



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 10:35 AM UTC

PDB ID : 9M3J / pdb_00009m3j
EMDB ID : EMD-63604
Title : structure of bundle-shaped PBS with both long rod and (ApcA2B3ApcD) trimer
Authors : Ma, J.; Sui, S.-F.
Deposited on : 2025-03-02
Resolution : 3.37 Å(reported)
Based on initial model : .

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

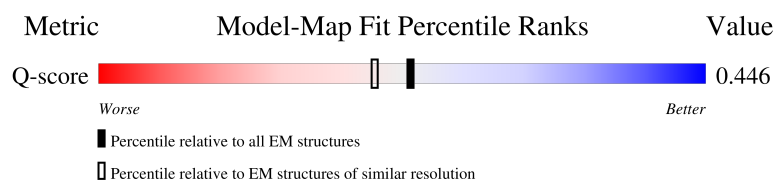
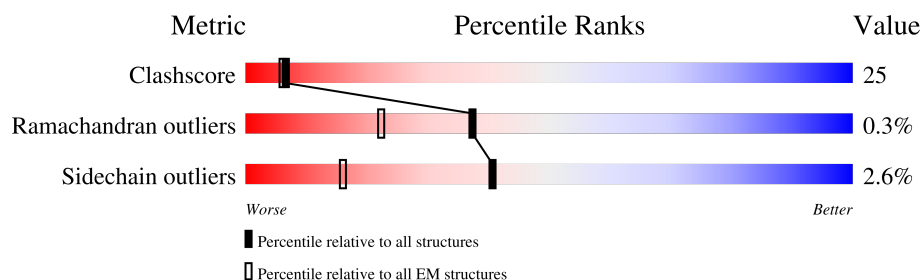
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.37 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	14287 (2.87 - 3.87)

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

Mol	Chain	Length	Quality of chain
1	A1	161	50% 48% ..
1	A2	161	60% 39% ..
1	A3	161	55% 42% ..
1	C1	161	45% 50% ..

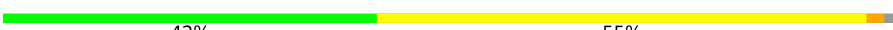
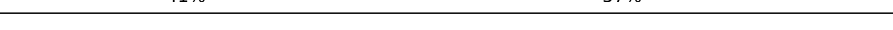
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Mol	Chain	Length	Quality of chain
1	C2	161	 60% 38% ..
1	C3	161	 53% 44% ..
1	E1	161	 63% 36% .
1	E2	161	 71% 28% ..
1	E3	161	 56% 41% ..
1	G2	161	 62% 37% ..
1	G3	161	 58% 41% ..
1	H1	161	 42% 56% ..
1	I2	161	 62% 35% ..
1	I3	161	 57% 40% ..
1	K2	161	 67% 30% ...
1	K3	161	 47% 50% ..
1	M2	161	 57% 41% ..
1	M3	161	 62% 37% .
1	O2	161	 55% 43% ..
1	O3	161	 64% 35% ..
1	Q2	161	 54% 42% ..
1	Q3	161	 62% 37% .
1	S2	161	 52% 47% ..
1	S3	161	 62% 36% ..
1	U2	161	 52% 47% ..
1	U3	161	 61% 36% ..
1	W2	161	 53% 43% ..
1	W3	161	 61% 35% ..
1	Y2	161	 53% 46% .

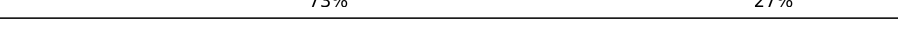
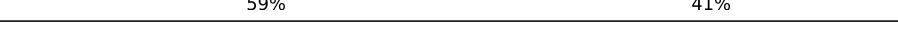
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Mol	Chain	Length	Quality of chain
1	Y3	161	 54% 45% .
1	a2	161	 50% 47% ..
1	a3	161	 60% 35% . .
1	c2	161	 42% 55% ..
1	c3	161	 57% 42% ..
1	e2	161	 54% 43% ..
1	e3	161	 61% 34% 5% .
1	g2	161	 48% 50% ..
1	i2	161	 50% 47% ..
1	k2	161	 52% 47% ..
1	m2	161	 42% 56% ..
1	o2	161	 51% 47% ..
1	q2	161	 55% 42% ..
1	s2	161	 41% 57% ..
1	u2	161	 56% 43% ..
2	B1	161	 49% 48% .
2	B2	161	 71% 28% .
2	B3	161	 65% 35%
2	D1	161	 5% 48% 51% .
2	D2	161	 69% 30% .
2	D3	161	 58% 40% .
2	F1	161	 49% 50% .
2	F2	161	 63% 37% .
2	F3	161	 56% 43% .
2	G1	161	 45% 53% .

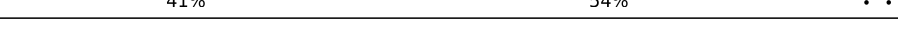
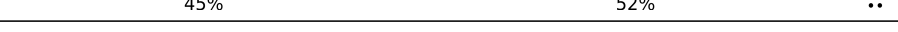
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Mol	Chain	Length	Quality of chain
2	H2	161	 63% 37%
2	H3	161	 66% 32% .
2	I1	161	 52% 48% .
2	J1	161	 49% 50% .
2	J2	161	 76% 24%
2	J3	161	 57% 41% .
2	L2	161	 68% 31% .
2	L3	161	 62% 37% .
2	N2	161	 60% 40%
2	N3	161	 71% 29% .
2	P2	161	 59% 40% .
2	P3	161	 66% 33% .
2	R2	161	 60% 40% .
2	R3	161	 71% 29%
2	T2	161	 50% 49% .
2	T3	161	 73% 27%
2	V2	161	 59% 41%
2	V3	161	 63% 36% .
2	X2	161	 61% 37% .
2	X3	161	 70% 30%
2	Z2	161	 63% 37% .
2	Z3	161	 70% 30% .
2	b2	161	 64% 36%
2	b3	161	 54% 45% .
2	d2	161	 57% 42% .

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Mol	Chain	Length	Quality of chain
2	d3	161	 68% 30% .
2	f2	161	 60% 39% .
2	f3	161	 56% 43% .
2	g3	161	 50% 45% 6% .
2	h2	161	 63% 37% .
2	h3	161	 52% 42% 6% .
2	j2	161	 60% 39% .
2	l2	161	 55% 42% .
2	n2	161	 53% 45% .
2	p2	161	 54% 46% .
2	r2	161	 53% 45% .
2	t2	161	 59% 40% .
2	v2	161	 49% 50% .
3	K1	161	 43% 53% ..
3	L1	161	 49% 45% 5% .
4	M1	69	 41% 54% ..
4	i3	69	 45% 52% ..
4	w2	69	 58% 29% 12% .
4	x2	69	 51% 45% ..
4	y2	69	 55% 42% ..
4	z1	69	 48% 46% ..
4	z2	69	 61% 35% ..
4	z3	69	 51% 45% ..
5	j3	1155	 53% 40% . .
5	k3	1155	 53% 40% . .

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 140502 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 alpha subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A1	160	Total	C	N	O	S	0	0
			1222	771	209	237	5		
1	C1	160	Total	C	N	O	S	0	0
			1222	771	209	237	5		
1	E1	160	Total	C	N	O	S	0	0
			1222	771	209	237	5		
1	H1	160	Total	C	N	O	S	0	0
			1222	771	209	237	5		
1	A2	160	Total	C	N	O	S	0	0
			1222	771	209	237	5		
1	C2	160	Total	C	N	O	S	0	0
			1222	771	209	237	5		
1	E2	160	Total	C	N	O	S	0	0
			1222	771	209	237	5		
1	G2	160	Total	C	N	O	S	0	0
			1222	771	209	237	5		
1	I2	160	Total	C	N	O	S	0	0
			1222	771	209	237	5		
1	K2	160	Total	C	N	O	S	0	0
			1222	771	209	237	5		
1	M2	160	Total	C	N	O	S	0	0
			1222	771	209	237	5		
1	O2	160	Total	C	N	O	S	0	0
			1222	771	209	237	5		
1	Q2	160	Total	C	N	O	S	0	0
			1222	771	209	237	5		
1	S2	160	Total	C	N	O	S	0	0
			1222	771	209	237	5		
1	U2	160	Total	C	N	O	S	0	0
			1222	771	209	237	5		
1	W2	160	Total	C	N	O	S	0	0
			1222	771	209	237	5		
1	Y2	160	Total	C	N	O	S	0	0
			1222	771	209	237	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	a2	160	Total	C	N	O	S	0	0
			1222	771	209	237	5		
1	c2	160	Total	C	N	O	S	0	0
			1222	771	209	237	5		
1	e2	160	Total	C	N	O	S	0	0
			1222	771	209	237	5		
1	g2	160	Total	C	N	O	S	0	0
			1222	771	209	237	5		
1	i2	160	Total	C	N	O	S	0	0
			1222	771	209	237	5		
1	k2	160	Total	C	N	O	S	0	0
			1222	771	209	237	5		
1	m2	160	Total	C	N	O	S	0	0
			1222	771	209	237	5		
1	o2	160	Total	C	N	O	S	0	0
			1222	771	209	237	5		
1	q2	160	Total	C	N	O	S	0	0
			1222	771	209	237	5		
1	s2	160	Total	C	N	O	S	0	0
			1222	771	209	237	5		
1	u2	160	Total	C	N	O	S	0	0
			1222	771	209	237	5		
1	A3	160	Total	C	N	O	S	0	0
			1222	771	209	237	5		
1	C3	160	Total	C	N	O	S	0	0
			1222	771	209	237	5		
1	E3	160	Total	C	N	O	S	0	0
			1222	771	209	237	5		
1	G3	160	Total	C	N	O	S	0	0
			1222	771	209	237	5		
1	I3	160	Total	C	N	O	S	0	0
			1222	771	209	237	5		
1	K3	160	Total	C	N	O	S	0	0
			1222	771	209	237	5		
1	M3	160	Total	C	N	O	S	0	0
			1222	771	209	237	5		
1	O3	160	Total	C	N	O	S	0	0
			1222	771	209	237	5		
1	Q3	160	Total	C	N	O	S	0	0
			1222	771	209	237	5		
1	S3	160	Total	C	N	O	S	0	0
			1222	771	209	237	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	U3	160	Total	C	N	O	S	0	0
			1222	771	209	237	5		
1	W3	160	Total	C	N	O	S	0	0
			1222	771	209	237	5		
1	Y3	160	Total	C	N	O	S	0	0
			1222	771	209	237	5		
1	a3	160	Total	C	N	O	S	0	0
			1222	771	209	237	5		
1	c3	160	Total	C	N	O	S	0	0
			1222	771	209	237	5		
1	e3	160	Total	C	N	O	S	0	0
			1222	771	209	237	5		

- Molecule 2 is a protein called Allophycocyanin beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B1	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
2	D1	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
2	F1	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
2	G1	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
2	I1	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
2	J1	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
2	B2	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
2	D2	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
2	F2	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
2	H2	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
2	J2	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
2	L2	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
2	N2	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	P2	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
2	R2	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
2	T2	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
2	V2	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
2	X2	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
2	Z2	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
2	b2	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
2	d2	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
2	f2	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
2	h2	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
2	j2	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
2	l2	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
2	n2	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
2	p2	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
2	r2	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
2	t2	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
2	v2	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
2	B3	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
2	D3	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
2	F3	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
2	H3	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	J3	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
2	L3	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
2	N3	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
2	P3	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
2	R3	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
2	T3	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
2	V3	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
2	X3	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
2	Z3	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
2	b3	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
2	d3	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
2	f3	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
2	g3	161	Total	C	N	O	S	0	0
			1209	767	202	234	6		
2	h3	161	Total	C	N	O	S	0	0
			1209	767	202	234	6		

- Molecule 3 is a protein called Allophycocyanin-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	K1	160	Total	C	N	O	S	0	0
			1255	796	215	237	7		
3	L1	160	Total	C	N	O	S	0	0
			1255	796	215	237	7		

- Molecule 4 is a protein called Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	z1	68	Total	C	N	O	S	0	0
			538	345	98	94	1		

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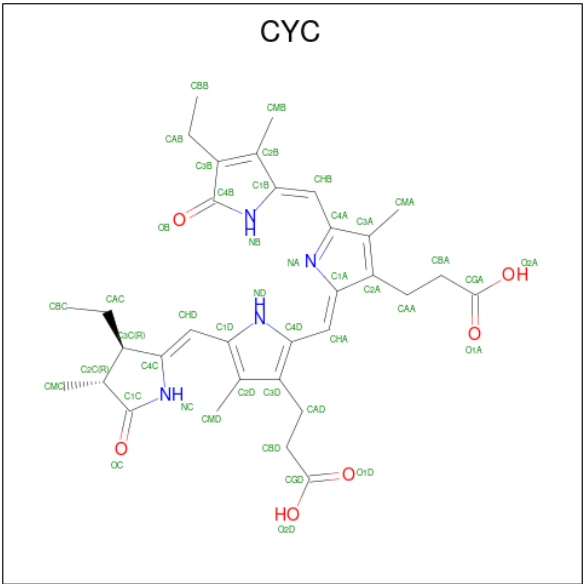
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Mol	Chain	Residues	Atoms					AltConf	Trace
4	M1	68	Total	C	N	O	S	0	0
			538	345	98	94	1		
4	z2	68	Total	C	N	O	S	0	0
			538	345	98	94	1		
4	w2	68	Total	C	N	O	S	0	0
			538	345	98	94	1		
4	x2	68	Total	C	N	O	S	0	0
			538	345	98	94	1		
4	y2	68	Total	C	N	O	S	0	0
			538	345	98	94	1		
4	z3	68	Total	C	N	O	S	0	0
			538	345	98	94	1		
4	i3	68	Total	C	N	O	S	0	0
			538	345	98	94	1		

- Molecule 5 is a protein called Phycobiliprotein ApcE.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	j3	1108	Total	C	N	O	S	0	0
			8819	5593	1559	1647	20		
5	k3	1108	Total	C	N	O	S	0	0
			8819	5593	1559	1647	20		

- Molecule 6 is PHYCOCYANOBILIN (CCD ID: CYC) (formula: C₃₃H₄₀N₄O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
6	A1	1	Total	C	N	O	0
			43	33	4	6	
6	C1	1	Total	C	N	O	0
			43	33	4	6	
6	F1	1	Total	C	N	O	0
			43	33	4	6	
6	E1	1	Total	C	N	O	0
			43	33	4	6	
6	H1	1	Total	C	N	O	0
			43	33	4	6	
6	J1	1	Total	C	N	O	0
			43	33	4	6	
6	K1	1	Total	C	N	O	0
			43	33	4	6	
6	L1	1	Total	C	N	O	0
			43	33	4	6	
6	z1	1	Total	C	N	O	0
			43	33	4	6	
6	M1	1	Total	C	N	O	0
			43	33	4	6	
6	A2	1	Total	C	N	O	0
			43	33	4	6	
6	B2	1	Total	C	N	O	0
			43	33	4	6	
6	C2	1	Total	C	N	O	0
			43	33	4	6	
6	E2	1	Total	C	N	O	0
			43	33	4	6	
6	F2	1	Total	C	N	O	0
			43	33	4	6	
6	G2	1	Total	C	N	O	0
			43	33	4	6	
6	H2	1	Total	C	N	O	0
			43	33	4	6	
6	I2	1	Total	C	N	O	0
			43	33	4	6	
6	K2	1	Total	C	N	O	0
			43	33	4	6	
6	L2	1	Total	C	N	O	0
			43	33	4	6	
6	M2	1	Total	C	N	O	0
			43	33	4	6	
6	N2	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
6	O2	1	Total	C	N	O	0
			43	33	4	6	
6	P2	1	Total	C	N	O	0
			43	33	4	6	
6	Q2	1	Total	C	N	O	0
			43	33	4	6	
6	R2	1	Total	C	N	O	0
			43	33	4	6	
6	S2	1	Total	C	N	O	0
			43	33	4	6	
6	T2	1	Total	C	N	O	0
			43	33	4	6	
6	U2	1	Total	C	N	O	0
			43	33	4	6	
6	V2	1	Total	C	N	O	0
			43	33	4	6	
6	W2	1	Total	C	N	O	0
			43	33	4	6	
6	X2	1	Total	C	N	O	0
			43	33	4	6	
6	Y2	1	Total	C	N	O	0
			43	33	4	6	
6	a2	1	Total	C	N	O	0
			43	33	4	6	
6	b2	1	Total	C	N	O	0
			43	33	4	6	
6	c2	1	Total	C	N	O	0
			43	33	4	6	
6	e2	1	Total	C	N	O	0
			43	33	4	6	
6	g2	1	Total	C	N	O	0
			43	33	4	6	
6	h2	1	Total	C	N	O	0
			43	33	4	6	
6	i2	1	Total	C	N	O	0
			43	33	4	6	
6	k2	1	Total	C	N	O	0
			43	33	4	6	
6	m2	1	Total	C	N	O	0
			43	33	4	6	
6	o2	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
6	p2	1	Total	C	N	O	0
			43	33	4	6	
6	q2	1	Total	C	N	O	0
			43	33	4	6	
6	s2	1	Total	C	N	O	0
			43	33	4	6	
6	u2	1	Total	C	N	O	0
			43	33	4	6	
6	v2	1	Total	C	N	O	0
			43	33	4	6	
6	x2	1	Total	C	N	O	0
			43	33	4	6	
6	y2	1	Total	C	N	O	0
			43	33	4	6	
6	A3	1	Total	C	N	O	0
			43	33	4	6	
6	C3	1	Total	C	N	O	0
			43	33	4	6	
6	D3	1	Total	C	N	O	0
			43	33	4	6	
6	E3	1	Total	C	N	O	0
			43	33	4	6	
6	F3	1	Total	C	N	O	0
			43	33	4	6	
6	G3	1	Total	C	N	O	0
			43	33	4	6	
6	H3	1	Total	C	N	O	0
			43	33	4	6	
6	I3	1	Total	C	N	O	0
			43	33	4	6	
6	J3	1	Total	C	N	O	0
			43	33	4	6	
6	K3	1	Total	C	N	O	0
			43	33	4	6	
6	L3	1	Total	C	N	O	0
			43	33	4	6	
6	M3	1	Total	C	N	O	0
			43	33	4	6	
6	N3	1	Total	C	N	O	0
			43	33	4	6	
6	O3	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
6	Q3	1	Total 43	C 33	N 4	O 6	0
6	R3	1	Total 43	C 33	N 4	O 6	0
6	S3	1	Total 43	C 33	N 4	O 6	0
6	T3	1	Total 43	C 33	N 4	O 6	0
6	U3	1	Total 43	C 33	N 4	O 6	0
6	V3	1	Total 43	C 33	N 4	O 6	0
6	W3	1	Total 43	C 33	N 4	O 6	0
6	X3	1	Total 43	C 33	N 4	O 6	0
6	Y3	1	Total 43	C 33	N 4	O 6	0
6	Z3	1	Total 43	C 33	N 4	O 6	0
6	a3	1	Total 43	C 33	N 4	O 6	0
6	b3	1	Total 43	C 33	N 4	O 6	0
6	c3	1	Total 43	C 33	N 4	O 6	0
6	d3	1	Total 43	C 33	N 4	O 6	0
6	e3	1	Total 43	C 33	N 4	O 6	0
6	f3	1	Total 43	C 33	N 4	O 6	0
6	g3	1	Total 43	C 33	N 4	O 6	0
6	z3	1	Total 43	C 33	N 4	O 6	0
6	j3	1	Total 43	C 33	N 4	O 6	0
6	j3	1	Total 43	C 33	N 4	O 6	0
6	j3	1	Total 43	C 33	N 4	O 6	0

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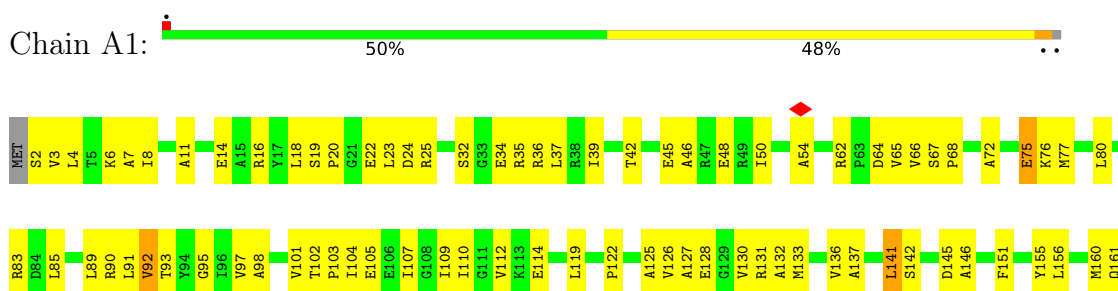
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Mol	Chain	Residues	Atoms					AltConf
6	j3	1	Total	C	N	O		0
			43	33	4	6		
6	j3	1	Total	C	N	O		0
			43	33	4	6		
6	j3	1	Total	C	H	N	O	0
			81	33	38	4	6	
6	k3	1	Total	C	N	O		0
			43	33	4	6		
6	k3	1	Total	C	N	O		0
			43	33	4	6		
6	k3	1	Total	C	N	O		0
			43	33	4	6		
6	k3	1	Total	C	N	O		0
			43	33	4	6		
6	k3	1	Total	C	N	O		0
			43	33	4	6		
6	k3	1	Total	C	H	N	O	0
			81	33	38	4	6	
6	h3	1	Total	C	N	O		0
			43	33	4	6		

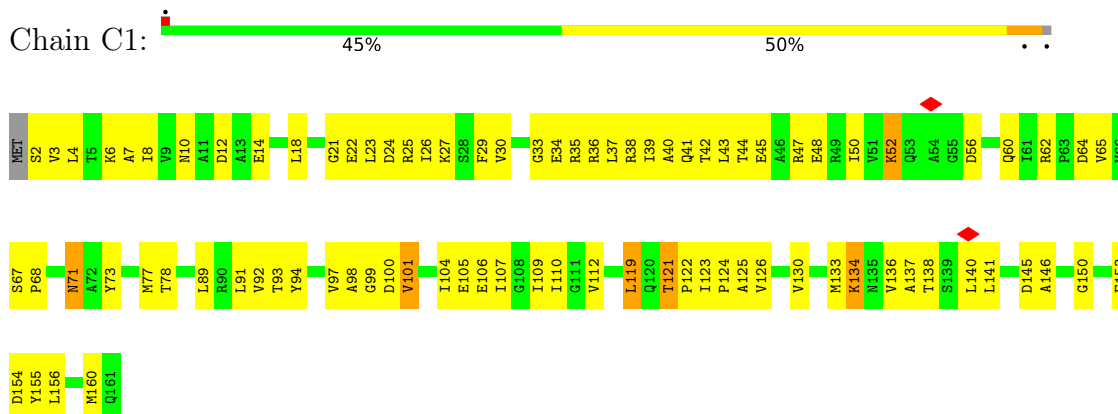
3 Residue-property plots [i](#)

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.

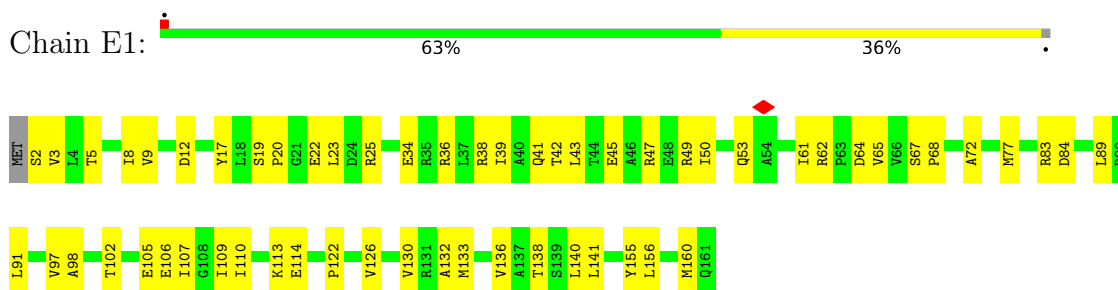
- Molecule 1: Allophycocyanin alpha subunit



- Molecule 1: Allophycocyanin alpha subunit



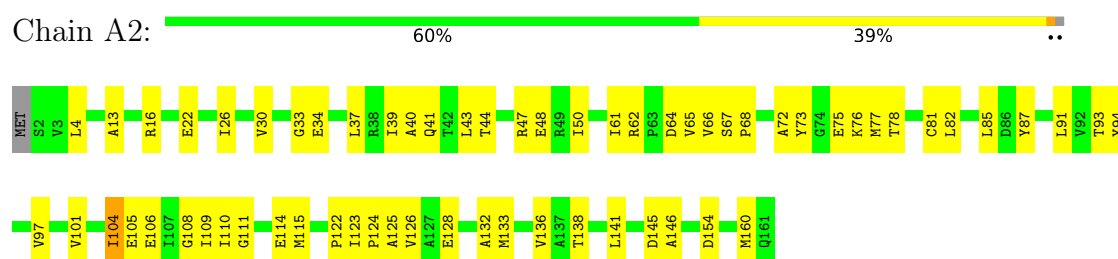
- Molecule 1: Allophycocyanin alpha subunit



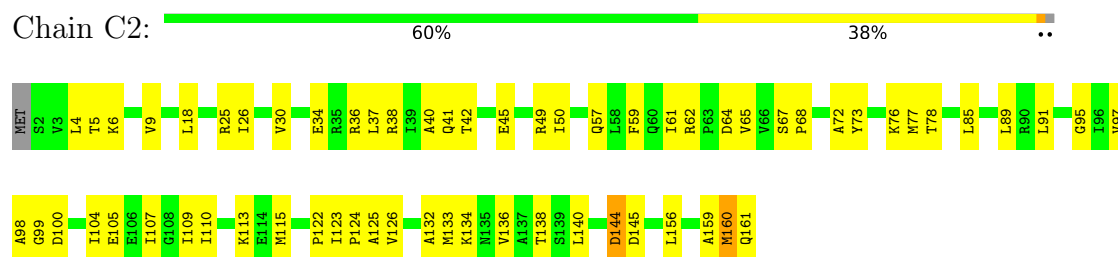
- Molecule 1: Allophycocyanin alpha subunit



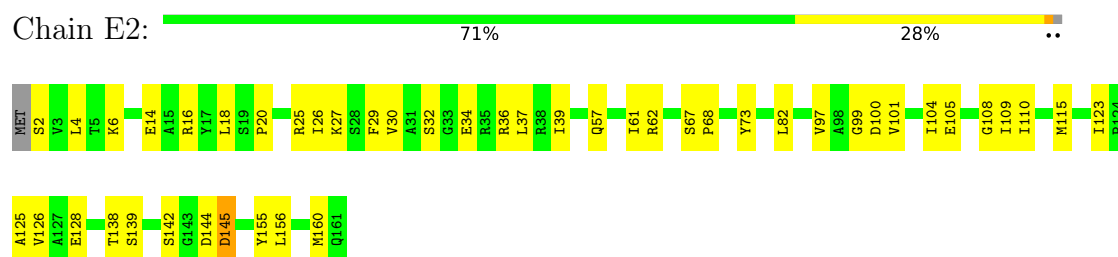
- Molecule 1: Allophycocyanin alpha subunit



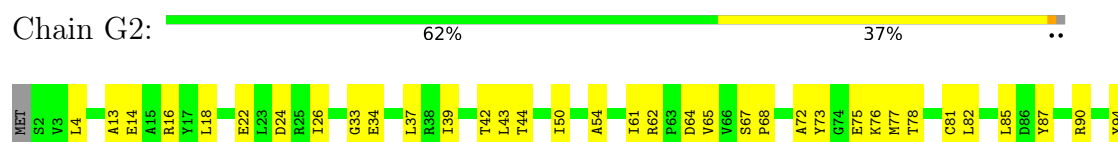
- Molecule 1: Allophycocyanin alpha subunit

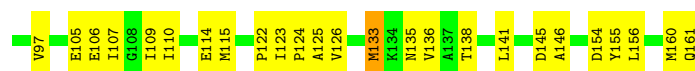


- Molecule 1: Allophycocyanin alpha subunit



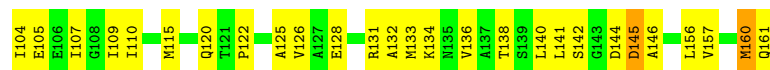
- Molecule 1: Allophycocyanin alpha subunit





- Molecule 1: Allophycocyanin alpha subunit

Chain I2: 62% 35% ..



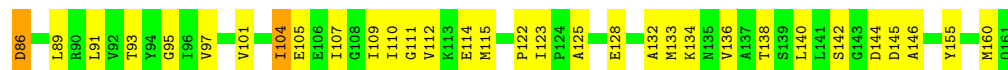
- Molecule 1: Allophycocyanin alpha subunit

Chain K2: 67% 30% ...



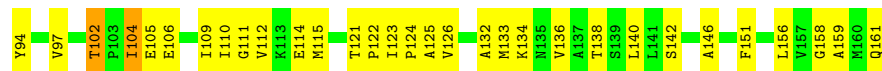
- Molecule 1: Allophycocyanin alpha subunit

Chain M2: 57% 41% ..



- Molecule 1: Allophycocyanin alpha subunit

Chain O2: 55% 43% ..



- Molecule 1: Allophycocyanin alpha subunit

Chain Q2: 54% 42% ..





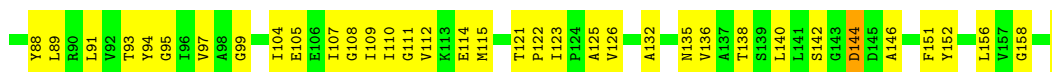
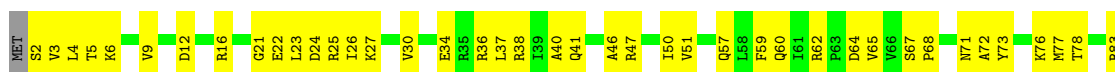
• Molecule 1: Allophycocyanin alpha subunit

Chain S2: 52% 47%



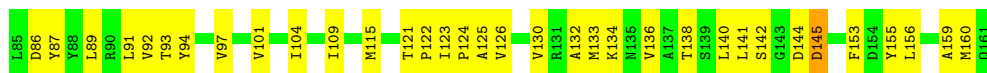
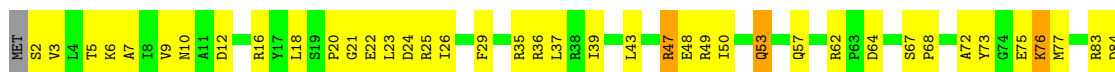
• Molecule 1: Allophycocyanin alpha subunit

Chain U2: 52% 47%



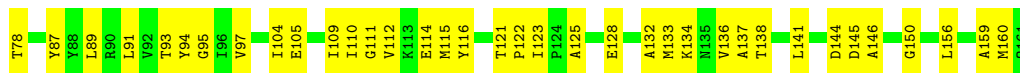
• Molecule 1: Allophycocyanin alpha subunit

Chain W2: 53% 43%



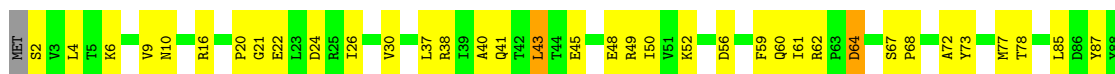
• Molecule 1: Allophycocyanin alpha subunit

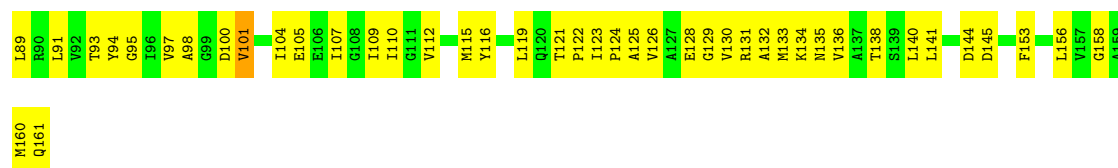
Chain Y2: 53% 46%



• Molecule 1: Allophycocyanin alpha subunit

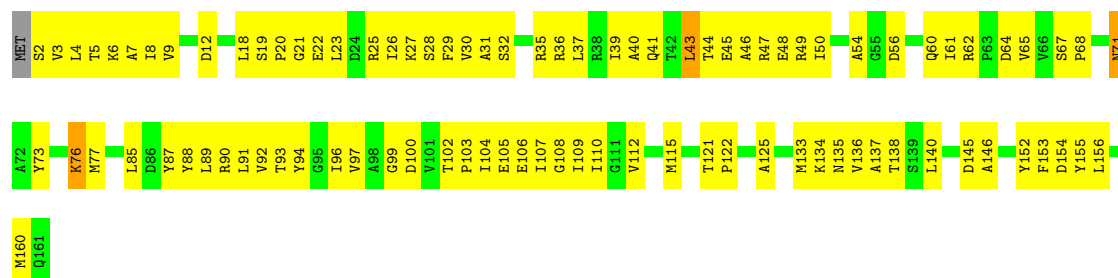
Chain a2: 50% 47%





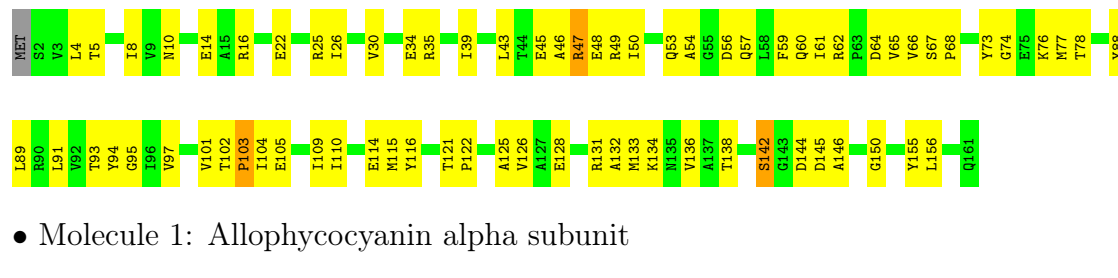
- Molecule 1: Allophycocyanin alpha subunit

Chain c2: 42% 55% ..



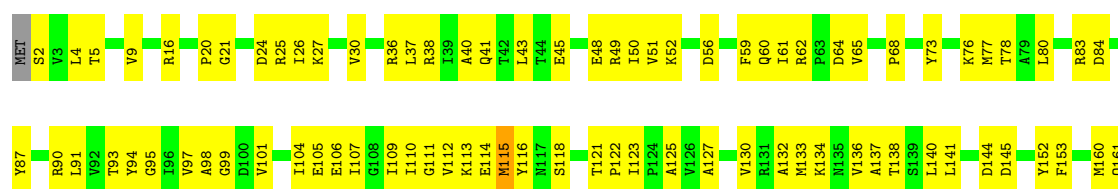
- Molecule 1: Allophycocyanin alpha subunit

Chain e2: 54% 43% ..



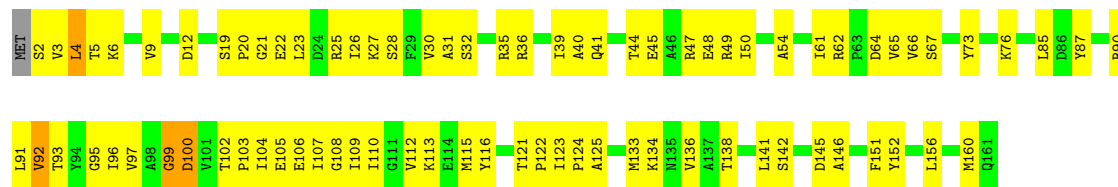
- Molecule 1: Allophycocyanin alpha subunit

Chain g2: 48% 50% ..

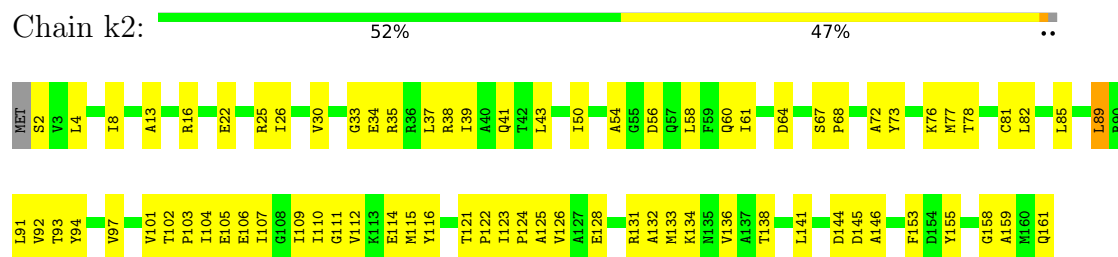


- Molecule 1: Allophycocyanin alpha subunit

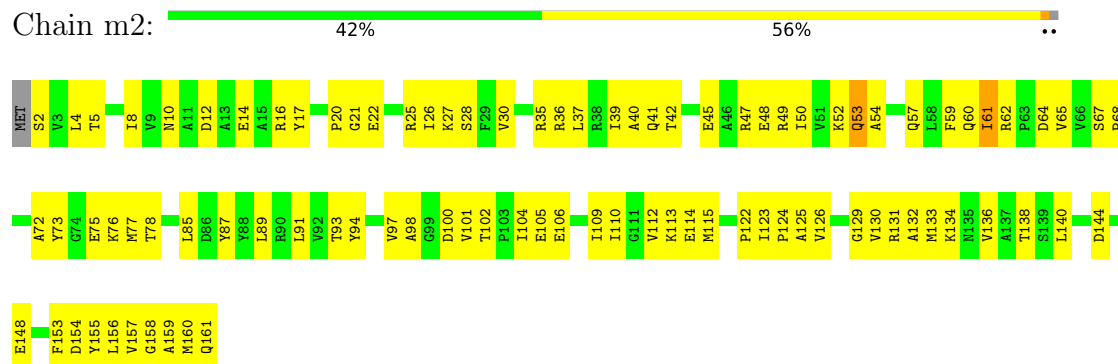
Chain i2: 50% 47% ..



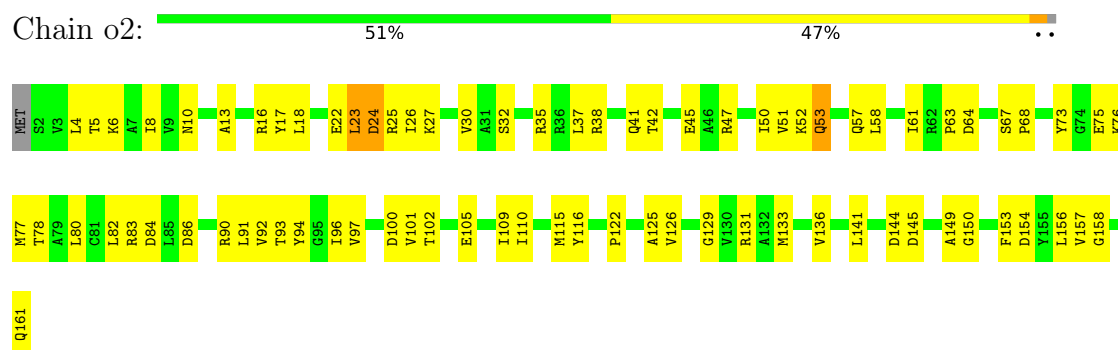
- Molecule 1: Allophycocyanin alpha subunit



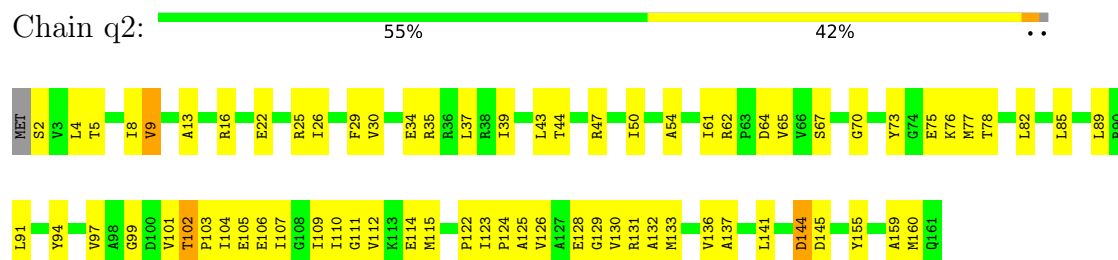
- Molecule 1: Allophycocyanin alpha subunit



- Molecule 1: Allophycocyanin alpha subunit

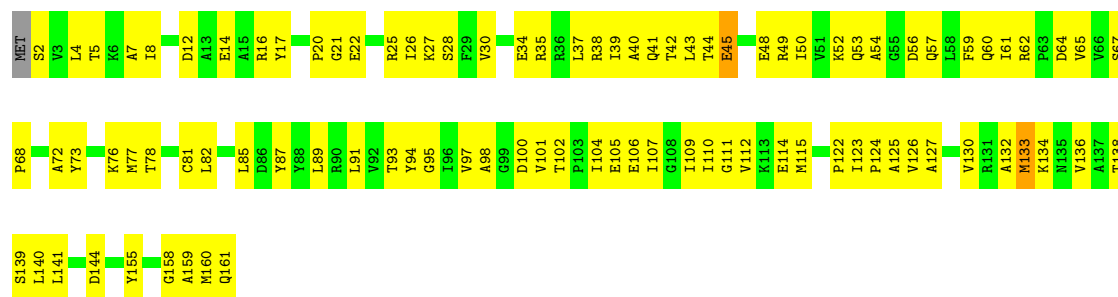


- Molecule 1: Allophycocyanin alpha subunit



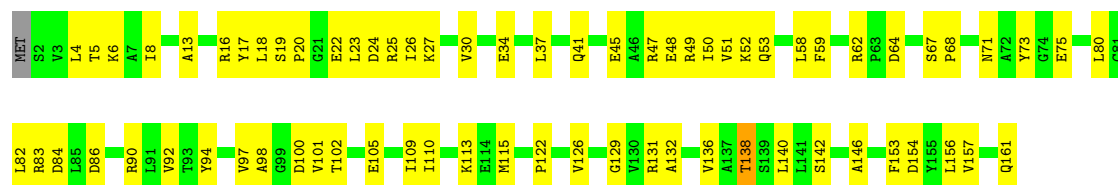
- Molecule 1: Allophycocyanin alpha subunit





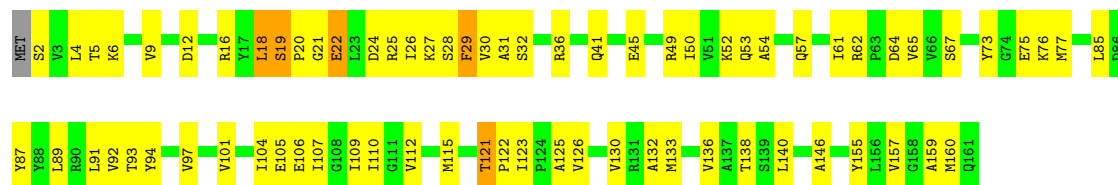
- Molecule 1: Allophycocyanin alpha subunit

Chain u2: ..



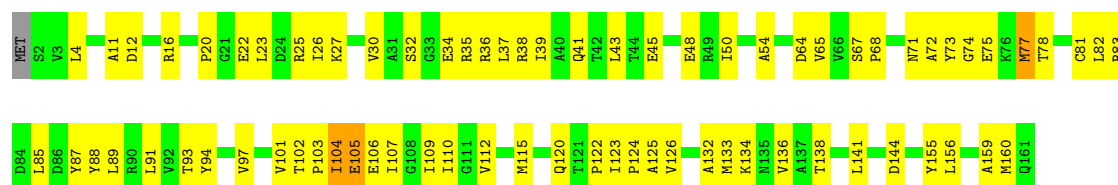
- Molecule 1: Allophycocyanin alpha subunit

Chain A3: ..



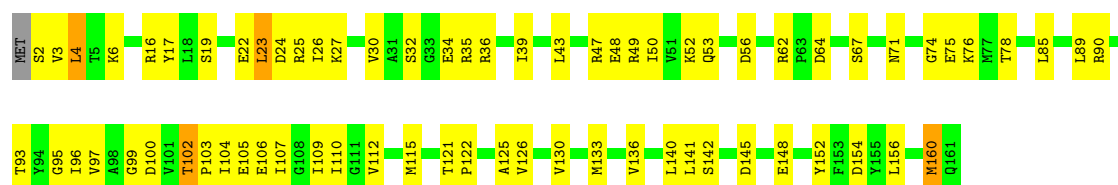
- Molecule 1: Allophycocyanin alpha subunit

Chain C3: ..

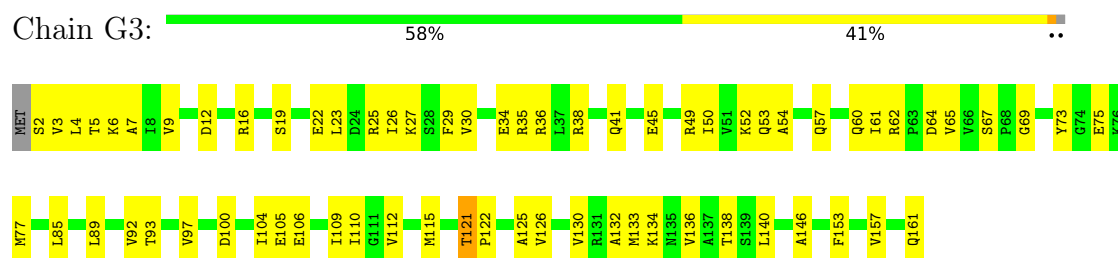


- Molecule 1: Allophycocyanin alpha subunit

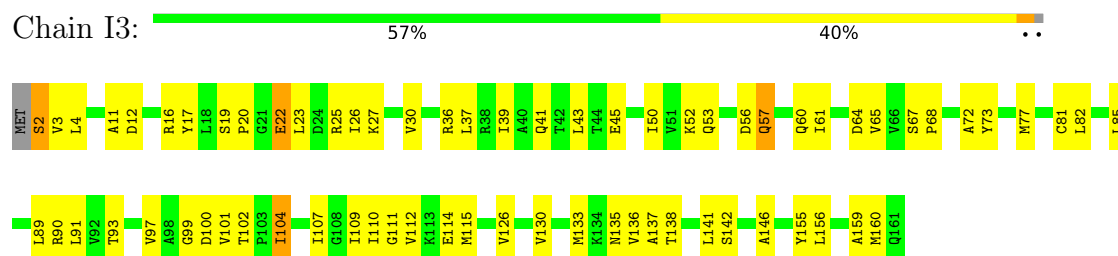
Chain E3: ..



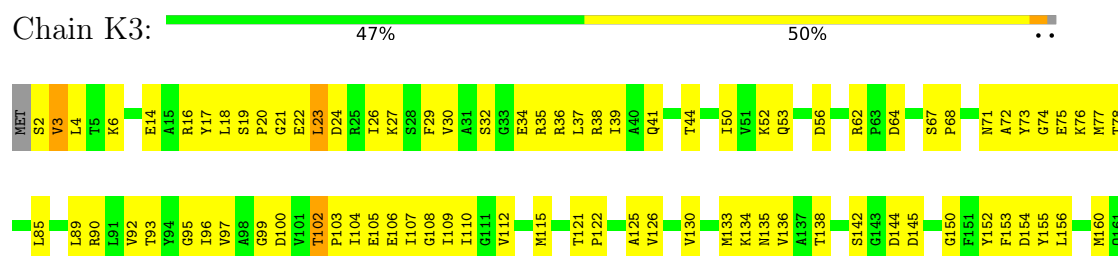
- Molecule 1: Allophycocyanin alpha subunit



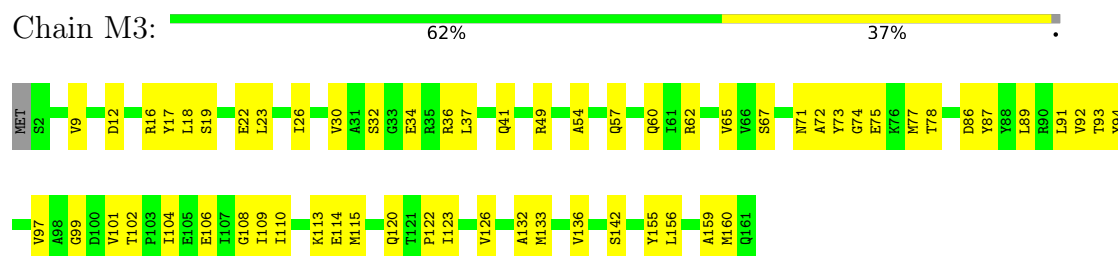
- Molecule 1: Allophycocyanin alpha subunit



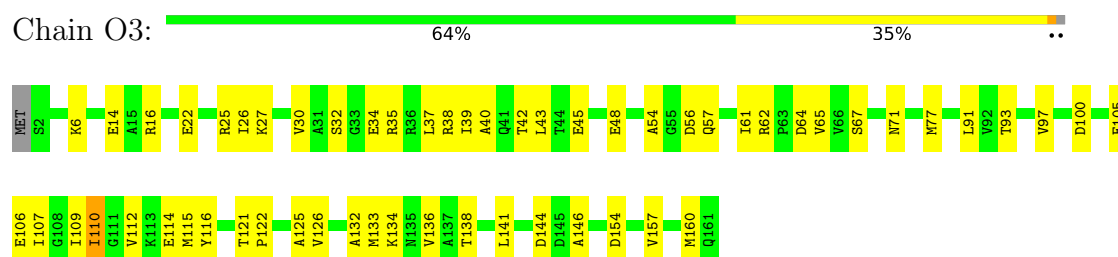
- Molecule 1: Allophycocyanin alpha subunit



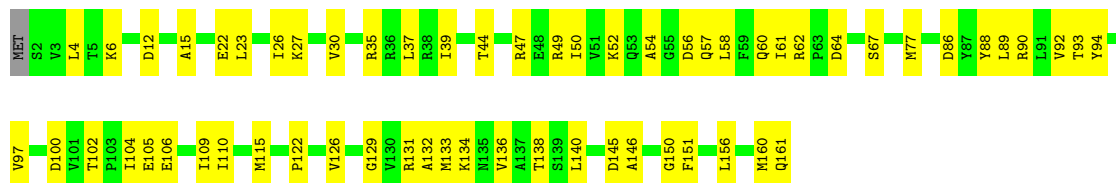
- Molecule 1: Allophycocyanin alpha subunit



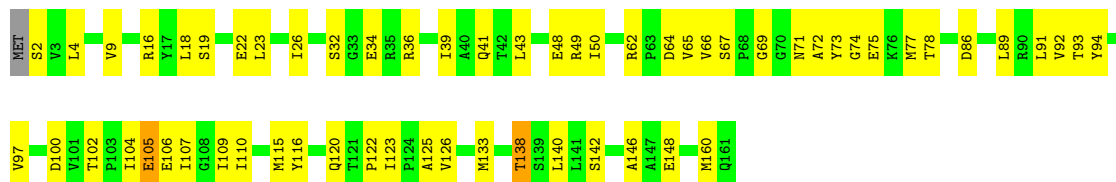
- Molecule 1: Allophycocyanin alpha subunit



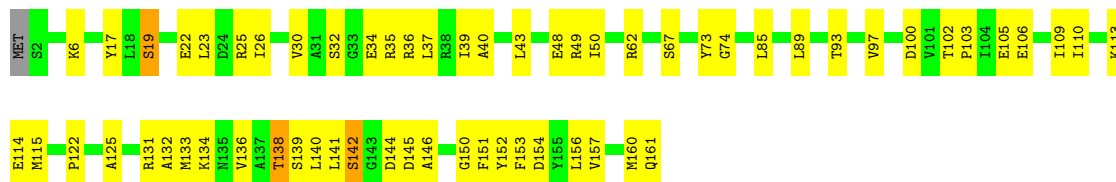
● Molecule 1: Allophycocyanin alpha subunit

Chain Q3:  62% 37%

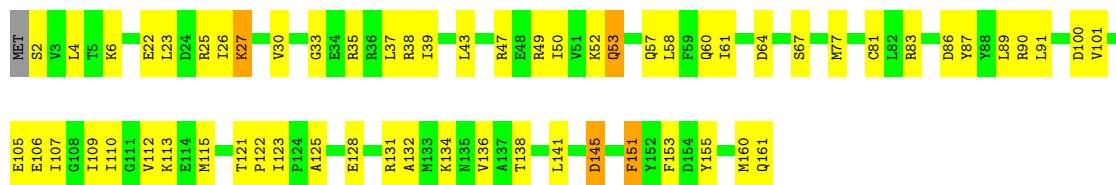
● Molecule 1: Allophycocyanin alpha subunit

Chain S3:  62% 36%

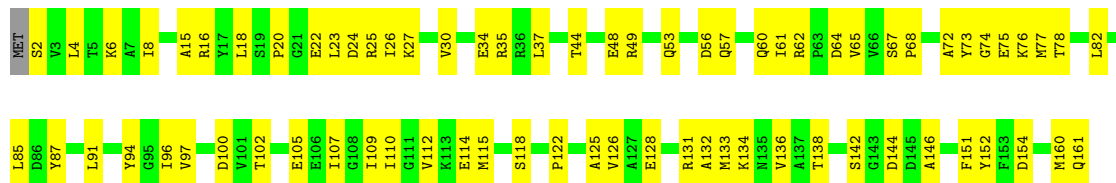
● Molecule 1: Allophycocyanin alpha subunit

Chain U3:  61% 36%

● Molecule 1: Allophycocyanin alpha subunit

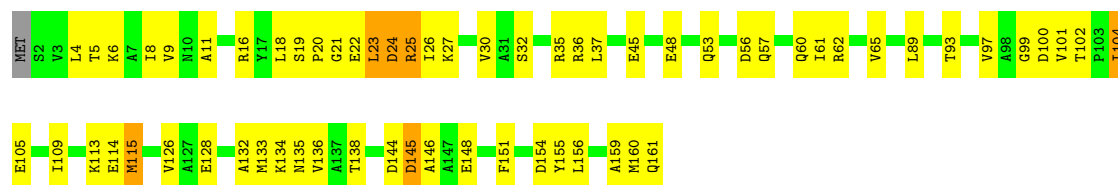
Chain W3:  61% 35%

● Molecule 1: Allophycocyanin alpha subunit

Chain Y3:  54% 45%

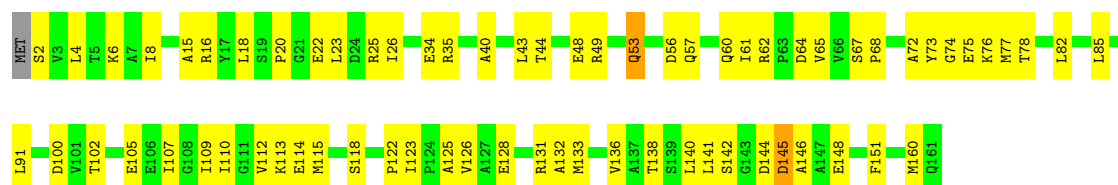
- Molecule 1: Allophycocyanin alpha subunit

Chain a3: 



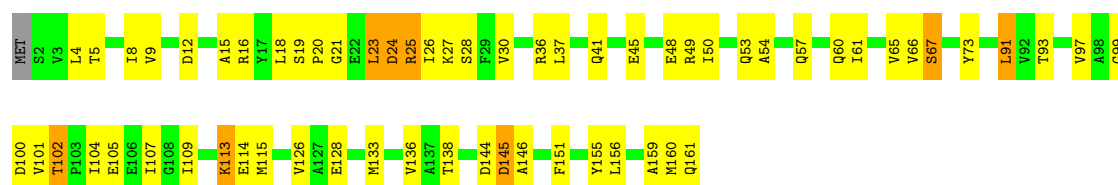
- Molecule 1: Allophycocyanin alpha subunit

Chain c3: 



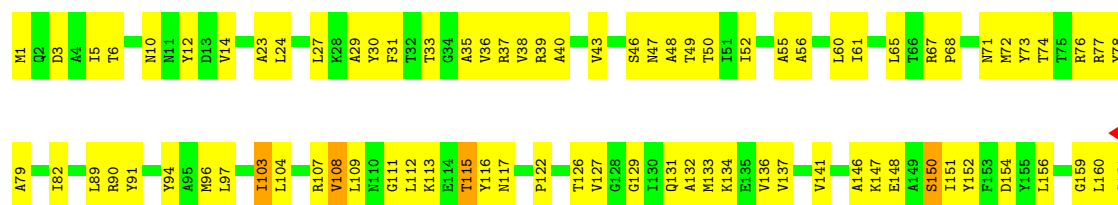
- Molecule 1: Allophycocyanin alpha subunit

Chain e3: 



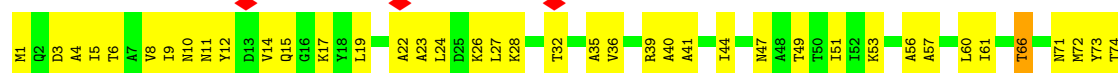
- Molecule 2: Allophycocyanin beta subunit

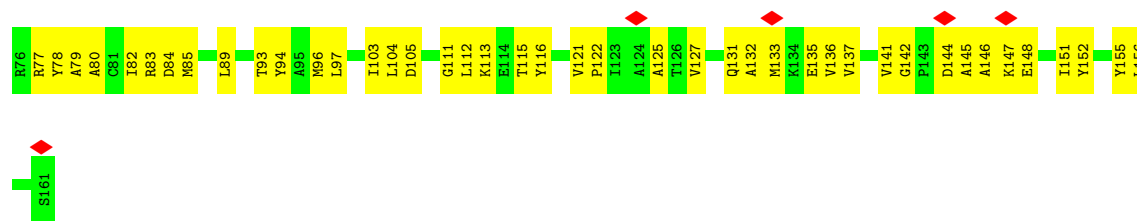
Chain B1: 



- Molecule 2: Allophycocyanin beta subunit

Chain D1: 

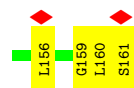
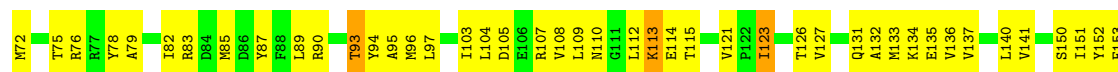
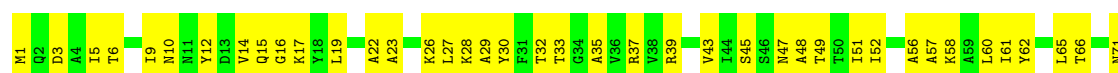




• Molecule 2: Allophycocyanin beta subunit



• Molecule 2: Allophycocyanin beta subunit

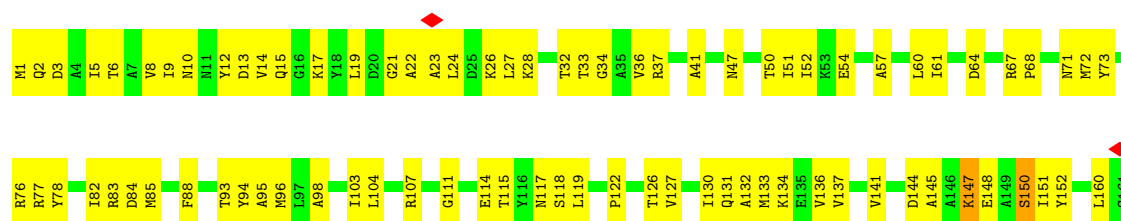


• Molecule 2: Allophycocyanin beta subunit



• Molecule 2: Allophycocyanin beta subunit





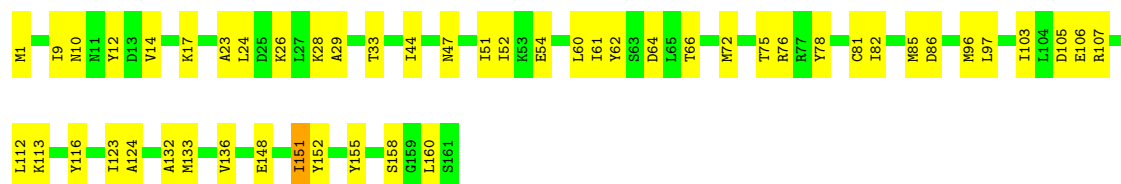
- Molecule 2: Allophycocyanin beta subunit

Chain B2: 71% 28%



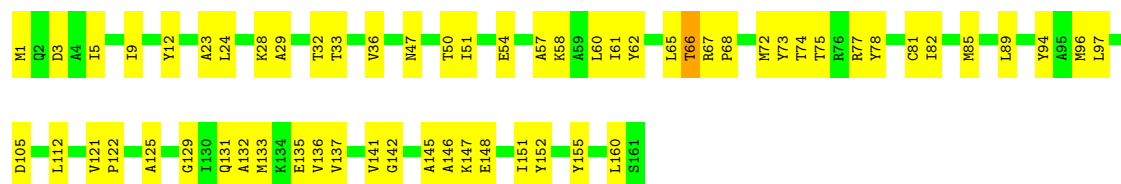
- Molecule 2: Allophycocyanin beta subunit

Chain D2: 69% 30%



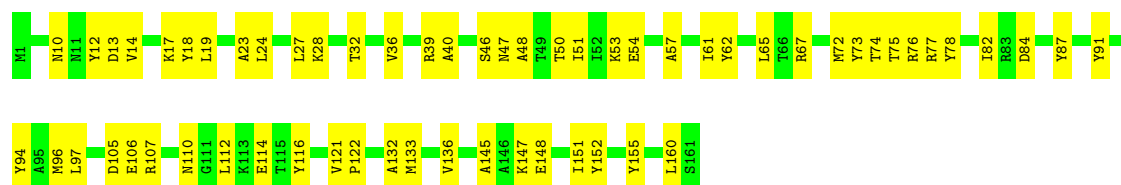
- Molecule 2: Allophycocyanin beta subunit

Chain F2: 63% 37%



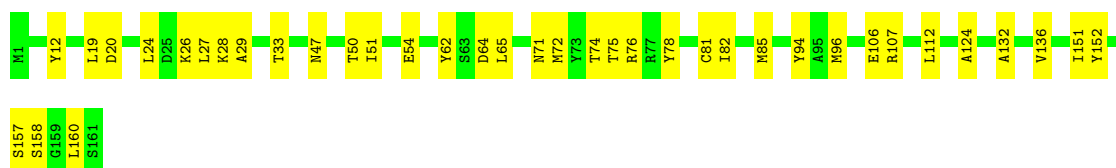
- Molecule 2: Allophycocyanin beta subunit

Chain H2: 63% 37%



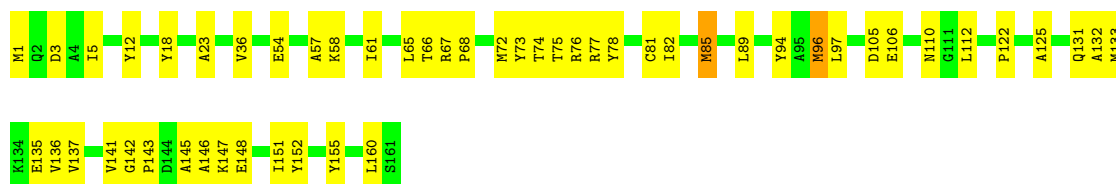
- Molecule 2: Allophycocyanin beta subunit

Chain J2:  76% 24%



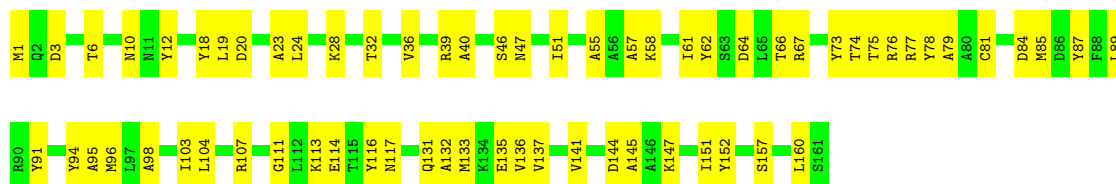
- Molecule 2: Allophycocyanin beta subunit

Chain L2:  68% 31% .



