



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 08:26 AM UTC

PDB ID : 9K9W / pdb_00009k9w
EMDB ID : EMD-62201
Title : structure of bundle-shaped PBS with short rod
Authors : Sui, S.-F.; Ma, J.; You, X.; Sun, S.
Deposited on : 2024-10-28
Resolution : 2.80 Å(reported)
Based on initial model : 6KGX

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

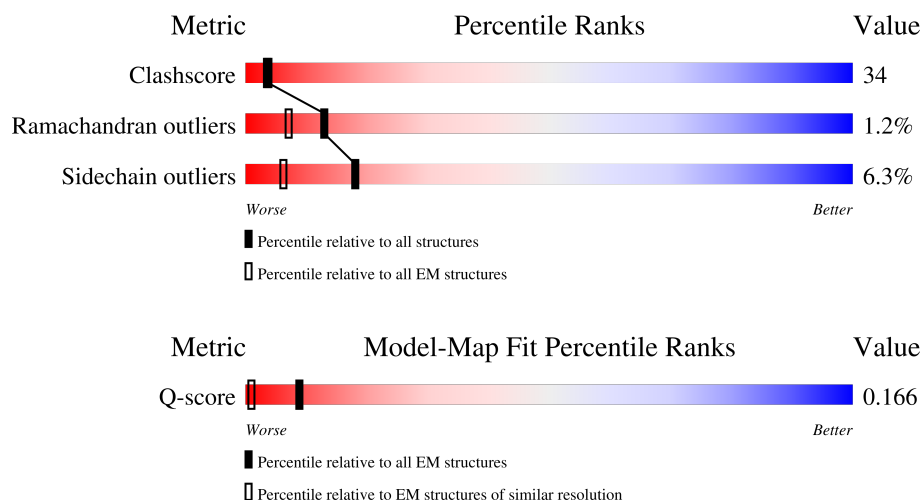
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.80 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.



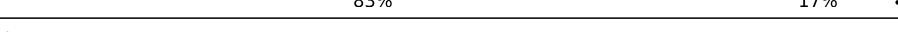
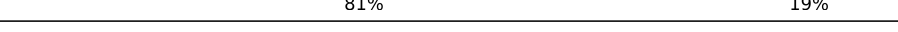
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11806 (2.30 - 3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	161	
1	B5	161	
1	B7	161	
1	D5	161	

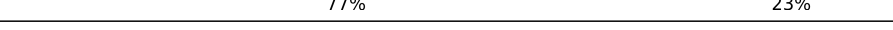
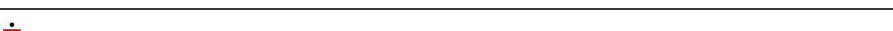
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Mol	Chain	Length	Quality of chain
1	D7	161	 73% 24% .
1	F5	161	 77% 21% .
1	F7	161	 85% 15%
1	H5	161	 78% 21% .
1	H7	161	 81% 18% .
1	J5	161	 66% 24% 8% .
1	J7	161	 73% 24% .
1	L5	161	 77% 21% .
1	L7	161	 85% 15%
1	N5	161	 84% 15% .
1	N7	161	 84% 16%
1	P5	161	 80% 20%
1	P7	161	 83% 17%
1	R5	161	 70% 29% .
1	R7	161	 84% 16%
1	T5	161	 83% 17% .
1	T7	161	 81% 19%
1	V5	161	 80% 20%
1	V7	161	 83% 16% .
1	X5	161	 70% 29% .
1	X7	161	 84% 16%
1	Z	161	 77% 22% .
1	Z5	161	 80% 20% .
1	Z7	161	 83% 17%
1	b5	161	 78% 21% .

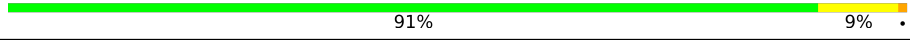
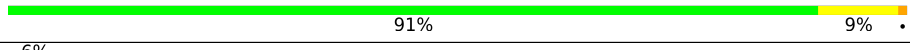
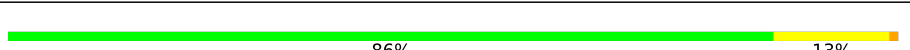
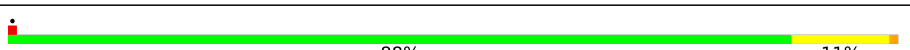
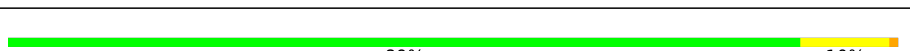
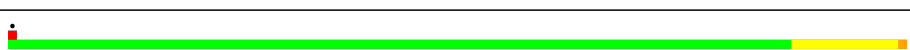
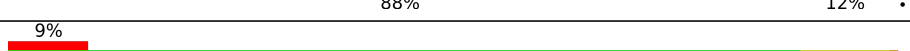
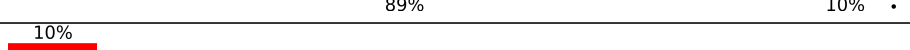
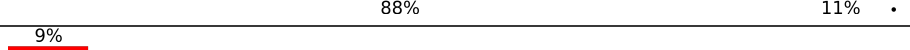
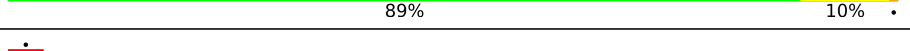
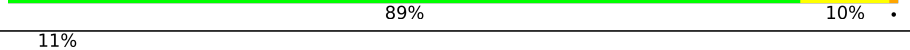
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Mol	Chain	Length	Quality of chain
1	b7	161	 68%25%6%
1	d5	161	 79%20%.
1	d7	161	 72%27%.
1	f5	161	 81%17%.
1	f7	161	 83%17%.
1	h7	161	 66%28%6%
1	j7	161	 78%21%.
1	l7	161	 80%19%.
1	n7	161	 79%21%
1	p7	161	 6%67%32%.
1	r7	161	 80%20%.
1	t7	161	 80%20%
1	v7	161	 8%66%32%.
2	A1	162	 77%23%.
2	A2	162	 75%23%.
2	A3	162	 76%22%.
2	A4	162	 76%23%.
2	A6	162	 75%23%.
2	A8	162	 75%23%.
2	A9	162	 75%24%.
2	AA	162	 73%26%.
2	C1	162	 5%88%10%.
2	C2	162	 88%11%.
2	C3	162	 5%90%9%.
2	C4	162	 12%88%12%.

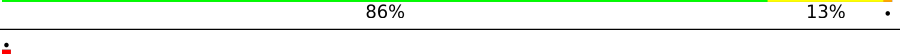
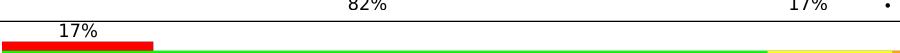
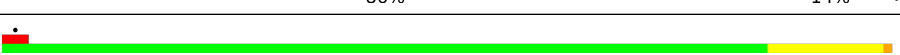
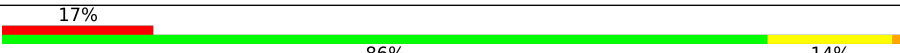
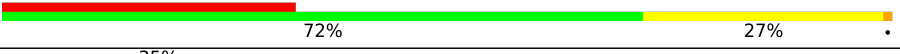
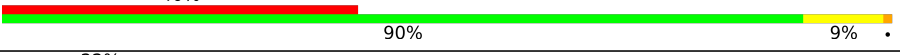
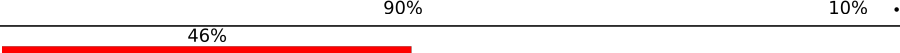
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Mol	Chain	Length	Quality of chain
2	C6	162	
2	C8	162	
2	C9	162	
2	CA	162	
2	E1	162	
2	E2	162	
2	E3	162	
2	E4	162	
2	E6	162	
2	E8	162	
2	E9	162	
2	EA	162	
2	G1	162	
2	G2	162	
2	G3	162	
2	G4	162	
2	G6	162	
2	G8	162	
2	G9	162	
2	GA	162	
2	I1	162	
2	I2	162	
2	I3	162	
2	I4	162	
2	I6	162	

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Mol	Chain	Length	Quality of chain
2	I8	162	 89% 10%
2	I9	162	 75% 22%
2	IA	162	 72% 25%
2	K1	162	 83% 17%
2	K2	162	 86% 13%
2	K3	162	 82% 17%
2	K4	162	 17% 86% 14%
2	K6	162	 86% 13%
2	K8	162	 17% 86% 14%
2	K9	162	 80% 15%
2	KA	162	 81% 15%
2	N4	162	 33% 72% 27%
2	N8	162	 35% 70% 28%
2	O1	162	 15% 78% 21%
2	O3	162	 14% 77% 22%
2	O9	162	 76% 23%
2	OA	162	 77% 22%
2	P4	162	 33% 86% 14%
2	P8	162	 33% 88% 11%
2	Q1	162	 42% 90% 9%
2	Q3	162	 40% 90% 9%
2	Q9	162	 22% 87% 12%
2	QA	162	 17% 70% 27%
2	R4	162	 46% 90% 10%
2	R8	162	 46% 88% 11%

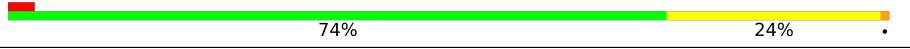
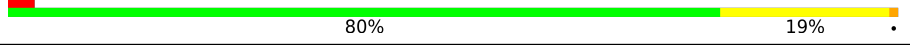
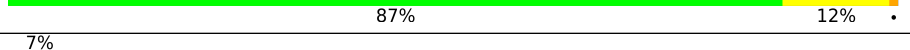
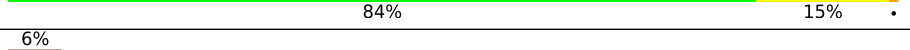
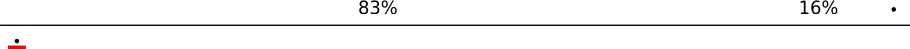
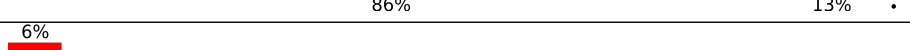
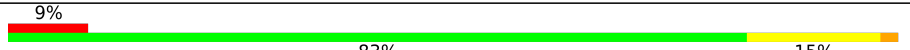
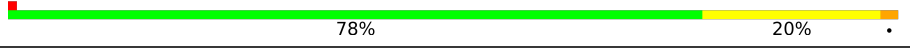
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Mol	Chain	Length	Quality of chain
2	S1	162	26% 90% 10% .
2	S3	162	25% 89% 10% .
2	S9	162	6% 88% 11% .
2	SA	162	6% 87% 12% .
2	T4	162	15% 88% 11% .
2	T8	162	14% 88% 10% .
2	U1	162	43% 83% 14% .
2	U3	162	43% 86% 12% ..
2	U9	162	5% 87% 12% .
2	UA	162	6% 79% 19% .
2	V4	162	47% 90% 10% .
2	V8	162	47% 91% 9% .
2	W1	162	36% 90% 10% .
2	W3	162	35% 91% 9% .
2	W9	162	54% 88% 11% .
2	WA	162	54% 88% 11% .
2	X4	162	40% 81% 19% .
2	X8	162	41% 78% 21% .
2	Y1	162	16% 87% 12% .
2	Y3	162	16% 88% 11% .
2	Y9	162	. 87% 12% .
2	YA	162	5% 86% 13% .
3	B1	172	. 77% 21% .
3	B2	172	. 84% 15% ..
3	B3	172	. 77% 22% .

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Mol	Chain	Length	Quality of chain
3	B4	172	
3	B6	172	
3	B8	172	
3	B9	172	
3	BA	172	
3	D1	172	
3	D2	172	
3	D3	172	
3	D4	172	
3	D6	172	
3	D8	172	
3	D9	172	
3	DA	172	
3	F1	172	
3	F2	172	
3	F3	172	
3	F4	172	
3	F6	172	
3	F8	172	
3	F9	172	
3	FA	172	
3	H1	172	
3	H2	172	
3	H3	172	
3	H4	172	

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Mol	Chain	Length	Quality of chain
3	H6	172	
3	H8	172	
3	H9	172	
3	HA	172	
3	J1	172	
3	J2	172	
3	J3	172	
3	J4	172	
3	J6	172	
3	J8	172	
3	J9	172	
3	JA	172	
3	L1	172	
3	L2	172	
3	L3	172	
3	L4	172	
3	L6	172	
3	L8	172	
3	L9	172	
3	LA	172	
3	O4	172	
3	O8	172	
3	P1	172	
3	P3	172	
3	P9	172	

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Mol	Chain	Length	Quality of chain
3	PA	172	
3	Q4	172	
3	Q8	172	
3	R1	172	
3	R3	172	
3	R9	172	
3	RA	172	
3	S4	172	
3	S8	172	
3	T1	172	
3	T3	172	
3	T9	172	
3	TA	172	
3	U4	172	
3	U8	172	
3	V1	172	
3	V3	172	
3	V9	172	
3	VA	172	
3	W4	172	
3	W8	172	
3	X1	172	
3	X3	172	
3	X9	172	
3	XA	172	

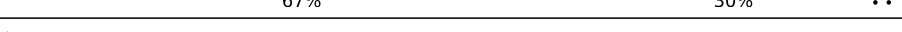
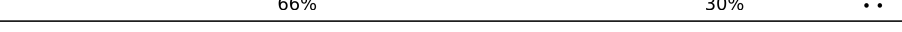
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Mol	Chain	Length	Quality of chain
3	Y4	172	
3	Y8	172	
3	Z1	172	
3	Z3	172	
3	Z9	172	
3	ZA	172	
4	M1	274	
4	M3	274	
4	M4	274	
4	M8	274	
4	M9	274	
4	MA	274	
5	N1	275	
5	N3	275	
5	N9	275	
5	NA	275	
5	Z4	275	
5	Z8	275	
6	M2	729	
6	M6	729	
7	N2	70	
7	N6	70	
8	A5	161	
8	A7	161	
8	C5	161	

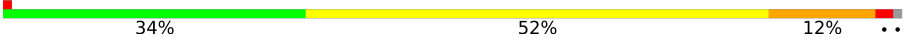
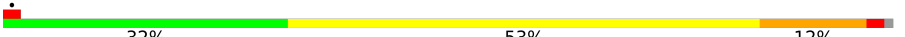
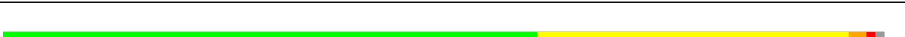
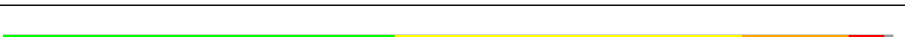
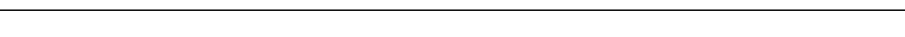
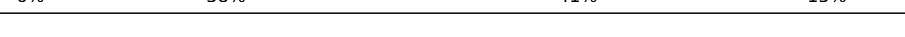
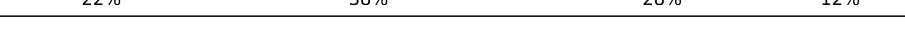
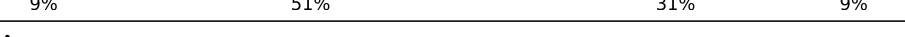
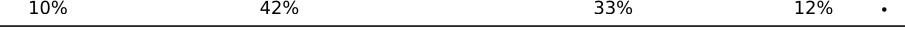
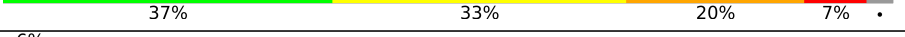
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Mol	Chain	Length	Quality of chain
8	C7	161	 63% 34% ...
8	E5	161	 52% 31% 13% ..
8	E7	161	 69% 27% ..
8	G5	161	 53% 39% 7% ..
8	G7	161	 69% 28% ..
8	I5	161	 58% 32% 6% ..
8	I7	161	 61% 35% ...
8	K5	161	 50% 34% 12% ..
8	K7	161	 70% 27% ..
8	M5	161	 66% 30% ..
8	M7	161	 68% 28% ..
8	O5	161	 59% 34%
8	O7	161	 60% 34%
8	Q5	161	 66% 28%
8	Q7	161	 66% 30% ..
8	S5	161	 67% 30% ..
8	S7	161	 66% 30% ..
8	U5	161	 54% 40%
8	U7	161	 62% 32%
8	W5	161	 66% 29%
8	W7	161	 66% 30% ..
8	Y5	161	 71% 26% ..
8	Y7	161	 70% 27% ..
8	a5	161	 58% 34%
8	a7	161	 60% 33% 6% ..

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Mol	Chain	Length	Quality of chain
8	c5	161	
8	c7	161	
8	e5	161	
8	e7	161	
8	g7	161	
8	i7	161	
8	k7	161	
8	m7	161	
8	o7	161	
8	q7	161	
8	s7	161	
8	u7	161	
9	i5	68	
9	w7	68	
9	x7	68	
9	y7	68	
9	z5	68	
9	z7	68	
10	j5	1155	
10	k5	1155	
11	a9	824	
11	aA	824	

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
1	MEN	D5	71	-	-	X	-
1	MEN	J5	71	-	-	X	-
1	MEN	v7	71	-	-	X	-
12	CYC	A5	201	-	-	X	-
12	CYC	B1	202	-	-	X	-
12	CYC	B3	202	-	-	X	-
12	CYC	B4	202	-	-	X	-
12	CYC	B5	201	-	-	X	-
12	CYC	B8	202	-	-	X	-
12	CYC	D7	201	-	-	X	-
12	CYC	D8	202	-	-	X	-
12	CYC	E5	201	-	-	X	-
12	CYC	F1	201	-	-	X	-
12	CYC	F2	201	-	-	X	-
12	CYC	F3	201	-	-	X	-
12	CYC	F6	201	-	-	X	-
12	CYC	F9	302	-	-	X	-
12	CYC	G5	201	-	-	X	-
12	CYC	H1	201	-	-	X	-
12	CYC	H4	201	-	-	X	-
12	CYC	H5	201	-	-	X	-
12	CYC	H8	201	-	-	X	-
12	CYC	H9	202	-	-	X	-
12	CYC	HA	202	-	-	X	-
12	CYC	J3	202	-	-	X	-
12	CYC	J7	201	-	-	X	-
12	CYC	J9	202	-	-	X	-
12	CYC	JA	202	-	-	X	-
12	CYC	K5	201	-	-	X	-
12	CYC	L3	202	-	-	X	-
12	CYC	L4	202	-	-	X	-
12	CYC	L9	202	-	-	X	-
12	CYC	LA	202	-	-	X	-
12	CYC	M4	301	-	-	X	-
12	CYC	M8	301	-	-	X	-
12	CYC	M8	302	-	-	X	-
12	CYC	O4	201	-	-	X	-
12	CYC	QA	201	-	-	X	-
12	CYC	R1	201	-	-	X	-
12	CYC	R3	201	-	-	X	-
12	CYC	S4	202	-	-	X	-
12	CYC	T1	301	-	-	X	-
12	CYC	T3	301	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	CYC	T9	301	-	-	X	-
12	CYC	TA	301	-	-	X	-
12	CYC	V9	201	-	-	X	-
12	CYC	VA	201	-	-	X	-
12	CYC	Z1	202	-	-	X	-
12	CYC	Z3	201	-	-	X	-
12	CYC	Z4	301	-	-	X	-
12	CYC	Z8	301	-	-	X	-
12	CYC	a9	901	-	-	X	-
12	CYC	aA	901	-	-	X	-
12	CYC	j5	1201	-	-	X	-
12	CYC	j5	1202	-	-	X	-
12	CYC	k5	1201	-	-	X	-
12	CYC	k5	1203	-	-	X	-
12	CYC	k5	1204	-	-	X	-
12	CYC	v7	201	-	-	X	-

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 382772 atoms, of which 76 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 Allophycocyanin beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	161	Total 1210	C 767	N 202	O 235	S 6	0	0
1	Z	161	Total 1210	C 767	N 202	O 235	S 6	0	0
1	L5	161	Total 1210	C 767	N 202	O 235	S 6	0	0
1	N5	161	Total 1210	C 767	N 202	O 235	S 6	0	0
1	B5	161	Total 1210	C 767	N 202	O 235	S 6	0	0
1	D5	161	Total 1210	C 767	N 202	O 235	S 6	0	0
1	F5	161	Total 1210	C 767	N 202	O 235	S 6	0	0
1	H5	161	Total 1210	C 767	N 202	O 235	S 6	0	0
1	J5	161	Total 1210	C 767	N 202	O 235	S 6	0	0
1	d5	161	Total 1210	C 767	N 202	O 235	S 6	0	0
1	f5	161	Total 1210	C 767	N 202	O 235	S 6	0	0
1	P5	161	Total 1210	C 767	N 202	O 235	S 6	0	0
1	R5	161	Total 1210	C 767	N 202	O 235	S 6	0	0
1	T5	161	Total 1210	C 767	N 202	O 235	S 6	0	0
1	V5	161	Total 1210	C 767	N 202	O 235	S 6	0	0
1	X5	161	Total 1210	C 767	N 202	O 235	S 6	0	0
1	Z5	161	Total 1210	C 767	N 202	O 235	S 6	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	b5	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
1	P7	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
1	R7	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
1	B7	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
1	D7	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
1	F7	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
1	H7	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
1	J7	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
1	L7	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
1	N7	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
1	h7	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
1	j7	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
1	T7	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
1	V7	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
1	X7	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
1	Z7	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
1	b7	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
1	d7	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
1	f7	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
1	l7	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
1	n7	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	p7	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
1	r7	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
1	t7	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
1	v7	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		

- Molecule 2 is a protein called Phycocyanin alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AA	162	Total	C	N	O	S	0	0
			1243	779	217	242	5		
2	CA	162	Total	C	N	O	S	0	0
			1243	779	217	242	5		
2	EA	162	Total	C	N	O	S	0	0
			1243	779	217	242	5		
2	GA	162	Total	C	N	O	S	0	0
			1243	779	217	242	5		
2	IA	162	Total	C	N	O	S	0	0
			1243	779	217	242	5		
2	KA	162	Total	C	N	O	S	0	0
			1243	779	217	242	5		
2	OA	162	Total	C	N	O	S	0	0
			1243	779	217	242	5		
2	QA	162	Total	C	N	O	S	0	0
			1243	779	217	242	5		
2	SA	162	Total	C	N	O	S	0	0
			1243	779	217	242	5		
2	UA	162	Total	C	N	O	S	0	0
			1243	779	217	242	5		
2	WA	162	Total	C	N	O	S	0	0
			1243	779	217	242	5		
2	YA	162	Total	C	N	O	S	0	0
			1243	779	217	242	5		
2	O1	162	Total	C	N	O	S	0	0
			1243	779	217	242	5		
2	Q1	162	Total	C	N	O	S	0	0
			1243	779	217	242	5		
2	S1	162	Total	C	N	O	S	0	0
			1243	779	217	242	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	A1	162	Total	C	N	O	S	0	0
			1243	779	217	242	5		
2	G3	162	Total	C	N	O	S	0	0
			1243	779	217	242	5		
2	I3	162	Total	C	N	O	S	0	0
			1243	779	217	242	5		
2	K3	162	Total	C	N	O	S	0	0
			1243	779	217	242	5		
2	G2	162	Total	C	N	O	S	0	0
			1243	779	217	242	5		
2	I2	162	Total	C	N	O	S	0	0
			1243	779	217	242	5		
2	K2	162	Total	C	N	O	S	0	0
			1243	779	217	242	5		
2	A3	162	Total	C	N	O	S	0	0
			1243	779	217	242	5		
2	C3	162	Total	C	N	O	S	0	0
			1243	779	217	242	5		
2	E3	162	Total	C	N	O	S	0	0
			1243	779	217	242	5		
2	A4	162	Total	C	N	O	S	0	0
			1243	779	217	242	5		
2	C4	162	Total	C	N	O	S	0	0
			1243	779	217	242	5		
2	O3	162	Total	C	N	O	S	0	0
			1243	779	217	242	5		
2	Q3	162	Total	C	N	O	S	0	0
			1243	779	217	242	5		
2	S3	162	Total	C	N	O	S	0	0
			1243	779	217	242	5		
2	U3	162	Total	C	N	O	S	0	0
			1243	779	217	242	5		
2	W3	162	Total	C	N	O	S	0	0
			1243	779	217	242	5		
2	Y3	162	Total	C	N	O	S	0	0
			1243	779	217	242	5		
2	T4	162	Total	C	N	O	S	0	0
			1243	779	217	242	5		
2	V4	162	Total	C	N	O	S	0	0
			1243	779	217	242	5		
2	E4	162	Total	C	N	O	S	0	0
			1243	779	217	242	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	G4	162	Total	C	N	O	S	0	0
			1243	779	217	242	5		
2	I4	162	Total	C	N	O	S	0	0
			1243	779	217	242	5		
2	K4	162	Total	C	N	O	S	0	0
			1243	779	217	242	5		
2	N4	162	Total	C	N	O	S	0	0
			1243	779	217	242	5		
2	P4	162	Total	C	N	O	S	0	0
			1243	779	217	242	5		
2	R4	162	Total	C	N	O	S	0	0
			1243	779	217	242	5		
2	X4	162	Total	C	N	O	S	0	0
			1243	779	217	242	5		
2	C1	162	Total	C	N	O	S	0	0
			1243	779	217	242	5		
2	K6	162	Total	C	N	O	S	0	0
			1243	779	217	242	5		
2	A6	162	Total	C	N	O	S	0	0
			1243	779	217	242	5		
2	C6	162	Total	C	N	O	S	0	0
			1243	779	217	242	5		
2	E6	162	Total	C	N	O	S	0	0
			1243	779	217	242	5		
2	G6	162	Total	C	N	O	S	0	0
			1243	779	217	242	5		
2	I6	162	Total	C	N	O	S	0	0
			1243	779	217	242	5		
2	E1	162	Total	C	N	O	S	0	0
			1243	779	217	242	5		
2	A8	162	Total	C	N	O	S	0	0
			1243	779	217	242	5		
2	C8	162	Total	C	N	O	S	0	0
			1243	779	217	242	5		
2	E8	162	Total	C	N	O	S	0	0
			1243	779	217	242	5		
2	T8	162	Total	C	N	O	S	0	0
			1243	779	217	242	5		
2	V8	162	Total	C	N	O	S	0	0
			1243	779	217	242	5		
2	X8	162	Total	C	N	O	S	0	0
			1243	779	217	242	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	G8	162	Total 1243	C 779	N 217	O 242	S 5	0	0
2	I8	162	Total 1243	C 779	N 217	O 242	S 5	0	0
2	K8	162	Total 1243	C 779	N 217	O 242	S 5	0	0
2	N8	162	Total 1243	C 779	N 217	O 242	S 5	0	0
2	P8	162	Total 1243	C 779	N 217	O 242	S 5	0	0
2	R8	162	Total 1243	C 779	N 217	O 242	S 5	0	0
2	O9	162	Total 1243	C 779	N 217	O 242	S 5	0	0
2	Q9	162	Total 1243	C 779	N 217	O 242	S 5	0	0
2	A9	162	Total 1243	C 779	N 217	O 242	S 5	0	0
2	C9	162	Total 1243	C 779	N 217	O 242	S 5	0	0
2	E9	162	Total 1243	C 779	N 217	O 242	S 5	0	0
2	G9	162	Total 1243	C 779	N 217	O 242	S 5	0	0
2	I9	162	Total 1243	C 779	N 217	O 242	S 5	0	0
2	K9	162	Total 1243	C 779	N 217	O 242	S 5	0	0
2	S9	162	Total 1243	C 779	N 217	O 242	S 5	0	0
2	U9	162	Total 1243	C 779	N 217	O 242	S 5	0	0
2	W9	162	Total 1243	C 779	N 217	O 242	S 5	0	0
2	Y9	162	Total 1243	C 779	N 217	O 242	S 5	0	0
2	G1	162	Total 1243	C 779	N 217	O 242	S 5	0	0
2	I1	162	Total 1243	C 779	N 217	O 242	S 5	0	0
2	K1	162	Total 1243	C 779	N 217	O 242	S 5	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	U1	162	Total	C	N	O	S	0	0
			1243	779	217	242	5		
2	W1	162	Total	C	N	O	S	0	0
			1243	779	217	242	5		
2	Y1	162	Total	C	N	O	S	0	0
			1243	779	217	242	5		
2	A2	162	Total	C	N	O	S	0	0
			1243	779	217	242	5		
2	C2	162	Total	C	N	O	S	0	0
			1243	779	217	242	5		
2	E2	162	Total	C	N	O	S	0	0
			1243	779	217	242	5		

- Molecule 3 is a protein called Phycocyanin beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	BA	172	Total	C	N	O	S	0	0
			1293	802	229	255	7		
3	DA	172	Total	C	N	O	S	0	0
			1293	802	229	255	7		
3	FA	172	Total	C	N	O	S	0	0
			1293	802	229	255	7		
3	HA	172	Total	C	N	O	S	0	0
			1293	802	229	255	7		
3	JA	172	Total	C	N	O	S	0	0
			1293	802	229	255	7		
3	LA	172	Total	C	N	O	S	0	0
			1293	802	229	255	7		
3	PA	172	Total	C	N	O	S	0	0
			1293	802	229	255	7		
3	RA	172	Total	C	N	O	S	0	0
			1293	802	229	255	7		
3	TA	172	Total	C	N	O	S	0	0
			1293	802	229	255	7		
3	VA	172	Total	C	N	O	S	0	0
			1293	802	229	255	7		
3	XA	172	Total	C	N	O	S	0	0
			1293	802	229	255	7		
3	ZA	172	Total	C	N	O	S	0	0
			1293	802	229	255	7		
3	P1	172	Total	C	N	O	S	0	0
			1293	802	229	255	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	R1	172	Total	C	N	O	S	0	0
			1293	802	229	255	7		
3	H3	172	Total	C	N	O	S	0	0
			1293	802	229	255	7		
3	J3	172	Total	C	N	O	S	0	0
			1293	802	229	255	7		
3	H2	172	Total	C	N	O	S	0	0
			1293	802	229	255	7		
3	J2	172	Total	C	N	O	S	0	0
			1293	802	229	255	7		
3	L2	172	Total	C	N	O	S	0	0
			1293	802	229	255	7		
3	B3	172	Total	C	N	O	S	0	0
			1293	802	229	255	7		
3	D3	172	Total	C	N	O	S	0	0
			1293	802	229	255	7		
3	F3	172	Total	C	N	O	S	0	0
			1293	802	229	255	7		
3	Z3	172	Total	C	N	O	S	0	0
			1293	802	229	255	7		
3	B4	172	Total	C	N	O	S	0	0
			1293	802	229	255	7		
3	D4	172	Total	C	N	O	S	0	0
			1293	802	229	255	7		
3	L3	172	Total	C	N	O	S	0	0
			1293	802	229	255	7		
3	P3	172	Total	C	N	O	S	0	0
			1293	802	229	255	7		
3	R3	172	Total	C	N	O	S	0	0
			1293	802	229	255	7		
3	T3	172	Total	C	N	O	S	0	0
			1293	802	229	255	7		
3	V3	172	Total	C	N	O	S	0	0
			1293	802	229	255	7		
3	X3	172	Total	C	N	O	S	0	0
			1293	802	229	255	7		
3	B1	172	Total	C	N	O	S	0	0
			1293	802	229	255	7		
3	S4	172	Total	C	N	O	S	0	0
			1293	802	229	255	7		
3	U4	172	Total	C	N	O	S	0	0
			1293	802	229	255	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	W4	172	Total	C	N	O	S	0	0
			1293	802	229	255	7		
3	F4	172	Total	C	N	O	S	0	0
			1293	802	229	255	7		
3	H4	172	Total	C	N	O	S	0	0
			1293	802	229	255	7		
3	J4	172	Total	C	N	O	S	0	0
			1293	802	229	255	7		
3	L4	172	Total	C	N	O	S	0	0
			1293	802	229	255	7		
3	O4	172	Total	C	N	O	S	0	0
			1293	802	229	255	7		
3	Q4	172	Total	C	N	O	S	0	0
			1293	802	229	255	7		
3	Y4	172	Total	C	N	O	S	0	0
			1293	802	229	255	7		
3	J6	172	Total	C	N	O	S	0	0
			1293	802	229	255	7		
3	L6	172	Total	C	N	O	S	0	0
			1293	802	229	255	7		
3	B6	172	Total	C	N	O	S	0	0
			1293	802	229	255	7		
3	D6	172	Total	C	N	O	S	0	0
			1293	802	229	255	7		
3	F6	172	Total	C	N	O	S	0	0
			1293	802	229	255	7		
3	H6	172	Total	C	N	O	S	0	0
			1293	802	229	255	7		
3	D1	172	Total	C	N	O	S	0	0
			1293	802	229	255	7		
3	B8	172	Total	C	N	O	S	0	0
			1293	802	229	255	7		
3	D8	172	Total	C	N	O	S	0	0
			1293	802	229	255	7		
3	U8	172	Total	C	N	O	S	0	0
			1293	802	229	255	7		
3	W8	172	Total	C	N	O	S	0	0
			1293	802	229	255	7		
3	F8	172	Total	C	N	O	S	0	0
			1293	802	229	255	7		
3	H8	172	Total	C	N	O	S	0	0
			1293	802	229	255	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	J8	172	Total	C	N	O	S	0	0
			1293	802	229	255	7		
3	L8	172	Total	C	N	O	S	0	0
			1293	802	229	255	7		
3	O8	172	Total	C	N	O	S	0	0
			1293	802	229	255	7		
3	Q8	172	Total	C	N	O	S	0	0
			1293	802	229	255	7		
3	S8	172	Total	C	N	O	S	0	0
			1293	802	229	255	7		
3	F1	172	Total	C	N	O	S	0	0
			1293	802	229	255	7		
3	L9	172	Total	C	N	O	S	0	0
			1293	802	229	255	7		
3	P9	172	Total	C	N	O	S	0	0
			1293	802	229	255	7		
3	Y8	172	Total	C	N	O	S	0	0
			1293	802	229	255	7		
3	B9	172	Total	C	N	O	S	0	0
			1293	802	229	255	7		
3	D9	172	Total	C	N	O	S	0	0
			1293	802	229	255	7		
3	F9	172	Total	C	N	O	S	0	0
			1293	802	229	255	7		
3	H9	172	Total	C	N	O	S	0	0
			1293	802	229	255	7		
3	J9	172	Total	C	N	O	S	0	0
			1293	802	229	255	7		
3	R9	172	Total	C	N	O	S	0	0
			1293	802	229	255	7		
3	T9	172	Total	C	N	O	S	0	0
			1293	802	229	255	7		
3	V9	172	Total	C	N	O	S	0	0
			1293	802	229	255	7		
3	X9	172	Total	C	N	O	S	0	0
			1293	802	229	255	7		
3	Z9	172	Total	C	N	O	S	0	0
			1293	802	229	255	7		
3	H1	172	Total	C	N	O	S	0	0
			1293	802	229	255	7		
3	J1	172	Total	C	N	O	S	0	0
			1293	802	229	255	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	L1	172	Total	C	N	O	S	0	0
			1293	802	229	255	7		
3	T1	172	Total	C	N	O	S	0	0
			1293	802	229	255	7		
3	V1	172	Total	C	N	O	S	0	0
			1293	802	229	255	7		
3	X1	172	Total	C	N	O	S	0	0
			1293	802	229	255	7		
3	Z1	172	Total	C	N	O	S	0	0
			1293	802	229	255	7		
3	B2	172	Total	C	N	O	S	0	0
			1293	802	229	255	7		
3	D2	172	Total	C	N	O	S	0	0
			1293	802	229	255	7		
3	F2	172	Total	C	N	O	S	0	0
			1293	802	229	255	7		

- Molecule 4 is a protein called Phycocyanin-associated rod linker protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	MA	274	Total	C	N	O	S	0	0
			2178	1383	377	413	5		
4	M3	274	Total	C	N	O	S	0	0
			2178	1383	377	413	5		
4	M4	274	Total	C	N	O	S	0	0
			2178	1383	377	413	5		
4	M8	274	Total	C	N	O	S	0	0
			2178	1383	377	413	5		
4	M9	274	Total	C	N	O	S	0	0
			2178	1383	377	413	5		
4	M1	274	Total	C	N	O	S	0	0
			2178	1383	377	413	5		

There are 330 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
MA	1	MET	-	initiating methionine	UNP Q7NGF2
MA	2	ASN	-	expression tag	UNP Q7NGF2
MA	3	VAL	-	expression tag	UNP Q7NGF2
MA	4	LEU	-	expression tag	UNP Q7NGF2
MA	5	THR	-	expression tag	UNP Q7NGF2
MA	6	THR	-	expression tag	UNP Q7NGF2

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Chain	Residue	Modelled	Actual	Comment	Reference
MA	7	SER	-	expression tag	UNP Q7NGF2
MA	8	SER	-	expression tag	UNP Q7NGF2
MA	9	GLN	-	expression tag	UNP Q7NGF2
MA	10	ARG	-	expression tag	UNP Q7NGF2
MA	11	GLY	-	expression tag	UNP Q7NGF2
MA	12	GLY	-	expression tag	UNP Q7NGF2
MA	13	LYS	-	expression tag	UNP Q7NGF2
MA	14	LEU	-	expression tag	UNP Q7NGF2
MA	15	PHE	-	expression tag	UNP Q7NGF2
MA	16	LYS	-	expression tag	UNP Q7NGF2
MA	17	VAL	-	expression tag	UNP Q7NGF2
MA	18	THR	-	expression tag	UNP Q7NGF2
MA	19	MET	-	expression tag	UNP Q7NGF2
MA	20	THR	-	expression tag	UNP Q7NGF2
MA	21	LEU	-	expression tag	UNP Q7NGF2
MA	22	SER	-	expression tag	UNP Q7NGF2
MA	23	PRO	-	expression tag	UNP Q7NGF2
MA	24	ALA	-	expression tag	UNP Q7NGF2
MA	25	LEU	-	expression tag	UNP Q7NGF2
MA	26	SER	-	expression tag	UNP Q7NGF2
MA	27	HIS	-	expression tag	UNP Q7NGF2
MA	28	HIS	-	expression tag	UNP Q7NGF2
MA	29	PRO	-	expression tag	UNP Q7NGF2
MA	30	TRP	-	expression tag	UNP Q7NGF2
MA	31	PRO	-	expression tag	UNP Q7NGF2
MA	32	SER	-	expression tag	UNP Q7NGF2
MA	33	LEU	-	expression tag	UNP Q7NGF2
MA	34	ASP	-	expression tag	UNP Q7NGF2
MA	35	THR	-	expression tag	UNP Q7NGF2
MA	36	TYR	-	expression tag	UNP Q7NGF2
MA	37	GLU	-	expression tag	UNP Q7NGF2
MA	38	PRO	-	expression tag	UNP Q7NGF2
MA	39	SER	-	expression tag	UNP Q7NGF2
MA	40	GLN	-	expression tag	UNP Q7NGF2
MA	41	ASN	-	expression tag	UNP Q7NGF2
MA	42	SER	-	expression tag	UNP Q7NGF2
MA	43	TYR	-	expression tag	UNP Q7NGF2
MA	44	SER	-	expression tag	UNP Q7NGF2
MA	45	VAL	-	expression tag	UNP Q7NGF2
MA	46	VAL	-	expression tag	UNP Q7NGF2
MA	47	VAL	-	expression tag	UNP Q7NGF2
MA	48	PRO	-	expression tag	UNP Q7NGF2

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Chain	Residue	Modelled	Actual	Comment	Reference
MA	49	LEU	-	expression tag	UNP Q7NGF2
MA	50	ASP	-	expression tag	UNP Q7NGF2
MA	51	ARG	-	expression tag	UNP Q7NGF2
MA	52	LEU	-	expression tag	UNP Q7NGF2
MA	53	LEU	-	expression tag	UNP Q7NGF2
MA	54	ALA	-	expression tag	UNP Q7NGF2
MA	55	GLU	-	expression tag	UNP Q7NGF2
M3	1	MET	-	initiating methionine	UNP Q7NGF2
M3	2	ASN	-	expression tag	UNP Q7NGF2
M3	3	VAL	-	expression tag	UNP Q7NGF2
M3	4	LEU	-	expression tag	UNP Q7NGF2
M3	5	THR	-	expression tag	UNP Q7NGF2
M3	6	THR	-	expression tag	UNP Q7NGF2
M3	7	SER	-	expression tag	UNP Q7NGF2
M3	8	SER	-	expression tag	UNP Q7NGF2
M3	9	GLN	-	expression tag	UNP Q7NGF2
M3	10	ARG	-	expression tag	UNP Q7NGF2
M3	11	GLY	-	expression tag	UNP Q7NGF2
M3	12	GLY	-	expression tag	UNP Q7NGF2
M3	13	LYS	-	expression tag	UNP Q7NGF2
M3	14	LEU	-	expression tag	UNP Q7NGF2
M3	15	PHE	-	expression tag	UNP Q7NGF2
M3	16	LYS	-	expression tag	UNP Q7NGF2
M3	17	VAL	-	expression tag	UNP Q7NGF2
M3	18	THR	-	expression tag	UNP Q7NGF2
M3	19	MET	-	expression tag	UNP Q7NGF2
M3	20	THR	-	expression tag	UNP Q7NGF2
M3	21	LEU	-	expression tag	UNP Q7NGF2
M3	22	SER	-	expression tag	UNP Q7NGF2
M3	23	PRO	-	expression tag	UNP Q7NGF2
M3	24	ALA	-	expression tag	UNP Q7NGF2
M3	25	LEU	-	expression tag	UNP Q7NGF2
M3	26	SER	-	expression tag	UNP Q7NGF2
M3	27	HIS	-	expression tag	UNP Q7NGF2
M3	28	HIS	-	expression tag	UNP Q7NGF2
M3	29	PRO	-	expression tag	UNP Q7NGF2
M3	30	TRP	-	expression tag	UNP Q7NGF2
M3	31	PRO	-	expression tag	UNP Q7NGF2
M3	32	SER	-	expression tag	UNP Q7NGF2
M3	33	LEU	-	expression tag	UNP Q7NGF2
M3	34	ASP	-	expression tag	UNP Q7NGF2
M3	35	THR	-	expression tag	UNP Q7NGF2

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Chain	Residue	Modelled	Actual	Comment	Reference
M3	36	TYR	-	expression tag	UNP Q7NGF2
M3	37	GLU	-	expression tag	UNP Q7NGF2
M3	38	PRO	-	expression tag	UNP Q7NGF2
M3	39	SER	-	expression tag	UNP Q7NGF2
M3	40	GLN	-	expression tag	UNP Q7NGF2
M3	41	ASN	-	expression tag	UNP Q7NGF2
M3	42	SER	-	expression tag	UNP Q7NGF2
M3	43	TYR	-	expression tag	UNP Q7NGF2
M3	44	SER	-	expression tag	UNP Q7NGF2
M3	45	VAL	-	expression tag	UNP Q7NGF2
M3	46	VAL	-	expression tag	UNP Q7NGF2
M3	47	VAL	-	expression tag	UNP Q7NGF2
M3	48	PRO	-	expression tag	UNP Q7NGF2
M3	49	LEU	-	expression tag	UNP Q7NGF2
M3	50	ASP	-	expression tag	UNP Q7NGF2
M3	51	ARG	-	expression tag	UNP Q7NGF2
M3	52	LEU	-	expression tag	UNP Q7NGF2
M3	53	LEU	-	expression tag	UNP Q7NGF2
M3	54	ALA	-	expression tag	UNP Q7NGF2
M3	55	GLU	-	expression tag	UNP Q7NGF2
M4	1	MET	-	initiating methionine	UNP Q7NGF2
M4	2	ASN	-	expression tag	UNP Q7NGF2
M4	3	VAL	-	expression tag	UNP Q7NGF2
M4	4	LEU	-	expression tag	UNP Q7NGF2
M4	5	THR	-	expression tag	UNP Q7NGF2
M4	6	THR	-	expression tag	UNP Q7NGF2
M4	7	SER	-	expression tag	UNP Q7NGF2
M4	8	SER	-	expression tag	UNP Q7NGF2
M4	9	GLN	-	expression tag	UNP Q7NGF2
M4	10	ARG	-	expression tag	UNP Q7NGF2
M4	11	GLY	-	expression tag	UNP Q7NGF2
M4	12	GLY	-	expression tag	UNP Q7NGF2
M4	13	LYS	-	expression tag	UNP Q7NGF2
M4	14	LEU	-	expression tag	UNP Q7NGF2
M4	15	PHE	-	expression tag	UNP Q7NGF2
M4	16	LYS	-	expression tag	UNP Q7NGF2
M4	17	VAL	-	expression tag	UNP Q7NGF2
M4	18	THR	-	expression tag	UNP Q7NGF2
M4	19	MET	-	expression tag	UNP Q7NGF2
M4	20	THR	-	expression tag	UNP Q7NGF2
M4	21	LEU	-	expression tag	UNP Q7NGF2
M4	22	SER	-	expression tag	UNP Q7NGF2

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Chain	Residue	Modelled	Actual	Comment	Reference
M4	23	PRO	-	expression tag	UNP Q7NGF2
M4	24	ALA	-	expression tag	UNP Q7NGF2
M4	25	LEU	-	expression tag	UNP Q7NGF2
M4	26	SER	-	expression tag	UNP Q7NGF2
M4	27	HIS	-	expression tag	UNP Q7NGF2
M4	28	HIS	-	expression tag	UNP Q7NGF2
M4	29	PRO	-	expression tag	UNP Q7NGF2
M4	30	TRP	-	expression tag	UNP Q7NGF2
M4	31	PRO	-	expression tag	UNP Q7NGF2
M4	32	SER	-	expression tag	UNP Q7NGF2
M4	33	LEU	-	expression tag	UNP Q7NGF2
M4	34	ASP	-	expression tag	UNP Q7NGF2
M4	35	THR	-	expression tag	UNP Q7NGF2
M4	36	TYR	-	expression tag	UNP Q7NGF2
M4	37	GLU	-	expression tag	UNP Q7NGF2
M4	38	PRO	-	expression tag	UNP Q7NGF2
M4	39	SER	-	expression tag	UNP Q7NGF2
M4	40	GLN	-	expression tag	UNP Q7NGF2
M4	41	ASN	-	expression tag	UNP Q7NGF2
M4	42	SER	-	expression tag	UNP Q7NGF2
M4	43	TYR	-	expression tag	UNP Q7NGF2
M4	44	SER	-	expression tag	UNP Q7NGF2
M4	45	VAL	-	expression tag	UNP Q7NGF2
M4	46	VAL	-	expression tag	UNP Q7NGF2
M4	47	VAL	-	expression tag	UNP Q7NGF2
M4	48	PRO	-	expression tag	UNP Q7NGF2
M4	49	LEU	-	expression tag	UNP Q7NGF2
M4	50	ASP	-	expression tag	UNP Q7NGF2
M4	51	ARG	-	expression tag	UNP Q7NGF2
M4	52	LEU	-	expression tag	UNP Q7NGF2
M4	53	LEU	-	expression tag	UNP Q7NGF2
M4	54	ALA	-	expression tag	UNP Q7NGF2
M4	55	GLU	-	expression tag	UNP Q7NGF2
M8	1	MET	-	initiating methionine	UNP Q7NGF2
M8	2	ASN	-	expression tag	UNP Q7NGF2
M8	3	VAL	-	expression tag	UNP Q7NGF2
M8	4	LEU	-	expression tag	UNP Q7NGF2
M8	5	THR	-	expression tag	UNP Q7NGF2
M8	6	THR	-	expression tag	UNP Q7NGF2
M8	7	SER	-	expression tag	UNP Q7NGF2
M8	8	SER	-	expression tag	UNP Q7NGF2
M8	9	GLN	-	expression tag	UNP Q7NGF2

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Chain	Residue	Modelled	Actual	Comment	Reference
M8	10	ARG	-	expression tag	UNP Q7NGF2
M8	11	GLY	-	expression tag	UNP Q7NGF2
M8	12	GLY	-	expression tag	UNP Q7NGF2
M8	13	LYS	-	expression tag	UNP Q7NGF2
M8	14	LEU	-	expression tag	UNP Q7NGF2
M8	15	PHE	-	expression tag	UNP Q7NGF2
M8	16	LYS	-	expression tag	UNP Q7NGF2
M8	17	VAL	-	expression tag	UNP Q7NGF2
M8	18	THR	-	expression tag	UNP Q7NGF2
M8	19	MET	-	expression tag	UNP Q7NGF2
M8	20	THR	-	expression tag	UNP Q7NGF2
M8	21	LEU	-	expression tag	UNP Q7NGF2
M8	22	SER	-	expression tag	UNP Q7NGF2
M8	23	PRO	-	expression tag	UNP Q7NGF2
M8	24	ALA	-	expression tag	UNP Q7NGF2
M8	25	LEU	-	expression tag	UNP Q7NGF2
M8	26	SER	-	expression tag	UNP Q7NGF2
M8	27	HIS	-	expression tag	UNP Q7NGF2
M8	28	HIS	-	expression tag	UNP Q7NGF2
M8	29	PRO	-	expression tag	UNP Q7NGF2
M8	30	TRP	-	expression tag	UNP Q7NGF2
M8	31	PRO	-	expression tag	UNP Q7NGF2
M8	32	SER	-	expression tag	UNP Q7NGF2
M8	33	LEU	-	expression tag	UNP Q7NGF2
M8	34	ASP	-	expression tag	UNP Q7NGF2
M8	35	THR	-	expression tag	UNP Q7NGF2
M8	36	TYR	-	expression tag	UNP Q7NGF2
M8	37	GLU	-	expression tag	UNP Q7NGF2
M8	38	PRO	-	expression tag	UNP Q7NGF2
M8	39	SER	-	expression tag	UNP Q7NGF2
M8	40	GLN	-	expression tag	UNP Q7NGF2
M8	41	ASN	-	expression tag	UNP Q7NGF2
M8	42	SER	-	expression tag	UNP Q7NGF2
M8	43	TYR	-	expression tag	UNP Q7NGF2
M8	44	SER	-	expression tag	UNP Q7NGF2
M8	45	VAL	-	expression tag	UNP Q7NGF2
M8	46	VAL	-	expression tag	UNP Q7NGF2
M8	47	VAL	-	expression tag	UNP Q7NGF2
M8	48	PRO	-	expression tag	UNP Q7NGF2
M8	49	LEU	-	expression tag	UNP Q7NGF2
M8	50	ASP	-	expression tag	UNP Q7NGF2
M8	51	ARG	-	expression tag	UNP Q7NGF2

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Chain	Residue	Modelled	Actual	Comment	Reference
M8	52	LEU	-	expression tag	UNP Q7NGF2
M8	53	LEU	-	expression tag	UNP Q7NGF2
M8	54	ALA	-	expression tag	UNP Q7NGF2
M8	55	GLU	-	expression tag	UNP Q7NGF2
M9	1	MET	-	initiating methionine	UNP Q7NGF2
M9	2	ASN	-	expression tag	UNP Q7NGF2
M9	3	VAL	-	expression tag	UNP Q7NGF2
M9	4	LEU	-	expression tag	UNP Q7NGF2
M9	5	THR	-	expression tag	UNP Q7NGF2
M9	6	THR	-	expression tag	UNP Q7NGF2
M9	7	SER	-	expression tag	UNP Q7NGF2
M9	8	SER	-	expression tag	UNP Q7NGF2
M9	9	GLN	-	expression tag	UNP Q7NGF2
M9	10	ARG	-	expression tag	UNP Q7NGF2
M9	11	GLY	-	expression tag	UNP Q7NGF2
M9	12	GLY	-	expression tag	UNP Q7NGF2
M9	13	LYS	-	expression tag	UNP Q7NGF2
M9	14	LEU	-	expression tag	UNP Q7NGF2
M9	15	PHE	-	expression tag	UNP Q7NGF2
M9	16	LYS	-	expression tag	UNP Q7NGF2
M9	17	VAL	-	expression tag	UNP Q7NGF2
M9	18	THR	-	expression tag	UNP Q7NGF2
M9	19	MET	-	expression tag	UNP Q7NGF2
M9	20	THR	-	expression tag	UNP Q7NGF2
M9	21	LEU	-	expression tag	UNP Q7NGF2
M9	22	SER	-	expression tag	UNP Q7NGF2
M9	23	PRO	-	expression tag	UNP Q7NGF2
M9	24	ALA	-	expression tag	UNP Q7NGF2
M9	25	LEU	-	expression tag	UNP Q7NGF2
M9	26	SER	-	expression tag	UNP Q7NGF2
M9	27	HIS	-	expression tag	UNP Q7NGF2
M9	28	HIS	-	expression tag	UNP Q7NGF2
M9	29	PRO	-	expression tag	UNP Q7NGF2
M9	30	TRP	-	expression tag	UNP Q7NGF2
M9	31	PRO	-	expression tag	UNP Q7NGF2
M9	32	SER	-	expression tag	UNP Q7NGF2
M9	33	LEU	-	expression tag	UNP Q7NGF2
M9	34	ASP	-	expression tag	UNP Q7NGF2
M9	35	THR	-	expression tag	UNP Q7NGF2
M9	36	TYR	-	expression tag	UNP Q7NGF2
M9	37	GLU	-	expression tag	UNP Q7NGF2
M9	38	PRO	-	expression tag	UNP Q7NGF2

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Chain	Residue	Modelled	Actual	Comment	Reference
M9	39	SER	-	expression tag	UNP Q7NGF2
M9	40	GLN	-	expression tag	UNP Q7NGF2
M9	41	ASN	-	expression tag	UNP Q7NGF2
M9	42	SER	-	expression tag	UNP Q7NGF2
M9	43	TYR	-	expression tag	UNP Q7NGF2
M9	44	SER	-	expression tag	UNP Q7NGF2
M9	45	VAL	-	expression tag	UNP Q7NGF2
M9	46	VAL	-	expression tag	UNP Q7NGF2
M9	47	VAL	-	expression tag	UNP Q7NGF2
M9	48	PRO	-	expression tag	UNP Q7NGF2
M9	49	LEU	-	expression tag	UNP Q7NGF2
M9	50	ASP	-	expression tag	UNP Q7NGF2
M9	51	ARG	-	expression tag	UNP Q7NGF2
M9	52	LEU	-	expression tag	UNP Q7NGF2
M9	53	LEU	-	expression tag	UNP Q7NGF2
M9	54	ALA	-	expression tag	UNP Q7NGF2
M9	55	GLU	-	expression tag	UNP Q7NGF2
M1	1	MET	-	initiating methionine	UNP Q7NGF2
M1	2	ASN	-	expression tag	UNP Q7NGF2
M1	3	VAL	-	expression tag	UNP Q7NGF2
M1	4	LEU	-	expression tag	UNP Q7NGF2
M1	5	THR	-	expression tag	UNP Q7NGF2
M1	6	THR	-	expression tag	UNP Q7NGF2
M1	7	SER	-	expression tag	UNP Q7NGF2
M1	8	SER	-	expression tag	UNP Q7NGF2
M1	9	GLN	-	expression tag	UNP Q7NGF2
M1	10	ARG	-	expression tag	UNP Q7NGF2
M1	11	GLY	-	expression tag	UNP Q7NGF2
M1	12	GLY	-	expression tag	UNP Q7NGF2
M1	13	LYS	-	expression tag	UNP Q7NGF2
M1	14	LEU	-	expression tag	UNP Q7NGF2
M1	15	PHE	-	expression tag	UNP Q7NGF2
M1	16	LYS	-	expression tag	UNP Q7NGF2
M1	17	VAL	-	expression tag	UNP Q7NGF2
M1	18	THR	-	expression tag	UNP Q7NGF2
M1	19	MET	-	expression tag	UNP Q7NGF2
M1	20	THR	-	expression tag	UNP Q7NGF2
M1	21	LEU	-	expression tag	UNP Q7NGF2
M1	22	SER	-	expression tag	UNP Q7NGF2
M1	23	PRO	-	expression tag	UNP Q7NGF2
M1	24	ALA	-	expression tag	UNP Q7NGF2
M1	25	LEU	-	expression tag	UNP Q7NGF2

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Chain	Residue	Modelled	Actual	Comment	Reference
M1	26	SER	-	expression tag	UNP Q7NGF2
M1	27	HIS	-	expression tag	UNP Q7NGF2
M1	28	HIS	-	expression tag	UNP Q7NGF2
M1	29	PRO	-	expression tag	UNP Q7NGF2
M1	30	TRP	-	expression tag	UNP Q7NGF2
M1	31	PRO	-	expression tag	UNP Q7NGF2
M1	32	SER	-	expression tag	UNP Q7NGF2
M1	33	LEU	-	expression tag	UNP Q7NGF2
M1	34	ASP	-	expression tag	UNP Q7NGF2
M1	35	THR	-	expression tag	UNP Q7NGF2
M1	36	TYR	-	expression tag	UNP Q7NGF2
M1	37	GLU	-	expression tag	UNP Q7NGF2
M1	38	PRO	-	expression tag	UNP Q7NGF2
M1	39	SER	-	expression tag	UNP Q7NGF2
M1	40	GLN	-	expression tag	UNP Q7NGF2
M1	41	ASN	-	expression tag	UNP Q7NGF2
M1	42	SER	-	expression tag	UNP Q7NGF2
M1	43	TYR	-	expression tag	UNP Q7NGF2
M1	44	SER	-	expression tag	UNP Q7NGF2
M1	45	VAL	-	expression tag	UNP Q7NGF2
M1	46	VAL	-	expression tag	UNP Q7NGF2
M1	47	VAL	-	expression tag	UNP Q7NGF2
M1	48	PRO	-	expression tag	UNP Q7NGF2
M1	49	LEU	-	expression tag	UNP Q7NGF2
M1	50	ASP	-	expression tag	UNP Q7NGF2
M1	51	ARG	-	expression tag	UNP Q7NGF2
M1	52	LEU	-	expression tag	UNP Q7NGF2
M1	53	LEU	-	expression tag	UNP Q7NGF2
M1	54	ALA	-	expression tag	UNP Q7NGF2
M1	55	GLU	-	expression tag	UNP Q7NGF2

- Molecule 5 is a protein called Phycocyanin-associated rod linker protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	NA	74	Total	C	N	O	S	0	0
			578	361	104	111	2		
5	N3	74	Total	C	N	O	S	0	0
			578	361	104	111	2		
5	Z4	74	Total	C	N	O	S	0	0
			578	361	104	111	2		
5	N9	74	Total	C	N	O	S	0	0
			578	361	104	111	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	Z8	74	Total	C	N	O	S	0	0
			578	361	104	111	2		
5	N1	74	Total	C	N	O	S	0	0
			578	361	104	111	2		

There are 336 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
NA	1	MET	-	initiating methionine	UNP Q7NM19
NA	2	SER	-	expression tag	UNP Q7NM19
NA	3	VAL	-	expression tag	UNP Q7NM19
NA	4	LEU	-	expression tag	UNP Q7NM19
NA	5	THR	-	expression tag	UNP Q7NM19
NA	6	GLY	-	expression tag	UNP Q7NM19
NA	7	ASP	-	expression tag	UNP Q7NM19
NA	8	ASN	-	expression tag	UNP Q7NM19
NA	9	GLN	-	expression tag	UNP Q7NM19
NA	10	GLN	-	expression tag	UNP Q7NM19
NA	11	ARG	-	expression tag	UNP Q7NM19
NA	12	GLY	-	expression tag	UNP Q7NM19
NA	13	SER	-	expression tag	UNP Q7NM19
NA	14	LYS	-	expression tag	UNP Q7NM19
NA	15	LEU	-	expression tag	UNP Q7NM19
NA	16	PHE	-	expression tag	UNP Q7NM19
NA	17	LYS	-	expression tag	UNP Q7NM19
NA	18	ILE	-	expression tag	UNP Q7NM19
NA	19	THR	-	expression tag	UNP Q7NM19
NA	20	ILE	-	expression tag	UNP Q7NM19
NA	21	ALA	-	expression tag	UNP Q7NM19
NA	22	LEU	-	expression tag	UNP Q7NM19
NA	23	SER	-	expression tag	UNP Q7NM19
NA	24	PRO	-	expression tag	UNP Q7NM19
NA	25	THR	-	expression tag	UNP Q7NM19
NA	26	LEU	-	expression tag	UNP Q7NM19
NA	27	ALA	-	expression tag	UNP Q7NM19
NA	28	HIS	-	expression tag	UNP Q7NM19
NA	29	HIS	-	expression tag	UNP Q7NM19
NA	30	PRO	-	expression tag	UNP Q7NM19
NA	31	TRP	-	expression tag	UNP Q7NM19
NA	32	PRO	-	expression tag	UNP Q7NM19
NA	33	GLY	-	expression tag	UNP Q7NM19
NA	34	LEU	-	expression tag	UNP Q7NM19

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Chain	Residue	Modelled	Actual	Comment	Reference
NA	35	ASP	-	expression tag	UNP Q7NM19
NA	36	THR	-	expression tag	UNP Q7NM19
NA	37	HIS	-	expression tag	UNP Q7NM19
NA	38	GLU	-	expression tag	UNP Q7NM19
NA	39	PRO	-	expression tag	UNP Q7NM19
NA	40	SER	-	expression tag	UNP Q7NM19
NA	41	GLN	-	expression tag	UNP Q7NM19
NA	42	SER	-	expression tag	UNP Q7NM19
NA	43	SER	-	expression tag	UNP Q7NM19
NA	44	TYR	-	expression tag	UNP Q7NM19
NA	45	SER	-	expression tag	UNP Q7NM19
NA	46	THR	-	expression tag	UNP Q7NM19
NA	47	ILE	-	expression tag	UNP Q7NM19
NA	48	VAL	-	expression tag	UNP Q7NM19
NA	49	SER	-	expression tag	UNP Q7NM19
NA	50	LEU	-	expression tag	UNP Q7NM19
NA	51	GLU	-	expression tag	UNP Q7NM19
NA	52	ARG	-	expression tag	UNP Q7NM19
NA	53	LEU	-	expression tag	UNP Q7NM19
NA	54	LEU	-	expression tag	UNP Q7NM19
NA	55	PRO	-	expression tag	UNP Q7NM19
NA	56	GLU	-	expression tag	UNP Q7NM19
N3	1	MET	-	initiating methionine	UNP Q7NM19
N3	2	SER	-	expression tag	UNP Q7NM19
N3	3	VAL	-	expression tag	UNP Q7NM19
N3	4	LEU	-	expression tag	UNP Q7NM19
N3	5	THR	-	expression tag	UNP Q7NM19
N3	6	GLY	-	expression tag	UNP Q7NM19
N3	7	ASP	-	expression tag	UNP Q7NM19
N3	8	ASN	-	expression tag	UNP Q7NM19
N3	9	GLN	-	expression tag	UNP Q7NM19
N3	10	GLN	-	expression tag	UNP Q7NM19
N3	11	ARG	-	expression tag	UNP Q7NM19
N3	12	GLY	-	expression tag	UNP Q7NM19
N3	13	SER	-	expression tag	UNP Q7NM19
N3	14	LYS	-	expression tag	UNP Q7NM19
N3	15	LEU	-	expression tag	UNP Q7NM19
N3	16	PHE	-	expression tag	UNP Q7NM19
N3	17	LYS	-	expression tag	UNP Q7NM19
N3	18	ILE	-	expression tag	UNP Q7NM19
N3	19	THR	-	expression tag	UNP Q7NM19
N3	20	ILE	-	expression tag	UNP Q7NM19

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Chain	Residue	Modelled	Actual	Comment	Reference
N3	21	ALA	-	expression tag	UNP Q7NM19
N3	22	LEU	-	expression tag	UNP Q7NM19
N3	23	SER	-	expression tag	UNP Q7NM19
N3	24	PRO	-	expression tag	UNP Q7NM19
N3	25	THR	-	expression tag	UNP Q7NM19
N3	26	LEU	-	expression tag	UNP Q7NM19
N3	27	ALA	-	expression tag	UNP Q7NM19
N3	28	HIS	-	expression tag	UNP Q7NM19
N3	29	HIS	-	expression tag	UNP Q7NM19
N3	30	PRO	-	expression tag	UNP Q7NM19
N3	31	TRP	-	expression tag	UNP Q7NM19
N3	32	PRO	-	expression tag	UNP Q7NM19
N3	33	GLY	-	expression tag	UNP Q7NM19
N3	34	LEU	-	expression tag	UNP Q7NM19
N3	35	ASP	-	expression tag	UNP Q7NM19
N3	36	THR	-	expression tag	UNP Q7NM19
N3	37	HIS	-	expression tag	UNP Q7NM19
N3	38	GLU	-	expression tag	UNP Q7NM19
N3	39	PRO	-	expression tag	UNP Q7NM19
N3	40	SER	-	expression tag	UNP Q7NM19
N3	41	GLN	-	expression tag	UNP Q7NM19
N3	42	SER	-	expression tag	UNP Q7NM19
N3	43	SER	-	expression tag	UNP Q7NM19
N3	44	TYR	-	expression tag	UNP Q7NM19
N3	45	SER	-	expression tag	UNP Q7NM19
N3	46	THR	-	expression tag	UNP Q7NM19
N3	47	ILE	-	expression tag	UNP Q7NM19
N3	48	VAL	-	expression tag	UNP Q7NM19
N3	49	SER	-	expression tag	UNP Q7NM19
N3	50	LEU	-	expression tag	UNP Q7NM19
N3	51	GLU	-	expression tag	UNP Q7NM19
N3	52	ARG	-	expression tag	UNP Q7NM19
N3	53	LEU	-	expression tag	UNP Q7NM19
N3	54	LEU	-	expression tag	UNP Q7NM19
N3	55	PRO	-	expression tag	UNP Q7NM19
N3	56	GLU	-	expression tag	UNP Q7NM19
Z4	1	MET	-	initiating methionine	UNP Q7NM19
Z4	2	SER	-	expression tag	UNP Q7NM19
Z4	3	VAL	-	expression tag	UNP Q7NM19
Z4	4	LEU	-	expression tag	UNP Q7NM19
Z4	5	THR	-	expression tag	UNP Q7NM19
Z4	6	GLY	-	expression tag	UNP Q7NM19

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Chain	Residue	Modelled	Actual	Comment	Reference
Z4	7	ASP	-	expression tag	UNP Q7NM19
Z4	8	ASN	-	expression tag	UNP Q7NM19
Z4	9	GLN	-	expression tag	UNP Q7NM19
Z4	10	GLN	-	expression tag	UNP Q7NM19
Z4	11	ARG	-	expression tag	UNP Q7NM19
Z4	12	GLY	-	expression tag	UNP Q7NM19
Z4	13	SER	-	expression tag	UNP Q7NM19
Z4	14	LYS	-	expression tag	UNP Q7NM19
Z4	15	LEU	-	expression tag	UNP Q7NM19
Z4	16	PHE	-	expression tag	UNP Q7NM19
Z4	17	LYS	-	expression tag	UNP Q7NM19
Z4	18	ILE	-	expression tag	UNP Q7NM19
Z4	19	THR	-	expression tag	UNP Q7NM19
Z4	20	ILE	-	expression tag	UNP Q7NM19
Z4	21	ALA	-	expression tag	UNP Q7NM19
Z4	22	LEU	-	expression tag	UNP Q7NM19
Z4	23	SER	-	expression tag	UNP Q7NM19
Z4	24	PRO	-	expression tag	UNP Q7NM19
Z4	25	THR	-	expression tag	UNP Q7NM19
Z4	26	LEU	-	expression tag	UNP Q7NM19
Z4	27	ALA	-	expression tag	UNP Q7NM19
Z4	28	HIS	-	expression tag	UNP Q7NM19
Z4	29	HIS	-	expression tag	UNP Q7NM19
Z4	30	PRO	-	expression tag	UNP Q7NM19
Z4	31	TRP	-	expression tag	UNP Q7NM19
Z4	32	PRO	-	expression tag	UNP Q7NM19
Z4	33	GLY	-	expression tag	UNP Q7NM19
Z4	34	LEU	-	expression tag	UNP Q7NM19
Z4	35	ASP	-	expression tag	UNP Q7NM19
Z4	36	THR	-	expression tag	UNP Q7NM19
Z4	37	HIS	-	expression tag	UNP Q7NM19
Z4	38	GLU	-	expression tag	UNP Q7NM19
Z4	39	PRO	-	expression tag	UNP Q7NM19
Z4	40	SER	-	expression tag	UNP Q7NM19
Z4	41	GLN	-	expression tag	UNP Q7NM19
Z4	42	SER	-	expression tag	UNP Q7NM19
Z4	43	SER	-	expression tag	UNP Q7NM19
Z4	44	TYR	-	expression tag	UNP Q7NM19
Z4	45	SER	-	expression tag	UNP Q7NM19
Z4	46	THR	-	expression tag	UNP Q7NM19
Z4	47	ILE	-	expression tag	UNP Q7NM19
Z4	48	VAL	-	expression tag	UNP Q7NM19

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Chain	Residue	Modelled	Actual	Comment	Reference
Z4	49	SER	-	expression tag	UNP Q7NM19
Z4	50	LEU	-	expression tag	UNP Q7NM19
Z4	51	GLU	-	expression tag	UNP Q7NM19
Z4	52	ARG	-	expression tag	UNP Q7NM19
Z4	53	LEU	-	expression tag	UNP Q7NM19
Z4	54	LEU	-	expression tag	UNP Q7NM19
Z4	55	PRO	-	expression tag	UNP Q7NM19
Z4	56	GLU	-	expression tag	UNP Q7NM19
N9	1	MET	-	initiating methionine	UNP Q7NM19
N9	2	SER	-	expression tag	UNP Q7NM19
N9	3	VAL	-	expression tag	UNP Q7NM19
N9	4	LEU	-	expression tag	UNP Q7NM19
N9	5	THR	-	expression tag	UNP Q7NM19
N9	6	GLY	-	expression tag	UNP Q7NM19
N9	7	ASP	-	expression tag	UNP Q7NM19
N9	8	ASN	-	expression tag	UNP Q7NM19
N9	9	GLN	-	expression tag	UNP Q7NM19
N9	10	GLN	-	expression tag	UNP Q7NM19
N9	11	ARG	-	expression tag	UNP Q7NM19
N9	12	GLY	-	expression tag	UNP Q7NM19
N9	13	SER	-	expression tag	UNP Q7NM19
N9	14	LYS	-	expression tag	UNP Q7NM19
N9	15	LEU	-	expression tag	UNP Q7NM19
N9	16	PHE	-	expression tag	UNP Q7NM19
N9	17	LYS	-	expression tag	UNP Q7NM19
N9	18	ILE	-	expression tag	UNP Q7NM19
N9	19	THR	-	expression tag	UNP Q7NM19
N9	20	ILE	-	expression tag	UNP Q7NM19
N9	21	ALA	-	expression tag	UNP Q7NM19
N9	22	LEU	-	expression tag	UNP Q7NM19
N9	23	SER	-	expression tag	UNP Q7NM19
N9	24	PRO	-	expression tag	UNP Q7NM19
N9	25	THR	-	expression tag	UNP Q7NM19
N9	26	LEU	-	expression tag	UNP Q7NM19
N9	27	ALA	-	expression tag	UNP Q7NM19
N9	28	HIS	-	expression tag	UNP Q7NM19
N9	29	HIS	-	expression tag	UNP Q7NM19
N9	30	PRO	-	expression tag	UNP Q7NM19
N9	31	TRP	-	expression tag	UNP Q7NM19
N9	32	PRO	-	expression tag	UNP Q7NM19
N9	33	GLY	-	expression tag	UNP Q7NM19
N9	34	LEU	-	expression tag	UNP Q7NM19

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Chain	Residue	Modelled	Actual	Comment	Reference
N9	35	ASP	-	expression tag	UNP Q7NM19
N9	36	THR	-	expression tag	UNP Q7NM19
N9	37	HIS	-	expression tag	UNP Q7NM19
N9	38	GLU	-	expression tag	UNP Q7NM19
N9	39	PRO	-	expression tag	UNP Q7NM19
N9	40	SER	-	expression tag	UNP Q7NM19
N9	41	GLN	-	expression tag	UNP Q7NM19
N9	42	SER	-	expression tag	UNP Q7NM19
N9	43	SER	-	expression tag	UNP Q7NM19
N9	44	TYR	-	expression tag	UNP Q7NM19
N9	45	SER	-	expression tag	UNP Q7NM19
N9	46	THR	-	expression tag	UNP Q7NM19
N9	47	ILE	-	expression tag	UNP Q7NM19
N9	48	VAL	-	expression tag	UNP Q7NM19
N9	49	SER	-	expression tag	UNP Q7NM19
N9	50	LEU	-	expression tag	UNP Q7NM19
N9	51	GLU	-	expression tag	UNP Q7NM19
N9	52	ARG	-	expression tag	UNP Q7NM19
N9	53	LEU	-	expression tag	UNP Q7NM19
N9	54	LEU	-	expression tag	UNP Q7NM19
N9	55	PRO	-	expression tag	UNP Q7NM19
N9	56	GLU	-	expression tag	UNP Q7NM19
Z8	1	MET	-	initiating methionine	UNP Q7NM19
Z8	2	SER	-	expression tag	UNP Q7NM19
Z8	3	VAL	-	expression tag	UNP Q7NM19
Z8	4	LEU	-	expression tag	UNP Q7NM19
Z8	5	THR	-	expression tag	UNP Q7NM19
Z8	6	GLY	-	expression tag	UNP Q7NM19
Z8	7	ASP	-	expression tag	UNP Q7NM19
Z8	8	ASN	-	expression tag	UNP Q7NM19
Z8	9	GLN	-	expression tag	UNP Q7NM19
Z8	10	GLN	-	expression tag	UNP Q7NM19
Z8	11	ARG	-	expression tag	UNP Q7NM19
Z8	12	GLY	-	expression tag	UNP Q7NM19
Z8	13	SER	-	expression tag	UNP Q7NM19
Z8	14	LYS	-	expression tag	UNP Q7NM19
Z8	15	LEU	-	expression tag	UNP Q7NM19
Z8	16	PHE	-	expression tag	UNP Q7NM19
Z8	17	LYS	-	expression tag	UNP Q7NM19
Z8	18	ILE	-	expression tag	UNP Q7NM19
Z8	19	THR	-	expression tag	UNP Q7NM19
Z8	20	ILE	-	expression tag	UNP Q7NM19

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Chain	Residue	Modelled	Actual	Comment	Reference
Z8	21	ALA	-	expression tag	UNP Q7NM19
Z8	22	LEU	-	expression tag	UNP Q7NM19
Z8	23	SER	-	expression tag	UNP Q7NM19
Z8	24	PRO	-	expression tag	UNP Q7NM19
Z8	25	THR	-	expression tag	UNP Q7NM19
Z8	26	LEU	-	expression tag	UNP Q7NM19
Z8	27	ALA	-	expression tag	UNP Q7NM19
Z8	28	HIS	-	expression tag	UNP Q7NM19
Z8	29	HIS	-	expression tag	UNP Q7NM19
Z8	30	PRO	-	expression tag	UNP Q7NM19
Z8	31	TRP	-	expression tag	UNP Q7NM19
Z8	32	PRO	-	expression tag	UNP Q7NM19
Z8	33	GLY	-	expression tag	UNP Q7NM19
Z8	34	LEU	-	expression tag	UNP Q7NM19
Z8	35	ASP	-	expression tag	UNP Q7NM19
Z8	36	THR	-	expression tag	UNP Q7NM19
Z8	37	HIS	-	expression tag	UNP Q7NM19
Z8	38	GLU	-	expression tag	UNP Q7NM19
Z8	39	PRO	-	expression tag	UNP Q7NM19
Z8	40	SER	-	expression tag	UNP Q7NM19
Z8	41	GLN	-	expression tag	UNP Q7NM19
Z8	42	SER	-	expression tag	UNP Q7NM19
Z8	43	SER	-	expression tag	UNP Q7NM19
Z8	44	TYR	-	expression tag	UNP Q7NM19
Z8	45	SER	-	expression tag	UNP Q7NM19
Z8	46	THR	-	expression tag	UNP Q7NM19
Z8	47	ILE	-	expression tag	UNP Q7NM19
Z8	48	VAL	-	expression tag	UNP Q7NM19
Z8	49	SER	-	expression tag	UNP Q7NM19
Z8	50	LEU	-	expression tag	UNP Q7NM19
Z8	51	GLU	-	expression tag	UNP Q7NM19
Z8	52	ARG	-	expression tag	UNP Q7NM19
Z8	53	LEU	-	expression tag	UNP Q7NM19
Z8	54	LEU	-	expression tag	UNP Q7NM19
Z8	55	PRO	-	expression tag	UNP Q7NM19
Z8	56	GLU	-	expression tag	UNP Q7NM19
N1	1	MET	-	initiating methionine	UNP Q7NM19
N1	2	SER	-	expression tag	UNP Q7NM19
N1	3	VAL	-	expression tag	UNP Q7NM19
N1	4	LEU	-	expression tag	UNP Q7NM19
N1	5	THR	-	expression tag	UNP Q7NM19
N1	6	GLY	-	expression tag	UNP Q7NM19

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Chain	Residue	Modelled	Actual	Comment	Reference
N1	7	ASP	-	expression tag	UNP Q7NM19
N1	8	ASN	-	expression tag	UNP Q7NM19
N1	9	GLN	-	expression tag	UNP Q7NM19
N1	10	GLN	-	expression tag	UNP Q7NM19
N1	11	ARG	-	expression tag	UNP Q7NM19
N1	12	GLY	-	expression tag	UNP Q7NM19
N1	13	SER	-	expression tag	UNP Q7NM19
N1	14	LYS	-	expression tag	UNP Q7NM19
N1	15	LEU	-	expression tag	UNP Q7NM19
N1	16	PHE	-	expression tag	UNP Q7NM19
N1	17	LYS	-	expression tag	UNP Q7NM19
N1	18	ILE	-	expression tag	UNP Q7NM19
N1	19	THR	-	expression tag	UNP Q7NM19
N1	20	ILE	-	expression tag	UNP Q7NM19
N1	21	ALA	-	expression tag	UNP Q7NM19
N1	22	LEU	-	expression tag	UNP Q7NM19
N1	23	SER	-	expression tag	UNP Q7NM19
N1	24	PRO	-	expression tag	UNP Q7NM19
N1	25	THR	-	expression tag	UNP Q7NM19
N1	26	LEU	-	expression tag	UNP Q7NM19
N1	27	ALA	-	expression tag	UNP Q7NM19
N1	28	HIS	-	expression tag	UNP Q7NM19
N1	29	HIS	-	expression tag	UNP Q7NM19
N1	30	PRO	-	expression tag	UNP Q7NM19
N1	31	TRP	-	expression tag	UNP Q7NM19
N1	32	PRO	-	expression tag	UNP Q7NM19
N1	33	GLY	-	expression tag	UNP Q7NM19
N1	34	LEU	-	expression tag	UNP Q7NM19
N1	35	ASP	-	expression tag	UNP Q7NM19
N1	36	THR	-	expression tag	UNP Q7NM19
N1	37	HIS	-	expression tag	UNP Q7NM19
N1	38	GLU	-	expression tag	UNP Q7NM19
N1	39	PRO	-	expression tag	UNP Q7NM19
N1	40	SER	-	expression tag	UNP Q7NM19
N1	41	GLN	-	expression tag	UNP Q7NM19
N1	42	SER	-	expression tag	UNP Q7NM19
N1	43	SER	-	expression tag	UNP Q7NM19
N1	44	TYR	-	expression tag	UNP Q7NM19
N1	45	SER	-	expression tag	UNP Q7NM19
N1	46	THR	-	expression tag	UNP Q7NM19
N1	47	ILE	-	expression tag	UNP Q7NM19
N1	48	VAL	-	expression tag	UNP Q7NM19

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Chain	Residue	Modelled	Actual	Comment	Reference
N1	49	SER	-	expression tag	UNP Q7NM19
N1	50	LEU	-	expression tag	UNP Q7NM19
N1	51	GLU	-	expression tag	UNP Q7NM19
N1	52	ARG	-	expression tag	UNP Q7NM19
N1	53	LEU	-	expression tag	UNP Q7NM19
N1	54	LEU	-	expression tag	UNP Q7NM19
N1	55	PRO	-	expression tag	UNP Q7NM19
N1	56	GLU	-	expression tag	UNP Q7NM19

- Molecule 6 is a protein called Glr2806 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	M2	279	Total	C	N	O	S	0	0
			2190	1381	387	417	5		
6	M6	279	Total	C	N	O	S	0	0
			2190	1381	387	417	5		

- Molecule 7 is a protein called CpcD protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	N2	70	Total	C	N	O	S	0	0
			545	349	91	103	2		
7	N6	70	Total	C	N	O	S	0	0
			545	349	91	103	2		

- Molecule 8 is a protein called Allophycocyanin alpha subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	K5	160	Total	C	N	O	S	0	0
			1222	771	209	237	5		
8	M5	160	Total	C	N	O	S	0	0
			1222	771	209	237	5		
8	O5	160	Total	C	N	O	S	0	0
			1222	771	209	237	5		
8	A5	160	Total	C	N	O	S	0	0
			1222	771	209	237	5		
8	C5	160	Total	C	N	O	S	0	0
			1222	771	209	237	5		
8	E5	160	Total	C	N	O	S	0	0
			1222	771	209	237	5		
8	G5	160	Total	C	N	O	S	0	0
			1222	771	209	237	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
8	I5	160	Total	C	N	O	S	0	0
			1222	771	209	237	5		
8	c5	160	Total	C	N	O	S	0	0
			1222	771	209	237	5		
8	e5	160	Total	C	N	O	S	0	0
			1222	771	209	237	5		
8	Q5	160	Total	C	N	O	S	0	0
			1222	771	209	237	5		
8	S5	160	Total	C	N	O	S	0	0
			1222	771	209	237	5		
8	U5	160	Total	C	N	O	S	0	0
			1222	771	209	237	5		
8	W5	160	Total	C	N	O	S	0	0
			1222	771	209	237	5		
8	Y5	160	Total	C	N	O	S	0	0
			1222	771	209	237	5		
8	a5	160	Total	C	N	O	S	0	0
			1222	771	209	237	5		
8	A7	160	Total	C	N	O	S	0	0
			1222	771	209	237	5		
8	O7	160	Total	C	N	O	S	0	0
			1222	771	209	237	5		
8	Q7	160	Total	C	N	O	S	0	0
			1222	771	209	237	5		
8	S7	160	Total	C	N	O	S	0	0
			1222	771	209	237	5		
8	C7	160	Total	C	N	O	S	0	0
			1222	771	209	237	5		
8	E7	160	Total	C	N	O	S	0	0
			1222	771	209	237	5		
8	G7	160	Total	C	N	O	S	0	0
			1222	771	209	237	5		
8	I7	160	Total	C	N	O	S	0	0
			1222	771	209	237	5		
8	K7	160	Total	C	N	O	S	0	0
			1222	771	209	237	5		
8	M7	160	Total	C	N	O	S	0	0
			1222	771	209	237	5		
8	g7	160	Total	C	N	O	S	0	0
			1222	771	209	237	5		
8	i7	160	Total	C	N	O	S	0	0
			1222	771	209	237	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
8	k7	160	Total	C	N	O	S	0	0
			1222	771	209	237	5		
8	U7	160	Total	C	N	O	S	0	0
			1222	771	209	237	5		
8	W7	160	Total	C	N	O	S	0	0
			1222	771	209	237	5		
8	Y7	160	Total	C	N	O	S	0	0
			1222	771	209	237	5		
8	a7	160	Total	C	N	O	S	0	0
			1222	771	209	237	5		
8	c7	160	Total	C	N	O	S	0	0
			1222	771	209	237	5		
8	e7	160	Total	C	N	O	S	0	0
			1222	771	209	237	5		
8	m7	160	Total	C	N	O	S	0	0
			1222	771	209	237	5		
8	o7	160	Total	C	N	O	S	0	0
			1222	771	209	237	5		
8	q7	160	Total	C	N	O	S	0	0
			1222	771	209	237	5		
8	s7	160	Total	C	N	O	S	0	0
			1222	771	209	237	5		
8	u7	160	Total	C	N	O	S	0	0
			1222	771	209	237	5		

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K5	61	ILE	LYS	conflict	UNP Q7NL80
M5	61	ILE	LYS	conflict	UNP Q7NL80
O5	61	ILE	LYS	conflict	UNP Q7NL80
A5	61	ILE	LYS	conflict	UNP Q7NL80
C5	61	ILE	LYS	conflict	UNP Q7NL80
E5	61	ILE	LYS	conflict	UNP Q7NL80
G5	61	ILE	LYS	conflict	UNP Q7NL80
I5	61	ILE	LYS	conflict	UNP Q7NL80
c5	61	ILE	LYS	conflict	UNP Q7NL80
e5	61	ILE	LYS	conflict	UNP Q7NL80
Q5	61	ILE	LYS	conflict	UNP Q7NL80
S5	61	ILE	LYS	conflict	UNP Q7NL80
U5	61	ILE	LYS	conflict	UNP Q7NL80
W5	61	ILE	LYS	conflict	UNP Q7NL80
Y5	61	ILE	LYS	conflict	UNP Q7NL80

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Chain	Residue	Modelled	Actual	Comment	Reference
a5	61	ILE	LYS	conflict	UNP Q7NL80
A7	61	ILE	LYS	conflict	UNP Q7NL80
O7	61	ILE	LYS	conflict	UNP Q7NL80
Q7	61	ILE	LYS	conflict	UNP Q7NL80
S7	61	ILE	LYS	conflict	UNP Q7NL80
C7	61	ILE	LYS	conflict	UNP Q7NL80
E7	61	ILE	LYS	conflict	UNP Q7NL80
G7	61	ILE	LYS	conflict	UNP Q7NL80
I7	61	ILE	LYS	conflict	UNP Q7NL80
K7	61	ILE	LYS	conflict	UNP Q7NL80
M7	61	ILE	LYS	conflict	UNP Q7NL80
g7	61	ILE	LYS	conflict	UNP Q7NL80
i7	61	ILE	LYS	conflict	UNP Q7NL80
k7	61	ILE	LYS	conflict	UNP Q7NL80
U7	61	ILE	LYS	conflict	UNP Q7NL80
W7	61	ILE	LYS	conflict	UNP Q7NL80
Y7	61	ILE	LYS	conflict	UNP Q7NL80
a7	61	ILE	LYS	conflict	UNP Q7NL80
c7	61	ILE	LYS	conflict	UNP Q7NL80
e7	61	ILE	LYS	conflict	UNP Q7NL80
m7	61	ILE	LYS	conflict	UNP Q7NL80
o7	61	ILE	LYS	conflict	UNP Q7NL80
q7	61	ILE	LYS	conflict	UNP Q7NL80
s7	61	ILE	LYS	conflict	UNP Q7NL80
u7	61	ILE	LYS	conflict	UNP Q7NL80

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	z5	68	Total	C	N	O	S	0	0
			538	345	98	94	1		
9	i5	68	Total	C	N	O	S	0	0
			538	345	98	94	1		
9	z7	68	Total	C	N	O	S	0	0
			538	345	98	94	1		
9	w7	68	Total	C	N	O	S	0	0
			538	345	98	94	1		
9	x7	68	Total	C	N	O	S	0	0
			538	345	98	94	1		
9	y7	68	Total	C	N	O	S	0	0
			538	345	98	94	1		

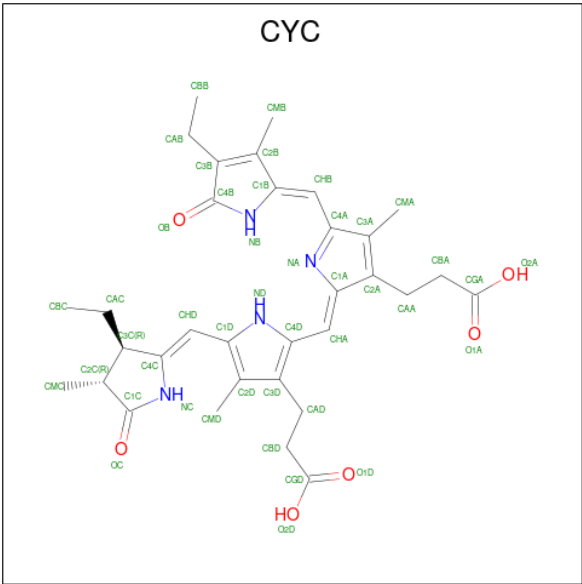
- Molecule 10 is a protein called Phycobiliprotein ApcE.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	j5	1108	8819	5593	1559	1647	20	0	0
10	k5	1108	8819	5593	1559	1647	20	0	0

- Molecule 11 is a protein called Glr1262 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	a9	800	6326	3959	1137	1218	12	0	0
11	aA	800	6326	3959	1137	1218	12	0	0

- Molecule 12 is PHYCOCYANOBILIN (CCD ID: CYC) (formula: C₃₃H₄₀N₄O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
12	A	1	43	33	4	6	0
12	Z	1	43	33	4	6	0
12	AA	1	43	33	4	6	0
12	BA	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
12	BA	1	43	33	4	6	0
12	CA	1	43	33	4	6	0
12	DA	1	43	33	4	6	0
12	DA	1	43	33	4	6	0
12	EA	1	43	33	4	6	0
12	FA	1	43	33	4	6	0
12	GA	1	43	33	4	6	0
12	HA	1	43	33	4	6	0
12	HA	1	43	33	4	6	0
12	IA	1	43	33	4	6	0
12	JA	1	43	33	4	6	0
12	JA	1	43	33	4	6	0
12	KA	1	43	33	4	6	0
12	LA	1	43	33	4	6	0
12	LA	1	43	33	4	6	0
12	OA	1	43	33	4	6	0
12	PA	1	43	33	4	6	0
12	PA	1	43	33	4	6	0
12	QA	1	43	33	4	6	0
12	RA	1	43	33	4	6	0
12	RA	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
12	SA	1	Total 43	C 33	N 4	O 6	0
12	TA	1	Total 43	C 33	N 4	O 6	0
12	TA	1	Total 43	C 33	N 4	O 6	0
12	UA	1	Total 43	C 33	N 4	O 6	0
12	VA	1	Total 43	C 33	N 4	O 6	0
12	VA	1	Total 43	C 33	N 4	O 6	0
12	WA	1	Total 43	C 33	N 4	O 6	0
12	XA	1	Total 43	C 33	N 4	O 6	0
12	XA	1	Total 43	C 33	N 4	O 6	0
12	YA	1	Total 43	C 33	N 4	O 6	0
12	ZA	1	Total 43	C 33	N 4	O 6	0
12	ZA	1	Total 43	C 33	N 4	O 6	0
12	O1	1	Total 43	C 33	N 4	O 6	0
12	P1	1	Total 43	C 33	N 4	O 6	0
12	P1	1	Total 43	C 33	N 4	O 6	0
12	Q1	1	Total 43	C 33	N 4	O 6	0
12	R1	1	Total 43	C 33	N 4	O 6	0
12	R1	1	Total 43	C 33	N 4	O 6	0
12	S1	1	Total 43	C 33	N 4	O 6	0
12	A1	1	Total 43	C 33	N 4	O 6	0
12	G3	1	Total 43	C 33	N 4	O 6	0

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Mol	Chain	Residues	Atoms				AltConf
12	H3	1	Total 43	C 33	N 4	O 6	0
12	H3	1	Total 43	C 33	N 4	O 6	0
12	I3	1	Total 43	C 33	N 4	O 6	0
12	J3	1	Total 43	C 33	N 4	O 6	0
12	J3	1	Total 43	C 33	N 4	O 6	0
12	K3	1	Total 43	C 33	N 4	O 6	0
12	G2	1	Total 43	C 33	N 4	O 6	0
12	H2	1	Total 43	C 33	N 4	O 6	0
12	H2	1	Total 43	C 33	N 4	O 6	0
12	I2	1	Total 43	C 33	N 4	O 6	0
12	J2	1	Total 43	C 33	N 4	O 6	0
12	J2	1	Total 43	C 33	N 4	O 6	0
12	K2	1	Total 43	C 33	N 4	O 6	0
12	L2	1	Total 43	C 33	N 4	O 6	0
12	L2	1	Total 43	C 33	N 4	O 6	0
12	N2	1	Total 43	C 33	N 4	O 6	0
12	A3	1	Total 43	C 33	N 4	O 6	0
12	B3	1	Total 43	C 33	N 4	O 6	0
12	B3	1	Total 43	C 33	N 4	O 6	0
12	C3	1	Total 43	C 33	N 4	O 6	0
12	D3	1	Total 43	C 33	N 4	O 6	0

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Mol	Chain	Residues	Atoms				AltConf
12	D3	1	Total 43	C 33	N 4	O 6	0
12	E3	1	Total 43	C 33	N 4	O 6	0
12	F3	1	Total 43	C 33	N 4	O 6	0
12	F3	1	Total 43	C 33	N 4	O 6	0
12	Z3	1	Total 43	C 33	N 4	O 6	0
12	Z3	1	Total 43	C 33	N 4	O 6	0
12	A4	1	Total 43	C 33	N 4	O 6	0
12	B4	1	Total 43	C 33	N 4	O 6	0
12	B4	1	Total 43	C 33	N 4	O 6	0
12	C4	1	Total 43	C 33	N 4	O 6	0
12	D4	1	Total 43	C 33	N 4	O 6	0
12	D4	1	Total 43	C 33	N 4	O 6	0
12	L3	1	Total 43	C 33	N 4	O 6	0
12	L3	1	Total 43	C 33	N 4	O 6	0
12	O3	1	Total 43	C 33	N 4	O 6	0
12	P3	1	Total 43	C 33	N 4	O 6	0
12	P3	1	Total 43	C 33	N 4	O 6	0
12	Q3	1	Total 43	C 33	N 4	O 6	0
12	R3	1	Total 43	C 33	N 4	O 6	0
12	R3	1	Total 43	C 33	N 4	O 6	0
12	S3	1	Total 43	C 33	N 4	O 6	0

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Mol	Chain	Residues	Atoms				AltConf
12	T3	1	Total	C	N	O	0
			43	33	4	6	
12	T3	1	Total	C	N	O	0
			43	33	4	6	
12	U3	1	Total	C	N	O	0
			43	33	4	6	
12	V3	1	Total	C	N	O	0
			43	33	4	6	
12	V3	1	Total	C	N	O	0
			43	33	4	6	
12	W3	1	Total	C	N	O	0
			43	33	4	6	
12	X3	1	Total	C	N	O	0
			43	33	4	6	
12	X3	1	Total	C	N	O	0
			43	33	4	6	
12	Y3	1	Total	C	N	O	0
			43	33	4	6	
12	B1	1	Total	C	N	O	0
			43	33	4	6	
12	B1	1	Total	C	N	O	0
			43	33	4	6	
12	S4	1	Total	C	N	O	0
			43	33	4	6	
12	S4	1	Total	C	N	O	0
			43	33	4	6	
12	T4	1	Total	C	N	O	0
			43	33	4	6	
12	U4	1	Total	C	N	O	0
			43	33	4	6	
12	U4	1	Total	C	N	O	0
			43	33	4	6	
12	V4	1	Total	C	N	O	0
			43	33	4	6	
12	W4	1	Total	C	N	O	0
			43	33	4	6	
12	W4	1	Total	C	N	O	0
			43	33	4	6	
12	E4	1	Total	C	N	O	0
			43	33	4	6	
12	F4	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
12	F4	1	Total 43	C 33	N 4	O 6	0
12	G4	1	Total 43	C 33	N 4	O 6	0
12	H4	1	Total 43	C 33	N 4	O 6	0
12	H4	1	Total 43	C 33	N 4	O 6	0
12	I4	1	Total 43	C 33	N 4	O 6	0
12	J4	1	Total 43	C 33	N 4	O 6	0
12	J4	1	Total 43	C 33	N 4	O 6	0
12	K4	1	Total 43	C 33	N 4	O 6	0
12	L4	1	Total 43	C 33	N 4	O 6	0
12	L4	1	Total 43	C 33	N 4	O 6	0
12	M4	1	Total 43	C 33	N 4	O 6	0
12	N4	1	Total 43	C 33	N 4	O 6	0
12	O4	1	Total 43	C 33	N 4	O 6	0
12	O4	1	Total 43	C 33	N 4	O 6	0
12	P4	1	Total 43	C 33	N 4	O 6	0
12	Q4	1	Total 43	C 33	N 4	O 6	0
12	R4	1	Total 43	C 33	N 4	O 6	0
12	K5	1	Total 43	C 33	N 4	O 6	0
12	L5	1	Total 43	C 33	N 4	O 6	0
12	M5	1	Total 43	C 33	N 4	O 6	0
12	N5	1	Total 43	C 33	N 4	O 6	0

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Mol	Chain	Residues	Atoms				AltConf
12	O5	1	Total 43	C 33	N 4	O 6	0
12	X4	1	Total 43	C 33	N 4	O 6	0
12	Y4	1	Total 43	C 33	N 4	O 6	0
12	Z4	1	Total 43	C 33	N 4	O 6	0
12	A5	1	Total 43	C 33	N 4	O 6	0
12	B5	1	Total 43	C 33	N 4	O 6	0
12	C5	1	Total 43	C 33	N 4	O 6	0
12	D5	1	Total 43	C 33	N 4	O 6	0
12	E5	1	Total 43	C 33	N 4	O 6	0
12	F5	1	Total 43	C 33	N 4	O 6	0
12	G5	1	Total 43	C 33	N 4	O 6	0
12	H5	1	Total 43	C 33	N 4	O 6	0
12	I5	1	Total 43	C 33	N 4	O 6	0
12	J5	1	Total 43	C 33	N 4	O 6	0
12	C1	1	Total 43	C 33	N 4	O 6	0
12	c5	1	Total 43	C 33	N 4	O 6	0
12	d5	1	Total 43	C 33	N 4	O 6	0
12	e5	1	Total 43	C 33	N 4	O 6	0
12	f5	1	Total 43	C 33	N 4	O 6	0
12	P5	1	Total 43	C 33	N 4	O 6	0
12	Q5	1	Total 43	C 33	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
12	R5	1	Total 43	C 33	N 4	O 6	0	
12	S5	1	Total 43	C 33	N 4	O 6	0	
12	T5	1	Total 43	C 33	N 4	O 6	0	
12	U5	1	Total 43	C 33	N 4	O 6	0	
12	V5	1	Total 43	C 33	N 4	O 6	0	
12	W5	1	Total 43	C 33	N 4	O 6	0	
12	X5	1	Total 43	C 33	N 4	O 6	0	
12	Y5	1	Total 43	C 33	N 4	O 6	0	
12	Z5	1	Total 43	C 33	N 4	O 6	0	
12	a5	1	Total 43	C 33	N 4	O 6	0	
12	b5	1	Total 43	C 33	N 4	O 6	0	
12	J6	1	Total 43	C 33	N 4	O 6	0	
12	J6	1	Total 43	C 33	N 4	O 6	0	
12	K6	1	Total 43	C 33	N 4	O 6	0	
12	L6	1	Total 43	C 33	N 4	O 6	0	
12	L6	1	Total 43	C 33	N 4	O 6	0	
12	N6	1	Total 43	C 33	N 4	O 6	0	
12	A7	1	Total 43	C 33	N 4	O 6	0	
12	j5	1	Total 81	C 33	H 38	N 4 O 6	0	
12	j5	1	Total 43	C 33	N 4	O 6	0	
12	k5	1	Total 81	C 33	H 38	N 4 O 6	0	

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Mol	Chain	Residues	Atoms				AltConf
12	k5	1	Total	C	N	O	0
			43	33	4	6	
12	k5	1	Total	C	N	O	0
			43	33	4	6	
12	k5	1	Total	C	N	O	0
			43	33	4	6	
12	A6	1	Total	C	N	O	0
			43	33	4	6	
12	B6	1	Total	C	N	O	0
			43	33	4	6	
12	C6	1	Total	C	N	O	0
			43	33	4	6	
12	D6	1	Total	C	N	O	0
			43	33	4	6	
12	D6	1	Total	C	N	O	0
			43	33	4	6	
12	E6	1	Total	C	N	O	0
			43	33	4	6	
12	F6	1	Total	C	N	O	0
			43	33	4	6	
12	F6	1	Total	C	N	O	0
			43	33	4	6	
12	G6	1	Total	C	N	O	0
			43	33	4	6	
12	H6	1	Total	C	N	O	0
			43	33	4	6	
12	H6	1	Total	C	N	O	0
			43	33	4	6	
12	I6	1	Total	C	N	O	0
			43	33	4	6	
12	D1	1	Total	C	N	O	0
			43	33	4	6	
12	D1	1	Total	C	N	O	0
			43	33	4	6	
12	O7	1	Total	C	N	O	0
			43	33	4	6	
12	P7	1	Total	C	N	O	0
			43	33	4	6	
12	Q7	1	Total	C	N	O	0
			43	33	4	6	
12	R7	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
12	S7	1	Total 43	C 33	N 4	O 6	0
12	B7	1	Total 43	C 33	N 4	O 6	0
12	C7	1	Total 43	C 33	N 4	O 6	0
12	D7	1	Total 43	C 33	N 4	O 6	0
12	E7	1	Total 43	C 33	N 4	O 6	0
12	F7	1	Total 43	C 33	N 4	O 6	0
12	G7	1	Total 43	C 33	N 4	O 6	0
12	H7	1	Total 43	C 33	N 4	O 6	0
12	I7	1	Total 43	C 33	N 4	O 6	0
12	J7	1	Total 43	C 33	N 4	O 6	0
12	K7	1	Total 43	C 33	N 4	O 6	0
12	L7	1	Total 43	C 33	N 4	O 6	0
12	M7	1	Total 43	C 33	N 4	O 6	0
12	N7	1	Total 43	C 33	N 4	O 6	0
12	g7	1	Total 43	C 33	N 4	O 6	0
12	h7	1	Total 43	C 33	N 4	O 6	0
12	i7	1	Total 43	C 33	N 4	O 6	0
12	j7	1	Total 43	C 33	N 4	O 6	0
12	k7	1	Total 43	C 33	N 4	O 6	0
12	T7	1	Total 43	C 33	N 4	O 6	0
12	U7	1	Total 43	C 33	N 4	O 6	0

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Mol	Chain	Residues	Atoms				AltConf
12	V7	1	Total 43	C 33	N 4	O 6	0
12	W7	1	Total 43	C 33	N 4	O 6	0
12	X7	1	Total 43	C 33	N 4	O 6	0
12	Y7	1	Total 43	C 33	N 4	O 6	0
12	a7	1	Total 43	C 33	N 4	O 6	0
12	b7	1	Total 43	C 33	N 4	O 6	0
12	c7	1	Total 43	C 33	N 4	O 6	0
12	d7	1	Total 43	C 33	N 4	O 6	0
12	e7	1	Total 43	C 33	N 4	O 6	0
12	f7	1	Total 43	C 33	N 4	O 6	0
12	E1	1	Total 43	C 33	N 4	O 6	0
12	A8	1	Total 43	C 33	N 4	O 6	0
12	B8	1	Total 43	C 33	N 4	O 6	0
12	B8	1	Total 43	C 33	N 4	O 6	0
12	C8	1	Total 43	C 33	N 4	O 6	0
12	D8	1	Total 43	C 33	N 4	O 6	0
12	D8	1	Total 43	C 33	N 4	O 6	0
12	E8	1	Total 43	C 33	N 4	O 6	0
12	m7	1	Total 43	C 33	N 4	O 6	0
12	o7	1	Total 43	C 33	N 4	O 6	0
12	p7	1	Total 43	C 33	N 4	O 6	0

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Mol	Chain	Residues	Atoms				AltConf
12	q7	1	Total	C	N	O	0
			43	33	4	6	
12	r7	1	Total	C	N	O	0
			43	33	4	6	
12	s7	1	Total	C	N	O	0
			43	33	4	6	
12	u7	1	Total	C	N	O	0
			43	33	4	6	
12	v7	1	Total	C	N	O	0
			43	33	4	6	
12	T8	1	Total	C	N	O	0
			43	33	4	6	
12	U8	1	Total	C	N	O	0
			43	33	4	6	
12	U8	1	Total	C	N	O	0
			43	33	4	6	
12	V8	1	Total	C	N	O	0
			43	33	4	6	
12	W8	1	Total	C	N	O	0
			43	33	4	6	
12	W8	1	Total	C	N	O	0
			43	33	4	6	
12	X8	1	Total	C	N	O	0
			43	33	4	6	
12	F8	1	Total	C	N	O	0
			43	33	4	6	
12	F8	1	Total	C	N	O	0
			43	33	4	6	
12	G8	1	Total	C	N	O	0
			43	33	4	6	
12	H8	1	Total	C	N	O	0
			43	33	4	6	
12	H8	1	Total	C	N	O	0
			43	33	4	6	
12	I8	1	Total	C	N	O	0
			43	33	4	6	
12	J8	1	Total	C	N	O	0
			43	33	4	6	
12	J8	1	Total	C	N	O	0
			43	33	4	6	
12	K8	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
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12	M8	1	Total 43	C 33	N 4	O 6	0
12	M8	1	Total 43	C 33	N 4	O 6	0
12	N8	1	Total 43	C 33	N 4	O 6	0
12	O8	1	Total 43	C 33	N 4	O 6	0
12	O8	1	Total 43	C 33	N 4	O 6	0
12	P8	1	Total 43	C 33	N 4	O 6	0
12	Q8	1	Total 43	C 33	N 4	O 6	0
12	R8	1	Total 43	C 33	N 4	O 6	0
12	S8	1	Total 43	C 33	N 4	O 6	0
12	F1	1	Total 43	C 33	N 4	O 6	0
12	F1	1	Total 43	C 33	N 4	O 6	0
12	L9	1	Total 43	C 33	N 4	O 6	0
12	L9	1	Total 43	C 33	N 4	O 6	0
12	O9	1	Total 43	C 33	N 4	O 6	0
12	P9	1	Total 43	C 33	N 4	O 6	0
12	P9	1	Total 43	C 33	N 4	O 6	0
12	Q9	1	Total 43	C 33	N 4	O 6	0
12	Y8	1	Total 43	C 33	N 4	O 6	0
12	Z8	1	Total 43	C 33	N 4	O 6	0
12	A9	1	Total 43	C 33	N 4	O 6	0

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Mol	Chain	Residues	Atoms				AltConf
12	B9	1	Total 43	C 33	N 4	O 6	0
12	B9	1	Total 43	C 33	N 4	O 6	0
12	C9	1	Total 43	C 33	N 4	O 6	0
12	D9	1	Total 43	C 33	N 4	O 6	0
12	D9	1	Total 43	C 33	N 4	O 6	0
12	E9	1	Total 43	C 33	N 4	O 6	0
12	F9	1	Total 43	C 33	N 4	O 6	0
12	F9	1	Total 43	C 33	N 4	O 6	0
12	F9	1	Total 43	C 33	N 4	O 6	0
12	G9	1	Total 43	C 33	N 4	O 6	0
12	H9	1	Total 43	C 33	N 4	O 6	0
12	H9	1	Total 43	C 33	N 4	O 6	0
12	I9	1	Total 43	C 33	N 4	O 6	0
12	J9	1	Total 43	C 33	N 4	O 6	0
12	J9	1	Total 43	C 33	N 4	O 6	0
12	K9	1	Total 43	C 33	N 4	O 6	0
12	R9	1	Total 43	C 33	N 4	O 6	0
12	R9	1	Total 43	C 33	N 4	O 6	0
12	S9	1	Total 43	C 33	N 4	O 6	0
12	T9	1	Total 43	C 33	N 4	O 6	0
12	T9	1	Total 43	C 33	N 4	O 6	0

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Mol	Chain	Residues	Atoms				AltConf
12	U9	1	Total 43	C 33	N 4	O 6	0
12	V9	1	Total 43	C 33	N 4	O 6	0
12	V9	1	Total 43	C 33	N 4	O 6	0
12	W9	1	Total 43	C 33	N 4	O 6	0
12	X9	1	Total 43	C 33	N 4	O 6	0
12	X9	1	Total 43	C 33	N 4	O 6	0
12	Y9	1	Total 43	C 33	N 4	O 6	0
12	Z9	1	Total 43	C 33	N 4	O 6	0
12	Z9	1	Total 43	C 33	N 4	O 6	0
12	G1	1	Total 43	C 33	N 4	O 6	0
12	a9	1	Total 43	C 33	N 4	O 6	0
12	aA	1	Total 43	C 33	N 4	O 6	0
12	aA	1	Total 43	C 33	N 4	O 6	0
12	H1	1	Total 43	C 33	N 4	O 6	0
12	H1	1	Total 43	C 33	N 4	O 6	0
12	I1	1	Total 43	C 33	N 4	O 6	0
12	J1	1	Total 43	C 33	N 4	O 6	0
12	K1	1	Total 43	C 33	N 4	O 6	0
12	L1	1	Total 43	C 33	N 4	O 6	0
12	T1	1	Total 43	C 33	N 4	O 6	0
12	T1	1	Total 43	C 33	N 4	O 6	0

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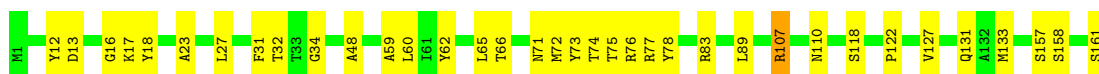
Mol	Chain	Residues	Atoms				AltConf
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12	V1	1	Total 43	C 33	N 4	O 6	0
12	V1	1	Total 43	C 33	N 4	O 6	0
12	W1	1	Total 43	C 33	N 4	O 6	0
12	X1	1	Total 43	C 33	N 4	O 6	0
12	X1	1	Total 43	C 33	N 4	O 6	0
12	Y1	1	Total 43	C 33	N 4	O 6	0
12	Z1	1	Total 43	C 33	N 4	O 6	0
12	Z1	1	Total 43	C 33	N 4	O 6	0
12	A2	1	Total 43	C 33	N 4	O 6	0
12	B2	1	Total 43	C 33	N 4	O 6	0
12	C2	1	Total 43	C 33	N 4	O 6	0
12	D2	1	Total 43	C 33	N 4	O 6	0
12	D2	1	Total 43	C 33	N 4	O 6	0
12	E2	1	Total 43	C 33	N 4	O 6	0
12	F2	1	Total 43	C 33	N 4	O 6	0
12	F2	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: Allophycocyanin beta subunit

Chain A: 



- Molecule 1: Allophycocyanin beta subunit

Chain Z: 



- Molecule 1: Allophycocyanin beta subunit

Chain L5: 



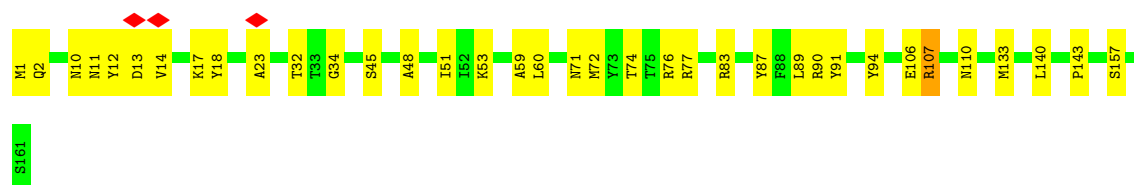
- Molecule 1: Allophycocyanin beta subunit

Chain N5: 



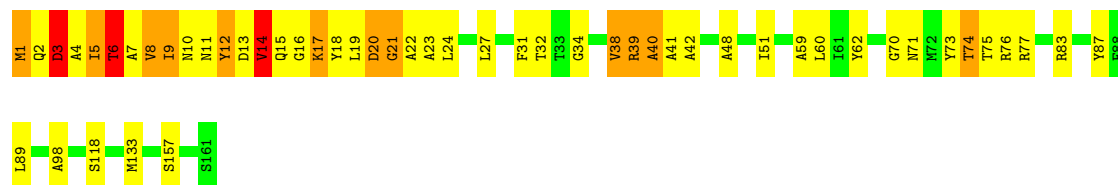
- Molecule 1: Allophycocyanin beta subunit

Chain B5: 



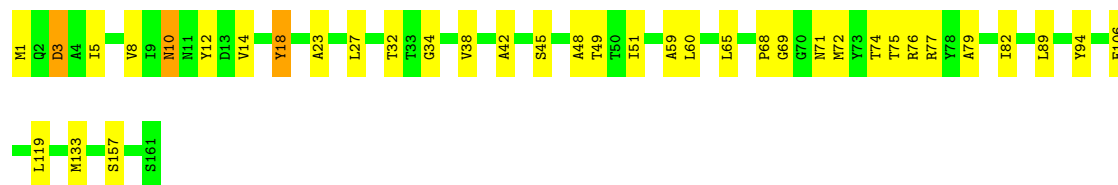
- Molecule 1: Allophycocyanin beta subunit

Chain D5: .



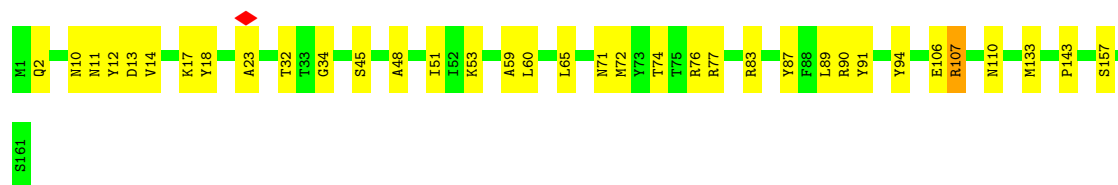
- Molecule 1: Allophycocyanin beta subunit

Chain F5: .



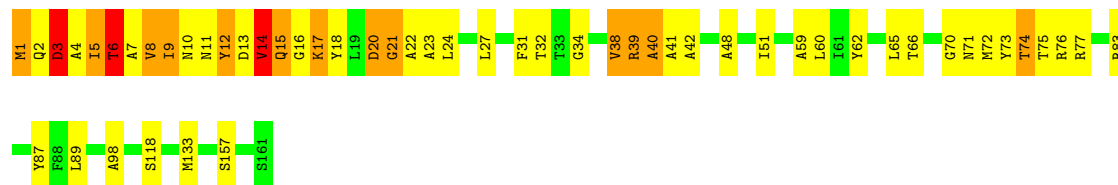
- Molecule 1: Allophycocyanin beta subunit

Chain H5: .



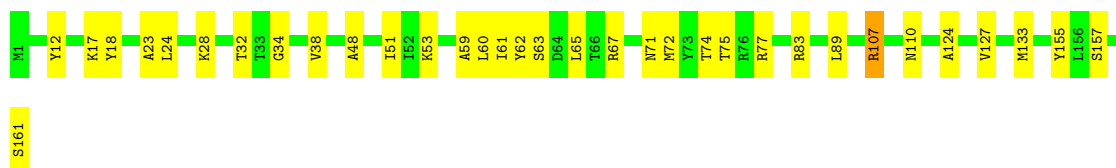
- Molecule 1: Allophycocyanin beta subunit

Chain J5: .

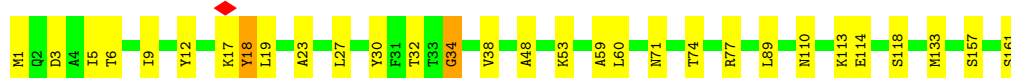
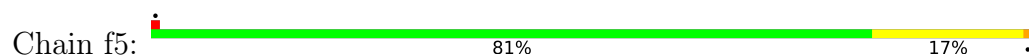


- Molecule 1: Allophycocyanin beta subunit

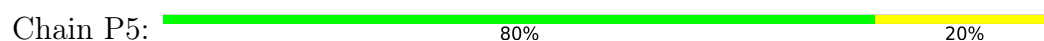
Chain d5: .



- Molecule 1: Allophycocyanin beta subunit



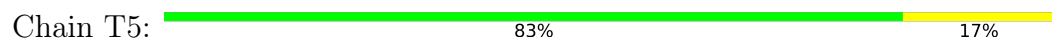
- Molecule 1: Allophycocyanin beta subunit



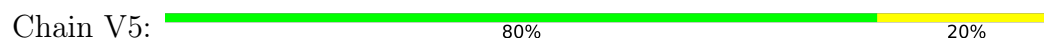
- Molecule 1: Allophycocyanin beta subunit



- Molecule 1: Allophycocyanin beta subunit

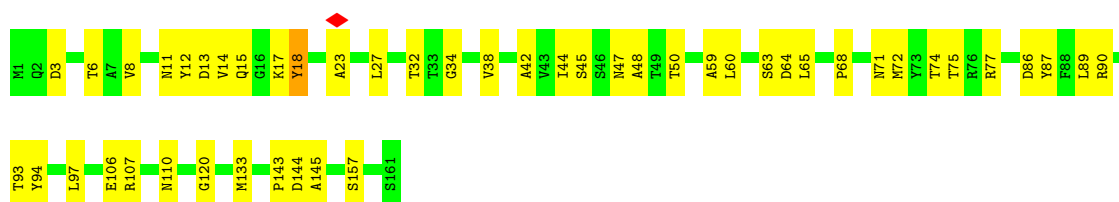


- Molecule 1: Allophycocyanin beta subunit



- Molecule 1: Allophycocyanin beta subunit





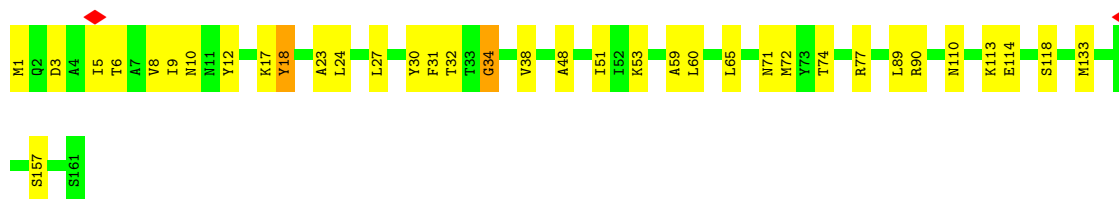
- Molecule 1: Allophycocyanin beta subunit

Chain Z5: 80% 20%



- Molecule 1: Allophycocyanin beta subunit

Chain b5: 78% 21%



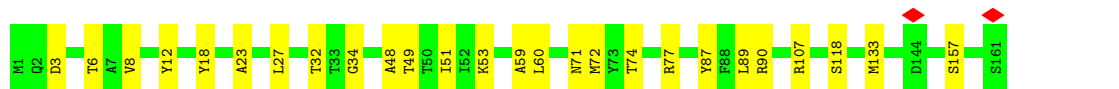
- Molecule 1: Allophycocyanin beta subunit

Chain P7: 83% 17%



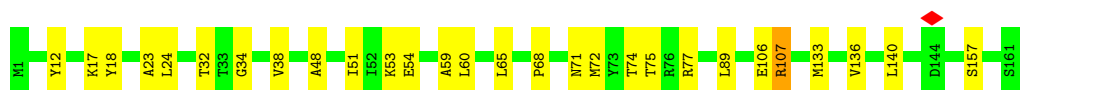
- Molecule 1: Allophycocyanin beta subunit

Chain R7: 84% 16%



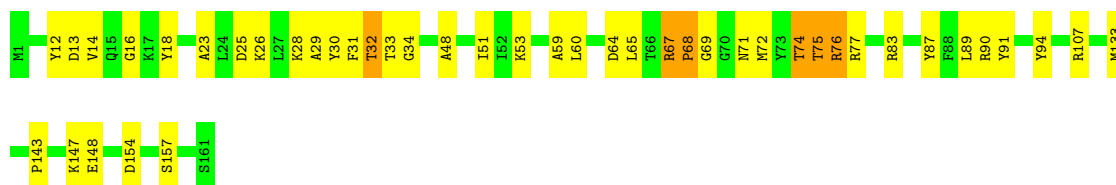
- Molecule 1: Allophycocyanin beta subunit

Chain B7: 83% 17%



- Molecule 1: Allophycocyanin beta subunit

Chain D7: 73% 24%



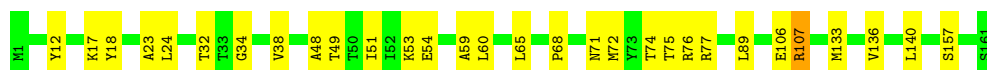
- Molecule 1: Allophycocyanin beta subunit

Chain F7: 85% 15%



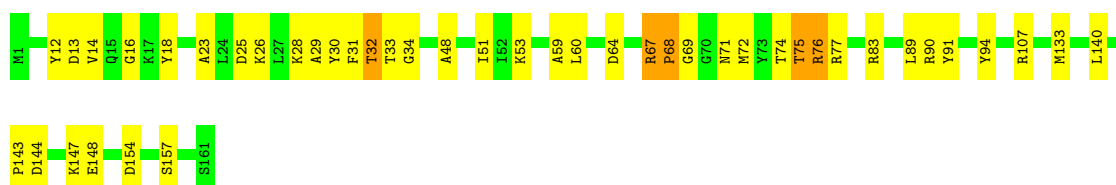
- Molecule 1: Allophycocyanin beta subunit

Chain H7: 81% 18%



- Molecule 1: Allophycocyanin beta subunit

Chain J7: 73% 24%



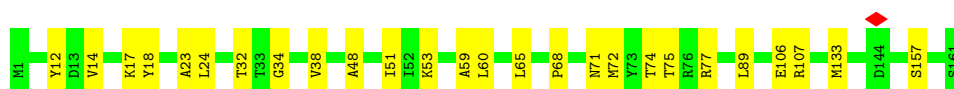
- Molecule 1: Allophycocyanin beta subunit

Chain L7: 85% 15%



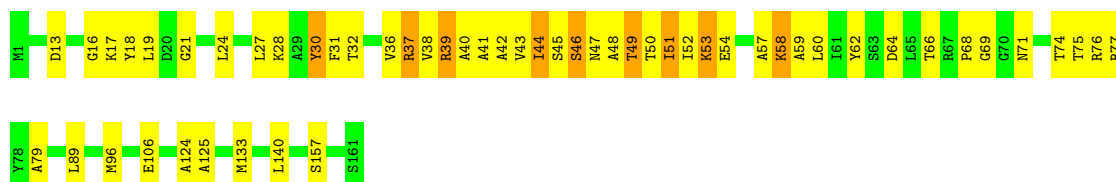
- Molecule 1: Allophycocyanin beta subunit

Chain N7: 84% 16%



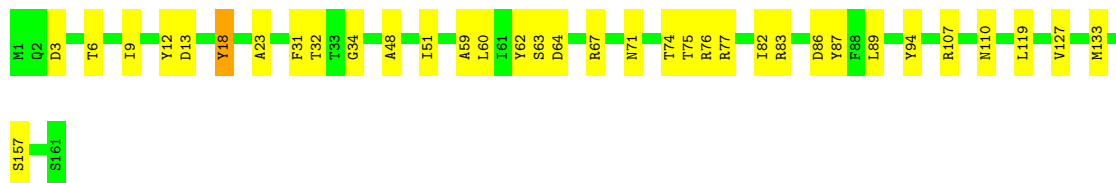
- Molecule 1: Allophycocyanin beta subunit

Chain h7: 66% 28% 6%



- Molecule 1: Allophycocyanin beta subunit

Chain j7: 78% 21% .



- Molecule 1: Allophycocyanin beta subunit

Chain T7: 81% 19%



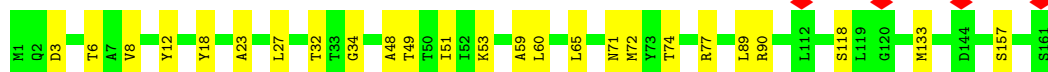
- Molecule 1: Allophycocyanin beta subunit

Chain V7: 83% 16% .



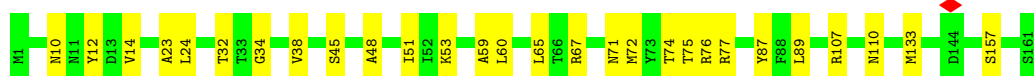
- Molecule 1: Allophycocyanin beta subunit

Chain X7: 84% 16%



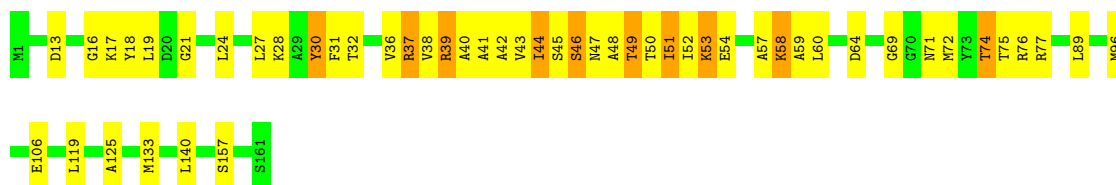
- Molecule 1: Allophycocyanin beta subunit

Chain Z7: 83% 17%



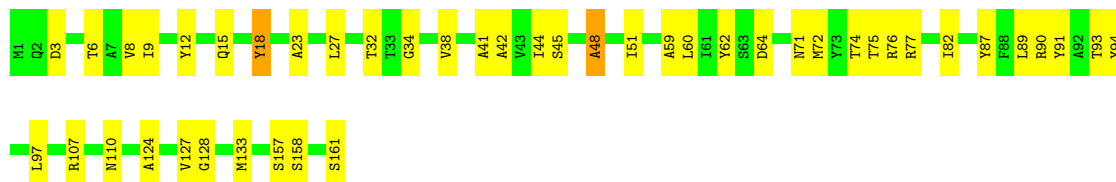
- Molecule 1: Allophycocyanin beta subunit

Chain b7: 68% 25% 6%



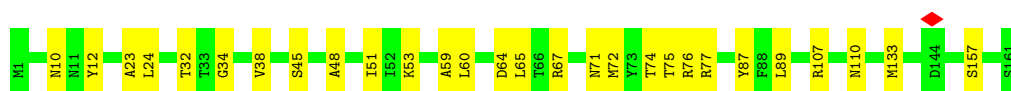
- Molecule 1: Allophycocyanin beta subunit

Chain d7: 72% 27%



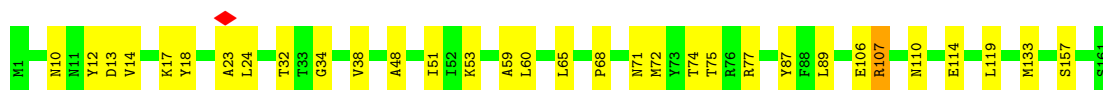
- Molecule 1: Allophycocyanin beta subunit

Chain f7: 83% 17%



- Molecule 1: Allophycocyanin beta subunit

Chain i7: 80% 19%



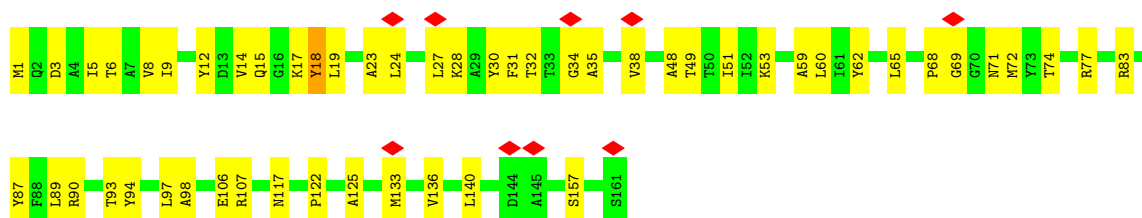
- Molecule 1: Allophycocyanin beta subunit

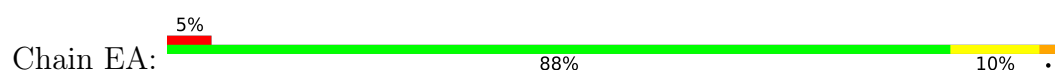
Chain n7: 79% 21%



- Molecule 1: Allophycocyanin beta subunit

Chain p7: 6% 67% 32%

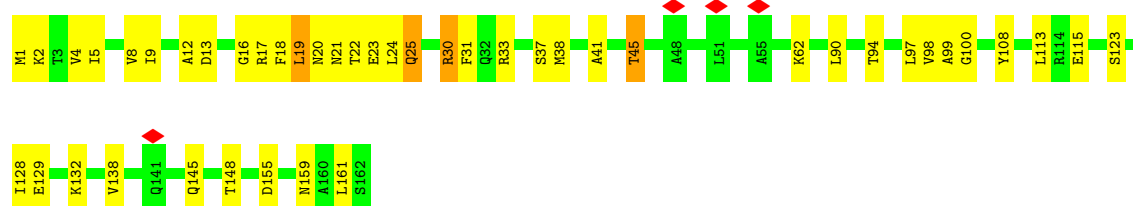




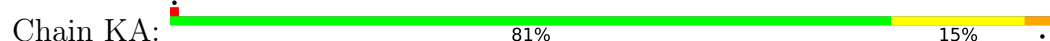
- Molecule 2: Phycocyanin alpha chain



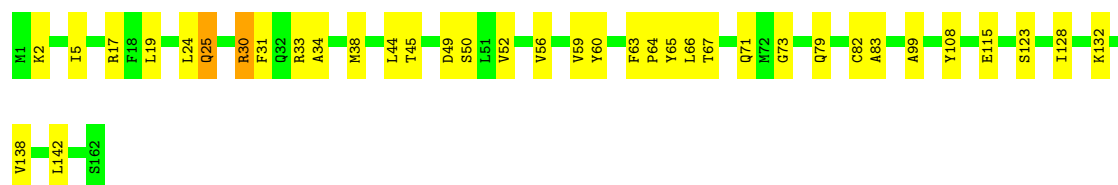
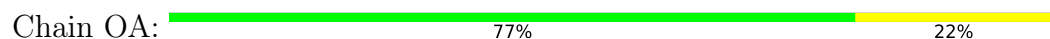
- Molecule 2: Phycocyanin alpha chain



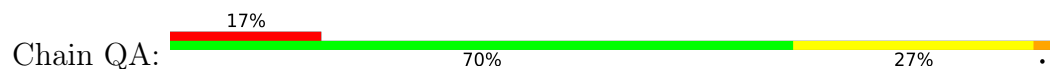
- Molecule 2: Phycocyanin alpha chain



- Molecule 2: Phycocyanin alpha chain

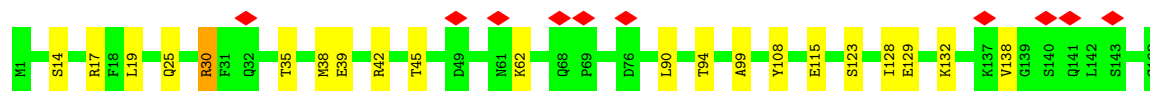
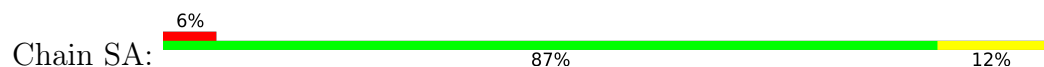


- Molecule 2: Phycocyanin alpha chain

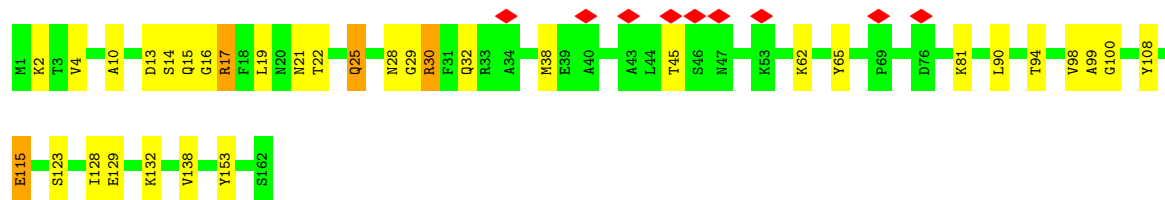
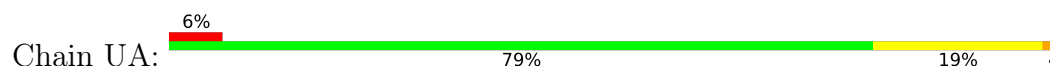




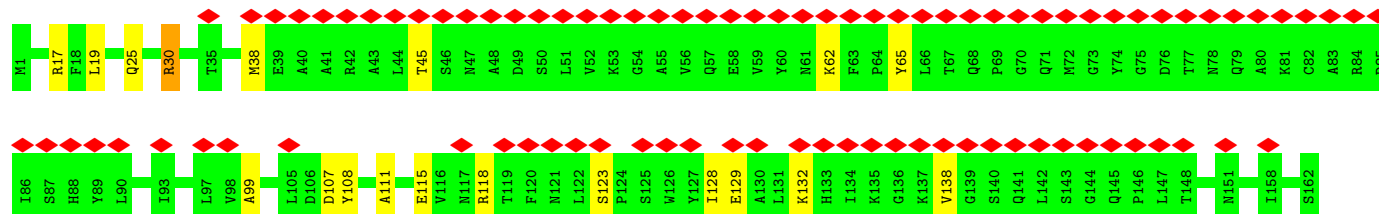
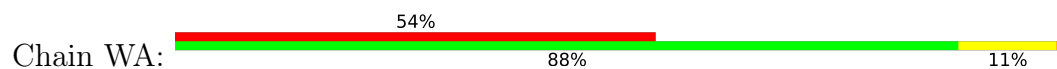
- Molecule 2: Phycocyanin alpha chain



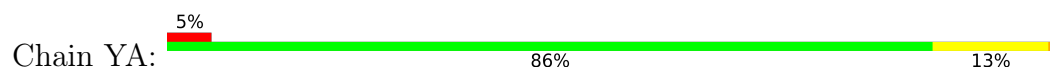
- Molecule 2: Phycocyanin alpha chain



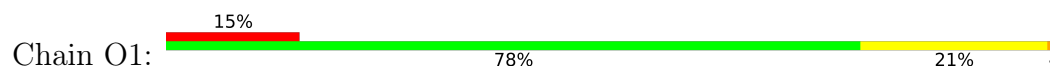
- Molecule 2: Phycocyanin alpha chain



- Molecule 2: Phycocyanin alpha chain

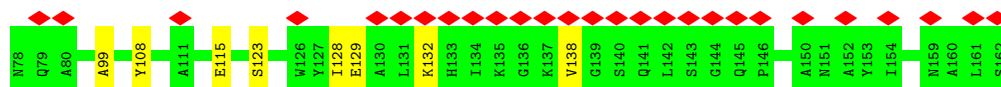
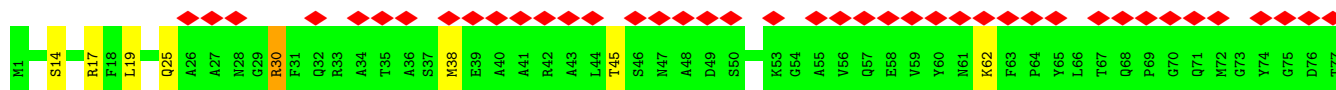
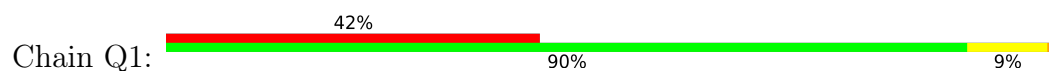


- Molecule 2: Phycocyanin alpha chain

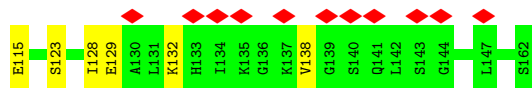
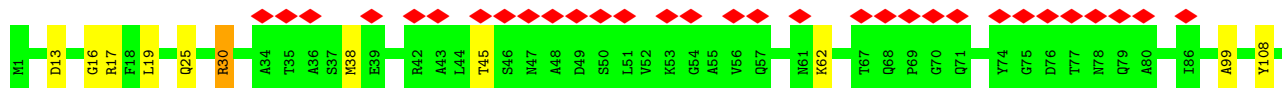
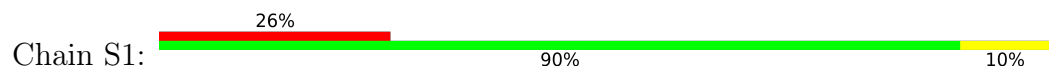




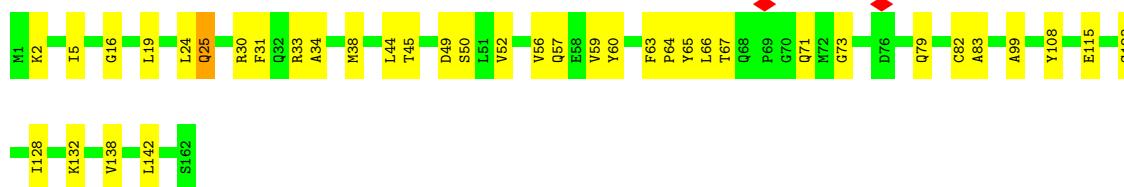
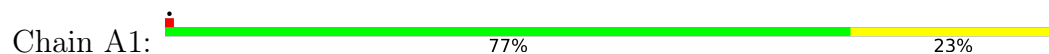
- Molecule 2: Phycocyanin alpha chain



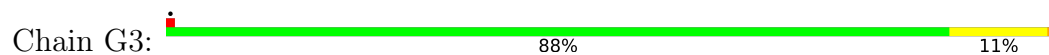
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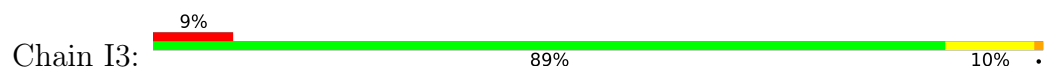
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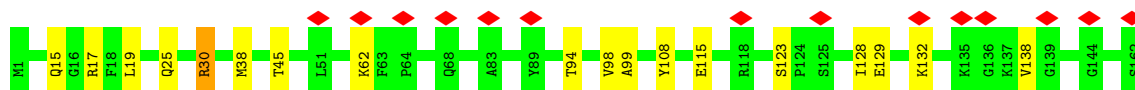


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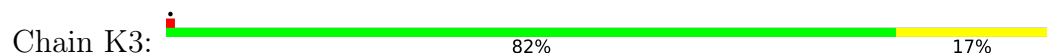


- Molecule 2: Phycocyanin alpha chain





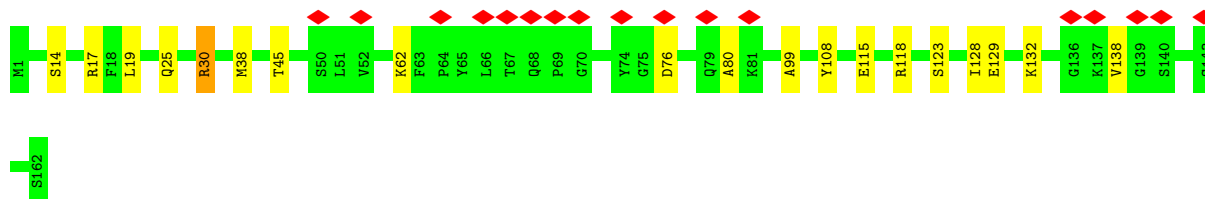
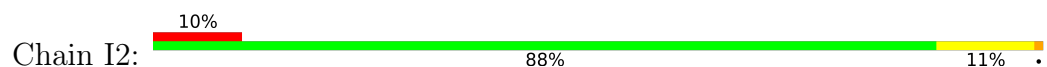
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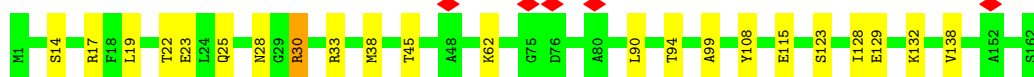
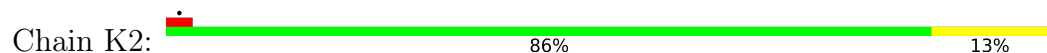
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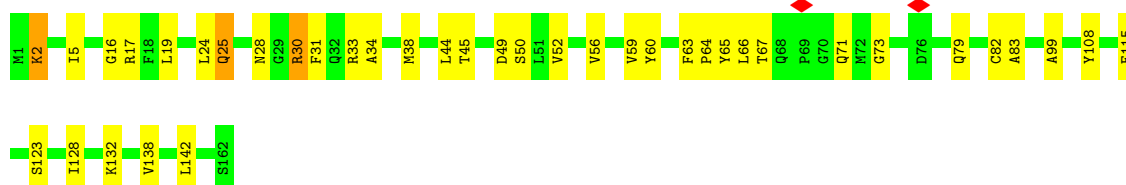
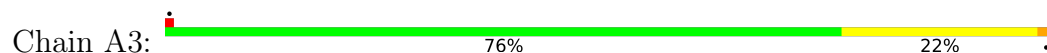
- Molecule 2: Phycocyanin alpha chain



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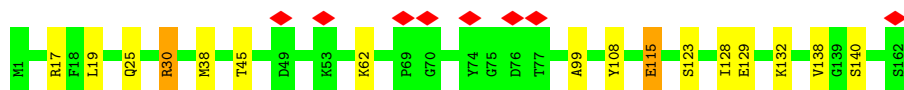


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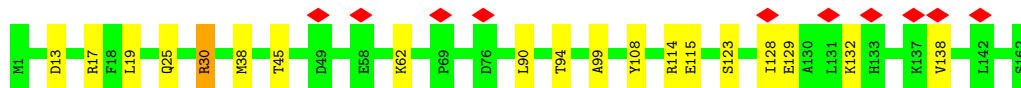
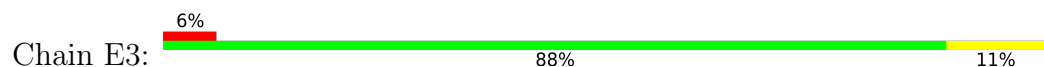


- Molecule 2: Phycocyanin alpha chain

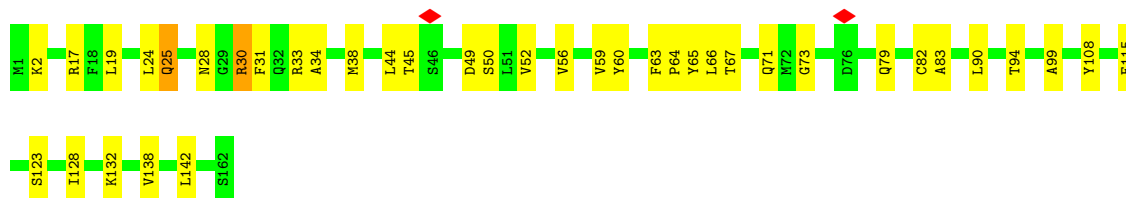
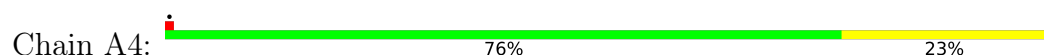




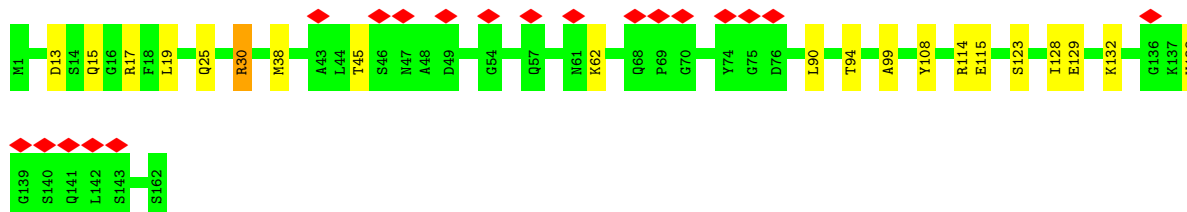
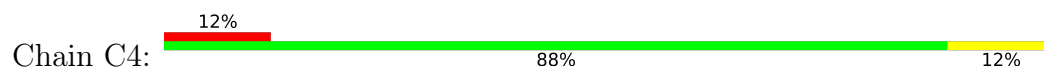
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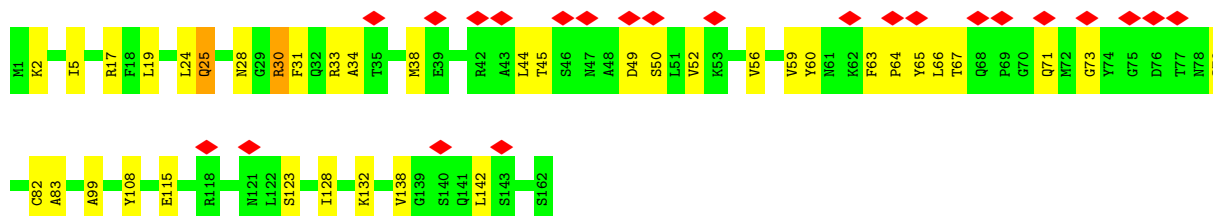
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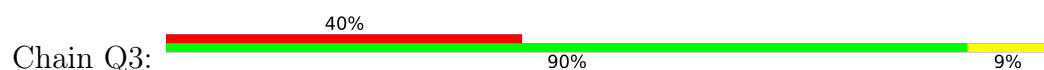
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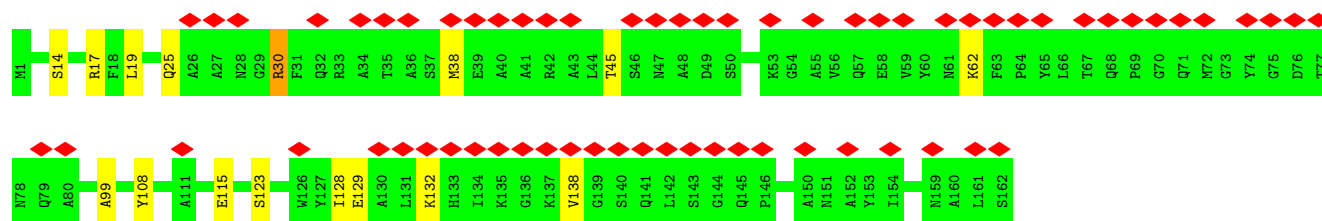


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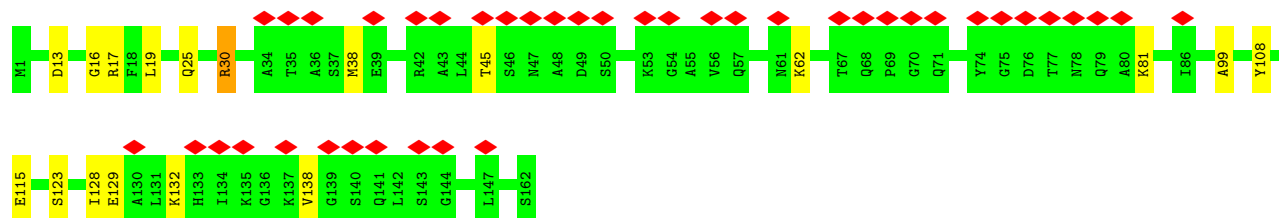
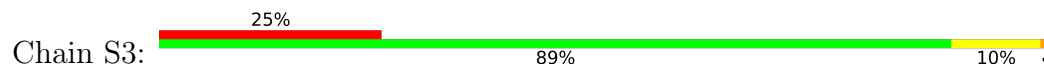


- Molecule 2: Phycocyanin alpha chain

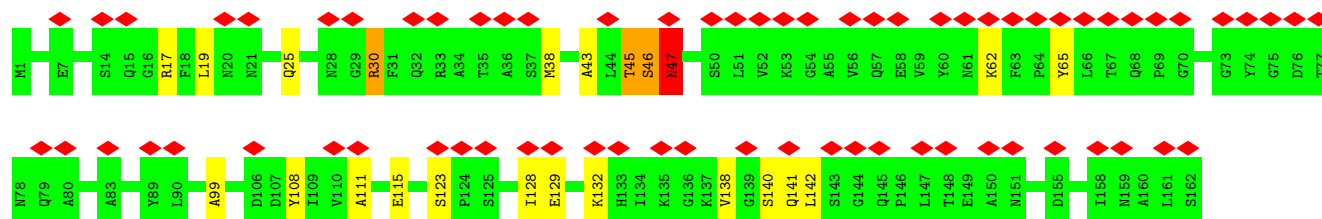
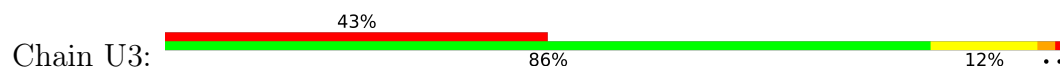




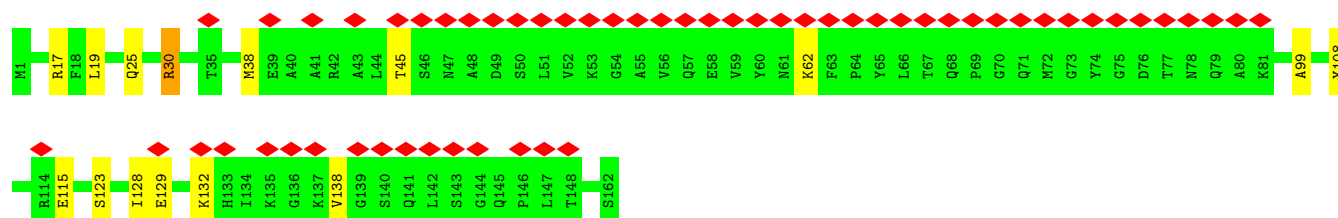
• Molecule 2: Phycocyanin alpha chain



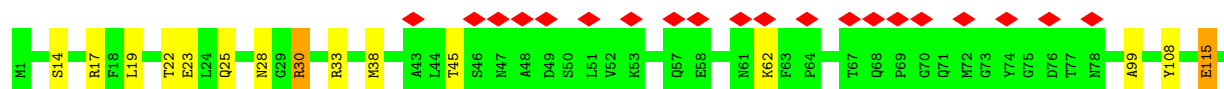
• Molecule 2: Phycocyanin alpha chain



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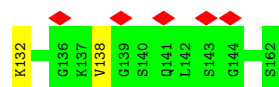
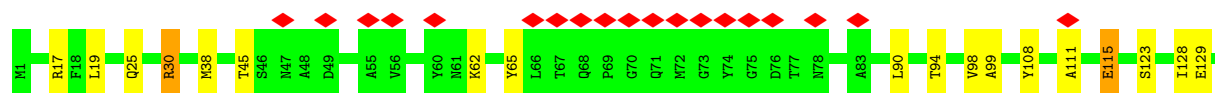
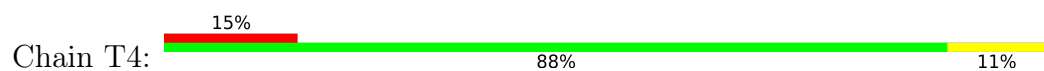


• Molecule 2: Phycocyanin alpha chain

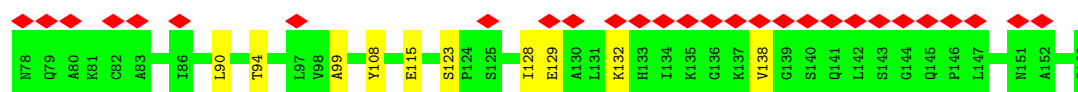
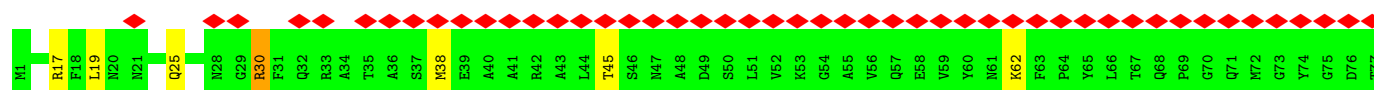
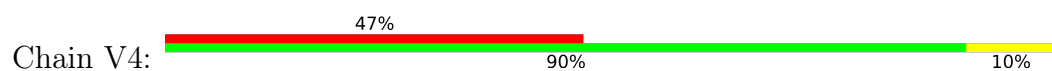




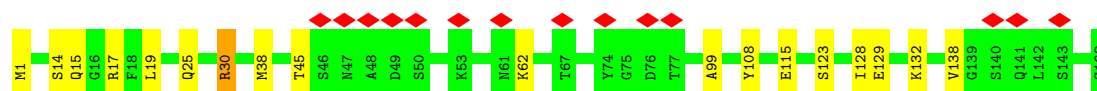
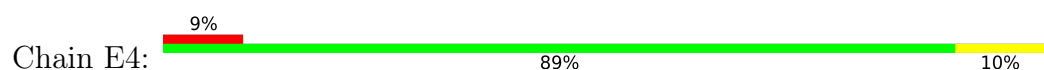
- Molecule 2: Phycocyanin alpha chain



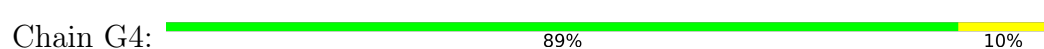
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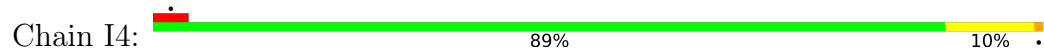
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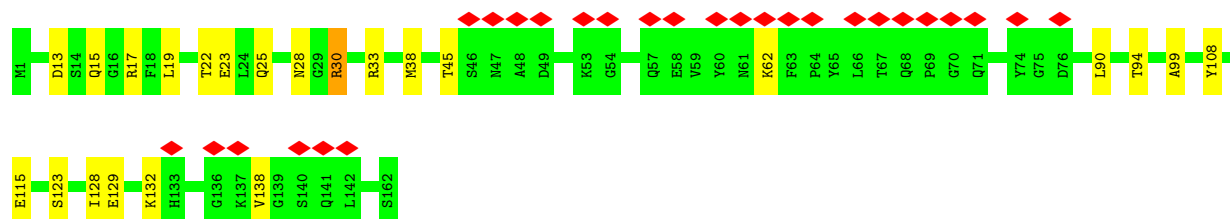
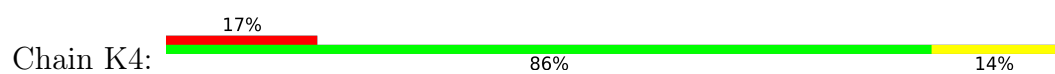
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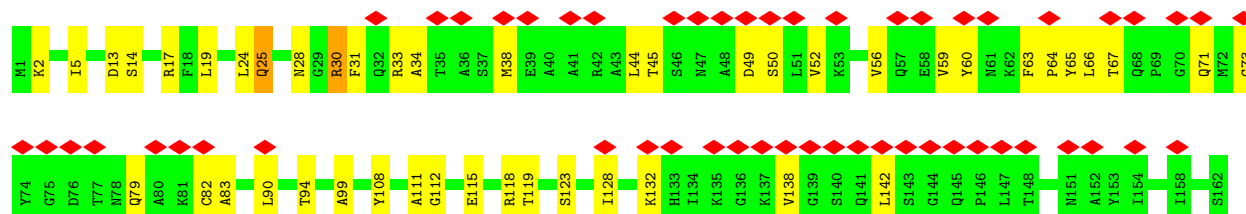
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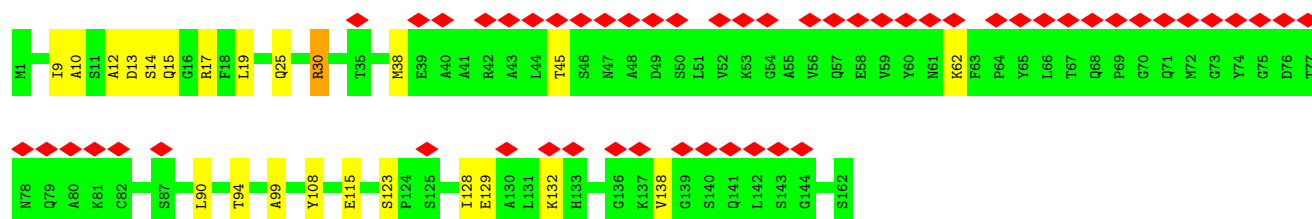
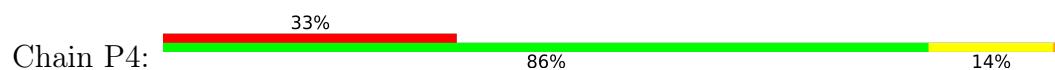
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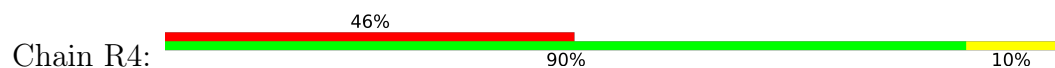
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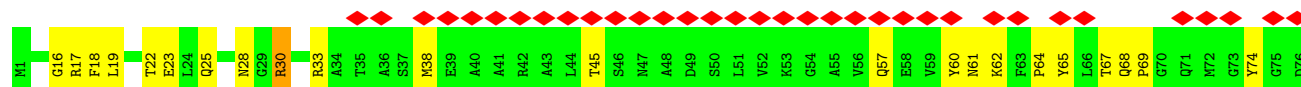
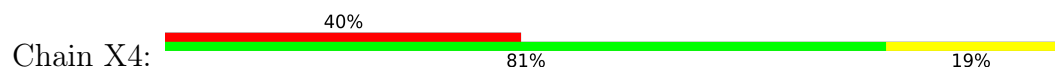
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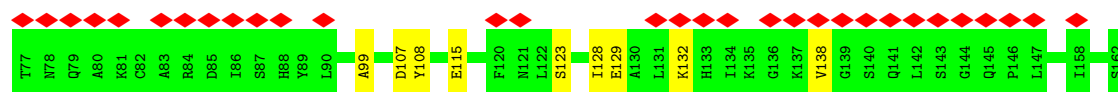


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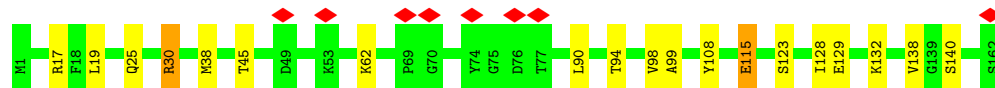
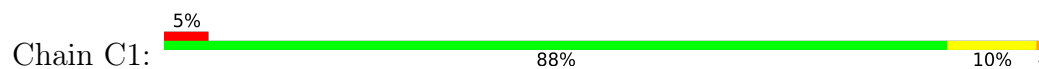


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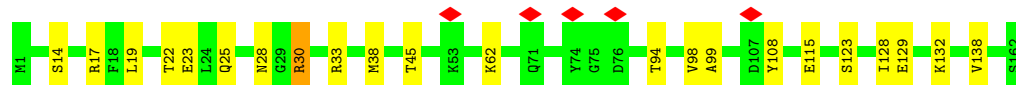




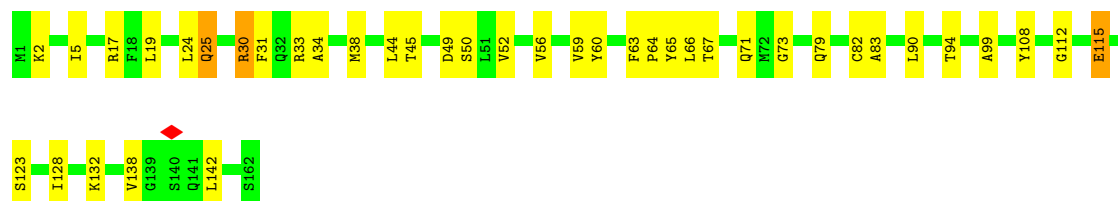
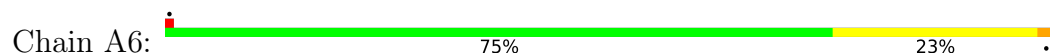
- Molecule 2: Phycocyanin alpha chain



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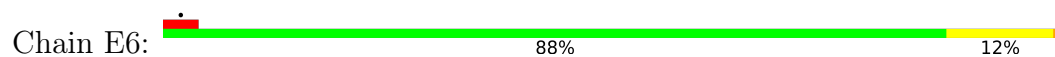
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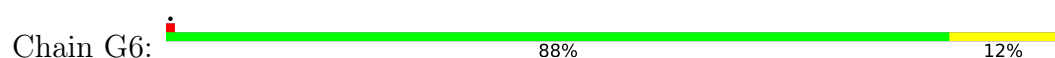
- Molecule 2: Phycocyanin alpha chain



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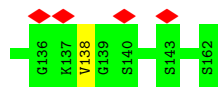
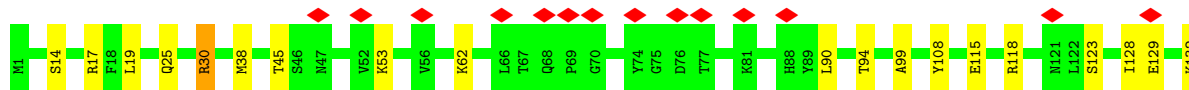
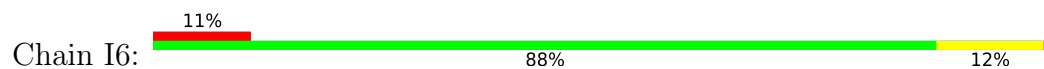


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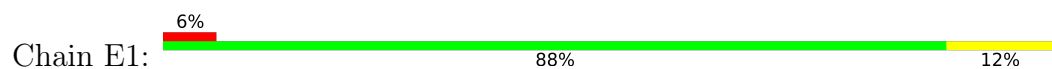




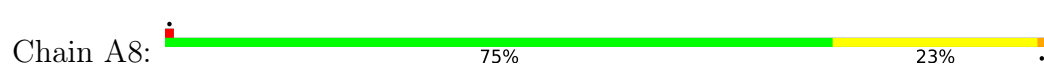
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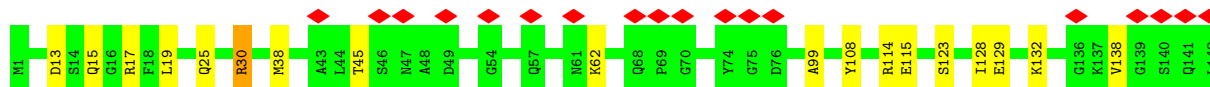
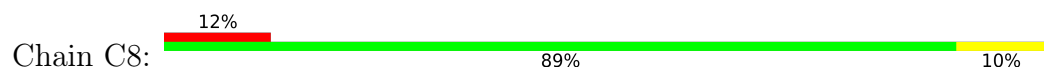
- Molecule 2: Phycocyanin alpha chain



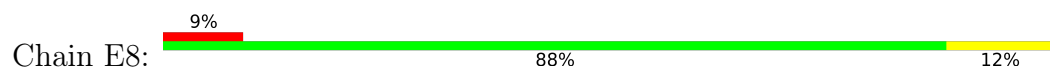
- Molecule 2: Phycocyanin alpha chain

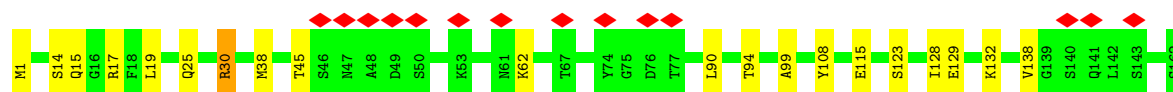


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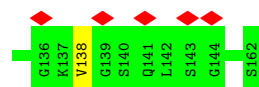
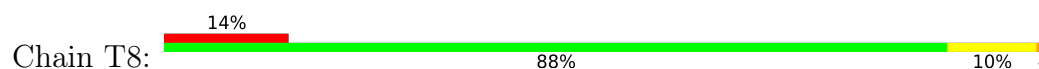


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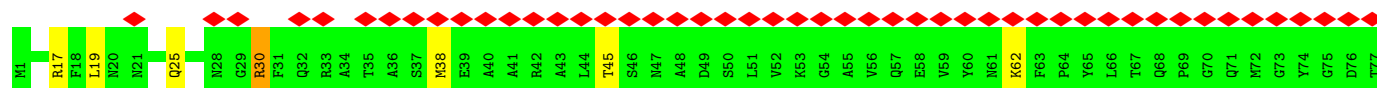
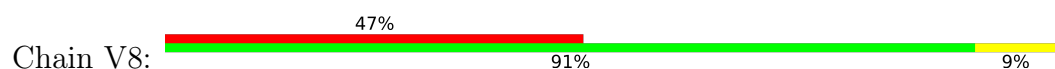




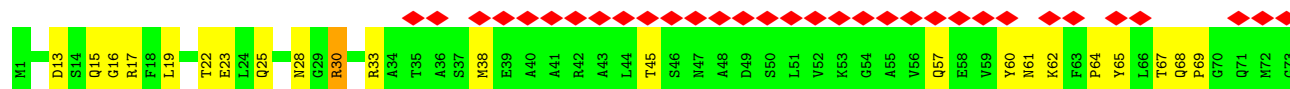
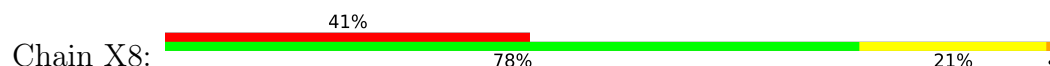
- Molecule 2: Phycocyanin alpha chain



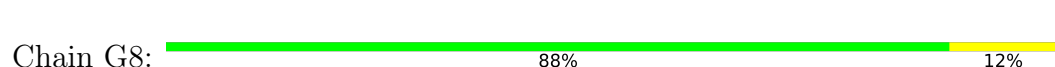
- Molecule 2: Phycocyanin alpha chain



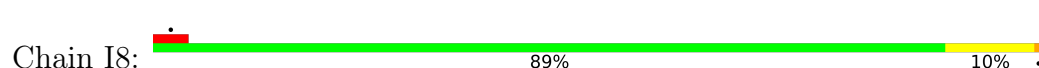
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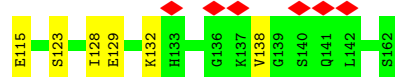
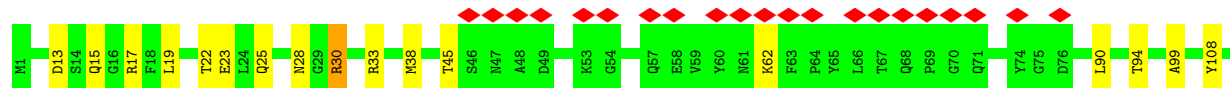
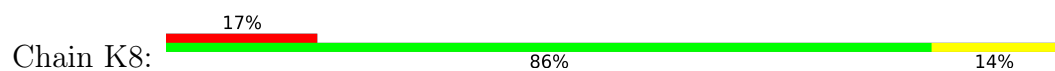


- Molecule 2: Phycocyanin alpha chain

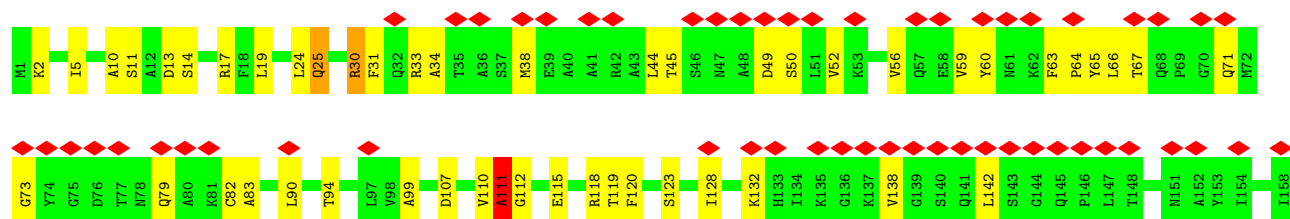




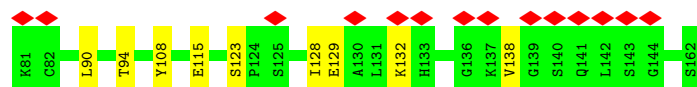
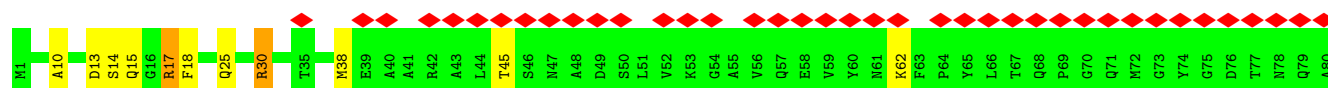
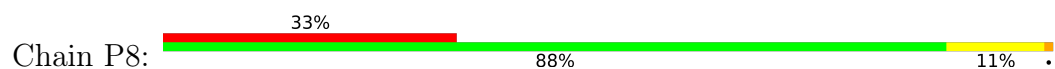
- Molecule 2: Phycocyanin alpha chain



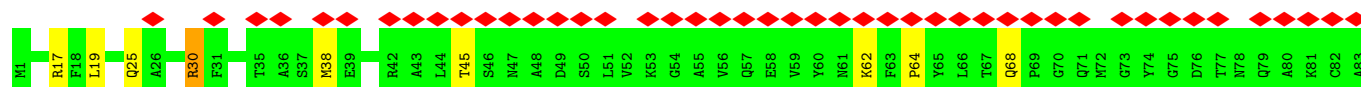
- Molecule 2: Phycocyanin alpha chain

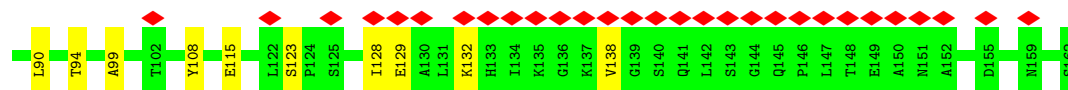


- Molecule 2: Phycocyanin alpha chain



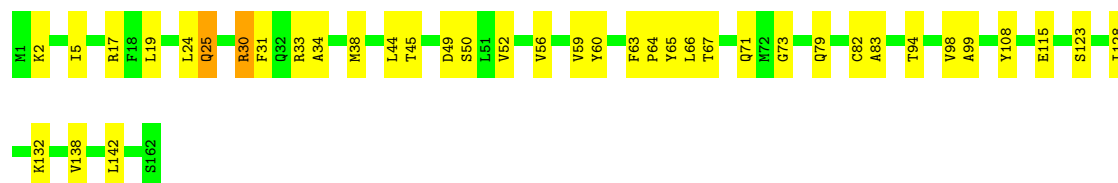
- Molecule 2: Phycocyanin alpha chain





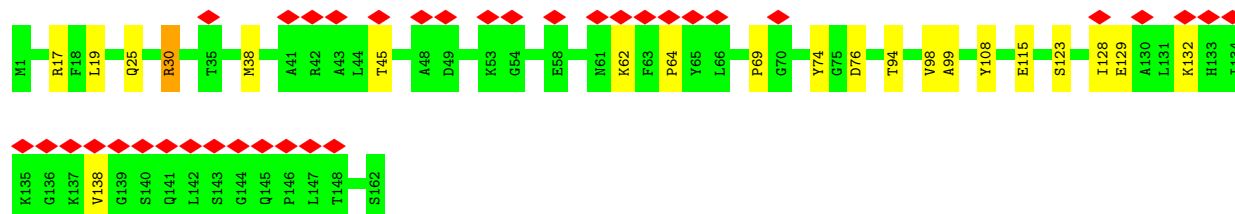
• Molecule 2: Phycocyanin alpha chain

Chain O9: 76% 23% .



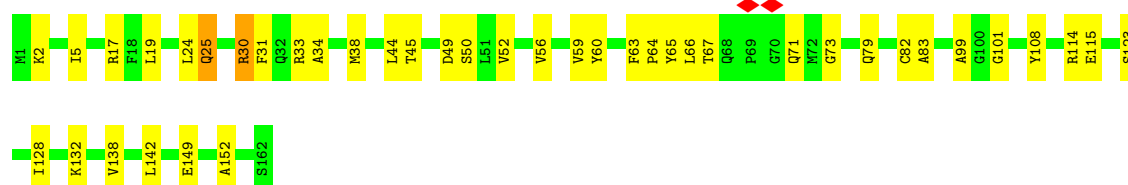
• Molecule 2: Phycocyanin alpha chain

Chain Q9: 22% 87% 12% .



• Molecule 2: Phycocyanin alpha chain

Chain A9: 75% 24% .



• Molecule 2: Phycocyanin alpha chain

Chain C9: 91% 9% .



• Molecule 2: Phycocyanin alpha chain

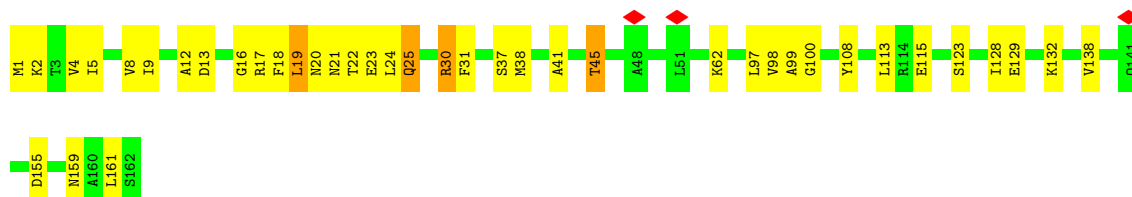
Chain E9: 5% 87% 11% .



● Molecule 2: Phycocyanin alpha chain

Chain G9:  89% 10%

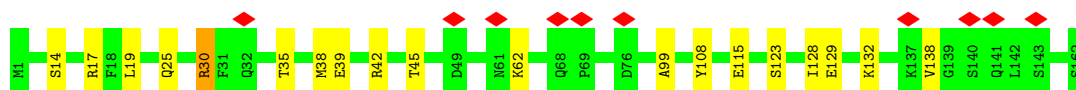
● Molecule 2: Phycocyanin alpha chain

Chain I9:  75% 22%

● Molecule 2: Phycocyanin alpha chain

Chain K9:  80% 15%

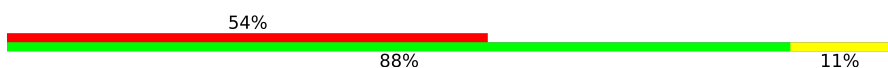
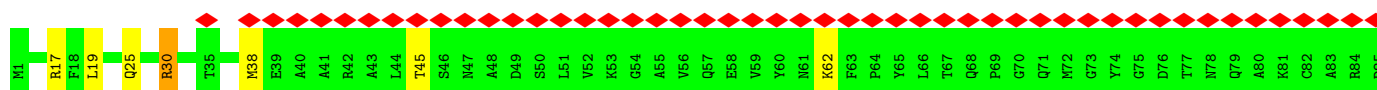
● Molecule 2: Phycocyanin alpha chain

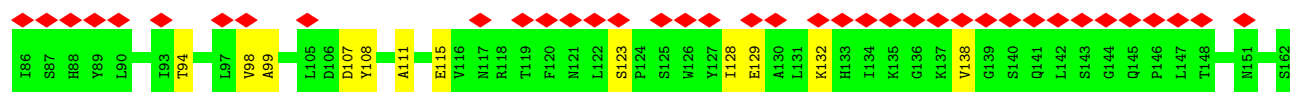
Chain S9:  6% 88% 11%

● Molecule 2: Phycocyanin alpha chain

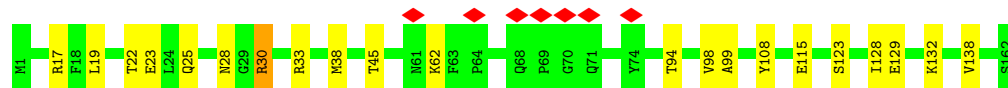
Chain U9:  5% 87% 12%

● Molecule 2: Phycocyanin alpha chain

Chain W9:  54% 88% 11%



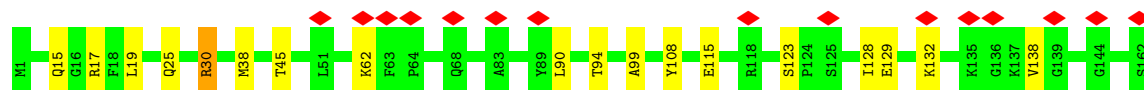
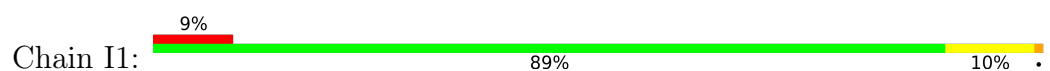
- Molecule 2: Phycocyanin alpha chain



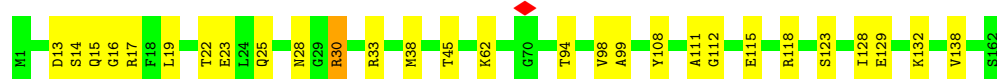
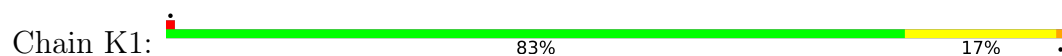
- Molecule 2: Phycocyanin alpha chain



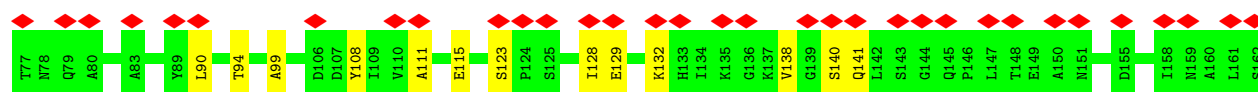
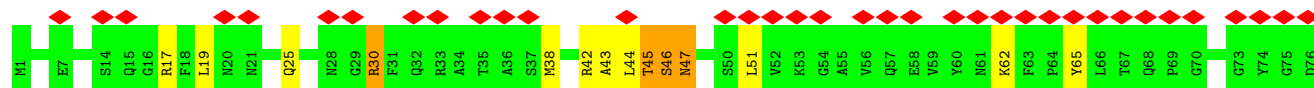
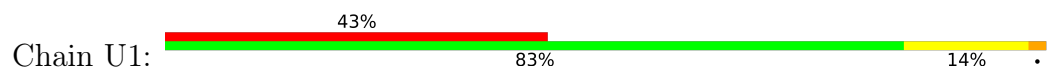
- Molecule 2: Phycocyanin alpha chain



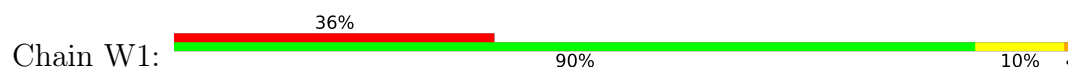
- Molecule 2: Phycocyanin alpha chain

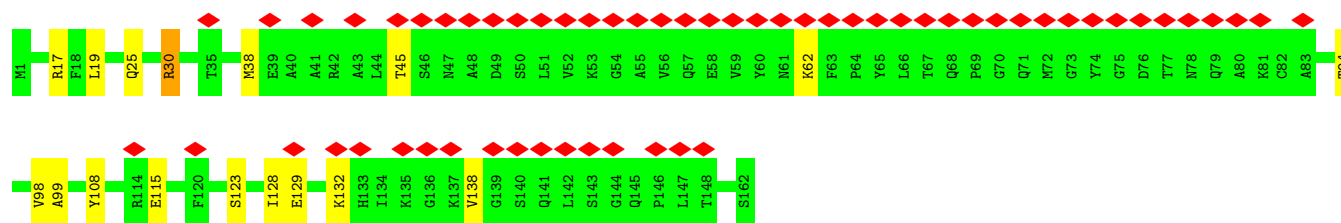


- Molecule 2: Phycocyanin alpha chain

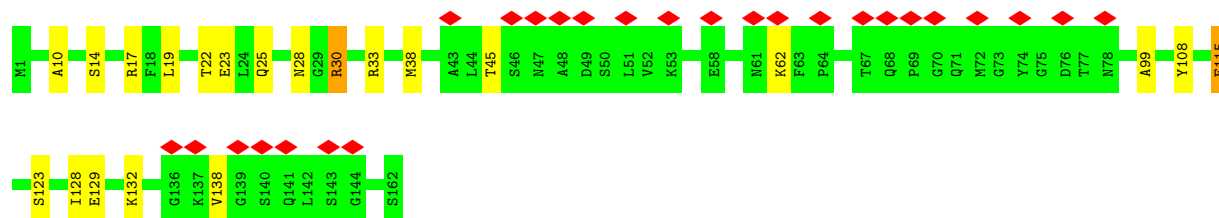
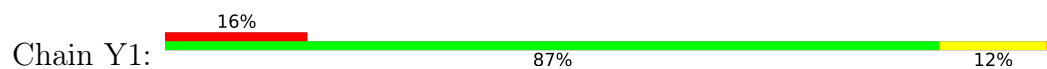


- Molecule 2: Phycocyanin alpha chain

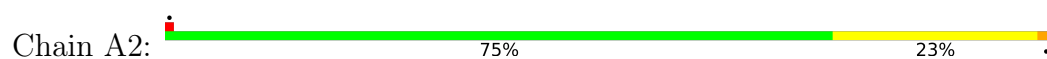




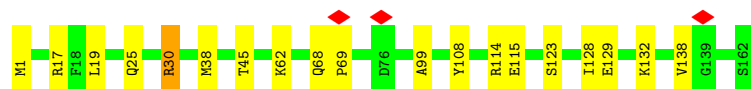
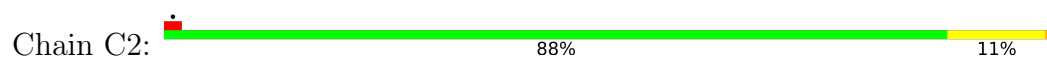
• Molecule 2: Phycocyanin alpha chain



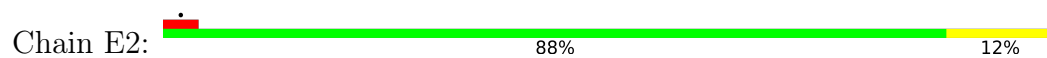
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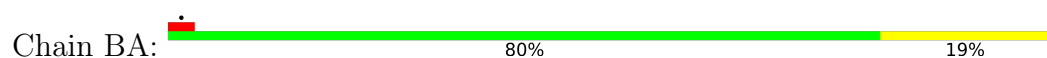
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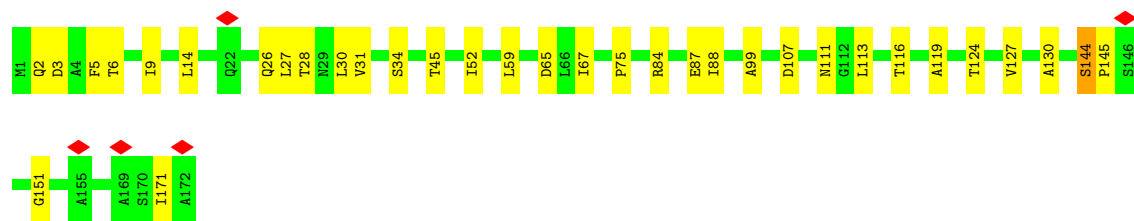


• Molecule 2: Phycocyanin alpha chain

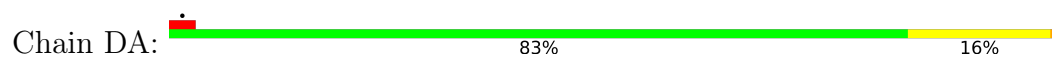


• Molecule 3: Phycocyanin beta chain

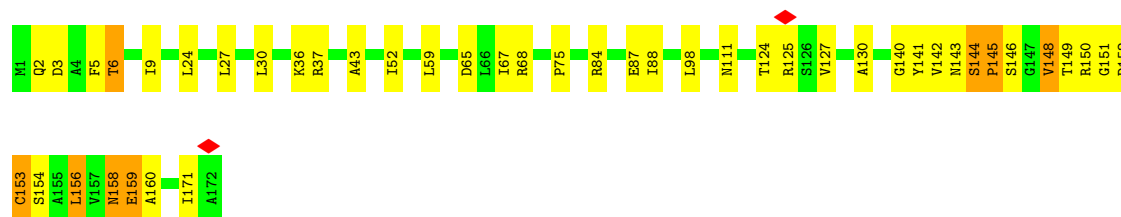
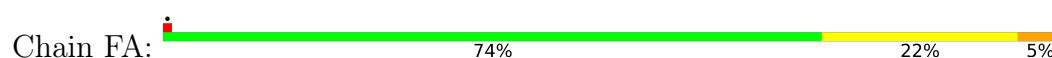




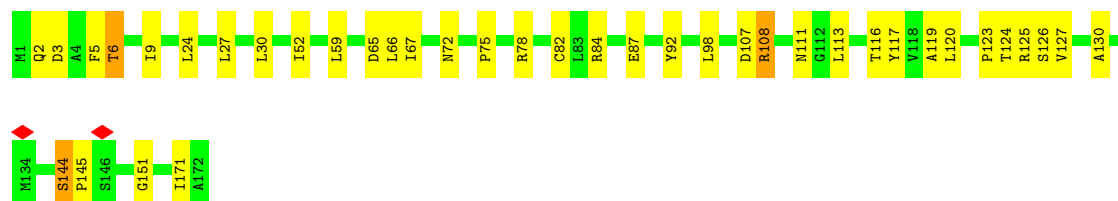
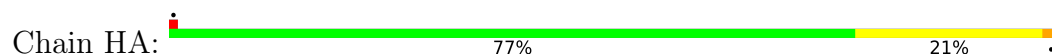
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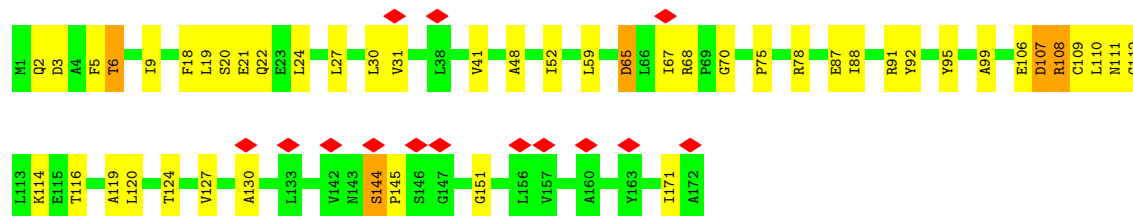
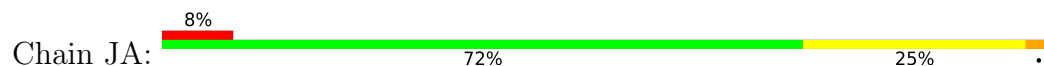
• Molecule 3: Phycocyanin beta chain



• Molecule 3: Phycocyanin beta chain

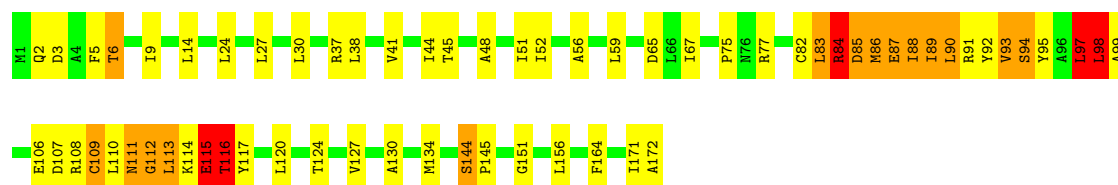


• Molecule 3: Phycocyanin beta chain



• Molecule 3: Phycocyanin beta chain

Chain LA: 



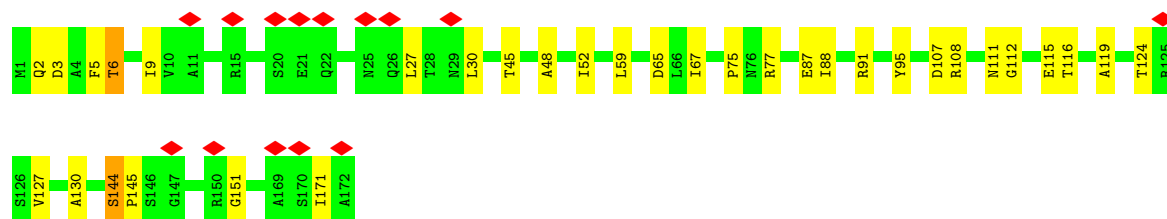
• Molecule 3: Phycocyanin beta chain

Chain PA: 



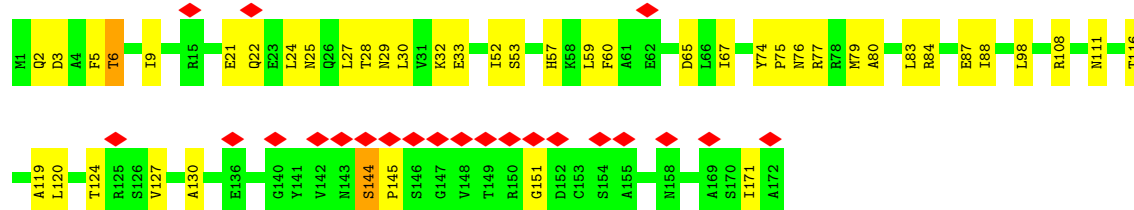
• Molecule 3: Phycocyanin beta chain

Chain RA: 



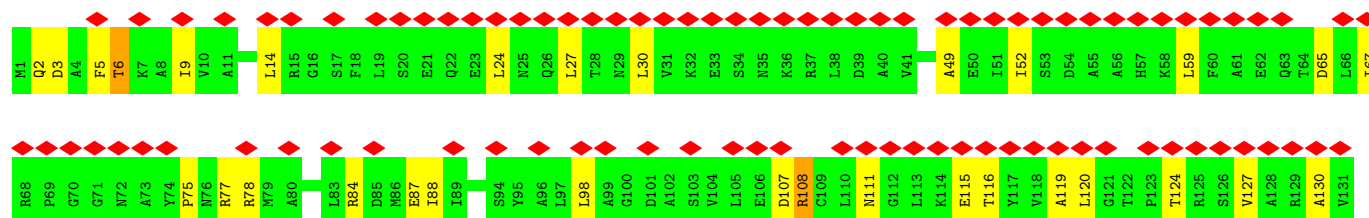
• Molecule 3: Phycocyanin beta chain

Chain TA: 



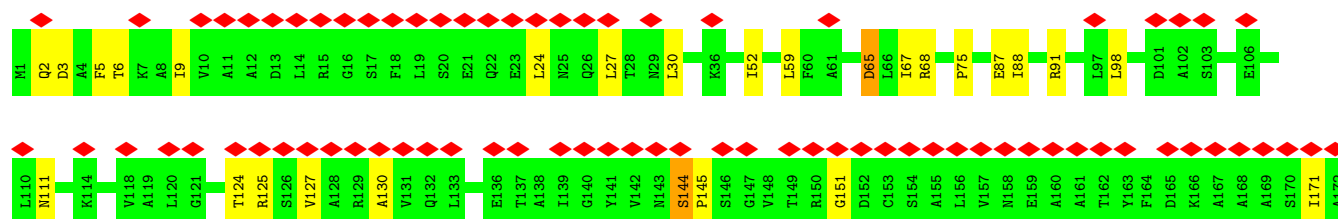
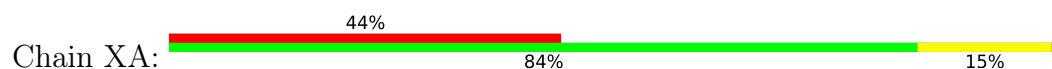
• Molecule 3: Phycocyanin beta chain

Chain VA: 

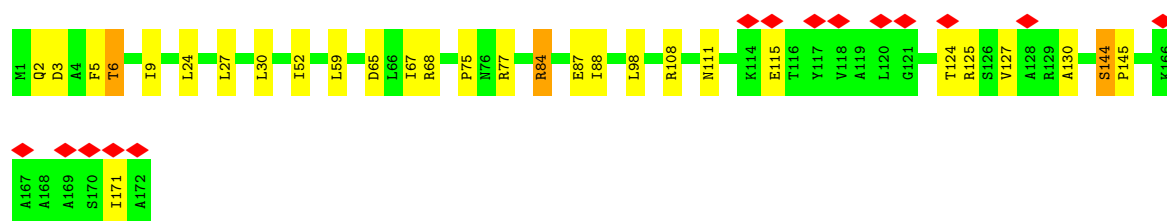
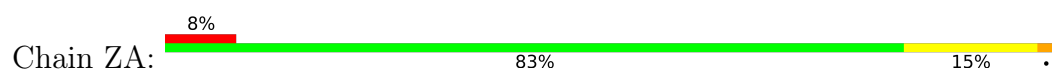




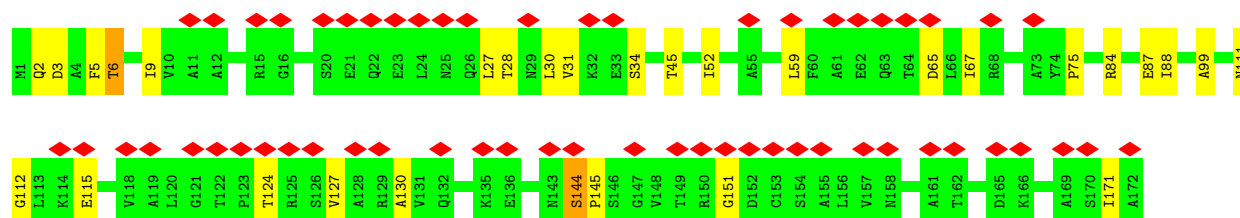
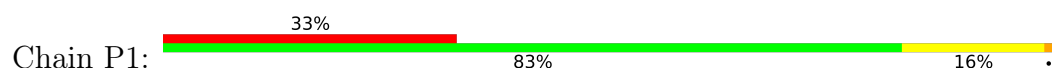
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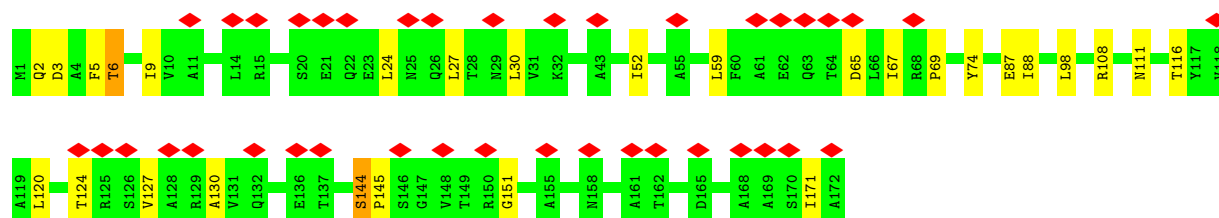
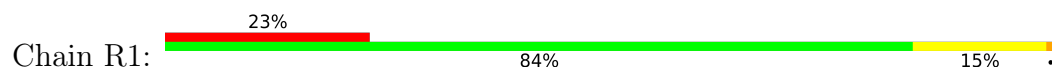
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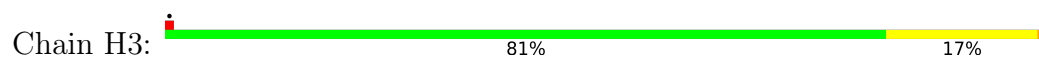
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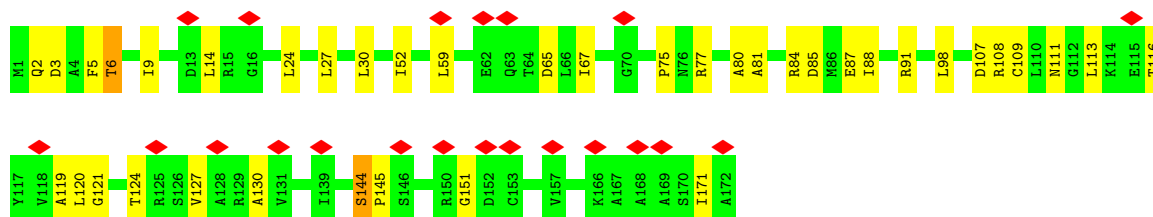
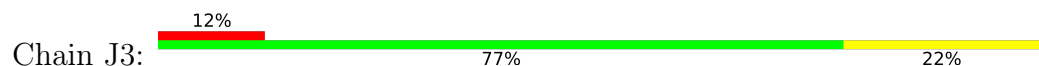
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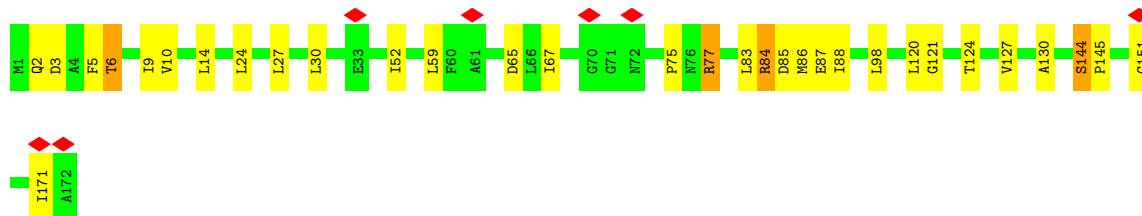
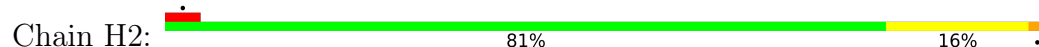
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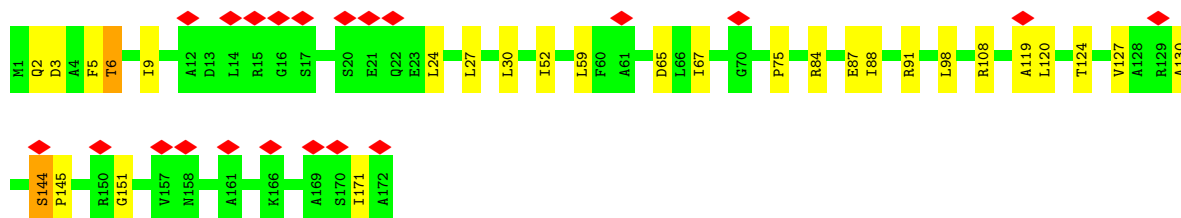
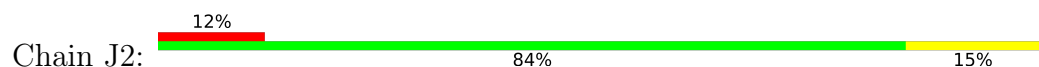
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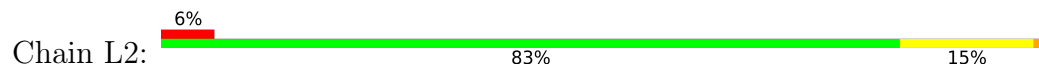
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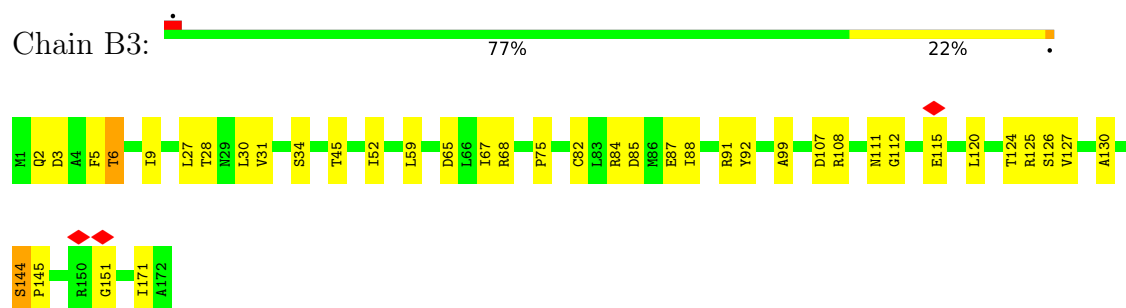
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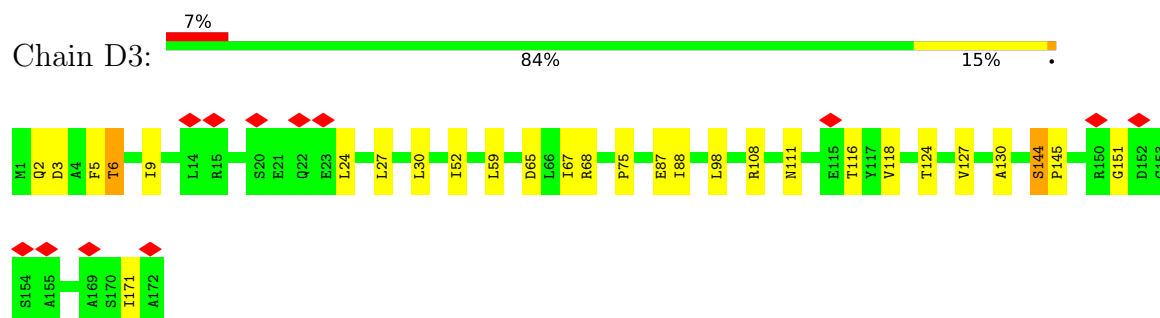
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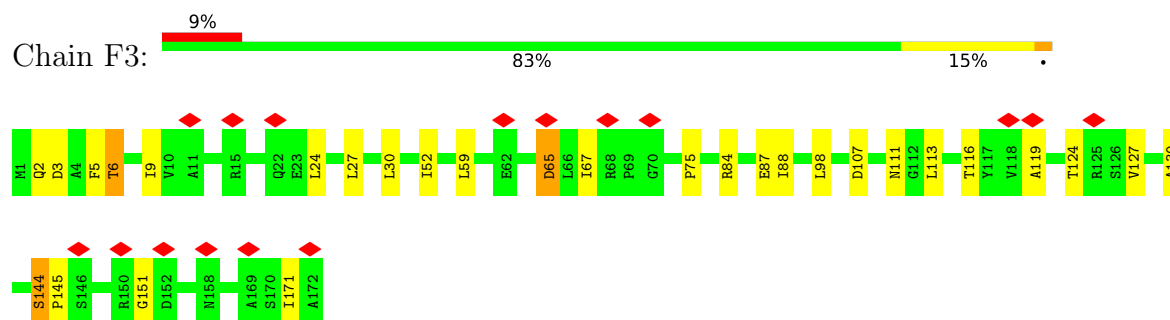
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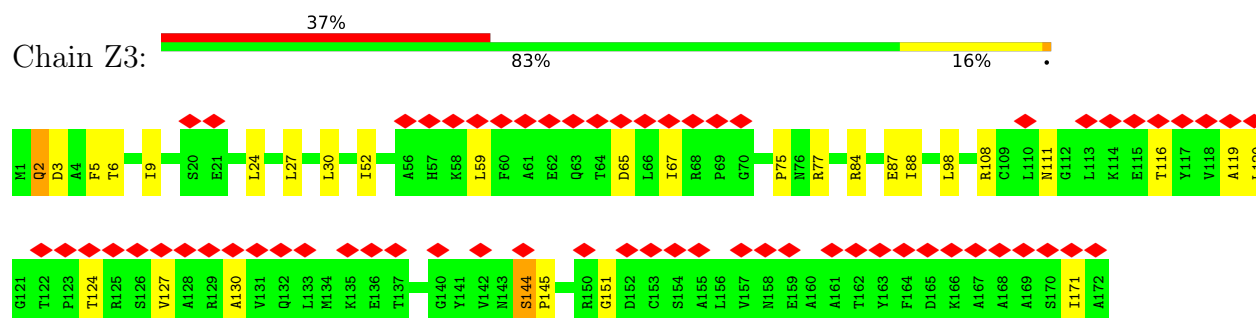
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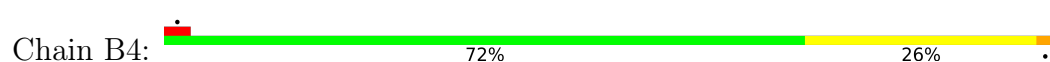
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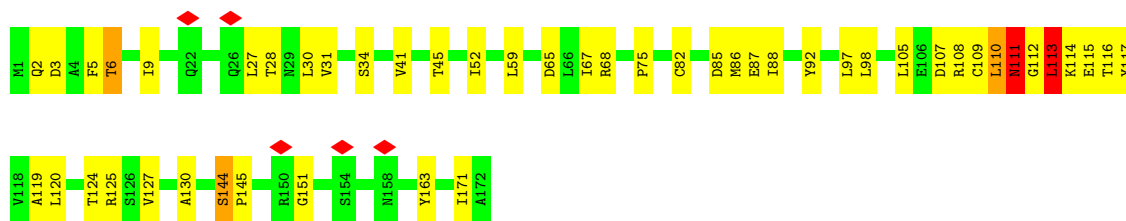


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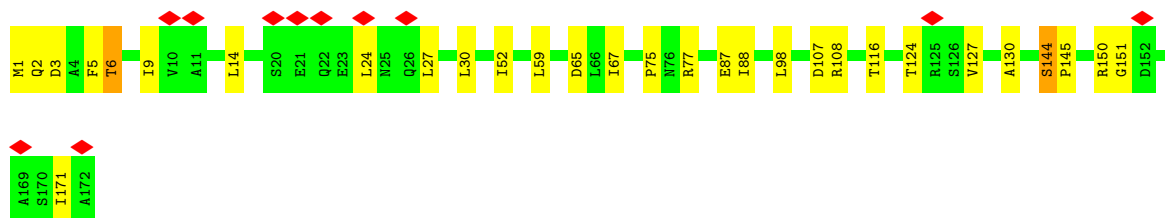
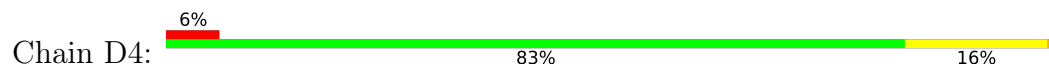


- Molecule 3: Phycocyanin beta chain

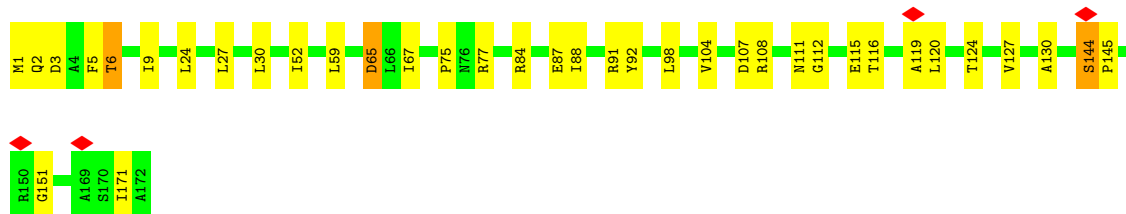
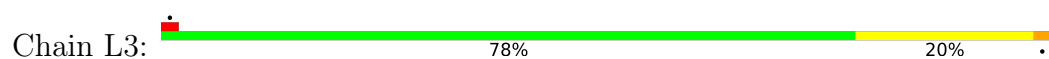




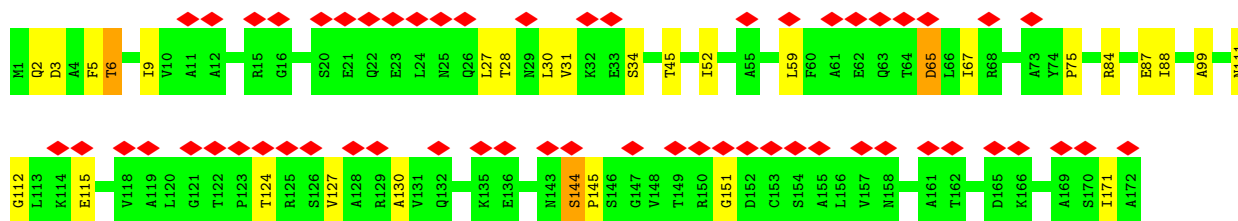
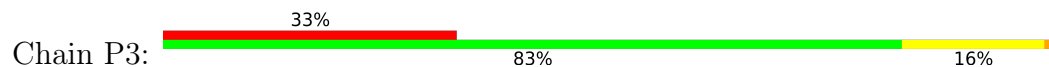
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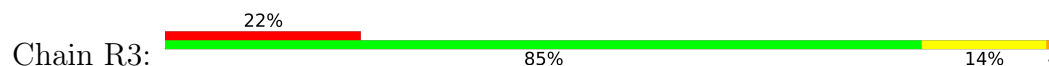
- Molecule 3: Phycocyanin beta chain

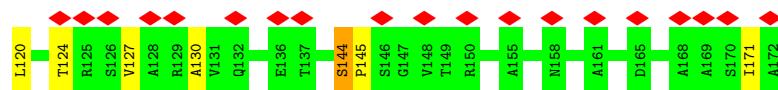


- Molecule 3: Phycocyanin beta chain

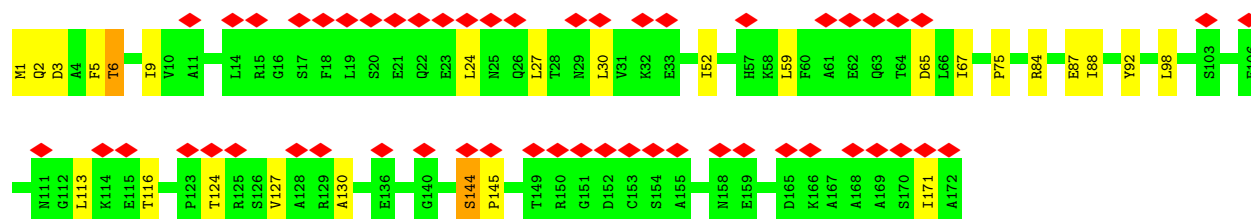
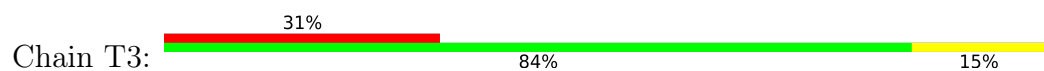


- Molecule 3: Phycocyanin beta chain

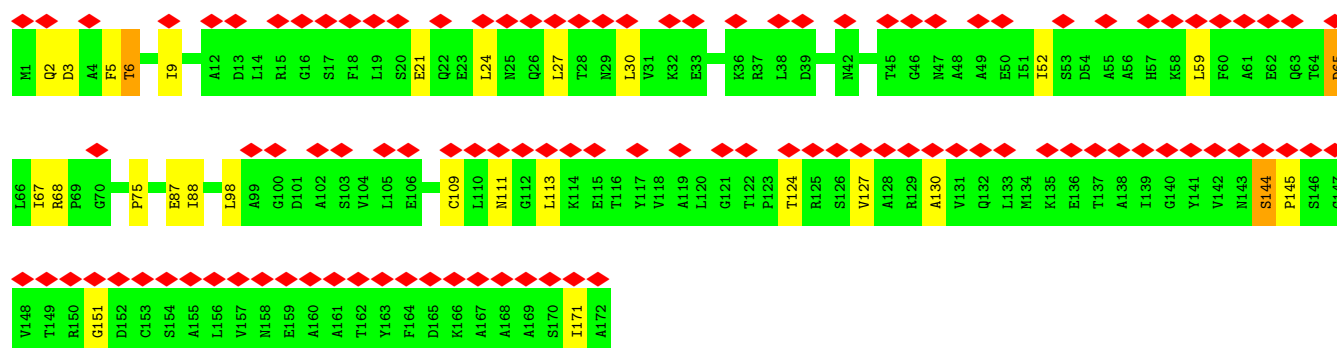
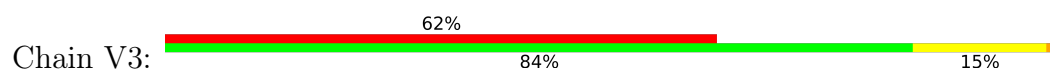




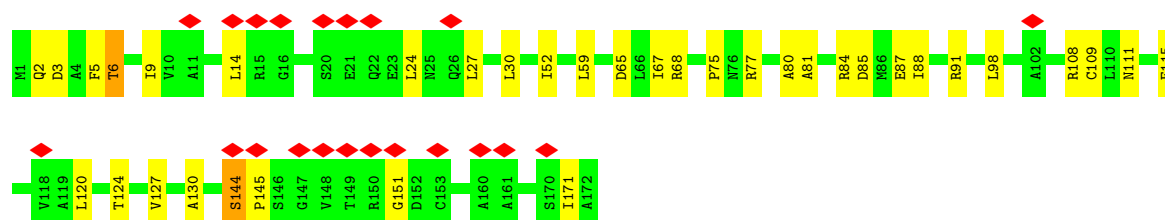
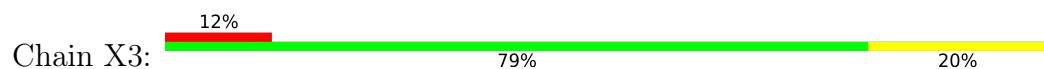
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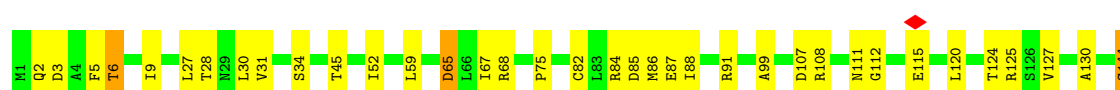
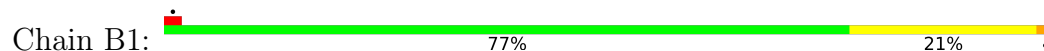
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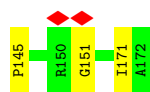


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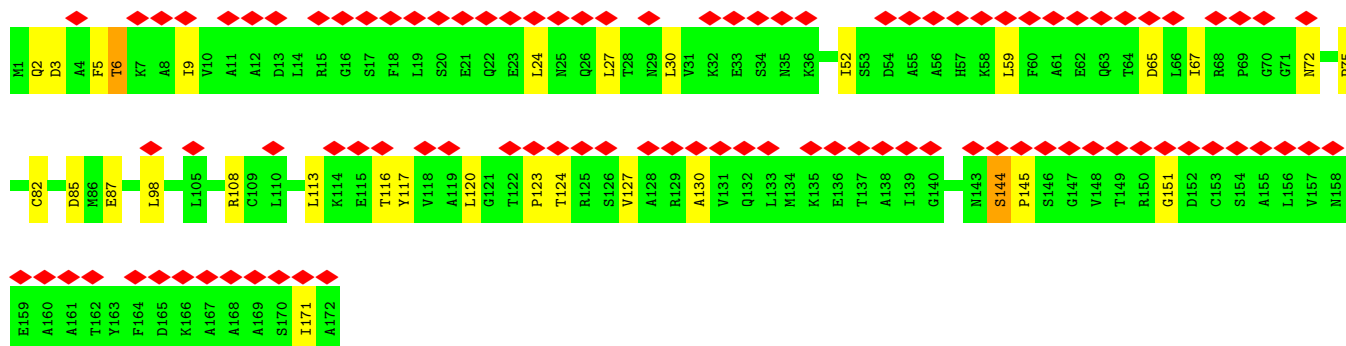
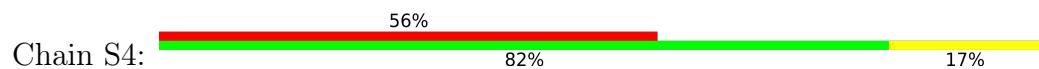


- Molecule 3: Phycocyanin beta chain

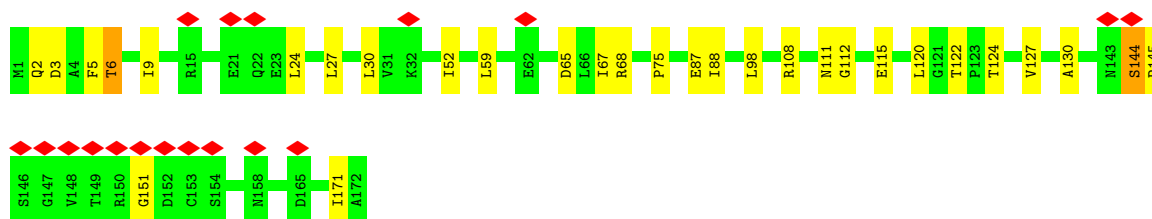
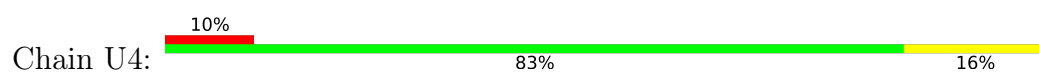




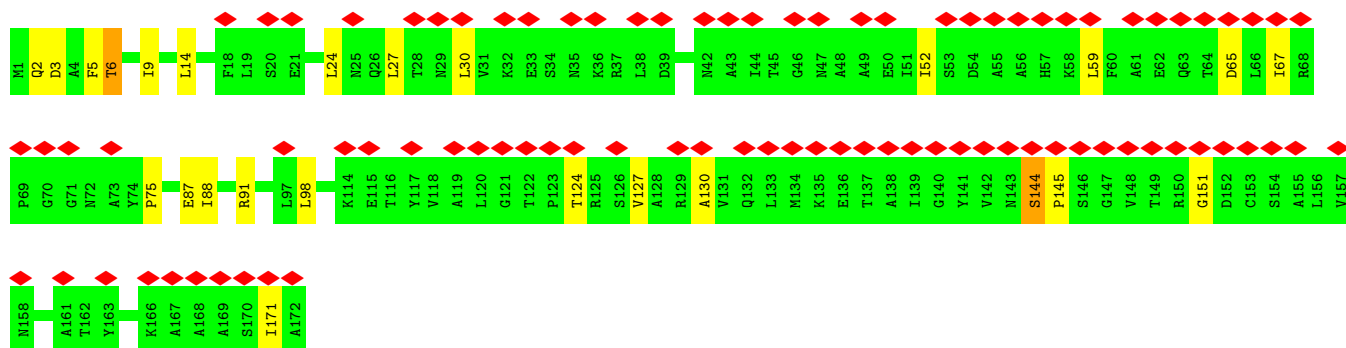
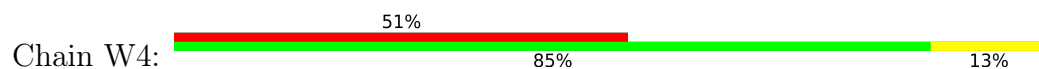
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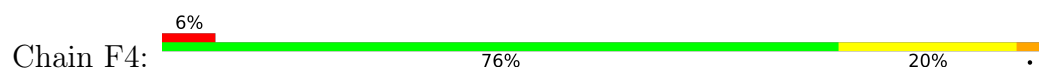
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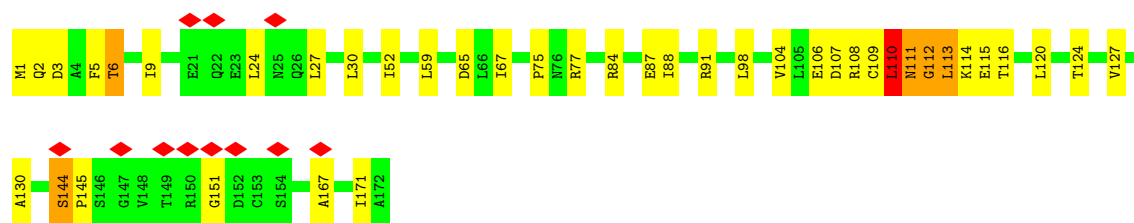


- Molecule 3: Phycocyanin beta chain

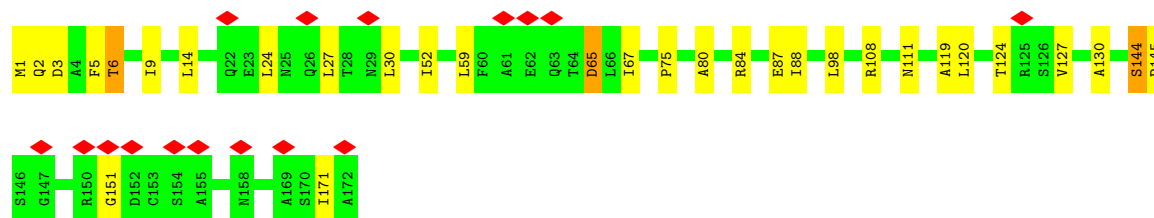
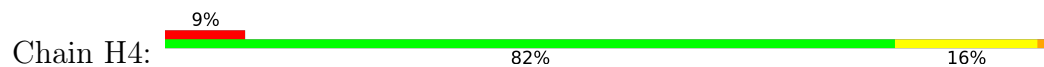


- Molecule 3: Phycocyanin beta chain

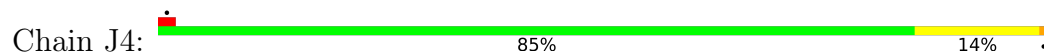




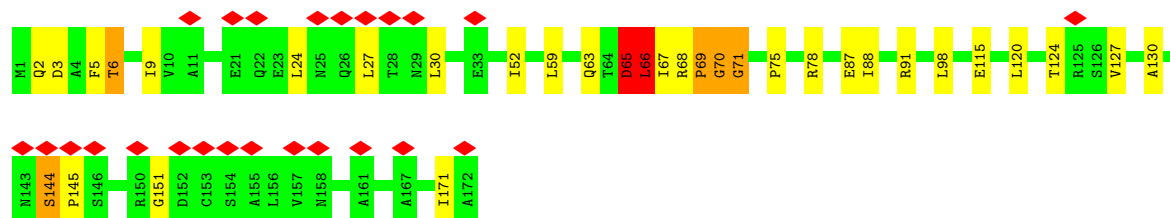
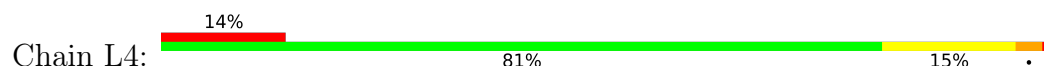
- Molecule 3: Phycocyanin beta chain



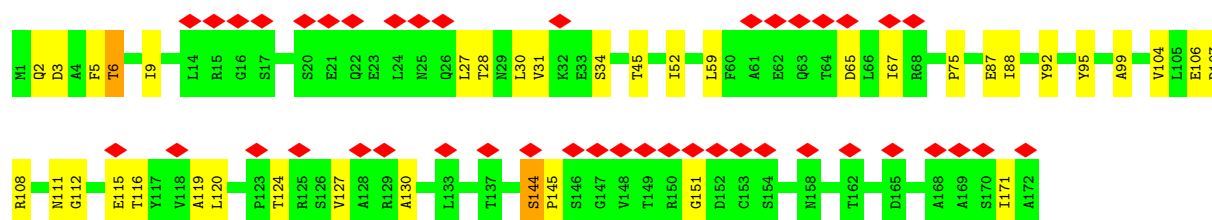
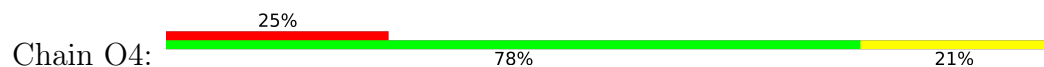
- Molecule 3: Phycocyanin beta chain



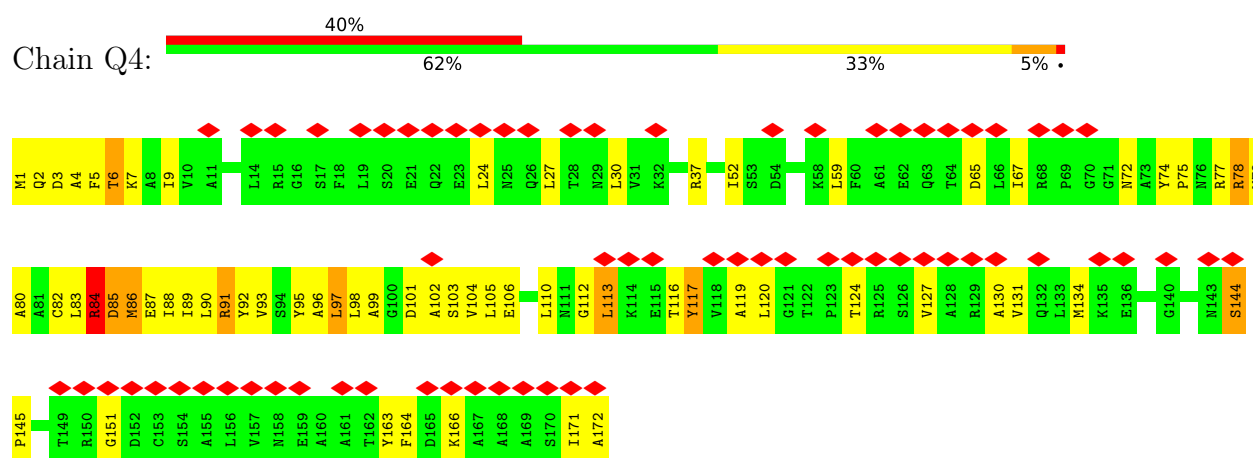
- Molecule 3: Phycocyanin beta chain



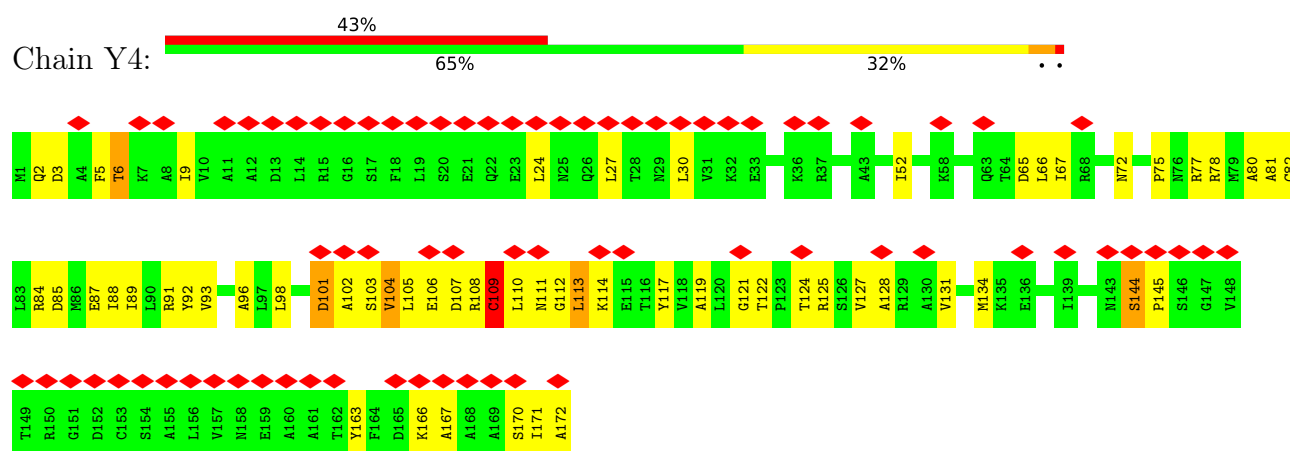
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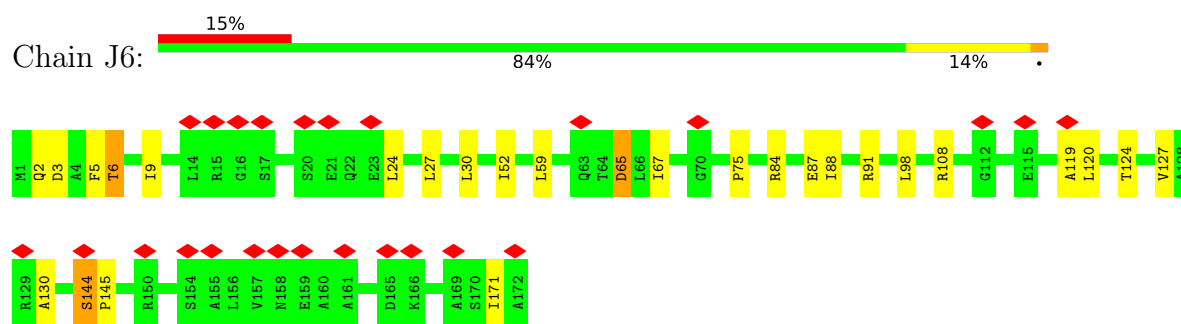
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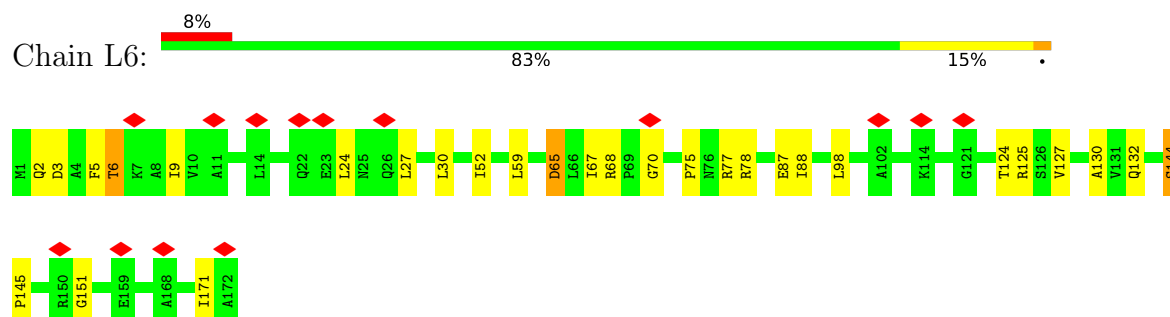
• Molecule 3: Phycocyanin beta chain



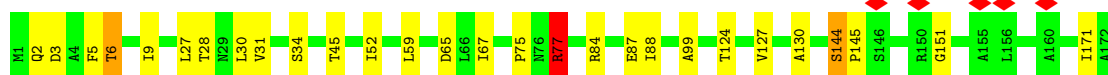
• Molecule 3: Phycocyanin beta chain



• Molecule 3: Phycocyanin beta chain



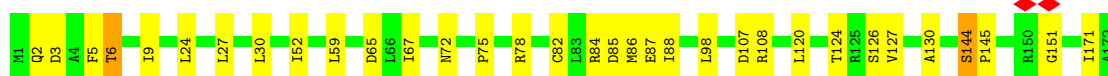
● Molecule 3: Phycocyanin beta chain

Chain B6:  84% 15% ..

