	0
8	M8	1201	0	1217	39	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	M9	1201	0	1217	35	0
8	O9	1201	0	1217	34	0
8	P8	1192	0	1209	43	0
8	R8	1201	0	1217	35	0
8	S9	1201	0	1217	25	0
8	T8	1201	0	1217	43	0
8	U9	1201	0	1217	26	0
8	W8	1201	0	1217	86	0
8	W9	1201	0	1217	27	0
8	Y8	1201	0	1217	28	0
8	Y9	1201	0	1217	20	0
8	a8	1201	0	1217	50	0
8	a9	1201	0	1217	27	0
8	c9	1201	0	1217	24	0
8	d8	1201	0	1216	73	0
8	e9	1201	0	1217	33	0
8	f8	1201	0	1217	42	0
8	h8	1201	0	1215	42	0
8	h9	1201	0	1217	29	0
8	j9	1201	0	1217	21	0
8	k8	1201	0	1217	70	0
8	l9	1201	0	1217	34	0
8	m8	1201	0	1217	75	0
8	n9	1201	0	1217	29	0
8	o8	1192	0	1209	109	0
8	p9	1201	0	1217	27	0
8	q8	1192	0	1208	51	0
8	r9	1201	0	1217	33	0
8	s8	1201	0	1217	68	0
8	t9	1201	0	1215	57	0
8	u8	1201	0	1214	57	0
8	v9	1201	0	1217	22	0
8	x9	1201	0	1217	31	0
8	z9	1201	0	1215	50	0
9	29	529	0	554	35	0
9	39	529	0	555	21	0
9	49	529	0	554	64	0
9	G8	529	0	556	33	0
9	N8	529	0	556	28	0
9	U8	529	0	556	51	0
9	b8	529	0	556	45	0
9	i8	529	0	556	60	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	09	8352	0	8386	557	0
10	19	8299	0	8332	427	0
11	Q9	1304	0	1298	24	0
11	g9	1312	0	1310	27	0
12	V9	1244	0	1261	21	0
12	m9	1244	0	1261	24	0
13	09	129	0	114	42	0
13	19	215	0	188	75	0
13	29	43	0	37	14	0
13	39	43	0	37	9	0
13	A3	43	0	38	24	0
13	A5	172	0	152	127	0
13	A7	43	0	38	24	0
13	A8	43	0	38	16	0
13	A9	43	0	38	19	0
13	AA	172	0	152	123	0
13	B1	43	0	38	18	0
13	B2	43	0	38	24	0
13	B3	43	0	38	26	0
13	B4	43	0	38	18	0
13	B5	43	0	38	6	0
13	B6	43	0	38	27	0
13	B7	43	0	38	27	0
13	B8	43	0	38	35	0
13	B9	43	0	38	11	0
13	C1	86	0	74	46	0
13	C2	86	0	76	71	0
13	C3	43	0	38	42	0
13	C4	86	0	74	46	0
13	C5	43	0	35	30	0
13	C6	86	0	76	71	0
13	C7	43	0	38	42	0
13	C8	43	0	38	16	0
13	C9	43	0	38	19	0
13	CA	43	0	35	29	0
13	D1	43	0	38	30	0
13	D2	43	0	38	17	0
13	D3	43	0	38	17	0
13	D4	43	0	38	30	0
13	D5	43	0	38	11	0
13	D6	43	0	38	17	0
13	D7	43	0	38	17	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	D8	43	0	38	29	0
13	D9	43	0	38	22	0
13	DA	43	0	38	11	0
13	E1	86	0	75	46	0
13	E2	86	0	73	54	0
13	E3	86	0	73	61	0
13	E4	86	0	75	45	0
13	E5	86	0	76	53	0
13	E6	86	0	73	53	0
13	E7	86	0	73	61	0
13	E8	43	0	38	16	0
13	E9	43	0	38	19	0
13	EA	86	0	76	53	0
13	F1	43	0	38	18	0
13	F2	43	0	38	16	0
13	F3	43	0	38	16	0
13	F4	43	0	38	19	0
13	F6	43	0	38	17	0
13	F7	43	0	38	18	0
13	F8	43	0	38	28	0
13	F9	43	0	38	16	0
13	G1	86	0	76	67	0
13	G2	86	0	75	73	0
13	G3	86	0	75	67	0
13	G4	86	0	76	68	0
13	G5	43	0	38	41	0
13	G6	86	0	75	75	0
13	G7	86	0	75	69	0
13	G9	43	0	38	19	0
13	GA	86	0	76	46	0
13	H1	43	0	38	7	0
13	H2	43	0	38	20	0
13	H3	43	0	38	20	0
13	H4	43	0	38	7	0
13	H6	43	0	38	20	0
13	H7	43	0	38	20	0
13	H8	43	0	38	18	0
13	H9	43	0	38	10	0
13	I1	86	0	75	53	0
13	I2	86	0	76	60	0
13	I3	86	0	76	58	0
13	I4	86	0	75	57	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	I5	86	0	76	49	0
13	I6	86	0	76	59	0
13	I7	86	0	76	61	0
13	I8	43	0	38	26	0
13	I9	43	0	38	19	0
13	IA	86	0	76	48	0
13	J1	43	0	38	27	0
13	J2	43	0	38	25	0
13	J3	43	0	38	24	0
13	J4	43	0	38	26	0
13	J5	43	0	38	2	0
13	J6	43	0	38	24	0
13	J7	43	0	38	24	0
13	J8	43	0	38	16	0
13	J9	43	0	38	10	0
13	JA	43	0	38	2	0
13	K1	86	0	76	85	0
13	K2	86	0	76	82	0
13	K3	86	0	76	80	0
13	K4	86	0	76	87	0
13	K5	43	0	38	27	0
13	K6	86	0	76	81	0
13	K7	86	0	76	82	0
13	K8	43	0	38	29	0
13	K9	43	0	38	19	0
13	KA	43	0	38	27	0
13	L1	43	0	38	13	0
13	L2	43	0	38	17	0
13	L3	43	0	38	17	0
13	L4	43	0	38	13	0
13	L5	43	0	38	9	0
13	L6	43	0	38	17	0
13	L7	43	0	38	17	0
13	L8	43	0	38	16	0
13	L9	43	0	38	9	0
13	LA	43	0	38	9	0
13	M1	86	0	75	52	0
13	M2	43	0	38	28	0
13	M3	43	0	38	28	0
13	M4	86	0	75	50	0
13	M5	129	0	114	68	0
13	M6	43	0	38	29	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	M7	43	0	38	27	0
13	M8	43	0	38	28	0
13	MA	129	0	114	70	0
13	N2	86	0	76	44	0
13	N3	43	0	38	30	0
13	N5	43	0	38	19	0
13	N6	86	0	76	47	0
13	N7	43	0	38	29	0
13	N9	43	0	38	19	0
13	NA	43	0	38	18	0
13	O1	43	0	38	27	0
13	O2	43	0	38	13	0
13	O4	43	0	38	26	0
13	O5	43	0	38	1	0
13	O6	43	0	38	14	0
13	O8	43	0	38	16	0
13	O9	43	0	38	11	0
13	OA	43	0	38	1	0
13	P1	86	0	74	61	0
13	P2	43	0	38	22	0
13	P4	86	0	74	60	0
13	P5	129	0	114	70	0
13	P6	43	0	38	22	0
13	P8	43	0	38	29	0
13	P9	43	0	38	20	0
13	PA	129	0	114	70	0
13	Q1	86	0	76	47	0
13	Q2	43	0	38	39	0
13	Q4	86	0	76	47	0
13	Q6	43	0	38	40	0
13	Q8	43	0	38	16	0
13	Q9	43	0	37	1	0
13	R1	43	0	37	6	0
13	R2	43	0	38	23	0
13	R4	43	0	37	6	0
13	R5	43	0	38	58	0
13	R6	43	0	38	25	0
13	R8	43	0	38	28	0
13	R9	43	0	38	19	0
13	RA	43	0	38	56	0
13	S1	43	0	38	20	0
13	S2	43	0	38	25	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	S4	43	0	38	21	0
13	S5	43	0	38	11	0
13	S6	43	0	38	24	0
13	S8	43	0	38	16	0
13	S9	43	0	38	10	0
13	SA	43	0	38	11	0
13	T1	86	0	76	92	0
13	T2	43	0	38	41	0
13	T4	86	0	76	94	0
13	T5	86	0	73	81	0
13	T6	43	0	38	39	0
13	T8	43	0	38	27	0
13	T9	43	0	38	19	0
13	TA	86	0	73	83	0
13	U1	43	0	38	7	0
13	U2	86	0	74	61	0
13	U4	43	0	38	7	0
13	U5	43	0	38	10	0
13	U6	86	0	74	61	0
13	U9	43	0	38	8	0
13	UA	43	0	38	10	0
13	V1	86	0	76	79	0
13	V2	86	0	76	68	0
13	V4	86	0	76	80	0
13	V5	86	0	76	69	0
13	V6	86	0	76	68	0
13	V8	43	0	38	16	0
13	V9	43	0	36	2	0
13	VA	86	0	76	70	0
13	W1	43	0	38	21	0
13	W2	129	0	114	117	0
13	W4	43	0	38	23	0
13	W5	43	0	38	8	0
13	W6	86	0	76	63	0
13	W8	43	0	38	26	0
13	WA	43	0	38	8	0
13	X1	86	0	76	52	0
13	X2	43	0	38	17	0
13	X4	86	0	75	41	0
13	X5	86	0	76	49	0
13	X6	86	0	76	66	0
13	X8	43	0	38	16	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	X9	43	0	38	19	0
13	XA	86	0	76	49	0
13	Y1	43	0	38	4	0
13	Y2	43	0	38	30	0
13	Y4	43	0	38	4	0
13	Y5	43	0	38	8	0
13	Y6	43	0	38	30	0
13	Y8	43	0	38	30	0
13	YA	43	0	38	8	0
13	Z1	86	0	76	46	0
13	Z2	86	0	76	66	0
13	Z4	86	0	76	45	0
13	Z5	86	0	76	54	0
13	Z6	86	0	76	66	0
13	Z8	43	0	38	16	0
13	Z9	43	0	38	15	0
13	ZA	86	0	76	55	0
13	b8	43	0	38	32	0
13	b9	43	0	38	19	0
13	c8	43	0	38	16	0
13	c9	43	0	38	10	0
13	d8	43	0	38	34	0
13	d9	43	0	38	15	0
13	e8	43	0	38	15	0
13	e9	43	0	38	10	0
13	f8	43	0	38	31	0
13	f9	43	0	38	20	0
13	g8	43	0	38	16	0
13	g9	43	0	37	0	0
13	h8	43	0	38	25	0
13	i9	43	0	38	15	0
13	j8	43	0	38	16	0
13	j9	43	0	38	10	0
13	k8	43	0	38	34	0
13	k9	43	0	38	19	0
13	l8	43	0	38	16	0
13	l9	43	0	38	6	0
13	m9	43	0	36	2	0
13	n8	43	0	38	15	0
13	o8	43	0	38	43	0
13	o9	43	0	38	19	0
13	p8	43	0	38	16	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	p9	43	0	38	10	0
13	q8	43	0	38	35	0
13	q9	43	0	38	19	0
13	r8	43	0	38	16	0
13	r9	43	0	38	11	0
13	s8	43	0	38	35	0
13	s9	43	0	38	19	0
13	t8	43	0	38	16	0
13	t9	43	0	38	10	0
13	u9	43	0	38	19	0
13	v9	43	0	38	10	0
13	w9	43	0	38	19	0
13	x9	43	0	38	10	0
13	y9	43	0	38	19	0
13	z9	43	0	38	10	0
All	All	387586	0	384517	19363	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 25.

The worst 5 of 19363 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G1:154:CYS:SG	13:G1:201:CYC:HBC2	1.33	1.68
3:G4:154:CYS:SG	13:G4:201:CYC:HBC2	1.33	1.68
3:E5:154:CYS:SG	13:E5:201:CYC:H2C	1.25	1.65
3:EA:154:CYS:SG	13:EA:201:CYC:H2C	1.25	1.65
3:I6:87:MET:CE	13:I6:201:CYC:HBC1	1.19	1.65

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A1	211/247 (85%)	189 (90%)	21 (10%)	1 (0%)	24	59
1	A4	211/247 (85%)	189 (90%)	21 (10%)	1 (0%)	24	59
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	21	55
2	L3	160/163 (98%)	157 (98%)	2 (1%)	1 (1%)	21	55
2	L4	160/163 (98%)	156 (98%)	4 (2%)	0	100	100
2	L5	160/163 (98%)	159 (99%)	1 (1%)	0	100	100
2	L6	160/163 (98%)	157 (98%)	2 (1%)	1 (1%)	21	55
2	L7	160/163 (98%)	157 (98%)	2 (1%)	1 (1%)	21	55
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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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%)	21	55
3	C3	170/173 (98%)	167 (98%)	2 (1%)	1 (1%)	21	55
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%)	21	55
3	C7	170/173 (98%)	167 (98%)	2 (1%)	1 (1%)	21	55
3	CA	170/173 (98%)	168 (99%)	2 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	E1	170/173 (98%)	166 (98%)	4 (2%)	0	100	100
3	E2	171/173 (99%)	166 (97%)	4 (2%)	1 (1%)	21	55
3	E3	171/173 (99%)	166 (97%)	4 (2%)	1 (1%)	21	55
3	E4	170/173 (98%)	166 (98%)	4 (2%)	0	100	100
3	E5	170/173 (98%)	169 (99%)	0	1 (1%)	21	55
3	E6	171/173 (99%)	166 (97%)	4 (2%)	1 (1%)	21	55
3	E7	171/173 (99%)	166 (97%)	4 (2%)	1 (1%)	21	55
3	EA	170/173 (98%)	169 (99%)	0	1 (1%)	21	55
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%)	21	55
3	G6	171/173 (99%)	168 (98%)	3 (2%)	0	100	100
3	G7	171/173 (99%)	168 (98%)	3 (2%)	0	100	100
3	GA	170/173 (98%)	168 (99%)	1 (1%)	1 (1%)	21	55
3	I1	171/173 (99%)	165 (96%)	4 (2%)	2 (1%)	10	41
3	I2	171/173 (99%)	167 (98%)	3 (2%)	1 (1%)	21	55
3	I3	171/173 (99%)	167 (98%)	3 (2%)	1 (1%)	21	55
3	I4	171/173 (99%)	165 (96%)	4 (2%)	2 (1%)	10	41
3	I5	170/173 (98%)	169 (99%)	1 (1%)	0	100	100
3	I6	171/173 (99%)	167 (98%)	3 (2%)	1 (1%)	21	55
3	I7	171/173 (99%)	167 (98%)	3 (2%)	1 (1%)	21	55
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%)	21	55
3	K3	170/173 (98%)	166 (98%)	3 (2%)	1 (1%)	21	55
3	K4	170/173 (98%)	166 (98%)	4 (2%)	0	100	100
3	K5	170/173 (98%)	169 (99%)	0	1 (1%)	21	55
3	K6	170/173 (98%)	166 (98%)	3 (2%)	1 (1%)	21	55
3	K7	170/173 (98%)	166 (98%)	3 (2%)	1 (1%)	21	55

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	KA	170/173 (98%)	169 (99%)	0	1 (1%)	21	55
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%)	21	55
3	P6	170/173 (98%)	166 (98%)	4 (2%)	0	100	100
3	PA	170/173 (98%)	169 (99%)	0	1 (1%)	21	55
3	R1	170/173 (98%)	166 (98%)	4 (2%)	0	100	100
3	R2	170/173 (98%)	165 (97%)	4 (2%)	1 (1%)	21	55
3	R4	170/173 (98%)	166 (98%)	4 (2%)	0	100	100
3	R5	170/173 (98%)	168 (99%)	1 (1%)	1 (1%)	21	55
3	R6	170/173 (98%)	165 (97%)	4 (2%)	1 (1%)	21	55
3	RA	170/173 (98%)	168 (99%)	1 (1%)	1 (1%)	21	55
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%)	21	55
3	T6	170/173 (98%)	166 (98%)	4 (2%)	0	100	100
3	TA	170/173 (98%)	169 (99%)	0	1 (1%)	21	55
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%)	21	55

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	V6	170/173 (98%)	166 (98%)	4 (2%)	0	100	100
3	VA	170/173 (98%)	169 (99%)	0	1 (1%)	21	55
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%)	21	55
3	X6	170/173 (98%)	166 (98%)	4 (2%)	0	100	100
3	XA	170/173 (98%)	169 (99%)	0	1 (1%)	21	55
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%)	18	53
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%)	18	53
4	N5	282/286 (99%)	257 (91%)	23 (8%)	2 (1%)	18	53
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%)	18	53
5	A2	247/253 (98%)	226 (92%)	18 (7%)	3 (1%)	10	41
5	A5	233/253 (92%)	218 (94%)	13 (6%)	2 (1%)	14	47
5	A6	247/253 (98%)	227 (92%)	18 (7%)	2 (1%)	16	50
5	AA	233/253 (92%)	218 (94%)	12 (5%)	3 (1%)	9	40
6	A3	134/279 (48%)	131 (98%)	1 (1%)	2 (2%)	8	37
6	A7	134/279 (48%)	131 (98%)	1 (1%)	2 (2%)	8	37
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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	36	69
10	19	1037/1132 (92%)	939 (90%)	93 (9%)	5 (0%)	24	59
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%)	44	74

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 ⓘ

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%)	188 (98%)	3 (2%)	55	69
1	A4	191/223 (86%)	188 (98%)	3 (2%)	55	69
2	B1	122/123 (99%)	108 (88%)	14 (12%)	5	22
2	B2	122/123 (99%)	108 (88%)	14 (12%)	5	22
2	B3	122/123 (99%)	108 (88%)	14 (12%)	5	22
2	B4	122/123 (99%)	107 (88%)	15 (12%)	4	20
2	B5	122/123 (99%)	107 (88%)	15 (12%)	4	20
2	B6	122/123 (99%)	108 (88%)	14 (12%)	5	22

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B7	122/123 (99%)	108 (88%)	14 (12%)	5	22
2	BA	122/123 (99%)	107 (88%)	15 (12%)	4	20
2	D1	122/123 (99%)	107 (88%)	15 (12%)	4	20
2	D2	122/123 (99%)	109 (89%)	13 (11%)	6	24
2	D3	122/123 (99%)	109 (89%)	13 (11%)	6	24
2	D4	122/123 (99%)	107 (88%)	15 (12%)	4	20
2	D5	122/123 (99%)	108 (88%)	14 (12%)	5	22
2	D6	122/123 (99%)	109 (89%)	13 (11%)	6	24
2	D7	122/123 (99%)	109 (89%)	13 (11%)	6	24
2	DA	122/123 (99%)	108 (88%)	14 (12%)	5	22
2	F1	122/123 (99%)	107 (88%)	15 (12%)	4	20
2	F2	122/123 (99%)	109 (89%)	13 (11%)	6	24
2	F3	122/123 (99%)	109 (89%)	13 (11%)	6	24
2	F4	122/123 (99%)	107 (88%)	15 (12%)	4	20
2	F5	122/123 (99%)	107 (88%)	15 (12%)	4	20
2	F6	122/123 (99%)	109 (89%)	13 (11%)	6	24
2	F7	122/123 (99%)	109 (89%)	13 (11%)	6	24
2	FA	122/123 (99%)	107 (88%)	15 (12%)	4	20
2	H1	122/123 (99%)	106 (87%)	16 (13%)	4	19
2	H2	122/123 (99%)	106 (87%)	16 (13%)	4	19
2	H3	122/123 (99%)	107 (88%)	15 (12%)	4	20
2	H4	122/123 (99%)	106 (87%)	16 (13%)	4	19
2	H5	122/123 (99%)	108 (88%)	14 (12%)	5	22
2	H6	122/123 (99%)	107 (88%)	15 (12%)	4	20
2	H7	122/123 (99%)	107 (88%)	15 (12%)	4	20
2	HA	122/123 (99%)	108 (88%)	14 (12%)	5	22
2	J1	122/123 (99%)	107 (88%)	15 (12%)	4	20
2	J2	122/123 (99%)	108 (88%)	14 (12%)	5	22
2	J3	122/123 (99%)	108 (88%)	14 (12%)	5	22
2	J4	122/123 (99%)	107 (88%)	15 (12%)	4	20
2	J5	122/123 (99%)	107 (88%)	15 (12%)	4	20

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	J6	122/123 (99%)	108 (88%)	14 (12%)	5	22
2	J7	122/123 (99%)	108 (88%)	14 (12%)	5	22
2	JA	122/123 (99%)	107 (88%)	15 (12%)	4	20
2	L1	122/123 (99%)	108 (88%)	14 (12%)	5	22
2	L2	122/123 (99%)	109 (89%)	13 (11%)	6	24
2	L3	122/123 (99%)	109 (89%)	13 (11%)	6	24
2	L4	122/123 (99%)	108 (88%)	14 (12%)	5	22
2	L5	122/123 (99%)	107 (88%)	15 (12%)	4	20
2	L6	122/123 (99%)	109 (89%)	13 (11%)	6	24
2	L7	122/123 (99%)	109 (89%)	13 (11%)	6	24
2	LA	122/123 (99%)	107 (88%)	15 (12%)	4	20
2	O1	122/123 (99%)	107 (88%)	15 (12%)	4	20
2	O2	122/123 (99%)	107 (88%)	15 (12%)	4	20
2	O4	122/123 (99%)	107 (88%)	15 (12%)	4	20
2	O5	122/123 (99%)	108 (88%)	14 (12%)	5	22
2	O6	122/123 (99%)	107 (88%)	15 (12%)	4	20
2	OA	122/123 (99%)	108 (88%)	14 (12%)	5	22
2	Q1	122/123 (99%)	107 (88%)	15 (12%)	4	20
2	Q2	122/123 (99%)	106 (87%)	16 (13%)	4	19
2	Q4	122/123 (99%)	107 (88%)	15 (12%)	4	20
2	Q5	122/123 (99%)	106 (87%)	16 (13%)	4	19
2	Q6	122/123 (99%)	106 (87%)	16 (13%)	4	19
2	QA	122/123 (99%)	106 (87%)	16 (13%)	4	19
2	S1	122/123 (99%)	107 (88%)	15 (12%)	4	20
2	S2	122/123 (99%)	107 (88%)	15 (12%)	4	20
2	S4	122/123 (99%)	107 (88%)	15 (12%)	4	20
2	S5	122/123 (99%)	106 (87%)	16 (13%)	4	19
2	S6	122/123 (99%)	107 (88%)	15 (12%)	4	20
2	SA	122/123 (99%)	106 (87%)	16 (13%)	4	19
2	U1	122/123 (99%)	106 (87%)	16 (13%)	4	19
2	U2	122/123 (99%)	109 (89%)	13 (11%)	6	24

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	U4	122/123 (99%)	106 (87%)	16 (13%)	4	19
2	U5	122/123 (99%)	108 (88%)	14 (12%)	5	22
2	U6	122/123 (99%)	109 (89%)	13 (11%)	6	24
2	UA	122/123 (99%)	108 (88%)	14 (12%)	5	22
2	W1	122/123 (99%)	107 (88%)	15 (12%)	4	20
2	W2	122/123 (99%)	107 (88%)	15 (12%)	4	20
2	W4	122/123 (99%)	107 (88%)	15 (12%)	4	20
2	W5	122/123 (99%)	107 (88%)	15 (12%)	4	20
2	W6	122/123 (99%)	108 (88%)	14 (12%)	5	22
2	WA	122/123 (99%)	107 (88%)	15 (12%)	4	20
2	Y1	122/123 (99%)	107 (88%)	15 (12%)	4	20
2	Y2	122/123 (99%)	108 (88%)	14 (12%)	5	22
2	Y4	122/123 (99%)	107 (88%)	15 (12%)	4	20
2	Y5	122/123 (99%)	107 (88%)	15 (12%)	4	20
2	Y6	122/123 (99%)	108 (88%)	14 (12%)	5	22
2	YA	122/123 (99%)	107 (88%)	15 (12%)	4	20
3	C1	134/135 (99%)	122 (91%)	12 (9%)	9	31
3	C2	134/135 (99%)	115 (86%)	19 (14%)	3	17
3	C3	134/135 (99%)	115 (86%)	19 (14%)	3	17
3	C4	134/135 (99%)	122 (91%)	12 (9%)	9	31
3	C5	134/135 (99%)	113 (84%)	21 (16%)	2	15
3	C6	134/135 (99%)	115 (86%)	19 (14%)	3	17
3	C7	134/135 (99%)	115 (86%)	19 (14%)	3	17
3	CA	134/135 (99%)	113 (84%)	21 (16%)	2	15
3	E1	134/135 (99%)	121 (90%)	13 (10%)	8	28
3	E2	135/135 (100%)	113 (84%)	22 (16%)	2	14
3	E3	135/135 (100%)	113 (84%)	22 (16%)	2	14
3	E4	134/135 (99%)	121 (90%)	13 (10%)	8	28
3	E5	134/135 (99%)	113 (84%)	21 (16%)	2	15
3	E6	135/135 (100%)	113 (84%)	22 (16%)	2	14
3	E7	135/135 (100%)	113 (84%)	22 (16%)	2	14

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	EA	134/135 (99%)	113 (84%)	21 (16%)	2	15
3	G1	134/135 (99%)	120 (90%)	14 (10%)	7	26
3	G2	135/135 (100%)	115 (85%)	20 (15%)	3	16
3	G3	135/135 (100%)	115 (85%)	20 (15%)	3	16
3	G4	134/135 (99%)	120 (90%)	14 (10%)	7	26
3	G5	134/135 (99%)	113 (84%)	21 (16%)	2	15
3	G6	135/135 (100%)	115 (85%)	20 (15%)	3	16
3	G7	135/135 (100%)	115 (85%)	20 (15%)	3	16
3	GA	134/135 (99%)	114 (85%)	20 (15%)	3	16
3	I1	135/135 (100%)	123 (91%)	12 (9%)	9	32
3	I2	135/135 (100%)	113 (84%)	22 (16%)	2	14
3	I3	135/135 (100%)	113 (84%)	22 (16%)	2	14
3	I4	135/135 (100%)	123 (91%)	12 (9%)	9	32
3	I5	134/135 (99%)	114 (85%)	20 (15%)	3	16
3	I6	135/135 (100%)	113 (84%)	22 (16%)	2	14
3	I7	135/135 (100%)	113 (84%)	22 (16%)	2	14
3	IA	134/135 (99%)	114 (85%)	20 (15%)	3	16
3	K1	134/135 (99%)	121 (90%)	13 (10%)	8	28
3	K2	134/135 (99%)	111 (83%)	23 (17%)	2	12
3	K3	134/135 (99%)	111 (83%)	23 (17%)	2	12
3	K4	134/135 (99%)	121 (90%)	13 (10%)	8	28
3	K5	134/135 (99%)	114 (85%)	20 (15%)	3	16
3	K6	134/135 (99%)	111 (83%)	23 (17%)	2	12
3	K7	134/135 (99%)	111 (83%)	23 (17%)	2	12
3	KA	134/135 (99%)	114 (85%)	20 (15%)	3	16
3	M1	134/135 (99%)	122 (91%)	12 (9%)	9	31
3	M2	134/135 (99%)	115 (86%)	19 (14%)	3	17
3	M3	134/135 (99%)	115 (86%)	19 (14%)	3	17
3	M4	134/135 (99%)	122 (91%)	12 (9%)	9	31
3	M5	134/135 (99%)	113 (84%)	21 (16%)	2	15
3	M6	134/135 (99%)	116 (87%)	18 (13%)	4	19

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	M7	134/135 (99%)	116 (87%)	18 (13%)	4	19
3	MA	134/135 (99%)	113 (84%)	21 (16%)	2	15
3	P1	134/135 (99%)	122 (91%)	12 (9%)	9	31
3	P2	134/135 (99%)	112 (84%)	22 (16%)	2	13
3	P4	134/135 (99%)	122 (91%)	12 (9%)	9	31
3	P5	134/135 (99%)	114 (85%)	20 (15%)	3	16
3	P6	134/135 (99%)	112 (84%)	22 (16%)	2	13
3	PA	134/135 (99%)	114 (85%)	20 (15%)	3	16
3	R1	134/135 (99%)	123 (92%)	11 (8%)	10	34
3	R2	134/135 (99%)	112 (84%)	22 (16%)	2	13
3	R4	134/135 (99%)	123 (92%)	11 (8%)	10	34
3	R5	134/135 (99%)	114 (85%)	20 (15%)	3	16
3	R6	134/135 (99%)	112 (84%)	22 (16%)	2	13
3	RA	134/135 (99%)	114 (85%)	20 (15%)	3	16
3	T1	134/135 (99%)	123 (92%)	11 (8%)	10	34
3	T2	134/135 (99%)	114 (85%)	20 (15%)	3	16
3	T4	134/135 (99%)	123 (92%)	11 (8%)	10	34
3	T5	134/135 (99%)	113 (84%)	21 (16%)	2	15
3	T6	134/135 (99%)	114 (85%)	20 (15%)	3	16
3	TA	134/135 (99%)	113 (84%)	21 (16%)	2	15
3	V1	134/135 (99%)	122 (91%)	12 (9%)	9	31
3	V2	134/135 (99%)	116 (87%)	18 (13%)	4	19
3	V4	134/135 (99%)	122 (91%)	12 (9%)	9	31
3	V5	134/135 (99%)	115 (86%)	19 (14%)	3	17
3	V6	134/135 (99%)	115 (86%)	19 (14%)	3	17
3	VA	134/135 (99%)	115 (86%)	19 (14%)	3	17
3	X1	134/135 (99%)	123 (92%)	11 (8%)	10	34
3	X2	134/135 (99%)	113 (84%)	21 (16%)	2	15
3	X4	134/135 (99%)	123 (92%)	11 (8%)	10	34
3	X5	134/135 (99%)	112 (84%)	22 (16%)	2	13
3	X6	134/135 (99%)	113 (84%)	21 (16%)	2	15

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	XA	134/135 (99%)	113 (84%)	21 (16%)	2	15
3	Z1	134/135 (99%)	123 (92%)	11 (8%)	10	34
3	Z2	134/135 (99%)	114 (85%)	20 (15%)	3	16
3	Z4	134/135 (99%)	123 (92%)	11 (8%)	10	34
3	Z5	134/135 (99%)	114 (85%)	20 (15%)	3	16
3	Z6	134/135 (99%)	114 (85%)	20 (15%)	3	16
3	ZA	134/135 (99%)	114 (85%)	20 (15%)	3	16
4	N1	242/243 (100%)	240 (99%)	2 (1%)	73	77
4	N2	242/243 (100%)	239 (99%)	3 (1%)	63	72
4	N3	50/243 (21%)	49 (98%)	1 (2%)	48	65
4	N4	242/243 (100%)	240 (99%)	2 (1%)	73	77
4	N5	242/243 (100%)	241 (100%)	1 (0%)	84	83
4	N6	242/243 (100%)	239 (99%)	3 (1%)	63	72
4	N7	50/243 (21%)	49 (98%)	1 (2%)	48	65
4	NA	242/243 (100%)	241 (100%)	1 (0%)	84	83
5	A2	220/224 (98%)	217 (99%)	3 (1%)	59	71
5	A5	210/224 (94%)	204 (97%)	6 (3%)	37	58
5	A6	220/224 (98%)	218 (99%)	2 (1%)	70	75
5	AA	210/224 (94%)	206 (98%)	4 (2%)	50	66
6	A3	120/242 (50%)	113 (94%)	7 (6%)	18	44
6	A7	120/242 (50%)	113 (94%)	7 (6%)	18	44
7	A8	124/126 (98%)	111 (90%)	13 (10%)	6	25
7	A9	124/126 (98%)	113 (91%)	11 (9%)	9	32
7	C8	124/126 (98%)	111 (90%)	13 (10%)	6	25
7	C9	124/126 (98%)	112 (90%)	12 (10%)	8	28
7	E8	124/126 (98%)	111 (90%)	13 (10%)	6	25
7	E9	124/126 (98%)	113 (91%)	11 (9%)	9	32
7	G9	124/126 (98%)	113 (91%)	11 (9%)	9	32
7	H8	124/126 (98%)	111 (90%)	13 (10%)	6	25
7	I9	124/126 (98%)	113 (91%)	11 (9%)	9	32
7	J8	124/126 (98%)	111 (90%)	13 (10%)	6	25

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	K9	124/126 (98%)	113 (91%)	11 (9%)	9	32
7	L8	124/126 (98%)	111 (90%)	13 (10%)	6	25
7	N9	124/126 (98%)	113 (91%)	11 (9%)	9	32
7	O8	124/126 (98%)	111 (90%)	13 (10%)	6	25
7	P9	124/126 (98%)	113 (91%)	11 (9%)	9	32
7	Q8	124/126 (98%)	111 (90%)	13 (10%)	6	25
7	R9	124/126 (98%)	113 (91%)	11 (9%)	9	32
7	S8	124/126 (98%)	111 (90%)	13 (10%)	6	25
7	T9	124/126 (98%)	113 (91%)	11 (9%)	9	32
7	V8	124/126 (98%)	111 (90%)	13 (10%)	6	25
7	X8	124/126 (98%)	111 (90%)	13 (10%)	6	25
7	X9	124/126 (98%)	113 (91%)	11 (9%)	9	32
7	Z8	124/126 (98%)	111 (90%)	13 (10%)	6	25
7	Z9	124/126 (98%)	113 (91%)	11 (9%)	9	32
7	b9	124/126 (98%)	113 (91%)	11 (9%)	9	32
7	c8	124/126 (98%)	111 (90%)	13 (10%)	6	25
7	d9	124/126 (98%)	113 (91%)	11 (9%)	9	32
7	e8	124/126 (98%)	111 (90%)	13 (10%)	6	25
7	f9	124/126 (98%)	113 (91%)	11 (9%)	9	32
7	g8	124/126 (98%)	111 (90%)	13 (10%)	6	25
7	i9	124/126 (98%)	113 (91%)	11 (9%)	9	32
7	j8	124/126 (98%)	111 (90%)	13 (10%)	6	25
7	k9	124/126 (98%)	113 (91%)	11 (9%)	9	32
7	l8	124/126 (98%)	111 (90%)	13 (10%)	6	25
7	n8	124/126 (98%)	111 (90%)	13 (10%)	6	25
7	o9	124/126 (98%)	113 (91%)	11 (9%)	9	32
7	p8	124/126 (98%)	111 (90%)	13 (10%)	6	25
7	q9	124/126 (98%)	113 (91%)	11 (9%)	9	32
7	r8	124/126 (98%)	111 (90%)	13 (10%)	6	25
7	s9	124/126 (98%)	113 (91%)	11 (9%)	9	32
7	t8	124/126 (98%)	111 (90%)	13 (10%)	6	25

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	u9	124/126 (98%)	113 (91%)	11 (9%)	9	32
7	w9	124/126 (98%)	113 (91%)	11 (9%)	9	32
7	y9	124/126 (98%)	113 (91%)	11 (9%)	9	32
8	B8	123/124 (99%)	110 (89%)	13 (11%)	6	25
8	B9	123/124 (99%)	113 (92%)	10 (8%)	11	35
8	D8	123/124 (99%)	110 (89%)	13 (11%)	6	25
8	D9	123/124 (99%)	113 (92%)	10 (8%)	11	35
8	F8	123/124 (99%)	110 (89%)	13 (11%)	6	25
8	F9	123/124 (99%)	113 (92%)	10 (8%)	11	35
8	H9	123/124 (99%)	113 (92%)	10 (8%)	11	35
8	I8	123/124 (99%)	110 (89%)	13 (11%)	6	25
8	J9	123/124 (99%)	113 (92%)	10 (8%)	11	35
8	K8	123/124 (99%)	110 (89%)	13 (11%)	6	25
8	L9	123/124 (99%)	113 (92%)	10 (8%)	11	35
8	M8	123/124 (99%)	110 (89%)	13 (11%)	6	25
8	M9	123/124 (99%)	113 (92%)	10 (8%)	11	35
8	O9	123/124 (99%)	113 (92%)	10 (8%)	11	35
8	P8	122/124 (98%)	109 (89%)	13 (11%)	6	24
8	R8	123/124 (99%)	110 (89%)	13 (11%)	6	25
8	S9	123/124 (99%)	113 (92%)	10 (8%)	11	35
8	T8	123/124 (99%)	110 (89%)	13 (11%)	6	25
8	U9	123/124 (99%)	112 (91%)	11 (9%)	9	32
8	W8	123/124 (99%)	110 (89%)	13 (11%)	6	25
8	W9	123/124 (99%)	113 (92%)	10 (8%)	11	35
8	Y8	123/124 (99%)	110 (89%)	13 (11%)	6	25
8	Y9	123/124 (99%)	113 (92%)	10 (8%)	11	35
8	a8	123/124 (99%)	110 (89%)	13 (11%)	6	25
8	a9	123/124 (99%)	113 (92%)	10 (8%)	11	35
8	c9	123/124 (99%)	113 (92%)	10 (8%)	11	35
8	d8	123/124 (99%)	111 (90%)	12 (10%)	7	28
8	e9	123/124 (99%)	113 (92%)	10 (8%)	11	35

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	f8	123/124 (99%)	110 (89%)	13 (11%)	6	25
8	h8	123/124 (99%)	110 (89%)	13 (11%)	6	25
8	h9	123/124 (99%)	113 (92%)	10 (8%)	11	35
8	j9	123/124 (99%)	113 (92%)	10 (8%)	11	35
8	k8	123/124 (99%)	110 (89%)	13 (11%)	6	25
8	l9	123/124 (99%)	113 (92%)	10 (8%)	11	35
8	m8	123/124 (99%)	110 (89%)	13 (11%)	6	25
8	n9	123/124 (99%)	113 (92%)	10 (8%)	11	35
8	o8	122/124 (98%)	109 (89%)	13 (11%)	6	24
8	p9	123/124 (99%)	113 (92%)	10 (8%)	11	35
8	q8	122/124 (98%)	109 (89%)	13 (11%)	6	24
8	r9	123/124 (99%)	113 (92%)	10 (8%)	11	35
8	s8	123/124 (99%)	110 (89%)	13 (11%)	6	25
8	t9	123/124 (99%)	113 (92%)	10 (8%)	11	35
8	u8	123/124 (99%)	110 (89%)	13 (11%)	6	25
8	v9	123/124 (99%)	113 (92%)	10 (8%)	11	35
8	x9	123/124 (99%)	113 (92%)	10 (8%)	11	35
8	z9	123/124 (99%)	113 (92%)	10 (8%)	11	35
9	29	56/59 (95%)	51 (91%)	5 (9%)	9	32
9	39	56/59 (95%)	50 (89%)	6 (11%)	6	24
9	49	56/59 (95%)	49 (88%)	7 (12%)	4	20
9	G8	56/59 (95%)	52 (93%)	4 (7%)	13	40
9	N8	56/59 (95%)	52 (93%)	4 (7%)	13	40
9	U8	56/59 (95%)	52 (93%)	4 (7%)	13	40
9	b8	56/59 (95%)	53 (95%)	3 (5%)	20	46
9	i8	56/59 (95%)	52 (93%)	4 (7%)	13	40
10	09	888/954 (93%)	885 (100%)	3 (0%)	86	85
10	19	882/954 (92%)	880 (100%)	2 (0%)	87	87
11	Q9	135/136 (99%)	135 (100%)	0	100	100
11	g9	136/136 (100%)	135 (99%)	1 (1%)	76	78
12	V9	132/133 (99%)	123 (93%)	9 (7%)	14	41

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	m9	132/133 (99%)	123 (93%)	9 (7%)	14	41
All	All	38416/39608 (97%)	34512 (90%)	3904 (10%)	9	26

5 of 3904 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	I6	21	SER
3	EA	134	LYS
3	I7	107	ASP
3	CA	132	VAL
3	TA	54	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 598 such sidechains are listed below:

Mol	Chain	Res	Type
7	E9	34	GLN
2	LA	149	ASN
8	L9	3	GLN
8	D9	3	GLN
7	i9	57	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 oligosaccharides 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	K7	202	-	46,46,46	0.79	0	63,67,67	0.81	1 (1%)
13	CYC	G7	201	3	46,46,46	2.31	19 (41%)	63,67,67	3.11	29 (46%)
13	CYC	Y6	201	-	46,46,46	2.30	19 (41%)	63,67,67	3.11	29 (46%)
13	CYC	R9	1001	-	46,46,46	2.26	16 (34%)	63,67,67	3.41	30 (47%)
13	CYC	P1	201	-	46,46,46	0.81	0	63,67,67	0.85	2 (3%)
13	CYC	K4	202	-	46,46,46	0.81	0	63,67,67	0.81	1 (1%)
13	CYC	S2	1001	-	46,46,46	2.29	18 (39%)	63,67,67	3.09	29 (46%)
13	CYC	O5	1001	-	46,46,46	2.29	19 (41%)	63,67,67	3.10	29 (46%)
13	CYC	V8	1001	-	46,46,46	2.27	15 (32%)	63,67,67	3.14	30 (47%)
13	CYC	B9	1001	-	46,46,46	2.32	16 (34%)	63,67,67	3.82	31 (49%)
13	CYC	U5	1001	-	46,46,46	2.30	19 (41%)	63,67,67	3.10	29 (46%)
13	CYC	K1	202	-	46,46,46	0.80	0	63,67,67	0.81	1 (1%)
13	CYC	S6	1001	-	46,46,46	2.30	19 (41%)	63,67,67	3.08	29 (46%)
13	CYC	Q4	202	-	46,46,46	0.82	1 (2%)	63,67,67	0.81	1 (1%)
13	CYC	d8	1001	-	46,46,46	2.53	16 (34%)	63,67,67	2.90	26 (41%)
13	CYC	K4	201	-	46,46,46	0.81	1 (2%)	63,67,67	0.80	1 (1%)
13	CYC	Z1	202	-	46,46,46	2.30	19 (41%)	63,67,67	3.08	29 (46%)
13	CYC	O6	1001	-	46,46,46	2.30	19 (41%)	63,67,67	3.09	29 (46%)
13	CYC	g8	1001	-	46,46,46	2.27	15 (32%)	63,67,67	3.13	31 (49%)
13	CYC	M7	201	-	46,46,46	0.81	0	63,67,67	0.81	1 (1%)
13	CYC	L6	201	-	46,46,46	2.30	19 (41%)	63,67,67	3.10	29 (46%)
13	CYC	e9	1001	-	46,46,46	2.32	16 (34%)	63,67,67	3.82	31 (49%)
13	CYC	j9	1001	-	46,46,46	2.32	16 (34%)	63,67,67	3.82	31 (49%)
13	CYC	O9	1001	-	46,46,46	2.32	16 (34%)	63,67,67	3.82	31 (49%)
13	CYC	T1	201	-	46,46,46	0.82	0	63,67,67	0.81	1 (1%)
13	CYC	b8	1001	-	46,46,46	2.54	16 (34%)	63,67,67	2.89	26 (41%)
13	CYC	GA	1001	-	46,46,46	2.30	19 (41%)	63,67,67	3.10	29 (46%)
13	CYC	E3	202	3	46,46,46	0.80	0	63,67,67	0.84	1 (1%)
13	CYC	D8	1001	-	46,46,46	2.54	16 (34%)	63,67,67	2.89	26 (41%)
13	CYC	WA	1001	-	46,46,46	2.30	19 (41%)	63,67,67	3.10	29 (46%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CYC	E9	1001	-	46,46,46	2.26	16 (34%)	63,67,67	3.41	30 (47%)
13	CYC	E7	201	-	46,46,46	2.49	18 (39%)	63,67,67	3.02	28 (44%)
13	CYC	V4	202	-	46,46,46	2.31	19 (41%)	63,67,67	3.10	29 (46%)
13	CYC	R8	1001	-	46,46,46	2.54	16 (34%)	63,67,67	2.89	26 (41%)
13	CYC	Z6	202	-	46,46,46	2.30	19 (41%)	63,67,67	3.10	29 (46%)
13	CYC	M2	201	-	46,46,46	0.82	0	63,67,67	0.80	1 (1%)
13	CYC	G2	201	-	46,46,46	0.82	0	63,67,67	0.80	1 (1%)
13	CYC	B3	1001	-	46,46,46	2.30	19 (41%)	63,67,67	3.11	29 (46%)
13	CYC	19	1203	-	46,46,46	2.32	16 (34%)	63,67,67	3.82	31 (49%)
13	CYC	C9	1001	-	46,46,46	2.26	16 (34%)	63,67,67	3.41	29 (46%)
13	CYC	M1	201	3	46,46,46	0.80	0	63,67,67	0.91	4 (6%)
13	CYC	R5	201	-	46,46,46	0.81	0	63,67,67	0.81	1 (1%)
13	CYC	o9	1001	-	46,46,46	2.26	16 (34%)	63,67,67	3.41	30 (47%)
13	CYC	E1	202	-	46,46,46	0.79	0	63,67,67	0.83	1 (1%)
13	CYC	I3	201	-	46,46,46	2.68	17 (36%)	63,67,67	3.16	29 (46%)
13	CYC	AA	302	-	46,46,46	2.49	18 (39%)	63,67,67	3.01	28 (44%)
13	CYC	k8	1001	-	46,46,46	2.54	16 (34%)	63,67,67	2.89	26 (41%)
13	CYC	D3	1001	-	46,46,46	2.29	19 (41%)	63,67,67	3.10	29 (46%)
13	CYC	G6	201	-	46,46,46	0.82	1 (2%)	63,67,67	0.80	1 (1%)
13	CYC	OA	1001	-	46,46,46	2.30	19 (41%)	63,67,67	3.09	29 (46%)
13	CYC	N5	301	-	46,46,46	2.68	17 (36%)	63,67,67	3.17	29 (46%)
13	CYC	Z6	201	-	46,46,46	0.82	1 (2%)	63,67,67	0.82	1 (1%)
13	CYC	P1	202	-	46,46,46	0.79	1 (2%)	63,67,67	0.81	1 (1%)
13	CYC	I4	202	-	46,46,46	0.80	0	63,67,67	0.81	1 (1%)
13	CYC	T4	202	-	46,46,46	2.31	19 (41%)	63,67,67	3.10	29 (46%)
13	CYC	T8	1001	-	46,46,46	2.54	16 (34%)	63,67,67	2.89	26 (41%)
13	CYC	XA	201	-	46,46,46	2.69	18 (39%)	63,67,67	3.18	30 (47%)
13	CYC	W6	202	-	46,46,46	2.31	19 (41%)	63,67,67	3.10	29 (46%)
13	CYC	Y1	201	-	46,46,46	2.30	19 (41%)	63,67,67	3.09	29 (46%)
13	CYC	T6	201	-	46,46,46	0.81	0	63,67,67	0.81	1 (1%)
13	CYC	A9	1001	-	46,46,46	2.26	16 (34%)	63,67,67	3.41	30 (47%)
13	CYC	K3	202	-	46,46,46	0.79	0	63,67,67	0.81	1 (1%)
13	CYC	c9	1001	-	46,46,46	2.32	16 (34%)	63,67,67	3.83	31 (49%)
13	CYC	D1	1001	-	46,46,46	2.29	18 (39%)	63,67,67	3.10	29 (46%)
13	CYC	LA	201	-	46,46,46	2.30	19 (41%)	63,67,67	3.10	29 (46%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CYC	I5	201	-	46,46,46	2.68	17 (36%)	63,67,67	3.17	29 (46%)
13	CYC	VA	201	-	46,46,46	2.68	16 (34%)	63,67,67	3.16	29 (46%)
13	CYC	Y5	201	-	46,46,46	2.30	19 (41%)	63,67,67	3.10	29 (46%)
13	CYC	p9	1001	-	46,46,46	2.32	16 (34%)	63,67,67	3.82	31 (49%)
13	CYC	C6	202	-	46,46,46	0.83	1 (2%)	63,67,67	0.80	1 (1%)
13	CYC	PA	202	-	46,46,46	0.78	0	63,67,67	0.81	1 (1%)
13	CYC	X1	202	-	46,46,46	0.82	0	63,67,67	0.80	1 (1%)
13	CYC	Q1	201	-	46,46,46	2.30	18 (39%)	63,67,67	3.09	29 (46%)
13	CYC	B4	1001	-	46,46,46	2.30	19 (41%)	63,67,67	3.10	29 (46%)
13	CYC	E6	201	-	46,46,46	2.49	18 (39%)	63,67,67	3.02	28 (44%)
13	CYC	ZA	201	-	46,46,46	2.69	17 (36%)	63,67,67	3.16	29 (46%)
13	CYC	E2	201	-	46,46,46	2.49	17 (36%)	63,67,67	3.01	28 (44%)
13	CYC	c8	1001	-	46,46,46	2.26	15 (32%)	63,67,67	3.13	31 (49%)
13	CYC	W1	1001	-	46,46,46	2.31	19 (41%)	63,67,67	3.10	29 (46%)
13	CYC	W2	201	-	46,46,46	0.79	0	63,67,67	0.82	1 (1%)
13	CYC	m9	201	-	46,46,46	2.34	17 (36%)	63,67,67	3.18	25 (39%)
13	CYC	Y8	1001	-	46,46,46	2.54	16 (34%)	63,67,67	2.89	26 (41%)
13	CYC	G1	201	-	46,46,46	0.81	0	63,67,67	0.80	1 (1%)
13	CYC	V2	201	-	46,46,46	0.80	1 (2%)	63,67,67	0.79	1 (1%)
13	CYC	X8	1001	-	46,46,46	2.27	15 (32%)	63,67,67	3.14	31 (49%)
13	CYC	C6	201	-	46,46,46	2.31	19 (41%)	63,67,67	3.11	29 (46%)
13	CYC	K1	201	-	46,46,46	0.81	1 (2%)	63,67,67	0.79	1 (1%)
13	CYC	f9	1001	-	46,46,46	2.26	16 (34%)	63,67,67	3.41	30 (47%)
13	CYC	t9	1001	-	46,46,46	2.32	16 (34%)	63,67,67	3.82	31 (49%)
13	CYC	V9	201	-	46,46,46	2.34	17 (36%)	63,67,67	3.18	25 (39%)
13	CYC	TA	202	-	46,46,46	0.81	0	63,67,67	0.81	1 (1%)
13	CYC	C1	301	3	46,46,46	2.30	19 (41%)	63,67,67	3.10	29 (46%)
13	CYC	19	1204	-	46,46,46	2.32	16 (34%)	63,67,67	3.83	31 (49%)
13	CYC	C1	302	-	46,46,46	0.83	1 (2%)	63,67,67	0.80	1 (1%)
13	CYC	E4	202	-	46,46,46	0.79	0	63,67,67	0.83	1 (1%)
13	CYC	i9	1001	-	46,46,46	2.26	16 (34%)	63,67,67	3.41	30 (47%)
13	CYC	C4	302	-	46,46,46	0.83	0	63,67,67	0.80	1 (1%)
13	CYC	19	1201	-	46,46,46	2.54	16 (34%)	63,67,67	2.89	26 (41%)
13	CYC	l9	1001	-	46,46,46	2.32	16 (34%)	63,67,67	3.82	31 (49%)
13	CYC	x9	1001	-	46,46,46	2.31	16 (34%)	63,67,67	3.82	31 (49%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CYC	r9	1001	-	46,46,46	2.32	16 (34%)	63,67,67	3.82	31 (49%)
13	CYC	IA	201	-	46,46,46	2.68	17 (36%)	63,67,67	3.18	29 (46%)
13	CYC	W8	1001	-	46,46,46	2.54	16 (34%)	63,67,67	2.89	25 (39%)
13	CYC	AA	301	-	46,46,46	2.49	18 (39%)	63,67,67	3.03	28 (44%)
13	CYC	M3	201	-	46,46,46	0.81	0	63,67,67	0.82	1 (1%)
13	CYC	V1	201	-	46,46,46	0.81	1 (2%)	63,67,67	0.80	1 (1%)
13	CYC	H9	1001	-	46,46,46	2.32	16 (34%)	63,67,67	3.83	31 (49%)
13	CYC	D6	1001	-	46,46,46	2.29	19 (41%)	63,67,67	3.10	29 (46%)
13	CYC	L7	201	-	46,46,46	2.31	19 (41%)	63,67,67	3.10	29 (46%)
13	CYC	A5	303	-	46,46,46	2.68	17 (36%)	63,67,67	3.13	30 (47%)
13	CYC	19	1202	10	46,46,46	2.29	17 (36%)	63,67,67	3.47	32 (50%)
13	CYC	p8	1001	-	46,46,46	2.27	15 (32%)	63,67,67	3.13	30 (47%)
13	CYC	Z4	201	-	46,46,46	0.83	1 (2%)	63,67,67	0.81	1 (1%)
13	CYC	N9	1001	-	46,46,46	2.26	16 (34%)	63,67,67	3.41	30 (47%)
13	CYC	W2	203	-	46,46,46	0.82	0	63,67,67	0.81	1 (1%)
13	CYC	SA	1001	-	46,46,46	2.30	19 (41%)	63,67,67	3.10	29 (46%)
13	CYC	A5	301	-	46,46,46	2.49	18 (39%)	63,67,67	3.03	29 (46%)
13	CYC	B8	1001	-	46,46,46	2.53	16 (34%)	63,67,67	2.89	26 (41%)
13	CYC	H3	1001	-	46,46,46	2.29	19 (41%)	63,67,67	3.07	29 (46%)
13	CYC	C4	301	3	46,46,46	2.30	19 (41%)	63,67,67	3.10	29 (46%)
13	CYC	G4	201	-	46,46,46	0.82	1 (2%)	63,67,67	0.80	1 (1%)
13	CYC	L1	201	-	46,46,46	2.30	19 (41%)	63,67,67	3.11	29 (46%)
13	CYC	R1	1001	3	46,46,46	2.31	19 (41%)	63,67,67	3.11	29 (46%)
13	CYC	J4	1001	-	46,46,46	2.30	19 (41%)	63,67,67	3.09	29 (46%)
13	CYC	GA	1002	-	46,46,46	0.81	0	63,67,67	0.79	1 (1%)
13	CYC	U2	201	-	46,46,46	0.82	1 (2%)	63,67,67	0.81	1 (1%)
13	CYC	H4	1001	-	46,46,46	2.30	19 (41%)	63,67,67	3.08	29 (46%)
13	CYC	L4	201	-	46,46,46	2.30	19 (41%)	63,67,67	3.10	29 (46%)
13	CYC	X5	201	-	46,46,46	2.69	17 (36%)	63,67,67	3.18	30 (47%)
13	CYC	M5	1003	-	46,46,46	0.83	0	63,67,67	0.80	1 (1%)
13	CYC	VA	202	-	46,46,46	0.80	1 (2%)	63,67,67	0.79	1 (1%)
13	CYC	I8	1001	-	46,46,46	2.54	16 (34%)	63,67,67	2.89	26 (41%)
13	CYC	X1	201	-	46,46,46	2.69	17 (36%)	63,67,67	3.19	30 (47%)
13	CYC	A5	304	-	46,46,46	2.69	16 (34%)	63,67,67	3.16	29 (46%)
13	CYC	X9	1001	-	46,46,46	2.26	16 (34%)	63,67,67	3.41	30 (47%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CYC	g9	1001	11	46,46,46	2.35	19 (41%)	63,67,67	3.04	28 (44%)
13	CYC	T5	201	-	46,46,46	2.68	17 (36%)	63,67,67	3.17	29 (46%)
13	CYC	K7	201	-	46,46,46	0.81	0	63,67,67	0.80	1 (1%)
13	CYC	N6	301	-	46,46,46	0.81	0	63,67,67	0.90	3 (4%)
13	CYC	E8	1001	-	46,46,46	2.27	15 (32%)	63,67,67	3.13	31 (49%)
13	CYC	B1	1001	-	46,46,46	2.30	19 (41%)	63,67,67	3.10	29 (46%)
13	CYC	I6	202	-	46,46,46	0.80	0	63,67,67	0.81	1 (1%)
13	CYC	P9	1001	-	46,46,46	2.26	17 (36%)	63,67,67	3.41	30 (47%)
13	CYC	M6	201	-	46,46,46	0.82	0	63,67,67	0.81	1 (1%)
13	CYC	V2	202	-	46,46,46	2.30	19 (41%)	63,67,67	3.11	29 (46%)
13	CYC	O2	1001	-	46,46,46	2.30	19 (41%)	63,67,67	3.09	29 (46%)
13	CYC	I2	202	-	46,46,46	0.81	0	63,67,67	0.82	1 (1%)
13	CYC	Q8	1001	-	46,46,46	2.27	15 (32%)	63,67,67	3.12	30 (47%)
13	CYC	F6	1001	-	46,46,46	2.31	19 (41%)	63,67,67	3.11	29 (46%)
13	CYC	N2	301	-	46,46,46	0.81	0	63,67,67	0.91	2 (3%)
13	CYC	B7	1001	-	46,46,46	2.30	19 (41%)	63,67,67	3.11	29 (46%)
13	CYC	G7	202	-	46,46,46	0.82	0	63,67,67	0.80	1 (1%)
13	CYC	X5	202	-	46,46,46	0.82	0	63,67,67	0.80	1 (1%)
13	CYC	29	1001	-	46,46,46	2.31	16 (34%)	63,67,67	3.82	30 (47%)
13	CYC	Z1	201	-	46,46,46	0.82	1 (2%)	63,67,67	0.82	1 (1%)
13	CYC	k9	1001	-	46,46,46	2.26	16 (34%)	63,67,67	3.41	30 (47%)
13	CYC	R4	1001	3	46,46,46	2.31	19 (41%)	63,67,67	3.11	29 (46%)
13	CYC	P4	201	-	46,46,46	0.80	0	63,67,67	0.85	2 (3%)
13	CYC	S9	1001	-	46,46,46	2.32	16 (34%)	63,67,67	3.82	30 (47%)
13	CYC	IA	202	-	46,46,46	0.80	0	63,67,67	0.81	1 (1%)
13	CYC	39	1001	-	46,46,46	2.31	16 (34%)	63,67,67	3.83	31 (49%)
13	CYC	K2	202	-	46,46,46	0.80	0	63,67,67	0.81	1 (1%)
13	CYC	P2	201	-	46,46,46	0.80	0	63,67,67	0.84	2 (3%)
13	CYC	F4	1001	-	46,46,46	2.30	19 (41%)	63,67,67	3.09	29 (46%)
13	CYC	E4	201	3	46,46,46	2.49	18 (39%)	63,67,67	3.02	29 (46%)
13	CYC	JA	1001	-	46,46,46	2.29	19 (41%)	63,67,67	3.10	29 (46%)
13	CYC	J2	1001	-	46,46,46	2.31	19 (41%)	63,67,67	3.10	29 (46%)
13	CYC	UA	1001	-	46,46,46	2.30	19 (41%)	63,67,67	3.10	29 (46%)
13	CYC	M4	202	-	46,46,46	0.81	0	63,67,67	0.80	1 (1%)
13	CYC	q8	1001	-	46,46,46	2.53	16 (34%)	63,67,67	2.90	26 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CYC	A5	302	-	46,46,46	2.50	18 (39%)	63,67,67	3.01	27 (42%)
13	CYC	I9	1001	-	46,46,46	2.26	17 (36%)	63,67,67	3.41	29 (46%)
13	CYC	F2	1001	-	46,46,46	2.31	19 (41%)	63,67,67	3.11	29 (46%)
13	CYC	C7	201	-	46,46,46	0.83	1 (2%)	63,67,67	0.81	1 (1%)
13	CYC	b9	1001	-	46,46,46	2.26	17 (36%)	63,67,67	3.41	30 (47%)
13	CYC	N2	302	-	46,46,46	2.31	19 (41%)	63,67,67	3.11	29 (46%)
13	CYC	G9	1001	-	46,46,46	2.26	16 (34%)	63,67,67	3.42	30 (47%)
13	CYC	D4	1001	-	46,46,46	2.29	19 (41%)	63,67,67	3.09	29 (46%)
13	CYC	H1	1001	-	46,46,46	2.30	20 (43%)	63,67,67	3.08	29 (46%)
13	CYC	q9	1001	-	46,46,46	2.26	17 (36%)	63,67,67	3.41	30 (47%)
13	CYC	U4	1001	-	46,46,46	2.30	19 (41%)	63,67,67	3.10	29 (46%)
13	CYC	E3	201	-	46,46,46	2.49	18 (39%)	63,67,67	3.02	29 (46%)
13	CYC	PA	201	-	46,46,46	0.80	0	63,67,67	0.84	2 (3%)
13	CYC	P6	201	-	46,46,46	0.80	0	63,67,67	0.84	2 (3%)
13	CYC	EA	202	-	46,46,46	2.30	19 (41%)	63,67,67	3.10	29 (46%)
13	CYC	M1	202	-	46,46,46	0.81	0	63,67,67	0.80	1 (1%)
13	CYC	B5	1001	-	46,46,46	2.30	19 (41%)	63,67,67	3.10	29 (46%)
13	CYC	G4	202	-	46,46,46	2.30	19 (41%)	63,67,67	3.10	29 (46%)
13	CYC	Z9	1001	-	46,46,46	2.26	17 (36%)	63,67,67	3.41	29 (46%)
13	CYC	09	1201	-	46,46,46	2.53	16 (34%)	63,67,67	2.89	26 (41%)
13	CYC	s9	1001	-	46,46,46	2.26	16 (34%)	63,67,67	3.41	30 (47%)
13	CYC	I4	201	3	46,46,46	2.69	17 (36%)	63,67,67	3.17	29 (46%)
13	CYC	d9	1001	-	46,46,46	2.26	16 (34%)	63,67,67	3.41	30 (47%)
13	CYC	Z2	202	-	46,46,46	2.30	19 (41%)	63,67,67	3.10	29 (46%)
13	CYC	E2	202	3	46,46,46	0.79	0	63,67,67	0.83	1 (1%)
13	CYC	A3	301	-	46,46,46	2.30	19 (41%)	63,67,67	3.09	29 (46%)
13	CYC	H2	1001	-	46,46,46	2.30	19 (41%)	63,67,67	3.08	29 (46%)
13	CYC	S5	1001	-	46,46,46	2.29	19 (41%)	63,67,67	3.09	29 (46%)
13	CYC	KA	201	-	46,46,46	0.81	0	63,67,67	0.80	1 (1%)
13	CYC	Z8	1001	-	46,46,46	2.27	15 (32%)	63,67,67	3.13	30 (47%)
13	CYC	T5	202	-	46,46,46	0.82	0	63,67,67	0.81	1 (1%)
13	CYC	D5	1001	-	46,46,46	2.29	19 (41%)	63,67,67	3.10	29 (46%)
13	CYC	G3	202	-	46,46,46	0.82	0	63,67,67	0.80	1 (1%)
13	CYC	e8	1001	-	46,46,46	2.27	15 (32%)	63,67,67	3.13	30 (47%)
13	CYC	r8	1001	-	46,46,46	2.27	15 (32%)	63,67,67	3.13	30 (47%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CYC	G6	202	3	46,46,46	2.31	19 (41%)	63,67,67	3.11	29 (46%)
13	CYC	N3	301	-	46,46,46	0.81	0	63,67,67	0.90	3 (4%)
13	CYC	H8	1001	-	46,46,46	2.27	15 (32%)	63,67,67	3.14	31 (49%)
13	CYC	AA	304	-	46,46,46	2.69	17 (36%)	63,67,67	3.16	29 (46%)
13	CYC	D9	1001	-	46,46,46	2.32	16 (34%)	63,67,67	3.82	31 (49%)
13	CYC	I3	202	-	46,46,46	0.80	0	63,67,67	0.81	1 (1%)
13	CYC	P5	201	-	46,46,46	0.80	0	63,67,67	0.84	2 (3%)
13	CYC	K9	1001	-	46,46,46	2.26	17 (36%)	63,67,67	3.41	30 (47%)
13	CYC	Z5	202	-	46,46,46	0.82	1 (2%)	63,67,67	0.81	1 (1%)
13	CYC	W5	1001	-	46,46,46	2.30	19 (41%)	63,67,67	3.09	29 (46%)
13	CYC	G1	202	-	46,46,46	2.30	19 (41%)	63,67,67	3.09	29 (46%)
13	CYC	TA	201	-	46,46,46	2.68	16 (34%)	63,67,67	3.17	29 (46%)
13	CYC	L2	201	-	46,46,46	2.30	19 (41%)	63,67,67	3.10	29 (46%)
13	CYC	C2	202	-	46,46,46	0.83	0	63,67,67	0.80	1 (1%)
13	CYC	l8	1001	-	46,46,46	2.27	15 (32%)	63,67,67	3.13	30 (47%)
13	CYC	V6	202	-	46,46,46	2.30	18 (39%)	63,67,67	3.11	29 (46%)
13	CYC	I1	202	-	46,46,46	0.80	0	63,67,67	0.81	1 (1%)
13	CYC	A7	301	-	46,46,46	2.30	19 (41%)	63,67,67	3.08	29 (46%)
13	CYC	CA	201	-	46,46,46	0.82	0	63,67,67	0.80	1 (1%)
13	CYC	E1	201	3	46,46,46	2.49	18 (39%)	63,67,67	3.02	28 (44%)
13	CYC	B6	1001	-	46,46,46	2.29	19 (41%)	63,67,67	3.10	29 (46%)
13	CYC	MA	1001	-	46,46,46	2.29	19 (41%)	63,67,67	3.09	29 (46%)
13	CYC	MA	1003	-	46,46,46	0.82	0	63,67,67	0.80	1 (1%)
13	CYC	N7	301	-	46,46,46	0.81	0	63,67,67	0.90	2 (3%)
13	CYC	O4	1001	-	46,46,46	2.30	19 (41%)	63,67,67	3.10	29 (46%)
13	CYC	Q6	201	-	46,46,46	2.30	19 (41%)	63,67,67	3.12	29 (46%)
13	CYC	K6	202	-	46,46,46	0.80	0	63,67,67	0.81	1 (1%)
13	CYC	DA	1001	-	46,46,46	2.29	19 (41%)	63,67,67	3.10	29 (46%)
13	CYC	PA	203	-	46,46,46	2.30	19 (41%)	63,67,67	3.10	29 (46%)
13	CYC	F3	1001	-	46,46,46	2.31	19 (41%)	63,67,67	3.11	29 (46%)
13	CYC	h8	1001	-	46,46,46	2.54	16 (34%)	63,67,67	2.90	26 (41%)
13	CYC	T9	1001	-	46,46,46	2.26	17 (36%)	63,67,67	3.41	30 (47%)
13	CYC	YA	201	-	46,46,46	2.30	19 (41%)	63,67,67	3.09	29 (46%)
13	CYC	f8	1001	-	46,46,46	2.54	16 (34%)	63,67,67	2.90	26 (41%)
13	CYC	D2	1001	-	46,46,46	2.29	19 (41%)	63,67,67	3.10	29 (46%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CYC	G5	201	-	46,46,46	0.81	0	63,67,67	0.80	1 (1%)
13	CYC	L8	1001	-	46,46,46	2.27	15 (32%)	63,67,67	3.13	30 (47%)
13	CYC	C5	201	-	46,46,46	0.83	0	63,67,67	0.79	1 (1%)
13	CYC	F1	1001	-	46,46,46	2.30	19 (41%)	63,67,67	3.09	29 (46%)
13	CYC	t8	1001	-	46,46,46	2.27	15 (32%)	63,67,67	3.13	30 (47%)
13	CYC	G3	201	3	46,46,46	2.31	19 (41%)	63,67,67	3.11	29 (46%)
13	CYC	S8	1001	-	46,46,46	2.27	15 (32%)	63,67,67	3.13	31 (49%)
13	CYC	F8	1001	-	46,46,46	2.54	16 (34%)	63,67,67	2.89	26 (41%)
13	CYC	U9	1001	-	46,46,46	2.31	16 (34%)	63,67,67	3.82	31 (49%)
13	CYC	v9	1001	-	46,46,46	2.32	16 (34%)	63,67,67	3.83	31 (49%)
13	CYC	X2	201	-	46,46,46	2.68	17 (36%)	63,67,67	3.18	30 (47%)
13	CYC	MA	1002	-	46,46,46	0.80	0	63,67,67	0.91	3 (4%)
13	CYC	NA	301	-	46,46,46	2.69	17 (36%)	63,67,67	3.18	30 (47%)
13	CYC	09	1203	-	46,46,46	2.32	15 (32%)	63,67,67	3.83	31 (49%)
13	CYC	J7	1001	-	46,46,46	2.31	19 (41%)	63,67,67	3.10	29 (46%)
13	CYC	RA	201	-	46,46,46	0.81	0	63,67,67	0.80	1 (1%)
13	CYC	j8	1001	-	46,46,46	2.27	15 (32%)	63,67,67	3.13	31 (49%)
13	CYC	X6	201	-	46,46,46	2.68	17 (36%)	63,67,67	3.18	29 (46%)
13	CYC	K5	201	-	46,46,46	0.80	0	63,67,67	0.81	1 (1%)
13	CYC	P5	202	-	46,46,46	0.78	0	63,67,67	0.81	1 (1%)
13	CYC	F9	1001	-	46,46,46	2.32	16 (34%)	63,67,67	3.83	31 (49%)
13	CYC	P5	203	-	46,46,46	2.30	19 (41%)	63,67,67	3.10	29 (46%)
13	CYC	Y4	201	-	46,46,46	2.30	19 (41%)	63,67,67	3.09	29 (46%)
13	CYC	L9	1001	-	46,46,46	2.32	16 (34%)	63,67,67	3.83	31 (49%)
13	CYC	Z5	201	-	46,46,46	2.69	18 (39%)	63,67,67	3.16	29 (46%)
13	CYC	I7	201	-	46,46,46	2.68	17 (36%)	63,67,67	3.16	29 (46%)
13	CYC	O1	1001	-	46,46,46	2.30	19 (41%)	63,67,67	3.10	29 (46%)
13	CYC	P8	1001	-	46,46,46	2.54	16 (34%)	63,67,67	2.88	26 (41%)
13	CYC	K2	201	-	46,46,46	0.82	0	63,67,67	0.81	1 (1%)
13	CYC	T2	201	-	46,46,46	0.81	0	63,67,67	0.81	1 (1%)
13	CYC	X4	201	-	46,46,46	2.69	17 (36%)	63,67,67	3.18	30 (47%)
13	CYC	M4	201	3	46,46,46	0.80	0	63,67,67	0.90	3 (4%)
13	CYC	J1	1001	-	46,46,46	2.30	19 (41%)	63,67,67	3.09	29 (46%)
13	CYC	I7	202	-	46,46,46	0.80	0	63,67,67	0.81	1 (1%)
13	CYC	U6	201	-	46,46,46	0.82	1 (2%)	63,67,67	0.81	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CYC	J9	1001	-	46,46,46	2.32	16 (34%)	63,67,67	3.83	31 (49%)
13	CYC	J6	1001	-	46,46,46	2.31	19 (41%)	63,67,67	3.10	29 (46%)
13	CYC	s8	1001	-	46,46,46	2.54	16 (34%)	63,67,67	2.90	26 (41%)
13	CYC	w9	1001	-	46,46,46	2.26	16 (34%)	63,67,67	3.41	30 (47%)
13	CYC	Z4	202	-	46,46,46	2.30	19 (41%)	63,67,67	3.10	29 (46%)
13	CYC	K8	1001	-	46,46,46	2.53	16 (34%)	63,67,67	2.89	26 (41%)
13	CYC	X4	202	-	46,46,46	0.82	0	63,67,67	0.80	1 (1%)
13	CYC	E5	201	-	46,46,46	0.80	0	63,67,67	0.83	1 (1%)
13	CYC	W2	202	-	46,46,46	2.31	19 (41%)	63,67,67	3.10	29 (46%)
13	CYC	J8	1001	-	46,46,46	2.27	15 (32%)	63,67,67	3.13	30 (47%)
13	CYC	Y2	201	-	46,46,46	2.30	19 (41%)	63,67,67	3.11	29 (46%)
13	CYC	J5	1001	-	46,46,46	2.30	19 (41%)	63,67,67	3.10	29 (46%)
13	CYC	n8	1001	-	46,46,46	2.27	15 (32%)	63,67,67	3.13	30 (47%)
13	CYC	y9	1001	-	46,46,46	2.26	16 (34%)	63,67,67	3.41	30 (47%)
13	CYC	EA	201	-	46,46,46	0.80	0	63,67,67	0.83	1 (1%)
13	CYC	I5	202	-	46,46,46	0.81	0	63,67,67	0.81	1 (1%)
13	CYC	Z2	201	-	46,46,46	0.83	1 (2%)	63,67,67	0.82	1 (1%)
13	CYC	E6	202	3	46,46,46	0.79	0	63,67,67	0.83	1 (1%)
13	CYC	ZA	202	-	46,46,46	0.83	1 (2%)	63,67,67	0.81	1 (1%)
13	CYC	AA	303	-	46,46,46	2.67	17 (36%)	63,67,67	3.13	30 (47%)
13	CYC	I6	201	-	46,46,46	2.68	17 (36%)	63,67,67	3.17	29 (46%)
13	CYC	M5	1001	-	46,46,46	2.30	19 (41%)	63,67,67	3.10	29 (46%)
13	CYC	H6	1001	-	46,46,46	2.29	19 (41%)	63,67,67	3.07	29 (46%)
13	CYC	S1	1001	-	46,46,46	2.29	19 (41%)	63,67,67	3.08	29 (46%)
13	CYC	09	1202	-	46,46,46	2.27	17 (36%)	63,67,67	3.18	28 (44%)
13	CYC	V1	202	-	46,46,46	2.31	19 (41%)	63,67,67	3.10	29 (46%)
13	CYC	X6	202	-	46,46,46	0.81	0	63,67,67	0.81	1 (1%)
13	CYC	T1	202	-	46,46,46	2.31	19 (41%)	63,67,67	3.10	29 (46%)
13	CYC	E5	202	-	46,46,46	2.30	19 (41%)	63,67,67	3.10	29 (46%)
13	CYC	P4	202	-	46,46,46	0.79	1 (2%)	63,67,67	0.82	1 (1%)
13	CYC	D7	1001	-	46,46,46	2.30	19 (41%)	63,67,67	3.09	29 (46%)
13	CYC	V6	201	-	46,46,46	0.81	1 (2%)	63,67,67	0.79	1 (1%)
13	CYC	I1	201	3	46,46,46	2.68	17 (36%)	63,67,67	3.17	30 (47%)
13	CYC	Q9	201	11	46,46,46	2.37	17 (36%)	63,67,67	2.91	26 (41%)
13	CYC	O8	1001	-	46,46,46	2.27	15 (32%)	63,67,67	3.13	30 (47%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CYC	M5	1002	-	46,46,46	0.80	0	63,67,67	0.90	3 (4%)
13	CYC	19	1205	-	46,46,46	2.32	16 (34%)	63,67,67	3.83	31 (49%)
13	CYC	U1	1001	-	46,46,46	2.29	19 (41%)	63,67,67	3.09	29 (46%)
13	CYC	V4	201	-	46,46,46	0.81	1 (2%)	63,67,67	0.79	1 (1%)
13	CYC	o8	1001	-	46,46,46	2.53	16 (34%)	63,67,67	2.89	26 (41%)
13	CYC	W6	201	-	46,46,46	0.78	0	63,67,67	0.82	1 (1%)
13	CYC	S4	1001	-	46,46,46	2.30	19 (41%)	63,67,67	3.09	29 (46%)
13	CYC	G2	202	3	46,46,46	2.30	19 (41%)	63,67,67	3.11	29 (46%)
13	CYC	Q4	201	-	46,46,46	2.30	19 (41%)	63,67,67	3.10	29 (46%)
13	CYC	I2	201	-	46,46,46	2.69	17 (36%)	63,67,67	3.17	29 (46%)
13	CYC	W4	1001	-	46,46,46	2.31	19 (41%)	63,67,67	3.10	29 (46%)
13	CYC	K3	201	-	46,46,46	0.81	0	63,67,67	0.80	1 (1%)
13	CYC	C3	201	-	46,46,46	0.83	1 (2%)	63,67,67	0.80	1 (1%)
13	CYC	M8	1001	-	46,46,46	2.54	16 (34%)	63,67,67	2.90	26 (41%)
13	CYC	A8	1001	-	46,46,46	2.27	15 (32%)	63,67,67	3.13	31 (49%)
13	CYC	z9	1001	-	46,46,46	2.32	16 (34%)	63,67,67	3.83	31 (49%)
13	CYC	C2	201	-	46,46,46	2.31	19 (41%)	63,67,67	3.10	29 (46%)
13	CYC	J3	1001	-	46,46,46	2.31	19 (41%)	63,67,67	3.09	29 (46%)
13	CYC	Q1	202	-	46,46,46	0.82	1 (2%)	63,67,67	0.81	1 (1%)
13	CYC	XA	202	-	46,46,46	0.82	0	63,67,67	0.80	1 (1%)
13	CYC	C8	1001	-	46,46,46	2.27	15 (32%)	63,67,67	3.13	30 (47%)
13	CYC	L5	201	-	46,46,46	2.30	19 (41%)	63,67,67	3.10	29 (46%)
13	CYC	H7	1001	-	46,46,46	2.30	19 (41%)	63,67,67	3.08	29 (46%)
13	CYC	R6	1001	-	46,46,46	2.31	19 (41%)	63,67,67	3.10	29 (46%)
13	CYC	N6	302	-	46,46,46	2.31	19 (41%)	63,67,67	3.11	29 (46%)
13	CYC	U2	202	-	46,46,46	2.30	19 (41%)	63,67,67	3.09	29 (46%)
13	CYC	B2	1001	-	46,46,46	2.29	19 (41%)	63,67,67	3.10	29 (46%)
13	CYC	T4	201	-	46,46,46	0.82	0	63,67,67	0.80	1 (1%)
13	CYC	Q2	201	-	46,46,46	2.30	19 (41%)	63,67,67	3.10	29 (46%)
13	CYC	R2	1001	-	46,46,46	2.31	19 (41%)	63,67,67	3.11	29 (46%)
13	CYC	u9	1001	-	46,46,46	2.26	16 (34%)	63,67,67	3.41	29 (46%)
13	CYC	F7	1001	-	46,46,46	2.31	19 (41%)	63,67,67	3.12	29 (46%)
13	CYC	K6	201	-	46,46,46	0.81	0	63,67,67	0.80	1 (1%)
13	CYC	L3	201	-	46,46,46	2.30	19 (41%)	63,67,67	3.11	29 (46%)
13	CYC	U6	202	-	46,46,46	2.30	19 (41%)	63,67,67	3.09	29 (46%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CYC	V5	201	-	46,46,46	2.68	16 (34%)	63,67,67	3.16	29 (46%)
13	CYC	E7	202	3	46,46,46	0.79	0	63,67,67	0.83	1 (1%)
13	CYC	V5	202	-	46,46,46	0.80	0	63,67,67	0.79	1 (1%)

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	K7	202	-	-	12/26/74/74	0/4/4/4
13	CYC	G7	201	3	-	8/26/74/74	0/4/4/4
13	CYC	Y6	201	-	-	8/26/74/74	0/4/4/4
13	CYC	R9	1001	-	-	9/26/74/74	0/4/4/4
13	CYC	P1	201	-	-	8/26/74/74	0/4/4/4
13	CYC	K4	202	-	-	12/26/74/74	0/4/4/4
13	CYC	S2	1001	-	-	8/26/74/74	0/4/4/4
13	CYC	O5	1001	-	-	8/26/74/74	0/4/4/4
13	CYC	V8	1001	-	-	9/26/74/74	0/4/4/4
13	CYC	B9	1001	-	-	8/26/74/74	0/4/4/4
13	CYC	U5	1001	-	-	8/26/74/74	0/4/4/4
13	CYC	K1	202	-	-	12/26/74/74	0/4/4/4
13	CYC	S6	1001	-	-	8/26/74/74	0/4/4/4
13	CYC	Q4	202	-	-	12/26/74/74	0/4/4/4
13	CYC	d8	1001	-	-	9/26/74/74	0/4/4/4
13	CYC	K4	201	-	-	12/26/74/74	0/4/4/4
13	CYC	Z1	202	-	-	8/26/74/74	0/4/4/4
13	CYC	O6	1001	-	-	8/26/74/74	0/4/4/4
13	CYC	g8	1001	-	-	9/26/74/74	0/4/4/4
13	CYC	M7	201	-	-	12/26/74/74	0/4/4/4
13	CYC	L6	201	-	-	8/26/74/74	0/4/4/4
13	CYC	e9	1001	-	-	8/26/74/74	0/4/4/4
13	CYC	j9	1001	-	-	8/26/74/74	0/4/4/4
13	CYC	O9	1001	-	-	8/26/74/74	0/4/4/4
13	CYC	T1	201	-	-	12/26/74/74	0/4/4/4
13	CYC	b8	1001	-	-	9/26/74/74	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CYC	GA	1001	-	-	8/26/74/74	0/4/4/4
13	CYC	E3	202	3	-	12/26/74/74	0/4/4/4
13	CYC	D8	1001	-	-	9/26/74/74	0/4/4/4
13	CYC	WA	1001	-	-	8/26/74/74	0/4/4/4
13	CYC	E9	1001	-	-	9/26/74/74	0/4/4/4
13	CYC	E7	201	-	-	8/26/74/74	0/4/4/4
13	CYC	V4	202	-	-	8/26/74/74	0/4/4/4
13	CYC	R8	1001	-	-	9/26/74/74	0/4/4/4
13	CYC	Z6	202	-	-	8/26/74/74	0/4/4/4
13	CYC	M2	201	-	-	12/26/74/74	0/4/4/4
13	CYC	G2	201	-	-	12/26/74/74	0/4/4/4
13	CYC	B3	1001	-	-	8/26/74/74	0/4/4/4
13	CYC	19	1203	-	-	9/26/74/74	0/4/4/4
13	CYC	C9	1001	-	-	9/26/74/74	0/4/4/4
13	CYC	M1	201	3	-	10/26/74/74	0/4/4/4
13	CYC	R5	201	-	-	12/26/74/74	0/4/4/4
13	CYC	o9	1001	-	-	9/26/74/74	0/4/4/4
13	CYC	E1	202	-	-	12/26/74/74	0/4/4/4
13	CYC	I3	201	-	-	9/26/74/74	0/4/4/4
13	CYC	AA	302	-	-	8/26/74/74	0/4/4/4
13	CYC	k8	1001	-	-	9/26/74/74	0/4/4/4
13	CYC	D3	1001	-	-	8/26/74/74	0/4/4/4
13	CYC	G6	201	-	-	12/26/74/74	0/4/4/4
13	CYC	OA	1001	-	-	8/26/74/74	0/4/4/4
13	CYC	N5	301	-	-	9/26/74/74	0/4/4/4
13	CYC	Z6	201	-	-	12/26/74/74	0/4/4/4
13	CYC	P1	202	-	-	12/26/74/74	0/4/4/4
13	CYC	I4	202	-	-	12/26/74/74	0/4/4/4
13	CYC	T4	202	-	-	8/26/74/74	0/4/4/4
13	CYC	T8	1001	-	-	9/26/74/74	0/4/4/4
13	CYC	XA	201	-	-	9/26/74/74	0/4/4/4
13	CYC	W6	202	-	-	8/26/74/74	0/4/4/4
13	CYC	Y1	201	-	-	8/26/74/74	0/4/4/4
13	CYC	T6	201	-	-	12/26/74/74	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CYC	A9	1001	-	-	9/26/74/74	0/4/4/4
13	CYC	K3	202	-	-	12/26/74/74	0/4/4/4
13	CYC	c9	1001	-	-	8/26/74/74	0/4/4/4
13	CYC	D1	1001	-	-	8/26/74/74	0/4/4/4
13	CYC	LA	201	-	-	8/26/74/74	0/4/4/4
13	CYC	I5	201	-	-	9/26/74/74	0/4/4/4
13	CYC	VA	201	-	-	9/26/74/74	0/4/4/4
13	CYC	Y5	201	-	-	8/26/74/74	0/4/4/4
13	CYC	p9	1001	-	-	8/26/74/74	0/4/4/4
13	CYC	C6	202	-	-	12/26/74/74	0/4/4/4
13	CYC	PA	202	-	-	12/26/74/74	0/4/4/4
13	CYC	X1	202	-	-	12/26/74/74	0/4/4/4
13	CYC	Q1	201	-	-	8/26/74/74	0/4/4/4
13	CYC	B4	1001	-	-	8/26/74/74	0/4/4/4
13	CYC	E6	201	-	-	8/26/74/74	0/4/4/4
13	CYC	ZA	201	-	-	9/26/74/74	0/4/4/4
13	CYC	E2	201	-	-	8/26/74/74	0/4/4/4
13	CYC	c8	1001	-	-	9/26/74/74	0/4/4/4
13	CYC	W1	1001	-	-	8/26/74/74	0/4/4/4
13	CYC	W2	201	-	-	12/26/74/74	0/4/4/4
13	CYC	m9	201	-	-	8/26/74/74	0/4/4/4
13	CYC	Y8	1001	-	-	9/26/74/74	0/4/4/4
13	CYC	G1	201	-	-	12/26/74/74	0/4/4/4
13	CYC	V2	201	-	-	12/26/74/74	0/4/4/4
13	CYC	X8	1001	-	-	9/26/74/74	0/4/4/4
13	CYC	C6	201	-	-	8/26/74/74	0/4/4/4
13	CYC	K1	201	-	-	12/26/74/74	0/4/4/4
13	CYC	f9	1001	-	-	9/26/74/74	0/4/4/4
13	CYC	t9	1001	-	-	8/26/74/74	0/4/4/4
13	CYC	V9	201	-	-	8/26/74/74	0/4/4/4
13	CYC	TA	202	-	-	12/26/74/74	0/4/4/4
13	CYC	C1	301	3	-	8/26/74/74	0/4/4/4
13	CYC	19	1204	-	-	8/26/74/74	0/4/4/4
13	CYC	C1	302	-	-	12/26/74/74	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CYC	E4	202	-	-	12/26/74/74	0/4/4/4
13	CYC	i9	1001	-	-	9/26/74/74	0/4/4/4
13	CYC	C4	302	-	-	12/26/74/74	0/4/4/4
13	CYC	19	1201	-	-	9/26/74/74	0/4/4/4
13	CYC	l9	1001	-	-	8/26/74/74	0/4/4/4
13	CYC	x9	1001	-	-	8/26/74/74	0/4/4/4
13	CYC	r9	1001	-	-	8/26/74/74	0/4/4/4
13	CYC	IA	201	-	-	9/26/74/74	0/4/4/4
13	CYC	W8	1001	-	-	9/26/74/74	0/4/4/4
13	CYC	AA	301	-	-	8/26/74/74	0/4/4/4
13	CYC	M3	201	-	-	12/26/74/74	0/4/4/4
13	CYC	V1	201	-	-	12/26/74/74	0/4/4/4
13	CYC	H9	1001	-	-	9/26/74/74	0/4/4/4
13	CYC	D6	1001	-	-	8/26/74/74	0/4/4/4
13	CYC	L7	201	-	-	8/26/74/74	0/4/4/4
13	CYC	A5	303	-	-	9/26/74/74	0/4/4/4
13	CYC	19	1202	10	-	8/26/74/74	0/4/4/4
13	CYC	p8	1001	-	-	9/26/74/74	0/4/4/4
13	CYC	Z4	201	-	-	12/26/74/74	0/4/4/4
13	CYC	N9	1001	-	-	9/26/74/74	0/4/4/4
13	CYC	W2	203	-	-	12/26/74/74	0/4/4/4
13	CYC	SA	1001	-	-	8/26/74/74	0/4/4/4
13	CYC	A5	301	-	-	8/26/74/74	0/4/4/4
13	CYC	B8	1001	-	-	9/26/74/74	0/4/4/4
13	CYC	H3	1001	-	-	8/26/74/74	0/4/4/4
13	CYC	C4	301	3	-	8/26/74/74	0/4/4/4
13	CYC	G4	201	-	-	12/26/74/74	0/4/4/4
13	CYC	L1	201	-	-	8/26/74/74	0/4/4/4
13	CYC	R1	1001	3	-	8/26/74/74	0/4/4/4
13	CYC	J4	1001	-	-	8/26/74/74	0/4/4/4
13	CYC	GA	1002	-	-	12/26/74/74	0/4/4/4
13	CYC	U2	201	-	-	12/26/74/74	0/4/4/4
13	CYC	H4	1001	-	-	8/26/74/74	0/4/4/4
13	CYC	L4	201	-	-	8/26/74/74	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CYC	X5	201	-	-	9/26/74/74	0/4/4/4
13	CYC	M5	1003	-	-	12/26/74/74	0/4/4/4
13	CYC	VA	202	-	-	12/26/74/74	0/4/4/4
13	CYC	I8	1001	-	-	9/26/74/74	0/4/4/4
13	CYC	X1	201	-	-	9/26/74/74	0/4/4/4
13	CYC	A5	304	-	-	9/26/74/74	0/4/4/4
13	CYC	X9	1001	-	-	9/26/74/74	0/4/4/4
13	CYC	g9	1001	11	-	9/26/74/74	0/4/4/4
13	CYC	T5	201	-	-	9/26/74/74	0/4/4/4
13	CYC	K7	201	-	-	12/26/74/74	0/4/4/4
13	CYC	N6	301	-	-	10/26/74/74	0/4/4/4
13	CYC	E8	1001	-	-	9/26/74/74	0/4/4/4
13	CYC	B1	1001	-	-	8/26/74/74	0/4/4/4
13	CYC	I6	202	-	-	12/26/74/74	0/4/4/4
13	CYC	P9	1001	-	-	9/26/74/74	0/4/4/4
13	CYC	M6	201	-	-	12/26/74/74	0/4/4/4
13	CYC	V2	202	-	-	8/26/74/74	0/4/4/4
13	CYC	O2	1001	-	-	8/26/74/74	0/4/4/4
13	CYC	I2	202	-	-	12/26/74/74	0/4/4/4
13	CYC	Q8	1001	-	-	9/26/74/74	0/4/4/4
13	CYC	F6	1001	-	-	8/26/74/74	0/4/4/4
13	CYC	N2	301	-	-	10/26/74/74	0/4/4/4
13	CYC	B7	1001	-	-	8/26/74/74	0/4/4/4
13	CYC	G7	202	-	-	12/26/74/74	0/4/4/4
13	CYC	X5	202	-	-	12/26/74/74	0/4/4/4
13	CYC	29	1001	-	-	8/26/74/74	0/4/4/4
13	CYC	Z1	201	-	-	12/26/74/74	0/4/4/4
13	CYC	k9	1001	-	-	9/26/74/74	0/4/4/4
13	CYC	R4	1001	3	-	8/26/74/74	0/4/4/4
13	CYC	P4	201	-	-	8/26/74/74	0/4/4/4
13	CYC	S9	1001	-	-	8/26/74/74	0/4/4/4
13	CYC	IA	202	-	-	12/26/74/74	0/4/4/4
13	CYC	39	1001	-	-	8/26/74/74	0/4/4/4
13	CYC	K2	202	-	-	12/26/74/74	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CYC	P2	201	-	-	8/26/74/74	0/4/4/4
13	CYC	F4	1001	-	-	8/26/74/74	0/4/4/4
13	CYC	E4	201	3	-	8/26/74/74	0/4/4/4
13	CYC	JA	1001	-	-	8/26/74/74	0/4/4/4
13	CYC	J2	1001	-	-	8/26/74/74	0/4/4/4
13	CYC	UA	1001	-	-	8/26/74/74	0/4/4/4
13	CYC	M4	202	-	-	12/26/74/74	0/4/4/4
13	CYC	q8	1001	-	-	9/26/74/74	0/4/4/4
13	CYC	A5	302	-	-	8/26/74/74	0/4/4/4
13	CYC	I9	1001	-	-	9/26/74/74	0/4/4/4
13	CYC	F2	1001	-	-	8/26/74/74	0/4/4/4
13	CYC	C7	201	-	-	12/26/74/74	0/4/4/4
13	CYC	b9	1001	-	-	9/26/74/74	0/4/4/4
13	CYC	N2	302	-	-	8/26/74/74	0/4/4/4
13	CYC	G9	1001	-	-	9/26/74/74	0/4/4/4
13	CYC	D4	1001	-	-	8/26/74/74	0/4/4/4
13	CYC	H1	1001	-	-	8/26/74/74	0/4/4/4
13	CYC	q9	1001	-	-	9/26/74/74	0/4/4/4
13	CYC	U4	1001	-	-	8/26/74/74	0/4/4/4
13	CYC	E3	201	-	-	8/26/74/74	0/4/4/4
13	CYC	PA	201	-	-	8/26/74/74	0/4/4/4
13	CYC	P6	201	-	-	8/26/74/74	0/4/4/4
13	CYC	EA	202	-	-	8/26/74/74	0/4/4/4
13	CYC	M1	202	-	-	12/26/74/74	0/4/4/4
13	CYC	B5	1001	-	-	8/26/74/74	0/4/4/4
13	CYC	G4	202	-	-	8/26/74/74	0/4/4/4
13	CYC	Z9	1001	-	-	9/26/74/74	0/4/4/4
13	CYC	09	1201	-	-	9/26/74/74	0/4/4/4
13	CYC	s9	1001	-	-	9/26/74/74	0/4/4/4
13	CYC	I4	201	3	-	9/26/74/74	0/4/4/4
13	CYC	d9	1001	-	-	9/26/74/74	0/4/4/4
13	CYC	Z2	202	-	-	8/26/74/74	0/4/4/4
13	CYC	E2	202	3	-	12/26/74/74	0/4/4/4
13	CYC	A3	301	-	-	8/26/74/74	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CYC	H2	1001	-	-	8/26/74/74	0/4/4/4
13	CYC	S5	1001	-	-	8/26/74/74	0/4/4/4
13	CYC	KA	201	-	-	12/26/74/74	0/4/4/4
13	CYC	Z8	1001	-	-	9/26/74/74	0/4/4/4
13	CYC	T5	202	-	-	12/26/74/74	0/4/4/4
13	CYC	D5	1001	-	-	8/26/74/74	0/4/4/4
13	CYC	G3	202	-	-	12/26/74/74	0/4/4/4
13	CYC	e8	1001	-	-	9/26/74/74	0/4/4/4
13	CYC	r8	1001	-	-	9/26/74/74	0/4/4/4
13	CYC	G6	202	3	-	8/26/74/74	0/4/4/4
13	CYC	N3	301	-	-	10/26/74/74	0/4/4/4
13	CYC	H8	1001	-	-	9/26/74/74	0/4/4/4
13	CYC	AA	304	-	-	9/26/74/74	0/4/4/4
13	CYC	D9	1001	-	-	8/26/74/74	0/4/4/4
13	CYC	I3	202	-	-	12/26/74/74	0/4/4/4
13	CYC	P5	201	-	-	8/26/74/74	0/4/4/4
13	CYC	K9	1001	-	-	9/26/74/74	0/4/4/4
13	CYC	Z5	202	-	-	12/26/74/74	0/4/4/4
13	CYC	W5	1001	-	-	8/26/74/74	0/4/4/4
13	CYC	G1	202	-	-	8/26/74/74	0/4/4/4
13	CYC	TA	201	-	-	9/26/74/74	0/4/4/4
13	CYC	L2	201	-	-	8/26/74/74	0/4/4/4
13	CYC	C2	202	-	-	12/26/74/74	0/4/4/4
13	CYC	l8	1001	-	-	9/26/74/74	0/4/4/4
13	CYC	V6	202	-	-	8/26/74/74	0/4/4/4
13	CYC	I1	202	-	-	12/26/74/74	0/4/4/4
13	CYC	A7	301	-	-	8/26/74/74	0/4/4/4
13	CYC	CA	201	-	-	12/26/74/74	0/4/4/4
13	CYC	E1	201	3	-	8/26/74/74	0/4/4/4
13	CYC	B6	1001	-	-	8/26/74/74	0/4/4/4
13	CYC	MA	1001	-	-	8/26/74/74	0/4/4/4
13	CYC	MA	1003	-	-	12/26/74/74	0/4/4/4
13	CYC	N7	301	-	-	10/26/74/74	0/4/4/4
13	CYC	O4	1001	-	-	8/26/74/74	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CYC	Q6	201	-	-	8/26/74/74	0/4/4/4
13	CYC	K6	202	-	-	12/26/74/74	0/4/4/4
13	CYC	DA	1001	-	-	8/26/74/74	0/4/4/4
13	CYC	PA	203	-	-	8/26/74/74	0/4/4/4
13	CYC	F3	1001	-	-	8/26/74/74	0/4/4/4
13	CYC	h8	1001	-	-	9/26/74/74	0/4/4/4
13	CYC	T9	1001	-	-	9/26/74/74	0/4/4/4
13	CYC	YA	201	-	-	8/26/74/74	0/4/4/4
13	CYC	f8	1001	-	-	9/26/74/74	0/4/4/4
13	CYC	D2	1001	-	-	8/26/74/74	0/4/4/4
13	CYC	G5	201	-	-	12/26/74/74	0/4/4/4
13	CYC	L8	1001	-	-	9/26/74/74	0/4/4/4
13	CYC	C5	201	-	-	12/26/74/74	0/4/4/4
13	CYC	F1	1001	-	-	8/26/74/74	0/4/4/4
13	CYC	t8	1001	-	-	9/26/74/74	0/4/4/4
13	CYC	G3	201	3	-	8/26/74/74	0/4/4/4
13	CYC	S8	1001	-	-	9/26/74/74	0/4/4/4
13	CYC	F8	1001	-	-	9/26/74/74	0/4/4/4
13	CYC	U9	1001	-	-	9/26/74/74	0/4/4/4
13	CYC	v9	1001	-	-	8/26/74/74	0/4/4/4
13	CYC	X2	201	-	-	9/26/74/74	0/4/4/4
13	CYC	MA	1002	-	-	10/26/74/74	0/4/4/4
13	CYC	NA	301	-	-	9/26/74/74	0/4/4/4
13	CYC	09	1203	-	-	8/26/74/74	0/4/4/4
13	CYC	J7	1001	-	-	8/26/74/74	0/4/4/4
13	CYC	RA	201	-	-	12/26/74/74	0/4/4/4
13	CYC	j8	1001	-	-	9/26/74/74	0/4/4/4
13	CYC	X6	201	-	-	9/26/74/74	0/4/4/4
13	CYC	K5	201	-	-	12/26/74/74	0/4/4/4
13	CYC	P5	202	-	-	12/26/74/74	0/4/4/4
13	CYC	F9	1001	-	-	8/26/74/74	0/4/4/4
13	CYC	P5	203	-	-	8/26/74/74	0/4/4/4
13	CYC	Y4	201	-	-	8/26/74/74	0/4/4/4
13	CYC	L9	1001	-	-	9/26/74/74	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CYC	Z5	201	-	-	9/26/74/74	0/4/4/4
13	CYC	I7	201	-	-	9/26/74/74	0/4/4/4
13	CYC	O1	1001	-	-	8/26/74/74	0/4/4/4
13	CYC	P8	1001	-	-	9/26/74/74	0/4/4/4
13	CYC	K2	201	-	-	12/26/74/74	0/4/4/4
13	CYC	T2	201	-	-	12/26/74/74	0/4/4/4
13	CYC	X4	201	-	-	9/26/74/74	0/4/4/4
13	CYC	M4	201	3	-	10/26/74/74	0/4/4/4
13	CYC	J1	1001	-	-	8/26/74/74	0/4/4/4
13	CYC	I7	202	-	-	12/26/74/74	0/4/4/4
13	CYC	U6	201	-	-	12/26/74/74	0/4/4/4
13	CYC	J9	1001	-	-	8/26/74/74	0/4/4/4
13	CYC	J6	1001	-	-	8/26/74/74	0/4/4/4
13	CYC	s8	1001	-	-	9/26/74/74	0/4/4/4
13	CYC	w9	1001	-	-	9/26/74/74	0/4/4/4
13	CYC	Z4	202	-	-	8/26/74/74	0/4/4/4
13	CYC	K8	1001	-	-	9/26/74/74	0/4/4/4
13	CYC	X4	202	-	-	12/26/74/74	0/4/4/4
13	CYC	E5	201	-	-	12/26/74/74	0/4/4/4
13	CYC	W2	202	-	-	8/26/74/74	0/4/4/4
13	CYC	J8	1001	-	-	9/26/74/74	0/4/4/4
13	CYC	Y2	201	-	-	8/26/74/74	0/4/4/4
13	CYC	J5	1001	-	-	8/26/74/74	0/4/4/4
13	CYC	n8	1001	-	-	9/26/74/74	0/4/4/4
13	CYC	y9	1001	-	-	9/26/74/74	0/4/4/4
13	CYC	EA	201	-	-	12/26/74/74	0/4/4/4
13	CYC	I5	202	-	-	12/26/74/74	0/4/4/4
13	CYC	Z2	201	-	-	12/26/74/74	0/4/4/4
13	CYC	E6	202	3	-	12/26/74/74	0/4/4/4
13	CYC	ZA	202	-	-	12/26/74/74	0/4/4/4
13	CYC	AA	303	-	-	9/26/74/74	0/4/4/4
13	CYC	I6	201	-	-	9/26/74/74	0/4/4/4
13	CYC	M5	1001	-	-	8/26/74/74	0/4/4/4
13	CYC	H6	1001	-	-	8/26/74/74	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CYC	S1	1001	-	-	8/26/74/74	0/4/4/4
13	CYC	09	1202	-	-	6/26/74/74	0/4/4/4
13	CYC	V1	202	-	-	8/26/74/74	0/4/4/4
13	CYC	X6	202	-	-	12/26/74/74	0/4/4/4
13	CYC	T1	202	-	-	8/26/74/74	0/4/4/4
13	CYC	E5	202	-	-	8/26/74/74	0/4/4/4
13	CYC	P4	202	-	-	12/26/74/74	0/4/4/4
13	CYC	D7	1001	-	-	8/26/74/74	0/4/4/4
13	CYC	V6	201	-	-	12/26/74/74	0/4/4/4
13	CYC	I1	201	3	-	9/26/74/74	0/4/4/4
13	CYC	Q9	201	11	-	11/26/74/74	0/4/4/4
13	CYC	O8	1001	-	-	9/26/74/74	0/4/4/4
13	CYC	M5	1002	-	-	10/26/74/74	0/4/4/4
13	CYC	19	1205	-	-	9/26/74/74	0/4/4/4
13	CYC	U1	1001	-	-	8/26/74/74	0/4/4/4
13	CYC	V4	201	-	-	12/26/74/74	0/4/4/4
13	CYC	o8	1001	-	-	9/26/74/74	0/4/4/4
13	CYC	W6	201	-	-	12/26/74/74	0/4/4/4
13	CYC	S4	1001	-	-	8/26/74/74	0/4/4/4
13	CYC	G2	202	3	-	8/26/74/74	0/4/4/4
13	CYC	Q4	201	-	-	8/26/74/74	0/4/4/4
13	CYC	I2	201	-	-	9/26/74/74	0/4/4/4
13	CYC	W4	1001	-	-	8/26/74/74	0/4/4/4
13	CYC	K3	201	-	-	12/26/74/74	0/4/4/4
13	CYC	C3	201	-	-	12/26/74/74	0/4/4/4
13	CYC	M8	1001	-	-	9/26/74/74	0/4/4/4
13	CYC	A8	1001	-	-	9/26/74/74	0/4/4/4
13	CYC	z9	1001	-	-	8/26/74/74	0/4/4/4
13	CYC	C2	201	-	-	8/26/74/74	0/4/4/4
13	CYC	J3	1001	-	-	8/26/74/74	0/4/4/4
13	CYC	Q1	202	-	-	12/26/74/74	0/4/4/4
13	CYC	XA	202	-	-	12/26/74/74	0/4/4/4
13	CYC	C8	1001	-	-	9/26/74/74	0/4/4/4
13	CYC	L5	201	-	-	8/26/74/74	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CYC	H7	1001	-	-	8/26/74/74	0/4/4/4
13	CYC	R6	1001	-	-	8/26/74/74	0/4/4/4
13	CYC	N6	302	-	-	8/26/74/74	0/4/4/4
13	CYC	U2	202	-	-	8/26/74/74	0/4/4/4
13	CYC	B2	1001	-	-	8/26/74/74	0/4/4/4
13	CYC	T4	201	-	-	12/26/74/74	0/4/4/4
13	CYC	Q2	201	-	-	8/26/74/74	0/4/4/4
13	CYC	R2	1001	-	-	8/26/74/74	0/4/4/4
13	CYC	u9	1001	-	-	9/26/74/74	0/4/4/4
13	CYC	F7	1001	-	-	8/26/74/74	0/4/4/4
13	CYC	K6	201	-	-	12/26/74/74	0/4/4/4
13	CYC	L3	201	-	-	8/26/74/74	0/4/4/4
13	CYC	U6	202	-	-	8/26/74/74	0/4/4/4
13	CYC	V5	201	-	-	9/26/74/74	0/4/4/4
13	CYC	E7	202	3	-	12/26/74/74	0/4/4/4
13	CYC	V5	202	-	-	12/26/74/74	0/4/4/4

The worst 5 of 4298 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	TA	201	CYC	CHD-C1D	6.18	1.54	1.40
13	VA	201	CYC	CHD-C1D	6.17	1.54	1.40
13	T5	201	CYC	CHD-C1D	6.15	1.54	1.40
13	V5	201	CYC	CHD-C1D	6.14	1.54	1.40
13	Z5	201	CYC	CHD-C1D	6.14	1.54	1.40

The worst 5 of 7224 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	39	1001	CYC	C3B-C4B-NB	16.68	120.07	106.77
13	c9	1001	CYC	C3B-C4B-NB	16.65	120.05	106.77
13	z9	1001	CYC	C3B-C4B-NB	16.65	120.05	106.77
13	09	1203	CYC	C3B-C4B-NB	16.65	120.05	106.77
13	19	1205	CYC	C3B-C4B-NB	16.65	120.05	106.77

There are no chirality outliers.

5 of 3258 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	B1	1001	CYC	NA-C4A-CHB-C1B
13	C1	301	CYC	NA-C4A-CHB-C1B
13	C1	302	CYC	C3A-C2A-CAA-CBA
13	D1	1001	CYC	NA-C4A-CHB-C1B
13	E1	202	CYC	C3A-C2A-CAA-CBA

There are no ring outliers.

346 monomers are involved in 8394 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	K7	202	CYC	29	0
13	G7	201	CYC	16	0
13	Y6	201	CYC	30	0
13	R9	1001	CYC	19	0
13	P1	201	CYC	29	0
13	K4	202	CYC	33	0
13	S2	1001	CYC	25	0
13	O5	1001	CYC	1	0
13	V8	1001	CYC	16	0
13	B9	1001	CYC	11	0
13	U5	1001	CYC	10	0
13	K1	202	CYC	33	0
13	S6	1001	CYC	24	0
13	Q4	202	CYC	33	0
13	d8	1001	CYC	34	0
13	K4	201	CYC	54	0
13	Z1	202	CYC	15	0
13	O6	1001	CYC	14	0
13	g8	1001	CYC	16	0
13	M7	201	CYC	27	0
13	L6	201	CYC	17	0
13	e9	1001	CYC	10	0
13	j9	1001	CYC	10	0
13	O9	1001	CYC	11	0
13	T1	201	CYC	50	0
13	b8	1001	CYC	32	0
13	GA	1001	CYC	5	0
13	E3	202	CYC	29	0
13	D8	1001	CYC	29	0
13	WA	1001	CYC	8	0
13	E9	1001	CYC	19	0
13	E7	201	CYC	33	0
13	V4	202	CYC	35	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	R8	1001	CYC	28	0
13	Z6	202	CYC	22	0
13	M2	201	CYC	28	0
13	G2	201	CYC	54	0
13	B3	1001	CYC	26	0
13	19	1203	CYC	10	0
13	C9	1001	CYC	19	0
13	M1	201	CYC	21	0
13	R5	201	CYC	58	0
13	o9	1001	CYC	19	0
13	E1	202	CYC	38	0
13	I3	201	CYC	22	0
13	AA	302	CYC	29	0
13	k8	1001	CYC	34	0
13	D3	1001	CYC	17	0
13	G6	201	CYC	55	0
13	OA	1001	CYC	1	0
13	N5	301	CYC	19	0
13	Z6	201	CYC	44	0
13	P1	202	CYC	32	0
13	I4	202	CYC	39	0
13	T4	202	CYC	42	0
13	T8	1001	CYC	27	0
13	XA	201	CYC	16	0
13	W6	202	CYC	24	0
13	Y1	201	CYC	4	0
13	T6	201	CYC	39	0
13	A9	1001	CYC	19	0
13	K3	202	CYC	29	0
13	c9	1001	CYC	10	0
13	D1	1001	CYC	30	0
13	LA	201	CYC	9	0
13	I5	201	CYC	16	0
13	VA	201	CYC	40	0
13	Y5	201	CYC	8	0
13	p9	1001	CYC	10	0
13	C6	202	CYC	42	0
13	PA	202	CYC	29	0
13	X1	202	CYC	22	0
13	Q1	201	CYC	14	0
13	B4	1001	CYC	18	0
13	E6	201	CYC	25	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	ZA	201	CYC	18	0
13	E2	201	CYC	24	0
13	c8	1001	CYC	16	0
13	W1	1001	CYC	21	0
13	W2	201	CYC	39	0
13	m9	201	CYC	2	0
13	Y8	1001	CYC	30	0
13	G1	201	CYC	39	0
13	V2	201	CYC	45	0
13	X8	1001	CYC	16	0
13	C6	201	CYC	29	0
13	K1	201	CYC	52	0
13	f9	1001	CYC	20	0
13	t9	1001	CYC	10	0
13	V9	201	CYC	2	0
13	TA	202	CYC	42	0
13	C1	301	CYC	15	0
13	19	1204	CYC	10	0
13	C1	302	CYC	31	0
13	E4	202	CYC	36	0
13	i9	1001	CYC	15	0
13	C4	302	CYC	30	0
13	19	1201	CYC	40	0
13	l9	1001	CYC	6	0
13	x9	1001	CYC	10	0
13	r9	1001	CYC	11	0
13	IA	201	CYC	16	0
13	W8	1001	CYC	26	0
13	AA	301	CYC	18	0
13	M3	201	CYC	28	0
13	V1	201	CYC	43	0
13	H9	1001	CYC	10	0
13	D6	1001	CYC	17	0
13	L7	201	CYC	17	0
13	A5	303	CYC	42	0
13	19	1202	CYC	3	0
13	p8	1001	CYC	16	0
13	Z4	201	CYC	31	0
13	N9	1001	CYC	19	0
13	W2	203	CYC	53	0
13	SA	1001	CYC	11	0
13	A5	301	CYC	18	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	B8	1001	CYC	35	0
13	H3	1001	CYC	20	0
13	C4	301	CYC	16	0
13	G4	201	CYC	39	0
13	L1	201	CYC	13	0
13	R1	1001	CYC	6	0
13	J4	1001	CYC	26	0
13	GA	1002	CYC	41	0
13	U2	201	CYC	37	0
13	H4	1001	CYC	7	0
13	L4	201	CYC	13	0
13	X5	201	CYC	16	0
13	M5	1003	CYC	40	0
13	VA	202	CYC	30	0
13	I8	1001	CYC	26	0
13	X1	201	CYC	30	0
13	A5	304	CYC	40	0
13	X9	1001	CYC	19	0
13	T5	201	CYC	40	0
13	K7	201	CYC	53	0
13	N6	301	CYC	31	0
13	E8	1001	CYC	16	0
13	B1	1001	CYC	18	0
13	I6	202	CYC	37	0
13	P9	1001	CYC	20	0
13	M6	201	CYC	29	0
13	V2	202	CYC	23	0
13	O2	1001	CYC	13	0
13	I2	202	CYC	37	0
13	Q8	1001	CYC	16	0
13	F6	1001	CYC	17	0
13	N2	301	CYC	29	0
13	B7	1001	CYC	27	0
13	G7	202	CYC	53	0
13	X5	202	CYC	33	0
13	29	1001	CYC	14	0
13	Z1	201	CYC	31	0
13	k9	1001	CYC	19	0
13	R4	1001	CYC	6	0
13	P4	201	CYC	28	0
13	S9	1001	CYC	10	0
13	IA	202	CYC	32	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	39	1001	CYC	9	0
13	K2	202	CYC	29	0
13	P2	201	CYC	22	0
13	F4	1001	CYC	19	0
13	E4	201	CYC	9	0
13	JA	1001	CYC	2	0
13	J2	1001	CYC	25	0
13	UA	1001	CYC	10	0
13	M4	202	CYC	29	0
13	q8	1001	CYC	35	0
13	A5	302	CYC	27	0
13	I9	1001	CYC	19	0
13	F2	1001	CYC	16	0
13	C7	201	CYC	42	0
13	b9	1001	CYC	19	0
13	N2	302	CYC	15	0
13	G9	1001	CYC	19	0
13	D4	1001	CYC	30	0
13	H1	1001	CYC	7	0
13	q9	1001	CYC	19	0
13	U4	1001	CYC	7	0
13	E3	201	CYC	32	0
13	PA	201	CYC	32	0
13	P6	201	CYC	22	0
13	EA	202	CYC	1	0
13	M1	202	CYC	31	0
13	B5	1001	CYC	6	0
13	G4	202	CYC	29	0
13	Z9	1001	CYC	15	0
13	09	1201	CYC	30	0
13	s9	1001	CYC	19	0
13	I4	201	CYC	18	0
13	d9	1001	CYC	15	0
13	Z2	202	CYC	22	0
13	E2	202	CYC	30	0
13	A3	301	CYC	24	0
13	H2	1001	CYC	20	0
13	S5	1001	CYC	11	0
13	KA	201	CYC	27	0
13	Z8	1001	CYC	16	0
13	T5	202	CYC	41	0
13	D5	1001	CYC	11	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	G3	202	CYC	52	0
13	e8	1001	CYC	15	0
13	r8	1001	CYC	16	0
13	G6	202	CYC	20	0
13	N3	301	CYC	30	0
13	H8	1001	CYC	18	0
13	AA	304	CYC	34	0
13	D9	1001	CYC	22	0
13	I3	202	CYC	36	0
13	P5	201	CYC	30	0
13	K9	1001	CYC	19	0
13	Z5	202	CYC	36	0
13	W5	1001	CYC	8	0
13	G1	202	CYC	28	0
13	TA	201	CYC	41	0
13	L2	201	CYC	17	0
13	C2	202	CYC	42	0
13	l8	1001	CYC	16	0
13	V6	202	CYC	24	0
13	I1	202	CYC	37	0
13	A7	301	CYC	24	0
13	CA	201	CYC	29	0
13	E1	201	CYC	8	0
13	B6	1001	CYC	27	0
13	MA	1001	CYC	1	0
13	MA	1003	CYC	42	0
13	N7	301	CYC	29	0
13	O4	1001	CYC	26	0
13	Q6	201	CYC	40	0
13	K6	202	CYC	29	0
13	DA	1001	CYC	11	0
13	PA	203	CYC	9	0
13	F3	1001	CYC	16	0
13	h8	1001	CYC	25	0
13	T9	1001	CYC	19	0
13	YA	201	CYC	8	0
13	f8	1001	CYC	31	0
13	D2	1001	CYC	17	0
13	G5	201	CYC	41	0
13	L8	1001	CYC	16	0
13	C5	201	CYC	30	0
13	F1	1001	CYC	18	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	t8	1001	CYC	16	0
13	G3	201	CYC	15	0
13	S8	1001	CYC	16	0
13	F8	1001	CYC	28	0
13	U9	1001	CYC	8	0
13	v9	1001	CYC	10	0
13	X2	201	CYC	17	0
13	MA	1002	CYC	27	0
13	NA	301	CYC	18	0
13	09	1203	CYC	12	0
13	J7	1001	CYC	24	0
13	RA	201	CYC	56	0
13	j8	1001	CYC	16	0
13	X6	201	CYC	17	0
13	K5	201	CYC	27	0
13	P5	202	CYC	31	0
13	F9	1001	CYC	16	0
13	P5	203	CYC	9	0
13	Y4	201	CYC	4	0
13	L9	1001	CYC	9	0
13	Z5	201	CYC	18	0
13	I7	201	CYC	25	0
13	O1	1001	CYC	27	0
13	P8	1001	CYC	29	0
13	K2	201	CYC	53	0
13	T2	201	CYC	41	0
13	X4	201	CYC	19	0
13	M4	201	CYC	21	0
13	J1	1001	CYC	27	0
13	I7	202	CYC	36	0
13	U6	201	CYC	37	0
13	J9	1001	CYC	10	0
13	J6	1001	CYC	24	0
13	s8	1001	CYC	35	0
13	w9	1001	CYC	19	0
13	Z4	202	CYC	14	0
13	K8	1001	CYC	29	0
13	X4	202	CYC	22	0
13	E5	201	CYC	52	0
13	W2	202	CYC	25	0
13	J8	1001	CYC	16	0
13	Y2	201	CYC	30	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	J5	1001	CYC	2	0
13	n8	1001	CYC	15	0
13	y9	1001	CYC	19	0
13	EA	201	CYC	52	0
13	I5	202	CYC	33	0
13	Z2	201	CYC	44	0
13	E6	202	CYC	28	0
13	ZA	202	CYC	37	0
13	AA	303	CYC	42	0
13	I6	201	CYC	22	0
13	M5	1001	CYC	1	0
13	H6	1001	CYC	20	0
13	S1	1001	CYC	20	0
13	V1	202	CYC	36	0
13	X6	202	CYC	49	0
13	T1	202	CYC	42	0
13	E5	202	CYC	1	0
13	P4	202	CYC	32	0
13	D7	1001	CYC	17	0
13	V6	201	CYC	44	0
13	I1	201	CYC	16	0
13	Q9	201	CYC	1	0
13	O8	1001	CYC	16	0
13	M5	1002	CYC	27	0
13	19	1205	CYC	12	0
13	U1	1001	CYC	7	0
13	V4	201	CYC	45	0
13	o8	1001	CYC	43	0
13	W6	201	CYC	39	0
13	S4	1001	CYC	21	0
13	G2	202	CYC	19	0
13	Q4	201	CYC	14	0
13	I2	201	CYC	23	0
13	W4	1001	CYC	23	0
13	K3	201	CYC	51	0
13	C3	201	CYC	42	0
13	M8	1001	CYC	28	0
13	A8	1001	CYC	16	0
13	z9	1001	CYC	10	0
13	C2	201	CYC	29	0
13	J3	1001	CYC	24	0
13	Q1	202	CYC	33	0

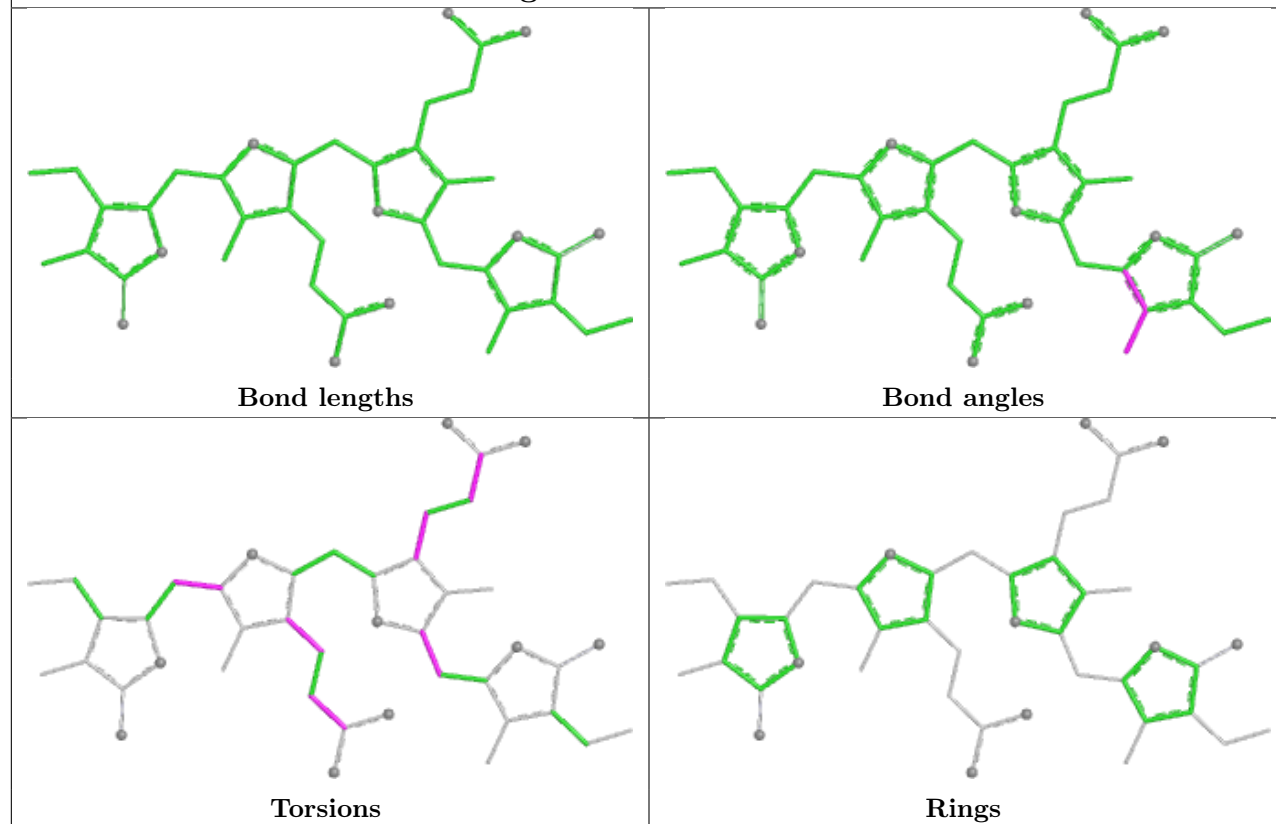
Continued on next page...

Continued from previous page...

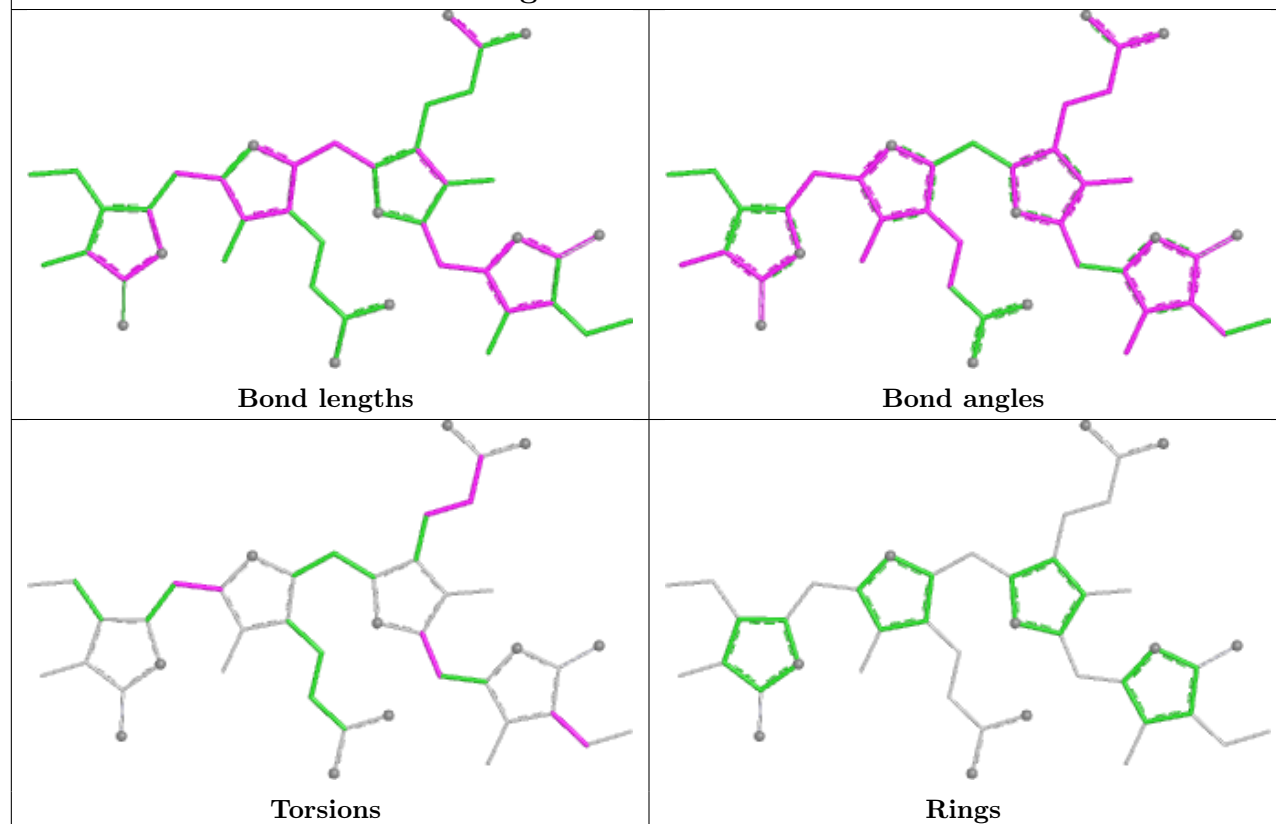
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	XA	202	CYC	33	0
13	C8	1001	CYC	16	0
13	L5	201	CYC	9	0
13	H7	1001	CYC	20	0
13	R6	1001	CYC	25	0
13	N6	302	CYC	16	0
13	U2	202	CYC	24	0
13	B2	1001	CYC	24	0
13	T4	201	CYC	52	0
13	Q2	201	CYC	39	0
13	R2	1001	CYC	23	0
13	u9	1001	CYC	19	0
13	F7	1001	CYC	18	0
13	K6	201	CYC	52	0
13	L3	201	CYC	17	0
13	U6	202	CYC	24	0
13	V5	201	CYC	39	0
13	E7	202	CYC	28	0
13	V5	202	CYC	30	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

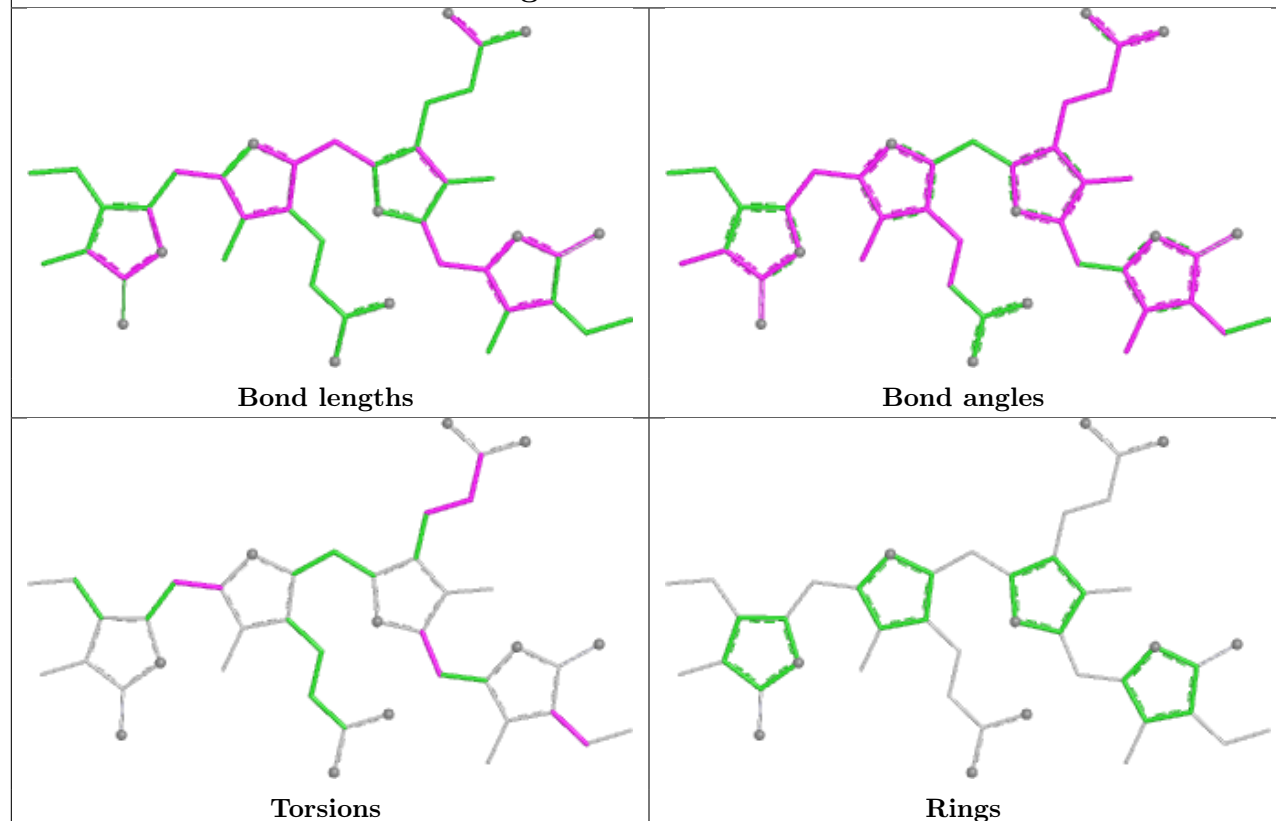
Ligand CYC K7 202



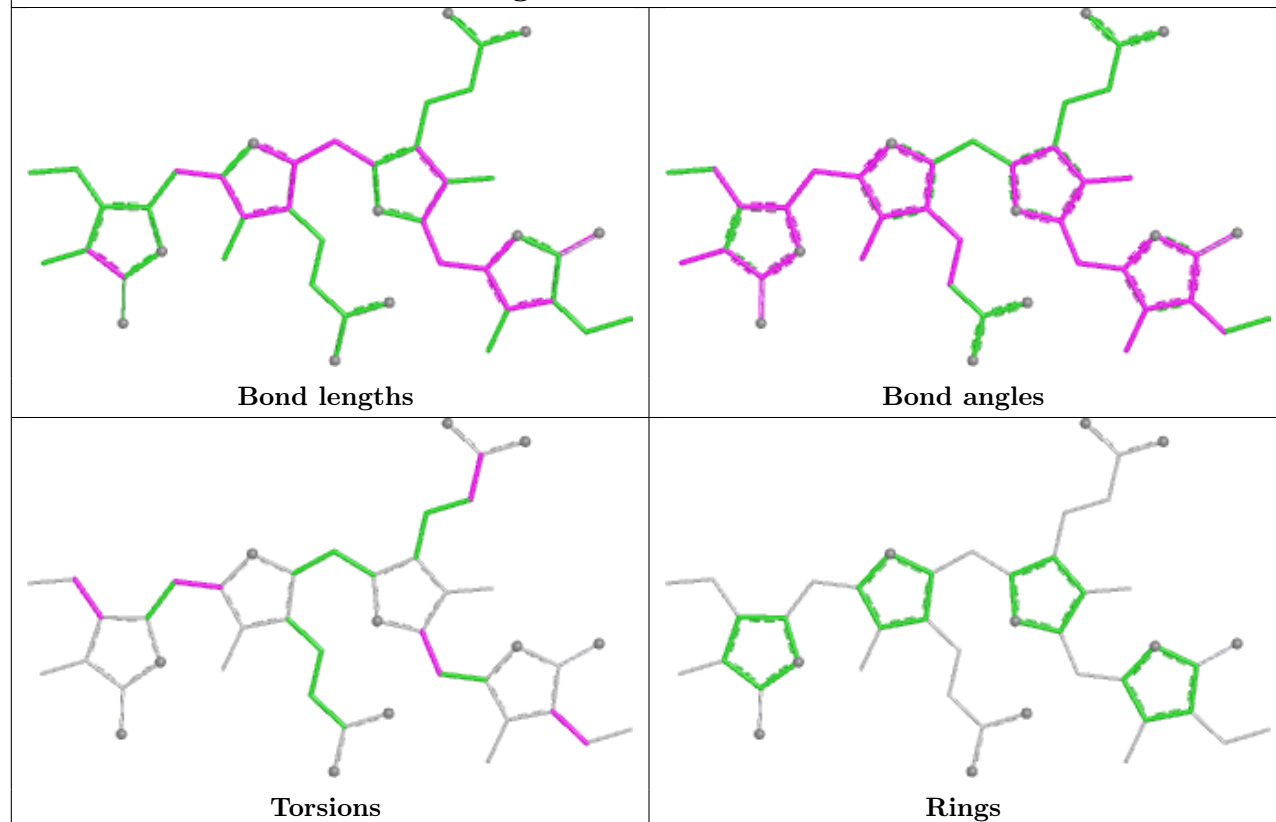
Ligand CYC G7 201

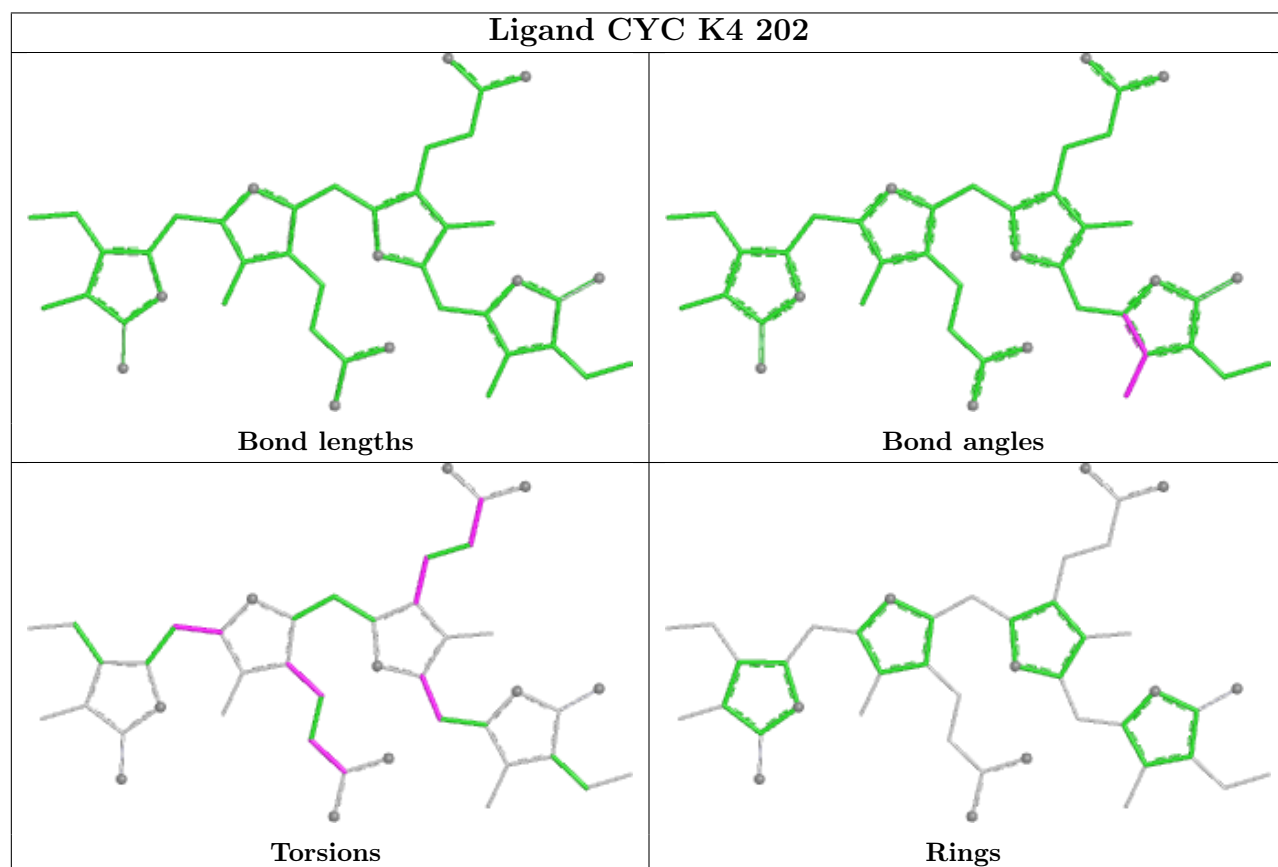
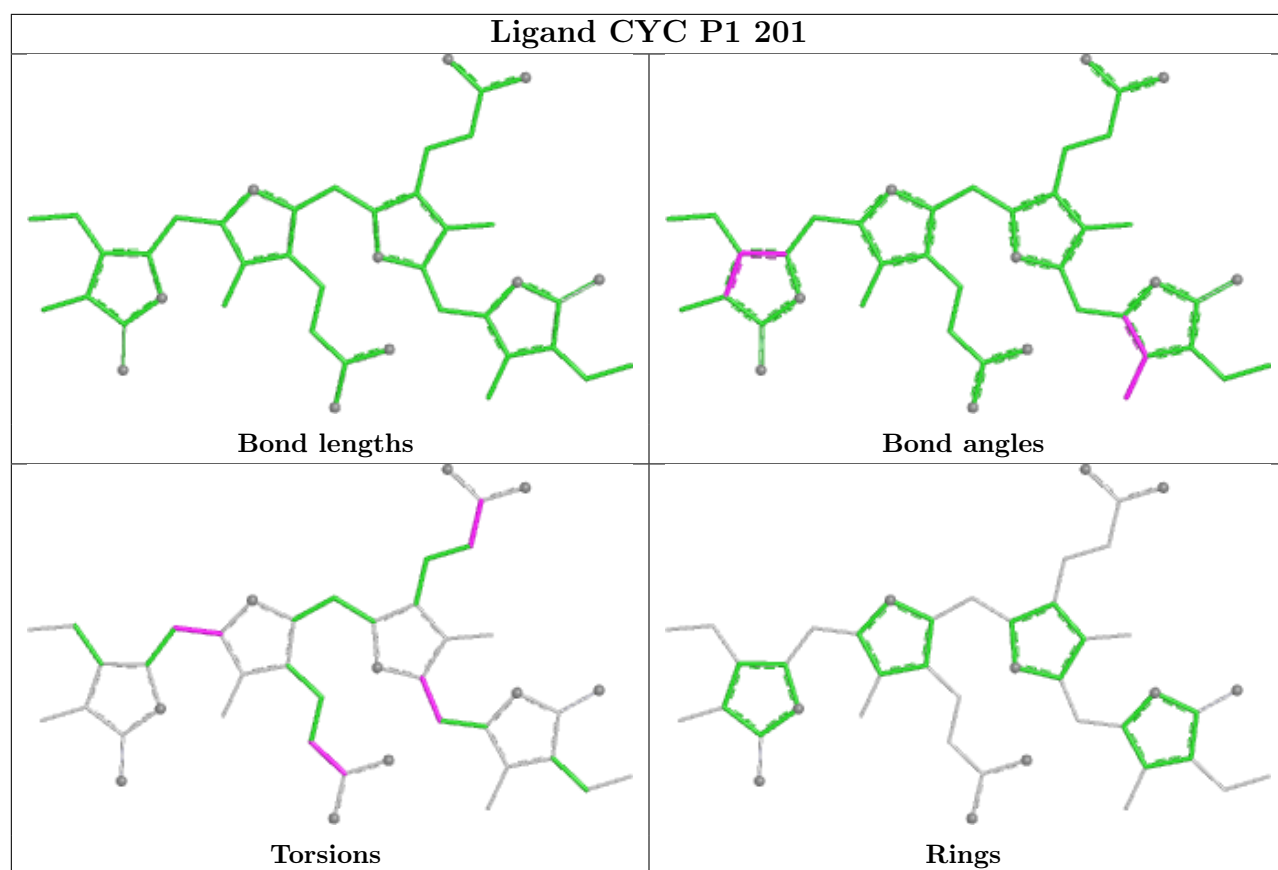


Ligand CYC Y6 201

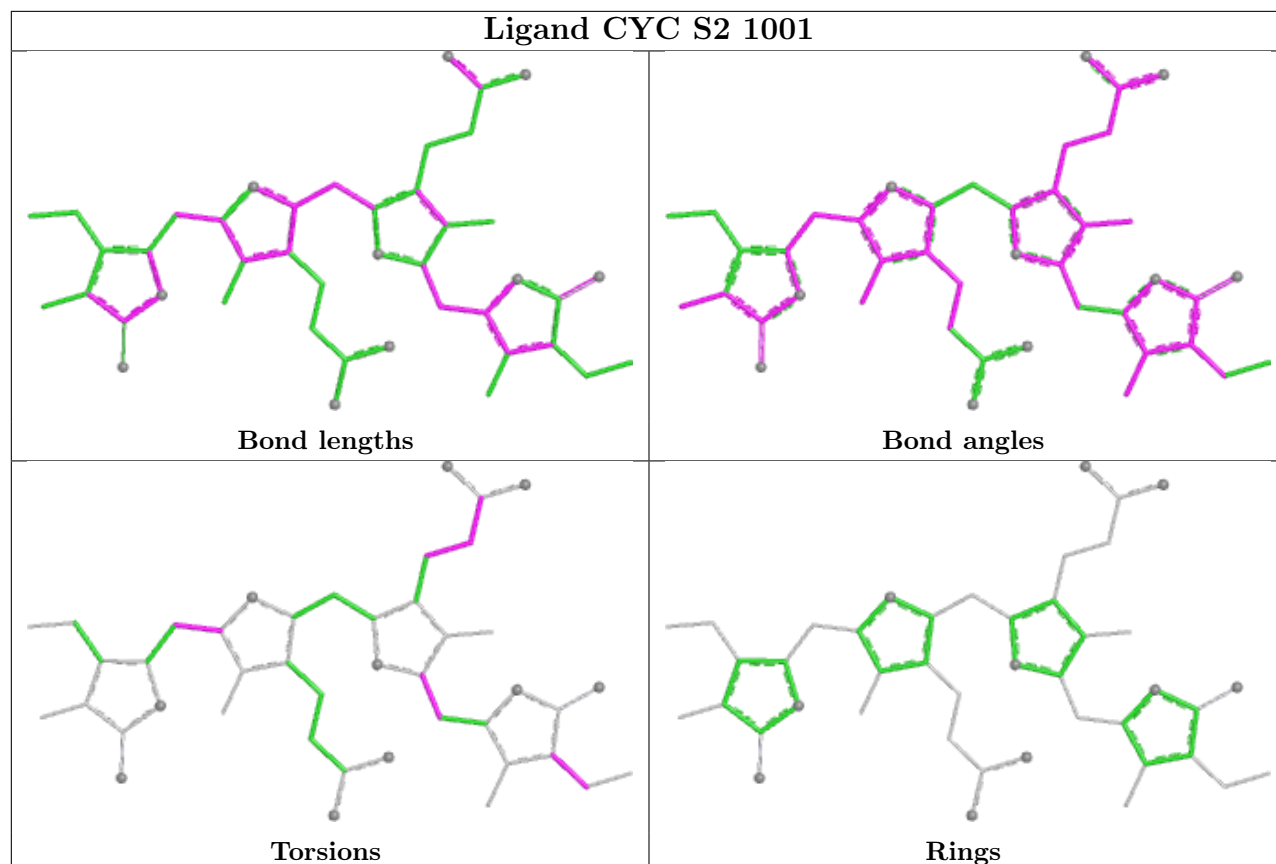


Ligand CYC R9 1001

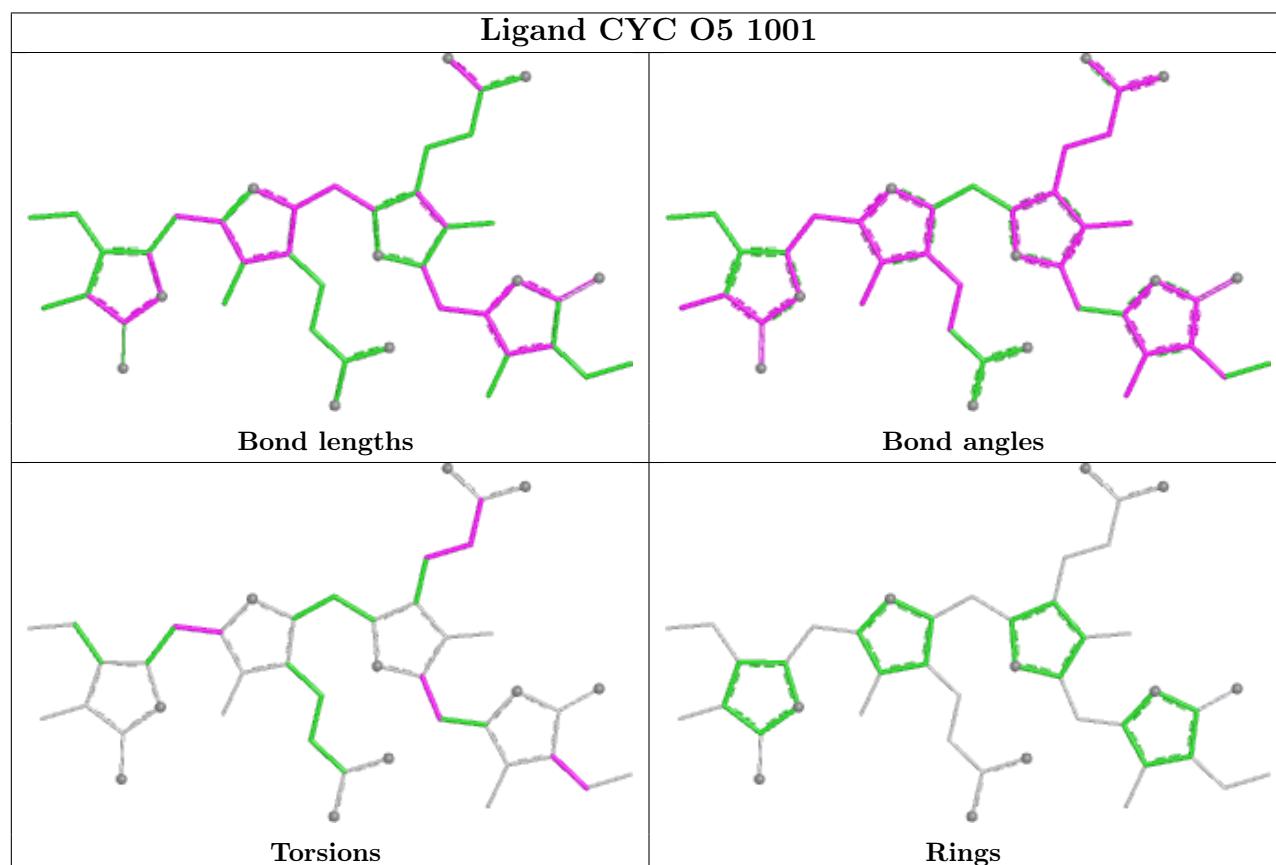




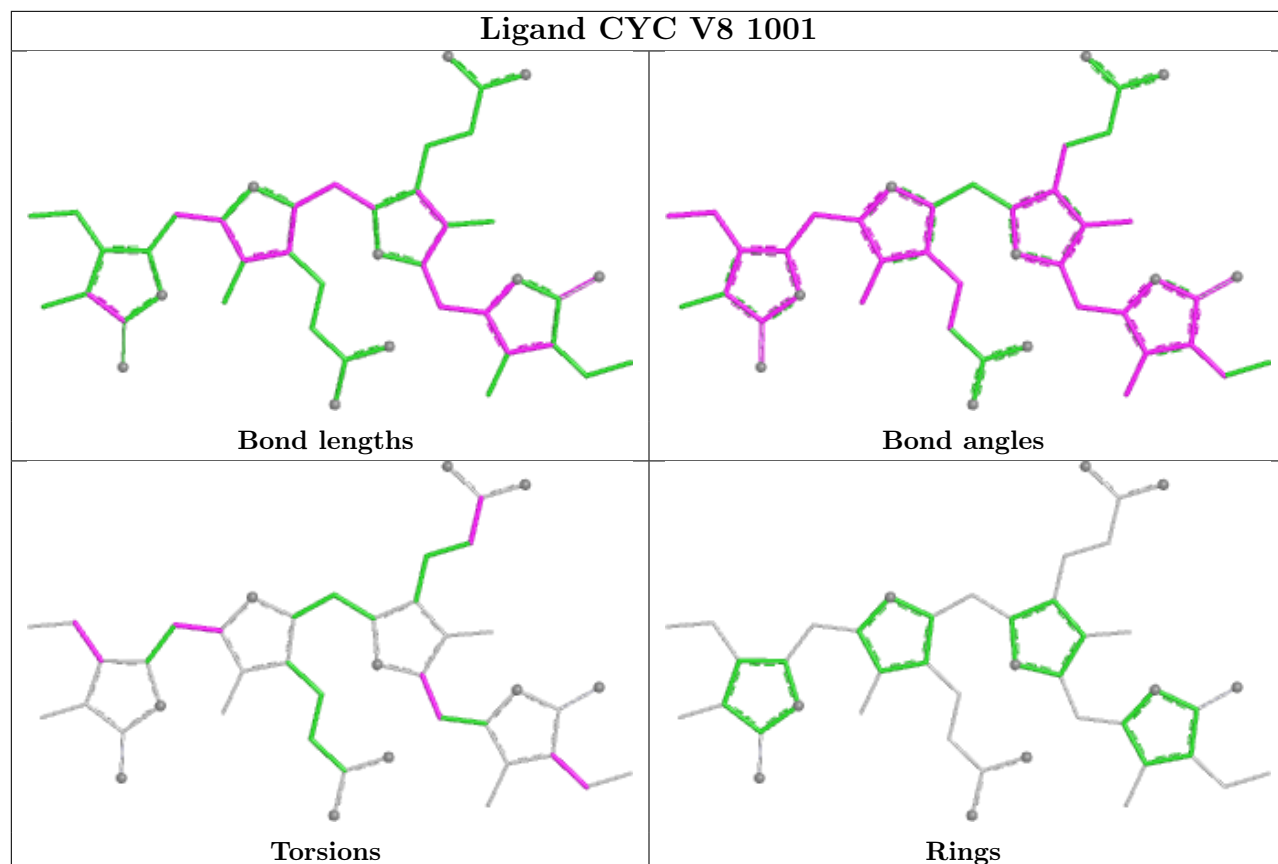
Ligand CYC S2 1001



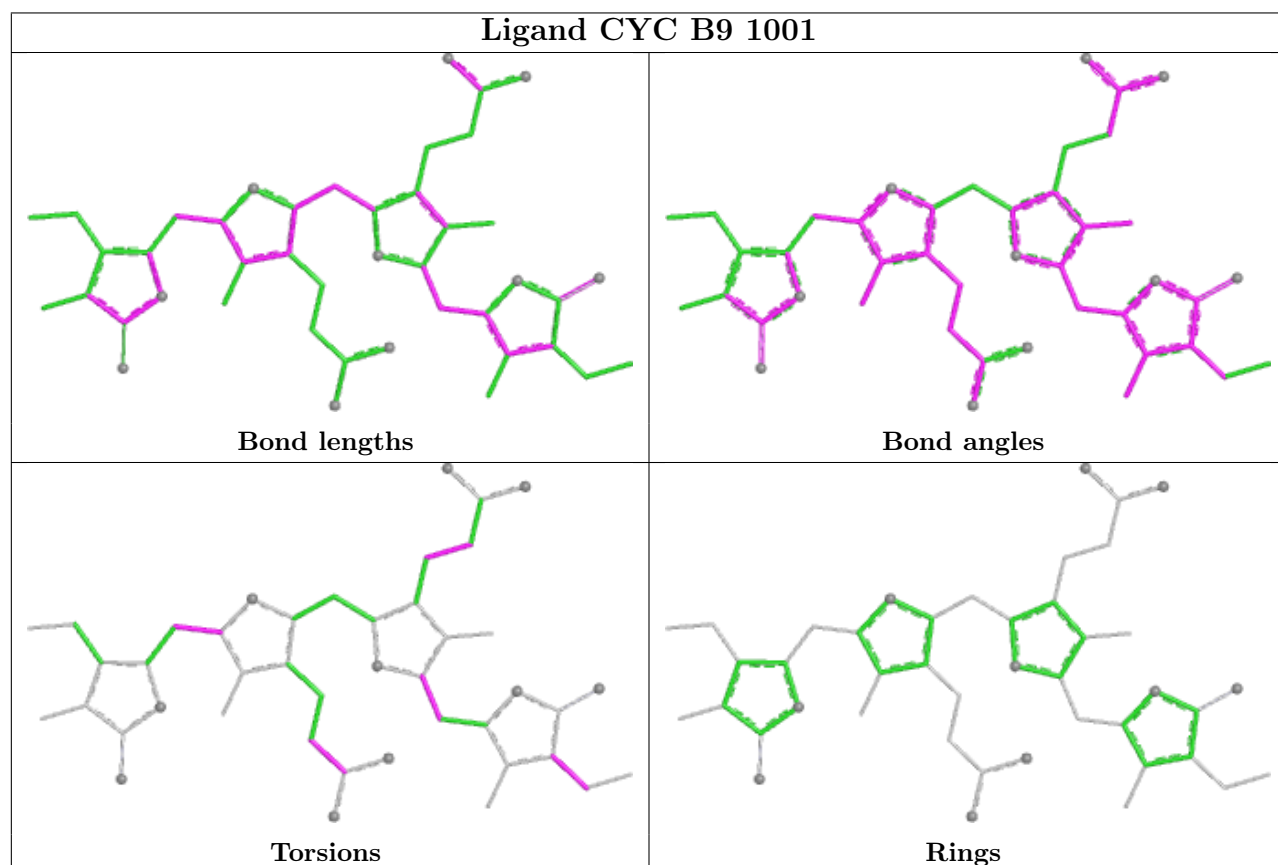
Ligand CYC O5 1001



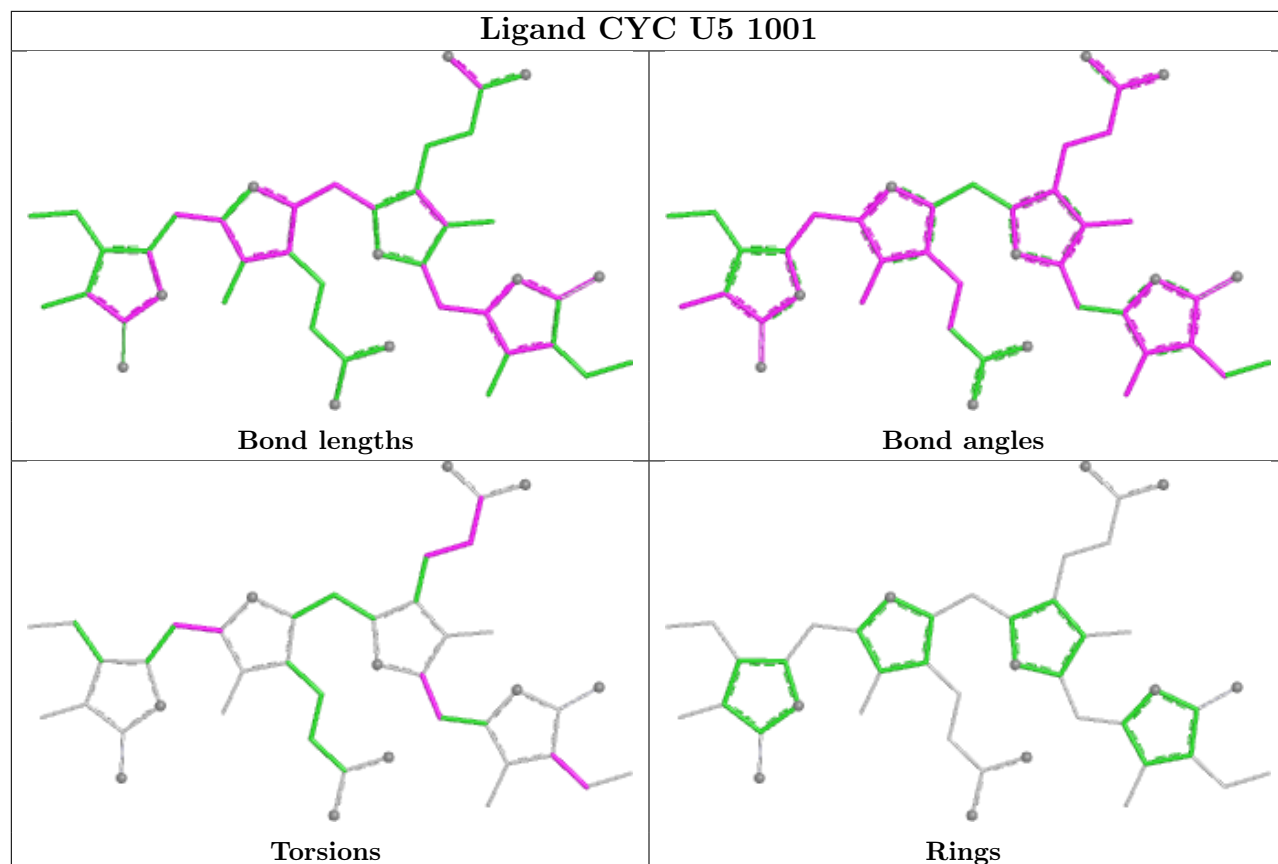
Ligand CYC V8 1001



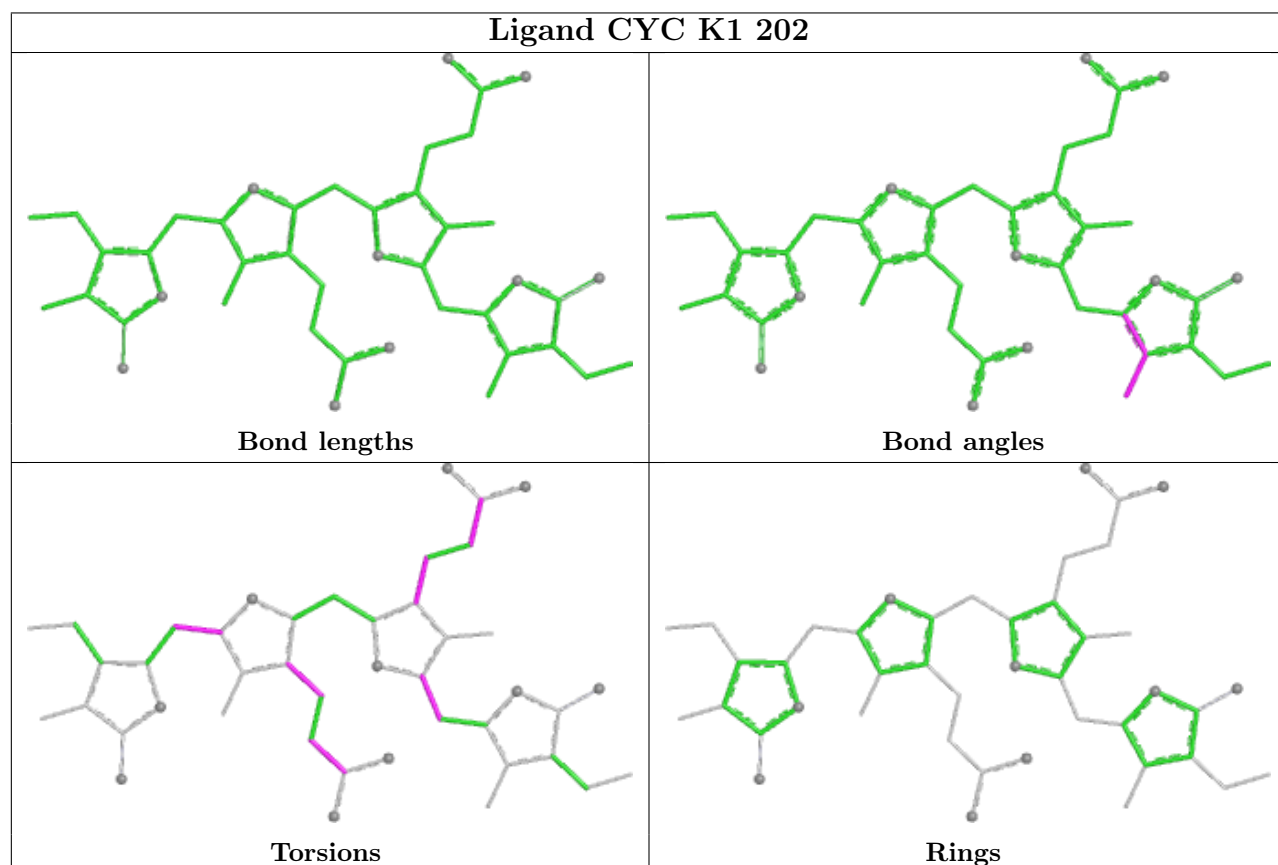
Ligand CYC B9 1001



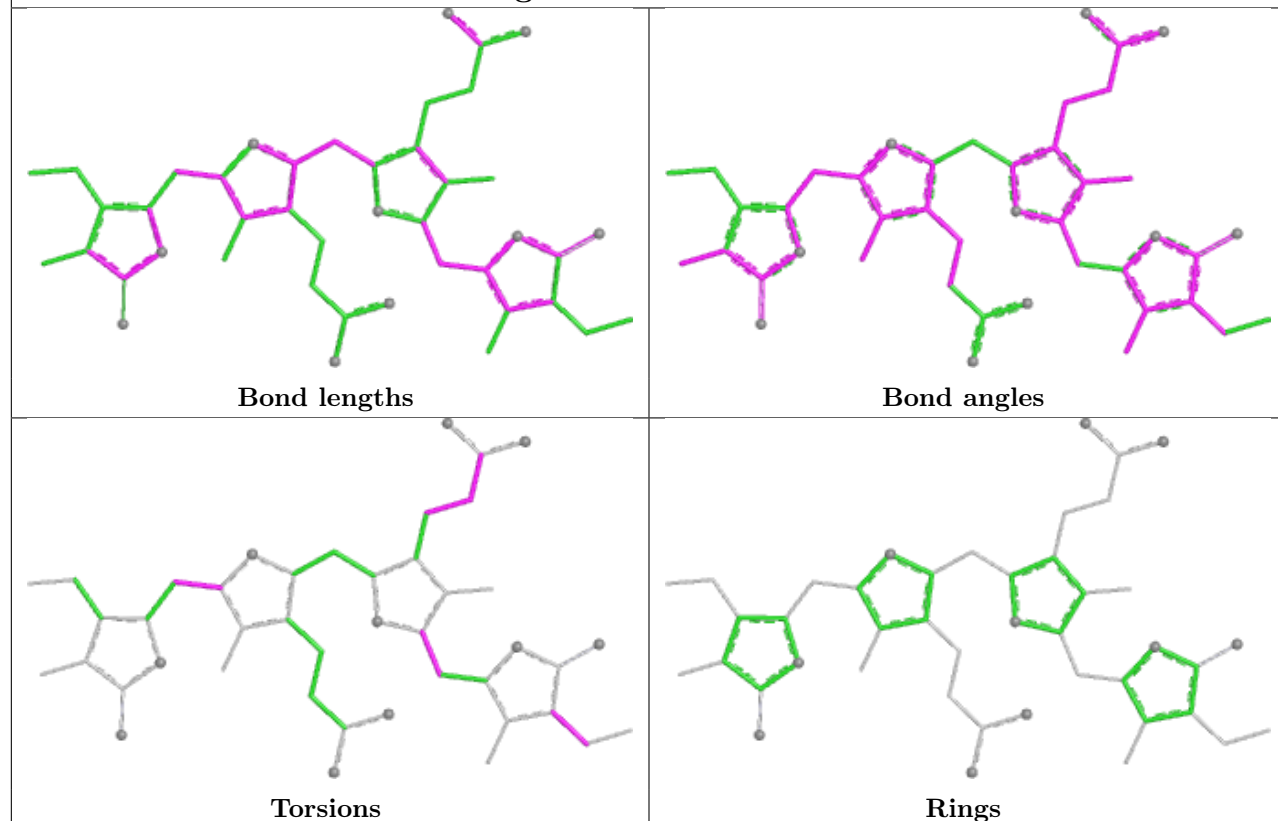
Ligand CYC U5 1001



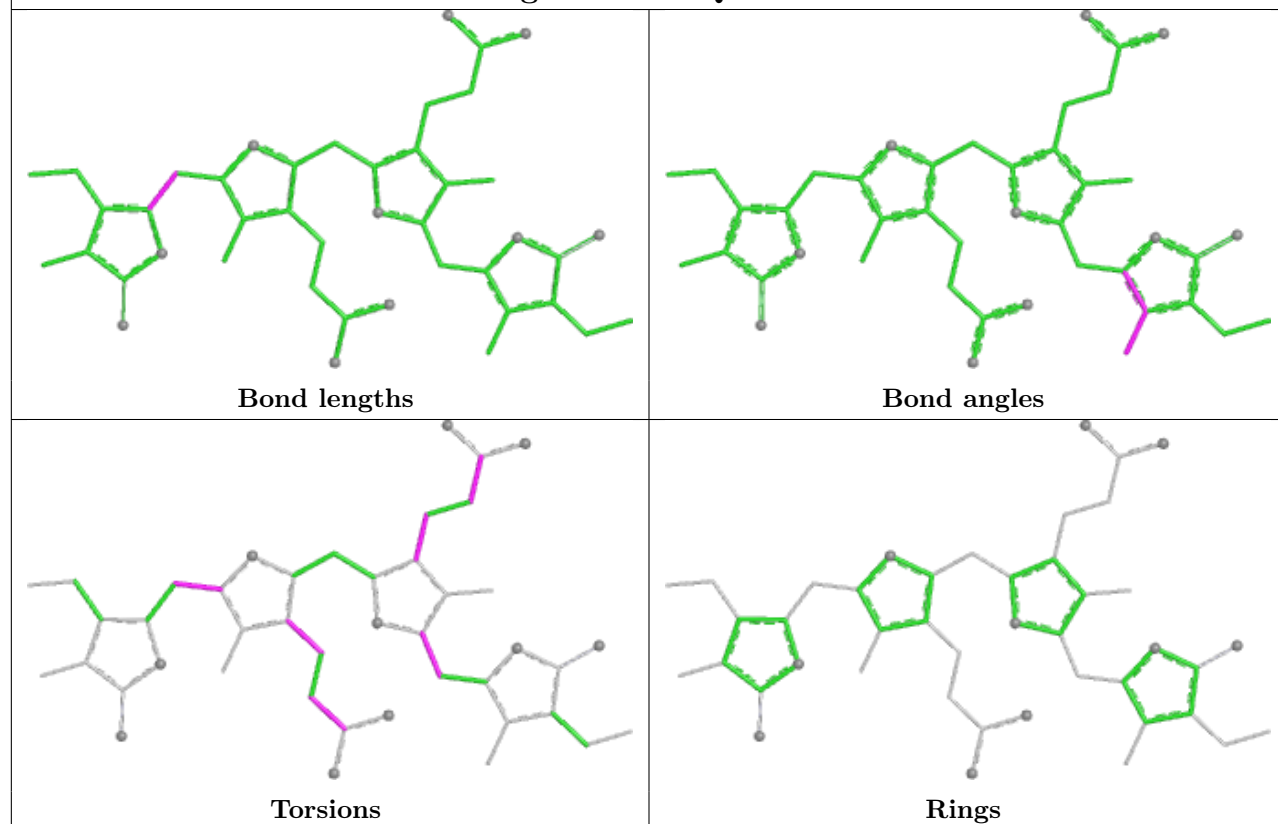
Ligand CYC K1 202



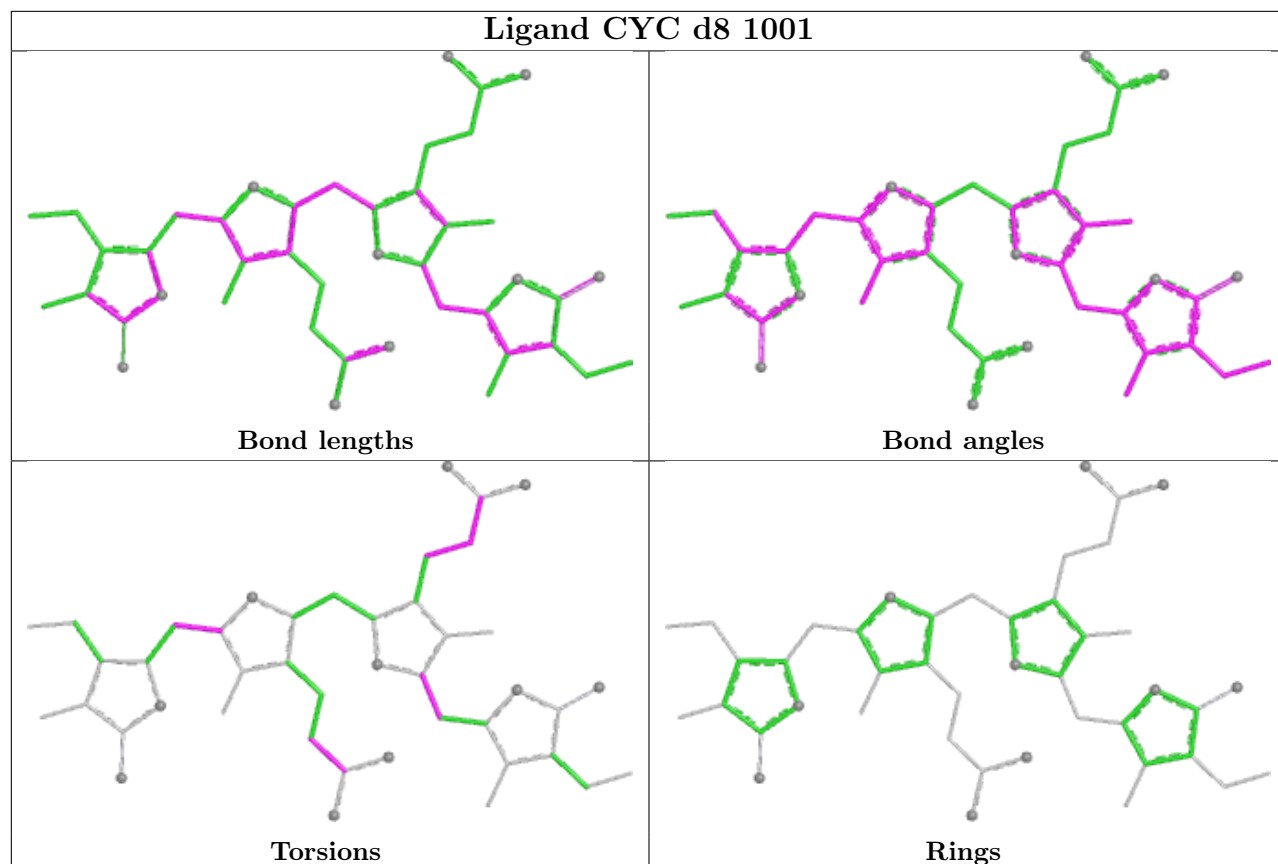
Ligand CYC S6 1001



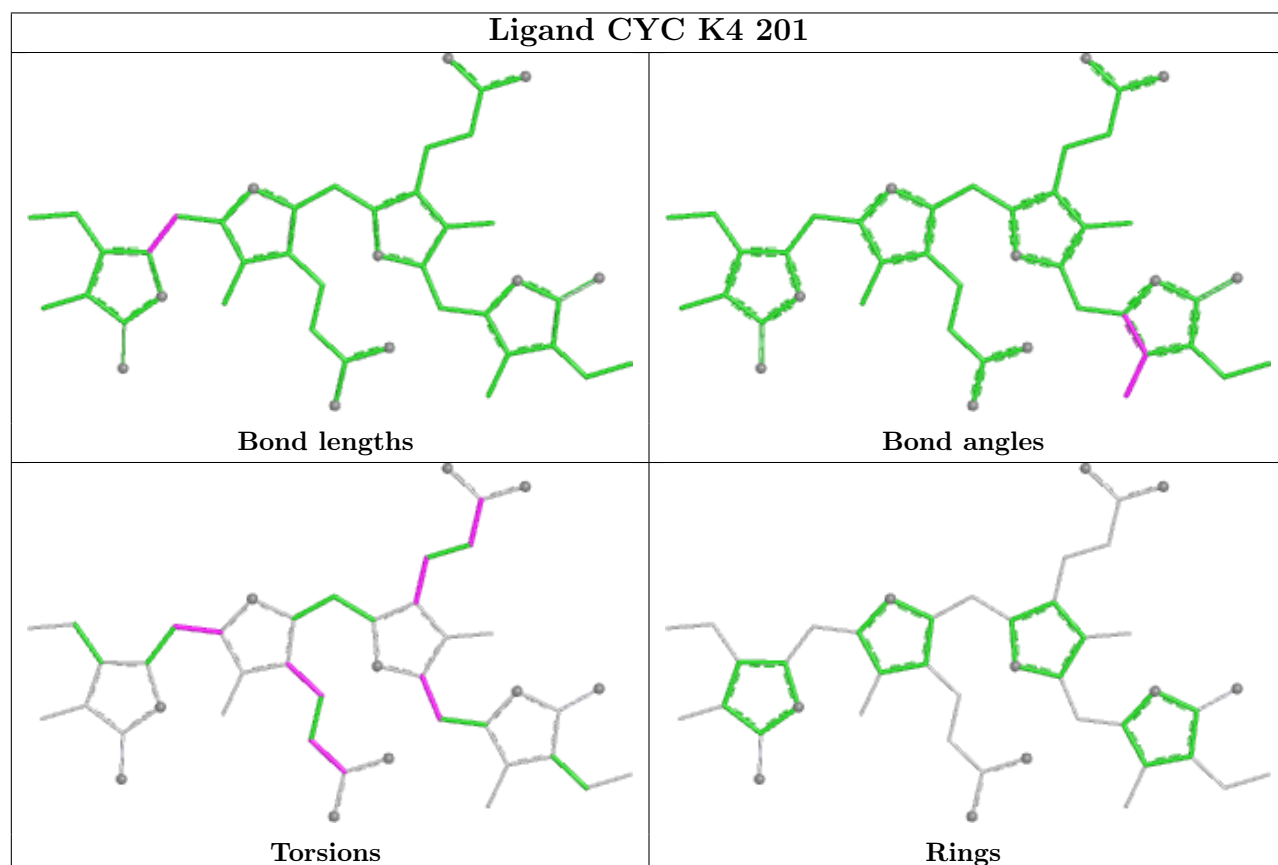
Ligand CYC Q4 202



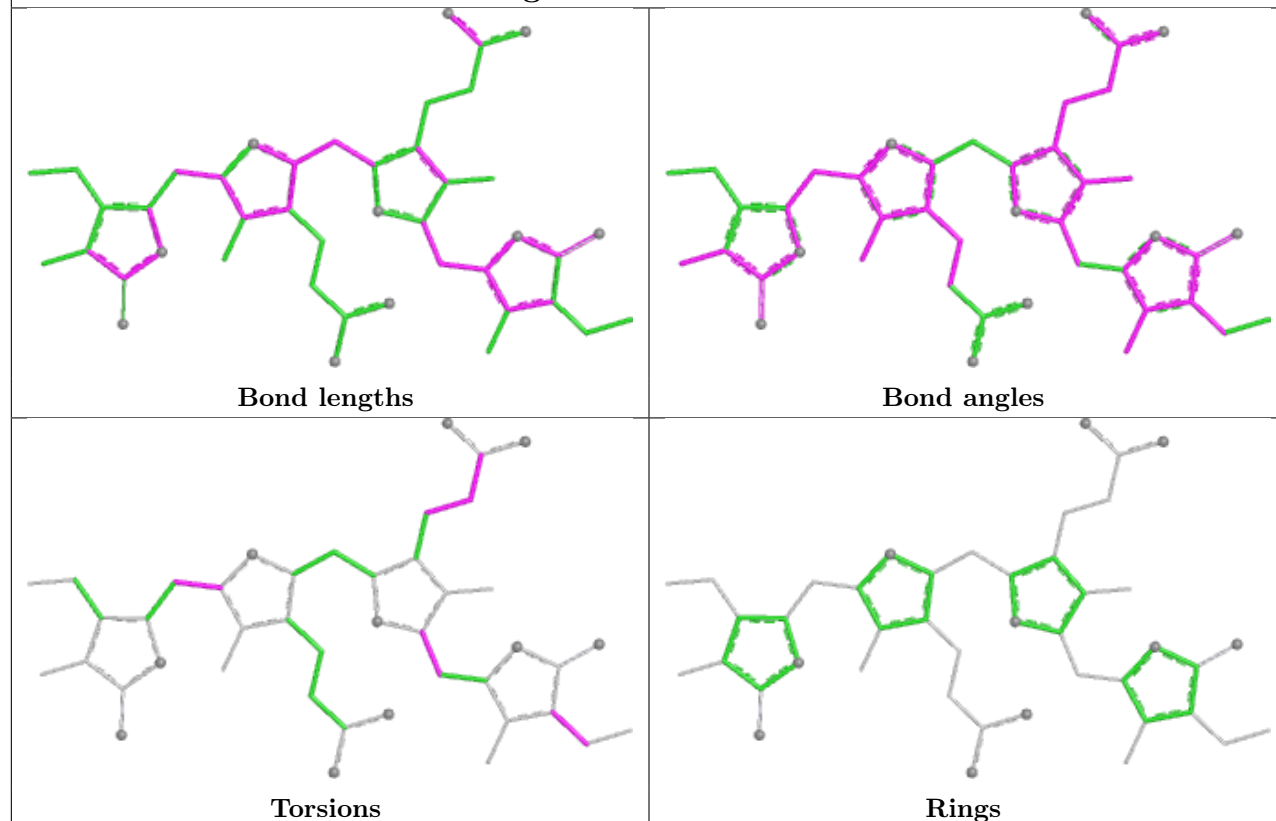
Ligand CYC d8 1001



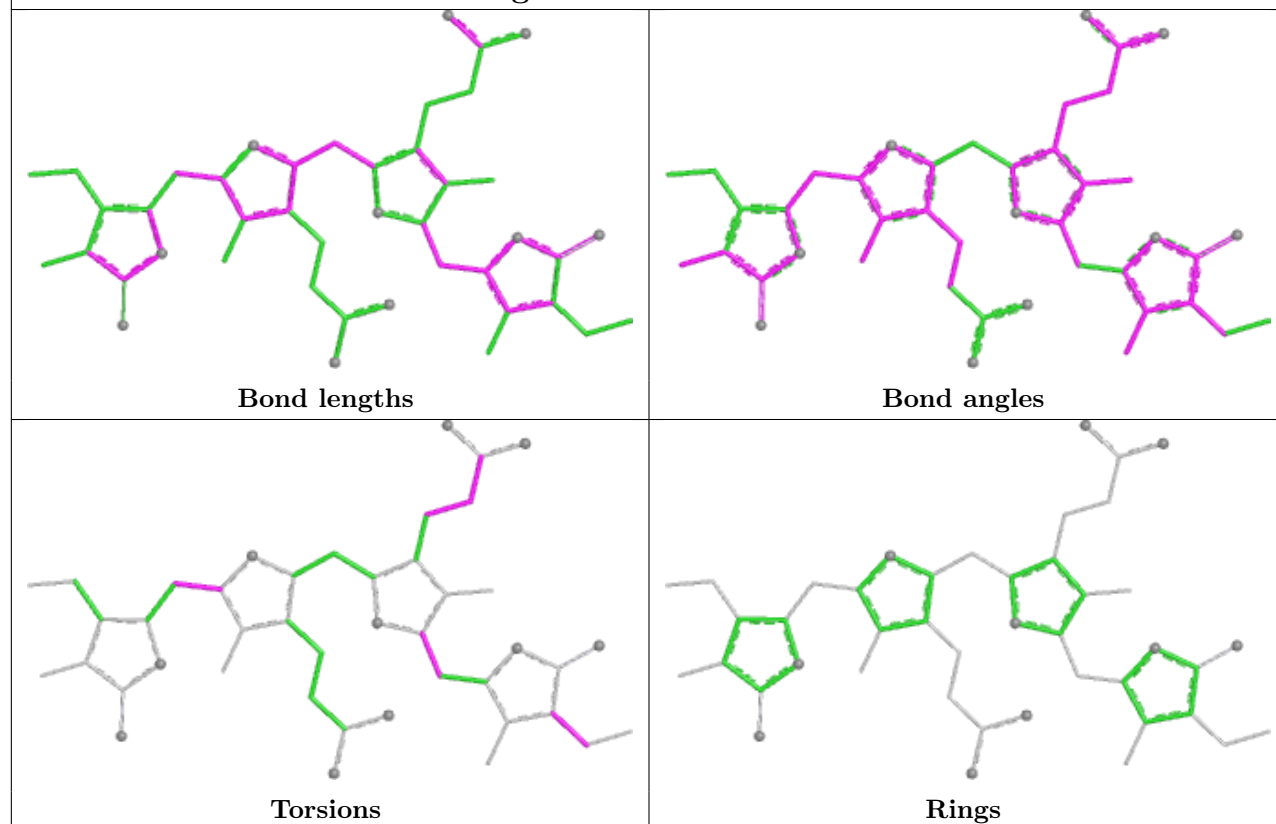
Ligand CYC K4 201

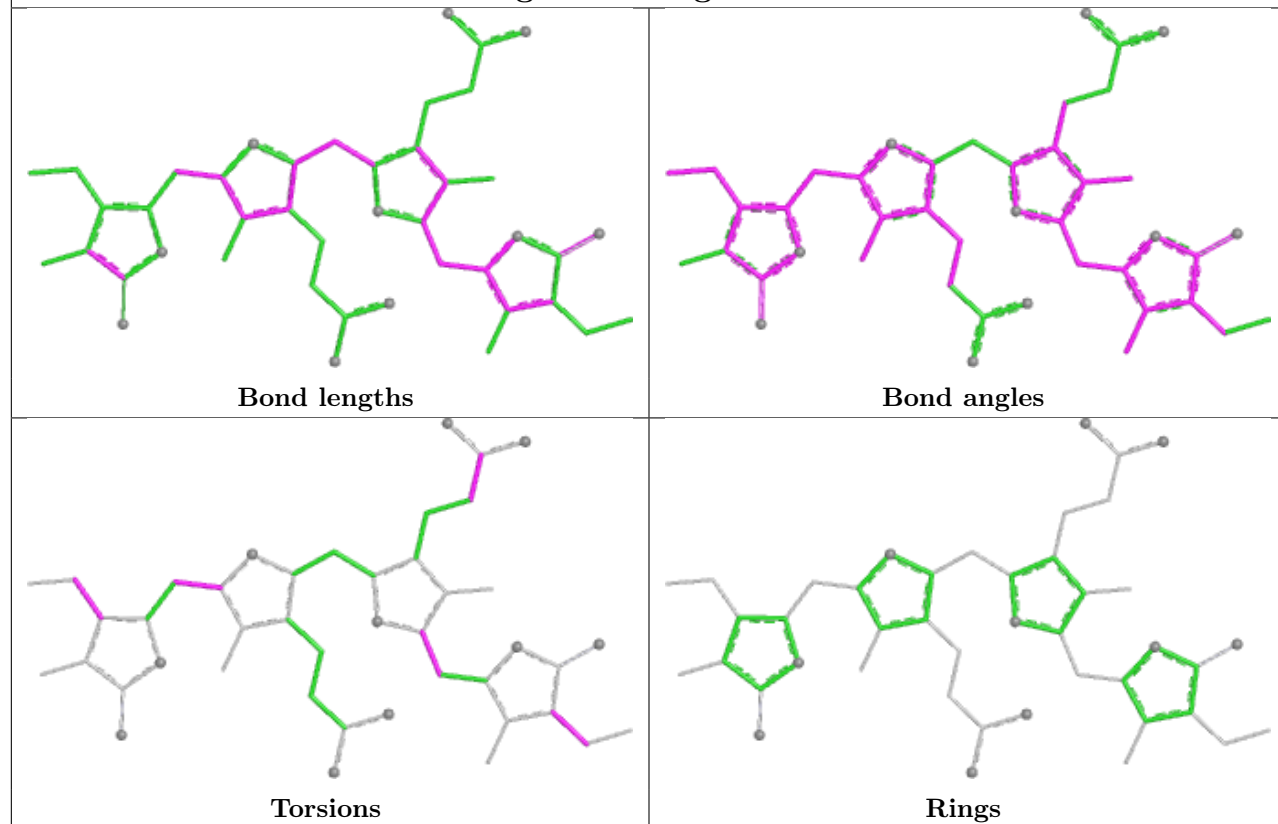
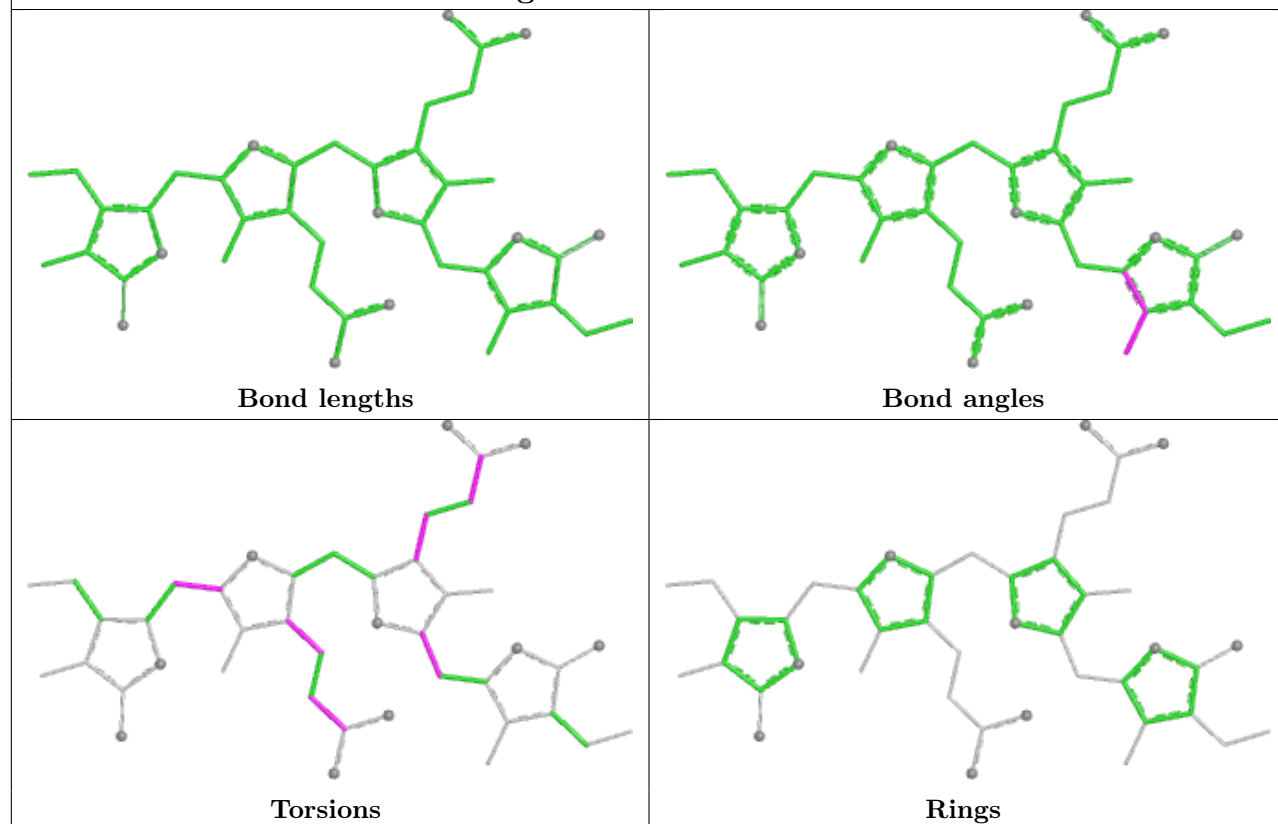