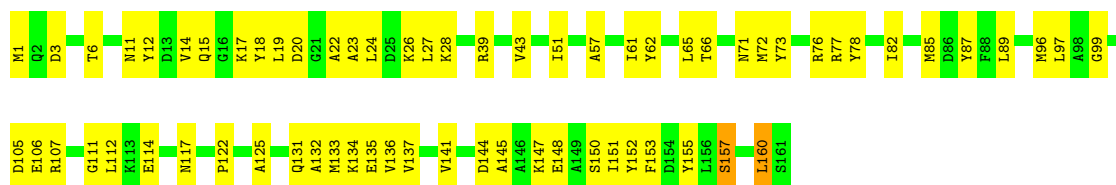
- Molecule 2: Allophycocyanin beta subunit

Chain N2:  60% 40%



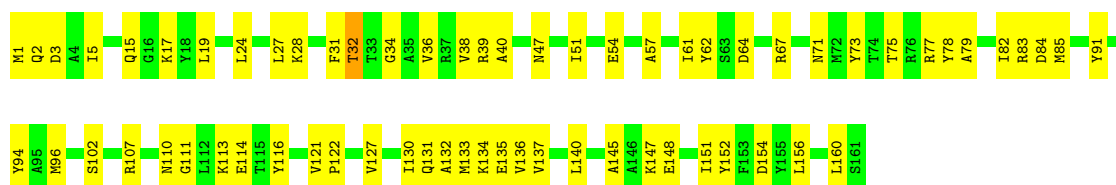
- Molecule 2: Allophycocyanin beta subunit

Chain P2:  59% 40% .



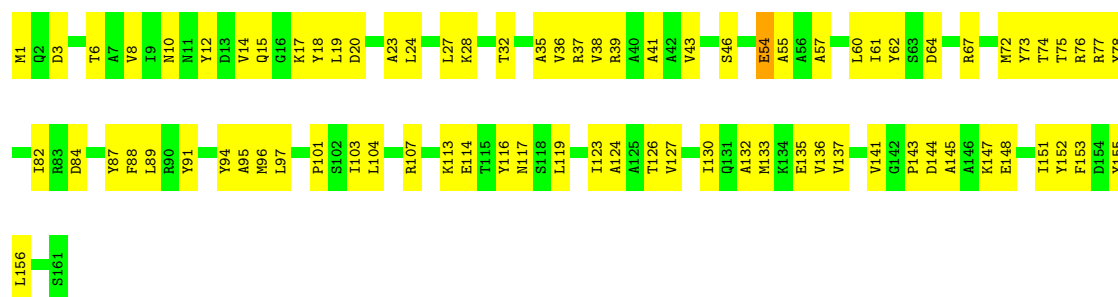
- Molecule 2: Allophycocyanin beta subunit

Chain R2:  60% 40% .



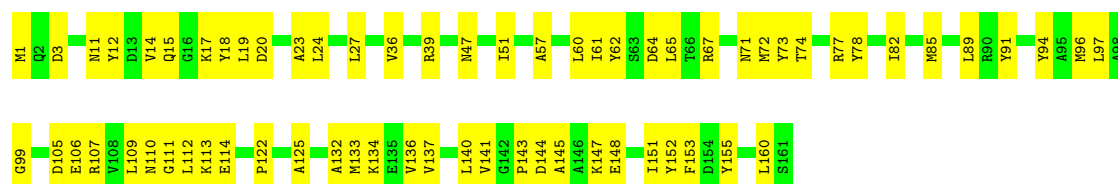
- Molecule 2: Allophycocyanin beta subunit

Chain T2:  50% 49% .



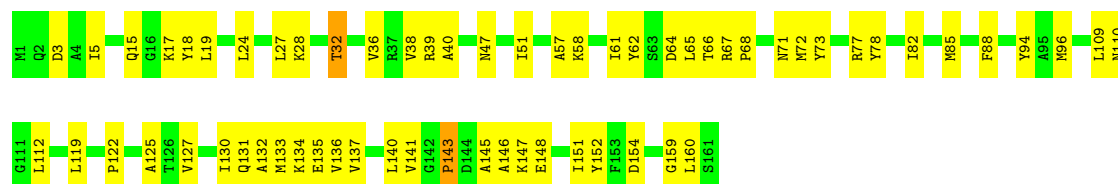
• Molecule 2: Allophycocyanin beta subunit

Chain V2:  59% 41%



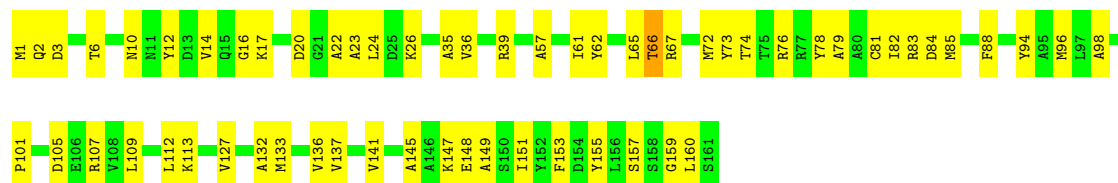
• Molecule 2: Allophycocyanin beta subunit

Chain X2:  61% 37% .



• Molecule 2: Allophycocyanin beta subunit

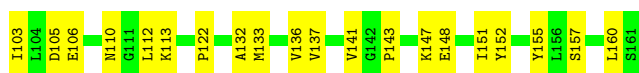
Chain Z2:  63% 37% .



• Molecule 2: Allophycocyanin beta subunit

Chain b2:  64% 36%





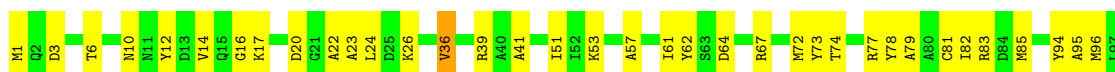
• Molecule 2: Allophycocyanin beta subunit

Chain d2: 57% 42%



• Molecule 2: Allophycocyanin beta subunit

Chain f2: 60% 39%



• Molecule 2: Allophycocyanin beta subunit

Chain h2: 63% 37%



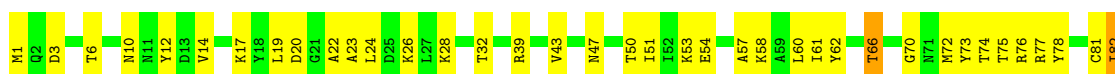
• Molecule 2: Allophycocyanin beta subunit

Chain j2: 60% 39%



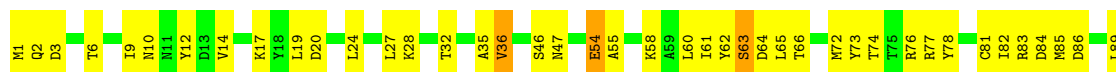
• Molecule 2: Allophycocyanin beta subunit

Chain l2: 55% 42%





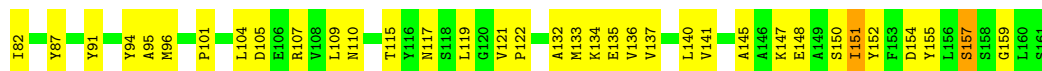
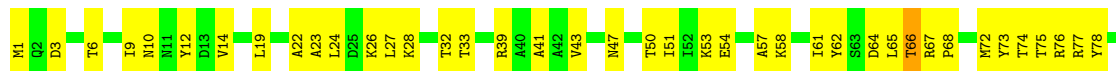
• Molecule 2: Allophycocyanin beta subunit



• Molecule 2: Allophycocyanin beta subunit



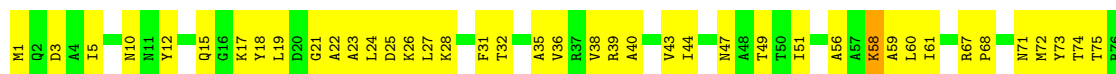
• Molecule 2: Allophycocyanin beta subunit



• Molecule 2: Allophycocyanin beta subunit

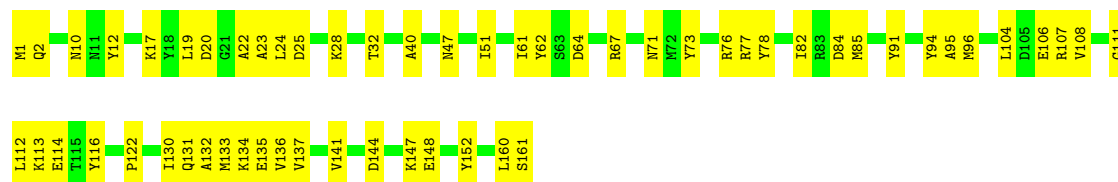


• Molecule 2: Allophycocyanin beta subunit

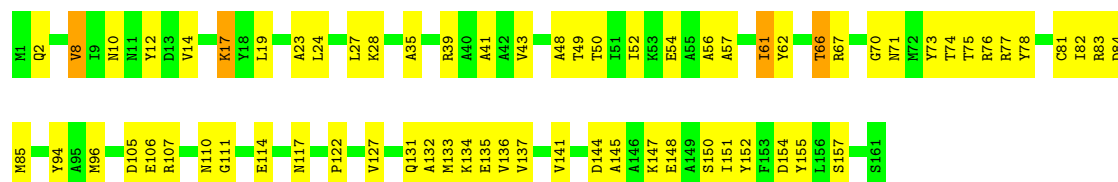




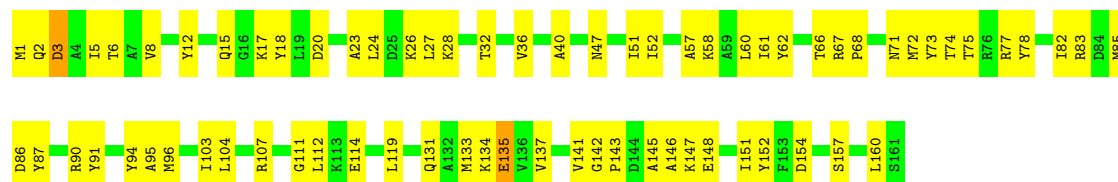
• Molecule 2: Allophycocyanin beta subunit



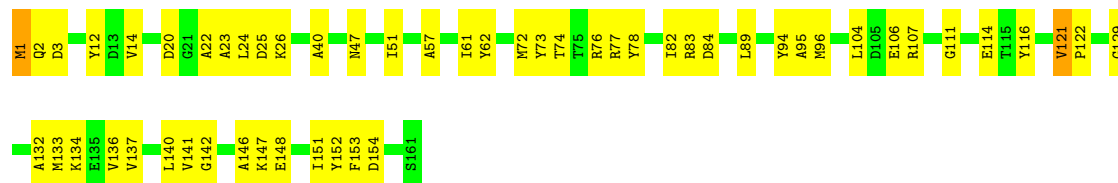
• Molecule 2: Allophycocyanin beta subunit



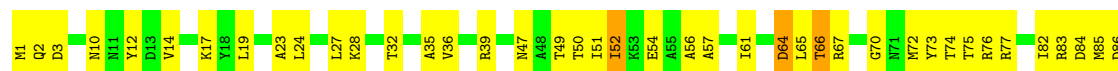
• Molecule 2: Allophycocyanin beta subunit

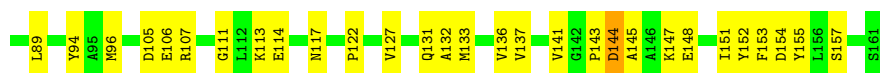


• Molecule 2: Allophycocyanin beta subunit



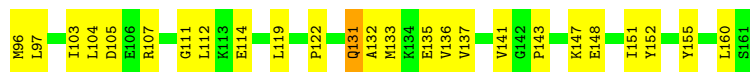
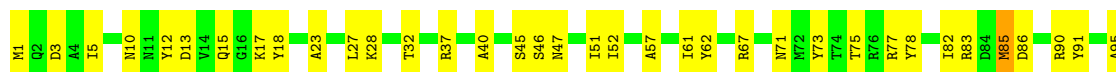
• Molecule 2: Allophycocyanin beta subunit





- Molecule 2: Allophycocyanin beta subunit

Chain L3: 62% 37% .



- Molecule 2: Allophycocyanin beta subunit

Chain N3: 71% 29% .



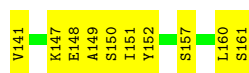
- Molecule 2: Allophycocyanin beta subunit

Chain P3: 66% 33% .



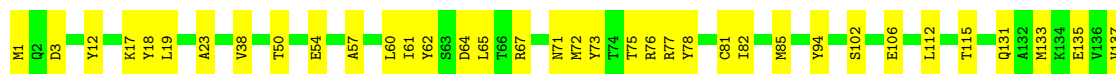
- Molecule 2: Allophycocyanin beta subunit

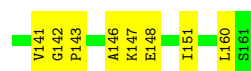
Chain R3: 71% 29%



- Molecule 2: Allophycocyanin beta subunit

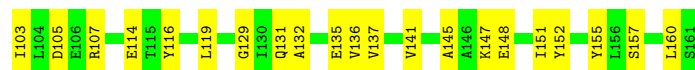
Chain T3: 73% 27%





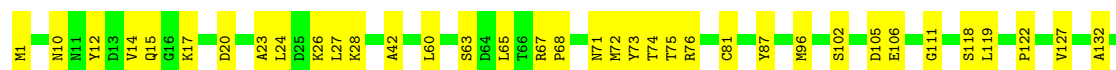
• Molecule 2: Allophycocyanin beta subunit

Chain V3: 63% 36% .



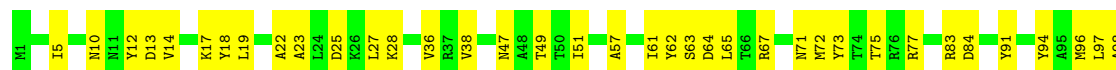
• Molecule 2: Allophycocyanin beta subunit

Chain X3: 70% 30% .



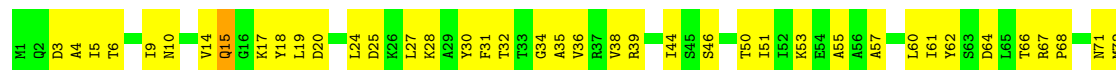
• Molecule 2: Allophycocyanin beta subunit

Chain Z3: 70% 30% .



• Molecule 2: Allophycocyanin beta subunit

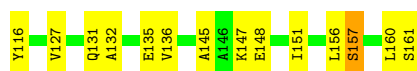
Chain b3: 54% 45% .



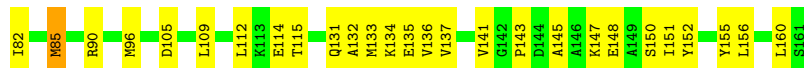
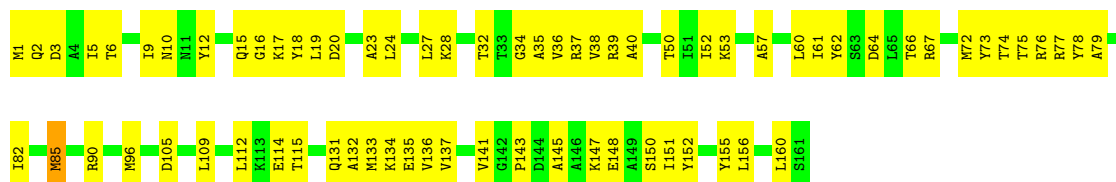
• Molecule 2: Allophycocyanin beta subunit

Chain d3: 68% 30% .

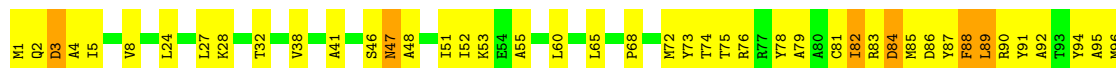




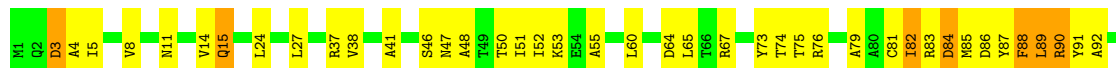
• Molecule 2: Allophycocyanin beta subunit



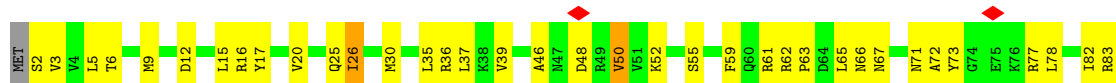
• Molecule 2: Allophycocyanin beta subunit



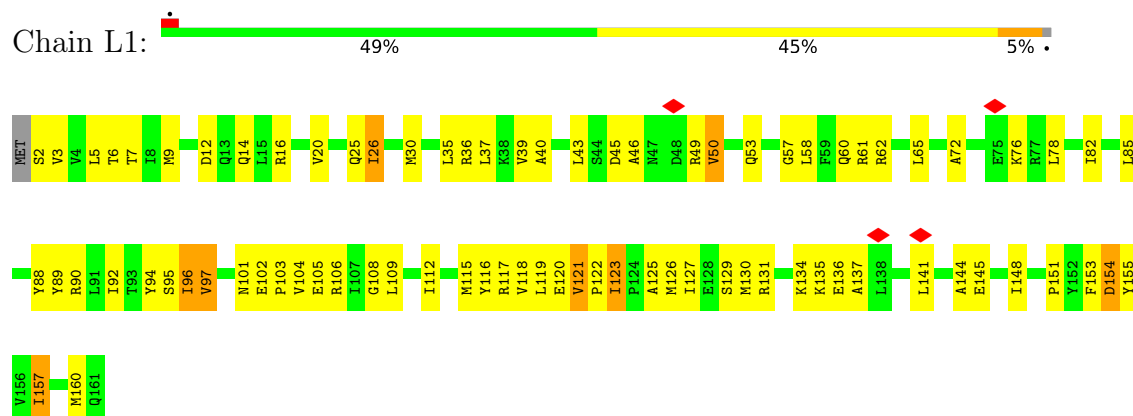
• Molecule 2: Allophycocyanin beta subunit



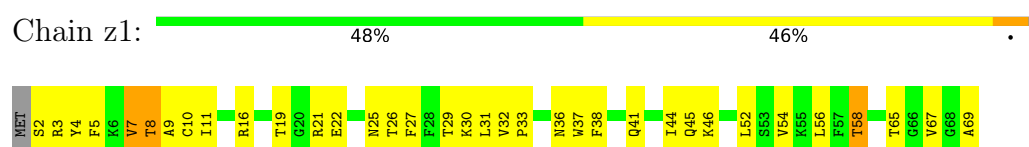
• Molecule 3: Allophycocyanin-B



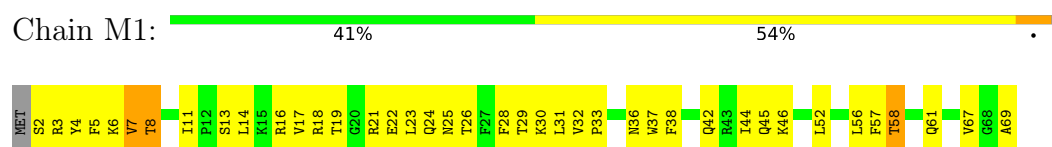
• Molecule 3: Allophycocyanin-B



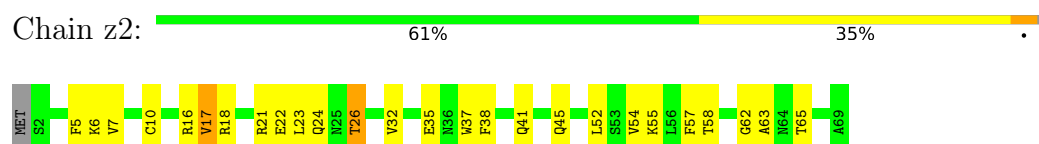
- Molecule 4: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core



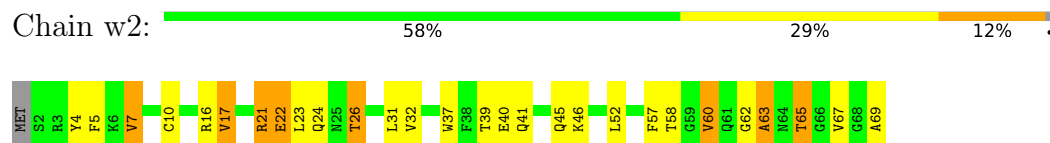
- Molecule 4: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core



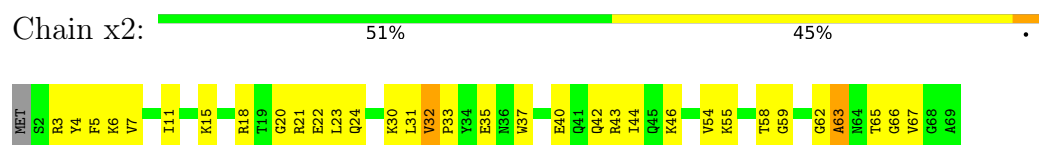
- Molecule 4: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core



- Molecule 4: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core

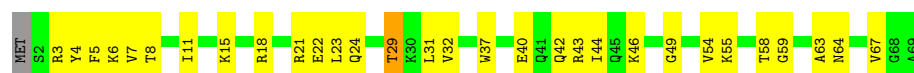


- Molecule 4: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core



- Molecule 4: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core

Chain y2:  55% 42% ..



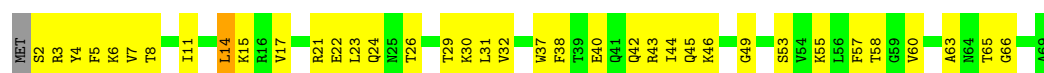
- Molecule 4: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core

Chain z3:  51% 45% ..



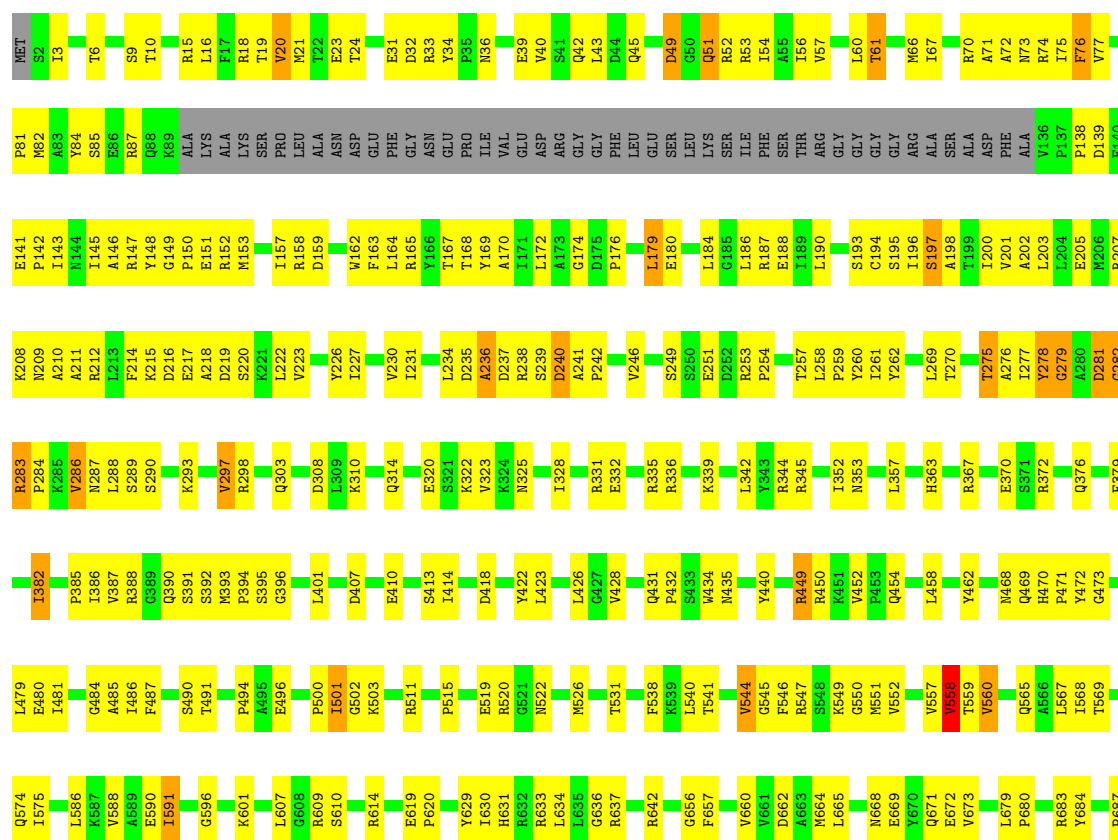
- Molecule 4: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core

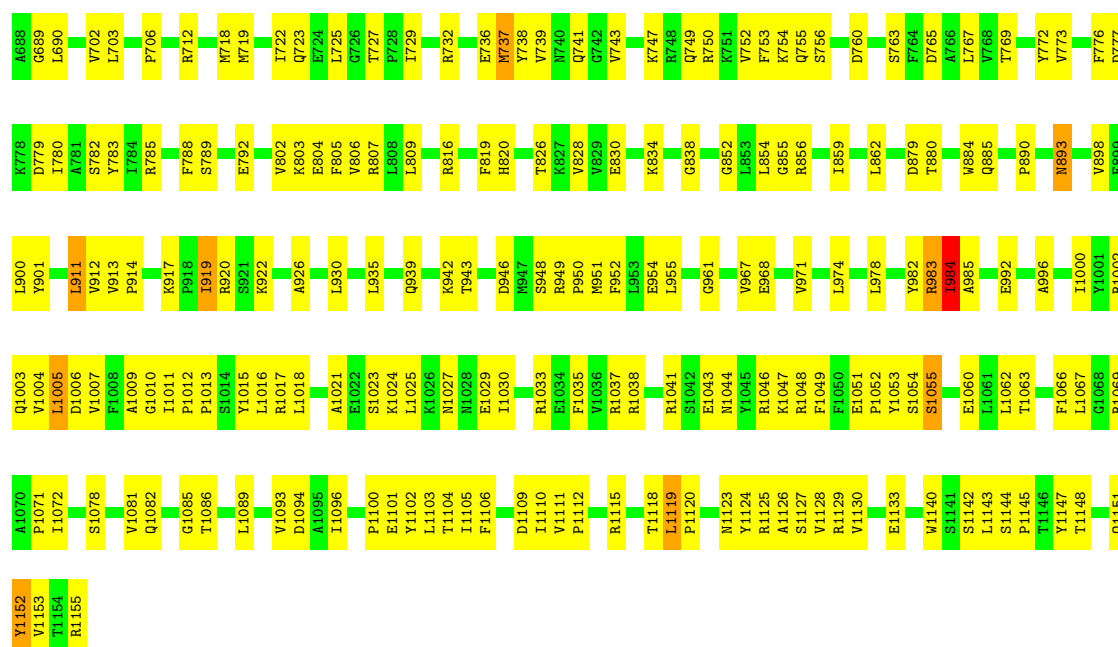
Chain i3:  45% 52% ..



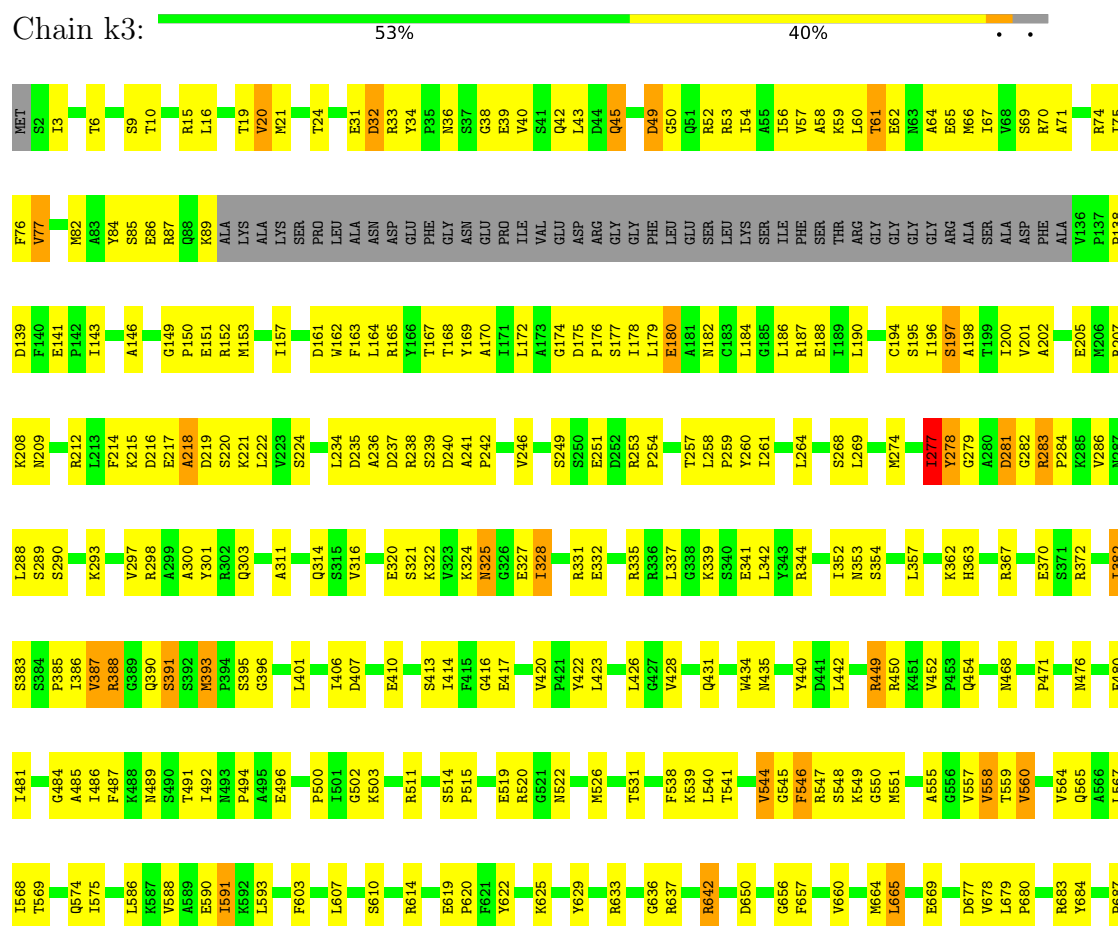
- Molecule 5: Phycobiliprotein ApCp

Chain j3:  53% 40% . .





- Molecule 5: Phycobiliprotein ApcE



T1148	F1066	E992	L900	D779	A688
Y1152	L1067	A996	Y901	I760	G689
R1155	G1068	A1009	L911	A781	L690
	R1069	I1000	V912	S782	
	A1070	Y1001	V913	Y783	V702
	P1071	R1002	P914	F788	L703
	S1078	Q1003	I919	S789	T704
	V1081	V1004	R920	E792	T705
	I1083	L1005	M923	L795	P706
	L1084	A1009	A926	I722	R712
	G1085	P1012	S927	Q723	
	T1086	P1013	M928	E724	I722
	A1090	L1016	P929	R802	Q725
	V1093	R1017	L930	R803	E724
	D1094	L1018	L935	E804	T727
	A1095	S1019	A936	F805	P728
	I1096	A1021	E937	V806	I729
	P1100	E1022	Q938	R807	
	F1101	S1023	Q939	L808	R732
	Y1102	K1024	A940	L809	
	L1103	L1025	T941	R816	E736
	T1104	K1026	K942	F819	M737
	I1105	N1027	T943	H820	Y738
	F1106	N1028	T943	D821	V739
	D1109	E1029	D946	R822	R740
	I1110	I1030	M947	T826	Q741
	V1111	R1033	S948	K827	G742
	P1112	E1034	R949	V828	V743
	R1115	F1035	P950	K834	K747
		V1036	M951	L837	R748
		R1037	F952	G838	Q749
		R1038	L953	L837	R750
			E954	G838	K751
			L955	G852	V752
			G961	L853	F753
			E1043	L854	K754
			E1044	G855	S756
			Y1045	R856	T759
			R1046	I859	D760
			K1047	V969	
			R1048	G970	S763
			F1049	V971	F764
			F1050	G972	D765
			E1051	T973	A766
			P1052	L974	L767
			Y1053	L978	V768
			S1054	T980	T769
			S1055	V881	
			E1060	Y982	Y772
			L1061	R983	V773
			L1062	I984	Q774
			T1063	S885	V775
				F886	F776
				R990	D777
				S991	K778

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	192814	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 K3 (6k x 4k)	Depositor
Maximum map value	1.670	Depositor
Minimum map value	-0.518	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.066	Depositor
Recommended contour level	0.15	Depositor
Map size ($\text{\AA}$)	636.78204, 636.78204, 636.78204	wwPDB
Map dimensions	580, 580, 580	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: CYC, MEN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A1	0.21	0/1239	0.50	0/1676
1	A2	0.21	0/1239	0.52	1/1676 (0.1%)
1	A3	0.44	1/1239 (0.1%)	0.69	4/1676 (0.2%)
1	C1	0.19	0/1239	0.50	1/1676 (0.1%)
1	C2	0.18	0/1239	0.44	0/1676
1	C3	0.19	0/1239	0.49	0/1676
1	E1	0.17	0/1239	0.43	0/1676
1	E2	0.22	0/1239	0.50	0/1676
1	E3	0.19	0/1239	0.47	0/1676
1	G2	0.19	0/1239	0.50	0/1676
1	G3	0.21	0/1239	0.50	0/1676
1	H1	0.20	0/1239	0.56	0/1676
1	I2	0.18	0/1239	0.46	0/1676
1	I3	0.22	0/1239	0.54	0/1676
1	K2	0.27	0/1239	0.58	0/1676
1	K3	0.22	0/1239	0.53	0/1676
1	M2	0.18	0/1239	0.50	0/1676
1	M3	0.25	0/1239	0.51	0/1676
1	O2	0.18	0/1239	0.48	0/1676
1	O3	0.20	0/1239	0.49	0/1676
1	Q2	0.21	0/1239	0.49	0/1676
1	Q3	0.20	0/1239	0.52	0/1676
1	S2	0.20	0/1239	0.51	0/1676
1	S3	0.25	0/1239	0.56	0/1676
1	U2	0.21	0/1239	0.53	0/1676
1	U3	0.21	0/1239	0.49	0/1676
1	W2	0.19	0/1239	0.48	0/1676
1	W3	0.19	0/1239	0.51	1/1676 (0.1%)
1	Y2	0.17	0/1239	0.48	0/1676
1	Y3	0.21	0/1239	0.50	0/1676
1	a2	0.17	0/1239	0.52	0/1676
1	a3	0.24	0/1239	0.58	3/1676 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	c2	0.20	0/1239	0.50	0/1676
1	c3	0.20	0/1239	0.48	0/1676
1	e2	0.25	0/1239	0.55	1/1676 (0.1%)
1	e3	0.24	0/1239	0.59	3/1676 (0.2%)
1	g2	0.18	0/1239	0.53	1/1676 (0.1%)
1	i2	0.28	0/1239	0.66	1/1676 (0.1%)
1	k2	0.16	0/1239	0.48	0/1676
1	m2	0.17	0/1239	0.51	0/1676
1	o2	0.22	0/1239	0.54	0/1676
1	q2	0.17	0/1239	0.45	0/1676
1	s2	0.20	0/1239	0.57	0/1676
1	u2	0.25	0/1239	0.54	0/1676
2	B1	0.16	0/1218	0.43	0/1648
2	B2	0.19	0/1218	0.52	1/1648 (0.1%)
2	B3	0.18	0/1218	0.45	0/1648
2	D1	0.14	0/1218	0.43	0/1648
2	D2	0.22	0/1218	0.48	0/1648
2	D3	0.18	0/1218	0.48	0/1648
2	F1	0.15	0/1218	0.43	0/1648
2	F2	0.19	0/1218	0.44	0/1648
2	F3	0.22	0/1218	0.54	1/1648 (0.1%)
2	G1	0.15	0/1218	0.47	0/1648
2	H2	0.18	0/1218	0.46	0/1648
2	H3	0.19	0/1218	0.47	0/1648
2	I1	0.18	0/1218	0.49	1/1648 (0.1%)
2	J1	0.17	0/1218	0.48	0/1648
2	J2	0.22	0/1218	0.44	0/1648
2	J3	0.17	0/1218	0.46	0/1648
2	L2	0.21	0/1218	0.50	1/1648 (0.1%)
2	L3	0.20	0/1218	0.51	1/1648 (0.1%)
2	N2	0.19	0/1218	0.47	0/1648
2	N3	0.22	0/1218	0.48	0/1648
2	P2	0.18	0/1218	0.47	0/1648
2	P3	0.19	0/1218	0.46	0/1648
2	R2	0.17	0/1218	0.46	0/1648
2	R3	0.23	0/1218	0.48	0/1648
2	T2	0.21	0/1218	0.53	1/1648 (0.1%)
2	T3	0.21	0/1218	0.44	0/1648
2	V2	0.17	0/1218	0.47	0/1648
2	V3	0.18	0/1218	0.43	0/1648
2	X2	0.20	0/1218	0.56	1/1648 (0.1%)
2	X3	0.24	0/1218	0.50	0/1648
2	Z2	0.16	0/1218	0.43	0/1648

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	Z3	0.22	0/1218	0.48	0/1648
2	b2	0.17	0/1218	0.43	0/1648
2	b3	0.25	0/1218	0.67	2/1648 (0.1%)
2	d2	0.16	0/1218	0.50	0/1648
2	d3	0.23	0/1218	0.48	0/1648
2	f2	0.15	0/1218	0.41	0/1648
2	f3	0.22	0/1218	0.57	2/1648 (0.1%)
2	g3	0.26	0/1217	0.75	3/1648 (0.2%)
2	h2	0.18	0/1218	0.46	0/1648
2	h3	0.25	0/1217	0.76	3/1648 (0.2%)
2	j2	0.16	0/1218	0.50	0/1648
2	l2	0.17	0/1218	0.46	0/1648
2	n2	0.18	0/1218	0.48	0/1648
2	p2	0.22	0/1218	0.51	0/1648
2	r2	0.16	0/1218	0.43	0/1648
2	t2	0.17	0/1218	0.46	0/1648
2	v2	0.22	0/1218	0.55	0/1648
3	K1	0.18	0/1276	0.56	0/1723
3	L1	0.22	0/1276	0.64	0/1723
4	M1	0.18	0/548	0.58	0/737
4	i3	0.21	0/548	0.51	0/737
4	w2	0.21	0/548	0.64	1/737 (0.1%)
4	x2	0.20	0/548	0.52	0/737
4	y2	0.22	0/548	0.60	0/737
4	z1	0.19	0/548	0.59	0/737
4	z2	0.21	0/548	0.69	1/737 (0.1%)
4	z3	0.22	0/548	0.61	0/737
5	j3	0.25	0/9003	0.60	8/12173 (0.1%)
5	k3	0.26	0/9003	0.61	8/12173 (0.1%)
All	All	0.21	1/137920 (0.0%)	0.53	51/186536 (0.0%)

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	K2	0	1
1	i2	0	1
2	g3	0	3
2	h3	0	3
4	w2	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
5	j3	0	6
5	k3	0	7
All	All	0	22

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A3	18	LEU	C-O	6.62	1.32	1.24

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b3	143	PRO	CA-N-CD	-10.79	96.90	112.00
2	X2	143	PRO	CA-N-CD	-10.56	97.22	112.00
2	f3	143	PRO	CA-N-CD	-9.15	99.19	112.00
2	g3	147	LYS	CA-C-N	7.89	136.62	121.54
2	g3	147	LYS	C-N-CA	7.89	136.62	121.54

There are no chirality outliers.

5 of 22 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	K2	49	ARG	Sidechain
2	g3	82	ILE	Peptide
2	g3	86	ASP	Peptide
1	i2	99	GLY	Peptide
4	w2	21	ARG	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A1	1222	0	1233	85	0
1	A2	1222	0	1233	63	0
1	A3	1222	0	1234	74	0
1	C1	1222	0	1233	101	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C2	1222	0	1233	54	0
1	C3	1222	0	1233	65	0
1	E1	1222	0	1233	59	0
1	E2	1222	0	1233	47	0
1	E3	1222	0	1233	64	0
1	G2	1222	0	1233	70	0
1	G3	1222	0	1234	65	0
1	H1	1222	0	1233	119	0
1	I2	1222	0	1233	52	0
1	I3	1222	0	1233	69	0
1	K2	1222	0	1233	53	0
1	K3	1222	0	1233	76	0
1	M2	1222	0	1233	85	0
1	M3	1222	0	1233	47	0
1	O2	1222	0	1233	78	0
1	O3	1222	0	1233	47	0
1	Q2	1222	0	1233	69	0
1	Q3	1222	0	1233	58	0
1	S2	1222	0	1233	91	0
1	S3	1222	0	1233	44	0
1	U2	1222	0	1233	79	0
1	U3	1222	0	1233	56	0
1	W2	1222	0	1233	66	0
1	W3	1222	0	1233	69	0
1	Y2	1222	0	1233	80	0
1	Y3	1222	0	1233	81	0
1	a2	1222	0	1233	82	0
1	a3	1222	0	1233	73	0
1	c2	1222	0	1233	113	0
1	c3	1222	0	1233	74	0
1	e2	1222	0	1233	64	0
1	e3	1222	0	1233	57	0
1	g2	1222	0	1233	81	0
1	i2	1222	0	1233	89	0
1	k2	1222	0	1233	79	0
1	m2	1222	0	1233	126	0
1	o2	1222	0	1233	84	0
1	q2	1222	0	1233	81	0
1	s2	1222	0	1233	107	0
1	u2	1222	0	1233	77	0
2	B1	1210	0	1220	86	0
2	B2	1210	0	1220	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B3	1210	0	1220	49	0
2	D1	1210	0	1220	84	0
2	D2	1210	0	1220	46	0
2	D3	1210	0	1217	68	0
2	F1	1210	0	1220	92	0
2	F2	1210	0	1220	48	0
2	F3	1210	0	1220	66	0
2	G1	1210	0	1220	83	0
2	H2	1210	0	1220	55	0
2	H3	1210	0	1220	51	0
2	I1	1210	0	1220	72	0
2	J1	1210	0	1220	93	0
2	J2	1210	0	1220	31	0
2	J3	1210	0	1217	72	0
2	L2	1210	0	1220	40	0
2	L3	1210	0	1220	61	0
2	N2	1210	0	1220	73	0
2	N3	1210	0	1220	42	0
2	P2	1210	0	1220	52	0
2	P3	1210	0	1220	42	0
2	R2	1210	0	1220	74	0
2	R3	1210	0	1220	40	0
2	T2	1210	0	1220	75	0
2	T3	1210	0	1220	39	0
2	V2	1210	0	1220	60	0
2	V3	1210	0	1220	55	0
2	X2	1210	0	1220	71	0
2	X3	1210	0	1220	36	0
2	Z2	1210	0	1220	59	0
2	Z3	1210	0	1220	38	0
2	b2	1210	0	1220	53	0
2	b3	1210	0	1220	79	0
2	d2	1210	0	1220	66	0
2	d3	1210	0	1220	36	0
2	f2	1210	0	1220	51	0
2	f3	1210	0	1220	77	0
2	g3	1209	0	1220	96	0
2	h2	1210	0	1220	57	0
2	h3	1209	0	1220	87	0
2	j2	1210	0	1220	59	0
2	l2	1210	0	1220	82	0
2	n2	1210	0	1220	75	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	p2	1210	0	1220	83	0
2	r2	1210	0	1220	71	0
2	t2	1210	0	1220	56	0
2	v2	1210	0	1220	97	0
3	K1	1255	0	1265	114	0
3	L1	1255	0	1265	98	0
4	M1	538	0	555	43	0
4	i3	538	0	555	35	0
4	w2	538	0	555	24	0
4	x2	538	0	555	33	0
4	y2	538	0	555	34	0
4	z1	538	0	555	50	0
4	z2	538	0	555	20	0
4	z3	538	0	554	31	0
5	j3	8819	0	8827	520	0
5	k3	8819	0	8826	517	0
6	A1	43	0	37	5	0
6	A2	43	0	37	7	0
6	A3	43	0	35	10	0
6	B2	43	0	37	4	0
6	C1	43	0	37	7	0
6	C2	43	0	35	4	0
6	C3	43	0	36	5	0
6	D3	43	0	36	4	0
6	E1	43	0	37	6	0
6	E2	43	0	37	5	0
6	E3	43	0	37	4	0
6	F1	43	0	37	5	0
6	F2	43	0	35	2	0
6	F3	43	0	37	5	0
6	G2	43	0	37	6	0
6	G3	43	0	35	9	0
6	H1	43	0	36	7	0
6	H2	43	0	37	7	0
6	H3	43	0	37	11	0
6	I2	43	0	35	3	0
6	I3	43	0	36	5	0
6	J1	43	0	37	7	0
6	J3	43	0	37	6	0
6	K1	43	0	37	10	0
6	K2	43	0	37	7	0
6	K3	43	0	37	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	L1	43	0	37	12	0
6	L2	43	0	36	2	0
6	L3	43	0	37	7	0
6	M1	43	0	37	6	0
6	M2	43	0	37	4	0
6	M3	43	0	37	4	0
6	N2	43	0	36	5	0
6	N3	43	0	37	4	0
6	O2	43	0	37	3	0
6	O3	43	0	35	6	0
6	P2	43	0	37	2	0
6	Q2	43	0	37	6	0
6	Q3	43	0	36	5	0
6	R2	43	0	37	2	0
6	R3	43	0	37	3	0
6	S2	43	0	37	8	0
6	S3	43	0	37	4	0
6	T2	43	0	37	6	0
6	T3	43	0	37	3	0
6	U2	43	0	35	3	0
6	U3	43	0	35	5	0
6	V2	43	0	36	3	0
6	V3	43	0	35	5	0
6	W2	43	0	37	7	0
6	W3	43	0	36	9	0
6	X2	43	0	37	5	0
6	X3	43	0	37	3	0
6	Y2	43	0	37	5	0
6	Y3	43	0	37	5	0
6	Z3	43	0	36	2	0
6	a2	43	0	36	6	0
6	a3	43	0	35	3	0
6	b2	43	0	37	8	0
6	b3	43	0	37	1	0
6	c2	43	0	37	4	0
6	c3	43	0	37	5	0
6	d3	43	0	35	3	0
6	e2	43	0	37	5	0
6	e3	43	0	35	4	0
6	f3	43	0	37	2	0
6	g2	43	0	35	4	0
6	g3	43	0	37	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	h2	43	0	37	5	0
6	h3	43	0	37	13	0
6	i2	43	0	37	4	0
6	j3	258	38	212	41	0
6	k2	43	0	36	5	0
6	k3	301	38	248	28	0
6	m2	43	0	37	5	0
6	o2	43	0	36	8	0
6	p2	43	0	36	7	0
6	q2	43	0	37	7	0
6	s2	43	0	36	7	0
6	u2	43	0	36	8	0
6	v2	43	0	36	7	0
6	x2	43	0	33	7	0
6	y2	43	0	33	8	0
6	z1	43	0	37	5	0
6	z3	43	0	37	7	0
All	All	140426	76	140910	6997	0

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

The worst 5 of 6997 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:e2:105:GLU:HA	1:e2:109:ILE:HG12	1.34	1.08
2:P3:60:LEU:HB3	2:P3:72:MET:HE1	1.40	1.02
1:e3:27:LYS:HE2	2:h3:38:VAL:HG11	1.43	1.01
2:b2:85:MET:HE1	6:b2:201:CYC:HBC1	1.43	1.00
4:x2:7:VAL:HG12	4:x2:54:VAL:HG13	1.44	1.00

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A1	158/161 (98%)	153 (97%)	5 (3%)	0	100	100
1	A2	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
1	A3	158/161 (98%)	148 (94%)	8 (5%)	2 (1%)	9	32
1	C1	158/161 (98%)	152 (96%)	6 (4%)	0	100	100
1	C2	158/161 (98%)	153 (97%)	5 (3%)	0	100	100
1	C3	158/161 (98%)	151 (96%)	7 (4%)	0	100	100
1	E1	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
1	E2	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
1	E3	158/161 (98%)	157 (99%)	1 (1%)	0	100	100
1	G2	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
1	G3	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
1	H1	158/161 (98%)	153 (97%)	5 (3%)	0	100	100
1	I2	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
1	I3	158/161 (98%)	153 (97%)	5 (3%)	0	100	100
1	K2	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
1	K3	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
1	M2	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
1	M3	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
1	O2	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
1	O3	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
1	Q2	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
1	Q3	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
1	S2	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
1	S3	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
1	U2	158/161 (98%)	157 (99%)	1 (1%)	0	100	100
1	U3	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
1	W2	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
1	W3	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
1	Y2	158/161 (98%)	157 (99%)	1 (1%)	0	100	100
1	Y3	158/161 (98%)	154 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	a2	158/161 (98%)	151 (96%)	7 (4%)	0	100	100
1	a3	158/161 (98%)	152 (96%)	5 (3%)	1 (1%)	21	49
1	c2	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
1	c3	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
1	e2	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
1	e3	158/161 (98%)	152 (96%)	5 (3%)	1 (1%)	21	49
1	g2	158/161 (98%)	152 (96%)	6 (4%)	0	100	100
1	i2	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
1	k2	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
1	m2	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
1	o2	158/161 (98%)	153 (97%)	5 (3%)	0	100	100
1	q2	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
1	s2	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
1	u2	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
2	B1	158/161 (98%)	153 (97%)	5 (3%)	0	100	100
2	B2	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
2	B3	158/161 (98%)	153 (97%)	5 (3%)	0	100	100
2	D1	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
2	D2	158/161 (98%)	151 (96%)	7 (4%)	0	100	100
2	D3	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
2	F1	158/161 (98%)	151 (96%)	7 (4%)	0	100	100
2	F2	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
2	F3	158/161 (98%)	153 (97%)	5 (3%)	0	100	100
2	G1	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
2	H2	158/161 (98%)	153 (97%)	5 (3%)	0	100	100
2	H3	158/161 (98%)	152 (96%)	6 (4%)	0	100	100
2	I1	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
2	J1	158/161 (98%)	153 (97%)	5 (3%)	0	100	100
2	J2	158/161 (98%)	152 (96%)	6 (4%)	0	100	100
2	J3	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
2	L2	158/161 (98%)	154 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	L3	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
2	N2	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
2	N3	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
2	P2	158/161 (98%)	151 (96%)	7 (4%)	0	100	100
2	P3	158/161 (98%)	153 (97%)	5 (3%)	0	100	100
2	R2	158/161 (98%)	152 (96%)	6 (4%)	0	100	100
2	R3	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
2	T2	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
2	T3	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
2	V2	158/161 (98%)	151 (96%)	7 (4%)	0	100	100
2	V3	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
2	X2	158/161 (98%)	153 (97%)	5 (3%)	0	100	100
2	X3	158/161 (98%)	153 (97%)	5 (3%)	0	100	100
2	Z2	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
2	Z3	158/161 (98%)	153 (97%)	5 (3%)	0	100	100
2	b2	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
2	b3	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
2	d2	158/161 (98%)	153 (97%)	5 (3%)	0	100	100
2	d3	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
2	f2	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
2	f3	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
2	g3	158/161 (98%)	130 (82%)	25 (16%)	3 (2%)	6	25
2	h2	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
2	h3	158/161 (98%)	130 (82%)	25 (16%)	3 (2%)	6	25
2	j2	158/161 (98%)	153 (97%)	5 (3%)	0	100	100
2	l2	158/161 (98%)	152 (96%)	6 (4%)	0	100	100
2	n2	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
2	p2	158/161 (98%)	153 (97%)	5 (3%)	0	100	100
2	r2	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
2	t2	158/161 (98%)	152 (96%)	6 (4%)	0	100	100
2	v2	158/161 (98%)	154 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	K1	158/161 (98%)	150 (95%)	8 (5%)	0	100	100
3	L1	158/161 (98%)	150 (95%)	8 (5%)	0	100	100
4	M1	66/69 (96%)	58 (88%)	7 (11%)	1 (2%)	8	29
4	i3	66/69 (96%)	59 (89%)	6 (9%)	1 (2%)	8	29
4	w2	66/69 (96%)	56 (85%)	7 (11%)	3 (4%)	2	12
4	x2	66/69 (96%)	57 (86%)	8 (12%)	1 (2%)	8	29
4	y2	66/69 (96%)	57 (86%)	9 (14%)	0	100	100
4	z1	66/69 (96%)	58 (88%)	8 (12%)	0	100	100
4	z2	66/69 (96%)	56 (85%)	8 (12%)	2 (3%)	3	18
4	z3	66/69 (96%)	59 (89%)	6 (9%)	1 (2%)	8	29
5	j3	1104/1155 (96%)	971 (88%)	119 (11%)	14 (1%)	9	32
5	k3	1104/1155 (96%)	973 (88%)	115 (10%)	16 (1%)	9	30
All	All	17588/17996 (98%)	16814 (96%)	725 (4%)	49 (0%)	37	64