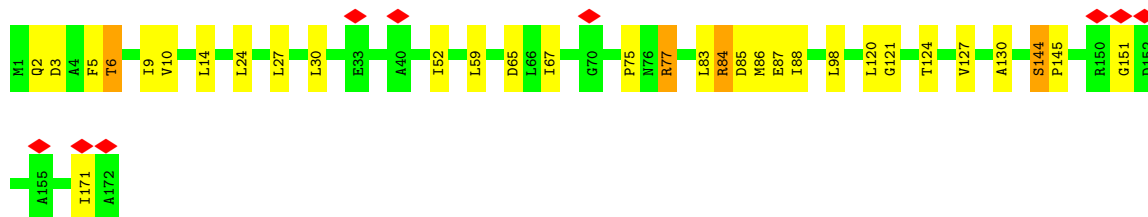
● Molecule 3: Phycocyanin beta chain

Chain D6:  86% 13% .

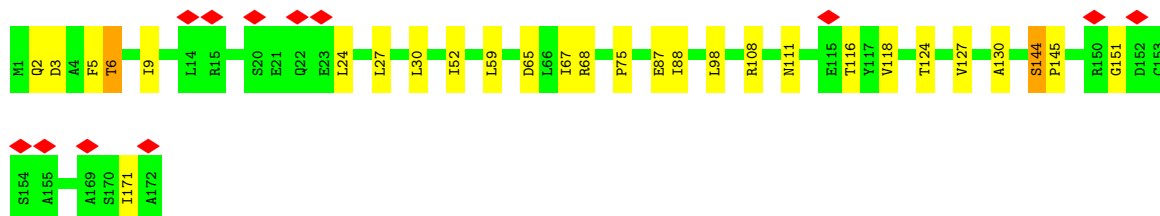
● Molecule 3: Phycocyanin beta chain

Chain F6:  81% 18% .

● Molecule 3: Phycocyanin beta chain

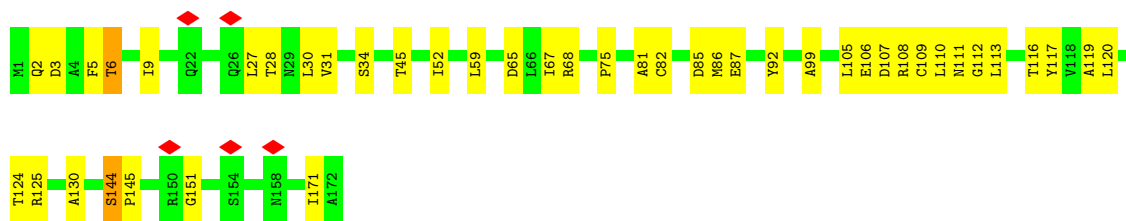
Chain H6:  81% 16% .

● Molecule 3: Phycocyanin beta chain

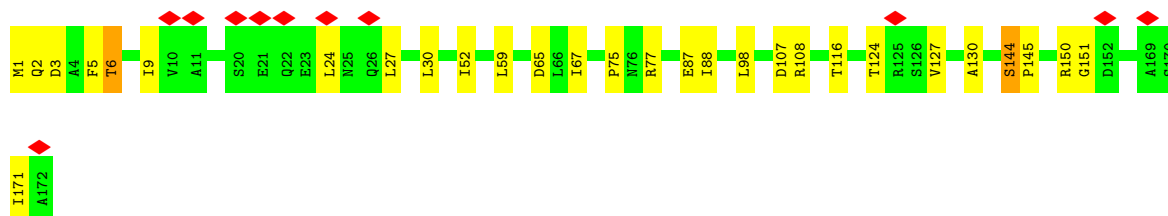
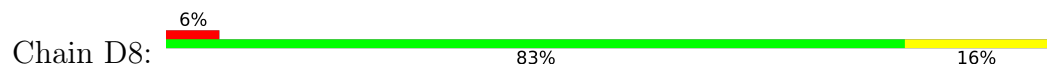
Chain D1:  84% 15% .

● Molecule 3: Phycocyanin beta chain

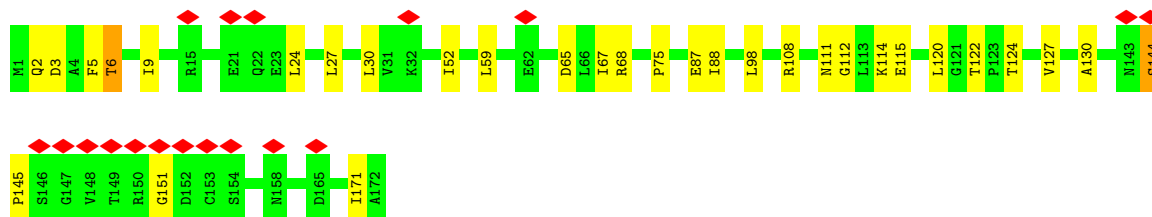
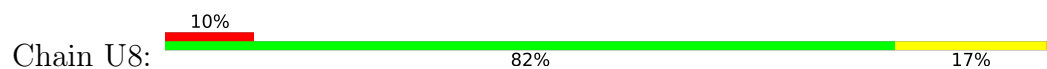
Chain B8:  74% 24% .



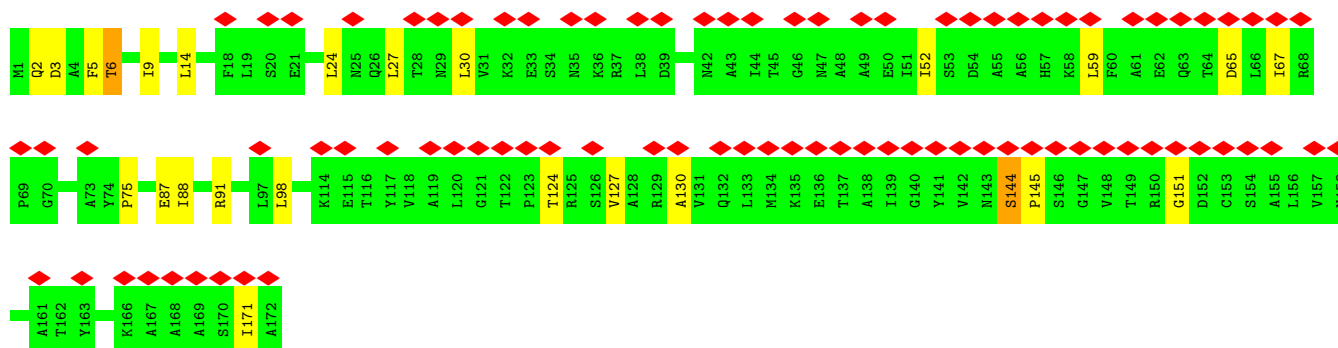
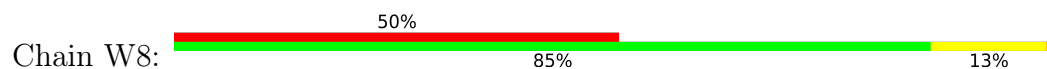
- Molecule 3: Phycocyanin beta chain



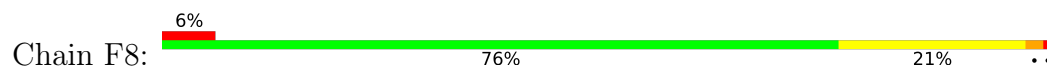
- Molecule 3: Phycocyanin beta chain

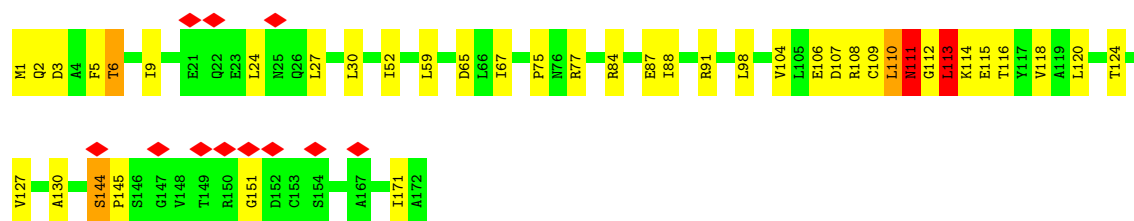


- Molecule 3: Phycocyanin beta chain

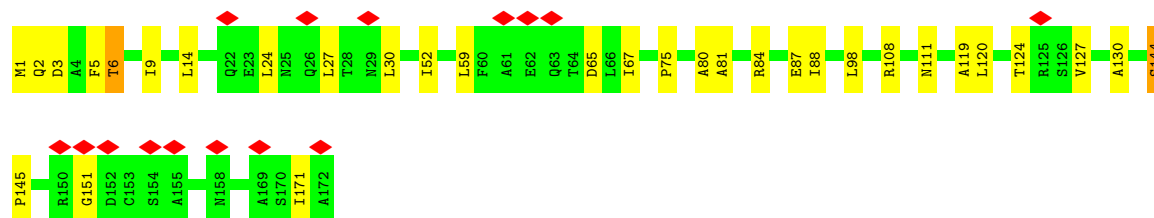
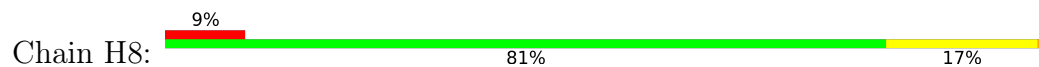


- Molecule 3: Phycocyanin beta chain

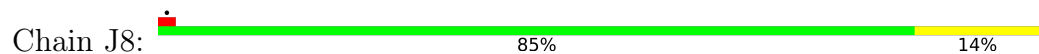




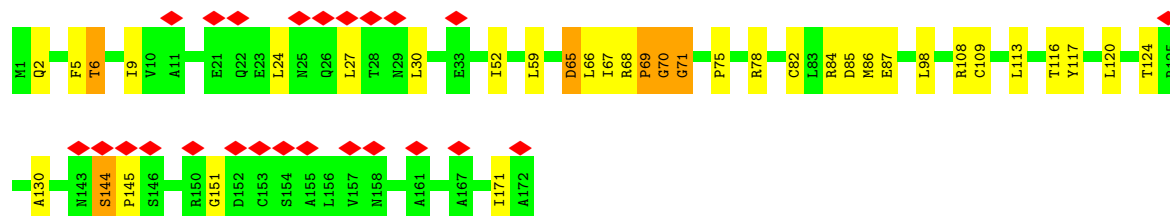
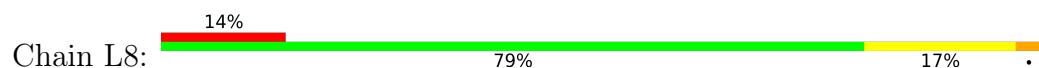
- Molecule 3: Phycocyanin beta chain



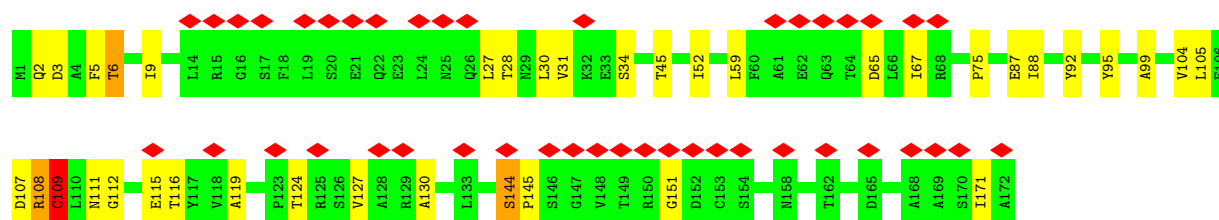
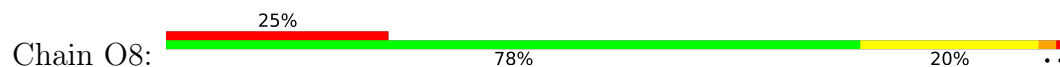
- Molecule 3: Phycocyanin beta chain



- Molecule 3: Phycocyanin beta chain

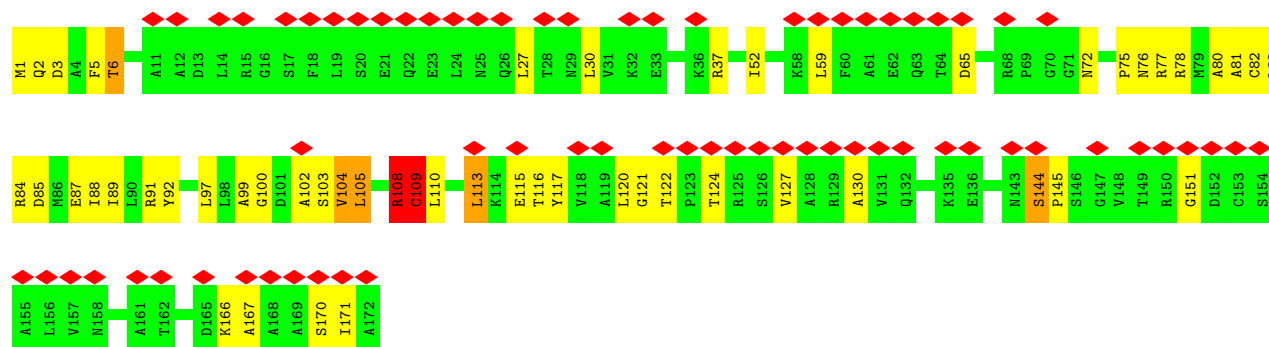


- Molecule 3: Phycocyanin beta chain



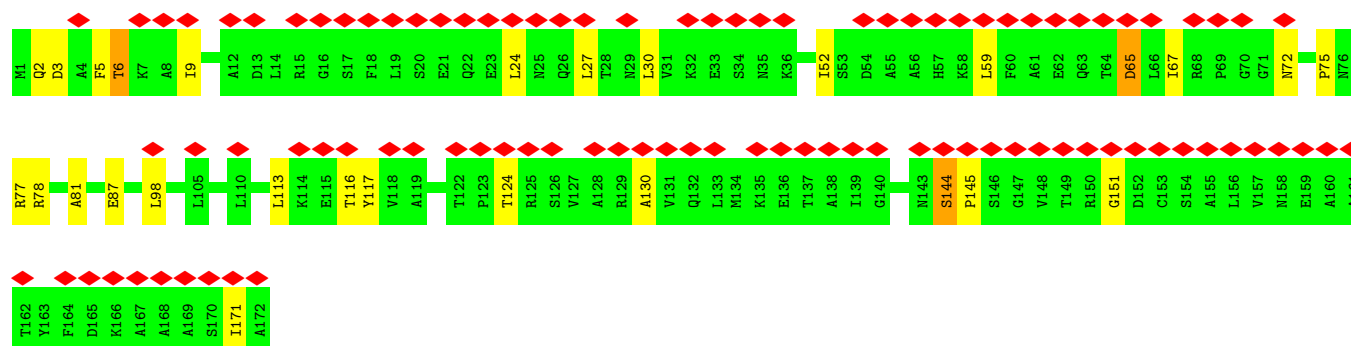
- Molecule 3: Phycocyanin beta chain

Chain Q8: 



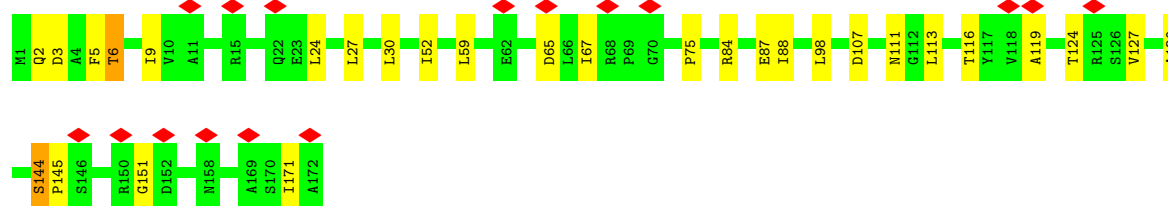
• Molecule 3: Phycocyanin beta chain

Chain S8: 



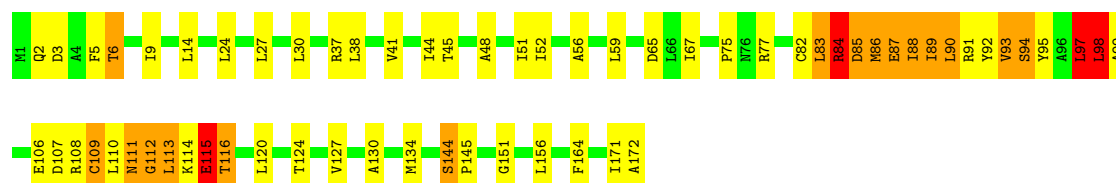
• Molecule 3: Phycocyanin beta chain

Chain F1: 



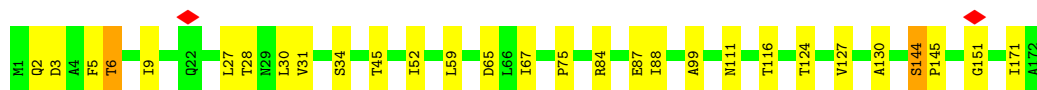
• Molecule 3: Phycocyanin beta chain

Chain L9: 



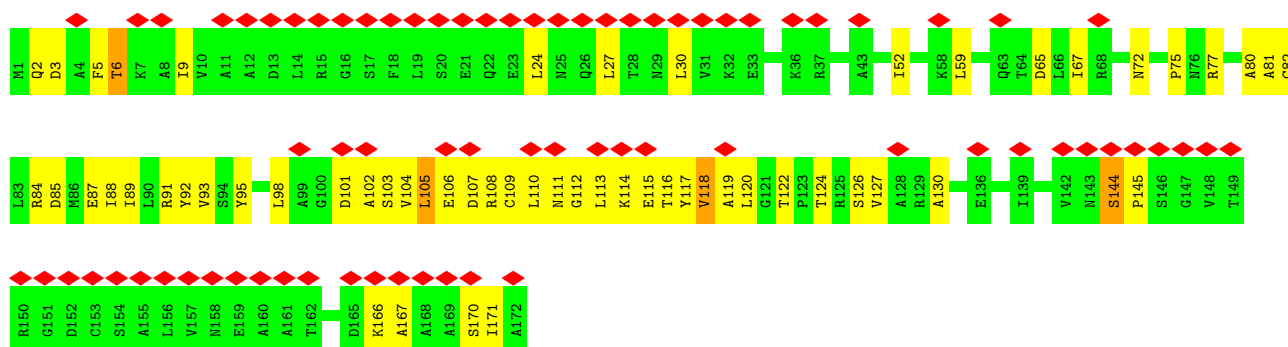
• Molecule 3: Phycocyanin beta chain

Chain P9: 



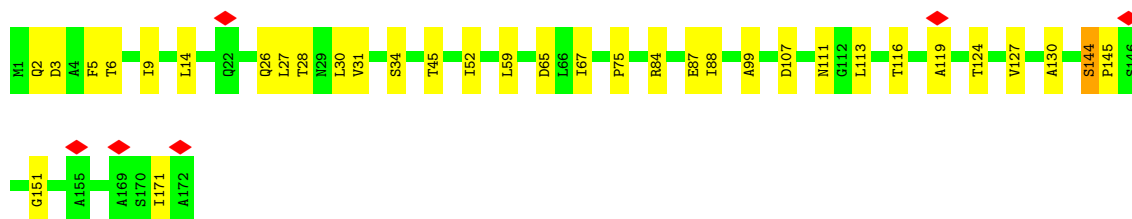
• Molecule 3: Phycocyanin beta chain

Chain Y8: 



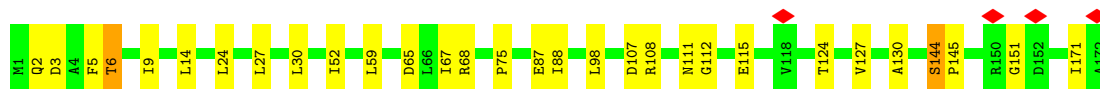
• Molecule 3: Phycocyanin beta chain

Chain B9: 



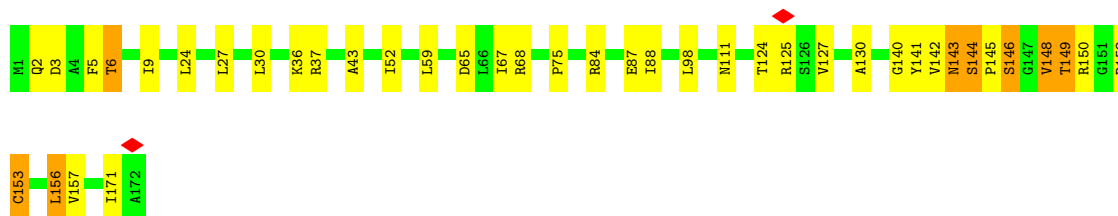
• Molecule 3: Phycocyanin beta chain

Chain D9: 

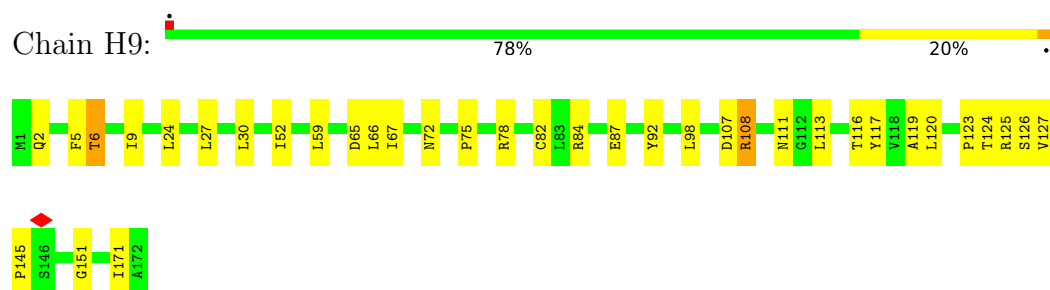


• Molecule 3: Phycocyanin beta chain

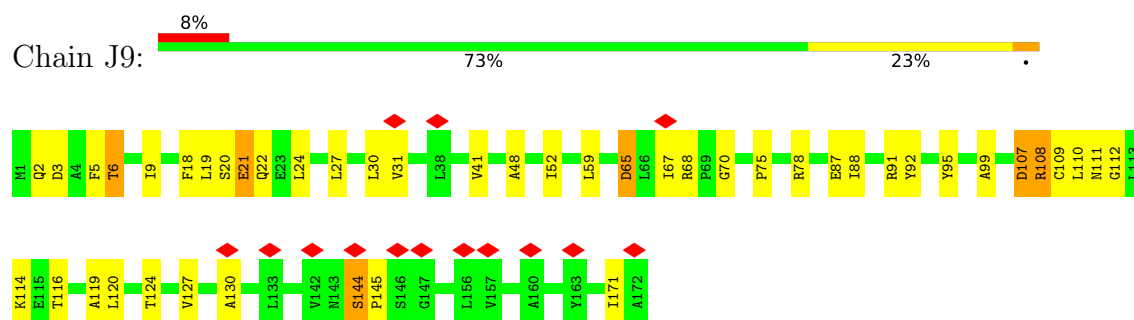
Chain F9: 



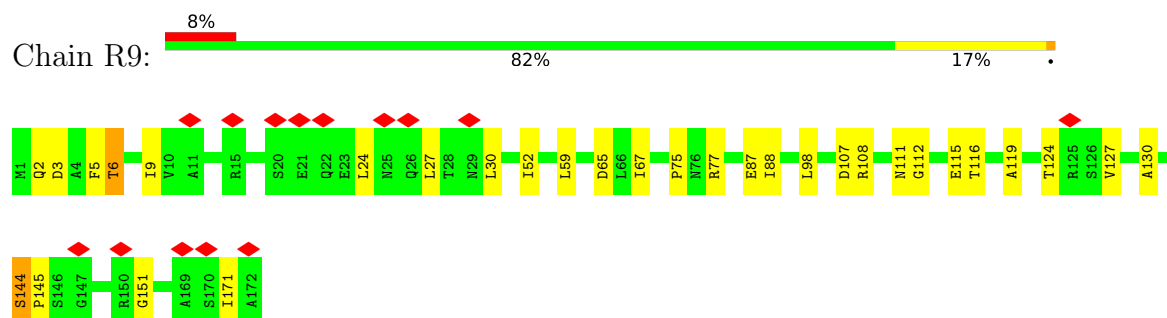
- Molecule 3: Phycocyanin beta chain



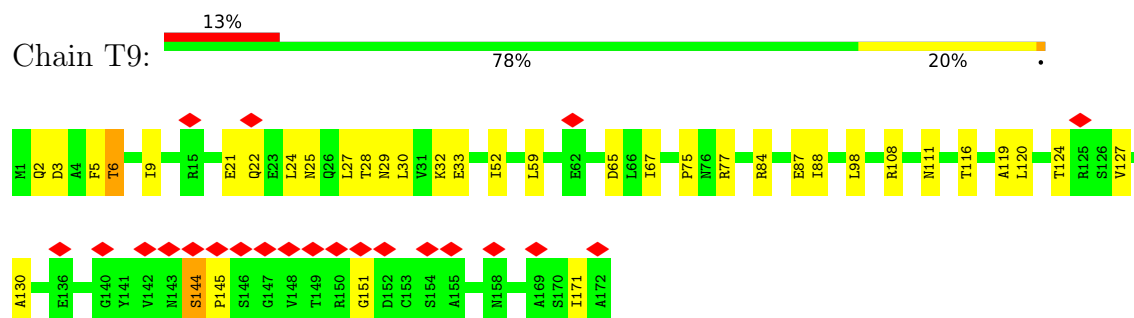
- Molecule 3: Phycocyanin beta chain



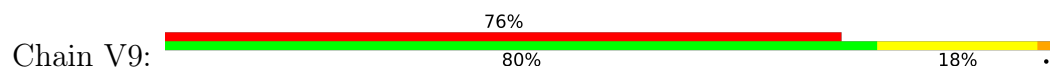
- Molecule 3: Phycocyanin beta chain

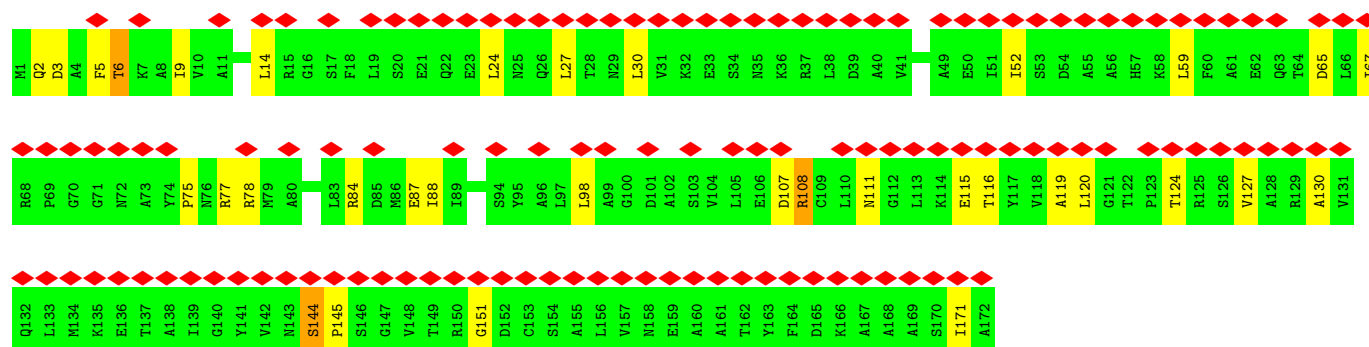


- Molecule 3: Phycocyanin beta chain

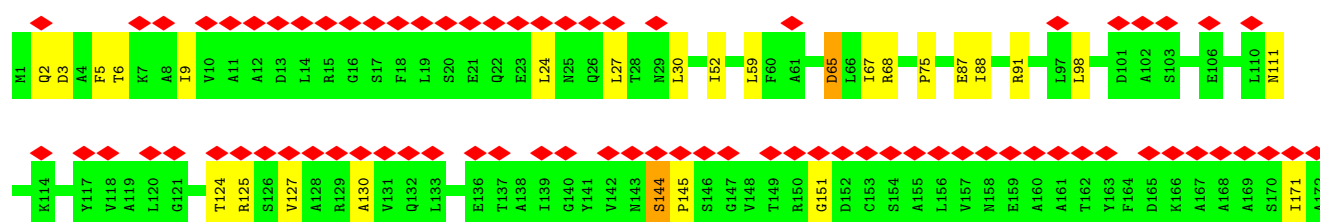
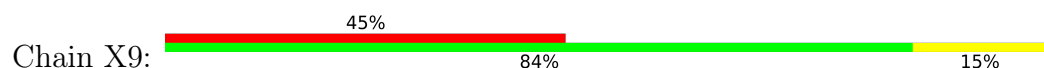


- Molecule 3: Phycocyanin beta chain

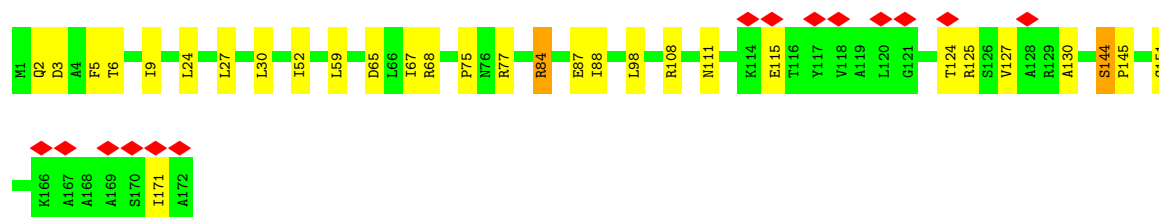
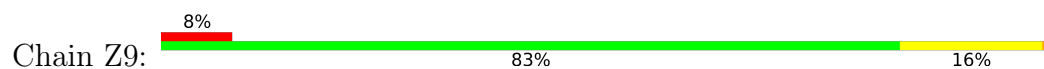




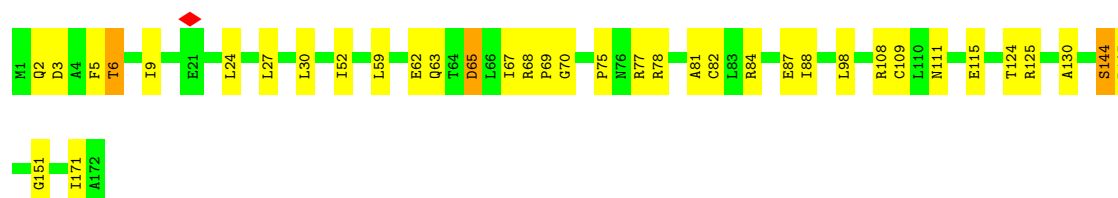
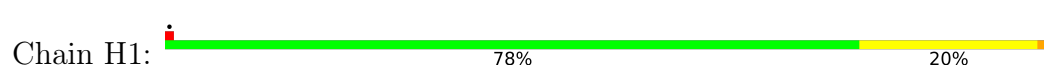
• Molecule 3: Phycocyanin beta chain



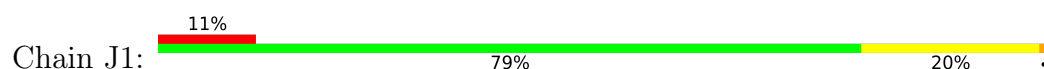
• Molecule 3: Phycocyanin beta chain



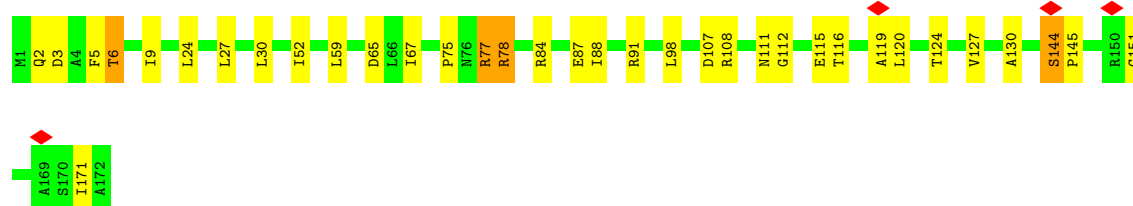
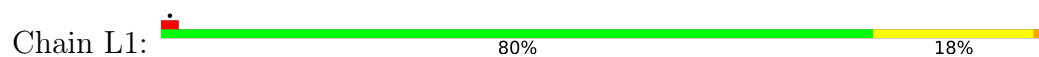
• Molecule 3: Phycocyanin beta chain



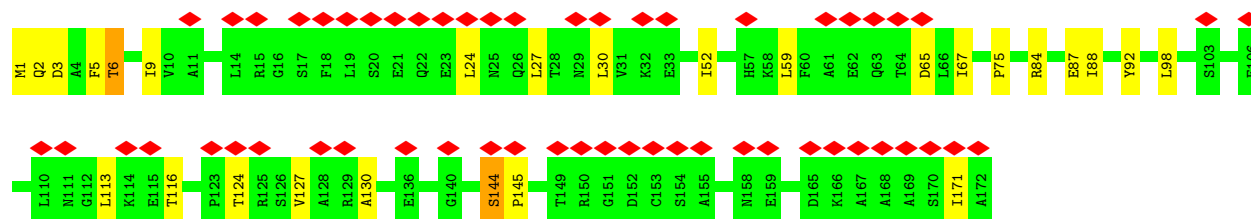
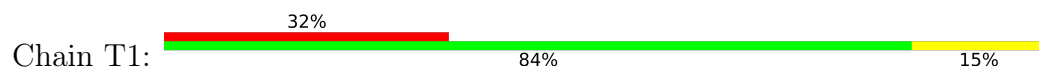
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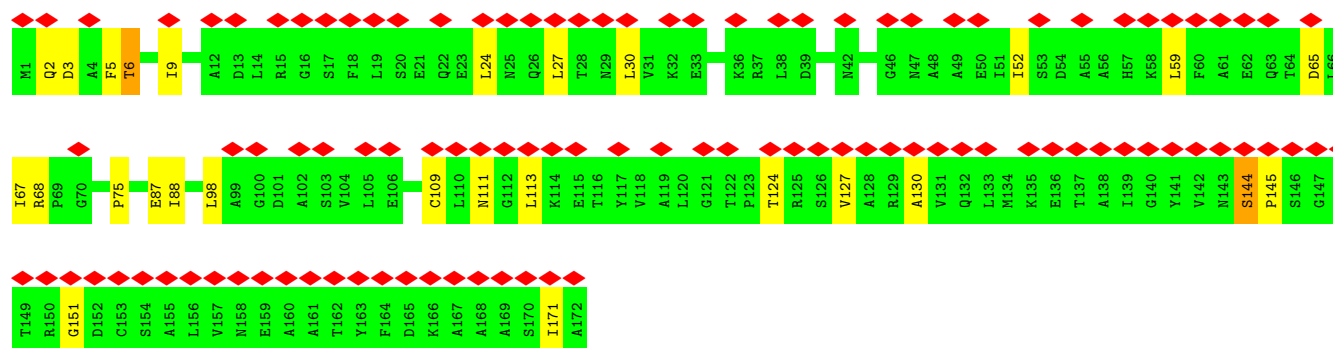
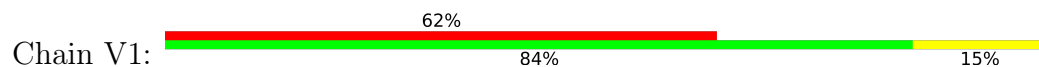
- Molecule 3: Phycocyanin beta chain



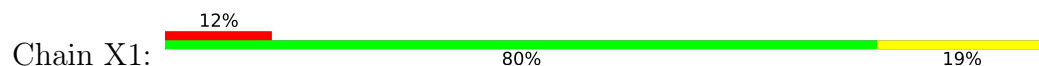
- Molecule 3: Phycocyanin beta chain

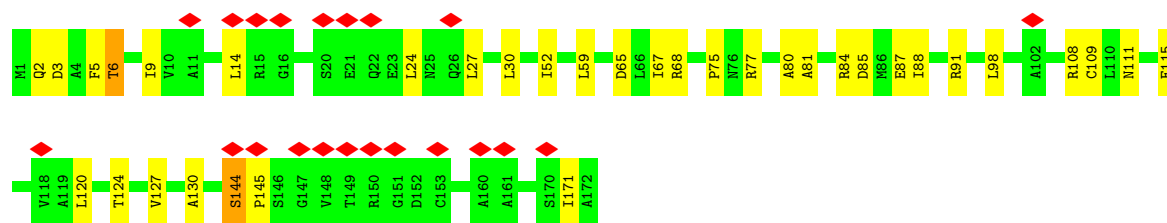


- Molecule 3: Phycocyanin beta chain

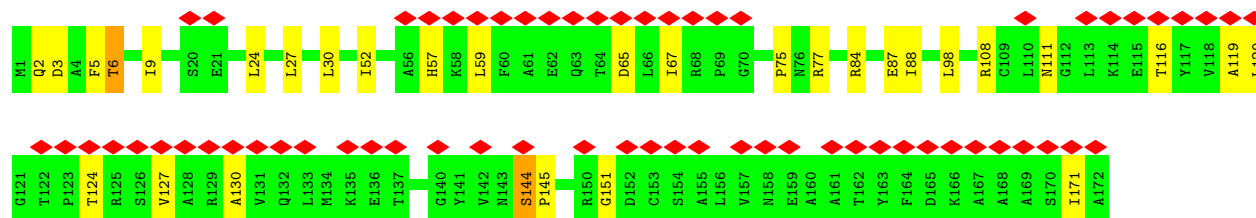
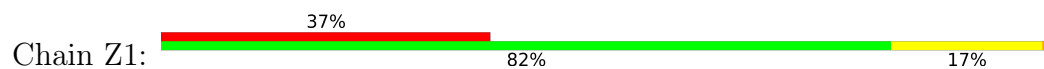


- Molecule 3: Phycocyanin beta chain

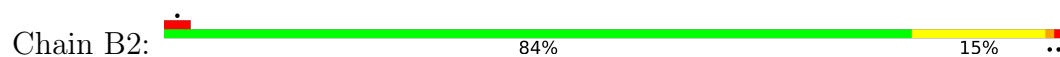




- Molecule 3: Phycocyanin beta chain



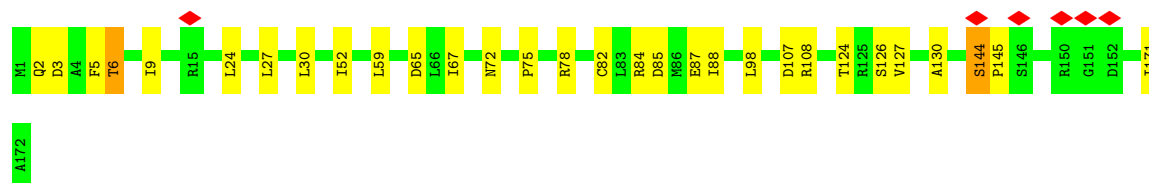
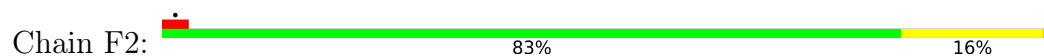
- Molecule 3: Phycocyanin beta chain



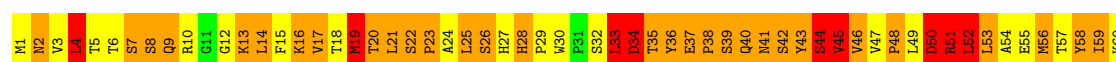
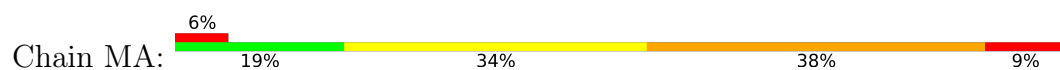
- Molecule 3: Phycocyanin beta chain

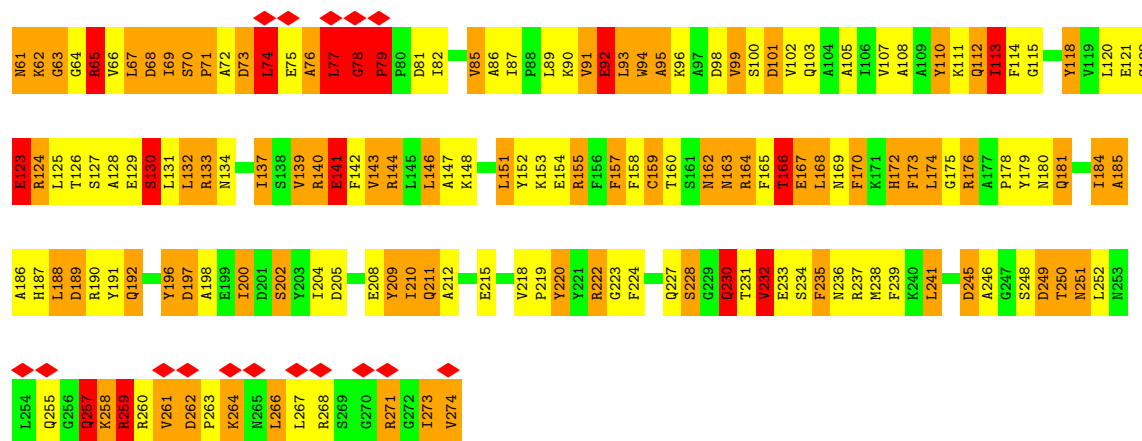


- Molecule 3: Phycocyanin beta chain

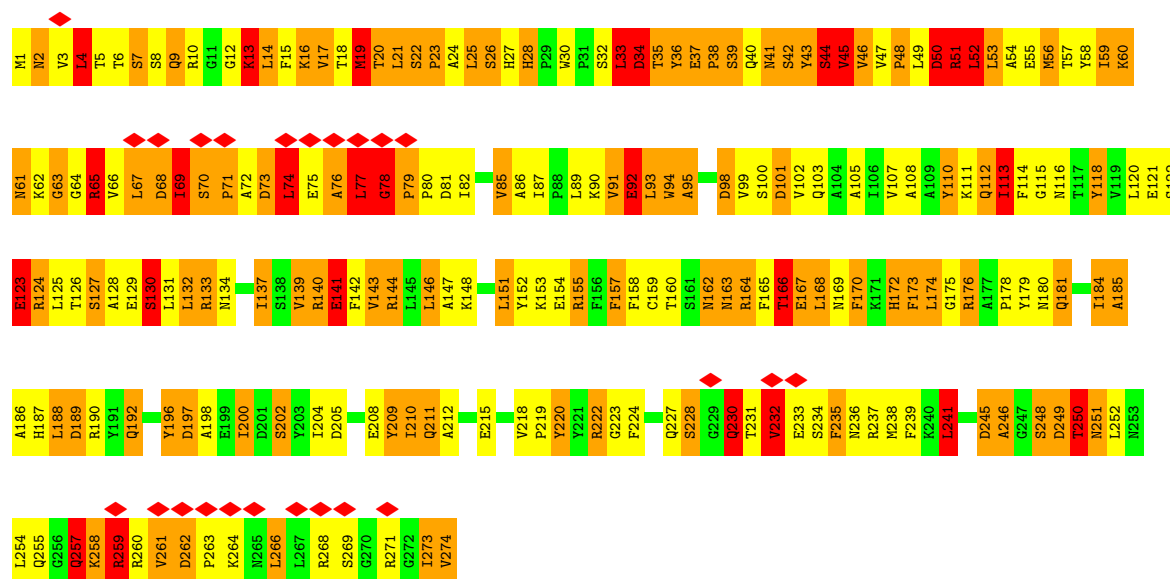
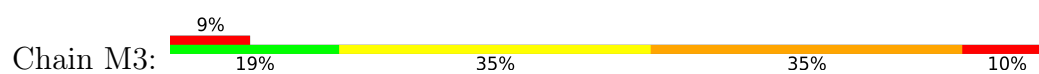


- Molecule 4: Phycocyanin-associated rod linker protein

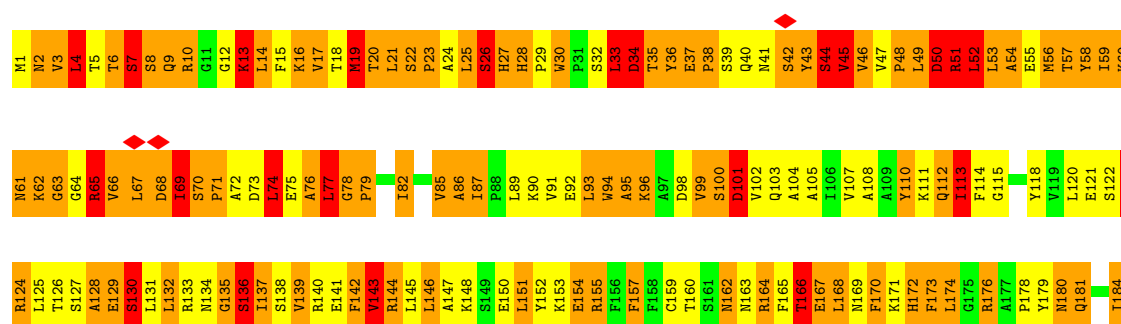




• Molecule 4: Phycocyanin-associated rod linker protein

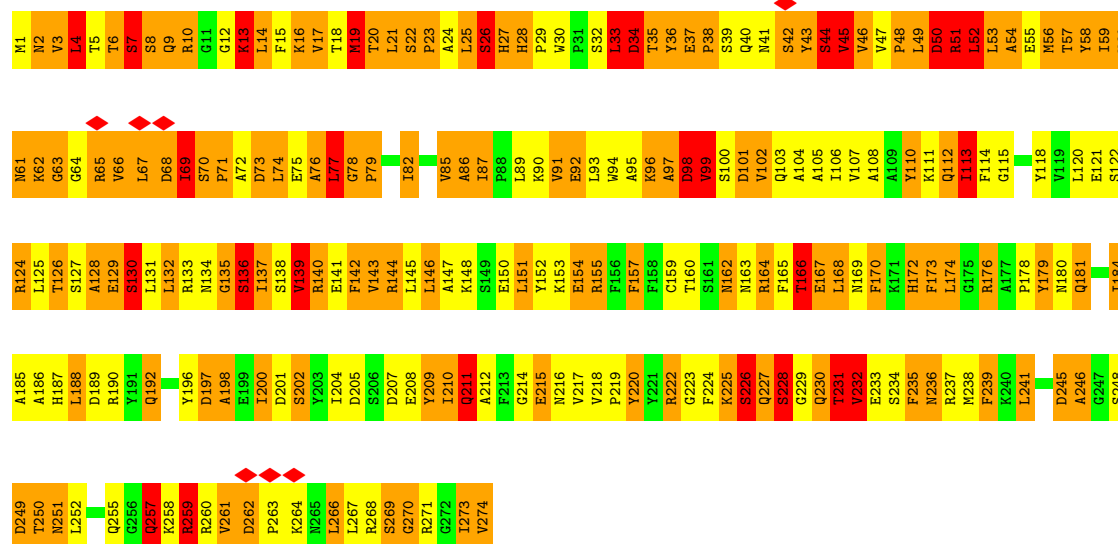


• Molecule 4: Phycocyanin-associated rod linker protein

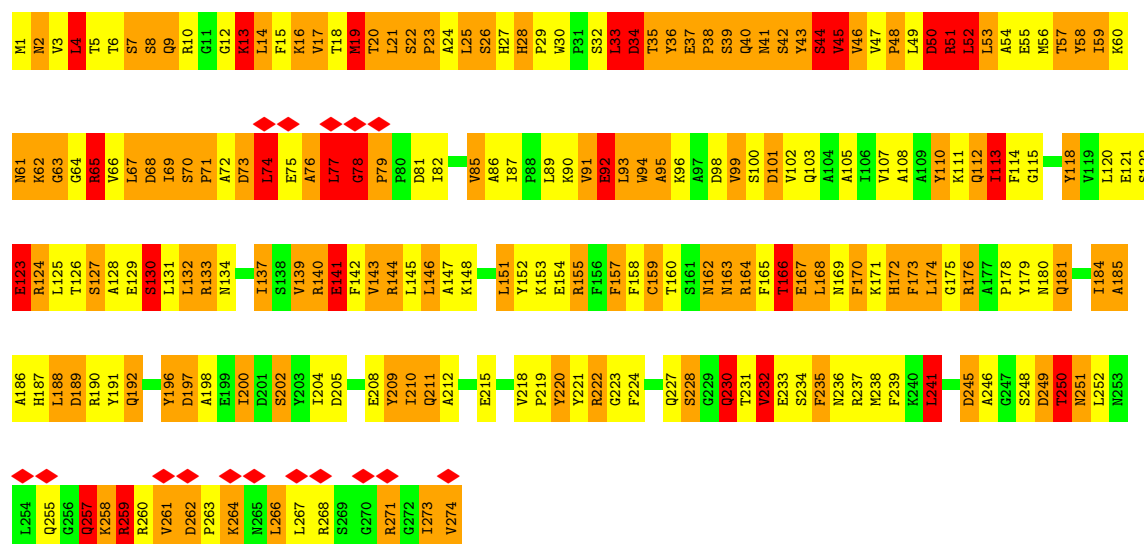
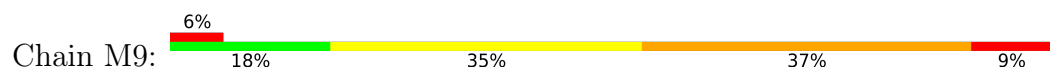




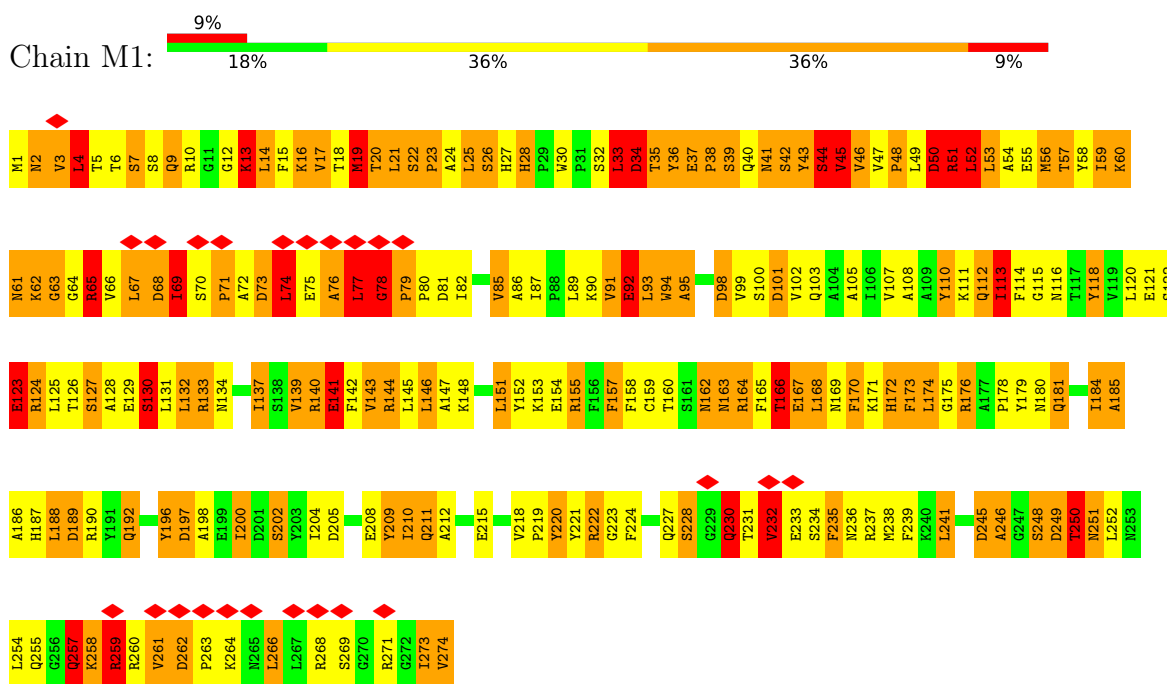
• Molecule 4: Phycocyanin-associated rod linker protein



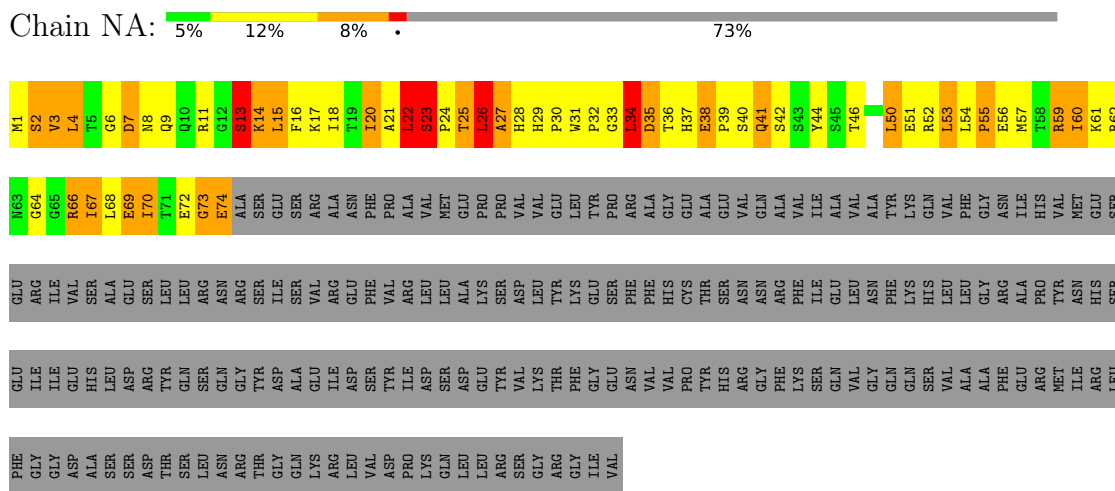
• Molecule 4: Phycocyanin-associated rod linker protein



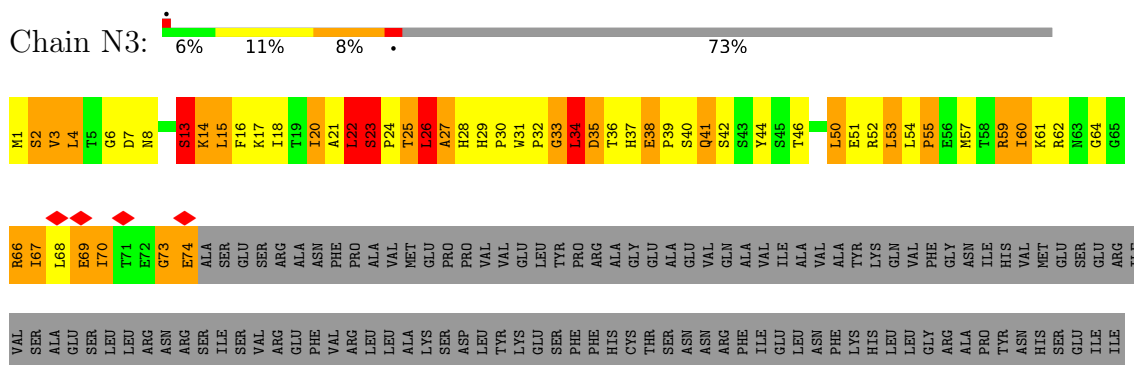
• Molecule 4: Phycocyanin-associated rod linker protein



- Molecule 5: Phycocyanin-associated rod linker protein



- Molecule 5: Phycocyanin-associated rod linker protein



[illegible]

- Molecule 5: Phycocyanin-associated rod linker protein

Chain Z4: 6% 9% 8% 73%

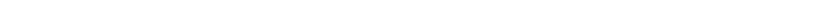
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	ARG	SER	170	V3
	THR	TYR	T71	L4
	SER	LEU	E72	
	LEU	ARG	G73	N8
	ASN	ASN	E74	
	ARG	ARG	ALA	S13
	GLY	SER	GLU	K14
	THR	TYR	ILE	L15
GLN	ALA	SER	SER	F16
	GLU	VAL	ARG	K17
	ILE	ARG	ALA	I18
	LEU	GLU	ASN	T19
	SER	PHE	PHE	G19
	VAL	VAL	PRO	A21
	ASP	ARG	ALA	L22
	PRO	LEU	VAL	S23
	LYS	LEU	VAL	
	GLN	SER	MET	P24
LEU	ASP	ALA	GLU	T25
	LEU	LYS	PRO	L26
	GLU	SER	PRO	A27
	VAL	ASP	VAL	H28
	LYS	LEU	VAL	H29
	THR	TYR	GLU	P30
	PHE	LYS	LEU	W31
	GLY	GLU	TYR	P32
	ILE	GLU	PRO	G33
	VAL	GLU	ARG	L34
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	VAL	HIS	GLU	H37
	PRO	CYS	GLU	E38
	THR	THR	ALA	P39
	HIS	SER	GLU	S40
	ARG	ASN	VAL	Q41
	GLY	ASN	GLN	S42
	PHE	ARG	ALA	S43
	GLN	PHE	VAL	G44
GLN	SER	ILE	ILE	Y44
	GLN	GLU	ALA	S45
	VAL	LEU	VAL	T46
	VAL	LEU	ALA	
	GLY	ASN	ALA	
	GLN	PHE	TYR	L50
	GLN	LYS	LYS	E51
	SER	HIS	GLN	R52
	VAL	VAL	VAL	L53
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	PHE	ARG	ASN	E56
	GLU	ALA	ILE	M57
	ARG	PRO	HIS	T58
	ARG	TYR	VAL	R59
	MET	ASN	VAL	L60
	GLY	VAL	GLU	K61
	ARG	HIS	GLU	R62
	LEU	SER	GLU	N63
	PHE	GLU	ARG	G64
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- Molecule 5: Phycocyanin-associated rod linker protein

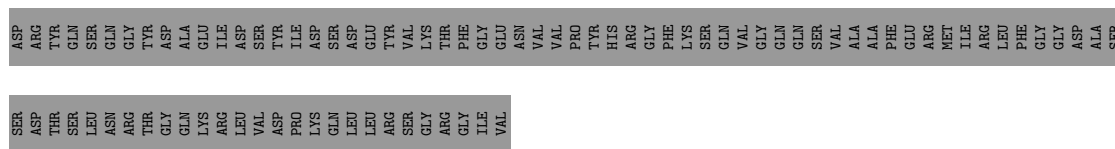
Chain N9: 5% 12% 8% . 73%

[illegible]

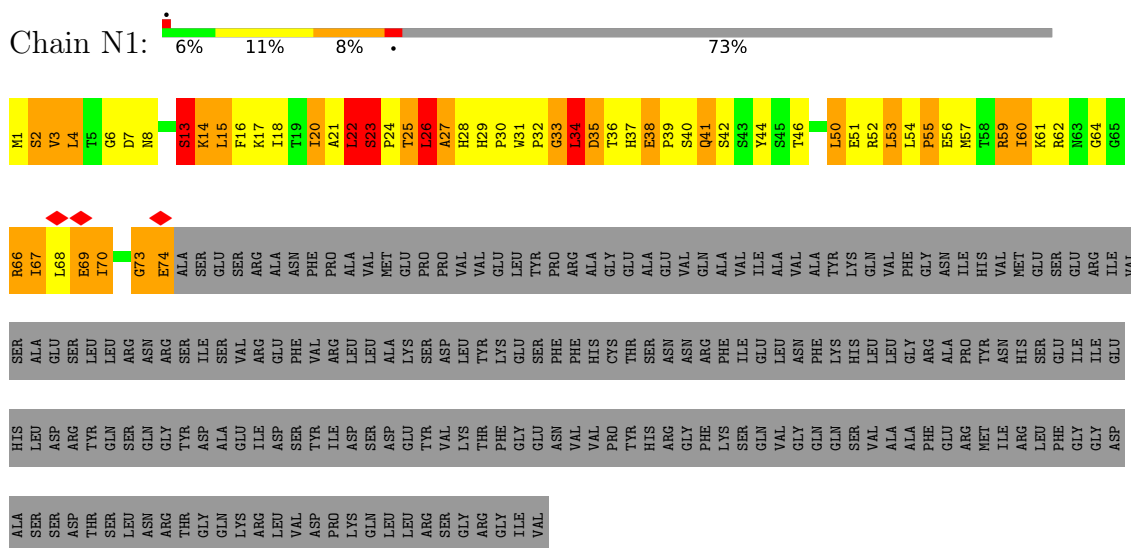
- Molecule 5: Phycocyanin-associated rod linker protein

Chain Z8:  6% 12% 8% . 73%

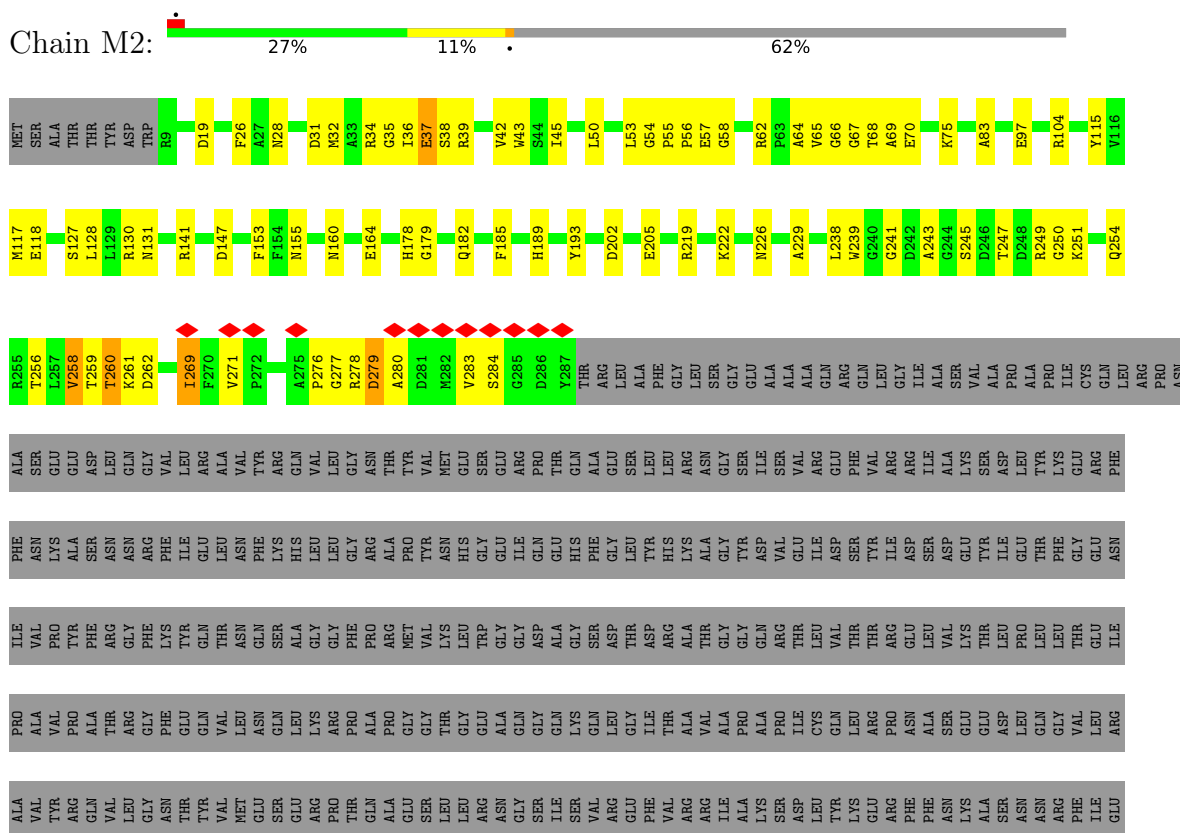
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T70	S2
I71	V3
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G73	T5
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ALA	Q9
SER	
SER	S13
ILE	K14
GLU	L15
VAL	F16
ARG	K17
ASN	N18
ASP	P19
LEU	T19
LEU	I20
VAL	A21
MET	L22
GLU	S23
LYS	P24
PRO	T25
PRO	L26
ASP	A27
LEU	H28
TYR	H29
GLU	P30
GLU	W31
SER	P32
PHE	G33
PHE	G33
HIS	L34
CYS	D35
THR	T36
GLU	H37
ASN	H38
ASN	P39
ASN	S40
ARG	Q41
PHE	I42
ILE	S42
GLU	S43
GLU	Y44
LEU	
ASN	
ALA	
ASN	L50
PHE	E51
PHE	R52
HIS	L53
LYS	L54
LEU	P55
LEU	G56
GLY	M57
GLY	ASN
ARG	ILE
ALA	
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PRO	H59
TYR	VAL
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HIS	L60
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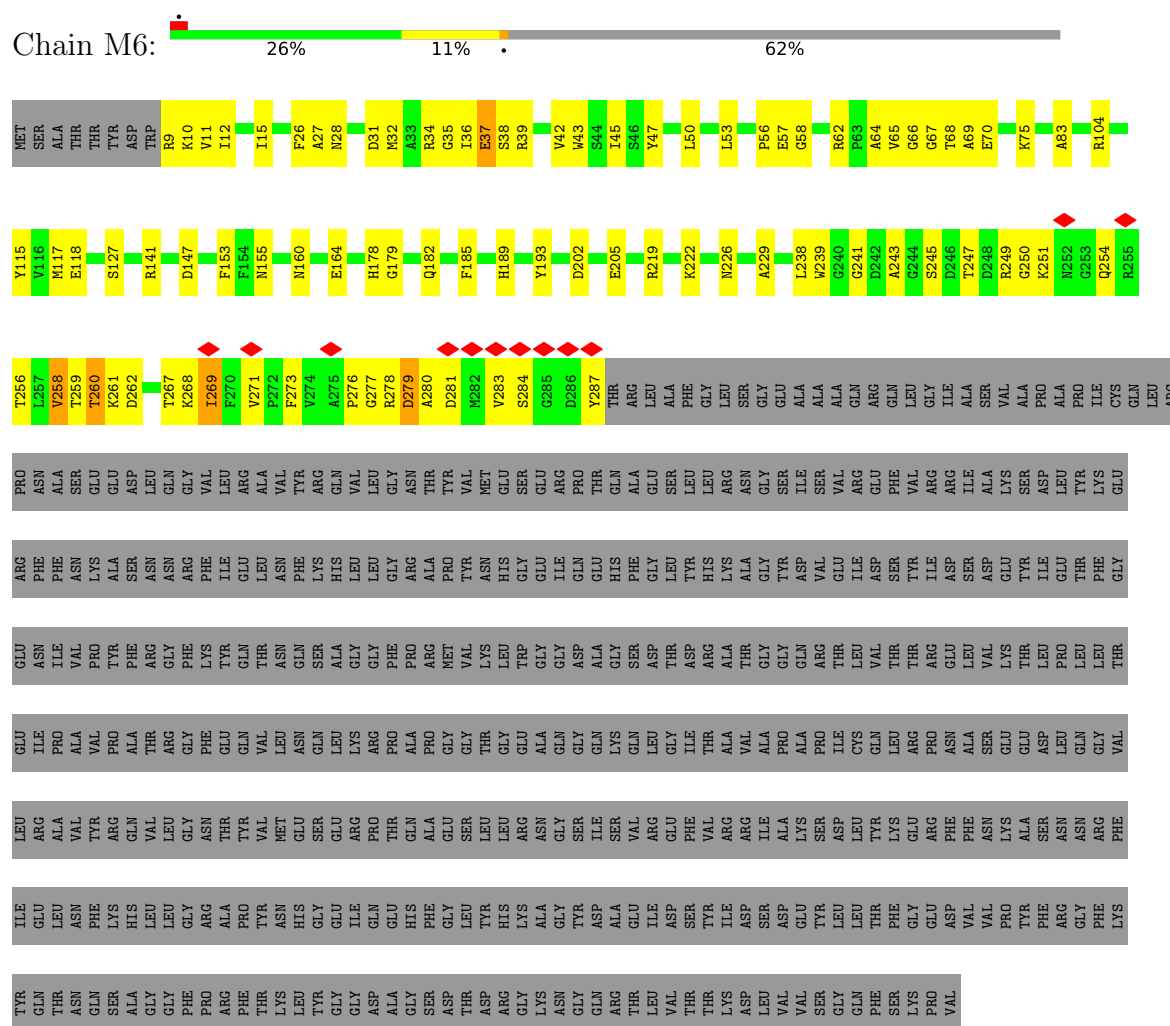
- Molecule 5: Phycocyanin-associated rod linker protein



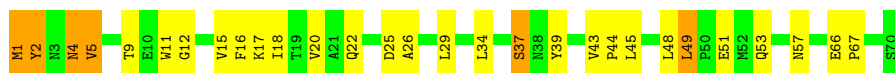
- Molecule 6: Glr2806 protein



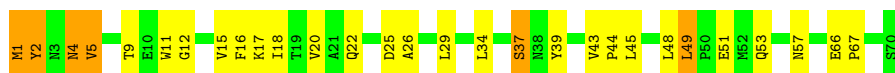
- Molecule 6: Glr2806 protein



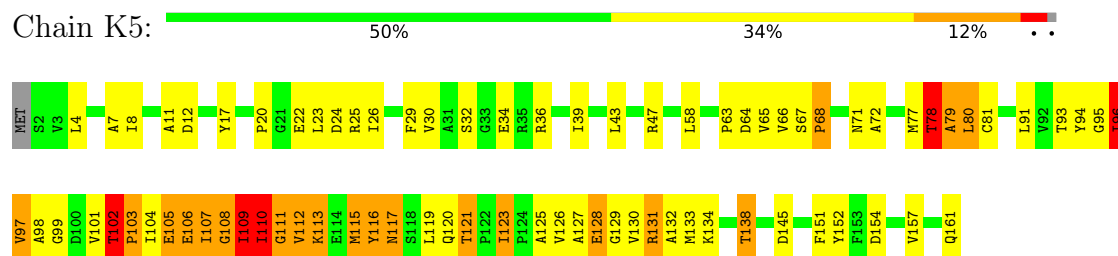
- Molecule 7: CpcD protein



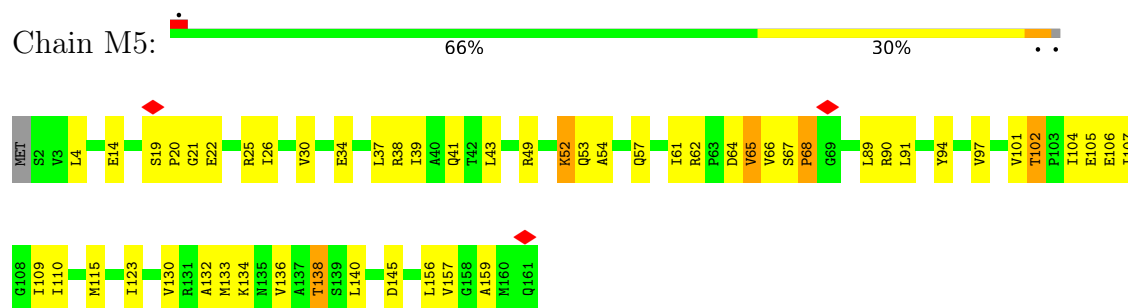
- Molecule 7: CpcD protein



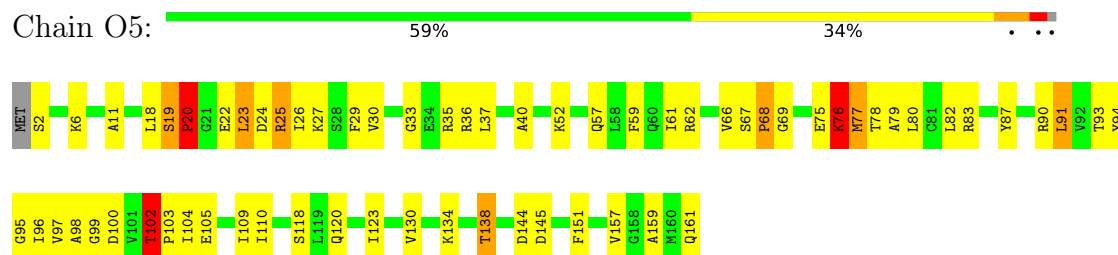
- Molecule 8: Allophycocyanin alpha subunit



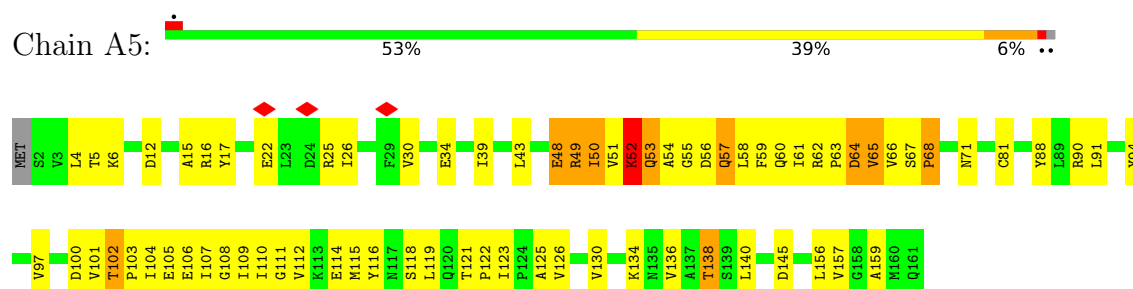
- Molecule 8: Allophycocyanin alpha subunit



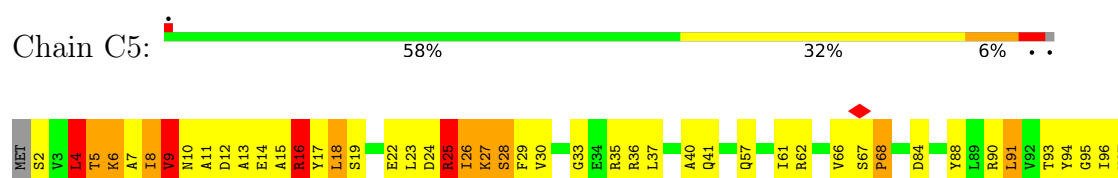
- Molecule 8: Allophycocyanin alpha subunit



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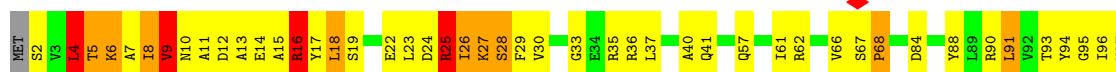
• Molecule 8: Allophycocyanin alpha subunit



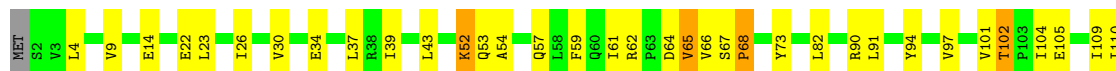
• Molecule 8: Allophycocyanin alpha subunit



• Molecule 8: Allophycocyanin alpha subunit

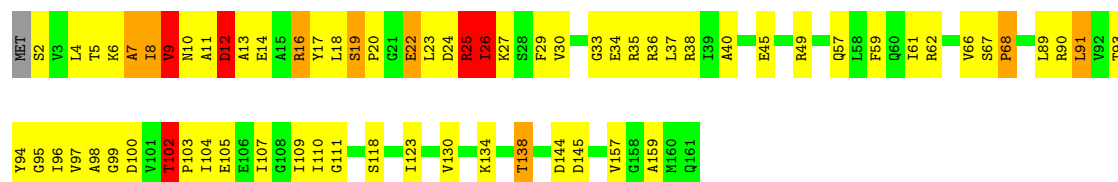


• Molecule 8: Allophycocyanin alpha subunit



• Molecule 8: Allophycocyanin alpha subunit

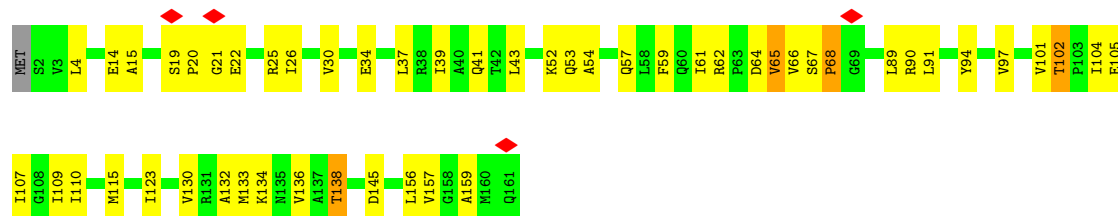




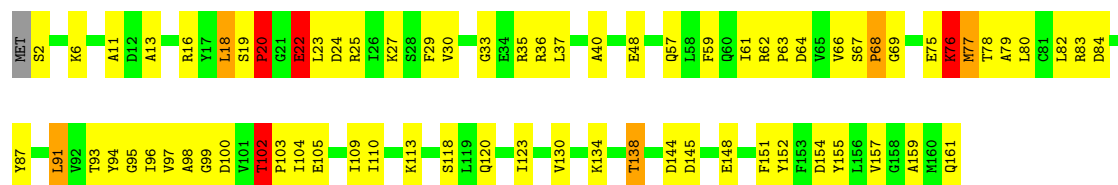
• Molecule 8: Allophycocyanin alpha subunit



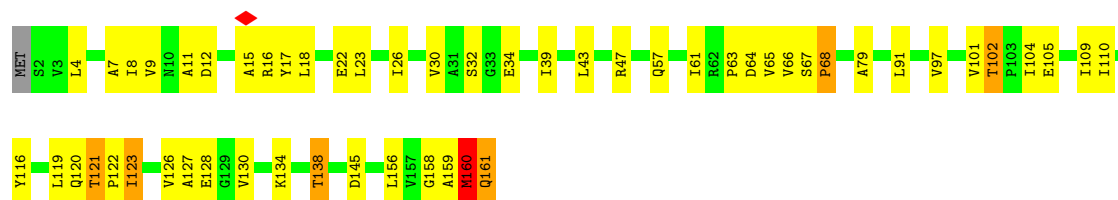
• Molecule 8: Allophycocyanin alpha subunit



• Molecule 8: Allophycocyanin alpha subunit

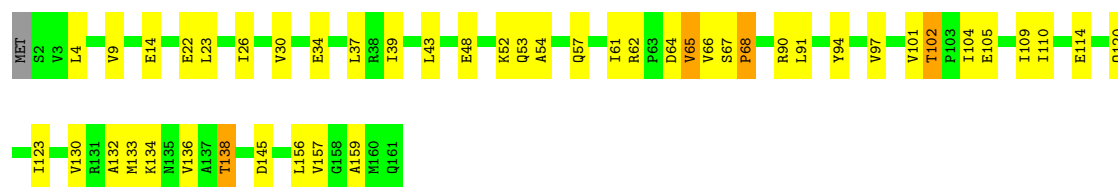


• Molecule 8: Allophycocyanin alpha subunit



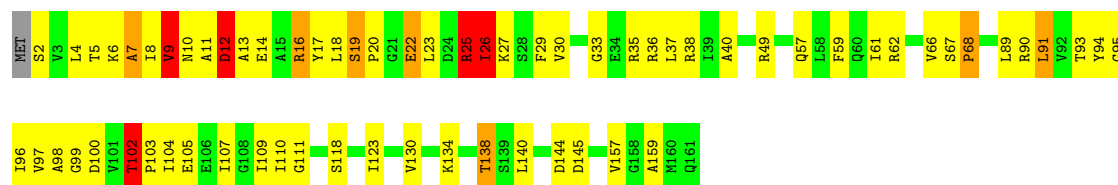
• Molecule 8: Allophycocyanin alpha subunit

Chain Y5:  71% 26% ..



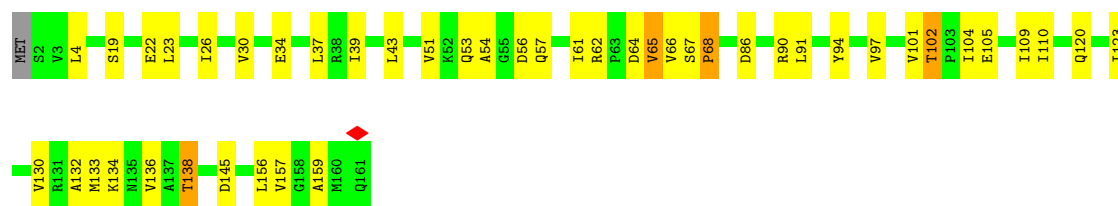
• Molecule 8: Allophycocyanin alpha subunit

Chain a5:  58% 34% . . .



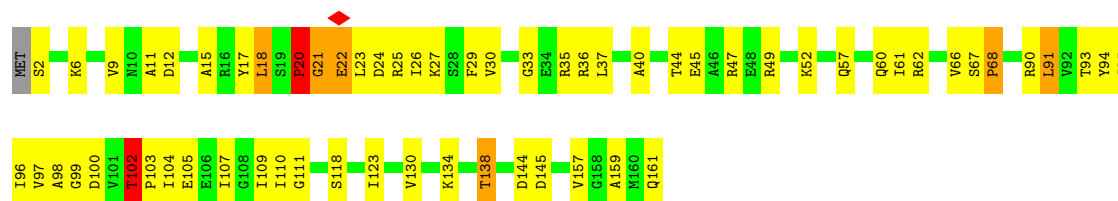
• Molecule 8: Allophycocyanin alpha subunit

Chain A7:  71% 25% ..



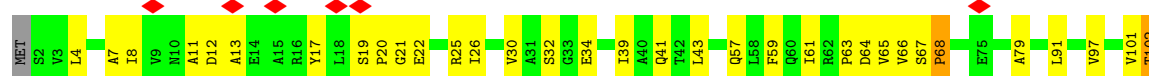
• Molecule 8: Allophycocyanin alpha subunit

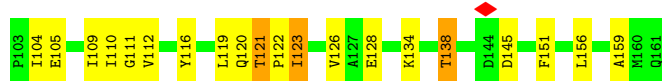
Chain O7:  60% 34% . . .



• Molecule 8: Allophycocyanin alpha subunit

Chain Q7:  66% 30% . . .

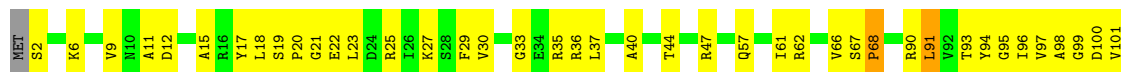




- Molecule 8: Allophycocyanin alpha subunit



- Molecule 8: Allophycocyanin alpha subunit



- Molecule 8: Allophycocyanin alpha subunit

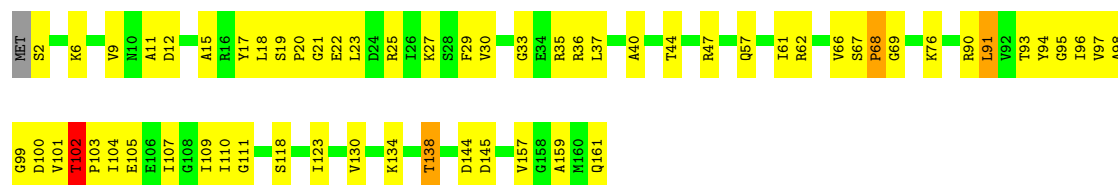


- Molecule 8: Allophycocyanin alpha subunit



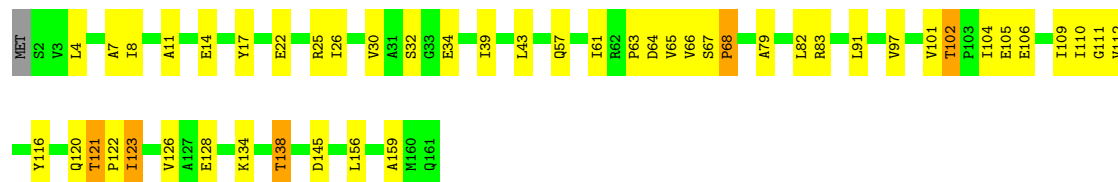
- Molecule 8: Allophycocyanin alpha subunit





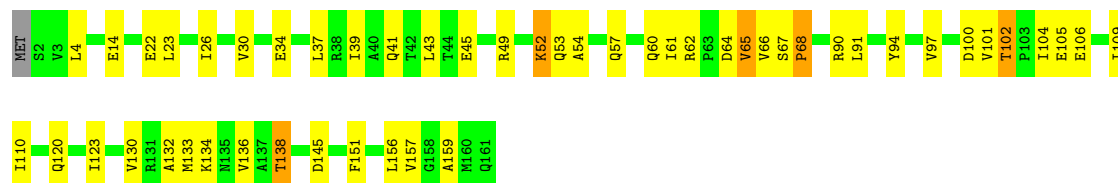
• Molecule 8: Allophycocyanin alpha subunit

Chain K7: 70% 27% ..



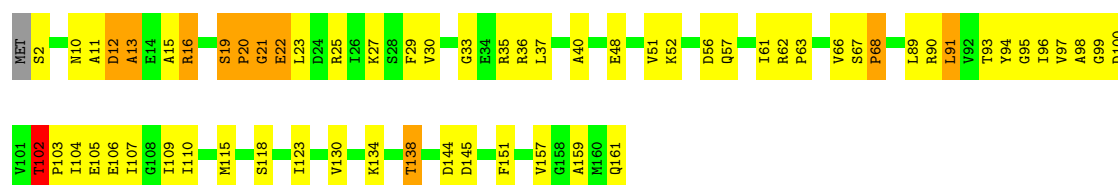
• Molecule 8: Allophycocyanin alpha subunit

Chain M7: 68% 28% ..



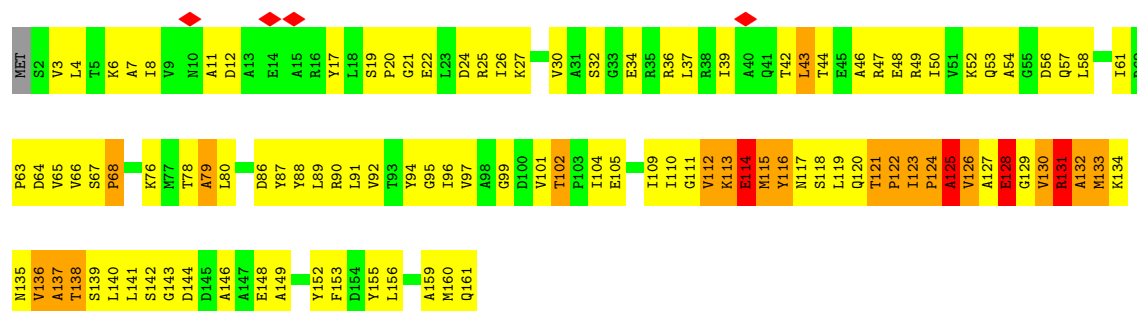
• Molecule 8: Allophycocyanin alpha subunit

Chain g7: 60% 32% 6% ..

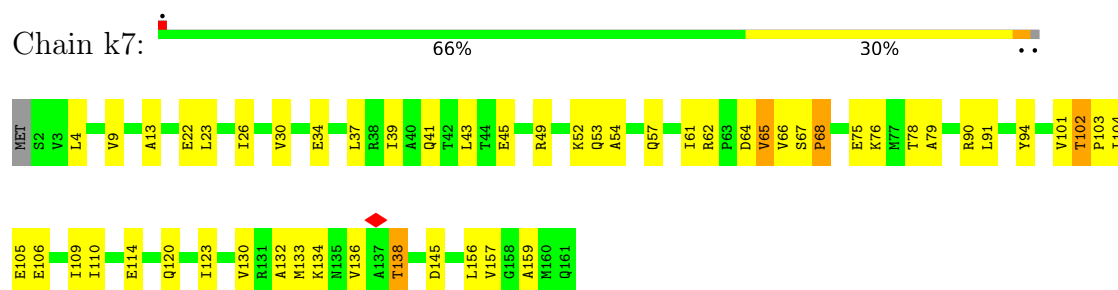


• Molecule 8: Allophycocyanin alpha subunit

Chain i7: 32% 53% 12% ..



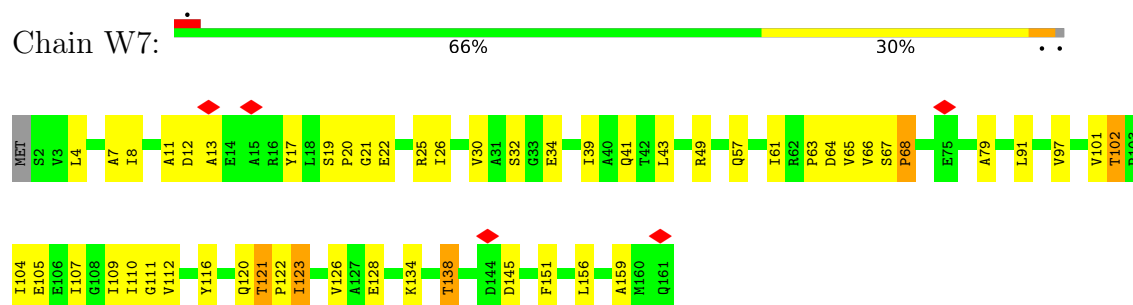
- Molecule 8: Allophycocyanin alpha subunit



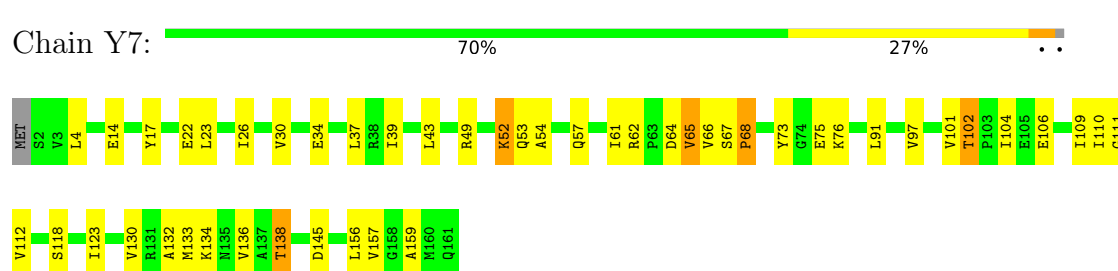
- Molecule 8: Allophycocyanin alpha subunit



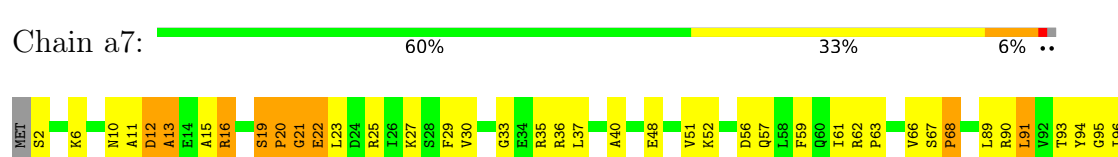
- Molecule 8: Allophycocyanin alpha subunit



- Molecule 8: Allophycocyanin alpha subunit



- Molecule 8: Allophycocyanin alpha subunit





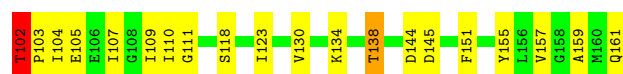
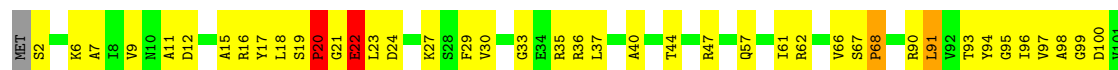
• Molecule 8: Allophycocyanin alpha subunit



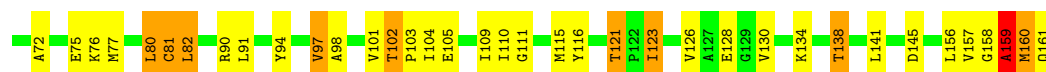
• Molecule 8: Allophycocyanin alpha subunit



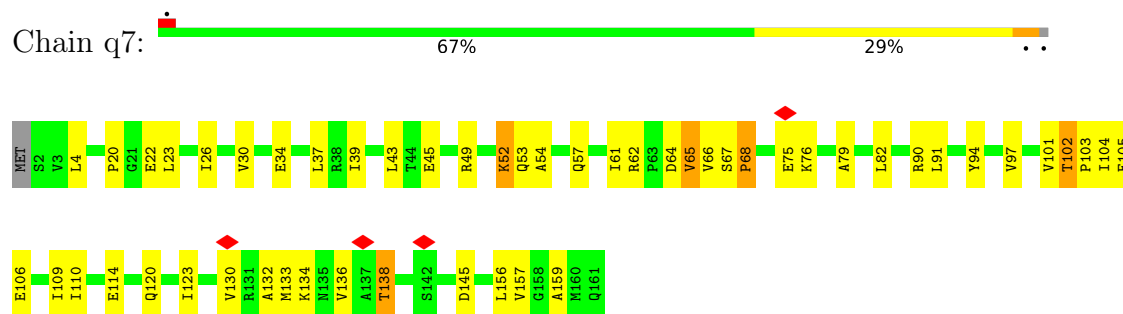
• Molecule 8: Allophycocyanin alpha subunit



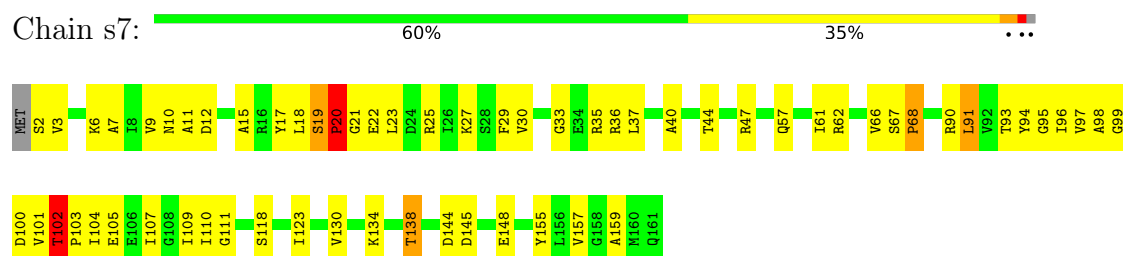
• Molecule 8: Allophycocyanin alpha subunit



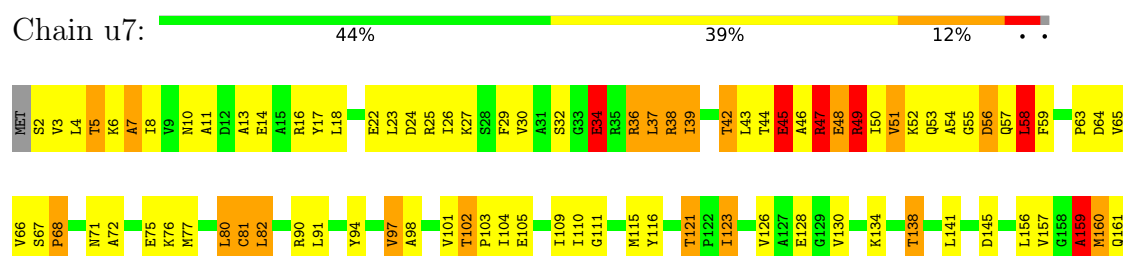
• Molecule 8: Allophycocyanin alpha subunit



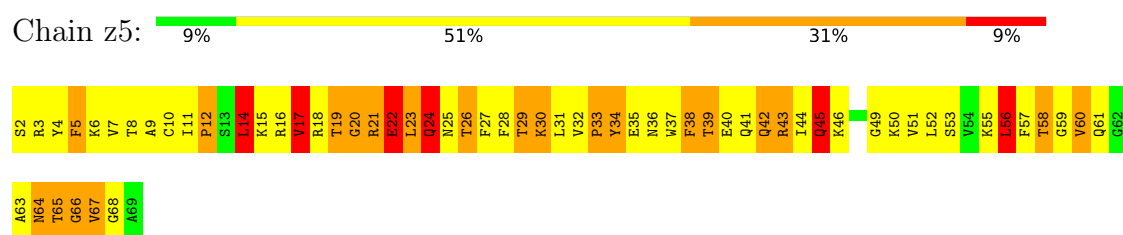
- Molecule 8: Allophycocyanin alpha subunit



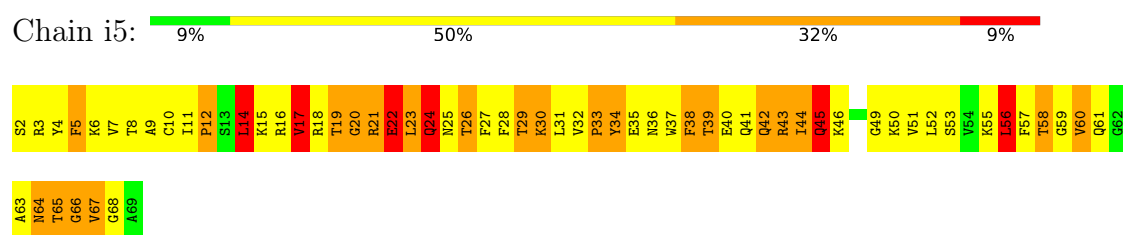
- Molecule 8: Allophycocyanin alpha subunit



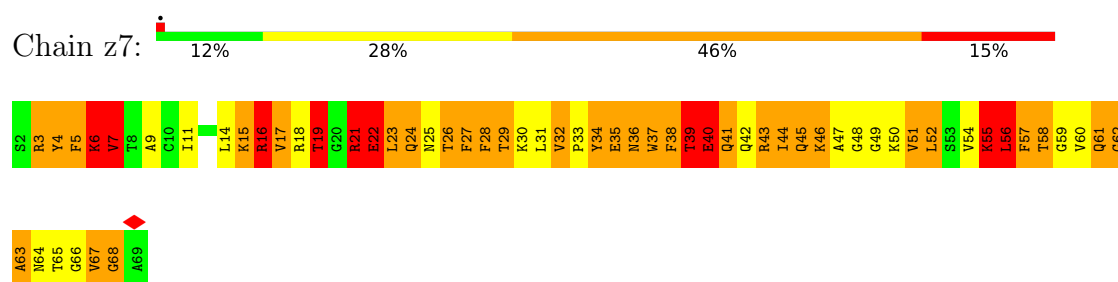
- Molecule 9: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core



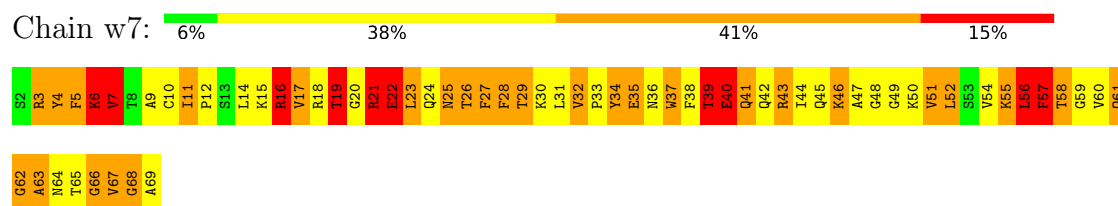
- Molecule 9: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core



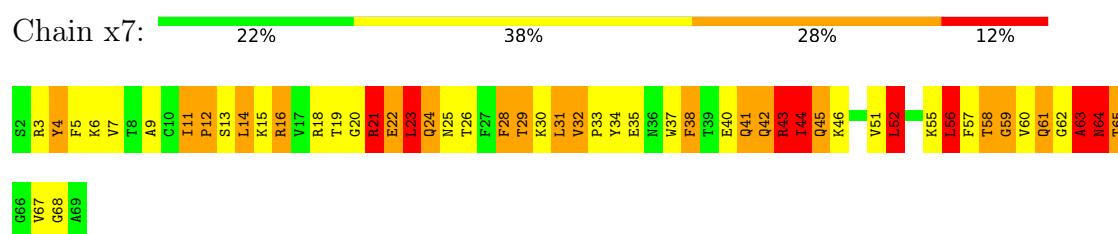
- Molecule 9: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core



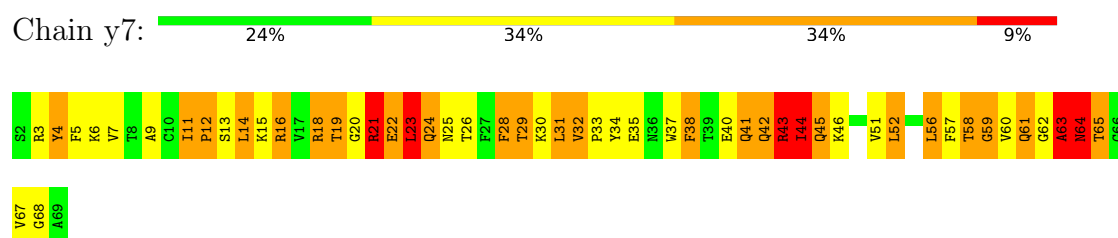
- Molecule 9: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core



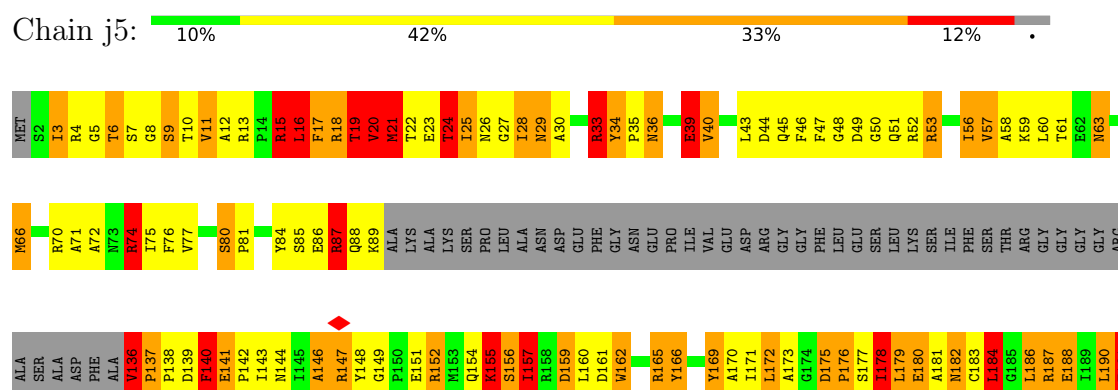
- Molecule 9: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core

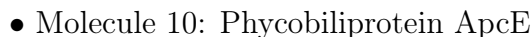


- Molecule 9: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core

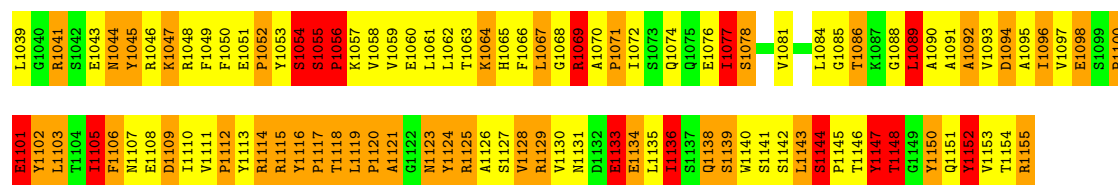


- Molecule 10: Phycobiliprotein ApcE

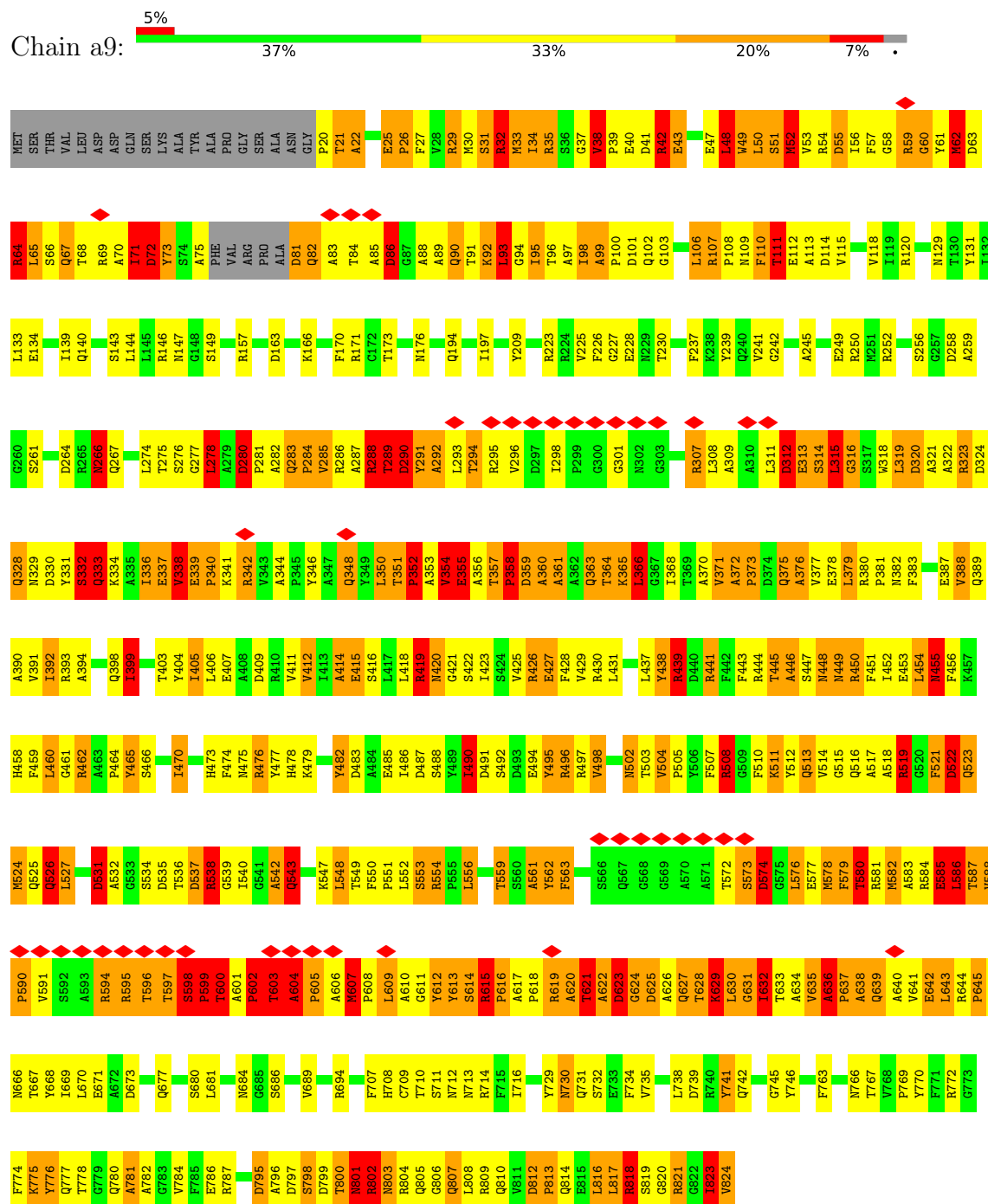




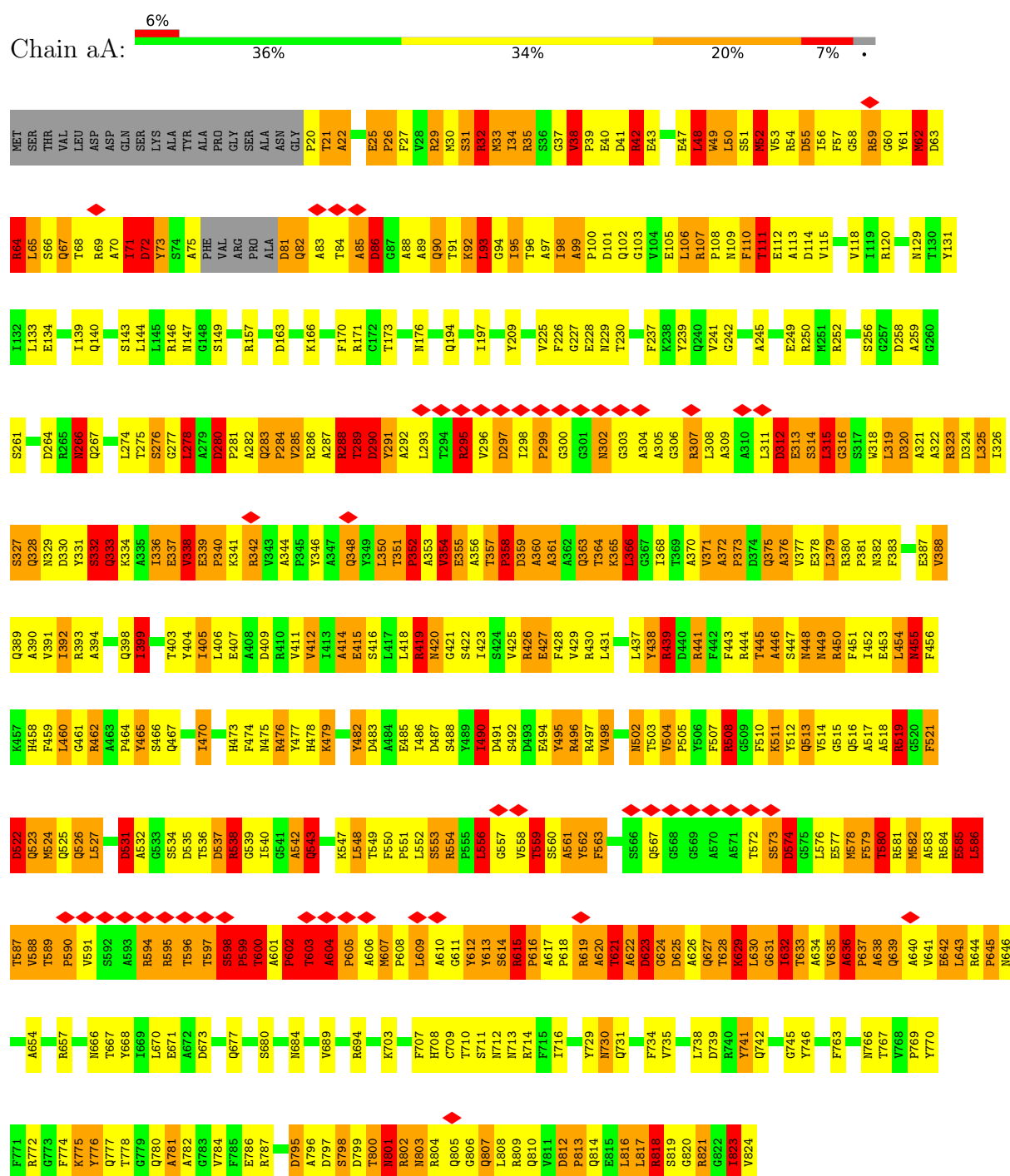
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I981	R920	R860	S801	M740	L679	E619	T559	A499	A439	F379	Q313	E252	L191	ALA	I3
Y982	G921	A861	S802	M741	P680	P620	V560	P580	G314	R253	Q314	R253	K192	SER	R4
R983	K922	R862	V802	G742	V681	F621	E561	I601	D441	I381	S315	P254	G193	ALA	T5
I984	N923	T863	K803	V743	E682	V622	G562	G502	L442	I382	V316	G255	C194	ASP	A71
A985	N924	G864	E804	V744	R683	V623	S563	K503	Y443	S383	S317	L256	S195	ASP	A72
P986	I925	A865	F805	A745	V684	G624	V564	D504	N444	S384	E318	T257	I196	PHE	S7
D987	A926	L866	V806	L746	L685	K625	G565	V505	Y445	P385	A319	L258	L197	ALA	G8
A988	G927	V867	R807	R747	T686	A626	A566	K506	A446	I387	S321	P259	A198	V136	S9
T989	N928	D868	L808	R748	P687	L627	L567	R507	A447	R388	G322	Y260	T199	P138	T10
R990	P929	G869	L809	G749	E688	E628	I568	I508	P448	R389	V323	Y261	T199	P139	V11
S991	L930	E870	G810	R750	G689	V629	T569	L509	R449	G390	V324	Y262	I200	D139	A12
E992	V931	E871	F811	K751	L690	L630	A570	I510	R450	Q390	K324	K263	A202	E141	R13
K993	Q932	H872	S812	V752	S691	H631	A571	R511	K451	S391	N325	K264	A203	P142	F14
D994	A933	G873	A813	F753	L692	R632	V572	N512	V452	S392	G326	L264	L203	P143	R15
V995	A934	R874	L814	K754	R693	R633	G573	G513	P453	E327	S325	S265	L204	I143	L16
A996	L935	L875	Y815	O755	K694	L634	Q574	S514	Q454	K394	I328	A266	M206	Y84	F17
A997	K936	Y876	R816	S756	R695	L635	I575	P515	F455	S395	S329	S268	M205	I145	R18
I998	E937	G877	K817	Q757	R696	G636	F576	T516	L456	G396	S329	S269	K208	A146	T19
A999	Q938	E878	K818	A758	F697	R637	G577	S517	T457	G397	F333	T270	N209	R147	R21
I1000	Q939	D879	F819	T759	G698	P638	R578	N518	L458	L398	R336	T271	A211	Q89	M21
Y1001	A940	T880	H820	D760	S699	T639	Q579	E519	F459	Y399	R337	F272	K89	Y148	E22
R1002	T941	V881	D821	R761	S700	Y640	L580	R520	A460	L337	K273	F273	A212	G149	E23
Q1003	K942	R822	R822	E762	D701	D641	Y581	G521	D461	L401	G338	M274	L213	E151	T24
Y1004	T943	S823	Y823	S763	V702	R642	Q582	N522	Y482	L402	K339	T275	F214	R152	I25
L1005	A944	K884	P824	F764	L703	V643	G584	P523	T463	D403	L342	A276	K215	M153	N26
D1006	L945	N825	N825	D765	T704	E644	Q584	T524	Q464	A404	L343	T277	D216	K155	G27
Y1007	R946	F886	T826	A766	T705	N645	R586	G525	P465	L405	Y343	Y278	E217	R156	I28
F1008	N947	R827	K827	L767	R706	N646	L586	M526	L406	R344	R344	G279	A218	S157	N29
A1009	S948	T888	V828	V768	G707	R647	K587	S527	P467	D407	R345	A280	D219	I157	ALA
I1010	R949	L889	V829	T768	G708	V648	V588	E528	N468	S408	E346	A281	S220	R158	ASN
I1011	P950	F990	E830	A770	G709	F649	A589	G529	N469	E409	F347	R283	K221	D159	ASP
P1012	F951	A891	F831	A771	L710	D650	E590	A530	H470	E410	Y348	P284	L160	L160	GLU
P1013	L952	R892	A832	V772	P711	L651	I591	T531	P471	Y411	Q349	K285	L222	D161	PHE
S1014	L953	K893	R833	V773	R712	A652	K592	T532	Y472	T412	P350	N286	V223	W162	N36
Y1015	E954	V894	K834	Q774	G713	S653	L593	L533	G473	S413	F351	N287	S225	ASN	E38
L1016	L955	P895	H835	V775	D714	K654	E594	G534	A474	I414	I352	L288	Y226	GLU	V40
R1017	G956	K896	F836	F776	A715	K655	N595	P535	G475	F415	N353	S289	I227	ILE	F39
L1018		S897	L837	D777	A716	G656	G596	K536	R476	G416	S354	S290	V230	T168	VAL
S1019	F959	R898	G838	K778	R717	F657	E597	F537	D477	E417	R355	D291	I231	Y169	GLU
E1020	G960	E899	R839	D779	M718	V658	T598	F538	P478	D418	V356	E292	I231	A170	ASP
A1021	L961	L900	A840	T780	M719	G659	T599	K539	L479	T419	L357	K293	R232	ARG	F46
E1022	A962	Y901	V841	A781	D720	V660	V600	L540	E480	V420	E358	E294	R233	GLY	F47
S1023	D963	R902	K842	S782	K721	V661	K601	T541	I481	P421	F361	R295	L234	A173	G48
K1024	G964	R903	N843	Y783	I722	D662	E602	Q542	Q482	Y422	F362	V296	D235	G174	D49
L1025	Q965	F904	Q844	I784	Q723	A663	F603	N543	F483	L423	K362	V297	A236	D175	G50
K1026	S966	T905	A845	R785	E724	N664	V604	V544	G484	R424	H363	R298	D237	P176	GLU
N1027	V967	R906	E846	S786	L725	L665	G605	G545	A485	N425	F364	A299	R238	GLY	Q51
I1028	E968	Q907	L847	E787	G726	N666	A606	F546	I486	L426	R372	A300	S239	S177	R52
E1029	V969	D908	I848	F788	R728	S667	L607	R547	F487	Q427	K367	Y301	D240	L178	R53
I1030	G970	P909	R849	S789	P728	E668	G608	S548	K488	V428	A368	R302	A241	L179	LEU
S1031	V971	S910	Y850	A790	L729	E669	R609	K549	N489	E429	P369	Q303	P242	E180	SER
Y1032	G972	L911	H851	L791	N730	V670	S610	G550	S490	V370	F369	Q304	P243	I16	ILE
R1033	T973	V912	G852	E792	E731	G671	E611	M511	T491	Q431	S371	V304	A243	N182	PHE
E1034	L974	V913	L853	S793	R732	E672	T612	V552	I492	P432	R372	F305	D244	C183	SER
F1035	R975	P914	L854	R794	S733	V673	F613	Q553	N493	S433	A373	R307	V246	L184	THR
V1036	R976	G915	G855	L795	F674	F674	R614	N554	P494	W494	E375	D308	R247	G185	ARG
R1037	Q977	F916	R856	R796	E736	F675	K615	A555	A495	V375	V375	L309	P248	L186	GLY
R1038	L978	K917	K857	N797	M737	E576	L616	G556	E496	W436	Q376	K310	S249	R187	E62
														GLY	N63



• Molecule 11: Glr1262 protein



• Molecule 11: Glr1262 protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	389430	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	64000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.900	Depositor
Minimum map value	-1.411	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.067	Depositor
Recommended contour level	0.15	Depositor
Map size ($\text{\AA}$)	614.82404, 614.82404, 614.82404	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.0979, 1.0979, 1.0979	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MEN, 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	A	0.73	0/1218	0.94	2/1648 (0.1%)
1	B5	0.74	0/1218	0.94	2/1648 (0.1%)
1	B7	0.74	0/1218	0.94	2/1648 (0.1%)
1	D5	1.39	22/1218 (1.8%)	1.17	7/1648 (0.4%)
1	D7	0.98	4/1218 (0.3%)	1.07	9/1648 (0.5%)
1	F5	1.04	5/1218 (0.4%)	1.24	5/1648 (0.3%)
1	F7	0.90	1/1218 (0.1%)	1.19	4/1648 (0.2%)
1	H5	0.74	0/1218	0.94	2/1648 (0.1%)
1	H7	0.74	0/1218	0.94	2/1648 (0.1%)
1	J5	1.39	21/1218 (1.7%)	1.17	7/1648 (0.4%)
1	J7	0.98	4/1218 (0.3%)	1.07	9/1648 (0.5%)
1	L5	1.05	5/1218 (0.4%)	1.24	5/1648 (0.3%)
1	L7	0.90	1/1218 (0.1%)	1.19	4/1648 (0.2%)
1	N5	0.74	0/1218	0.93	2/1648 (0.1%)
1	N7	0.74	0/1218	0.94	2/1648 (0.1%)
1	P5	0.75	0/1218	0.93	1/1648 (0.1%)
1	P7	0.74	0/1218	0.93	1/1648 (0.1%)
1	R5	0.90	1/1218 (0.1%)	1.19	4/1648 (0.2%)
1	R7	0.90	1/1218 (0.1%)	1.19	4/1648 (0.2%)
1	T5	0.74	0/1218	0.93	2/1648 (0.1%)
1	T7	0.74	0/1218	0.93	2/1648 (0.1%)
1	V5	0.75	0/1218	0.93	1/1648 (0.1%)
1	V7	0.75	0/1218	0.93	1/1648 (0.1%)
1	X5	0.91	1/1218 (0.1%)	1.19	4/1648 (0.2%)
1	X7	0.90	1/1218 (0.1%)	1.19	4/1648 (0.2%)
1	Z	0.73	0/1218	0.94	2/1648 (0.1%)
1	Z5	0.73	0/1218	0.94	2/1648 (0.1%)
1	Z7	0.74	0/1218	0.94	2/1648 (0.1%)
1	b5	0.90	1/1218 (0.1%)	1.19	4/1648 (0.2%)
1	b7	1.51	29/1218 (2.4%)	1.13	3/1648 (0.2%)
1	d5	0.74	0/1218	0.94	2/1648 (0.1%)
1	d7	0.90	1/1218 (0.1%)	1.19	4/1648 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	f5	0.90	1/1218 (0.1%)	1.19	4/1648 (0.2%)
1	f7	0.74	0/1218	0.93	2/1648 (0.1%)
1	h7	1.51	29/1218 (2.4%)	1.13	3/1648 (0.2%)
1	j7	0.90	1/1218 (0.1%)	1.19	4/1648 (0.2%)
1	l7	0.74	0/1218	0.94	2/1648 (0.1%)
1	n7	0.74	0/1218	0.93	1/1648 (0.1%)
1	p7	0.90	1/1218 (0.1%)	1.19	4/1648 (0.2%)
1	r7	0.74	0/1218	0.94	2/1648 (0.1%)
1	t7	0.74	0/1218	0.92	1/1648 (0.1%)
1	v7	0.90	1/1218 (0.1%)	1.19	4/1648 (0.2%)
2	A1	0.72	0/1265	0.86	0/1713
2	A2	0.72	0/1265	0.86	0/1713
2	A3	0.72	0/1265	0.86	0/1713
2	A4	0.72	0/1265	0.86	0/1713
2	A6	0.72	0/1265	0.86	0/1713
2	A8	0.72	0/1265	0.86	0/1713
2	A9	0.72	0/1265	0.86	0/1713
2	AA	0.72	0/1265	0.86	0/1713
2	C1	0.73	0/1265	0.87	0/1713
2	C2	0.73	0/1265	0.86	0/1713
2	C3	0.73	0/1265	0.86	0/1713
2	C4	0.73	0/1265	0.86	0/1713
2	C6	0.73	0/1265	0.87	0/1713
2	C8	0.73	0/1265	0.86	0/1713
2	C9	0.73	0/1265	0.86	0/1713
2	CA	0.73	0/1265	0.86	0/1713
2	E1	0.73	0/1265	0.86	0/1713
2	E2	0.73	0/1265	0.86	0/1713
2	E3	0.73	0/1265	0.86	0/1713
2	E4	0.73	0/1265	0.86	0/1713
2	E6	0.73	0/1265	0.86	0/1713
2	E8	0.73	0/1265	0.86	0/1713
2	E9	0.73	0/1265	0.86	0/1713
2	EA	0.73	0/1265	0.86	0/1713
2	G1	0.73	0/1265	0.86	0/1713
2	G2	0.73	0/1265	0.86	0/1713
2	G3	0.73	0/1265	0.86	0/1713
2	G4	0.74	0/1265	0.86	0/1713
2	G6	0.73	0/1265	0.86	0/1713
2	G8	0.74	0/1265	0.86	0/1713
2	G9	0.73	0/1265	0.86	0/1713
2	GA	0.73	0/1265	0.86	0/1713
2	I1	0.72	0/1265	0.87	0/1713

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	I2	0.73	0/1265	0.86	0/1713
2	I3	0.73	0/1265	0.87	0/1713
2	I4	0.73	0/1265	0.86	0/1713
2	I6	0.73	0/1265	0.86	0/1713
2	I8	0.73	0/1265	0.86	0/1713
2	I9	0.65	0/1265	0.84	0/1713
2	IA	0.65	0/1265	0.84	0/1713
2	K1	0.73	0/1265	0.86	0/1713
2	K2	0.73	0/1265	0.86	0/1713
2	K3	0.73	0/1265	0.86	0/1713
2	K4	0.73	0/1265	0.86	0/1713
2	K6	0.73	0/1265	0.86	0/1713
2	K8	0.73	0/1265	0.86	0/1713
2	K9	0.92	1/1265 (0.1%)	1.03	6/1713 (0.4%)
2	KA	0.92	1/1265 (0.1%)	1.03	6/1713 (0.4%)
2	N4	0.72	0/1265	0.86	0/1713
2	N8	0.72	0/1265	0.88	2/1713 (0.1%)
2	O1	0.72	0/1265	0.86	0/1713
2	O3	0.72	0/1265	0.86	0/1713
2	O9	0.72	0/1265	0.86	0/1713
2	OA	0.72	0/1265	0.86	0/1713
2	P4	0.73	0/1265	0.87	0/1713
2	P8	0.73	0/1265	0.87	0/1713
2	Q1	0.73	0/1265	0.87	0/1713
2	Q3	0.73	0/1265	0.87	0/1713
2	Q9	0.73	0/1265	0.87	0/1713
2	QA	0.73	0/1265	0.88	0/1713
2	R4	0.73	0/1265	0.86	0/1713
2	R8	0.73	0/1265	0.86	0/1713
2	S1	0.73	0/1265	0.86	0/1713
2	S3	0.73	0/1265	0.86	0/1713
2	S9	0.73	0/1265	0.86	0/1713
2	SA	0.73	0/1265	0.86	0/1713
2	T4	0.73	0/1265	0.86	0/1713
2	T8	0.73	0/1265	0.86	0/1713
2	U1	0.73	0/1265	0.90	3/1713 (0.2%)
2	U3	0.73	0/1265	1.09	2/1713 (0.1%)
2	U9	0.73	0/1265	0.86	0/1713
2	UA	0.73	0/1265	0.86	0/1713
2	V4	0.73	0/1265	0.86	0/1713
2	V8	0.73	0/1265	0.86	0/1713
2	W1	0.73	0/1265	0.86	0/1713
2	W3	0.73	0/1265	0.86	0/1713

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	W9	0.72	0/1265	0.86	0/1713
2	WA	0.73	0/1265	0.86	0/1713
2	X4	0.73	0/1265	0.86	0/1713
2	X8	0.73	0/1265	0.86	0/1713
2	Y1	0.73	0/1265	0.86	0/1713
2	Y3	0.73	0/1265	0.86	0/1713
2	Y9	0.73	0/1265	0.86	0/1713
2	YA	0.73	0/1265	0.86	0/1713
3	B1	0.79	0/1307	0.90	2/1768 (0.1%)
3	B2	0.82	1/1307 (0.1%)	0.92	2/1768 (0.1%)
3	B3	0.79	0/1307	0.90	2/1768 (0.1%)
3	B4	0.81	0/1307	0.94	3/1768 (0.2%)
3	B6	0.82	1/1307 (0.1%)	0.92	2/1768 (0.1%)
3	B8	0.80	0/1307	0.92	2/1768 (0.1%)
3	B9	0.79	0/1307	0.91	2/1768 (0.1%)
3	BA	0.79	0/1307	0.91	2/1768 (0.1%)
3	D1	0.78	0/1307	0.90	2/1768 (0.1%)
3	D2	0.78	0/1307	0.90	2/1768 (0.1%)
3	D3	0.78	0/1307	0.90	2/1768 (0.1%)
3	D4	0.79	0/1307	0.90	2/1768 (0.1%)
3	D6	0.78	0/1307	0.90	2/1768 (0.1%)
3	D8	0.79	0/1307	0.90	2/1768 (0.1%)
3	D9	0.79	0/1307	0.90	2/1768 (0.1%)
3	DA	0.79	0/1307	0.90	2/1768 (0.1%)
3	F1	0.79	0/1307	0.90	2/1768 (0.1%)
3	F2	0.79	0/1307	0.90	2/1768 (0.1%)
3	F3	0.79	0/1307	0.90	2/1768 (0.1%)
3	F4	0.78	0/1307	0.96	3/1768 (0.2%)
3	F6	0.79	0/1307	0.90	2/1768 (0.1%)
3	F8	0.79	0/1307	0.95	4/1768 (0.2%)
3	F9	1.03	4/1307 (0.3%)	1.30	9/1768 (0.5%)
3	FA	1.04	3/1307 (0.2%)	1.13	10/1768 (0.6%)
3	H1	0.78	0/1307	0.90	2/1768 (0.1%)
3	H2	0.98	4/1307 (0.3%)	1.05	6/1768 (0.3%)
3	H3	0.78	0/1307	0.90	2/1768 (0.1%)
3	H4	0.79	0/1307	0.90	2/1768 (0.1%)
3	H6	0.98	4/1307 (0.3%)	1.05	6/1768 (0.3%)
3	H8	0.79	0/1307	0.90	2/1768 (0.1%)
3	H9	0.81	0/1307	0.91	2/1768 (0.1%)
3	HA	0.81	0/1307	0.91	2/1768 (0.1%)
3	J1	0.78	0/1307	0.90	2/1768 (0.1%)
3	J2	0.78	0/1307	0.90	2/1768 (0.1%)
3	J3	0.78	0/1307	0.90	2/1768 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	J4	0.78	0/1307	0.90	2/1768 (0.1%)
3	J6	0.78	0/1307	0.90	2/1768 (0.1%)
3	J8	0.78	0/1307	0.90	2/1768 (0.1%)
3	J9	0.82	1/1307 (0.1%)	0.93	4/1768 (0.2%)
3	JA	0.82	1/1307 (0.1%)	0.93	4/1768 (0.2%)
3	L1	0.78	0/1307	1.08	5/1768 (0.3%)
3	L2	0.80	0/1307	0.97	5/1768 (0.3%)
3	L3	0.78	0/1307	0.90	2/1768 (0.1%)
3	L4	0.78	0/1307	1.12	5/1768 (0.3%)
3	L6	0.79	0/1307	0.91	2/1768 (0.1%)
3	L8	0.78	0/1307	0.91	2/1768 (0.1%)
3	L9	1.39	24/1307 (1.8%)	1.11	11/1768 (0.6%)
3	LA	1.39	24/1307 (1.8%)	1.11	11/1768 (0.6%)
3	O4	0.79	0/1307	0.90	2/1768 (0.1%)
3	O8	0.79	0/1307	1.08	4/1768 (0.2%)
3	P1	0.79	0/1307	0.90	2/1768 (0.1%)
3	P3	0.79	0/1307	0.90	2/1768 (0.1%)
3	P9	0.79	0/1307	0.90	2/1768 (0.1%)
3	PA	0.79	0/1307	0.90	2/1768 (0.1%)
3	Q4	0.84	0/1307	1.12	4/1768 (0.2%)
3	Q8	0.82	0/1307	1.03	4/1768 (0.2%)
3	R1	0.77	0/1307	0.90	2/1768 (0.1%)
3	R3	0.78	0/1307	0.91	2/1768 (0.1%)
3	R9	0.79	0/1307	0.90	2/1768 (0.1%)
3	RA	0.79	0/1307	0.90	2/1768 (0.1%)
3	S4	0.79	0/1307	0.90	2/1768 (0.1%)
3	S8	0.79	0/1307	0.90	2/1768 (0.1%)
3	T1	0.78	0/1307	0.90	2/1768 (0.1%)
3	T3	0.78	0/1307	0.90	2/1768 (0.1%)
3	T9	0.78	0/1307	0.90	2/1768 (0.1%)
3	TA	0.78	0/1307	0.90	2/1768 (0.1%)
3	U4	0.79	0/1307	0.90	2/1768 (0.1%)
3	U8	0.79	0/1307	0.90	2/1768 (0.1%)
3	V1	0.79	0/1307	0.90	2/1768 (0.1%)
3	V3	0.79	0/1307	0.90	2/1768 (0.1%)
3	V9	0.79	0/1307	0.91	2/1768 (0.1%)
3	VA	0.79	0/1307	0.91	2/1768 (0.1%)
3	W4	0.78	0/1307	0.90	2/1768 (0.1%)
3	W8	0.78	0/1307	0.90	2/1768 (0.1%)
3	X1	0.78	0/1307	0.90	2/1768 (0.1%)
3	X3	0.78	0/1307	0.90	2/1768 (0.1%)
3	X9	0.78	0/1307	0.90	2/1768 (0.1%)
3	XA	0.78	0/1307	0.90	2/1768 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	Y4	0.82	0/1307	1.14	5/1768 (0.3%)
3	Y8	0.81	0/1307	0.99	2/1768 (0.1%)
3	Z1	0.78	0/1307	0.90	2/1768 (0.1%)
3	Z3	0.78	0/1307	0.90	2/1768 (0.1%)
3	Z9	0.79	0/1307	0.91	2/1768 (0.1%)
3	ZA	0.79	0/1307	0.91	2/1768 (0.1%)
4	M1	2.88	178/2225 (8.0%)	2.02	94/3011 (3.1%)
4	M3	2.88	178/2225 (8.0%)	2.02	94/3011 (3.1%)
4	M4	2.85	171/2225 (7.7%)	2.15	99/3011 (3.3%)
4	M8	2.85	171/2225 (7.7%)	2.41	114/3011 (3.8%)
4	M9	2.88	180/2225 (8.1%)	2.02	95/3011 (3.2%)
4	MA	2.88	178/2225 (8.0%)	2.02	95/3011 (3.2%)
5	N1	1.66	3/589 (0.5%)	1.84	13/797 (1.6%)
5	N3	1.66	3/589 (0.5%)	1.84	13/797 (1.6%)
5	N9	1.66	3/589 (0.5%)	1.84	13/797 (1.6%)
5	NA	1.66	3/589 (0.5%)	1.84	13/797 (1.6%)
5	Z4	1.66	3/589 (0.5%)	2.83	19/797 (2.4%)
5	Z8	1.64	3/589 (0.5%)	1.83	13/797 (1.6%)
6	M2	0.34	0/2237	0.74	3/3022 (0.1%)
6	M6	0.34	0/2237	0.74	3/3022 (0.1%)
7	N2	0.43	0/555	0.90	1/755 (0.1%)
7	N6	0.43	0/555	0.90	1/755 (0.1%)
8	A5	1.45	28/1239 (2.3%)	1.12	7/1676 (0.4%)
8	A7	0.73	2/1239 (0.2%)	0.99	1/1676 (0.1%)
8	C5	1.50	30/1239 (2.4%)	1.28	15/1676 (0.9%)
8	C7	0.65	1/1239 (0.1%)	1.00	4/1676 (0.2%)
8	E5	1.74	34/1239 (2.7%)	1.40	21/1676 (1.3%)
8	E7	0.78	3/1239 (0.2%)	1.12	6/1676 (0.4%)
8	G5	1.45	28/1239 (2.3%)	1.12	7/1676 (0.4%)
8	G7	0.73	2/1239 (0.2%)	0.99	1/1676 (0.1%)
8	I5	1.50	29/1239 (2.3%)	1.28	15/1676 (0.9%)
8	I7	0.66	1/1239 (0.1%)	1.01	4/1676 (0.2%)
8	K5	1.74	34/1239 (2.7%)	1.39	21/1676 (1.3%)
8	K7	0.78	3/1239 (0.2%)	1.12	6/1676 (0.4%)
8	M5	0.73	2/1239 (0.2%)	1.00	3/1676 (0.2%)
8	M7	0.72	2/1239 (0.2%)	0.98	1/1676 (0.1%)
8	O5	0.67	1/1239 (0.1%)	1.15	9/1676 (0.5%)
8	O7	0.66	1/1239 (0.1%)	1.01	6/1676 (0.4%)
8	Q5	0.85	4/1239 (0.3%)	1.15	7/1676 (0.4%)
8	Q7	0.78	3/1239 (0.2%)	1.12	6/1676 (0.4%)
8	S5	0.73	2/1239 (0.2%)	0.98	1/1676 (0.1%)
8	S7	0.73	2/1239 (0.2%)	0.99	1/1676 (0.1%)
8	U5	0.68	1/1239 (0.1%)	1.17	8/1676 (0.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
8	U7	0.65	1/1239 (0.1%)	1.03	6/1676 (0.4%)
8	W5	0.85	4/1239 (0.3%)	1.15	7/1676 (0.4%)
8	W7	0.78	3/1239 (0.2%)	1.12	6/1676 (0.4%)
8	Y5	0.72	2/1239 (0.2%)	0.98	1/1676 (0.1%)
8	Y7	0.73	2/1239 (0.2%)	0.98	1/1676 (0.1%)
8	a5	1.24	14/1239 (1.1%)	1.19	7/1676 (0.4%)
8	a7	1.03	10/1239 (0.8%)	1.06	7/1676 (0.4%)
8	c5	0.72	2/1239 (0.2%)	0.99	1/1676 (0.1%)
8	c7	1.73	38/1239 (3.1%)	1.53	21/1676 (1.3%)
8	e5	1.24	16/1239 (1.3%)	1.21	8/1676 (0.5%)
8	e7	0.72	1/1239 (0.1%)	0.98	1/1676 (0.1%)
8	g7	1.03	10/1239 (0.8%)	1.06	7/1676 (0.4%)
8	i7	1.73	38/1239 (3.1%)	1.53	21/1676 (1.3%)
8	k7	0.73	1/1239 (0.1%)	1.00	1/1676 (0.1%)
8	m7	0.65	1/1239 (0.1%)	1.00	4/1676 (0.2%)
8	o7	1.84	43/1239 (3.5%)	1.41	18/1676 (1.1%)
8	q7	0.73	2/1239 (0.2%)	1.01	1/1676 (0.1%)
8	s7	0.65	1/1239 (0.1%)	1.03	5/1676 (0.3%)
8	u7	1.84	43/1239 (3.5%)	1.41	18/1676 (1.1%)
9	i5	3.44	74/548 (13.5%)	2.43	20/737 (2.7%)
9	w7	3.26	66/548 (12.0%)	2.44	37/737 (5.0%)
9	x7	2.30	19/548 (3.5%)	1.99	16/737 (2.2%)
9	y7	2.30	19/548 (3.5%)	1.99	16/737 (2.2%)
9	z5	3.44	77/548 (14.1%)	2.44	20/737 (2.7%)
9	z7	3.26	66/548 (12.0%)	2.44	37/737 (5.0%)
10	j5	3.83	1446/9003 (16.1%)	2.36	479/12173 (3.9%)
10	k5	3.83	1453/9003 (16.1%)	2.35	474/12173 (3.9%)
11	a9	1.67	107/6453 (1.7%)	2.08	198/8728 (2.3%)
11	aA	1.67	107/6453 (1.7%)	2.09	200/8728 (2.3%)
All	All	1.35	5153/373432 (1.4%)	1.21	2859/505286 (0.6%)

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	D5	0	1
1	J5	0	1
3	L9	0	1
3	LA	0	1
3	Q4	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	Q8	0	1
4	M1	0	2
4	M3	0	2
4	M4	0	2
4	M8	0	2
4	M9	0	2
4	MA	0	2
5	Z4	0	2
6	M2	0	5
6	M6	0	5
7	N2	0	1
7	N6	0	1
8	E7	0	1
8	K7	0	1
8	O5	0	1
8	Q5	0	1
8	Q7	0	1
8	U7	0	1
8	W5	0	1
8	W7	0	1
8	a5	0	3
8	c7	0	3
8	e5	0	3
8	i7	0	3
8	o7	0	2
8	u7	0	2
9	i5	0	1
9	x7	0	2
9	y7	0	2
9	z5	0	1
10	j5	0	23
10	k5	0	23
11	a9	0	16
11	aA	0	17
All	All	0	143

The worst 5 of 5153 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	j5	897	SER	C-O	-20.50	1.00	1.24
10	k5	897	SER	C-O	-20.50	1.00	1.24
1	L5	18	TYR	C-N	18.60	1.58	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	p7	18	TYR	C-N	18.58	1.58	1.33
1	v7	18	TYR	C-N	18.55	1.58	1.33

The worst 5 of 2859 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	aA	354	VAL	O-C-N	-47.09	63.71	122.57
11	a9	354	VAL	O-C-N	-47.06	63.75	122.57
5	Z4	23	SER	CA-C-N	36.90	155.98	119.82
5	Z4	23	SER	C-N-CA	36.90	155.98	119.82
10	j5	743	VAL	CA-C-N	33.24	161.38	119.84

There are no chirality outliers.

5 of 143 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	LA	109	CYS	Mainchain
6	M2	37	GLU	Peptide
6	M2	58	GLY	Peptide
4	MA	20	THR	Mainchain
4	MA	228	SER	Mainchain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1210	0	1220	112	0
1	B5	1210	0	1218	97	0
1	B7	1210	0	1219	59	0
1	D5	1210	0	1219	89	0
1	D7	1210	0	1219	151	0
1	F5	1210	0	1220	69	0
1	F7	1210	0	1220	21	0
1	H5	1210	0	1218	77	0
1	H7	1210	0	1219	59	0
1	J5	1210	0	1219	91	0
1	J7	1210	0	1220	149	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L5	1210	0	1220	74	0
1	L7	1210	0	1220	19	0
1	N5	1210	0	1220	82	0
1	N7	1210	0	1218	28	0
1	P5	1210	0	1218	63	0
1	P7	1210	0	1220	51	0
1	R5	1210	0	1216	184	0
1	R7	1210	0	1219	31	0
1	T5	1210	0	1220	90	0
1	T7	1210	0	1218	44	0
1	V5	1210	0	1219	64	0
1	V7	1210	0	1220	51	0
1	X5	1210	0	1219	181	0
1	X7	1210	0	1219	30	0
1	Z	1210	0	1219	115	0
1	Z5	1210	0	1215	100	0
1	Z7	1210	0	1218	44	0
1	b5	1210	0	1218	118	0
1	b7	1210	0	1219	105	0
1	d5	1210	0	1217	91	0
1	d7	1210	0	1215	163	0
1	f5	1210	0	1219	110	0
1	f7	1210	0	1218	46	0
1	h7	1210	0	1219	108	0
1	j7	1210	0	1217	100	0
1	l7	1210	0	1217	73	0
1	n7	1210	0	1220	109	0
1	p7	1210	0	1219	339	0
1	r7	1210	0	1219	55	0
1	t7	1210	0	1218	126	0
1	v7	1210	0	1218	335	0
2	A1	1243	0	1225	84	0
2	A2	1243	0	1225	84	0
2	A3	1243	0	1225	87	0
2	A4	1243	0	1225	82	0
2	A6	1243	0	1225	84	0
2	A8	1243	0	1225	83	0
2	A9	1243	0	1225	85	0
2	AA	1243	0	1225	84	0
2	C1	1243	0	1225	29	0
2	C2	1243	0	1225	17	0
2	C3	1243	0	1225	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C4	1243	0	1225	18	0
2	C6	1243	0	1225	15	0
2	C8	1243	0	1225	17	0
2	C9	1243	0	1225	12	0
2	CA	1243	0	1225	12	0
2	E1	1243	0	1225	19	0
2	E2	1243	0	1225	17	0
2	E3	1243	0	1225	19	0
2	E4	1243	0	1224	32	0
2	E6	1243	0	1225	17	0
2	E8	1243	0	1224	27	0
2	E9	1243	0	1225	40	0
2	EA	1243	0	1225	40	0
2	G1	1243	0	1225	43	0
2	G2	1243	0	1225	34	0
2	G3	1243	0	1225	42	0
2	G4	1243	0	1225	21	0
2	G6	1243	0	1225	26	0
2	G8	1243	0	1225	20	0
2	G9	1243	0	1225	20	0
2	GA	1243	0	1225	21	0
2	I1	1243	0	1225	15	0
2	I2	1243	0	1225	18	0
2	I3	1243	0	1225	15	0
2	I4	1243	0	1225	25	0
2	I6	1243	0	1225	17	0
2	I8	1243	0	1225	27	0
2	I9	1243	0	1225	99	0
2	IA	1243	0	1225	106	0
2	K1	1243	0	1224	68	0
2	K2	1243	0	1225	29	0
2	K3	1243	0	1224	91	0
2	K4	1243	0	1225	32	0
2	K6	1243	0	1225	30	0
2	K8	1243	0	1225	32	0
2	K9	1243	0	1225	76	0
2	KA	1243	0	1225	58	0
2	N4	1243	0	1225	152	0
2	N8	1243	0	1225	174	0
2	O1	1243	0	1225	78	0
2	O3	1243	0	1225	82	0
2	O9	1243	0	1225	81	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	OA	1243	0	1225	80	0
2	P4	1243	0	1223	67	0
2	P8	1243	0	1223	54	0
2	Q1	1243	0	1225	19	0
2	Q3	1243	0	1225	18	0
2	Q9	1243	0	1224	39	0
2	QA	1243	0	1223	164	0
2	R4	1243	0	1225	18	0
2	R8	1243	0	1225	18	0
2	S1	1243	0	1225	21	0
2	S3	1243	0	1225	22	0
2	S9	1243	0	1223	60	0
2	SA	1243	0	1223	59	0
2	T4	1243	0	1225	19	0
2	T8	1243	0	1225	18	0
2	U1	1243	0	1224	45	0
2	U3	1243	0	1222	42	0
2	U9	1243	0	1225	29	0
2	UA	1243	0	1225	67	0
2	V4	1243	0	1225	13	0
2	V8	1243	0	1225	11	0
2	W1	1243	0	1225	12	0
2	W3	1243	0	1225	11	0
2	W9	1243	0	1225	22	0
2	WA	1243	0	1225	30	0
2	X4	1243	0	1224	152	0
2	X8	1243	0	1224	162	0
2	Y1	1243	0	1225	32	0
2	Y3	1243	0	1225	32	0
2	Y9	1243	0	1225	29	0
2	YA	1243	0	1225	30	0
3	B1	1293	0	1300	113	0
3	B2	1293	0	1301	42	0
3	B3	1293	0	1301	108	0
3	B4	1293	0	1300	216	0
3	B6	1293	0	1301	42	0
3	B8	1293	0	1298	136	0
3	B9	1293	0	1301	67	0
3	BA	1293	0	1301	66	0
3	D1	1293	0	1301	42	0
3	D2	1293	0	1301	19	0
3	D3	1293	0	1301	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D4	1293	0	1301	54	0
3	D6	1293	0	1301	20	0
3	D8	1293	0	1301	46	0
3	D9	1293	0	1300	62	0
3	DA	1293	0	1300	63	0
3	F1	1293	0	1301	37	0
3	F2	1293	0	1302	62	0
3	F3	1293	0	1301	39	0
3	F4	1293	0	1298	175	0
3	F6	1293	0	1302	81	0
3	F8	1293	0	1299	145	0
3	F9	1293	0	1301	122	0
3	FA	1293	0	1302	133	0
3	H1	1293	0	1301	81	0
3	H2	1293	0	1301	55	0
3	H3	1293	0	1299	52	0
3	H4	1293	0	1299	104	0
3	H6	1293	0	1301	56	0
3	H8	1293	0	1300	100	0
3	H9	1293	0	1301	120	0
3	HA	1293	0	1300	123	0
3	J1	1293	0	1297	82	0
3	J2	1293	0	1301	43	0
3	J3	1293	0	1300	148	0
3	J4	1293	0	1301	33	0
3	J6	1293	0	1301	42	0
3	J8	1293	0	1301	31	0
3	J9	1293	0	1294	144	0
3	JA	1293	0	1294	150	0
3	L1	1293	0	1301	140	0
3	L2	1293	0	1301	82	0
3	L3	1293	0	1301	137	0
3	L4	1293	0	1301	100	0
3	L6	1293	0	1301	45	0
3	L8	1293	0	1302	139	0
3	L9	1293	0	1301	154	0
3	LA	1293	0	1301	156	0
3	O4	1293	0	1299	122	0
3	O8	1293	0	1298	145	0
3	P1	1293	0	1301	40	0
3	P3	1293	0	1301	41	0
3	P9	1293	0	1301	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	PA	1293	0	1301	38	0
3	Q4	1293	0	1301	208	0
3	Q8	1293	0	1301	243	0
3	R1	1293	0	1301	34	0
3	R3	1293	0	1301	30	0
3	R9	1293	0	1301	46	0
3	RA	1293	0	1301	52	0
3	S4	1293	0	1302	57	0
3	S8	1293	0	1302	77	0
3	T1	1293	0	1301	41	0
3	T3	1293	0	1301	43	0
3	T9	1293	0	1297	144	0
3	TA	1293	0	1297	238	0
3	U4	1293	0	1299	92	0
3	U8	1293	0	1301	103	0
3	V1	1293	0	1301	39	0
3	V3	1293	0	1301	41	0
3	V9	1293	0	1298	143	0
3	VA	1293	0	1298	146	0
3	W4	1293	0	1301	21	0
3	W8	1293	0	1301	21	0
3	X1	1293	0	1301	77	0
3	X3	1293	0	1301	77	0
3	X9	1293	0	1301	45	0
3	XA	1293	0	1301	46	0
3	Y4	1293	0	1301	221	0
3	Y8	1293	0	1299	162	0
3	Z1	1293	0	1299	48	0
3	Z3	1293	0	1299	46	0
3	Z9	1293	0	1301	52	0
3	ZA	1293	0	1301	51	0
4	M1	2178	0	2143	394	0
4	M3	2178	0	2143	377	0
4	M4	2178	0	2139	967	0
4	M8	2178	0	2139	873	0
4	M9	2178	0	2140	513	0
4	MA	2178	0	2140	513	0
5	N1	578	0	587	206	0
5	N3	578	0	587	201	0
5	N9	578	0	584	235	0
5	NA	578	0	584	231	0
5	Z4	578	0	584	469	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	Z8	578	0	584	536	0
6	M2	2190	0	2142	289	0
6	M6	2190	0	2137	317	0
7	N2	545	0	552	43	0
7	N6	545	0	552	43	0
8	A5	1222	0	1234	174	0
8	A7	1222	0	1233	50	0
8	C5	1222	0	1232	109	0
8	C7	1222	0	1231	119	0
8	E5	1222	0	1231	105	0
8	E7	1222	0	1231	76	0
8	G5	1222	0	1234	216	0
8	G7	1222	0	1233	68	0
8	I5	1222	0	1232	109	0
8	I7	1222	0	1232	130	0
8	K5	1222	0	1231	123	0
8	K7	1222	0	1231	77	0
8	M5	1222	0	1233	110	0
8	M7	1222	0	1233	64	0
8	O5	1222	0	1233	176	0
8	O7	1222	0	1230	131	0
8	Q5	1222	0	1230	125	0
8	Q7	1222	0	1231	105	0
8	S5	1222	0	1233	127	0
8	S7	1222	0	1233	85	0
8	U5	1222	0	1230	222	0
8	U7	1222	0	1231	120	0
8	W5	1222	0	1230	123	0
8	W7	1222	0	1231	96	0
8	Y5	1222	0	1233	55	0
8	Y7	1222	0	1233	59	0
8	a5	1222	0	1232	126	0
8	a7	1222	0	1230	173	0
8	c5	1222	0	1233	64	0
8	c7	1222	0	1228	335	0
8	e5	1222	0	1232	124	0
8	e7	1222	0	1233	51	0
8	g7	1222	0	1232	175	0
8	i7	1222	0	1229	362	0
8	k7	1222	0	1233	107	0
8	m7	1222	0	1232	123	0
8	o7	1222	0	1226	310	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	q7	1222	0	1233	105	0
8	s7	1222	0	1229	172	0
8	u7	1222	0	1228	301	0
9	i5	538	0	555	145	0
9	w7	538	0	552	106	0
9	x7	538	0	552	115	0
9	y7	538	0	553	99	0
9	z5	538	0	555	152	0
9	z7	538	0	554	99	0
10	j5	8819	0	8820	1743	0
10	k5	8819	0	8823	1832	0
11	a9	6326	0	6124	1826	0
11	aA	6326	0	6123	1862	0
12	A	43	0	37	9	0
12	A1	43	0	37	8	0
12	A2	43	0	37	8	0
12	A3	43	0	37	8	0
12	A4	43	0	37	8	0
12	A5	43	0	38	69	0
12	A6	43	0	37	8	0
12	A7	43	0	37	3	0
12	A8	43	0	37	8	0
12	A9	43	0	37	8	0
12	AA	43	0	37	8	0
12	B1	86	0	74	75	0
12	B2	43	0	37	7	0
12	B3	86	0	75	75	0
12	B4	86	0	69	124	0
12	B5	43	0	37	26	0
12	B6	43	0	37	7	0
12	B7	43	0	37	12	0
12	B8	86	0	68	92	0
12	B9	86	0	74	27	0
12	BA	86	0	74	26	0
12	C1	43	0	37	8	0
12	C2	43	0	37	8	0
12	C3	43	0	37	8	0
12	C4	43	0	37	8	0
12	C5	43	0	37	7	0
12	C6	43	0	37	8	0
12	C7	43	0	37	4	0
12	C8	43	0	37	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	C9	43	0	37	8	0
12	CA	43	0	37	8	0
12	D1	86	0	74	15	0
12	D2	86	0	74	15	0
12	D3	86	0	74	15	0
12	D4	86	0	73	15	0
12	D5	43	0	37	11	0
12	D6	86	0	74	14	0
12	D7	43	0	35	32	0
12	D8	86	0	73	27	0
12	D9	86	0	74	21	0
12	DA	86	0	74	20	0
12	E1	43	0	37	8	0
12	E2	43	0	37	7	0
12	E3	43	0	37	8	0
12	E4	43	0	37	8	0
12	E5	43	0	37	27	0
12	E6	43	0	37	8	0
12	E7	43	0	37	13	0
12	E8	43	0	37	8	0
12	E9	43	0	37	7	0
12	EA	43	0	37	7	0
12	F1	86	0	74	31	0
12	F2	86	0	75	59	0
12	F3	86	0	74	31	0
12	F4	86	0	70	17	0
12	F5	43	0	37	17	0
12	F6	86	0	75	69	0
12	F7	43	0	37	17	0
12	F8	86	0	70	14	0
12	F9	129	0	112	73	0
12	FA	43	0	37	19	0
12	G1	43	0	37	8	0
12	G2	43	0	37	11	0
12	G3	43	0	37	8	0
12	G4	43	0	37	8	0
12	G5	43	0	38	70	0
12	G6	43	0	37	8	0
12	G7	43	0	37	3	0
12	G8	43	0	37	8	0
12	G9	43	0	37	8	0
12	GA	43	0	37	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	H1	86	0	73	62	0
12	H2	86	0	74	27	0
12	H3	86	0	74	20	0
12	H4	86	0	74	35	0
12	H5	43	0	37	21	0
12	H6	86	0	74	25	0
12	H7	43	0	37	11	0
12	H8	86	0	74	34	0
12	H9	86	0	72	88	0
12	HA	86	0	73	88	0
12	I1	43	0	37	8	0
12	I2	43	0	37	8	0
12	I3	43	0	37	8	0
12	I4	43	0	37	8	0
12	I5	43	0	37	8	0
12	I6	43	0	37	8	0
12	I7	43	0	37	3	0
12	I8	43	0	37	8	0
12	I9	43	0	37	8	0
12	IA	43	0	37	8	0
12	J1	43	0	37	7	0
12	J2	86	0	74	18	0
12	J3	86	0	74	51	0
12	J4	86	0	74	18	0
12	J5	43	0	37	12	0
12	J6	86	0	74	17	0
12	J7	43	0	35	23	0
12	J8	86	0	74	20	0
12	J9	86	0	73	48	0
12	JA	86	0	73	47	0
12	K1	43	0	37	8	0
12	K2	43	0	37	8	0
12	K3	43	0	37	8	0
12	K4	43	0	37	8	0
12	K5	43	0	37	28	0
12	K6	43	0	37	8	0
12	K7	43	0	37	14	0
12	K8	43	0	37	8	0
12	K9	43	0	37	8	0
12	KA	43	0	37	8	0
12	L1	43	0	37	9	0
12	L2	86	0	74	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	L3	86	0	71	30	0
12	L4	86	0	74	30	0
12	L5	43	0	37	14	0
12	L6	86	0	74	18	0
12	L7	43	0	37	13	0
12	L8	43	0	37	10	0
12	L9	86	0	74	35	0
12	LA	86	0	74	33	0
12	M4	43	0	37	76	0
12	M5	43	0	37	4	0
12	M7	43	0	37	3	0
12	M8	86	0	72	181	0
12	N2	43	0	37	13	0
12	N4	43	0	37	8	0
12	N5	43	0	37	14	0
12	N6	43	0	37	13	0
12	N7	43	0	37	10	0
12	N8	43	0	37	12	0
12	O1	43	0	37	11	0
12	O3	43	0	37	8	0
12	O4	86	0	74	32	0
12	O5	43	0	37	4	0
12	O7	43	0	37	3	0
12	O8	86	0	74	27	0
12	O9	43	0	37	8	0
12	OA	43	0	37	8	0
12	P1	86	0	74	25	0
12	P3	86	0	74	25	0
12	P4	43	0	37	8	0
12	P5	43	0	37	18	0
12	P7	43	0	37	13	0
12	P8	43	0	37	8	0
12	P9	86	0	74	20	0
12	PA	86	0	74	19	0
12	Q1	43	0	37	8	0
12	Q3	43	0	37	8	0
12	Q4	43	0	37	6	0
12	Q5	43	0	37	15	0
12	Q7	43	0	37	14	0
12	Q8	43	0	37	6	0
12	Q9	43	0	37	8	0
12	QA	43	0	37	49	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	R1	86	0	74	33	0
12	R3	86	0	74	32	0
12	R4	43	0	37	8	0
12	R5	43	0	37	15	0
12	R7	43	0	37	9	0
12	R8	43	0	37	8	0
12	R9	86	0	74	25	0
12	RA	86	0	74	27	0
12	S1	43	0	37	8	0
12	S3	43	0	37	9	0
12	S4	86	0	75	39	0
12	S5	43	0	37	3	0
12	S7	43	0	37	4	0
12	S8	43	0	37	6	0
12	S9	43	0	37	8	0
12	SA	43	0	37	8	0
12	T1	86	0	74	28	0
12	T3	86	0	74	28	0
12	T4	43	0	37	8	0
12	T5	43	0	37	19	0
12	T7	43	0	37	16	0
12	T8	43	0	37	8	0
12	T9	86	0	74	52	0
12	TA	86	0	74	53	0
12	U1	43	0	37	8	0
12	U3	43	0	37	8	0
12	U4	86	0	74	19	0
12	U5	43	0	37	3	0
12	U7	43	0	37	3	0
12	U8	86	0	74	21	0
12	U9	43	0	37	8	0
12	UA	43	0	37	9	0
12	V1	86	0	74	13	0
12	V3	86	0	74	13	0
12	V4	43	0	37	8	0
12	V5	43	0	37	18	0
12	V7	43	0	37	10	0
12	V8	43	0	37	8	0
12	V9	86	0	74	48	0
12	VA	86	0	74	60	0
12	W1	43	0	37	8	0
12	W3	43	0	37	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	W4	86	0	74	14	0
12	W5	43	0	37	14	0
12	W7	43	0	37	14	0
12	W8	86	0	74	15	0
12	W9	43	0	37	8	0
12	WA	43	0	37	8	0
12	X1	86	0	74	23	0
12	X3	86	0	74	26	0
12	X4	43	0	37	8	0
12	X5	43	0	37	16	0
12	X7	43	0	37	8	0
12	X8	43	0	37	8	0
12	X9	86	0	74	15	0
12	XA	86	0	74	13	0
12	Y1	43	0	37	8	0
12	Y3	43	0	37	8	0
12	Y4	43	0	37	8	0
12	Y5	43	0	37	3	0
12	Y7	43	0	37	3	0
12	Y8	43	0	37	10	0
12	Y9	43	0	37	8	0
12	YA	43	0	37	8	0
12	Z	43	0	37	8	0
12	Z1	86	0	74	37	0
12	Z3	86	0	74	38	0
12	Z4	43	0	38	104	0
12	Z5	43	0	37	15	0
12	Z8	43	0	37	163	0
12	Z9	86	0	74	20	0
12	ZA	86	0	74	21	0
12	a5	43	0	37	8	0
12	a7	43	0	37	3	0
12	a9	43	0	36	106	0
12	aA	86	0	71	72	0
12	b5	43	0	37	7	0
12	b7	43	0	37	18	0
12	c5	43	0	37	3	0
12	c7	43	0	37	10	0
12	d5	43	0	37	16	0
12	d7	43	0	37	19	0
12	e5	43	0	37	8	0
12	e7	43	0	37	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	f5	43	0	37	6	0
12	f7	43	0	35	16	0
12	g7	43	0	37	3	0
12	h7	43	0	37	15	0
12	i7	43	0	37	13	0
12	j5	86	38	75	57	0
12	j7	43	0	37	15	0
12	k5	172	38	147	119	0
12	k7	43	0	37	3	0
12	m7	43	0	37	4	0
12	o7	43	0	35	18	0
12	p7	43	0	37	16	0
12	q7	43	0	37	3	0
12	r7	43	0	37	17	0
12	s7	43	0	37	3	0
12	u7	43	0	35	19	0
12	v7	43	0	37	22	0
All	All	382696	76	379888	26296	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 34.

The worst 5 of 26296 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)
1:A:73:TYR:HE1	10:k5:162:TRP:CZ2	1.10	1.70
10:k5:1152:TYR:CE2	8:G7:68:PRO:HG2	1.24	1.70
10:k5:1008:PHE:CE1	1:p7:87:TYR:CE2	1.76	1.68
10:j5:1008:PHE:CE1	1:v7:87:TYR:CE2	1.77	1.68
3:TA:32:LYS:HE3	2:X4:60:TYR:CD2	1.25	1.68

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	158/161 (98%)	150 (95%)	6 (4%)	2 (1%)	9	31
1	B5	158/161 (98%)	150 (95%)	6 (4%)	2 (1%)	9	31
1	B7	158/161 (98%)	150 (95%)	6 (4%)	2 (1%)	9	31
1	D5	158/161 (98%)	145 (92%)	9 (6%)	4 (2%)	4	16
1	D7	158/161 (98%)	149 (94%)	6 (4%)	3 (2%)	6	22
1	F5	158/161 (98%)	150 (95%)	6 (4%)	2 (1%)	9	31
1	F7	158/161 (98%)	151 (96%)	5 (3%)	2 (1%)	9	31
1	H5	158/161 (98%)	150 (95%)	6 (4%)	2 (1%)	9	31
1	H7	158/161 (98%)	150 (95%)	6 (4%)	2 (1%)	9	31
1	J5	158/161 (98%)	145 (92%)	9 (6%)	4 (2%)	4	16
1	J7	158/161 (98%)	149 (94%)	6 (4%)	3 (2%)	6	22
1	L5	158/161 (98%)	150 (95%)	6 (4%)	2 (1%)	9	31
1	L7	158/161 (98%)	151 (96%)	5 (3%)	2 (1%)	9	31
1	N5	158/161 (98%)	150 (95%)	6 (4%)	2 (1%)	9	31
1	N7	158/161 (98%)	150 (95%)	6 (4%)	2 (1%)	9	31
1	P5	158/161 (98%)	150 (95%)	6 (4%)	2 (1%)	9	31
1	P7	158/161 (98%)	150 (95%)	6 (4%)	2 (1%)	9	31
1	R5	158/161 (98%)	151 (96%)	5 (3%)	2 (1%)	9	31
1	R7	158/161 (98%)	151 (96%)	5 (3%)	2 (1%)	9	31
1	T5	158/161 (98%)	150 (95%)	6 (4%)	2 (1%)	9	31
1	T7	158/161 (98%)	150 (95%)	6 (4%)	2 (1%)	9	31
1	V5	158/161 (98%)	150 (95%)	6 (4%)	2 (1%)	9	31
1	V7	158/161 (98%)	150 (95%)	6 (4%)	2 (1%)	9	31
1	X5	158/161 (98%)	151 (96%)	5 (3%)	2 (1%)	9	31
1	X7	158/161 (98%)	151 (96%)	5 (3%)	2 (1%)	9	31
1	Z	158/161 (98%)	150 (95%)	6 (4%)	2 (1%)	9	31
1	Z5	158/161 (98%)	150 (95%)	6 (4%)	2 (1%)	9	31
1	Z7	158/161 (98%)	150 (95%)	6 (4%)	2 (1%)	9	31
1	b5	158/161 (98%)	151 (96%)	5 (3%)	2 (1%)	9	31
1	b7	158/161 (98%)	150 (95%)	7 (4%)	1 (1%)	21	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	d5	158/161 (98%)	150 (95%)	6 (4%)	2 (1%)	9	31
1	d7	158/161 (98%)	151 (96%)	5 (3%)	2 (1%)	9	31
1	f5	158/161 (98%)	151 (96%)	5 (3%)	2 (1%)	9	31
1	f7	158/161 (98%)	150 (95%)	6 (4%)	2 (1%)	9	31
1	h7	158/161 (98%)	150 (95%)	7 (4%)	1 (1%)	21	51
1	j7	158/161 (98%)	151 (96%)	5 (3%)	2 (1%)	9	31
1	l7	158/161 (98%)	150 (95%)	6 (4%)	2 (1%)	9	31
1	n7	158/161 (98%)	150 (95%)	6 (4%)	2 (1%)	9	31
1	p7	158/161 (98%)	151 (96%)	5 (3%)	2 (1%)	9	31
1	r7	158/161 (98%)	150 (95%)	6 (4%)	2 (1%)	9	31
1	t7	158/161 (98%)	150 (95%)	6 (4%)	2 (1%)	9	31
1	v7	158/161 (98%)	151 (96%)	5 (3%)	2 (1%)	9	31
2	A1	160/162 (99%)	155 (97%)	5 (3%)	0	100	100
2	A2	160/162 (99%)	155 (97%)	5 (3%)	0	100	100
2	A3	160/162 (99%)	155 (97%)	5 (3%)	0	100	100
2	A4	160/162 (99%)	155 (97%)	5 (3%)	0	100	100
2	A6	160/162 (99%)	155 (97%)	5 (3%)	0	100	100
2	A8	160/162 (99%)	155 (97%)	5 (3%)	0	100	100
2	A9	160/162 (99%)	155 (97%)	5 (3%)	0	100	100
2	AA	160/162 (99%)	155 (97%)	5 (3%)	0	100	100
2	C1	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
2	C2	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
2	C3	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
2	C4	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
2	C6	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
2	C8	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
2	C9	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
2	CA	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
2	E1	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
2	E2	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
2	E3	160/162 (99%)	158 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E4	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
2	E6	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
2	E8	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
2	E9	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
2	EA	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
2	G1	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
2	G2	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
2	G3	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
2	G4	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
2	G6	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
2	G8	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
2	G9	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
2	GA	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
2	I1	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
2	I2	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
2	I3	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
2	I4	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
2	I6	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
2	I8	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
2	I9	160/162 (99%)	153 (96%)	6 (4%)	1 (1%)	21	51
2	IA	160/162 (99%)	153 (96%)	6 (4%)	1 (1%)	21	51
2	K1	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
2	K2	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
2	K3	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
2	K4	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
2	K6	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
2	K8	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
2	K9	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
2	KA	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
2	N4	160/162 (99%)	155 (97%)	5 (3%)	0	100	100
2	N8	160/162 (99%)	154 (96%)	5 (3%)	1 (1%)	21	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	O1	160/162 (99%)	155 (97%)	5 (3%)	0	100	100
2	O3	160/162 (99%)	155 (97%)	5 (3%)	0	100	100
2	O9	160/162 (99%)	155 (97%)	5 (3%)	0	100	100
2	OA	160/162 (99%)	155 (97%)	5 (3%)	0	100	100
2	P4	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
2	P8	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
2	Q1	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
2	Q3	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
2	Q9	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
2	QA	160/162 (99%)	156 (98%)	4 (2%)	0	100	100
2	R4	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
2	R8	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
2	S1	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
2	S3	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
2	S9	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
2	SA	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
2	T4	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
2	T8	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
2	U1	160/162 (99%)	157 (98%)	3 (2%)	0	100	100
2	U3	160/162 (99%)	157 (98%)	2 (1%)	1 (1%)	21	51
2	U9	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
2	UA	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
2	V4	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
2	V8	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
2	W1	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
2	W3	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
2	W9	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
2	WA	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
2	X4	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
2	X8	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
2	Y1	160/162 (99%)	158 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	Y3	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
2	Y9	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
2	YA	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
3	B1	170/172 (99%)	162 (95%)	7 (4%)	1 (1%)	21	51
3	B2	170/172 (99%)	162 (95%)	7 (4%)	1 (1%)	21	51
3	B3	170/172 (99%)	162 (95%)	7 (4%)	1 (1%)	21	51
3	B4	170/172 (99%)	159 (94%)	9 (5%)	2 (1%)	10	34
3	B6	170/172 (99%)	162 (95%)	7 (4%)	1 (1%)	21	51
3	B8	170/172 (99%)	160 (94%)	9 (5%)	1 (1%)	21	51
3	B9	170/172 (99%)	162 (95%)	7 (4%)	1 (1%)	21	51
3	BA	170/172 (99%)	162 (95%)	7 (4%)	1 (1%)	21	51
3	D1	170/172 (99%)	162 (95%)	7 (4%)	1 (1%)	21	51
3	D2	170/172 (99%)	162 (95%)	7 (4%)	1 (1%)	21	51
3	D3	170/172 (99%)	162 (95%)	7 (4%)	1 (1%)	21	51
3	D4	170/172 (99%)	162 (95%)	7 (4%)	1 (1%)	21	51
3	D6	170/172 (99%)	162 (95%)	7 (4%)	1 (1%)	21	51
3	D8	170/172 (99%)	162 (95%)	7 (4%)	1 (1%)	21	51
3	D9	170/172 (99%)	162 (95%)	7 (4%)	1 (1%)	21	51
3	DA	170/172 (99%)	162 (95%)	7 (4%)	1 (1%)	21	51
3	F1	170/172 (99%)	162 (95%)	7 (4%)	1 (1%)	21	51
3	F2	170/172 (99%)	162 (95%)	7 (4%)	1 (1%)	21	51
3	F3	170/172 (99%)	162 (95%)	7 (4%)	1 (1%)	21	51
3	F4	170/172 (99%)	158 (93%)	7 (4%)	5 (3%)	3	13
3	F6	170/172 (99%)	162 (95%)	7 (4%)	1 (1%)	21	51
3	F8	170/172 (99%)	159 (94%)	7 (4%)	4 (2%)	4	17
3	F9	170/172 (99%)	160 (94%)	8 (5%)	2 (1%)	10	34
3	FA	170/172 (99%)	162 (95%)	7 (4%)	1 (1%)	21	51
3	H1	170/172 (99%)	162 (95%)	7 (4%)	1 (1%)	21	51
3	H2	170/172 (99%)	161 (95%)	8 (5%)	1 (1%)	21	51
3	H3	170/172 (99%)	162 (95%)	7 (4%)	1 (1%)	21	51
3	H4	170/172 (99%)	162 (95%)	7 (4%)	1 (1%)	21	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	H6	170/172 (99%)	161 (95%)	8 (5%)	1 (1%)	21	51
3	H8	170/172 (99%)	162 (95%)	7 (4%)	1 (1%)	21	51
3	H9	170/172 (99%)	162 (95%)	7 (4%)	1 (1%)	21	51
3	HA	170/172 (99%)	162 (95%)	7 (4%)	1 (1%)	21	51
3	J1	170/172 (99%)	162 (95%)	7 (4%)	1 (1%)	21	51
3	J2	170/172 (99%)	162 (95%)	7 (4%)	1 (1%)	21	51
3	J3	170/172 (99%)	162 (95%)	7 (4%)	1 (1%)	21	51
3	J4	170/172 (99%)	162 (95%)	7 (4%)	1 (1%)	21	51
3	J6	170/172 (99%)	162 (95%)	7 (4%)	1 (1%)	21	51
3	J8	170/172 (99%)	162 (95%)	7 (4%)	1 (1%)	21	51
3	J9	170/172 (99%)	163 (96%)	5 (3%)	2 (1%)	10	34
3	JA	170/172 (99%)	163 (96%)	5 (3%)	2 (1%)	10	34
3	L1	170/172 (99%)	161 (95%)	7 (4%)	2 (1%)	10	34
3	L2	170/172 (99%)	163 (96%)	6 (4%)	1 (1%)	21	51
3	L3	170/172 (99%)	162 (95%)	7 (4%)	1 (1%)	21	51
3	L4	170/172 (99%)	158 (93%)	7 (4%)	5 (3%)	3	13
3	L6	170/172 (99%)	162 (95%)	7 (4%)	1 (1%)	21	51
3	L8	170/172 (99%)	159 (94%)	7 (4%)	4 (2%)	4	17
3	L9	170/172 (99%)	162 (95%)	7 (4%)	1 (1%)	21	51
3	LA	170/172 (99%)	162 (95%)	7 (4%)	1 (1%)	21	51
3	O4	170/172 (99%)	162 (95%)	7 (4%)	1 (1%)	21	51
3	O8	170/172 (99%)	162 (95%)	6 (4%)	2 (1%)	10	34
3	P1	170/172 (99%)	162 (95%)	7 (4%)	1 (1%)	21	51
3	P3	170/172 (99%)	162 (95%)	7 (4%)	1 (1%)	21	51
3	P9	170/172 (99%)	162 (95%)	7 (4%)	1 (1%)	21	51
3	PA	170/172 (99%)	162 (95%)	7 (4%)	1 (1%)	21	51
3	Q4	170/172 (99%)	156 (92%)	11 (6%)	3 (2%)	6	23
3	Q8	170/172 (99%)	156 (92%)	12 (7%)	2 (1%)	10	34
3	R1	170/172 (99%)	162 (95%)	7 (4%)	1 (1%)	21	51
3	R3	170/172 (99%)	162 (95%)	7 (4%)	1 (1%)	21	51
3	R9	170/172 (99%)	162 (95%)	7 (4%)	1 (1%)	21	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	RA	170/172 (99%)	162 (95%)	7 (4%)	1 (1%)	21	51
3	S4	170/172 (99%)	162 (95%)	7 (4%)	1 (1%)	21	51
3	S8	170/172 (99%)	162 (95%)	7 (4%)	1 (1%)	21	51
3	T1	170/172 (99%)	162 (95%)	7 (4%)	1 (1%)	21	51
3	T3	170/172 (99%)	162 (95%)	7 (4%)	1 (1%)	21	51
3	T9	170/172 (99%)	162 (95%)	7 (4%)	1 (1%)	21	51
3	TA	170/172 (99%)	162 (95%)	7 (4%)	1 (1%)	21	51
3	U4	170/172 (99%)	162 (95%)	7 (4%)	1 (1%)	21	51
3	U8	170/172 (99%)	162 (95%)	7 (4%)	1 (1%)	21	51
3	V1	170/172 (99%)	162 (95%)	7 (4%)	1 (1%)	21	51
3	V3	170/172 (99%)	162 (95%)	7 (4%)	1 (1%)	21	51
3	V9	170/172 (99%)	162 (95%)	7 (4%)	1 (1%)	21	51
3	VA	170/172 (99%)	162 (95%)	7 (4%)	1 (1%)	21	51
3	W4	170/172 (99%)	162 (95%)	7 (4%)	1 (1%)	21	51
3	W8	170/172 (99%)	162 (95%)	7 (4%)	1 (1%)	21	51
3	X1	170/172 (99%)	162 (95%)	7 (4%)	1 (1%)	21	51
3	X3	170/172 (99%)	162 (95%)	7 (4%)	1 (1%)	21	51
3	X9	170/172 (99%)	162 (95%)	7 (4%)	1 (1%)	21	51
3	XA	170/172 (99%)	162 (95%)	7 (4%)	1 (1%)	21	51
3	Y4	170/172 (99%)	153 (90%)	15 (9%)	2 (1%)	10	34
3	Y8	170/172 (99%)	155 (91%)	14 (8%)	1 (1%)	21	51
3	Z1	170/172 (99%)	162 (95%)	7 (4%)	1 (1%)	21	51
3	Z3	170/172 (99%)	162 (95%)	7 (4%)	1 (1%)	21	51
3	Z9	170/172 (99%)	162 (95%)	7 (4%)	1 (1%)	21	51
3	ZA	170/172 (99%)	162 (95%)	7 (4%)	1 (1%)	21	51
4	M1	272/274 (99%)	253 (93%)	10 (4%)	9 (3%)	3	11
4	M3	272/274 (99%)	253 (93%)	10 (4%)	9 (3%)	3	11
4	M4	272/274 (99%)	251 (92%)	10 (4%)	11 (4%)	2	8
4	M8	272/274 (99%)	245 (90%)	11 (4%)	16 (6%)	1	3
4	M9	272/274 (99%)	253 (93%)	10 (4%)	9 (3%)	3	11
4	MA	272/274 (99%)	253 (93%)	10 (4%)	9 (3%)	3	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	N1	72/275 (26%)	65 (90%)	5 (7%)	2 (3%)	4	14
5	N3	72/275 (26%)	65 (90%)	5 (7%)	2 (3%)	4	14
5	N9	72/275 (26%)	65 (90%)	5 (7%)	2 (3%)	4	14
5	NA	72/275 (26%)	65 (90%)	5 (7%)	2 (3%)	4	14
5	Z4	72/275 (26%)	59 (82%)	7 (10%)	6 (8%)	0	1
5	Z8	72/275 (26%)	65 (90%)	5 (7%)	2 (3%)	4	14
6	M2	277/729 (38%)	246 (89%)	30 (11%)	1 (0%)	30	60
6	M6	277/729 (38%)	246 (89%)	30 (11%)	1 (0%)	30	60
7	N2	68/70 (97%)	54 (79%)	13 (19%)	1 (2%)	8	28
7	N6	68/70 (97%)	54 (79%)	13 (19%)	1 (2%)	8	28
8	A5	158/161 (98%)	154 (98%)	3 (2%)	1 (1%)	21	51
8	A7	158/161 (98%)	154 (98%)	3 (2%)	1 (1%)	21	51
8	C5	158/161 (98%)	145 (92%)	9 (6%)	4 (2%)	4	16
8	C7	158/161 (98%)	154 (98%)	2 (1%)	2 (1%)	9	31
8	E5	158/161 (98%)	152 (96%)	3 (2%)	3 (2%)	6	22
8	E7	158/161 (98%)	151 (96%)	5 (3%)	2 (1%)	9	31
8	G5	158/161 (98%)	154 (98%)	3 (2%)	1 (1%)	21	51
8	G7	158/161 (98%)	154 (98%)	3 (2%)	1 (1%)	21	51
8	I5	158/161 (98%)	145 (92%)	9 (6%)	4 (2%)	4	16
8	I7	158/161 (98%)	154 (98%)	2 (1%)	2 (1%)	9	31
8	K5	158/161 (98%)	152 (96%)	3 (2%)	3 (2%)	6	22
8	K7	158/161 (98%)	151 (96%)	5 (3%)	2 (1%)	9	31
8	M5	158/161 (98%)	154 (98%)	3 (2%)	1 (1%)	21	51
8	M7	158/161 (98%)	154 (98%)	3 (2%)	1 (1%)	21	51
8	O5	158/161 (98%)	148 (94%)	6 (4%)	4 (2%)	4	16
8	O7	158/161 (98%)	151 (96%)	2 (1%)	5 (3%)	3	11
8	Q5	158/161 (98%)	150 (95%)	5 (3%)	3 (2%)	6	22
8	Q7	158/161 (98%)	151 (96%)	5 (3%)	2 (1%)	9	31
8	S5	158/161 (98%)	154 (98%)	3 (2%)	1 (1%)	21	51
8	S7	158/161 (98%)	154 (98%)	3 (2%)	1 (1%)	21	51
8	U5	158/161 (98%)	151 (96%)	3 (2%)	4 (2%)	4	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	U7	158/161 (98%)	151 (96%)	3 (2%)	4 (2%)	4	16
8	W5	158/161 (98%)	150 (95%)	5 (3%)	3 (2%)	6	22
8	W7	158/161 (98%)	151 (96%)	5 (3%)	2 (1%)	9	31
8	Y5	158/161 (98%)	154 (98%)	3 (2%)	1 (1%)	21	51
8	Y7	158/161 (98%)	154 (98%)	3 (2%)	1 (1%)	21	51
8	a5	158/161 (98%)	149 (94%)	5 (3%)	4 (2%)	4	16
8	a7	158/161 (98%)	152 (96%)	4 (2%)	2 (1%)	9	31
8	c5	158/161 (98%)	154 (98%)	3 (2%)	1 (1%)	21	51
8	c7	158/161 (98%)	149 (94%)	7 (4%)	2 (1%)	9	31
8	e5	158/161 (98%)	149 (94%)	5 (3%)	4 (2%)	4	16
8	e7	158/161 (98%)	154 (98%)	3 (2%)	1 (1%)	21	51
8	g7	158/161 (98%)	152 (96%)	4 (2%)	2 (1%)	9	31
8	i7	158/161 (98%)	149 (94%)	7 (4%)	2 (1%)	9	31
8	k7	158/161 (98%)	154 (98%)	3 (2%)	1 (1%)	21	51
8	m7	158/161 (98%)	150 (95%)	4 (2%)	4 (2%)	4	16
8	o7	158/161 (98%)	150 (95%)	6 (4%)	2 (1%)	9	31
8	q7	158/161 (98%)	154 (98%)	3 (2%)	1 (1%)	21	51
8	s7	158/161 (98%)	152 (96%)	3 (2%)	3 (2%)	6	22
8	u7	158/161 (98%)	150 (95%)	6 (4%)	2 (1%)	9	31
9	i5	66/68 (97%)	61 (92%)	3 (4%)	2 (3%)	3	12
9	w7	66/68 (97%)	55 (83%)	8 (12%)	3 (4%)	2	7
9	x7	66/68 (97%)	53 (80%)	11 (17%)	2 (3%)	3	12
9	y7	66/68 (97%)	53 (80%)	11 (17%)	2 (3%)	3	12
9	z5	66/68 (97%)	61 (92%)	3 (4%)	2 (3%)	3	12
9	z7	66/68 (97%)	55 (83%)	8 (12%)	3 (4%)	2	7
10	j5	1104/1155 (96%)	967 (88%)	88 (8%)	49 (4%)	2	7
10	k5	1104/1155 (96%)	966 (88%)	88 (8%)	50 (4%)	2	7
11	a9	796/824 (97%)	691 (87%)	70 (9%)	35 (4%)	2	7
11	aA	796/824 (97%)	688 (86%)	70 (9%)	38 (5%)	2	6
All	All	47626/50516 (94%)	45281 (95%)	1786 (4%)	559 (1%)	13	34

5 of 559 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	FA	145	PRO
3	JA	21	GLU
4	MA	2	ASN
4	MA	78	GLY
4	MA	79	PRO

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	A	121/121 (100%)	119 (98%)	2 (2%)	53	83
1	B5	121/121 (100%)	119 (98%)	2 (2%)	53	83
1	B7	121/121 (100%)	119 (98%)	2 (2%)	53	83
1	D5	121/121 (100%)	114 (94%)	7 (6%)	18	49
1	D7	121/121 (100%)	119 (98%)	2 (2%)	53	83
1	F5	121/121 (100%)	118 (98%)	3 (2%)	42	76
1	F7	121/121 (100%)	119 (98%)	2 (2%)	53	83
1	H5	121/121 (100%)	119 (98%)	2 (2%)	53	83
1	H7	121/121 (100%)	119 (98%)	2 (2%)	53	83
1	J5	121/121 (100%)	114 (94%)	7 (6%)	18	49
1	J7	121/121 (100%)	119 (98%)	2 (2%)	53	83
1	L5	121/121 (100%)	118 (98%)	3 (2%)	42	76
1	L7	121/121 (100%)	119 (98%)	2 (2%)	53	83
1	N5	121/121 (100%)	119 (98%)	2 (2%)	53	83
1	N7	121/121 (100%)	119 (98%)	2 (2%)	53	83
1	P5	121/121 (100%)	119 (98%)	2 (2%)	53	83
1	P7	121/121 (100%)	119 (98%)	2 (2%)	53	83
1	R5	121/121 (100%)	119 (98%)	2 (2%)	53	83
1	R7	121/121 (100%)	119 (98%)	2 (2%)	53	83
1	T5	121/121 (100%)	119 (98%)	2 (2%)	53	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	T7	121/121 (100%)	119 (98%)	2 (2%)	53	83
1	V5	121/121 (100%)	119 (98%)	2 (2%)	53	83
1	V7	121/121 (100%)	119 (98%)	2 (2%)	53	83
1	X5	121/121 (100%)	119 (98%)	2 (2%)	53	83
1	X7	121/121 (100%)	119 (98%)	2 (2%)	53	83
1	Z	121/121 (100%)	119 (98%)	2 (2%)	53	83
1	Z5	121/121 (100%)	119 (98%)	2 (2%)	53	83
1	Z7	121/121 (100%)	119 (98%)	2 (2%)	53	83
1	b5	121/121 (100%)	119 (98%)	2 (2%)	53	83
1	b7	121/121 (100%)	114 (94%)	7 (6%)	18	49
1	d5	121/121 (100%)	119 (98%)	2 (2%)	53	83
1	d7	121/121 (100%)	119 (98%)	2 (2%)	53	83
1	f5	121/121 (100%)	119 (98%)	2 (2%)	53	83
1	f7	121/121 (100%)	119 (98%)	2 (2%)	53	83
1	h7	121/121 (100%)	114 (94%)	7 (6%)	18	49
1	j7	121/121 (100%)	119 (98%)	2 (2%)	53	83
1	l7	121/121 (100%)	119 (98%)	2 (2%)	53	83
1	n7	121/121 (100%)	119 (98%)	2 (2%)	53	83
1	p7	121/121 (100%)	119 (98%)	2 (2%)	53	83
1	r7	121/121 (100%)	119 (98%)	2 (2%)	53	83
1	t7	121/121 (100%)	119 (98%)	2 (2%)	53	83
1	v7	121/121 (100%)	119 (98%)	2 (2%)	53	83
2	A1	130/130 (100%)	125 (96%)	5 (4%)	29	64
2	A2	130/130 (100%)	124 (95%)	6 (5%)	24	58
2	A3	130/130 (100%)	123 (95%)	7 (5%)	20	51
2	A4	130/130 (100%)	124 (95%)	6 (5%)	24	58
2	A6	130/130 (100%)	124 (95%)	6 (5%)	24	58
2	A8	130/130 (100%)	124 (95%)	6 (5%)	24	58
2	A9	130/130 (100%)	124 (95%)	6 (5%)	24	58
2	AA	130/130 (100%)	124 (95%)	6 (5%)	24	58
2	C1	130/130 (100%)	124 (95%)	6 (5%)	24	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C2	130/130 (100%)	124 (95%)	6 (5%)	24	58
2	C3	130/130 (100%)	124 (95%)	6 (5%)	24	58
2	C4	130/130 (100%)	124 (95%)	6 (5%)	24	58
2	C6	130/130 (100%)	124 (95%)	6 (5%)	24	58
2	C8	130/130 (100%)	124 (95%)	6 (5%)	24	58
2	C9	130/130 (100%)	124 (95%)	6 (5%)	24	58
2	CA	130/130 (100%)	124 (95%)	6 (5%)	24	58
2	E1	130/130 (100%)	124 (95%)	6 (5%)	24	58
2	E2	130/130 (100%)	124 (95%)	6 (5%)	24	58
2	E3	130/130 (100%)	124 (95%)	6 (5%)	24	58
2	E4	130/130 (100%)	124 (95%)	6 (5%)	24	58
2	E6	130/130 (100%)	124 (95%)	6 (5%)	24	58
2	E8	130/130 (100%)	124 (95%)	6 (5%)	24	58
2	E9	130/130 (100%)	124 (95%)	6 (5%)	24	58
2	EA	130/130 (100%)	124 (95%)	6 (5%)	24	58
2	G1	130/130 (100%)	124 (95%)	6 (5%)	24	58
2	G2	130/130 (100%)	124 (95%)	6 (5%)	24	58
2	G3	130/130 (100%)	124 (95%)	6 (5%)	24	58
2	G4	130/130 (100%)	124 (95%)	6 (5%)	24	58
2	G6	130/130 (100%)	124 (95%)	6 (5%)	24	58
2	G8	130/130 (100%)	124 (95%)	6 (5%)	24	58
2	G9	130/130 (100%)	124 (95%)	6 (5%)	24	58
2	GA	130/130 (100%)	124 (95%)	6 (5%)	24	58
2	I1	130/130 (100%)	124 (95%)	6 (5%)	24	58
2	I2	130/130 (100%)	124 (95%)	6 (5%)	24	58
2	I3	130/130 (100%)	124 (95%)	6 (5%)	24	58
2	I4	130/130 (100%)	124 (95%)	6 (5%)	24	58
2	I6	130/130 (100%)	124 (95%)	6 (5%)	24	58
2	I8	130/130 (100%)	124 (95%)	6 (5%)	24	58
2	I9	130/130 (100%)	125 (96%)	5 (4%)	29	64
2	IA	130/130 (100%)	125 (96%)	5 (4%)	29	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	K1	130/130 (100%)	125 (96%)	5 (4%)	29	64
2	K2	130/130 (100%)	124 (95%)	6 (5%)	24	58
2	K3	130/130 (100%)	124 (95%)	6 (5%)	24	58
2	K4	130/130 (100%)	124 (95%)	6 (5%)	24	58
2	K6	130/130 (100%)	124 (95%)	6 (5%)	24	58
2	K8	130/130 (100%)	124 (95%)	6 (5%)	24	58
2	K9	130/130 (100%)	124 (95%)	6 (5%)	24	58
2	KA	130/130 (100%)	124 (95%)	6 (5%)	24	58
2	N4	130/130 (100%)	125 (96%)	5 (4%)	29	64
2	N8	130/130 (100%)	125 (96%)	5 (4%)	29	64
2	O1	130/130 (100%)	124 (95%)	6 (5%)	24	58
2	O3	130/130 (100%)	124 (95%)	6 (5%)	24	58
2	O9	130/130 (100%)	124 (95%)	6 (5%)	24	58
2	OA	130/130 (100%)	124 (95%)	6 (5%)	24	58
2	P4	130/130 (100%)	124 (95%)	6 (5%)	24	58
2	P8	130/130 (100%)	124 (95%)	6 (5%)	24	58
2	Q1	130/130 (100%)	124 (95%)	6 (5%)	24	58
2	Q3	130/130 (100%)	124 (95%)	6 (5%)	24	58
2	Q9	130/130 (100%)	124 (95%)	6 (5%)	24	58
2	QA	130/130 (100%)	123 (95%)	7 (5%)	20	51
2	R4	130/130 (100%)	124 (95%)	6 (5%)	24	58
2	R8	130/130 (100%)	124 (95%)	6 (5%)	24	58
2	S1	130/130 (100%)	124 (95%)	6 (5%)	24	58
2	S3	130/130 (100%)	124 (95%)	6 (5%)	24	58
2	S9	130/130 (100%)	124 (95%)	6 (5%)	24	58
2	SA	130/130 (100%)	124 (95%)	6 (5%)	24	58
2	T4	130/130 (100%)	124 (95%)	6 (5%)	24	58
2	T8	130/130 (100%)	124 (95%)	6 (5%)	24	58
2	U1	130/130 (100%)	122 (94%)	8 (6%)	16	45
2	U3	130/130 (100%)	124 (95%)	6 (5%)	24	58
2	U9	130/130 (100%)	124 (95%)	6 (5%)	24	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	UA	130/130 (100%)	124 (95%)	6 (5%)	24	58
2	V4	130/130 (100%)	124 (95%)	6 (5%)	24	58
2	V8	130/130 (100%)	124 (95%)	6 (5%)	24	58
2	W1	130/130 (100%)	124 (95%)	6 (5%)	24	58
2	W3	130/130 (100%)	124 (95%)	6 (5%)	24	58
2	W9	130/130 (100%)	124 (95%)	6 (5%)	24	58
2	WA	130/130 (100%)	124 (95%)	6 (5%)	24	58
2	X4	130/130 (100%)	124 (95%)	6 (5%)	24	58
2	X8	130/130 (100%)	124 (95%)	6 (5%)	24	58
2	Y1	130/130 (100%)	124 (95%)	6 (5%)	24	58
2	Y3	130/130 (100%)	124 (95%)	6 (5%)	24	58
2	Y9	130/130 (100%)	124 (95%)	6 (5%)	24	58
2	YA	130/130 (100%)	124 (95%)	6 (5%)	24	58
3	B1	134/134 (100%)	131 (98%)	3 (2%)	45	78
3	B2	134/134 (100%)	130 (97%)	4 (3%)	36	72
3	B3	134/134 (100%)	131 (98%)	3 (2%)	45	78
3	B4	134/134 (100%)	128 (96%)	6 (4%)	24	58
3	B6	134/134 (100%)	130 (97%)	4 (3%)	36	72
3	B8	134/134 (100%)	131 (98%)	3 (2%)	45	78
3	B9	134/134 (100%)	132 (98%)	2 (2%)	57	84
3	BA	134/134 (100%)	132 (98%)	2 (2%)	57	84
3	D1	134/134 (100%)	131 (98%)	3 (2%)	45	78
3	D2	134/134 (100%)	131 (98%)	3 (2%)	45	78
3	D3	134/134 (100%)	131 (98%)	3 (2%)	45	78
3	D4	134/134 (100%)	131 (98%)	3 (2%)	45	78
3	D6	134/134 (100%)	131 (98%)	3 (2%)	45	78
3	D8	134/134 (100%)	131 (98%)	3 (2%)	45	78
3	D9	134/134 (100%)	131 (98%)	3 (2%)	45	78
3	DA	134/134 (100%)	131 (98%)	3 (2%)	45	78
3	F1	134/134 (100%)	131 (98%)	3 (2%)	45	78
3	F2	134/134 (100%)	131 (98%)	3 (2%)	45	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	F3	134/134 (100%)	131 (98%)	3 (2%)	45	78
3	F4	134/134 (100%)	130 (97%)	4 (3%)	36	72
3	F6	134/134 (100%)	131 (98%)	3 (2%)	45	78
3	F8	134/134 (100%)	129 (96%)	5 (4%)	30	65
3	F9	134/134 (100%)	129 (96%)	5 (4%)	30	65
3	FA	134/134 (100%)	129 (96%)	5 (4%)	30	65
3	H1	134/134 (100%)	131 (98%)	3 (2%)	45	78
3	H2	134/134 (100%)	131 (98%)	3 (2%)	45	78
3	H3	134/134 (100%)	131 (98%)	3 (2%)	45	78
3	H4	134/134 (100%)	131 (98%)	3 (2%)	45	78
3	H6	134/134 (100%)	131 (98%)	3 (2%)	45	78
3	H8	134/134 (100%)	131 (98%)	3 (2%)	45	78
3	H9	134/134 (100%)	130 (97%)	4 (3%)	36	72
3	HA	134/134 (100%)	130 (97%)	4 (3%)	36	72
3	J1	134/134 (100%)	131 (98%)	3 (2%)	45	78
3	J2	134/134 (100%)	131 (98%)	3 (2%)	45	78
3	J3	134/134 (100%)	131 (98%)	3 (2%)	45	78
3	J4	134/134 (100%)	131 (98%)	3 (2%)	45	78
3	J6	134/134 (100%)	131 (98%)	3 (2%)	45	78
3	J8	134/134 (100%)	131 (98%)	3 (2%)	45	78
3	J9	134/134 (100%)	131 (98%)	3 (2%)	45	78
3	JA	134/134 (100%)	131 (98%)	3 (2%)	45	78
3	L1	134/134 (100%)	131 (98%)	3 (2%)	45	78
3	L2	134/134 (100%)	131 (98%)	3 (2%)	45	78
3	L3	134/134 (100%)	131 (98%)	3 (2%)	45	78
3	L4	134/134 (100%)	131 (98%)	3 (2%)	45	78
3	L6	134/134 (100%)	131 (98%)	3 (2%)	45	78
3	L8	134/134 (100%)	131 (98%)	3 (2%)	45	78
3	L9	134/134 (100%)	124 (92%)	10 (8%)	12	37
3	LA	134/134 (100%)	124 (92%)	10 (8%)	12	37
3	O4	134/134 (100%)	131 (98%)	3 (2%)	45	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	O8	134/134 (100%)	130 (97%)	4 (3%)	36	72
3	P1	134/134 (100%)	131 (98%)	3 (2%)	45	78
3	P3	134/134 (100%)	131 (98%)	3 (2%)	45	78
3	P9	134/134 (100%)	131 (98%)	3 (2%)	45	78
3	PA	134/134 (100%)	131 (98%)	3 (2%)	45	78
3	Q4	134/134 (100%)	129 (96%)	5 (4%)	30	65
3	Q8	134/134 (100%)	127 (95%)	7 (5%)	21	53
3	R1	134/134 (100%)	131 (98%)	3 (2%)	45	78
3	R3	134/134 (100%)	131 (98%)	3 (2%)	45	78
3	R9	134/134 (100%)	131 (98%)	3 (2%)	45	78
3	RA	134/134 (100%)	131 (98%)	3 (2%)	45	78
3	S4	134/134 (100%)	131 (98%)	3 (2%)	45	78
3	S8	134/134 (100%)	131 (98%)	3 (2%)	45	78
3	T1	134/134 (100%)	131 (98%)	3 (2%)	45	78
3	T3	134/134 (100%)	131 (98%)	3 (2%)	45	78
3	T9	134/134 (100%)	131 (98%)	3 (2%)	45	78
3	TA	134/134 (100%)	131 (98%)	3 (2%)	45	78
3	U4	134/134 (100%)	131 (98%)	3 (2%)	45	78
3	U8	134/134 (100%)	131 (98%)	3 (2%)	45	78
3	V1	134/134 (100%)	131 (98%)	3 (2%)	45	78
3	V3	134/134 (100%)	131 (98%)	3 (2%)	45	78
3	V9	134/134 (100%)	130 (97%)	4 (3%)	36	72
3	VA	134/134 (100%)	130 (97%)	4 (3%)	36	72
3	W4	134/134 (100%)	131 (98%)	3 (2%)	45	78
3	W8	134/134 (100%)	131 (98%)	3 (2%)	45	78
3	X1	134/134 (100%)	131 (98%)	3 (2%)	45	78
3	X3	134/134 (100%)	131 (98%)	3 (2%)	45	78
3	X9	134/134 (100%)	132 (98%)	2 (2%)	57	84
3	XA	134/134 (100%)	132 (98%)	2 (2%)	57	84
3	Y4	134/134 (100%)	129 (96%)	5 (4%)	30	65
3	Y8	134/134 (100%)	128 (96%)	6 (4%)	24	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	Z1	134/134 (100%)	130 (97%)	4 (3%)	36	72
3	Z3	134/134 (100%)	131 (98%)	3 (2%)	45	78
3	Z9	134/134 (100%)	131 (98%)	3 (2%)	45	78
3	ZA	134/134 (100%)	130 (97%)	4 (3%)	36	72
4	M1	235/238 (99%)	182 (77%)	53 (23%)	1	3
4	M3	235/238 (99%)	182 (77%)	53 (23%)	1	3
4	M4	235/238 (99%)	181 (77%)	54 (23%)	1	3
4	M8	235/238 (99%)	182 (77%)	53 (23%)	1	3
4	M9	235/238 (99%)	182 (77%)	53 (23%)	1	3
4	MA	235/238 (99%)	182 (77%)	53 (23%)	1	3
5	N1	66/240 (28%)	40 (61%)	26 (39%)	0	0
5	N3	66/240 (28%)	40 (61%)	26 (39%)	0	0
5	N9	66/240 (28%)	39 (59%)	27 (41%)	0	0
5	NA	66/240 (28%)	39 (59%)	27 (41%)	0	0
5	Z4	66/240 (28%)	43 (65%)	23 (35%)	0	0
5	Z8	66/240 (28%)	46 (70%)	20 (30%)	0	1
6	M2	230/603 (38%)	228 (99%)	2 (1%)	70	89
6	M6	230/603 (38%)	228 (99%)	2 (1%)	70	89
7	N2	61/62 (98%)	57 (93%)	4 (7%)	15	43
7	N6	61/62 (98%)	57 (93%)	4 (7%)	15	43
8	A5	127/128 (99%)	120 (94%)	7 (6%)	19	51
8	A7	127/128 (99%)	122 (96%)	5 (4%)	28	64
8	C5	127/128 (99%)	120 (94%)	7 (6%)	19	51
8	C7	127/128 (99%)	124 (98%)	3 (2%)	43	77
8	E5	127/128 (99%)	115 (91%)	12 (9%)	8	27
8	E7	127/128 (99%)	122 (96%)	5 (4%)	28	64
8	G5	127/128 (99%)	120 (94%)	7 (6%)	19	51
8	G7	127/128 (99%)	122 (96%)	5 (4%)	28	64
8	I5	127/128 (99%)	120 (94%)	7 (6%)	19	51
8	I7	127/128 (99%)	124 (98%)	3 (2%)	43	77
8	K5	127/128 (99%)	115 (91%)	12 (9%)	8	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	K7	127/128 (99%)	122 (96%)	5 (4%)	28	64
8	M5	127/128 (99%)	121 (95%)	6 (5%)	23	57
8	M7	127/128 (99%)	121 (95%)	6 (5%)	23	57
8	O5	127/128 (99%)	123 (97%)	4 (3%)	35	70
8	O7	127/128 (99%)	124 (98%)	3 (2%)	43	77
8	Q5	127/128 (99%)	121 (95%)	6 (5%)	23	57
8	Q7	127/128 (99%)	122 (96%)	5 (4%)	28	64
8	S5	127/128 (99%)	121 (95%)	6 (5%)	23	57
8	S7	127/128 (99%)	121 (95%)	6 (5%)	23	57
8	U5	127/128 (99%)	122 (96%)	5 (4%)	28	64
8	U7	127/128 (99%)	123 (97%)	4 (3%)	35	70
8	W5	127/128 (99%)	121 (95%)	6 (5%)	23	57
8	W7	127/128 (99%)	122 (96%)	5 (4%)	28	64
8	Y5	127/128 (99%)	121 (95%)	6 (5%)	23	57
8	Y7	127/128 (99%)	121 (95%)	6 (5%)	23	57
8	a5	127/128 (99%)	120 (94%)	7 (6%)	19	51
8	a7	127/128 (99%)	125 (98%)	2 (2%)	55	83
8	c5	127/128 (99%)	121 (95%)	6 (5%)	23	57
8	c7	127/128 (99%)	116 (91%)	11 (9%)	9	30
8	e5	127/128 (99%)	120 (94%)	7 (6%)	19	51
8	e7	127/128 (99%)	121 (95%)	6 (5%)	23	57
8	g7	127/128 (99%)	125 (98%)	2 (2%)	55	83
8	i7	127/128 (99%)	116 (91%)	11 (9%)	9	30
8	k7	127/128 (99%)	122 (96%)	5 (4%)	28	64
8	m7	127/128 (99%)	123 (97%)	4 (3%)	35	70
8	o7	127/128 (99%)	117 (92%)	10 (8%)	11	35
8	q7	127/128 (99%)	121 (95%)	6 (5%)	23	57
8	s7	127/128 (99%)	123 (97%)	4 (3%)	35	70
8	u7	127/128 (99%)	117 (92%)	10 (8%)	11	35
9	i5	57/57 (100%)	48 (84%)	9 (16%)	2	9
9	w7	57/57 (100%)	42 (74%)	15 (26%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	x7	57/57 (100%)	40 (70%)	17 (30%)	0	1
9	y7	57/57 (100%)	40 (70%)	17 (30%)	0	1
9	z5	57/57 (100%)	48 (84%)	9 (16%)	2	9
9	z7	57/57 (100%)	42 (74%)	15 (26%)	0	2
10	j5	941/977 (96%)	716 (76%)	225 (24%)	1	3
10	k5	941/977 (96%)	717 (76%)	224 (24%)	1	3
11	a9	652/670 (97%)	525 (80%)	127 (20%)	1	5
11	aA	652/670 (97%)	522 (80%)	130 (20%)	1	5
All	All	38254/40212 (95%)	35843 (94%)	2411 (6%)	18	45