Ligand CYC Z1 202

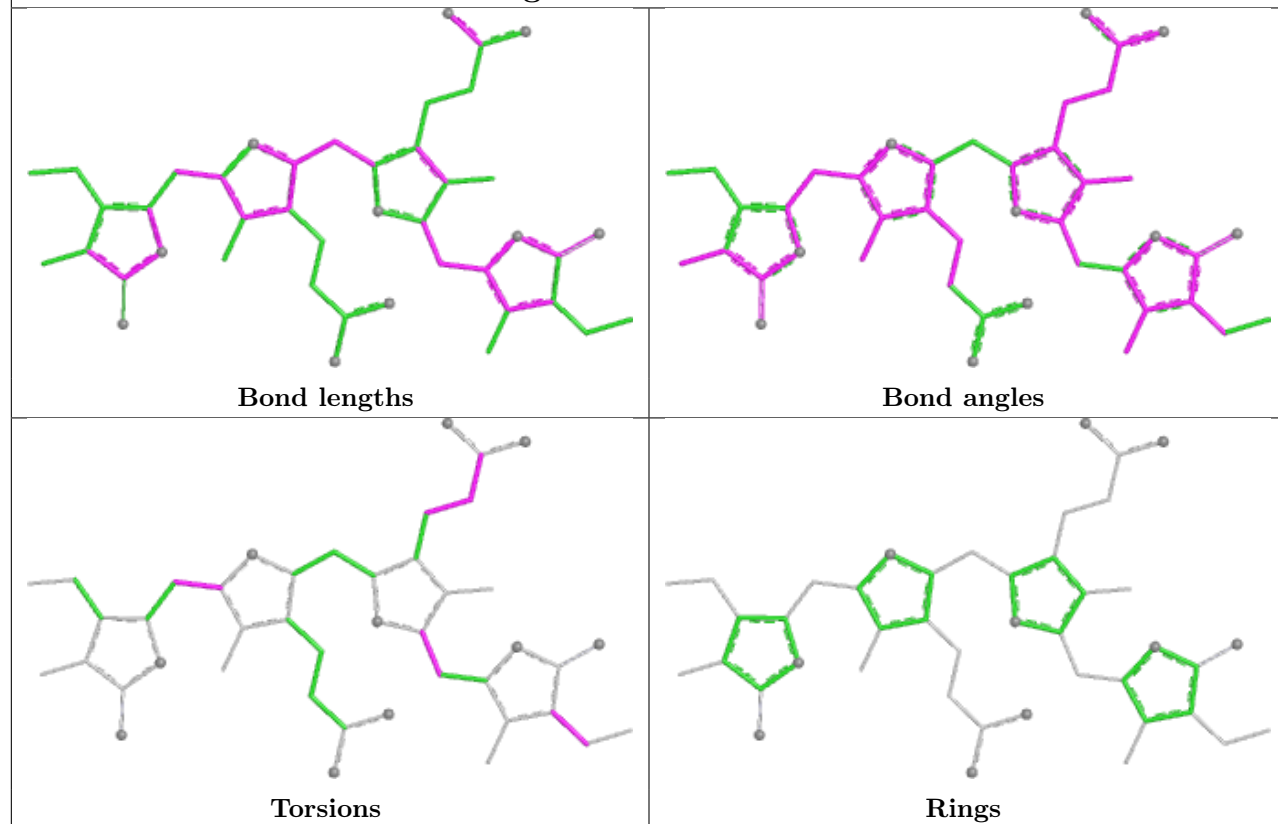


Ligand CYC O6 1001

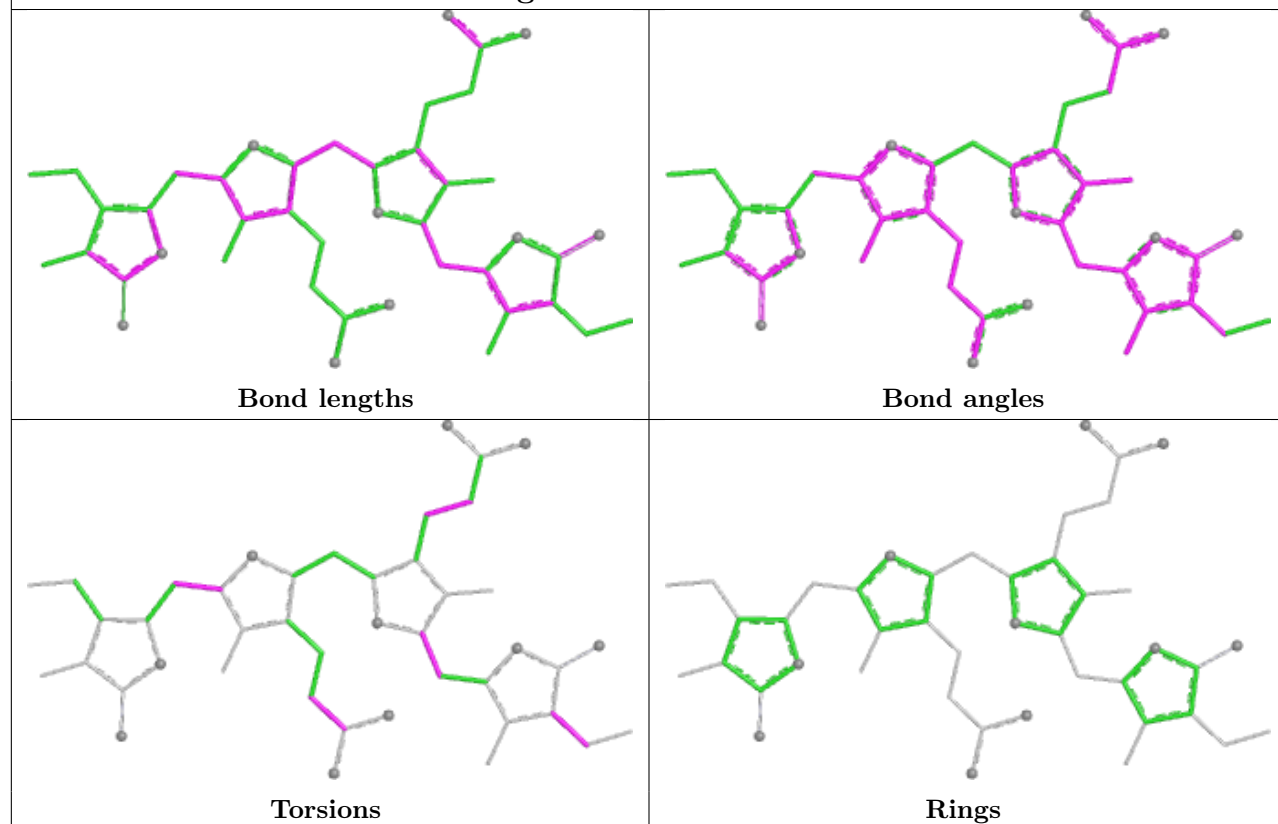


Ligand **CYC g8 1001**Ligand **CYC M7 201**

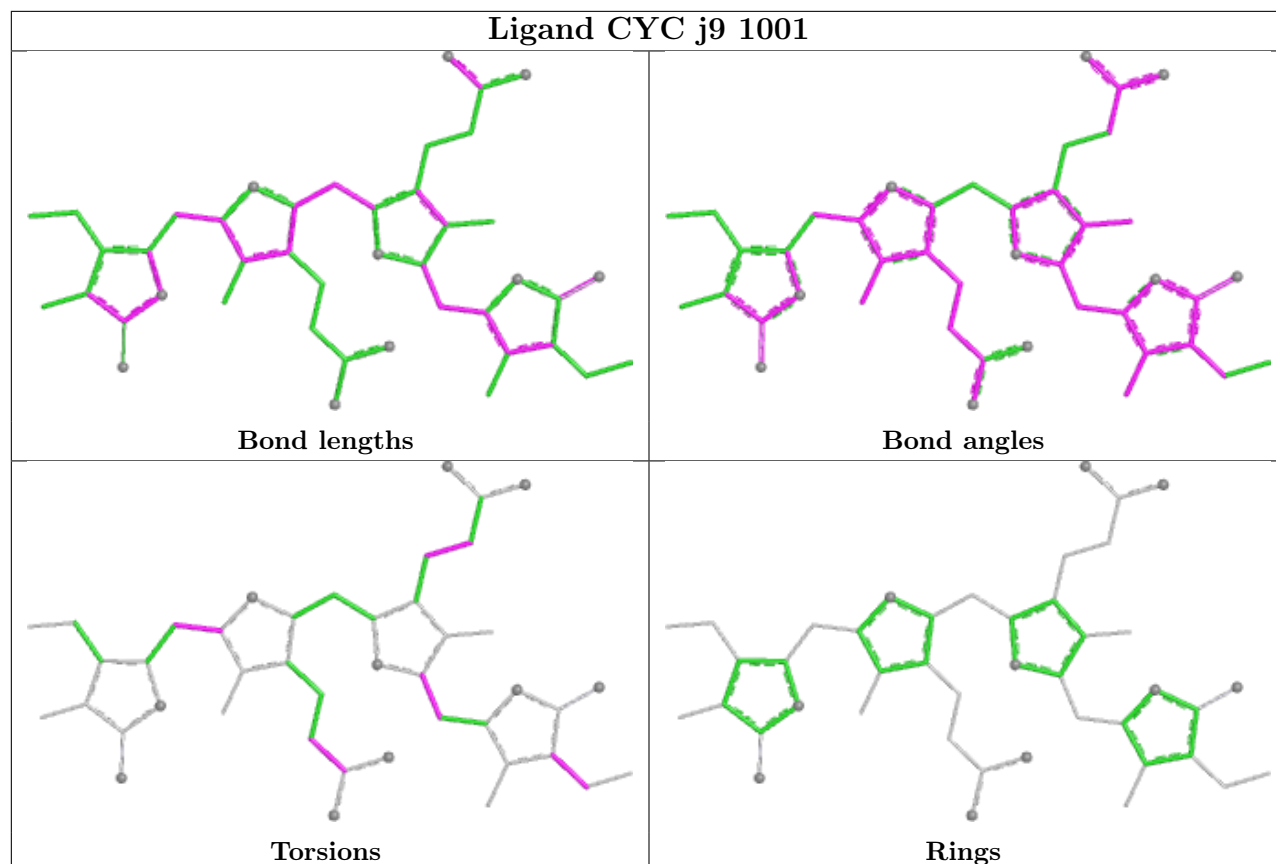
Ligand CYC L6 201



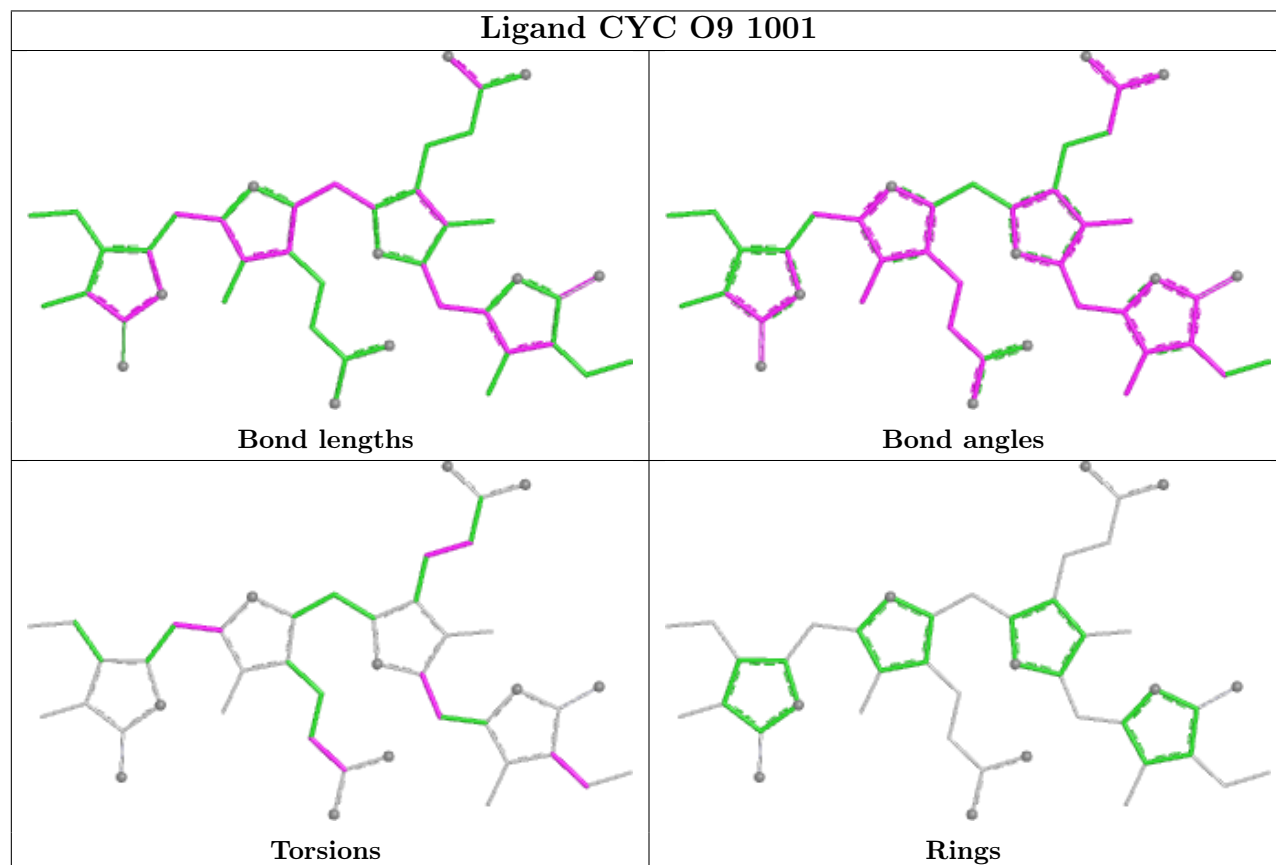
Ligand CYC e9 1001



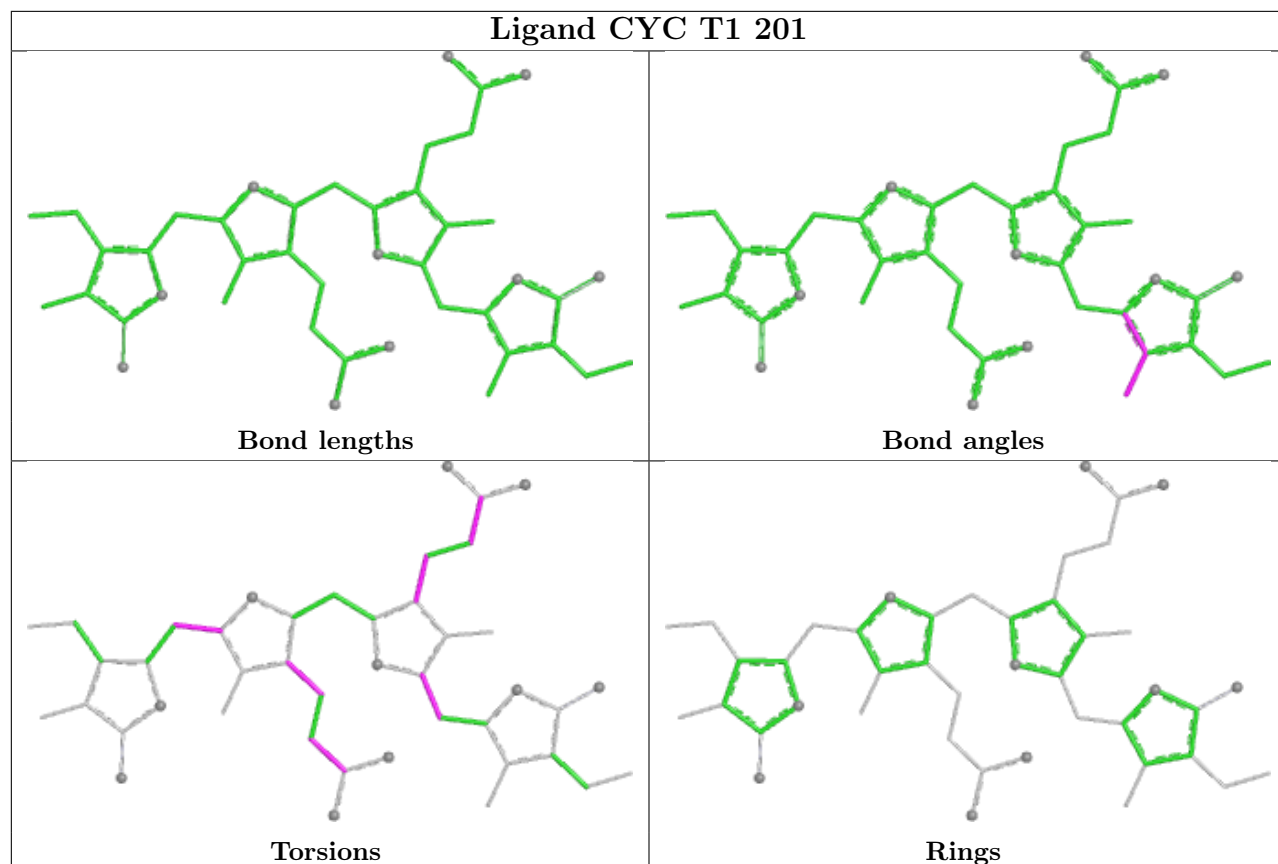
Ligand CYC j9 1001



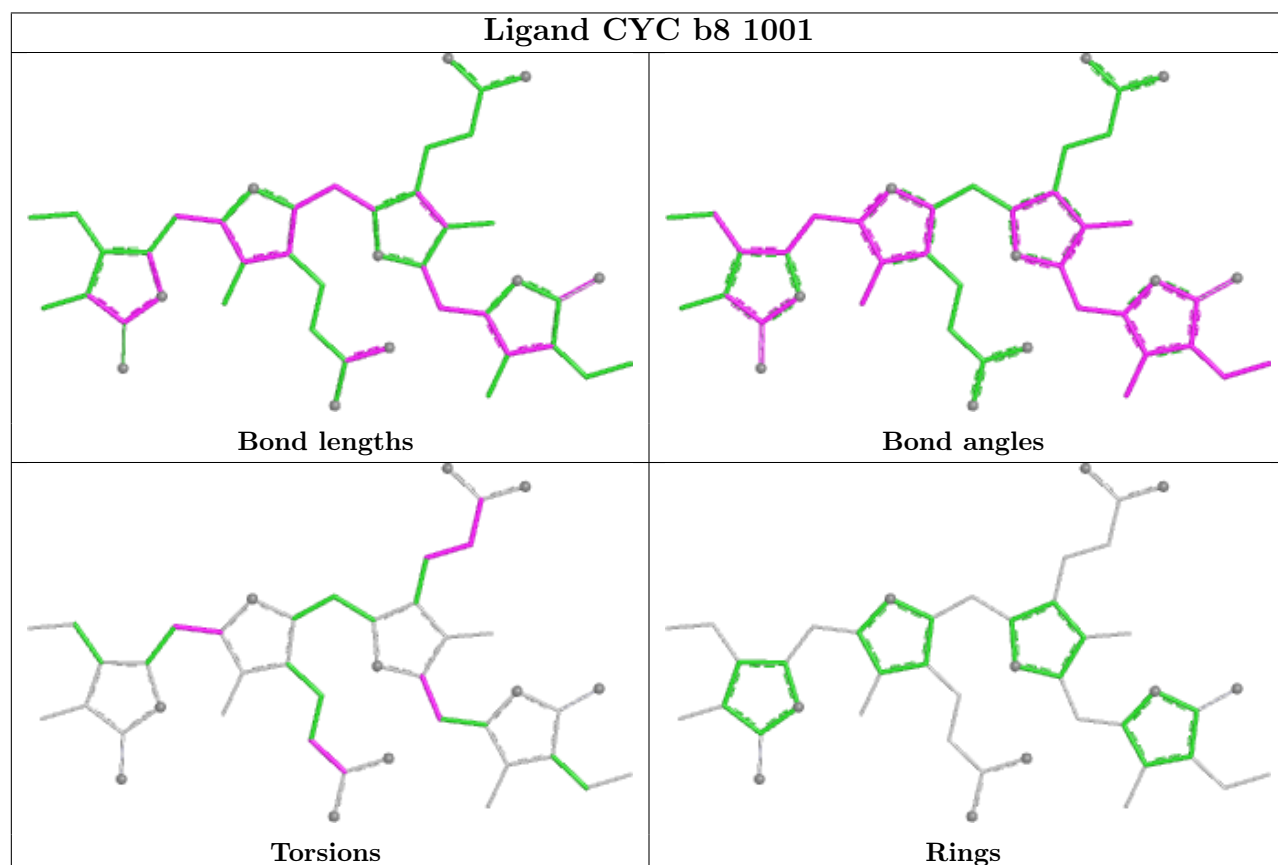
Ligand CYC O9 1001



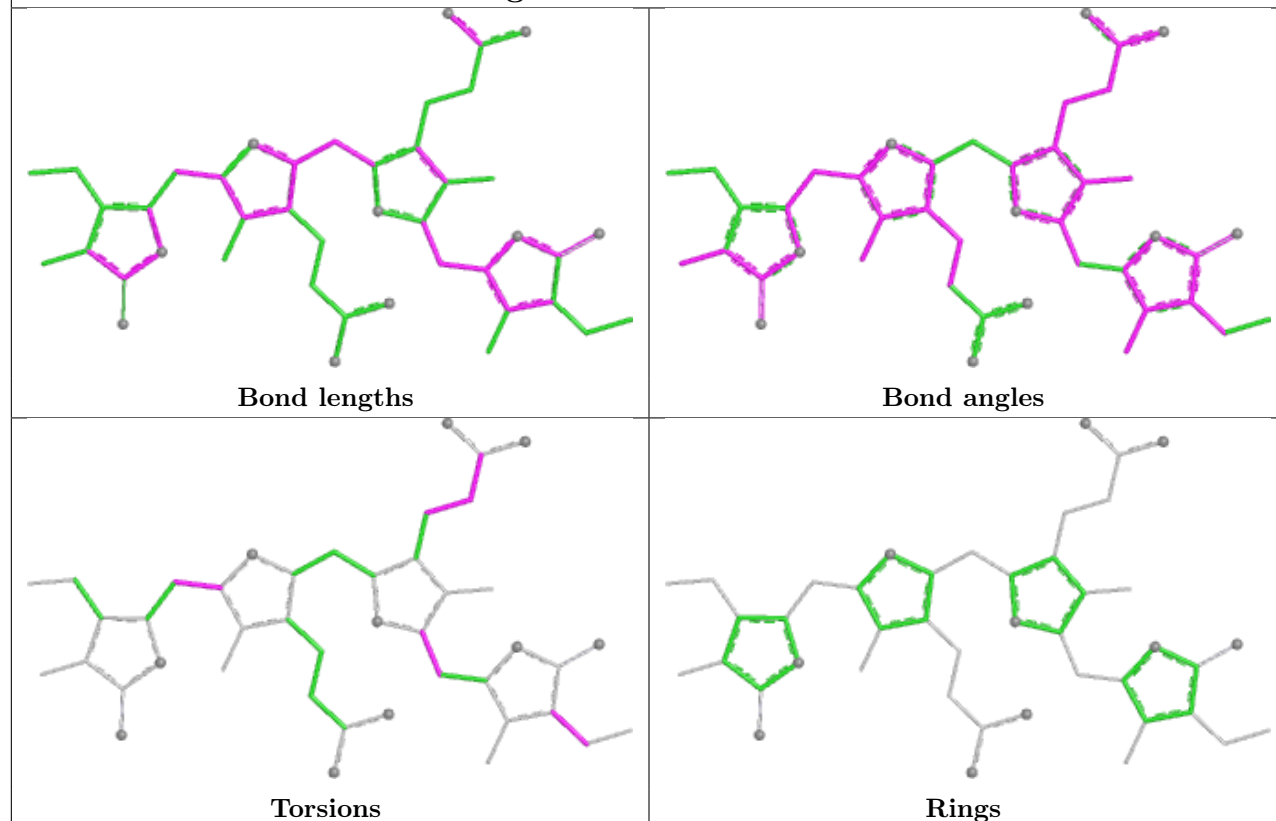
Ligand CYC T1 201



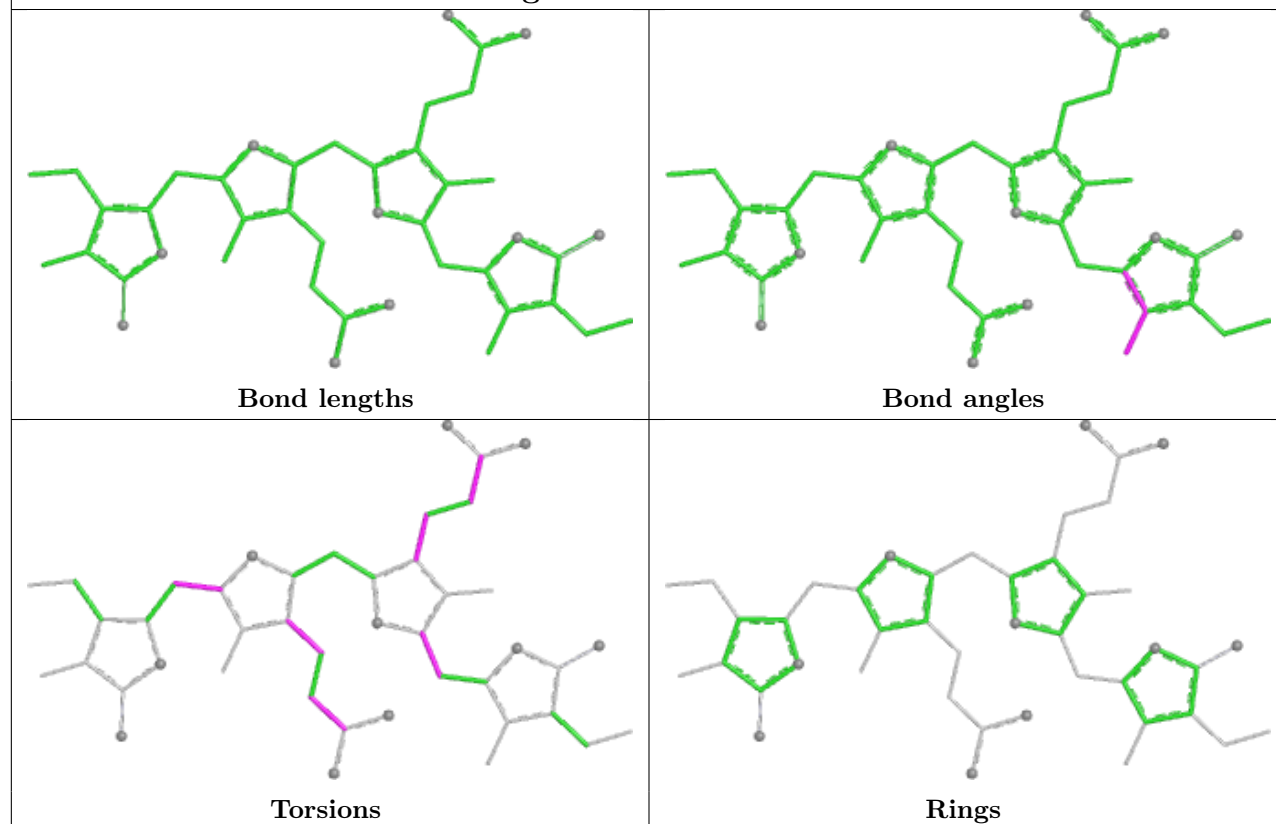
Ligand CYC b8 1001



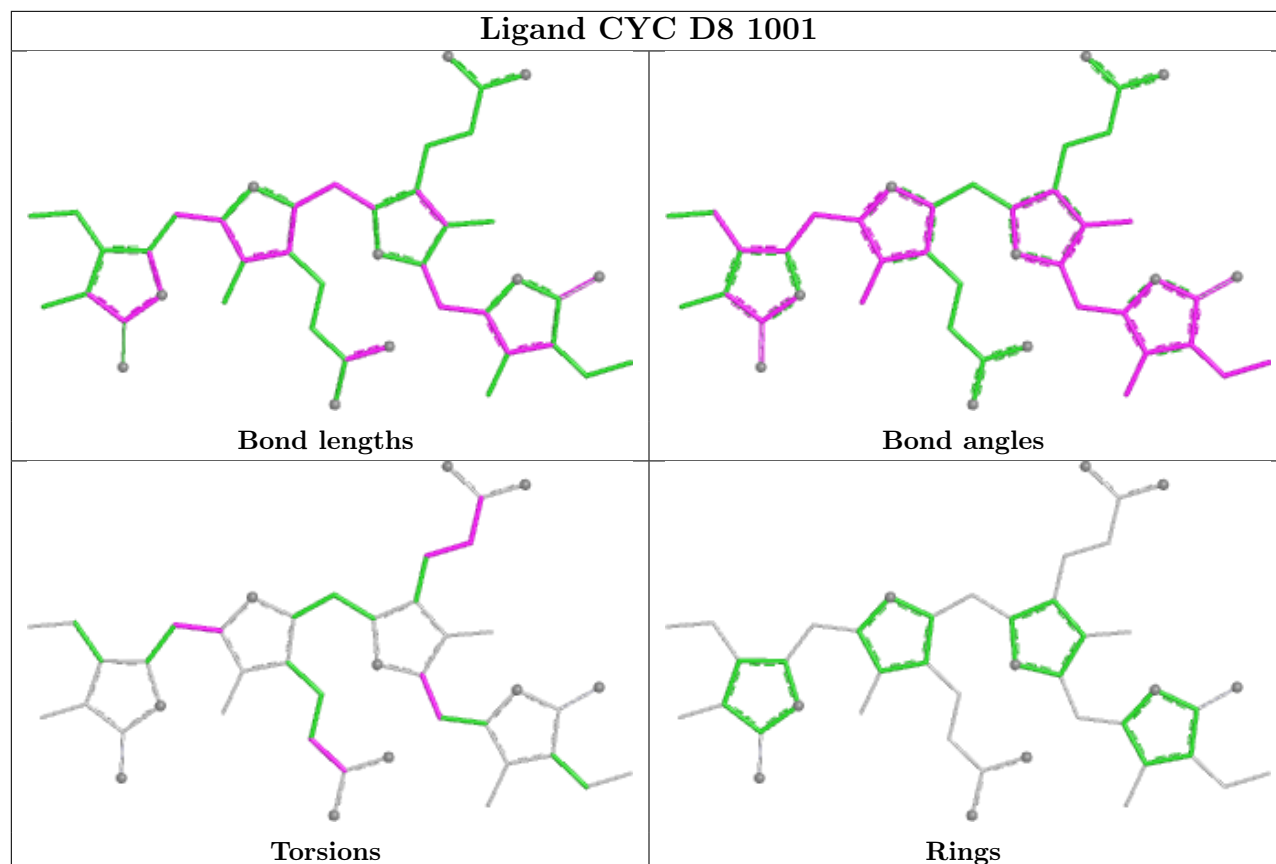
Ligand CYC GA 1001



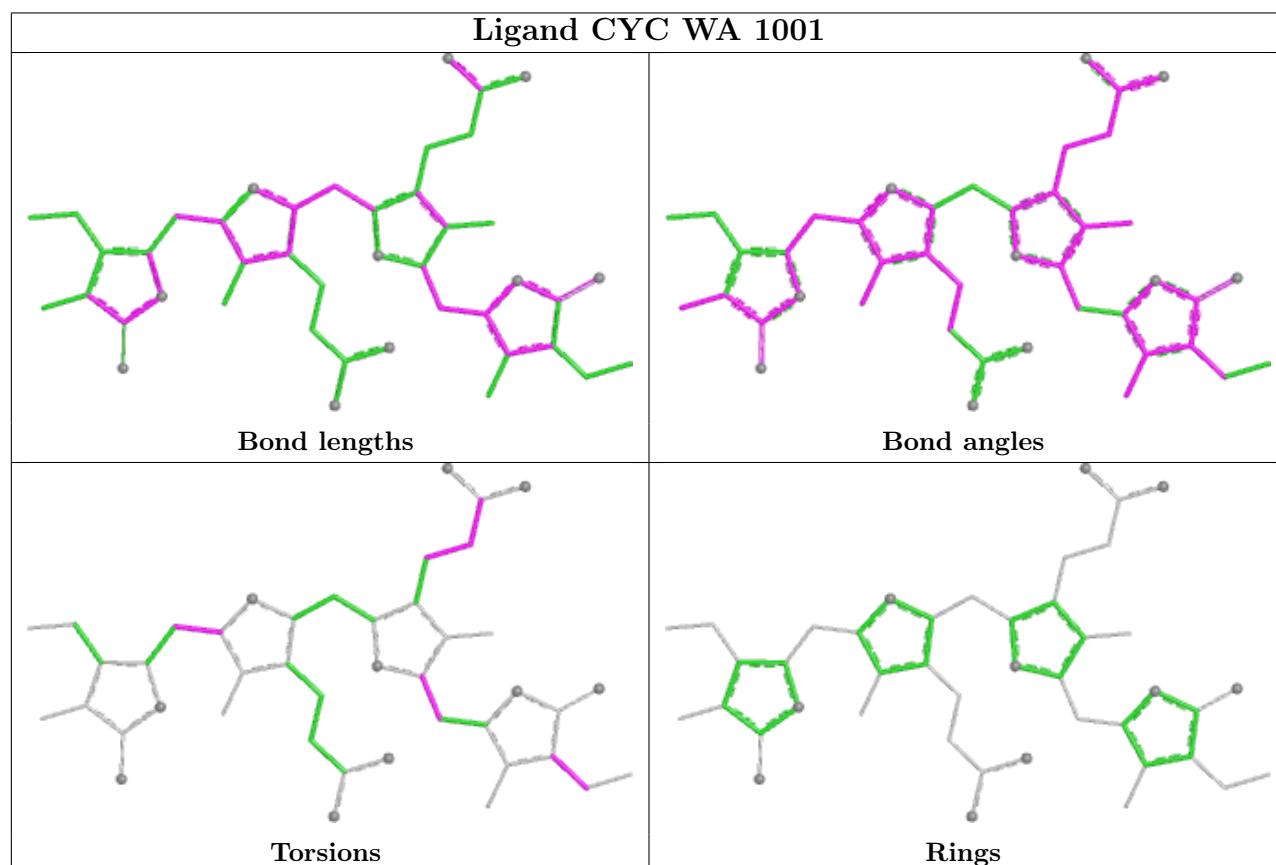
Ligand CYC E3 202



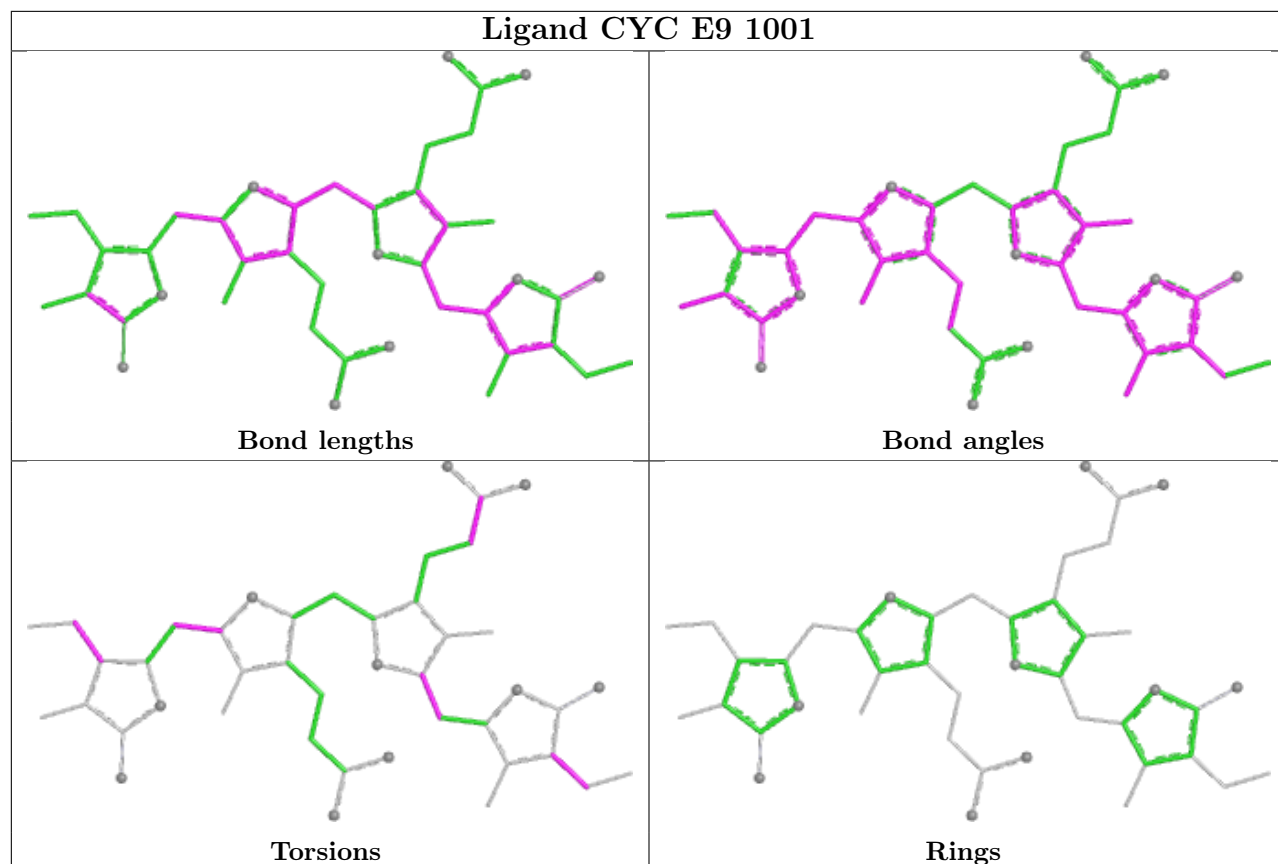
Ligand CYC D8 1001



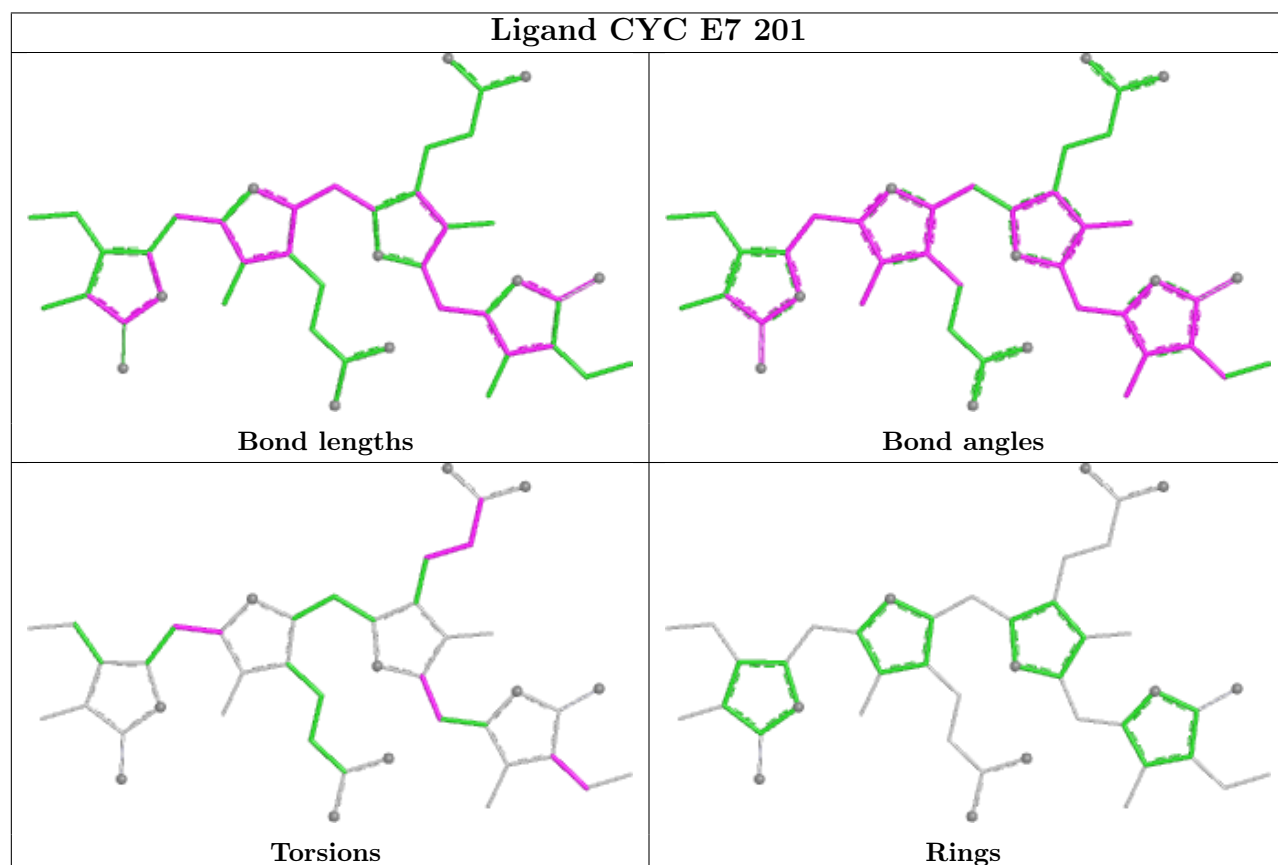
Ligand CYC WA 1001

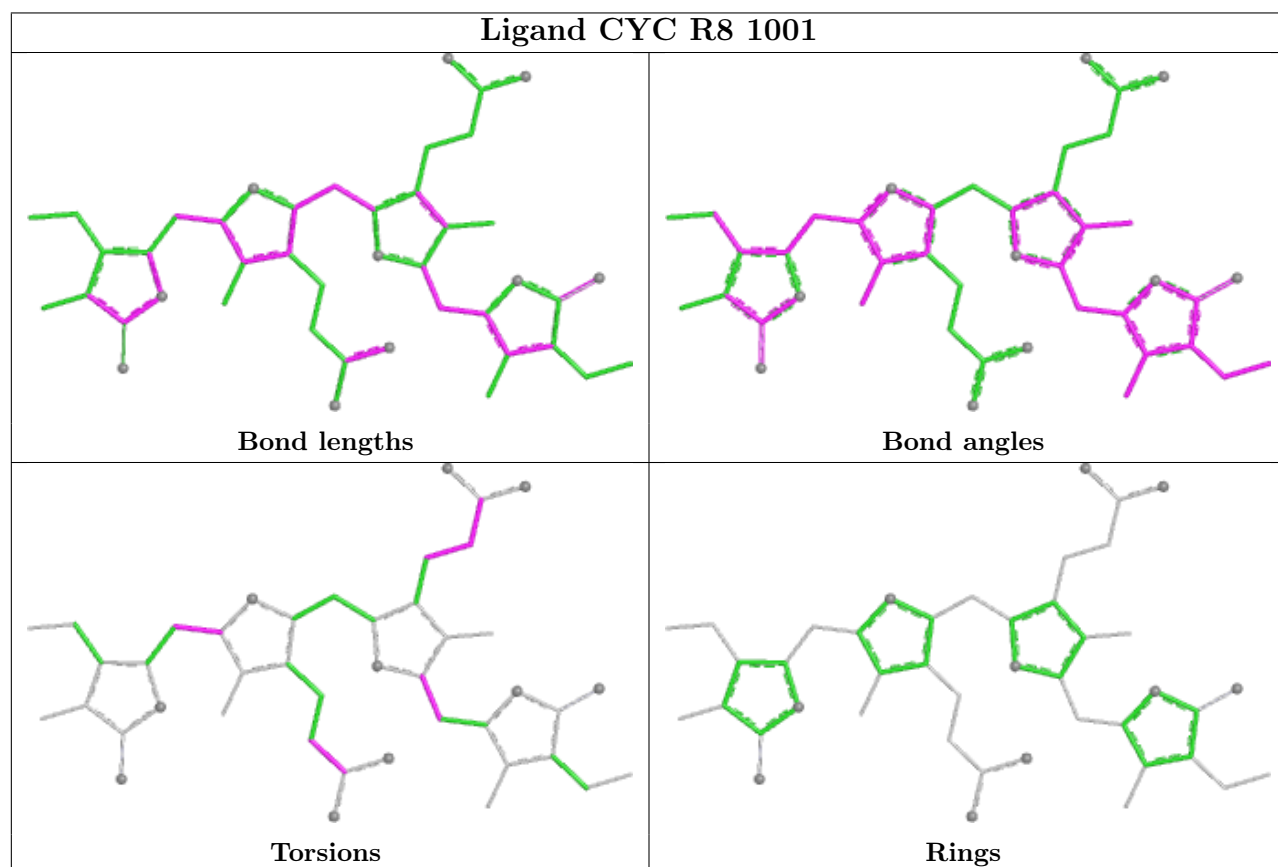
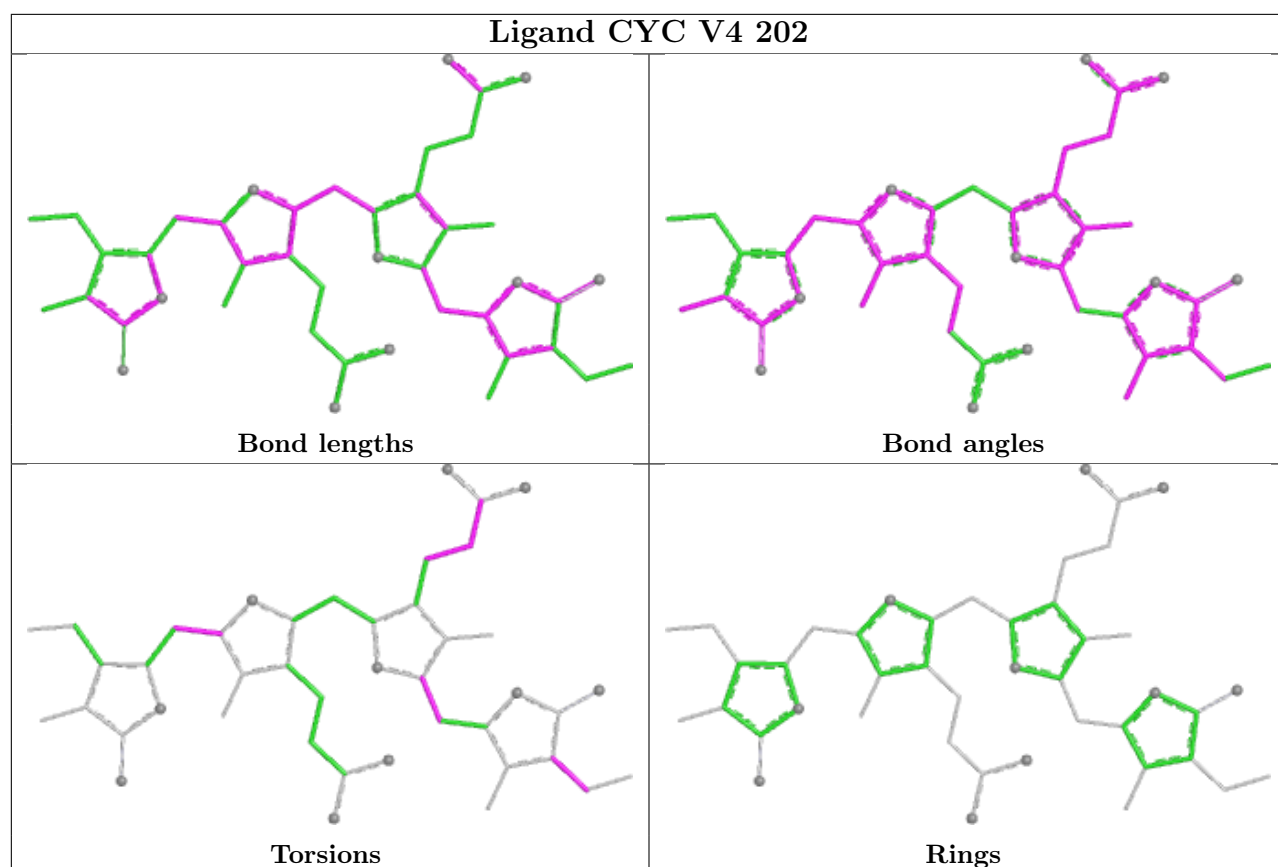


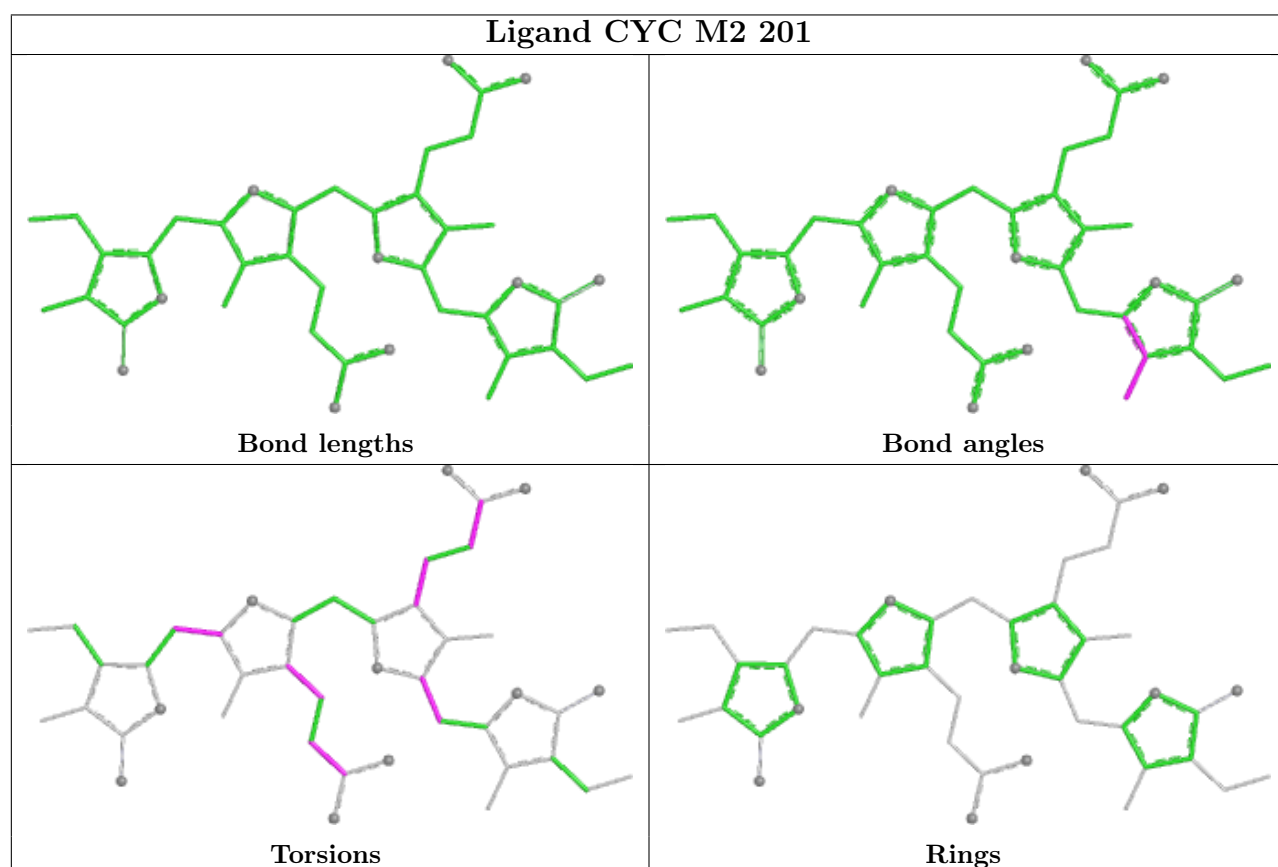
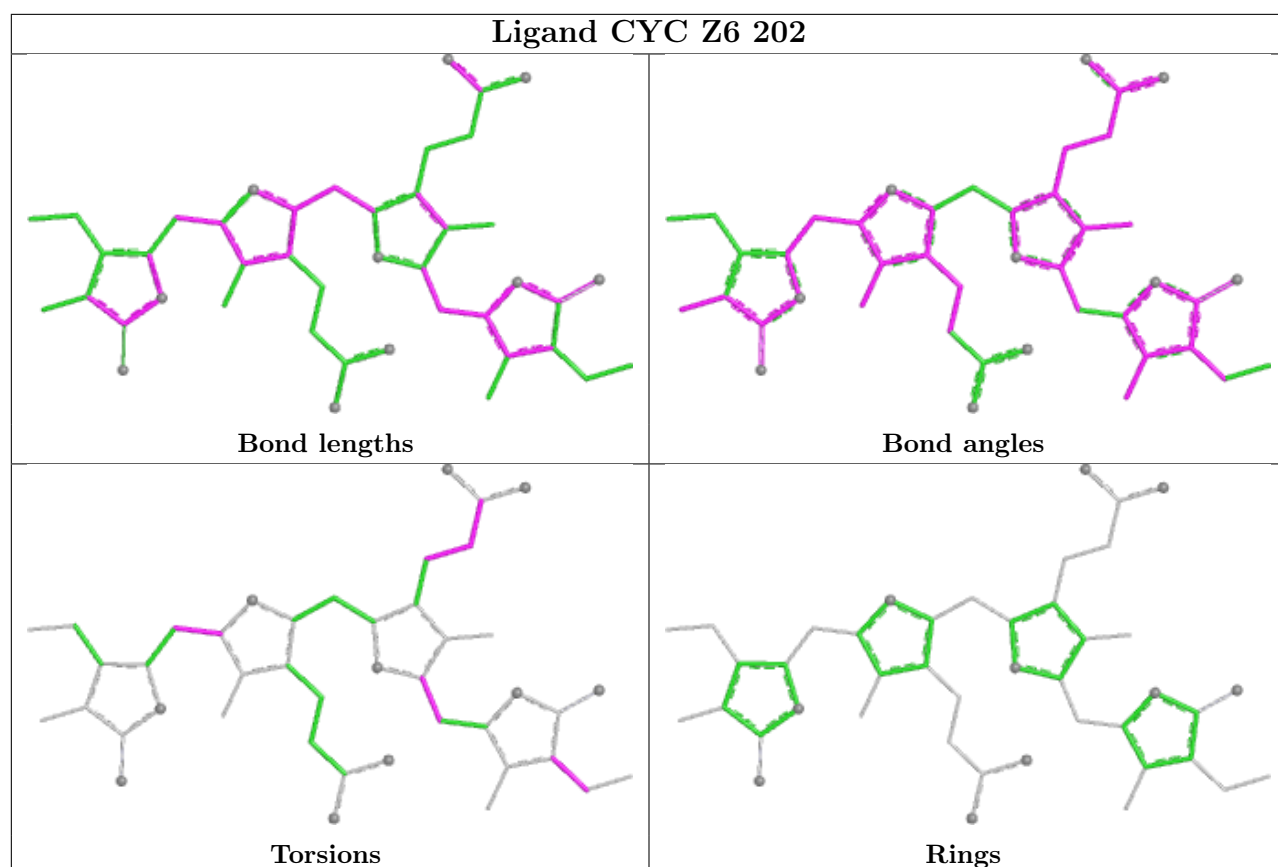
Ligand CYC E9 1001



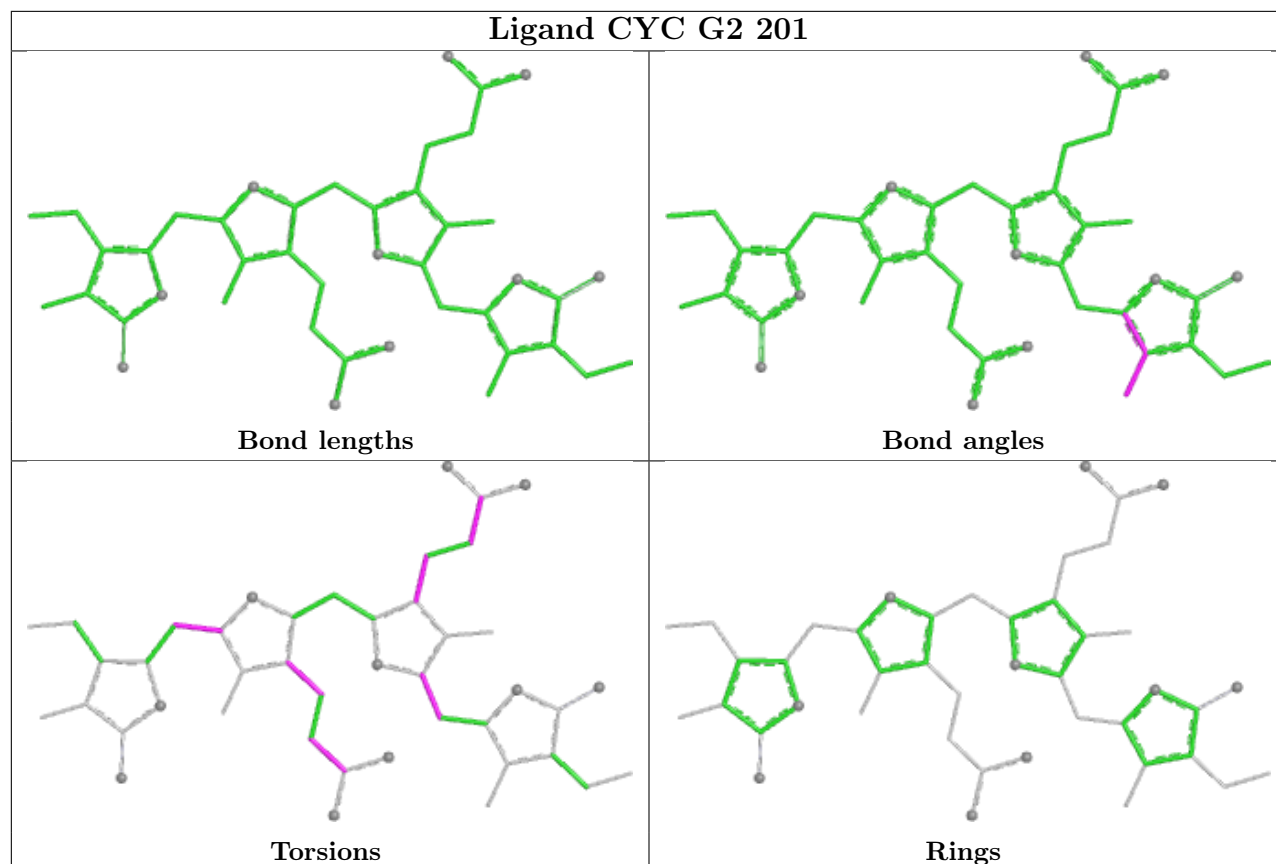
Ligand CYC E7 201



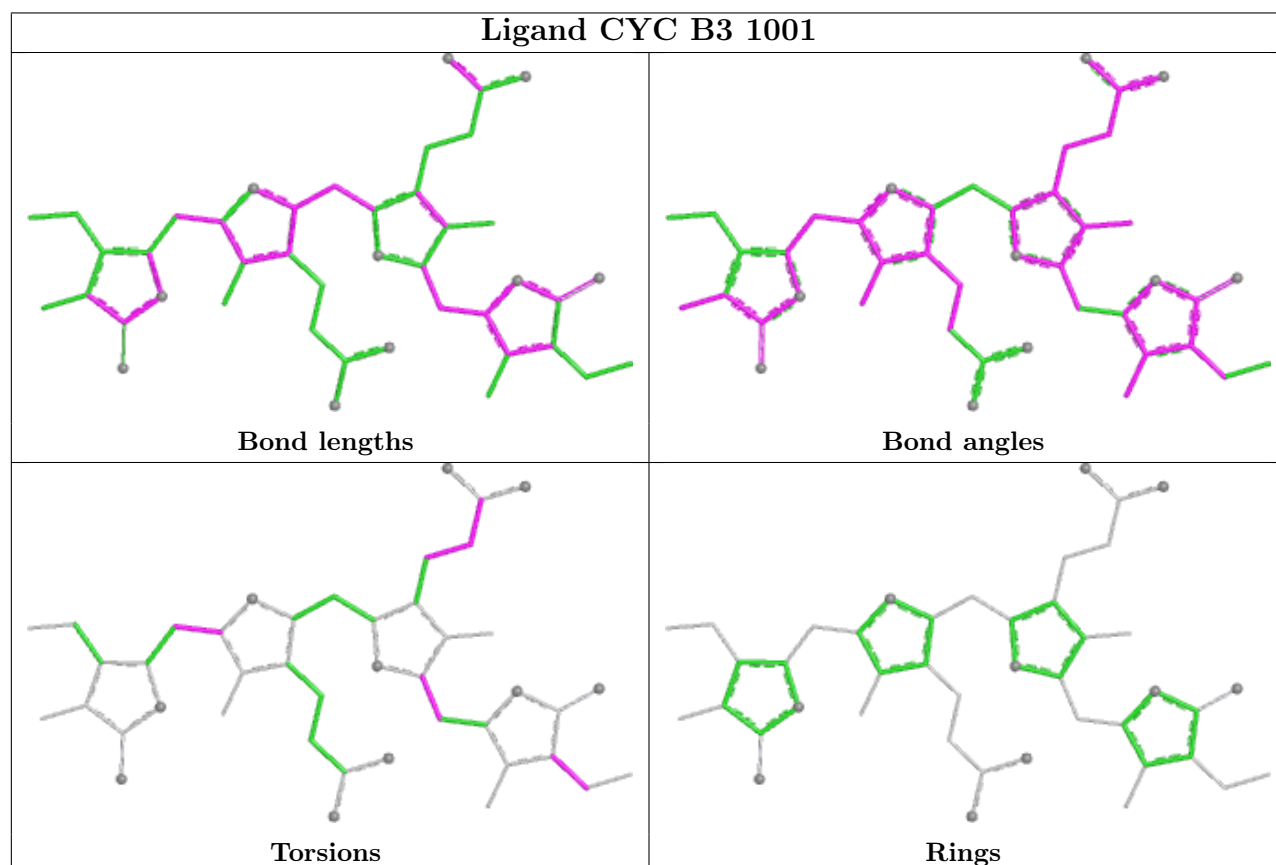




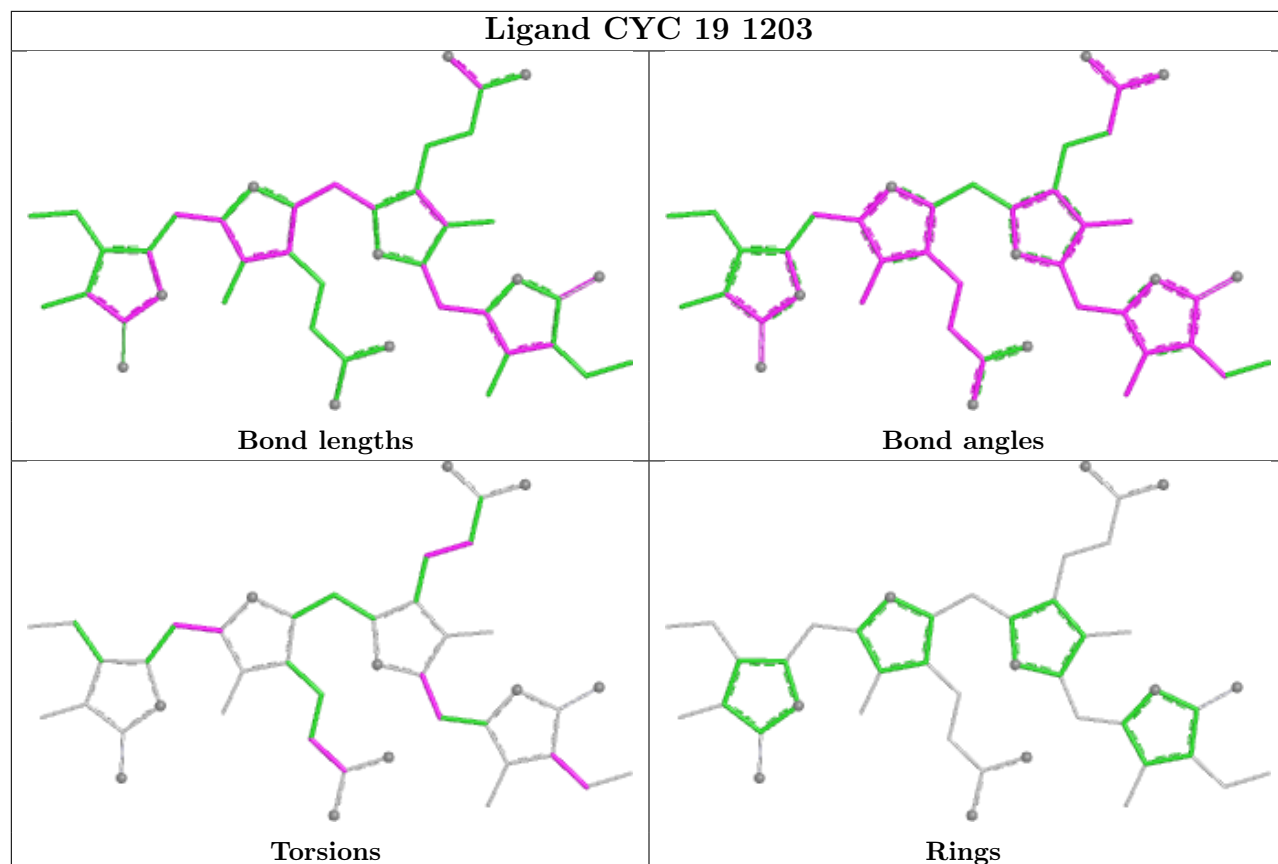
Ligand CYC G2 201



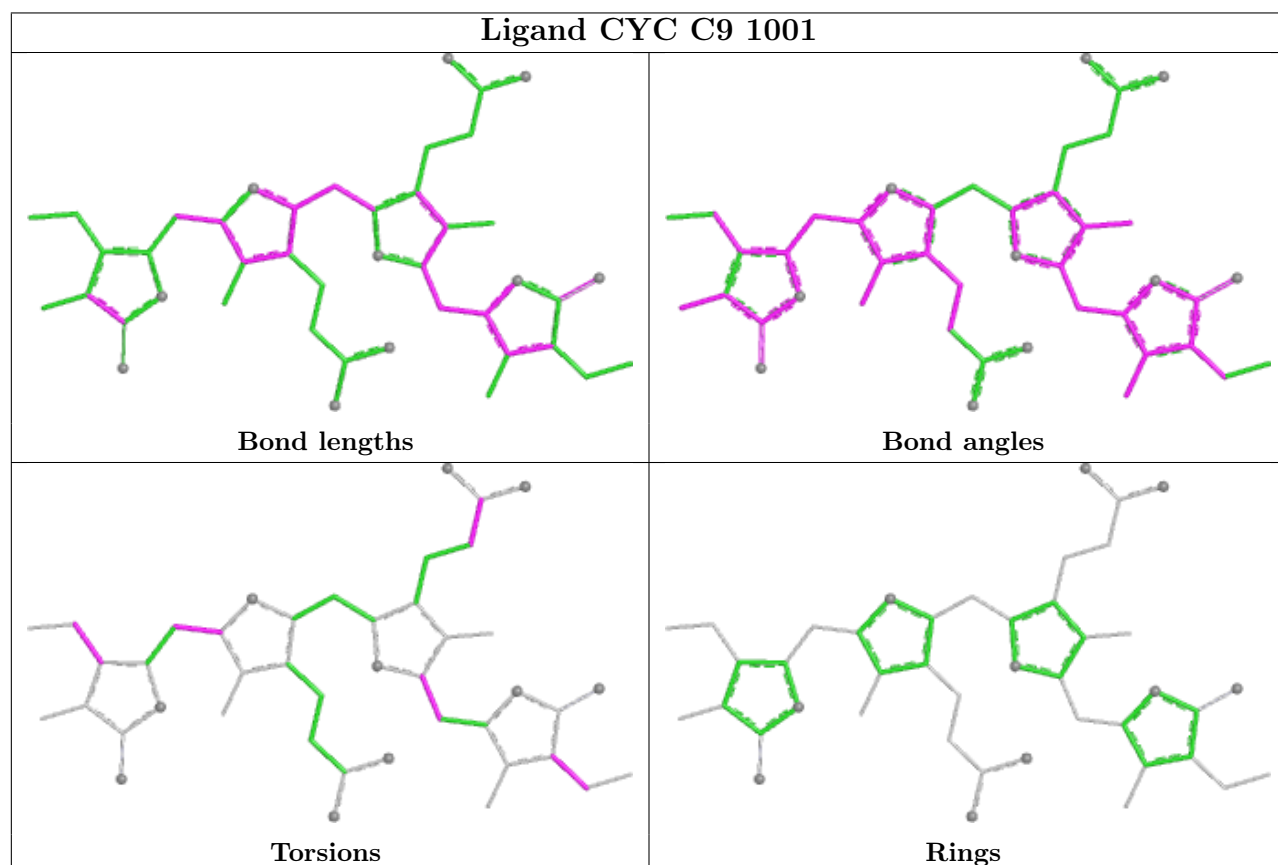
Ligand CYC B3 1001



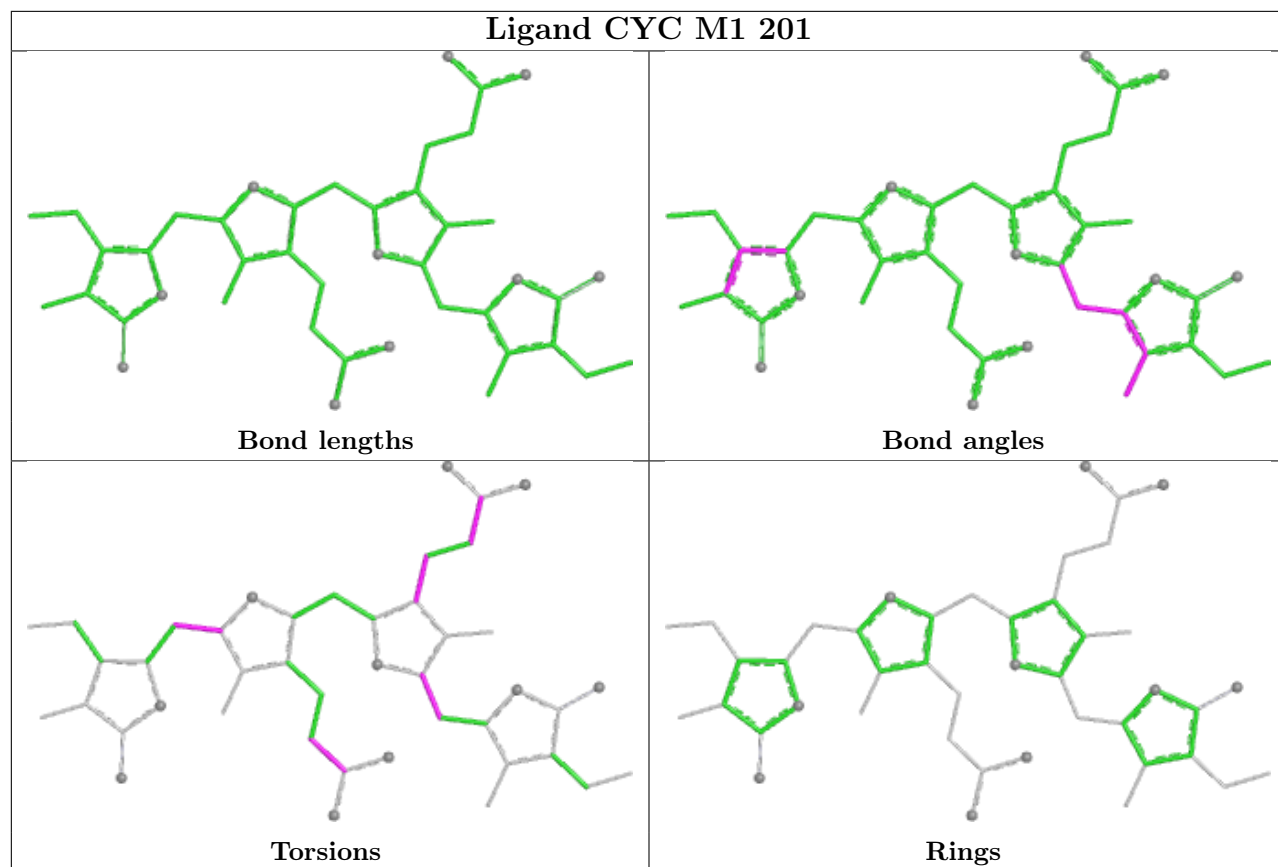
Ligand CYC 19 1203



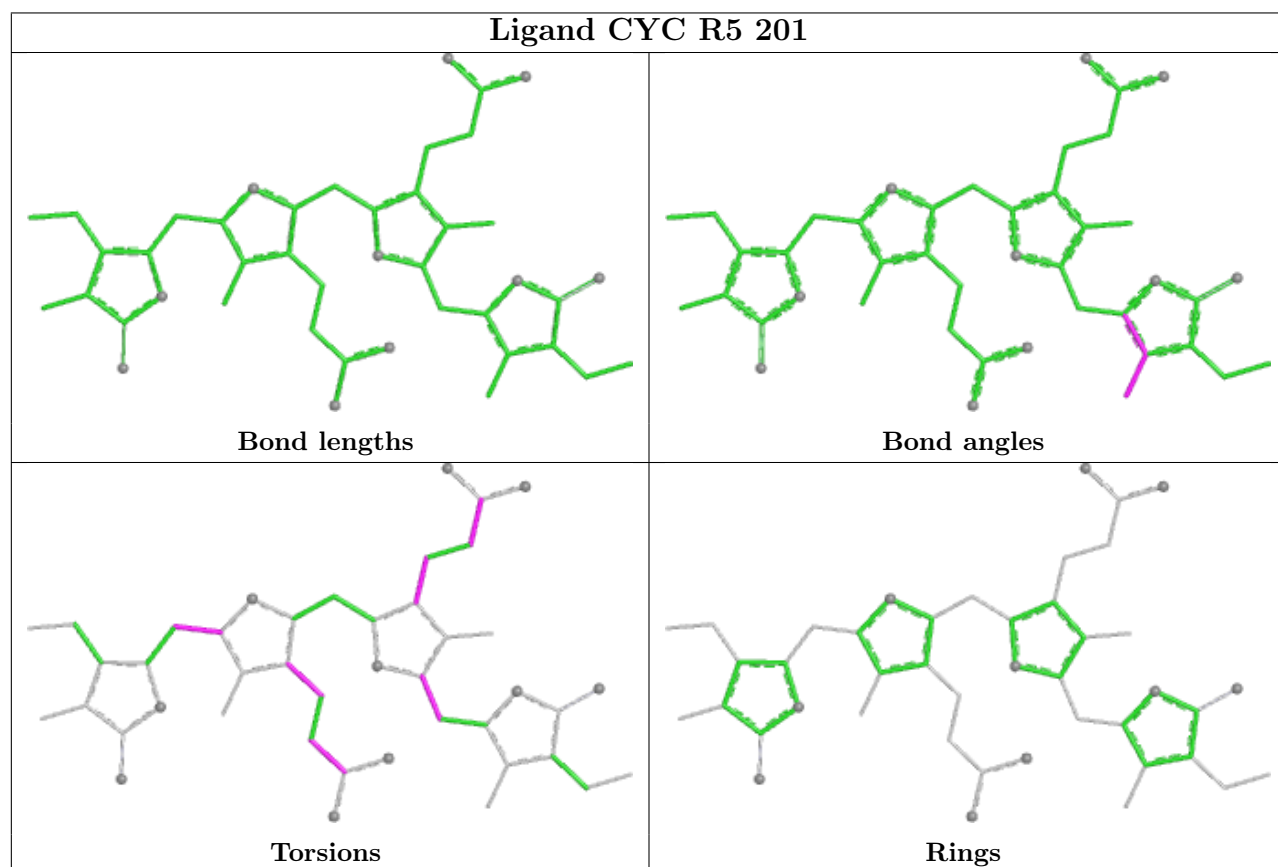
Ligand CYC C9 1001



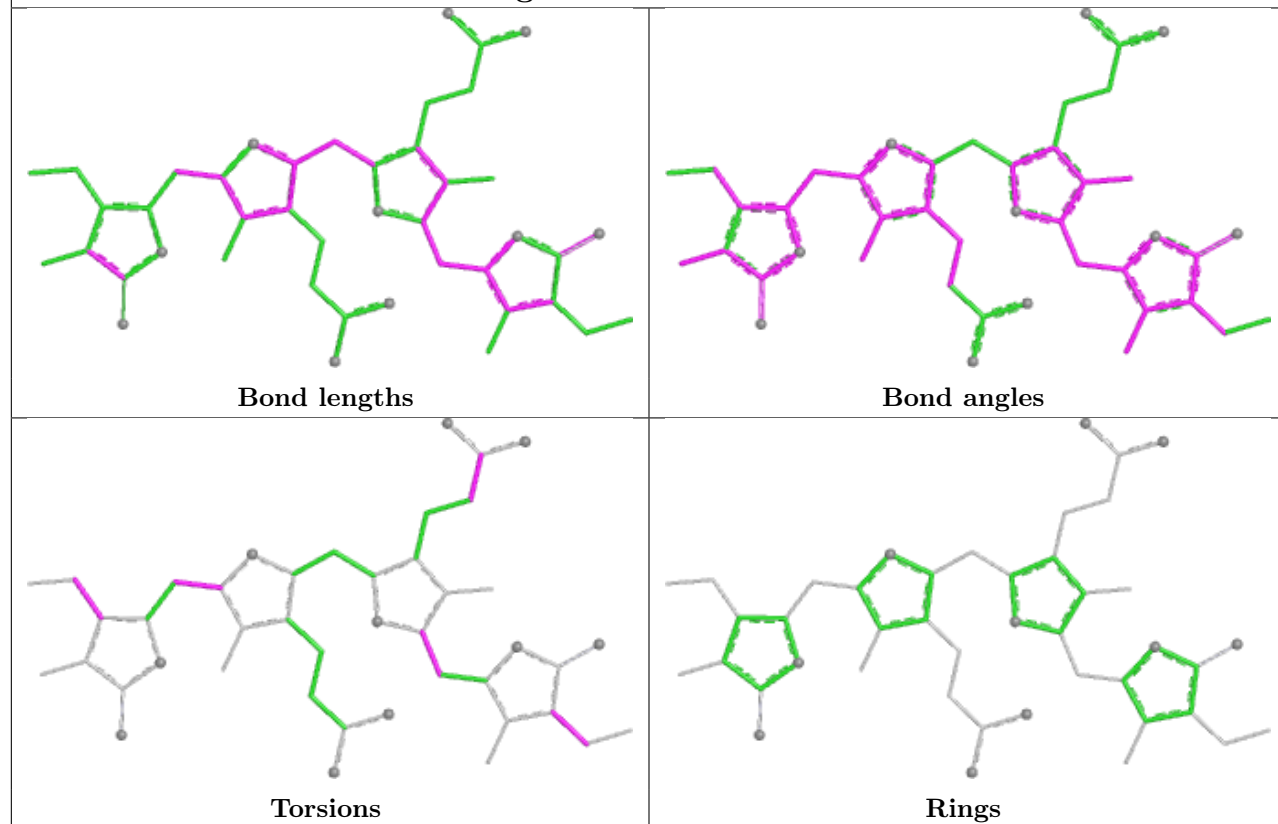
Ligand CYC M1 201



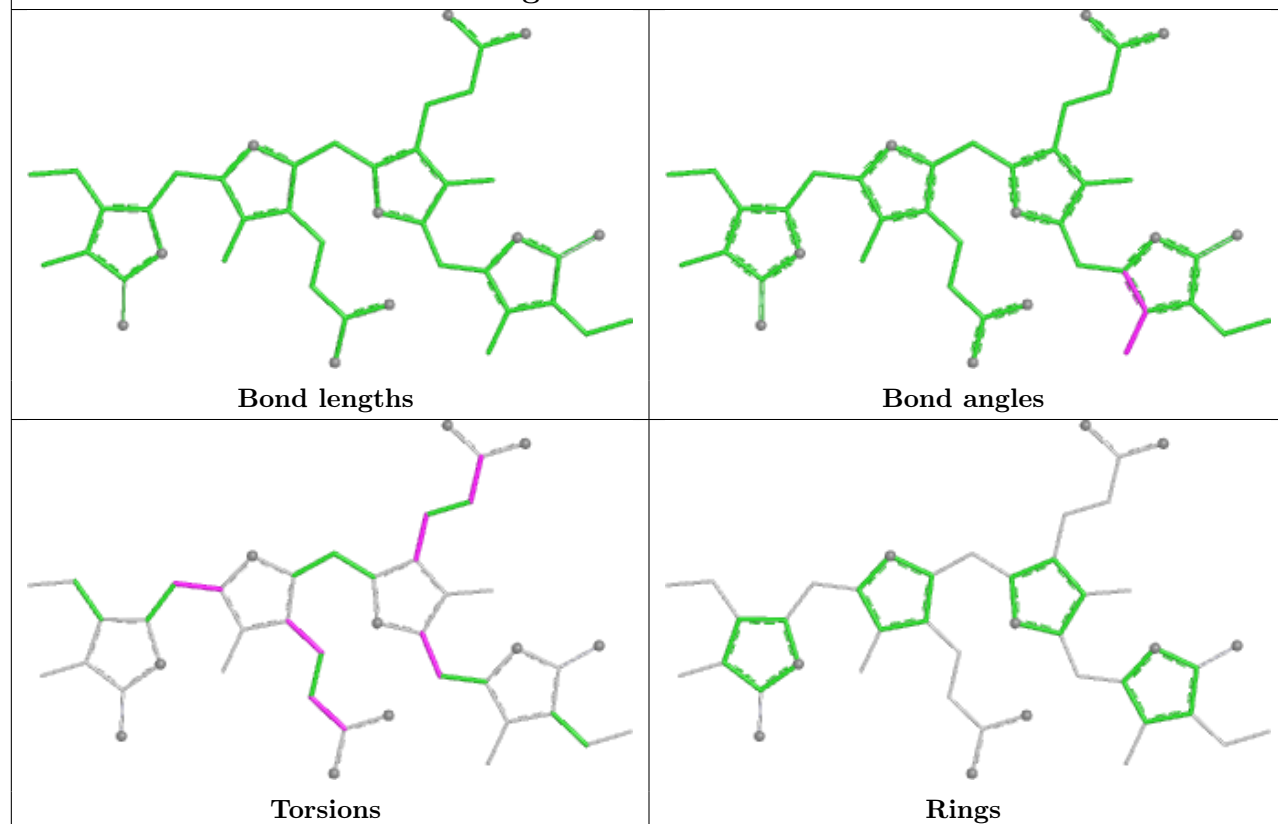
Ligand CYC R5 201

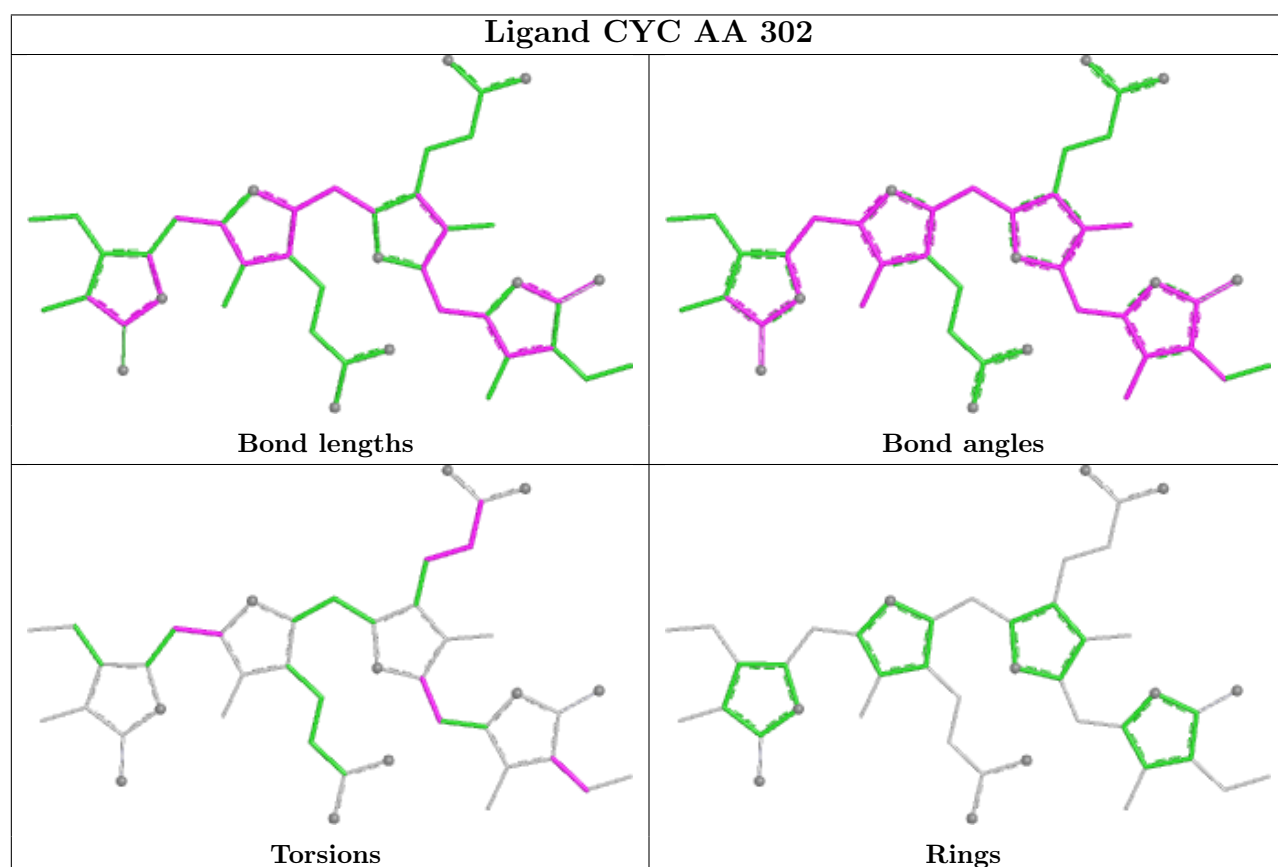
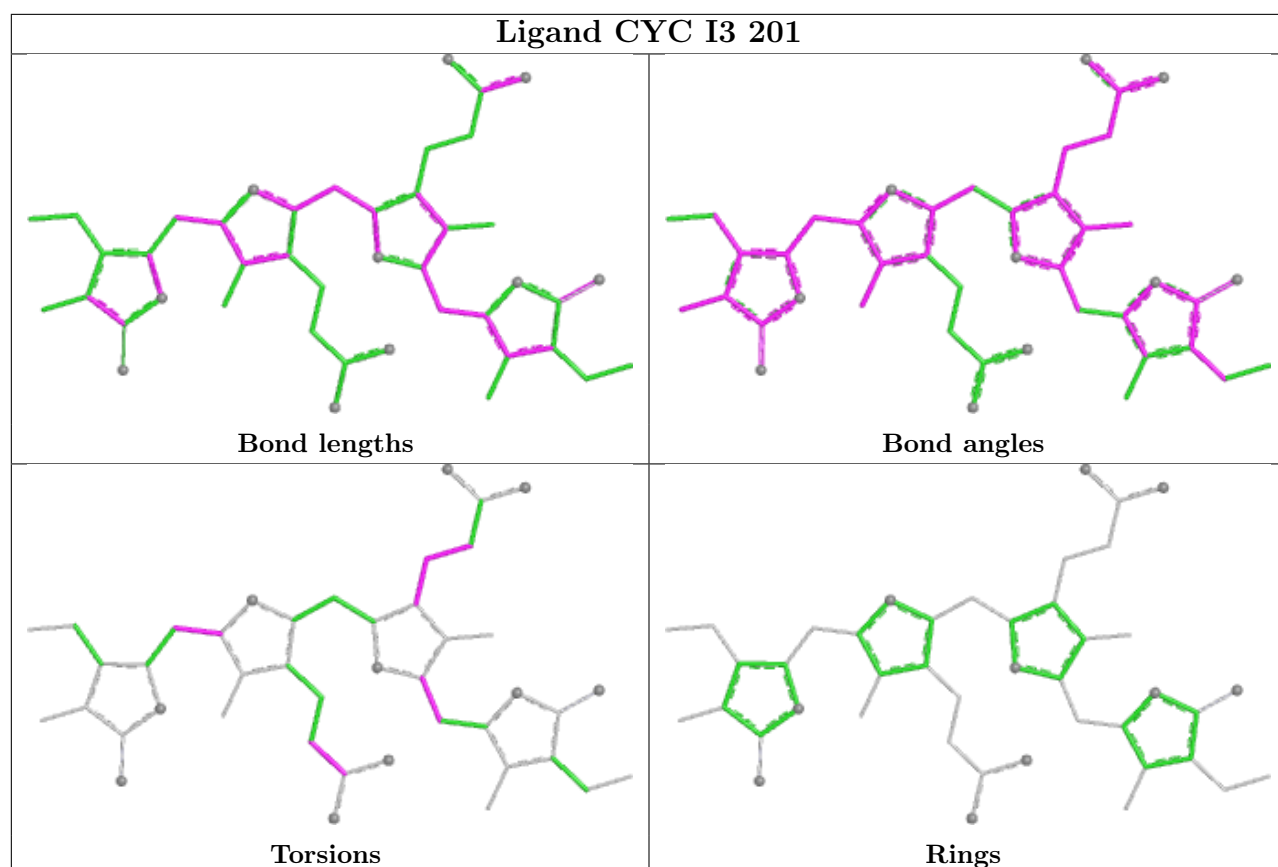


Ligand CYC o9 1001

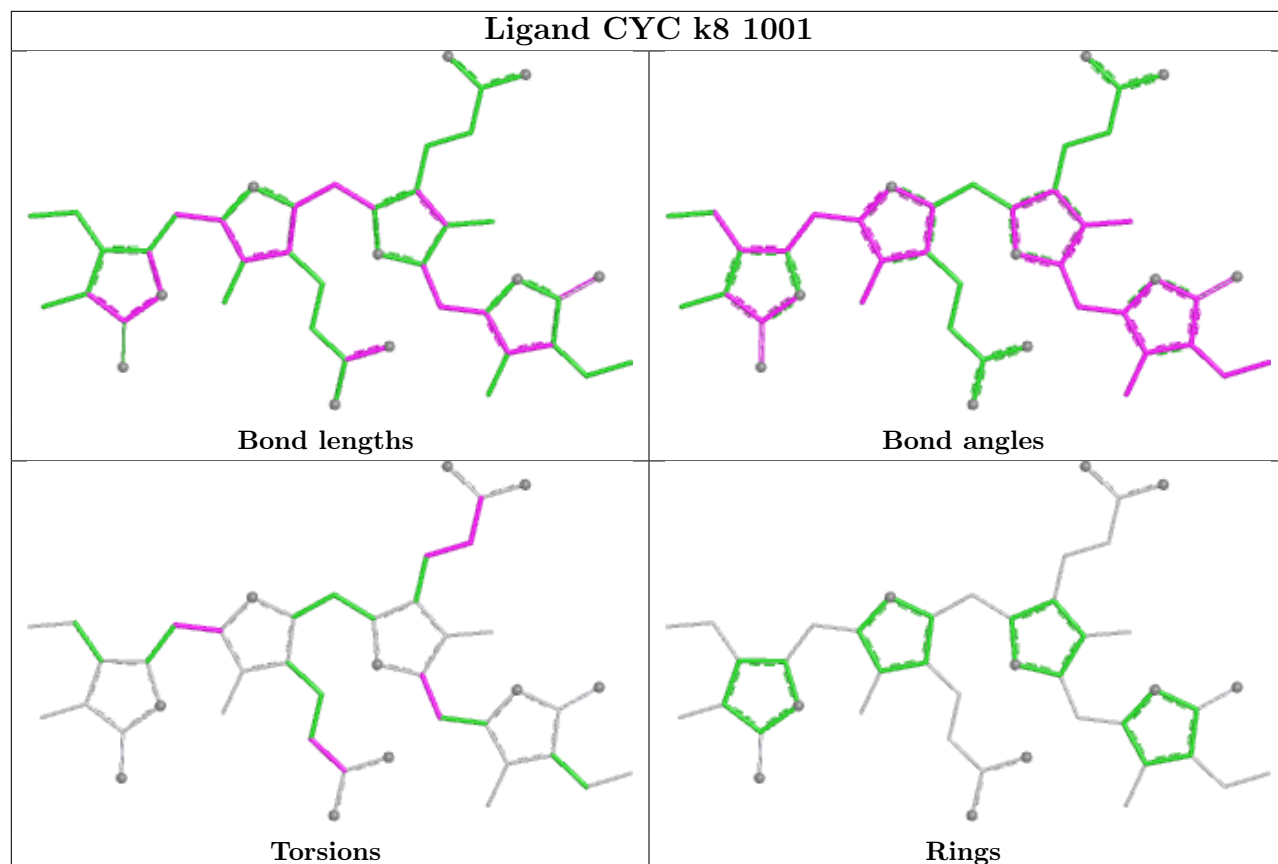


Ligand CYC E1 202

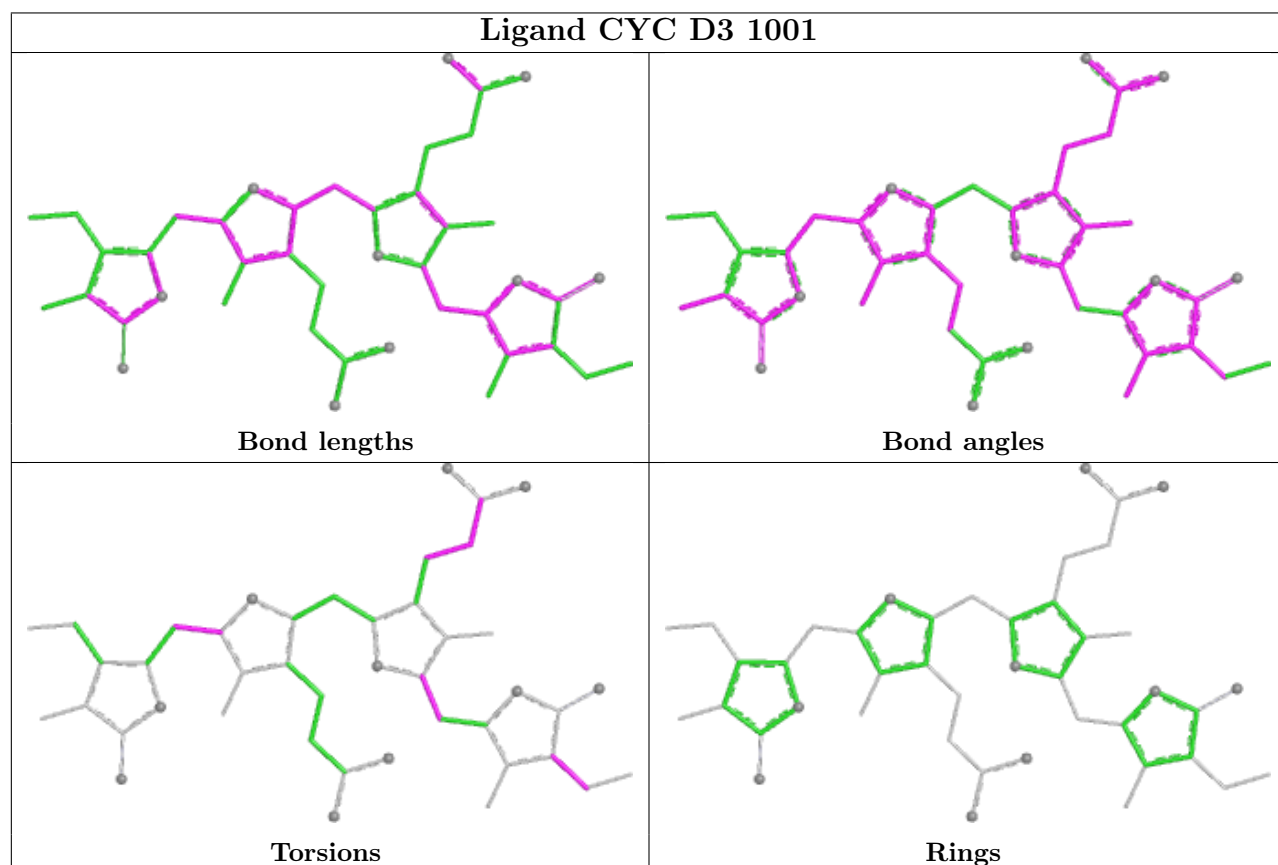


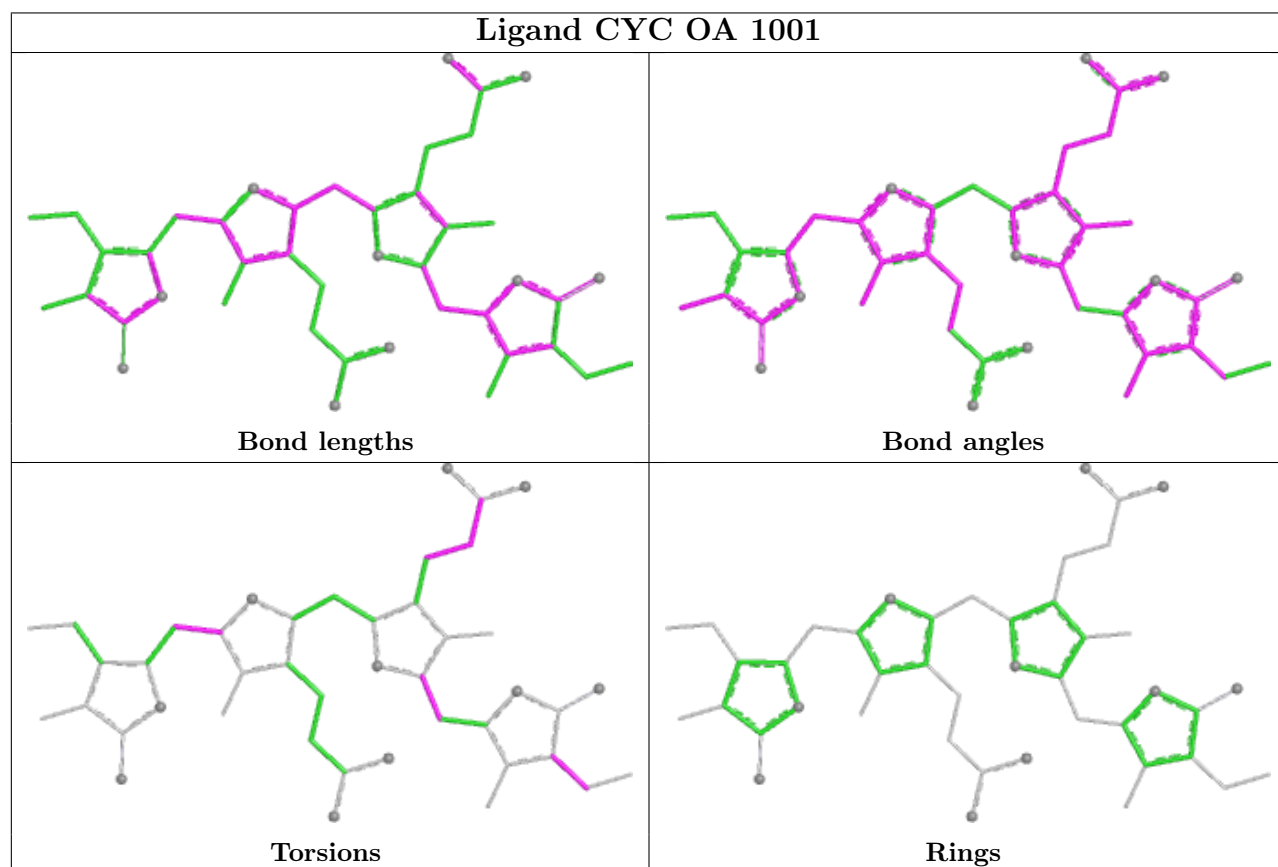
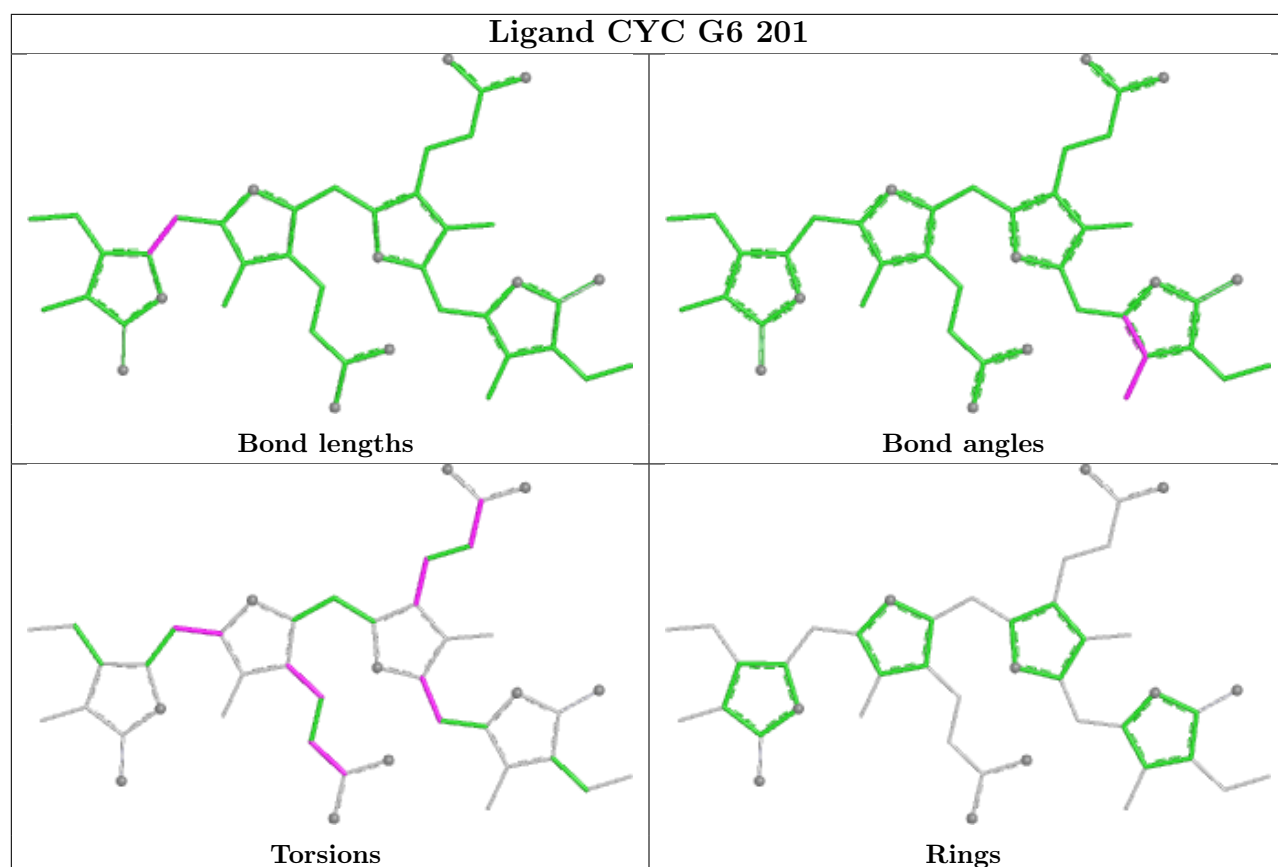


Ligand CYC k8 1001

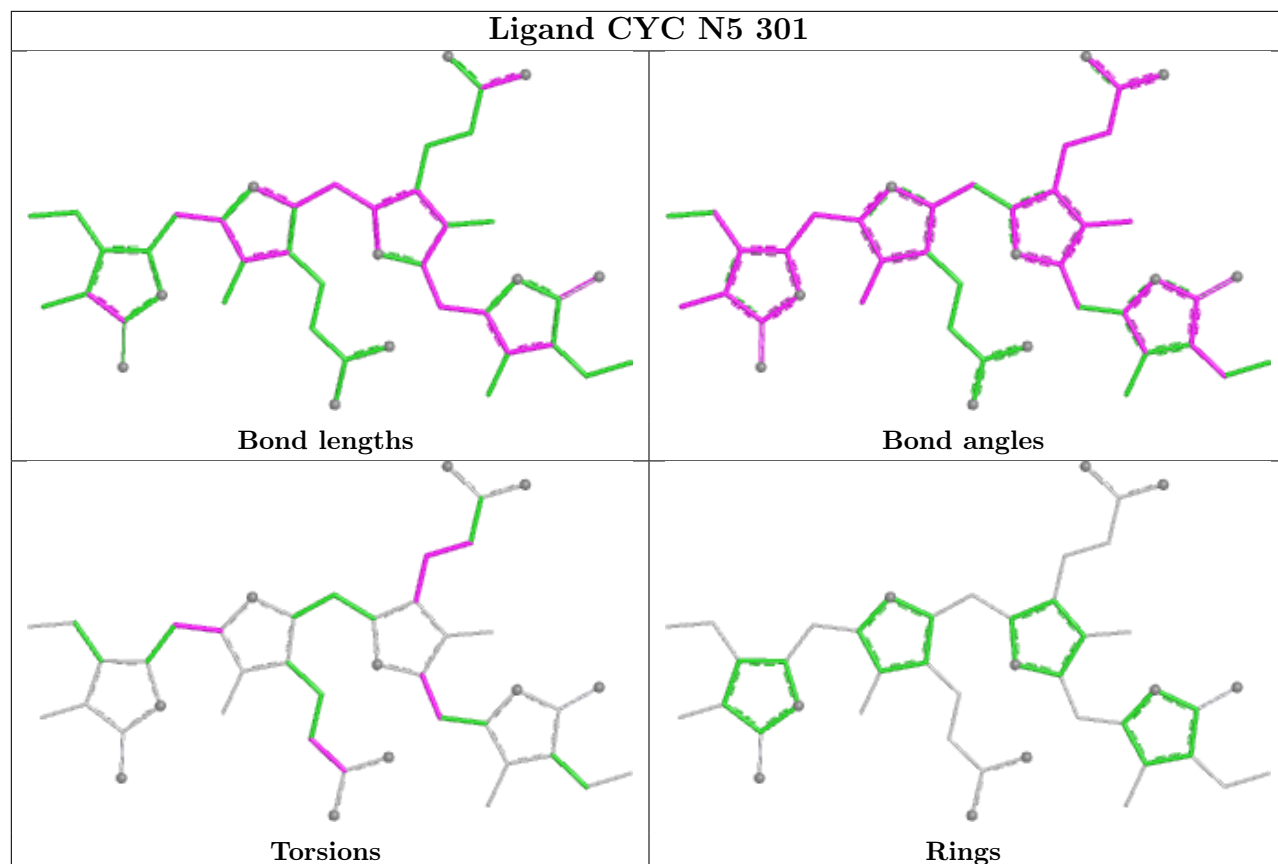


Ligand CYC D3 1001

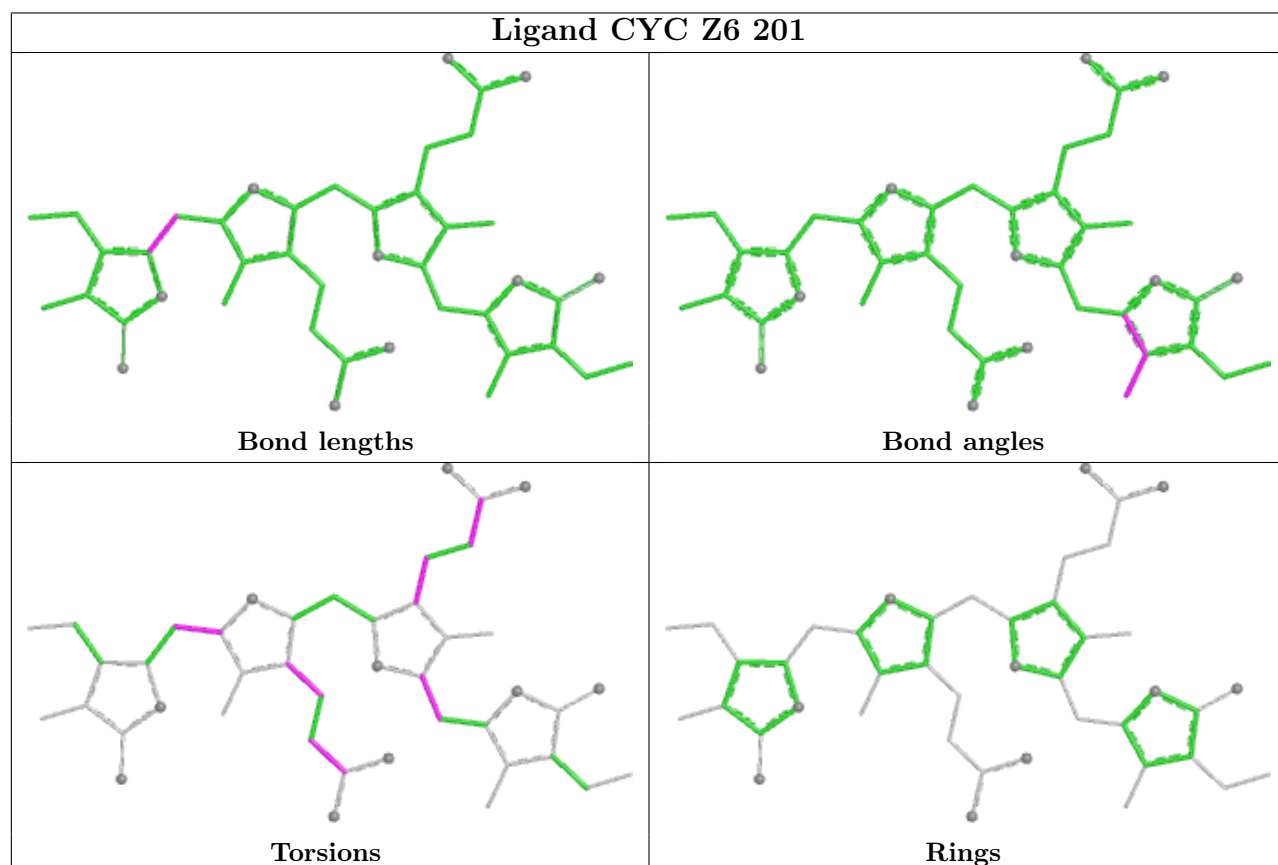


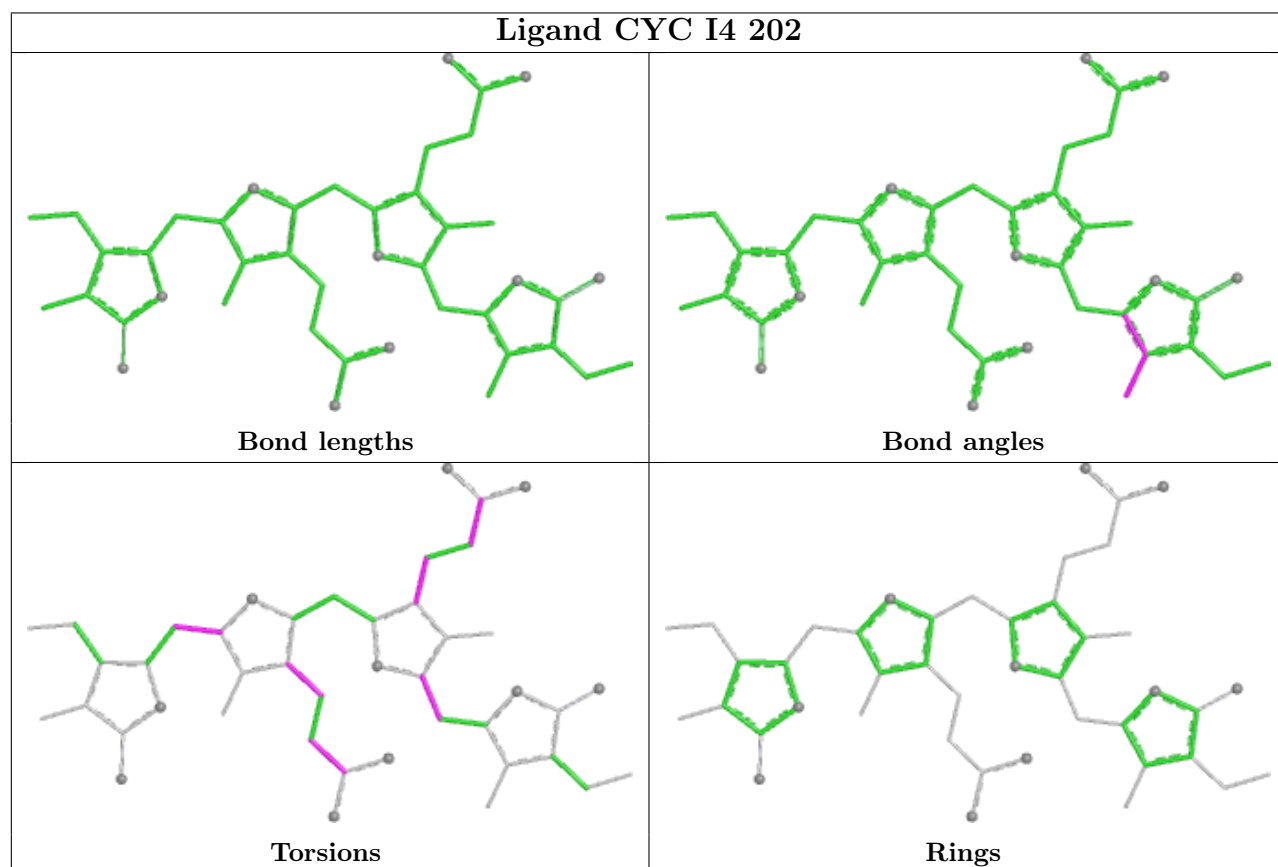
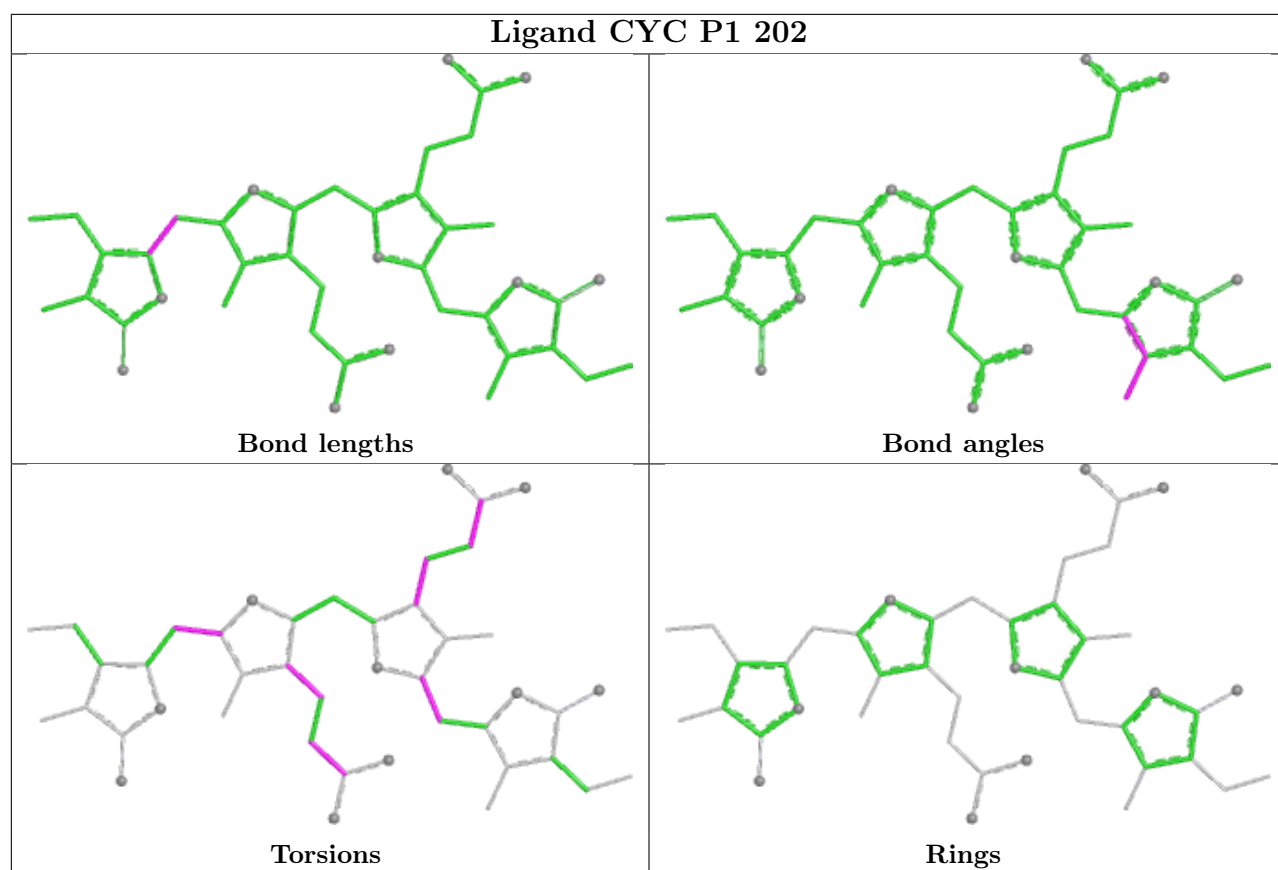


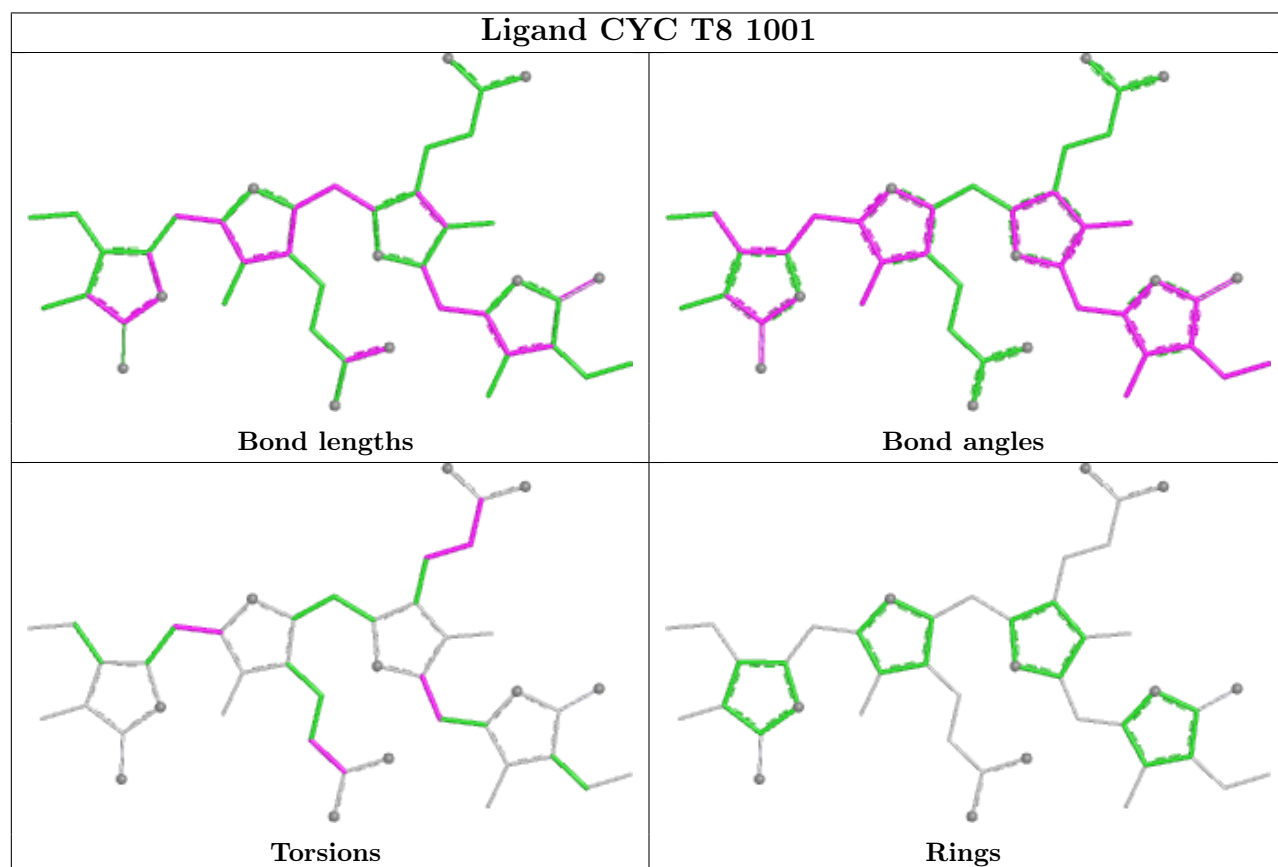
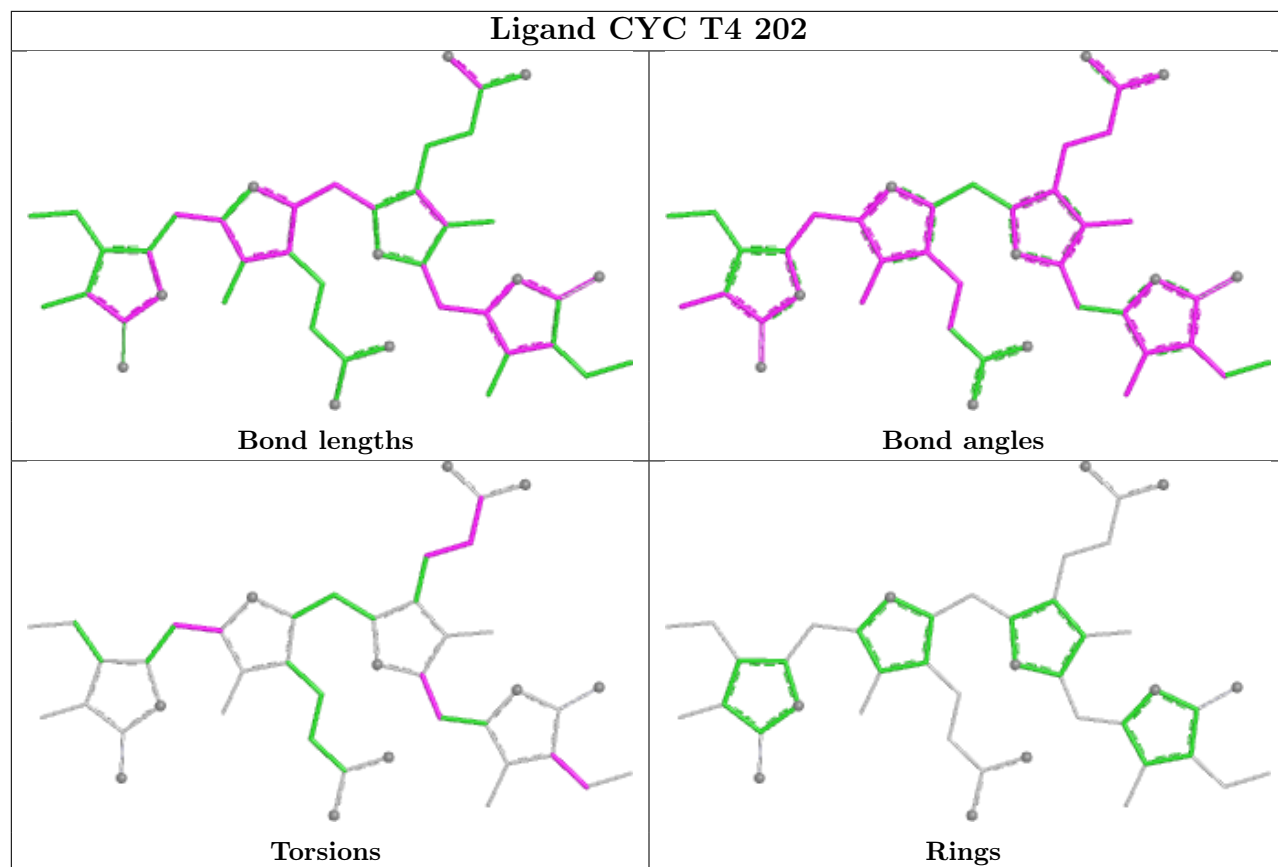
Ligand CYC N5 301



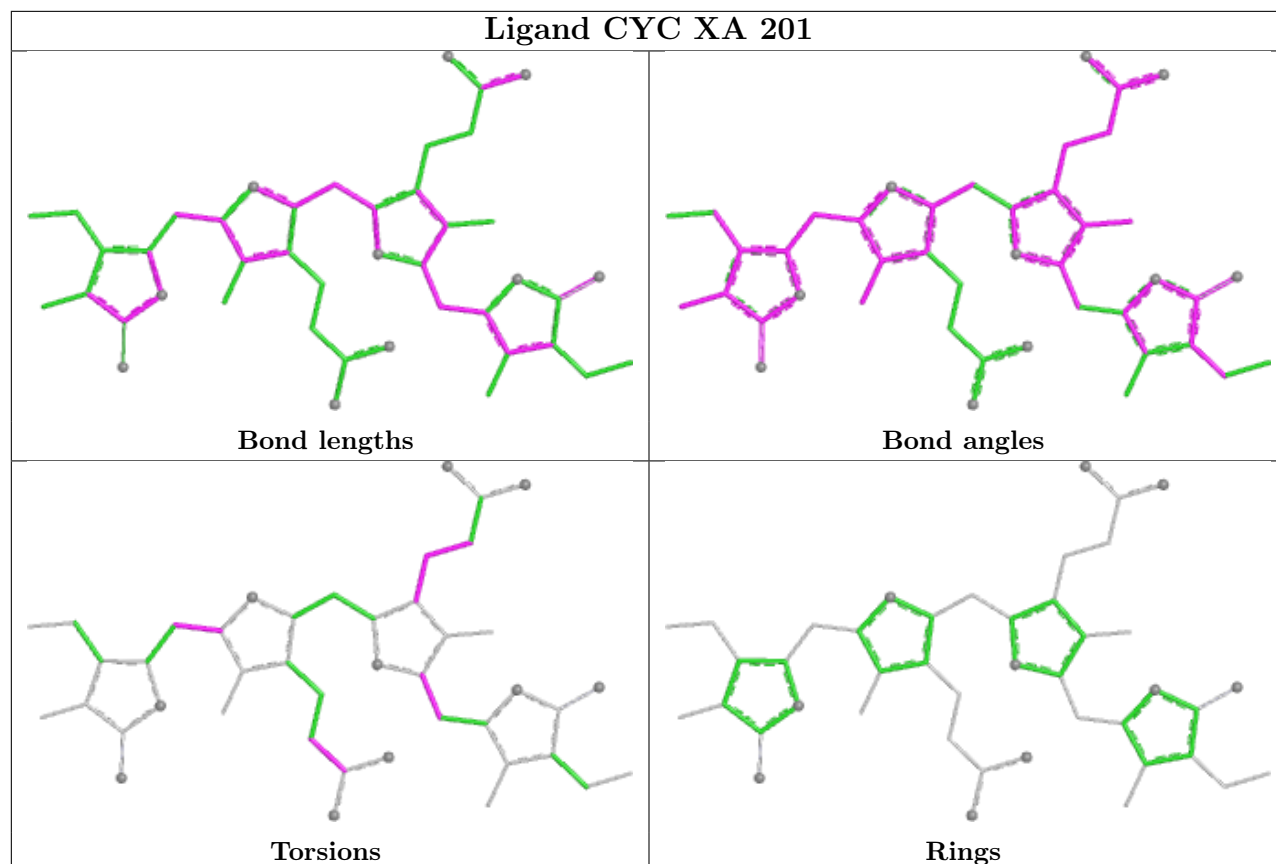
Ligand CYC Z6 201



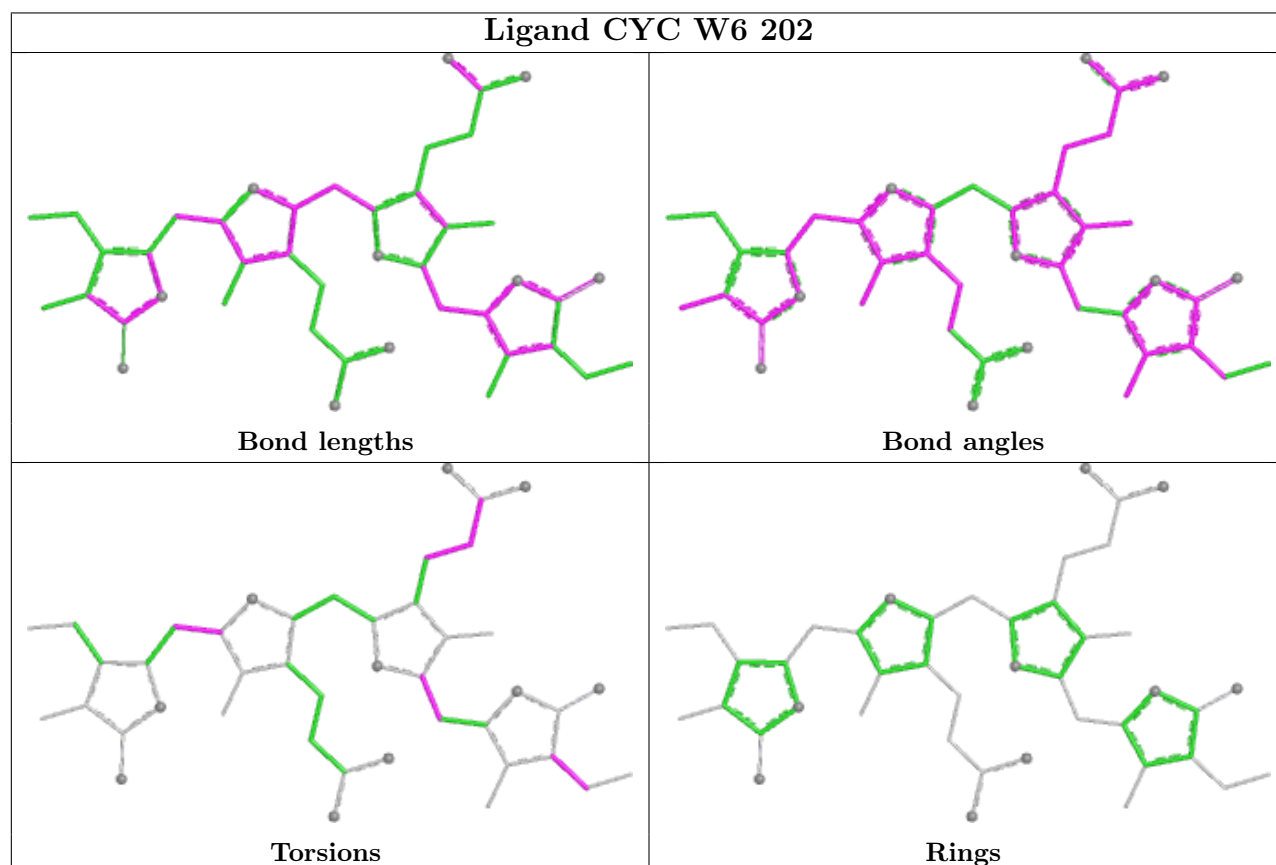


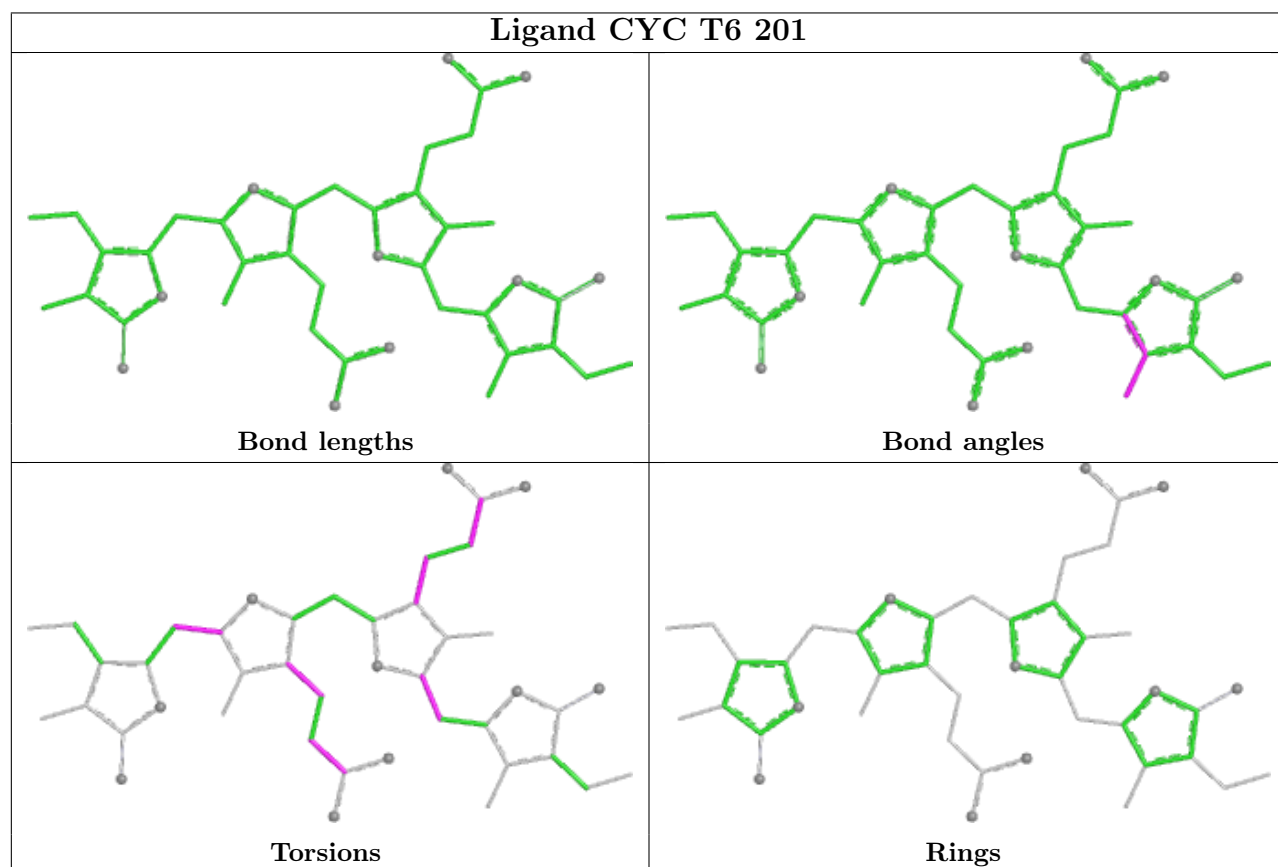
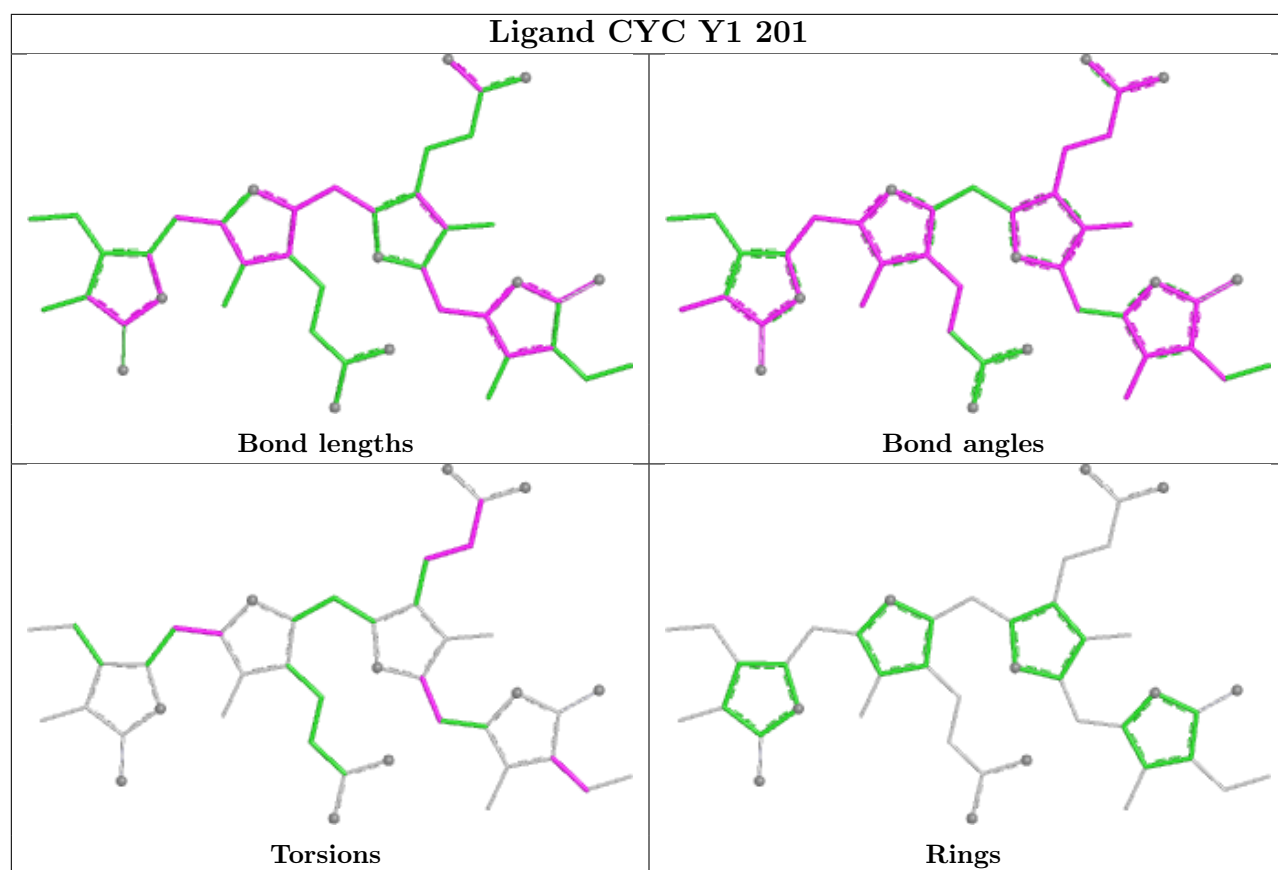