5 of 49 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	a3	25	ARG
1	e3	25	ARG
2	g3	90	ARG
2	g3	102	SER
5	j3	20	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A1	127/128 (99%)	122 (96%)	5 (4%)	28	53
1	A2	127/128 (99%)	126 (99%)	1 (1%)	73	77
1	A3	127/128 (99%)	126 (99%)	1 (1%)	73	77
1	C1	127/128 (99%)	120 (94%)	7 (6%)	19	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C2	127/128 (99%)	125 (98%)	2 (2%)	55	68
1	C3	127/128 (99%)	123 (97%)	4 (3%)	35	59
1	E1	127/128 (99%)	126 (99%)	1 (1%)	73	77
1	E2	127/128 (99%)	121 (95%)	6 (5%)	23	50
1	E3	127/128 (99%)	121 (95%)	6 (5%)	23	50
1	G2	127/128 (99%)	126 (99%)	1 (1%)	73	77
1	G3	127/128 (99%)	125 (98%)	2 (2%)	55	68
1	H1	127/128 (99%)	124 (98%)	3 (2%)	43	62
1	I2	127/128 (99%)	122 (96%)	5 (4%)	28	53
1	I3	127/128 (99%)	121 (95%)	6 (5%)	23	50
1	K2	127/128 (99%)	120 (94%)	7 (6%)	19	46
1	K3	127/128 (99%)	124 (98%)	3 (2%)	43	62
1	M2	111/128 (87%)	106 (96%)	5 (4%)	24	50
1	M3	127/128 (99%)	124 (98%)	3 (2%)	43	62
1	O2	127/128 (99%)	125 (98%)	2 (2%)	55	68
1	O3	127/128 (99%)	125 (98%)	2 (2%)	55	68
1	Q2	127/128 (99%)	121 (95%)	6 (5%)	23	50
1	Q3	127/128 (99%)	126 (99%)	1 (1%)	73	77
1	S2	127/128 (99%)	124 (98%)	3 (2%)	43	62
1	S3	127/128 (99%)	121 (95%)	6 (5%)	23	50
1	U2	127/128 (99%)	126 (99%)	1 (1%)	73	77
1	U3	127/128 (99%)	121 (95%)	6 (5%)	23	50
1	W2	127/128 (99%)	120 (94%)	7 (6%)	19	46
1	W3	127/128 (99%)	122 (96%)	5 (4%)	28	53
1	Y2	127/128 (99%)	127 (100%)	0	100	100
1	Y3	127/128 (99%)	127 (100%)	0	100	100
1	a2	127/128 (99%)	124 (98%)	3 (2%)	43	62
1	a3	127/128 (99%)	123 (97%)	4 (3%)	35	59
1	c2	127/128 (99%)	122 (96%)	5 (4%)	28	53
1	c3	127/128 (99%)	123 (97%)	4 (3%)	35	59
1	e2	127/128 (99%)	123 (97%)	4 (3%)	35	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	e3	127/128 (99%)	121 (95%)	6 (5%)	23	50
1	g2	127/128 (99%)	125 (98%)	2 (2%)	55	68
1	i2	127/128 (99%)	121 (95%)	6 (5%)	23	50
1	k2	127/128 (99%)	126 (99%)	1 (1%)	73	77
1	m2	127/128 (99%)	124 (98%)	3 (2%)	43	62
1	o2	127/128 (99%)	124 (98%)	3 (2%)	43	62
1	q2	127/128 (99%)	123 (97%)	4 (3%)	35	59
1	s2	127/128 (99%)	125 (98%)	2 (2%)	55	68
1	u2	127/128 (99%)	125 (98%)	2 (2%)	55	68
2	B1	121/121 (100%)	116 (96%)	5 (4%)	27	52
2	B2	121/121 (100%)	119 (98%)	2 (2%)	53	67
2	B3	121/121 (100%)	121 (100%)	0	100	100
2	D1	121/121 (100%)	118 (98%)	3 (2%)	42	62
2	D2	121/121 (100%)	119 (98%)	2 (2%)	53	67
2	D3	121/121 (100%)	117 (97%)	4 (3%)	33	58
2	F1	121/121 (100%)	120 (99%)	1 (1%)	73	77
2	F2	121/121 (100%)	120 (99%)	1 (1%)	73	77
2	F3	121/121 (100%)	120 (99%)	1 (1%)	73	77
2	G1	121/121 (100%)	115 (95%)	6 (5%)	22	48
2	H2	121/121 (100%)	120 (99%)	1 (1%)	73	77
2	H3	121/121 (100%)	119 (98%)	2 (2%)	53	67
2	I1	121/121 (100%)	120 (99%)	1 (1%)	73	77
2	J1	121/121 (100%)	119 (98%)	2 (2%)	53	67
2	J2	121/121 (100%)	119 (98%)	2 (2%)	53	67
2	J3	121/121 (100%)	117 (97%)	4 (3%)	33	58
2	L2	121/121 (100%)	120 (99%)	1 (1%)	73	77
2	L3	121/121 (100%)	120 (99%)	1 (1%)	73	77
2	N2	121/121 (100%)	121 (100%)	0	100	100
2	N3	121/121 (100%)	119 (98%)	2 (2%)	53	67
2	P2	121/121 (100%)	118 (98%)	3 (2%)	42	62
2	P3	121/121 (100%)	119 (98%)	2 (2%)	53	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	R2	121/121 (100%)	118 (98%)	3 (2%)	42	62
2	R3	121/121 (100%)	119 (98%)	2 (2%)	53	67
2	T2	121/121 (100%)	120 (99%)	1 (1%)	73	77
2	T3	121/121 (100%)	121 (100%)	0	100	100
2	V2	121/121 (100%)	121 (100%)	0	100	100
2	V3	121/121 (100%)	118 (98%)	3 (2%)	42	62
2	X2	121/121 (100%)	120 (99%)	1 (1%)	73	77
2	X3	121/121 (100%)	118 (98%)	3 (2%)	42	62
2	Z2	121/121 (100%)	120 (99%)	1 (1%)	73	77
2	Z3	121/121 (100%)	120 (99%)	1 (1%)	73	77
2	b2	121/121 (100%)	120 (99%)	1 (1%)	73	77
2	b3	121/121 (100%)	121 (100%)	0	100	100
2	d2	121/121 (100%)	116 (96%)	5 (4%)	27	52
2	d3	121/121 (100%)	119 (98%)	2 (2%)	53	67
2	f2	121/121 (100%)	119 (98%)	2 (2%)	53	67
2	f3	121/121 (100%)	120 (99%)	1 (1%)	73	77
2	g3	121/121 (100%)	116 (96%)	5 (4%)	27	52
2	h2	121/121 (100%)	118 (98%)	3 (2%)	42	62
2	h3	121/121 (100%)	114 (94%)	7 (6%)	18	44
2	j2	121/121 (100%)	118 (98%)	3 (2%)	42	62
2	l2	121/121 (100%)	117 (97%)	4 (3%)	33	58
2	n2	121/121 (100%)	116 (96%)	5 (4%)	27	52
2	p2	121/121 (100%)	120 (99%)	1 (1%)	73	77
2	r2	121/121 (100%)	117 (97%)	4 (3%)	33	58
2	t2	121/121 (100%)	117 (97%)	4 (3%)	33	58
2	v2	121/121 (100%)	117 (97%)	4 (3%)	33	58
3	K1	132/135 (98%)	123 (93%)	9 (7%)	14	40
3	L1	132/135 (98%)	122 (92%)	10 (8%)	12	38
4	M1	57/58 (98%)	51 (90%)	6 (10%)	6	24
4	i3	57/58 (98%)	55 (96%)	2 (4%)	32	56
4	w2	57/58 (98%)	52 (91%)	5 (9%)	9	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	x2	57/58 (98%)	55 (96%)	2 (4%)	32	56
4	y2	57/58 (98%)	56 (98%)	1 (2%)	51	67
4	z1	57/58 (98%)	53 (93%)	4 (7%)	14	39
4	z2	57/58 (98%)	56 (98%)	1 (2%)	51	67
4	z3	57/58 (98%)	55 (96%)	2 (4%)	32	56
5	j3	941/977 (96%)	912 (97%)	29 (3%)	35	59
5	k3	941/977 (96%)	913 (97%)	28 (3%)	36	60
All	All	13982/14128 (99%)	13615 (97%)	367 (3%)	41	61

5 of 367 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I3	104	ILE
2	d3	157	SER
1	K3	23	LEU
1	U3	32	SER
4	z3	23	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 88 such sidechains are listed below:

Mol	Chain	Res	Type
2	V3	110	ASN
5	j3	851	HIS
2	Z3	47	ASN
5	j3	26	ASN
5	k3	29	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

48 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	$\# Z > 2$
2	MEN	D3	71	2	7,8,9	0.92	0	4,9,11	1.03	0
2	MEN	B1	71	2	7,8,9	0.95	0	4,9,11	0.61	0
2	MEN	d3	71	2	7,8,9	0.91	0	4,9,11	0.93	0
2	MEN	R3	71	2	7,8,9	0.91	0	4,9,11	0.94	0
2	MEN	B3	71	2	7,8,9	0.90	0	4,9,11	1.10	0
2	MEN	J2	71	2	7,8,9	0.94	0	4,9,11	1.12	1 (25%)
2	MEN	v2	71	2	7,8,9	0.94	0	4,9,11	0.63	0
2	MEN	F1	71	2	7,8,9	0.93	0	4,9,11	0.78	0
2	MEN	l2	71	2	7,8,9	0.97	0	4,9,11	0.50	0
2	MEN	H3	71	2	7,8,9	0.92	0	4,9,11	0.80	0
2	MEN	L3	71	2	7,8,9	0.90	0	4,9,11	0.87	0
2	MEN	H2	71	2	7,8,9	0.91	0	4,9,11	0.92	0
2	MEN	Z3	71	2	7,8,9	0.92	0	4,9,11	0.95	0
2	MEN	j2	71	2	7,8,9	0.94	0	4,9,11	0.86	0
2	MEN	Z2	71	2	7,8,9	0.90	0	4,9,11	0.55	0
2	MEN	b3	71	2	7,8,9	0.94	0	4,9,11	0.70	0
2	MEN	B2	71	2	7,8,9	0.95	0	4,9,11	0.89	0
2	MEN	V2	71	2	7,8,9	0.90	0	4,9,11	0.80	0
2	MEN	J3	71	2	7,8,9	0.92	0	4,9,11	0.98	0
2	MEN	r2	71	2	7,8,9	0.96	0	4,9,11	0.97	0
2	MEN	N2	71	2	7,8,9	0.93	0	4,9,11	0.88	0
2	MEN	G1	71	2	7,8,9	0.92	0	4,9,11	1.06	0
2	MEN	L2	71	2	7,8,9	0.94	0	4,9,11	0.80	0
2	MEN	f2	71	2	7,8,9	0.96	0	4,9,11	0.71	0
2	MEN	g3	71	2	7,8,9	0.88	0	4,9,11	0.88	0
2	MEN	h3	71	2	7,8,9	0.90	0	4,9,11	0.94	0
2	MEN	D2	71	2	7,8,9	0.93	0	4,9,11	0.99	0
2	MEN	R2	71	2	7,8,9	0.90	0	4,9,11	0.76	0
2	MEN	T2	71	2	7,8,9	0.92	0	4,9,11	0.93	0
2	MEN	P2	71	2	7,8,9	0.99	0	4,9,11	0.96	0
2	MEN	h2	71	2	7,8,9	0.95	0	4,9,11	0.75	0
2	MEN	I1	71	2	7,8,9	0.95	0	4,9,11	0.83	0
2	MEN	n2	71	2	7,8,9	0.93	0	4,9,11	0.89	0
2	MEN	P3	71	2	7,8,9	0.92	0	4,9,11	0.74	0
2	MEN	D1	71	2	7,8,9	0.93	0	4,9,11	0.92	0
2	MEN	V3	71	2	7,8,9	0.92	0	4,9,11	0.56	0
2	MEN	J1	71	2	7,8,9	0.93	0	4,9,11	0.91	0
2	MEN	F3	71	2	7,8,9	0.92	0	4,9,11	0.87	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MEN	t2	71	2	7,8,9	0.91	0	4,9,11	0.89	0
2	MEN	F2	71	2	7,8,9	0.94	0	4,9,11	0.78	0
2	MEN	d2	71	2	7,8,9	0.96	0	4,9,11	0.96	0
2	MEN	b2	71	2	7,8,9	0.93	0	4,9,11	0.78	0
2	MEN	X2	71	2	7,8,9	0.90	0	4,9,11	0.85	0
2	MEN	T3	71	2	7,8,9	0.94	0	4,9,11	0.92	0
2	MEN	X3	71	2	7,8,9	0.89	0	4,9,11	0.99	0
2	MEN	f3	71	2	7,8,9	0.95	0	4,9,11	0.69	0
2	MEN	N3	71	2	7,8,9	0.92	0	4,9,11	0.95	0
2	MEN	p2	71	2	7,8,9	0.92	0	4,9,11	0.74	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
2	MEN	D3	71	2	-	1/7/8/10	-
2	MEN	B1	71	2	-	2/7/8/10	-
2	MEN	d3	71	2	-	1/7/8/10	-
2	MEN	R3	71	2	-	0/7/8/10	-
2	MEN	B3	71	2	-	0/7/8/10	-
2	MEN	J2	71	2	-	1/7/8/10	-
2	MEN	v2	71	2	-	0/7/8/10	-
2	MEN	F1	71	2	-	4/7/8/10	-
2	MEN	l2	71	2	-	2/7/8/10	-
2	MEN	H3	71	2	-	0/7/8/10	-
2	MEN	L3	71	2	-	2/7/8/10	-
2	MEN	H2	71	2	-	0/7/8/10	-
2	MEN	Z3	71	2	-	2/7/8/10	-
2	MEN	j2	71	2	-	2/7/8/10	-
2	MEN	Z2	71	2	-	3/7/8/10	-
2	MEN	b3	71	2	-	0/7/8/10	-
2	MEN	B2	71	2	-	0/7/8/10	-
2	MEN	V2	71	2	-	2/7/8/10	-
2	MEN	J3	71	2	-	2/7/8/10	-
2	MEN	r2	71	2	-	0/7/8/10	-
2	MEN	N2	71	2	-	0/7/8/10	-
2	MEN	G1	71	2	-	2/7/8/10	-
2	MEN	L2	71	2	-	2/7/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MEN	f2	71	2	-	3/7/8/10	-
2	MEN	g3	71	2	-	5/7/8/10	-
2	MEN	h3	71	2	-	5/7/8/10	-
2	MEN	D2	71	2	-	0/7/8/10	-
2	MEN	R2	71	2	-	0/7/8/10	-
2	MEN	T2	71	2	-	0/7/8/10	-
2	MEN	P2	71	2	-	1/7/8/10	-
2	MEN	h2	71	2	-	2/7/8/10	-
2	MEN	I1	71	2	-	2/7/8/10	-
2	MEN	n2	71	2	-	1/7/8/10	-
2	MEN	P3	71	2	-	2/7/8/10	-
2	MEN	D1	71	2	-	3/7/8/10	-
2	MEN	V3	71	2	-	0/7/8/10	-
2	MEN	J1	71	2	-	2/7/8/10	-
2	MEN	F3	71	2	-	3/7/8/10	-
2	MEN	t2	71	2	-	2/7/8/10	-
2	MEN	F2	71	2	-	3/7/8/10	-
2	MEN	d2	71	2	-	2/7/8/10	-
2	MEN	b2	71	2	-	2/7/8/10	-
2	MEN	X2	71	2	-	0/7/8/10	-
2	MEN	T3	71	2	-	1/7/8/10	-
2	MEN	X3	71	2	-	0/7/8/10	-
2	MEN	f3	71	2	-	3/7/8/10	-
2	MEN	N3	71	2	-	0/7/8/10	-
2	MEN	p2	71	2	-	2/7/8/10	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J2	71	MEN	CB-CG-ND2	2.04	118.20	115.53

There are no chirality outliers.

5 of 72 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B1	71	MEN	C-CA-CB-CG
2	D1	71	MEN	O-C-CA-CB

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Mol	Chain	Res	Type	Atoms
2	F1	71	MEN	C-CA-CB-CG
2	G1	71	MEN	C-CA-CB-CG
2	F2	71	MEN	O-C-CA-CB

There are no ring outliers.

27 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D3	71	MEN	1	0
2	B1	71	MEN	1	0
2	d3	71	MEN	1	0
2	R3	71	MEN	1	0
2	B3	71	MEN	1	0
2	v2	71	MEN	3	0
2	F1	71	MEN	1	0
2	L3	71	MEN	1	0
2	Z3	71	MEN	1	0
2	j2	71	MEN	1	0
2	b3	71	MEN	1	0
2	V2	71	MEN	1	0
2	G1	71	MEN	1	0
2	R2	71	MEN	1	0
2	P2	71	MEN	1	0
2	I1	71	MEN	1	0
2	D1	71	MEN	1	0
2	J1	71	MEN	1	0
2	F3	71	MEN	1	0
2	t2	71	MEN	1	0
2	d2	71	MEN	1	0
2	b2	71	MEN	1	0
2	X2	71	MEN	2	0
2	T3	71	MEN	1	0
2	X3	71	MEN	1	0
2	N3	71	MEN	1	0
2	p2	71	MEN	3	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

96 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
6	CYC	p2	201	2	46,46,46	0.82	1 (2%)	63,67,67	1.29	6 (9%)
6	CYC	Q2	201	1	46,46,46	0.81	1 (2%)	63,67,67	1.44	5 (7%)
6	CYC	H2	201	2	46,46,46	0.82	1 (2%)	63,67,67	1.37	4 (6%)
6	CYC	E3	201	1	46,46,46	0.81	1 (2%)	63,67,67	1.43	6 (9%)
6	CYC	F2	201	2	46,46,46	0.82	1 (2%)	63,67,67	1.31	5 (7%)
6	CYC	X2	201	2	46,46,46	0.84	1 (2%)	63,67,67	1.39	5 (7%)
6	CYC	I3	201	1	46,46,46	0.82	1 (2%)	63,67,67	1.39	5 (7%)
6	CYC	h2	201	2	46,46,46	0.83	1 (2%)	63,67,67	1.30	4 (6%)
6	CYC	C3	201	1	46,46,46	0.82	1 (2%)	63,67,67	1.40	5 (7%)
6	CYC	N3	201	2	46,46,46	0.83	1 (2%)	63,67,67	1.40	5 (7%)
6	CYC	P2	201	2	46,46,46	0.85	1 (2%)	63,67,67	1.40	5 (7%)
6	CYC	z1	101	2	46,46,46	0.83	1 (2%)	63,67,67	1.40	6 (9%)
6	CYC	g3	201	2	46,46,46	0.82	1 (2%)	63,67,67	1.38	5 (7%)
6	CYC	k3	1205	2	46,46,46	0.84	1 (2%)	63,67,67	1.33	5 (7%)
6	CYC	j3	1206	-	46,46,46	0.89	2 (4%)	63,67,67	1.24	7 (11%)
6	CYC	y2	101	2	46,46,46	0.86	1 (2%)	63,67,67	1.37	7 (11%)
6	CYC	R3	201	2	46,46,46	0.82	0	63,67,67	1.30	5 (7%)
6	CYC	K2	201	1	46,46,46	0.82	1 (2%)	63,67,67	1.37	5 (7%)
6	CYC	S2	201	1	46,46,46	0.81	1 (2%)	63,67,67	1.44	5 (7%)
6	CYC	Q3	201	1	46,46,46	0.82	1 (2%)	63,67,67	1.43	5 (7%)
6	CYC	M2	201	1	46,46,46	0.83	1 (2%)	63,67,67	1.44	5 (7%)
6	CYC	T2	201	2	46,46,46	0.88	2 (4%)	63,67,67	1.30	5 (7%)
6	CYC	L3	201	2	46,46,46	0.81	1 (2%)	63,67,67	1.39	6 (9%)
6	CYC	V2	201	2	46,46,46	0.84	1 (2%)	63,67,67	1.37	6 (9%)
6	CYC	G2	201	1	46,46,46	0.83	1 (2%)	63,67,67	1.42	5 (7%)
6	CYC	V3	201	2	46,46,46	0.81	1 (2%)	63,67,67	1.39	5 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	CYC	a2	201	1	46,46,46	0.81	1 (2%)	63,67,67	1.40	5 (7%)
6	CYC	U2	201	1	46,46,46	0.82	1 (2%)	63,67,67	1.42	5 (7%)
6	CYC	Y2	201	1	46,46,46	0.84	1 (2%)	63,67,67	1.44	5 (7%)
6	CYC	I2	201	1	46,46,46	0.82	1 (2%)	63,67,67	1.37	5 (7%)
6	CYC	B2	201	2	46,46,46	0.83	1 (2%)	63,67,67	1.43	4 (6%)
6	CYC	L1	201	3	46,46,46	0.88	2 (4%)	63,67,67	1.38	5 (7%)
6	CYC	T3	201	2	46,46,46	0.83	2 (4%)	63,67,67	1.40	5 (7%)
6	CYC	k3	1206	2	46,46,46	0.81	1 (2%)	63,67,67	1.40	5 (7%)
6	CYC	j3	1202	2	46,46,46	0.94	1 (2%)	63,67,67	1.44	8 (12%)
6	CYC	q2	201	1	46,46,46	0.81	1 (2%)	63,67,67	1.30	6 (9%)
6	CYC	W2	201	1	46,46,46	0.81	1 (2%)	63,67,67	1.42	6 (9%)
6	CYC	k3	1207	-	46,46,46	0.91	3 (6%)	63,67,67	1.50	10 (15%)
6	CYC	j3	1201	2	46,46,46	0.84	1 (2%)	63,67,67	1.28	5 (7%)
6	CYC	j3	1203	2	46,46,46	0.88	2 (4%)	63,67,67	1.39	6 (9%)
6	CYC	J1	201	2	46,46,46	0.86	1 (2%)	63,67,67	1.44	5 (7%)
6	CYC	K1	201	3	46,46,46	0.86	2 (4%)	63,67,67	1.43	5 (7%)
6	CYC	d3	201	2	46,46,46	0.81	0	63,67,67	1.38	5 (7%)
6	CYC	k3	1202	2	46,46,46	0.77	0	63,67,67	1.35	6 (9%)
6	CYC	m2	201	1	46,46,46	0.83	1 (2%)	63,67,67	1.44	5 (7%)
6	CYC	j3	1204	2	46,46,46	0.90	2 (4%)	63,67,67	1.36	5 (7%)
6	CYC	a3	201	1	46,46,46	0.82	1 (2%)	63,67,67	1.37	5 (7%)
6	CYC	k3	1203	2	46,46,46	0.89	1 (2%)	63,67,67	1.46	7 (11%)
6	CYC	H1	201	1	46,46,46	0.83	1 (2%)	63,67,67	1.44	5 (7%)
6	CYC	o2	201	1	46,46,46	0.86	1 (2%)	63,67,67	1.39	5 (7%)
6	CYC	u2	201	1	46,46,46	0.86	1 (2%)	63,67,67	1.37	5 (7%)
6	CYC	h3	201	2	46,46,46	0.83	1 (2%)	63,67,67	1.39	4 (6%)
6	CYC	F3	201	2	46,46,46	0.80	1 (2%)	63,67,67	1.40	6 (9%)
6	CYC	E2	201	1	46,46,46	0.81	1 (2%)	63,67,67	1.37	5 (7%)
6	CYC	c2	201	1	46,46,46	0.82	1 (2%)	63,67,67	1.43	5 (7%)
6	CYC	E1	201	1	46,46,46	0.86	2 (4%)	63,67,67	1.44	5 (7%)
6	CYC	c3	201	1	46,46,46	0.83	1 (2%)	63,67,67	1.42	5 (7%)
6	CYC	M1	101	2	46,46,46	0.84	1 (2%)	63,67,67	1.35	5 (7%)
6	CYC	G3	201	-	46,46,46	0.88	2 (4%)	63,67,67	1.47	4 (6%)
6	CYC	J3	201	2	46,46,46	0.86	1 (2%)	63,67,67	1.42	5 (7%)
6	CYC	k3	1204	2	46,46,46	0.85	2 (4%)	63,67,67	1.15	3 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	CYC	O3	201	1	46,46,46	0.81	1 (2%)	63,67,67	1.41	6 (9%)
6	CYC	A1	201	1	46,46,46	0.85	1 (2%)	63,67,67	1.41	5 (7%)
6	CYC	g2	201	1	46,46,46	0.81	1 (2%)	63,67,67	1.42	5 (7%)
6	CYC	j3	1205	2	46,46,46	0.85	1 (2%)	63,67,67	1.35	5 (7%)
6	CYC	N2	201	2	46,46,46	0.84	1 (2%)	63,67,67	1.32	5 (7%)
6	CYC	Y3	201	1	46,46,46	0.83	1 (2%)	63,67,67	1.44	5 (7%)
6	CYC	L2	201	2	46,46,46	0.82	1 (2%)	63,67,67	1.31	5 (7%)
6	CYC	f3	201	2	46,46,46	0.84	1 (2%)	63,67,67	1.30	5 (7%)
6	CYC	S3	201	1	46,46,46	0.82	1 (2%)	63,67,67	1.42	5 (7%)
6	CYC	D3	201	2	46,46,46	0.88	1 (2%)	63,67,67	1.38	5 (7%)
6	CYC	O2	201	1	46,46,46	0.81	1 (2%)	63,67,67	1.38	5 (7%)
6	CYC	C1	201	1	46,46,46	0.83	1 (2%)	63,67,67	1.45	5 (7%)
6	CYC	v2	201	2	46,46,46	0.82	1 (2%)	63,67,67	1.38	6 (9%)
6	CYC	b2	201	2	46,46,46	0.84	1 (2%)	63,67,67	1.27	5 (7%)
6	CYC	H3	201	2	46,46,46	0.84	1 (2%)	63,67,67	1.32	5 (7%)
6	CYC	W3	201	1	46,46,46	0.82	1 (2%)	63,67,67	1.45	6 (9%)
6	CYC	b3	201	2	46,46,46	0.83	1 (2%)	63,67,67	1.28	5 (7%)
6	CYC	U3	201	1	46,46,46	0.81	1 (2%)	63,67,67	1.41	6 (9%)
6	CYC	x2	101	2	46,46,46	0.83	1 (2%)	63,67,67	1.31	6 (9%)
6	CYC	k3	1201	2	46,46,46	1.11	3 (6%)	63,67,67	1.28	5 (7%)
6	CYC	e3	201	1	46,46,46	0.83	1 (2%)	63,67,67	1.37	5 (7%)
6	CYC	A2	201	1	46,46,46	0.83	1 (2%)	63,67,67	1.42	5 (7%)
6	CYC	K3	201	1	46,46,46	0.82	1 (2%)	63,67,67	1.43	6 (9%)
6	CYC	M3	201	1	46,46,46	0.81	1 (2%)	63,67,67	1.38	5 (7%)
6	CYC	R2	201	2	46,46,46	0.81	0	63,67,67	1.38	5 (7%)
6	CYC	i2	201	1	46,46,46	0.80	1 (2%)	63,67,67	1.39	5 (7%)
6	CYC	z3	101	2	46,46,46	0.85	2 (4%)	63,67,67	1.25	6 (9%)
6	CYC	k2	201	1	46,46,46	0.86	2 (4%)	63,67,67	1.40	4 (6%)
6	CYC	F1	201	2	46,46,46	0.84	1 (2%)	63,67,67	1.45	5 (7%)
6	CYC	Z3	201	2	46,46,46	0.80	0	63,67,67	1.36	5 (7%)
6	CYC	A3	201	-	46,46,46	0.89	2 (4%)	63,67,67	1.49	4 (6%)
6	CYC	s2	201	1	46,46,46	0.83	1 (2%)	63,67,67	1.41	5 (7%)
6	CYC	X3	201	2	46,46,46	0.83	0	63,67,67	1.31	5 (7%)
6	CYC	e2	201	1	46,46,46	0.83	1 (2%)	63,67,67	1.41	5 (7%)
6	CYC	C2	201	1	46,46,46	0.81	1 (2%)	63,67,67	1.38	4 (6%)

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
6	CYC	p2	201	2	-	10/26/74/74	0/4/4/4
6	CYC	Q2	201	1	-	6/26/74/74	0/4/4/4
6	CYC	H2	201	2	-	8/26/74/74	0/4/4/4
6	CYC	E3	201	1	-	6/26/74/74	0/4/4/4
6	CYC	F2	201	2	-	10/26/74/74	0/4/4/4
6	CYC	X2	201	2	-	10/26/74/74	0/4/4/4
6	CYC	I3	201	1	-	6/26/74/74	0/4/4/4
6	CYC	h2	201	2	-	10/26/74/74	0/4/4/4
6	CYC	C3	201	1	-	6/26/74/74	0/4/4/4
6	CYC	N3	201	2	-	10/26/74/74	0/4/4/4
6	CYC	P2	201	2	-	10/26/74/74	0/4/4/4
6	CYC	z1	101	2	-	10/26/74/74	0/4/4/4
6	CYC	g3	201	2	-	11/26/74/74	0/4/4/4
6	CYC	k3	1205	2	-	10/26/74/74	0/4/4/4
6	CYC	j3	1206	-	-	6/26/74/74	0/4/4/4
6	CYC	y2	101	2	-	10/26/74/74	0/4/4/4
6	CYC	R3	201	2	-	10/26/74/74	0/4/4/4
6	CYC	K2	201	1	-	6/26/74/74	0/4/4/4
6	CYC	S2	201	1	-	6/26/74/74	0/4/4/4
6	CYC	Q3	201	1	-	9/26/74/74	0/4/4/4
6	CYC	M2	201	1	-	6/26/74/74	0/4/4/4
6	CYC	T2	201	2	-	10/26/74/74	0/4/4/4
6	CYC	L3	201	2	-	10/26/74/74	0/4/4/4
6	CYC	V2	201	2	-	10/26/74/74	0/4/4/4
6	CYC	G2	201	1	-	6/26/74/74	0/4/4/4
6	CYC	V3	201	2	-	8/26/74/74	0/4/4/4
6	CYC	a2	201	1	-	6/26/74/74	0/4/4/4
6	CYC	U2	201	1	-	6/26/74/74	0/4/4/4
6	CYC	Y2	201	1	-	6/26/74/74	0/4/4/4
6	CYC	I2	201	1	-	6/26/74/74	0/4/4/4
6	CYC	B2	201	2	-	10/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	CYC	L1	201	3	-	6/26/74/74	0/4/4/4
6	CYC	T3	201	2	-	10/26/74/74	0/4/4/4
6	CYC	k3	1206	2	-	8/26/74/74	0/4/4/4
6	CYC	j3	1202	2	-	9/26/74/74	0/4/4/4
6	CYC	q2	201	1	-	6/26/74/74	0/4/4/4
6	CYC	W2	201	1	-	6/26/74/74	0/4/4/4
6	CYC	k3	1207	-	-	6/26/74/74	0/4/4/4
6	CYC	j3	1201	2	-	10/26/74/74	0/4/4/4
6	CYC	j3	1203	2	-	8/26/74/74	0/4/4/4
6	CYC	J1	201	2	-	10/26/74/74	0/4/4/4
6	CYC	K1	201	3	-	6/26/74/74	0/4/4/4
6	CYC	d3	201	2	-	10/26/74/74	0/4/4/4
6	CYC	k3	1202	2	-	6/26/74/74	0/4/4/4
6	CYC	m2	201	1	-	6/26/74/74	0/4/4/4
6	CYC	j3	1204	2	-	9/26/74/74	0/4/4/4
6	CYC	a3	201	1	-	6/26/74/74	0/4/4/4
6	CYC	k3	1203	2	-	8/26/74/74	0/4/4/4
6	CYC	H1	201	1	-	6/26/74/74	0/4/4/4
6	CYC	o2	201	1	-	6/26/74/74	0/4/4/4
6	CYC	u2	201	1	-	6/26/74/74	0/4/4/4
6	CYC	h3	201	2	-	10/26/74/74	0/4/4/4
6	CYC	F3	201	2	-	10/26/74/74	0/4/4/4
6	CYC	E2	201	1	-	6/26/74/74	0/4/4/4
6	CYC	c2	201	1	-	6/26/74/74	0/4/4/4
6	CYC	E1	201	1	-	6/26/74/74	0/4/4/4
6	CYC	c3	201	1	-	6/26/74/74	0/4/4/4
6	CYC	M1	101	2	-	10/26/74/74	0/4/4/4
6	CYC	G3	201	-	-	6/26/74/74	0/4/4/4
6	CYC	J3	201	2	-	10/26/74/74	0/4/4/4
6	CYC	k3	1204	2	-	10/26/74/74	0/4/4/4
6	CYC	O3	201	1	-	6/26/74/74	0/4/4/4
6	CYC	A1	201	1	-	6/26/74/74	0/4/4/4
6	CYC	g2	201	1	-	6/26/74/74	0/4/4/4
6	CYC	j3	1205	2	-	10/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	CYC	N2	201	2	-	10/26/74/74	0/4/4/4
6	CYC	Y3	201	1	-	6/26/74/74	0/4/4/4
6	CYC	L2	201	2	-	10/26/74/74	0/4/4/4
6	CYC	f3	201	2	-	10/26/74/74	0/4/4/4
6	CYC	S3	201	1	-	6/26/74/74	0/4/4/4
6	CYC	D3	201	2	-	12/26/74/74	0/4/4/4
6	CYC	O2	201	1	-	6/26/74/74	0/4/4/4
6	CYC	C1	201	1	-	6/26/74/74	0/4/4/4
6	CYC	v2	201	2	-	11/26/74/74	0/4/4/4
6	CYC	b2	201	2	-	11/26/74/74	0/4/4/4
6	CYC	H3	201	2	-	10/26/74/74	0/4/4/4
6	CYC	W3	201	1	-	6/26/74/74	0/4/4/4
6	CYC	b3	201	2	-	10/26/74/74	0/4/4/4
6	CYC	U3	201	1	-	6/26/74/74	0/4/4/4
6	CYC	x2	101	2	-	10/26/74/74	0/4/4/4
6	CYC	k3	1201	2	-	8/26/74/74	0/4/4/4
6	CYC	e3	201	1	-	6/26/74/74	0/4/4/4
6	CYC	A2	201	1	-	6/26/74/74	0/4/4/4
6	CYC	K3	201	1	-	6/26/74/74	0/4/4/4
6	CYC	M3	201	1	-	6/26/74/74	0/4/4/4
6	CYC	R2	201	2	-	10/26/74/74	0/4/4/4
6	CYC	i2	201	1	-	6/26/74/74	0/4/4/4
6	CYC	z3	101	2	-	10/26/74/74	0/4/4/4
6	CYC	k2	201	1	-	6/26/74/74	0/4/4/4
6	CYC	F1	201	2	-	8/26/74/74	0/4/4/4
6	CYC	Z3	201	2	-	10/26/74/74	0/4/4/4
6	CYC	A3	201	-	-	6/26/74/74	0/4/4/4
6	CYC	s2	201	1	-	6/26/74/74	0/4/4/4
6	CYC	X3	201	2	-	10/26/74/74	0/4/4/4
6	CYC	e2	201	1	-	6/26/74/74	0/4/4/4
6	CYC	C2	201	1	-	6/26/74/74	0/4/4/4

The worst 5 of 107 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	k3	1201	CYC	CHD-C4C	4.22	1.43	1.36
6	j3	1202	CYC	C1B-C2B	-3.39	1.39	1.45
6	A3	201	CYC	CHD-C4C	2.94	1.41	1.36
6	k3	1201	CYC	CHD-C1D	2.93	1.47	1.40
6	j3	1206	CYC	CHD-C4C	2.91	1.41	1.36

The worst 5 of 501 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A3	201	CYC	C1D-CHD-C4C	6.89	139.53	127.76
6	G3	201	CYC	C1D-CHD-C4C	6.87	139.49	127.76
6	h3	201	CYC	C1D-CHD-C4C	6.83	139.43	127.76
6	g3	201	CYC	C1D-CHD-C4C	6.63	139.09	127.76
6	F1	201	CYC	C1D-CHD-C4C	6.49	138.84	127.76

There are no chirality outliers.

5 of 756 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A1	201	CYC	NA-C4A-CHB-C1B
6	A1	201	CYC	C3A-C4A-CHB-C1B
6	C1	201	CYC	NA-C4A-CHB-C1B
6	C1	201	CYC	C3A-C4A-CHB-C1B
6	F1	201	CYC	NA-C4A-CHB-C1B

There are no ring outliers.

95 monomers are involved in 524 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	p2	201	CYC	7	0
6	Q2	201	CYC	6	0
6	H2	201	CYC	7	0
6	E3	201	CYC	4	0
6	F2	201	CYC	2	0
6	X2	201	CYC	5	0
6	I3	201	CYC	5	0
6	h2	201	CYC	5	0
6	C3	201	CYC	5	0
6	N3	201	CYC	4	0
6	P2	201	CYC	2	0
6	z1	101	CYC	5	0
6	g3	201	CYC	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	k3	1205	CYC	10	0
6	j3	1206	CYC	1	0
6	y2	101	CYC	8	0
6	R3	201	CYC	3	0
6	K2	201	CYC	7	0
6	S2	201	CYC	8	0
6	Q3	201	CYC	5	0
6	M2	201	CYC	4	0
6	T2	201	CYC	6	0
6	L3	201	CYC	7	0
6	V2	201	CYC	3	0
6	G2	201	CYC	6	0
6	V3	201	CYC	5	0
6	a2	201	CYC	6	0
6	U2	201	CYC	3	0
6	Y2	201	CYC	5	0
6	I2	201	CYC	3	0
6	B2	201	CYC	4	0
6	L1	201	CYC	12	0
6	T3	201	CYC	3	0
6	k3	1206	CYC	3	0
6	j3	1202	CYC	5	0
6	q2	201	CYC	7	0
6	W2	201	CYC	7	0
6	j3	1201	CYC	11	0
6	j3	1203	CYC	6	0
6	J1	201	CYC	7	0
6	K1	201	CYC	10	0
6	d3	201	CYC	3	0
6	k3	1202	CYC	4	0
6	m2	201	CYC	5	0
6	j3	1204	CYC	9	0
6	a3	201	CYC	3	0
6	k3	1203	CYC	2	0
6	H1	201	CYC	7	0
6	o2	201	CYC	8	0
6	u2	201	CYC	8	0
6	h3	201	CYC	13	0
6	F3	201	CYC	5	0
6	E2	201	CYC	5	0
6	c2	201	CYC	4	0
6	E1	201	CYC	6	0

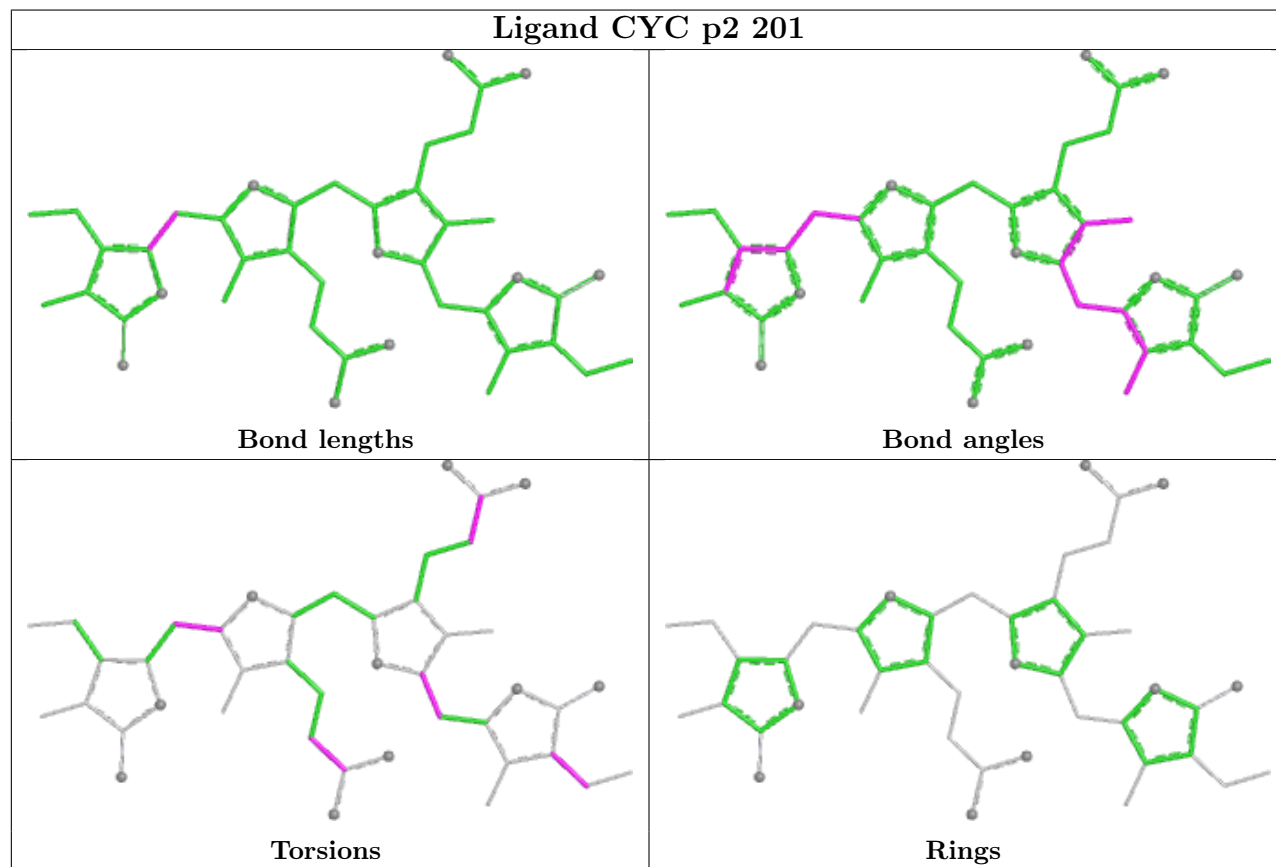
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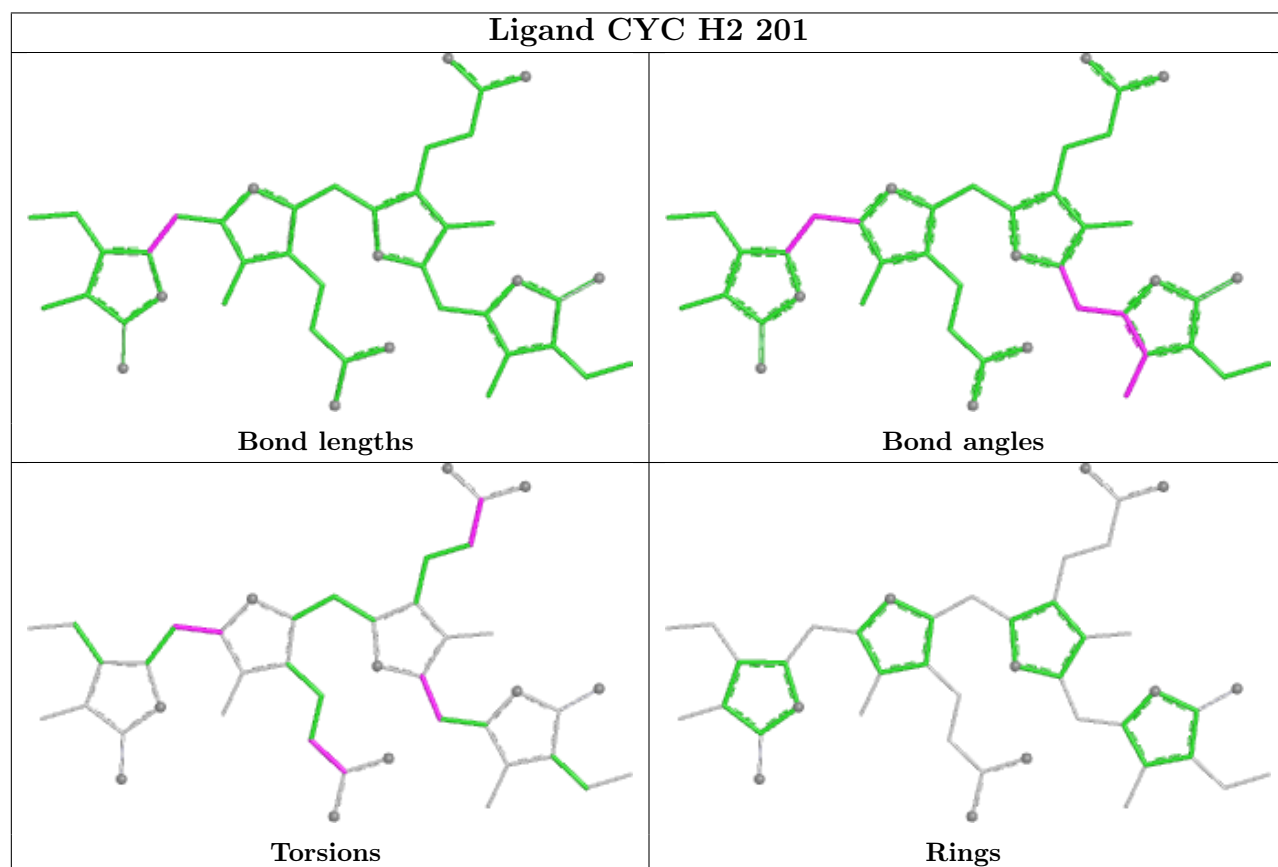
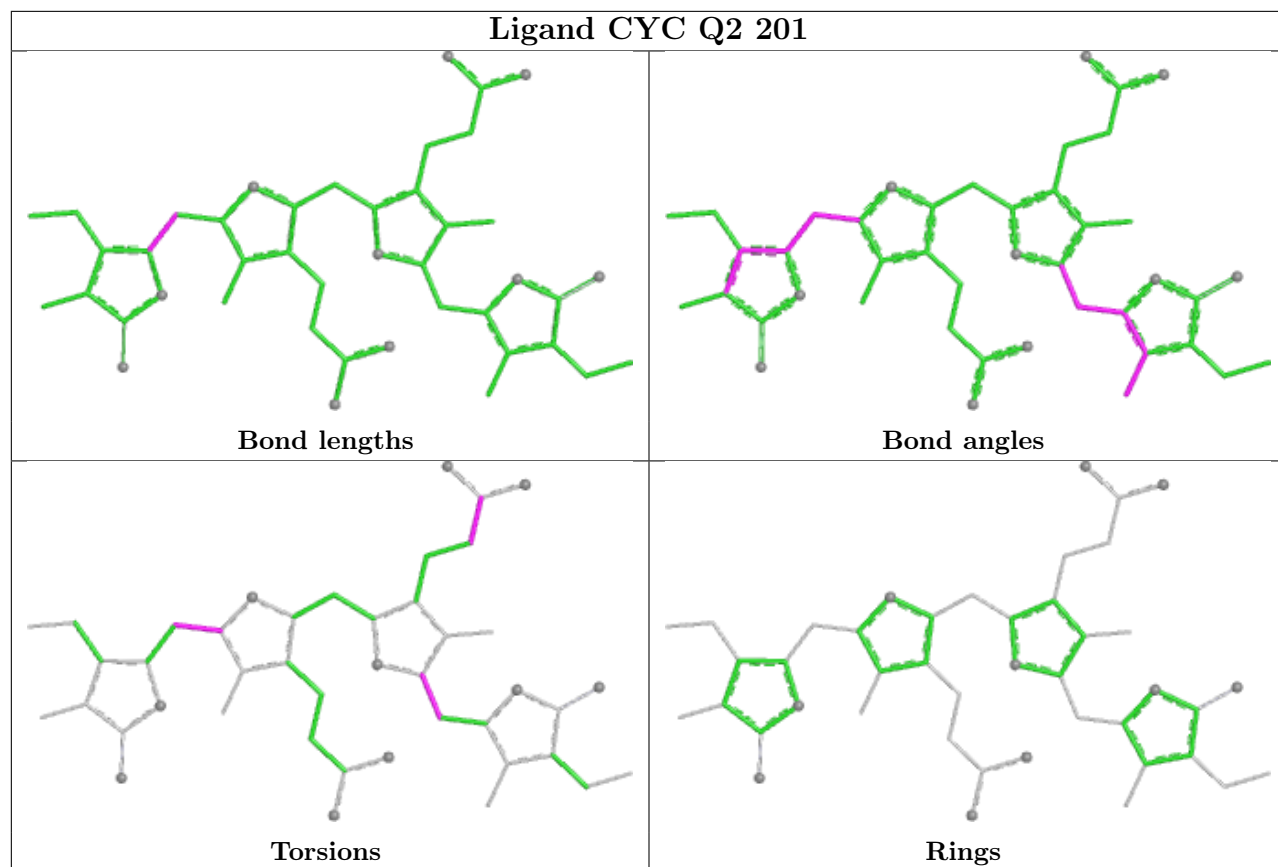
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	c3	201	CYC	5	0
6	M1	101	CYC	6	0
6	G3	201	CYC	9	0
6	J3	201	CYC	6	0
6	k3	1204	CYC	6	0
6	O3	201	CYC	6	0
6	A1	201	CYC	5	0
6	g2	201	CYC	4	0
6	j3	1205	CYC	9	0
6	N2	201	CYC	5	0
6	Y3	201	CYC	5	0
6	L2	201	CYC	2	0
6	f3	201	CYC	2	0
6	S3	201	CYC	4	0
6	D3	201	CYC	4	0
6	O2	201	CYC	3	0
6	C1	201	CYC	7	0
6	v2	201	CYC	7	0
6	b2	201	CYC	8	0
6	H3	201	CYC	11	0
6	W3	201	CYC	9	0
6	b3	201	CYC	1	0
6	U3	201	CYC	5	0
6	x2	101	CYC	7	0
6	k3	1201	CYC	3	0
6	e3	201	CYC	4	0
6	A2	201	CYC	7	0
6	K3	201	CYC	4	0
6	M3	201	CYC	4	0
6	R2	201	CYC	2	0
6	i2	201	CYC	4	0
6	z3	101	CYC	7	0
6	k2	201	CYC	5	0
6	F1	201	CYC	5	0
6	Z3	201	CYC	2	0
6	A3	201	CYC	10	0
6	s2	201	CYC	7	0
6	X3	201	CYC	3	0
6	e2	201	CYC	5	0
6	C2	201	CYC	4	0

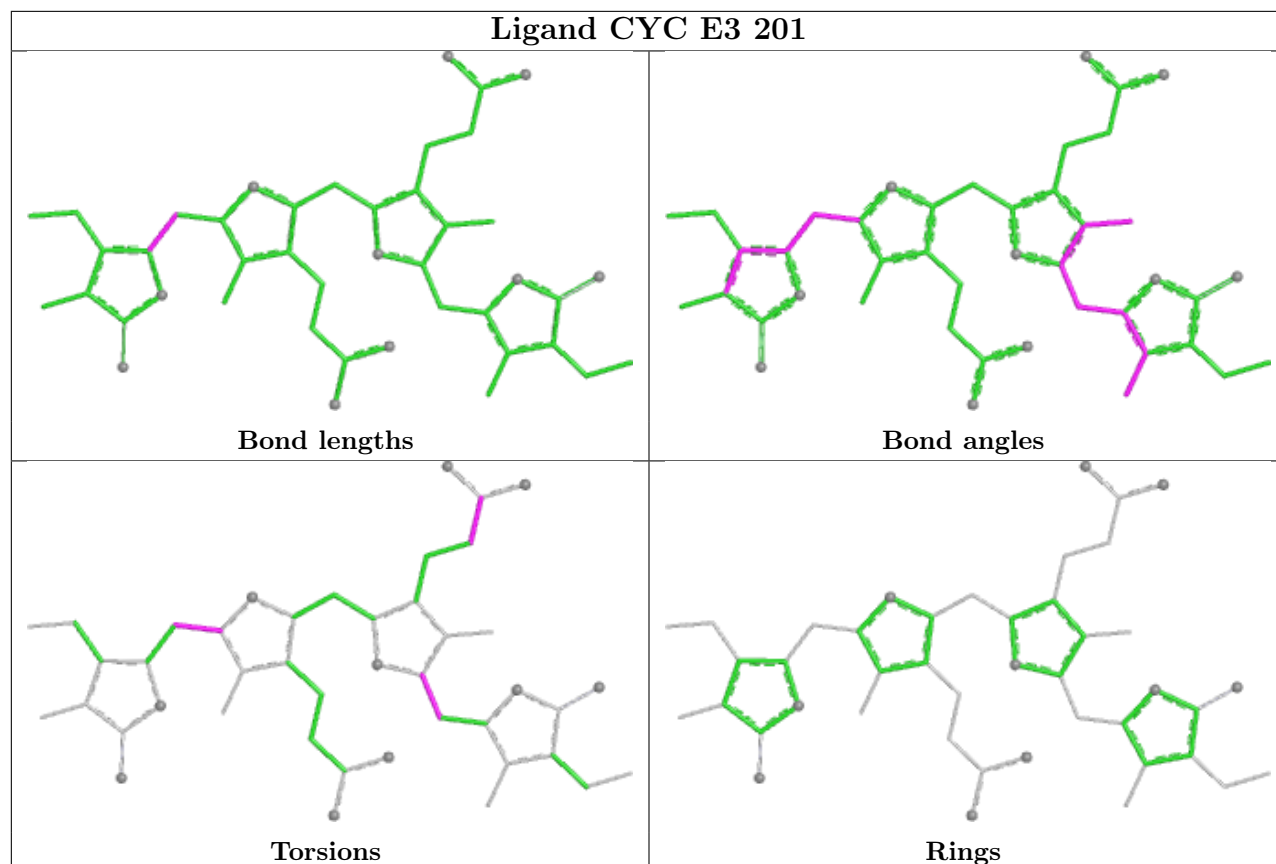
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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.