5 of 2411 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	N9	67	ILE
4	M1	113	ILE
2	C9	30	ARG
5	N9	60	ILE
11	a9	543	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 542 such sidechains are listed below:

Mol	Chain	Res	Type
11	a9	348	GLN
11	aA	176	ASN
11	a9	329	ASN
5	N1	29	HIS
1	T5	11	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

42 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	MEN	L5	71	1	7,8,9	0.34	0	4,9,11	0.42	0
1	MEN	D5	71	1	7,8,9	0.38	0	4,9,11	0.42	0
1	MEN	P7	71	1	7,8,9	0.37	0	4,9,11	0.39	0
1	MEN	D7	71	1	7,8,9	0.37	0	4,9,11	0.44	0
1	MEN	T7	71	1	7,8,9	0.38	0	4,9,11	0.37	0
1	MEN	X5	71	1	7,8,9	0.37	0	4,9,11	0.35	0
1	MEN	f5	71	1	7,8,9	0.34	0	4,9,11	0.37	0
1	MEN	J5	71	1	7,8,9	0.39	0	4,9,11	0.42	0
1	MEN	J7	71	1	7,8,9	0.38	0	4,9,11	0.44	0
1	MEN	L7	71	1	7,8,9	0.37	0	4,9,11	0.39	0
1	MEN	h7	71	1	7,8,9	0.34	0	4,9,11	0.37	0
1	MEN	V7	71	1	7,8,9	0.35	0	4,9,11	0.39	0
1	MEN	B7	71	1	7,8,9	0.37	0	4,9,11	0.38	0
1	MEN	p7	71	1	7,8,9	0.36	0	4,9,11	0.39	0
1	MEN	X7	71	1	7,8,9	0.38	0	4,9,11	0.43	0
1	MEN	F5	71	1	7,8,9	0.36	0	4,9,11	0.42	0
1	MEN	d7	71	1	7,8,9	0.37	0	4,9,11	0.38	0
1	MEN	V5	71	1	7,8,9	0.38	0	4,9,11	0.40	0
1	MEN	v7	71	1	7,8,9	0.35	0	4,9,11	0.40	0
1	MEN	P5	71	1	7,8,9	0.37	0	4,9,11	0.41	0
1	MEN	R5	71	1	7,8,9	0.37	0	4,9,11	0.36	0
1	MEN	l7	71	1	7,8,9	0.37	0	4,9,11	0.37	0
1	MEN	j7	71	1	7,8,9	0.36	0	4,9,11	0.38	0
1	MEN	d5	71	1	7,8,9	0.36	0	4,9,11	0.33	0
1	MEN	Z	71	1	7,8,9	0.36	0	4,9,11	0.31	0
1	MEN	Z5	71	1	7,8,9	0.36	0	4,9,11	0.32	0
1	MEN	R7	71	1	7,8,9	0.37	0	4,9,11	0.36	0
1	MEN	H7	71	1	7,8,9	0.38	0	4,9,11	0.38	0
1	MEN	Z7	71	1	7,8,9	0.37	0	4,9,11	0.39	0
1	MEN	r7	71	1	7,8,9	0.37	0	4,9,11	0.41	0
1	MEN	H5	71	1	7,8,9	0.38	0	4,9,11	0.37	0
1	MEN	N5	71	1	7,8,9	0.39	0	4,9,11	0.39	0
1	MEN	T5	71	1	7,8,9	0.39	0	4,9,11	0.40	0
1	MEN	B5	71	1	7,8,9	0.37	0	4,9,11	0.39	0
1	MEN	b5	71	1	7,8,9	0.33	0	4,9,11	0.37	0
1	MEN	F7	71	1	7,8,9	0.35	0	4,9,11	0.39	0
1	MEN	b7	71	1	7,8,9	0.34	0	4,9,11	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MEN	N7	71	1	7,8,9	0.38	0	4,9,11	0.41	0
1	MEN	n7	71	1	7,8,9	0.38	0	4,9,11	0.38	0
1	MEN	f7	71	1	7,8,9	0.38	0	4,9,11	0.39	0
1	MEN	A	71	1	7,8,9	0.37	0	4,9,11	0.34	0
1	MEN	t7	71	1	7,8,9	0.37	0	4,9,11	0.38	0

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
1	MEN	L5	71	1	-	0/7/8/10	-
1	MEN	D5	71	1	-	0/7/8/10	-
1	MEN	P7	71	1	-	0/7/8/10	-
1	MEN	D7	71	1	-	0/7/8/10	-
1	MEN	T7	71	1	-	0/7/8/10	-
1	MEN	X5	71	1	-	0/7/8/10	-
1	MEN	f5	71	1	-	0/7/8/10	-
1	MEN	J5	71	1	-	0/7/8/10	-
1	MEN	J7	71	1	-	0/7/8/10	-
1	MEN	L7	71	1	-	0/7/8/10	-
1	MEN	h7	71	1	-	0/7/8/10	-
1	MEN	V7	71	1	-	0/7/8/10	-
1	MEN	B7	71	1	-	0/7/8/10	-
1	MEN	p7	71	1	-	0/7/8/10	-
1	MEN	X7	71	1	-	0/7/8/10	-
1	MEN	F5	71	1	-	0/7/8/10	-
1	MEN	d7	71	1	-	0/7/8/10	-
1	MEN	V5	71	1	-	0/7/8/10	-
1	MEN	v7	71	1	-	0/7/8/10	-
1	MEN	P5	71	1	-	0/7/8/10	-
1	MEN	R5	71	1	-	0/7/8/10	-
1	MEN	l7	71	1	-	0/7/8/10	-
1	MEN	j7	71	1	-	0/7/8/10	-
1	MEN	d5	71	1	-	0/7/8/10	-
1	MEN	Z	71	1	-	0/7/8/10	-
1	MEN	Z5	71	1	-	0/7/8/10	-
1	MEN	R7	71	1	-	0/7/8/10	-
1	MEN	H7	71	1	-	0/7/8/10	-
1	MEN	Z7	71	1	-	0/7/8/10	-
1	MEN	r7	71	1	-	0/7/8/10	-
1	MEN	H5	71	1	-	0/7/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MEN	N5	71	1	-	0/7/8/10	-
1	MEN	T5	71	1	-	0/7/8/10	-
1	MEN	B5	71	1	-	0/7/8/10	-
1	MEN	b5	71	1	-	0/7/8/10	-
1	MEN	F7	71	1	-	0/7/8/10	-
1	MEN	b7	71	1	-	0/7/8/10	-
1	MEN	N7	71	1	-	0/7/8/10	-
1	MEN	n7	71	1	-	0/7/8/10	-
1	MEN	f7	71	1	-	0/7/8/10	-
1	MEN	A	71	1	-	0/7/8/10	-
1	MEN	t7	71	1	-	0/7/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

42 monomers are involved in 62 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	L5	71	MEN	1	0
1	D5	71	MEN	9	0
1	P7	71	MEN	1	0
1	D7	71	MEN	1	0
1	T7	71	MEN	1	0
1	X5	71	MEN	1	0
1	f5	71	MEN	1	0
1	J5	71	MEN	8	0
1	J7	71	MEN	1	0
1	L7	71	MEN	1	0
1	h7	71	MEN	1	0
1	V7	71	MEN	1	0
1	B7	71	MEN	1	0
1	p7	71	MEN	1	0
1	X7	71	MEN	1	0
1	F5	71	MEN	1	0
1	d7	71	MEN	1	0
1	V5	71	MEN	1	0
1	v7	71	MEN	6	0
1	P5	71	MEN	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	R5	71	MEN	1	0
1	l7	71	MEN	1	0
1	j7	71	MEN	1	0
1	d5	71	MEN	1	0
1	Z	71	MEN	1	0
1	Z5	71	MEN	1	0
1	R7	71	MEN	1	0
1	H7	71	MEN	1	0
1	Z7	71	MEN	1	0
1	r7	71	MEN	1	0
1	H5	71	MEN	1	0
1	N5	71	MEN	1	0
1	T5	71	MEN	1	0
1	B5	71	MEN	1	0
1	b5	71	MEN	1	0
1	F7	71	MEN	1	0
1	b7	71	MEN	1	0
1	N7	71	MEN	1	0
1	n7	71	MEN	1	0
1	f7	71	MEN	1	0
1	A	71	MEN	1	0
1	t7	71	MEN	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

336 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	$\# Z > 2$
12	CYC	W3	201	-	46,46,46	2.27	17 (36%)	63,67,67	2.77	30 (47%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	CYC	Y8	201	-	46,46,46	2.22	13 (28%)	63,67,67	2.92	25 (39%)
12	CYC	Q1	201	-	46,46,46	2.27	17 (36%)	63,67,67	2.78	28 (44%)
12	CYC	A5	201	-	46,46,46	2.30	14 (30%)	63,67,67	2.92	23 (36%)
12	CYC	U8	201	-	46,46,46	2.30	18 (39%)	63,67,67	2.84	27 (42%)
12	CYC	X9	202	-	46,46,46	2.21	12 (26%)	63,67,67	2.90	25 (39%)
12	CYC	J6	201	-	46,46,46	2.21	14 (30%)	63,67,67	2.90	25 (39%)
12	CYC	D1	202	-	46,46,46	2.31	18 (39%)	63,67,67	2.83	27 (42%)
12	CYC	S9	201	-	46,46,46	2.27	17 (36%)	63,67,67	2.80	29 (46%)
12	CYC	Y9	201	-	46,46,46	2.28	16 (34%)	63,67,67	2.81	29 (46%)
12	CYC	U7	201	-	46,46,46	2.31	14 (30%)	63,67,67	2.94	24 (38%)
12	CYC	Q4	201	-	46,46,46	2.21	13 (28%)	63,67,67	2.91	25 (39%)
12	CYC	O7	201	-	46,46,46	2.32	14 (30%)	63,67,67	2.93	24 (38%)
12	CYC	ZA	202	-	46,46,46	2.30	17 (36%)	63,67,67	2.85	26 (41%)
12	CYC	QA	201	-	46,46,46	2.28	17 (36%)	63,67,67	2.79	28 (44%)
12	CYC	H2	201	-	46,46,46	2.29	18 (39%)	63,67,67	2.81	26 (41%)
12	CYC	h7	201	-	46,46,46	2.41	18 (39%)	63,67,67	2.69	26 (41%)
12	CYC	Z1	201	-	46,46,46	2.22	14 (30%)	63,67,67	2.89	25 (39%)
12	CYC	WA	201	-	46,46,46	2.28	16 (34%)	63,67,67	2.77	29 (46%)
12	CYC	H6	201	-	46,46,46	2.28	18 (39%)	63,67,67	2.82	25 (39%)
12	CYC	p7	201	-	46,46,46	2.40	16 (34%)	63,67,67	2.72	26 (41%)
12	CYC	e5	201	-	46,46,46	2.33	14 (30%)	63,67,67	2.93	24 (38%)
12	CYC	L6	202	-	46,46,46	2.19	14 (30%)	63,67,67	2.89	24 (38%)
12	CYC	k5	1202	-	46,46,46	2.41	17 (36%)	63,67,67	2.71	26 (41%)
12	CYC	G3	201	-	46,46,46	2.28	16 (34%)	63,67,67	2.78	29 (46%)
12	CYC	k7	201	-	46,46,46	2.30	14 (30%)	63,67,67	2.92	24 (38%)
12	CYC	H9	201	-	46,46,46	2.20	13 (28%)	63,67,67	2.88	25 (39%)
12	CYC	r7	201	-	46,46,46	2.40	16 (34%)	63,67,67	2.70	25 (39%)
12	CYC	VA	201	-	46,46,46	2.29	18 (39%)	63,67,67	2.86	26 (41%)
12	CYC	k5	1204	-	46,46,46	2.40	17 (36%)	63,67,67	2.69	25 (39%)
12	CYC	J1	201	-	46,46,46	2.19	14 (30%)	63,67,67	2.87	25 (39%)
12	CYC	J9	202	-	46,46,46	2.29	17 (36%)	63,67,67	2.82	25 (39%)
12	CYC	G2	201	-	46,46,46	2.29	16 (34%)	63,67,67	2.80	29 (46%)
12	CYC	D6	202	-	46,46,46	2.19	13 (28%)	63,67,67	2.90	24 (38%)
12	CYC	N5	201	-	46,46,46	2.40	17 (36%)	63,67,67	2.71	25 (39%)
12	CYC	N6	101	-	46,46,46	2.29	18 (39%)	63,67,67	2.83	25 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	CYC	L3	202	-	46,46,46	2.29	18 (39%)	63,67,67	2.82	26 (41%)
12	CYC	J4	201	-	46,46,46	2.30	18 (39%)	63,67,67	2.83	25 (39%)
12	CYC	O4	202	-	46,46,46	2.20	13 (28%)	63,67,67	2.92	24 (38%)
12	CYC	Z8	301	-	46,46,46	2.30	17 (36%)	63,67,67	2.82	26 (41%)
12	CYC	C4	201	-	46,46,46	2.27	16 (34%)	63,67,67	2.80	28 (44%)
12	CYC	G7	201	-	46,46,46	2.30	15 (32%)	63,67,67	2.91	23 (36%)
12	CYC	J3	201	-	46,46,46	2.19	14 (30%)	63,67,67	2.87	25 (39%)
12	CYC	JA	201	-	46,46,46	2.21	14 (30%)	63,67,67	2.91	25 (39%)
12	CYC	G9	201	-	46,46,46	2.28	17 (36%)	63,67,67	2.79	28 (44%)
12	CYC	V9	201	-	46,46,46	2.29	18 (39%)	63,67,67	2.85	26 (41%)
12	CYC	I6	201	-	46,46,46	2.29	18 (39%)	63,67,67	2.79	29 (46%)
12	CYC	G5	201	-	46,46,46	2.31	14 (30%)	63,67,67	2.93	23 (36%)
12	CYC	O9	201	-	46,46,46	2.29	16 (34%)	63,67,67	2.79	29 (46%)
12	CYC	M5	201	-	46,46,46	2.30	14 (30%)	63,67,67	2.90	24 (38%)
12	CYC	T9	302	-	46,46,46	2.21	14 (30%)	63,67,67	2.89	25 (39%)
12	CYC	V1	201	-	46,46,46	2.29	18 (39%)	63,67,67	2.83	26 (41%)
12	CYC	A9	201	-	46,46,46	2.28	16 (34%)	63,67,67	2.78	30 (47%)
12	CYC	E4	201	-	46,46,46	2.28	17 (36%)	63,67,67	2.81	29 (46%)
12	CYC	H4	202	-	46,46,46	2.21	13 (28%)	63,67,67	2.89	25 (39%)
12	CYC	F9	303	-	46,46,46	2.19	12 (26%)	63,67,67	2.89	25 (39%)
12	CYC	I1	201	-	46,46,46	2.28	17 (36%)	63,67,67	2.80	28 (44%)
12	CYC	T8	201	-	46,46,46	2.28	16 (34%)	63,67,67	2.81	29 (46%)
12	CYC	G1	201	-	46,46,46	2.28	16 (34%)	63,67,67	2.79	29 (46%)
12	CYC	K2	201	-	46,46,46	2.28	15 (32%)	63,67,67	2.81	30 (47%)
12	CYC	R3	201	-	46,46,46	2.30	18 (39%)	63,67,67	2.82	27 (42%)
12	CYC	TA	302	-	46,46,46	2.21	14 (30%)	63,67,67	2.89	25 (39%)
12	CYC	J6	202	-	46,46,46	2.30	18 (39%)	63,67,67	2.83	25 (39%)
12	CYC	E1	201	-	46,46,46	2.28	17 (36%)	63,67,67	2.78	28 (44%)
12	CYC	F3	202	-	46,46,46	2.20	14 (30%)	63,67,67	2.87	25 (39%)
12	CYC	B7	201	-	46,46,46	2.40	17 (36%)	63,67,67	2.71	25 (39%)
12	CYC	H3	202	-	46,46,46	2.29	16 (34%)	63,67,67	2.82	25 (39%)
12	CYC	L6	201	-	46,46,46	2.29	17 (36%)	63,67,67	2.83	25 (39%)
12	CYC	U4	202	-	46,46,46	2.20	13 (28%)	63,67,67	2.88	25 (39%)
12	CYC	D5	201	-	46,46,46	2.41	16 (34%)	63,67,67	2.71	25 (39%)
12	CYC	B3	201	-	46,46,46	2.21	13 (28%)	63,67,67	2.91	25 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	CYC	G6	201	-	46,46,46	2.28	16 (34%)	63,67,67	2.79	28 (44%)
12	CYC	C8	201	-	46,46,46	2.27	16 (34%)	63,67,67	2.80	28 (44%)
12	CYC	f7	201	-	46,46,46	2.41	17 (36%)	63,67,67	2.71	26 (41%)
12	CYC	d5	201	-	46,46,46	2.40	17 (36%)	63,67,67	2.71	25 (39%)
12	CYC	a5	201	-	46,46,46	2.32	14 (30%)	63,67,67	2.93	24 (38%)
12	CYC	u7	201	-	46,46,46	2.32	14 (30%)	63,67,67	2.93	23 (36%)
12	CYC	L8	201	-	46,46,46	2.20	13 (28%)	63,67,67	2.90	24 (38%)
12	CYC	D8	202	-	46,46,46	2.31	18 (39%)	63,67,67	2.81	27 (42%)
12	CYC	a7	201	-	46,46,46	2.33	14 (30%)	63,67,67	2.95	23 (36%)
12	CYC	b5	201	-	46,46,46	2.39	16 (34%)	63,67,67	2.71	26 (41%)
12	CYC	P1	202	-	46,46,46	2.21	13 (28%)	63,67,67	2.91	25 (39%)
12	CYC	K5	201	-	46,46,46	2.32	14 (30%)	63,67,67	2.95	24 (38%)
12	CYC	D9	202	-	46,46,46	2.21	14 (30%)	63,67,67	2.87	25 (39%)
12	CYC	P1	201	-	46,46,46	2.29	17 (36%)	63,67,67	2.81	26 (41%)
12	CYC	H9	202	-	46,46,46	2.29	18 (39%)	63,67,67	2.81	25 (39%)
12	CYC	B2	201	-	46,46,46	2.21	14 (30%)	63,67,67	2.90	24 (38%)
12	CYC	D6	201	-	46,46,46	2.30	18 (39%)	63,67,67	2.81	25 (39%)
12	CYC	M7	201	-	46,46,46	2.31	14 (30%)	63,67,67	2.92	23 (36%)
12	CYC	H6	202	-	46,46,46	2.20	13 (28%)	63,67,67	2.88	25 (39%)
12	CYC	T3	301	-	46,46,46	2.29	18 (39%)	63,67,67	2.82	25 (39%)
12	CYC	Z	201	-	46,46,46	2.39	16 (34%)	63,67,67	2.71	26 (41%)
12	CYC	P4	201	-	46,46,46	2.27	17 (36%)	63,67,67	2.78	28 (44%)
12	CYC	BA	201	-	46,46,46	2.29	17 (36%)	63,67,67	2.82	26 (41%)
12	CYC	T1	301	-	46,46,46	2.29	18 (39%)	63,67,67	2.82	25 (39%)
12	CYC	j7	201	-	46,46,46	2.40	17 (36%)	63,67,67	2.72	26 (41%)
12	CYC	K9	201	-	46,46,46	2.28	17 (36%)	63,67,67	2.81	29 (46%)
12	CYC	S7	201	-	46,46,46	2.30	14 (30%)	63,67,67	2.89	23 (36%)
12	CYC	B5	201	-	46,46,46	2.42	17 (36%)	63,67,67	2.71	25 (39%)
12	CYC	g7	201	-	46,46,46	2.33	14 (30%)	63,67,67	2.96	24 (38%)
12	CYC	X4	201	-	46,46,46	2.28	15 (32%)	63,67,67	2.79	29 (46%)
12	CYC	J2	201	-	46,46,46	2.21	14 (30%)	63,67,67	2.90	25 (39%)
12	CYC	B1	202	-	46,46,46	2.30	18 (39%)	63,67,67	2.82	27 (42%)
12	CYC	R4	201	-	46,46,46	2.28	15 (32%)	63,67,67	2.82	29 (46%)
12	CYC	O5	201	-	46,46,46	2.31	14 (30%)	63,67,67	2.94	23 (36%)
12	CYC	M8	302	-	46,46,46	2.29	18 (39%)	63,67,67	2.84	25 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	CYC	XA	201	-	46,46,46	2.30	18 (39%)	63,67,67	2.85	25 (39%)
12	CYC	K4	201	-	46,46,46	2.29	16 (34%)	63,67,67	2.80	29 (46%)
12	CYC	D9	201	-	46,46,46	2.30	18 (39%)	63,67,67	2.82	26 (41%)
12	CYC	V9	202	-	46,46,46	2.19	14 (30%)	63,67,67	2.91	25 (39%)
12	CYC	a9	901	-	46,46,46	2.29	17 (36%)	63,67,67	2.82	25 (39%)
12	CYC	B4	202	-	46,46,46	2.29	16 (34%)	63,67,67	2.82	27 (42%)
12	CYC	Q3	201	-	46,46,46	2.27	17 (36%)	63,67,67	2.78	28 (44%)
12	CYC	D1	201	-	46,46,46	2.19	13 (28%)	63,67,67	2.89	25 (39%)
12	CYC	T4	201	-	46,46,46	2.28	16 (34%)	63,67,67	2.81	29 (46%)
12	CYC	F2	202	-	46,46,46	2.18	14 (30%)	63,67,67	2.87	24 (38%)
12	CYC	F2	201	-	46,46,46	2.30	18 (39%)	63,67,67	2.83	26 (41%)
12	CYC	X5	201	-	46,46,46	2.41	18 (39%)	63,67,67	2.72	26 (41%)
12	CYC	RA	202	-	46,46,46	2.20	13 (28%)	63,67,67	2.88	25 (39%)
12	CYC	S1	201	-	46,46,46	2.28	16 (34%)	63,67,67	2.79	29 (46%)
12	CYC	I2	201	-	46,46,46	2.29	17 (36%)	63,67,67	2.79	29 (46%)
12	CYC	j5	1201	-	46,46,46	2.59	18 (39%)	63,67,67	2.87	29 (46%)
12	CYC	O8	201	-	46,46,46	2.28	17 (36%)	63,67,67	2.81	27 (42%)
12	CYC	Y4	201	-	46,46,46	2.22	13 (28%)	63,67,67	2.92	25 (39%)
12	CYC	R8	201	-	46,46,46	2.28	15 (32%)	63,67,67	2.81	29 (46%)
12	CYC	V1	202	-	46,46,46	2.20	13 (28%)	63,67,67	2.89	25 (39%)
12	CYC	L9	202	-	46,46,46	2.31	18 (39%)	63,67,67	2.84	25 (39%)
12	CYC	J5	201	-	46,46,46	2.41	16 (34%)	63,67,67	2.72	25 (39%)
12	CYC	B8	201	-	46,46,46	2.20	13 (28%)	63,67,67	2.93	25 (39%)
12	CYC	C9	201	-	46,46,46	2.27	15 (32%)	63,67,67	2.80	30 (47%)
12	CYC	C5	201	-	46,46,46	2.32	14 (30%)	63,67,67	2.92	23 (36%)
12	CYC	GA	201	-	46,46,46	2.28	17 (36%)	63,67,67	2.79	29 (46%)
12	CYC	W8	202	-	46,46,46	2.22	14 (30%)	63,67,67	2.91	25 (39%)
12	CYC	H1	201	-	46,46,46	2.28	16 (34%)	63,67,67	2.82	26 (41%)
12	CYC	J8	202	-	46,46,46	2.23	13 (28%)	63,67,67	2.91	25 (39%)
12	CYC	C7	201	-	46,46,46	2.32	15 (32%)	63,67,67	2.93	24 (38%)
12	CYC	J8	201	-	46,46,46	2.30	18 (39%)	63,67,67	2.83	25 (39%)
12	CYC	S5	201	-	46,46,46	2.31	14 (30%)	63,67,67	2.90	24 (38%)
12	CYC	TA	301	-	46,46,46	2.28	18 (39%)	63,67,67	2.81	25 (39%)
12	CYC	V8	201	-	46,46,46	2.27	16 (34%)	63,67,67	2.78	28 (44%)
12	CYC	B3	202	-	46,46,46	2.30	18 (39%)	63,67,67	2.82	27 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	CYC	Z4	301	-	46,46,46	2.30	18 (39%)	63,67,67	2.82	26 (41%)
12	CYC	Y5	201	-	46,46,46	2.32	14 (30%)	63,67,67	2.95	23 (36%)
12	CYC	DA	202	-	46,46,46	2.21	14 (30%)	63,67,67	2.87	25 (39%)
12	CYC	N8	201	-	46,46,46	2.29	15 (32%)	63,67,67	2.80	28 (44%)
12	CYC	R9	202	-	46,46,46	2.20	13 (28%)	63,67,67	2.88	25 (39%)
12	CYC	o7	201	-	46,46,46	2.33	14 (30%)	63,67,67	2.93	23 (36%)
12	CYC	F7	201	-	46,46,46	2.41	17 (36%)	63,67,67	2.72	26 (41%)
12	CYC	E8	201	-	46,46,46	2.28	17 (36%)	63,67,67	2.81	29 (46%)
12	CYC	J3	202	-	46,46,46	2.30	18 (39%)	63,67,67	2.83	26 (41%)
12	CYC	Z3	201	-	46,46,46	2.30	17 (36%)	63,67,67	2.84	26 (41%)
12	CYC	F4	201	-	46,46,46	2.20	14 (30%)	63,67,67	2.89	25 (39%)
12	CYC	HA	202	-	46,46,46	2.29	18 (39%)	63,67,67	2.81	25 (39%)
12	CYC	O1	201	-	46,46,46	2.31	17 (36%)	63,67,67	2.81	29 (46%)
12	CYC	V7	201	-	46,46,46	2.40	16 (34%)	63,67,67	2.71	25 (39%)
12	CYC	I3	201	-	46,46,46	2.28	17 (36%)	63,67,67	2.80	28 (44%)
12	CYC	Y1	201	-	46,46,46	2.27	16 (34%)	63,67,67	2.79	29 (46%)
12	CYC	Z3	202	-	46,46,46	2.22	14 (30%)	63,67,67	2.89	25 (39%)
12	CYC	F4	202	-	46,46,46	2.29	19 (41%)	63,67,67	2.84	26 (41%)
12	CYC	A8	201	-	46,46,46	2.29	17 (36%)	63,67,67	2.79	29 (46%)
12	CYC	H3	201	-	46,46,46	2.20	14 (30%)	63,67,67	2.89	25 (39%)
12	CYC	X3	202	-	46,46,46	2.20	13 (28%)	63,67,67	2.88	25 (39%)
12	CYC	j5	1202	-	46,46,46	2.40	16 (34%)	63,67,67	2.69	25 (39%)
12	CYC	T3	302	-	46,46,46	2.20	14 (30%)	63,67,67	2.90	25 (39%)
12	CYC	A1	201	-	46,46,46	2.29	16 (34%)	63,67,67	2.81	29 (46%)
12	CYC	L1	201	-	46,46,46	2.20	13 (28%)	63,67,67	2.90	25 (39%)
12	CYC	m7	201	-	46,46,46	2.31	14 (30%)	63,67,67	2.92	23 (36%)
12	CYC	W7	201	-	46,46,46	2.32	14 (30%)	63,67,67	2.94	24 (38%)
12	CYC	ZA	201	-	46,46,46	2.20	14 (30%)	63,67,67	2.88	25 (39%)
12	CYC	C3	201	-	46,46,46	2.27	16 (34%)	63,67,67	2.79	29 (46%)
12	CYC	P9	202	-	46,46,46	2.20	13 (28%)	63,67,67	2.92	25 (39%)
12	CYC	O8	202	-	46,46,46	2.20	13 (28%)	63,67,67	2.92	24 (38%)
12	CYC	E7	201	-	46,46,46	2.33	14 (30%)	63,67,67	2.94	23 (36%)
12	CYC	AA	201	-	46,46,46	2.28	16 (34%)	63,67,67	2.78	30 (47%)
12	CYC	L5	201	-	46,46,46	2.41	17 (36%)	63,67,67	2.72	26 (41%)
12	CYC	q7	201	-	46,46,46	2.30	14 (30%)	63,67,67	2.92	23 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	CYC	VA	202	-	46,46,46	2.20	14 (30%)	63,67,67	2.91	25 (39%)
12	CYC	R5	201	-	46,46,46	2.40	18 (39%)	63,67,67	2.71	26 (41%)
12	CYC	XA	202	-	46,46,46	2.21	12 (26%)	63,67,67	2.90	25 (39%)
12	CYC	K6	201	-	46,46,46	2.28	15 (32%)	63,67,67	2.81	30 (47%)
12	CYC	T5	201	-	46,46,46	2.41	17 (36%)	63,67,67	2.72	25 (39%)
12	CYC	X1	202	-	46,46,46	2.19	13 (28%)	63,67,67	2.88	25 (39%)
12	CYC	D7	201	-	46,46,46	2.41	16 (34%)	63,67,67	2.70	25 (39%)
12	CYC	K7	201	-	46,46,46	2.33	14 (30%)	63,67,67	2.94	24 (38%)
12	CYC	A3	201	-	46,46,46	2.29	16 (34%)	63,67,67	2.81	29 (46%)
12	CYC	G8	201	-	46,46,46	2.28	17 (36%)	63,67,67	2.80	29 (46%)
12	CYC	H8	201	-	46,46,46	2.29	17 (36%)	63,67,67	2.83	26 (41%)
12	CYC	U4	201	-	46,46,46	2.30	18 (39%)	63,67,67	2.84	27 (42%)
12	CYC	IA	201	-	46,46,46	2.26	15 (32%)	63,67,67	2.79	29 (46%)
12	CYC	JA	202	-	46,46,46	2.29	17 (36%)	63,67,67	2.82	25 (39%)
12	CYC	i7	201	-	46,46,46	2.32	15 (32%)	63,67,67	2.96	24 (38%)
12	CYC	H2	202	-	46,46,46	2.19	13 (28%)	63,67,67	2.88	25 (39%)
12	CYC	F8	202	-	46,46,46	2.29	19 (41%)	63,67,67	2.84	26 (41%)
12	CYC	W1	201	-	46,46,46	2.27	17 (36%)	63,67,67	2.78	29 (46%)
12	CYC	F8	201	-	46,46,46	2.20	14 (30%)	63,67,67	2.89	25 (39%)
12	CYC	N2	101	-	46,46,46	2.29	18 (39%)	63,67,67	2.84	25 (39%)
12	CYC	I8	201	-	46,46,46	2.28	16 (34%)	63,67,67	2.79	29 (46%)
12	CYC	D4	202	-	46,46,46	2.31	18 (39%)	63,67,67	2.81	27 (42%)
12	CYC	A4	201	-	46,46,46	2.29	17 (36%)	63,67,67	2.79	29 (46%)
12	CYC	c5	201	-	46,46,46	2.32	15 (32%)	63,67,67	2.94	23 (36%)
12	CYC	LA	201	-	46,46,46	2.20	13 (28%)	63,67,67	2.89	25 (39%)
12	CYC	SA	201	-	46,46,46	2.27	17 (36%)	63,67,67	2.80	29 (46%)
12	CYC	H5	201	-	46,46,46	2.42	17 (36%)	63,67,67	2.71	25 (39%)
12	CYC	W8	201	-	46,46,46	2.29	17 (36%)	63,67,67	2.81	26 (41%)
12	CYC	B6	201	-	46,46,46	2.21	14 (30%)	63,67,67	2.90	24 (38%)
12	CYC	s7	201	-	46,46,46	2.30	14 (30%)	63,67,67	2.91	23 (36%)
12	CYC	X1	201	-	46,46,46	2.30	17 (36%)	63,67,67	2.83	26 (41%)
12	CYC	L3	201	-	46,46,46	2.20	13 (28%)	63,67,67	2.90	25 (39%)
12	CYC	DA	201	-	46,46,46	2.30	18 (39%)	63,67,67	2.83	27 (42%)
12	CYC	f5	201	-	46,46,46	2.40	17 (36%)	63,67,67	2.71	26 (41%)
12	CYC	D3	202	-	46,46,46	2.31	18 (39%)	63,67,67	2.82	27 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	CYC	X8	201	-	46,46,46	2.28	15 (32%)	63,67,67	2.80	29 (46%)
12	CYC	K1	201	-	46,46,46	2.27	15 (32%)	63,67,67	2.80	29 (46%)
12	CYC	B9	201	-	46,46,46	2.29	17 (36%)	63,67,67	2.82	26 (41%)
12	CYC	F5	201	-	46,46,46	2.41	16 (34%)	63,67,67	2.72	26 (41%)
12	CYC	E6	201	-	46,46,46	2.28	16 (34%)	63,67,67	2.81	30 (47%)
12	CYC	c7	201	-	46,46,46	2.32	14 (30%)	63,67,67	2.94	24 (38%)
12	CYC	U5	201	-	46,46,46	2.32	14 (30%)	63,67,67	2.95	24 (38%)
12	CYC	R7	201	-	46,46,46	2.40	17 (36%)	63,67,67	2.72	26 (41%)
12	CYC	Q5	201	-	46,46,46	2.33	14 (30%)	63,67,67	2.93	23 (36%)
12	CYC	P9	201	-	46,46,46	2.29	17 (36%)	63,67,67	2.85	26 (41%)
12	CYC	F9	301	-	46,46,46	2.28	18 (39%)	63,67,67	2.82	27 (42%)
12	CYC	R3	202	-	46,46,46	2.19	13 (28%)	63,67,67	2.89	25 (39%)
12	CYC	T9	301	-	46,46,46	2.28	18 (39%)	63,67,67	2.81	25 (39%)
12	CYC	W4	202	-	46,46,46	2.22	14 (30%)	63,67,67	2.91	25 (39%)
12	CYC	W4	201	-	46,46,46	2.29	17 (36%)	63,67,67	2.81	26 (41%)
12	CYC	H4	201	-	46,46,46	2.29	17 (36%)	63,67,67	2.83	26 (41%)
12	CYC	F1	202	-	46,46,46	2.20	14 (30%)	63,67,67	2.87	25 (39%)
12	CYC	F6	201	-	46,46,46	2.30	18 (39%)	63,67,67	2.83	27 (42%)
12	CYC	X7	201	-	46,46,46	2.40	17 (36%)	63,67,67	2.71	26 (41%)
12	CYC	F1	201	-	46,46,46	2.29	17 (36%)	63,67,67	2.82	26 (41%)
12	CYC	L4	201	-	46,46,46	2.20	13 (28%)	63,67,67	2.89	24 (38%)
12	CYC	U8	202	-	46,46,46	2.20	13 (28%)	63,67,67	2.88	25 (39%)
12	CYC	Z9	201	-	46,46,46	2.20	13 (28%)	63,67,67	2.88	25 (39%)
12	CYC	YA	201	-	46,46,46	2.28	16 (34%)	63,67,67	2.81	29 (46%)
12	CYC	PA	202	-	46,46,46	2.20	13 (28%)	63,67,67	2.91	25 (39%)
12	CYC	J9	201	-	46,46,46	2.21	14 (30%)	63,67,67	2.91	25 (39%)
12	CYC	U9	201	-	46,46,46	2.29	17 (36%)	63,67,67	2.79	29 (46%)
12	CYC	D4	201	-	46,46,46	2.20	14 (30%)	63,67,67	2.90	25 (39%)
12	CYC	RA	201	-	46,46,46	2.31	18 (39%)	63,67,67	2.81	25 (39%)
12	CYC	K3	201	-	46,46,46	2.28	15 (32%)	63,67,67	2.80	29 (46%)
12	CYC	L2	202	-	46,46,46	2.19	14 (30%)	63,67,67	2.88	25 (39%)
12	CYC	U1	201	-	46,46,46	2.28	17 (36%)	63,67,67	2.78	29 (46%)
12	CYC	V5	201	-	46,46,46	2.40	16 (34%)	63,67,67	2.71	26 (41%)
12	CYC	aA	902	-	46,46,46	2.29	18 (39%)	63,67,67	2.82	26 (41%)
12	CYC	aA	901	-	46,46,46	2.30	18 (39%)	63,67,67	2.84	27 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	CYC	S4	201	-	46,46,46	2.20	13 (28%)	63,67,67	2.89	25 (39%)
12	CYC	D3	201	-	46,46,46	2.20	13 (28%)	63,67,67	2.89	25 (39%)
12	CYC	E9	201	-	46,46,46	2.29	17 (36%)	63,67,67	2.81	29 (46%)
12	CYC	Z9	202	-	46,46,46	2.30	17 (36%)	63,67,67	2.85	26 (41%)
12	CYC	PA	201	-	46,46,46	2.30	17 (36%)	63,67,67	2.85	26 (41%)
12	CYC	F3	201	-	46,46,46	2.29	17 (36%)	63,67,67	2.82	26 (41%)
12	CYC	BA	202	-	46,46,46	2.22	14 (30%)	63,67,67	2.92	25 (39%)
12	CYC	KA	201	-	46,46,46	2.28	17 (36%)	63,67,67	2.81	29 (46%)
12	CYC	P3	202	-	46,46,46	2.21	13 (28%)	63,67,67	2.91	25 (39%)
12	CYC	C1	201	-	46,46,46	2.27	16 (34%)	63,67,67	2.79	29 (46%)
12	CYC	P7	201	-	46,46,46	2.40	16 (34%)	63,67,67	2.71	26 (41%)
12	CYC	I7	201	-	46,46,46	2.32	15 (32%)	63,67,67	2.93	24 (38%)
12	CYC	X9	201	-	46,46,46	2.29	18 (39%)	63,67,67	2.85	25 (39%)
12	CYC	P3	201	-	46,46,46	2.29	17 (36%)	63,67,67	2.81	26 (41%)
12	CYC	H8	202	-	46,46,46	2.21	13 (28%)	63,67,67	2.89	25 (39%)
12	CYC	D2	202	-	46,46,46	2.19	13 (28%)	63,67,67	2.90	24 (38%)
12	CYC	N7	201	-	46,46,46	2.40	16 (34%)	63,67,67	2.69	25 (39%)
12	CYC	Z1	202	-	46,46,46	2.30	17 (36%)	63,67,67	2.84	26 (41%)
12	CYC	K8	201	-	46,46,46	2.29	16 (34%)	63,67,67	2.81	29 (46%)
12	CYC	J2	202	-	46,46,46	2.30	18 (39%)	63,67,67	2.84	25 (39%)
12	CYC	Q9	201	-	46,46,46	2.27	17 (36%)	63,67,67	2.79	28 (44%)
12	CYC	k5	1203	-	46,46,46	2.40	16 (34%)	63,67,67	2.70	26 (41%)
12	CYC	LA	202	-	46,46,46	2.31	18 (39%)	63,67,67	2.85	26 (41%)
12	CYC	W5	201	-	46,46,46	2.33	14 (30%)	63,67,67	2.93	23 (36%)
12	CYC	V3	202	-	46,46,46	2.21	13 (28%)	63,67,67	2.89	25 (39%)
12	CYC	E5	201	-	46,46,46	2.33	14 (30%)	63,67,67	2.94	24 (38%)
12	CYC	J4	202	-	46,46,46	2.22	13 (28%)	63,67,67	2.91	25 (39%)
12	CYC	V3	201	-	46,46,46	2.29	18 (39%)	63,67,67	2.83	25 (39%)
12	CYC	B8	202	-	46,46,46	2.30	17 (36%)	63,67,67	2.81	26 (41%)
12	CYC	HA	201	-	46,46,46	2.20	13 (28%)	63,67,67	2.88	25 (39%)
12	CYC	P5	201	-	46,46,46	2.40	16 (34%)	63,67,67	2.70	26 (41%)
12	CYC	D8	201	-	46,46,46	2.20	14 (30%)	63,67,67	2.90	25 (39%)
12	CYC	Z5	201	-	46,46,46	2.40	17 (36%)	63,67,67	2.70	25 (39%)
12	CYC	UA	201	-	46,46,46	2.29	17 (36%)	63,67,67	2.79	29 (46%)
12	CYC	FA	301	-	46,46,46	2.28	18 (39%)	63,67,67	2.82	27 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	CYC	E3	201	-	46,46,46	2.28	17 (36%)	63,67,67	2.78	28 (44%)
12	CYC	X3	201	-	46,46,46	2.30	17 (36%)	63,67,67	2.83	26 (41%)
12	CYC	U3	201	-	46,46,46	2.28	17 (36%)	63,67,67	2.78	28 (44%)
12	CYC	Q7	201	-	46,46,46	2.33	14 (30%)	63,67,67	2.95	24 (38%)
12	CYC	Q8	201	-	46,46,46	2.21	13 (28%)	63,67,67	2.90	25 (39%)
12	CYC	R1	202	-	46,46,46	2.19	13 (28%)	63,67,67	2.89	25 (39%)
12	CYC	EA	201	-	46,46,46	2.29	17 (36%)	63,67,67	2.81	29 (46%)
12	CYC	J7	201	-	46,46,46	2.41	16 (34%)	63,67,67	2.71	26 (41%)
12	CYC	T1	302	-	46,46,46	2.20	14 (30%)	63,67,67	2.90	25 (39%)
12	CYC	C6	201	-	46,46,46	2.29	16 (34%)	63,67,67	2.80	27 (42%)
12	CYC	F6	202	-	46,46,46	2.18	14 (30%)	63,67,67	2.87	25 (39%)
12	CYC	S8	201	-	46,46,46	2.20	13 (28%)	63,67,67	2.89	25 (39%)
12	CYC	L4	202	-	46,46,46	2.28	17 (36%)	63,67,67	2.82	25 (39%)
12	CYC	A6	201	-	46,46,46	2.29	16 (34%)	63,67,67	2.80	29 (46%)
12	CYC	A	201	-	46,46,46	2.39	16 (34%)	63,67,67	2.71	26 (41%)
12	CYC	F9	302	-	46,46,46	2.20	13 (28%)	63,67,67	2.89	25 (39%)
12	CYC	B1	201	-	46,46,46	2.21	13 (28%)	63,67,67	2.91	25 (39%)
12	CYC	I4	201	-	46,46,46	2.28	16 (34%)	63,67,67	2.79	29 (46%)
12	CYC	S4	202	-	46,46,46	2.30	18 (39%)	63,67,67	2.85	25 (39%)
12	CYC	E2	201	-	46,46,46	2.28	17 (36%)	63,67,67	2.80	30 (47%)
12	CYC	T7	201	-	46,46,46	2.41	17 (36%)	63,67,67	2.71	26 (41%)
12	CYC	H7	201	-	46,46,46	2.41	17 (36%)	63,67,67	2.72	26 (41%)
12	CYC	B4	201	-	46,46,46	2.21	13 (28%)	63,67,67	2.93	25 (39%)
12	CYC	b7	201	-	46,46,46	2.41	18 (39%)	63,67,67	2.70	26 (41%)
12	CYC	V4	201	-	46,46,46	2.27	16 (34%)	63,67,67	2.78	28 (44%)
12	CYC	M8	301	-	46,46,46	2.28	18 (39%)	63,67,67	2.80	26 (41%)
12	CYC	O4	201	-	46,46,46	2.28	17 (36%)	63,67,67	2.81	27 (42%)
12	CYC	OA	201	-	46,46,46	2.29	16 (34%)	63,67,67	2.79	29 (46%)
12	CYC	CA	201	-	46,46,46	2.27	15 (32%)	63,67,67	2.80	30 (47%)
12	CYC	C2	201	-	46,46,46	2.28	16 (34%)	63,67,67	2.80	27 (42%)
12	CYC	R9	201	-	46,46,46	2.31	18 (39%)	63,67,67	2.81	25 (39%)
12	CYC	A7	201	-	46,46,46	2.31	15 (32%)	63,67,67	2.92	23 (36%)
12	CYC	Y7	201	-	46,46,46	2.31	14 (30%)	63,67,67	2.90	23 (36%)
12	CYC	d7	201	-	46,46,46	2.41	17 (36%)	63,67,67	2.72	26 (41%)
12	CYC	P8	201	-	46,46,46	2.28	17 (36%)	63,67,67	2.78	28 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	CYC	L2	201	-	46,46,46	2.29	18 (39%)	63,67,67	2.83	25 (39%)
12	CYC	G4	201	-	46,46,46	2.28	17 (36%)	63,67,67	2.80	29 (46%)
12	CYC	D2	201	-	46,46,46	2.30	18 (39%)	63,67,67	2.82	25 (39%)
12	CYC	L9	201	-	46,46,46	2.20	13 (28%)	63,67,67	2.90	25 (39%)
12	CYC	H1	202	-	46,46,46	2.21	14 (30%)	63,67,67	2.89	25 (39%)
12	CYC	W9	201	-	46,46,46	2.28	16 (34%)	63,67,67	2.77	29 (46%)
12	CYC	A2	201	-	46,46,46	2.29	16 (34%)	63,67,67	2.80	29 (46%)
12	CYC	k5	1201	-	46,46,46	2.59	18 (39%)	63,67,67	2.85	29 (46%)
12	CYC	M4	301	-	46,46,46	2.29	18 (39%)	63,67,67	2.81	26 (41%)
12	CYC	L7	201	-	46,46,46	2.41	17 (36%)	63,67,67	2.72	26 (41%)
12	CYC	N4	201	-	46,46,46	2.29	15 (32%)	63,67,67	2.80	28 (44%)
12	CYC	v7	201	-	46,46,46	2.39	16 (34%)	63,67,67	2.71	26 (41%)
12	CYC	B9	202	-	46,46,46	2.22	14 (30%)	63,67,67	2.92	25 (39%)
12	CYC	R1	201	-	46,46,46	2.30	18 (39%)	63,67,67	2.82	27 (42%)
12	CYC	I5	201	-	46,46,46	2.32	15 (32%)	63,67,67	2.92	23 (36%)
12	CYC	Y3	201	-	46,46,46	2.27	16 (34%)	63,67,67	2.79	29 (46%)
12	CYC	O3	201	-	46,46,46	2.31	17 (36%)	63,67,67	2.81	29 (46%)
12	CYC	I9	201	-	46,46,46	2.26	15 (32%)	63,67,67	2.79	29 (46%)
12	CYC	S3	201	-	46,46,46	2.28	16 (34%)	63,67,67	2.79	29 (46%)
12	CYC	e7	201	-	46,46,46	2.31	14 (30%)	63,67,67	2.90	23 (36%)

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
12	CYC	W3	201	-	-	10/26/74/74	0/4/4/4
12	CYC	Y8	201	-	-	10/26/74/74	0/4/4/4
12	CYC	Q1	201	-	-	10/26/74/74	0/4/4/4
12	CYC	A5	201	-	-	7/26/74/74	0/4/4/4
12	CYC	U8	201	-	-	6/26/74/74	0/4/4/4
12	CYC	X9	202	-	-	10/26/74/74	0/4/4/4
12	CYC	J6	201	-	-	10/26/74/74	0/4/4/4
12	CYC	D1	202	-	-	6/26/74/74	0/4/4/4
12	CYC	S9	201	-	-	10/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CYC	Y9	201	-	-	10/26/74/74	0/4/4/4
12	CYC	U7	201	-	-	7/26/74/74	0/4/4/4
12	CYC	Q4	201	-	-	10/26/74/74	0/4/4/4
12	CYC	O7	201	-	-	7/26/74/74	0/4/4/4
12	CYC	ZA	202	-	-	6/26/74/74	0/4/4/4
12	CYC	QA	201	-	-	10/26/74/74	0/4/4/4
12	CYC	H2	201	-	-	6/26/74/74	0/4/4/4
12	CYC	h7	201	-	-	10/26/74/74	0/4/4/4
12	CYC	Z1	201	-	-	10/26/74/74	0/4/4/4
12	CYC	WA	201	-	-	10/26/74/74	0/4/4/4
12	CYC	H6	201	-	-	6/26/74/74	0/4/4/4
12	CYC	p7	201	-	-	10/26/74/74	0/4/4/4
12	CYC	e5	201	-	-	7/26/74/74	0/4/4/4
12	CYC	L6	202	-	-	10/26/74/74	0/4/4/4
12	CYC	k5	1202	-	-	10/26/74/74	0/4/4/4
12	CYC	G3	201	-	-	10/26/74/74	0/4/4/4
12	CYC	k7	201	-	-	7/26/74/74	0/4/4/4
12	CYC	H9	201	-	-	10/26/74/74	0/4/4/4
12	CYC	r7	201	-	-	10/26/74/74	0/4/4/4
12	CYC	VA	201	-	-	6/26/74/74	0/4/4/4
12	CYC	k5	1204	-	-	10/26/74/74	0/4/4/4
12	CYC	J1	201	-	-	10/26/74/74	0/4/4/4
12	CYC	J9	202	-	-	6/26/74/74	0/4/4/4
12	CYC	G2	201	-	-	10/26/74/74	0/4/4/4
12	CYC	D6	202	-	-	10/26/74/74	0/4/4/4
12	CYC	N5	201	-	-	10/26/74/74	0/4/4/4
12	CYC	N6	101	-	-	6/26/74/74	0/4/4/4
12	CYC	L3	202	-	-	6/26/74/74	0/4/4/4
12	CYC	J4	201	-	-	6/26/74/74	0/4/4/4
12	CYC	O4	202	-	-	10/26/74/74	0/4/4/4
12	CYC	Z8	301	-	-	6/26/74/74	0/4/4/4
12	CYC	C4	201	-	-	10/26/74/74	0/4/4/4
12	CYC	G7	201	-	-	7/26/74/74	0/4/4/4
12	CYC	J3	201	-	-	10/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CYC	JA	201	-	-	10/26/74/74	0/4/4/4
12	CYC	G9	201	-	-	10/26/74/74	0/4/4/4
12	CYC	V9	201	-	-	6/26/74/74	0/4/4/4
12	CYC	I6	201	-	-	10/26/74/74	0/4/4/4
12	CYC	G5	201	-	-	7/26/74/74	0/4/4/4
12	CYC	O9	201	-	-	10/26/74/74	0/4/4/4
12	CYC	M5	201	-	-	7/26/74/74	0/4/4/4
12	CYC	T9	302	-	-	10/26/74/74	0/4/4/4
12	CYC	V1	201	-	-	6/26/74/74	0/4/4/4
12	CYC	A9	201	-	-	10/26/74/74	0/4/4/4
12	CYC	E4	201	-	-	10/26/74/74	0/4/4/4
12	CYC	H4	202	-	-	10/26/74/74	0/4/4/4
12	CYC	F9	303	-	-	10/26/74/74	0/4/4/4
12	CYC	I1	201	-	-	10/26/74/74	0/4/4/4
12	CYC	T8	201	-	-	10/26/74/74	0/4/4/4
12	CYC	G1	201	-	-	10/26/74/74	0/4/4/4
12	CYC	K2	201	-	-	10/26/74/74	0/4/4/4
12	CYC	R3	201	-	-	6/26/74/74	0/4/4/4
12	CYC	TA	302	-	-	10/26/74/74	0/4/4/4
12	CYC	J6	202	-	-	6/26/74/74	0/4/4/4
12	CYC	E1	201	-	-	10/26/74/74	0/4/4/4
12	CYC	F3	202	-	-	10/26/74/74	0/4/4/4
12	CYC	B7	201	-	-	10/26/74/74	0/4/4/4
12	CYC	H3	202	-	-	6/26/74/74	0/4/4/4
12	CYC	L6	201	-	-	6/26/74/74	0/4/4/4
12	CYC	U4	202	-	-	10/26/74/74	0/4/4/4
12	CYC	D5	201	-	-	10/26/74/74	0/4/4/4
12	CYC	B3	201	-	-	10/26/74/74	0/4/4/4
12	CYC	G6	201	-	-	10/26/74/74	0/4/4/4
12	CYC	C8	201	-	-	10/26/74/74	0/4/4/4
12	CYC	f7	201	-	-	10/26/74/74	0/4/4/4
12	CYC	d5	201	-	-	10/26/74/74	0/4/4/4
12	CYC	a5	201	-	-	7/26/74/74	0/4/4/4
12	CYC	u7	201	-	-	7/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CYC	L8	201	-	-	10/26/74/74	0/4/4/4
12	CYC	D8	202	-	-	6/26/74/74	0/4/4/4
12	CYC	a7	201	-	-	7/26/74/74	0/4/4/4
12	CYC	b5	201	-	-	10/26/74/74	0/4/4/4
12	CYC	P1	202	-	-	10/26/74/74	0/4/4/4
12	CYC	K5	201	-	-	7/26/74/74	0/4/4/4
12	CYC	D9	202	-	-	10/26/74/74	0/4/4/4
12	CYC	P1	201	-	-	6/26/74/74	0/4/4/4
12	CYC	H9	202	-	-	6/26/74/74	0/4/4/4
12	CYC	B2	201	-	-	10/26/74/74	0/4/4/4
12	CYC	D6	201	-	-	6/26/74/74	0/4/4/4
12	CYC	M7	201	-	-	7/26/74/74	0/4/4/4
12	CYC	H6	202	-	-	10/26/74/74	0/4/4/4
12	CYC	T3	301	-	-	6/26/74/74	0/4/4/4
12	CYC	Z	201	-	-	10/26/74/74	0/4/4/4
12	CYC	P4	201	-	-	10/26/74/74	0/4/4/4
12	CYC	BA	201	-	-	6/26/74/74	0/4/4/4
12	CYC	T1	301	-	-	6/26/74/74	0/4/4/4
12	CYC	j7	201	-	-	10/26/74/74	0/4/4/4
12	CYC	K9	201	-	-	10/26/74/74	0/4/4/4
12	CYC	S7	201	-	-	7/26/74/74	0/4/4/4
12	CYC	B5	201	-	-	10/26/74/74	0/4/4/4
12	CYC	g7	201	-	-	7/26/74/74	0/4/4/4
12	CYC	X4	201	-	-	10/26/74/74	0/4/4/4
12	CYC	J2	201	-	-	10/26/74/74	0/4/4/4
12	CYC	B1	202	-	-	6/26/74/74	0/4/4/4
12	CYC	R4	201	-	-	10/26/74/74	0/4/4/4
12	CYC	O5	201	-	-	7/26/74/74	0/4/4/4
12	CYC	M8	302	-	-	6/26/74/74	0/4/4/4
12	CYC	XA	201	-	-	6/26/74/74	0/4/4/4
12	CYC	K4	201	-	-	10/26/74/74	0/4/4/4
12	CYC	D9	201	-	-	6/26/74/74	0/4/4/4
12	CYC	V9	202	-	-	10/26/74/74	0/4/4/4
12	CYC	a9	901	-	-	6/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CYC	B4	202	-	-	6/26/74/74	0/4/4/4
12	CYC	Q3	201	-	-	10/26/74/74	0/4/4/4
12	CYC	D1	201	-	-	10/26/74/74	0/4/4/4
12	CYC	T4	201	-	-	10/26/74/74	0/4/4/4
12	CYC	F2	202	-	-	10/26/74/74	0/4/4/4
12	CYC	F2	201	-	-	6/26/74/74	0/4/4/4
12	CYC	X5	201	-	-	10/26/74/74	0/4/4/4
12	CYC	RA	202	-	-	10/26/74/74	0/4/4/4
12	CYC	S1	201	-	-	10/26/74/74	0/4/4/4
12	CYC	I2	201	-	-	10/26/74/74	0/4/4/4
12	CYC	j5	1201	-	-	7/26/74/74	0/4/4/4
12	CYC	O8	201	-	-	6/26/74/74	0/4/4/4
12	CYC	Y4	201	-	-	10/26/74/74	0/4/4/4
12	CYC	R8	201	-	-	10/26/74/74	0/4/4/4
12	CYC	V1	202	-	-	10/26/74/74	0/4/4/4
12	CYC	L9	202	-	-	6/26/74/74	0/4/4/4
12	CYC	J5	201	-	-	10/26/74/74	0/4/4/4
12	CYC	B8	201	-	-	10/26/74/74	0/4/4/4
12	CYC	C9	201	-	-	10/26/74/74	0/4/4/4
12	CYC	C5	201	-	-	7/26/74/74	0/4/4/4
12	CYC	GA	201	-	-	10/26/74/74	0/4/4/4
12	CYC	W8	202	-	-	10/26/74/74	0/4/4/4
12	CYC	H1	201	-	-	6/26/74/74	0/4/4/4
12	CYC	J8	202	-	-	10/26/74/74	0/4/4/4
12	CYC	C7	201	-	-	7/26/74/74	0/4/4/4
12	CYC	J8	201	-	-	6/26/74/74	0/4/4/4
12	CYC	S5	201	-	-	7/26/74/74	0/4/4/4
12	CYC	TA	301	-	-	6/26/74/74	0/4/4/4
12	CYC	V8	201	-	-	10/26/74/74	0/4/4/4
12	CYC	B3	202	-	-	6/26/74/74	0/4/4/4
12	CYC	Z4	301	-	-	6/26/74/74	0/4/4/4
12	CYC	Y5	201	-	-	7/26/74/74	0/4/4/4
12	CYC	DA	202	-	-	10/26/74/74	0/4/4/4
12	CYC	N8	201	-	-	10/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CYC	R9	202	-	-	10/26/74/74	0/4/4/4
12	CYC	o7	201	-	-	7/26/74/74	0/4/4/4
12	CYC	F7	201	-	-	10/26/74/74	0/4/4/4
12	CYC	E8	201	-	-	10/26/74/74	0/4/4/4
12	CYC	J3	202	-	-	6/26/74/74	0/4/4/4
12	CYC	Z3	201	-	-	6/26/74/74	0/4/4/4
12	CYC	F4	201	-	-	10/26/74/74	0/4/4/4
12	CYC	HA	202	-	-	6/26/74/74	0/4/4/4
12	CYC	O1	201	-	-	10/26/74/74	0/4/4/4
12	CYC	V7	201	-	-	10/26/74/74	0/4/4/4
12	CYC	I3	201	-	-	10/26/74/74	0/4/4/4
12	CYC	Y1	201	-	-	10/26/74/74	0/4/4/4
12	CYC	Z3	202	-	-	10/26/74/74	0/4/4/4
12	CYC	F4	202	-	-	6/26/74/74	0/4/4/4
12	CYC	A8	201	-	-	10/26/74/74	0/4/4/4
12	CYC	H3	201	-	-	10/26/74/74	0/4/4/4
12	CYC	X3	202	-	-	10/26/74/74	0/4/4/4
12	CYC	j5	1202	-	-	10/26/74/74	0/4/4/4
12	CYC	T3	302	-	-	10/26/74/74	0/4/4/4
12	CYC	A1	201	-	-	10/26/74/74	0/4/4/4
12	CYC	L1	201	-	-	10/26/74/74	0/4/4/4
12	CYC	m7	201	-	-	7/26/74/74	0/4/4/4
12	CYC	W7	201	-	-	7/26/74/74	0/4/4/4
12	CYC	ZA	201	-	-	10/26/74/74	0/4/4/4
12	CYC	C3	201	-	-	10/26/74/74	0/4/4/4
12	CYC	P9	202	-	-	10/26/74/74	0/4/4/4
12	CYC	O8	202	-	-	10/26/74/74	0/4/4/4
12	CYC	E7	201	-	-	7/26/74/74	0/4/4/4
12	CYC	AA	201	-	-	10/26/74/74	0/4/4/4
12	CYC	L5	201	-	-	10/26/74/74	0/4/4/4
12	CYC	q7	201	-	-	7/26/74/74	0/4/4/4
12	CYC	VA	202	-	-	10/26/74/74	0/4/4/4
12	CYC	R5	201	-	-	10/26/74/74	0/4/4/4
12	CYC	XA	202	-	-	10/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CYC	K6	201	-	-	10/26/74/74	0/4/4/4
12	CYC	T5	201	-	-	10/26/74/74	0/4/4/4
12	CYC	X1	202	-	-	10/26/74/74	0/4/4/4
12	CYC	D7	201	-	-	10/26/74/74	0/4/4/4
12	CYC	K7	201	-	-	7/26/74/74	0/4/4/4
12	CYC	A3	201	-	-	10/26/74/74	0/4/4/4
12	CYC	G8	201	-	-	10/26/74/74	0/4/4/4
12	CYC	H8	201	-	-	6/26/74/74	0/4/4/4
12	CYC	U4	201	-	-	6/26/74/74	0/4/4/4
12	CYC	IA	201	-	-	10/26/74/74	0/4/4/4
12	CYC	JA	202	-	-	6/26/74/74	0/4/4/4
12	CYC	i7	201	-	-	7/26/74/74	0/4/4/4
12	CYC	H2	202	-	-	10/26/74/74	0/4/4/4
12	CYC	F8	202	-	-	6/26/74/74	0/4/4/4
12	CYC	W1	201	-	-	10/26/74/74	0/4/4/4
12	CYC	F8	201	-	-	10/26/74/74	0/4/4/4
12	CYC	N2	101	-	-	6/26/74/74	0/4/4/4
12	CYC	I8	201	-	-	10/26/74/74	0/4/4/4
12	CYC	D4	202	-	-	6/26/74/74	0/4/4/4
12	CYC	A4	201	-	-	10/26/74/74	0/4/4/4
12	CYC	c5	201	-	-	7/26/74/74	0/4/4/4
12	CYC	LA	201	-	-	10/26/74/74	0/4/4/4
12	CYC	SA	201	-	-	10/26/74/74	0/4/4/4
12	CYC	H5	201	-	-	10/26/74/74	0/4/4/4
12	CYC	W8	201	-	-	6/26/74/74	0/4/4/4
12	CYC	B6	201	-	-	10/26/74/74	0/4/4/4
12	CYC	s7	201	-	-	7/26/74/74	0/4/4/4
12	CYC	X1	201	-	-	6/26/74/74	0/4/4/4
12	CYC	L3	201	-	-	10/26/74/74	0/4/4/4
12	CYC	DA	201	-	-	6/26/74/74	0/4/4/4
12	CYC	f5	201	-	-	10/26/74/74	0/4/4/4
12	CYC	D3	202	-	-	6/26/74/74	0/4/4/4
12	CYC	X8	201	-	-	10/26/74/74	0/4/4/4
12	CYC	K1	201	-	-	10/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CYC	B9	201	-	-	6/26/74/74	0/4/4/4
12	CYC	F5	201	-	-	10/26/74/74	0/4/4/4
12	CYC	E6	201	-	-	10/26/74/74	0/4/4/4
12	CYC	c7	201	-	-	7/26/74/74	0/4/4/4
12	CYC	U5	201	-	-	7/26/74/74	0/4/4/4
12	CYC	R7	201	-	-	10/26/74/74	0/4/4/4
12	CYC	Q5	201	-	-	7/26/74/74	0/4/4/4
12	CYC	P9	201	-	-	6/26/74/74	0/4/4/4
12	CYC	F9	301	-	-	6/26/74/74	0/4/4/4
12	CYC	R3	202	-	-	10/26/74/74	0/4/4/4
12	CYC	T9	301	-	-	6/26/74/74	0/4/4/4
12	CYC	W4	202	-	-	10/26/74/74	0/4/4/4
12	CYC	W4	201	-	-	6/26/74/74	0/4/4/4
12	CYC	H4	201	-	-	6/26/74/74	0/4/4/4
12	CYC	F1	202	-	-	10/26/74/74	0/4/4/4
12	CYC	F6	201	-	-	6/26/74/74	0/4/4/4
12	CYC	X7	201	-	-	10/26/74/74	0/4/4/4
12	CYC	F1	201	-	-	6/26/74/74	0/4/4/4
12	CYC	L4	201	-	-	10/26/74/74	0/4/4/4
12	CYC	U8	202	-	-	10/26/74/74	0/4/4/4
12	CYC	Z9	201	-	-	10/26/74/74	0/4/4/4
12	CYC	YA	201	-	-	10/26/74/74	0/4/4/4
12	CYC	PA	202	-	-	10/26/74/74	0/4/4/4
12	CYC	J9	201	-	-	10/26/74/74	0/4/4/4
12	CYC	U9	201	-	-	10/26/74/74	0/4/4/4
12	CYC	D4	201	-	-	10/26/74/74	0/4/4/4
12	CYC	RA	201	-	-	6/26/74/74	0/4/4/4
12	CYC	K3	201	-	-	10/26/74/74	0/4/4/4
12	CYC	L2	202	-	-	10/26/74/74	0/4/4/4
12	CYC	U1	201	-	-	10/26/74/74	0/4/4/4
12	CYC	V5	201	-	-	10/26/74/74	0/4/4/4
12	CYC	aA	902	-	-	6/26/74/74	0/4/4/4
12	CYC	aA	901	-	-	6/26/74/74	0/4/4/4
12	CYC	S4	201	-	-	10/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CYC	D3	201	-	-	10/26/74/74	0/4/4/4
12	CYC	E9	201	-	-	10/26/74/74	0/4/4/4
12	CYC	Z9	202	-	-	6/26/74/74	0/4/4/4
12	CYC	PA	201	-	-	6/26/74/74	0/4/4/4
12	CYC	F3	201	-	-	6/26/74/74	0/4/4/4
12	CYC	BA	202	-	-	10/26/74/74	0/4/4/4
12	CYC	KA	201	-	-	10/26/74/74	0/4/4/4
12	CYC	P3	202	-	-	10/26/74/74	0/4/4/4
12	CYC	C1	201	-	-	10/26/74/74	0/4/4/4
12	CYC	P7	201	-	-	10/26/74/74	0/4/4/4
12	CYC	I7	201	-	-	7/26/74/74	0/4/4/4
12	CYC	X9	201	-	-	6/26/74/74	0/4/4/4
12	CYC	P3	201	-	-	6/26/74/74	0/4/4/4
12	CYC	H8	202	-	-	10/26/74/74	0/4/4/4
12	CYC	D2	202	-	-	10/26/74/74	0/4/4/4
12	CYC	N7	201	-	-	10/26/74/74	0/4/4/4
12	CYC	Z1	202	-	-	6/26/74/74	0/4/4/4
12	CYC	K8	201	-	-	10/26/74/74	0/4/4/4
12	CYC	J2	202	-	-	6/26/74/74	0/4/4/4
12	CYC	Q9	201	-	-	10/26/74/74	0/4/4/4
12	CYC	k5	1203	-	-	10/26/74/74	0/4/4/4
12	CYC	LA	202	-	-	6/26/74/74	0/4/4/4
12	CYC	W5	201	-	-	7/26/74/74	0/4/4/4
12	CYC	V3	202	-	-	10/26/74/74	0/4/4/4
12	CYC	E5	201	-	-	7/26/74/74	0/4/4/4
12	CYC	J4	202	-	-	10/26/74/74	0/4/4/4
12	CYC	V3	201	-	-	6/26/74/74	0/4/4/4
12	CYC	B8	202	-	-	6/26/74/74	0/4/4/4
12	CYC	HA	201	-	-	10/26/74/74	0/4/4/4
12	CYC	P5	201	-	-	10/26/74/74	0/4/4/4
12	CYC	D8	201	-	-	10/26/74/74	0/4/4/4
12	CYC	Z5	201	-	-	10/26/74/74	0/4/4/4
12	CYC	UA	201	-	-	10/26/74/74	0/4/4/4
12	CYC	FA	301	-	-	6/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CYC	E3	201	-	-	10/26/74/74	0/4/4/4
12	CYC	X3	201	-	-	6/26/74/74	0/4/4/4
12	CYC	U3	201	-	-	10/26/74/74	0/4/4/4
12	CYC	Q7	201	-	-	7/26/74/74	0/4/4/4
12	CYC	Q8	201	-	-	10/26/74/74	0/4/4/4
12	CYC	R1	202	-	-	10/26/74/74	0/4/4/4
12	CYC	EA	201	-	-	10/26/74/74	0/4/4/4
12	CYC	J7	201	-	-	10/26/74/74	0/4/4/4
12	CYC	T1	302	-	-	10/26/74/74	0/4/4/4
12	CYC	C6	201	-	-	10/26/74/74	0/4/4/4
12	CYC	F6	202	-	-	10/26/74/74	0/4/4/4
12	CYC	S8	201	-	-	10/26/74/74	0/4/4/4
12	CYC	L4	202	-	-	6/26/74/74	0/4/4/4
12	CYC	A6	201	-	-	10/26/74/74	0/4/4/4
12	CYC	A	201	-	-	10/26/74/74	0/4/4/4
12	CYC	F9	302	-	-	10/26/74/74	0/4/4/4
12	CYC	B1	201	-	-	10/26/74/74	0/4/4/4
12	CYC	I4	201	-	-	10/26/74/74	0/4/4/4
12	CYC	S4	202	-	-	6/26/74/74	0/4/4/4
12	CYC	E2	201	-	-	10/26/74/74	0/4/4/4
12	CYC	T7	201	-	-	10/26/74/74	0/4/4/4
12	CYC	H7	201	-	-	10/26/74/74	0/4/4/4
12	CYC	B4	201	-	-	10/26/74/74	0/4/4/4
12	CYC	b7	201	-	-	10/26/74/74	0/4/4/4
12	CYC	V4	201	-	-	10/26/74/74	0/4/4/4
12	CYC	M8	301	-	-	6/26/74/74	0/4/4/4
12	CYC	O4	201	-	-	6/26/74/74	0/4/4/4
12	CYC	OA	201	-	-	10/26/74/74	0/4/4/4
12	CYC	CA	201	-	-	10/26/74/74	0/4/4/4
12	CYC	C2	201	-	-	10/26/74/74	0/4/4/4
12	CYC	R9	201	-	-	6/26/74/74	0/4/4/4
12	CYC	A7	201	-	-	7/26/74/74	0/4/4/4
12	CYC	Y7	201	-	-	7/26/74/74	0/4/4/4
12	CYC	d7	201	-	-	10/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CYC	P8	201	-	-	10/26/74/74	0/4/4/4
12	CYC	L2	201	-	-	6/26/74/74	0/4/4/4
12	CYC	G4	201	-	-	10/26/74/74	0/4/4/4
12	CYC	D2	201	-	-	6/26/74/74	0/4/4/4
12	CYC	L9	201	-	-	10/26/74/74	0/4/4/4
12	CYC	H1	202	-	-	10/26/74/74	0/4/4/4
12	CYC	W9	201	-	-	10/26/74/74	0/4/4/4
12	CYC	A2	201	-	-	10/26/74/74	0/4/4/4
12	CYC	k5	1201	-	-	7/26/74/74	0/4/4/4
12	CYC	M4	301	-	-	6/26/74/74	0/4/4/4
12	CYC	L7	201	-	-	10/26/74/74	0/4/4/4
12	CYC	N4	201	-	-	10/26/74/74	0/4/4/4
12	CYC	v7	201	-	-	10/26/74/74	0/4/4/4
12	CYC	B9	202	-	-	10/26/74/74	0/4/4/4
12	CYC	R1	201	-	-	6/26/74/74	0/4/4/4
12	CYC	I5	201	-	-	7/26/74/74	0/4/4/4
12	CYC	Y3	201	-	-	10/26/74/74	0/4/4/4
12	CYC	O3	201	-	-	10/26/74/74	0/4/4/4
12	CYC	I9	201	-	-	10/26/74/74	0/4/4/4
12	CYC	S3	201	-	-	10/26/74/74	0/4/4/4
12	CYC	e7	201	-	-	7/26/74/74	0/4/4/4

The worst 5 of 5274 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	k5	1201	CYC	CHA-C1A	6.08	1.50	1.38
12	j5	1201	CYC	CHA-C1A	6.07	1.50	1.38
12	F7	201	CYC	C3B-C2B	6.05	1.49	1.36
12	p7	201	CYC	C3B-C2B	6.05	1.49	1.36
12	F5	201	CYC	C3B-C2B	6.03	1.49	1.36

The worst 5 of 8757 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	i7	201	CYC	C3B-C4B-NB	12.38	116.64	106.77
12	g7	201	CYC	C3B-C4B-NB	12.33	116.60	106.77
12	K5	201	CYC	C3B-C4B-NB	12.32	116.59	106.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	Q7	201	CYC	C3B-C4B-NB	12.31	116.59	106.77
12	a7	201	CYC	C3B-C4B-NB	12.28	116.56	106.77

There are no chirality outliers.

5 of 2898 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	A	201	CYC	NA-C4A-CHB-C1B
12	Z	201	CYC	NA-C4A-CHB-C1B
12	AA	201	CYC	NA-C4A-CHB-C1B
12	AA	201	CYC	C3A-C4A-CHB-C1B
12	AA	201	CYC	C2B-C3B-CAB-CBB

There are no ring outliers.

336 monomers are involved in 5213 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	W3	201	CYC	8	0
12	Y8	201	CYC	10	0
12	Q1	201	CYC	8	0
12	A5	201	CYC	69	0
12	U8	201	CYC	13	0
12	X9	202	CYC	8	0
12	J6	201	CYC	7	0
12	D1	202	CYC	9	0
12	S9	201	CYC	8	0
12	Y9	201	CYC	8	0
12	U7	201	CYC	3	0
12	Q4	201	CYC	6	0
12	O7	201	CYC	3	0
12	ZA	202	CYC	12	0
12	QA	201	CYC	49	0
12	H2	201	CYC	19	0
12	h7	201	CYC	15	0
12	Z1	201	CYC	9	0
12	WA	201	CYC	8	0
12	H6	201	CYC	19	0
12	p7	201	CYC	16	0
12	e5	201	CYC	8	0
12	L6	202	CYC	10	0
12	k5	1202	CYC	15	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	G3	201	CYC	8	0
12	k7	201	CYC	3	0
12	H9	201	CYC	6	0
12	r7	201	CYC	17	0
12	VA	201	CYC	41	0
12	k5	1204	CYC	40	0
12	J1	201	CYC	7	0
12	J9	202	CYC	39	0
12	G2	201	CYC	11	0
12	D6	202	CYC	6	0
12	N5	201	CYC	14	0
12	N6	101	CYC	13	0
12	L3	202	CYC	21	0
12	J4	201	CYC	12	0
12	O4	202	CYC	10	0
12	Z8	301	CYC	163	0
12	C4	201	CYC	8	0
12	G7	201	CYC	3	0
12	J3	201	CYC	6	0
12	JA	201	CYC	8	0
12	G9	201	CYC	8	0
12	V9	201	CYC	42	0
12	I6	201	CYC	8	0
12	G5	201	CYC	70	0
12	O9	201	CYC	8	0
12	M5	201	CYC	4	0
12	T9	302	CYC	6	0
12	V1	201	CYC	7	0
12	A9	201	CYC	8	0
12	E4	201	CYC	8	0
12	H4	202	CYC	6	0
12	F9	303	CYC	18	0
12	I1	201	CYC	8	0
12	T8	201	CYC	8	0
12	G1	201	CYC	8	0
12	K2	201	CYC	8	0
12	R3	201	CYC	25	0
12	TA	302	CYC	8	0
12	J6	202	CYC	10	0
12	E1	201	CYC	8	0
12	F3	202	CYC	7	0
12	B7	201	CYC	12	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	H3	202	CYC	14	0
12	L6	201	CYC	8	0
12	U4	202	CYC	6	0
12	D5	201	CYC	11	0
12	B3	201	CYC	8	0
12	G6	201	CYC	8	0
12	C8	201	CYC	8	0
12	f7	201	CYC	16	0
12	d5	201	CYC	16	0
12	a5	201	CYC	8	0
12	u7	201	CYC	19	0
12	L8	201	CYC	10	0
12	D8	202	CYC	21	0
12	a7	201	CYC	3	0
12	b5	201	CYC	7	0
12	P1	202	CYC	7	0
12	K5	201	CYC	28	0
12	D9	202	CYC	7	0
12	P1	201	CYC	18	0
12	H9	202	CYC	82	0
12	B2	201	CYC	7	0
12	D6	201	CYC	8	0
12	M7	201	CYC	3	0
12	H6	202	CYC	6	0
12	T3	301	CYC	23	0
12	Z	201	CYC	8	0
12	P4	201	CYC	8	0
12	BA	201	CYC	18	0
12	T1	301	CYC	23	0
12	j7	201	CYC	15	0
12	K9	201	CYC	8	0
12	S7	201	CYC	4	0
12	B5	201	CYC	26	0
12	g7	201	CYC	3	0
12	X4	201	CYC	8	0
12	J2	201	CYC	8	0
12	B1	202	CYC	68	0
12	R4	201	CYC	8	0
12	O5	201	CYC	4	0
12	M8	302	CYC	80	0
12	XA	201	CYC	7	0
12	K4	201	CYC	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	D9	201	CYC	14	0
12	V9	202	CYC	6	0
12	a9	901	CYC	106	0
12	B4	202	CYC	116	0
12	Q3	201	CYC	8	0
12	D1	201	CYC	6	0
12	T4	201	CYC	8	0
12	F2	202	CYC	5	0
12	F2	201	CYC	54	0
12	X5	201	CYC	16	0
12	RA	202	CYC	8	0
12	S1	201	CYC	8	0
12	I2	201	CYC	8	0
12	j5	1201	CYC	26	0
12	O8	201	CYC	18	0
12	Y4	201	CYC	8	0
12	R8	201	CYC	8	0
12	V1	202	CYC	6	0
12	L9	202	CYC	21	0
12	J5	201	CYC	12	0
12	B8	201	CYC	8	0
12	C9	201	CYC	8	0
12	C5	201	CYC	7	0
12	GA	201	CYC	8	0
12	W8	202	CYC	8	0
12	H1	201	CYC	56	0
12	J8	202	CYC	8	0
12	C7	201	CYC	4	0
12	J8	201	CYC	12	0
12	S5	201	CYC	3	0
12	TA	301	CYC	45	0
12	V8	201	CYC	8	0
12	B3	202	CYC	67	0
12	Z4	301	CYC	104	0
12	Y5	201	CYC	3	0
12	DA	202	CYC	6	0
12	N8	201	CYC	12	0
12	R9	202	CYC	6	0
12	o7	201	CYC	18	0
12	F7	201	CYC	17	0
12	E8	201	CYC	8	0
12	J3	202	CYC	45	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	Z3	201	CYC	26	0
12	F4	201	CYC	8	0
12	HA	202	CYC	82	0
12	O1	201	CYC	11	0
12	V7	201	CYC	10	0
12	I3	201	CYC	8	0
12	Y1	201	CYC	8	0
12	Z3	202	CYC	12	0
12	F4	202	CYC	9	0
12	A8	201	CYC	8	0
12	H3	201	CYC	6	0
12	X3	202	CYC	8	0
12	j5	1202	CYC	31	0
12	T3	302	CYC	5	0
12	A1	201	CYC	8	0
12	L1	201	CYC	9	0
12	m7	201	CYC	4	0
12	W7	201	CYC	14	0
12	ZA	201	CYC	9	0
12	C3	201	CYC	8	0
12	P9	202	CYC	9	0
12	O8	202	CYC	9	0
12	E7	201	CYC	13	0
12	AA	201	CYC	8	0
12	L5	201	CYC	14	0
12	q7	201	CYC	3	0
12	VA	202	CYC	19	0
12	R5	201	CYC	15	0
12	XA	202	CYC	6	0
12	K6	201	CYC	8	0
12	T5	201	CYC	19	0
12	X1	202	CYC	5	0
12	D7	201	CYC	32	0
12	K7	201	CYC	14	0
12	A3	201	CYC	8	0
12	G8	201	CYC	8	0
12	H8	201	CYC	28	0
12	U4	201	CYC	13	0
12	IA	201	CYC	8	0
12	JA	202	CYC	39	0
12	i7	201	CYC	13	0
12	H2	202	CYC	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	F8	202	CYC	8	0
12	W1	201	CYC	8	0
12	F8	201	CYC	6	0
12	N2	101	CYC	13	0
12	I8	201	CYC	8	0
12	D4	202	CYC	9	0
12	A4	201	CYC	8	0
12	c5	201	CYC	3	0
12	LA	201	CYC	12	0
12	SA	201	CYC	8	0
12	H5	201	CYC	21	0
12	W8	201	CYC	7	0
12	B6	201	CYC	7	0
12	s7	201	CYC	3	0
12	X1	201	CYC	18	0
12	L3	201	CYC	9	0
12	DA	201	CYC	14	0
12	f5	201	CYC	6	0
12	D3	202	CYC	9	0
12	X8	201	CYC	8	0
12	K1	201	CYC	8	0
12	B9	201	CYC	20	0
12	F5	201	CYC	17	0
12	E6	201	CYC	8	0
12	c7	201	CYC	10	0
12	U5	201	CYC	3	0
12	R7	201	CYC	9	0
12	Q5	201	CYC	15	0
12	P9	201	CYC	11	0
12	F9	301	CYC	20	0
12	R3	202	CYC	7	0
12	T9	301	CYC	46	0
12	W4	202	CYC	7	0
12	W4	201	CYC	7	0
12	H4	201	CYC	29	0
12	F1	202	CYC	6	0
12	F6	201	CYC	63	0
12	X7	201	CYC	8	0
12	F1	201	CYC	25	0
12	L4	201	CYC	9	0
12	U8	202	CYC	8	0
12	Z9	201	CYC	9	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	YA	201	CYC	8	0
12	PA	202	CYC	7	0
12	J9	201	CYC	9	0
12	U9	201	CYC	8	0
12	D4	201	CYC	6	0
12	RA	201	CYC	19	0
12	K3	201	CYC	8	0
12	L2	202	CYC	10	0
12	U1	201	CYC	8	0
12	V5	201	CYC	18	0
12	aA	902	CYC	20	0
12	aA	901	CYC	52	0
12	S4	201	CYC	6	0
12	D3	201	CYC	6	0
12	E9	201	CYC	7	0
12	Z9	202	CYC	11	0
12	PA	201	CYC	12	0
12	F3	201	CYC	24	0
12	BA	202	CYC	8	0
12	KA	201	CYC	8	0
12	P3	202	CYC	8	0
12	C1	201	CYC	8	0
12	P7	201	CYC	13	0
12	I7	201	CYC	3	0
12	X9	201	CYC	7	0
12	P3	201	CYC	17	0
12	H8	202	CYC	6	0
12	D2	202	CYC	7	0
12	N7	201	CYC	10	0
12	Z1	202	CYC	28	0
12	K8	201	CYC	8	0
12	J2	202	CYC	10	0
12	Q9	201	CYC	8	0
12	k5	1203	CYC	34	0
12	LA	202	CYC	21	0
12	W5	201	CYC	14	0
12	V3	202	CYC	6	0
12	E5	201	CYC	27	0
12	J4	202	CYC	6	0
12	V3	201	CYC	7	0
12	B8	202	CYC	84	0
12	HA	201	CYC	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	P5	201	CYC	18	0
12	D8	201	CYC	6	0
12	Z5	201	CYC	15	0
12	UA	201	CYC	9	0
12	FA	301	CYC	19	0
12	E3	201	CYC	8	0
12	X3	201	CYC	18	0
12	U3	201	CYC	8	0
12	Q7	201	CYC	14	0
12	Q8	201	CYC	6	0
12	R1	202	CYC	7	0
12	EA	201	CYC	7	0
12	J7	201	CYC	23	0
12	T1	302	CYC	5	0
12	C6	201	CYC	8	0
12	F6	202	CYC	6	0
12	S8	201	CYC	6	0
12	L4	202	CYC	21	0
12	A6	201	CYC	8	0
12	A	201	CYC	9	0
12	F9	302	CYC	35	0
12	B1	201	CYC	7	0
12	I4	201	CYC	8	0
12	S4	202	CYC	33	0
12	E2	201	CYC	7	0
12	T7	201	CYC	16	0
12	H7	201	CYC	11	0
12	B4	201	CYC	8	0
12	b7	201	CYC	18	0
12	V4	201	CYC	8	0
12	M8	301	CYC	101	0
12	O4	201	CYC	22	0
12	OA	201	CYC	8	0
12	CA	201	CYC	8	0
12	C2	201	CYC	8	0
12	R9	201	CYC	19	0
12	A7	201	CYC	3	0
12	Y7	201	CYC	3	0
12	d7	201	CYC	19	0
12	P8	201	CYC	8	0
12	L2	201	CYC	8	0
12	G4	201	CYC	8	0

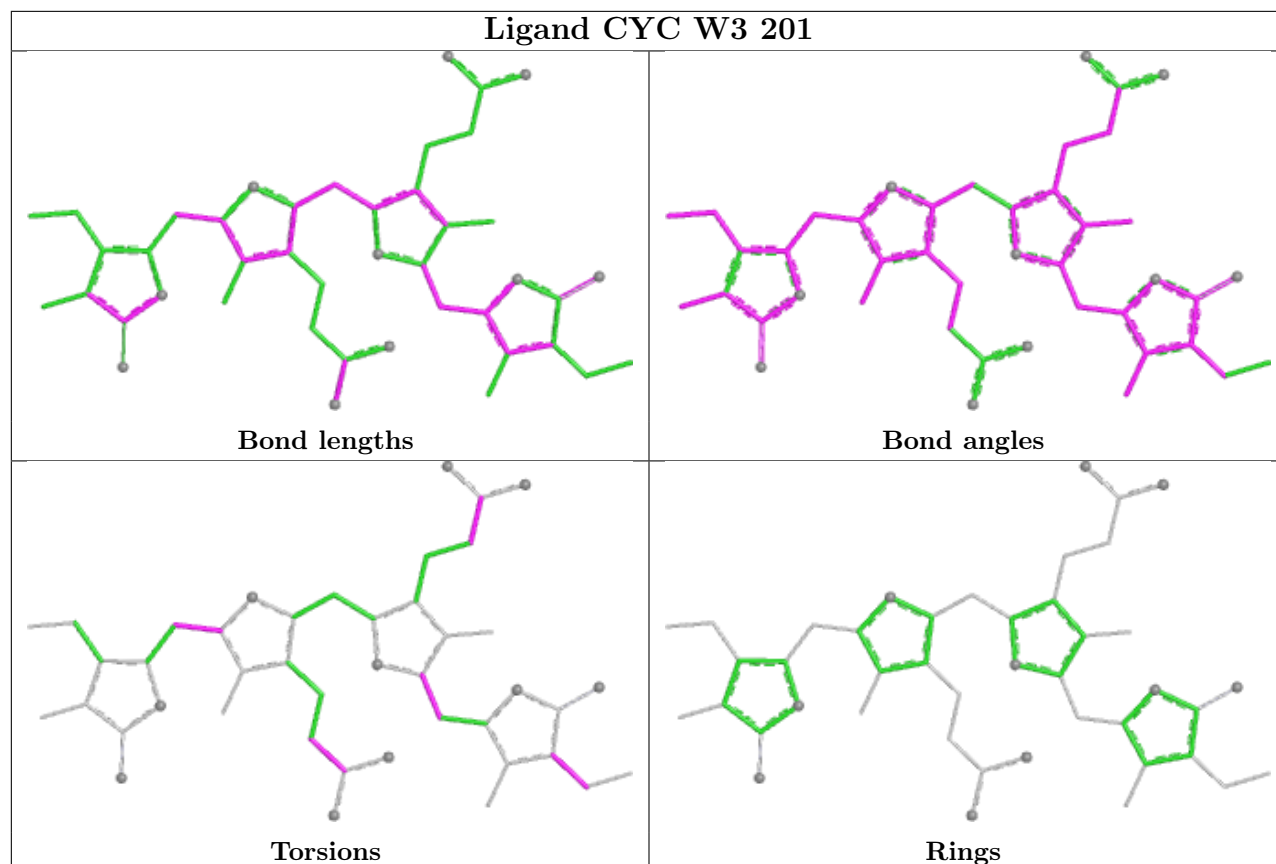
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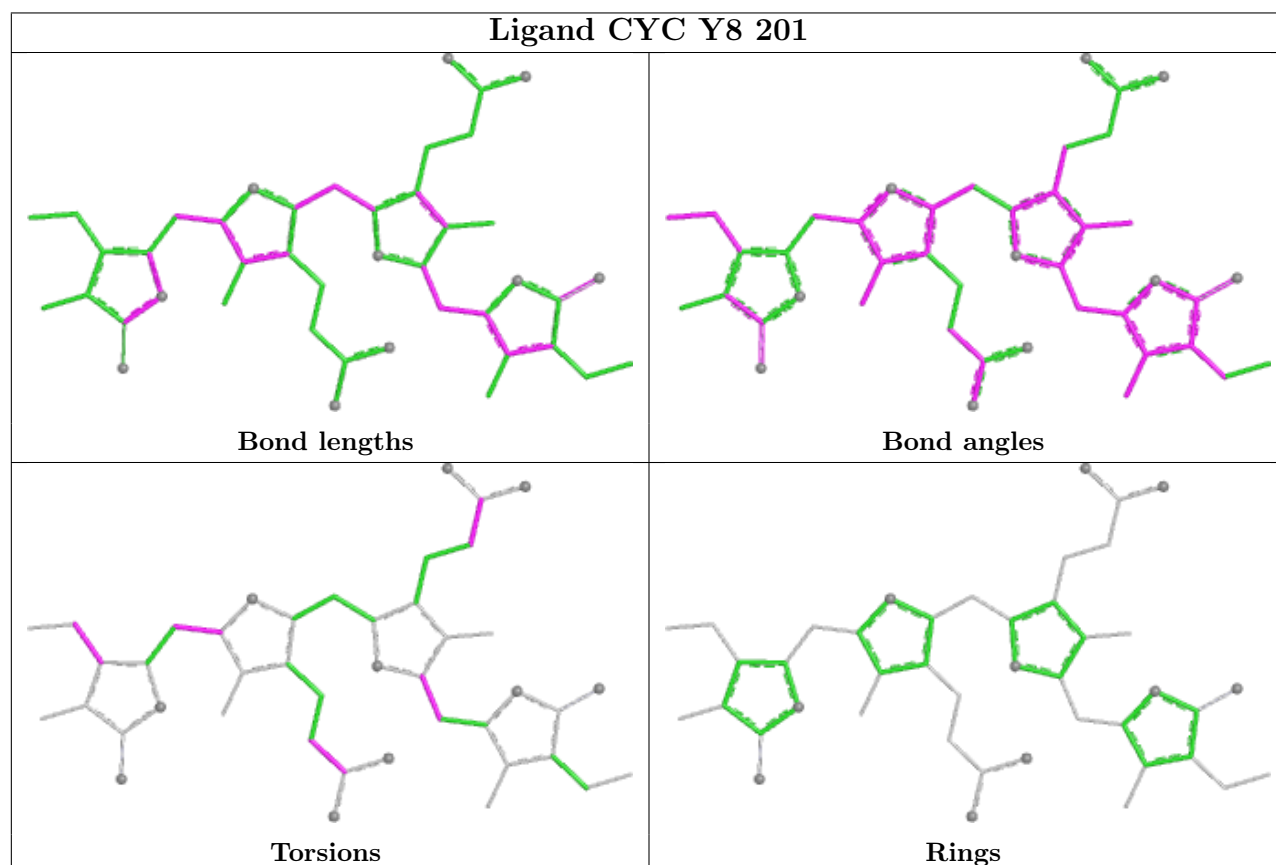
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	D2	201	CYC	8	0
12	L9	201	CYC	14	0
12	H1	202	CYC	6	0
12	W9	201	CYC	8	0
12	A2	201	CYC	8	0
12	k5	1201	CYC	30	0
12	M4	301	CYC	76	0
12	L7	201	CYC	13	0
12	N4	201	CYC	8	0
12	v7	201	CYC	22	0
12	B9	202	CYC	7	0
12	R1	201	CYC	26	0
12	I5	201	CYC	8	0
12	Y3	201	CYC	8	0
12	O3	201	CYC	8	0
12	I9	201	CYC	8	0
12	S3	201	CYC	9	0
12	e7	201	CYC	3	0

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

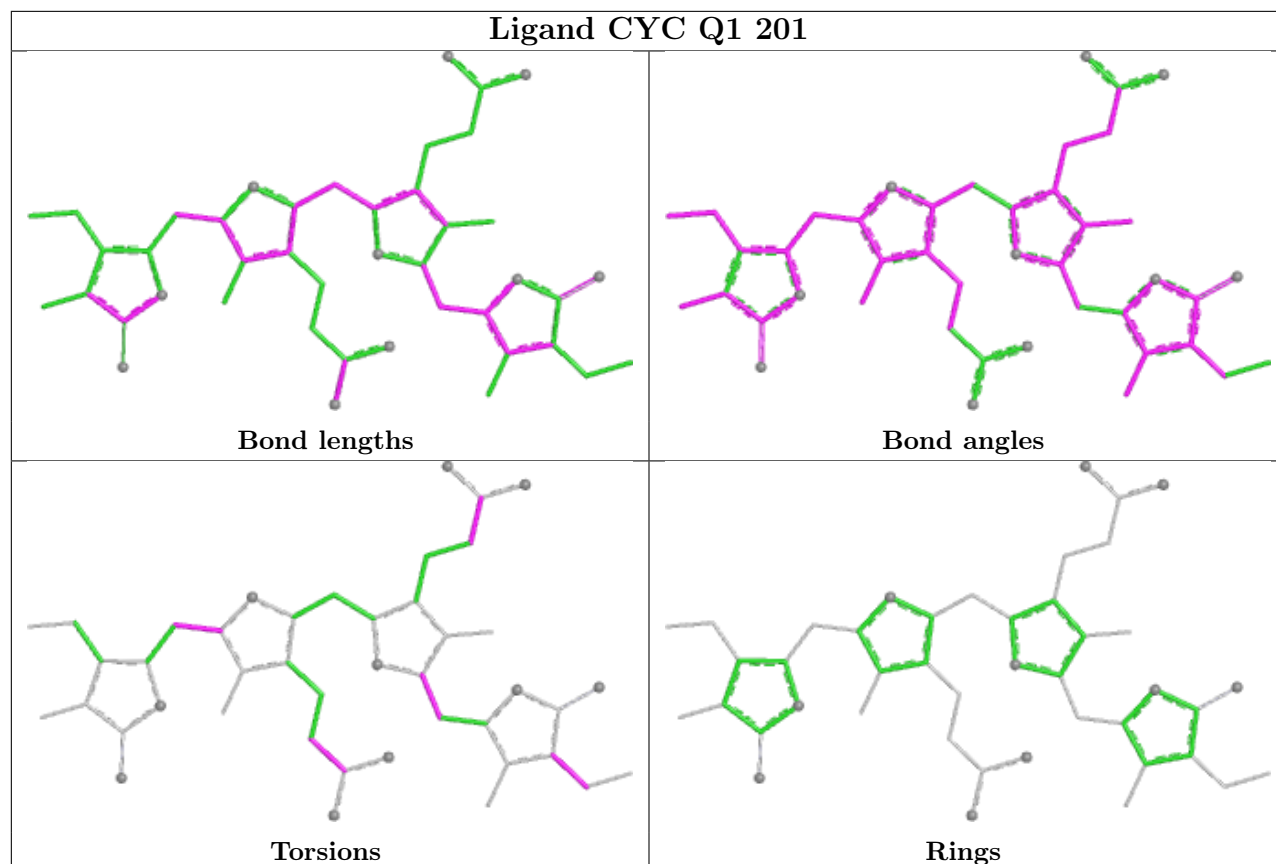
Ligand CYC W3 201



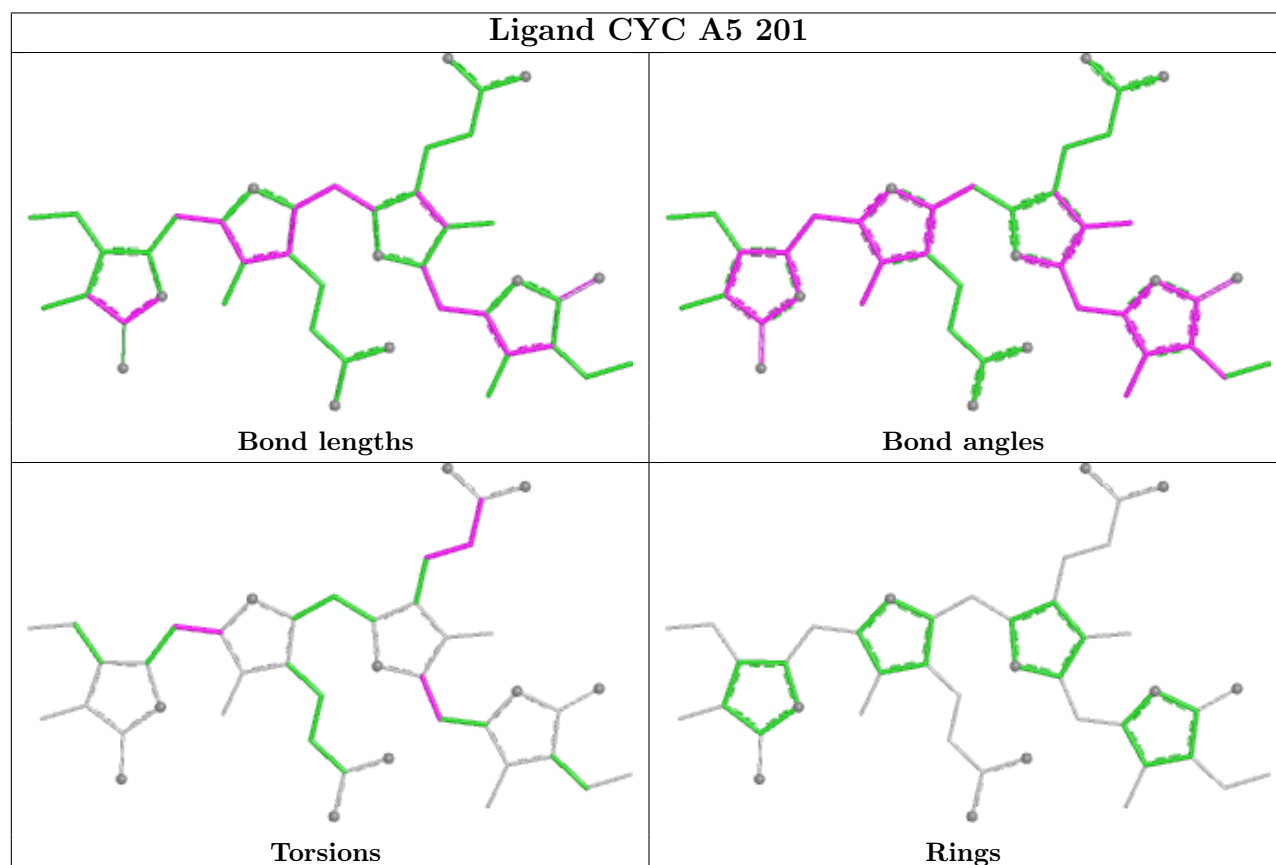
Ligand CYC Y8 201



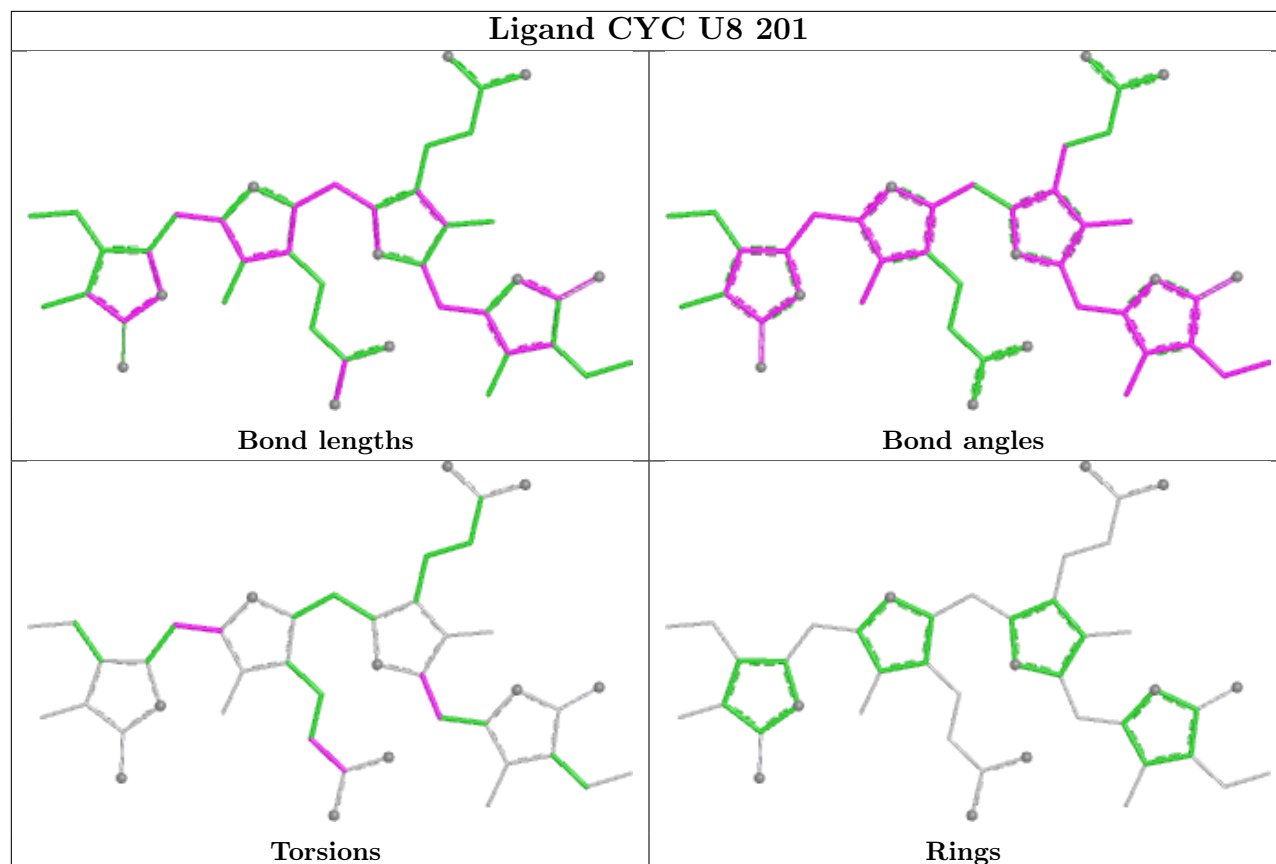
Ligand CYC Q1 201



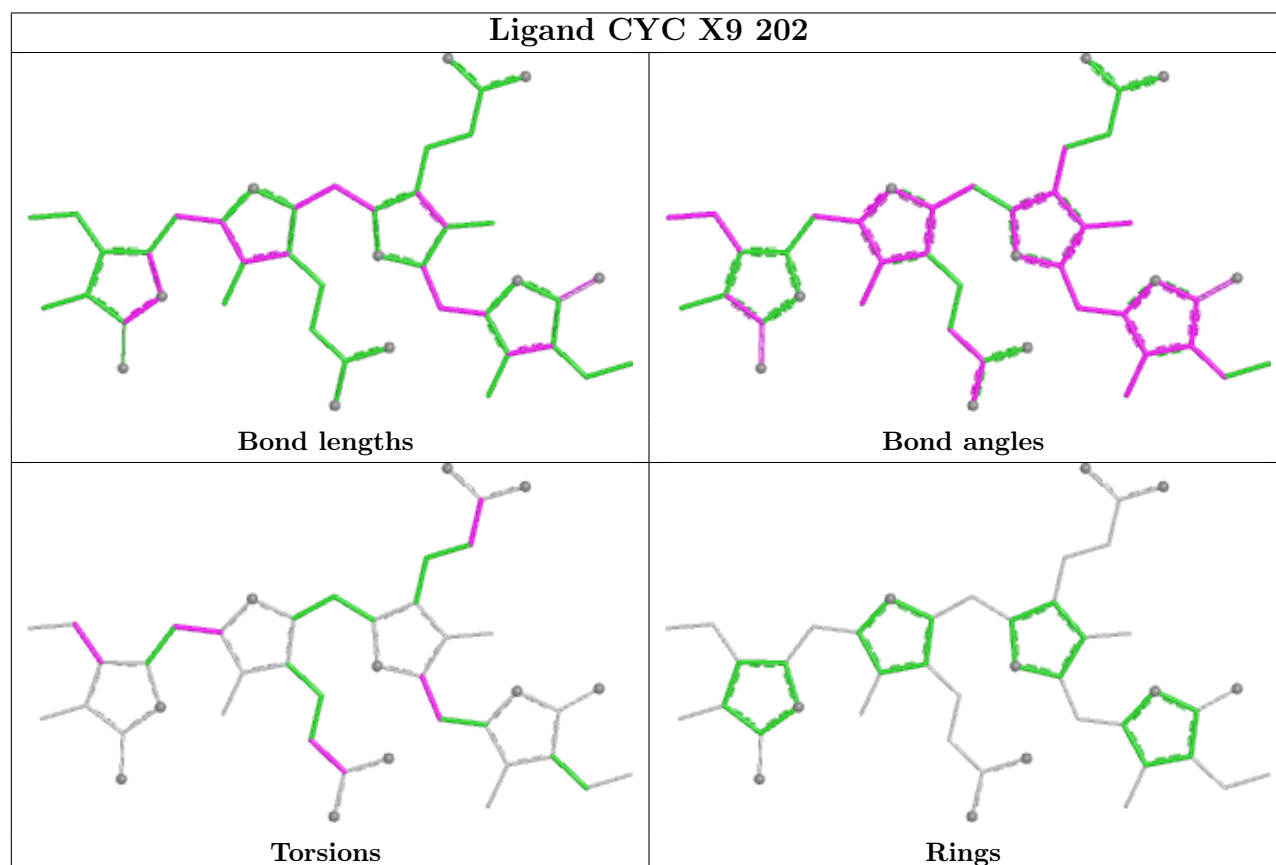
Ligand CYC A5 201

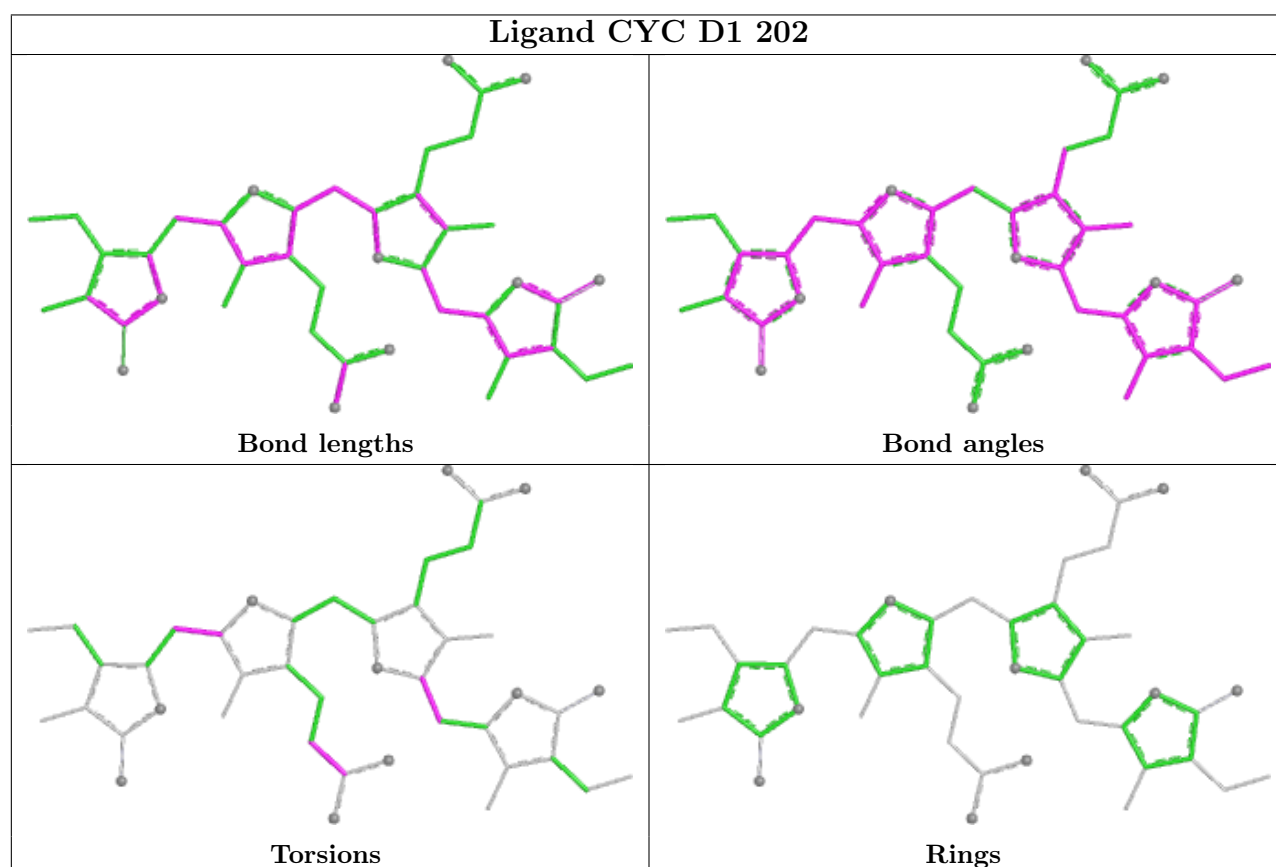
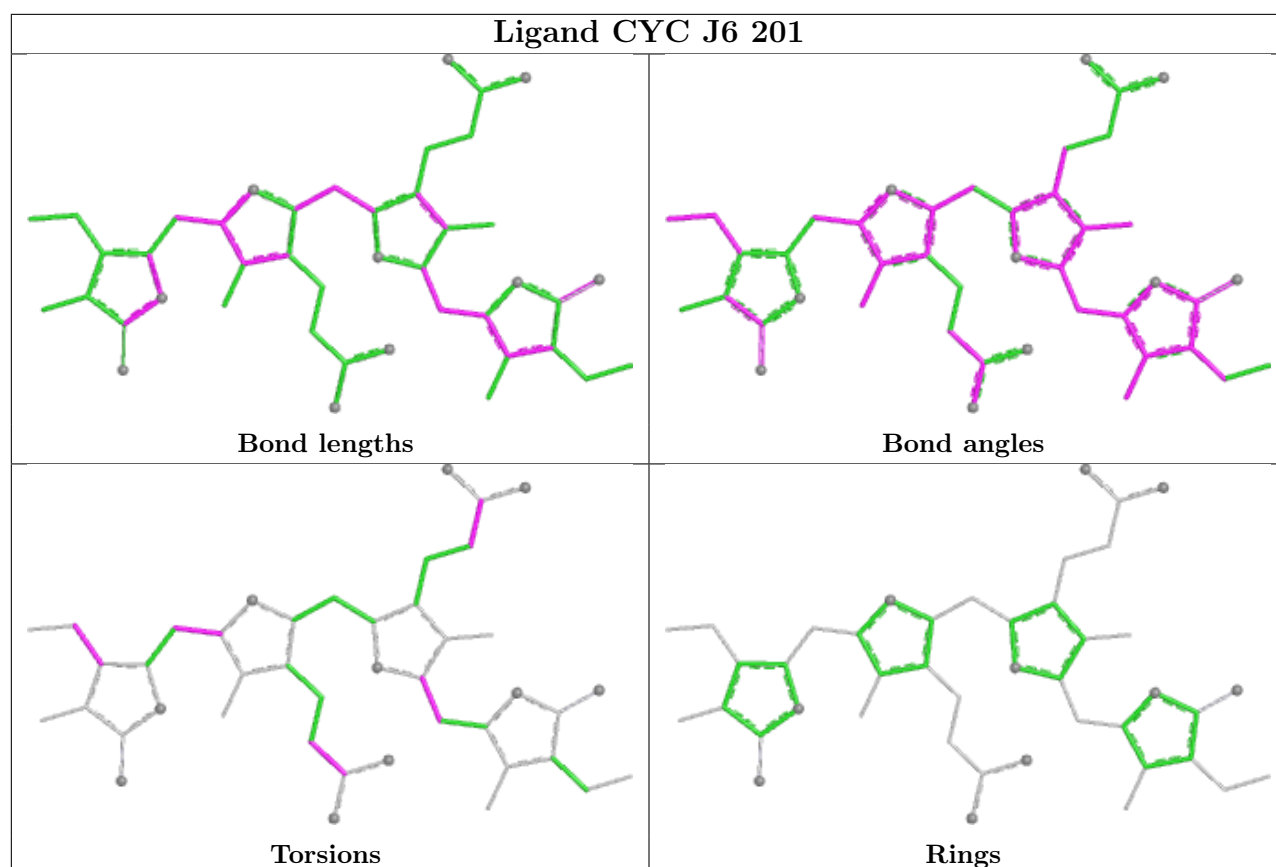


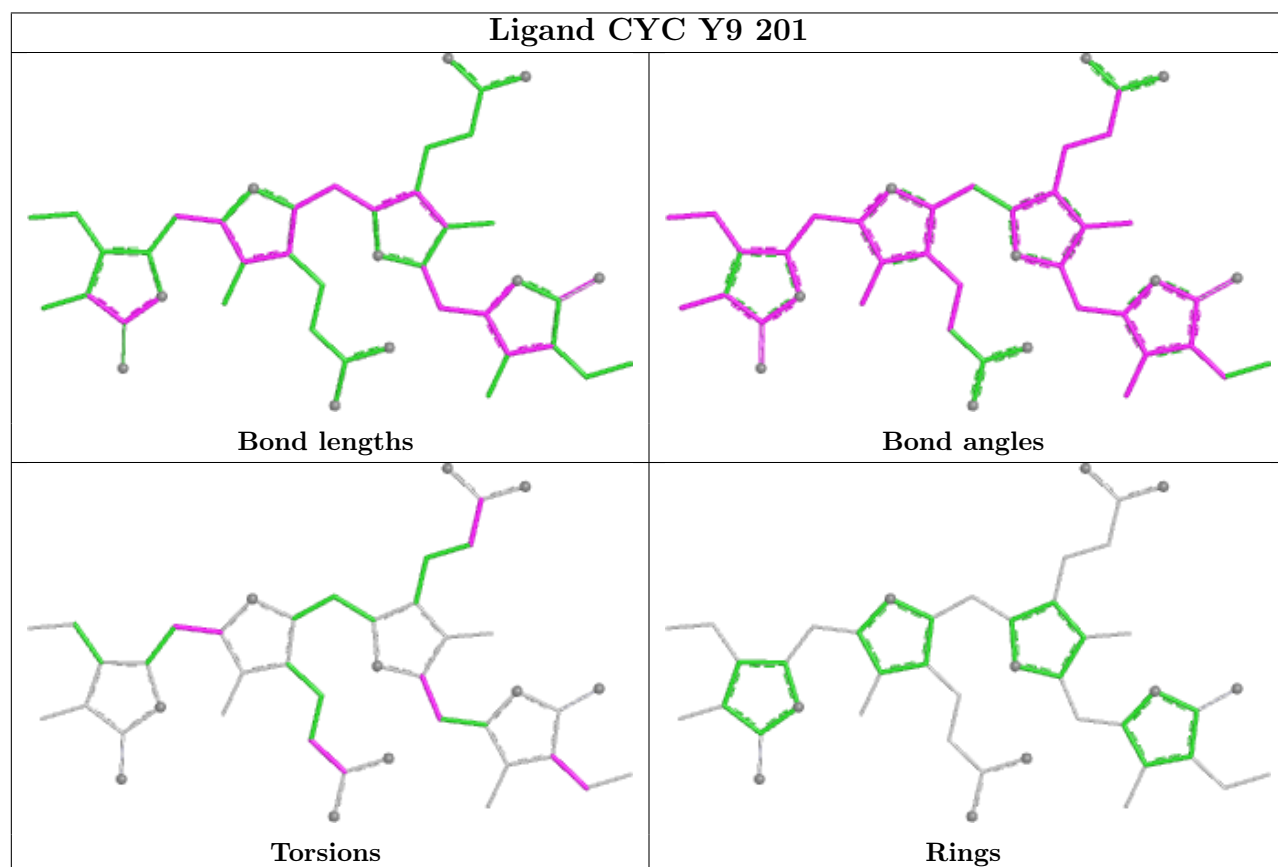
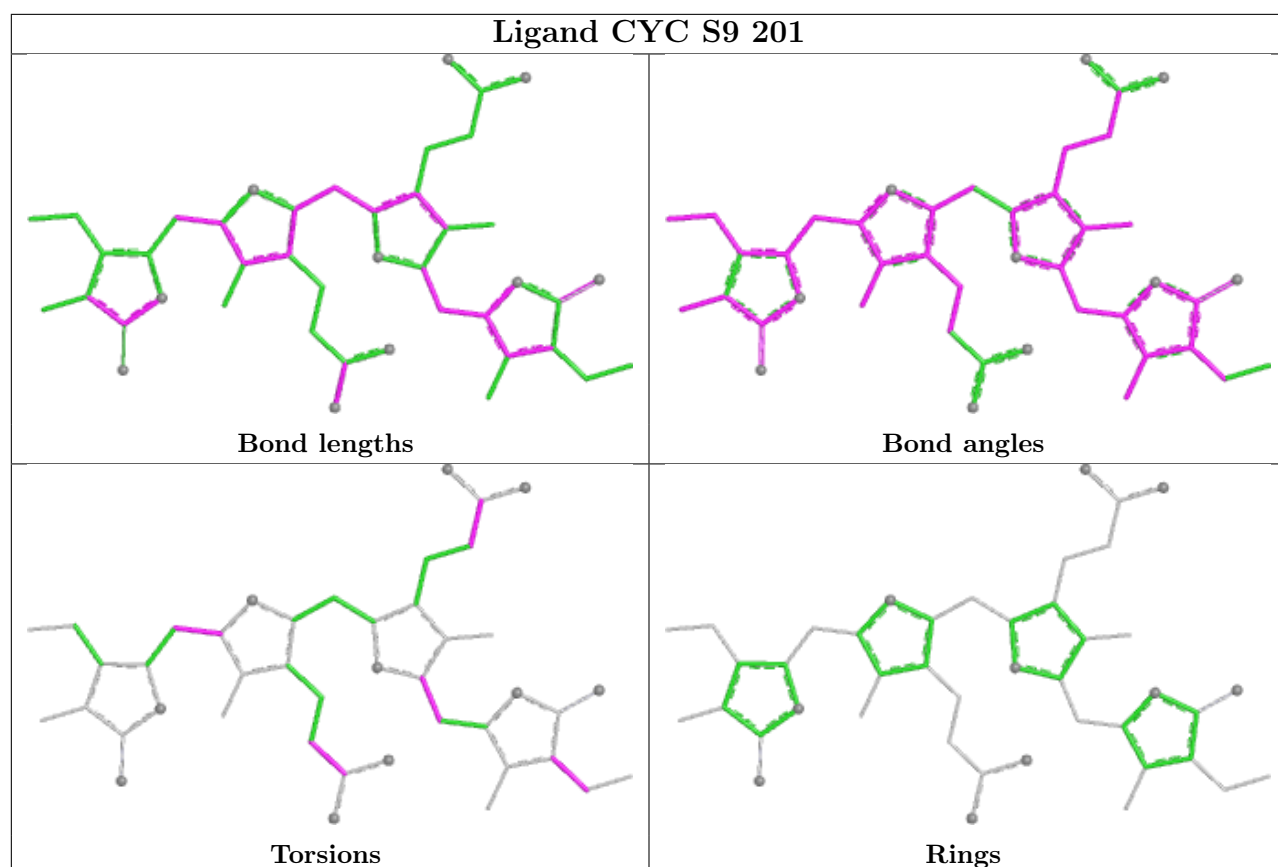
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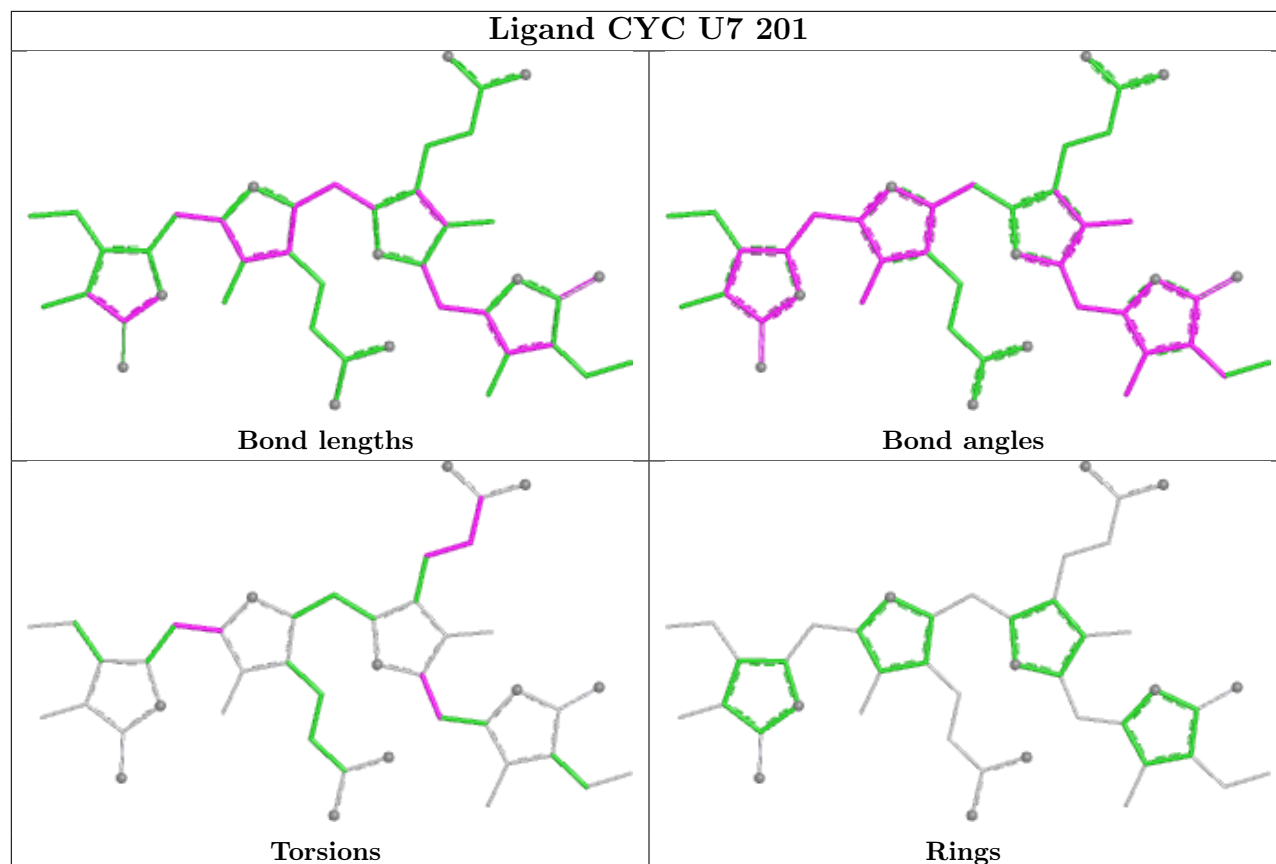
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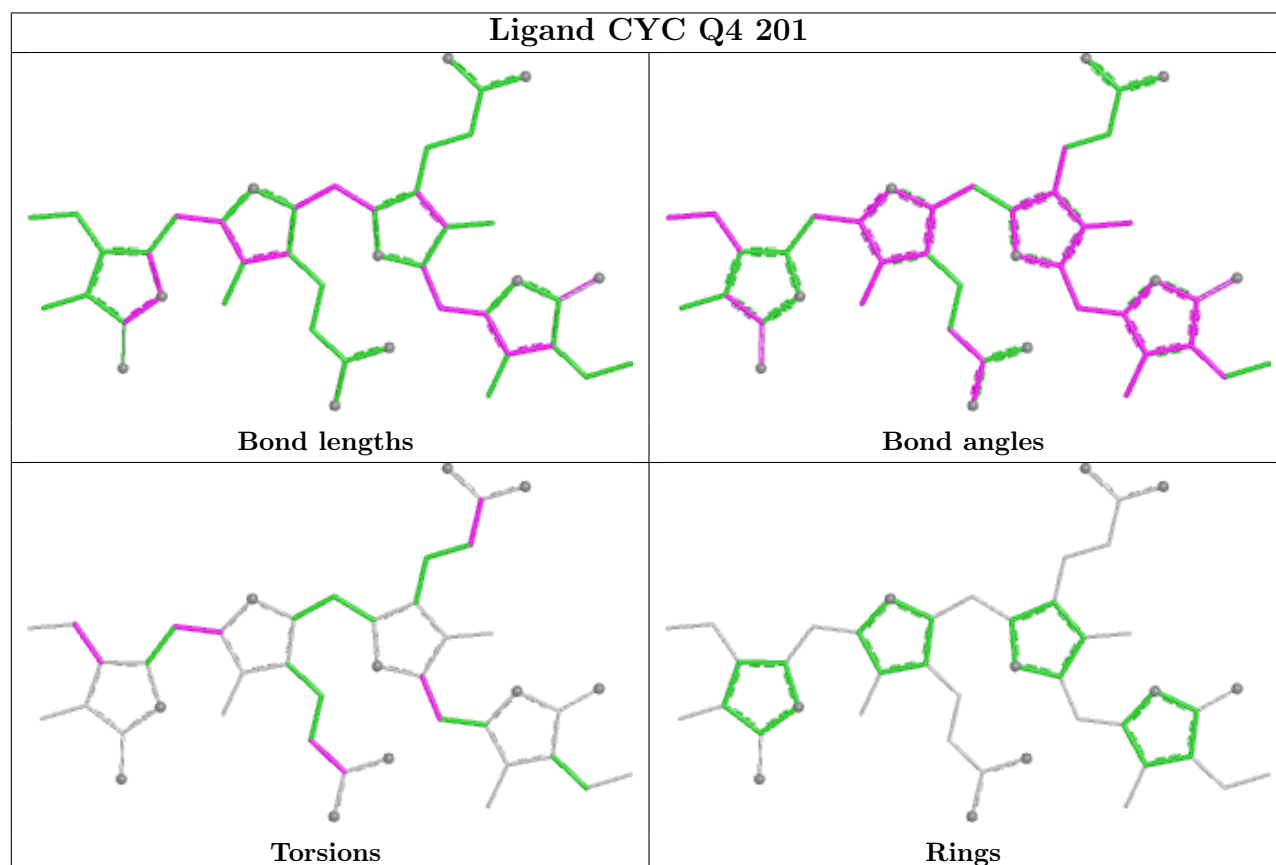




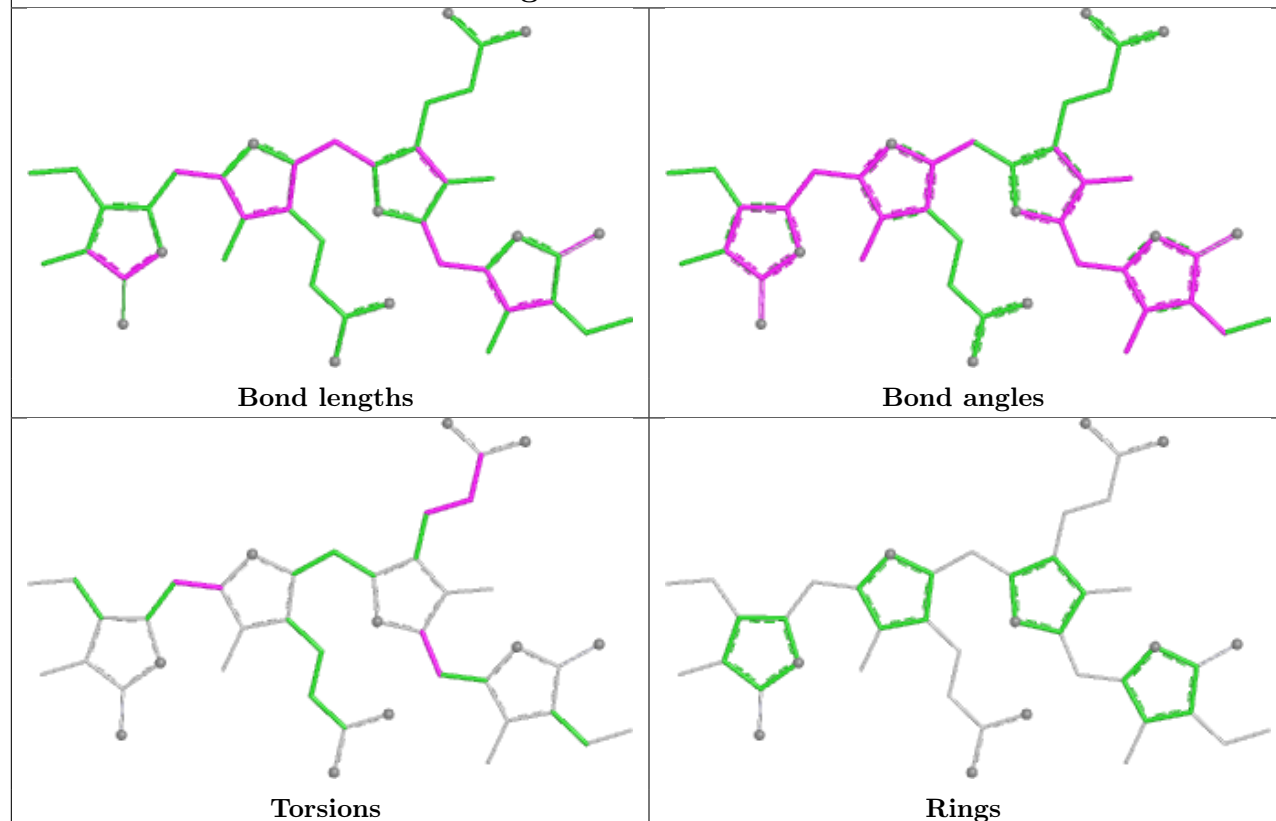
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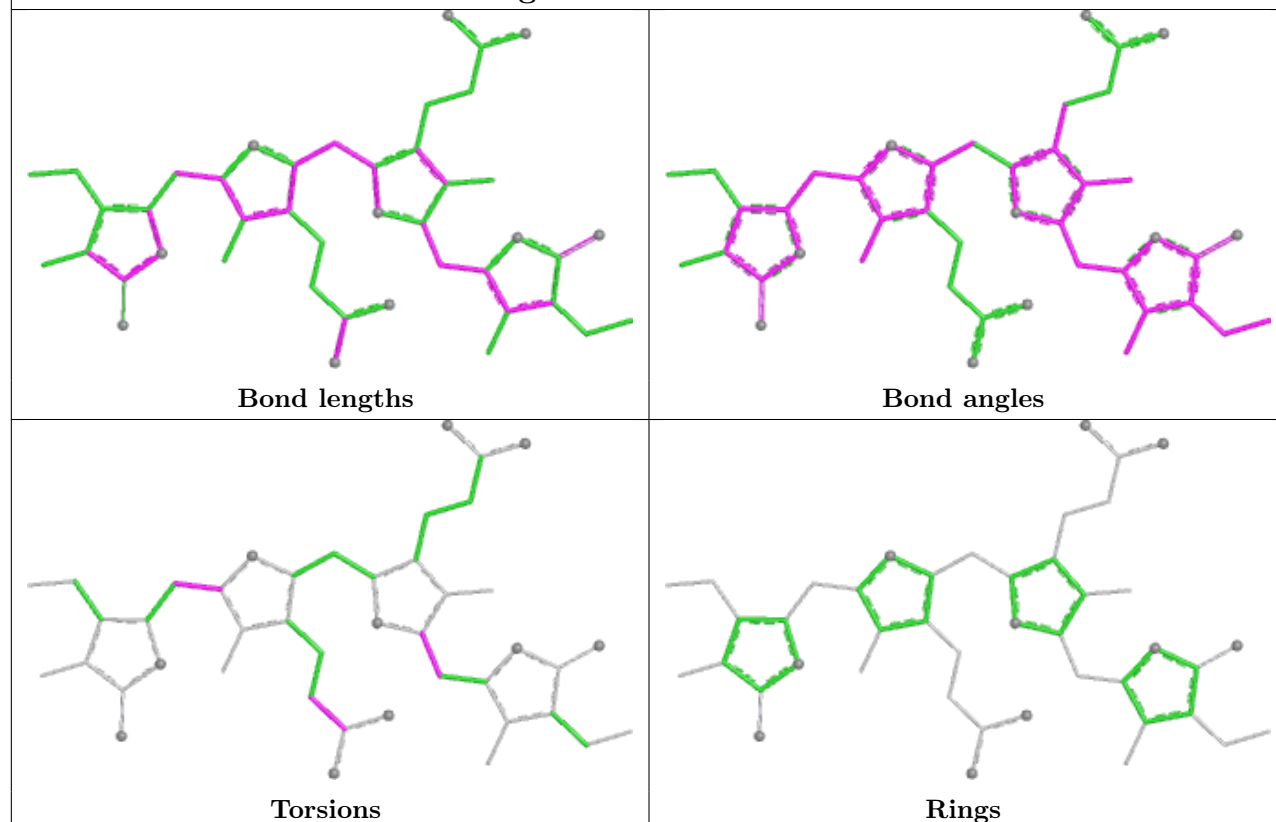
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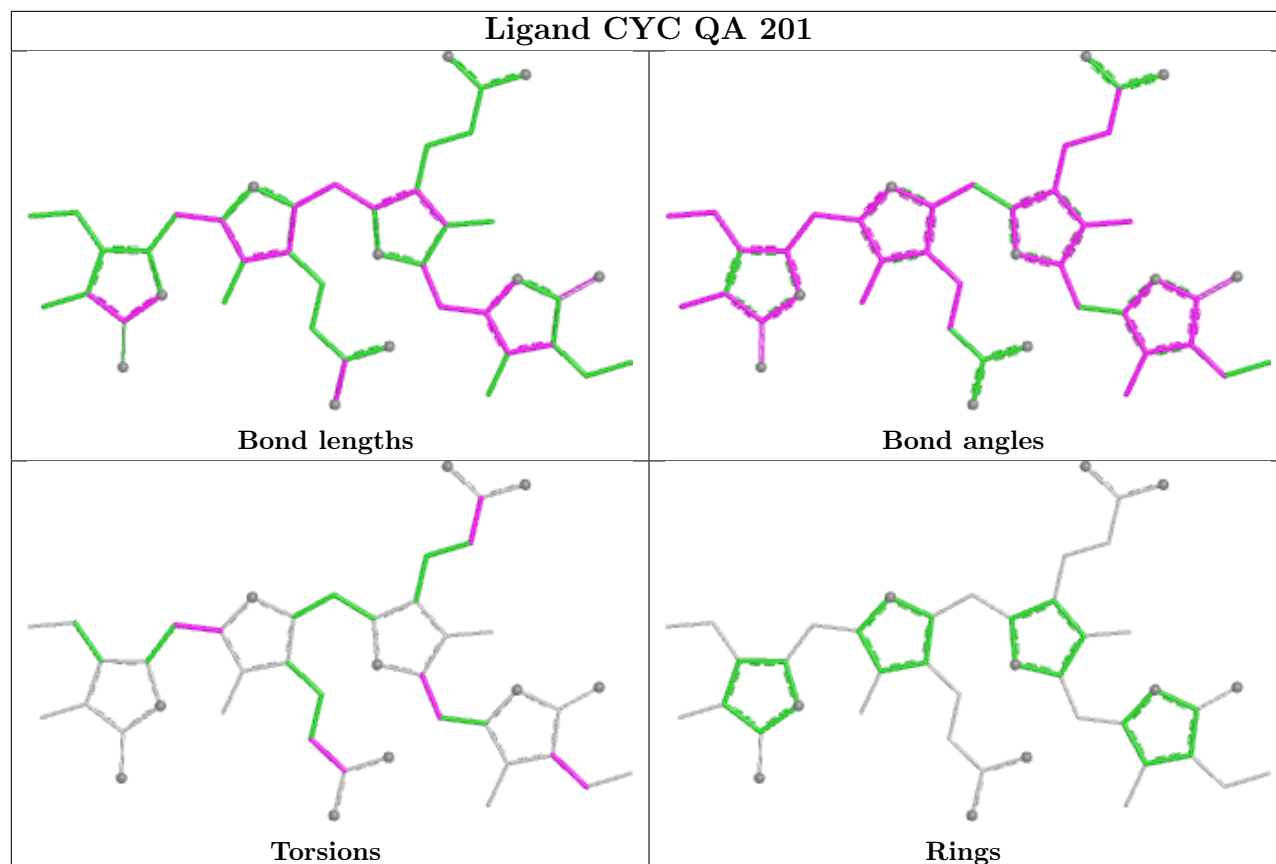
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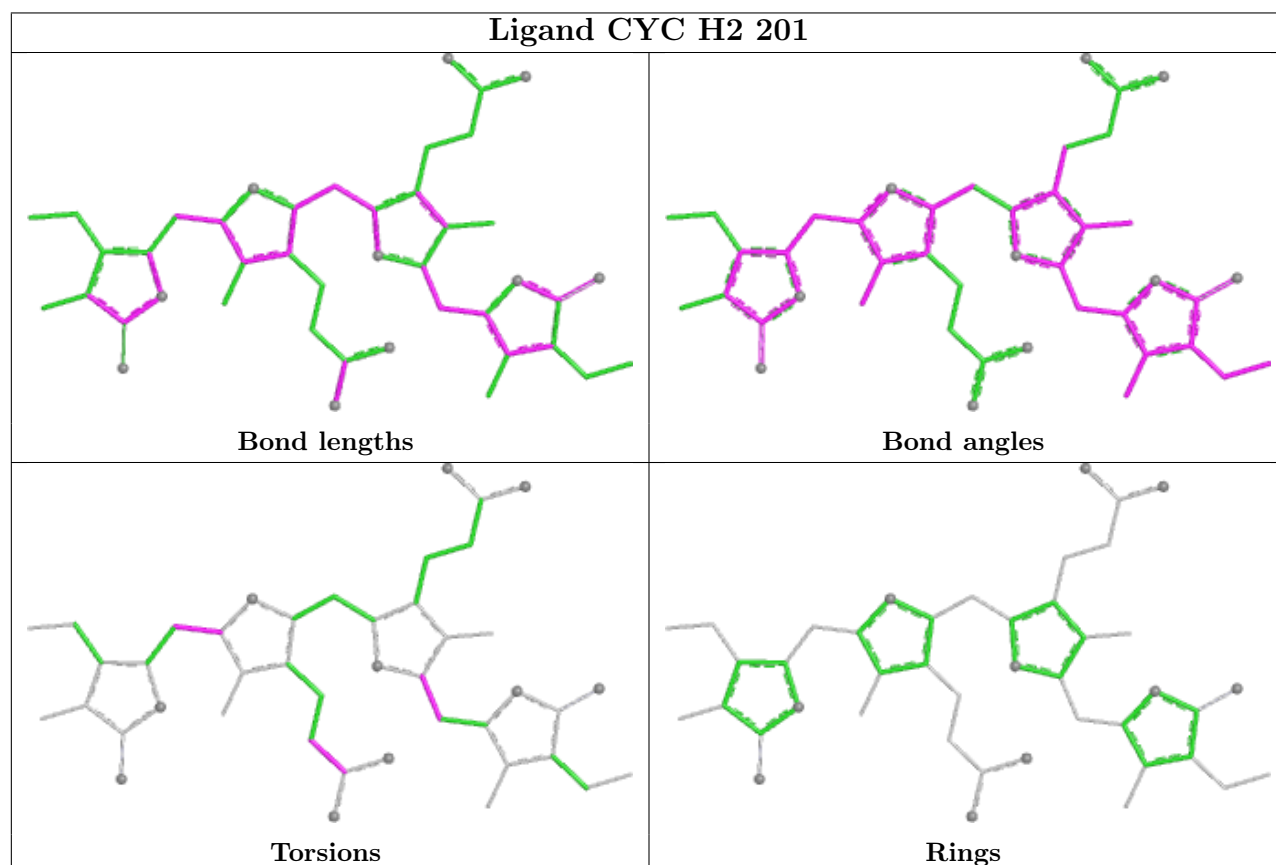
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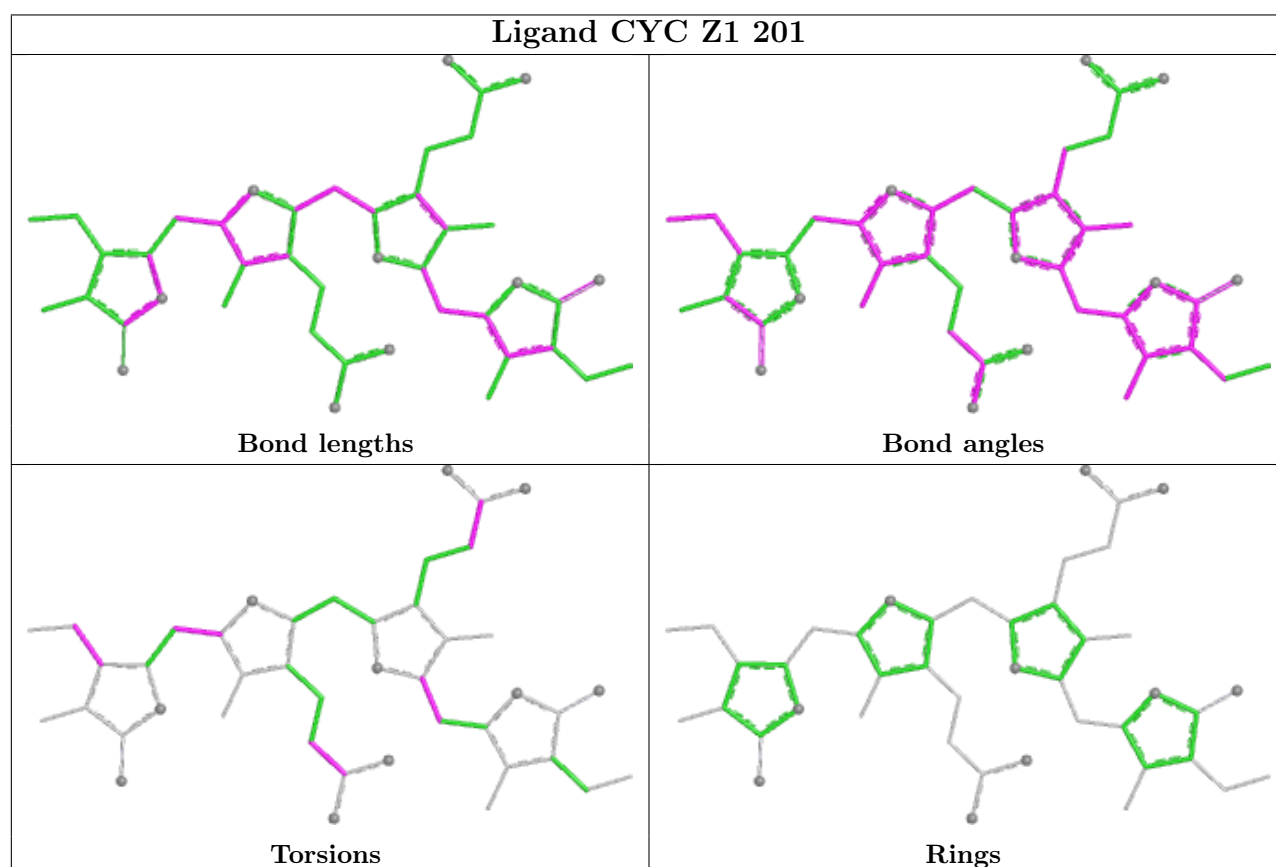
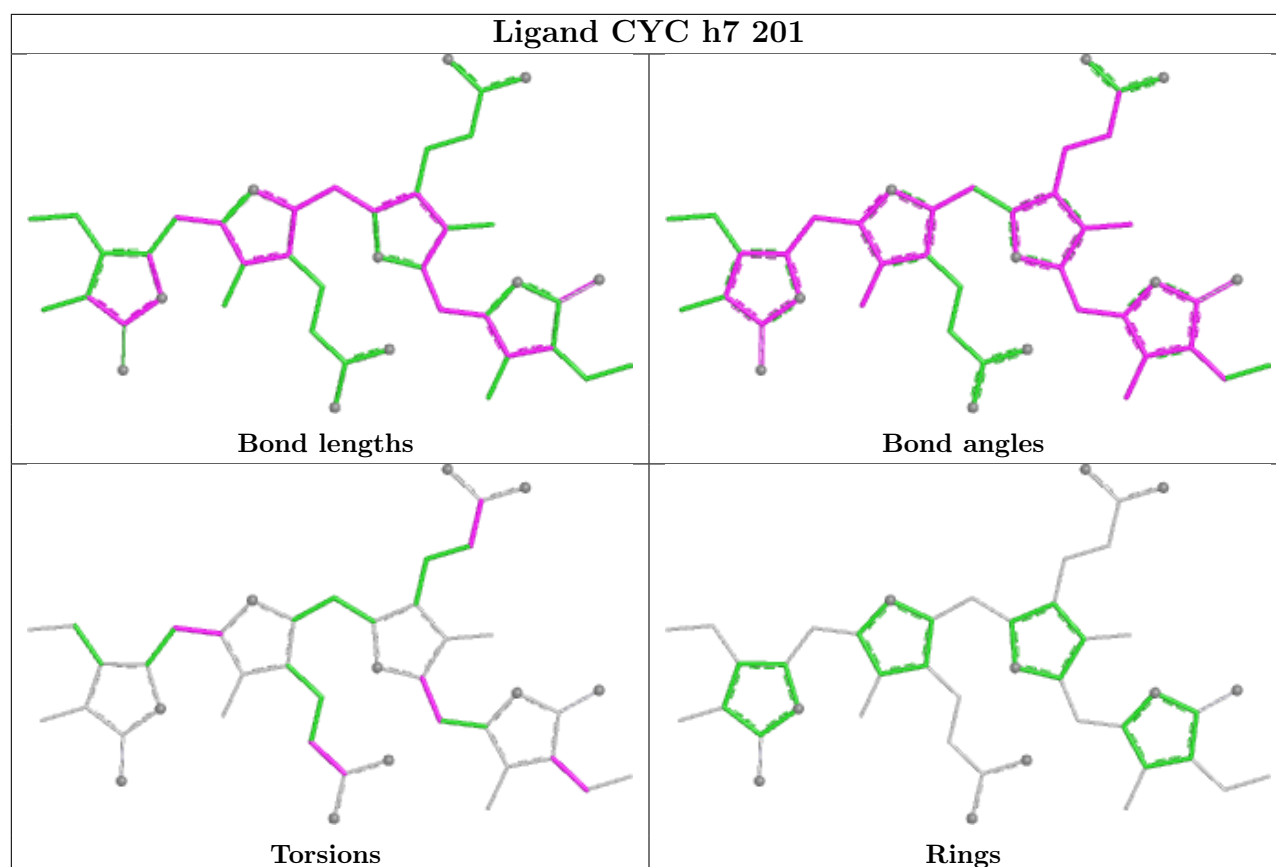


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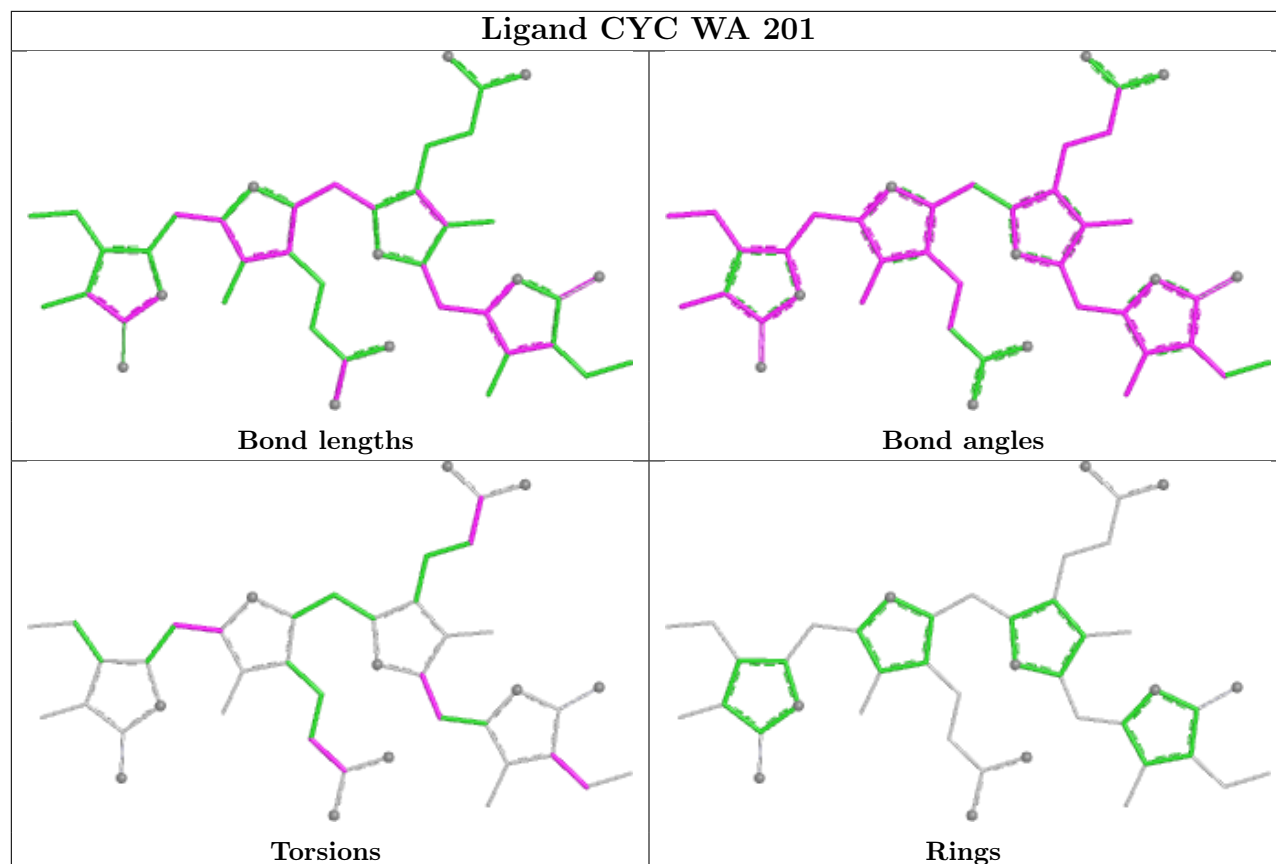


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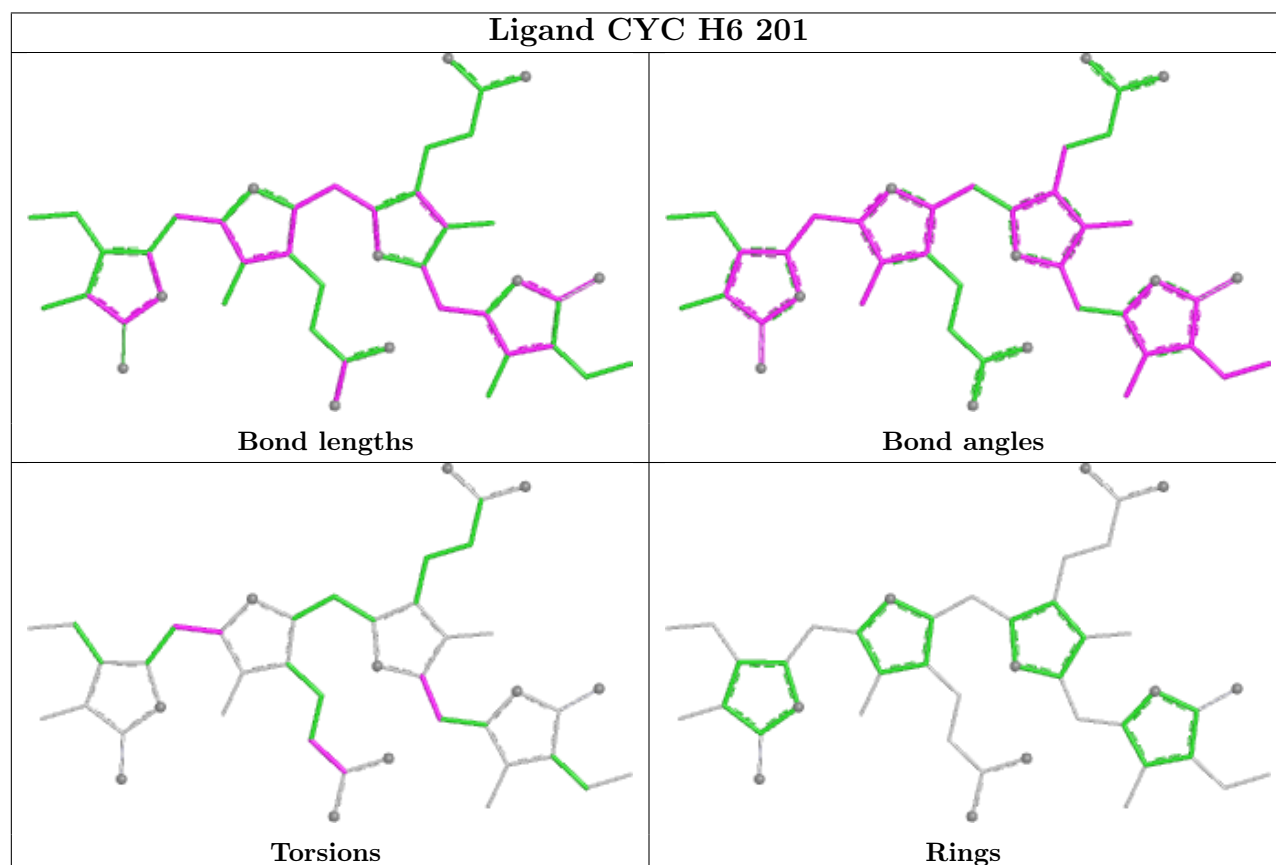




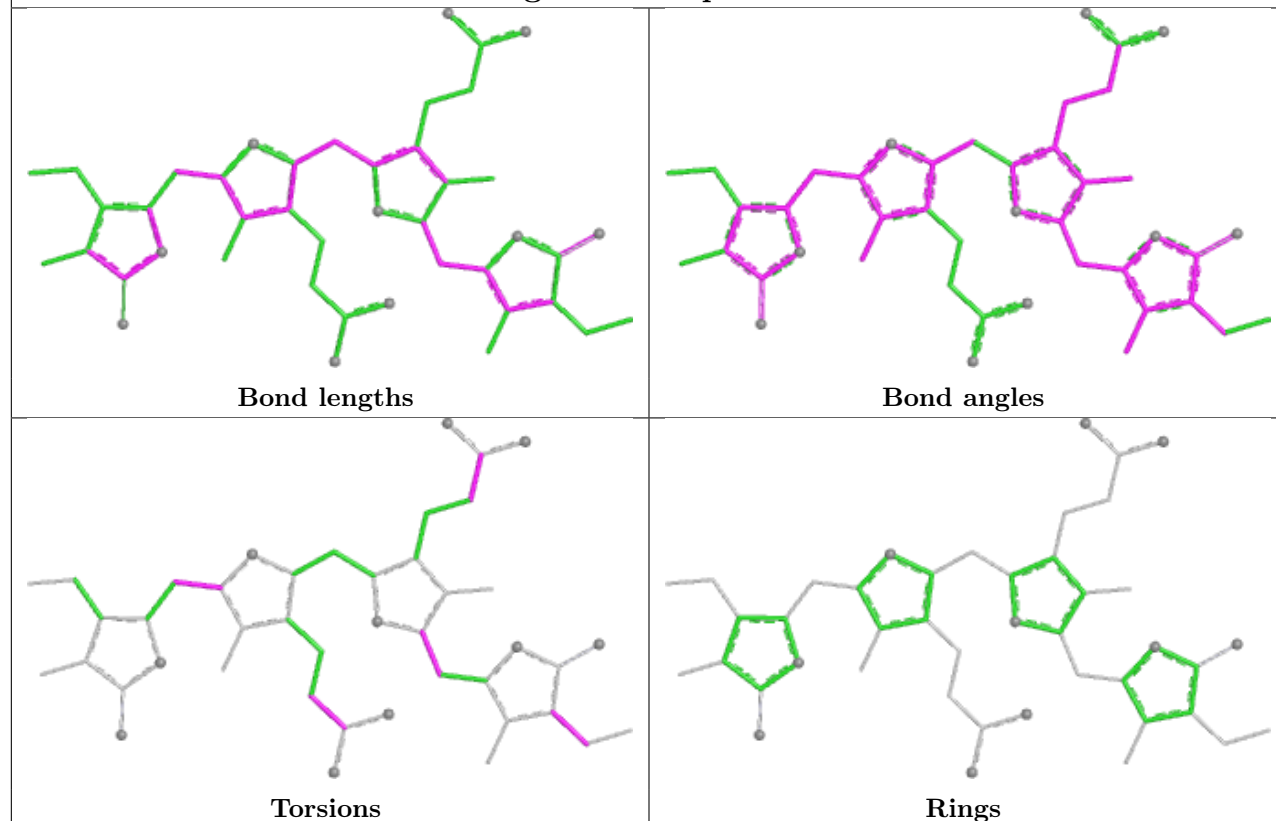
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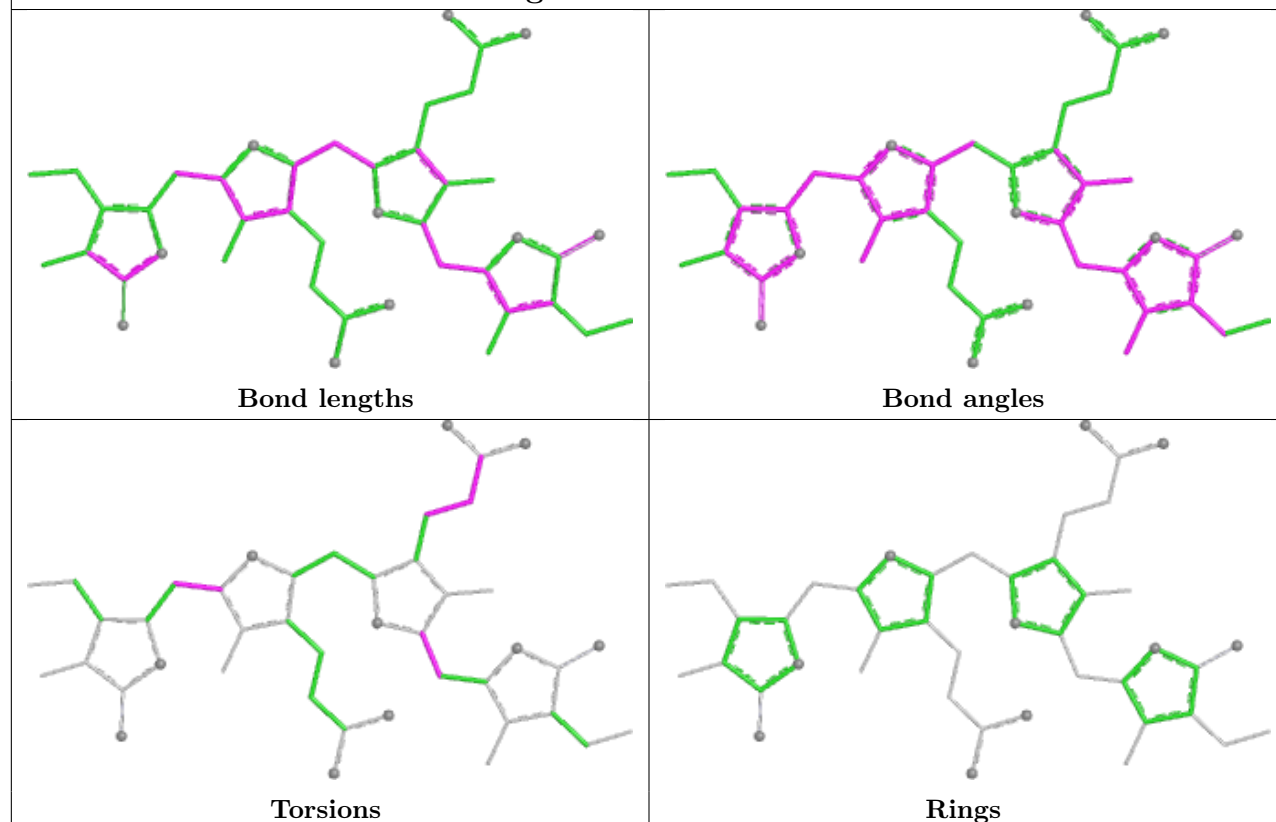
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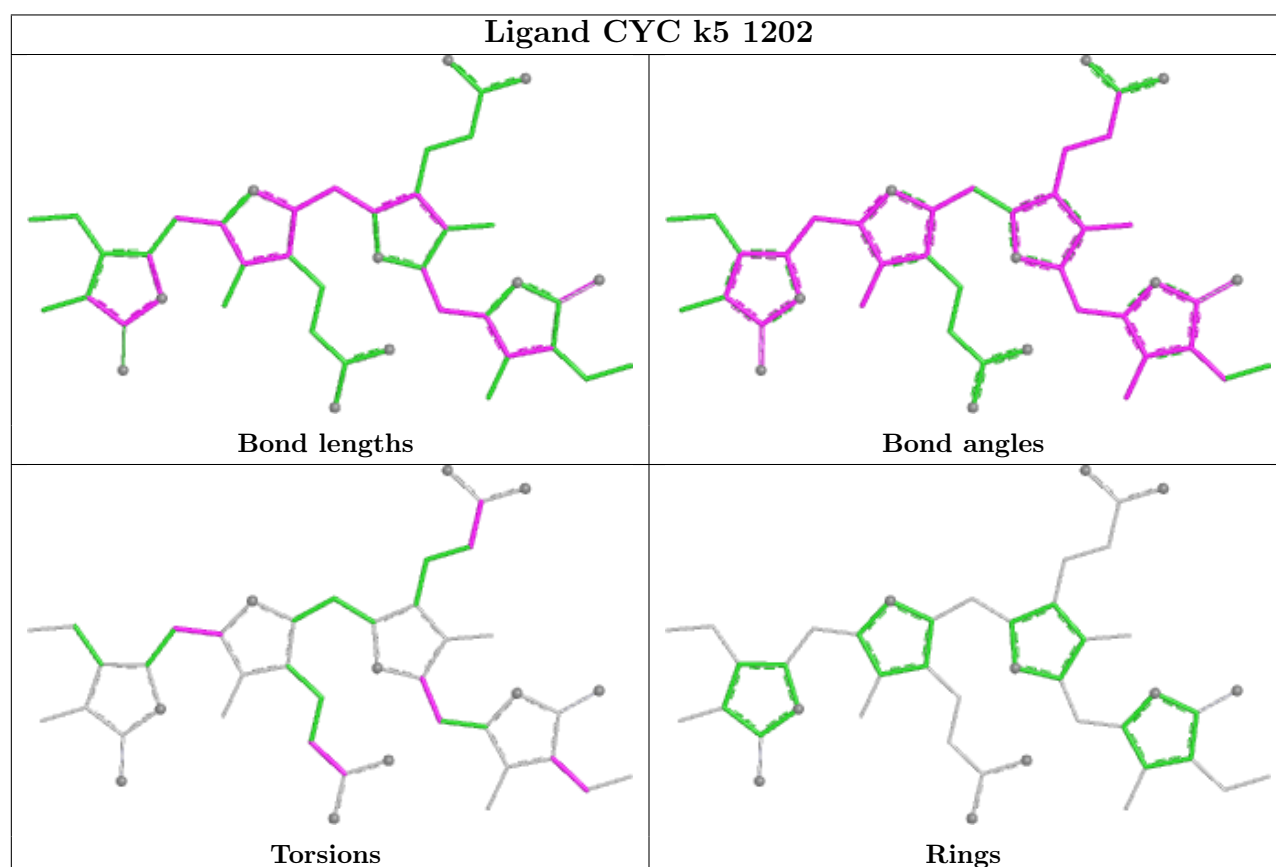
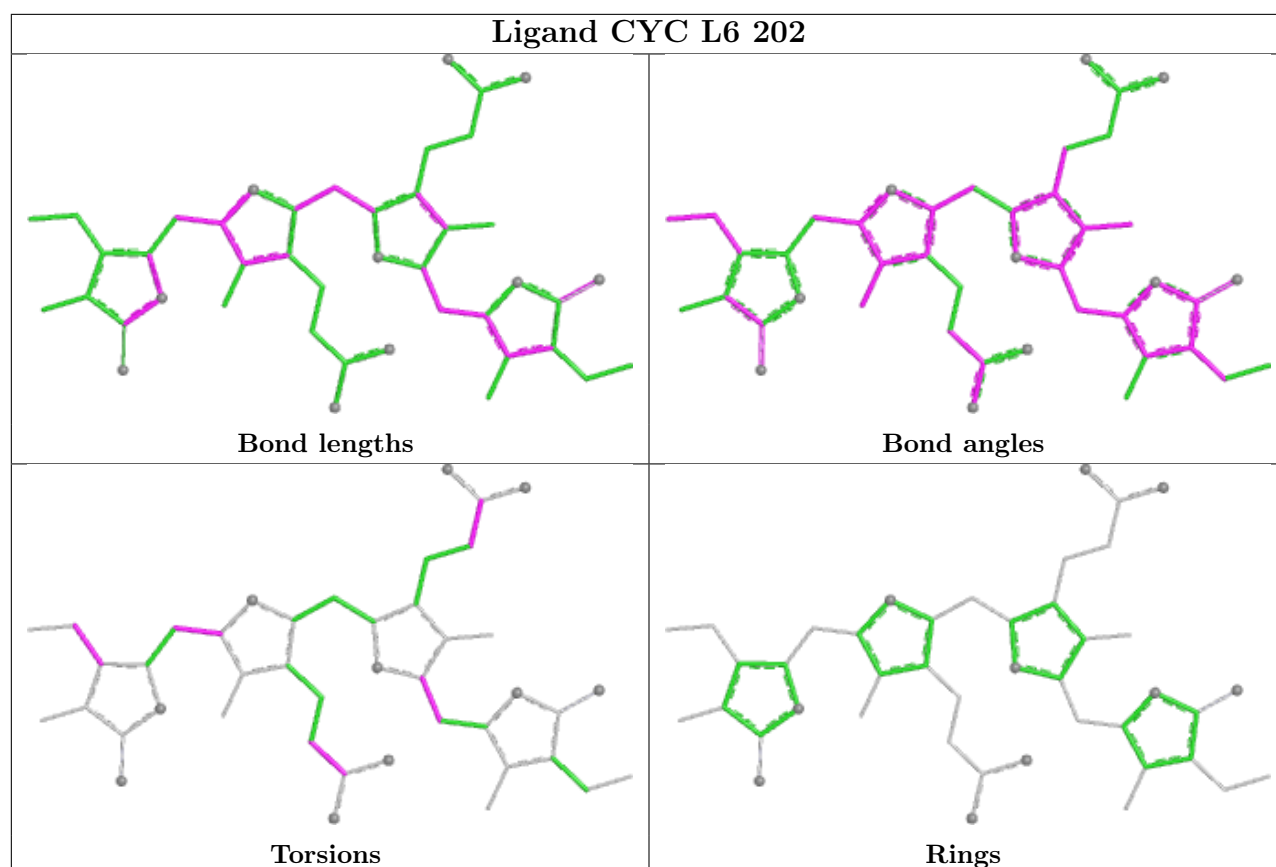


Ligand CYC p7 201

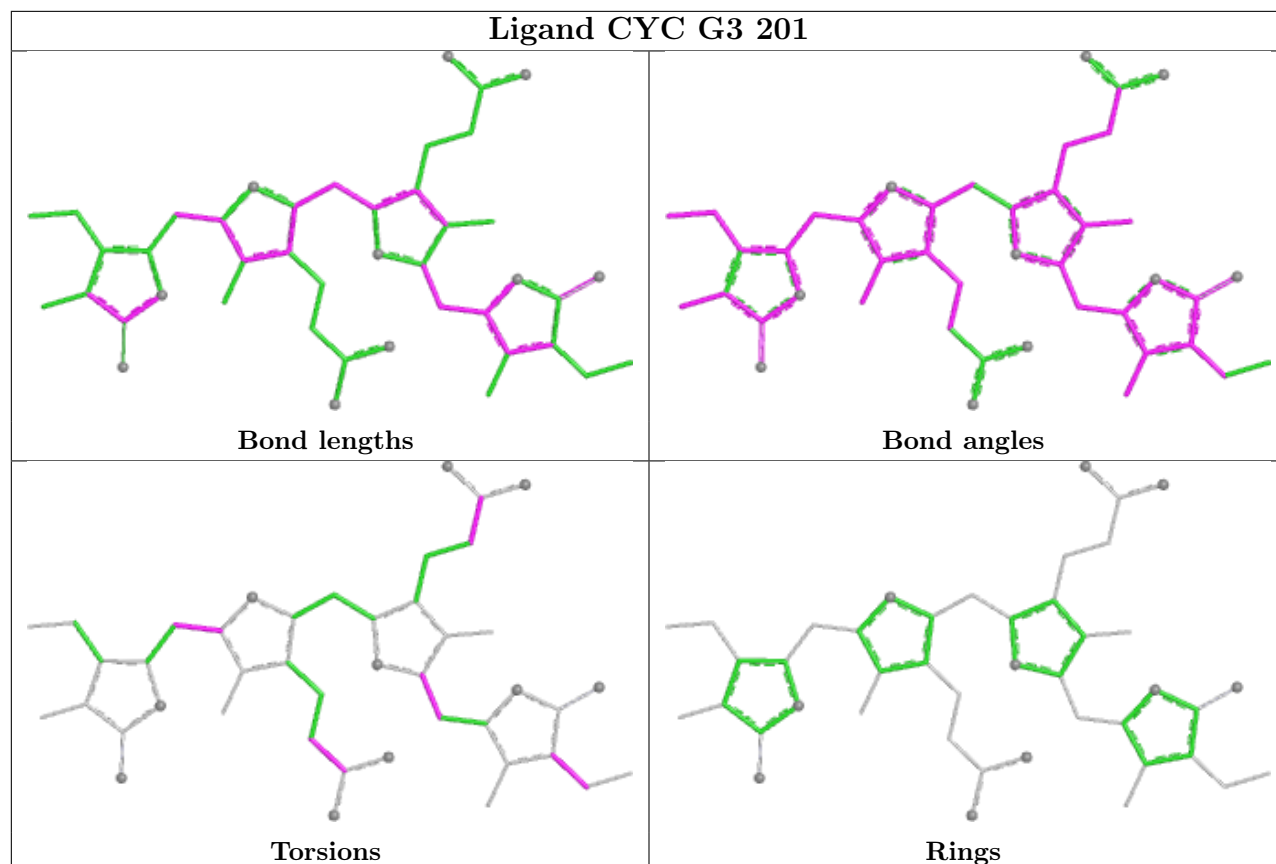


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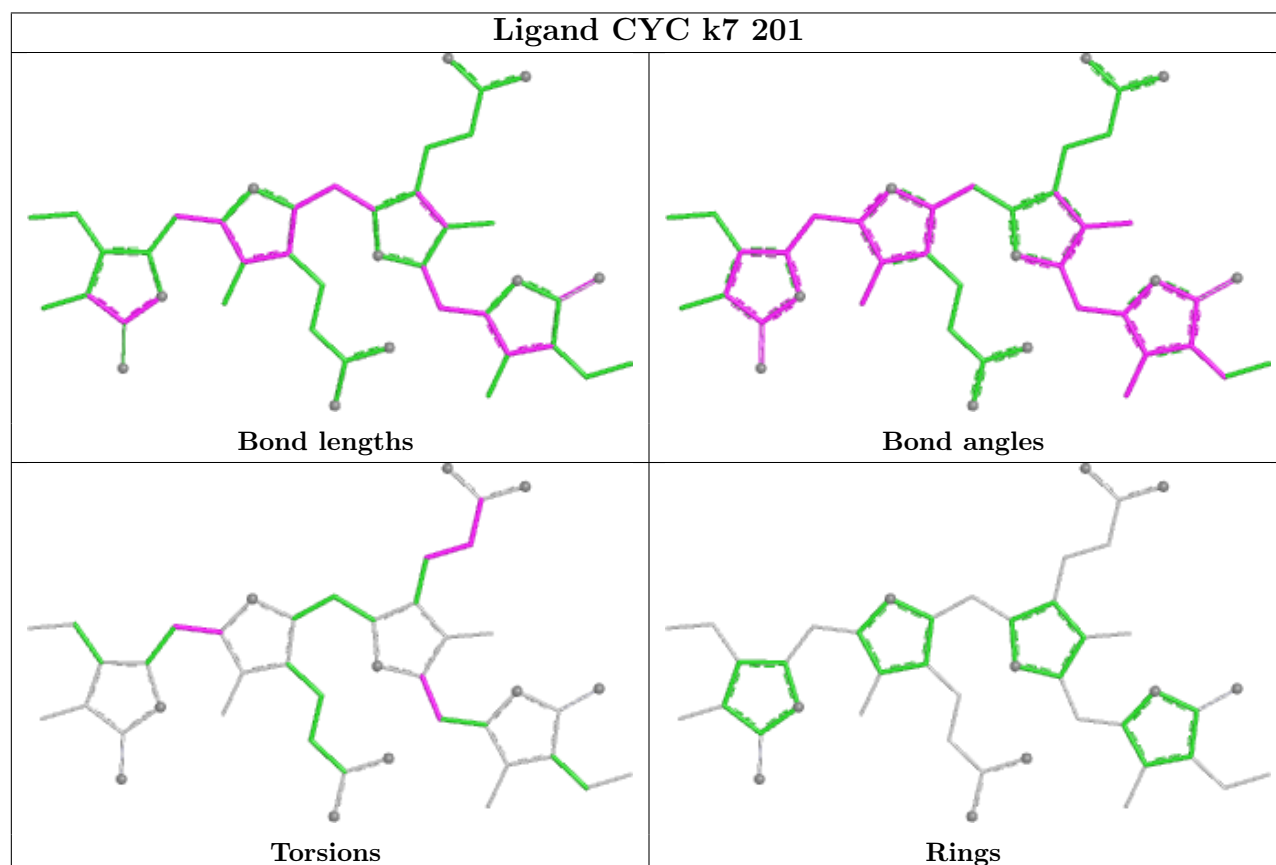




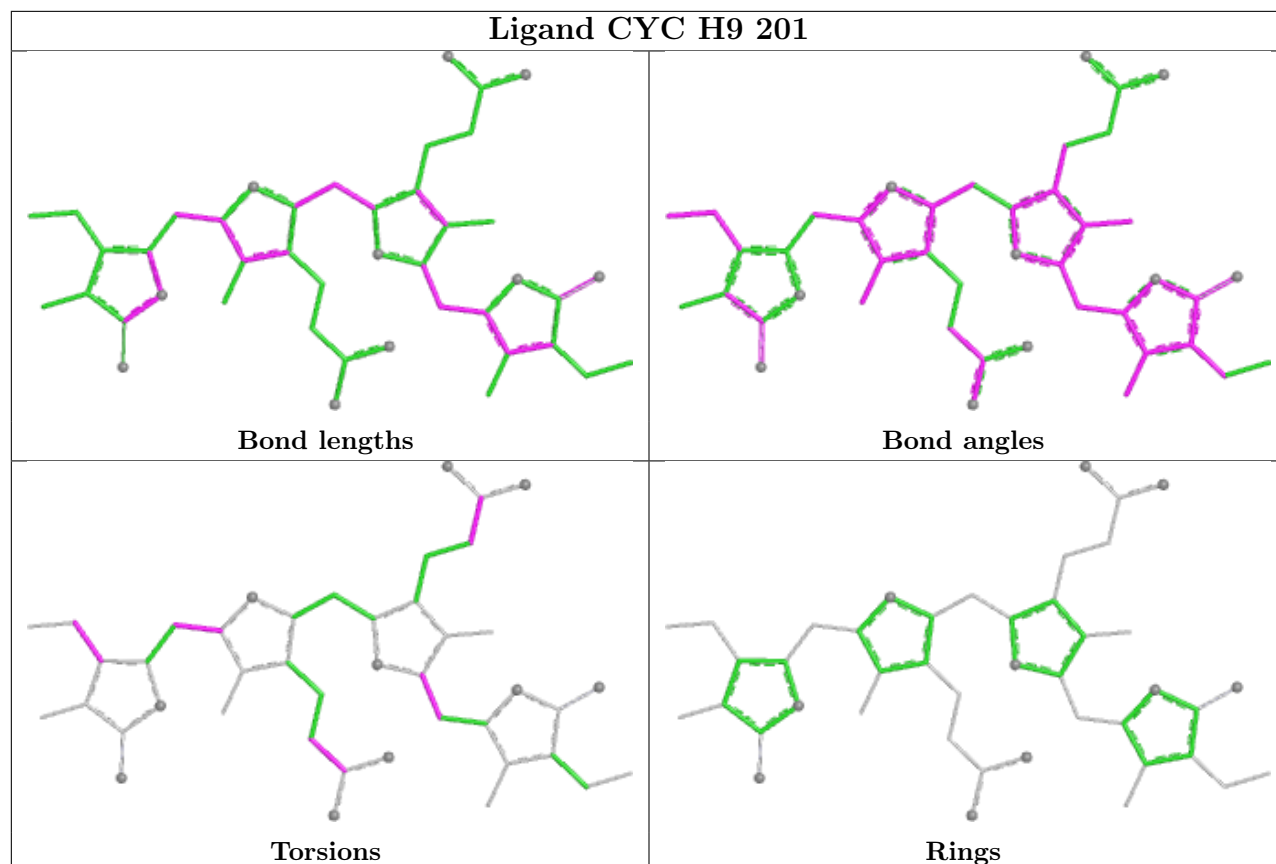
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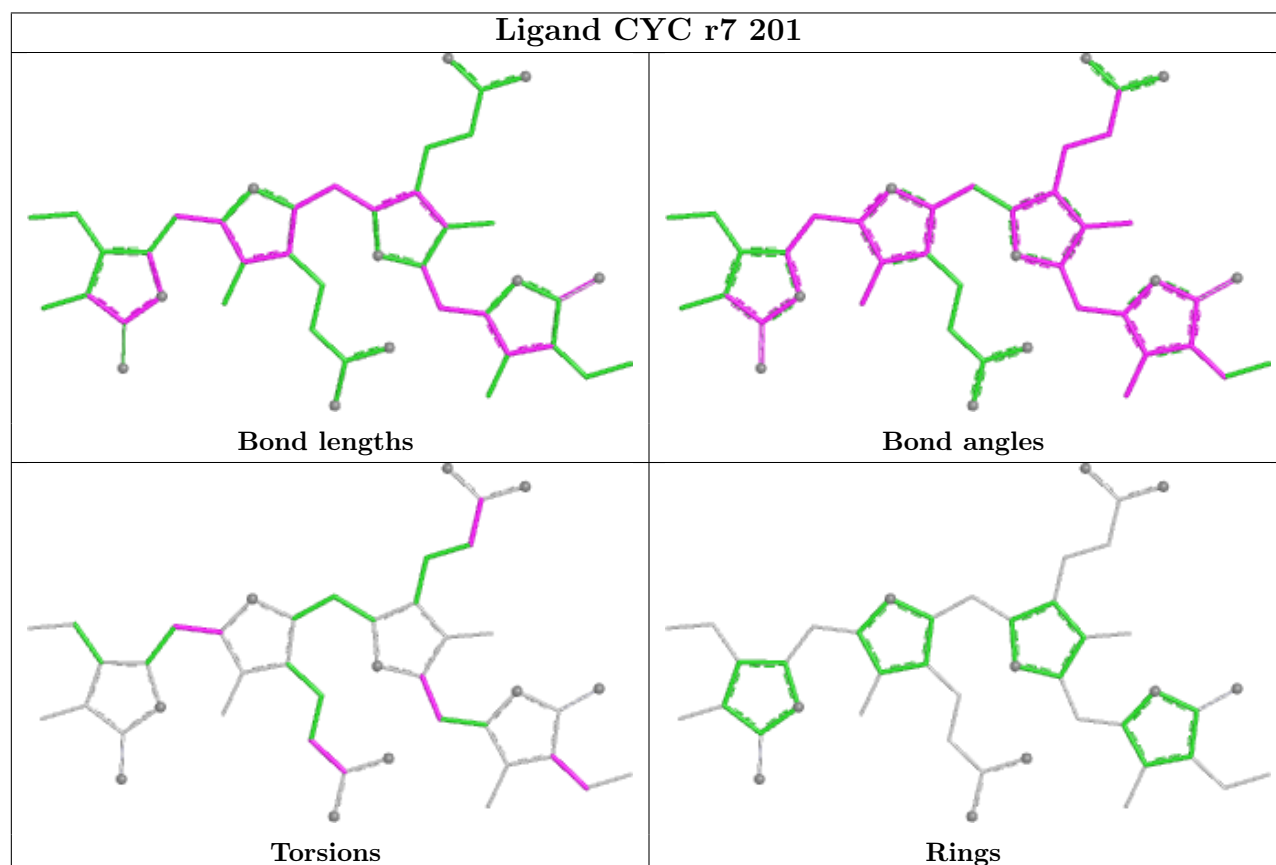
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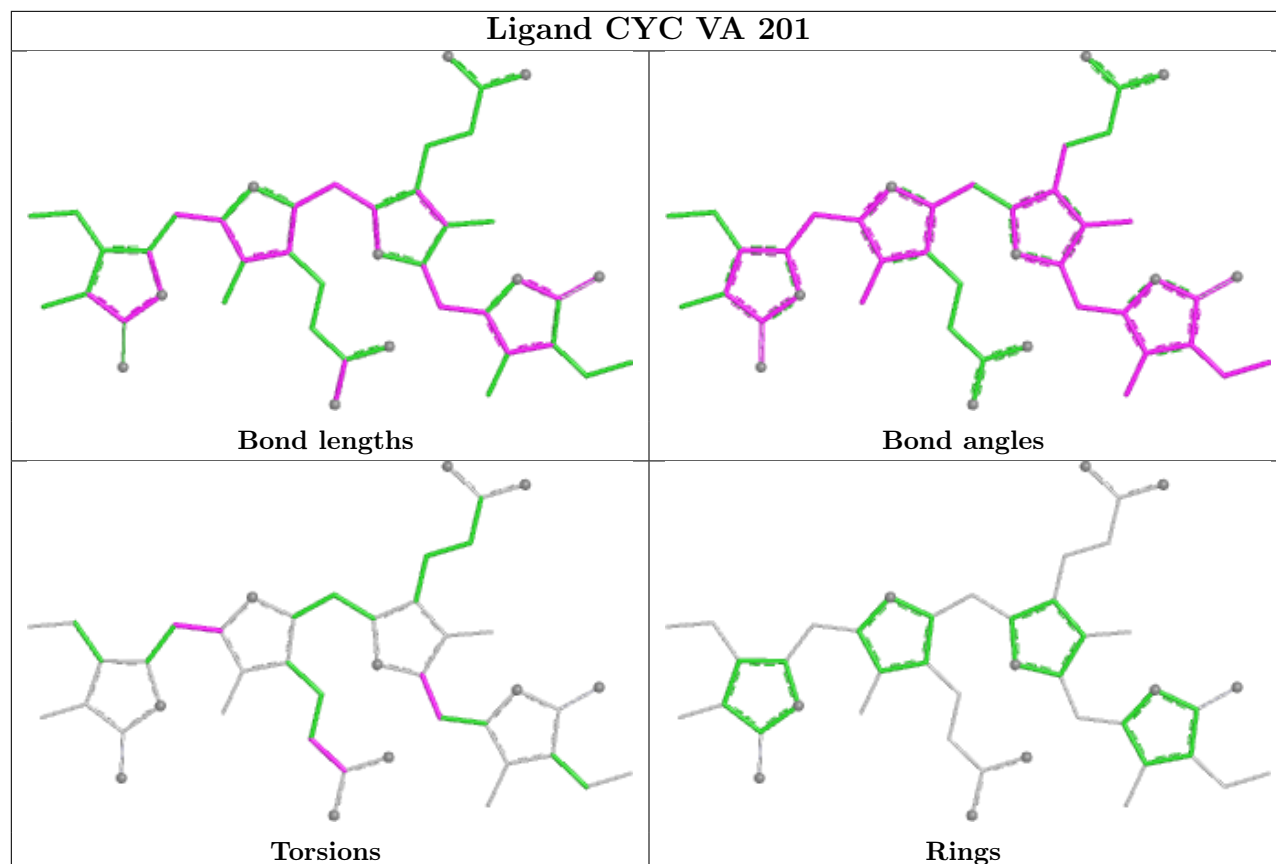
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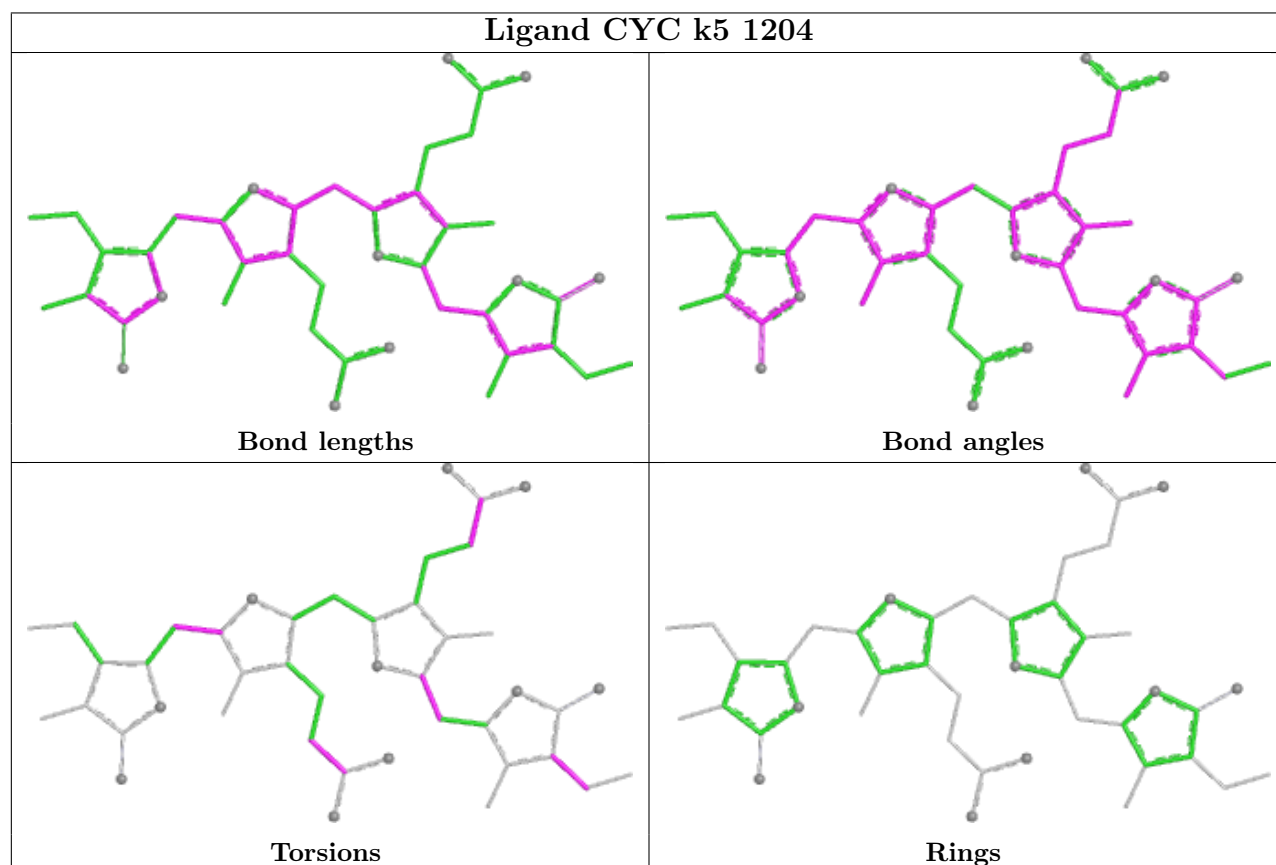
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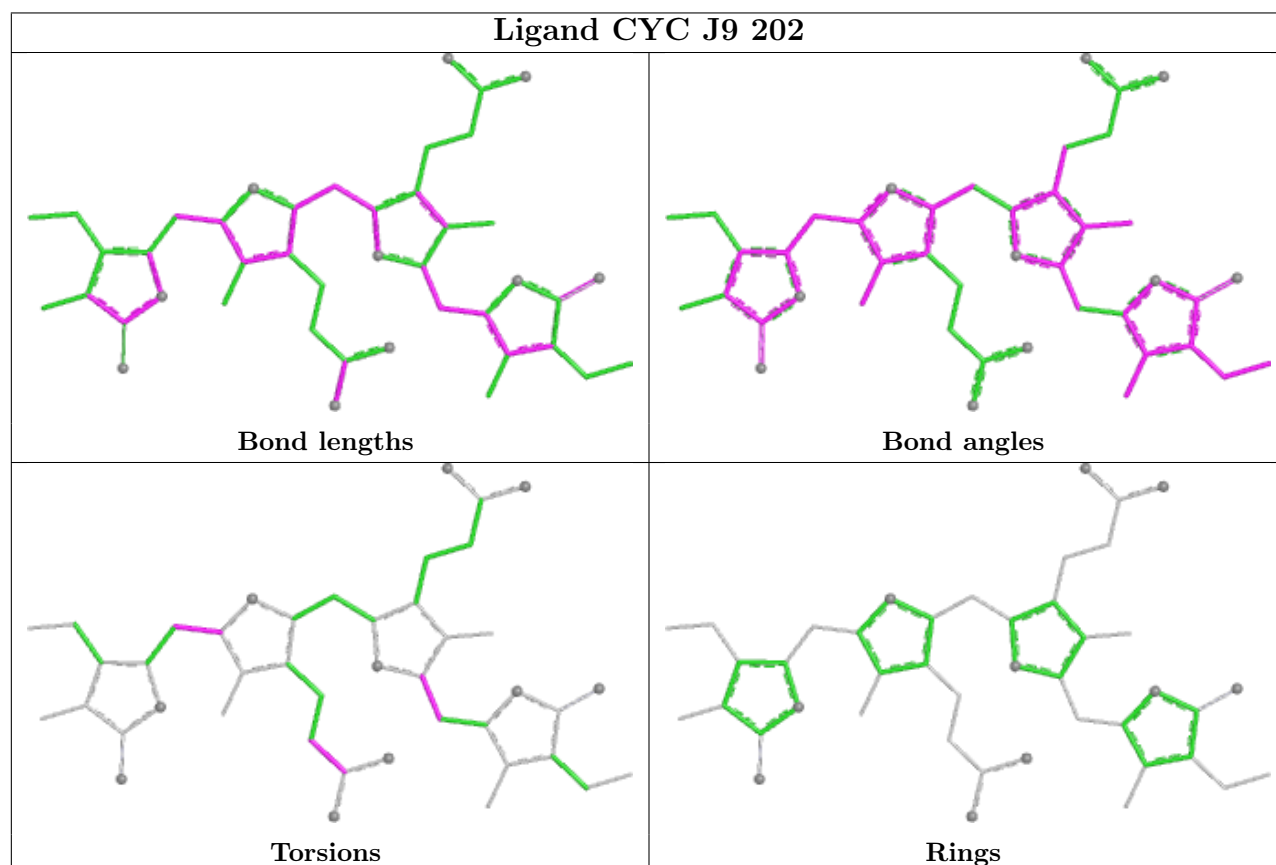
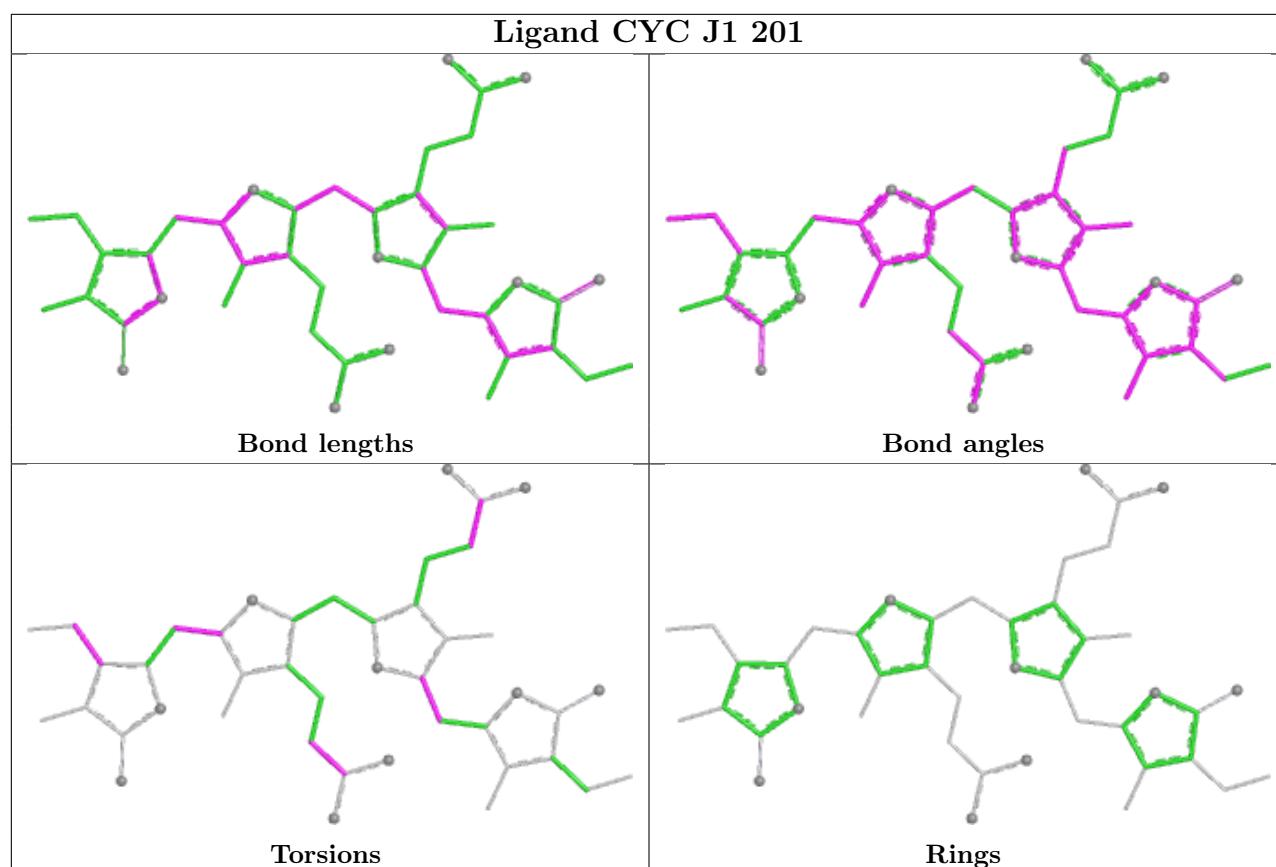


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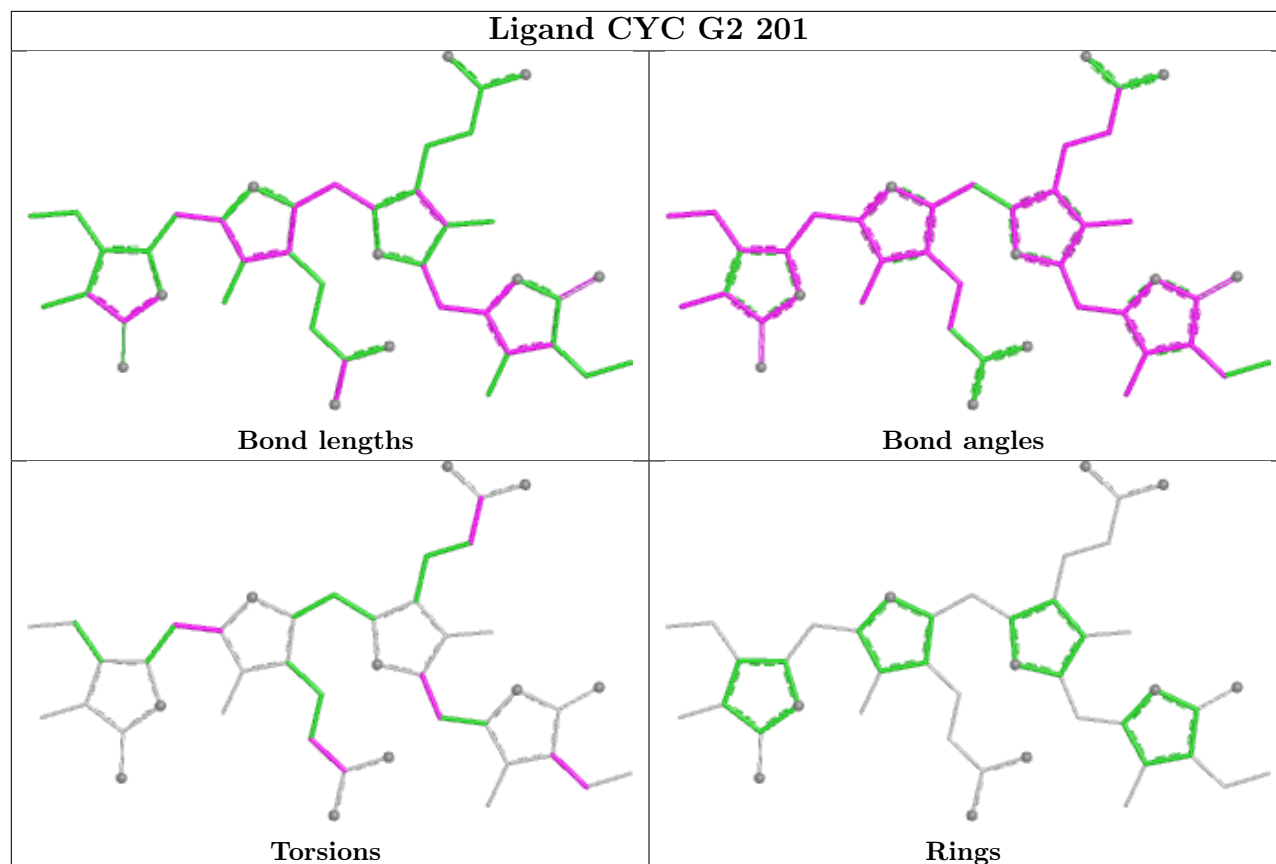


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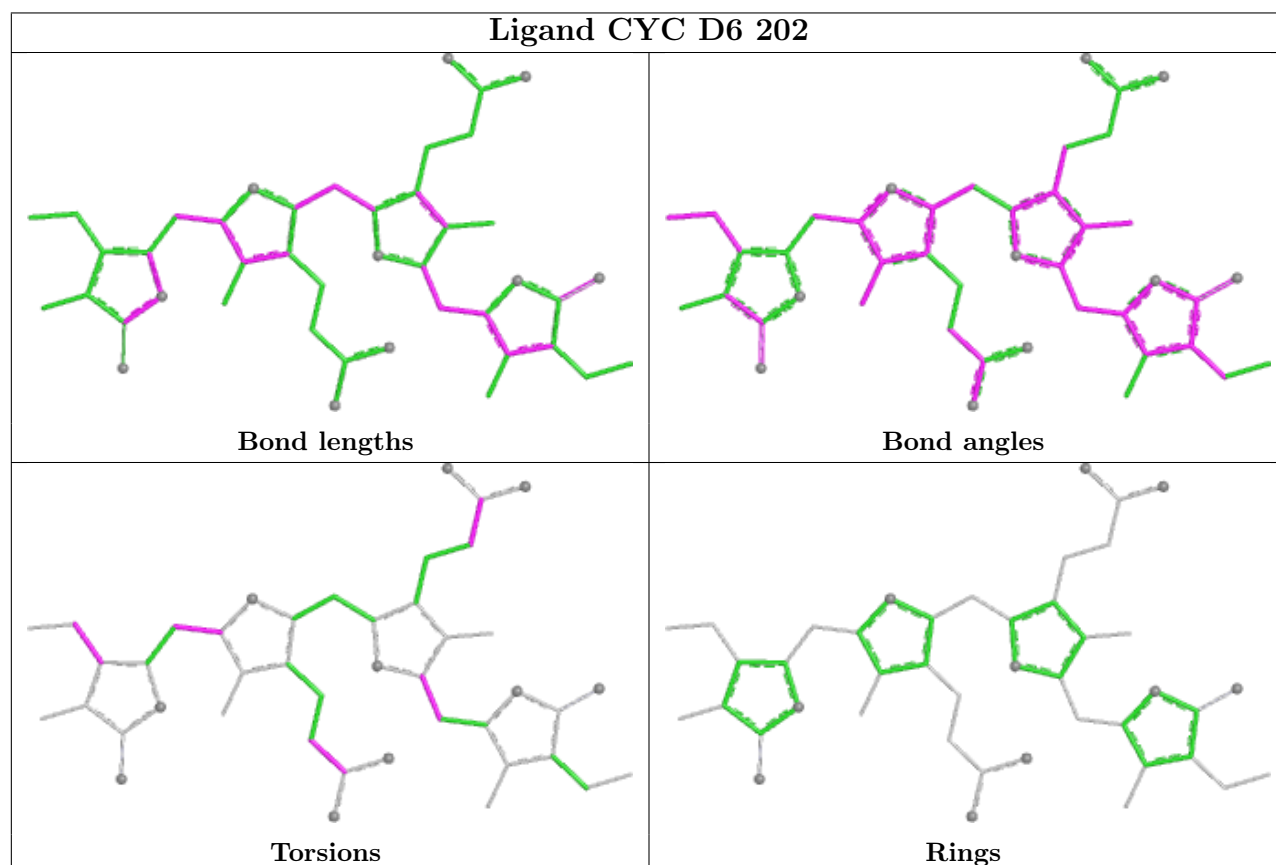