Ligand CYC XA 201

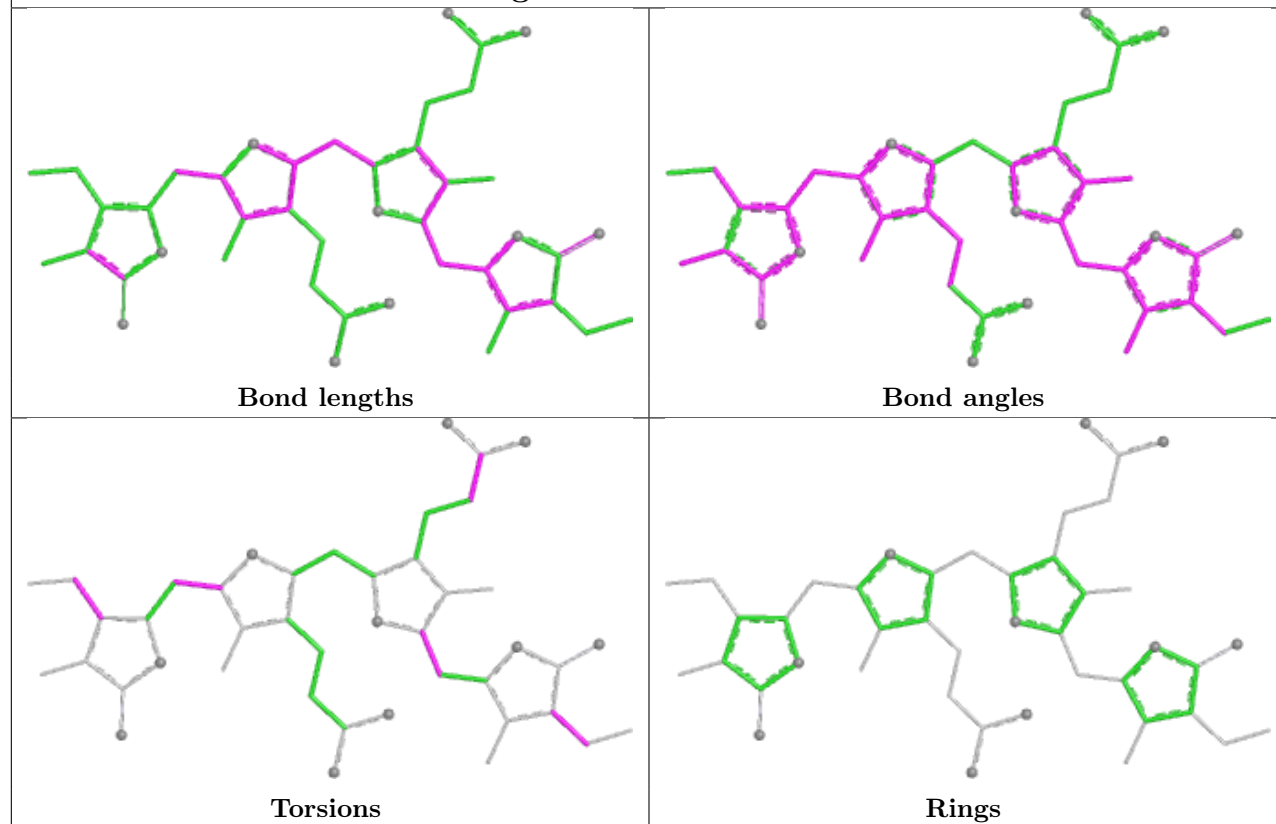


Ligand CYC W6 202

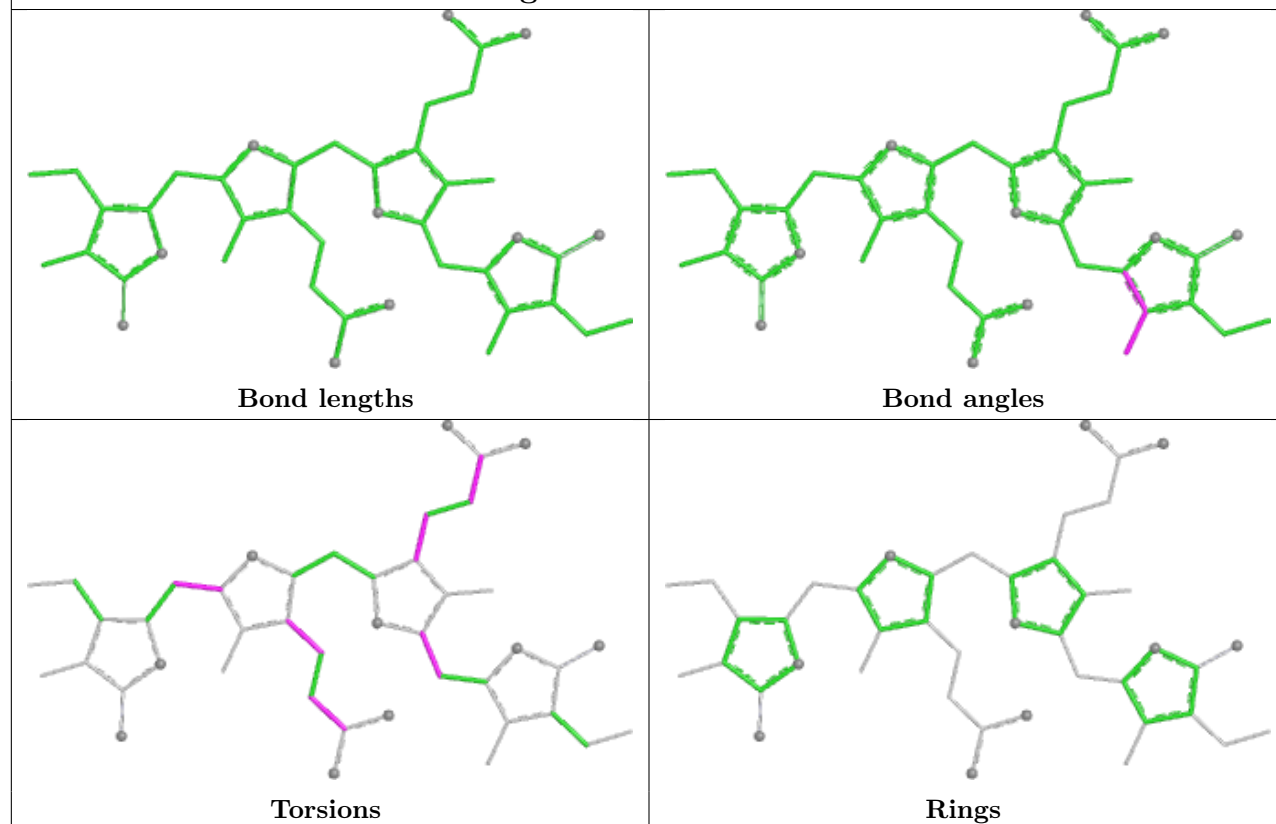




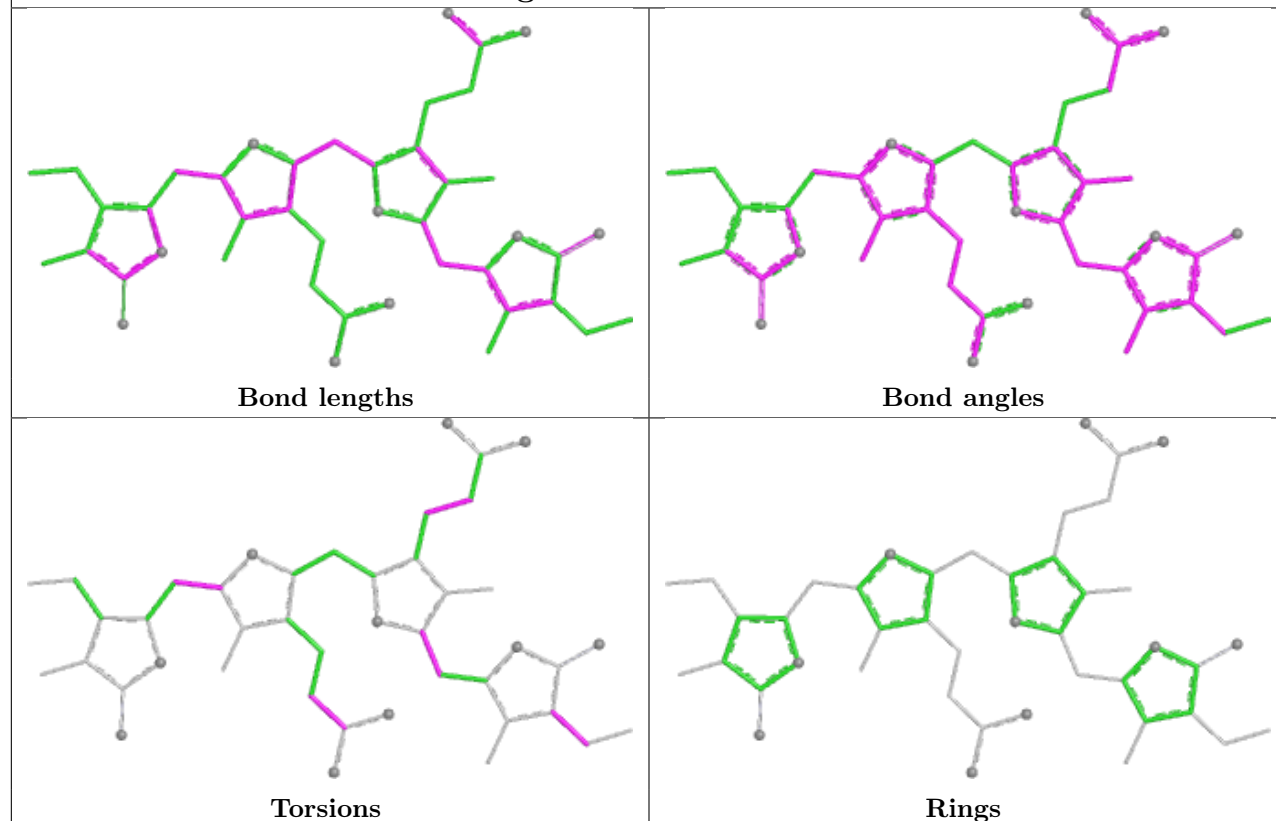
Ligand CYC A9 1001



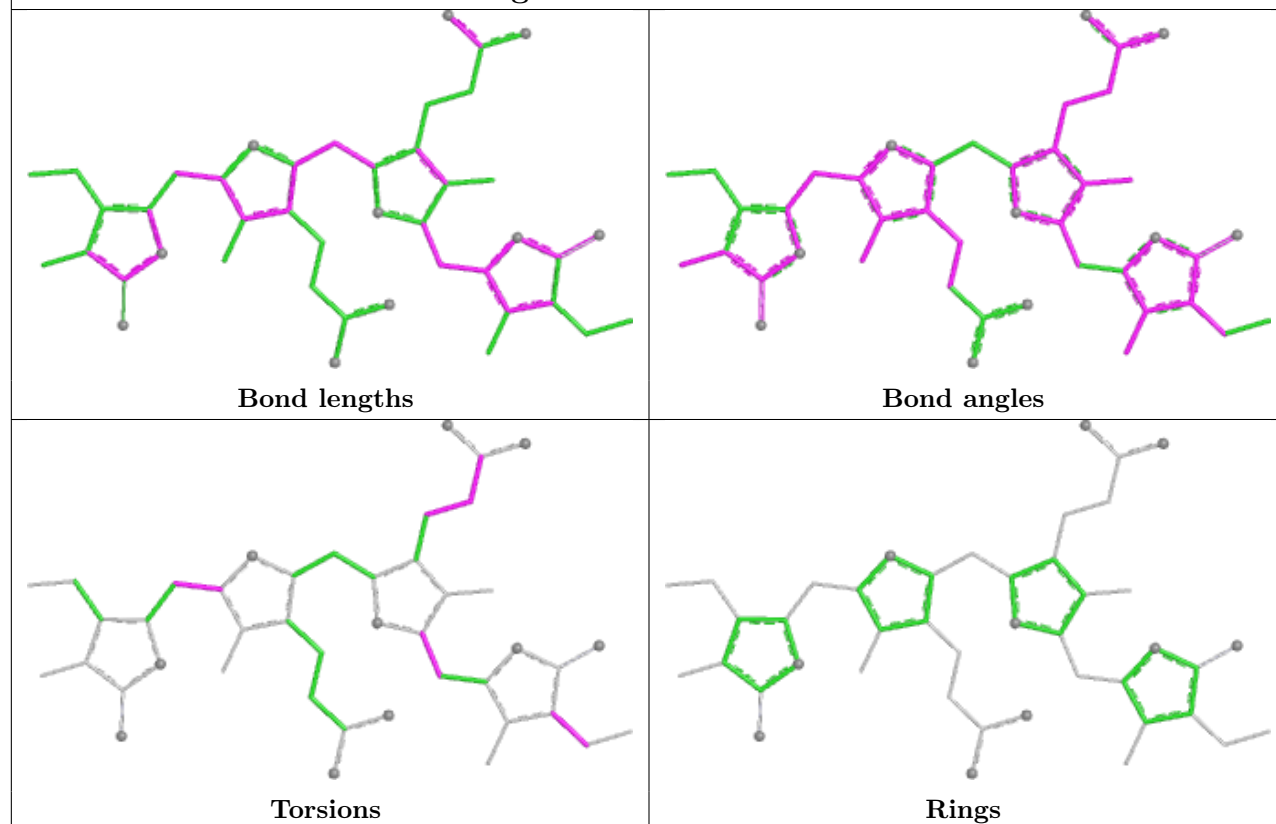
Ligand CYC K3 202



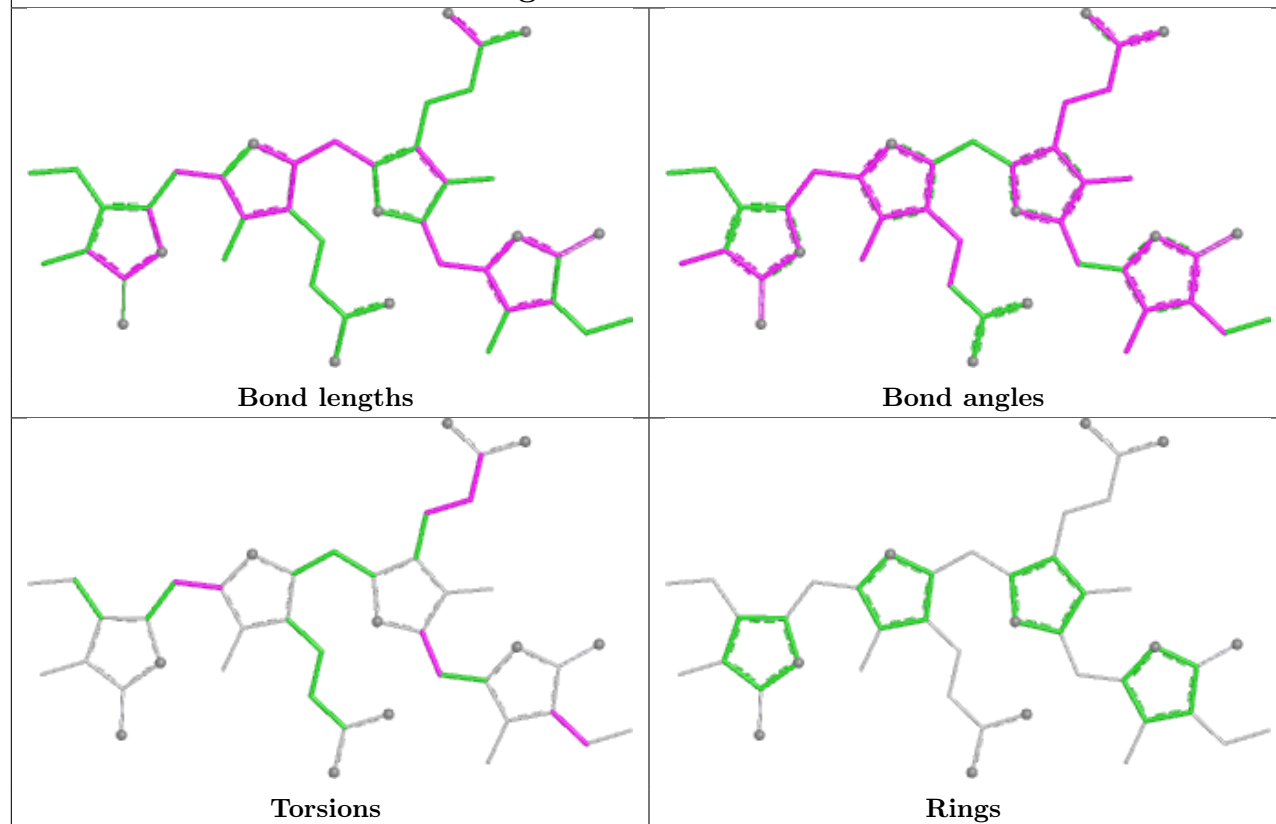
Ligand CYC c9 1001



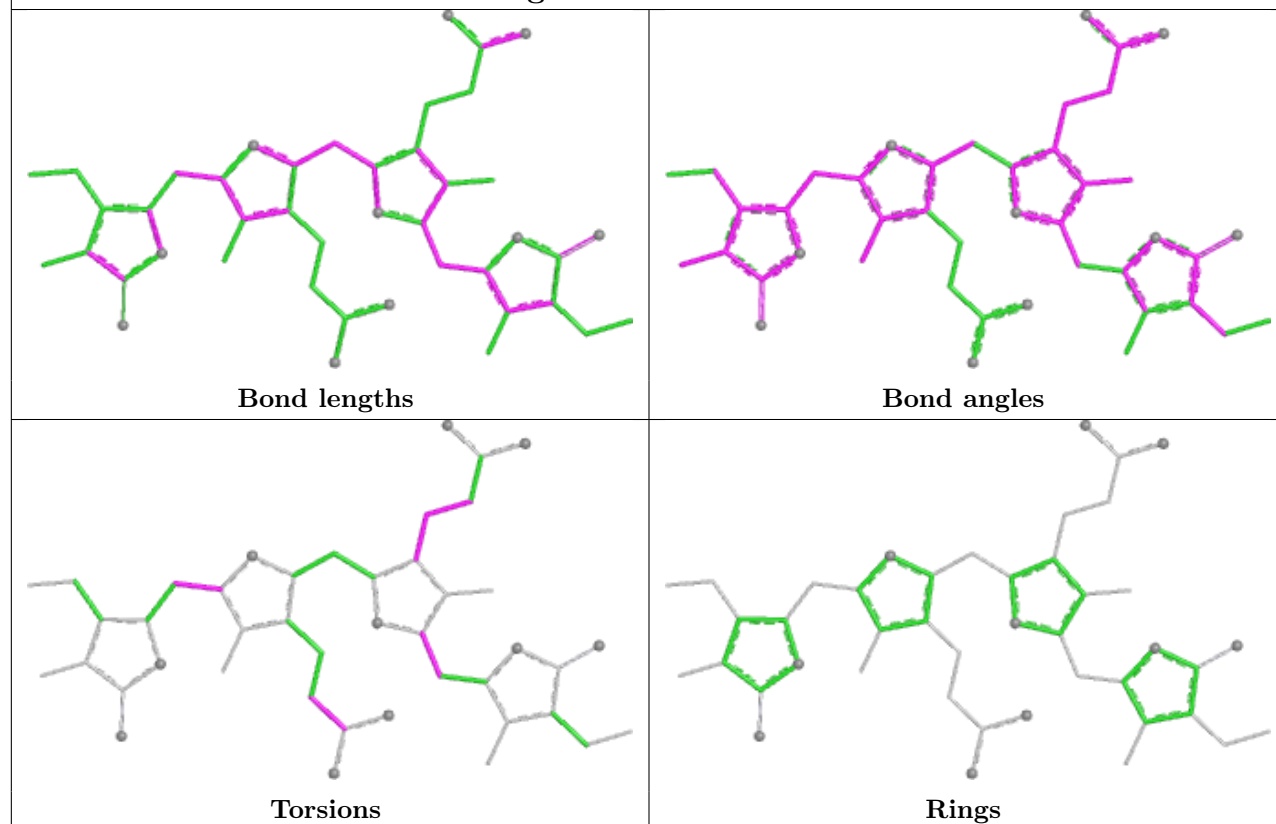
Ligand CYC D1 1001



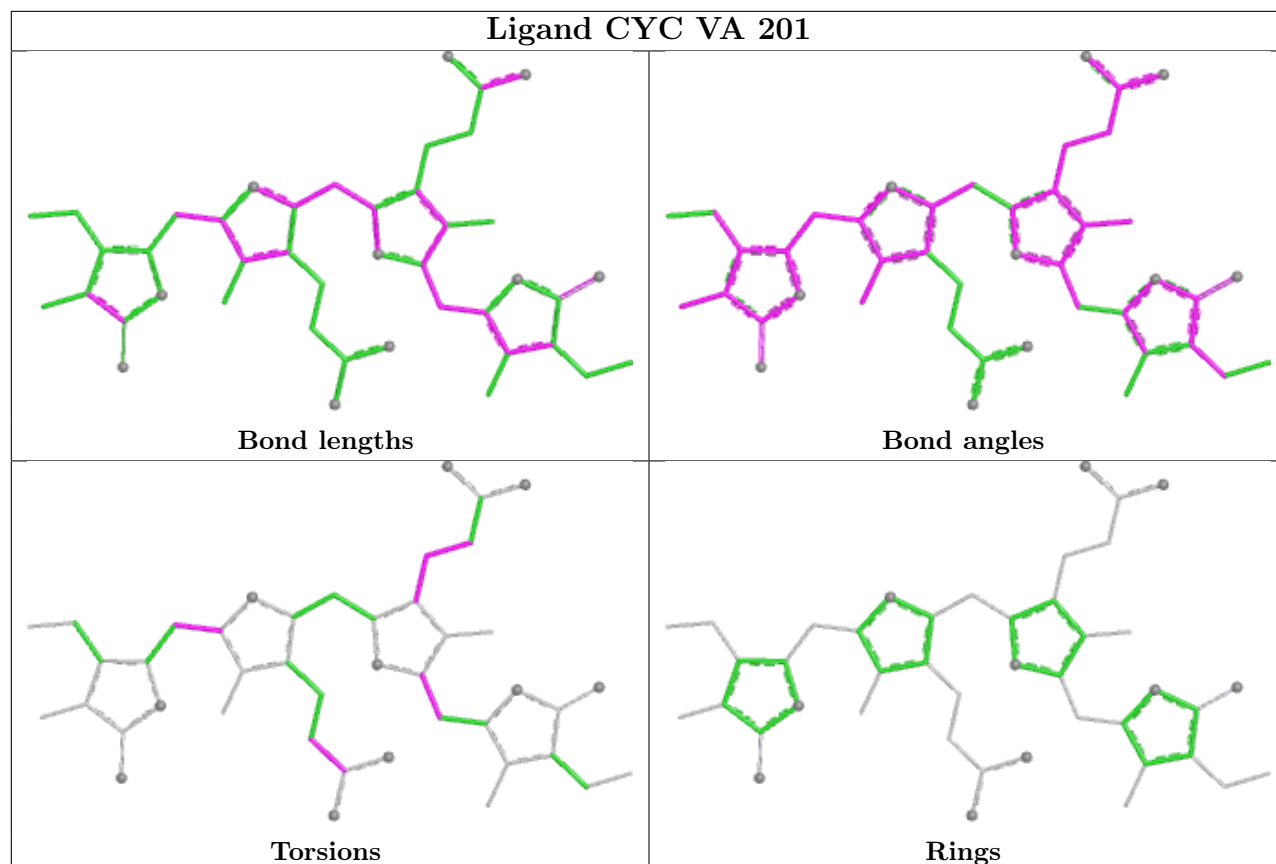
Ligand CYC LA 201



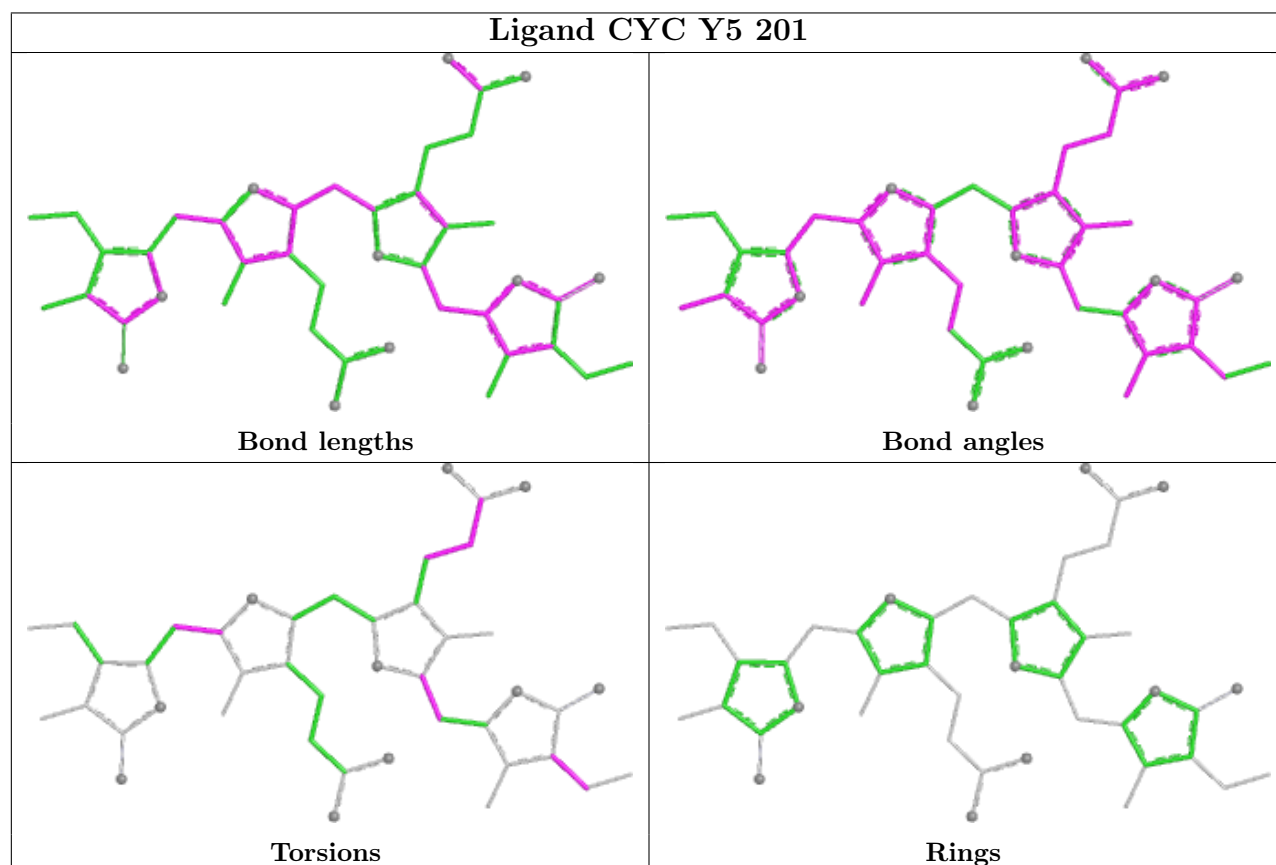
Ligand CYC I5 201



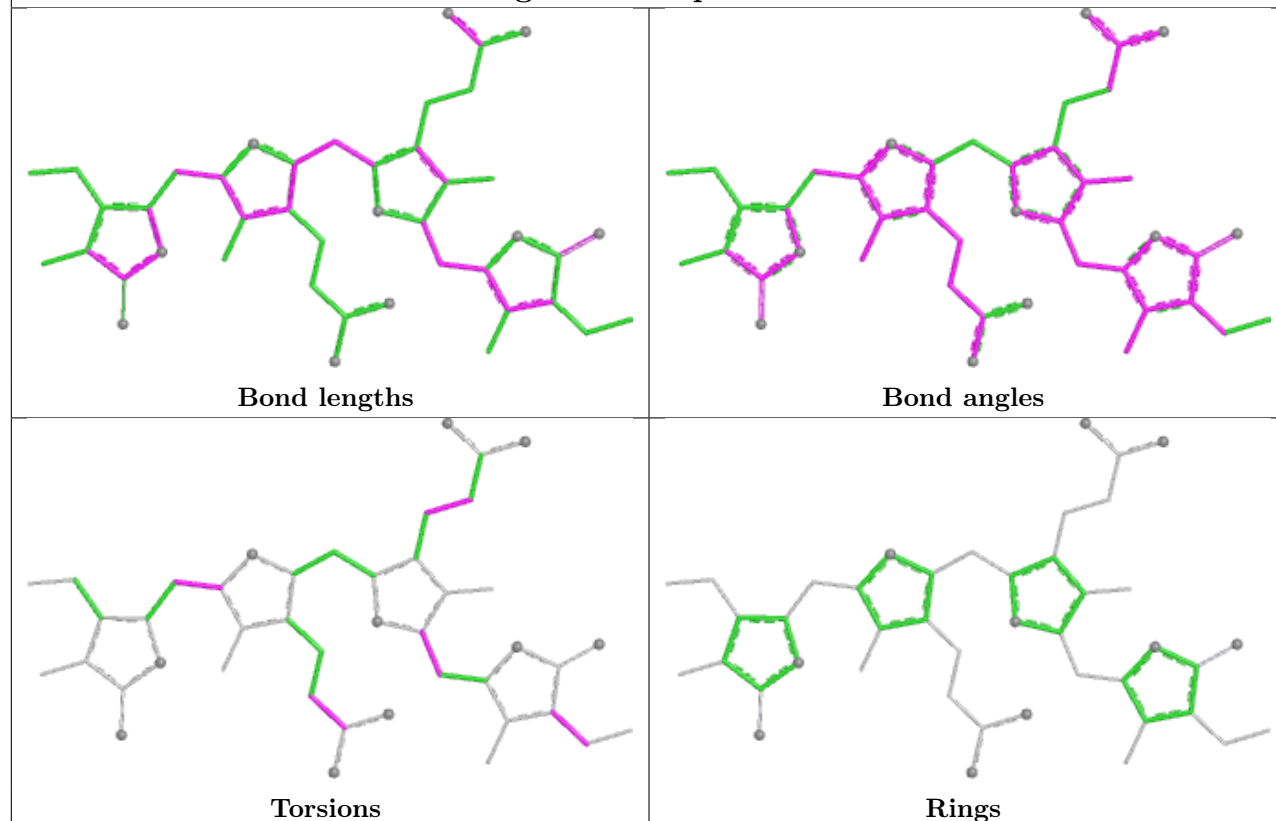
Ligand CYC VA 201



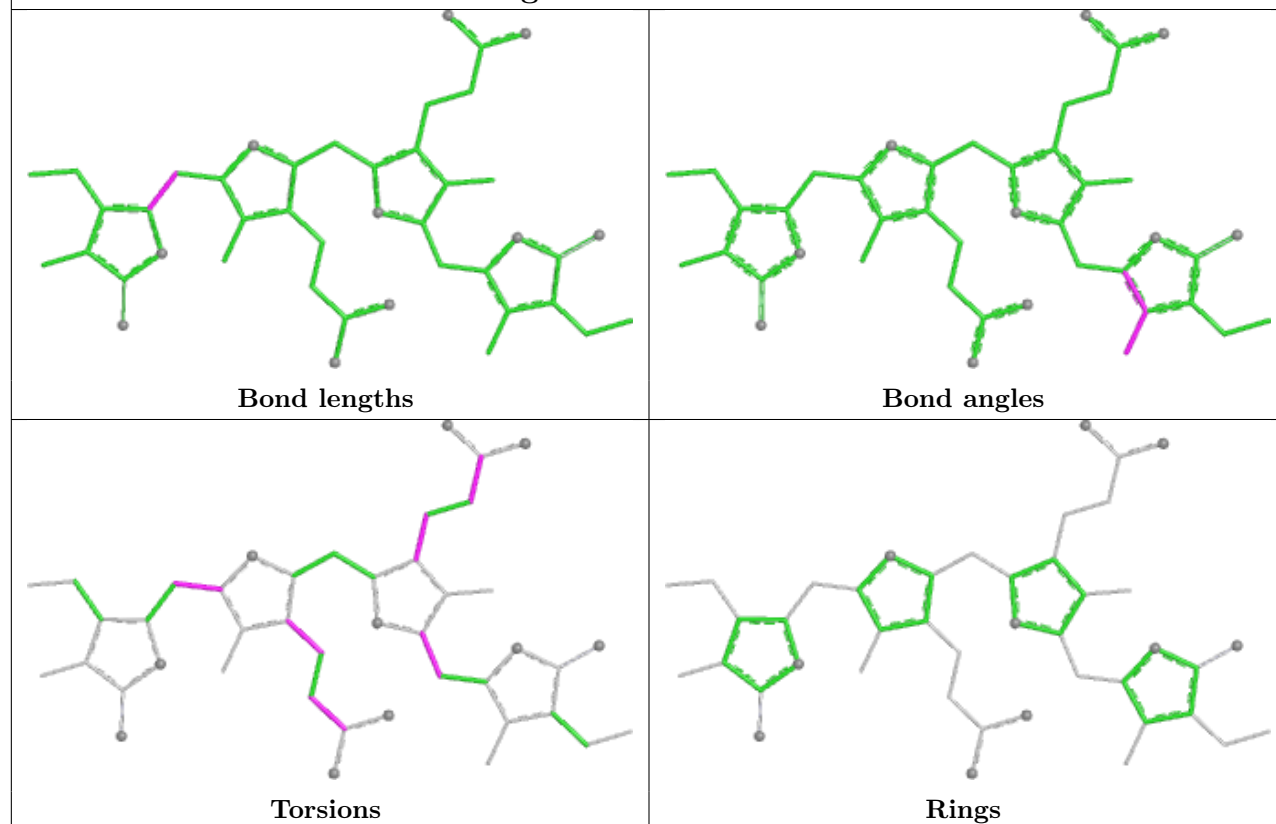
Ligand CYC Y5 201



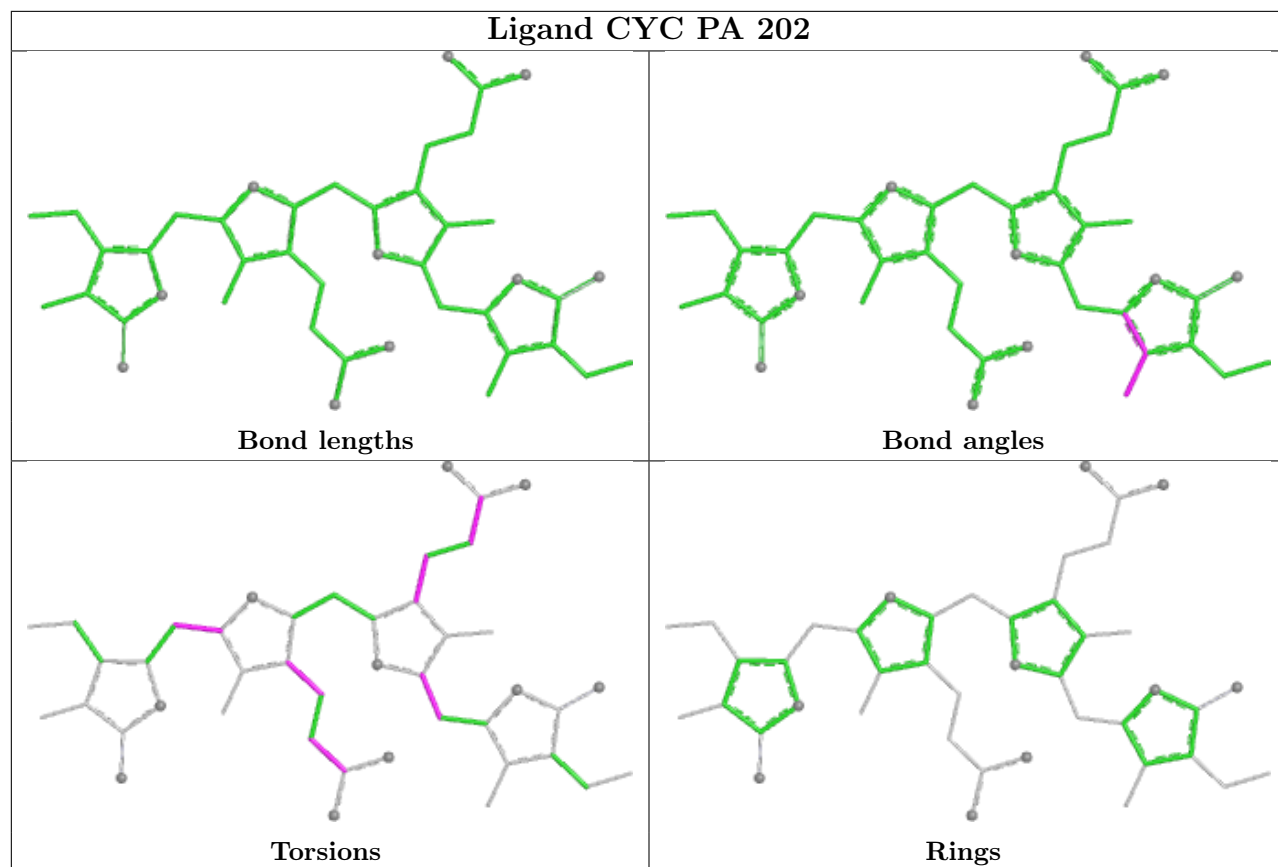
Ligand CYC p9 1001



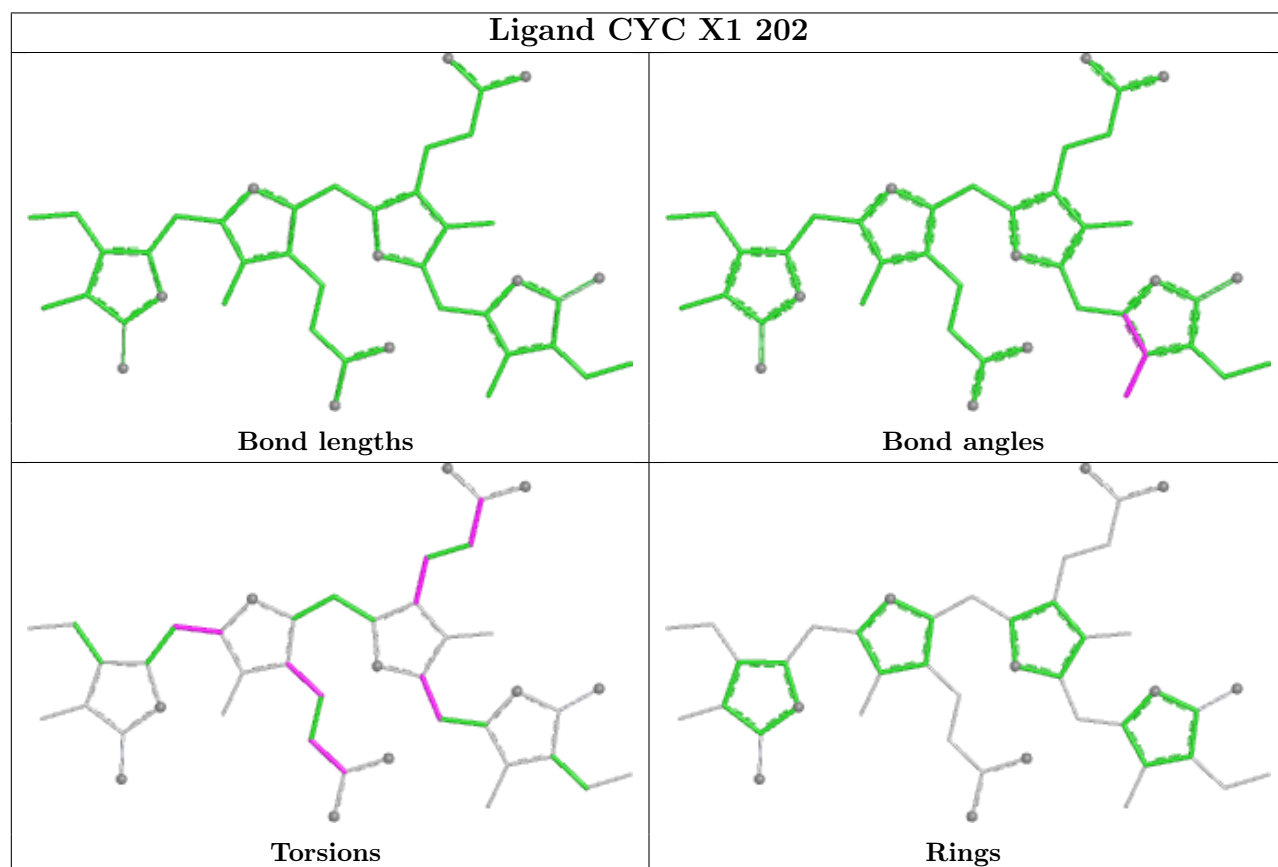
Ligand CYC C6 202



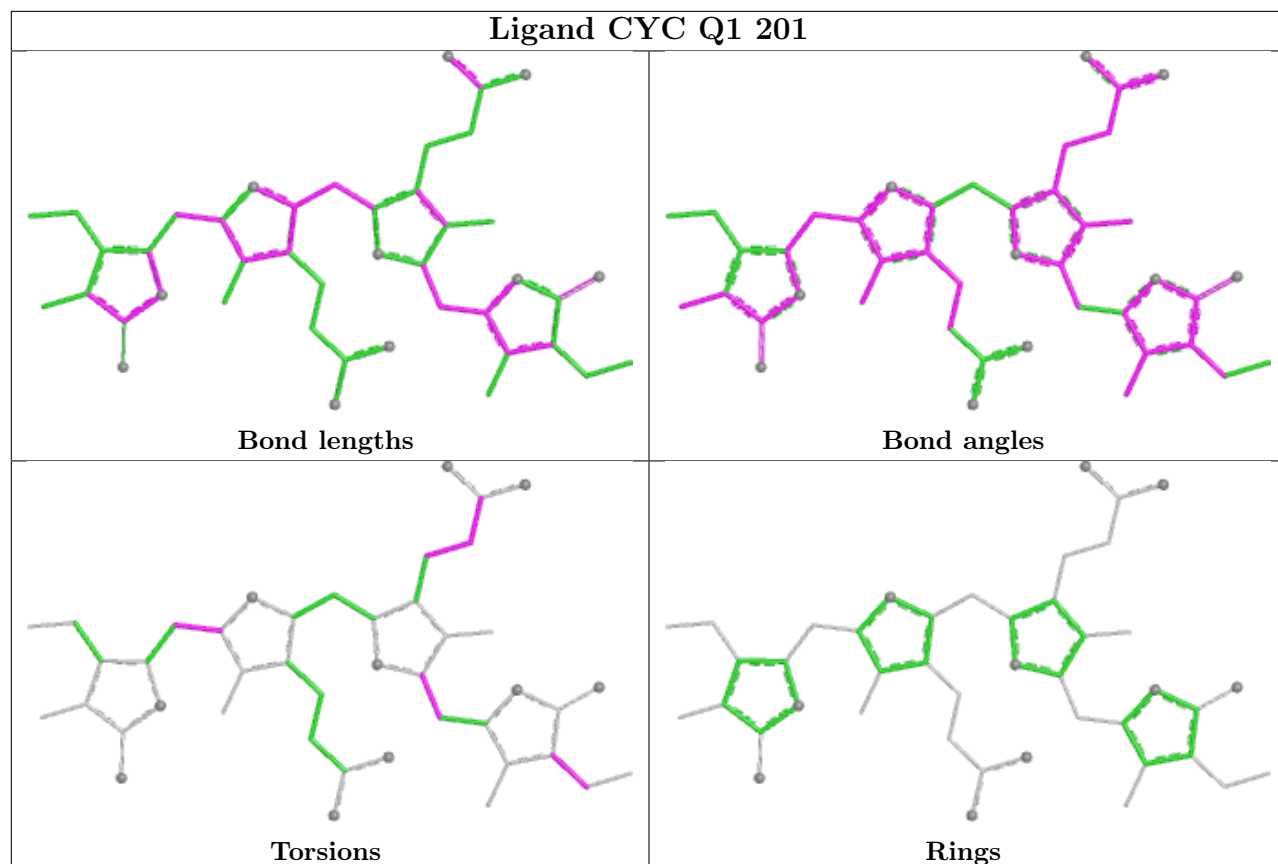
Ligand CYC PA 202



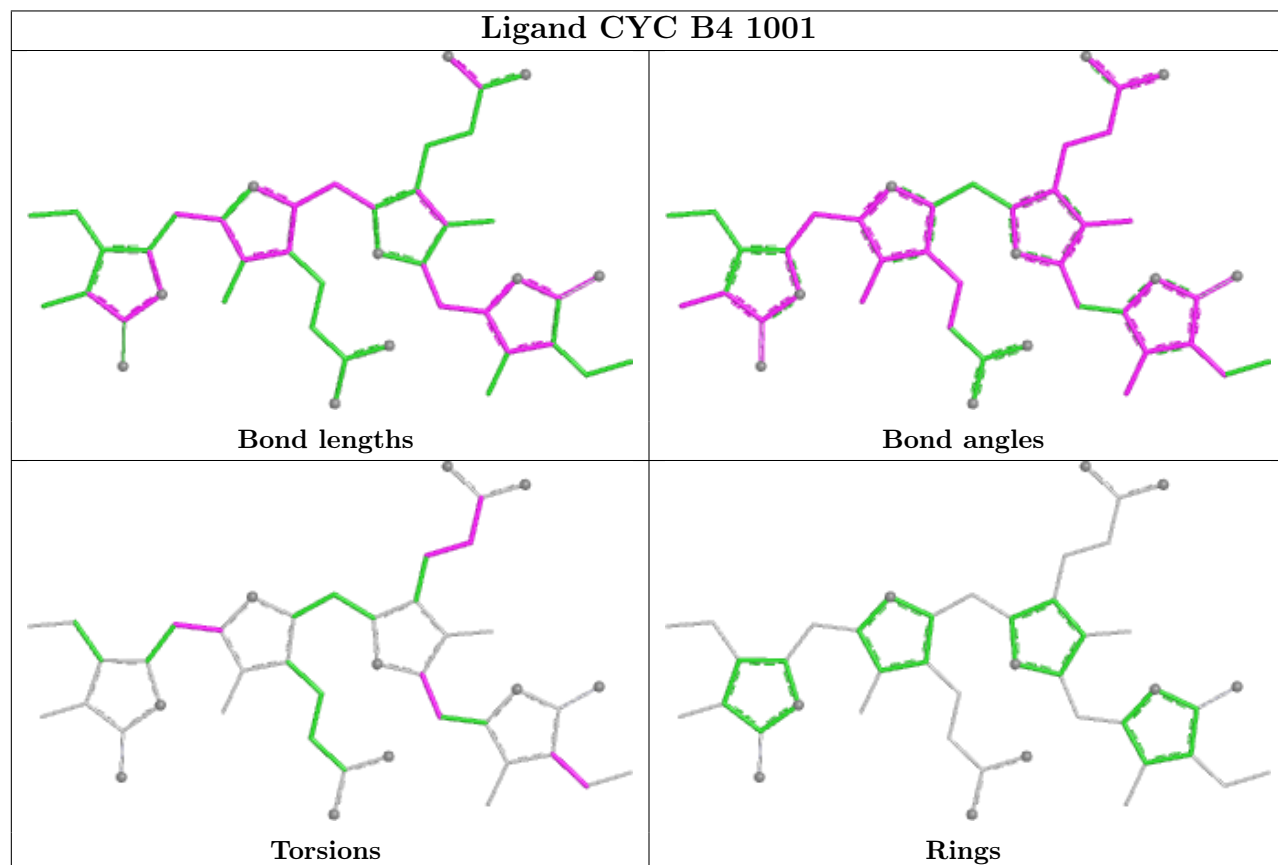
Ligand CYC X1 202



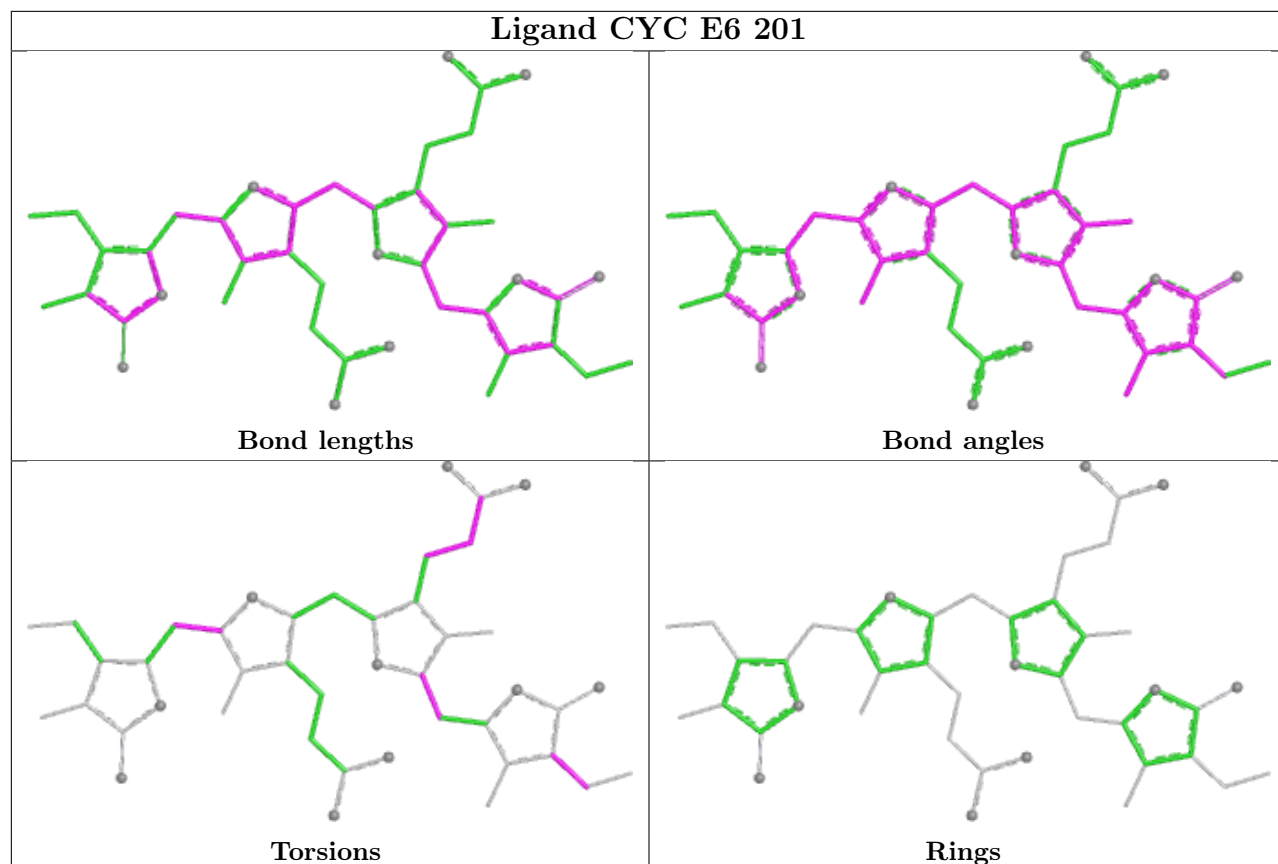
Ligand CYC Q1 201



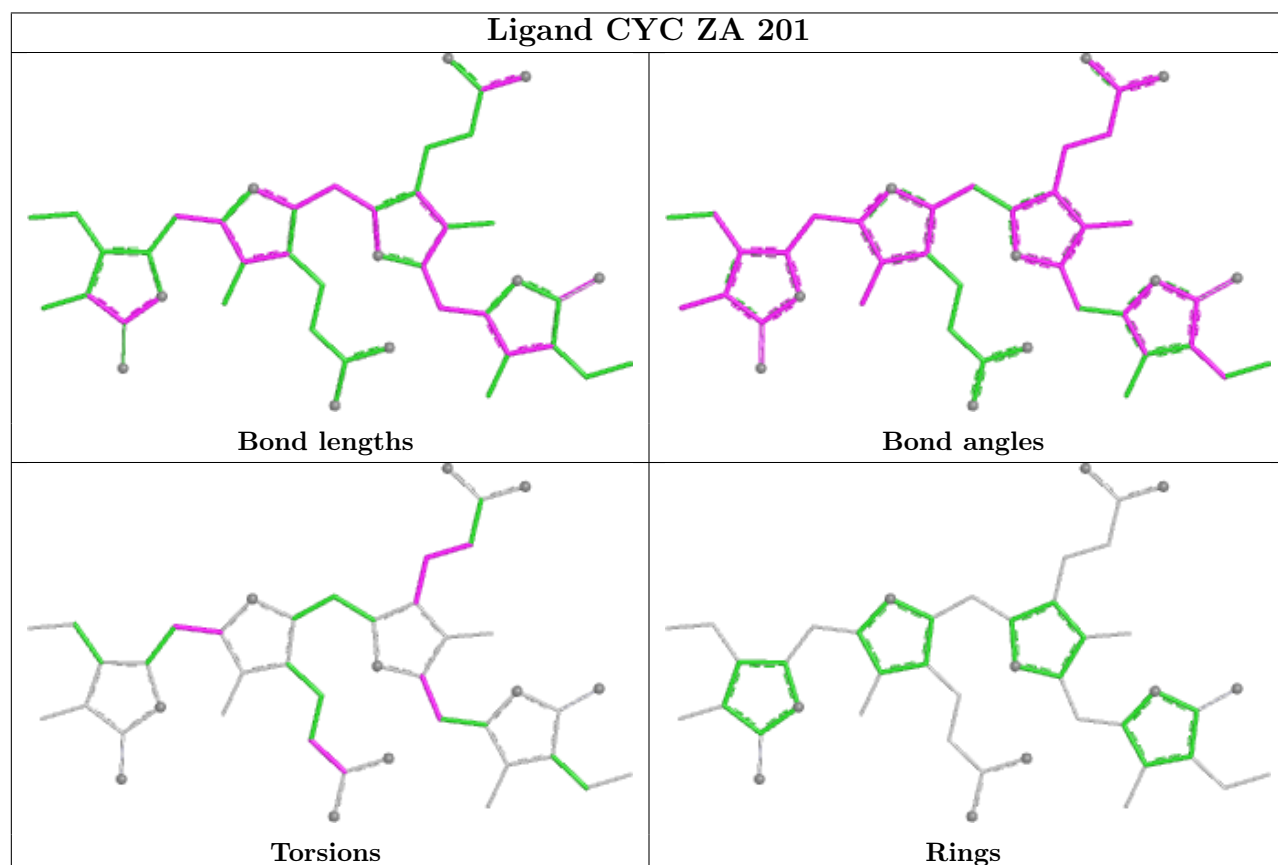
Ligand CYC B4 1001

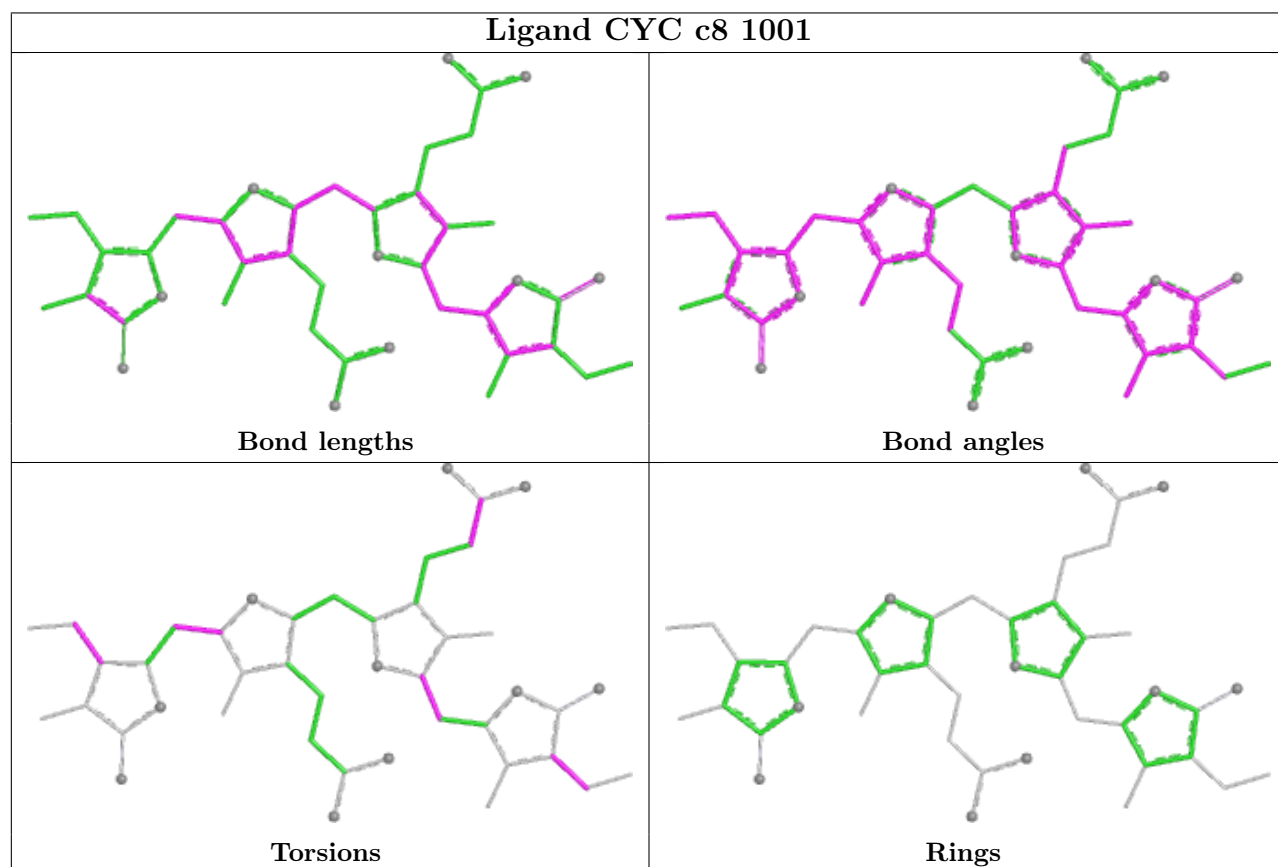
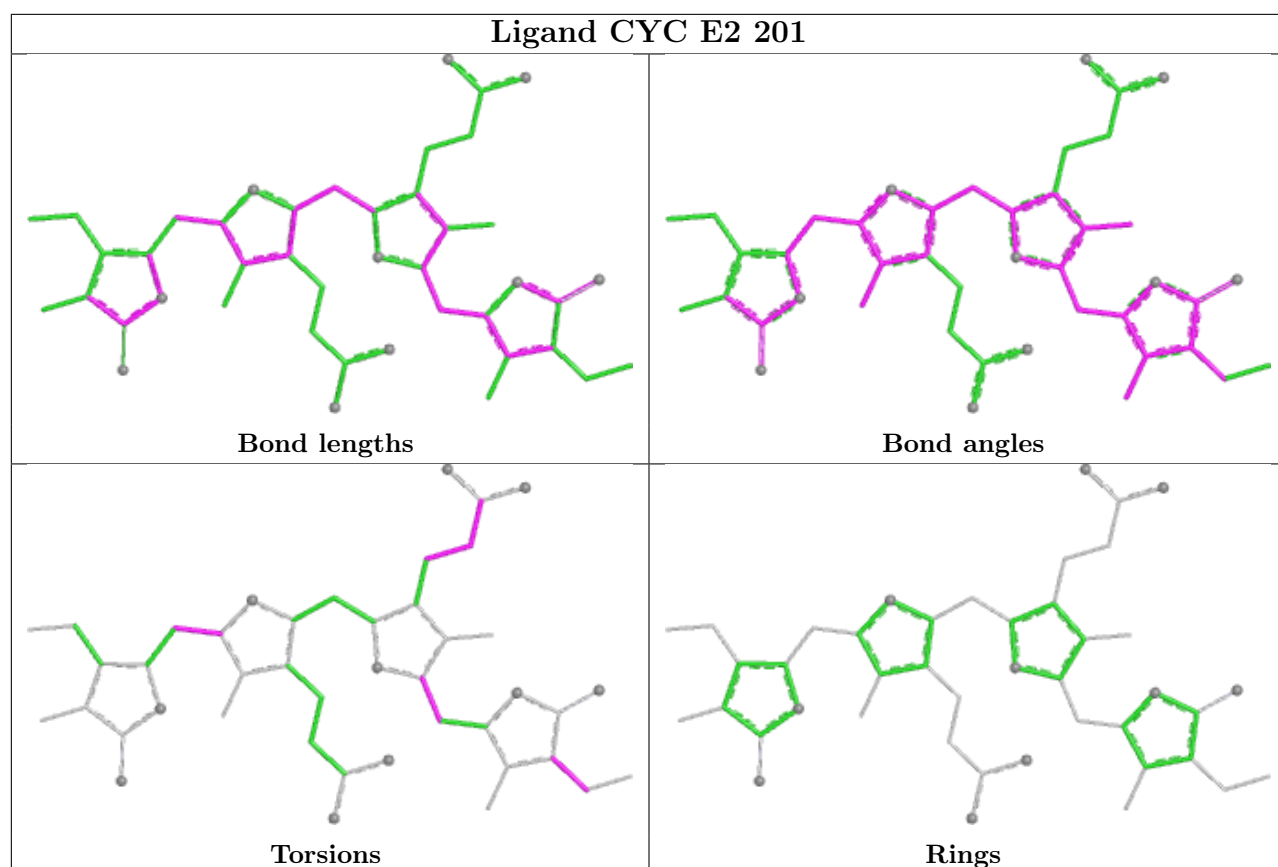


Ligand CYC E6 201

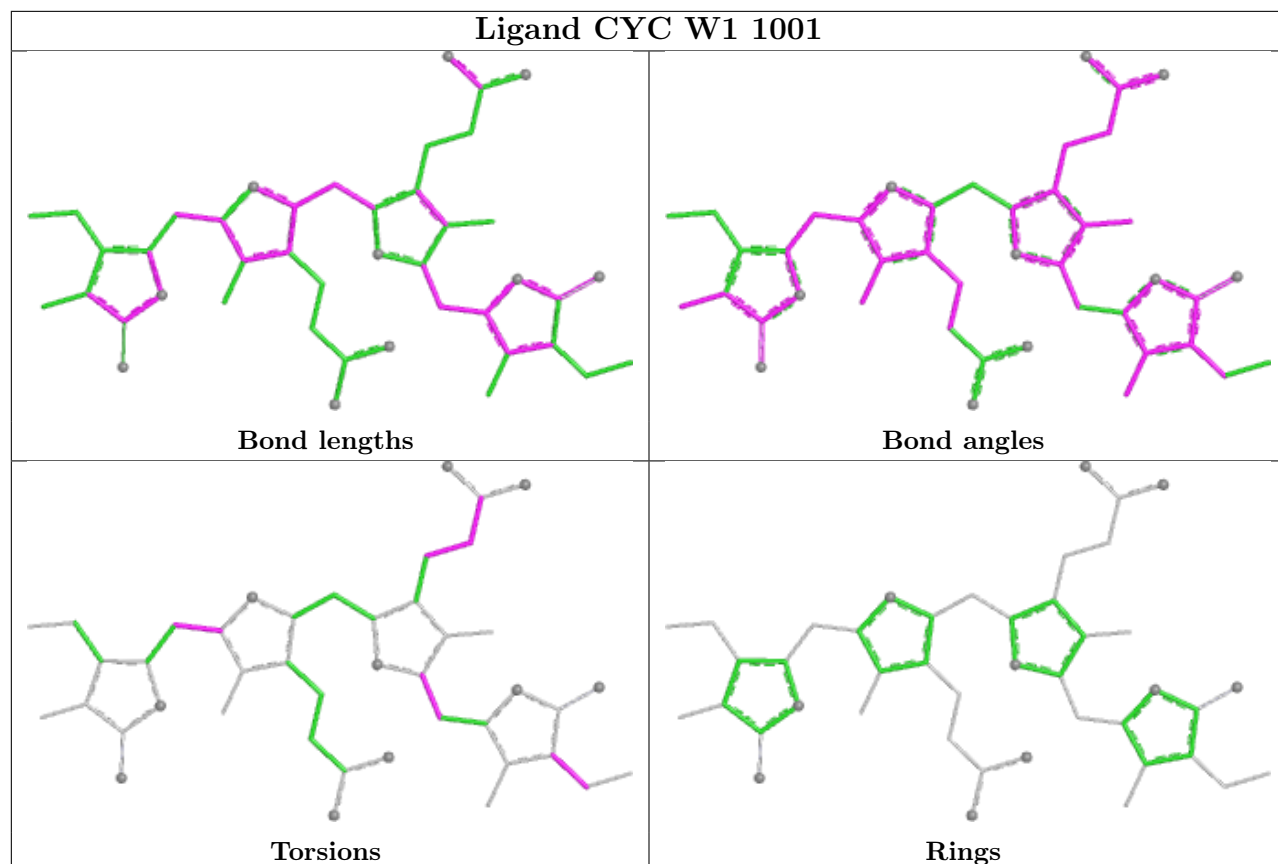


Ligand CYC ZA 201

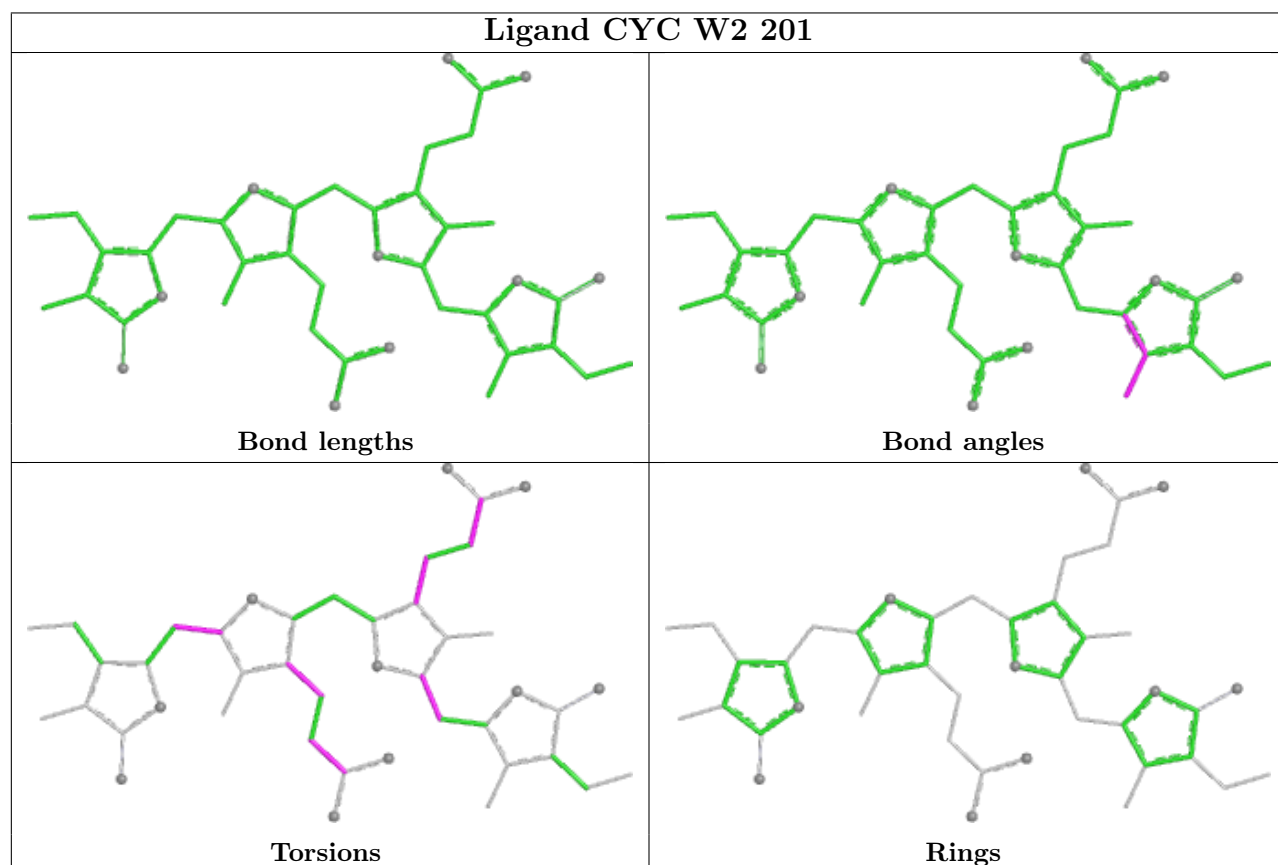




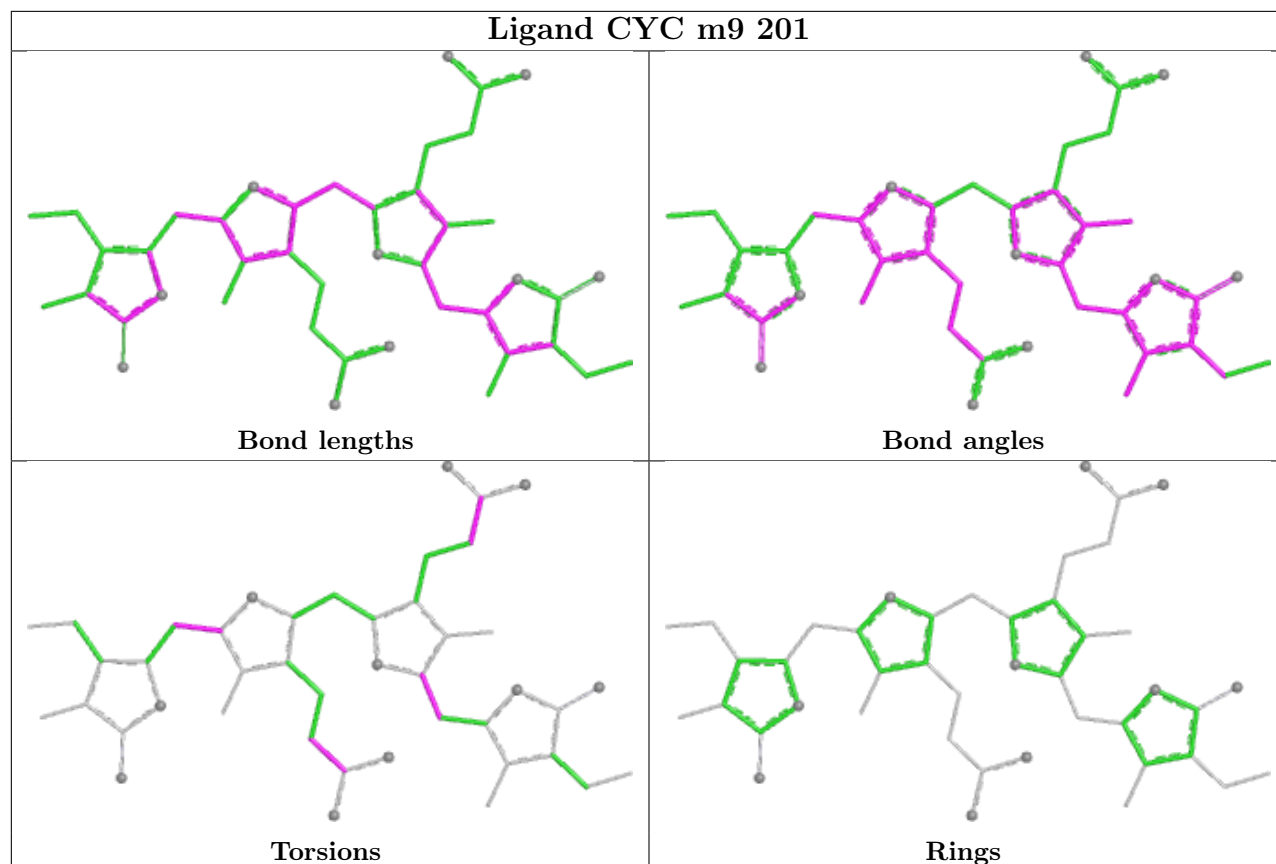
Ligand CYC W1 1001



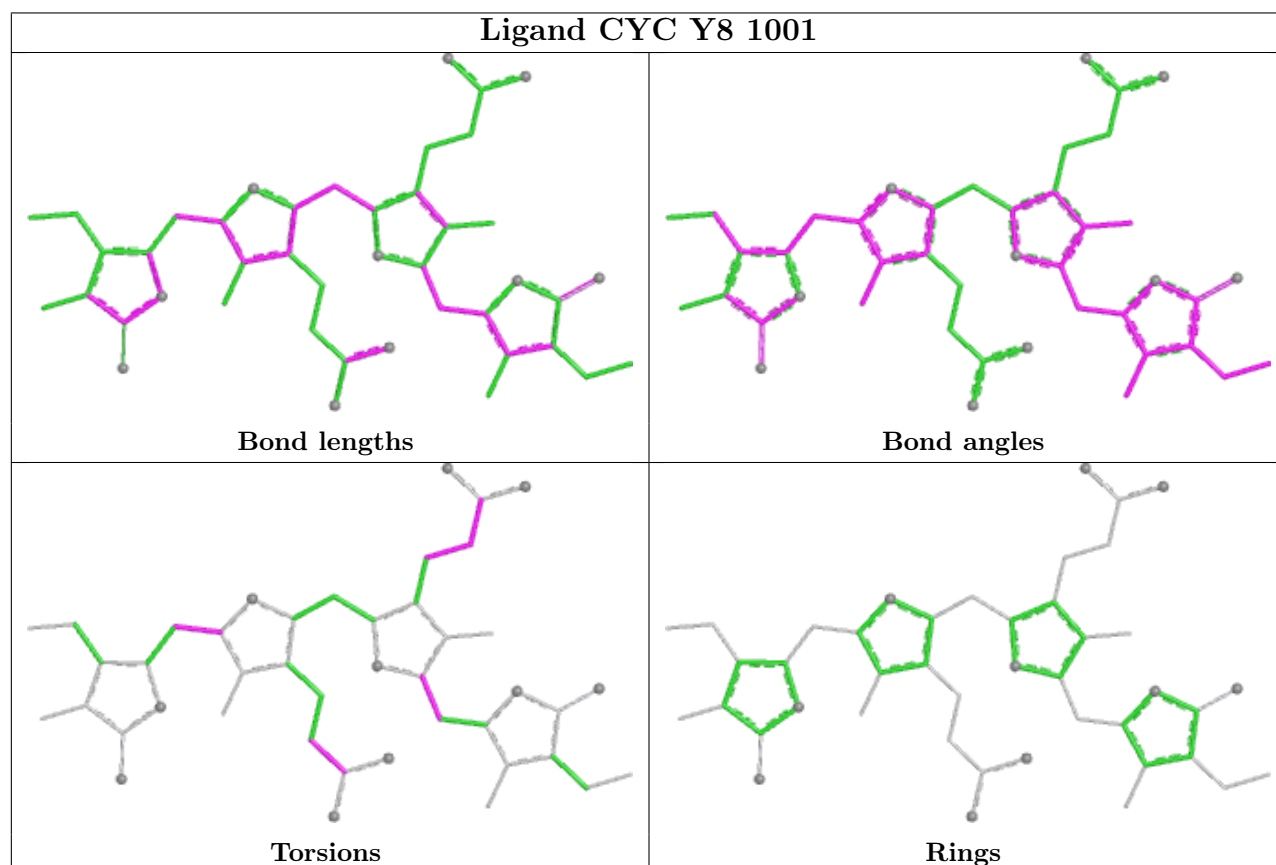
Ligand CYC W2 201

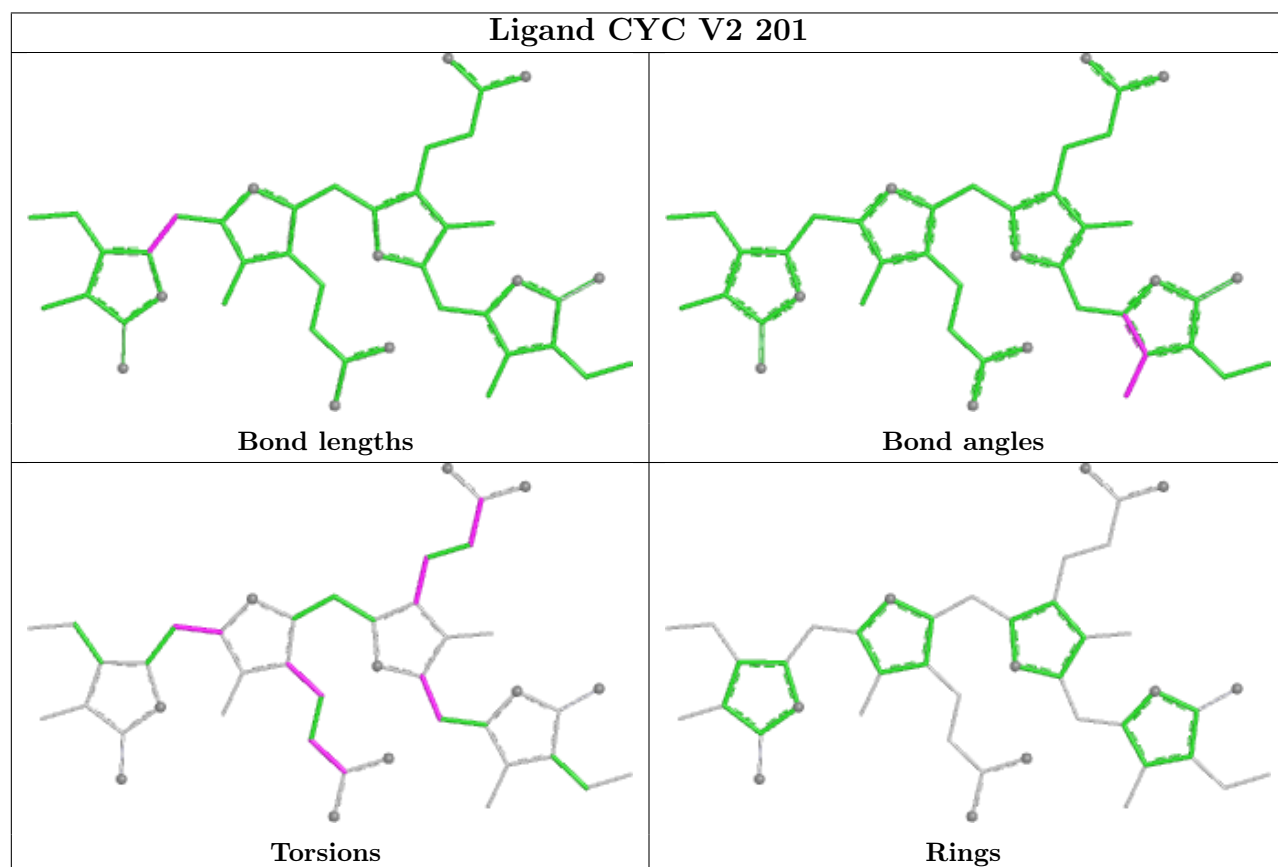
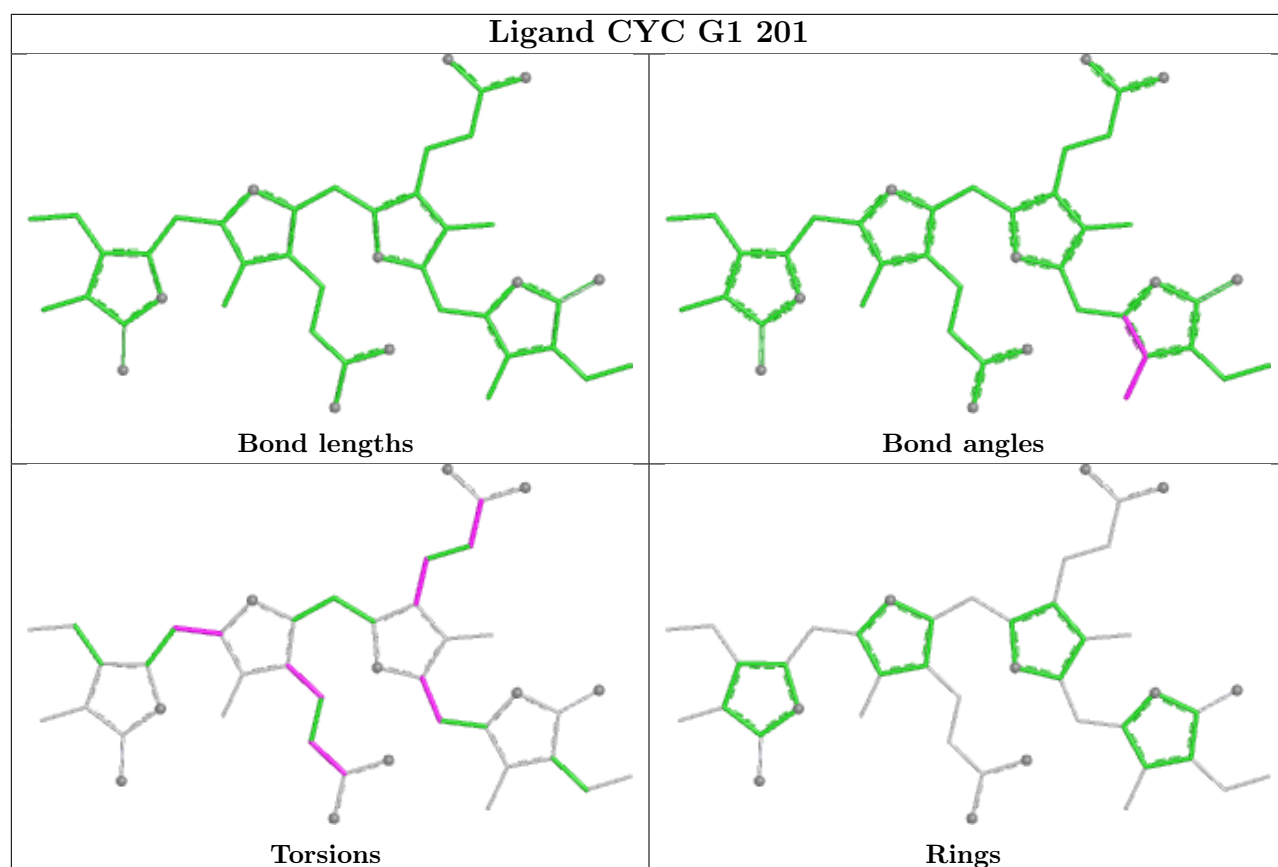


Ligand CYC m9 201

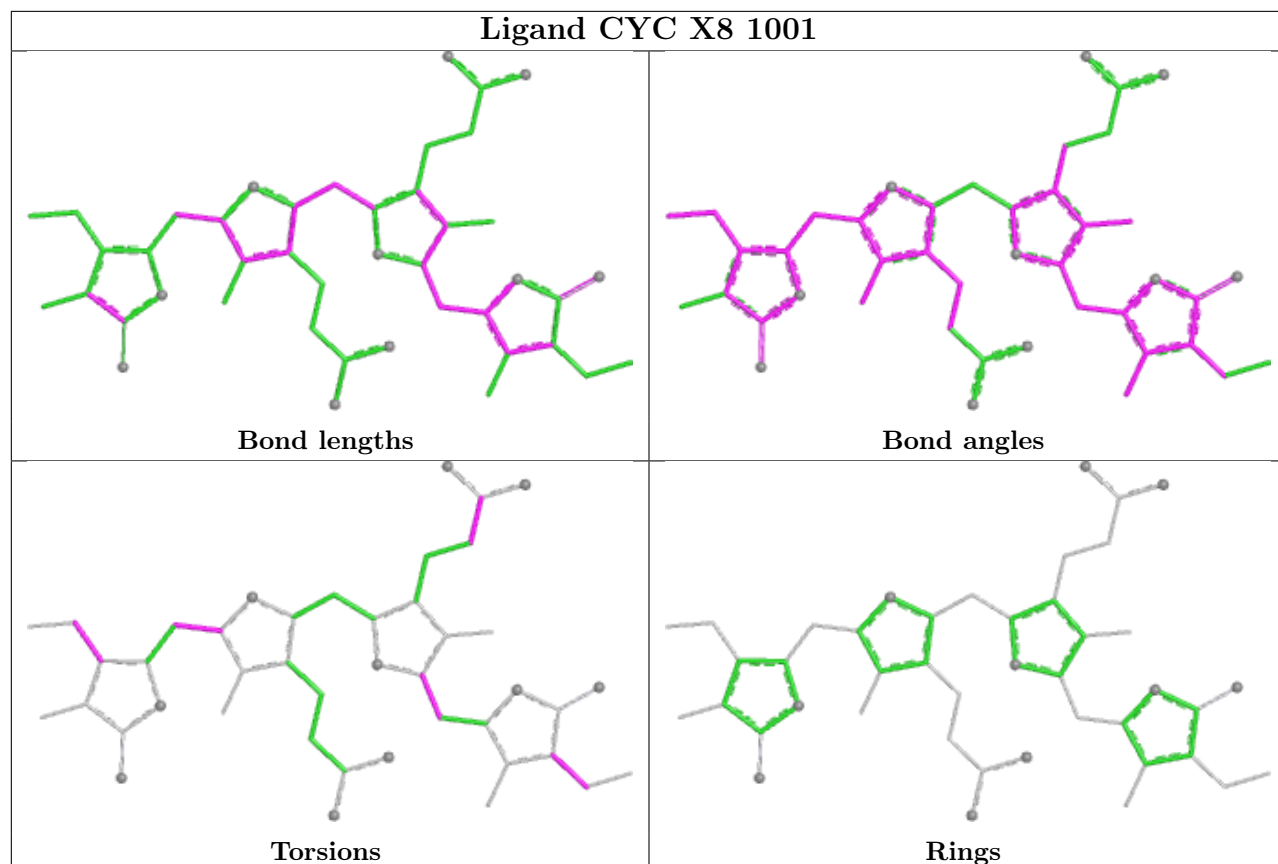


Ligand CYC Y8 1001

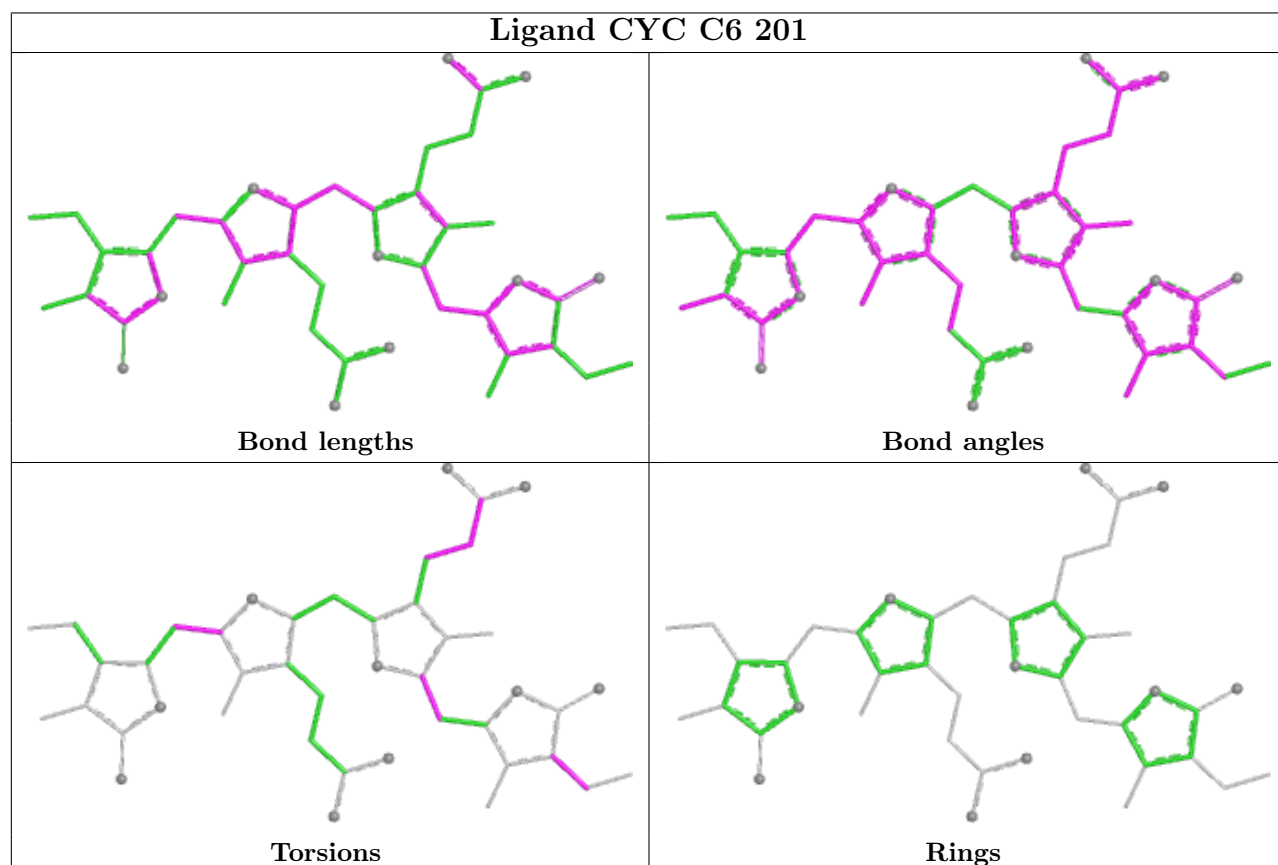




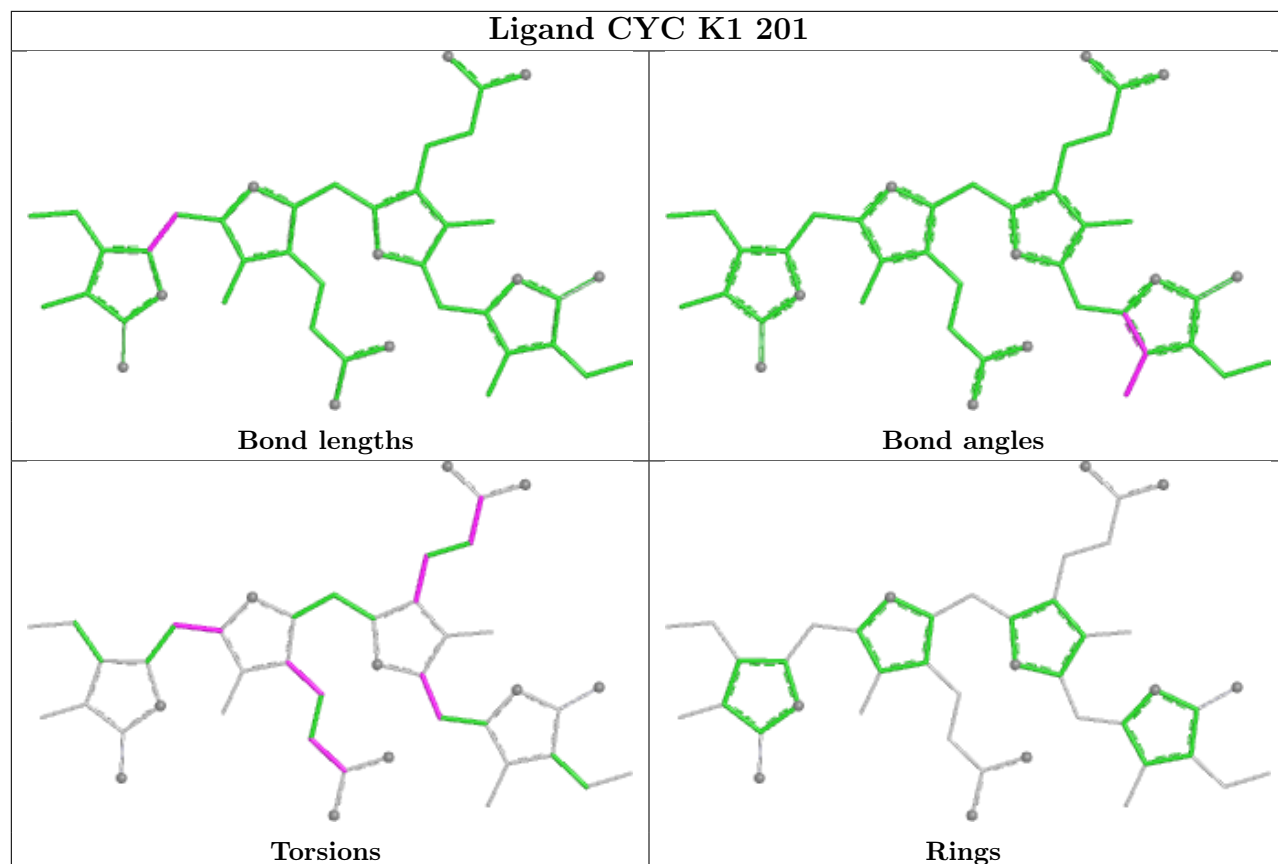
Ligand CYC X8 1001



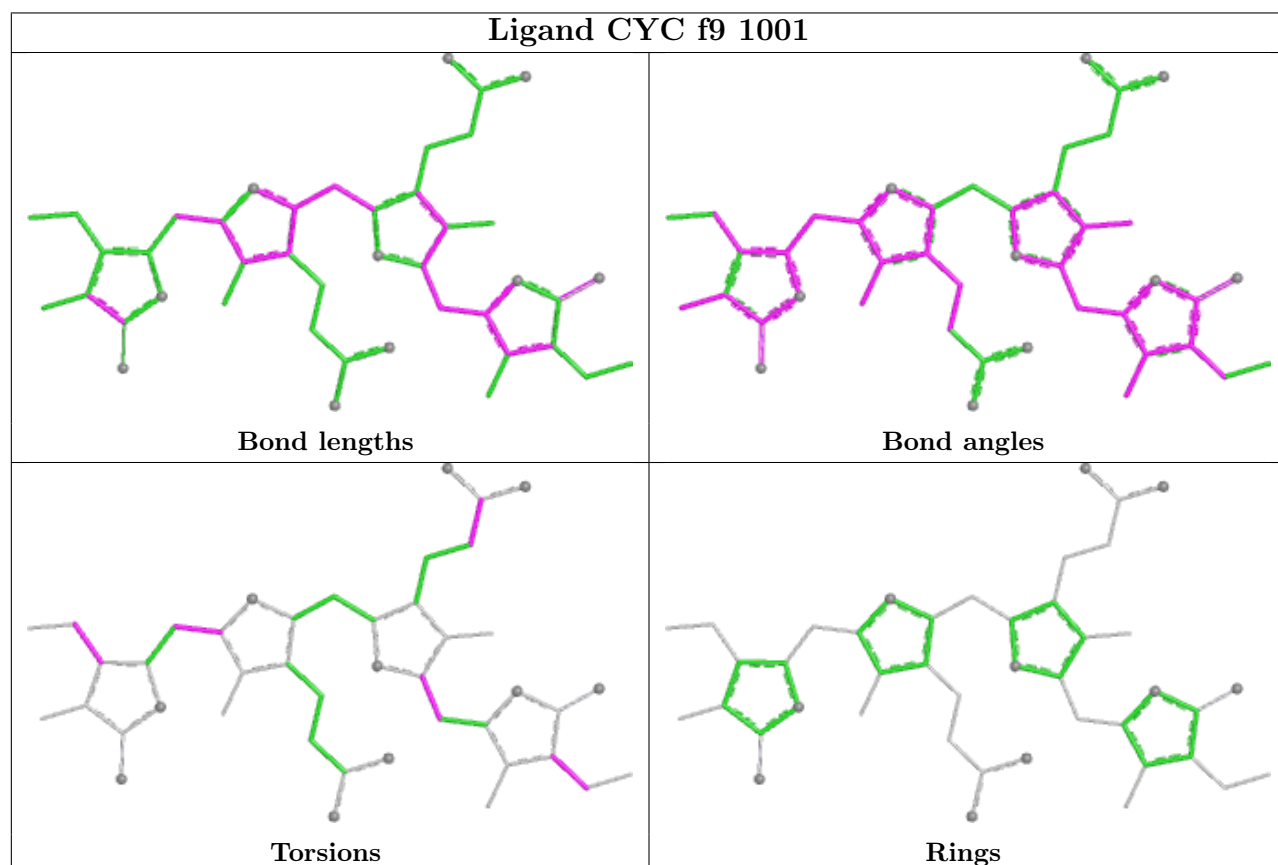
Ligand CYC C6 201



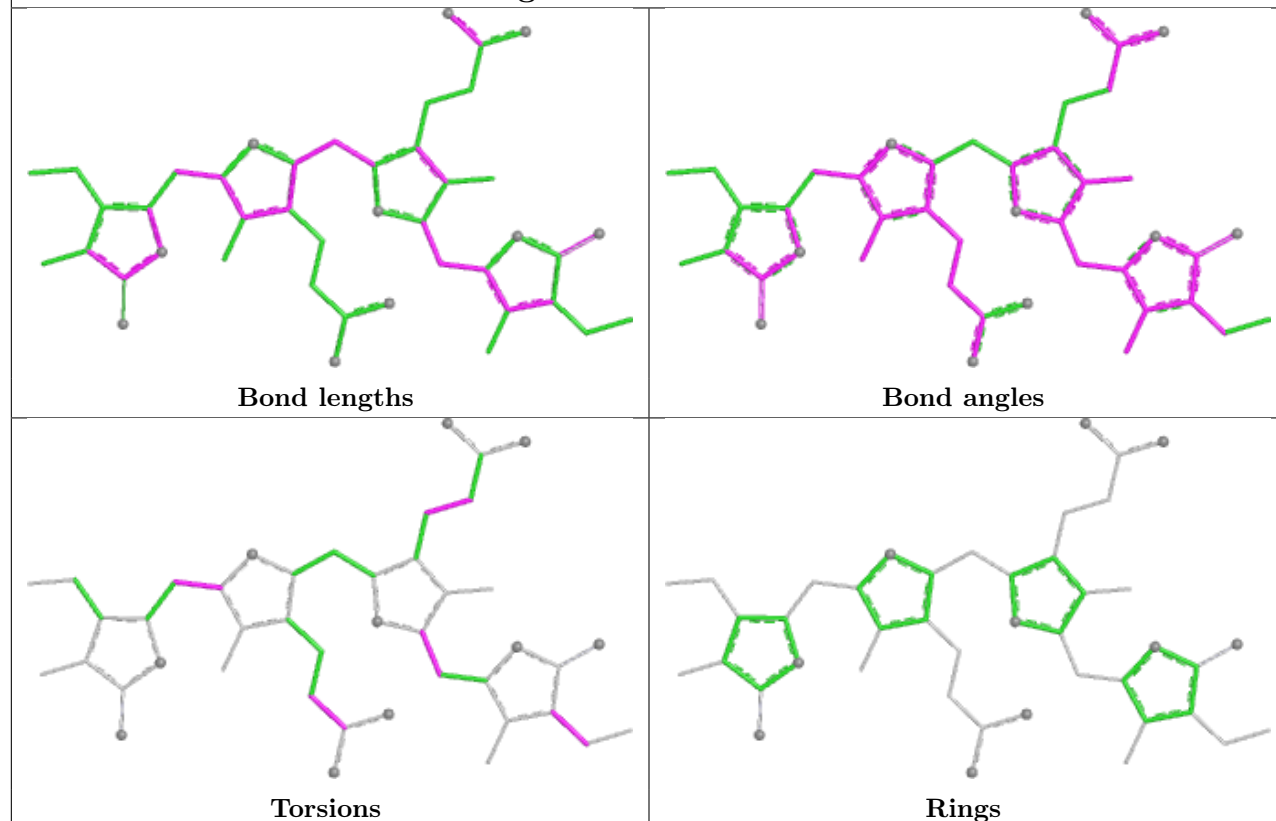
Ligand CYC K1 201



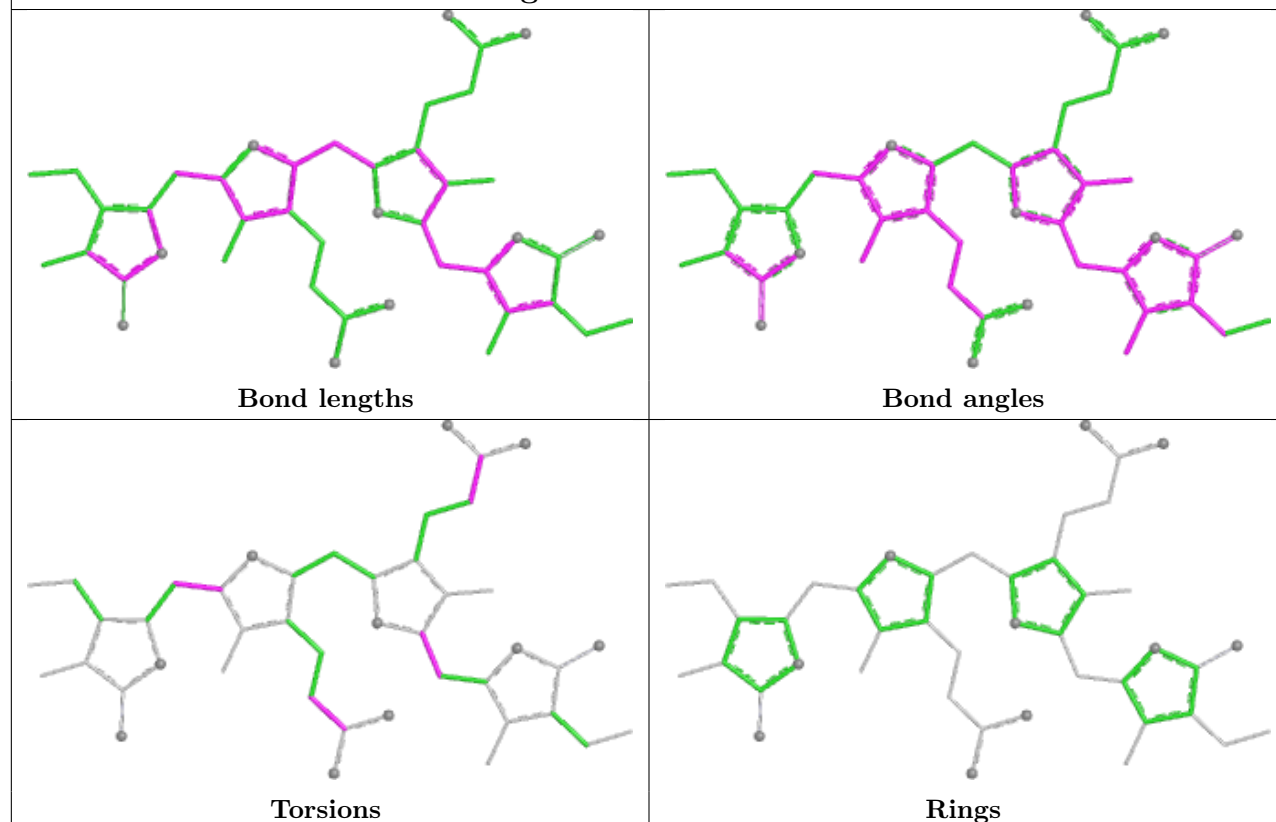
Ligand CYC f9 1001



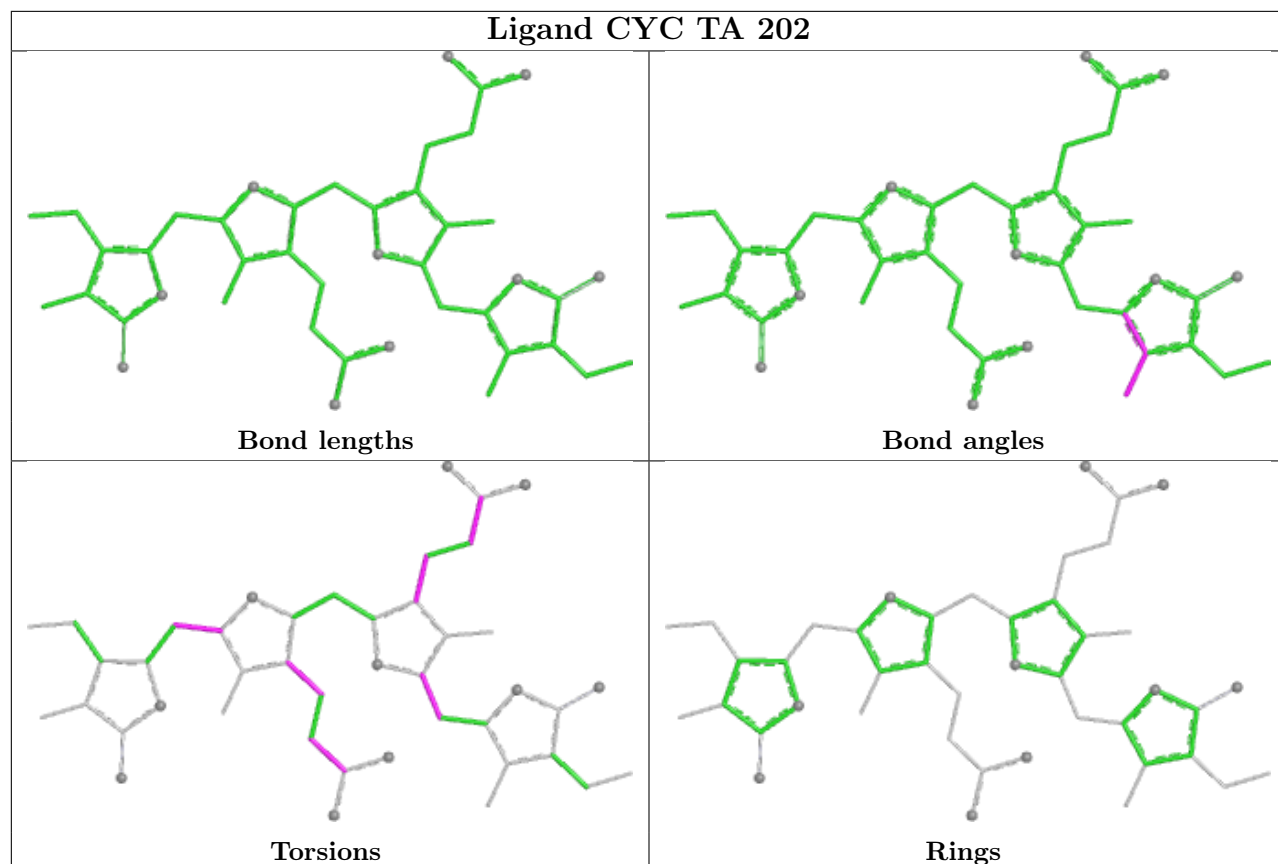
Ligand CYC t9 1001



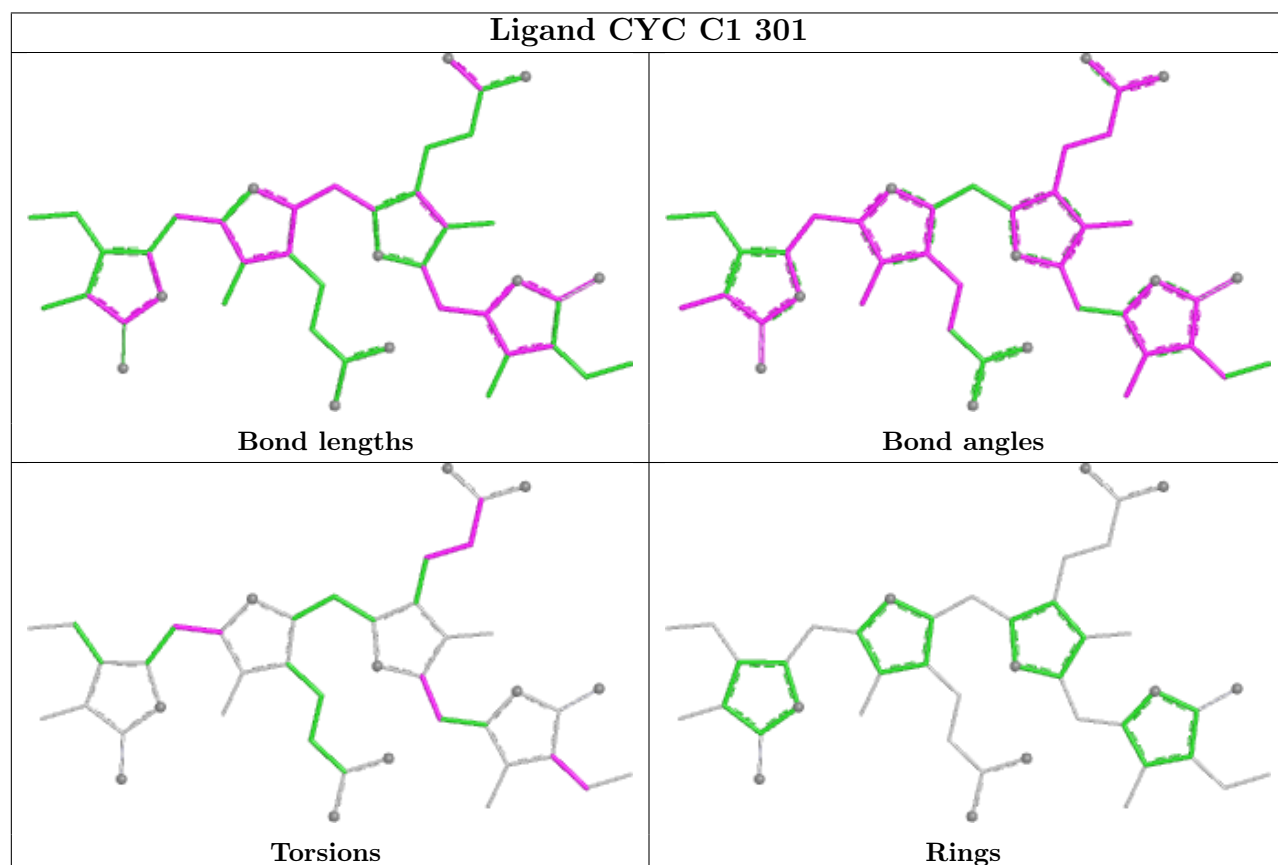
Ligand CYC V9 201



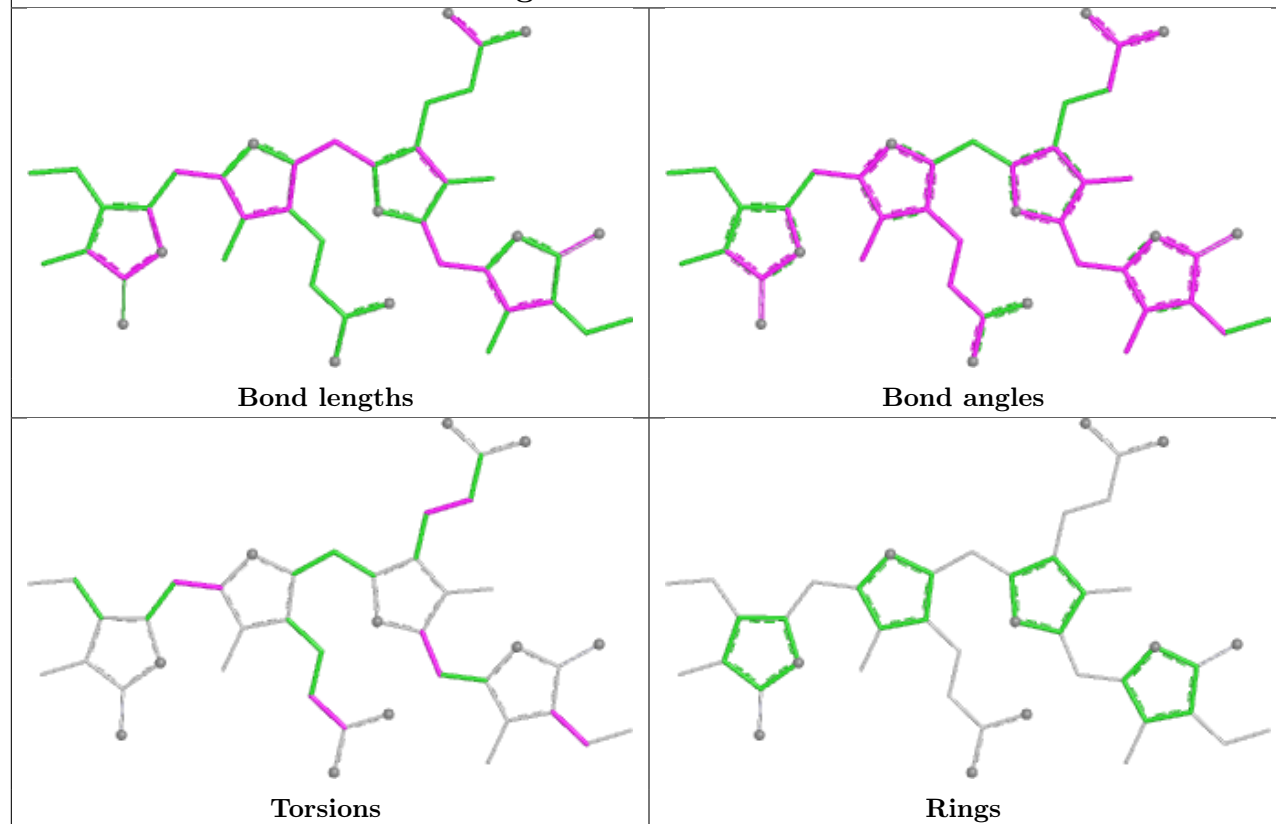
Ligand CYC TA 202



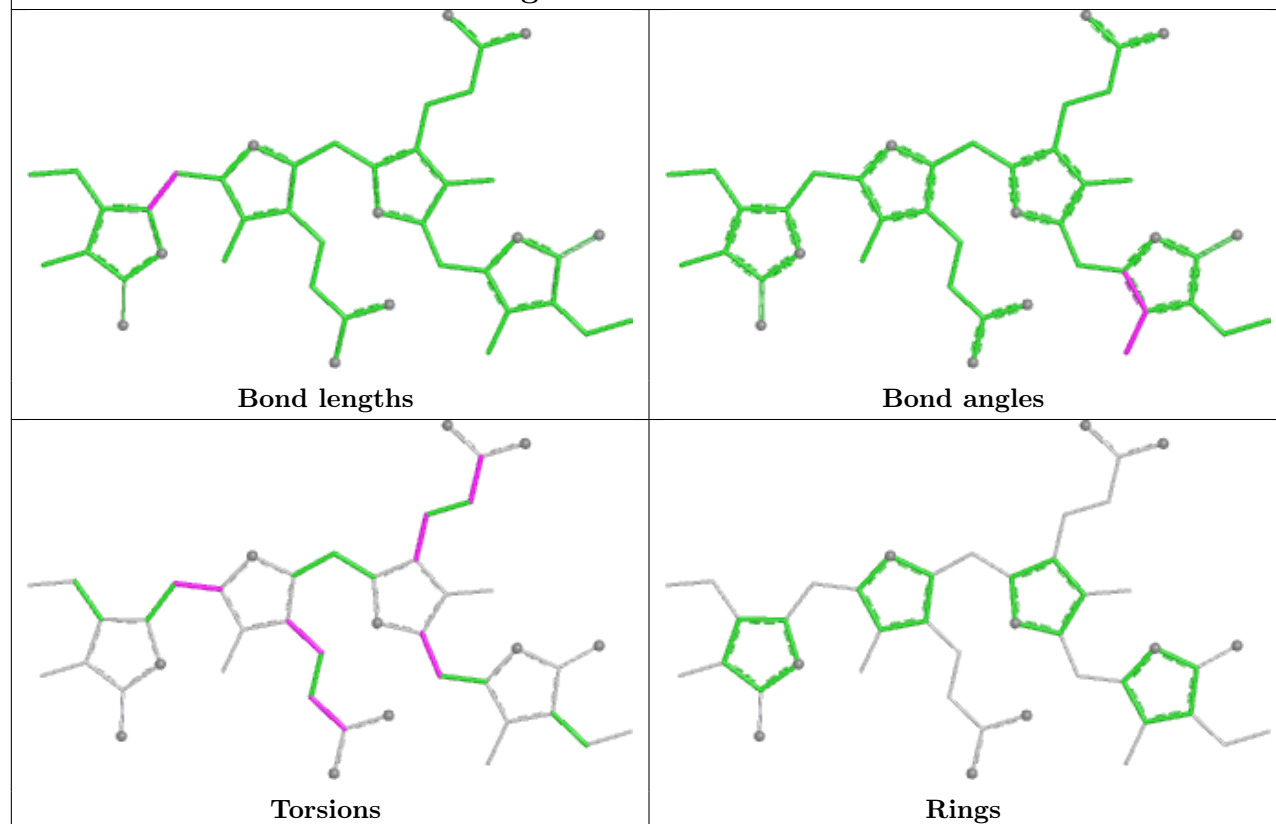
Ligand CYC C1 301

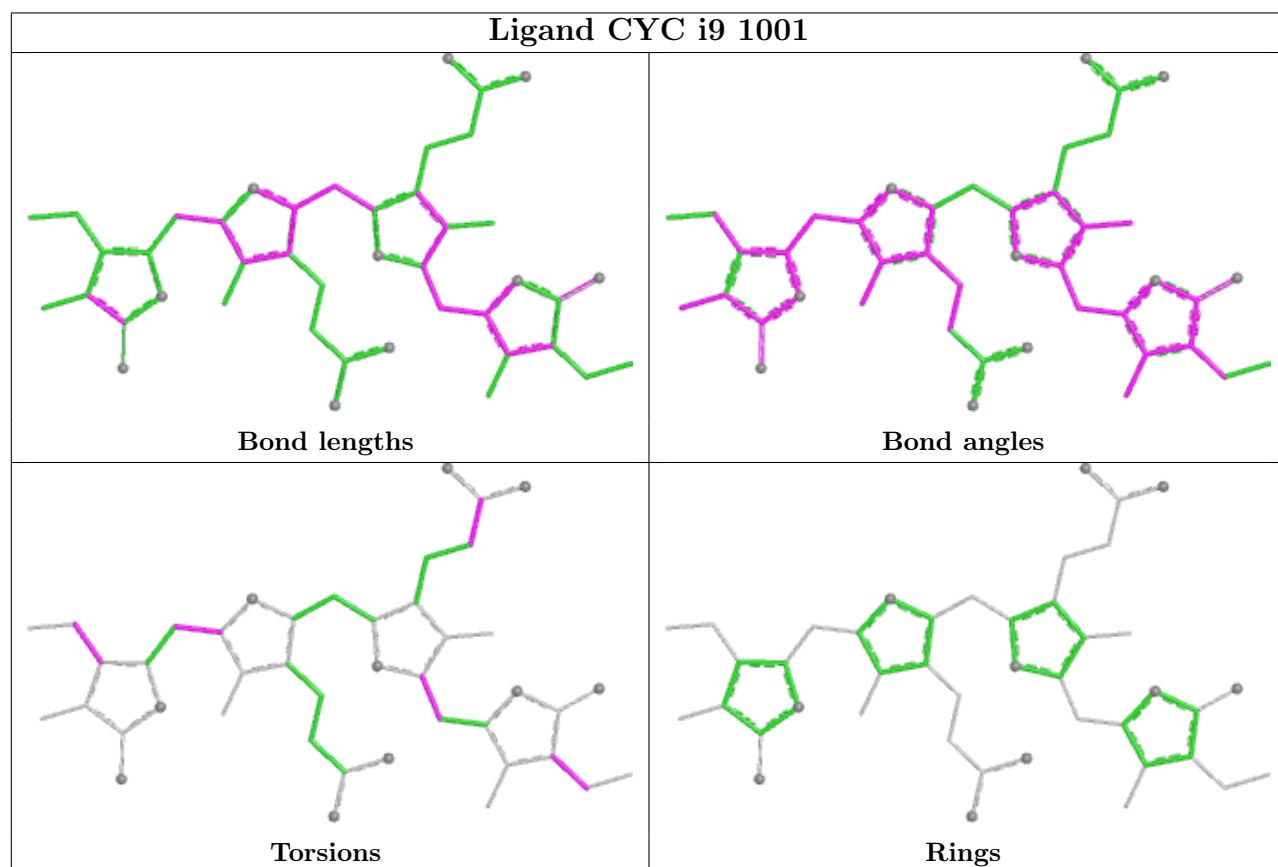
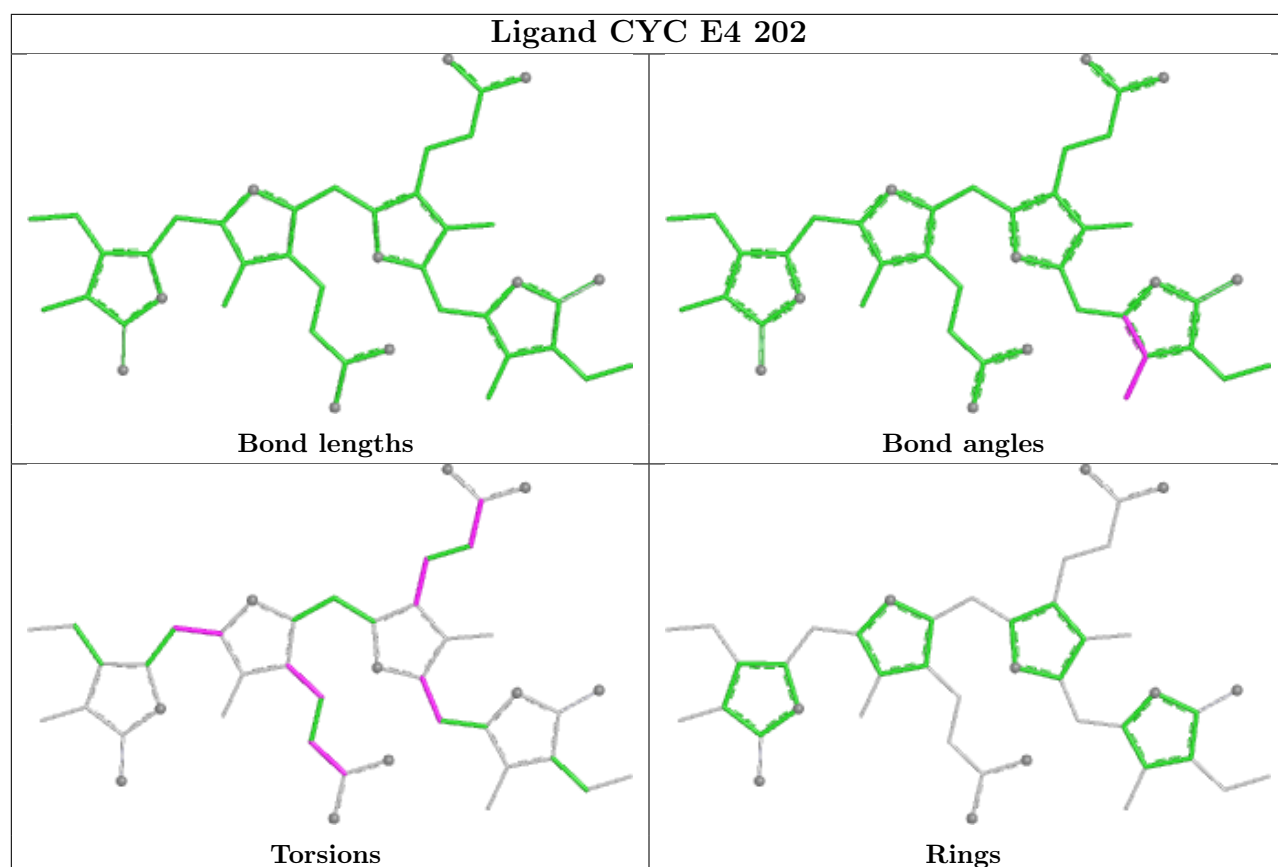


Ligand CYC 19 1204

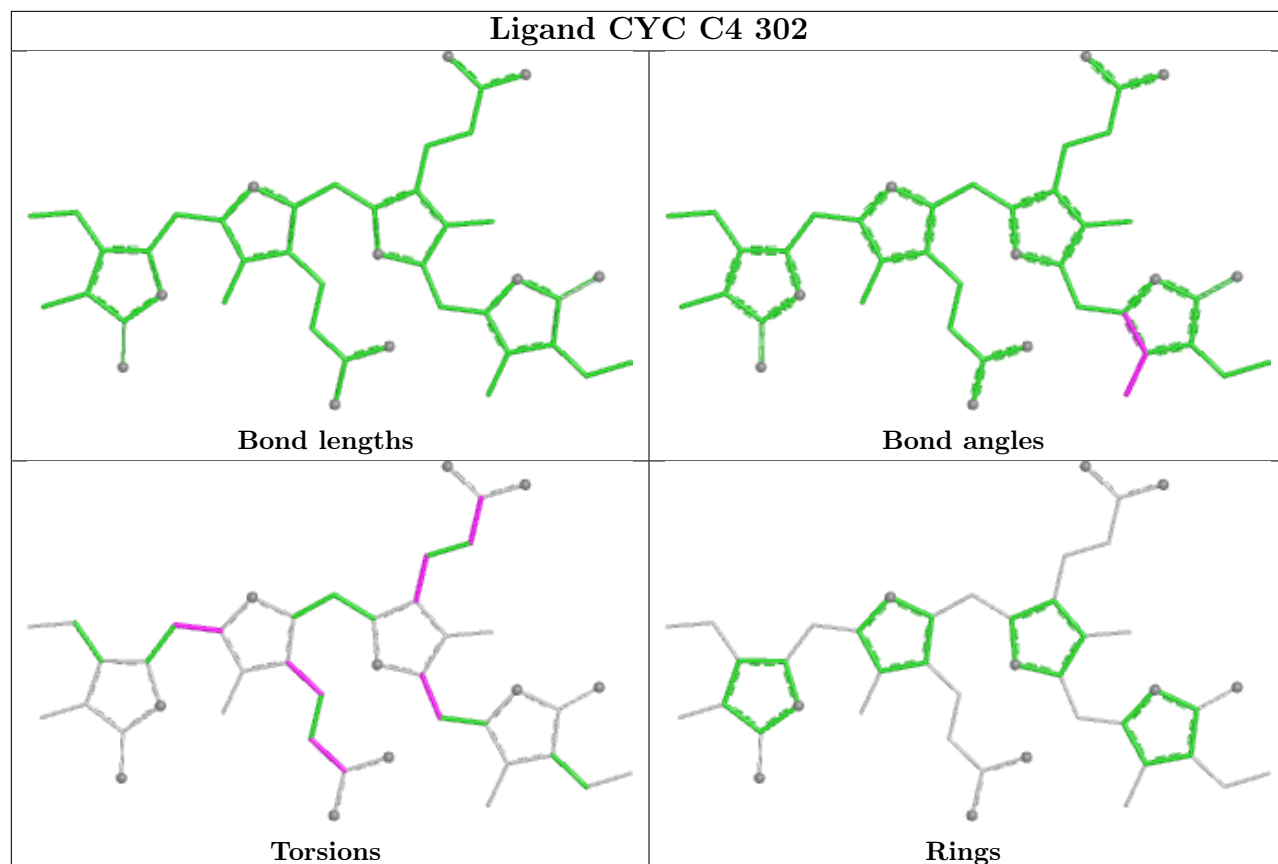


Ligand CYC C1 302

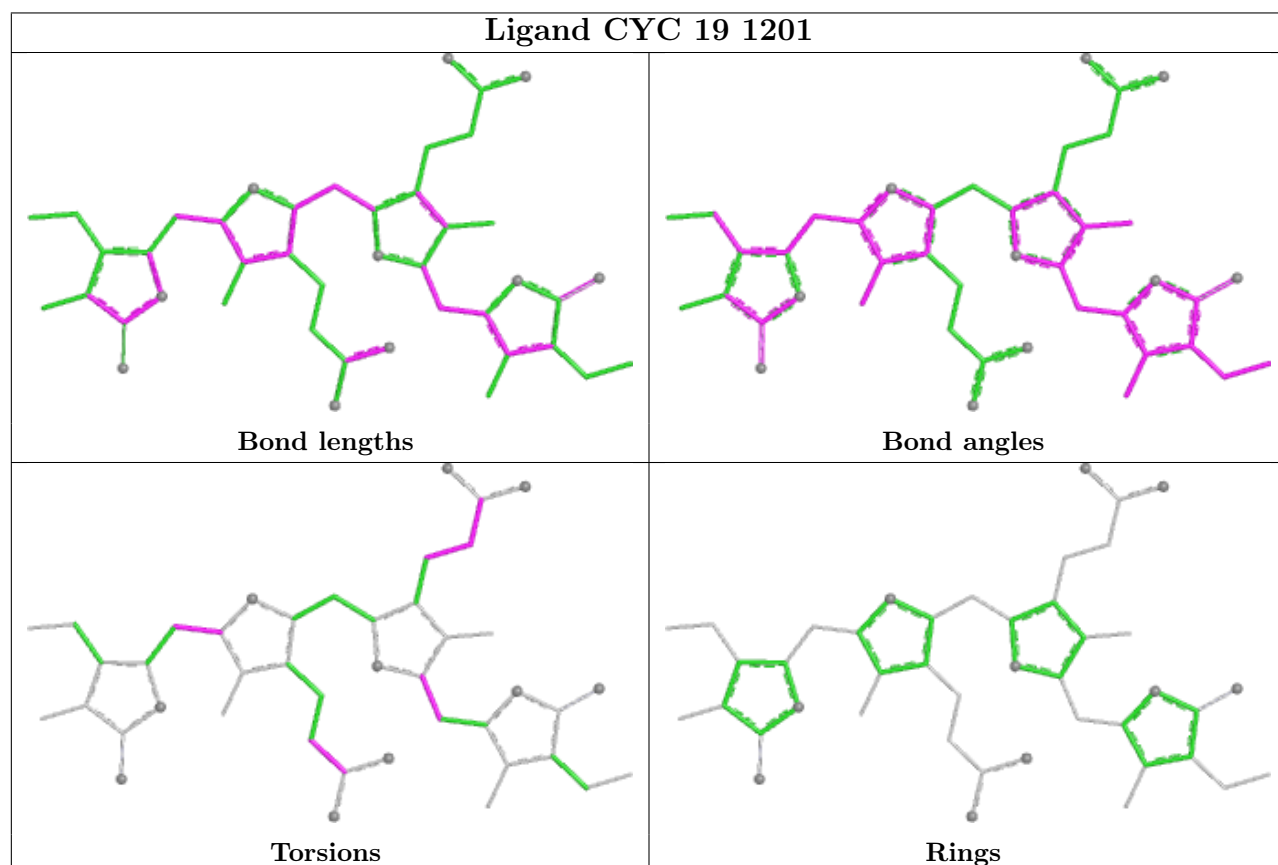




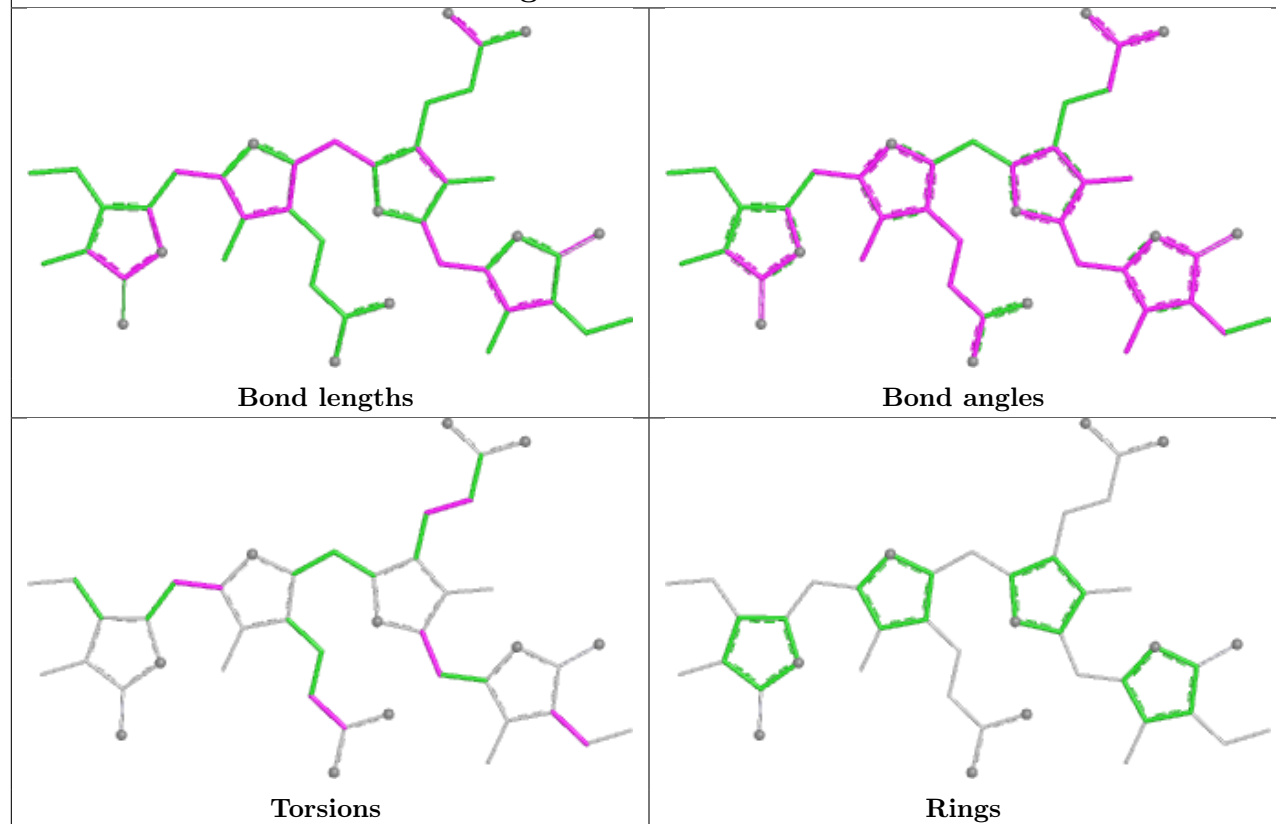
Ligand CYC C4 302



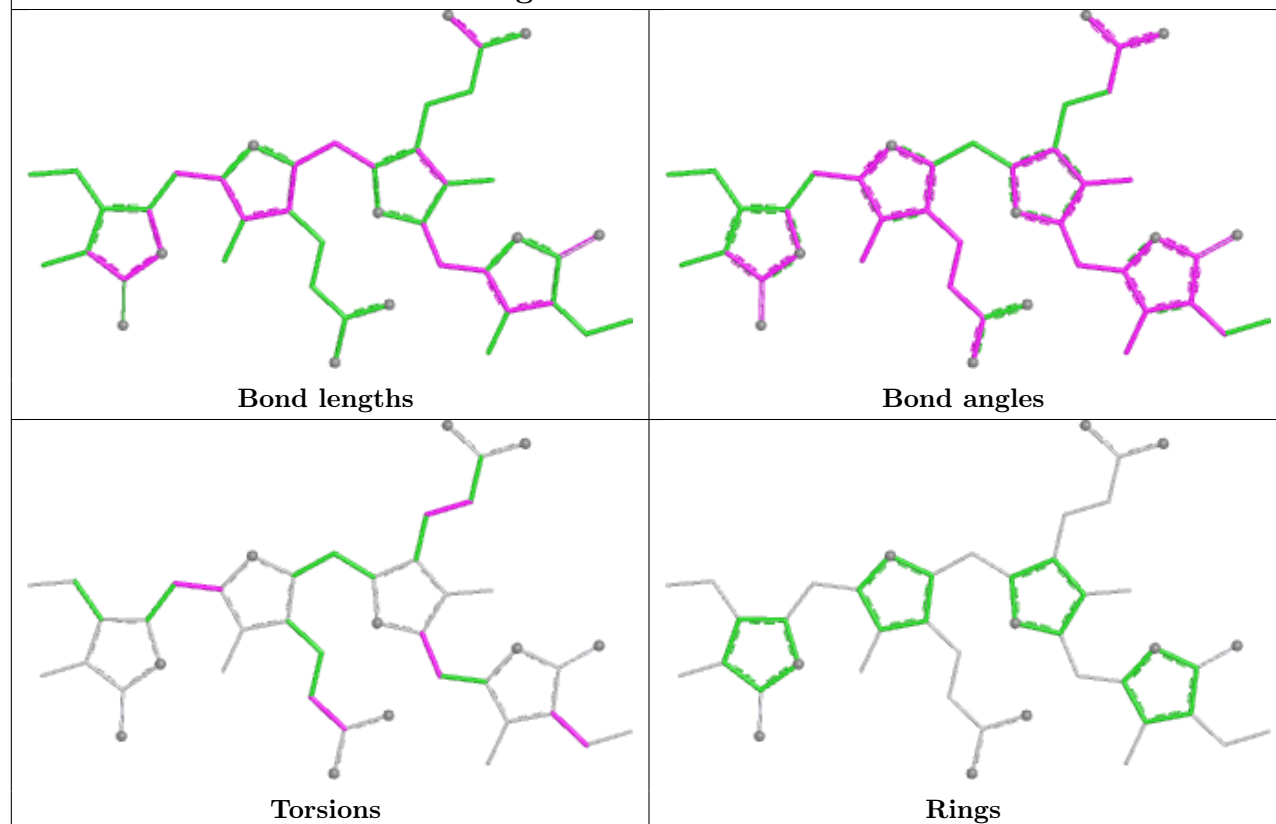
Ligand CYC 19 1201



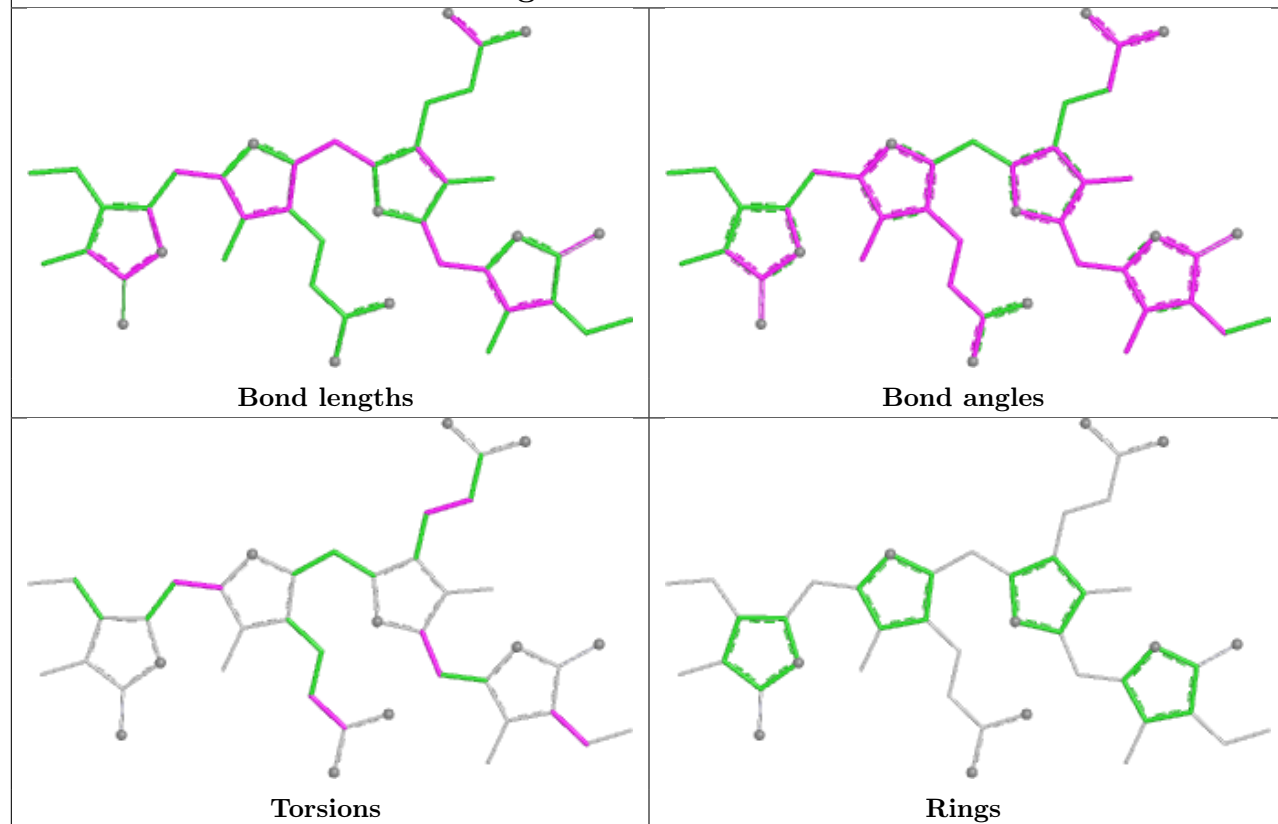
Ligand CYC l9 1001



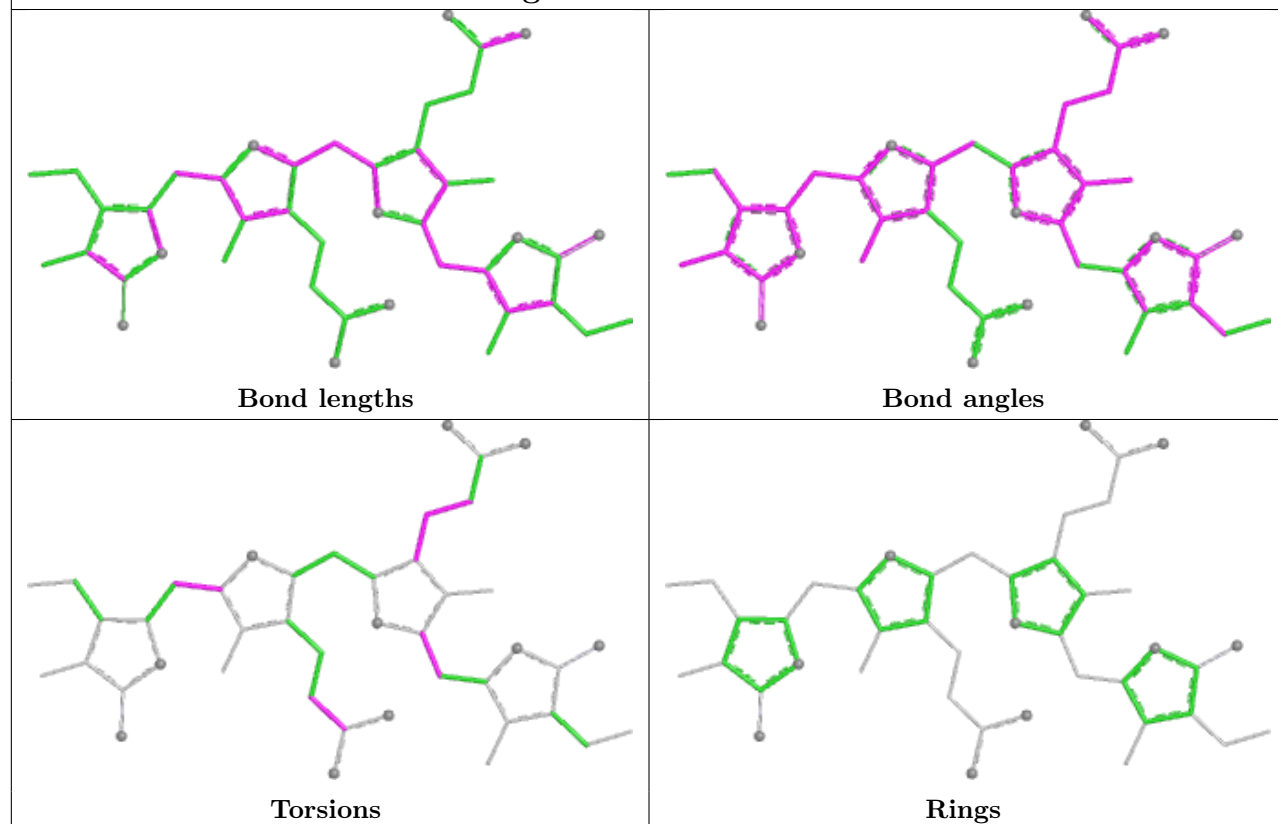
Ligand CYC x9 1001



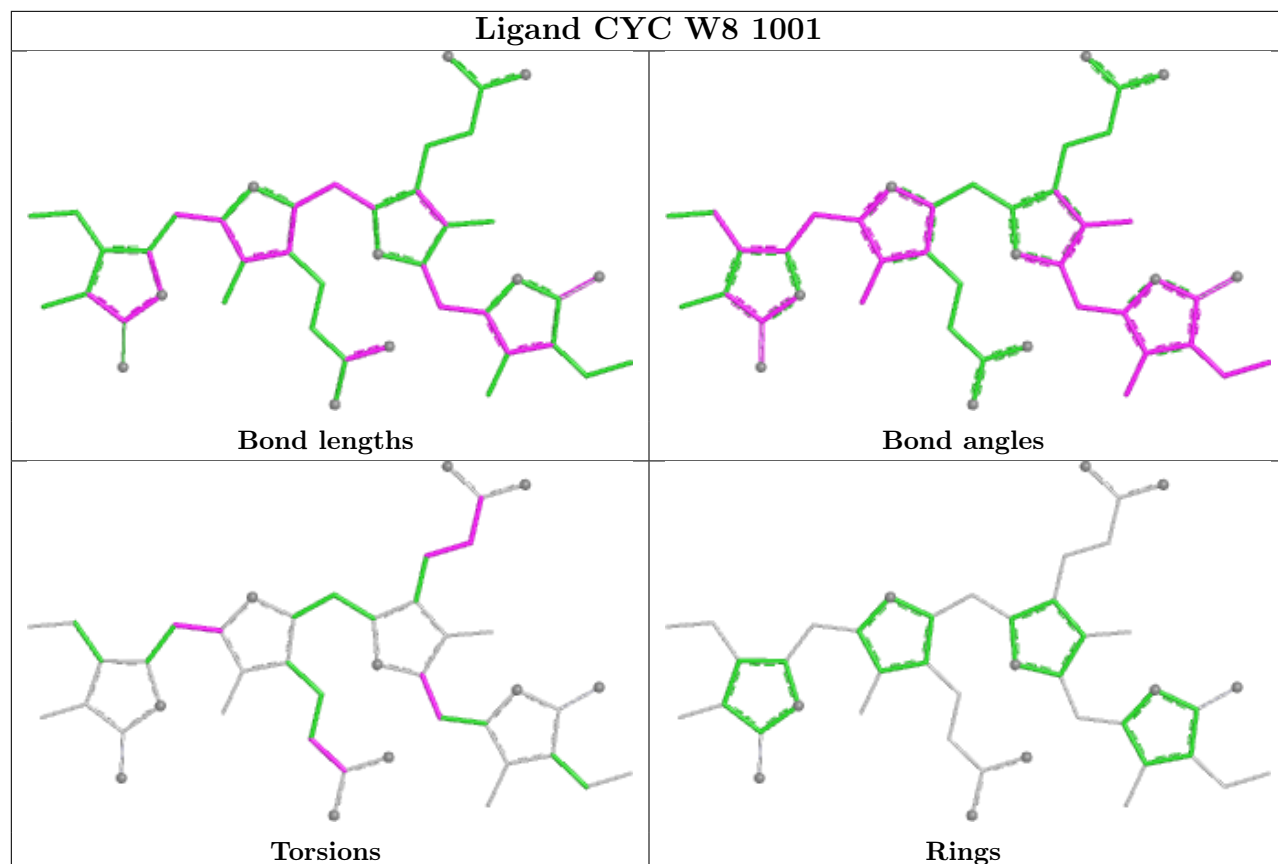
Ligand CYC r9 1001



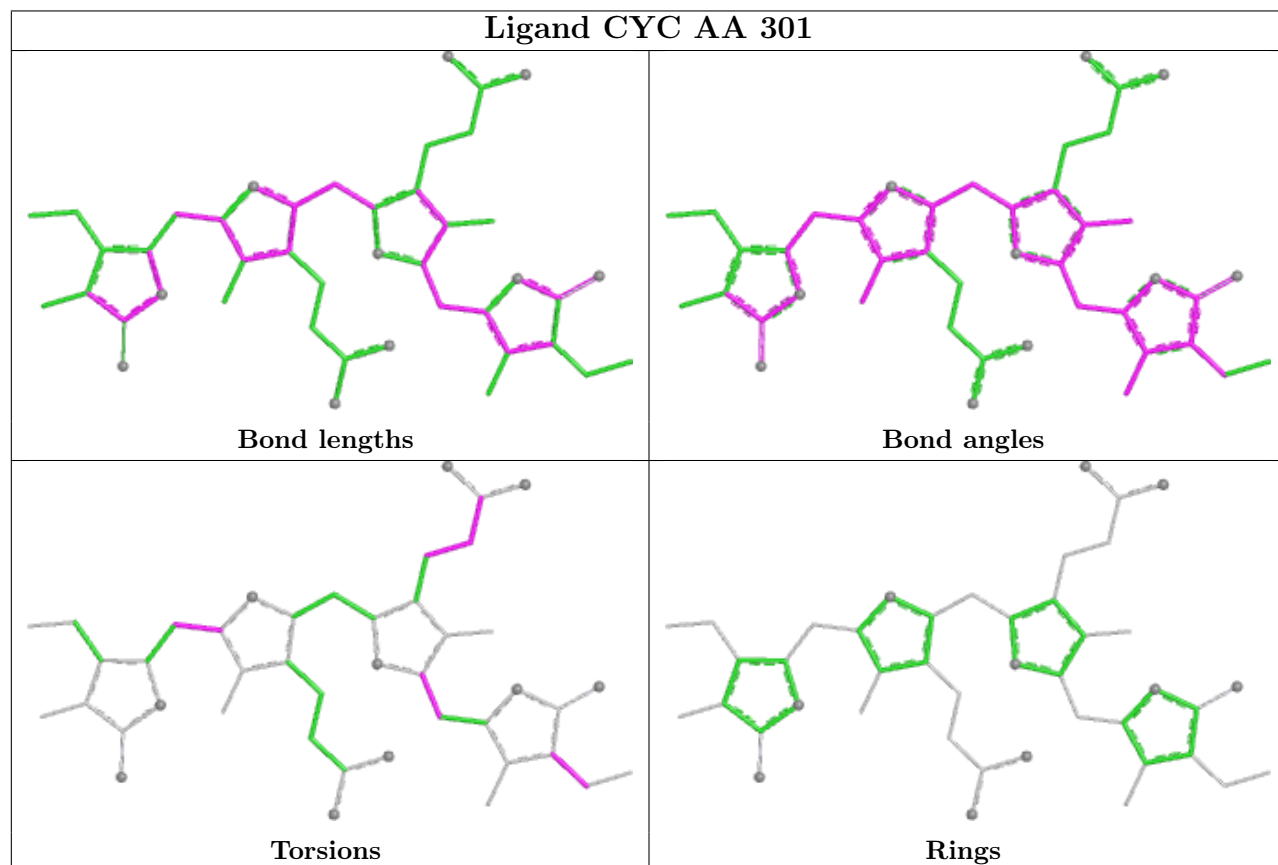
Ligand CYC IA 201



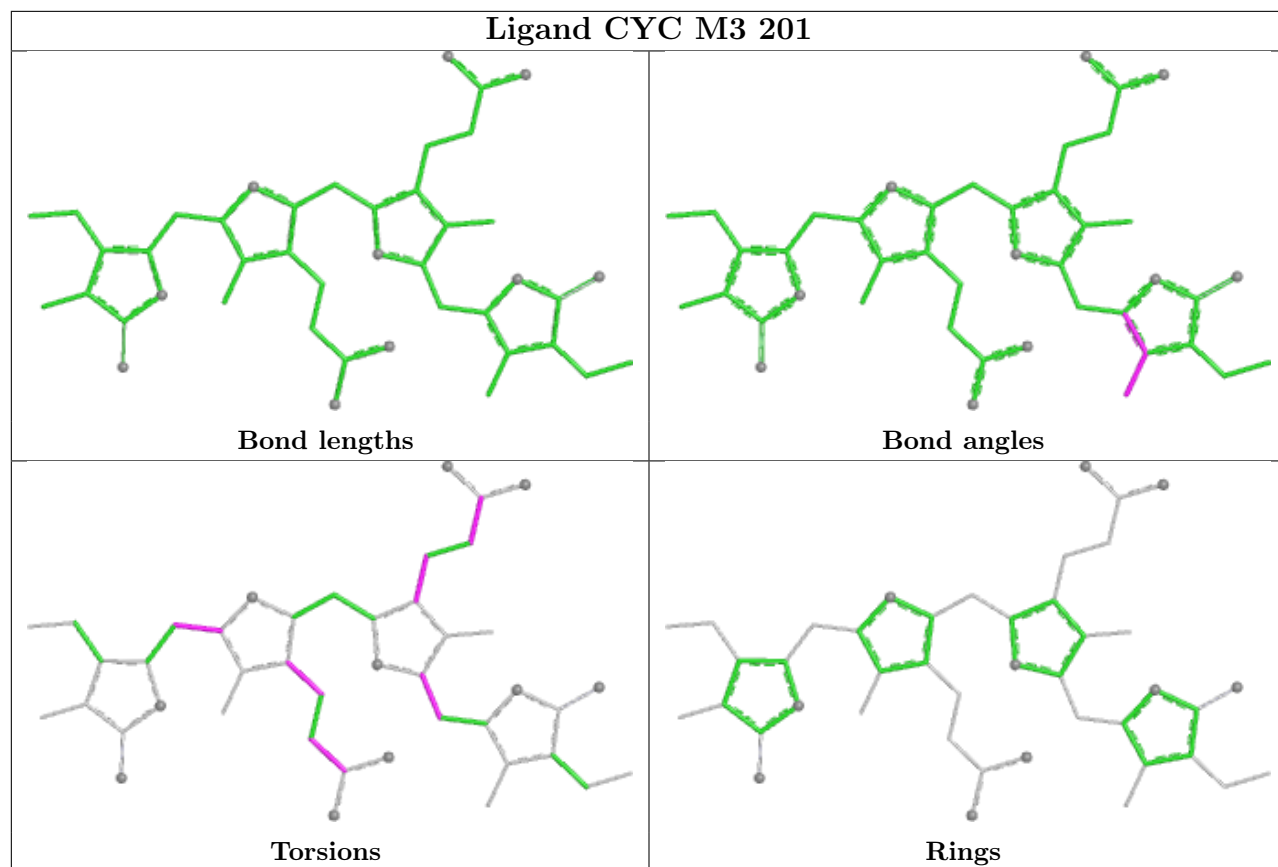
Ligand CYC W8 1001



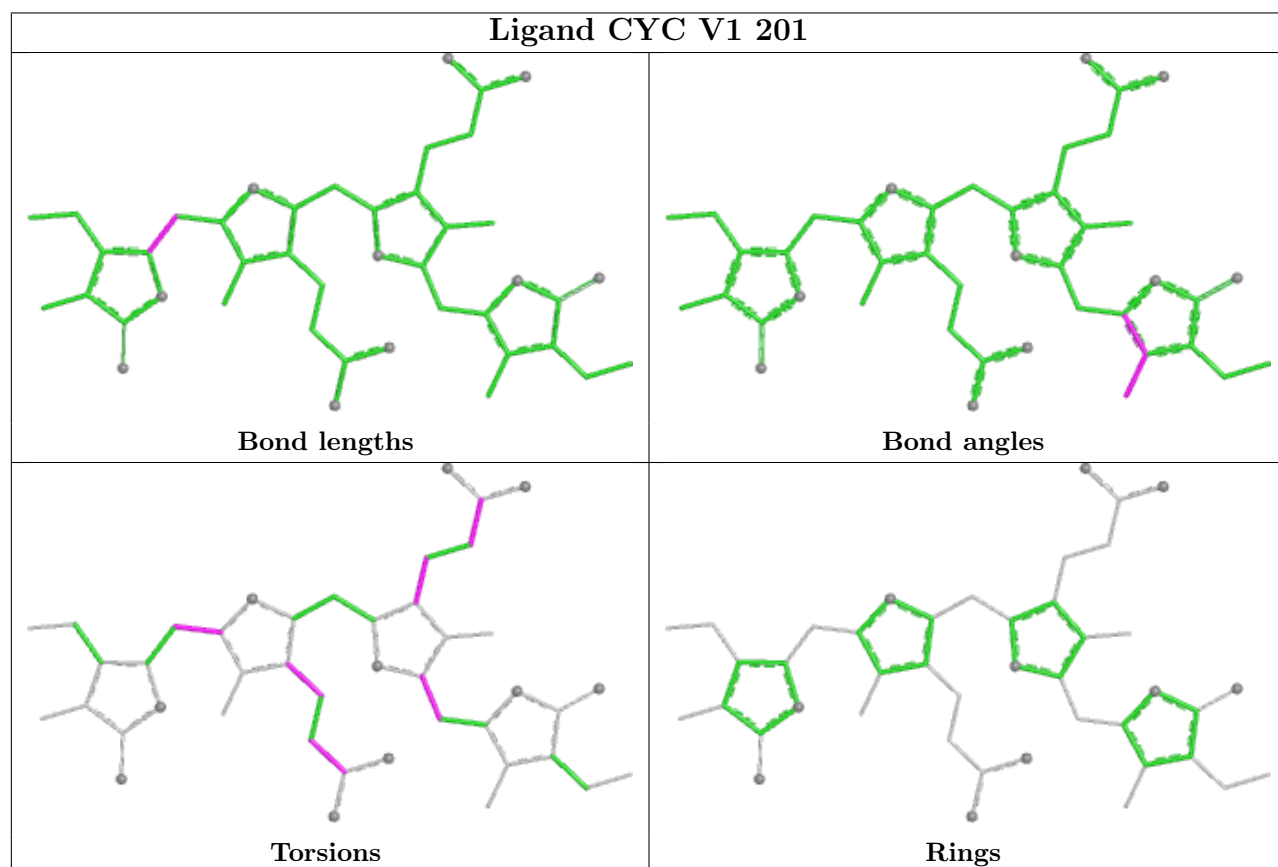
Ligand CYC AA 301



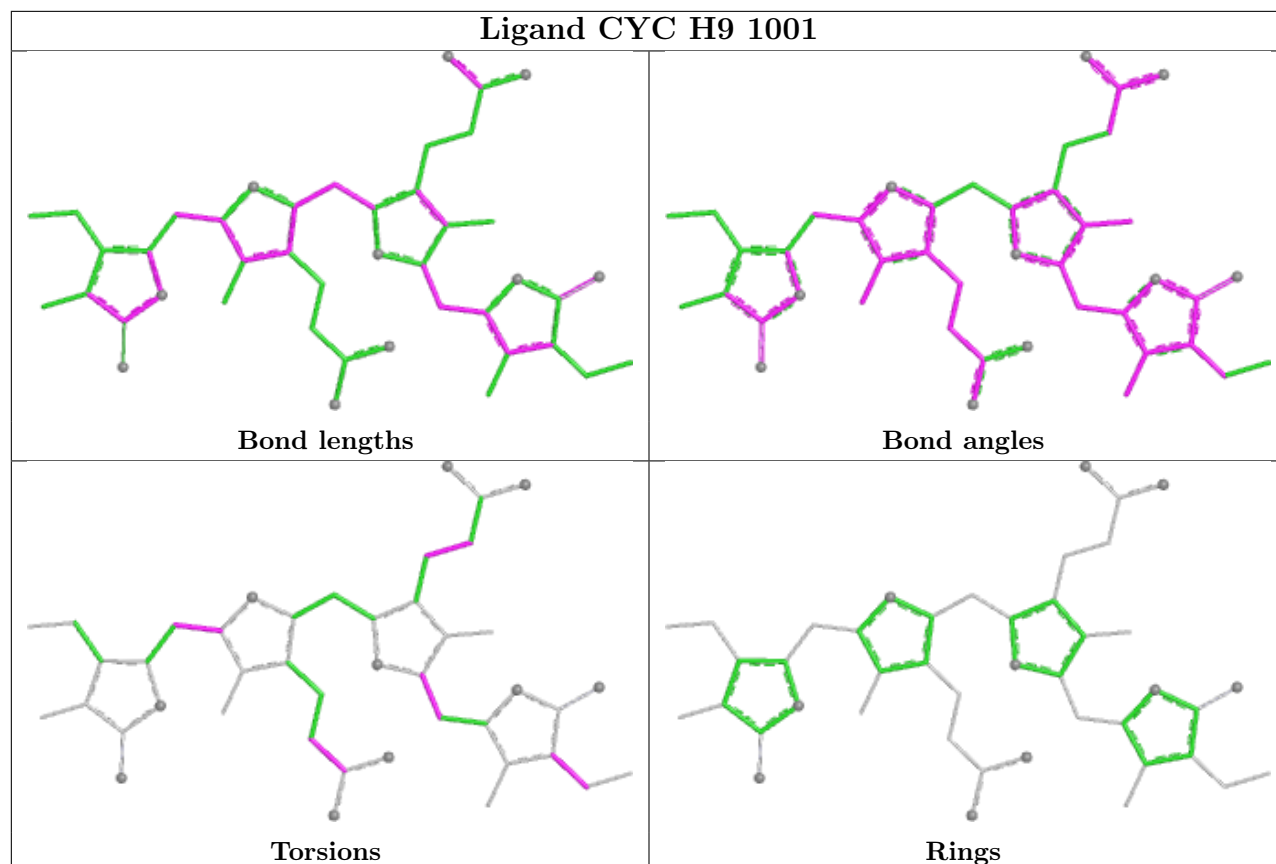
Ligand CYC M3 201



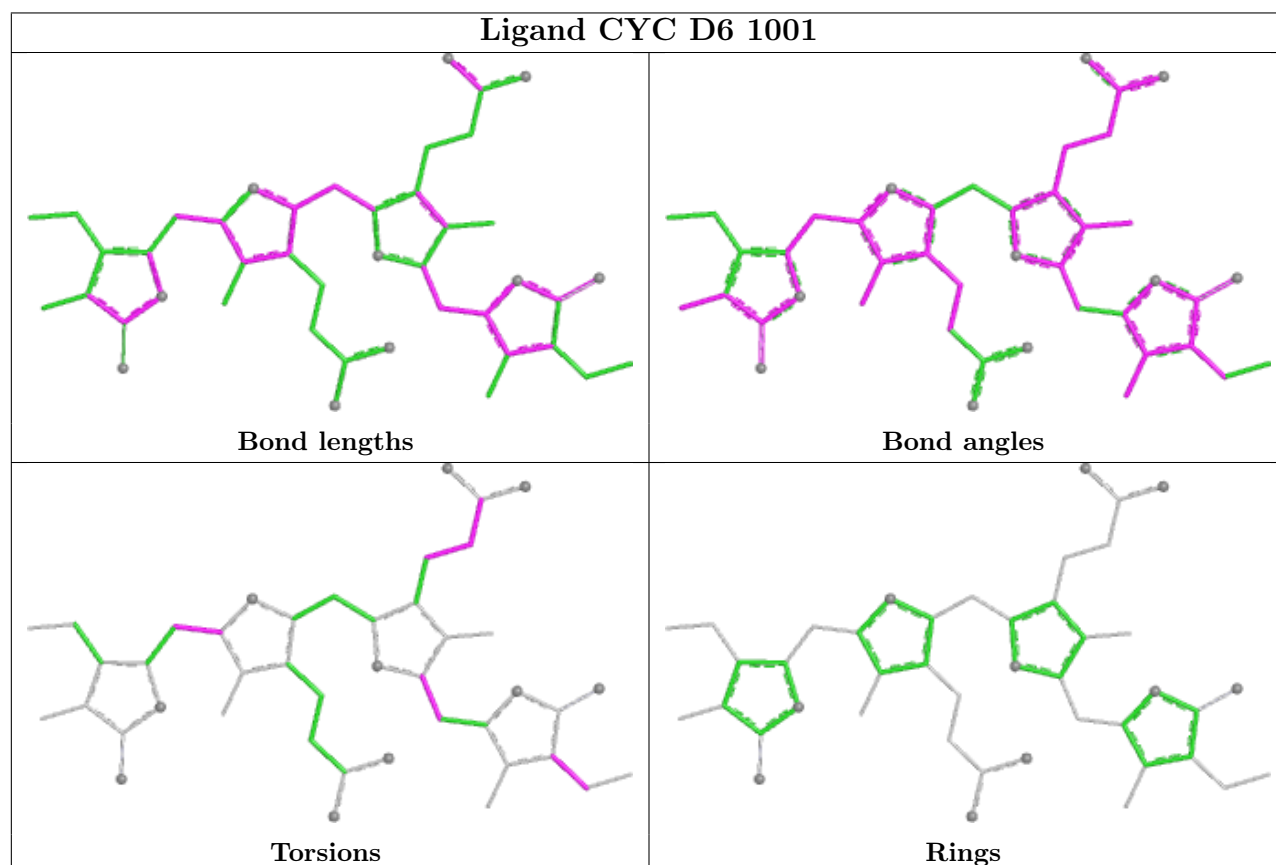
Ligand CYC V1 201



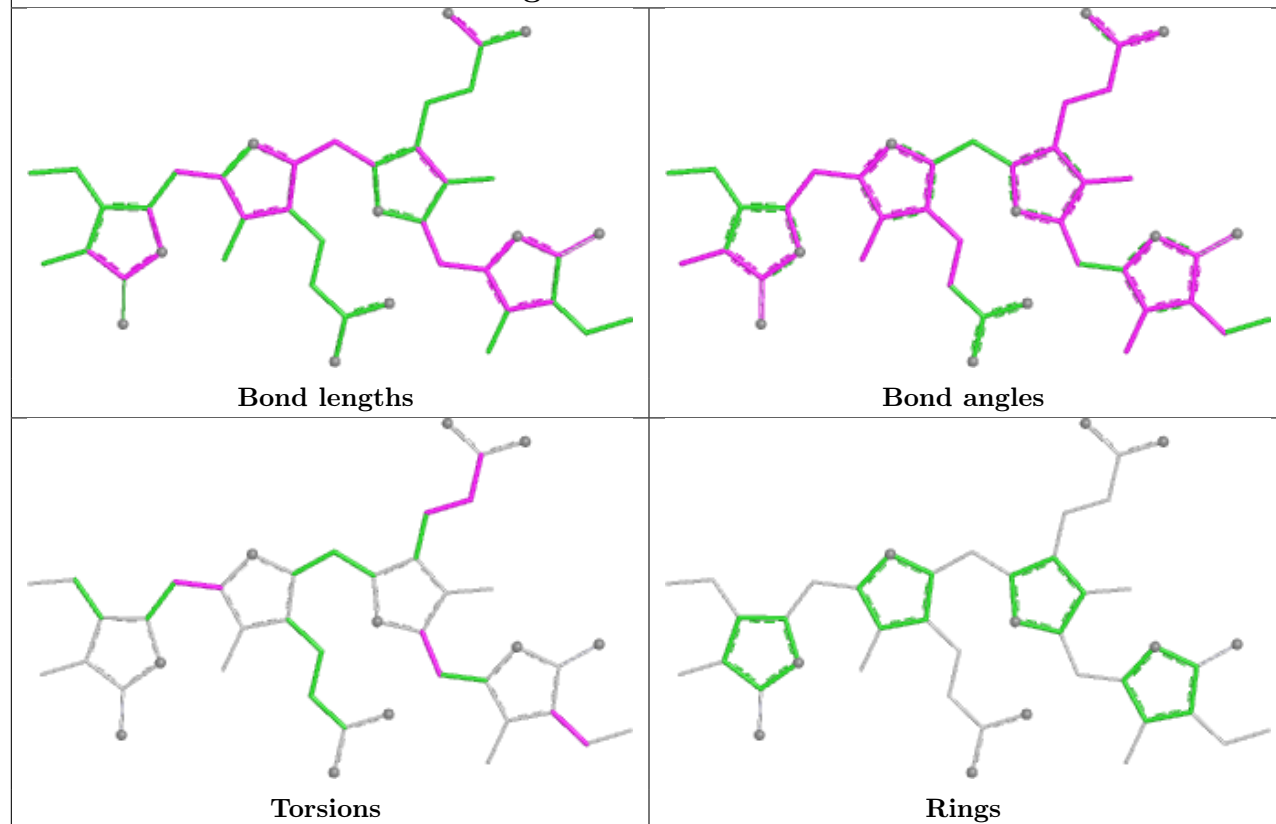
Ligand CYC H9 1001



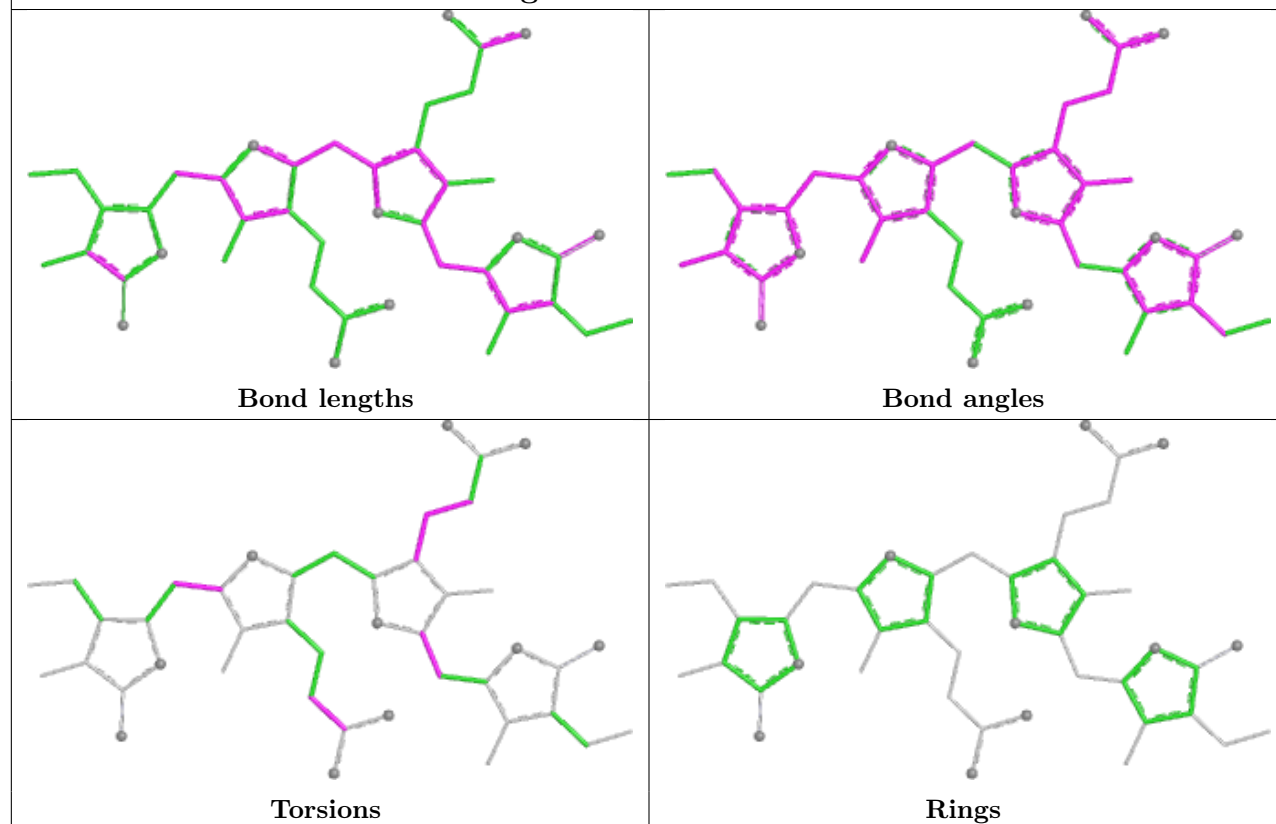
Ligand CYC D6 1001



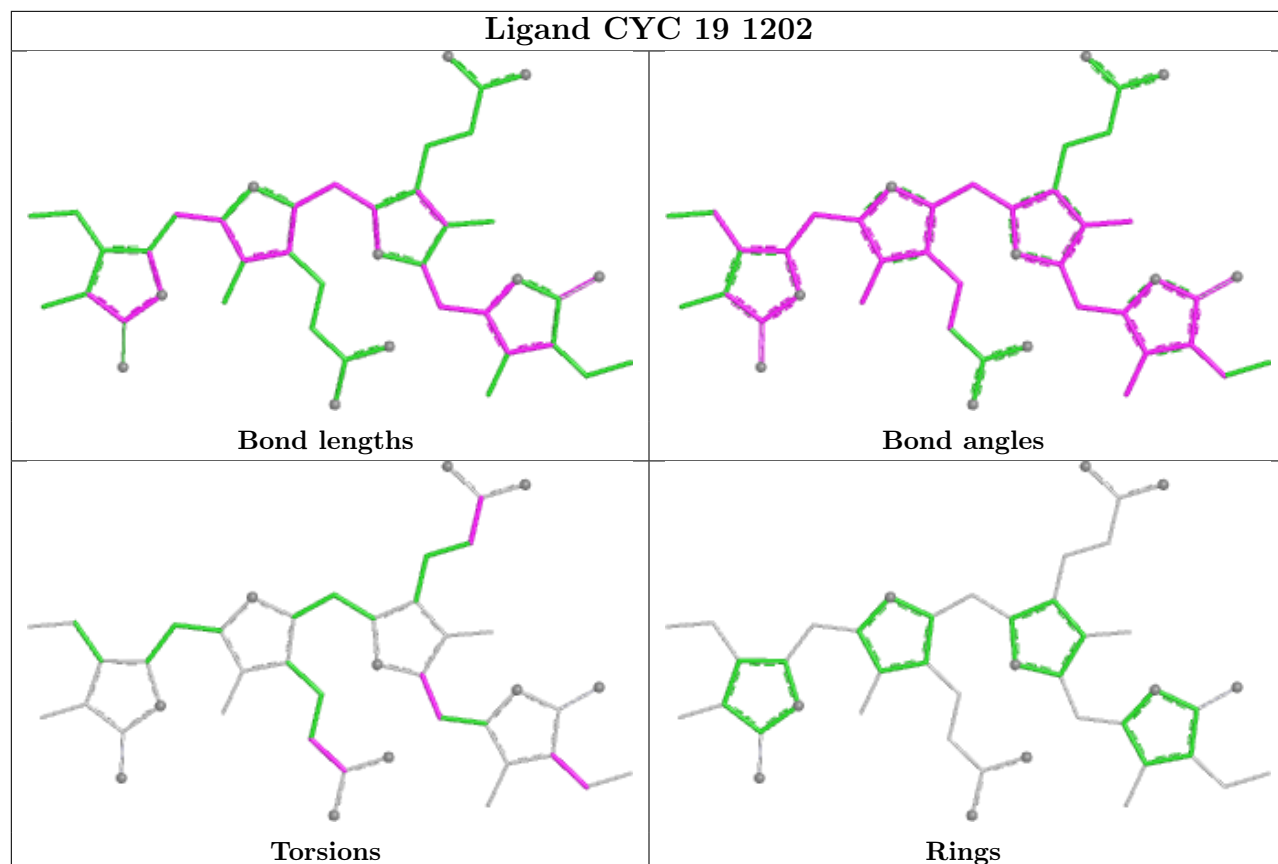
Ligand CYC L7 201



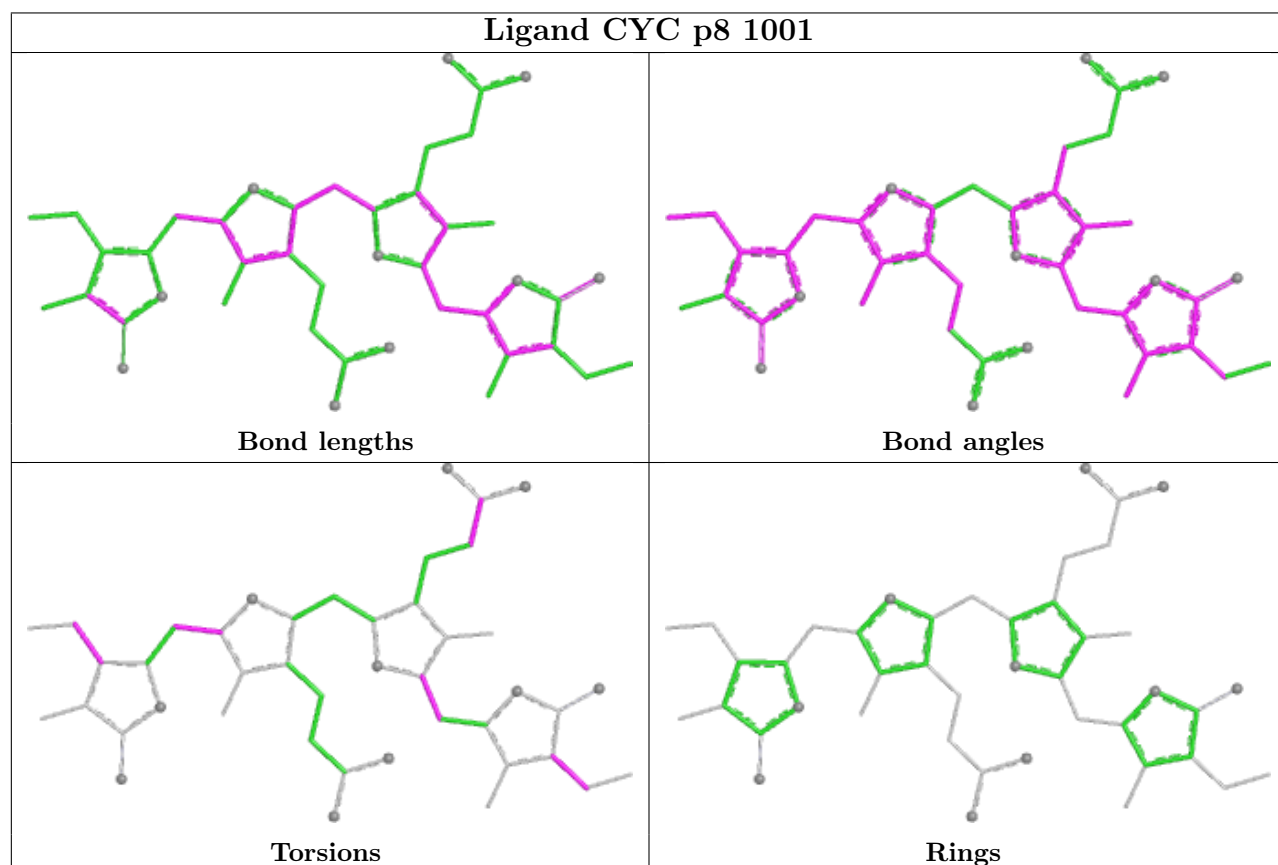
Ligand CYC A5 303

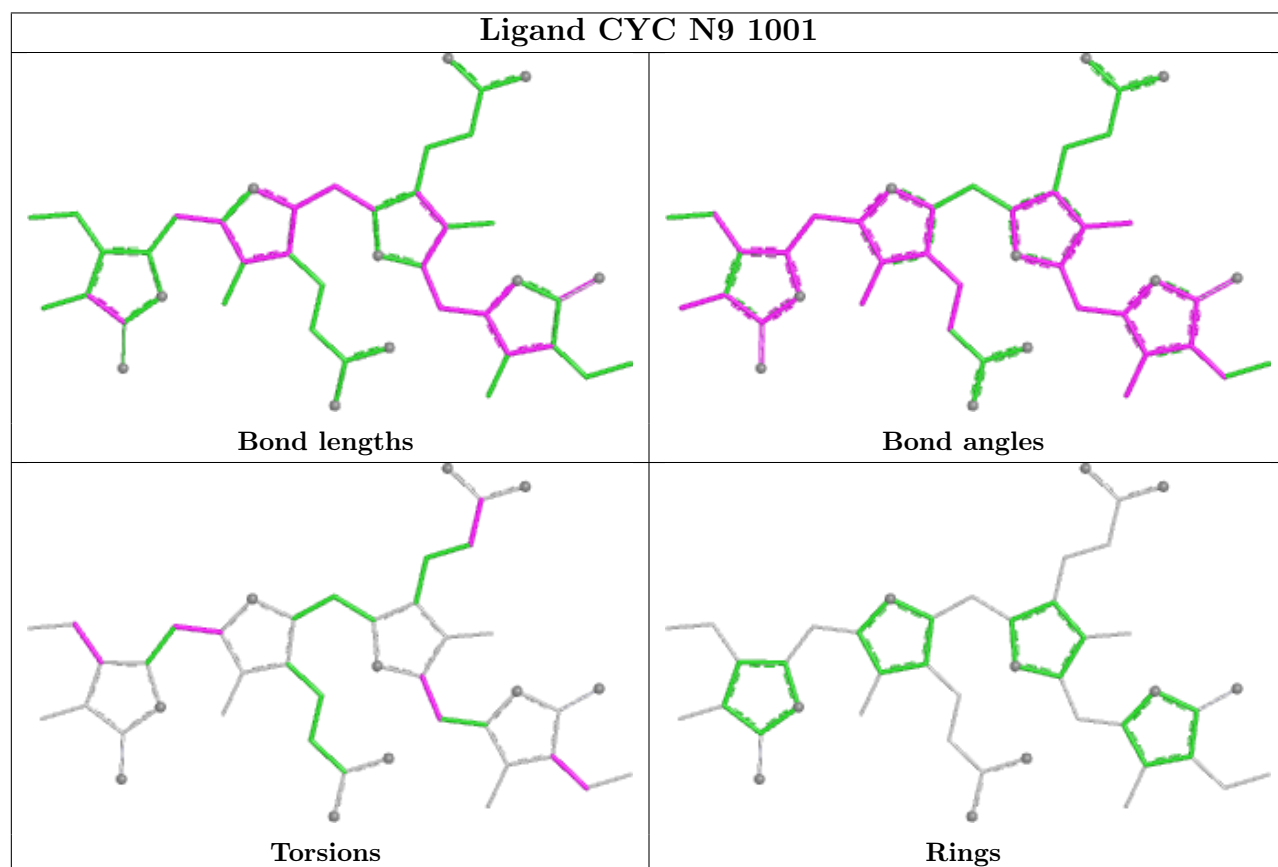
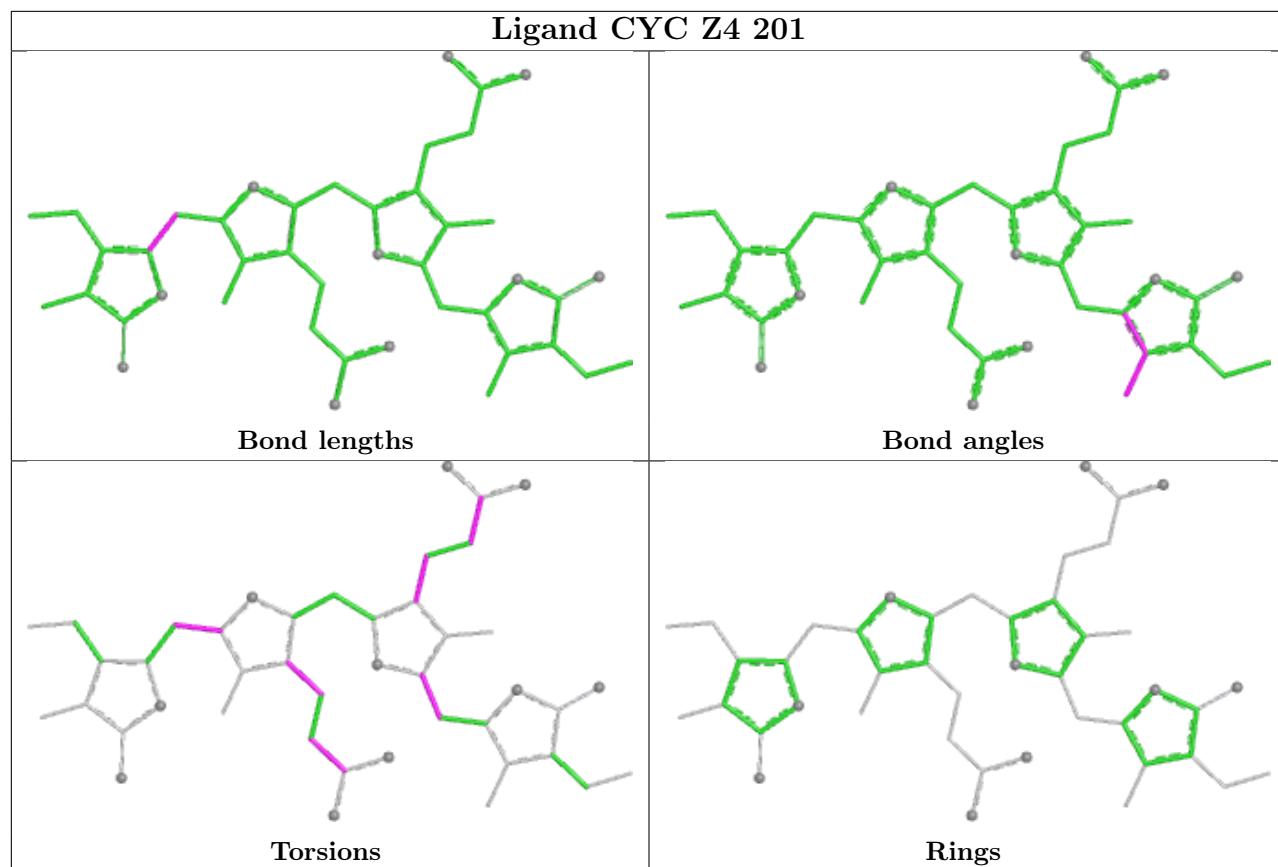