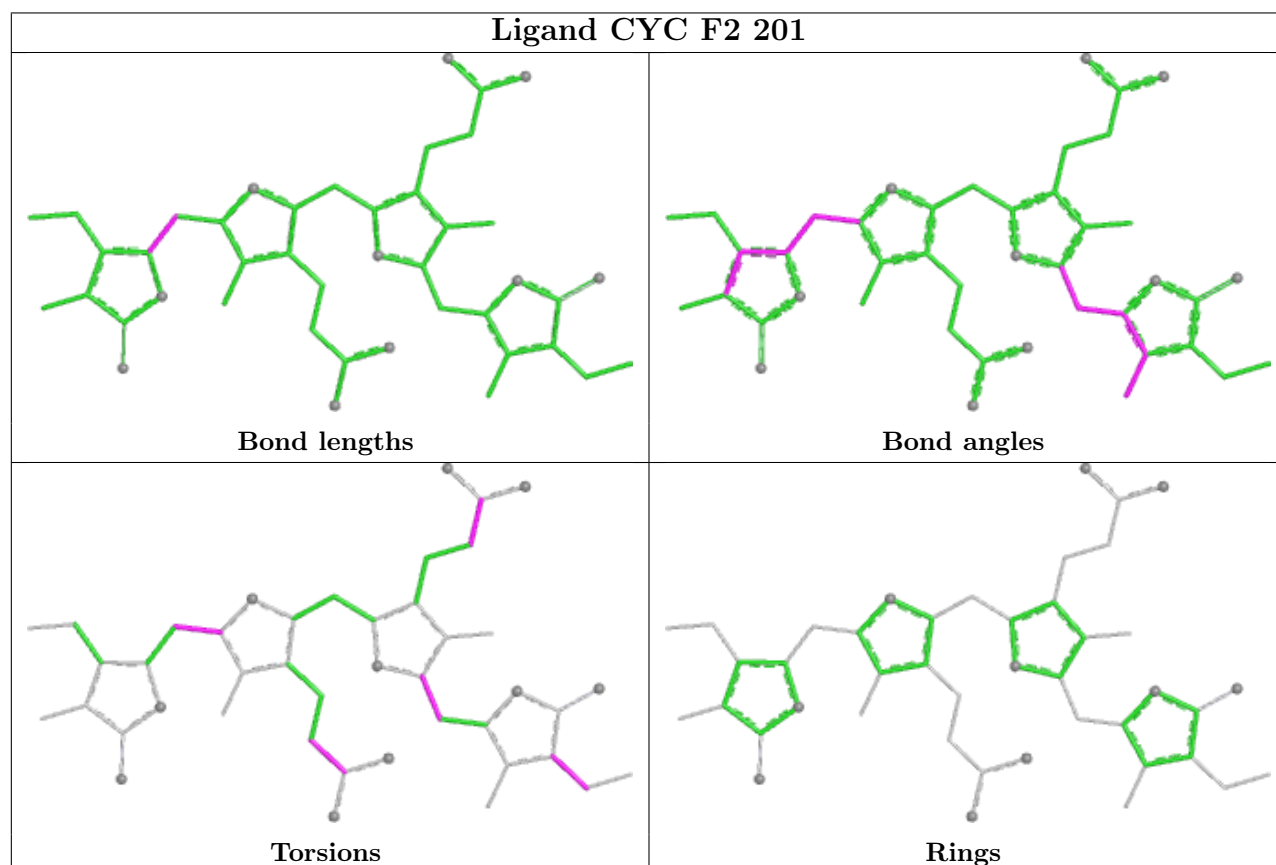




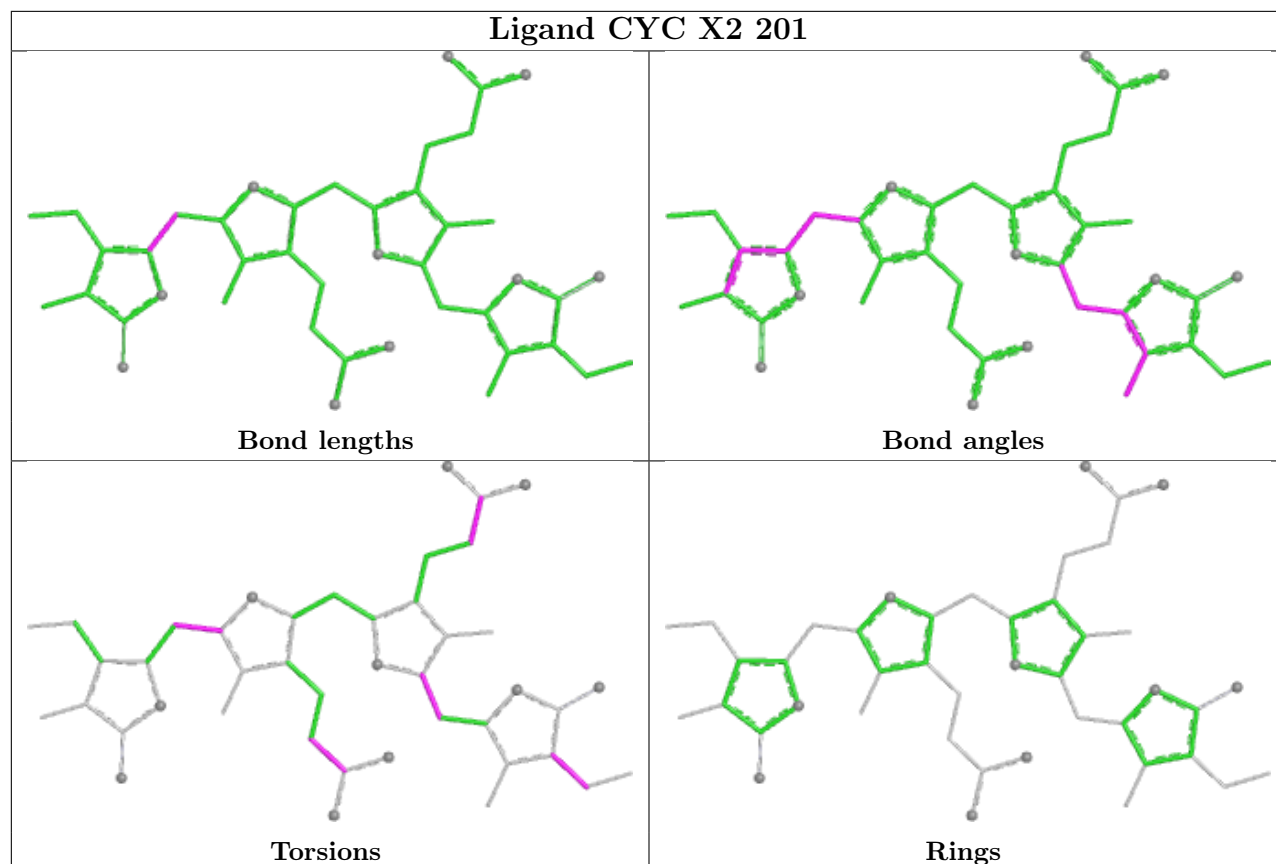
Ligand CYC E3 201



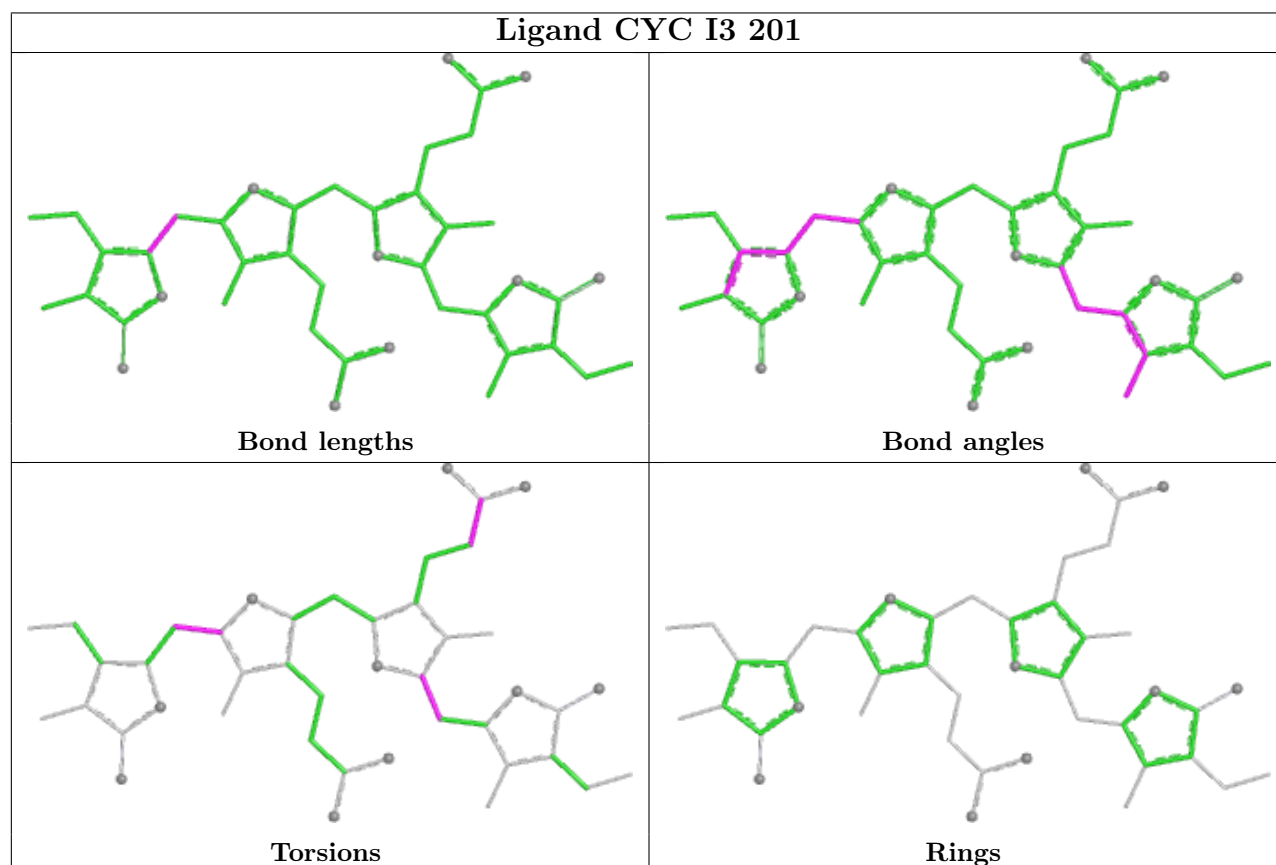
Ligand CYC F2 201

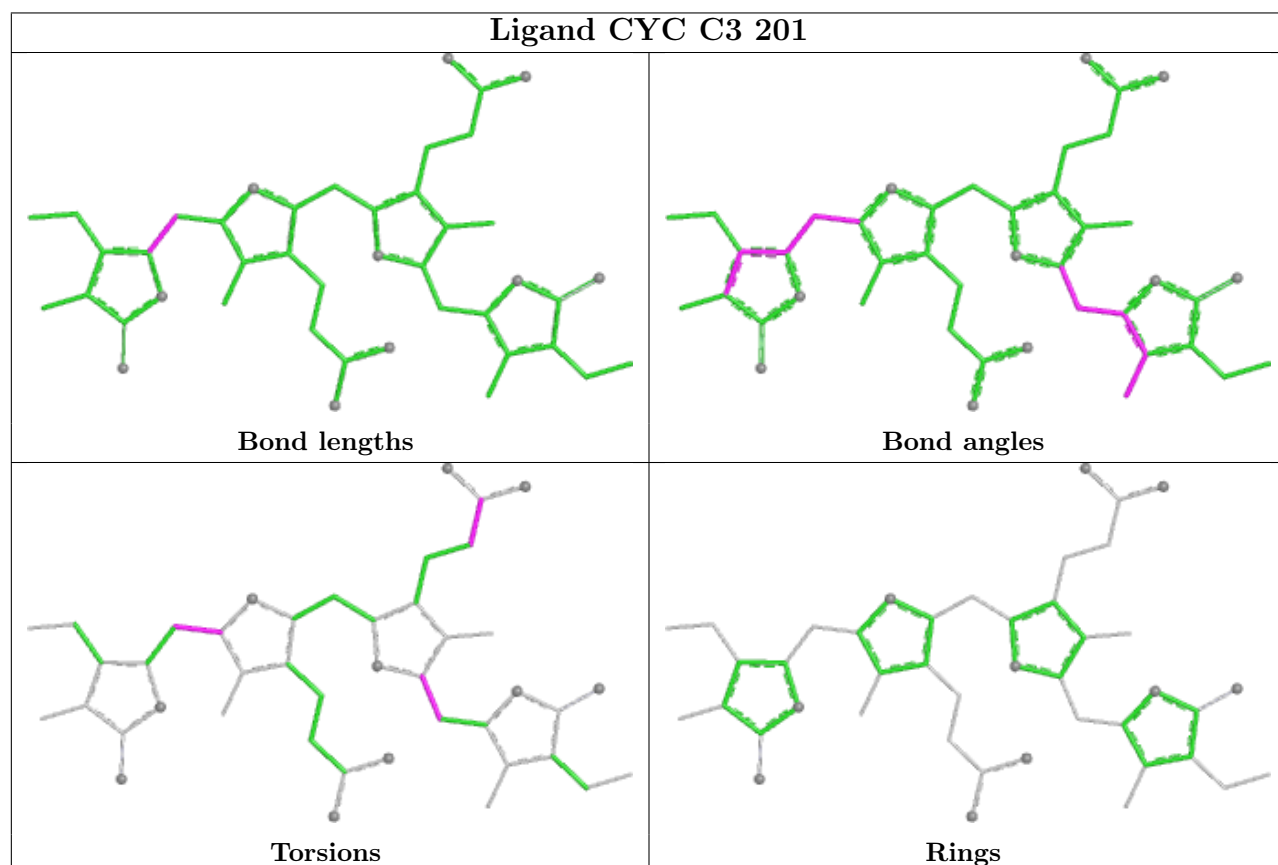
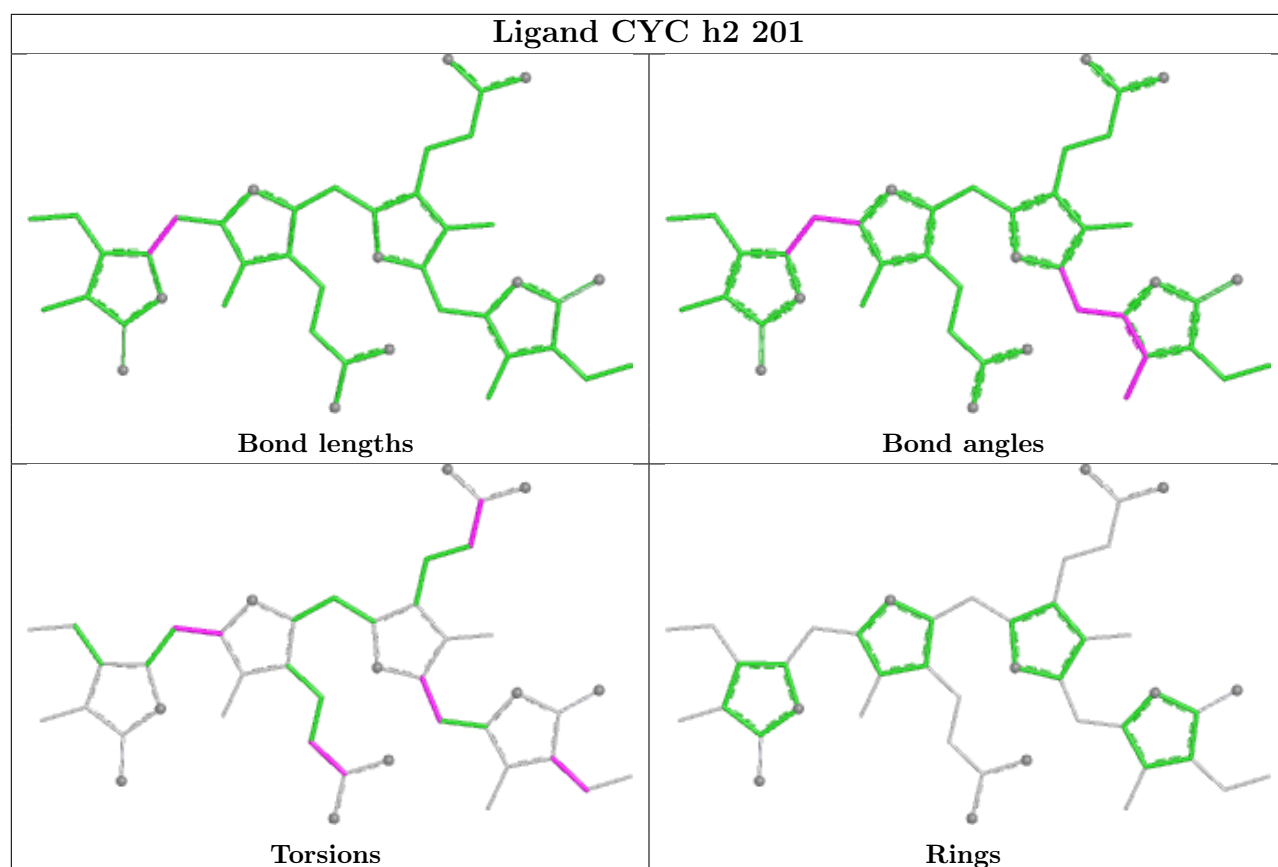


Ligand CYC X2 201

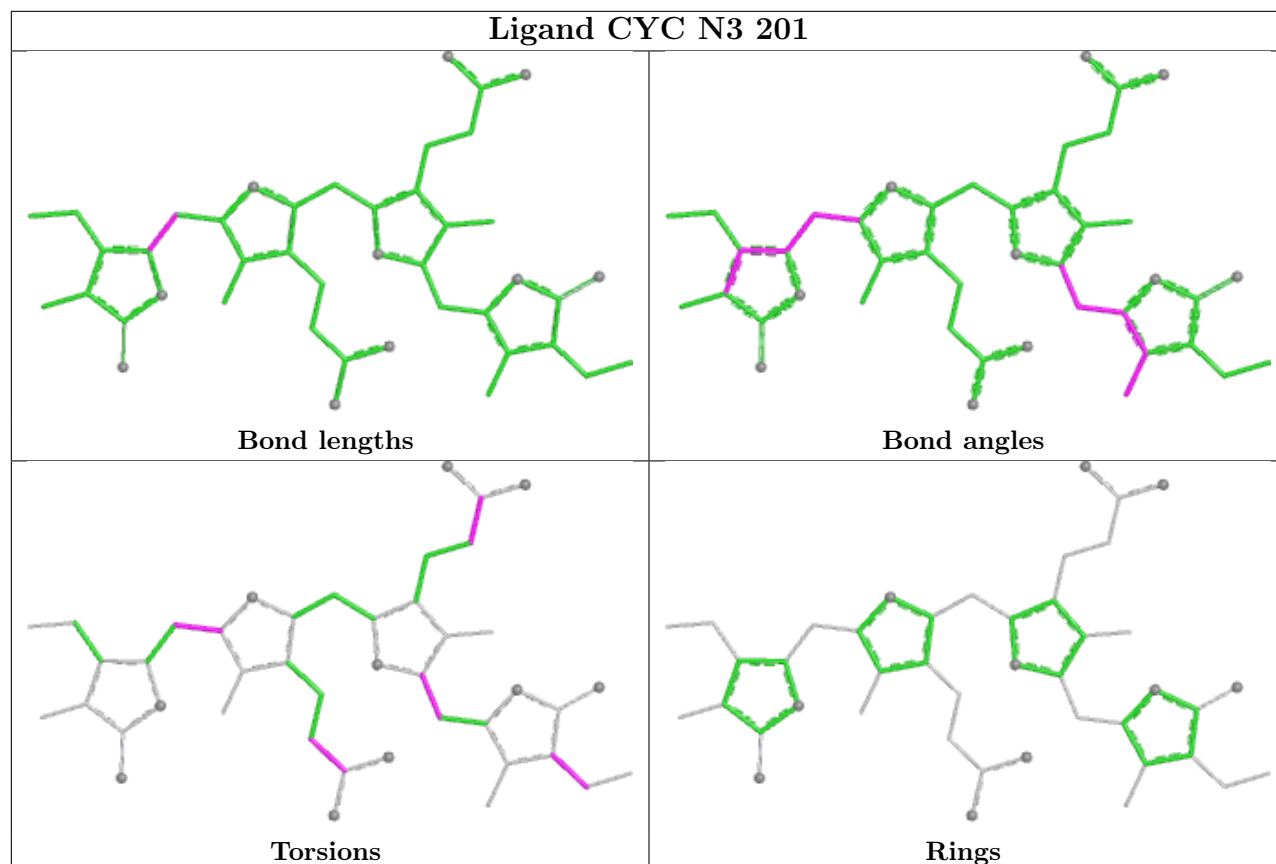


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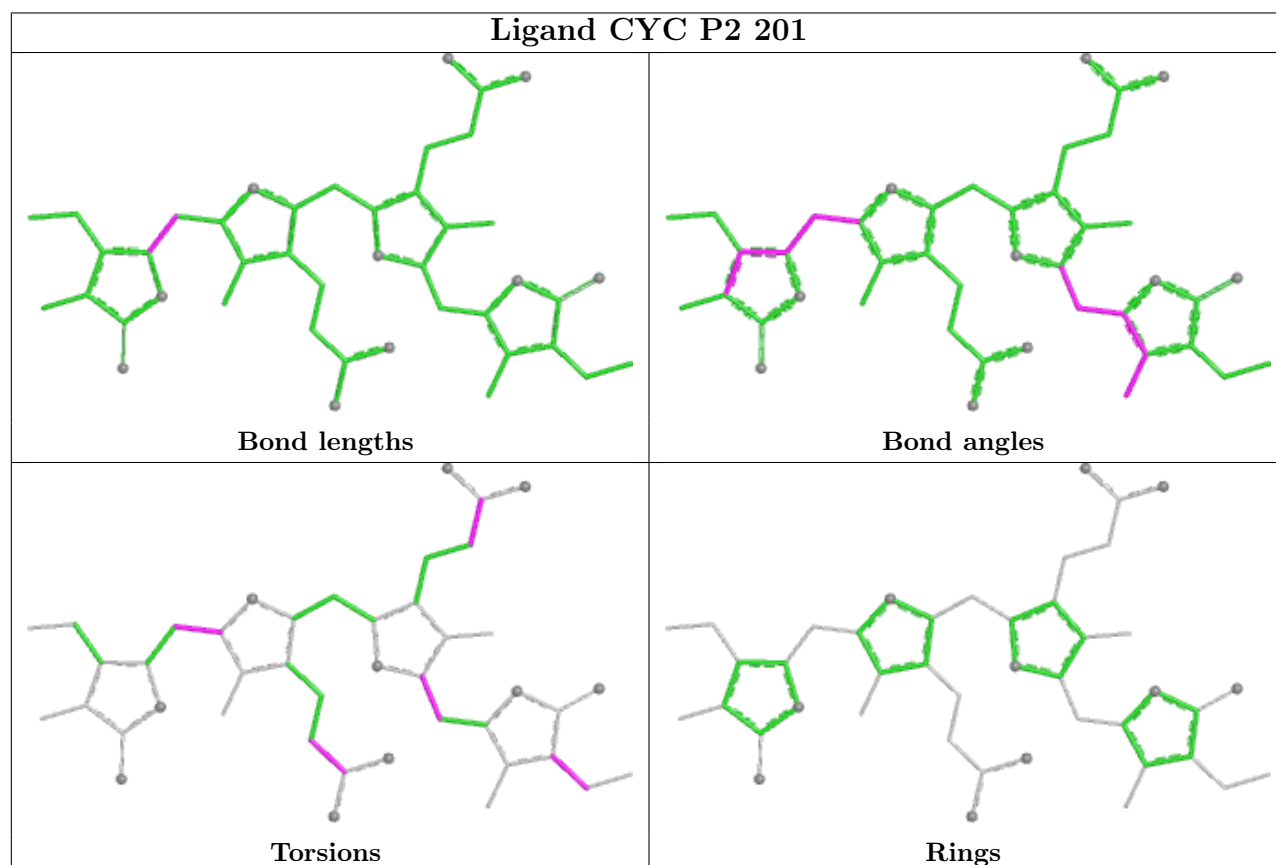


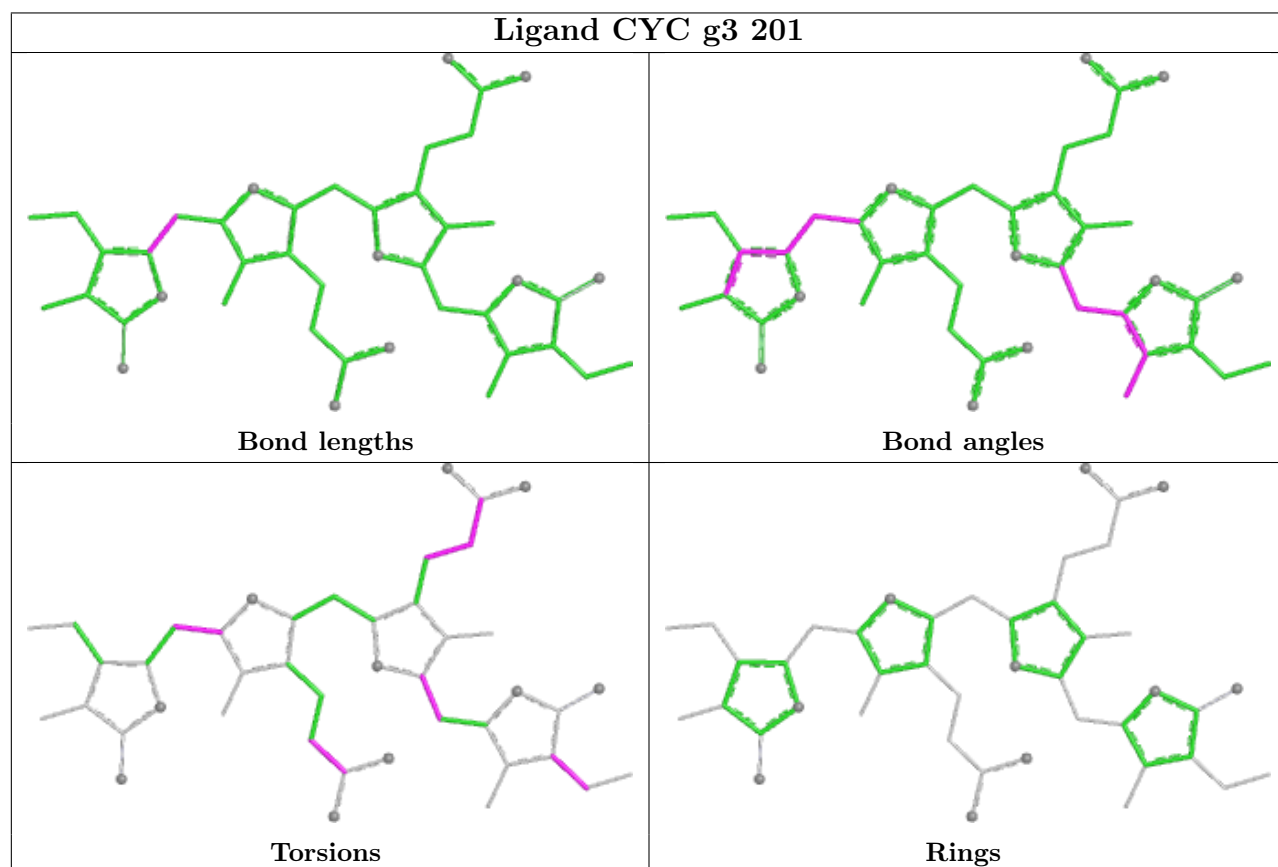
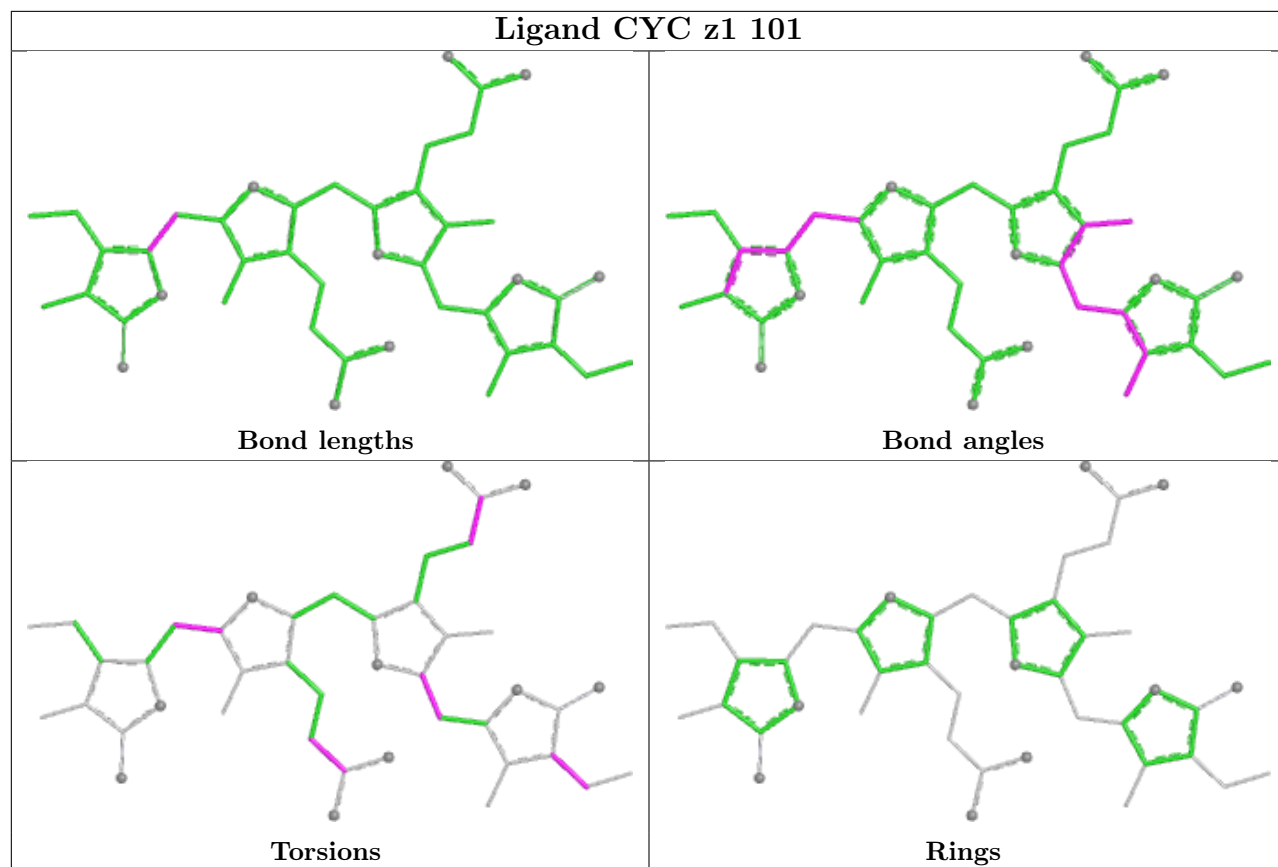


Ligand CYC N3 201

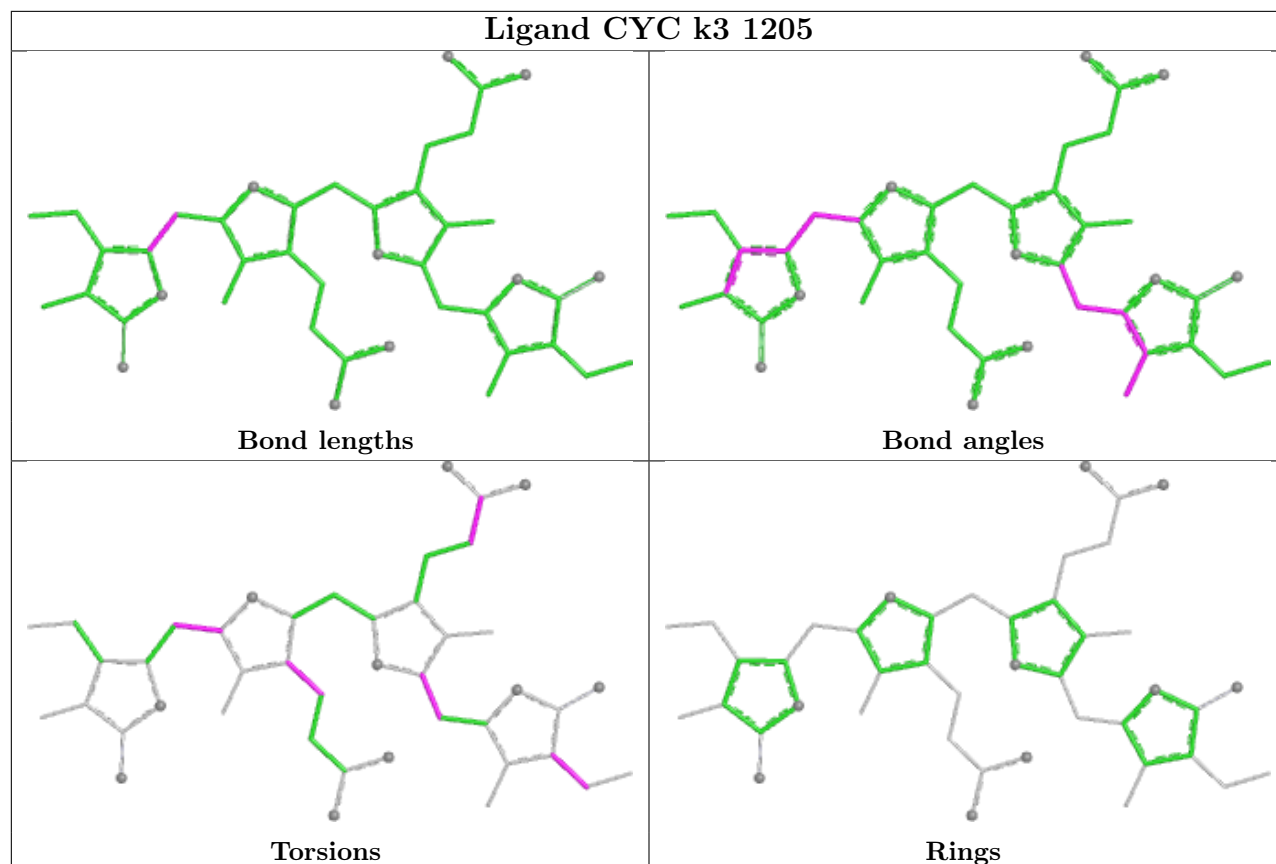


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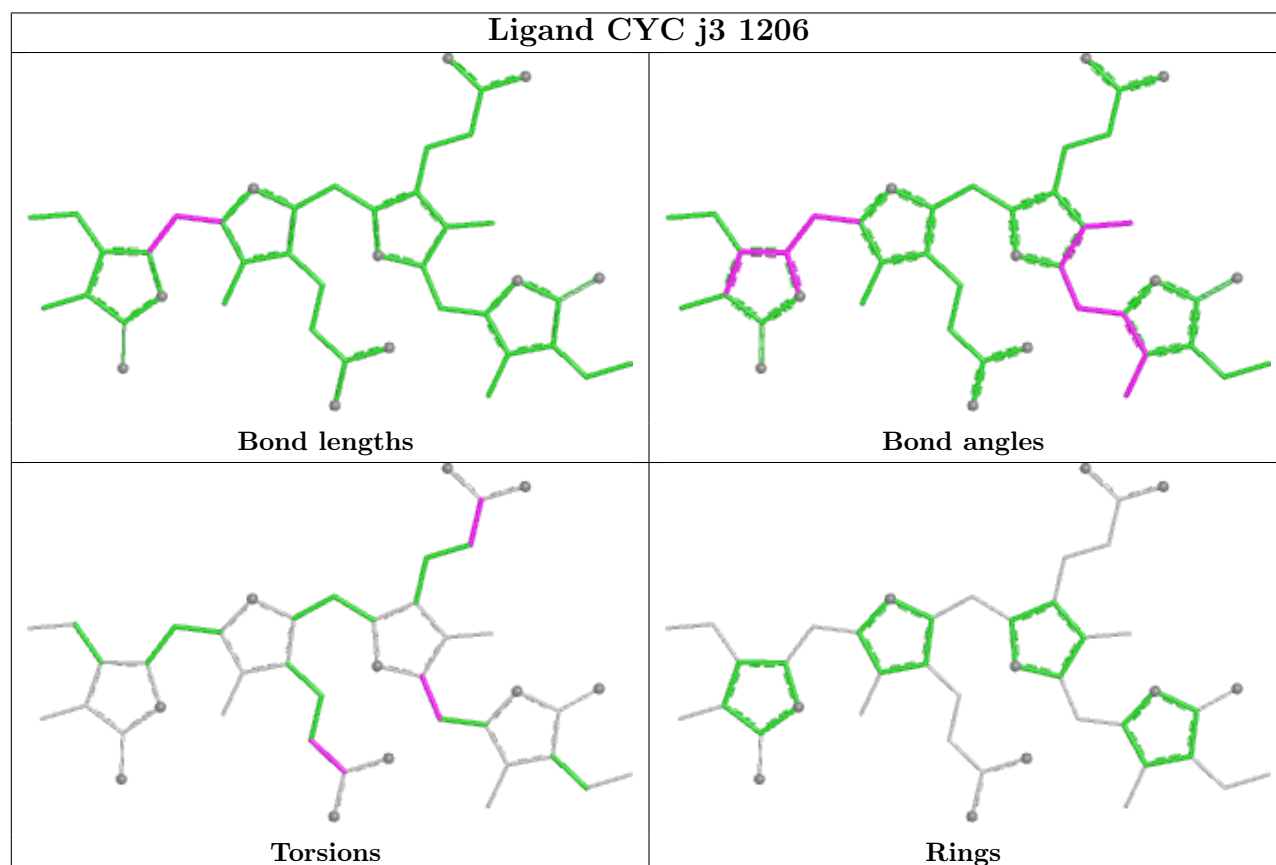


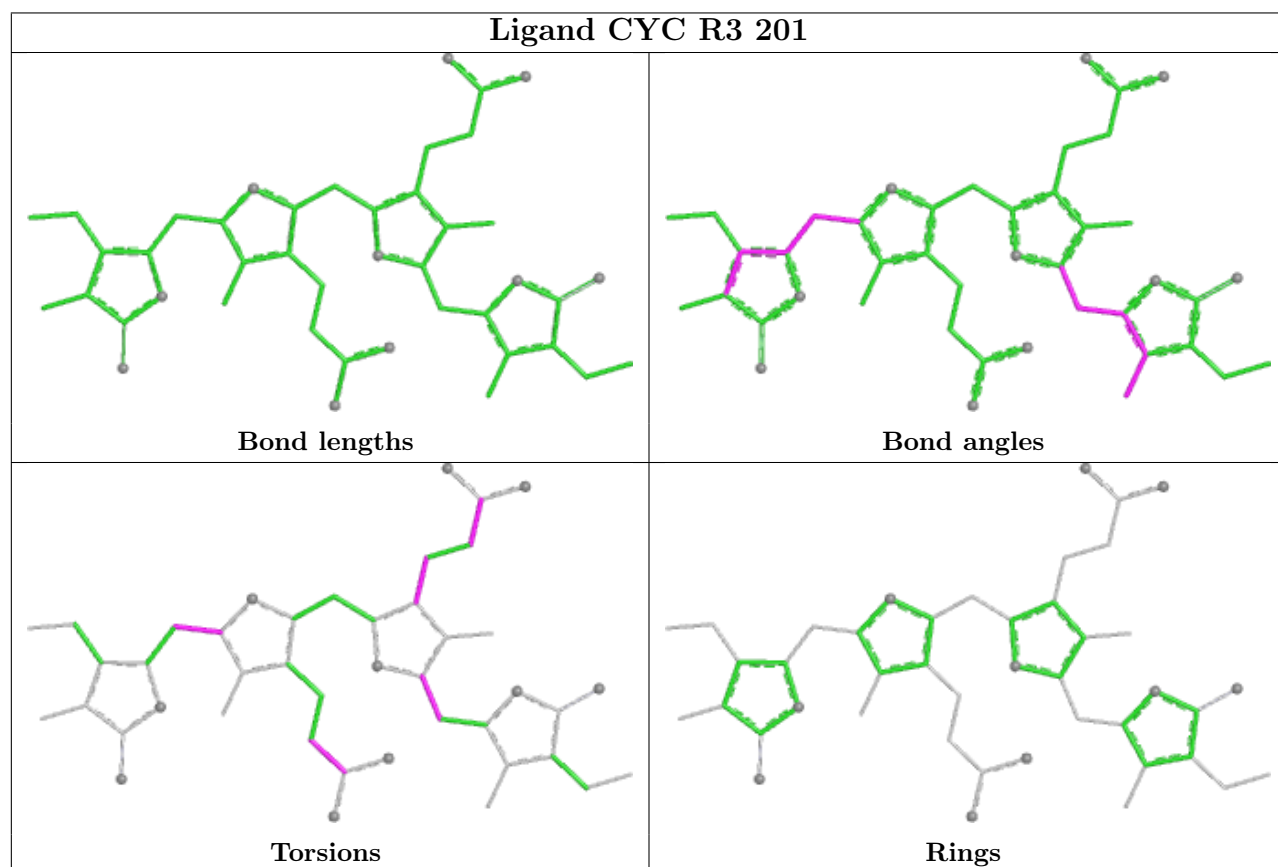
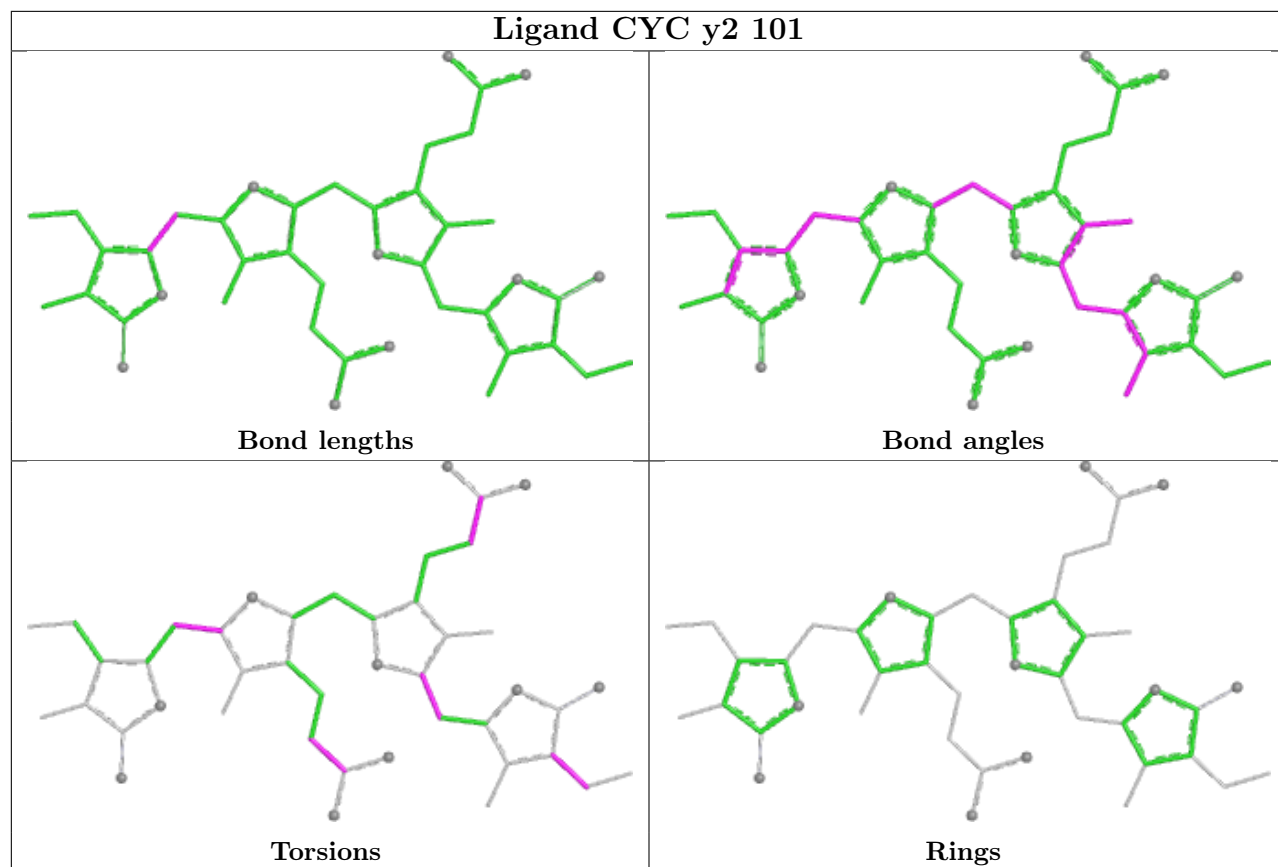


Ligand CYC k3 1205

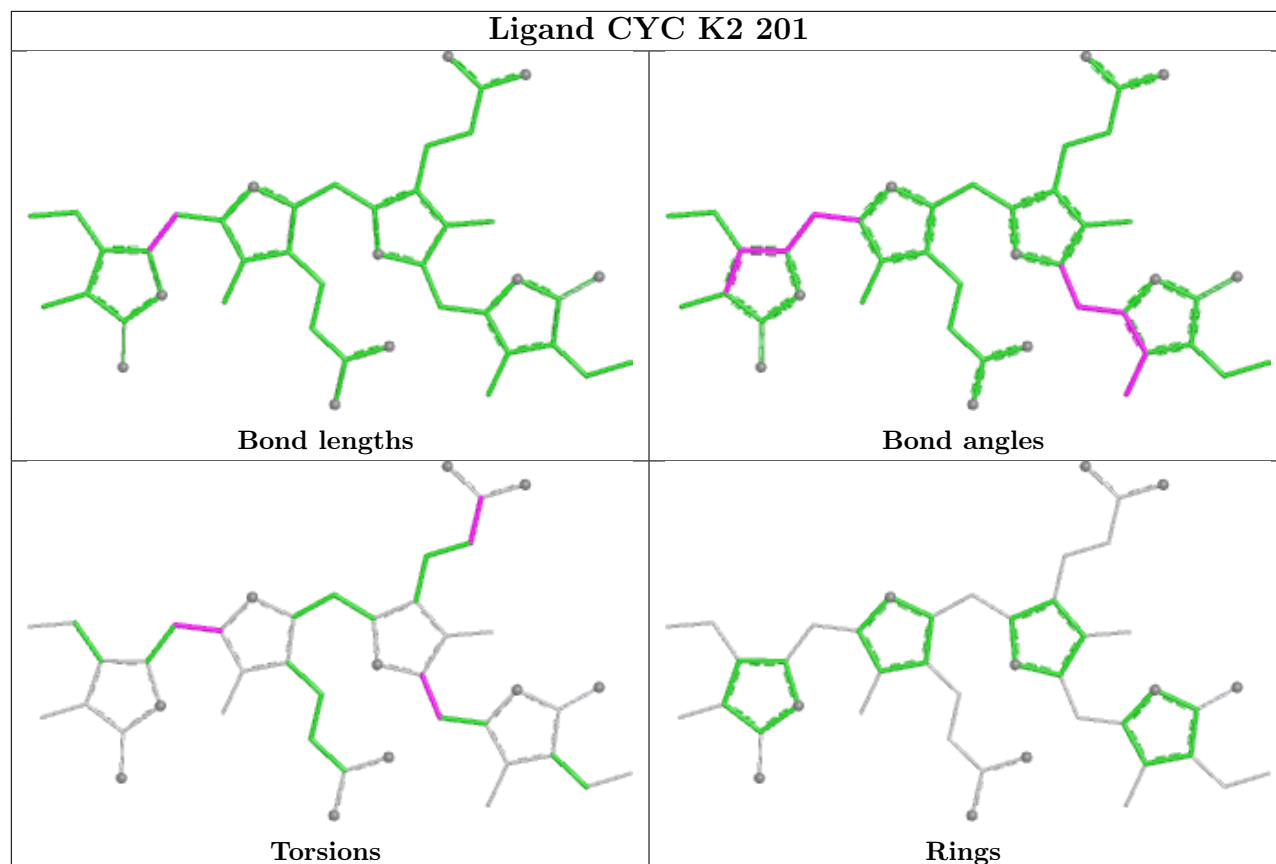


Ligand CYC j3 1206

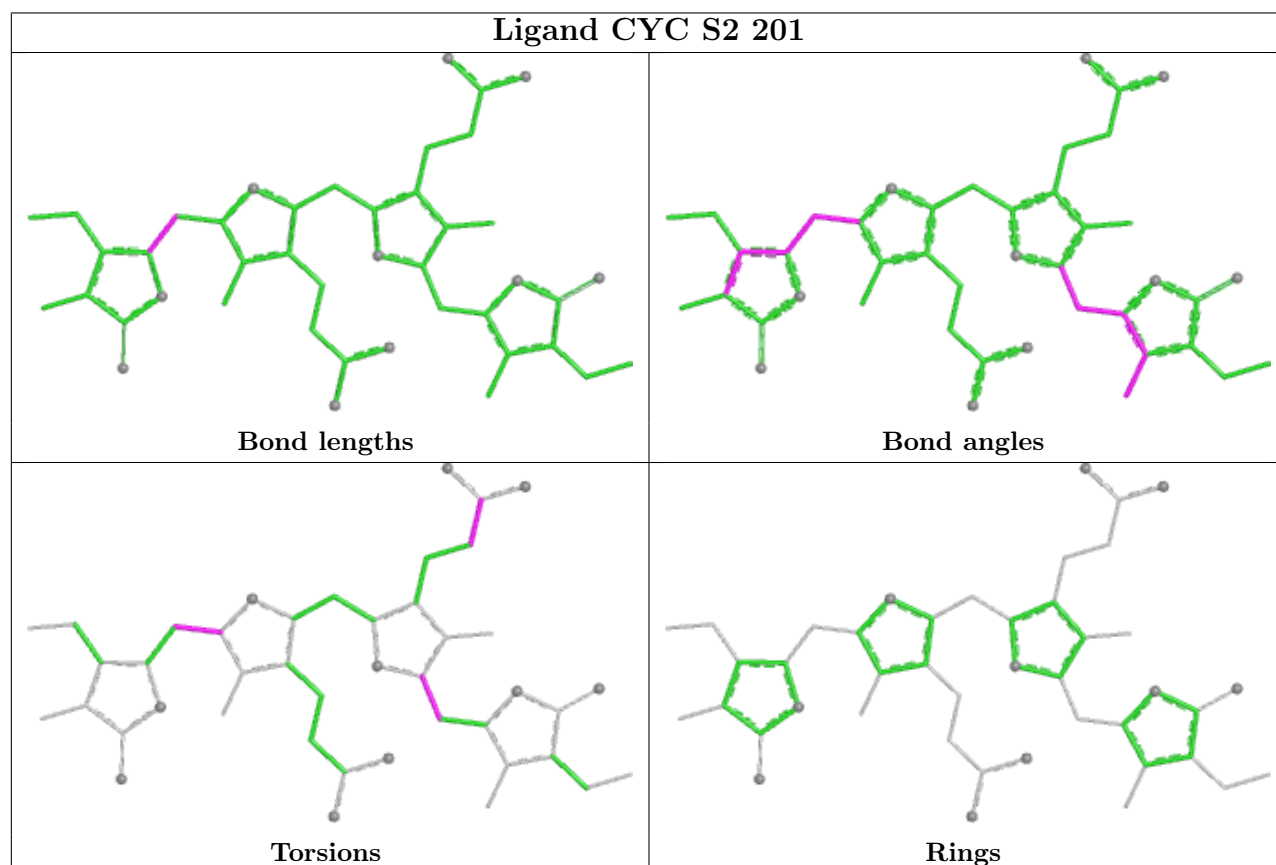


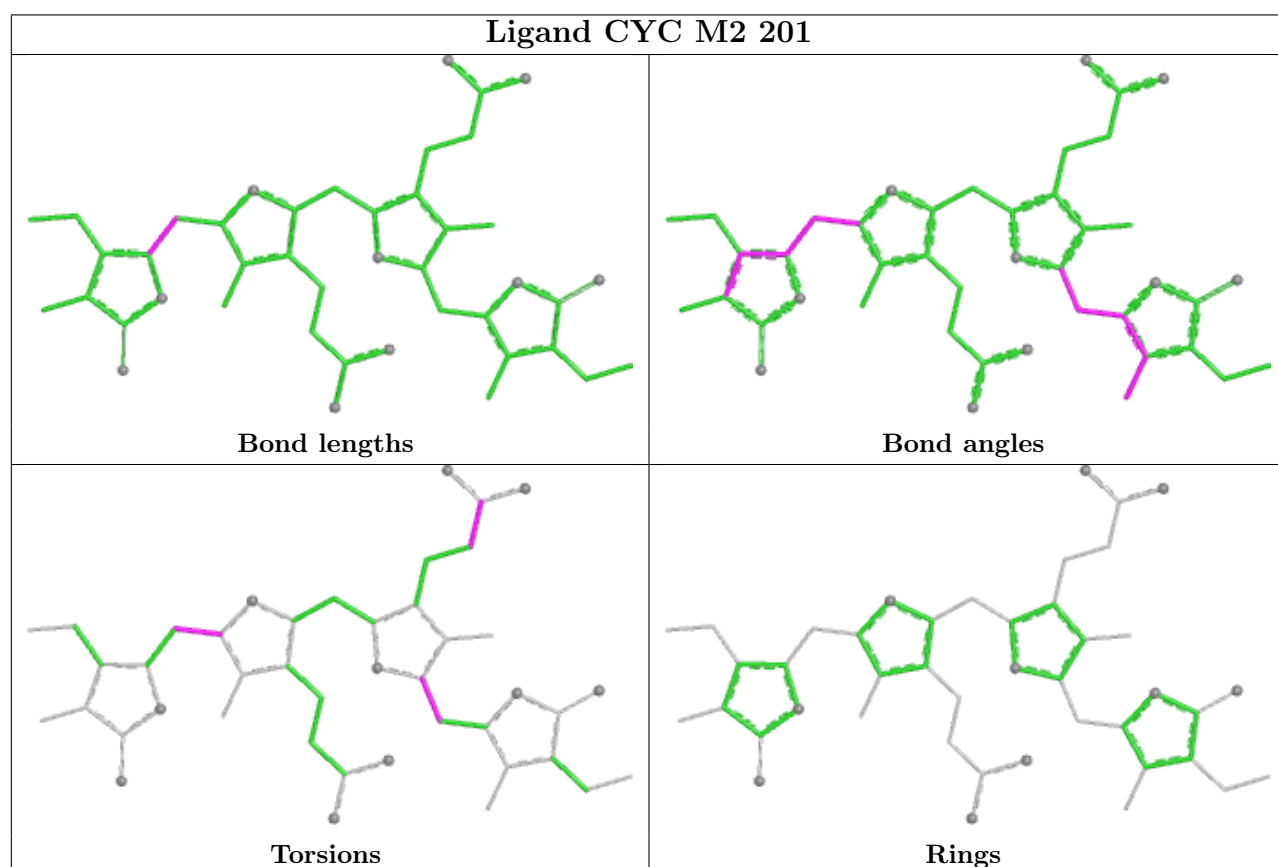
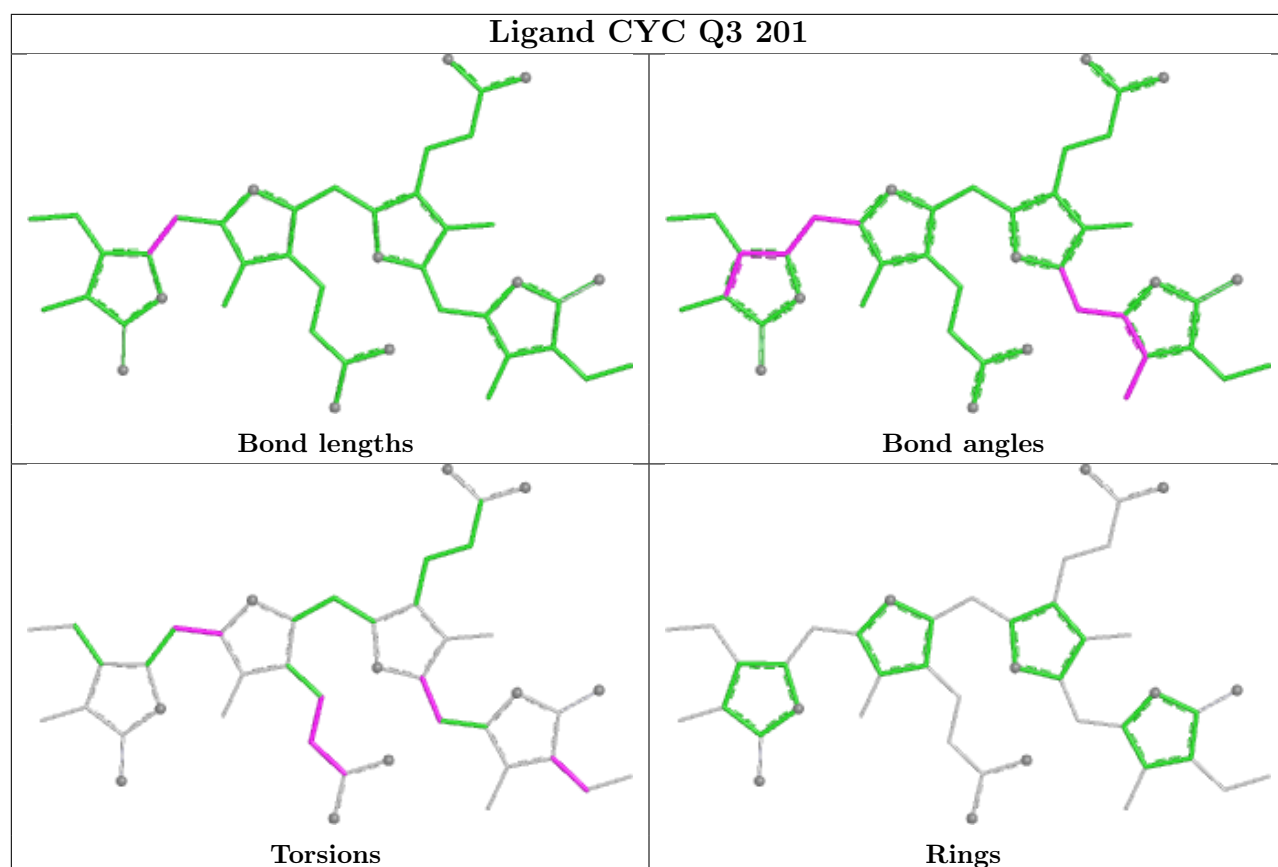