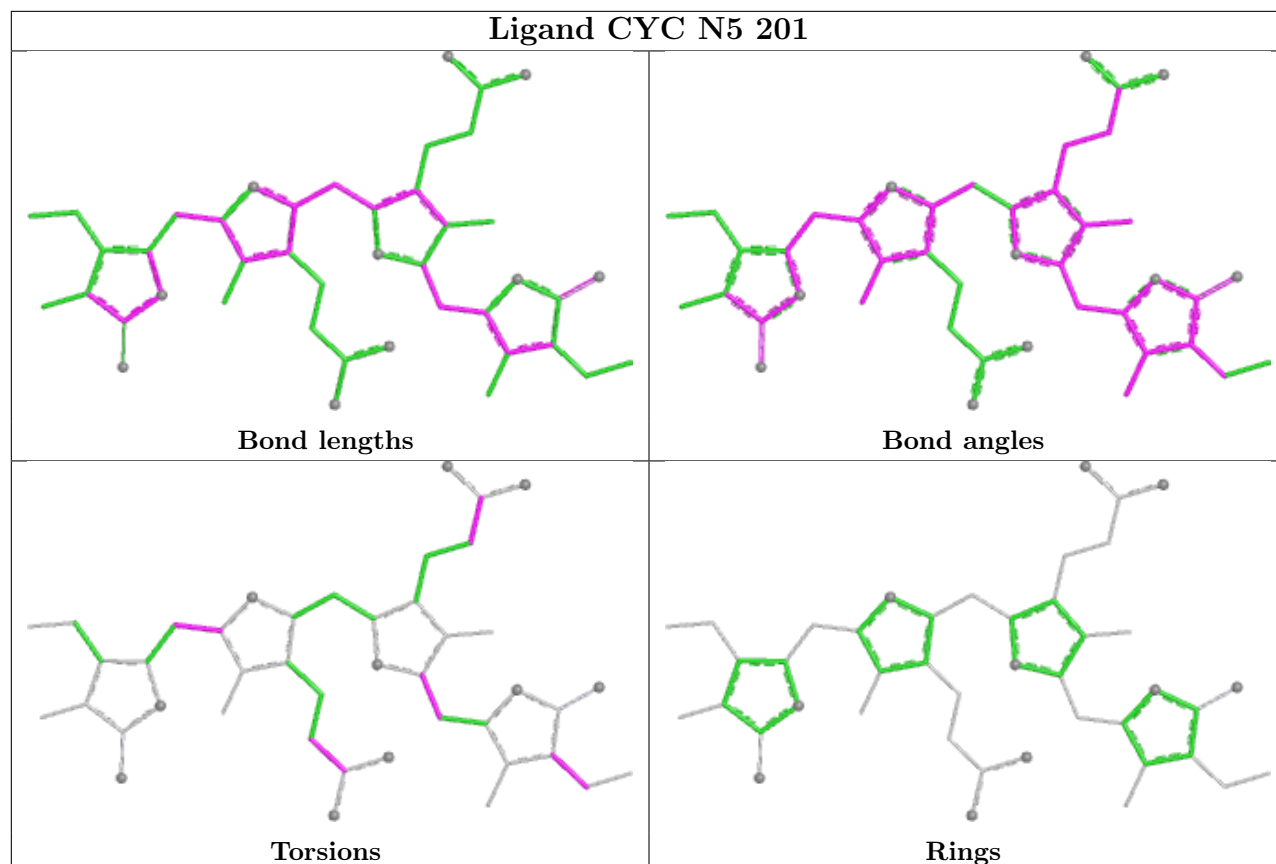
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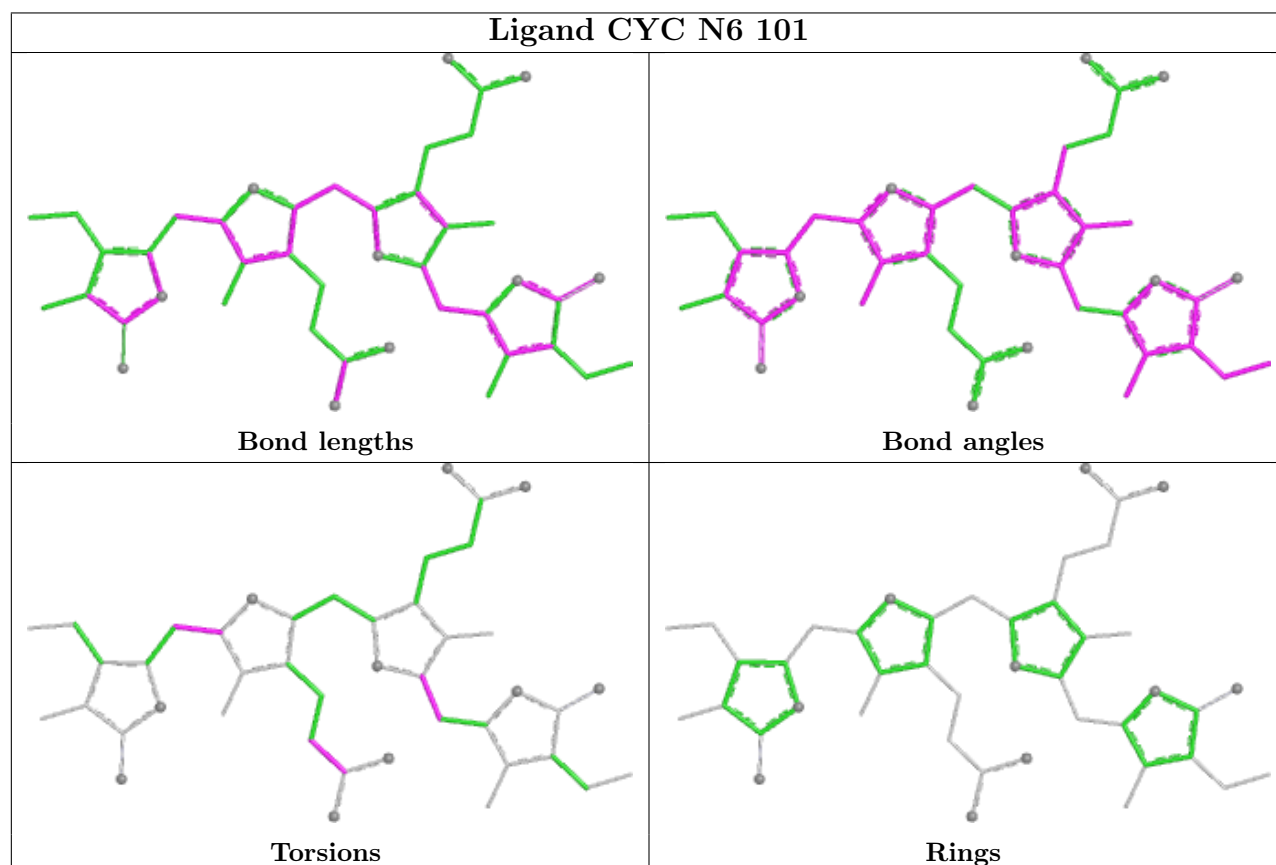
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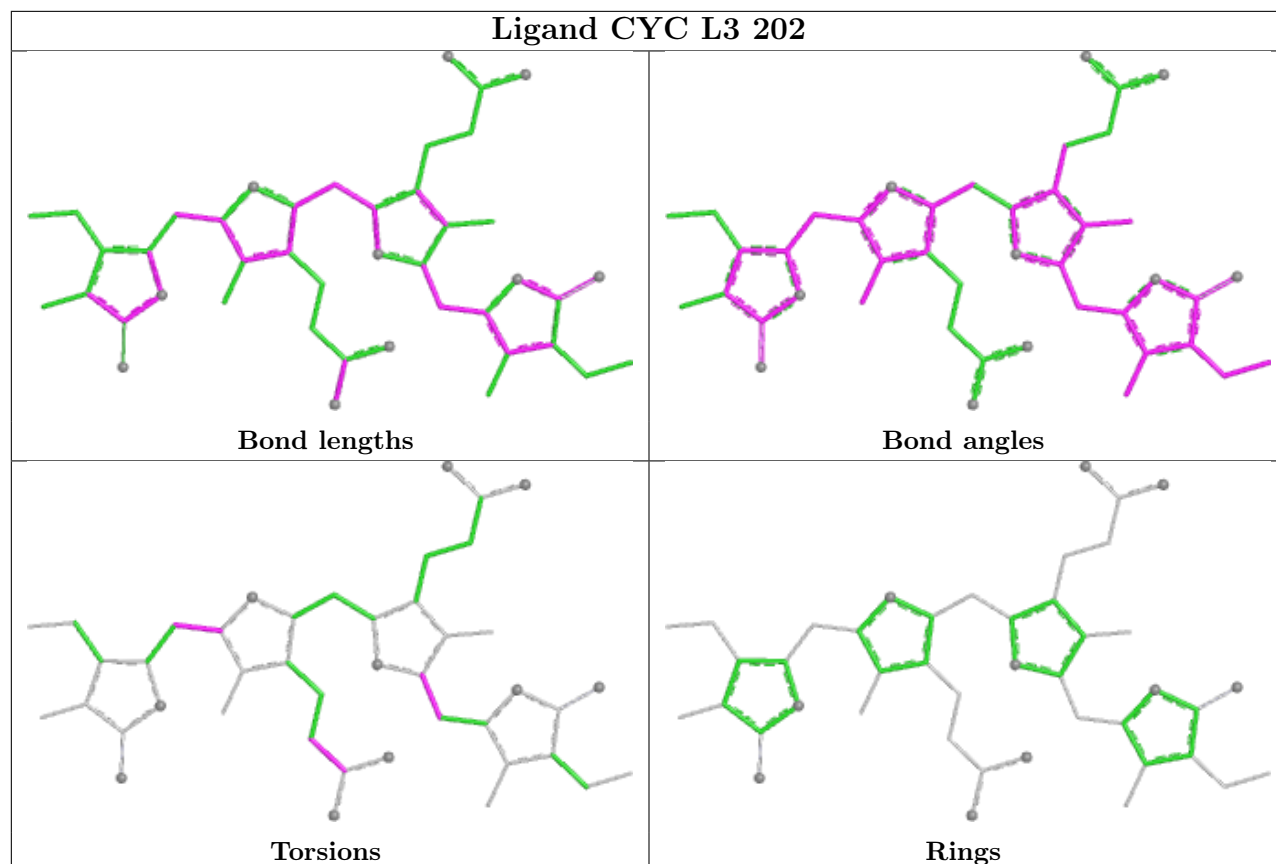
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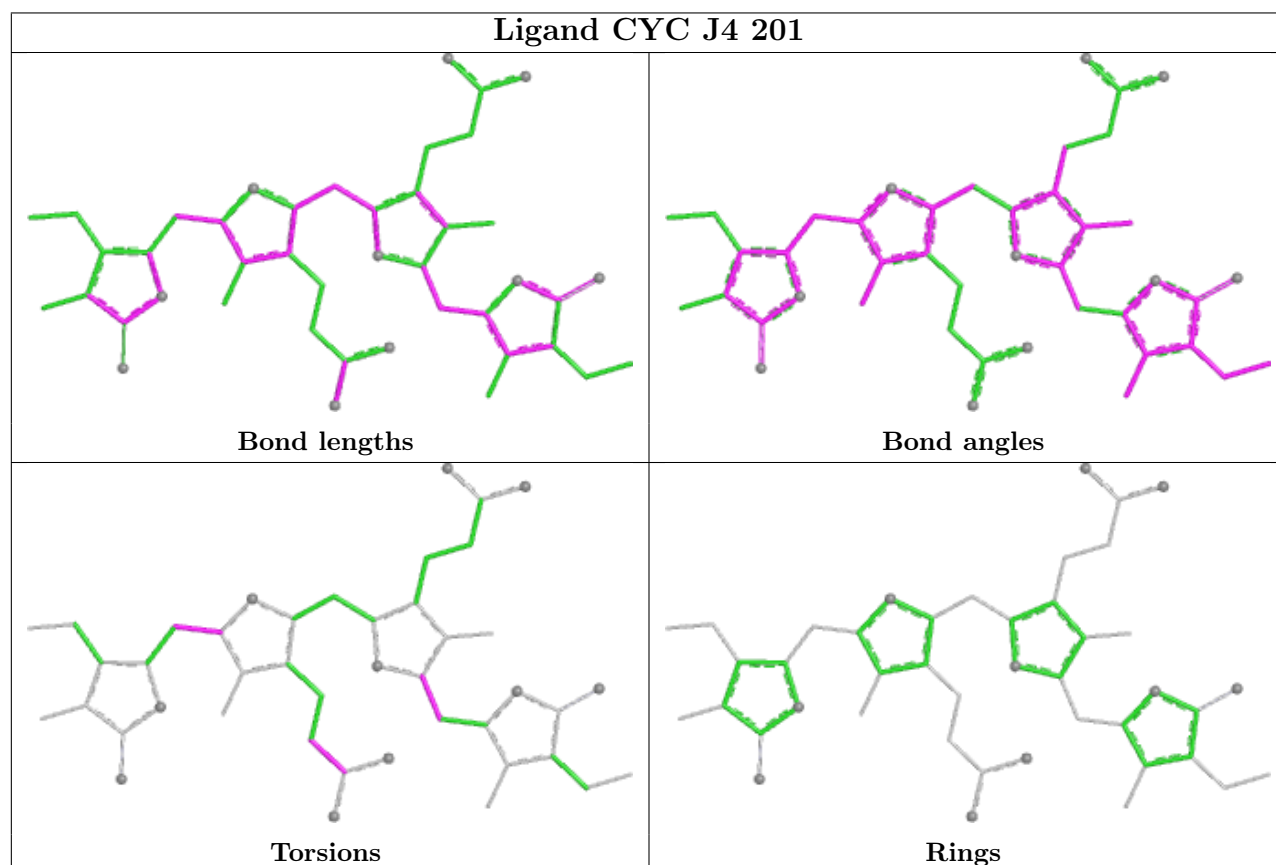
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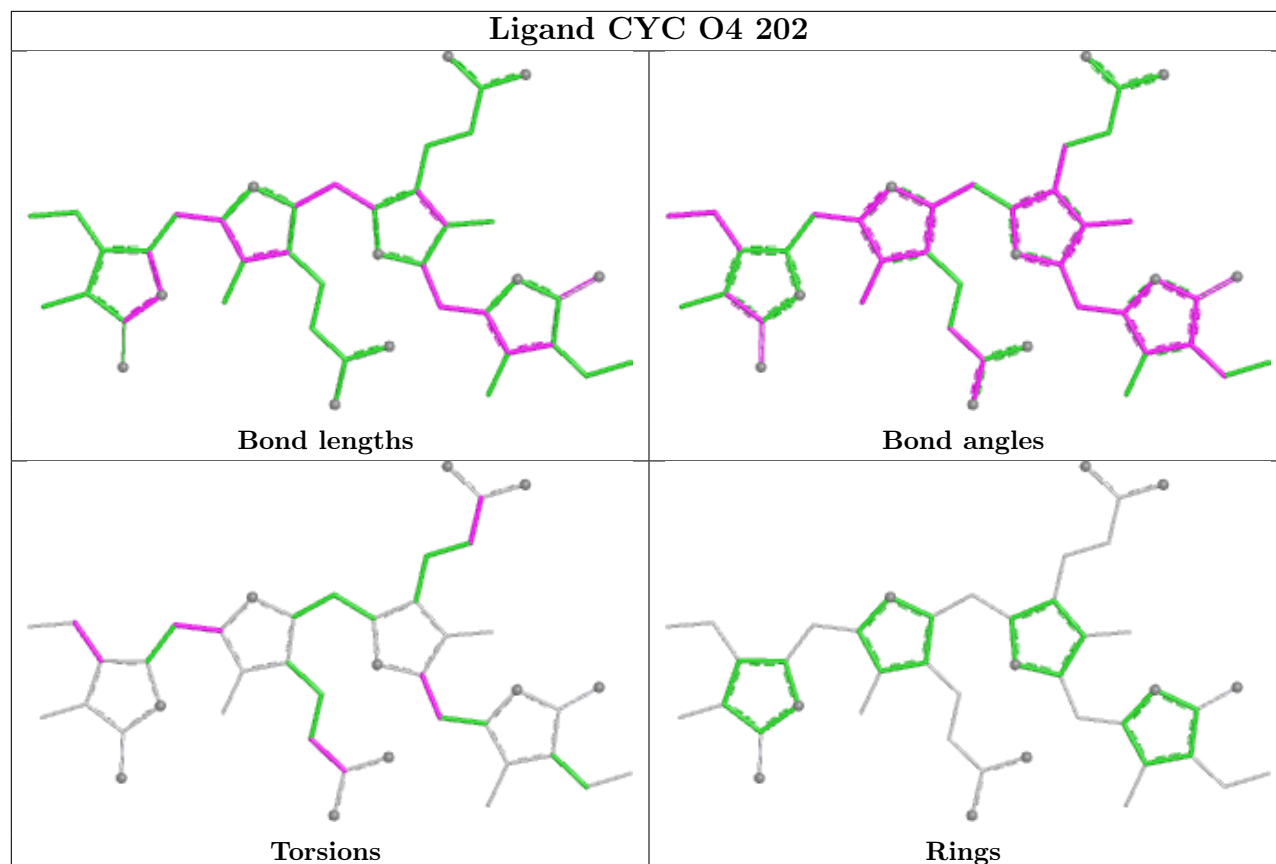
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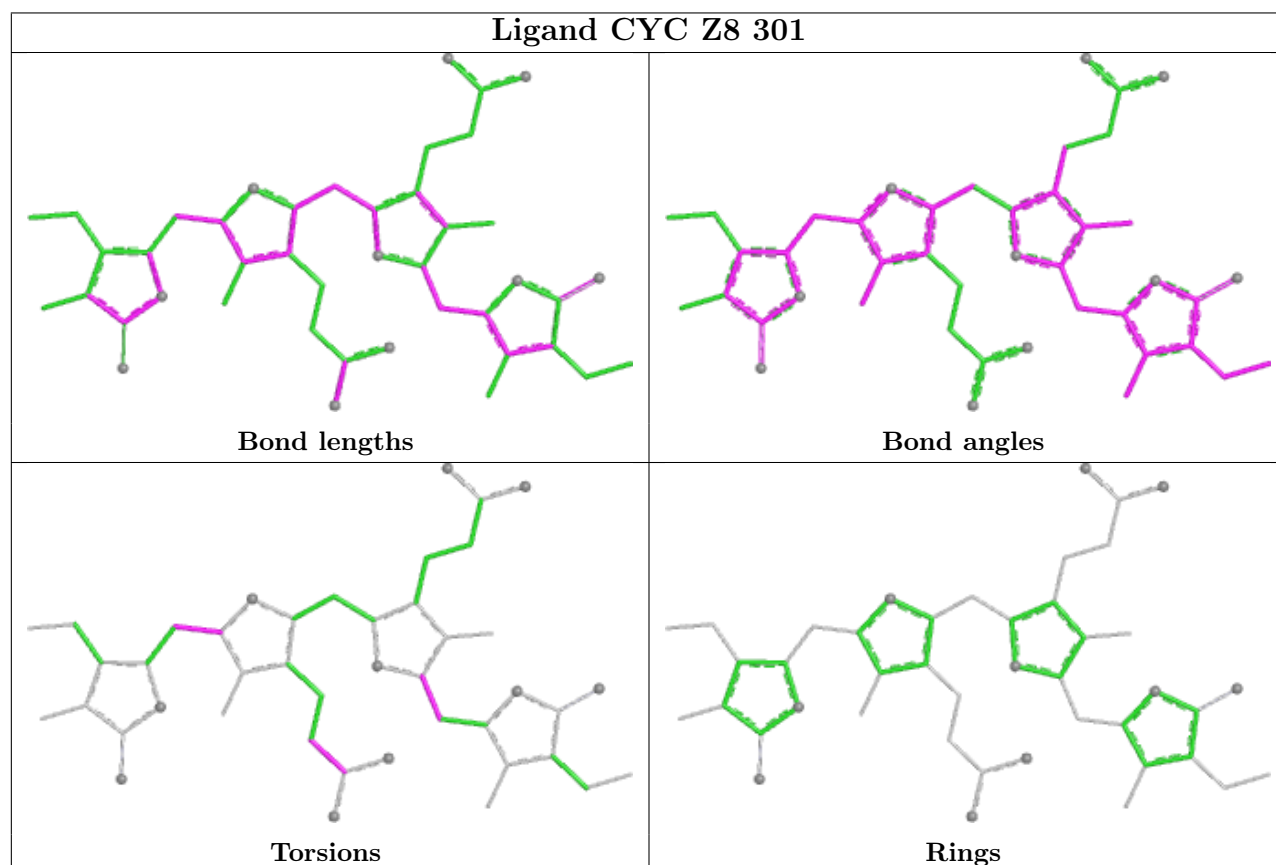
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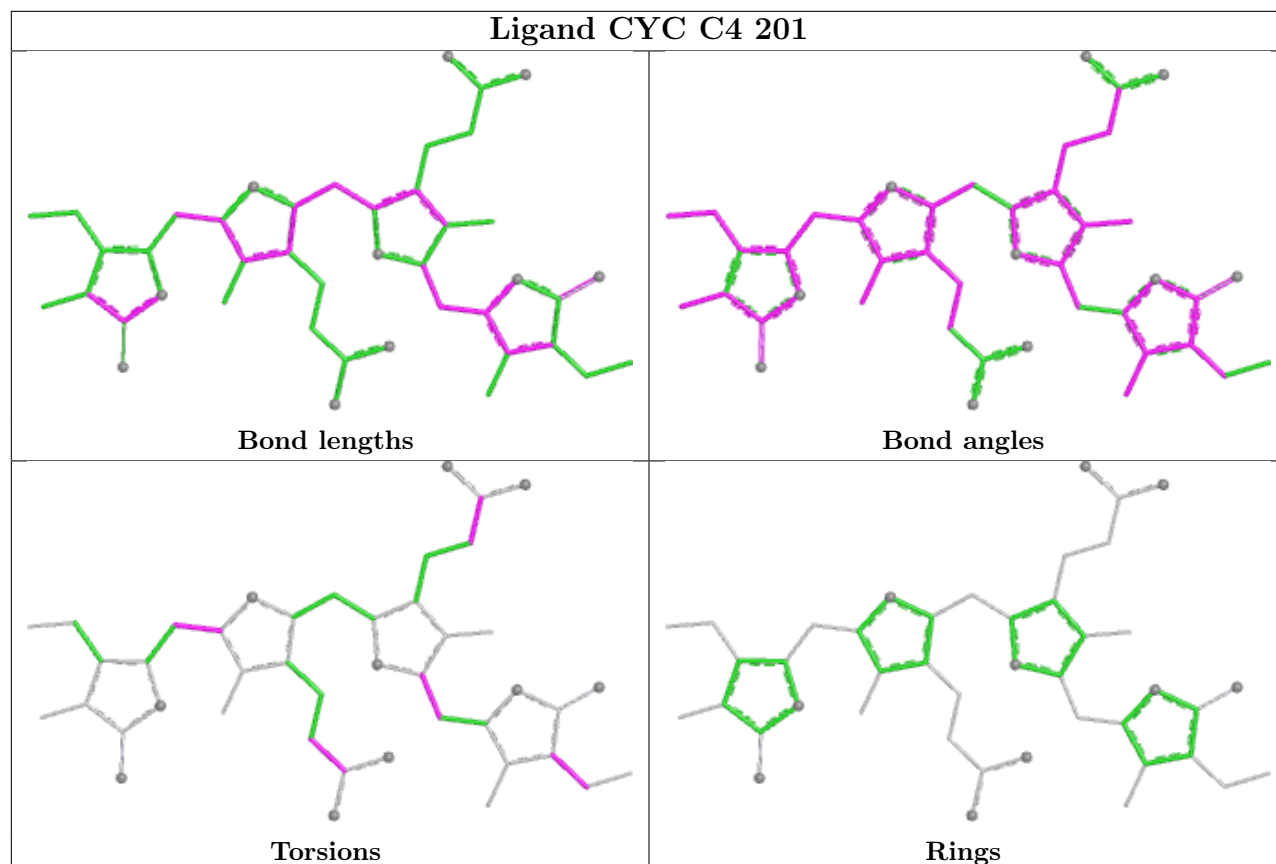
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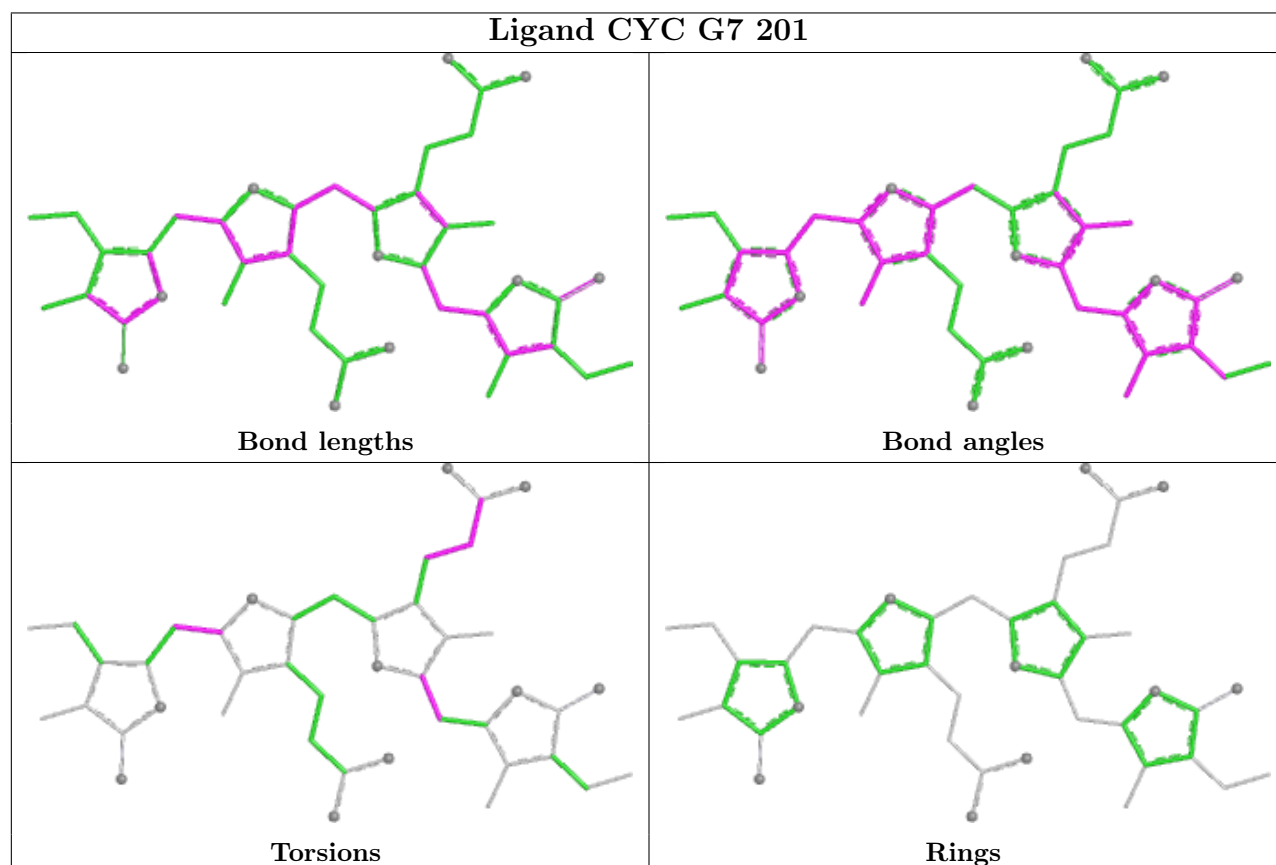
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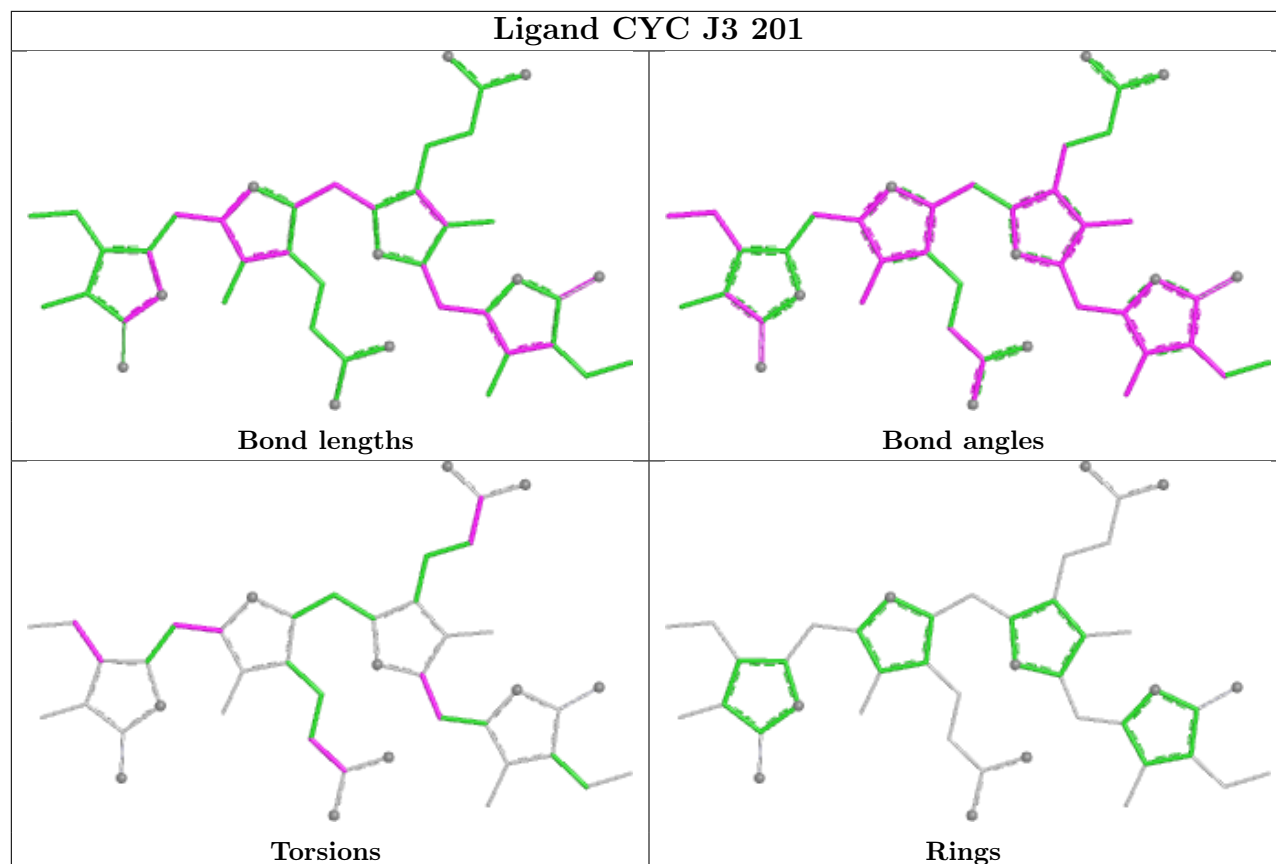
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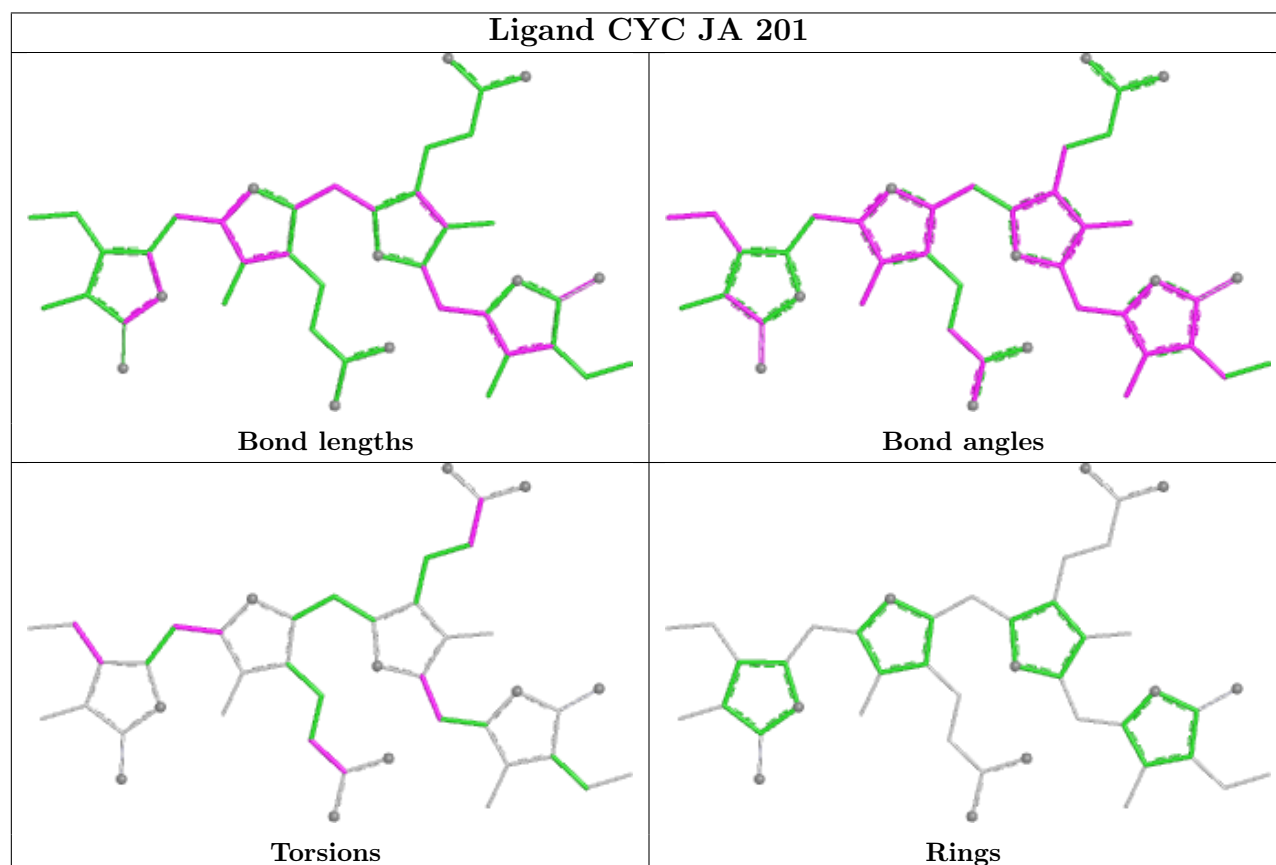
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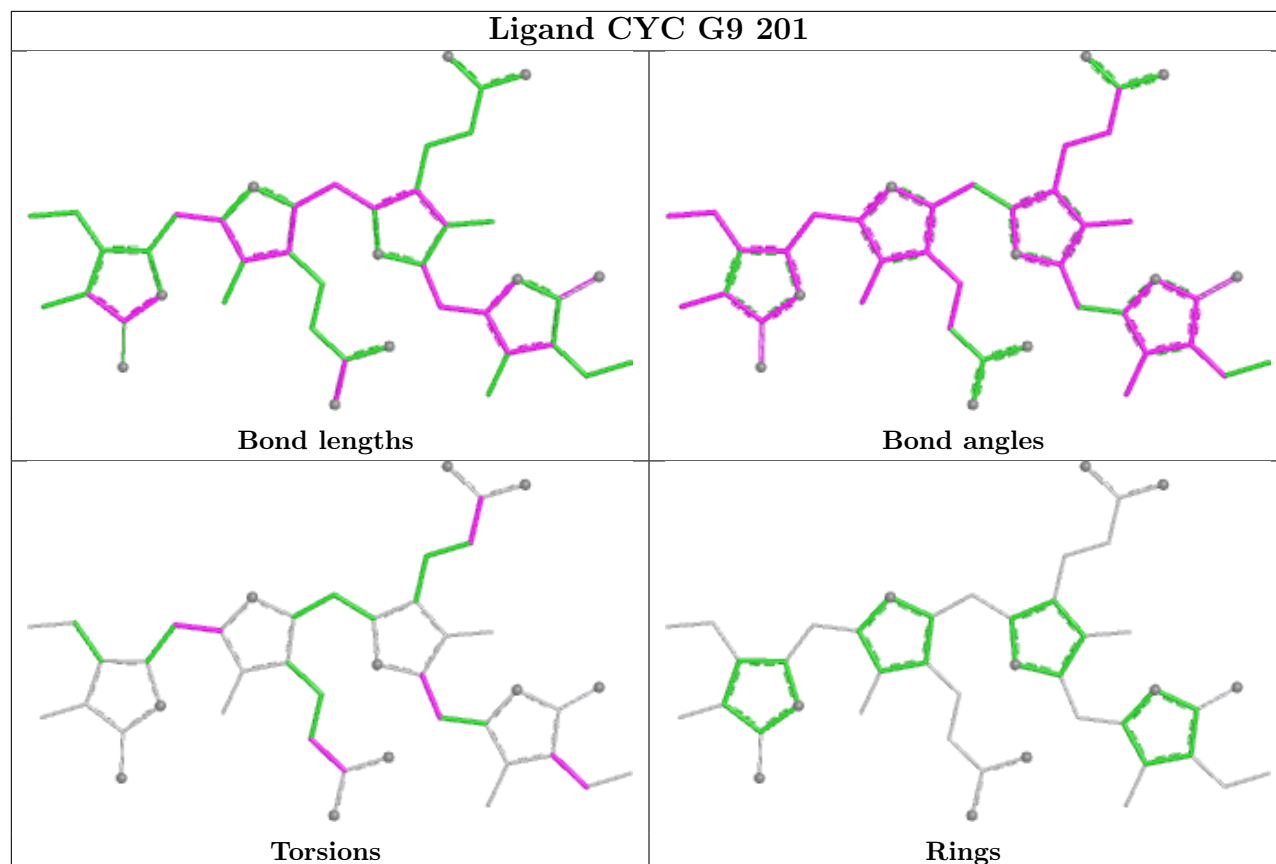
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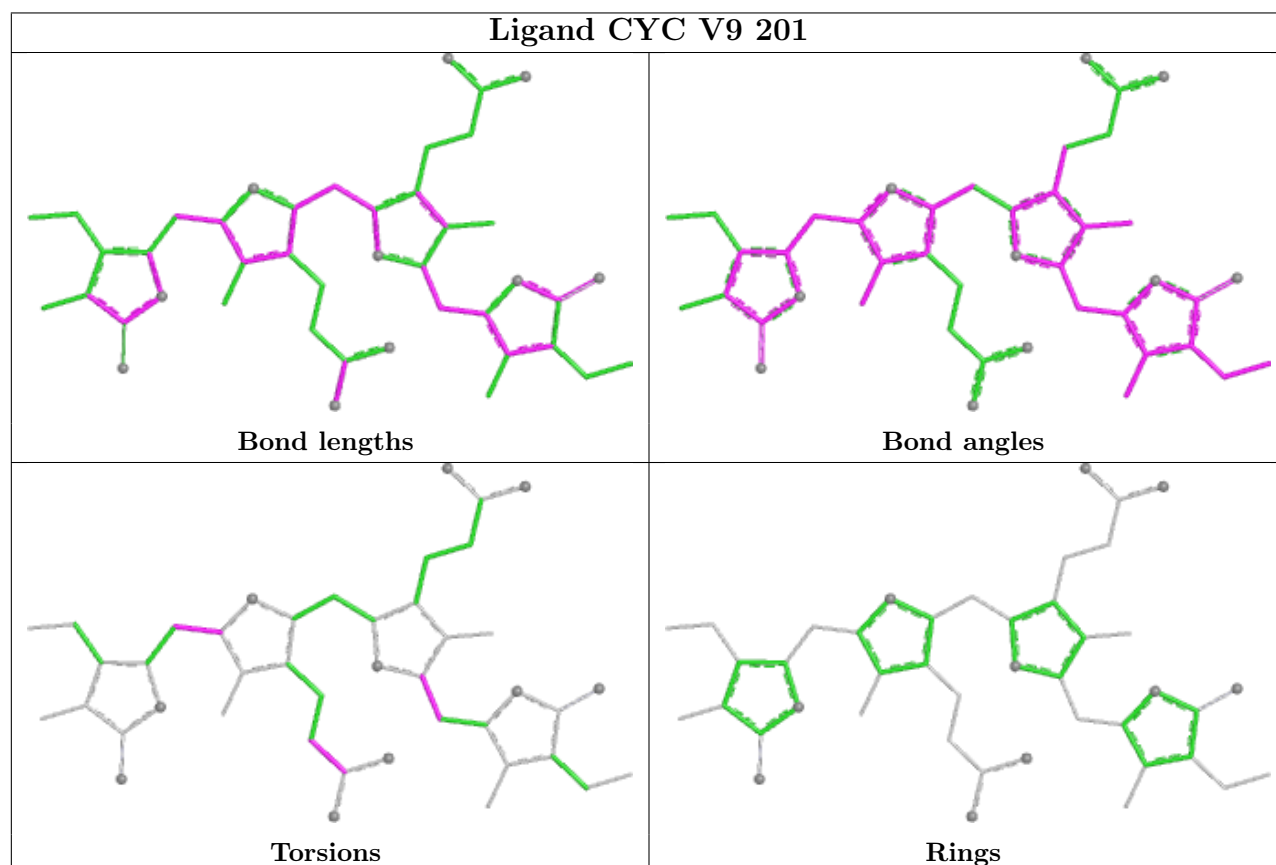
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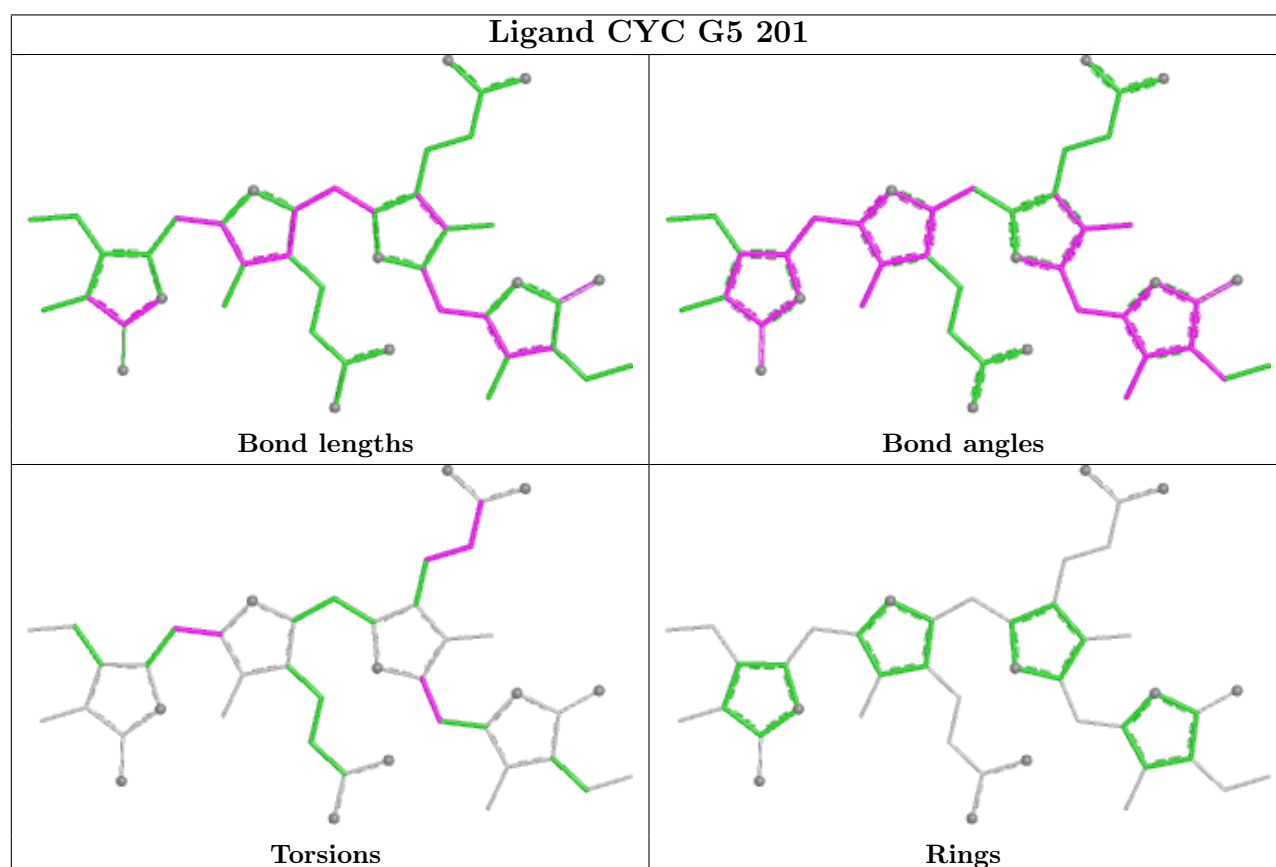
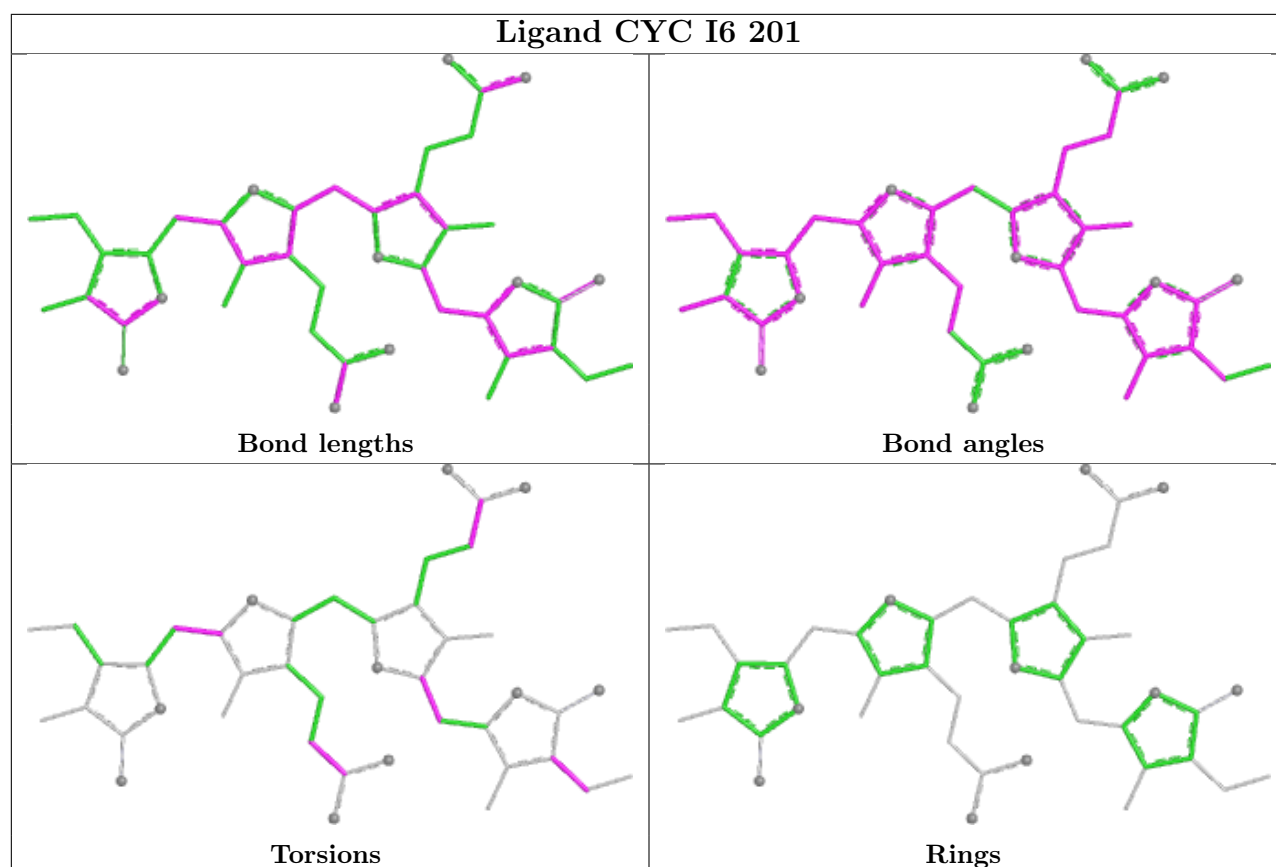


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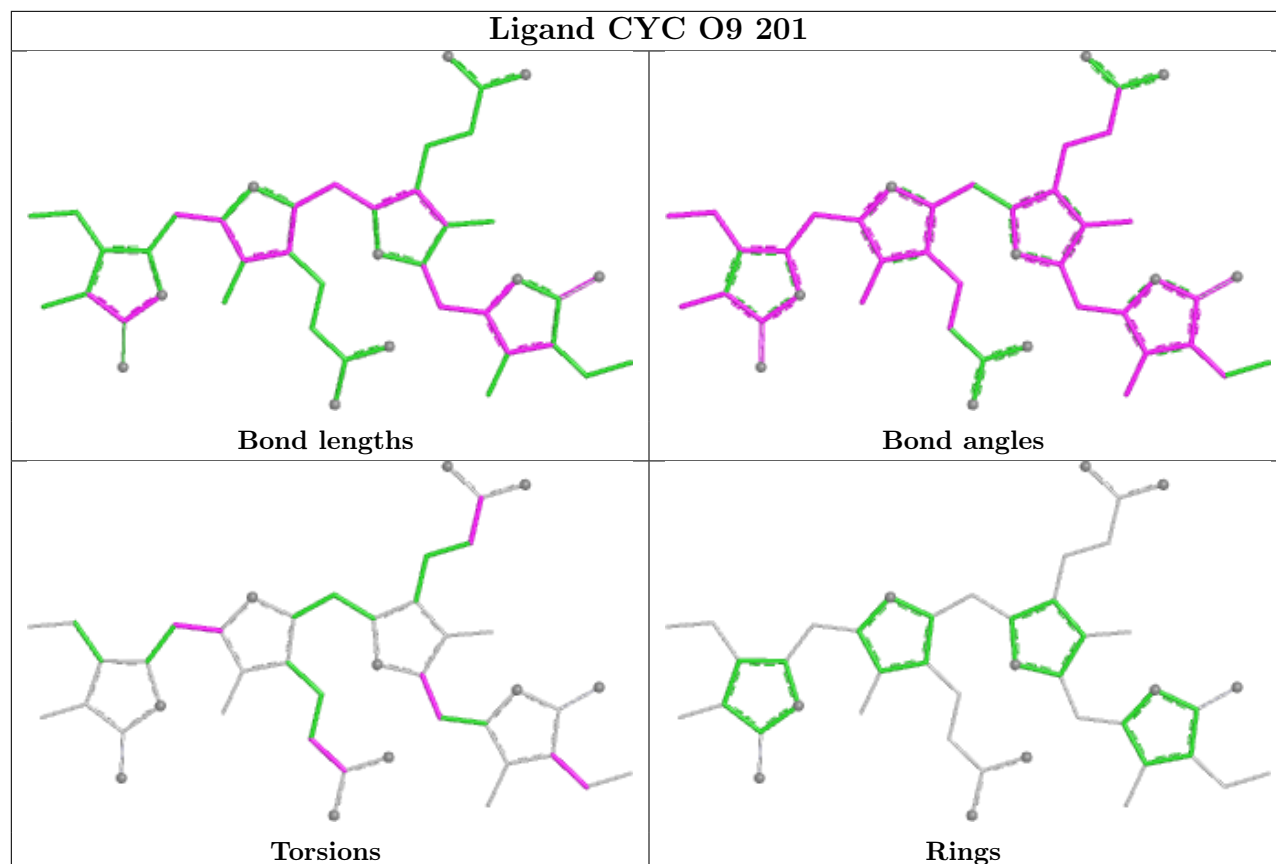


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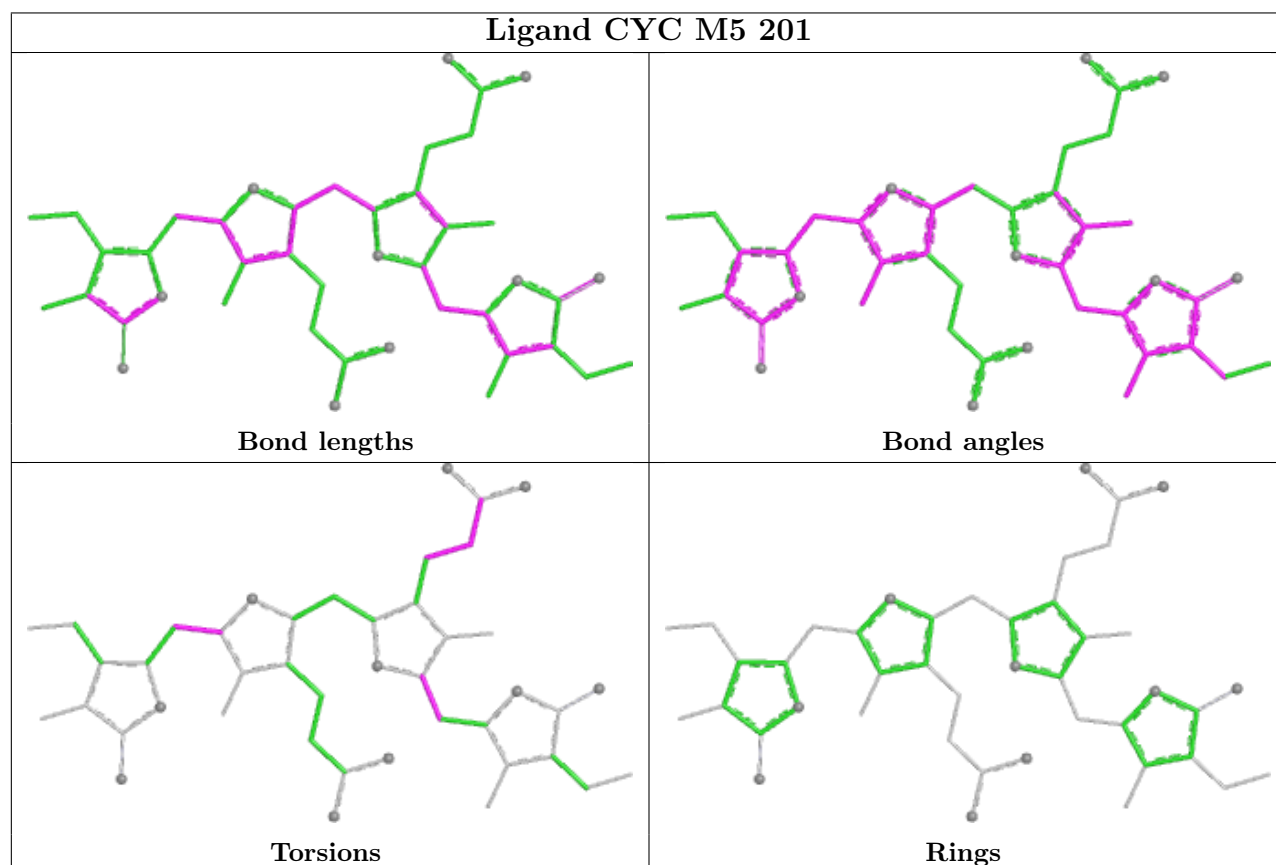




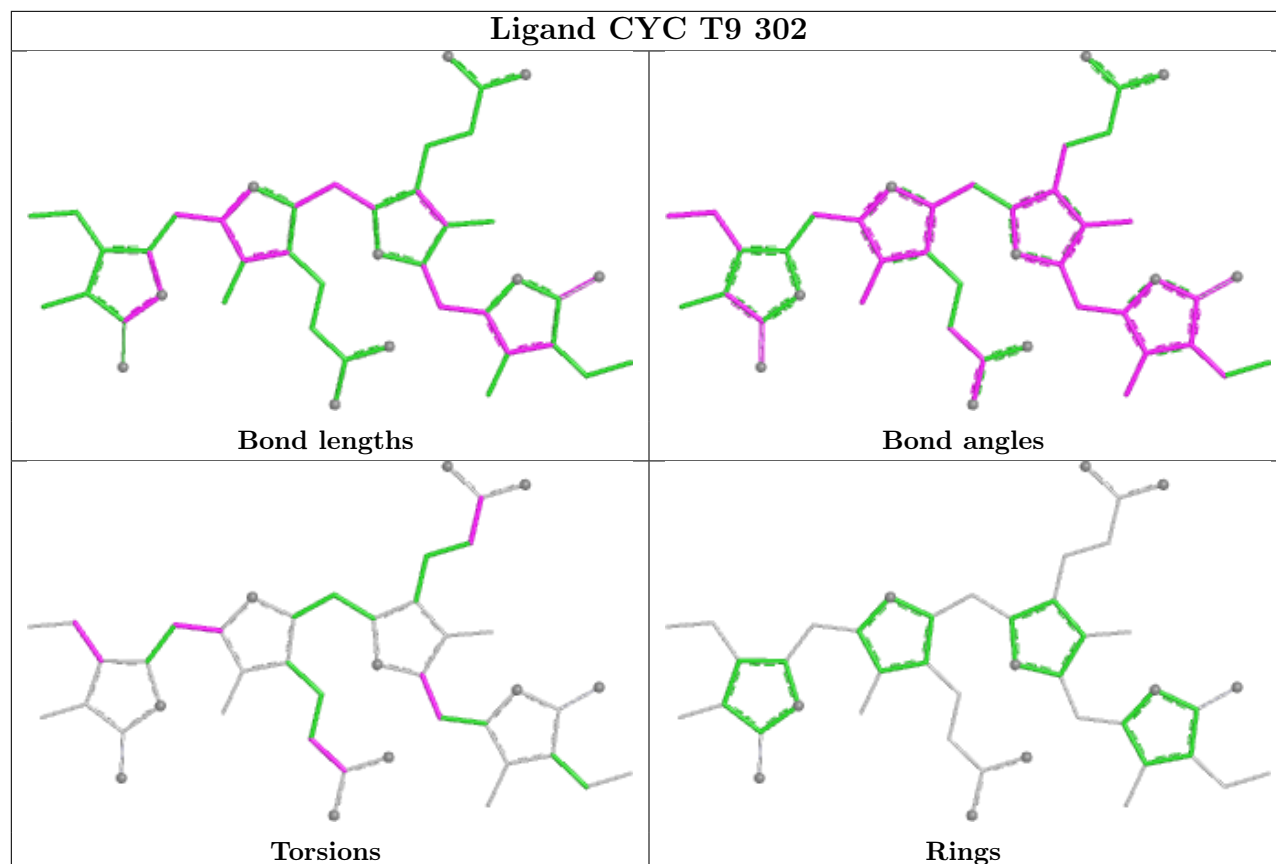
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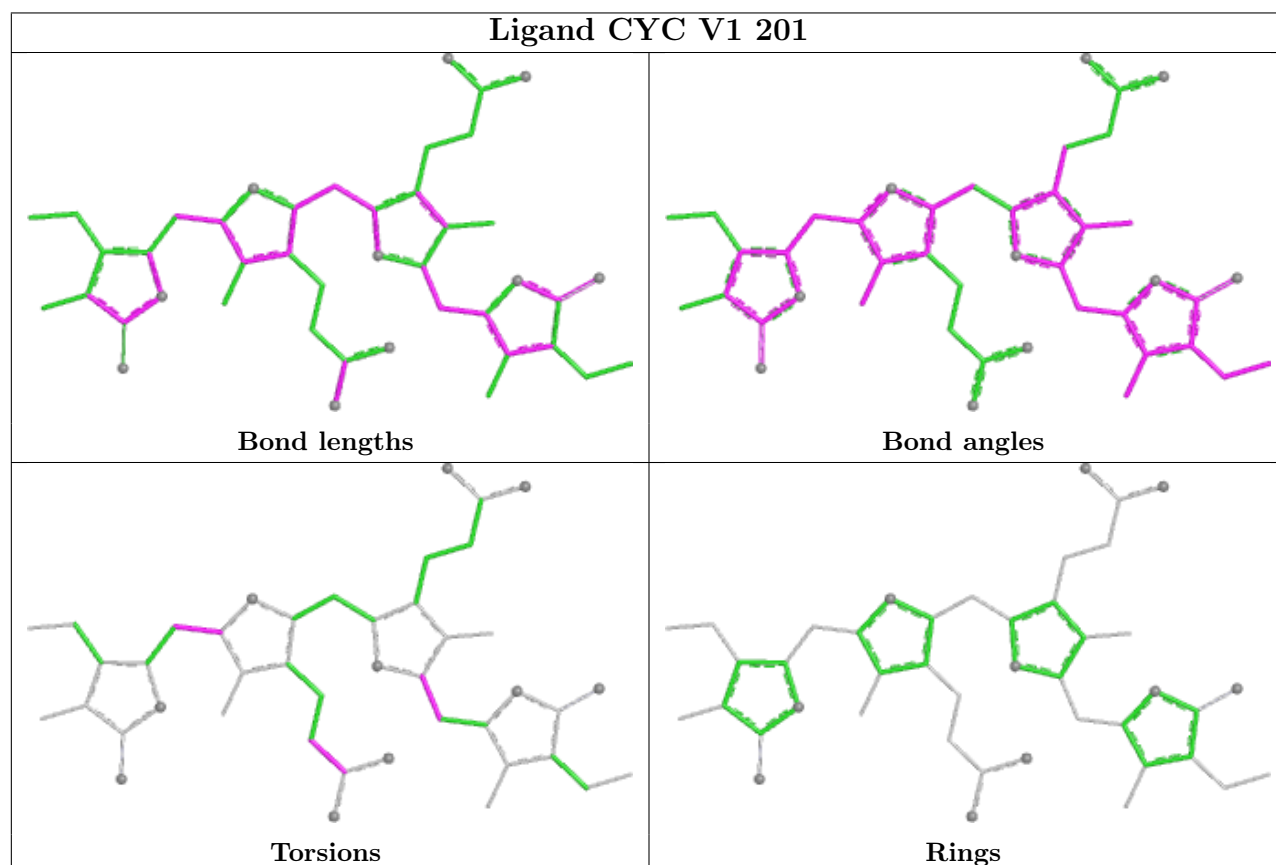
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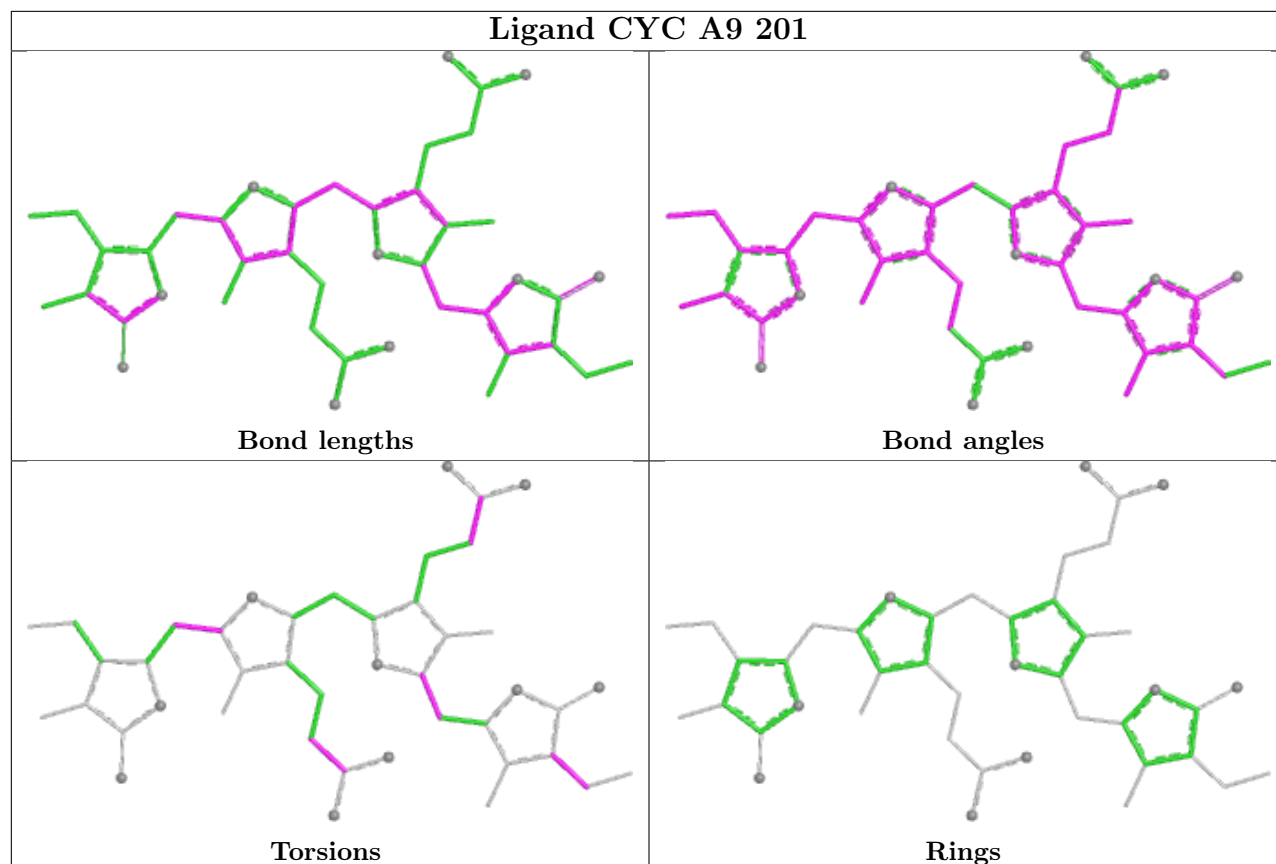
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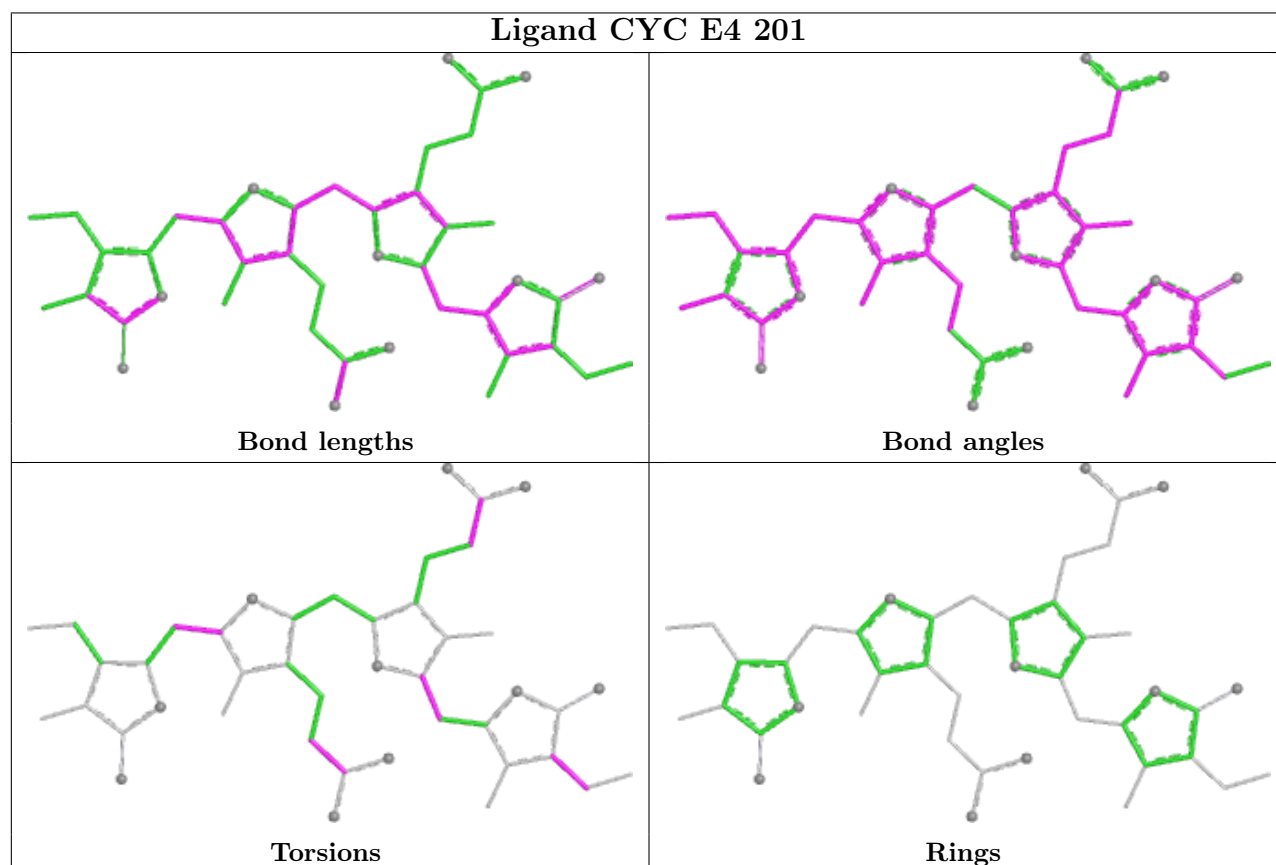
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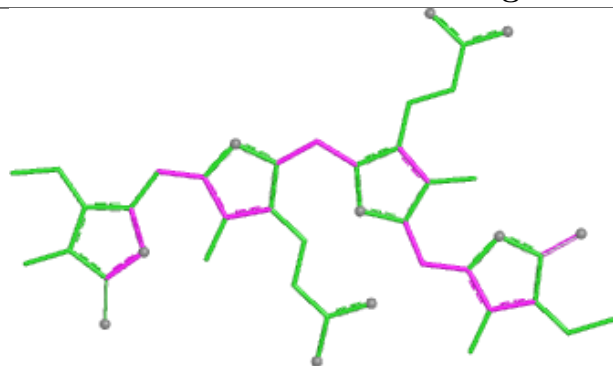
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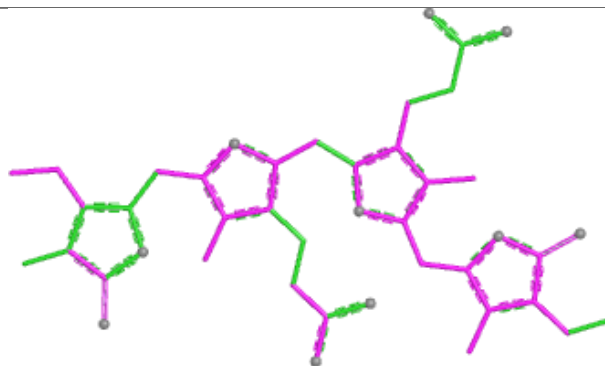
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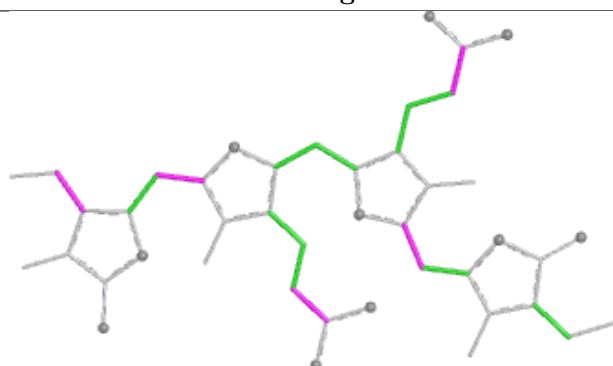
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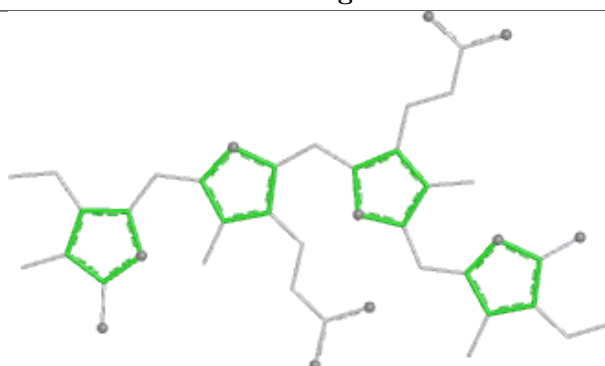
Bond lengths



Bond angles

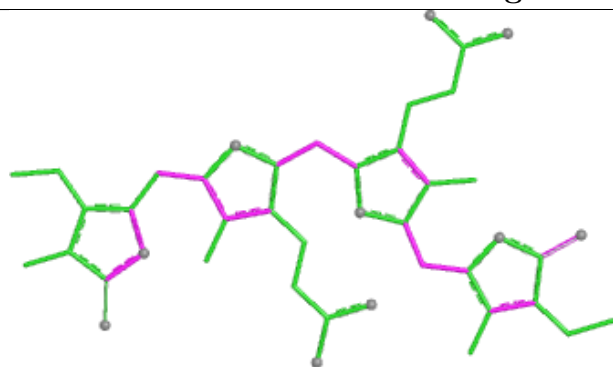


Torsions

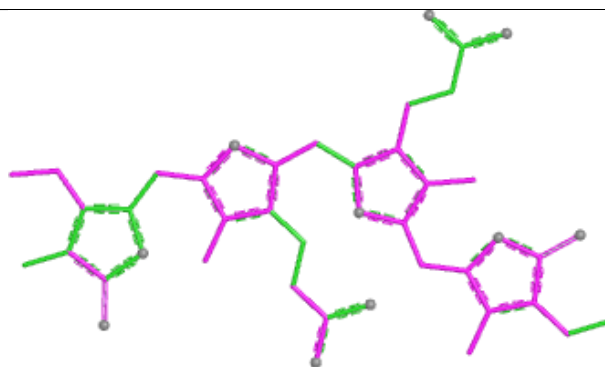


Rings

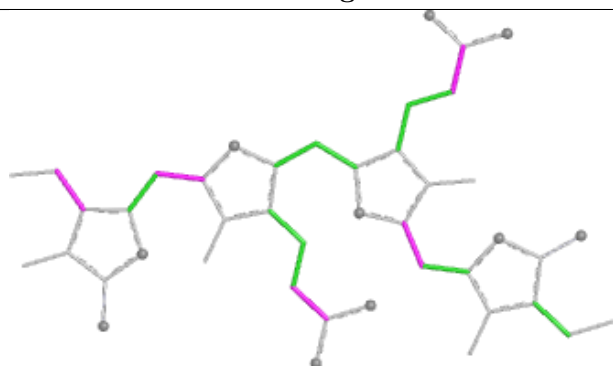
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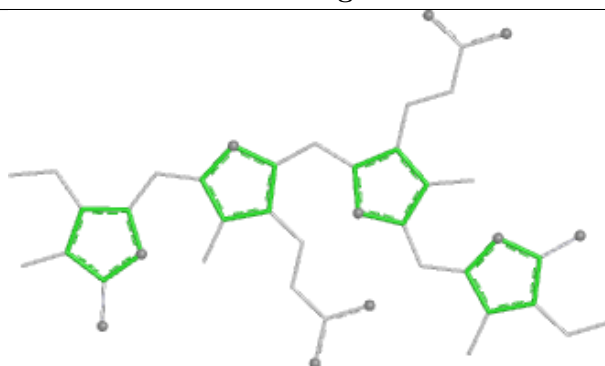
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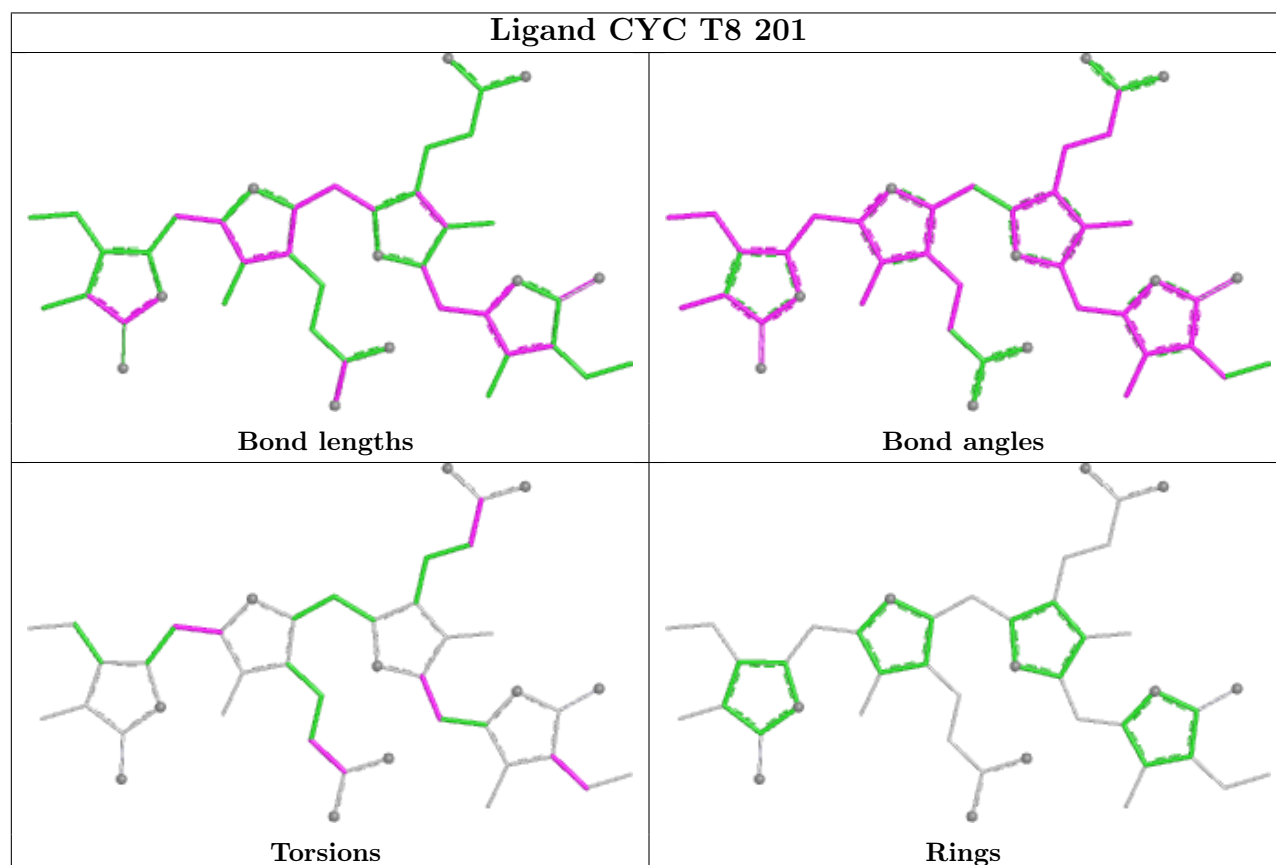
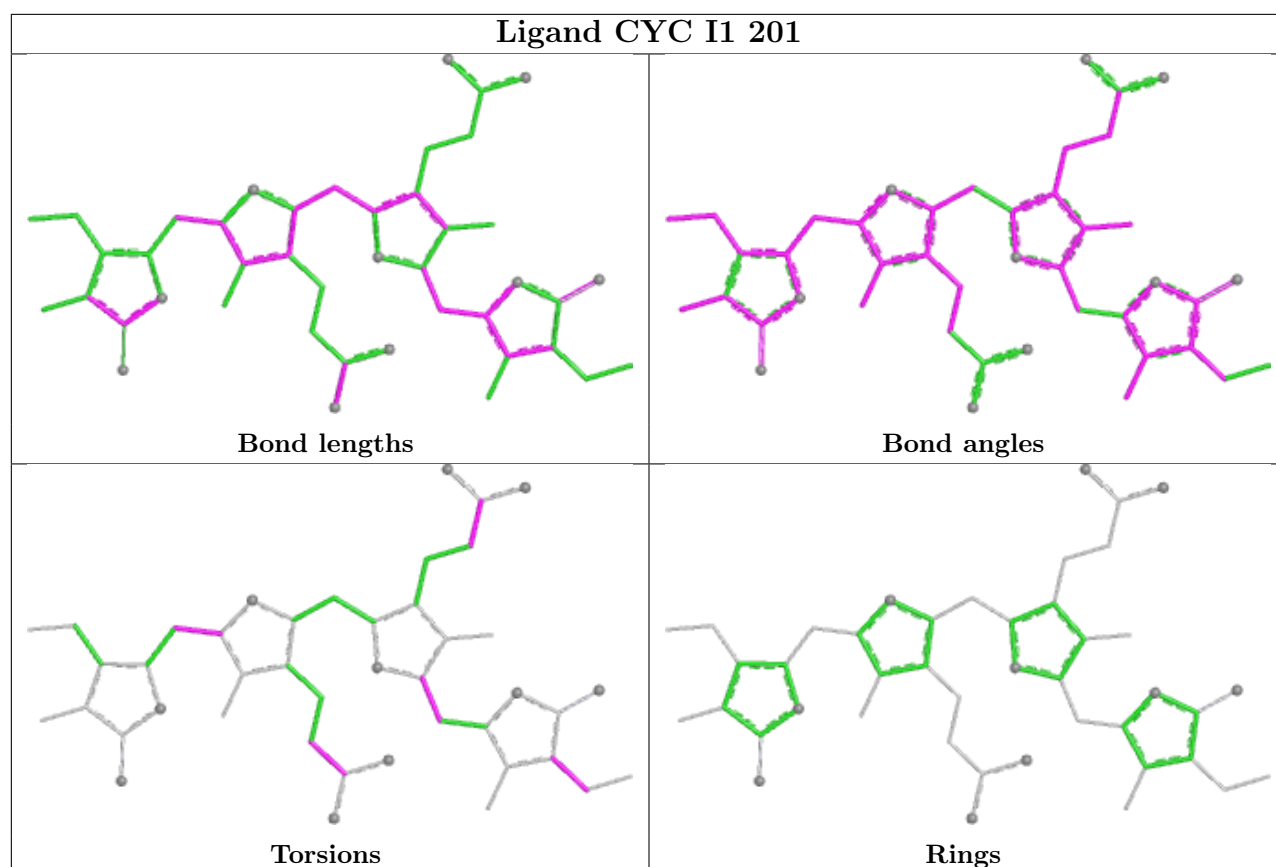
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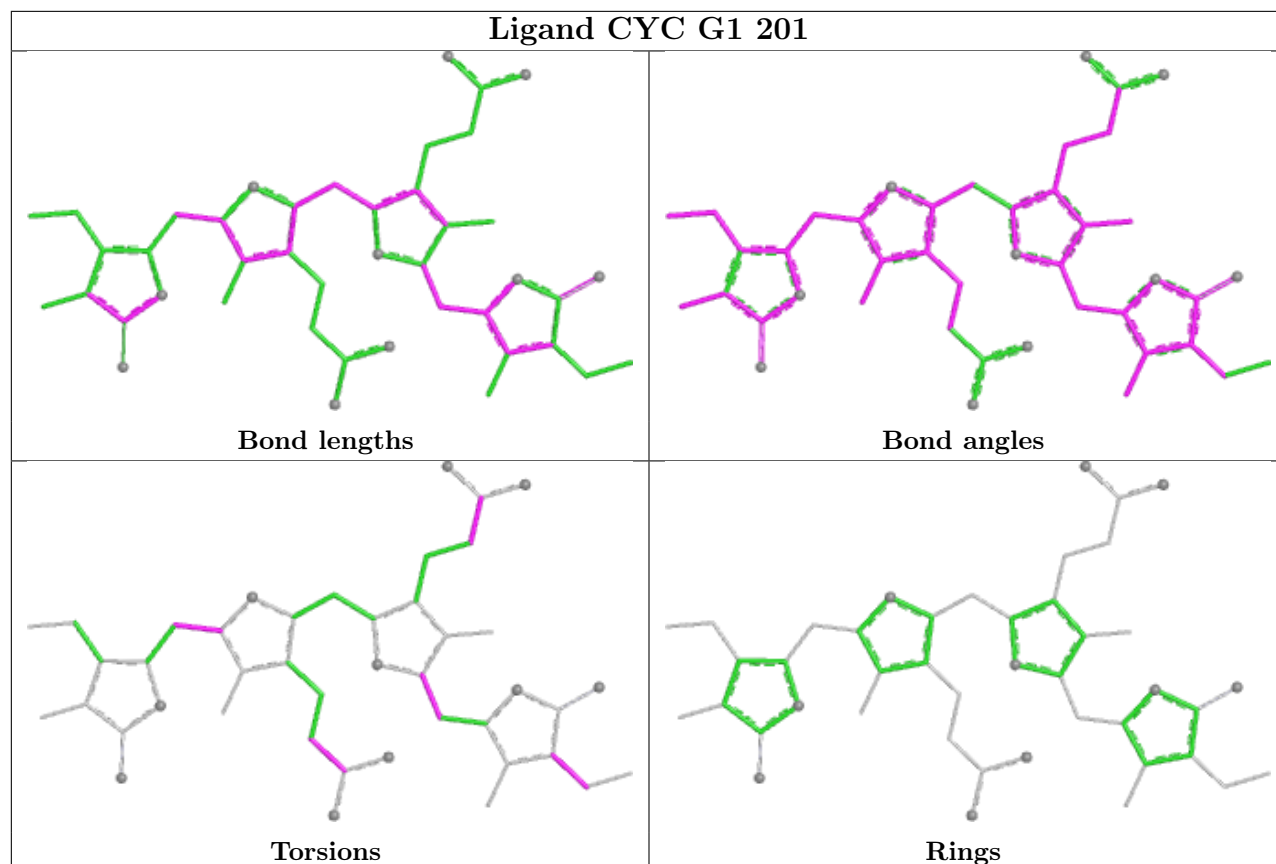
Torsions



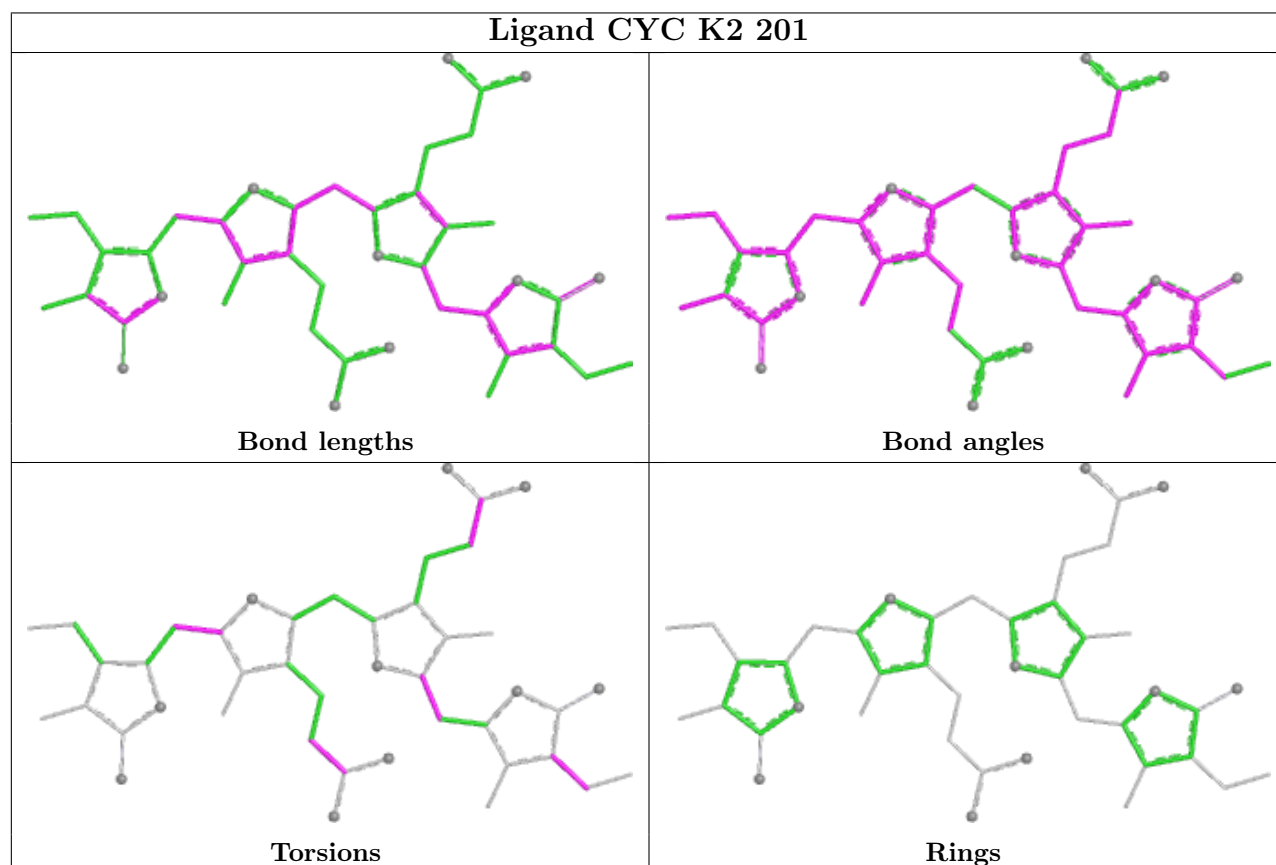
Rings



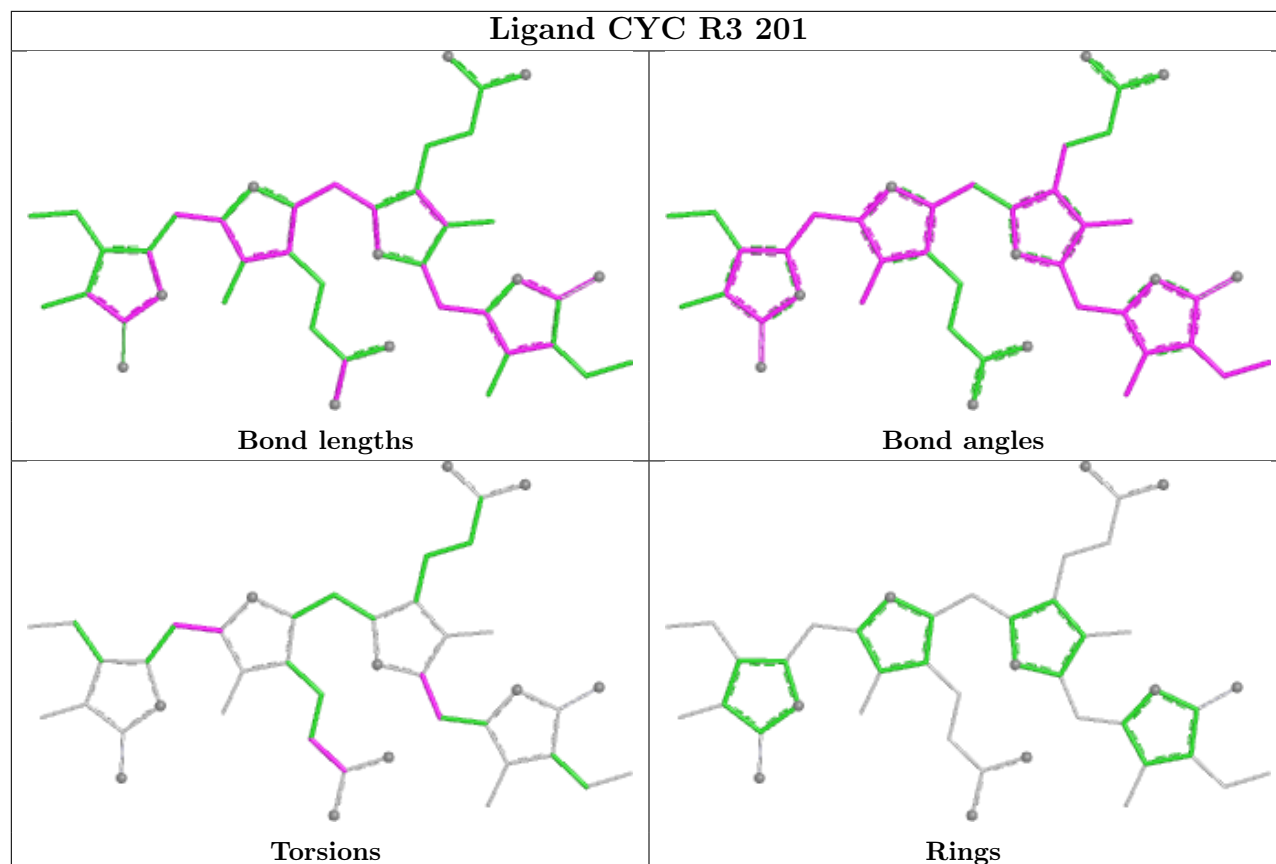
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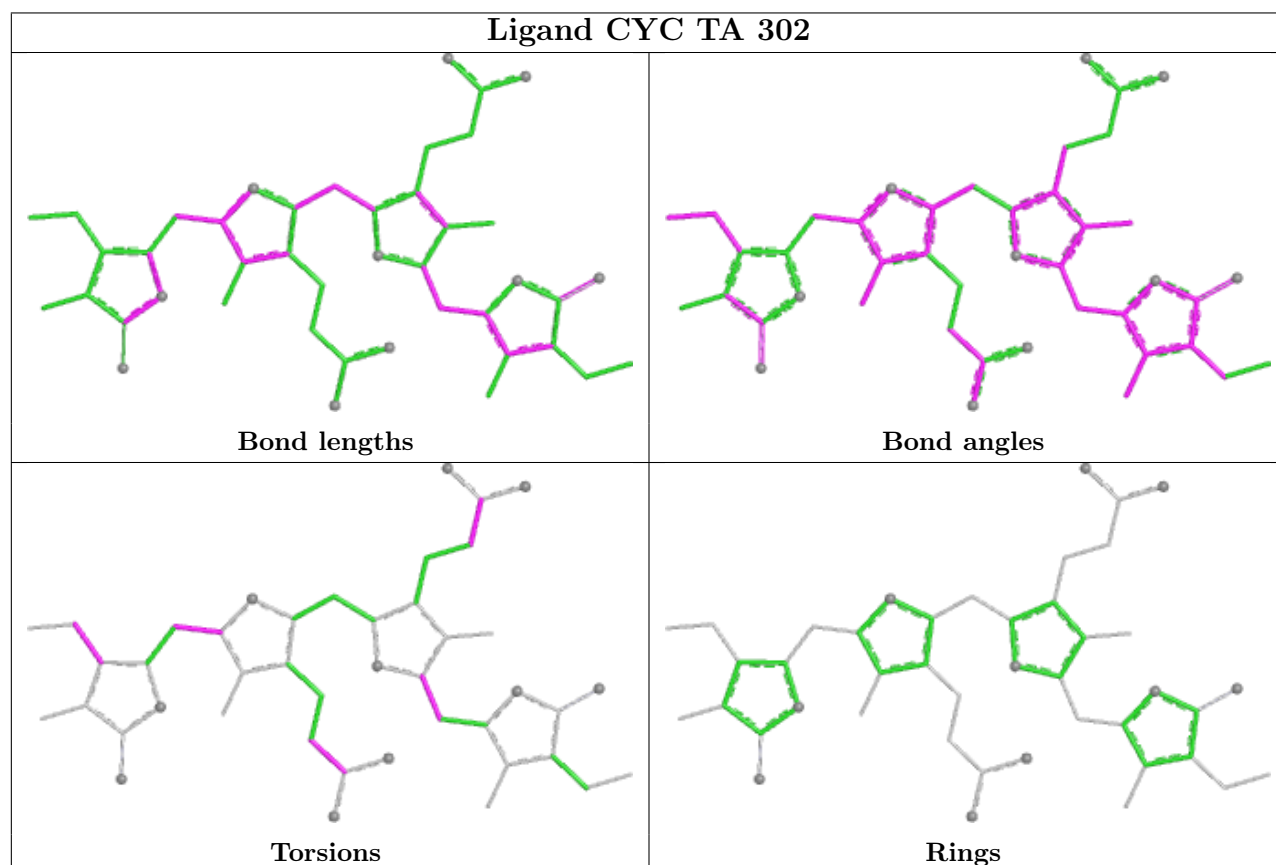
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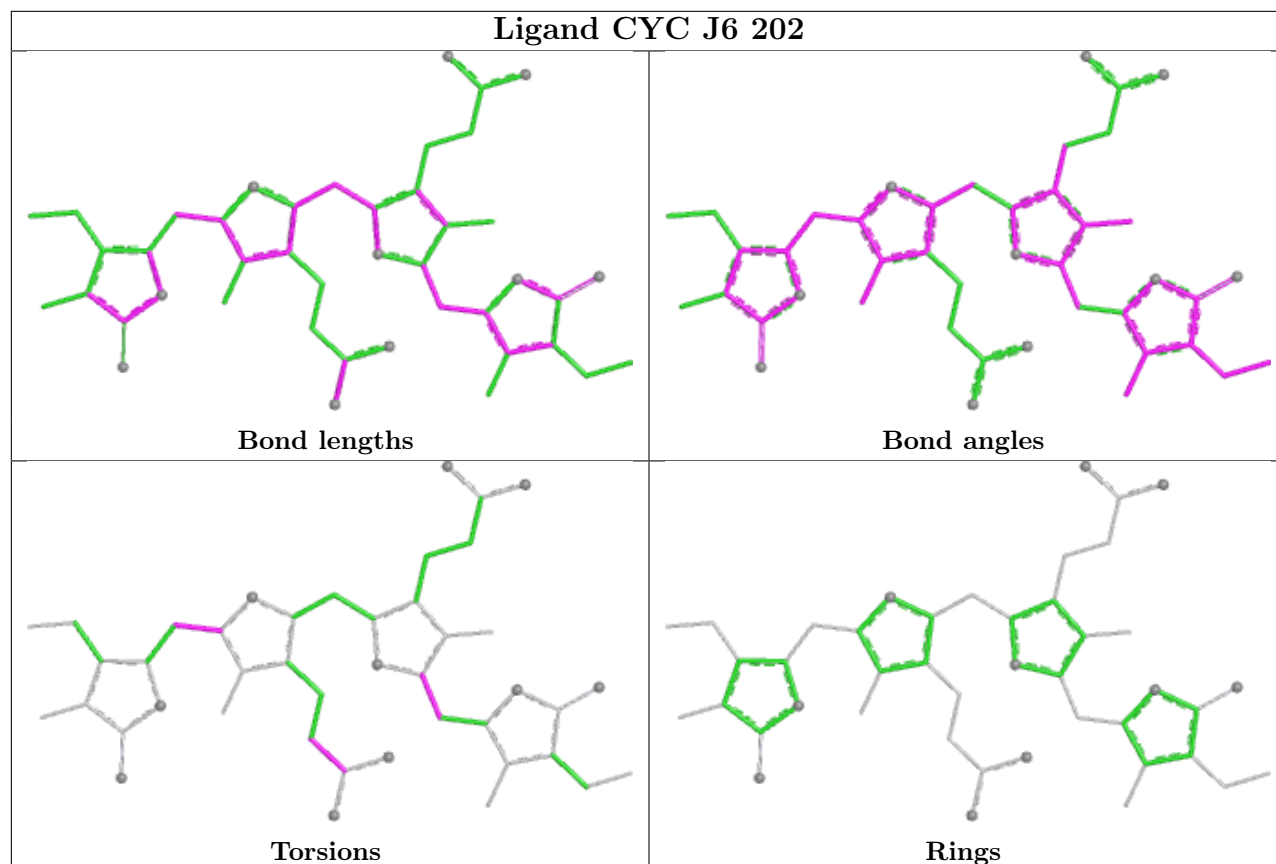
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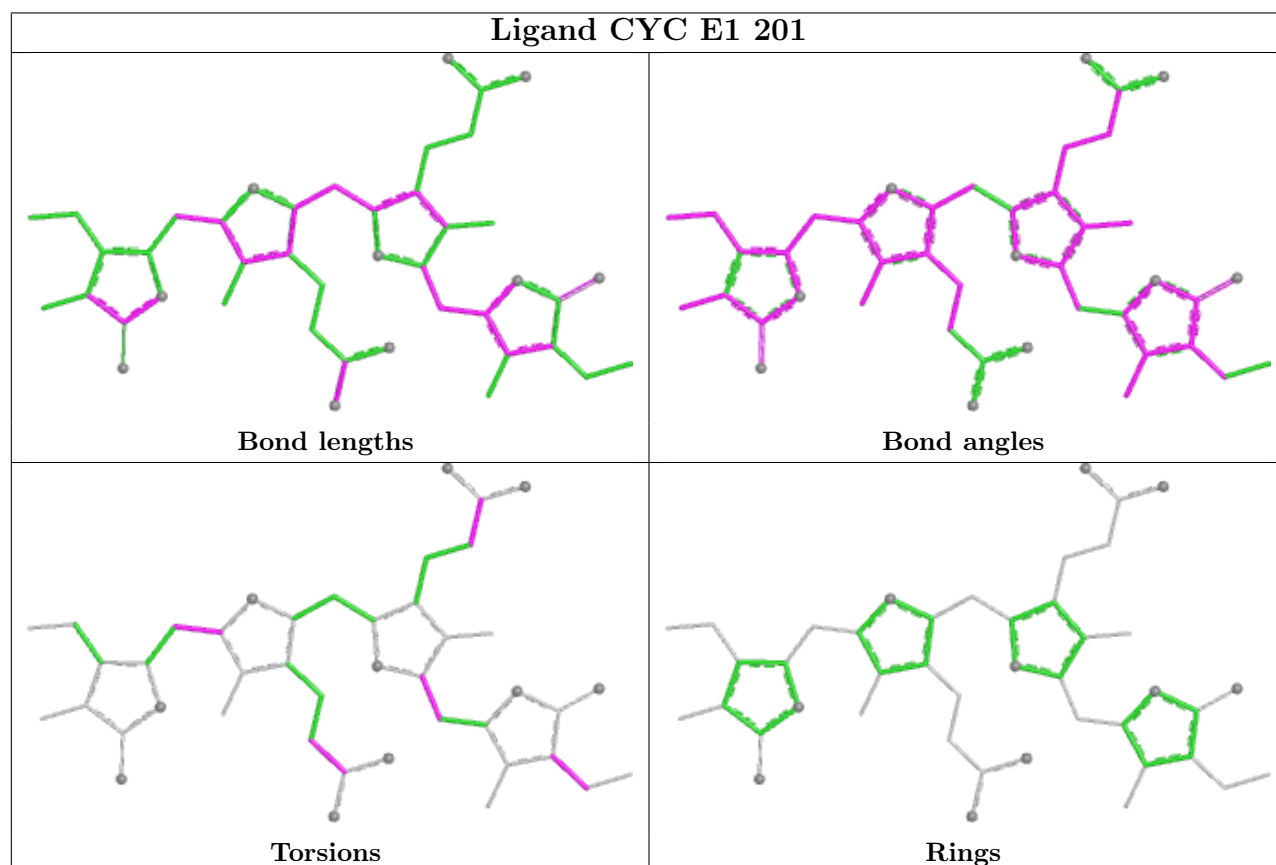
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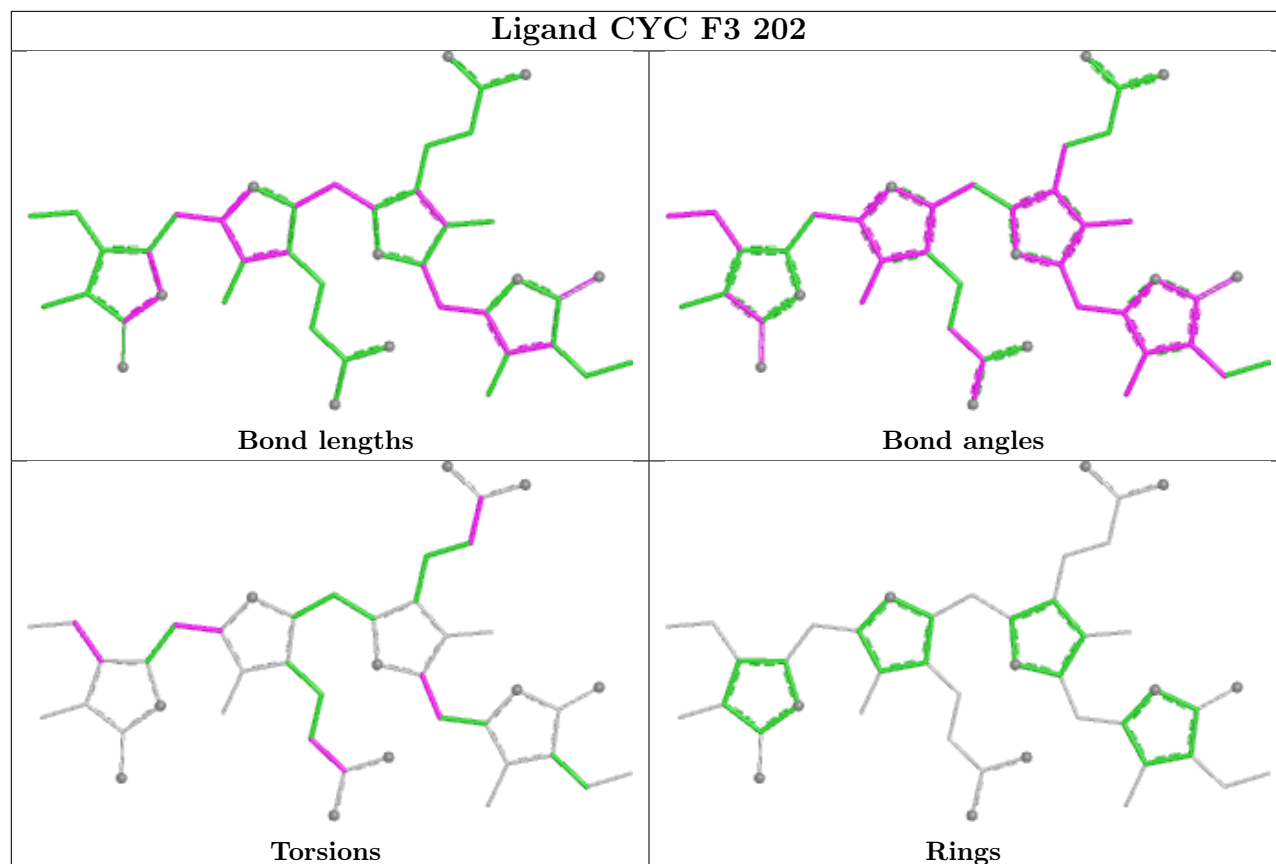
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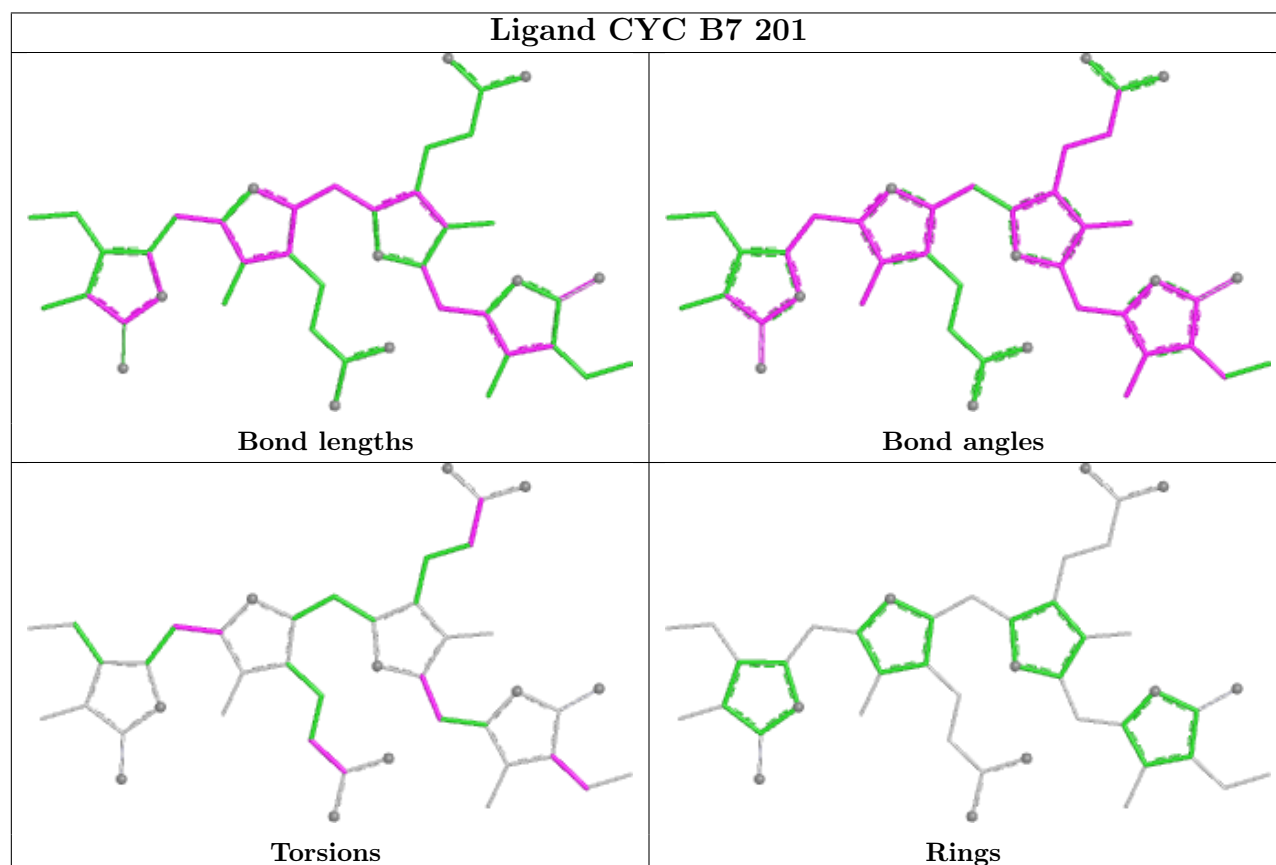
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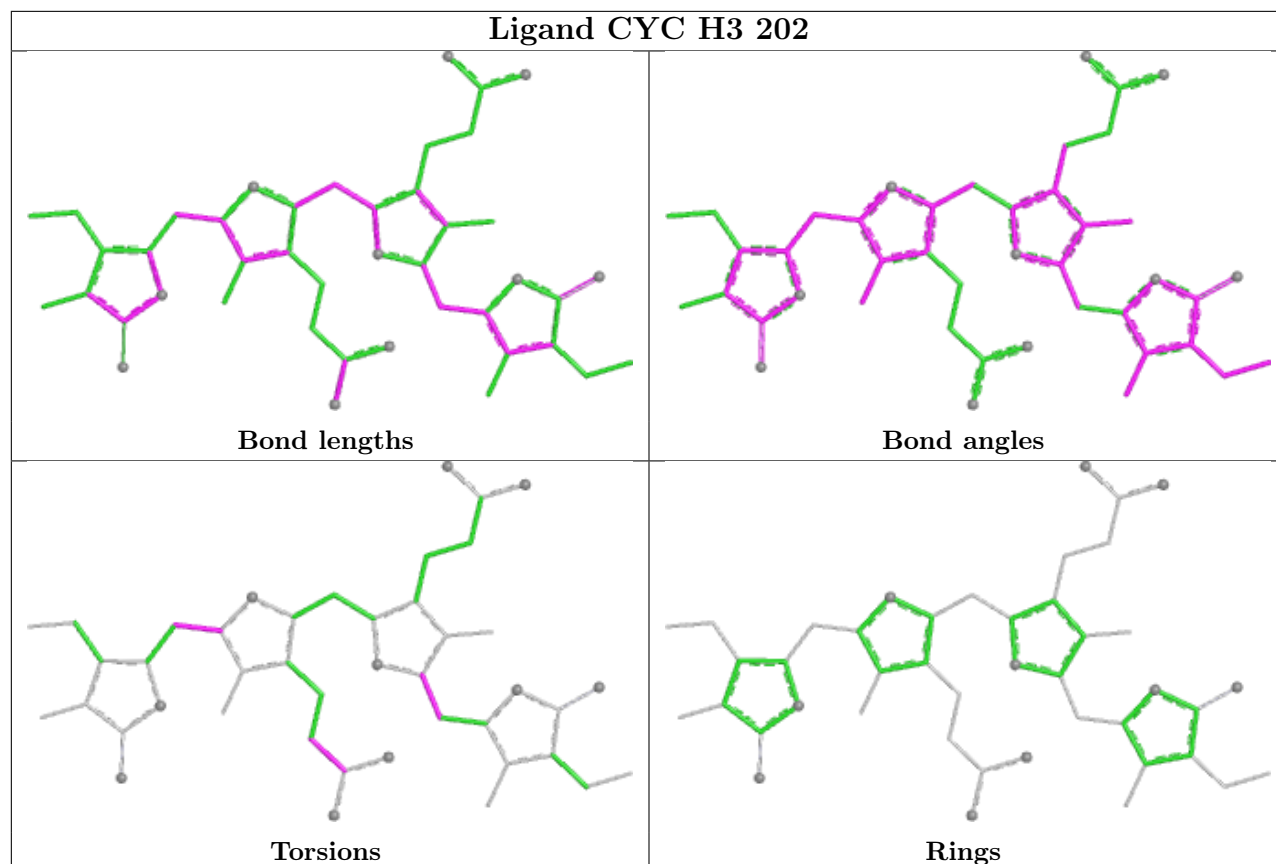
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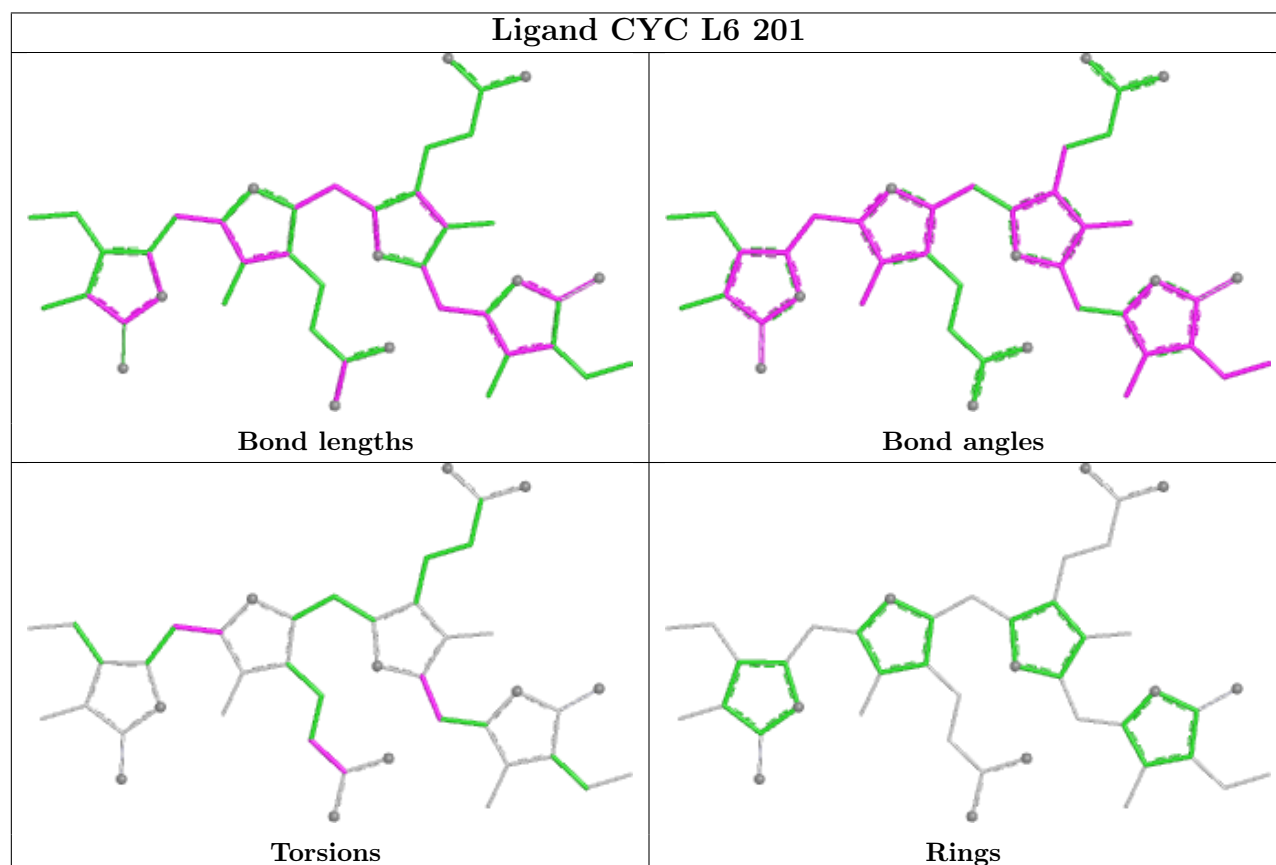
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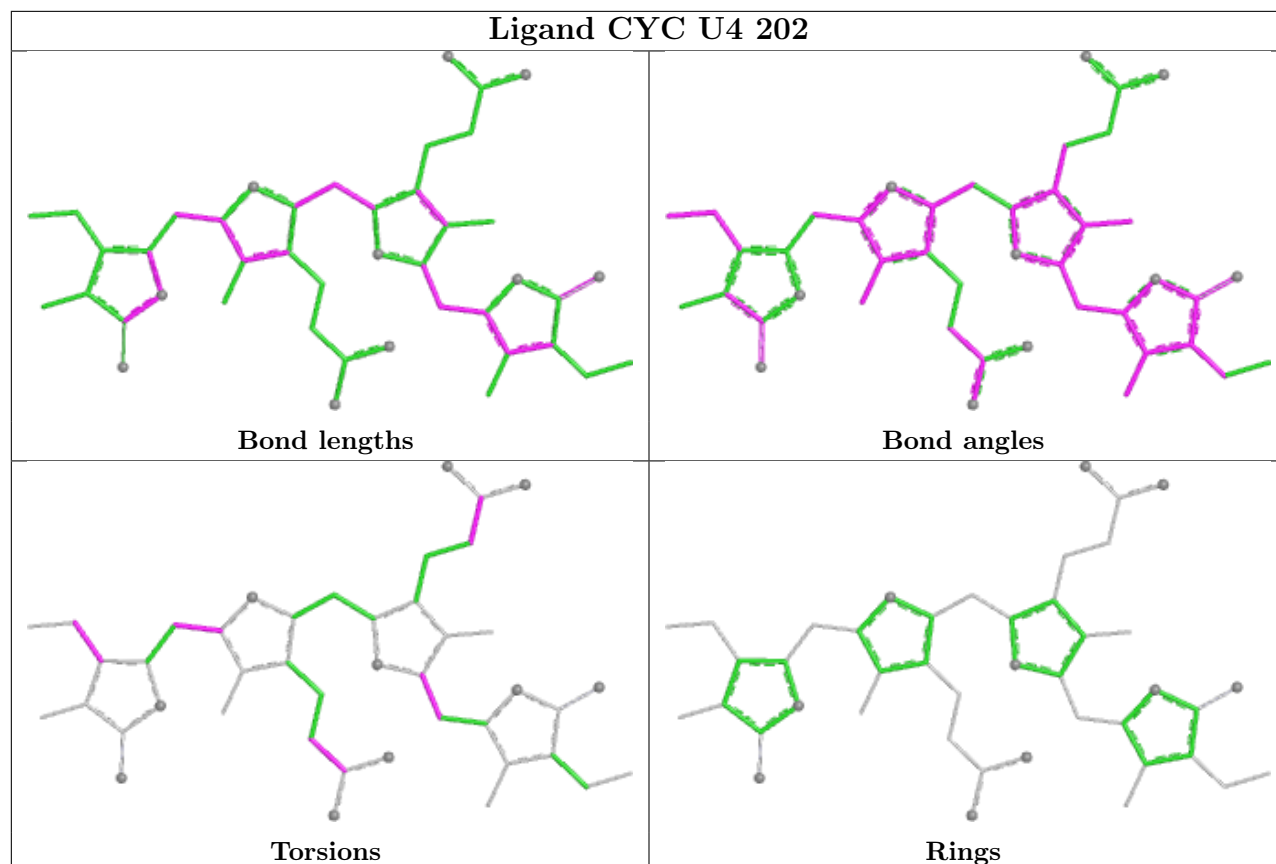
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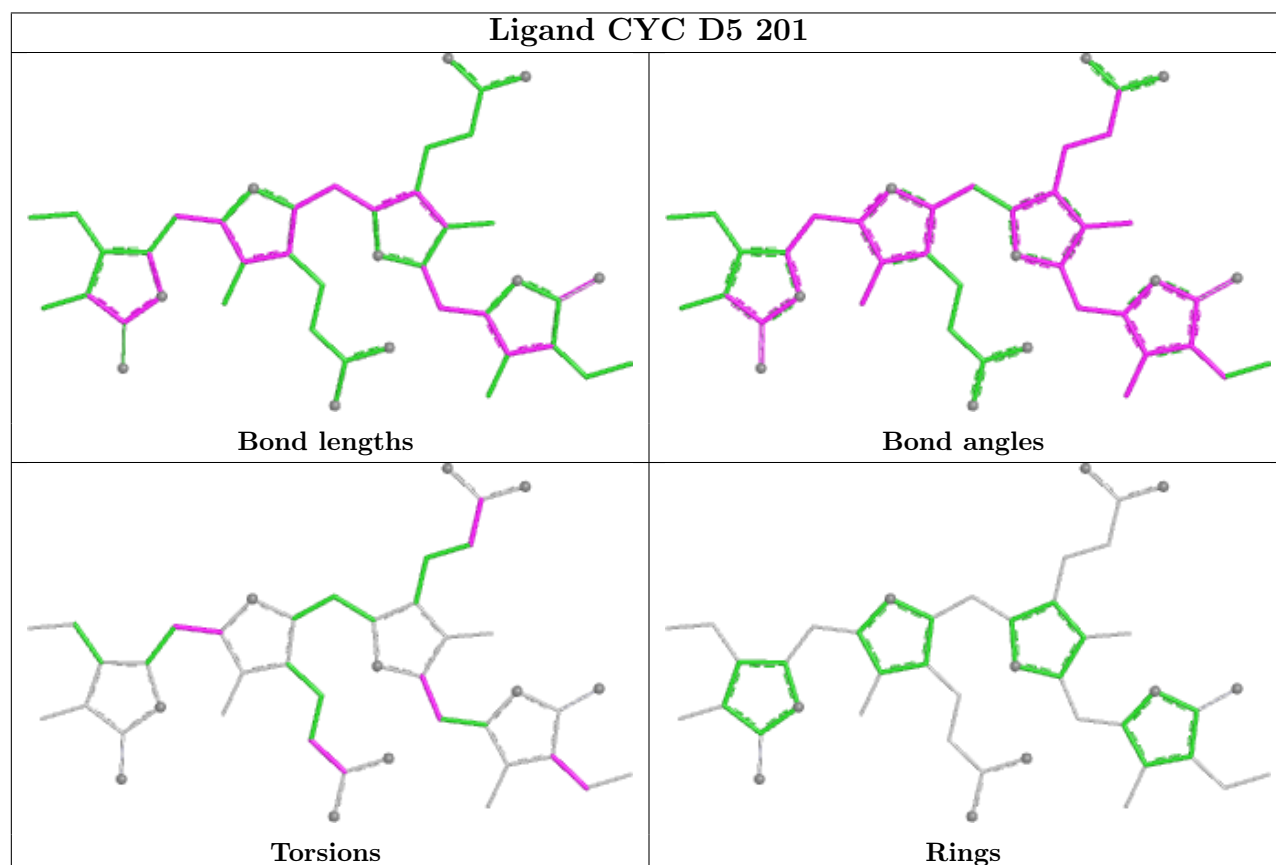
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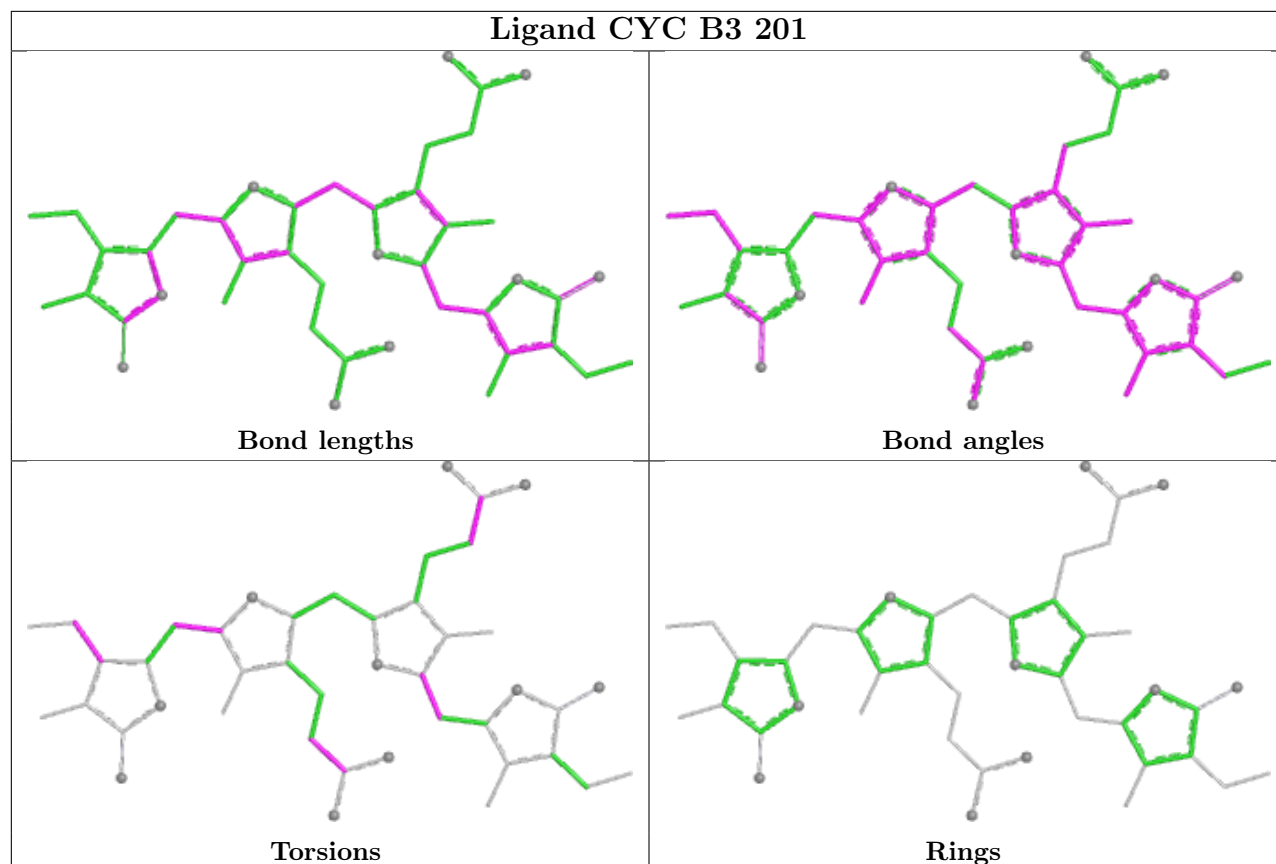
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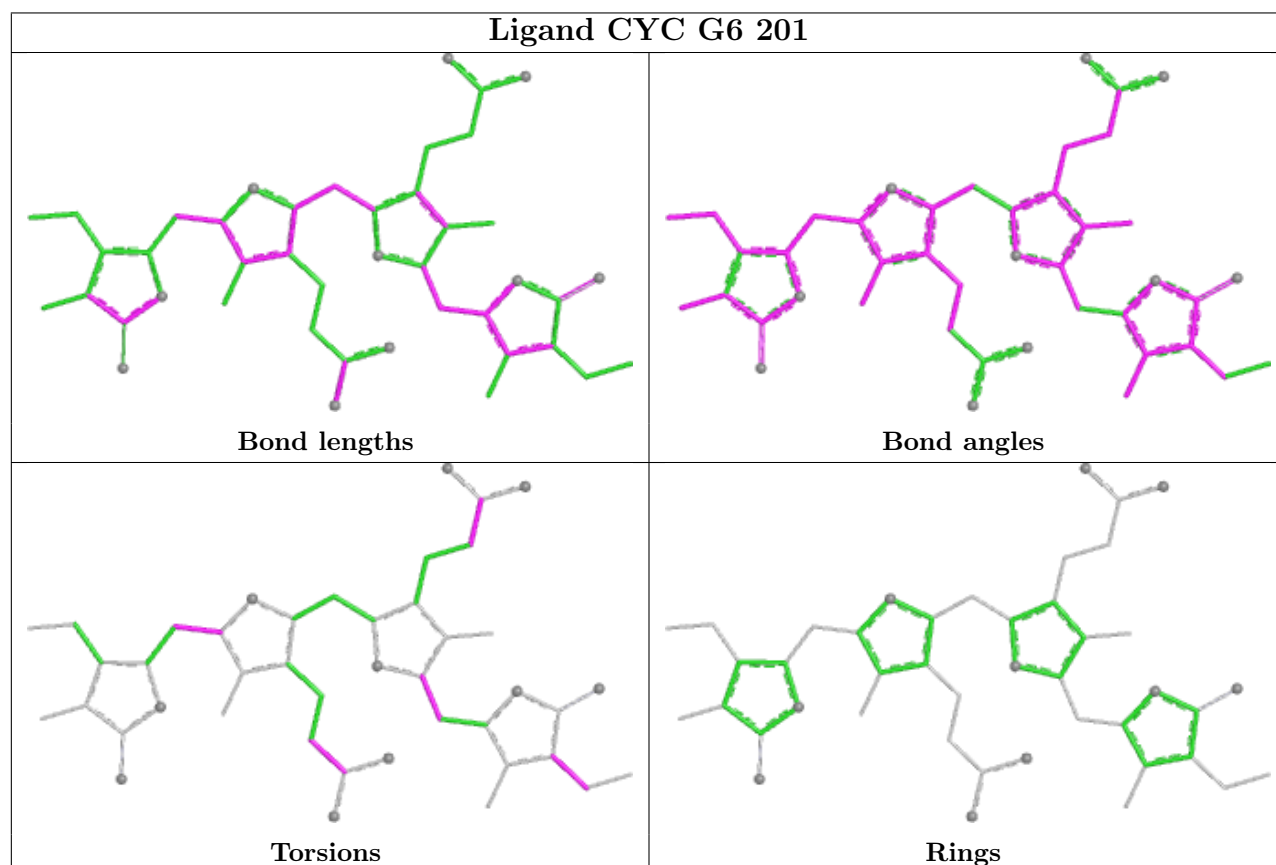
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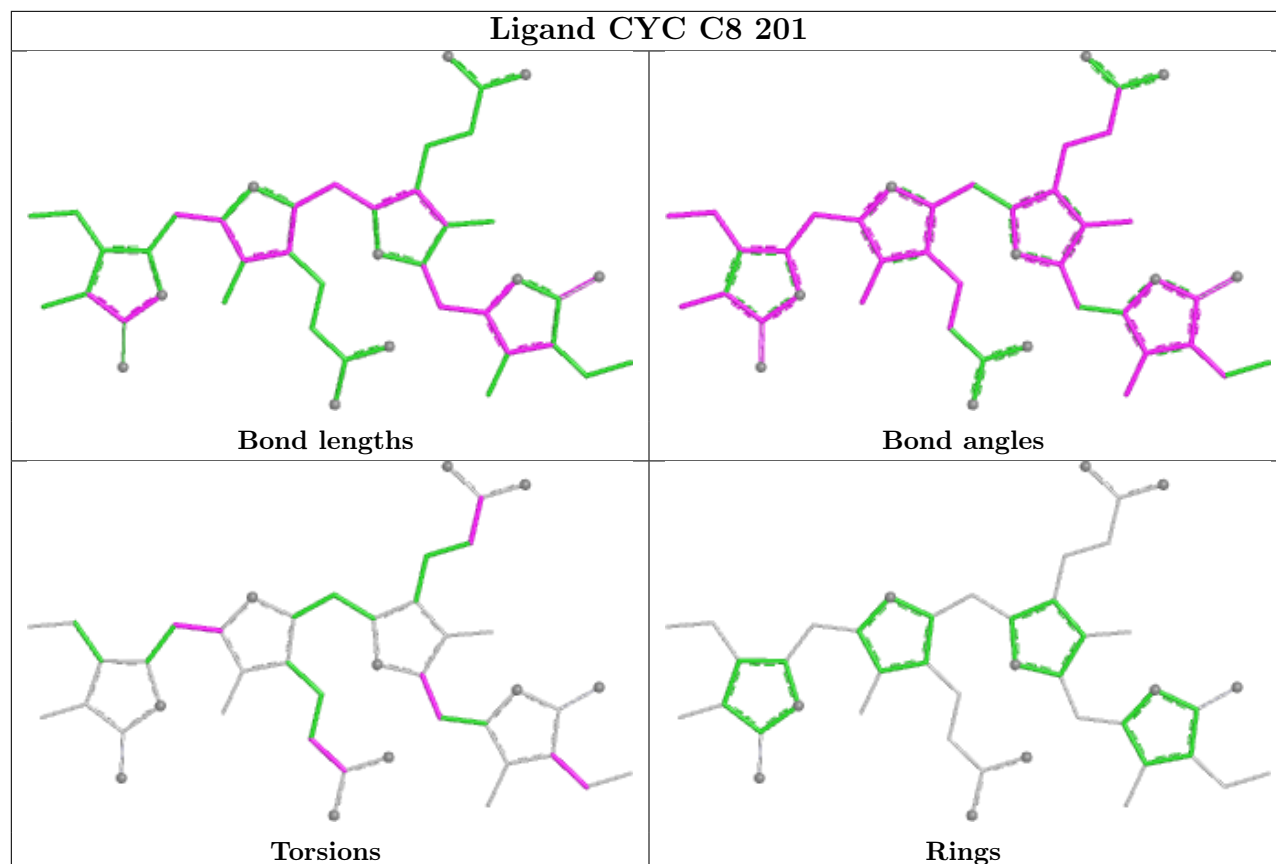
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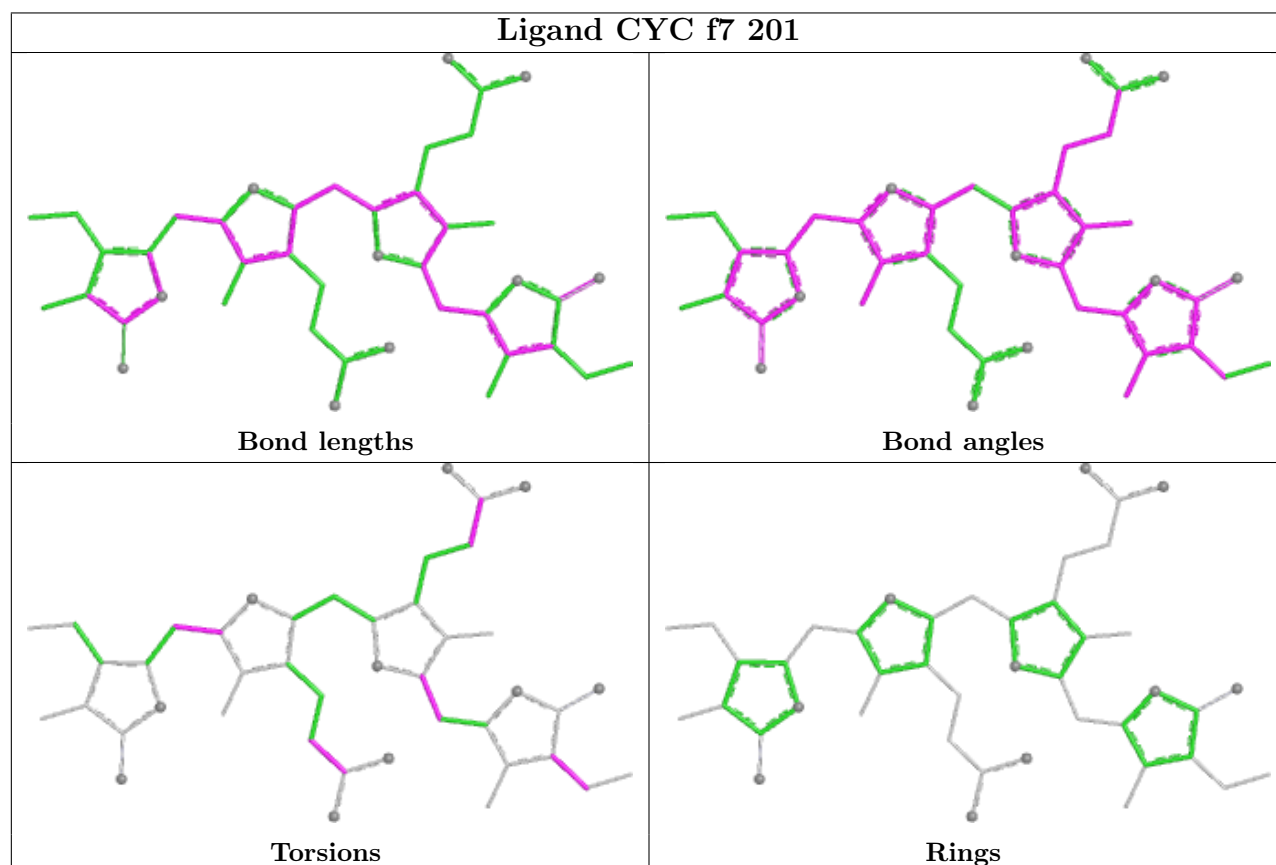
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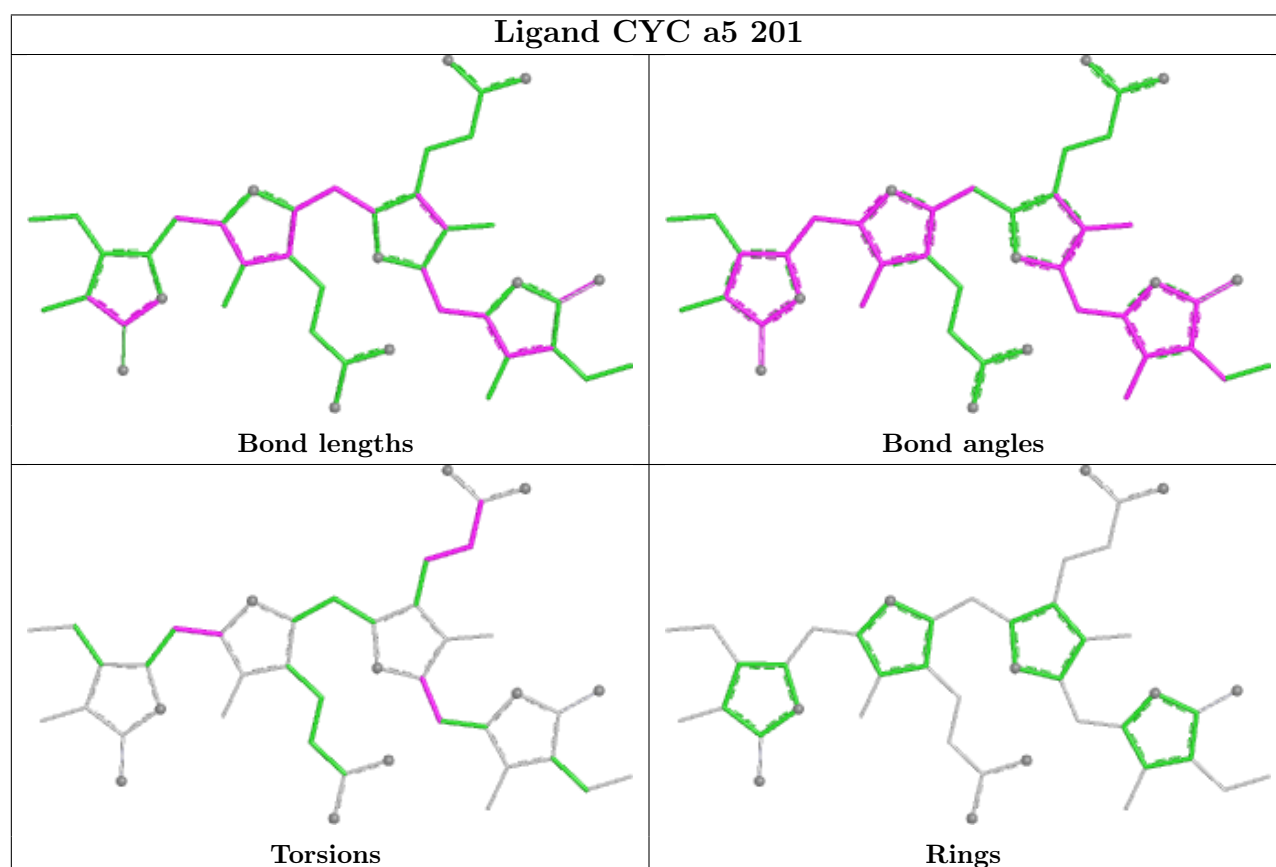
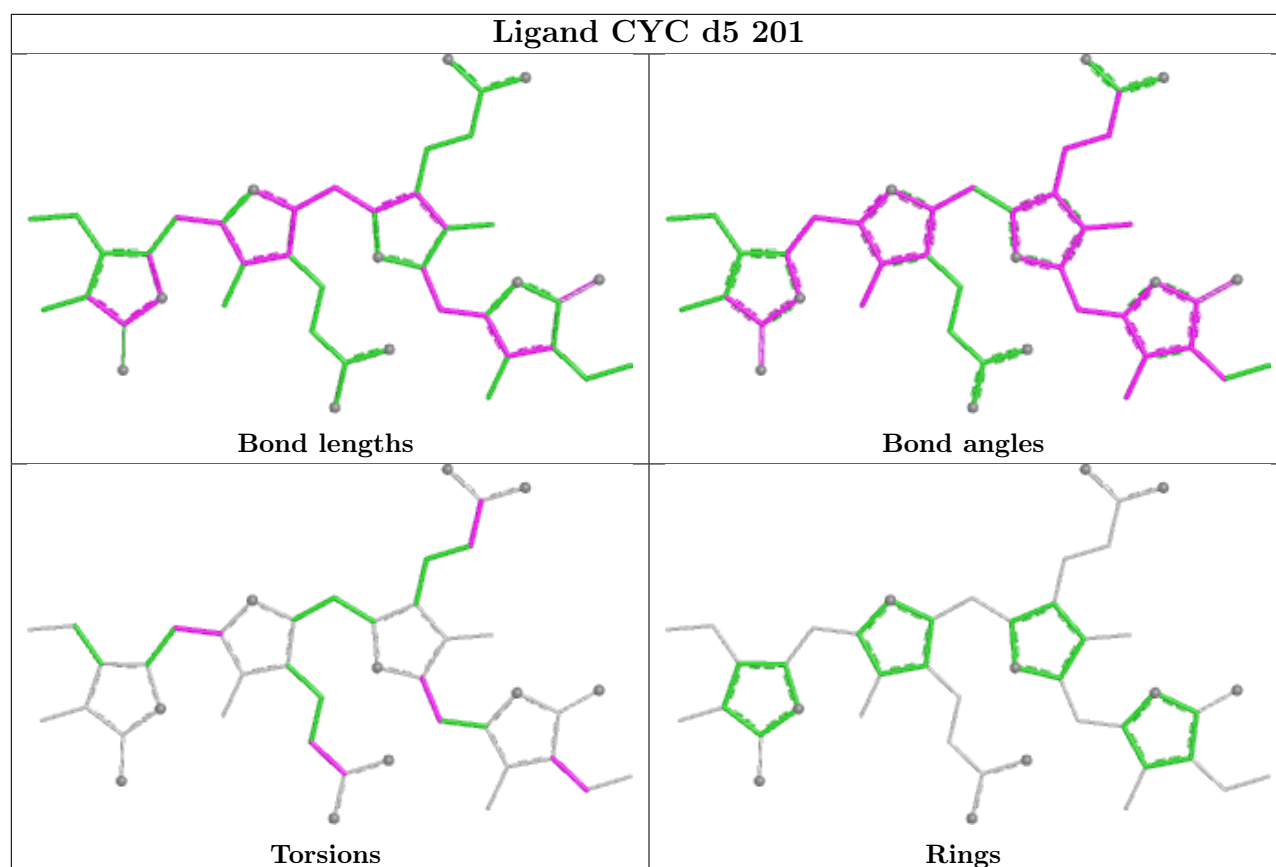


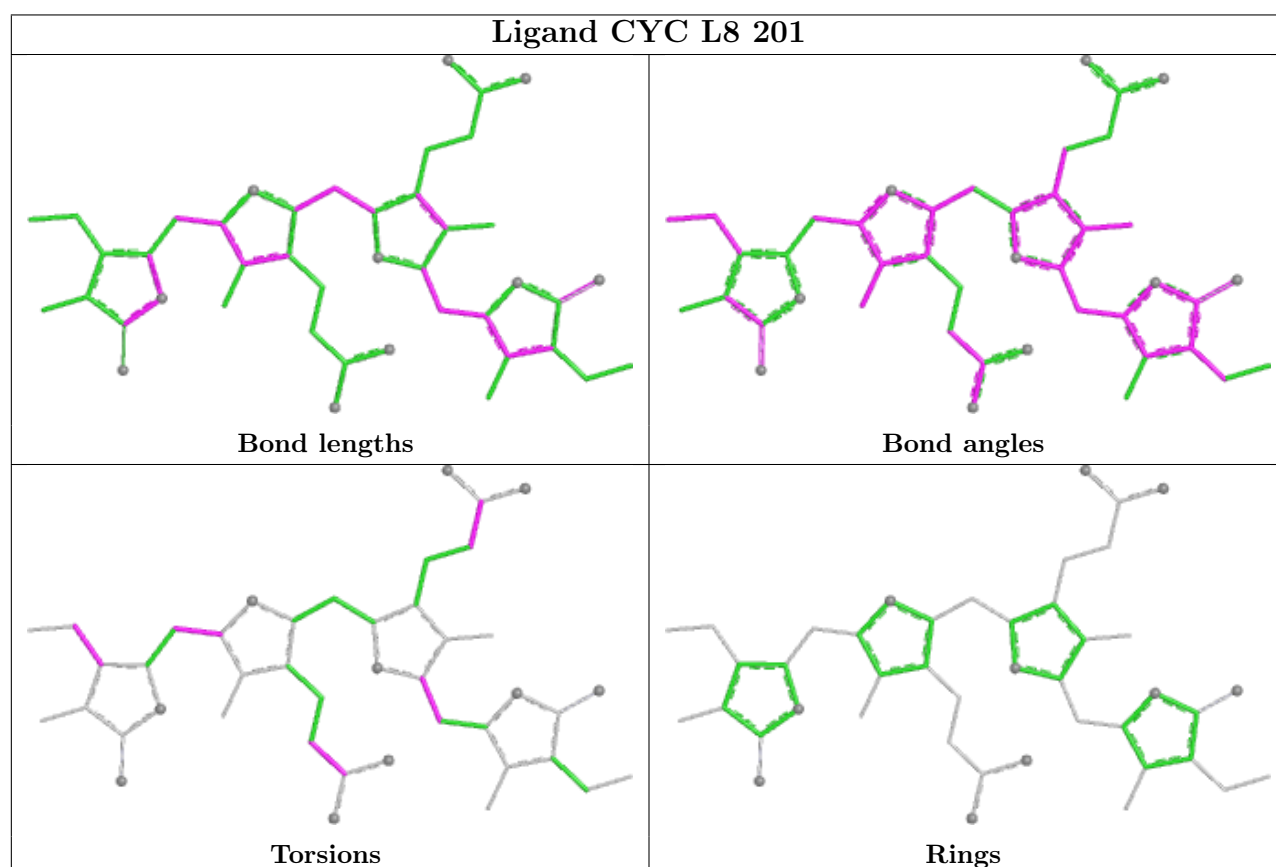
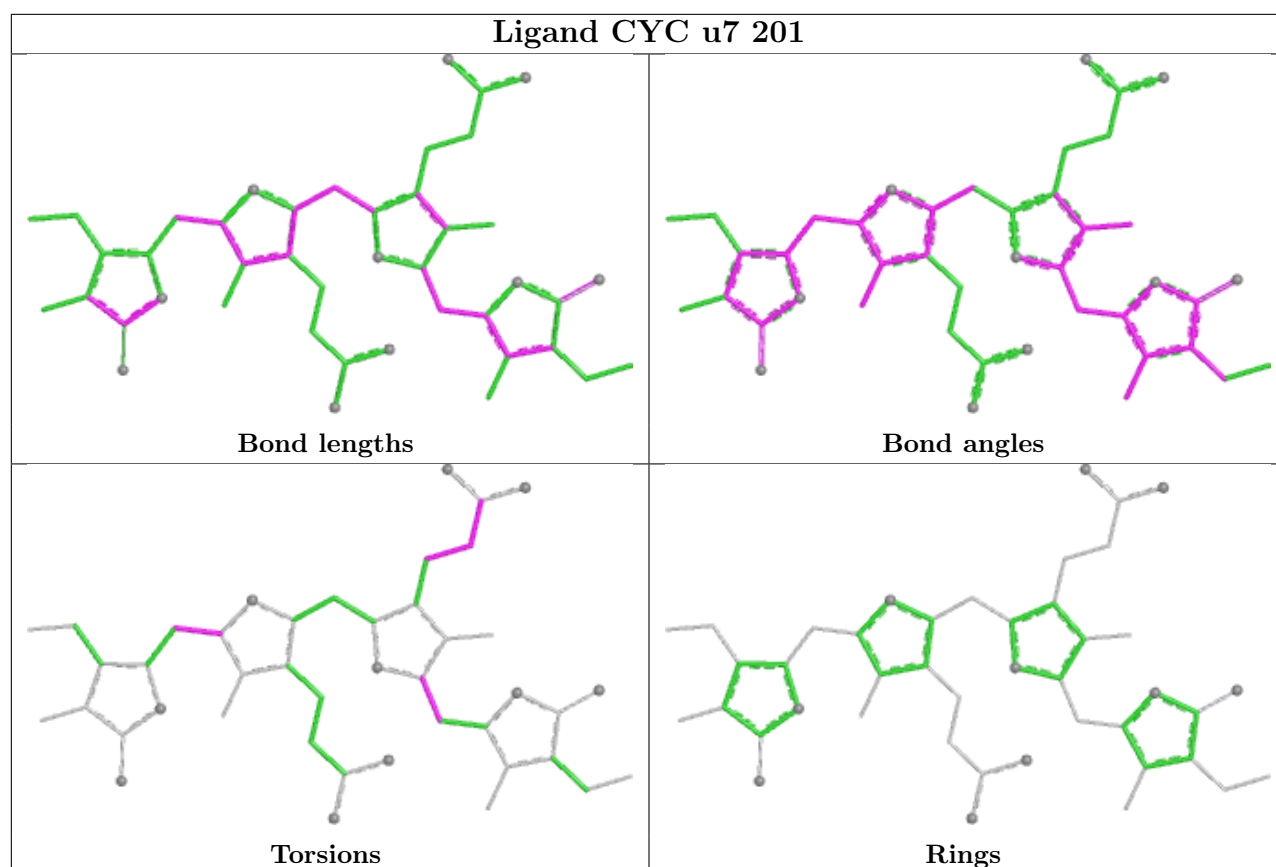
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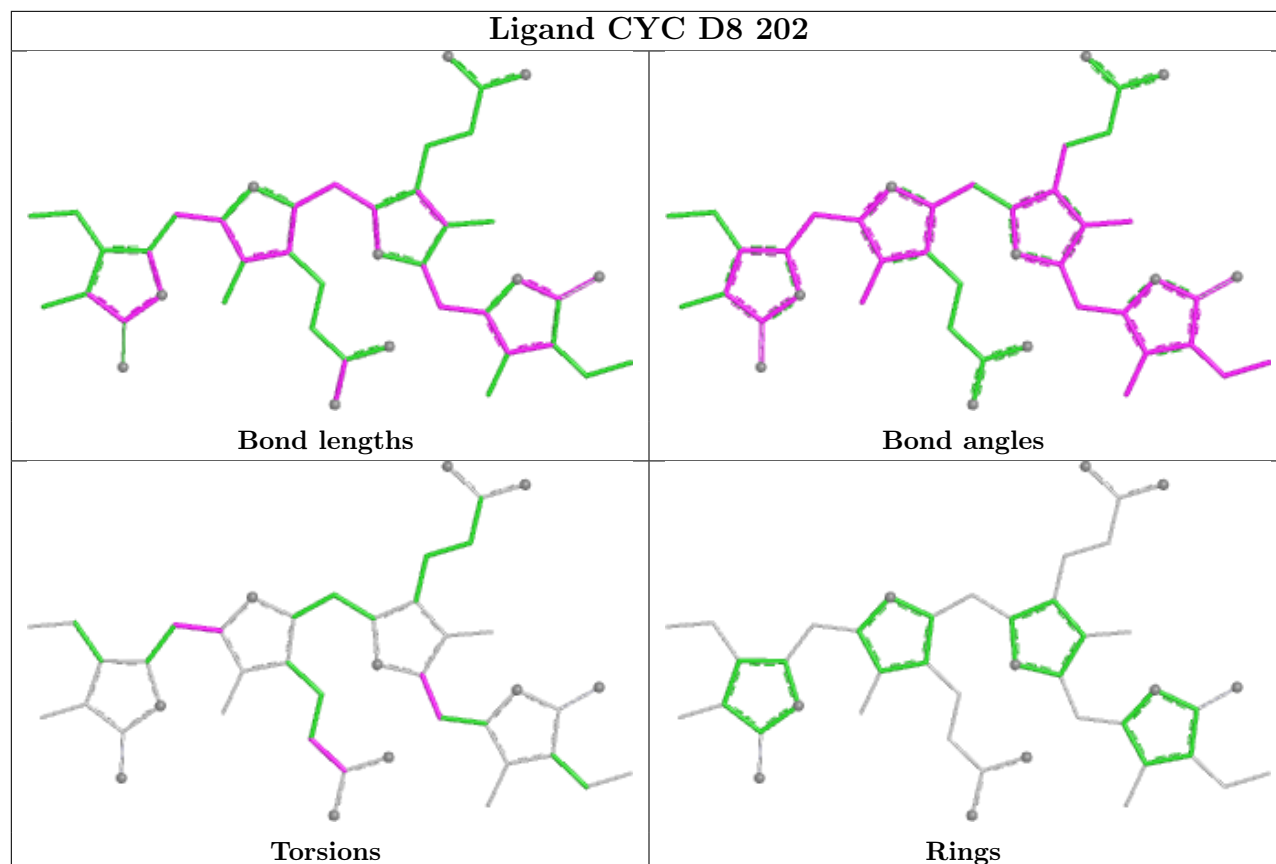
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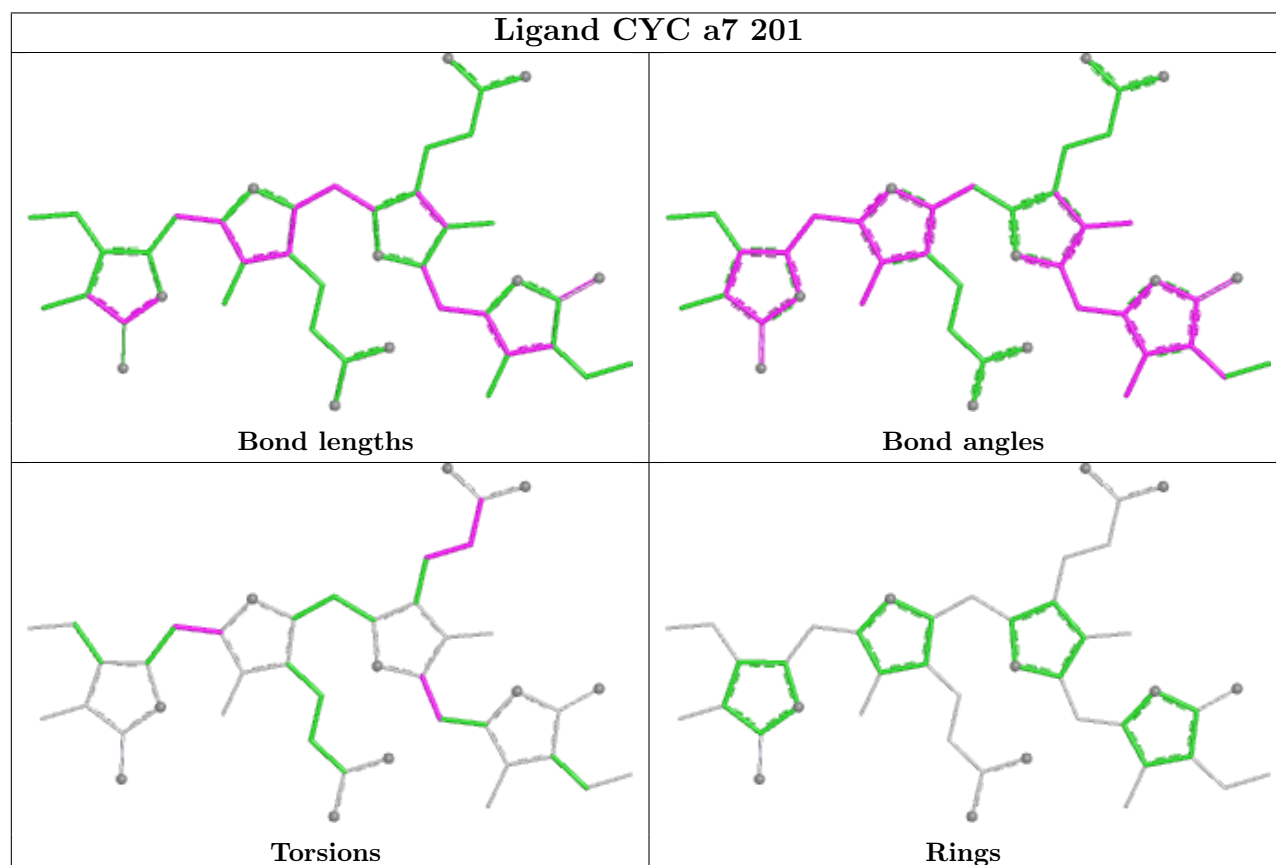


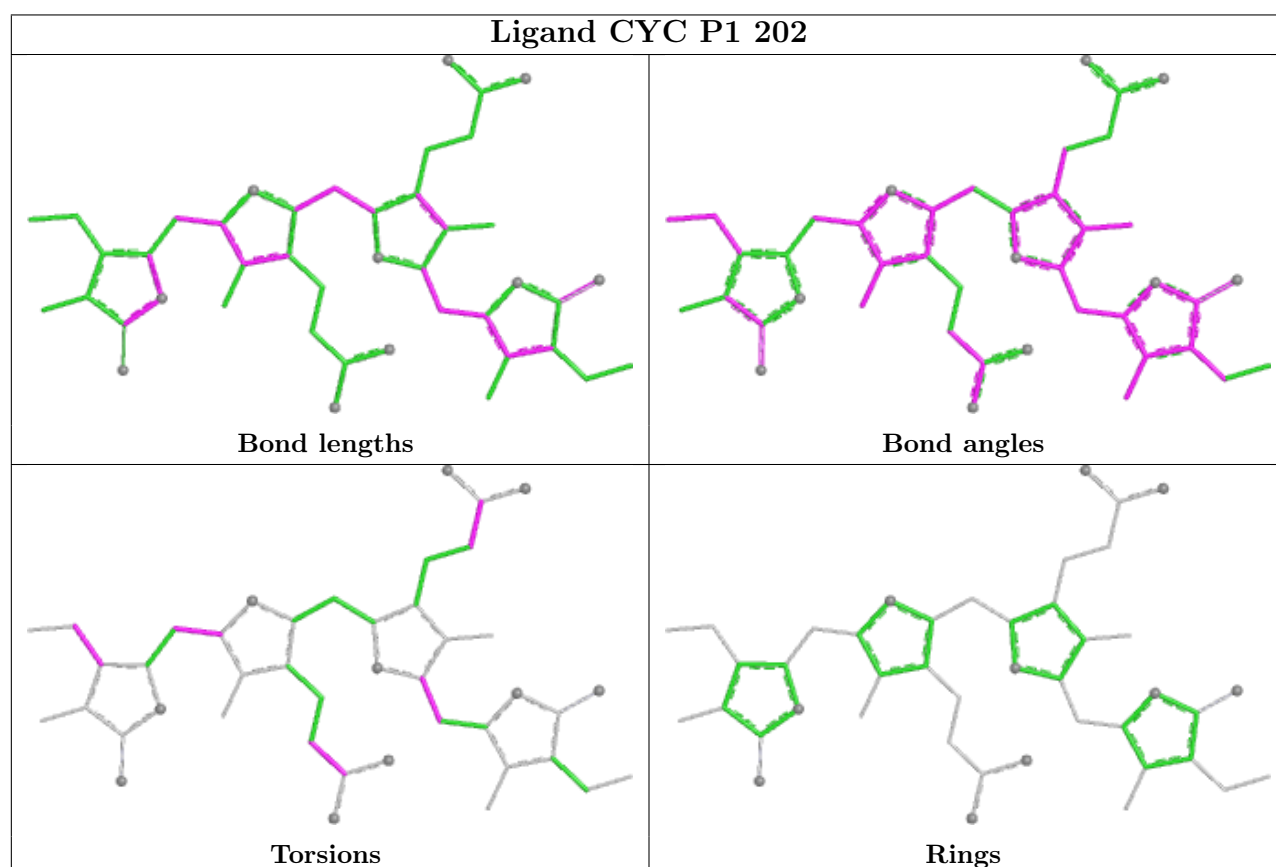
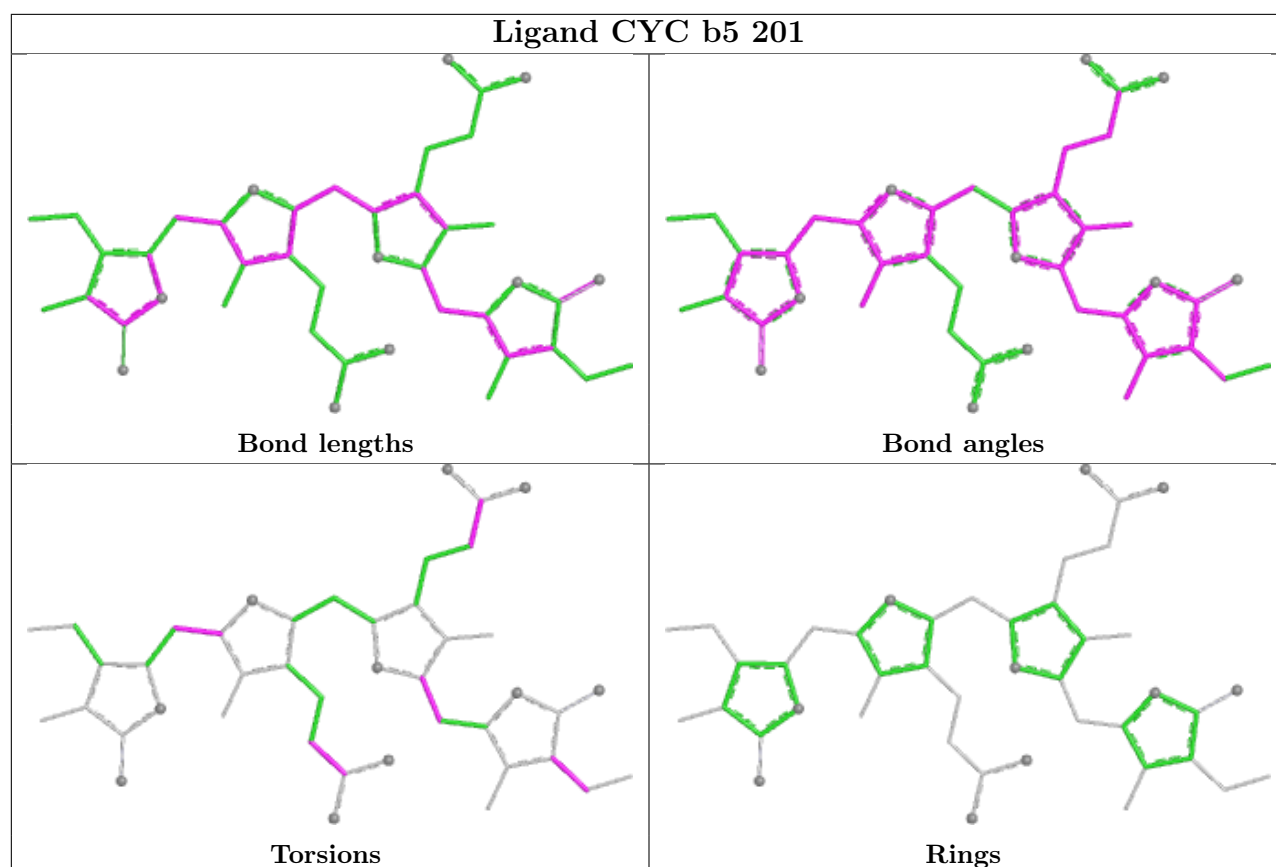


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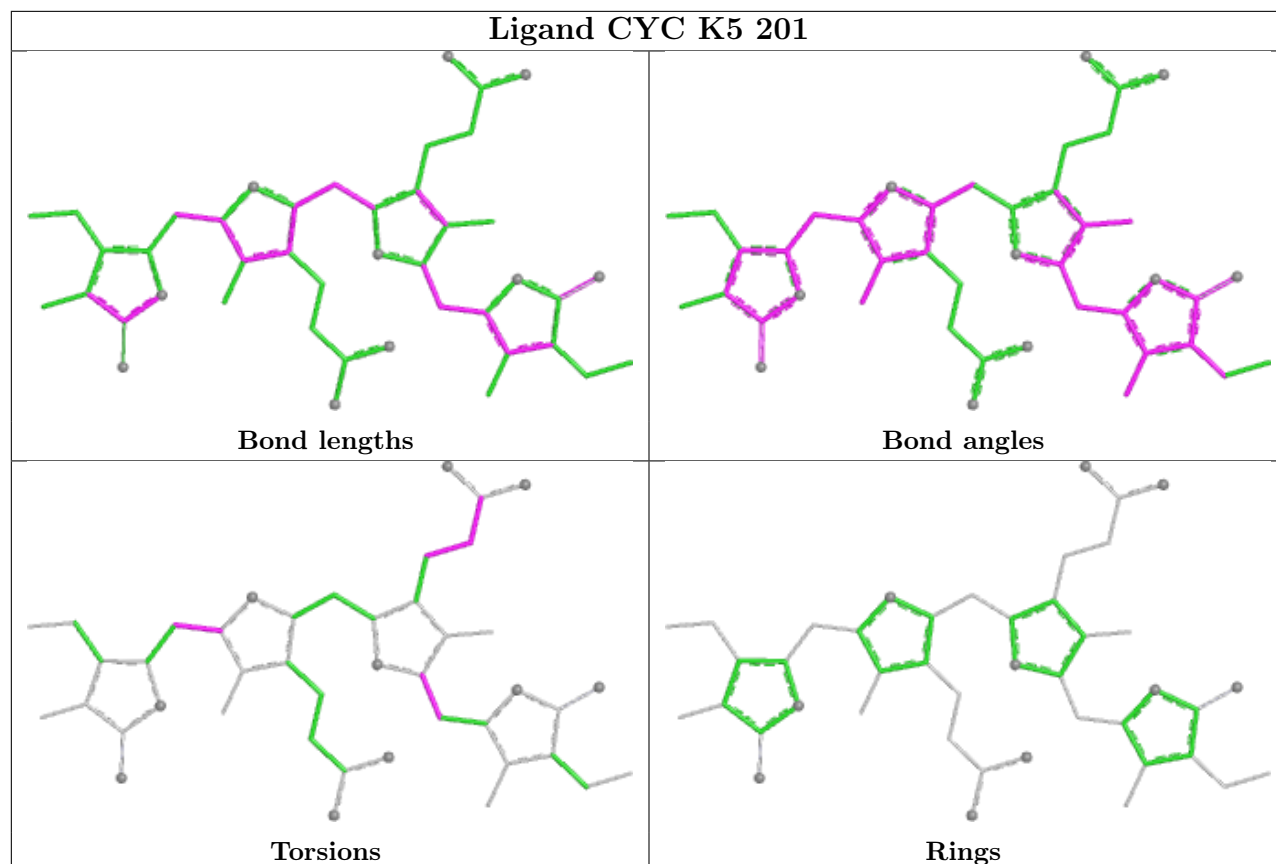


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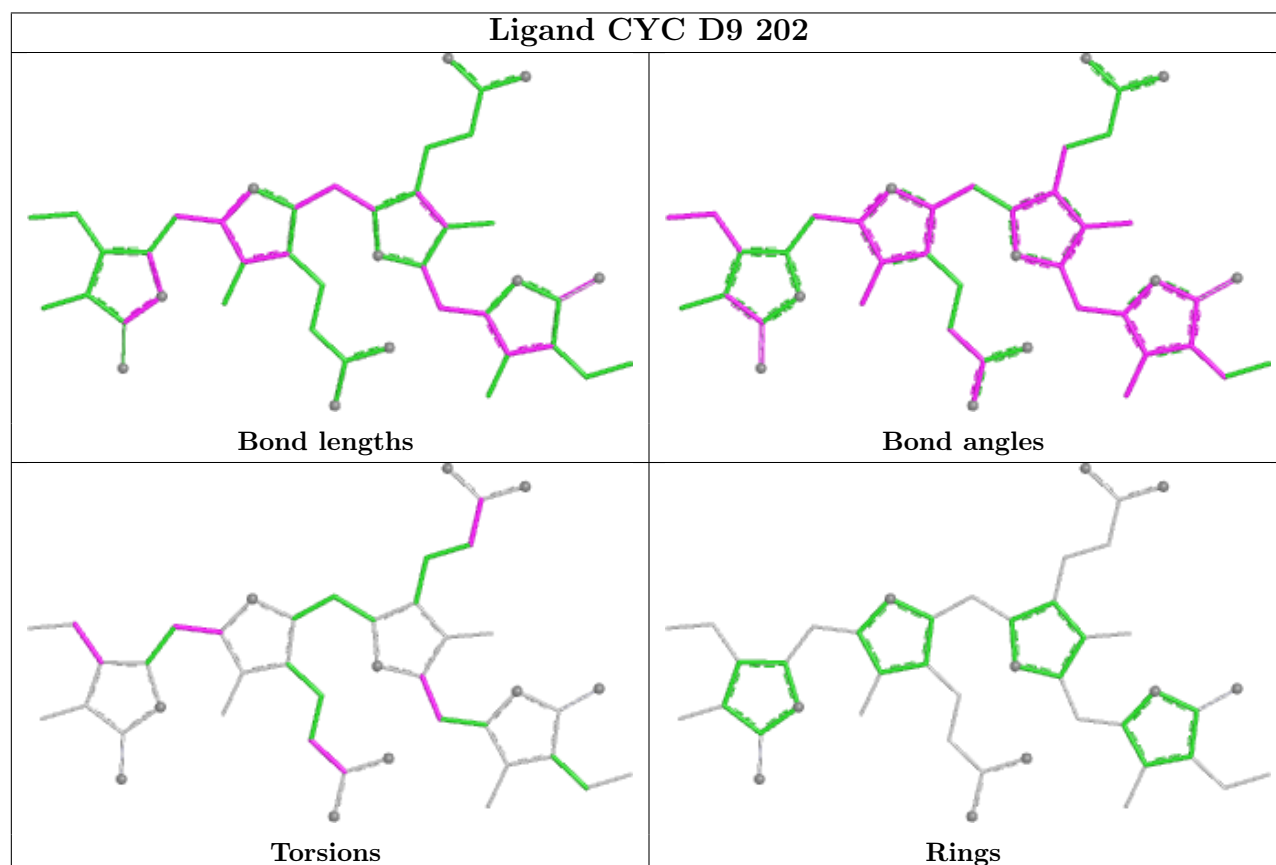




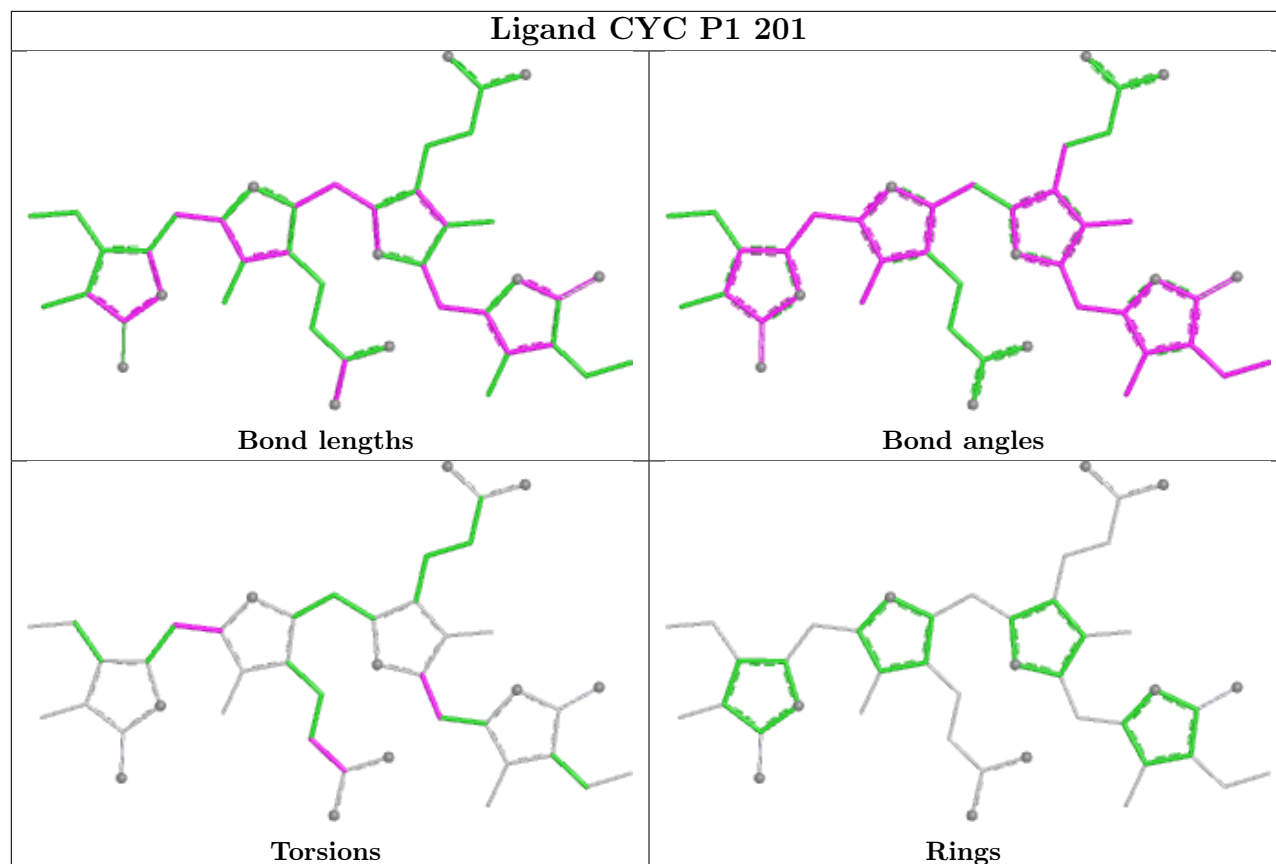
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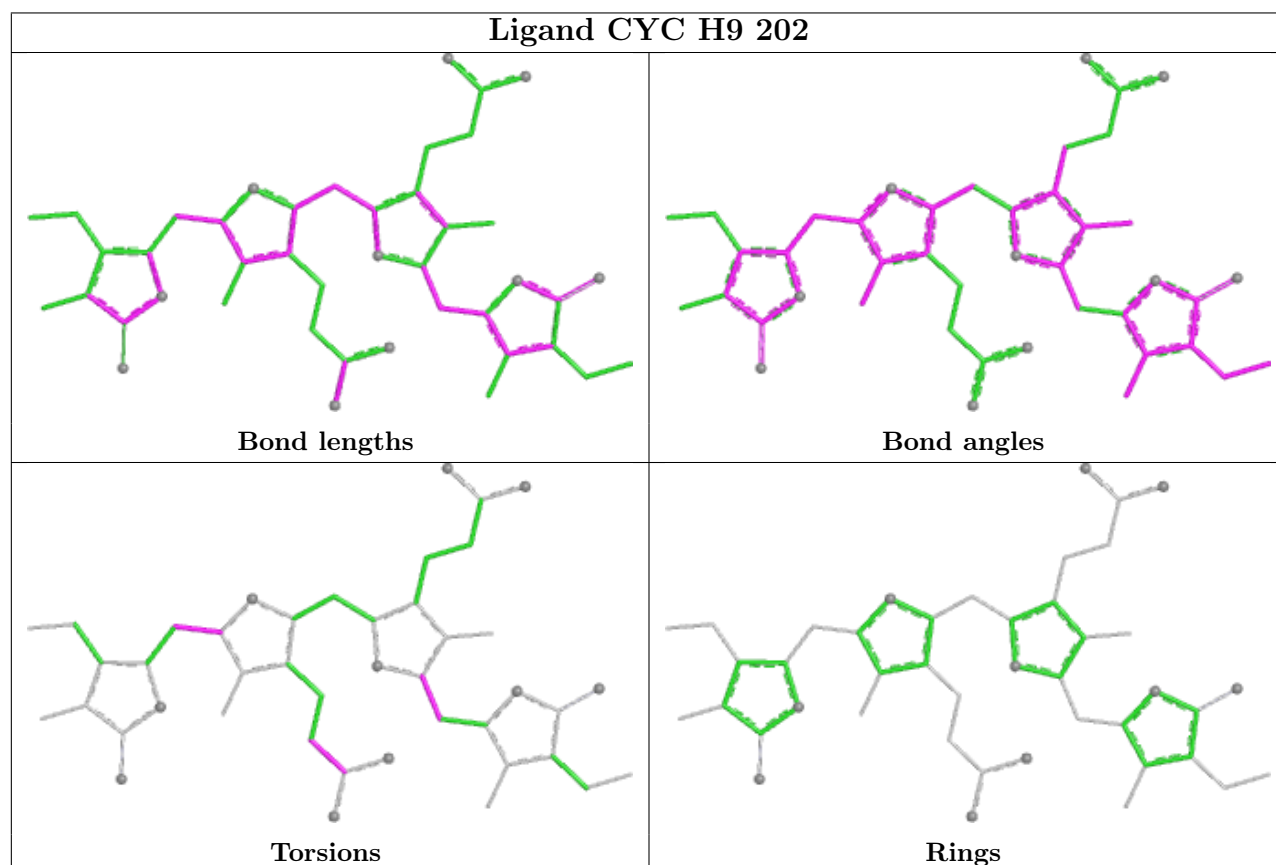
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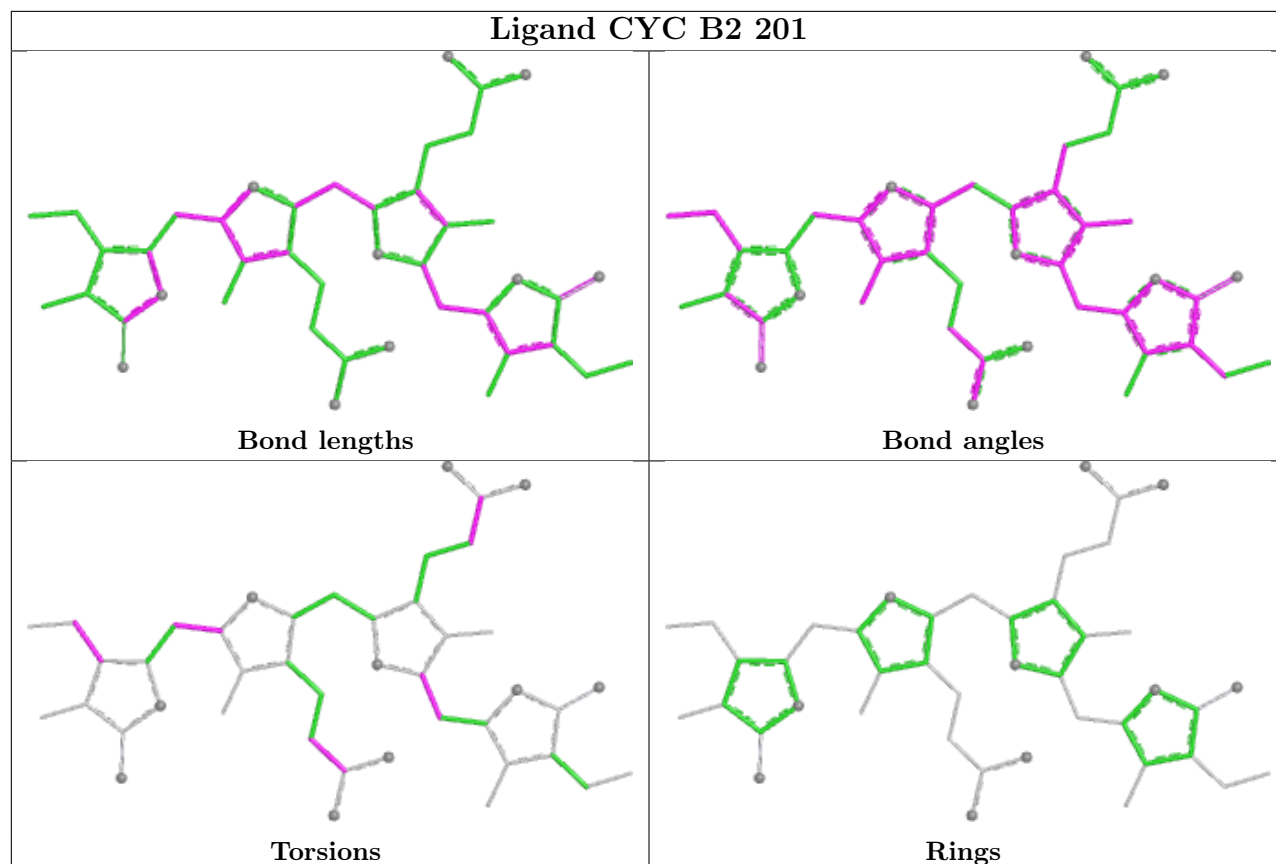
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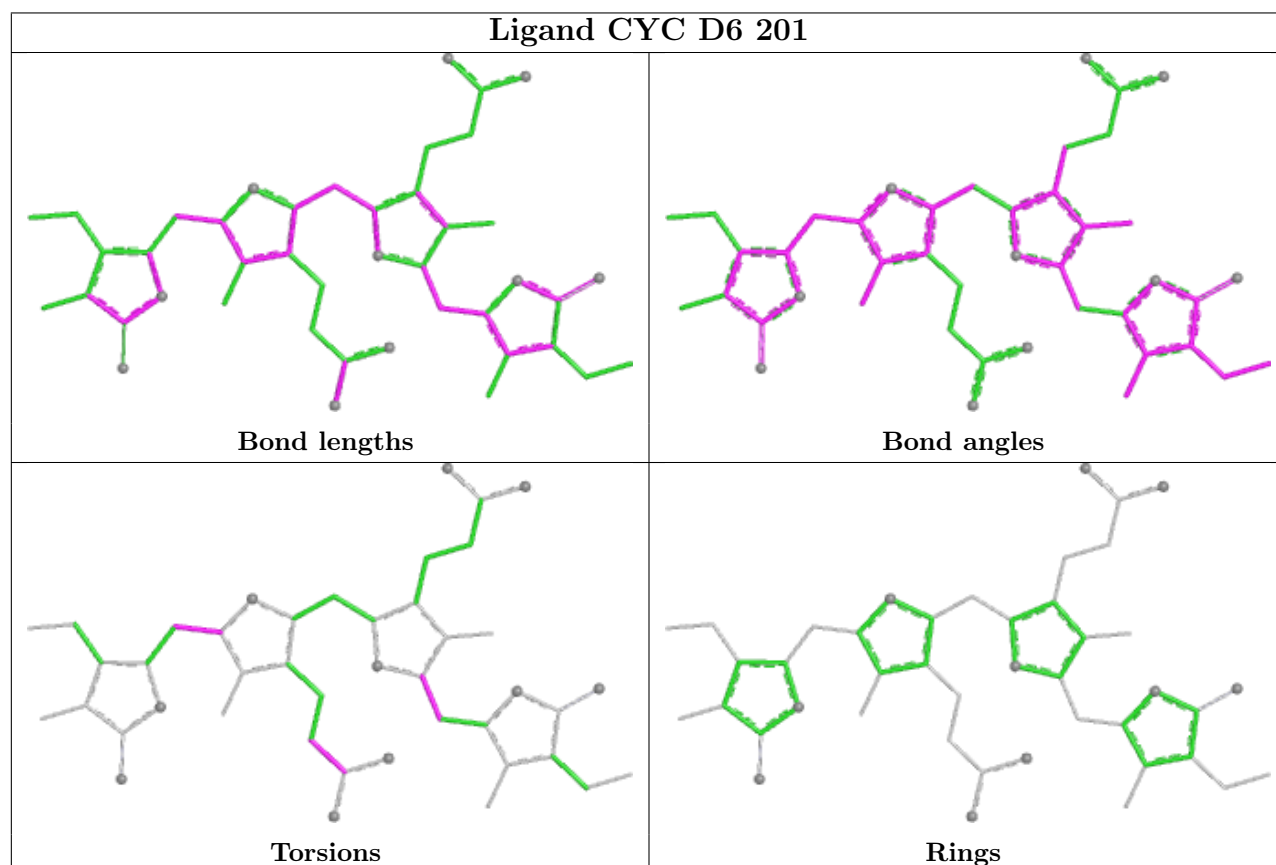
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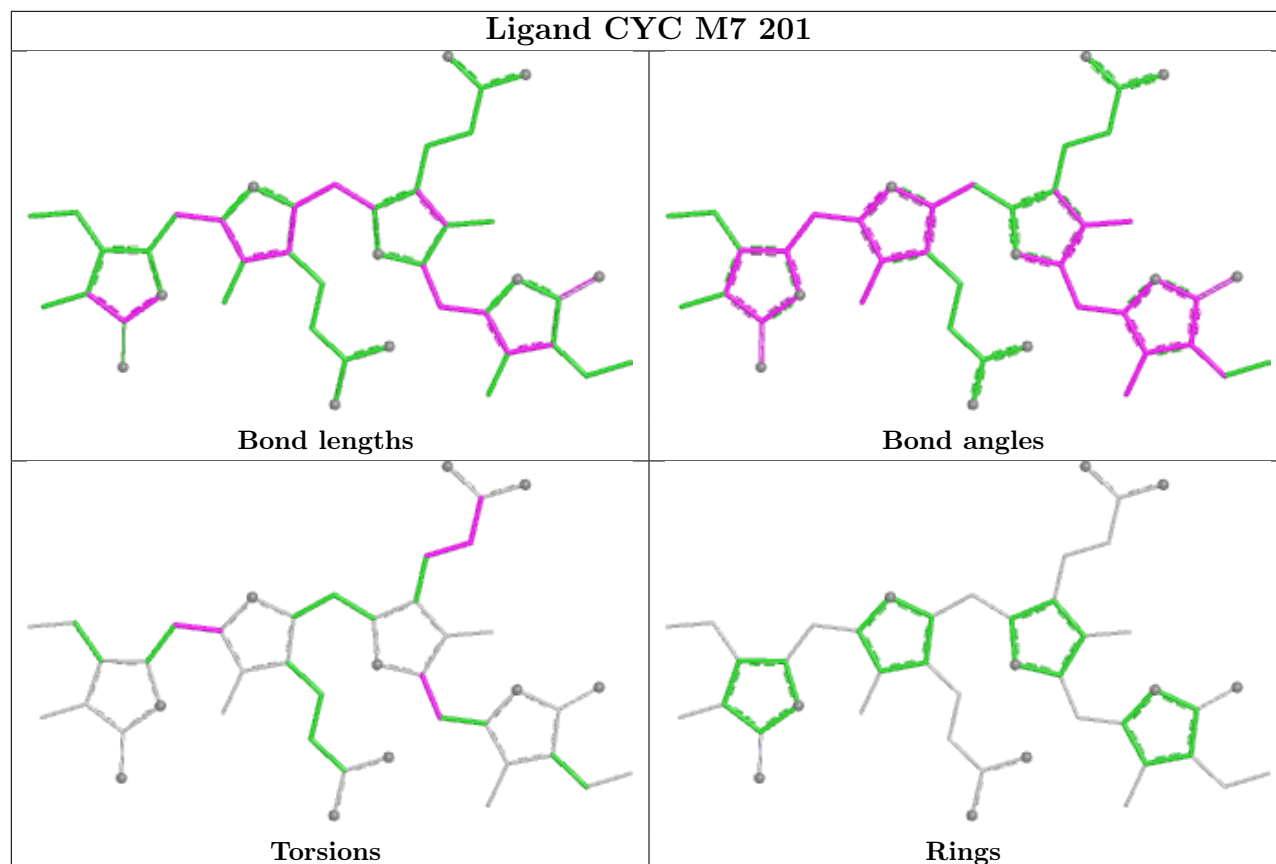
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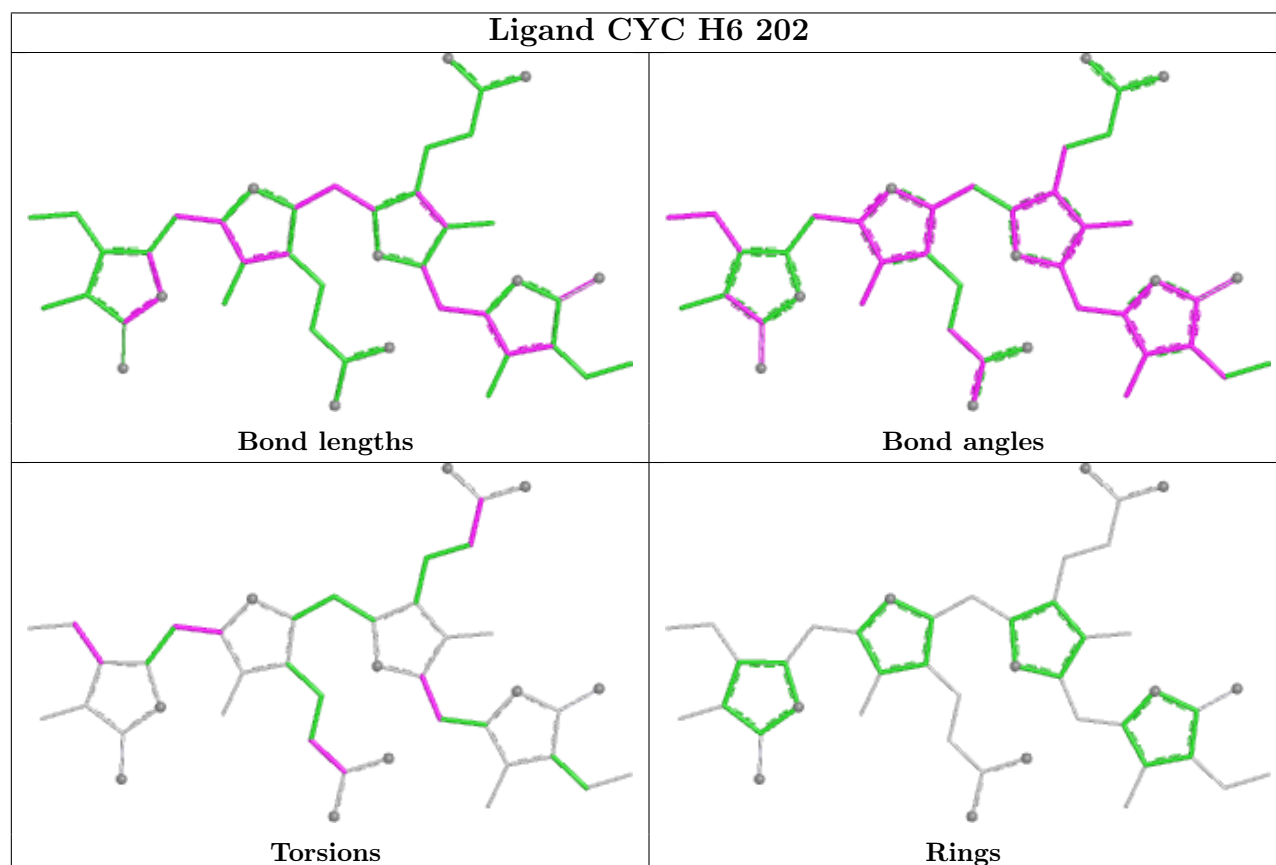
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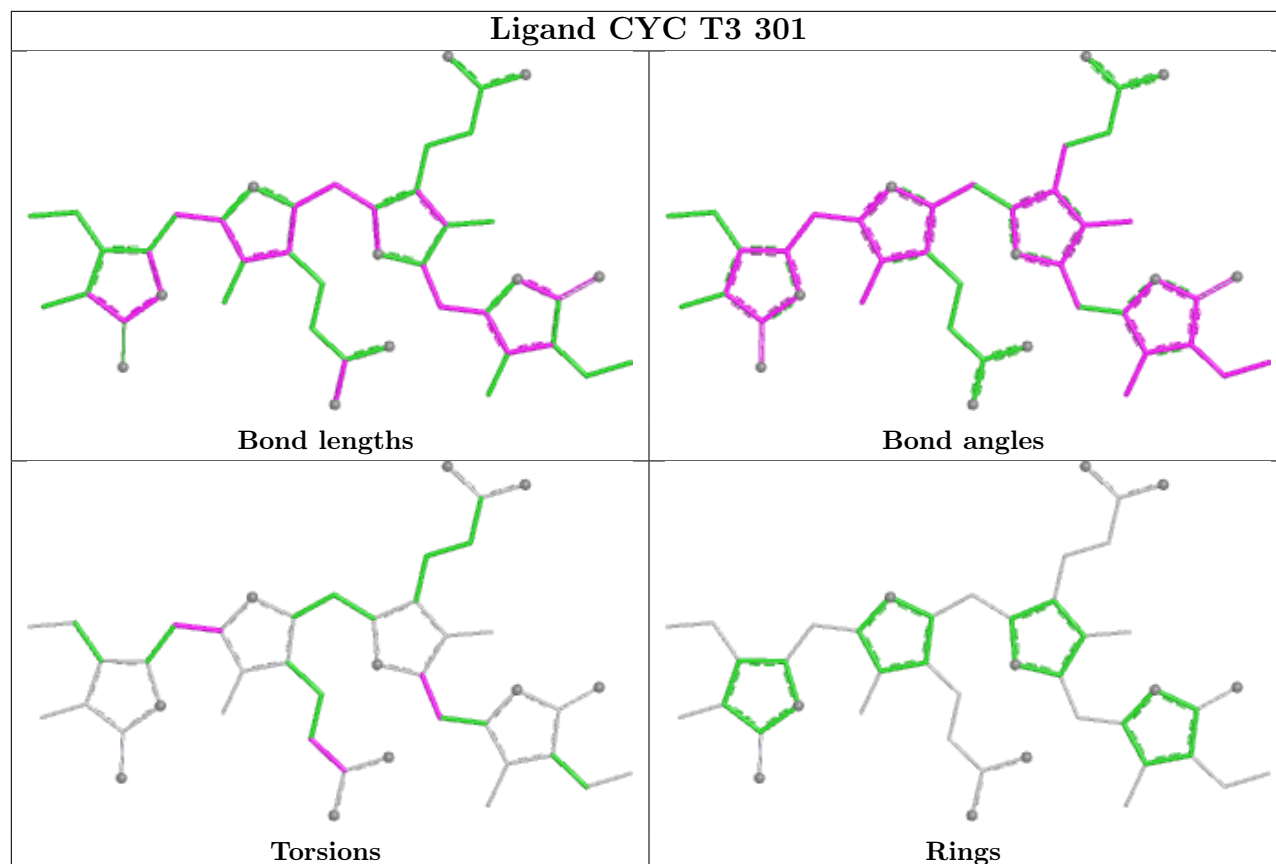
Ligand CYC M7 201



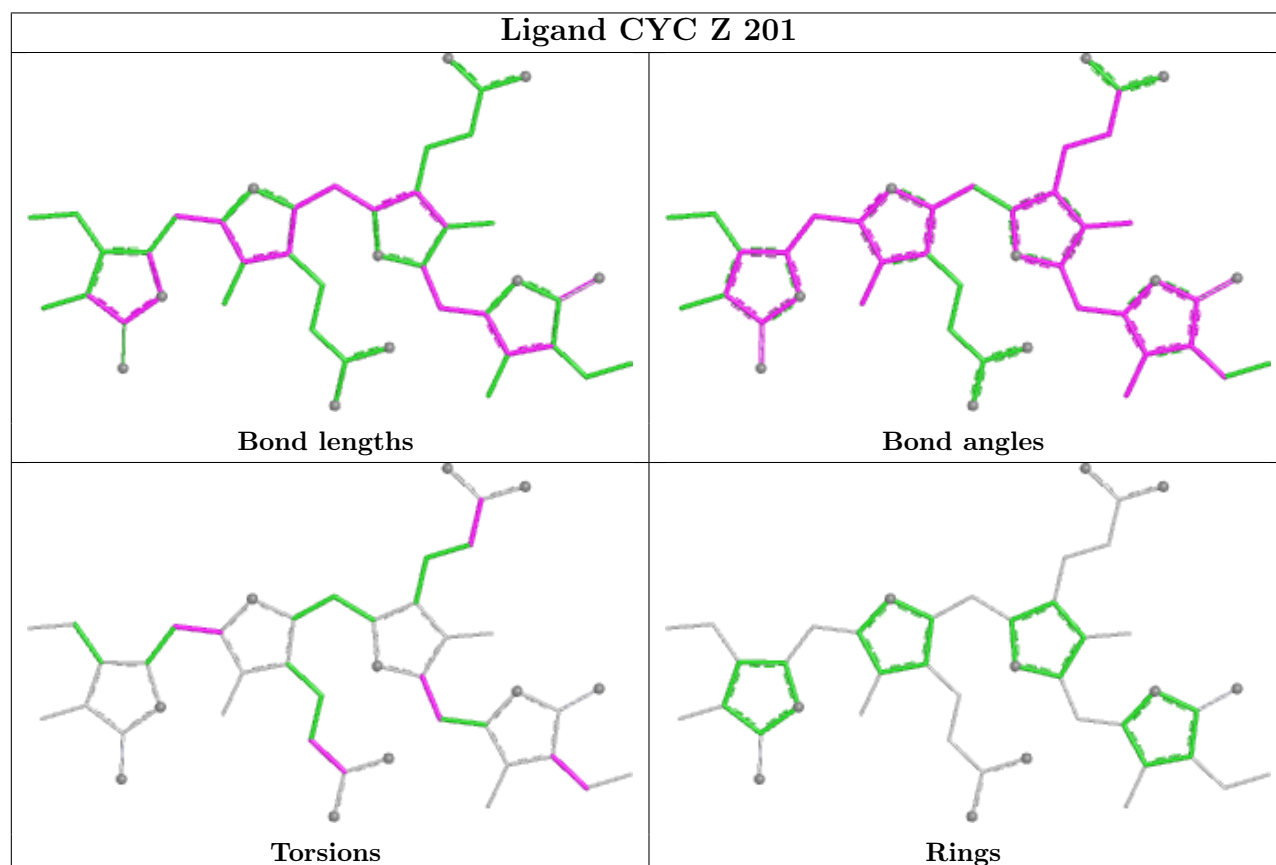
Ligand CYC H6 202



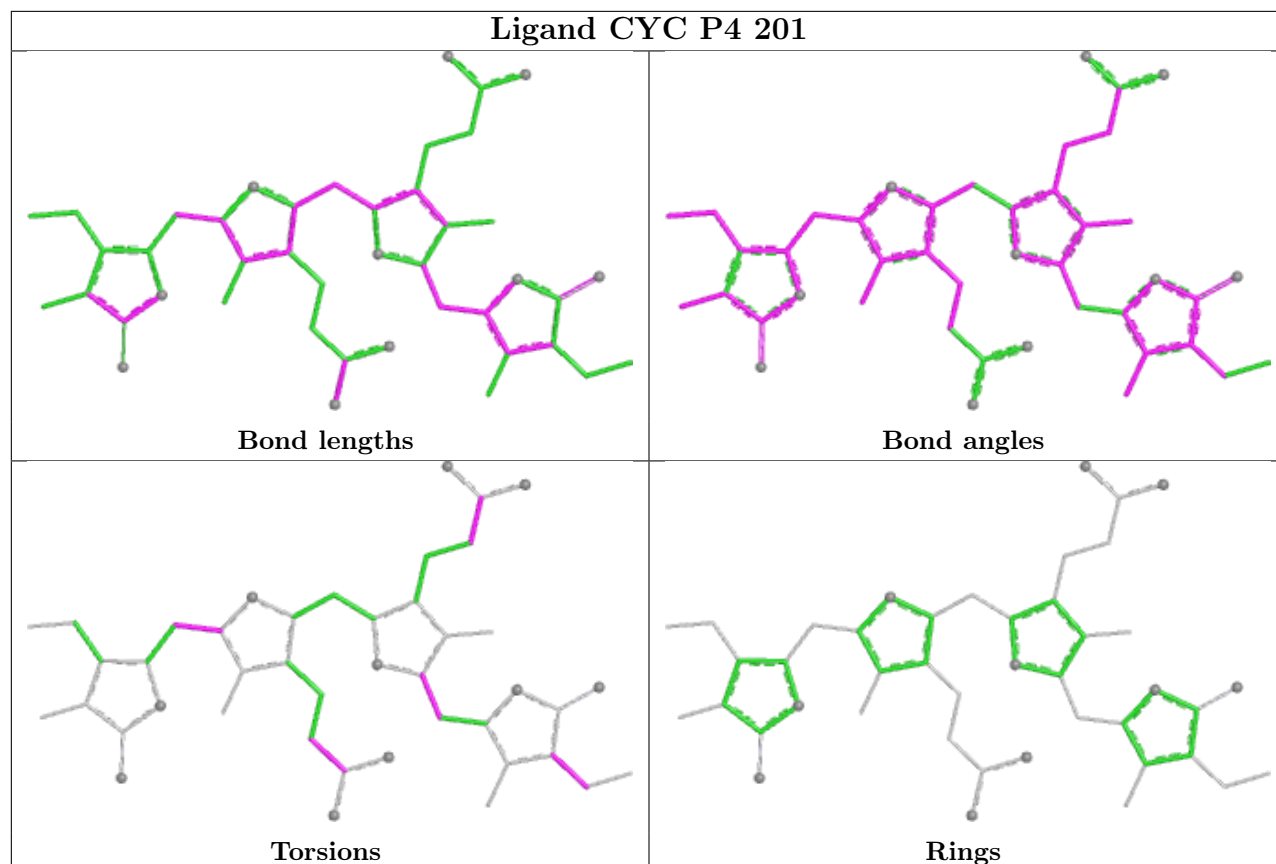
Ligand CYC T3 301



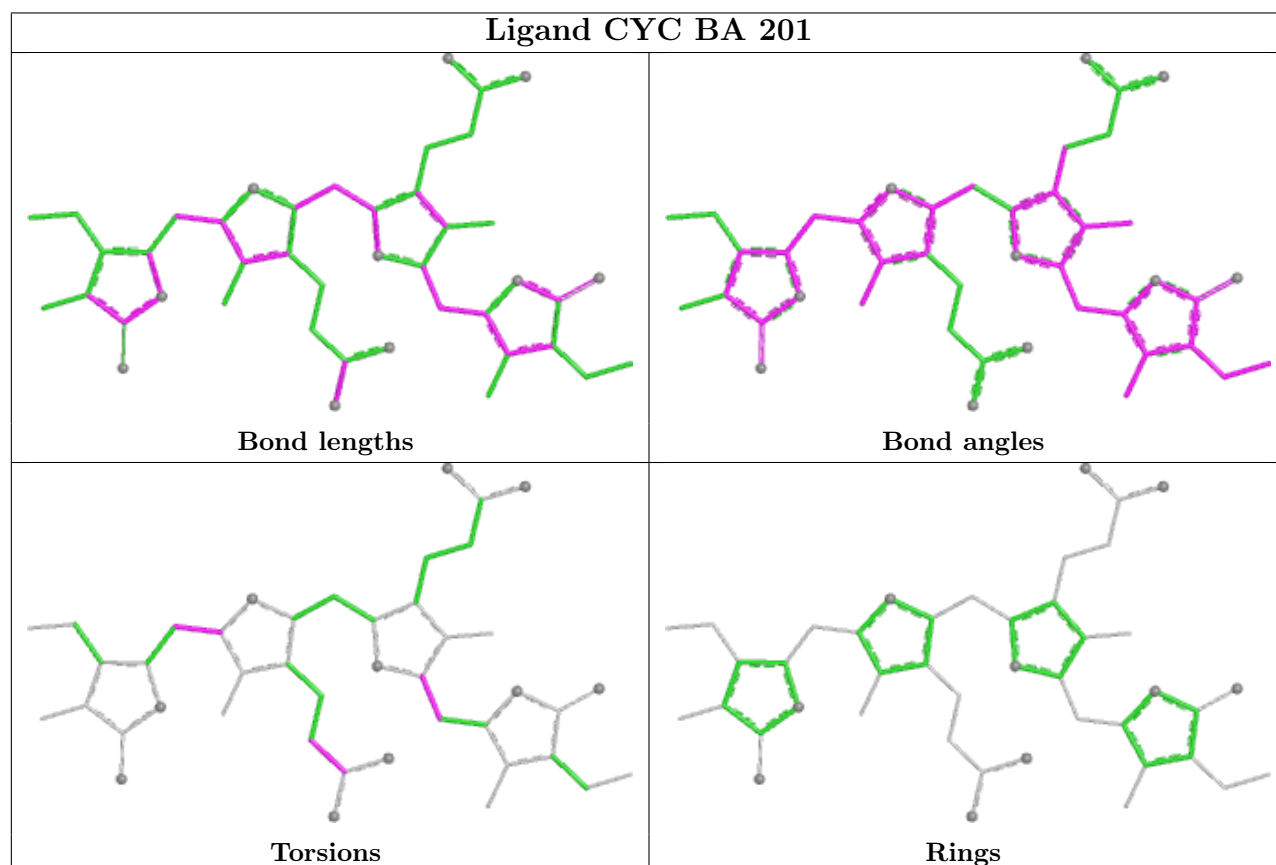
Ligand CYC Z 201



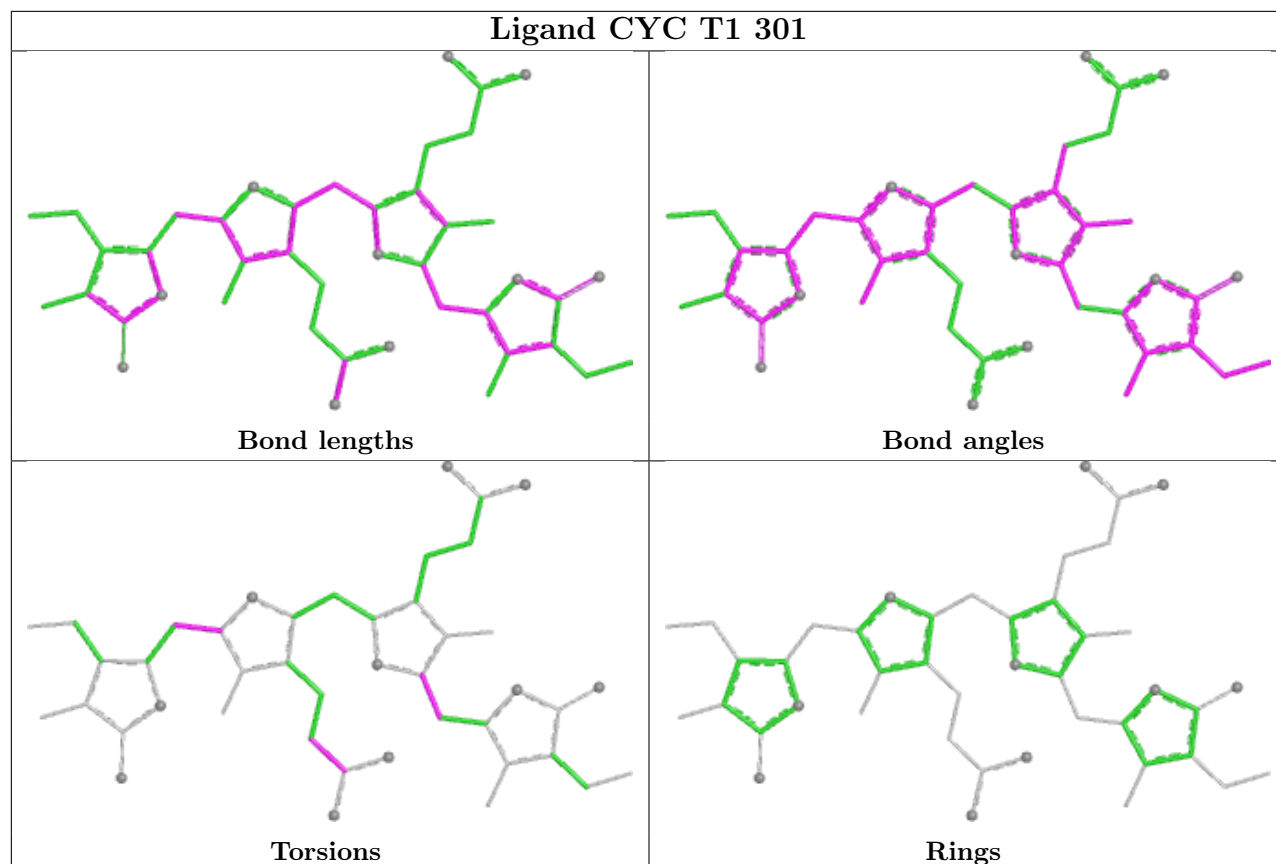
Ligand CYC P4 201



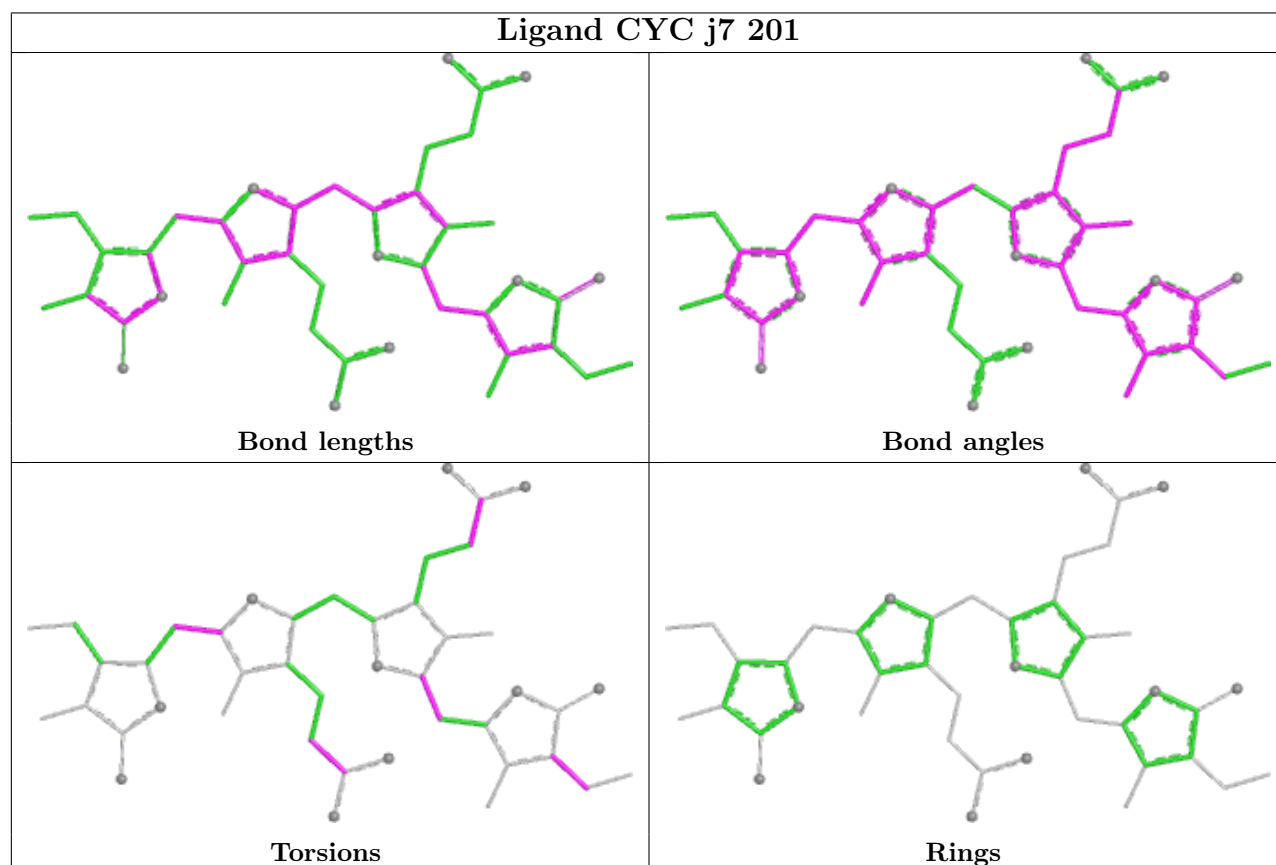
Ligand CYC BA 201



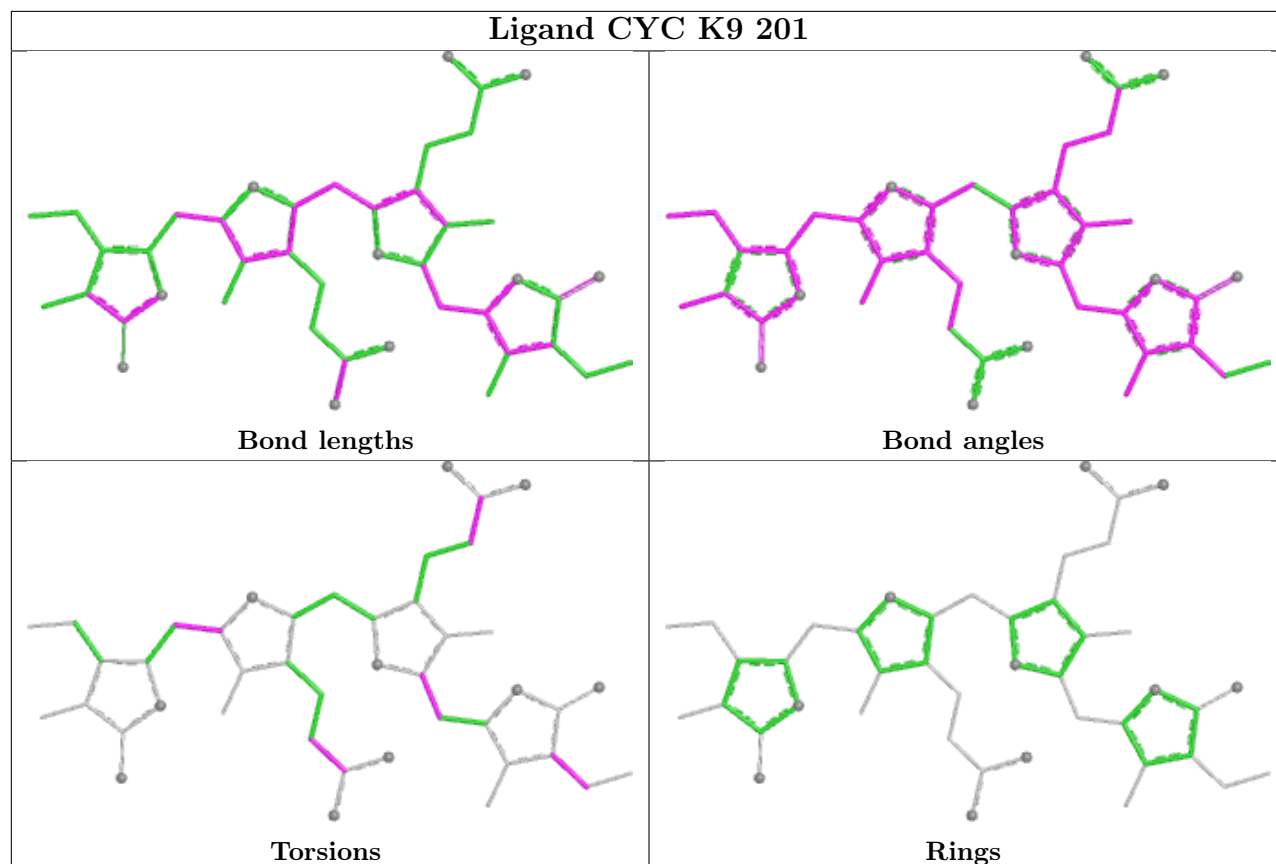
Ligand CYC T1 301



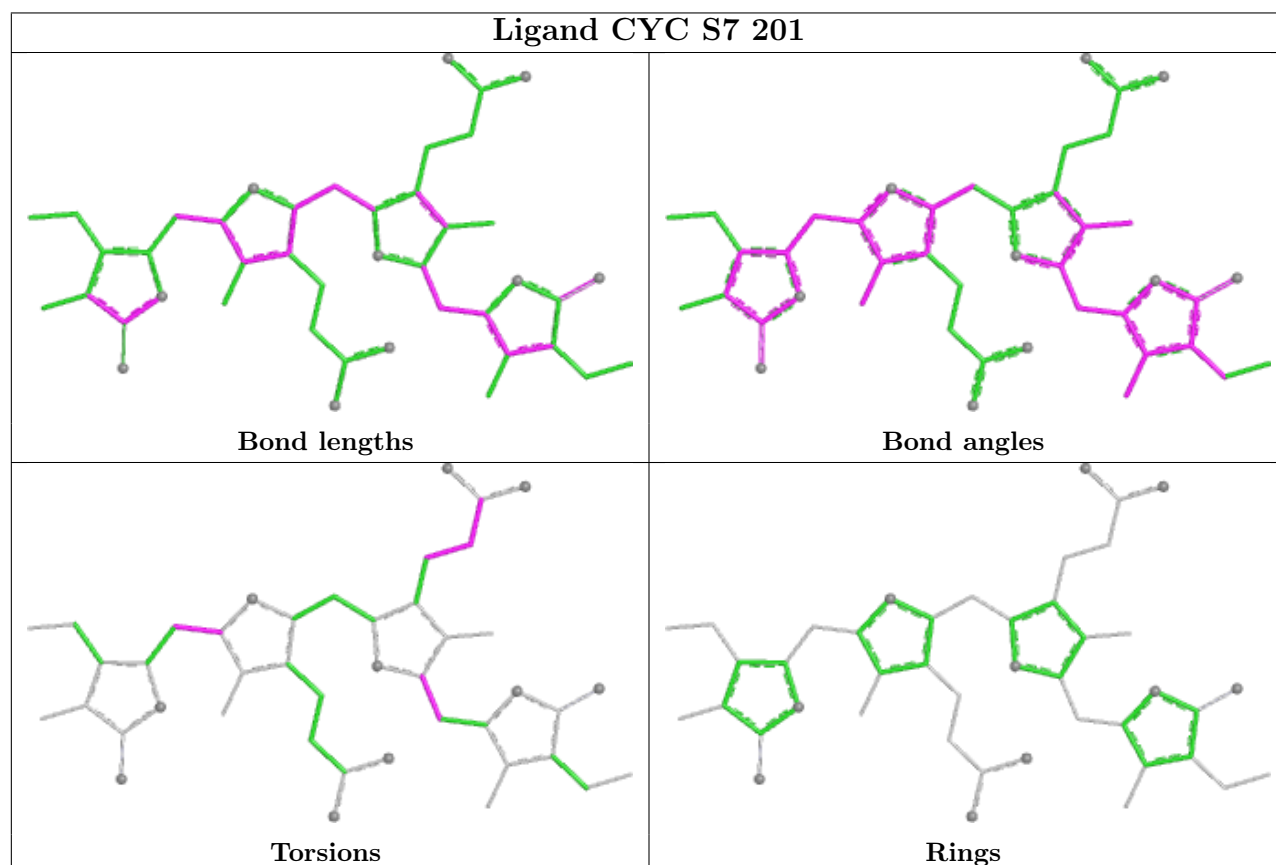
Ligand CYC j7 201



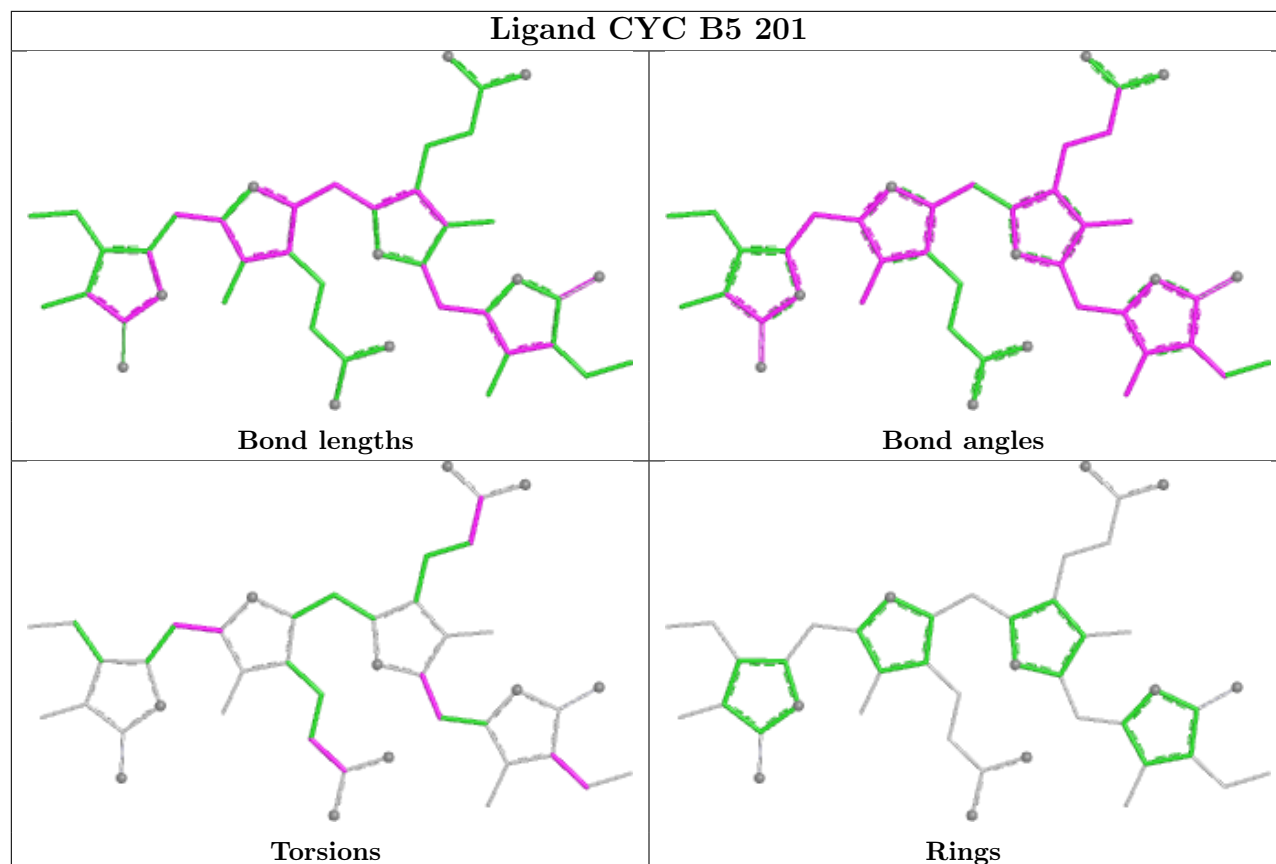
Ligand CYC K9 201



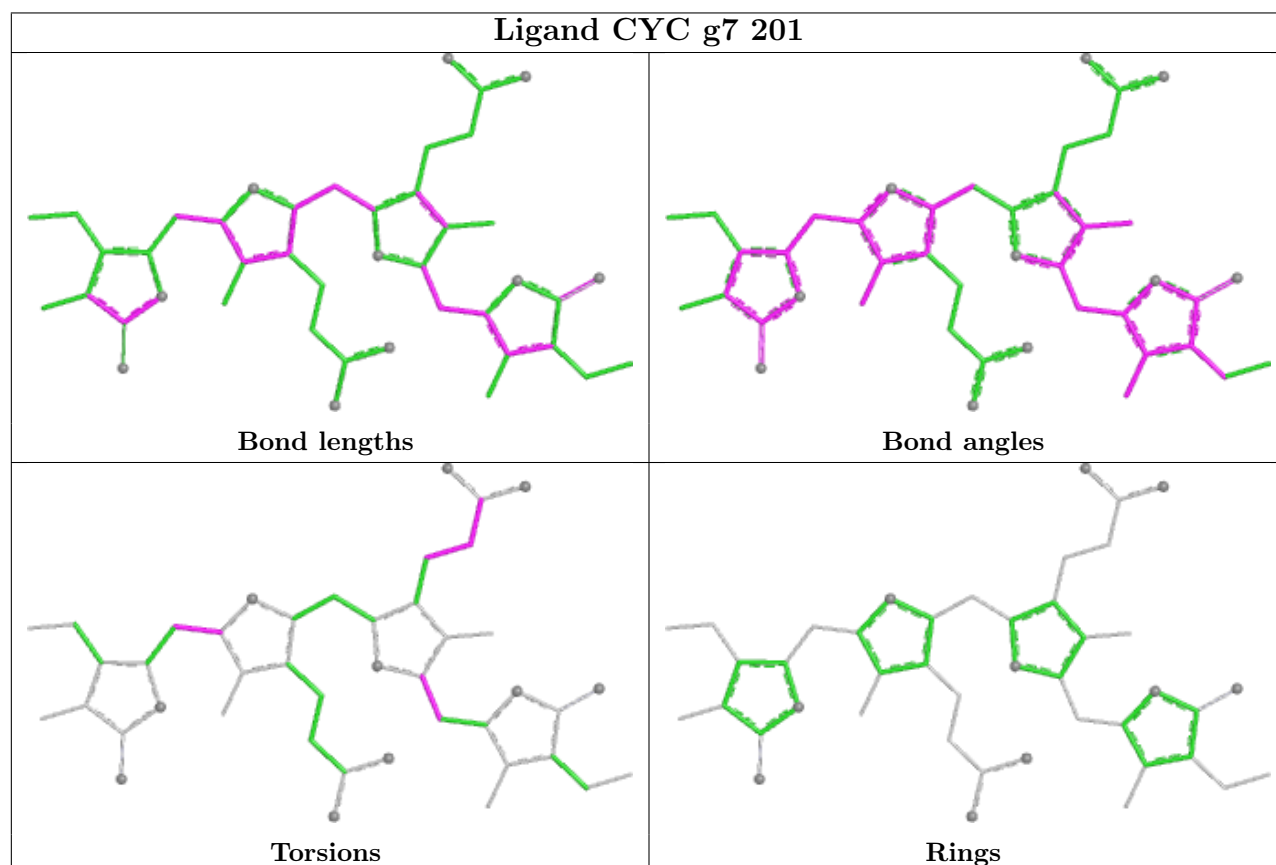
Ligand CYC S7 201



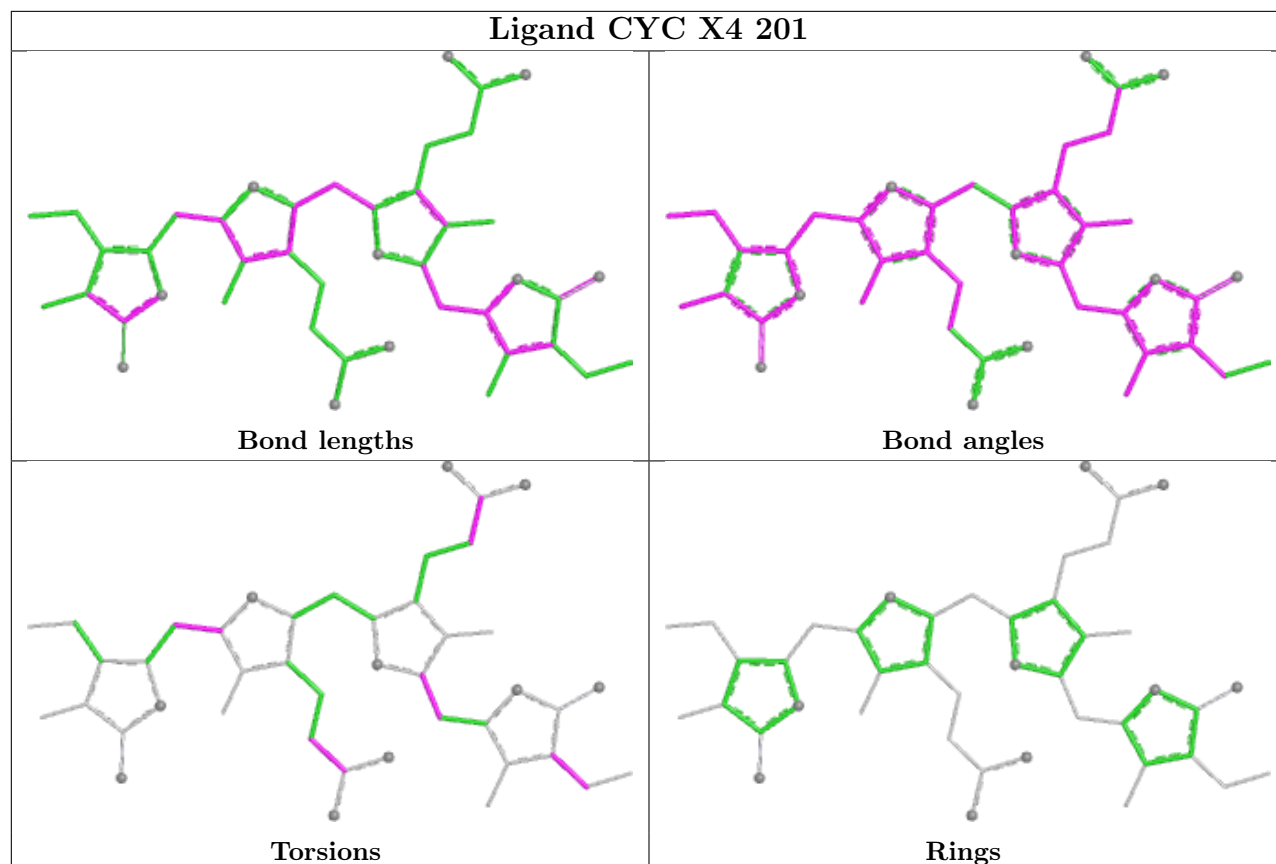
Ligand CYC B5 201



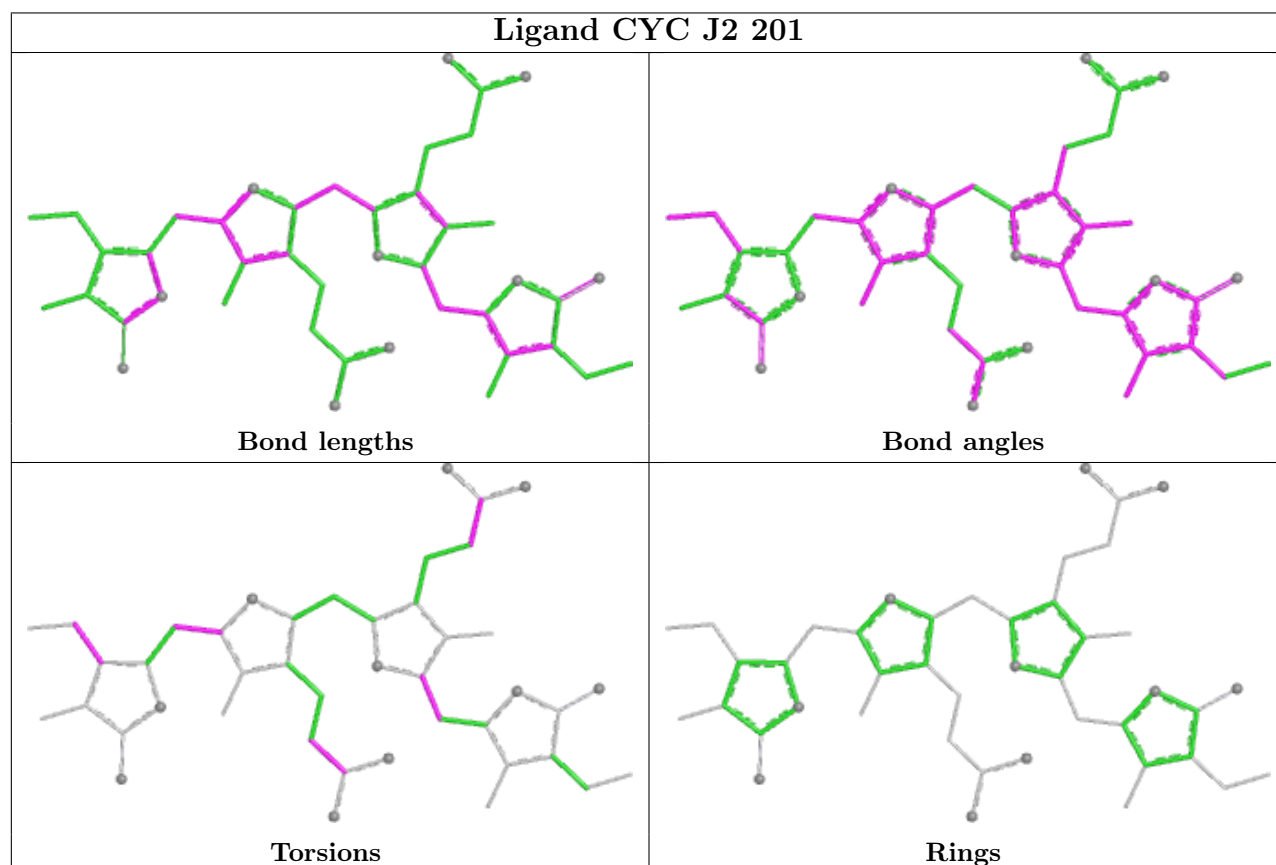
Ligand CYC g7 201



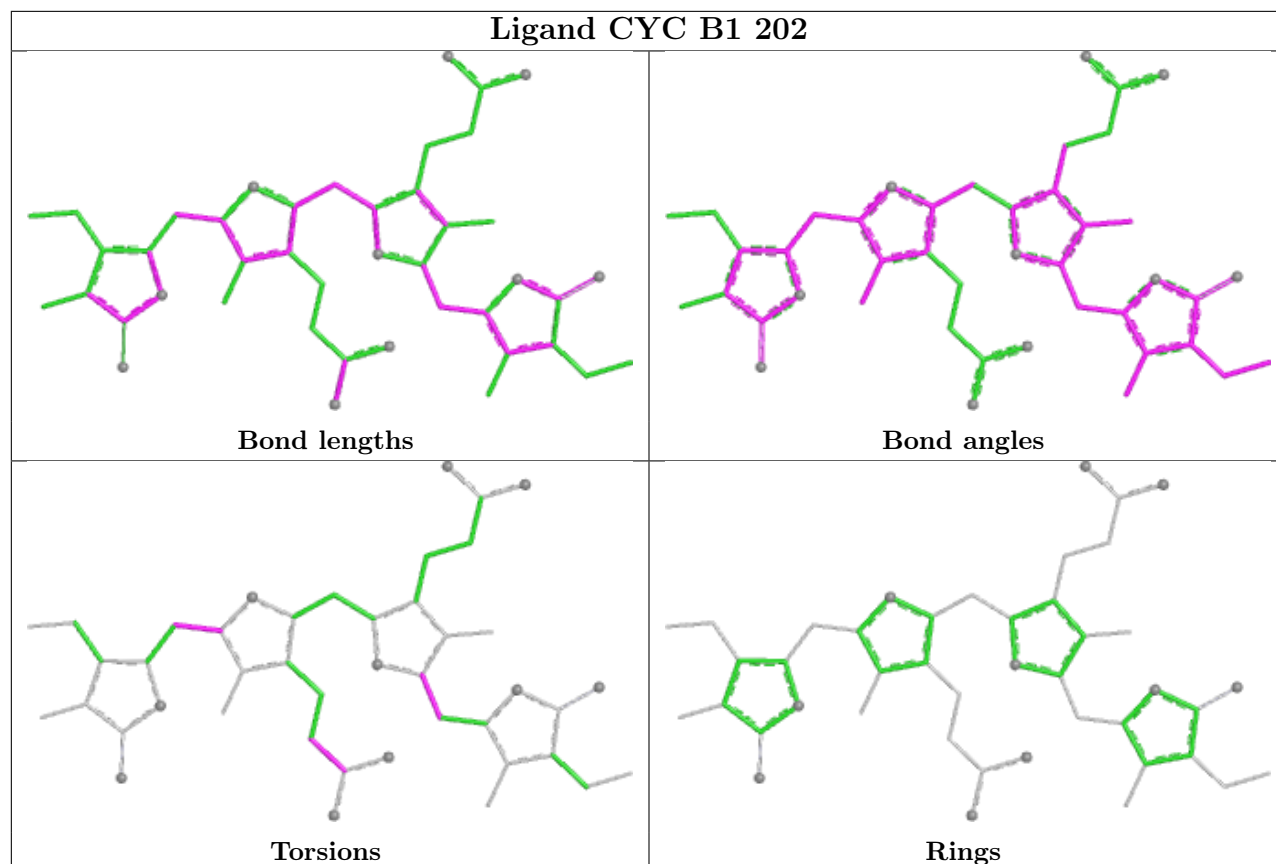
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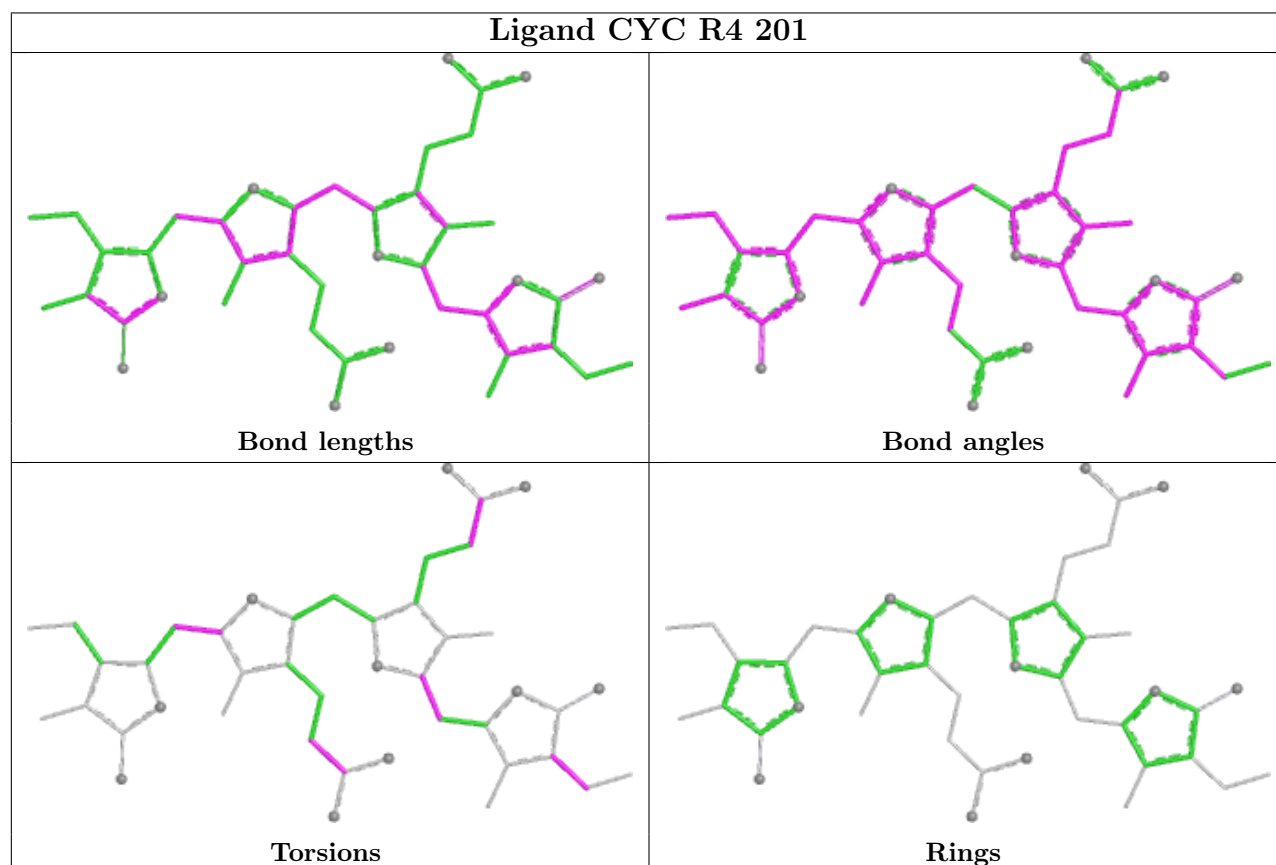
Ligand CYC J2 201