Ligand CYC 19 1202

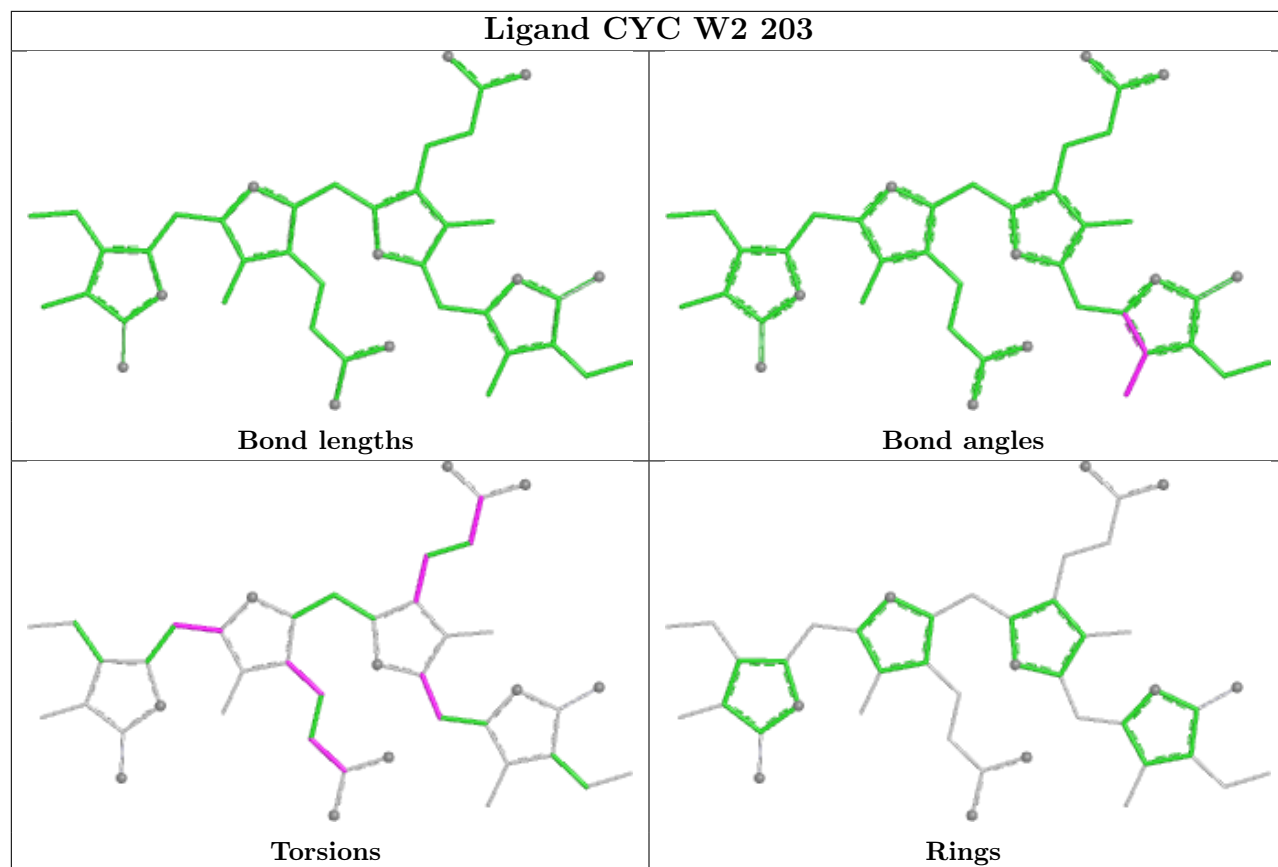


Ligand CYC p8 1001

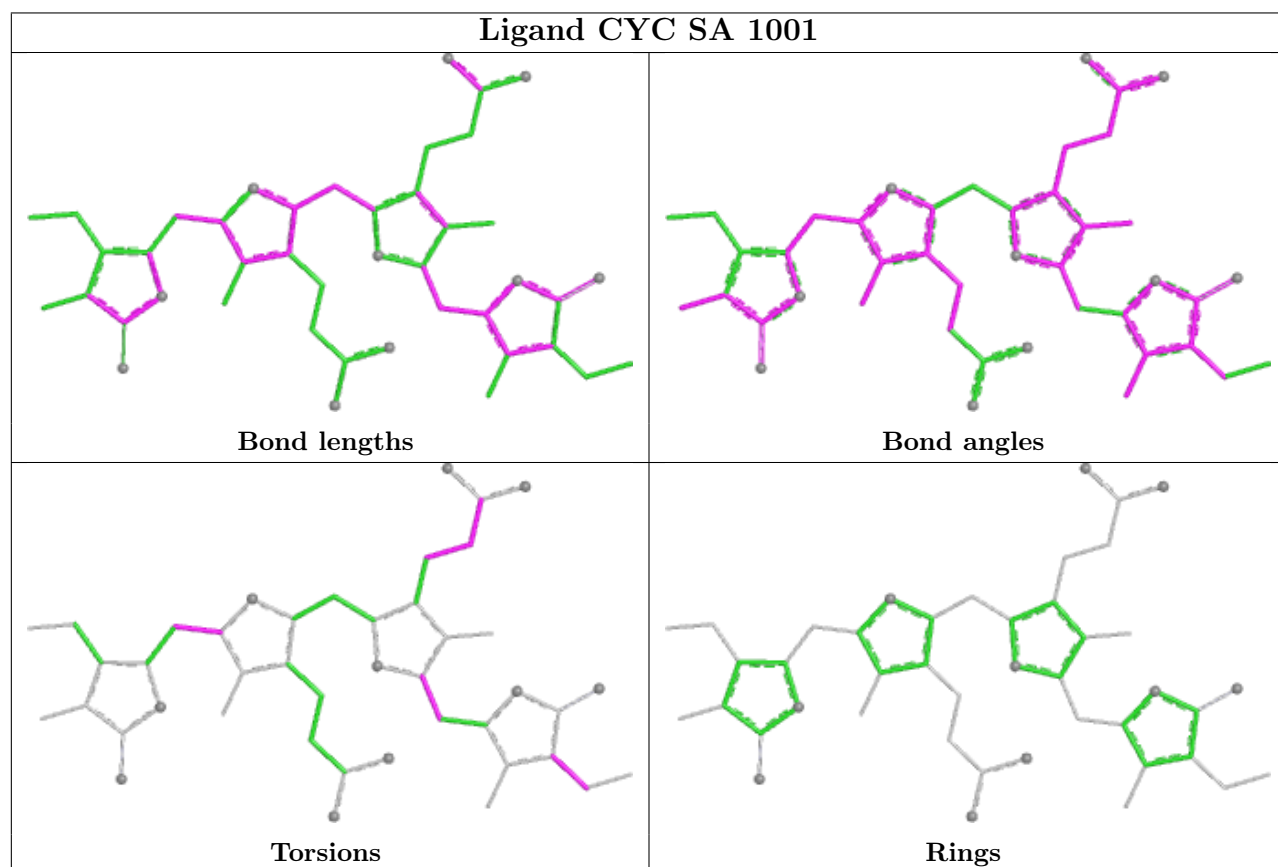




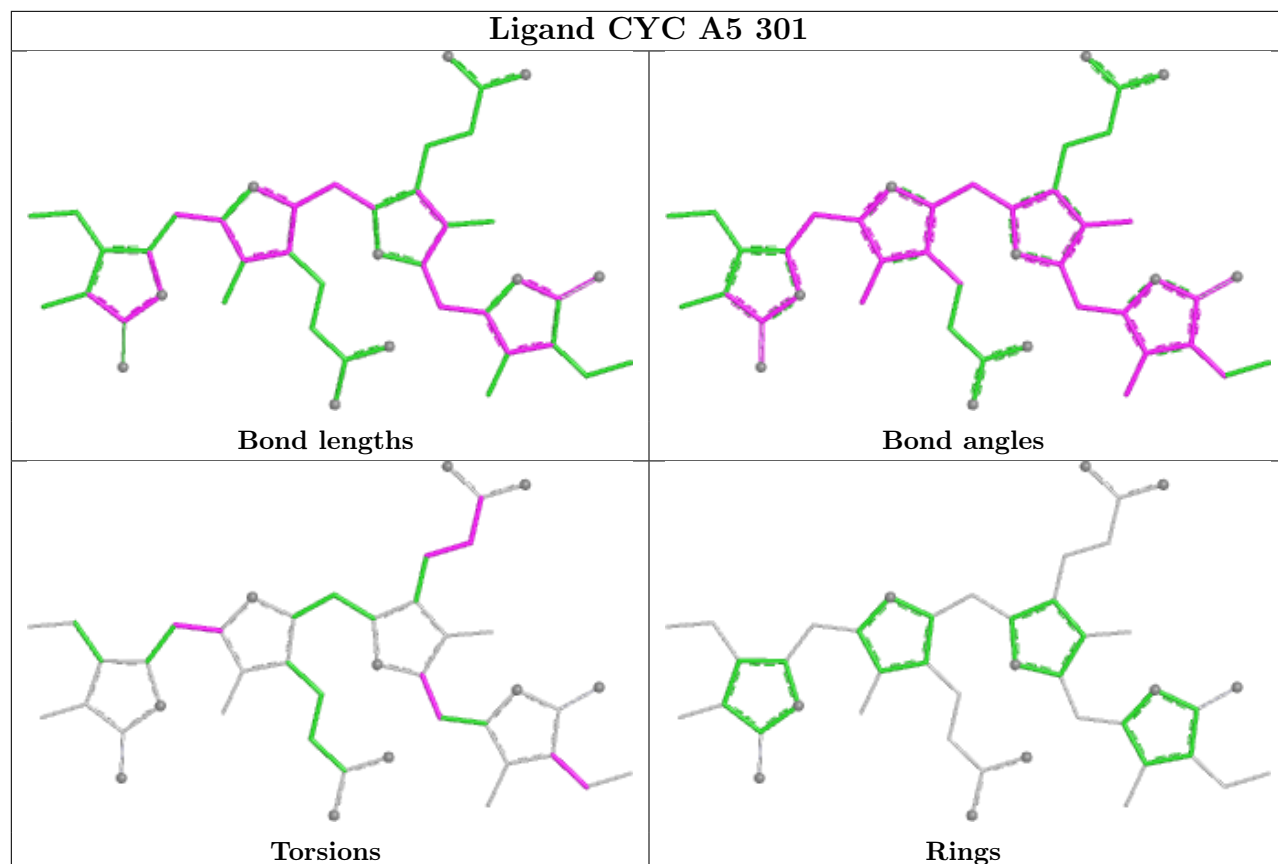
Ligand CYC W2 203



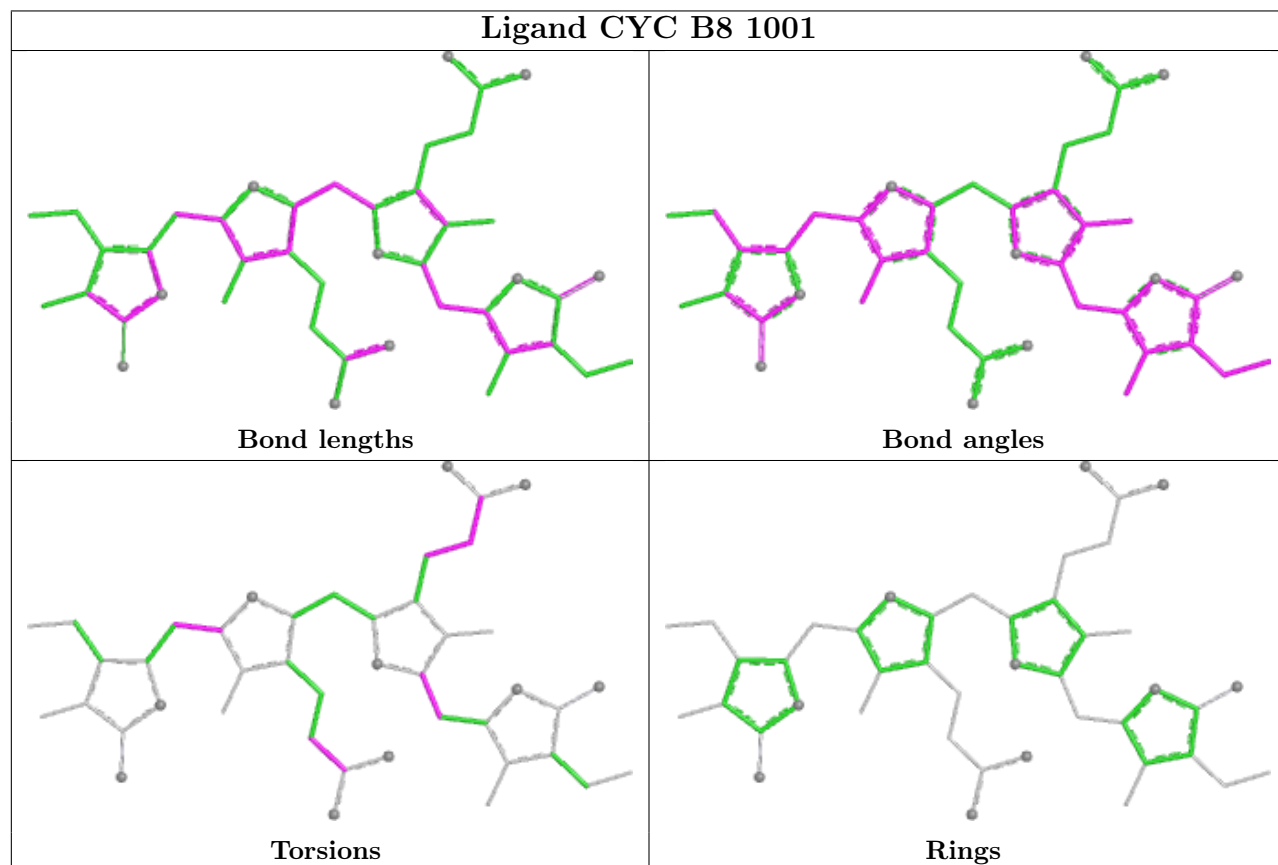
Ligand CYC SA 1001



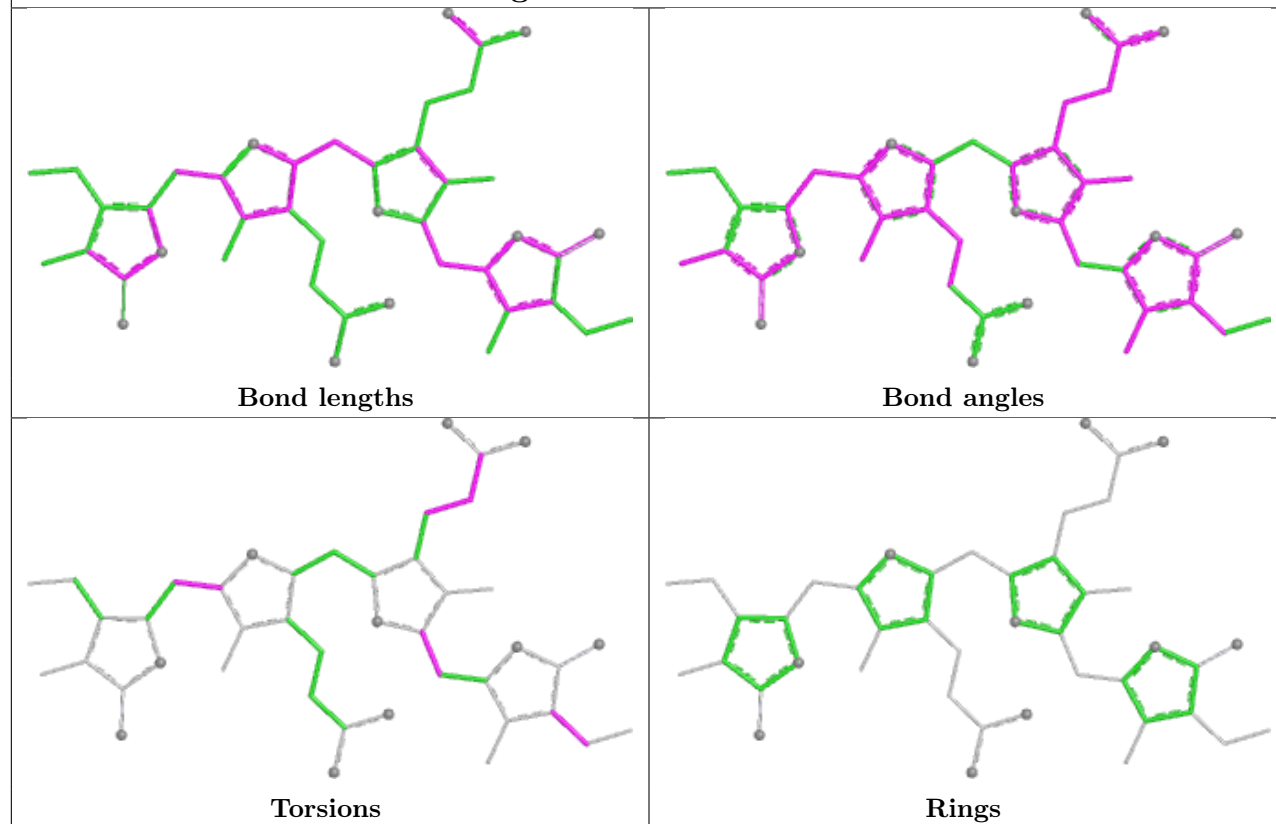
Ligand CYC A5 301



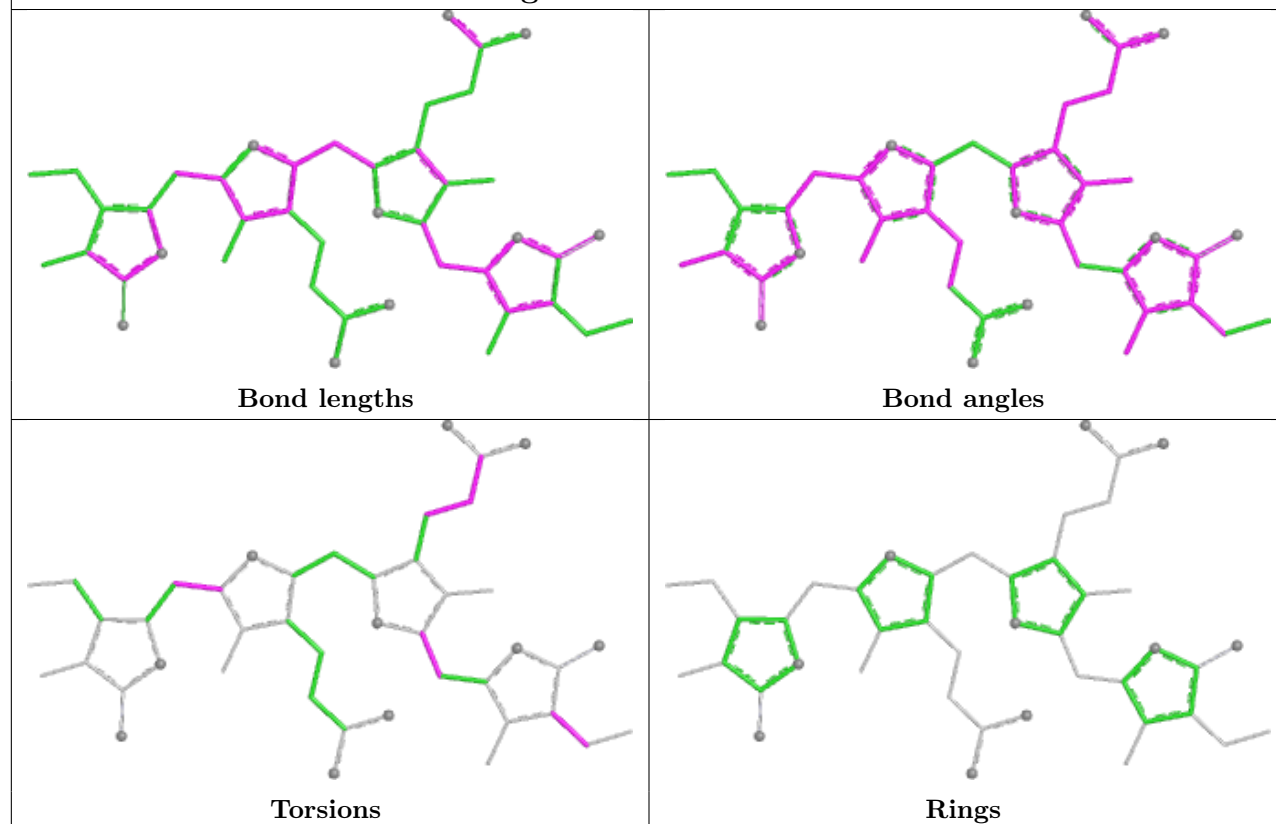
Ligand CYC B8 1001



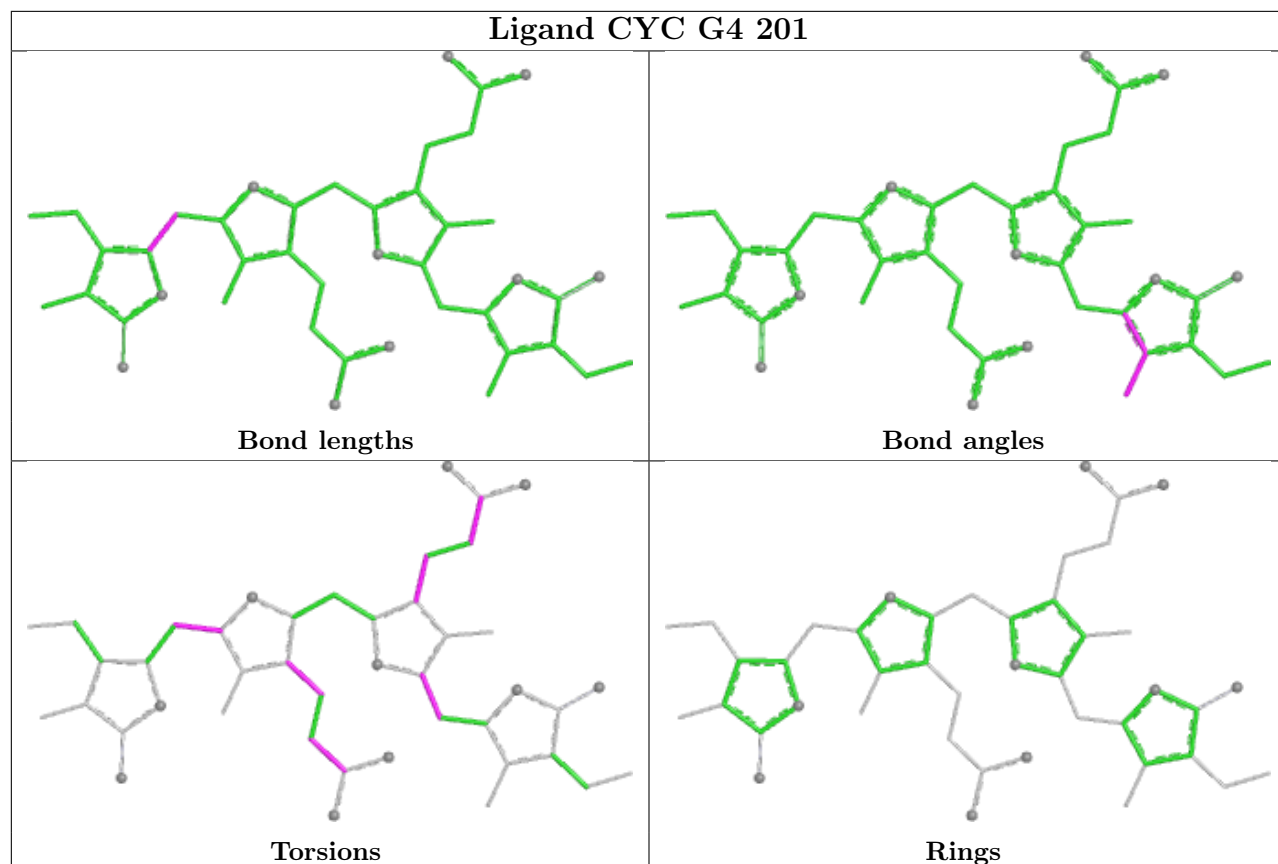
Ligand CYC H3 1001



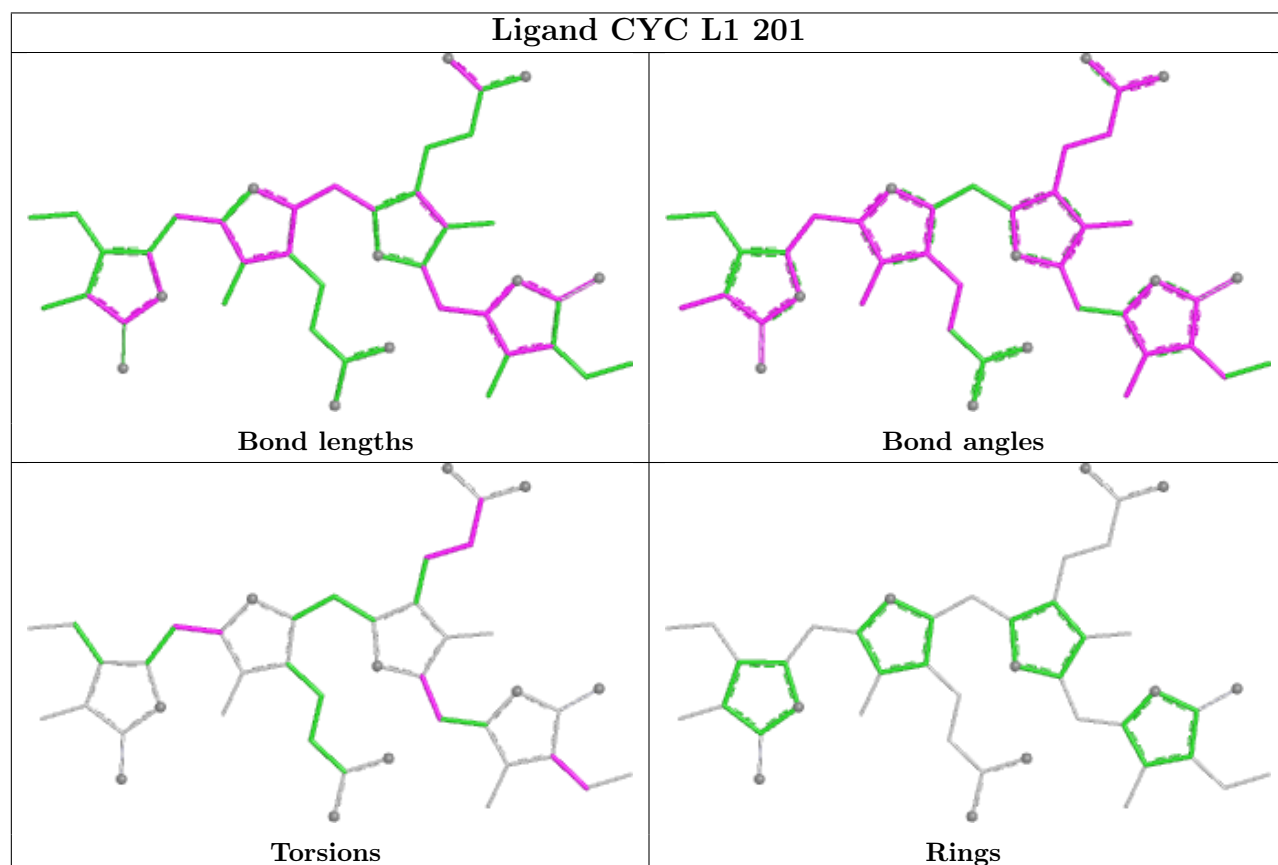
Ligand CYC C4 301



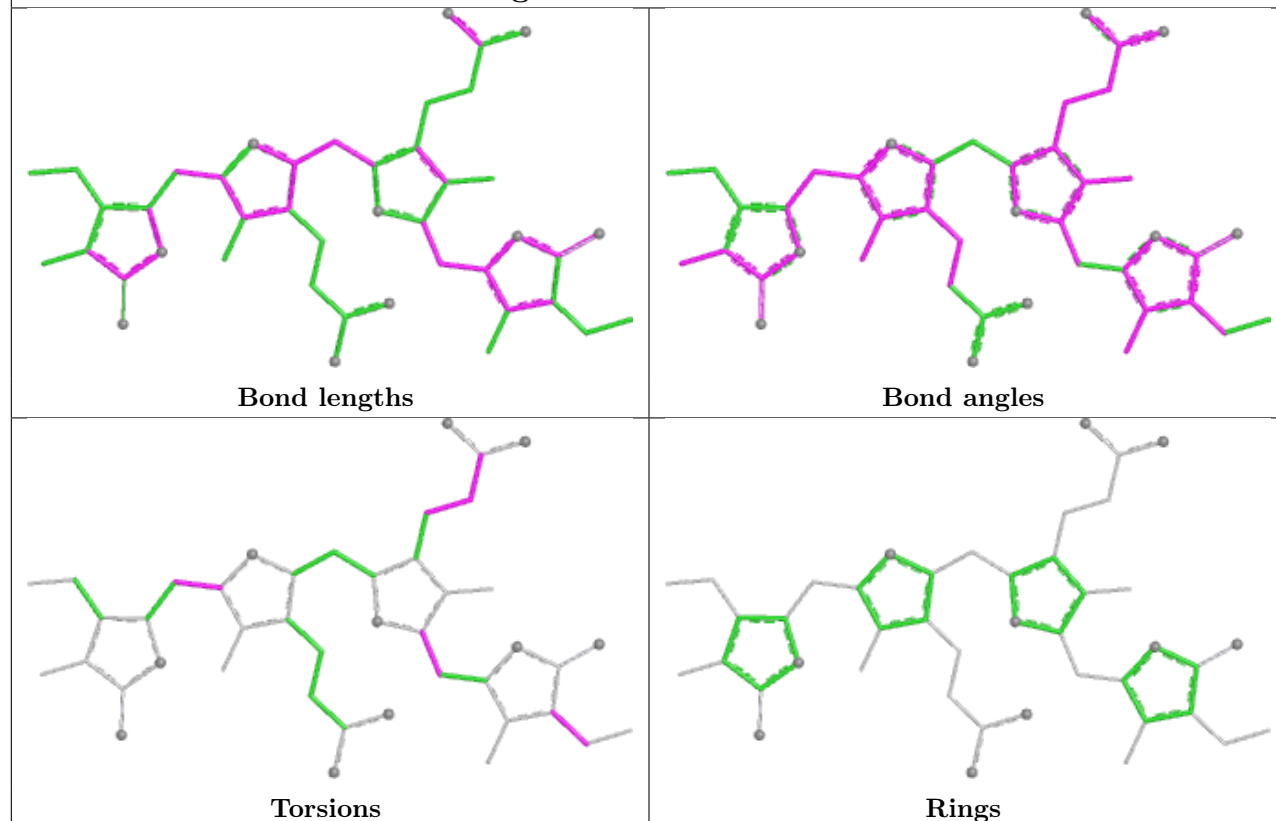
Ligand CYC G4 201



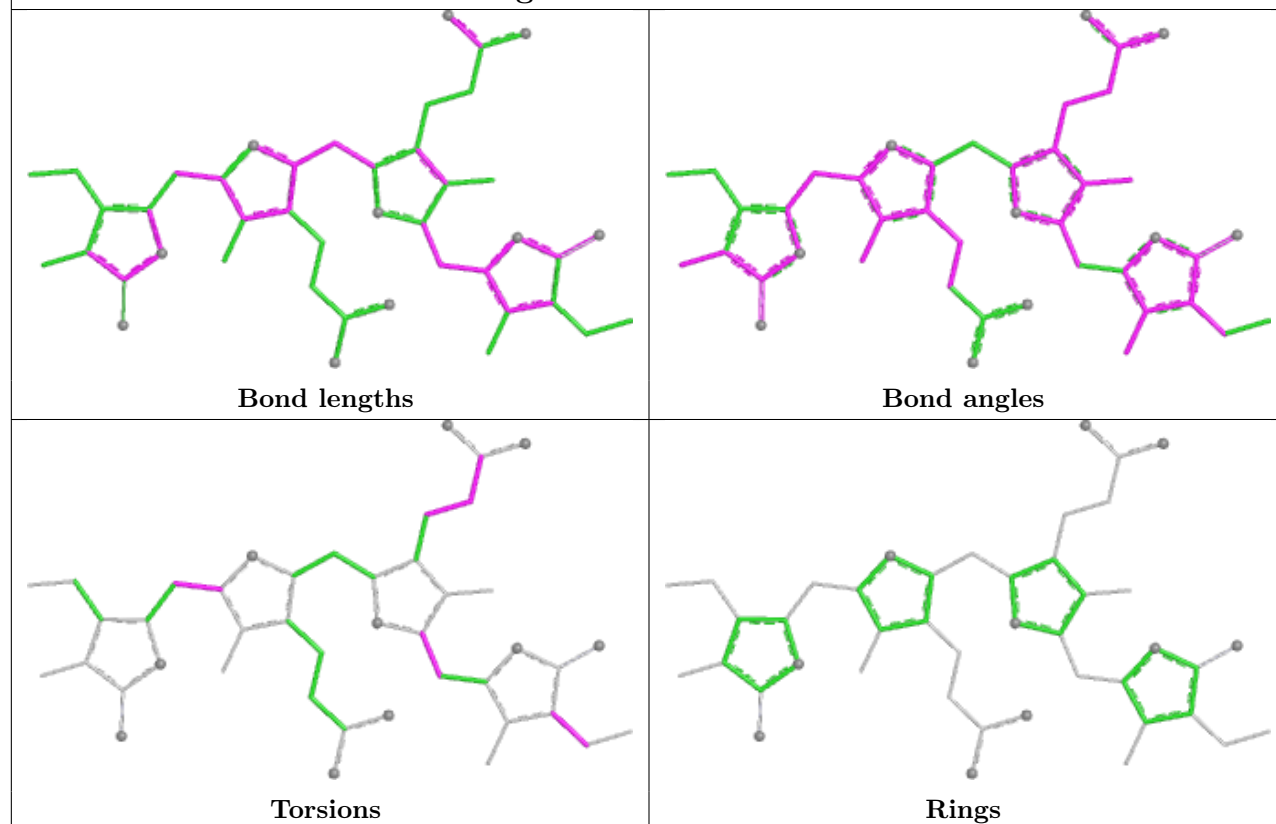
Ligand CYC L1 201



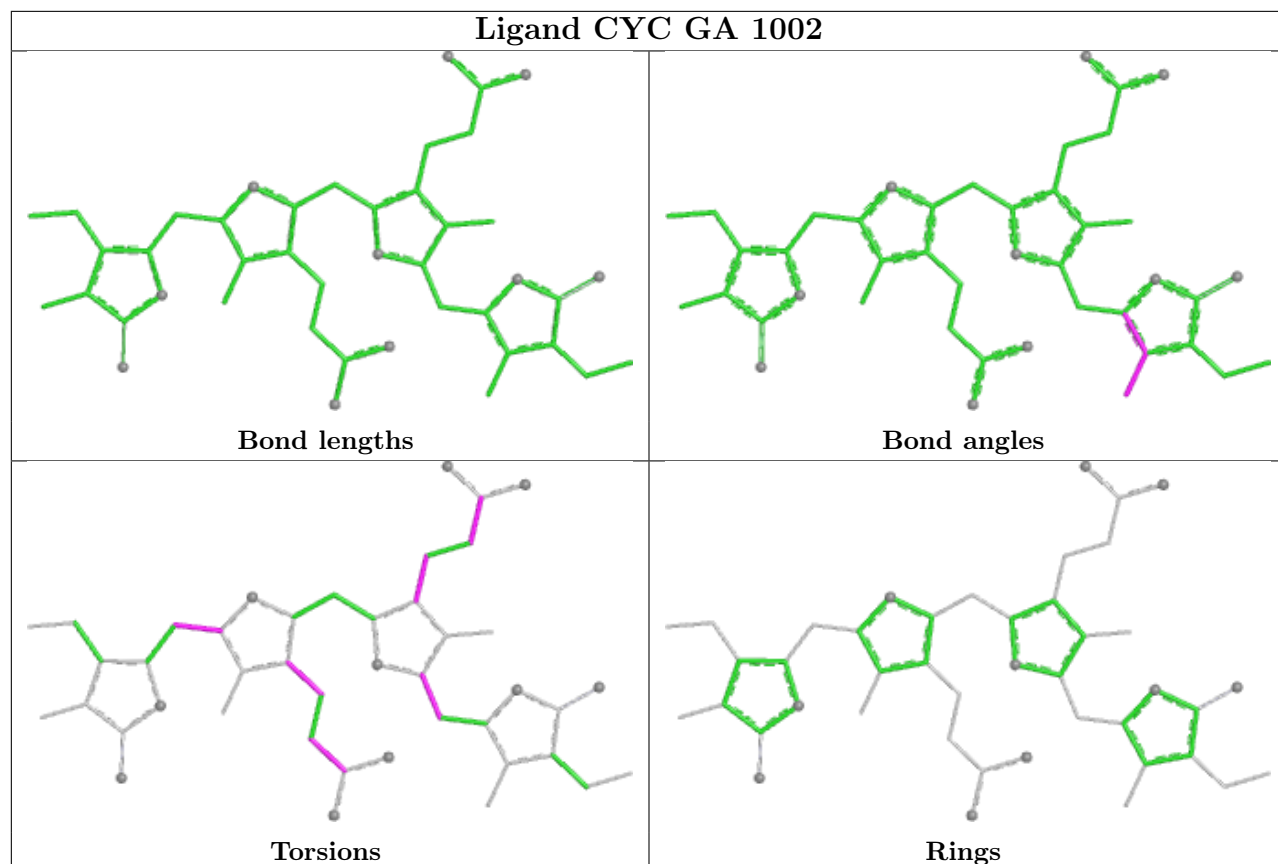
Ligand CYC R1 1001



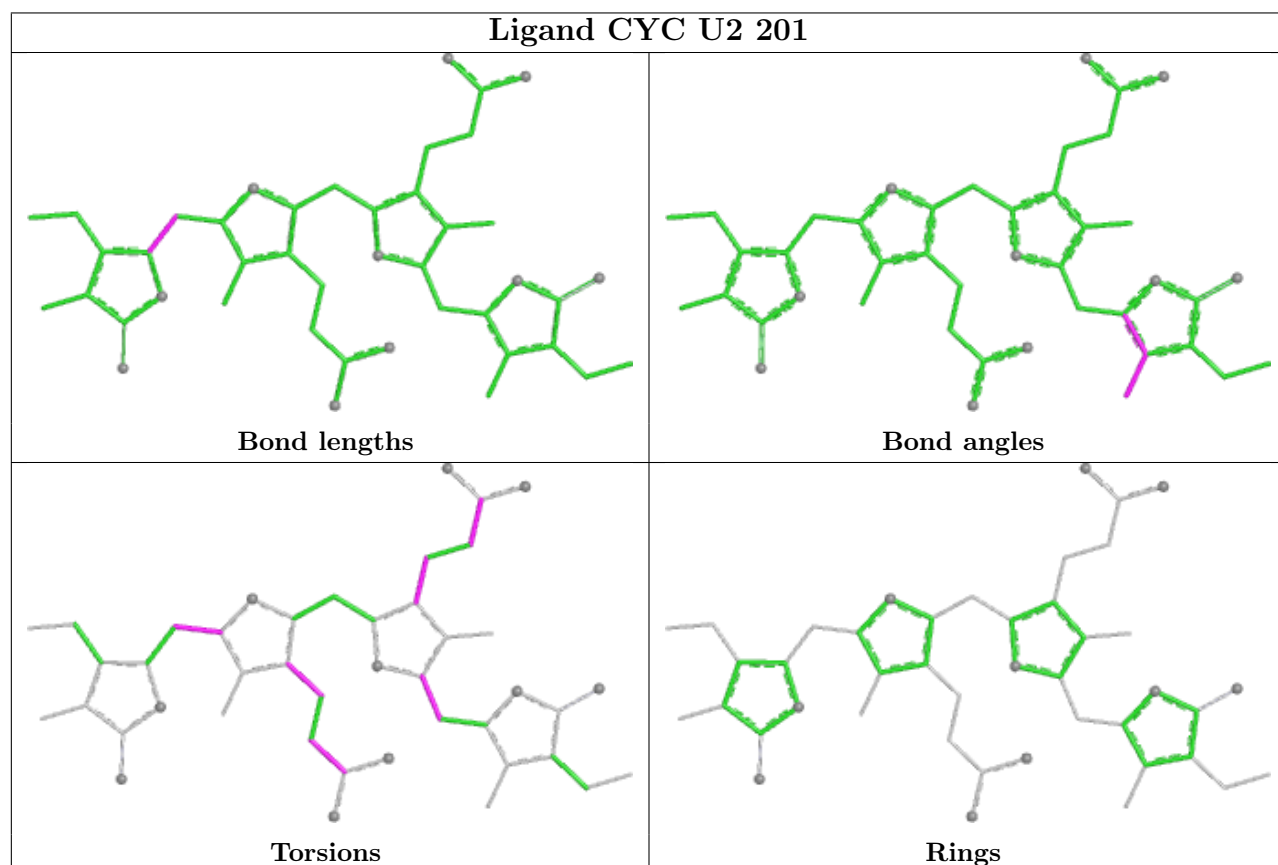
Ligand CYC J4 1001



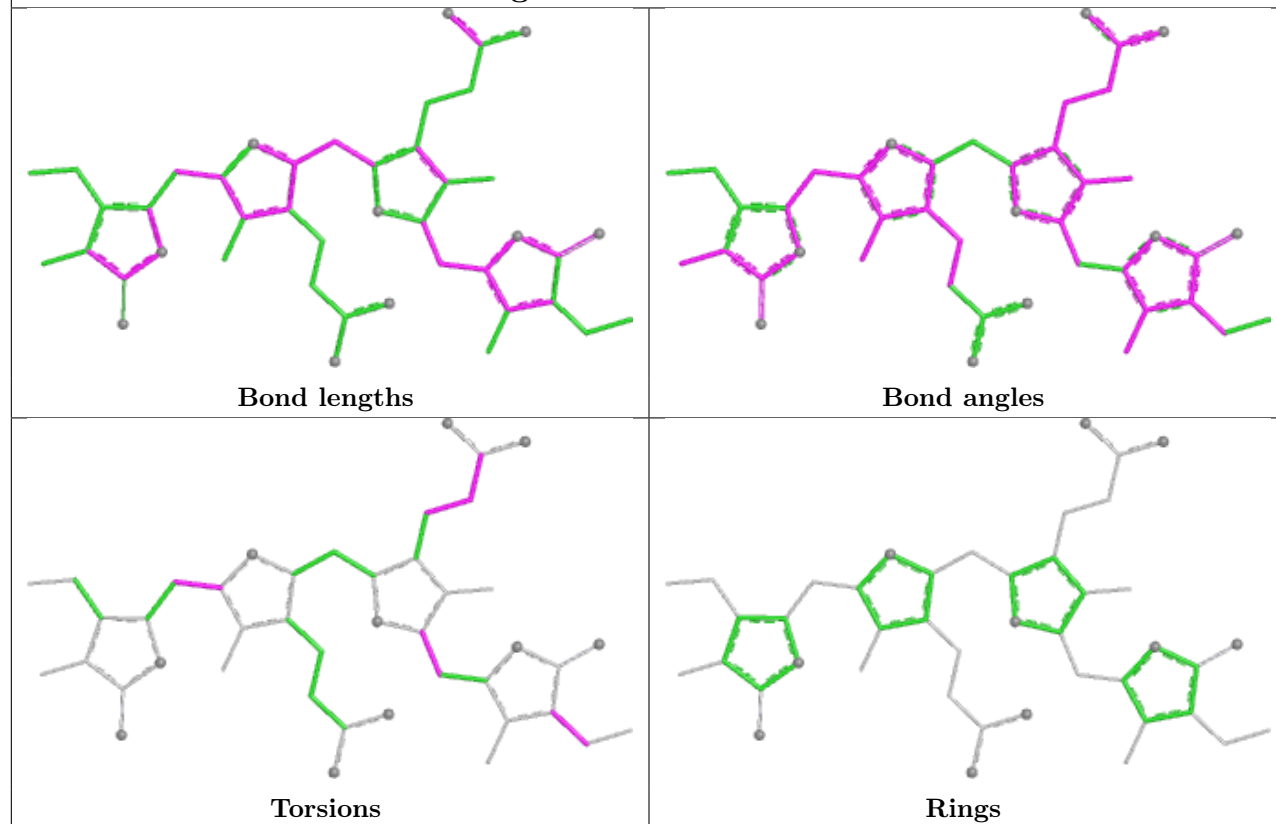
Ligand CYC GA 1002



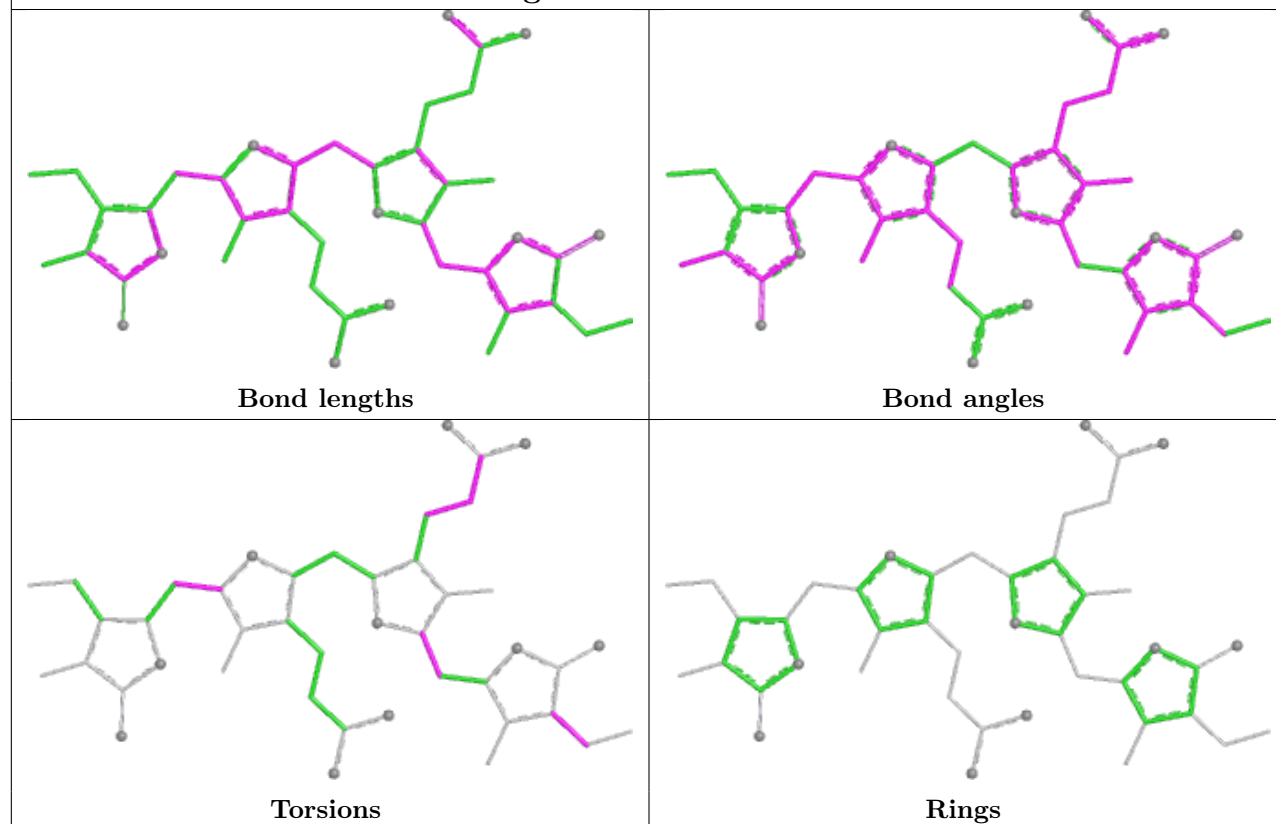
Ligand CYC U2 201

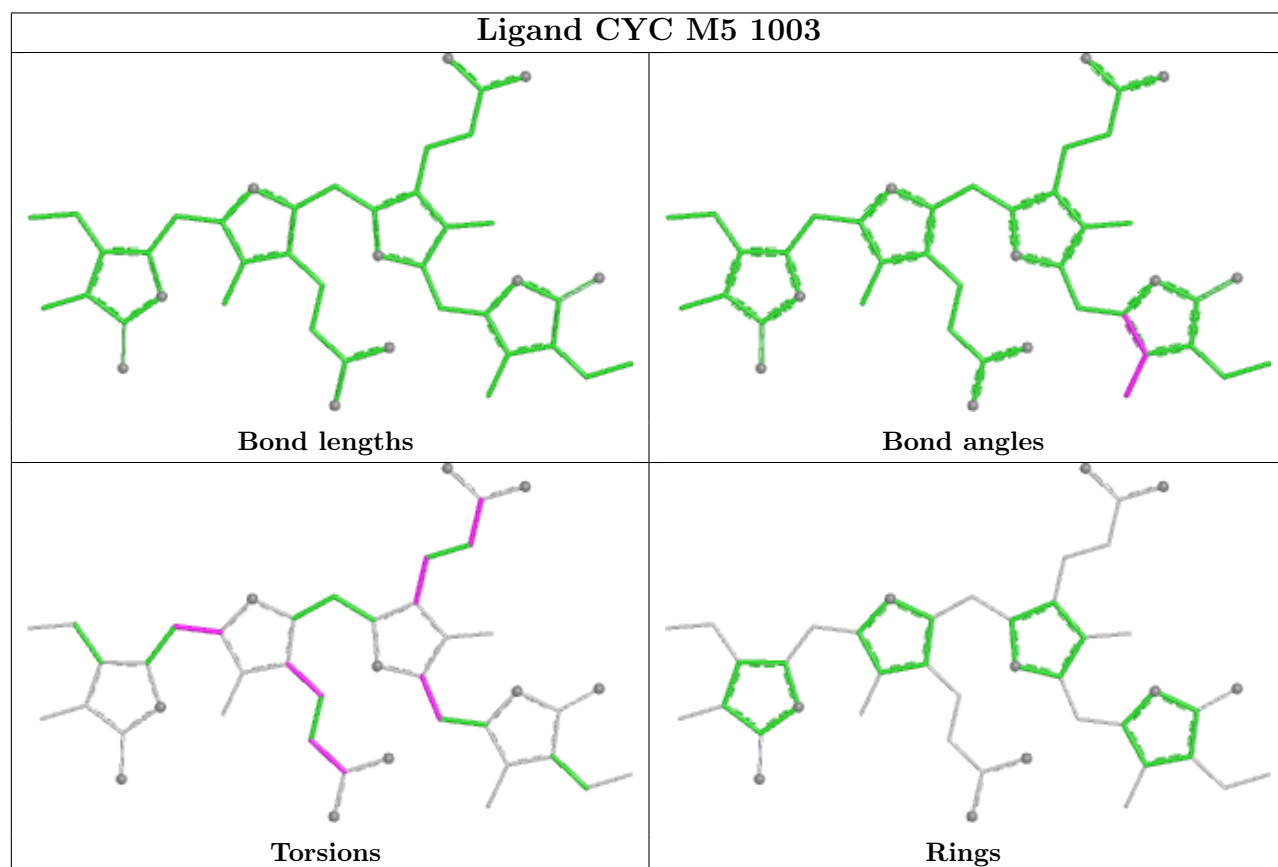
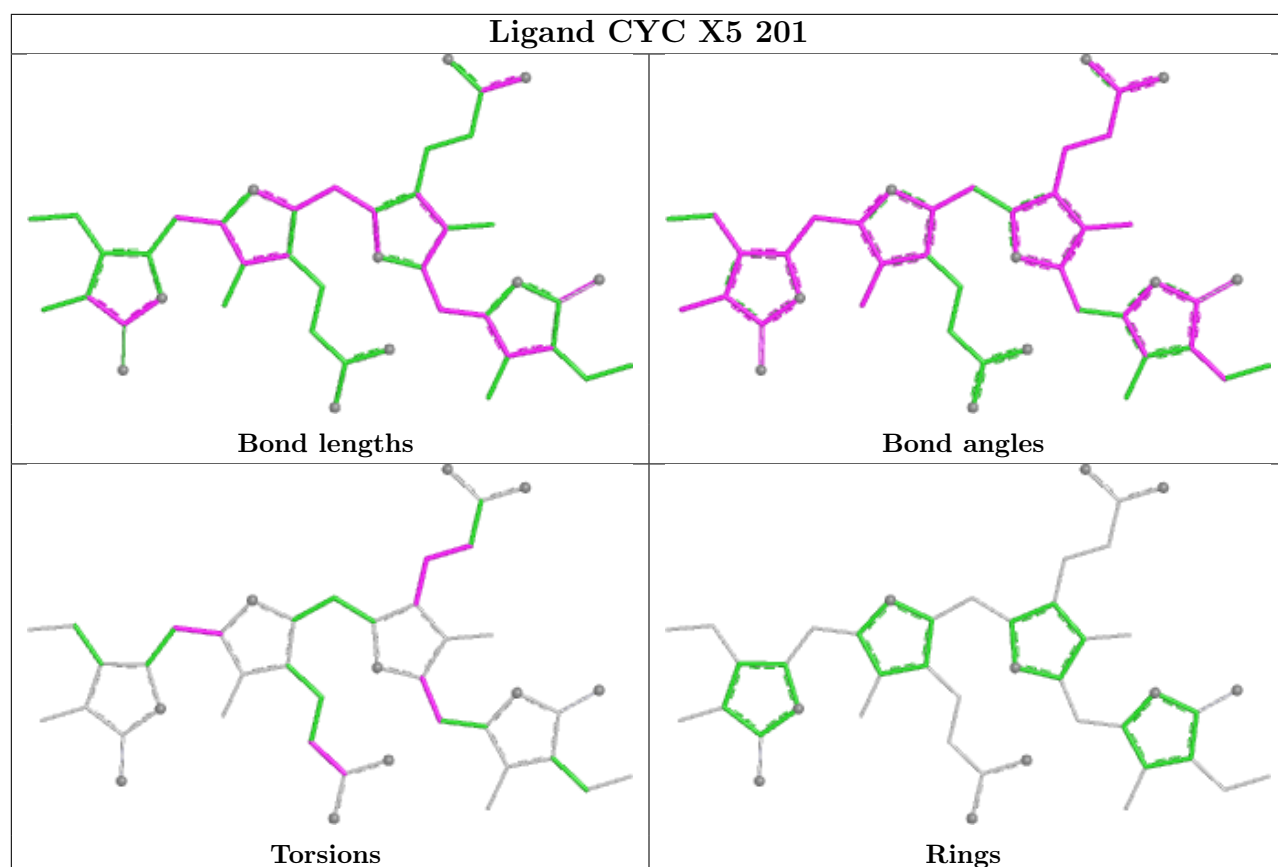


Ligand CYC H4 1001

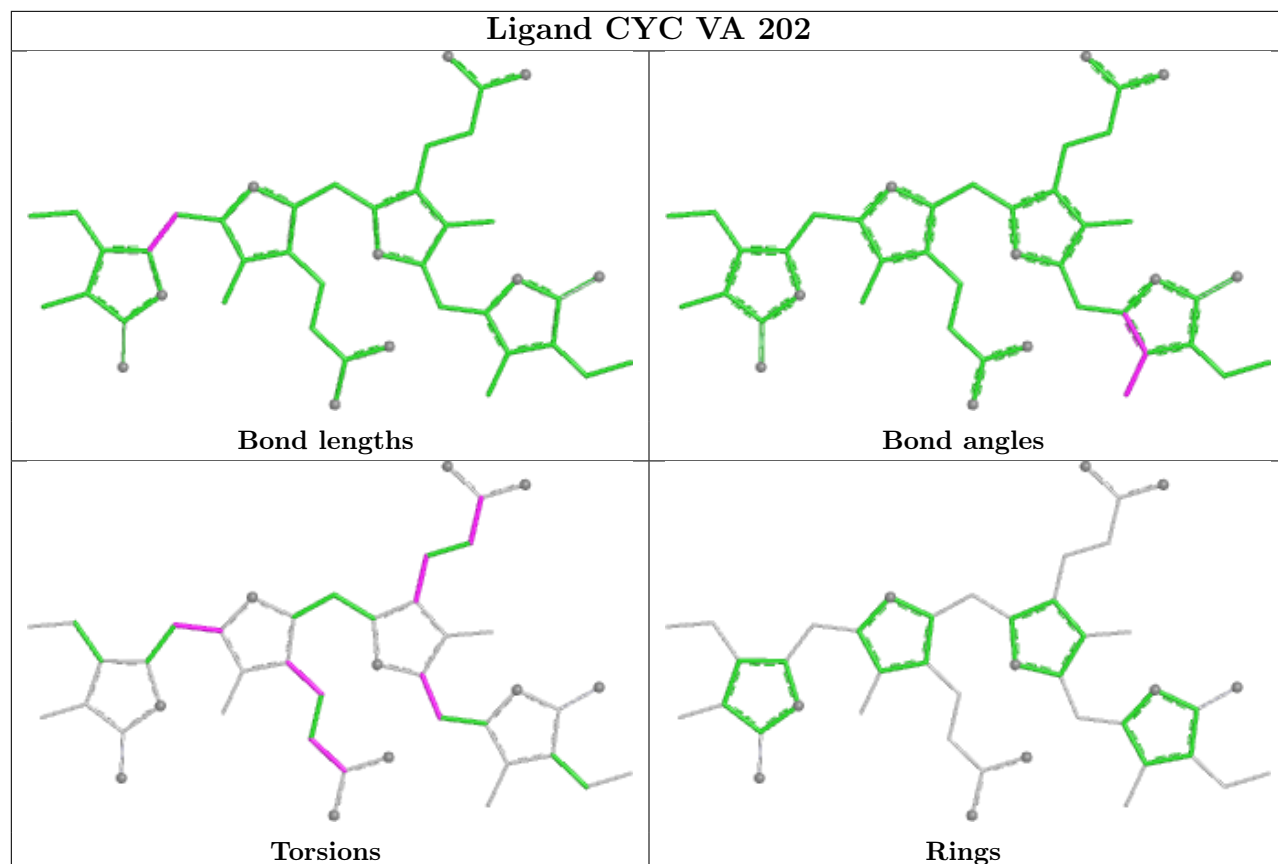


Ligand CYC L4 201

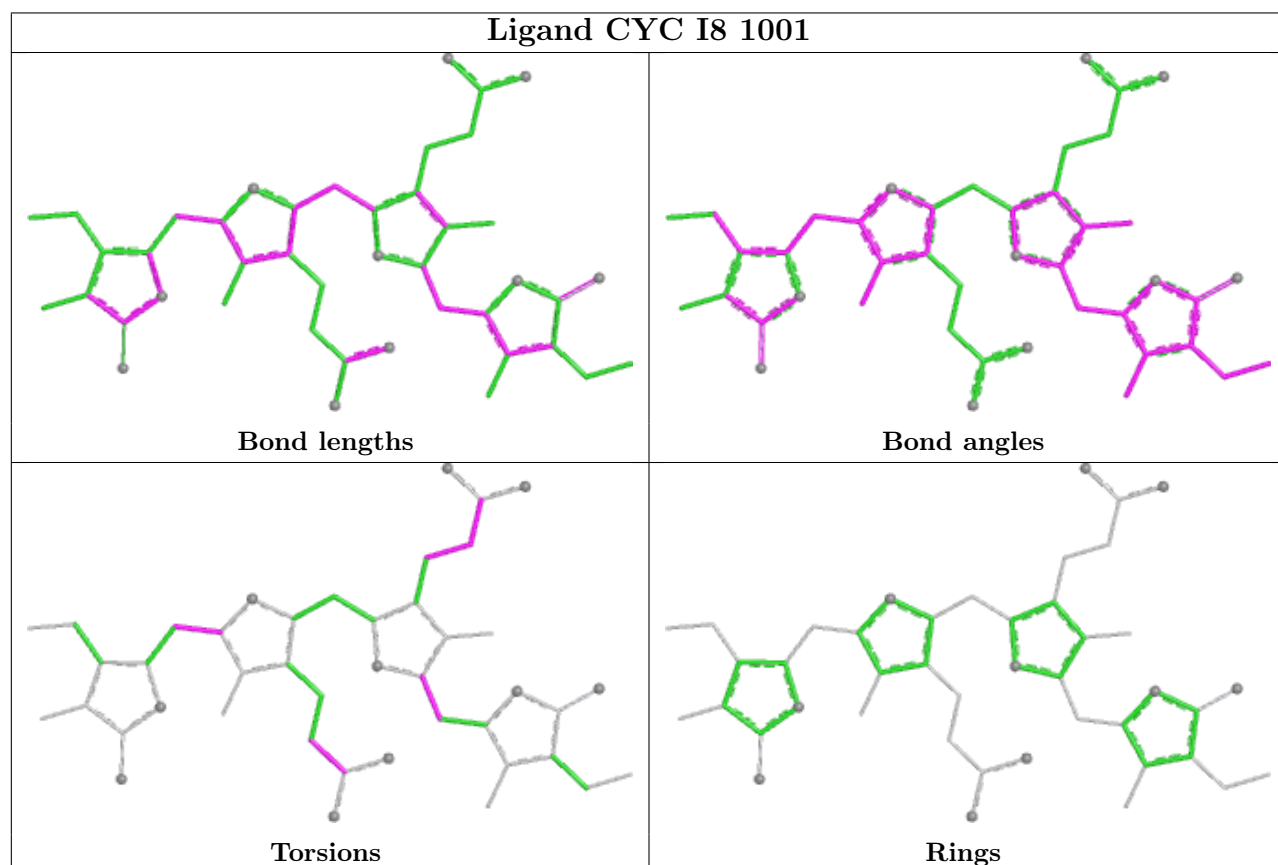




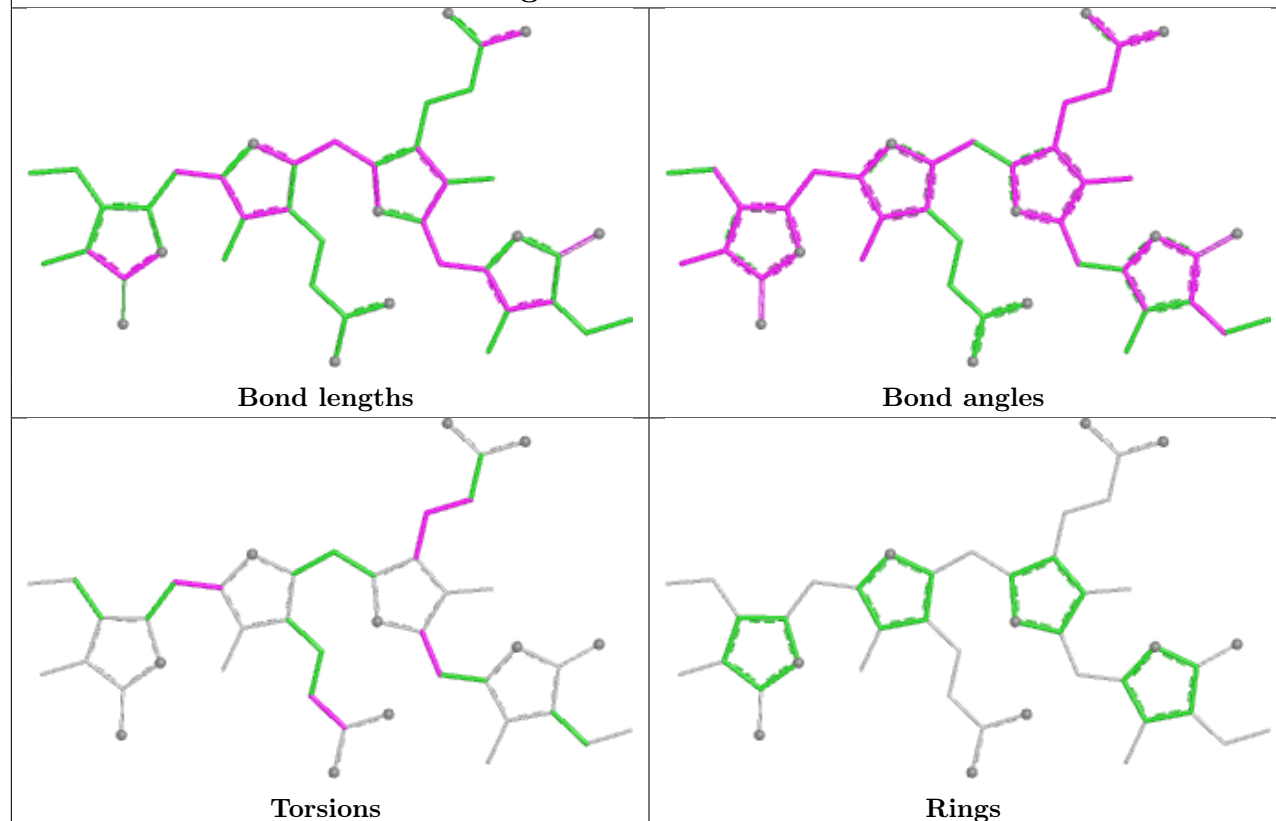
Ligand CYC VA 202



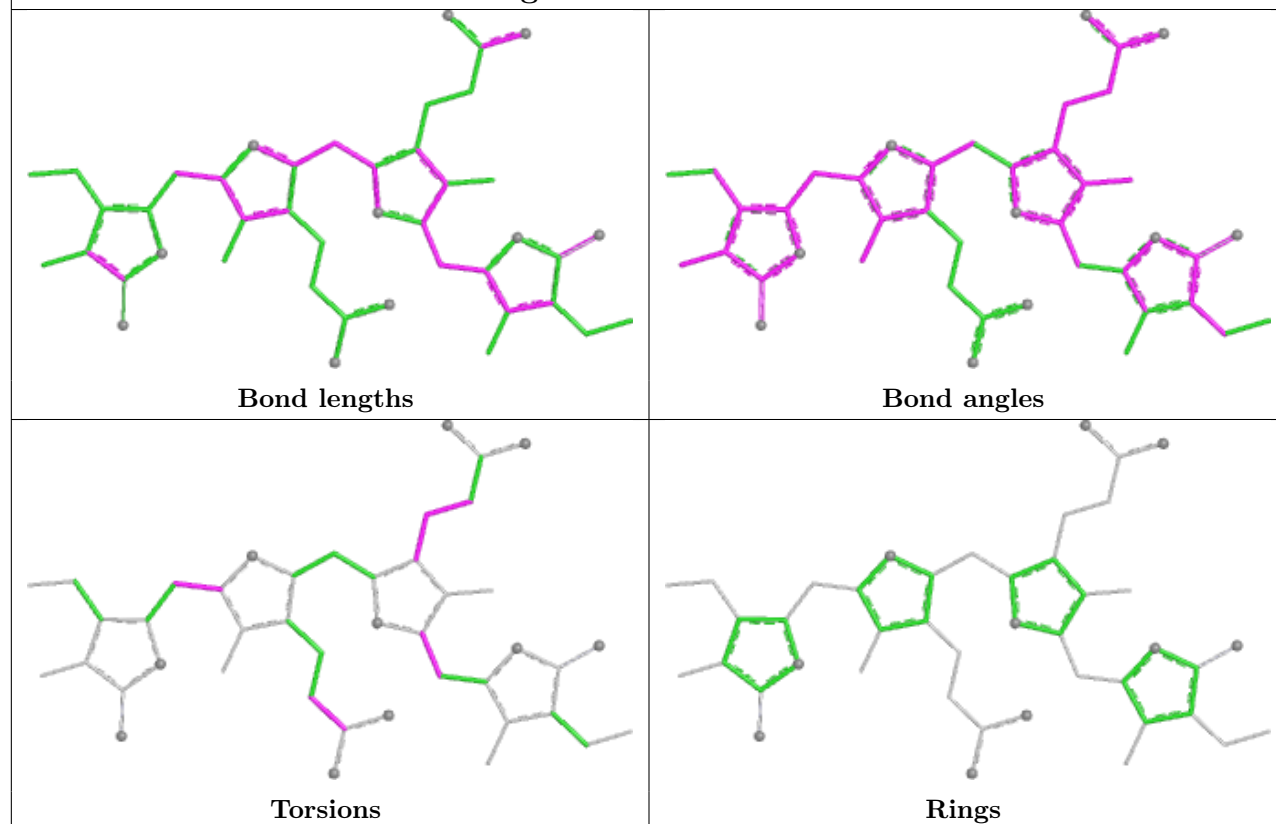
Ligand CYC I8 1001



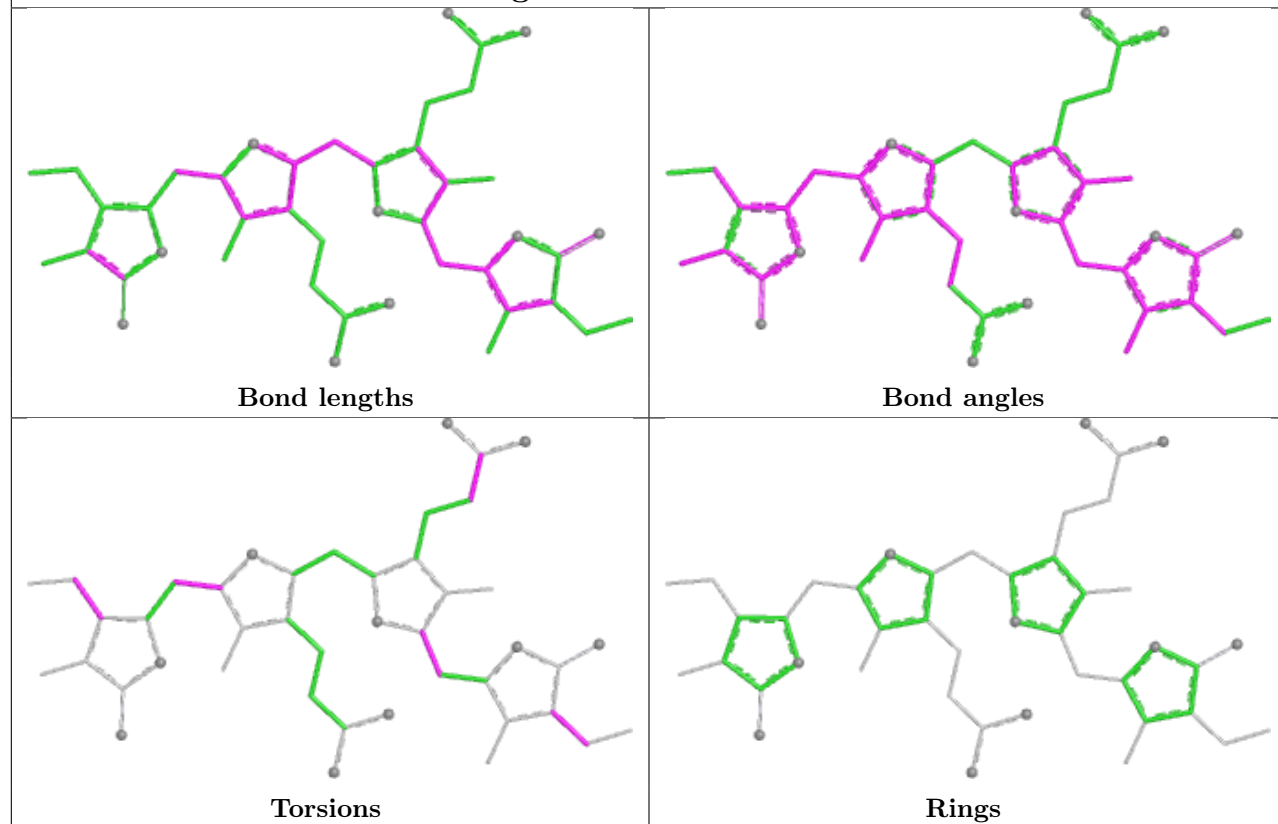
Ligand CYC X1 201



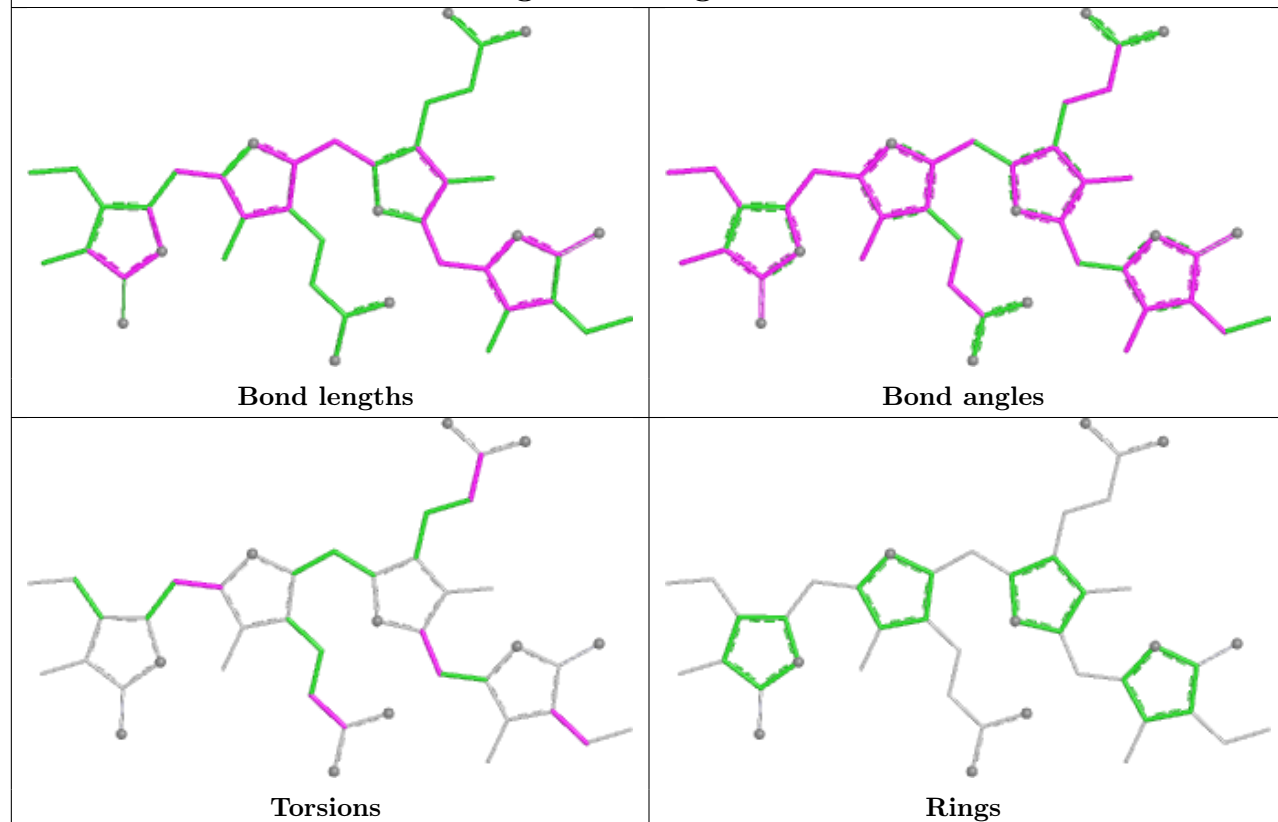
Ligand CYC A5 304

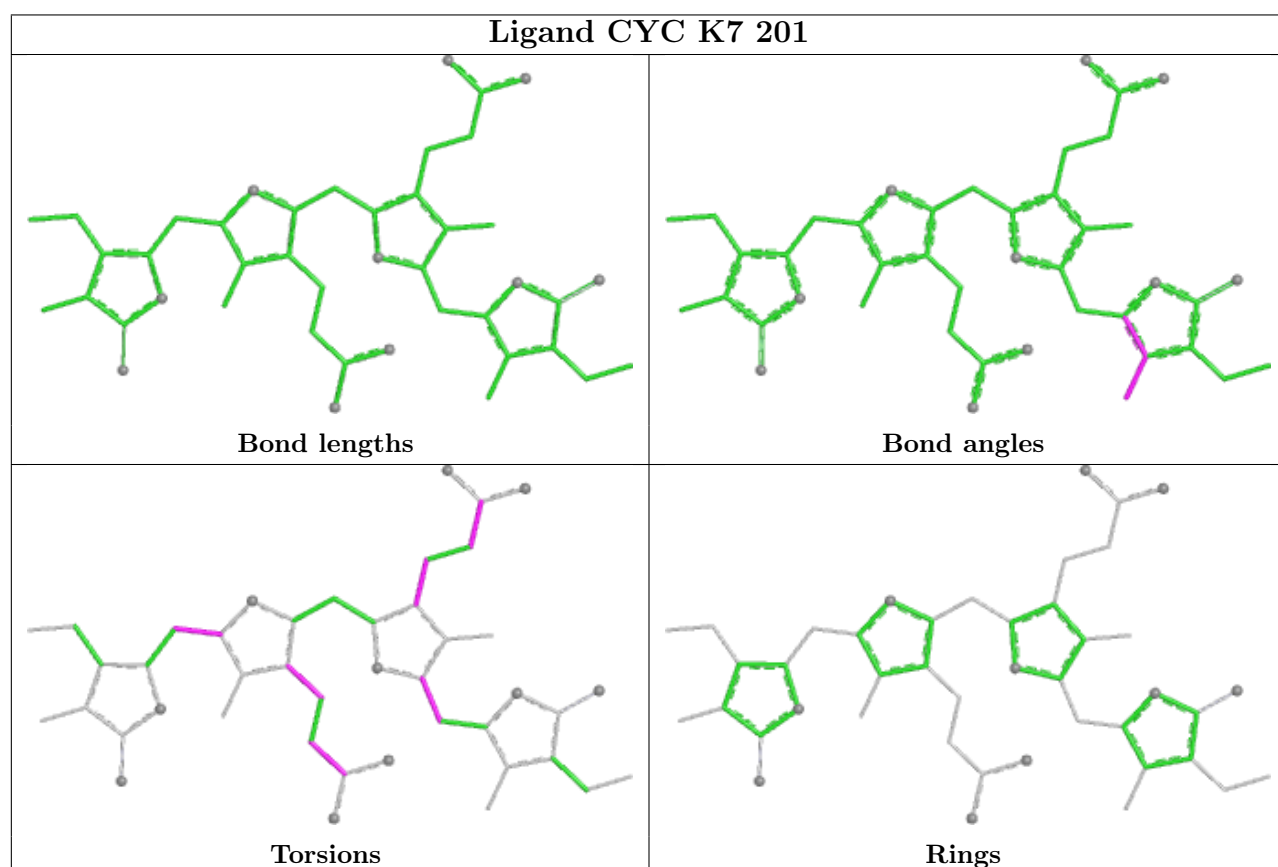
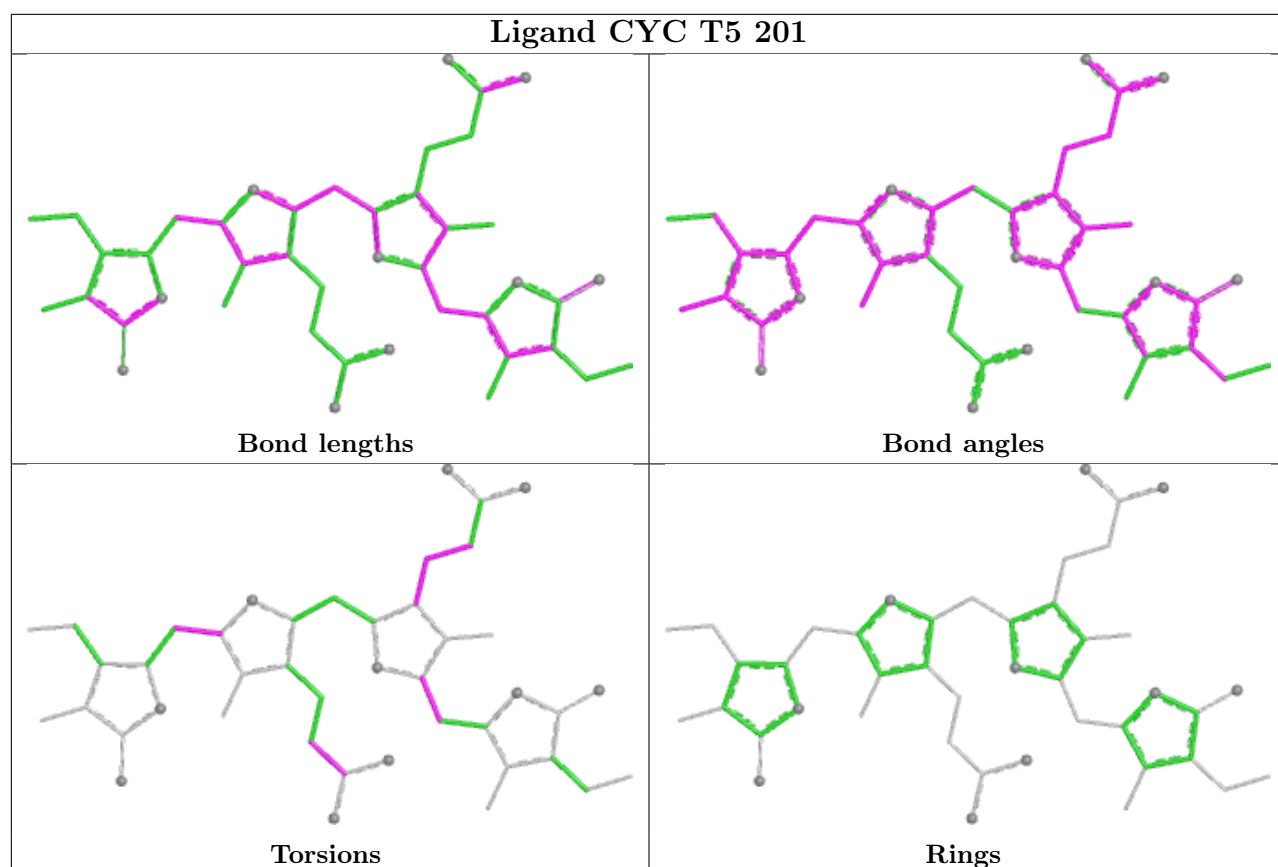


Ligand CYC X9 1001

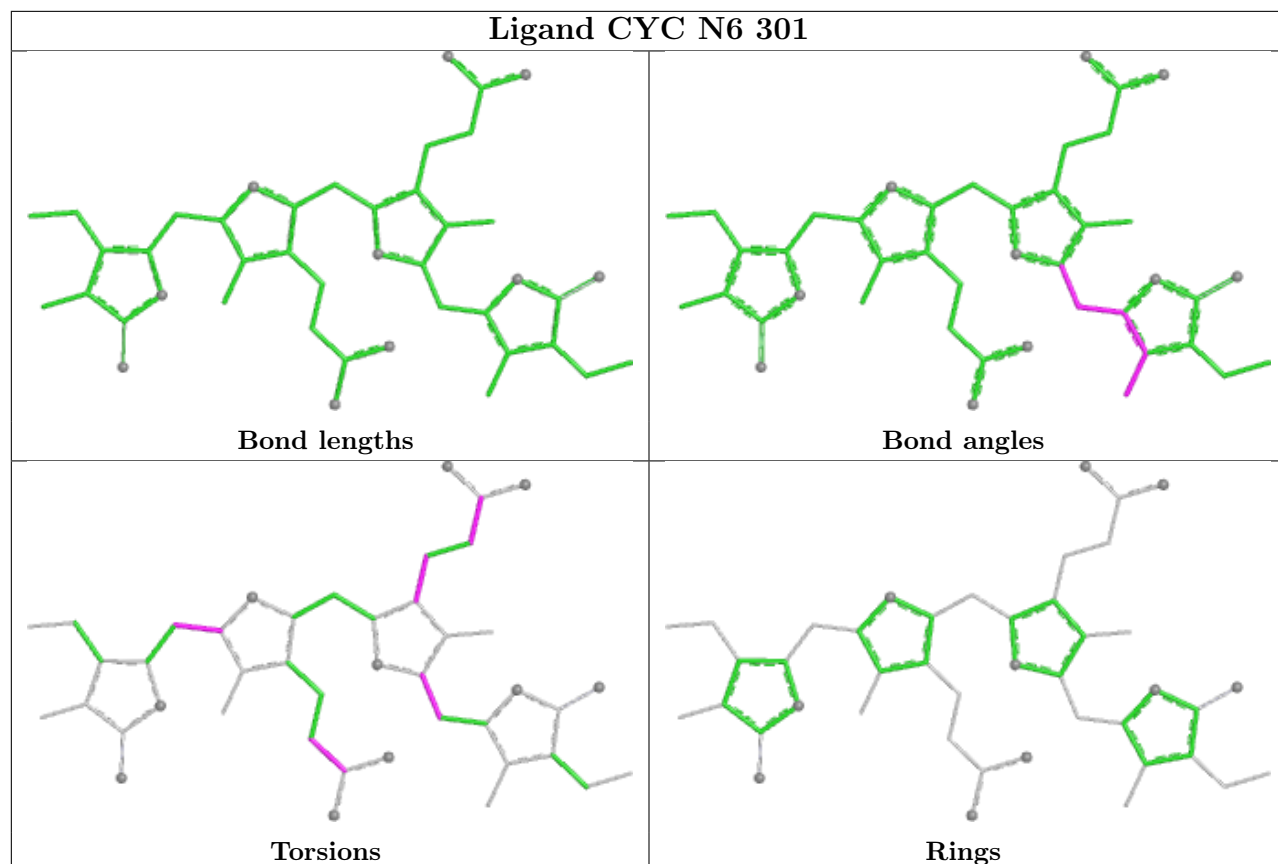


Ligand CYC g9 1001

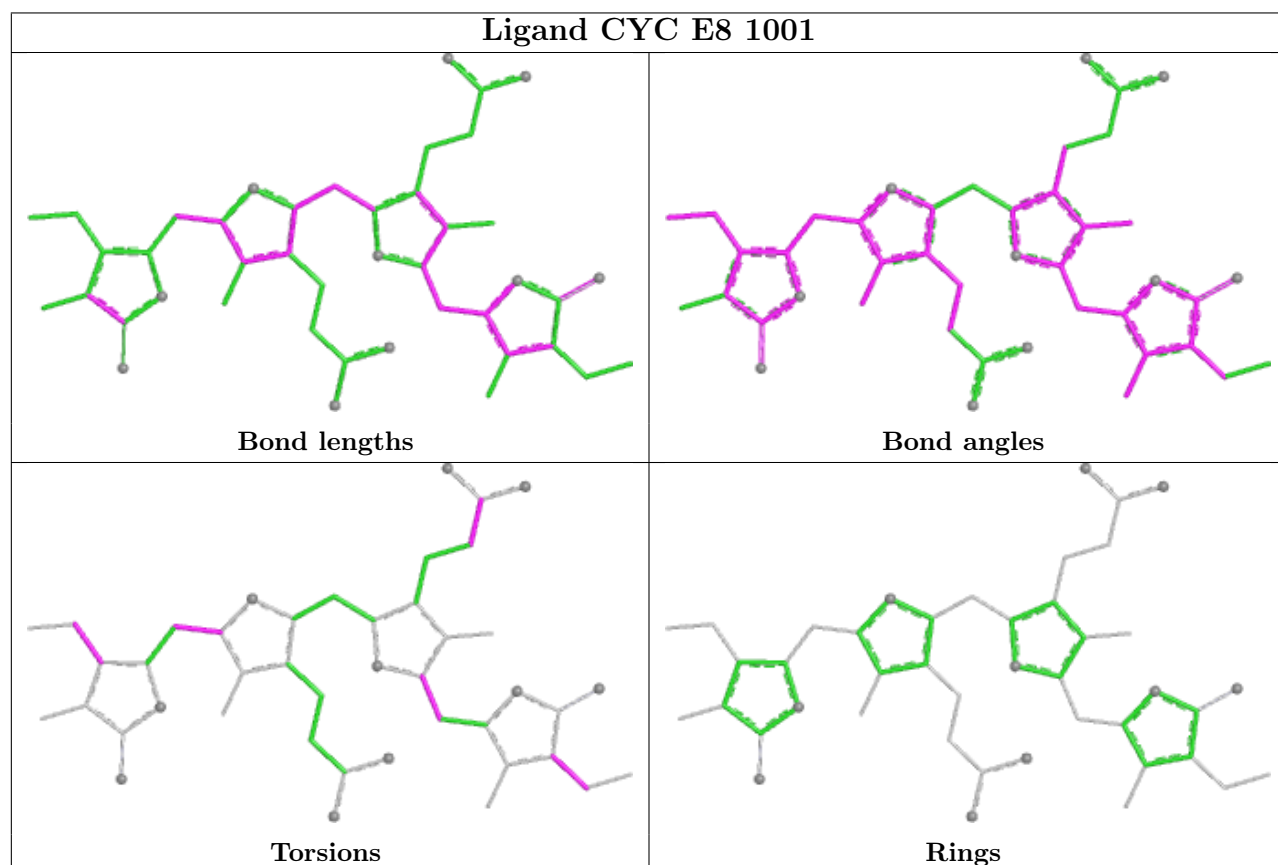




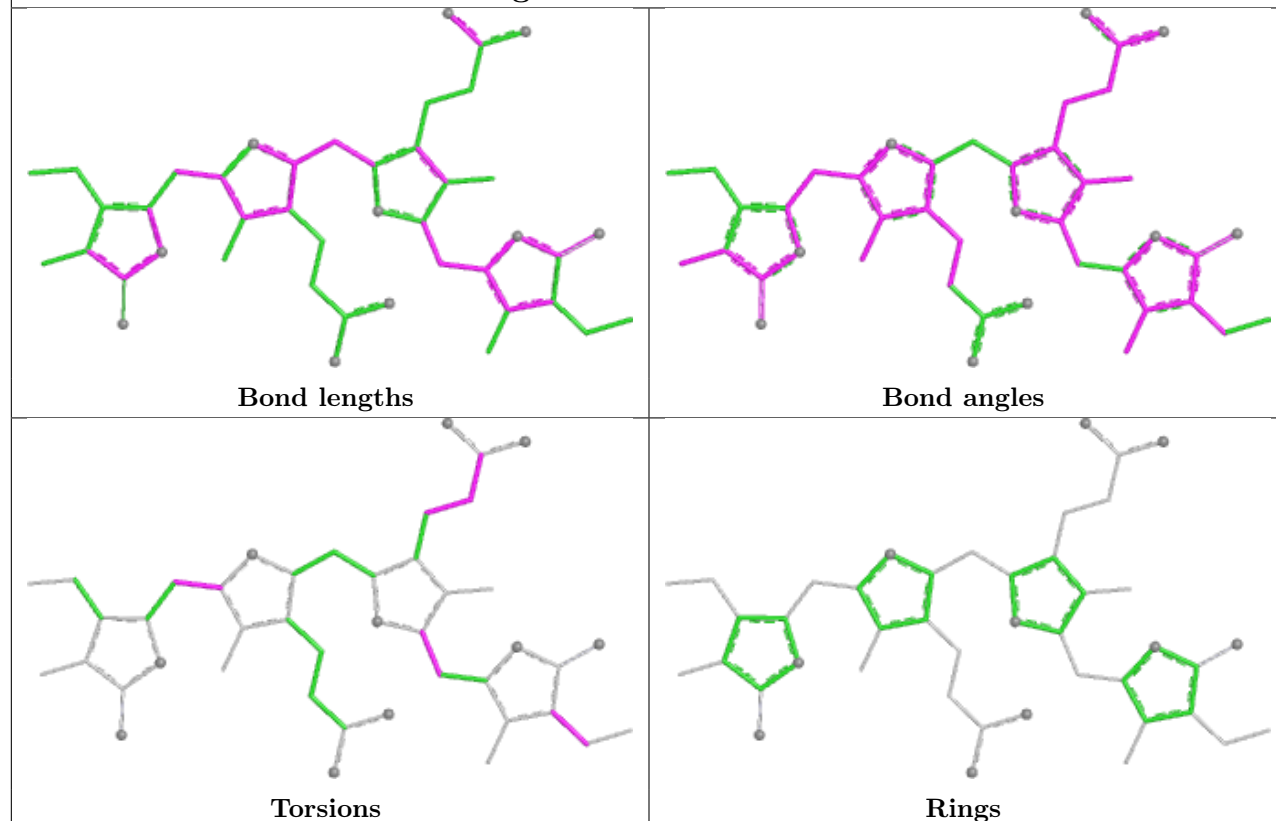
Ligand CYC N6 301



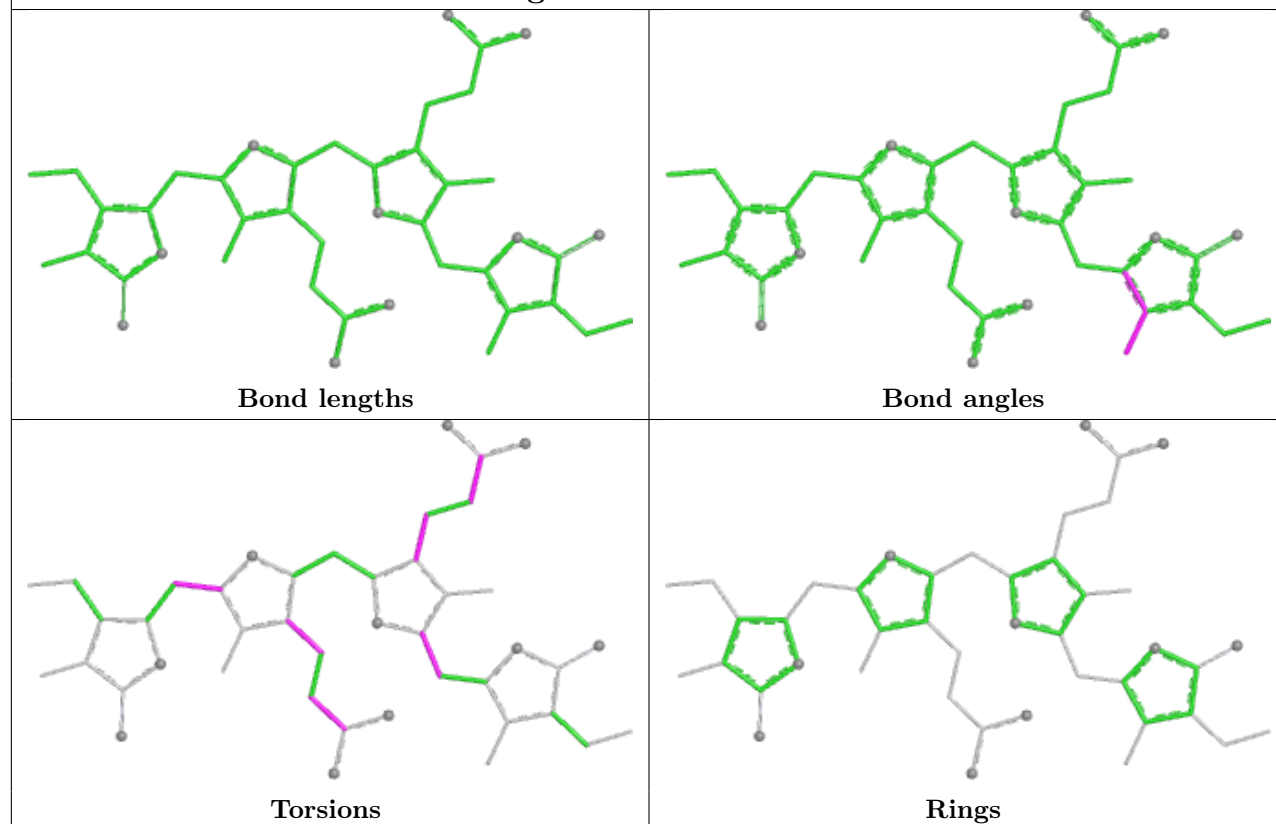
Ligand CYC E8 1001



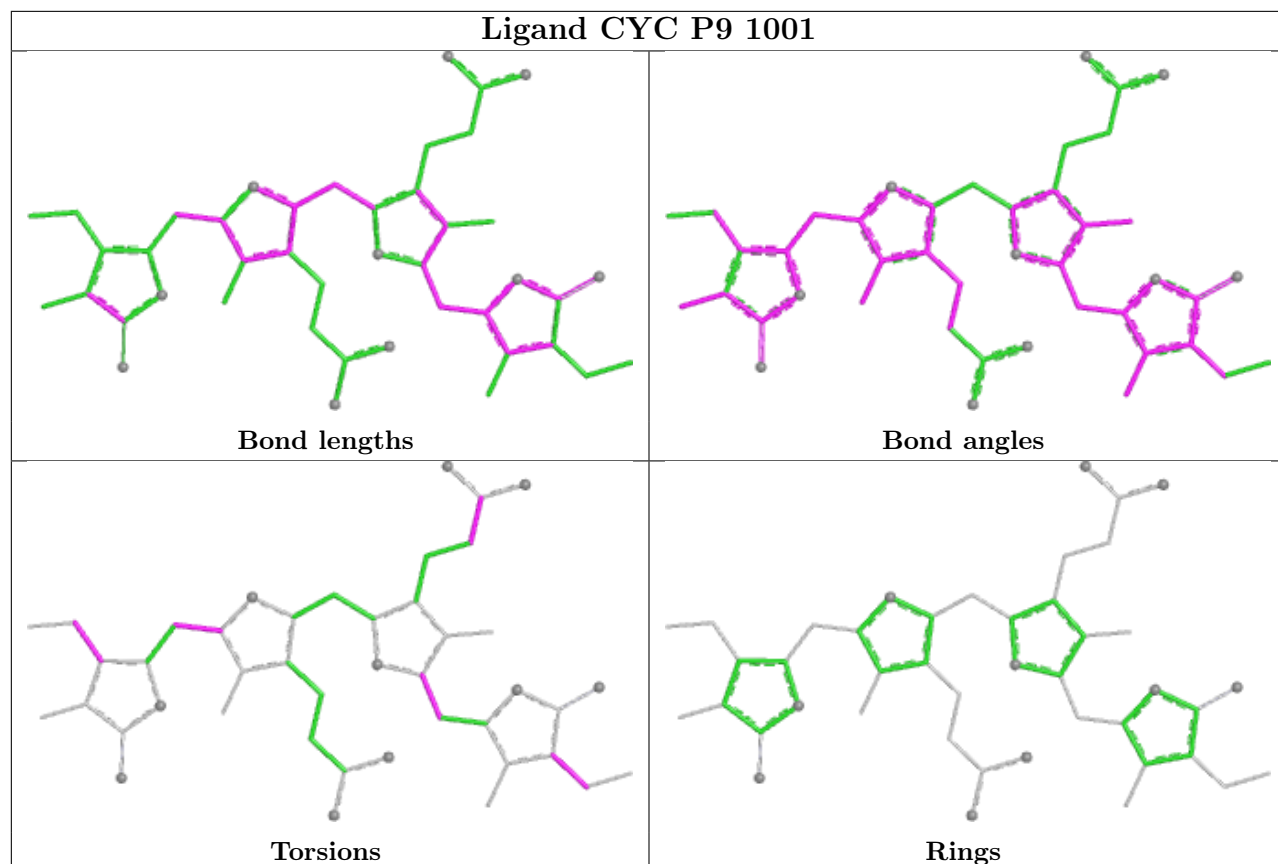
Ligand CYC B1 1001



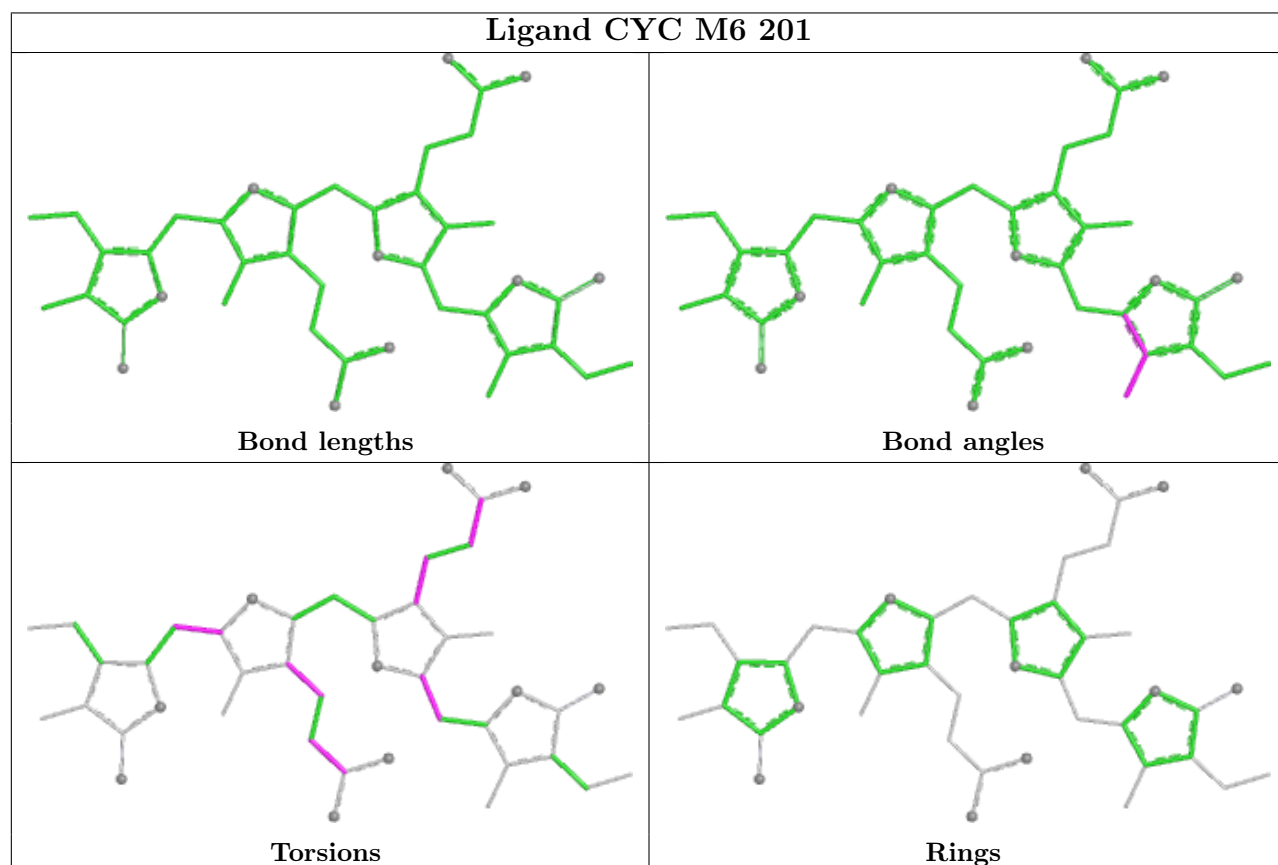
Ligand CYC I6 202

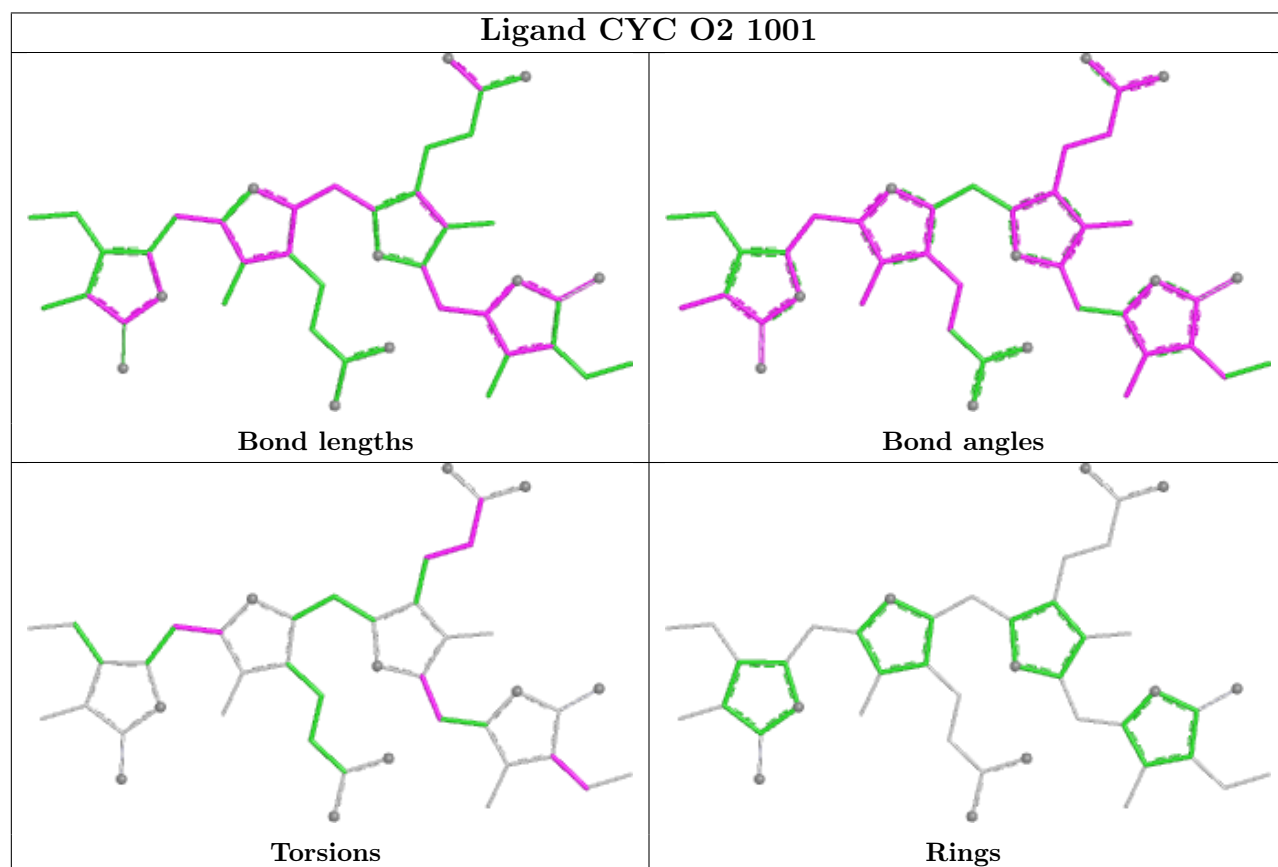
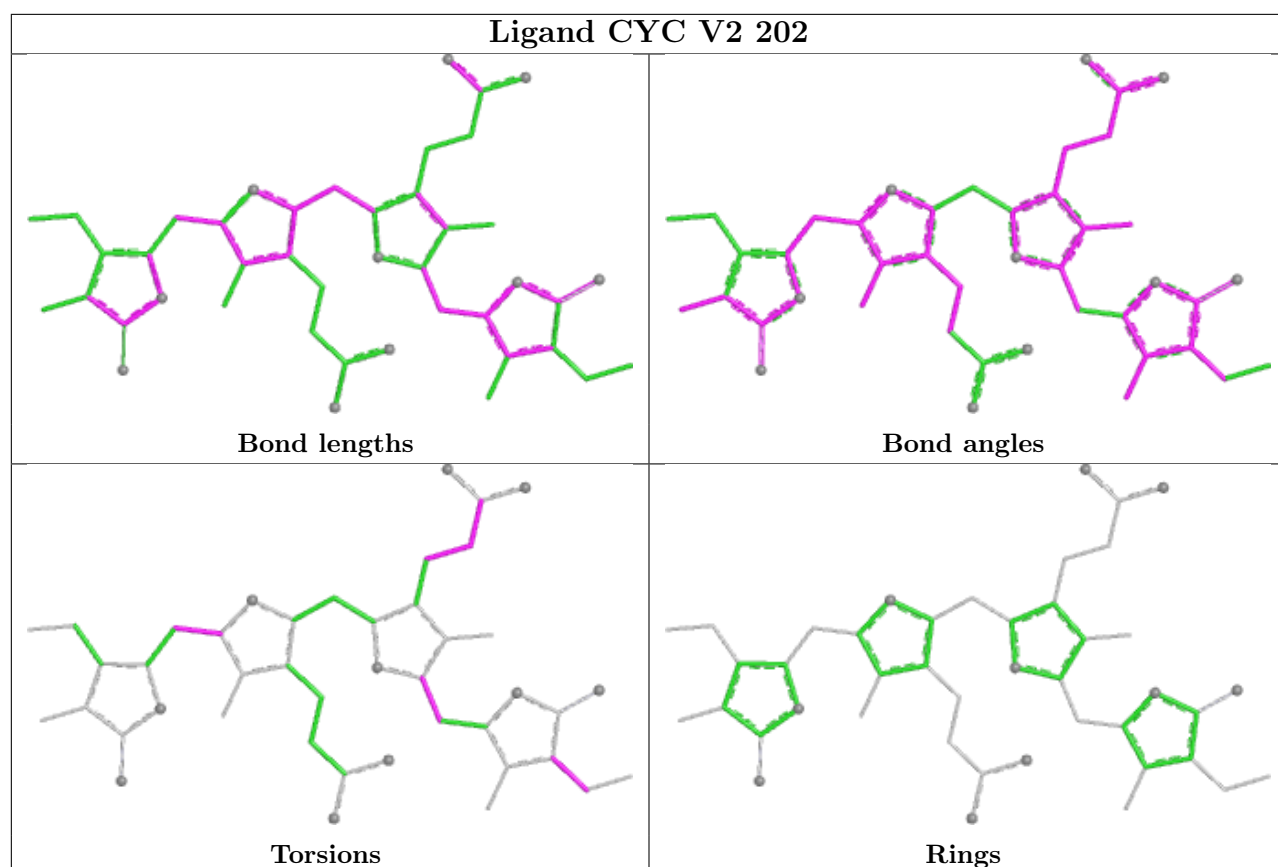


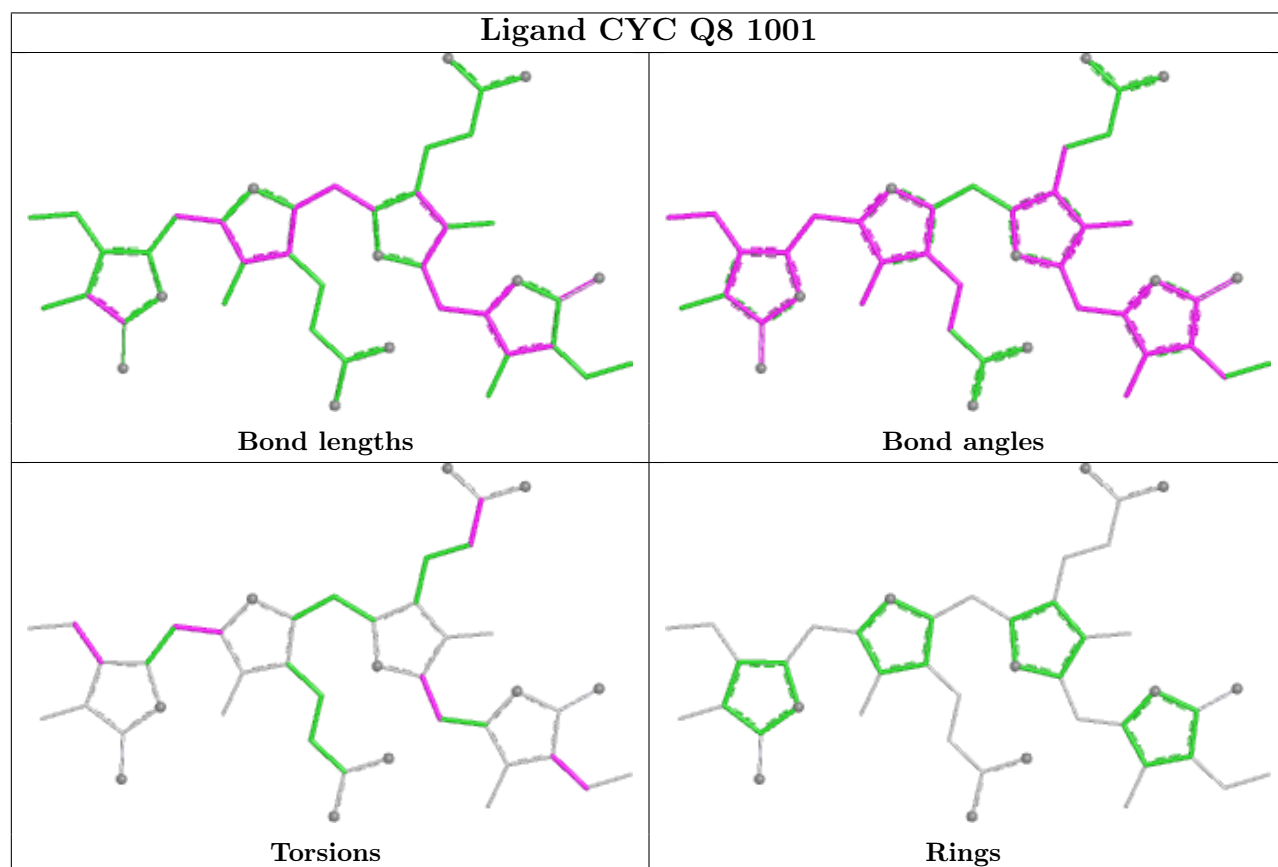
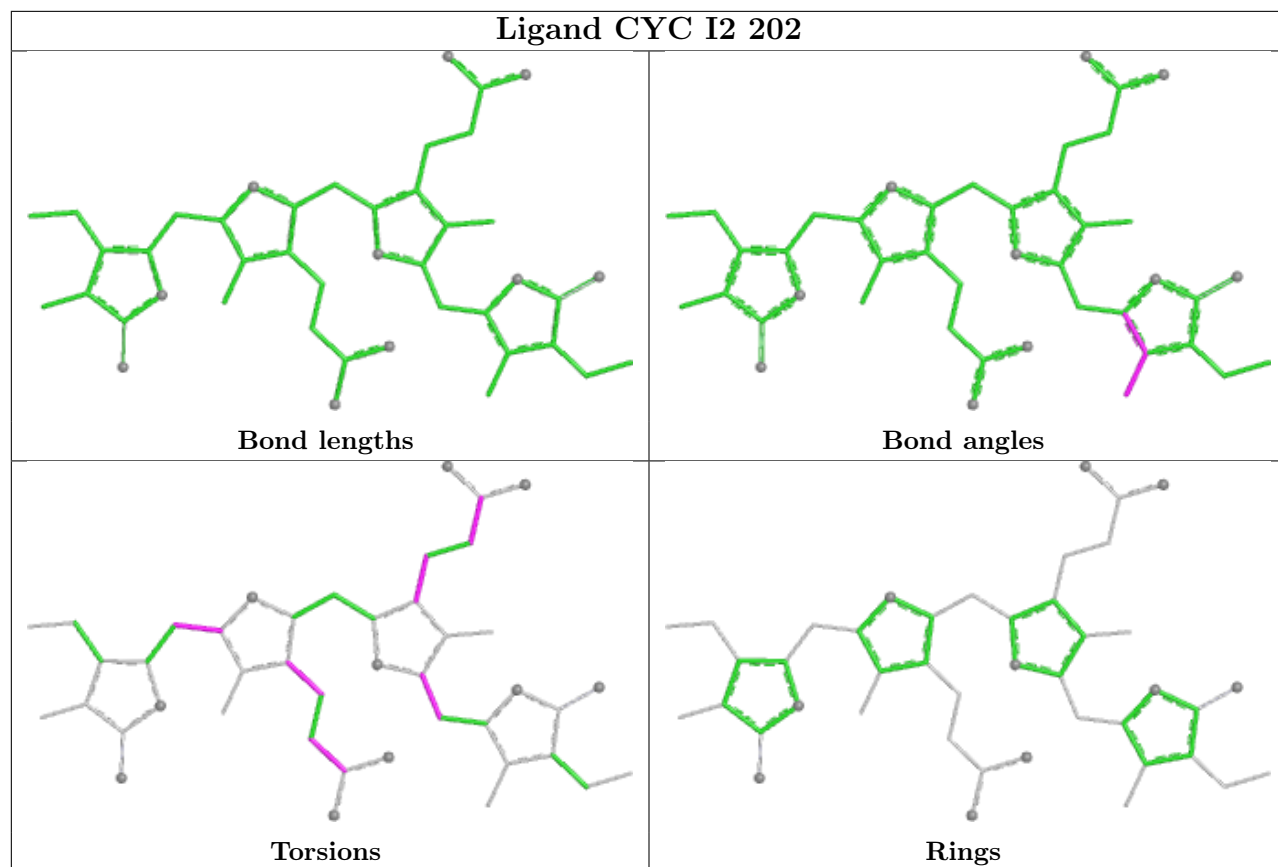
Ligand CYC P9 1001



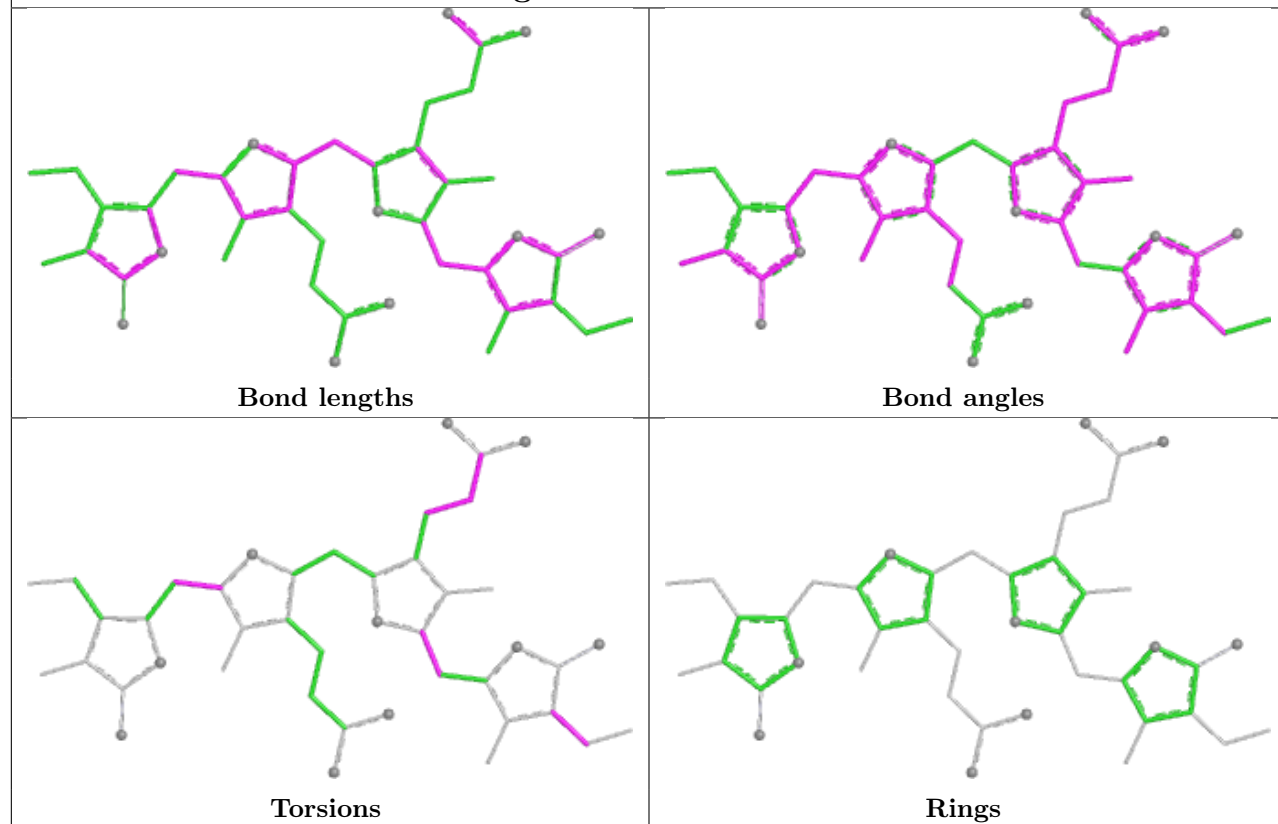
Ligand CYC M6 201



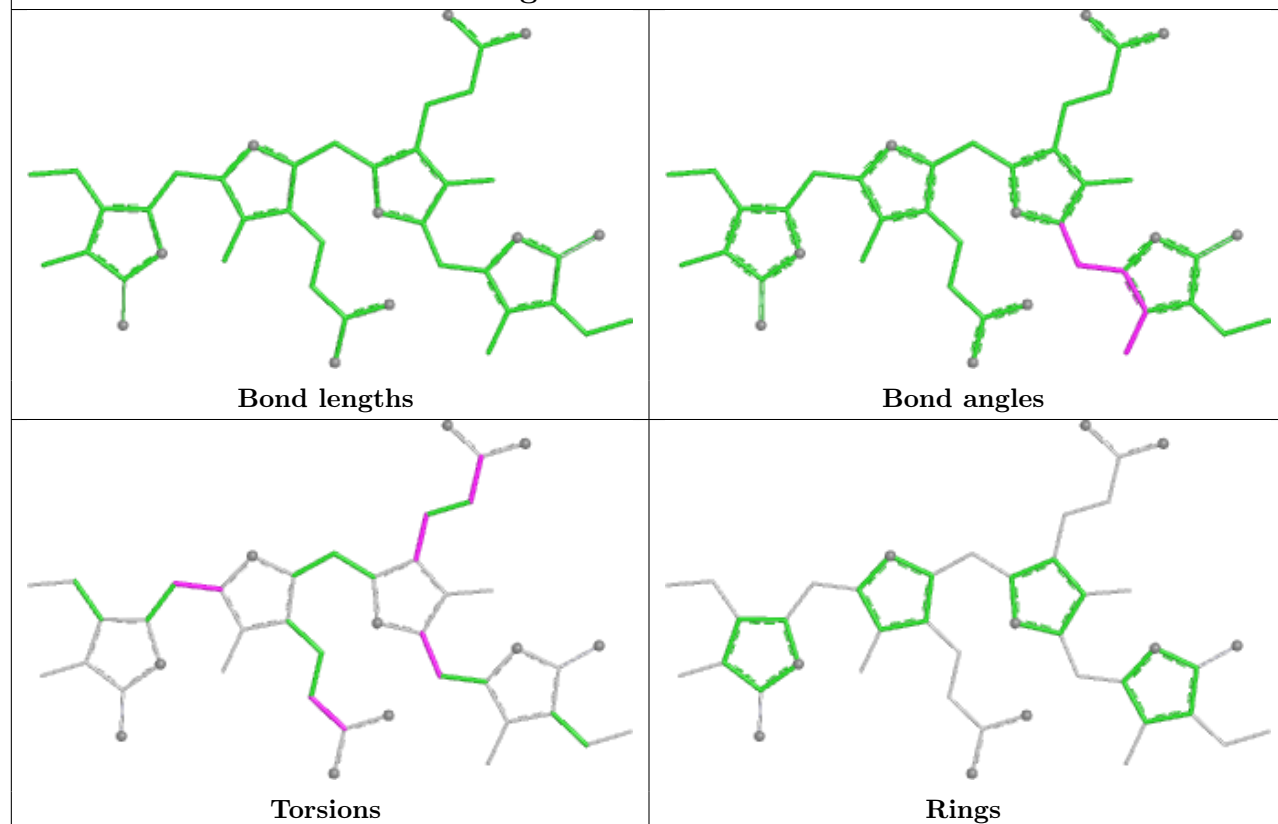




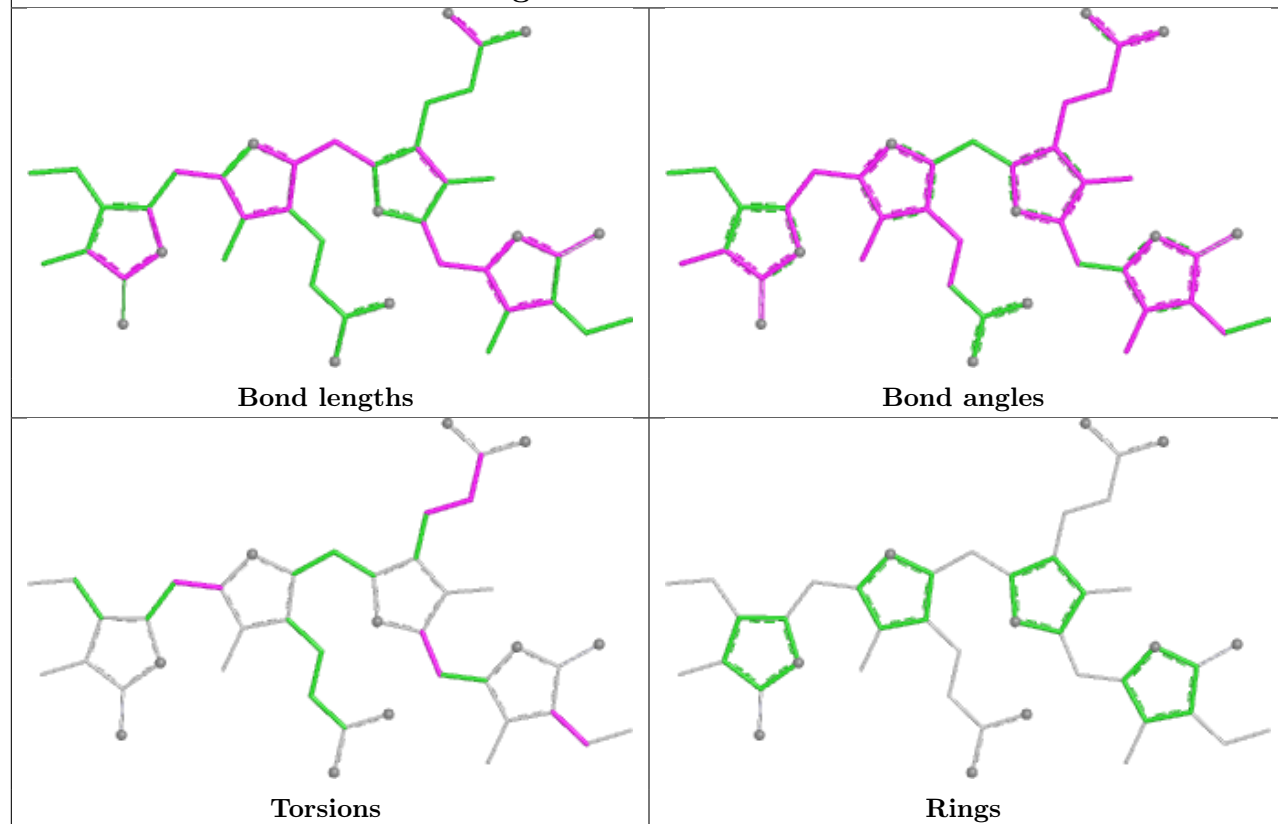
Ligand CYC F6 1001



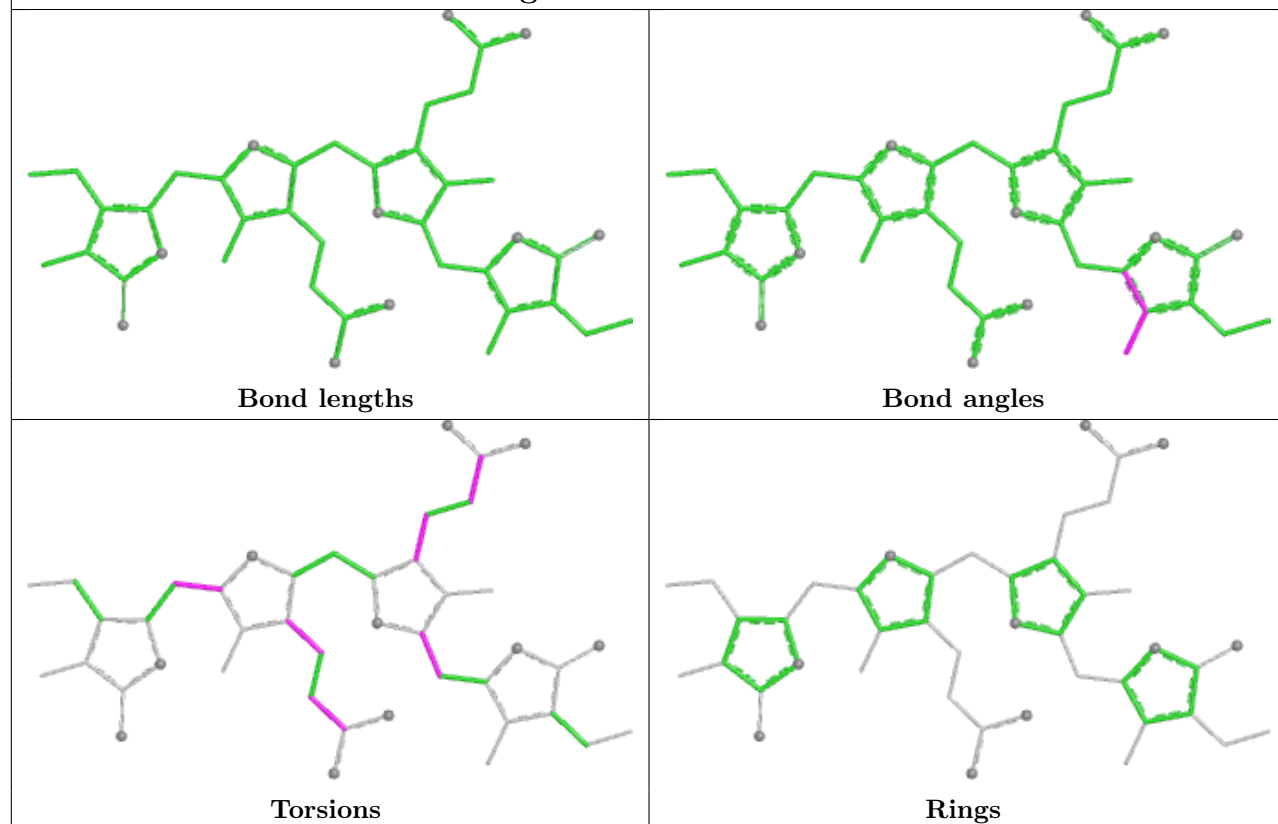
Ligand CYC N2 301

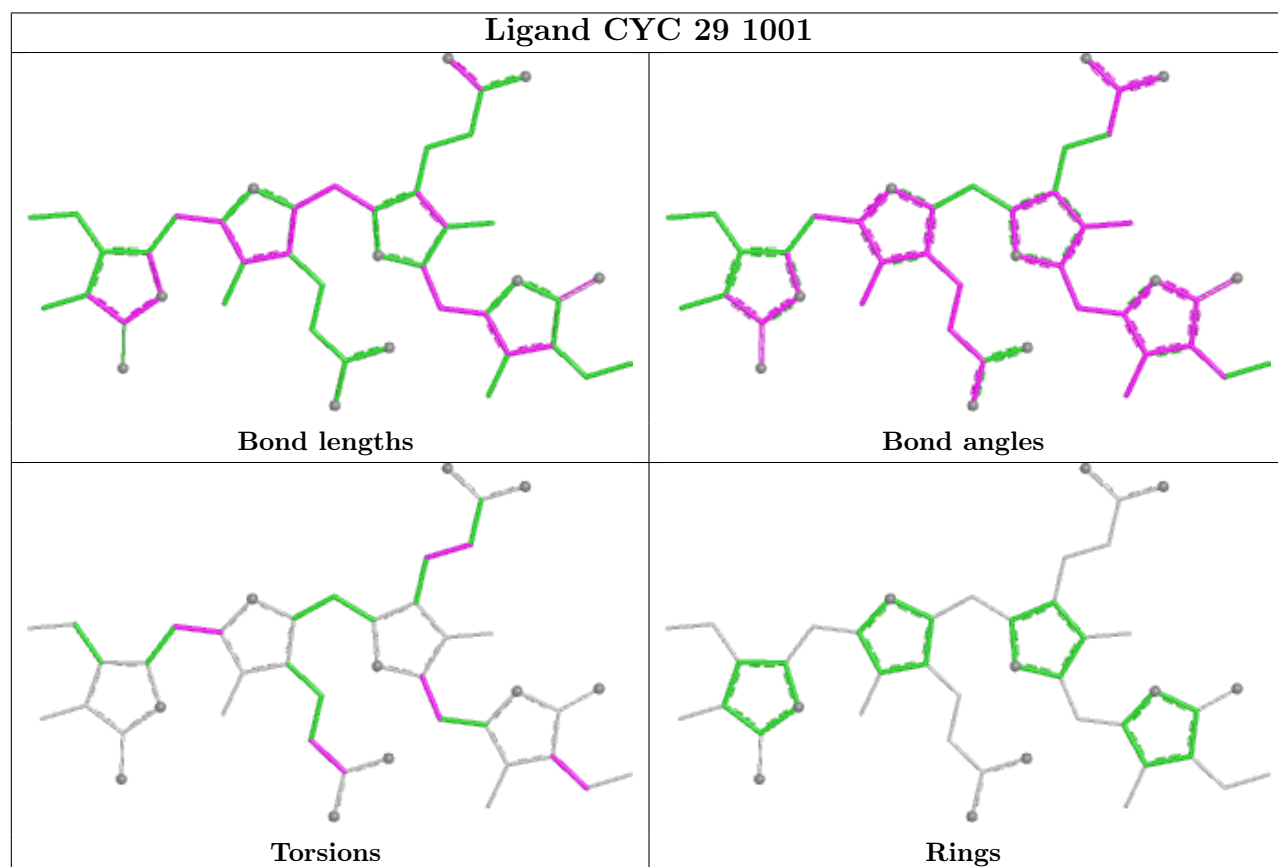
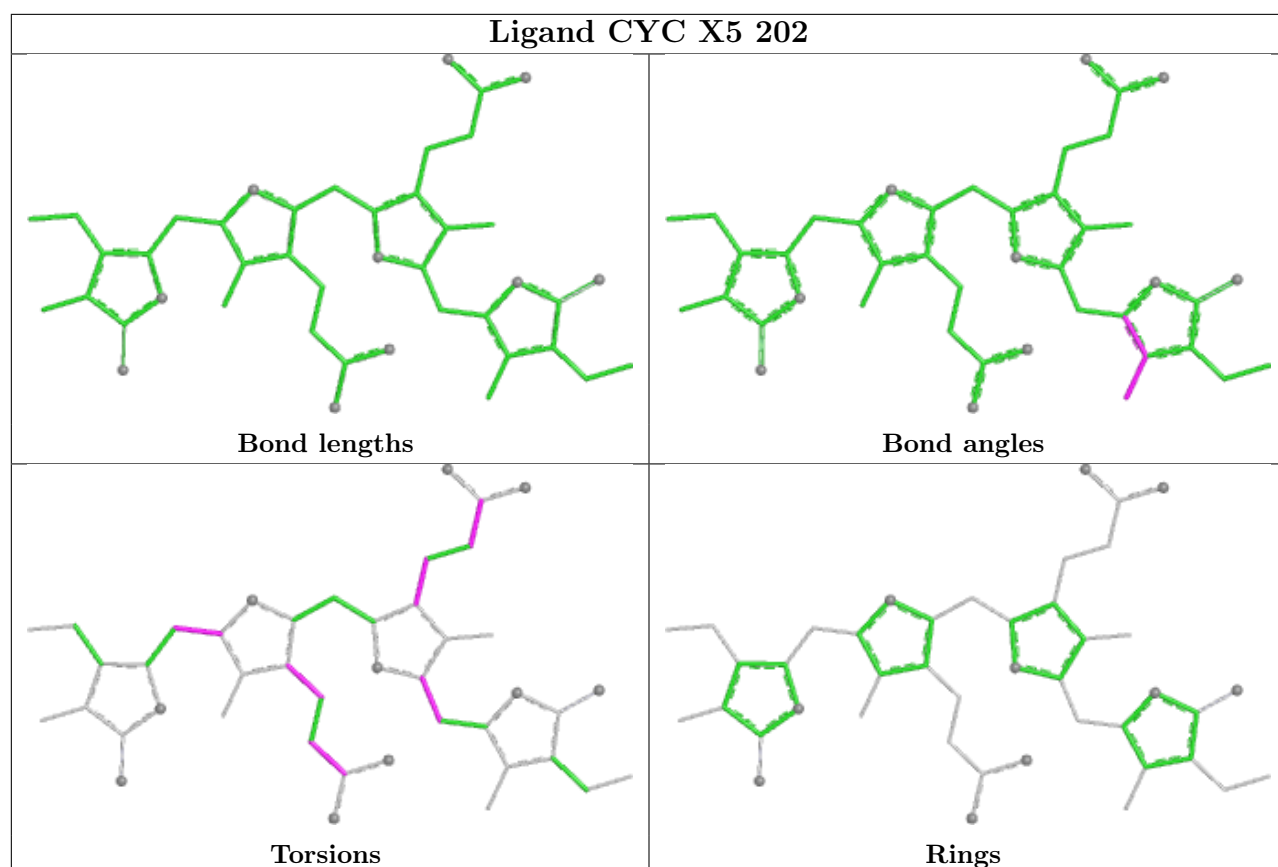


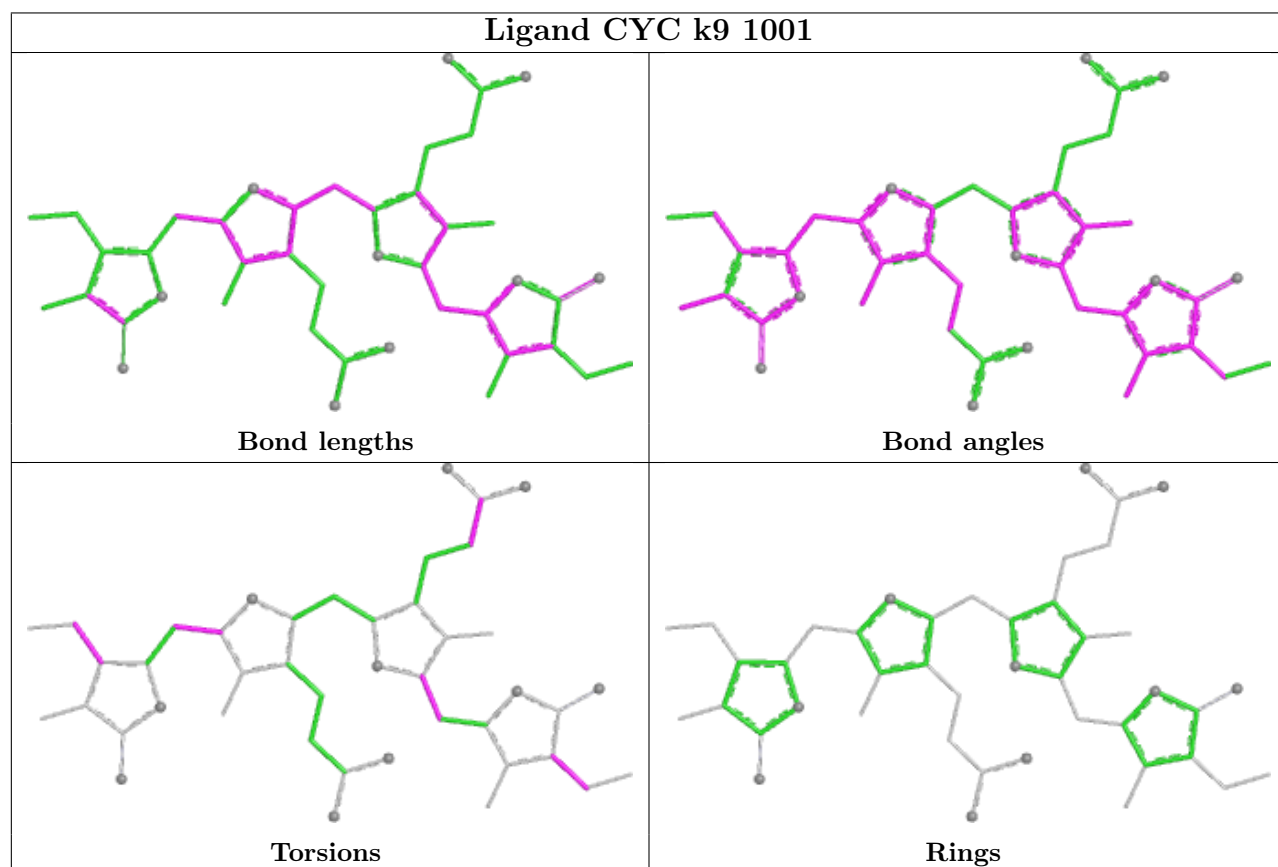
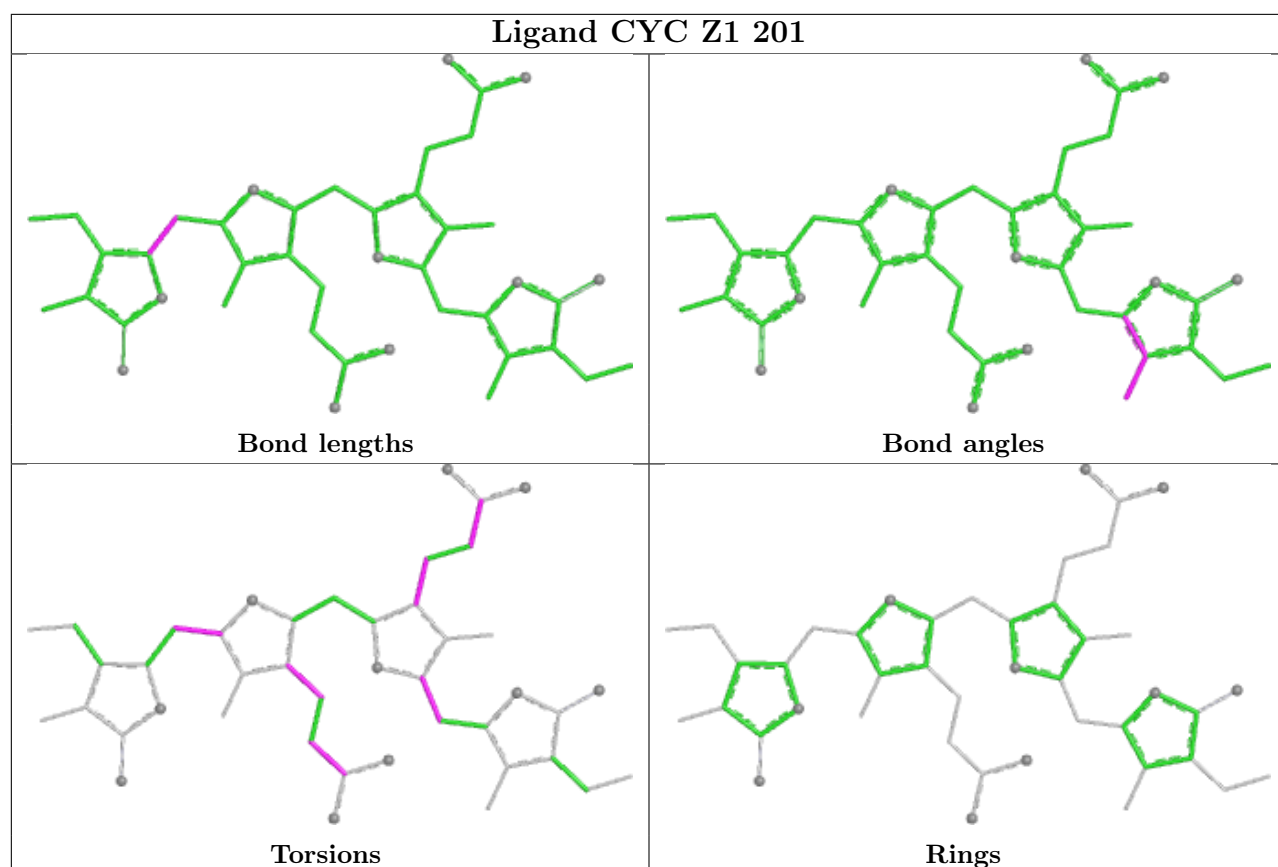
Ligand CYC B7 1001



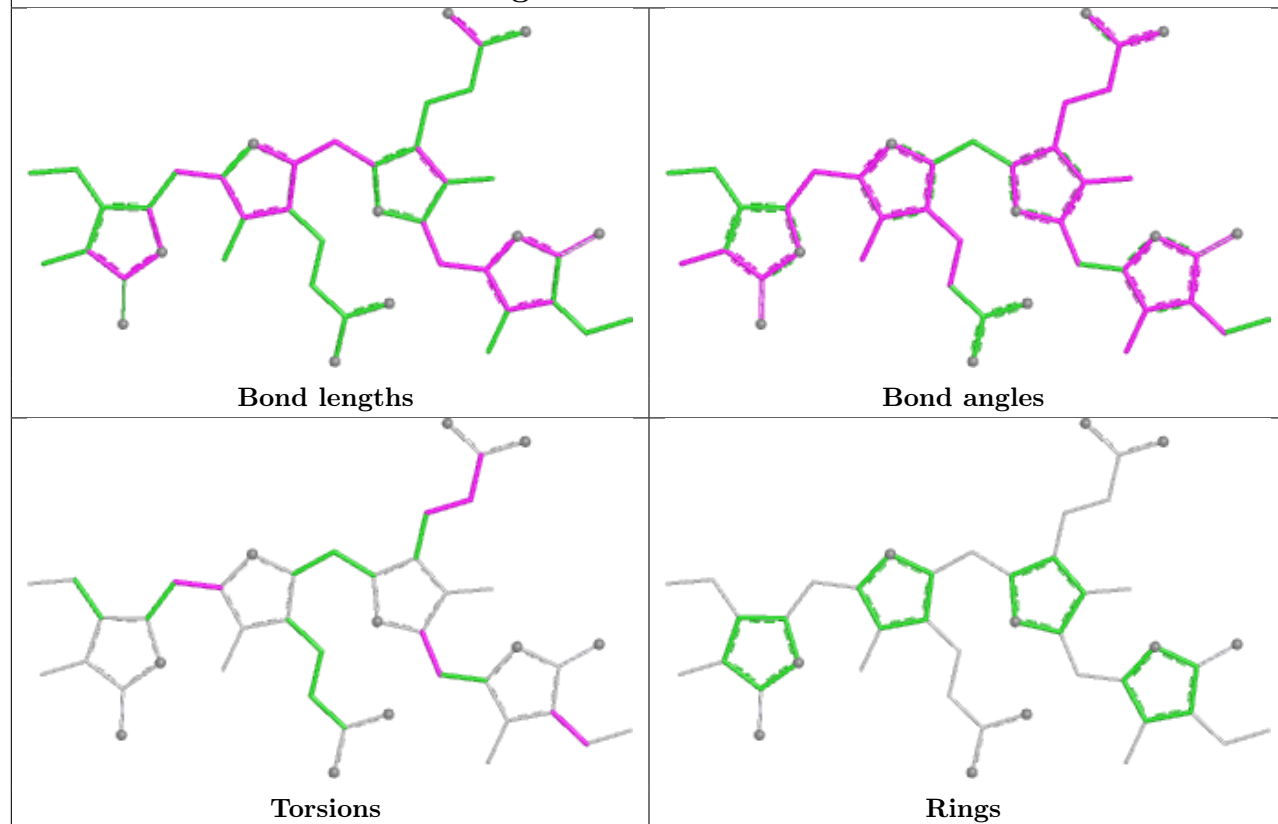
Ligand CYC G7 202



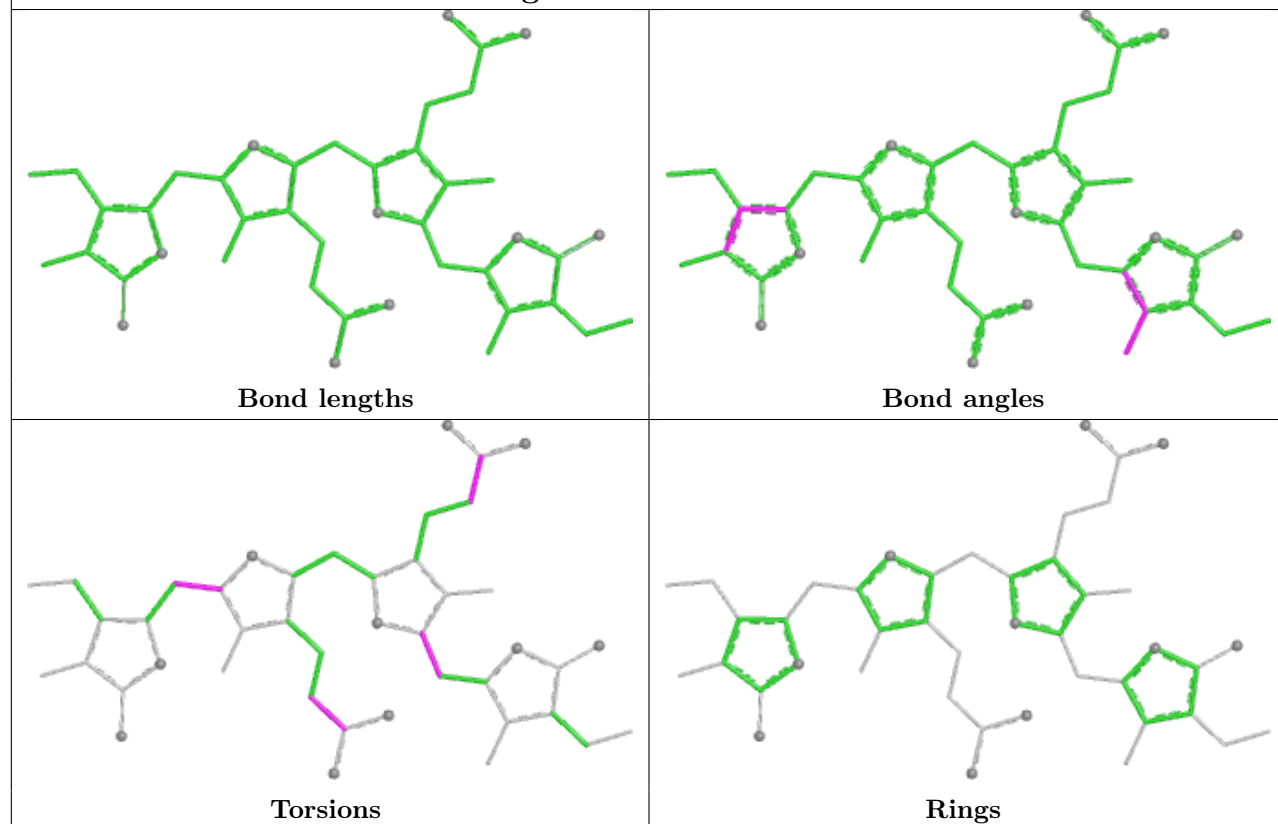




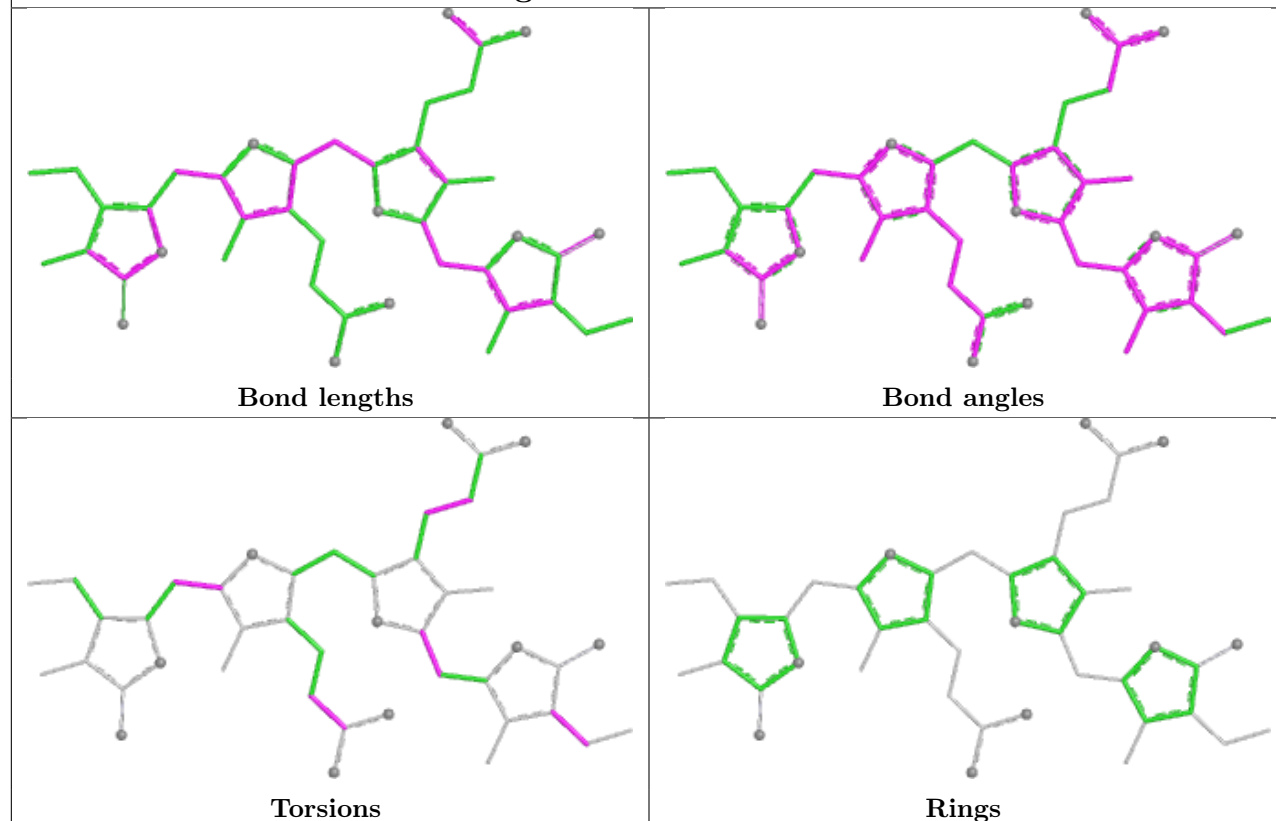
Ligand CYC R4 1001



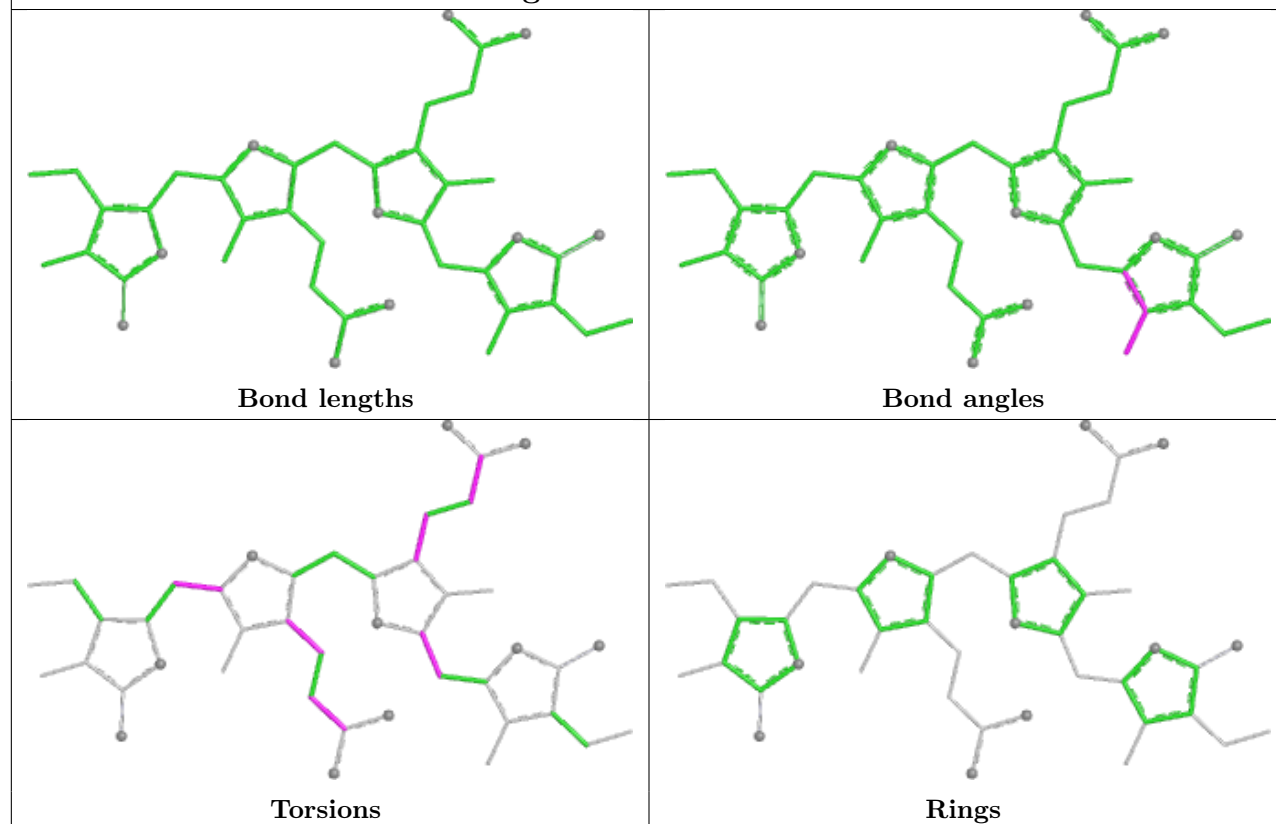
Ligand CYC P4 201



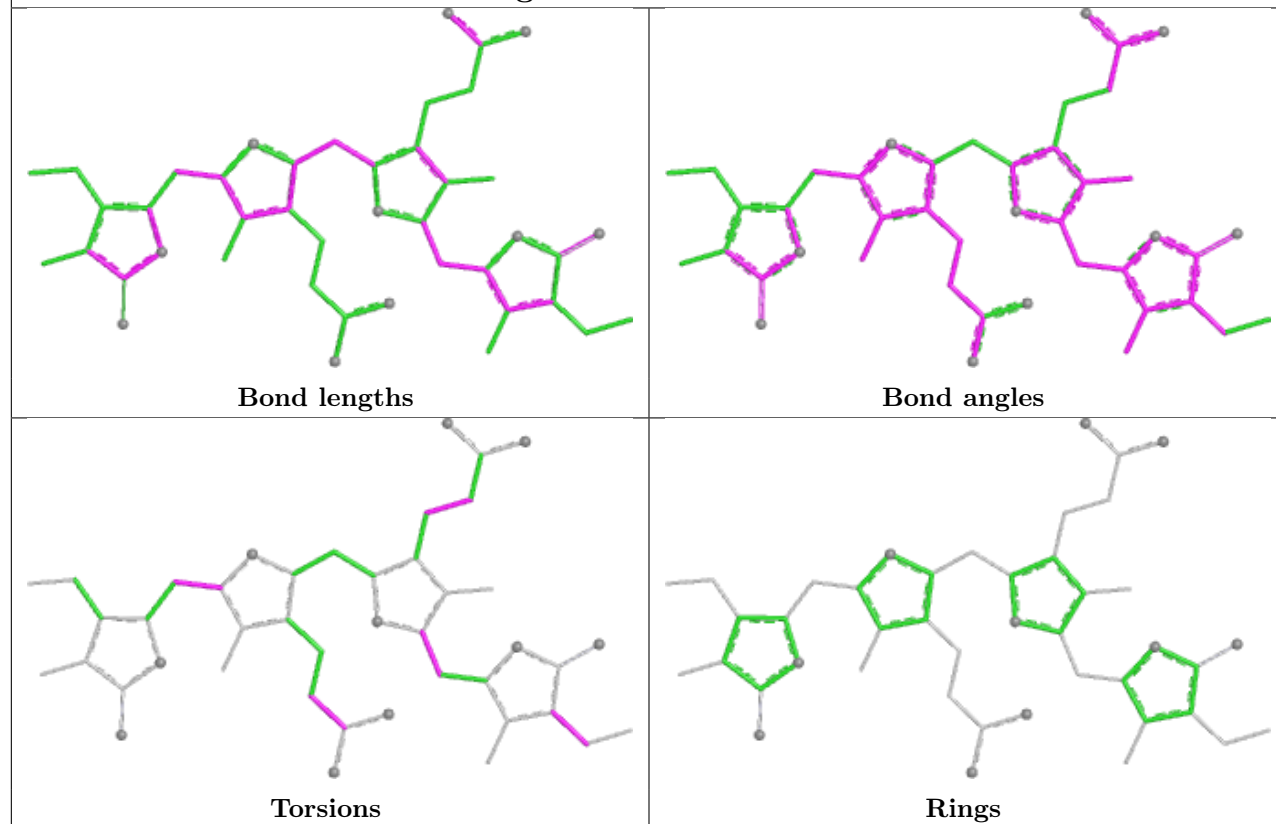
Ligand CYC S9 1001



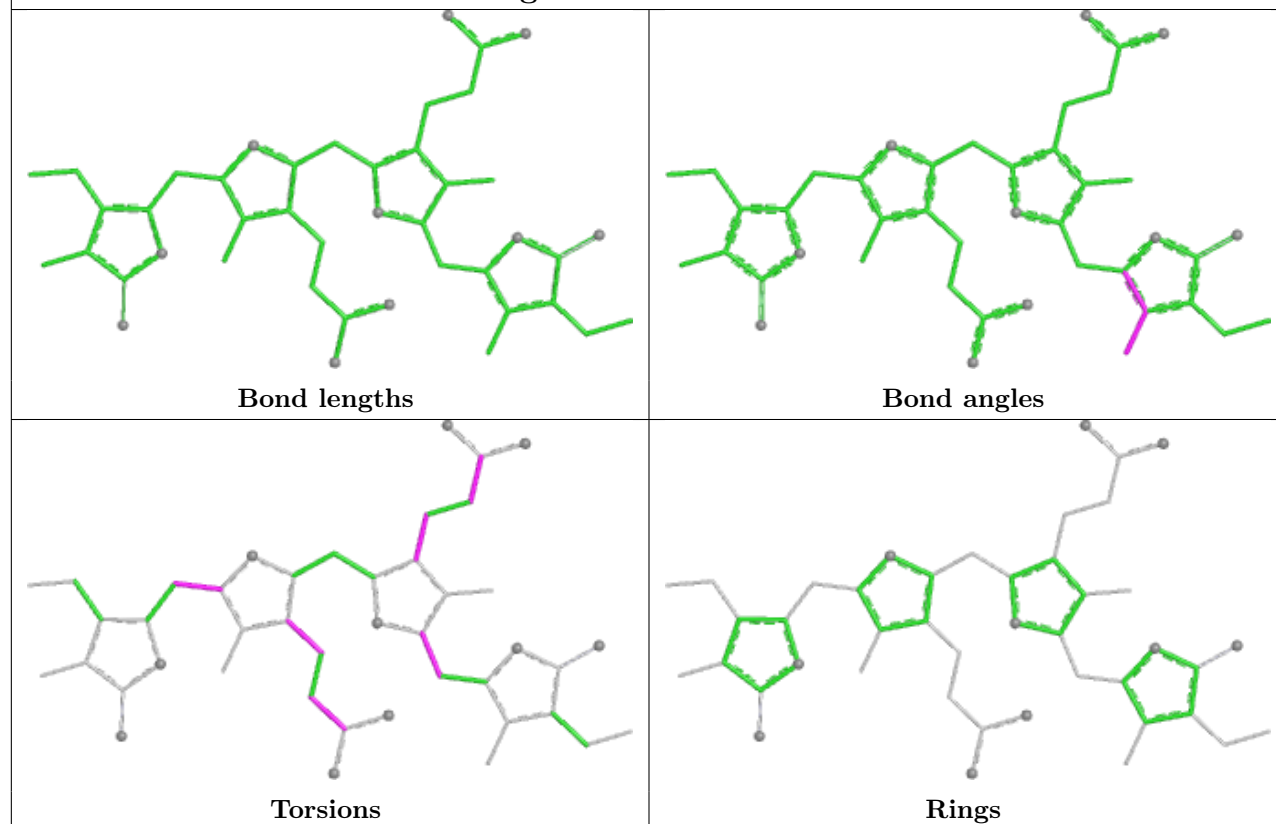
Ligand CYC IA 202

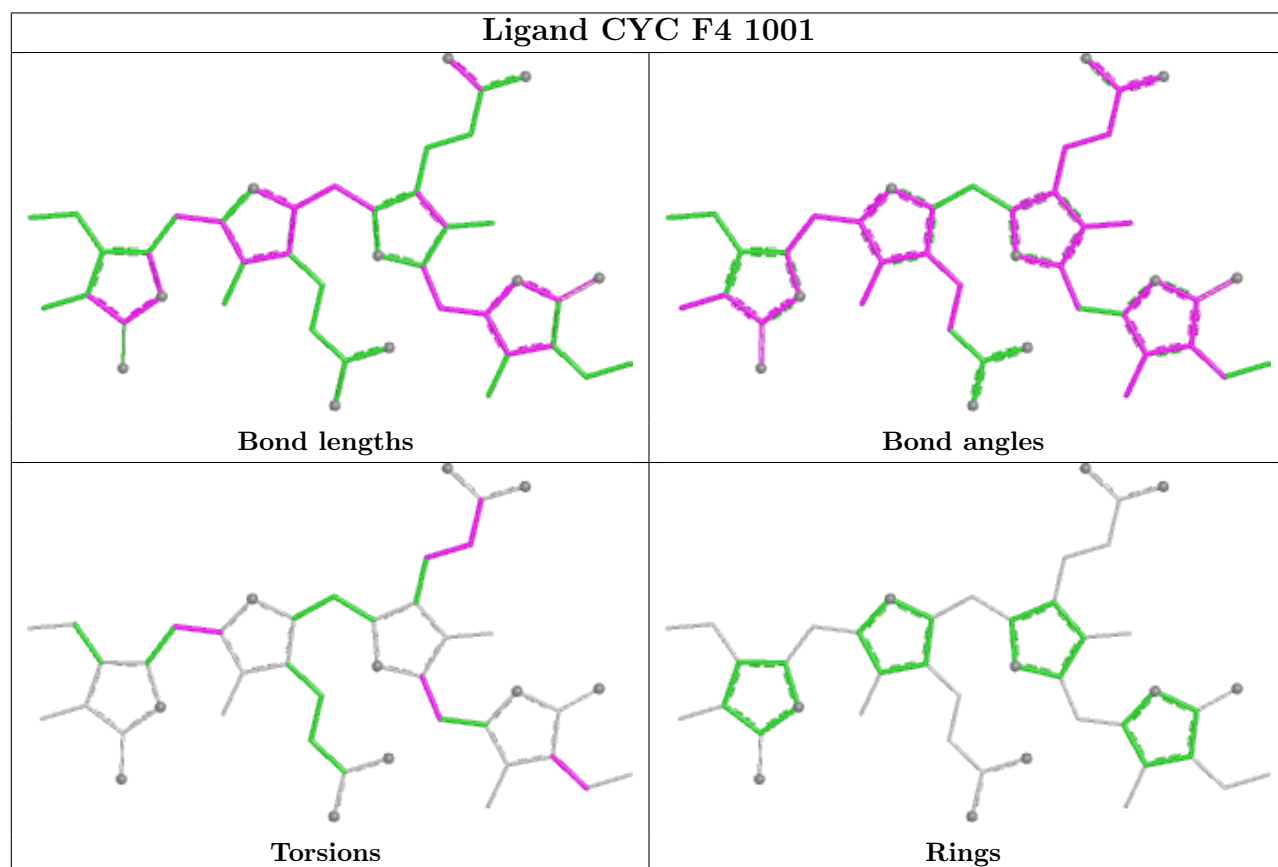
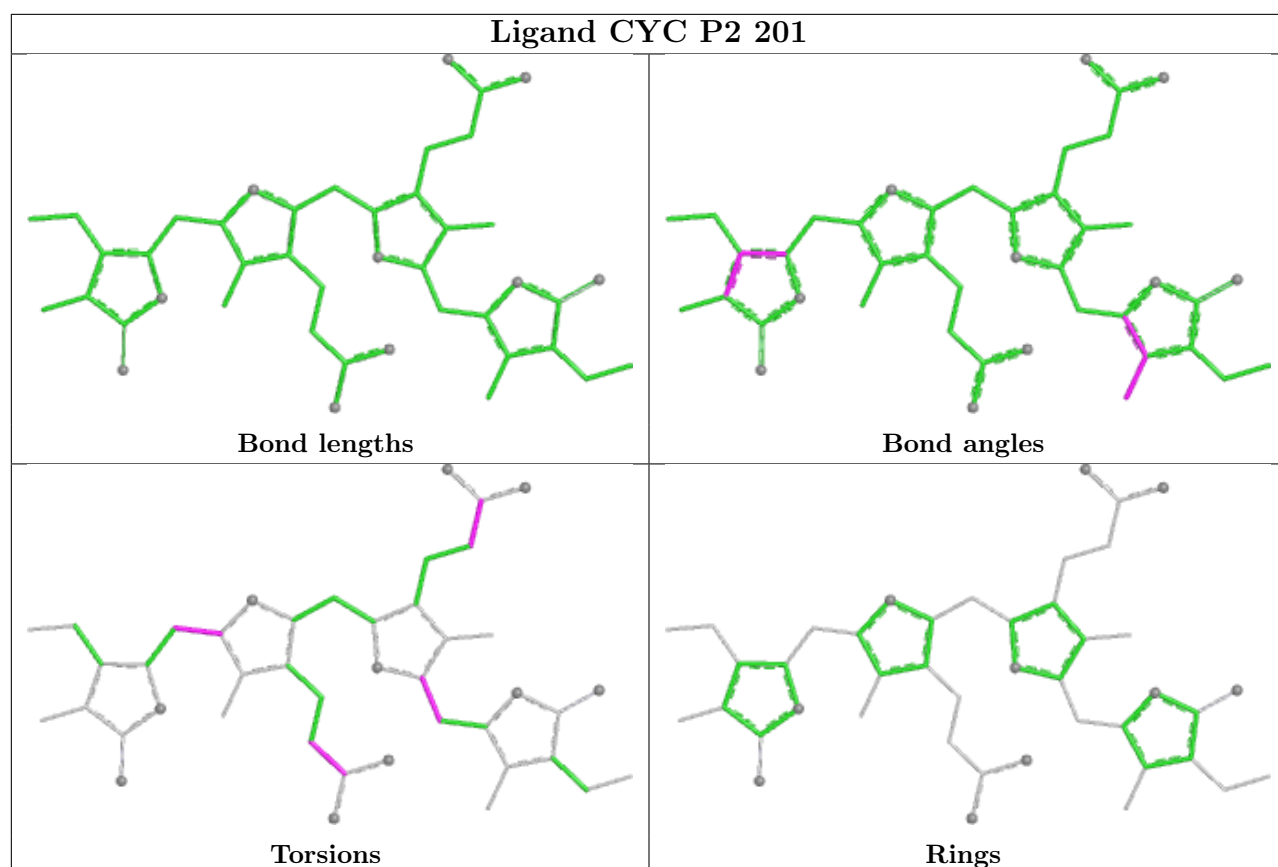