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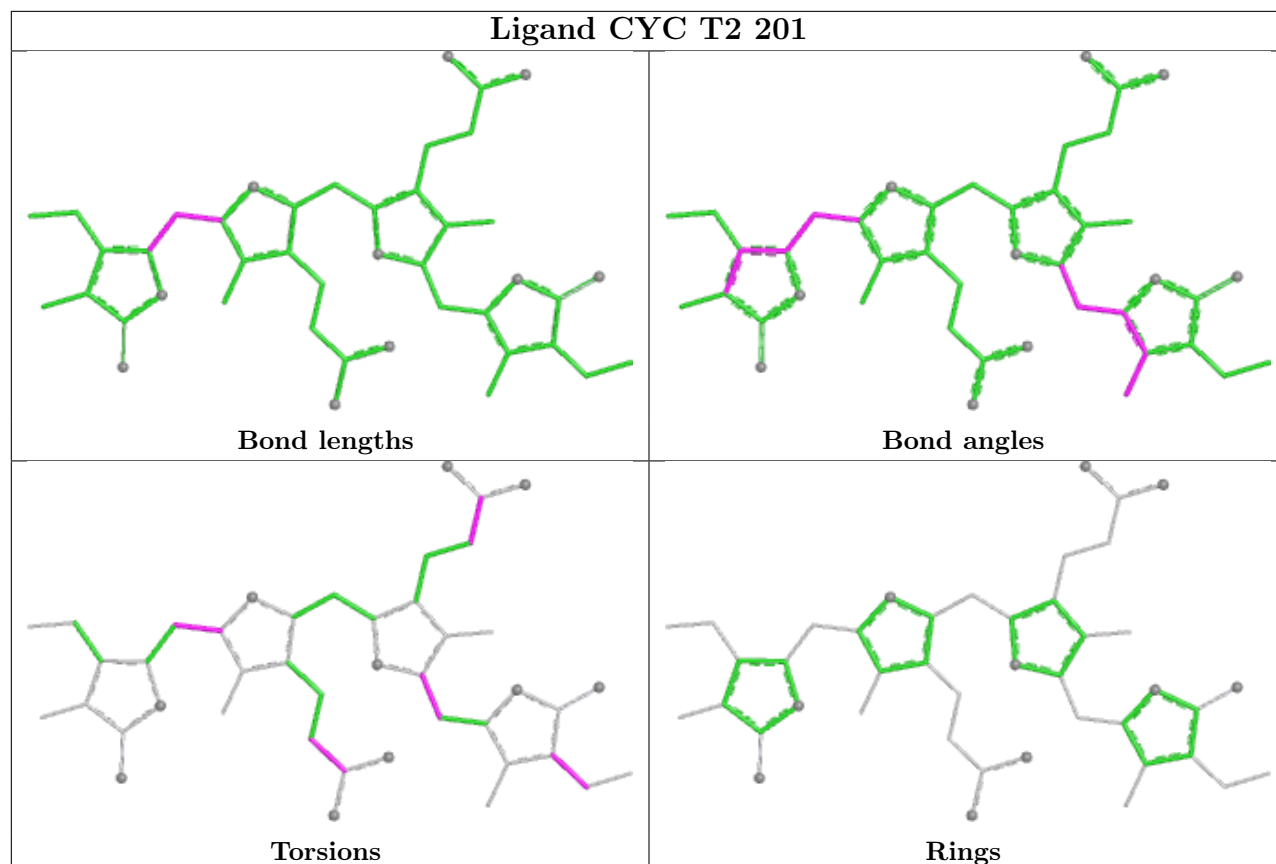


Ligand CYC S2 201

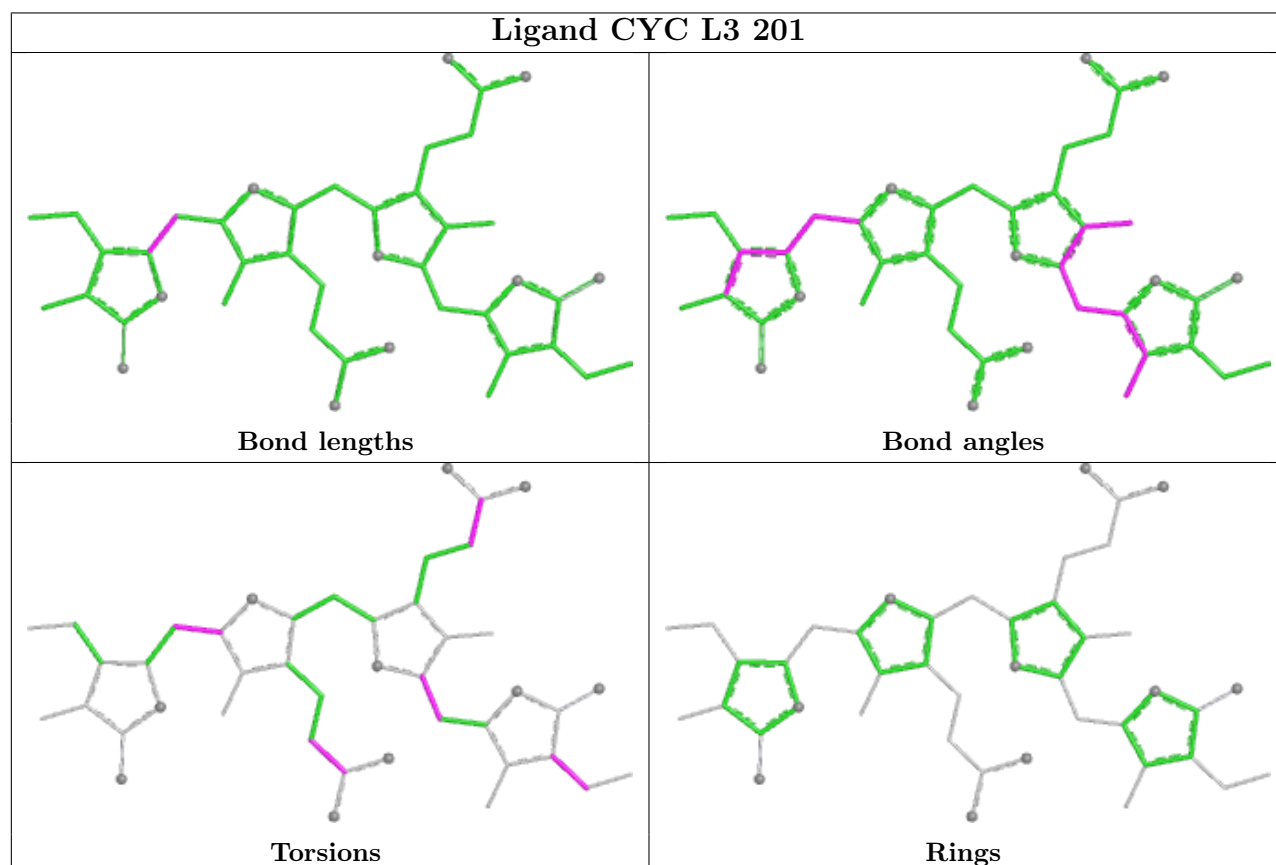


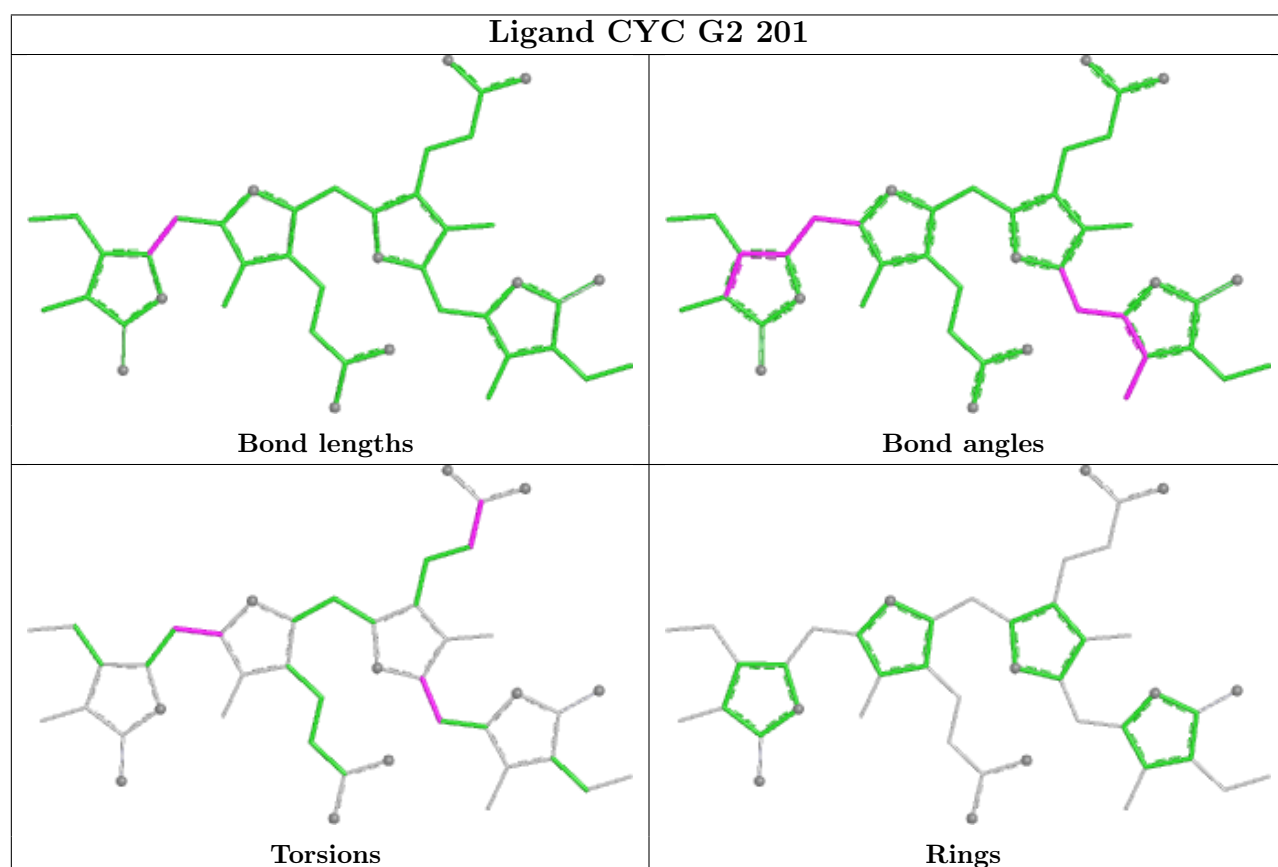
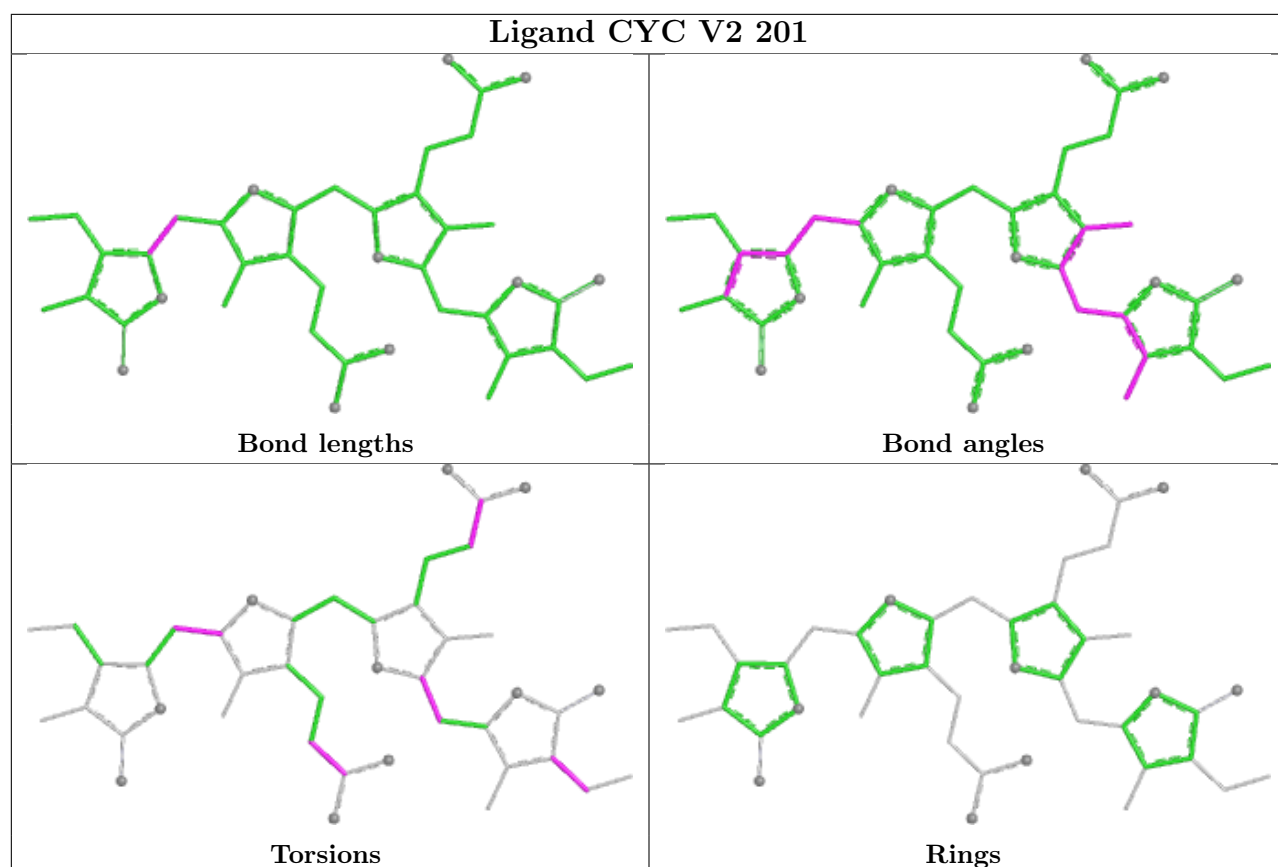


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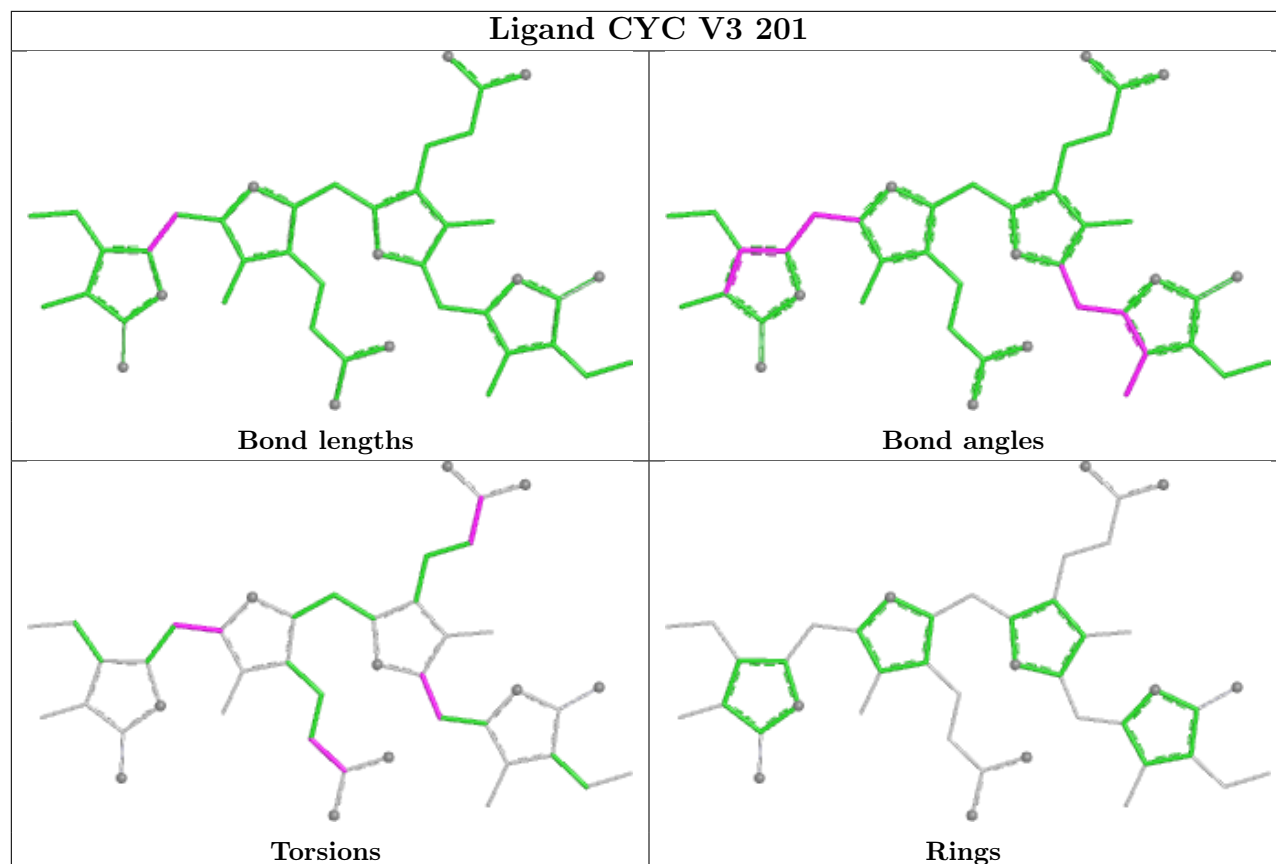


Ligand CYC L3 201

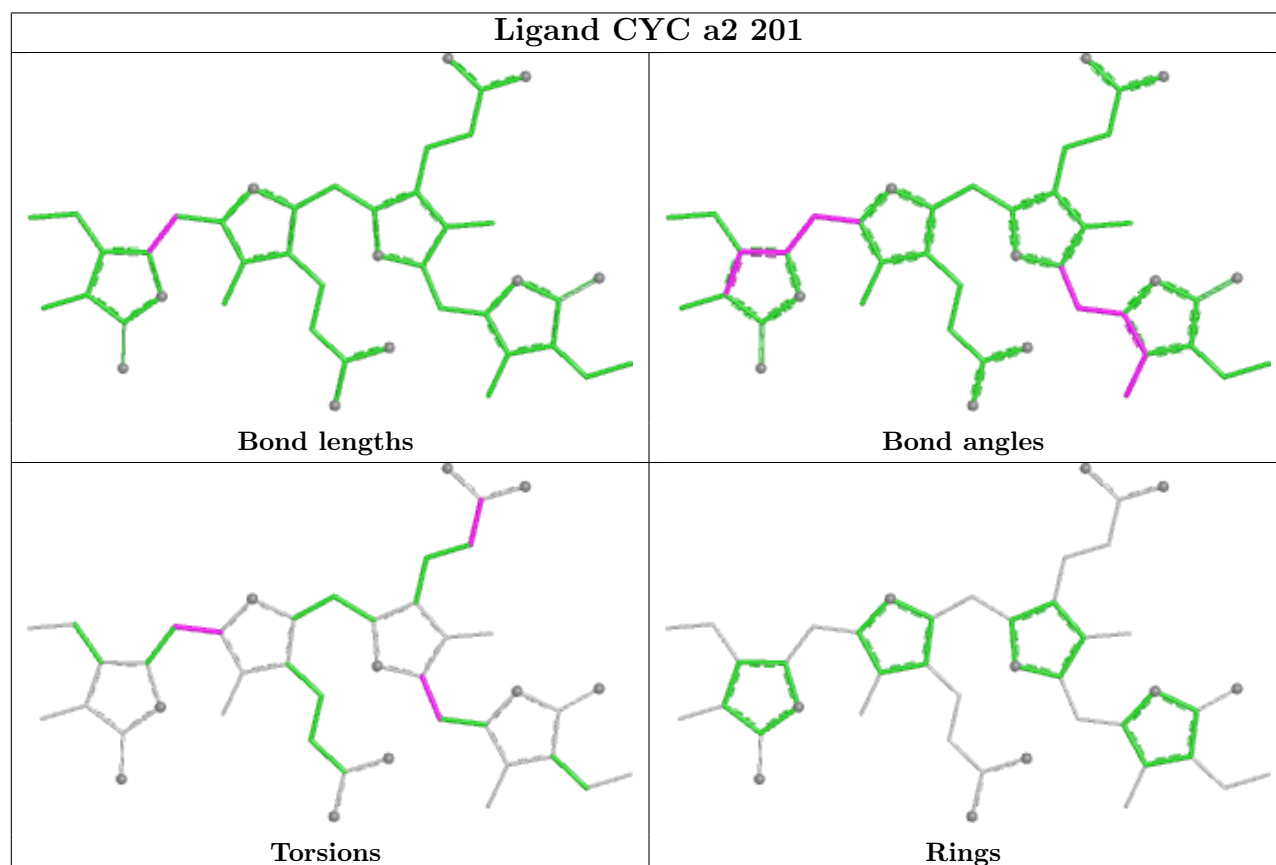


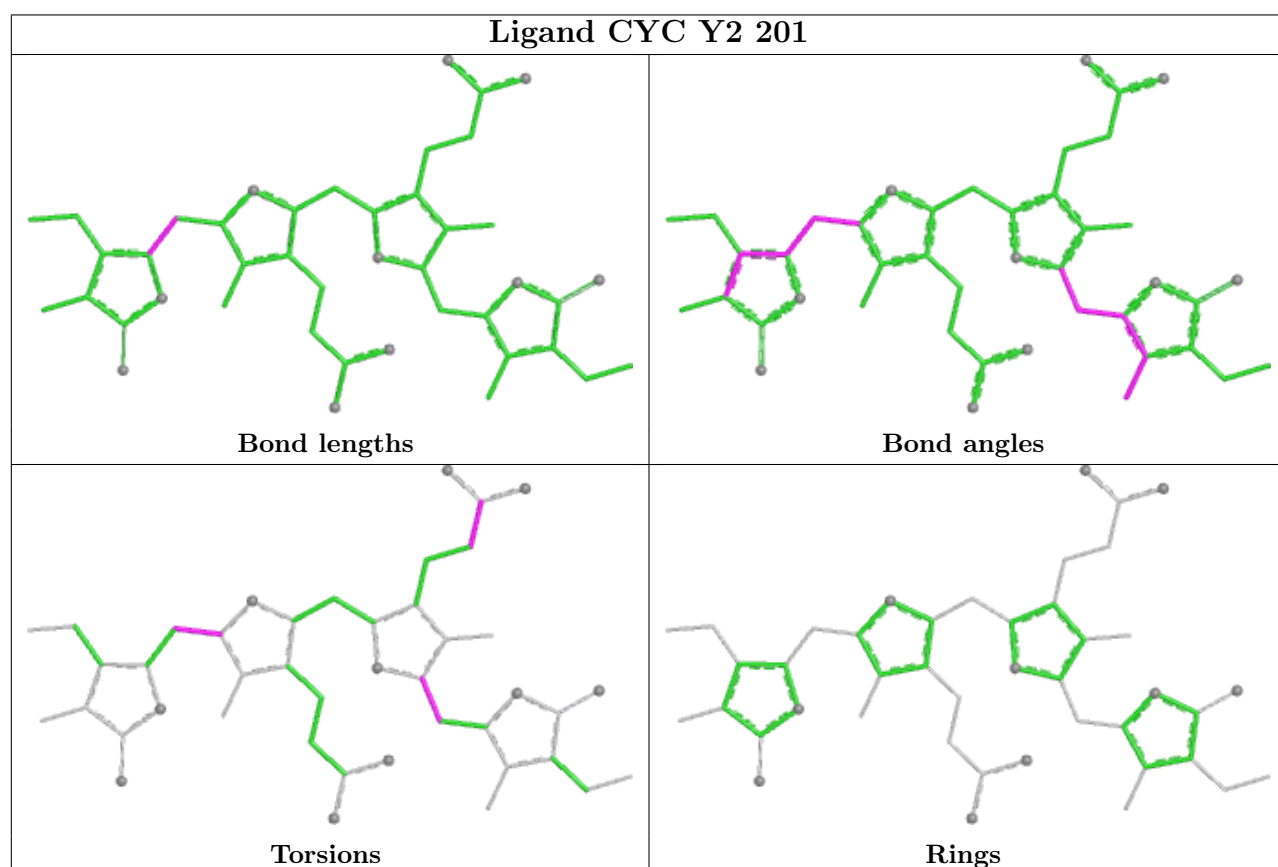
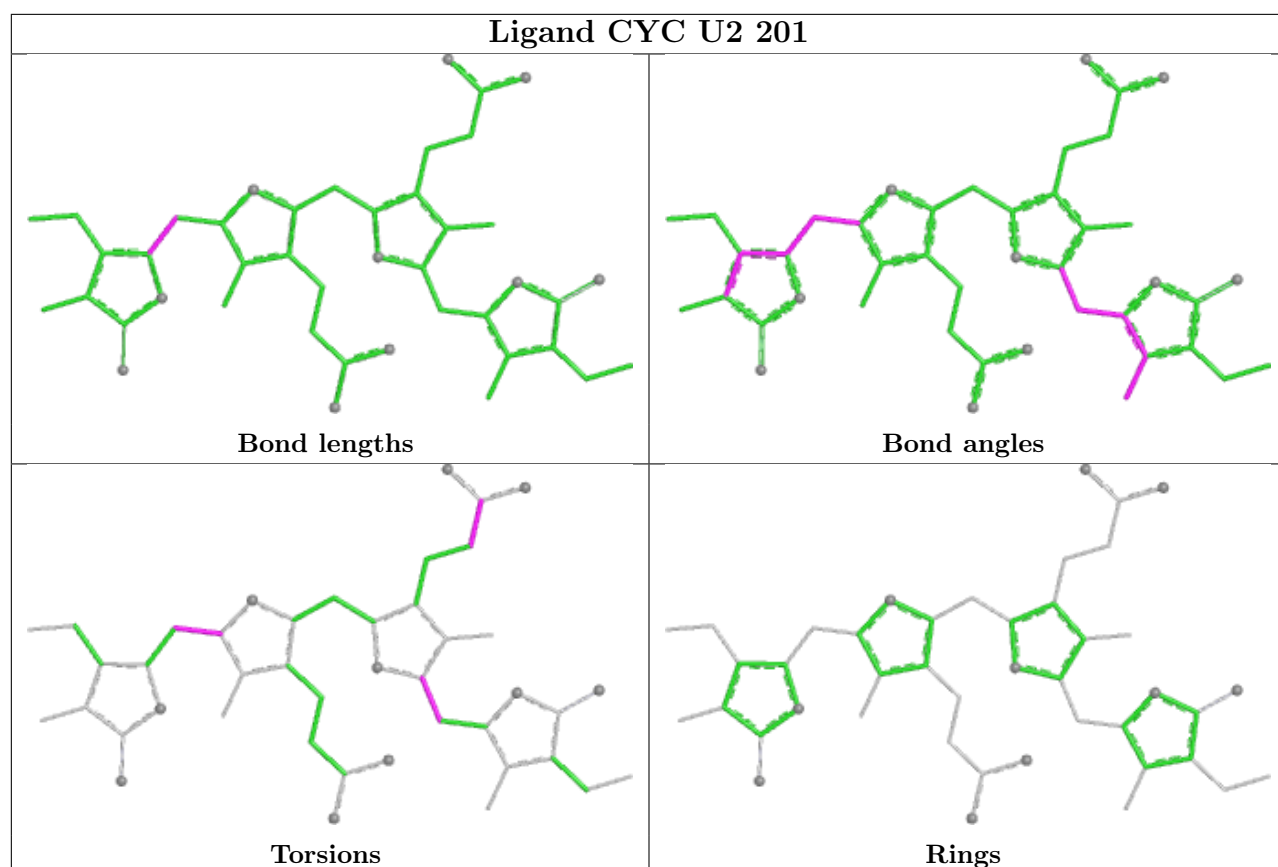


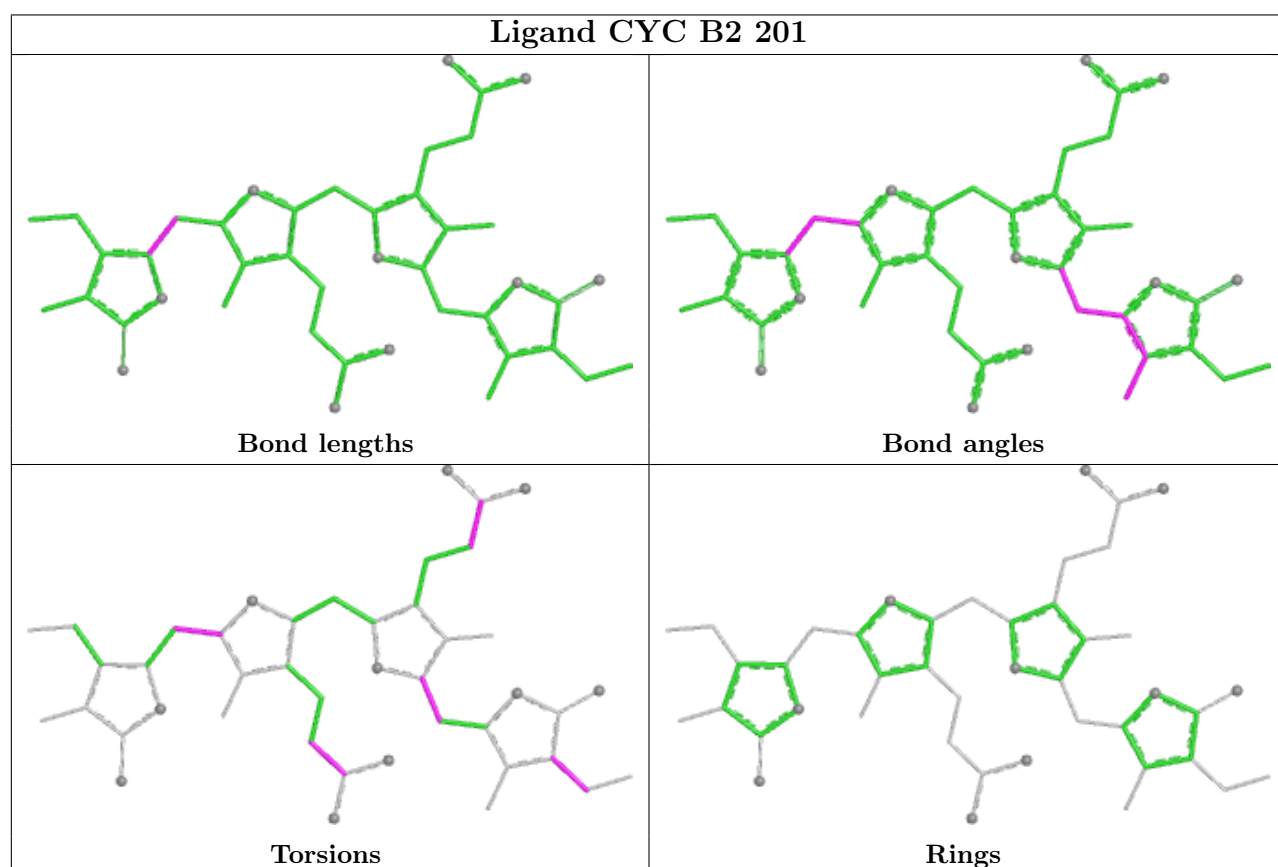
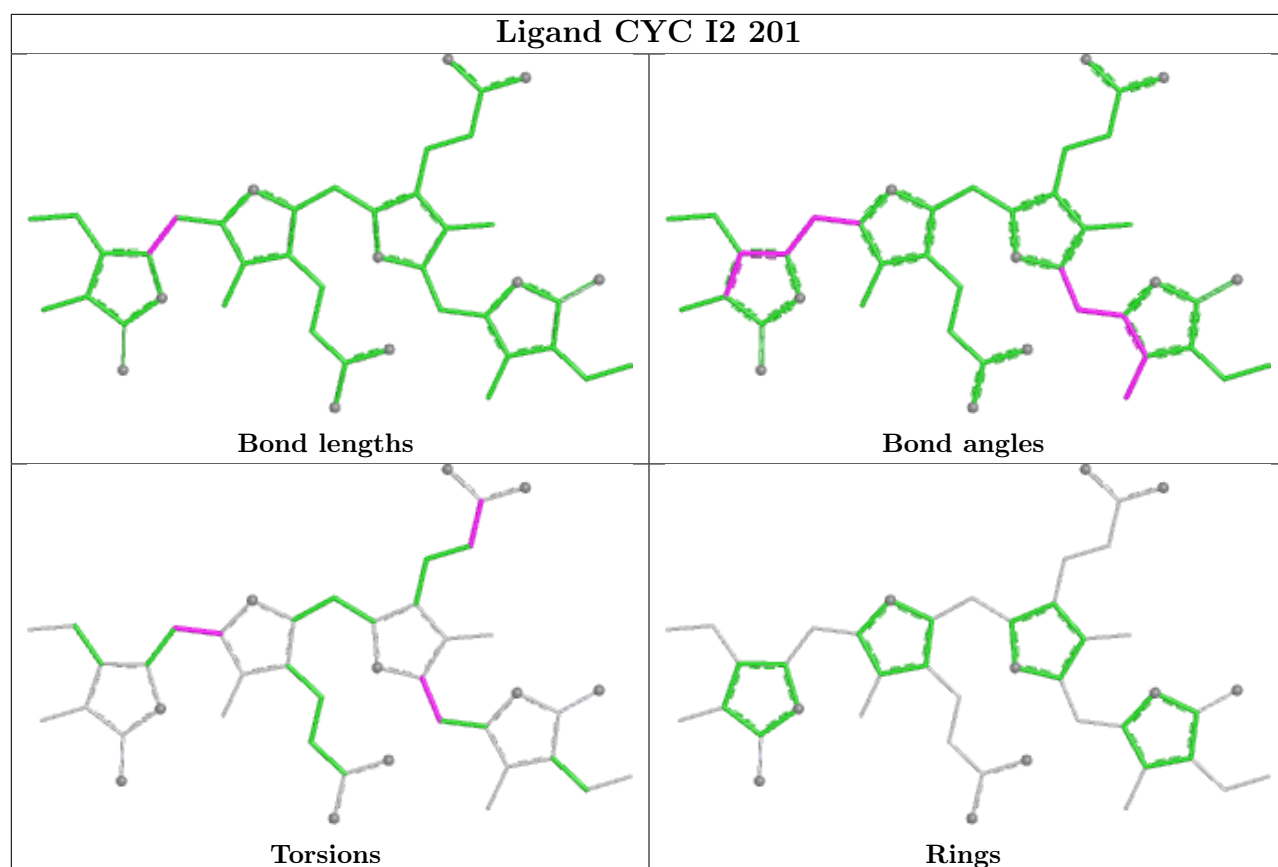
Ligand CYC V3 201

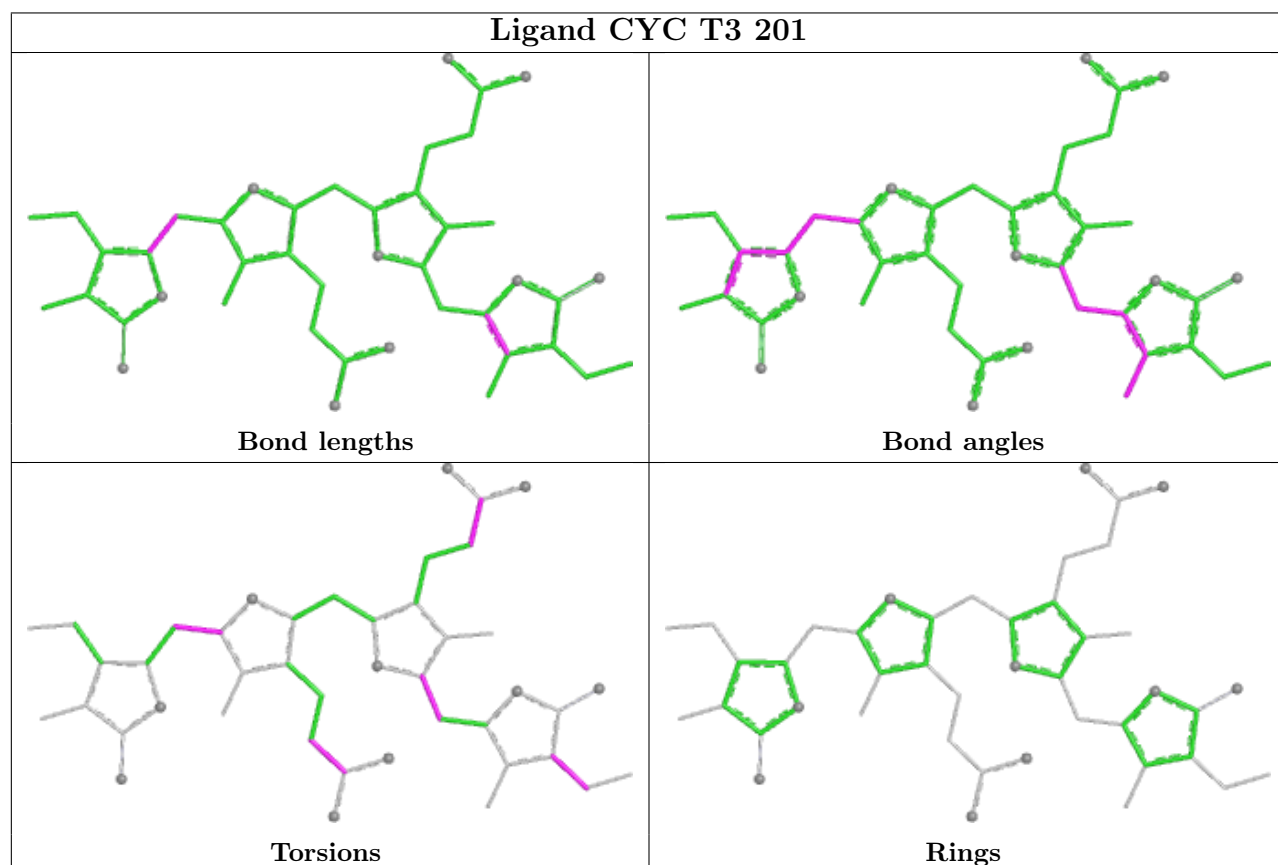
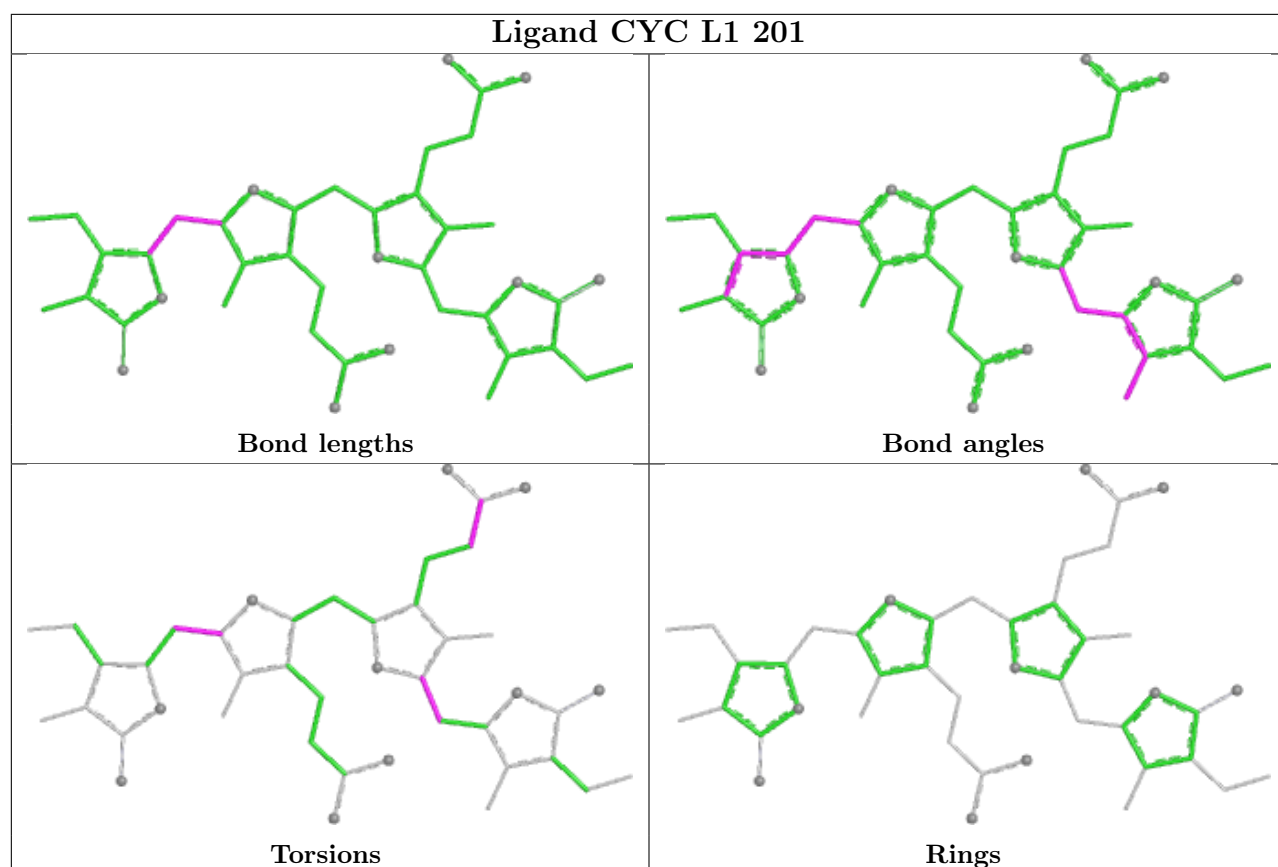


Ligand CYC a2 201

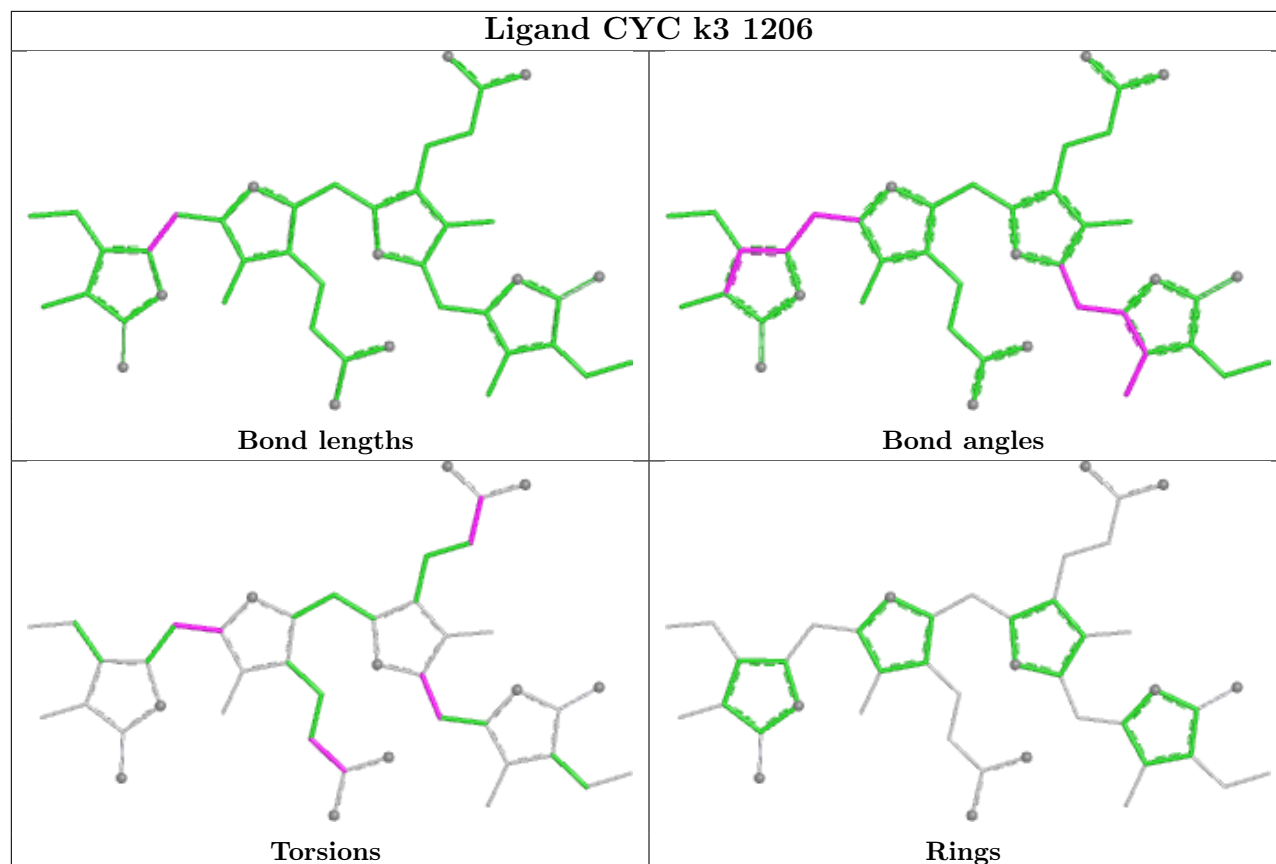




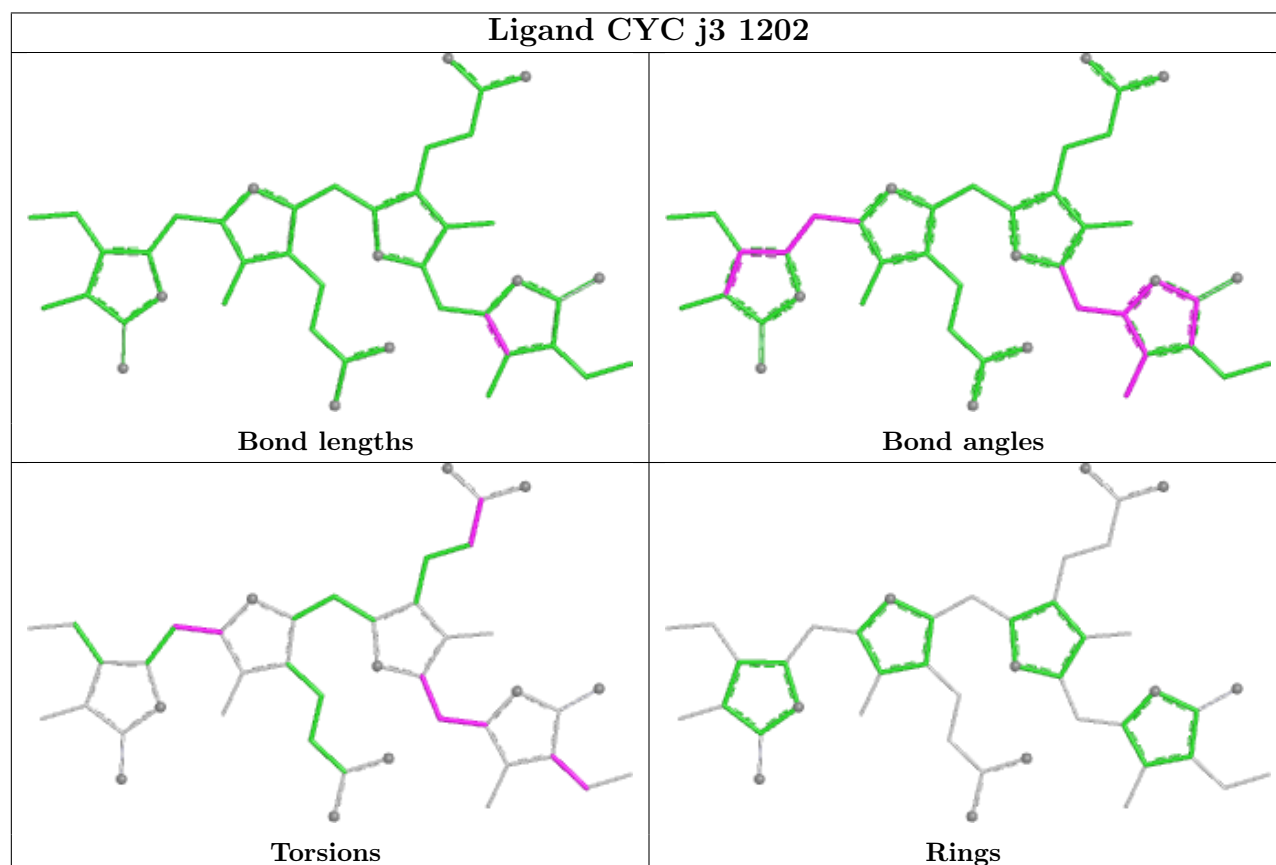


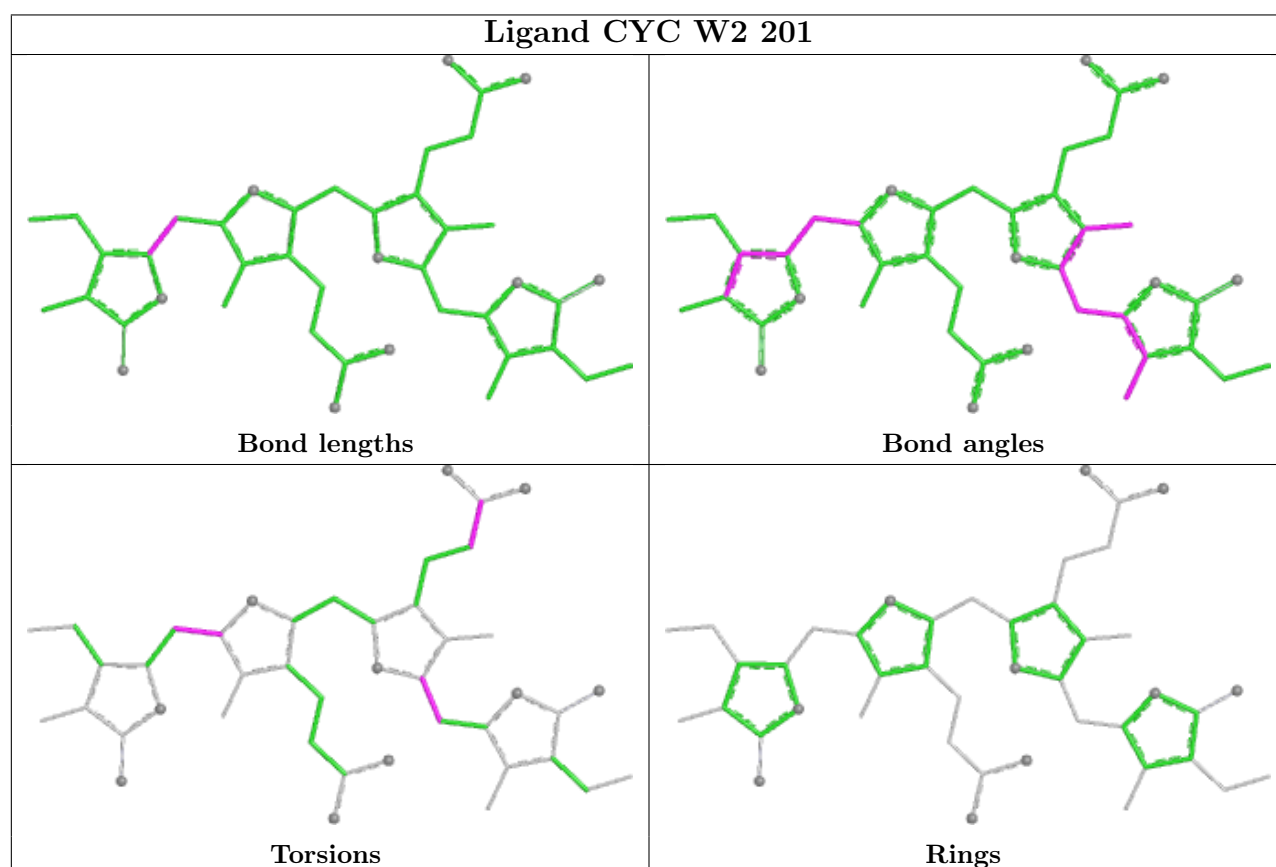
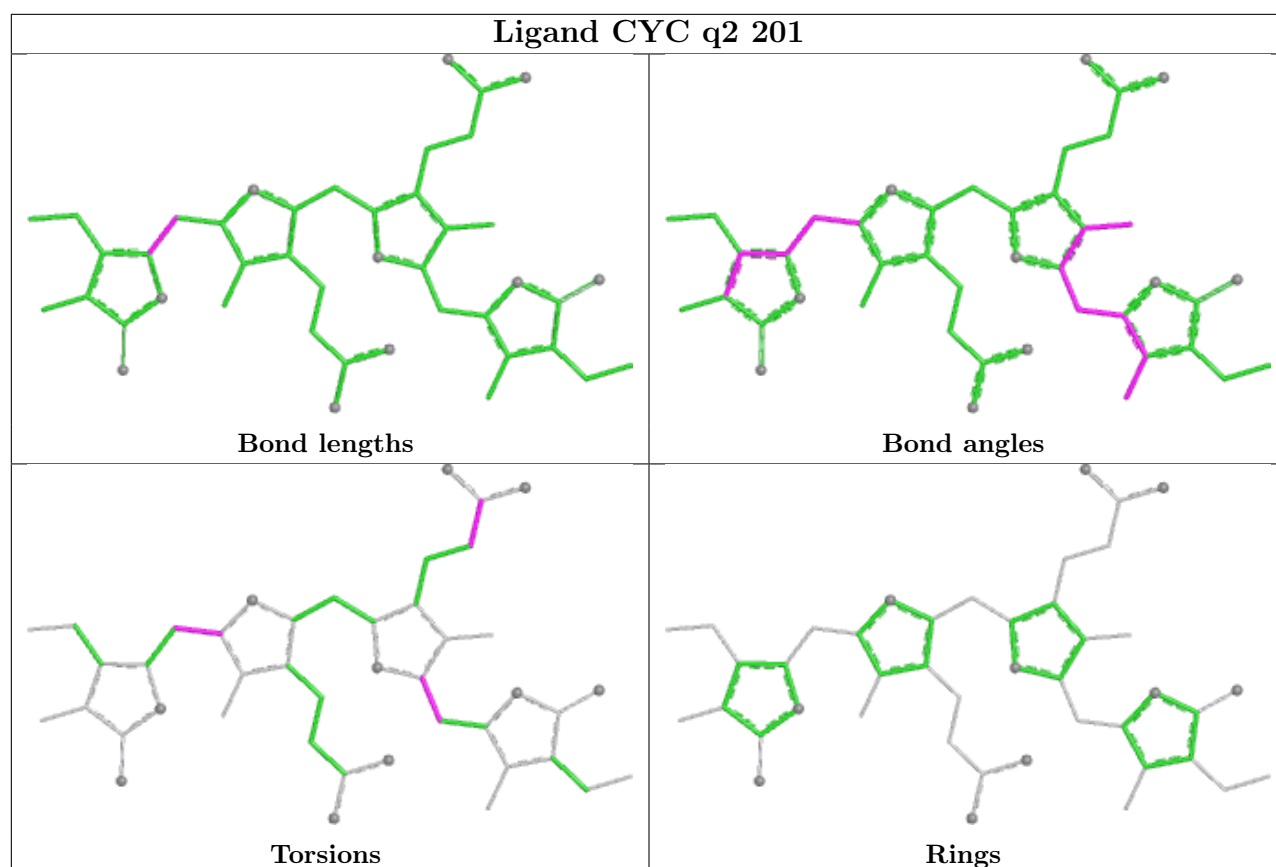


Ligand CYC k3 1206

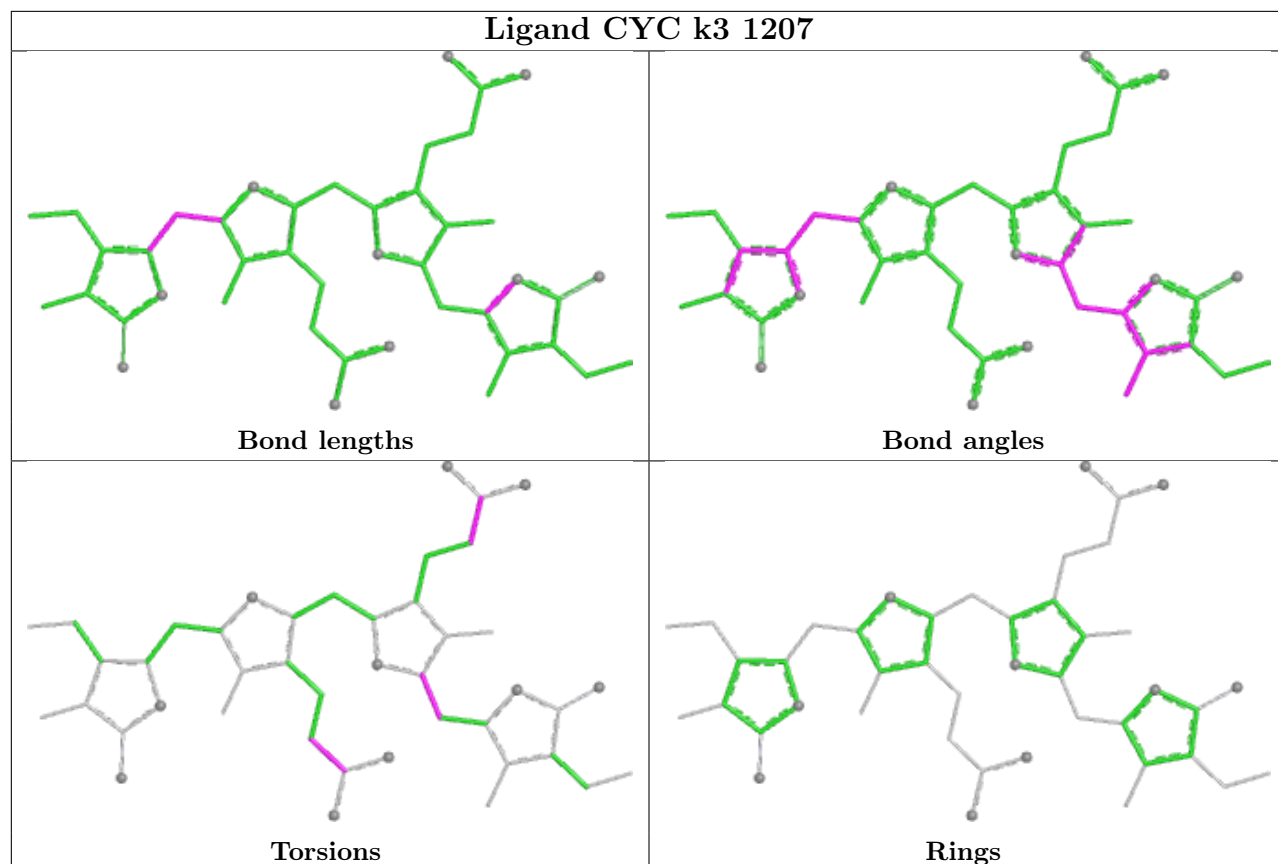


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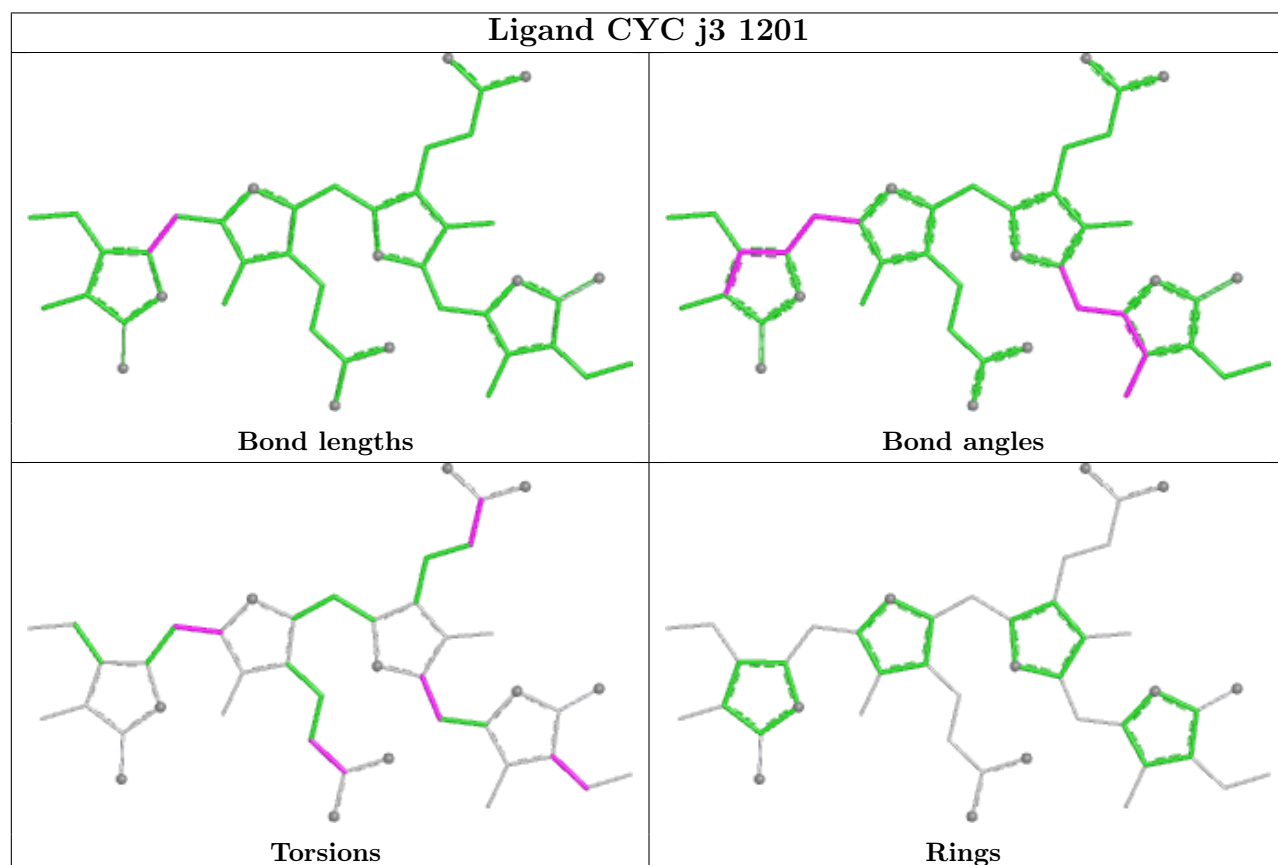