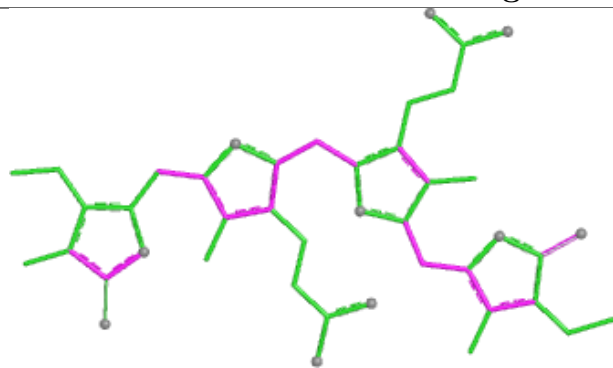
Ligand CYC B1 202



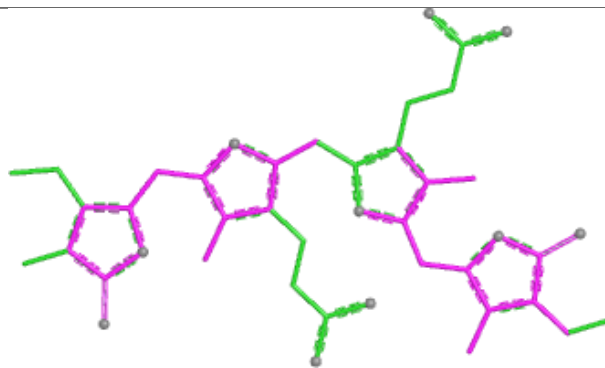
Ligand CYC R4 201



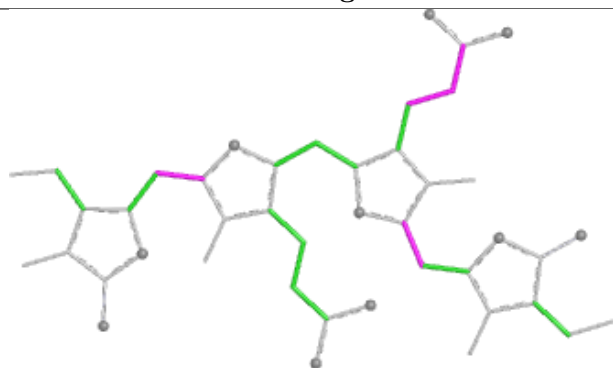
Ligand CYC O5 201



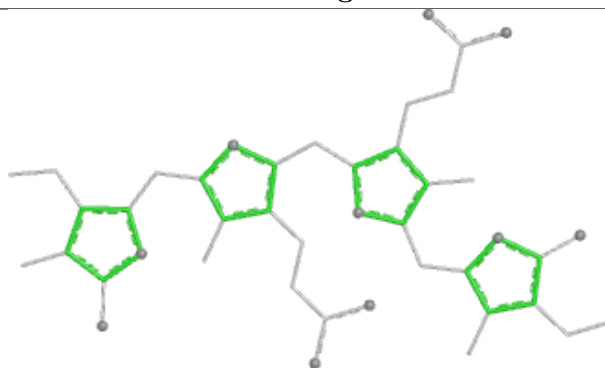
Bond lengths



Bond angles

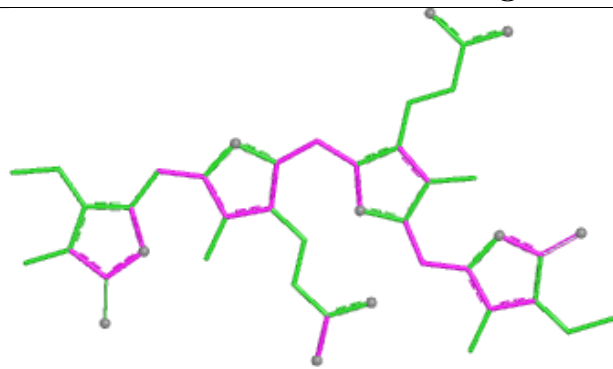


Torsions

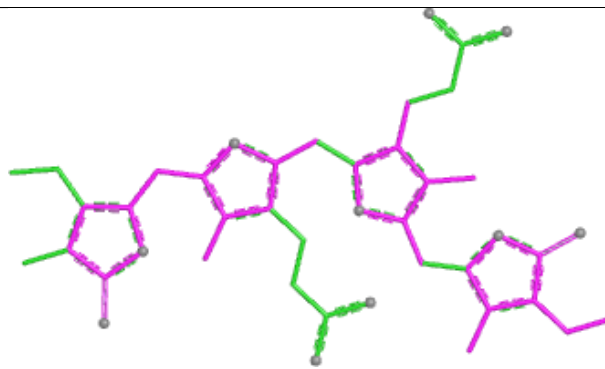


Rings

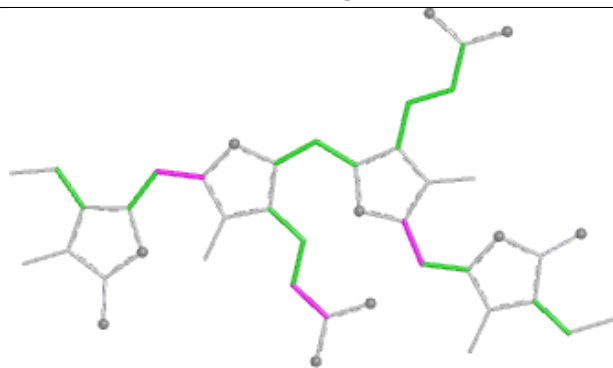
Ligand CYC M8 302



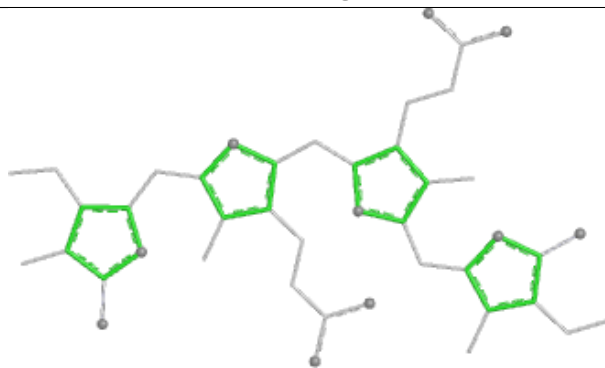
Bond lengths



Bond angles

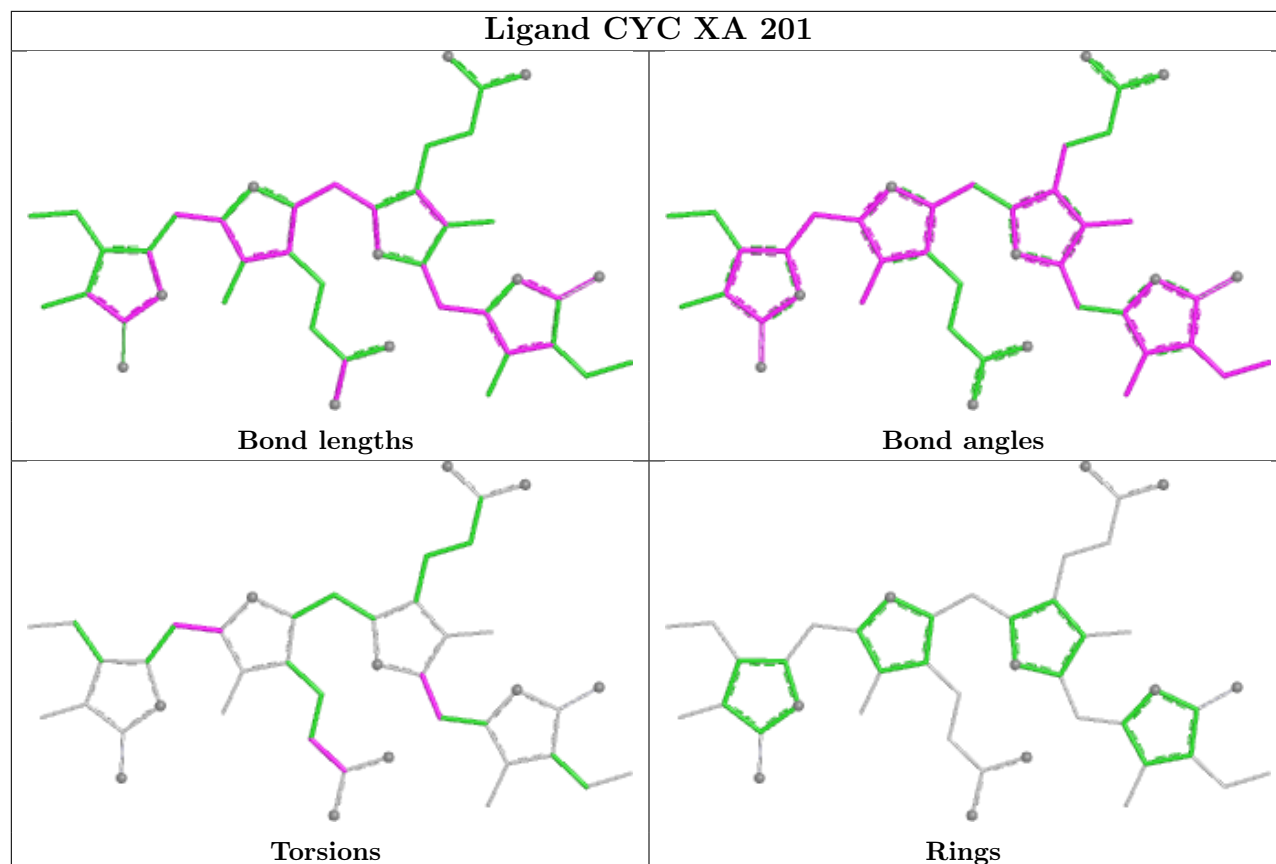


Torsions

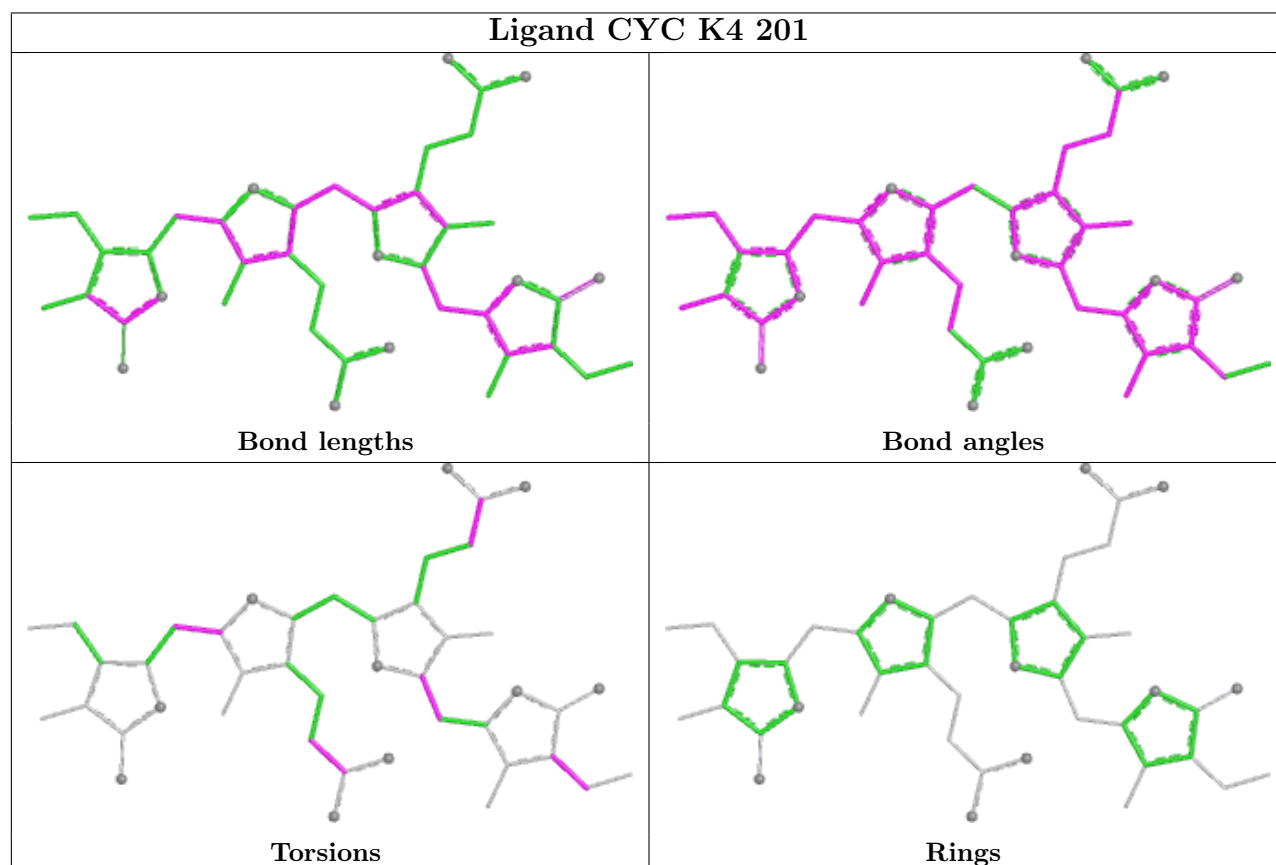


Rings

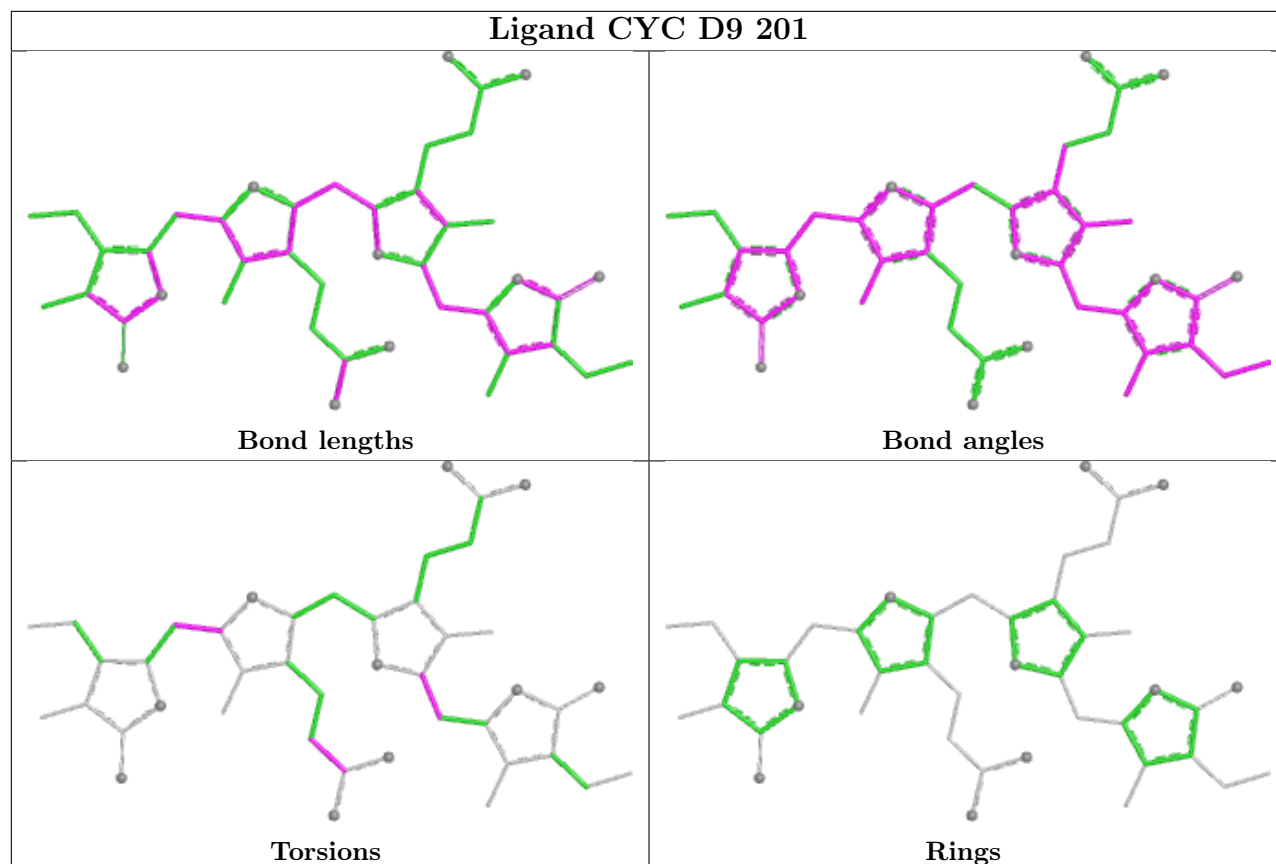
Ligand CYC XA 201



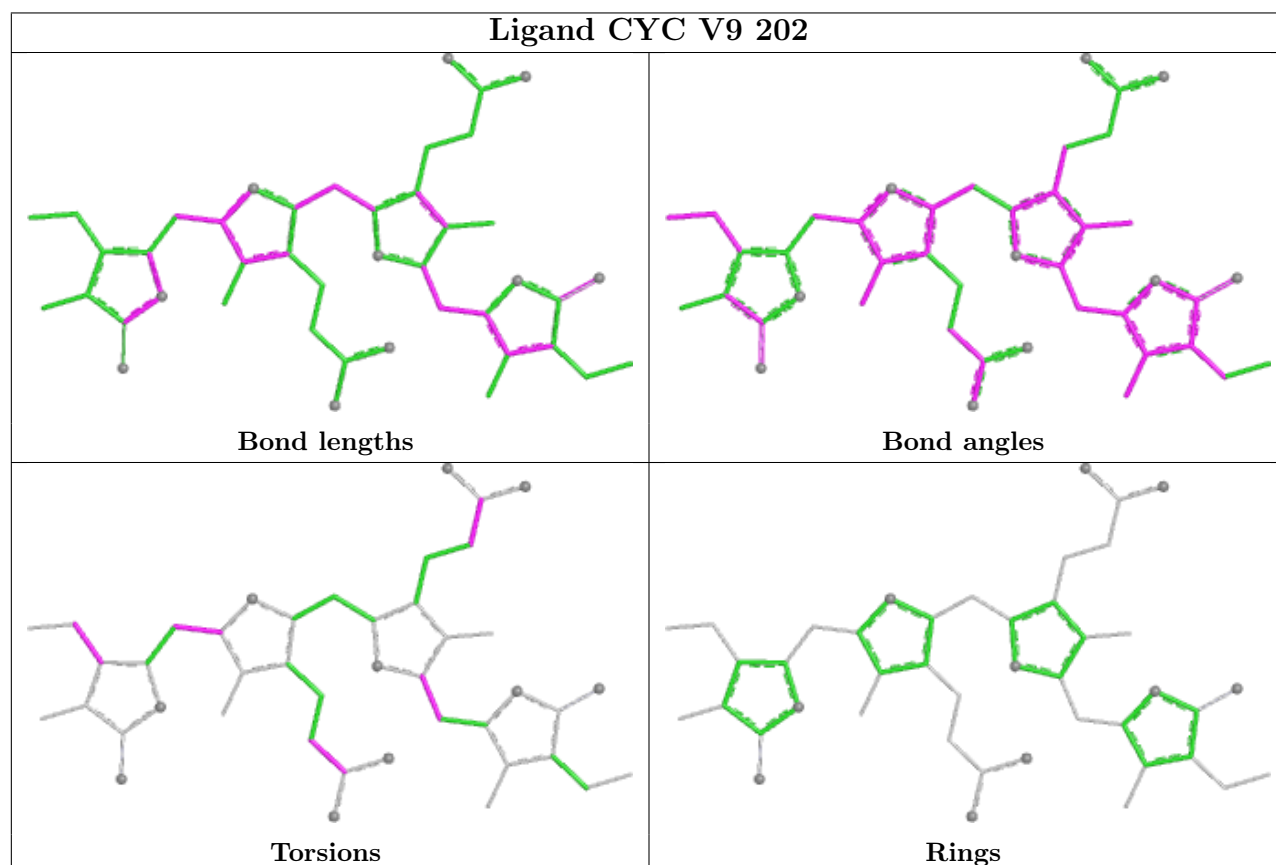
Ligand CYC K4 201

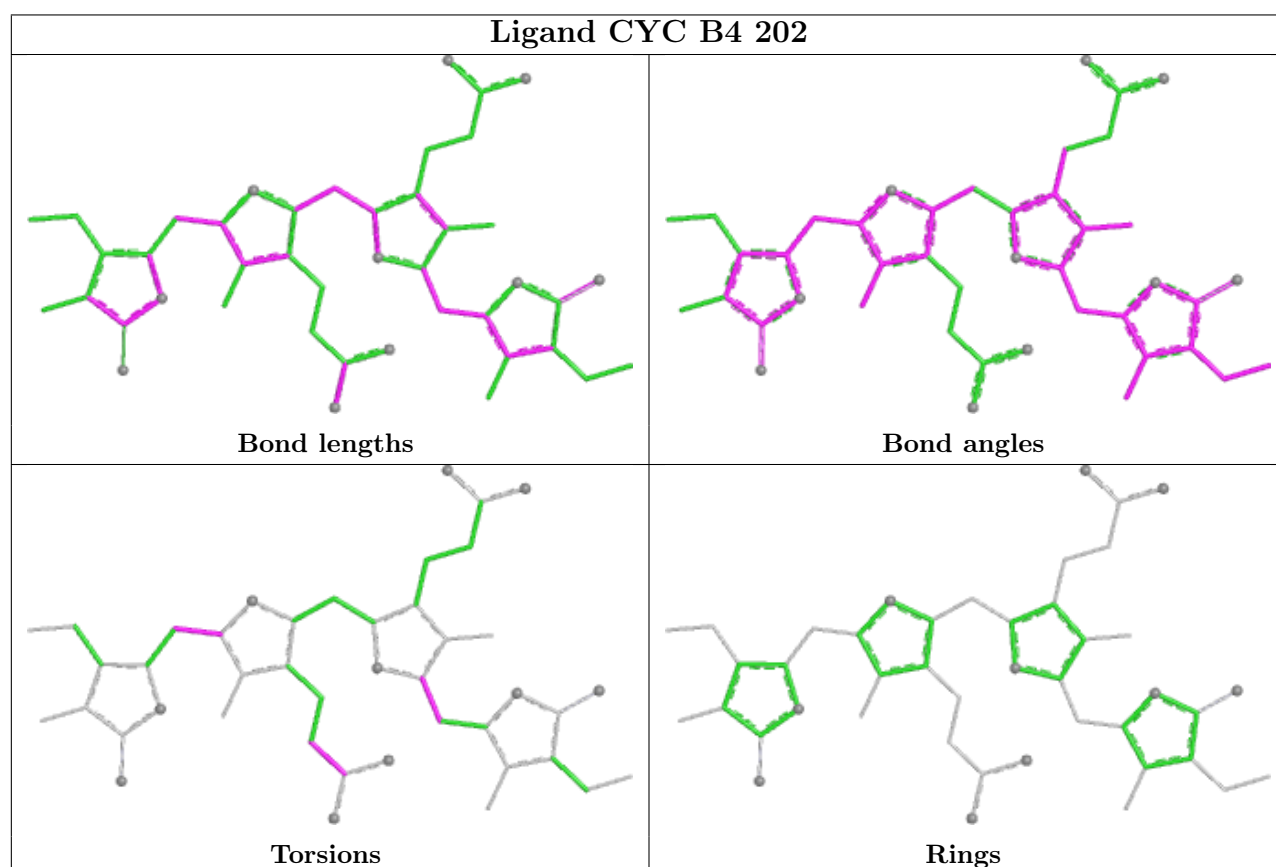
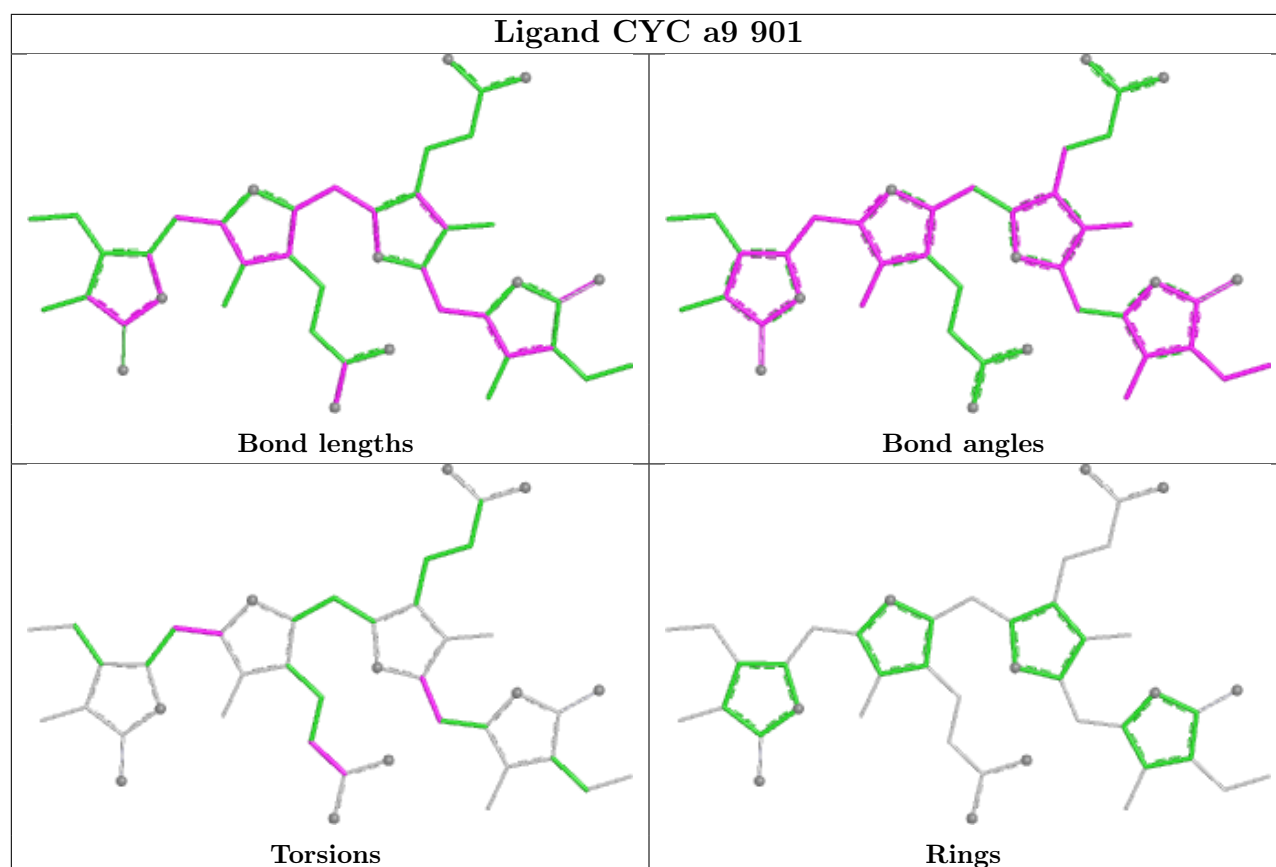


Ligand CYC D9 201

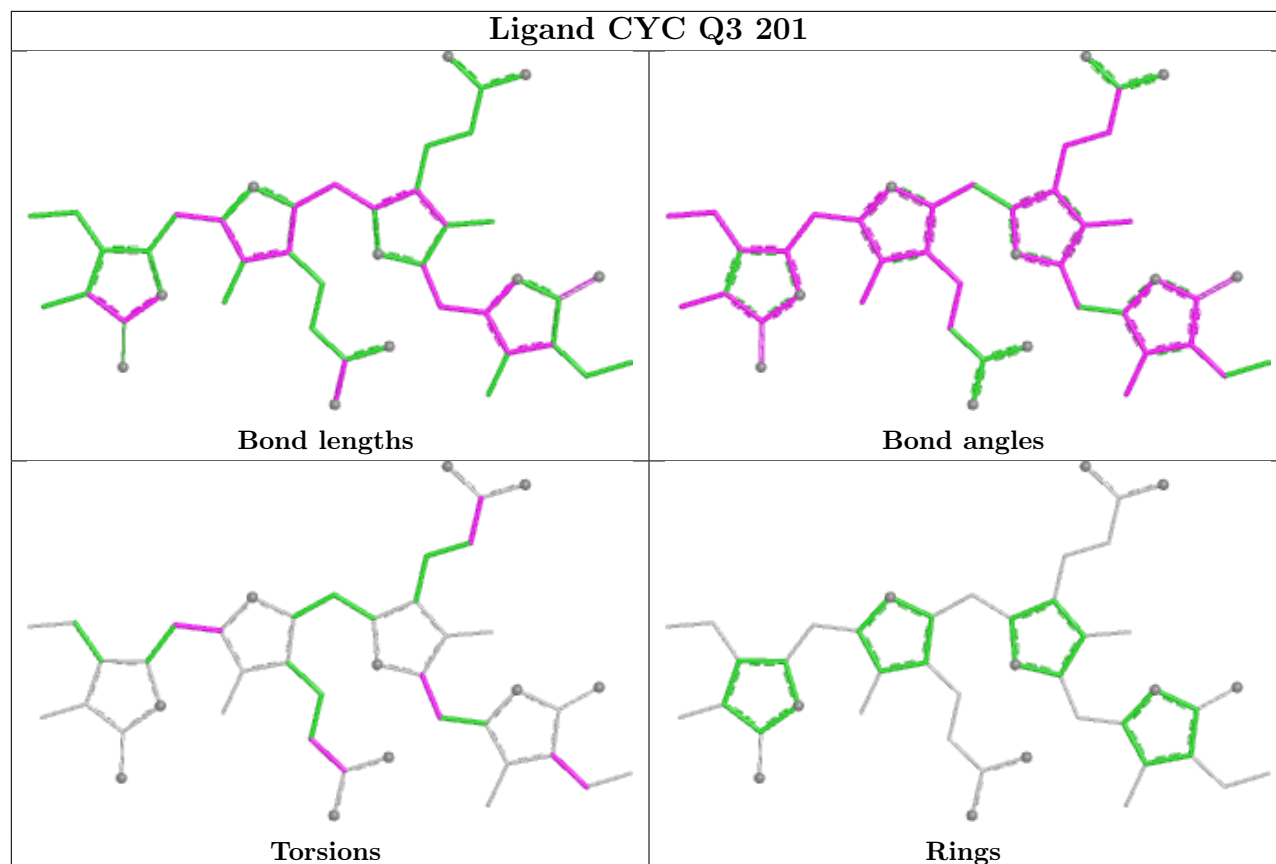


Ligand CYC V9 202

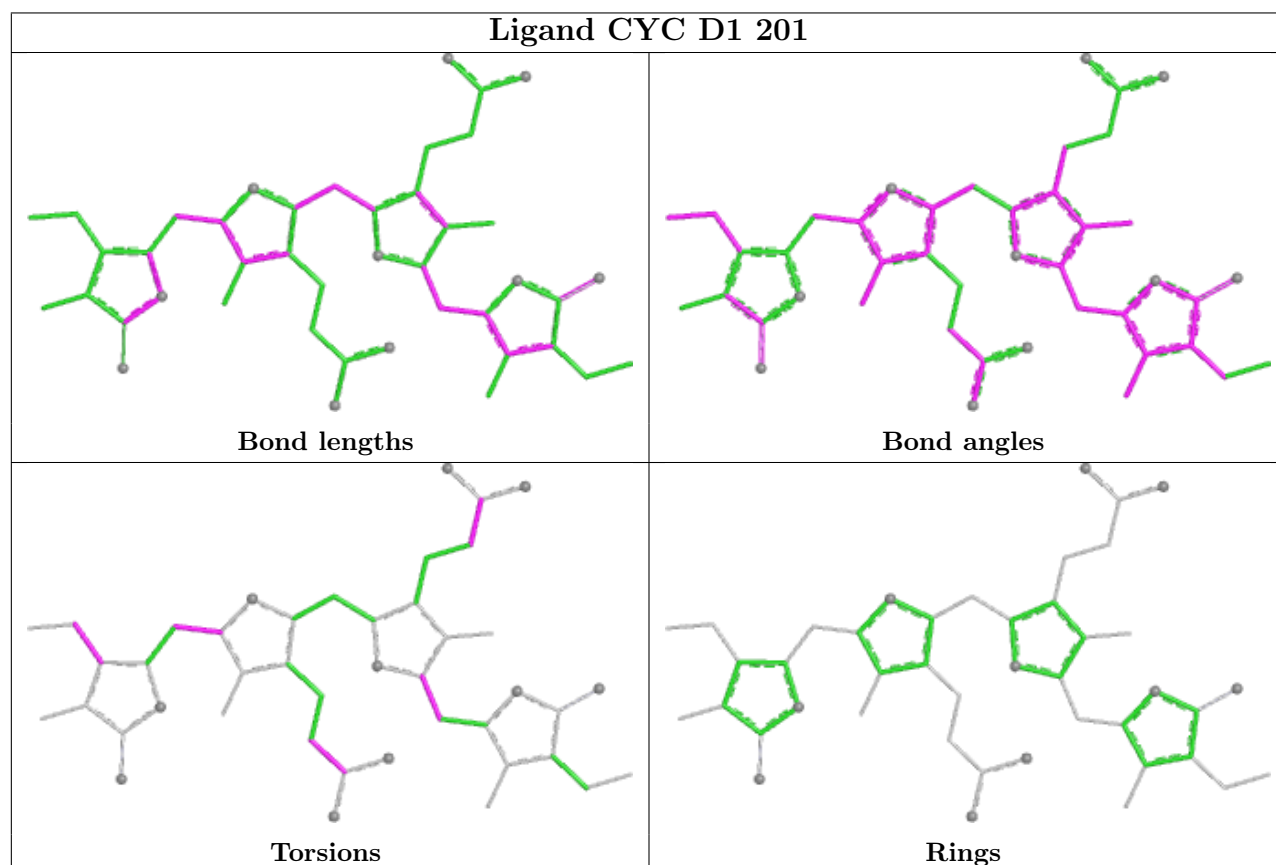




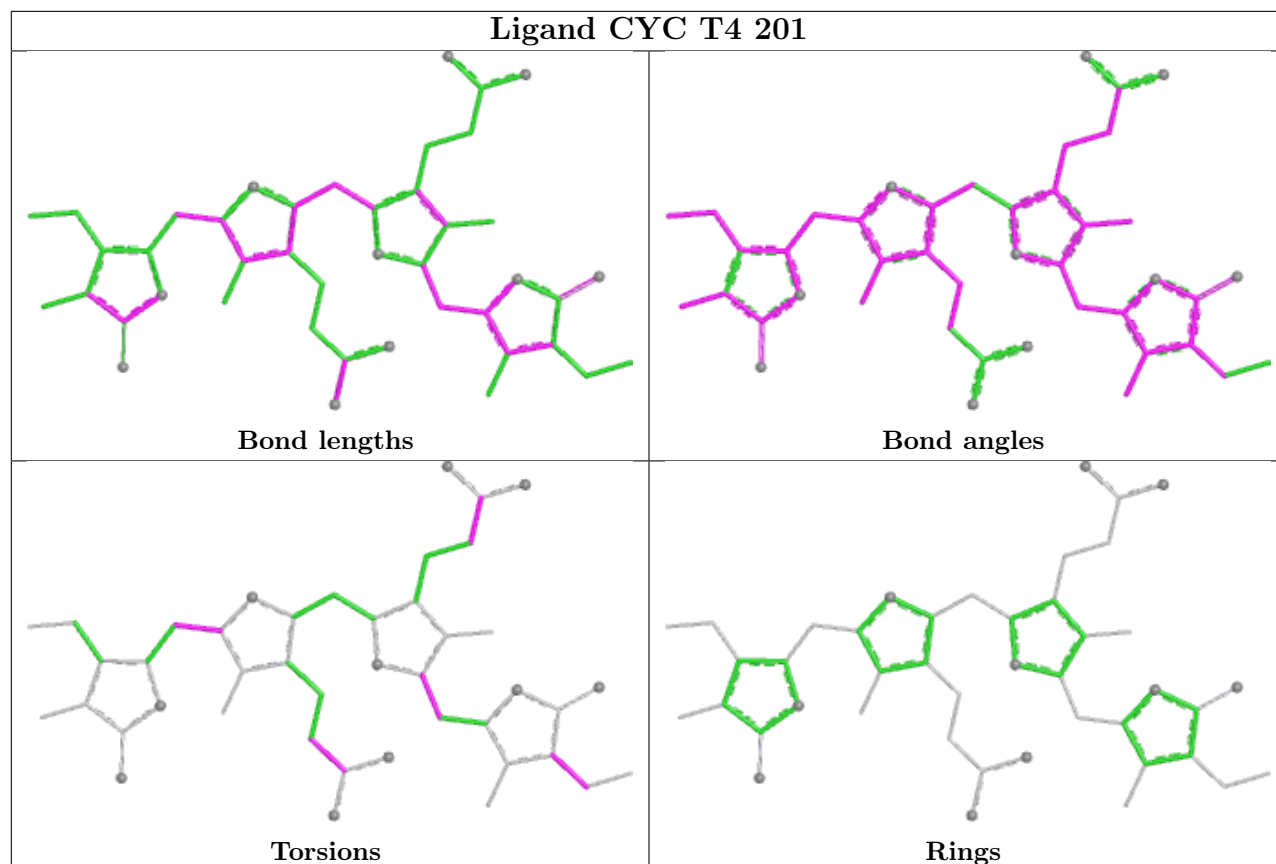
Ligand CYC Q3 201



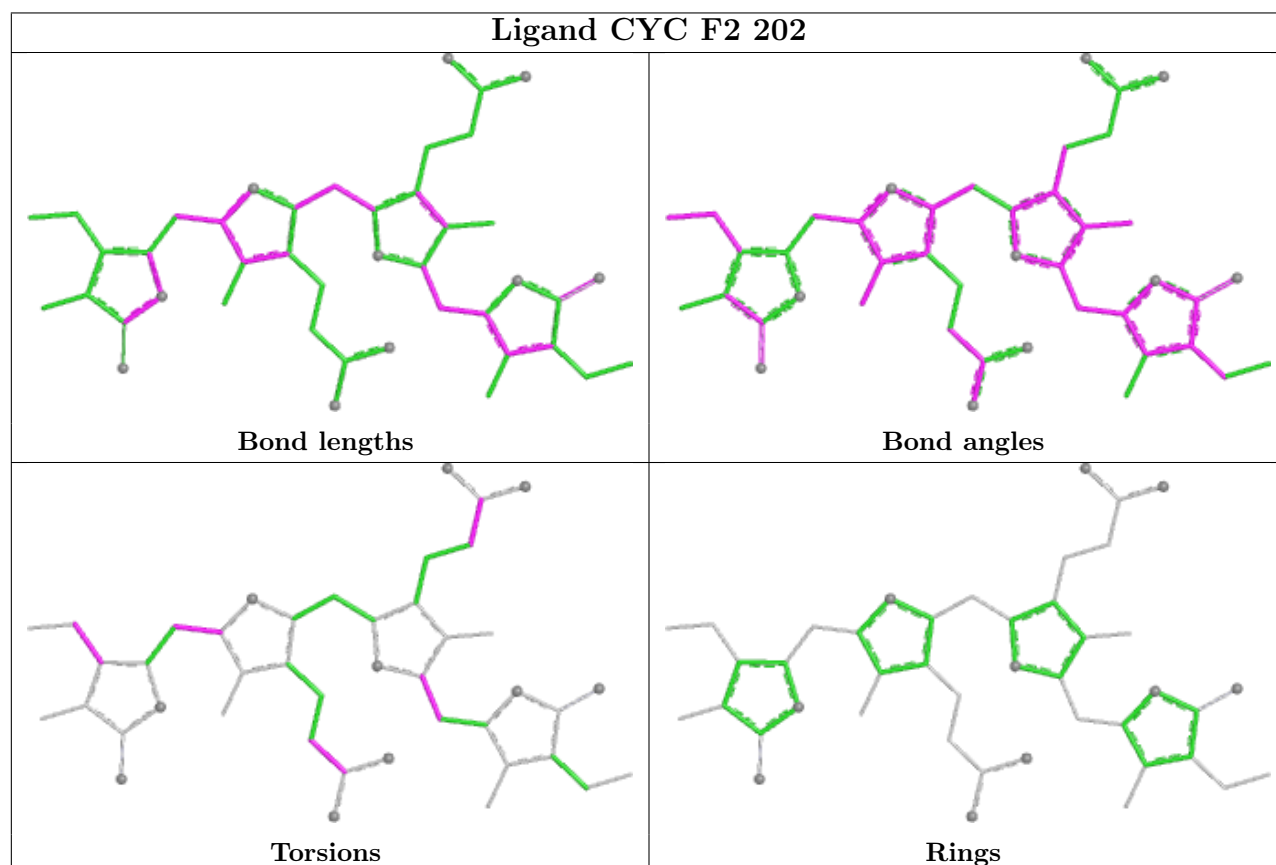
Ligand CYC D1 201



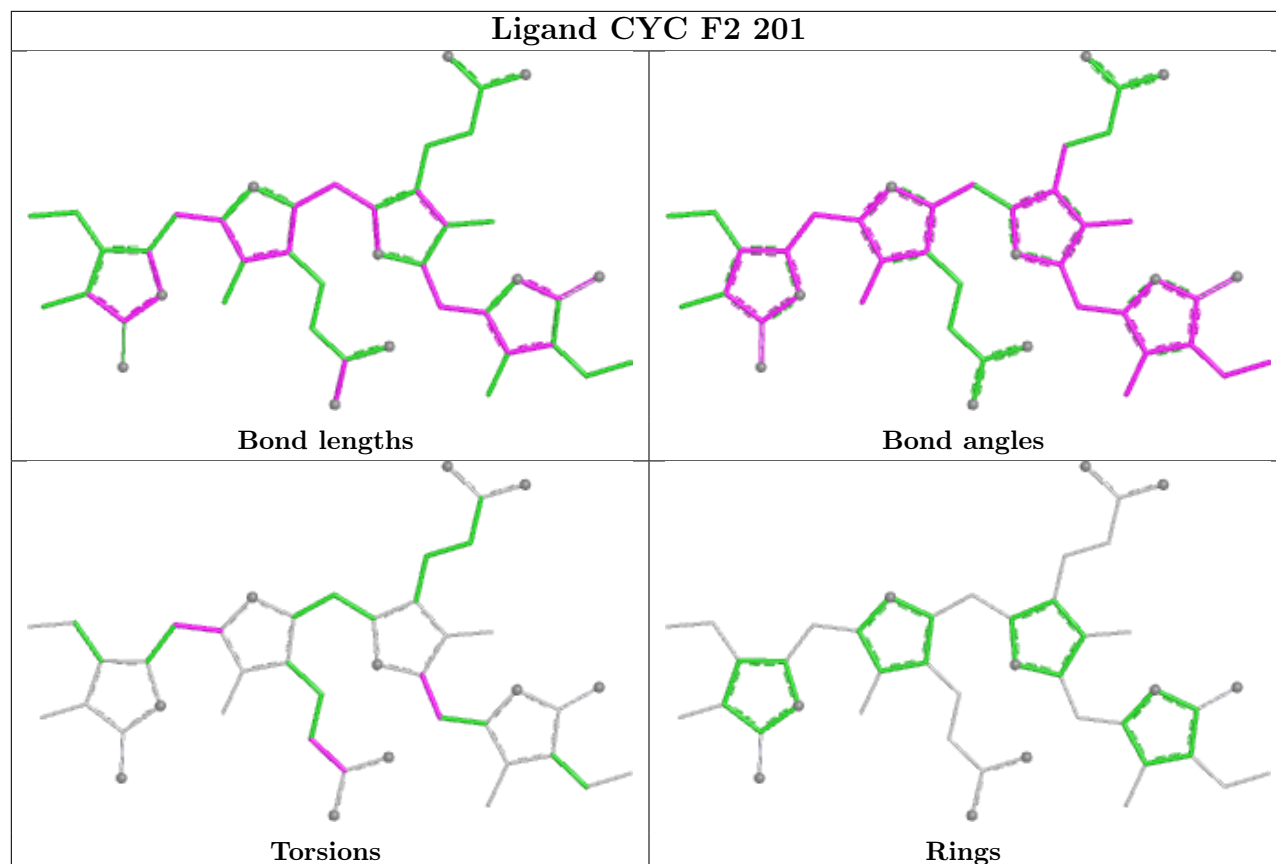
Ligand CYC T4 201



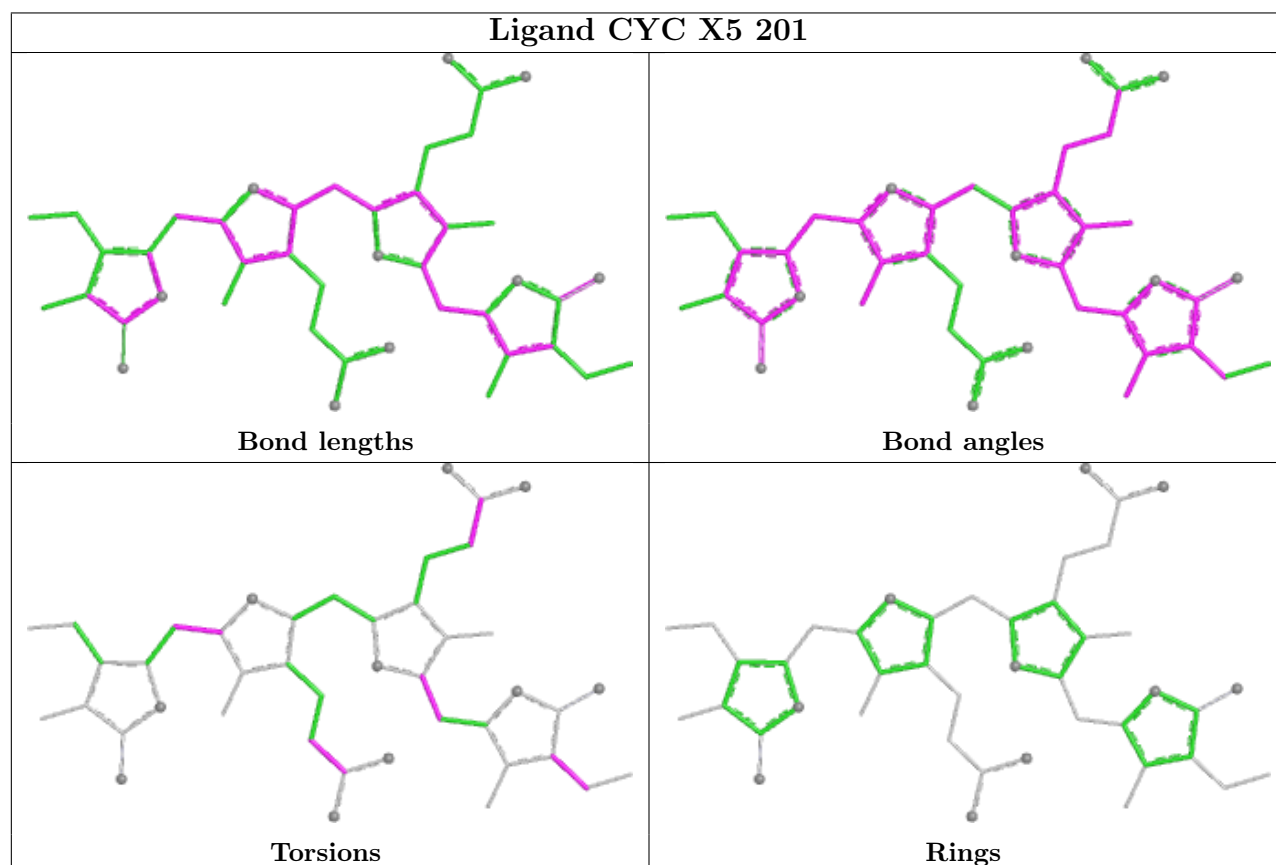
Ligand CYC F2 202



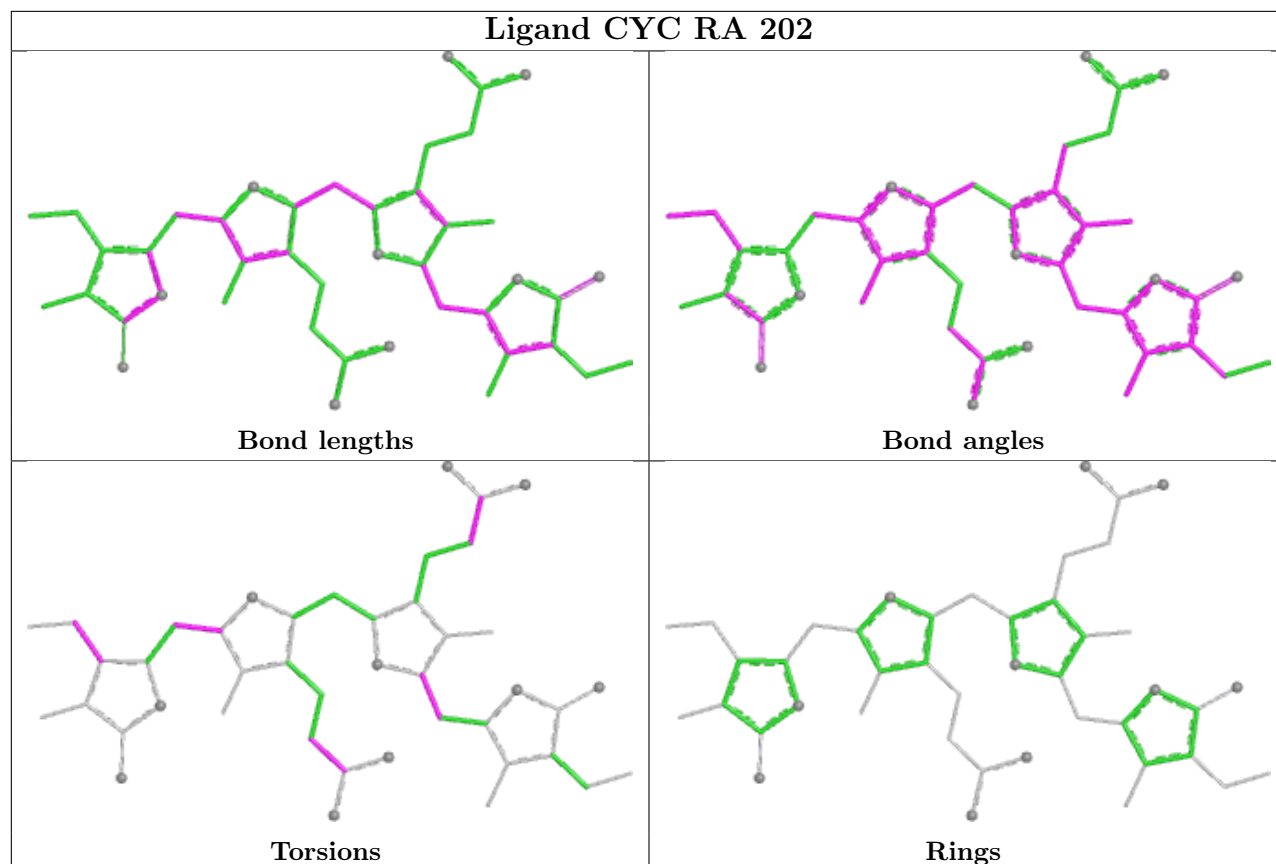
Ligand CYC F2 201



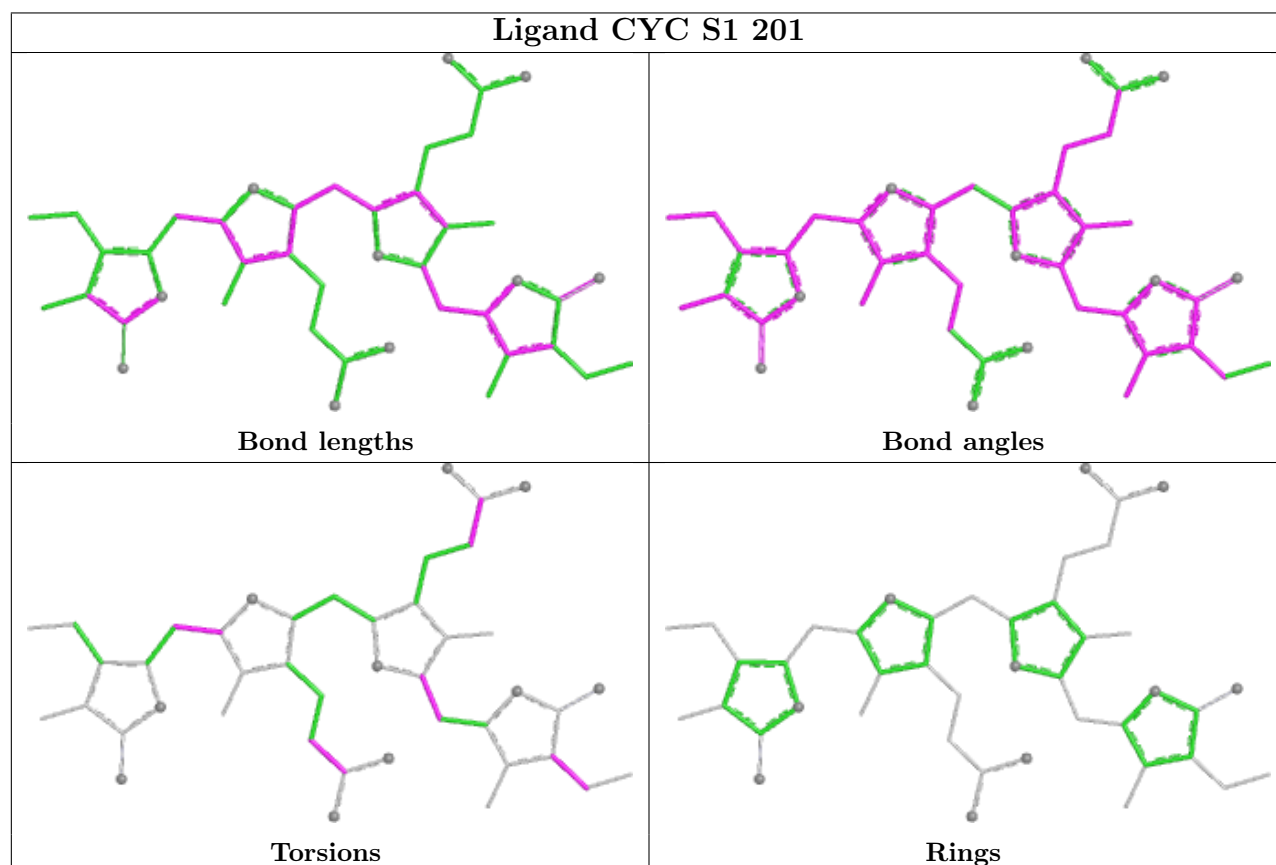
Ligand CYC X5 201

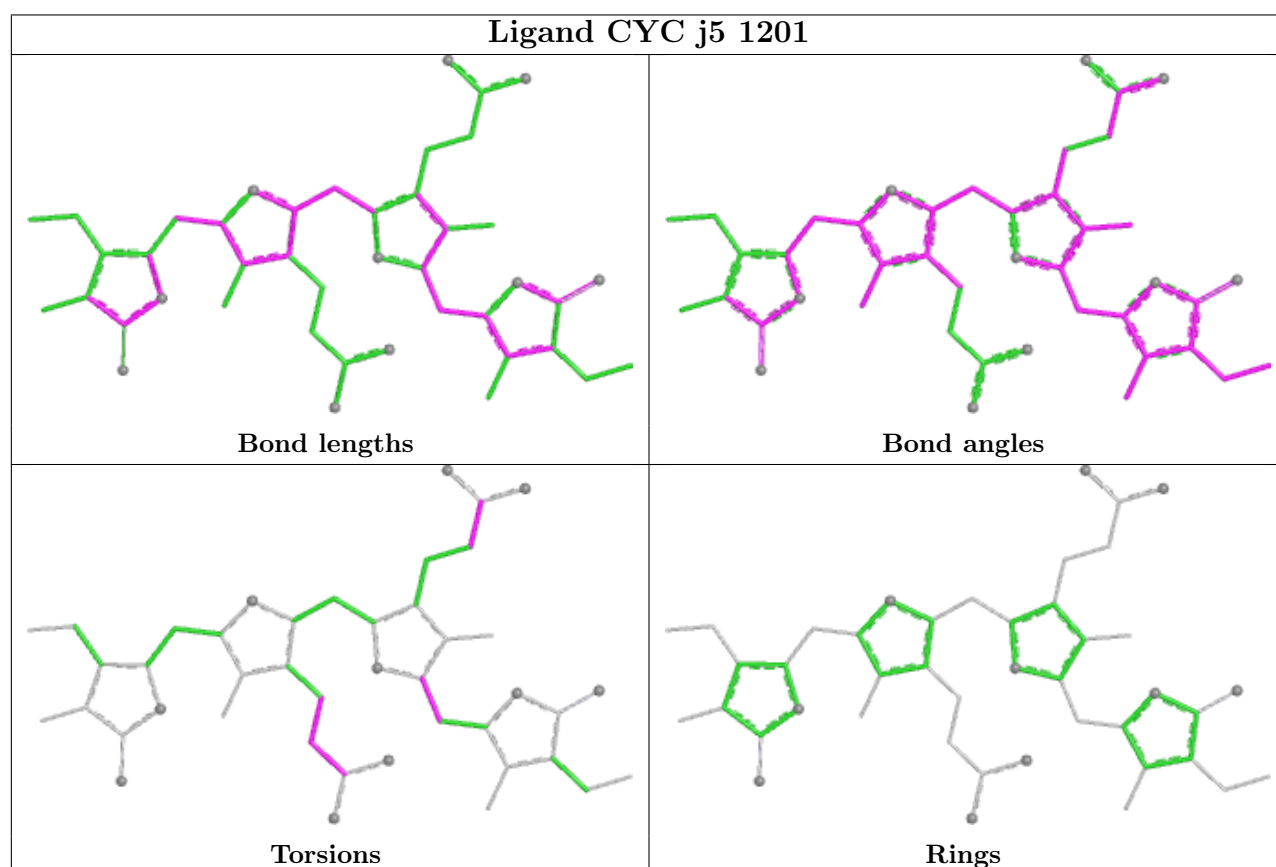
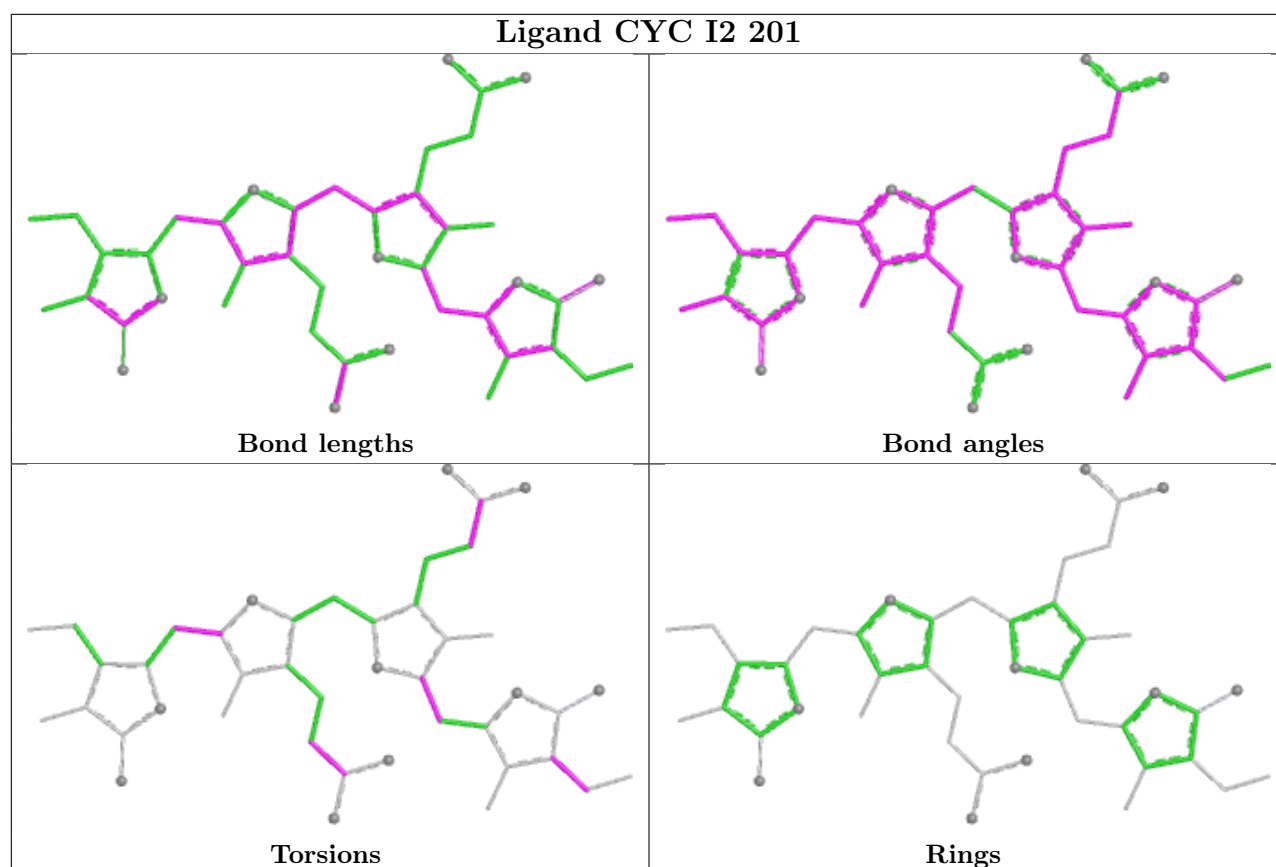


Ligand CYC RA 202

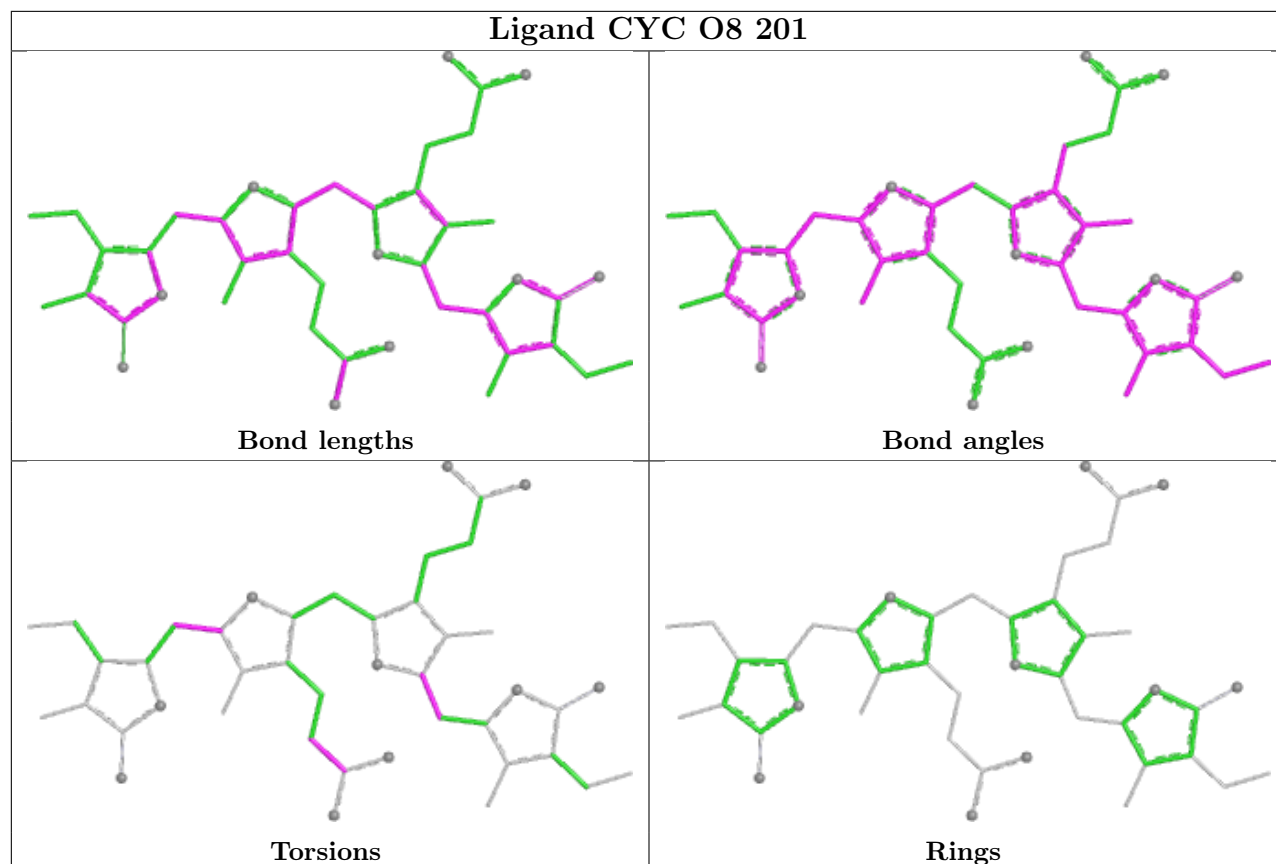


Ligand CYC S1 201

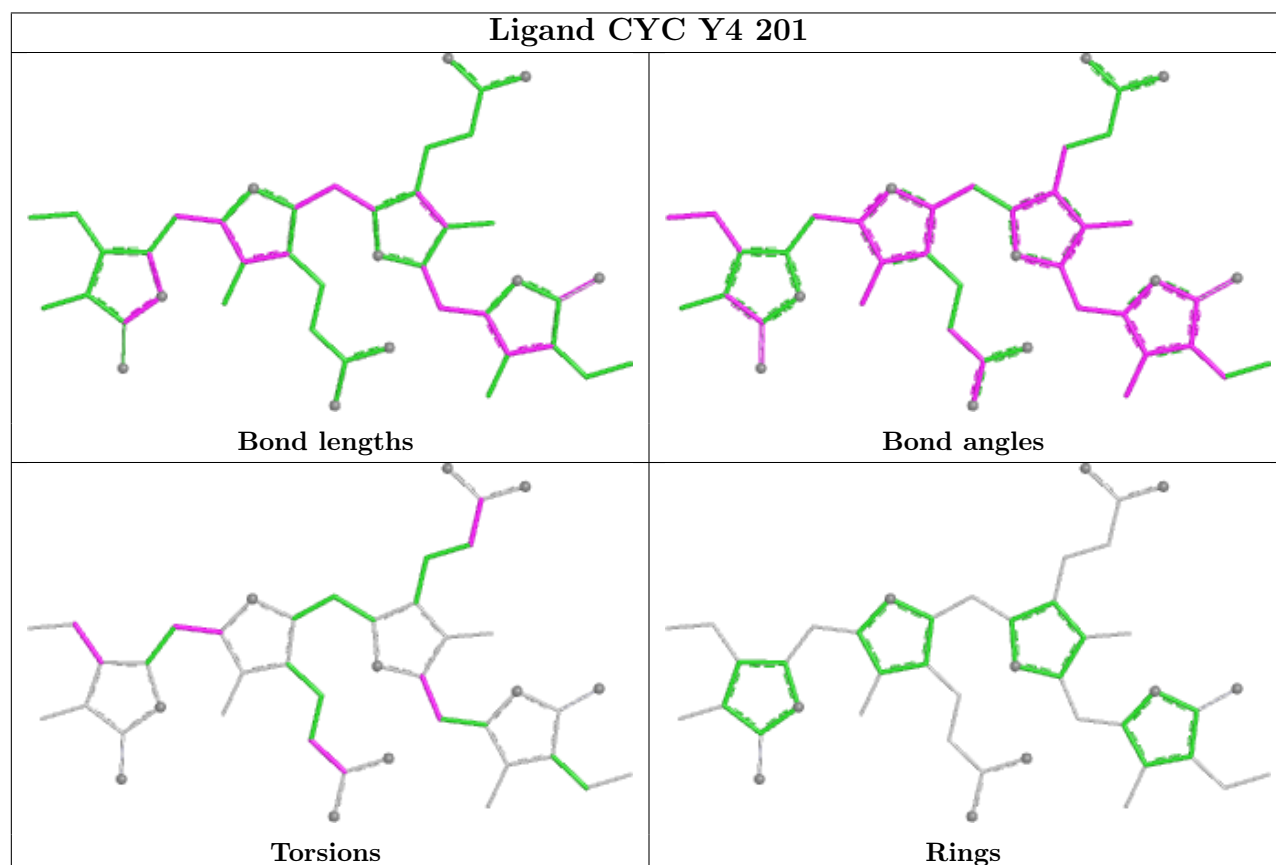




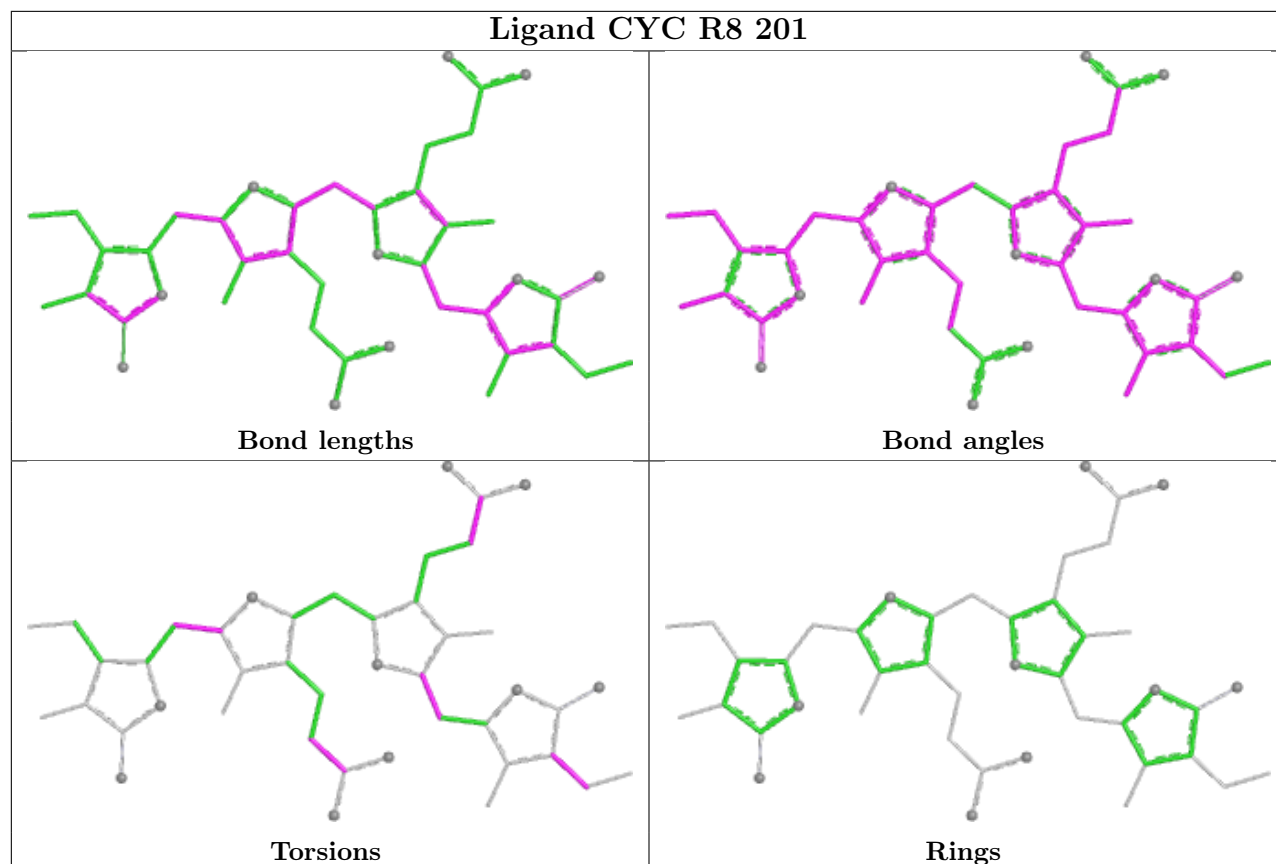
Ligand CYC O8 201



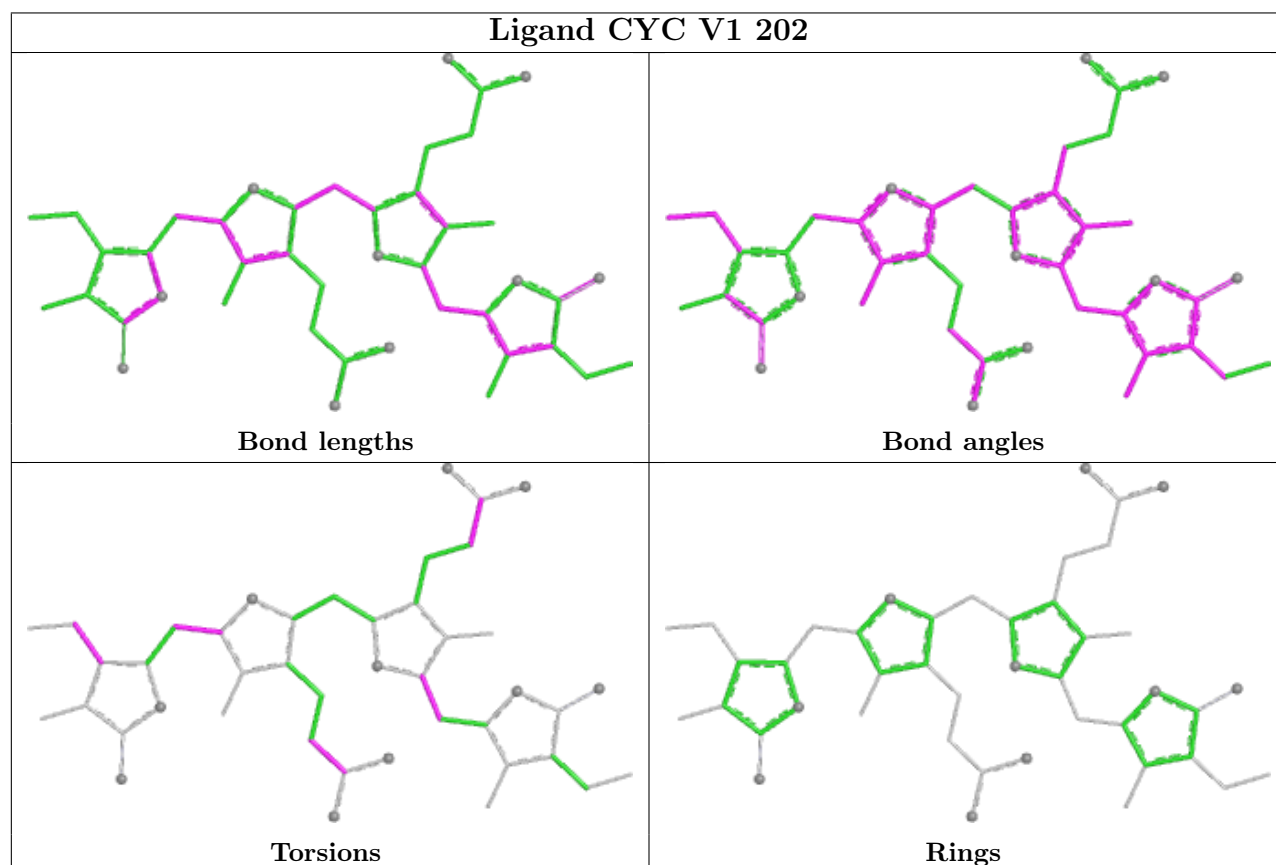
Ligand CYC Y4 201



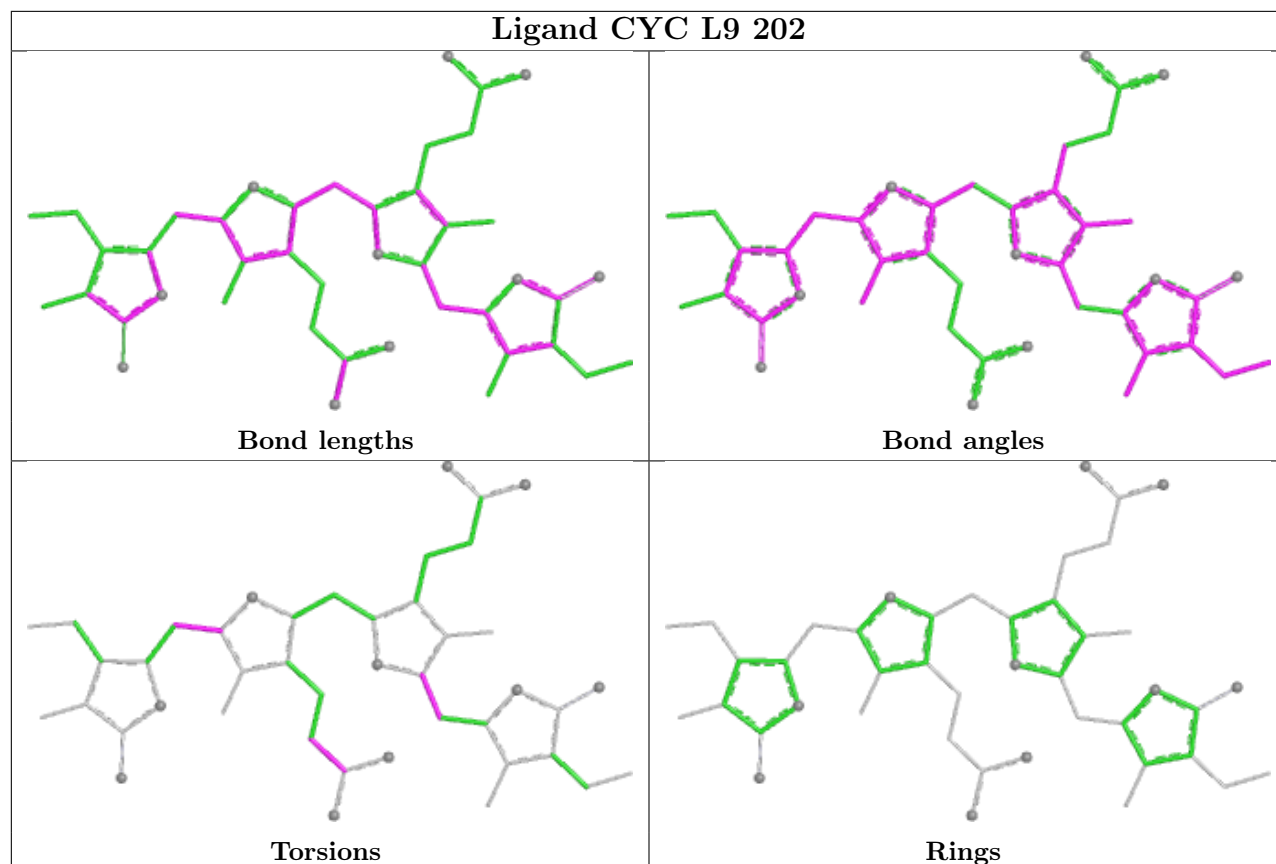
Ligand CYC R8 201



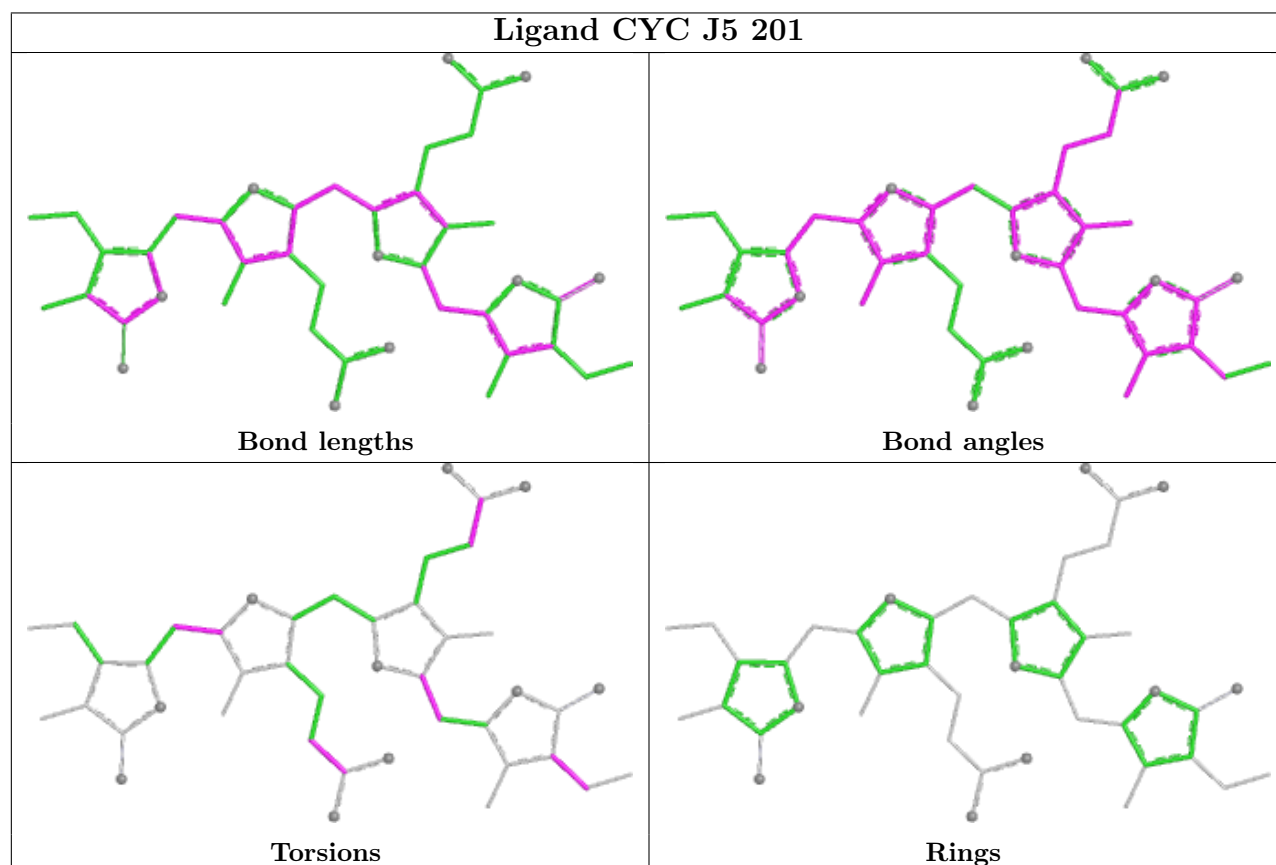
Ligand CYC V1 202



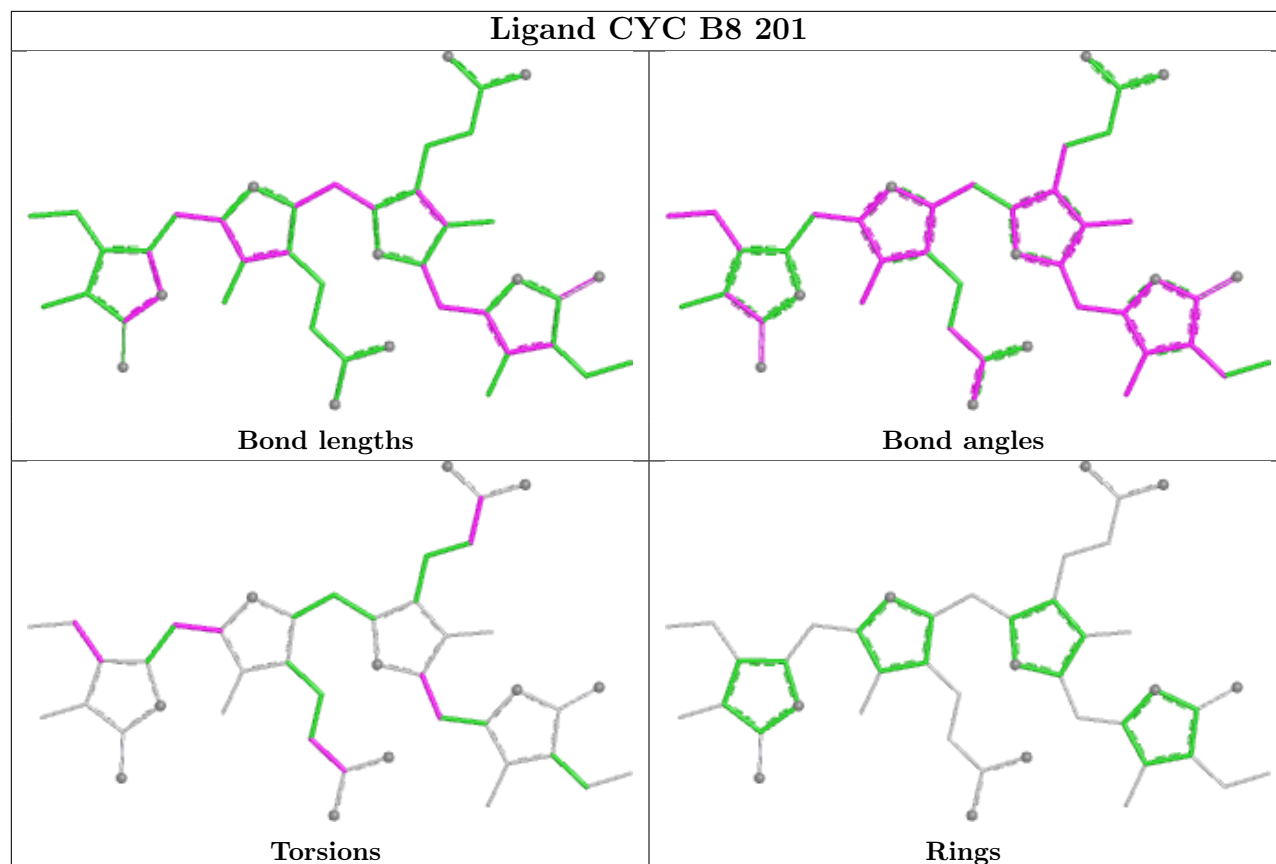
Ligand CYC L9 202



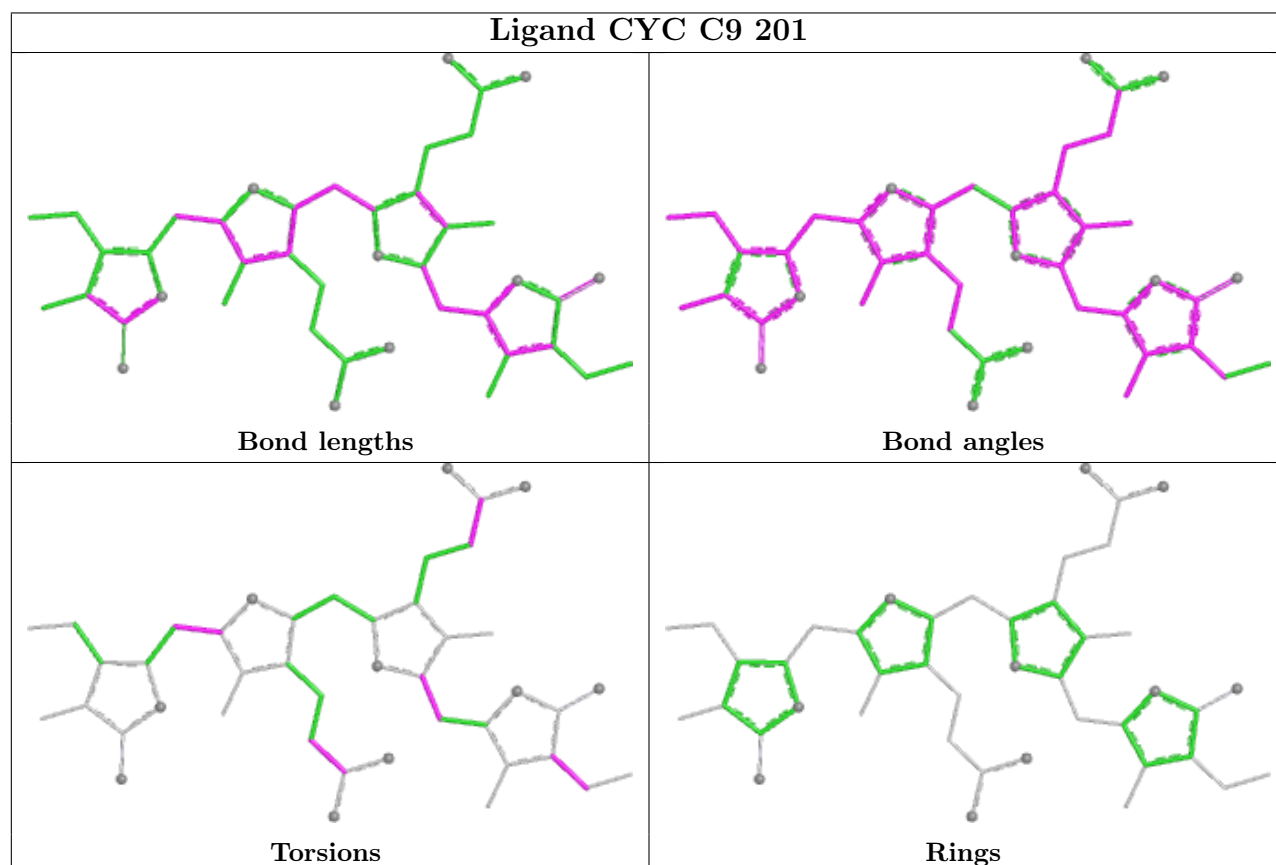
Ligand CYC J5 201



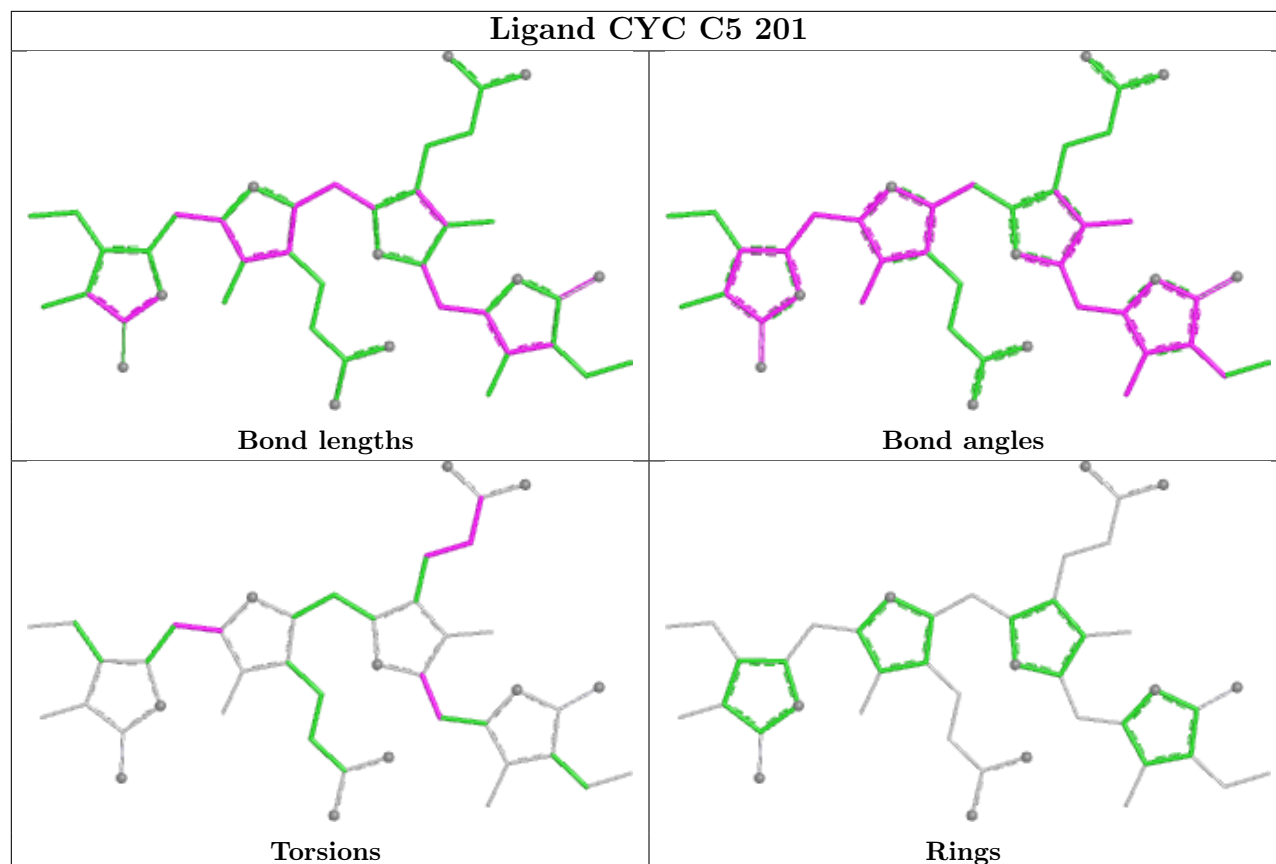
Ligand CYC B8 201



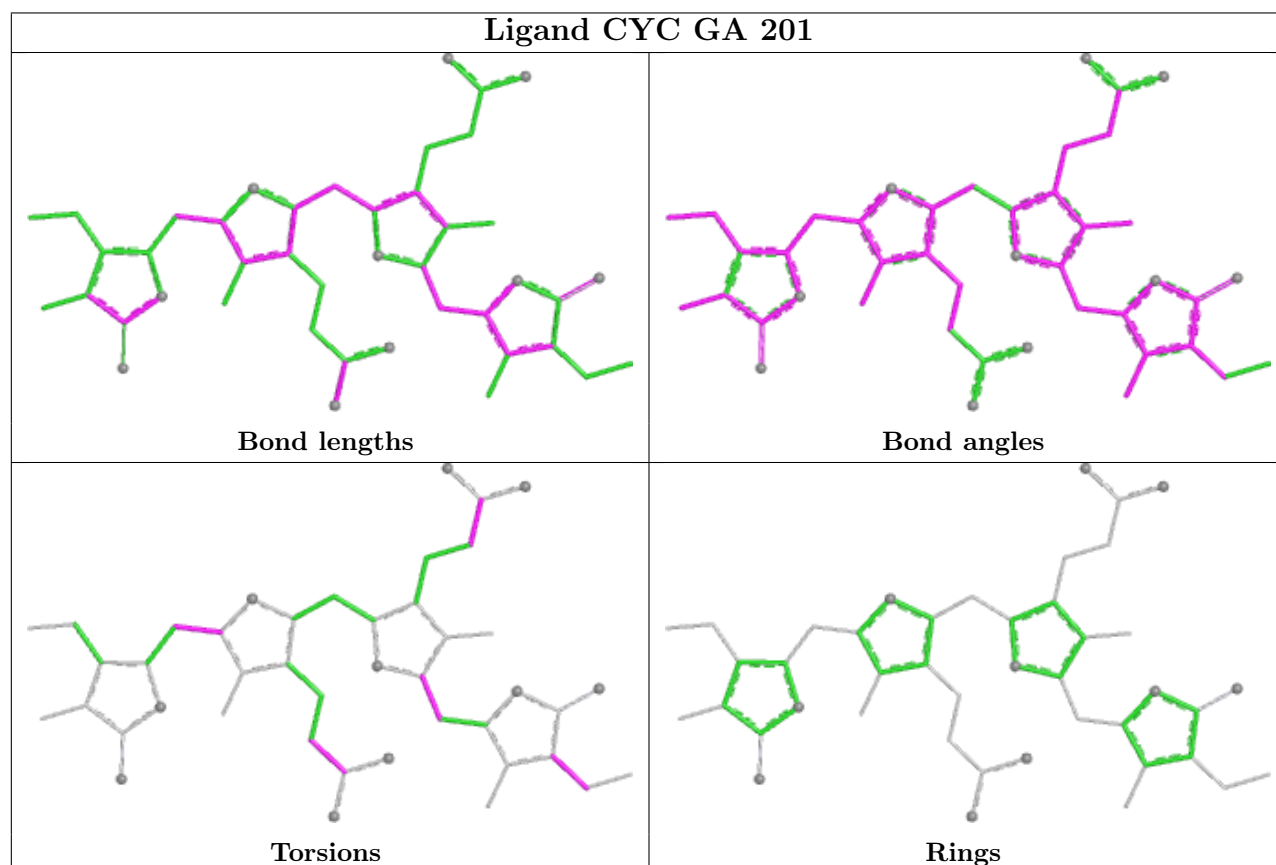
Ligand CYC C9 201



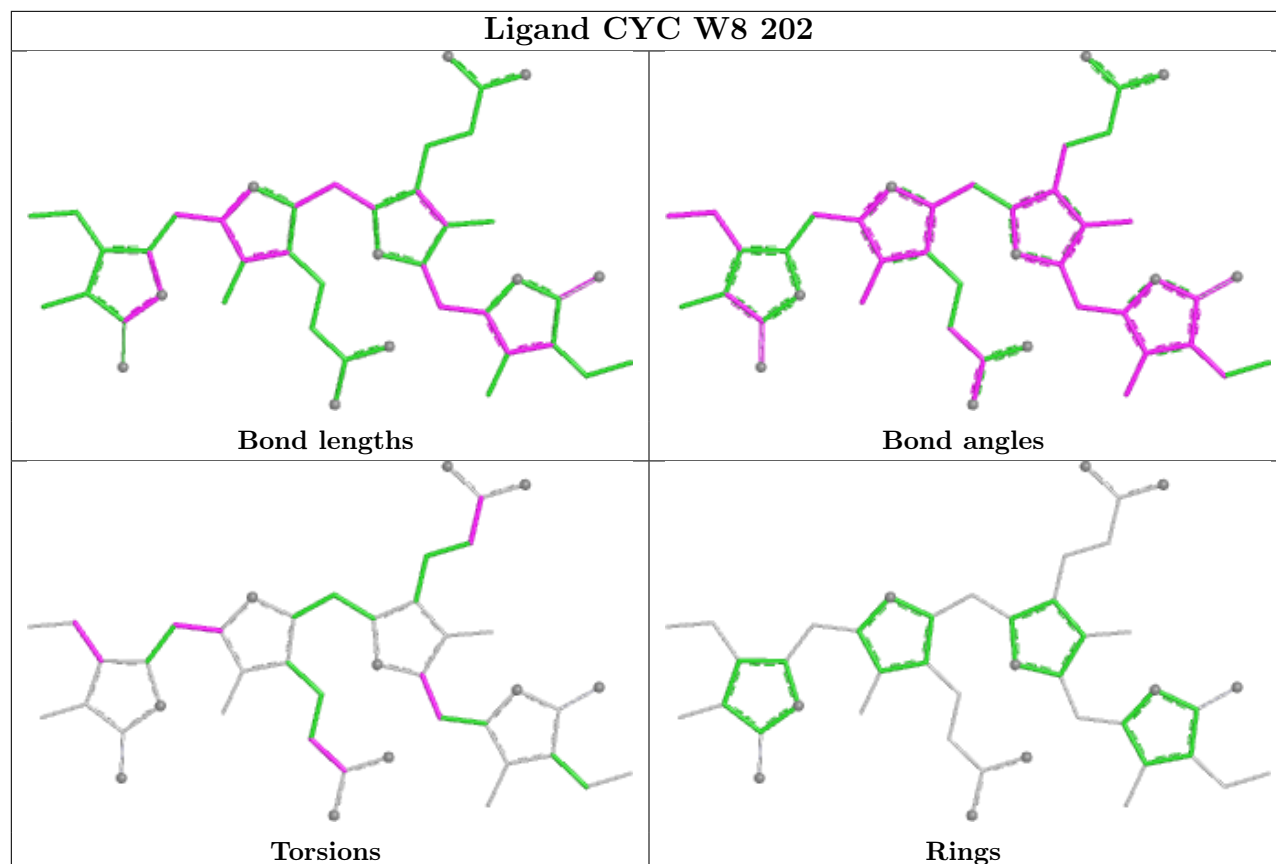
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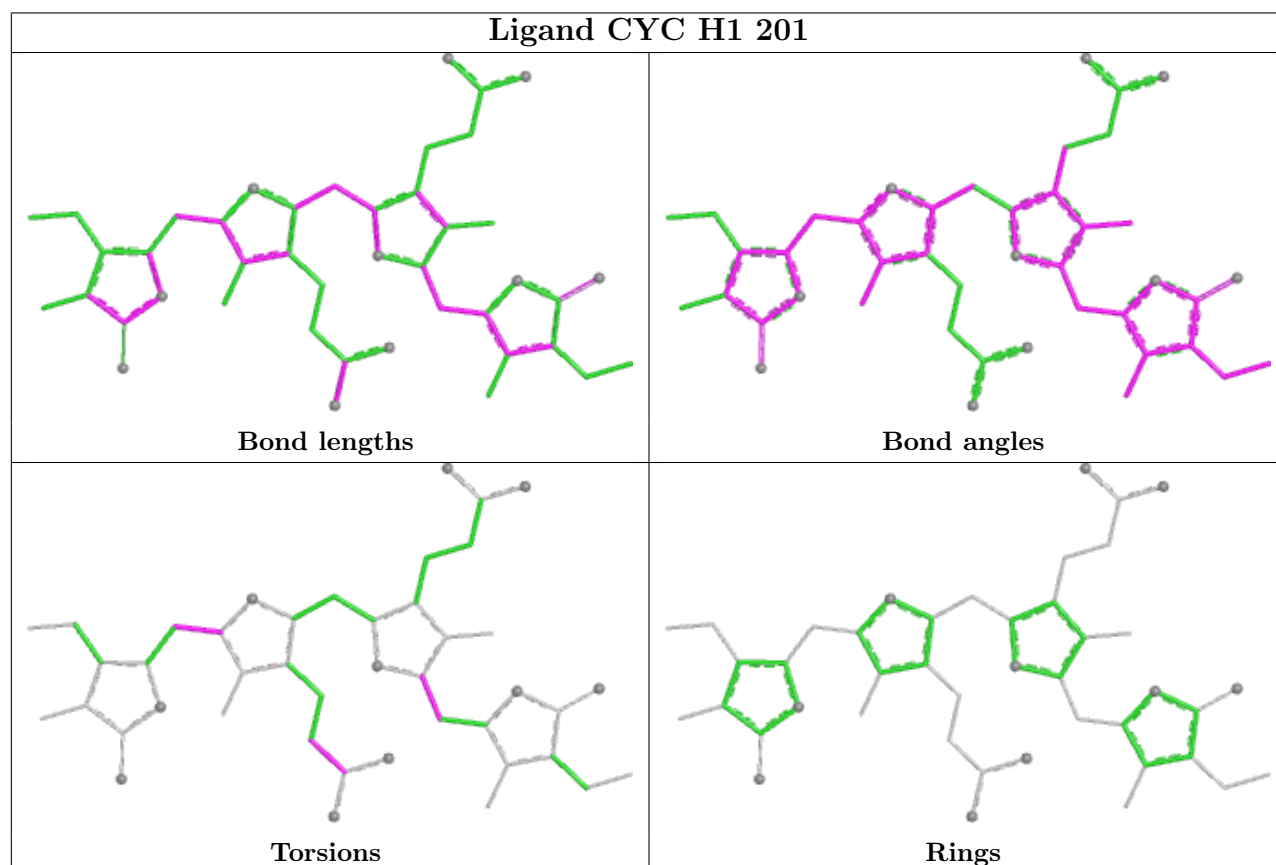
Ligand CYC GA 201



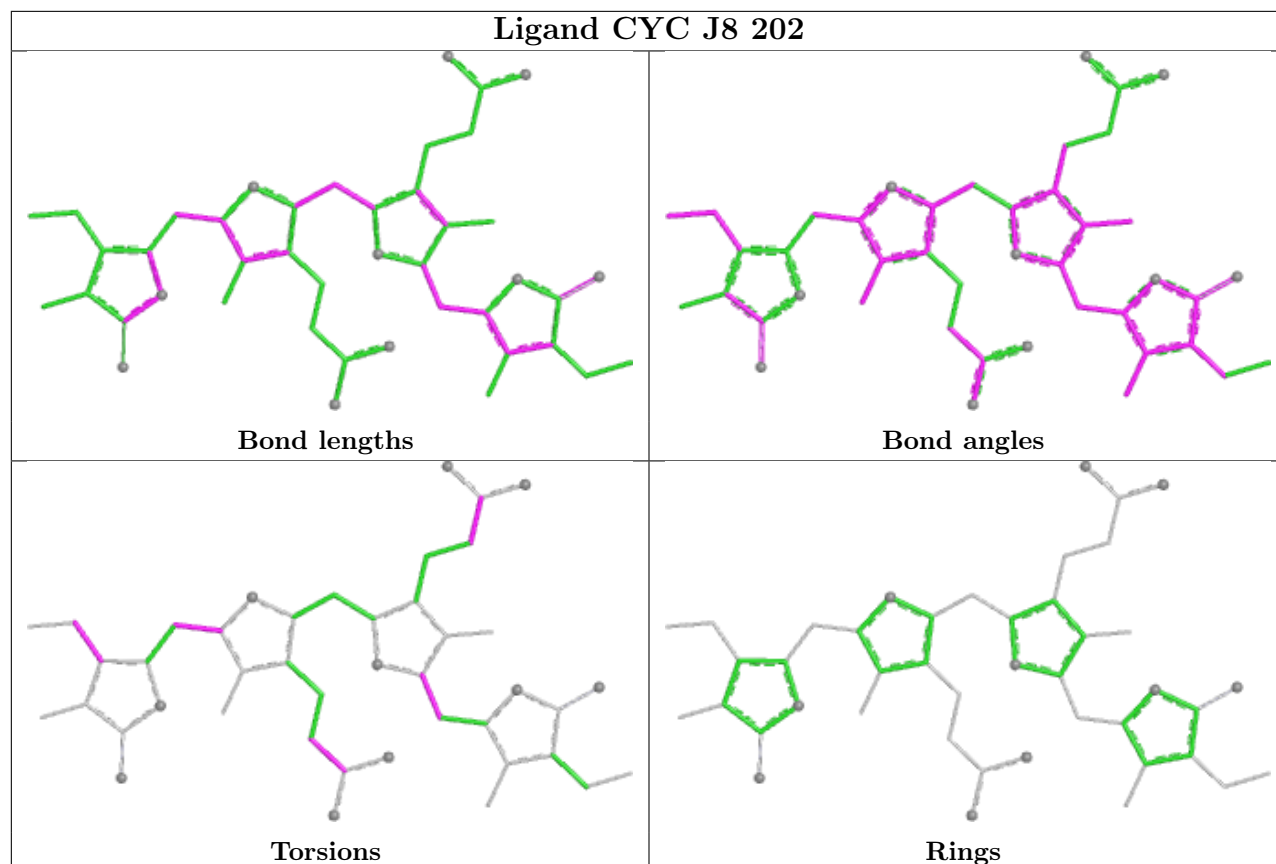
Ligand CYC W8 202



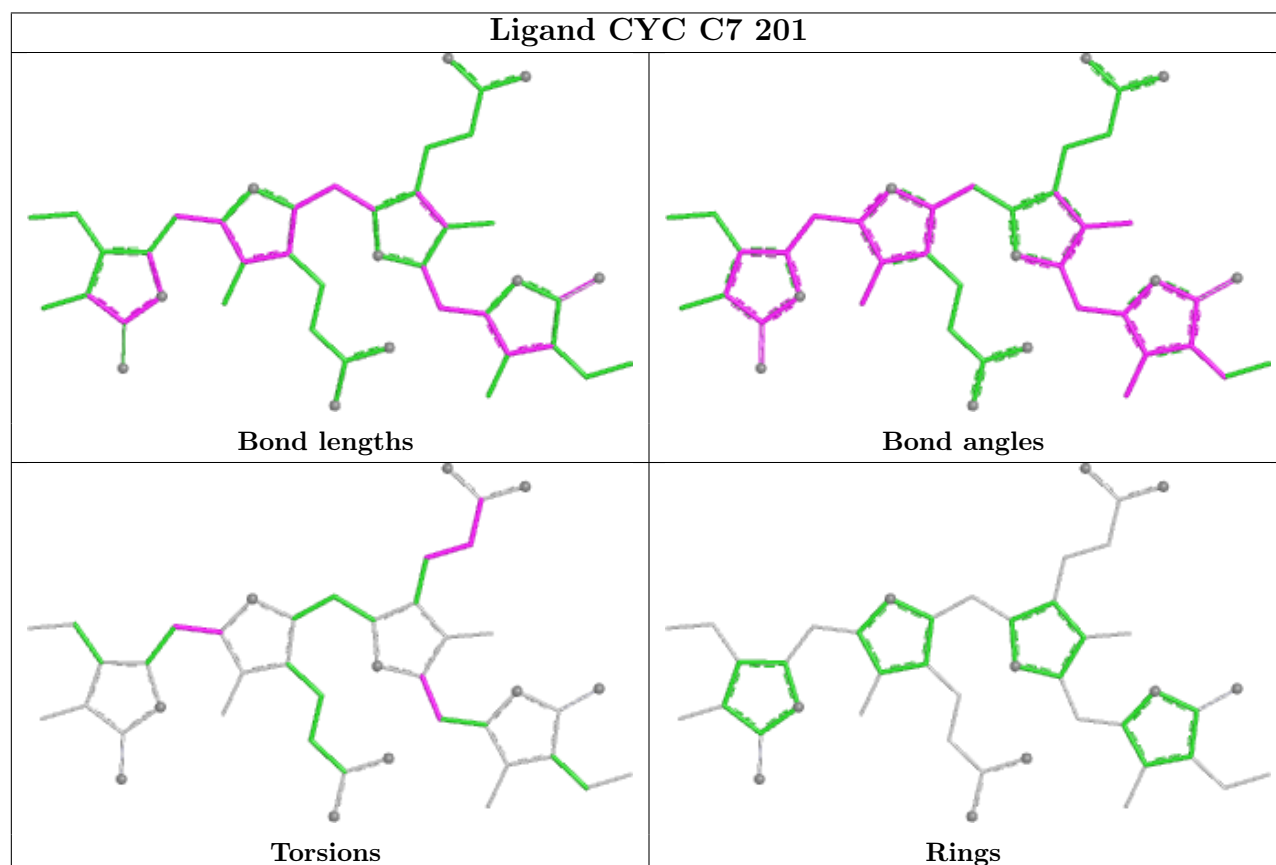
Ligand CYC H1 201



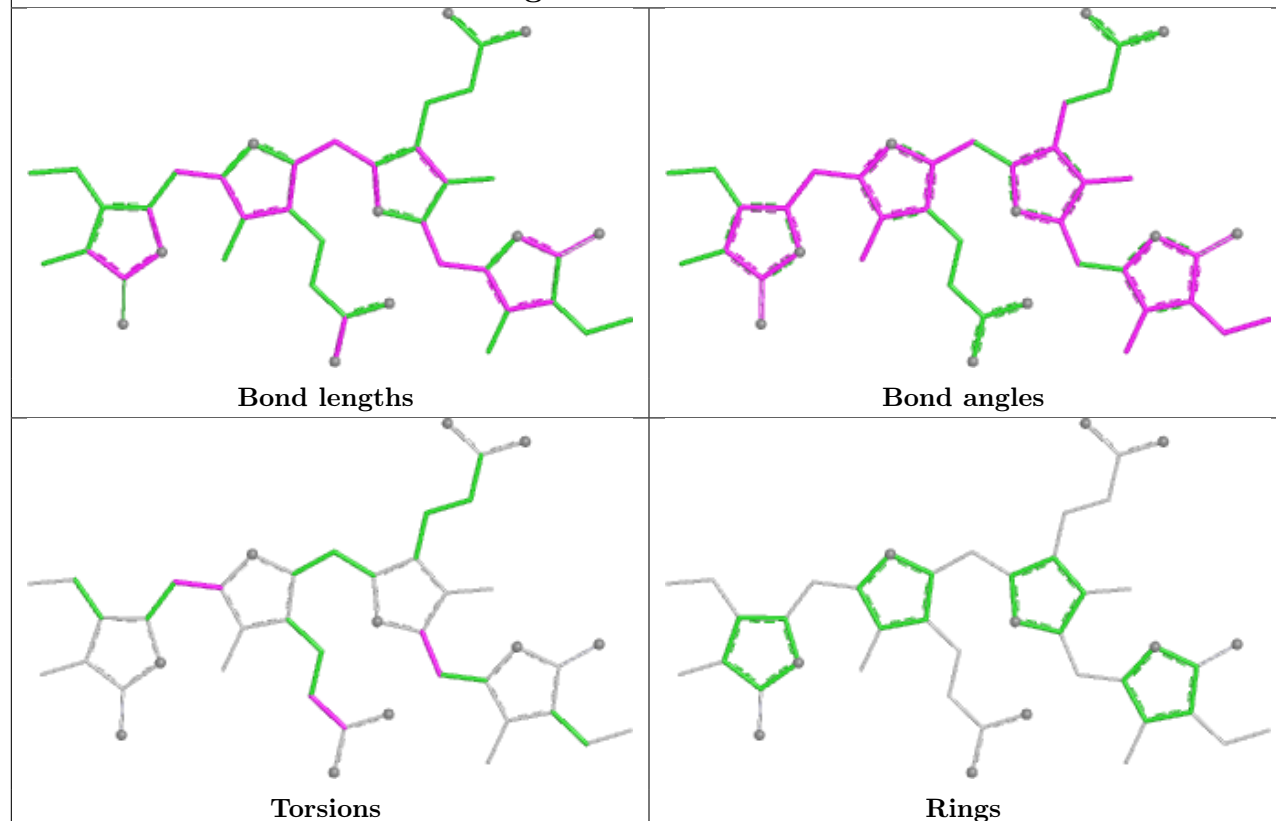
Ligand CYC J8 202



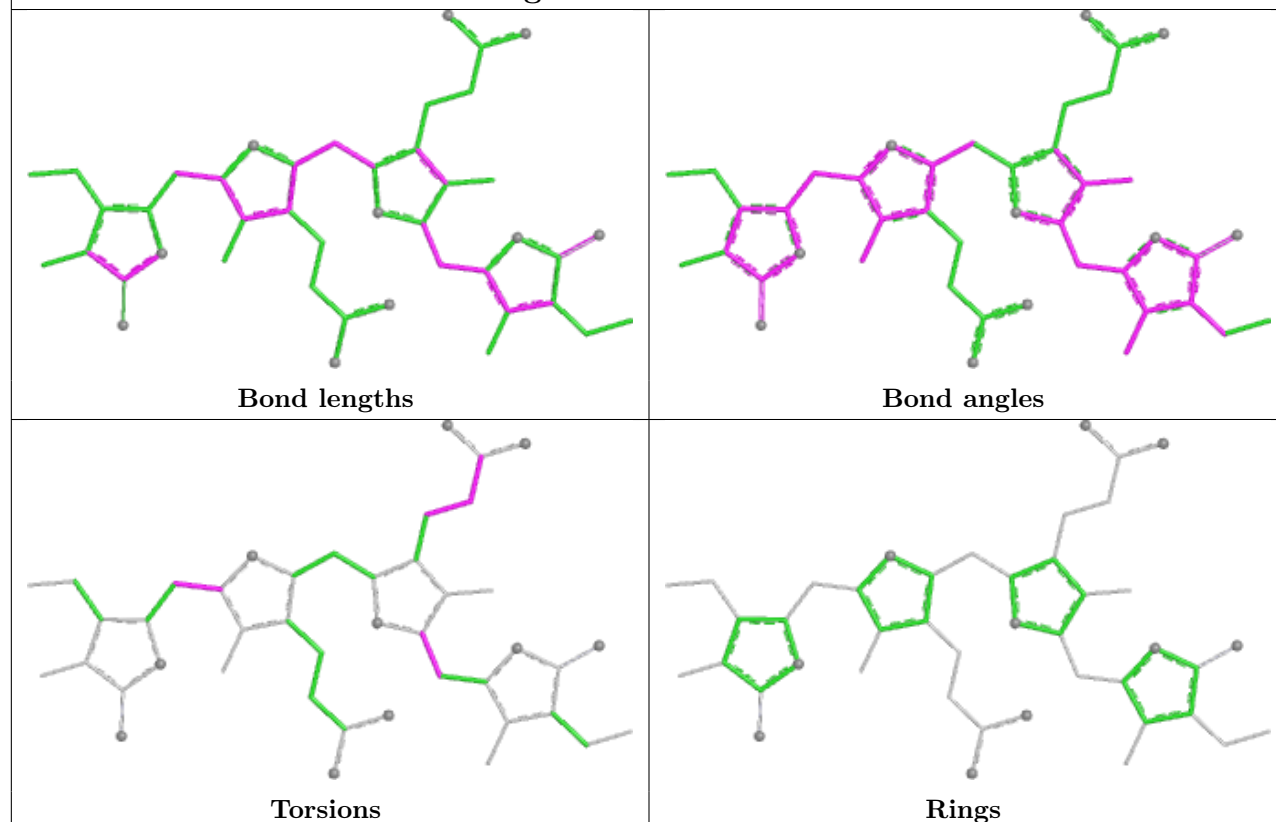
Ligand CYC C7 201



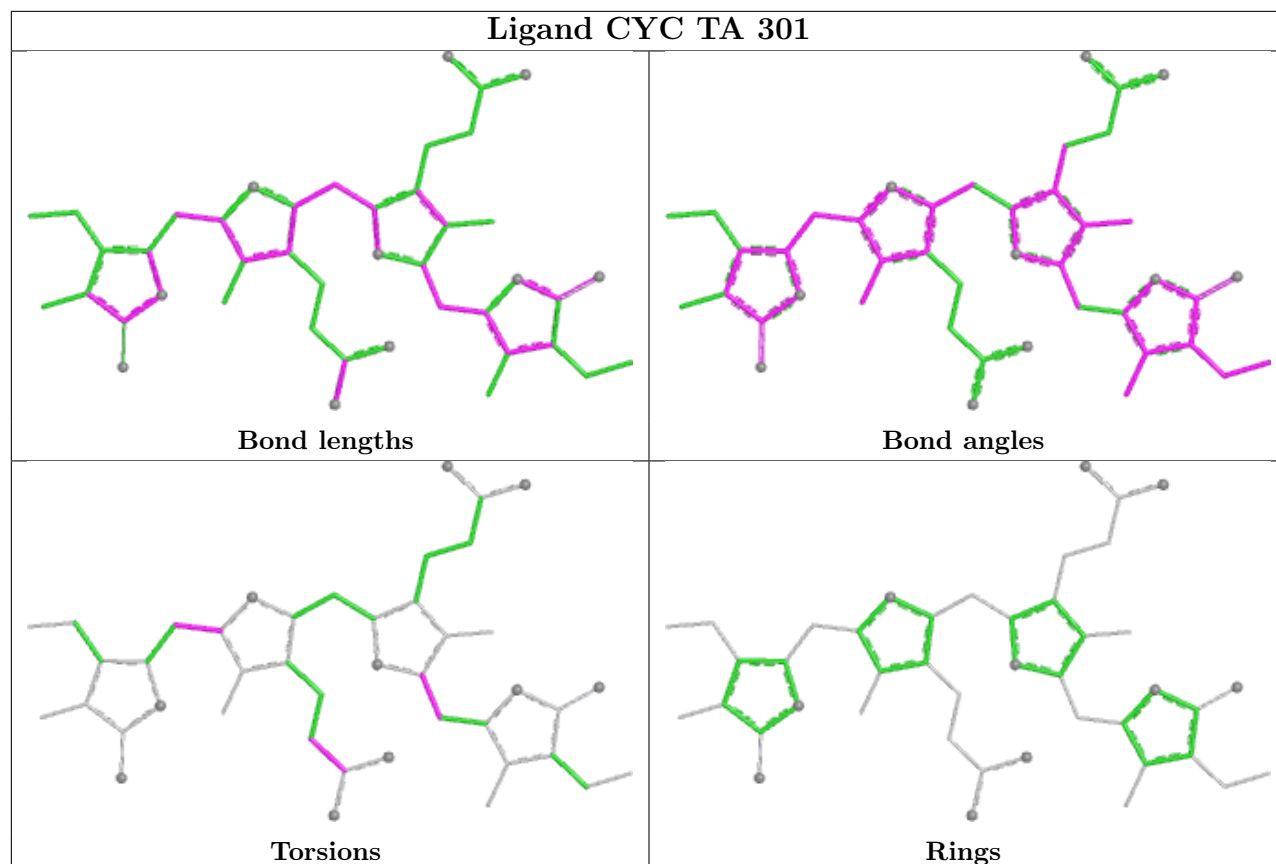
Ligand CYC J8 201



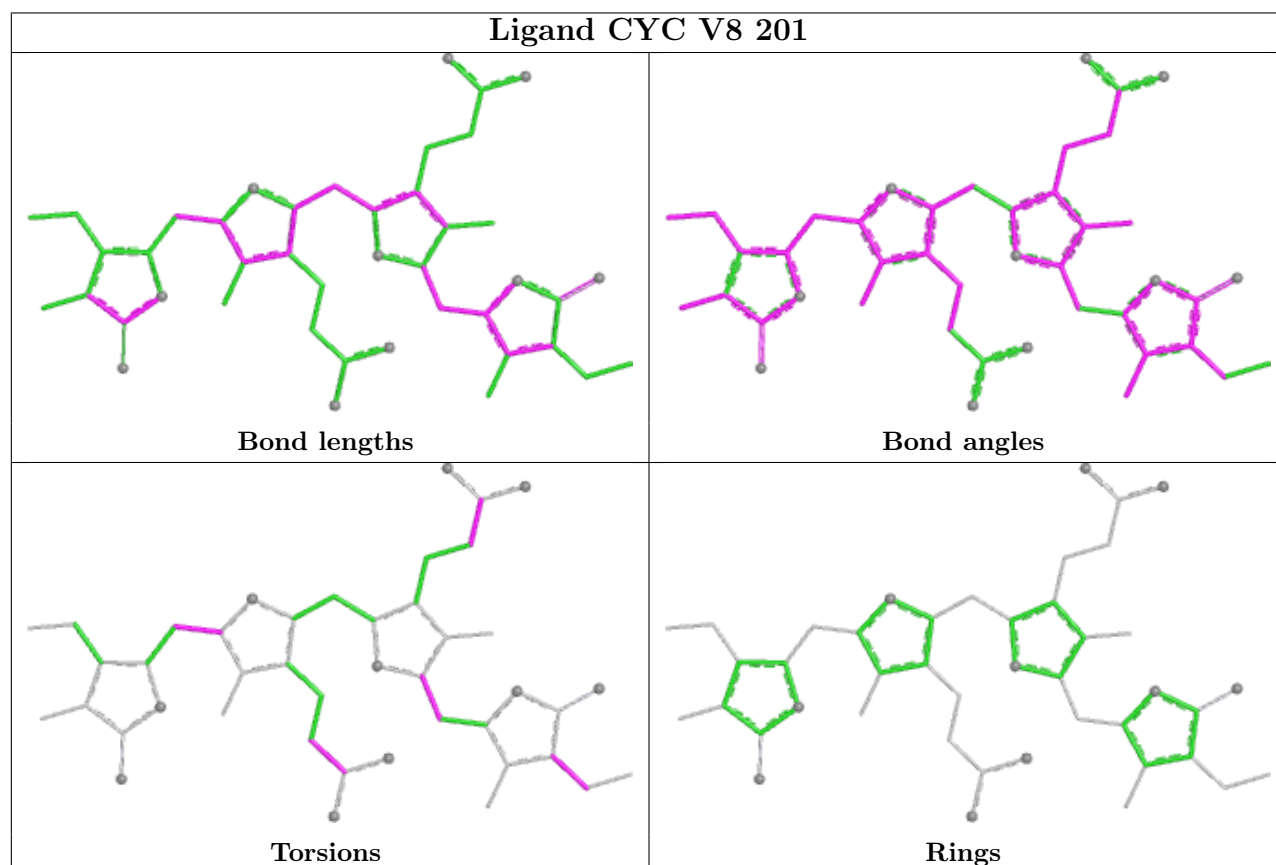
Ligand CYC S5 201



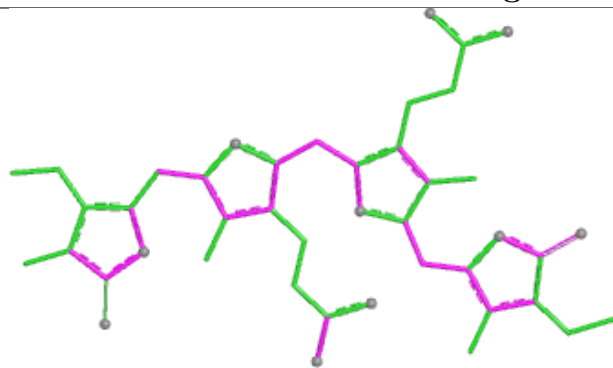
Ligand CYC TA 301



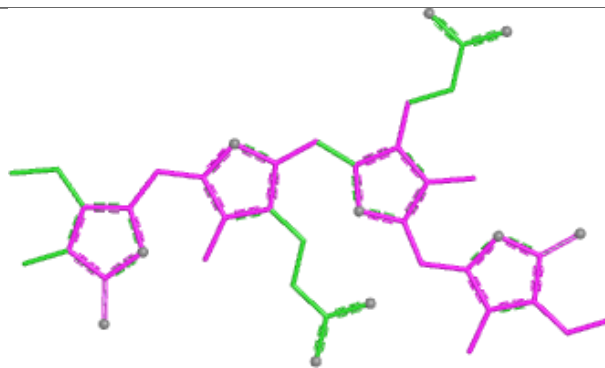
Ligand CYC V8 201



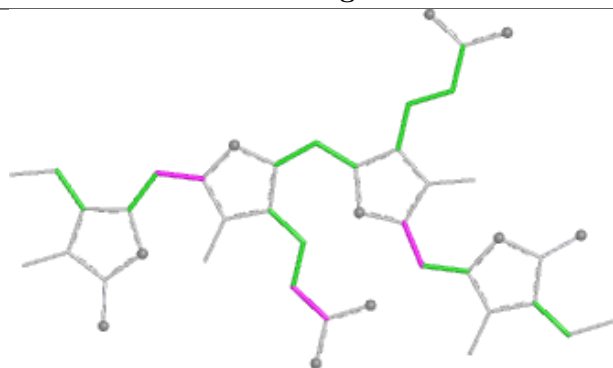
Ligand CYC B3 202



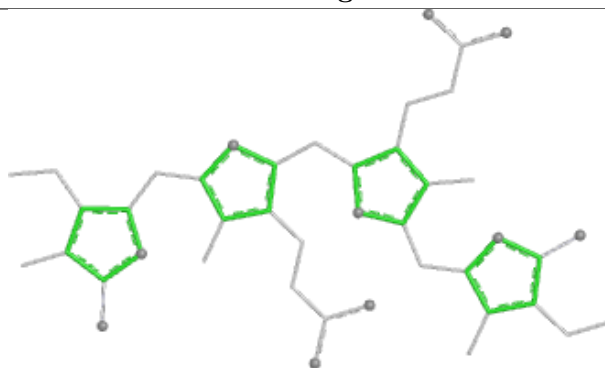
Bond lengths



Bond angles

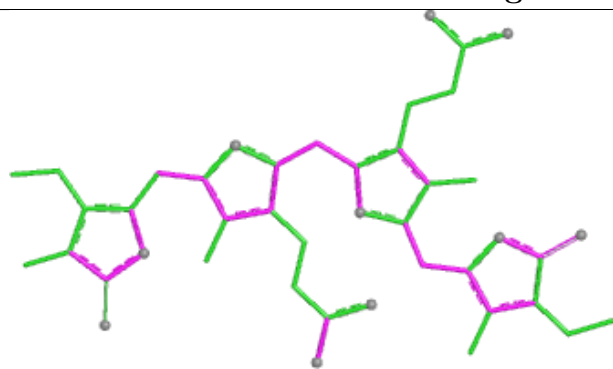


Torsions

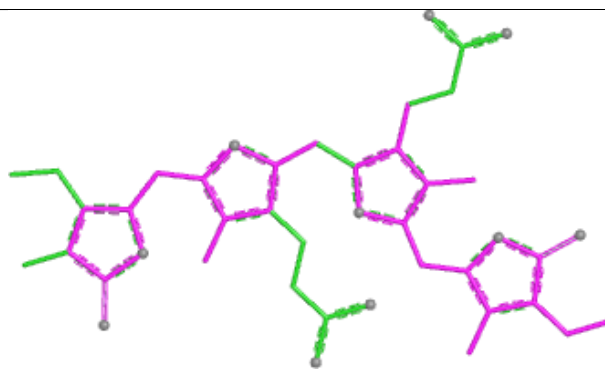


Rings

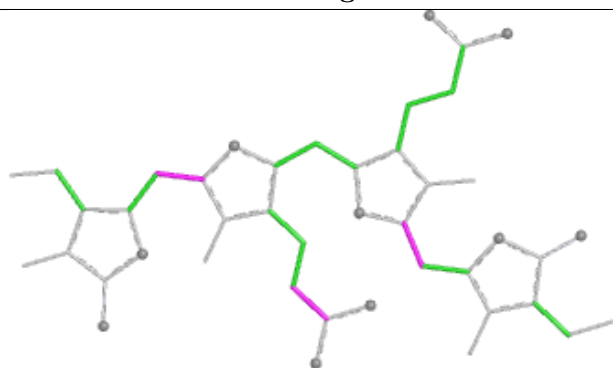
Ligand CYC Z4 301



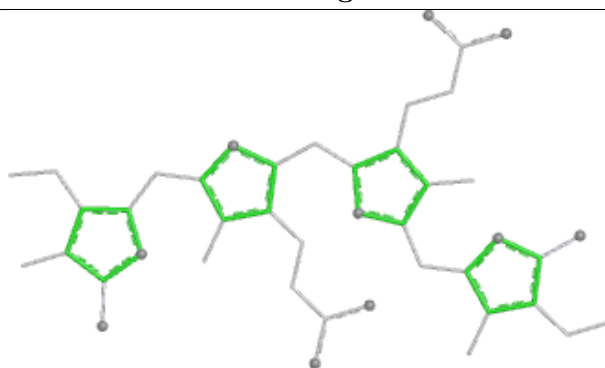
Bond lengths



Bond angles

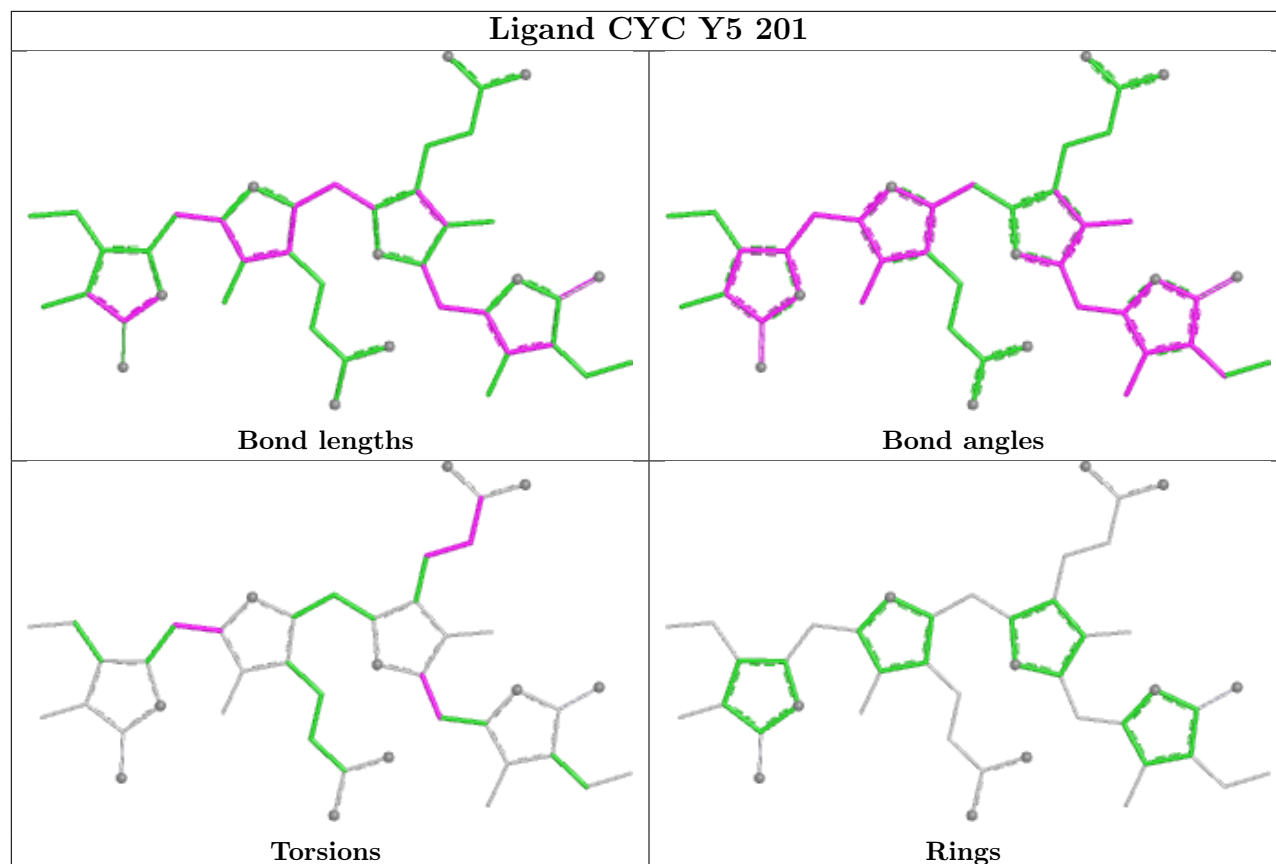


Torsions

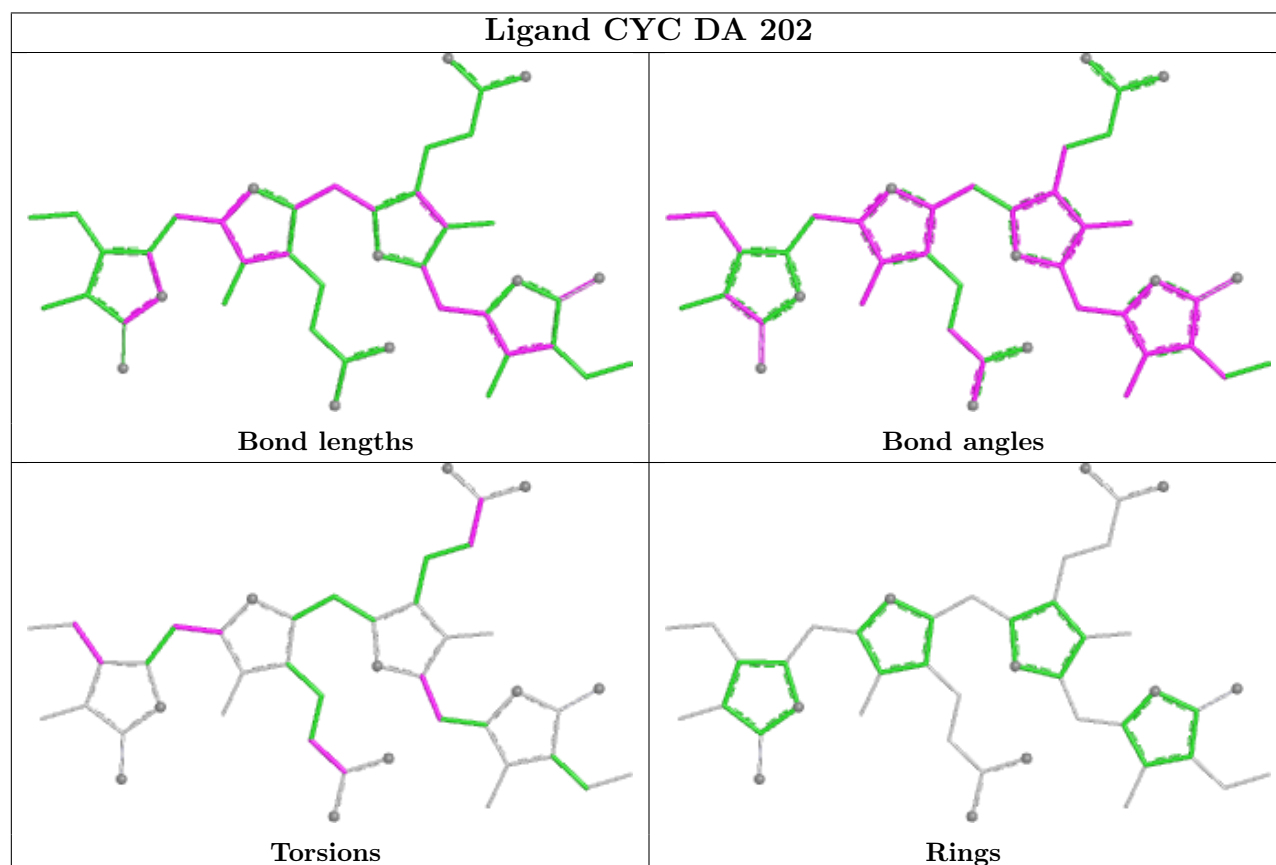


Rings

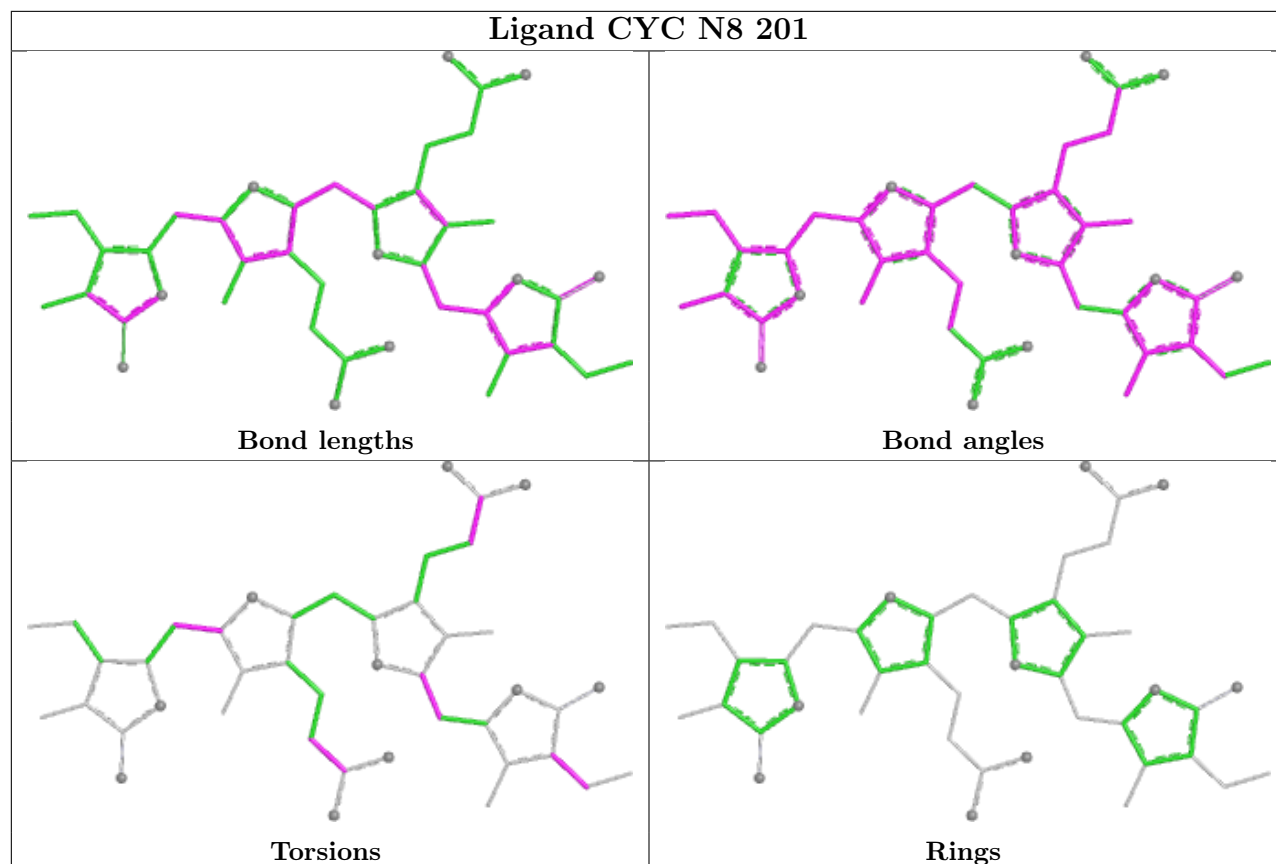
Ligand CYC Y5 201



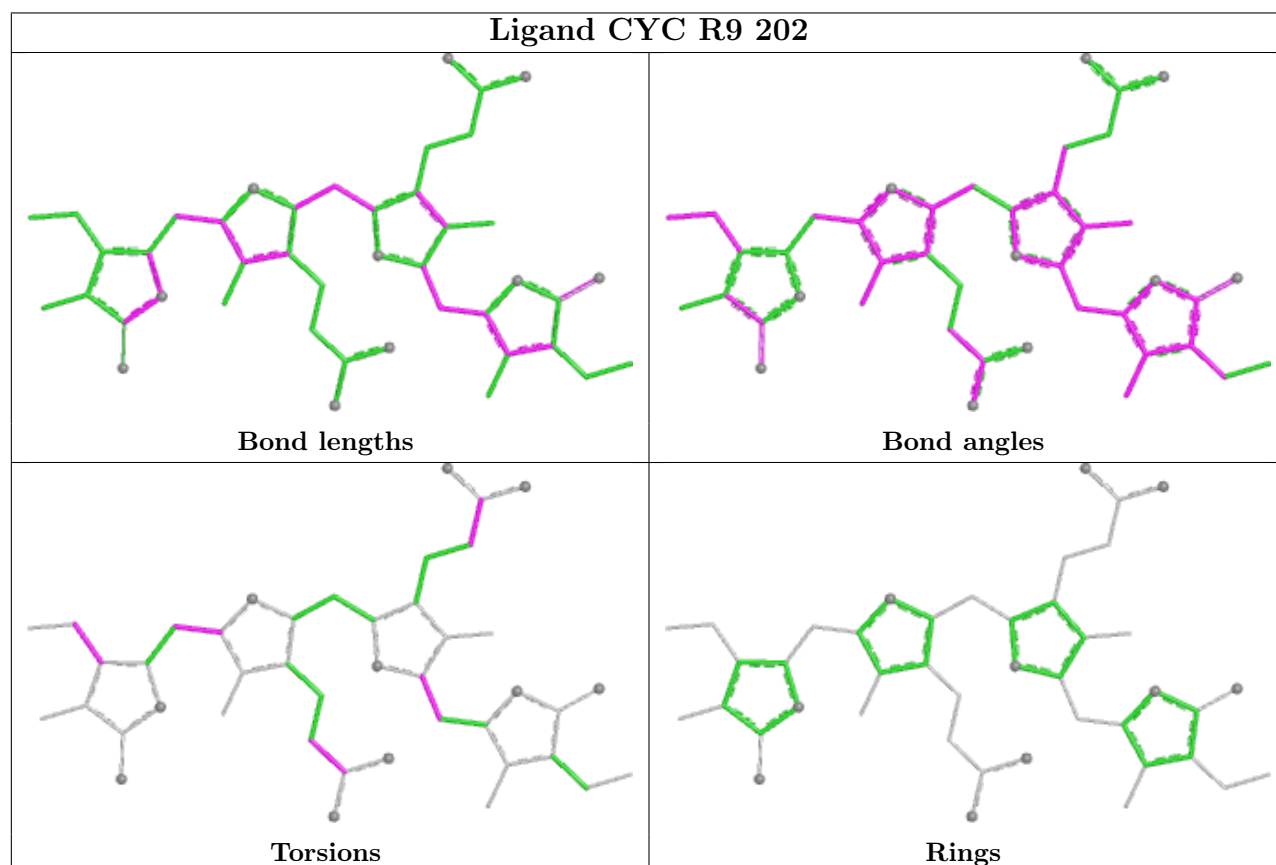
Ligand CYC DA 202

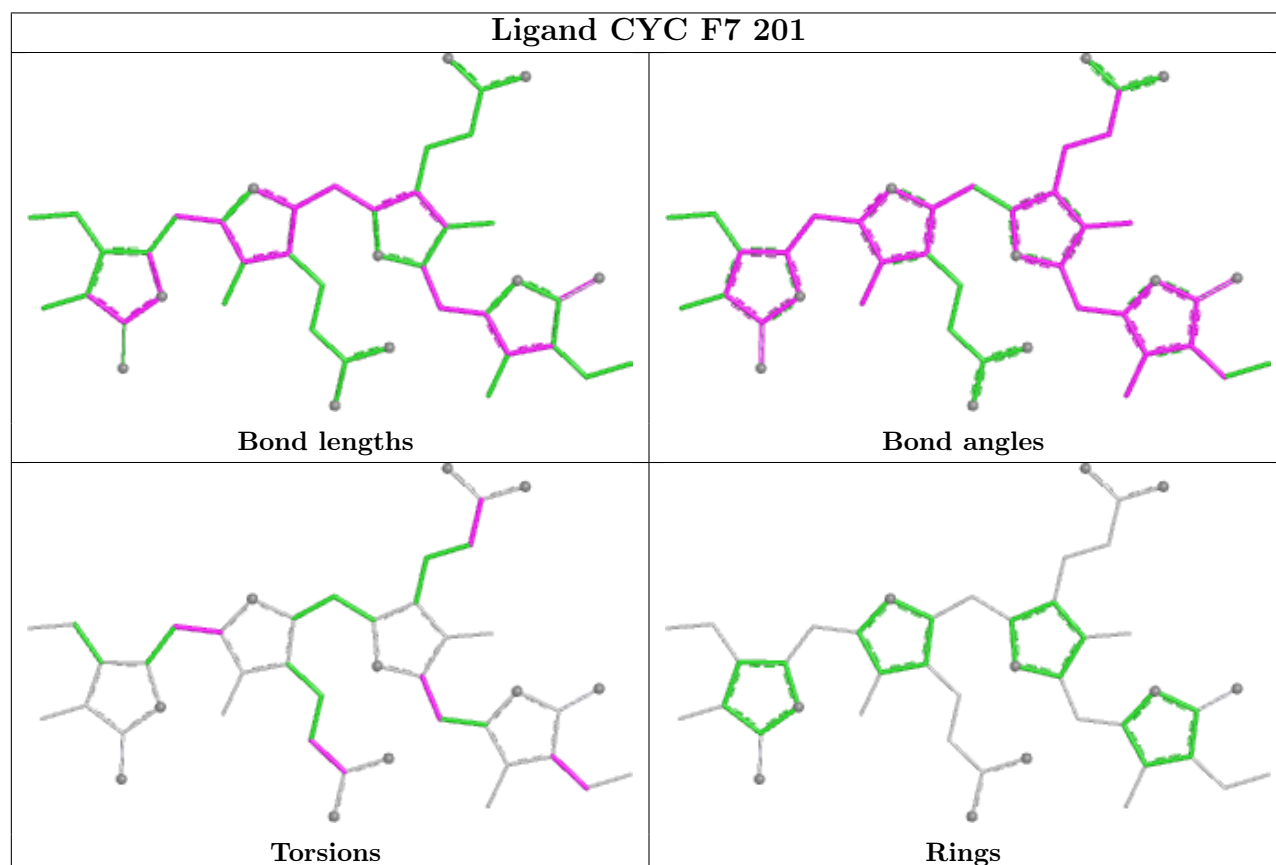
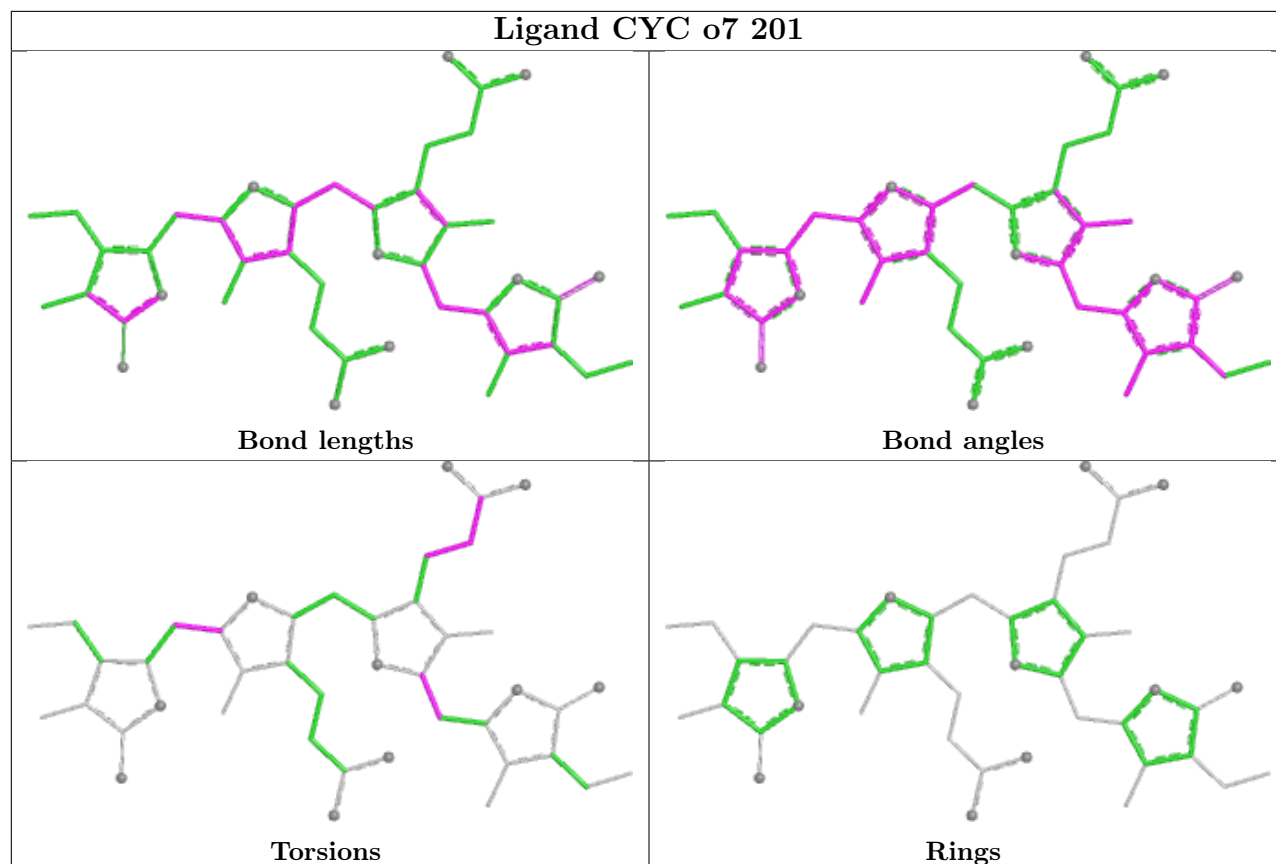