Ligand CYC 39 1001

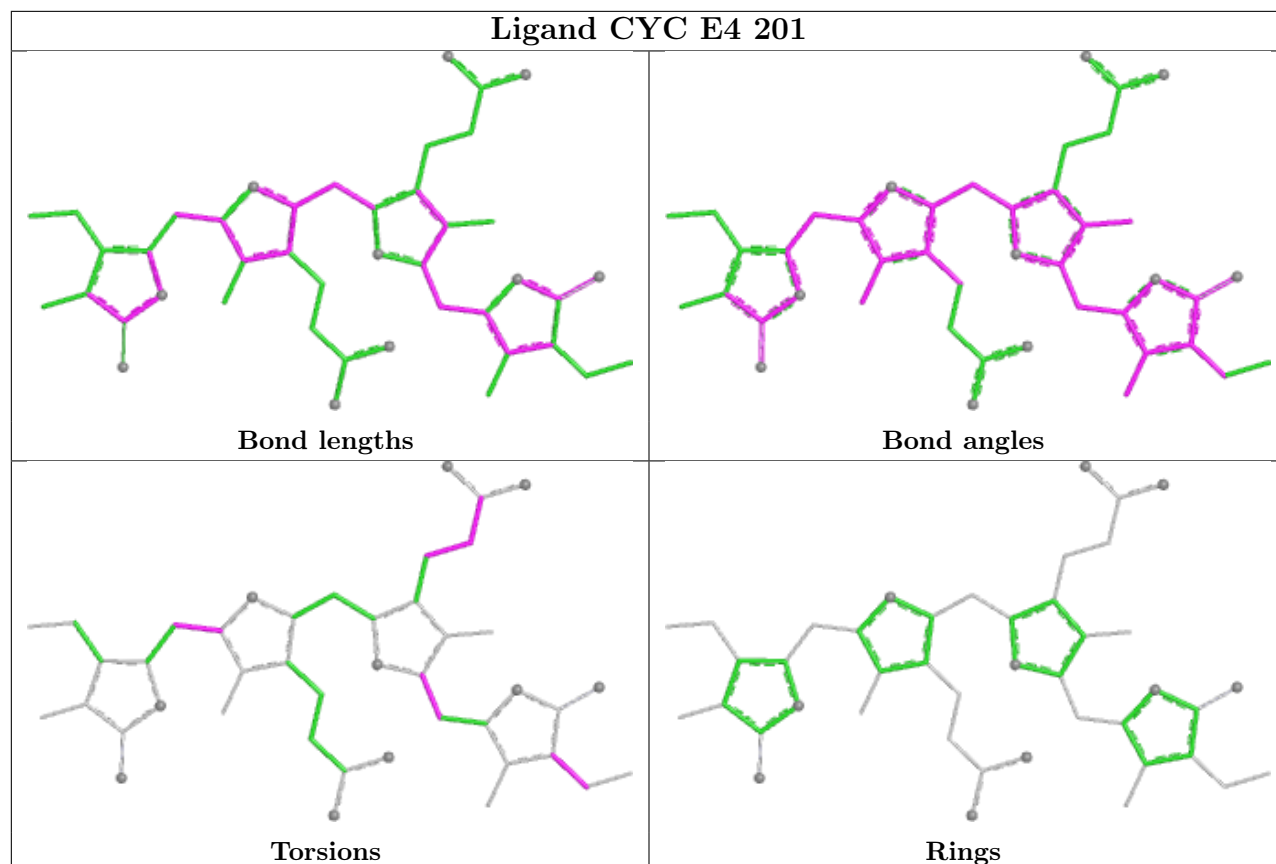


Ligand CYC K2 202

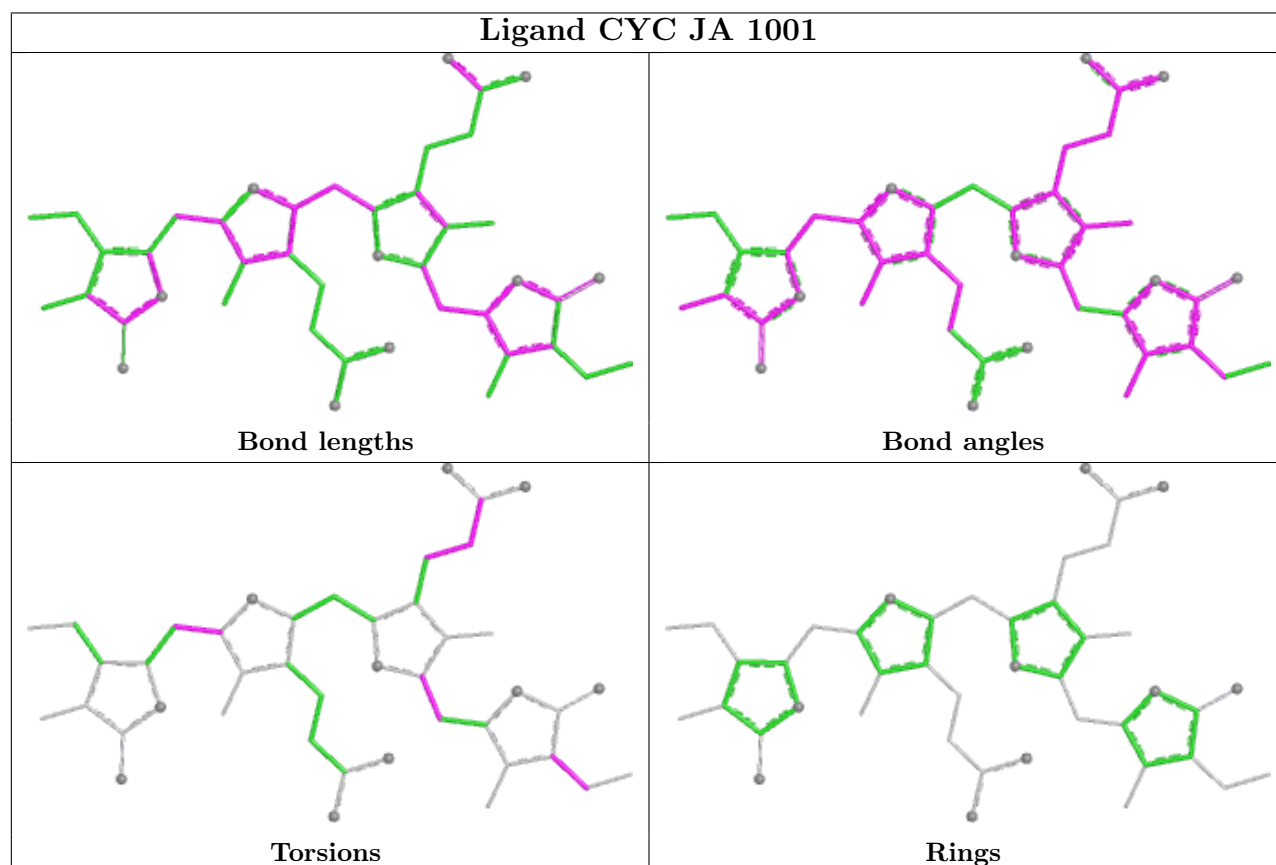




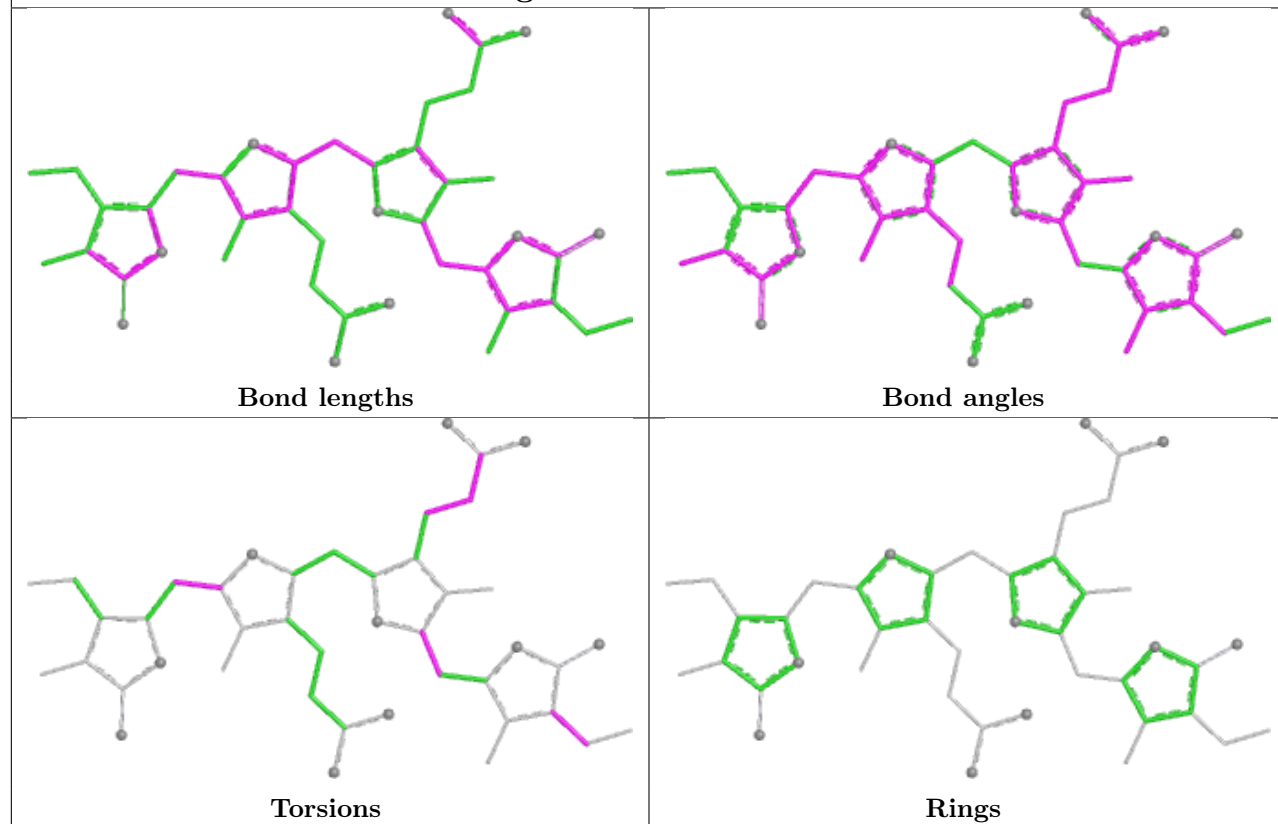
Ligand CYC E4 201



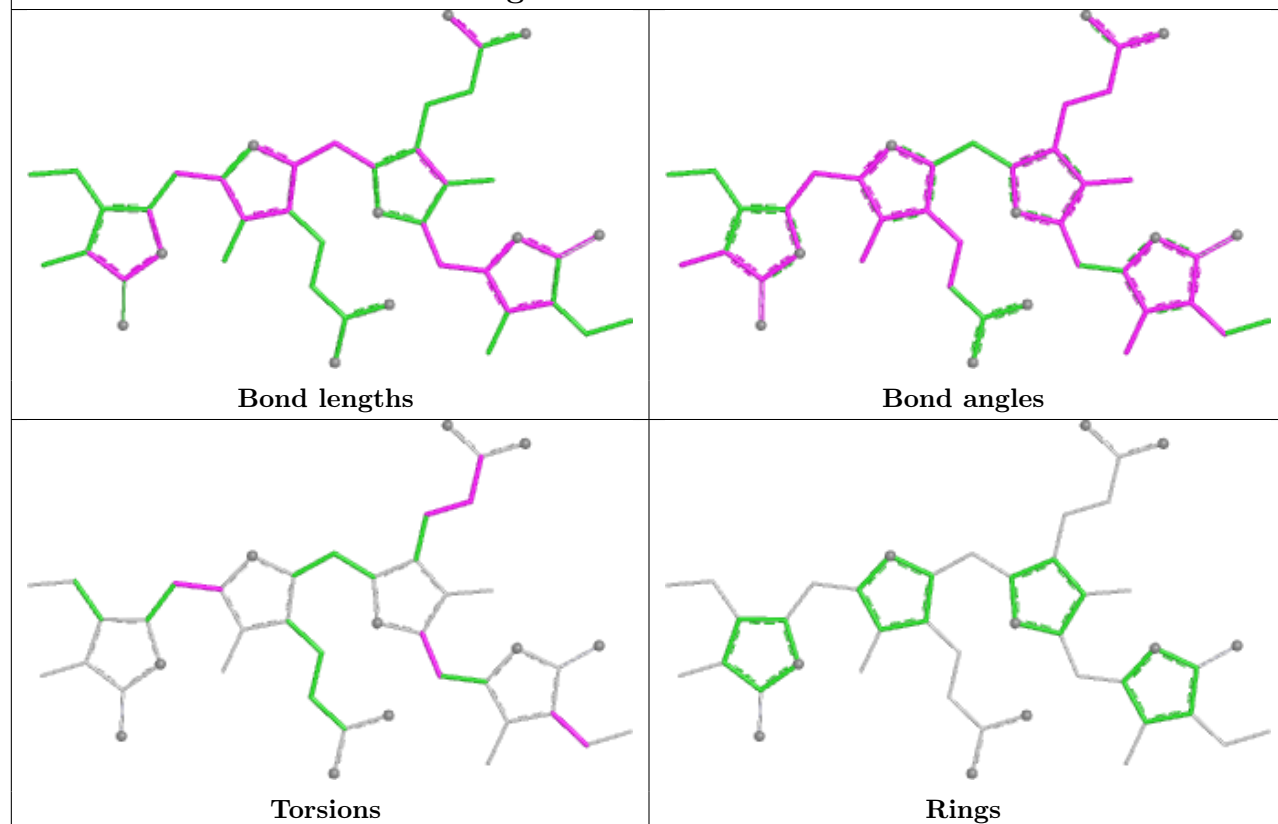
Ligand CYC JA 1001



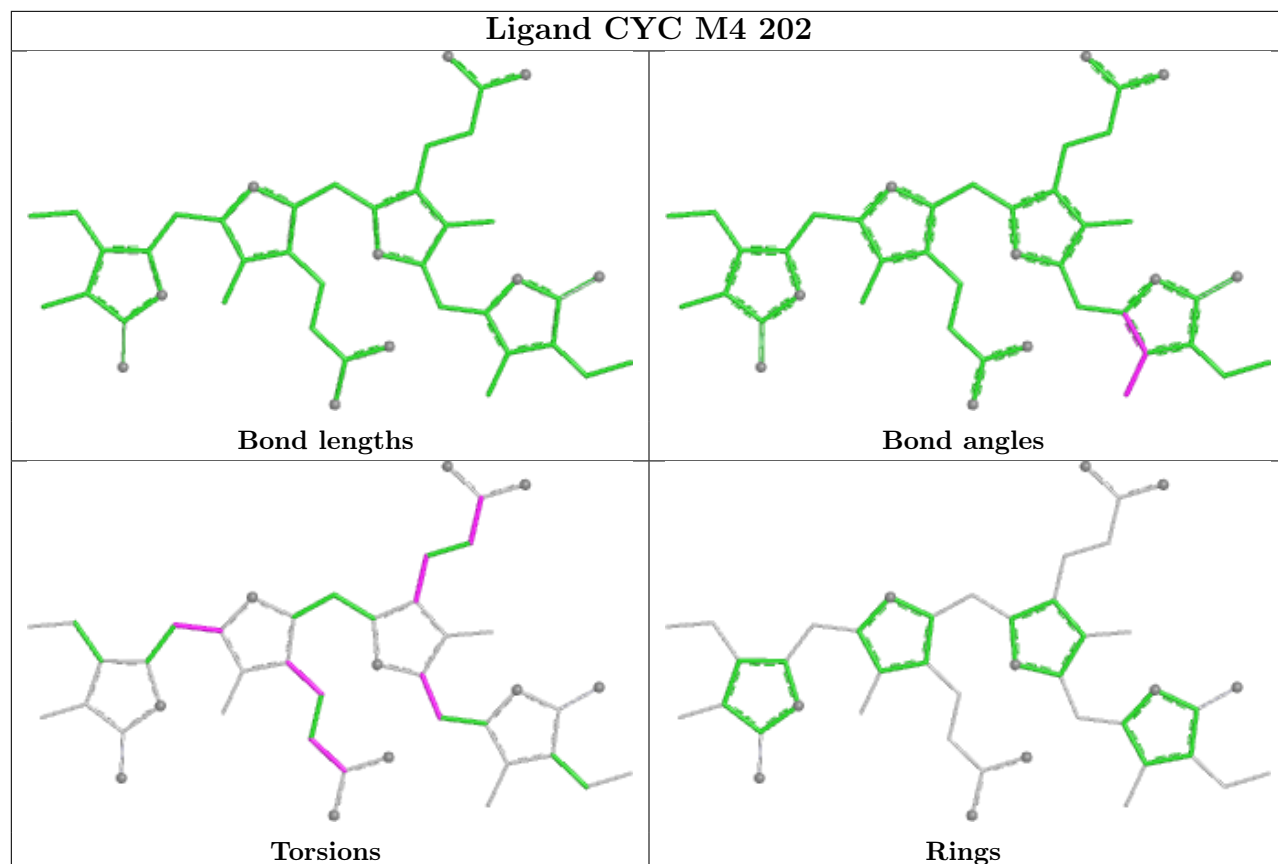
Ligand CYC J2 1001



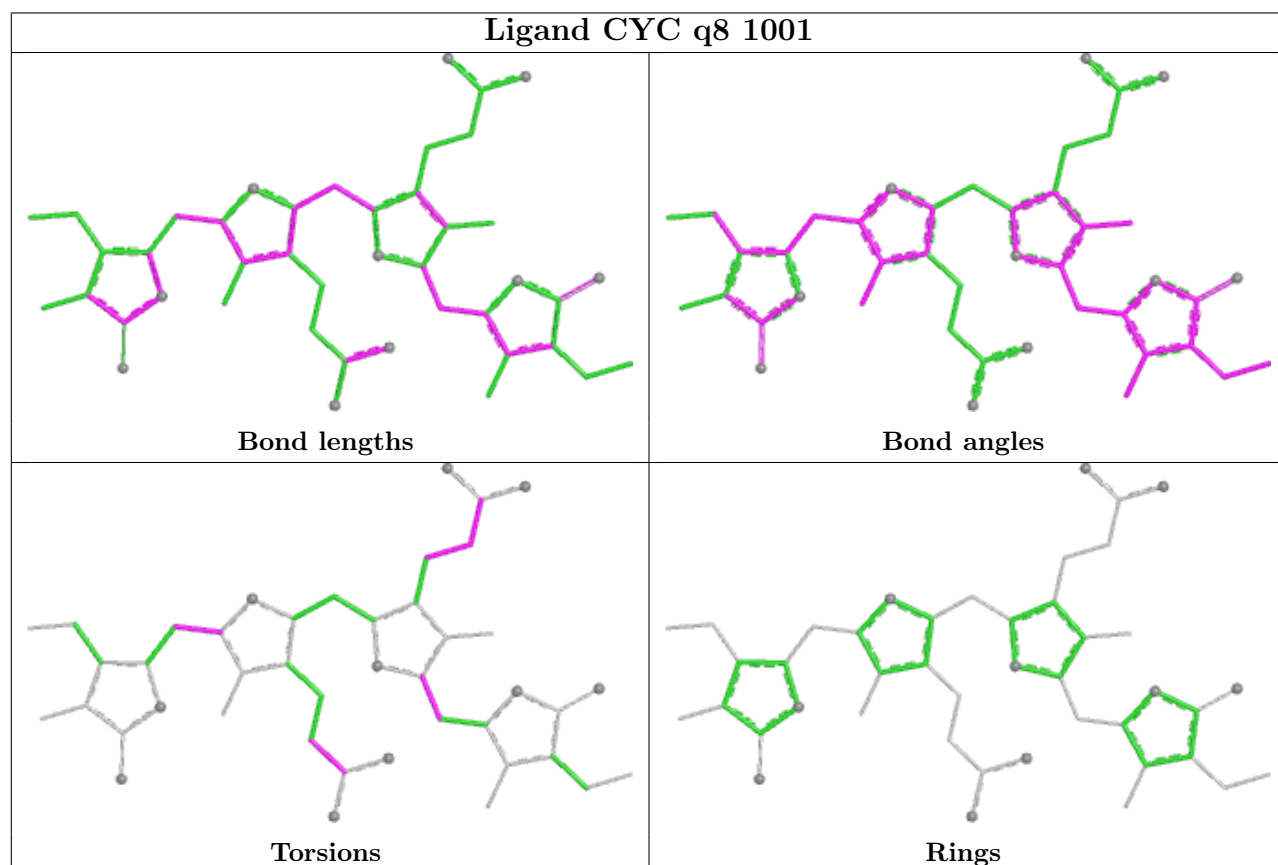
Ligand CYC UA 1001

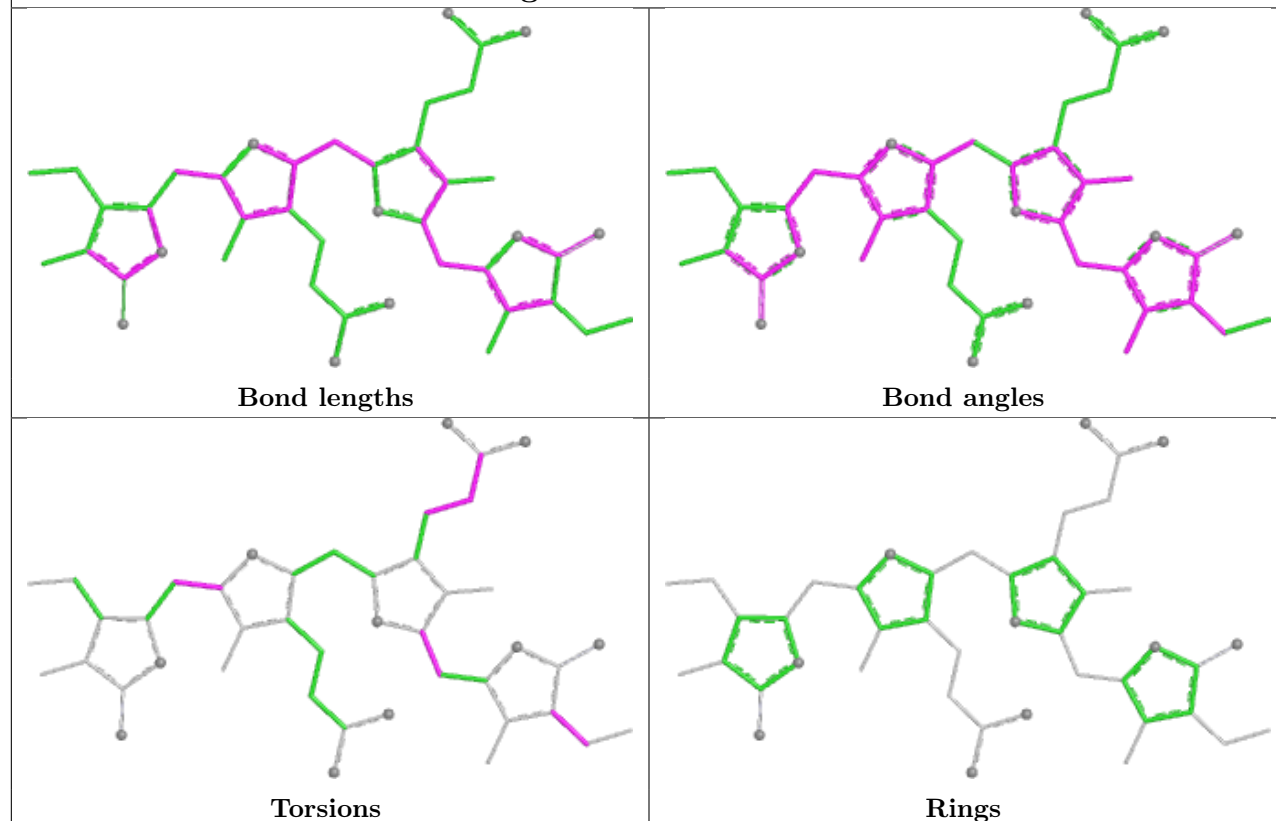
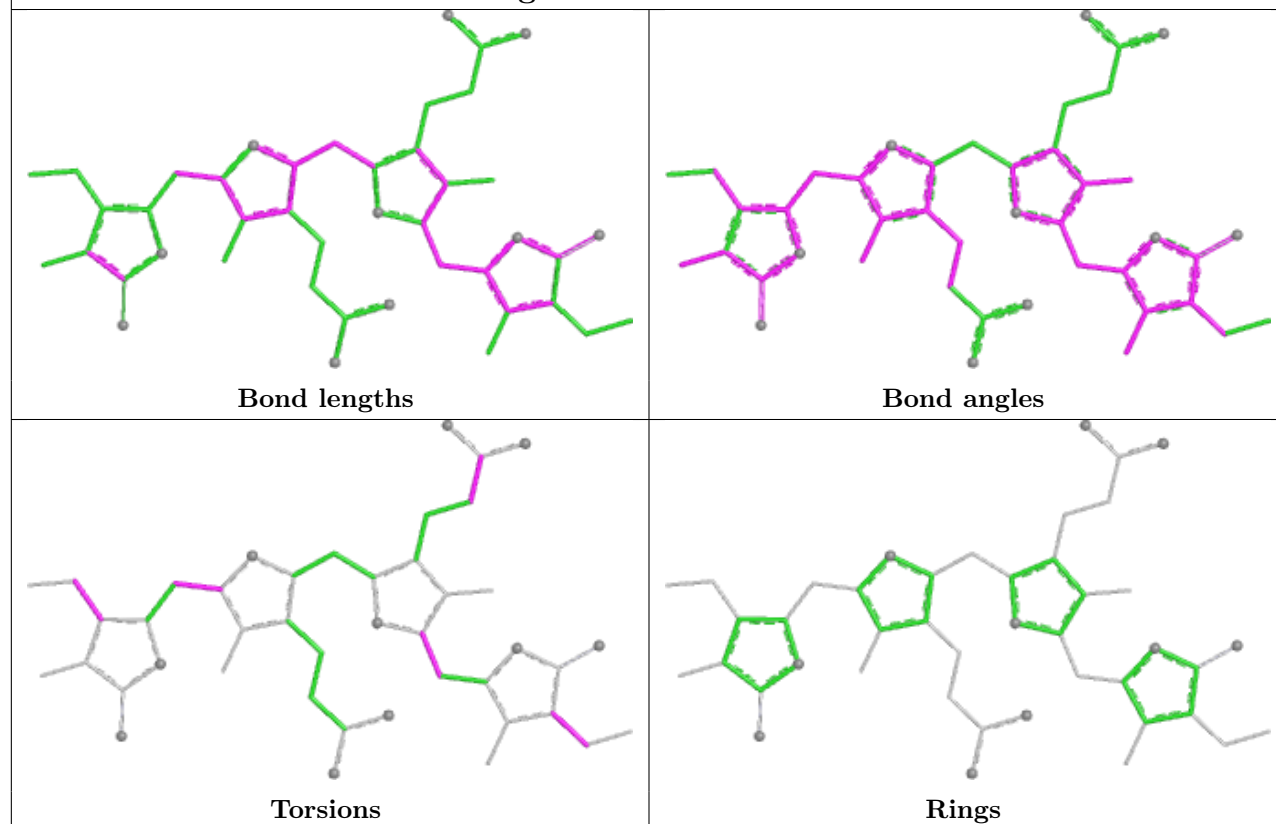


Ligand CYC M4 202

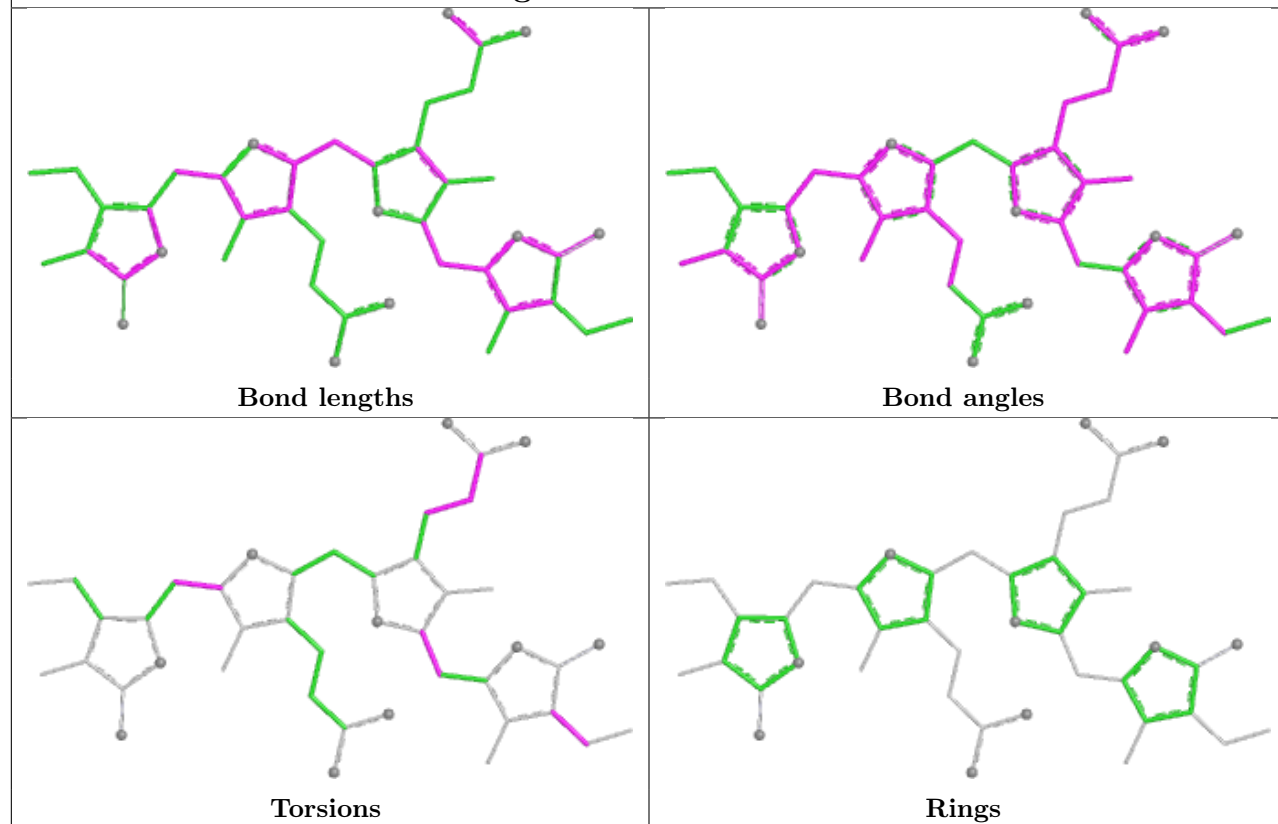


Ligand CYC q8 1001

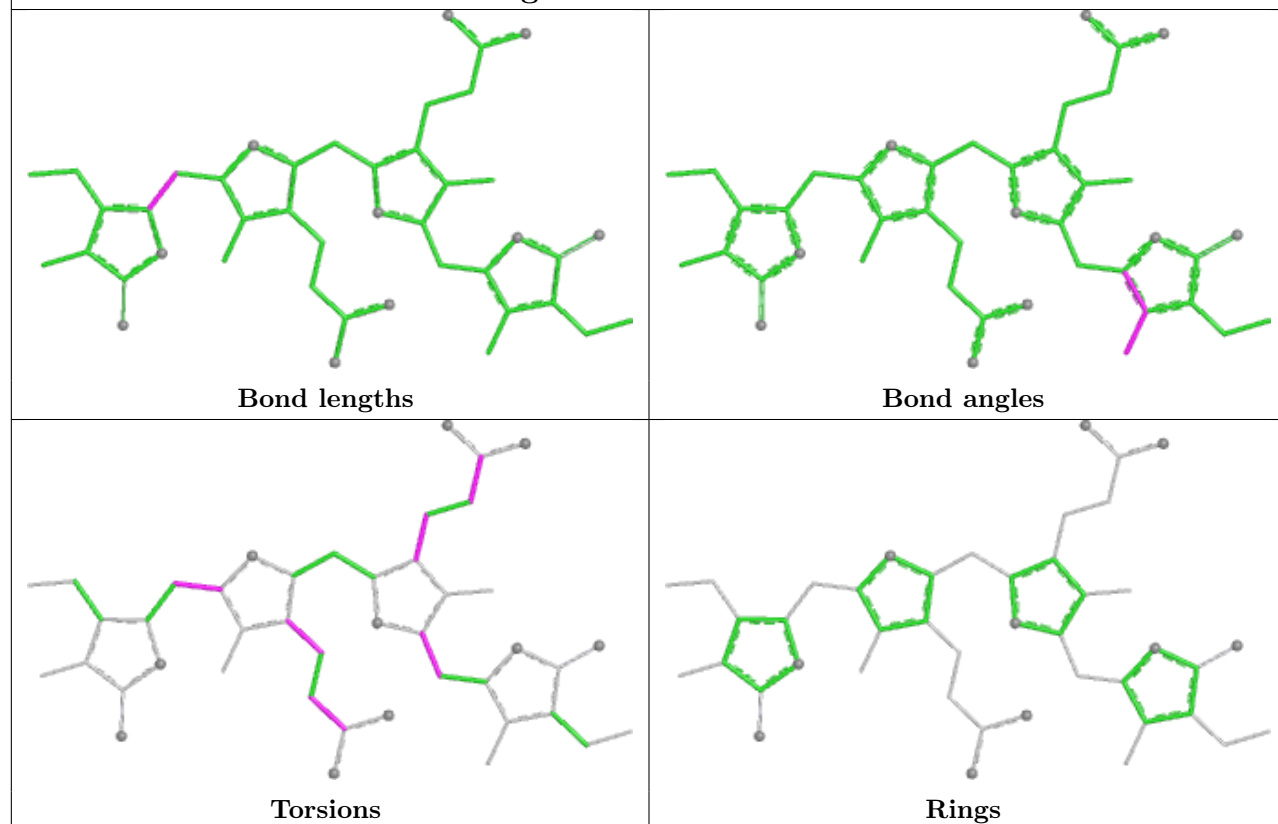


Ligand CYC A5 302**Ligand CYC I9 1001**

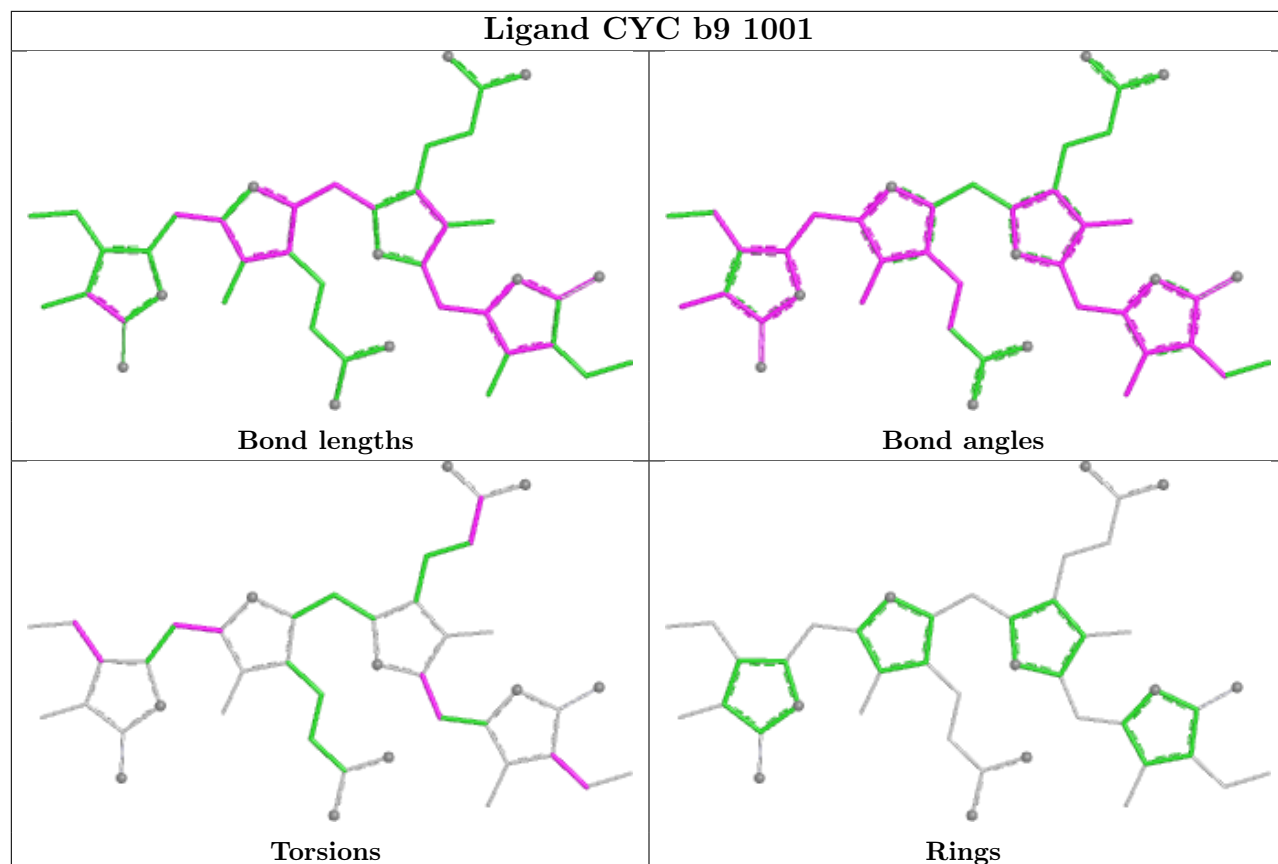
Ligand CYC F2 1001



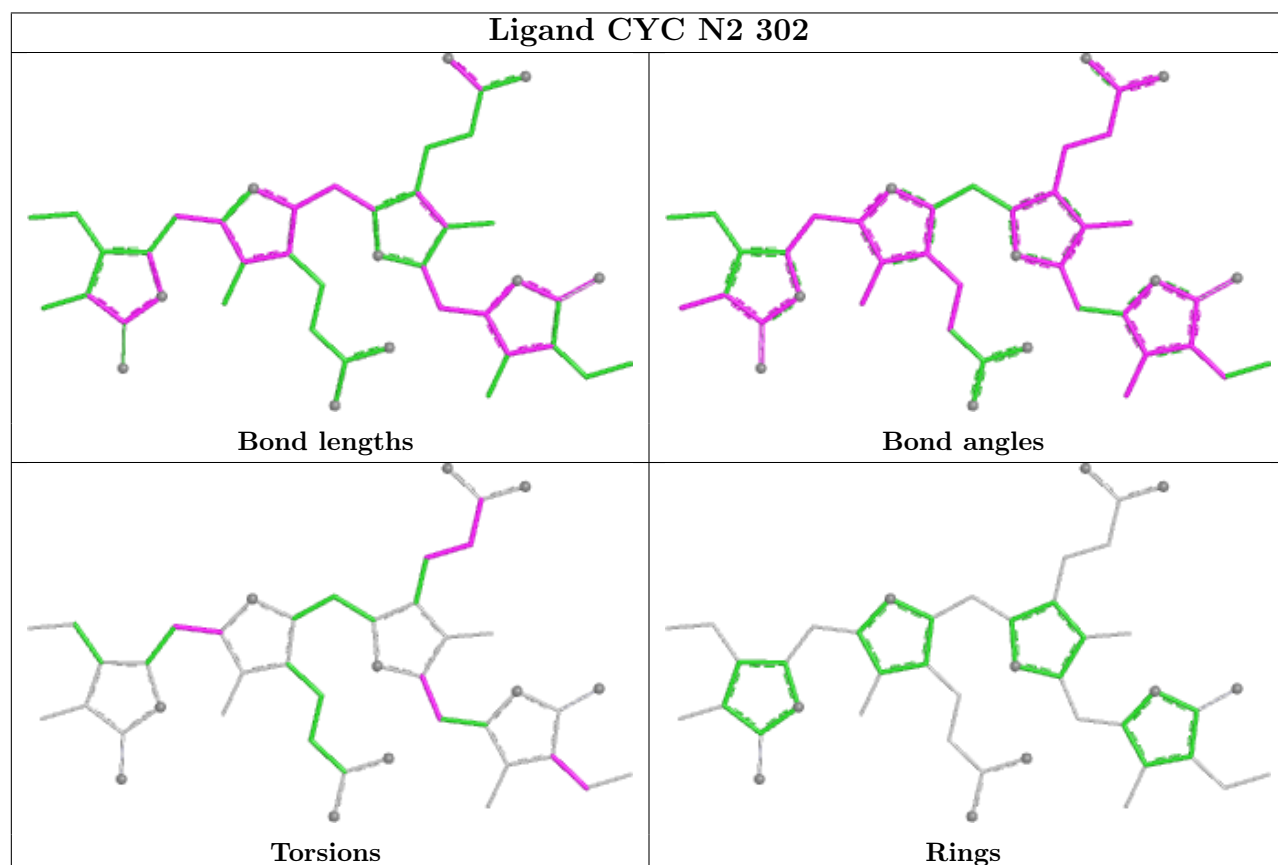
Ligand CYC C7 201



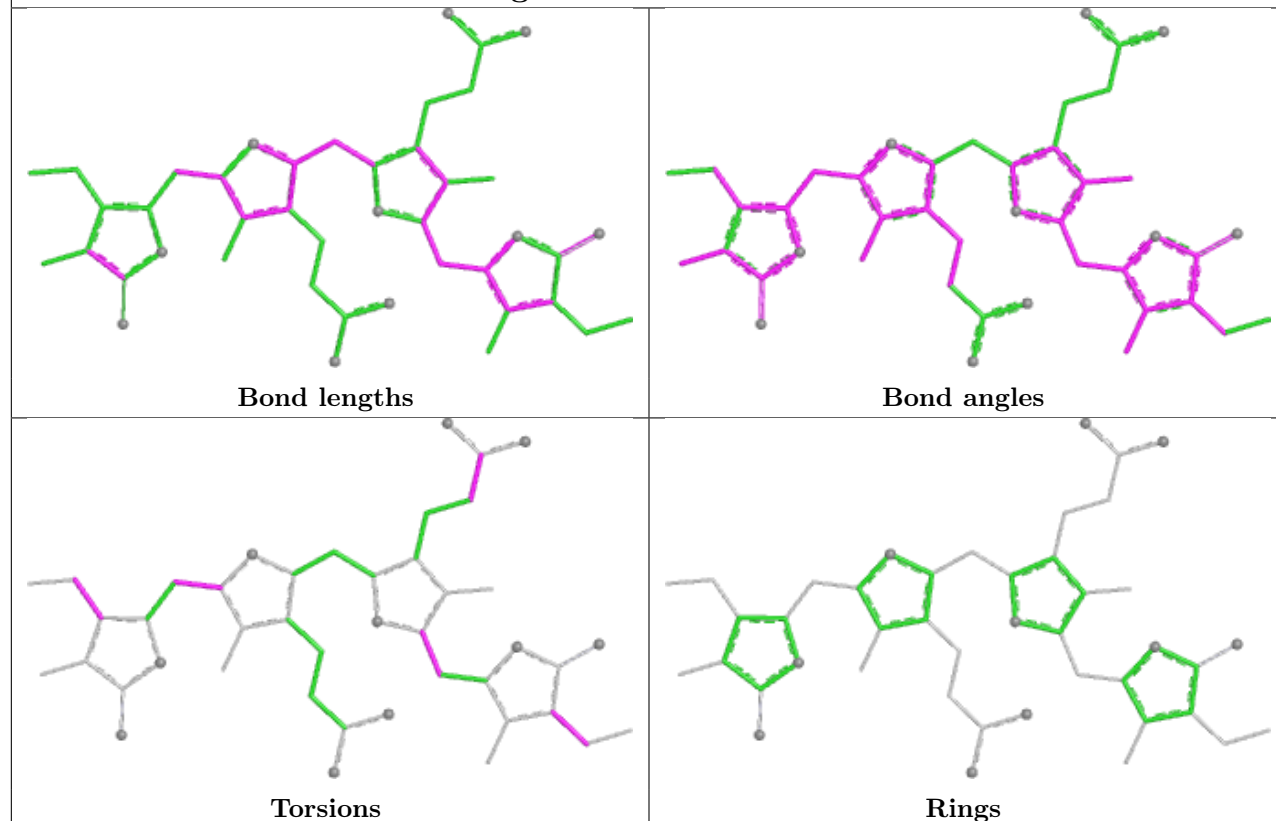
Ligand CYC b9 1001



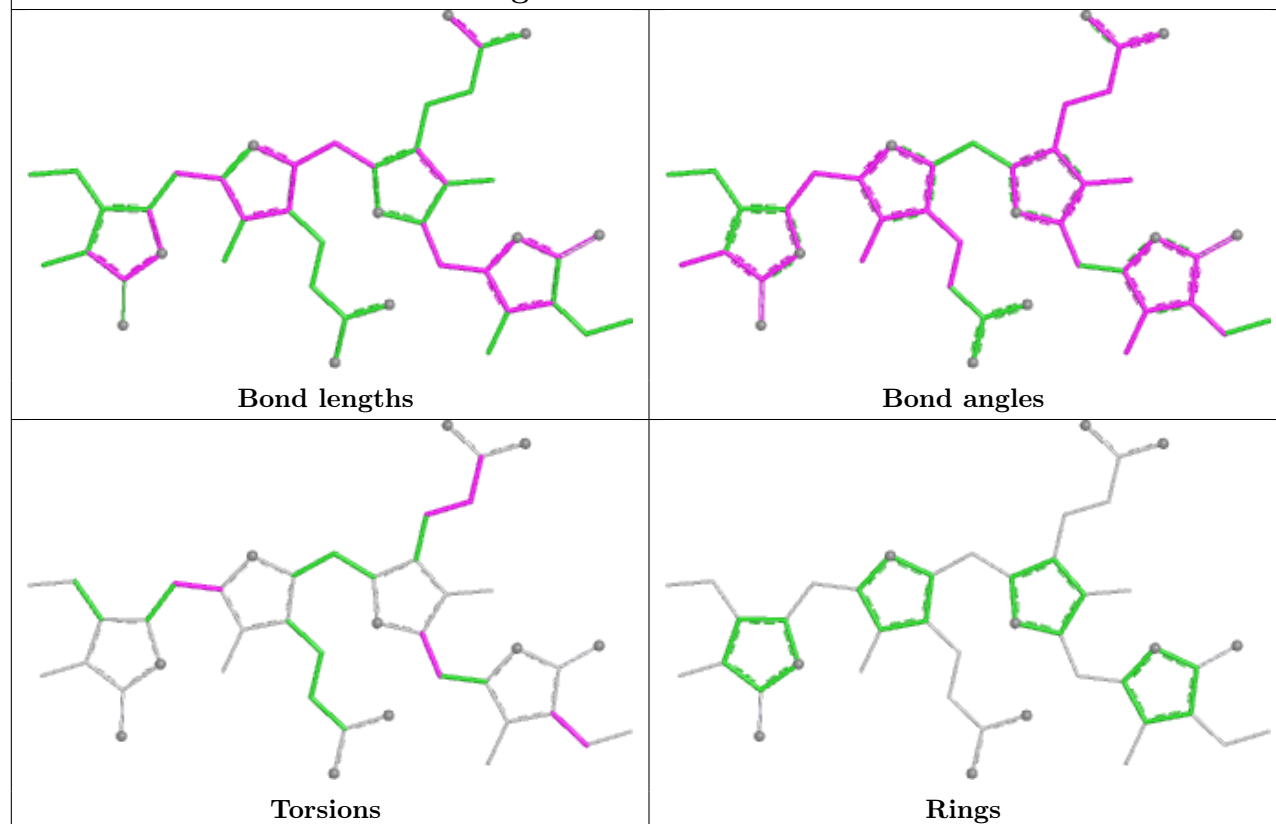
Ligand CYC N2 302



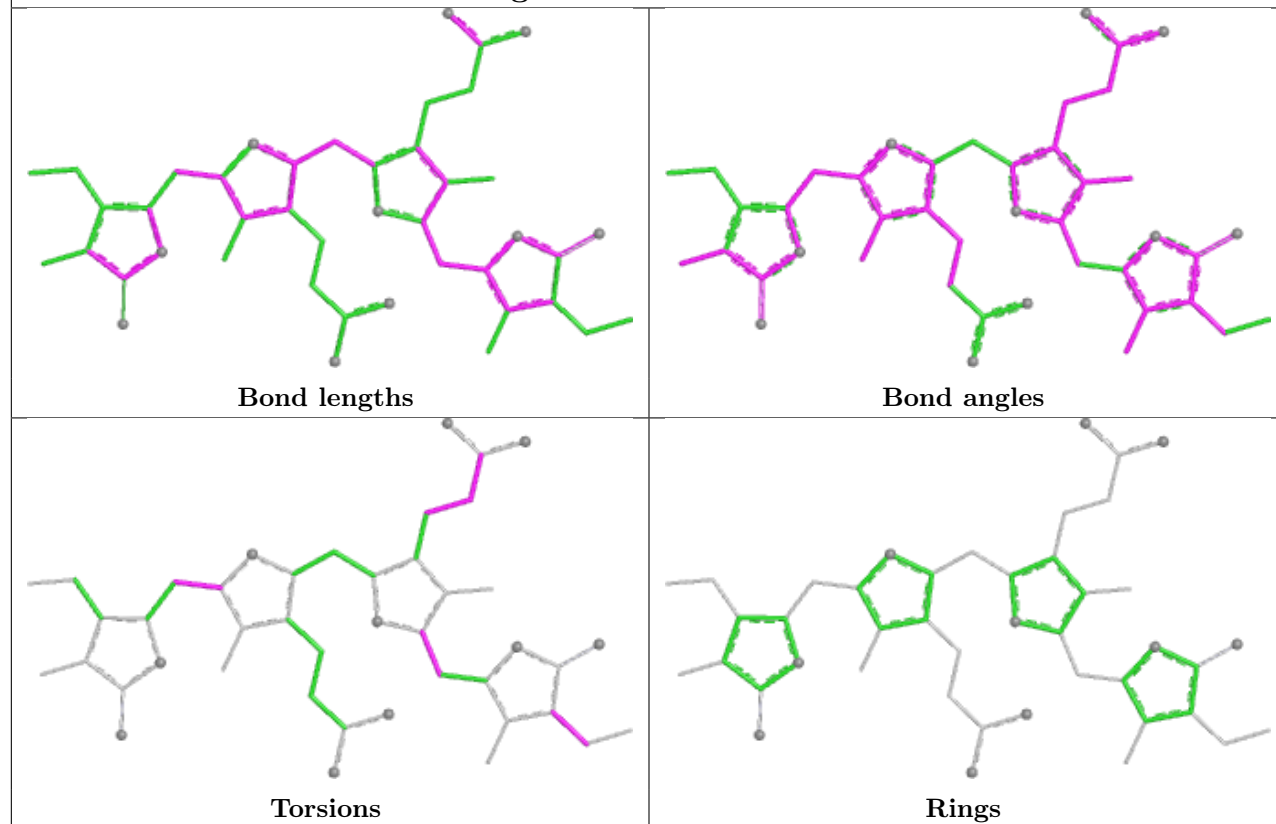
Ligand CYC G9 1001



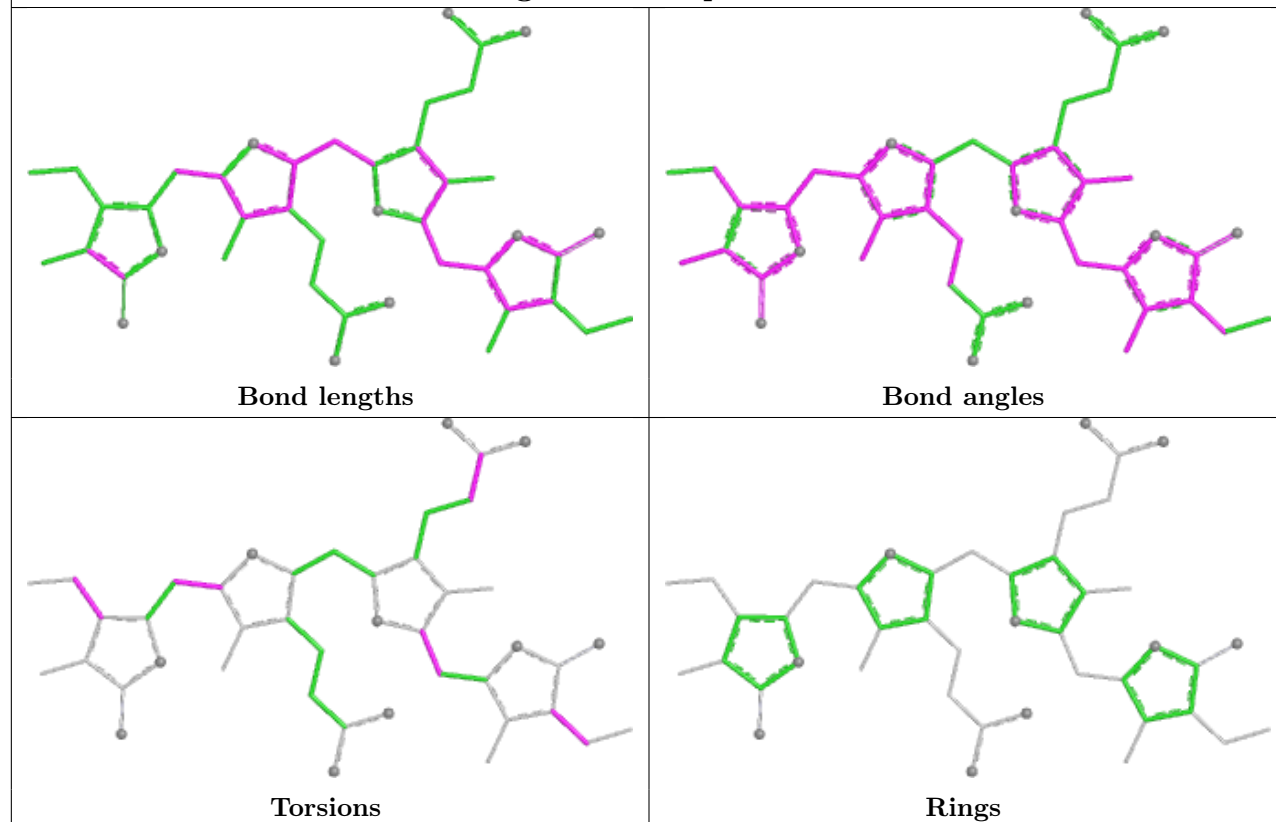
Ligand CYC D4 1001



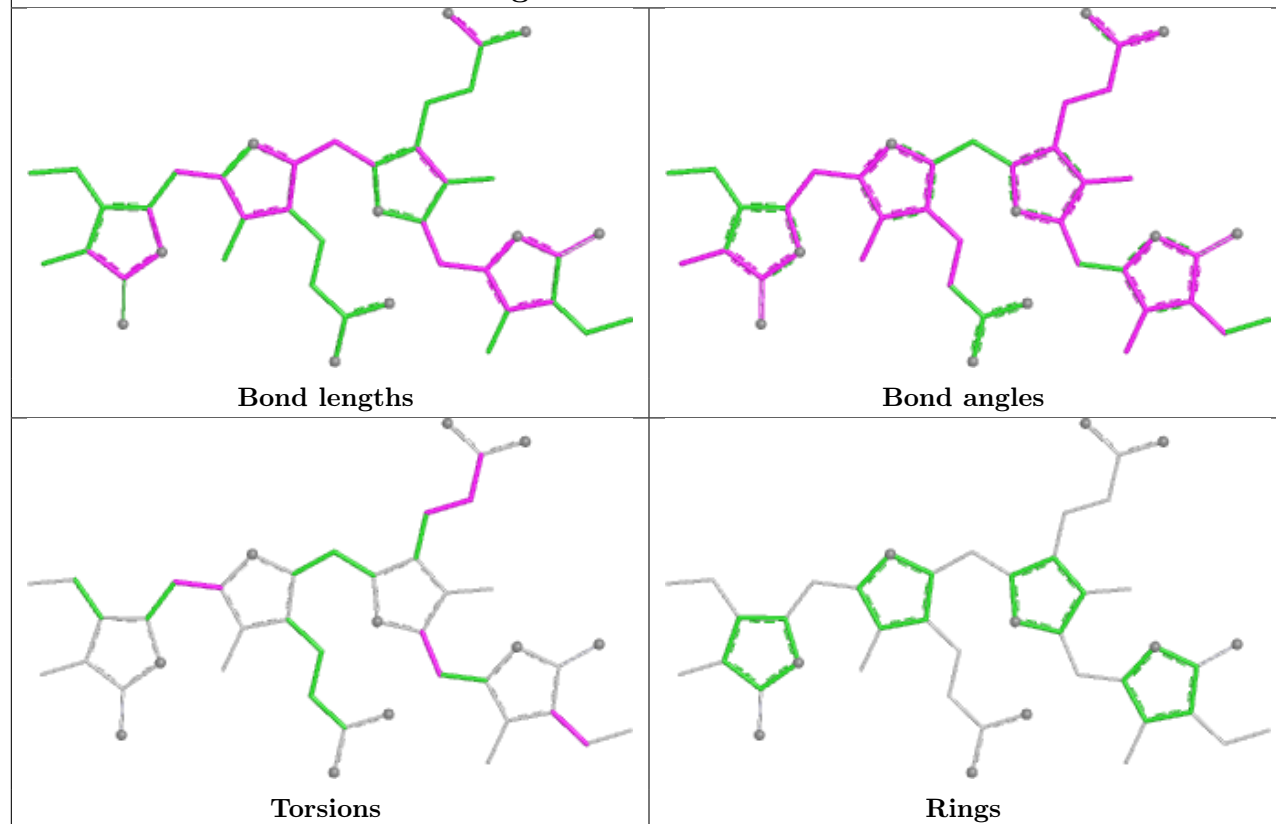
Ligand CYC H1 1001



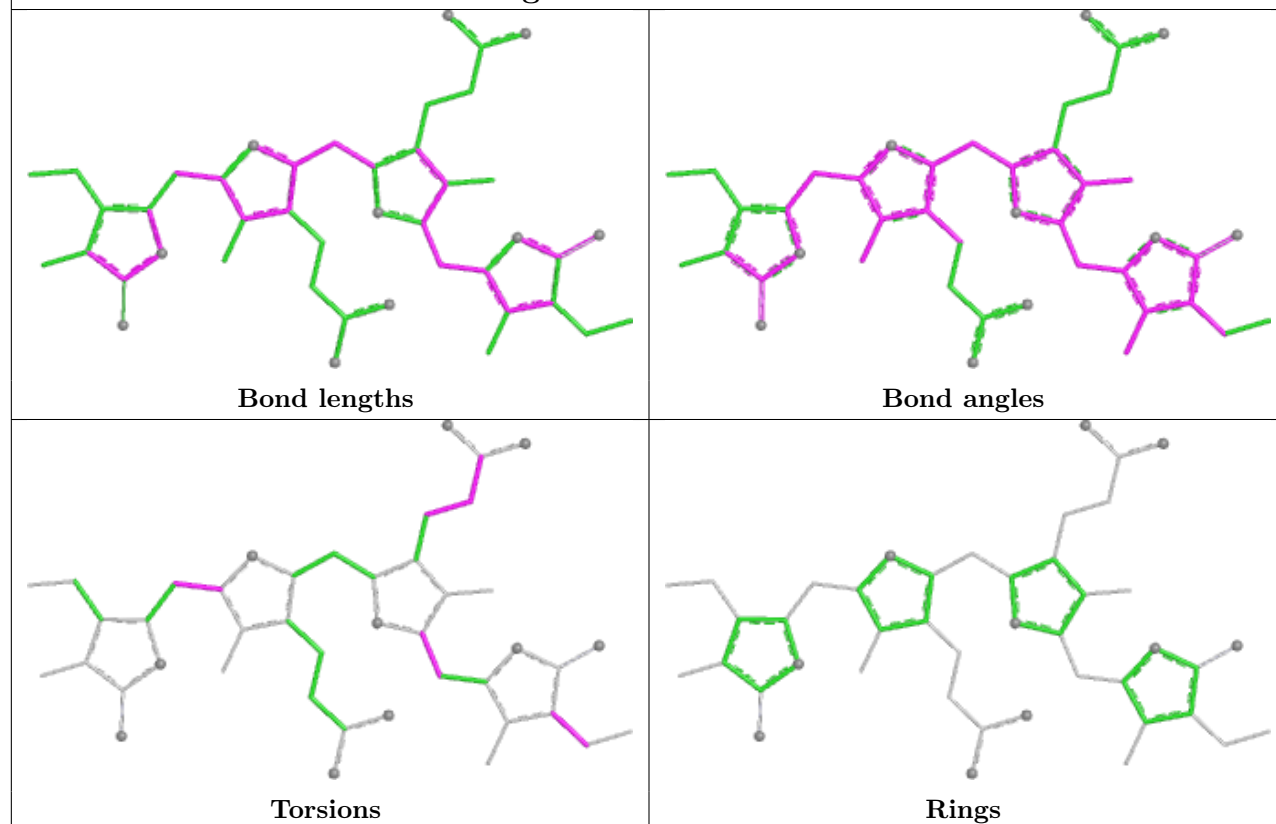
Ligand CYC q9 1001



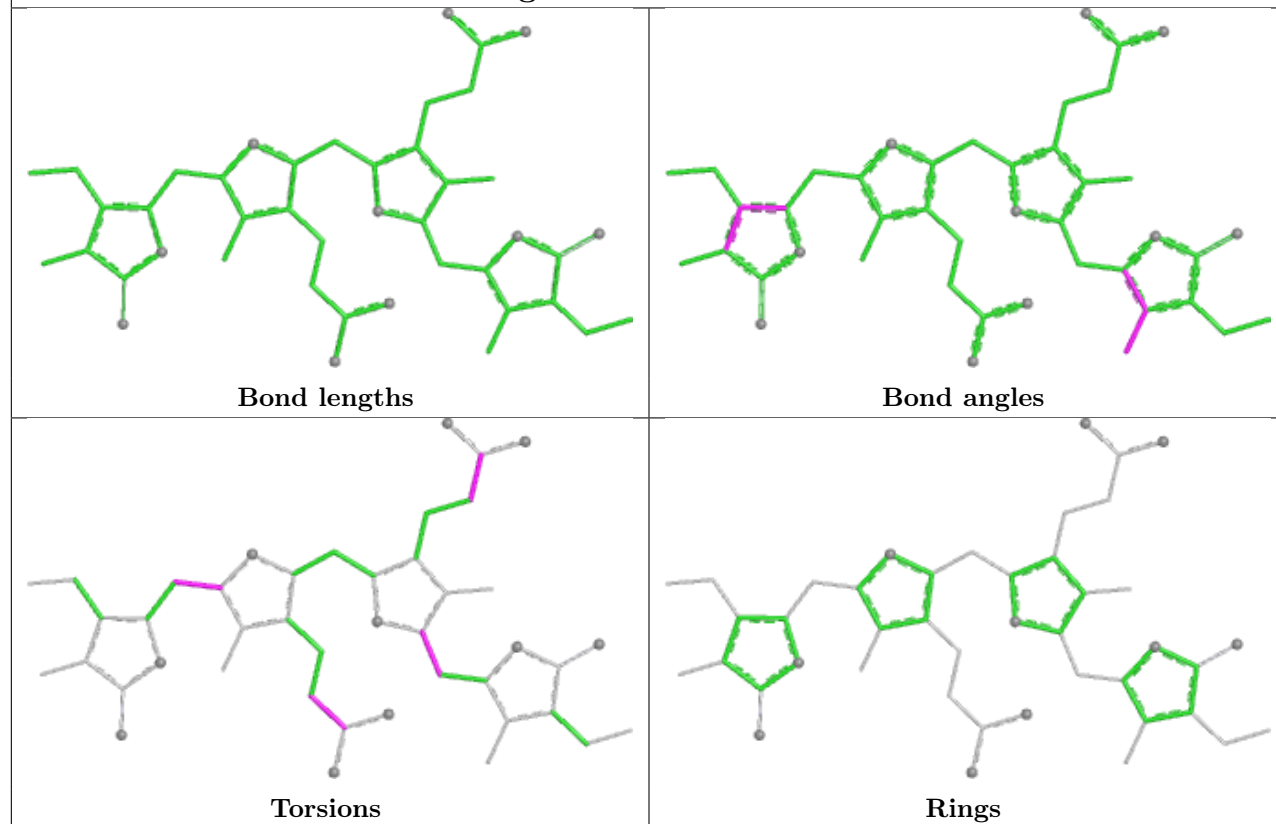
Ligand CYC U4 1001



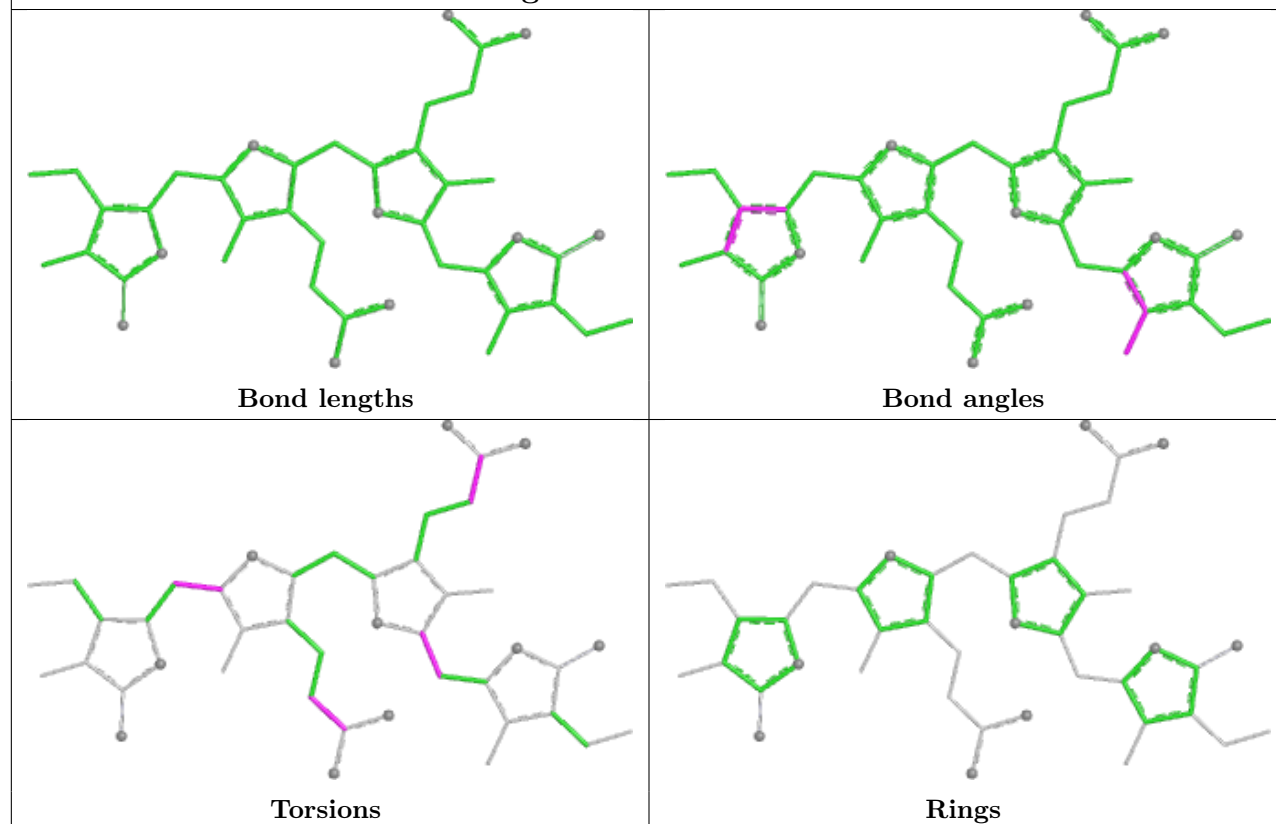
Ligand CYC E3 201



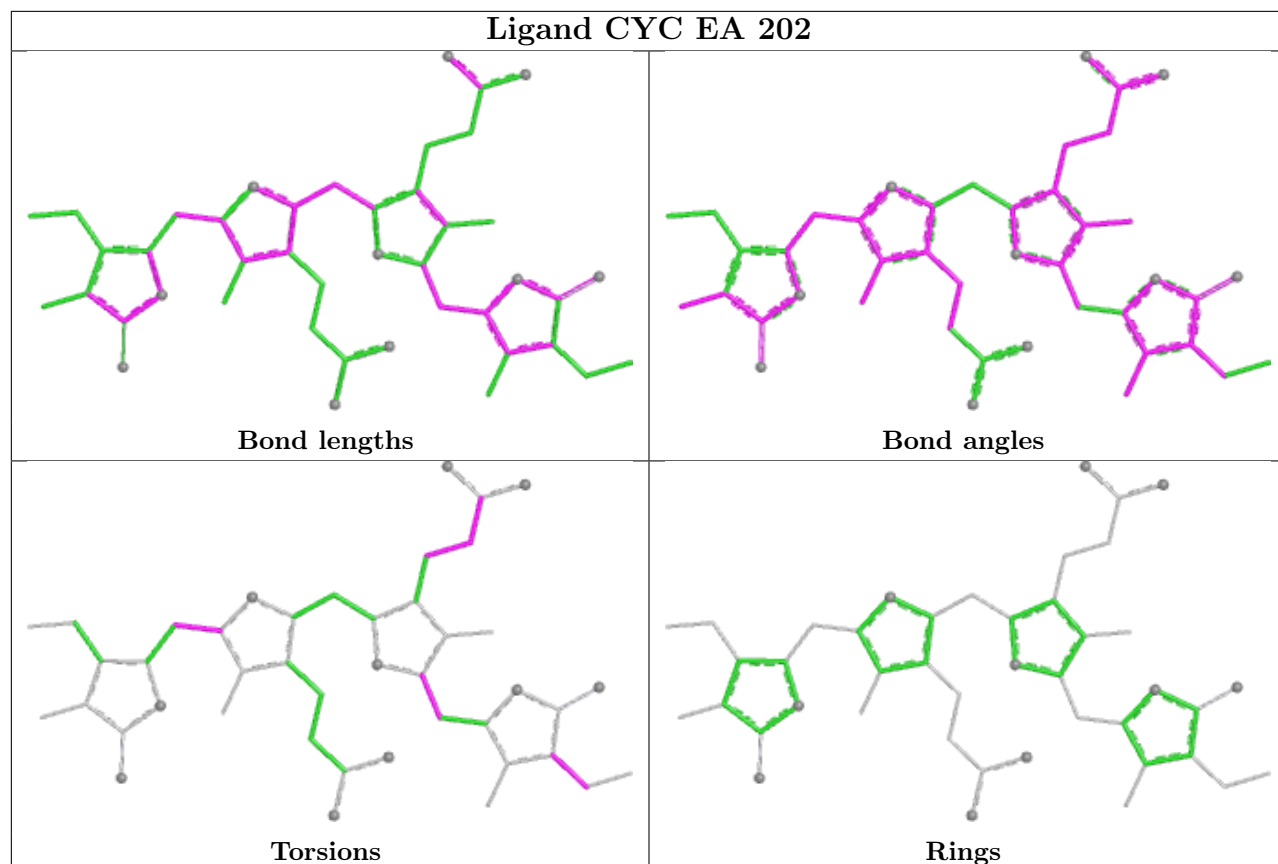
Ligand CYC PA 201



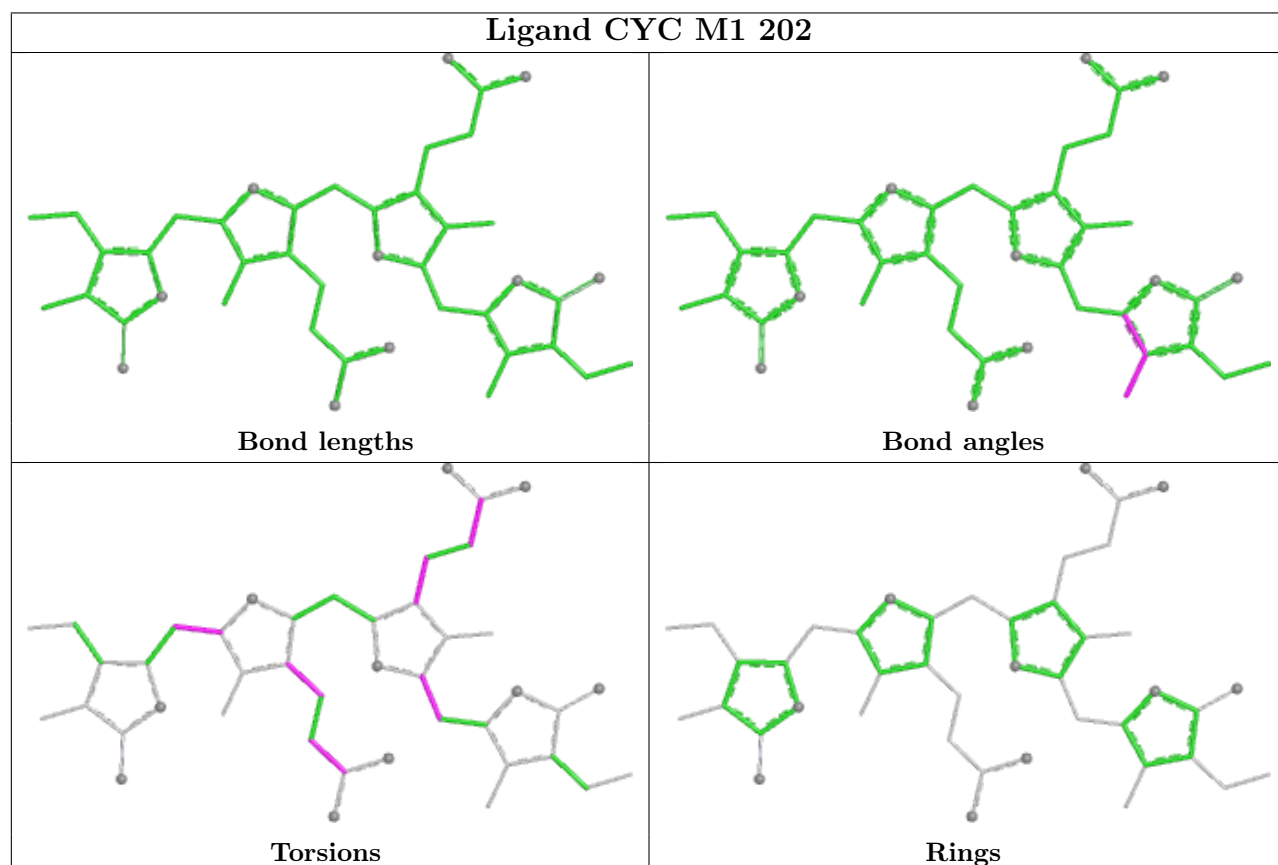
Ligand CYC P6 201



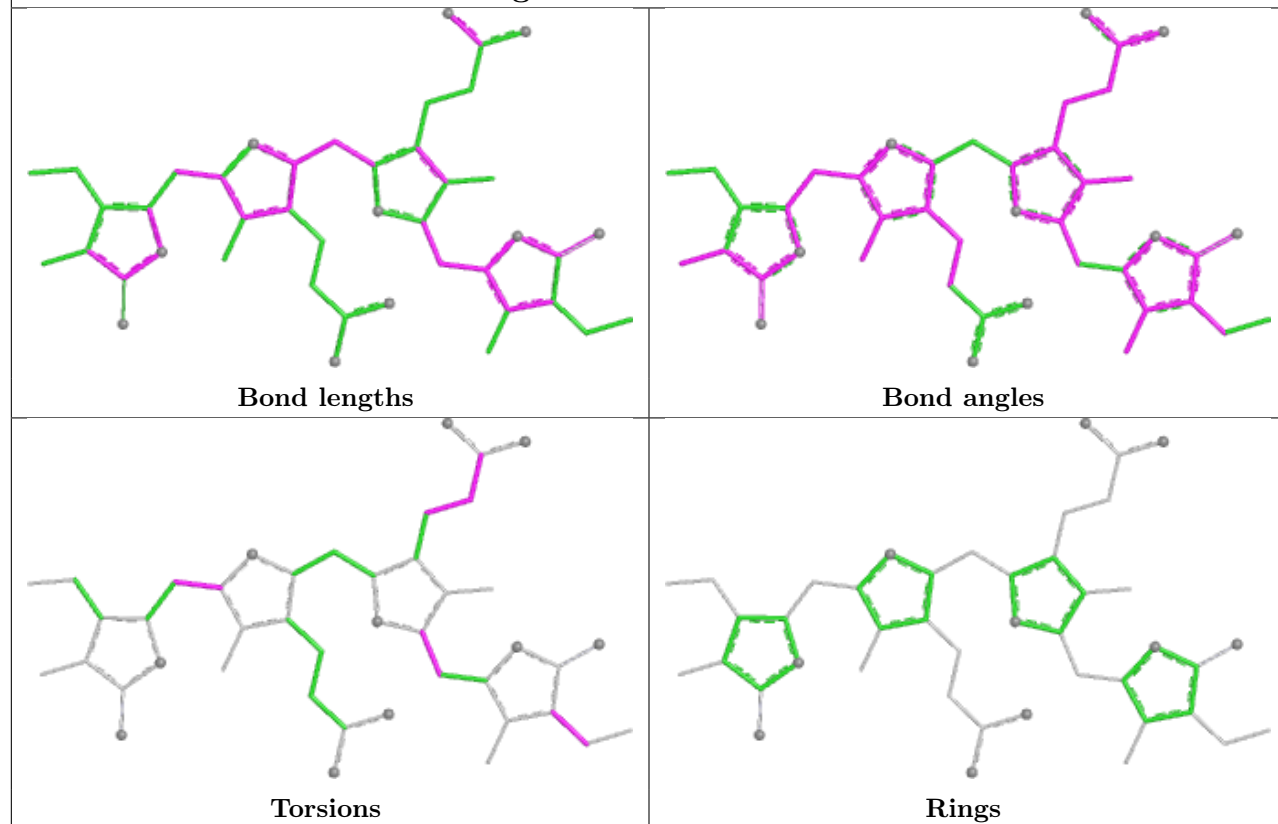
Ligand CYC EA 202



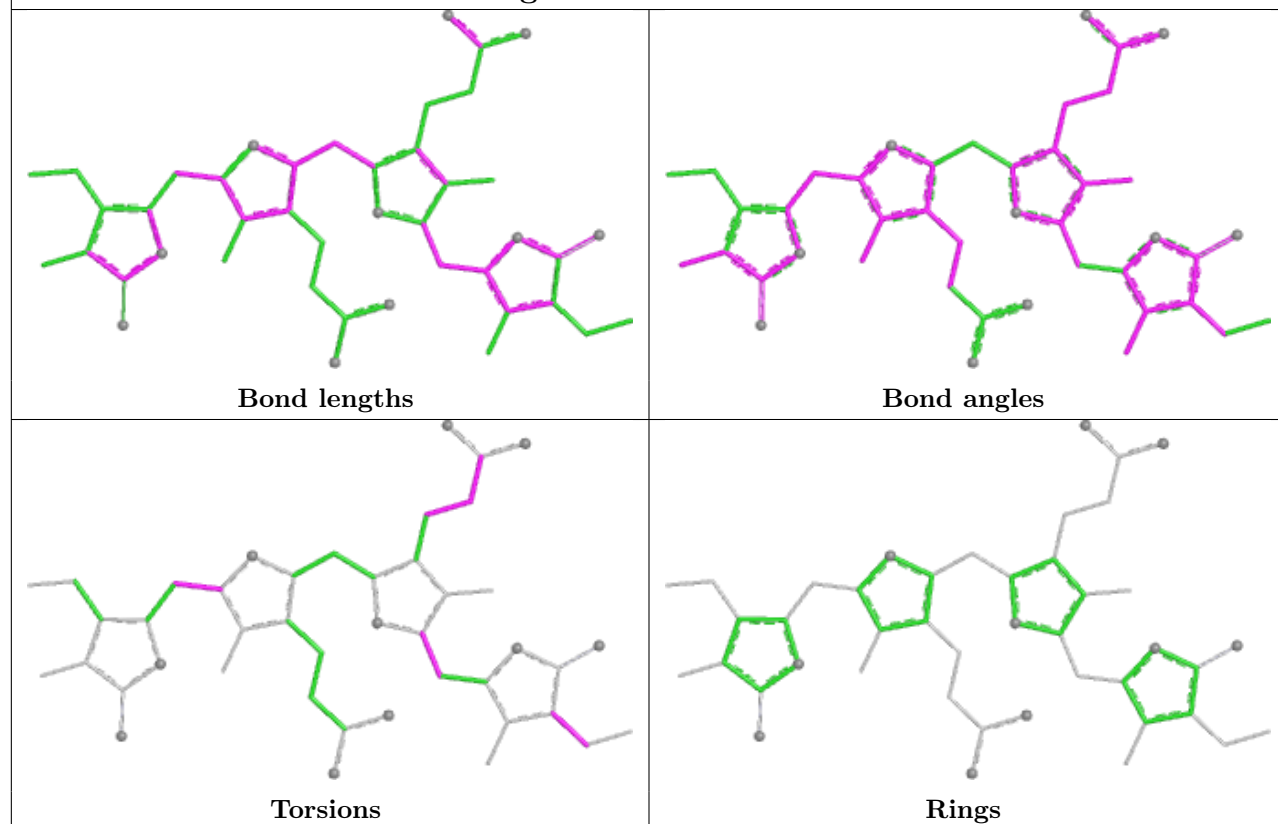
Ligand CYC M1 202



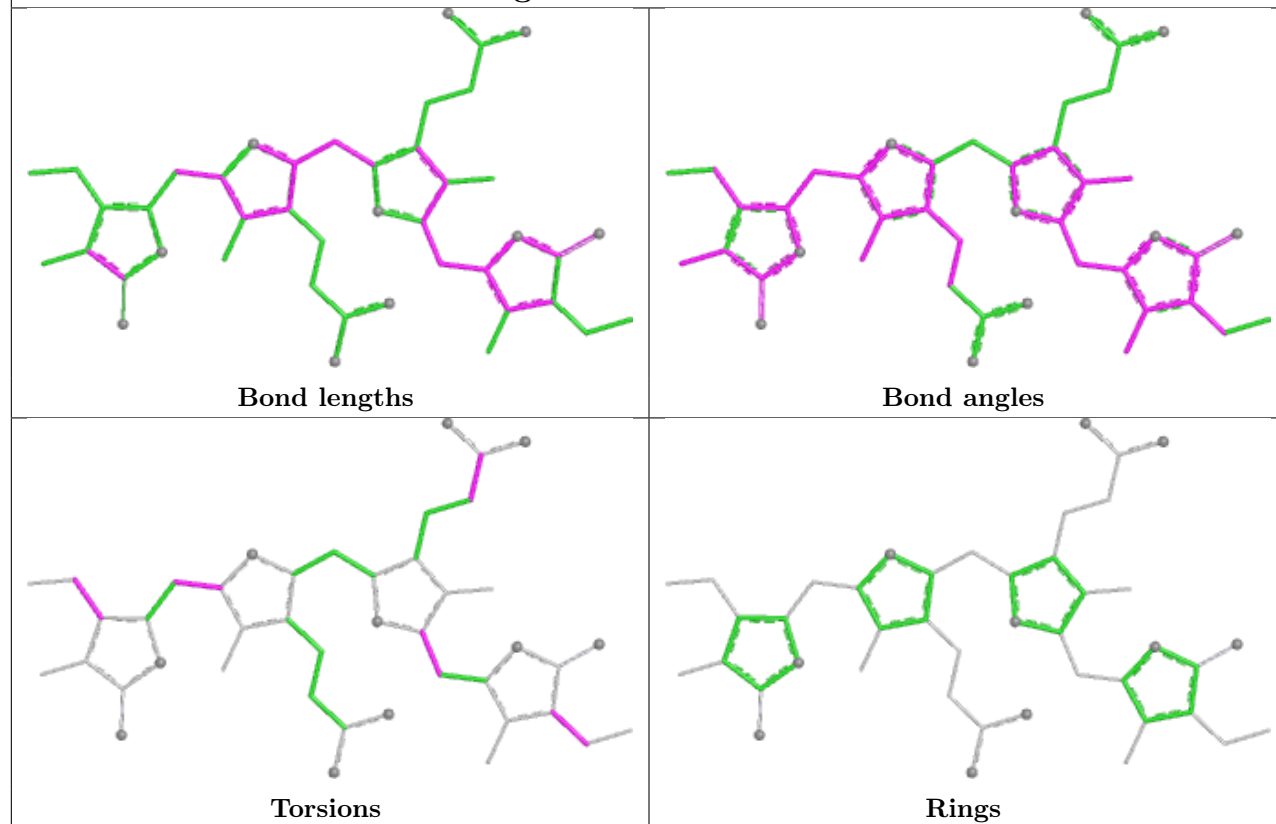
Ligand CYC B5 1001



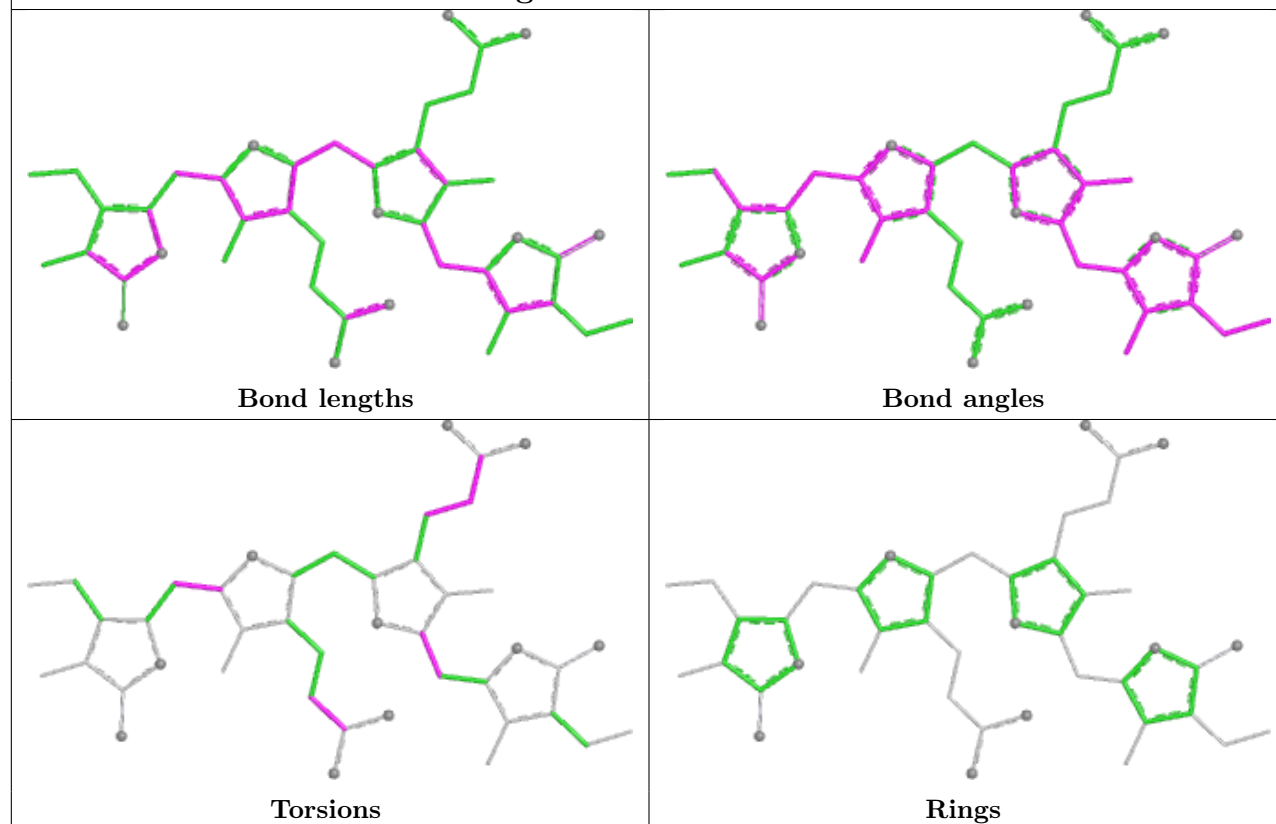
Ligand CYC G4 202



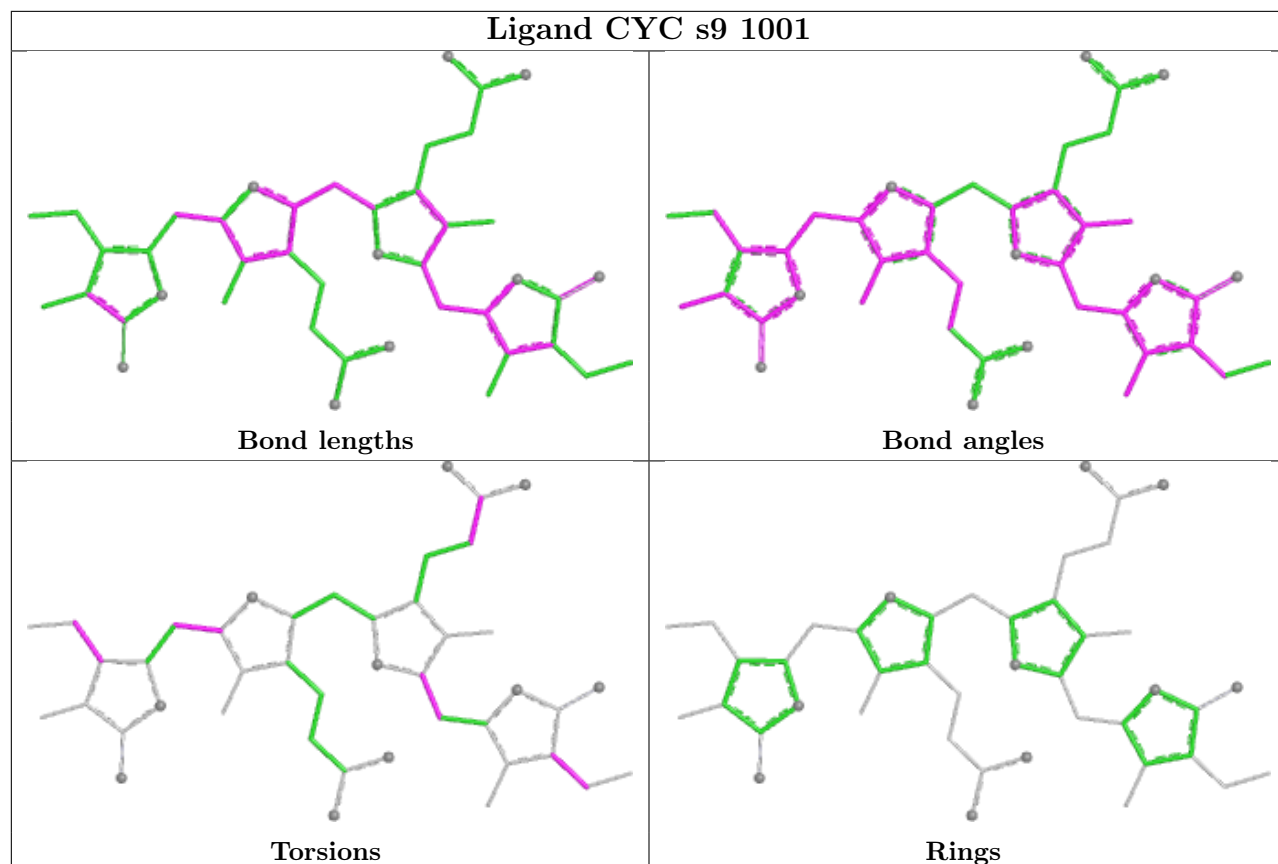
Ligand CYC Z9 1001



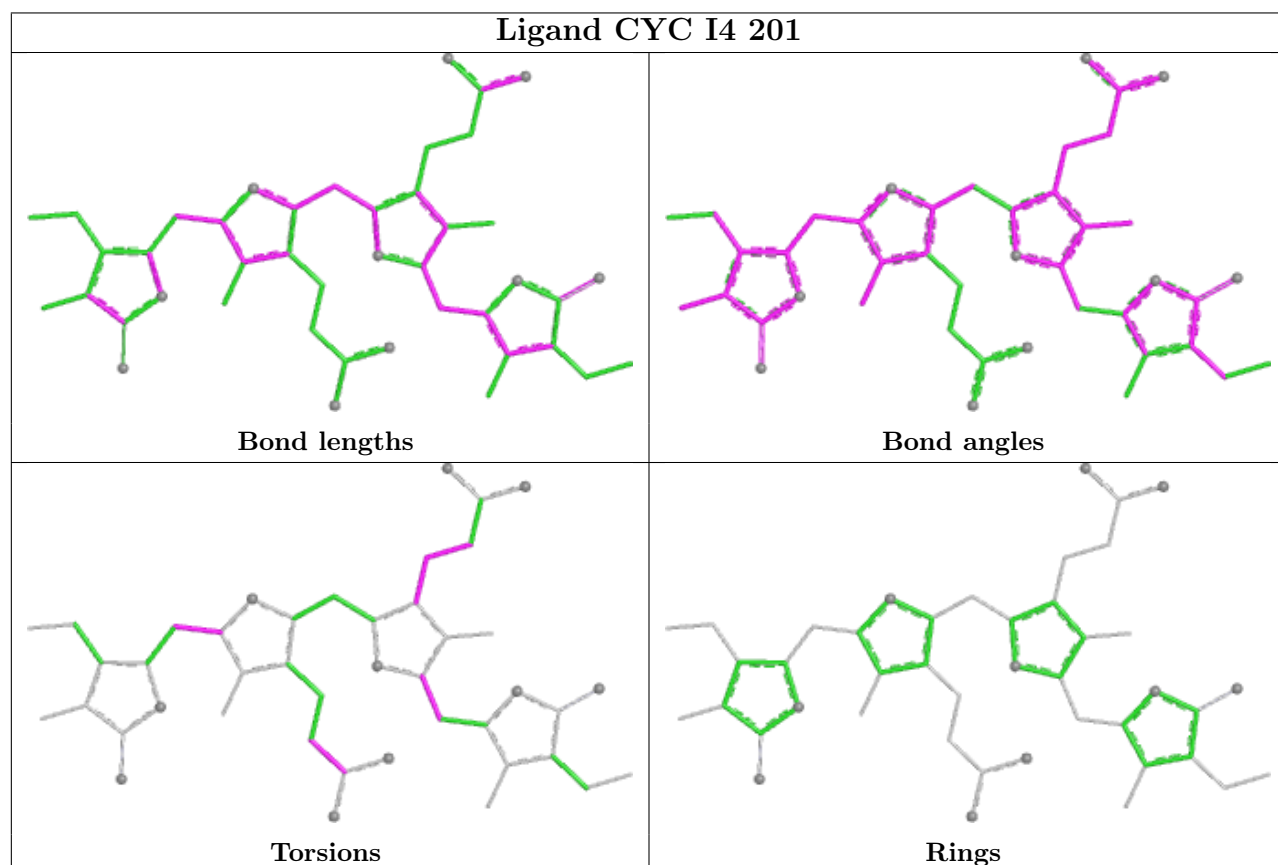
Ligand CYC 09 1201



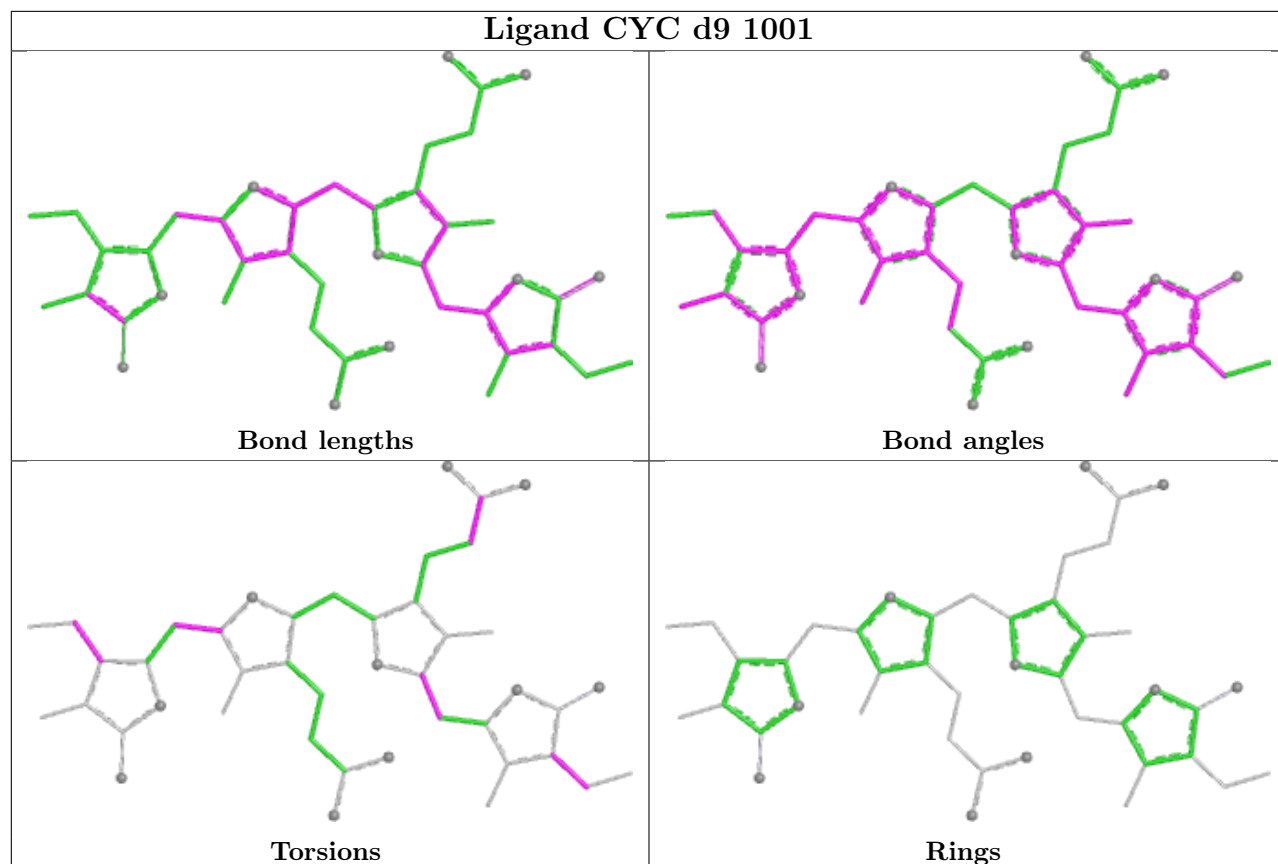
Ligand CYC s9 1001



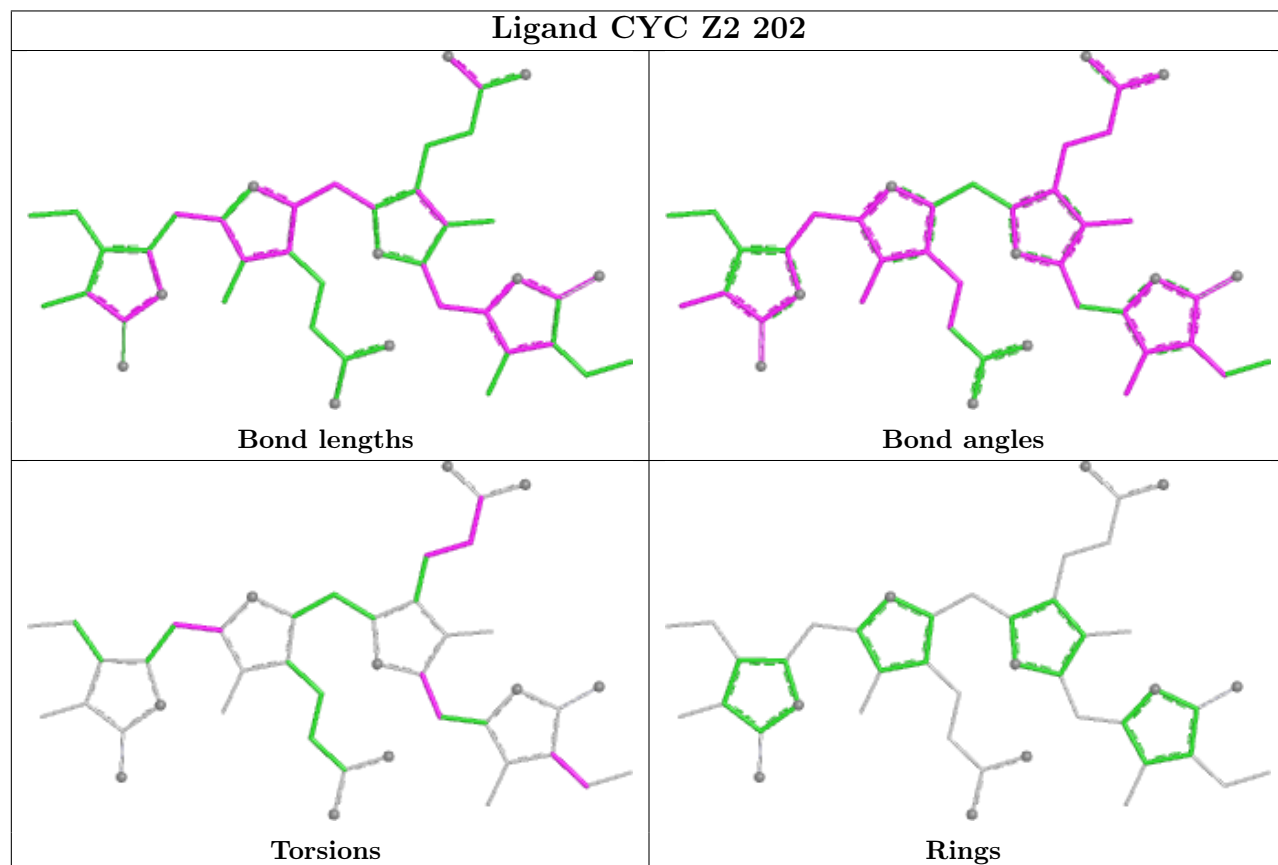
Ligand CYC I4 201

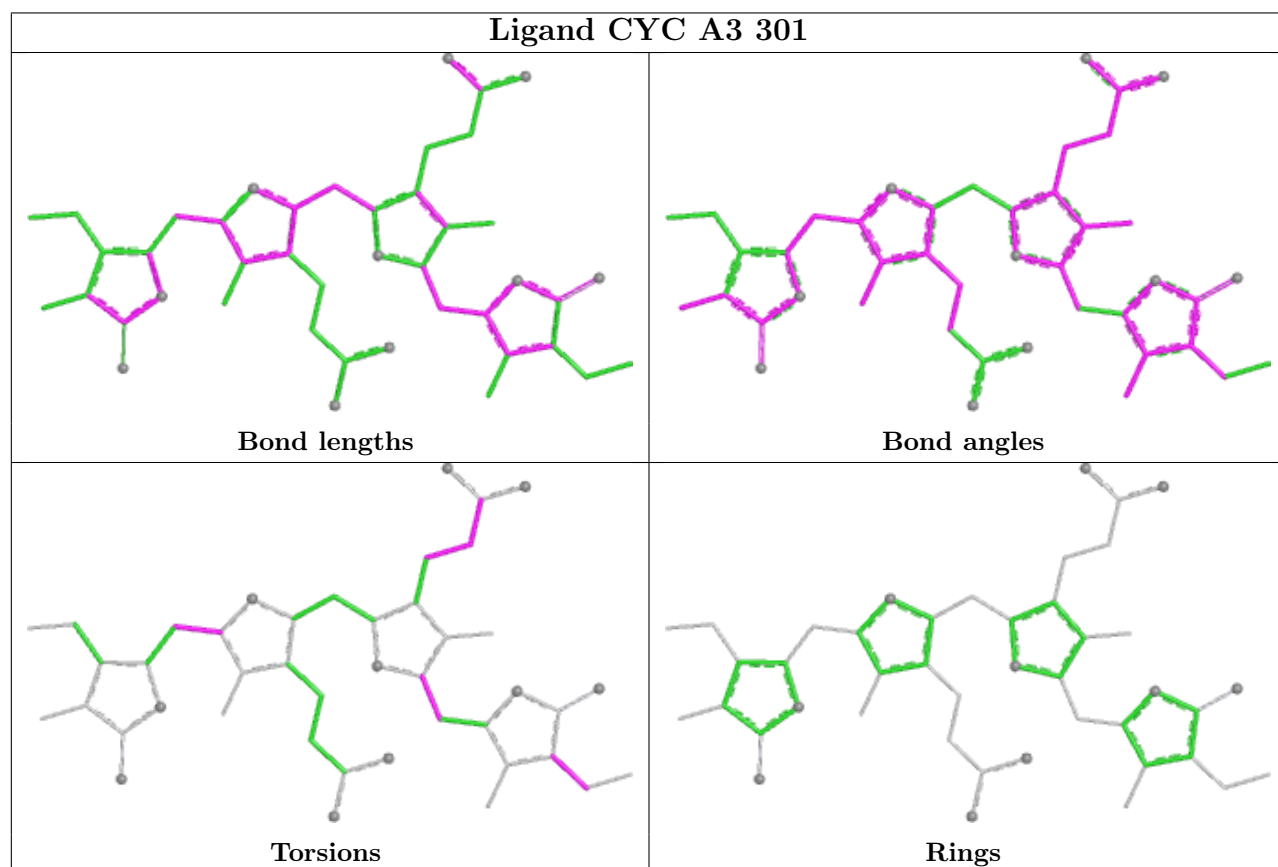
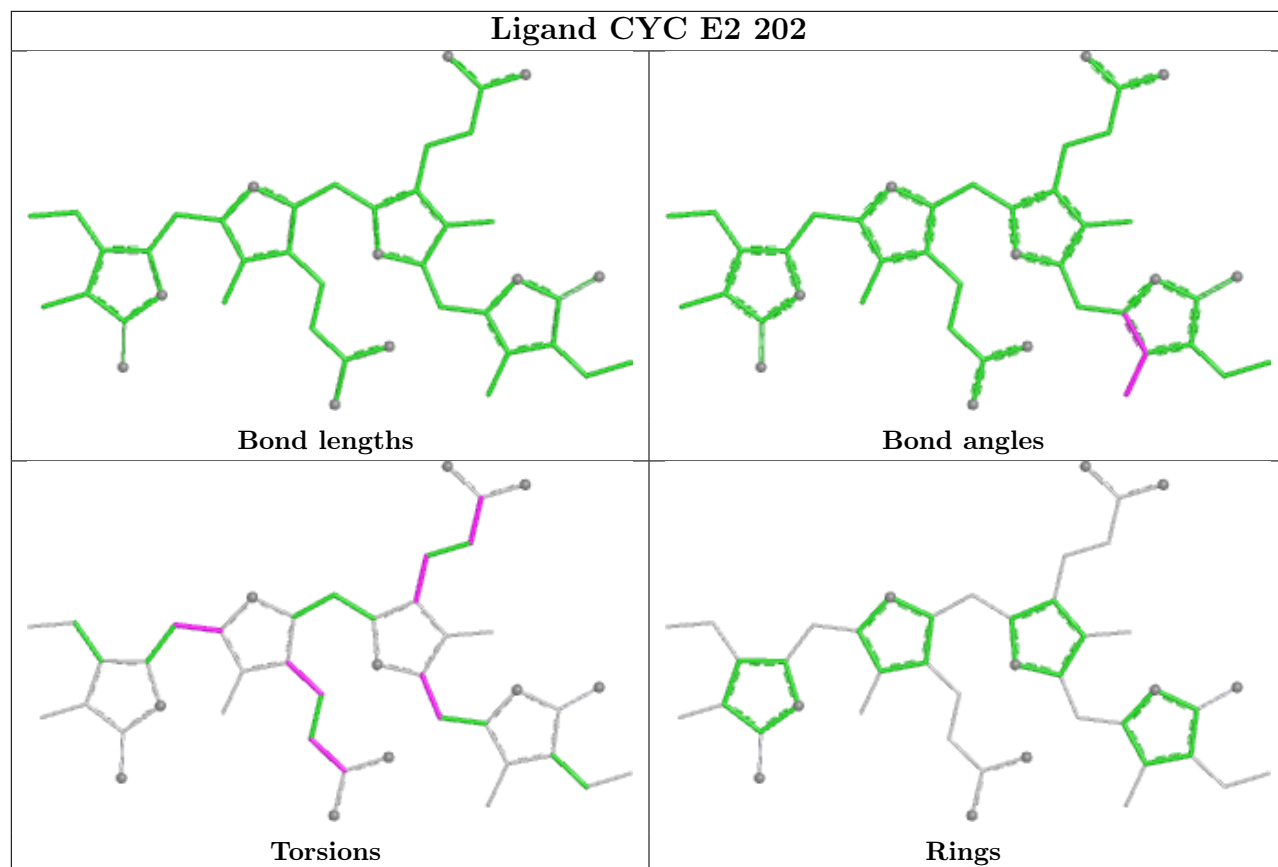


Ligand CYC d9 1001

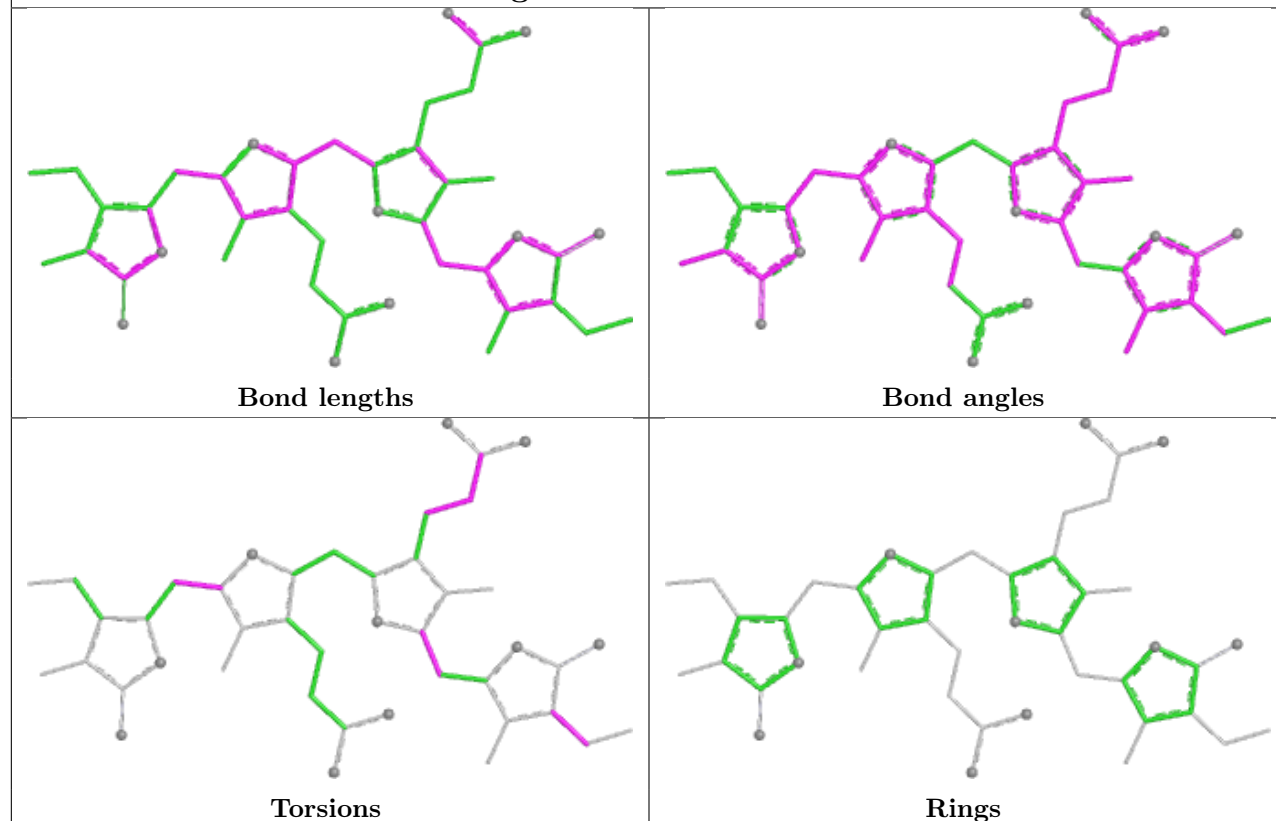


Ligand CYC Z2 202

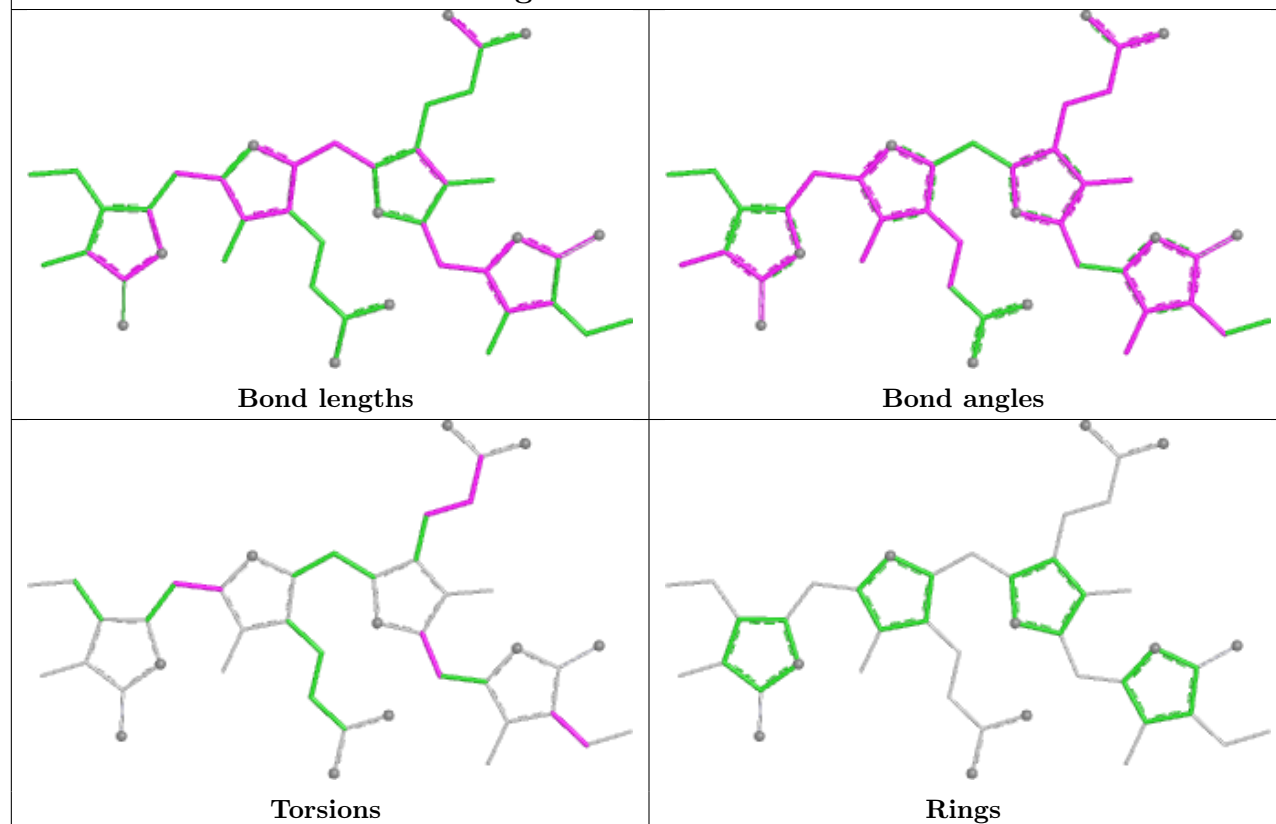




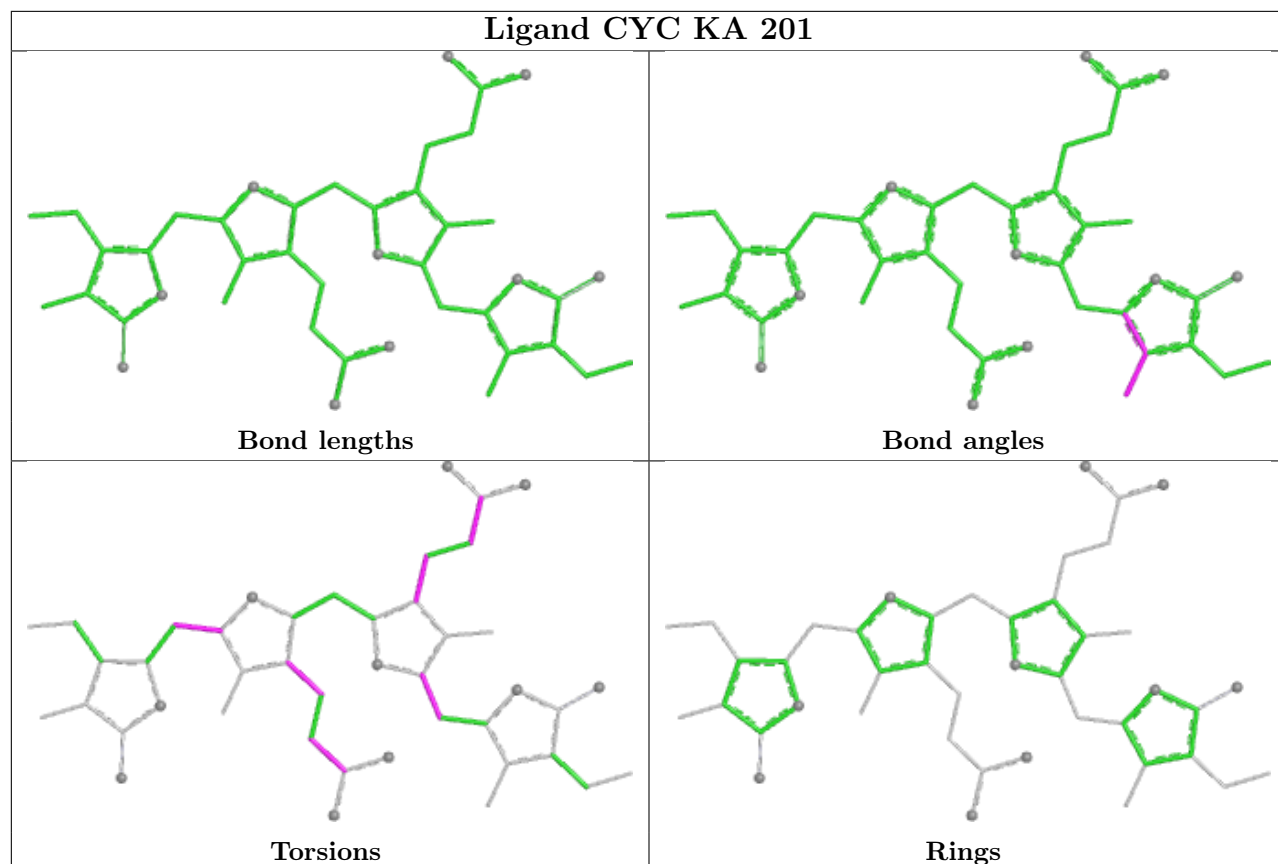
Ligand CYC H2 1001



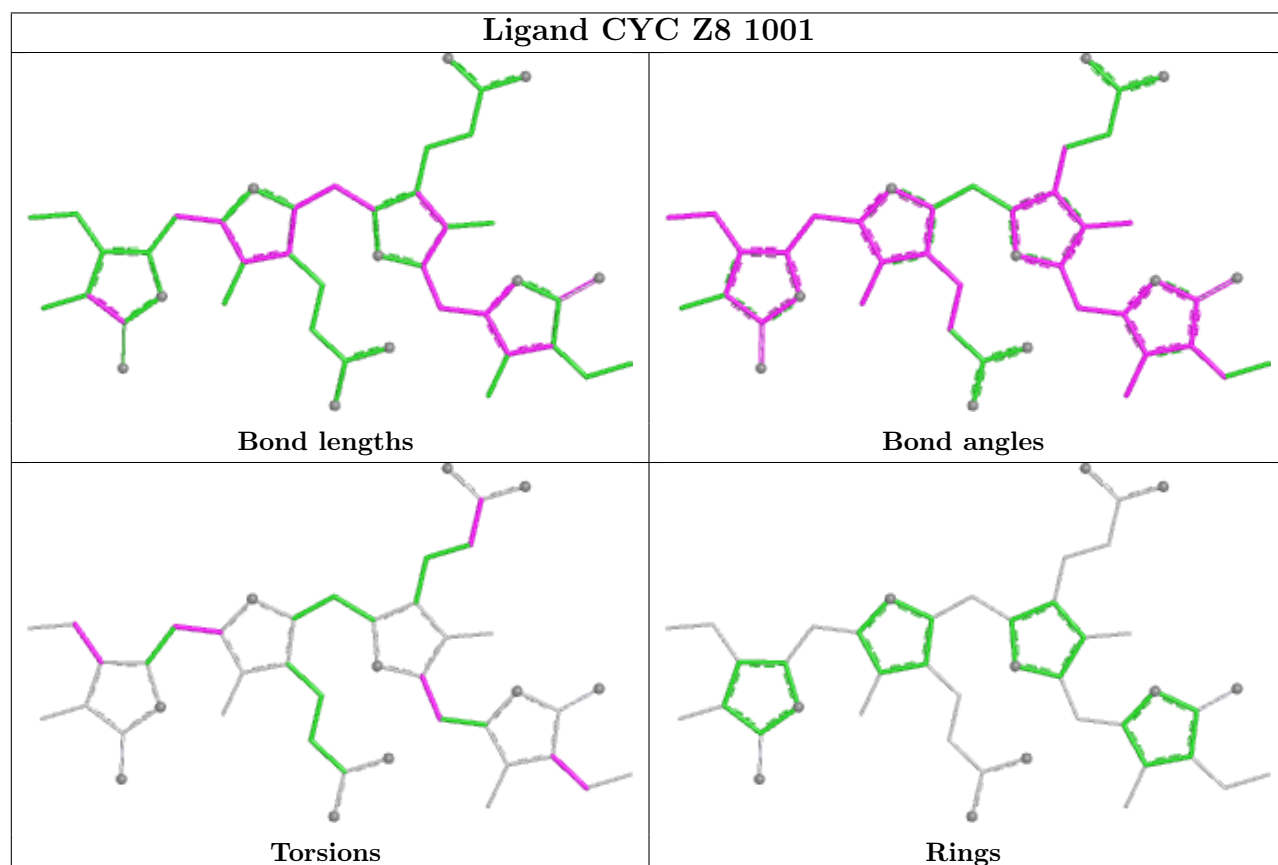
Ligand CYC S5 1001

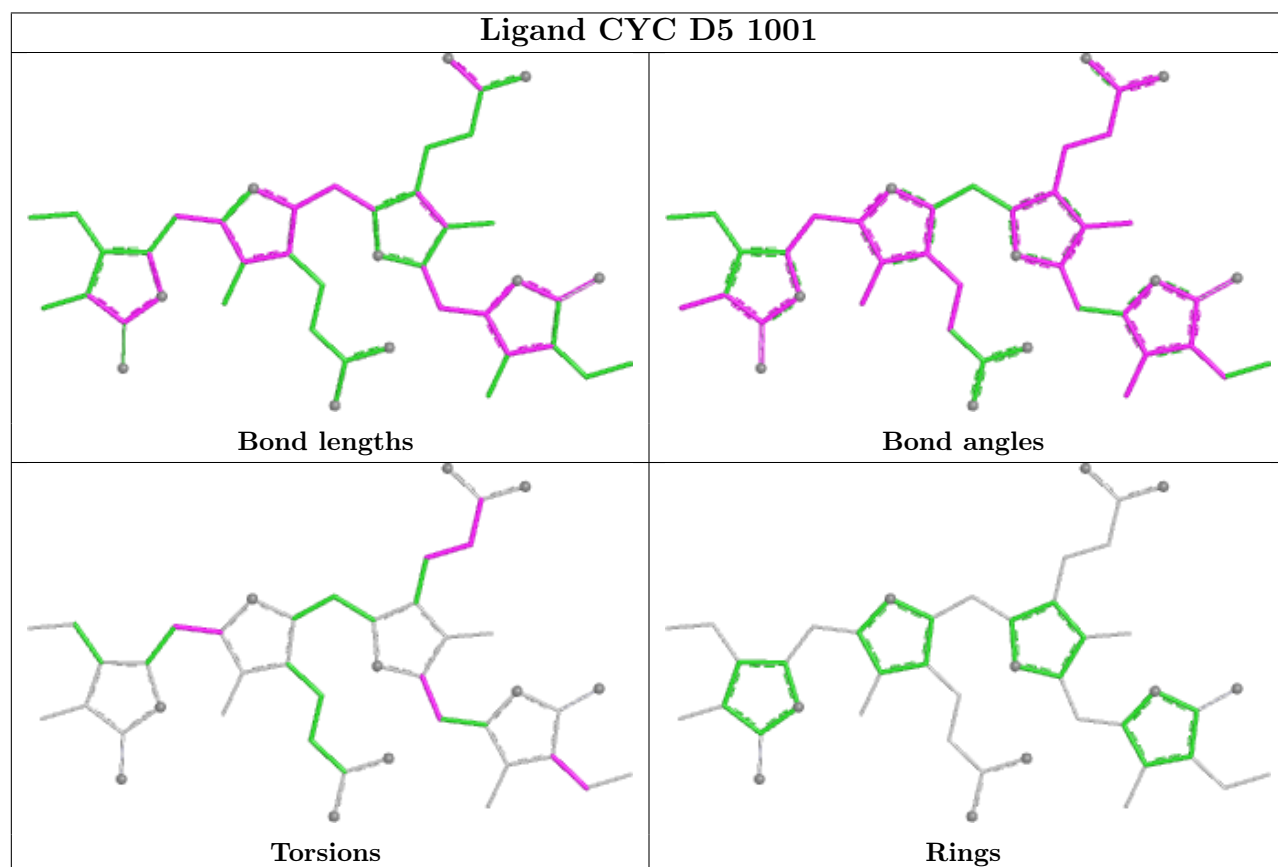
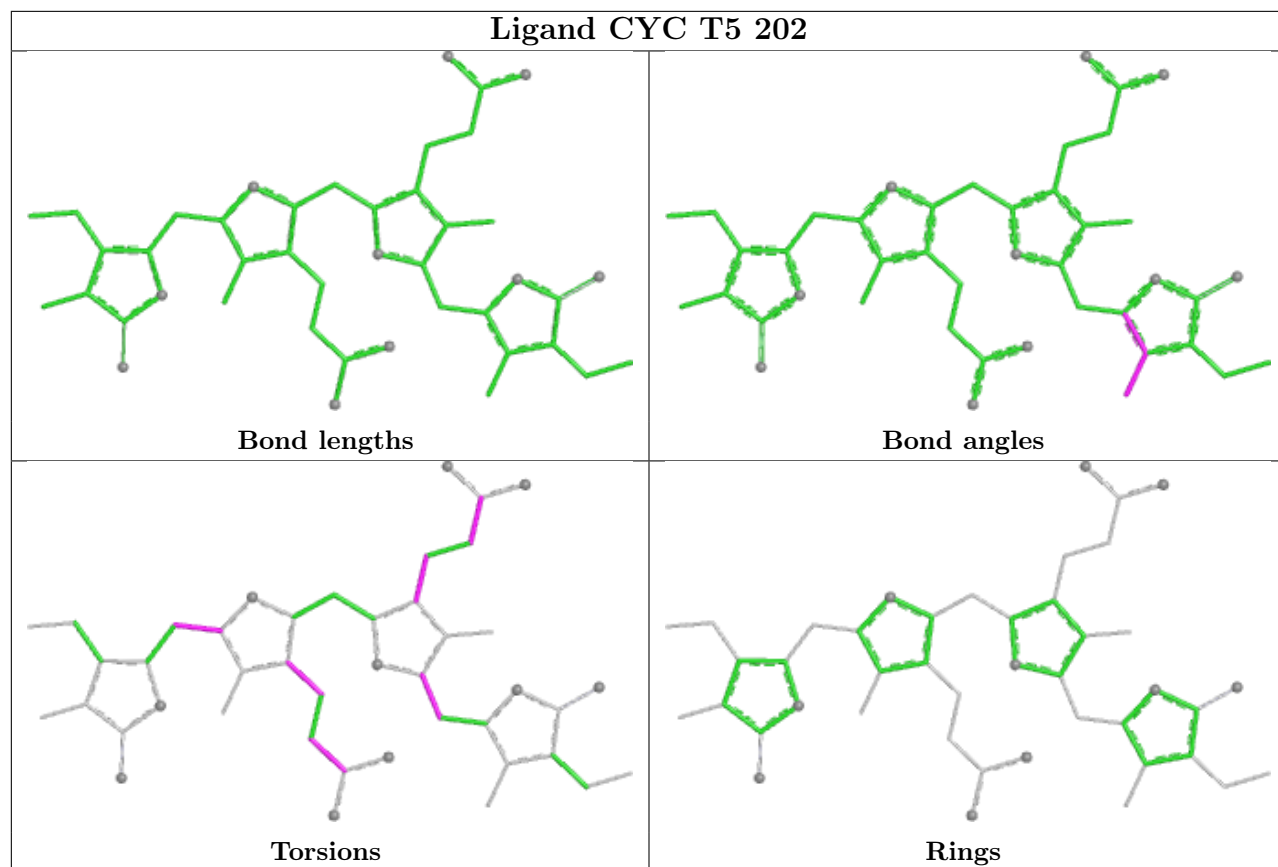


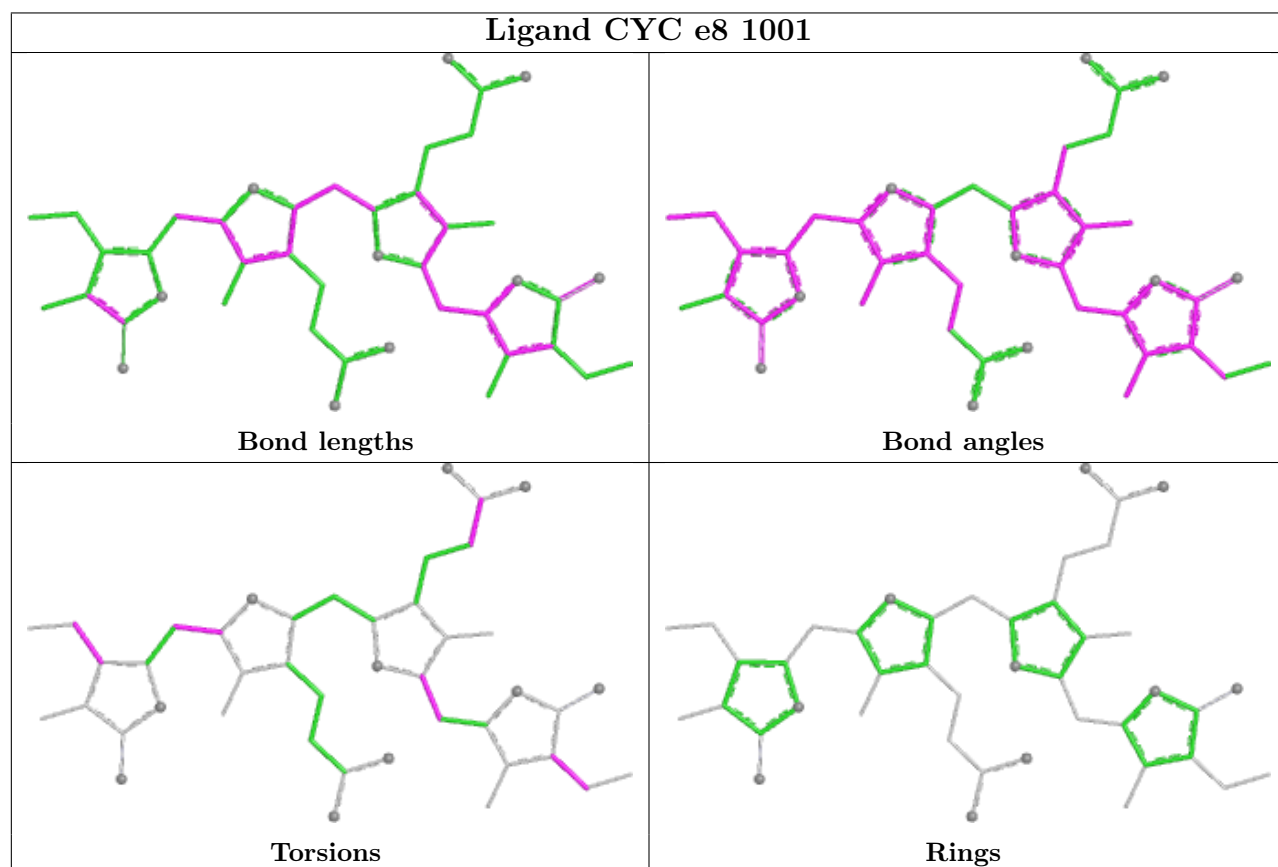
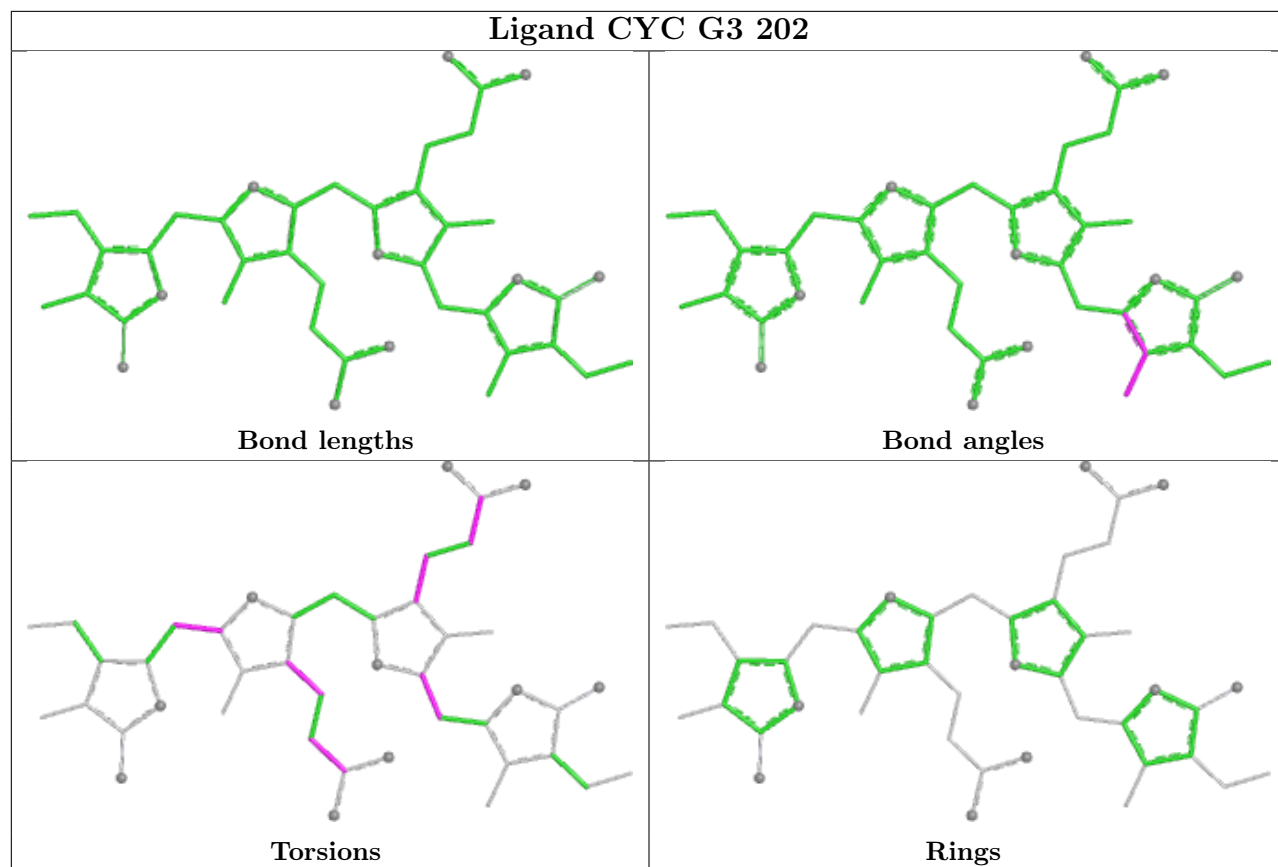
Ligand CYC KA 201

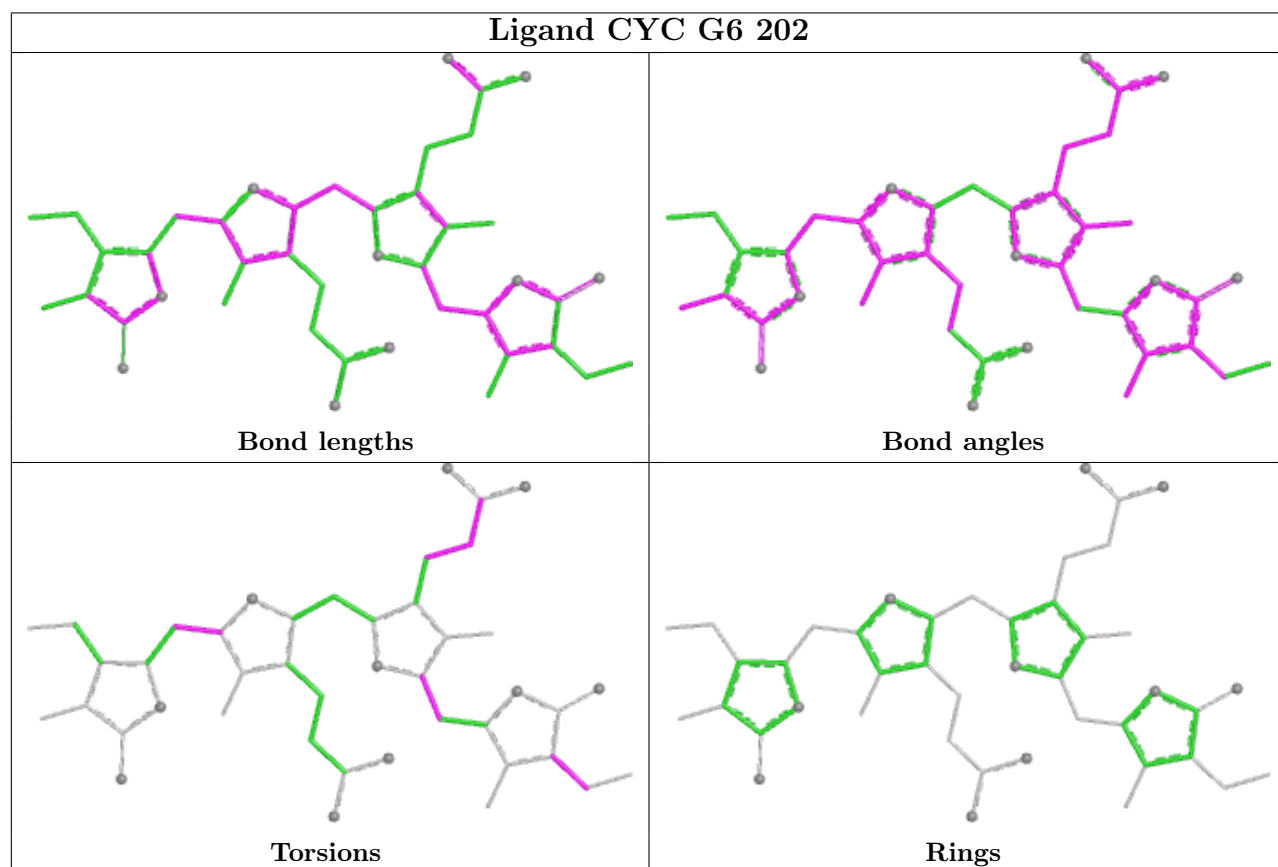
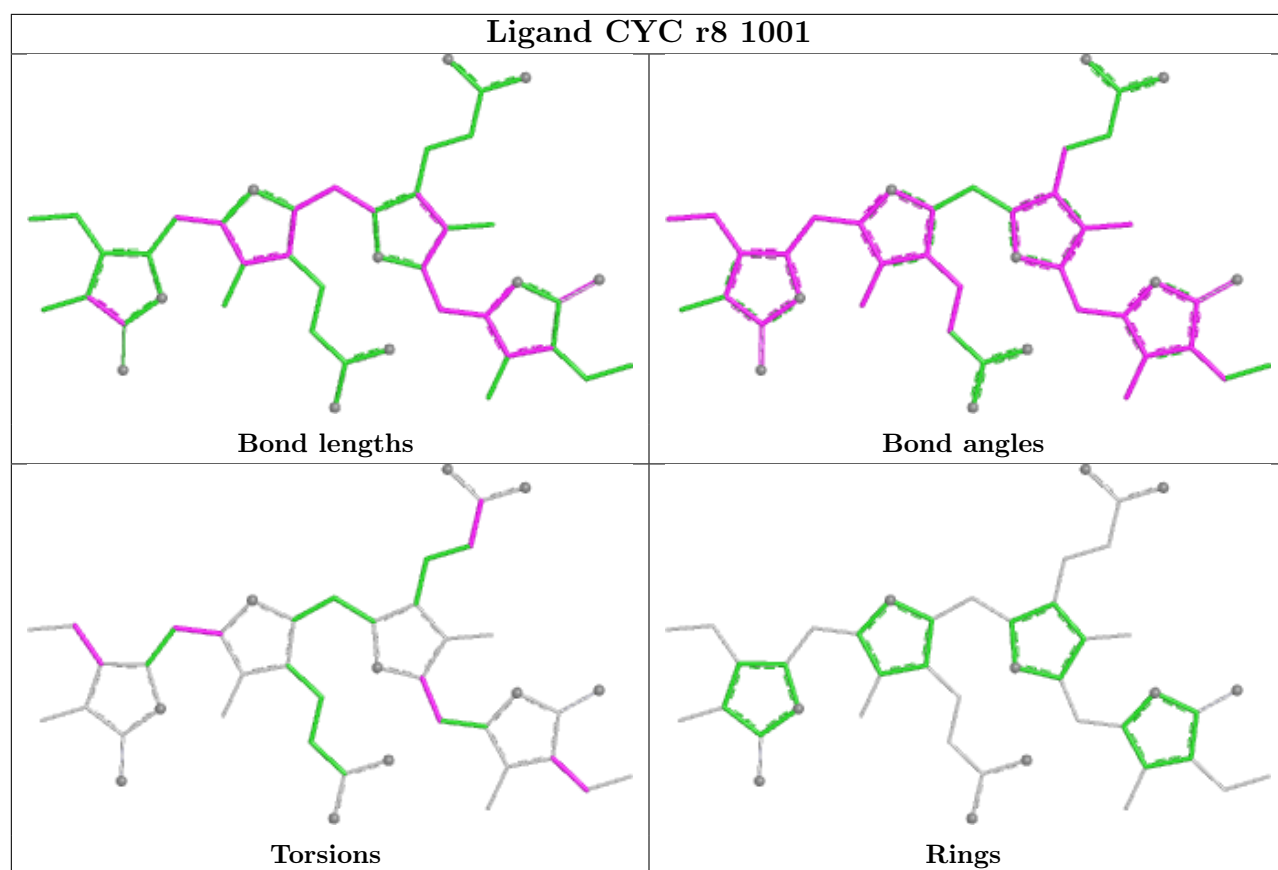


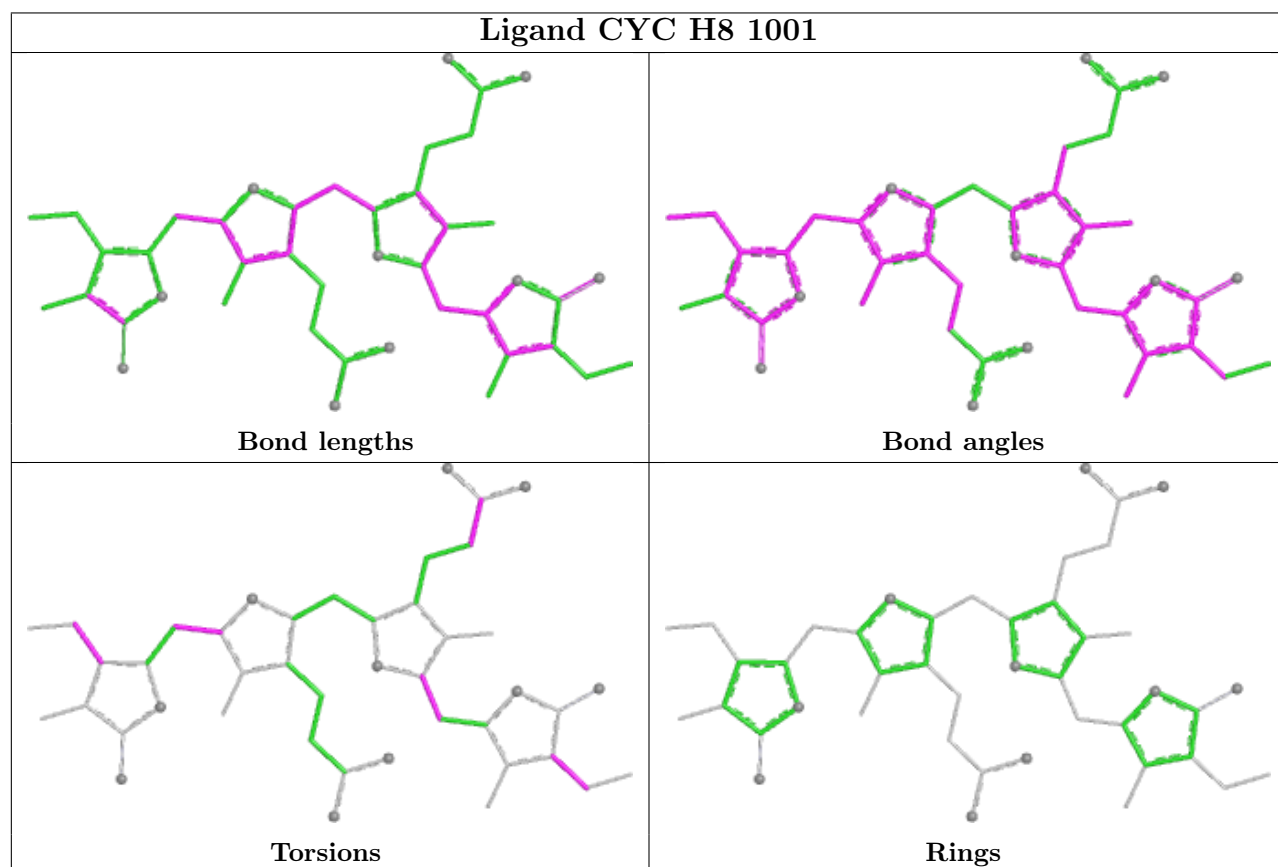
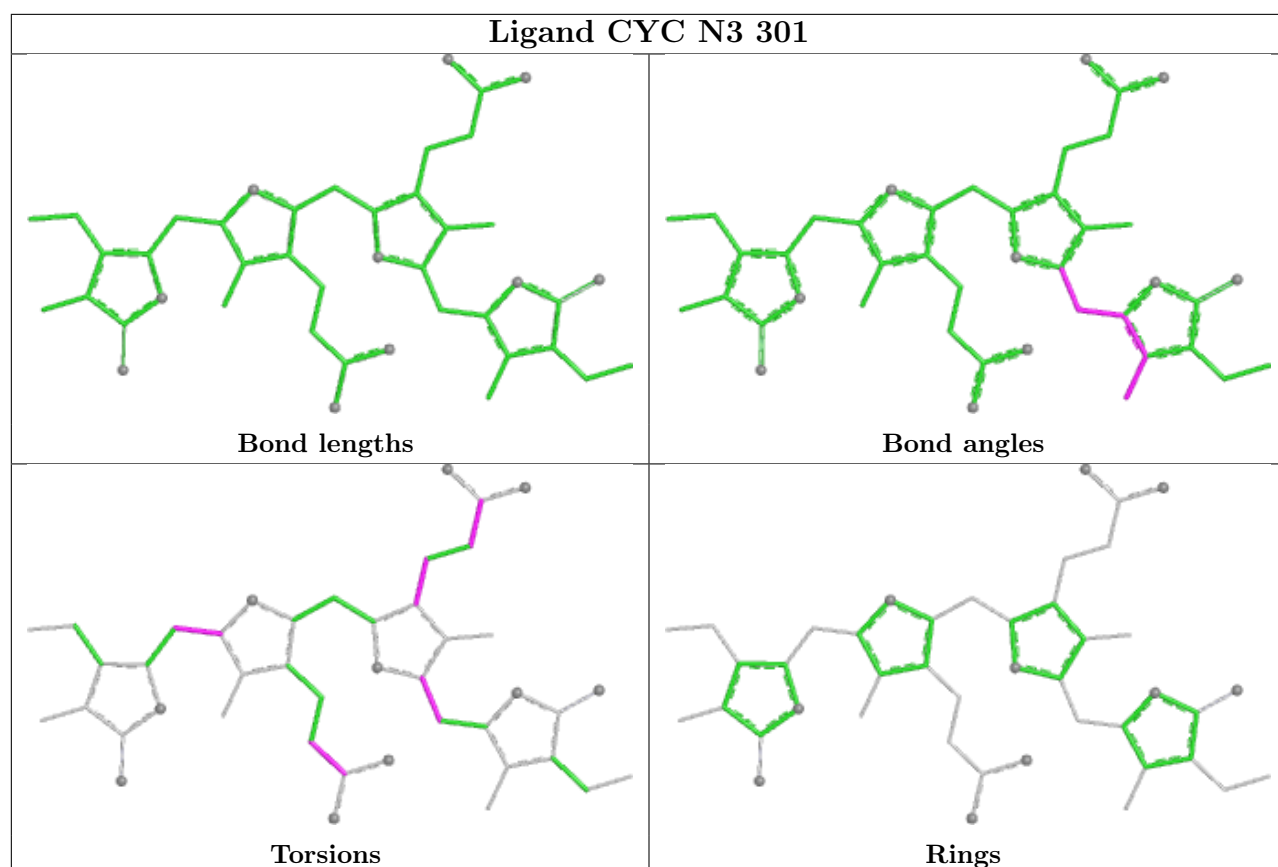
Ligand CYC Z8 1001



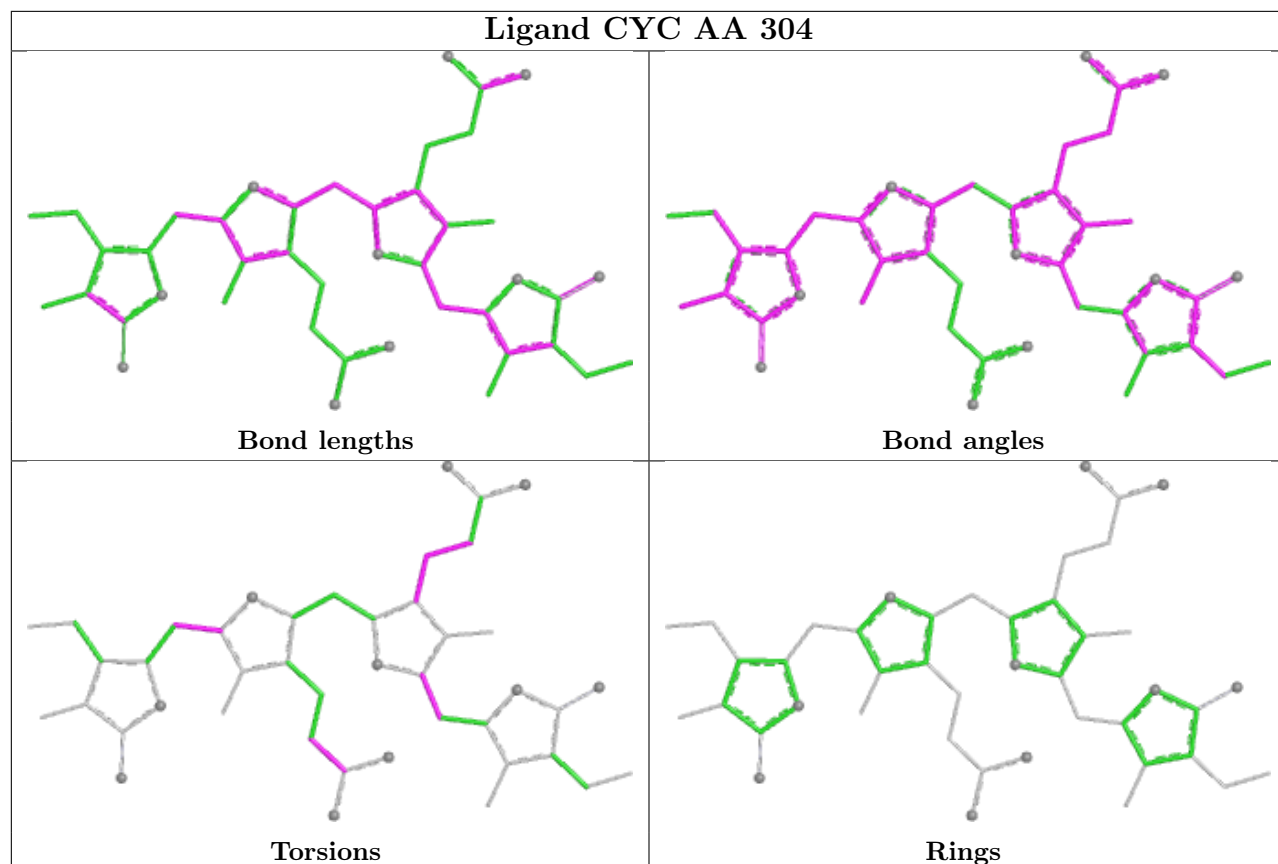




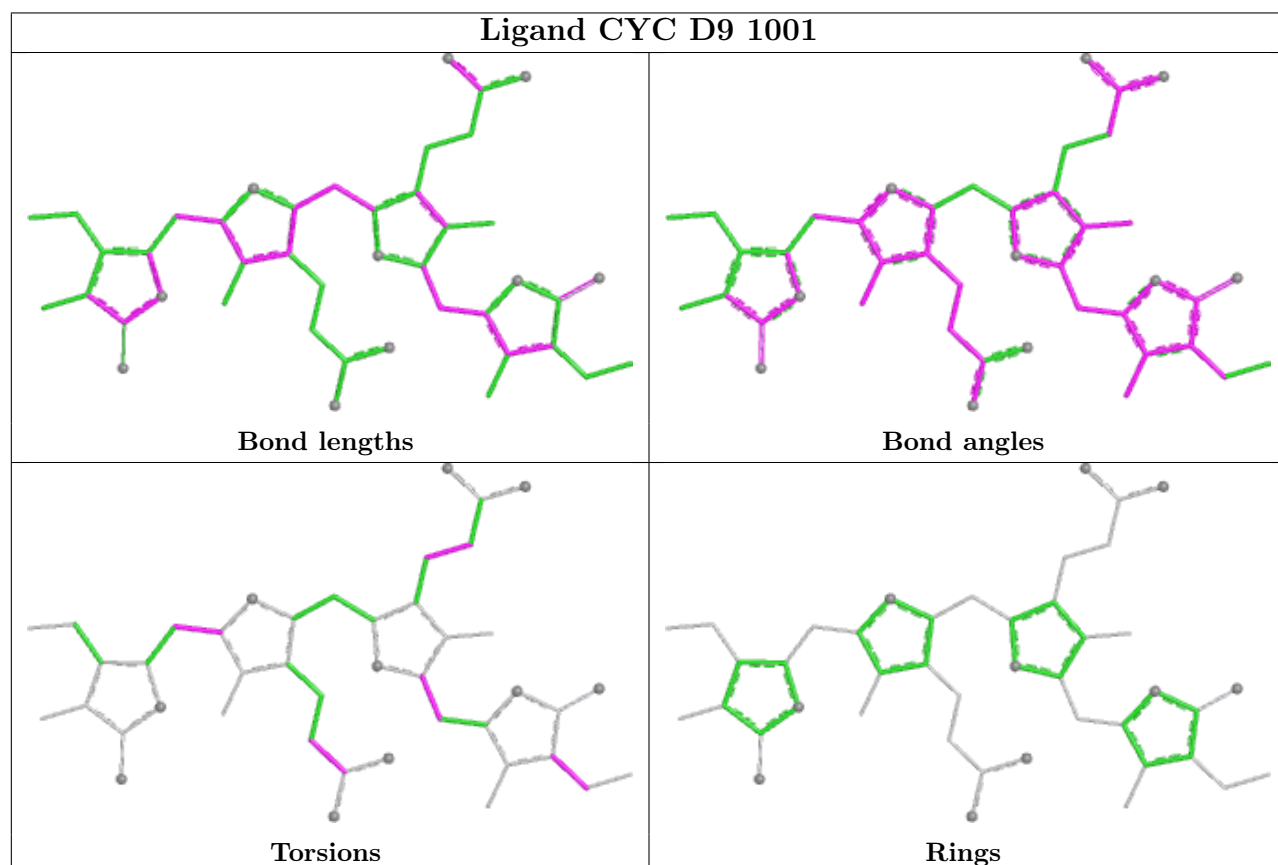


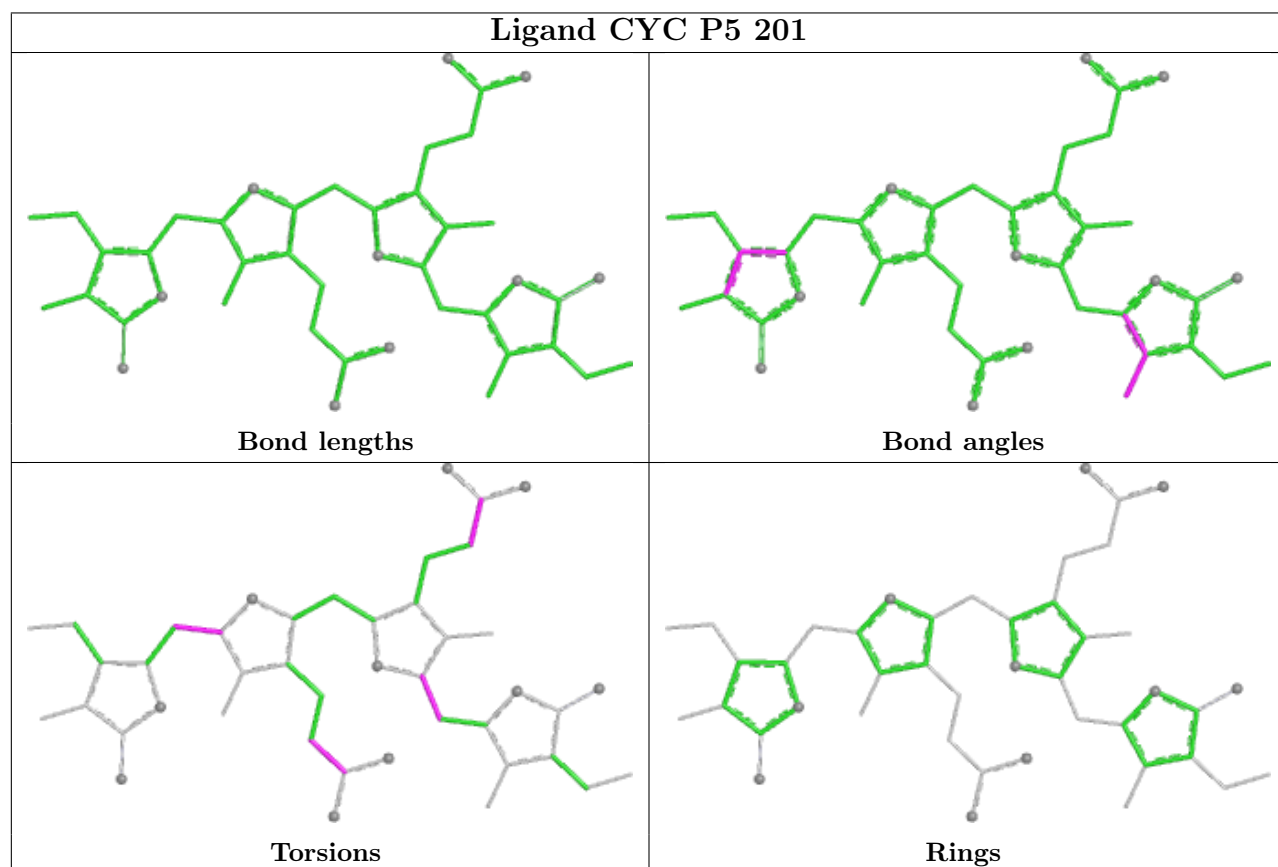
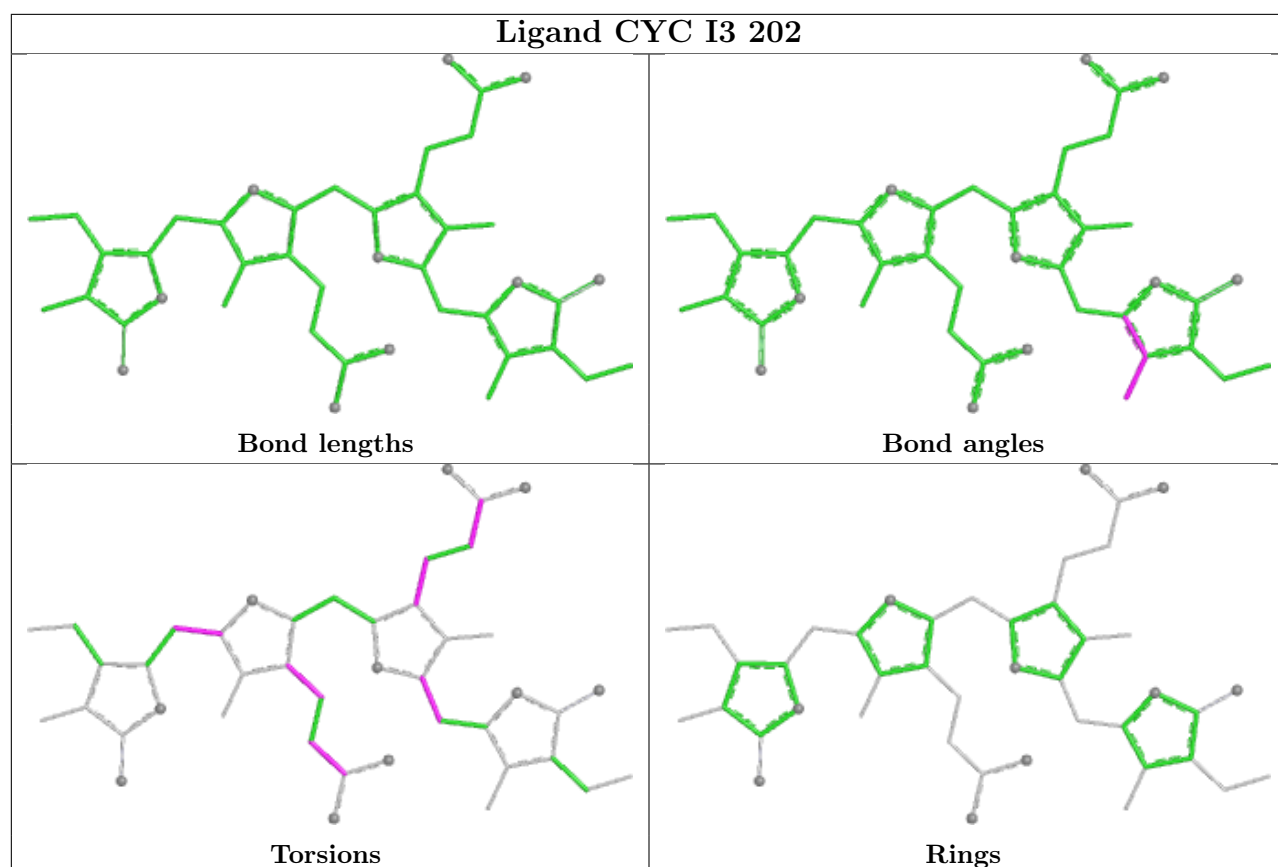