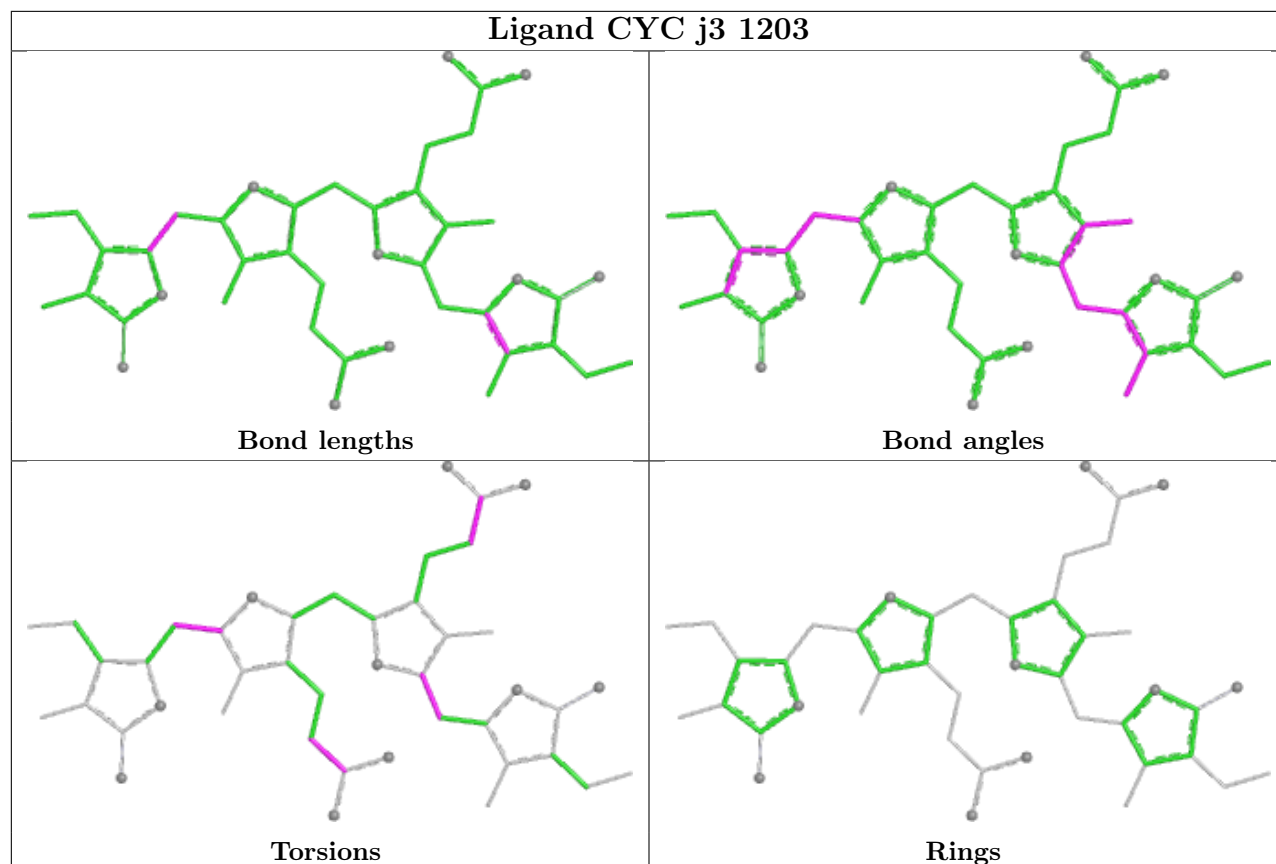
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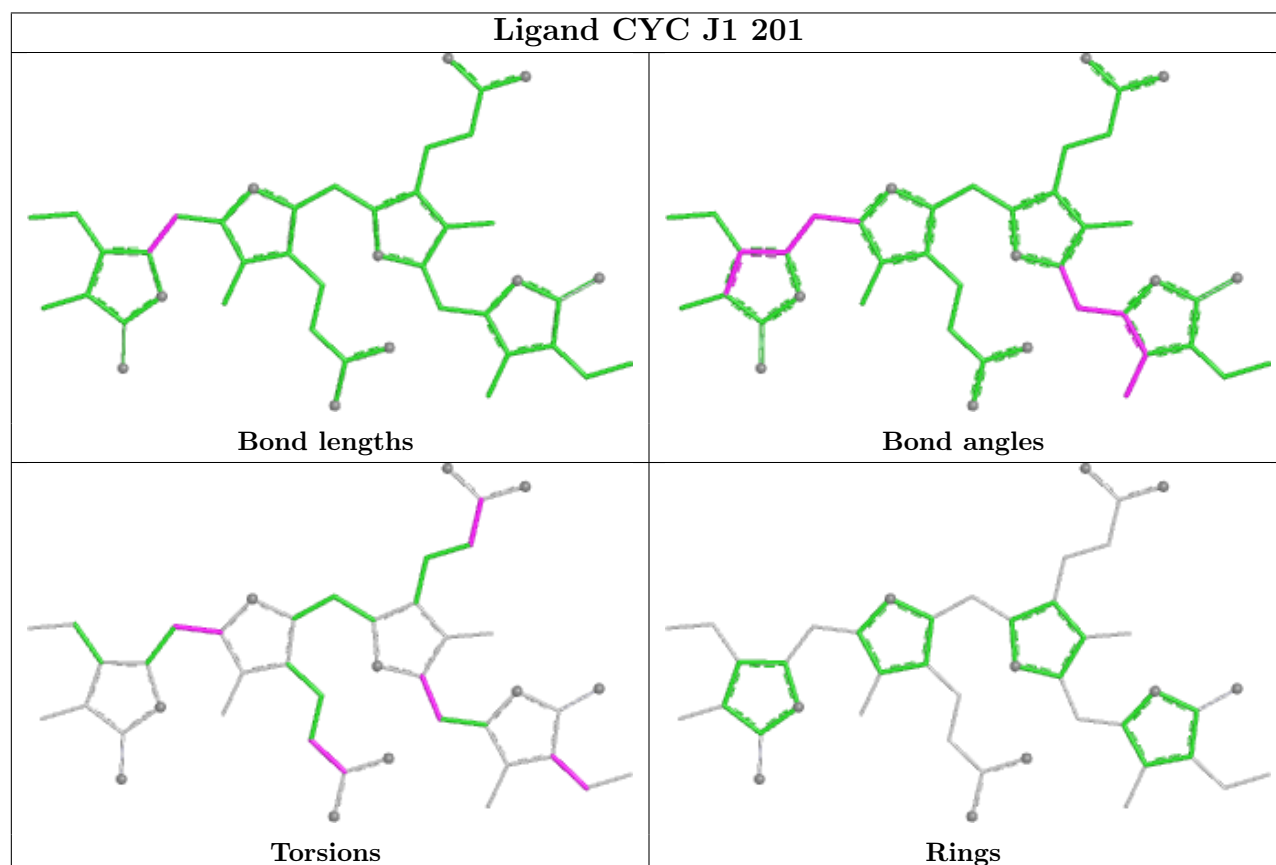
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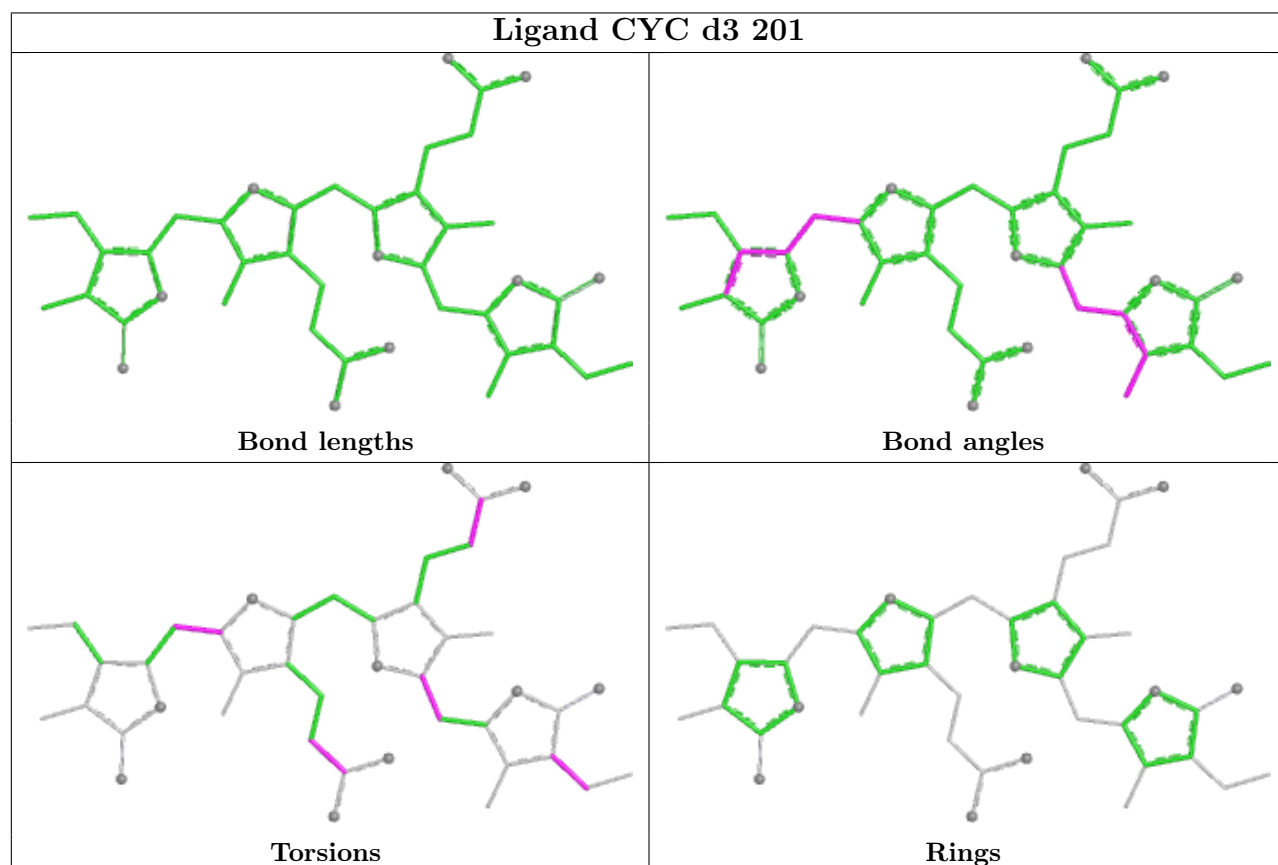
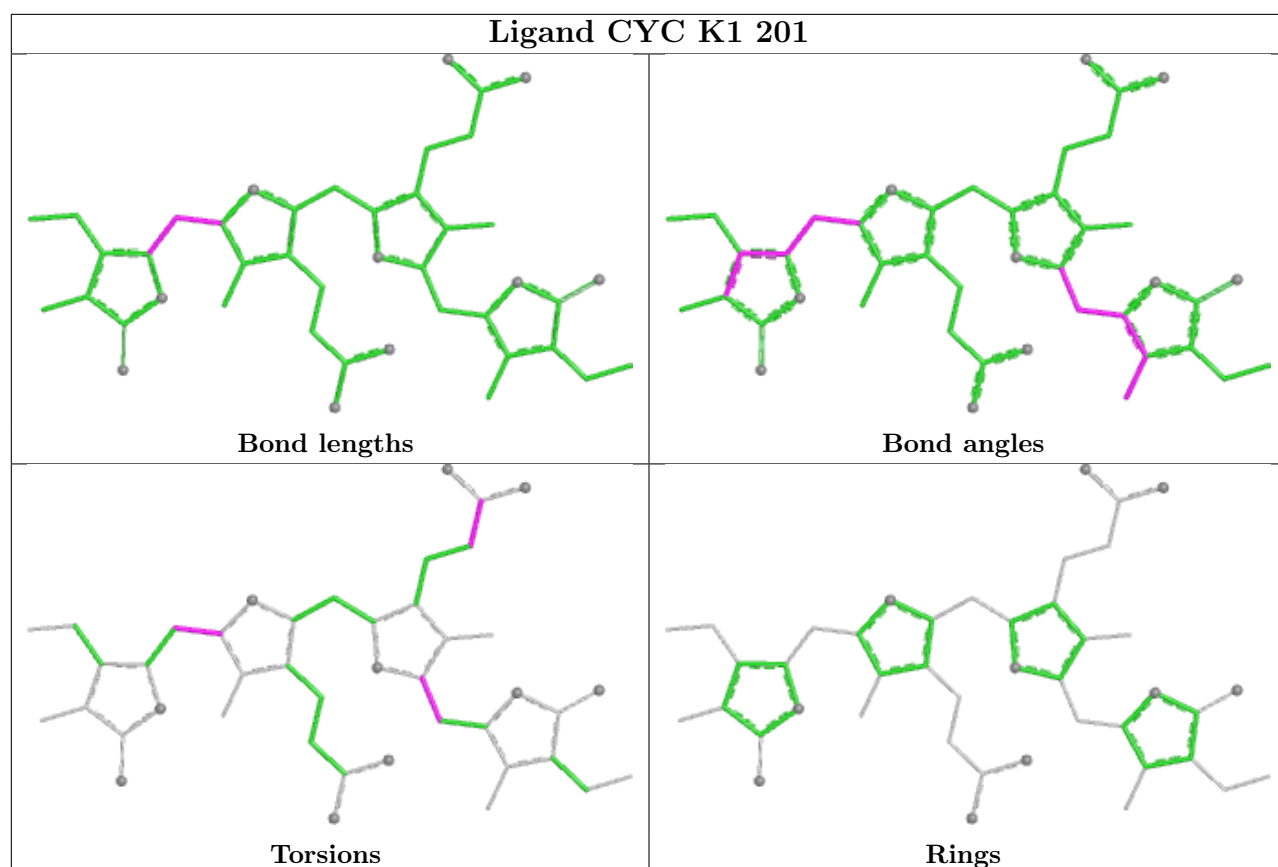


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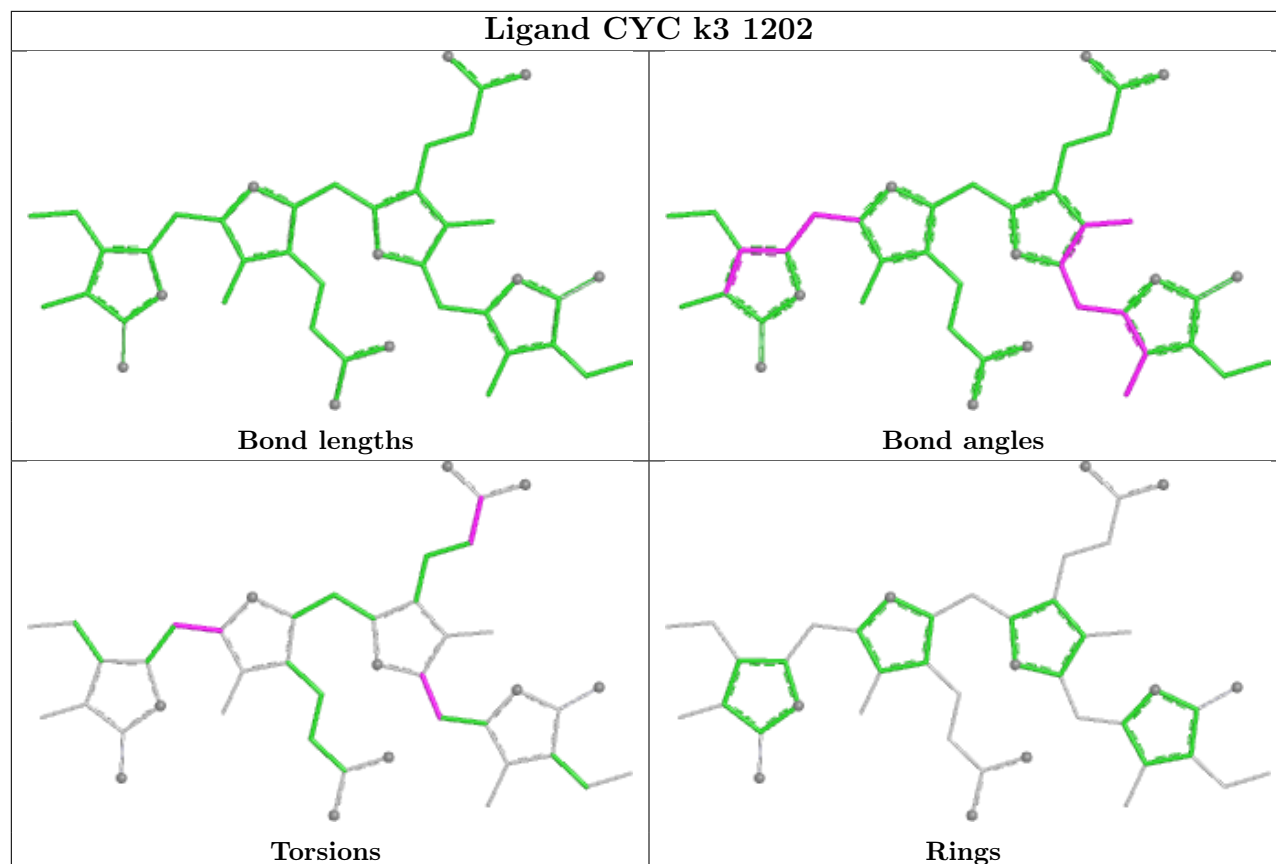


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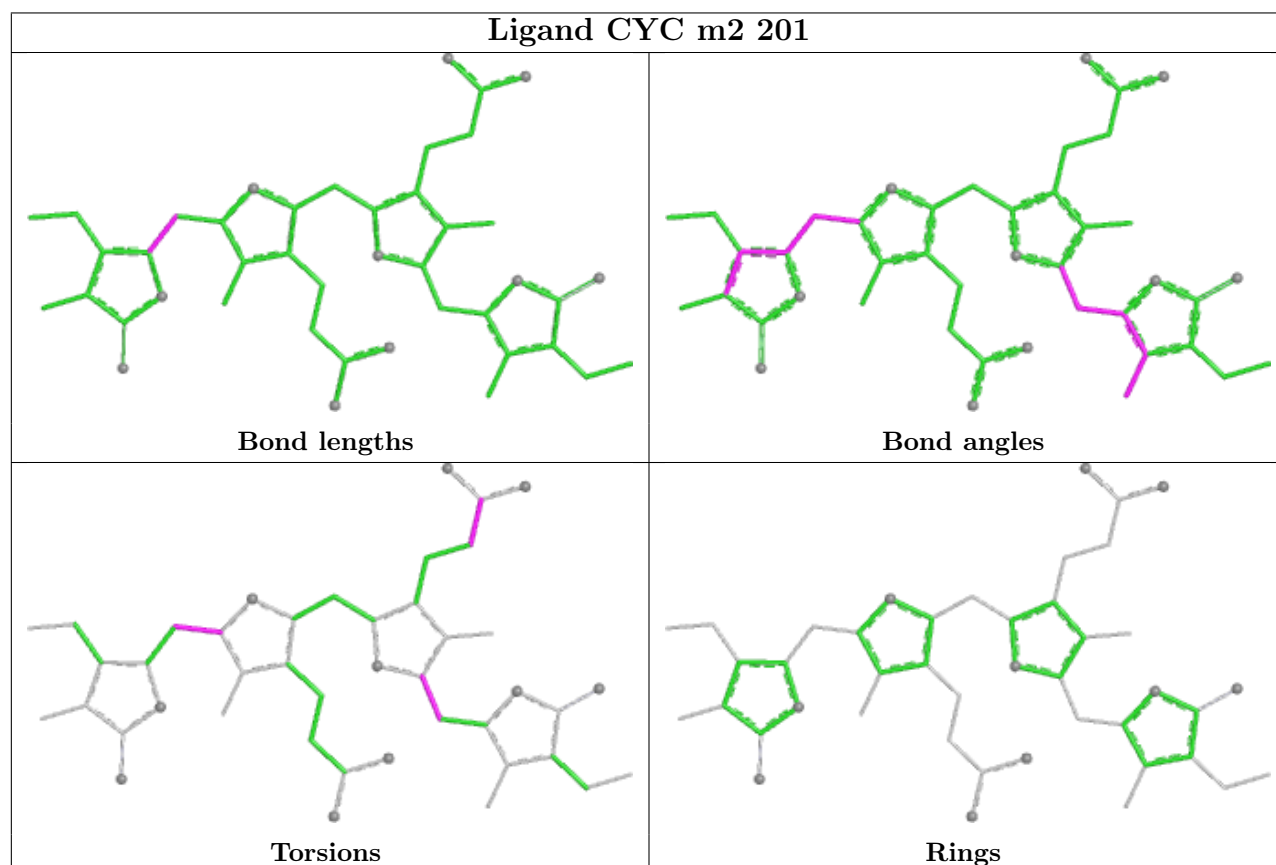




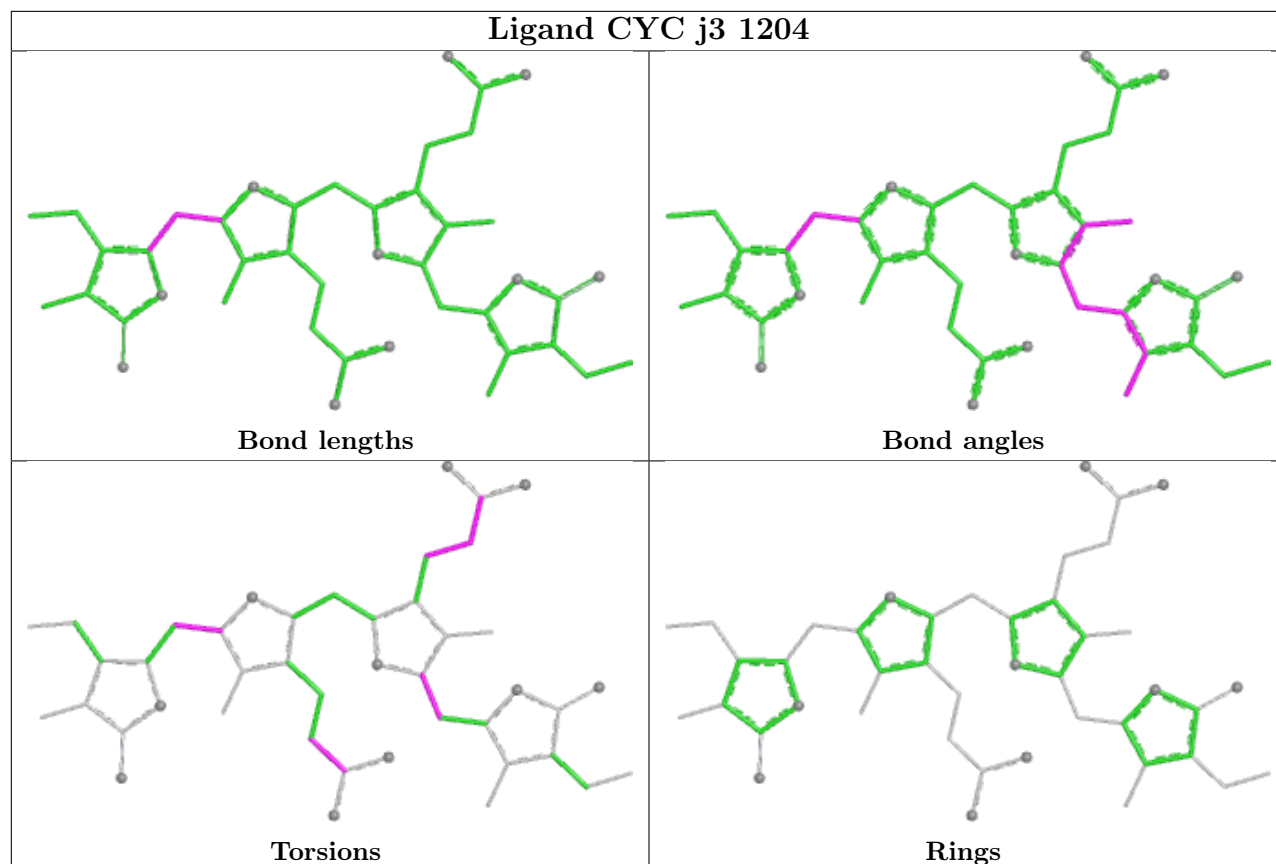
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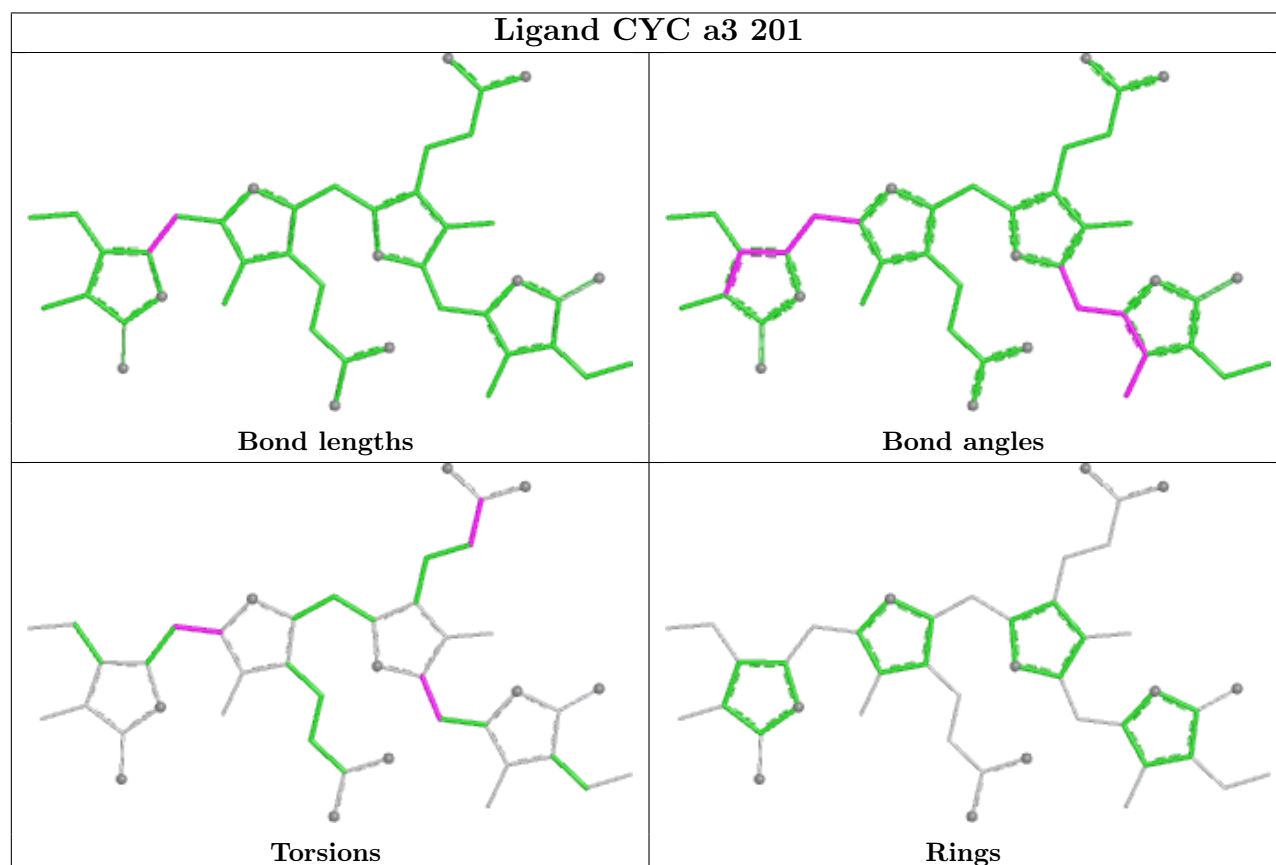
Ligand CYC m2 201



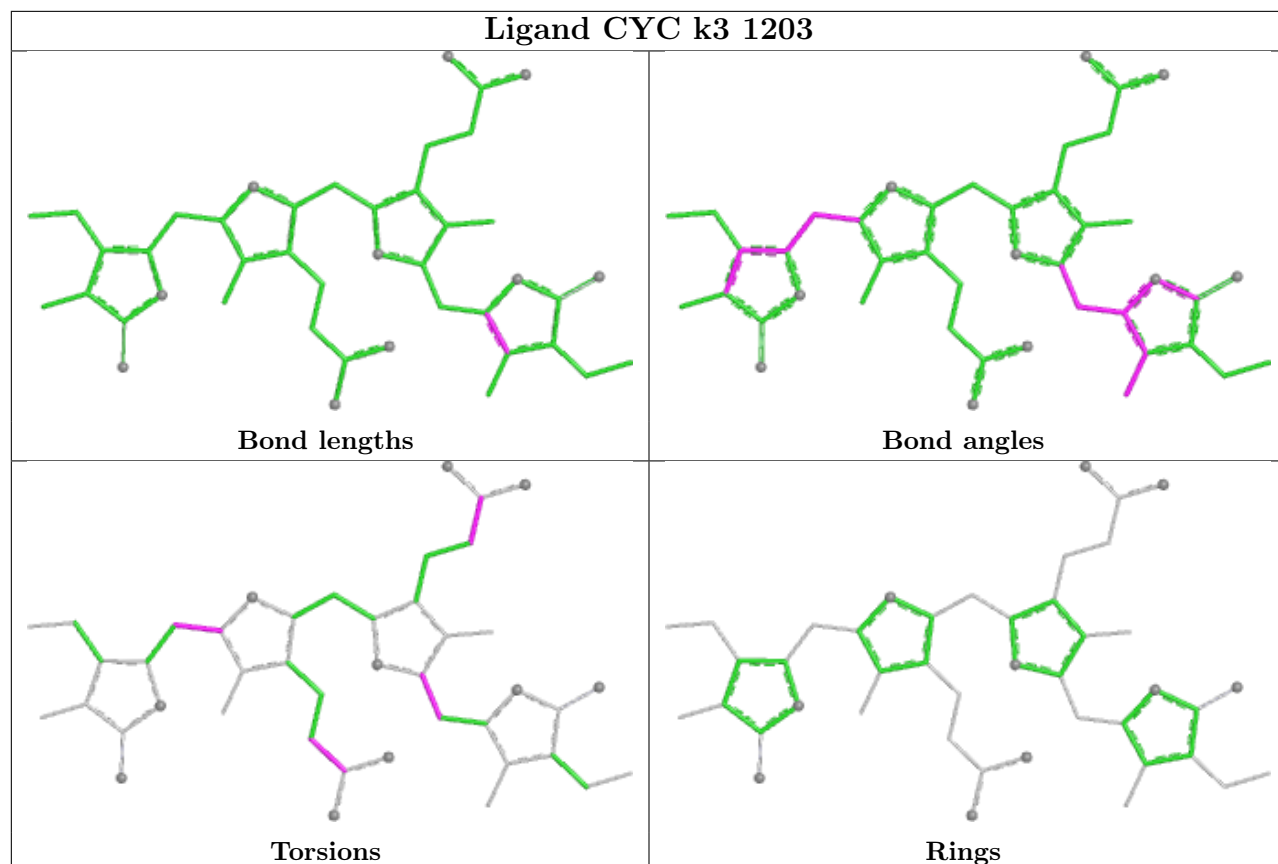
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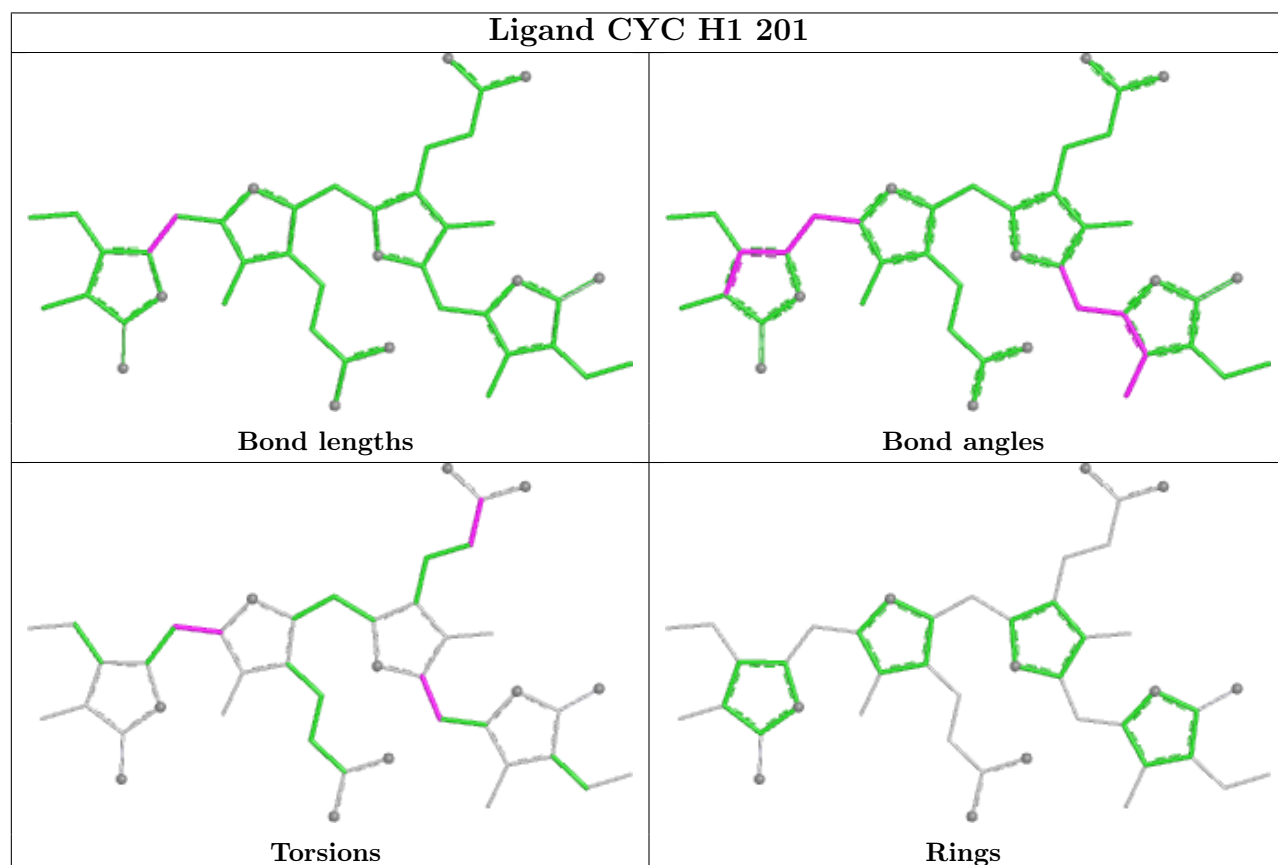
Ligand CYC a3 201

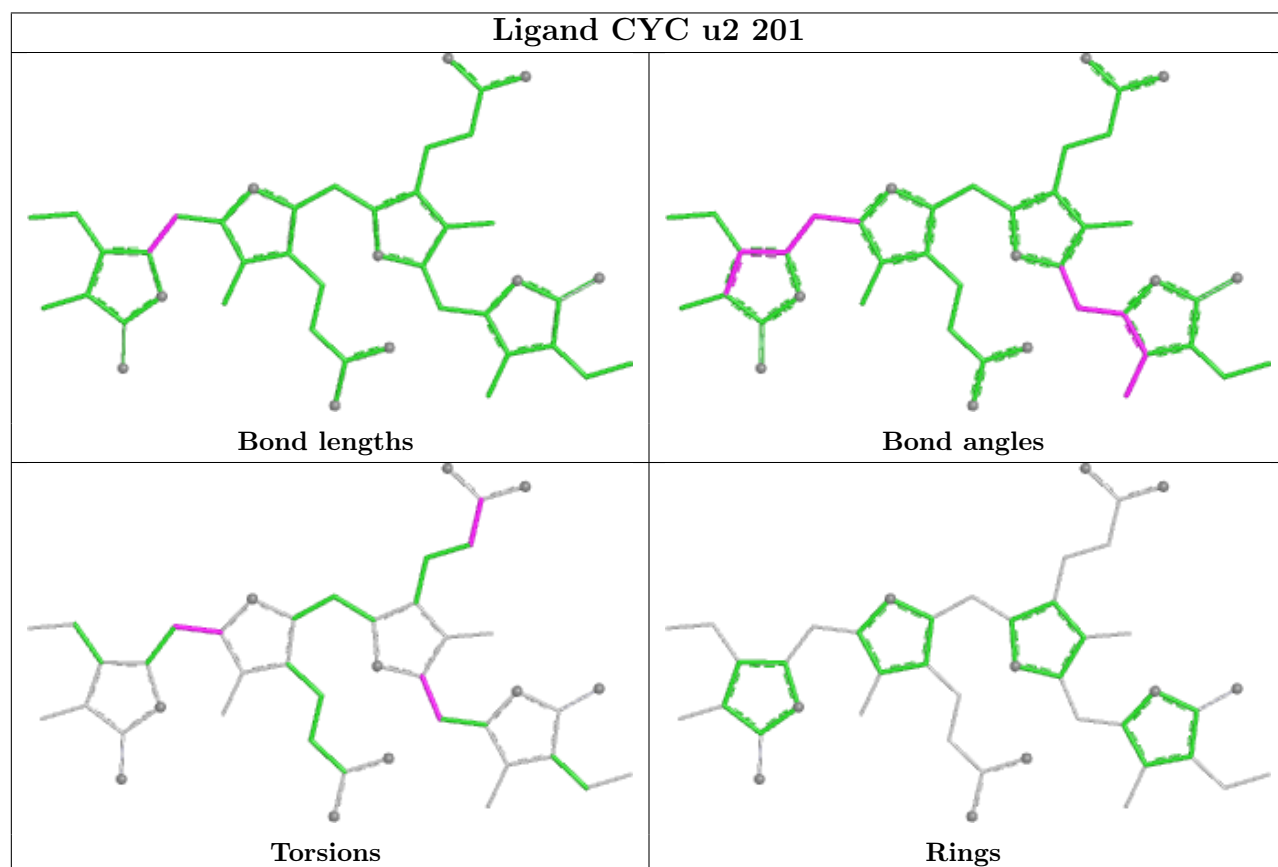
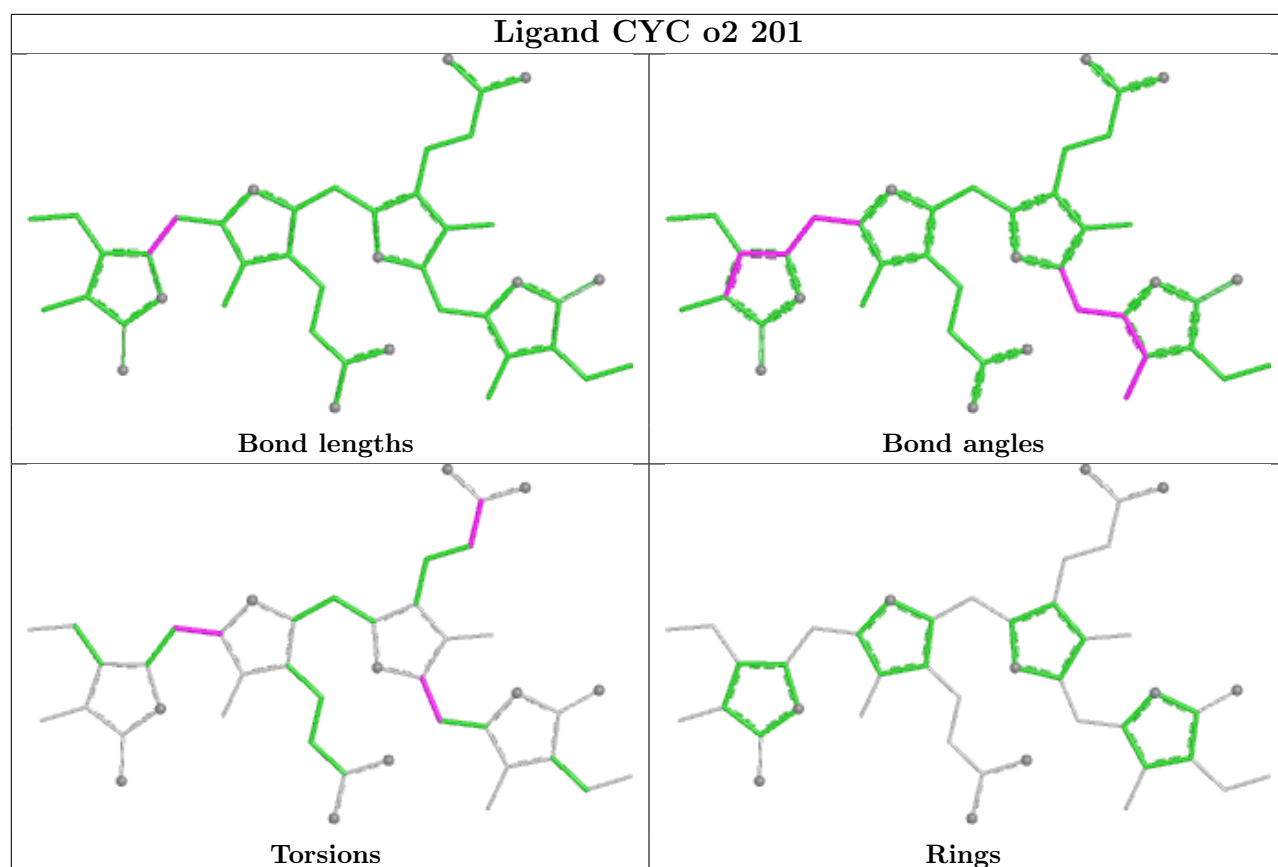


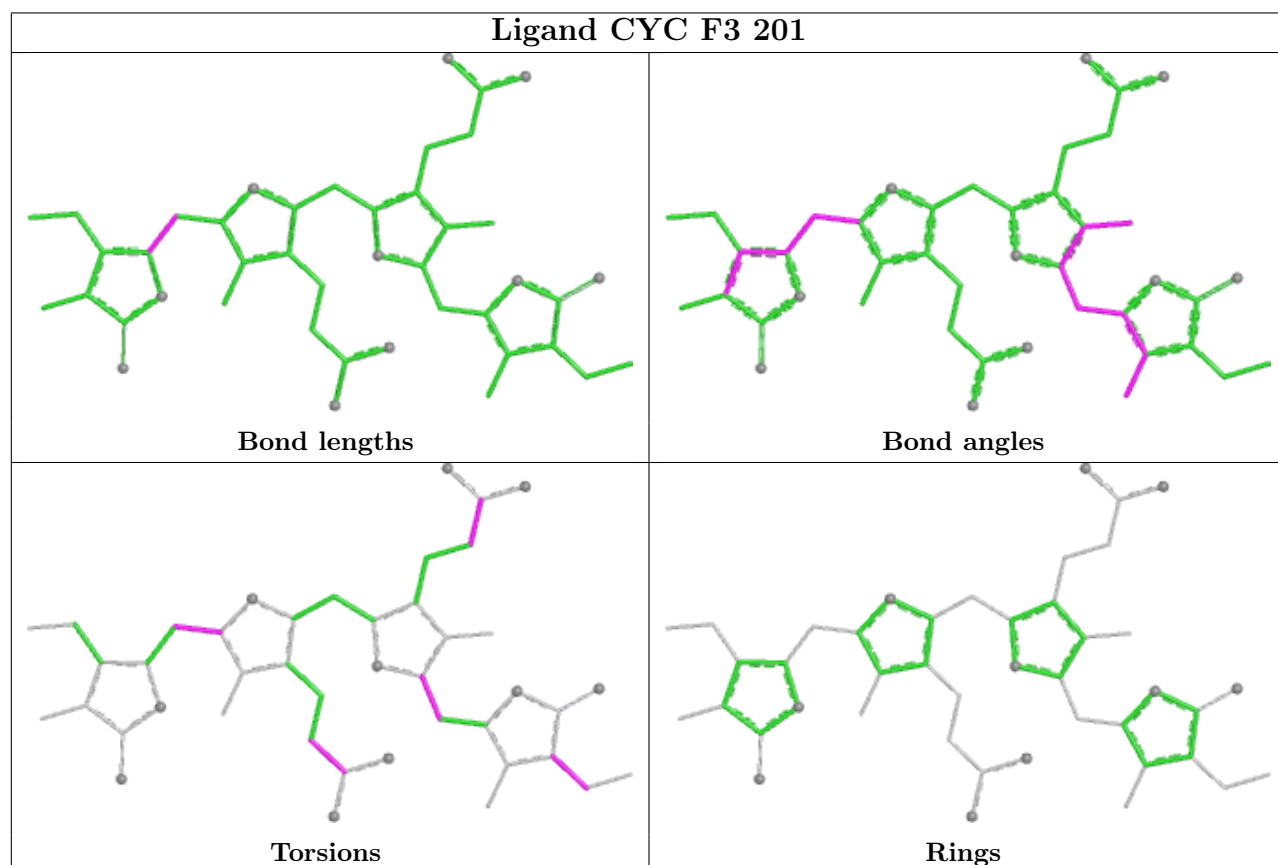
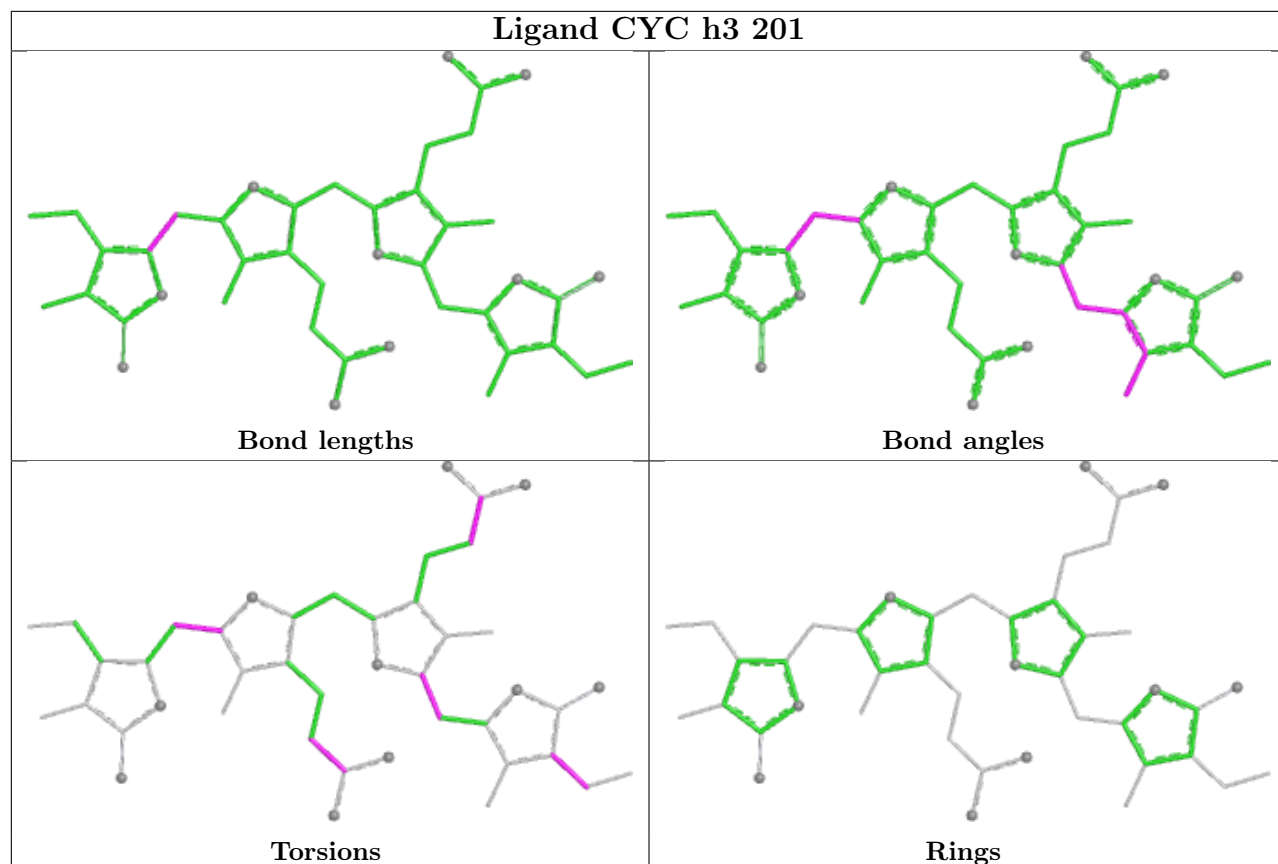
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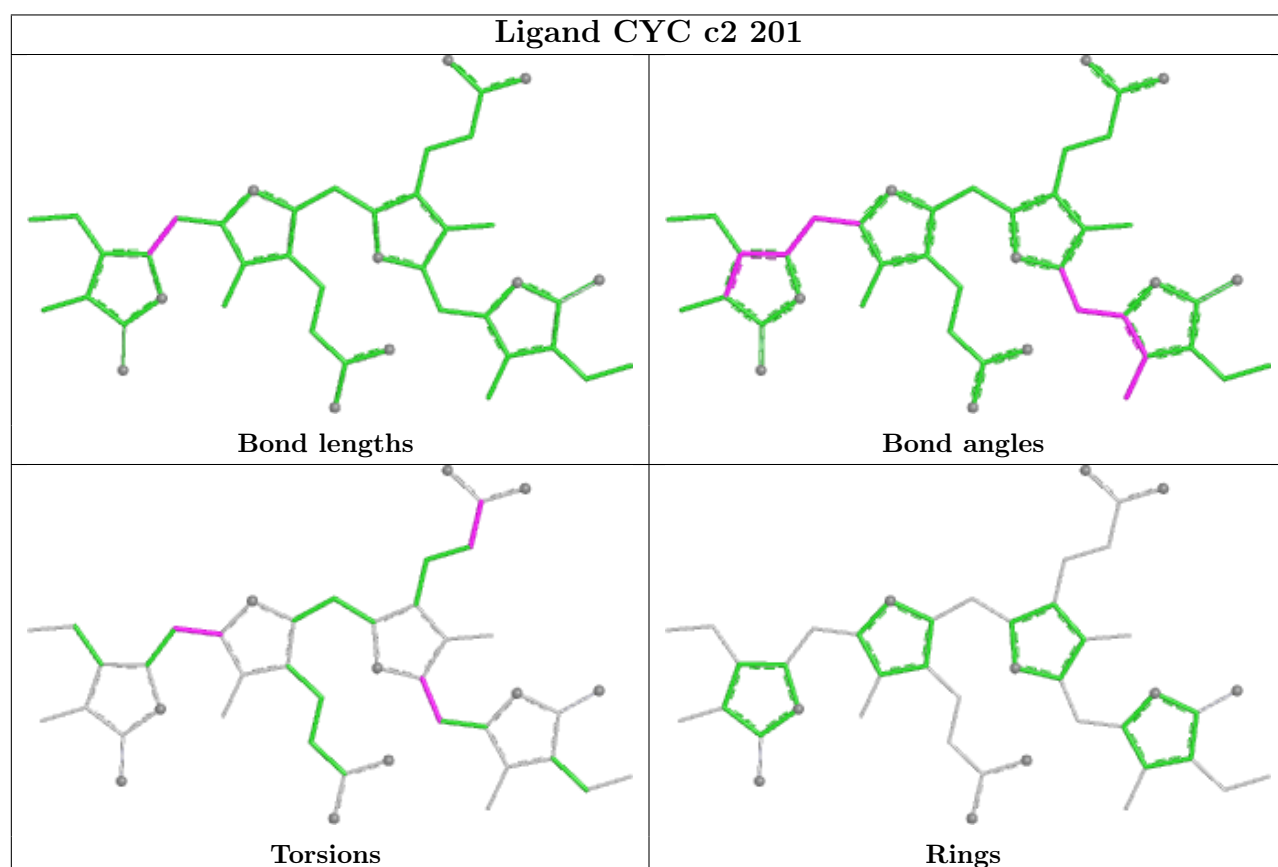
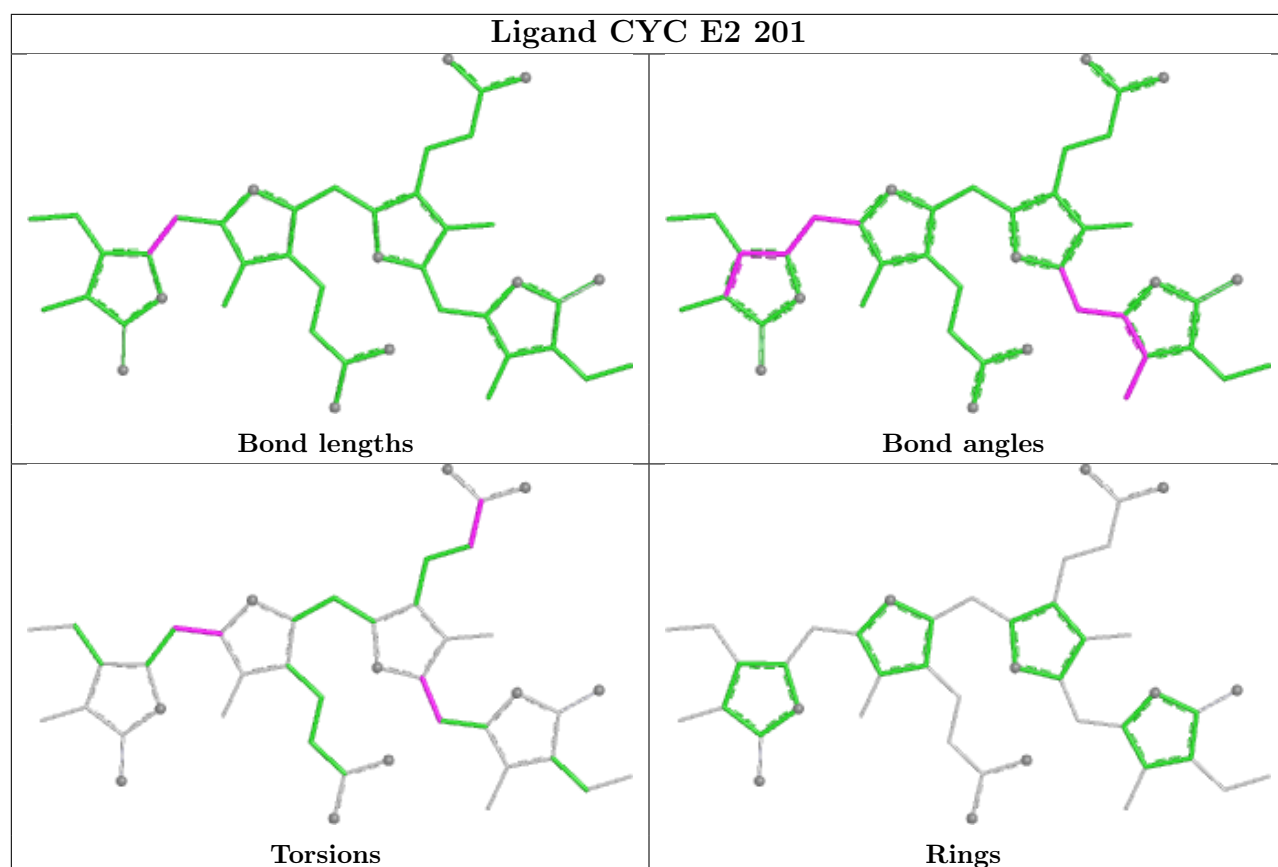