Ligand CYC N8 201

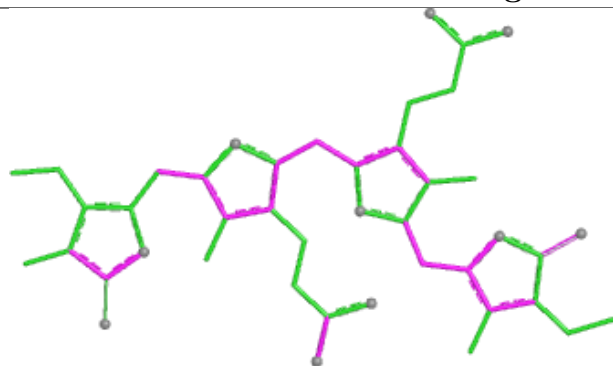


Ligand CYC R9 202

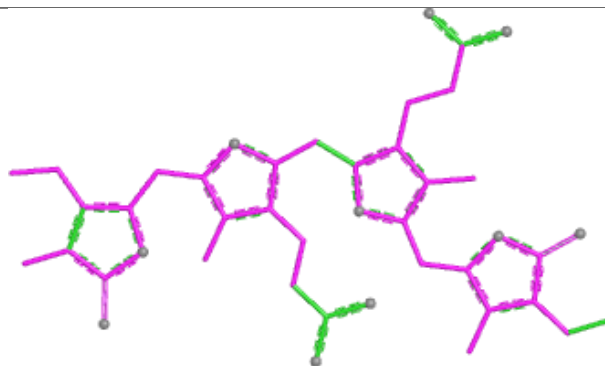




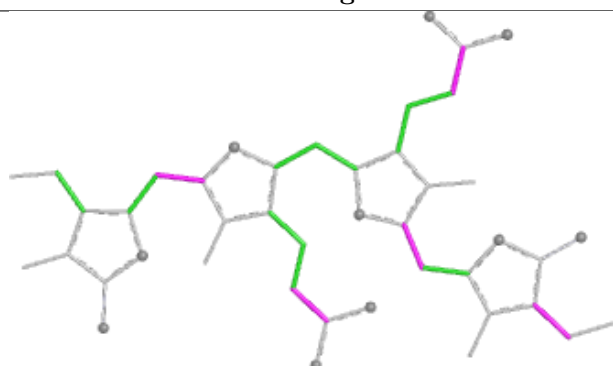
Ligand CYC E8 201



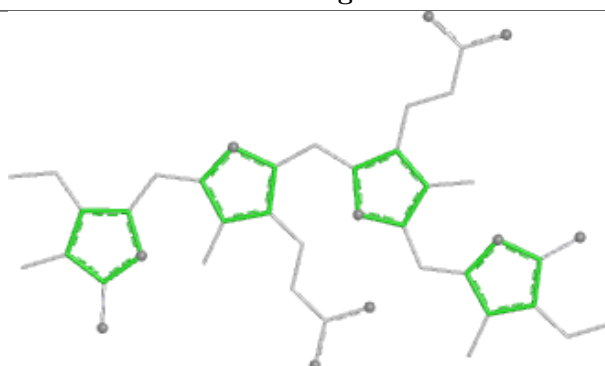
Bond lengths



Bond angles

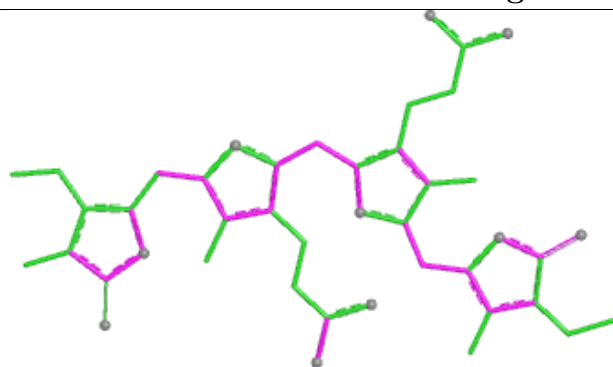


Torsions

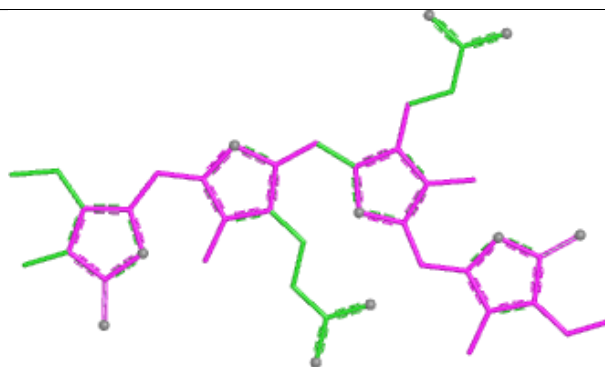


Rings

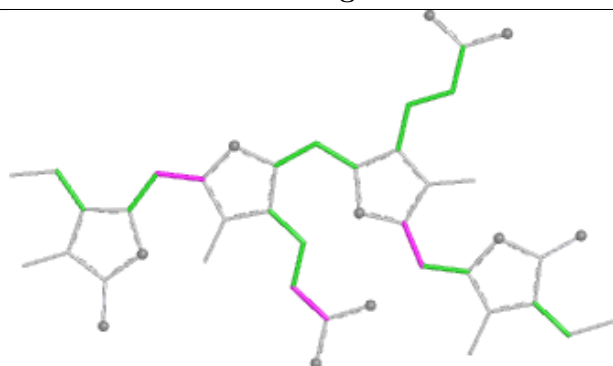
Ligand CYC J3 202



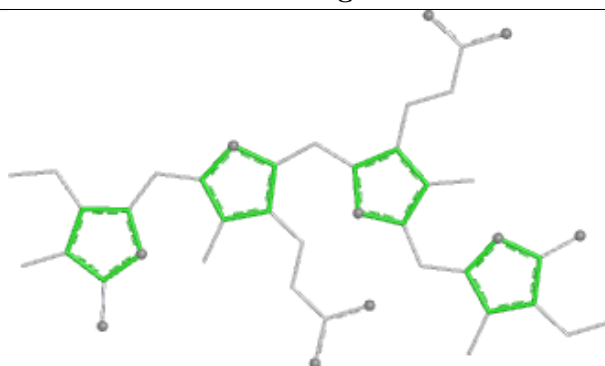
Bond lengths



Bond angles

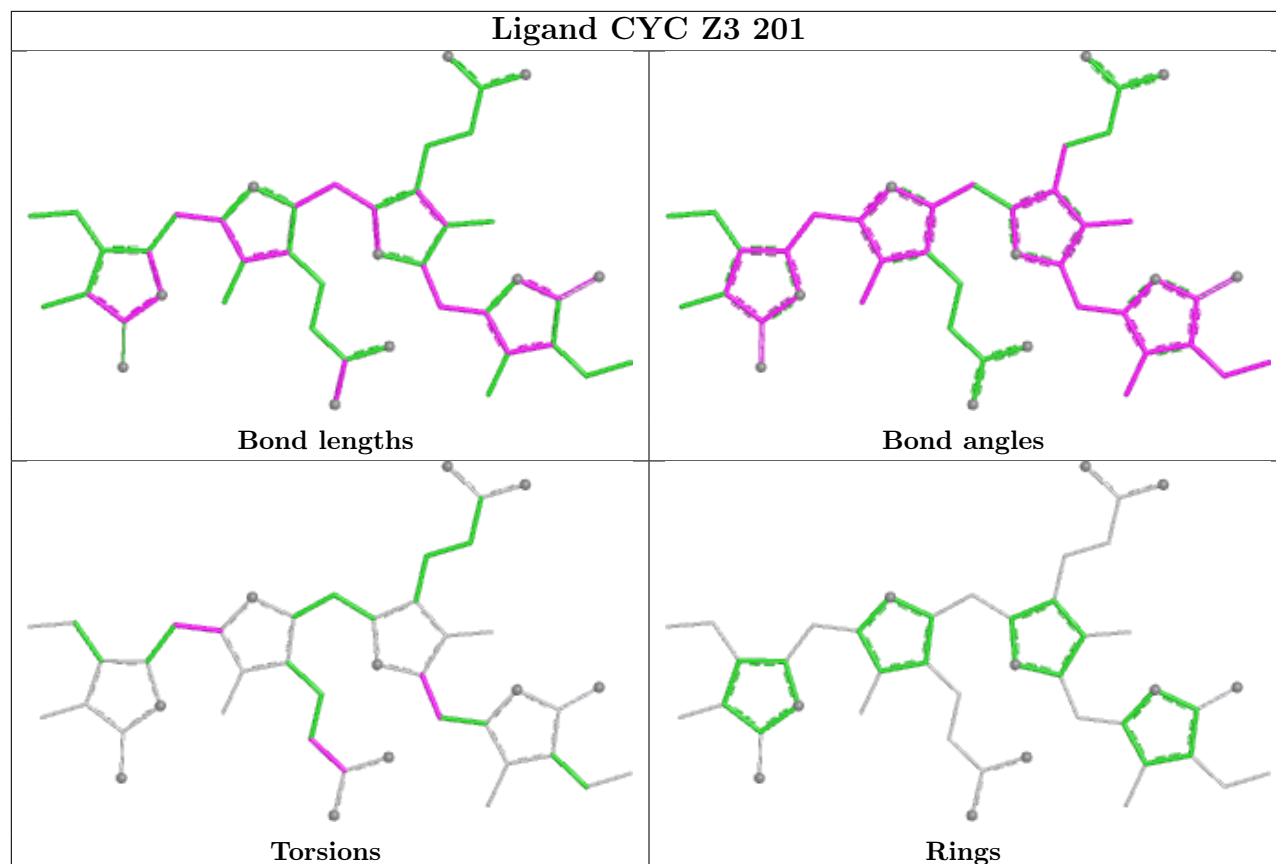


Torsions

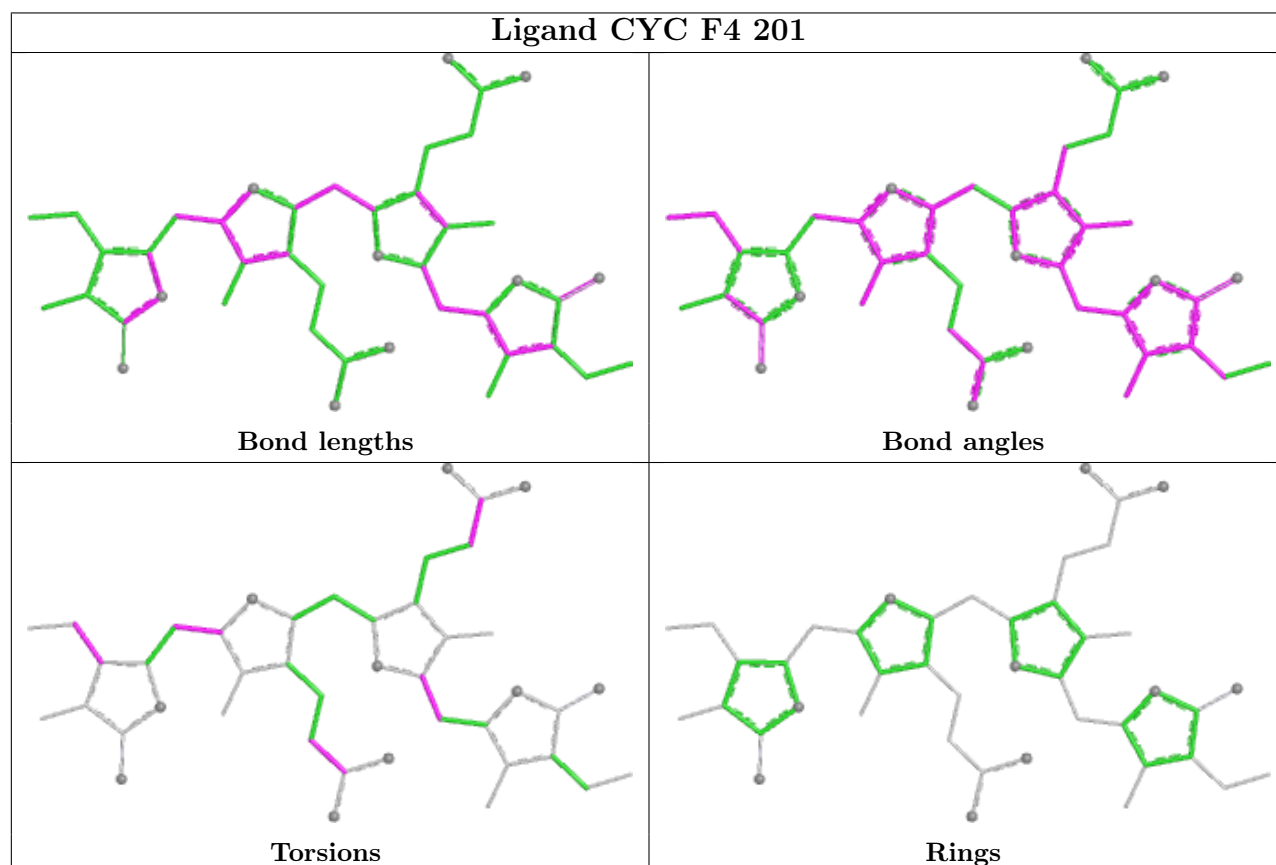


Rings

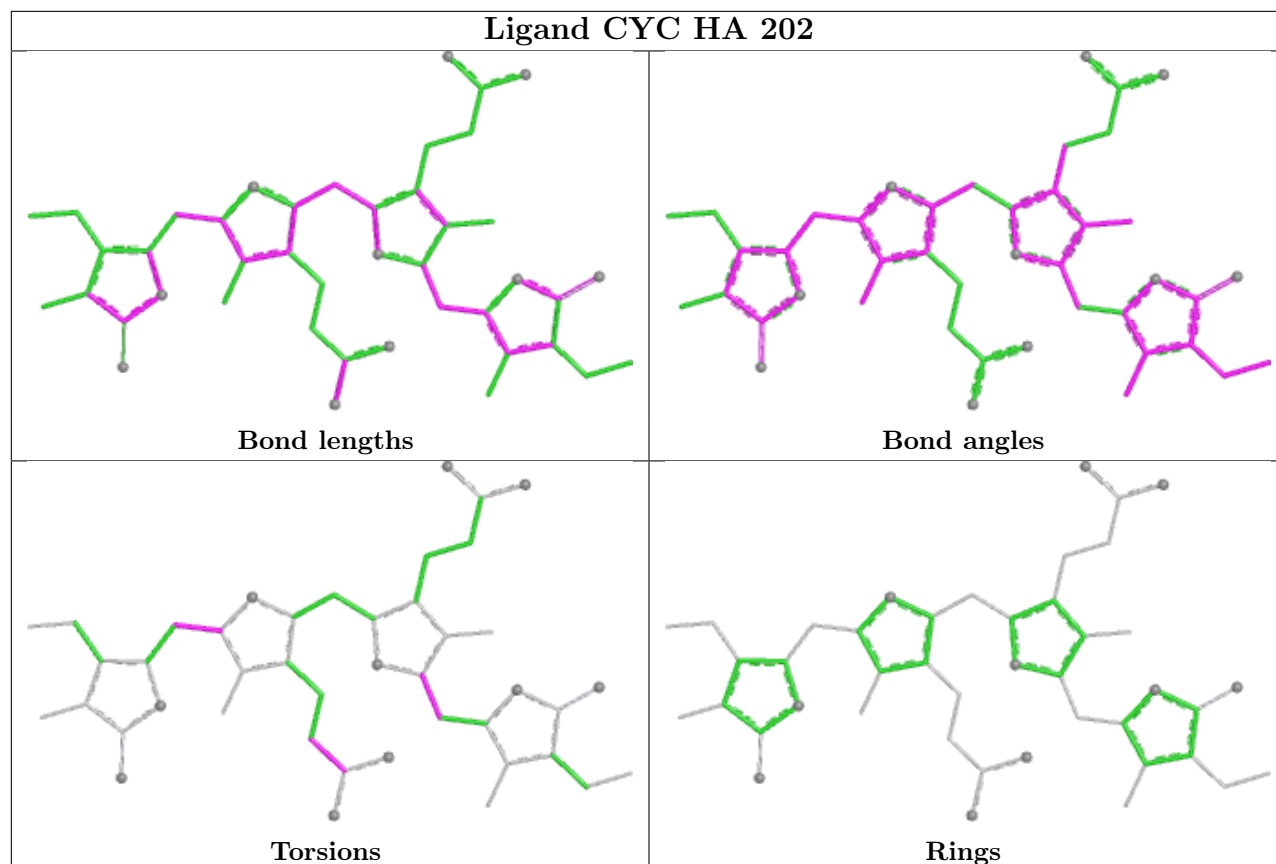
Ligand CYC Z3 201



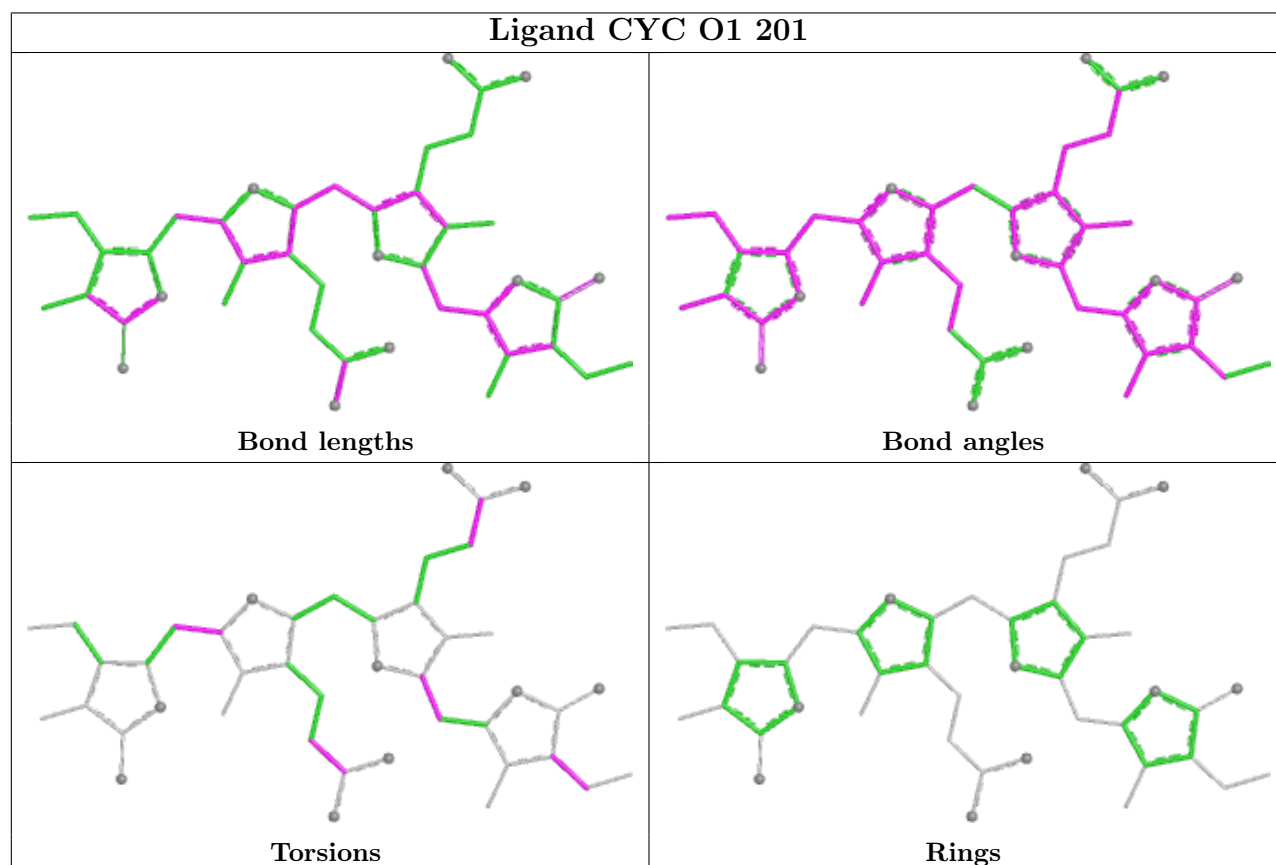
Ligand CYC F4 201



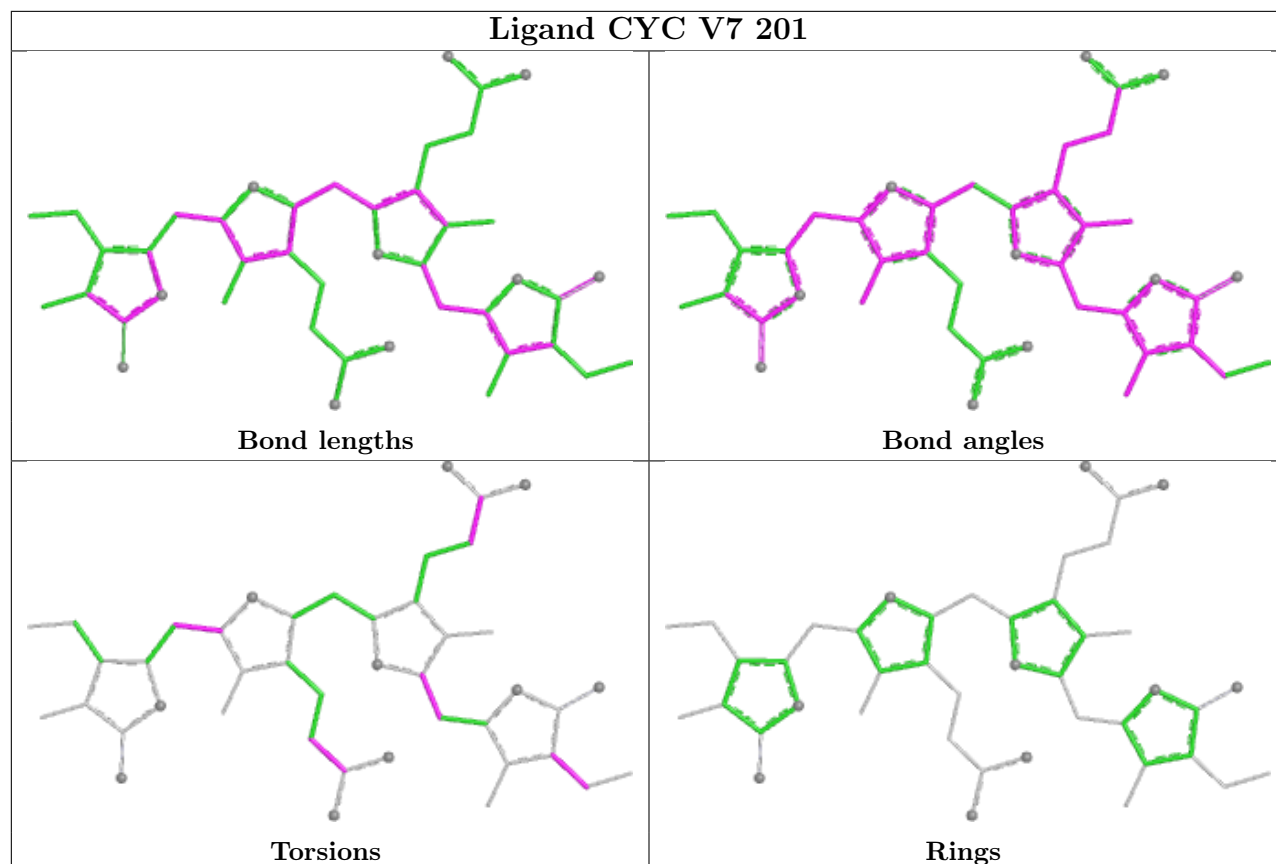
Ligand CYC HA 202



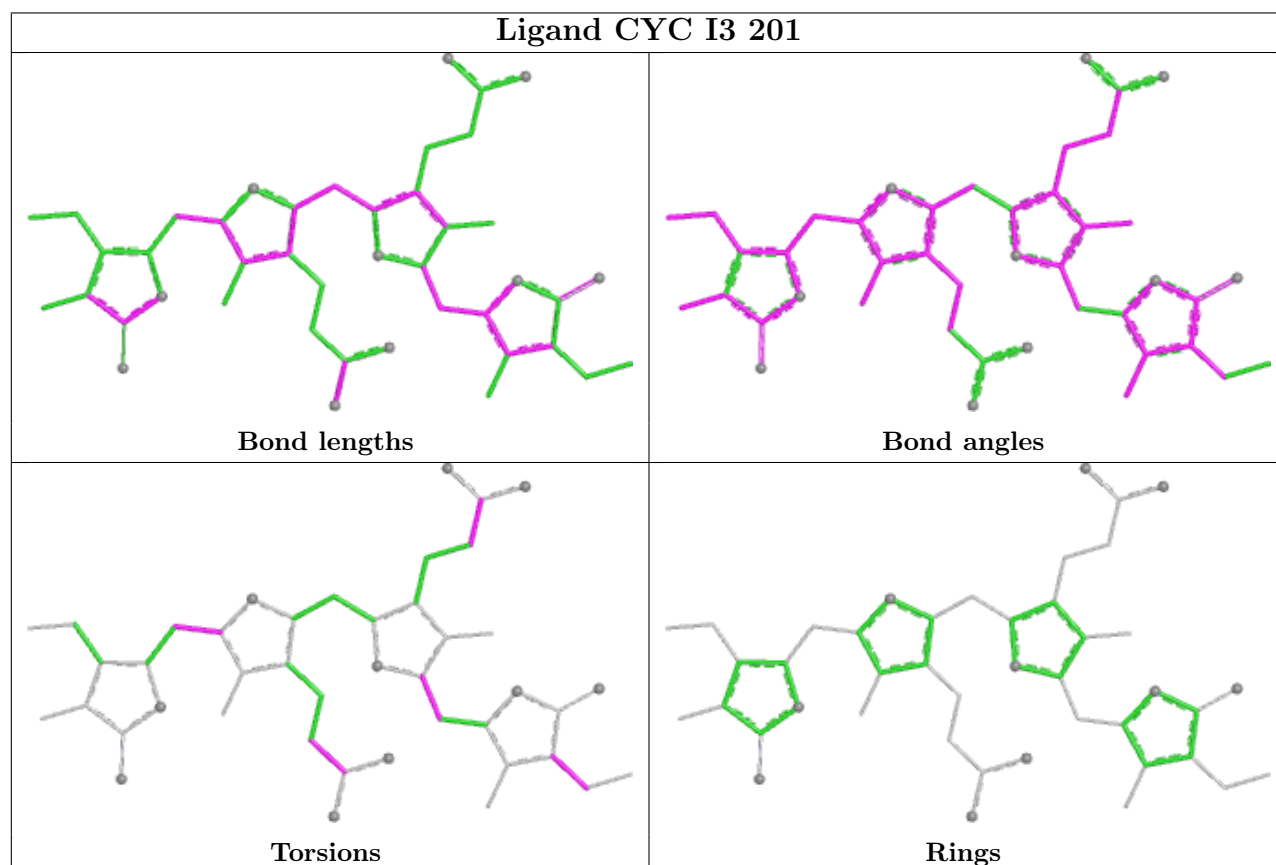
Ligand CYC O1 201



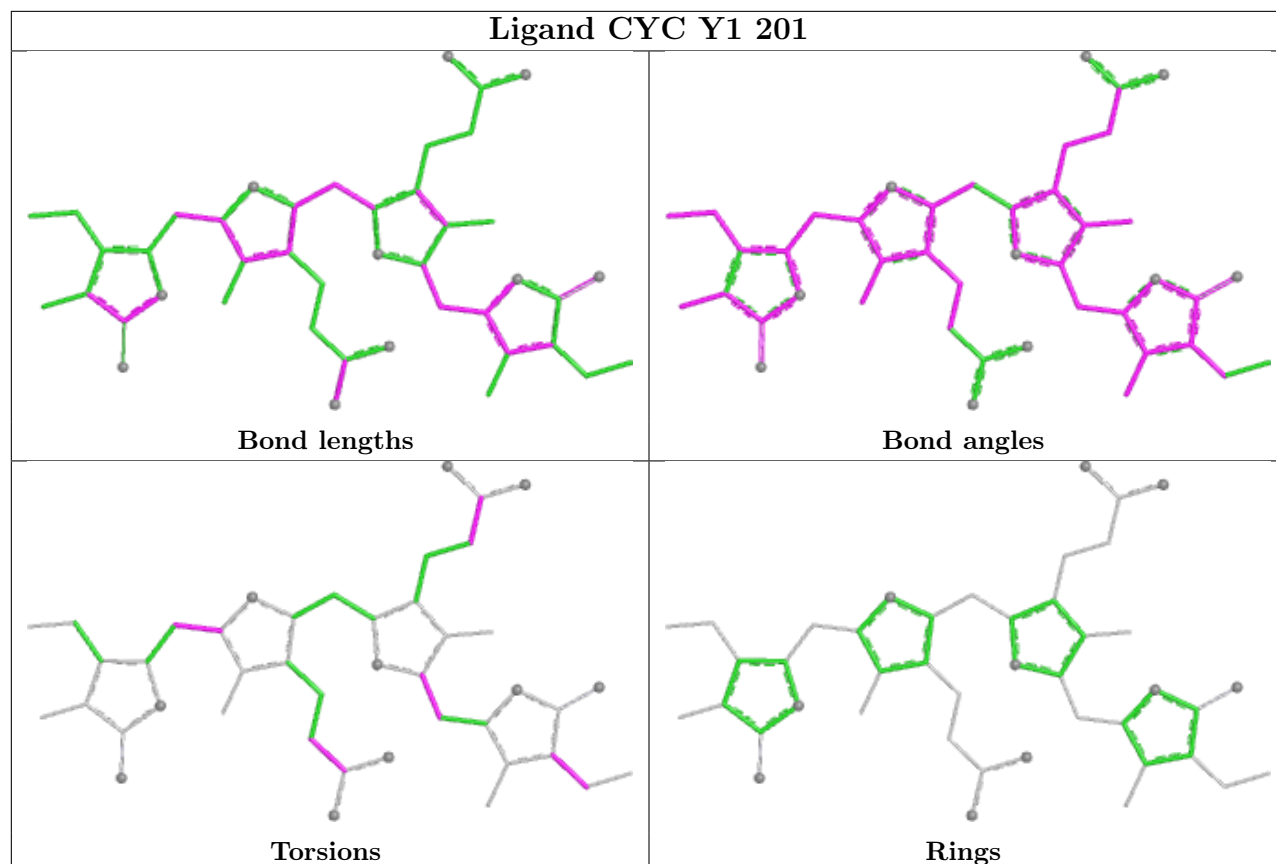
Ligand CYC V7 201



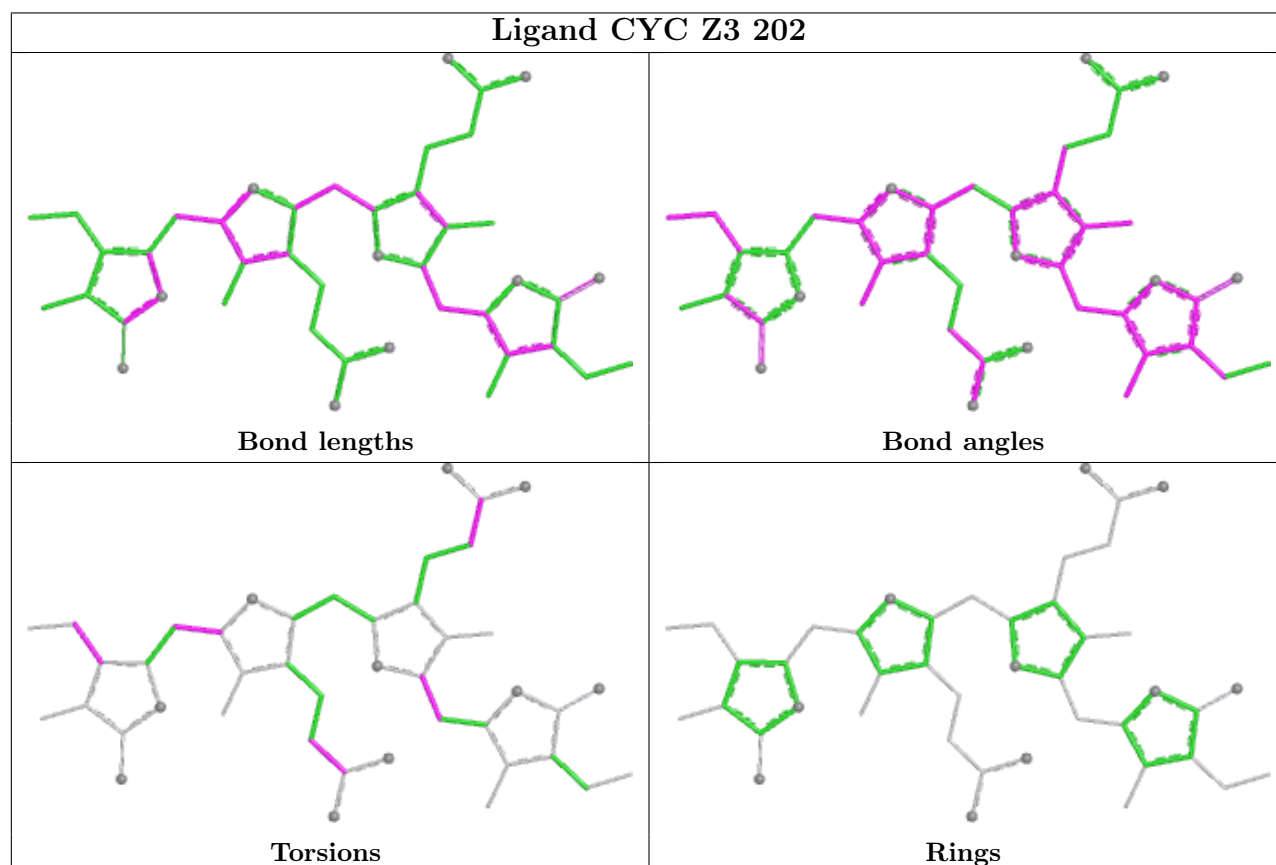
Ligand CYC I3 201



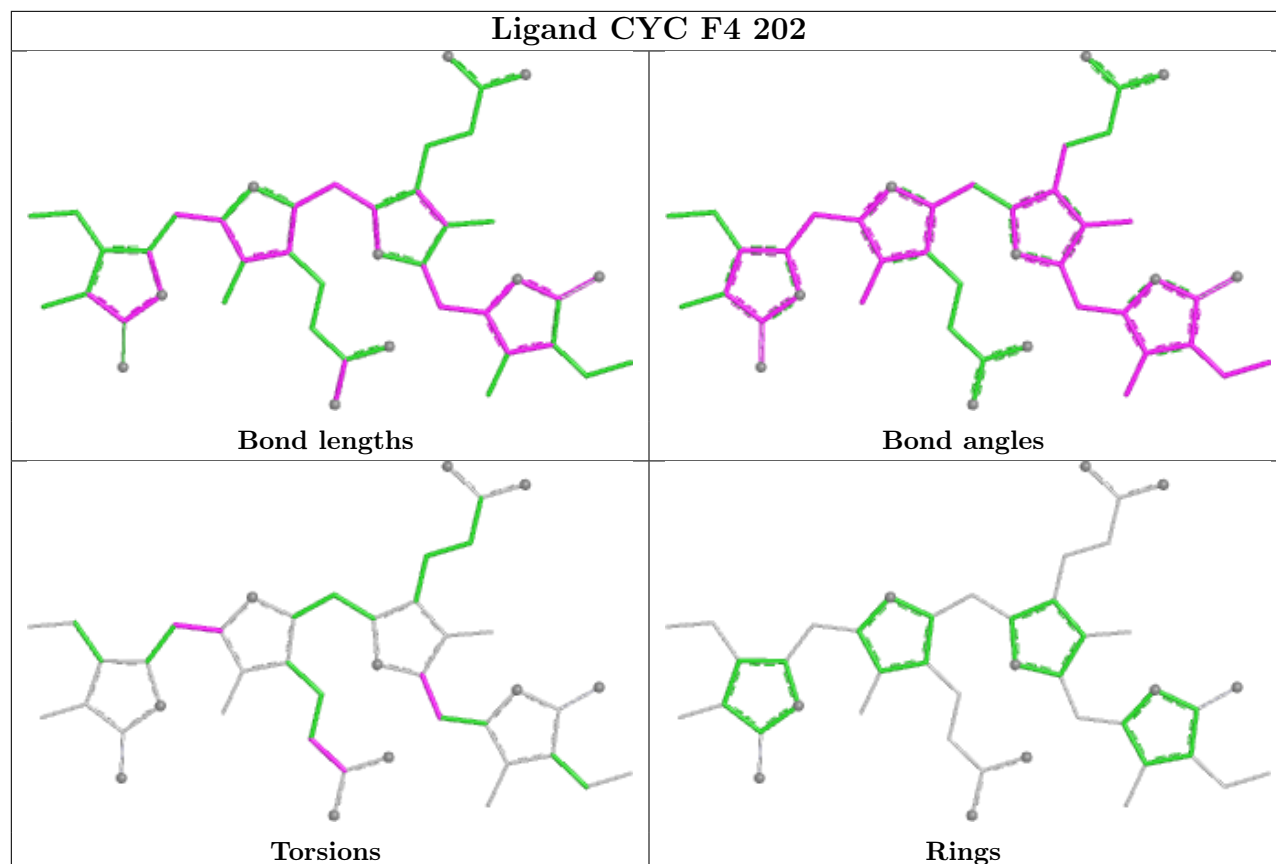
Ligand CYC Y1 201



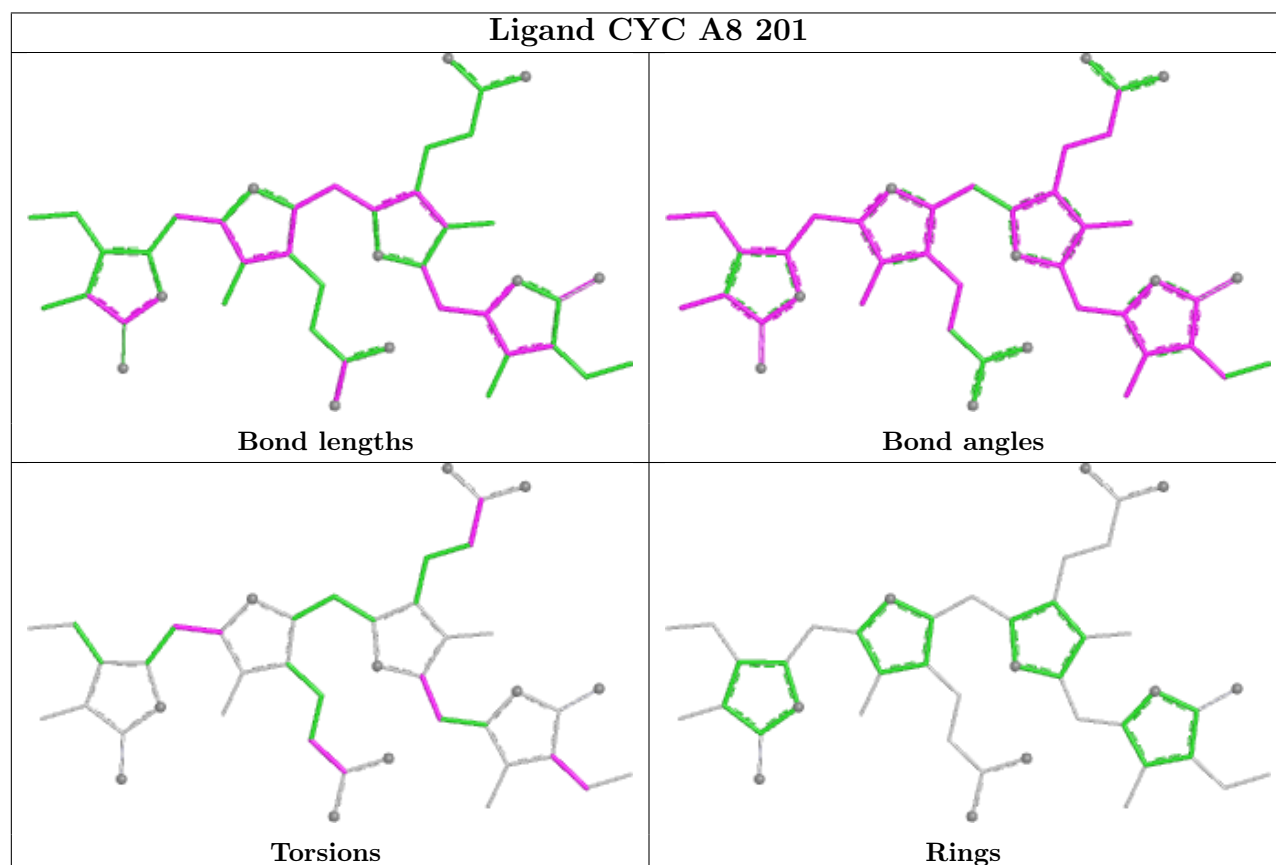
Ligand CYC Z3 202



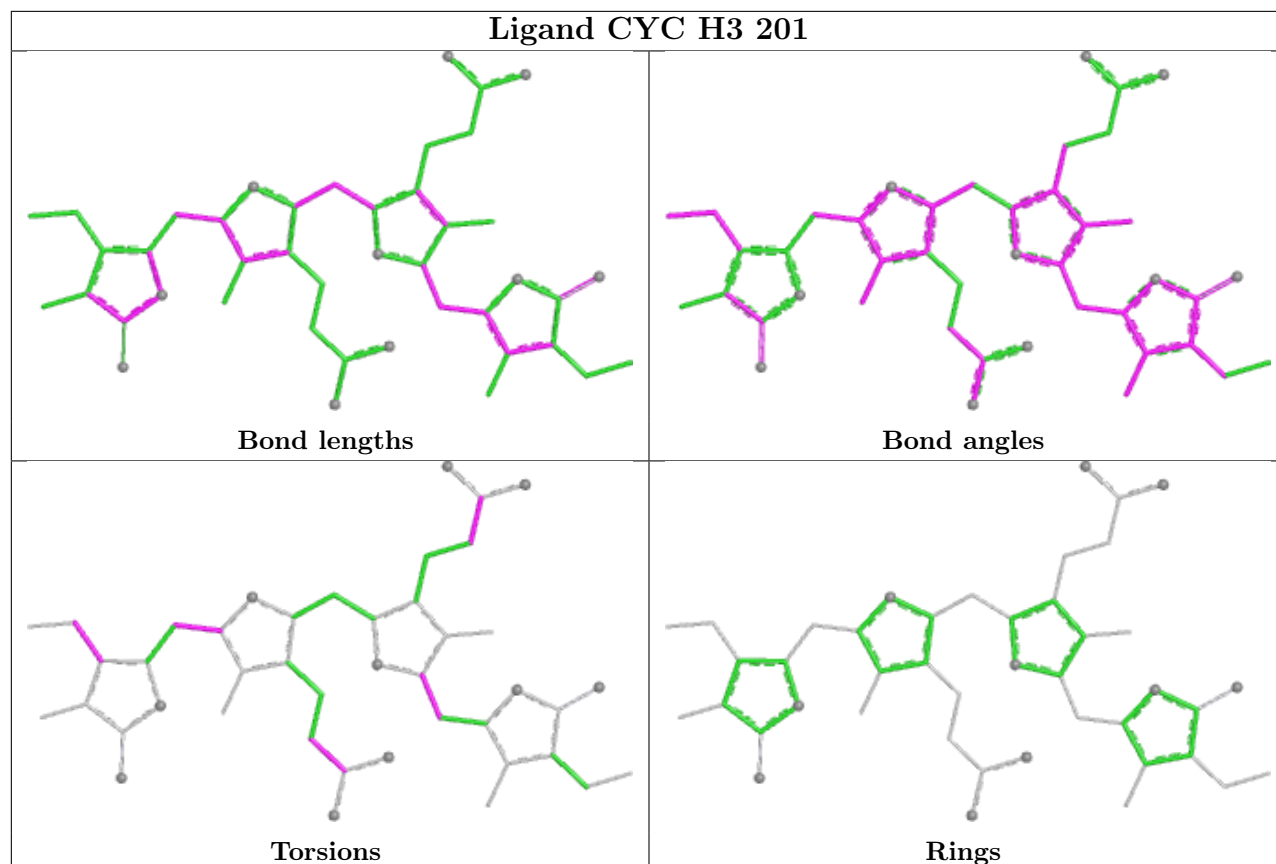
Ligand CYC F4 202



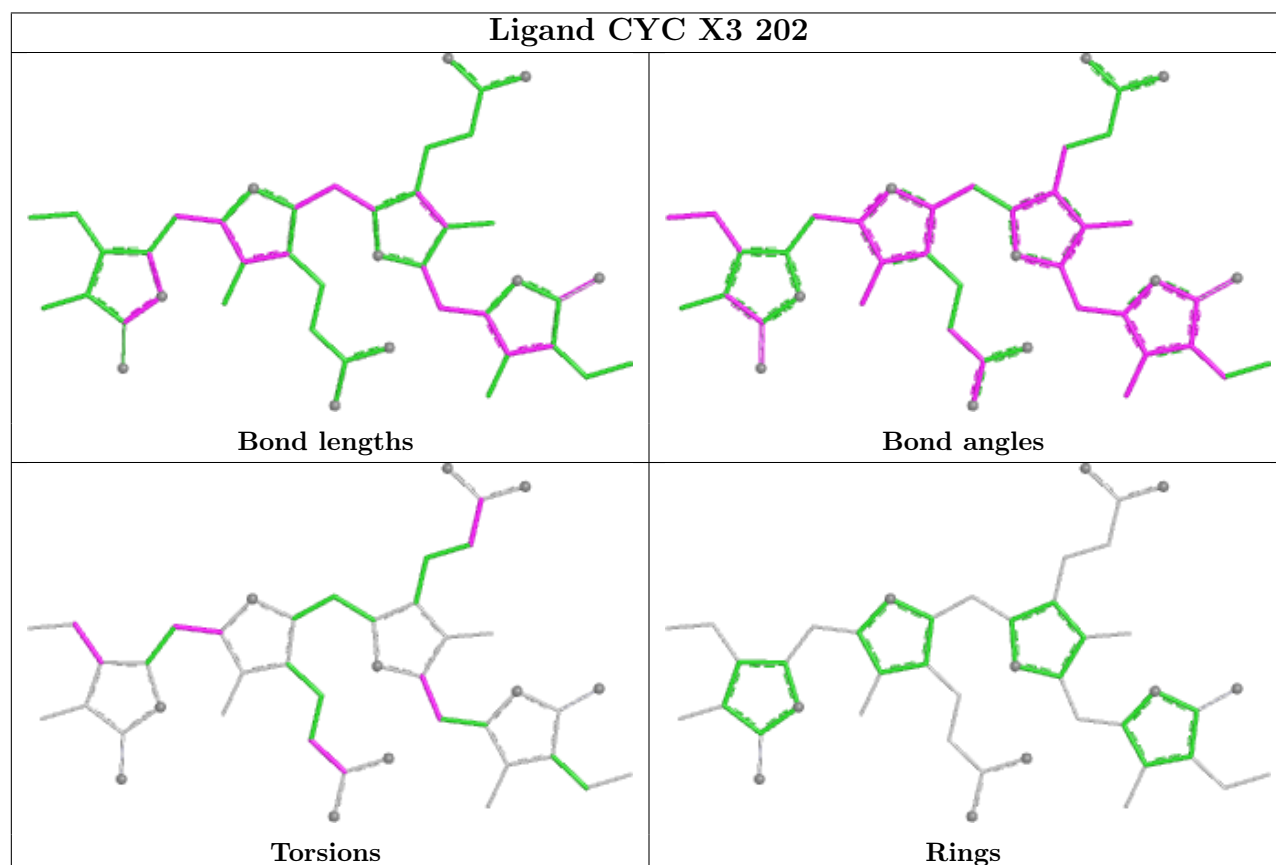
Ligand CYC A8 201



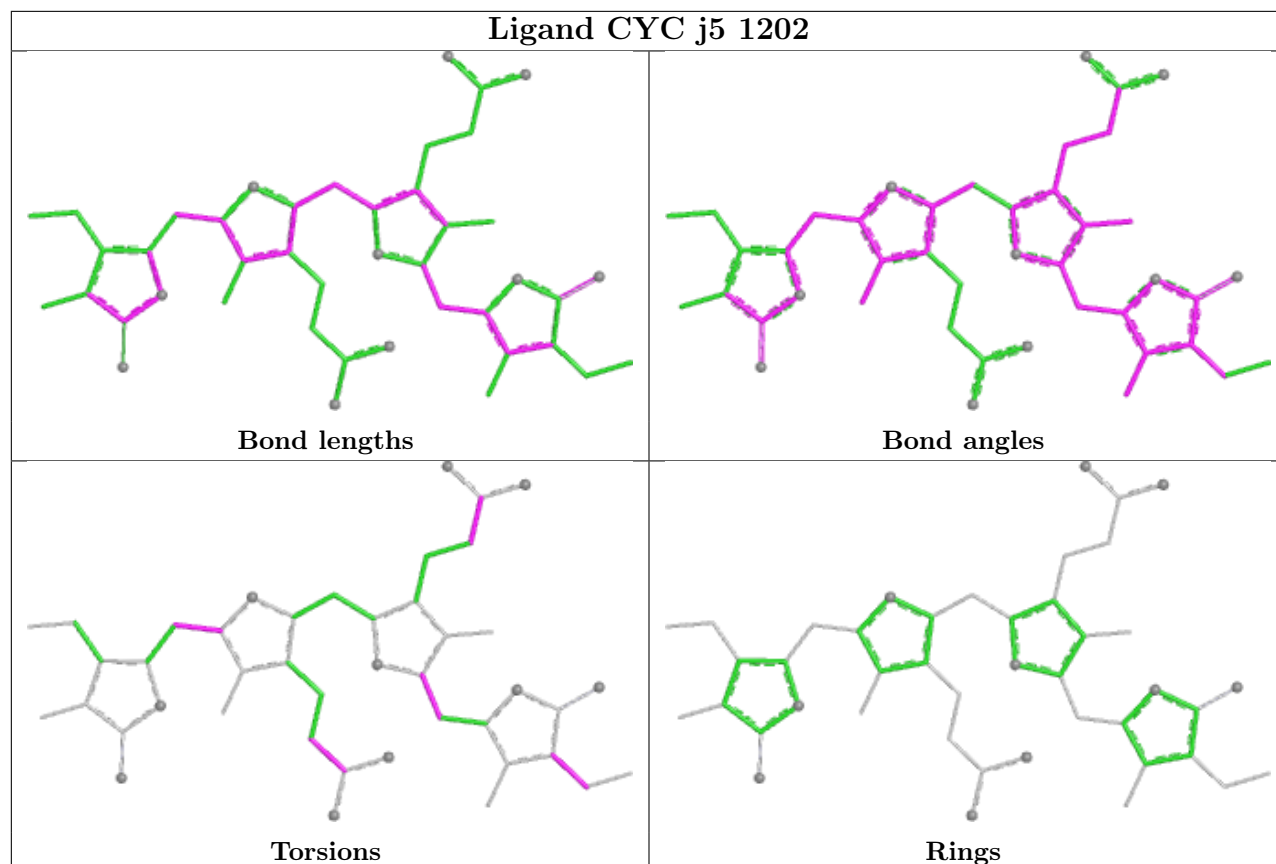
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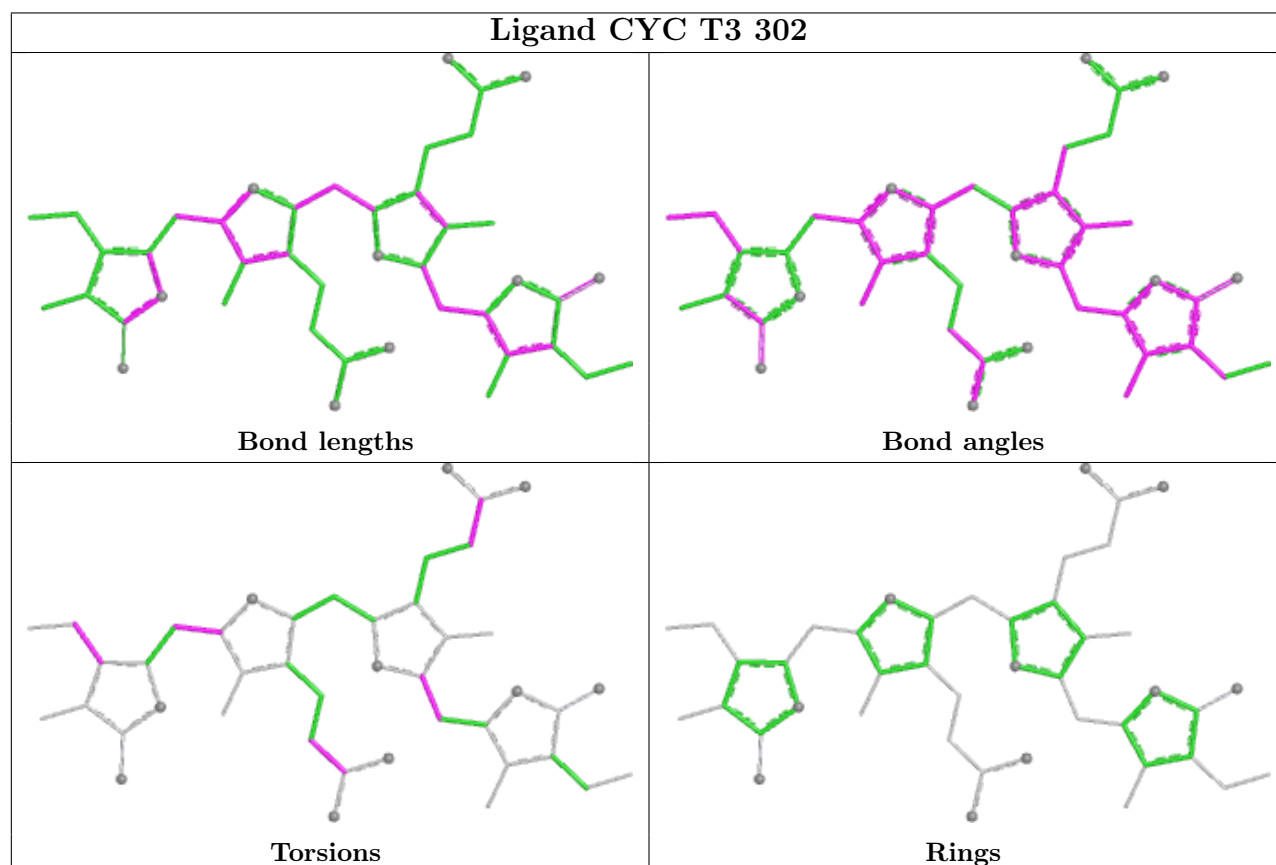
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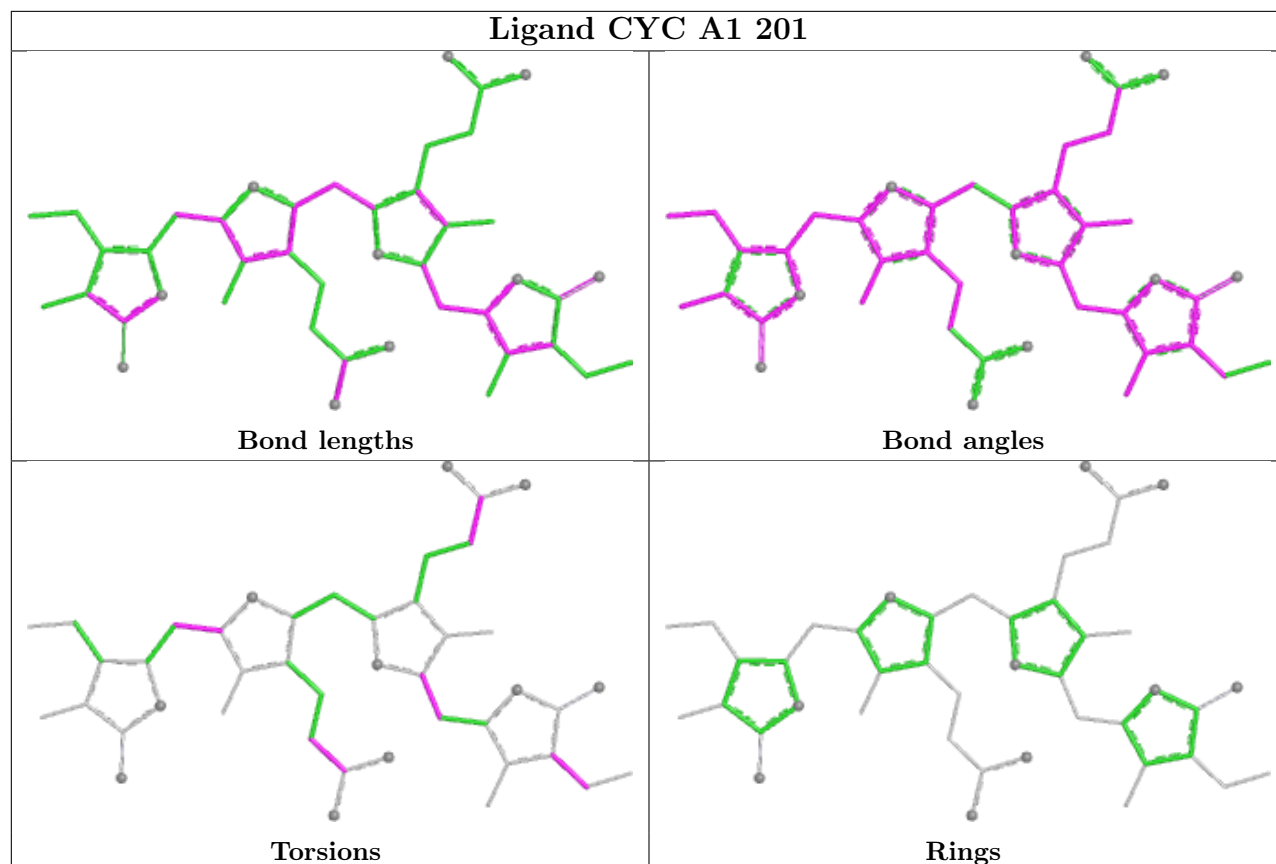
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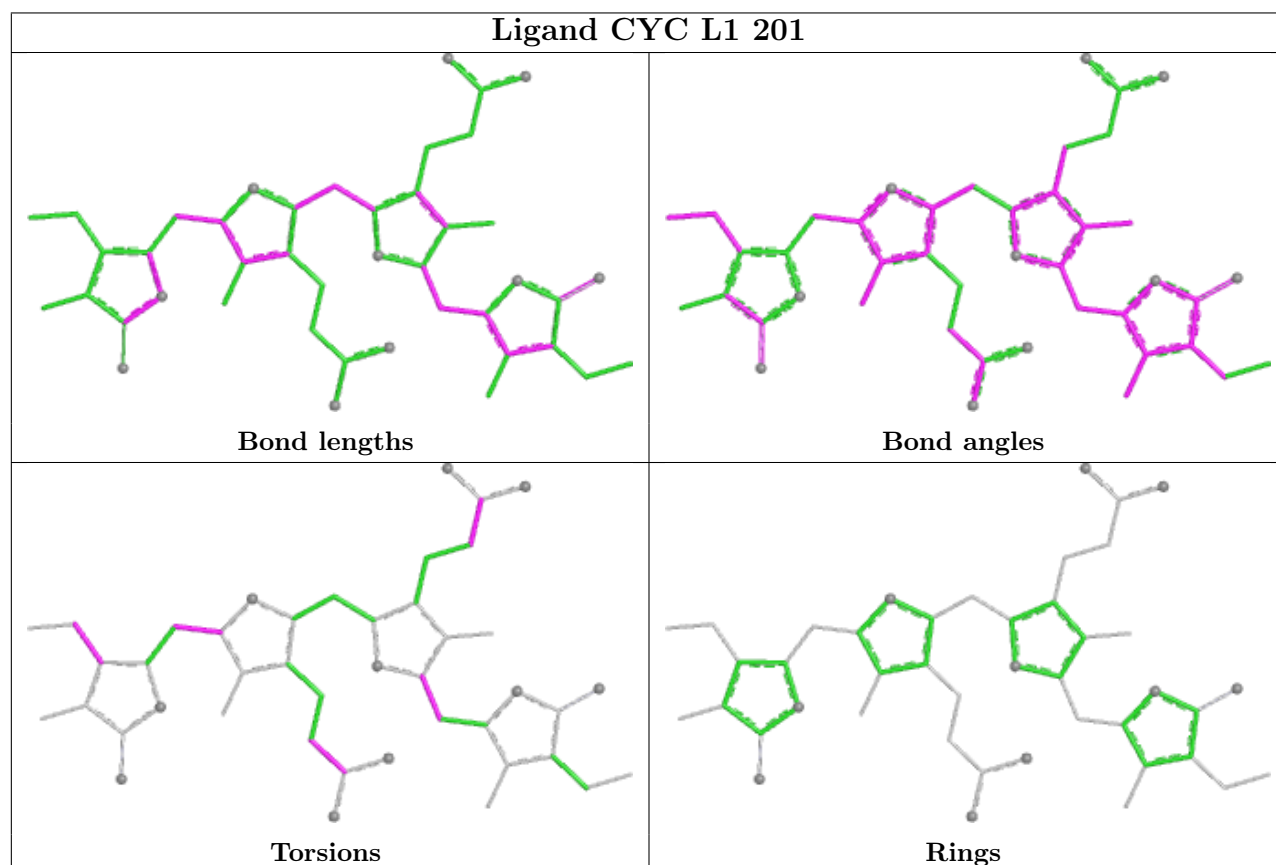
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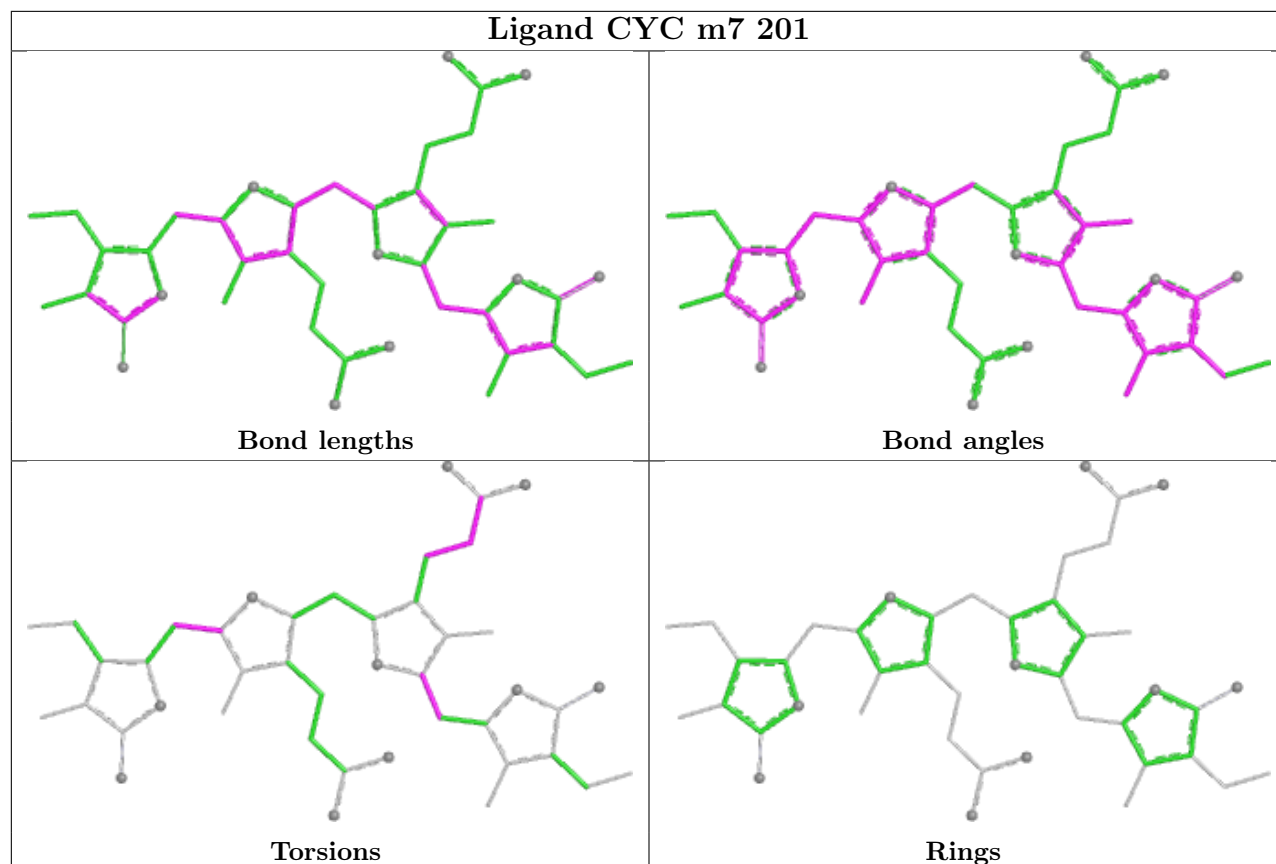
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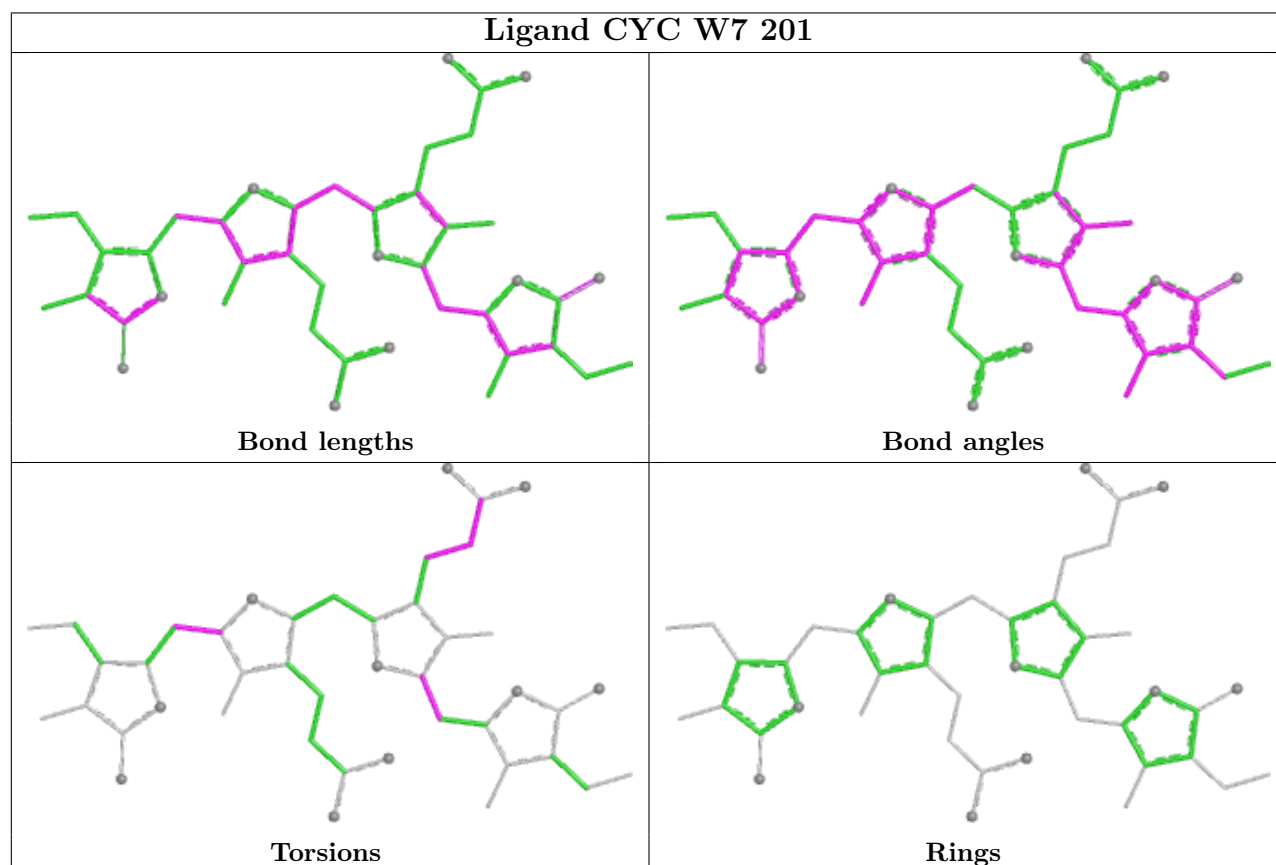
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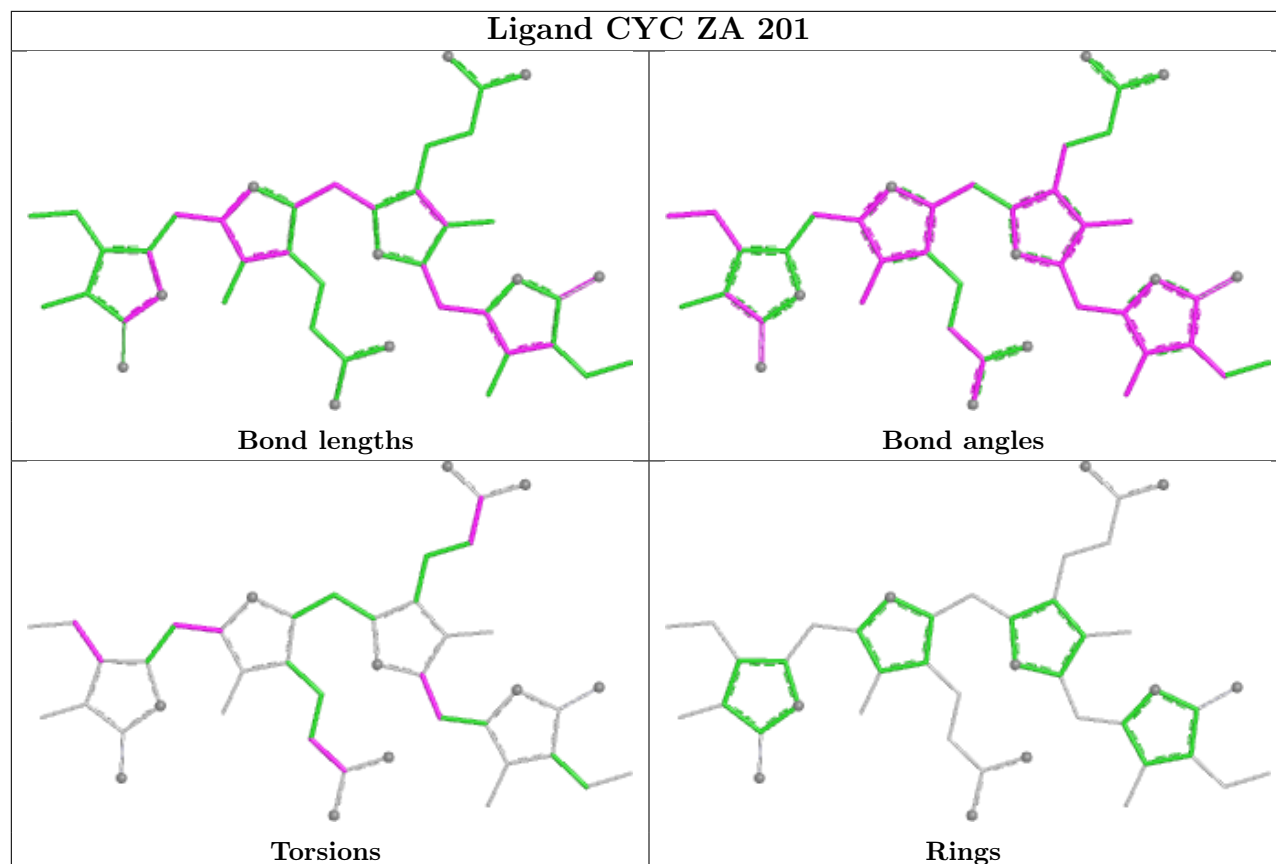
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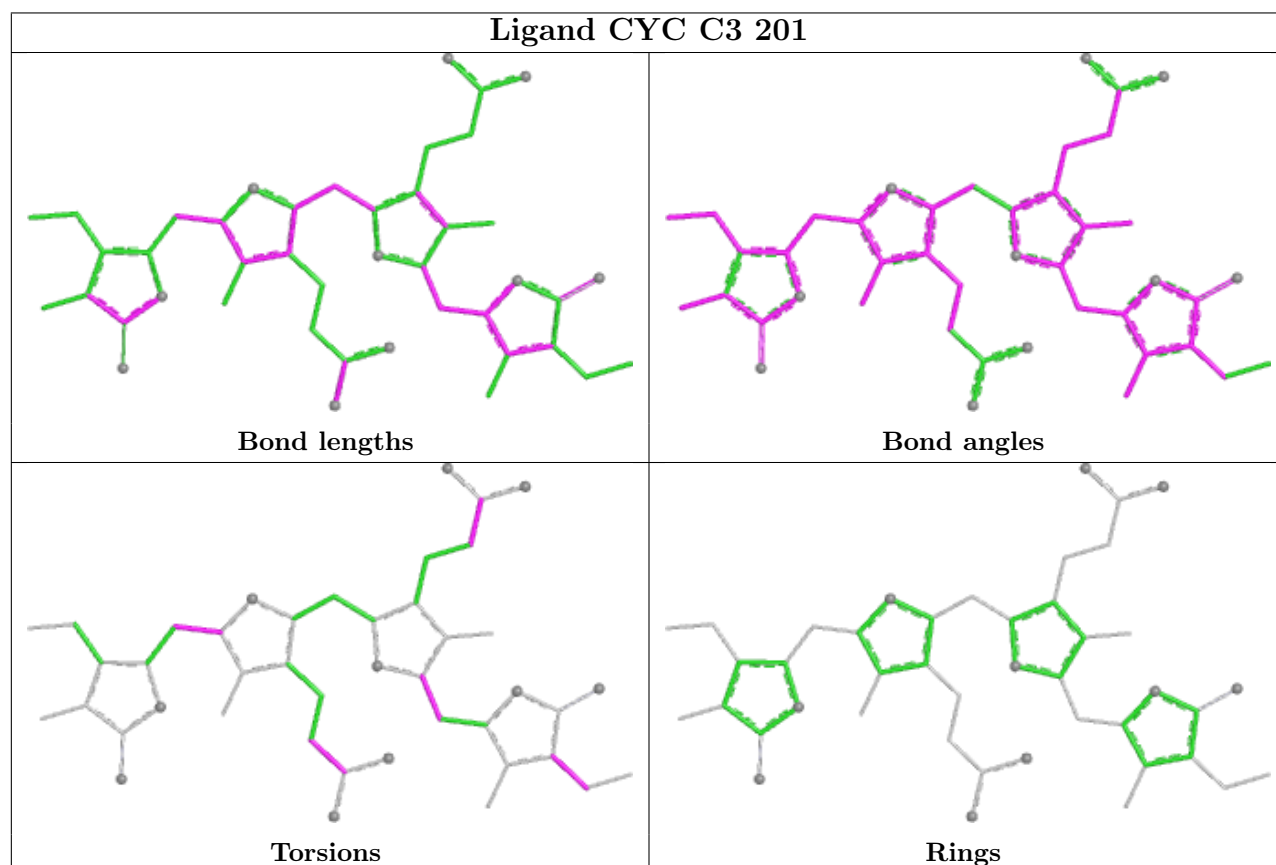
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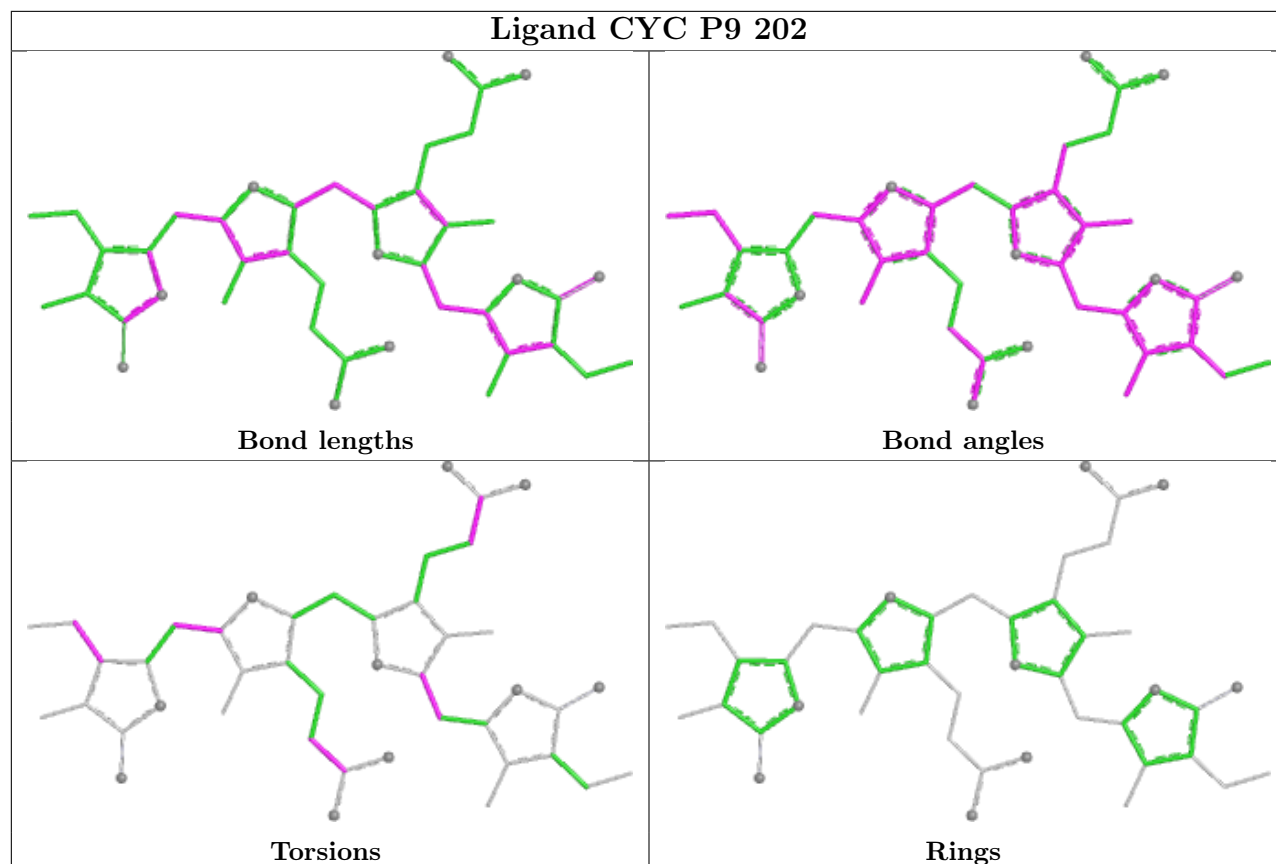
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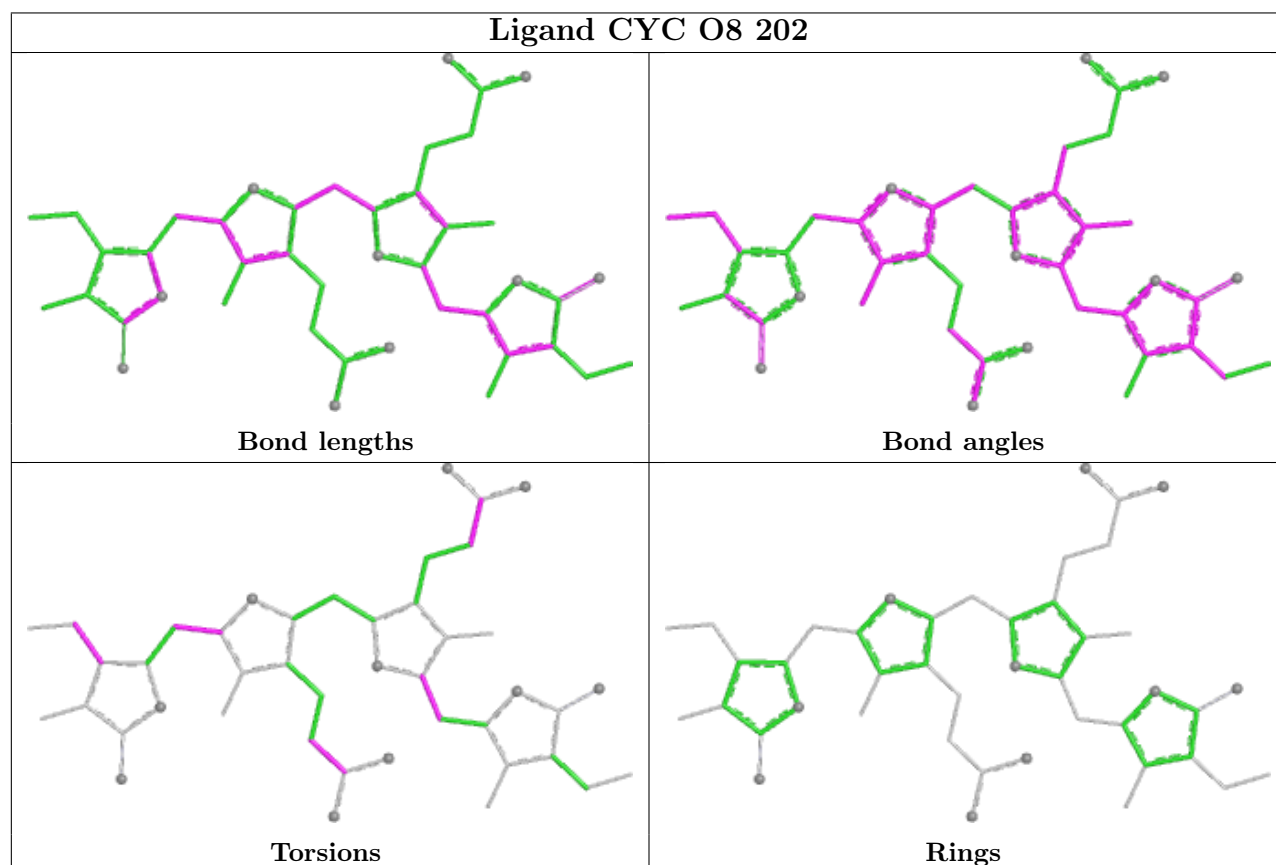
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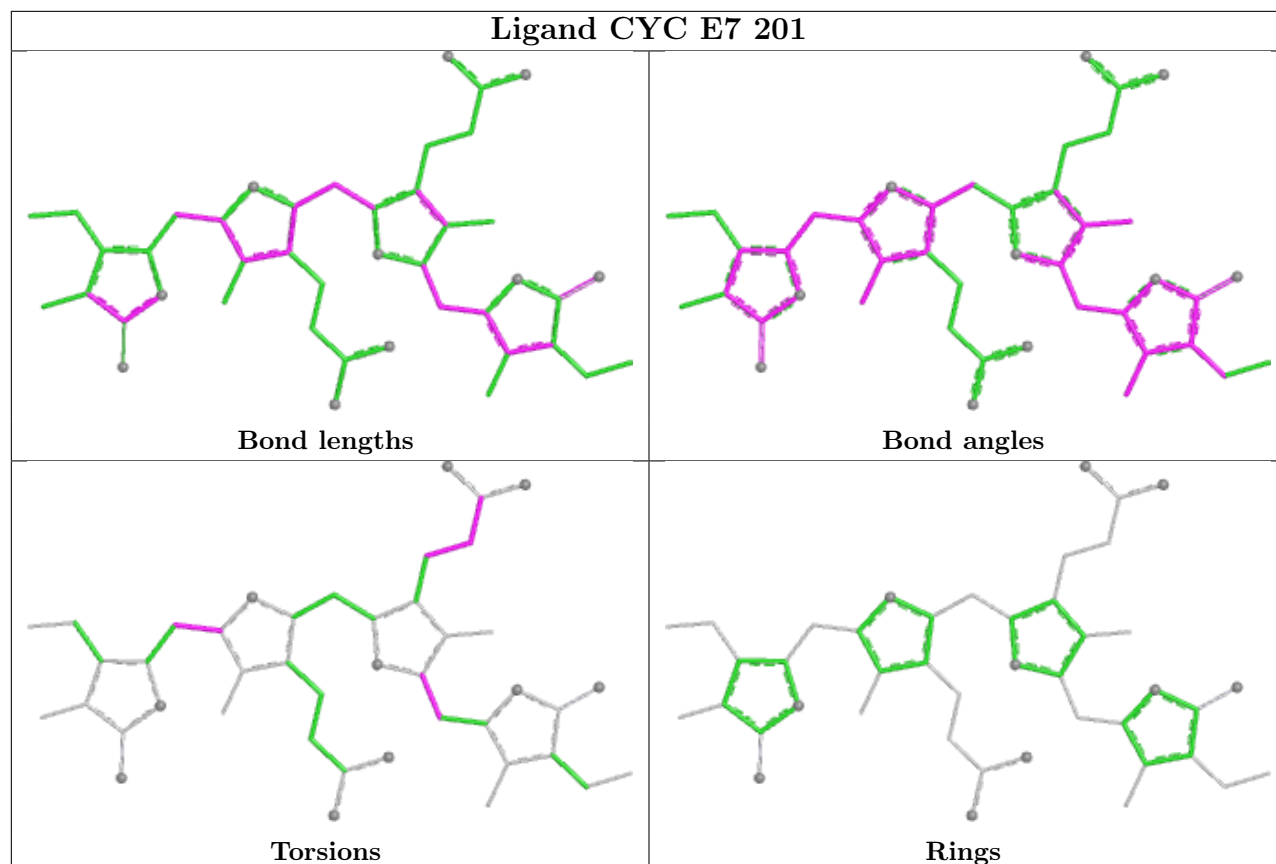
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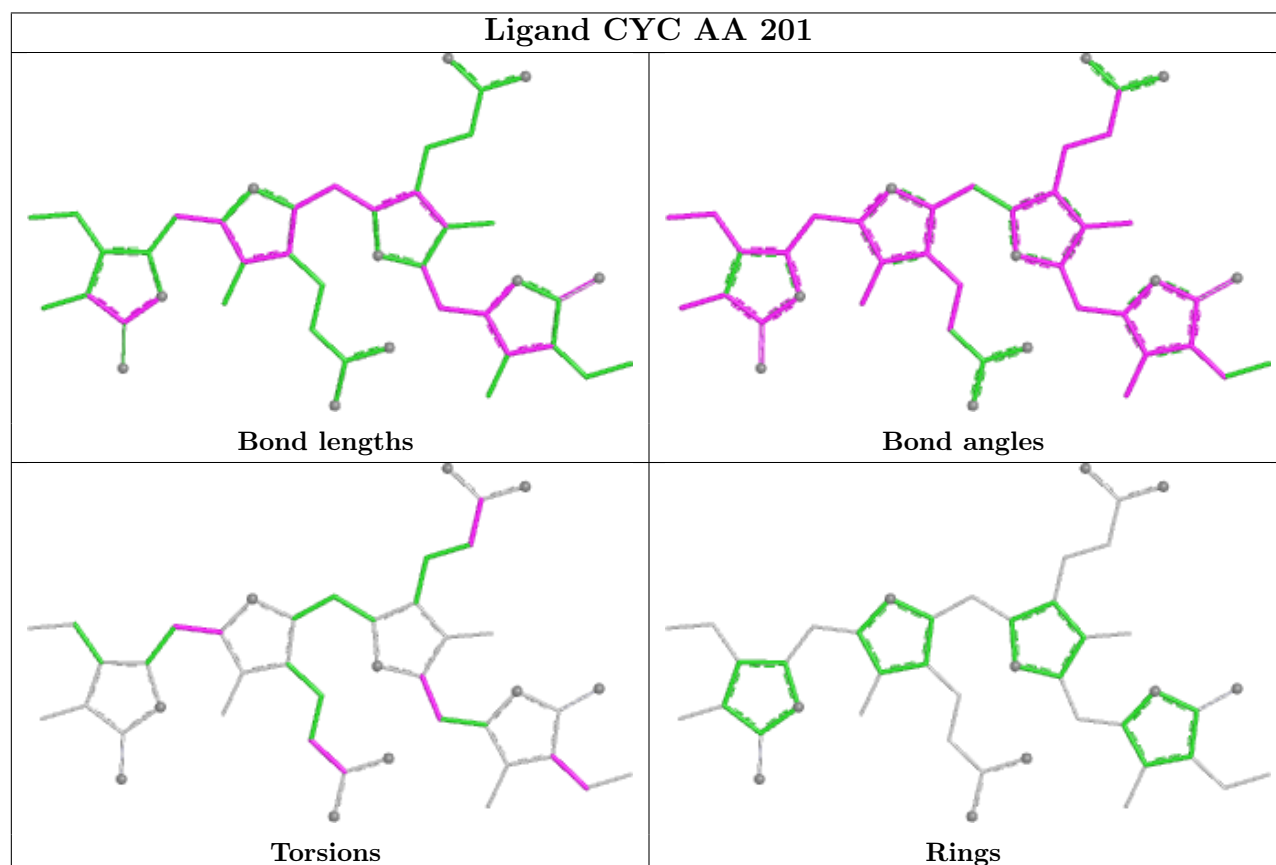
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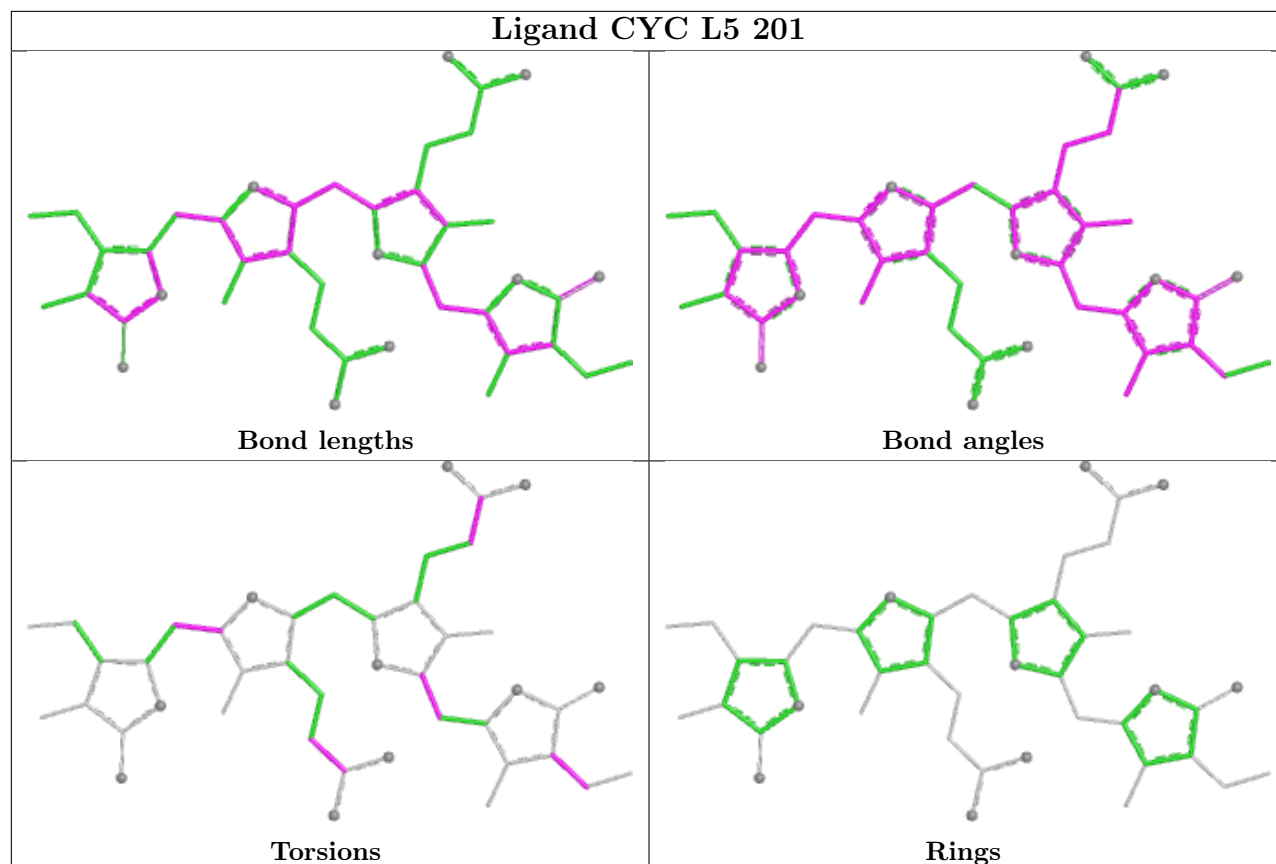
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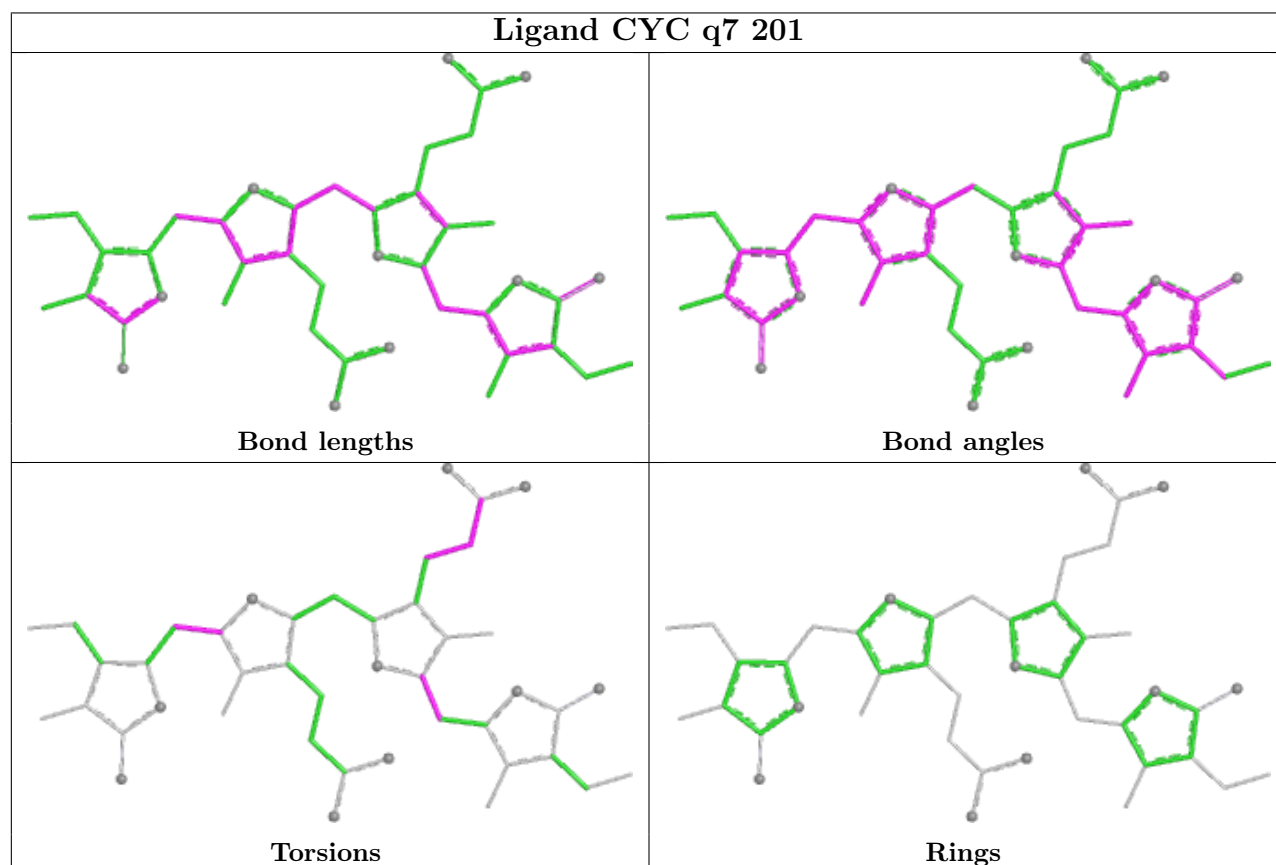
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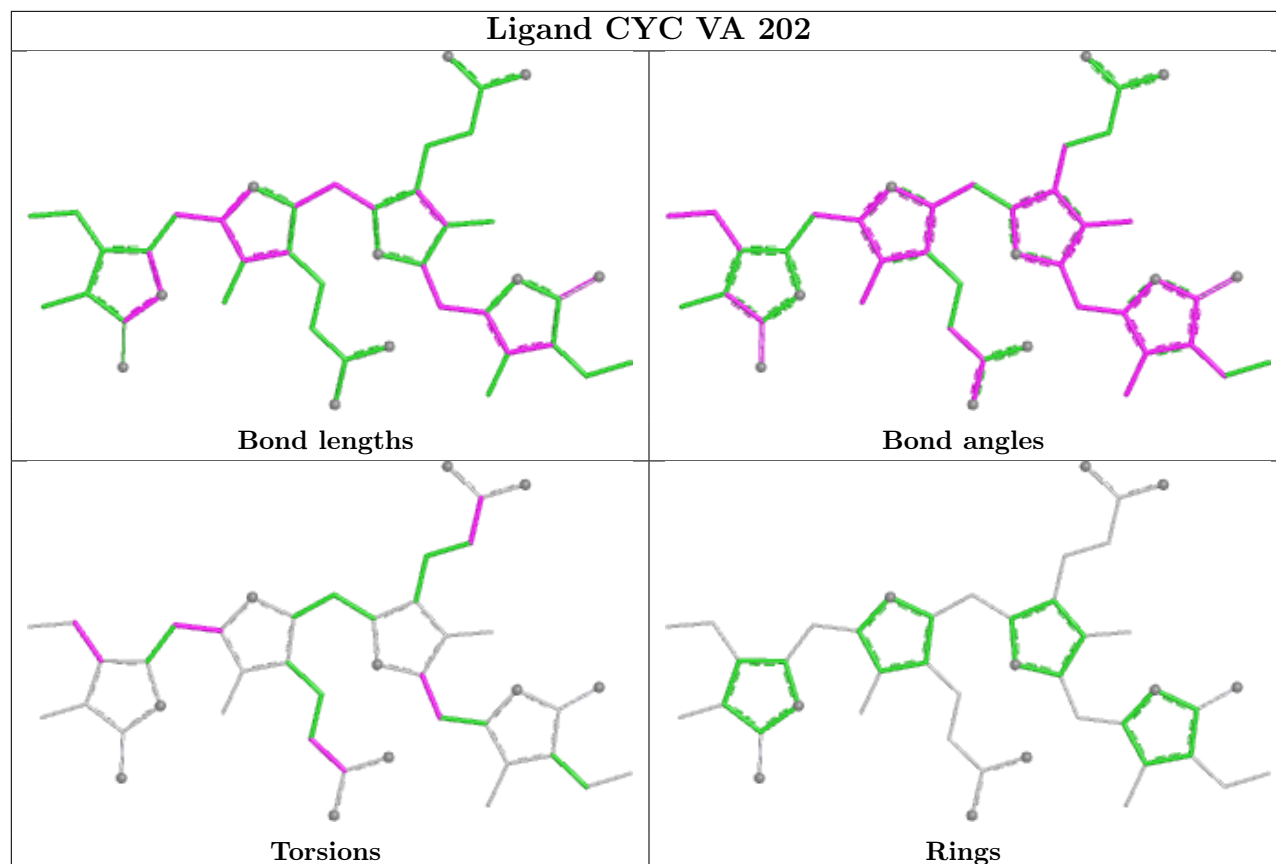
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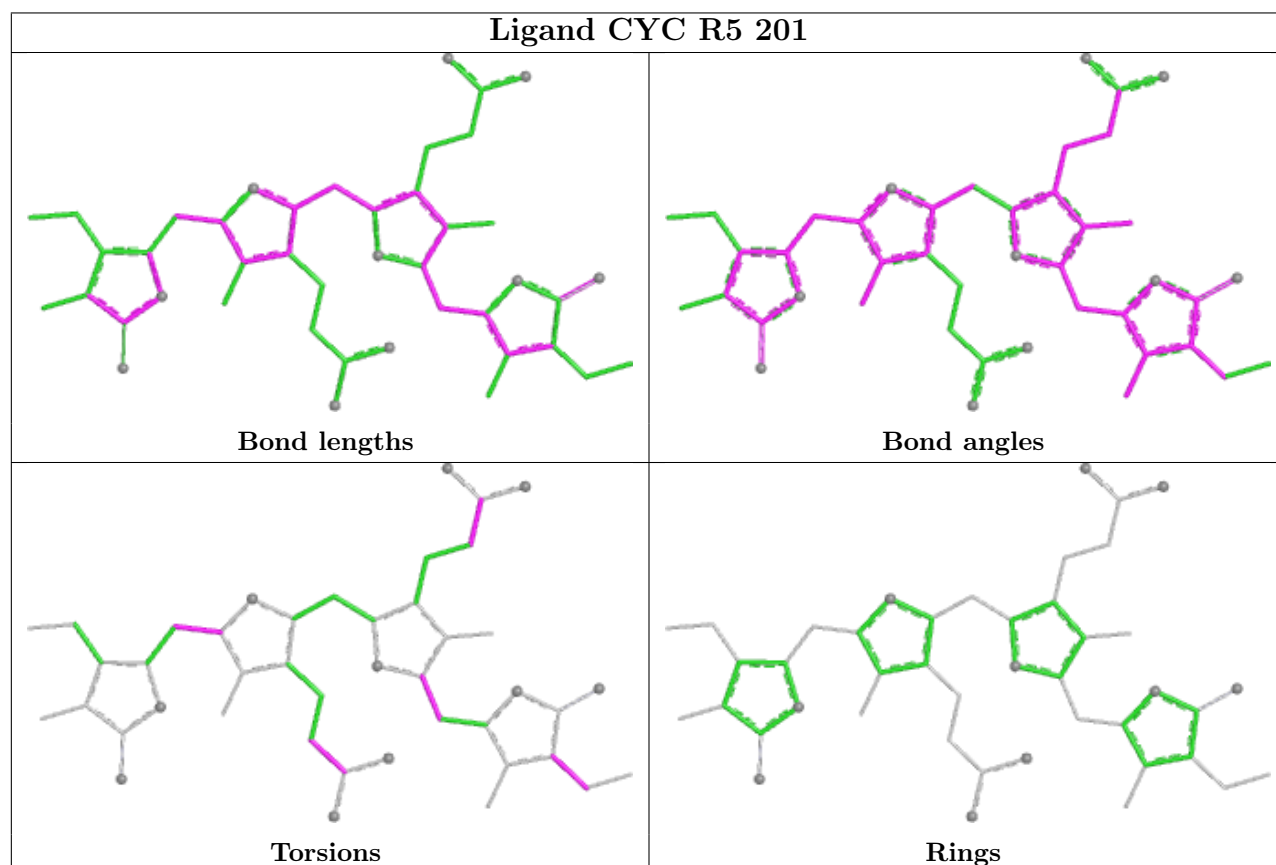
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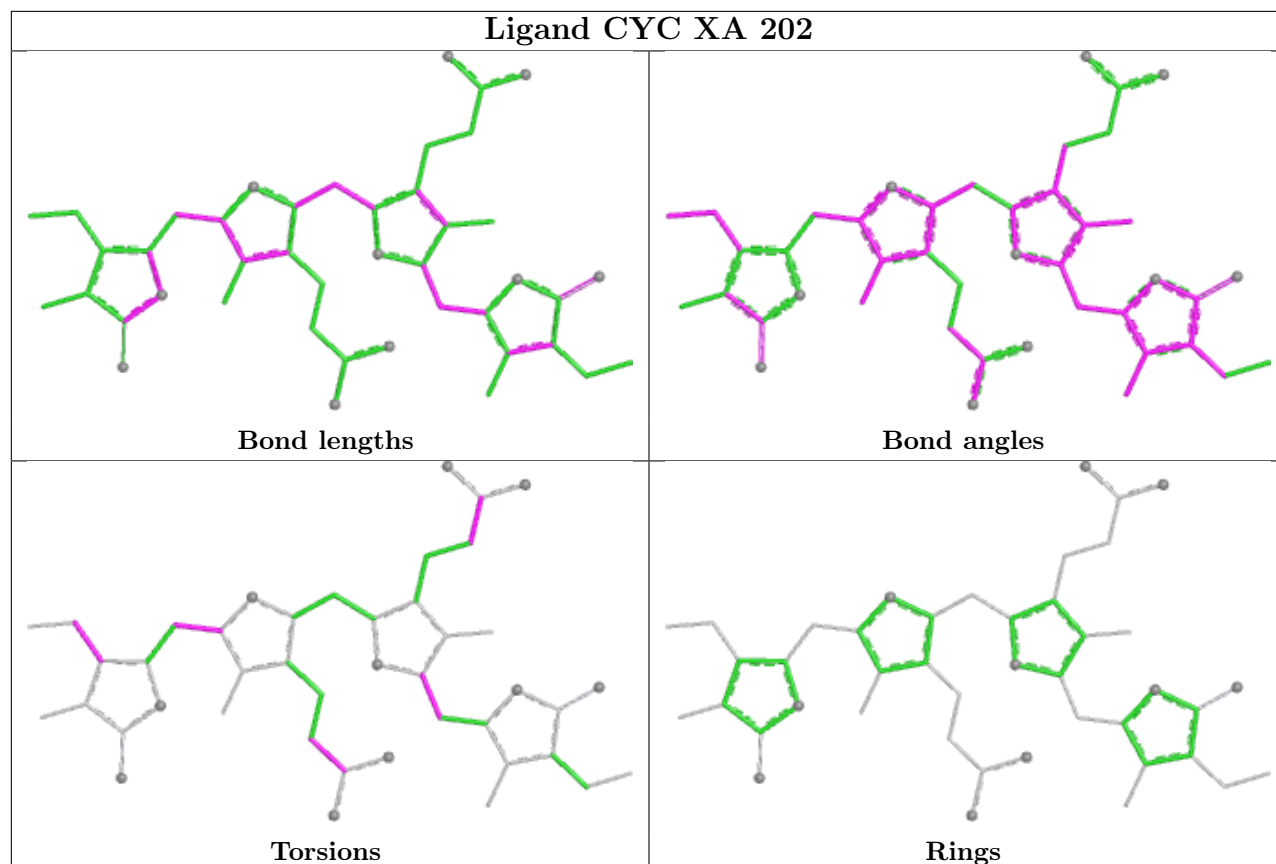
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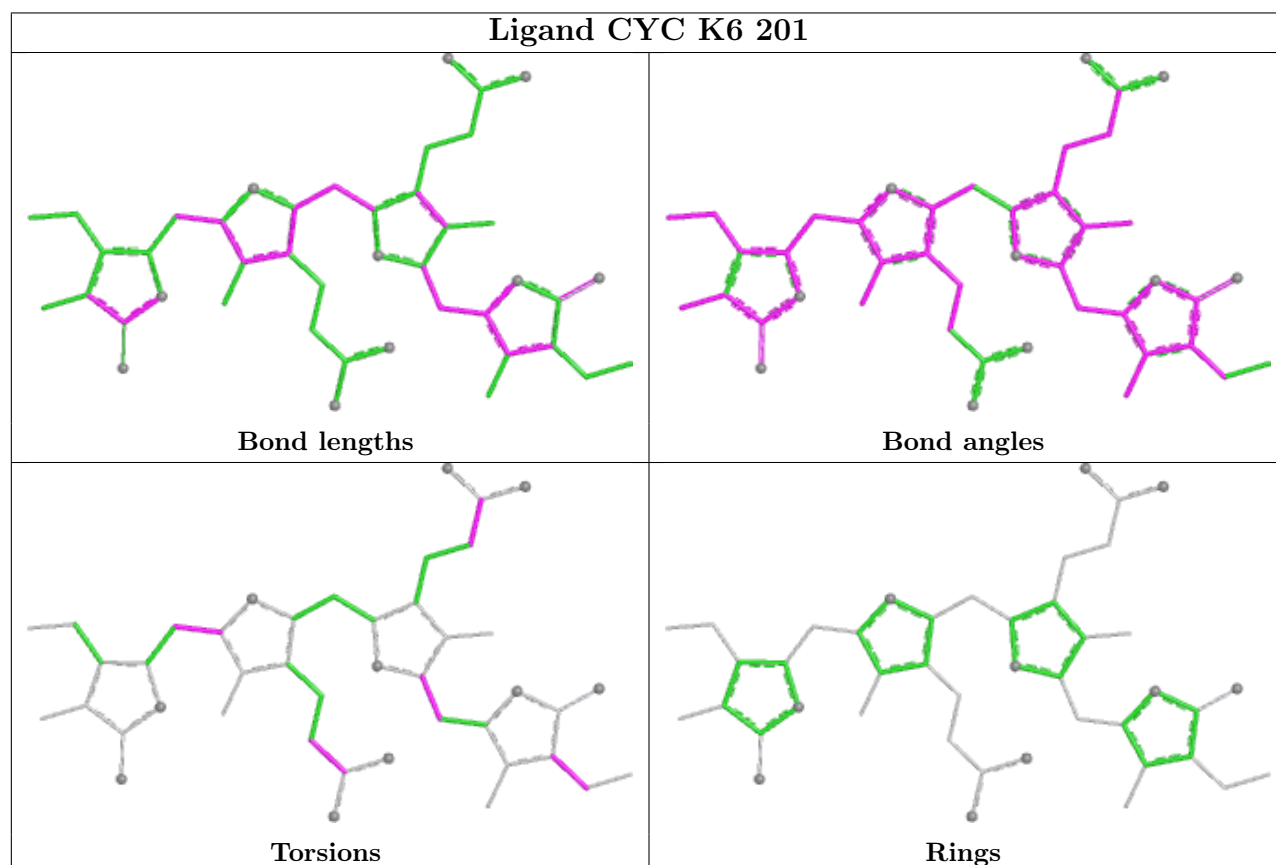
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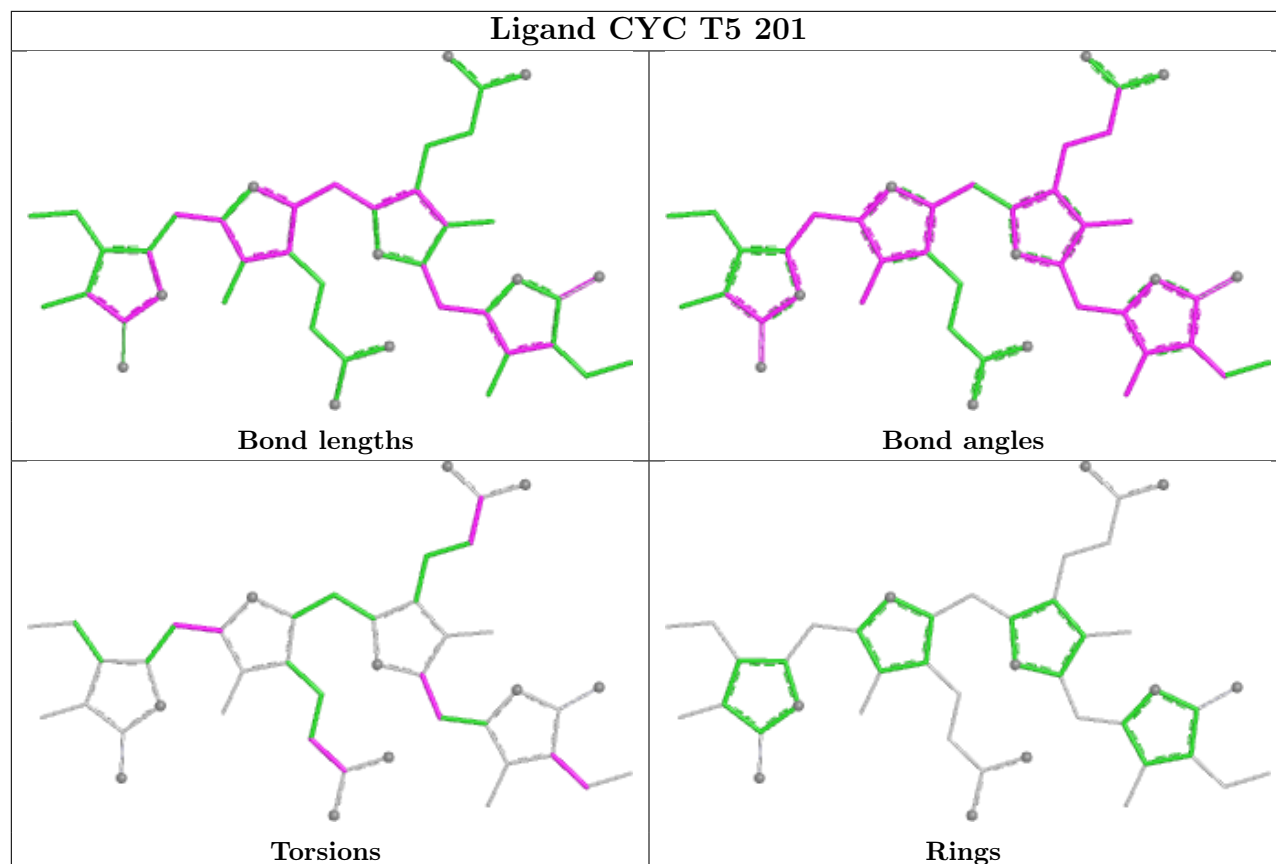
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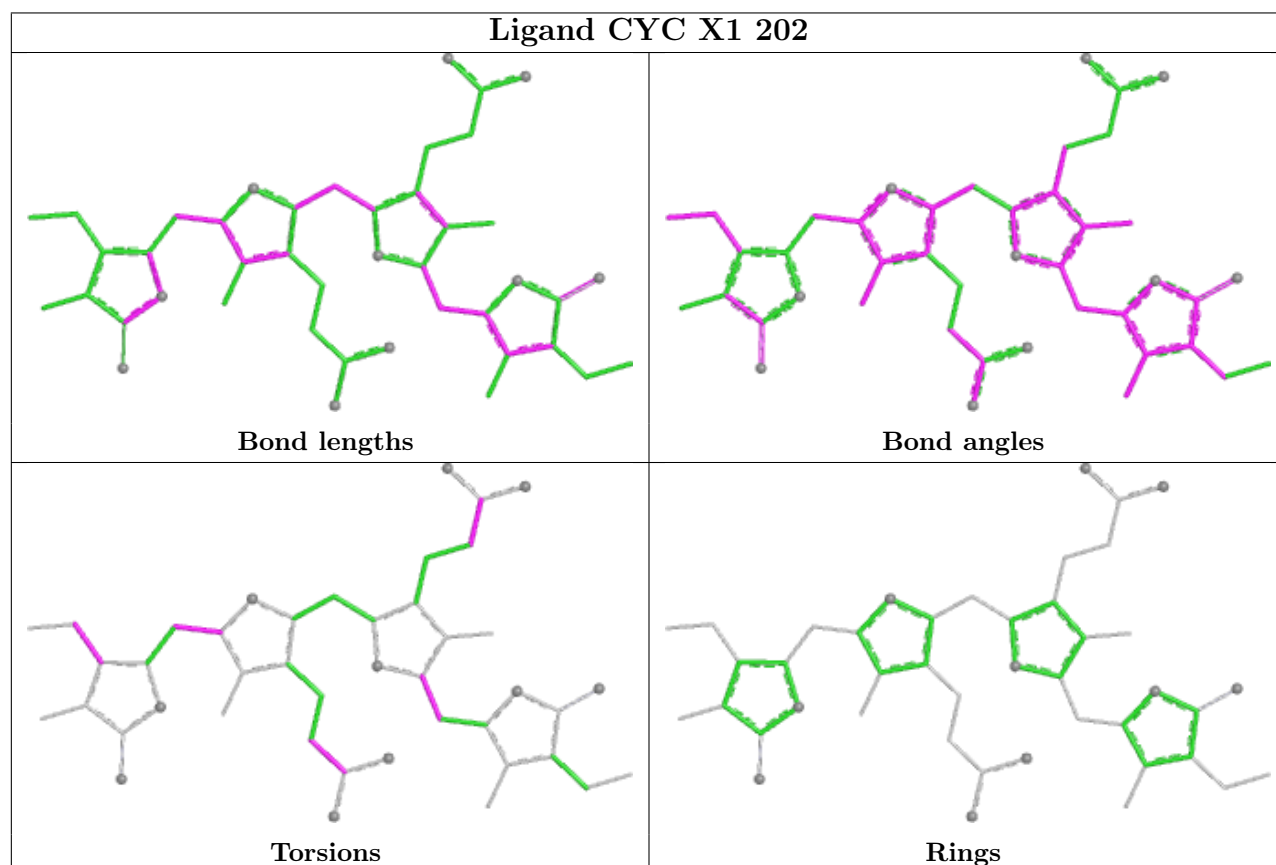
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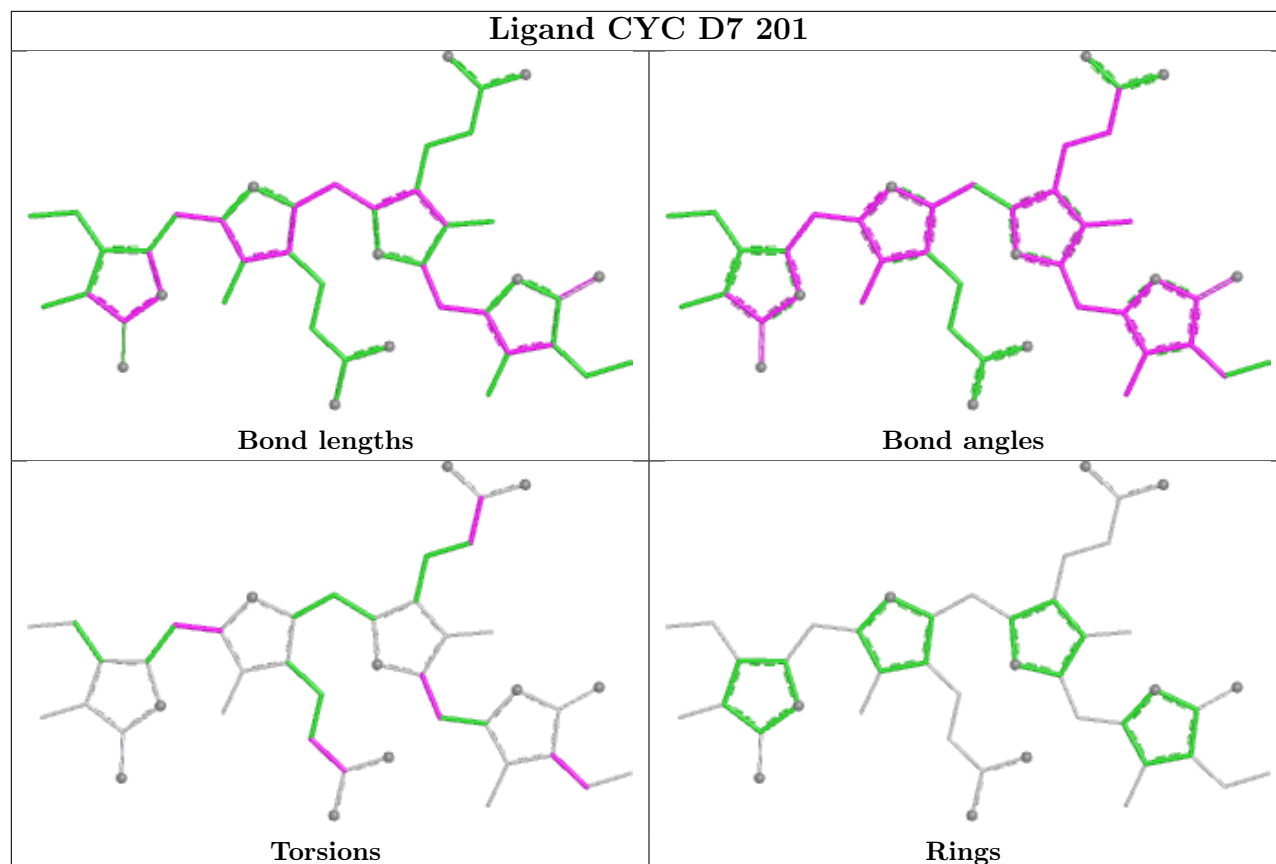
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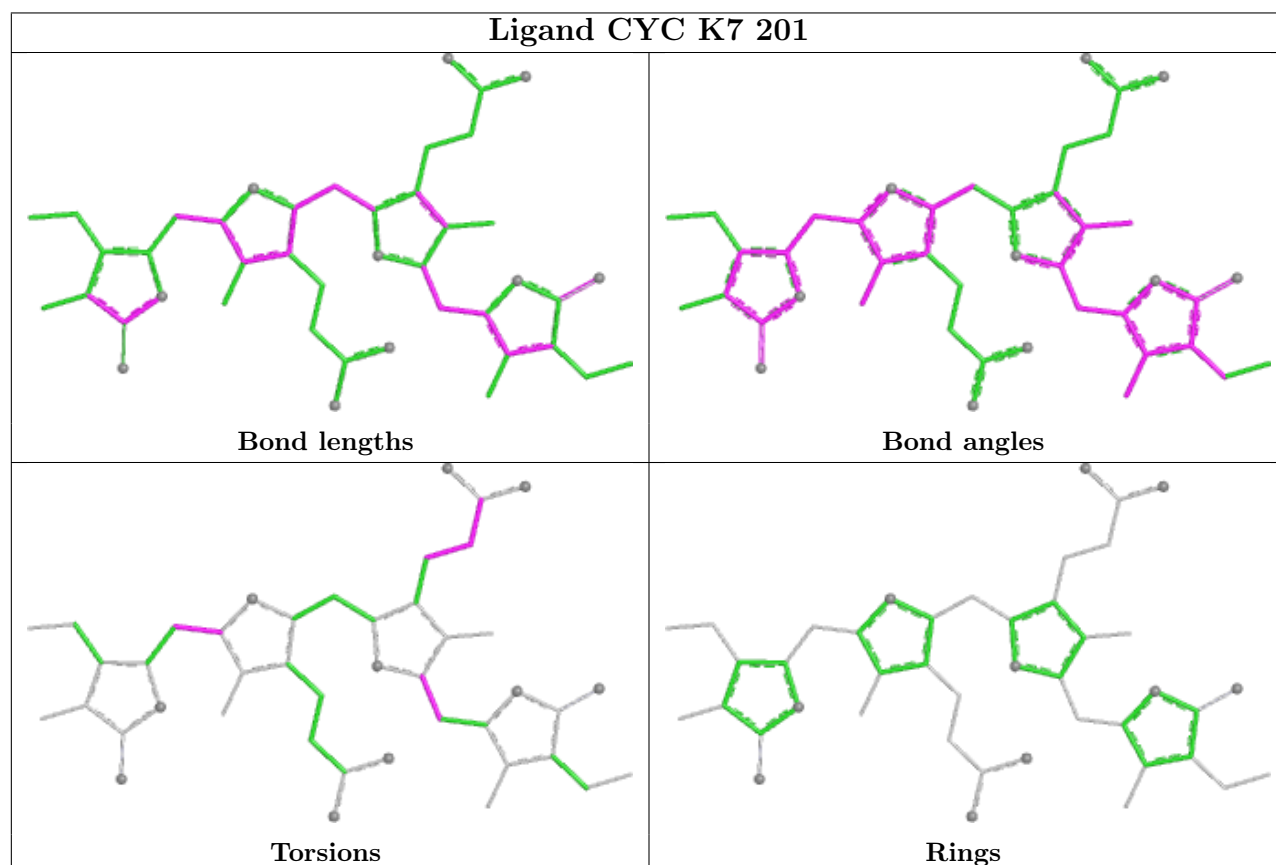
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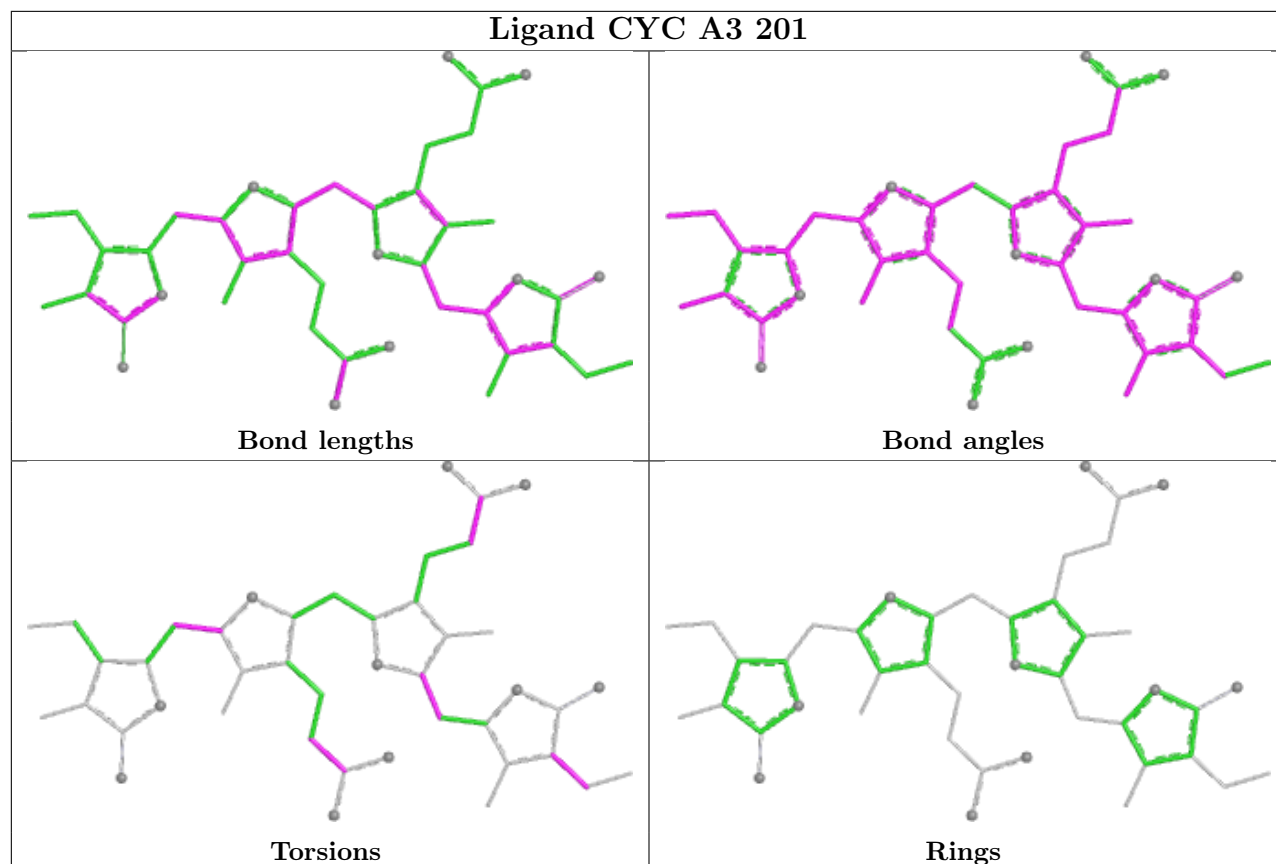
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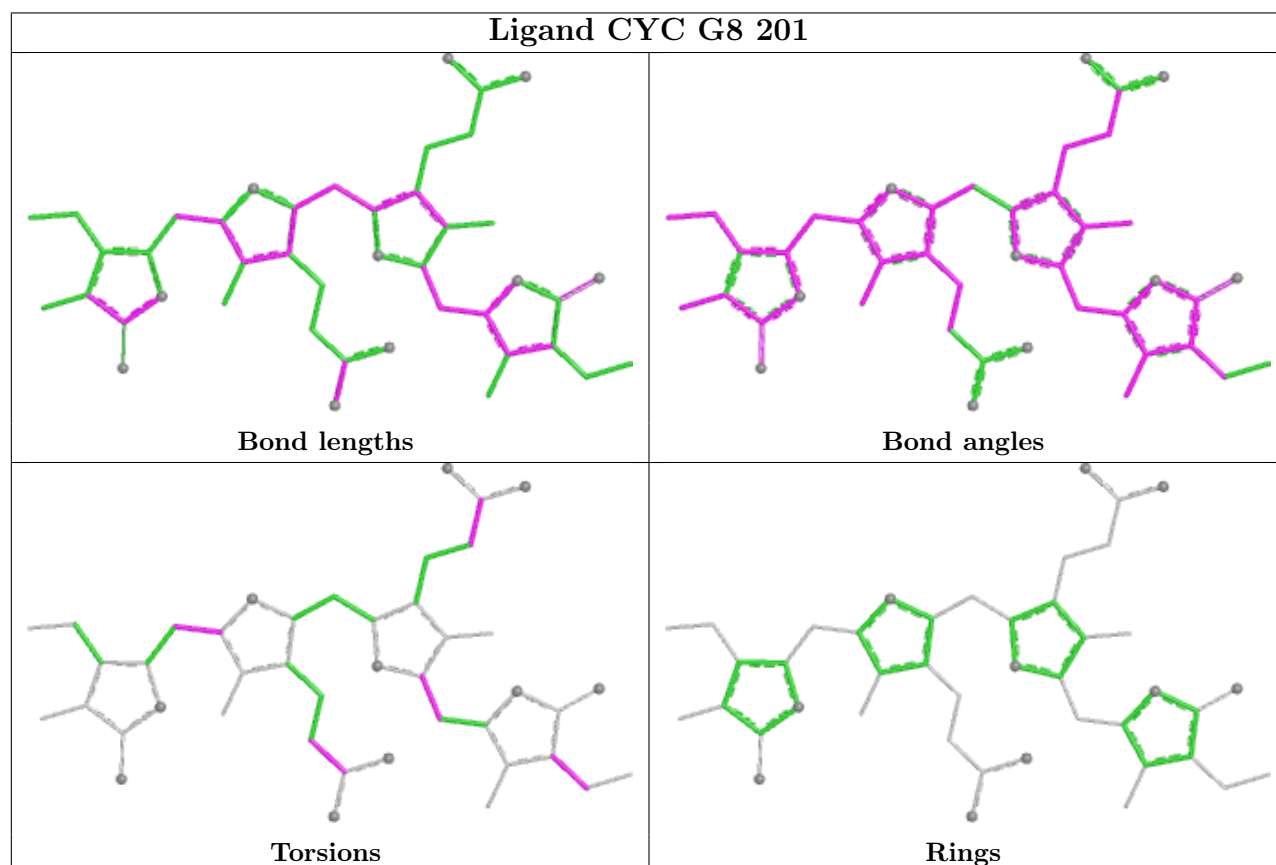
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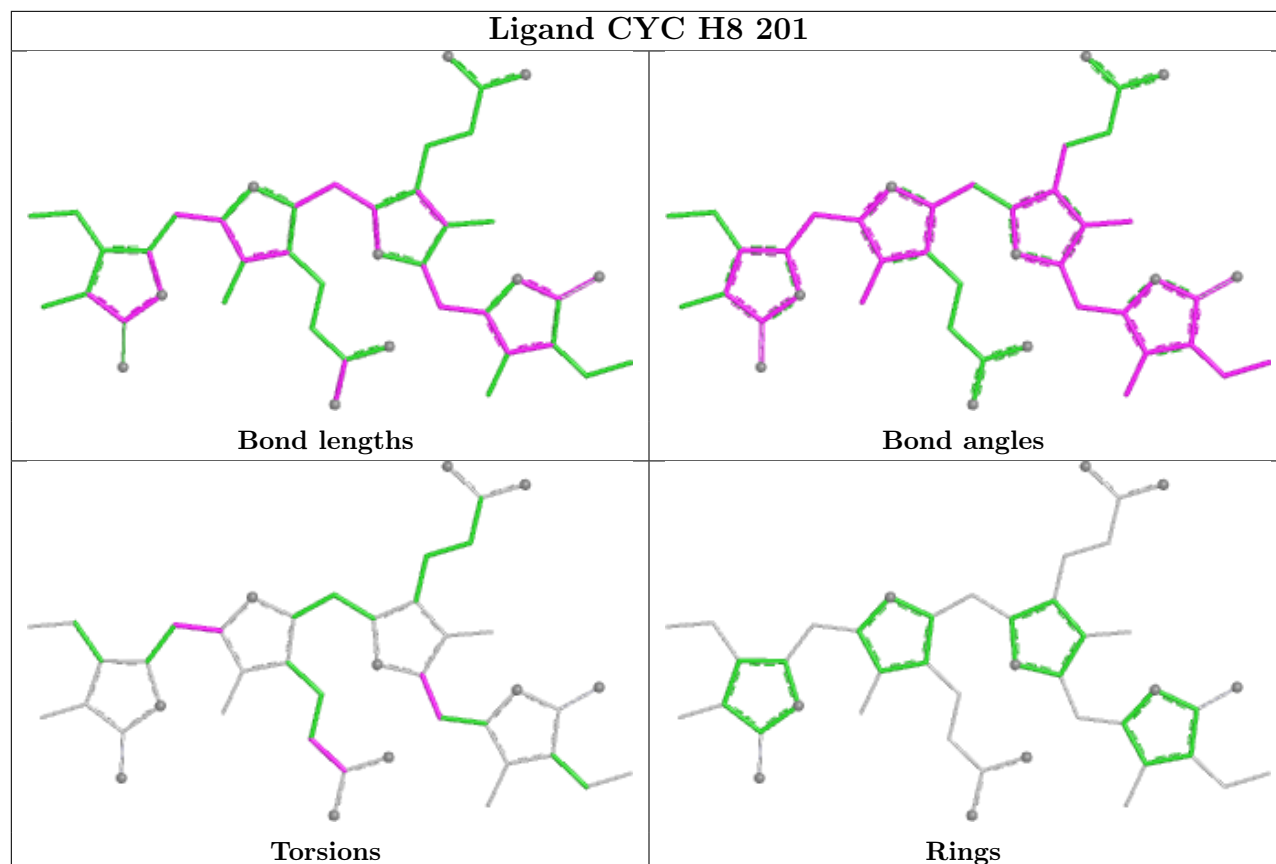
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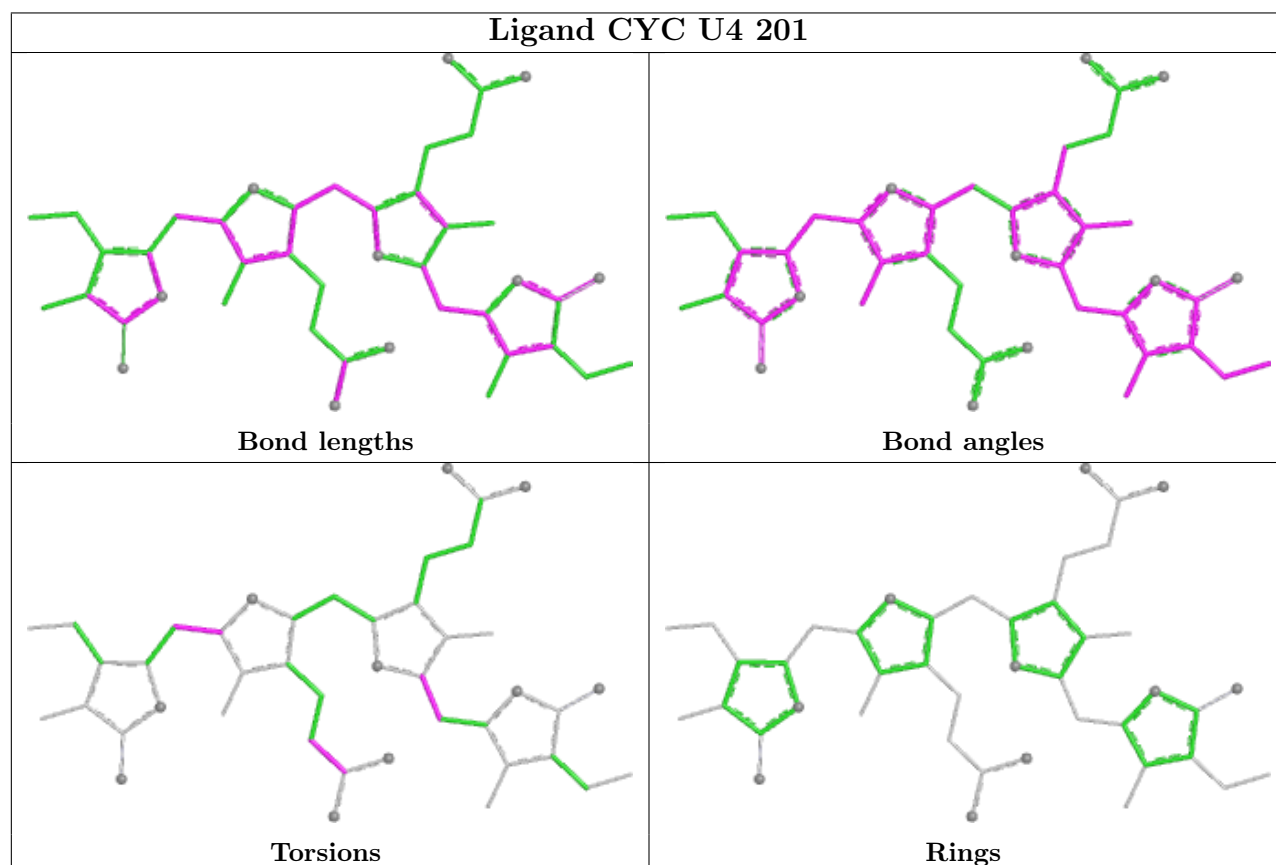
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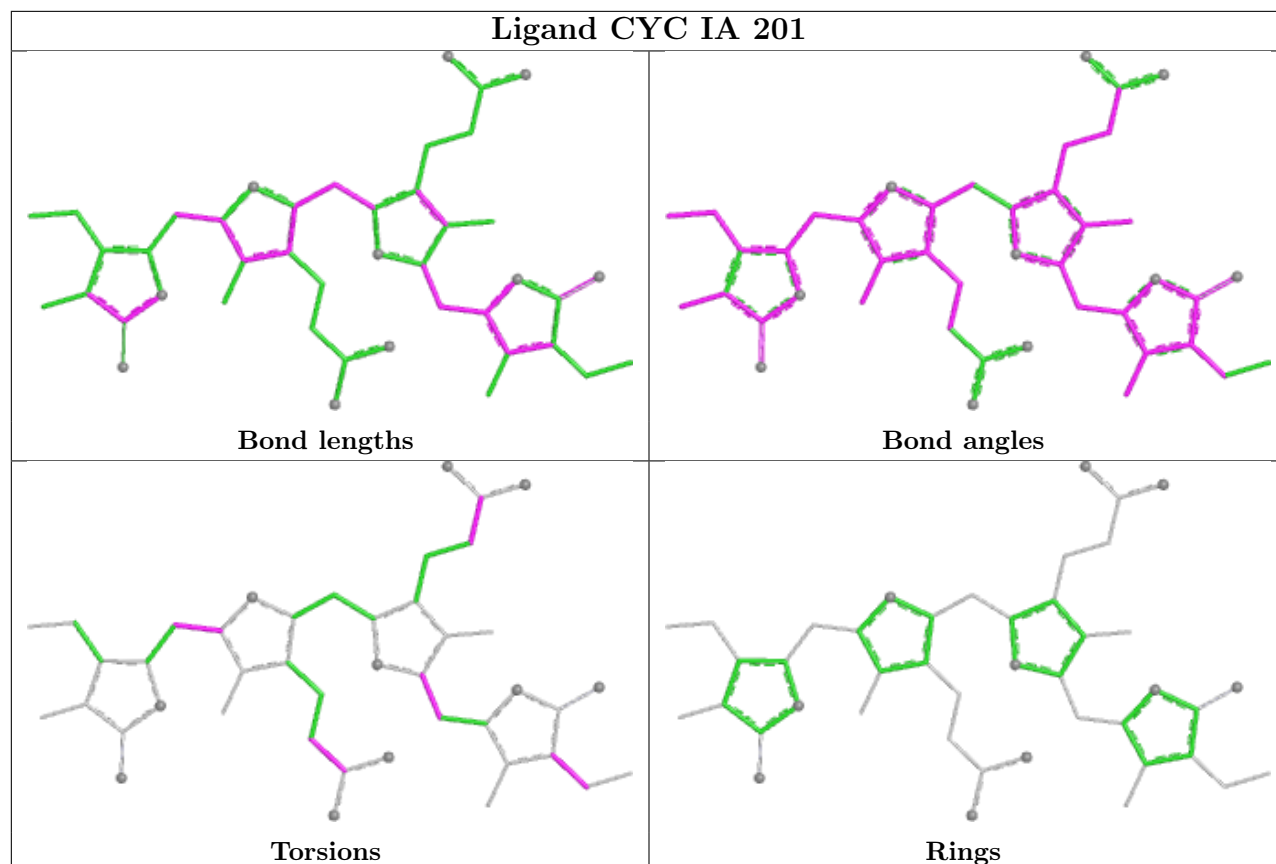
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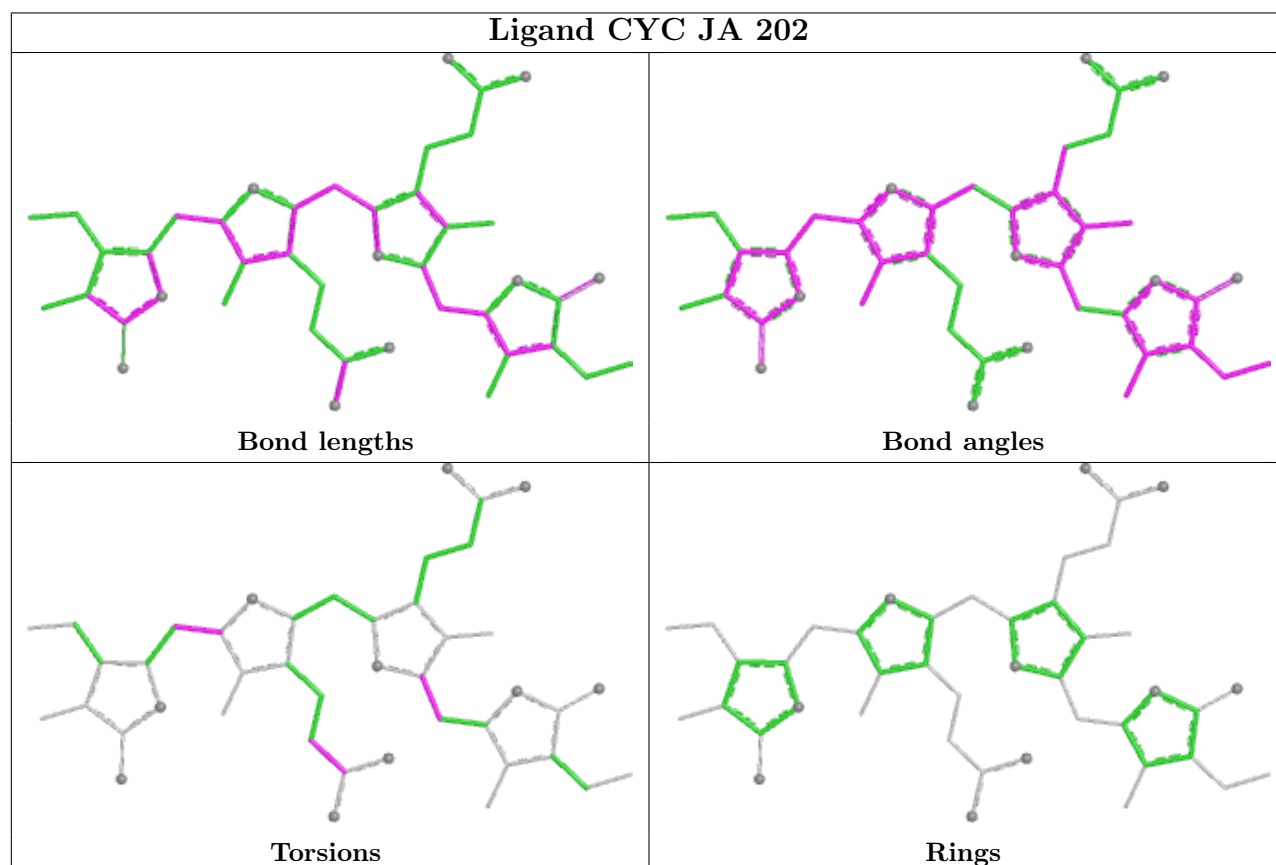
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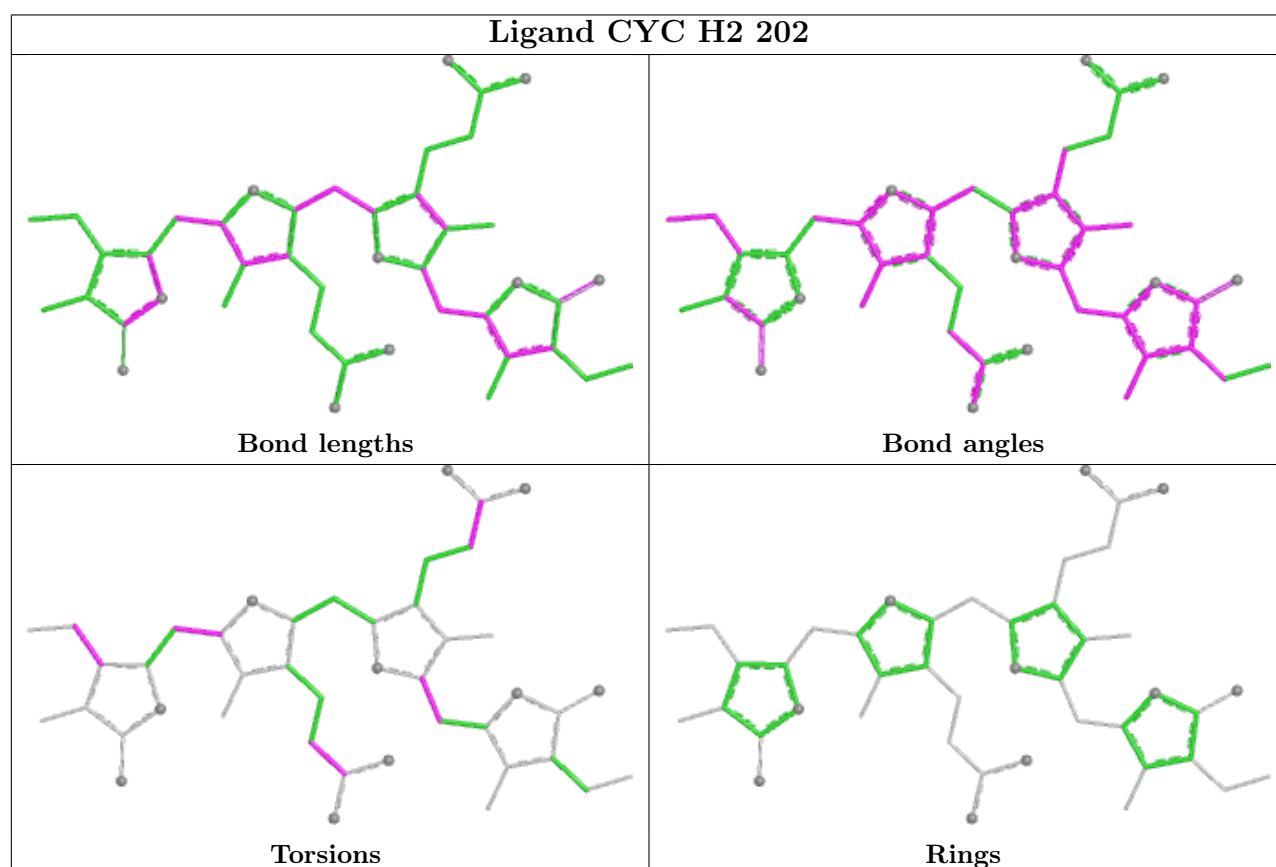
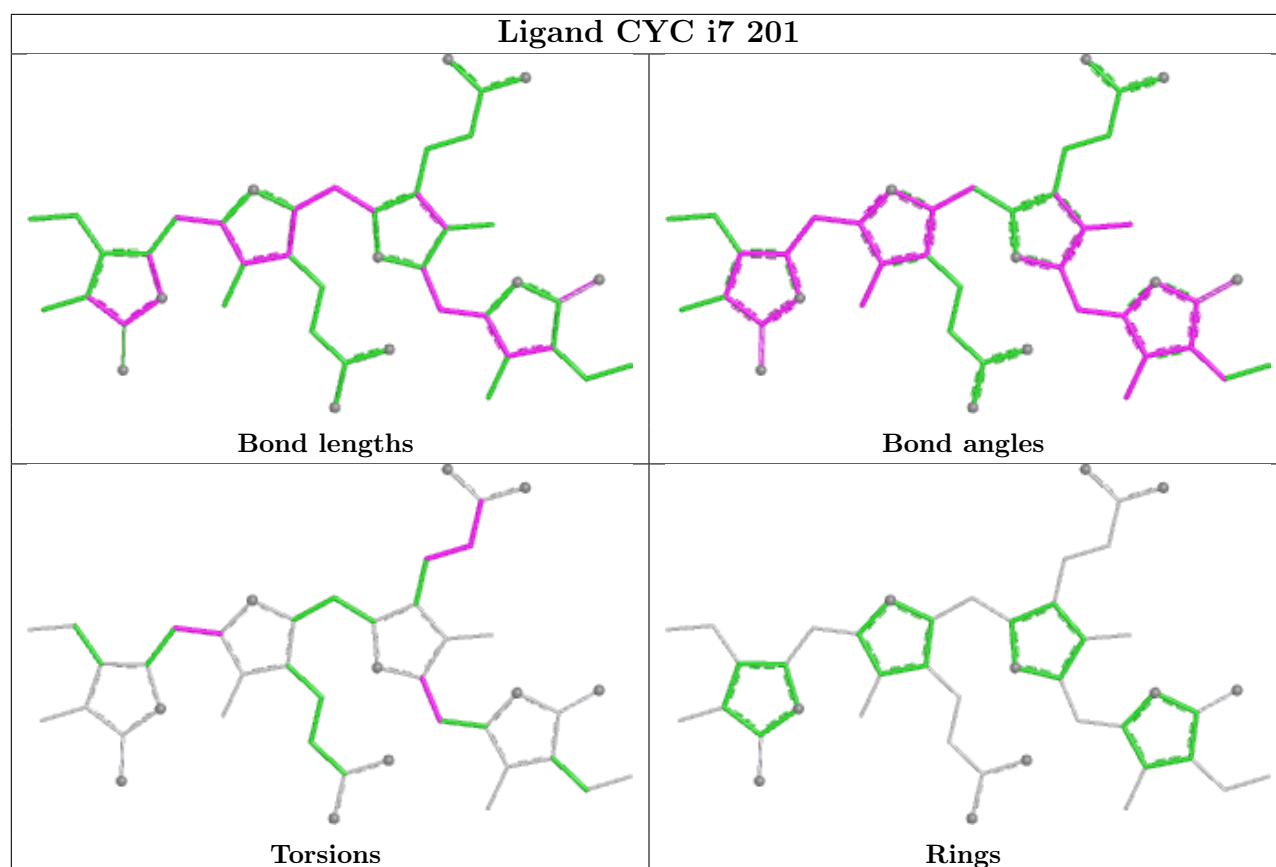


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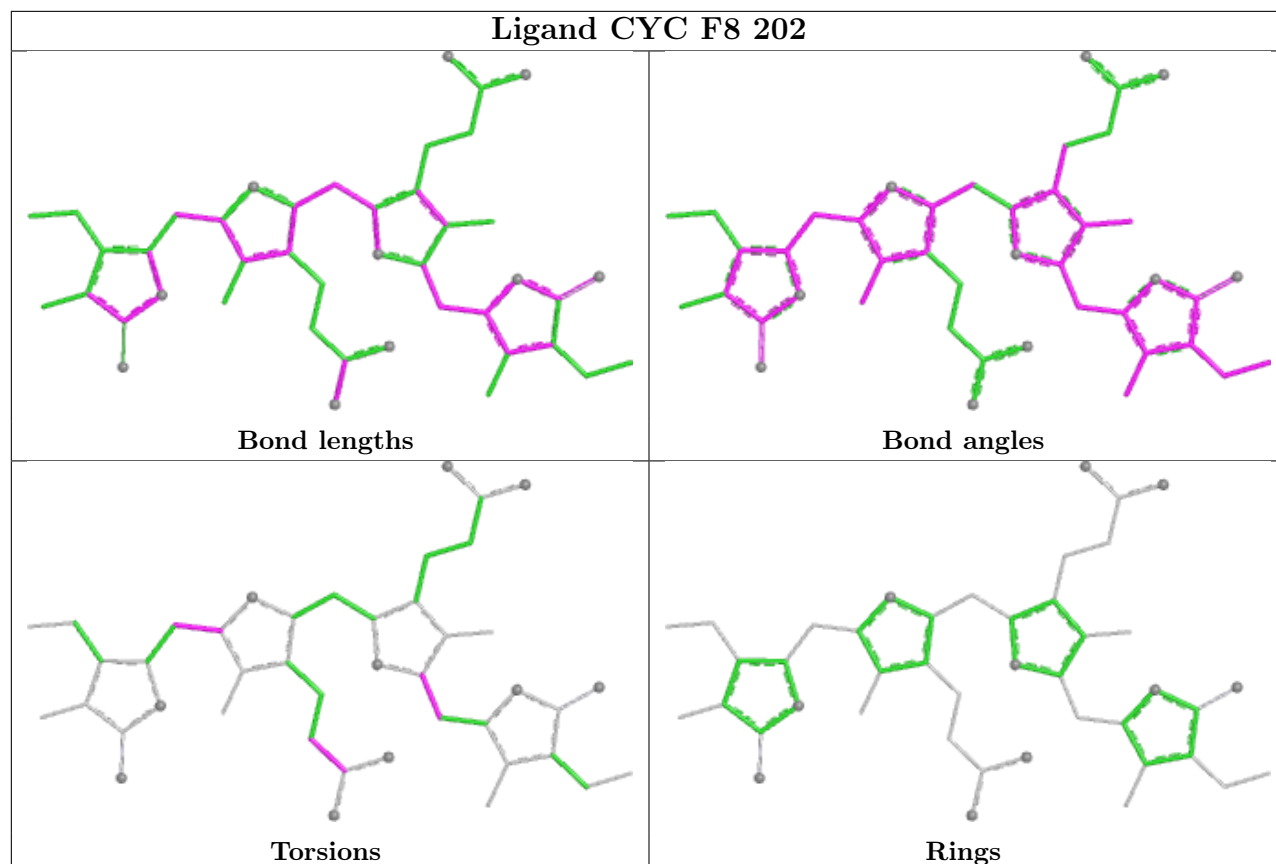


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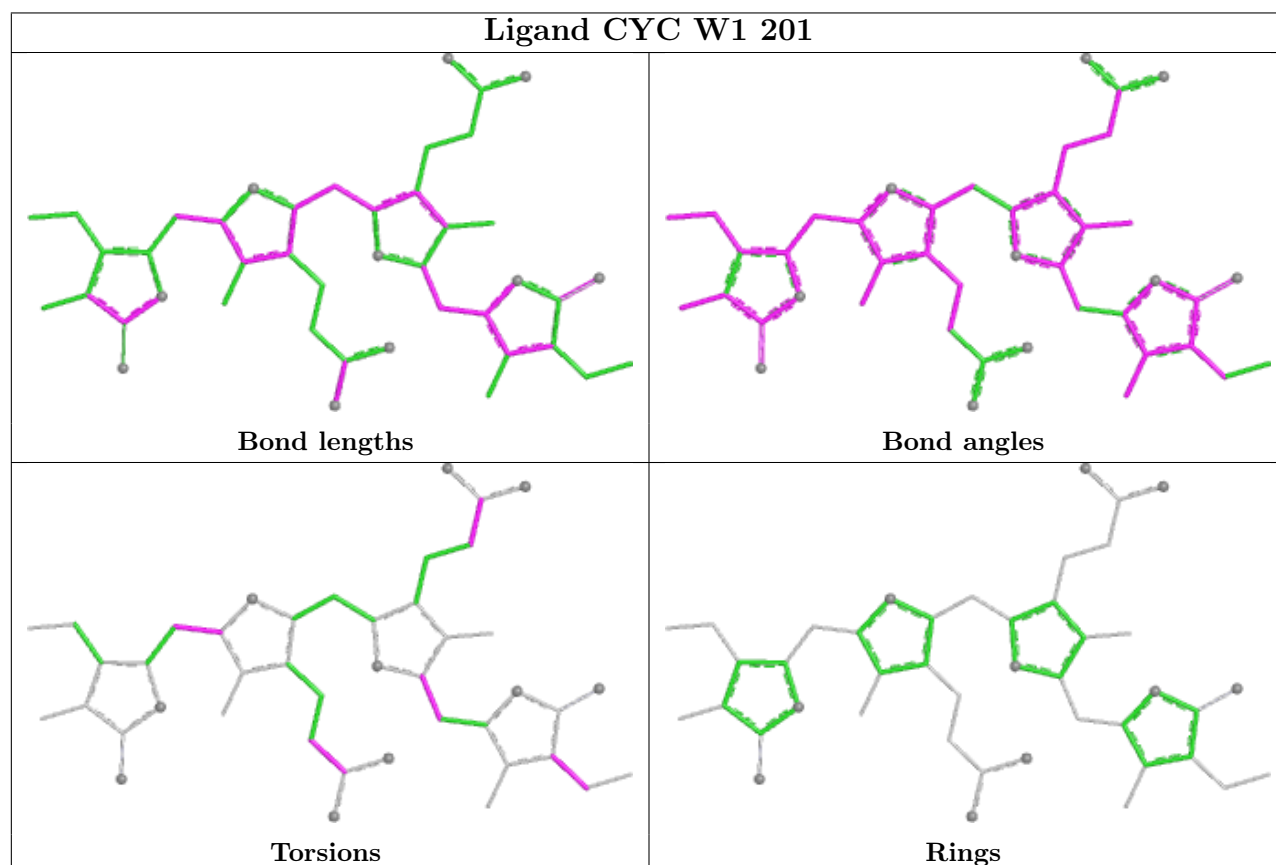




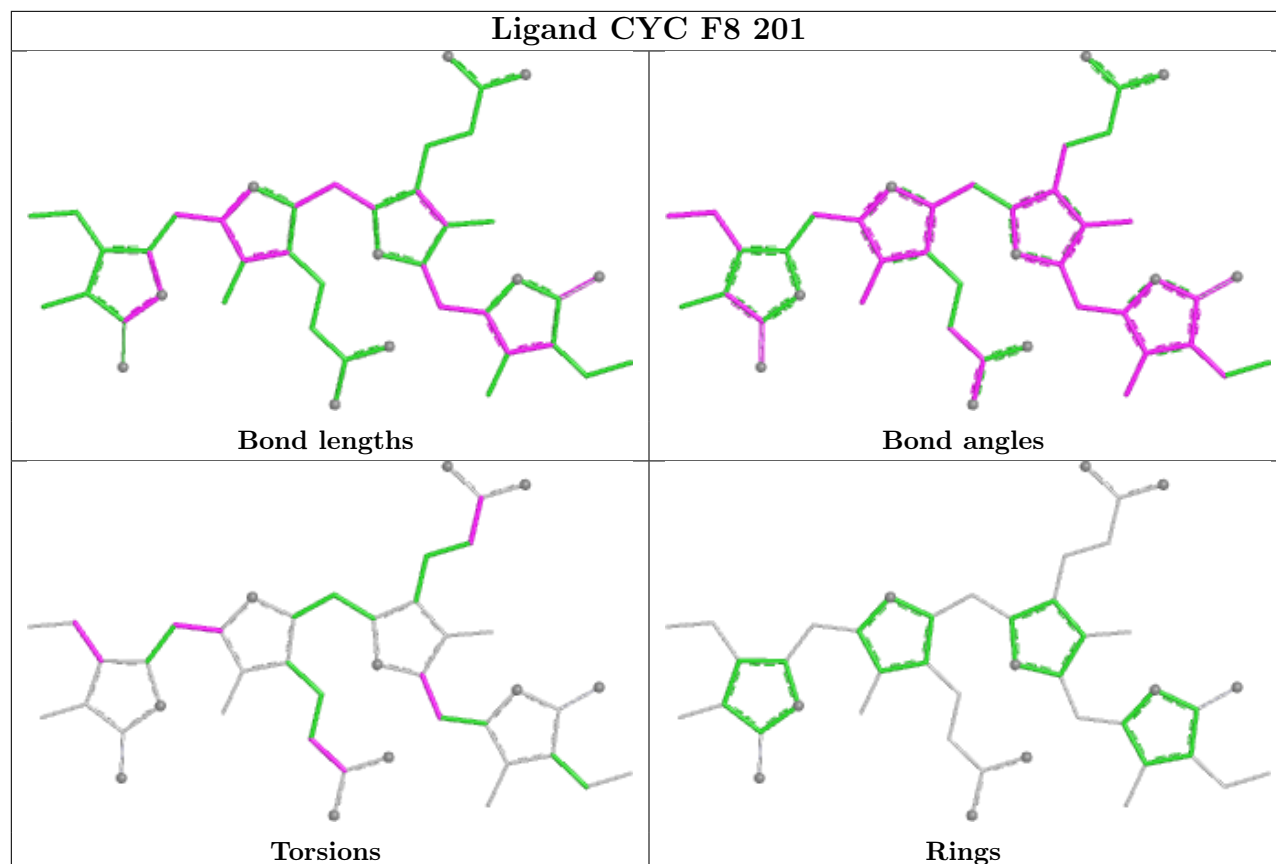
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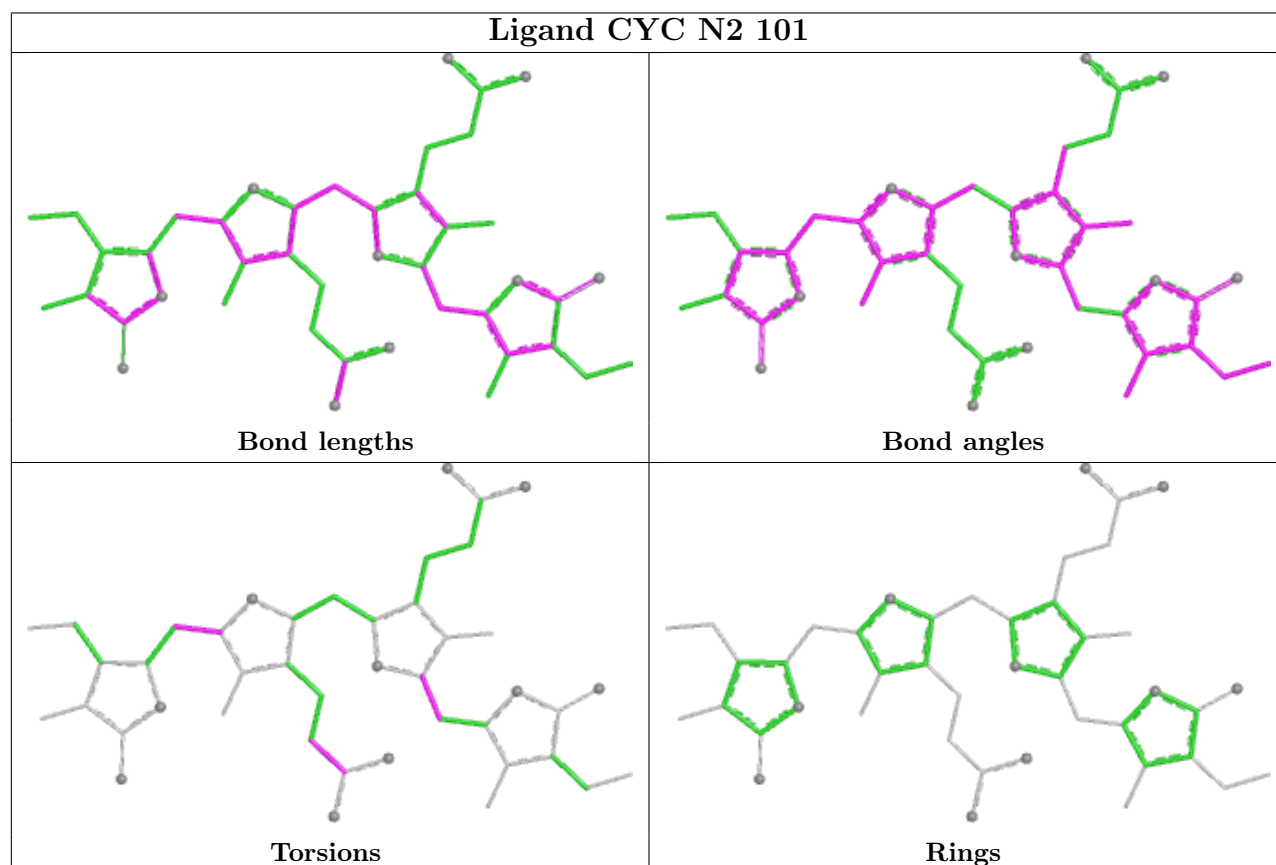
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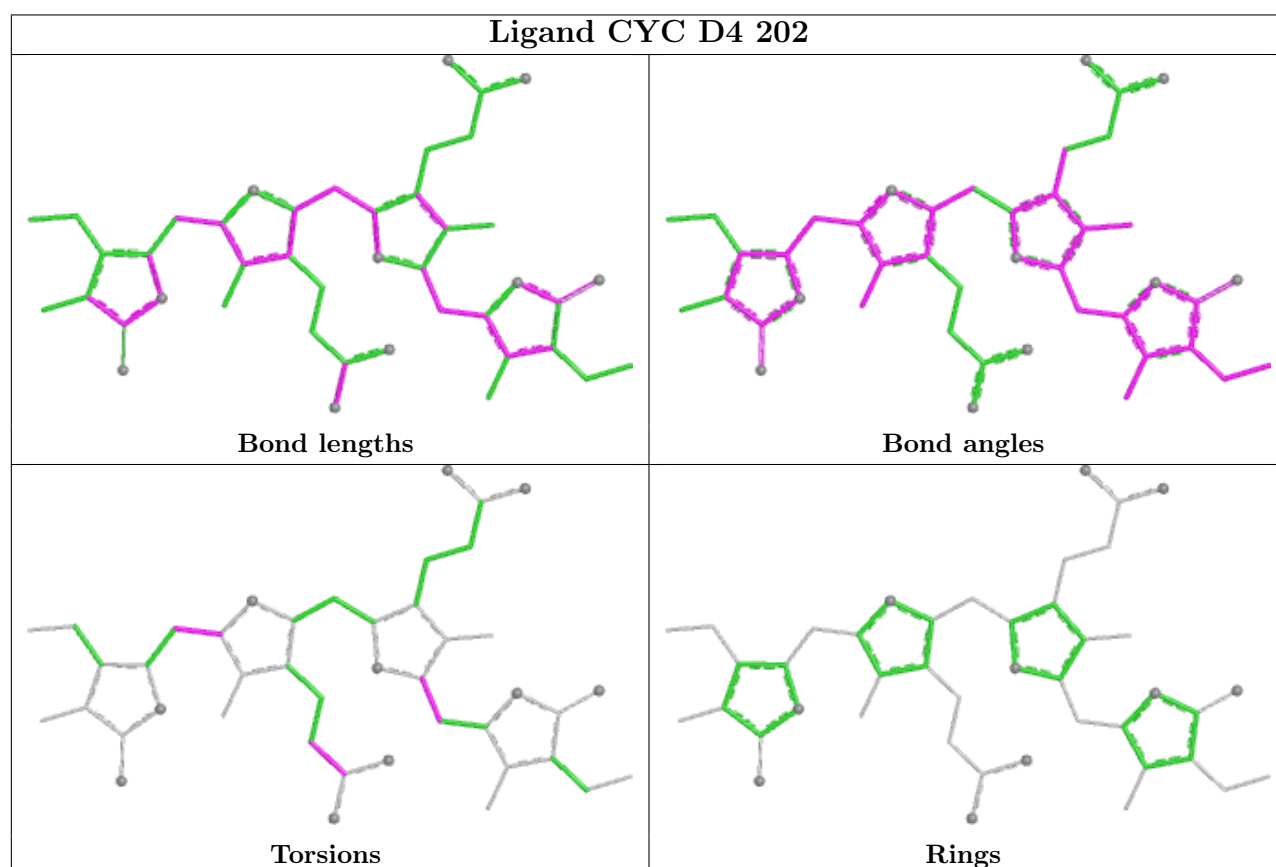
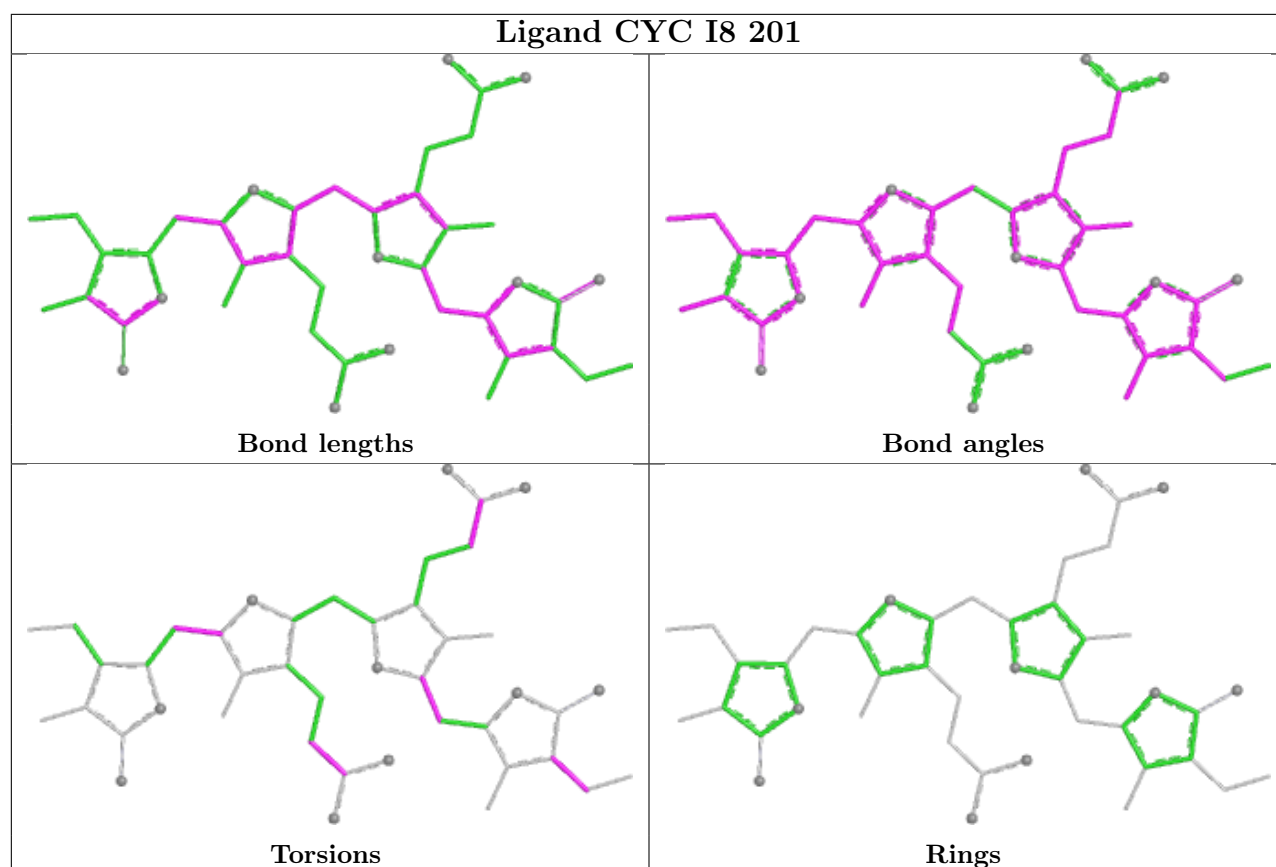


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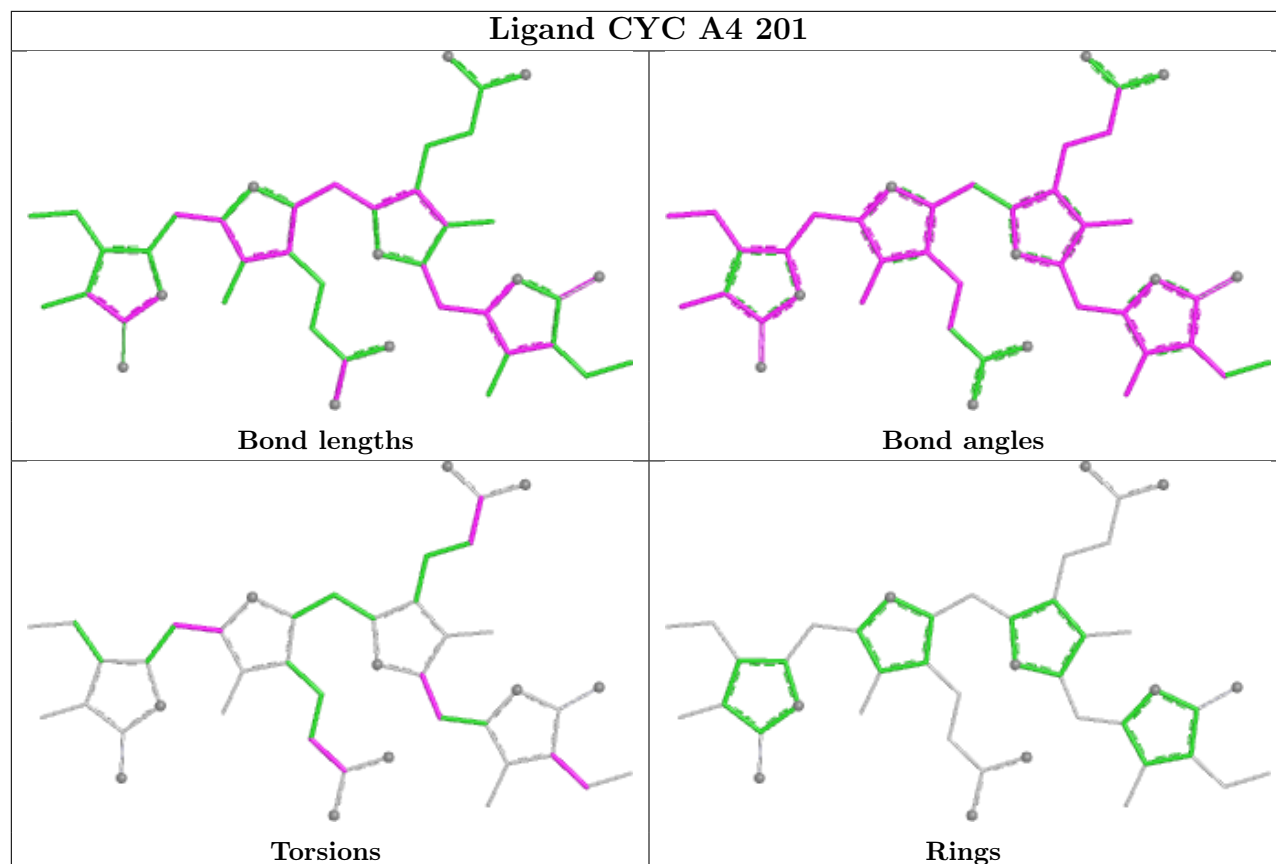


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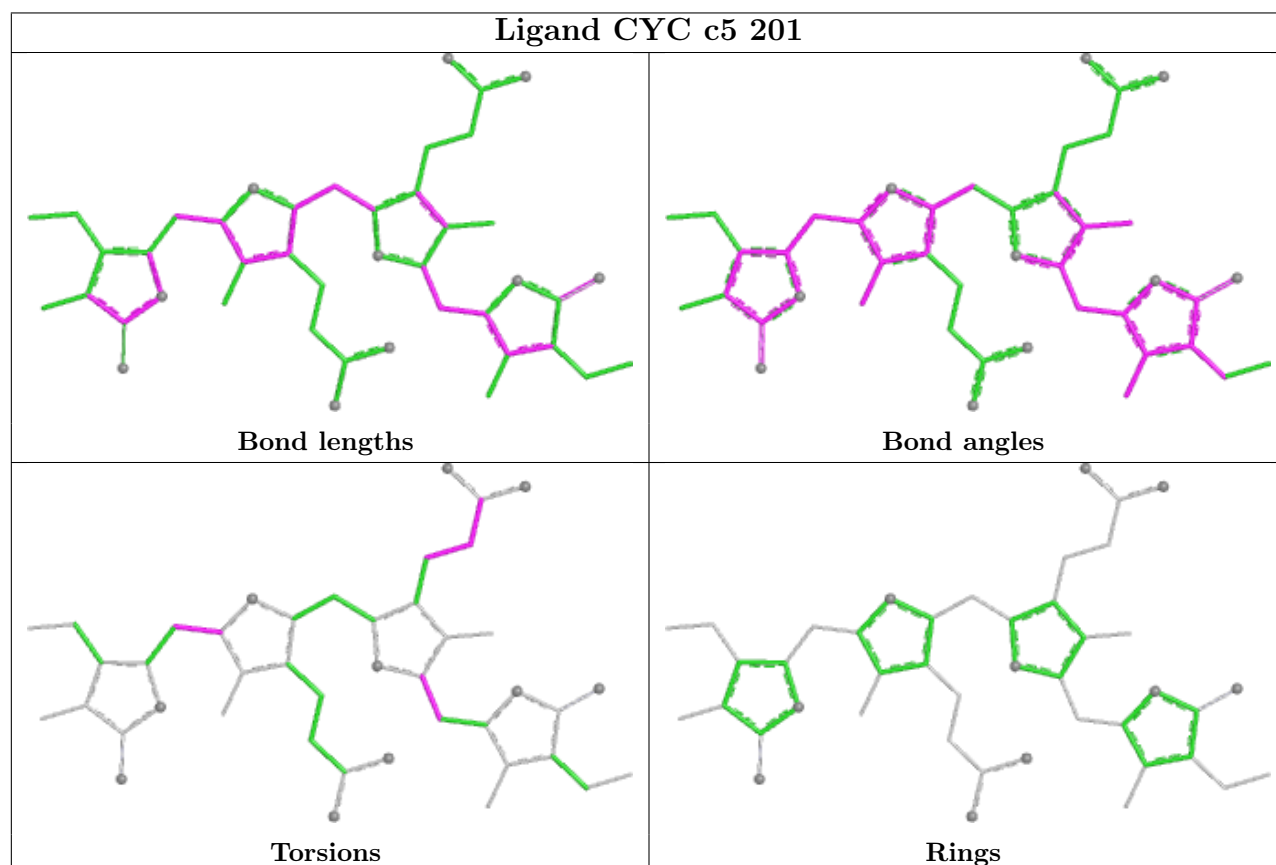




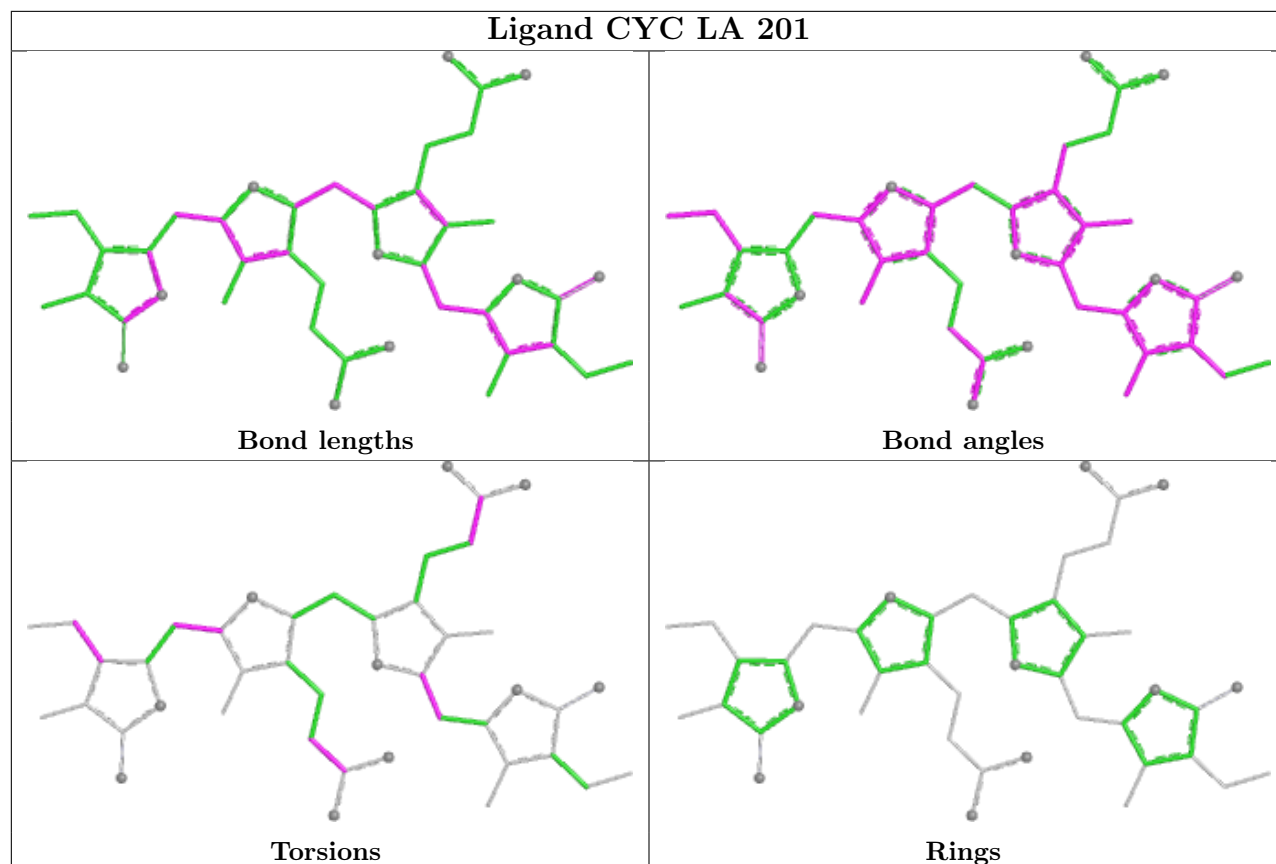
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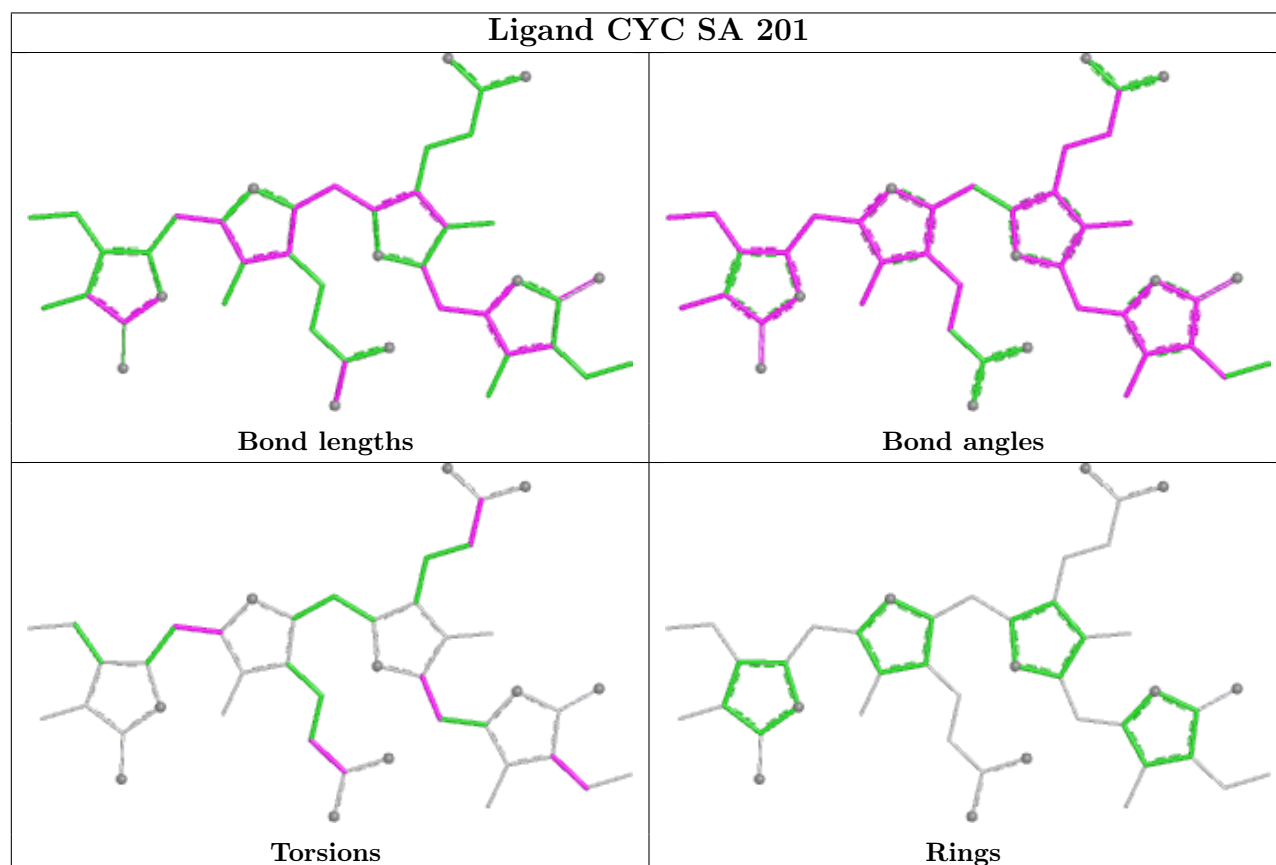
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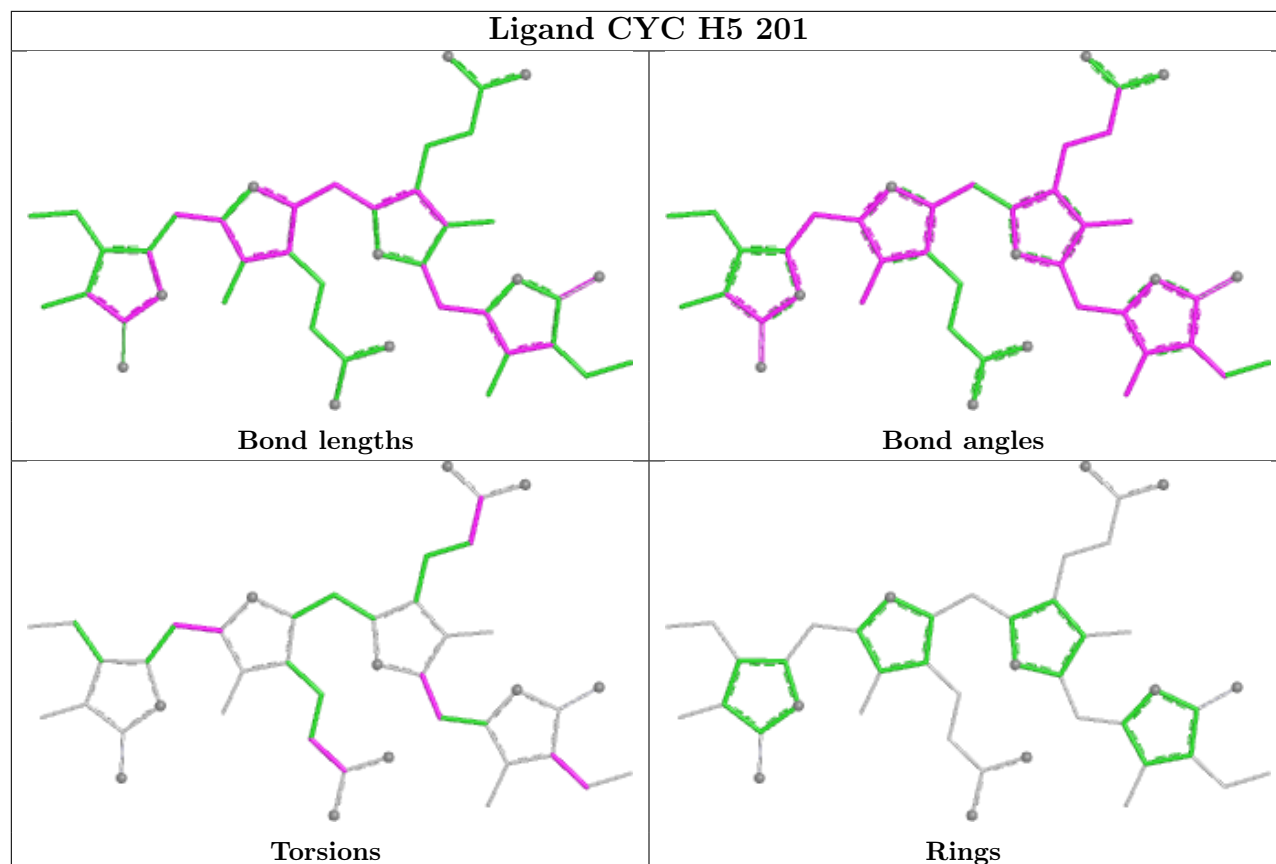
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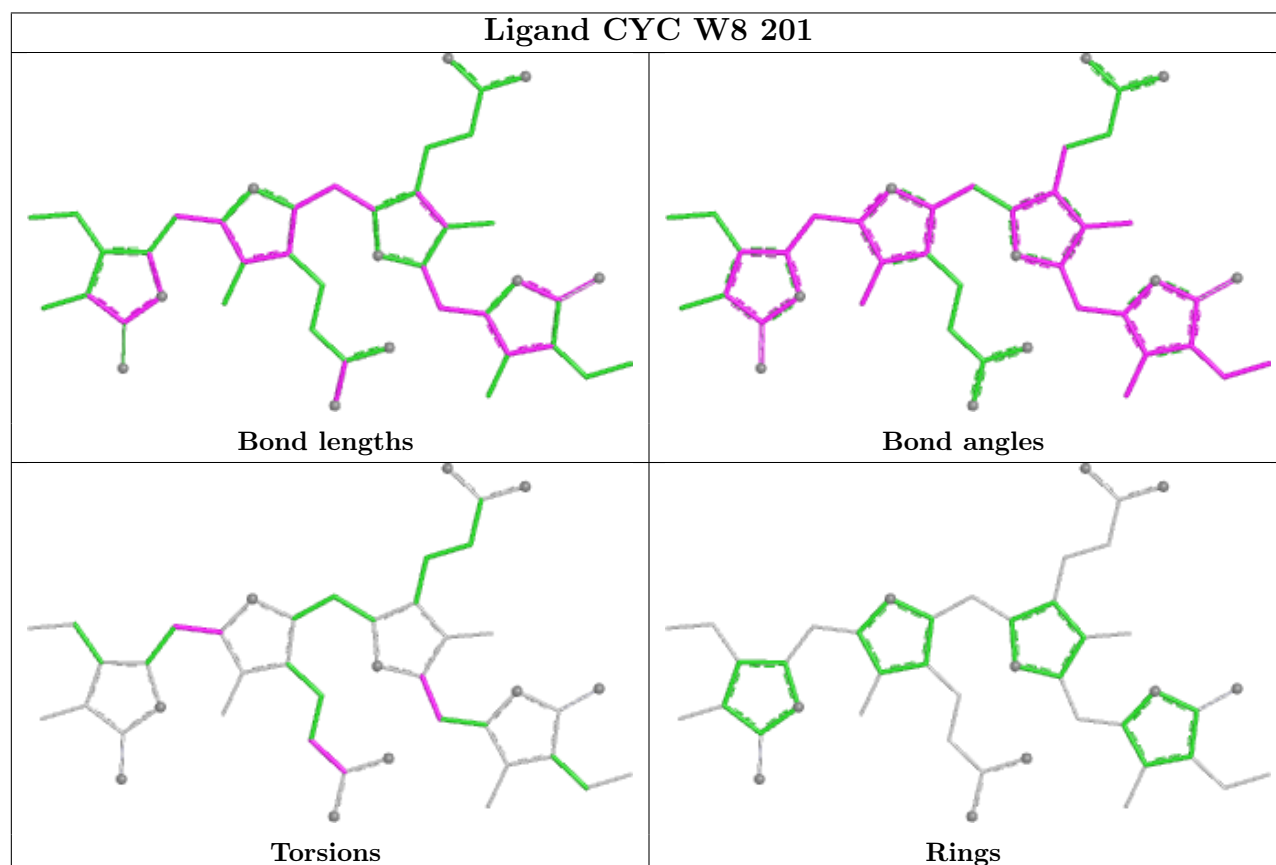
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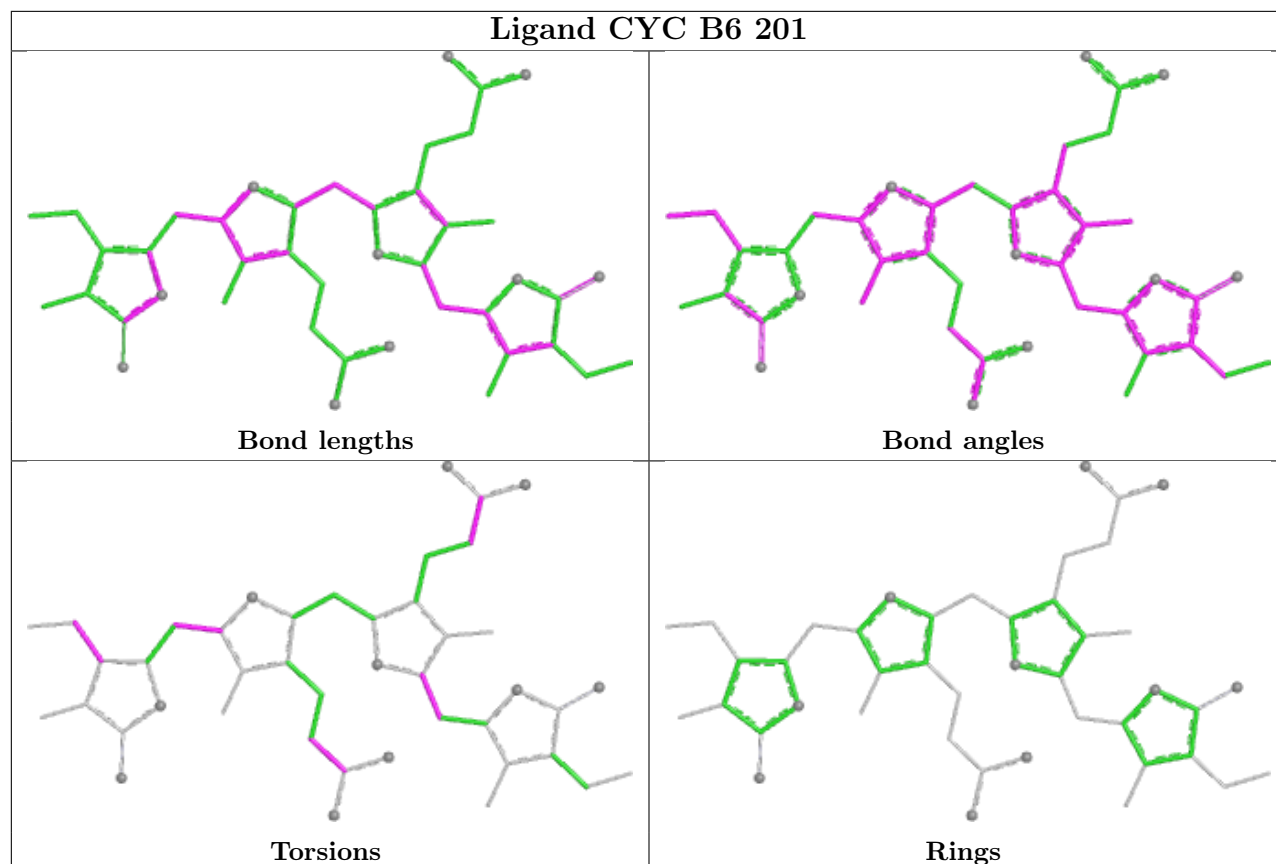
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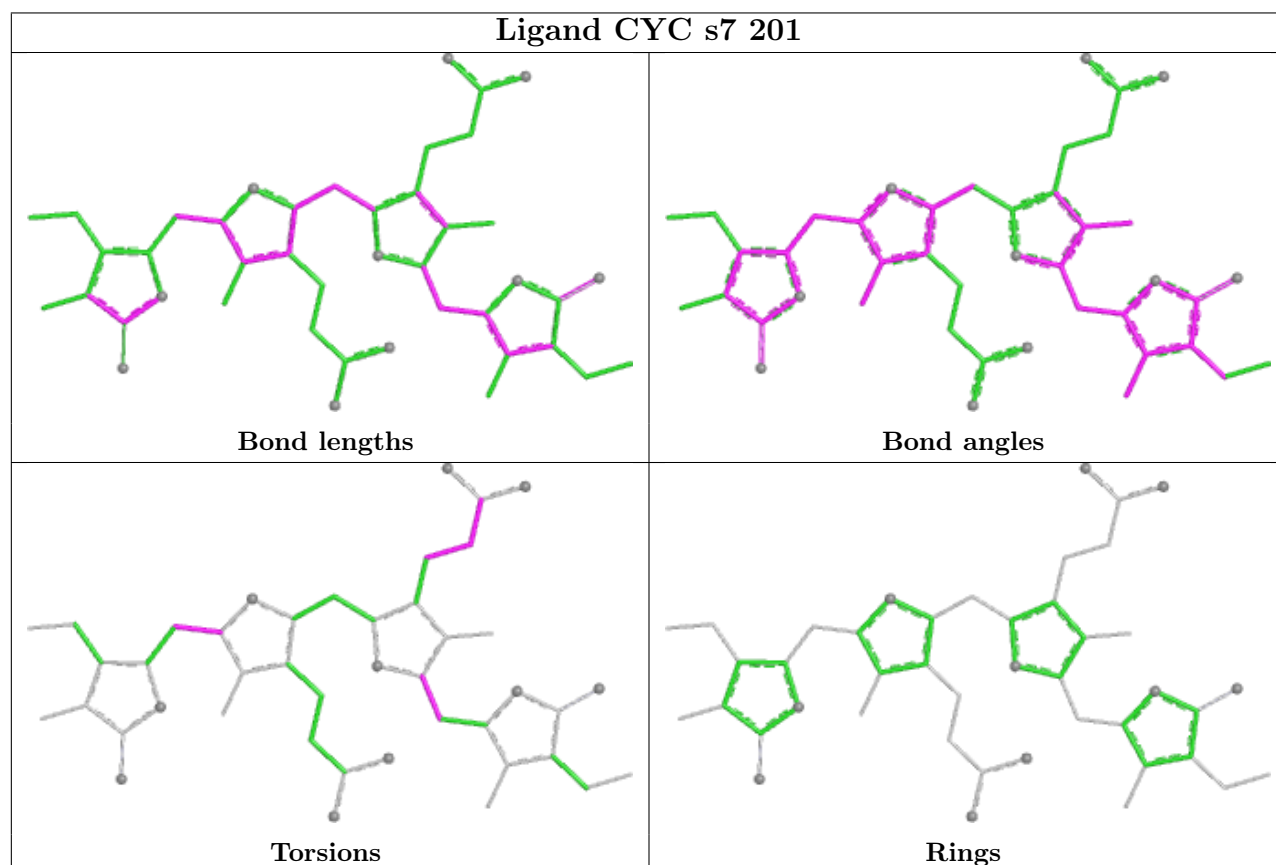
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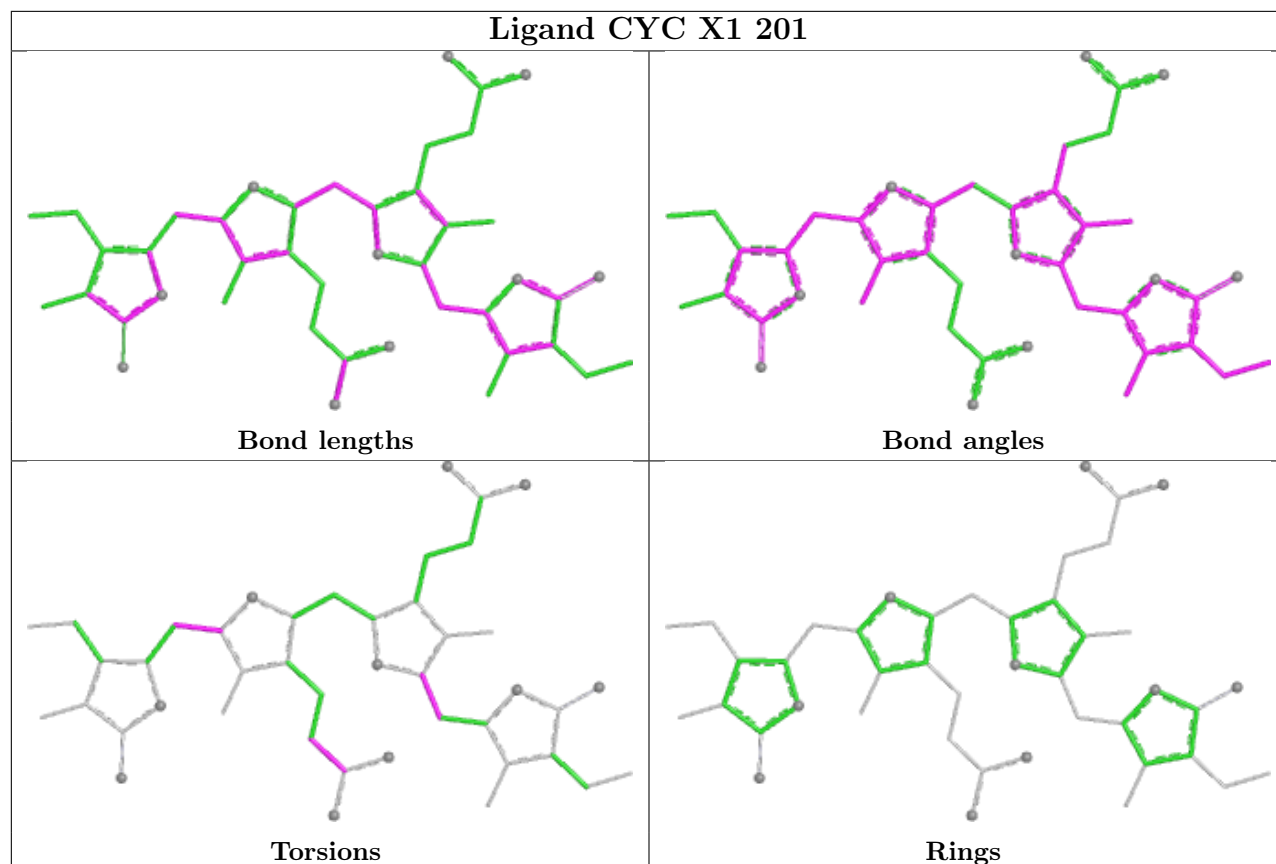
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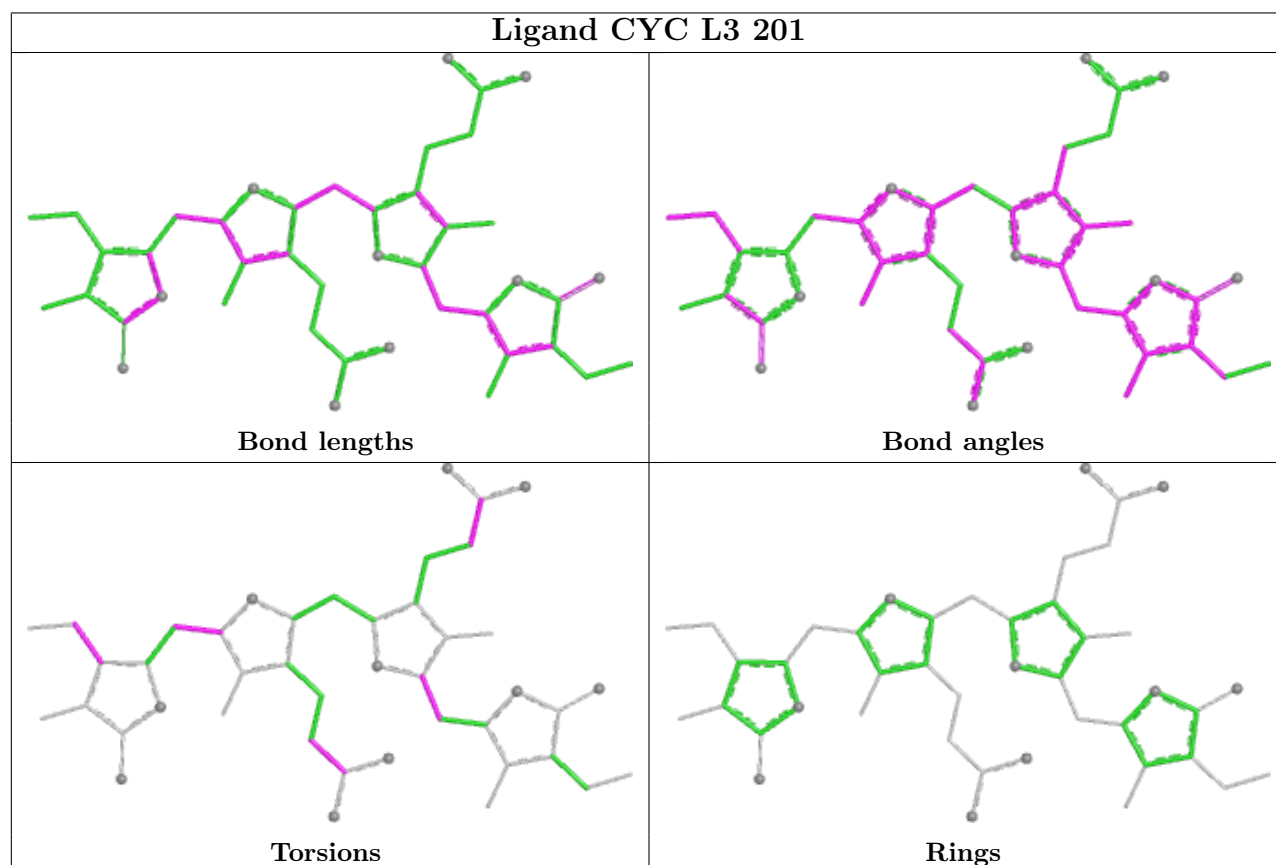
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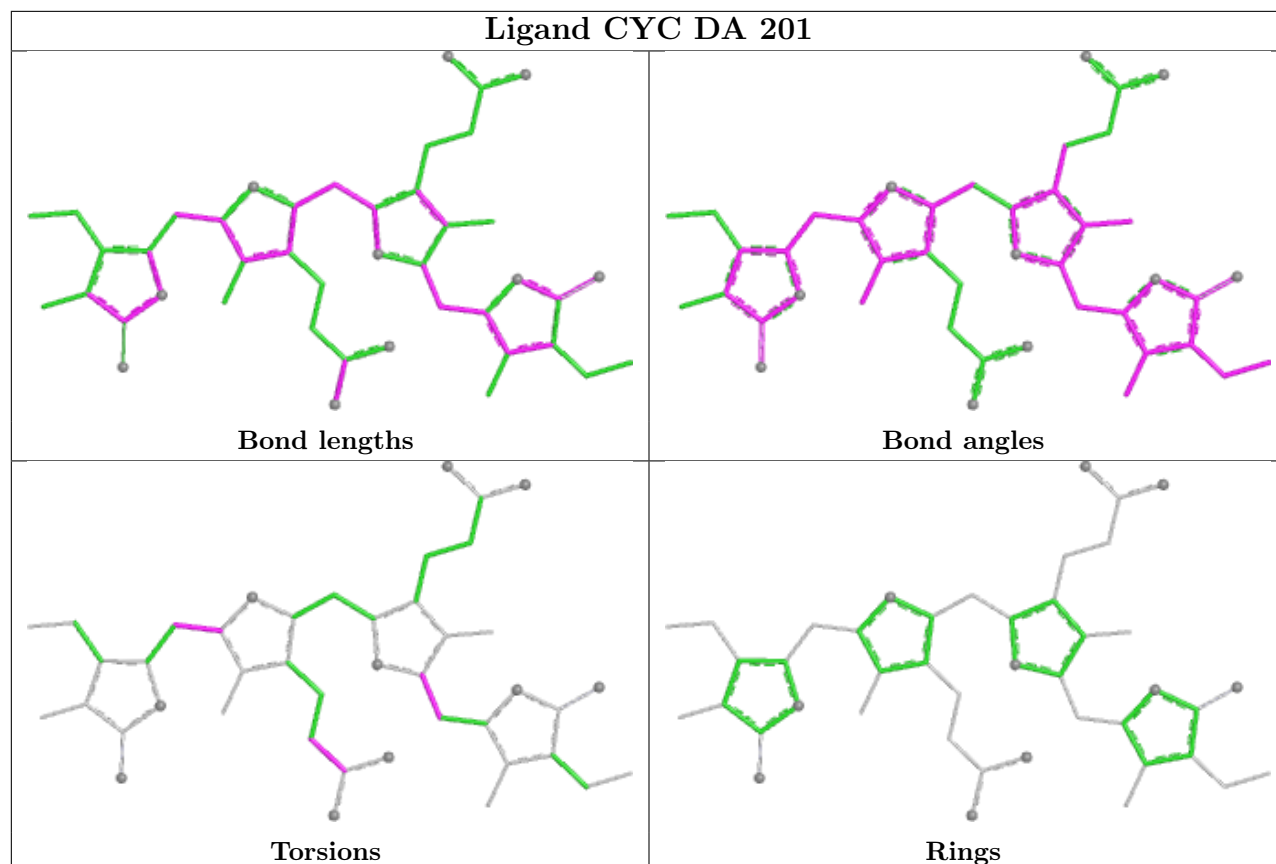
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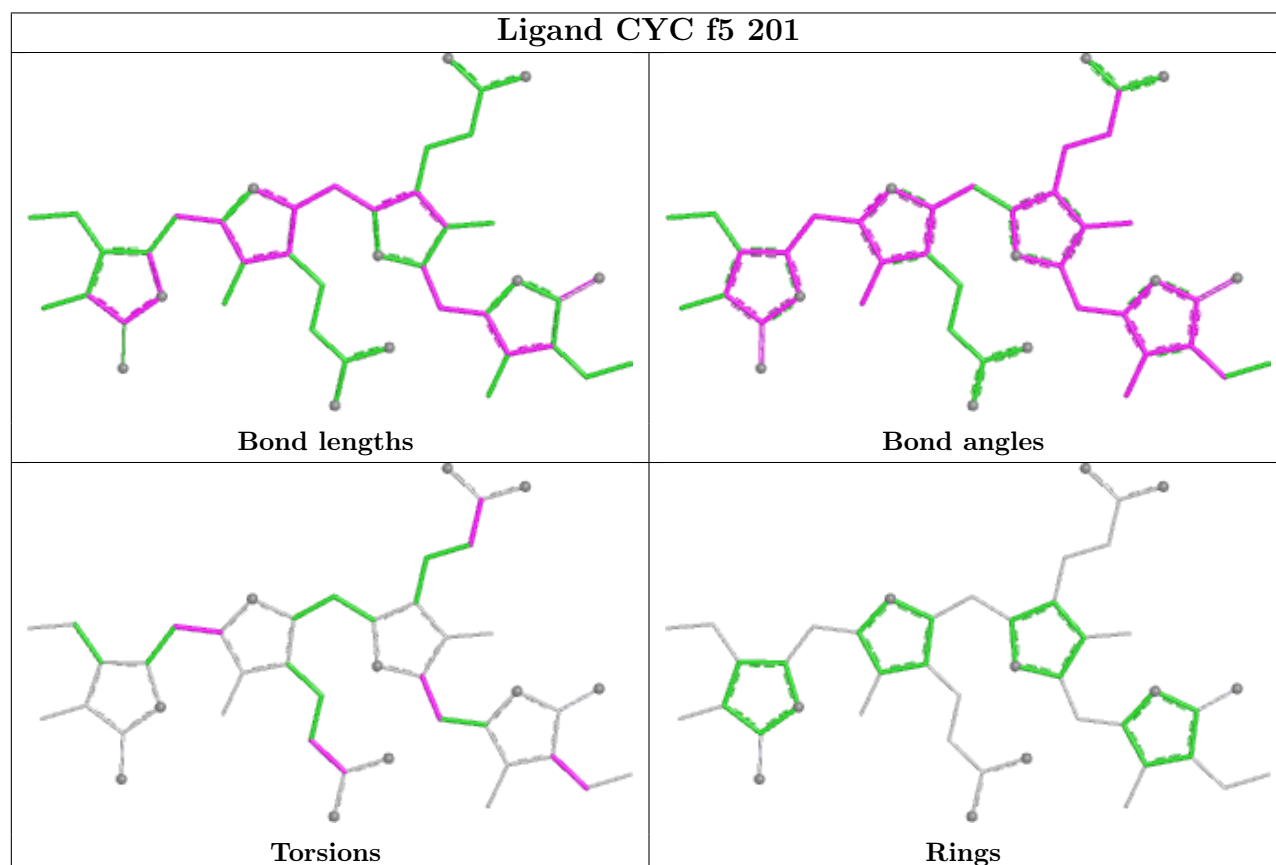
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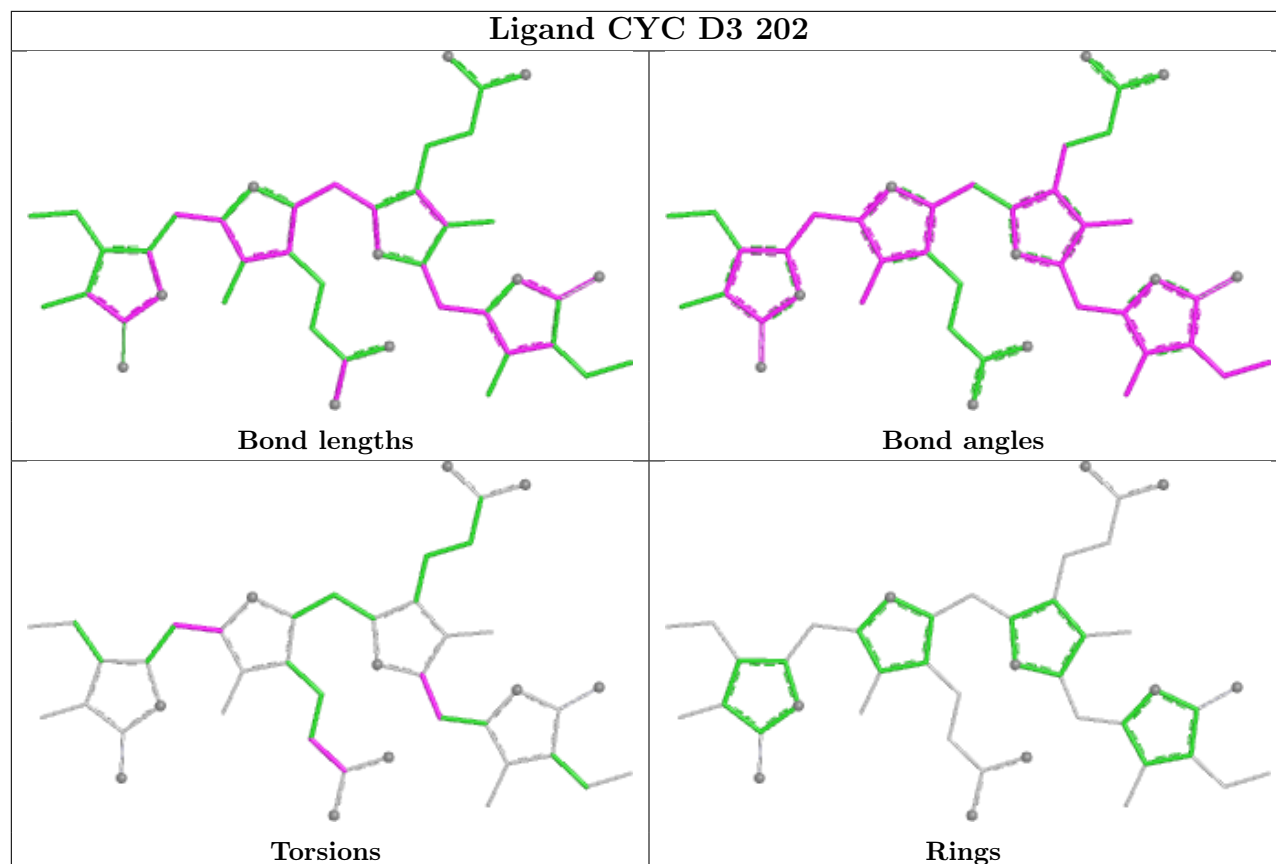
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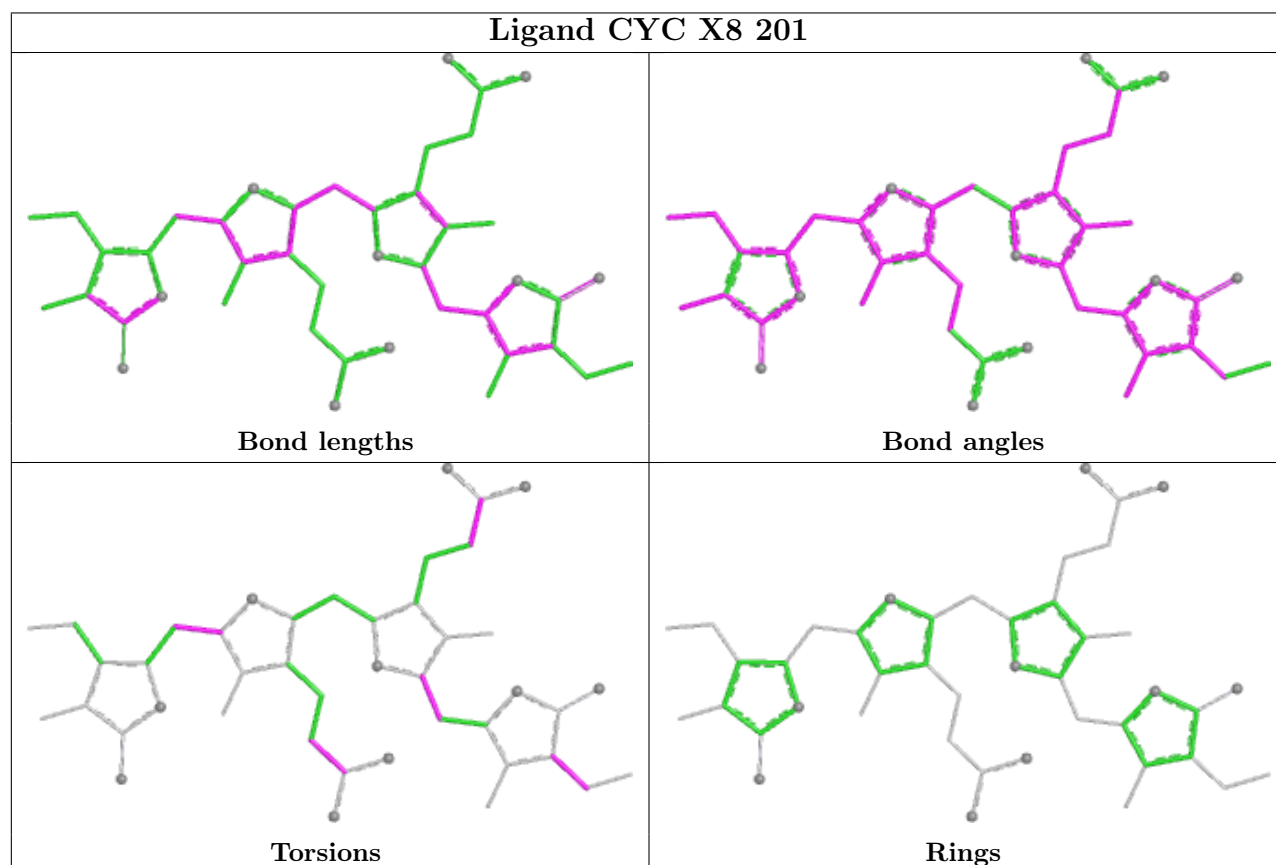
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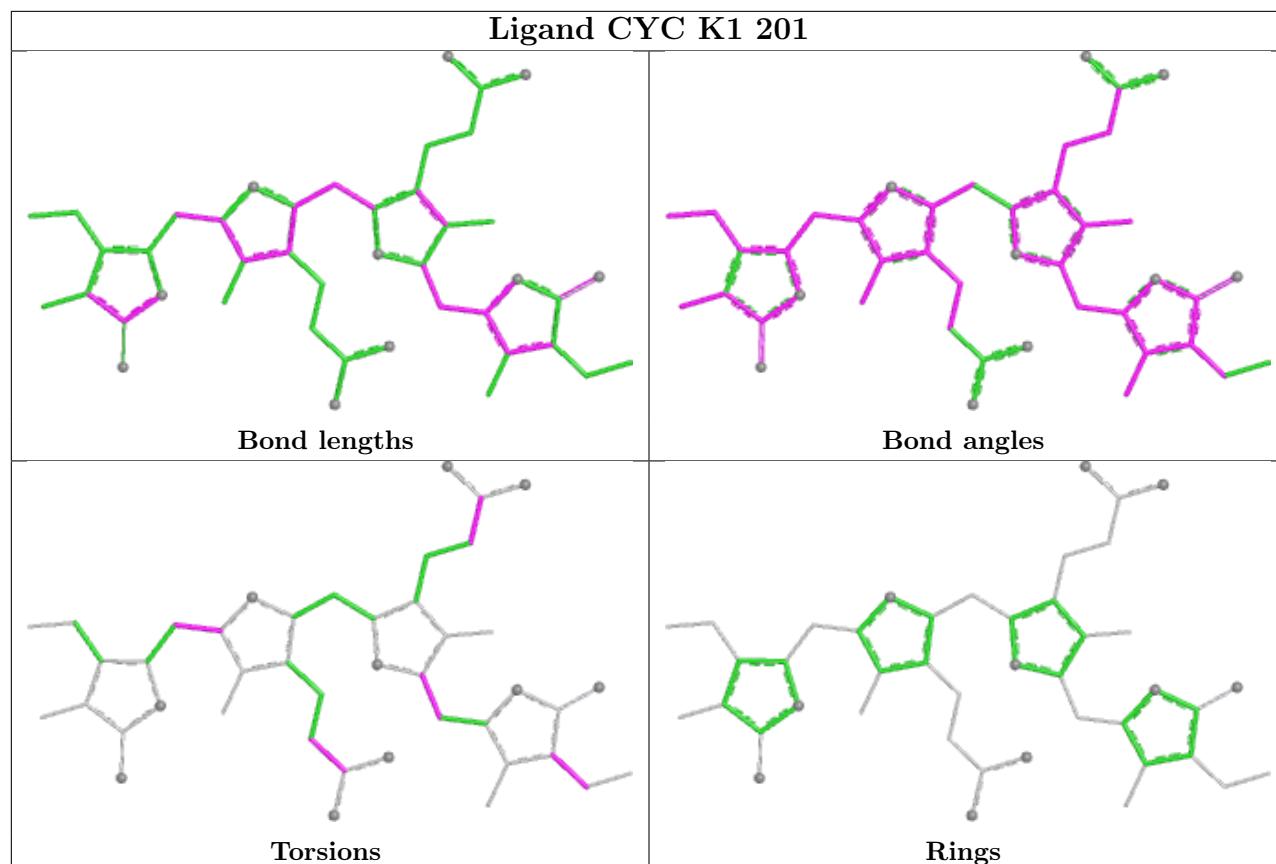
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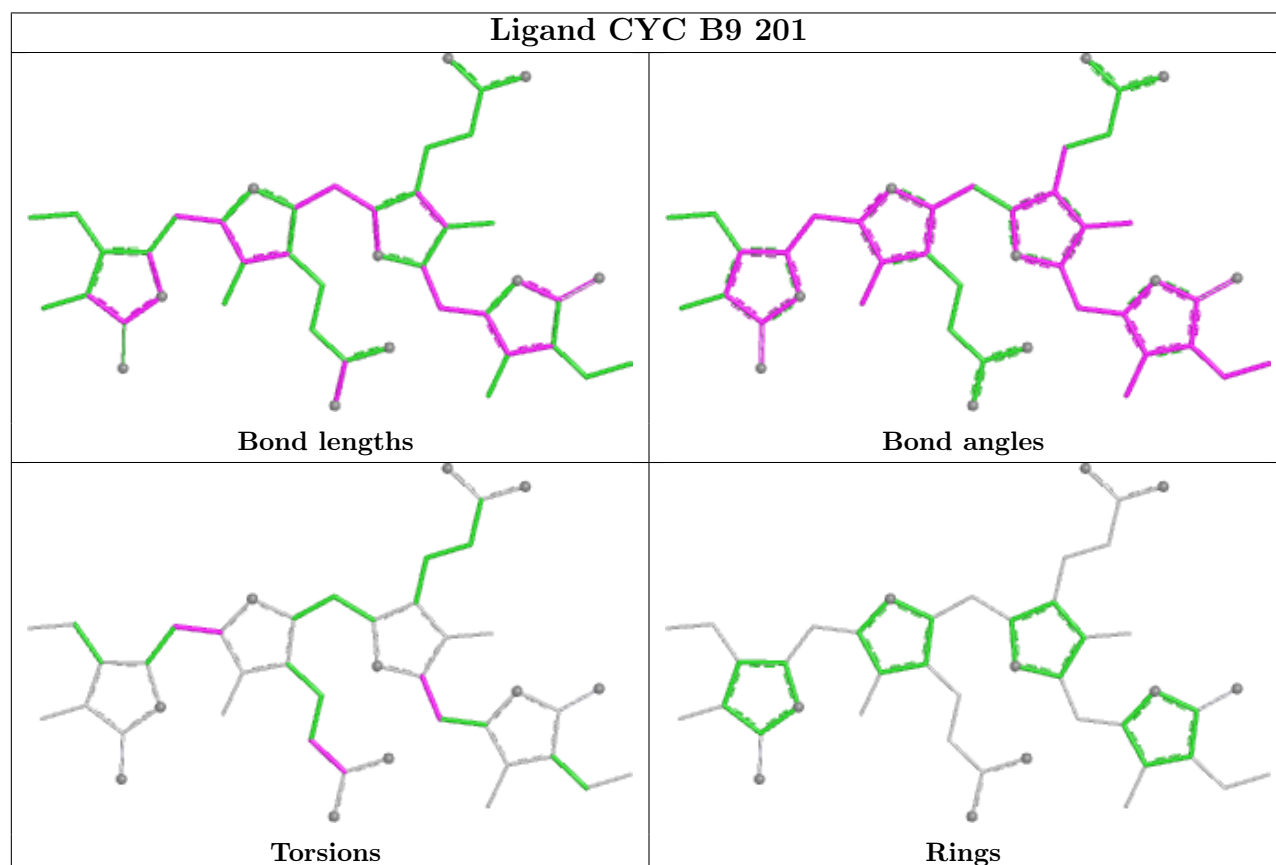
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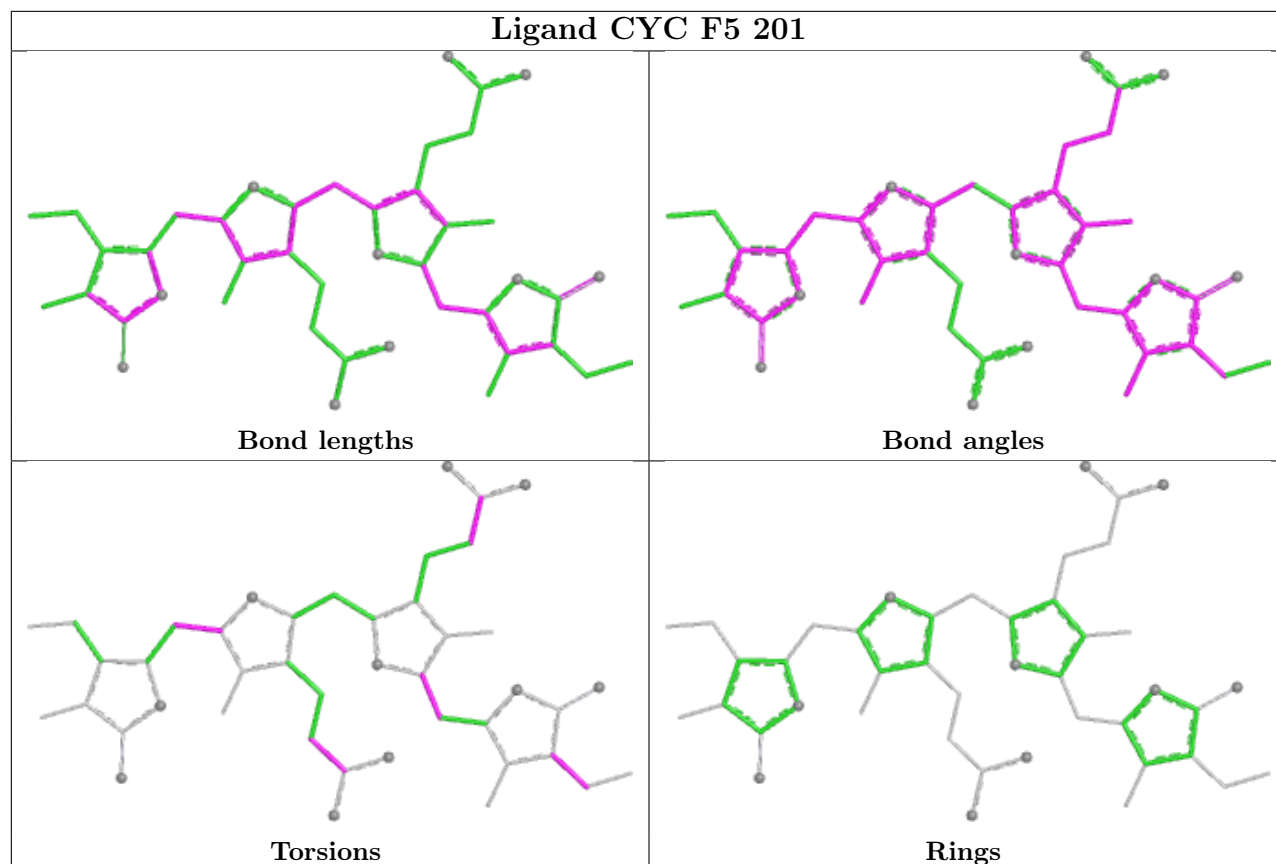
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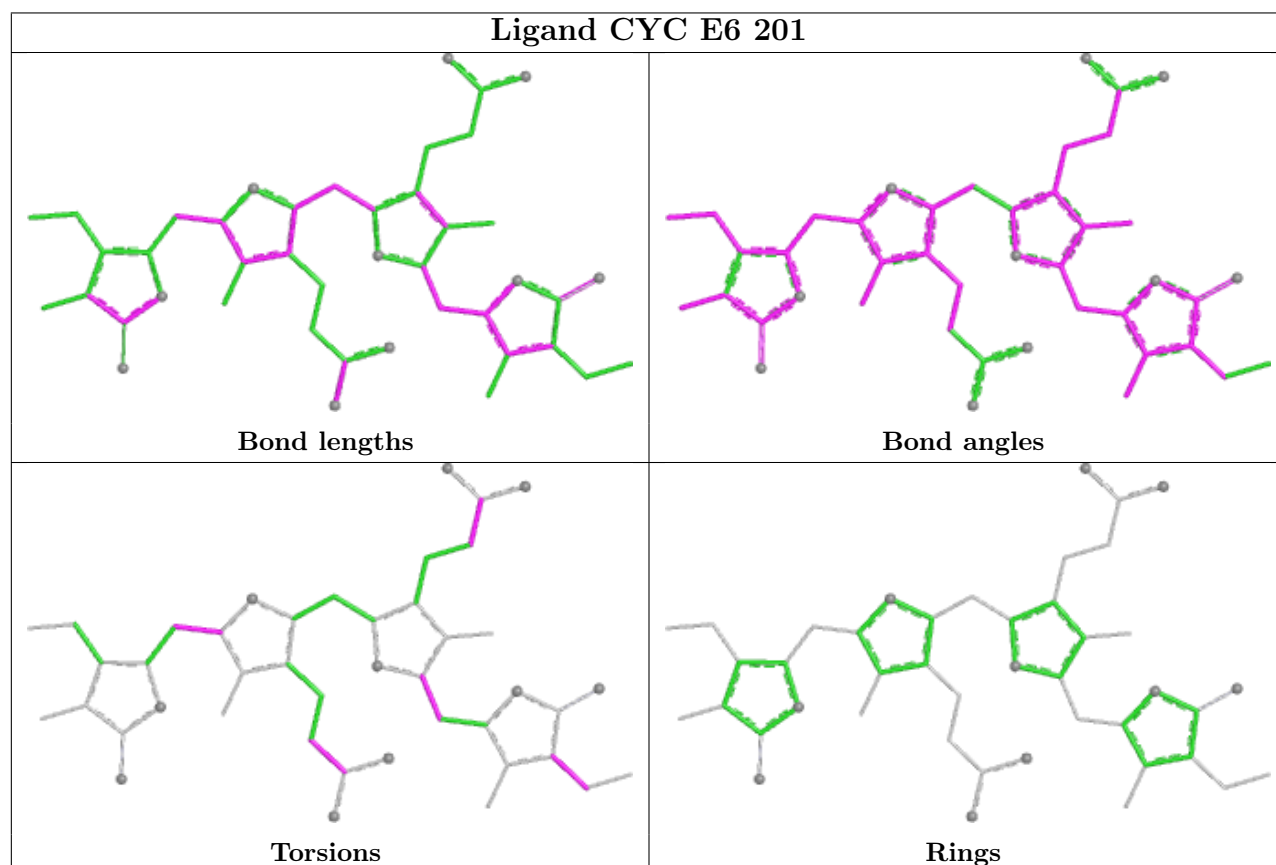
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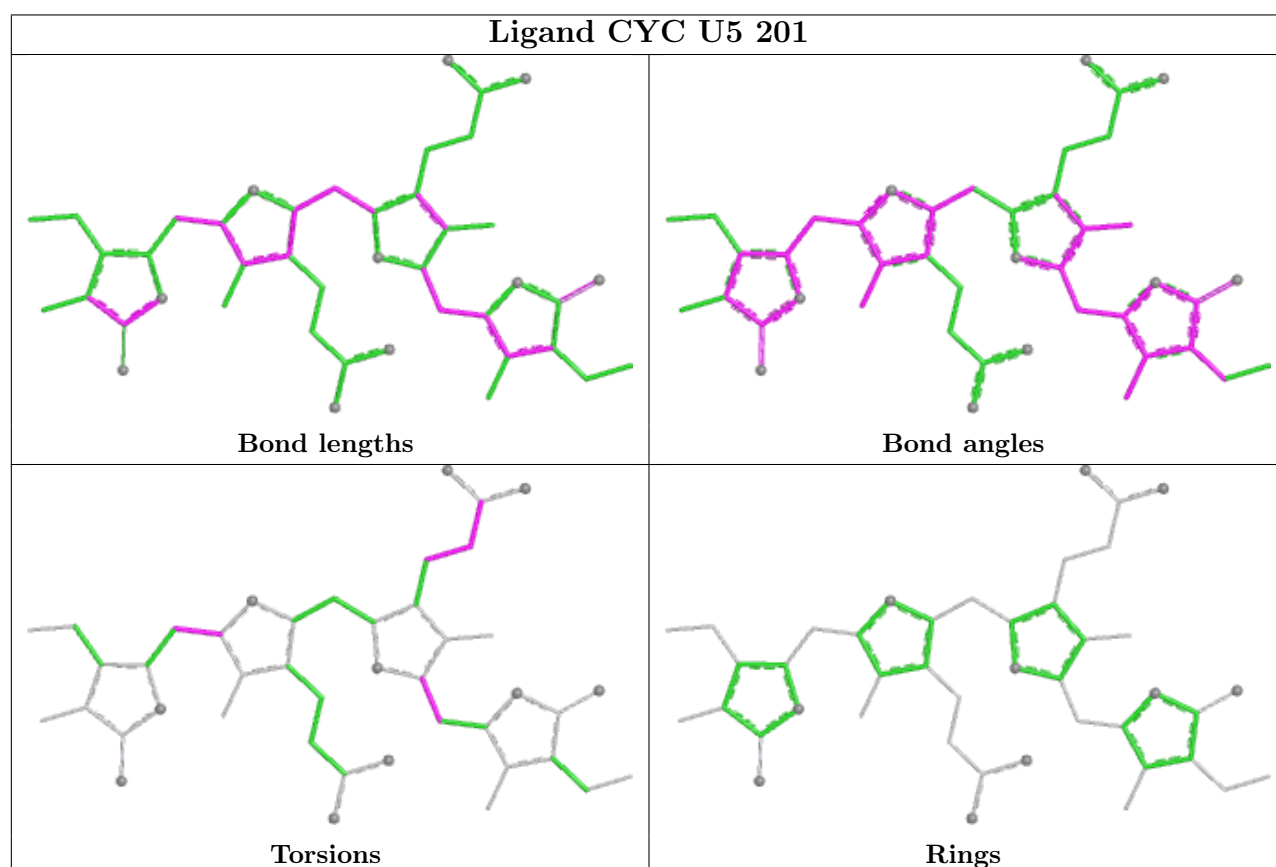
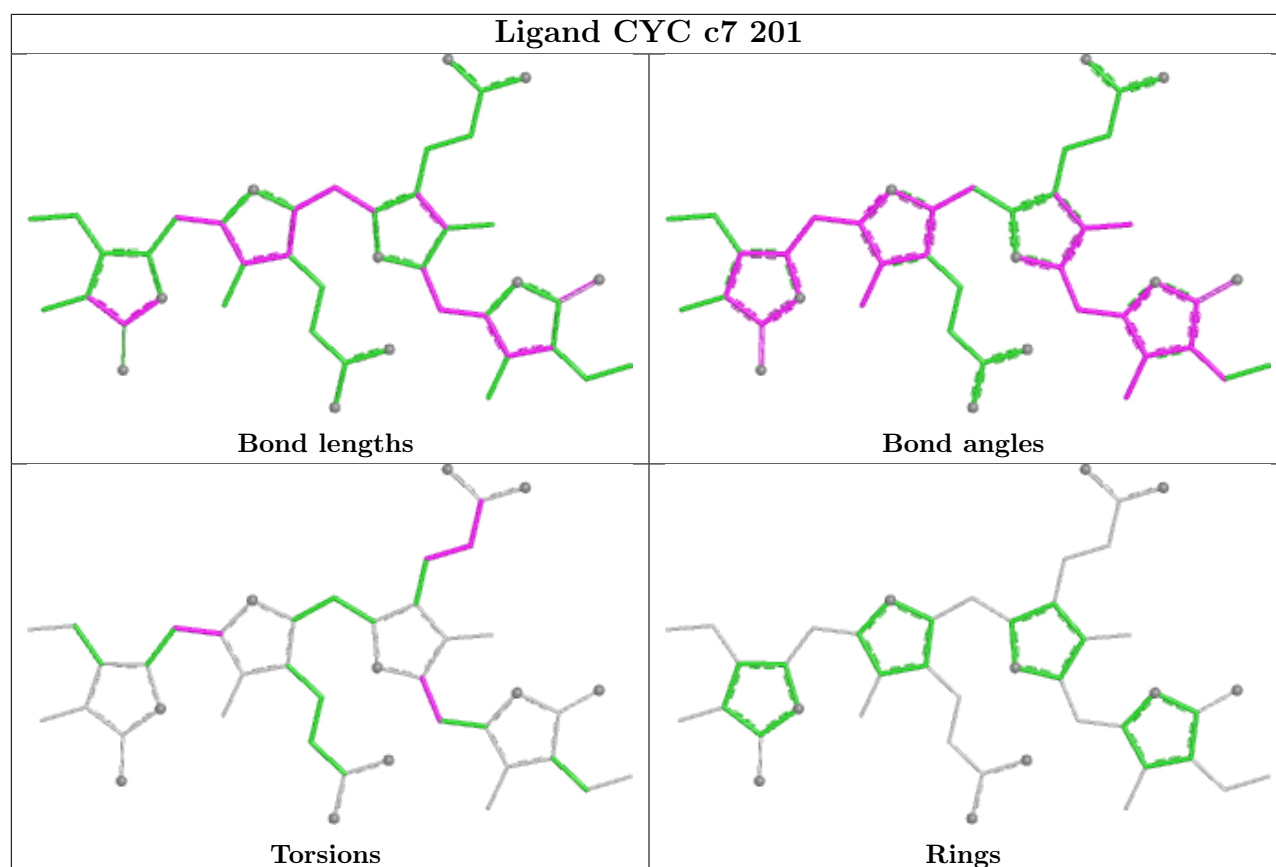


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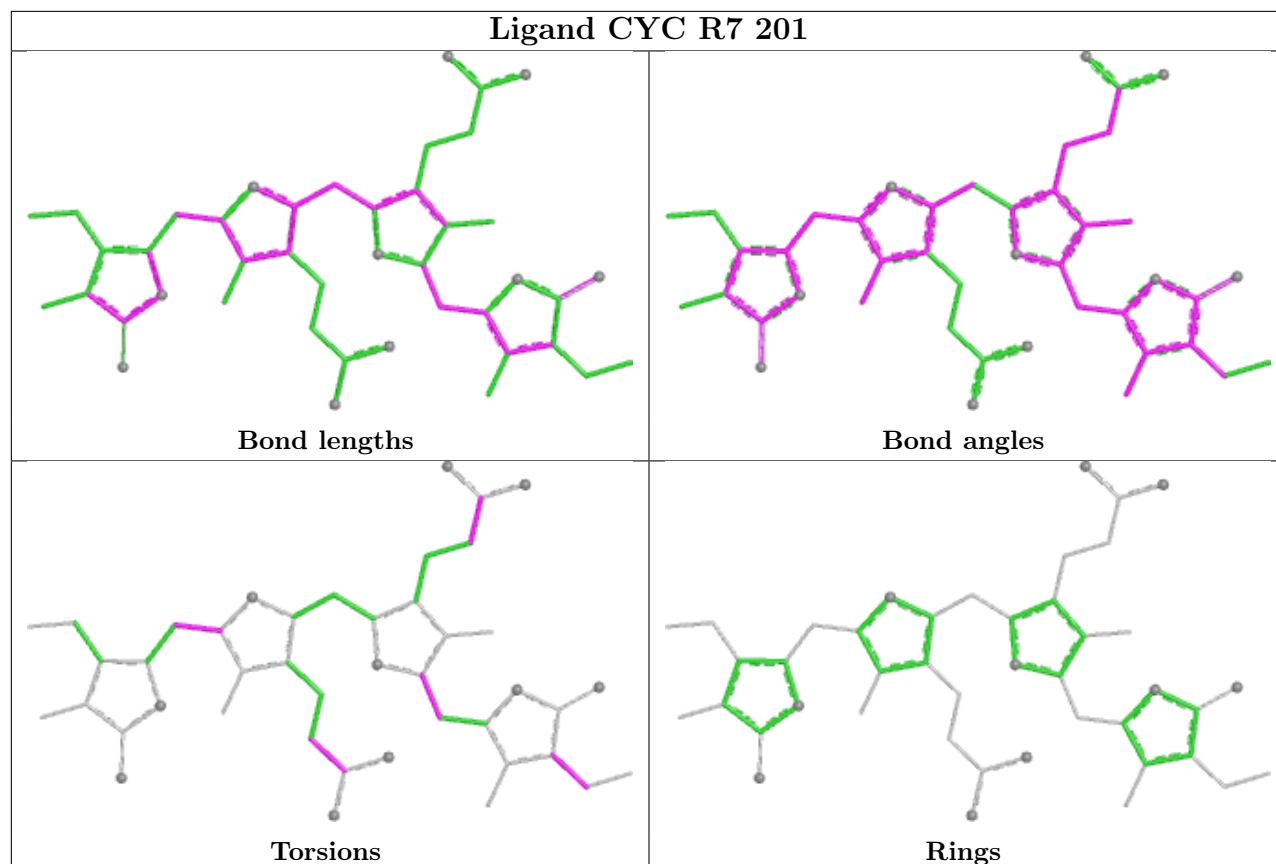