Ligand CYC AA 304

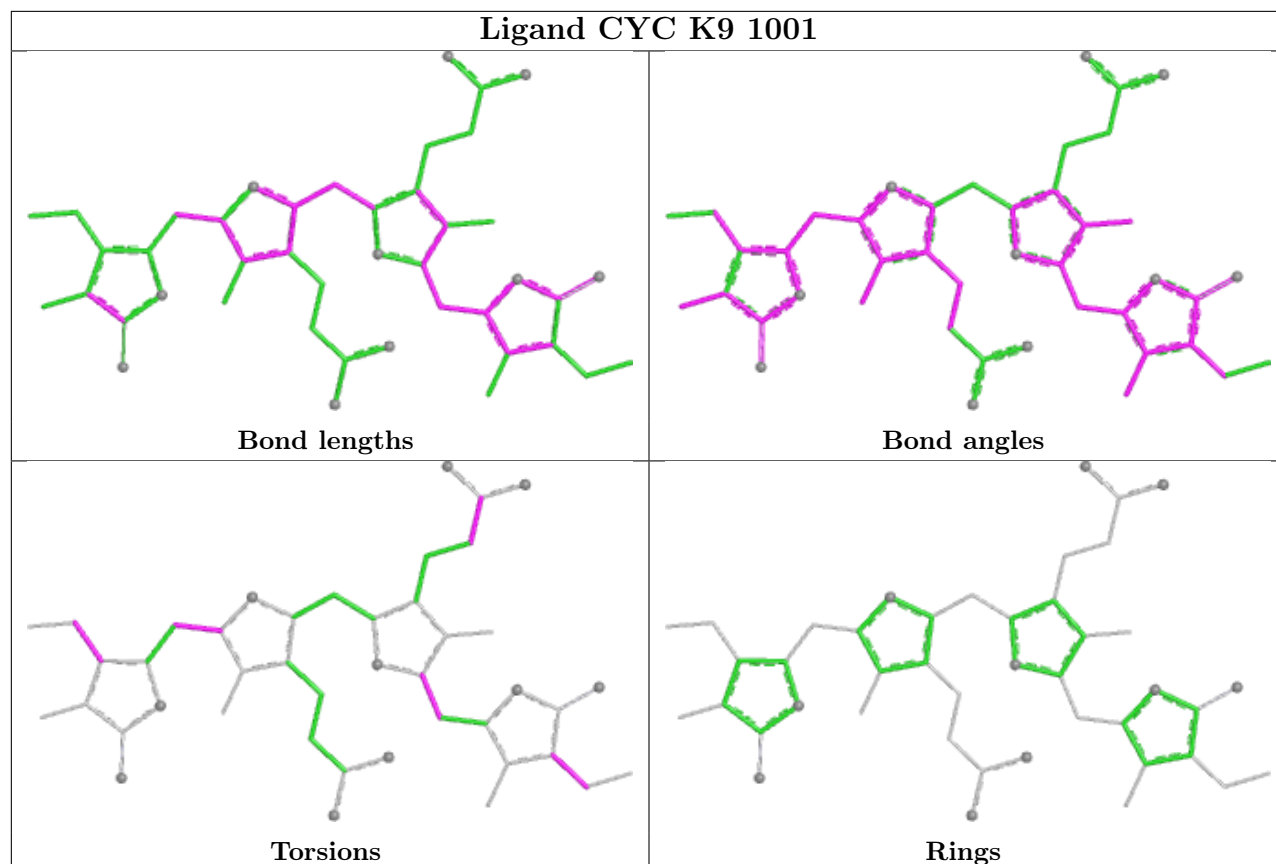


Ligand CYC D9 1001

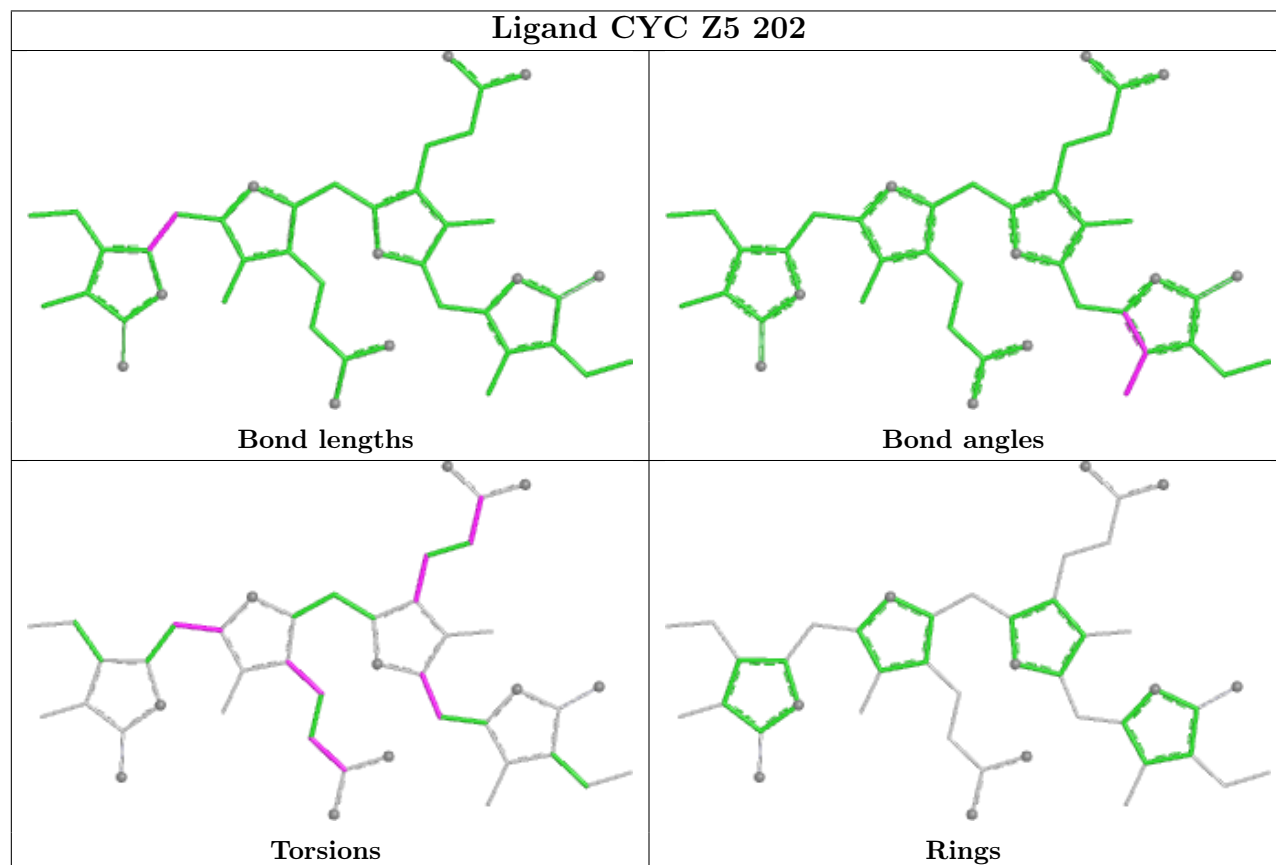




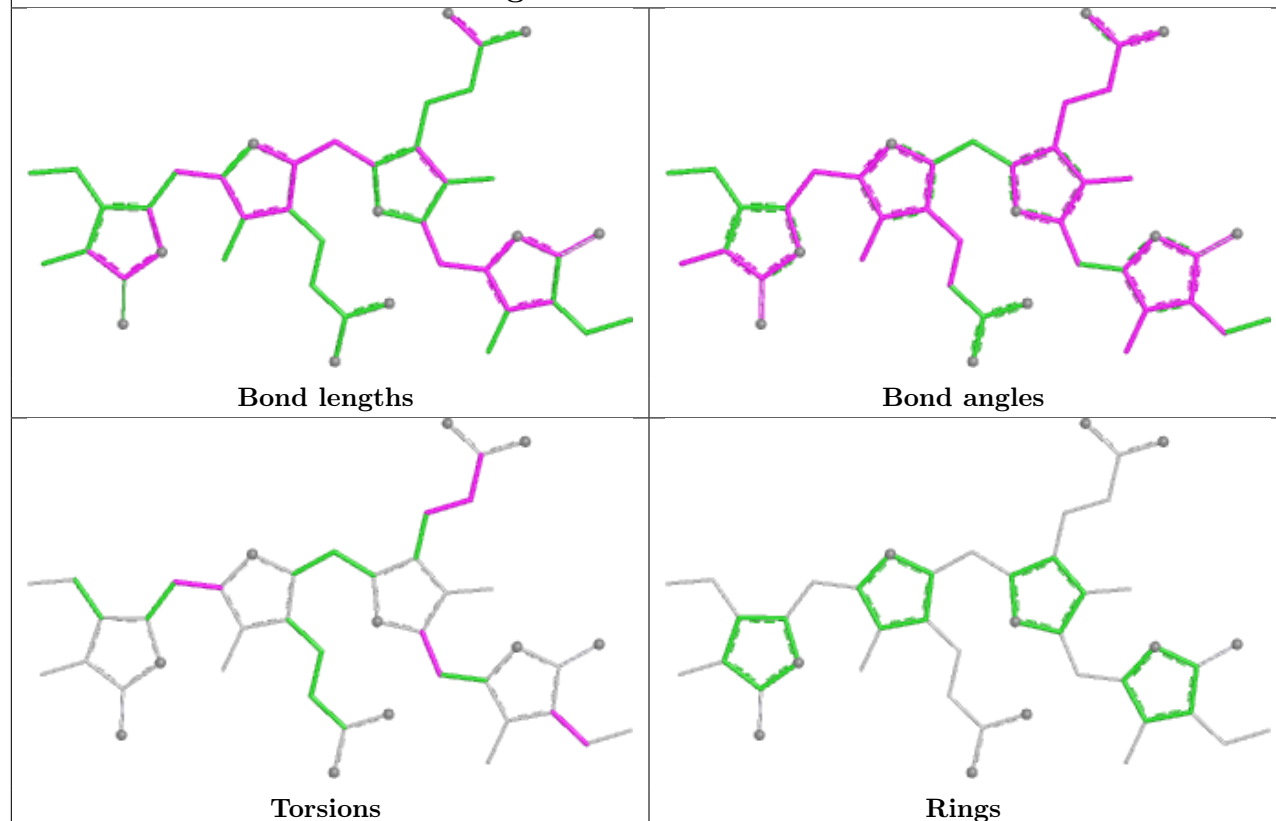
Ligand CYC K9 1001



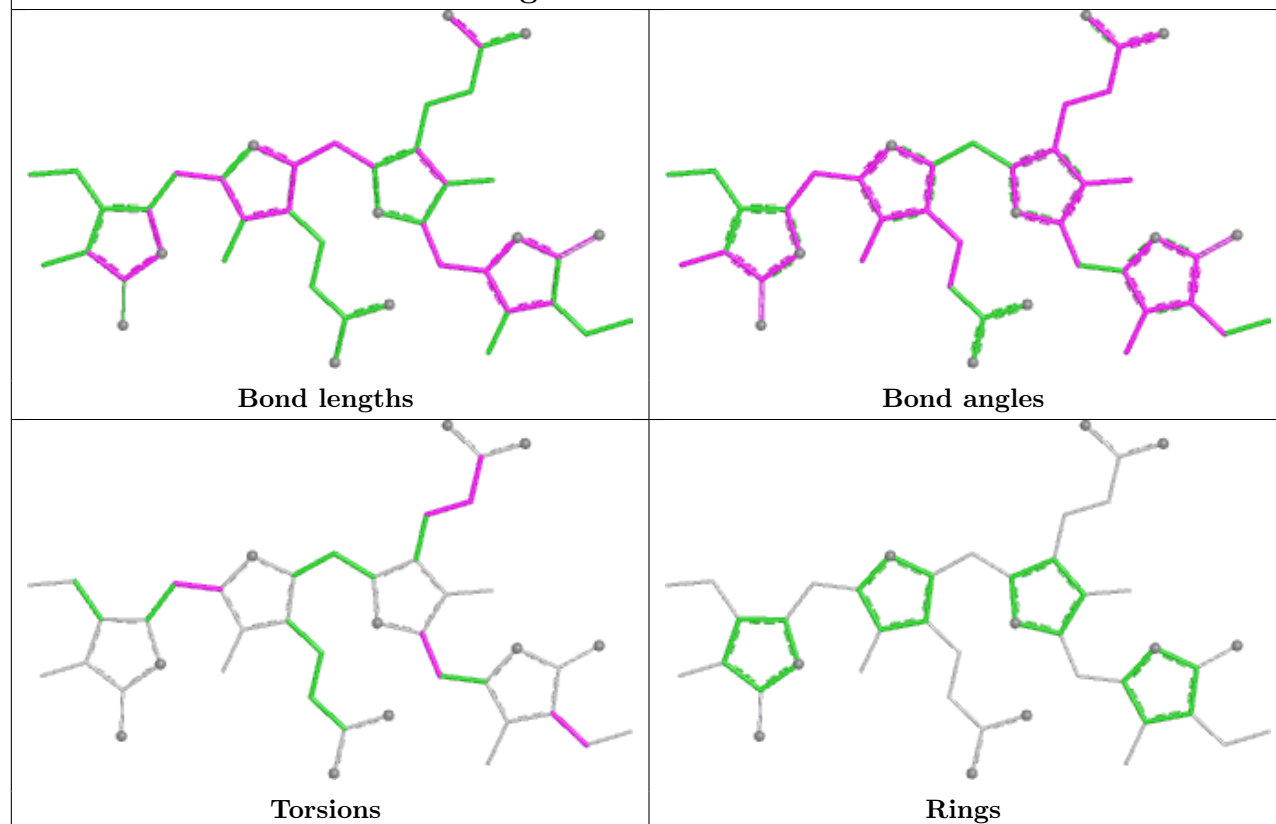
Ligand CYC Z5 202



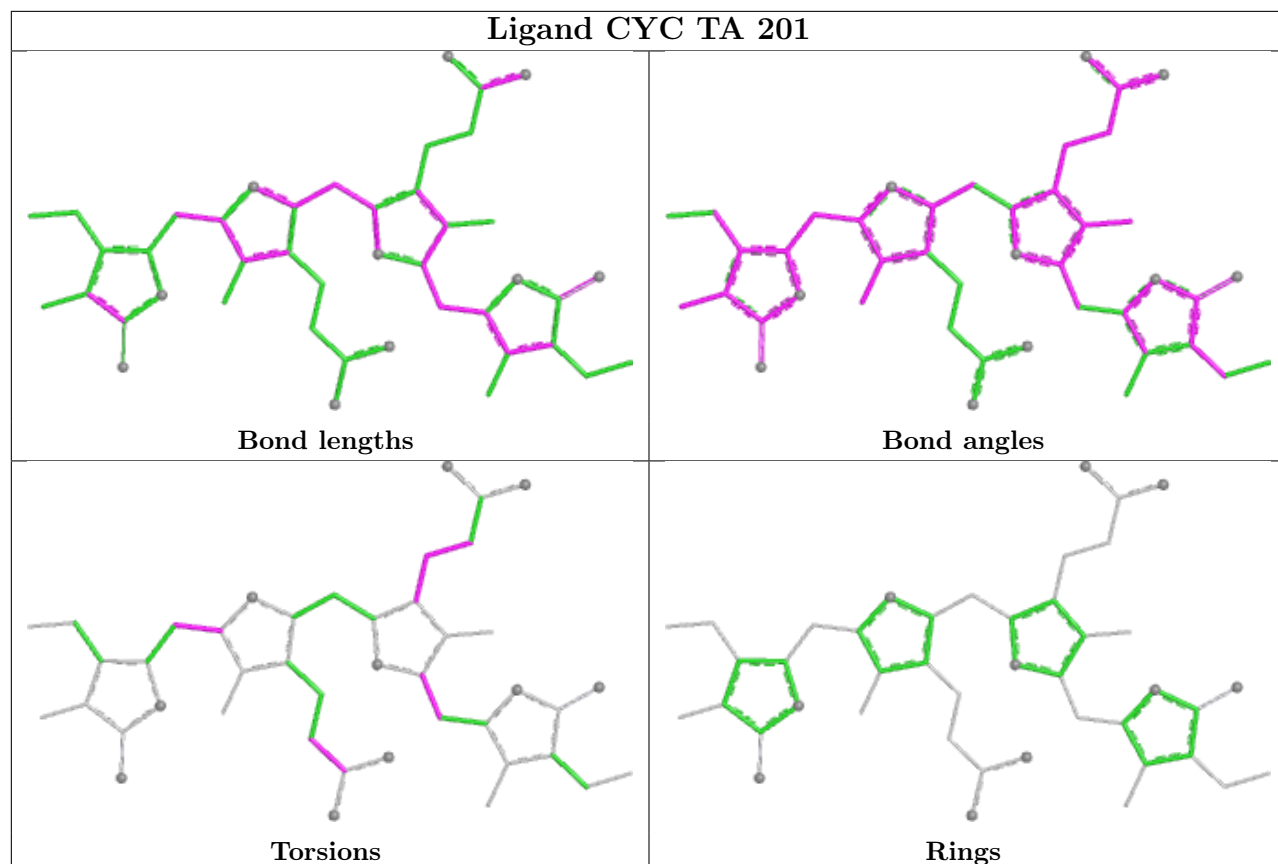
Ligand CYC W5 1001



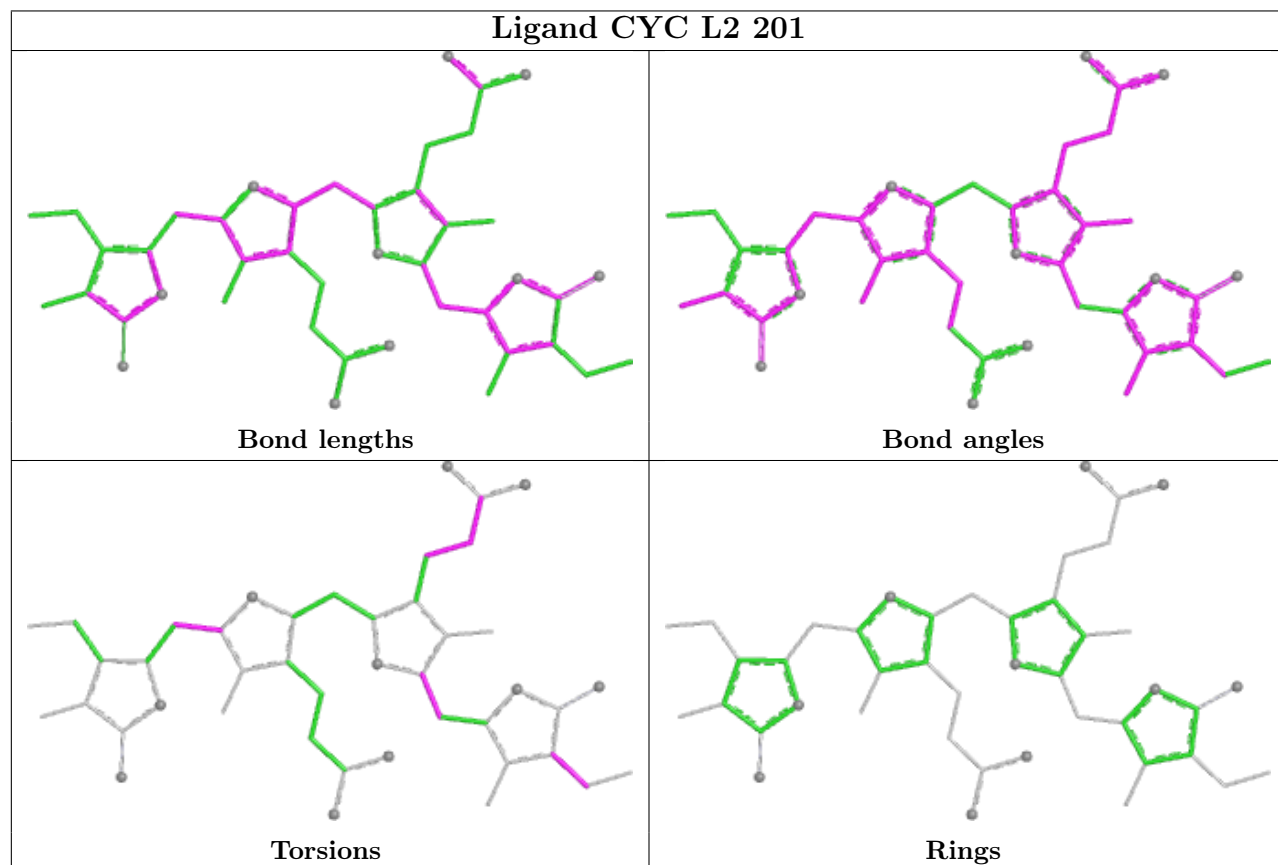
Ligand CYC G1 202

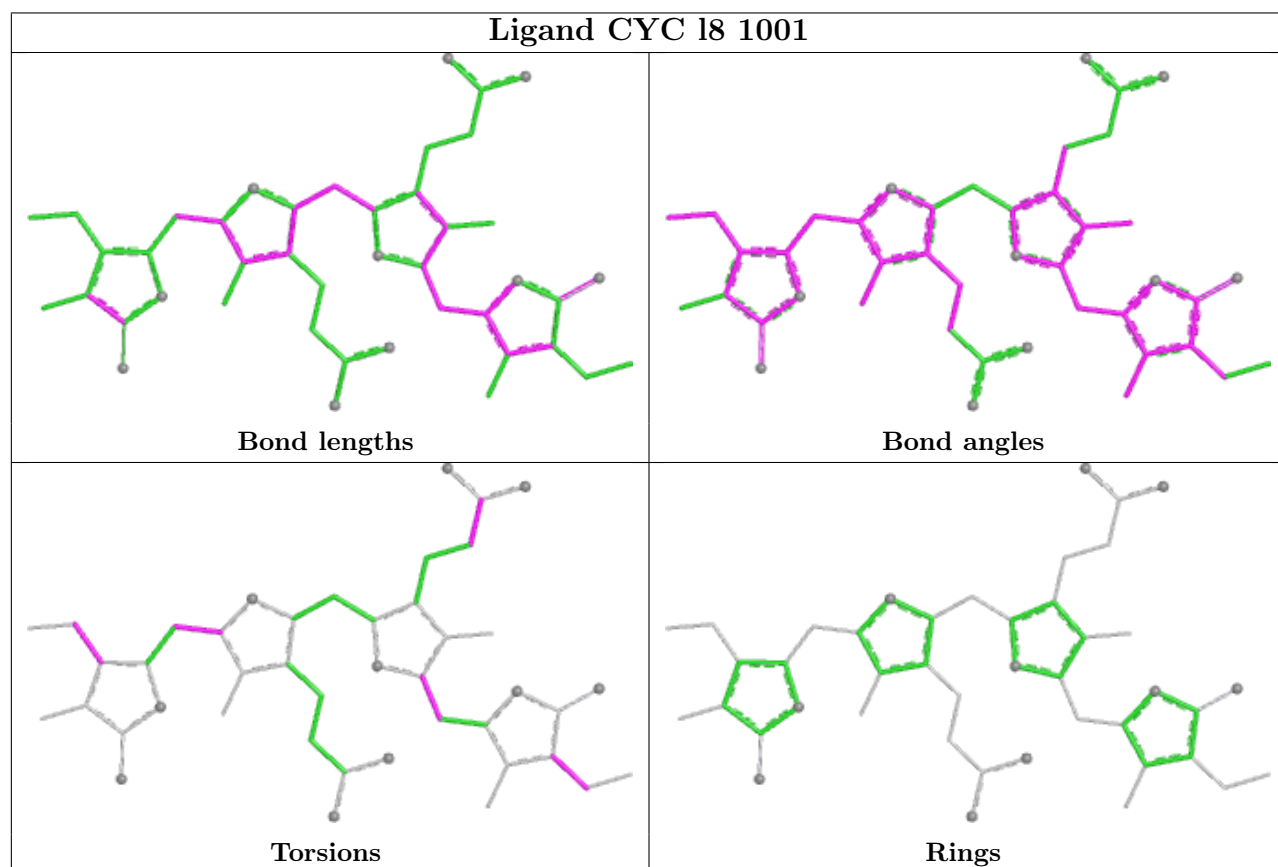
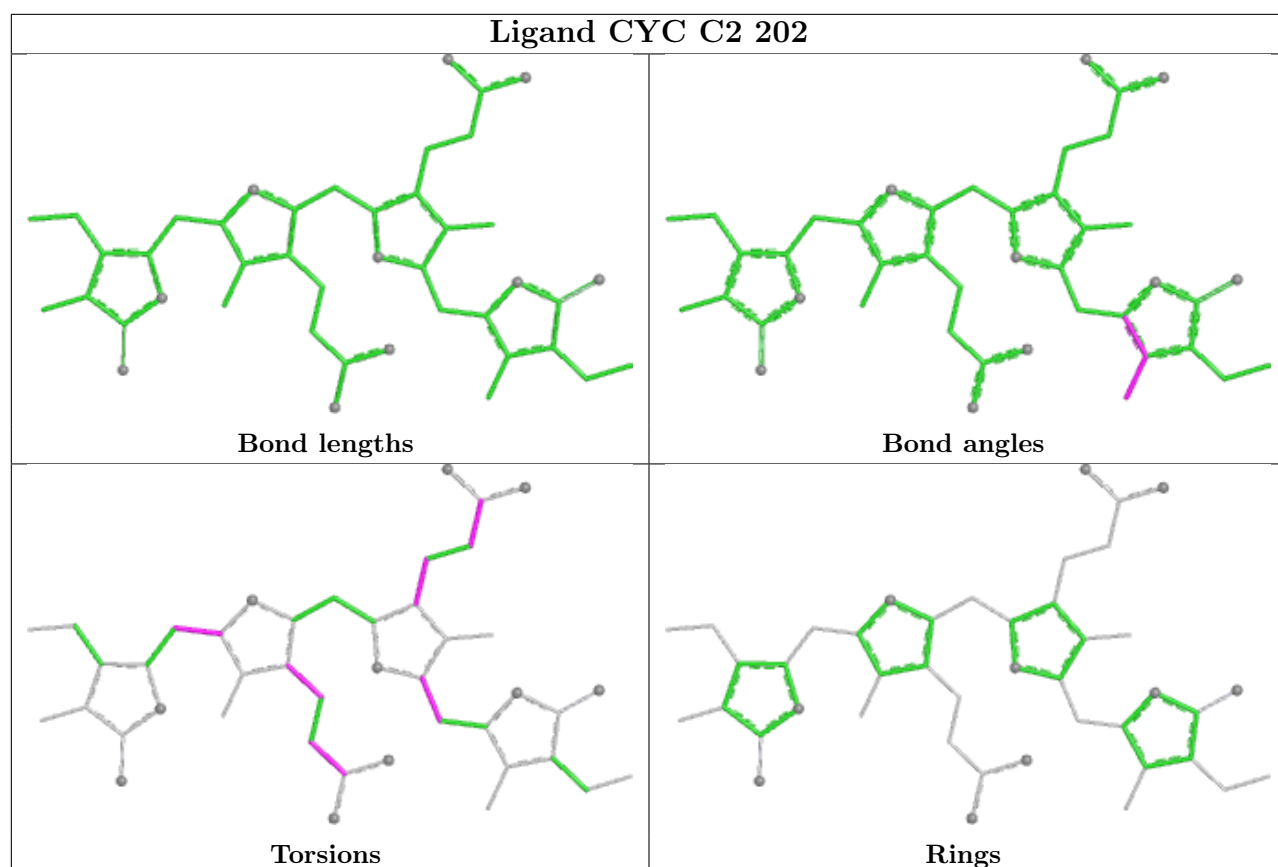


Ligand CYC TA 201

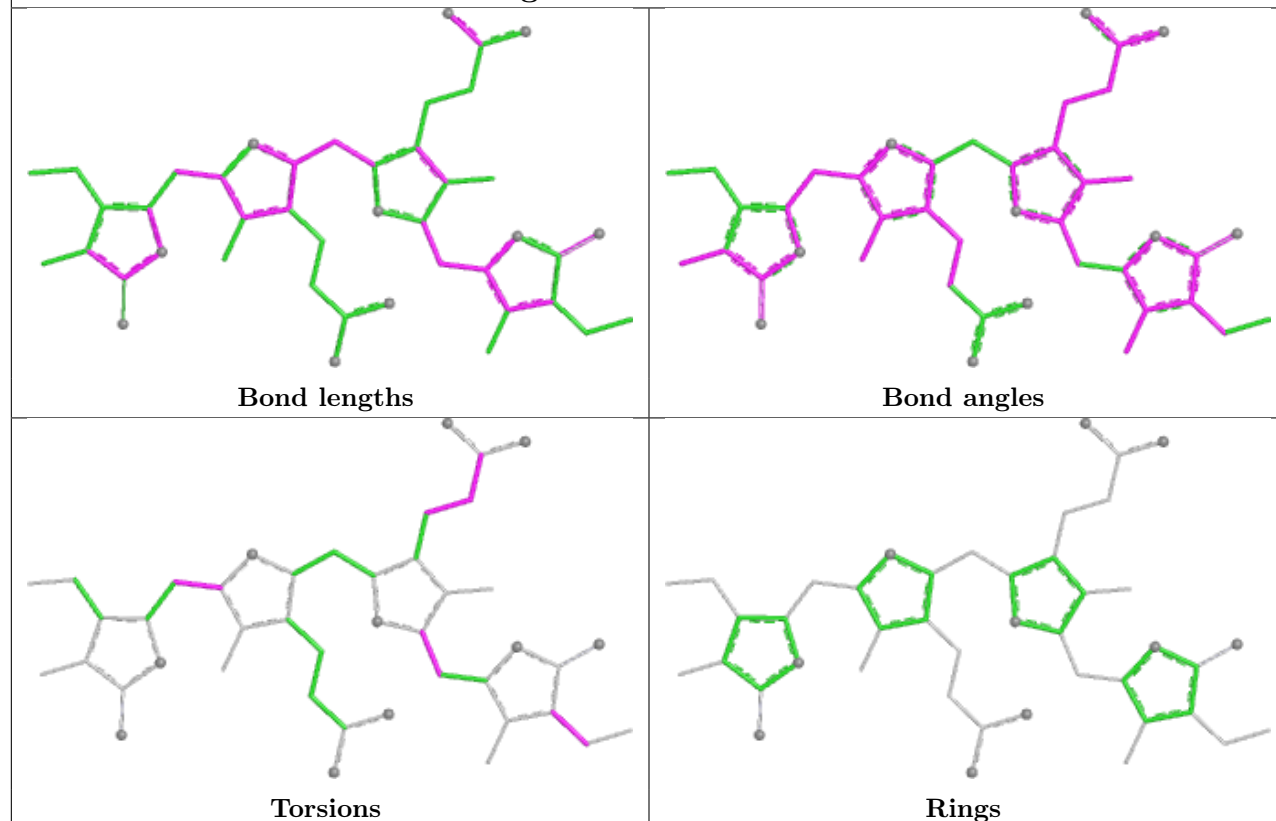


Ligand CYC L2 201

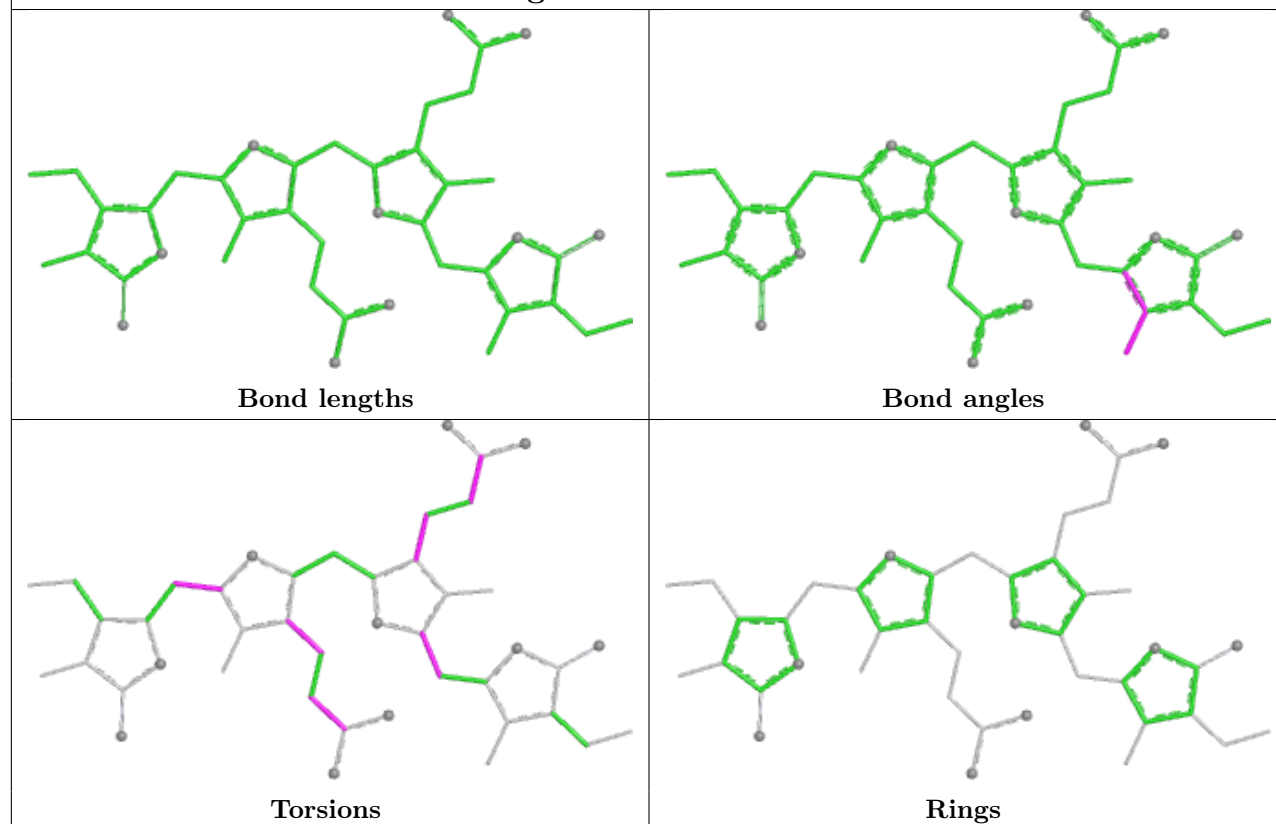




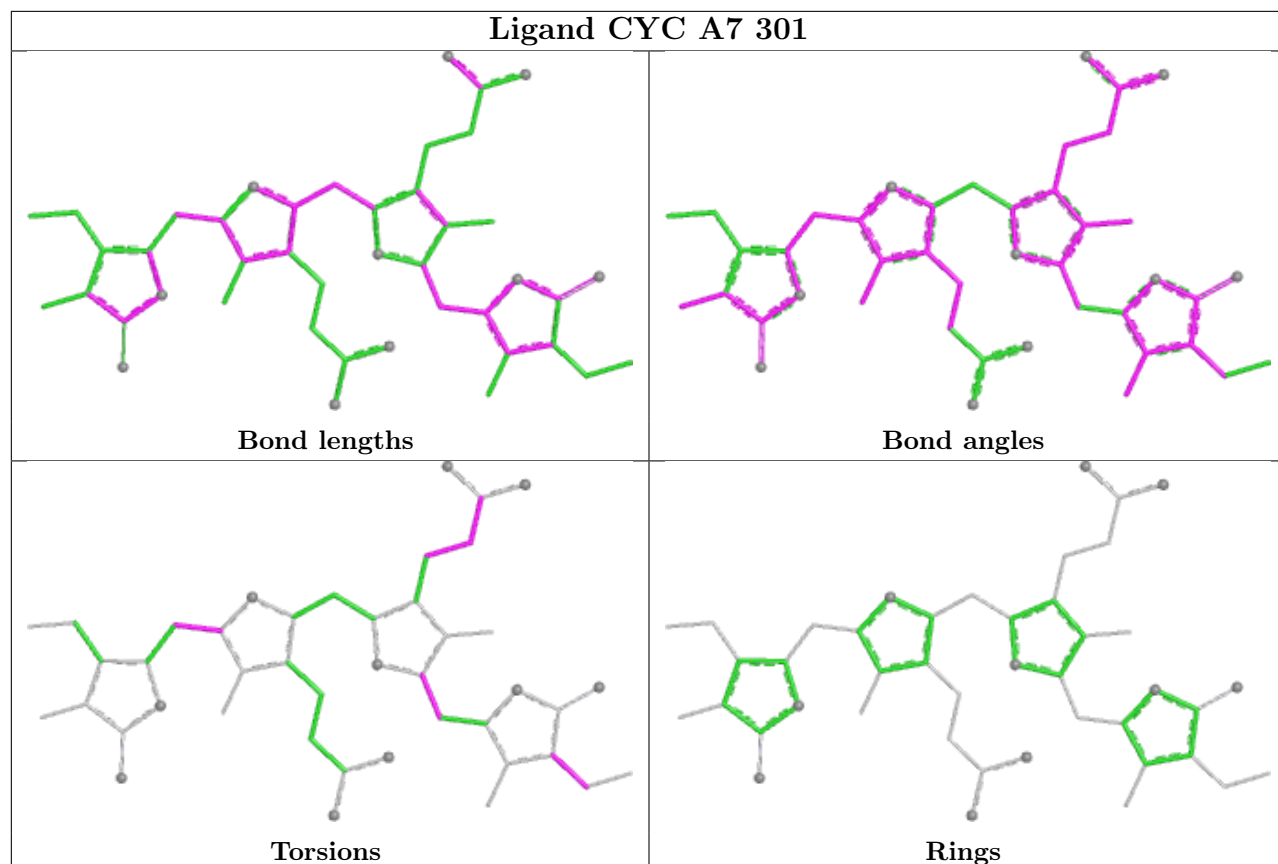
Ligand CYC V6 202



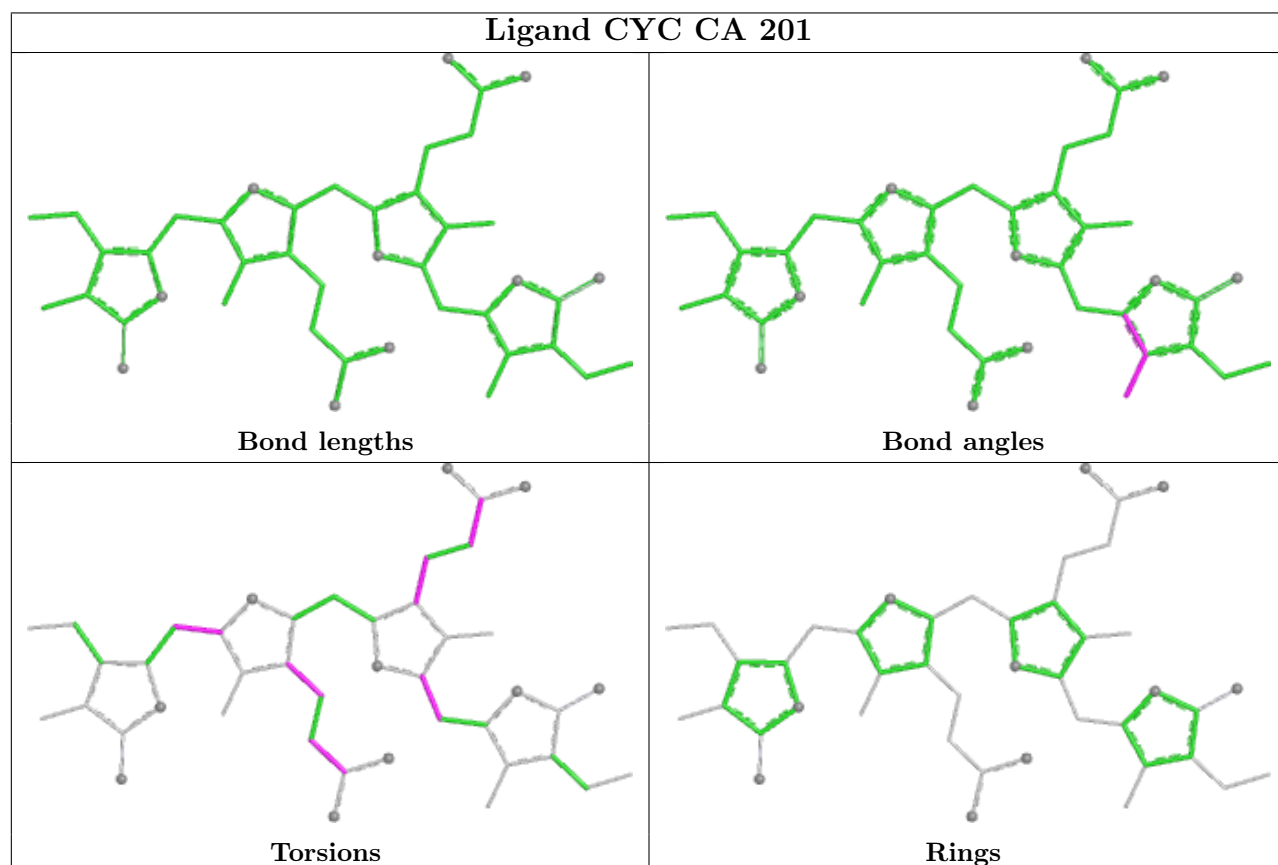
Ligand CYC I1 202

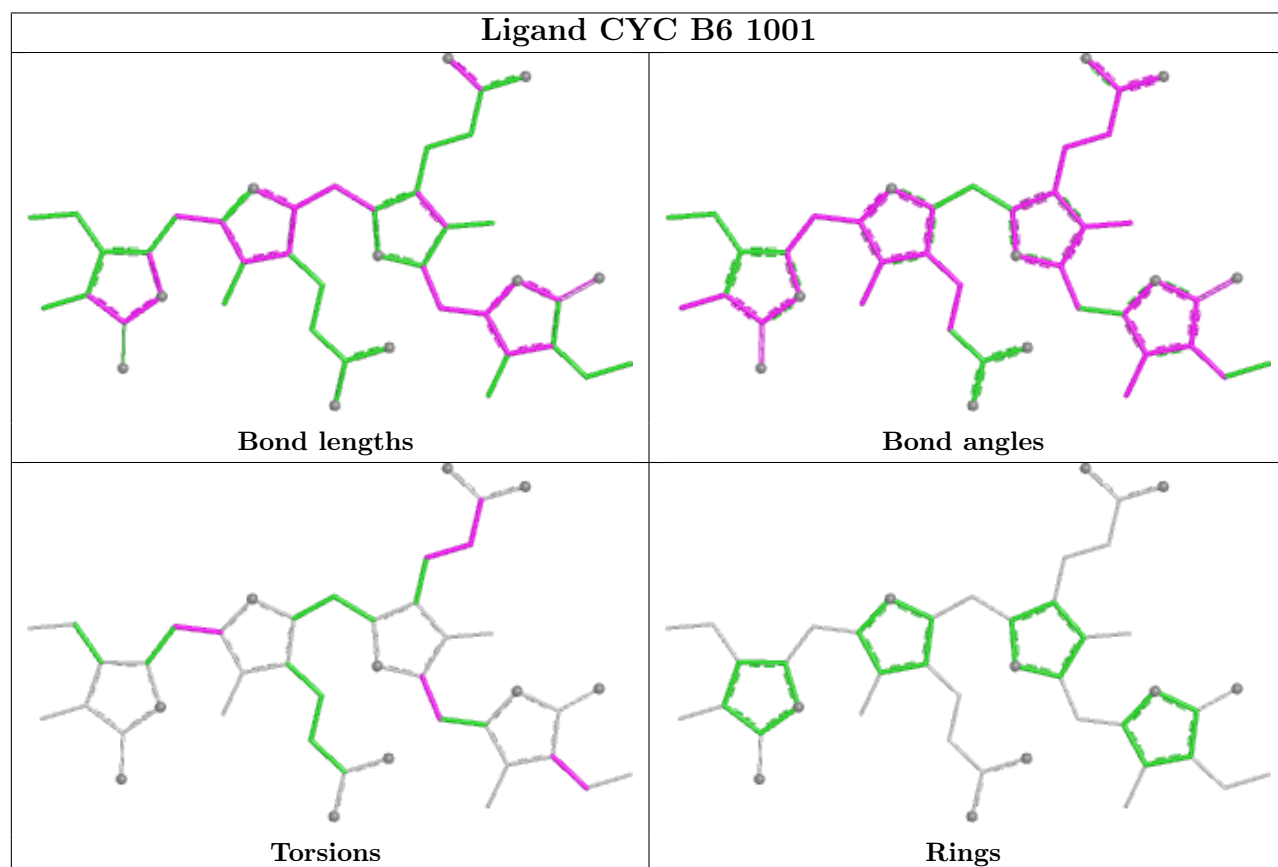
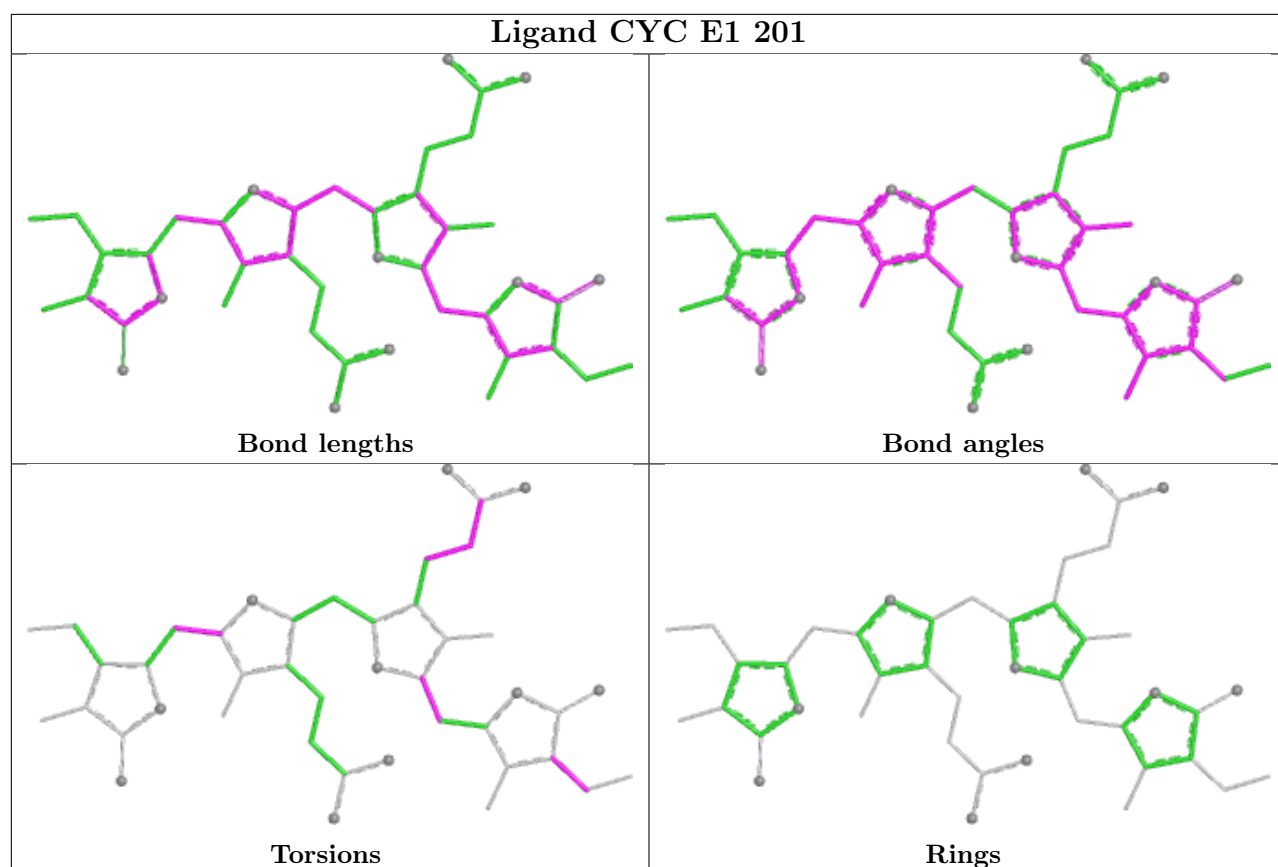


Ligand CYC A7 301

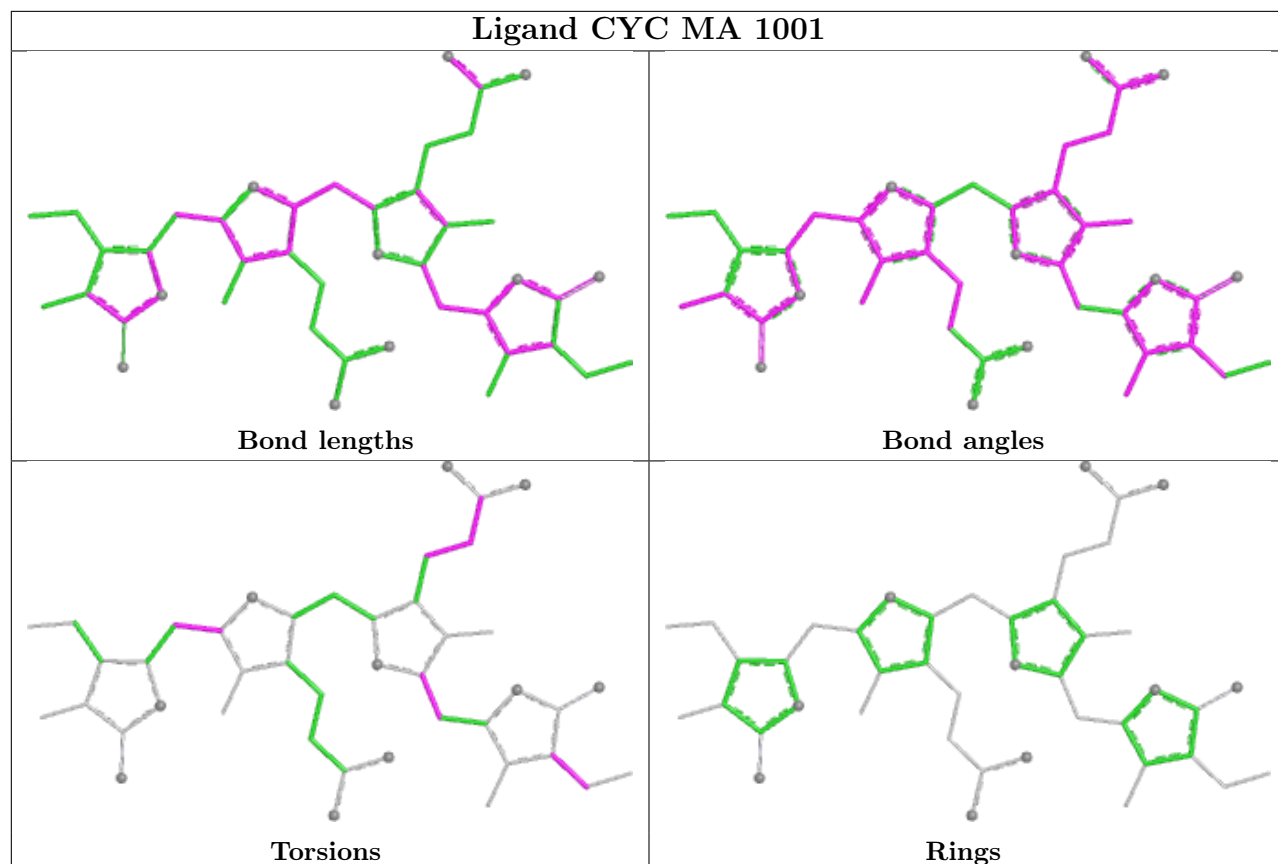


Ligand CYC CA 201

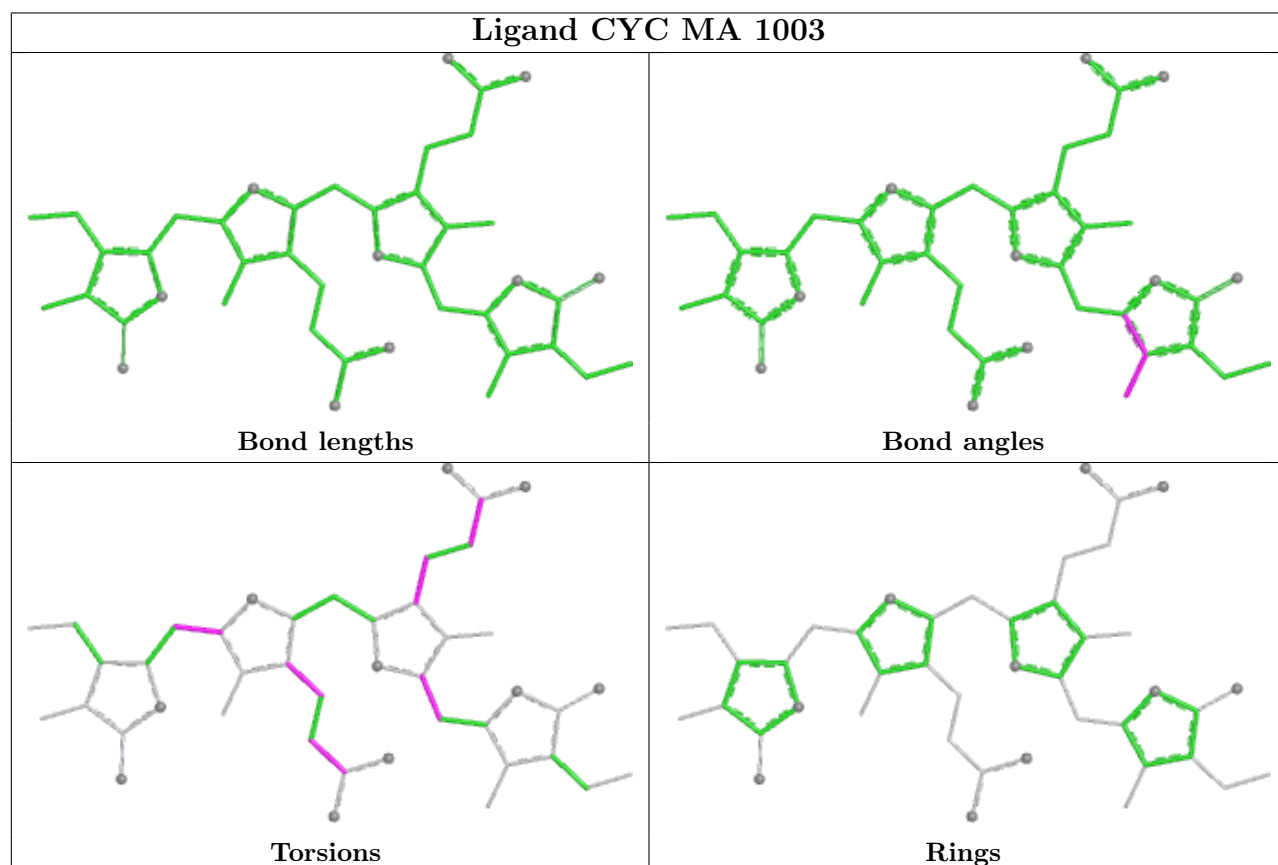


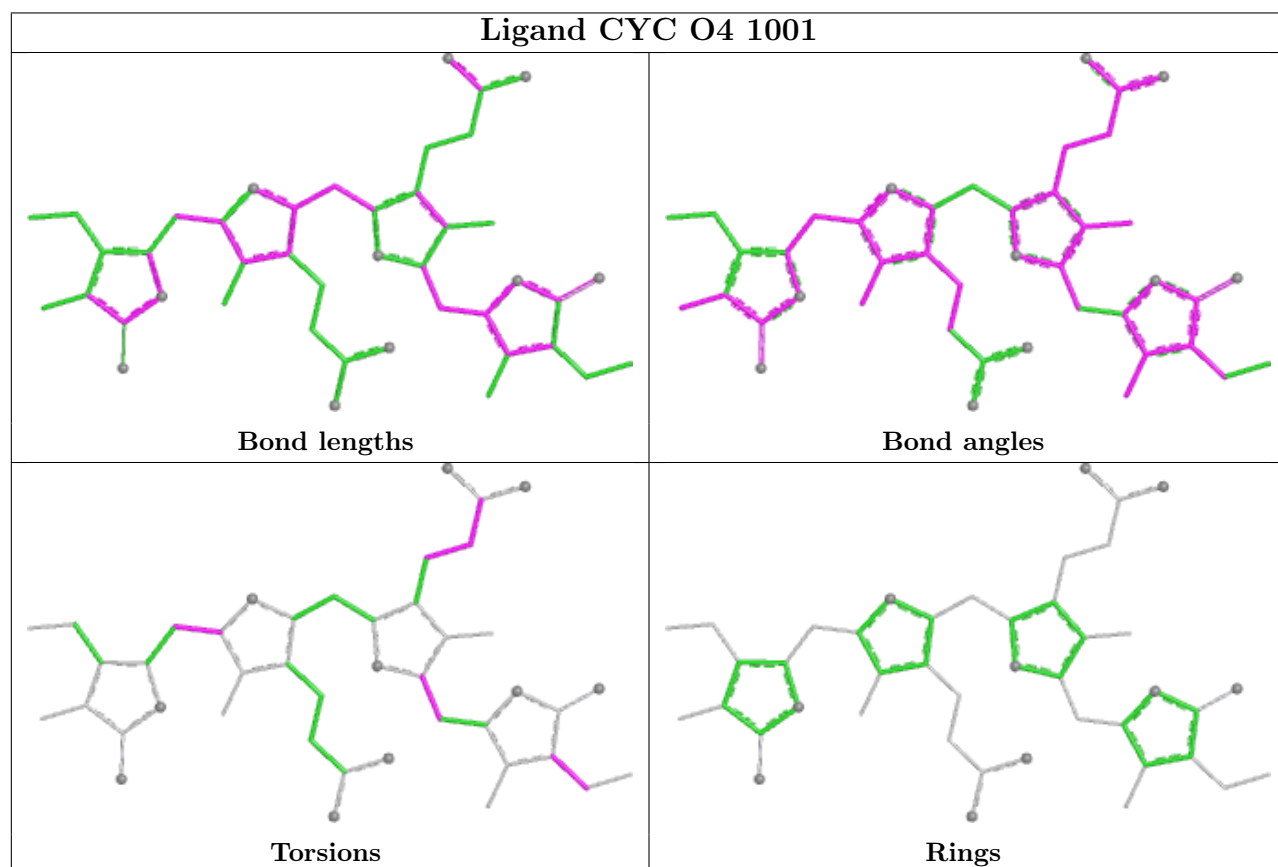
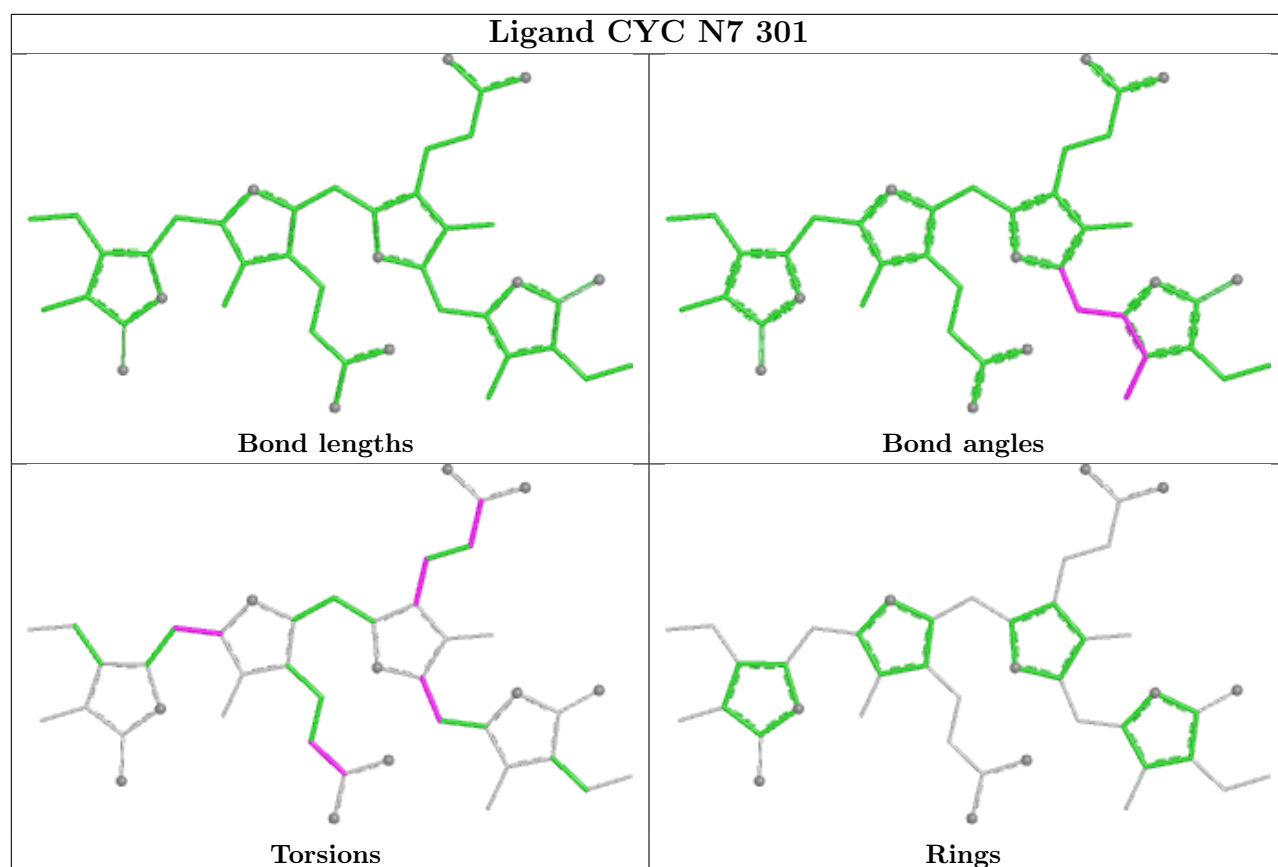


Ligand CYC MA 1001

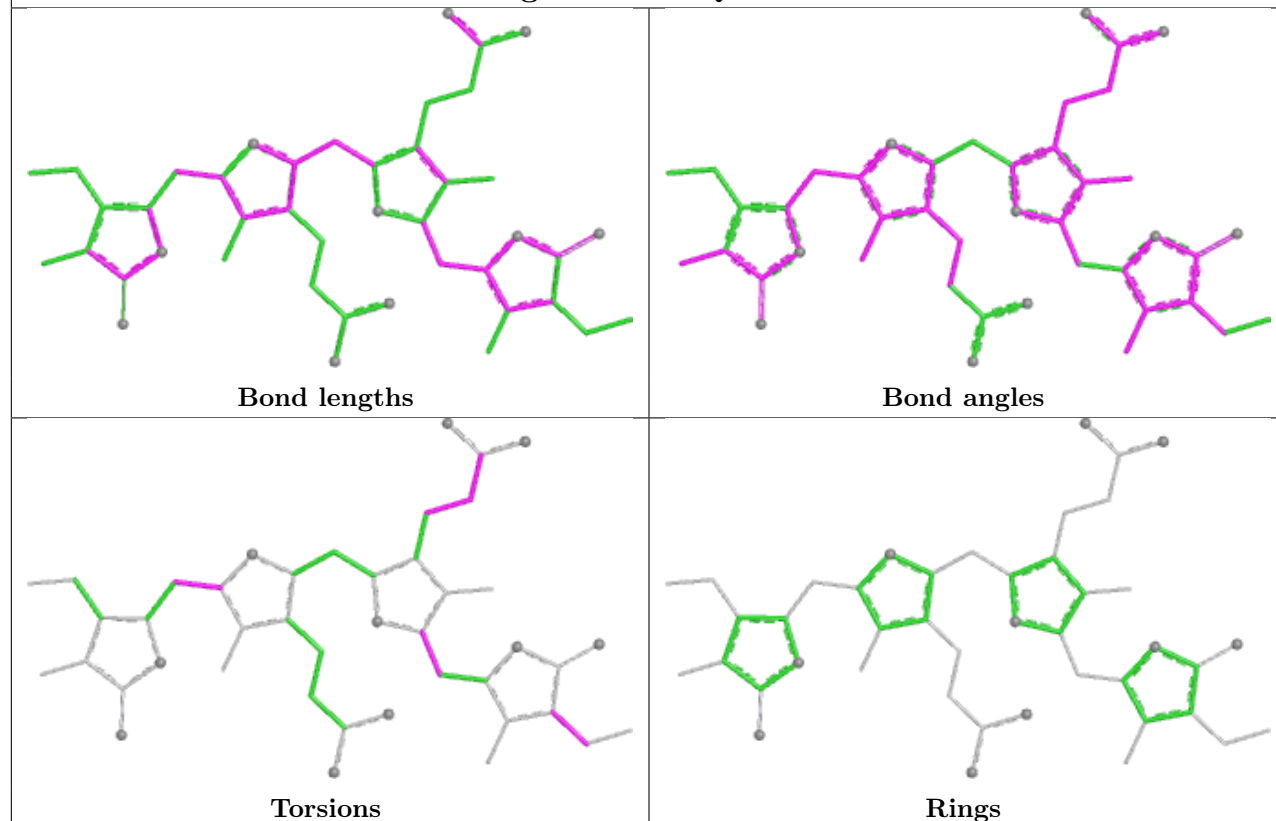


Ligand CYC MA 1003

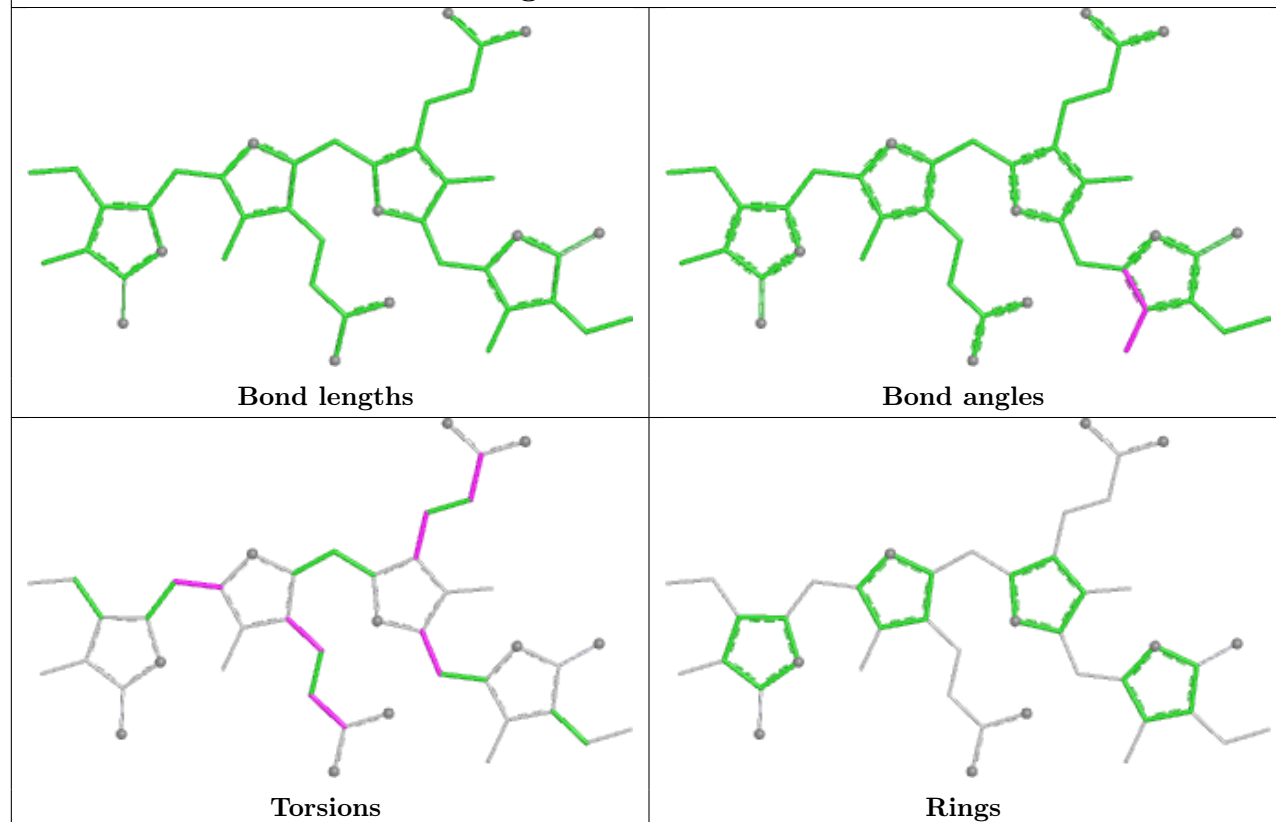




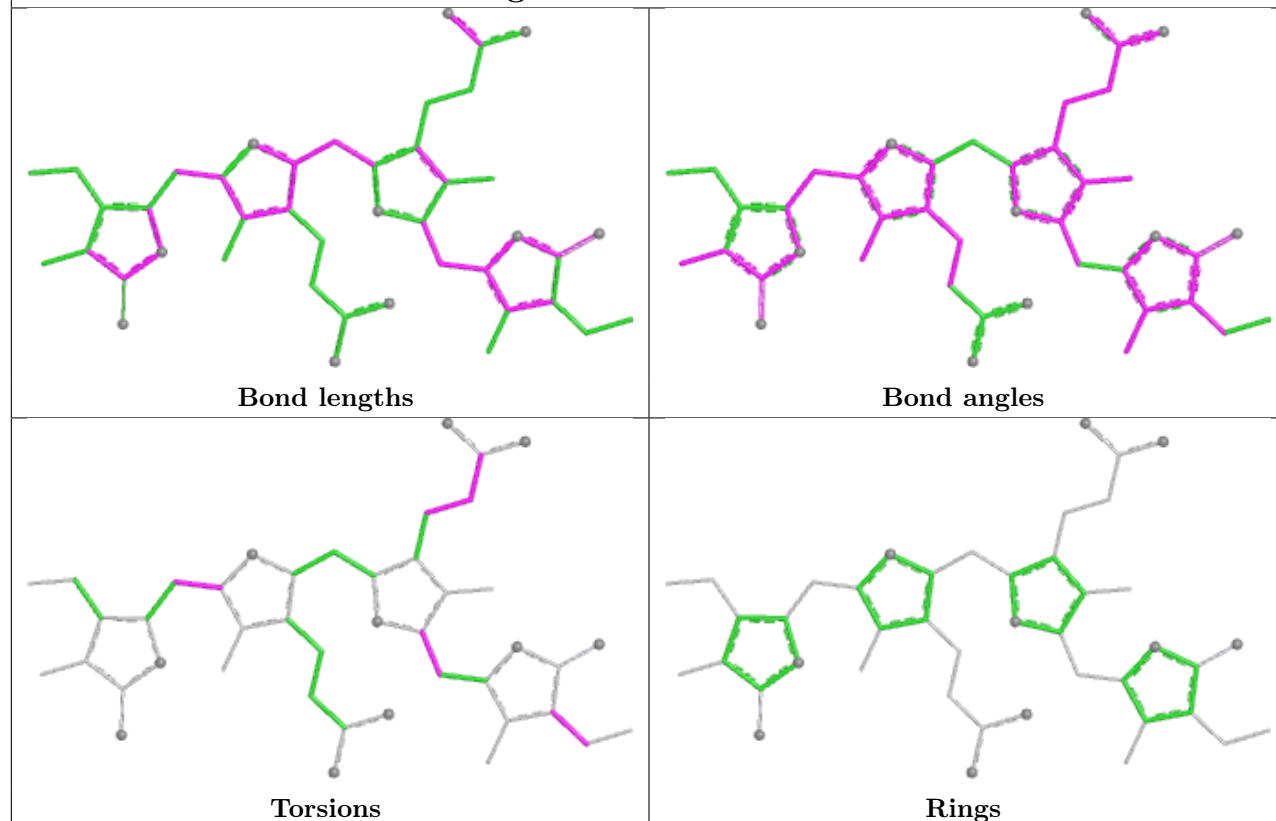
Ligand CYC Q6 201



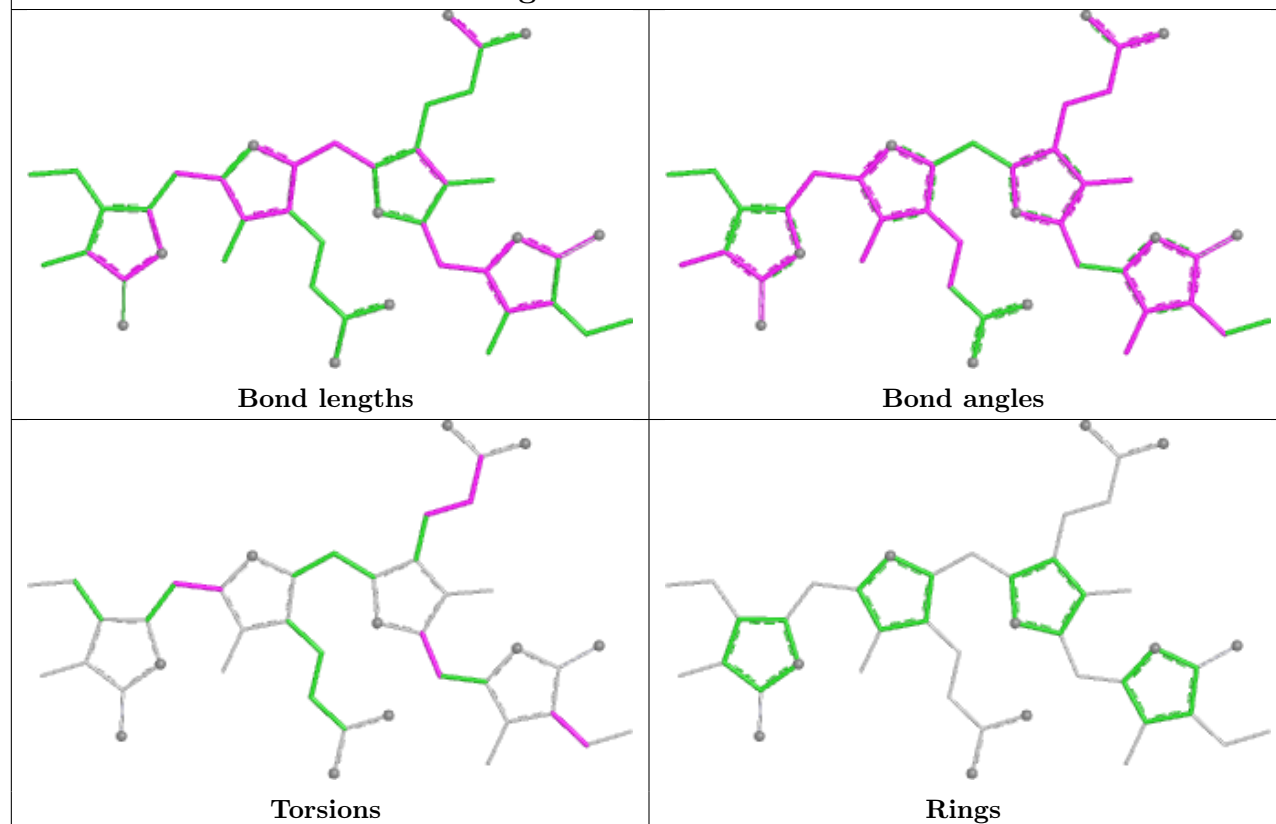
Ligand CYC K6 202



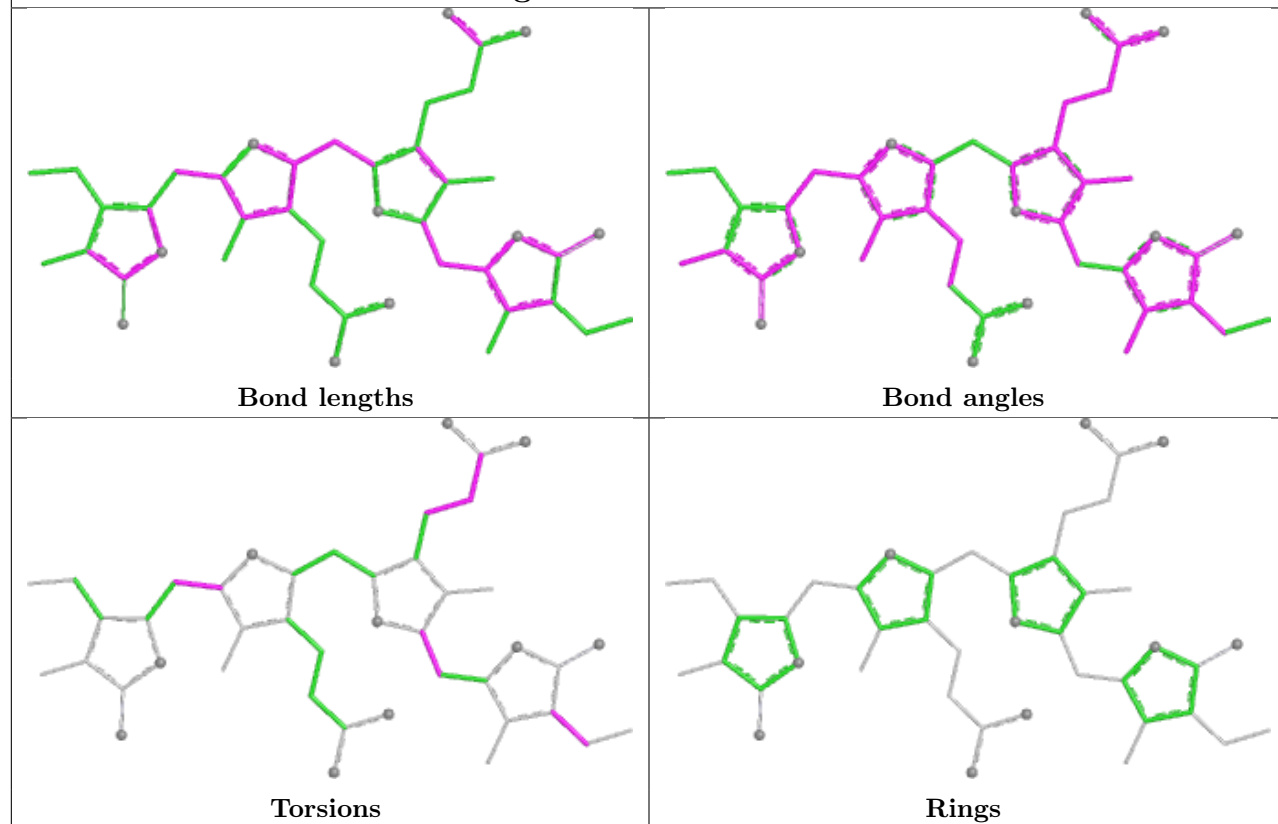
Ligand CYC DA 1001



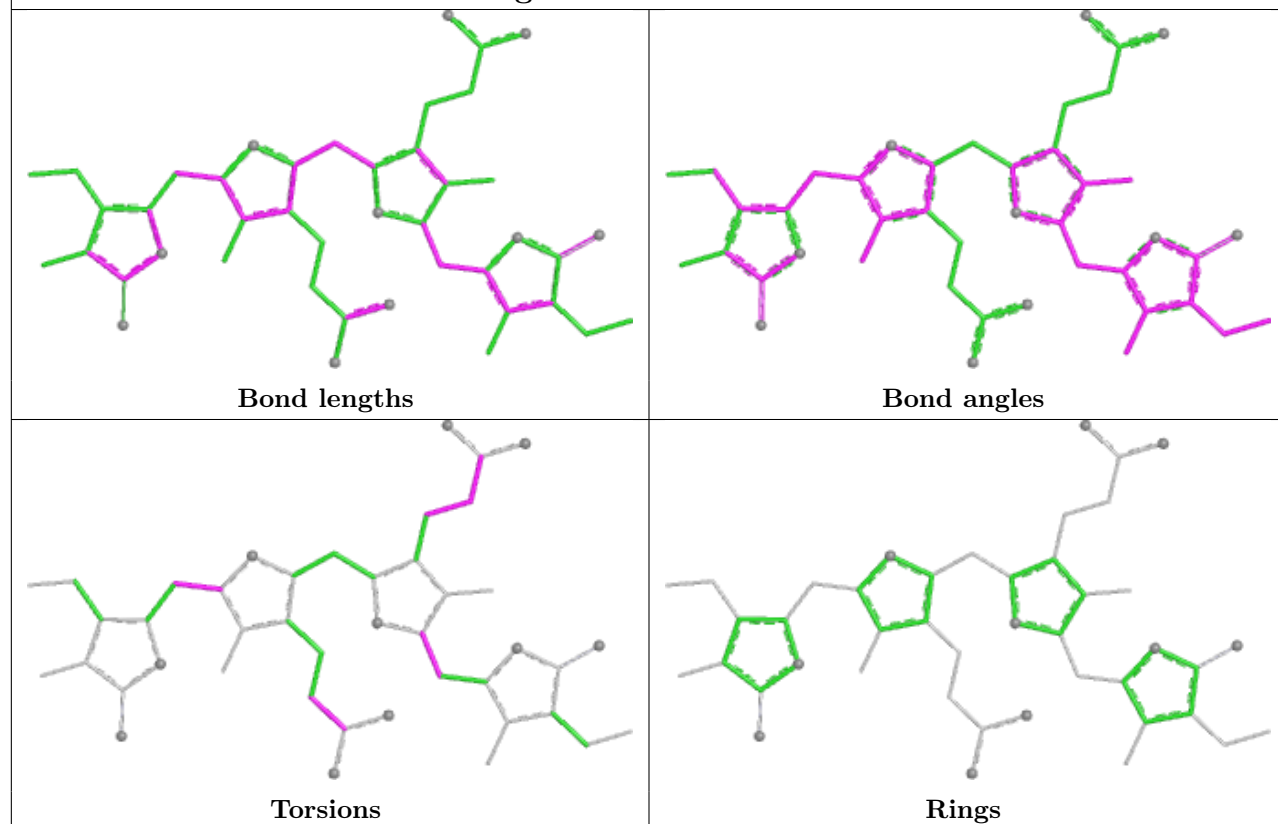
Ligand CYC PA 203



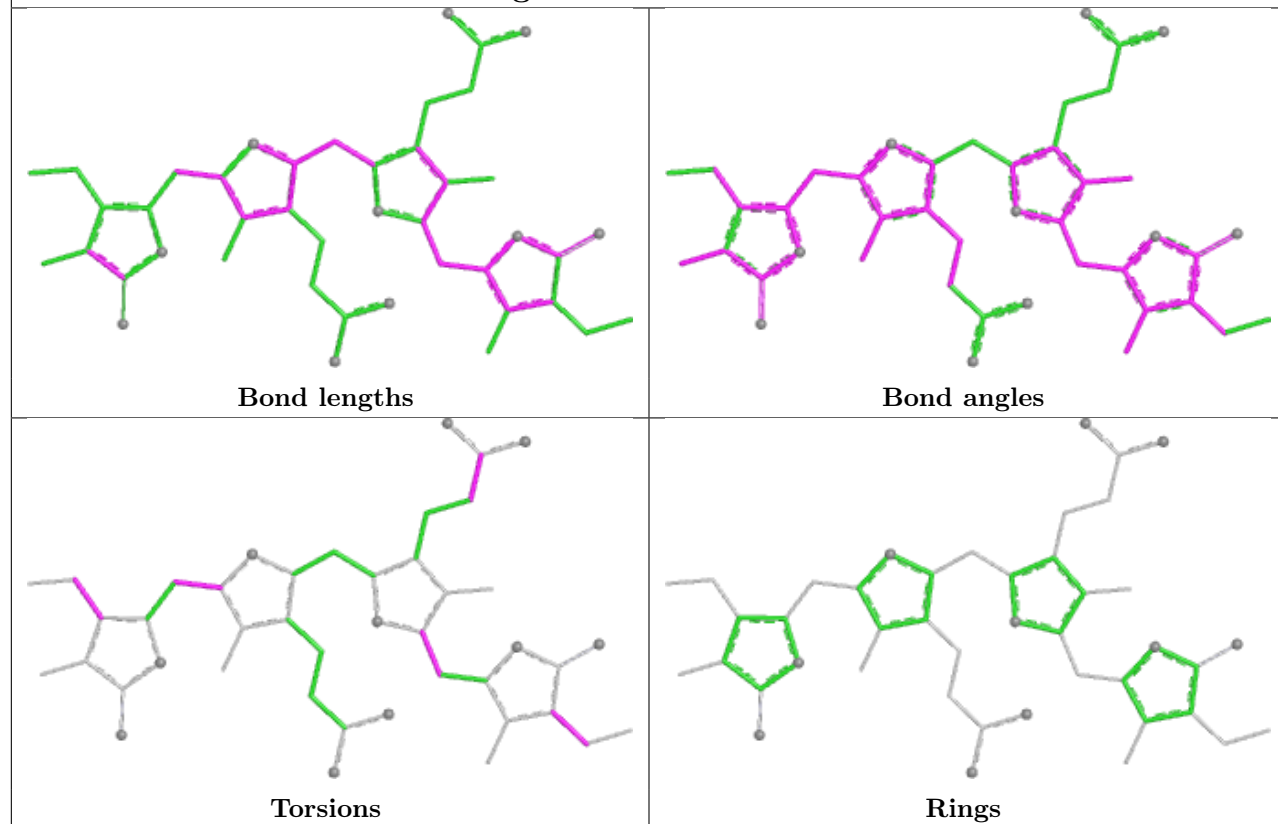
Ligand CYC F3 1001



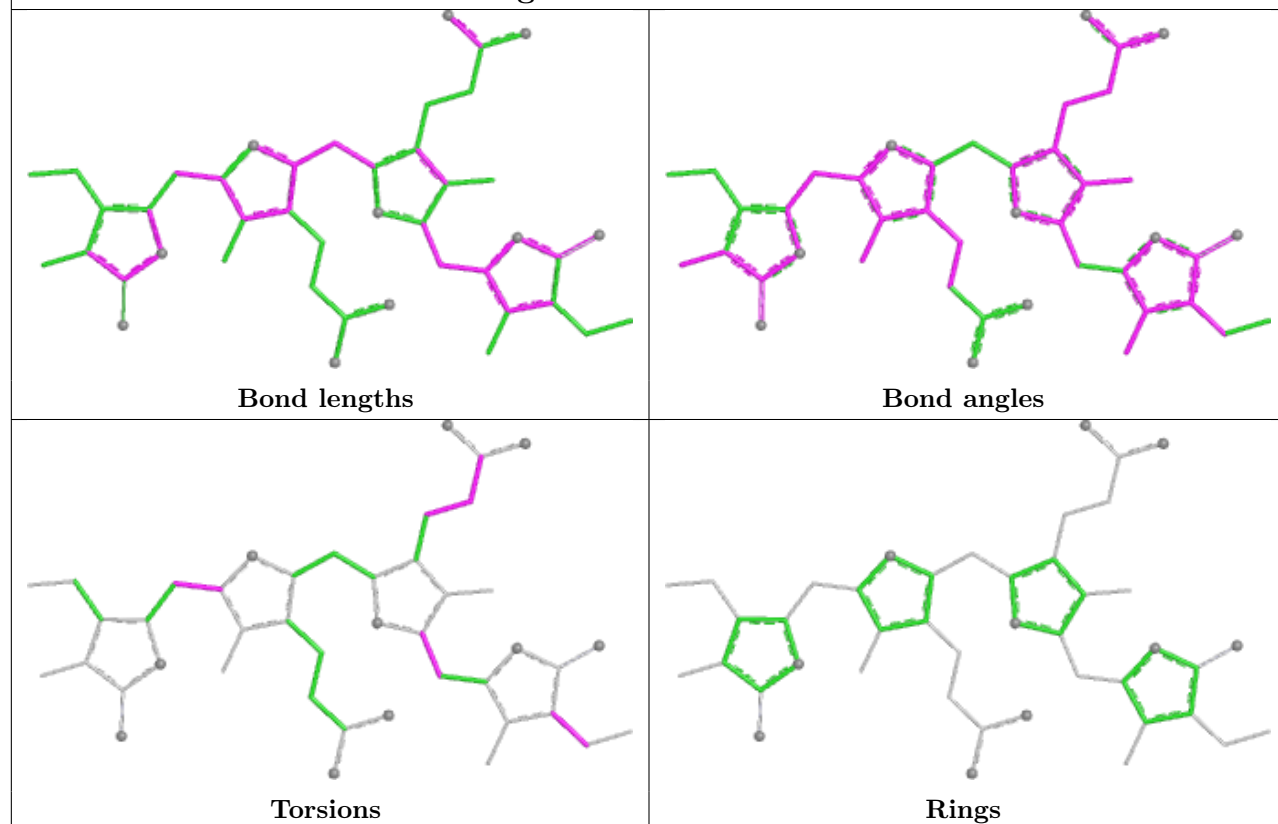
Ligand CYC h8 1001



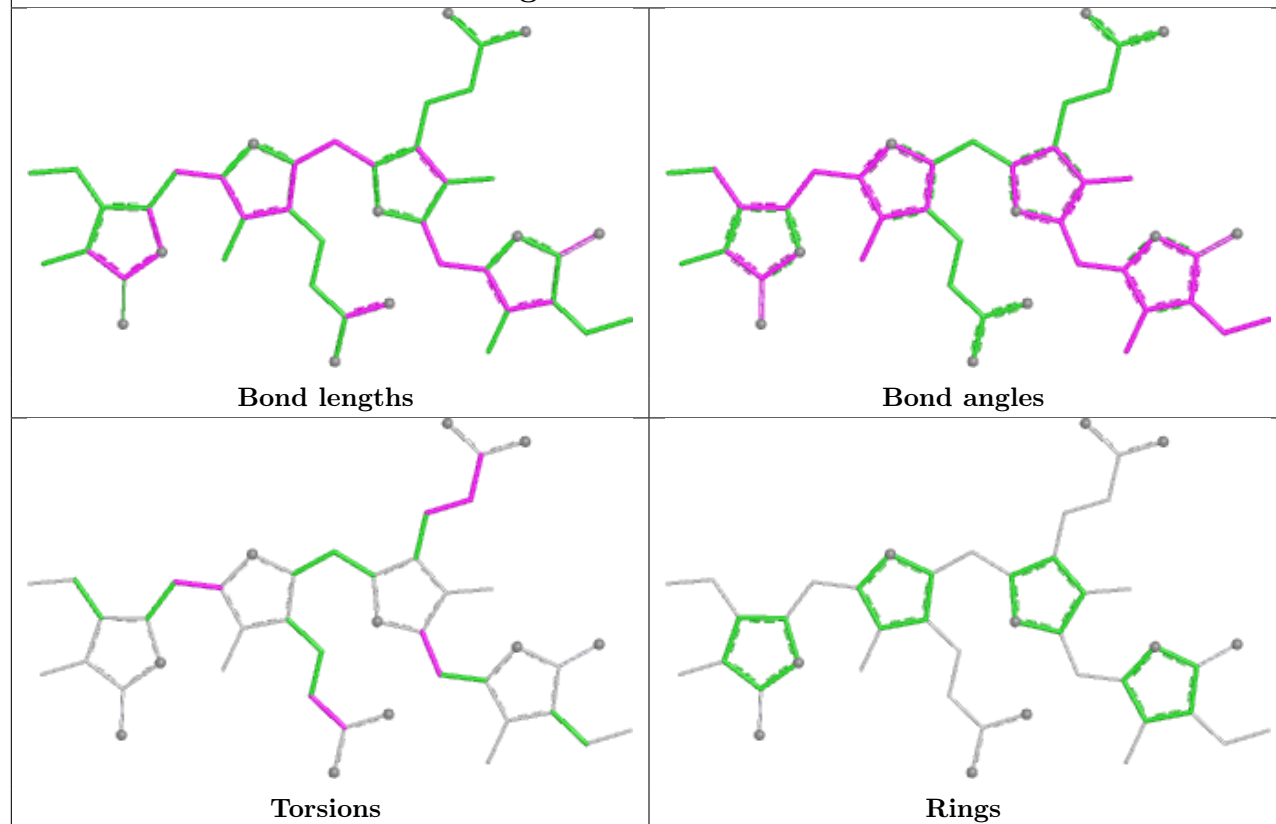
Ligand CYC T9 1001



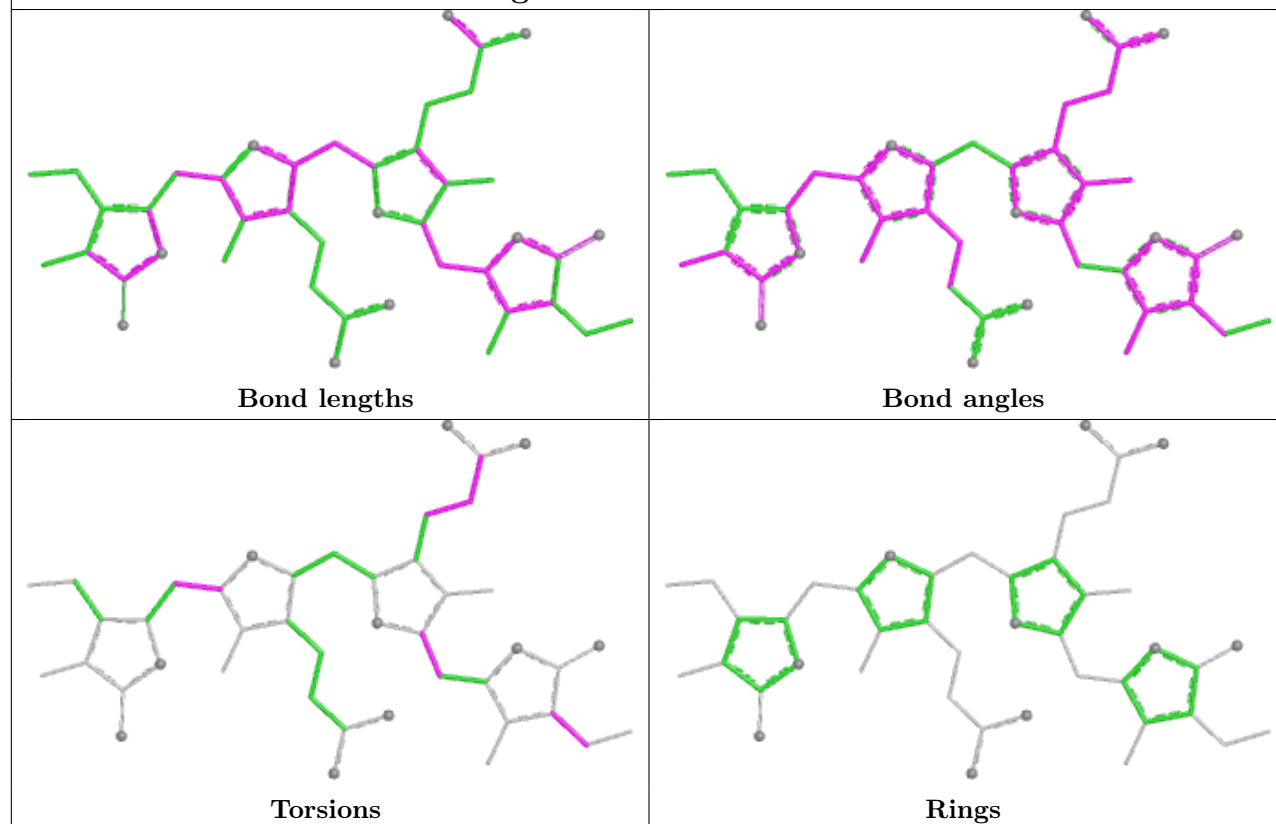
Ligand CYC YA 201



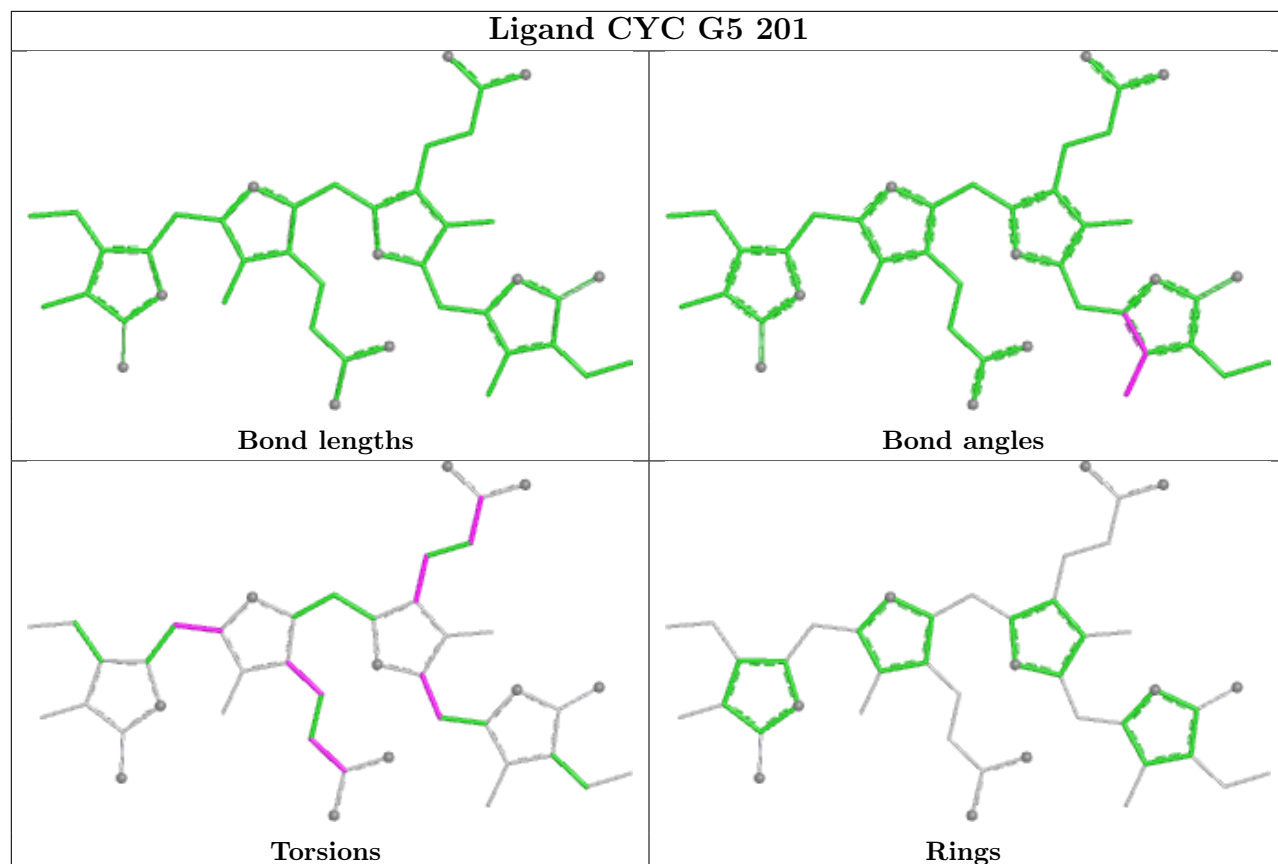
Ligand CYC f8 1001



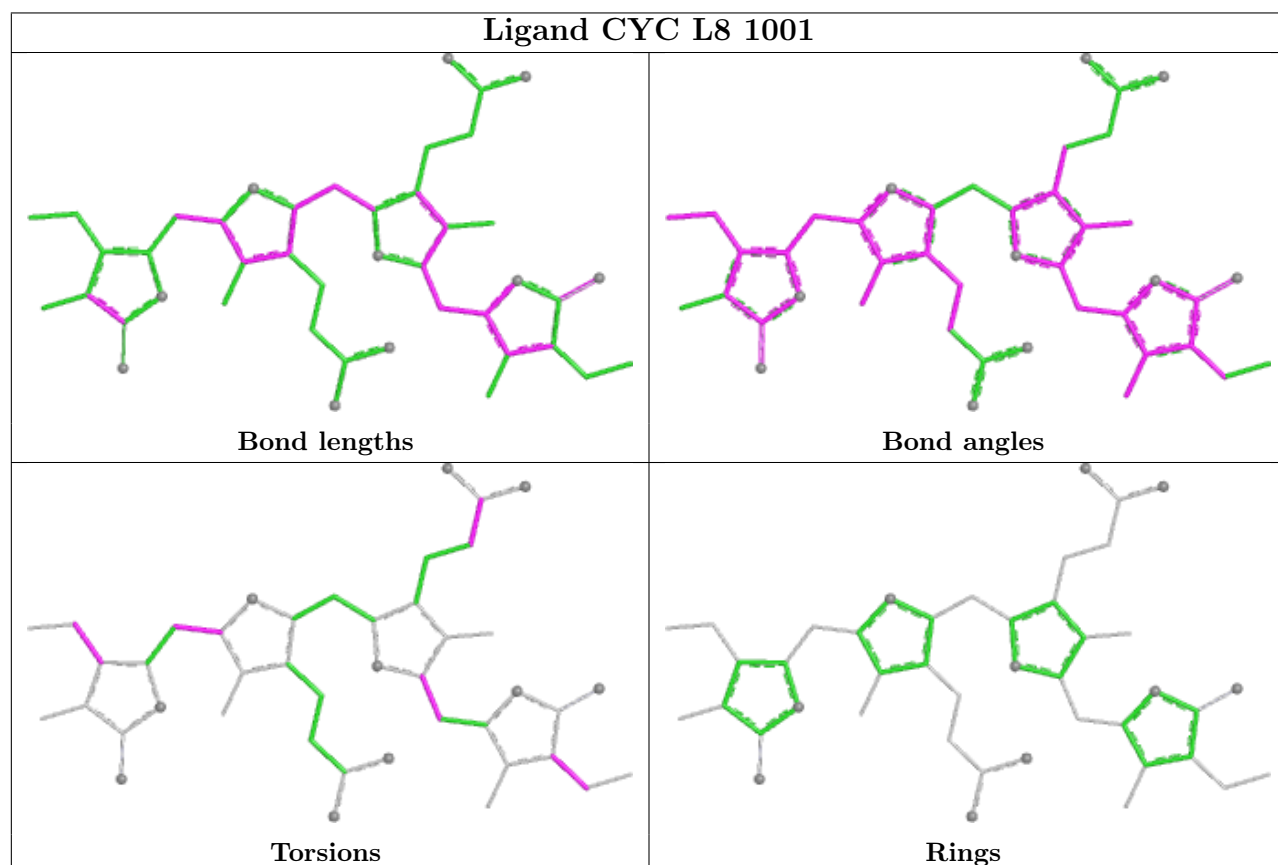
Ligand CYC D2 1001

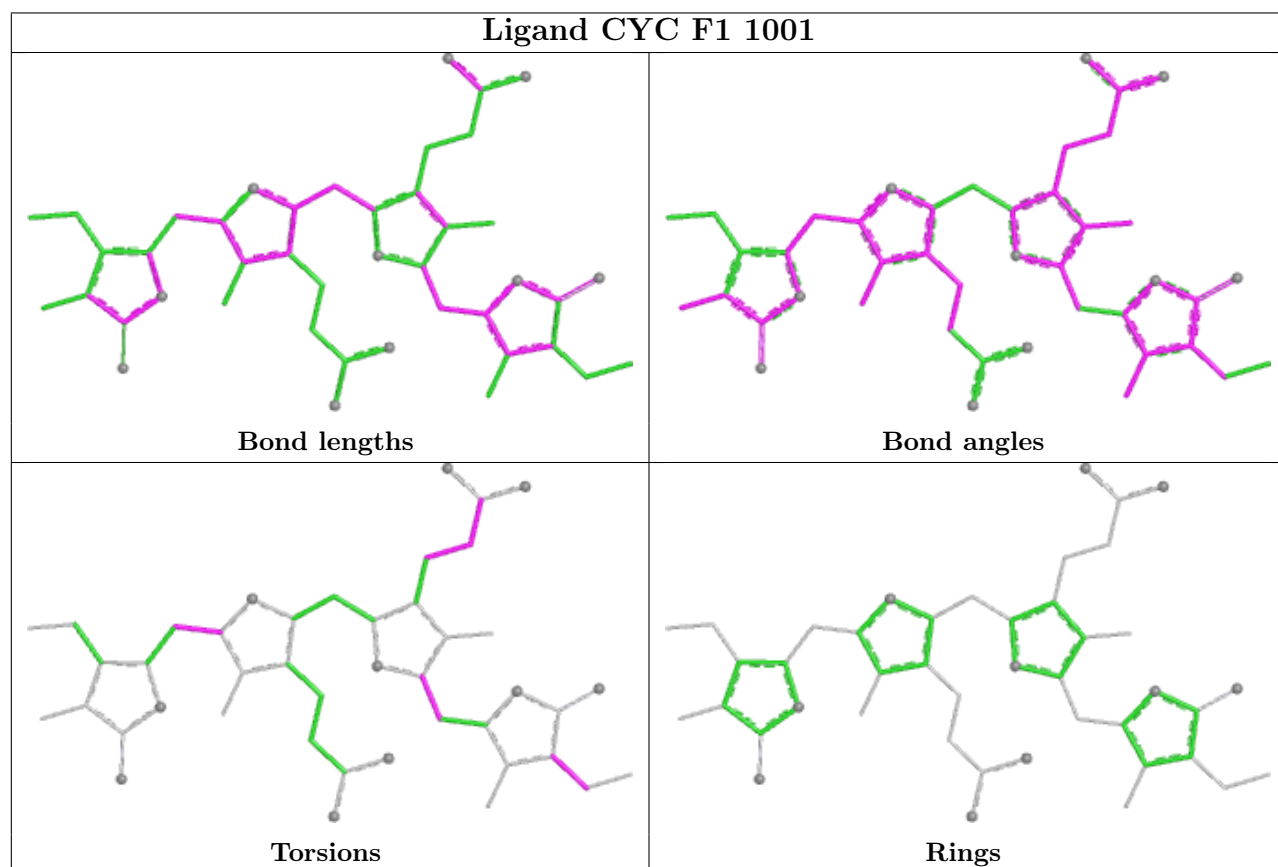
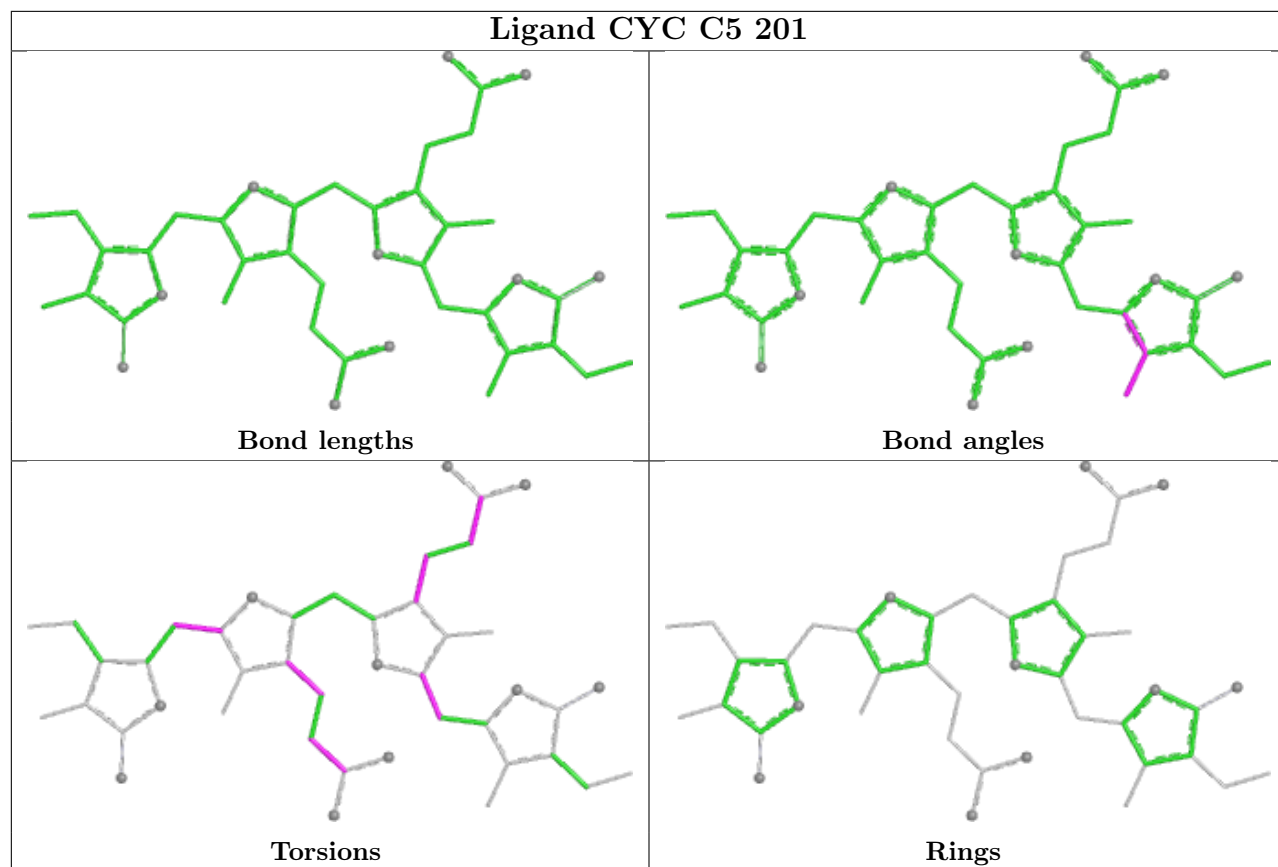


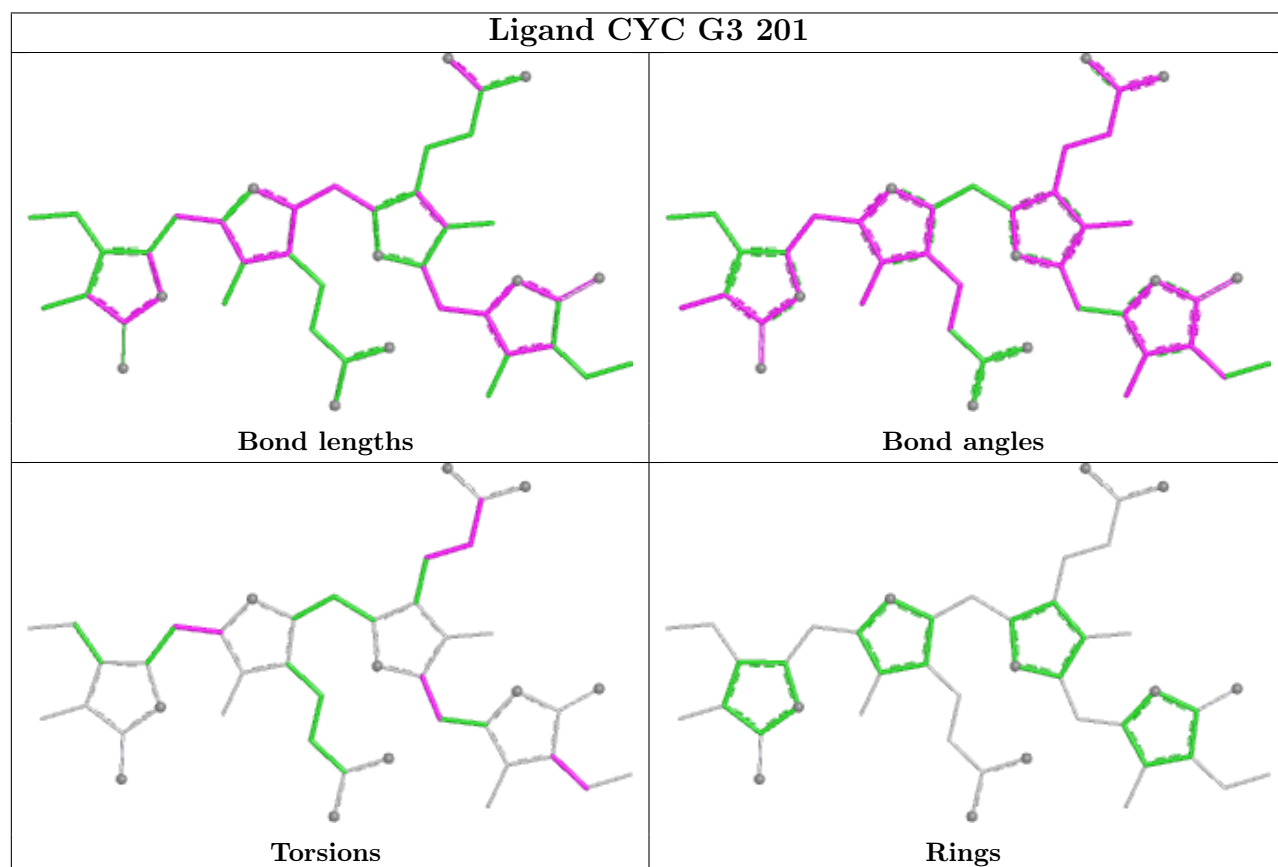
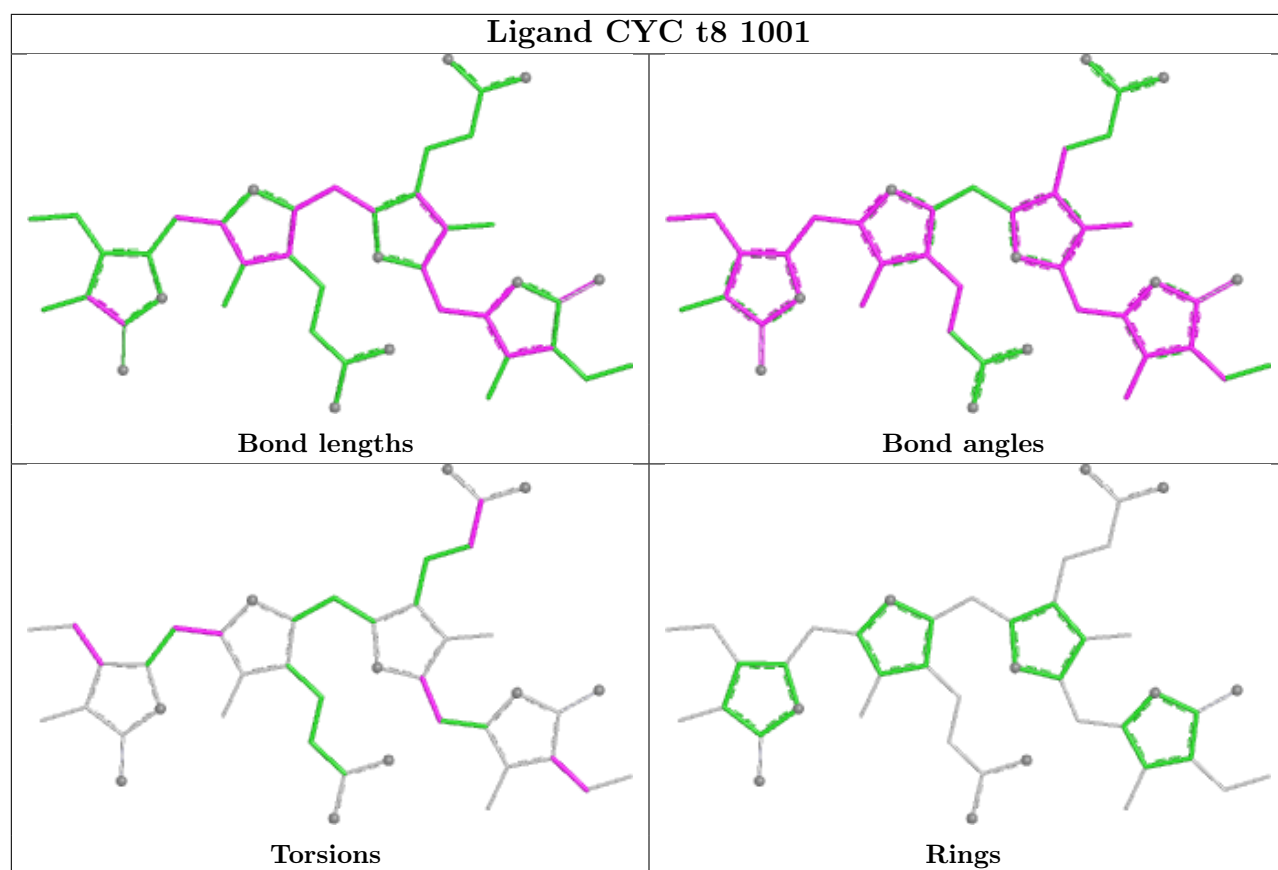
Ligand CYC G5 201



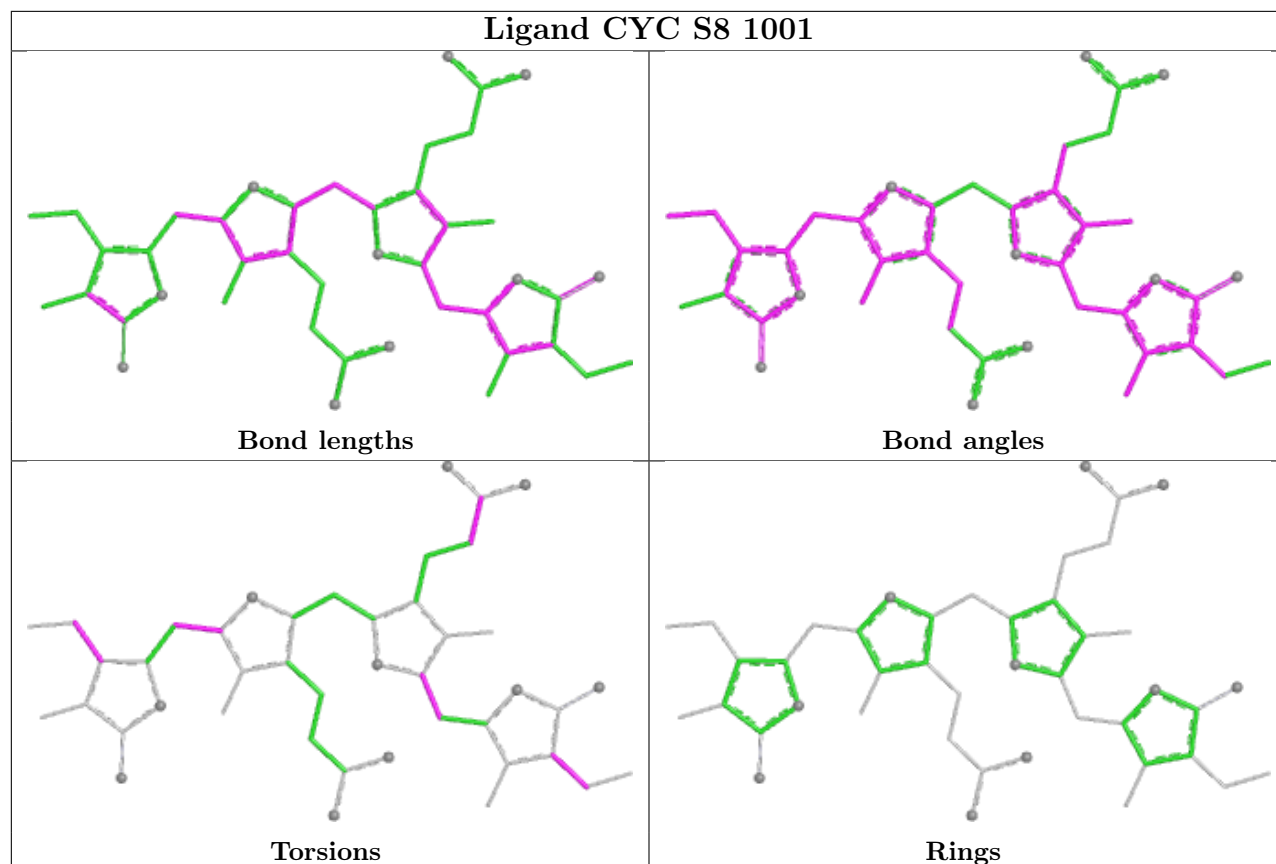
Ligand CYC L8 1001



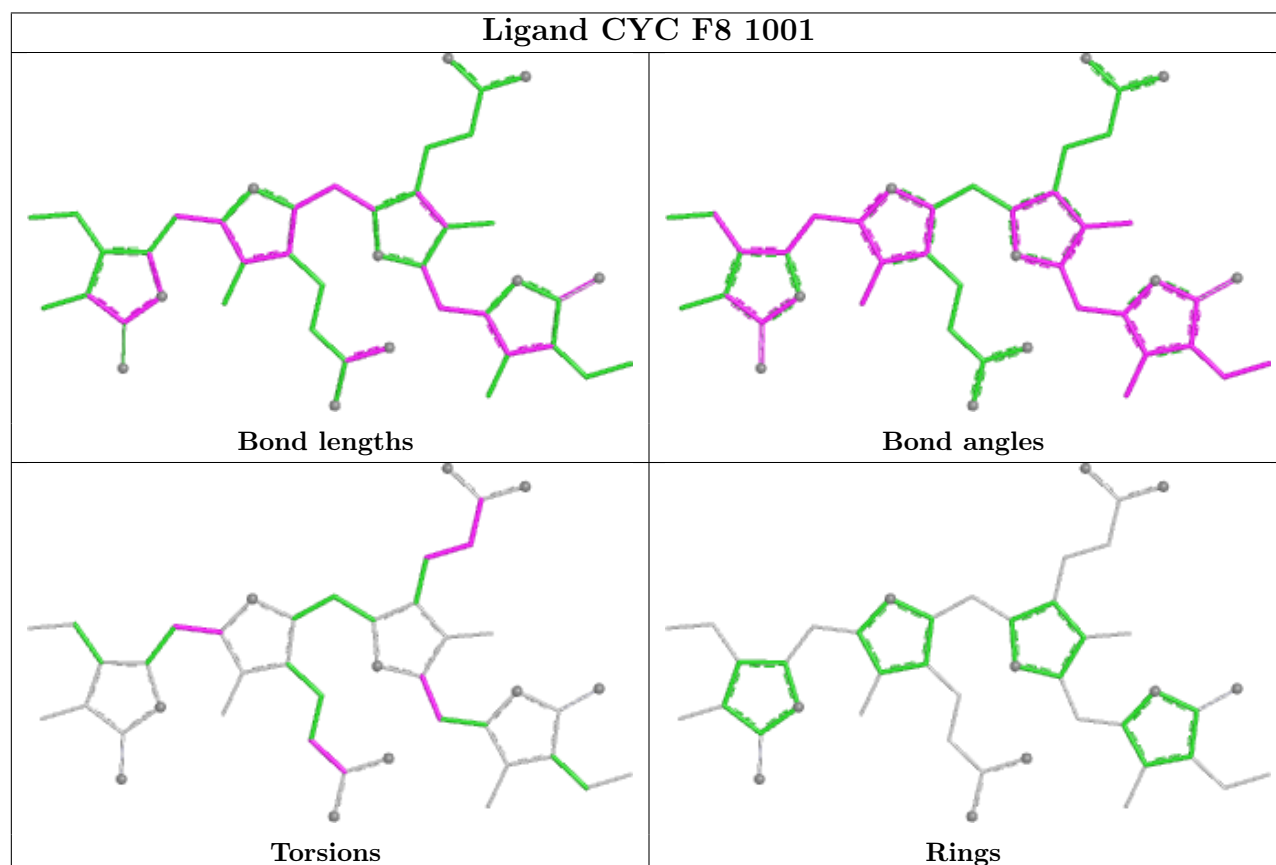




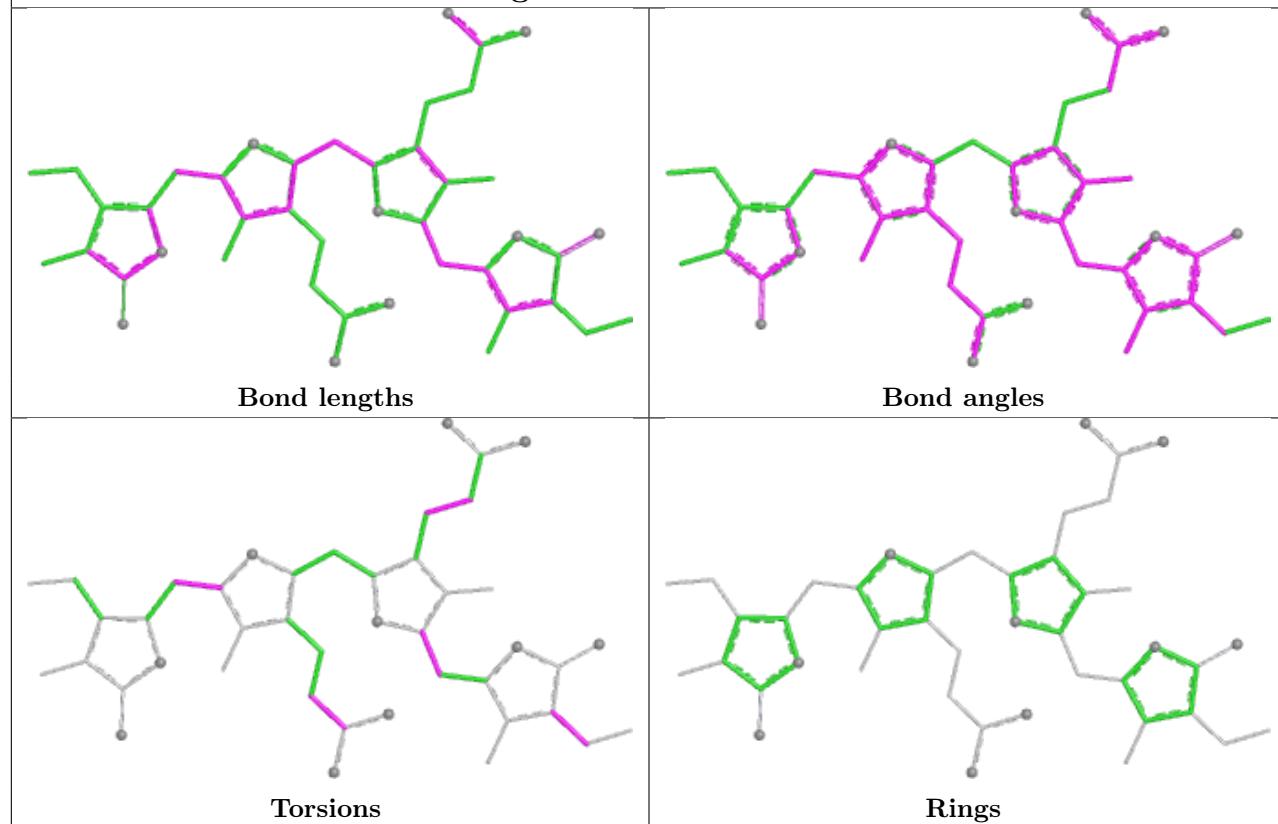
Ligand CYC S8 1001



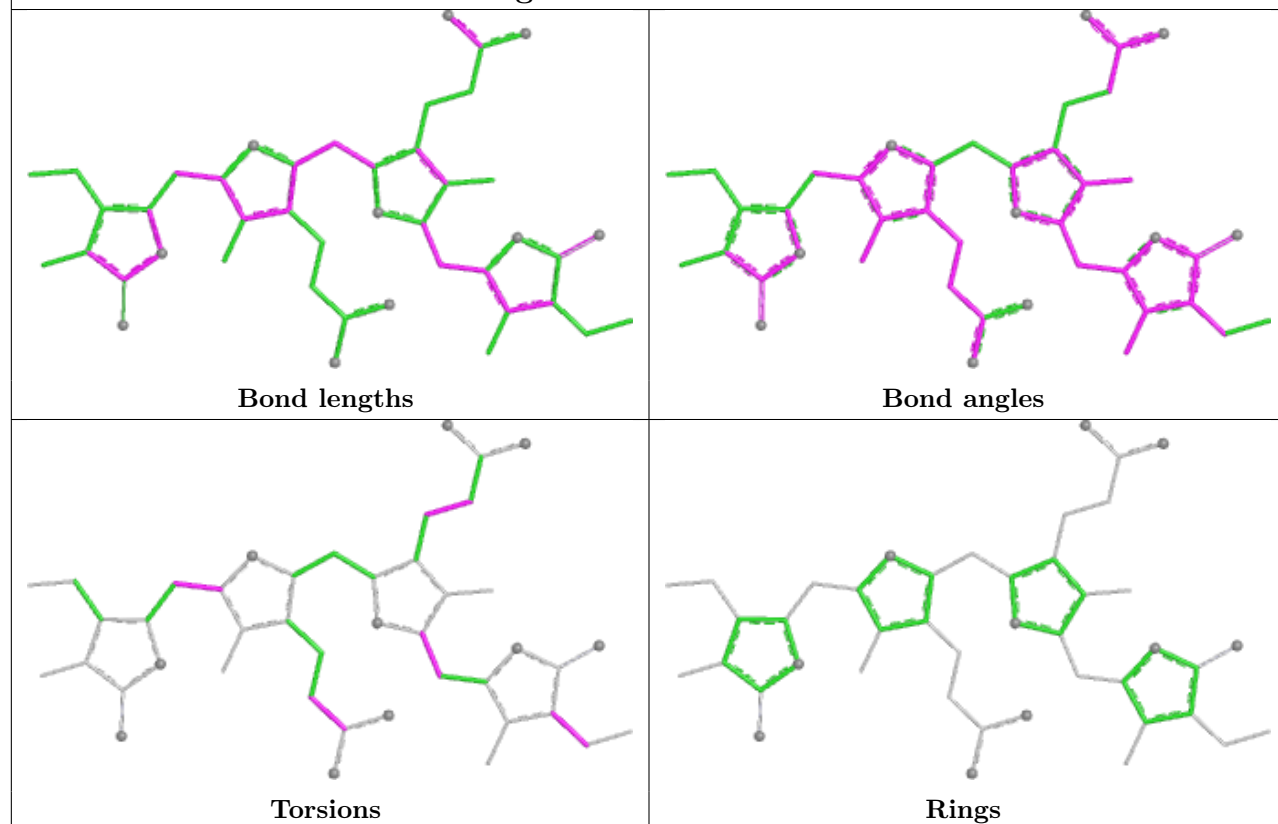
Ligand CYC F8 1001

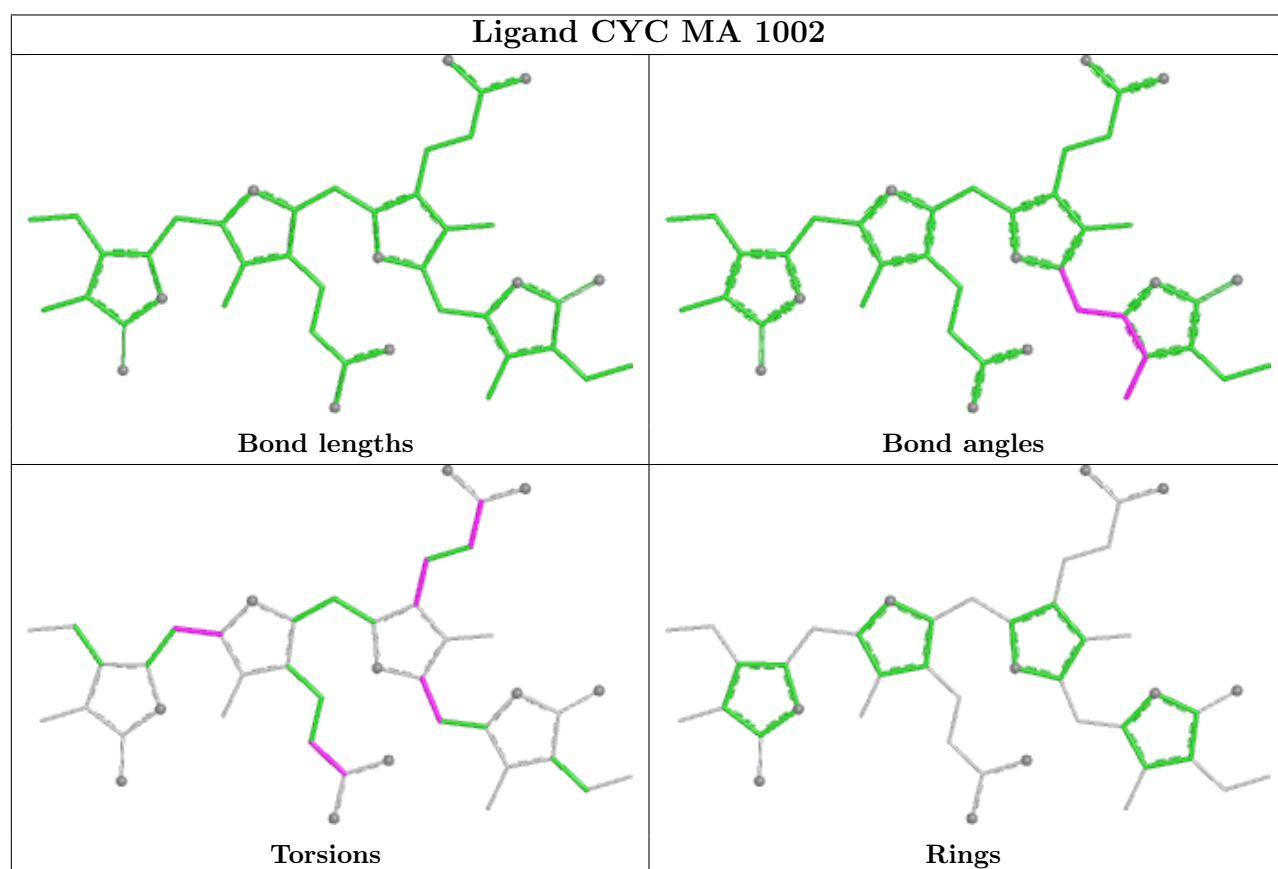
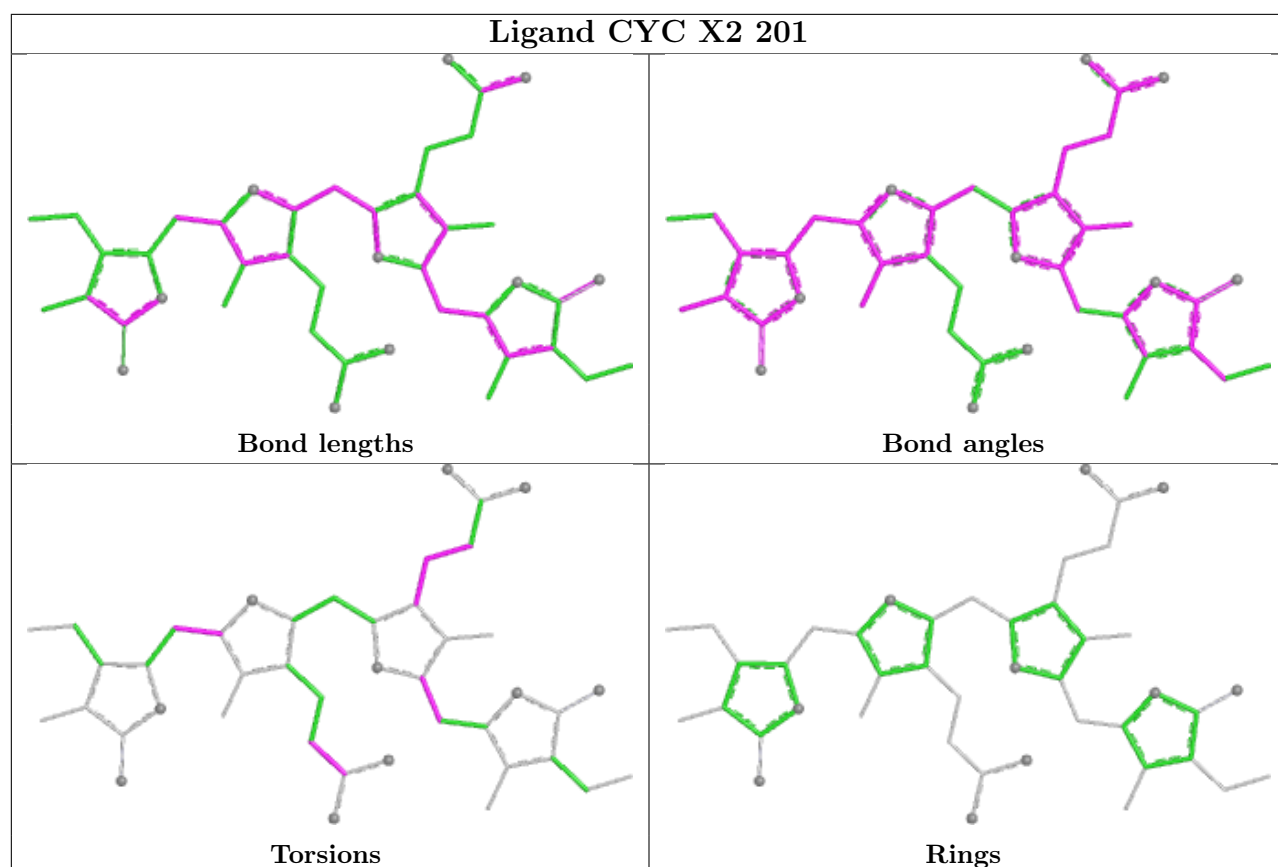