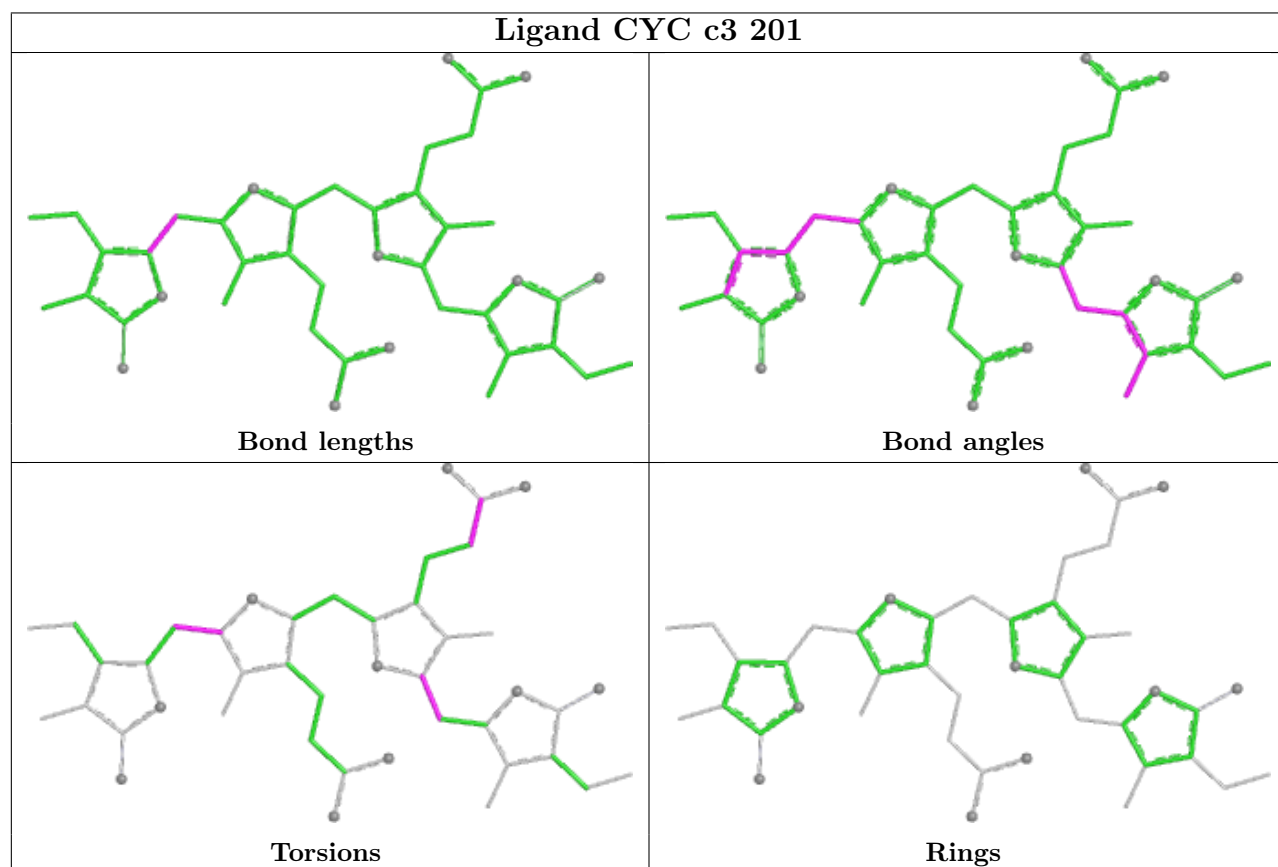
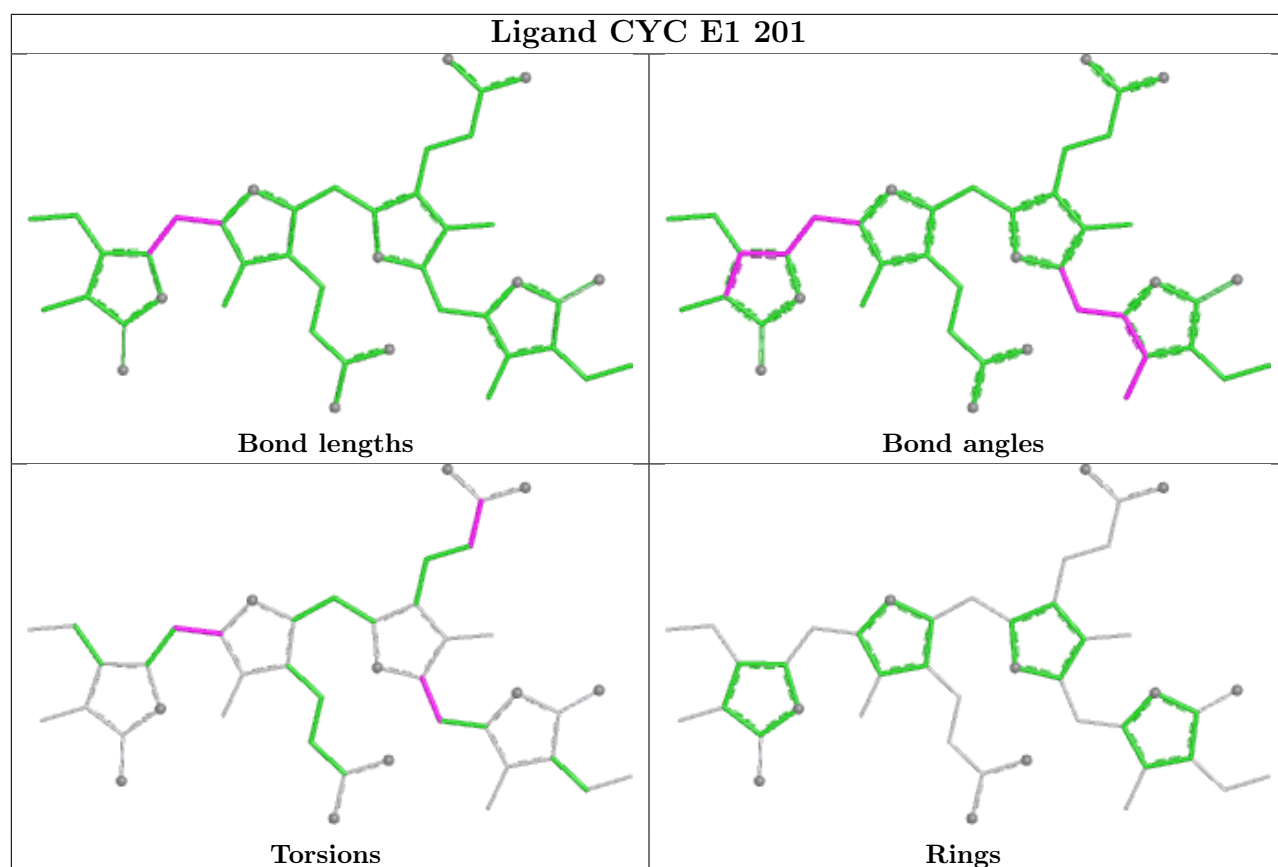
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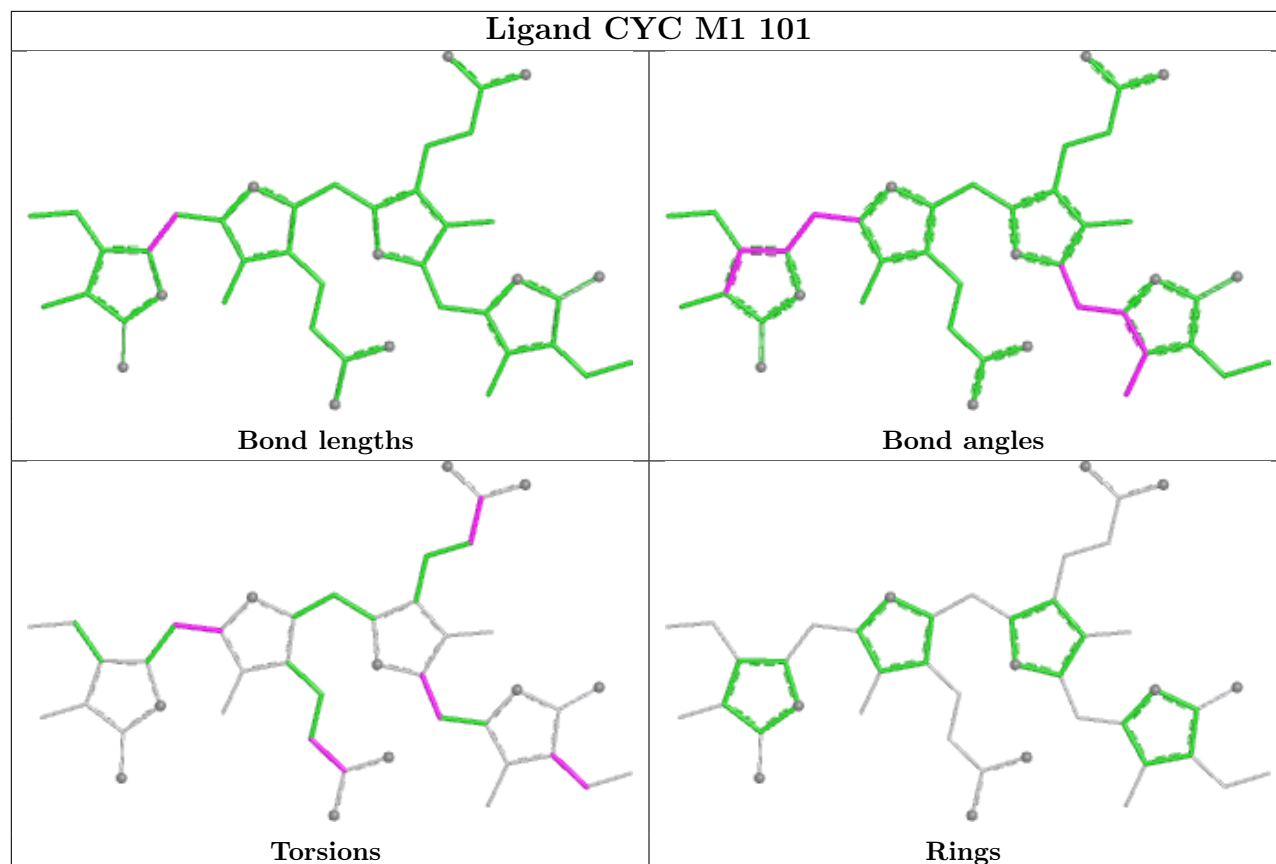




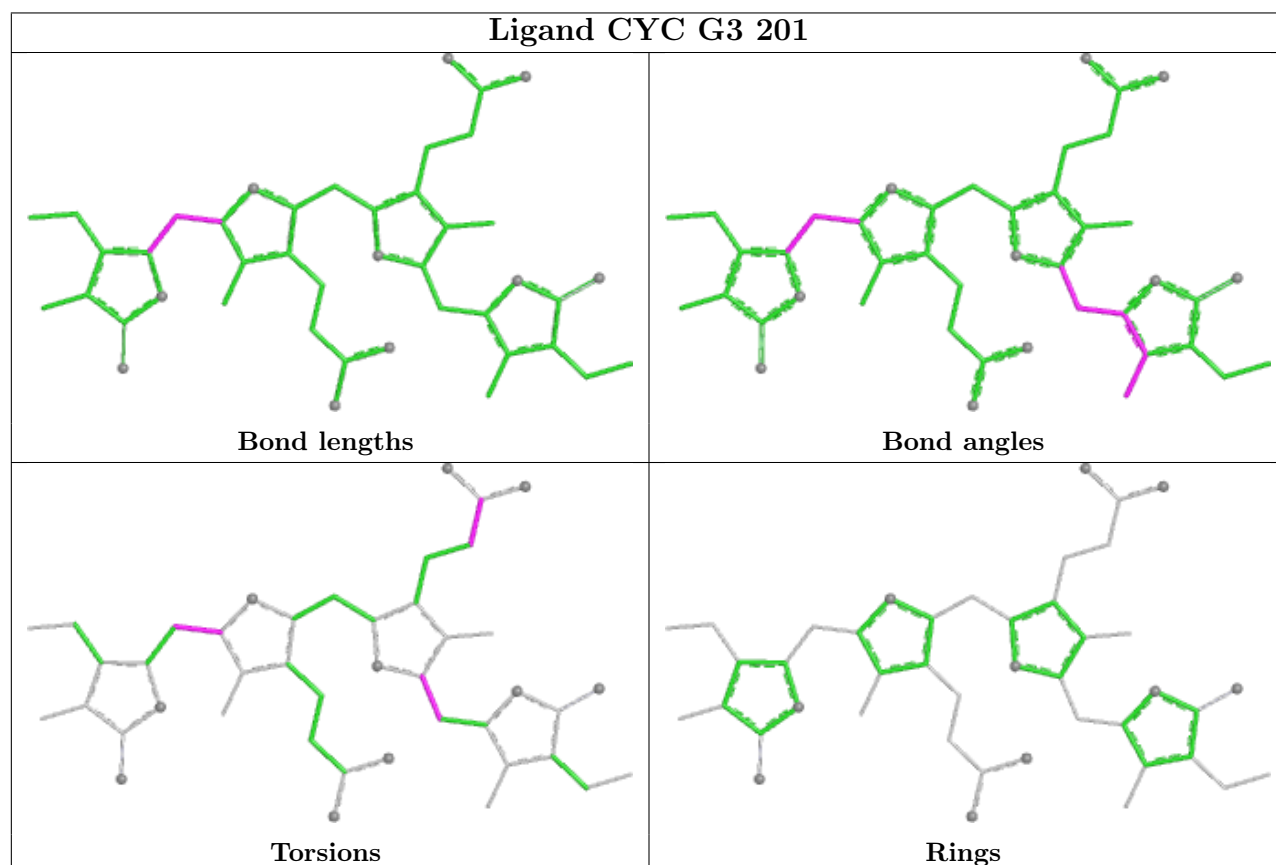


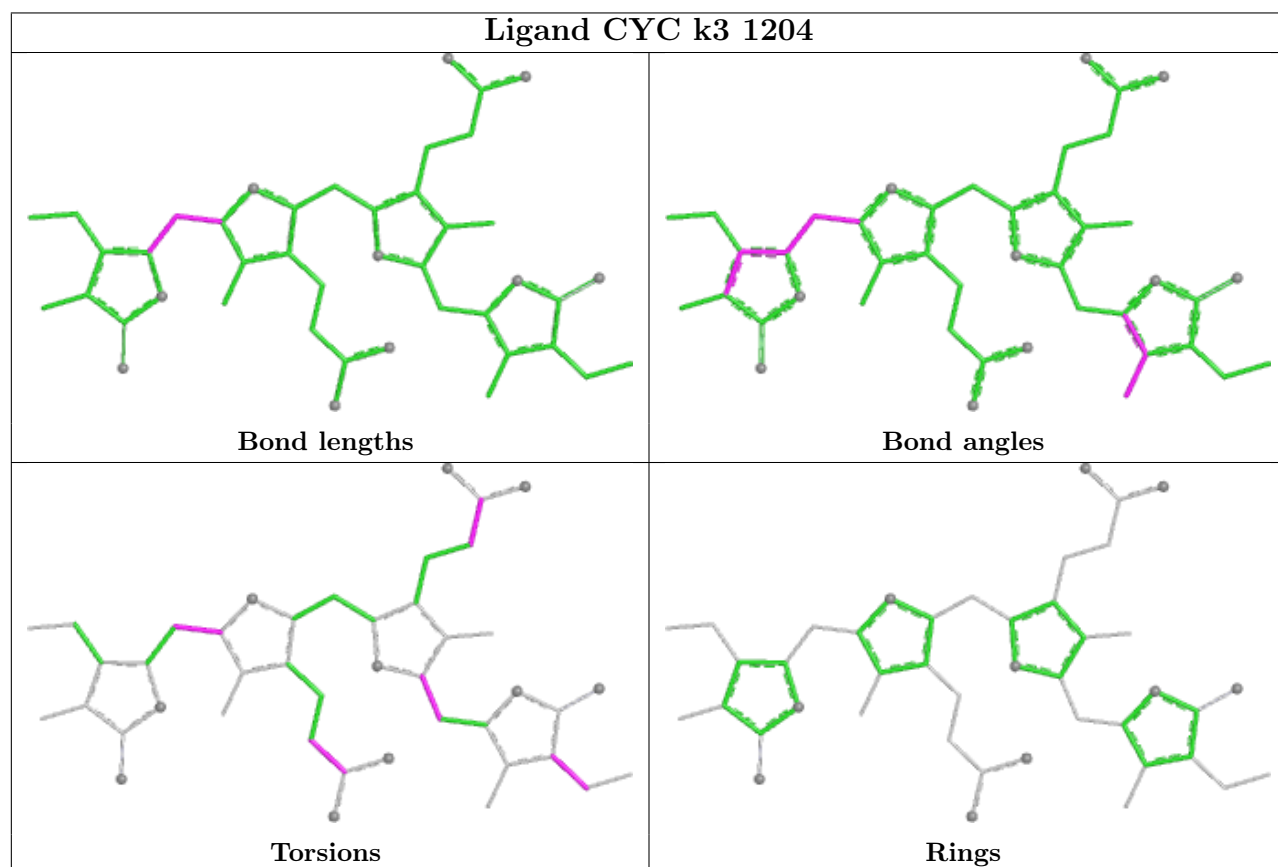
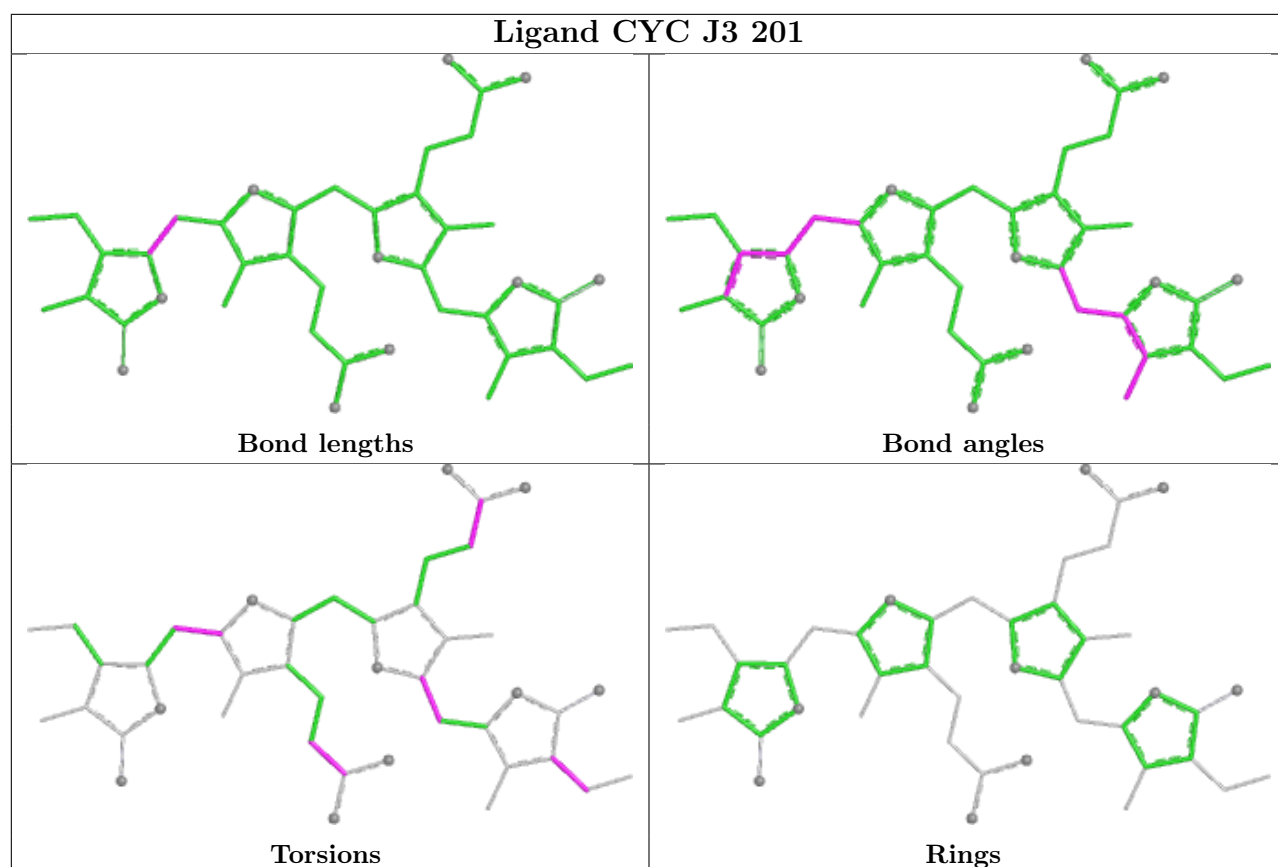


Ligand CYC M1 101

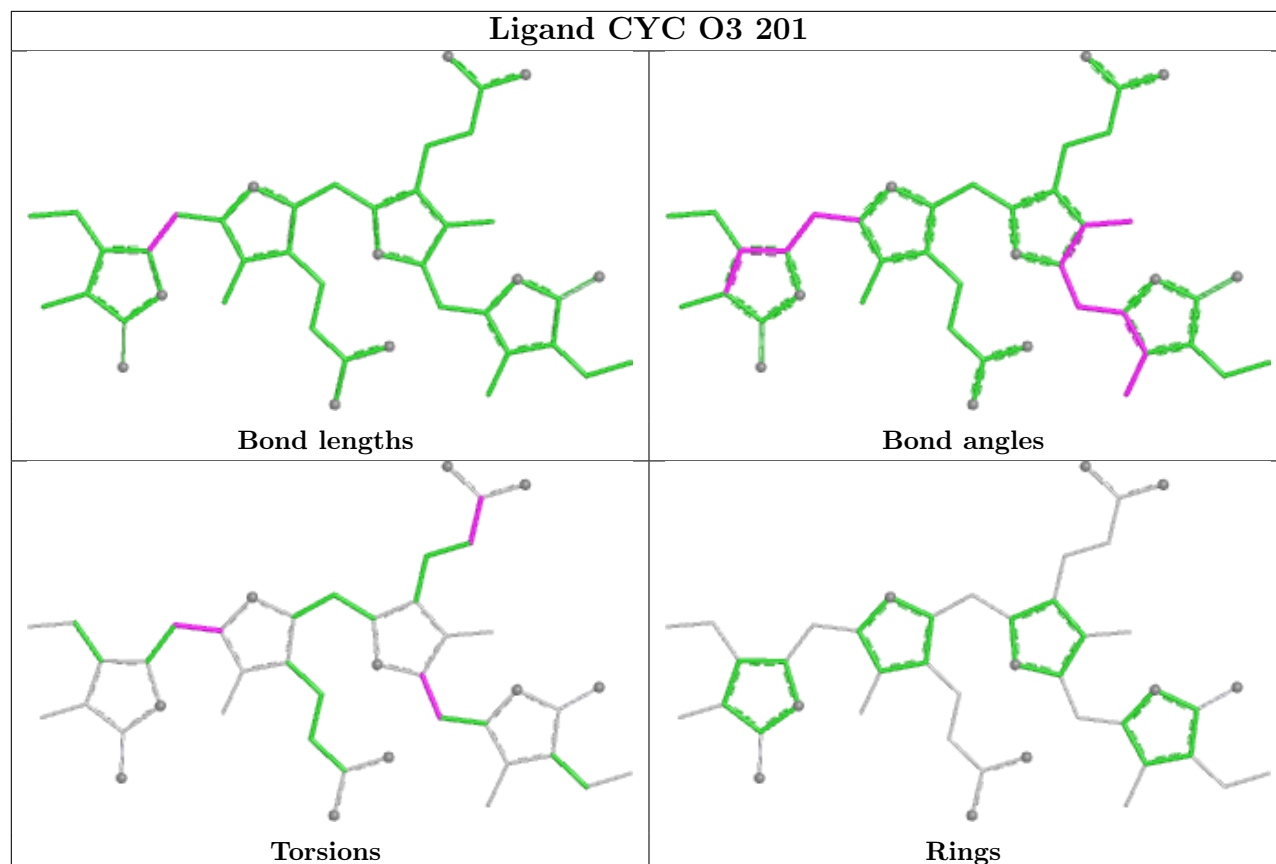


Ligand CYC G3 201

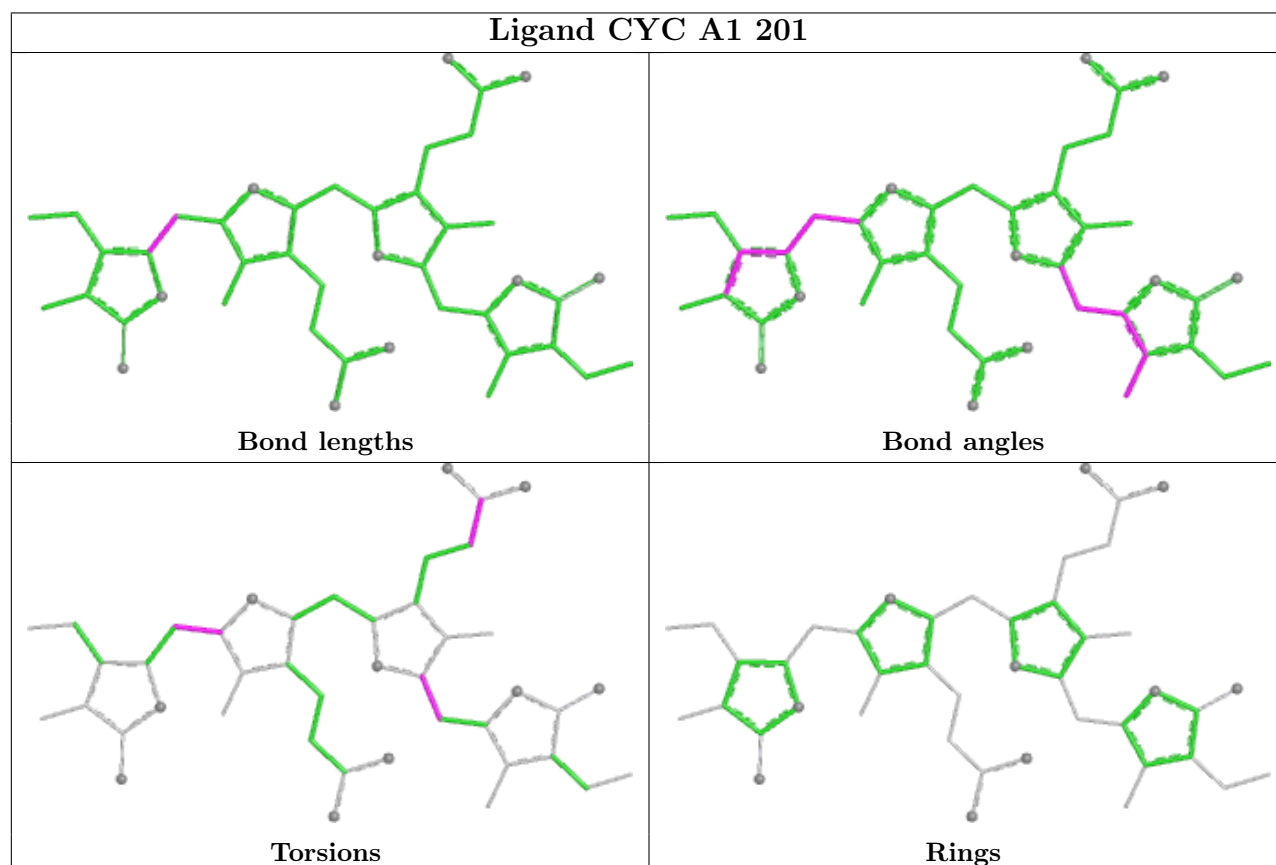


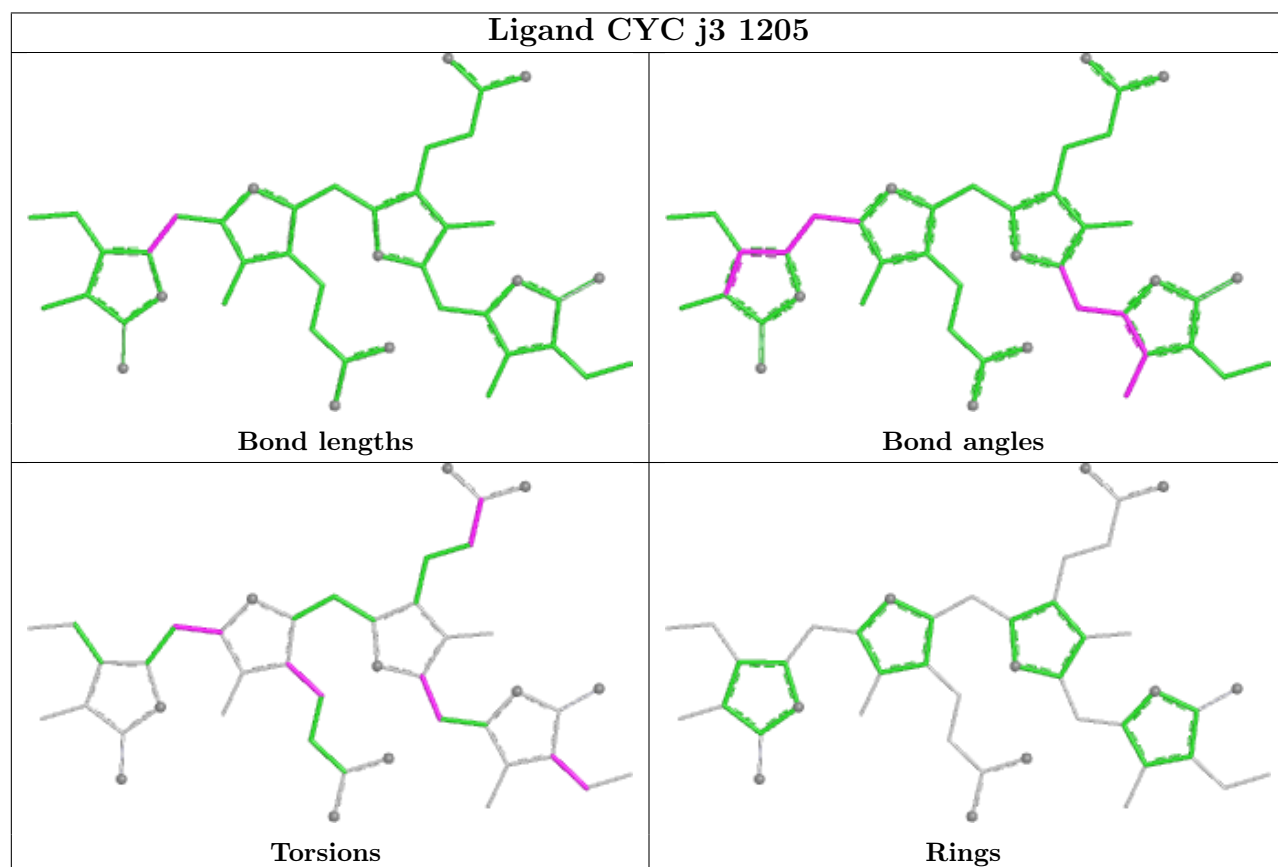
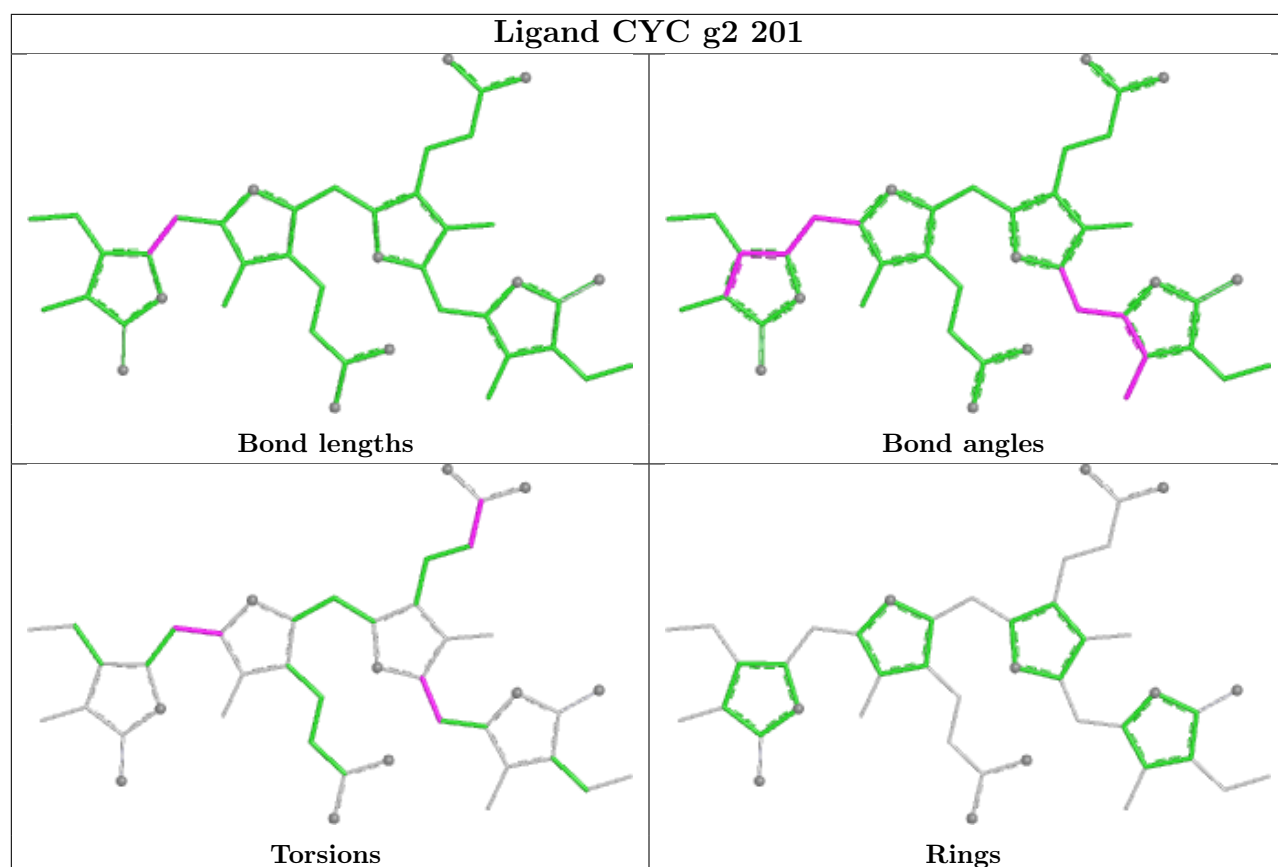


Ligand CYC O3 201

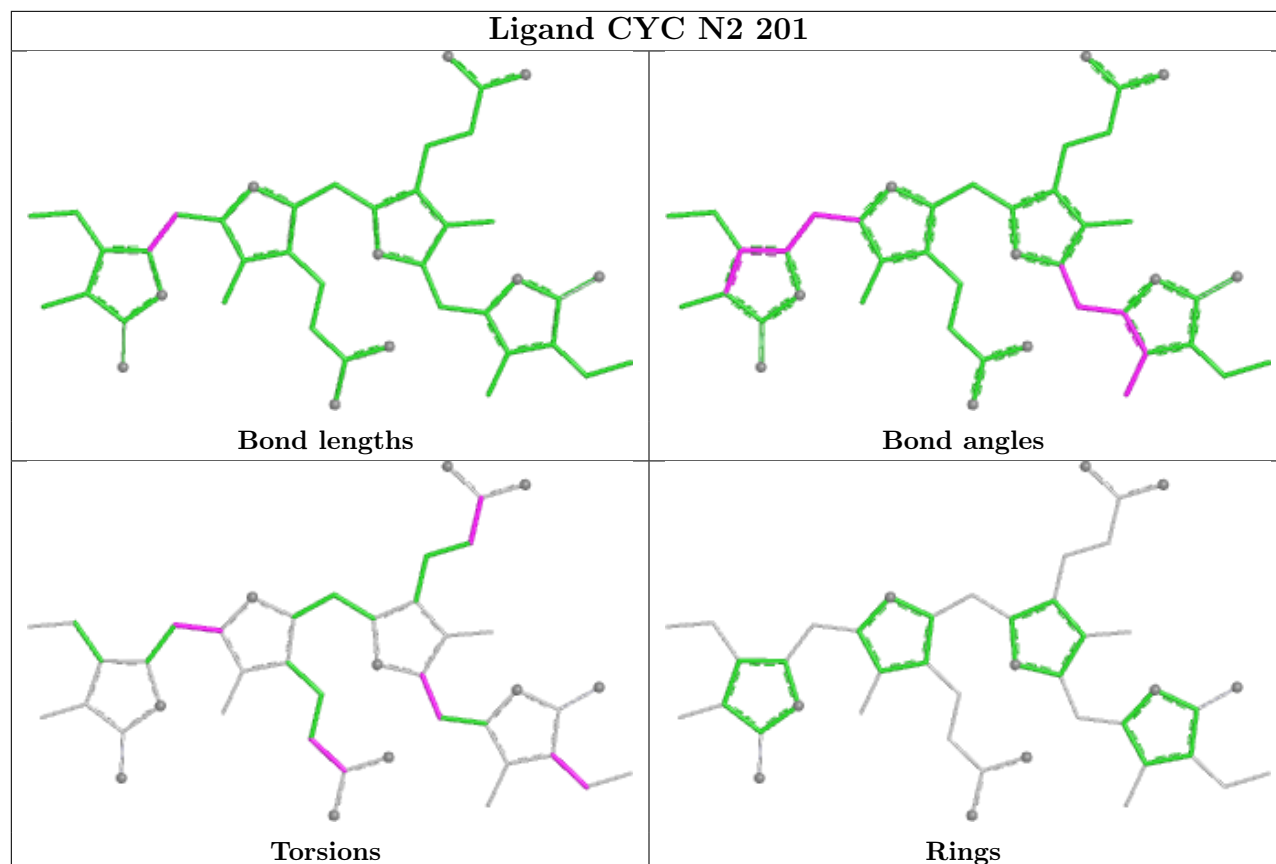


Ligand CYC A1 201

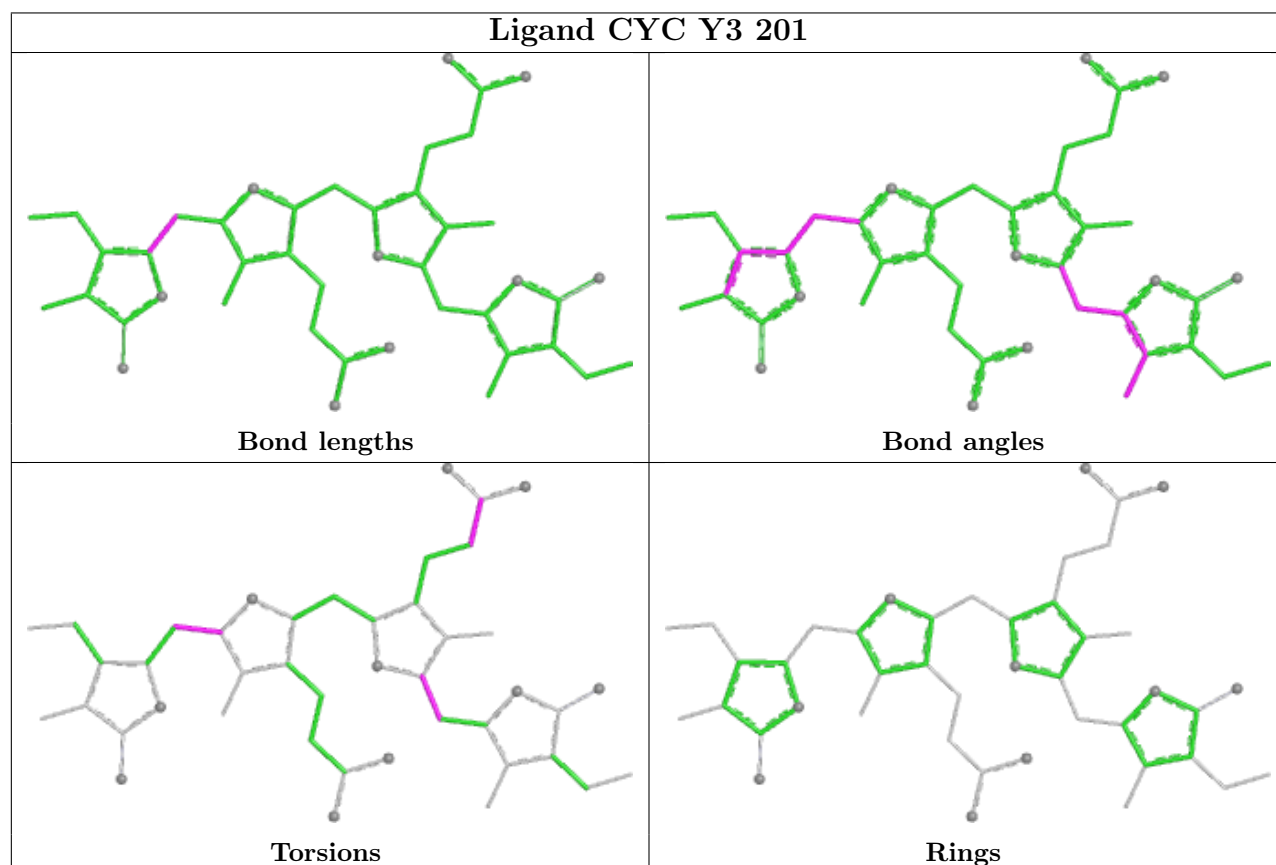




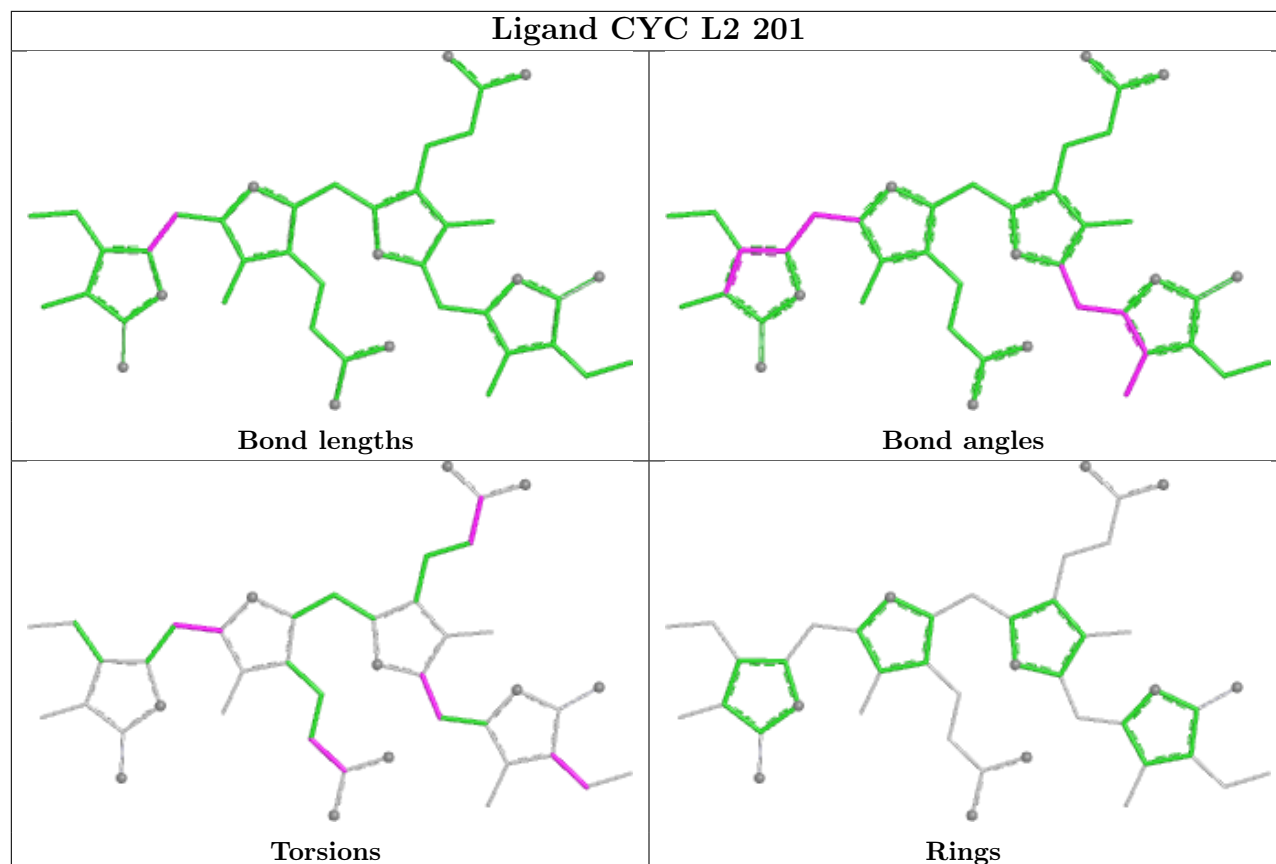
Ligand CYC N2 201



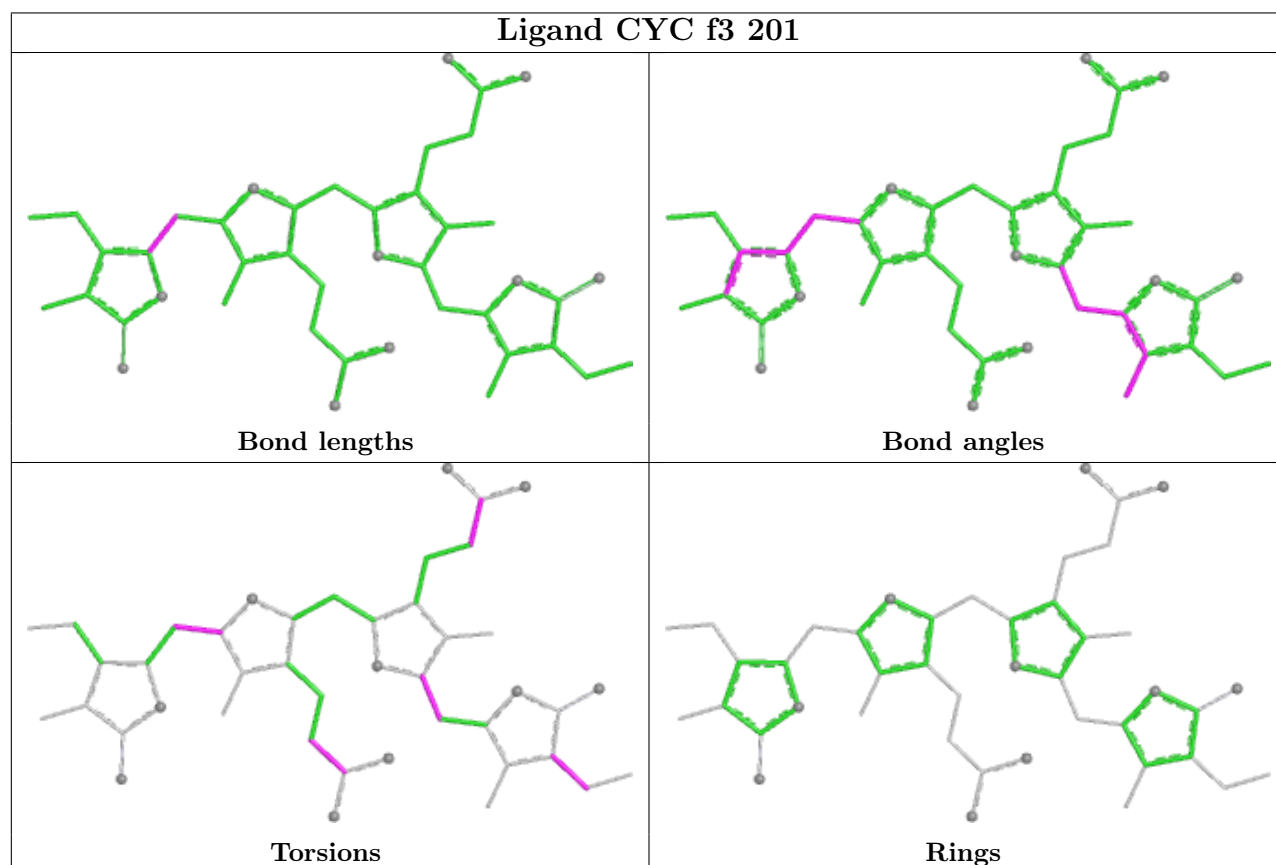
Ligand CYC Y3 201

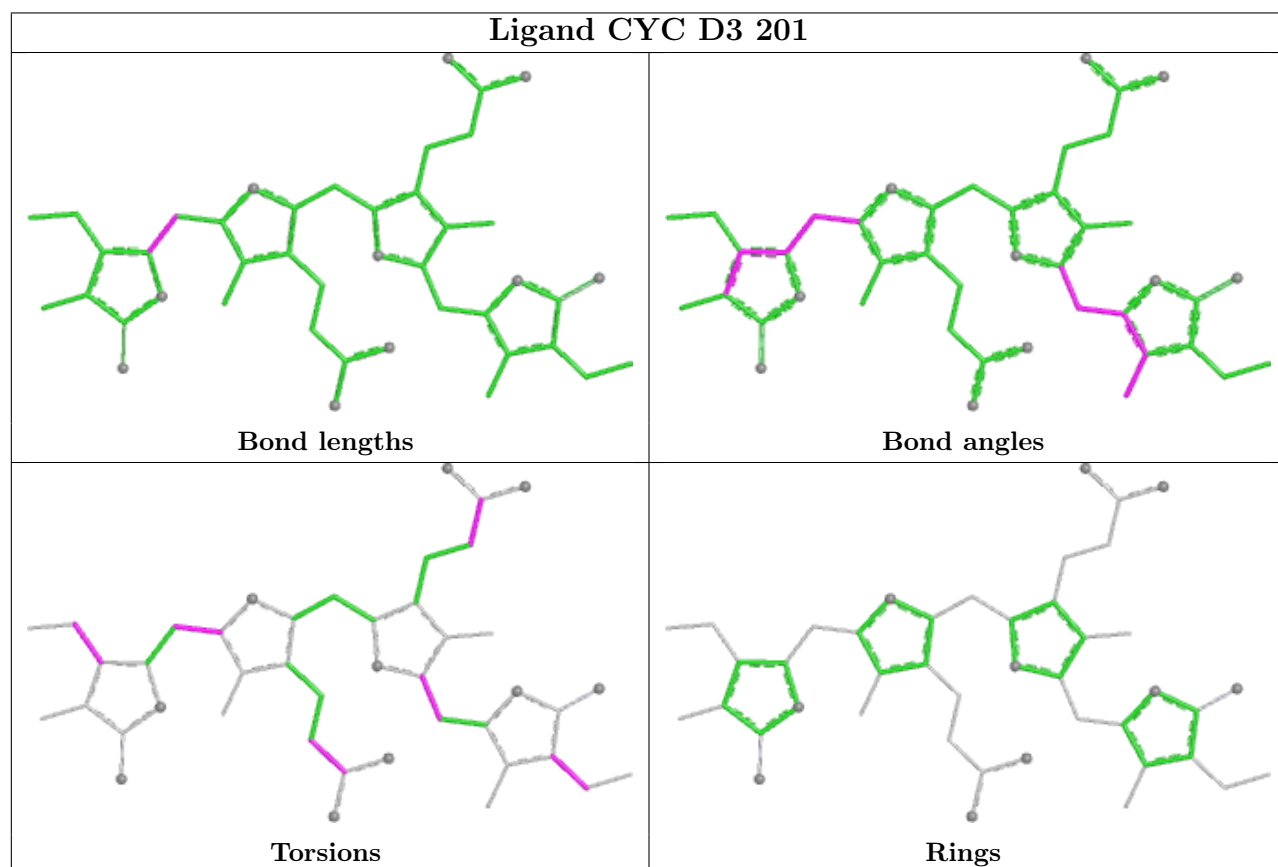
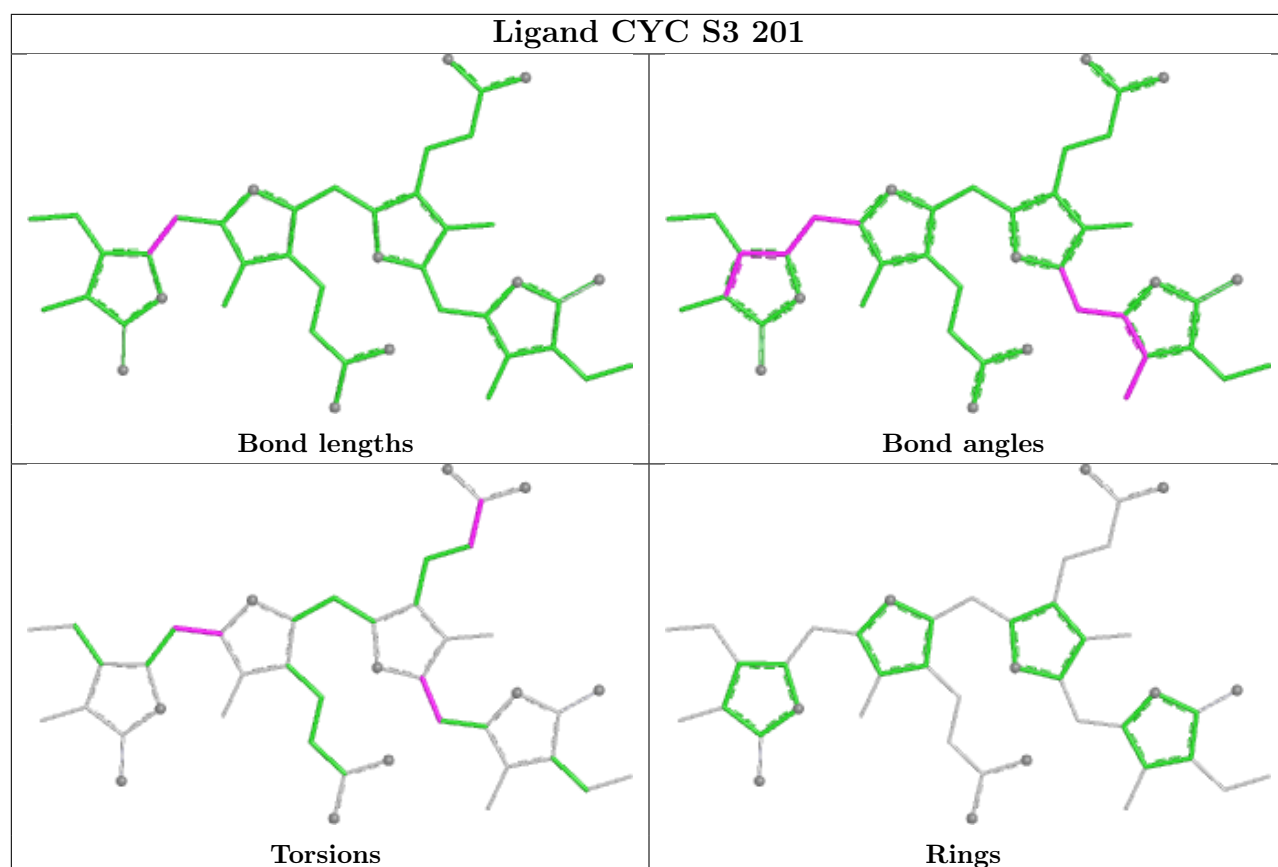