Ligand CYC E6 201

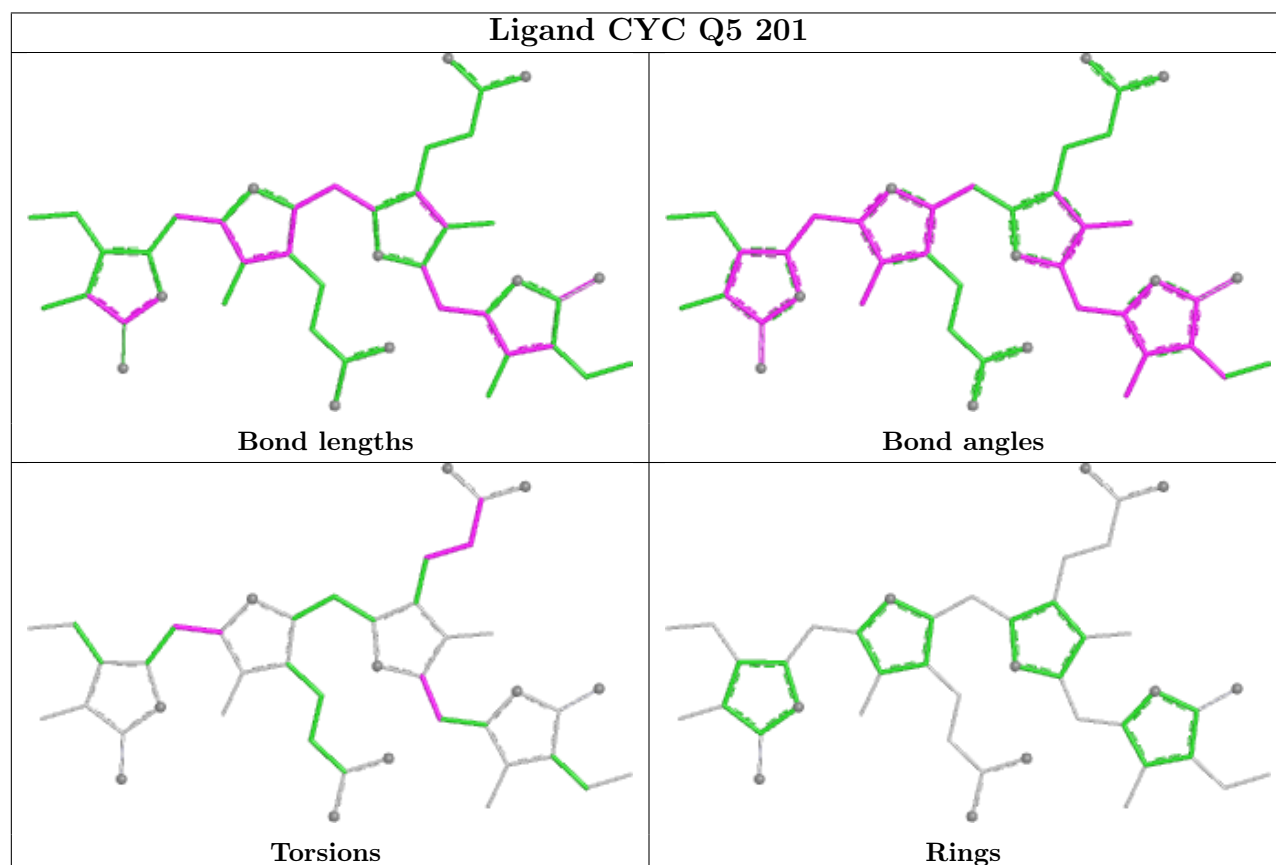




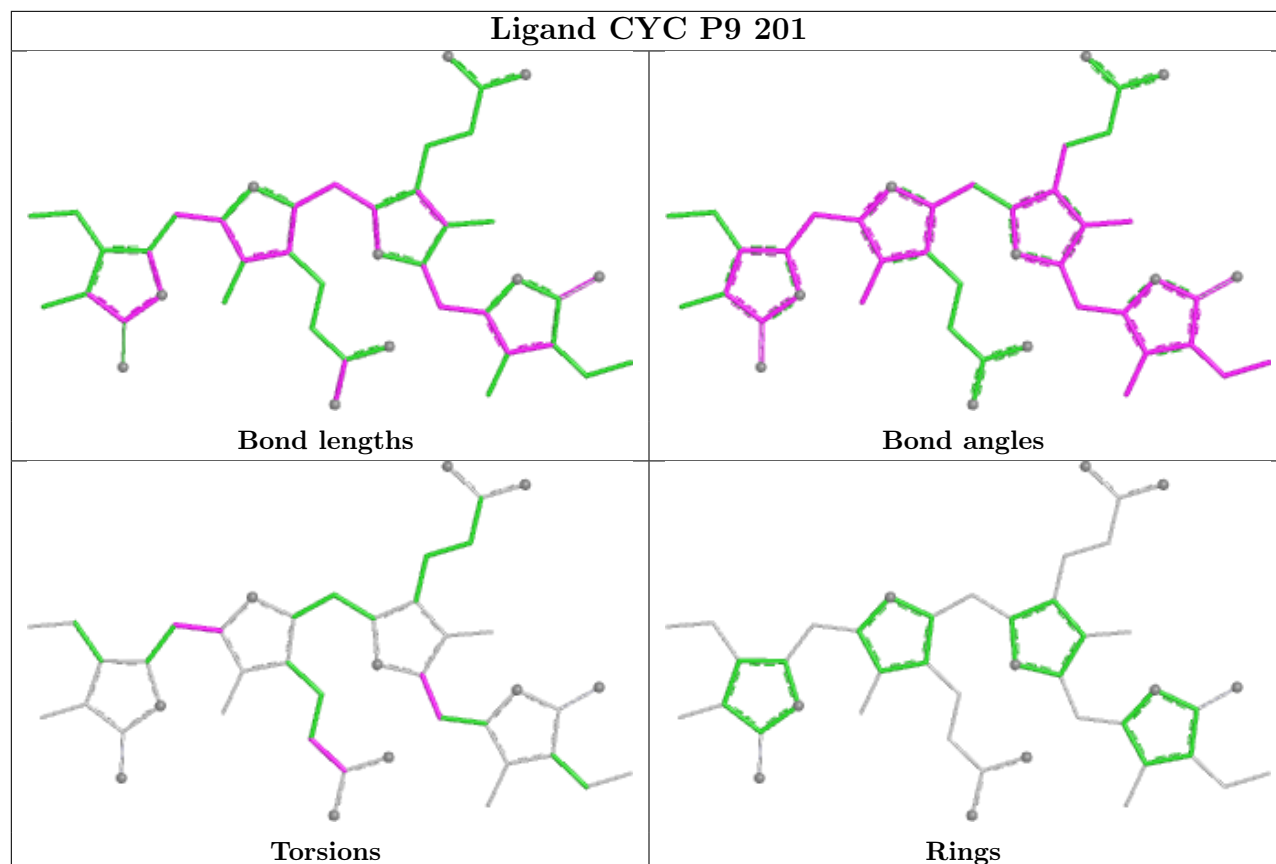
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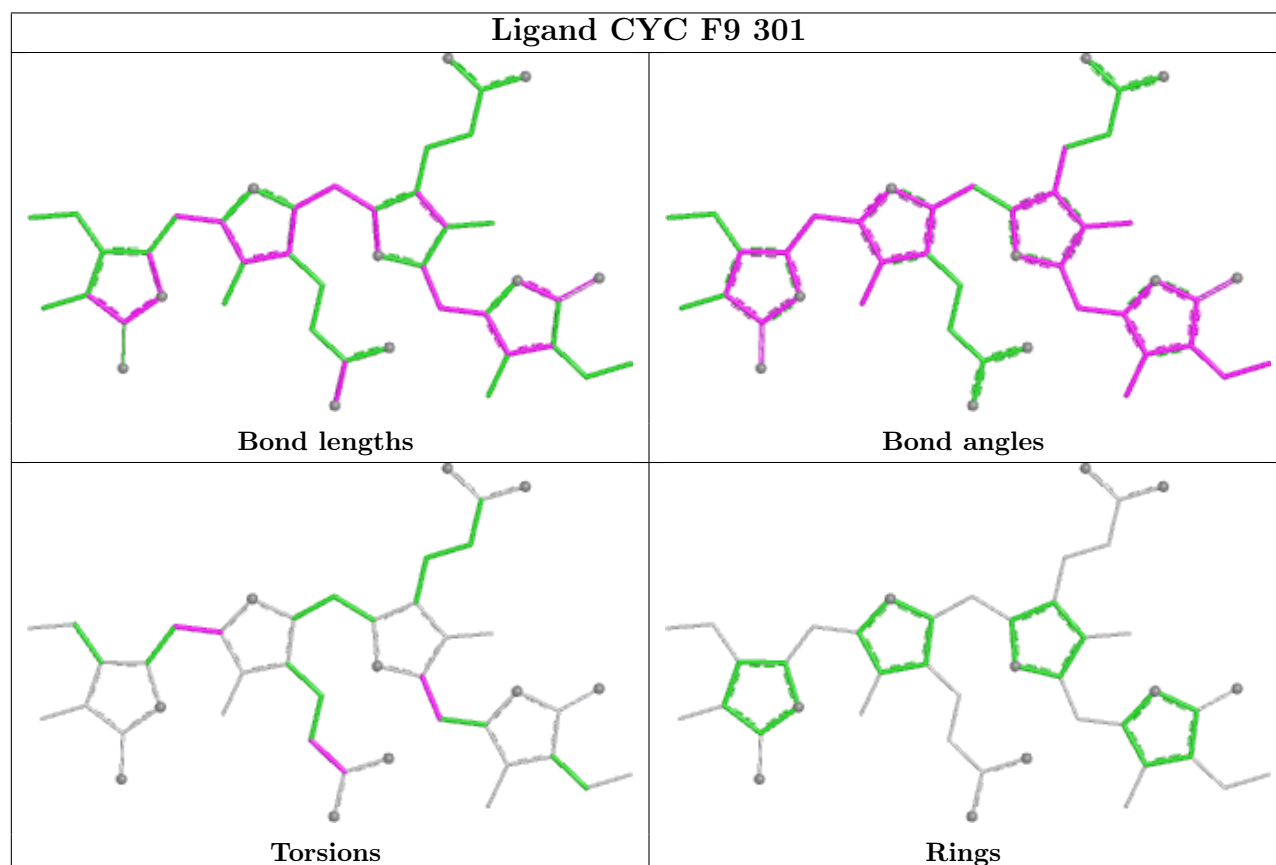
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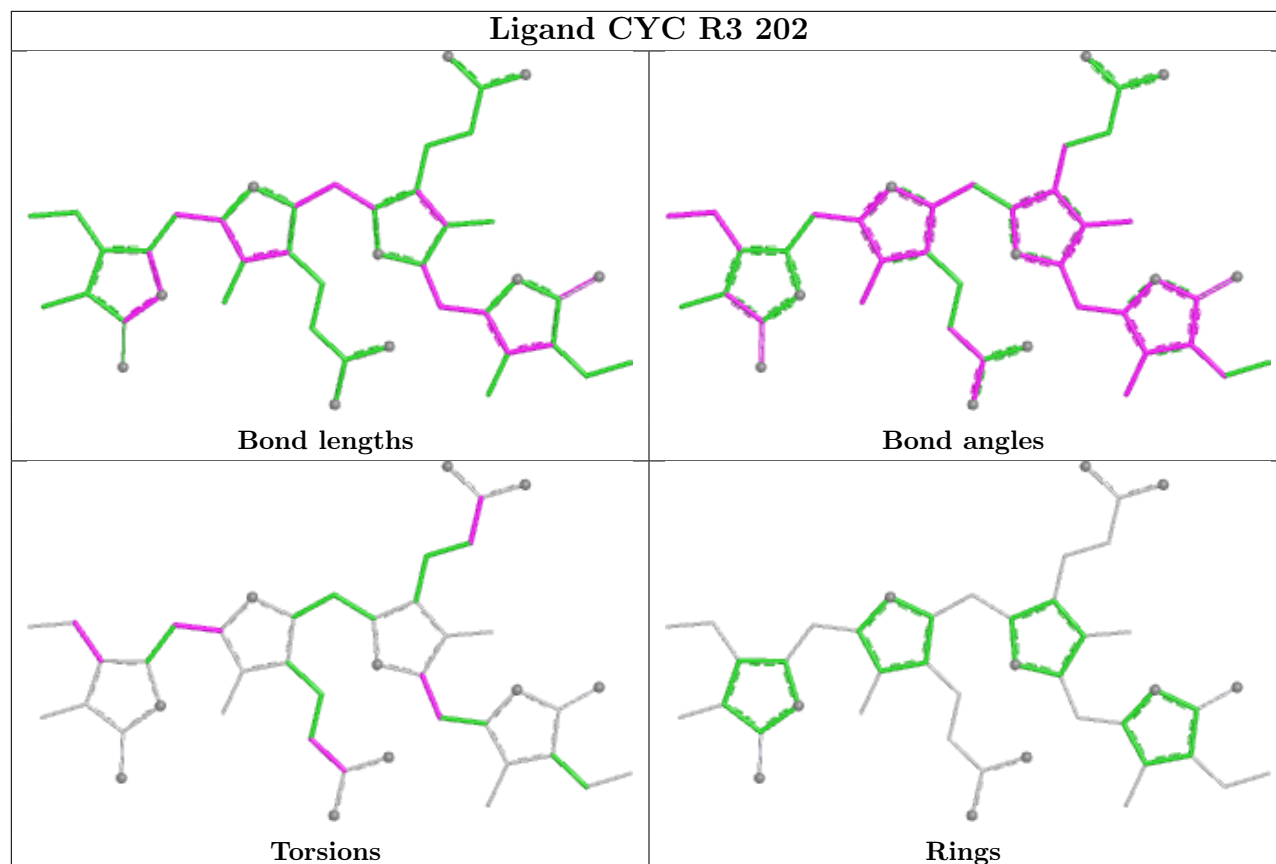
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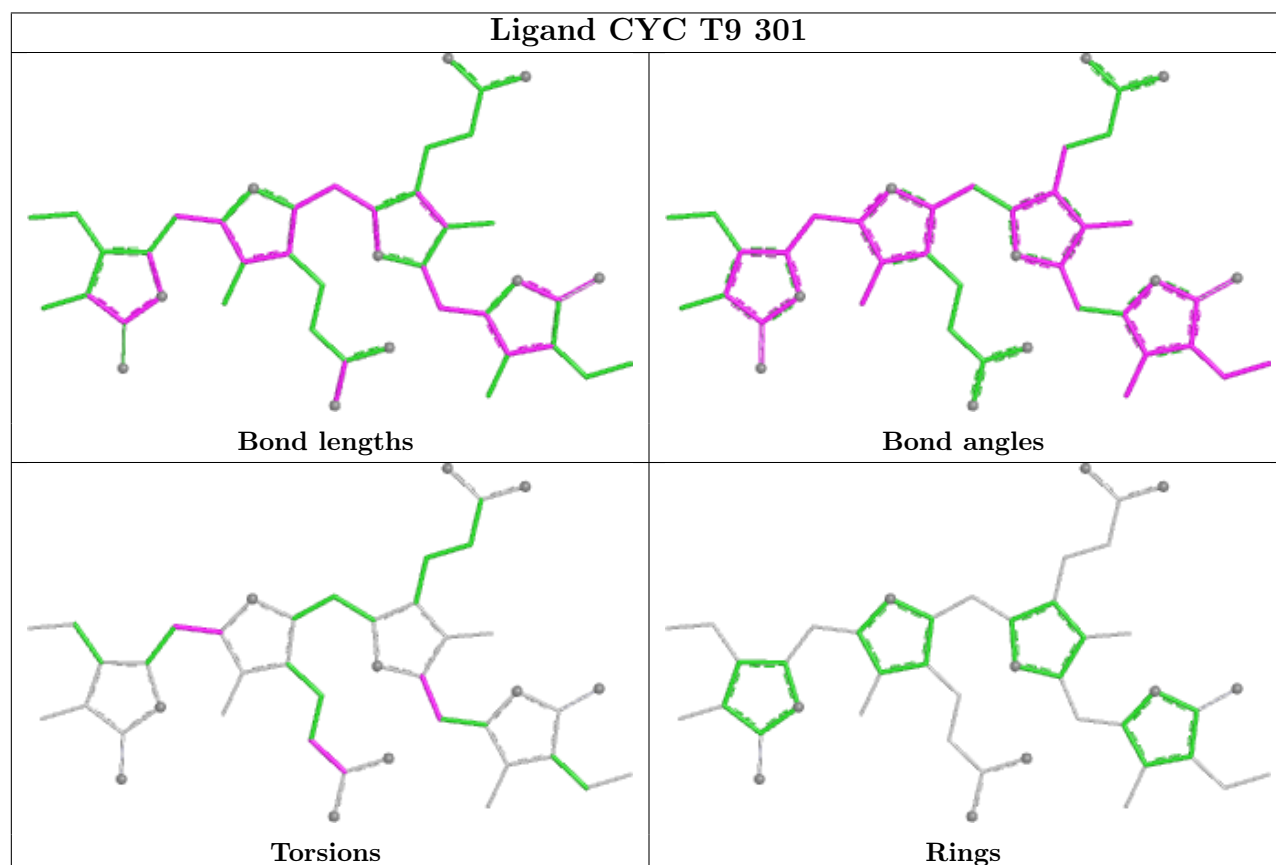
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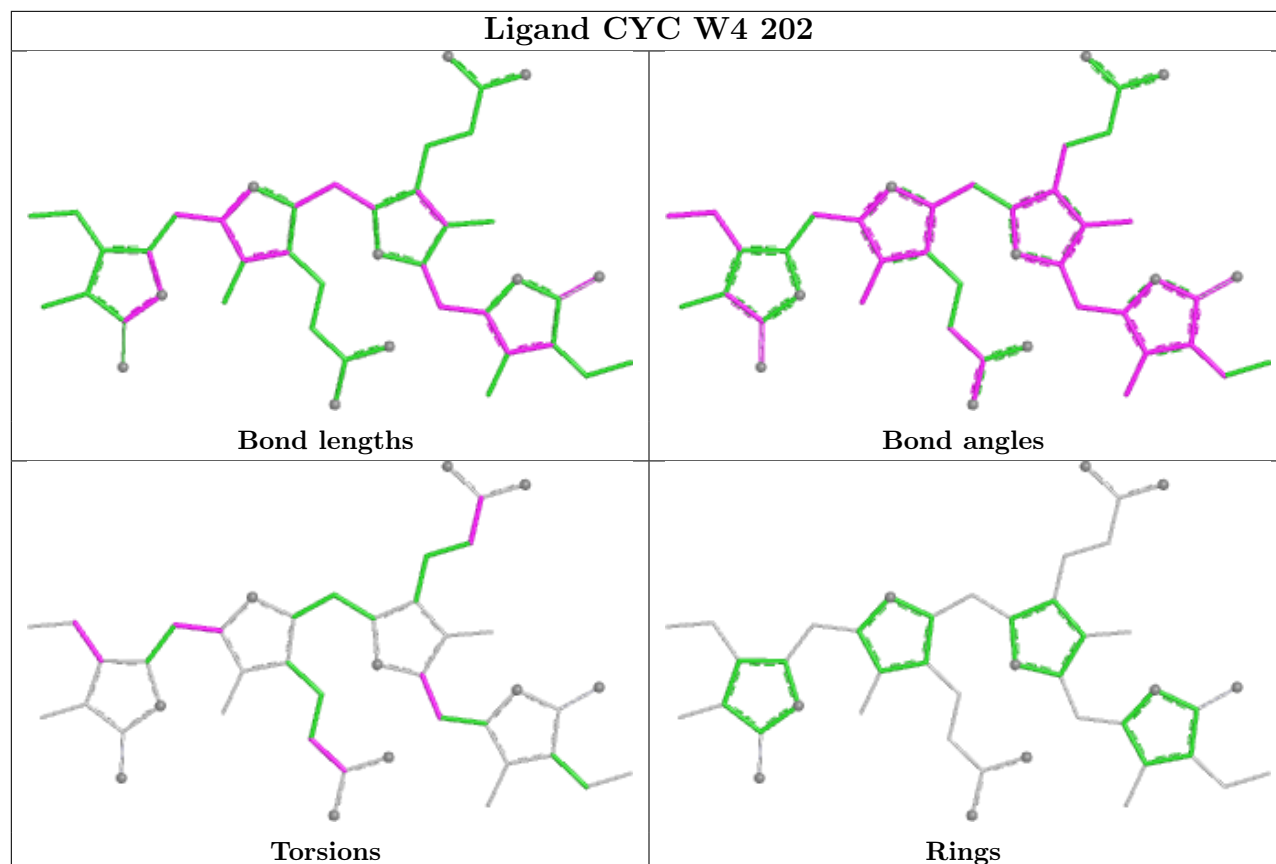
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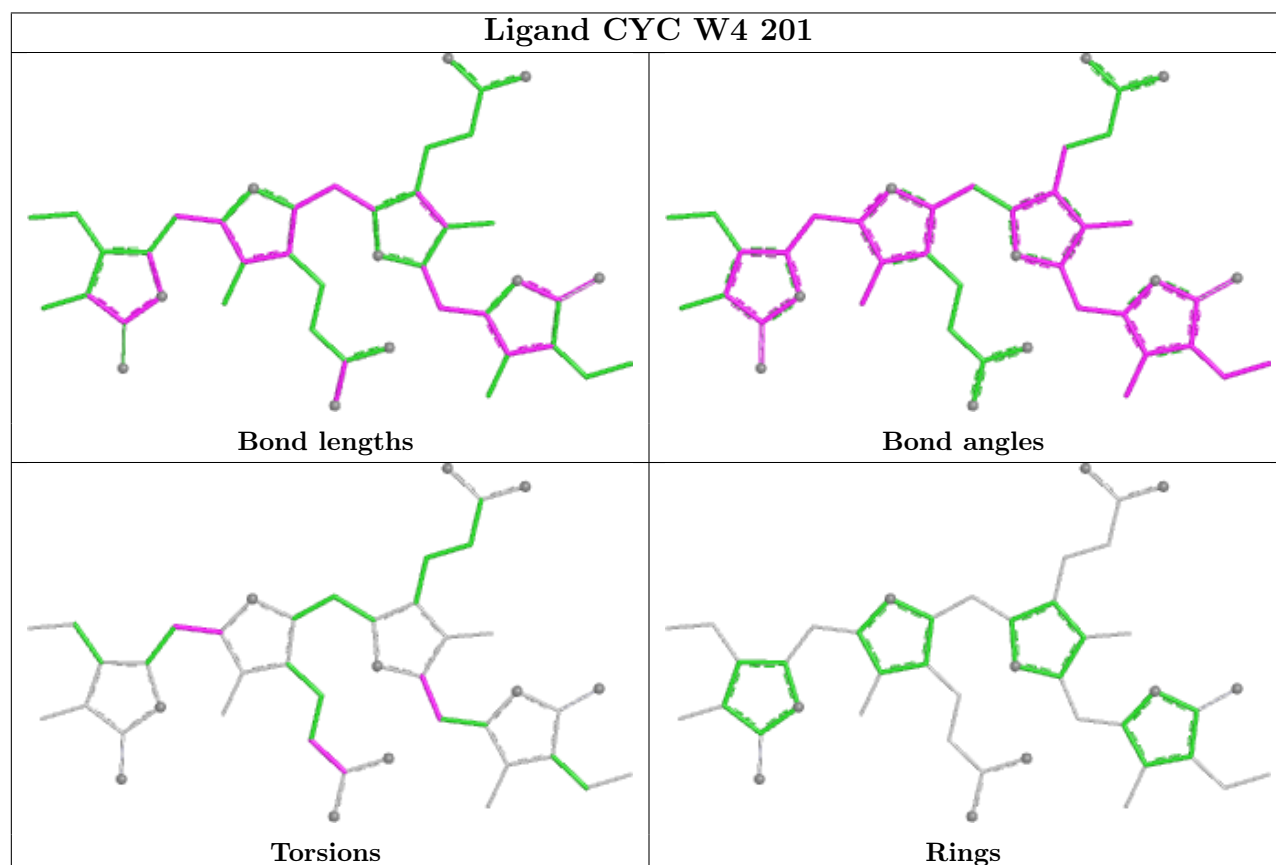
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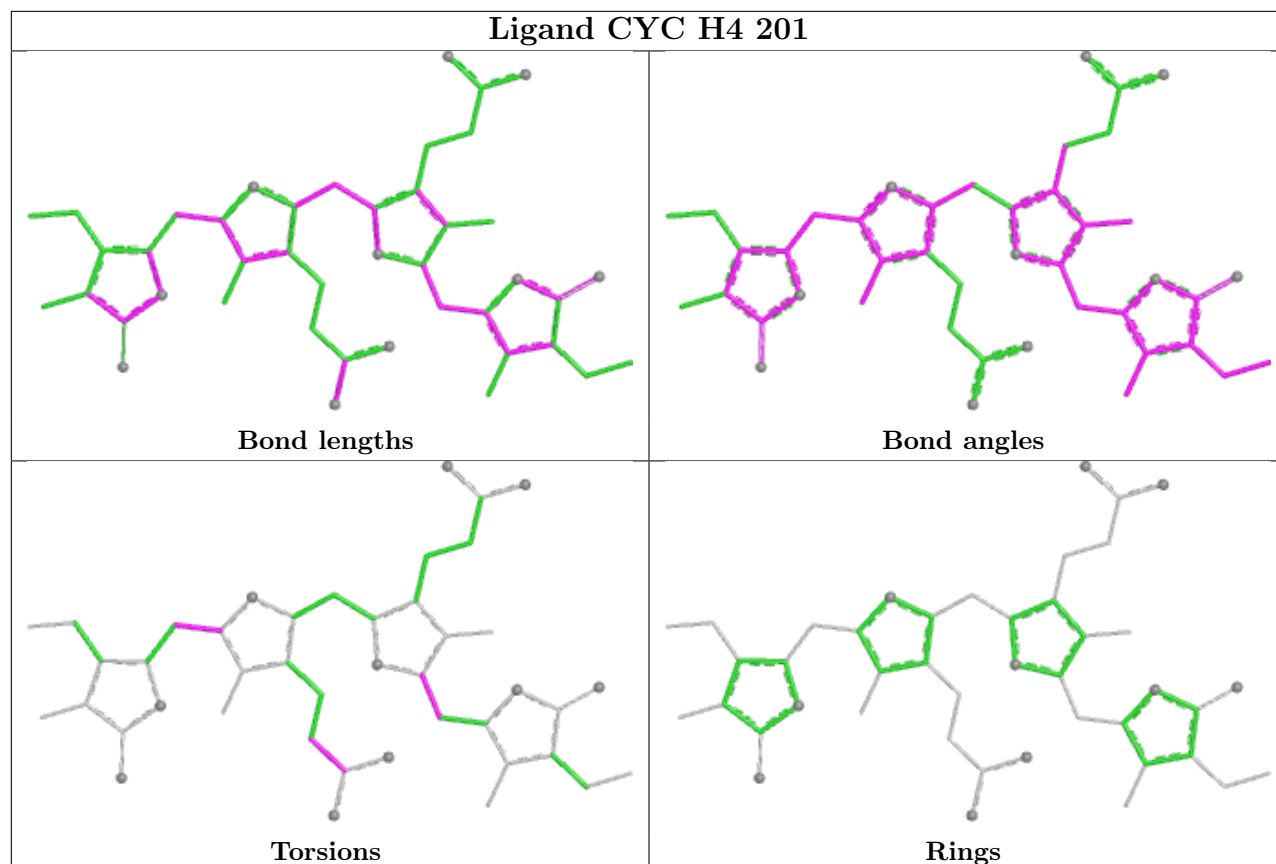
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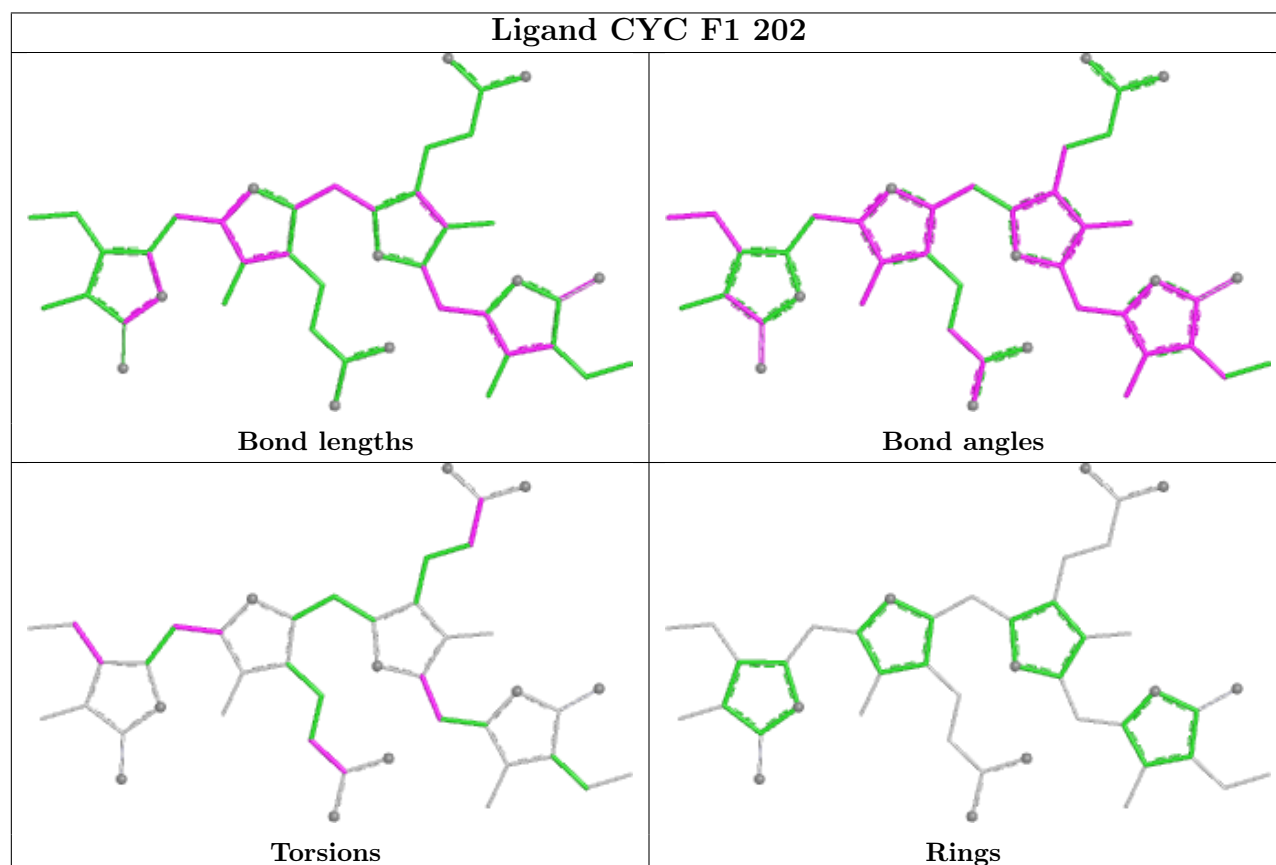
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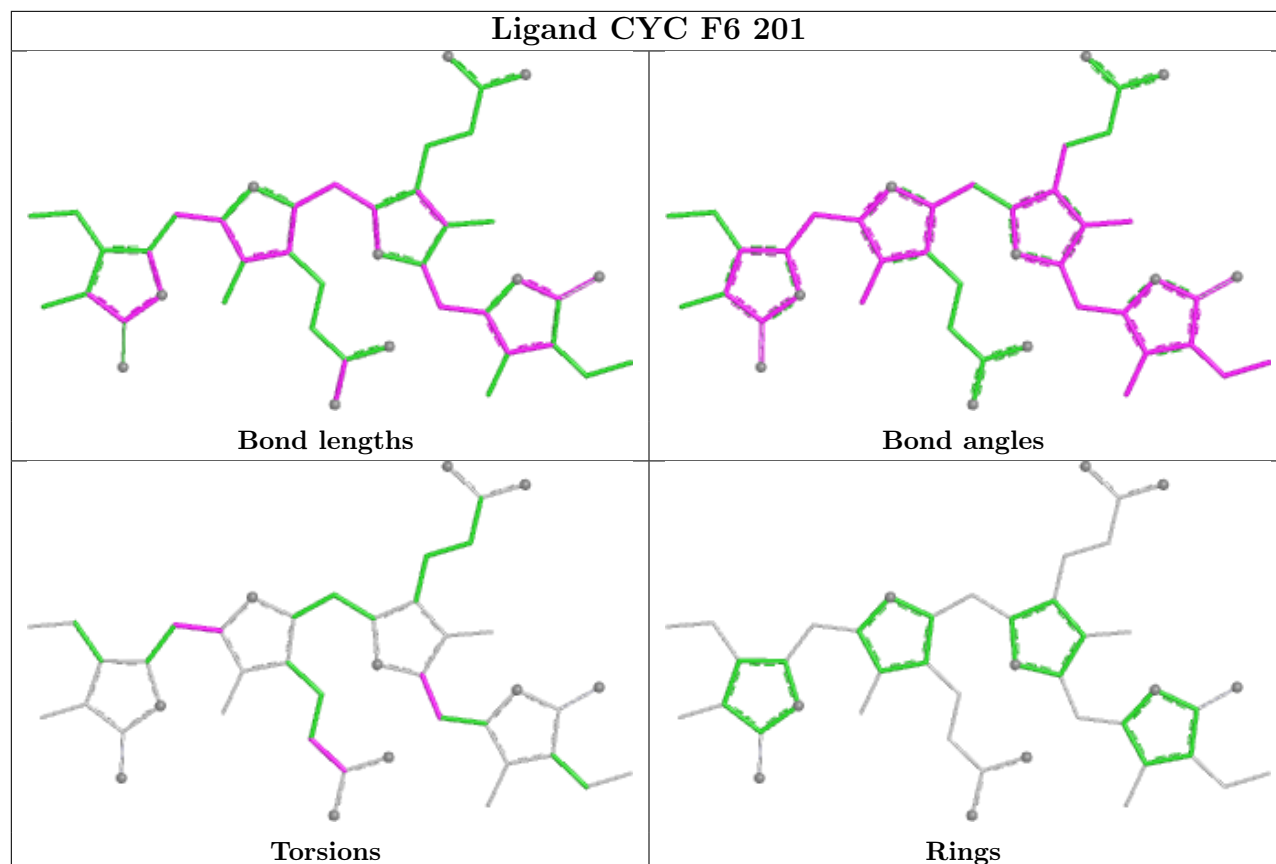
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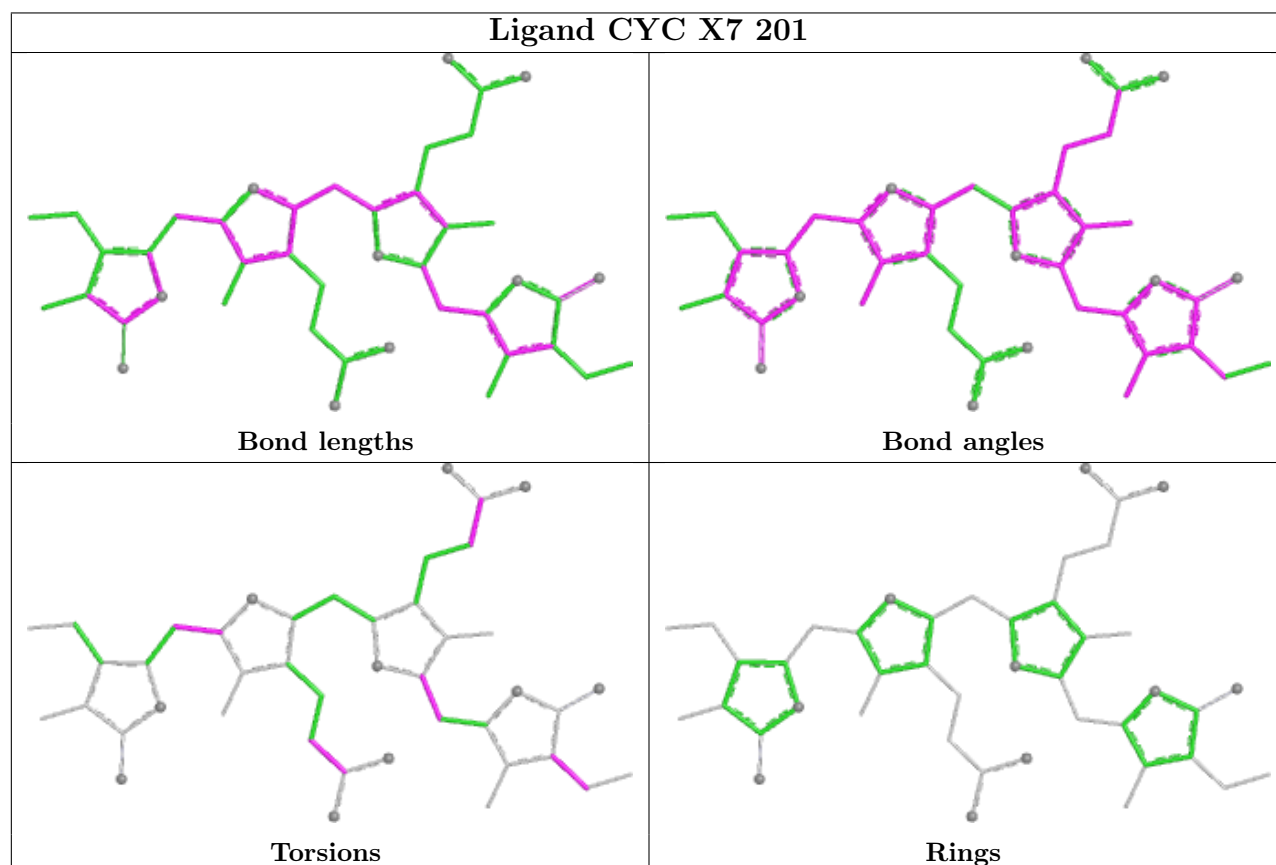
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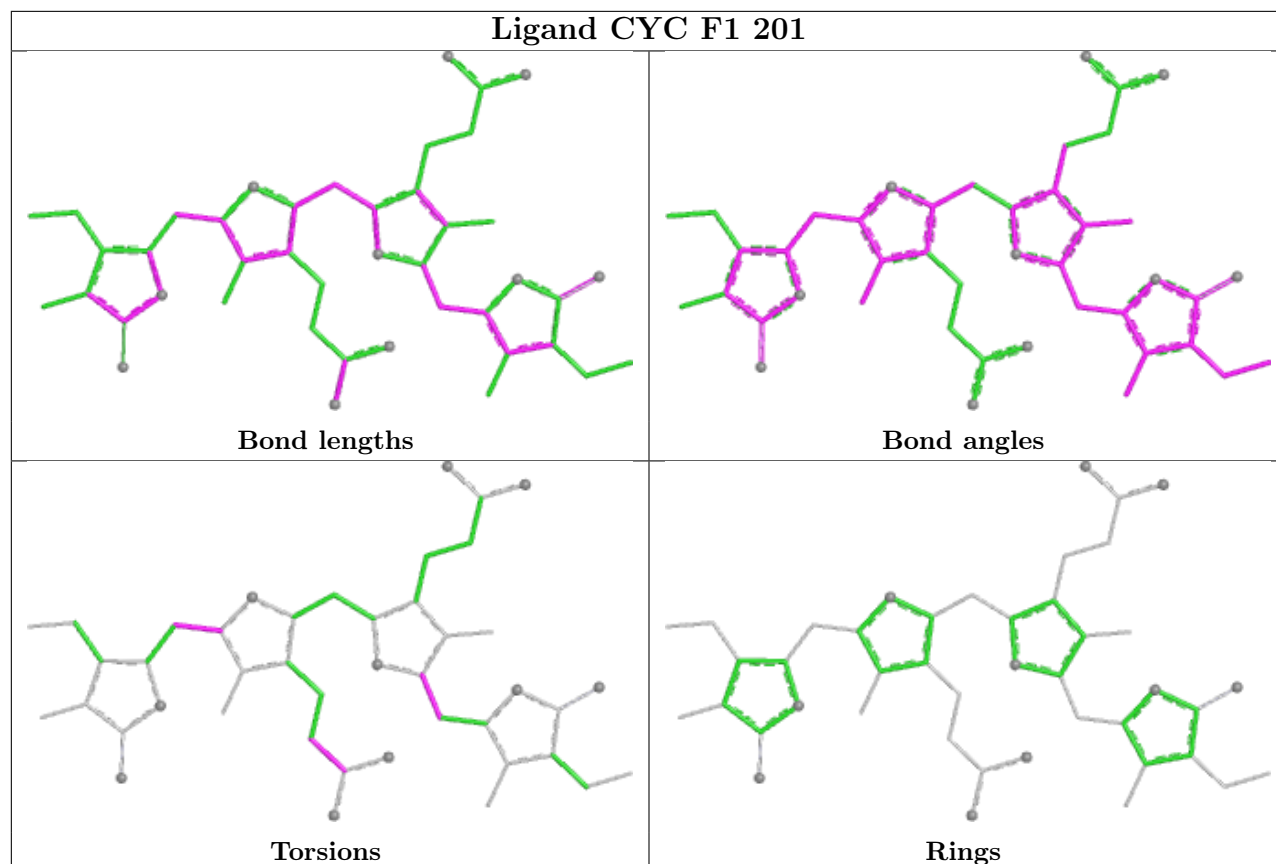
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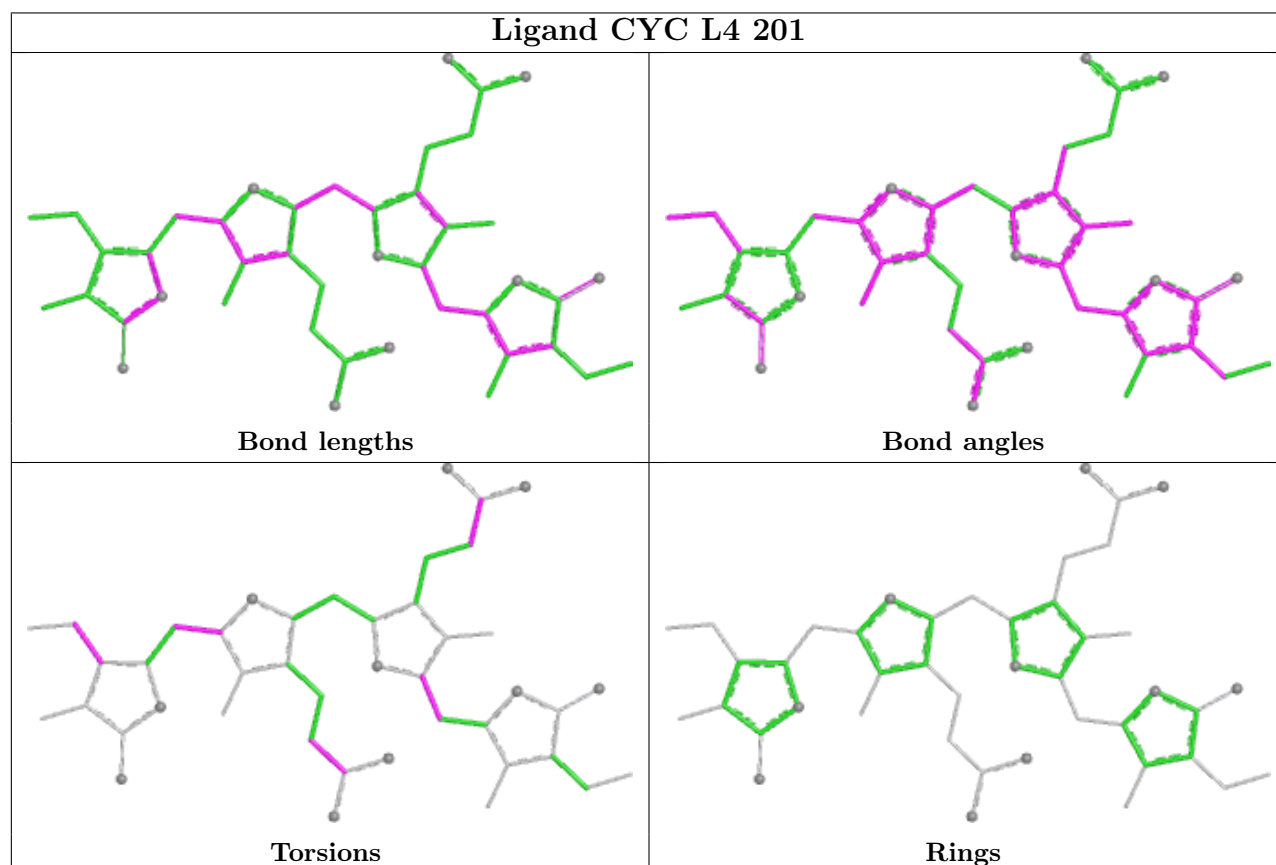
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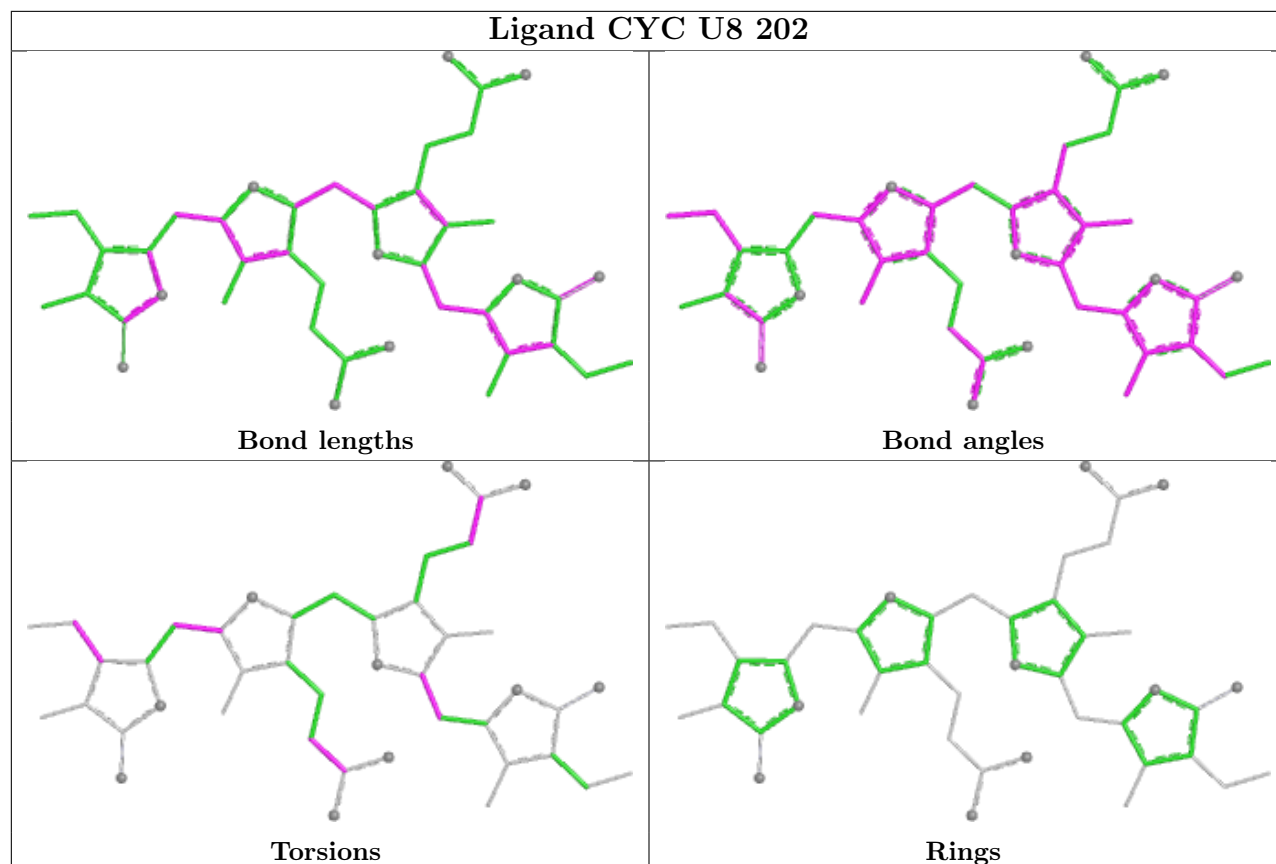
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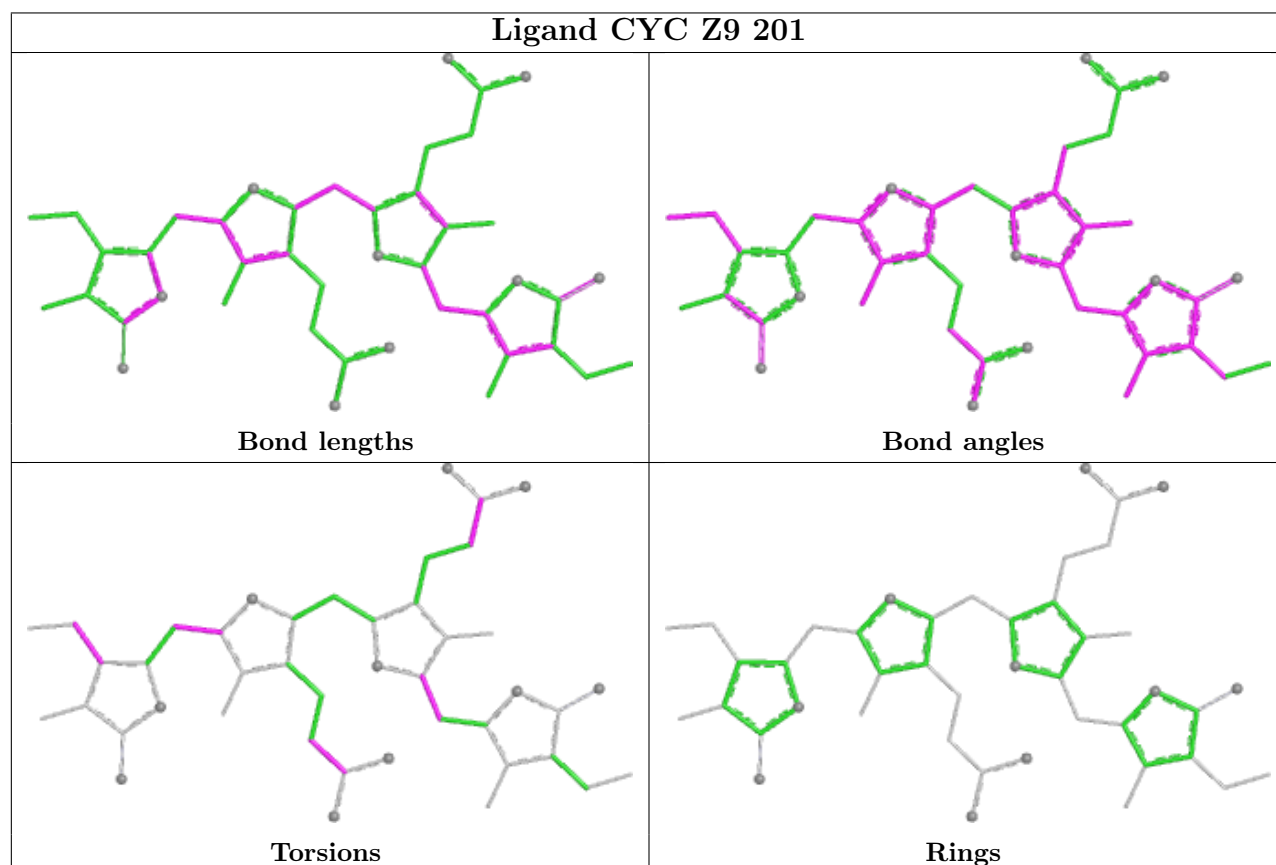
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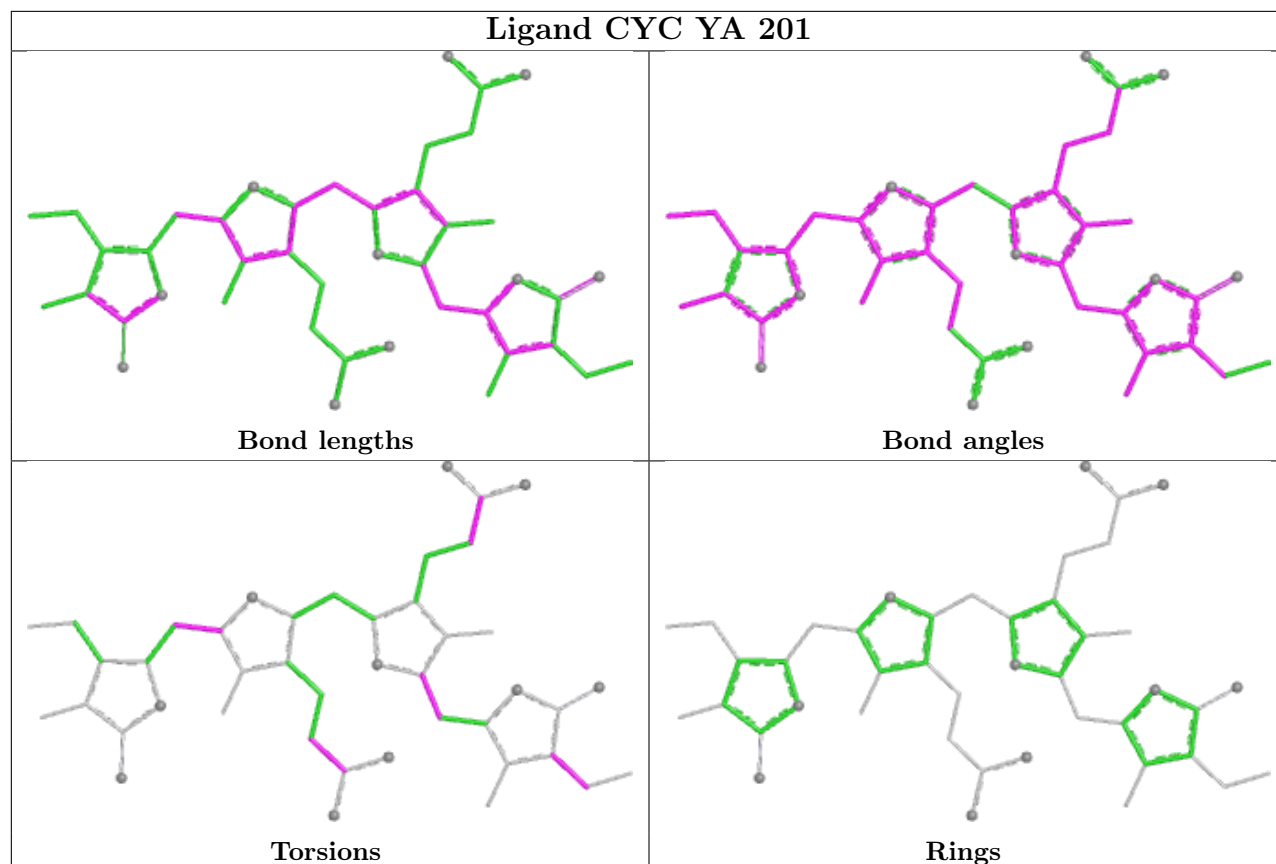
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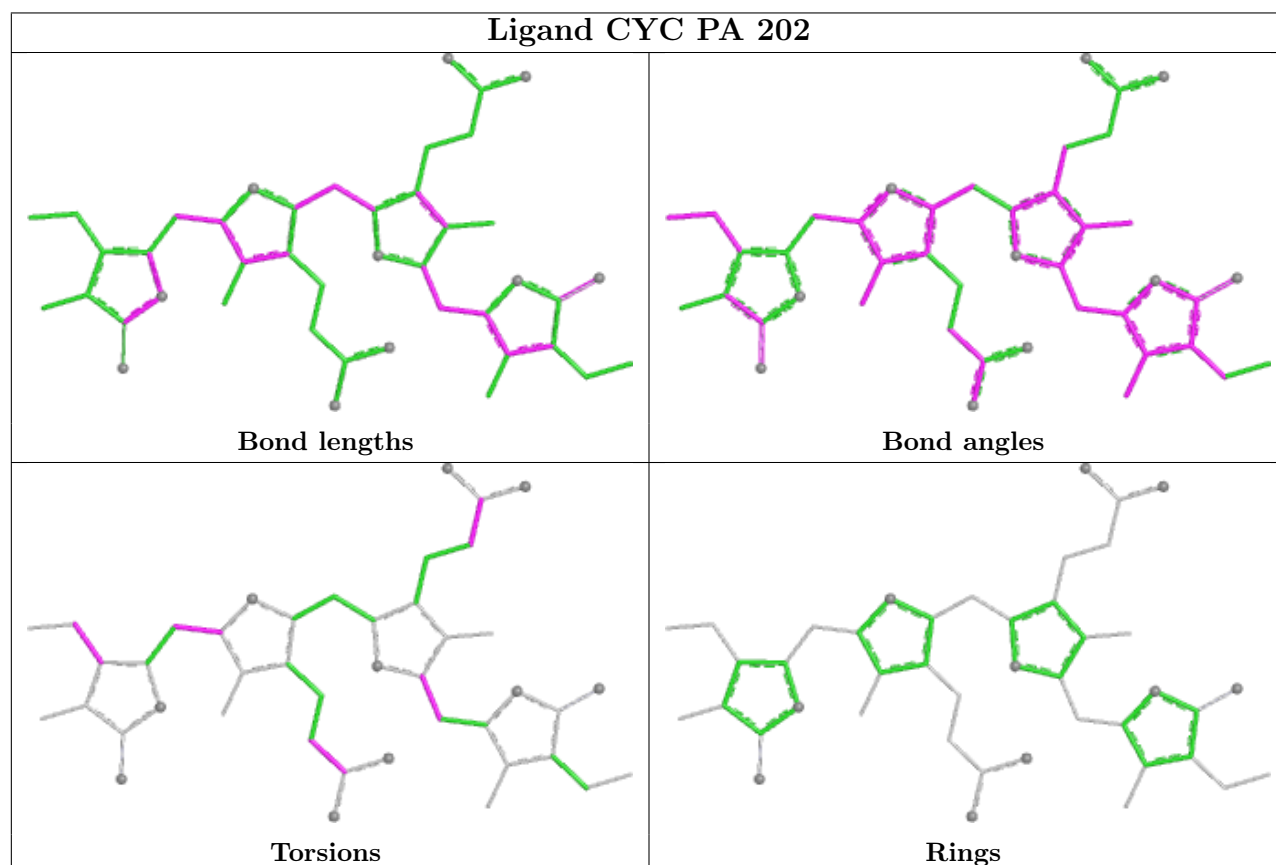
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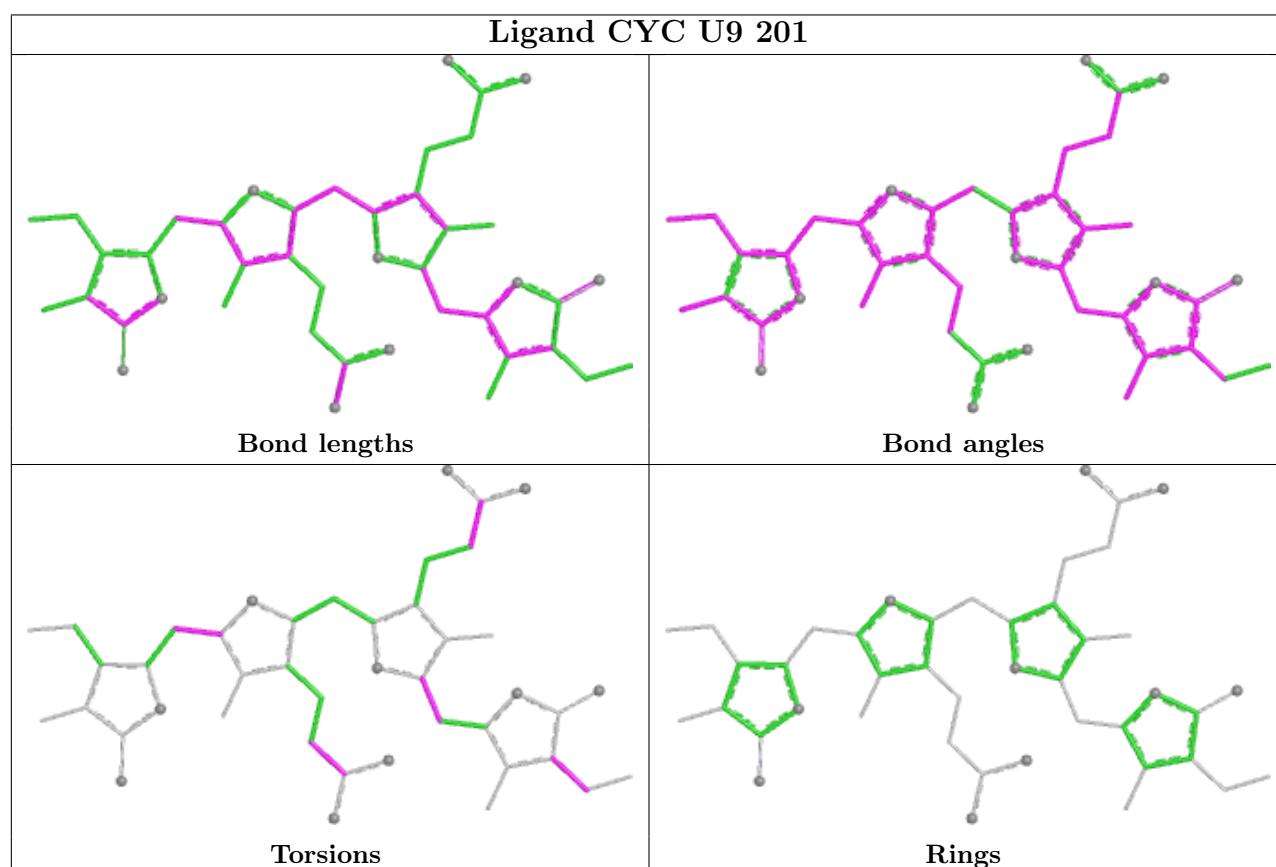
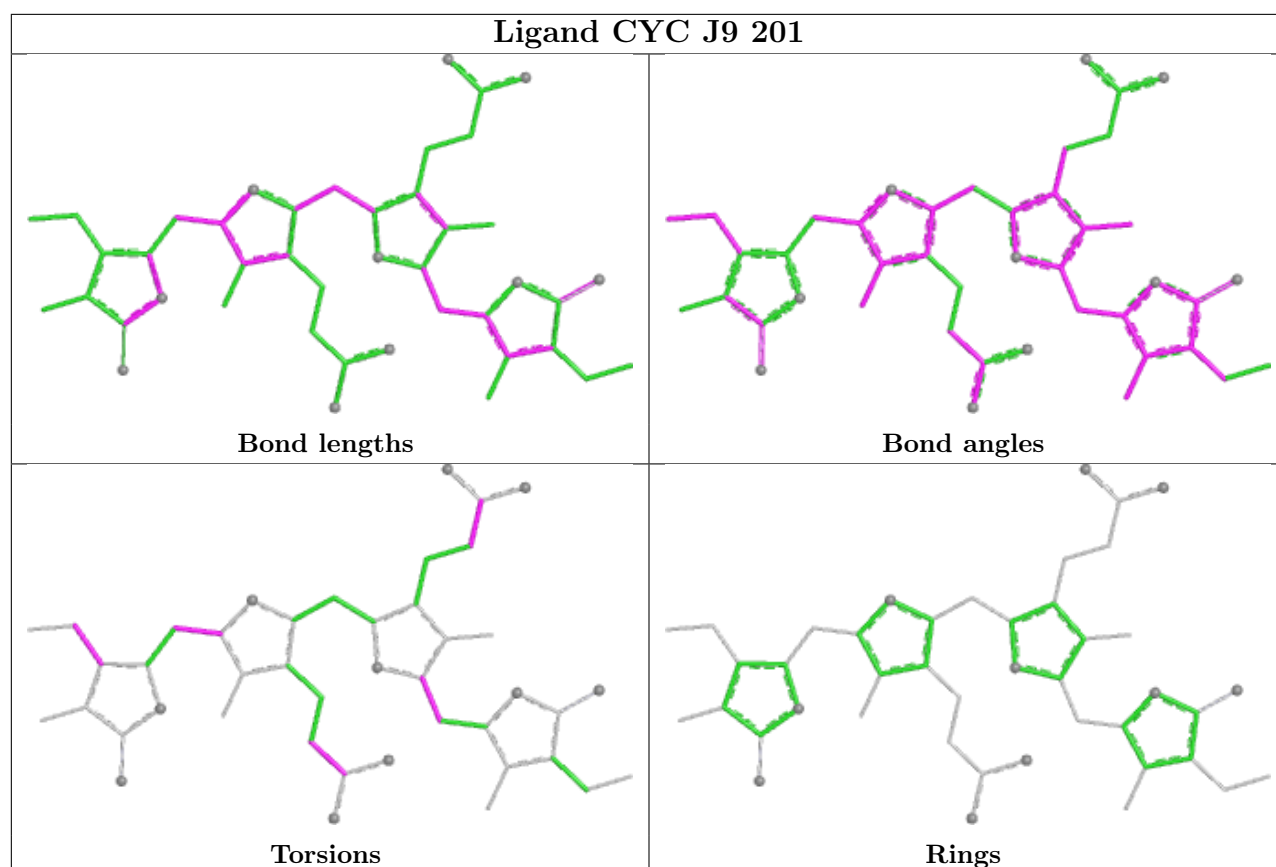


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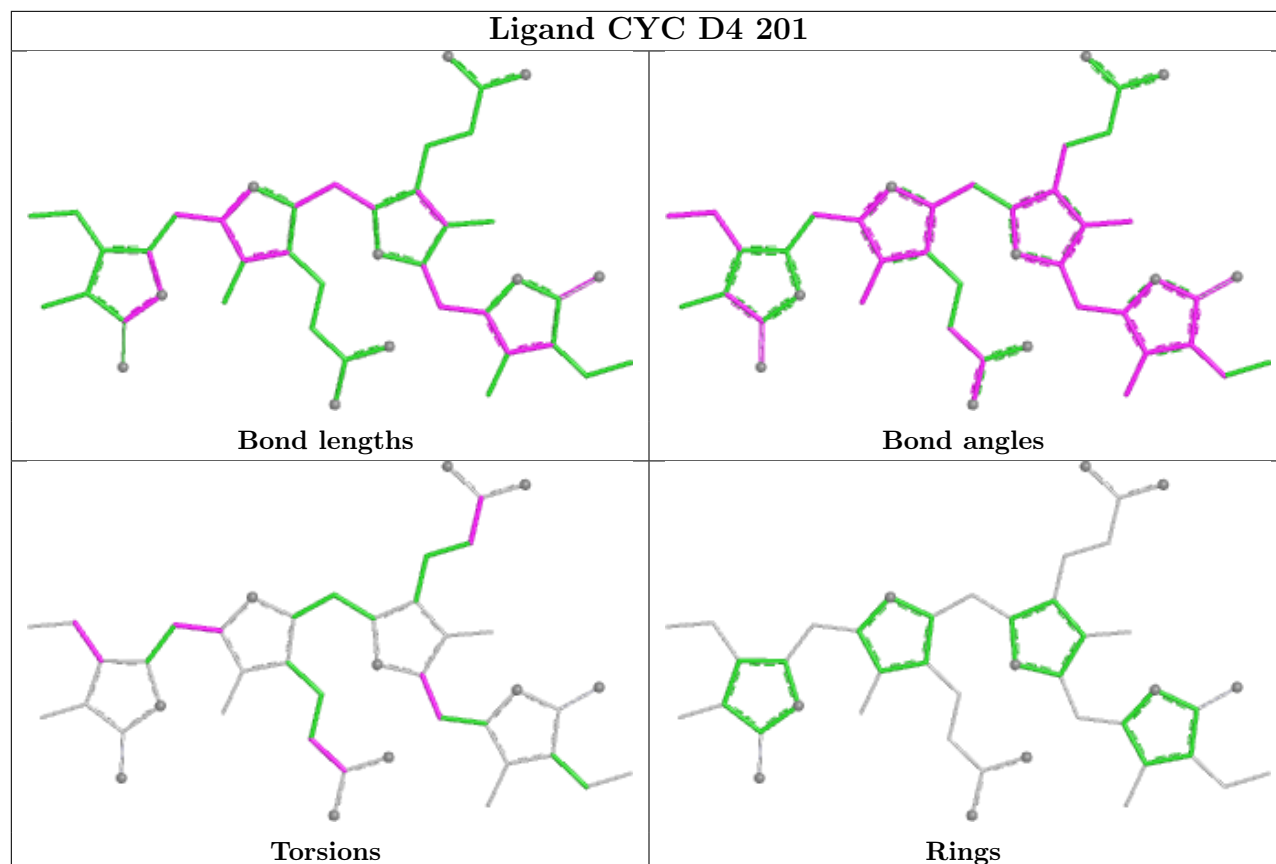


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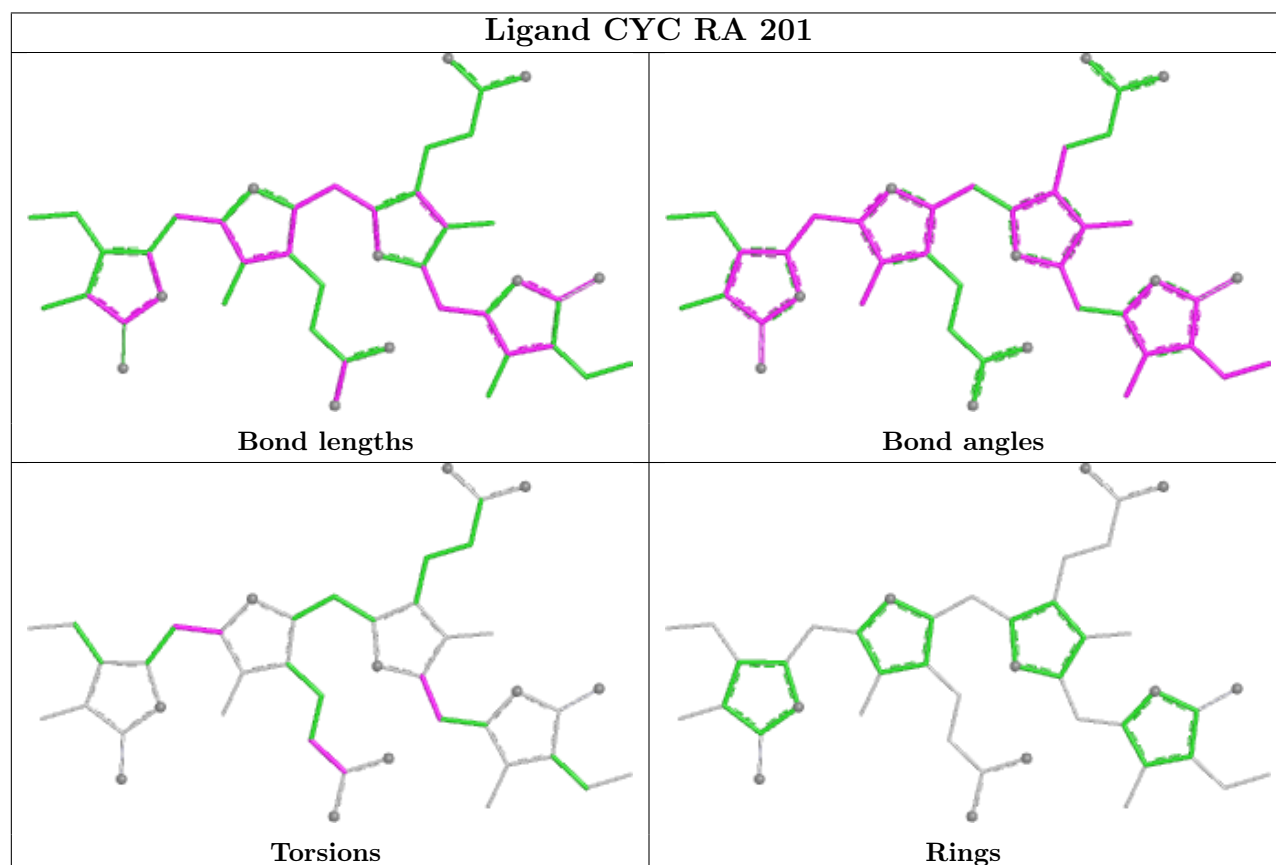




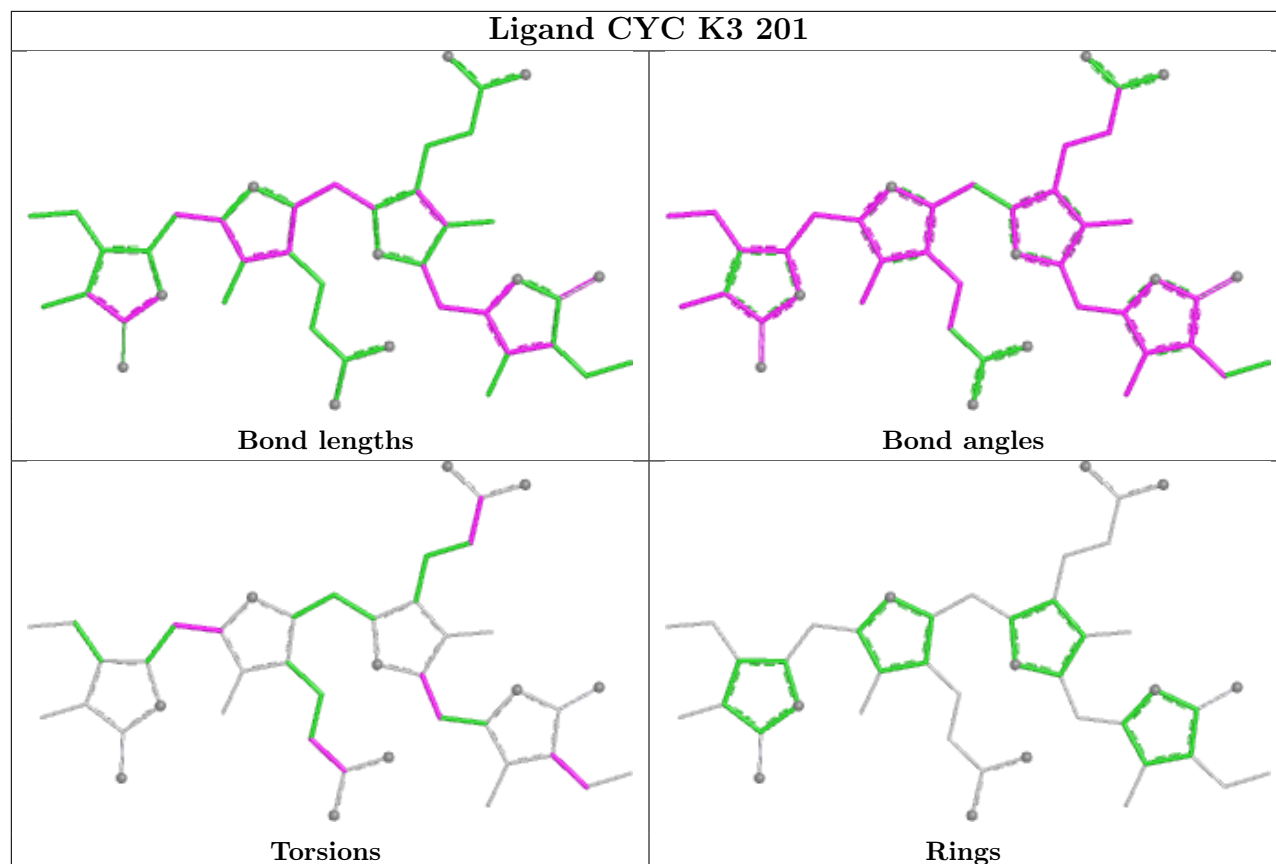
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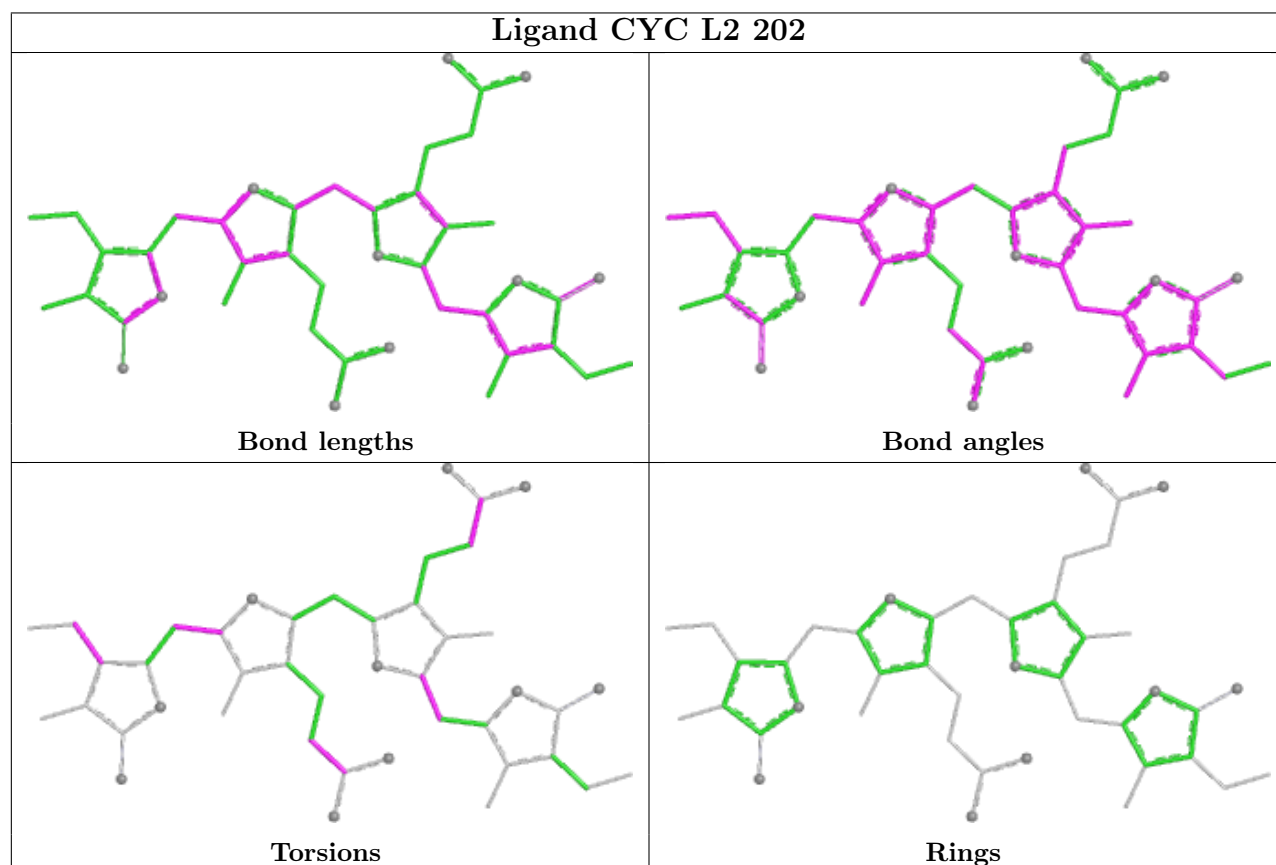
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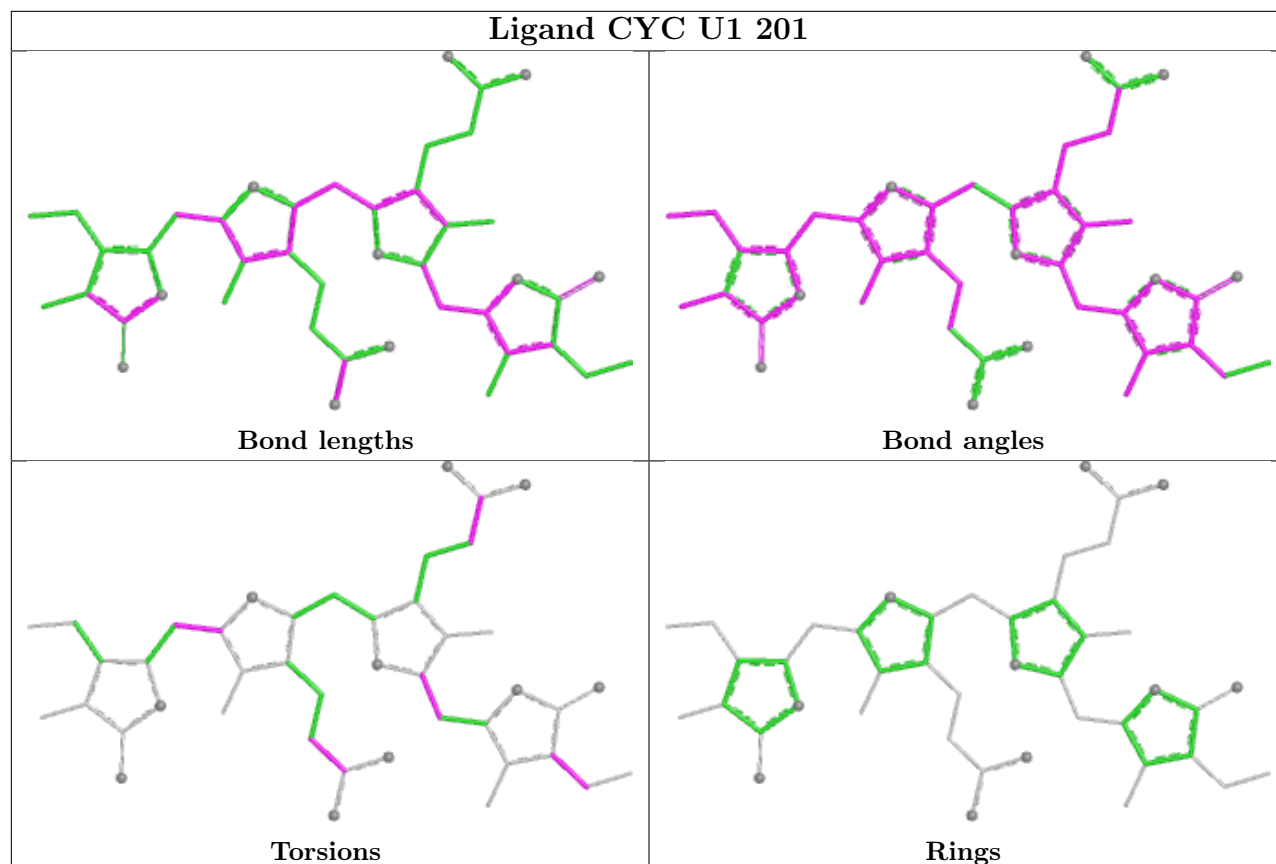
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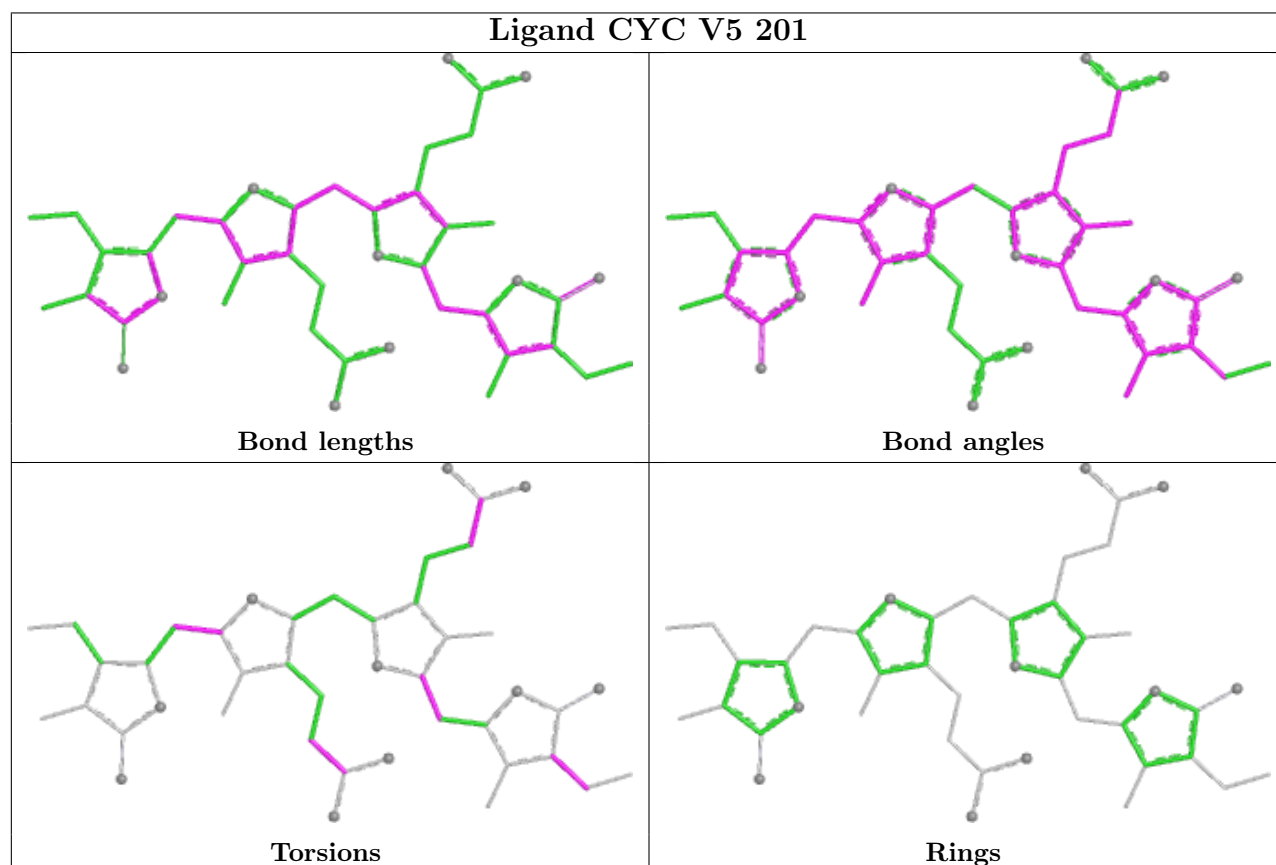
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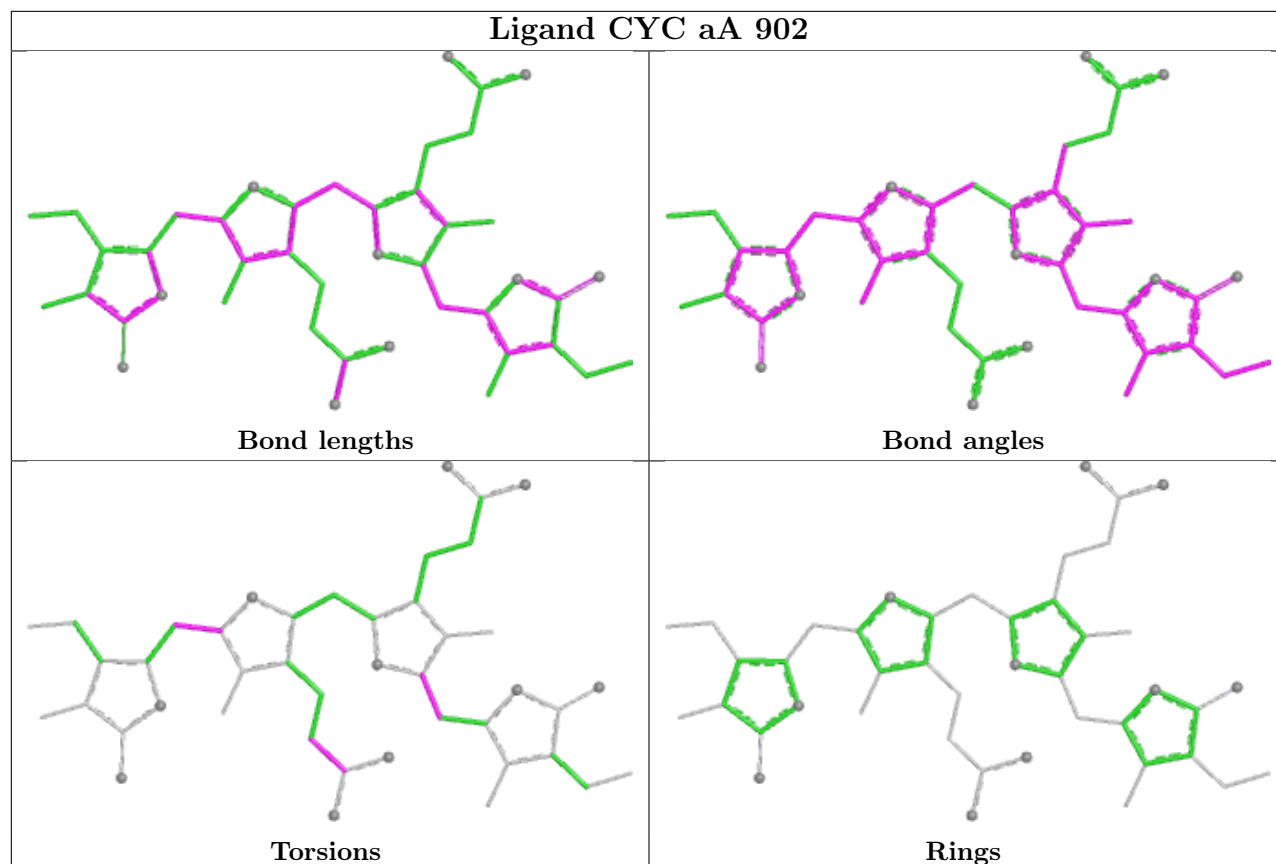
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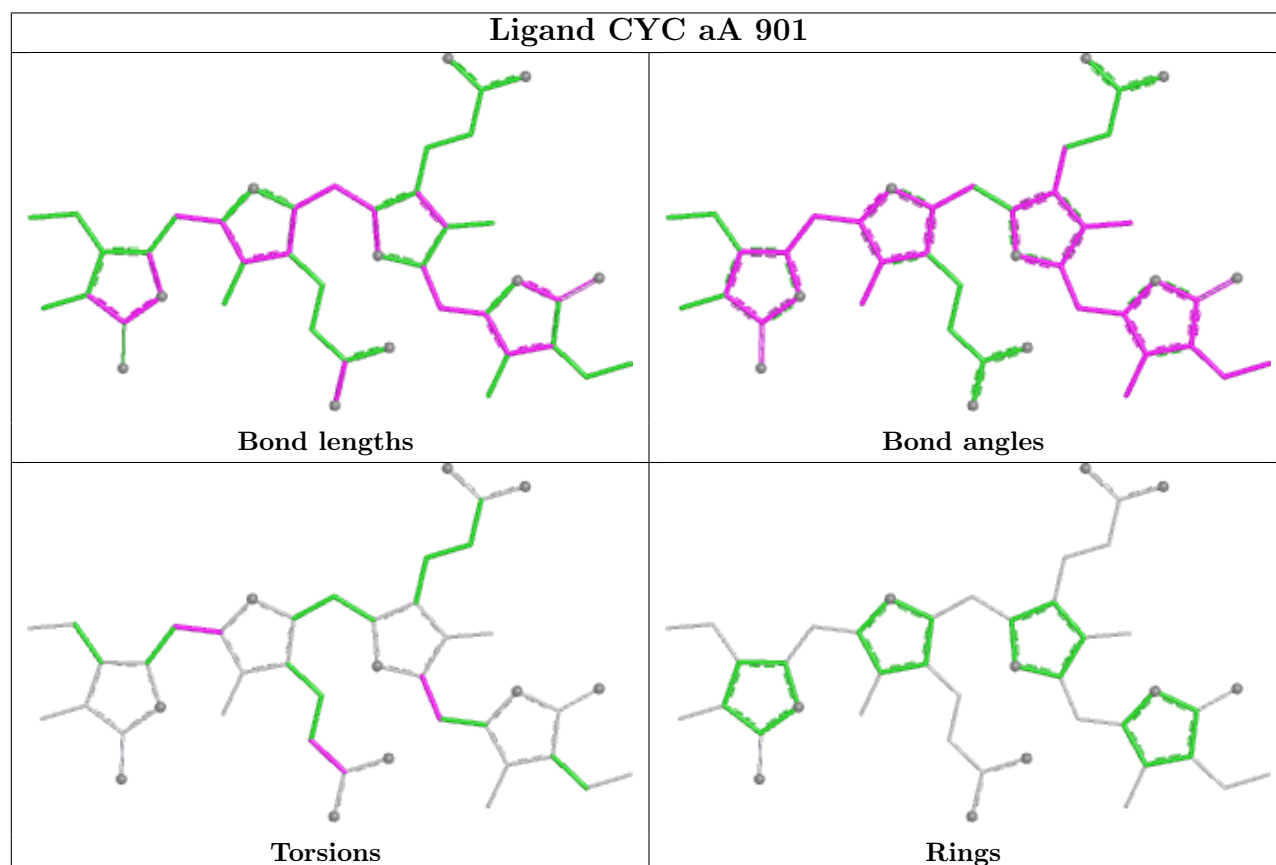
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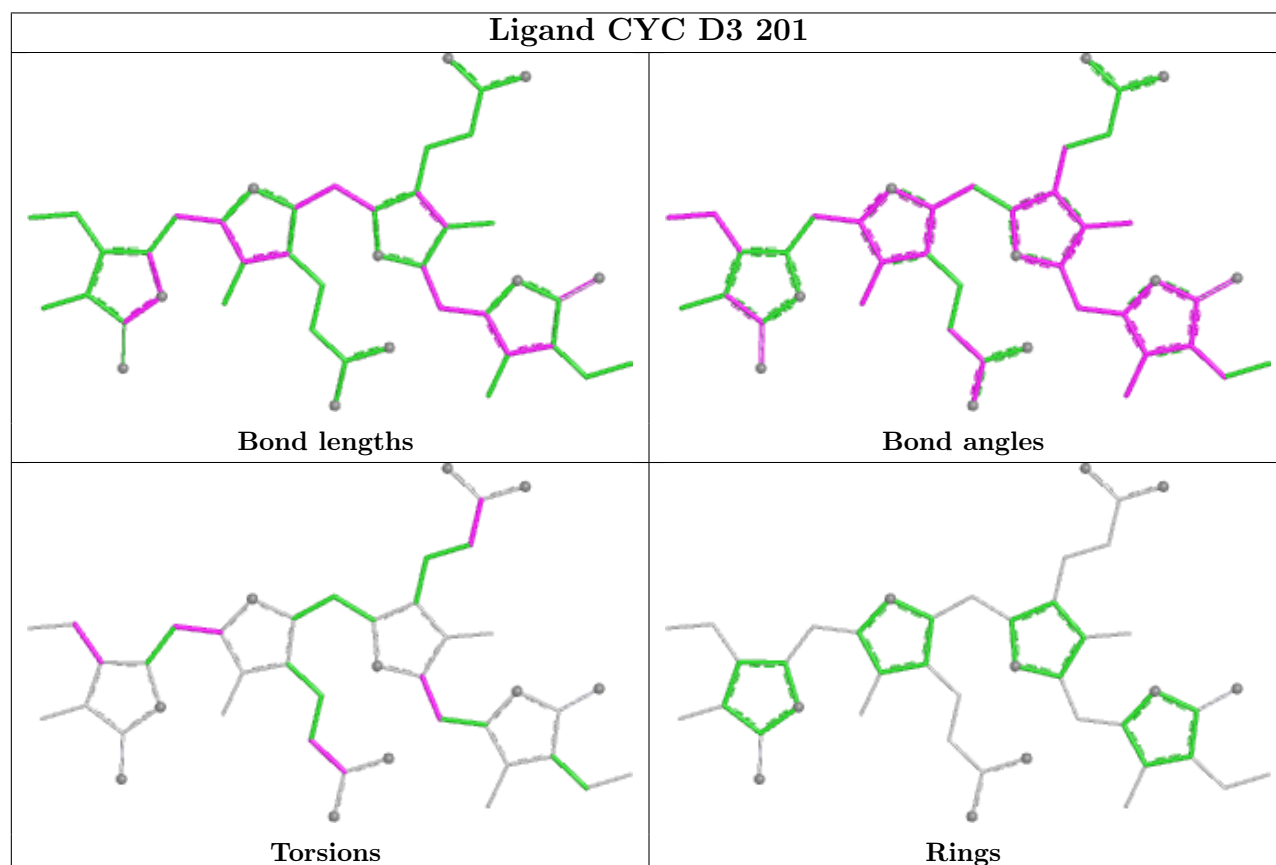
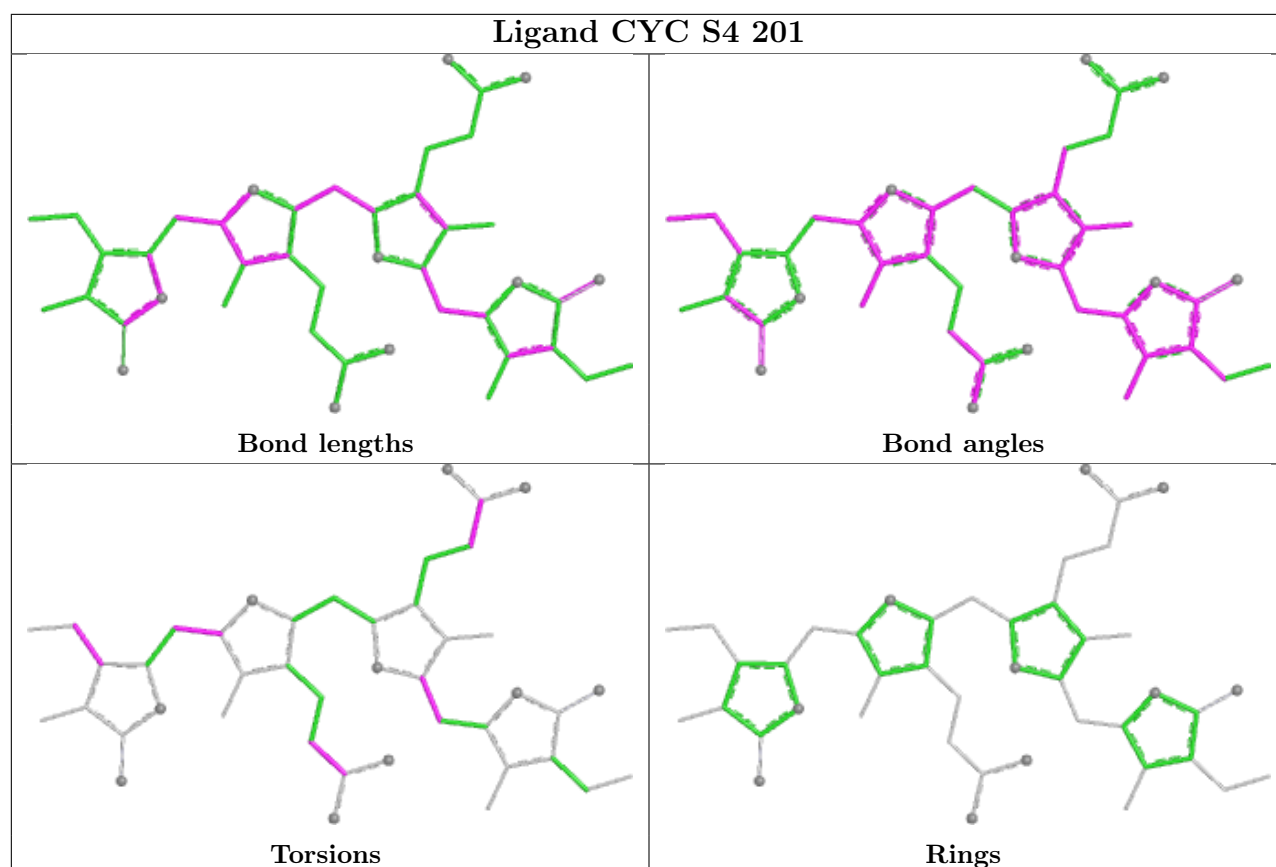


Ligand CYC aA 902

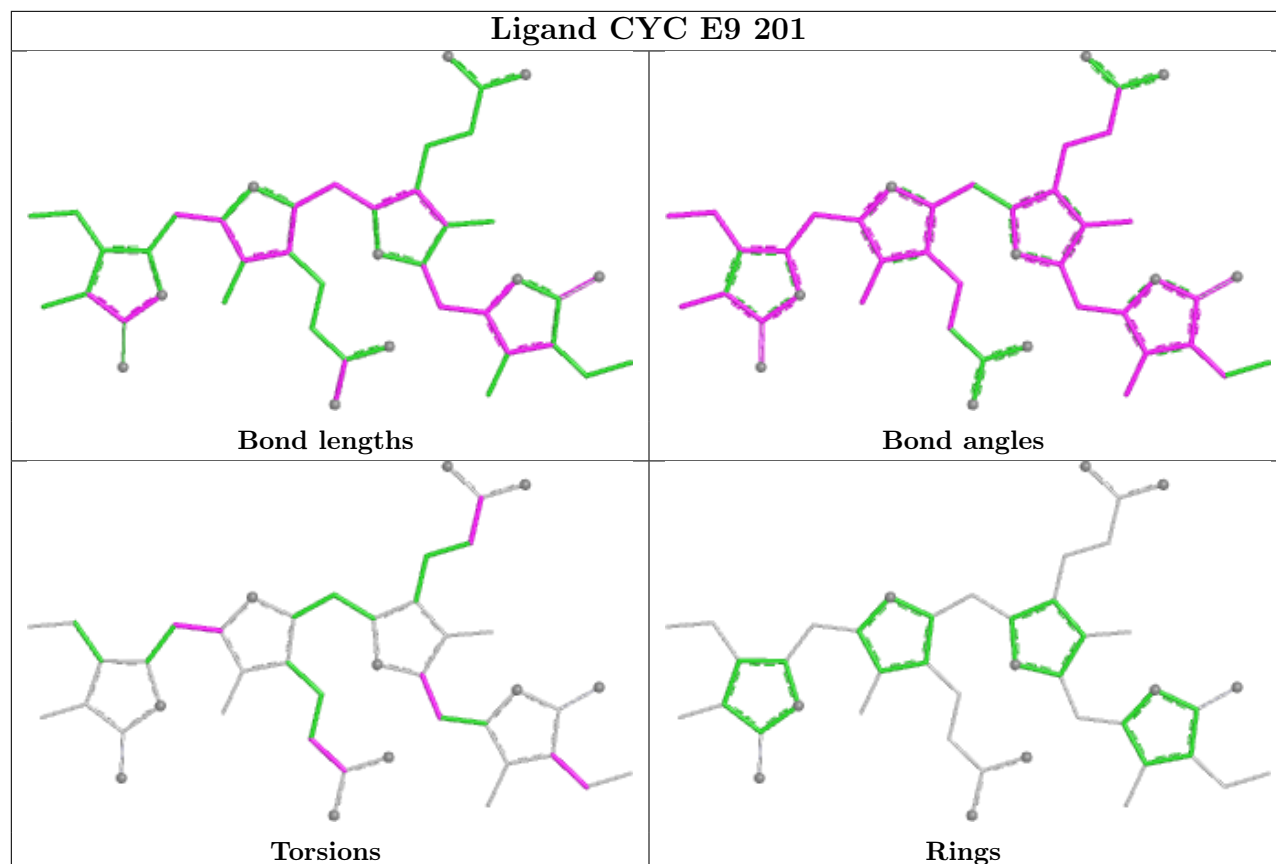


Ligand CYC aA 901

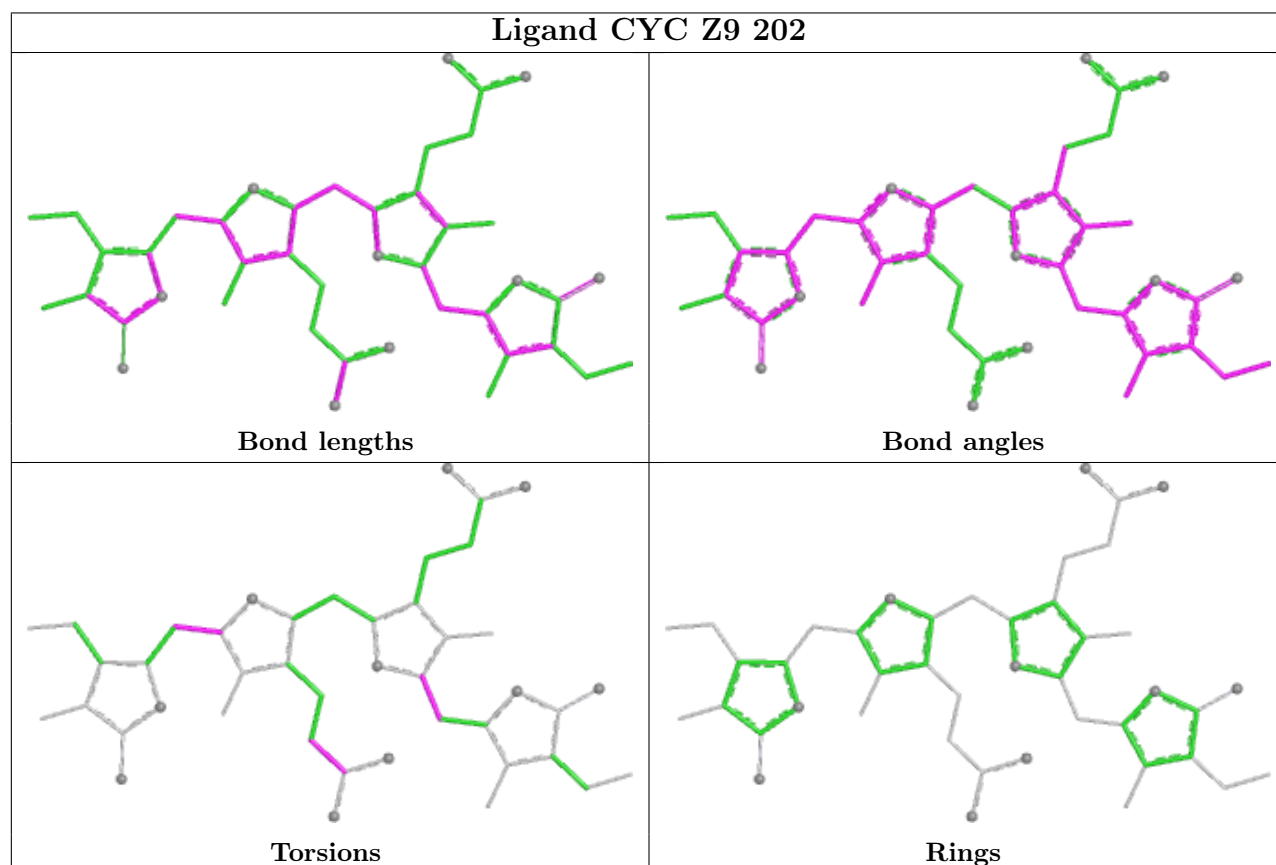




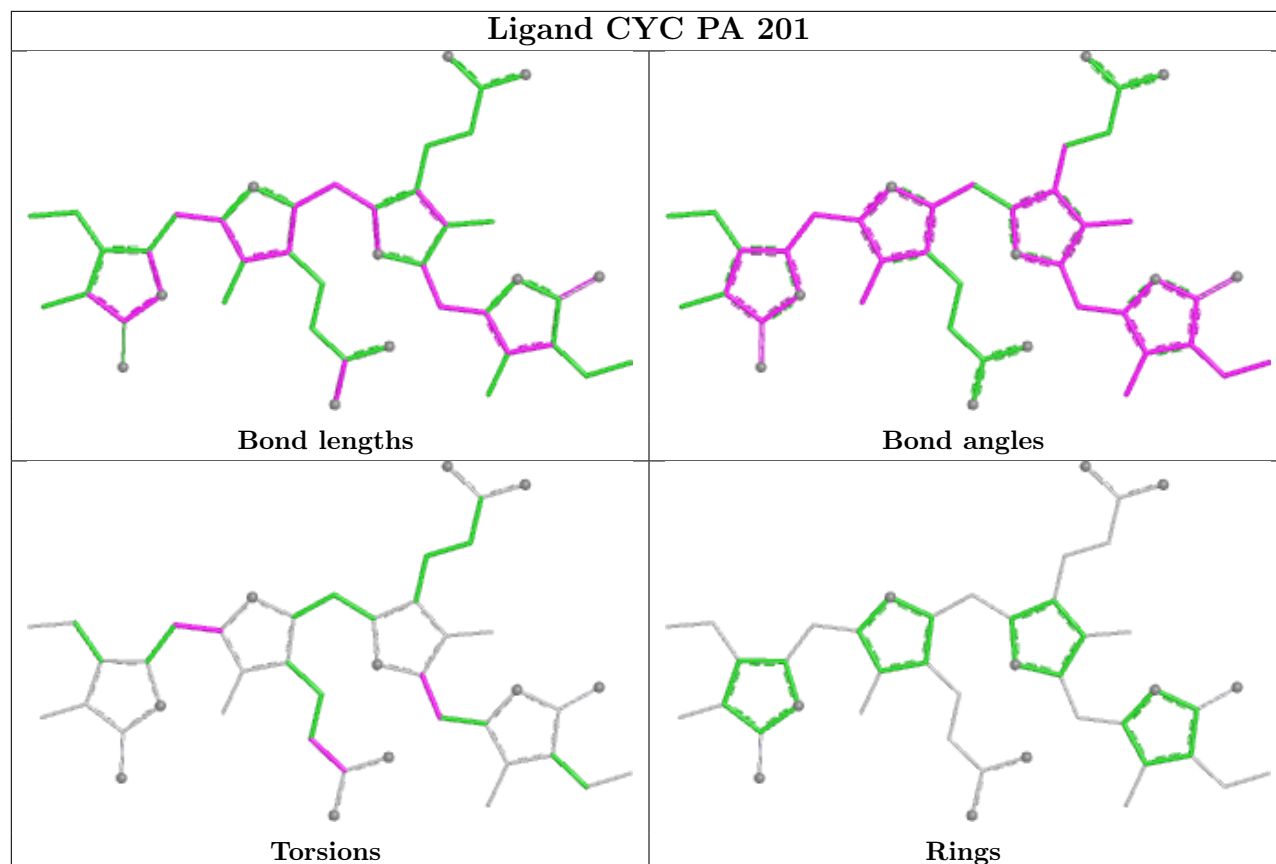
Ligand CYC E9 201



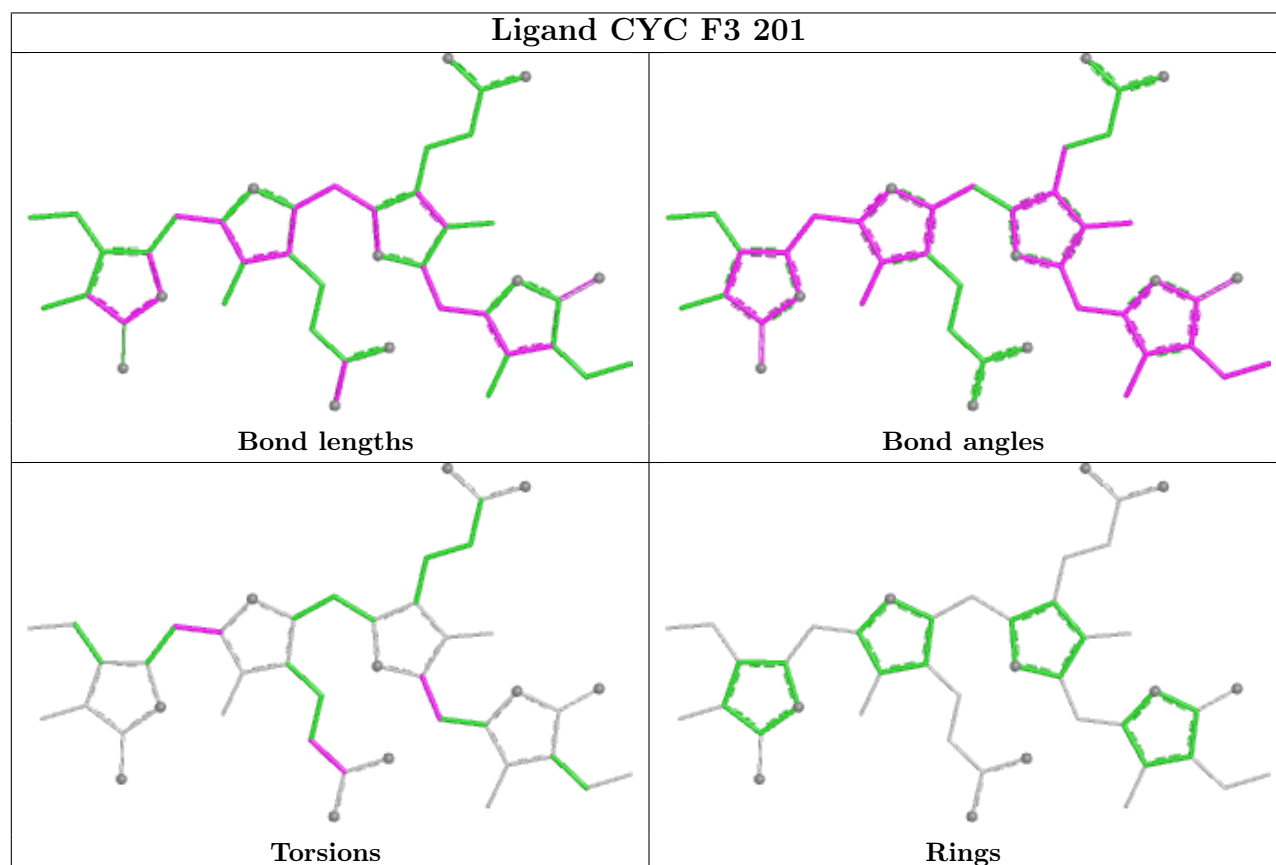
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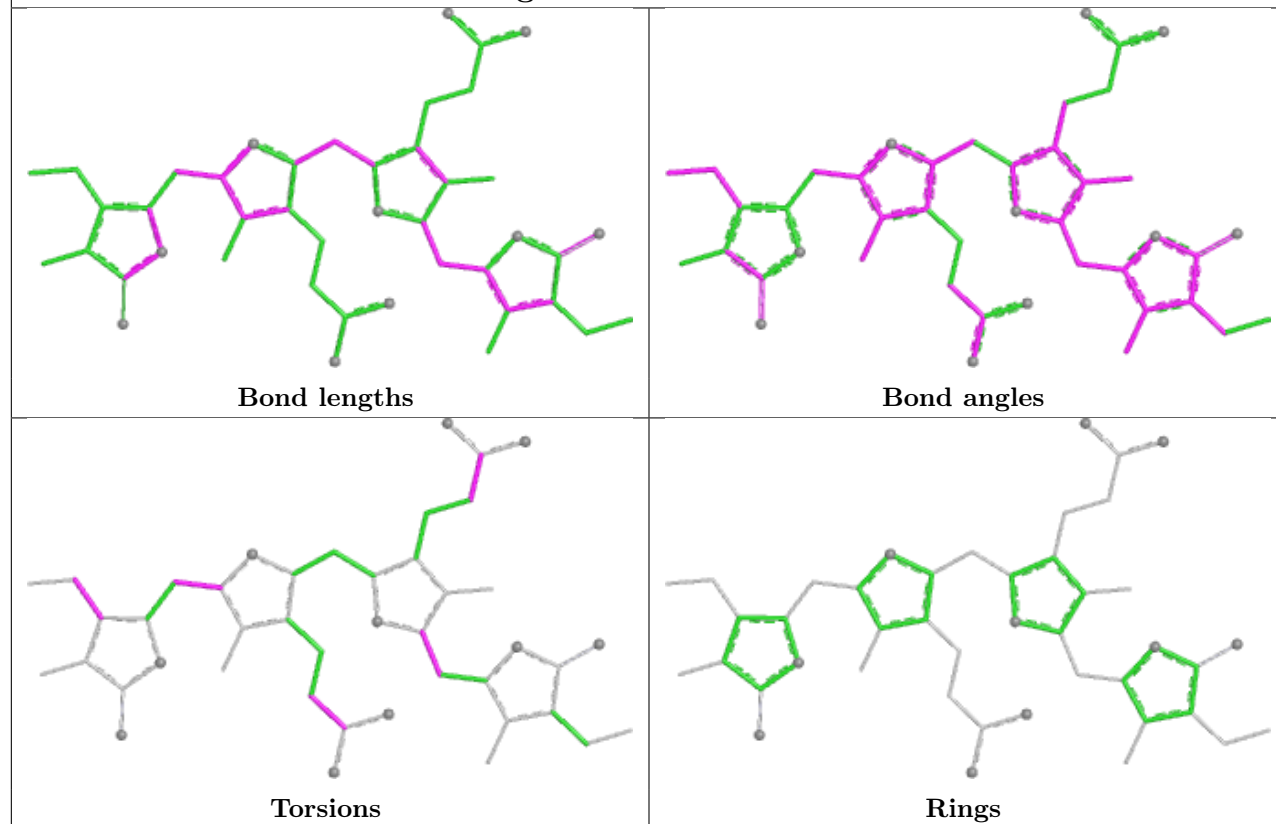
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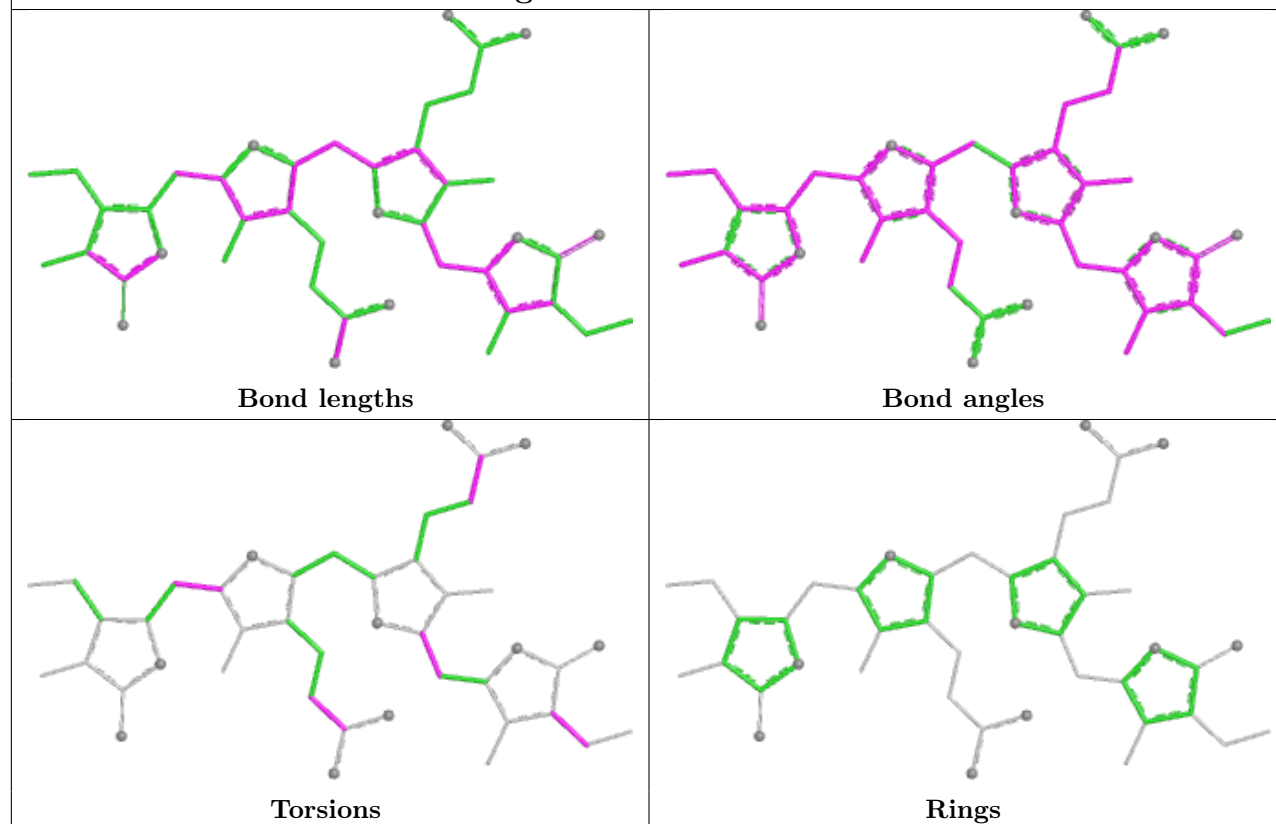
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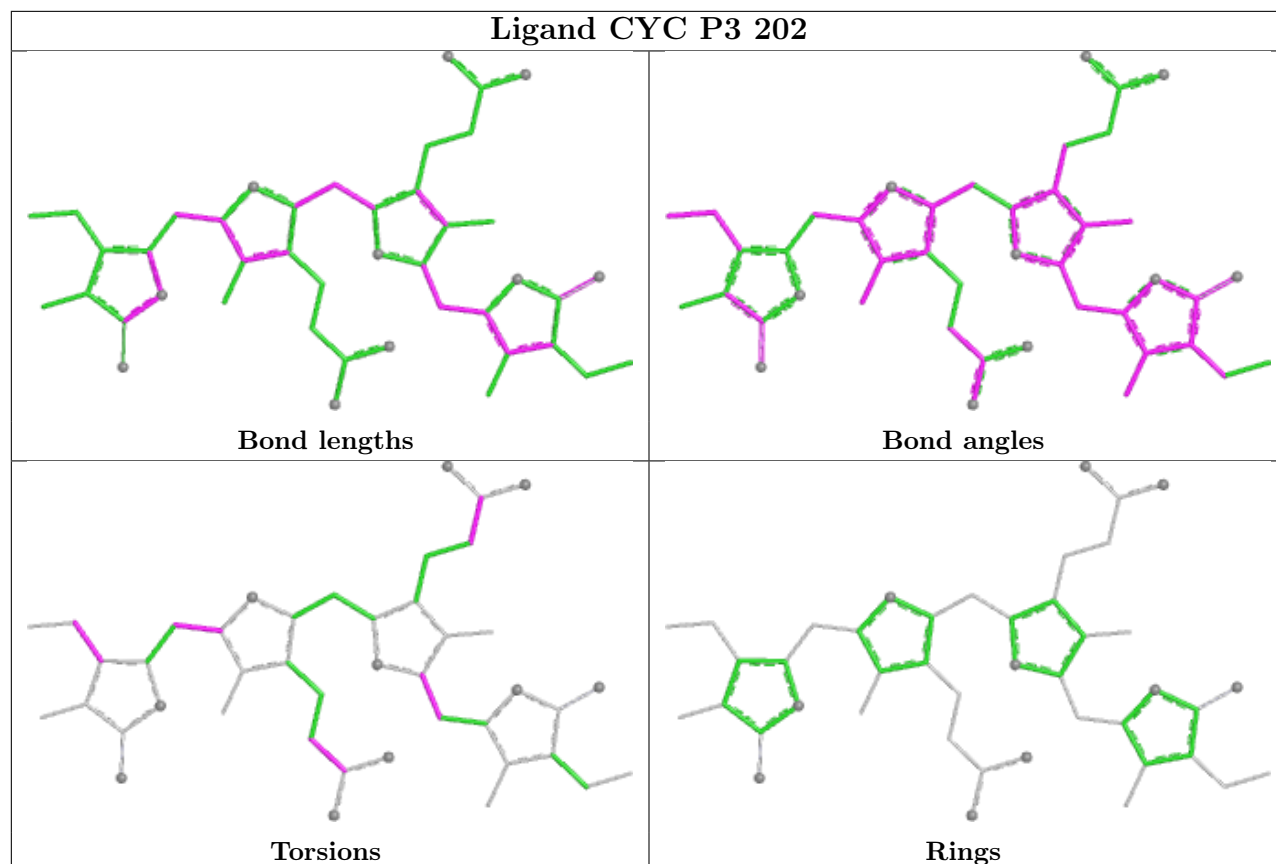
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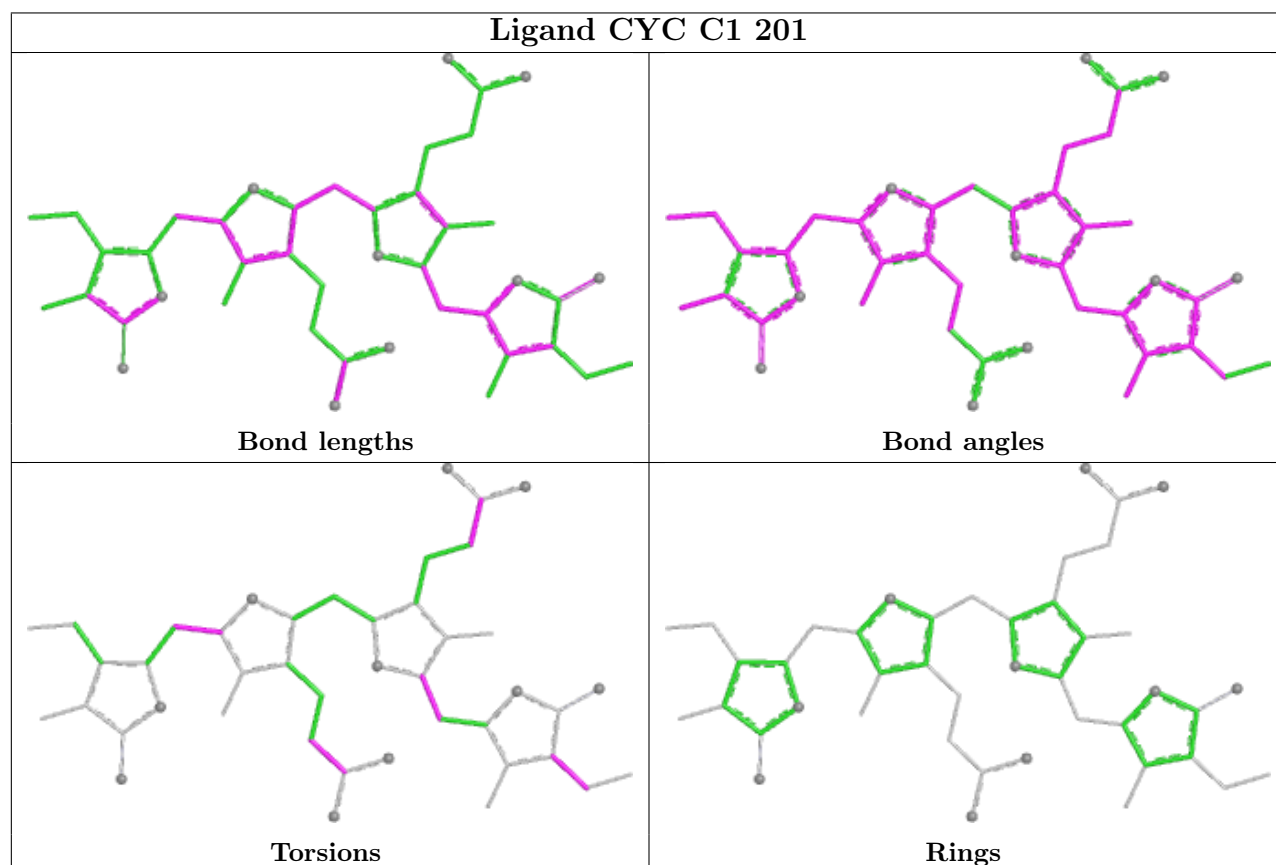
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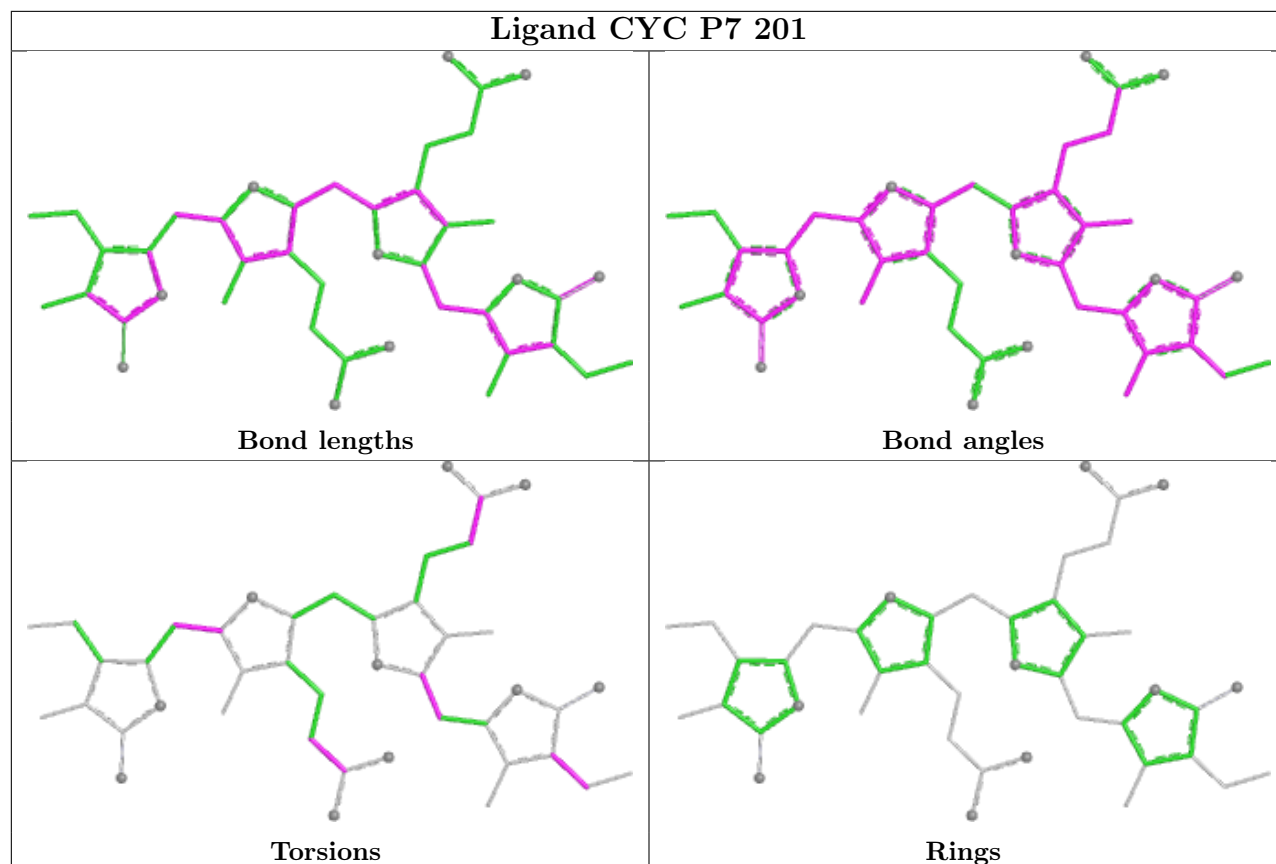
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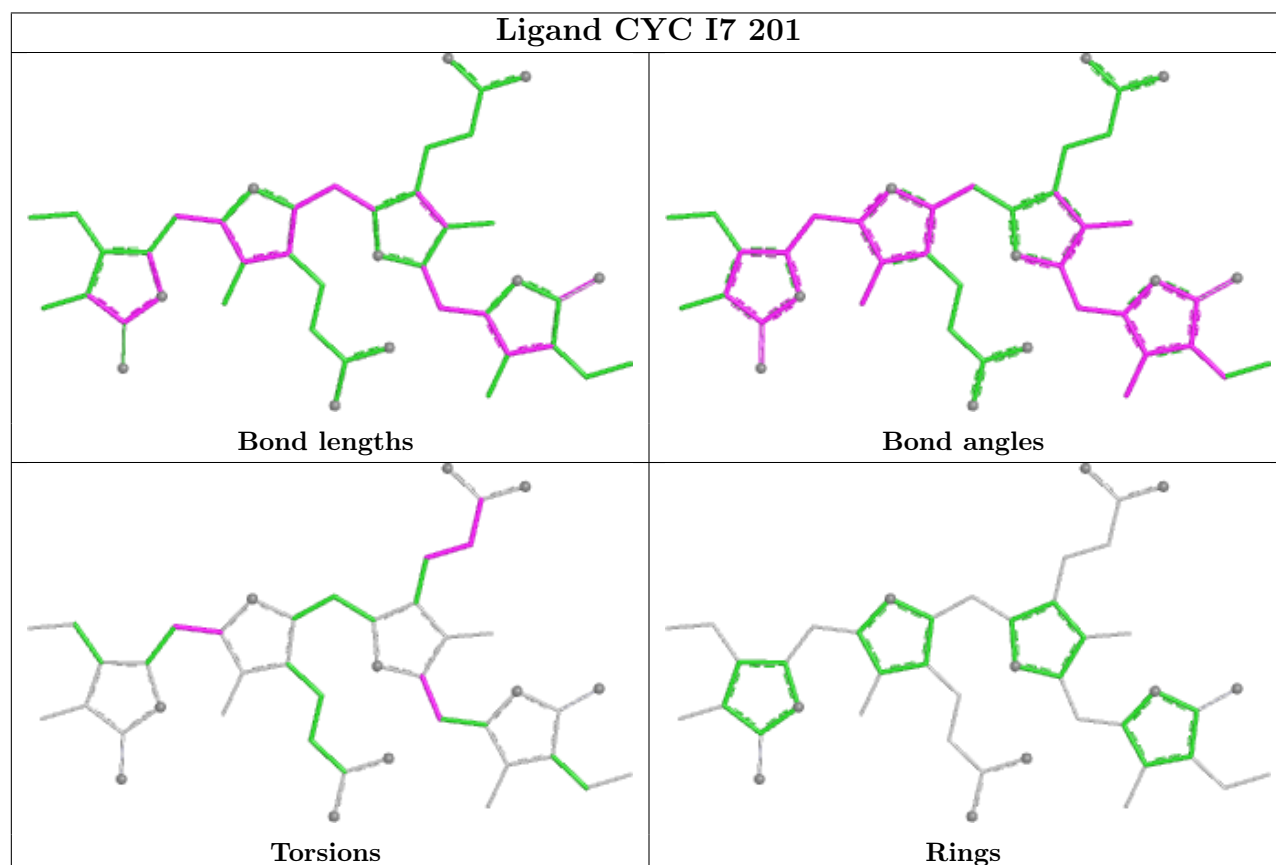
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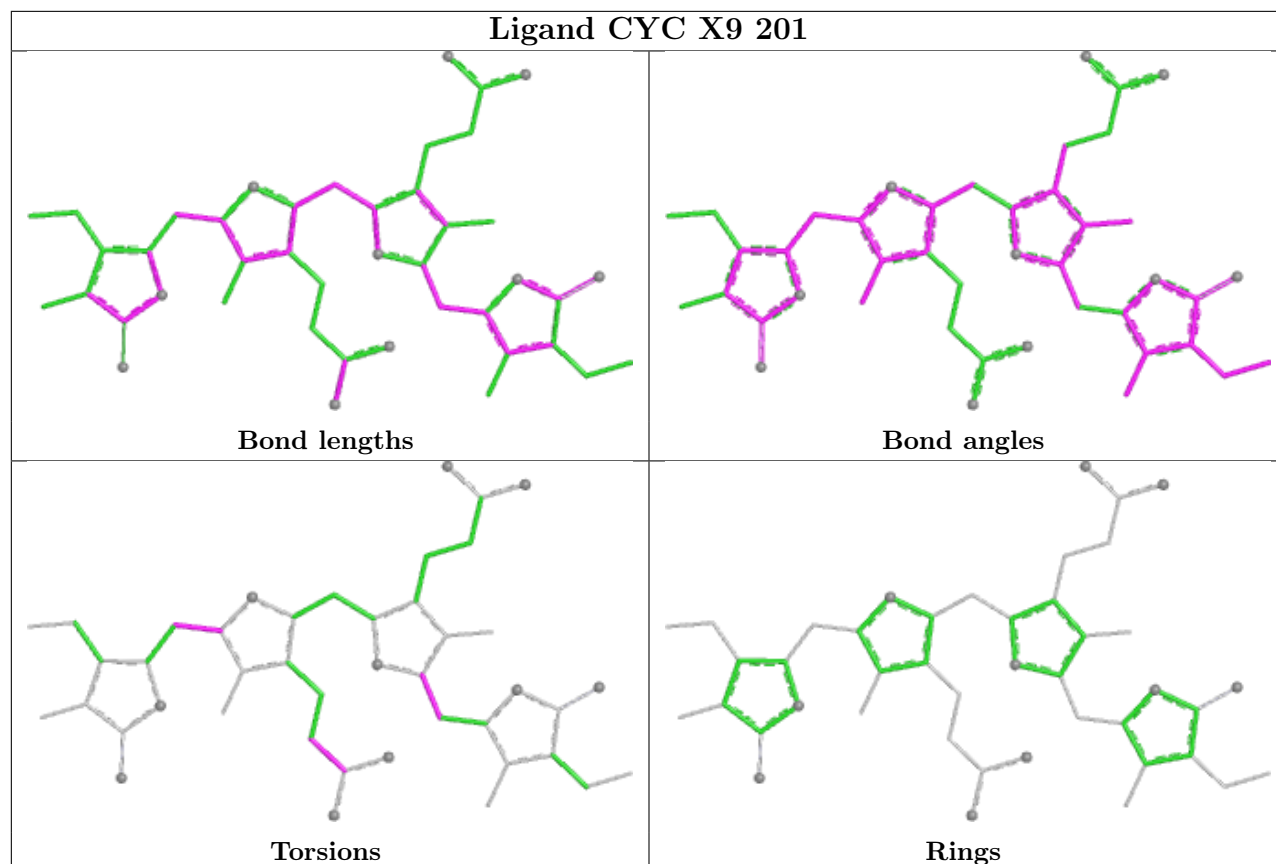
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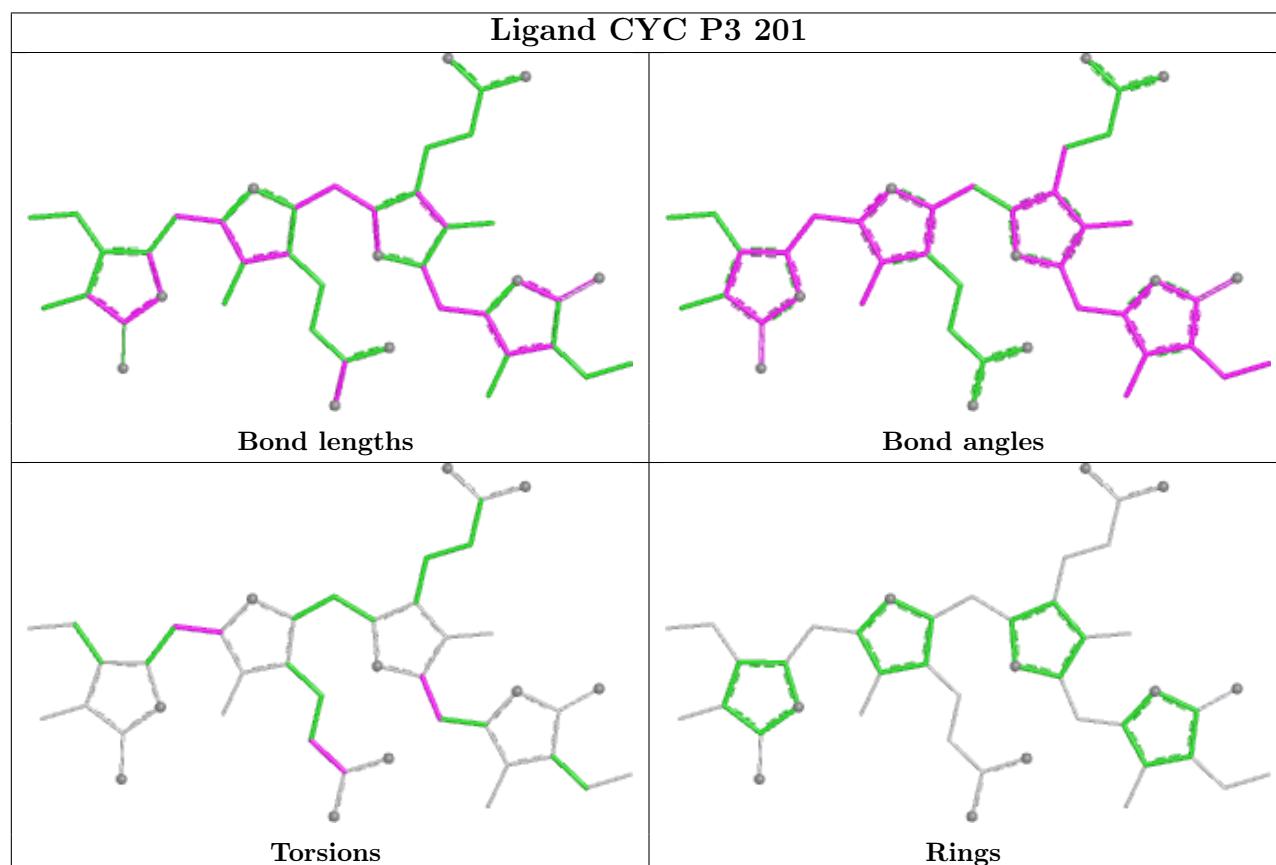
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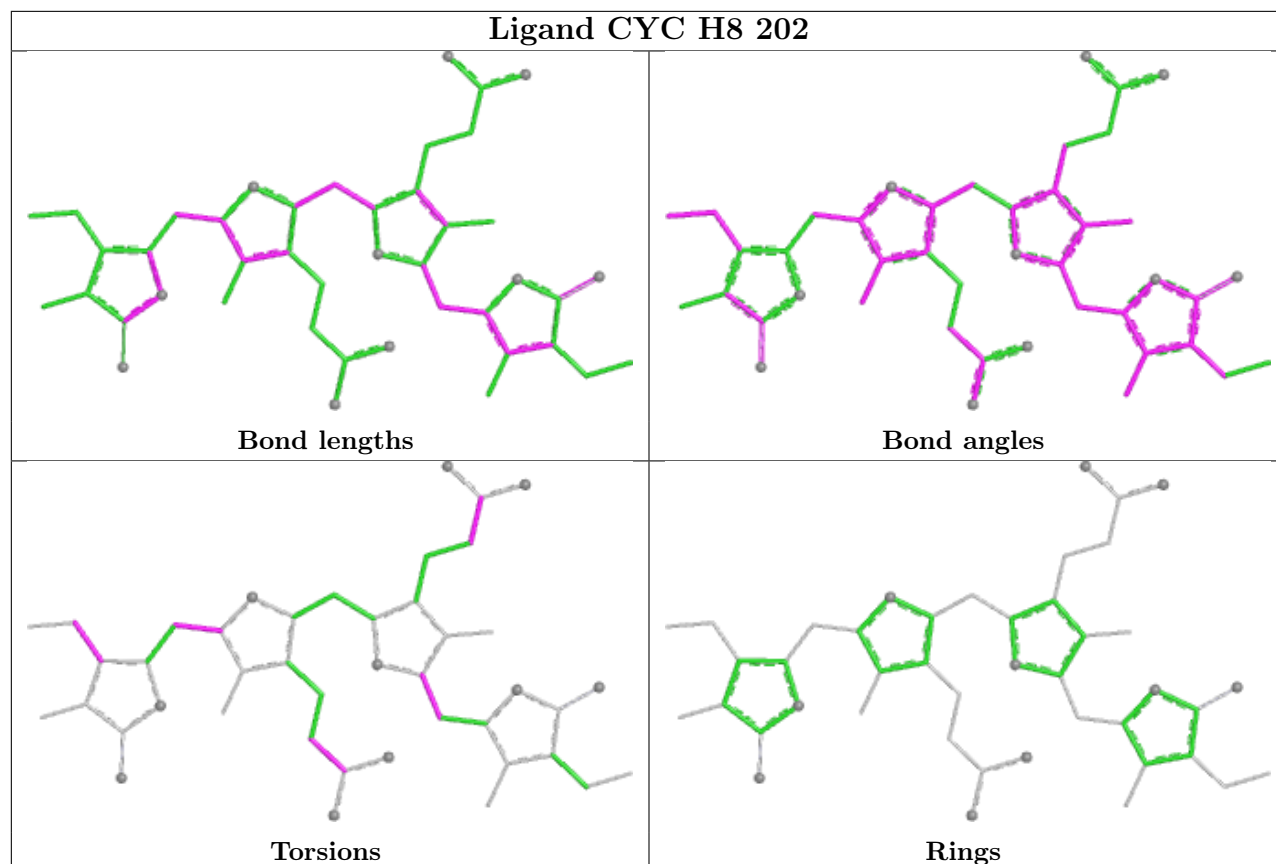
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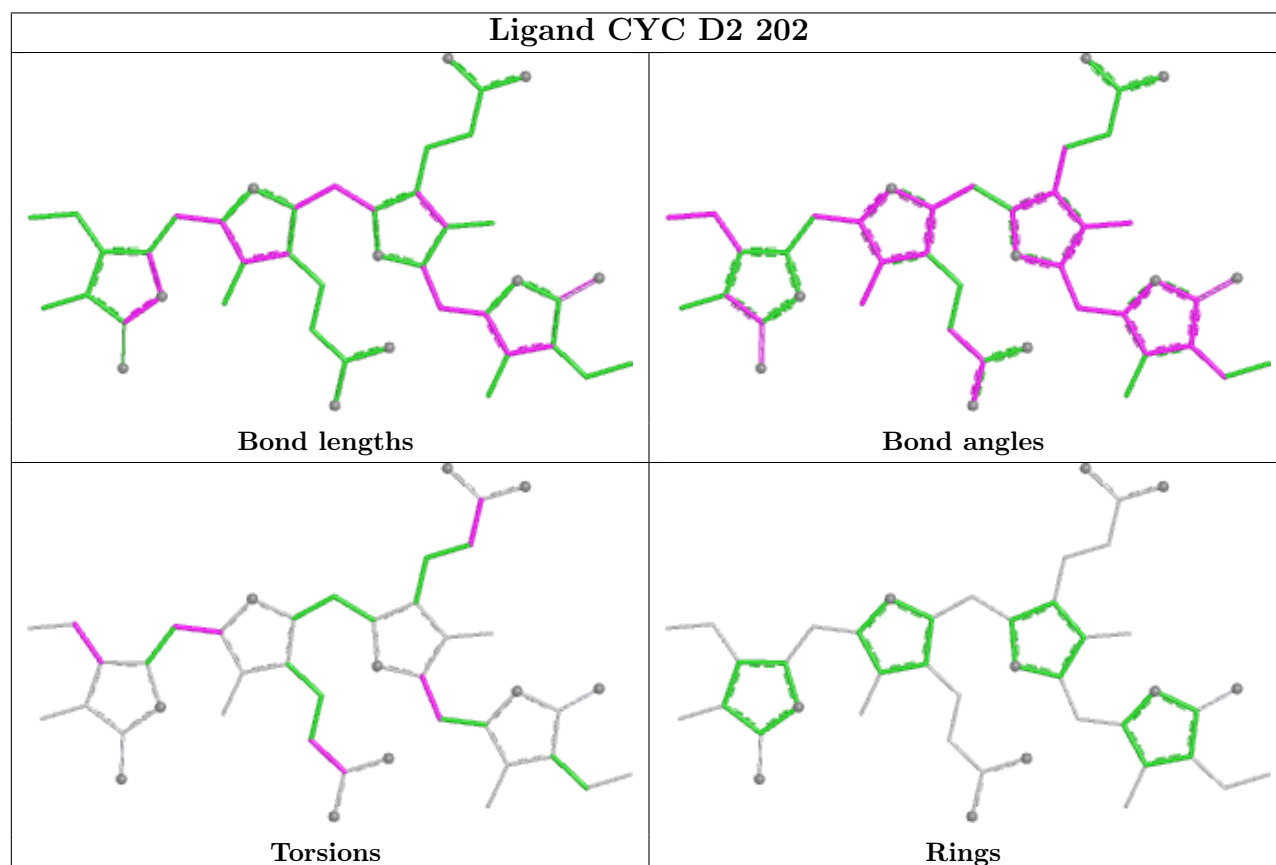
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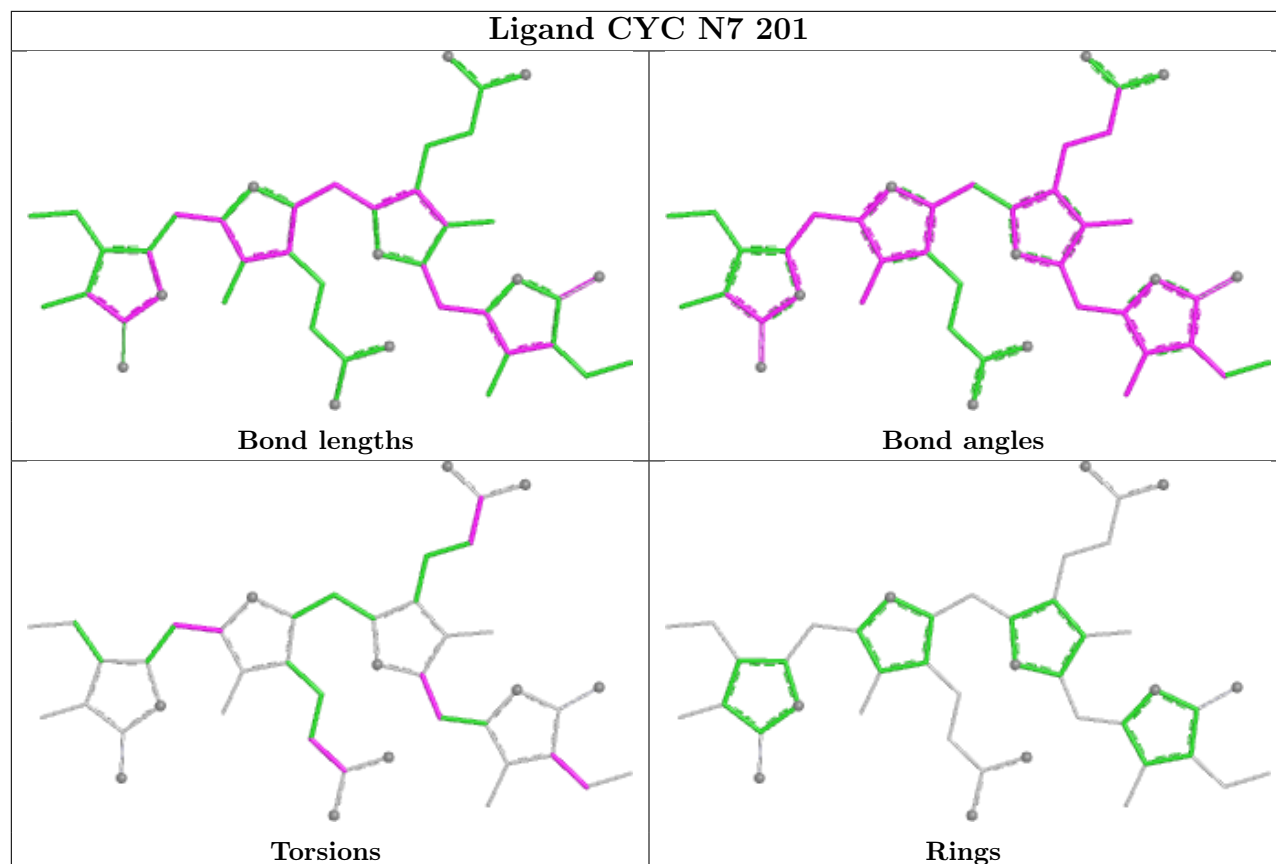
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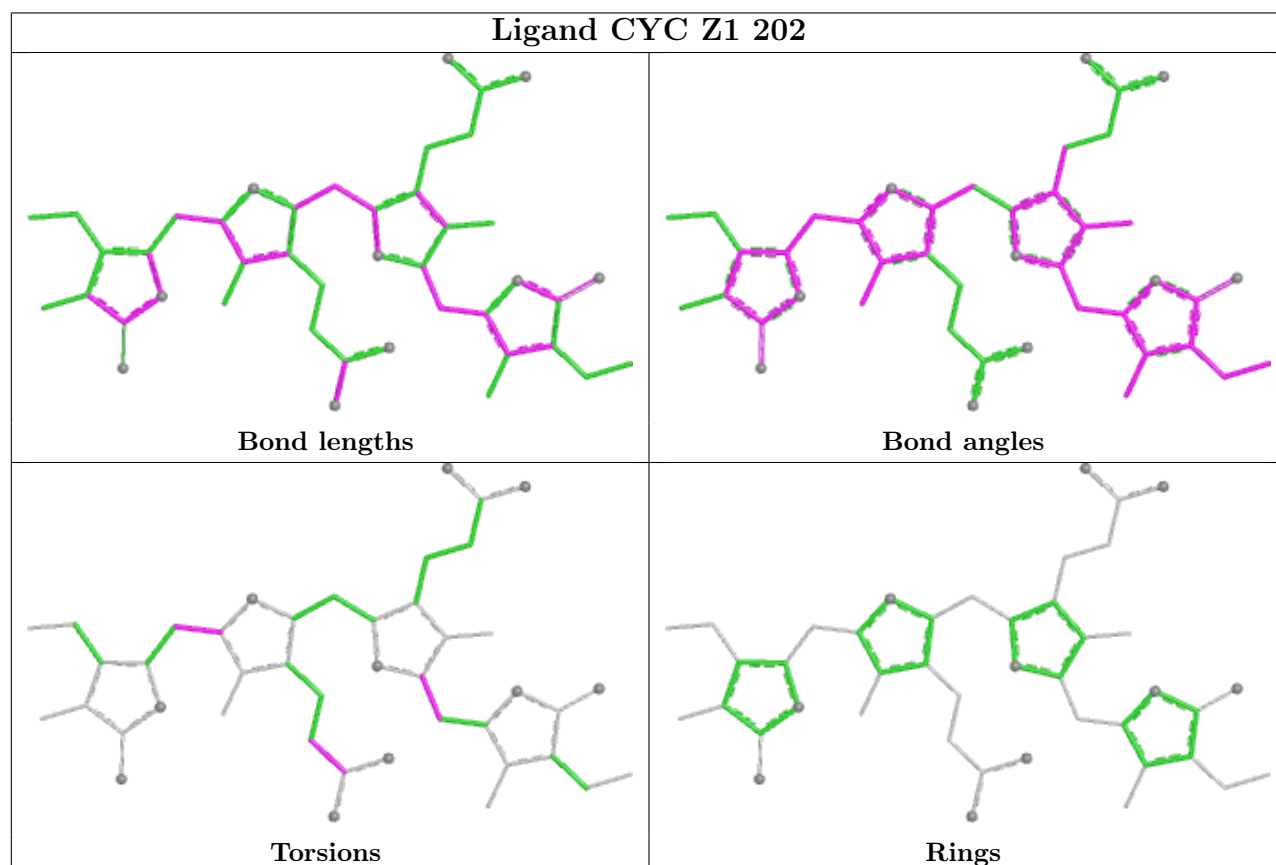
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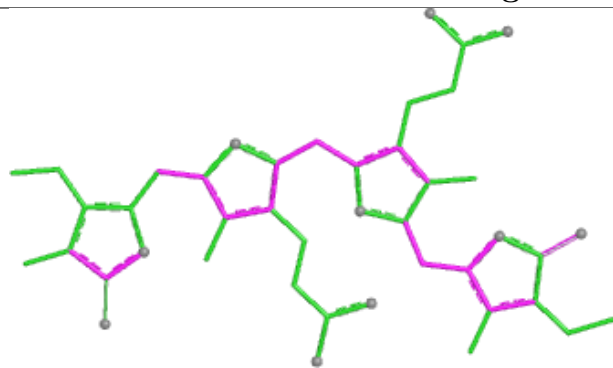
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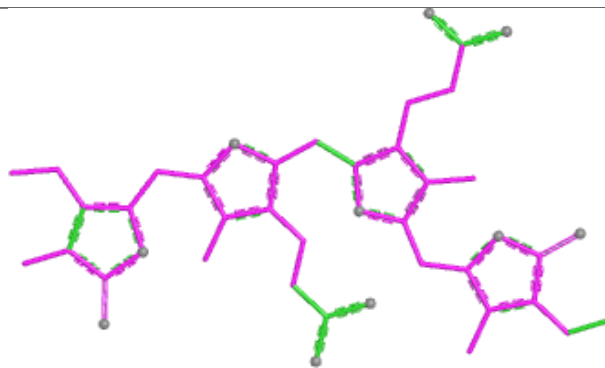
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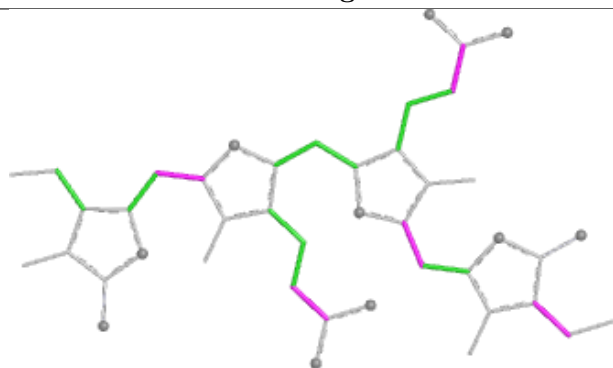
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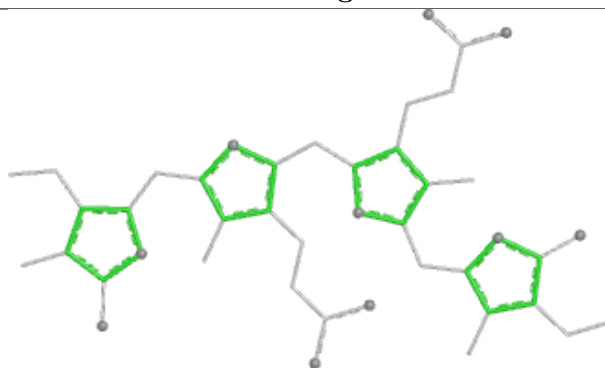
Bond lengths



Bond angles

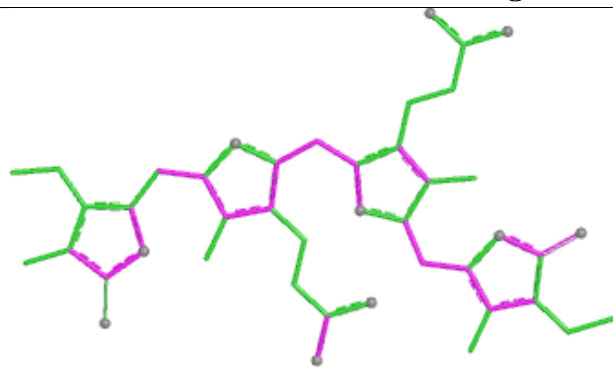


Torsions

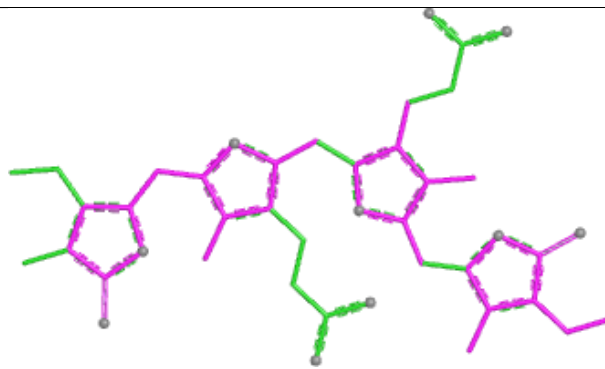


Rings

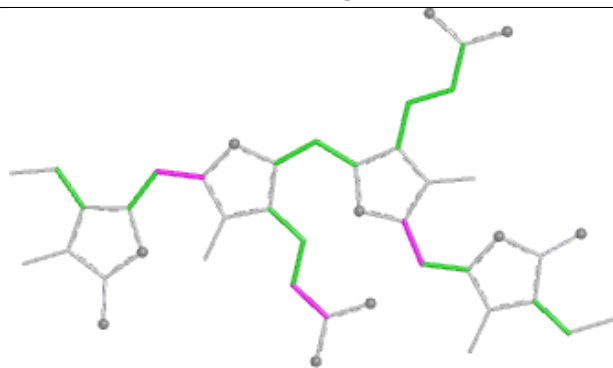
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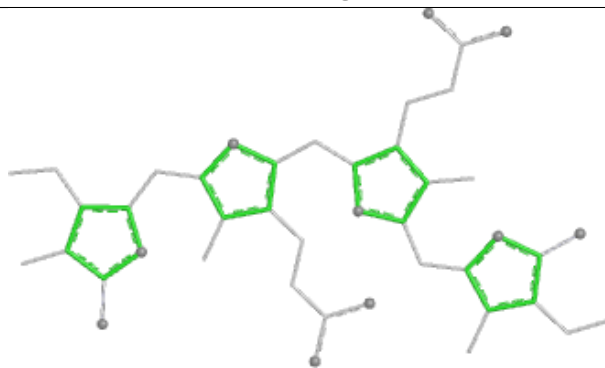
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Bond angles

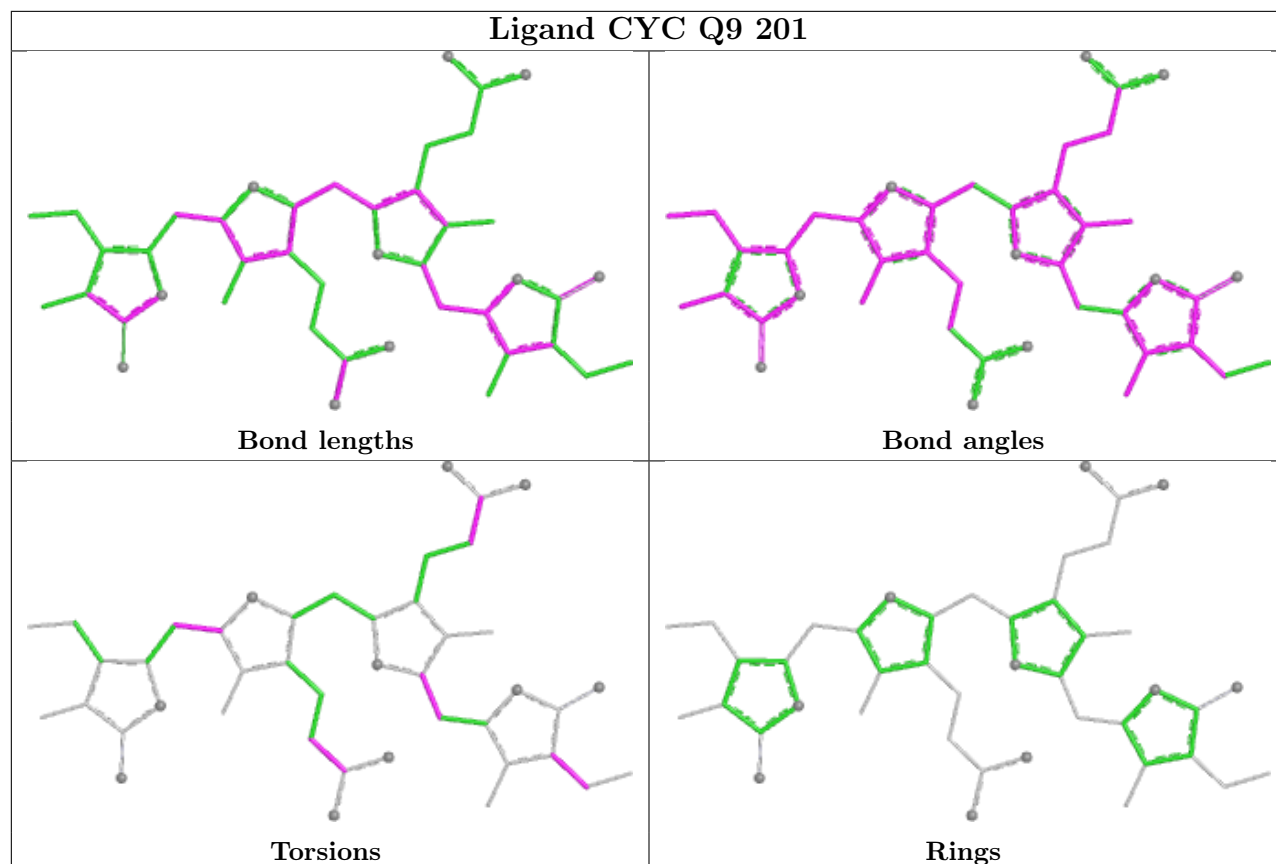


Torsions

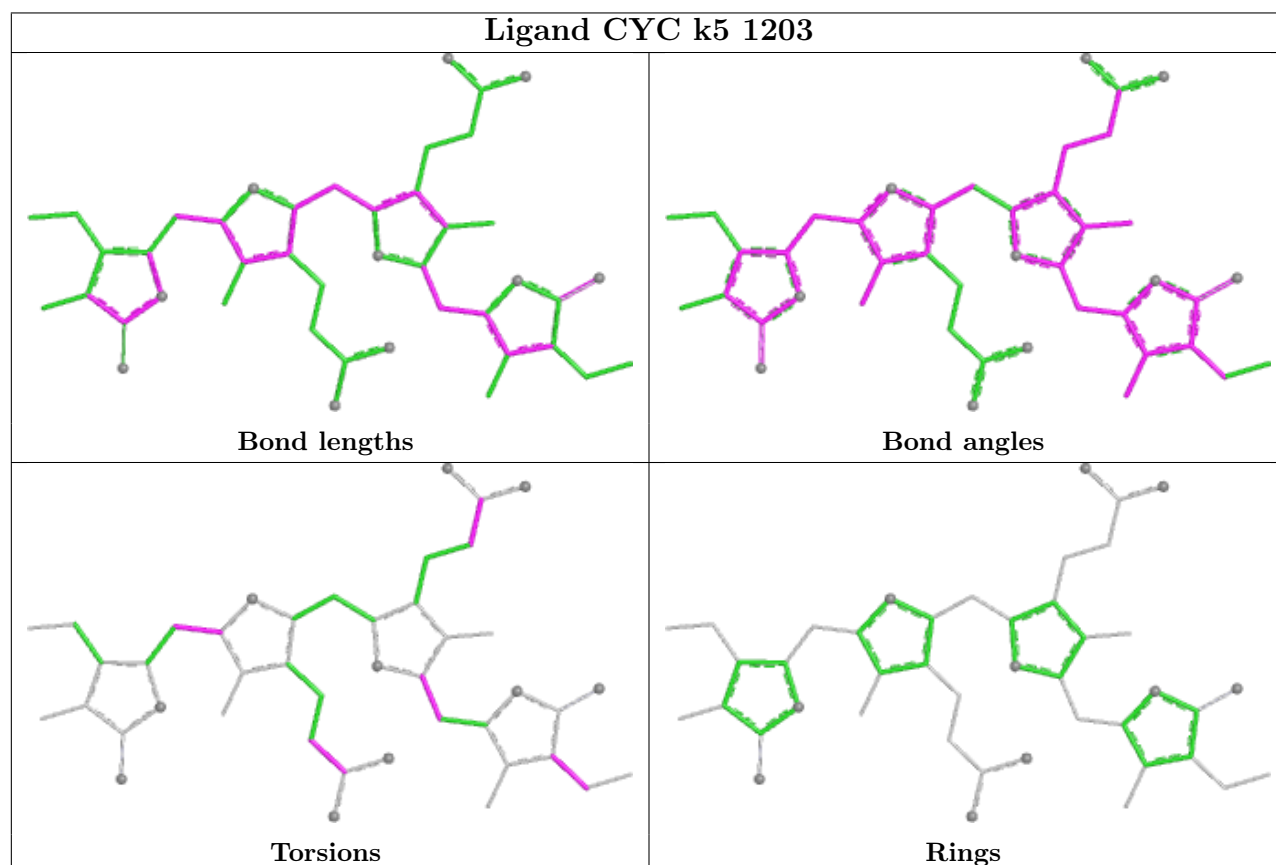


Rings

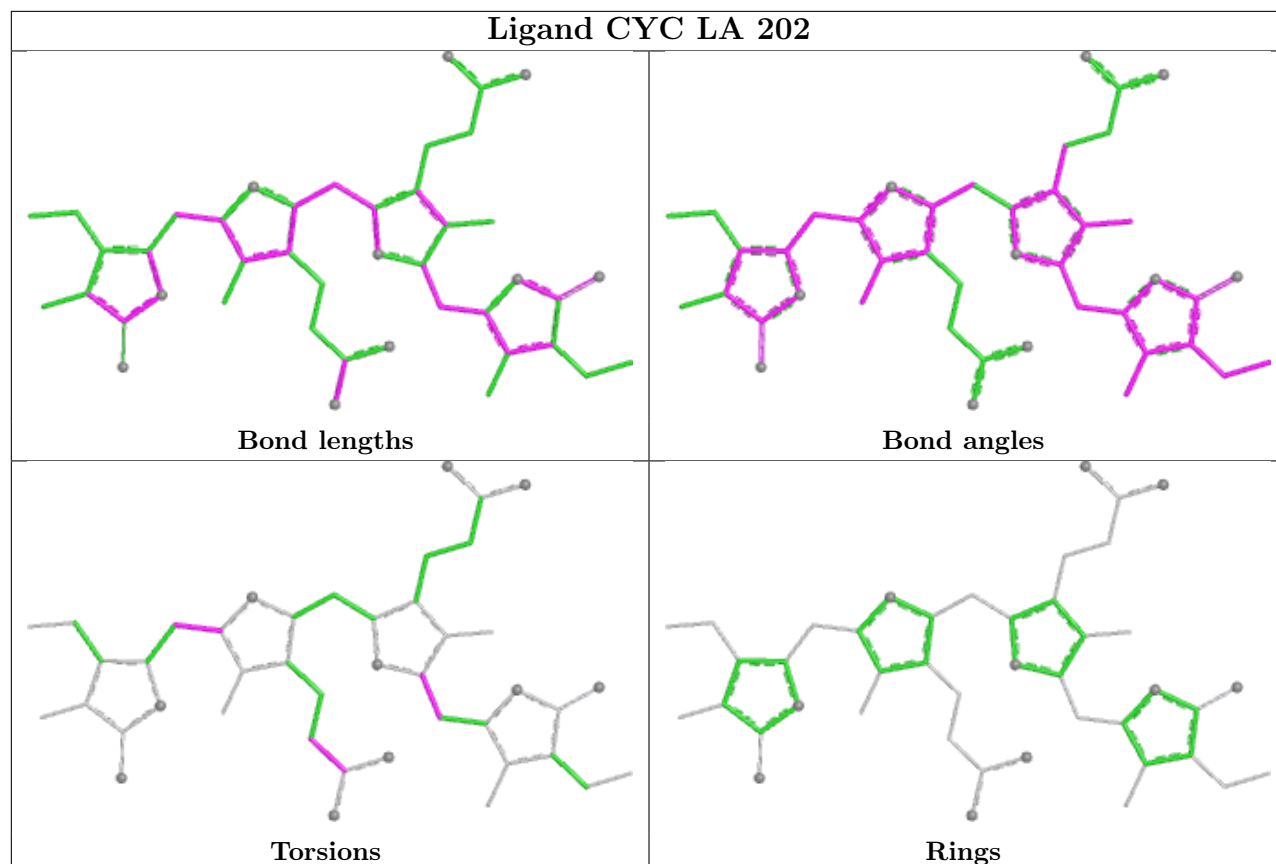
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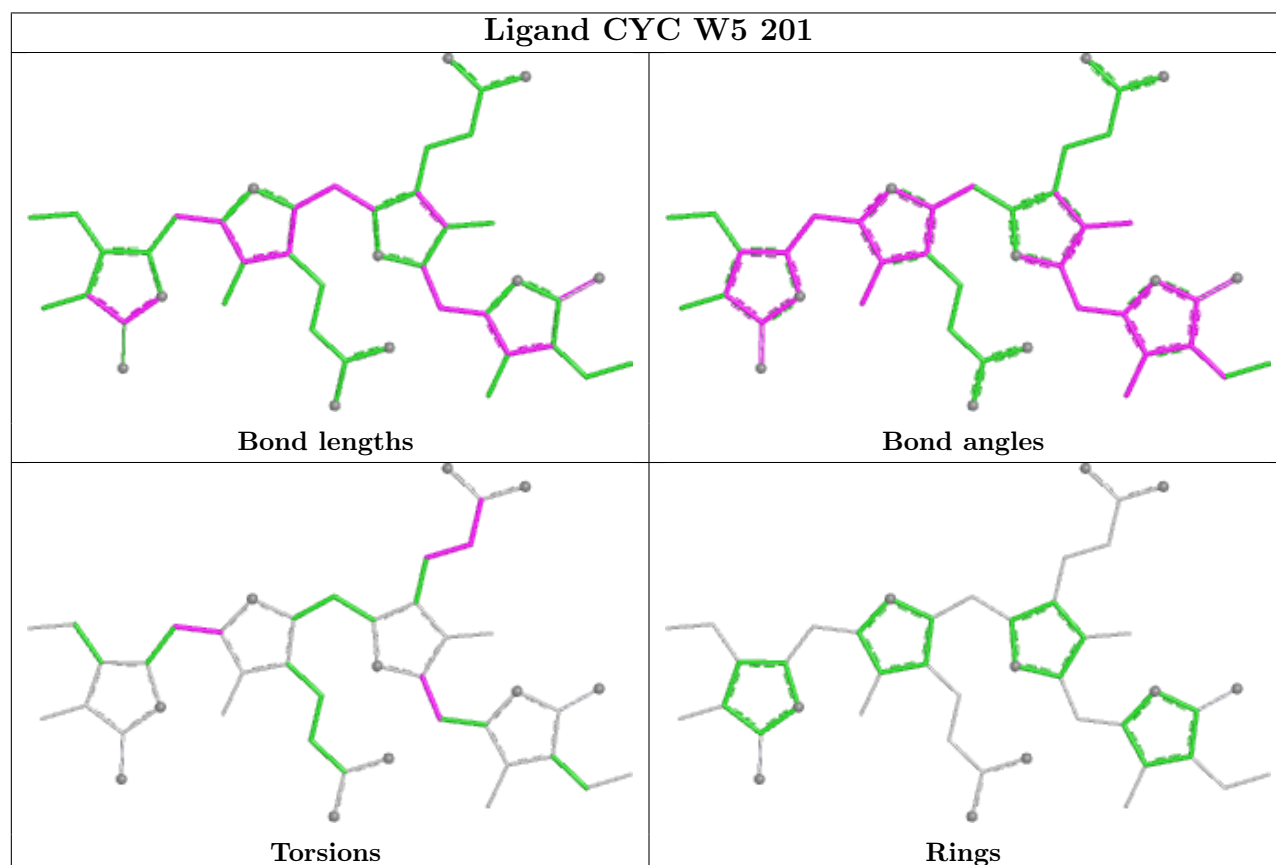
Ligand CYC k5 1203



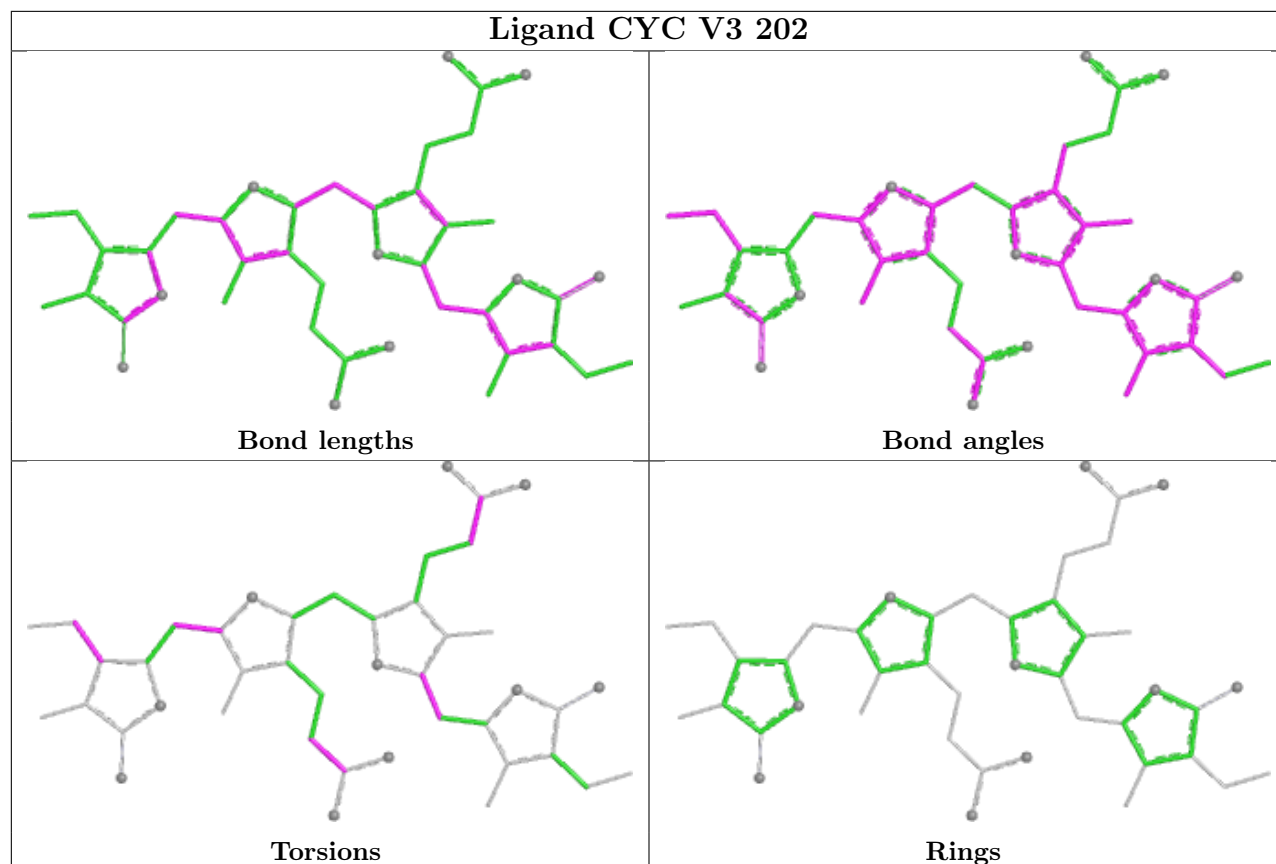
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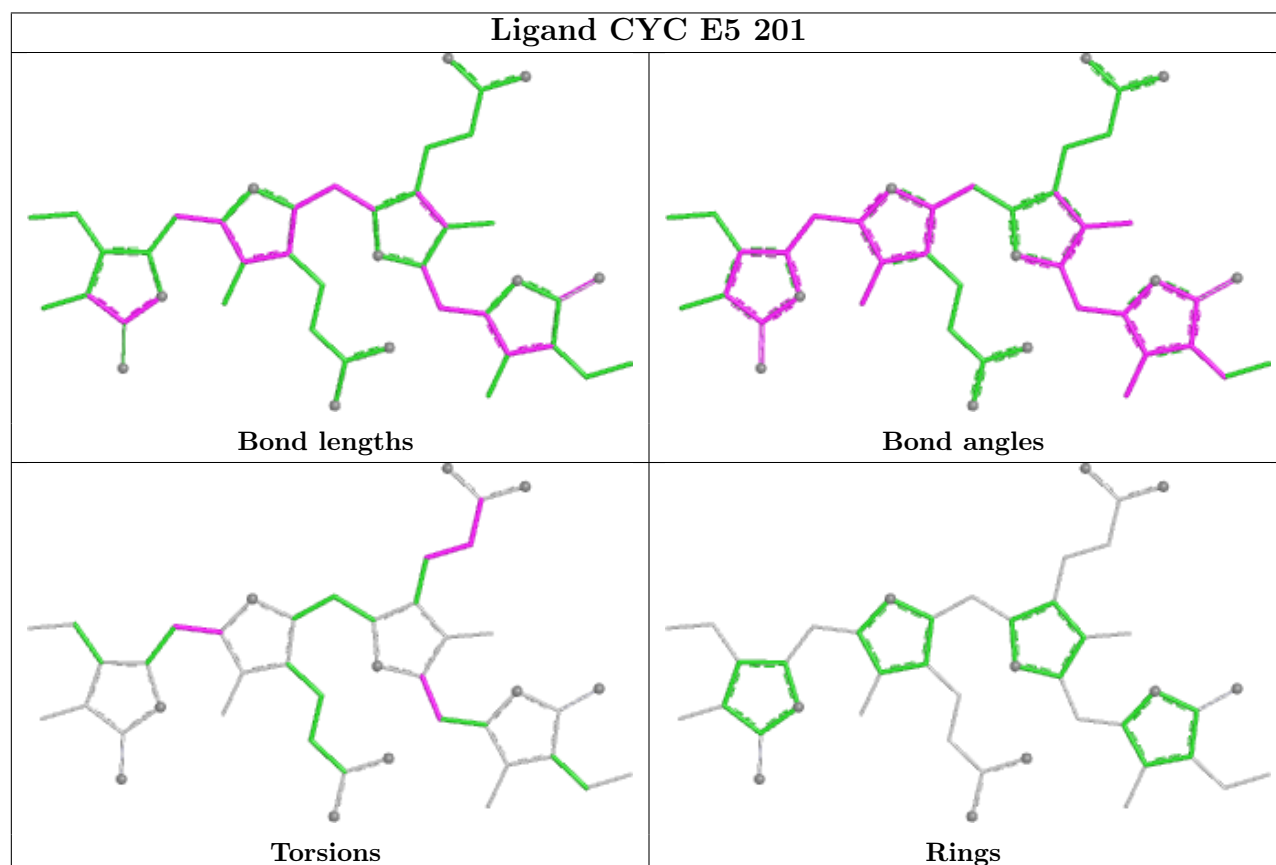
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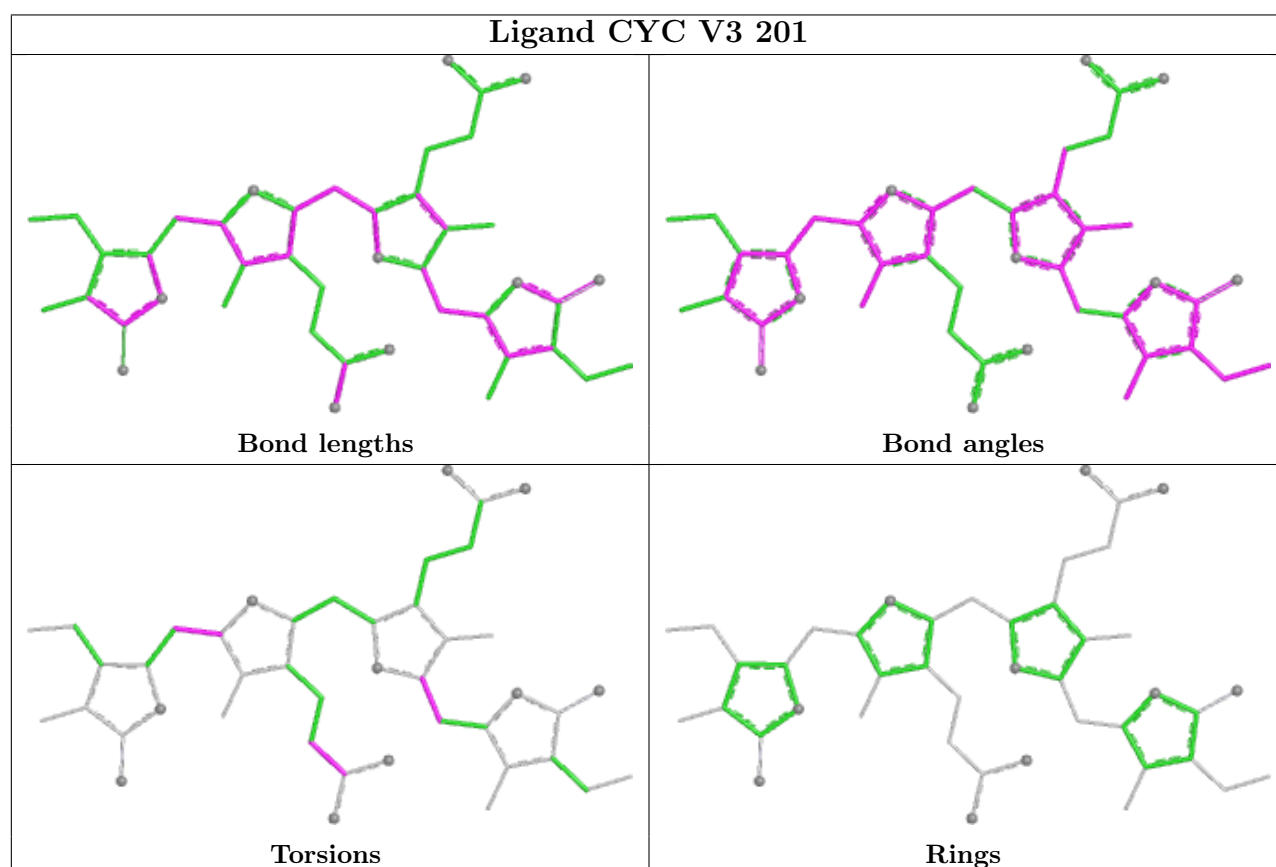
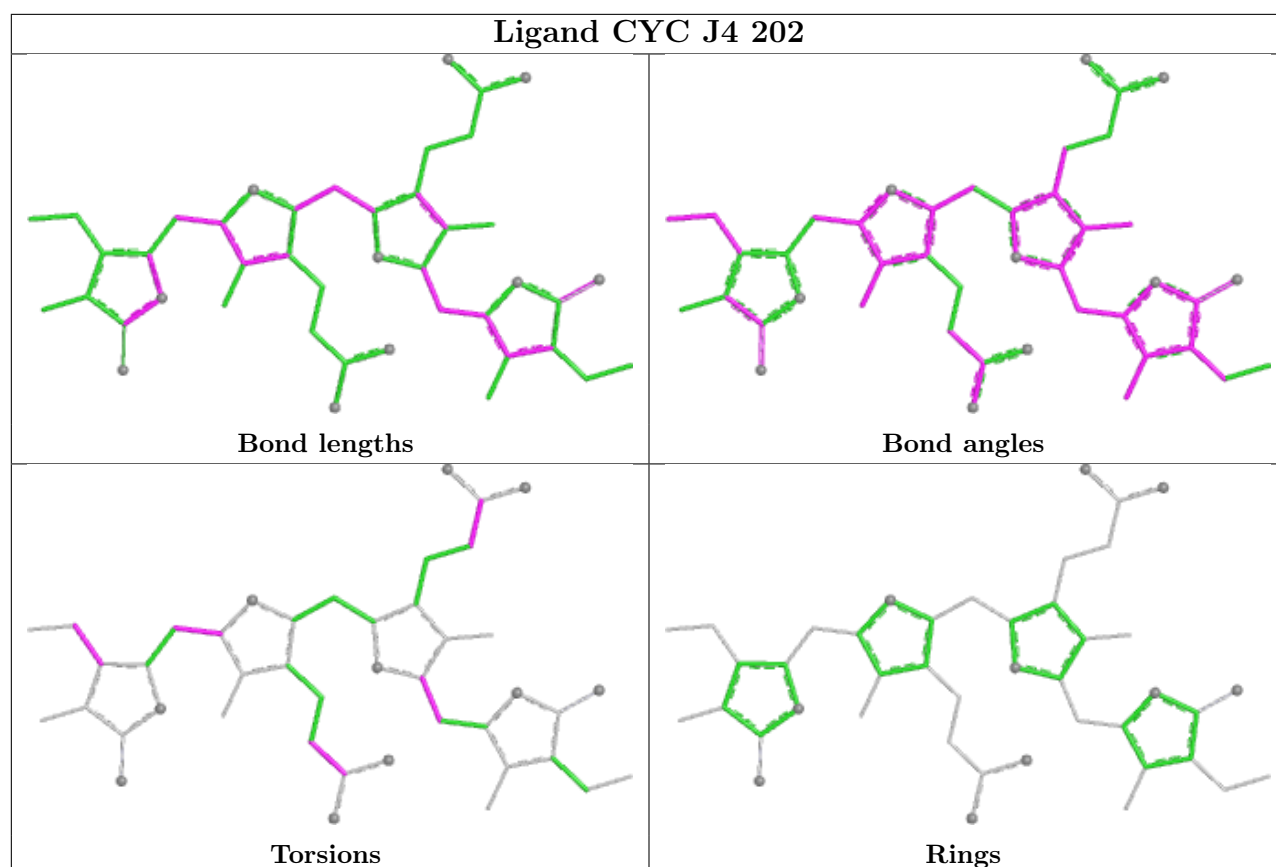


Ligand CYC V3 202

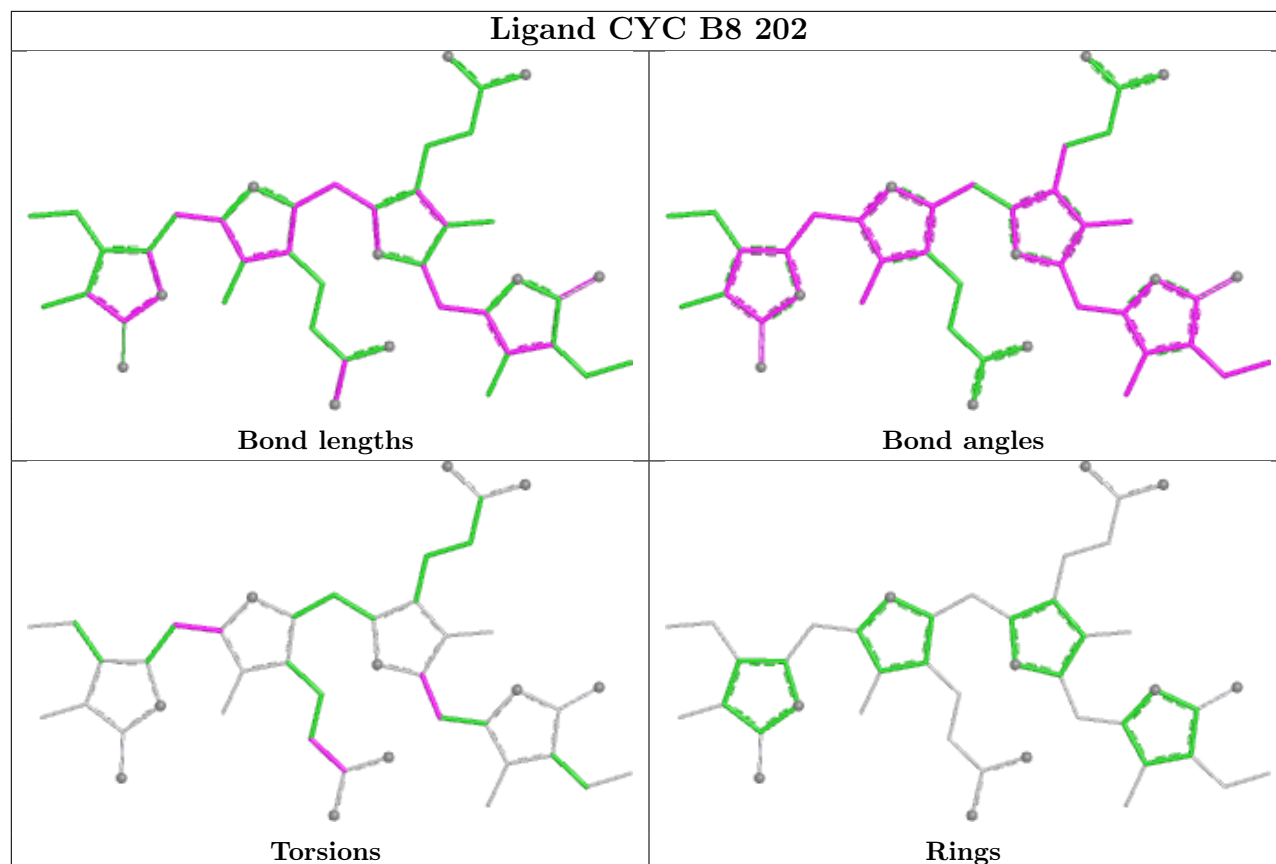


Ligand CYC E5 201

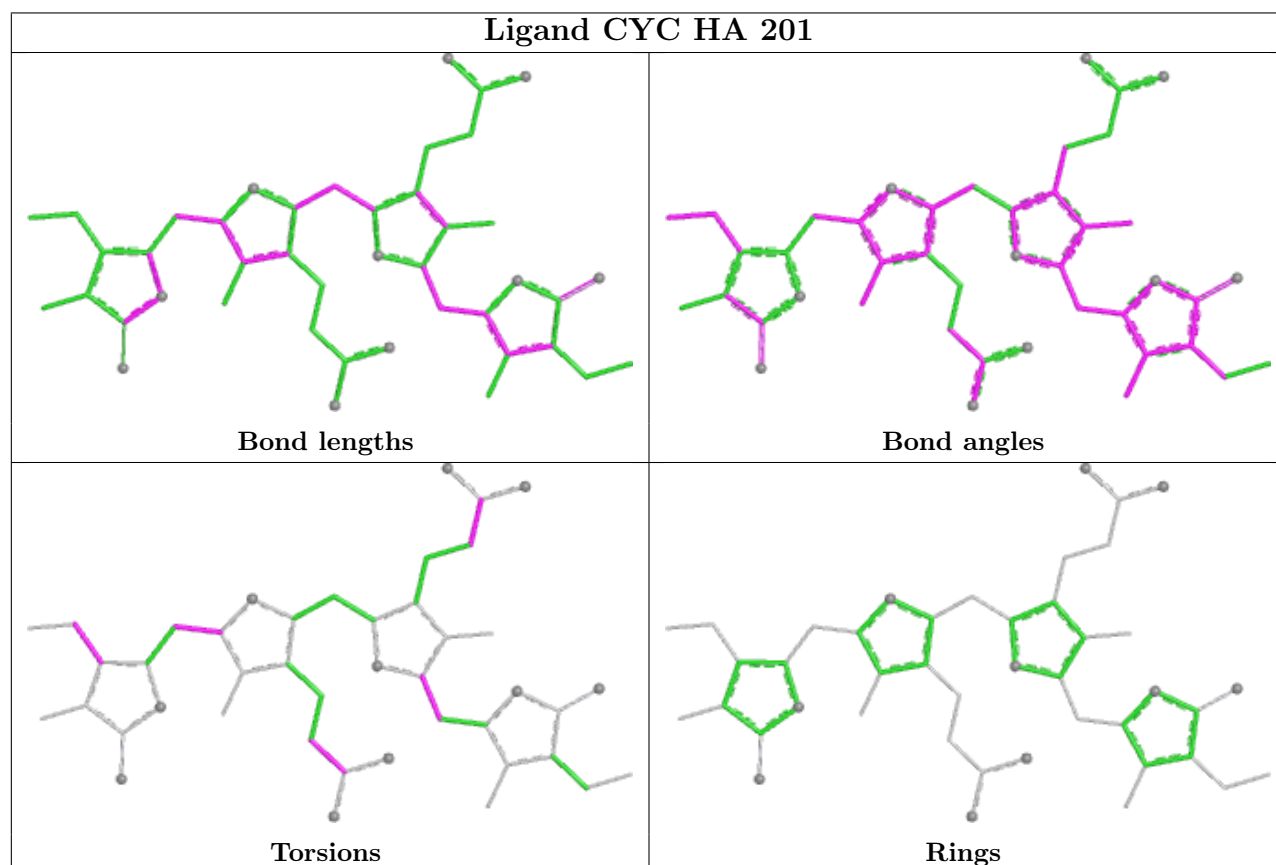




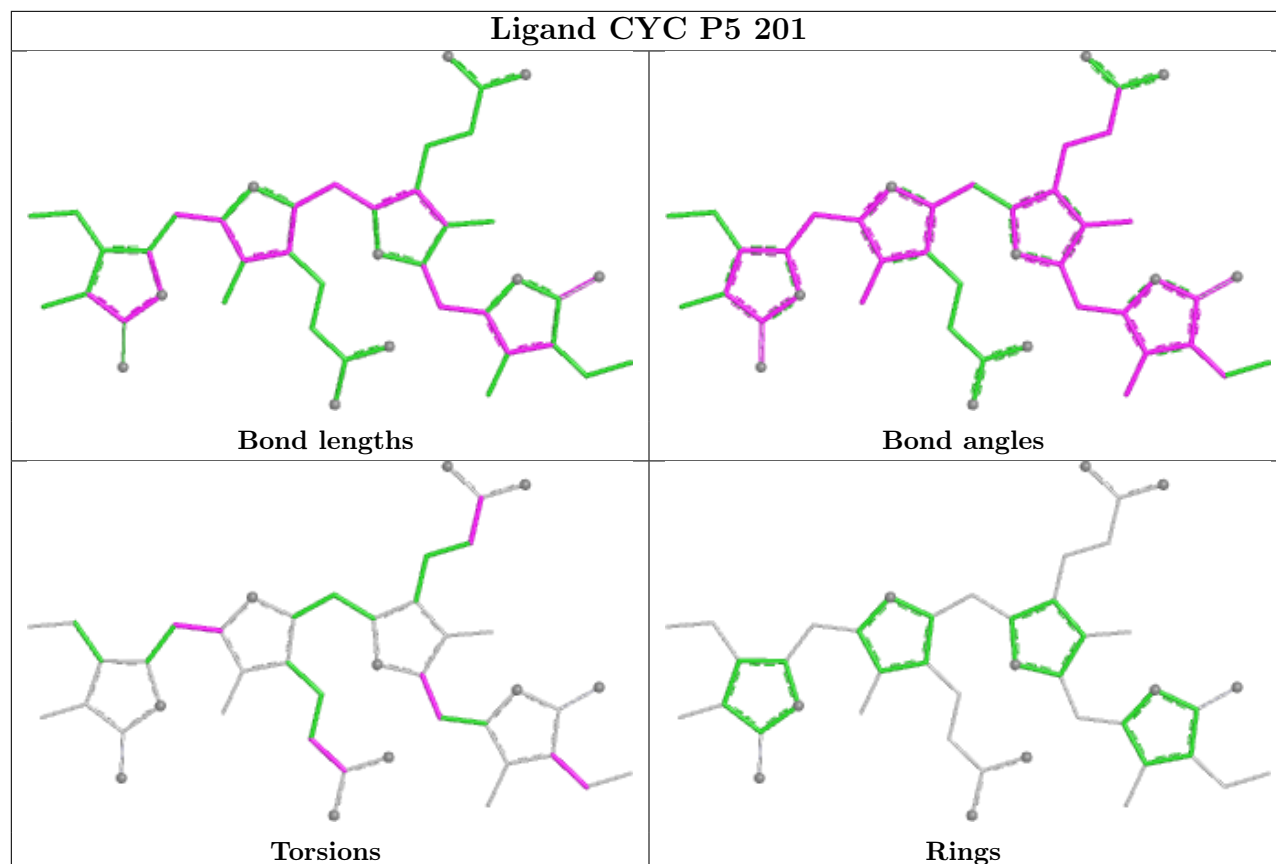
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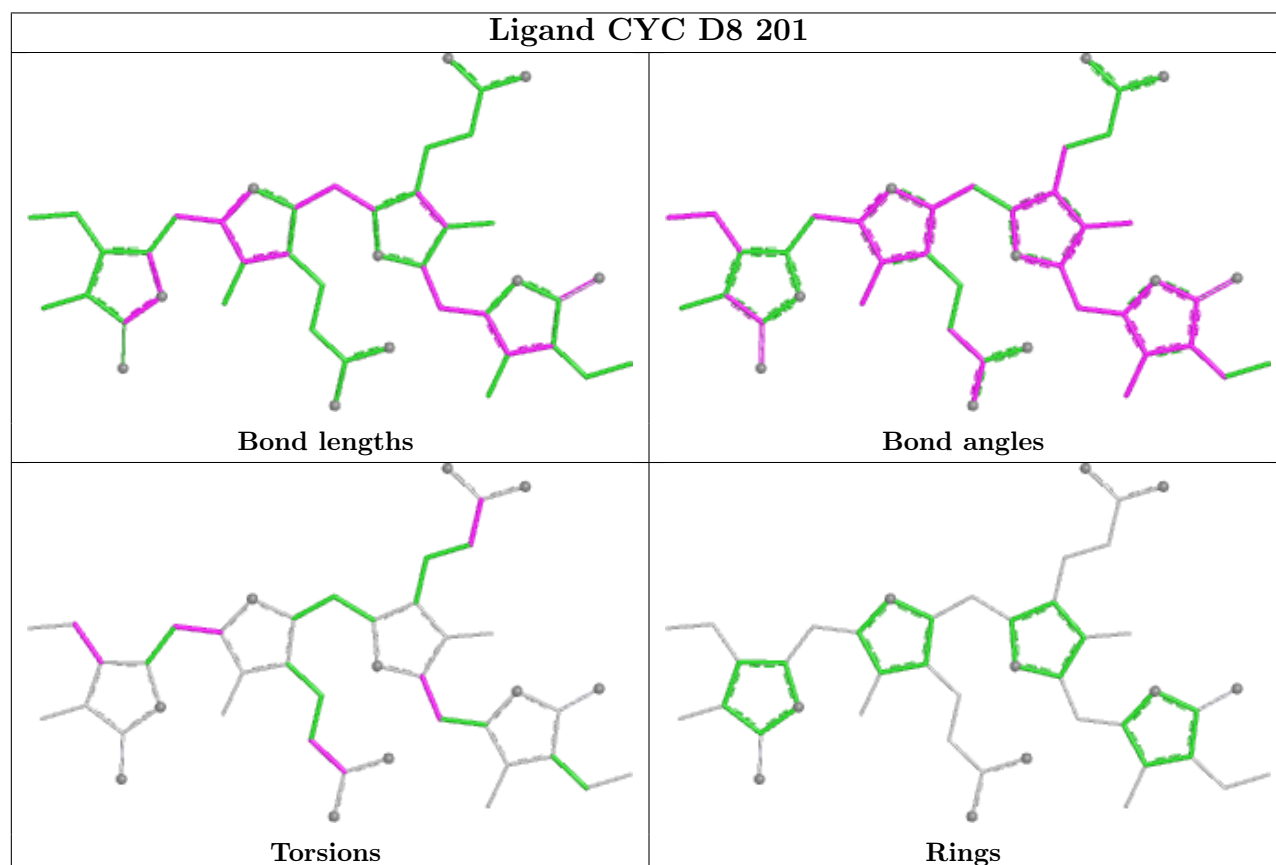
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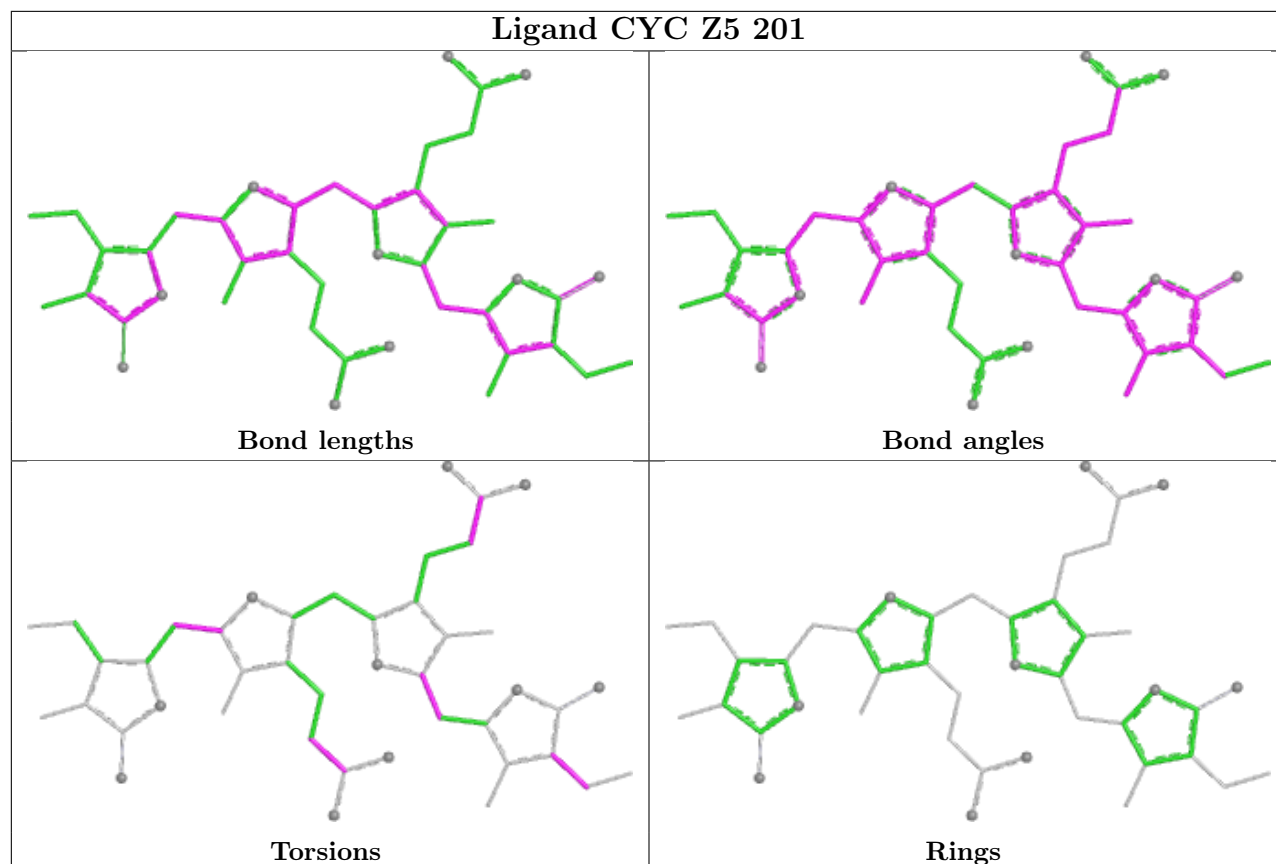
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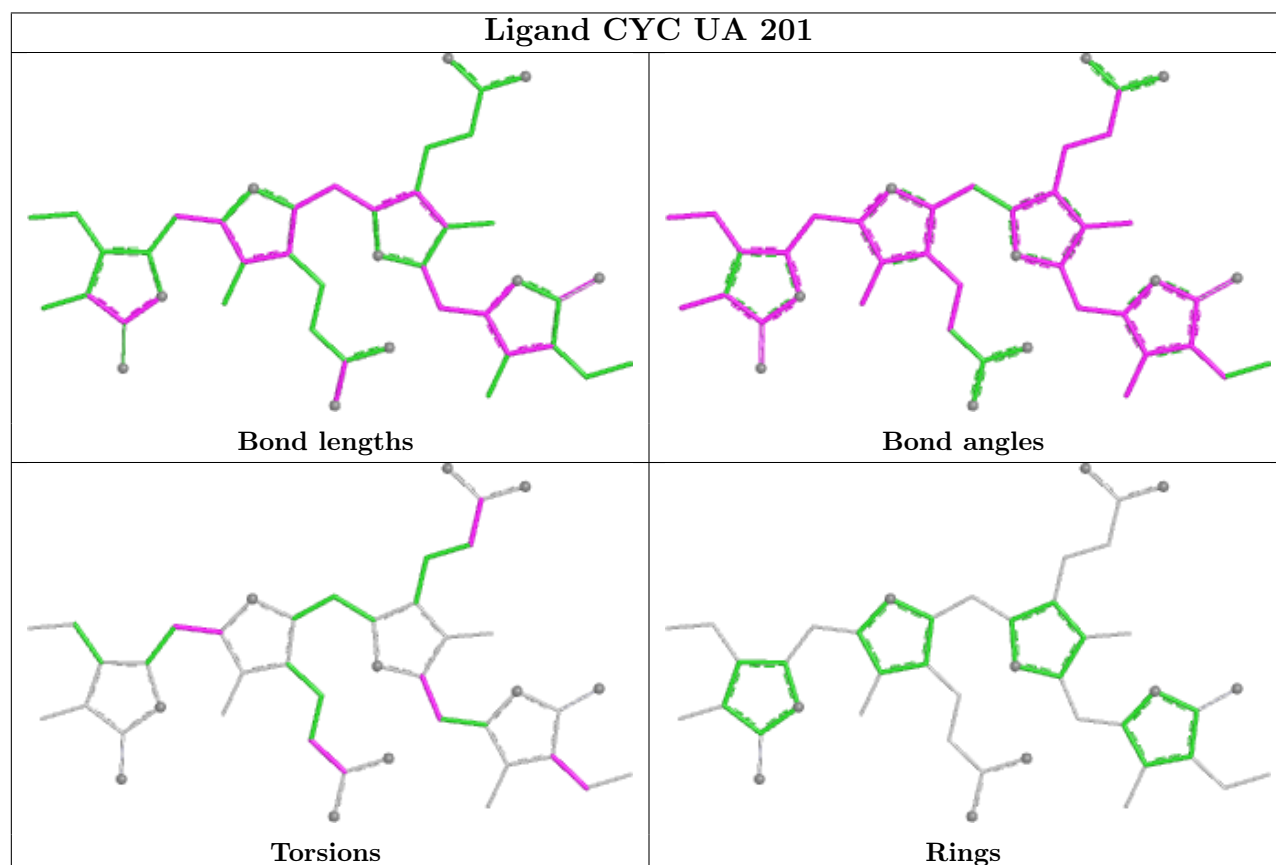
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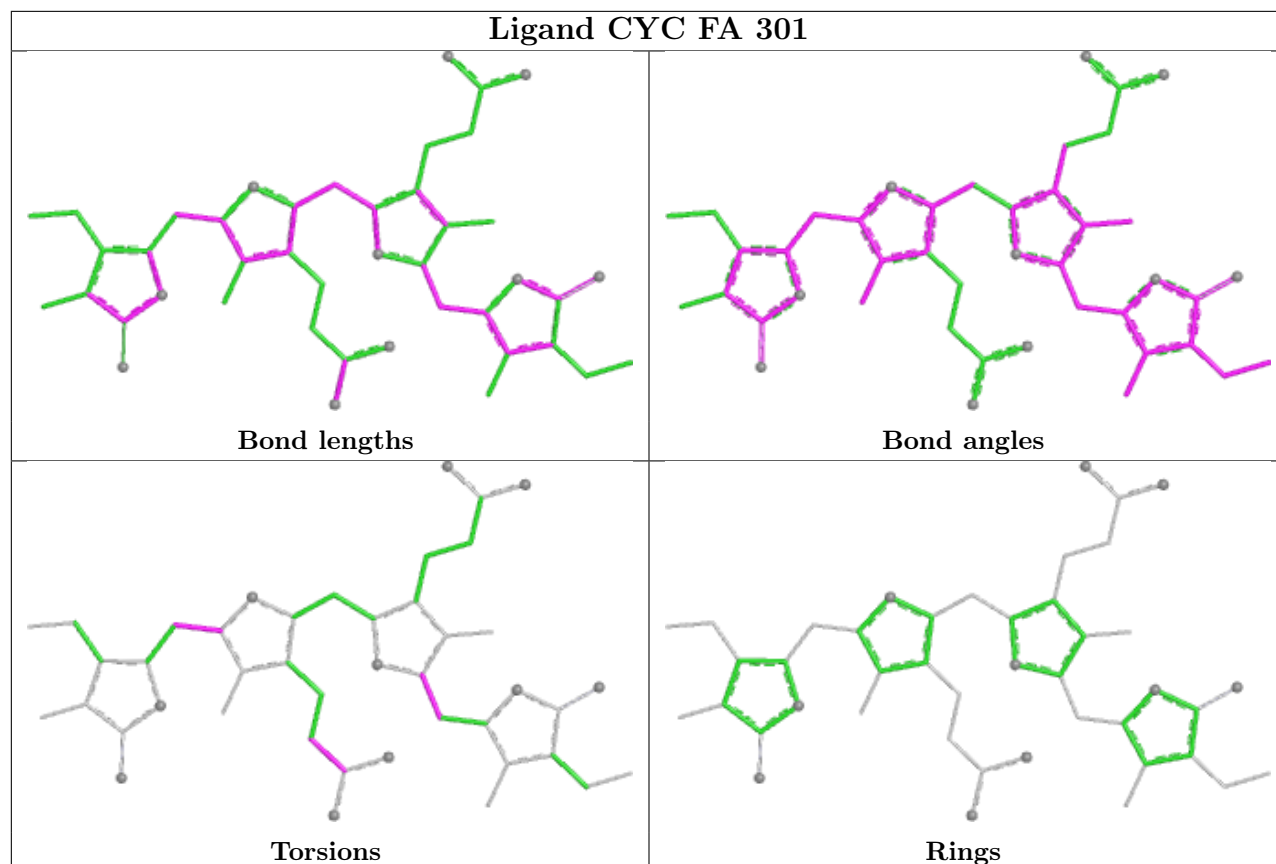
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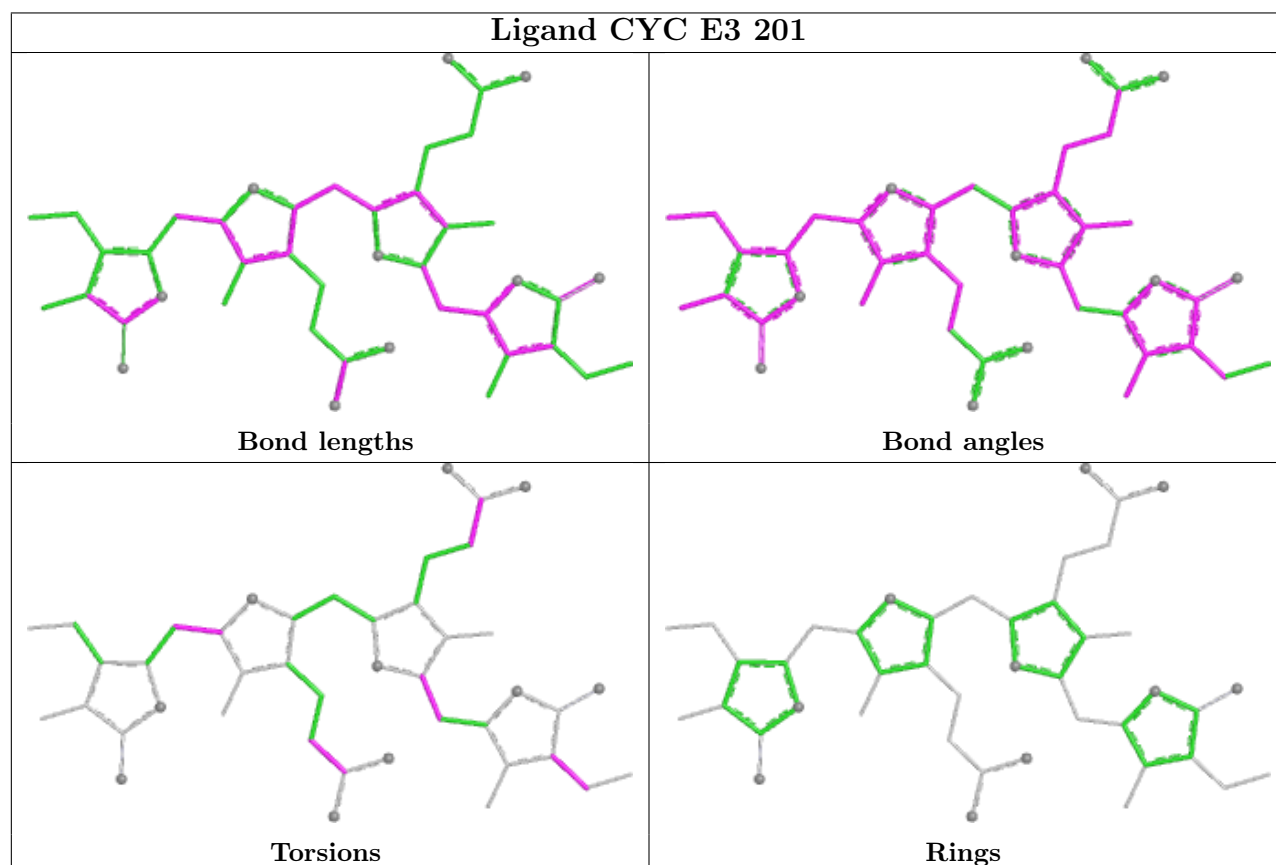
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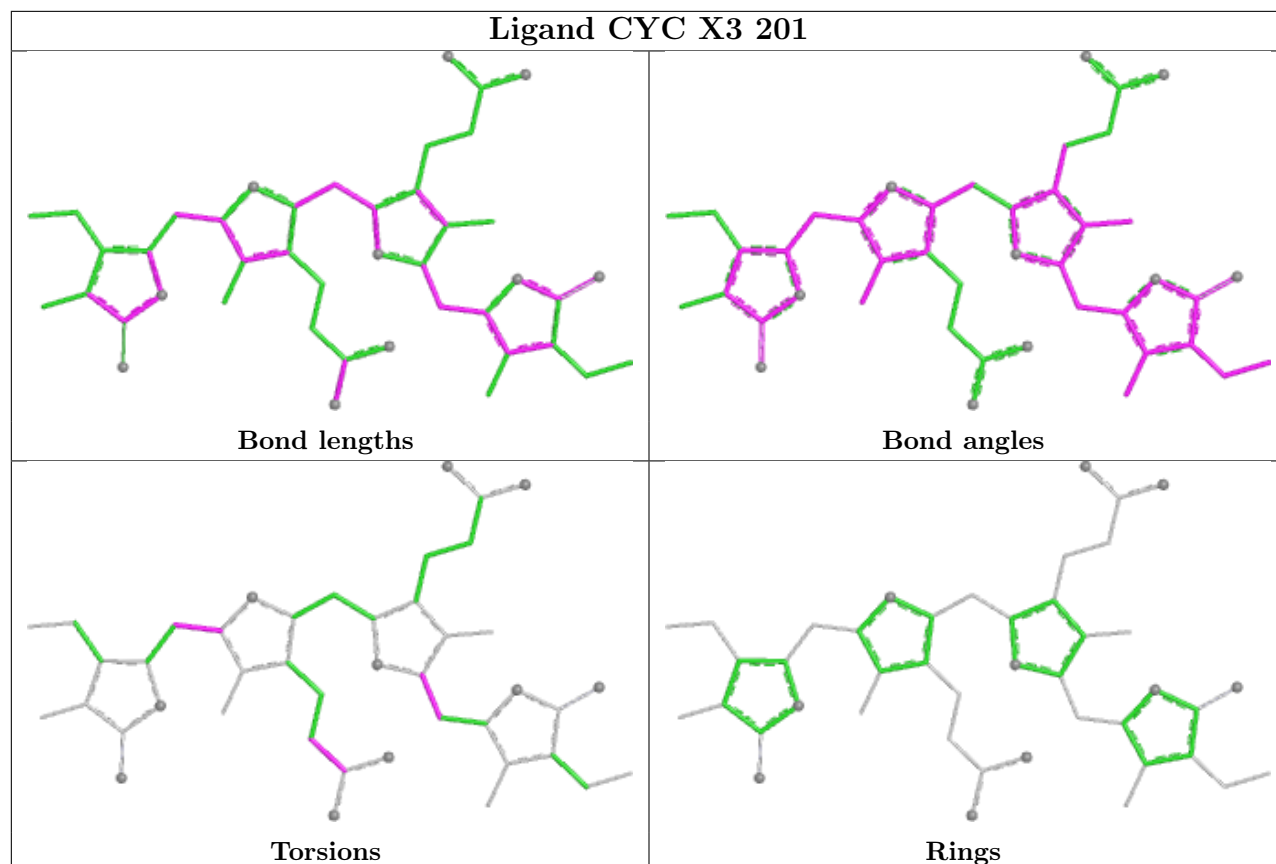
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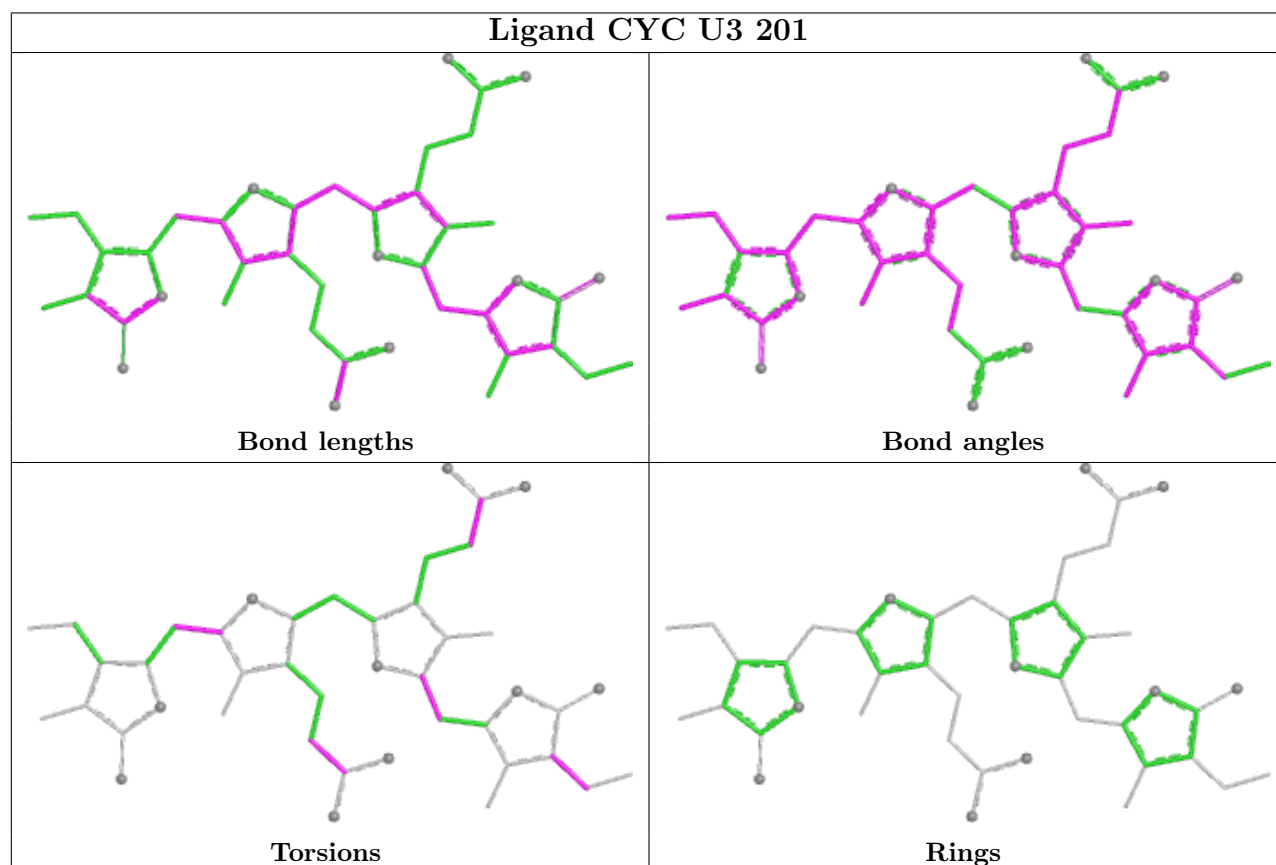
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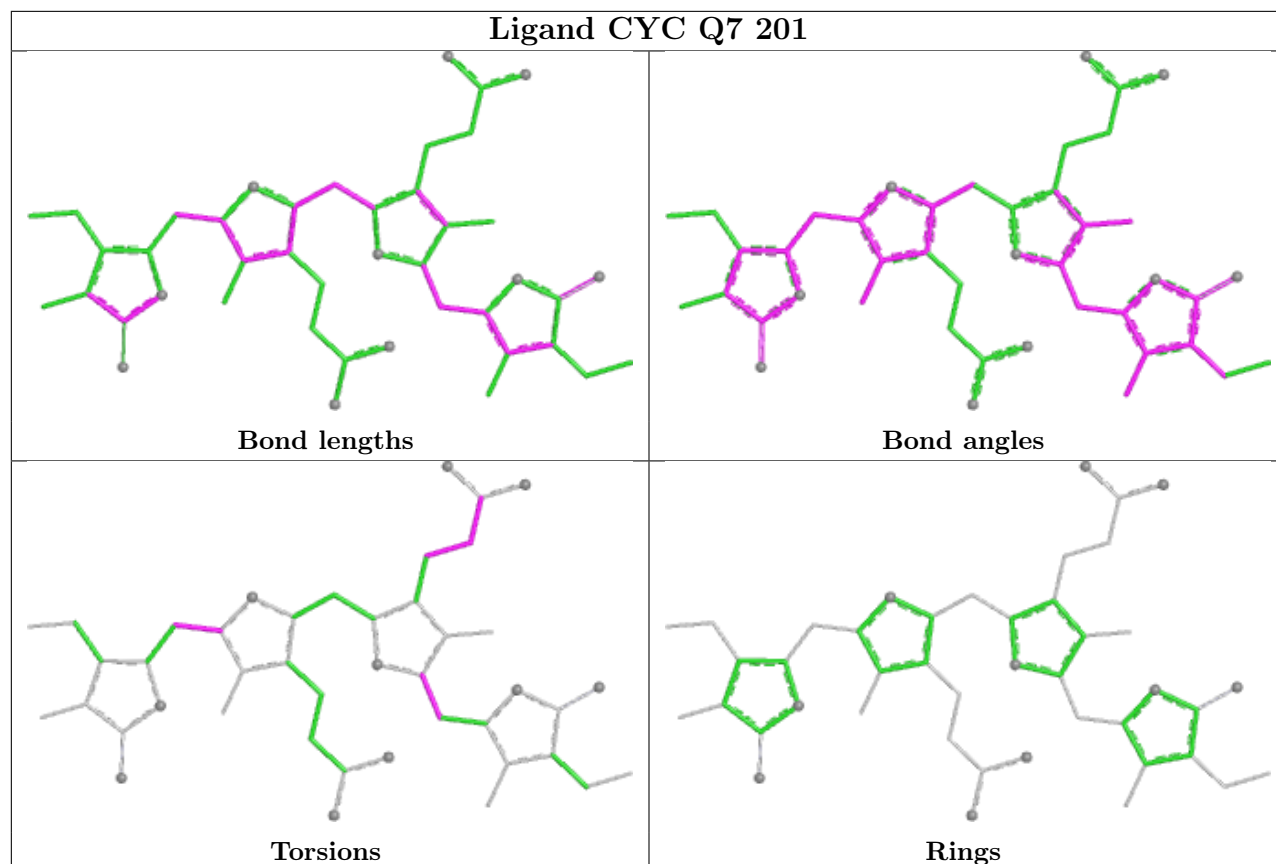
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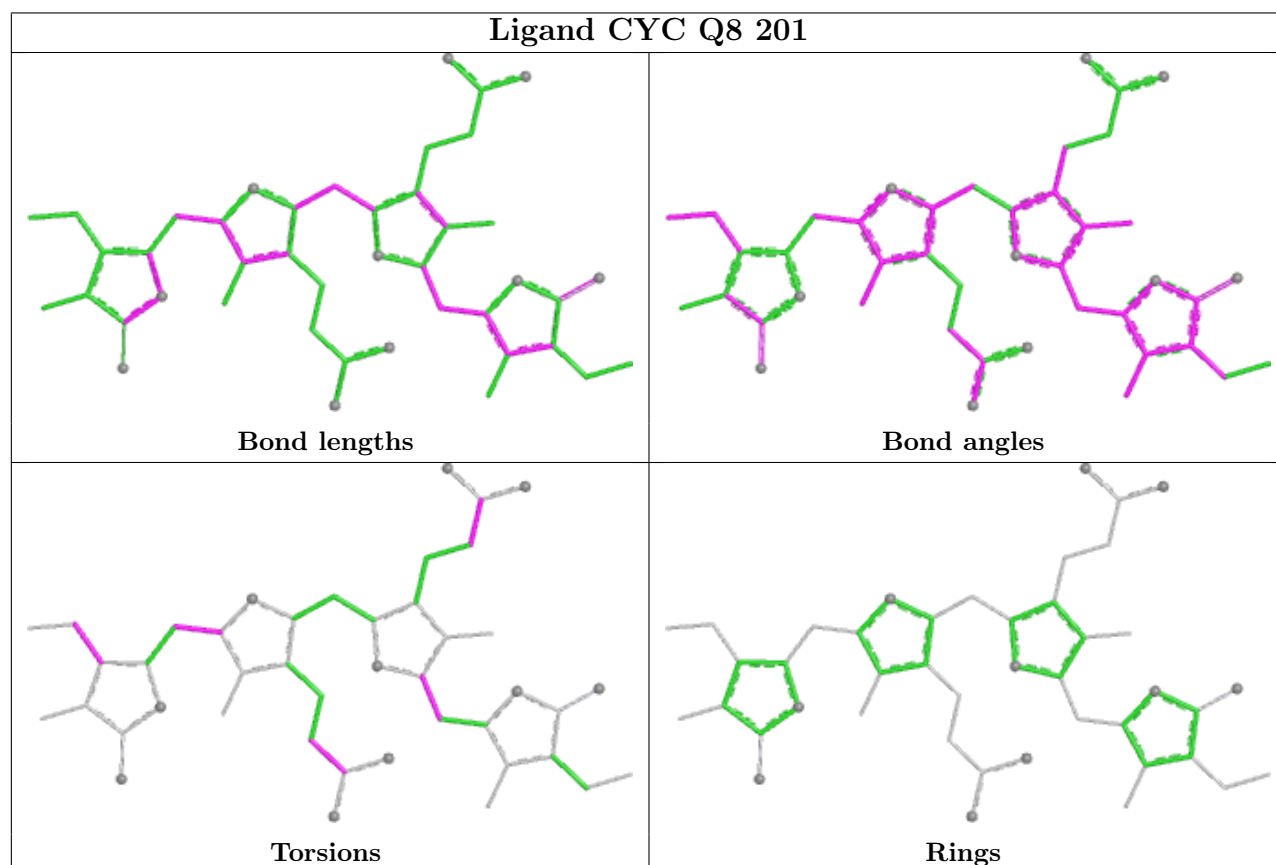
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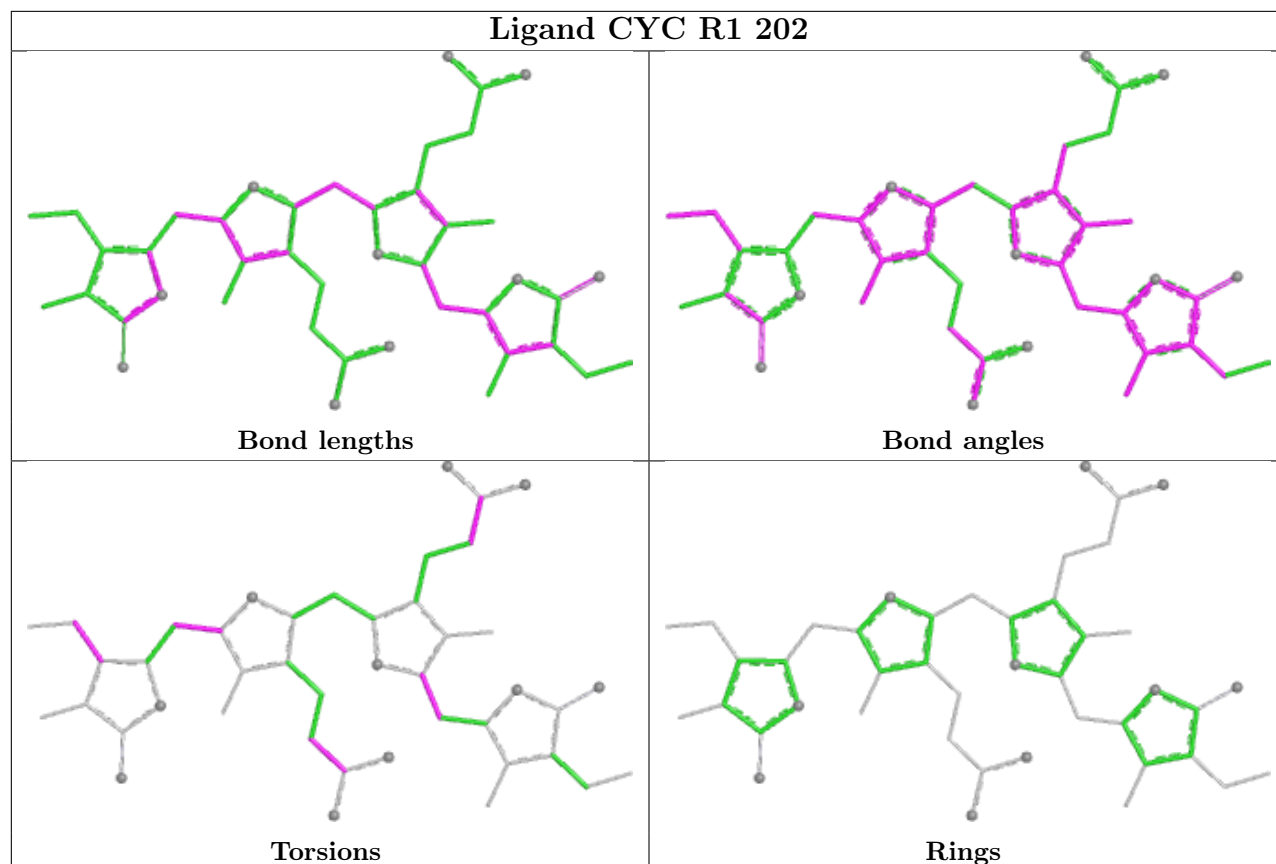
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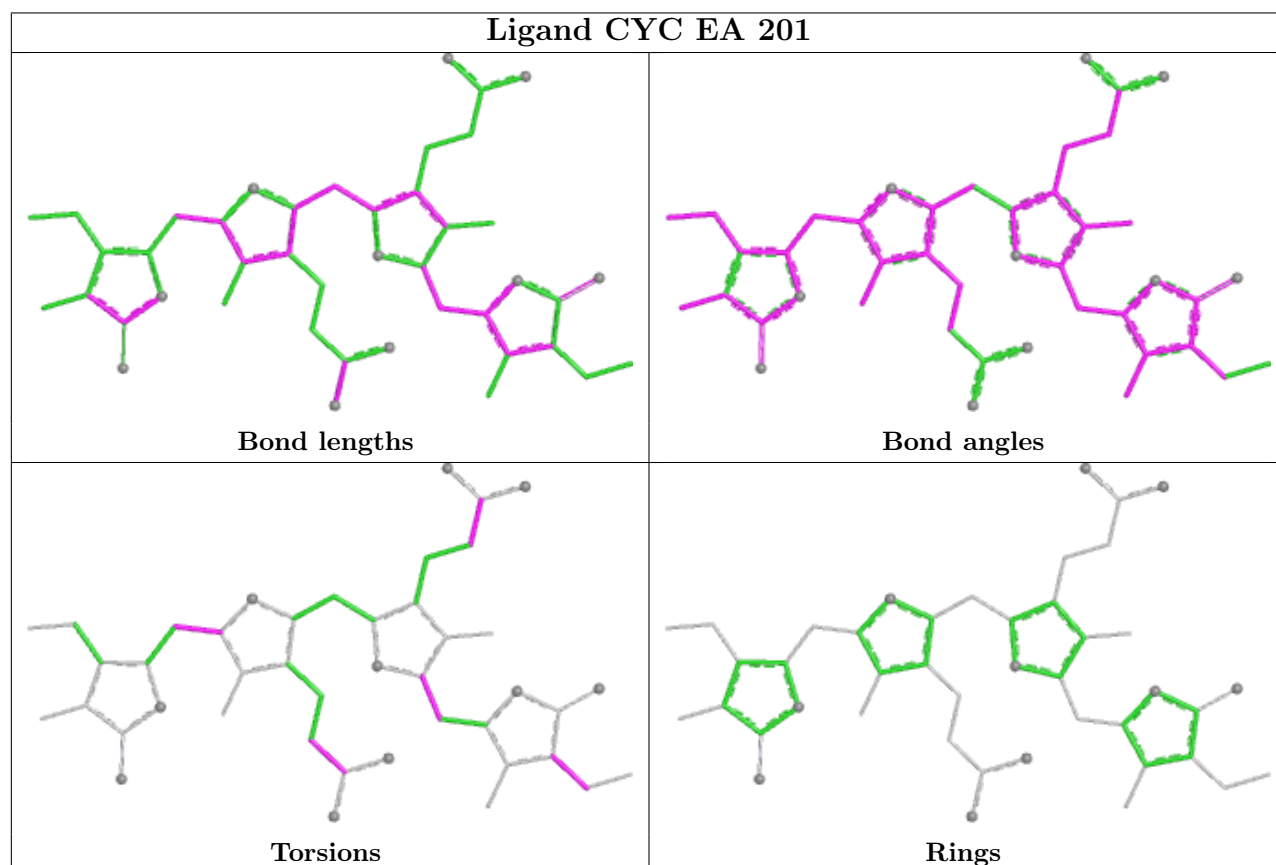
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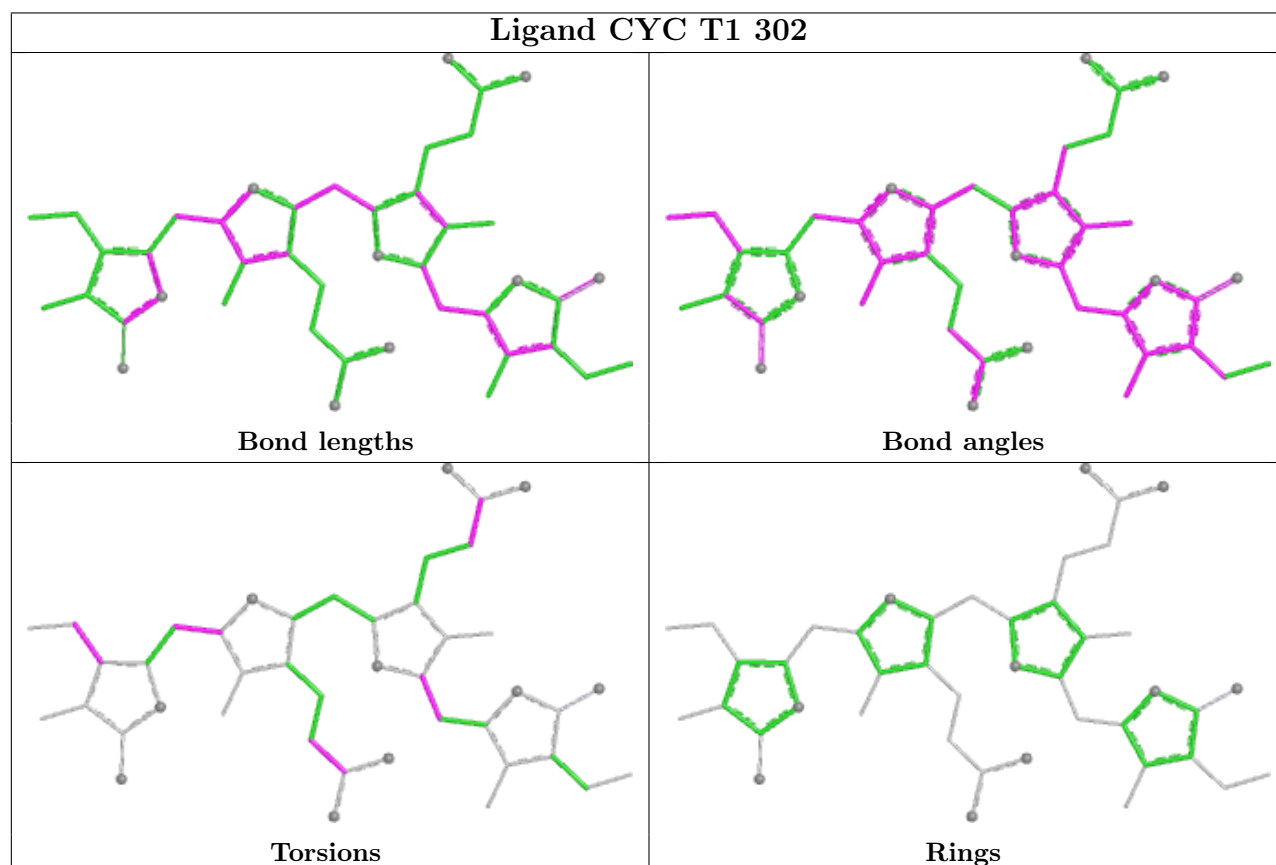
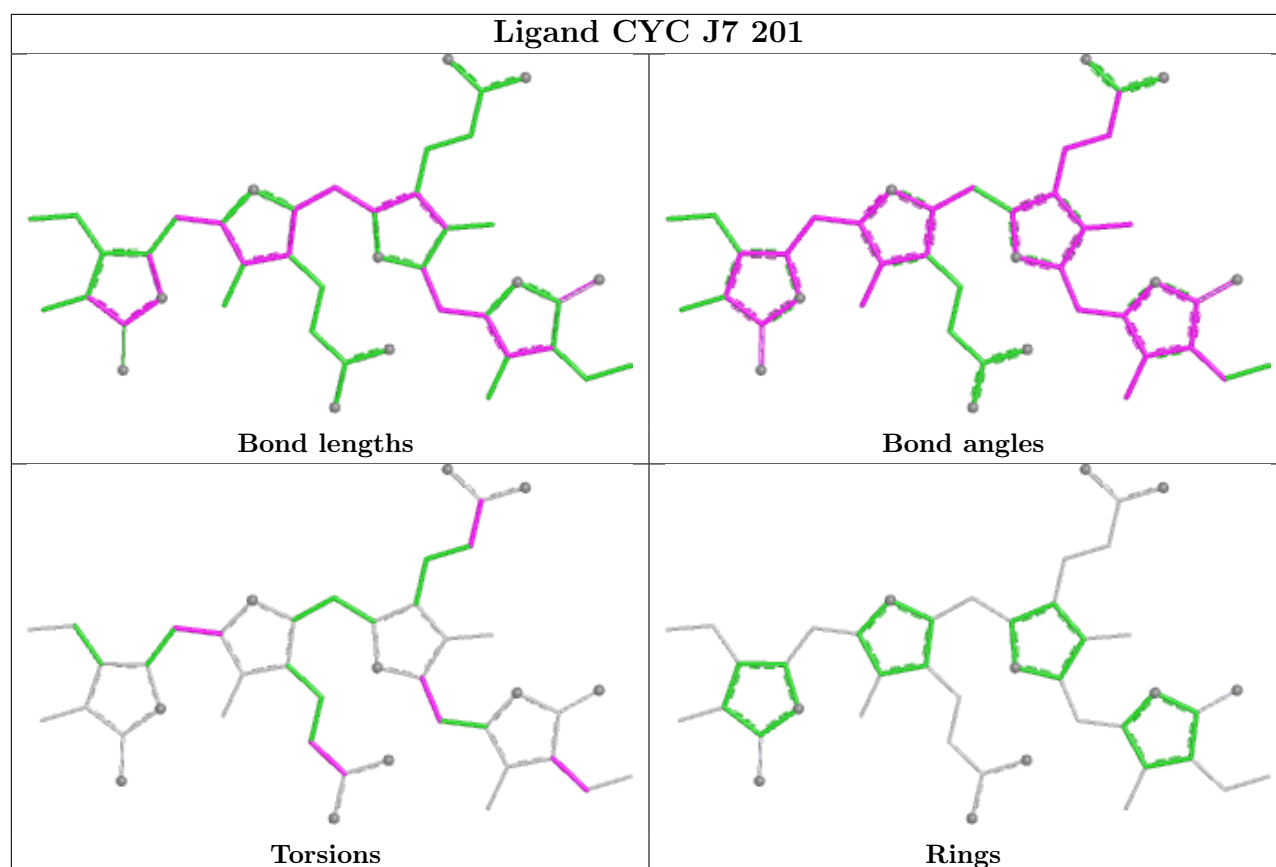