Ligand CYC U9 1001

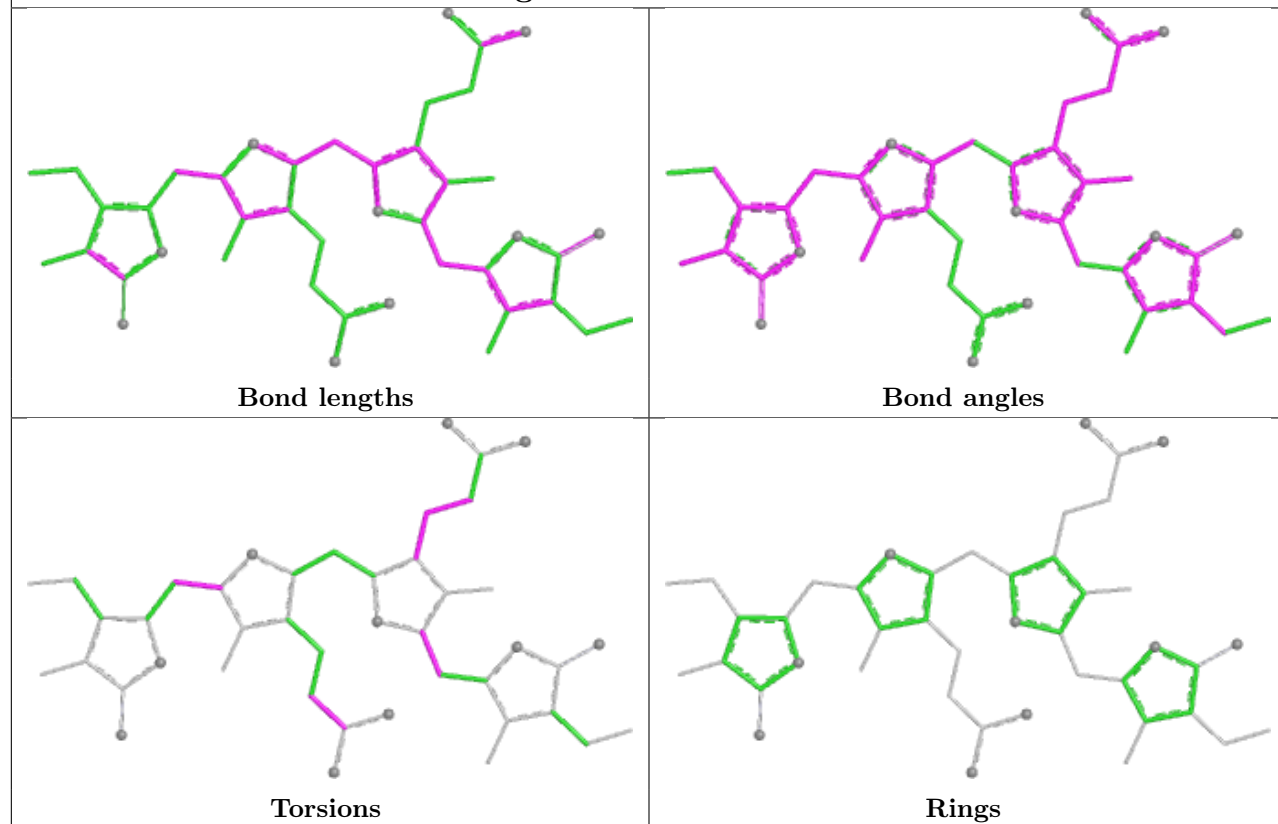


Ligand CYC v9 1001

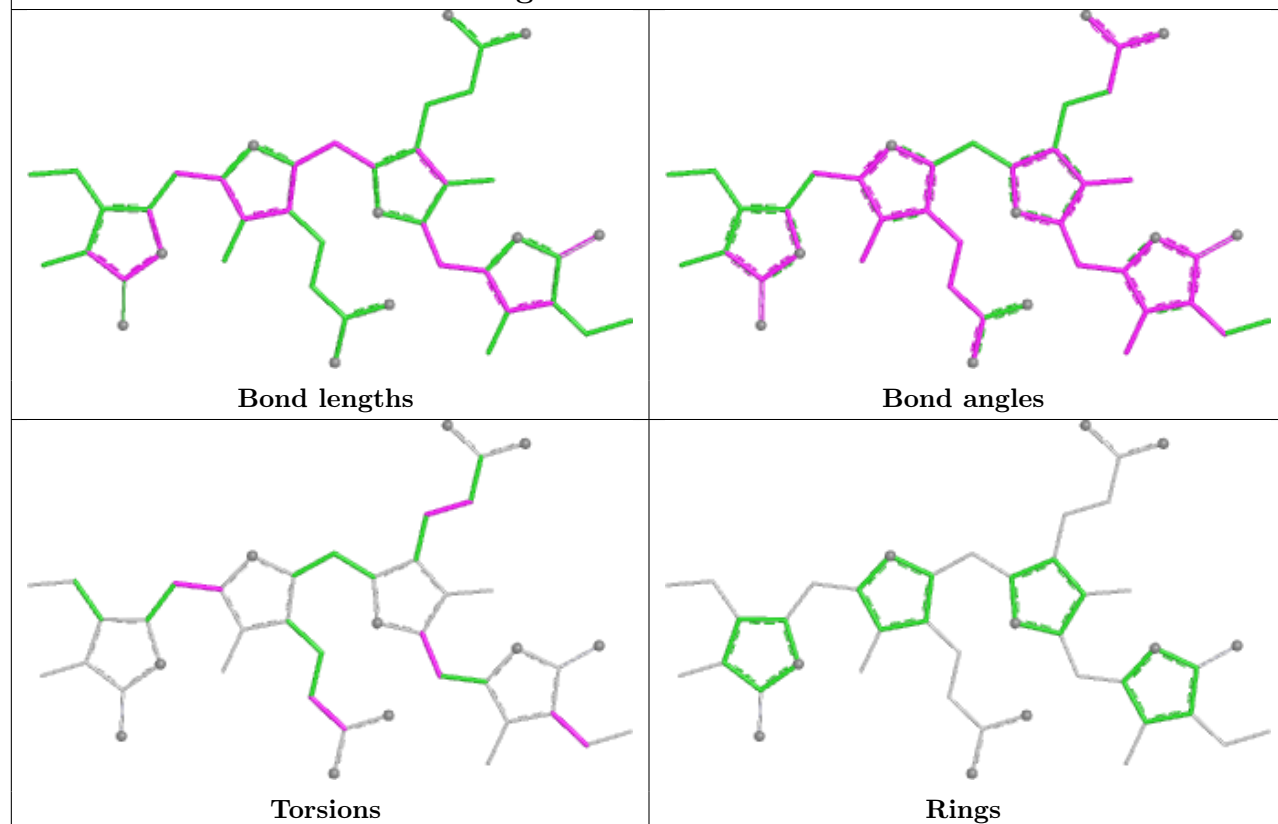




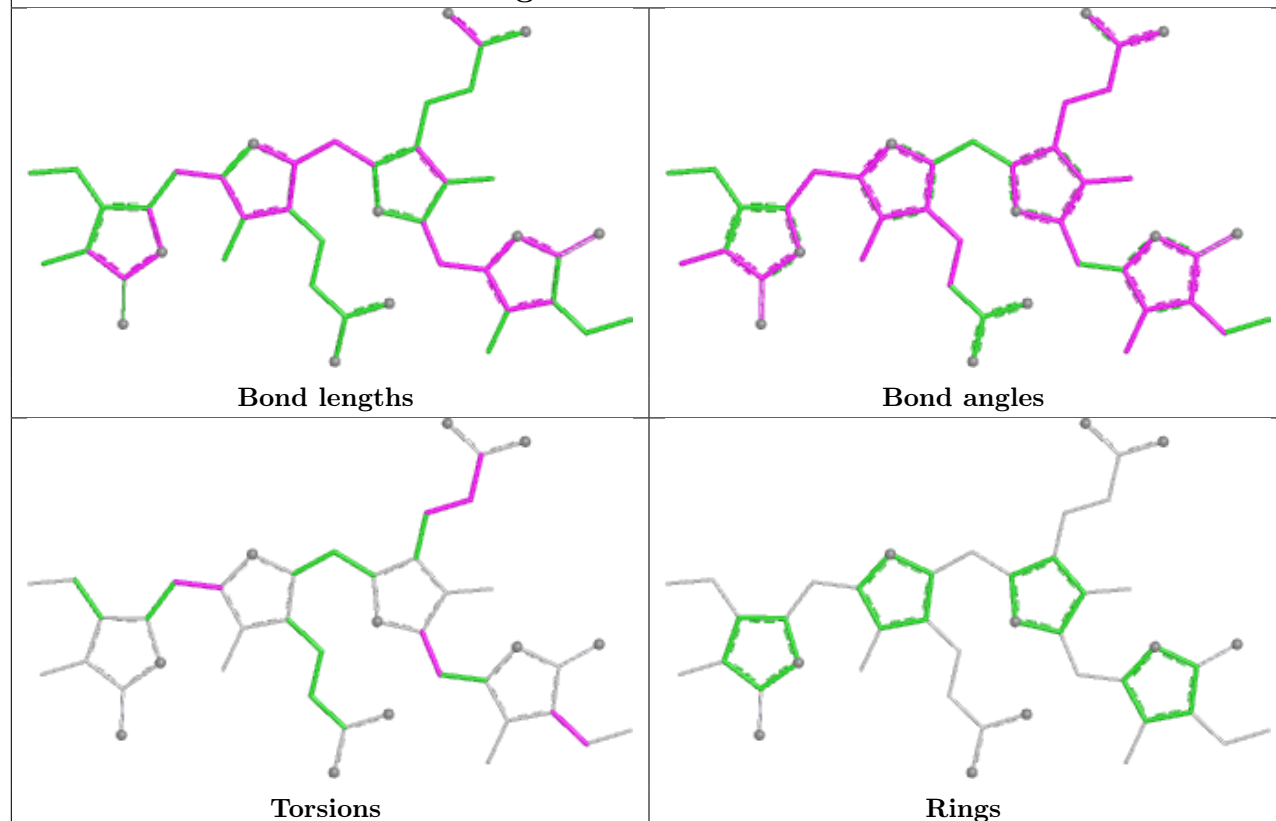
Ligand CYC NA 301



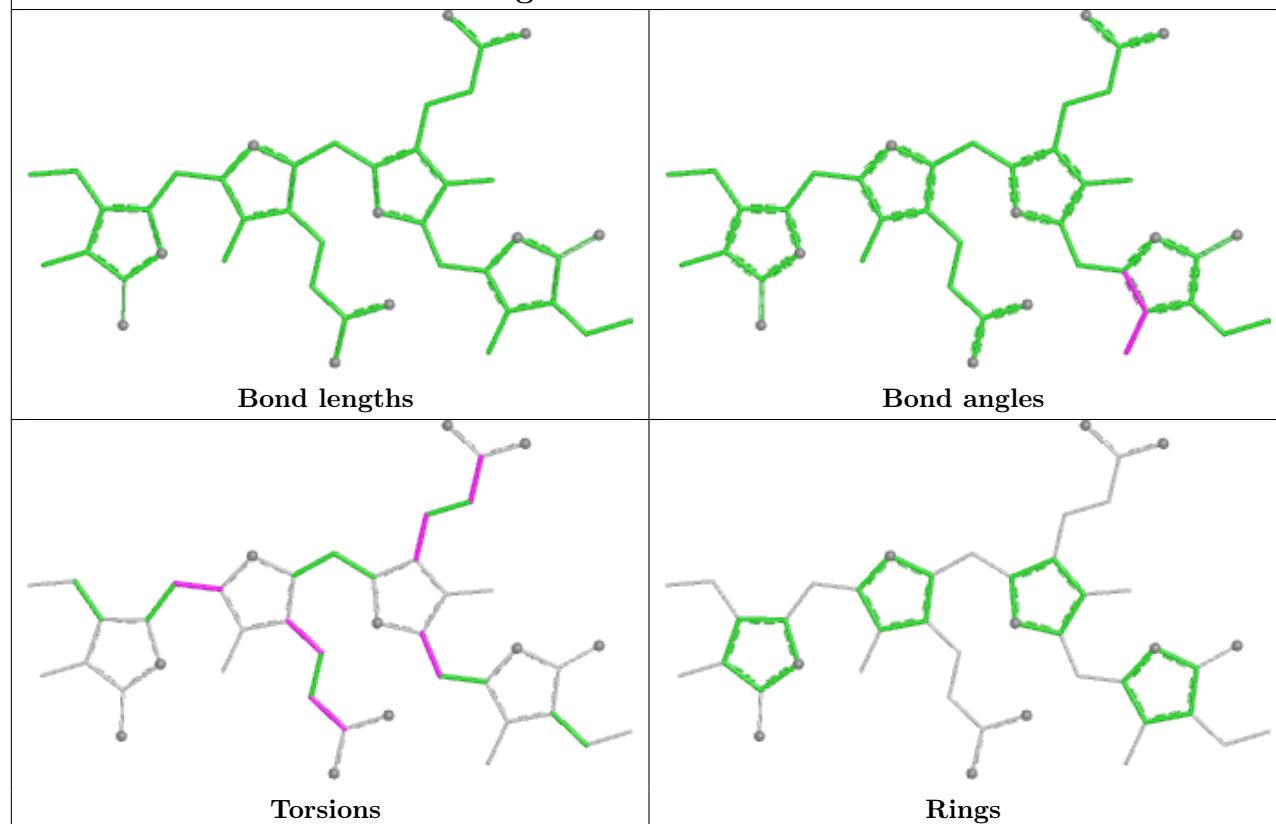
Ligand CYC 09 1203



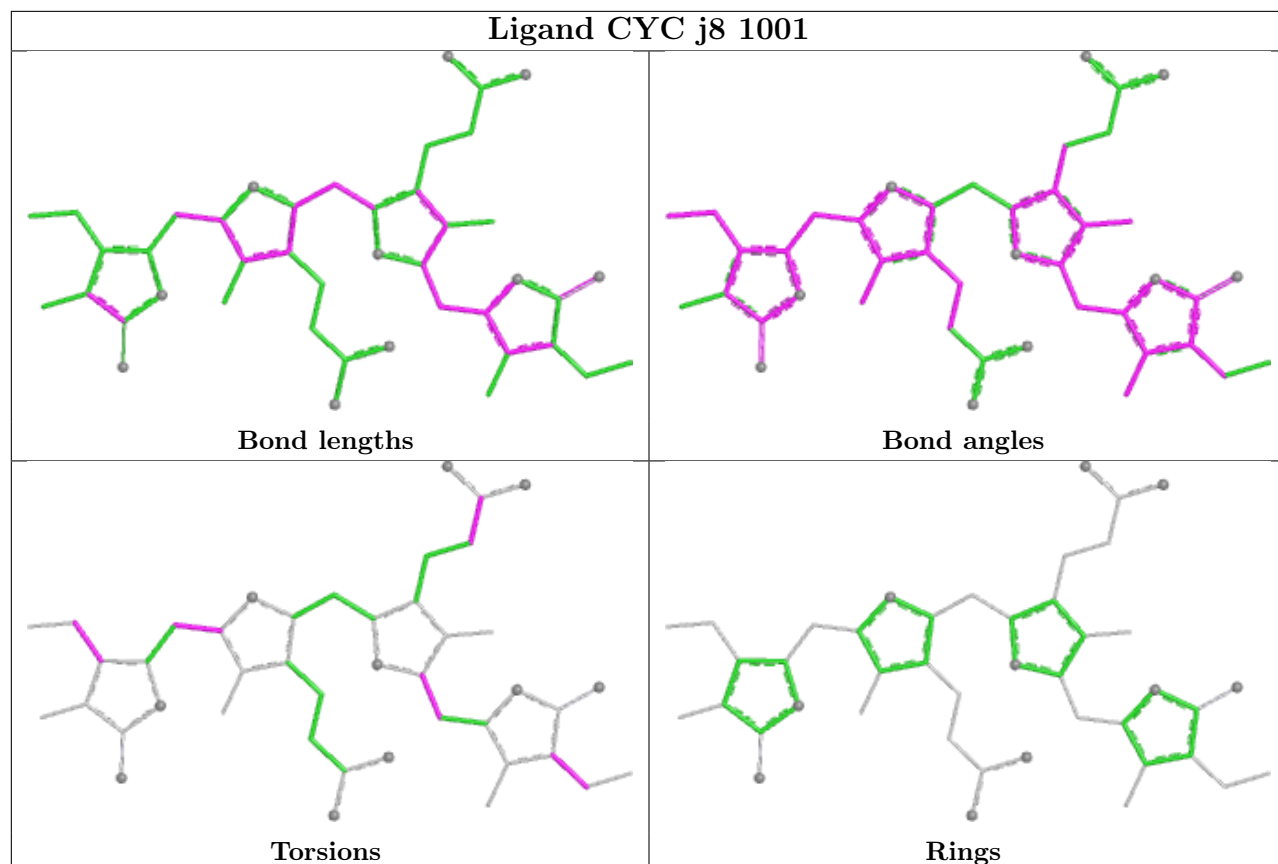
Ligand CYC J7 1001



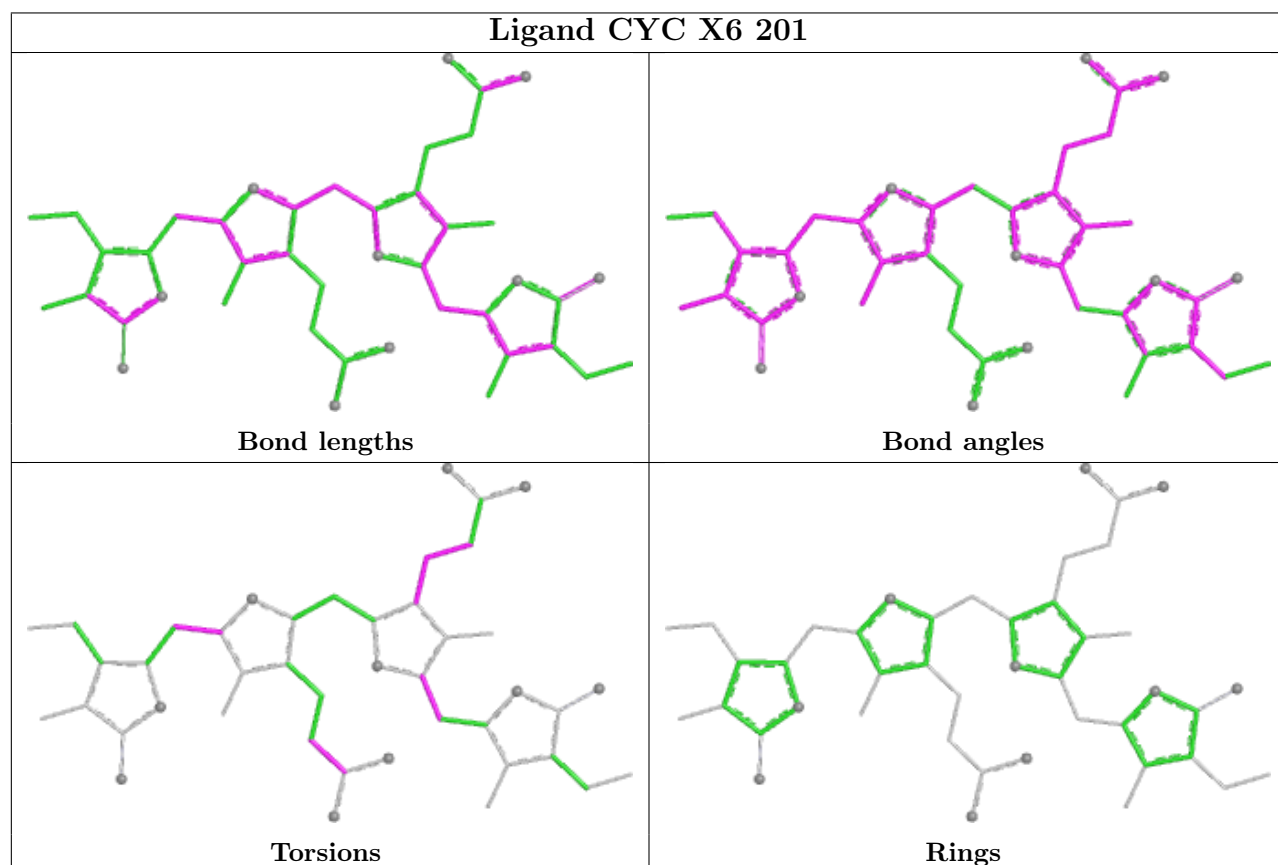
Ligand CYC RA 201



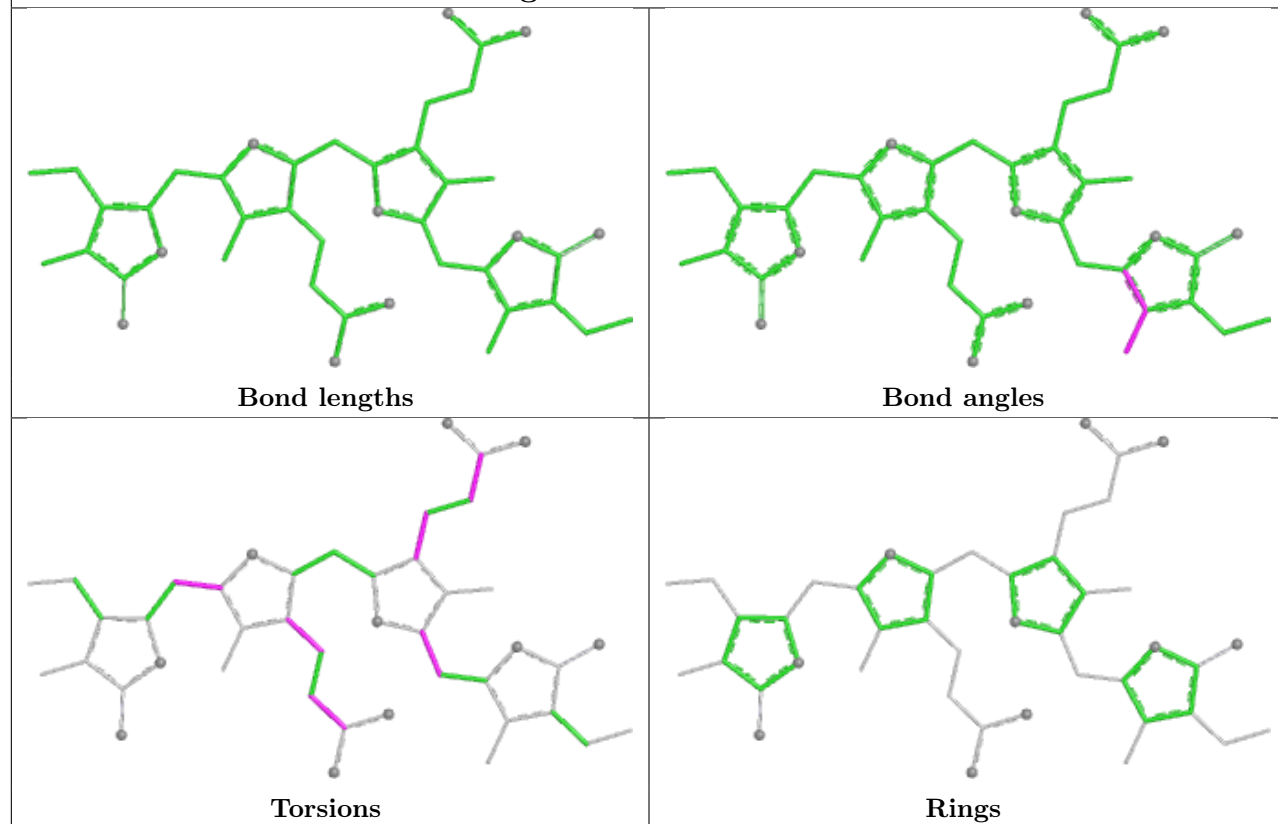
Ligand CYC j8 1001



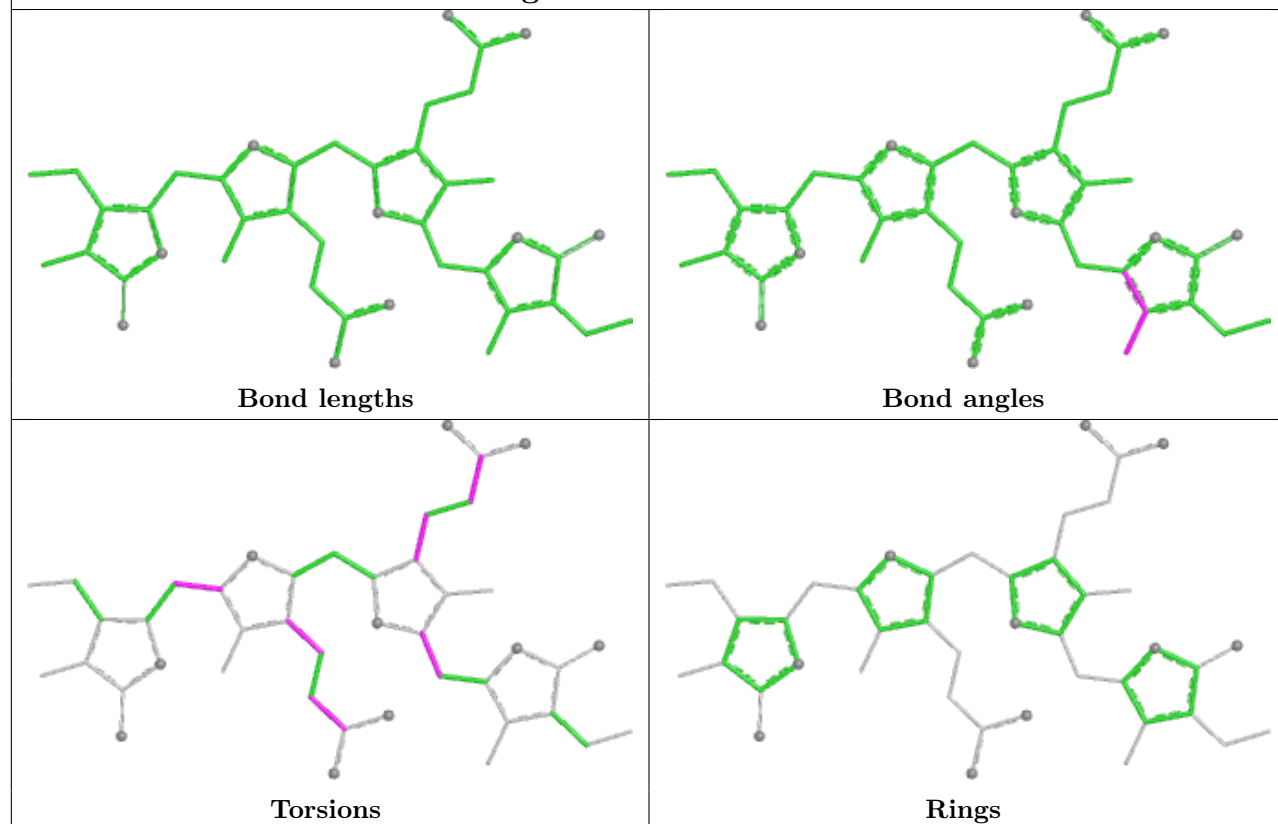
Ligand CYC X6 201



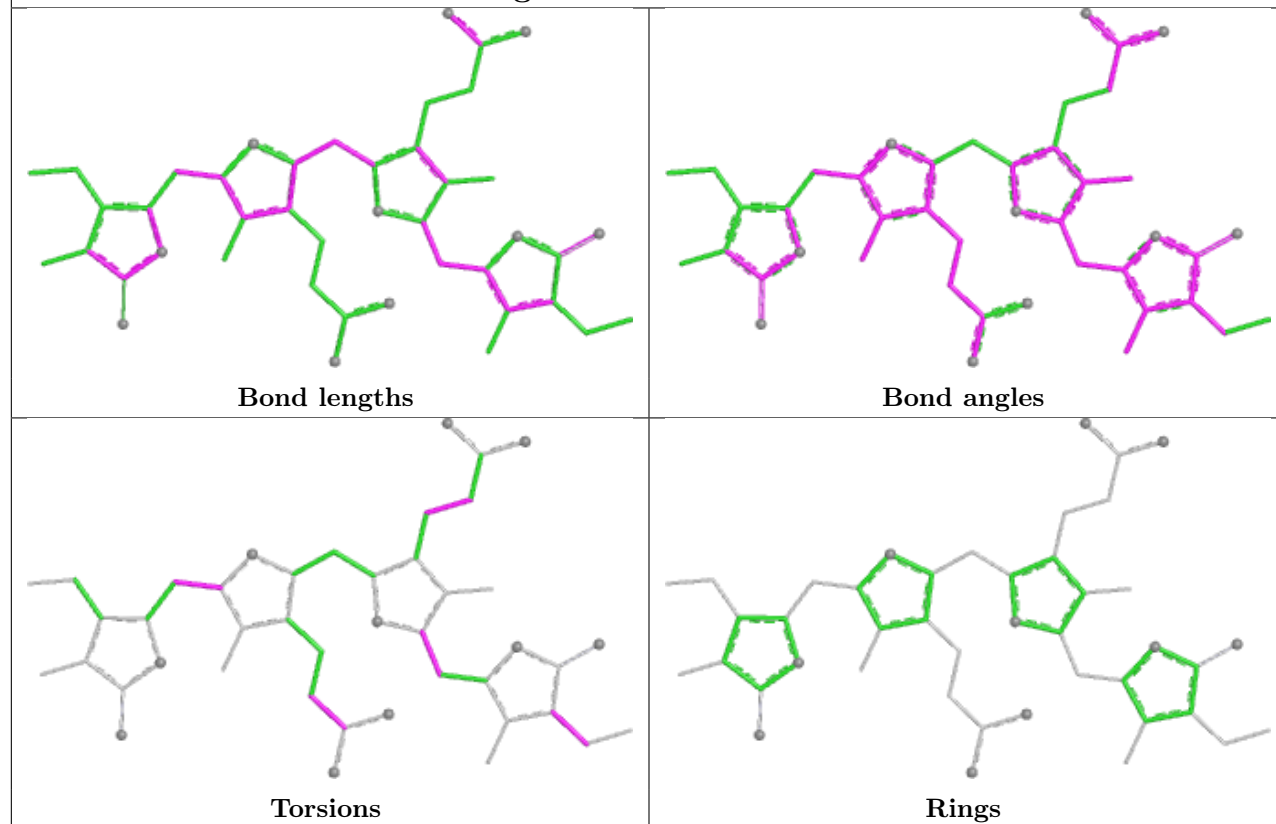
Ligand CYC K5 201



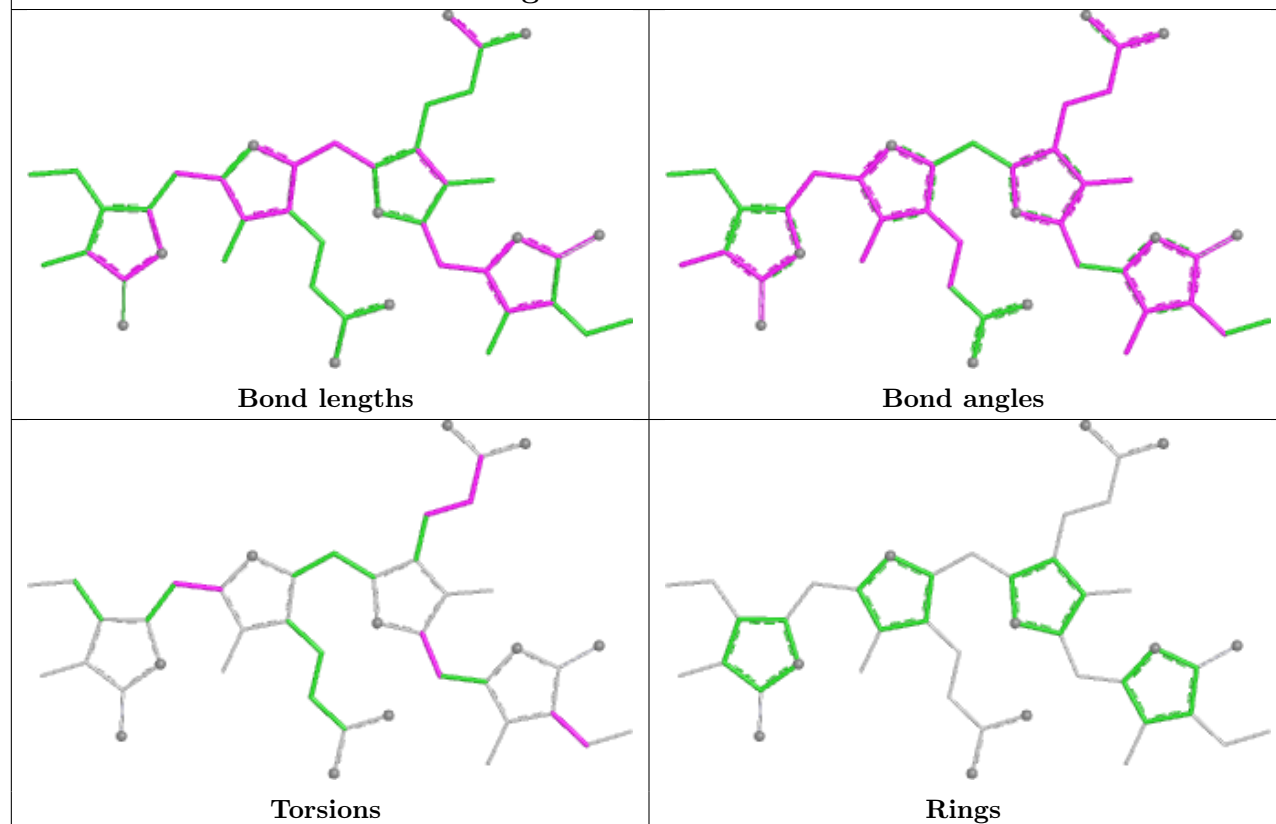
Ligand CYC P5 202



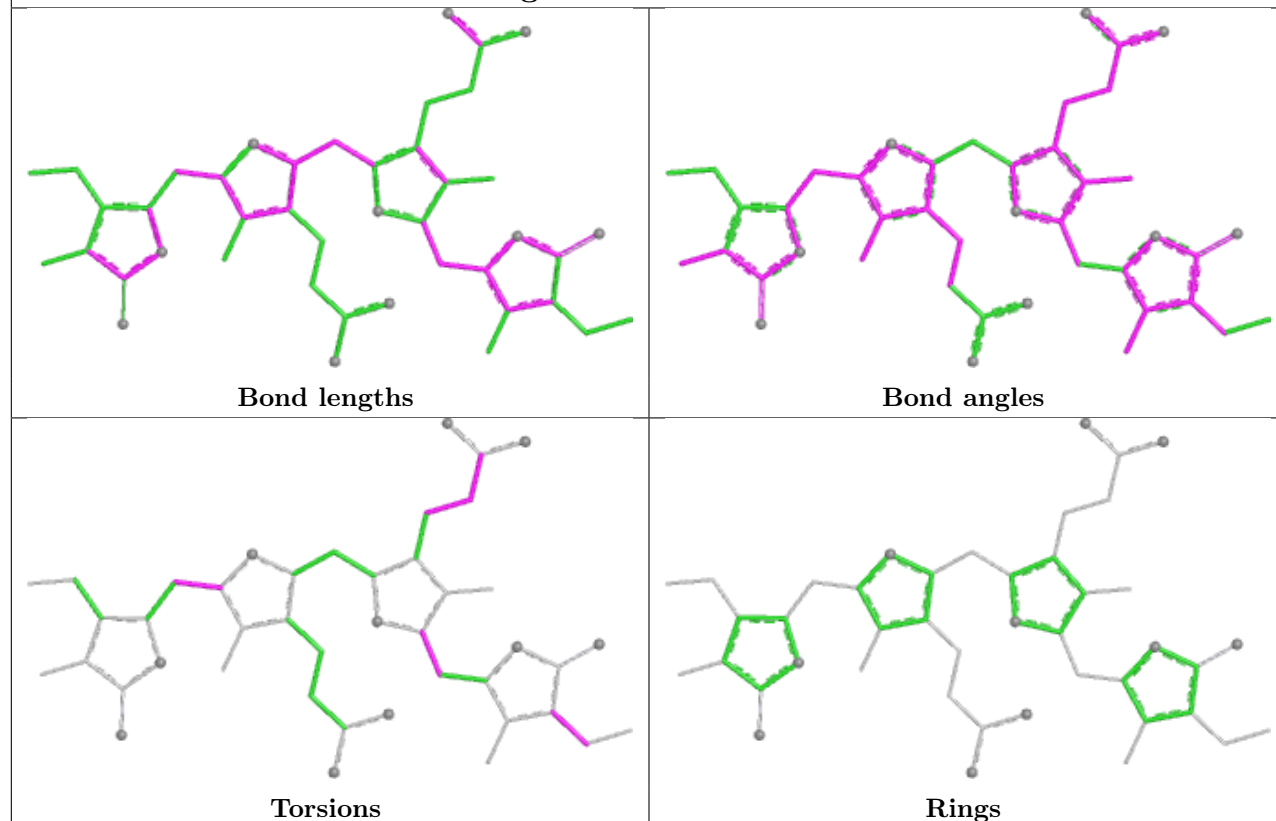
Ligand CYC F9 1001



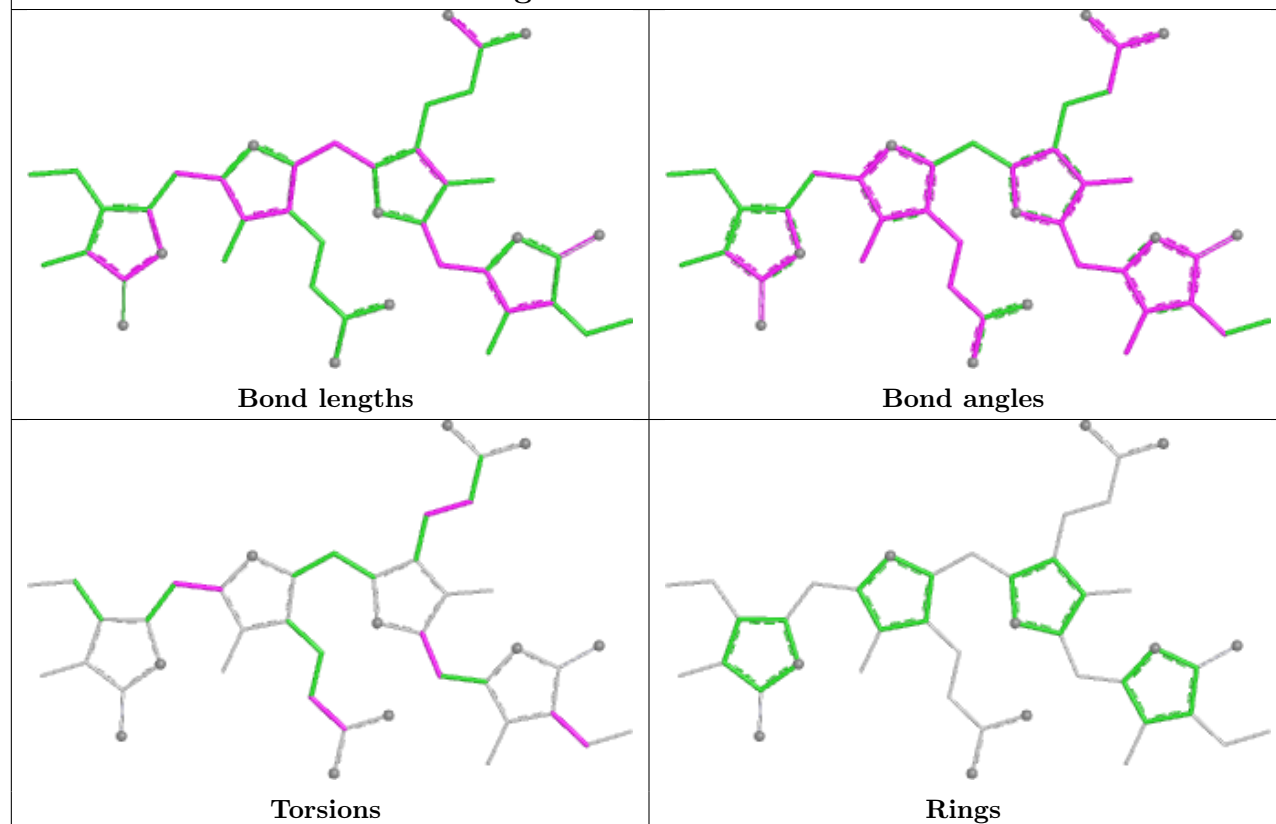
Ligand CYC P5 203



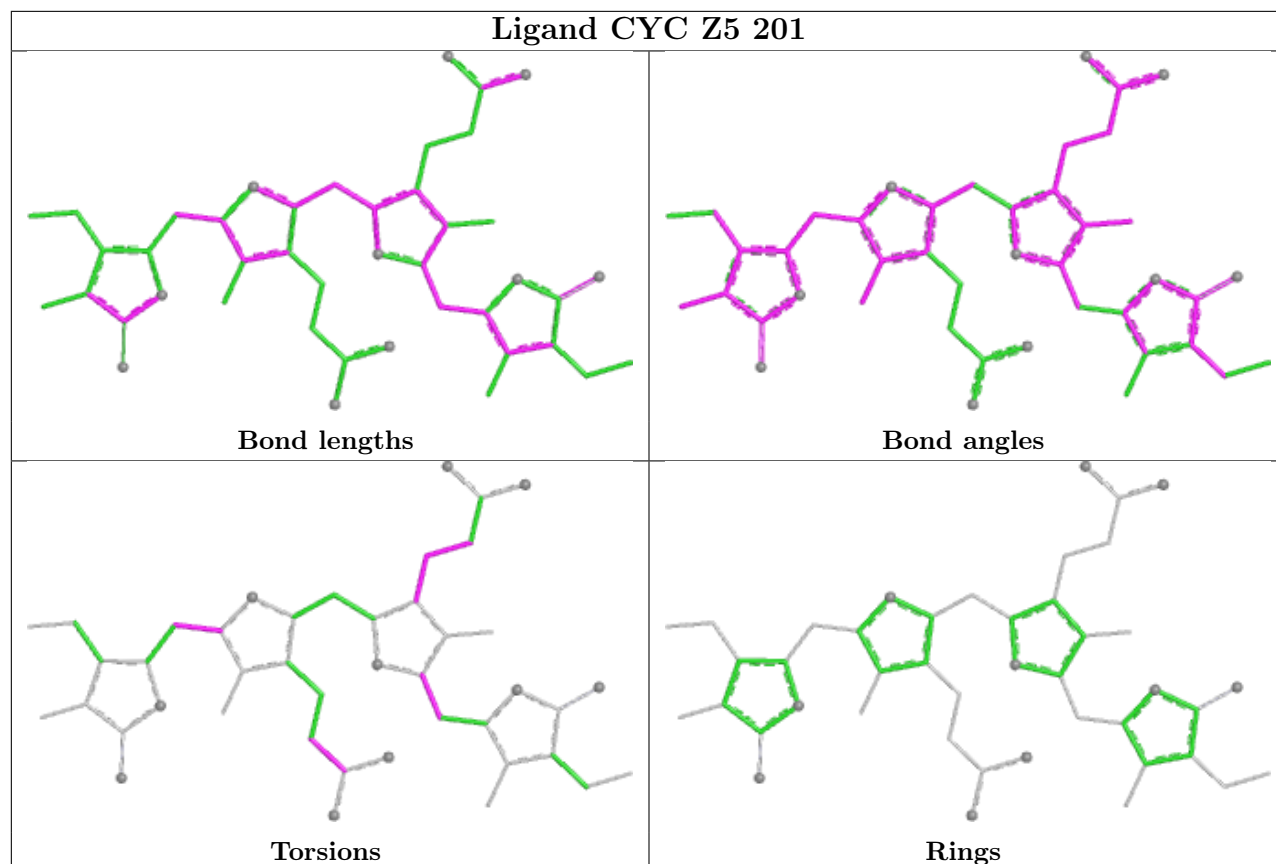
Ligand CYC Y4 201



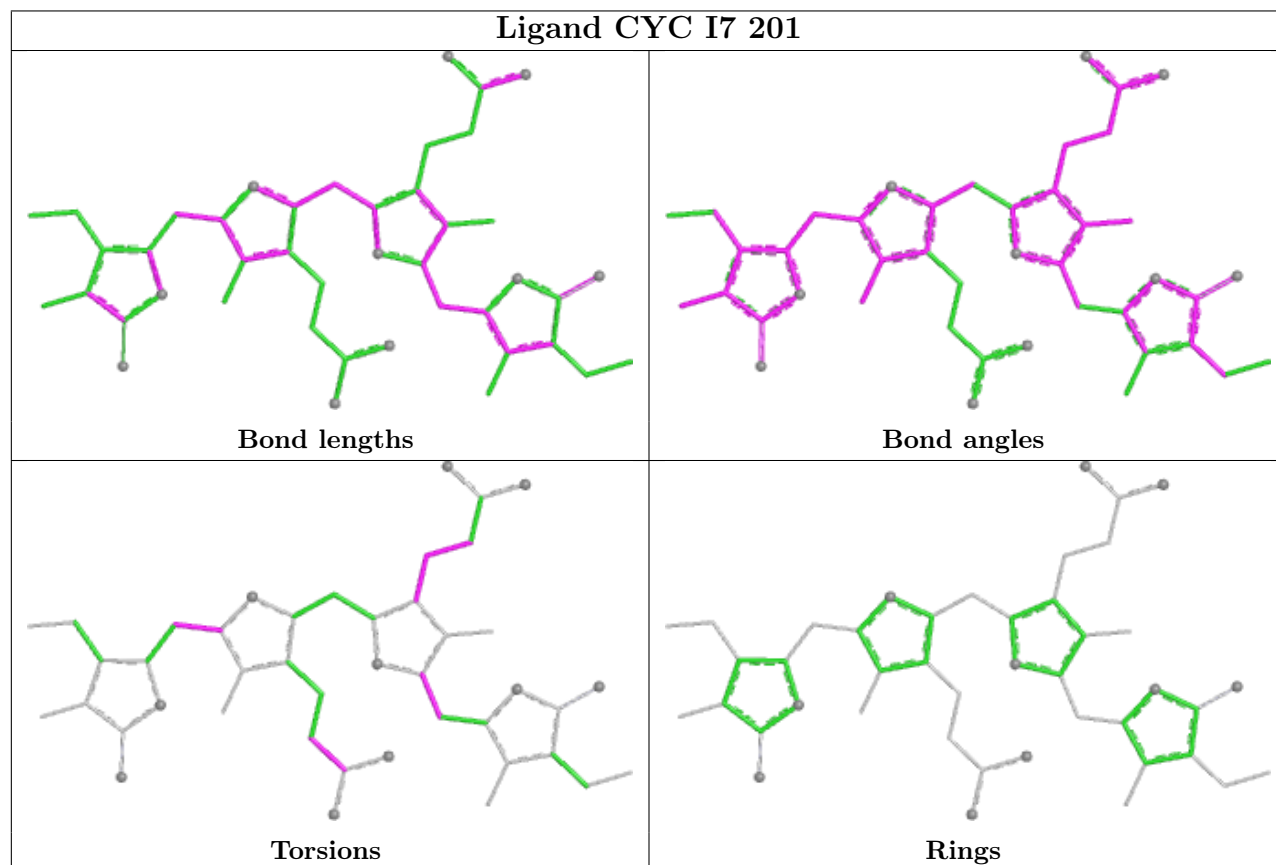
Ligand CYC L9 1001



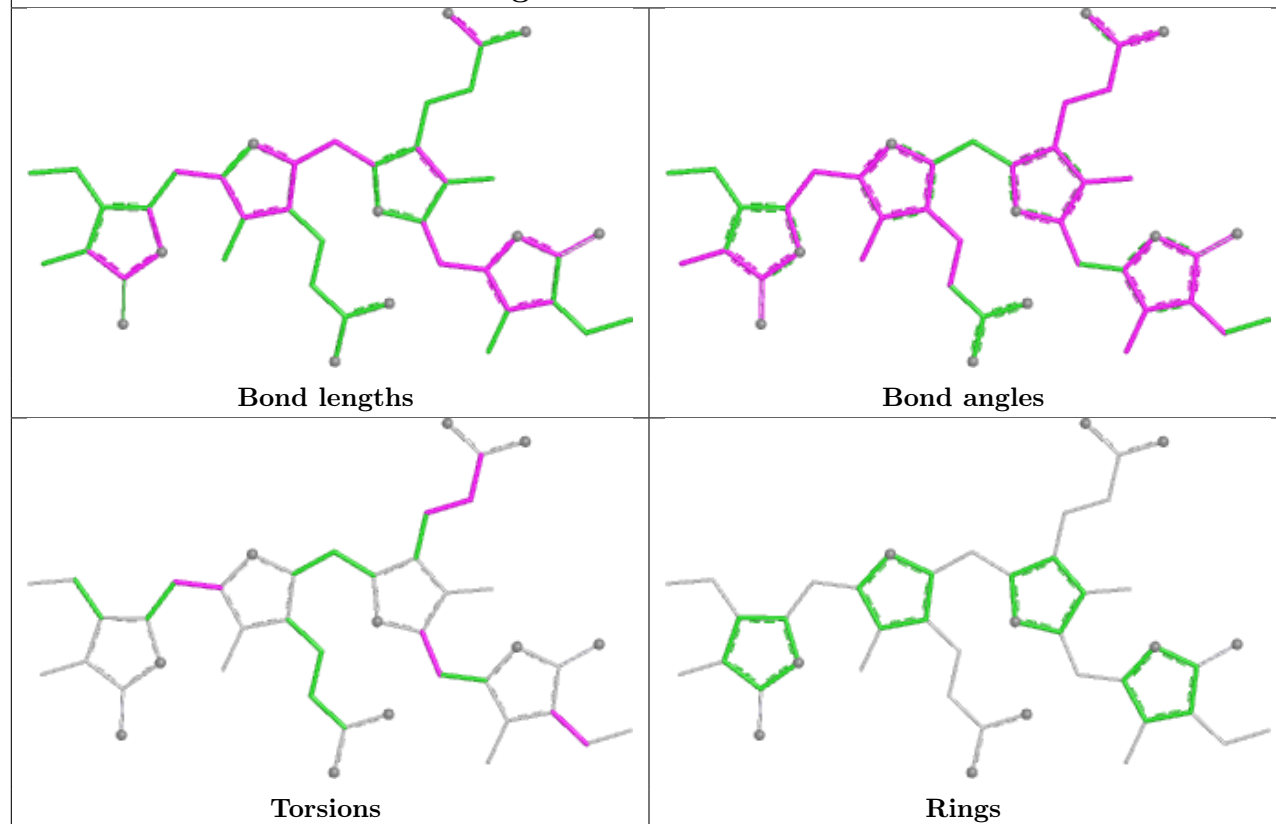
Ligand CYC Z5 201



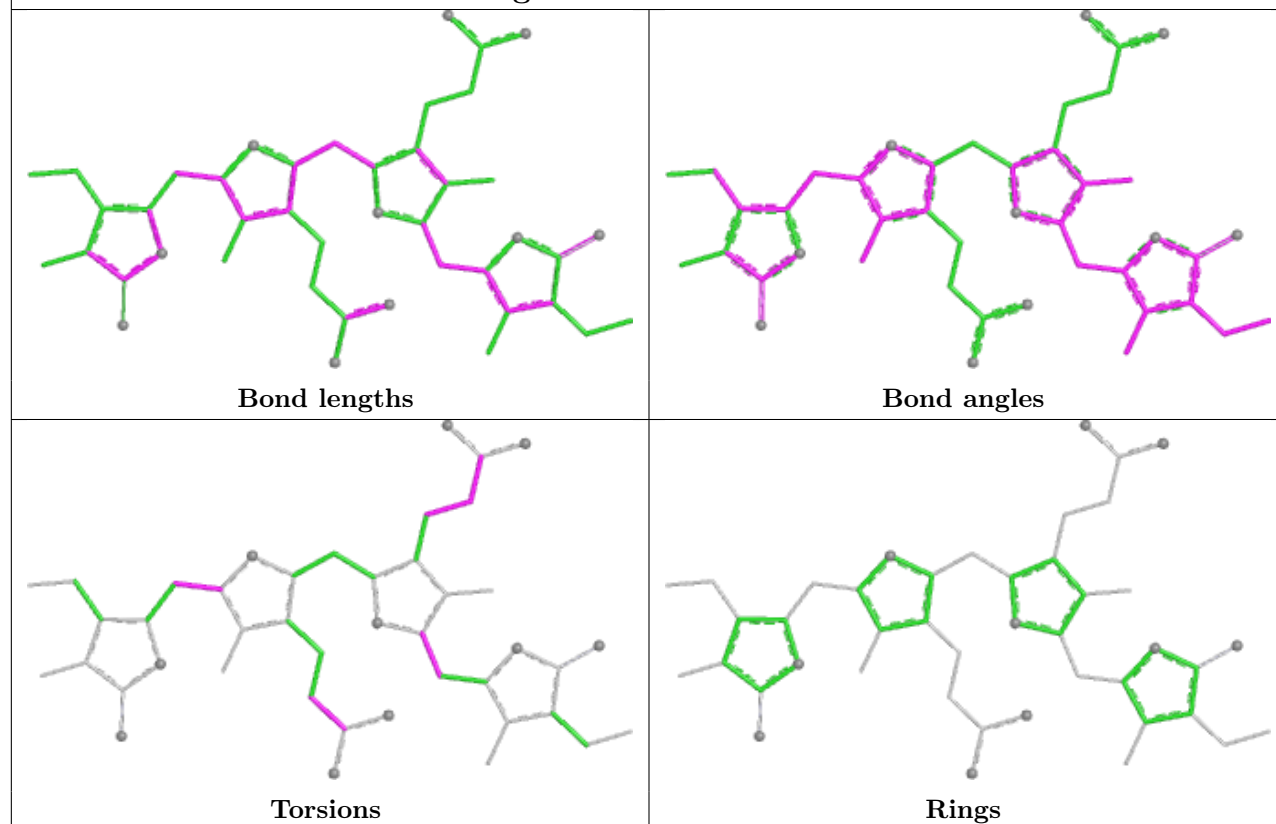
Ligand CYC I7 201



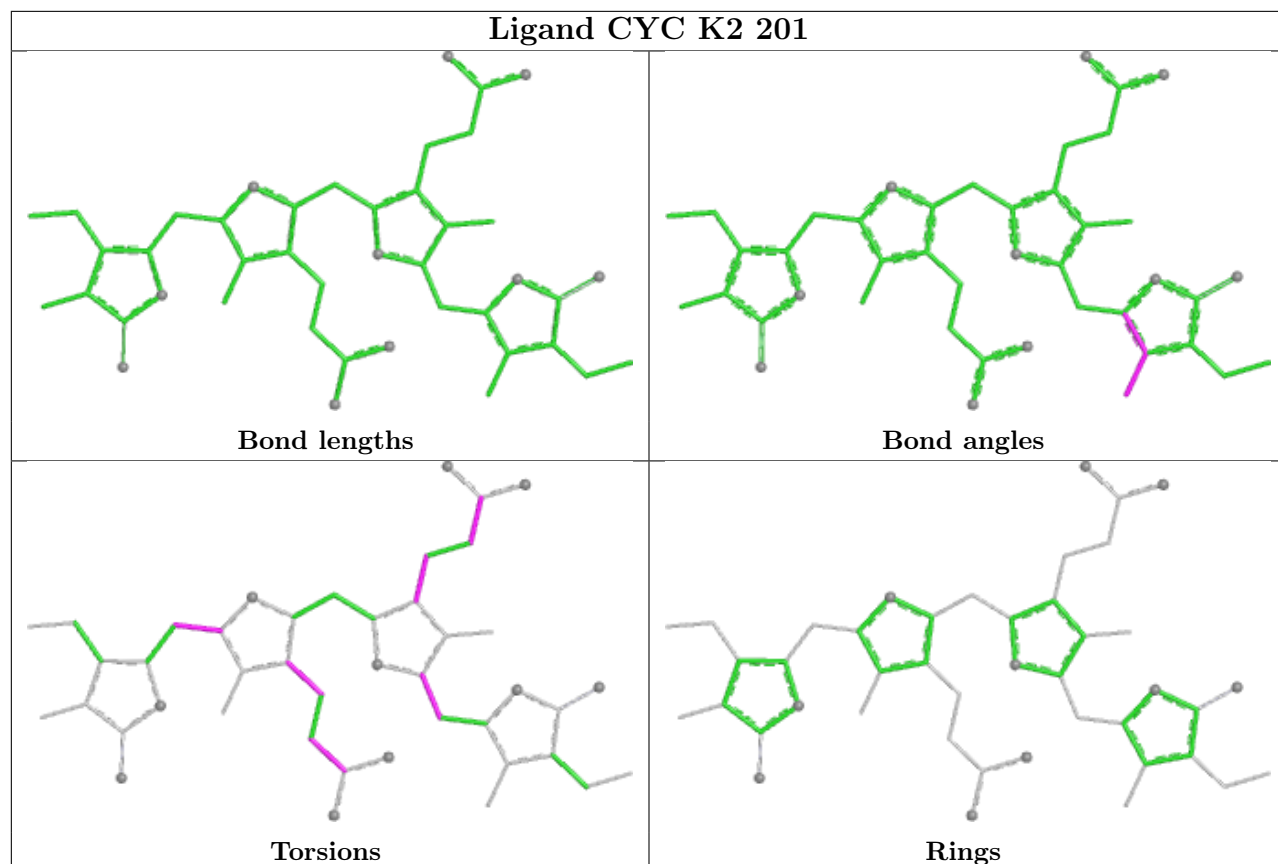
Ligand CYC O1 1001



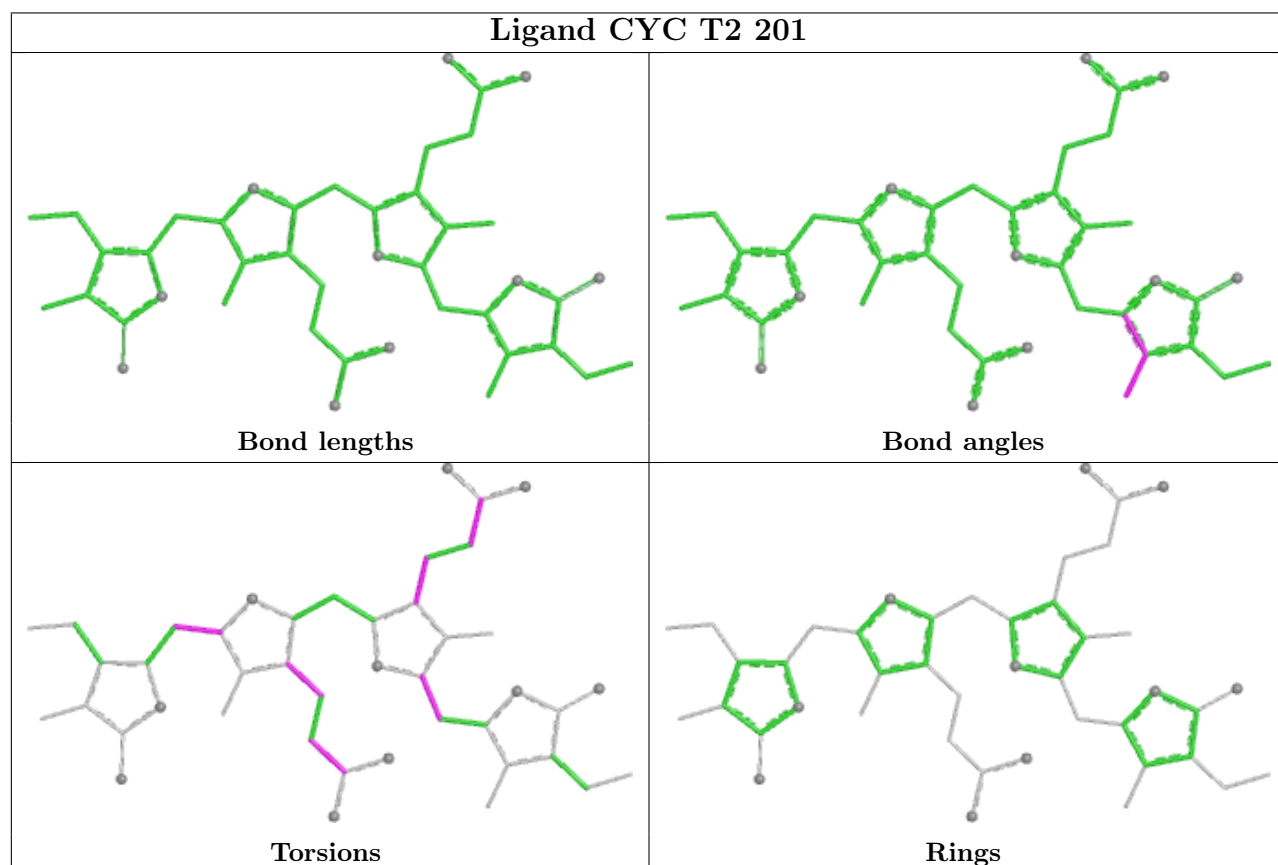
Ligand CYC P8 1001

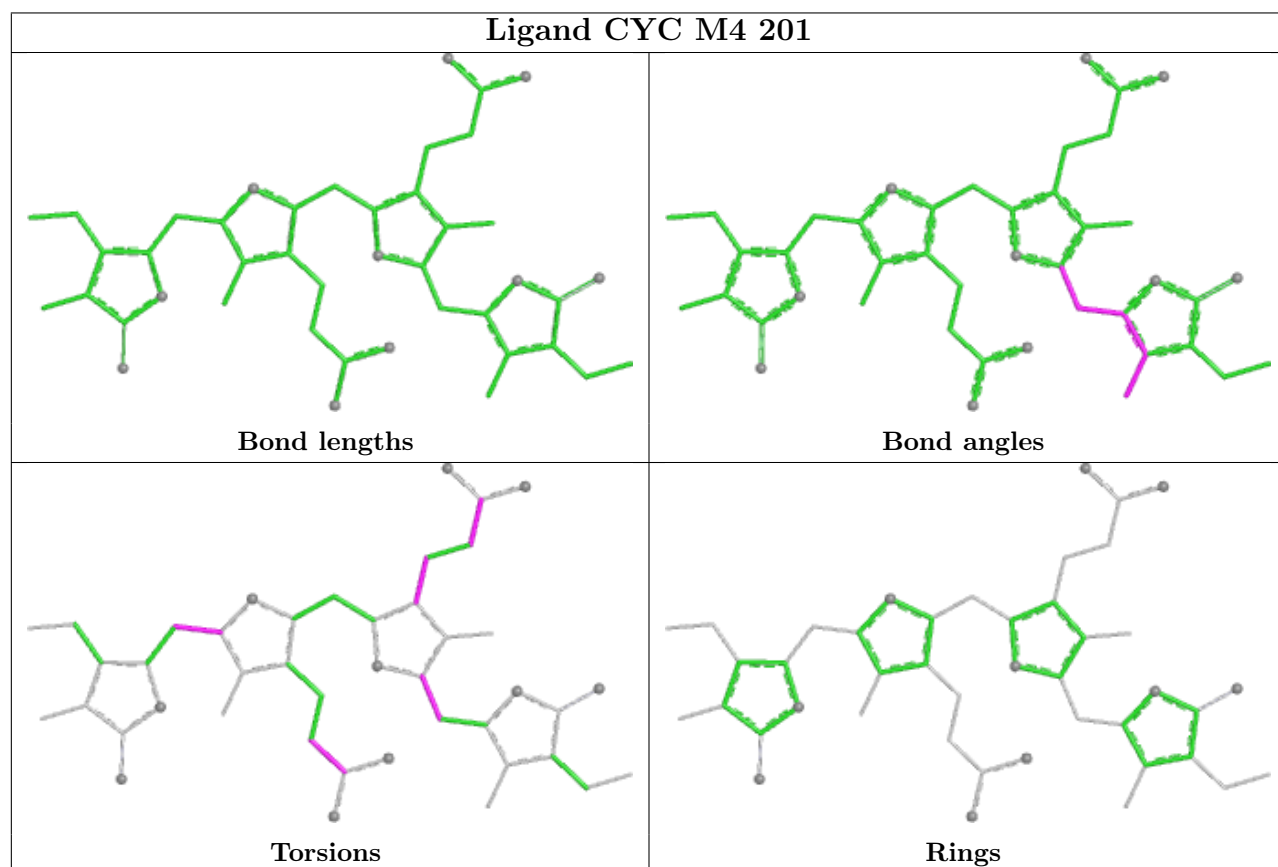
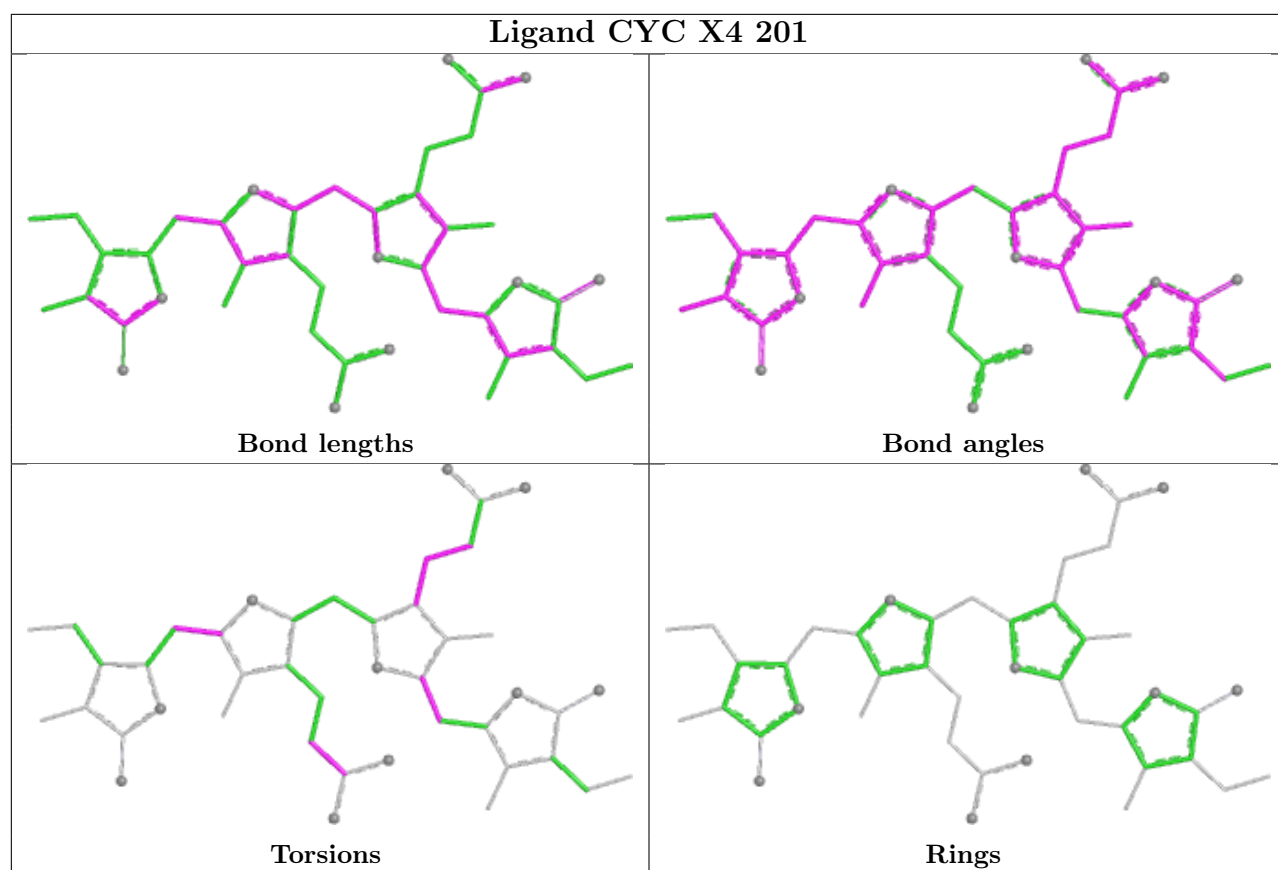


Ligand CYC K2 201

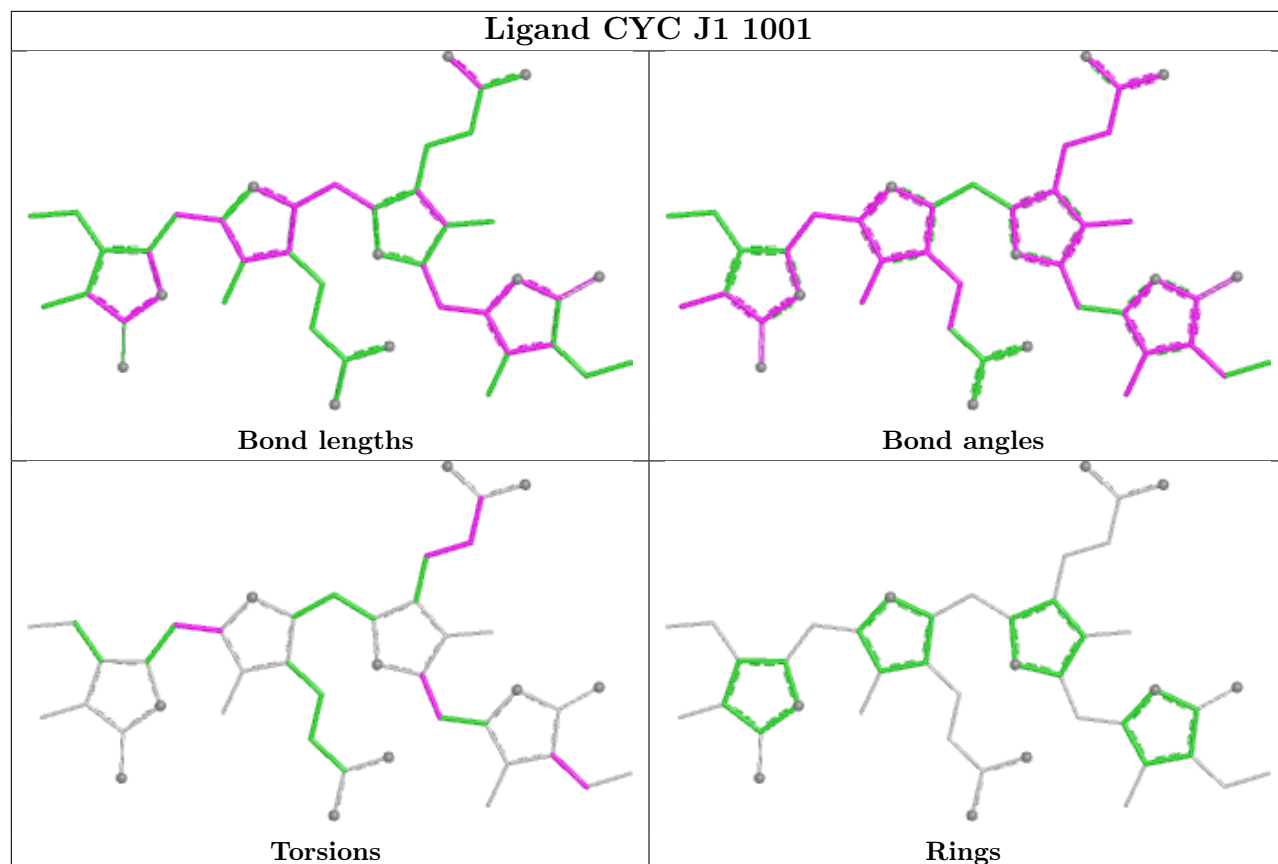


Ligand CYC T2 201

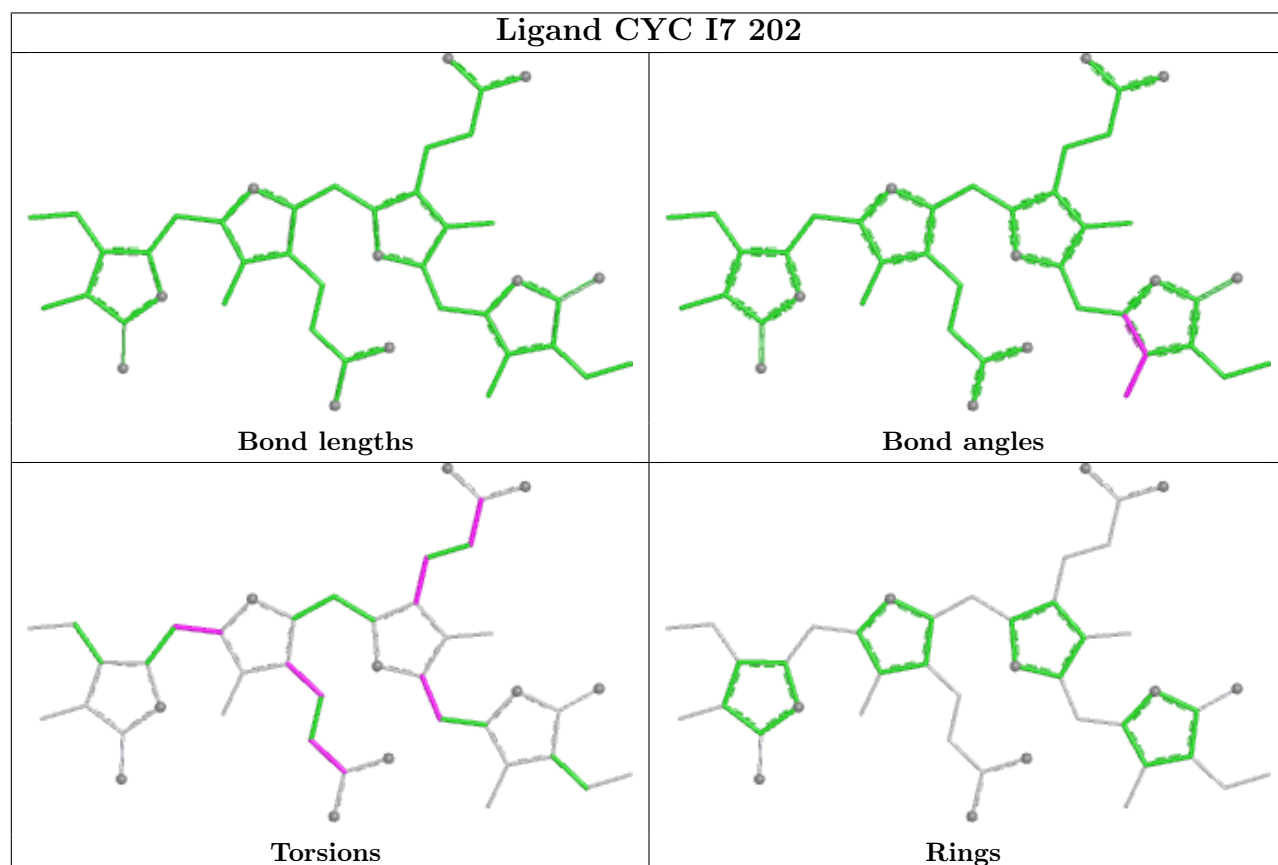




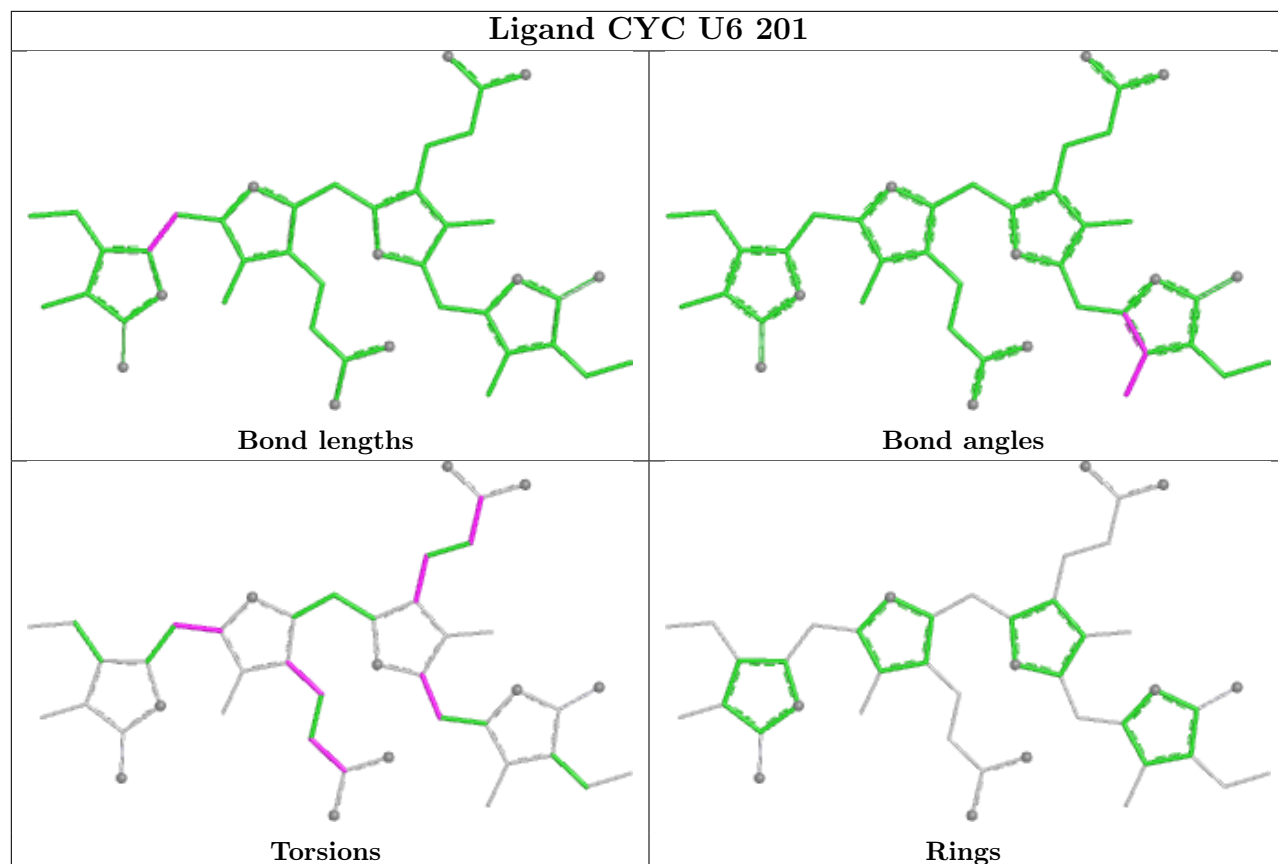
Ligand CYC J1 1001



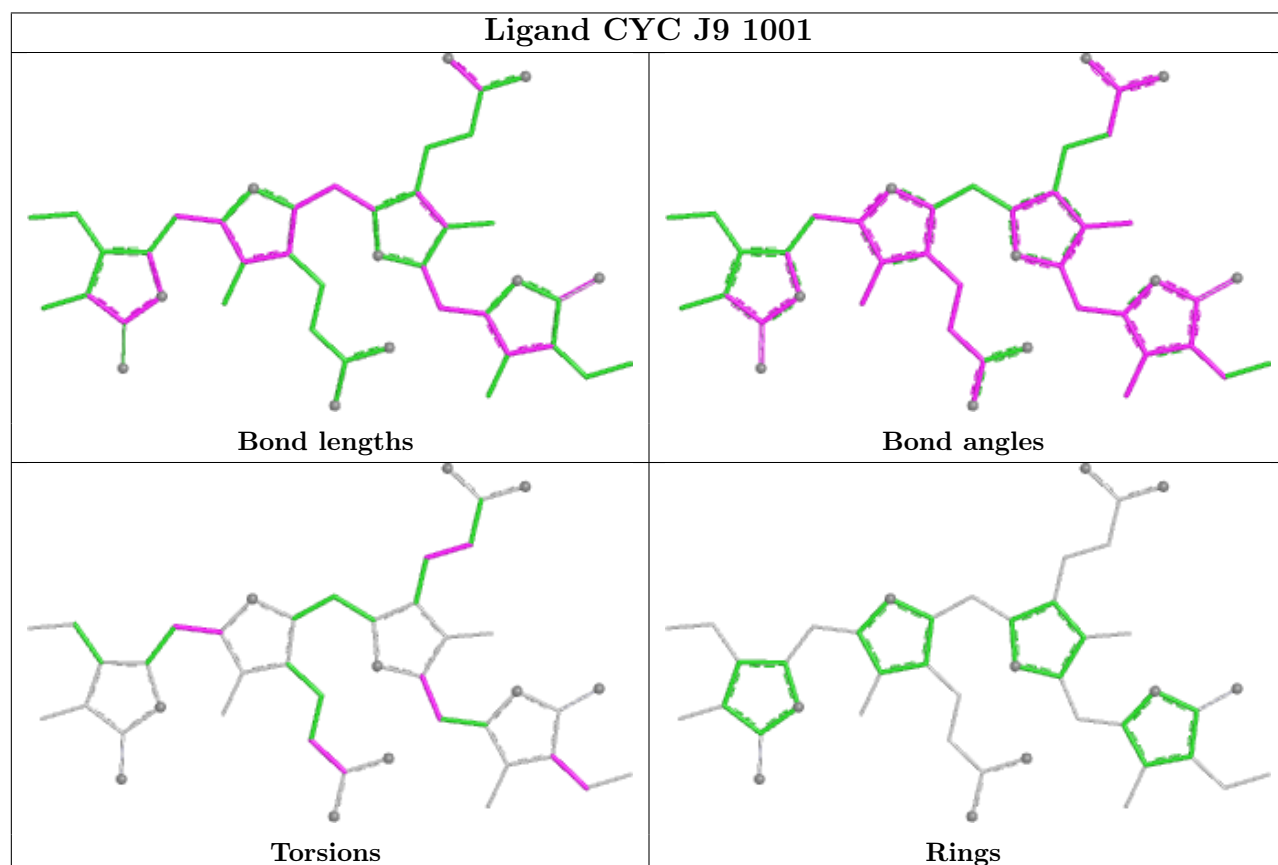
Ligand CYC I7 202



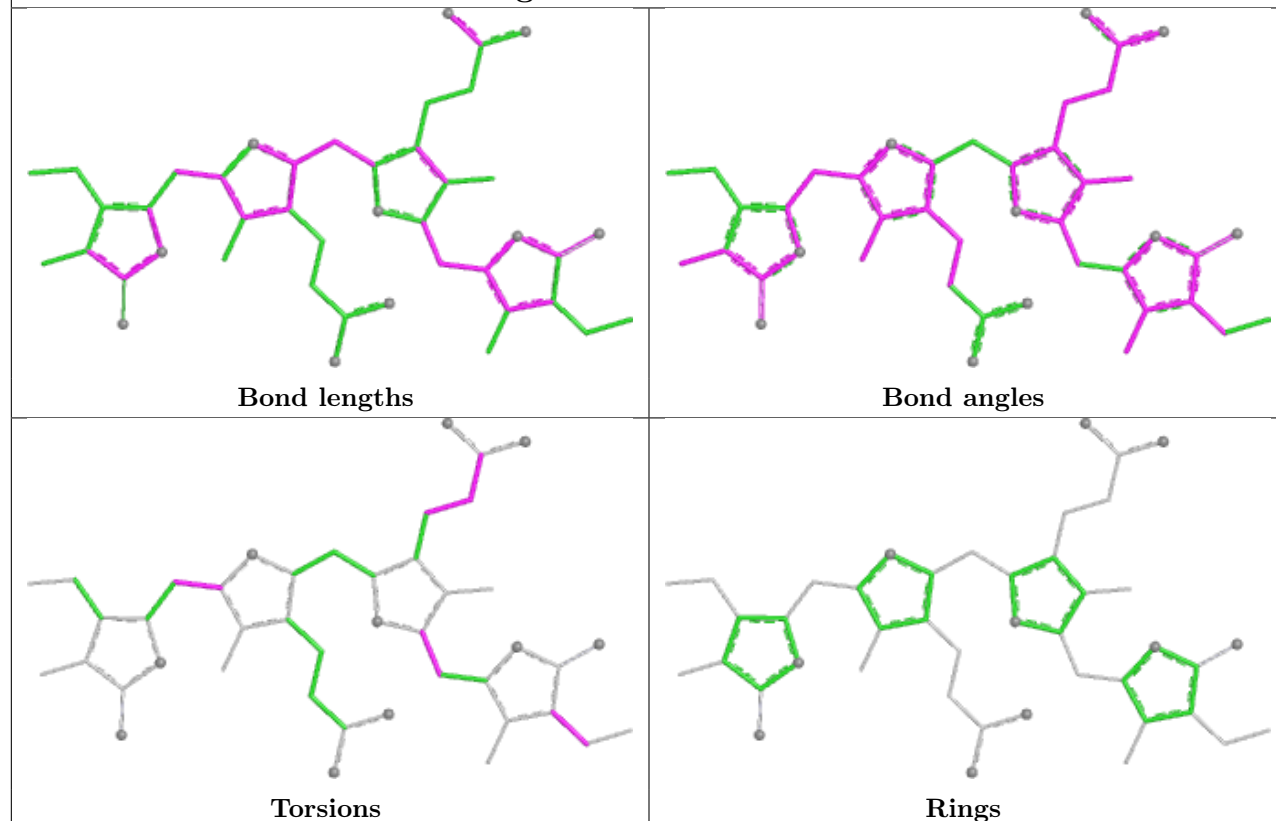
Ligand CYC U6 201



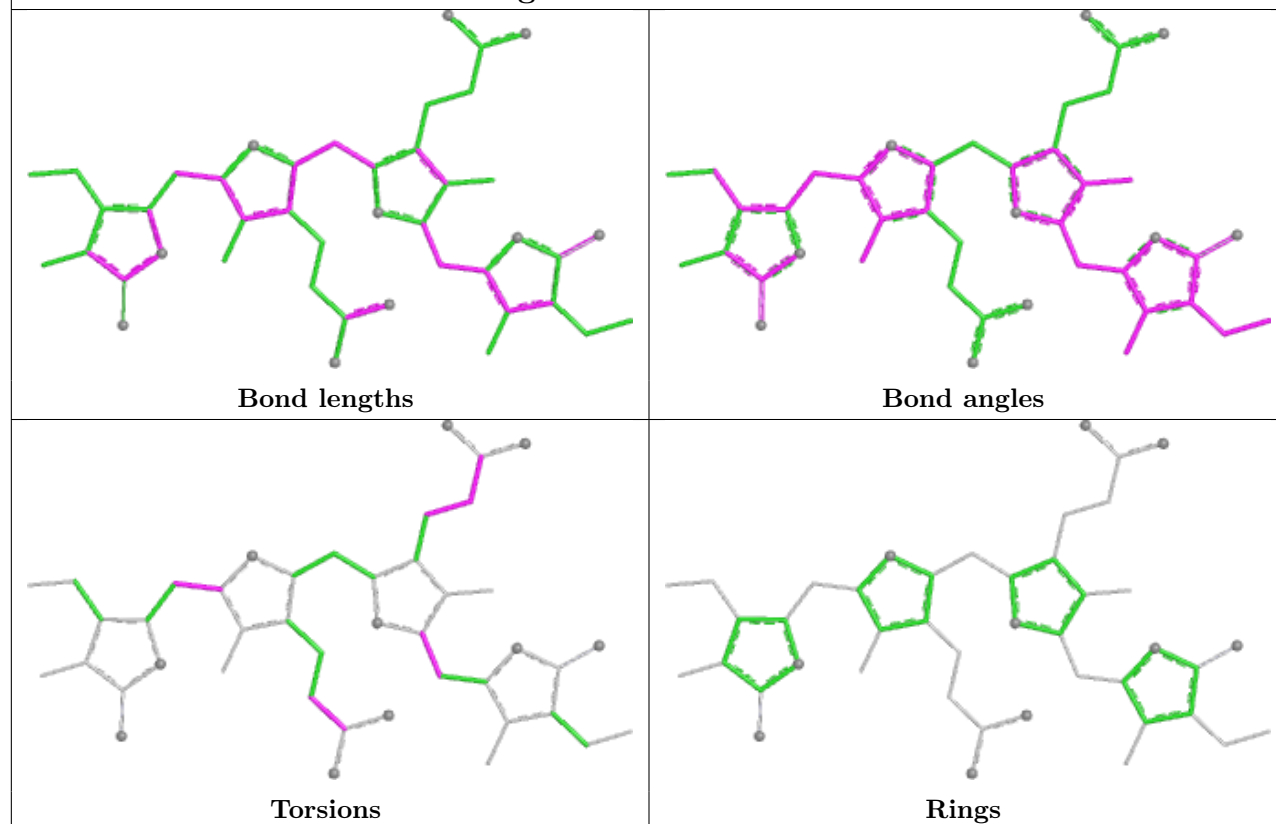
Ligand CYC J9 1001



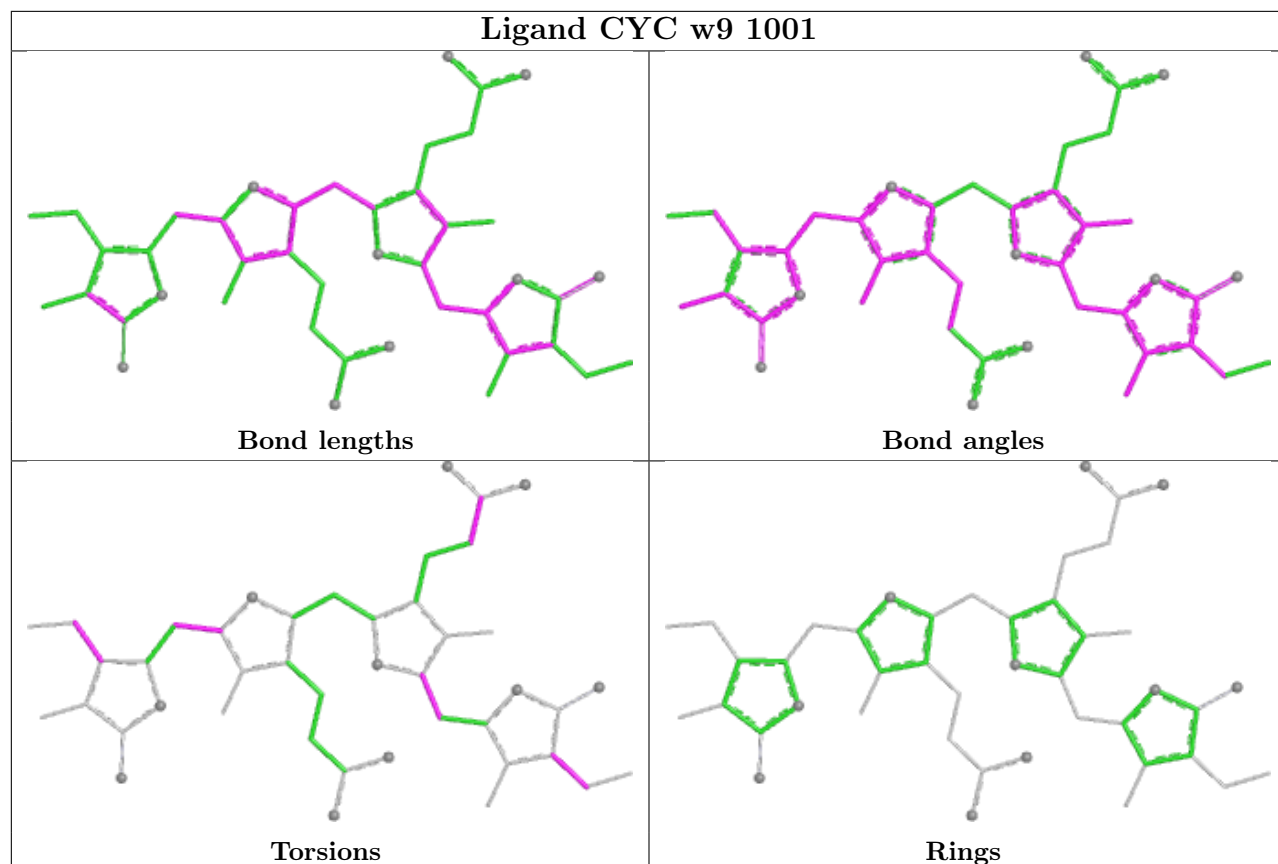
Ligand CYC J6 1001



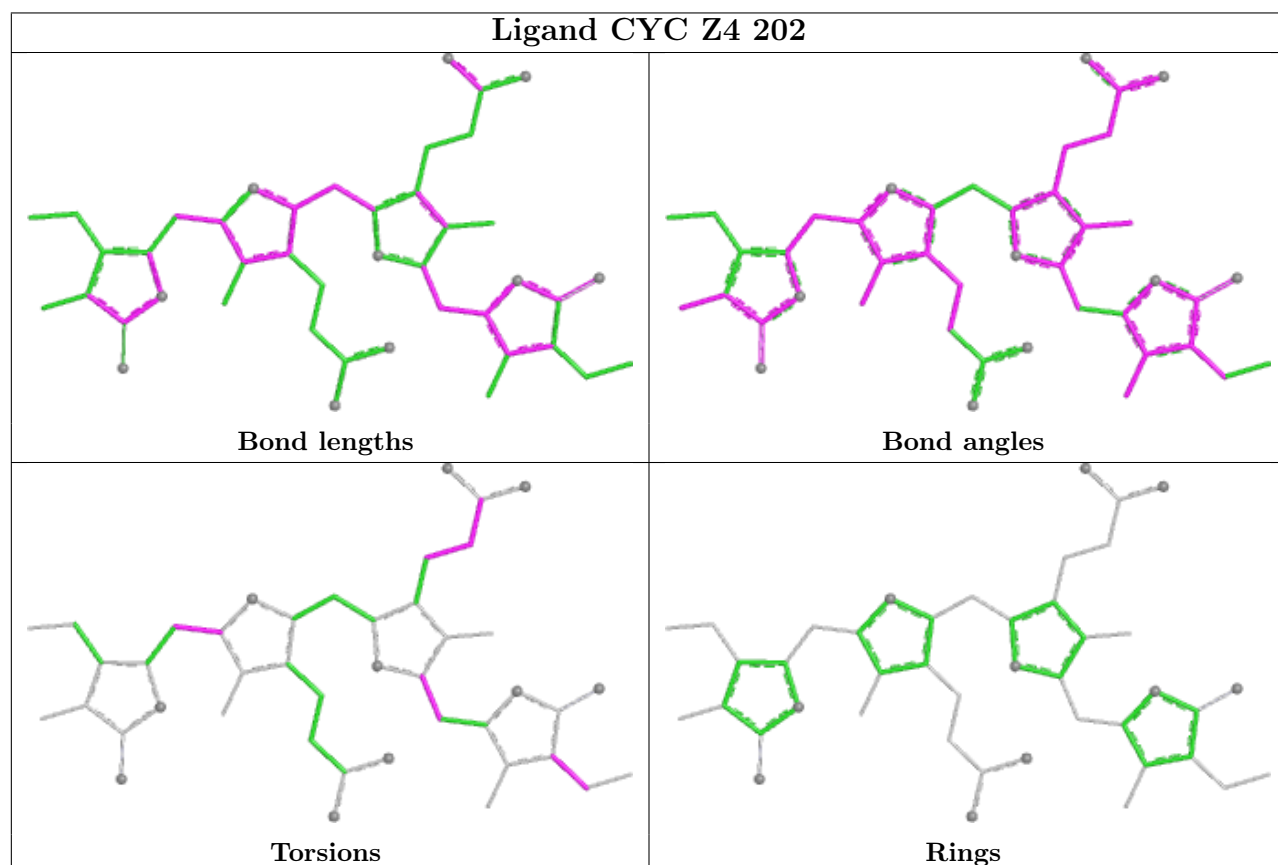
Ligand CYC s8 1001



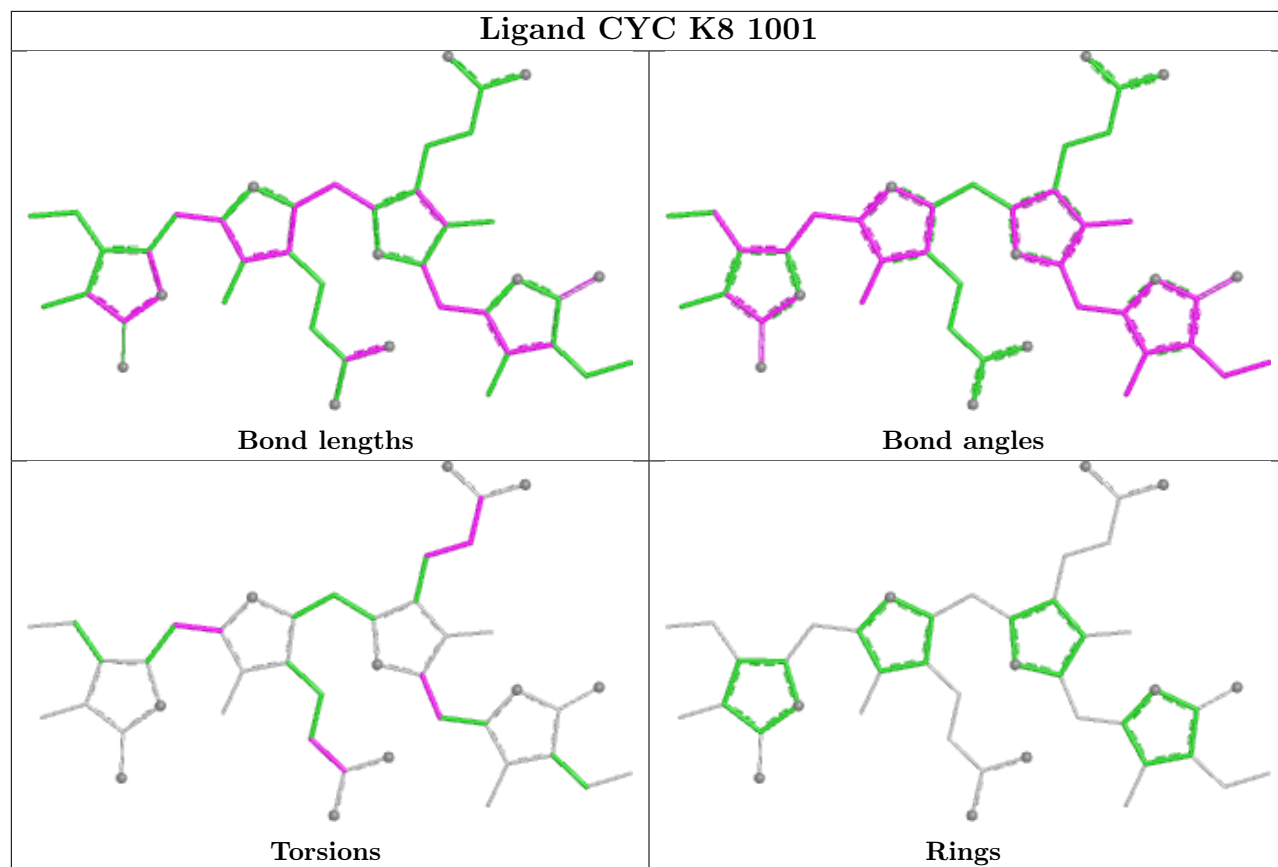
Ligand CYC w9 1001



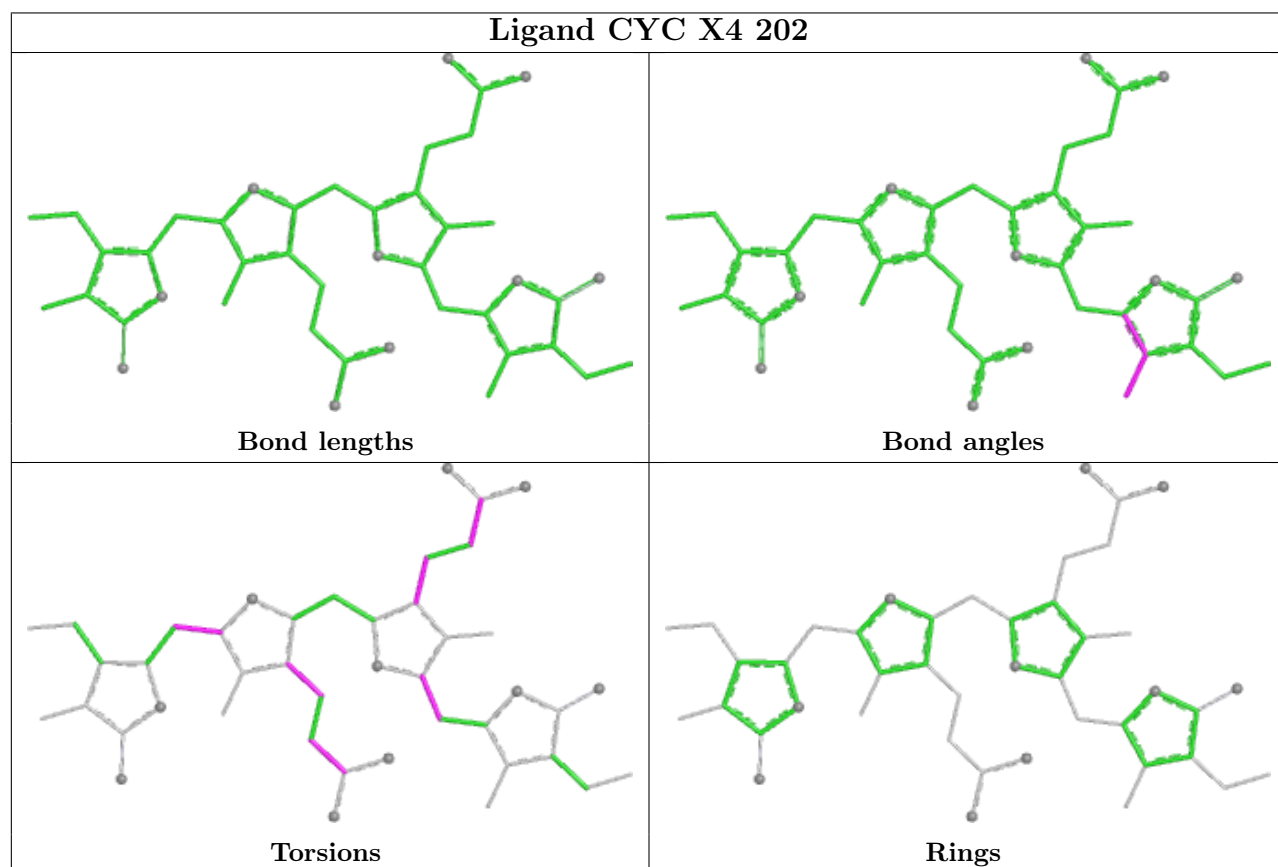
Ligand CYC Z4 202



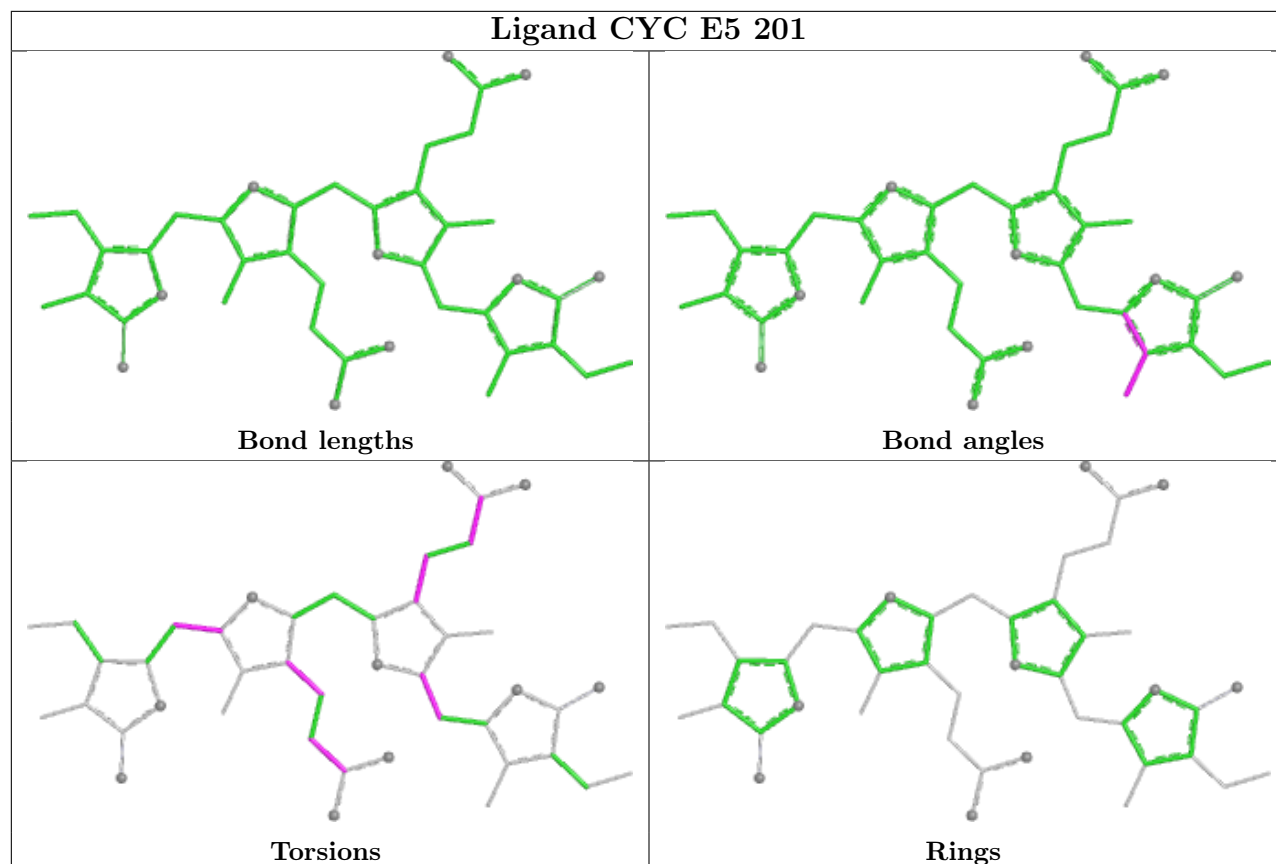
Ligand CYC K8 1001



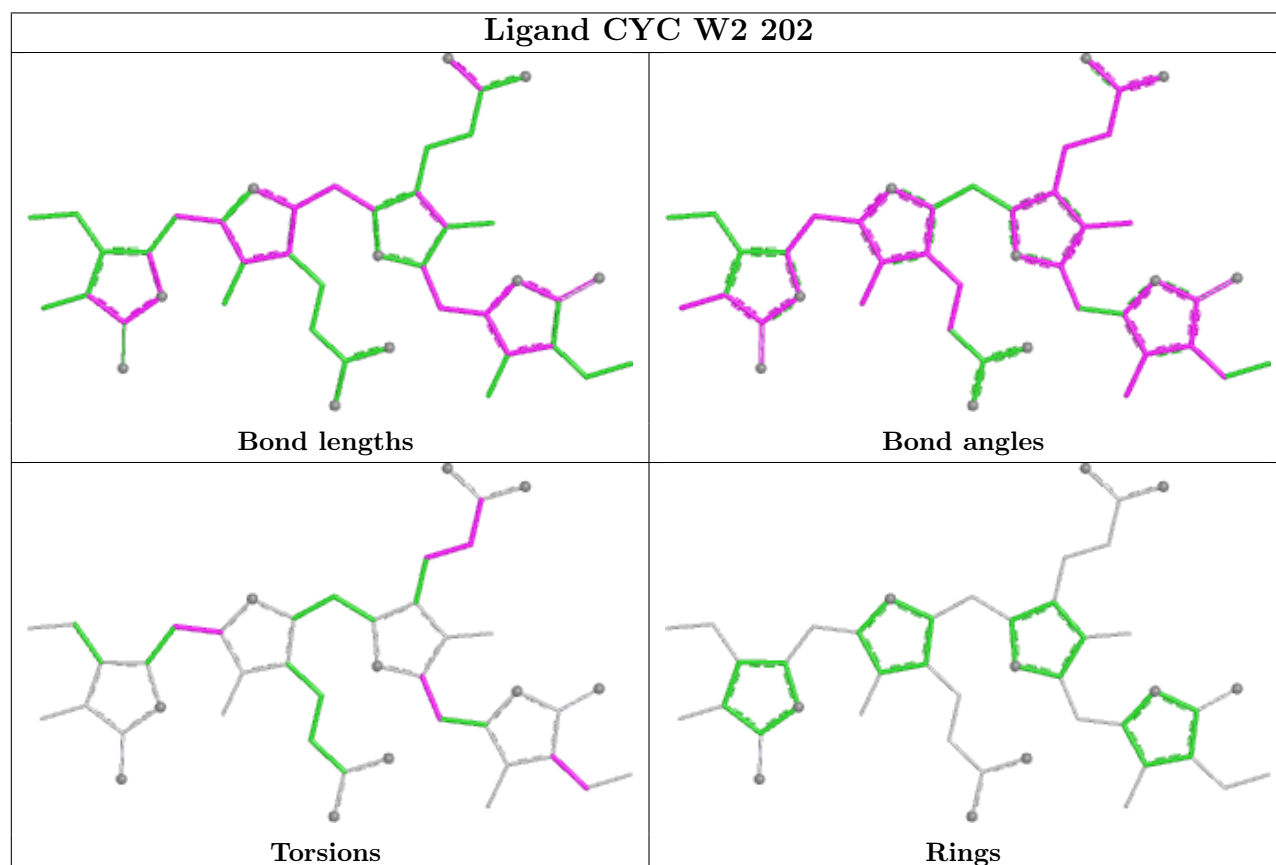
Ligand CYC X4 202



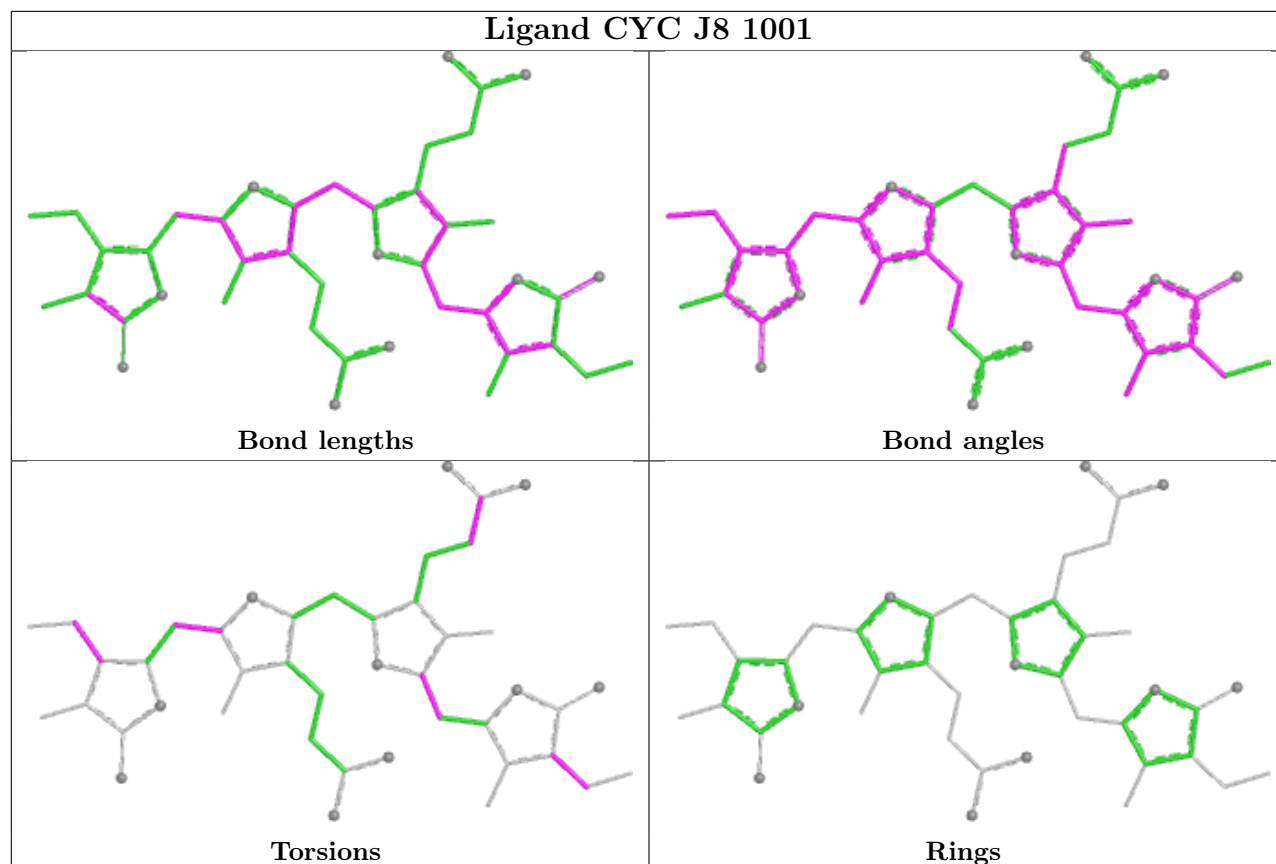
Ligand CYC E5 201



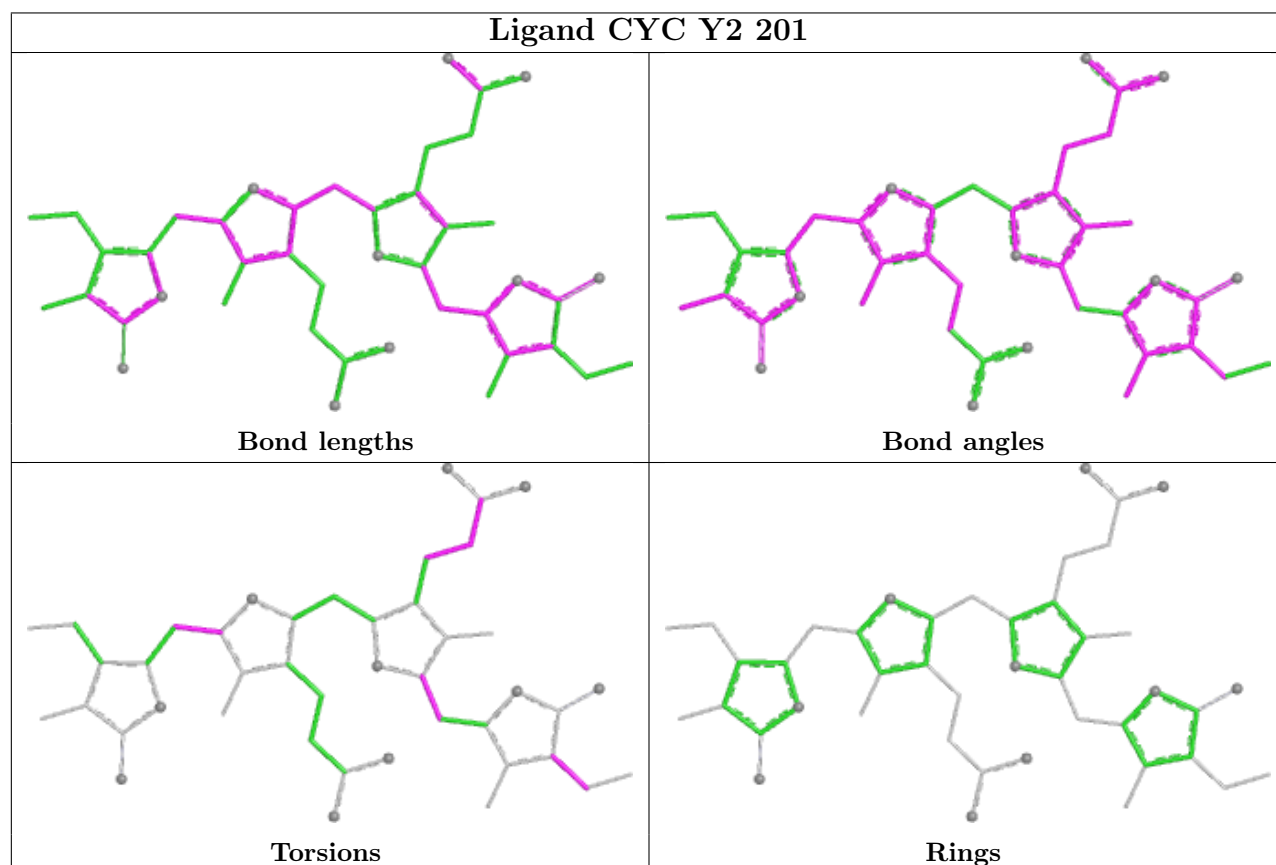
Ligand CYC W2 202



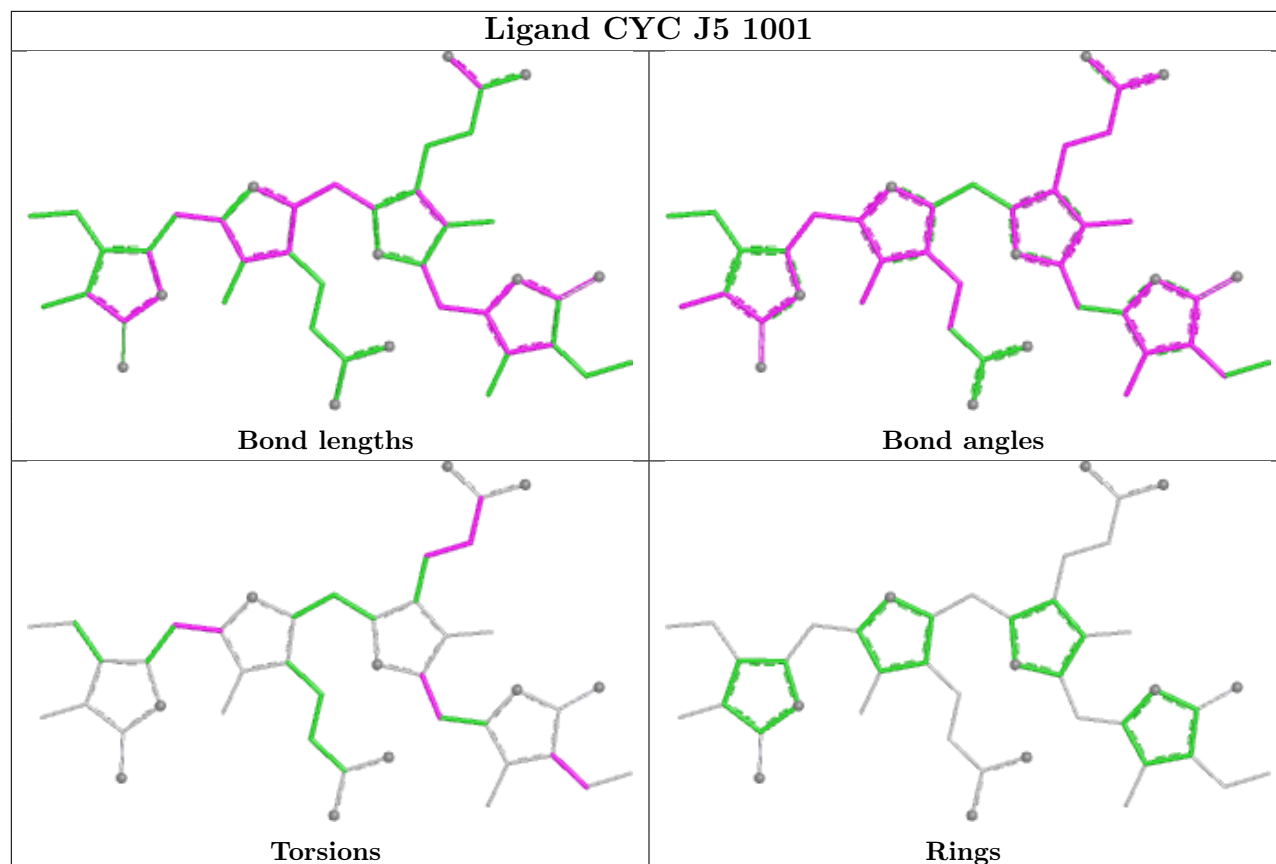
Ligand CYC J8 1001



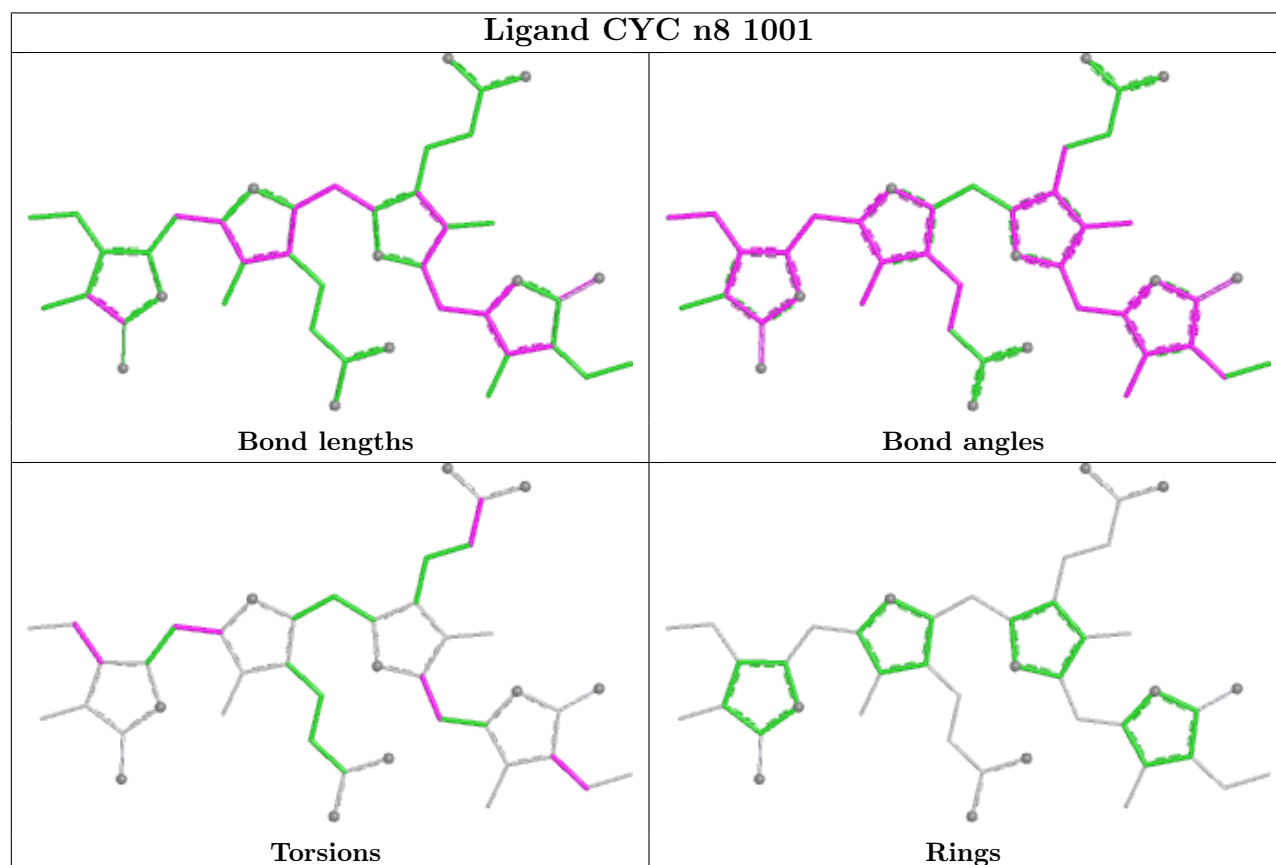
Ligand CYC Y2 201



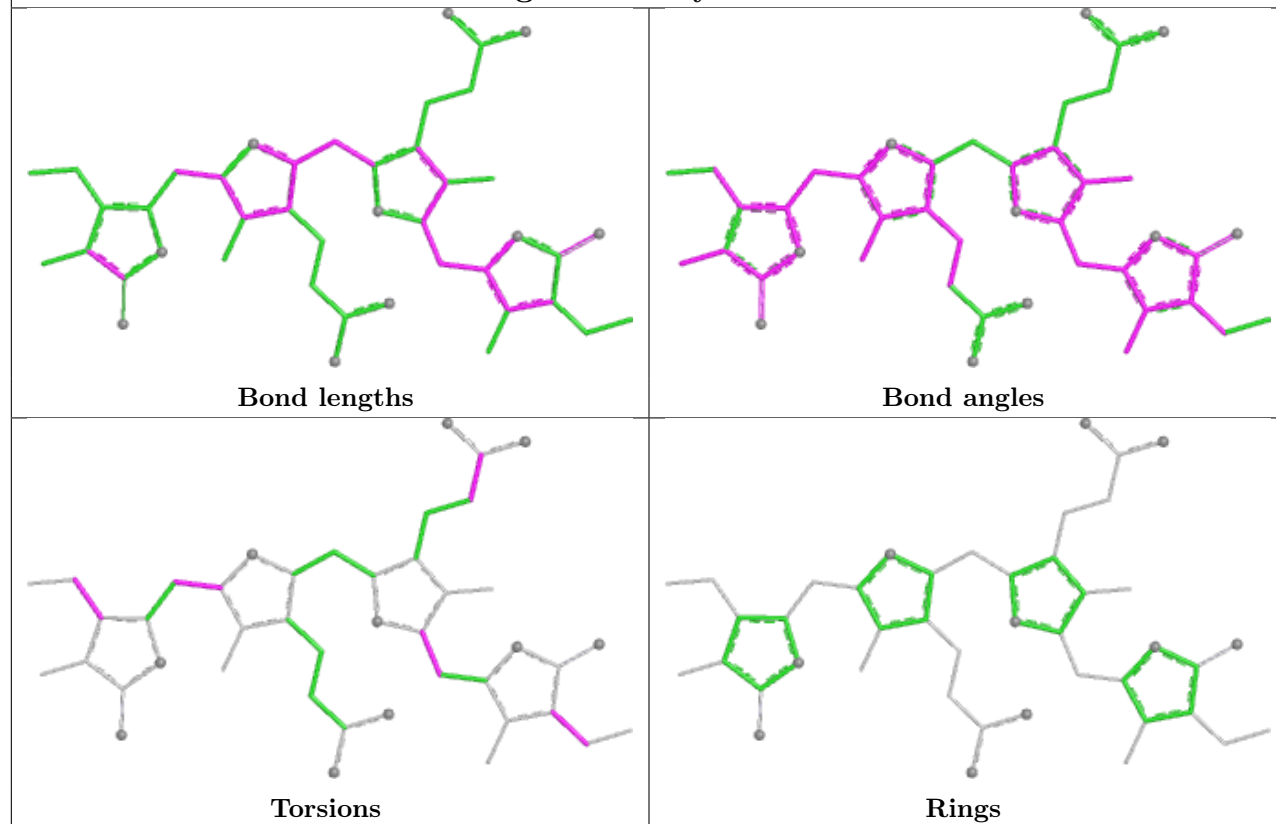
Ligand CYC J5 1001



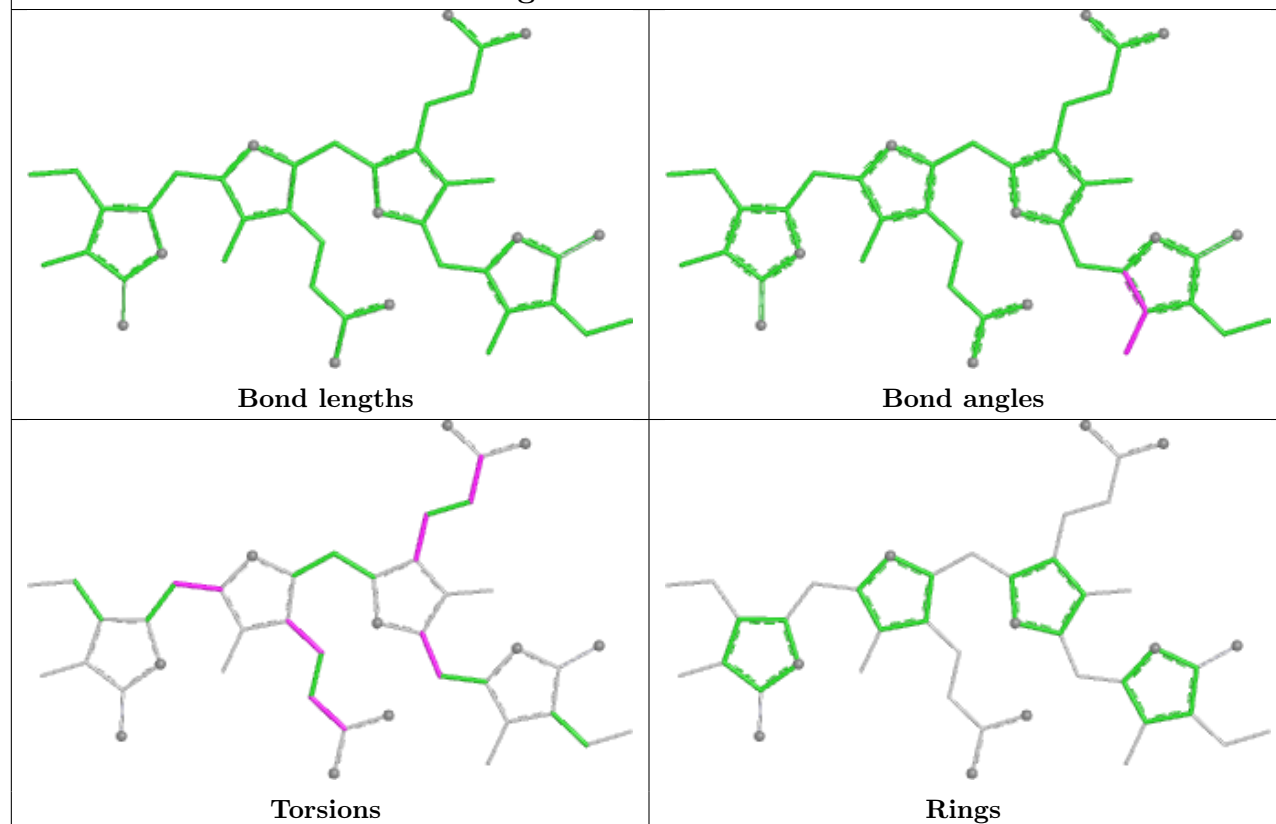
Ligand CYC n8 1001

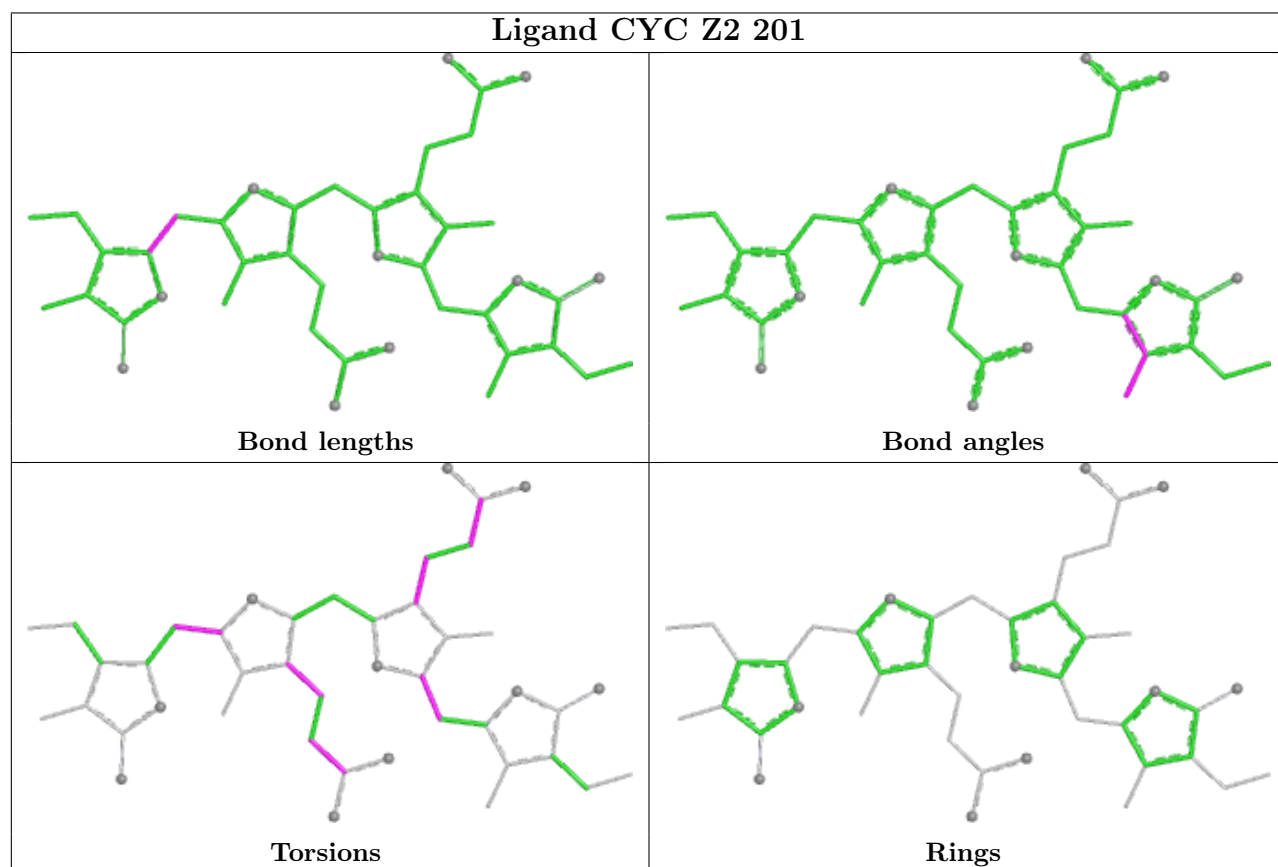
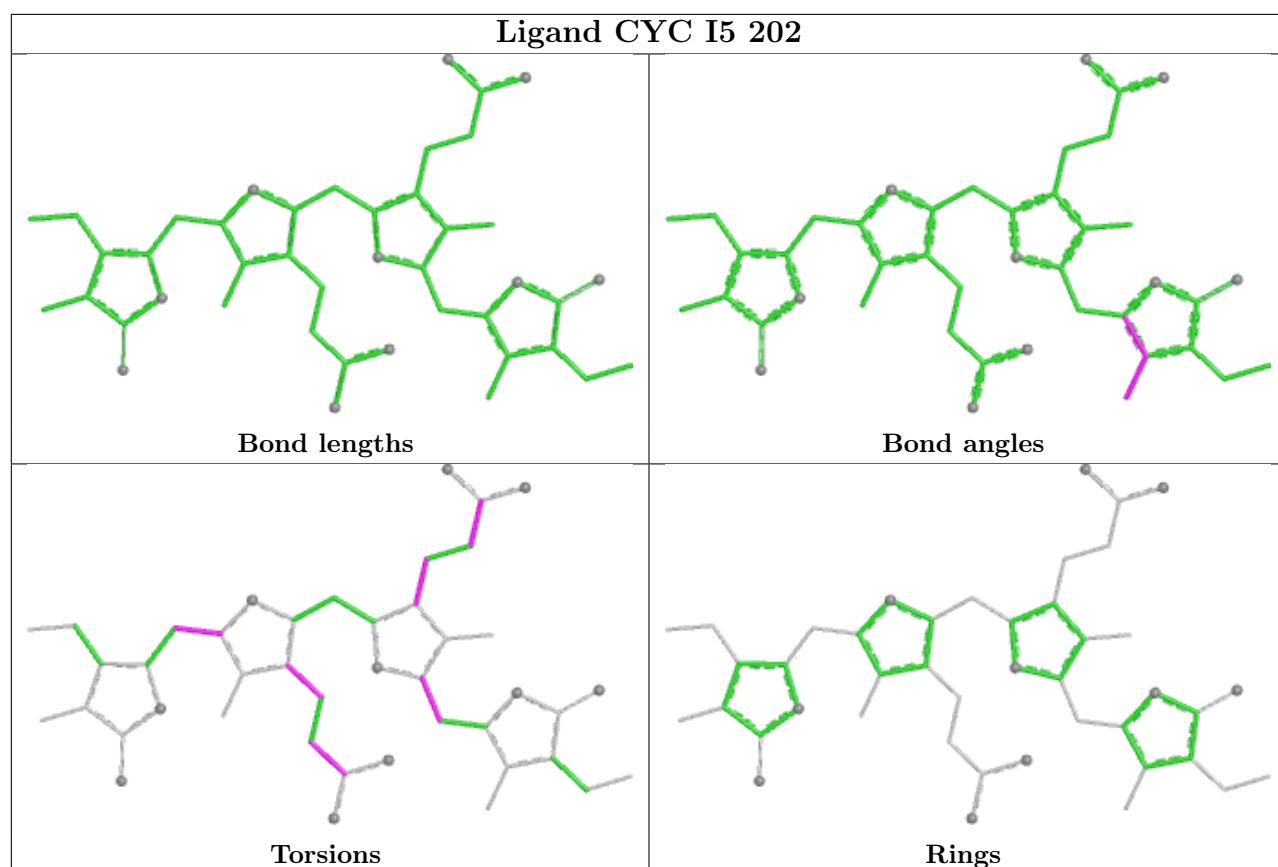


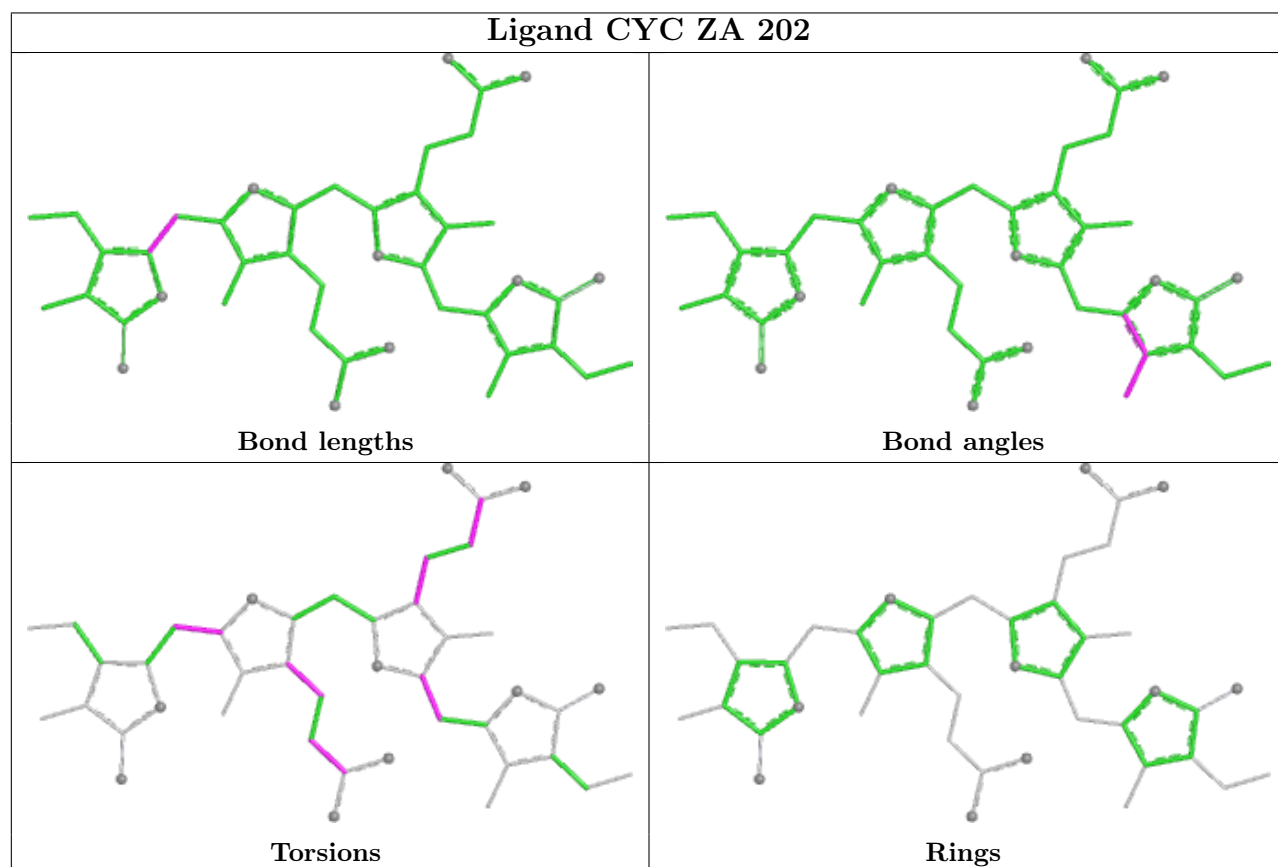
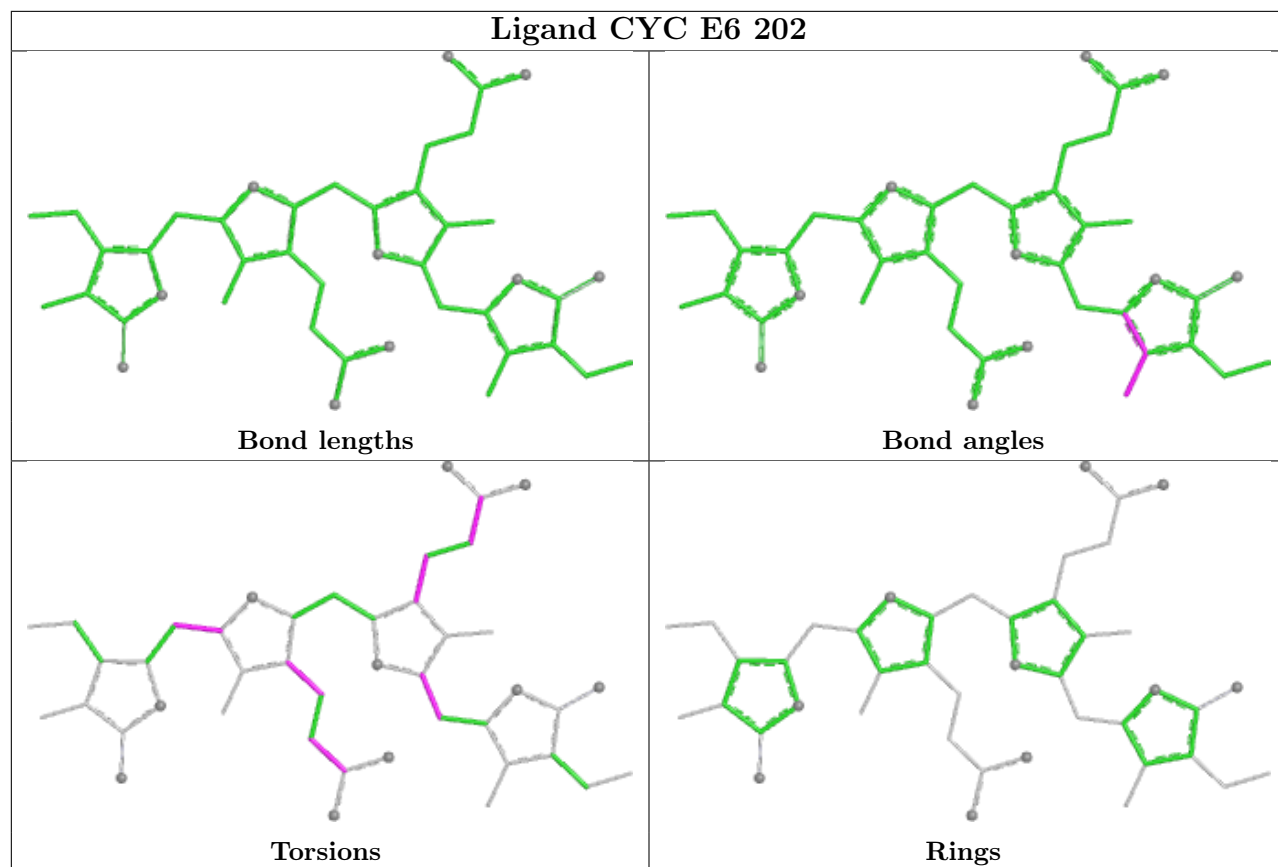
Ligand CYC y9 1001



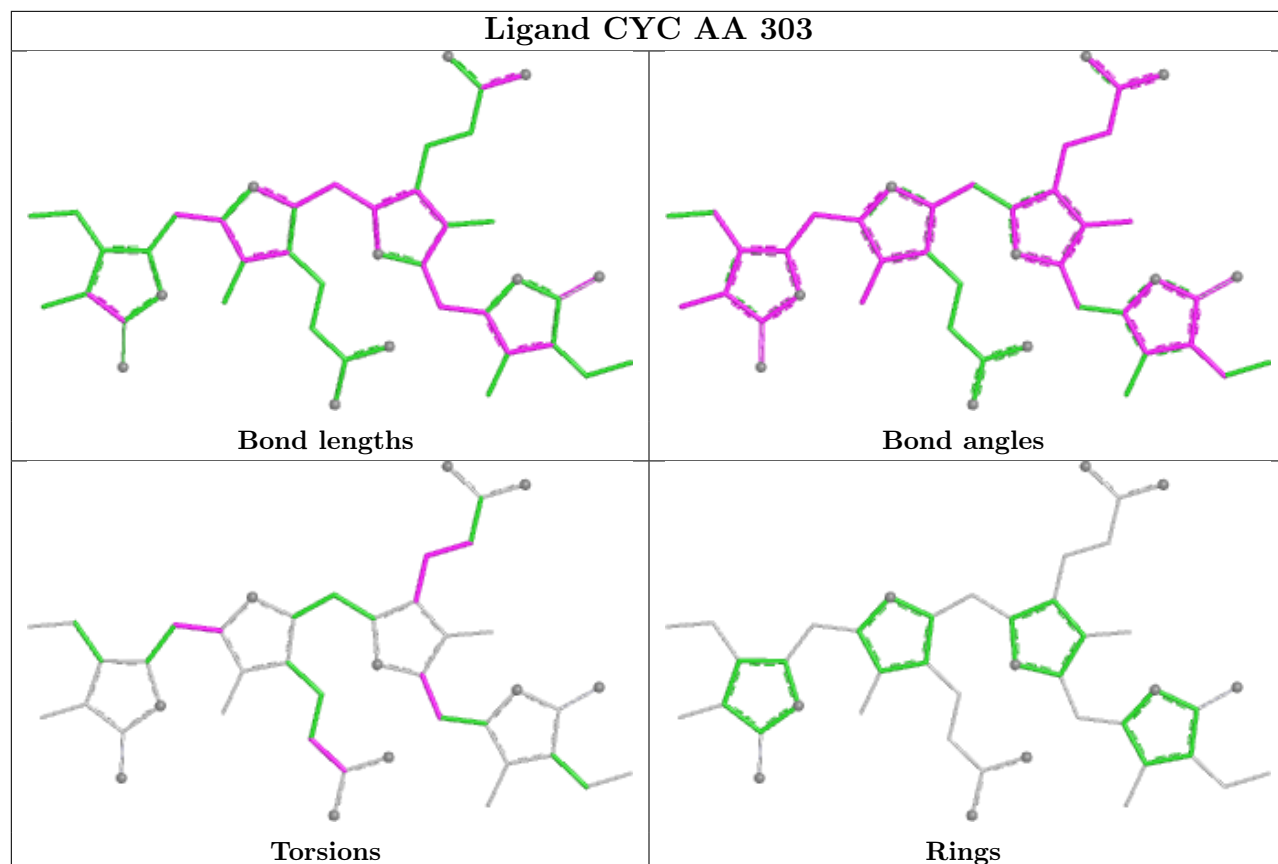
Ligand CYC EA 201



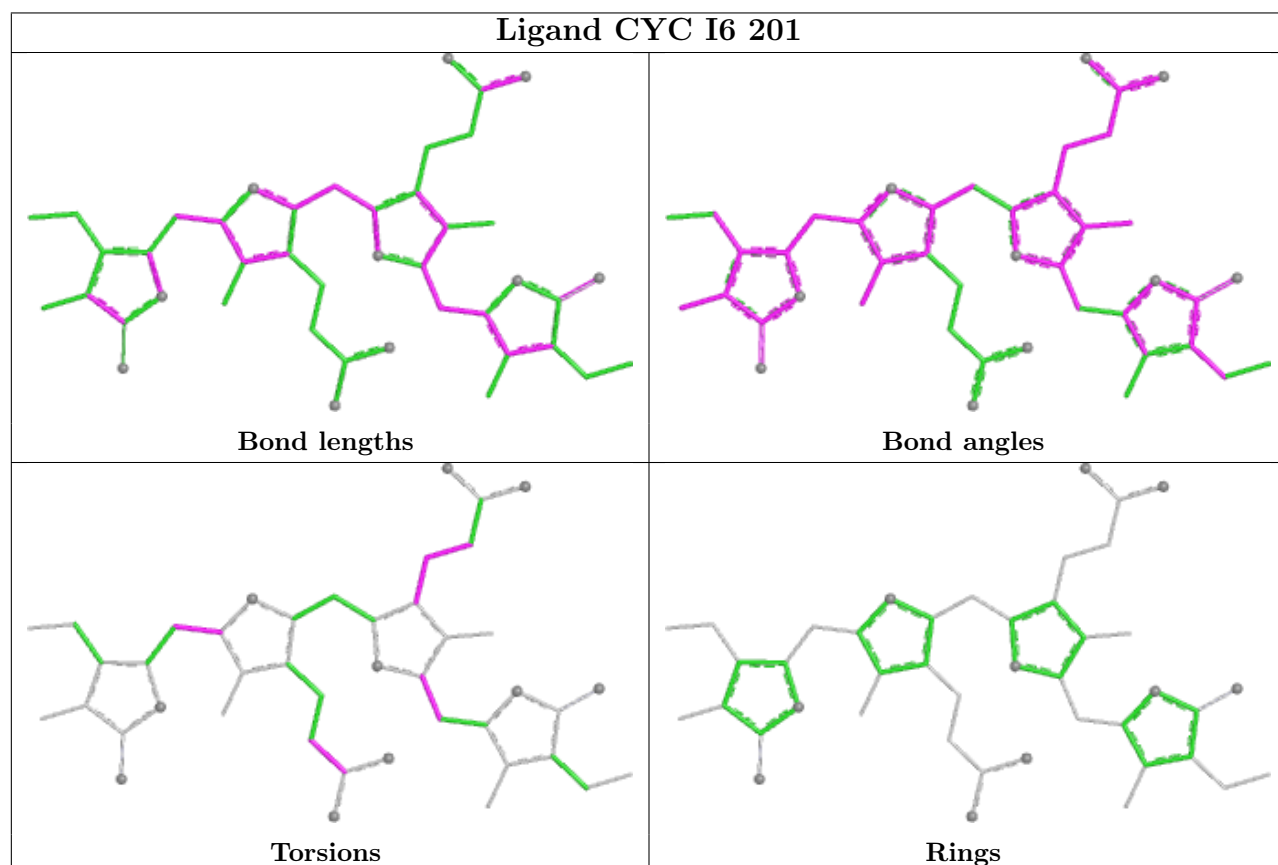




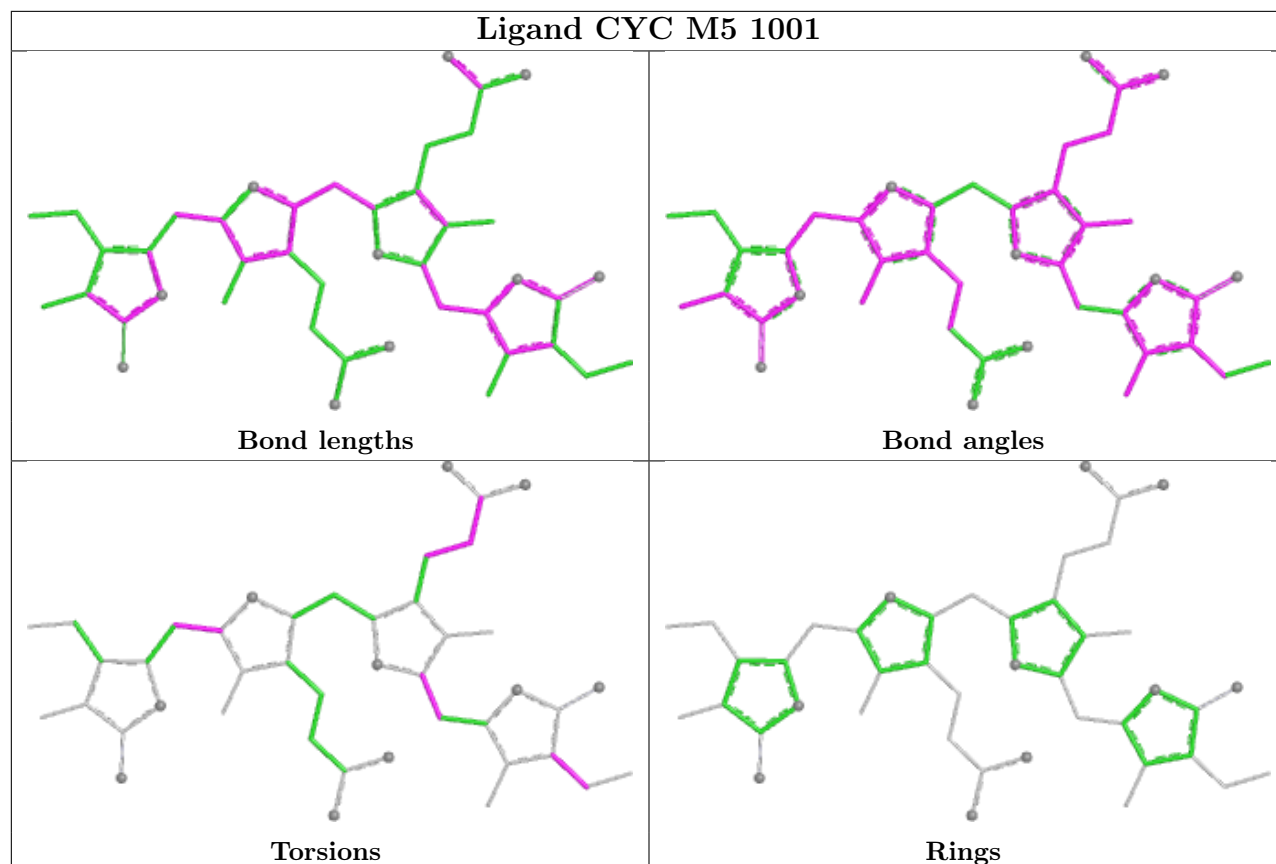
Ligand CYC AA 303



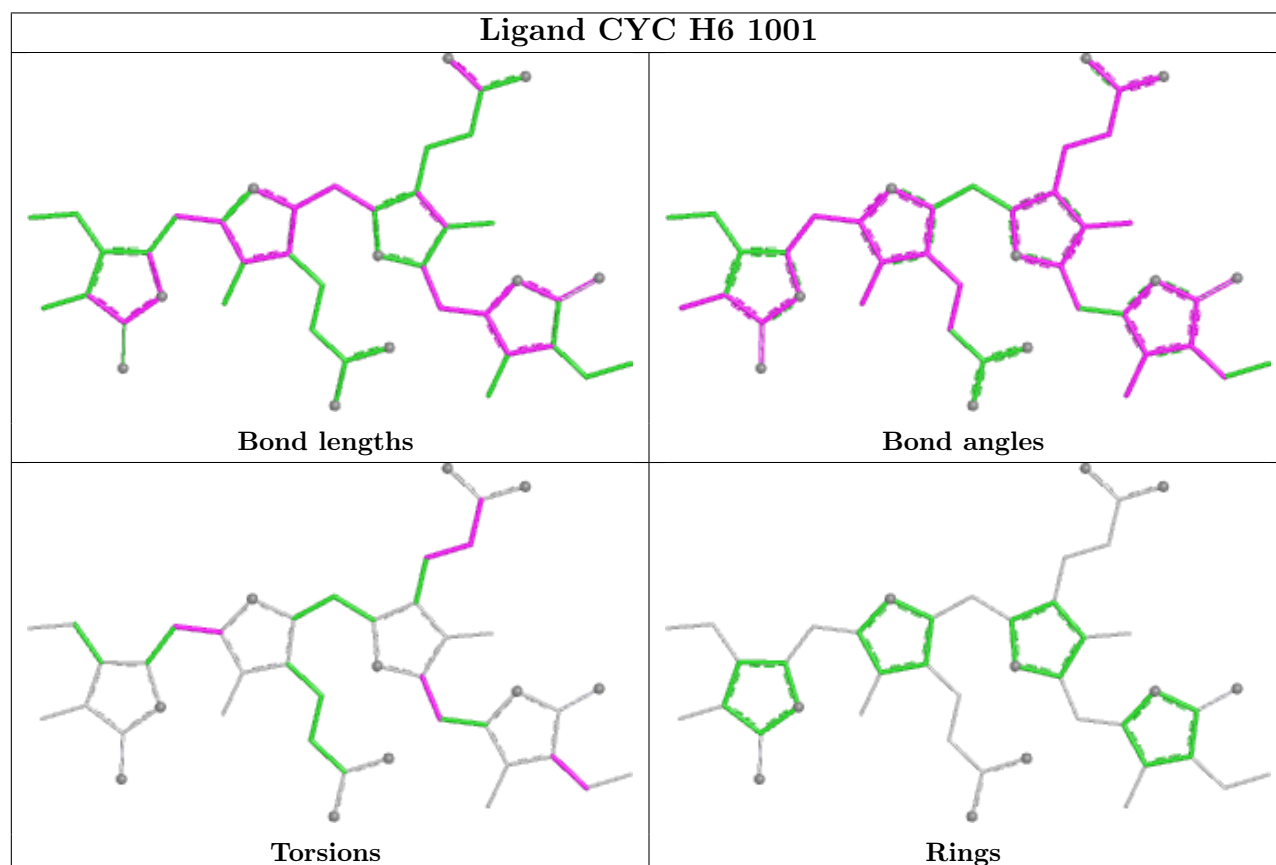
Ligand CYC I6 201



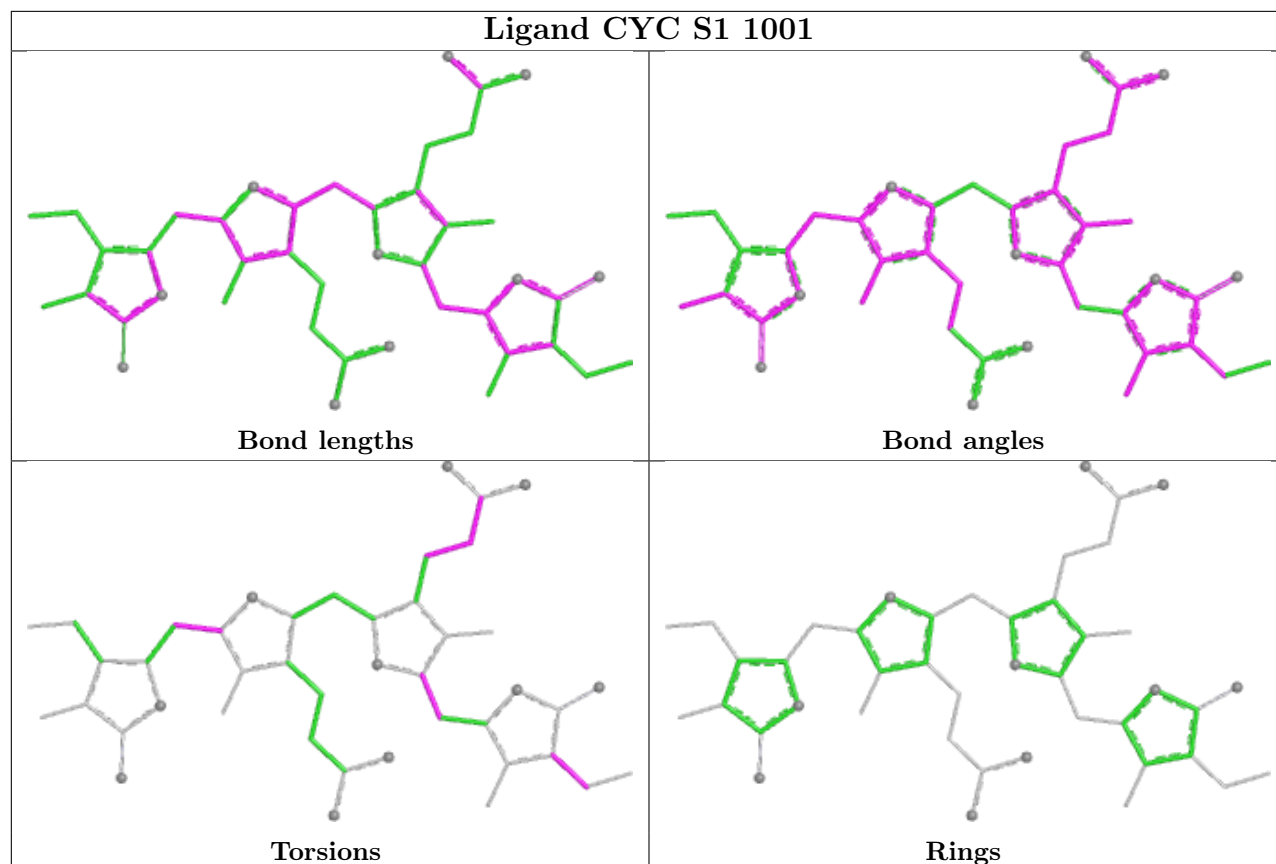
Ligand CYC M5 1001



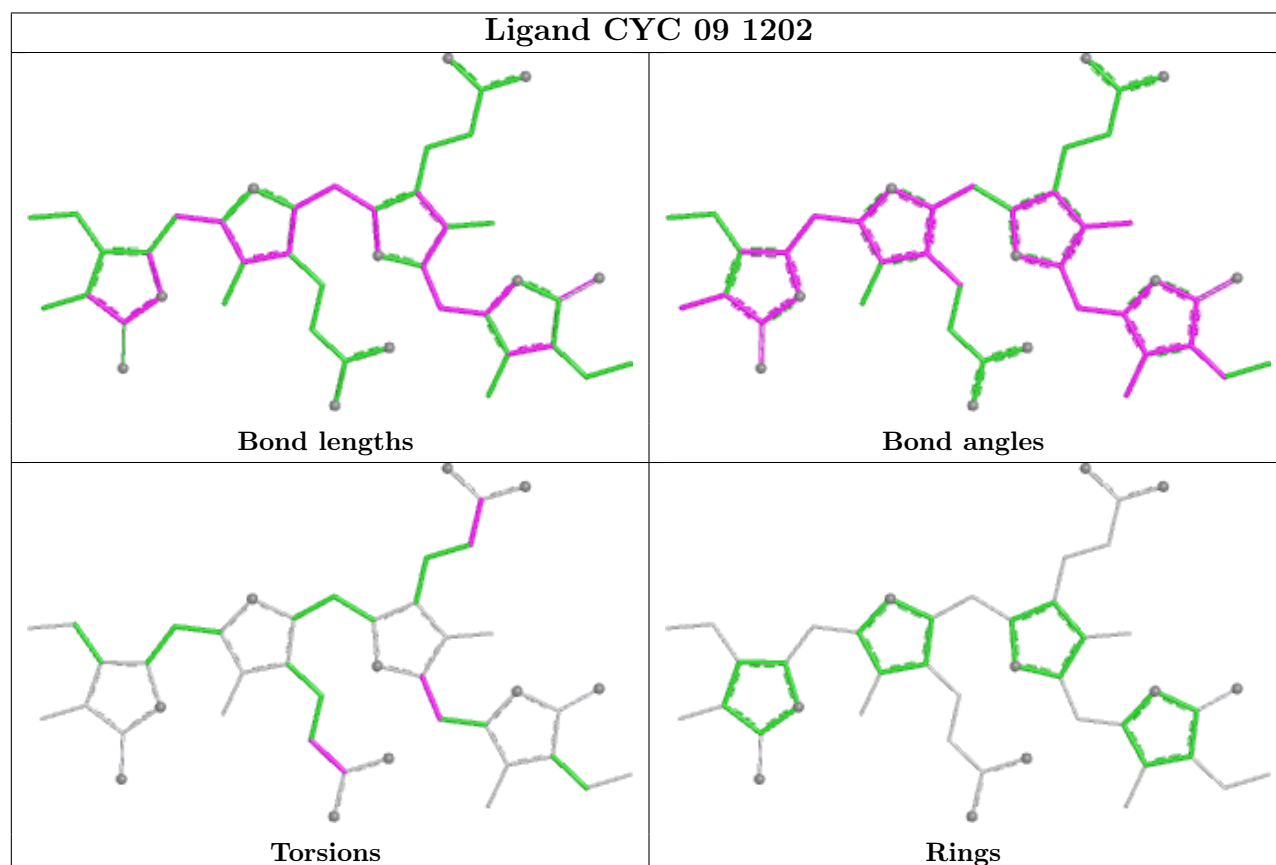
Ligand CYC H6 1001



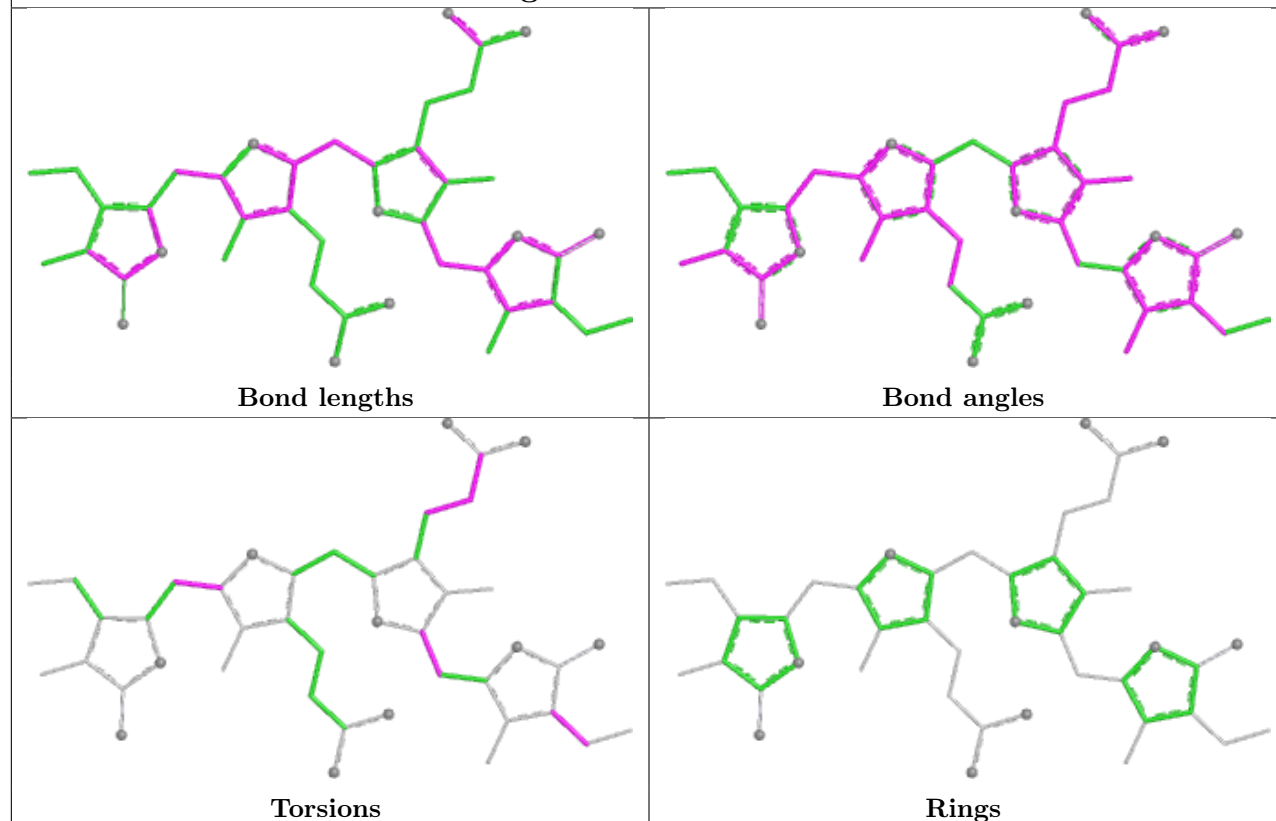
Ligand CYC S1 1001



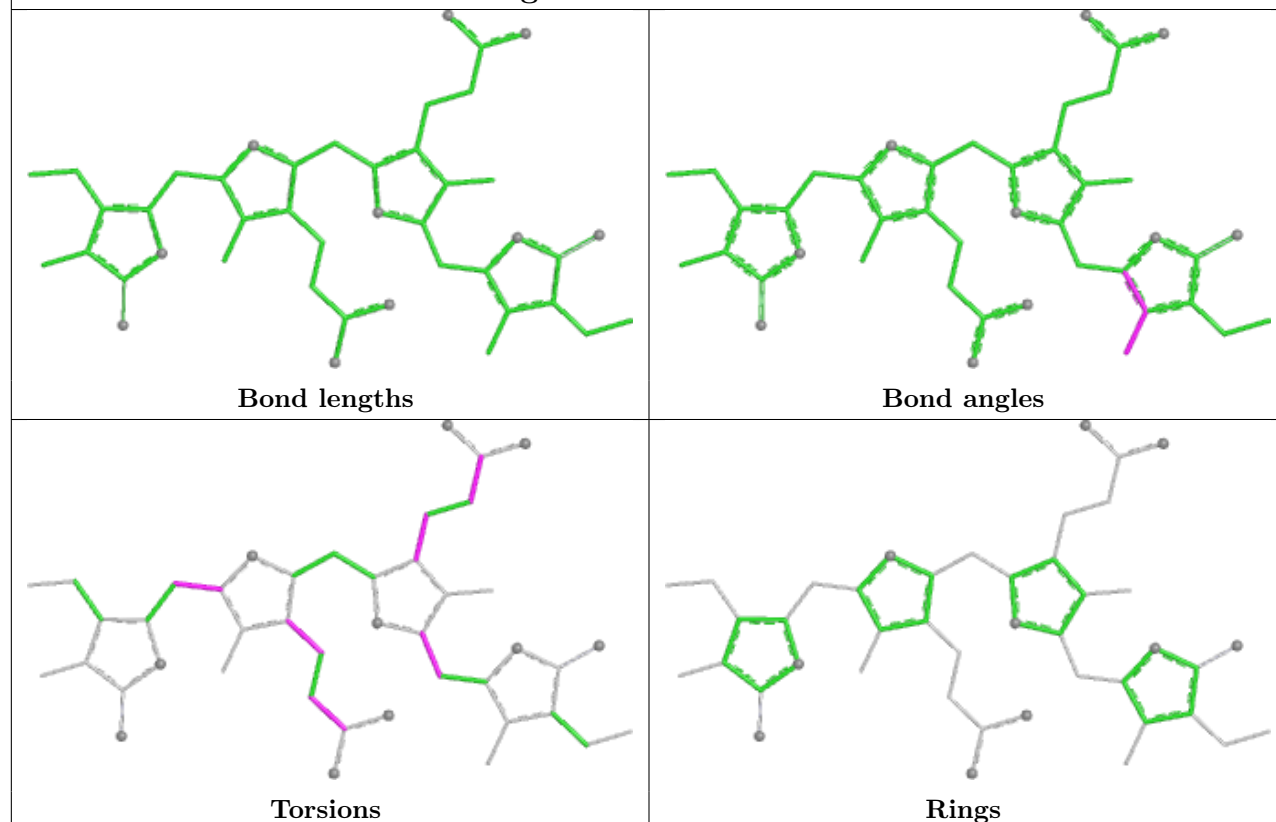
Ligand CYC 09 1202



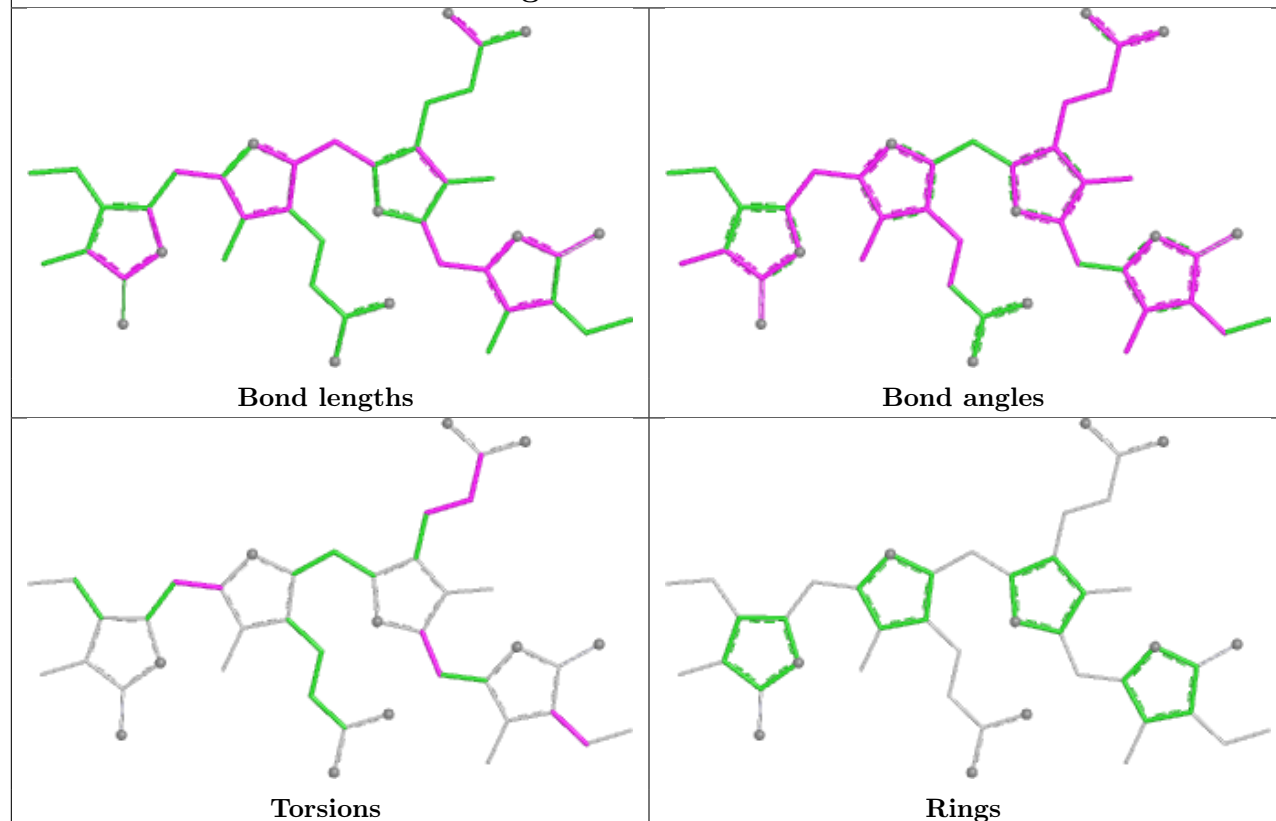
Ligand CYC V1 202



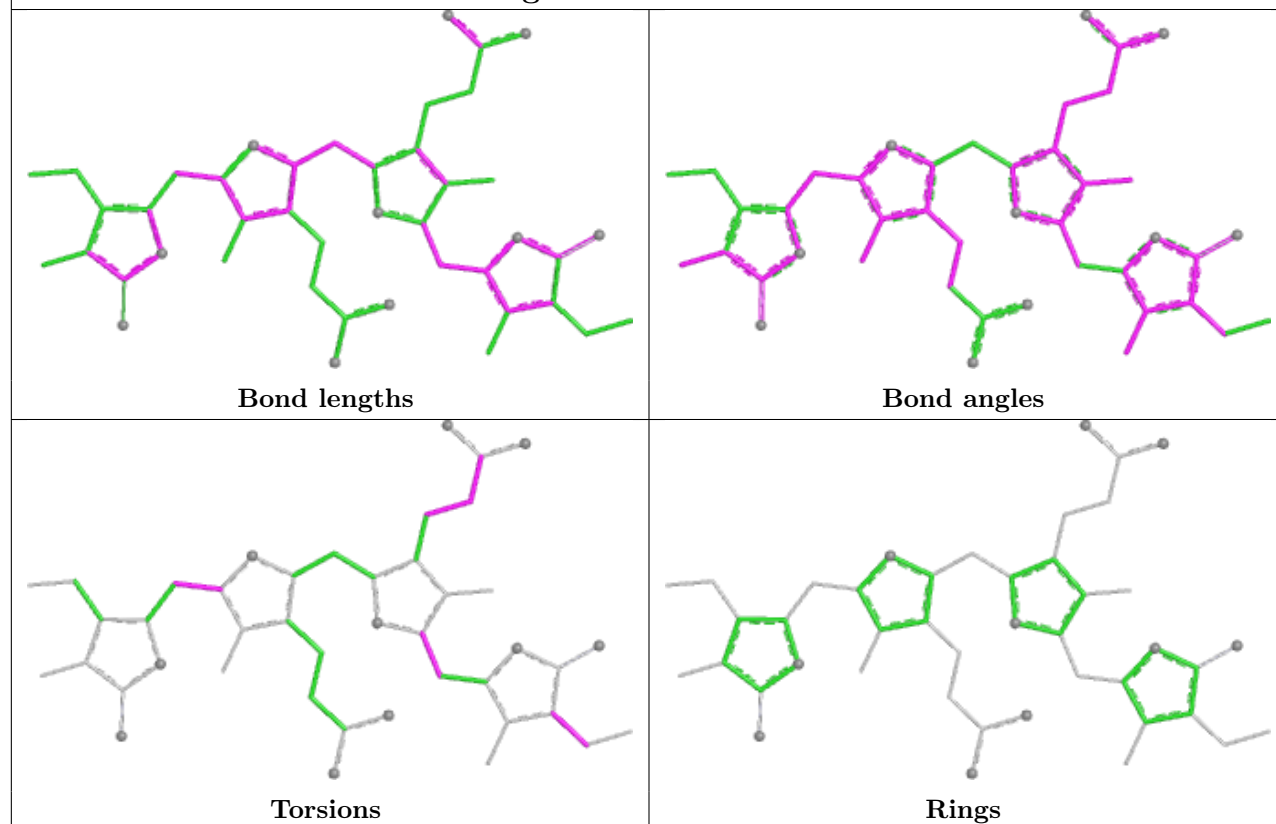
Ligand CYC X6 202



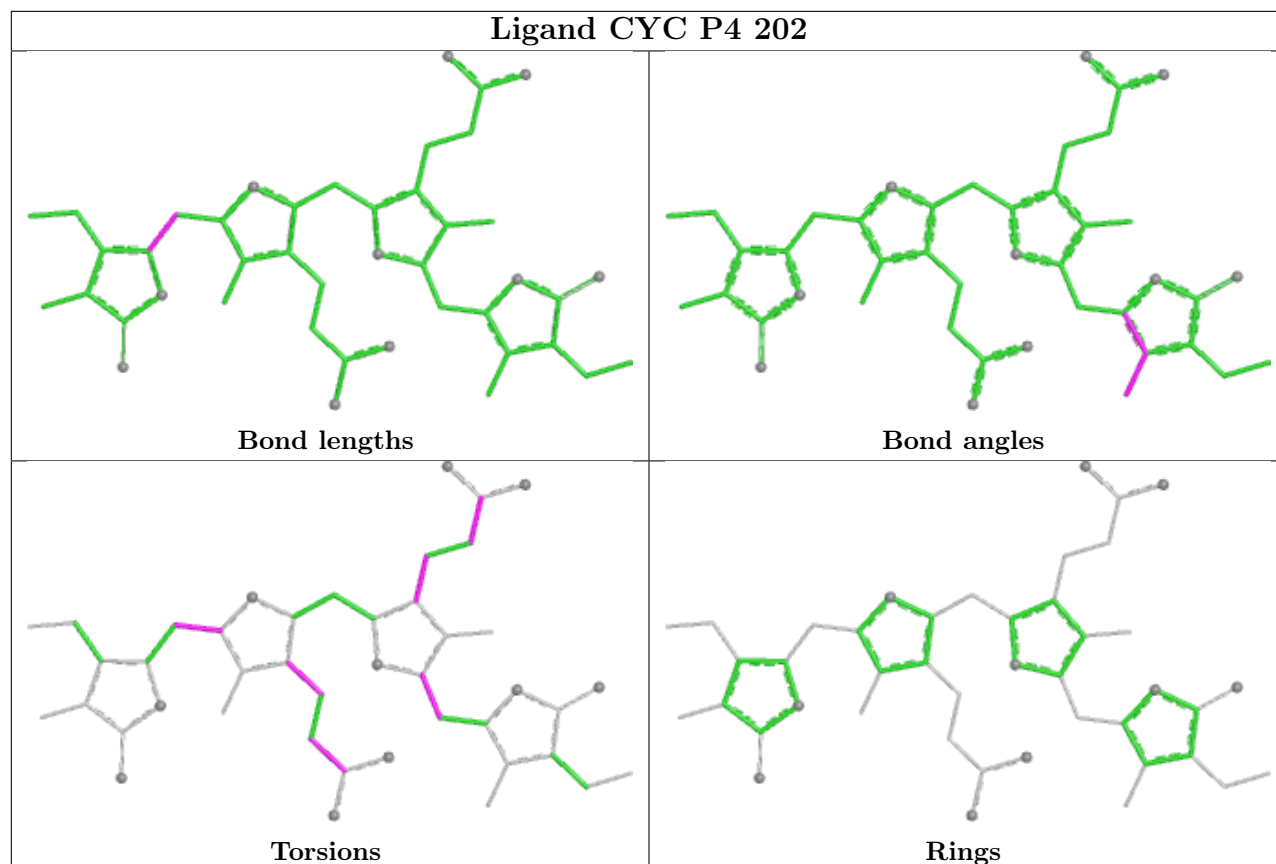
Ligand CYC T1 202



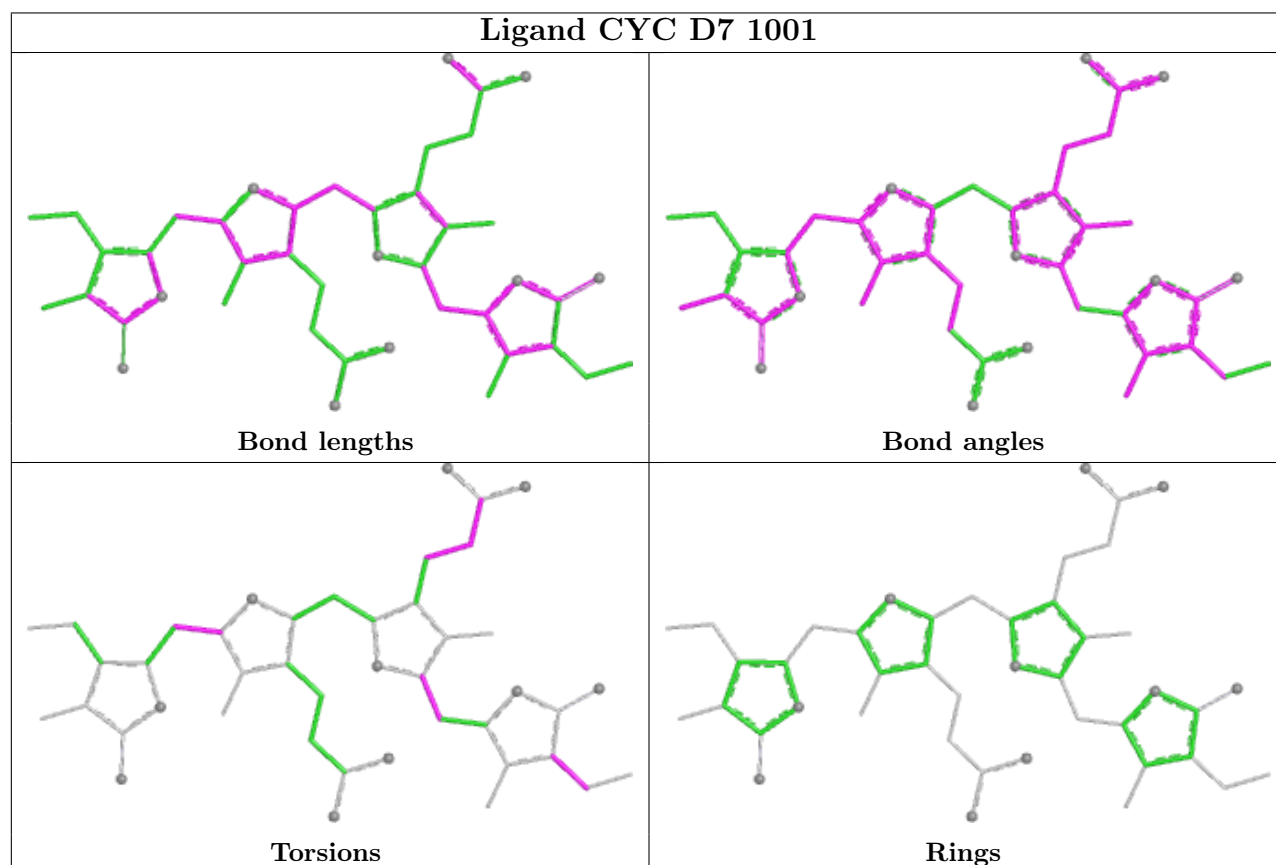
Ligand CYC E5 202



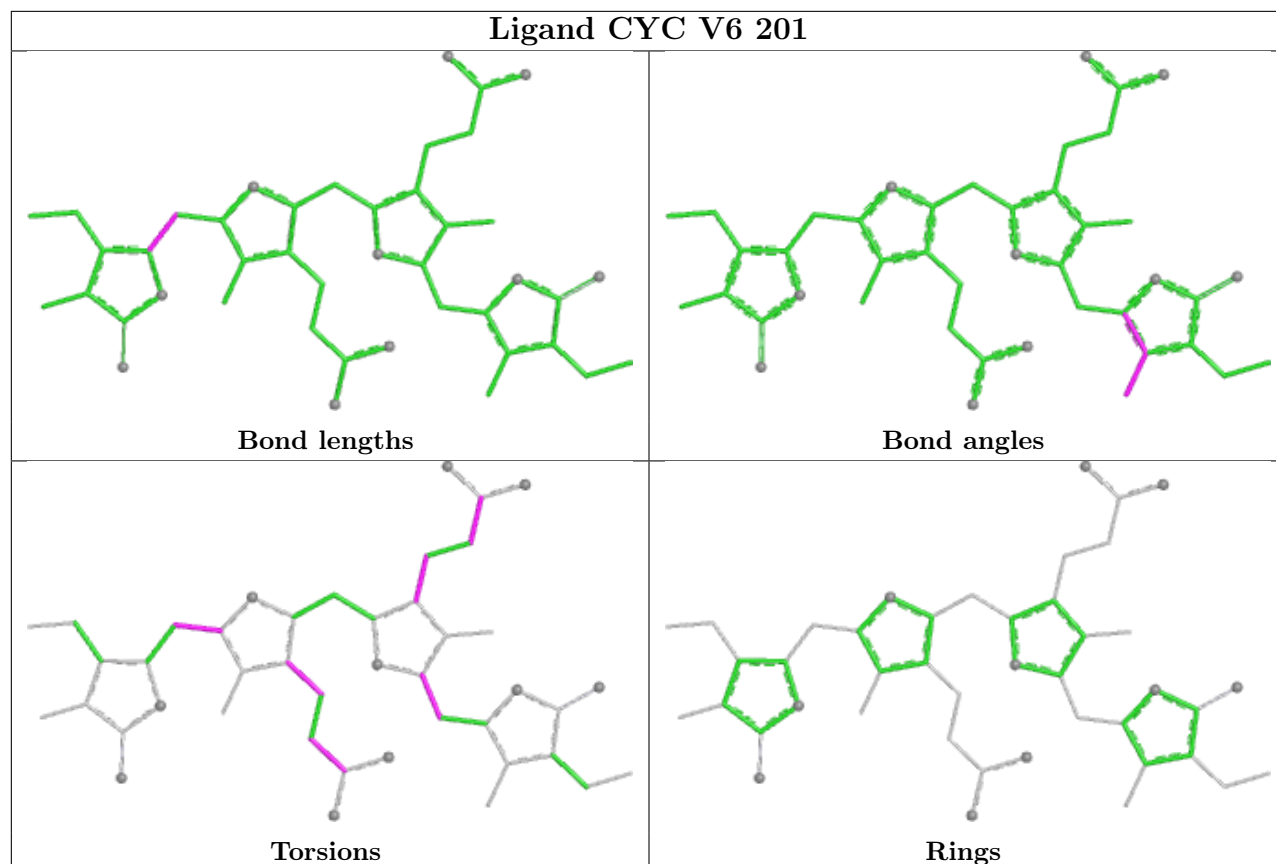
Ligand CYC P4 202



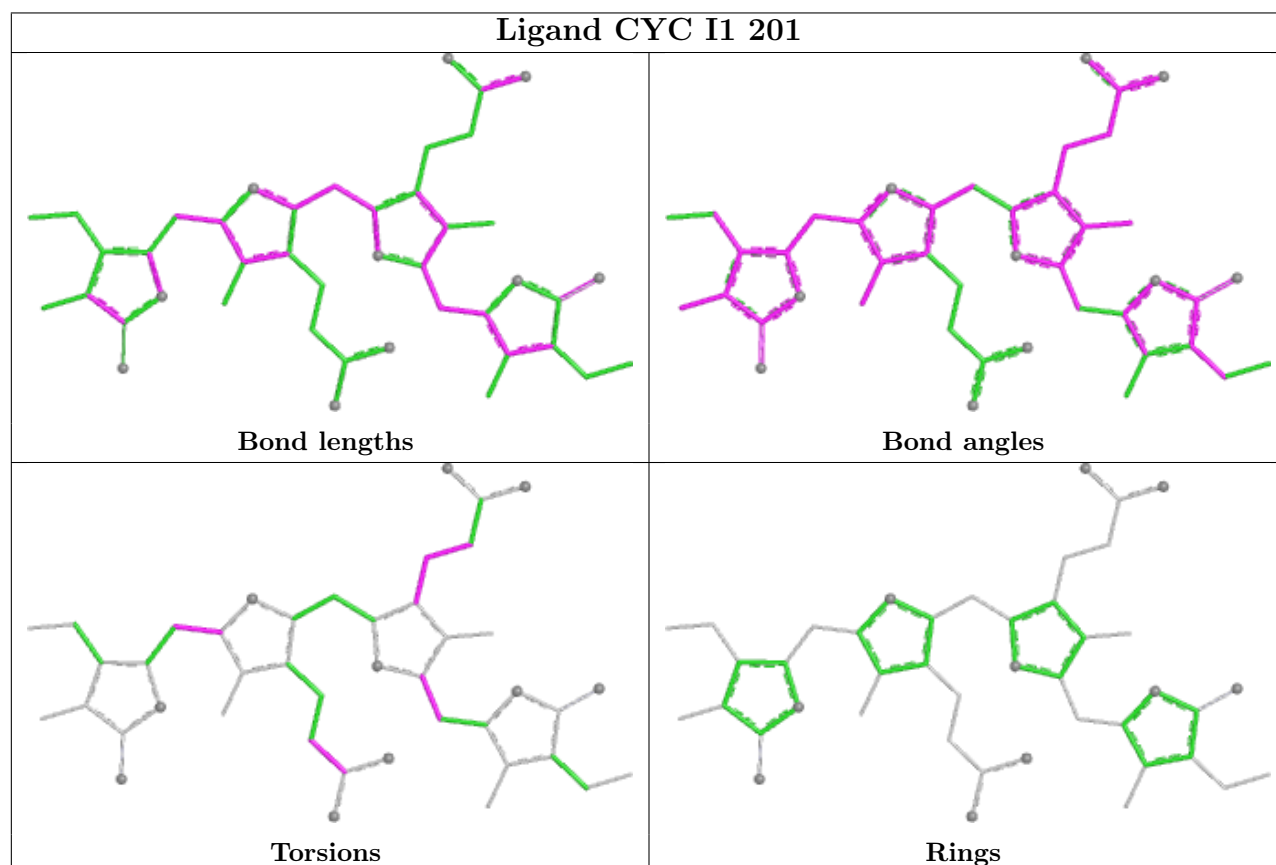
Ligand CYC D7 1001



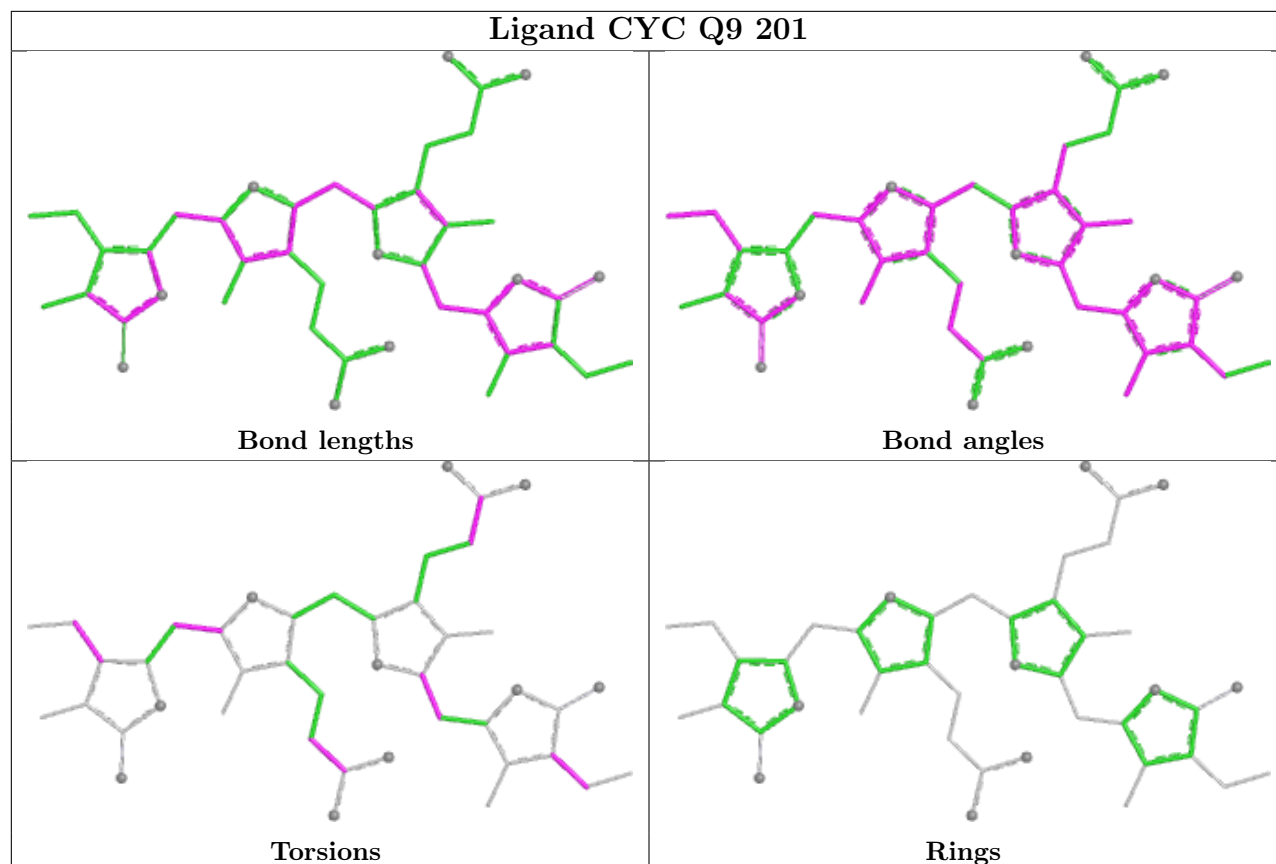
Ligand CYC V6 201



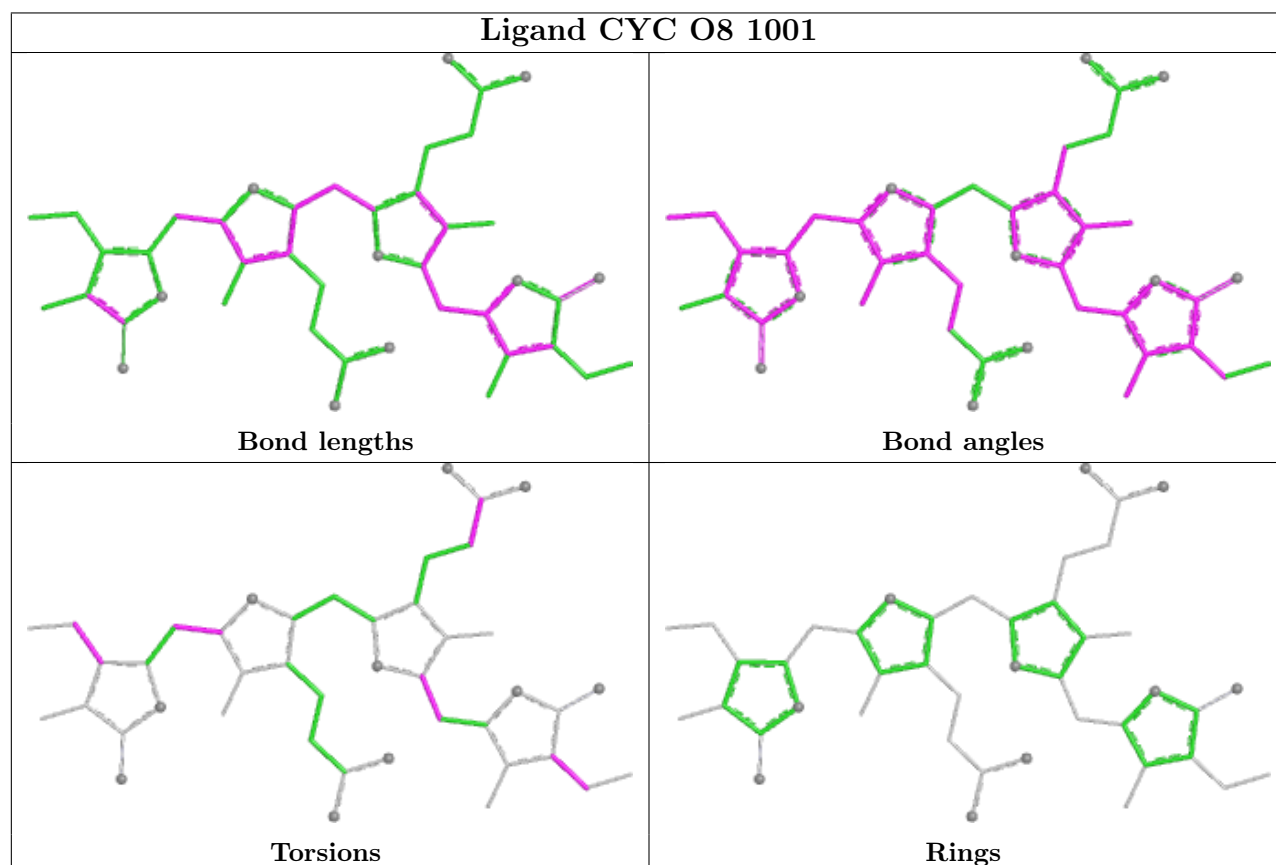
Ligand CYC I1 201



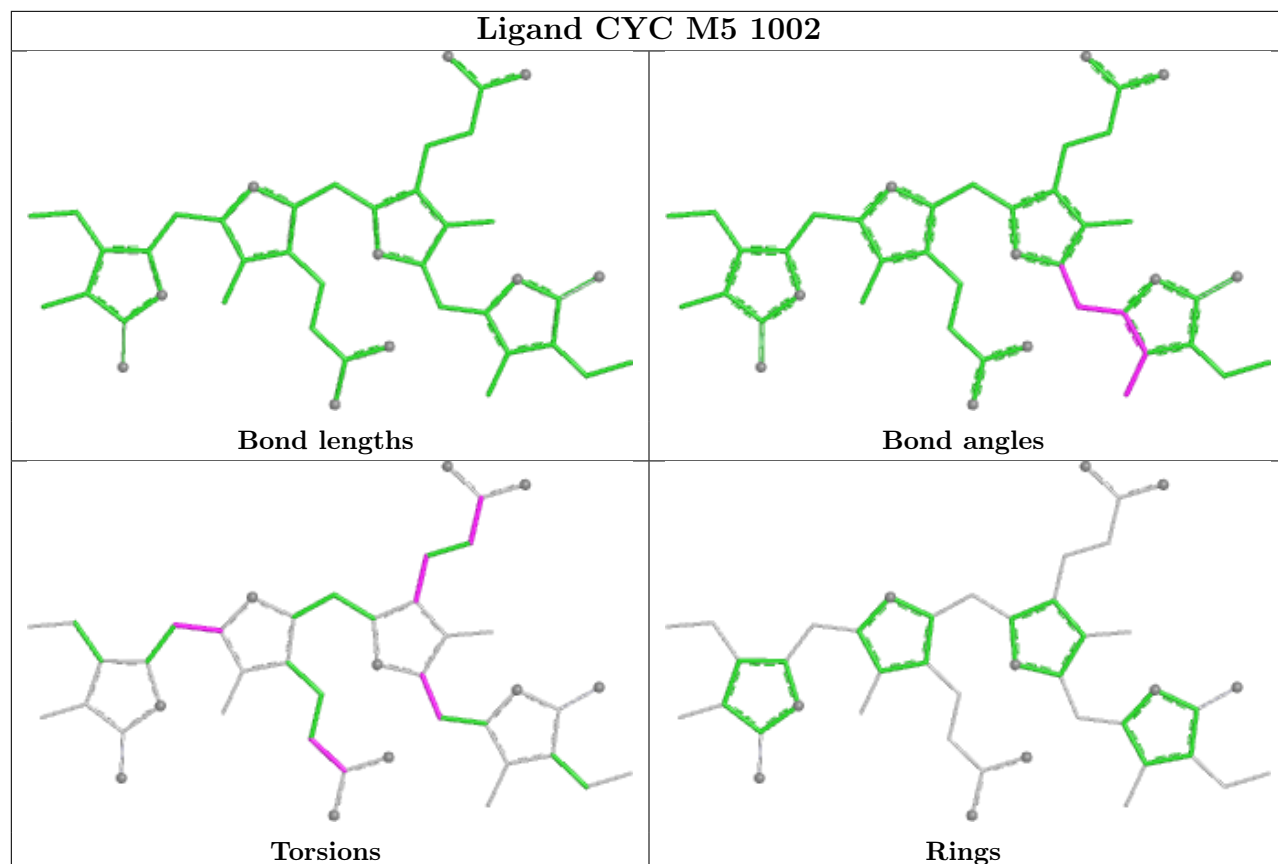
Ligand CYC Q9 201



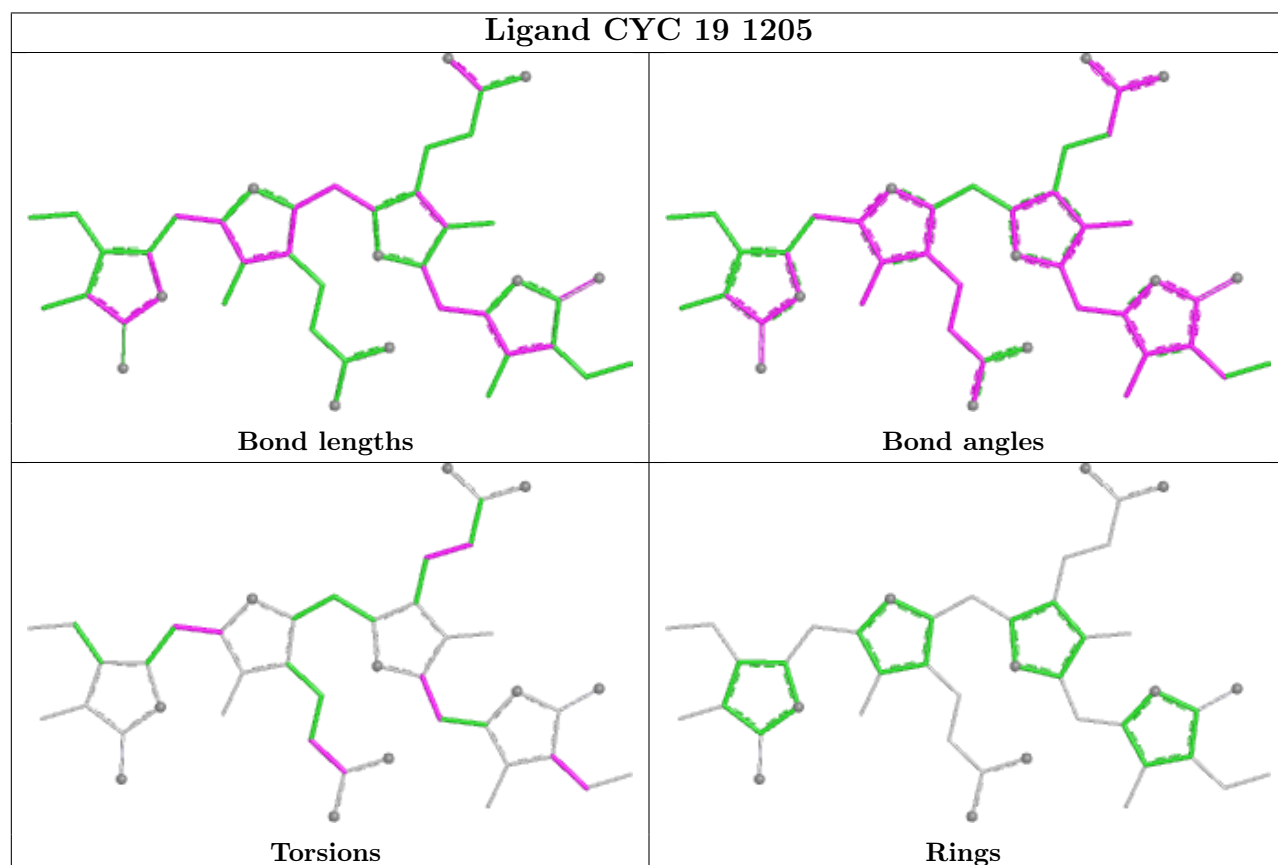
Ligand CYC O8 1001



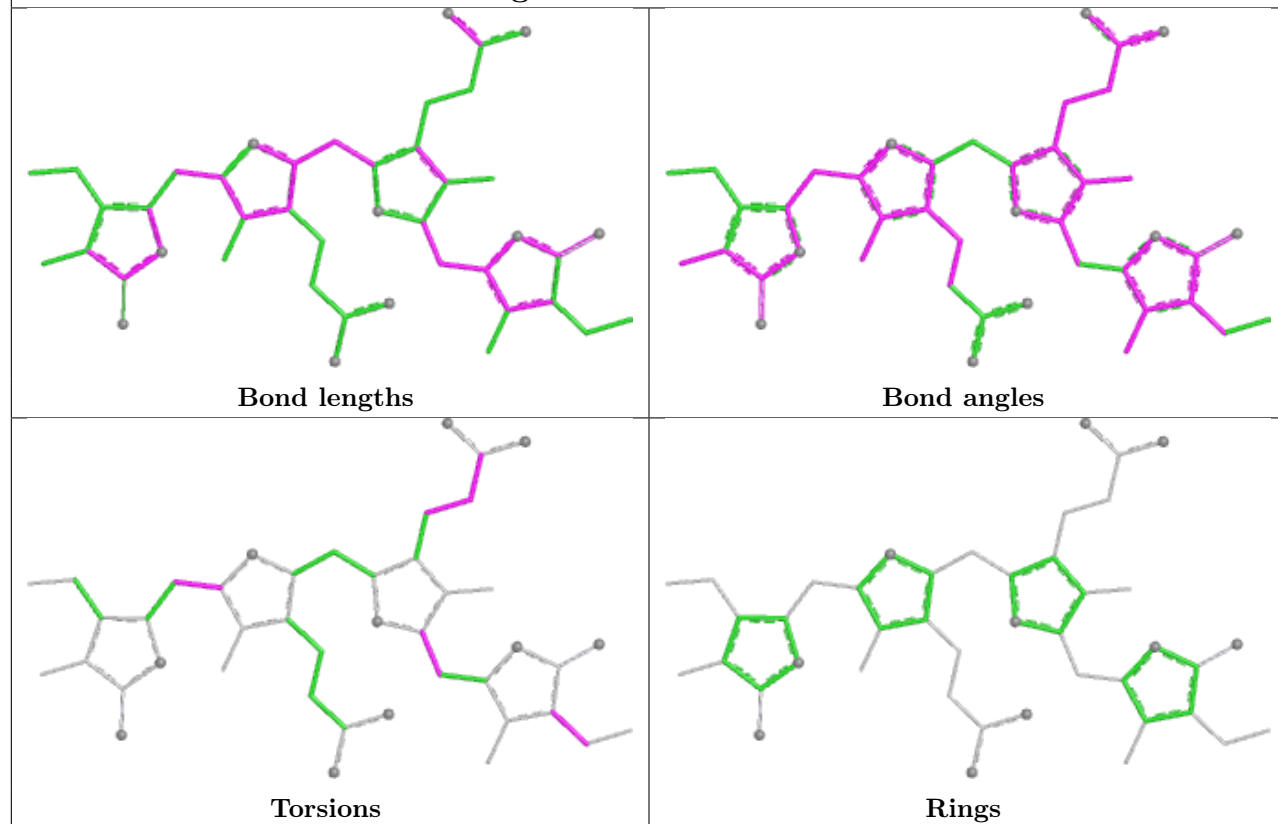
Ligand CYC M5 1002



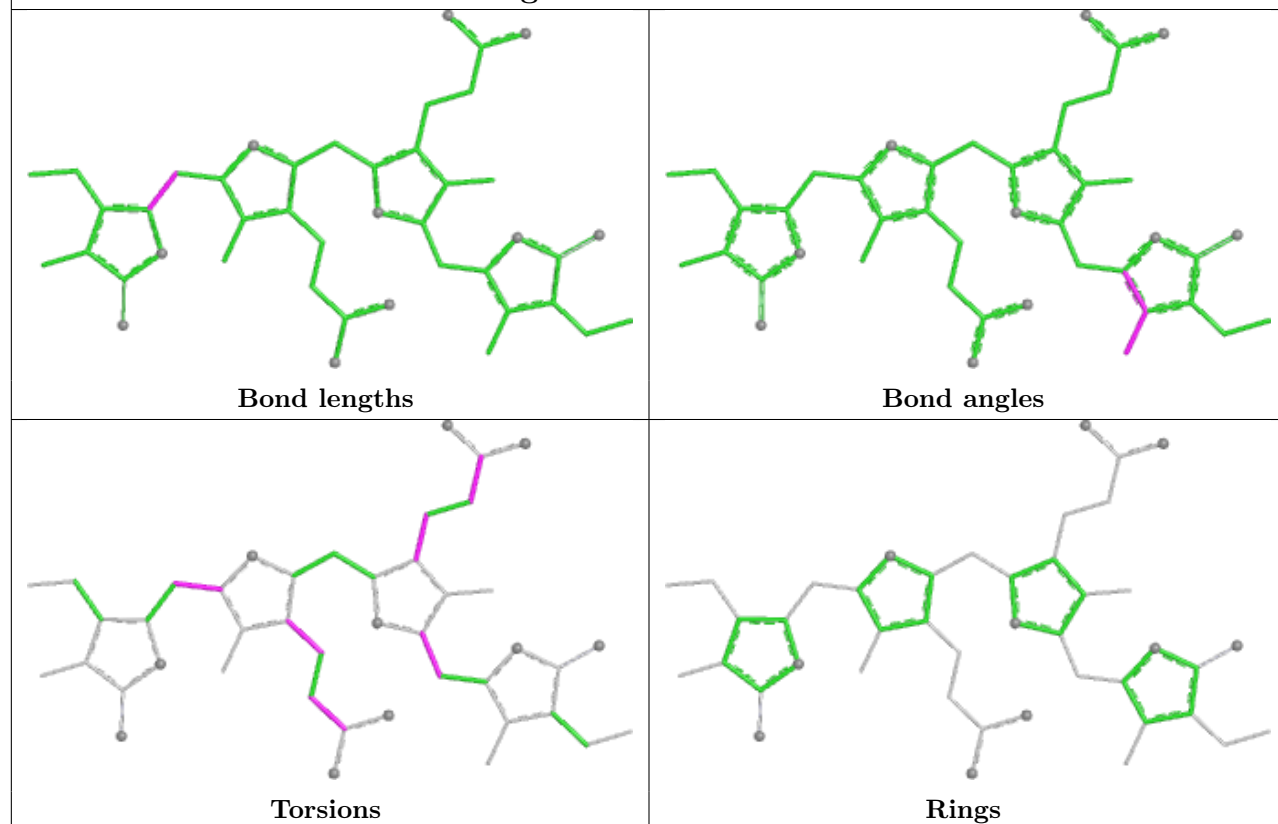
Ligand CYC 19 1205



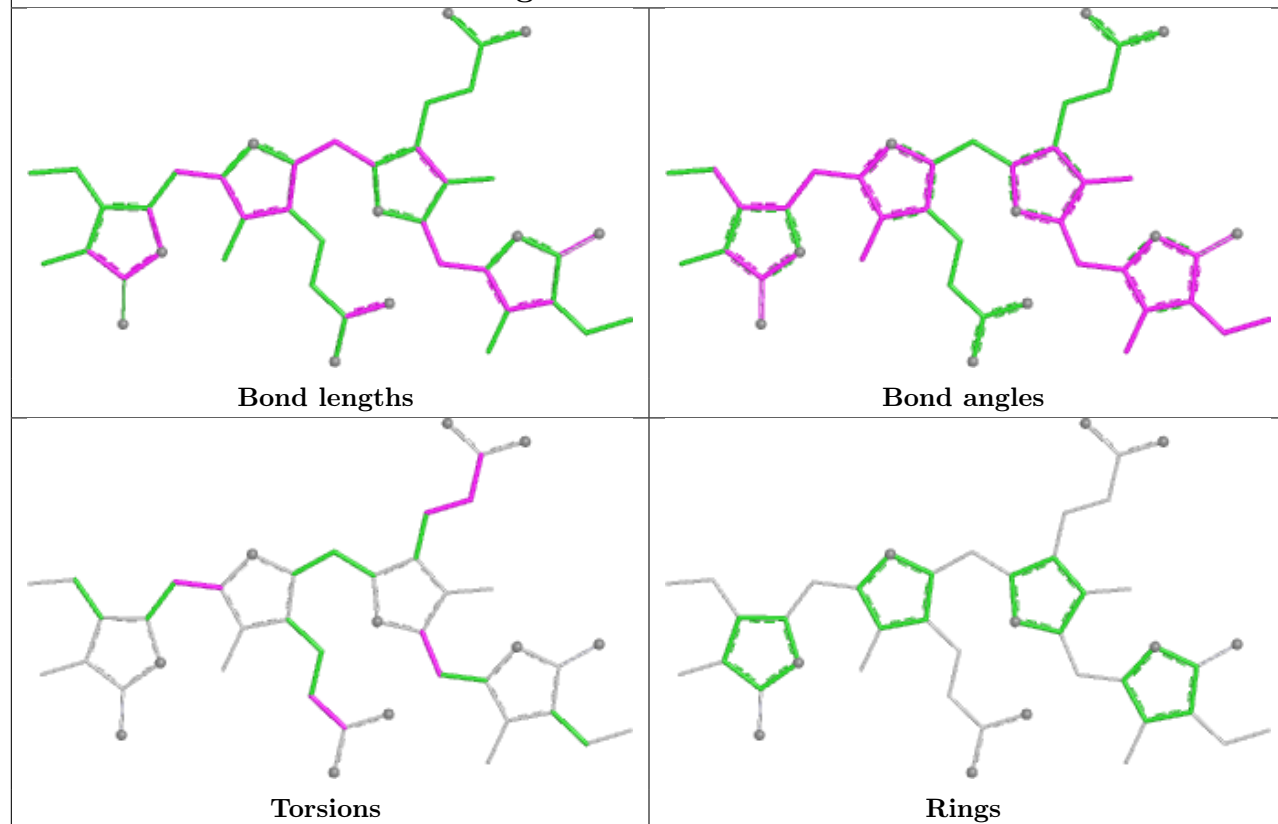
Ligand CYC U1 1001



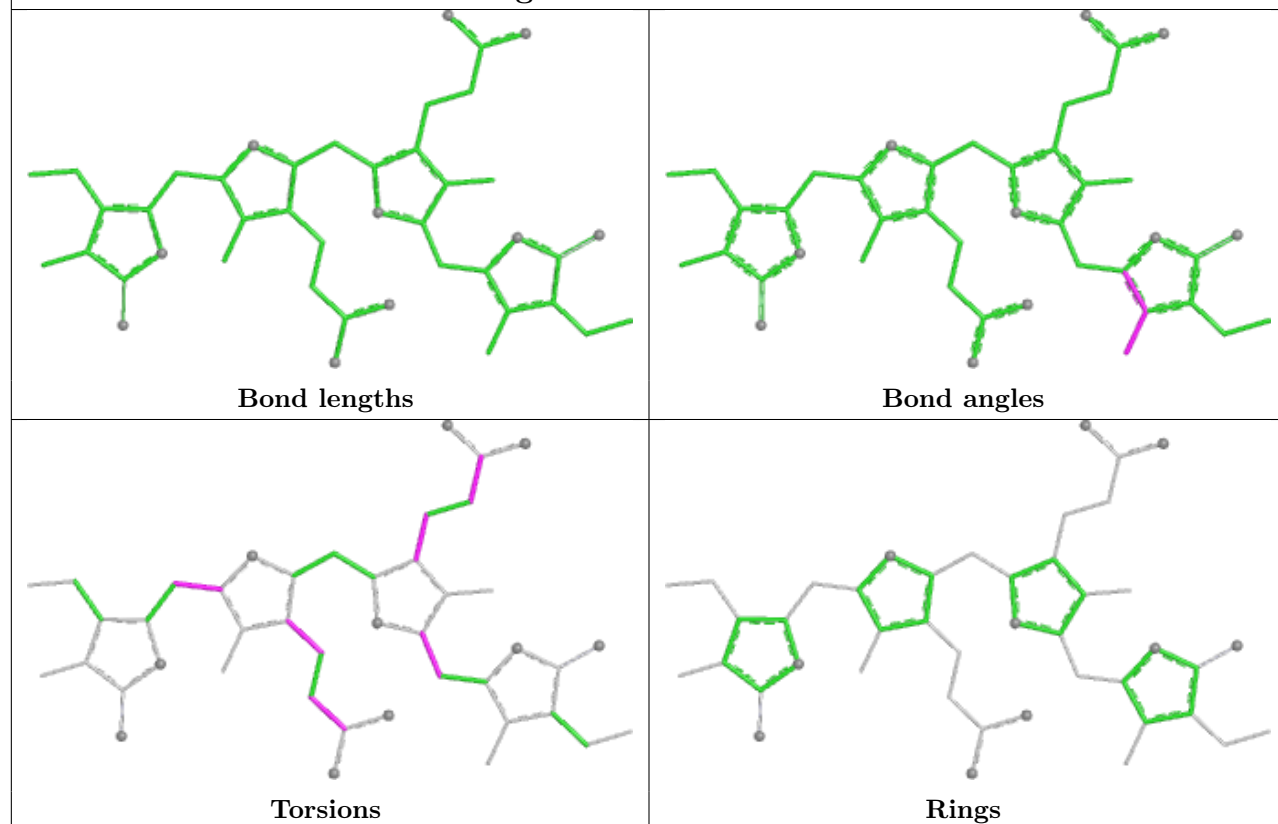
Ligand CYC V4 201



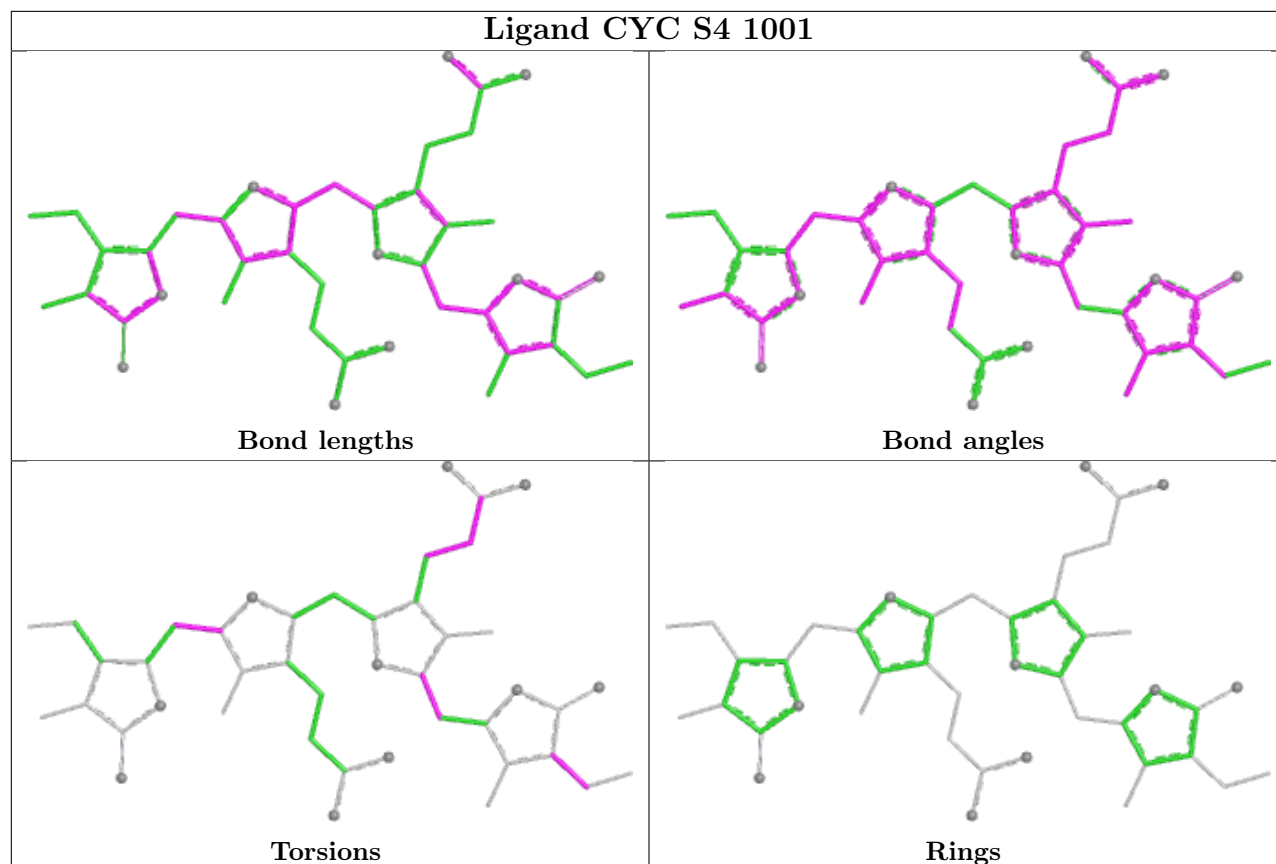
Ligand CYC o8 1001



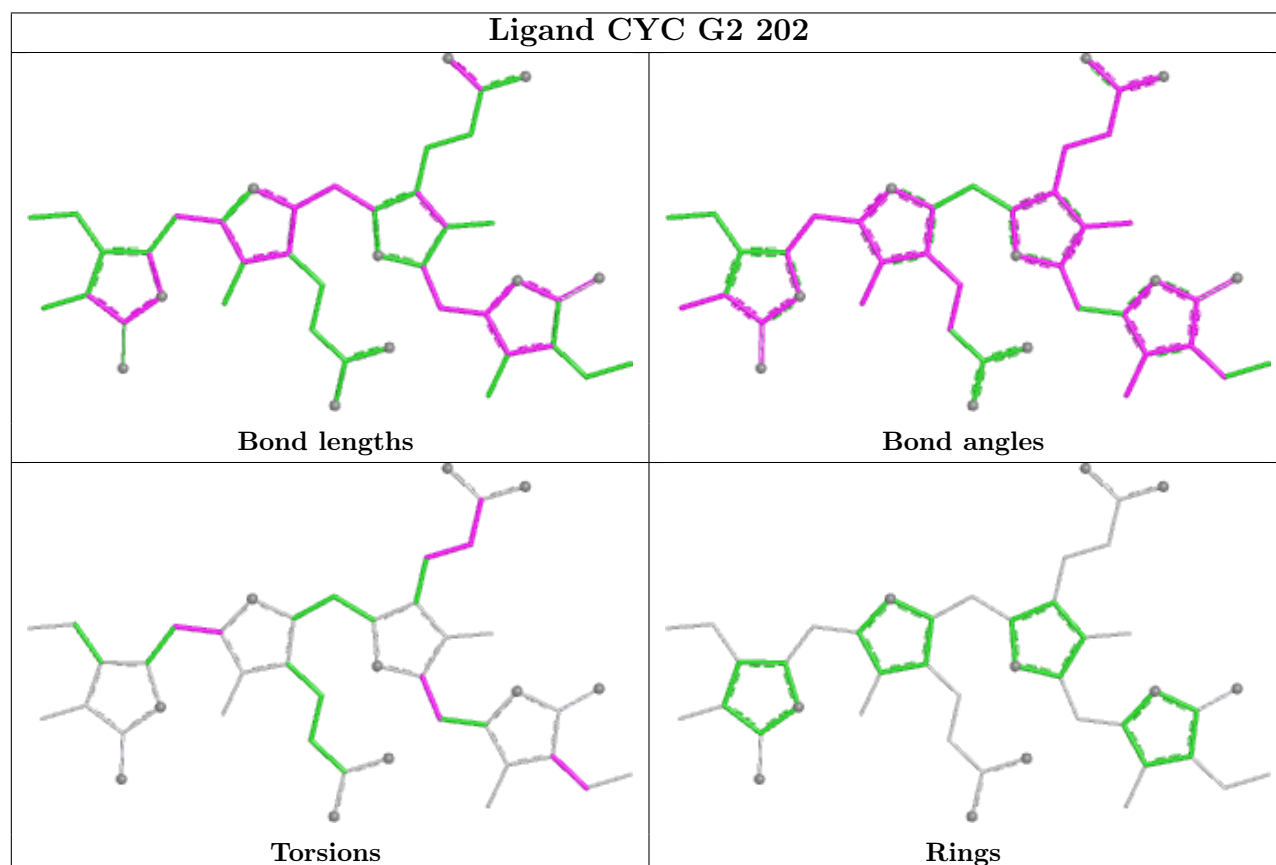
Ligand CYC W6 201



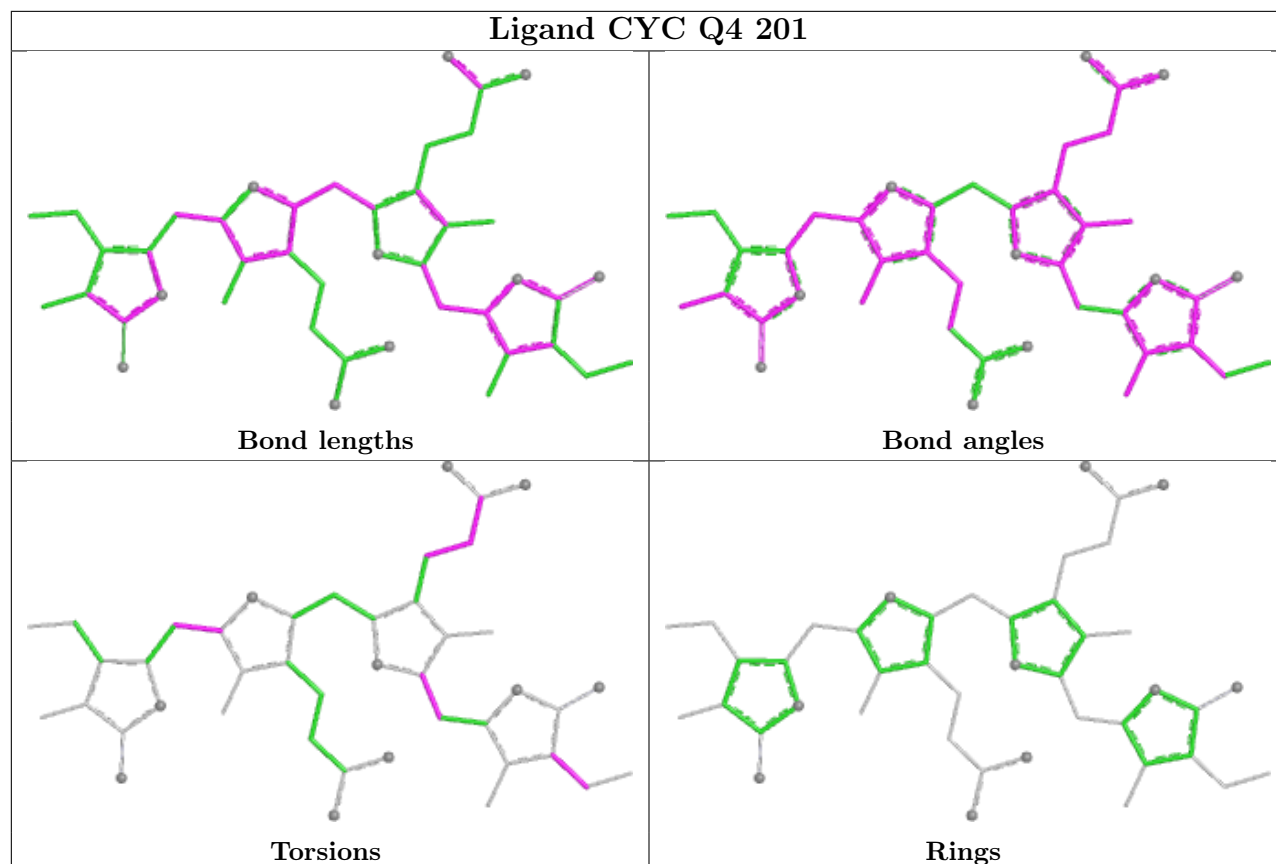
Ligand CYC S4 1001



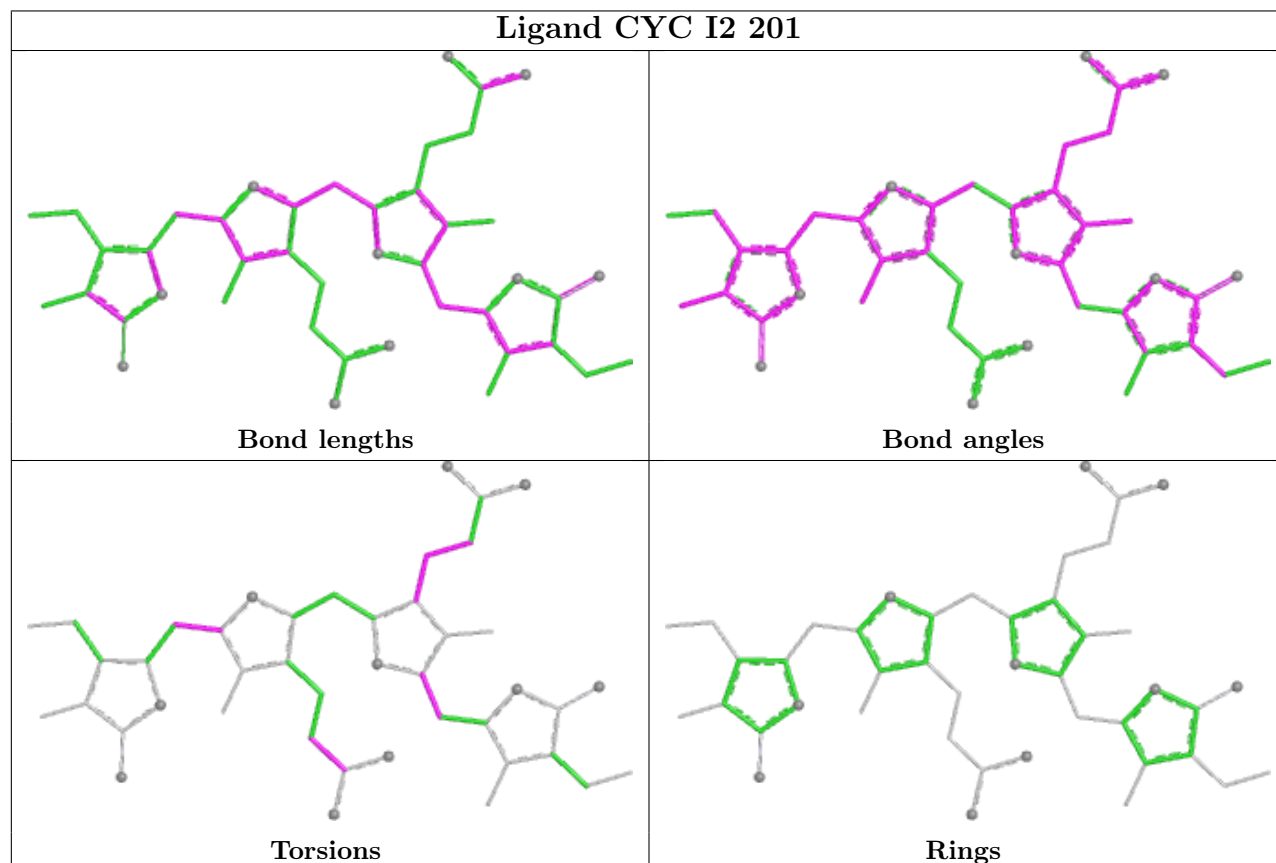
Ligand CYC G2 202



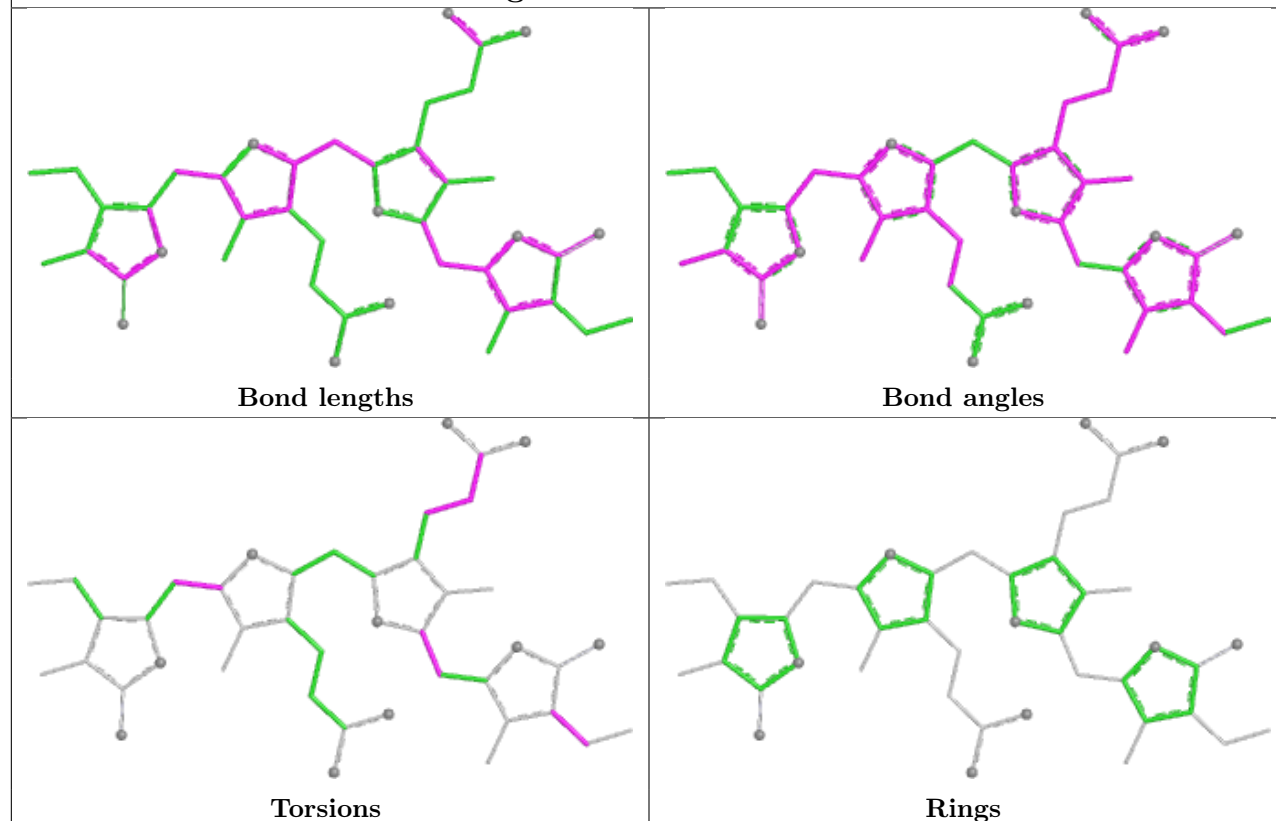
Ligand CYC Q4 201



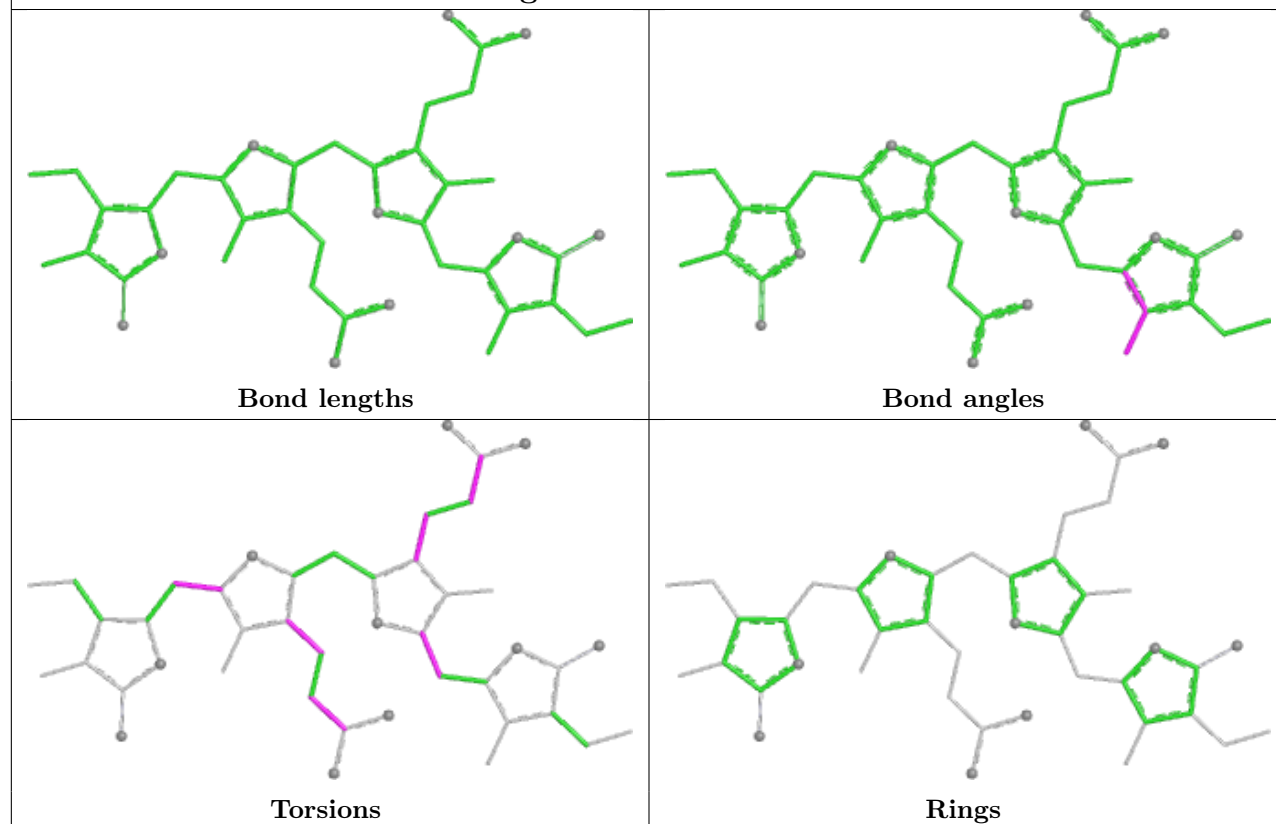
Ligand CYC I2 201



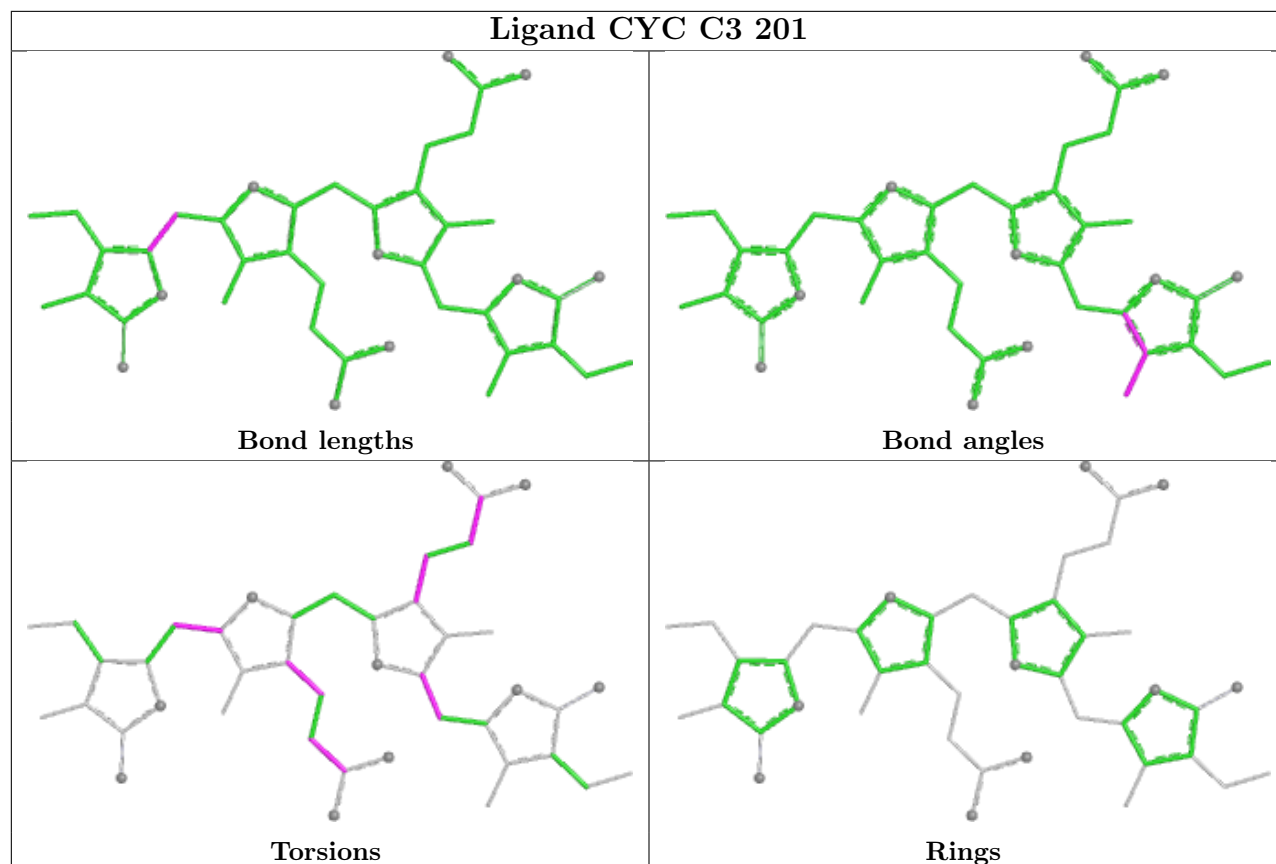
Ligand CYC W4 1001



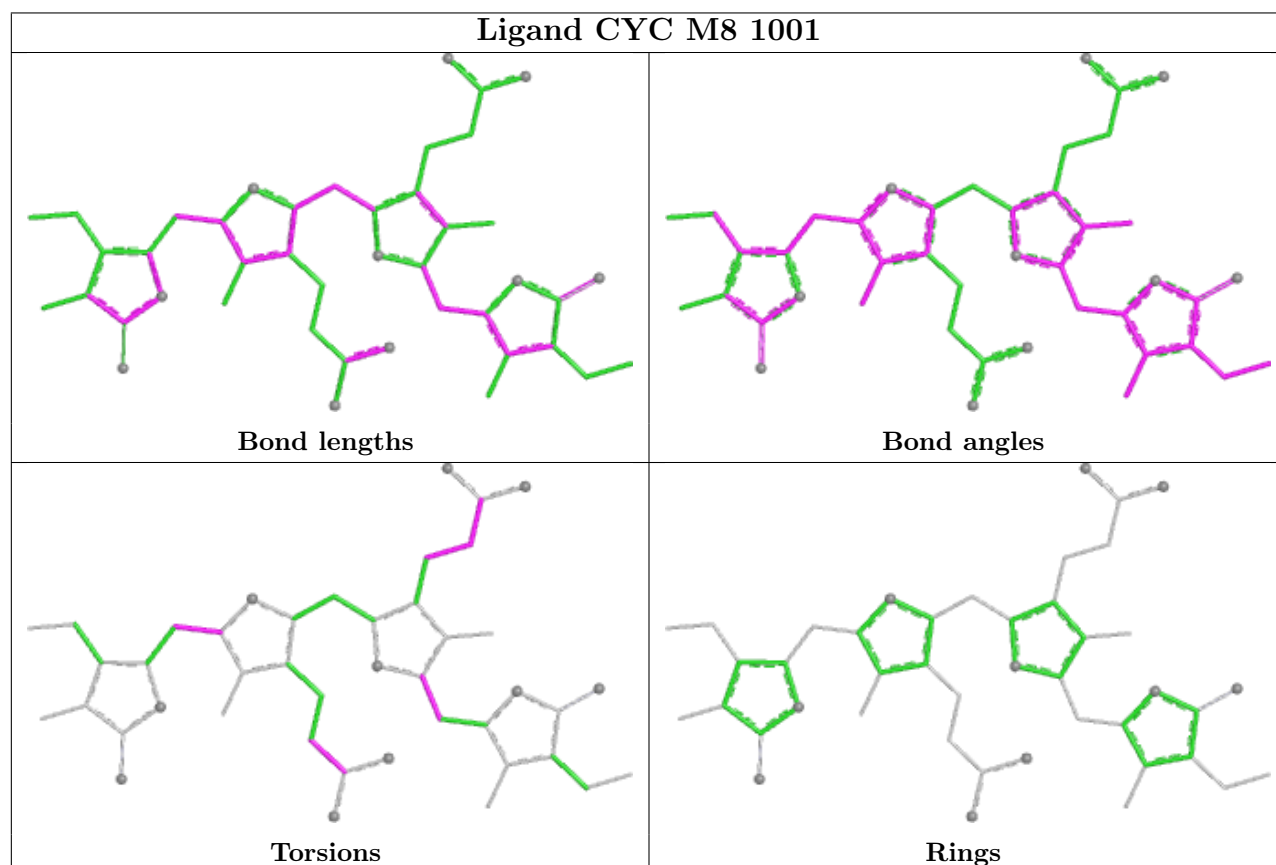
Ligand CYC K3 201



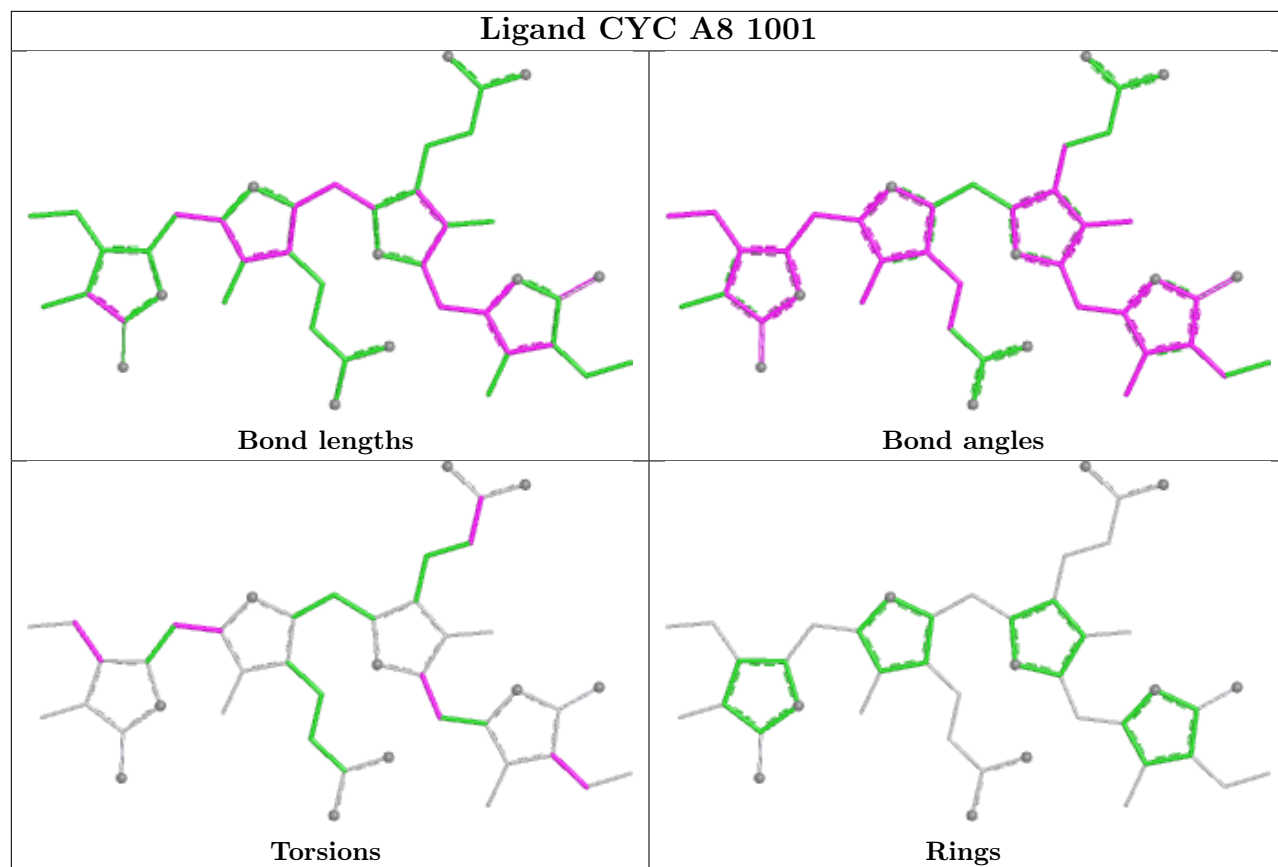
Ligand CYC C3 201



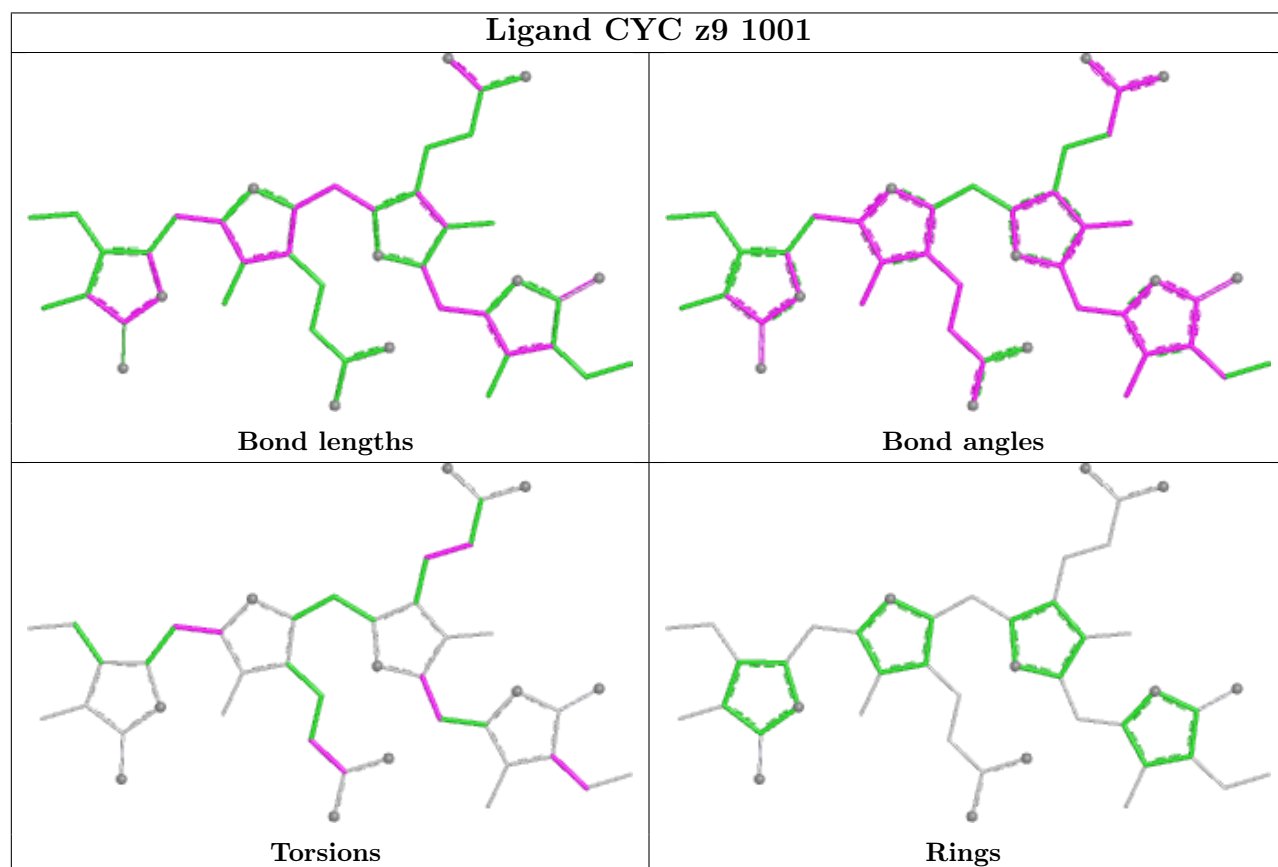
Ligand CYC M8 1001



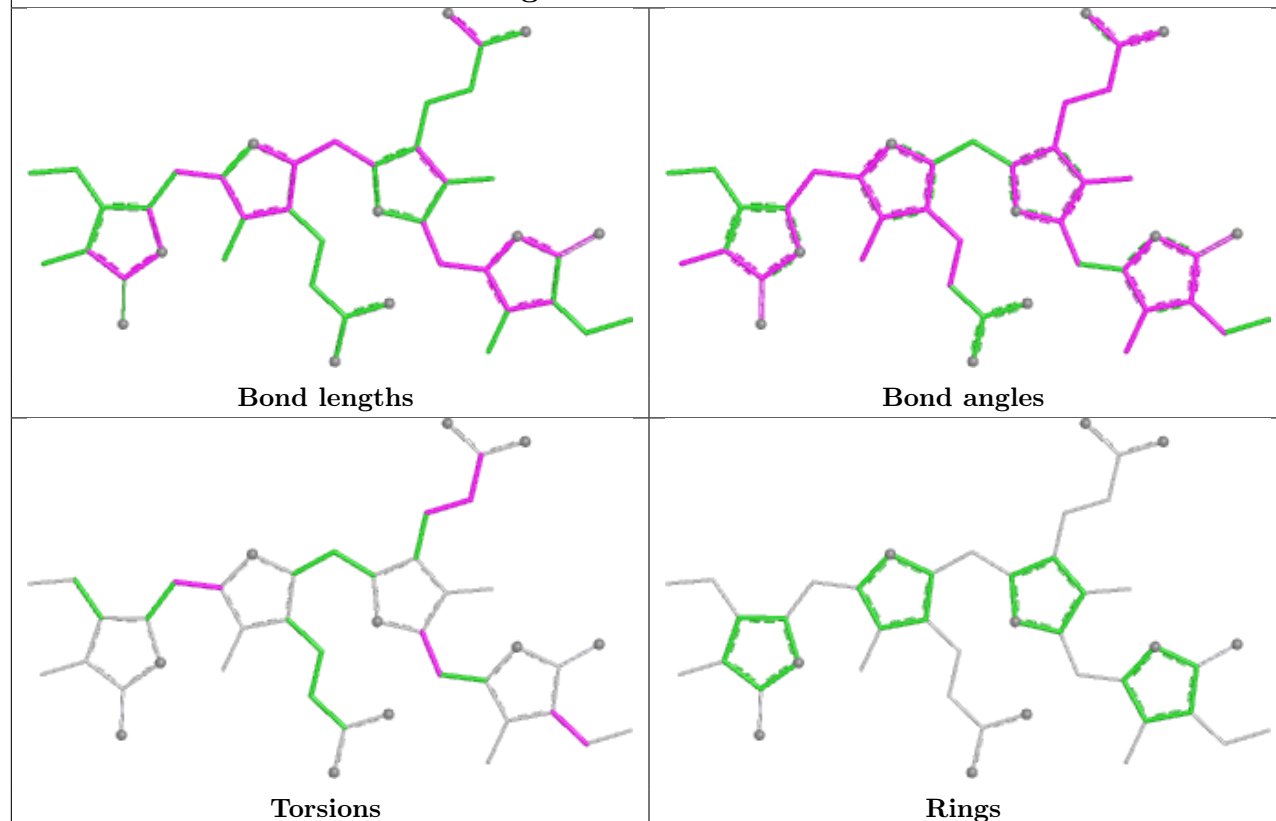
Ligand CYC A8 1001



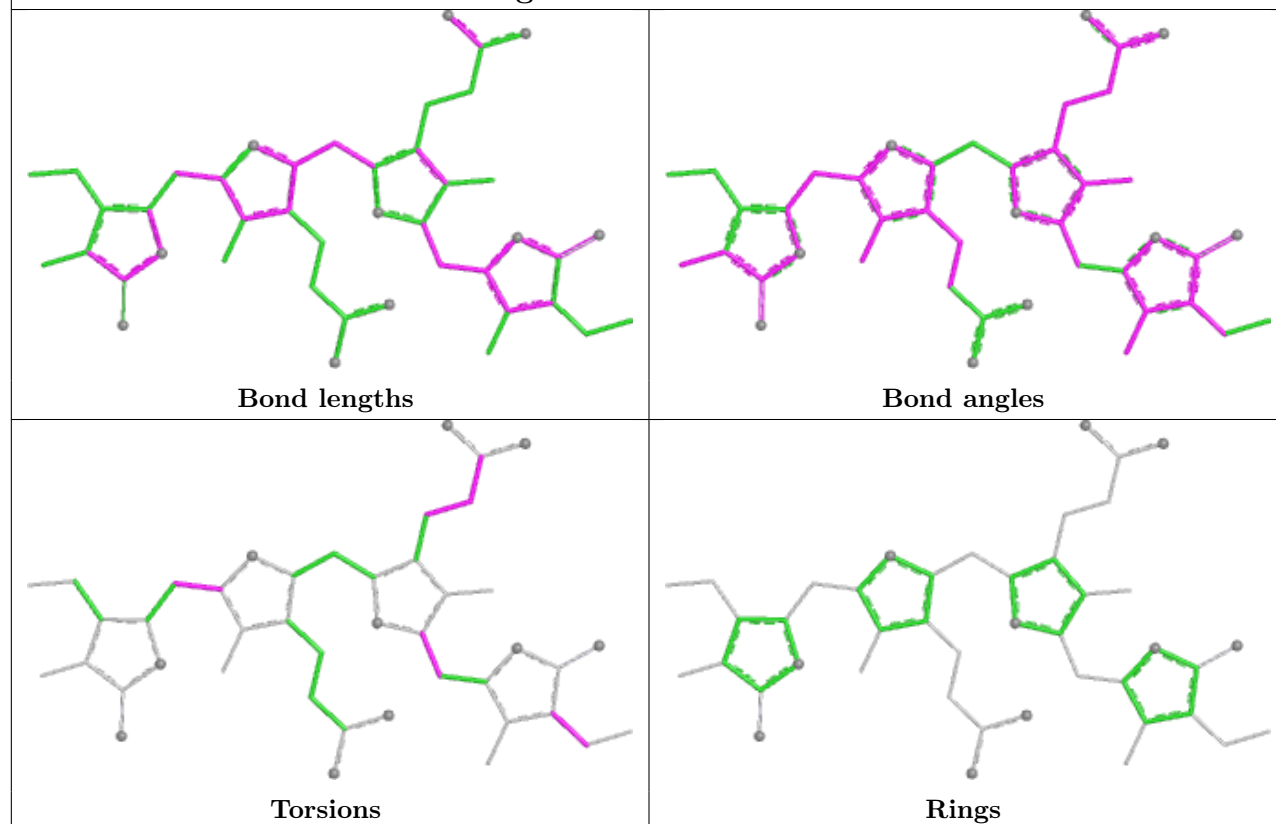
Ligand CYC z9 1001



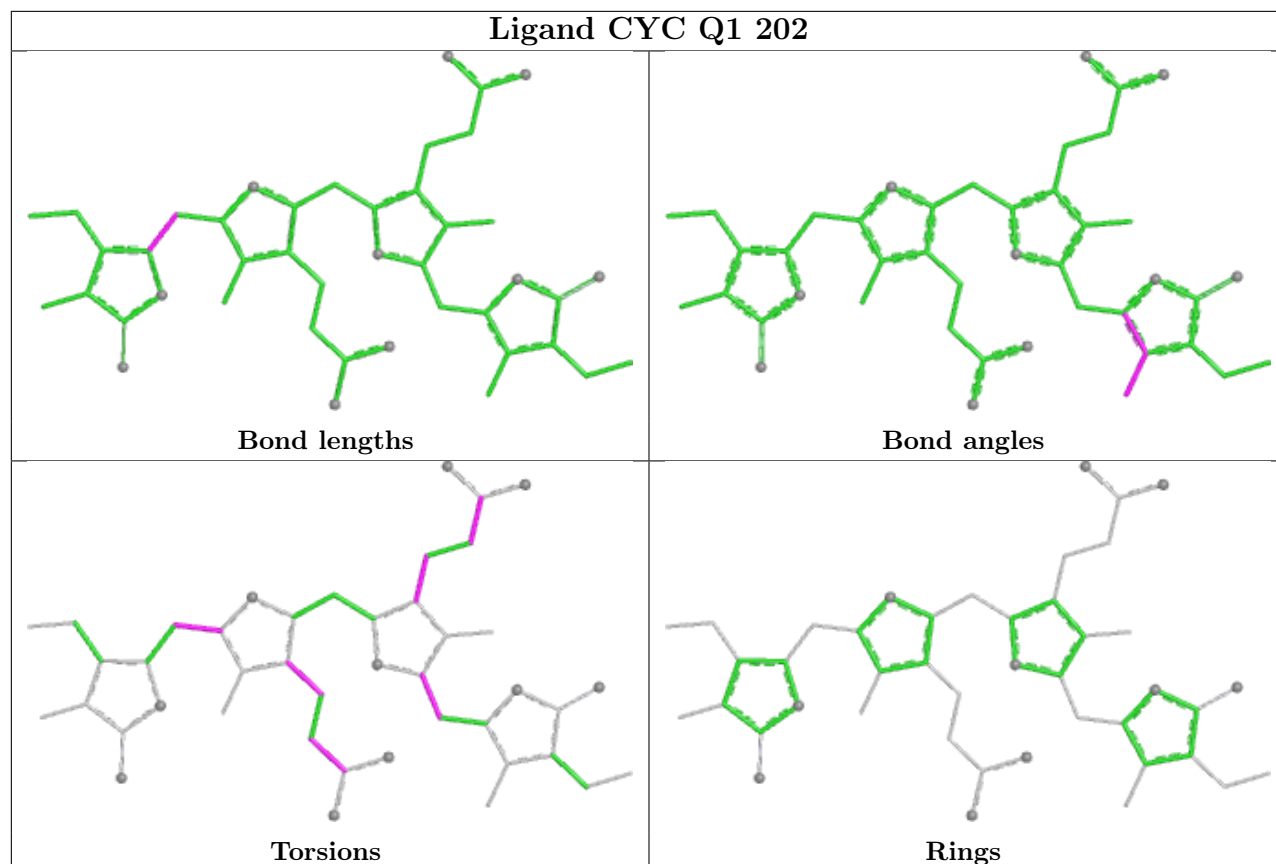
Ligand CYC C2 201



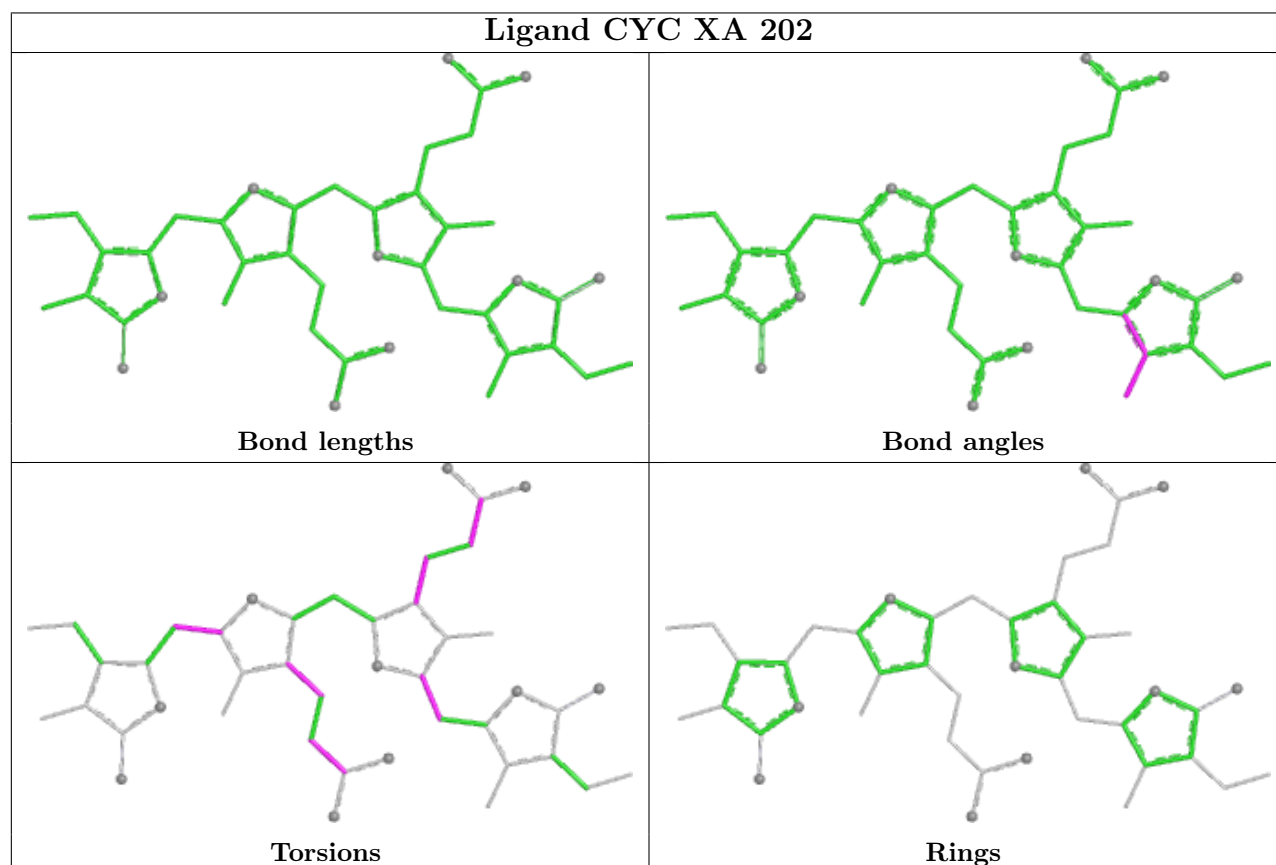
Ligand CYC J3 1001



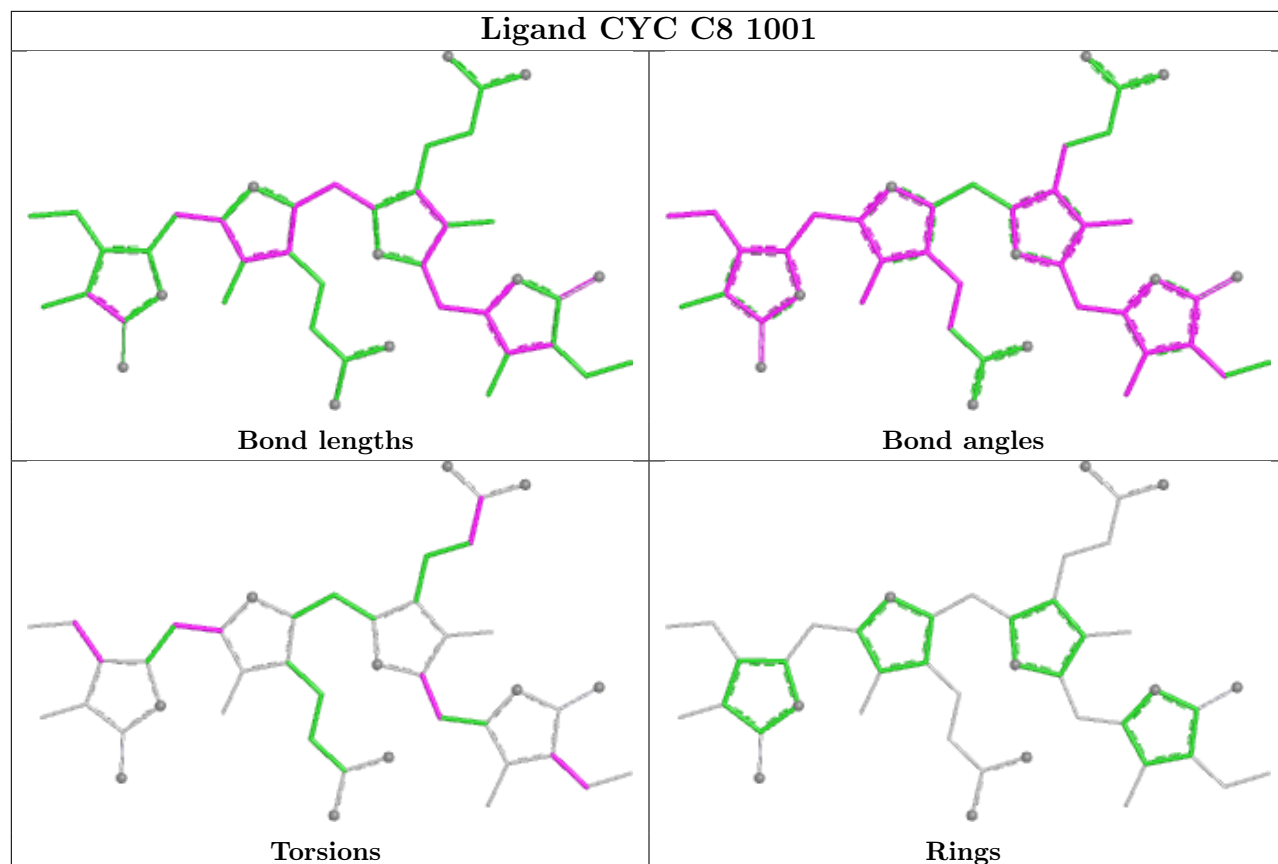
Ligand CYC Q1 202



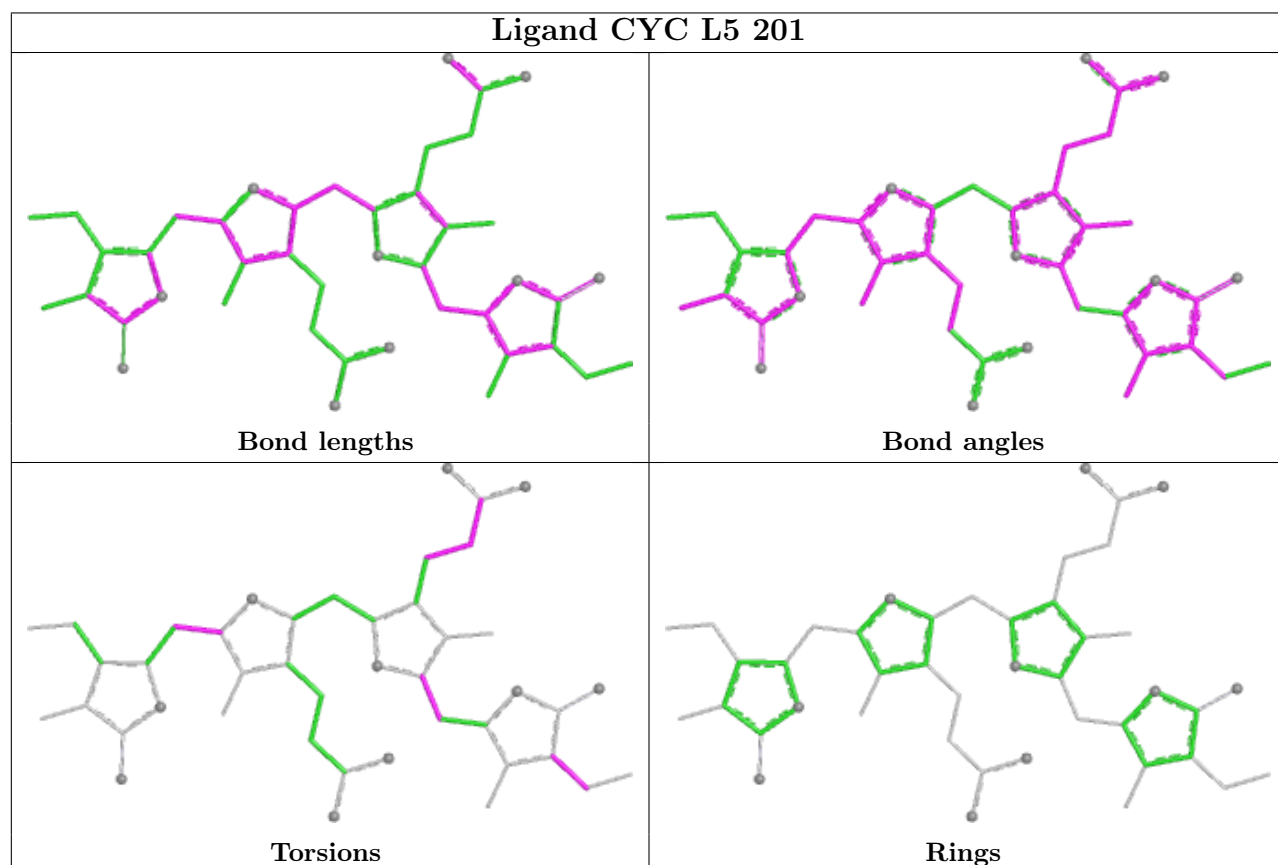
Ligand CYC XA 202



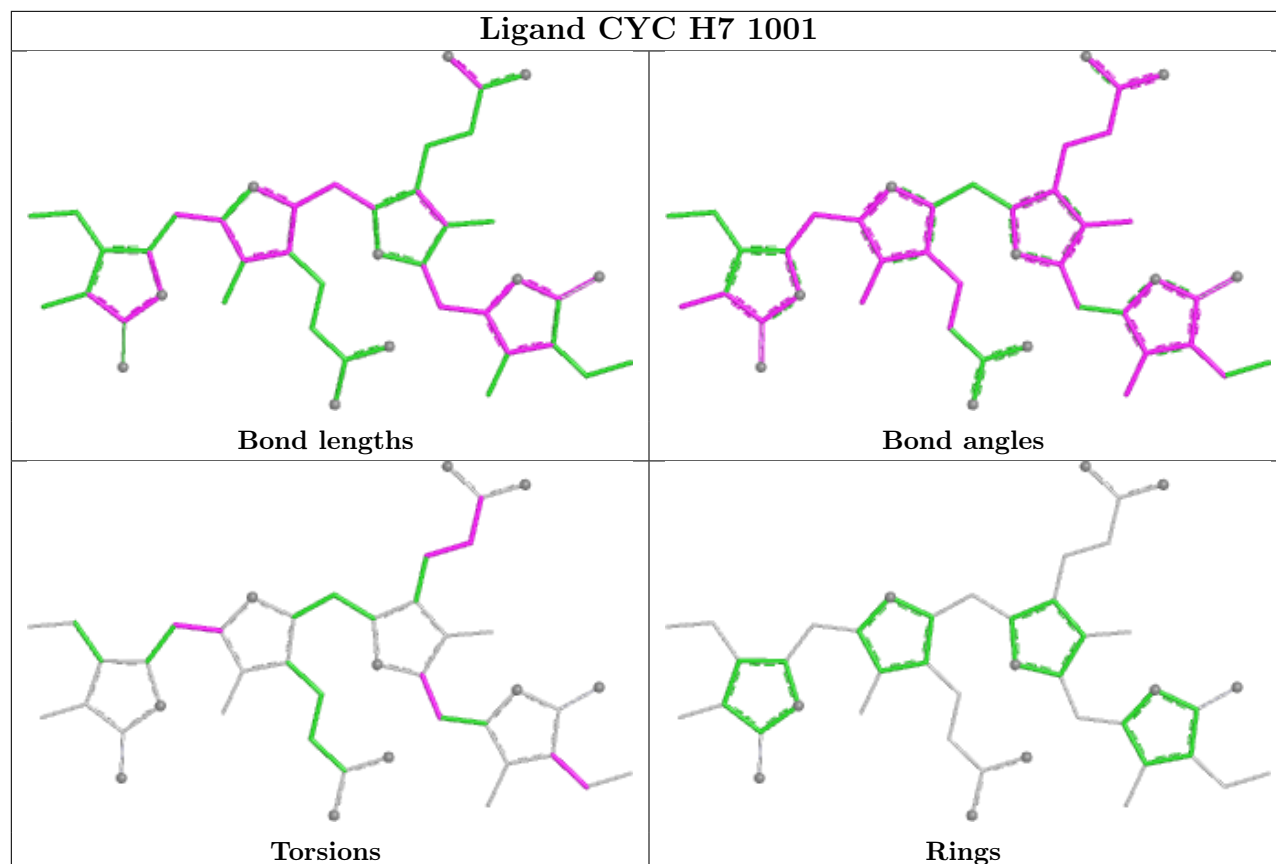
Ligand CYC C8 1001



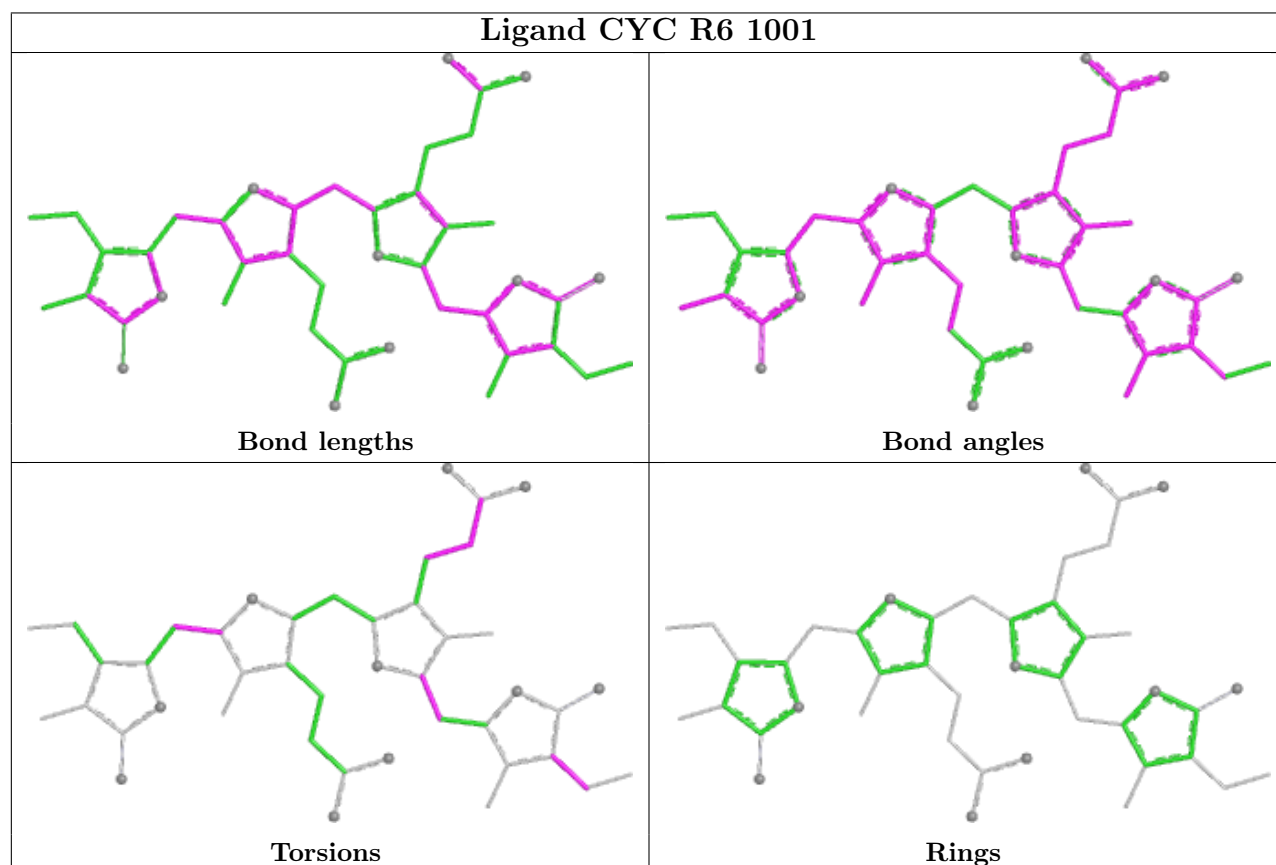
Ligand CYC L5 201



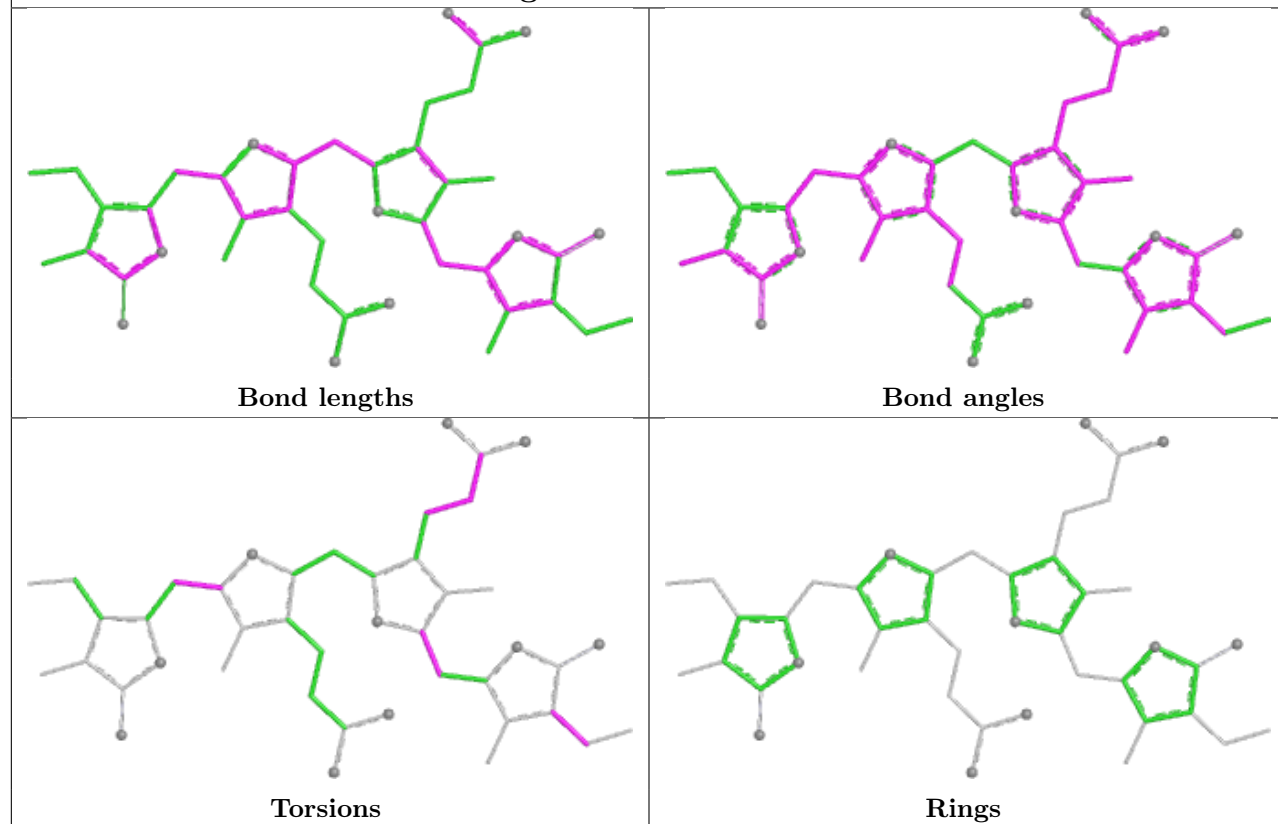
Ligand CYC H7 1001



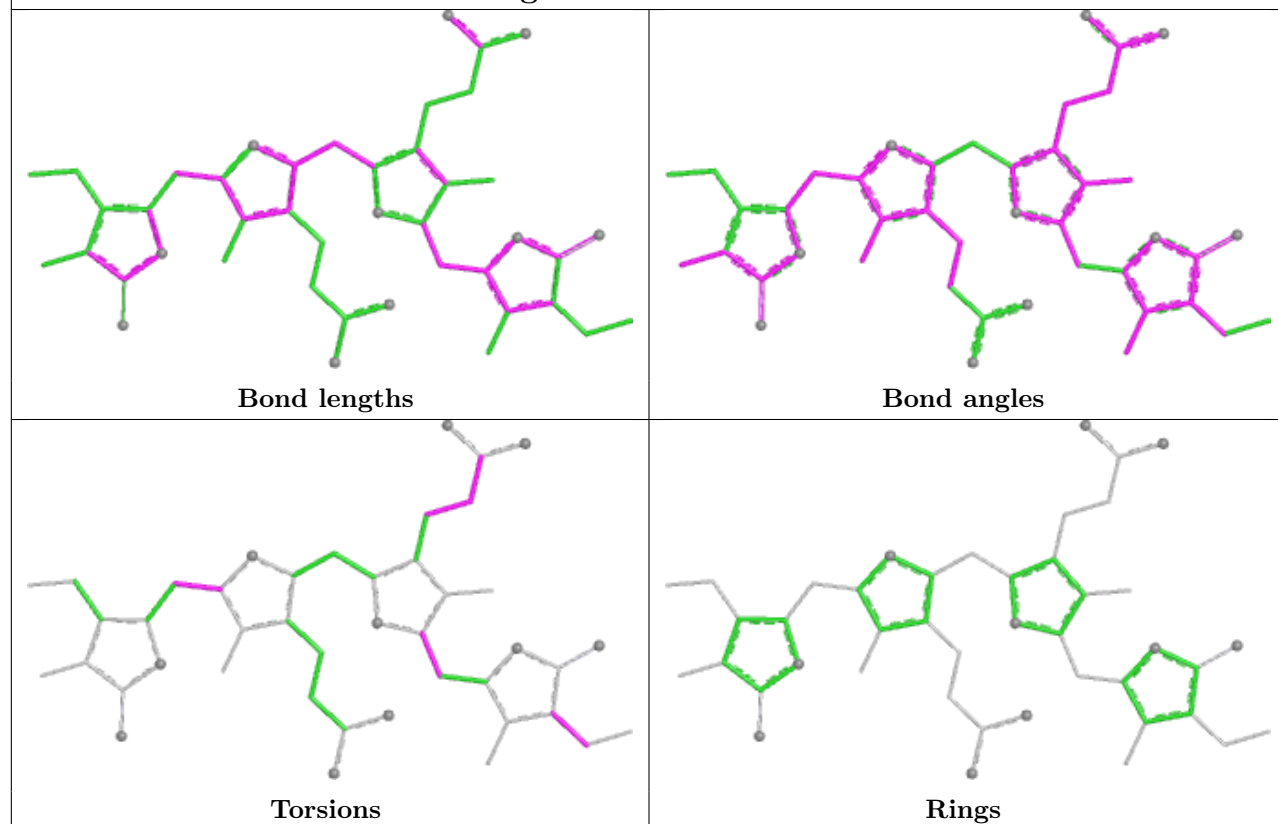
Ligand CYC R6 1001



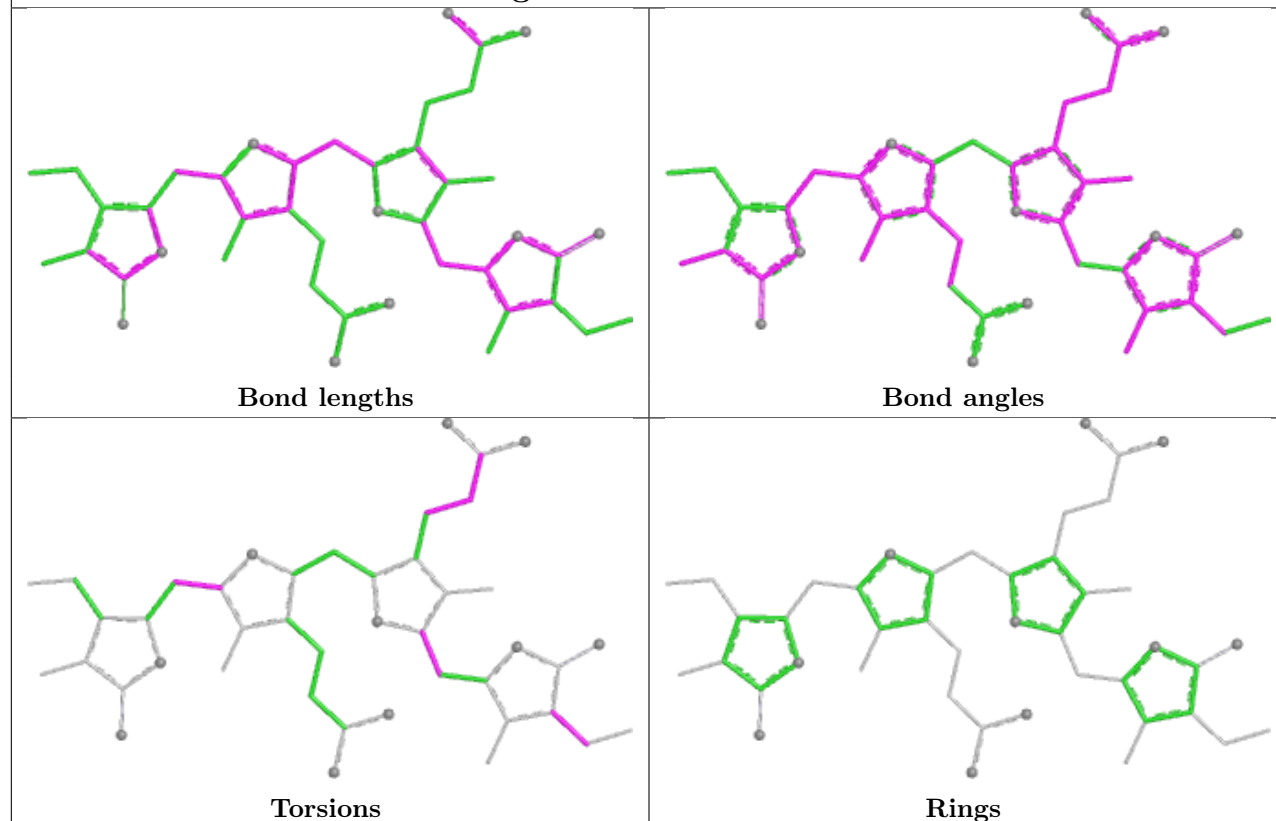
Ligand CYC N6 302



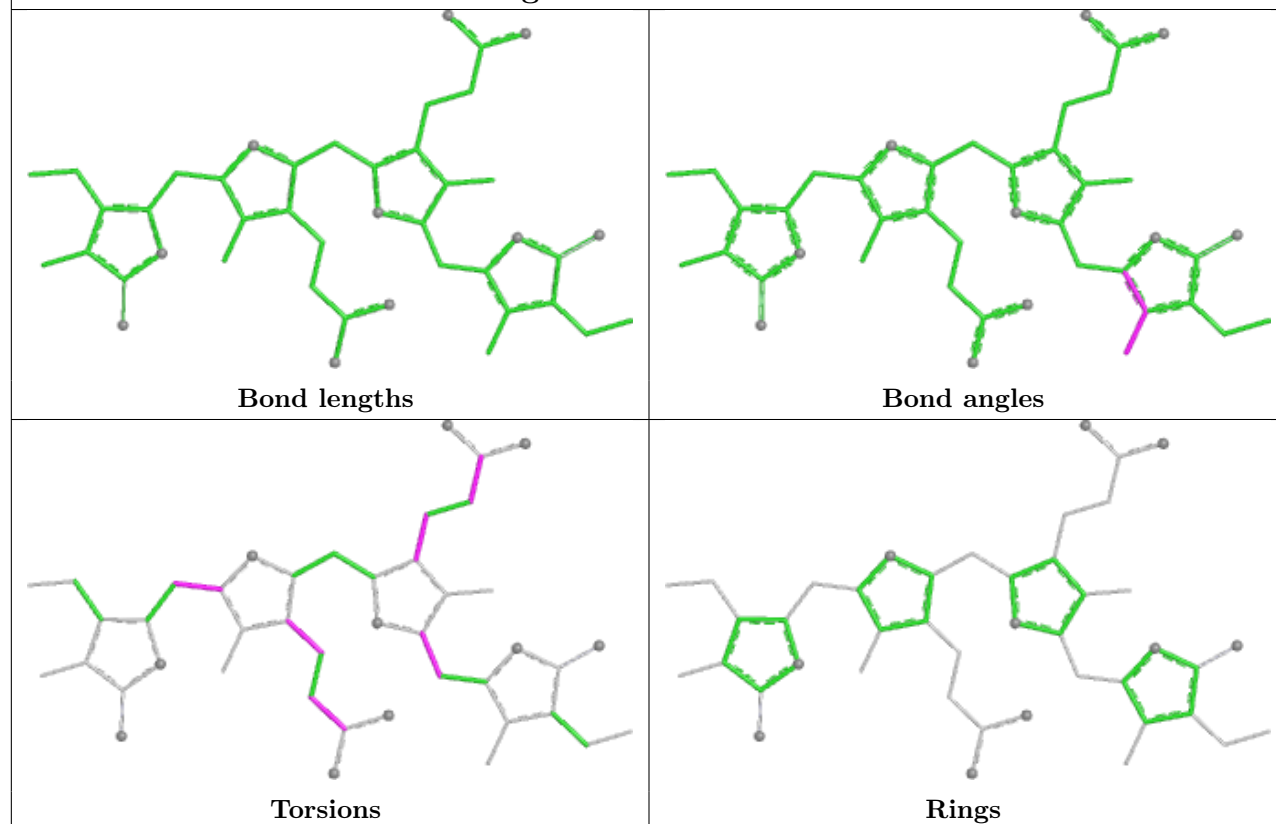
Ligand CYC U2 202



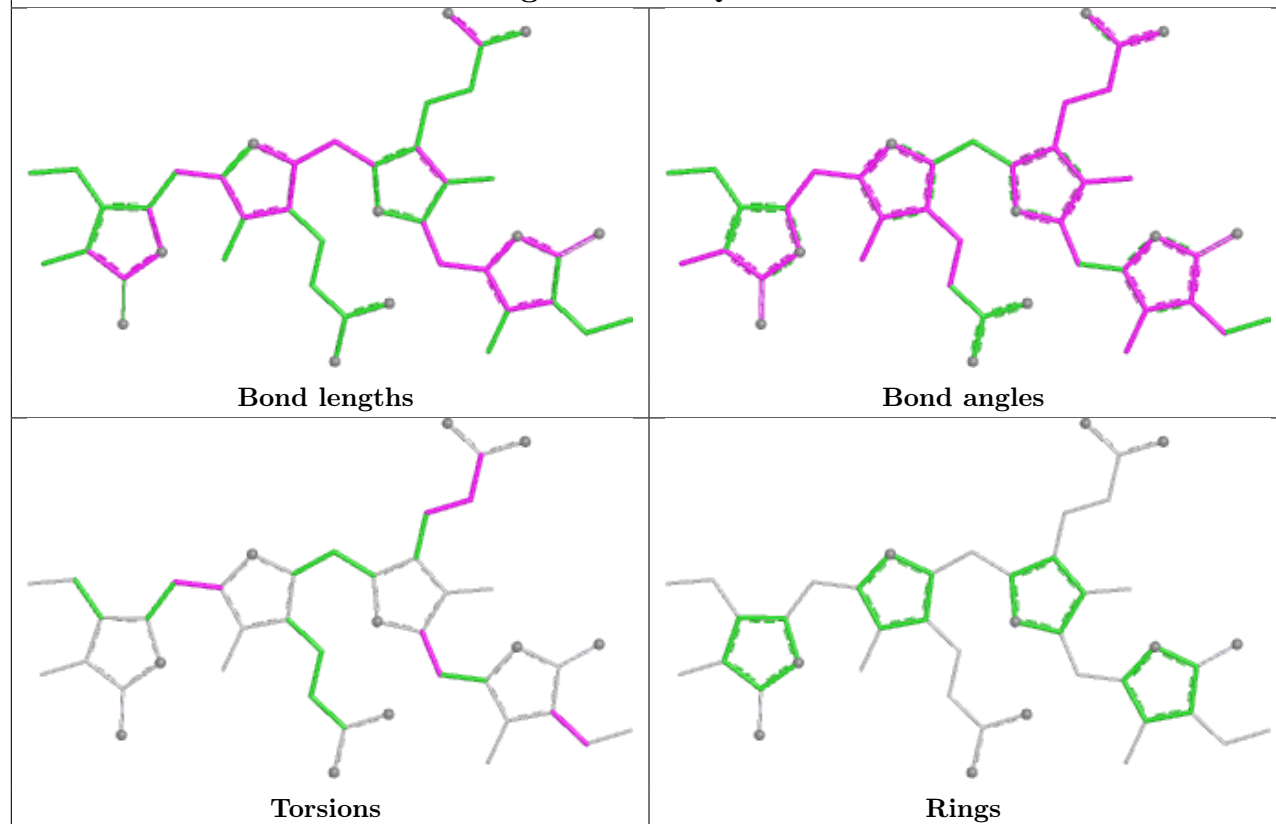
Ligand CYC B2 1001



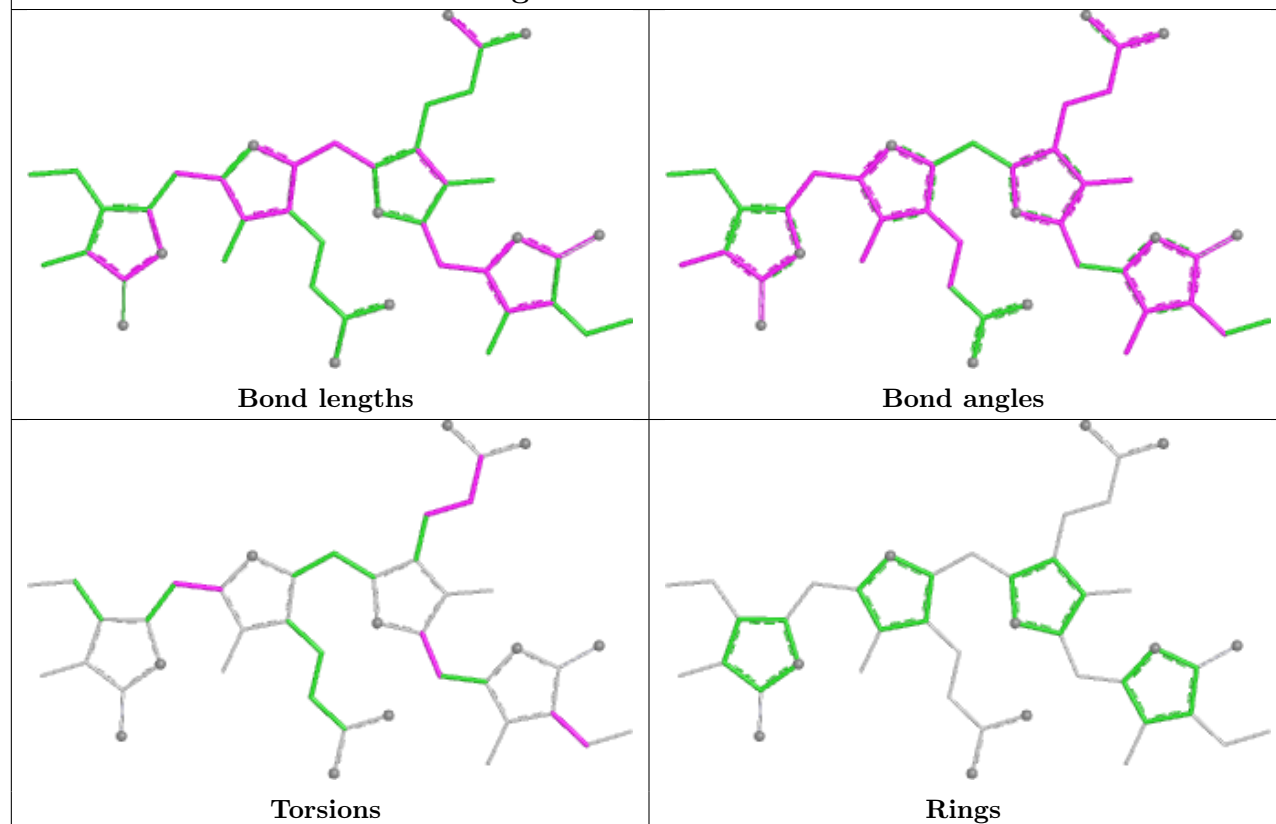
Ligand CYC T4 201



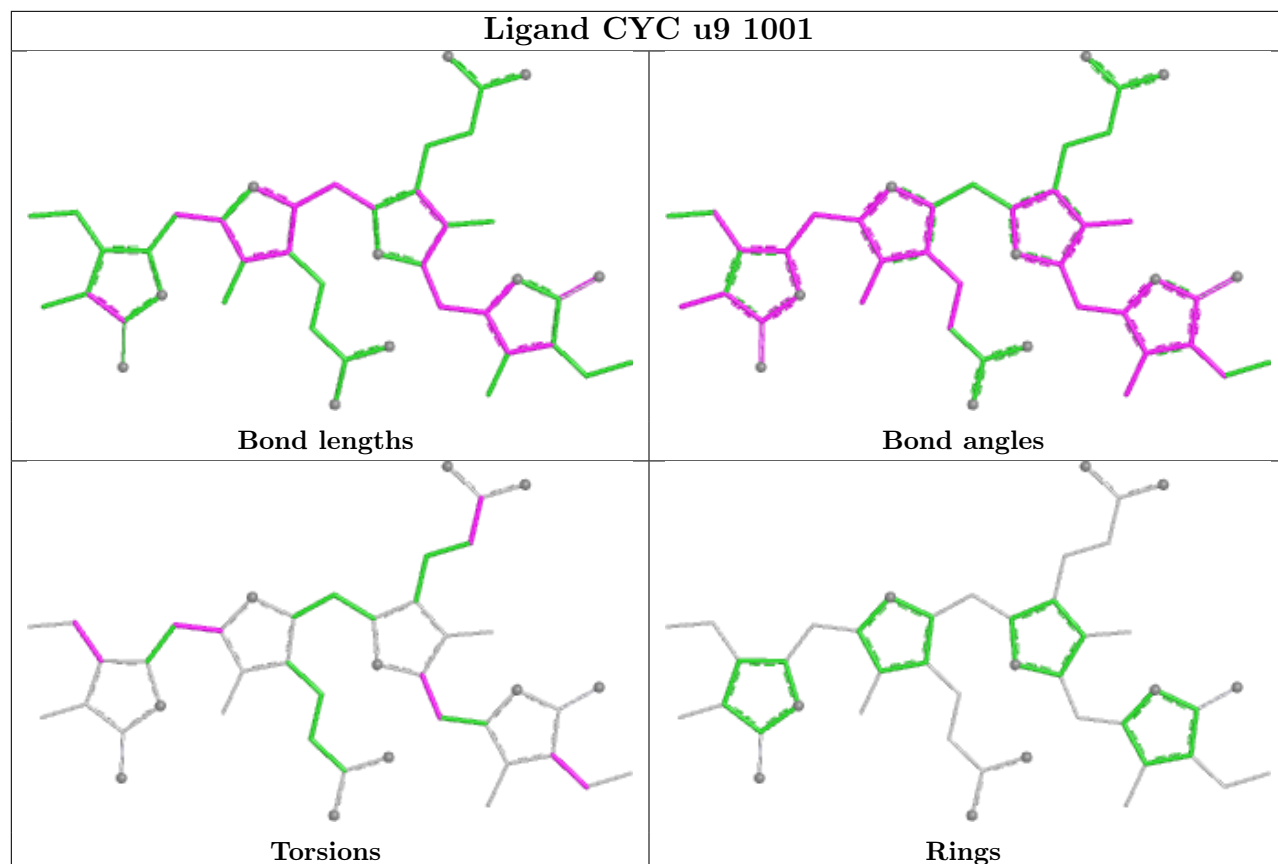
Ligand CYC Q2 201



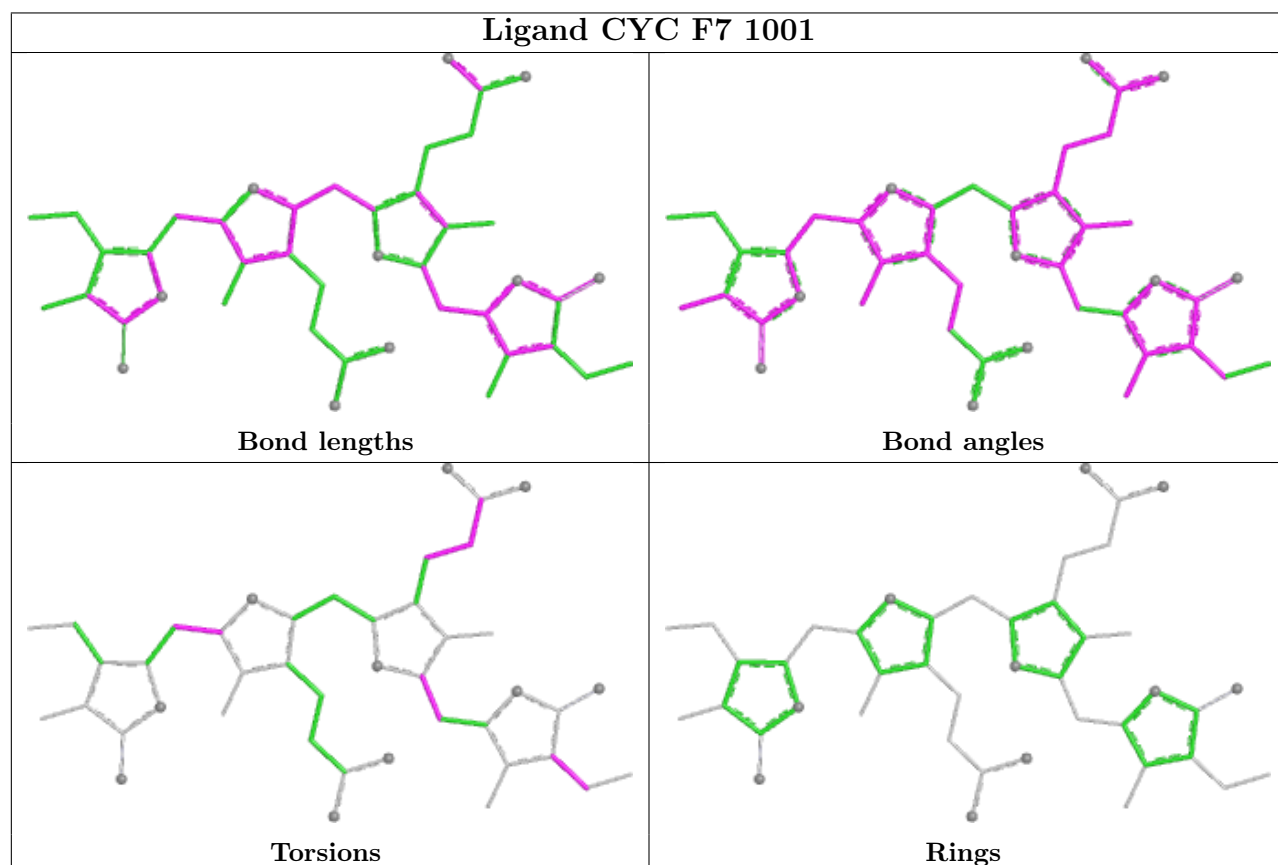
Ligand CYC R2 1001



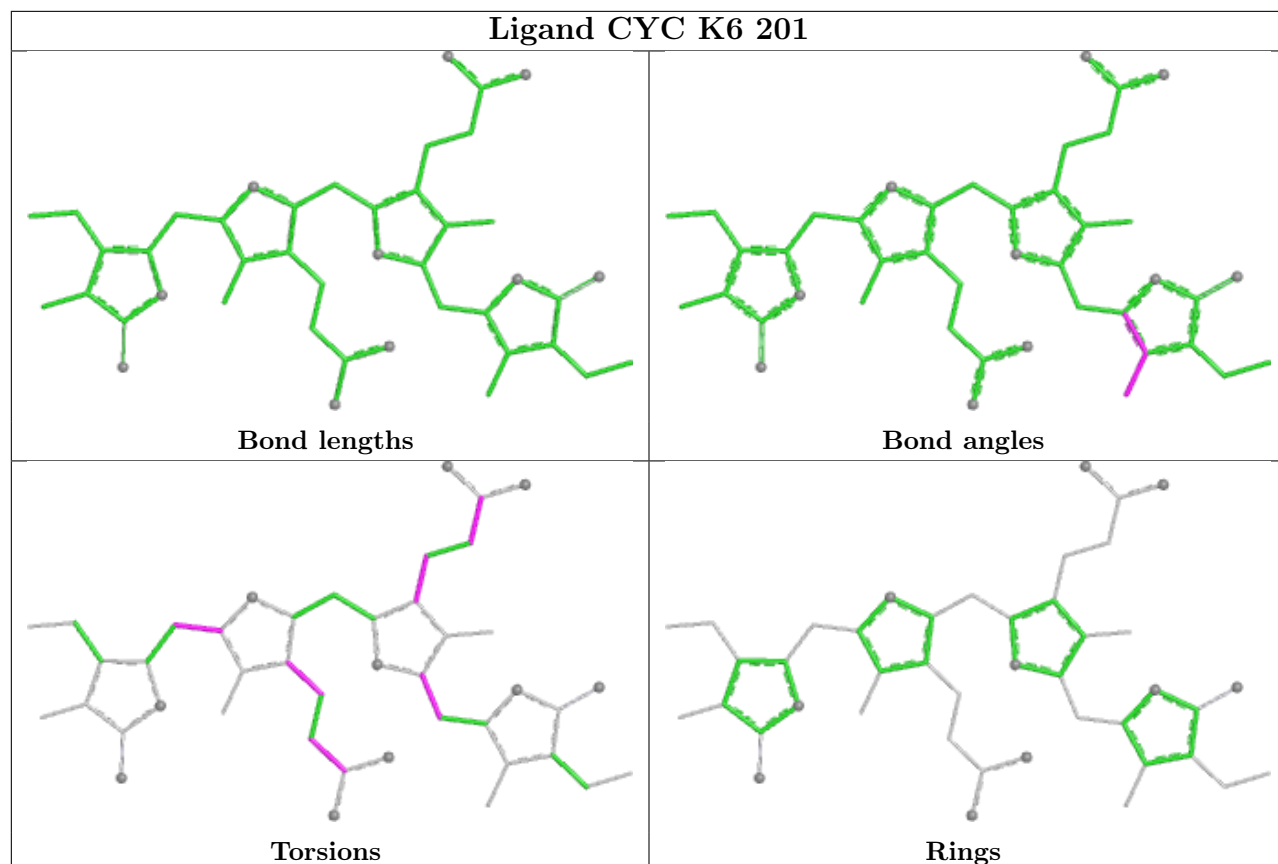
Ligand CYC u9 1001



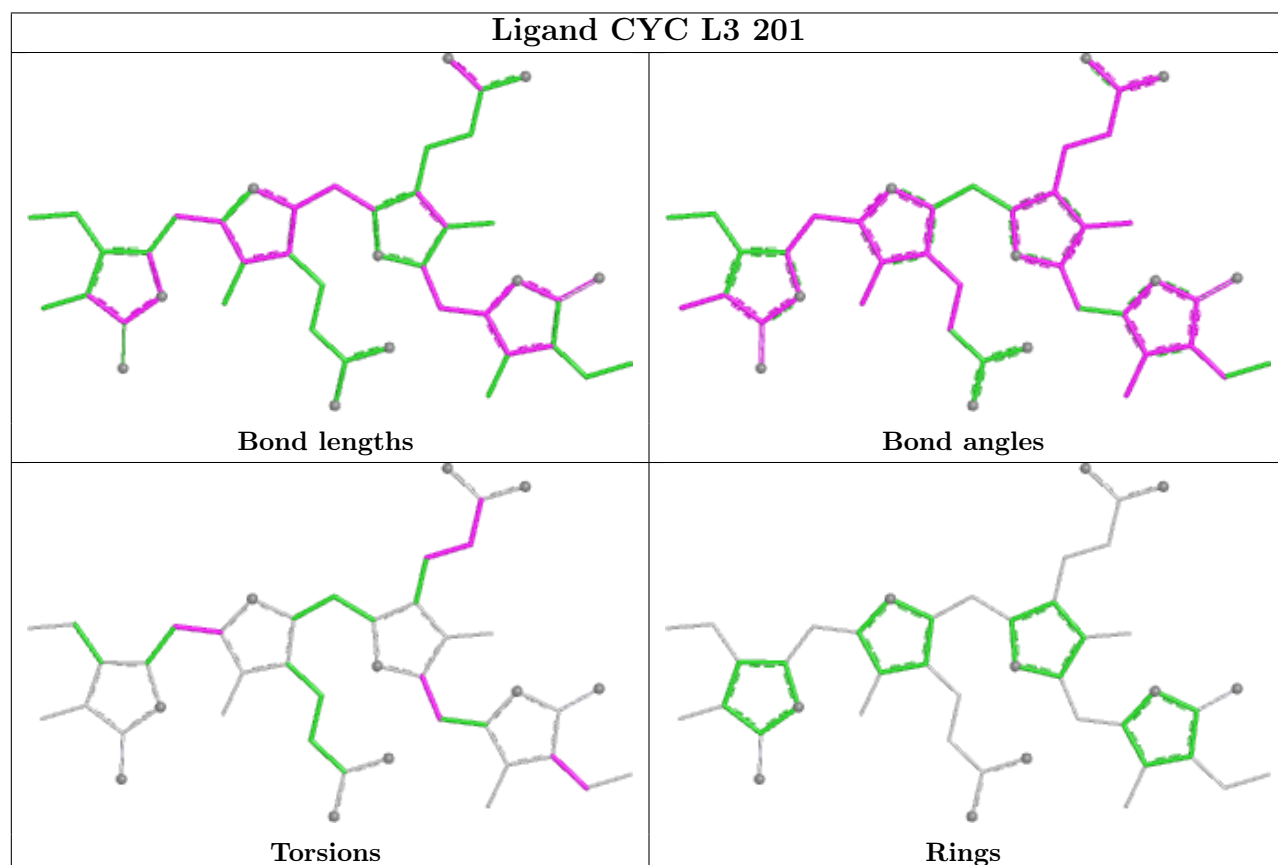
Ligand CYC F7 1001



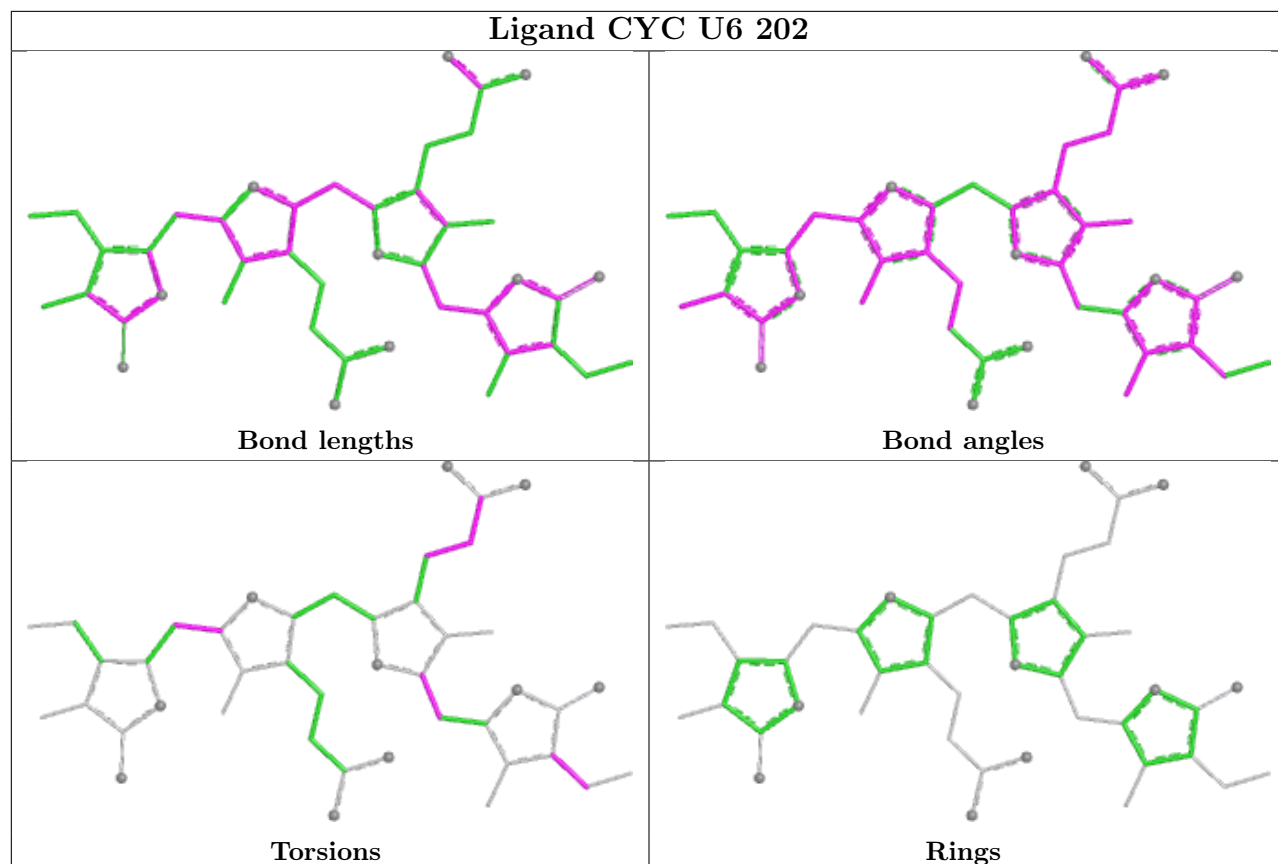
Ligand CYC K6 201



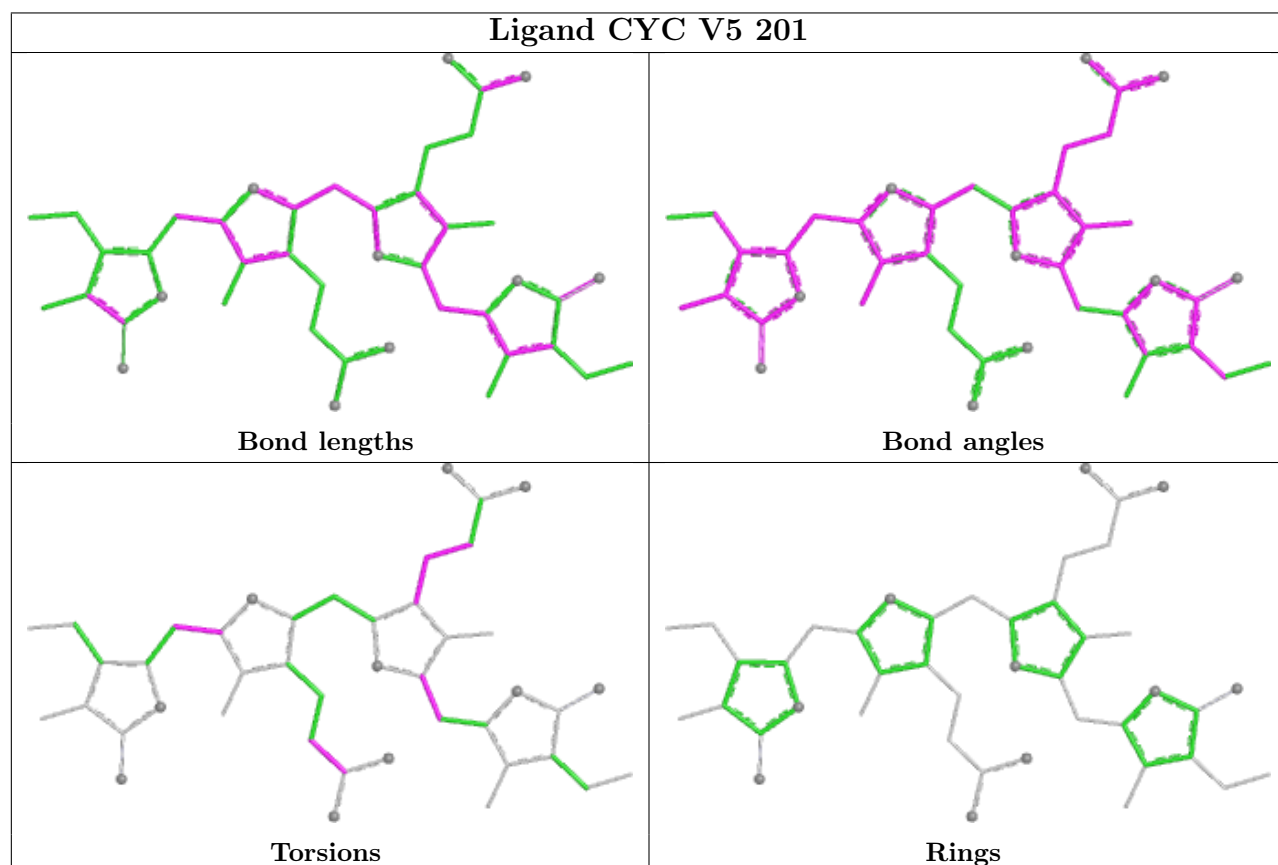
Ligand CYC L3 201

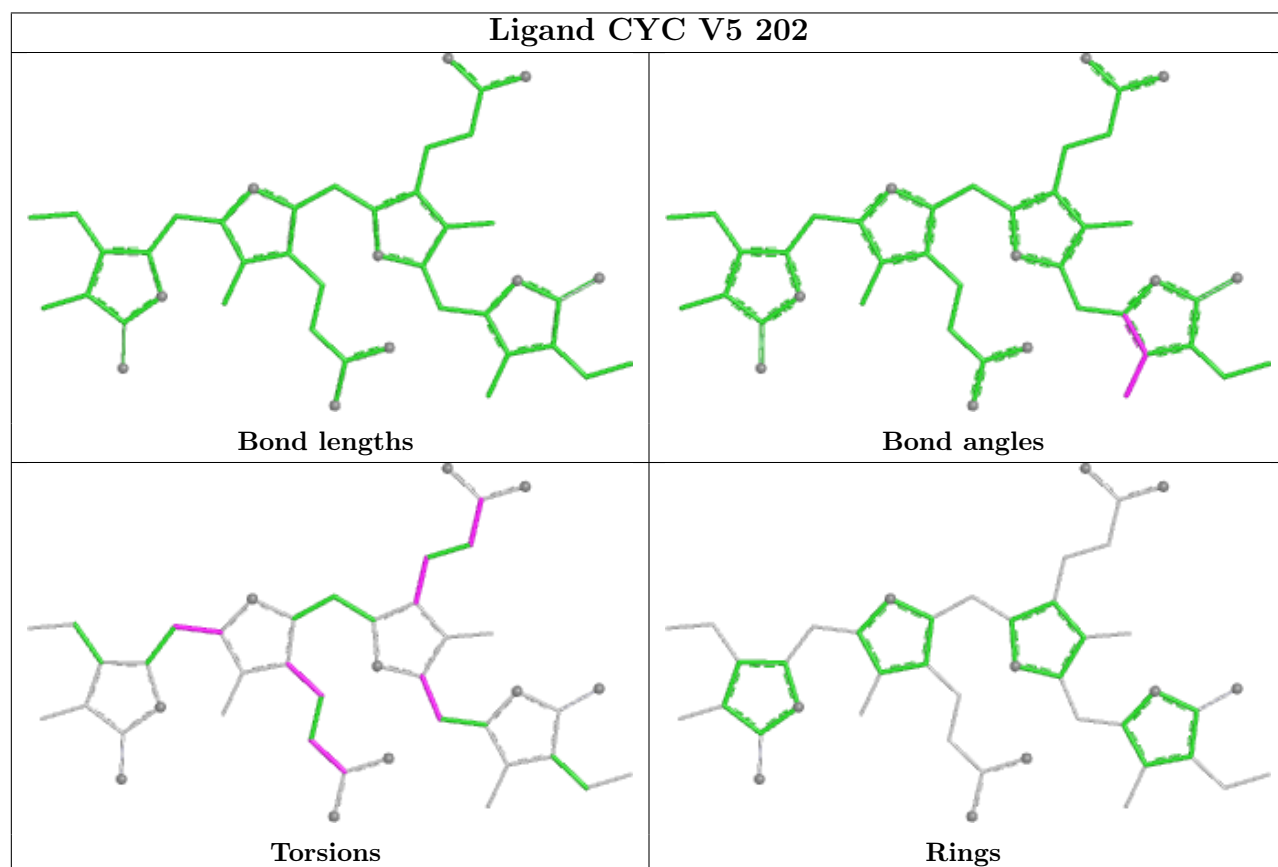
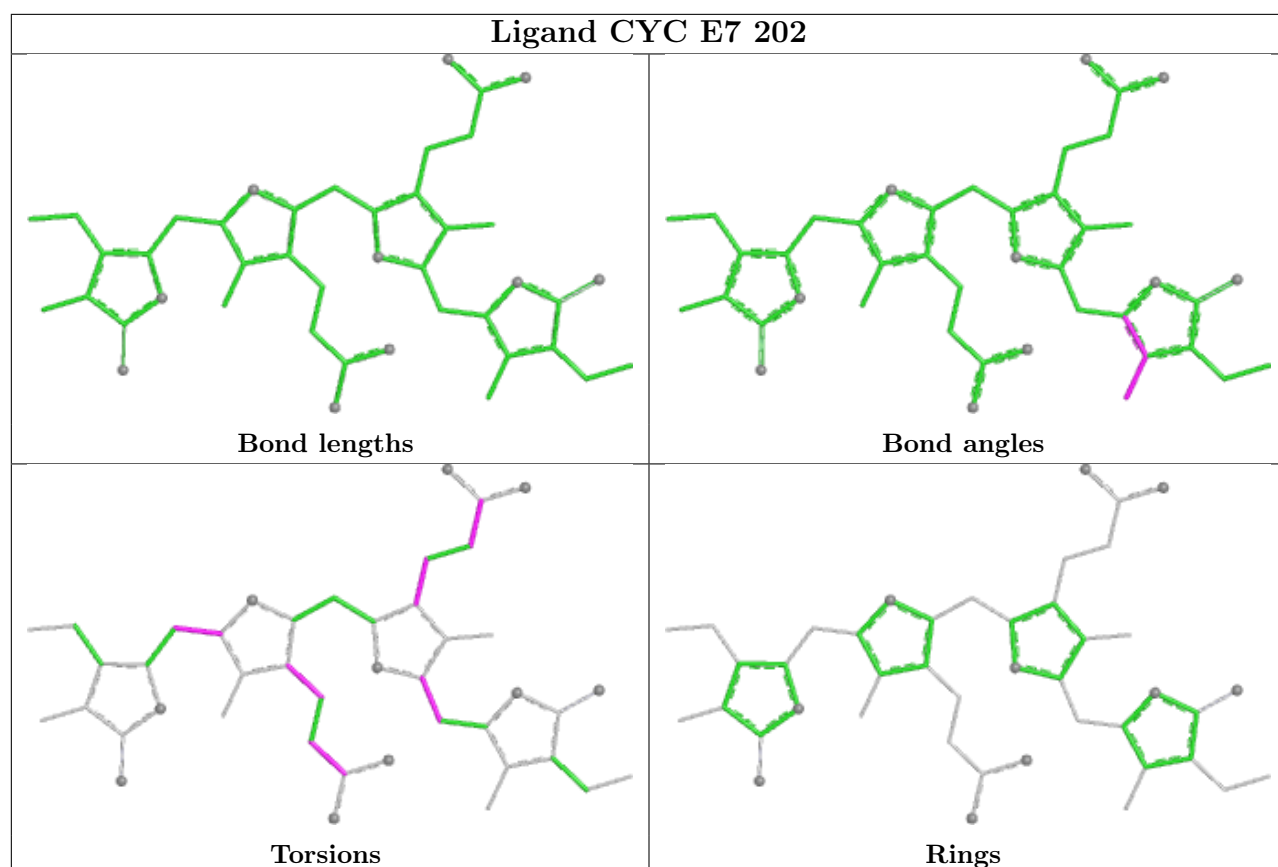


Ligand CYC U6 202



Ligand CYC V5 201





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.

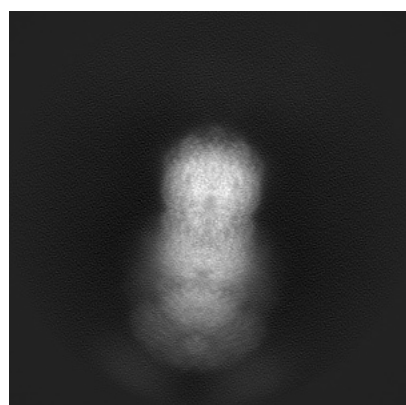
6 Map visualisation [i](#)

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.

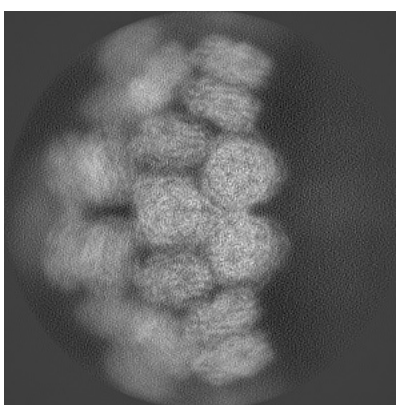
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

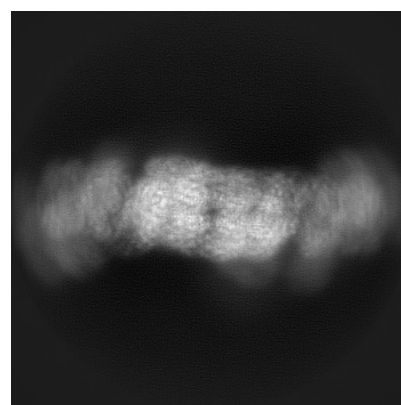
6.1.1 Primary map



X



Y

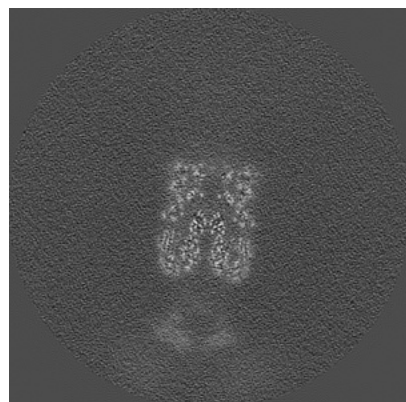


Z

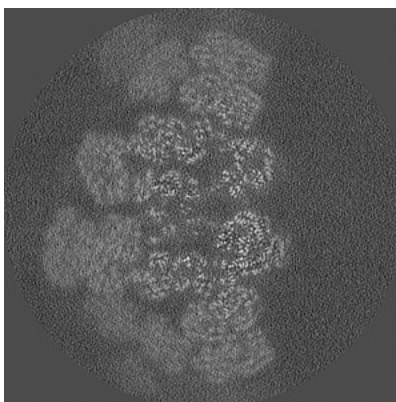
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

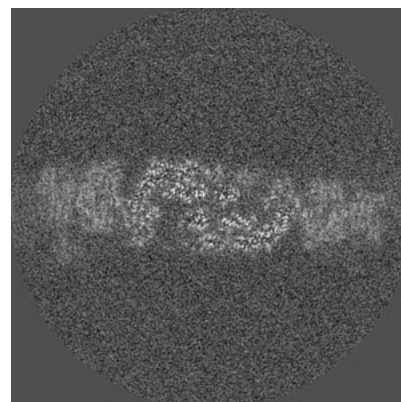
6.2.1 Primary map



X Index: 250



Y Index: 250

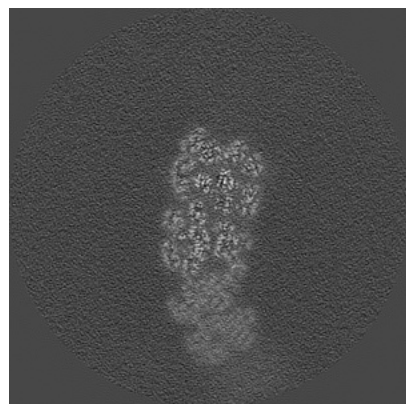


Z Index: 250

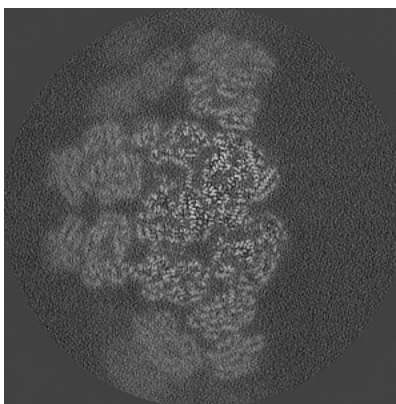
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

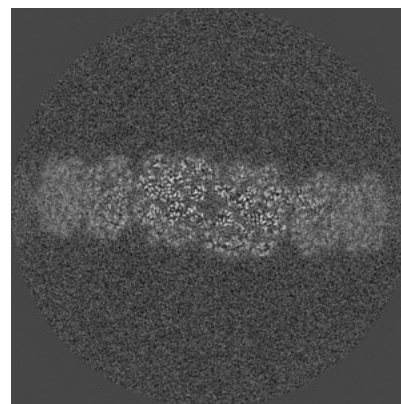
6.3.1 Primary map



X Index: 223



Y Index: 232

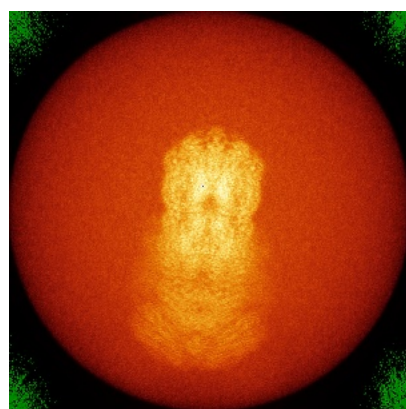


Z Index: 275

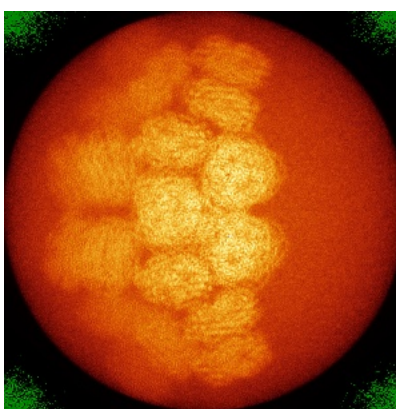
The images above show the largest variance slices of the map in three orthogonal directions.

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

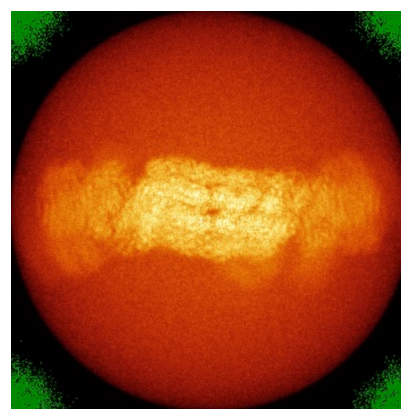
6.4.1 Primary map



X



Y

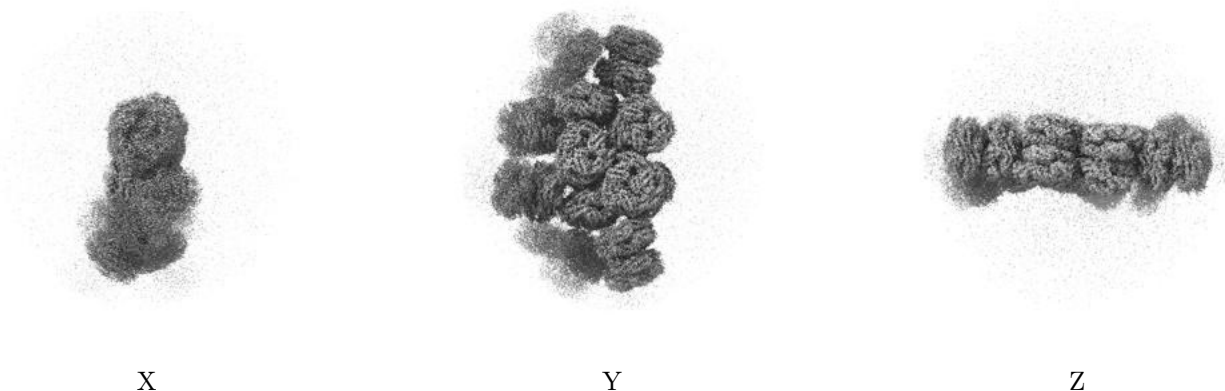


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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.

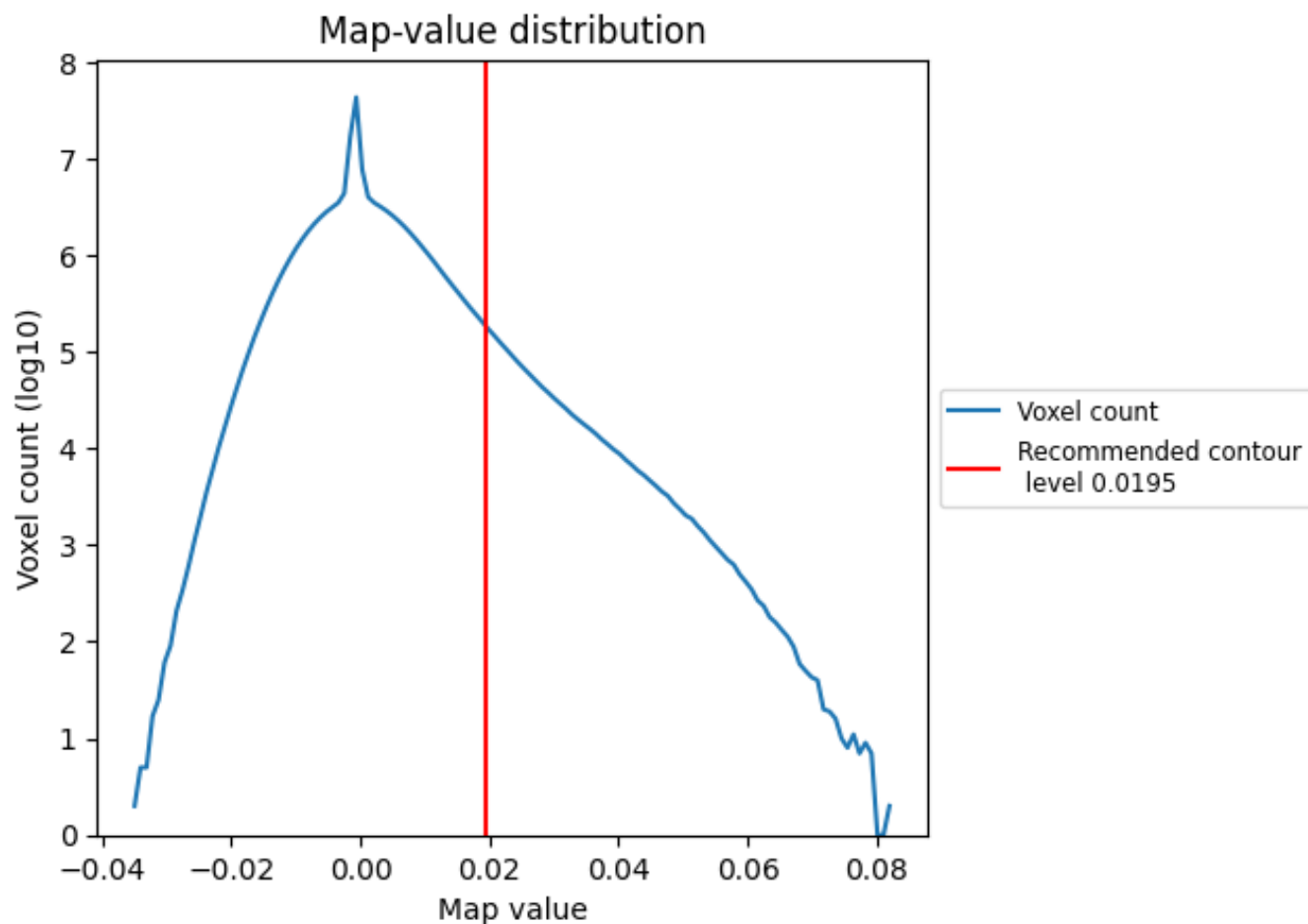
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

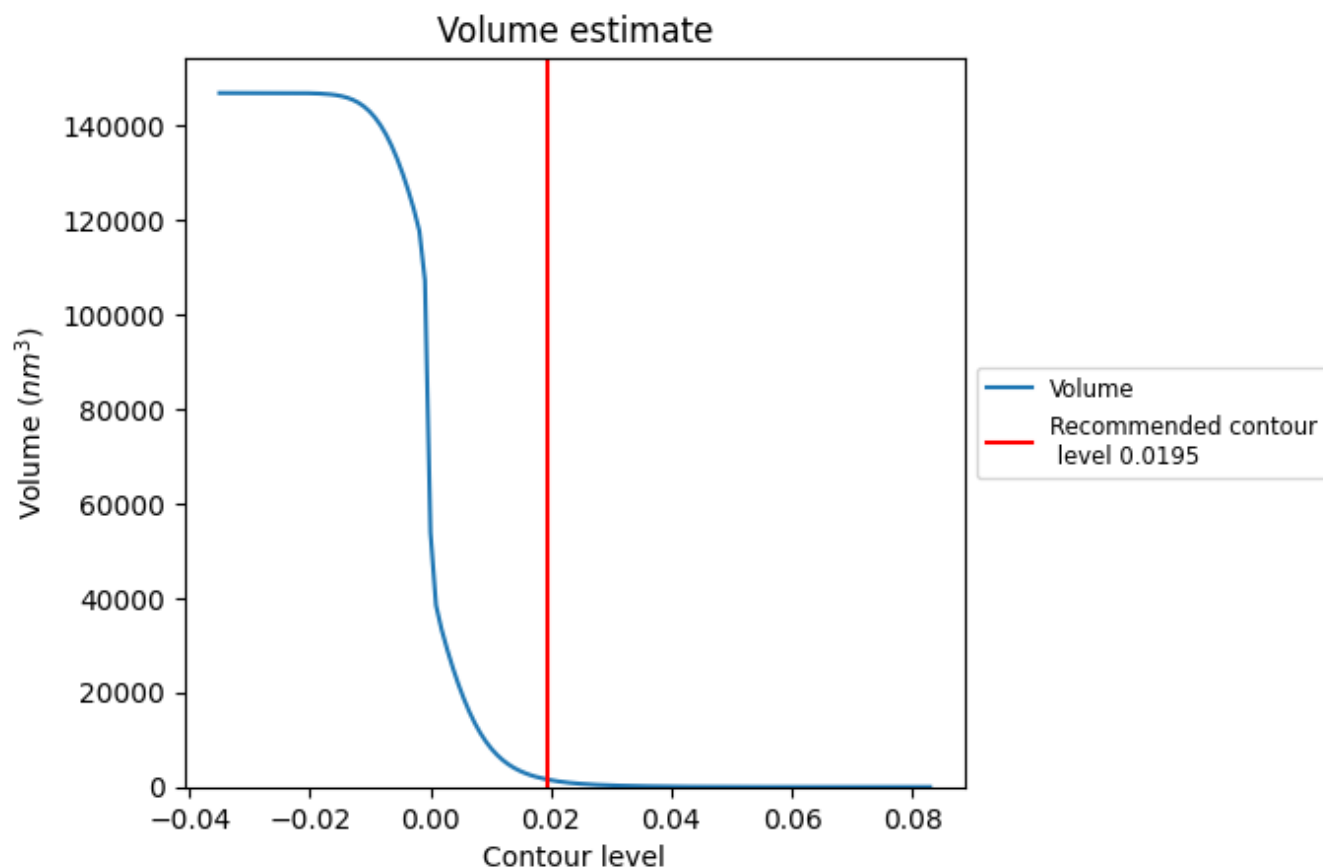
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

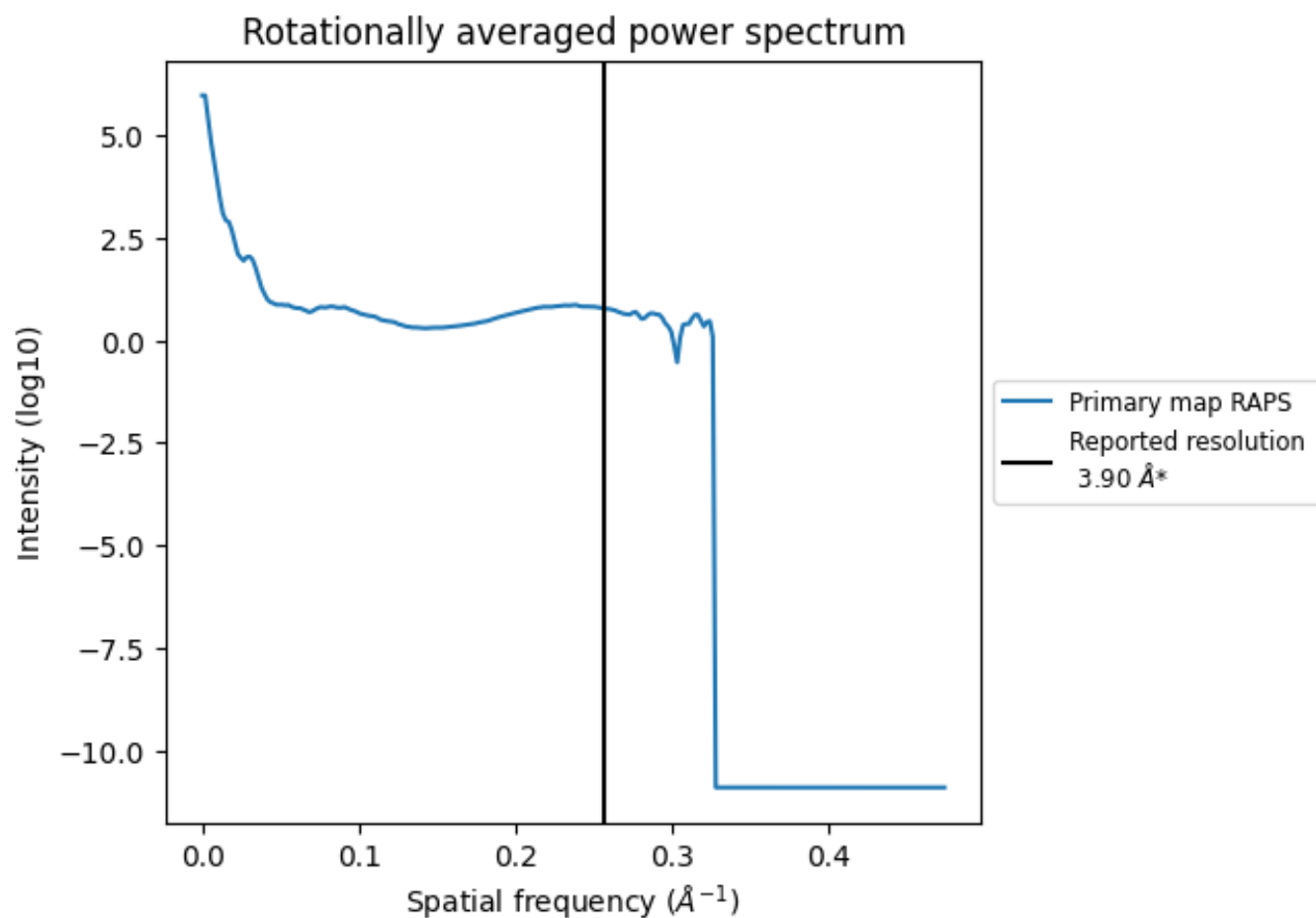
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

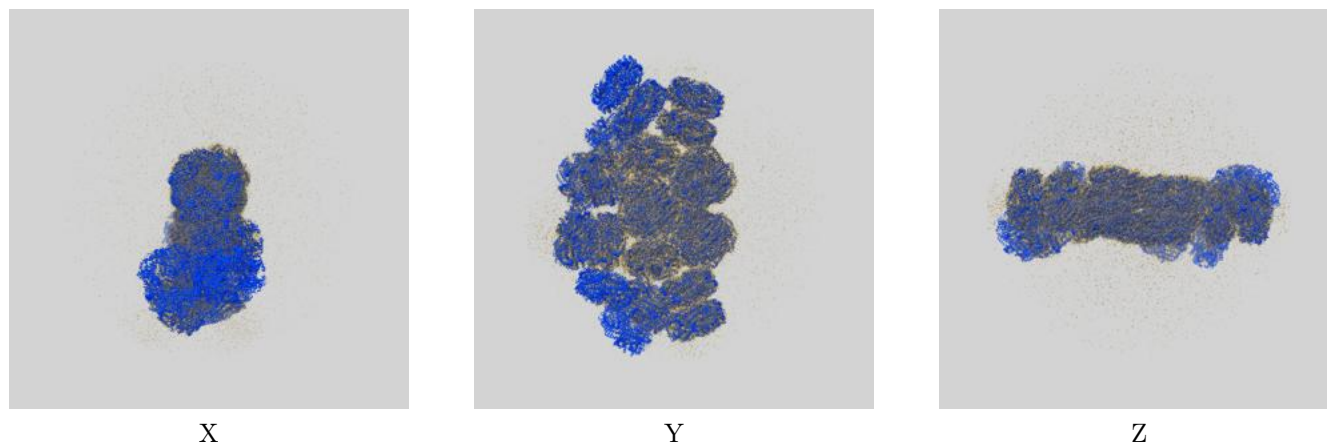
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

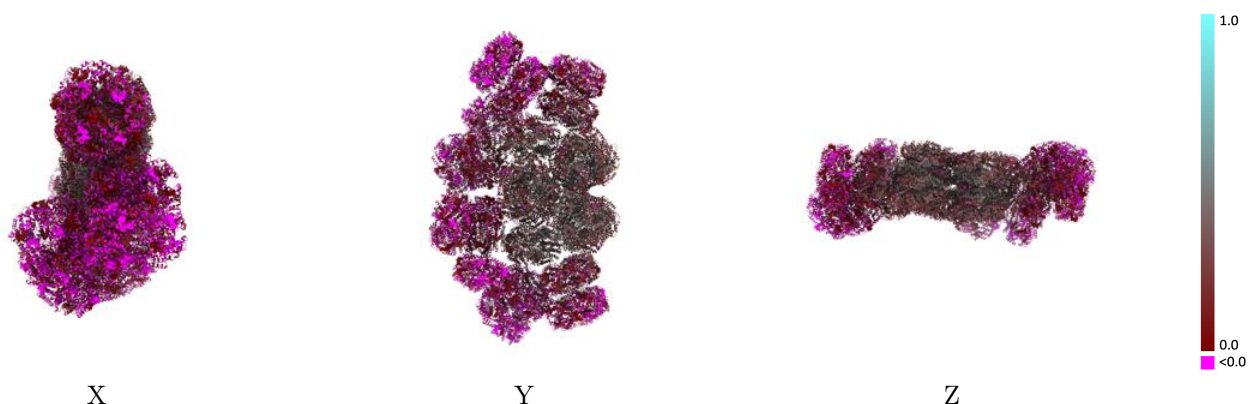
This section contains information regarding the fit between EMDB map EMD-31381 and PDB model 7EYD. Per-residue inclusion information can be found in section [3](#) on page [51](#).

9.1 Map-model overlay [i](#)



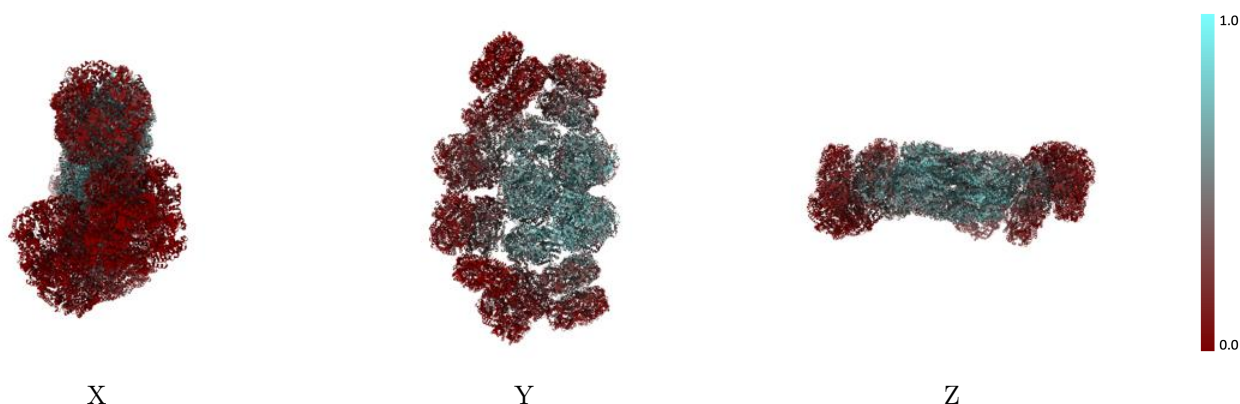
The images above show the 3D surface view of the map at the recommended contour level 0.0195 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



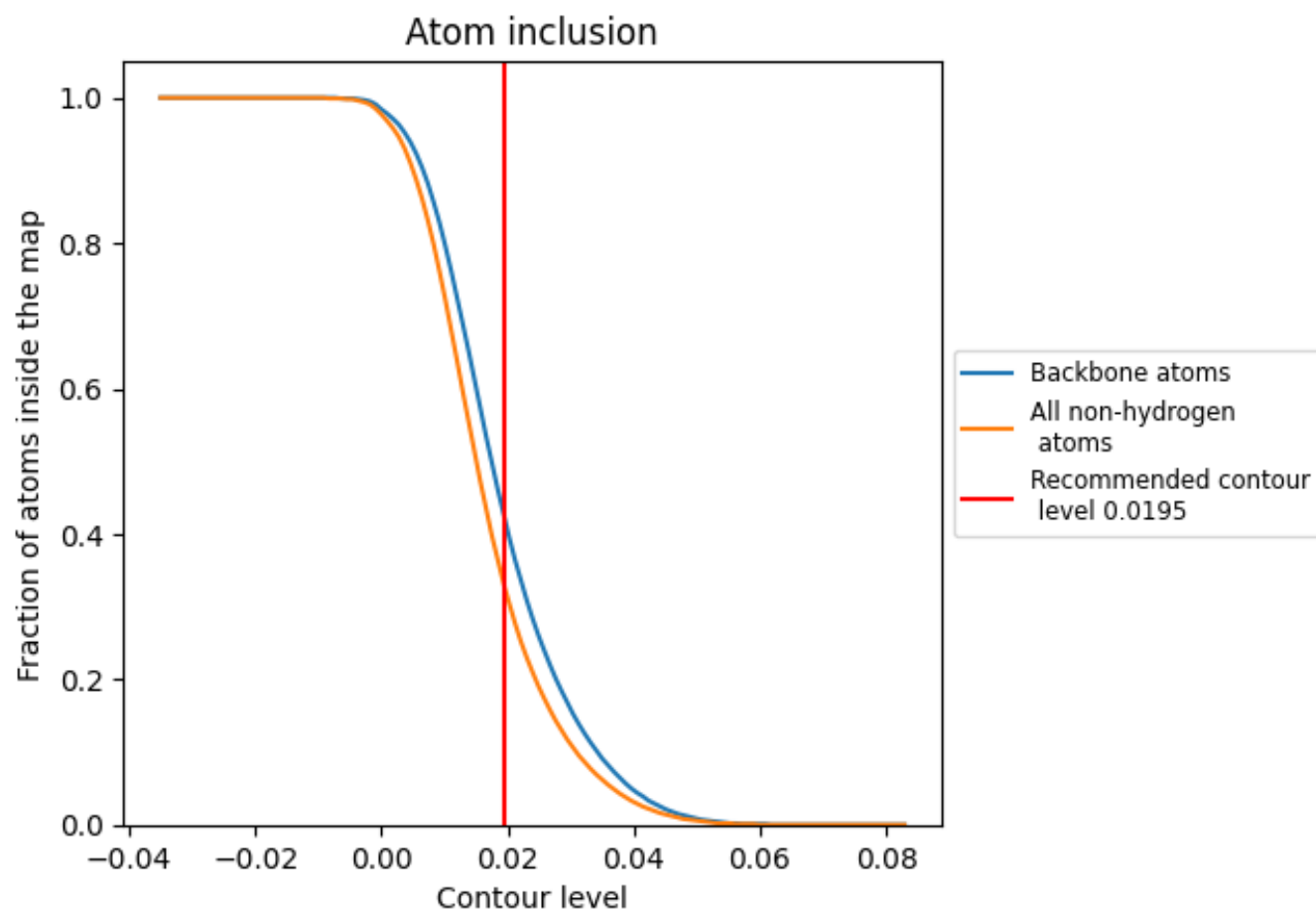
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	 0.3280	 0.1710
09	 0.7180	 0.4170
19	 0.7210	 0.4210
29	 0.5990	 0.3660
39	 0.6010	 0.3640
49	 0.6010	 0.3620
A1	 0.1480	 0.0850
A2	 0.5910	 0.2960
A3	 0.0480	 0.0430
A4	 0.1800	 0.0850
A5	 0.4510	 0.2120
A6	 0.6190	 0.3240
A7	 0.0650	 0.0430
A8	 0.5750	 0.3230
A9	 0.5390	 0.2580
AA	 0.4120	 0.1900
B1	 0.1310	 0.0820
B2	 0.5080	 0.2620
B3	 0.0170	 0.0290
B4	 0.1700	 0.1020
B5	 0.3090	 0.1060
B6	 0.5320	 0.2630
B7	 0.0270	 0.0450
B8	 0.6260	 0.3170
B9	 0.5420	 0.2620
BA	 0.2990	 0.0940
C1	 0.0770	 0.0520
C2	 0.4460	 0.2230
C3	 0.0430	 0.0570
C4	 0.1150	 0.0860
C5	 0.2910	 0.1280
C6	 0.4670	 0.2260
C7	 0.0430	 0.0560
C8	 0.7020	 0.3800
C9	 0.5680	 0.2990



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
CA	 0.2640	 0.1300
D1	 0.0680	 0.0370
D2	 0.2690	 0.1200
D3	 0.0360	 0.0310
D4	 0.1000	 0.0510
D5	 0.2580	 0.1100
D6	 0.3130	 0.1240
D7	 0.0540	 0.0580
D8	 0.6550	 0.3540
D9	 0.5650	 0.3090
DA	 0.2370	 0.1320
E1	 0.0710	 0.0500
E2	 0.2970	 0.1490
E3	 0.0160	 0.0020
E4	 0.1130	 0.0690
E5	 0.3040	 0.1270
E6	 0.3580	 0.1630
E7	 0.0290	 -0.0060
E8	 0.5570	 0.2740
E9	 0.6140	 0.3120
EA	 0.2730	 0.1400
F1	 0.0590	 0.0330
F2	 0.3860	 0.1720
F3	 0.0110	 0.0110
F4	 0.0700	 0.0440
F5	 0.3520	 0.1490
F6	 0.4090	 0.1890
F7	 0.0130	 0.0300
F8	 0.5950	 0.3160
F9	 0.5860	 0.2890
FA	 0.3200	 0.1400
G1	 0.0920	 0.0680
G2	 0.4580	 0.2460
G3	 0.0110	 0.0480
G4	 0.1380	 0.0990
G5	 0.4100	 0.1700
G6	 0.4930	 0.2600
G7	 0.0170	 0.0410
G8	 0.6280	 0.3440
G9	 0.7450	 0.4030
GA	 0.3710	 0.1660
H1	 0.0820	 0.0300

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
H2	 0.3170	 0.1240
H3	 0.0120	 0.0170
H4	 0.1080	 0.0620
H5	 0.2640	 0.1390
H6	 0.3250	 0.1270
H7	 0.0130	 -0.0010
H8	 0.5570	 0.2990
H9	 0.7640	 0.4470
HA	 0.2570	 0.1320
I1	 0.0600	 0.0160
I2	 0.2560	 0.0900
I3	 0.0210	 0.0390
I4	 0.0840	 0.0270
I5	 0.2590	 0.1110
I6	 0.3020	 0.1360
I7	 0.0280	 0.0460
I8	 0.6040	 0.3360
I9	 0.7270	 0.3750
IA	 0.2510	 0.0920
J1	 0.0560	 0.0470
J2	 0.3290	 0.1580
J3	 0.0280	 0.0130
J4	 0.0810	 0.0260
J5	 0.2730	 0.1470
J6	 0.3480	 0.1670
J7	 0.0410	 0.0470
J8	 0.7190	 0.3850
J9	 0.7260	 0.4090
JA	 0.2400	 0.1120
K1	 0.0820	 0.0480
K2	 0.3670	 0.1610
K3	 0.0130	 0.0040
K4	 0.0950	 0.0270
K5	 0.2260	 0.0730
K6	 0.4050	 0.1650
K7	 0.0250	 0.0160
K8	 0.6670	 0.3480
K9	 0.6520	 0.3410
KA	 0.2200	 0.0840
L1	 0.0950	 0.0680
L2	 0.4080	 0.2010
L3	 0.0110	 0.0190

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
L4	 0.1060	 0.0650
L5	 0.3310	 0.1370
L6	 0.4410	 0.2000
L7	 0.0110	 0.0160
L8	 0.5530	 0.2600
L9	 0.7310	 0.3890
LA	 0.2640	 0.0790
M1	 0.0660	 0.0260
M2	 0.3350	 0.1500
M3	 0.0050	 0.0260
M4	 0.0740	 0.0230
M5	 0.3130	 0.1240
M6	 0.3730	 0.1670
M7	 0.0120	 0.0300
M8	 0.5920	 0.3240
M9	 0.6750	 0.3630
MA	 0.2760	 0.0890
N1	 0.0260	 0.0130
N2	 0.2920	 0.1380
N3	 0.0210	 0.0050
N4	 0.0430	 0.0210
N5	 0.2170	 0.0930
N6	 0.3290	 0.1530
N7	 0.0600	 0.0210
N8	 0.6320	 0.3730
N9	 0.7160	 0.3840
NA	 0.1720	 0.0660
O1	 0.0030	 -0.0190
O2	 0.1310	 0.0460
O4	 0.0080	 0.0080
O5	 0.1230	 0.0590
O6	 0.1340	 0.0550
O8	 0.5320	 0.2600
O9	 0.7490	 0.4320
OA	 0.0950	 0.0440
P1	 0.0120	 0.0400
P2	 0.1630	 0.0820
P4	 0.0160	 0.0210
P5	 0.1390	 0.0580
P6	 0.1940	 0.0750
P8	 0.5510	 0.2850
P9	 0.7180	 0.4090

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
PA	 0.1300	 0.0600
Q1	 0.0050	 0.0140
Q2	 0.1640	 0.0570
Q4	 0.0040	 0.0120
Q5	 0.1180	 0.0710
Q6	 0.2160	 0.0740
Q8	 0.5900	 0.3140
Q9	 0.7460	 0.4380
QA	 0.0980	 0.0480
R1	 0.0120	 0.0010
R2	 0.2100	 0.1000
R4	 0.0130	 0.0070
R5	 0.1530	 0.0710
R6	 0.2600	 0.1410
R8	 0.5500	 0.2960
R9	 0.4620	 0.2610
RA	 0.1210	 0.0550
S1	 0.0060	 0.0200
S2	 0.1730	 0.0780
S4	 0.0080	 0.0250
S5	 0.1190	 0.0450
S6	 0.1720	 0.0800
S8	 0.5960	 0.2850
S9	 0.4950	 0.2790
SA	 0.0900	 0.0200
T1	 0.0110	 0.0090
T2	 0.2290	 0.1000
T4	 0.0110	 0.0210
T5	 0.1450	 0.0750
T6	 0.2260	 0.1020
T8	 0.5990	 0.2940
T9	 0.5040	 0.2570
TA	 0.1260	 0.0810
U1	 0.0050	 0.0090
U2	 0.1370	 0.0630
U4	 0.0040	 -0.0010
U5	 0.0990	 0.0550
U6	 0.1330	 0.0540
U8	 0.5800	 0.3130
U9	 0.5190	 0.2760
UA	 0.0690	 0.0180
V1	 0.0020	 -0.0020

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
V2	 0.1030	 0.0470
V4	 0.0020	 -0.0070
V5	 0.0860	 0.0150
V6	 0.1160	 0.0290
V8	 0.4040	 0.2150
V9	 0.5600	 0.3370
VA	 0.0650	 0.0370
W1	 0.0020	 0.0100
W2	 0.1000	 0.0610
W4	 0.0020	 -0.0350
W5	 0.0650	 0.0490
W6	 0.1260	 0.0430
W8	 0.4810	 0.2280
W9	 0.5870	 0.3180
WA	 0.0650	 0.0450
X1	 0.0040	 -0.0060
X2	 0.1050	 0.0670
X4	 0.0030	 -0.0050
X5	 0.0830	 0.0560
X6	 0.1100	 0.0550
X8	 0.5980	 0.2810
X9	 0.7000	 0.3700
XA	 0.0550	 0.0260
Y1	 0.0040	 0.0040
Y2	 0.1260	 0.0700
Y4	 0.0050	 0.0160
Y5	 0.1030	 0.0820
Y6	 0.1370	 0.0640
Y8	 0.6550	 0.3410
Y9	 0.7100	 0.3960
YA	 0.0520	 0.0450
Z1	 0.0020	 0.0270
Z2	 0.0980	 0.0300
Z4	 0.0090	 0.0150
Z5	 0.0970	 0.0380
Z6	 0.1380	 0.0750
Z8	 0.6540	 0.3560
Z9	 0.6430	 0.3330
ZA	 0.0600	 0.0230
a8	 0.5600	 0.2760
a9	 0.7210	 0.3780
b8	 0.6050	 0.3240

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
b9	 0.7160	 0.3840
c8	 0.4020	 0.1980
c9	 0.7790	 0.4430
d8	 0.4750	 0.2400
d9	 0.6730	 0.3610
e8	 0.5680	 0.2770
e9	 0.7530	 0.4400
f8	 0.6140	 0.3180
f9	 0.7040	 0.4060
g8	 0.6580	 0.3480
g9	 0.7160	 0.4280
h8	 0.5410	 0.2740
h9	 0.6890	 0.3730
i8	 0.5540	 0.2840
i9	 0.4100	 0.2230
j8	 0.5420	 0.2600
j9	 0.5000	 0.2670
k8	 0.5420	 0.2930
k9	 0.4560	 0.2150
l8	 0.4950	 0.2390
l9	 0.4770	 0.2580
m8	 0.6560	 0.3590
m9	 0.5200	 0.3020
n8	 0.6840	 0.3590
n9	 0.5520	 0.3010
o8	 0.6590	 0.3450
o9	 0.6200	 0.3040
p8	 0.5540	 0.2540
p9	 0.6970	 0.3700
q8	 0.5650	 0.2940
q9	 0.6660	 0.3330
r8	 0.4830	 0.2340
r9	 0.7440	 0.4080
s8	 0.6750	 0.3660
s9	 0.6830	 0.3710
t8	 0.7130	 0.3760
t9	 0.7170	 0.3990
u8	 0.6760	 0.3280
u9	 0.6100	 0.3020
v9	 0.6860	 0.3530
w9	 0.6610	 0.3310
x9	 0.7310	 0.3870

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
y9	 0.6930	 0.3650
z9	 0.7210	 0.3950