Ligand CYC R1 202

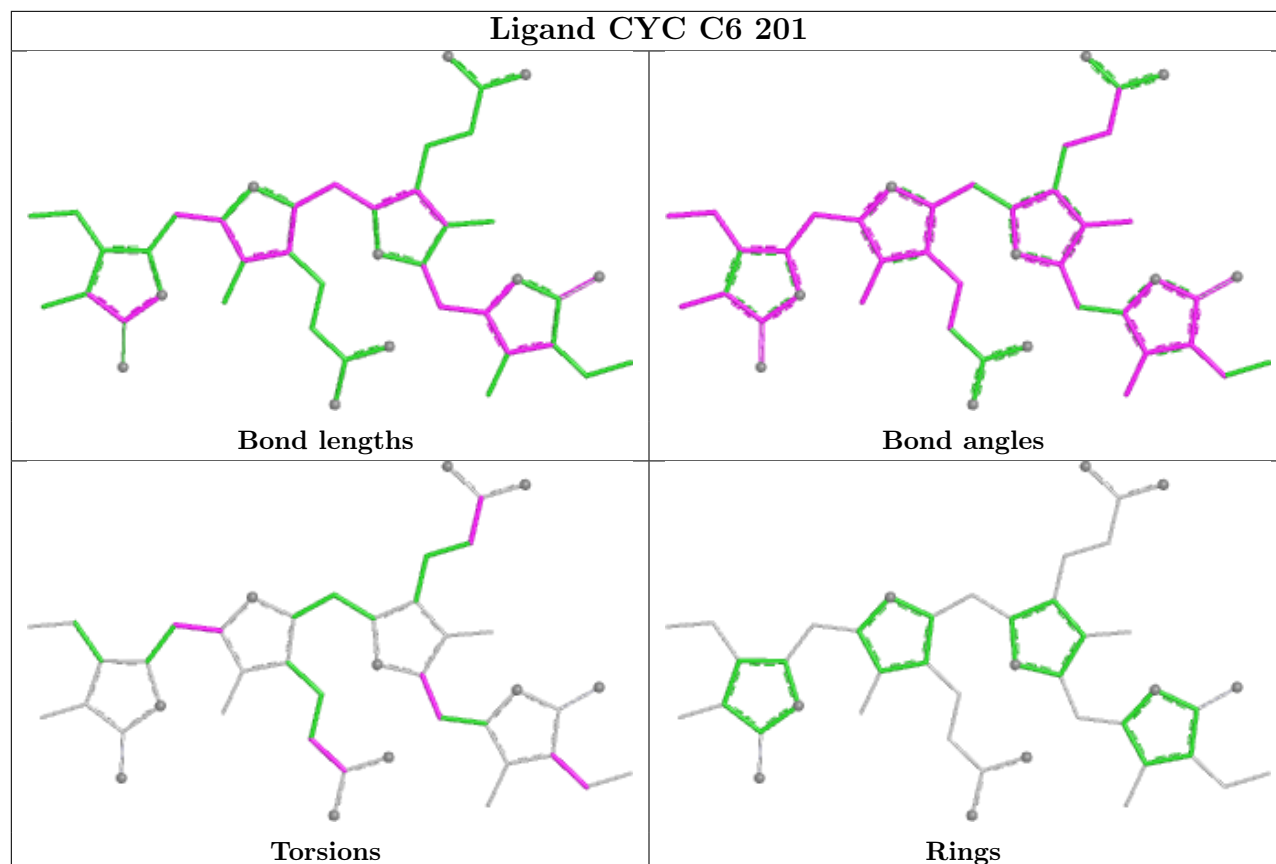


Ligand CYC EA 201

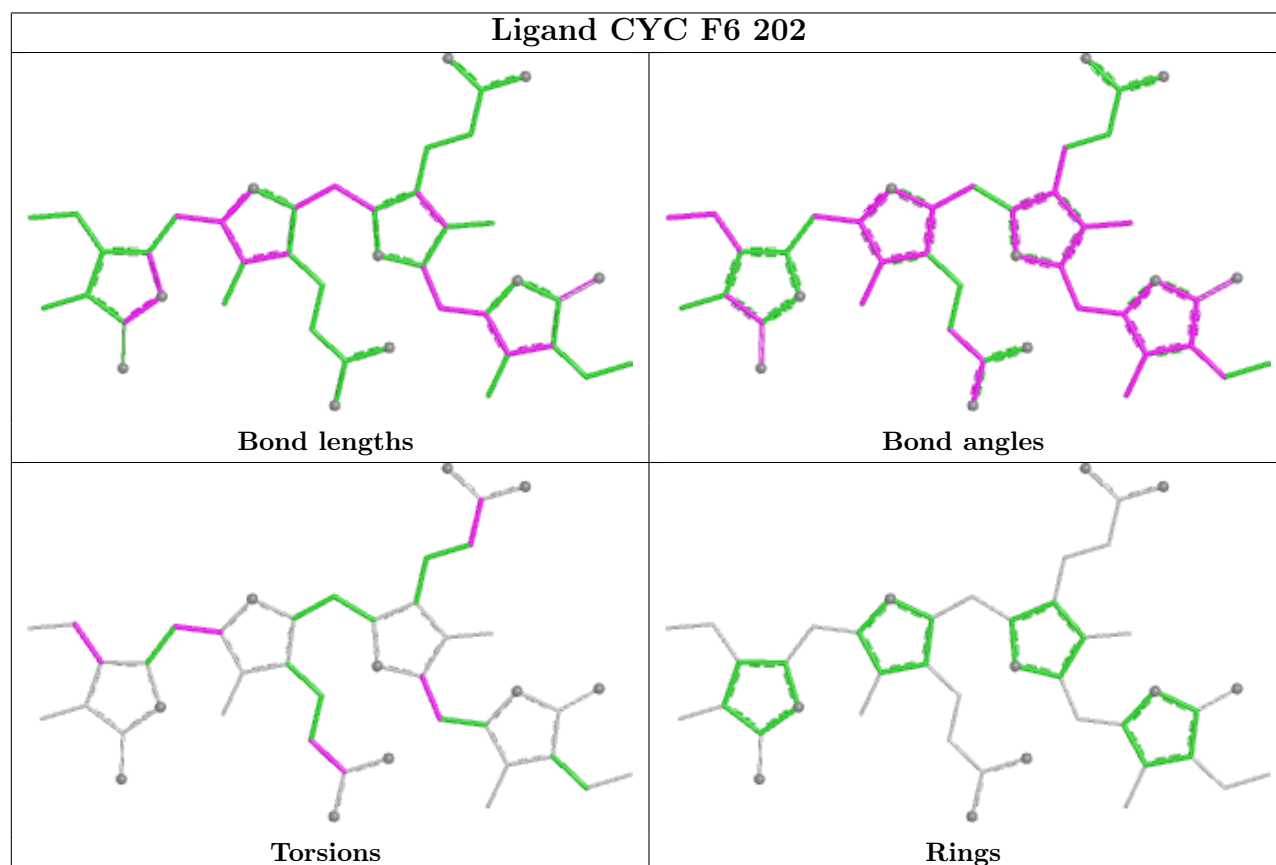




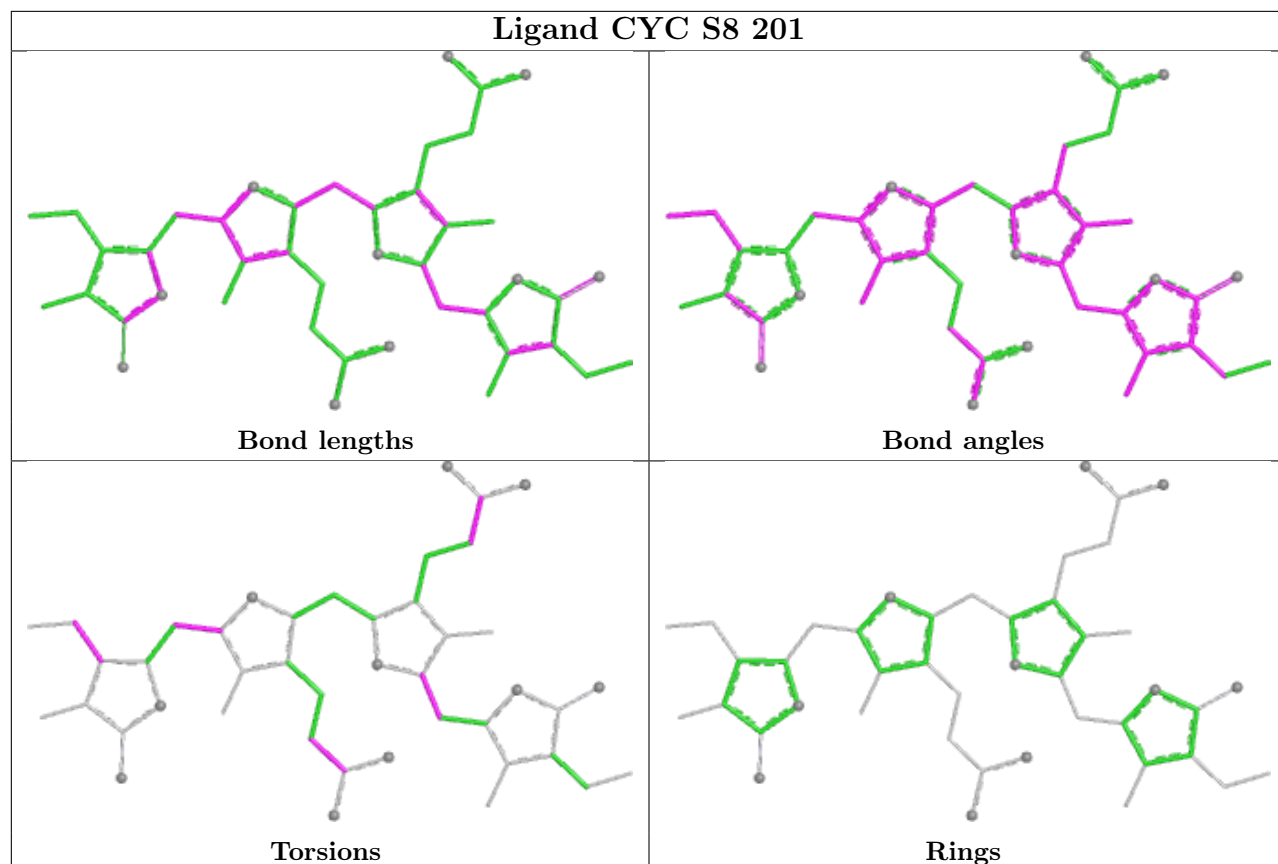
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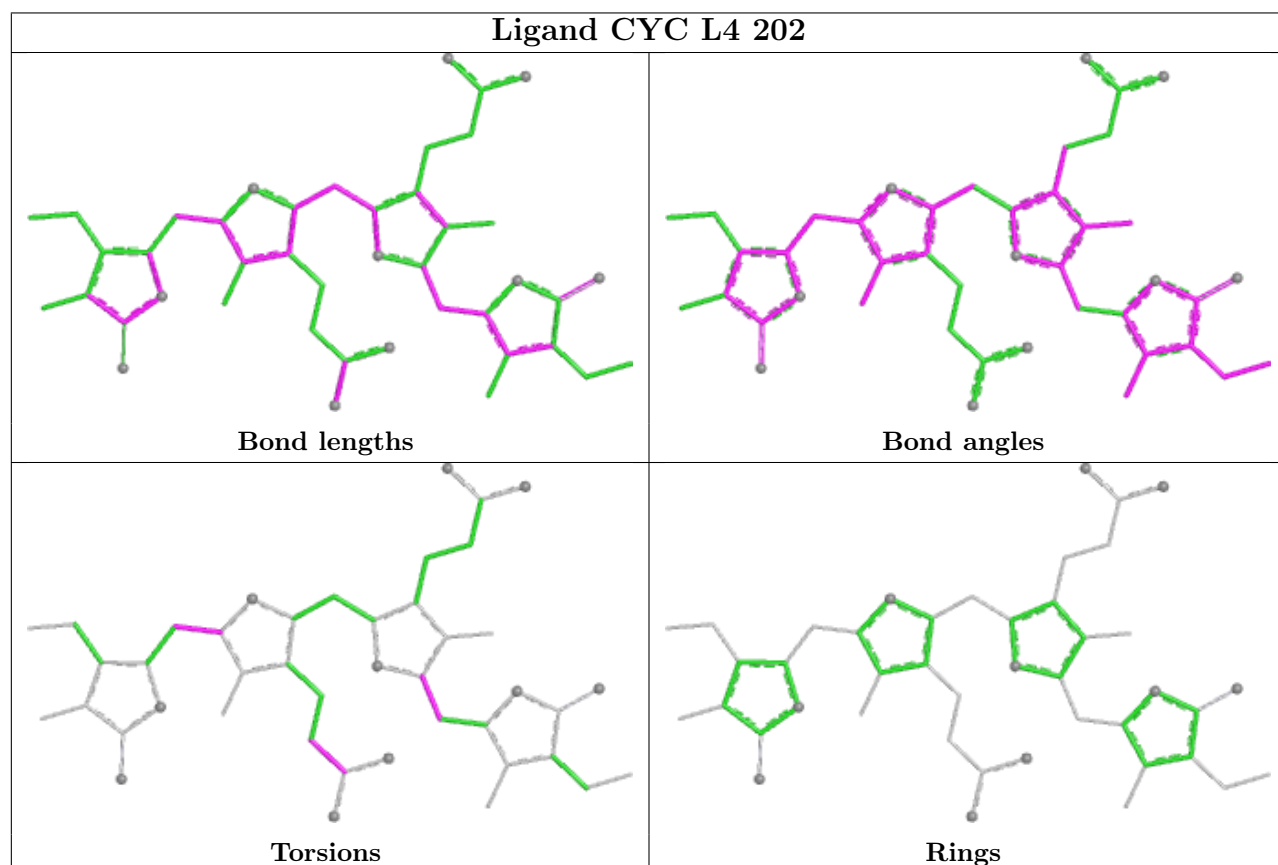
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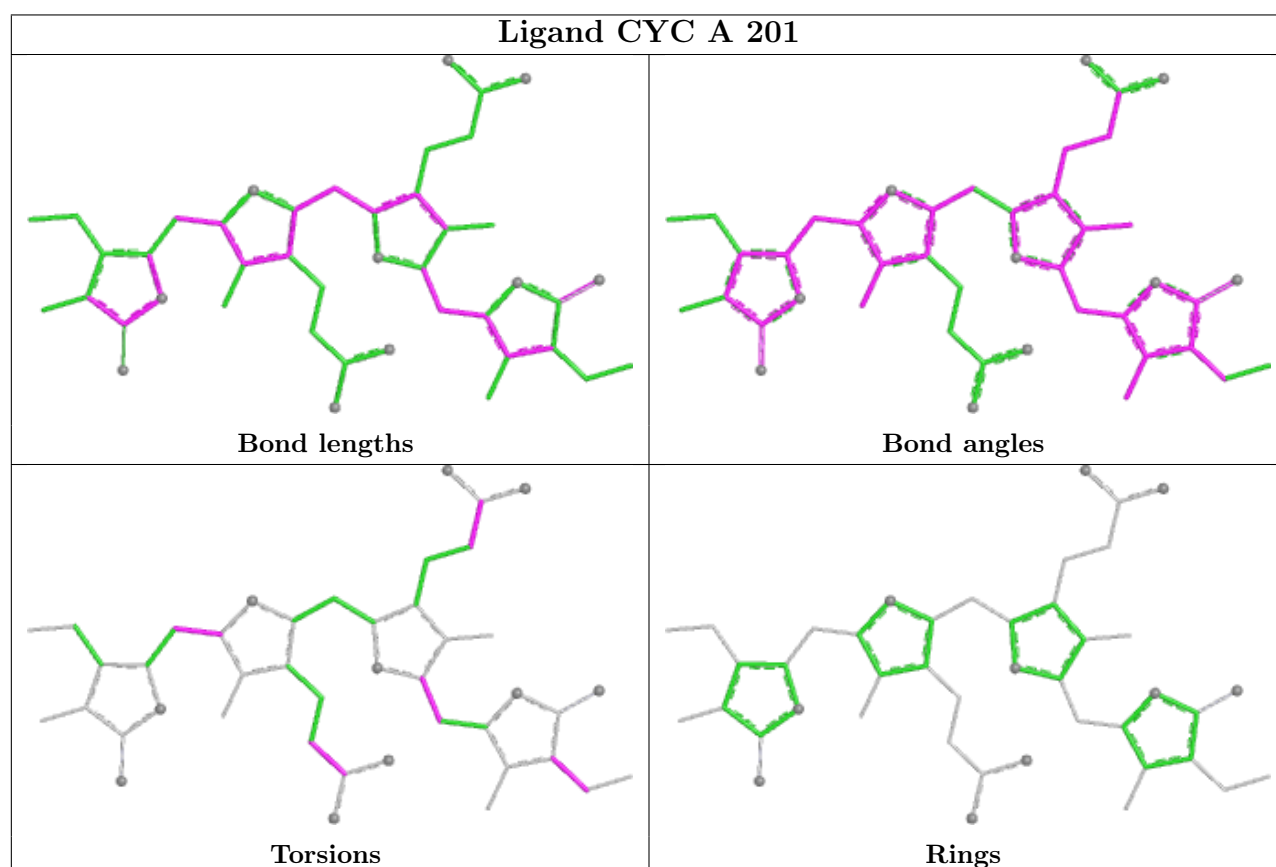
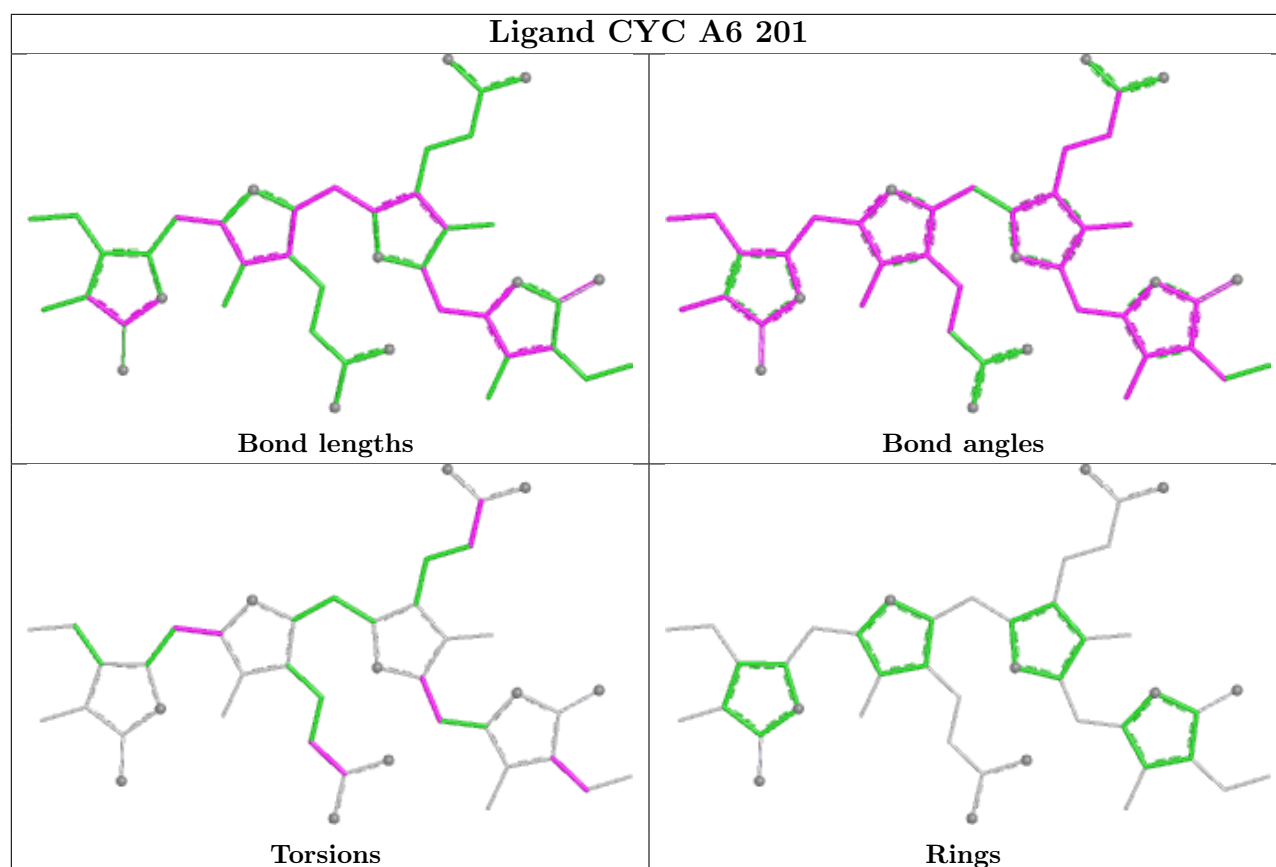


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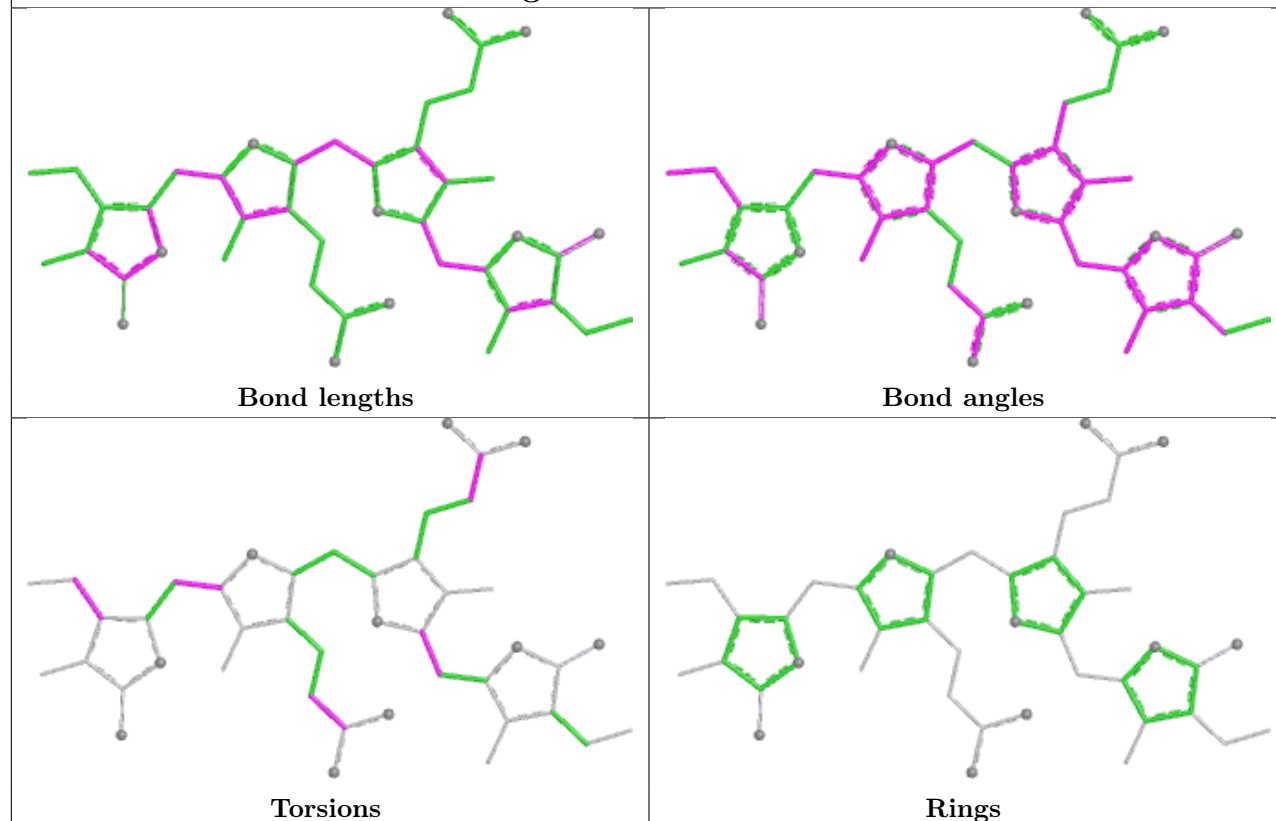


Ligand CYC L4 202

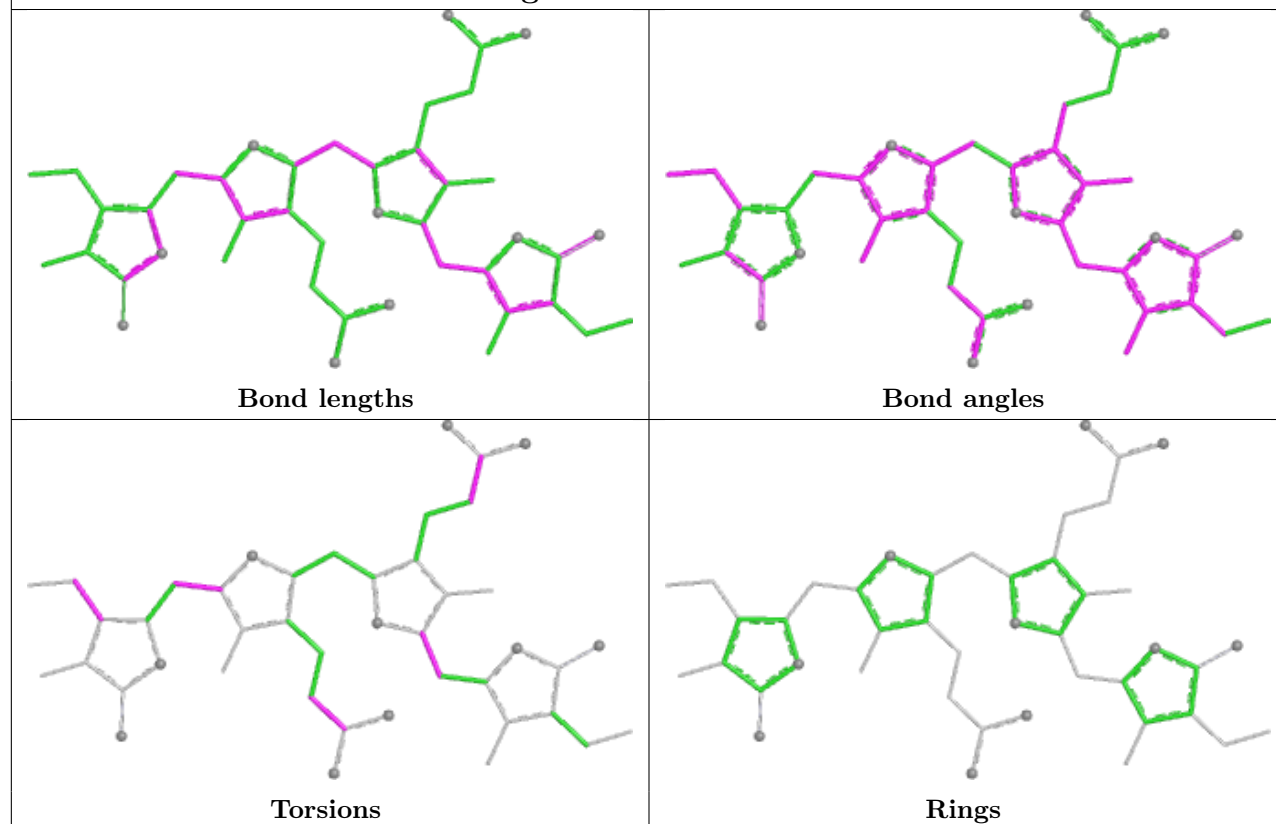


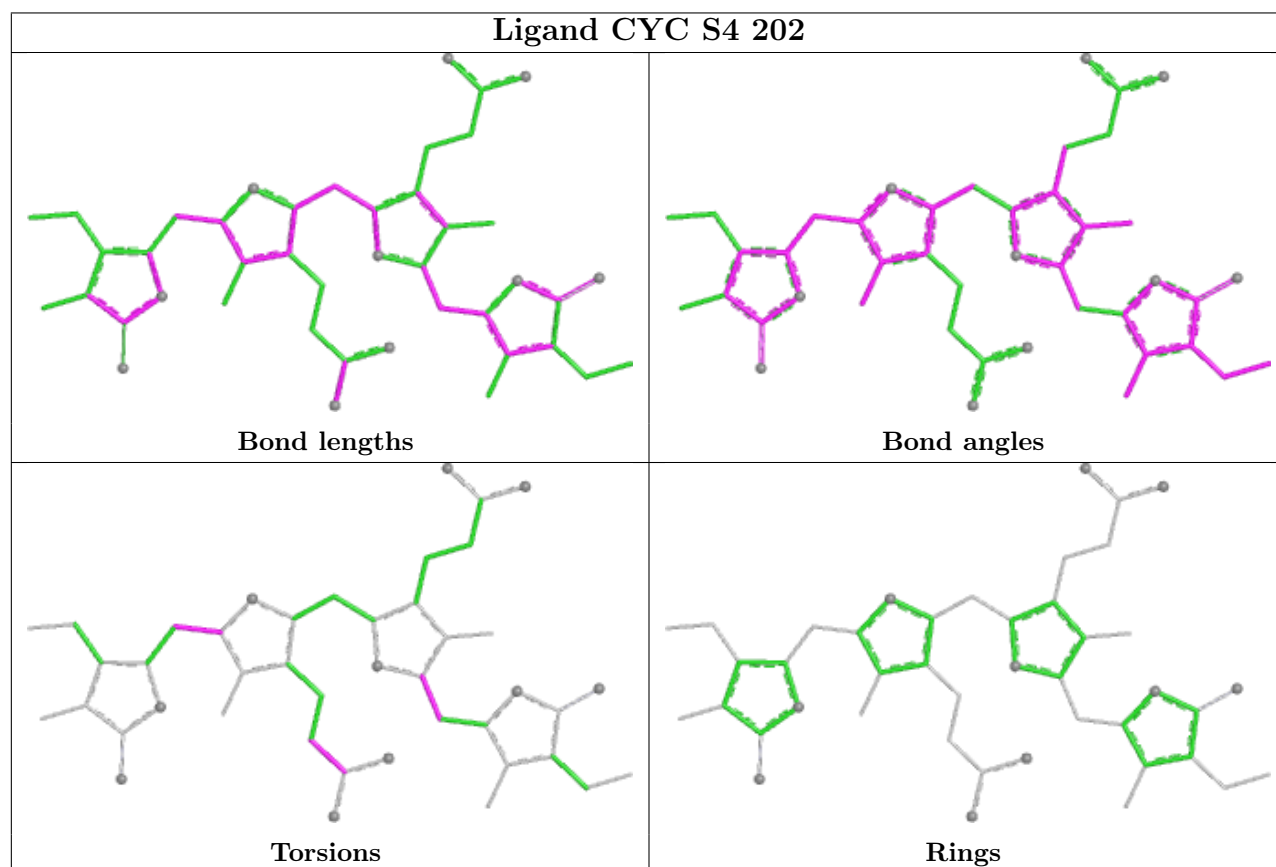
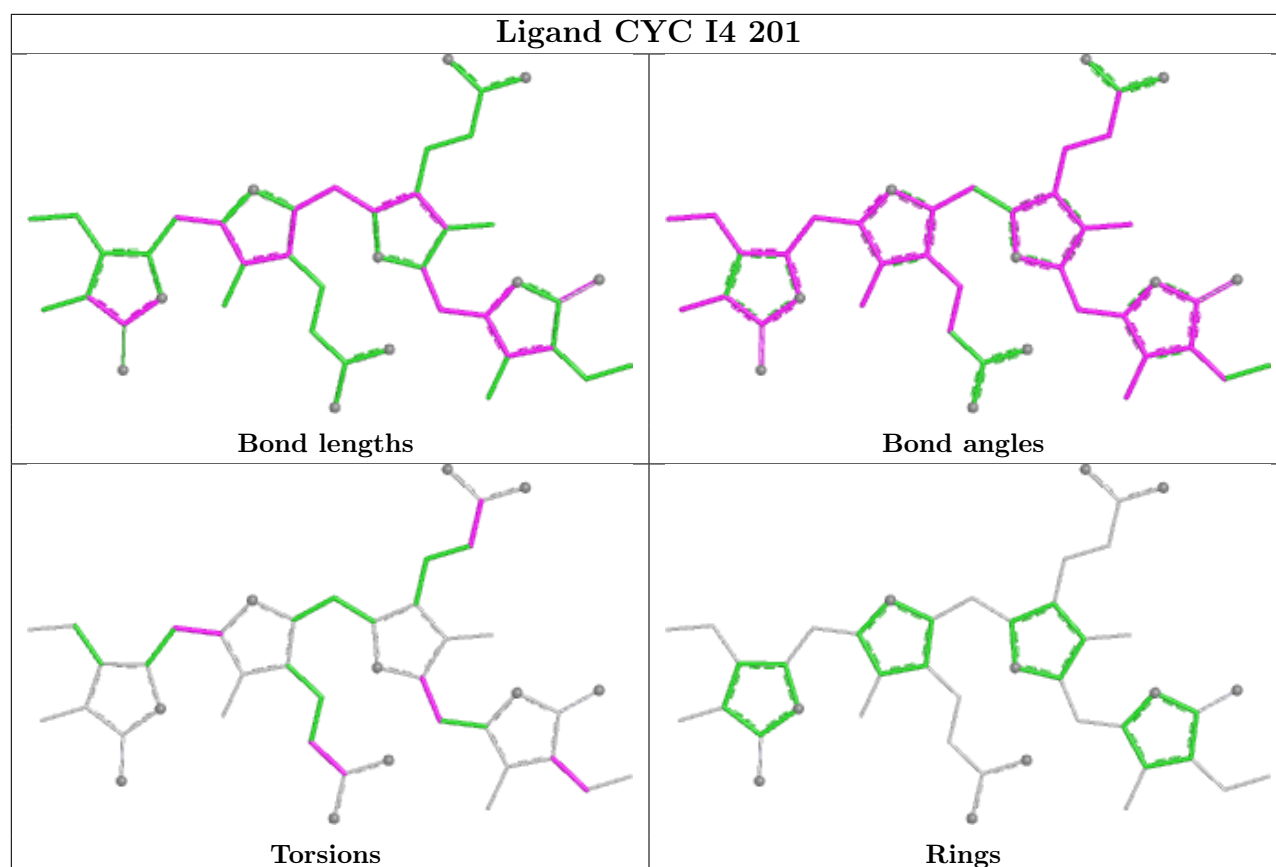


Ligand CYC F9 302

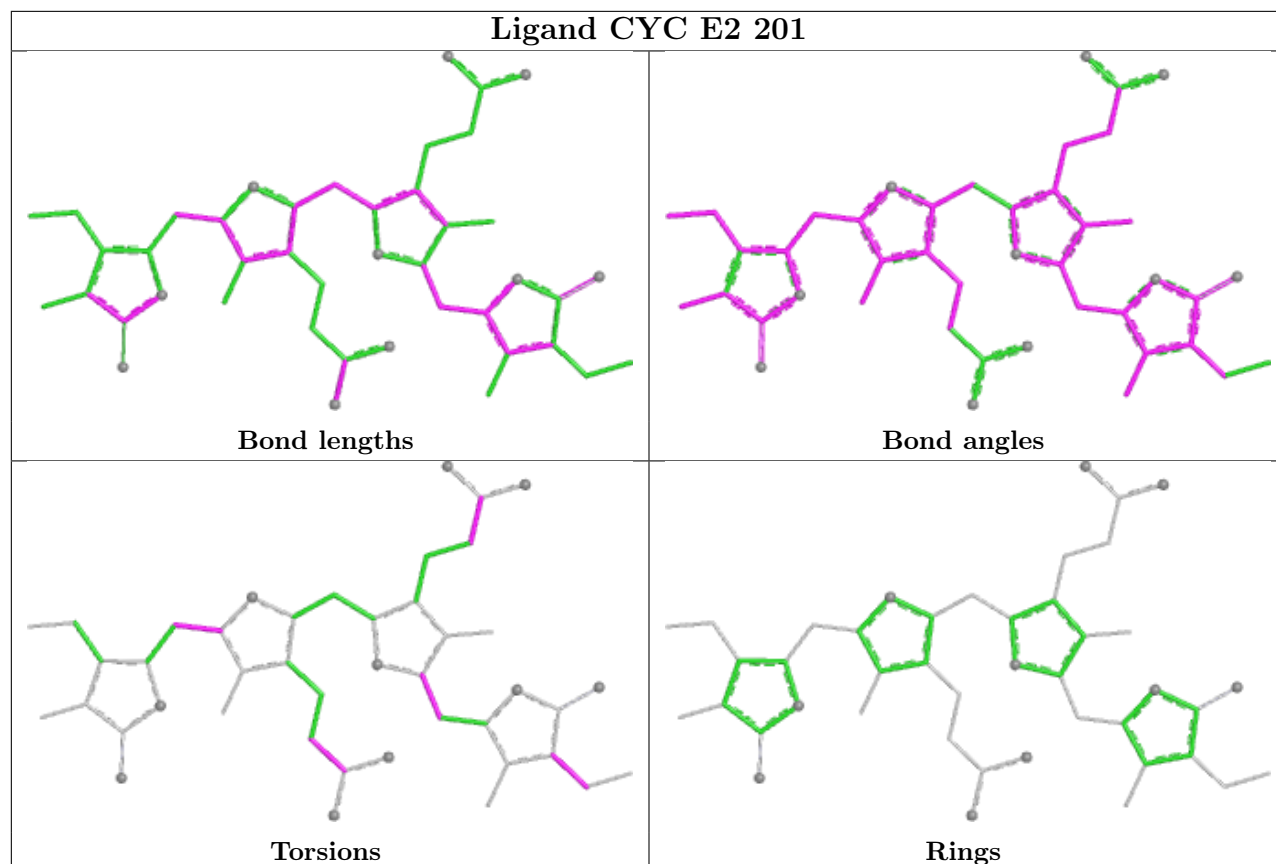


Ligand CYC B1 201

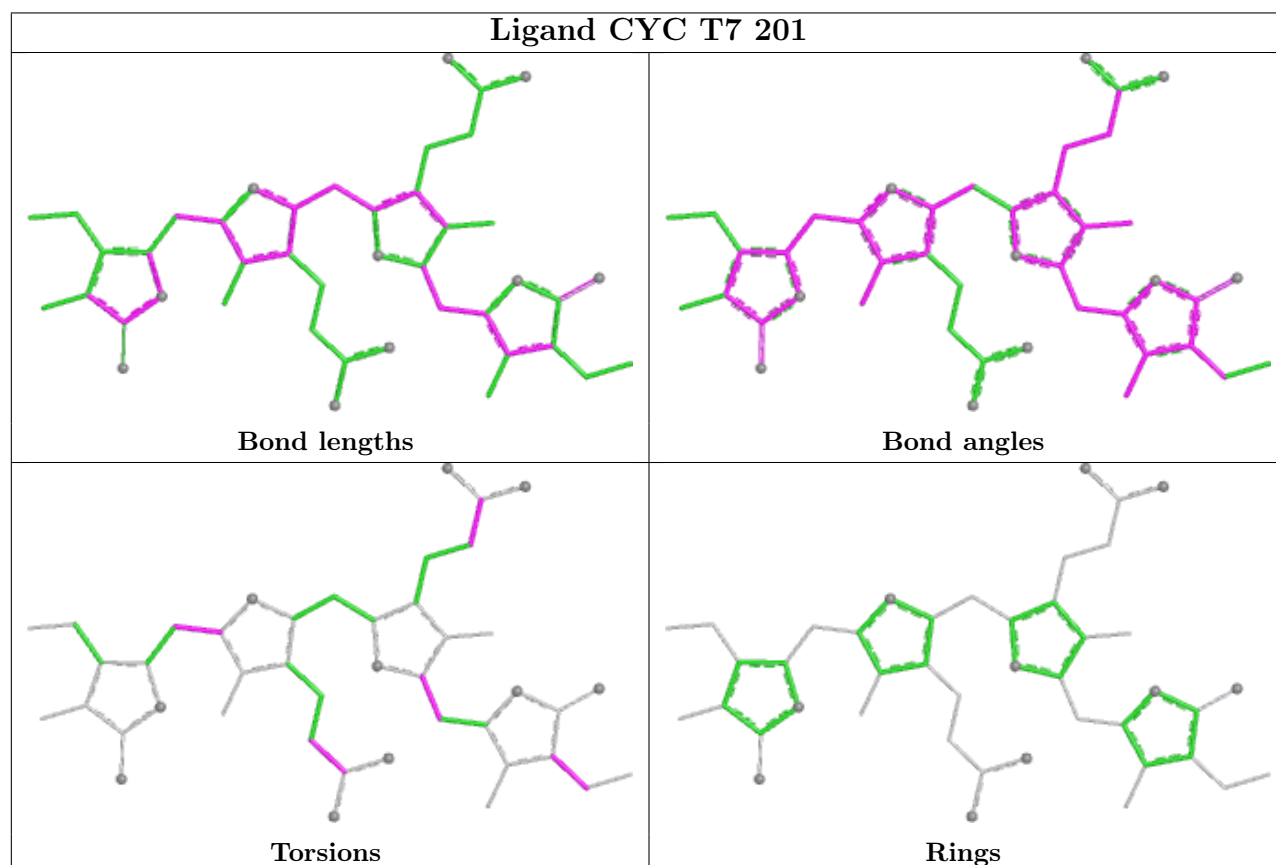




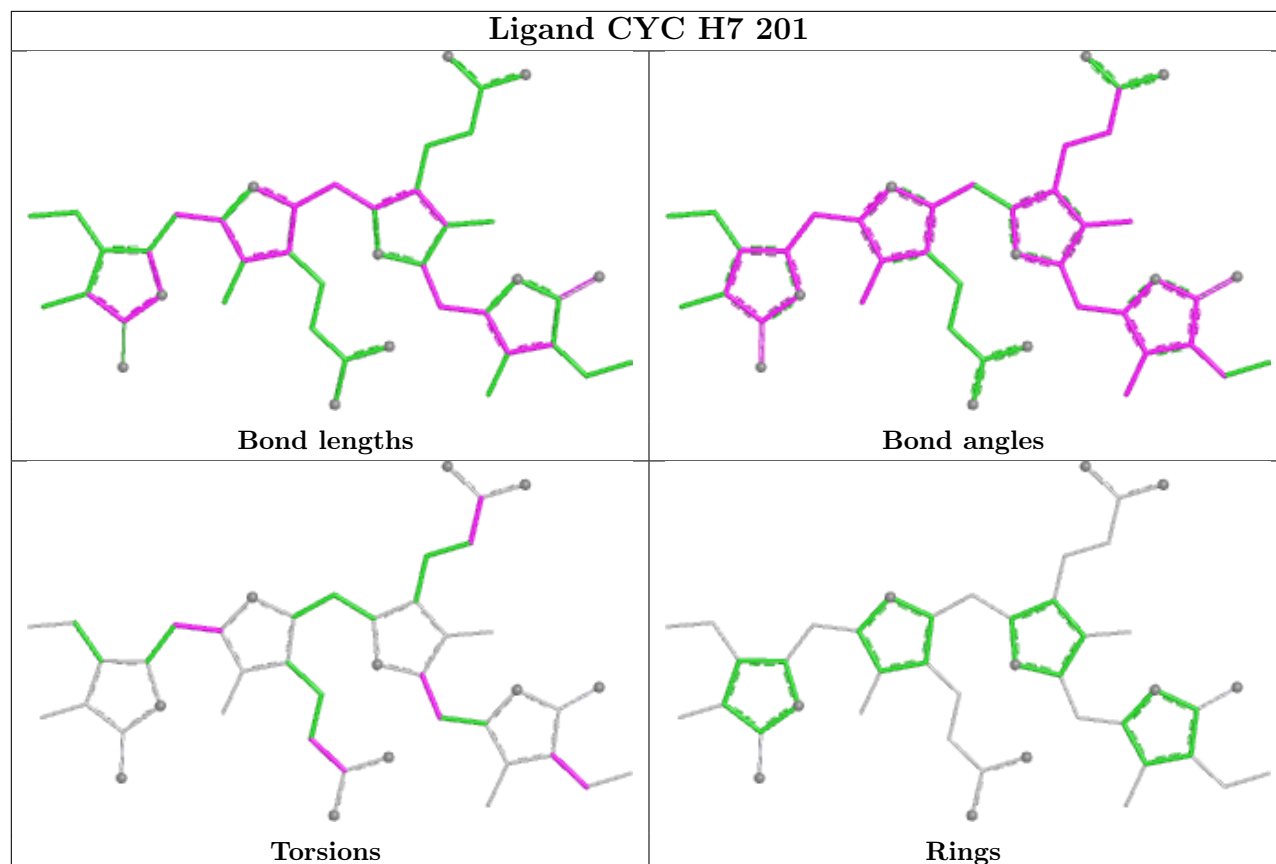
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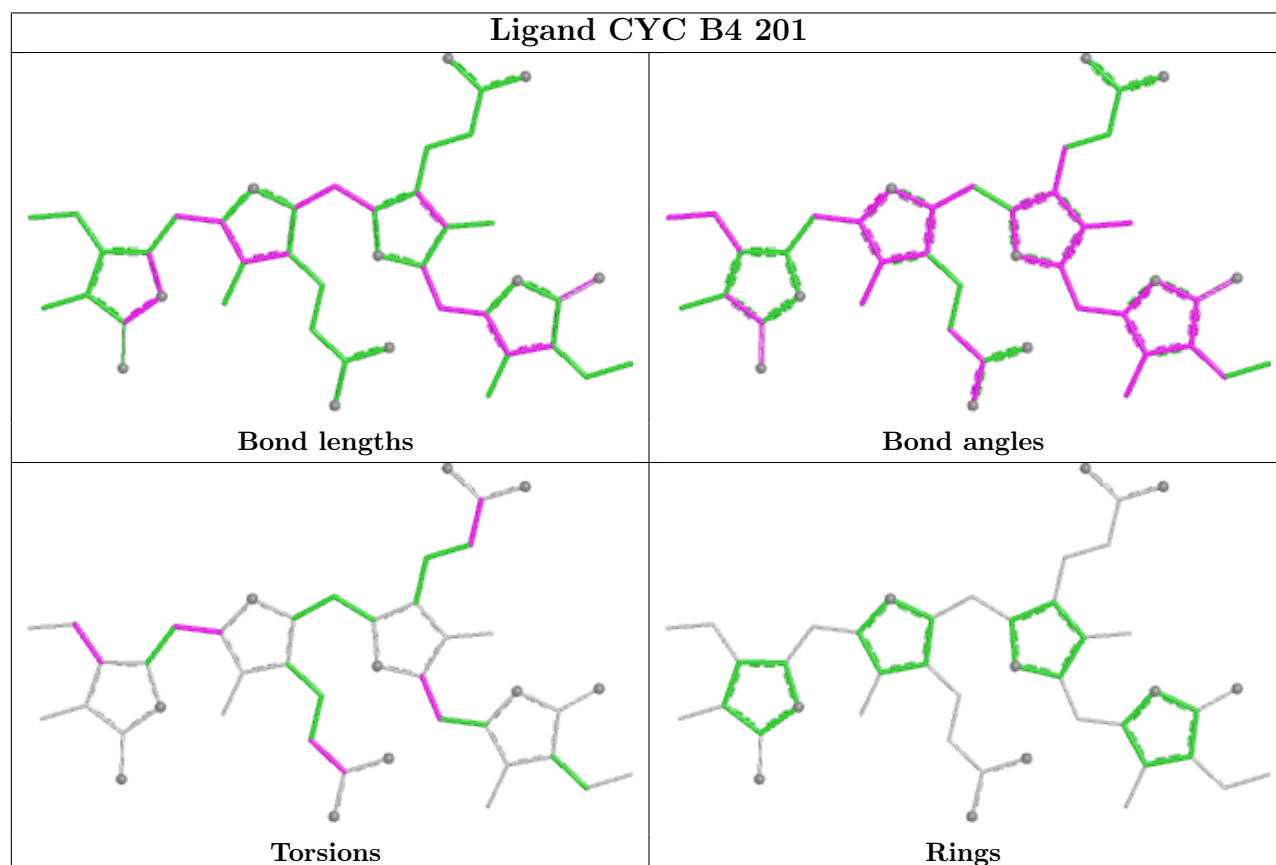
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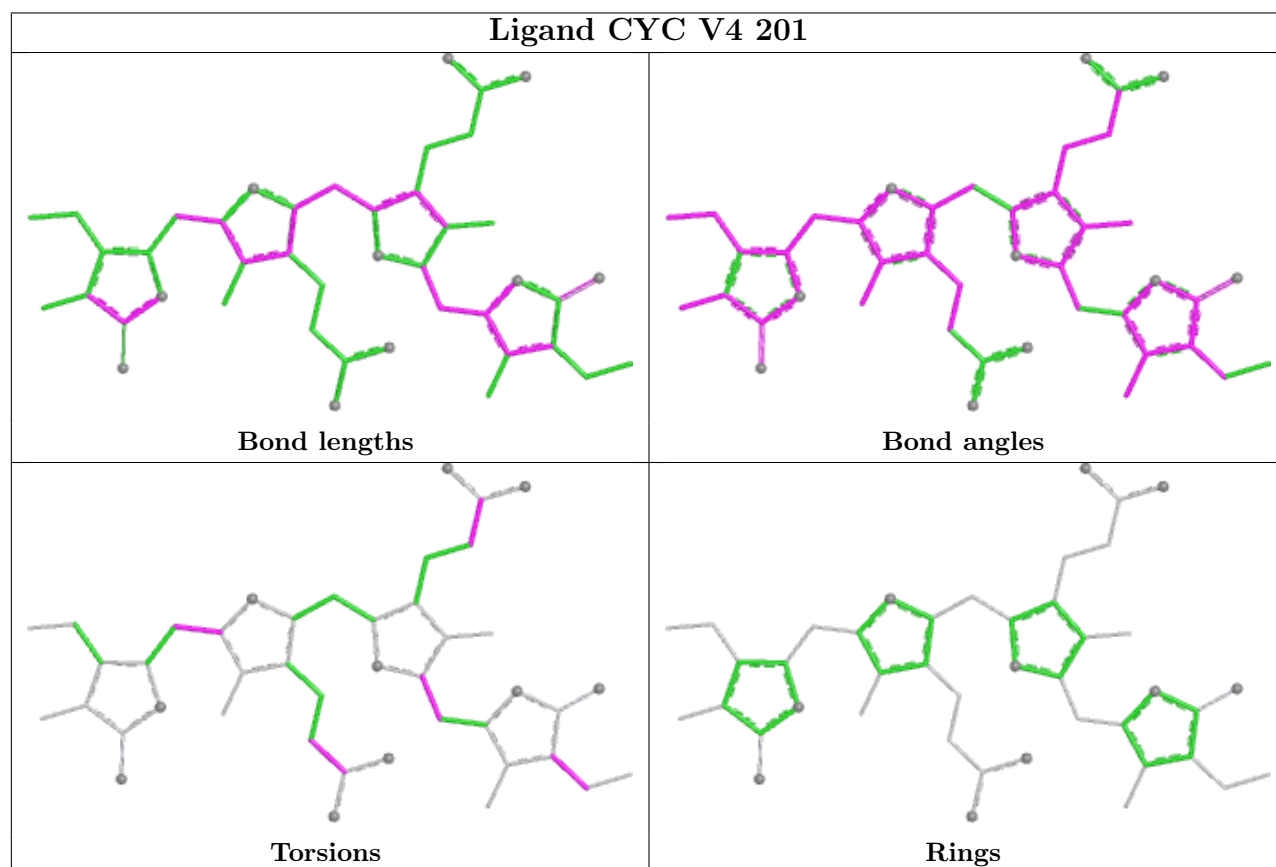
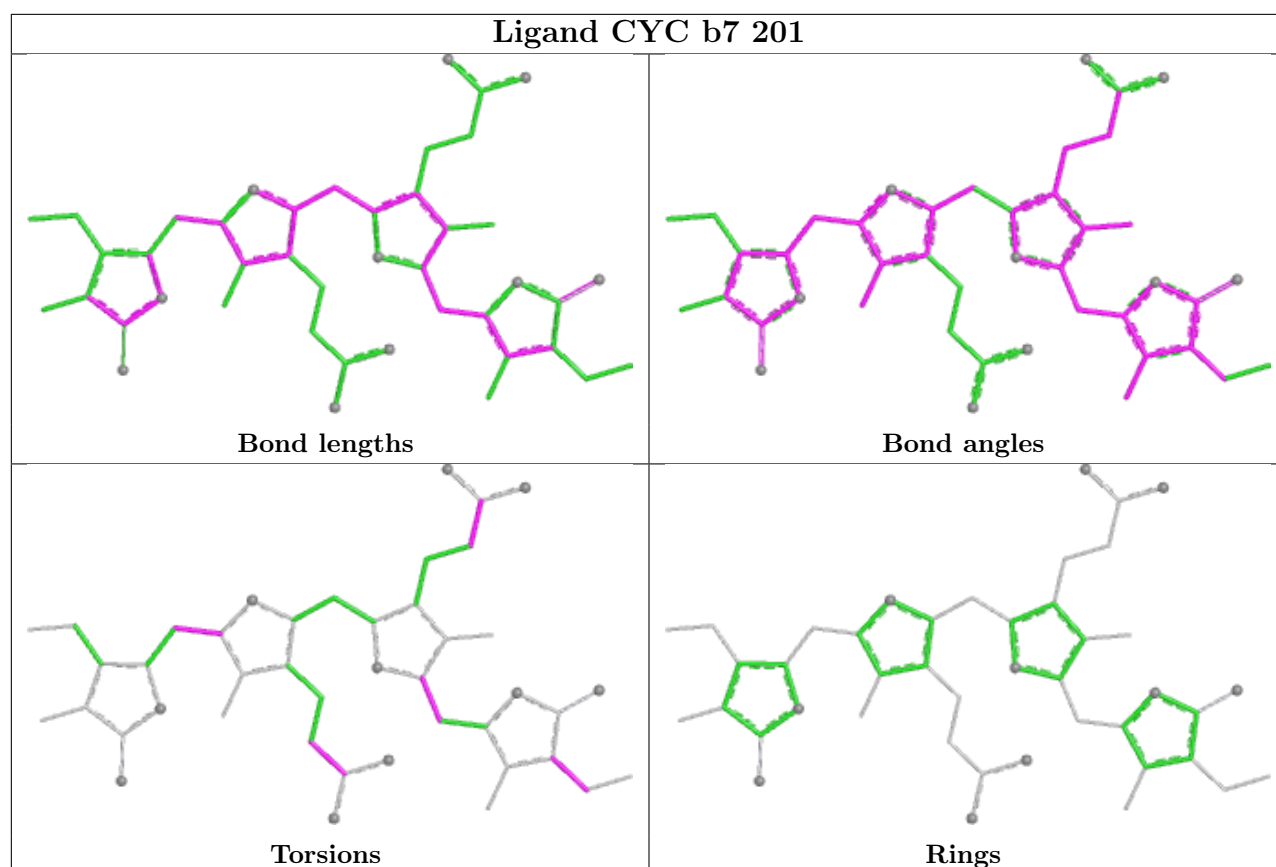


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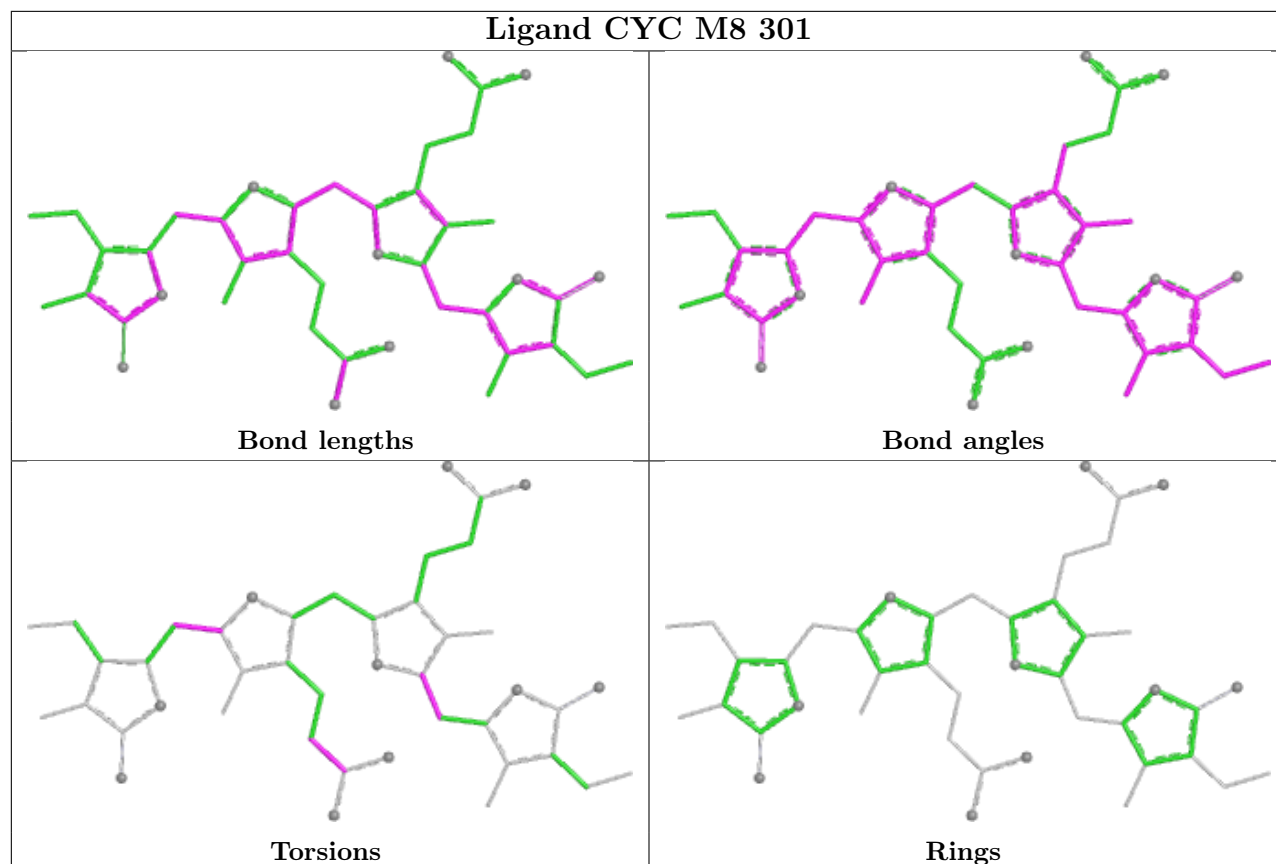


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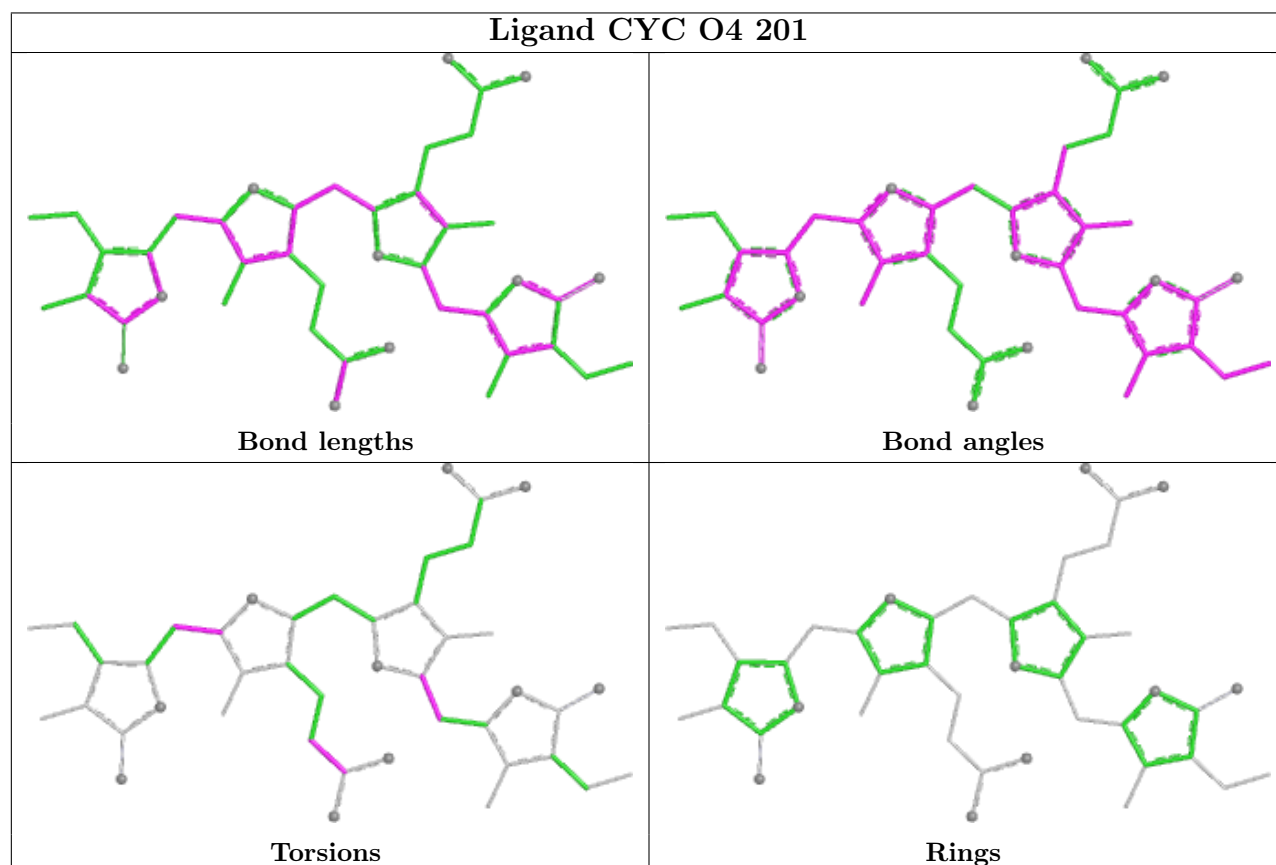




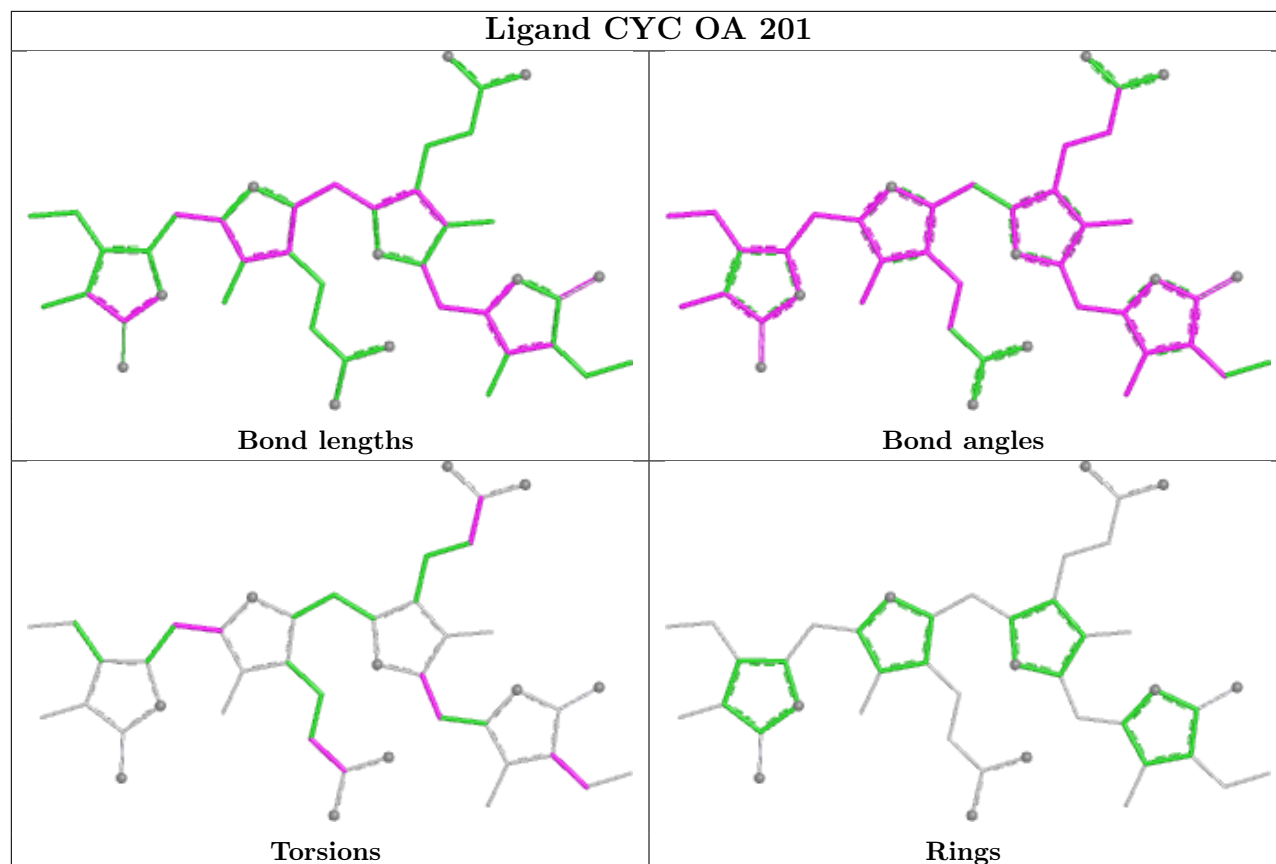
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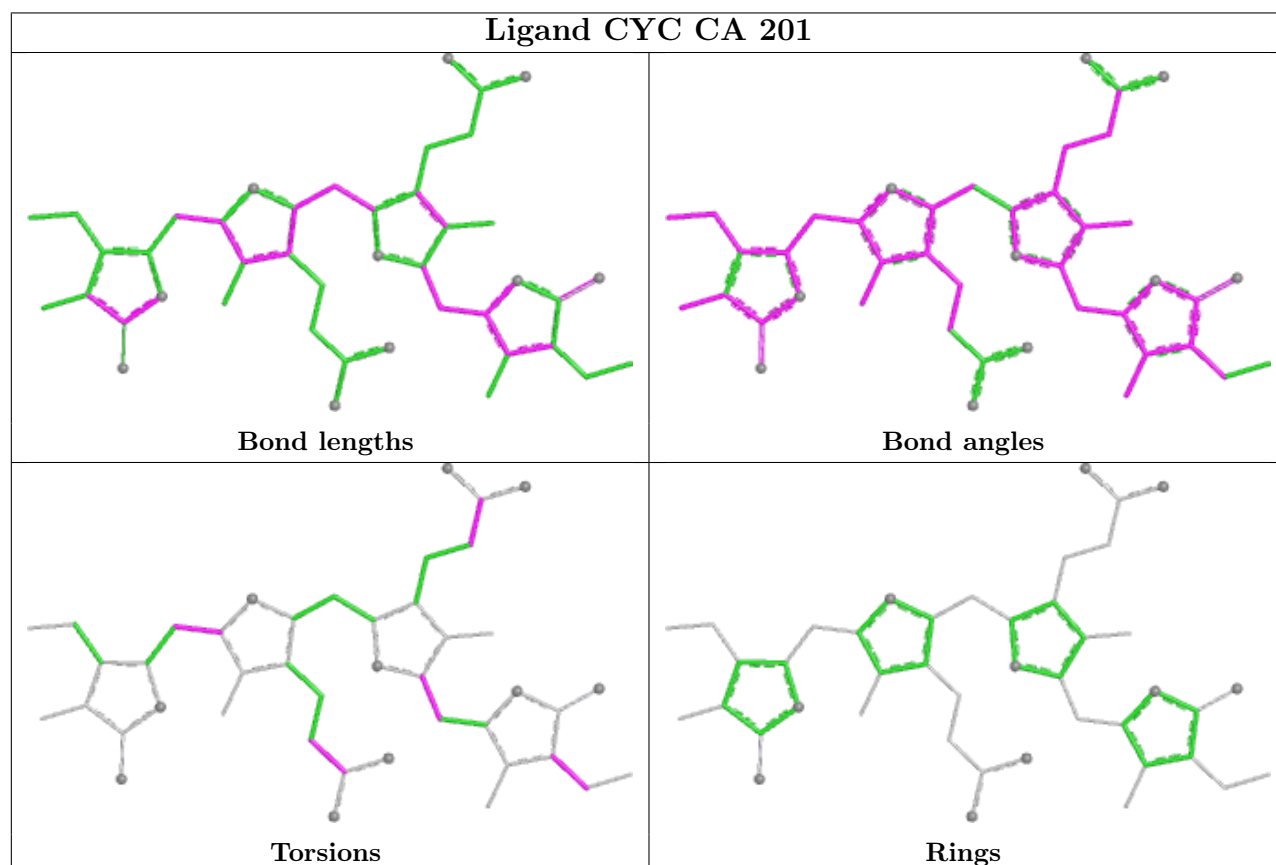
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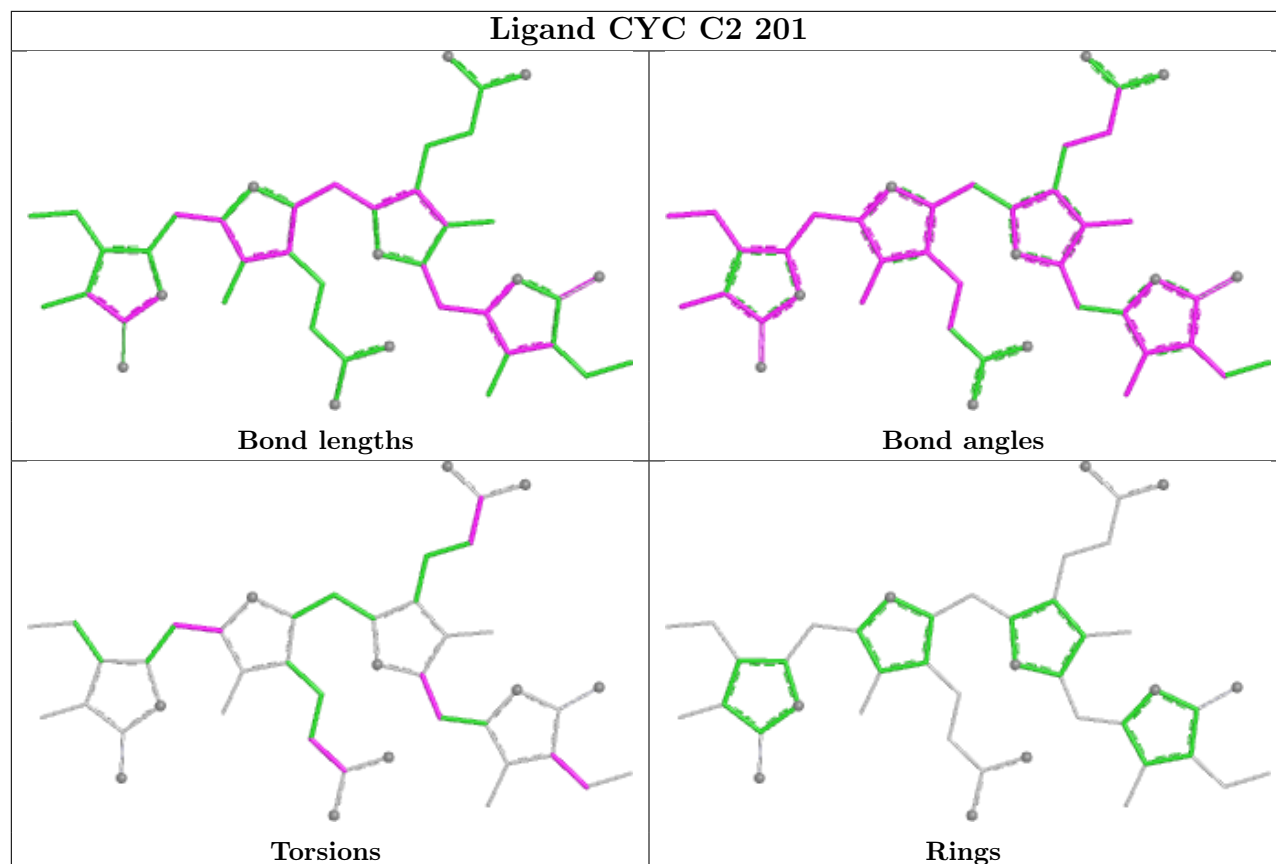
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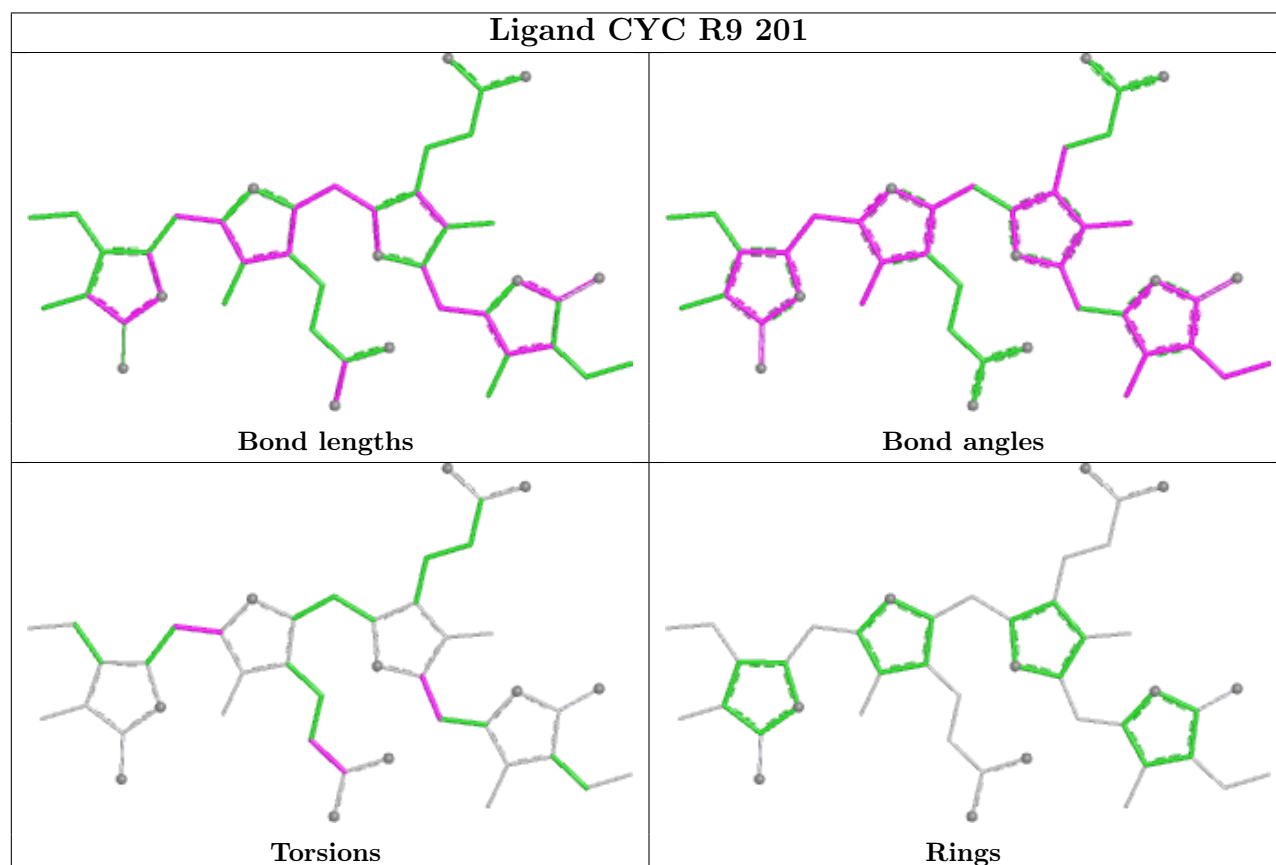
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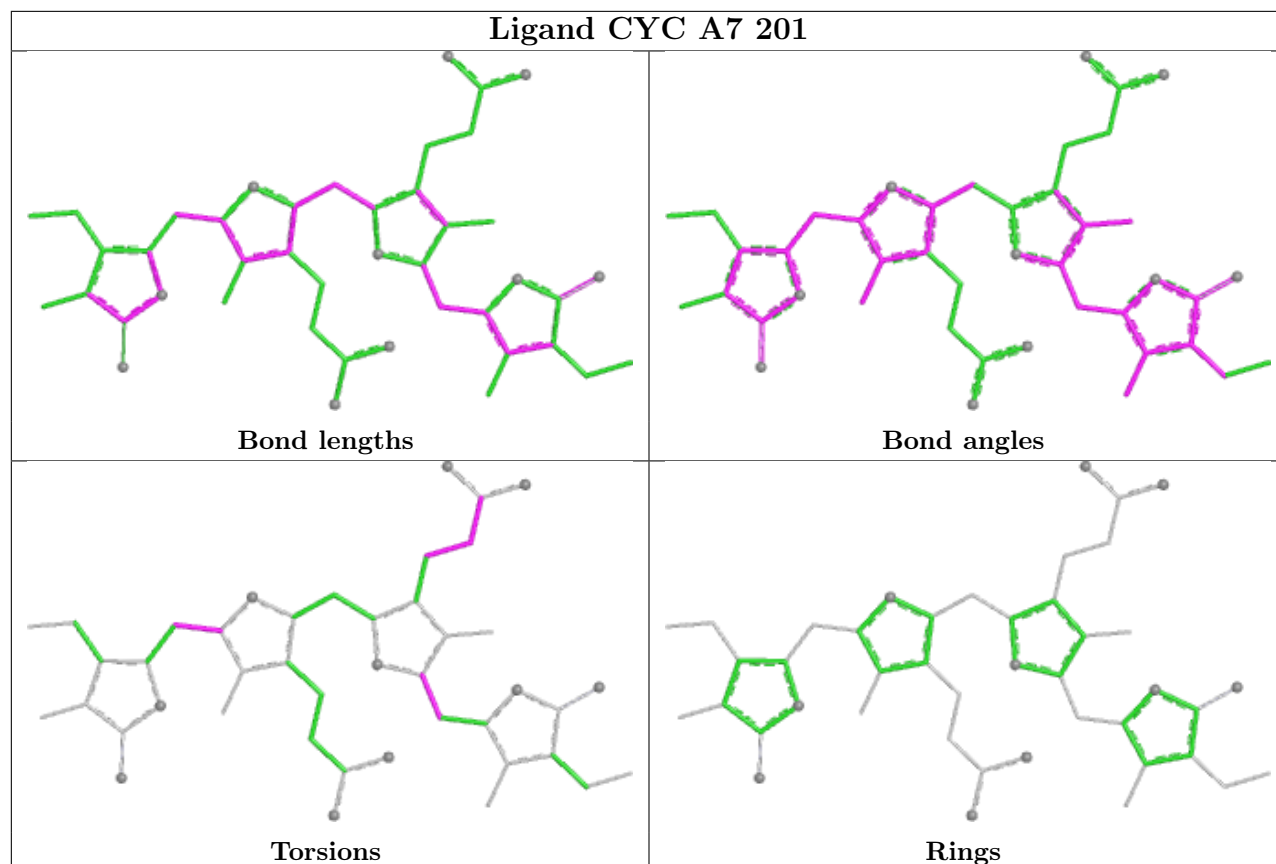
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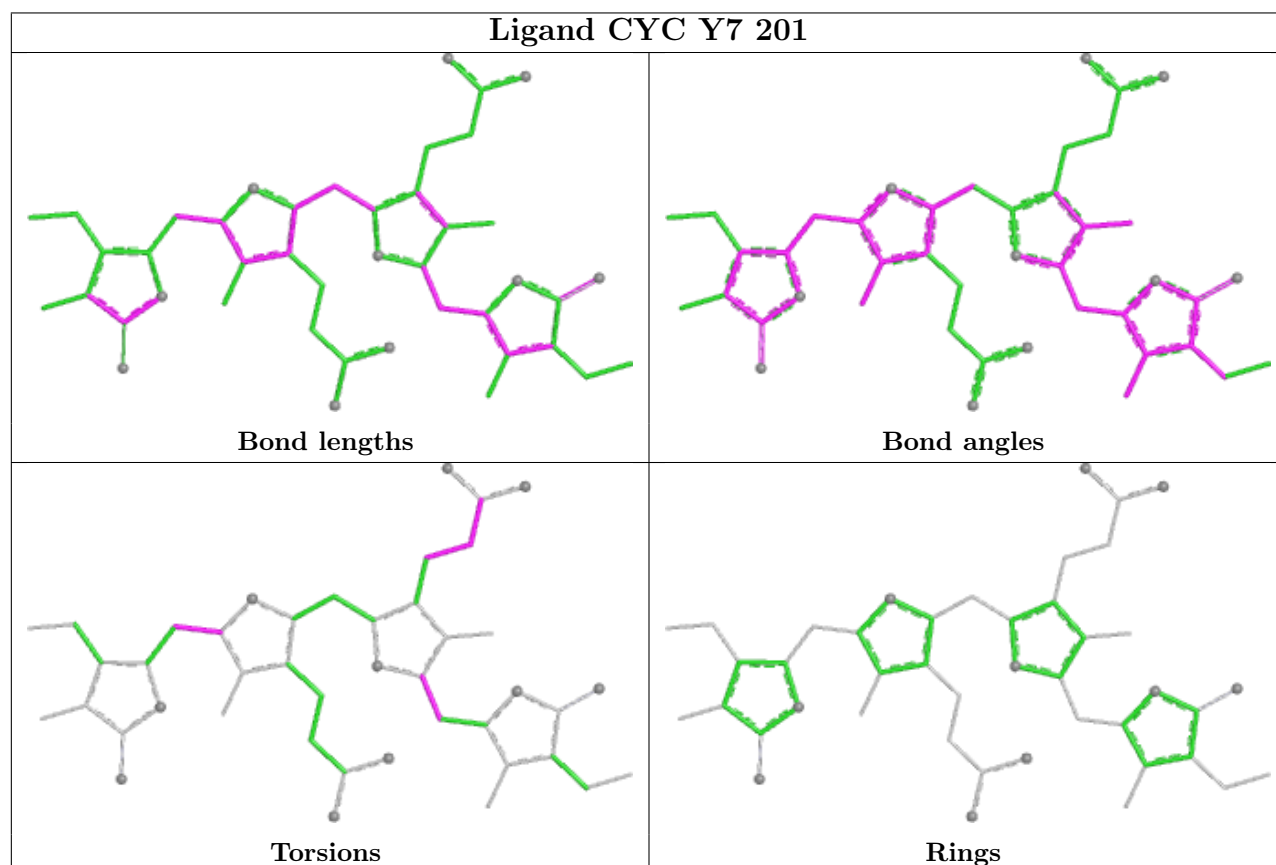
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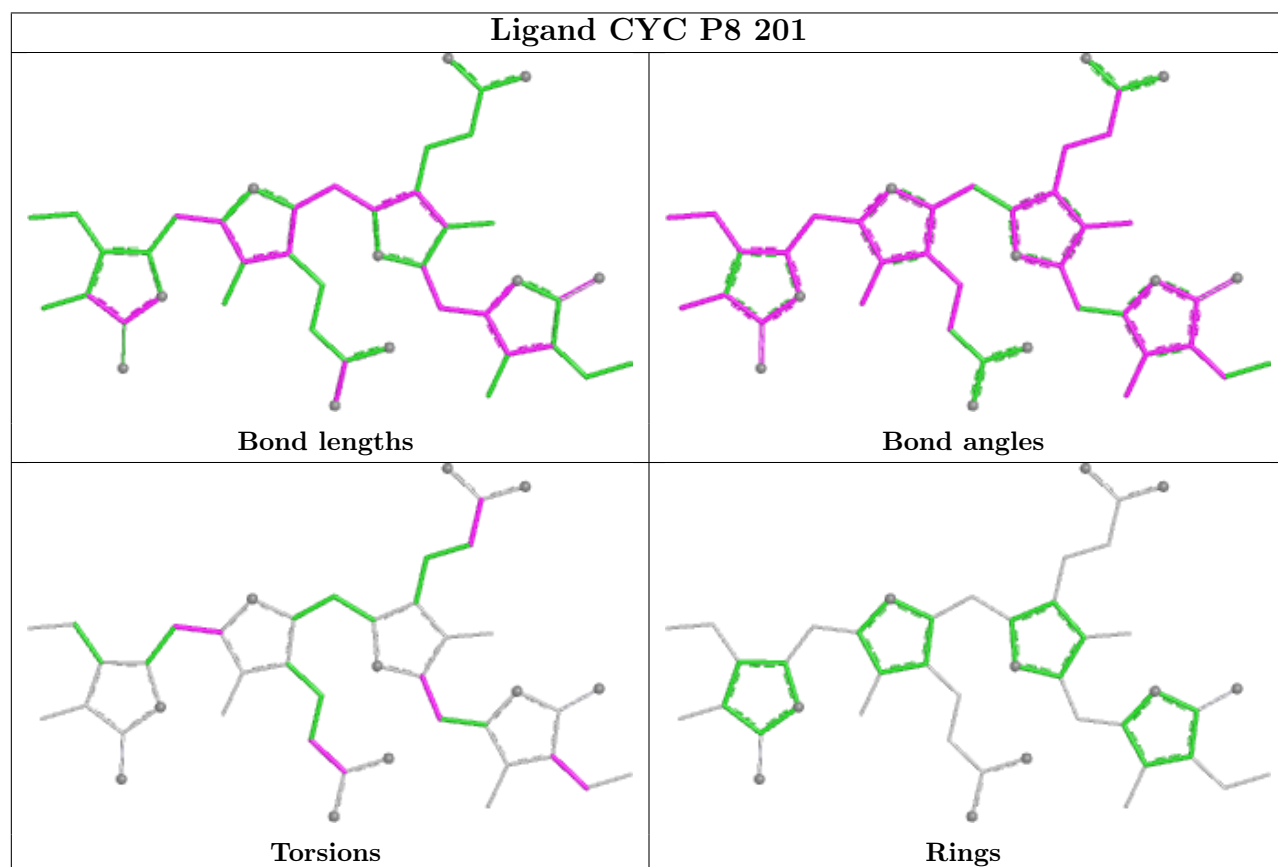
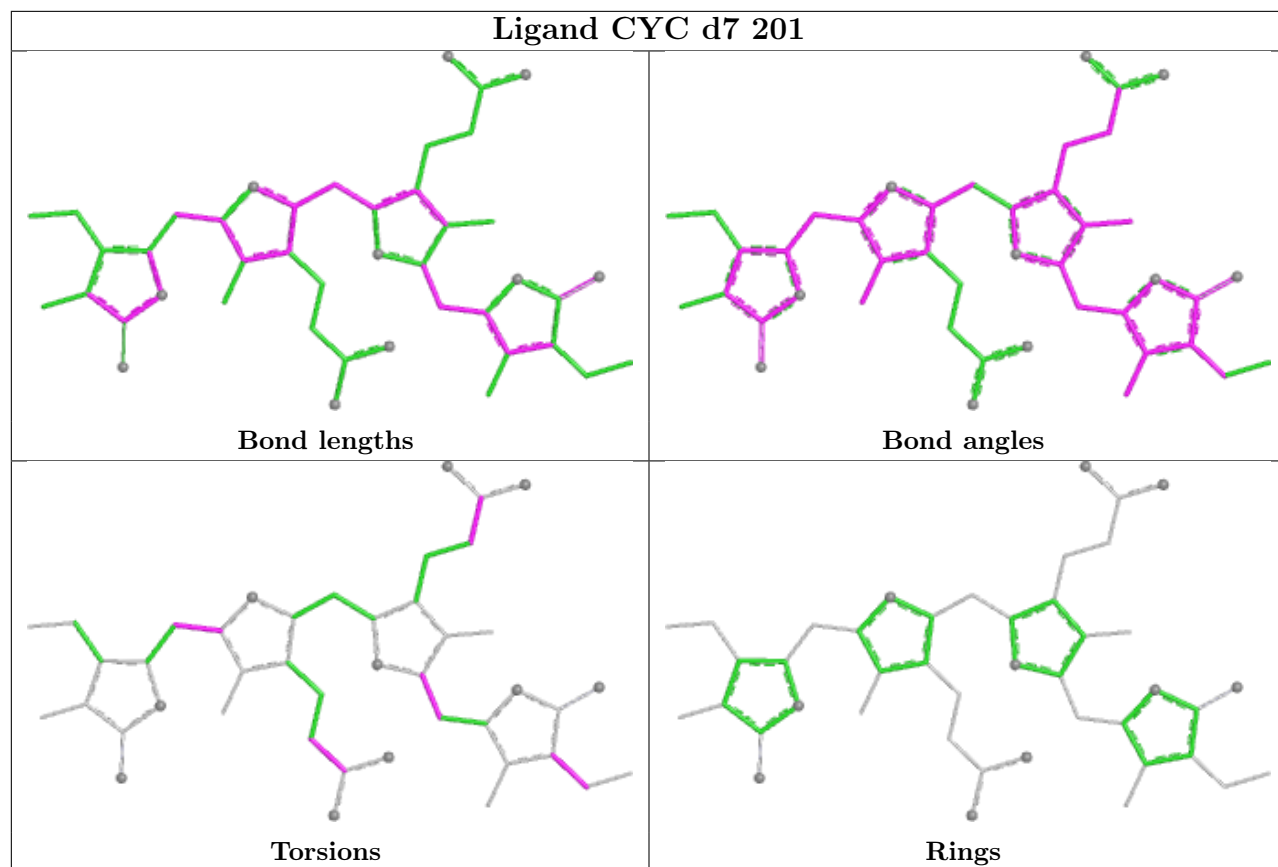


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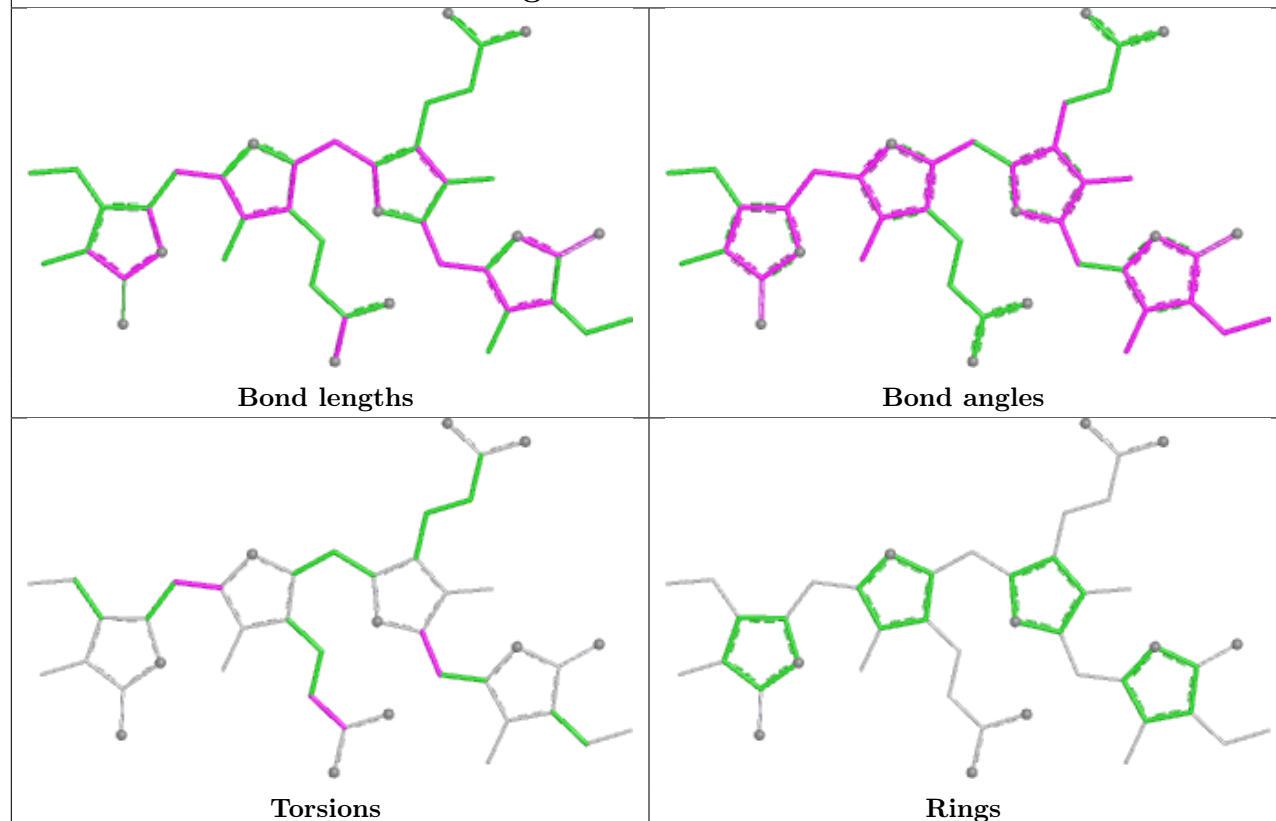


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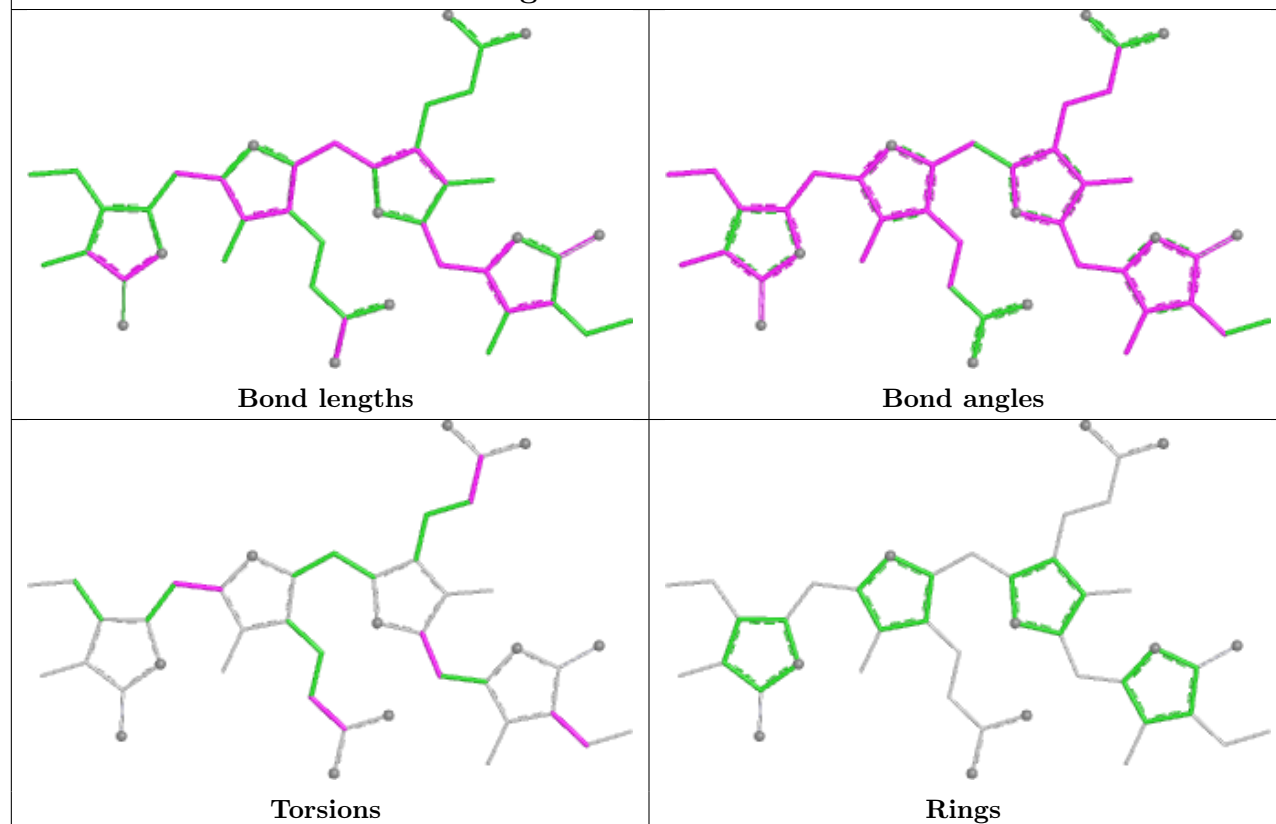




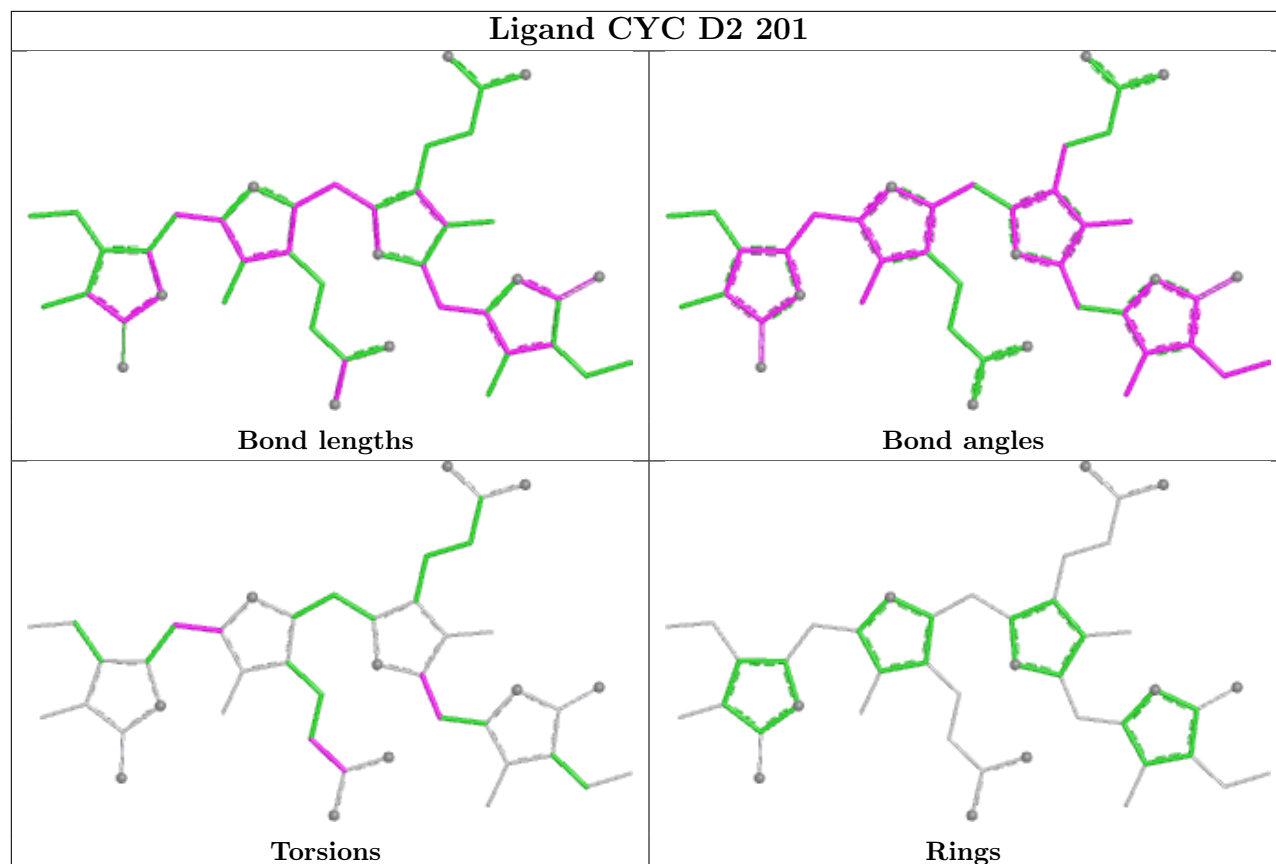
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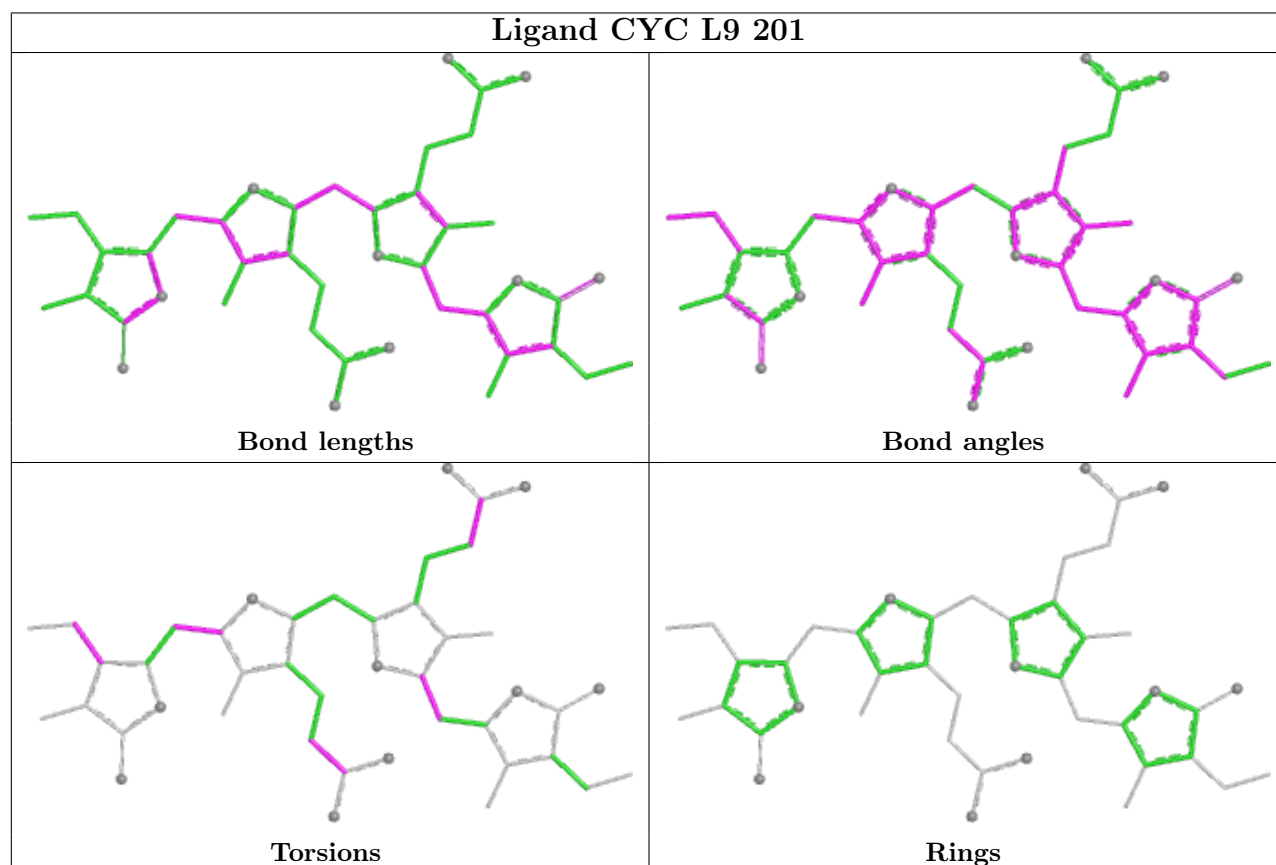
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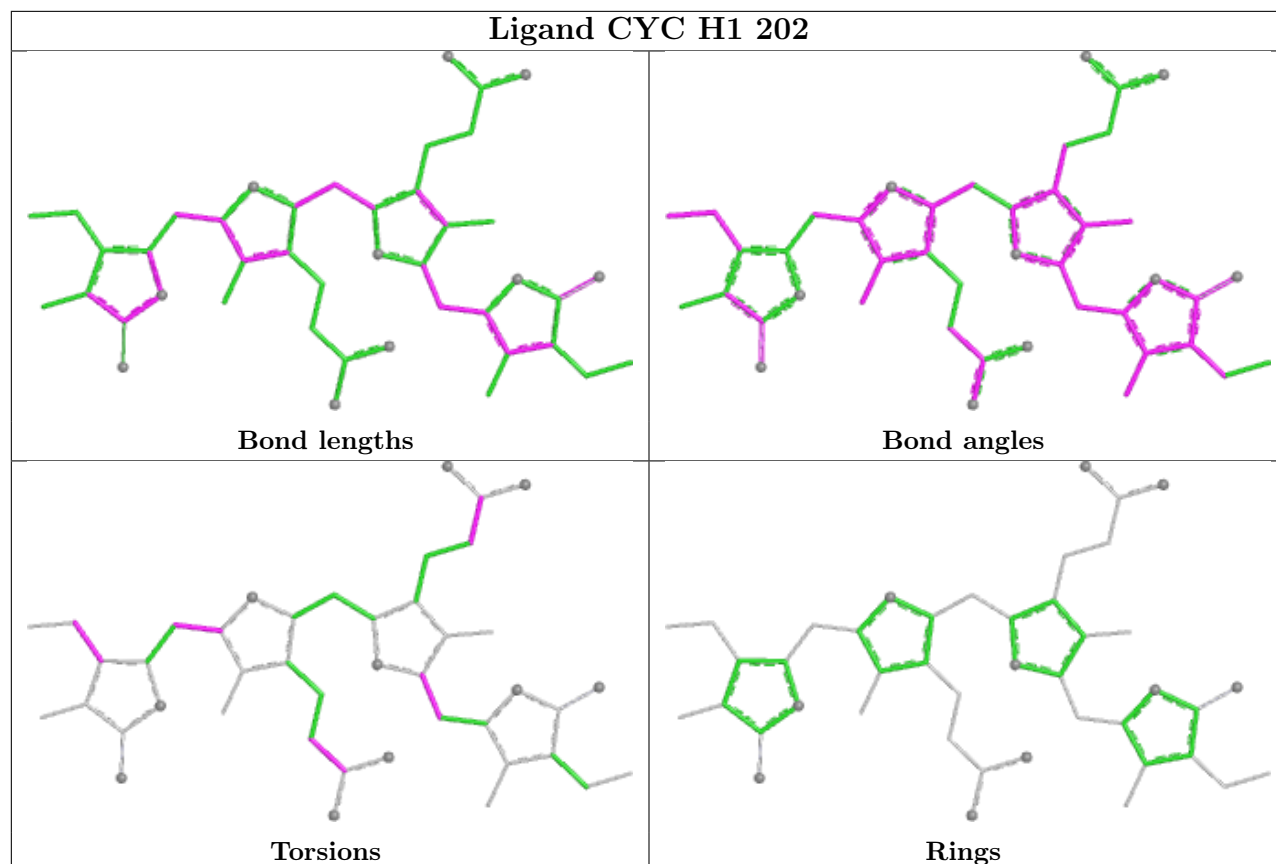
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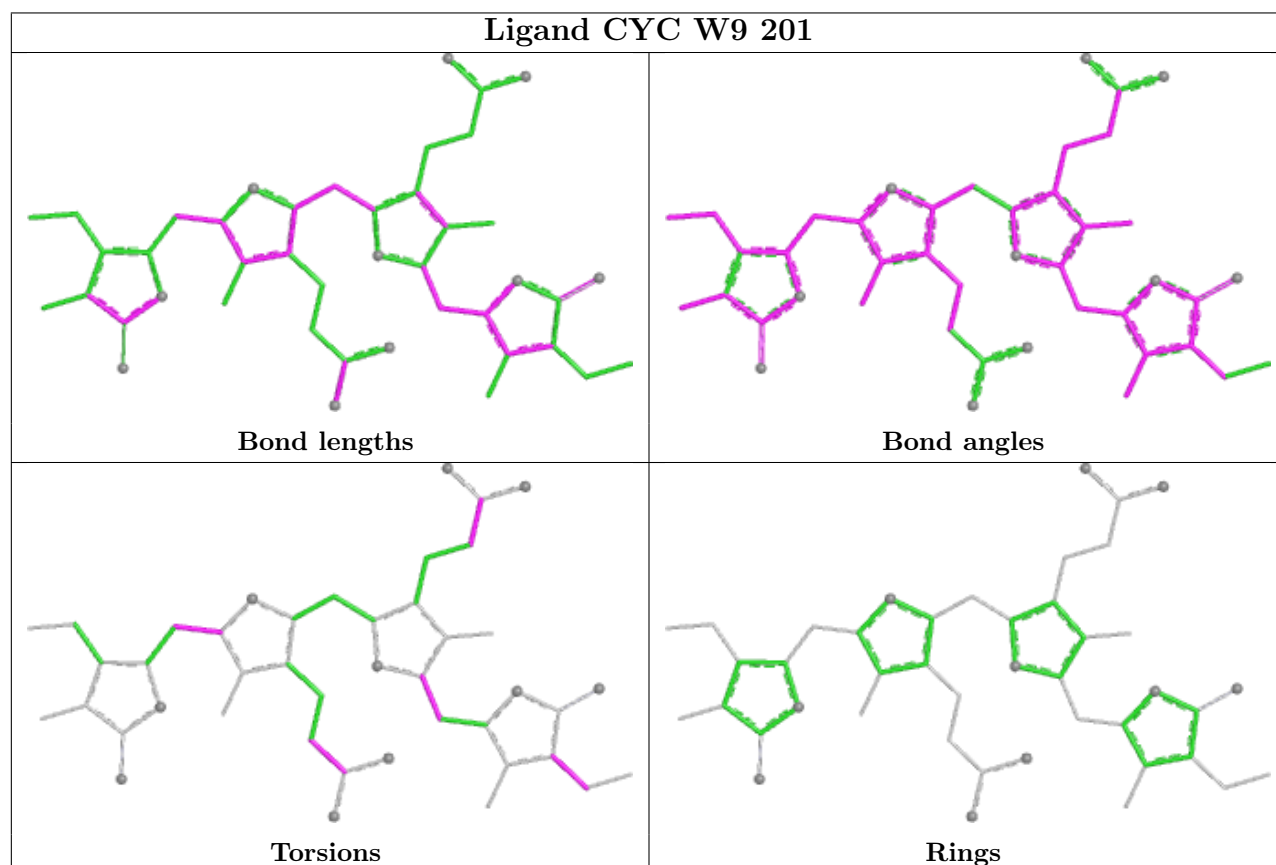
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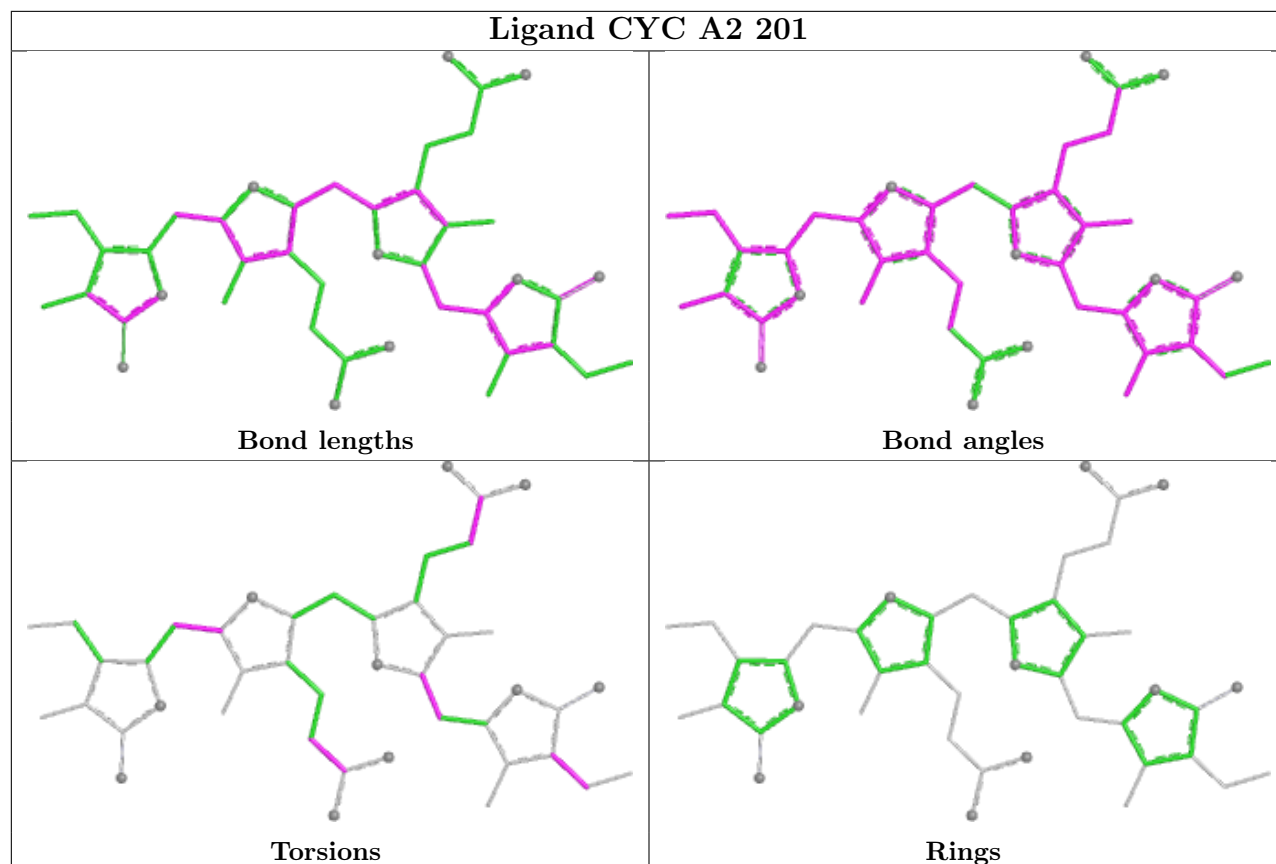
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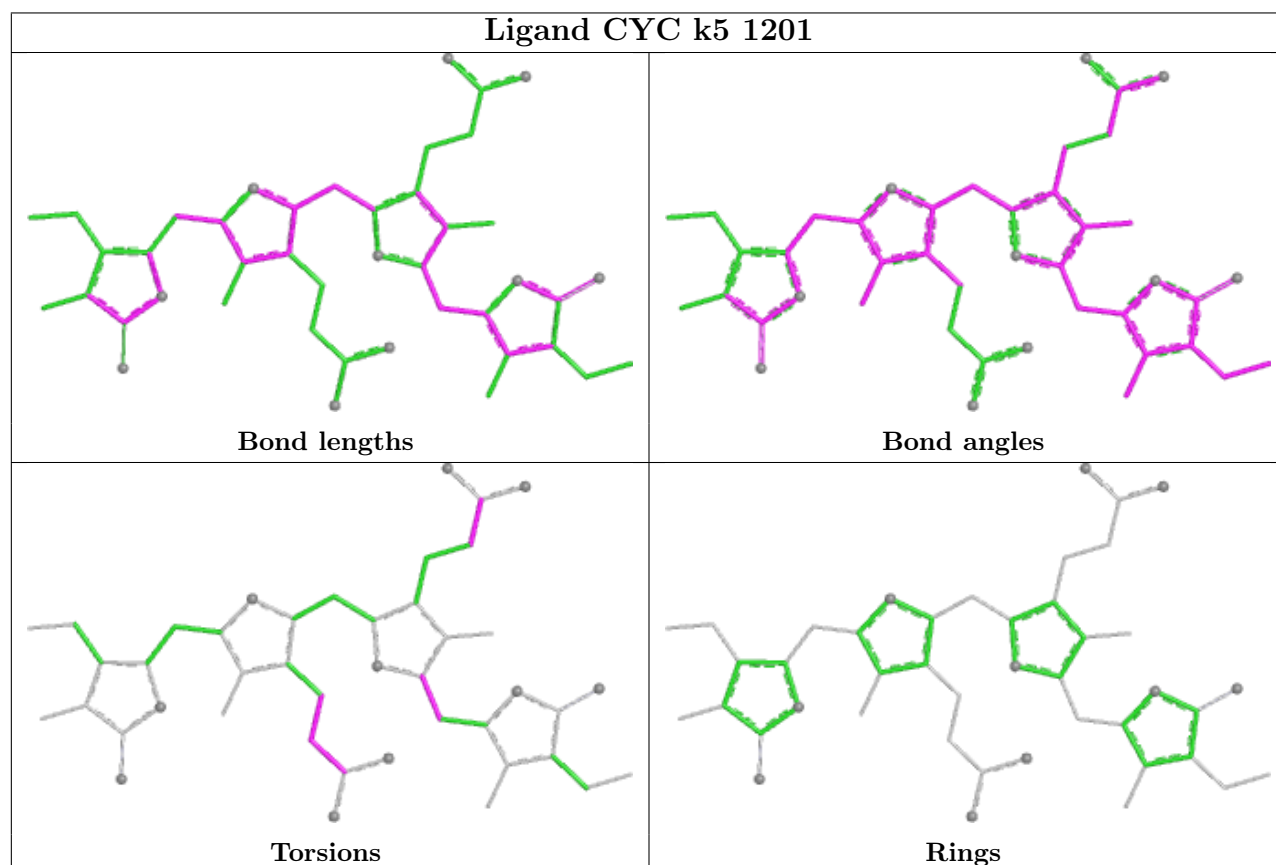
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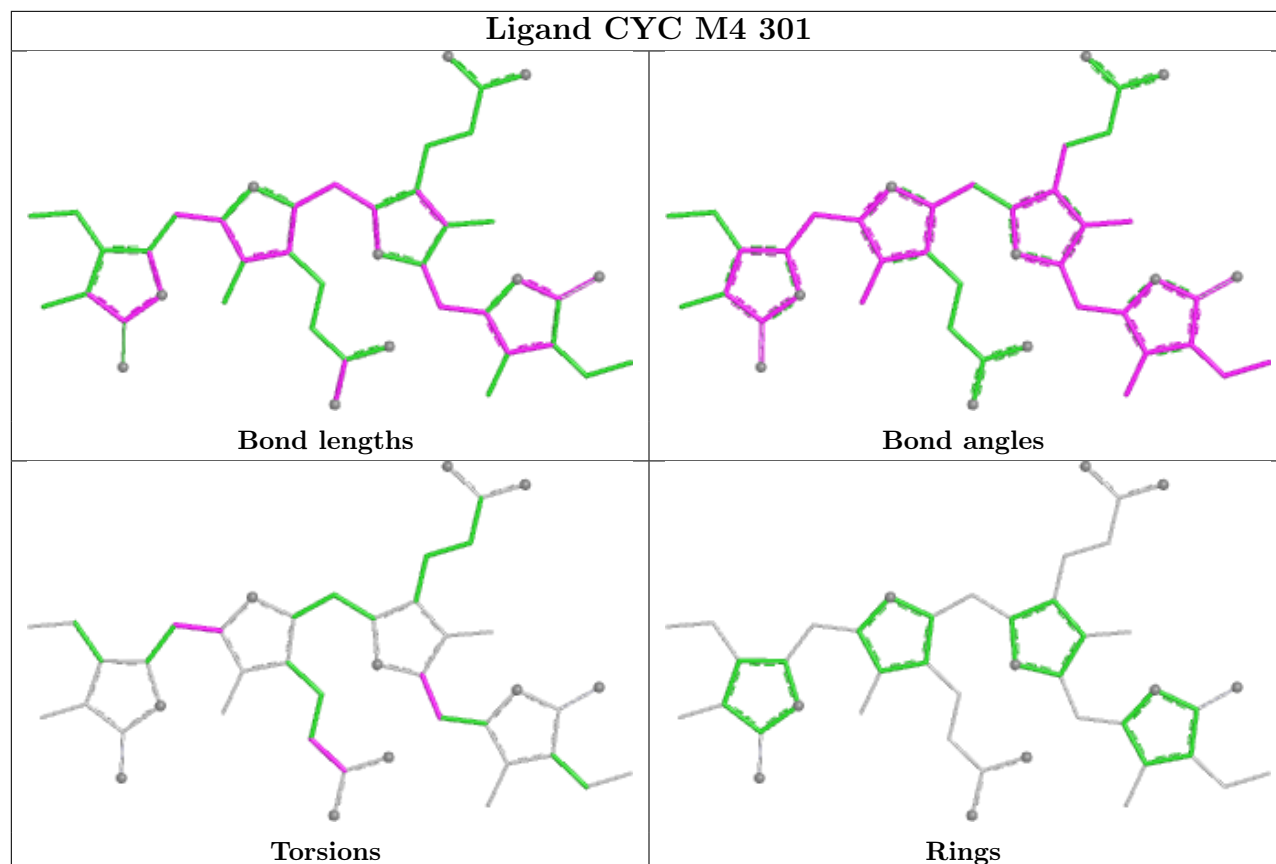
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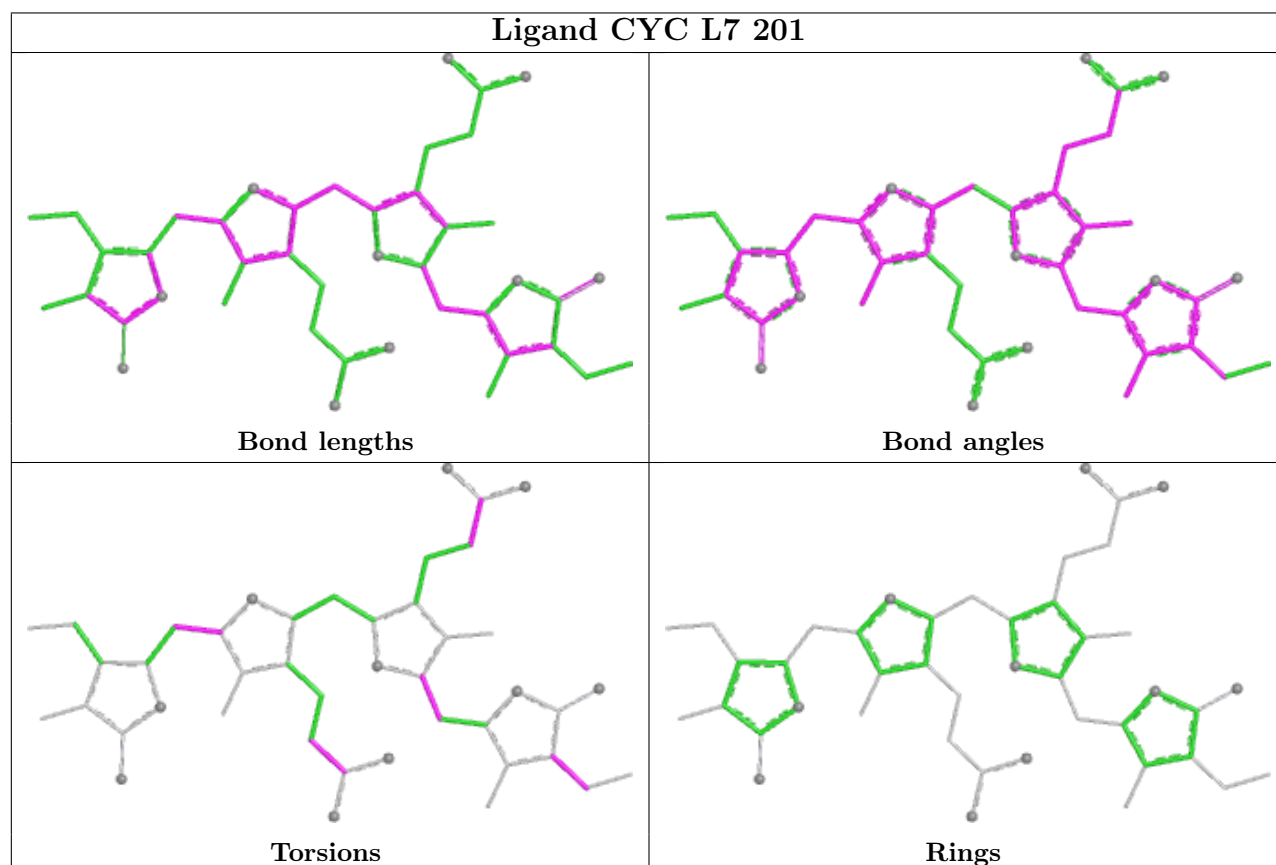
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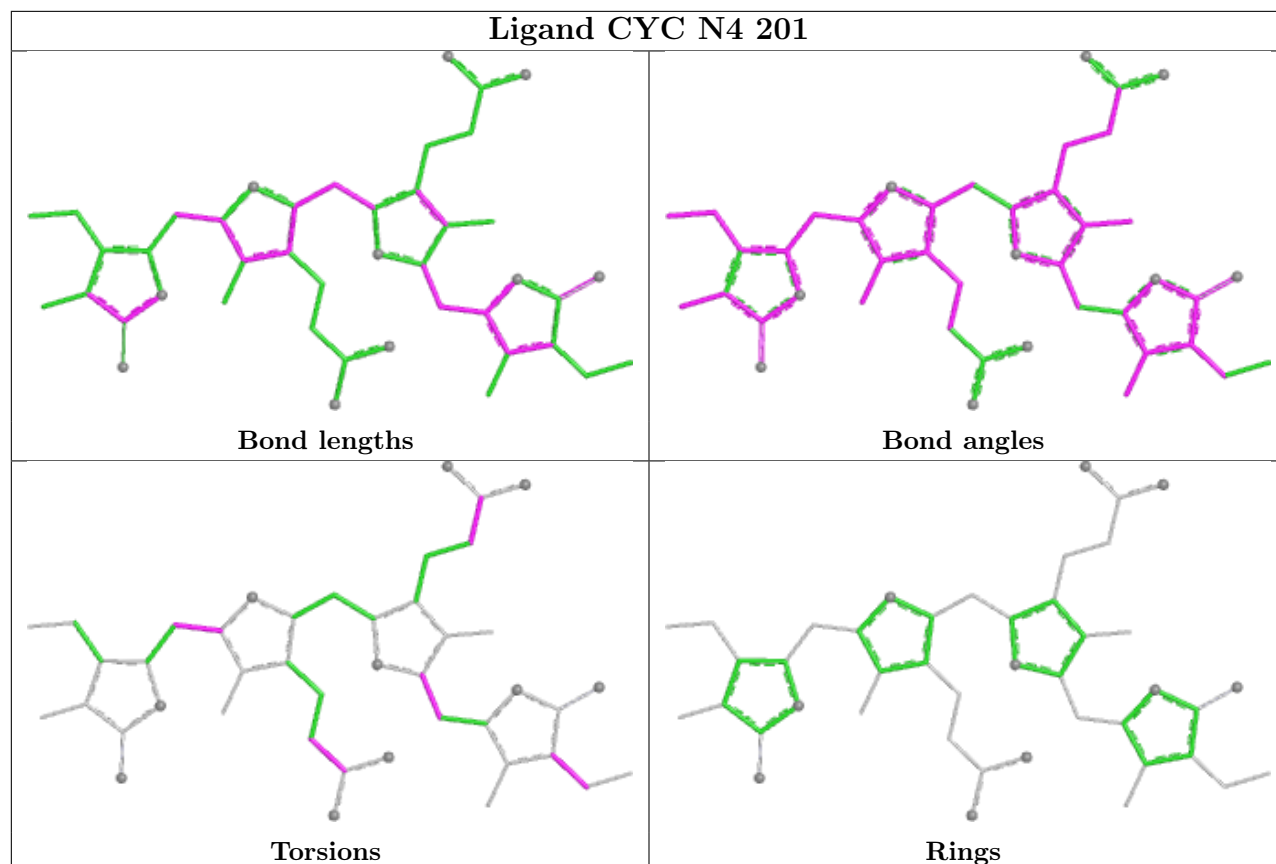
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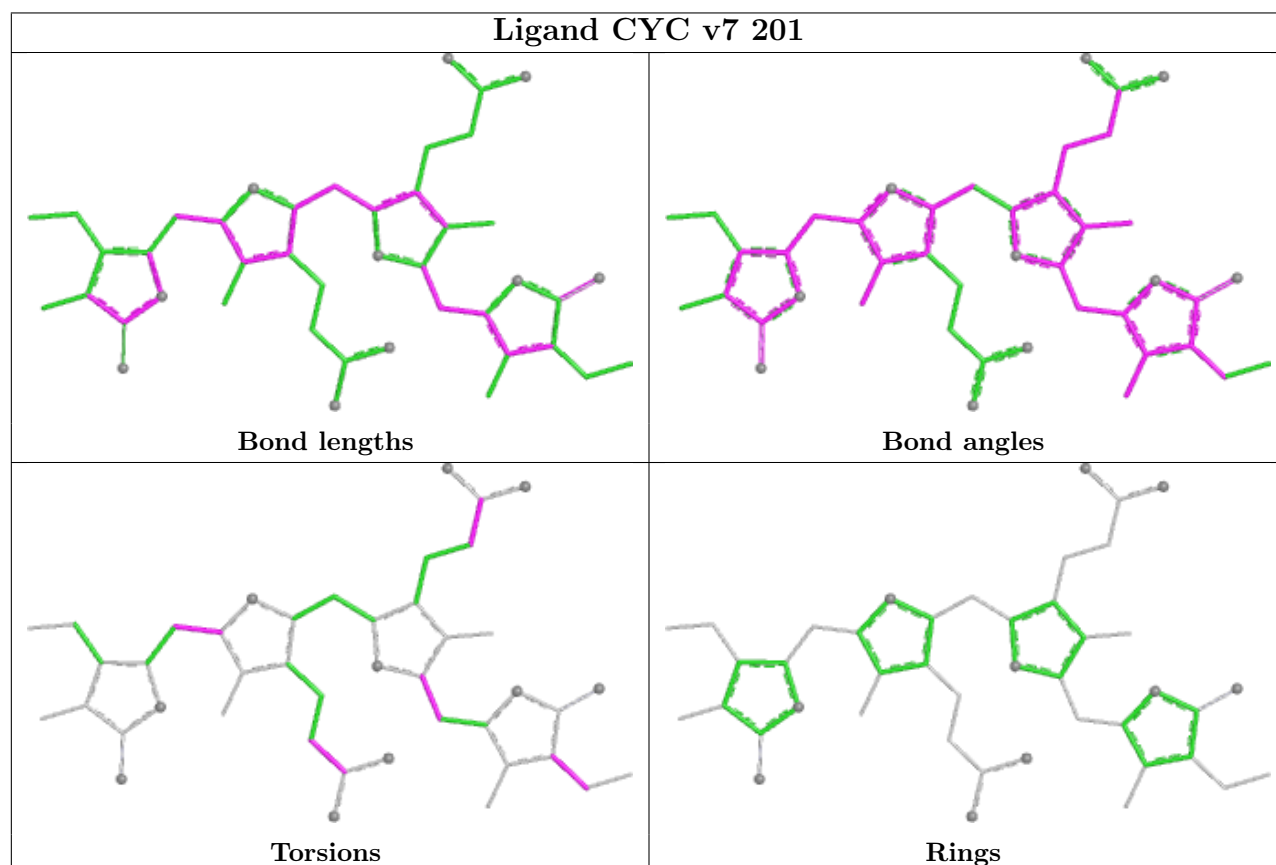
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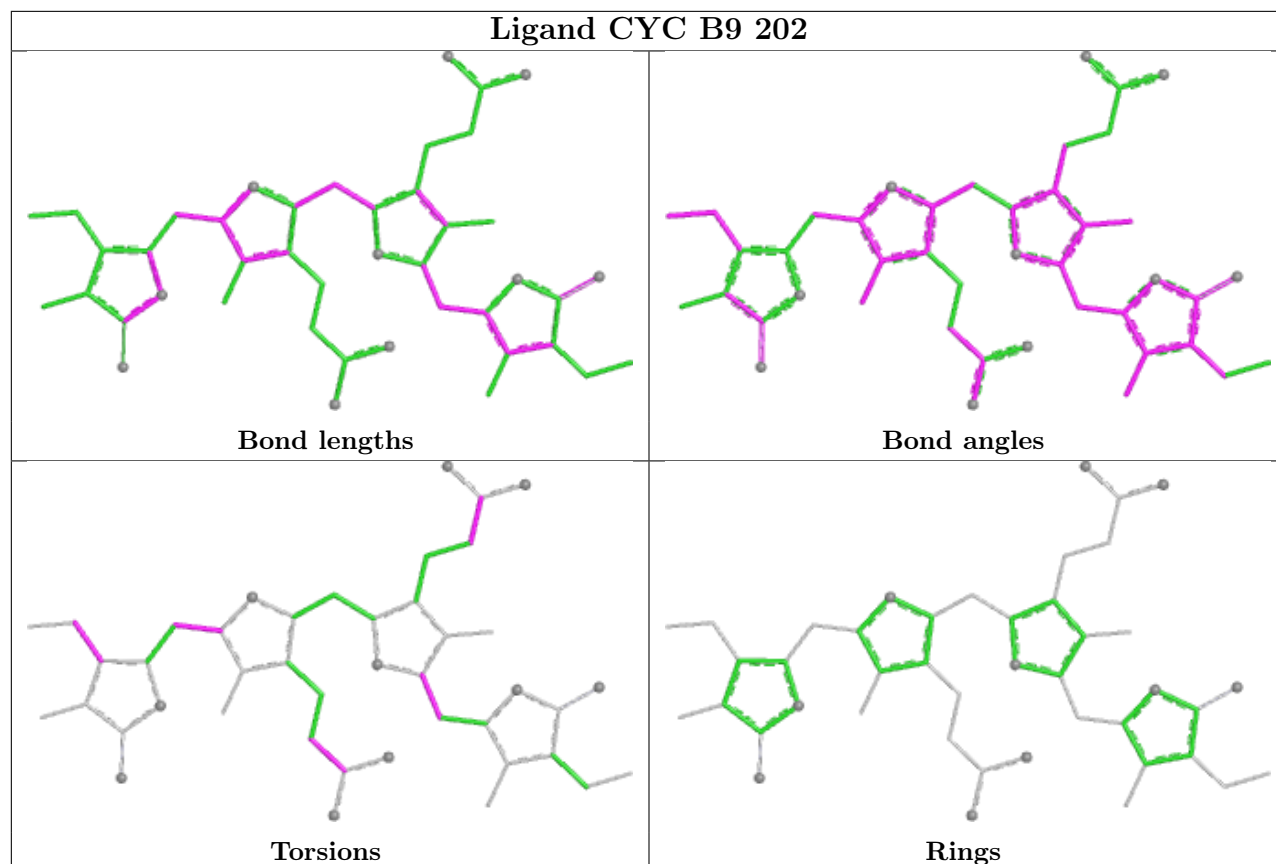
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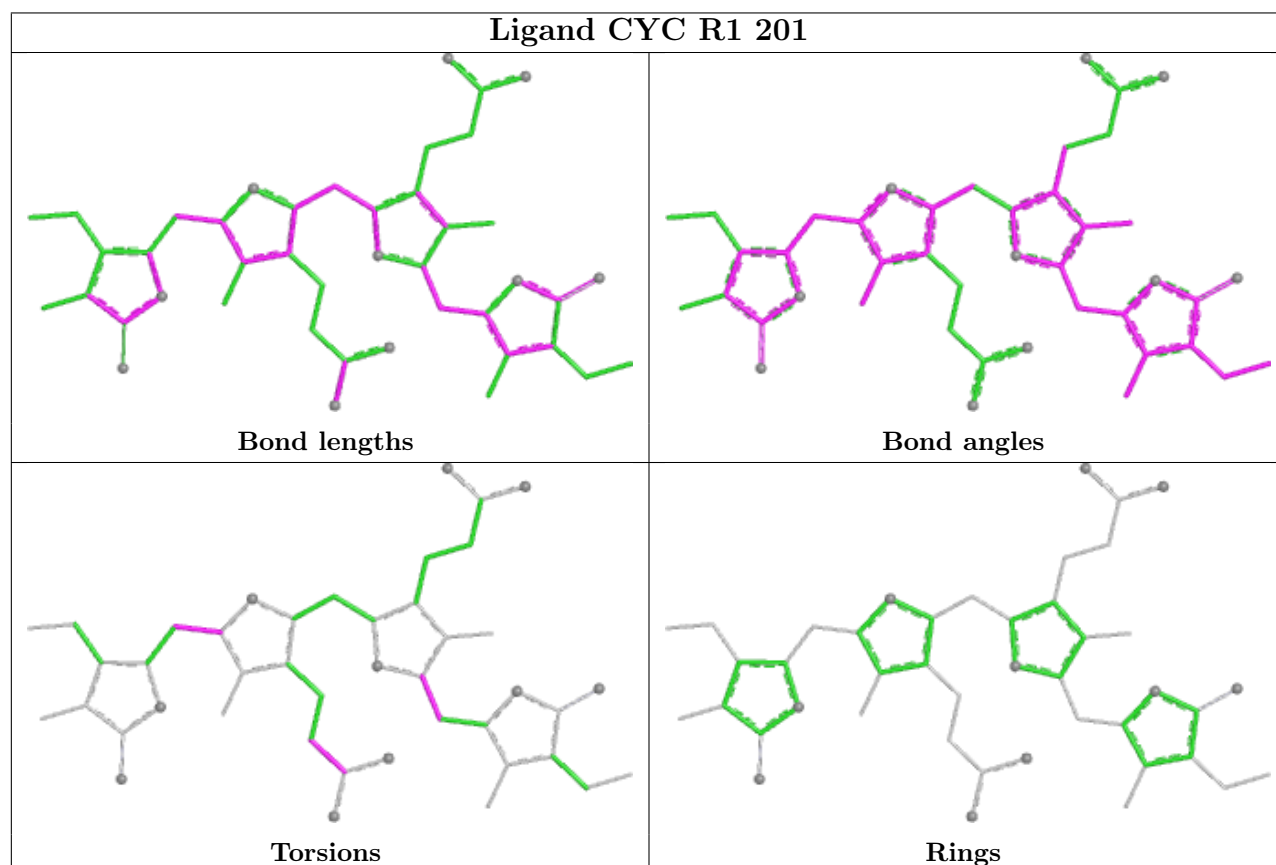
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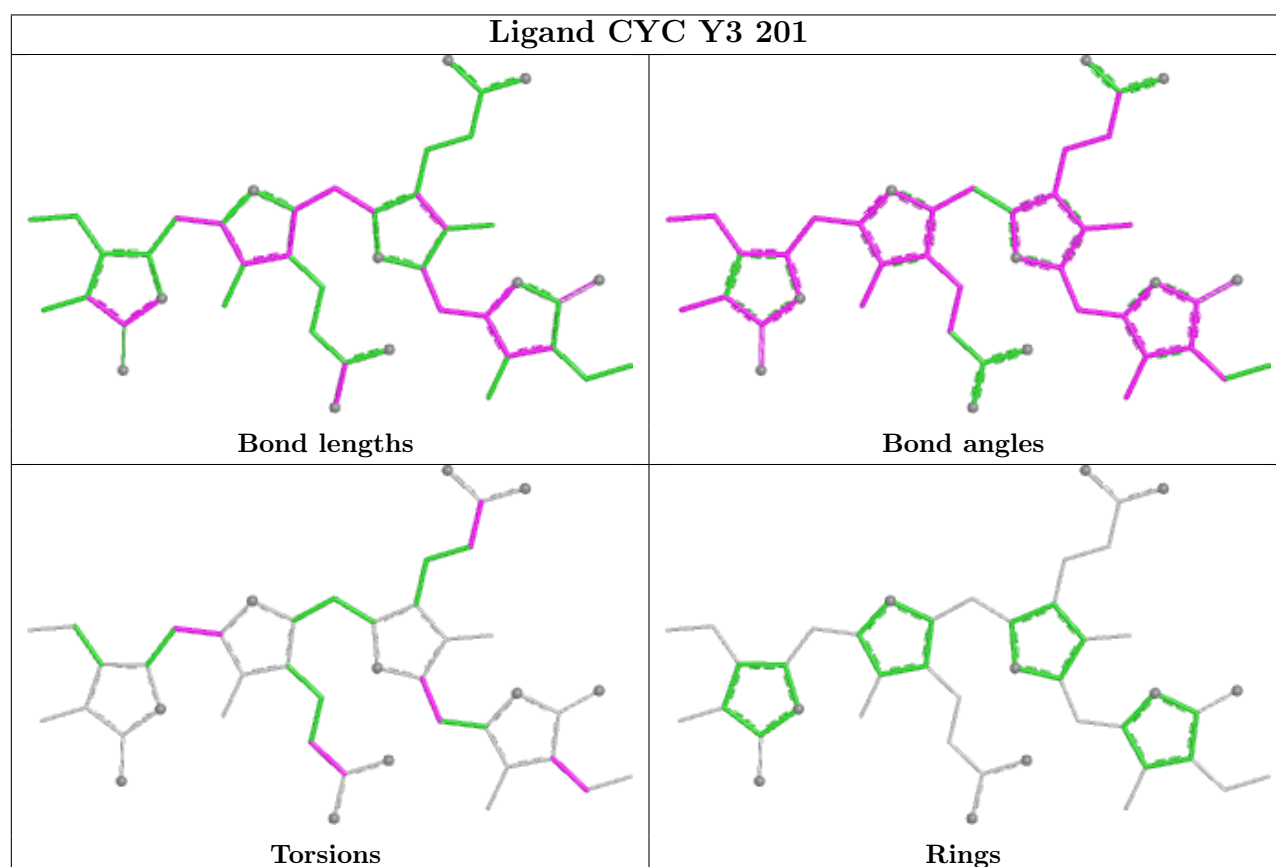
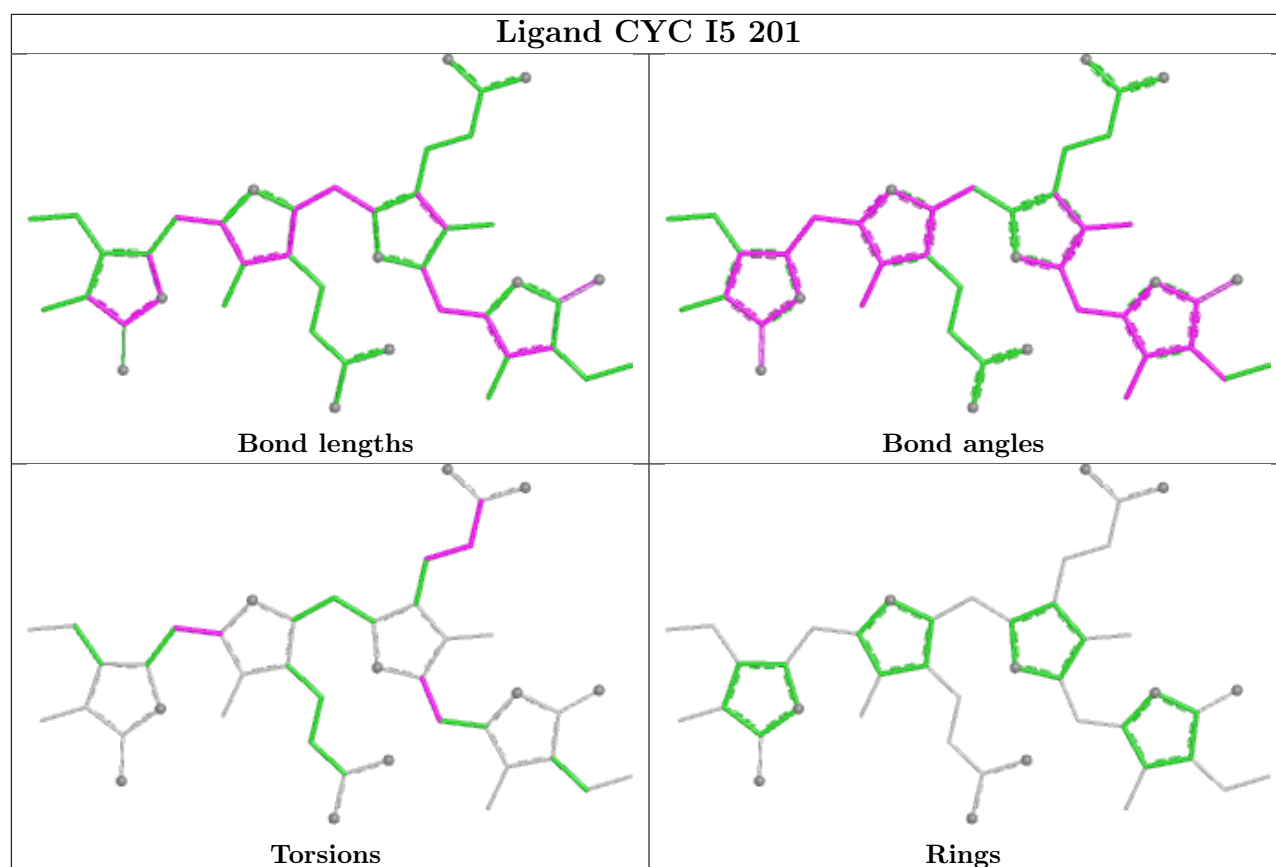


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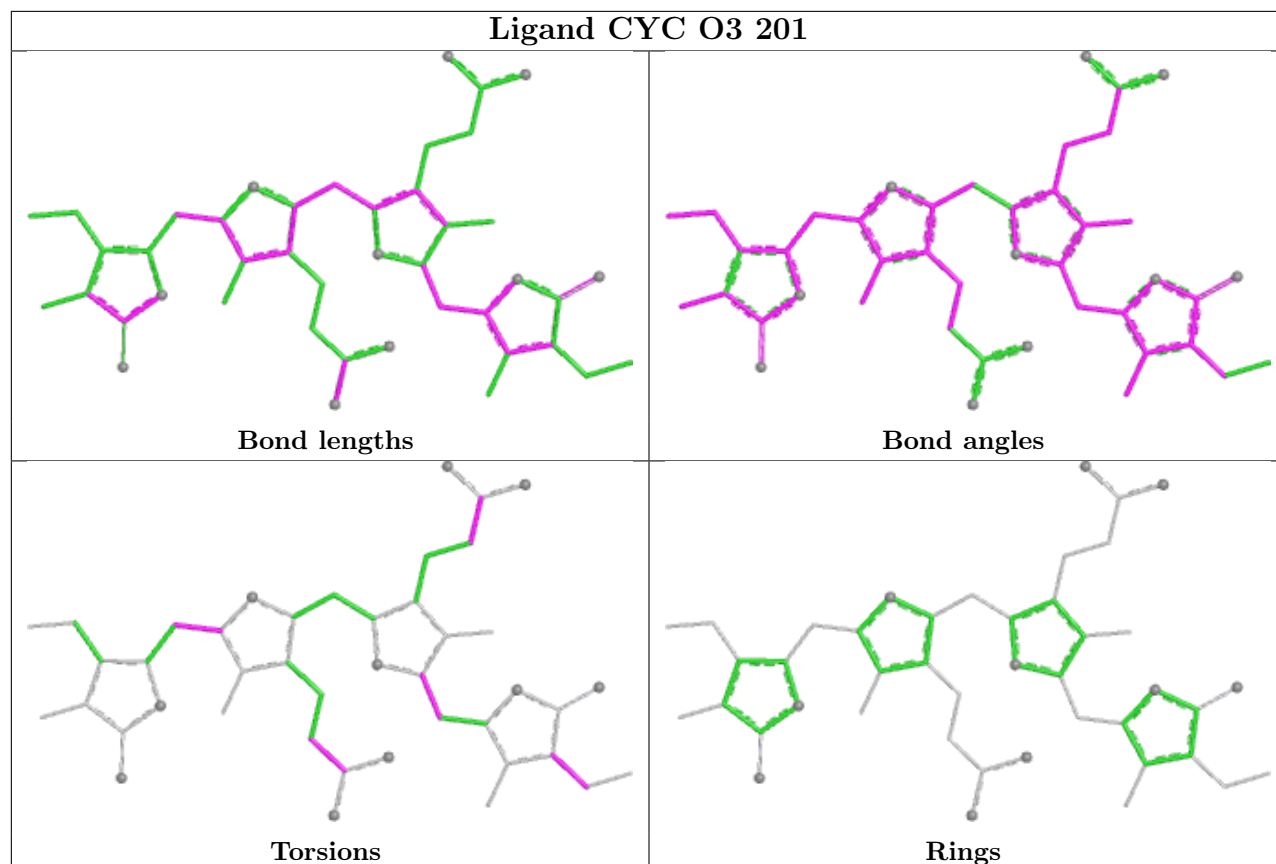


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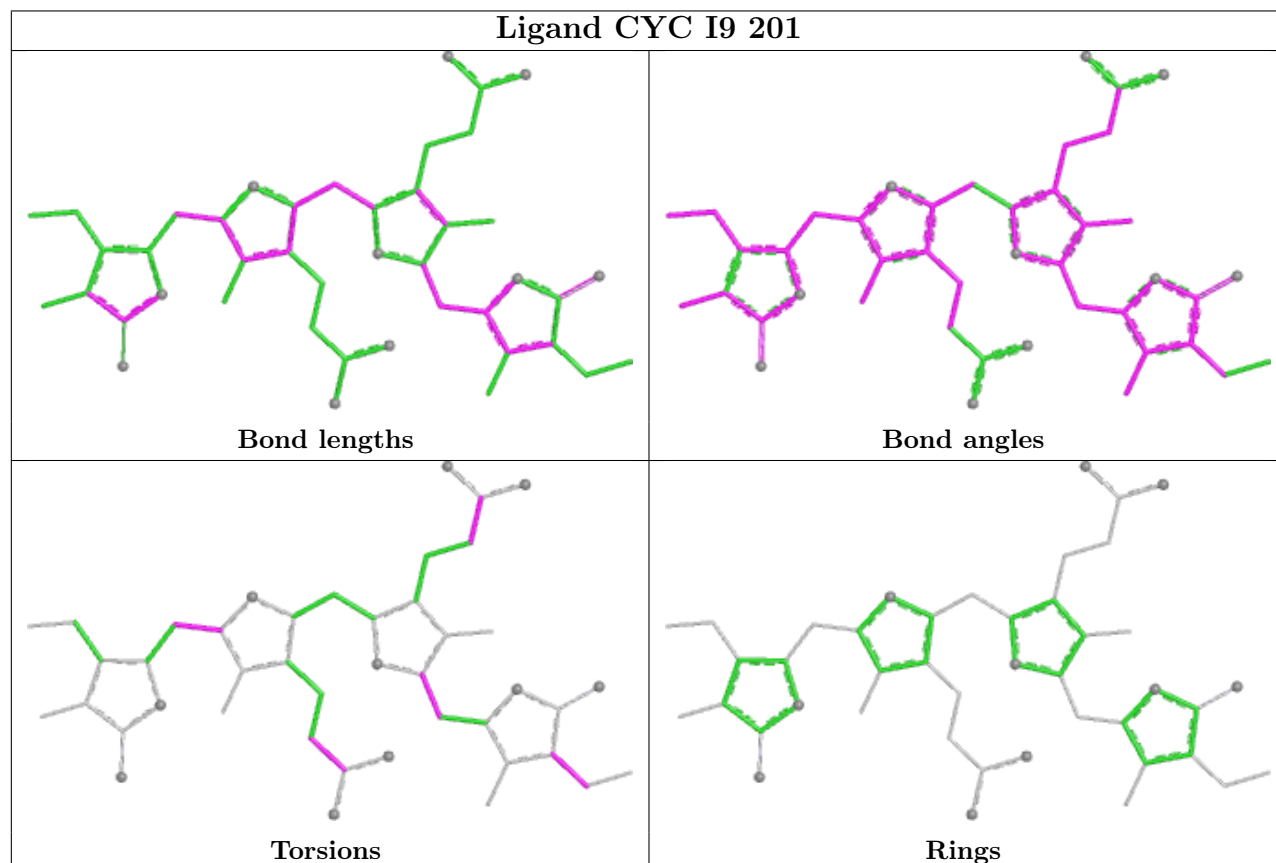


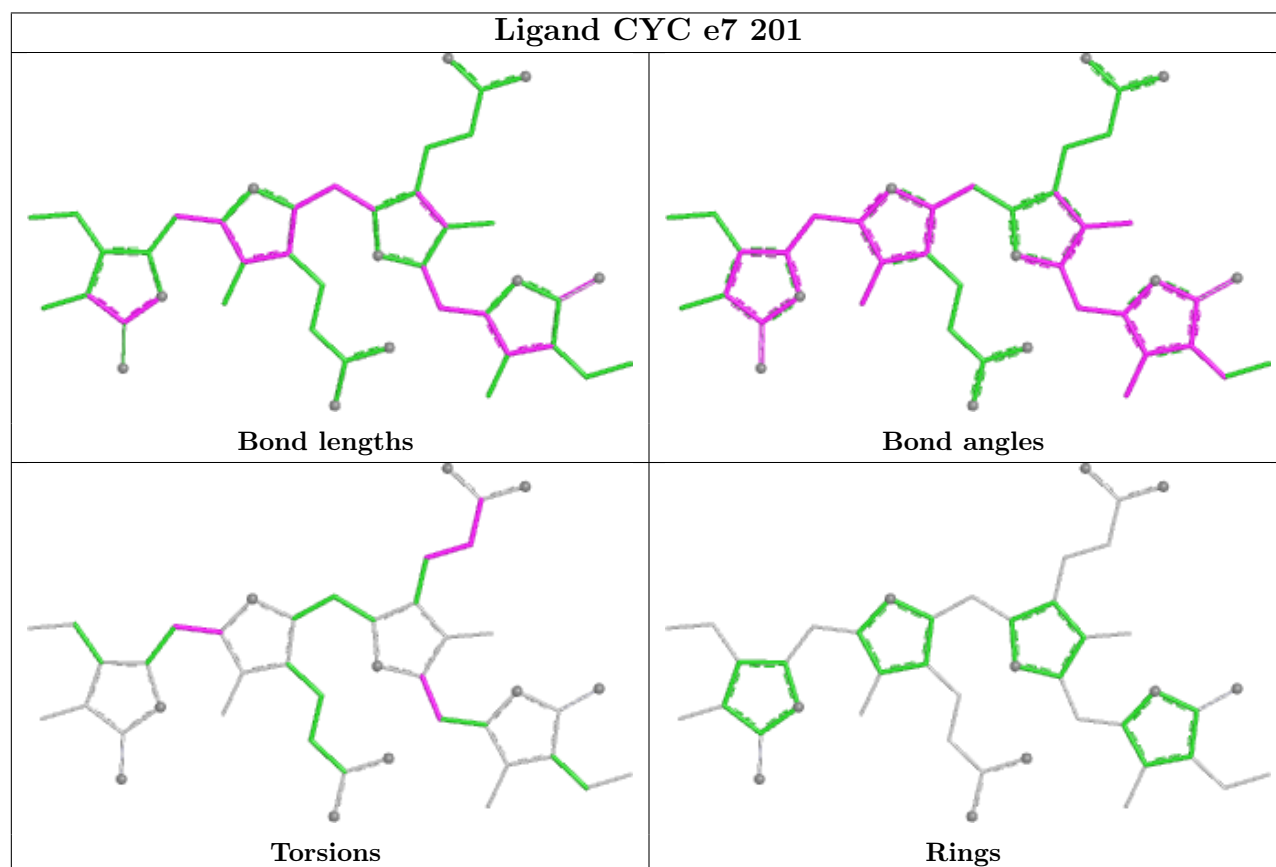
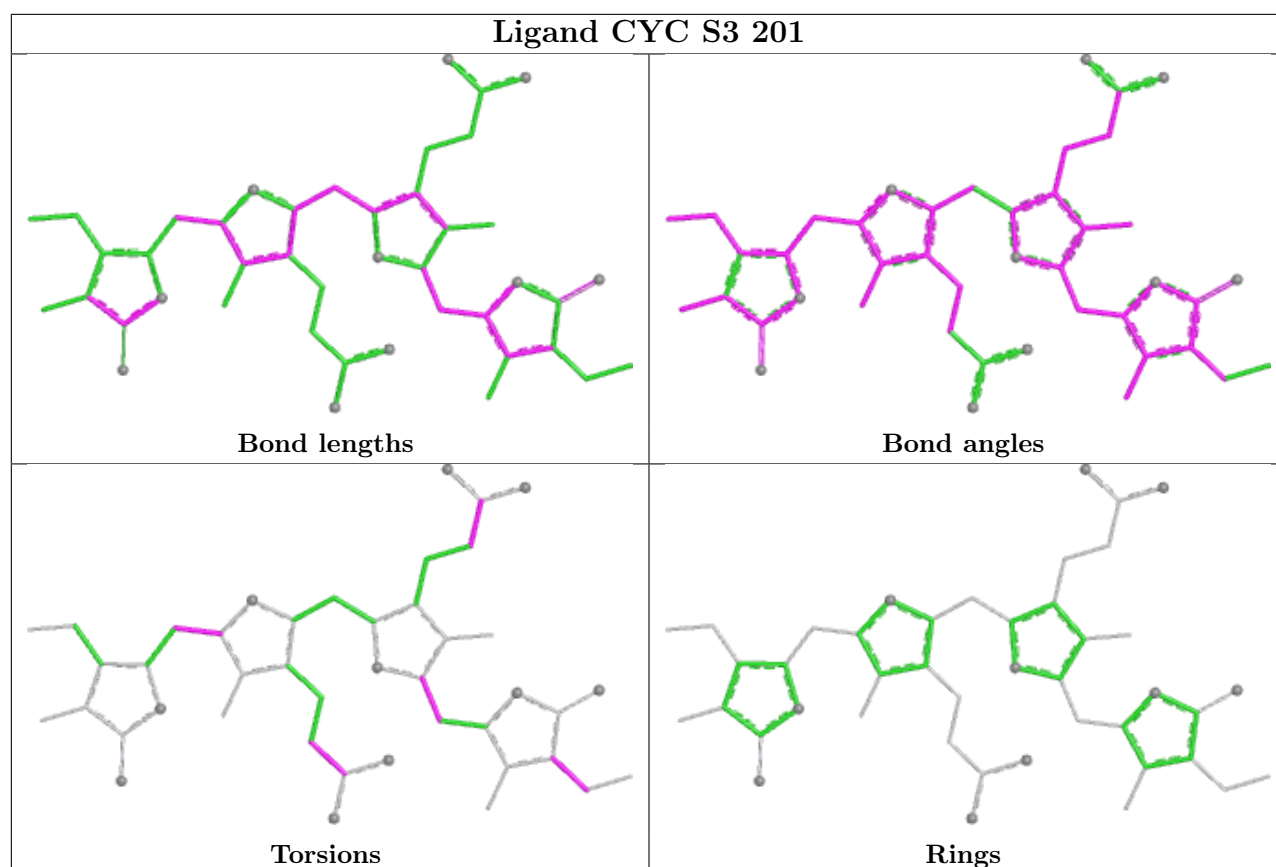


Ligand CYC O3 201



Ligand CYC I9 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.

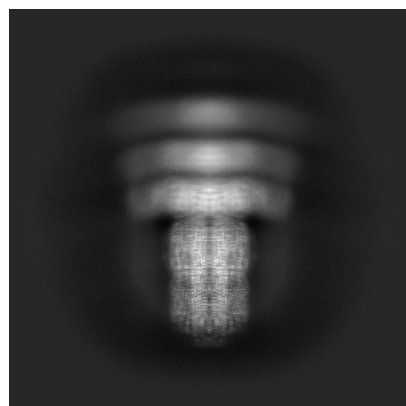
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62201. These allow visual inspection of the internal detail of the map and identification of artifacts.

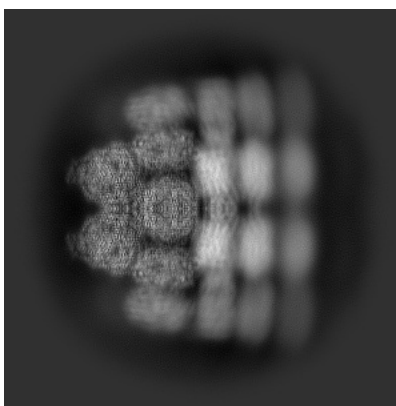
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

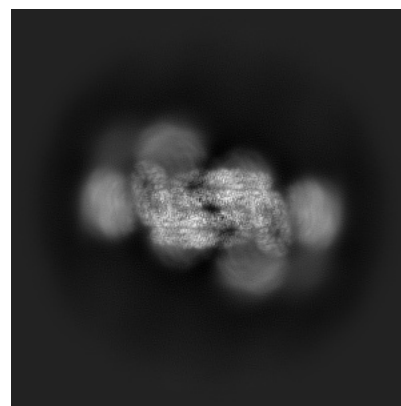
6.1.1 Primary map



X

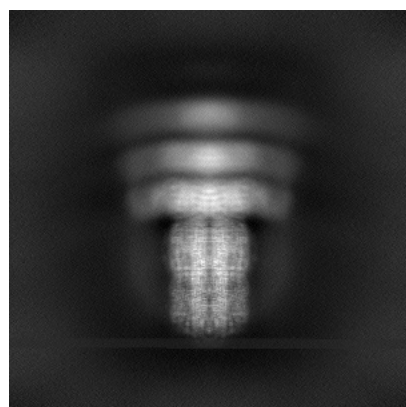


Y

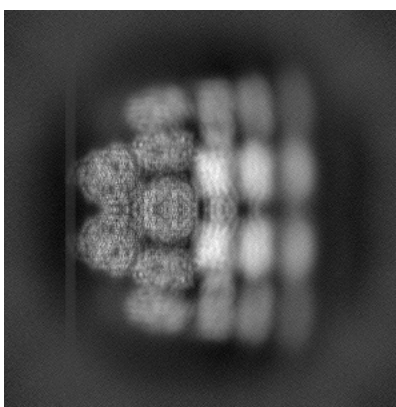


Z

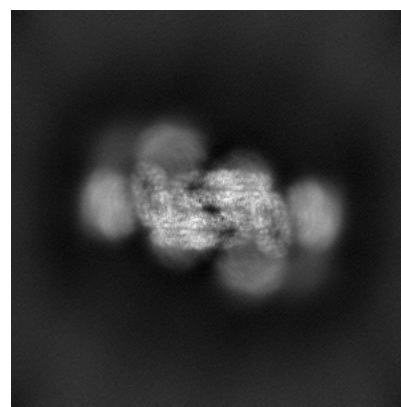
6.1.2 Raw map



X



Y

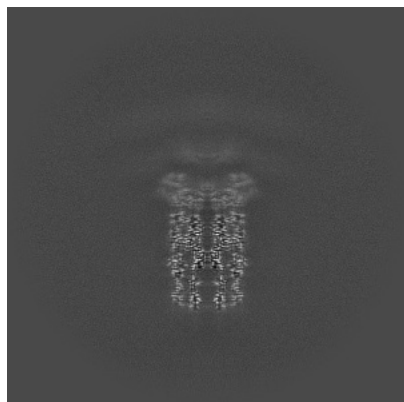


Z

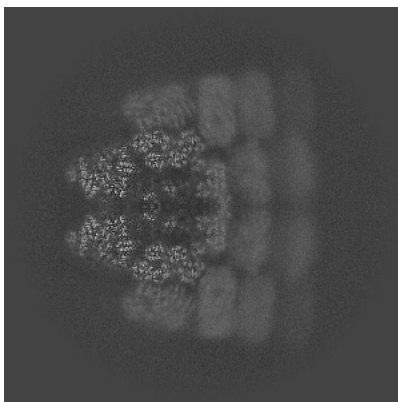
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

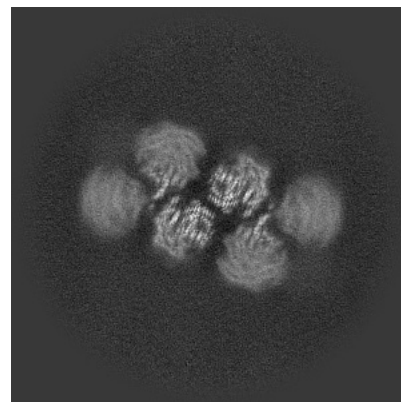
6.2.1 Primary map



X Index: 280

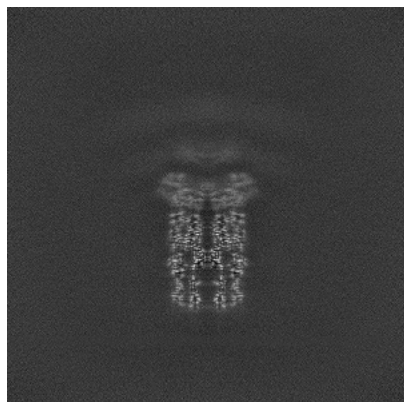


Y Index: 280

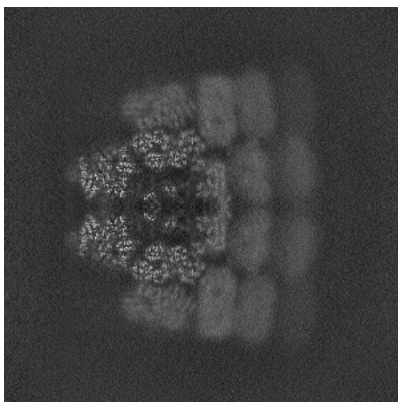


Z Index: 280

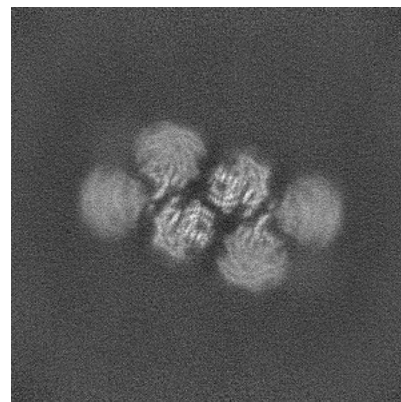
6.2.2 Raw map



X Index: 280



Y Index: 280



Z Index: 280

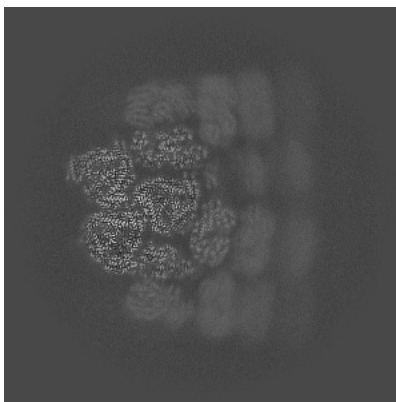
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

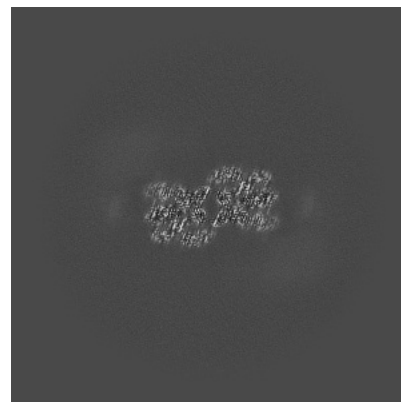
6.3.1 Primary map



X Index: 259



Y Index: 265

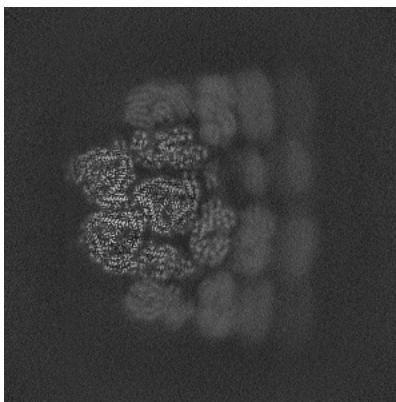


Z Index: 166

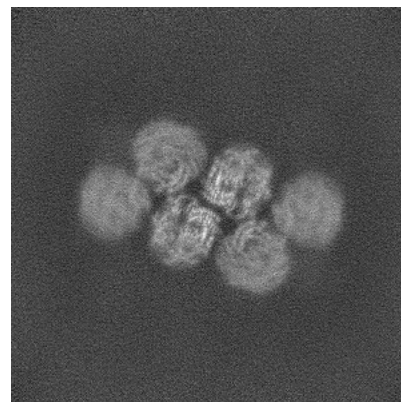
6.3.2 Raw map



X Index: 258



Y Index: 265

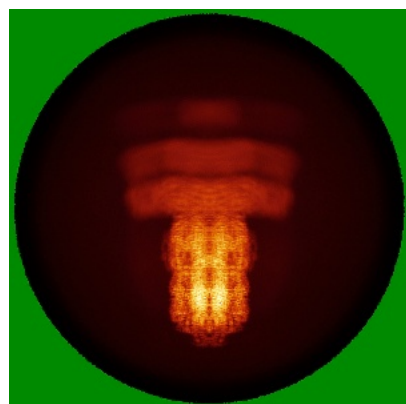


Z Index: 290

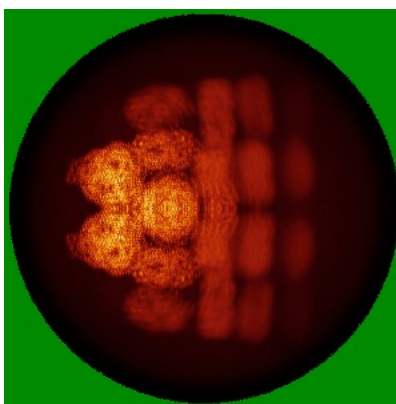
The images above show the largest variance slices of the map in three orthogonal directions.

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

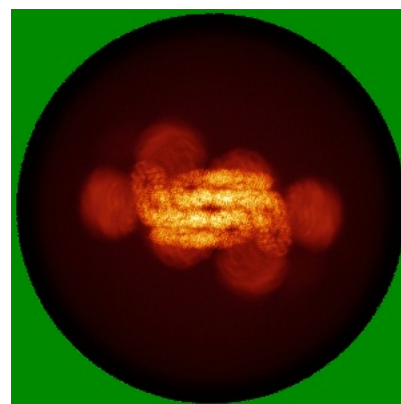
6.4.1 Primary map



X

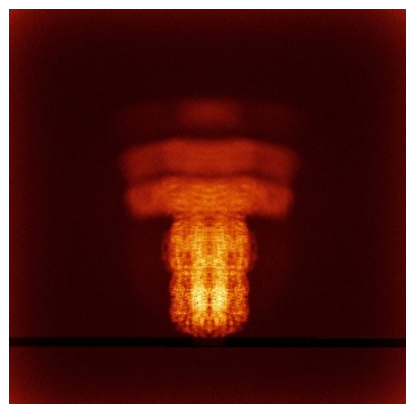


Y

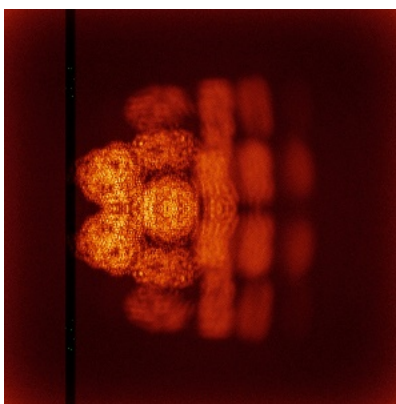


Z

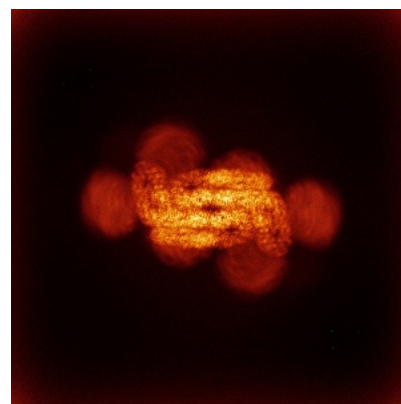
6.4.2 Raw map



X



Y

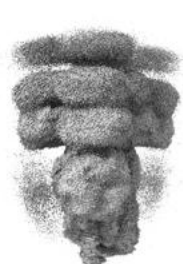


Z

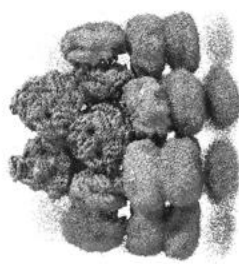
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

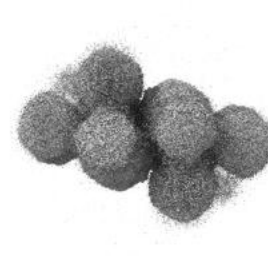
6.5.1 Primary map



X



Y



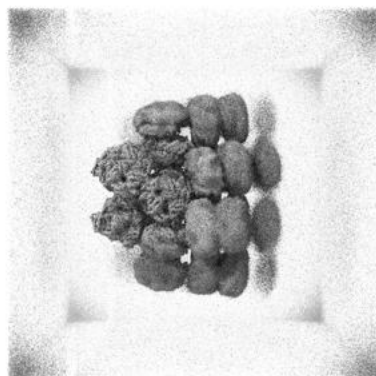
Z

The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

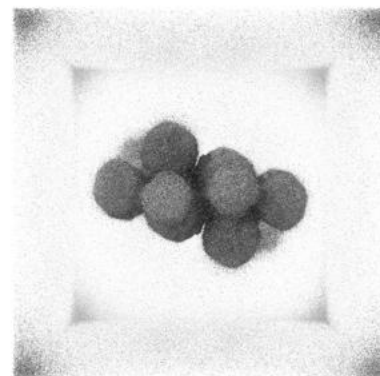
6.5.2 Raw map



X



Y



Z

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

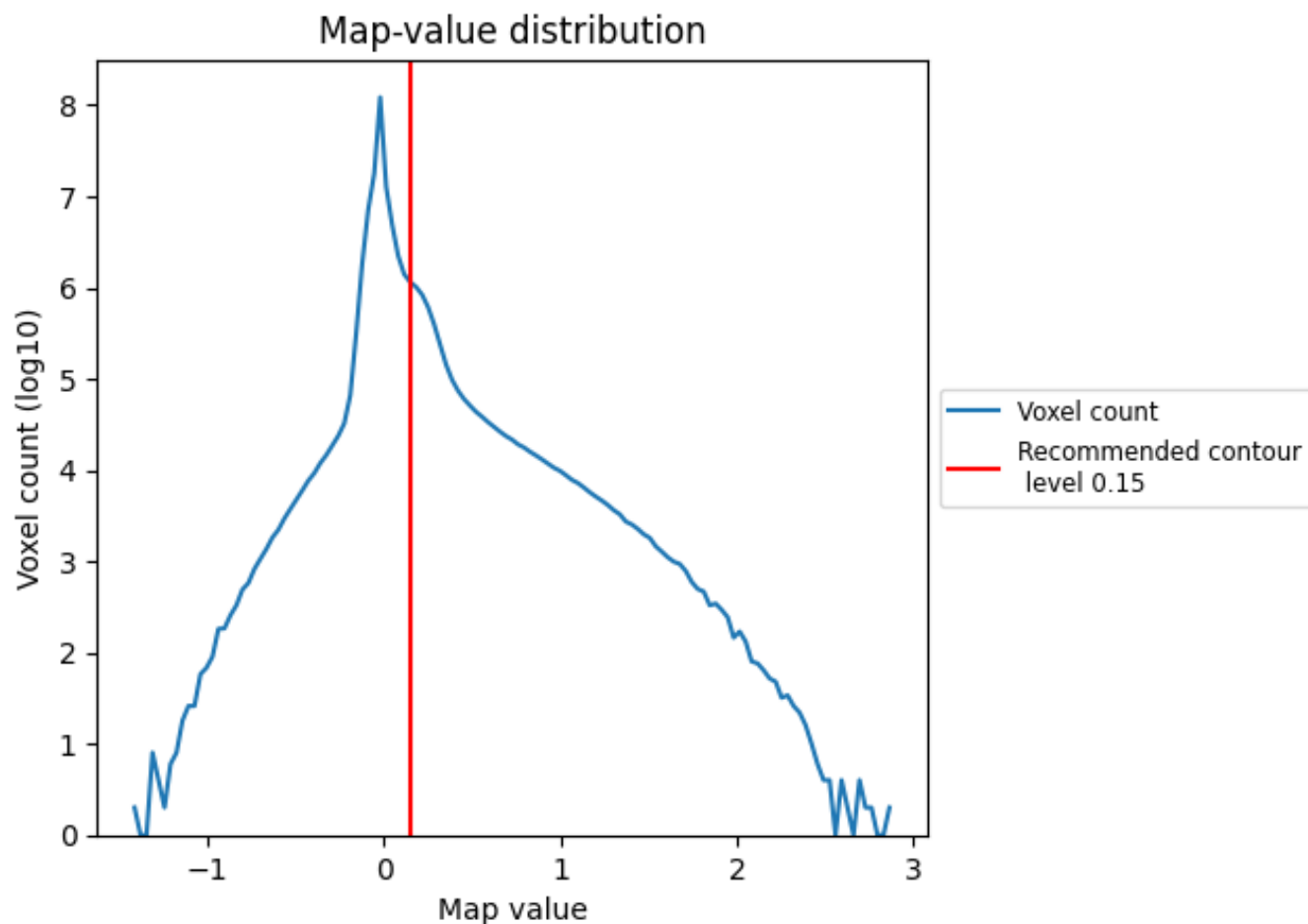
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

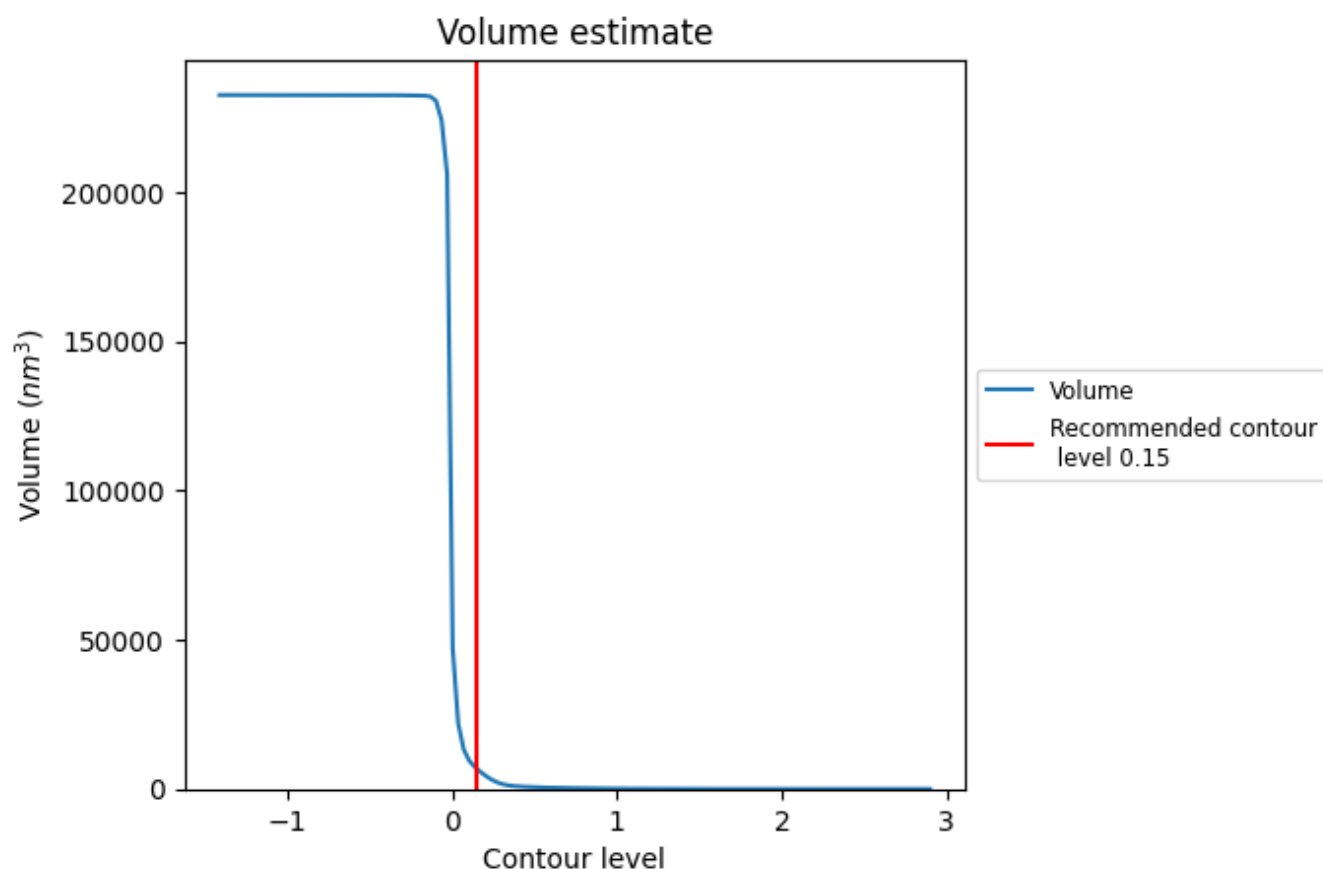
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

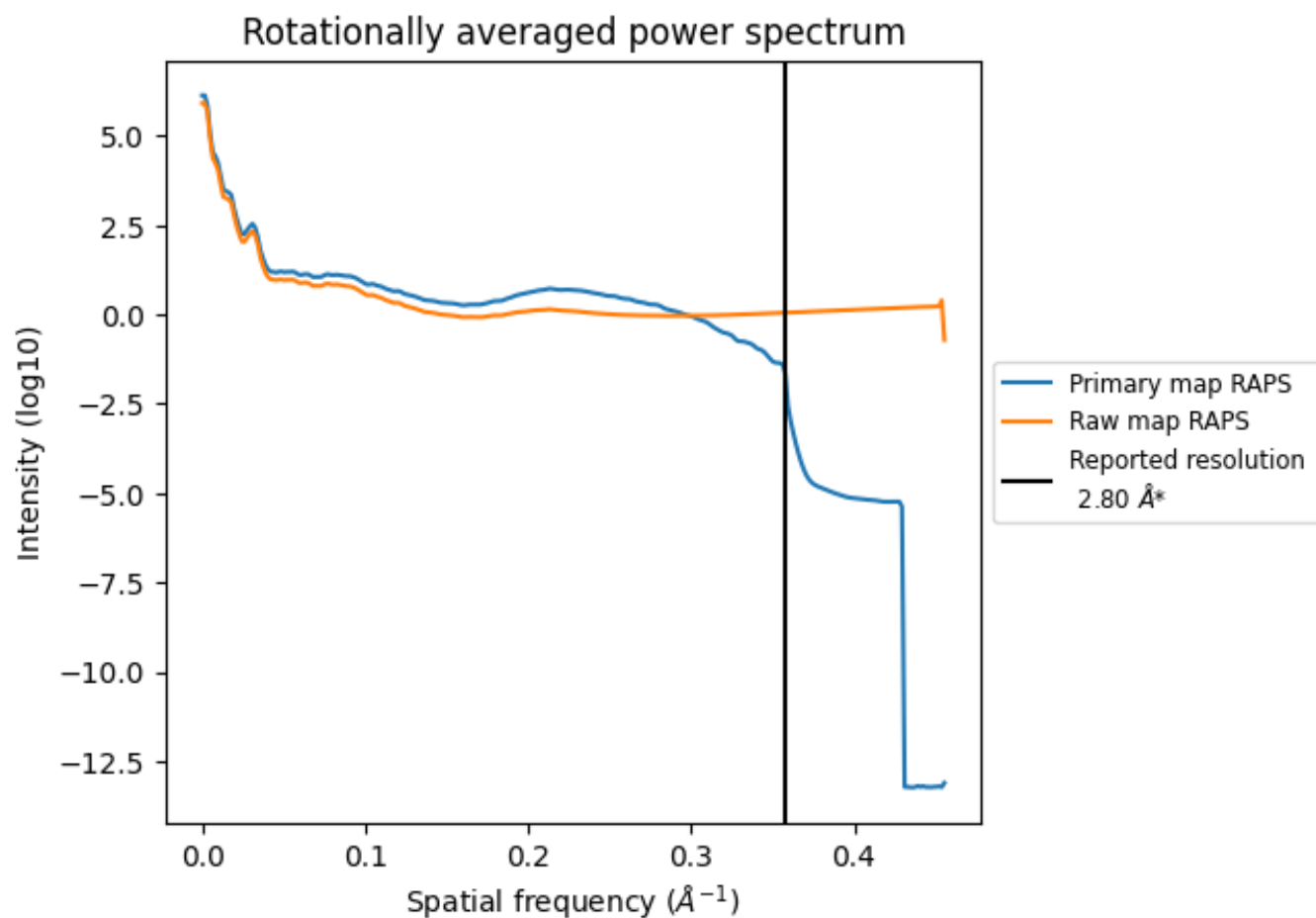
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 6773 nm³; this corresponds to an approximate mass of 6118 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 ⓘ

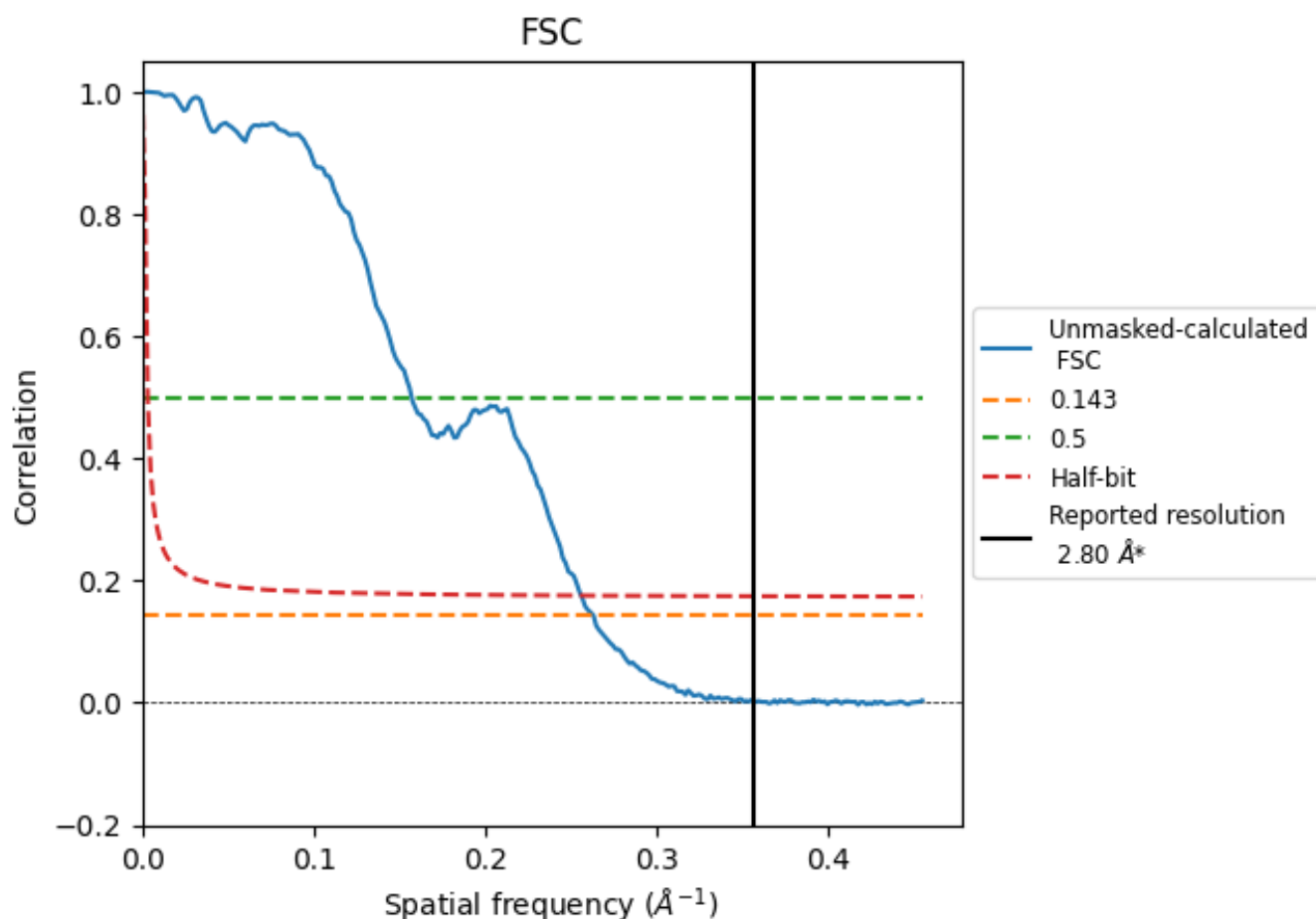


*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

8.2 Resolution estimates [i](#)

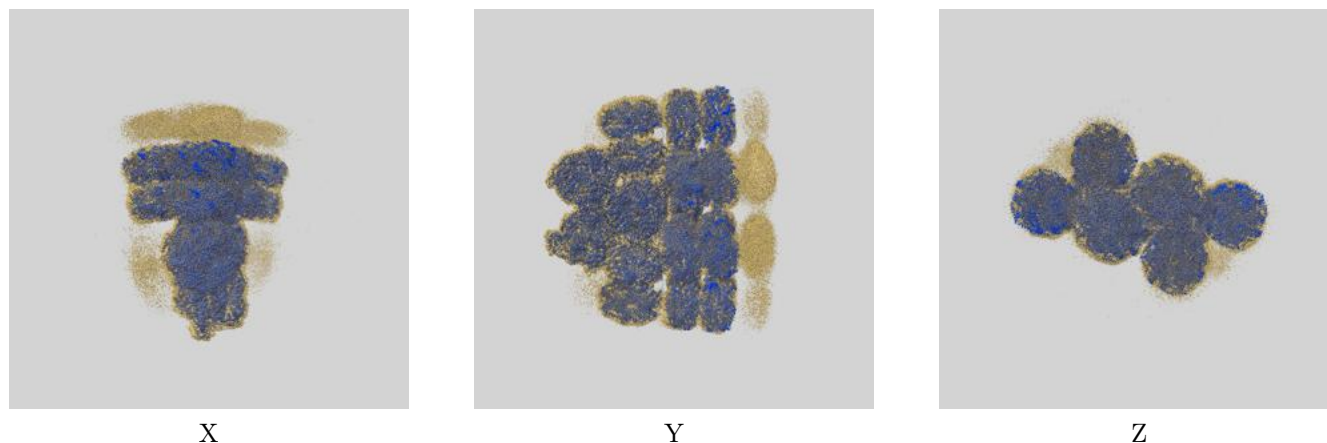
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.80	6.36	3.90

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.80 differs from the reported value 2.8 by more than 10 %

9 Map-model fit [i](#)

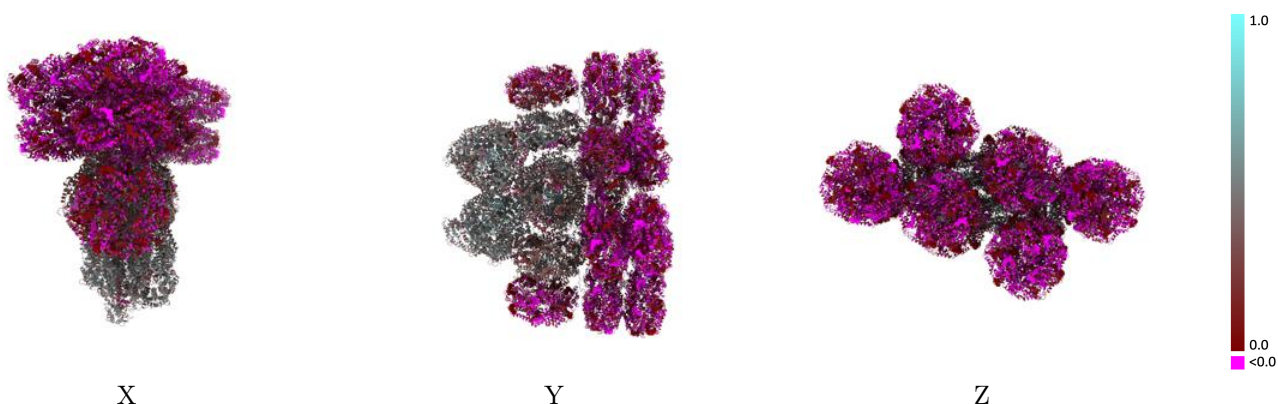
This section contains information regarding the fit between EMDB map EMD-62201 and PDB model 9K9W. Per-residue inclusion information can be found in section [3](#) on page [64](#).

9.1 Map-model overlay [i](#)



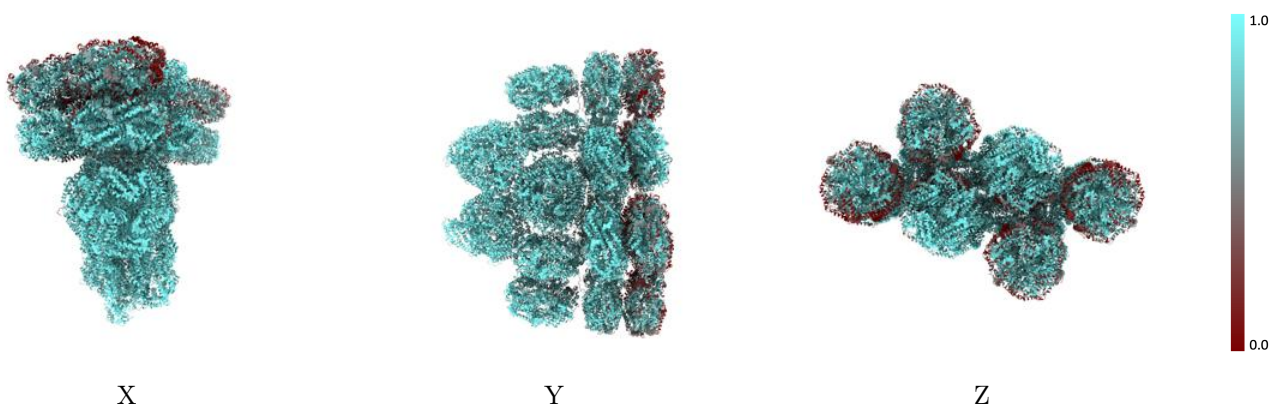
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



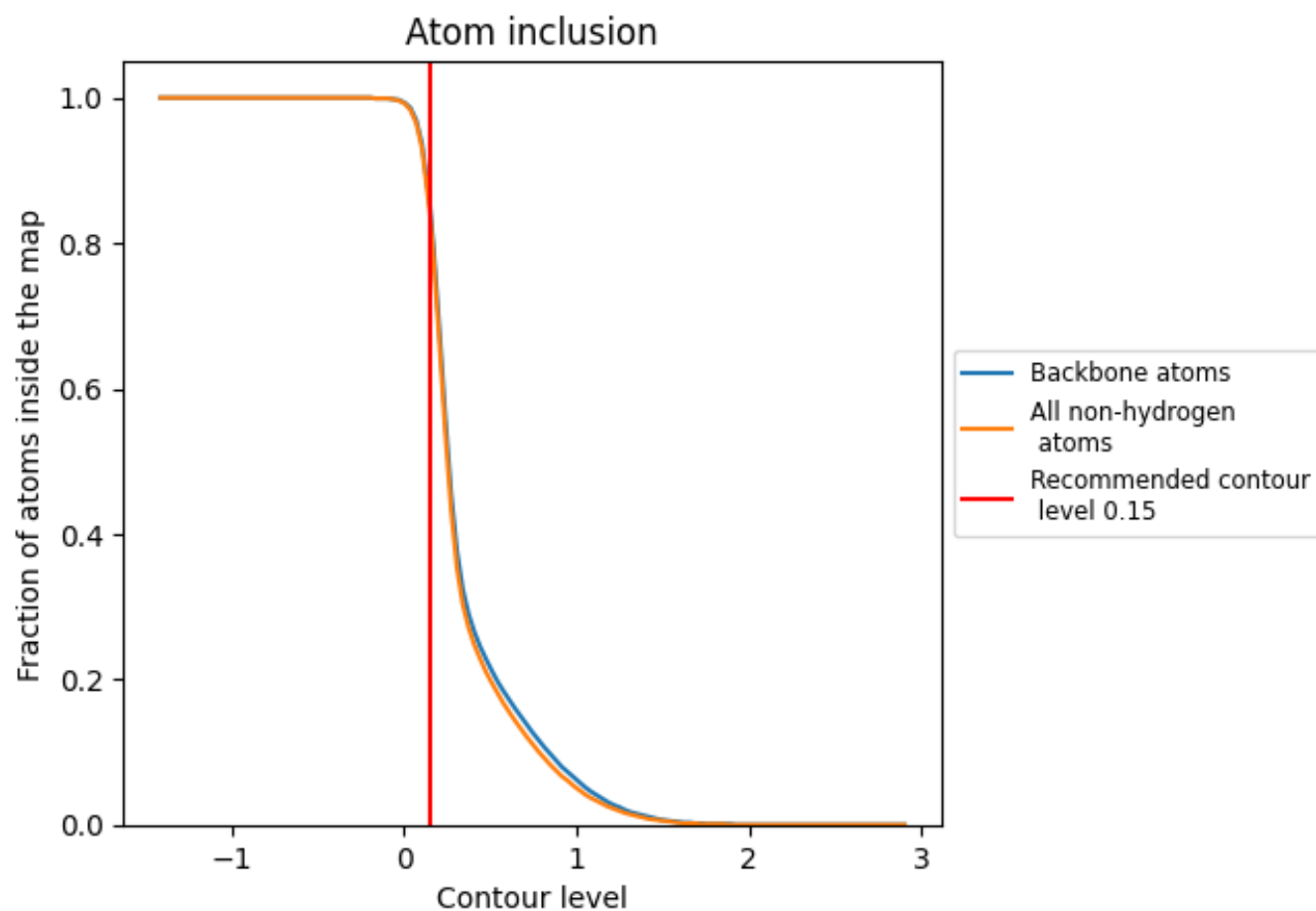
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.15).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 84% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8410	 0.1660
A	 0.9470	 0.4470
A1	 0.9680	 0.0200
A2	 0.9530	 0.0760
A3	 0.9680	 0.0180
A4	 0.9620	 0.0050
A5	 0.8880	 0.4010
A6	 0.9360	 0.0450
A7	 0.9070	 0.4410
A8	 0.9590	 0.0050
A9	 0.9710	 0.1020
AA	 0.9710	 0.1010
B1	 0.9110	 0.0460
B2	 0.9180	 0.0420
B3	 0.9100	 0.0450
B4	 0.8740	 0.0160
B5	 0.9300	 0.4250
B6	 0.9170	 0.0210
B7	 0.9140	 0.4480
B8	 0.8760	 0.0190
B9	 0.9190	 0.0640
BA	 0.9200	 0.0650
C1	 0.9070	 0.0260
C2	 0.9200	 0.0530
C3	 0.9060	 0.0270
C4	 0.8570	 0.0230
C5	 0.9150	 0.3900
C6	 0.9070	 0.0180
C7	 0.9290	 0.4230
C8	 0.8590	 0.0230
C9	 0.9440	 0.1850
CA	 0.9430	 0.1800
D1	 0.8770	 0.0390
D2	 0.9520	 0.0480
D3	 0.8740	 0.0390



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Chain	Atom inclusion	Q-score
D4	 0.8880	 0.0350
D5	 0.9400	 0.4380
D6	 0.9460	 0.0220
D7	 0.9270	 0.4710
D8	 0.8880	 0.0350
D9	 0.8880	 0.0870
DA	 0.8880	 0.0850
E1	 0.8780	 0.0440
E2	 0.8970	 0.0370
E3	 0.8770	 0.0470
E4	 0.8810	 0.0090
E5	 0.9490	 0.4440
E6	 0.8970	 -0.0060
E7	 0.9140	 0.4560
E8	 0.8810	 0.0120
E9	 0.8690	 0.0360
EA	 0.8690	 0.0270
F1	 0.8240	 0.0690
F2	 0.9320	 0.0730
F3	 0.8230	 0.0690
F4	 0.8870	 0.0200
F5	 0.9560	 0.4680
F6	 0.9450	 0.0640
F7	 0.9210	 0.4680
F8	 0.8850	 0.0200
F9	 0.9370	 0.1660
FA	 0.9350	 0.1630
G1	 0.9550	 0.0100
G2	 0.9540	 0.1620
G3	 0.9540	 0.0090
G4	 0.9650	 0.0600
G5	 0.8900	 0.3950
G6	 0.9410	 0.1340
G7	 0.9180	 0.4560
G8	 0.9650	 0.0560
G9	 0.9660	 0.0900
GA	 0.9670	 0.0890
H1	 0.9190	 0.0510
H2	 0.8170	 0.1580
H3	 0.9190	 0.0480
H4	 0.8680	 0.0340
H5	 0.9390	 0.4420

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Chain	Atom inclusion	Q-score
H6	 0.7890	 0.1510
H7	 0.9210	 0.4490
H8	 0.8710	 0.0340
H9	 0.9440	 0.1020
HA	 0.9440	 0.0970
I1	 0.8110	 0.0770
I2	 0.8180	 0.0700
I3	 0.8110	 0.0810
I4	 0.9300	 0.0210
I5	 0.9240	 0.4120
I6	 0.8090	 0.0620
I7	 0.9310	 0.4410
I8	 0.9310	 0.0240
I9	 0.9030	 0.1620
IA	 0.9000	 0.1510
J1	 0.8200	 0.0600
J2	 0.7860	 0.0510
J3	 0.8240	 0.0640
J4	 0.9200	 0.0180
J5	 0.9480	 0.4520
J6	 0.7540	 0.0390
J7	 0.9230	 0.4760
J8	 0.9220	 0.0190
J9	 0.7570	 0.0370
JA	 0.7580	 0.0260
K1	 0.9570	 0.0210
K2	 0.9160	 0.0640
K3	 0.9570	 0.0210
K4	 0.7970	 -0.0040
K5	 0.9510	 0.4480
K6	 0.8890	 0.0350
K7	 0.9200	 0.4690
K8	 0.7980	 -0.0030
K9	 0.8880	 0.0330
KA	 0.8860	 0.0320
L1	 0.9210	 0.0140
L2	 0.8740	 0.1670
L3	 0.9230	 0.0150
L4	 0.8280	 0.0190
L5	 0.9620	 0.4790
L6	 0.8280	 0.0950
L7	 0.9360	 0.4950

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Chain	Atom inclusion	Q-score
L8	 0.8210	 0.0170
L9	 0.9710	 0.0630
LA	 0.9710	 0.0640
M1	 0.8250	 0.0150
M2	 0.9060	 0.1810
M3	 0.8250	 0.0150
M4	 0.9250	 0.0060
M5	 0.8880	 0.3860
M6	 0.8900	 0.1380
M7	 0.9160	 0.4090
M8	 0.9220	 0.0070
M9	 0.8990	 0.0260
MA	 0.8970	 0.0250
N1	 0.8500	 0.0180
N2	 0.9640	 0.0580
N3	 0.8520	 0.0200
N4	 0.6060	 0.0320
N5	 0.9160	 0.4630
N6	 0.9390	 0.0140
N7	 0.9090	 0.4070
N8	 0.6050	 0.0360
N9	 0.9770	 -0.0350
NA	 0.9790	 -0.0330
O1	 0.7780	 -0.0010
O3	 0.7770	 -0.0040
O4	 0.6630	 0.0210
O5	 0.9230	 0.4090
O7	 0.8320	 0.3020
O8	 0.6660	 0.0190
O9	 0.9720	 0.0070
OA	 0.9730	 0.0100
P1	 0.6150	 0.0000
P3	 0.6130	 0.0020
P4	 0.6130	 0.0150
P5	 0.9370	 0.4400
P7	 0.9210	 0.3850
P8	 0.6150	 0.0170
P9	 0.9420	 0.0270
PA	 0.9380	 0.0260
Q1	 0.5190	 0.0250
Q3	 0.5230	 0.0260
Q4	 0.5520	 0.0070

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Chain	Atom inclusion	Q-score
Q5	 0.9170	 0.3890
Q7	 0.8470	 0.2750
Q8	 0.5340	 0.0200
Q9	 0.7250	 0.0060
QA	 0.7680	 0.0190
R1	 0.6870	 0.0350
R3	 0.6900	 0.0360
R4	 0.4480	 -0.0020
R5	 0.9230	 0.4280
R7	 0.8980	 0.3190
R8	 0.4500	 -0.0030
R9	 0.8570	 0.0320
RA	 0.8570	 0.0330
S1	 0.6770	 0.0090
S3	 0.6790	 0.0090
S4	 0.4190	 0.0200
S5	 0.8940	 0.4090
S7	 0.8710	 0.3170
S8	 0.4070	 0.0150
S9	 0.8810	 0.0320
SA	 0.8810	 0.0310
T1	 0.6030	 -0.0180
T3	 0.6070	 -0.0230
T4	 0.7530	 0.0090
T5	 0.9350	 0.5020
T7	 0.8800	 0.3090
T8	 0.7560	 0.0060
T9	 0.8300	 0.0220
TA	 0.8310	 0.0190
U1	 0.4790	 0.0270
U3	 0.4730	 0.0210
U4	 0.7550	 0.0020
U5	 0.9420	 0.4640
U7	 0.8160	 0.2730
U8	 0.7520	 0.0020
U9	 0.8550	 0.0250
UA	 0.8560	 0.0280
V1	 0.3550	 0.0020
V3	 0.3550	 0.0030
V4	 0.4840	 0.0010
V5	 0.9540	 0.4770
V7	 0.9130	 0.3600

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Chain	Atom inclusion	Q-score
V8	 0.4810	 0.0030
V9	 0.2500	 0.0030
VA	 0.2510	 0.0040
W1	 0.5900	 0.0200
W3	 0.5980	 0.0210
W4	 0.4270	 -0.0000
W5	 0.9240	 0.4160
W7	 0.8470	 0.2670
W8	 0.4280	 -0.0020
W9	 0.3970	 0.0280
WA	 0.3950	 0.0270
X1	 0.7710	 0.0070
X3	 0.7700	 0.0050
X4	 0.5080	 0.0090
X5	 0.9310	 0.4440
X7	 0.8850	 0.2980
X8	 0.5080	 0.0050
X9	 0.5140	 0.0210
XA	 0.5110	 0.0180
Y1	 0.7920	 0.0060
Y3	 0.7910	 0.0010
Y4	 0.4670	 -0.0060
Y5	 0.9370	 0.4230
Y7	 0.9380	 0.3320
Y8	 0.4750	 -0.0060
Y9	 0.9060	 0.0350
YA	 0.9050	 0.0340
Z	 0.9530	 0.4620
Z1	 0.5710	 -0.0020
Z3	 0.5700	 -0.0040
Z4	 0.9320	 0.0790
Z5	 0.9320	 0.4750
Z7	 0.9270	 0.3800
Z8	 0.9220	 0.0570
Z9	 0.8430	 0.0200
ZA	 0.8450	 0.0200
a5	 0.9420	 0.4730
a7	 0.9200	 0.3710
a9	 0.9110	 0.1690
aA	 0.9100	 0.1710
b5	 0.8930	 0.3450
b7	 0.9550	 0.4480

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Chain	Atom inclusion	Q-score
c5	 0.9370	 0.4260
c7	 0.9330	 0.3650
d5	 0.9340	 0.4700
d7	 0.9640	 0.3620
e5	 0.9400	 0.4680
e7	 0.9310	 0.3250
f5	 0.9080	 0.3800
f7	 0.9320	 0.3790
g7	 0.9180	 0.3670
h7	 0.9580	 0.4450
i5	 0.9710	 0.5210
i7	 0.8840	 0.2520
j5	 0.9730	 0.5350
j7	 0.9600	 0.3550
k5	 0.9720	 0.5330
k7	 0.8890	 0.3350
l7	 0.9090	 0.3360
m7	 0.9450	 0.2980
n7	 0.8880	 0.3070
o7	 0.9420	 0.4350
p7	 0.8300	 0.2650
q7	 0.8360	 0.2340
r7	 0.9070	 0.3460
s7	 0.9450	 0.2960
t7	 0.8720	 0.2670
u7	 0.9530	 0.4790
v7	 0.7890	 0.1970
w7	 0.9830	 0.5160
x7	 0.9810	 0.5000
y7	 0.9810	 0.5050
z5	 0.9680	 0.5260
z7	 0.9870	 0.5470