Ligand CYC L2 201

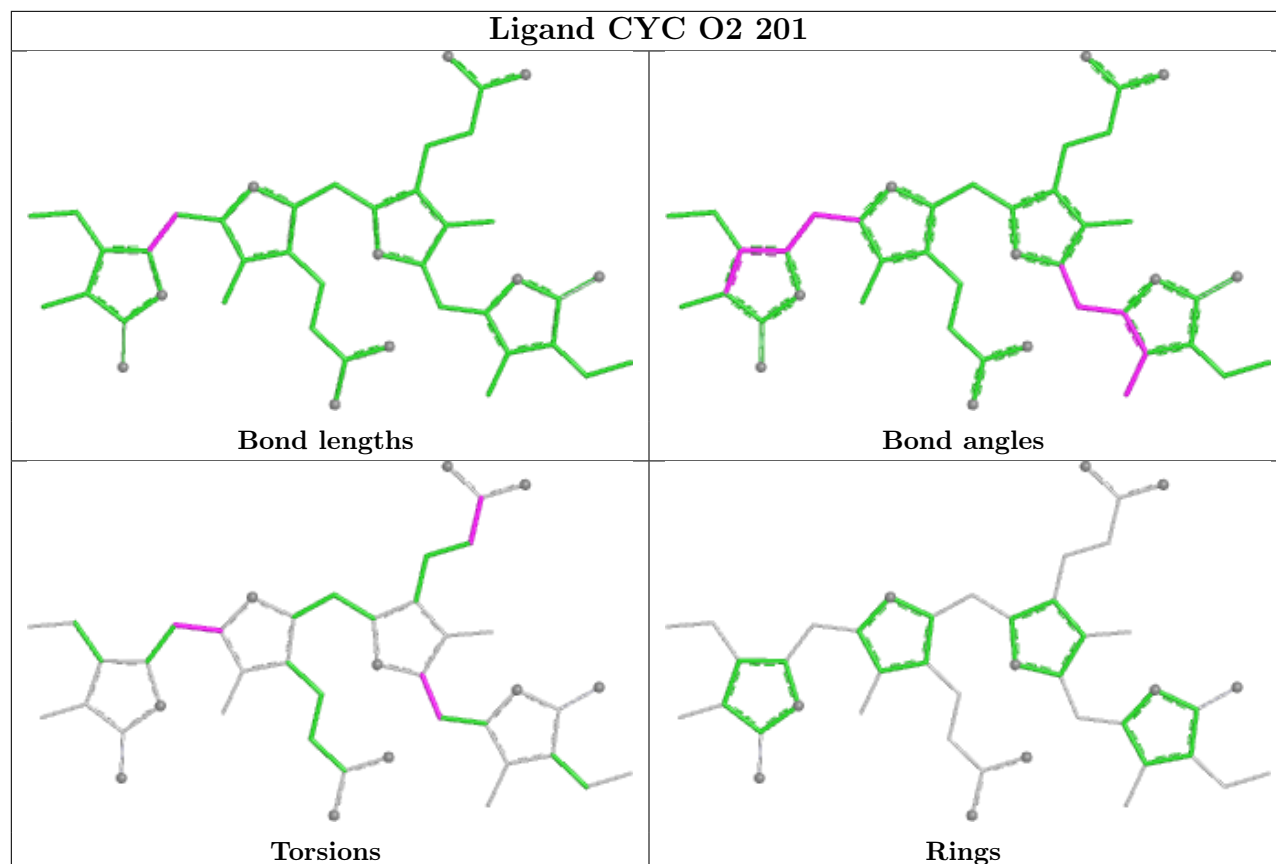


Ligand CYC f3 201

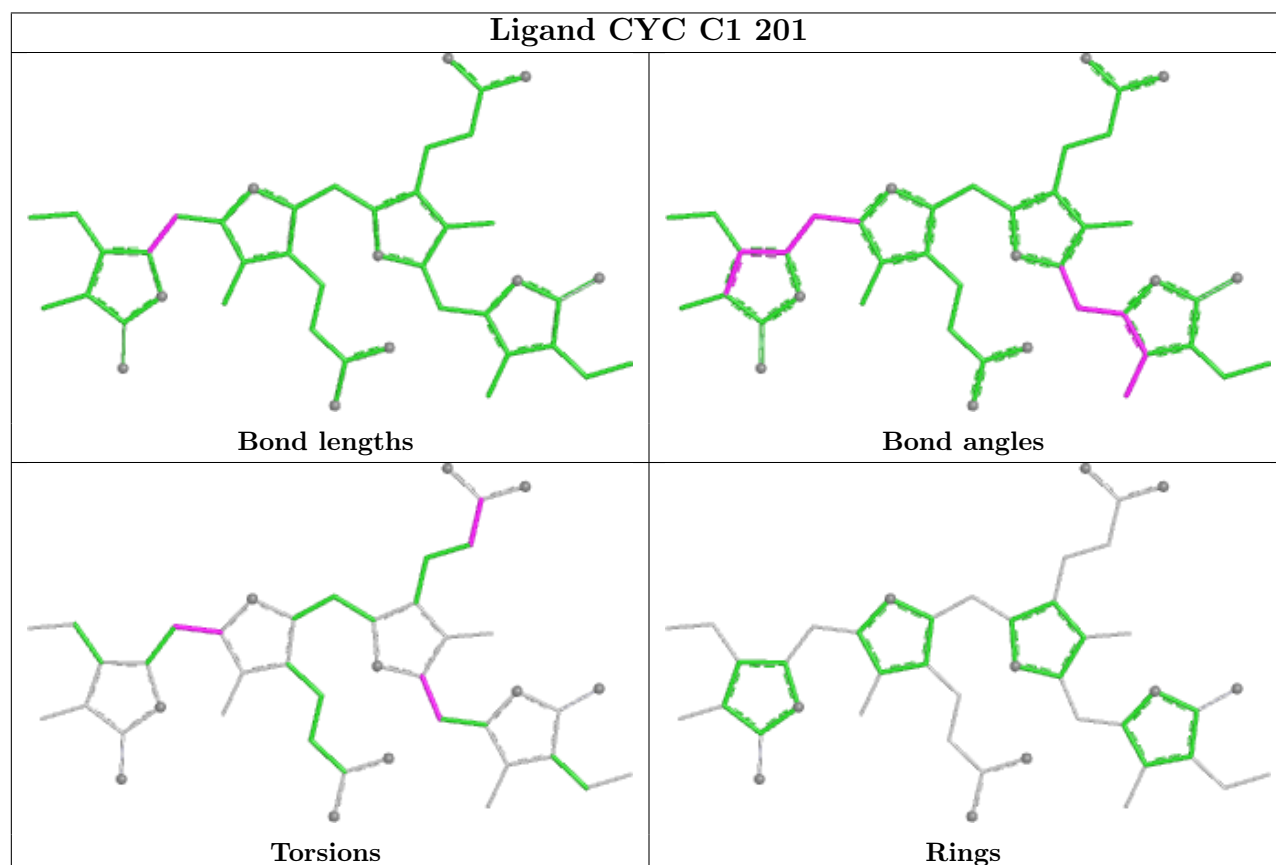


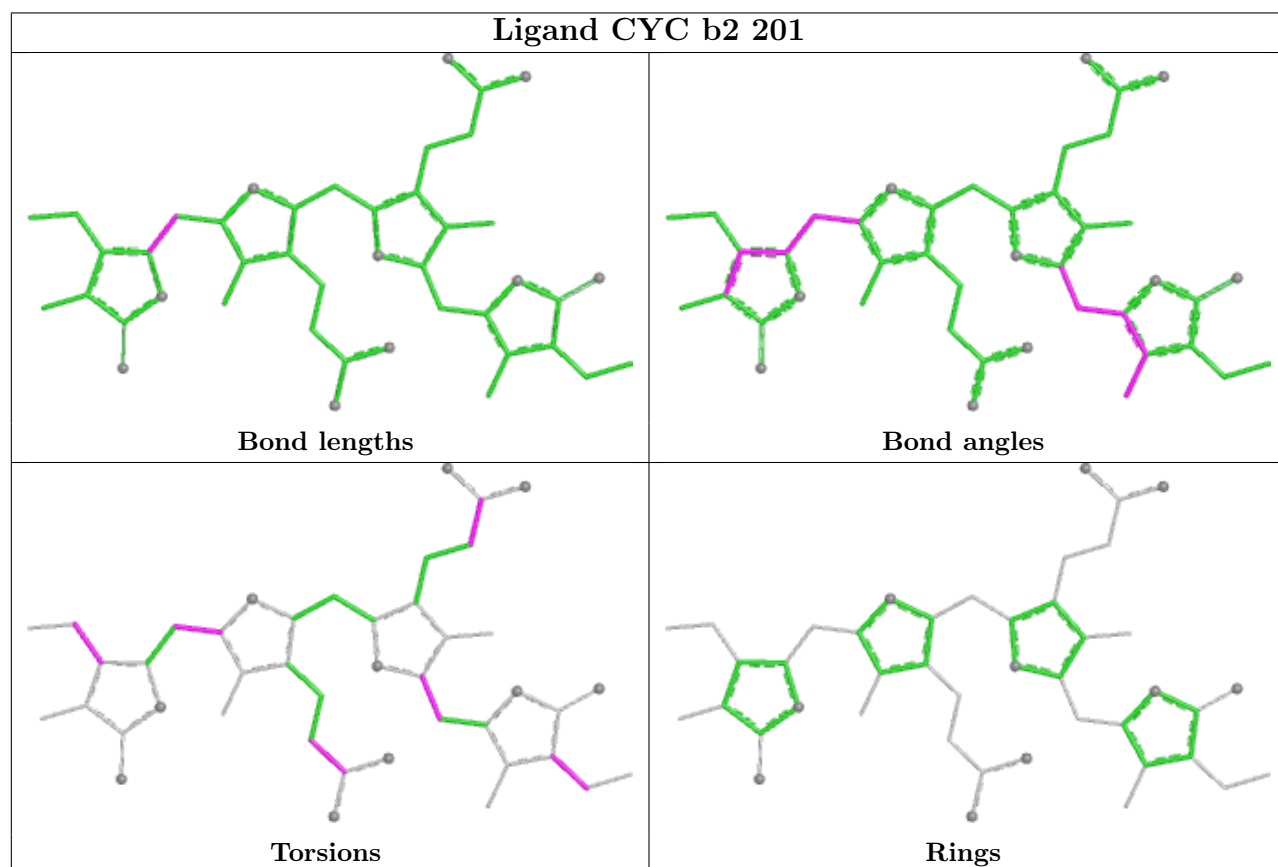
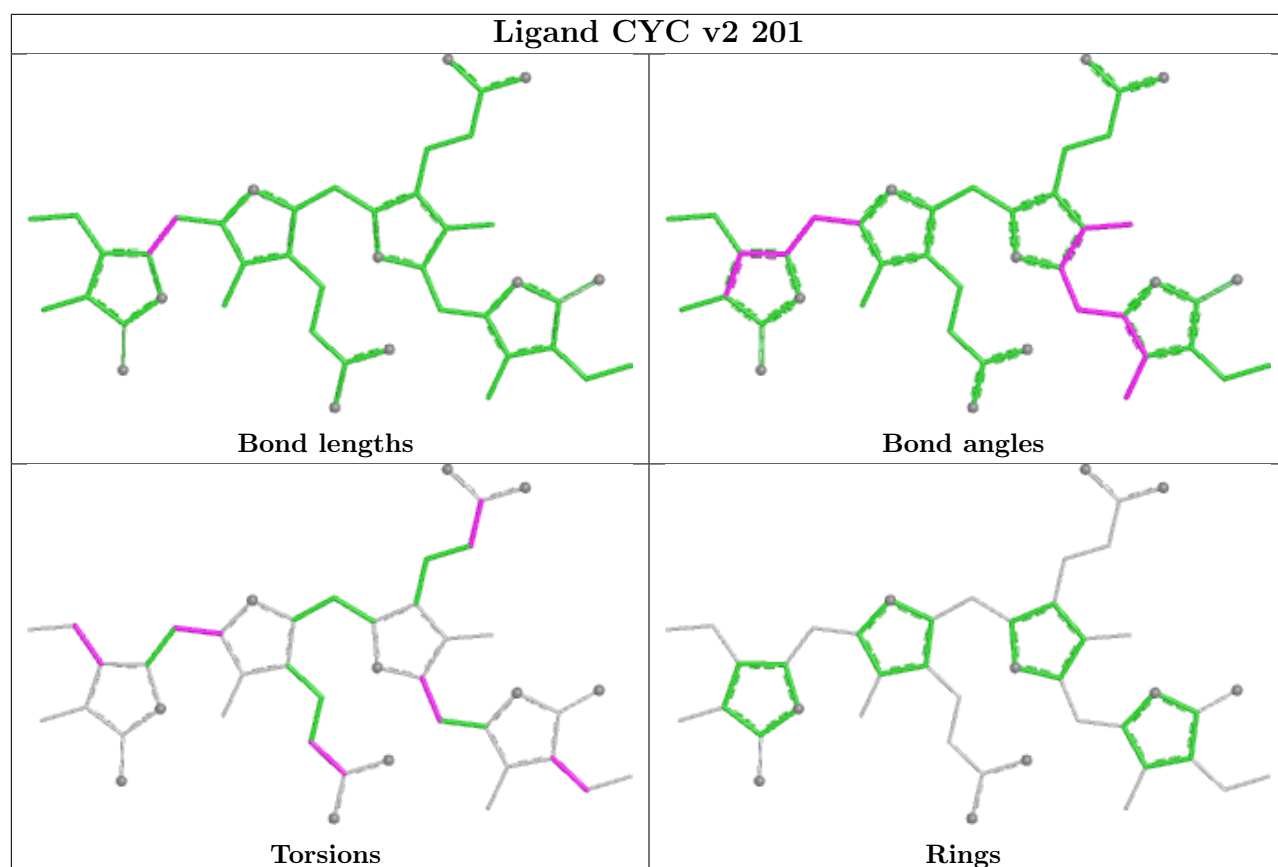


Ligand CYC O2 201

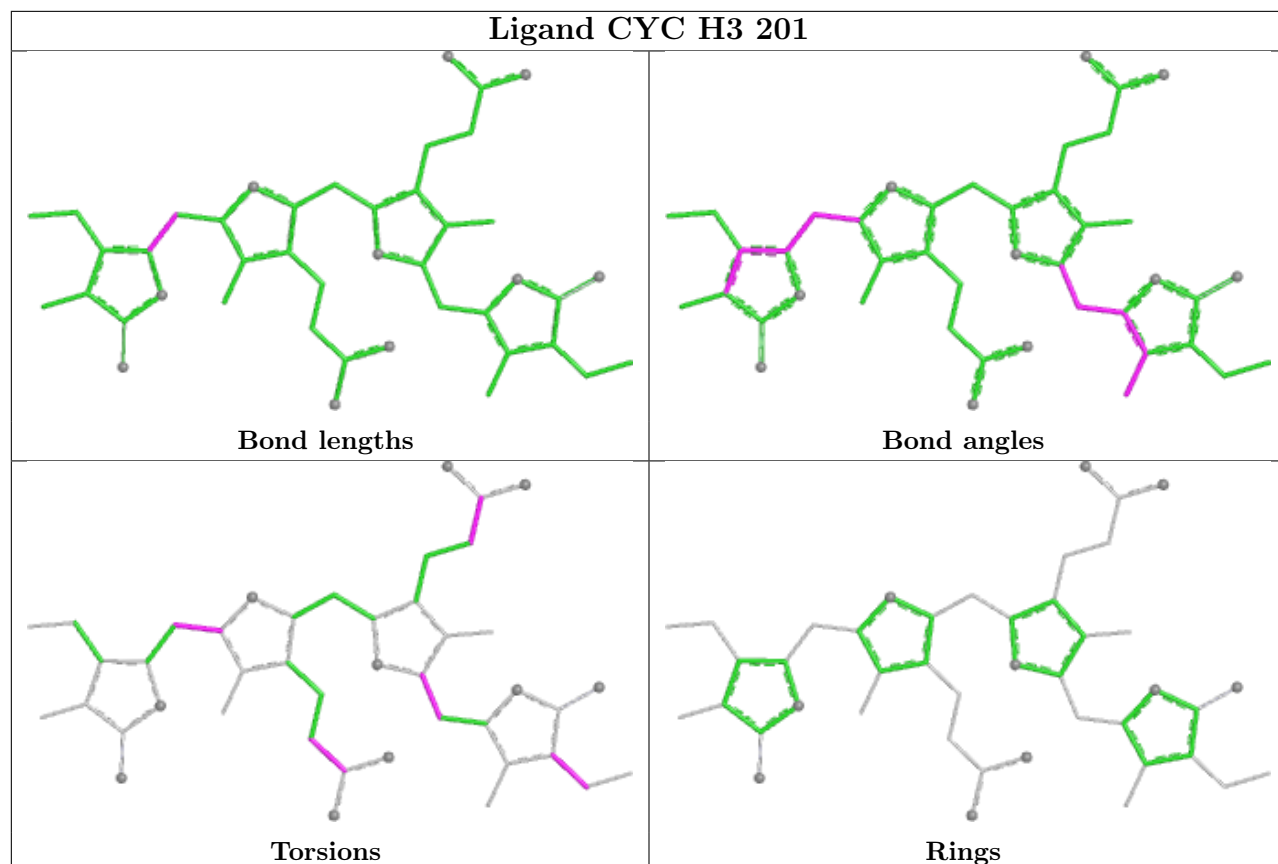


Ligand CYC C1 201

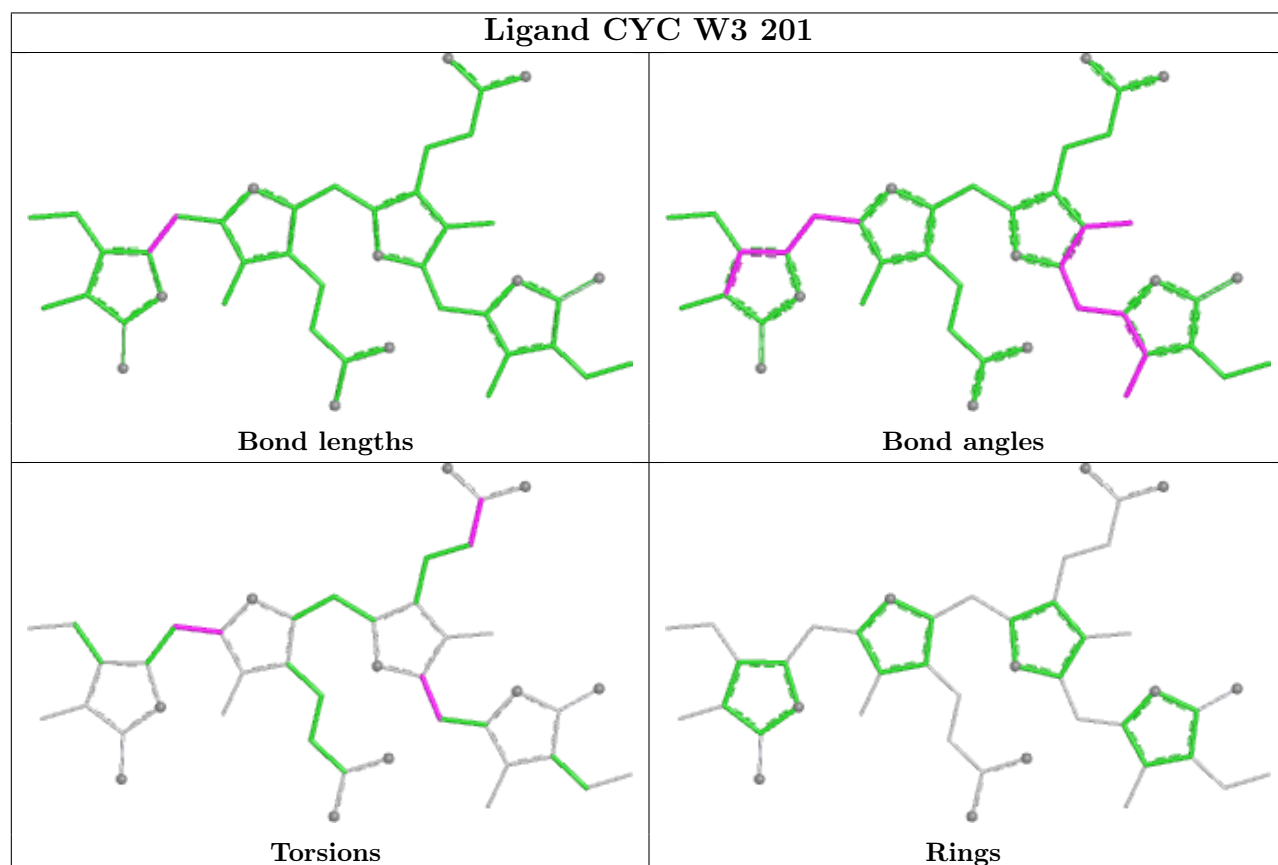


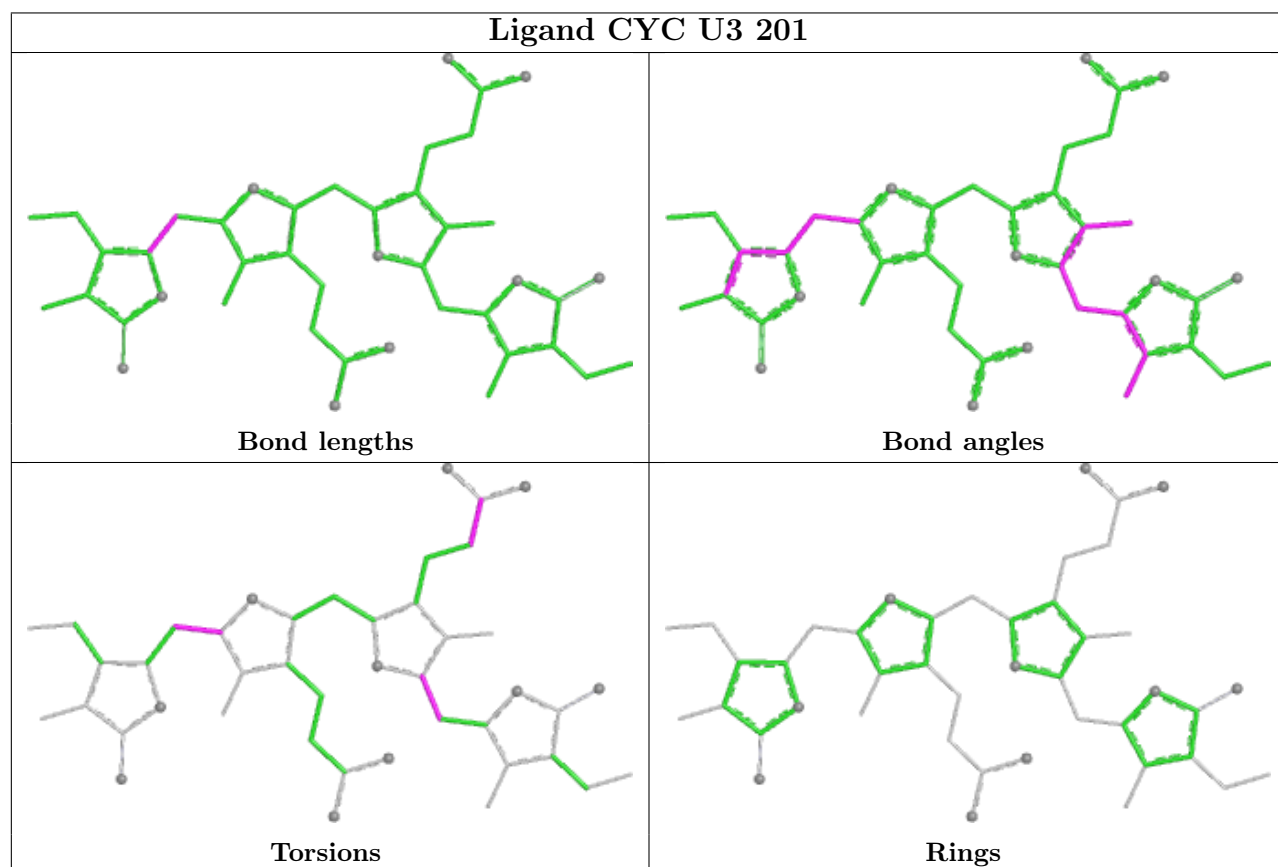
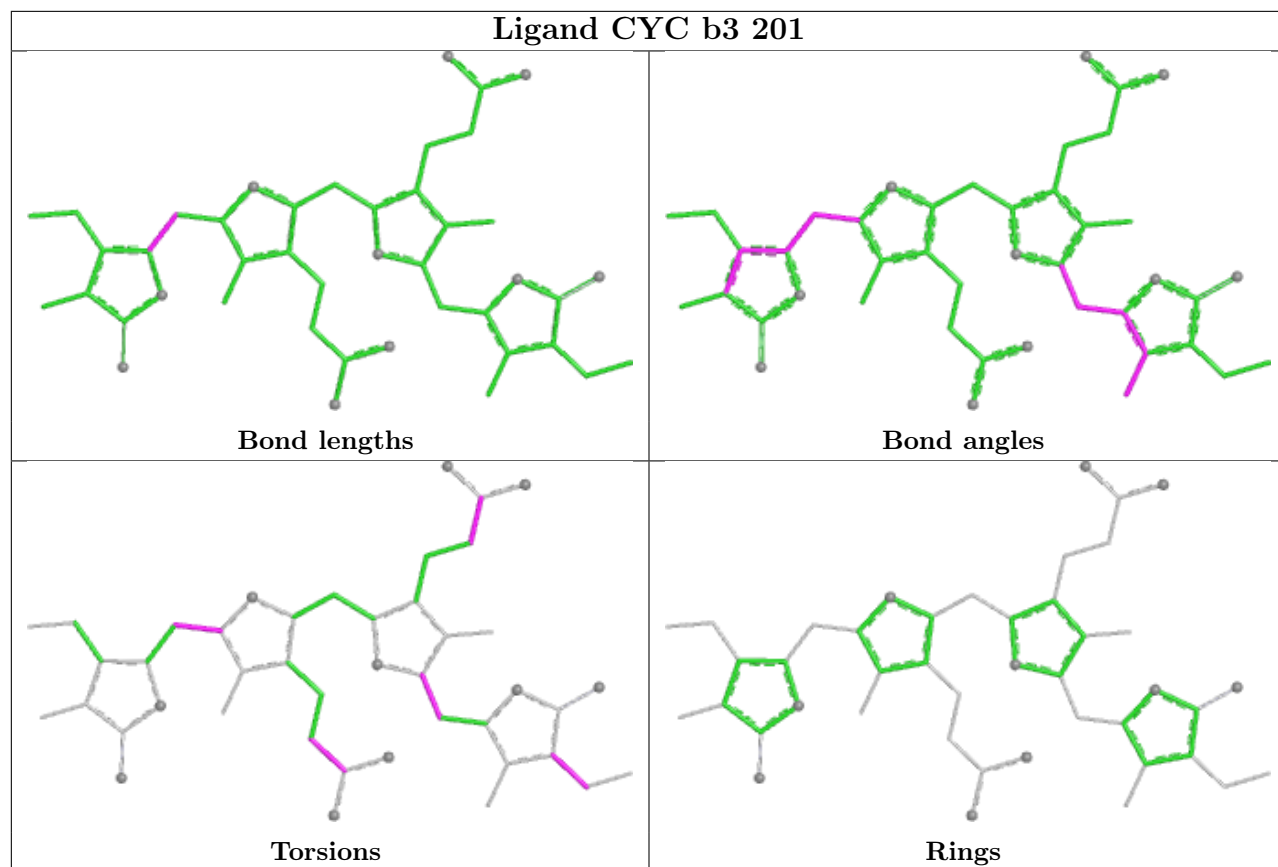


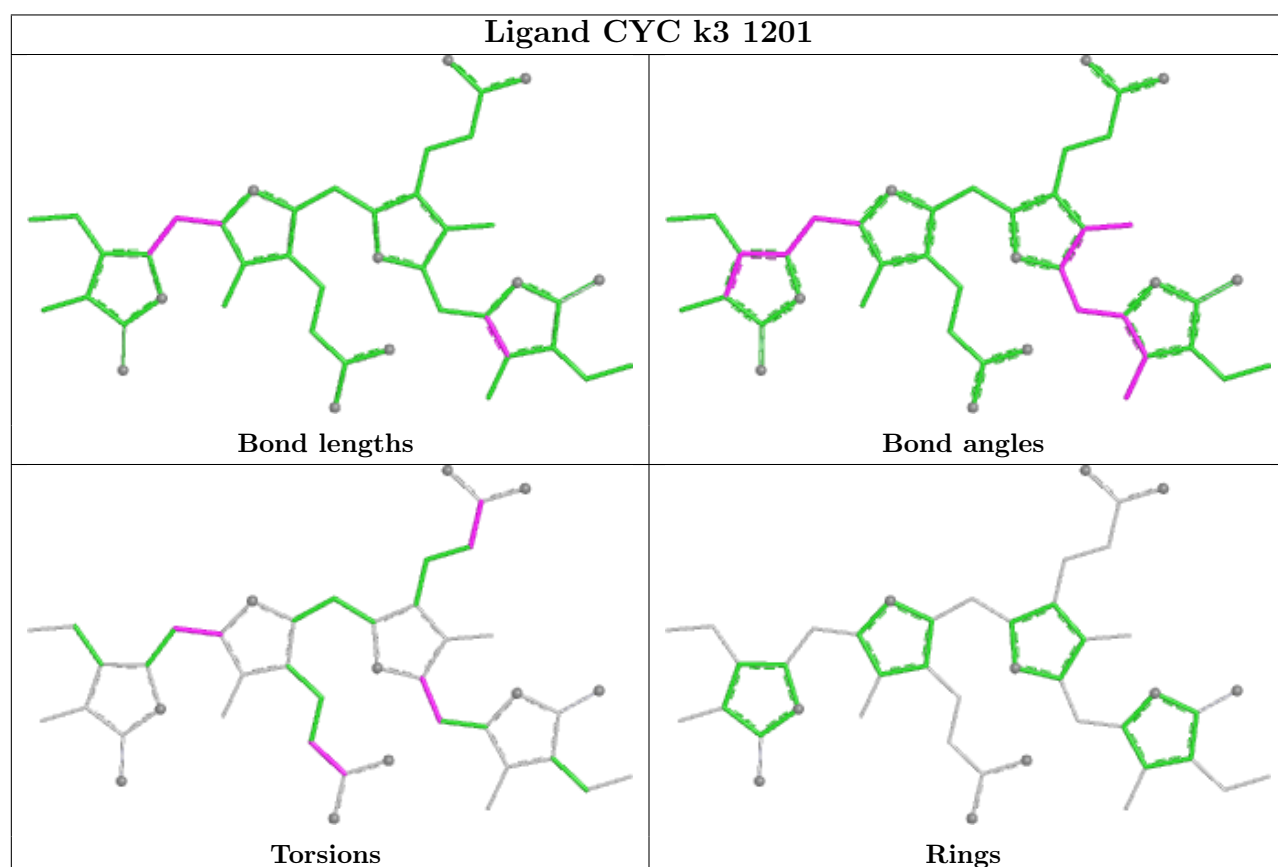
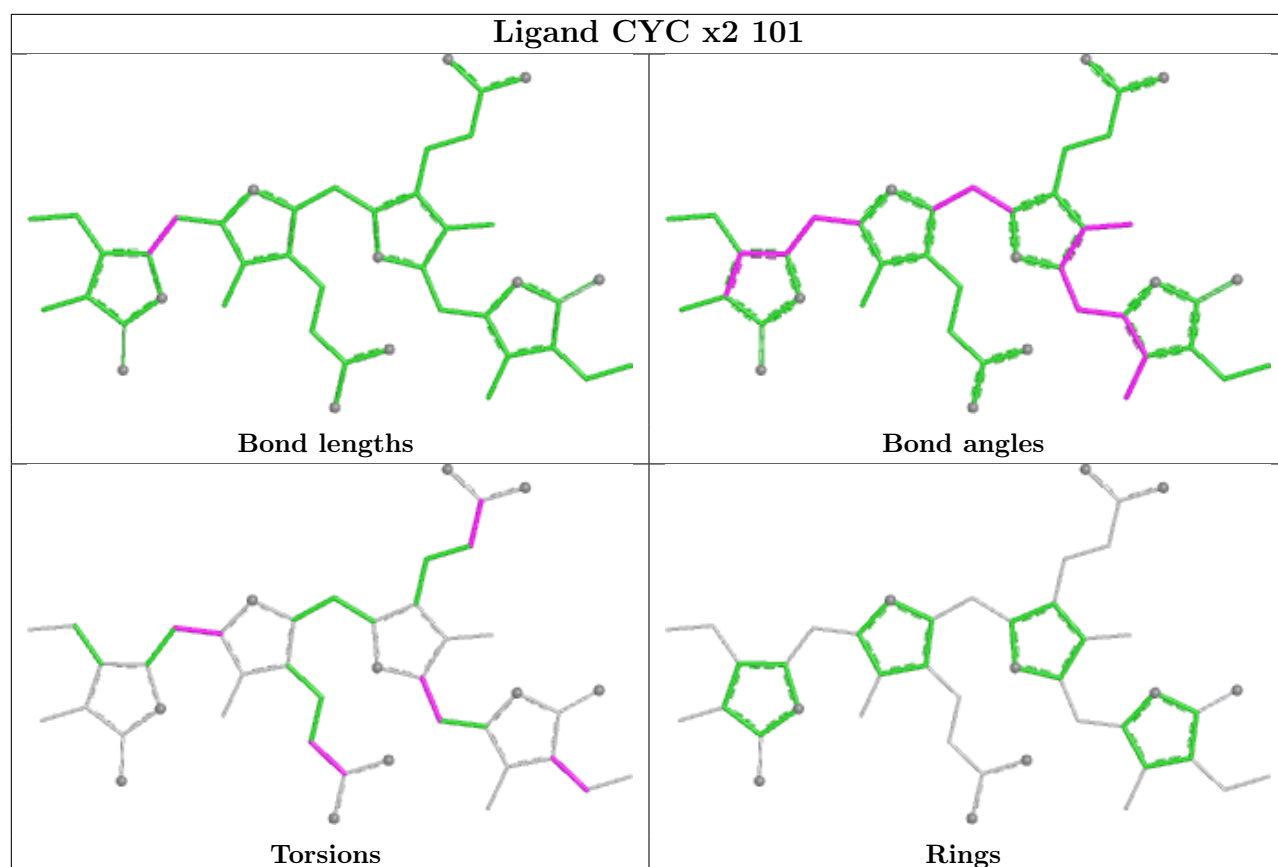
Ligand CYC H3 201

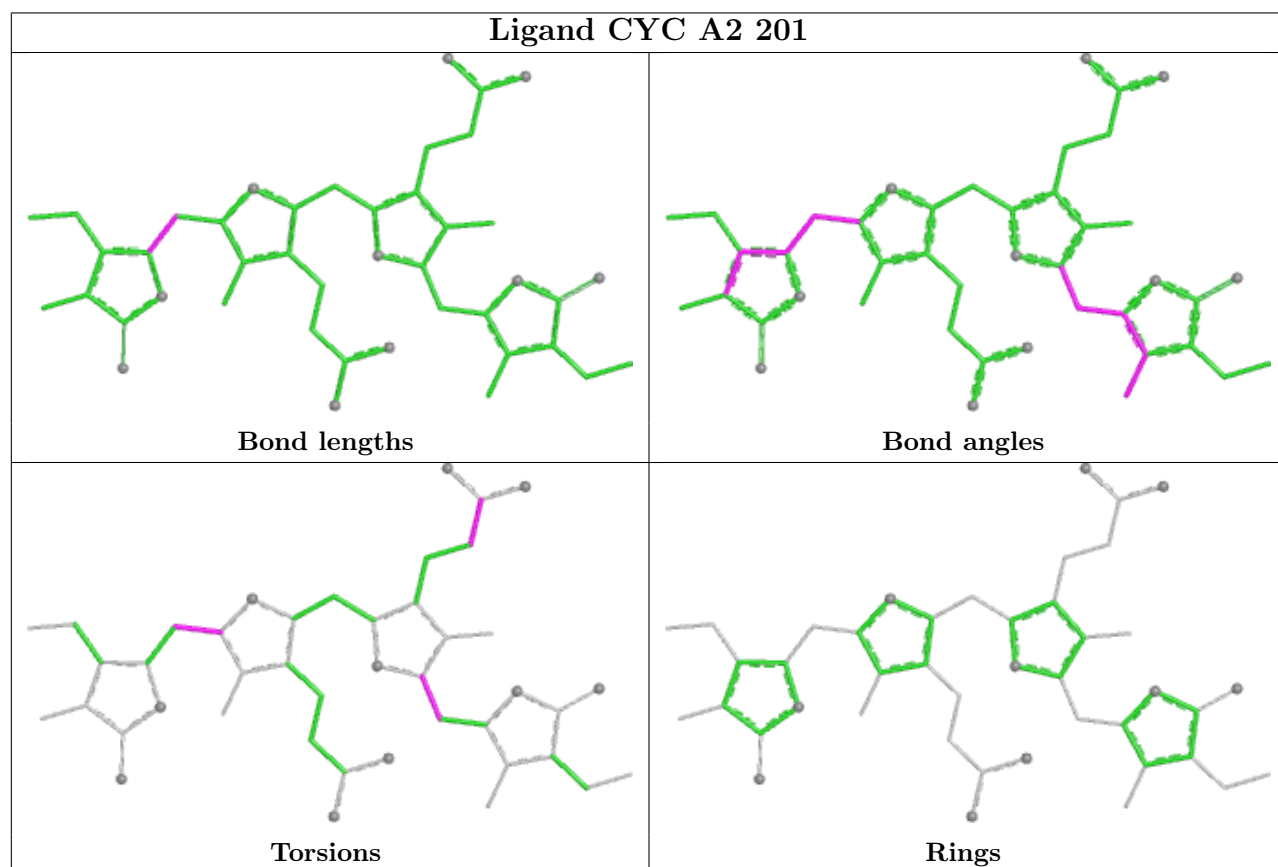
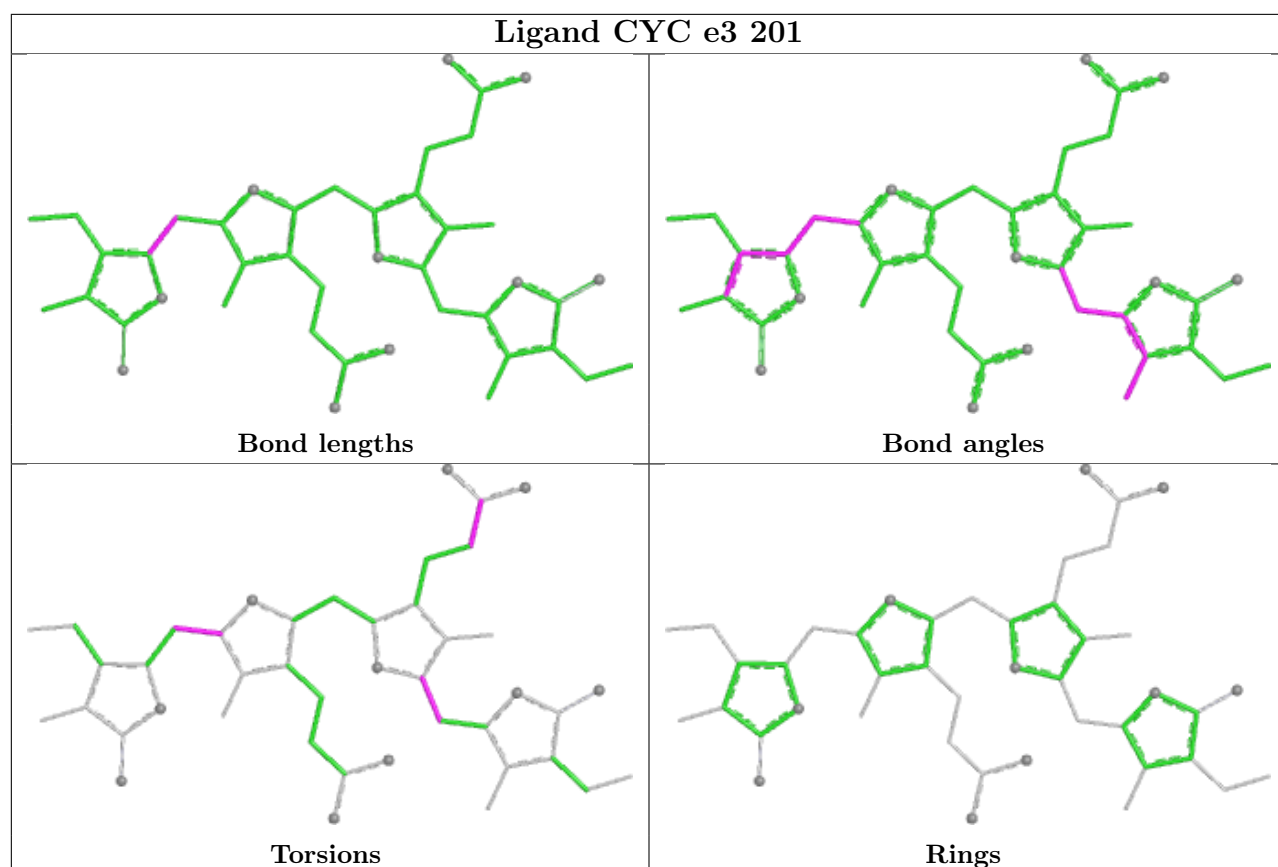


Ligand CYC W3 201

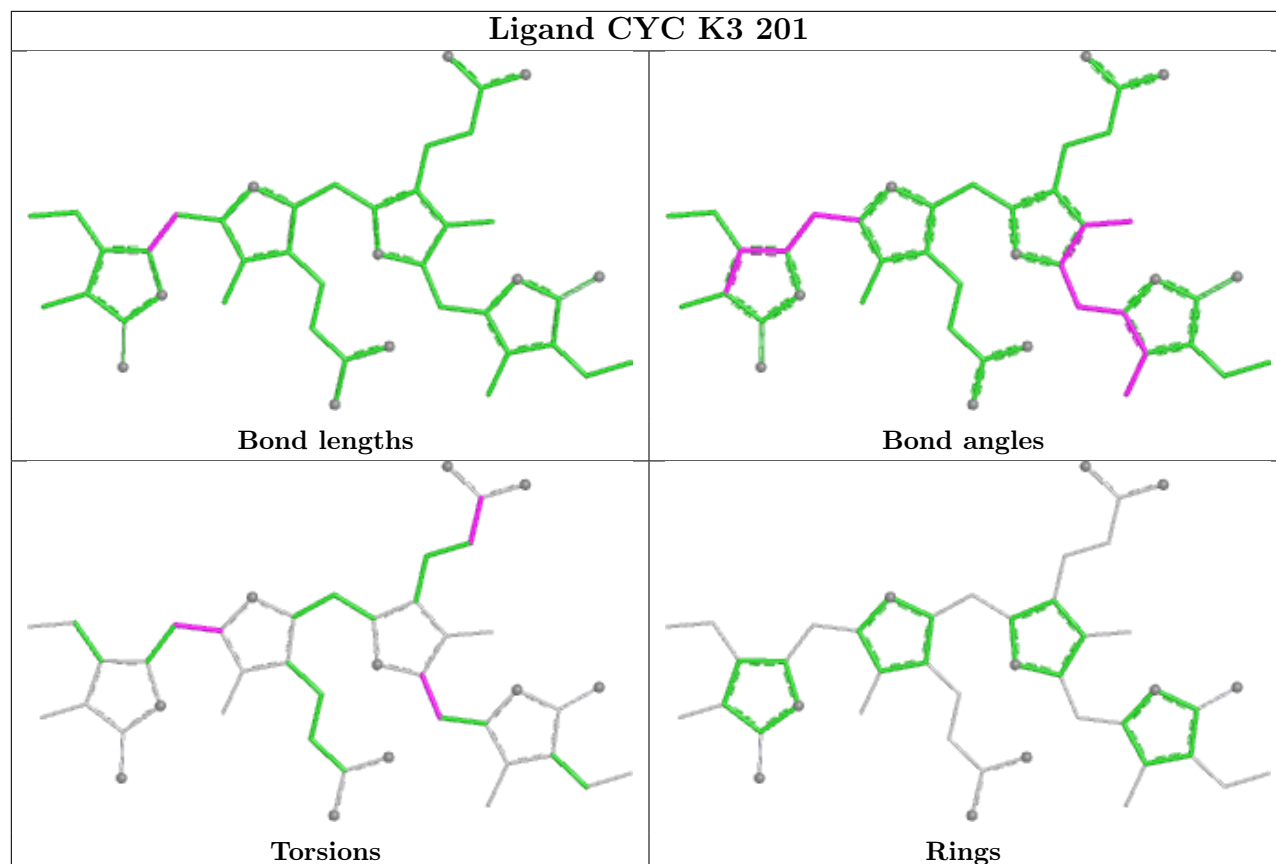




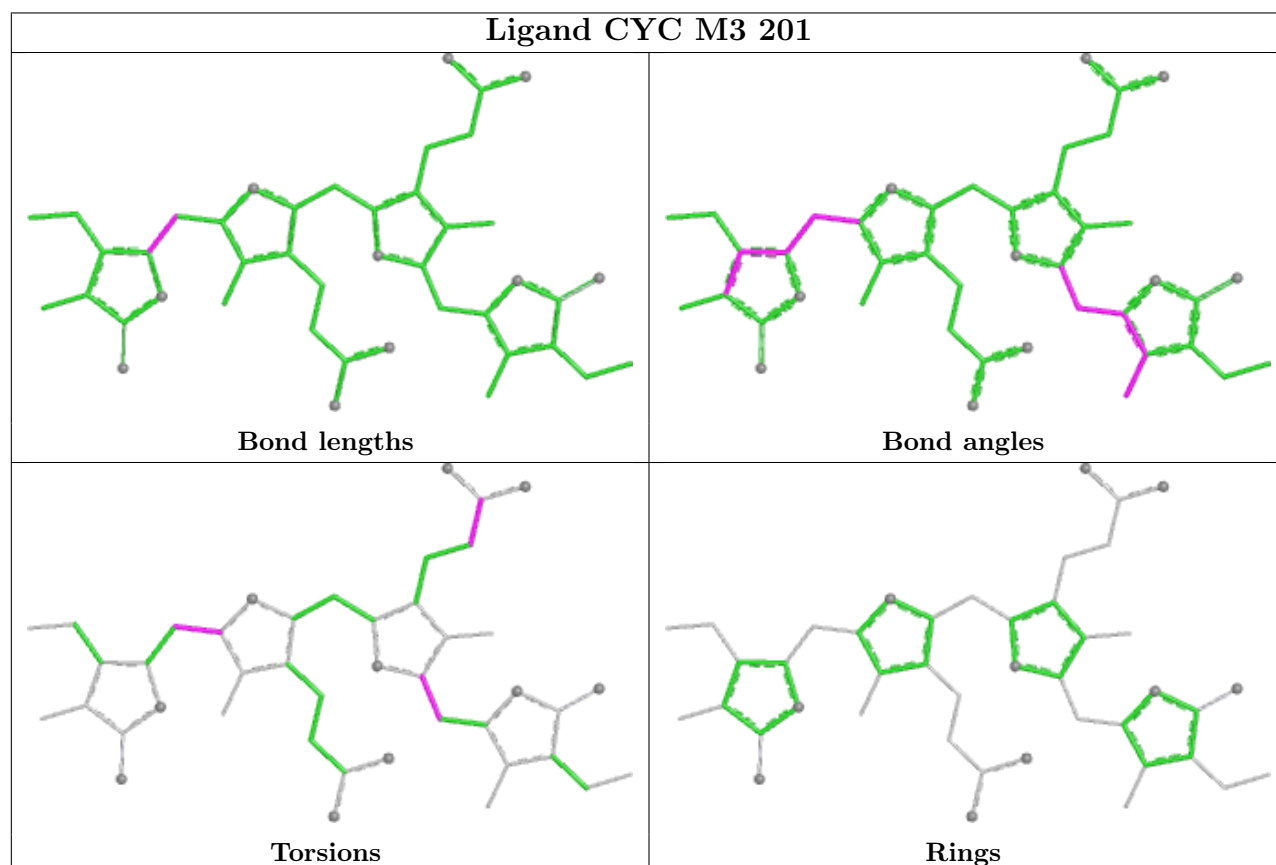


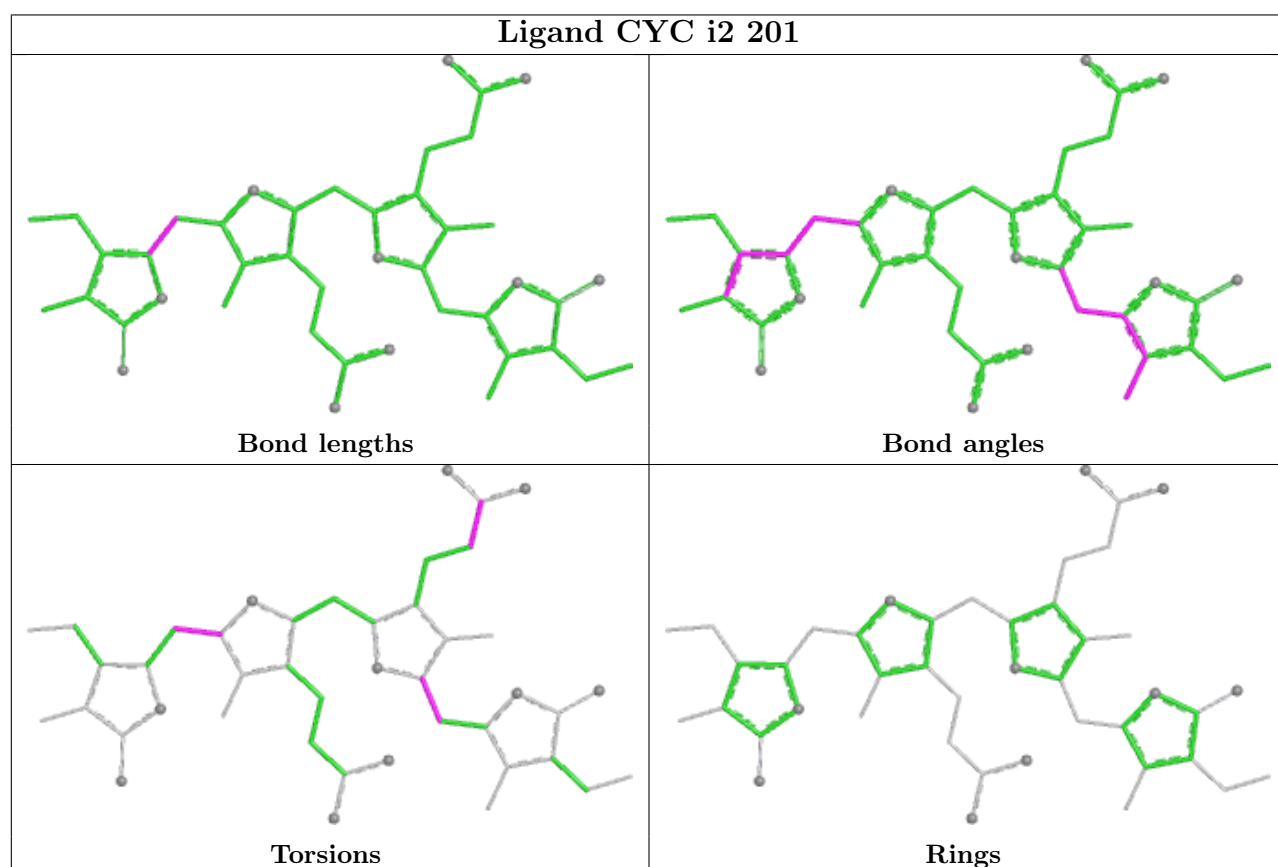
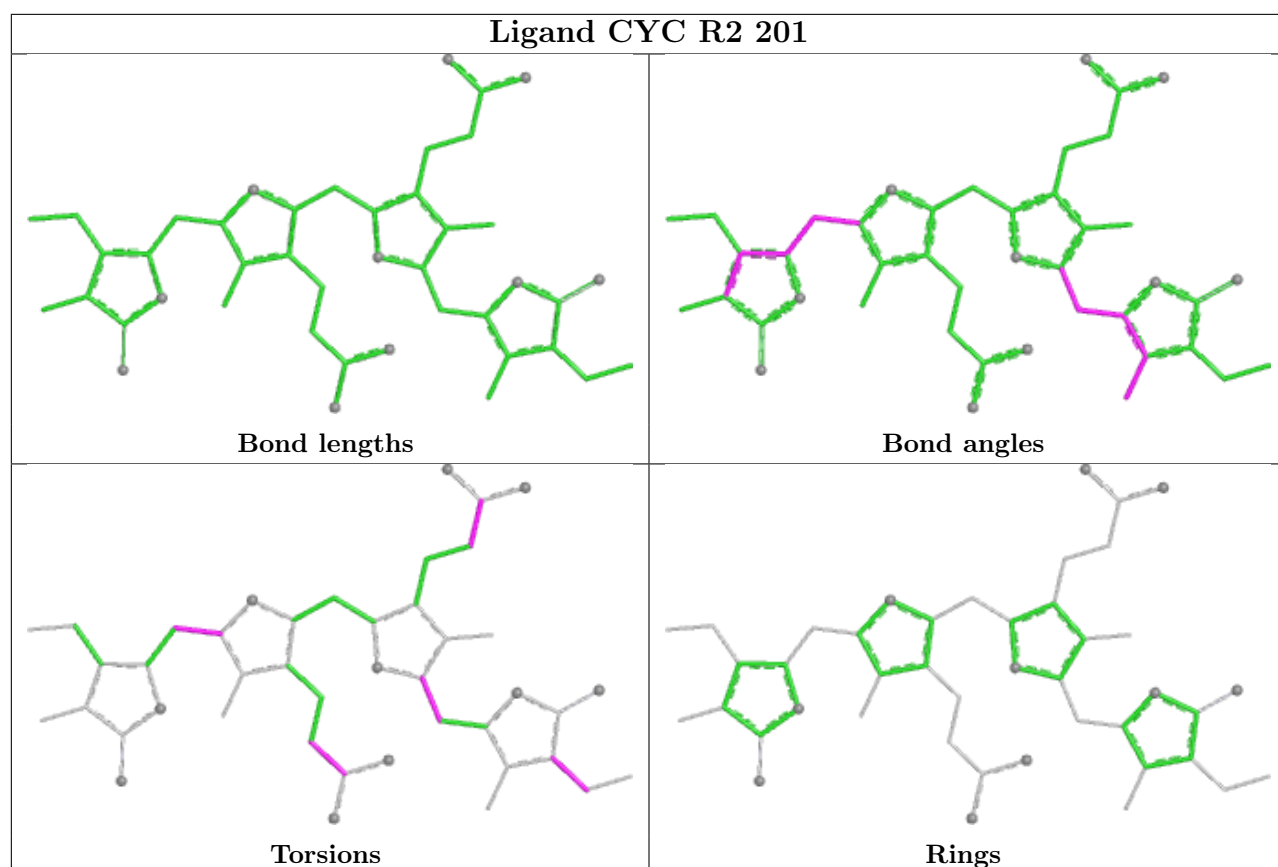


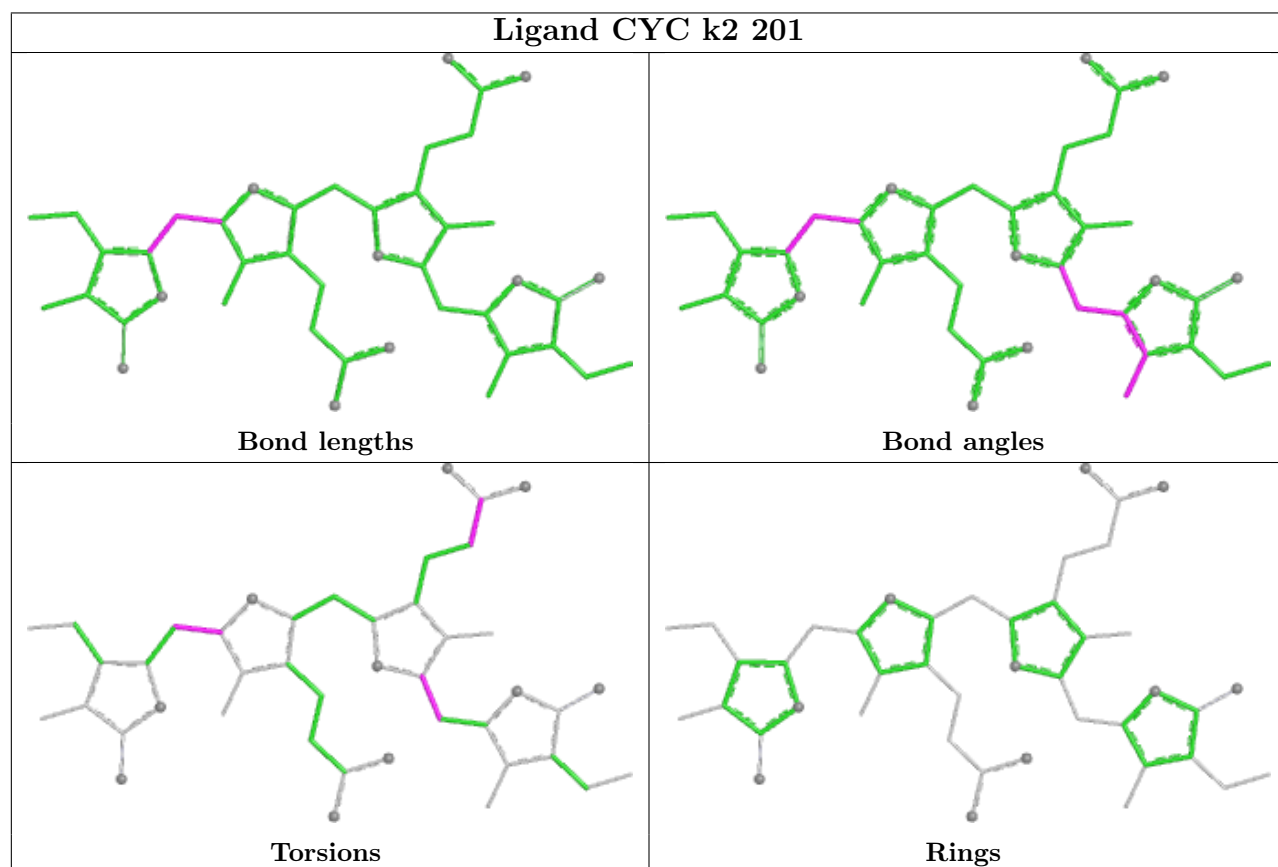
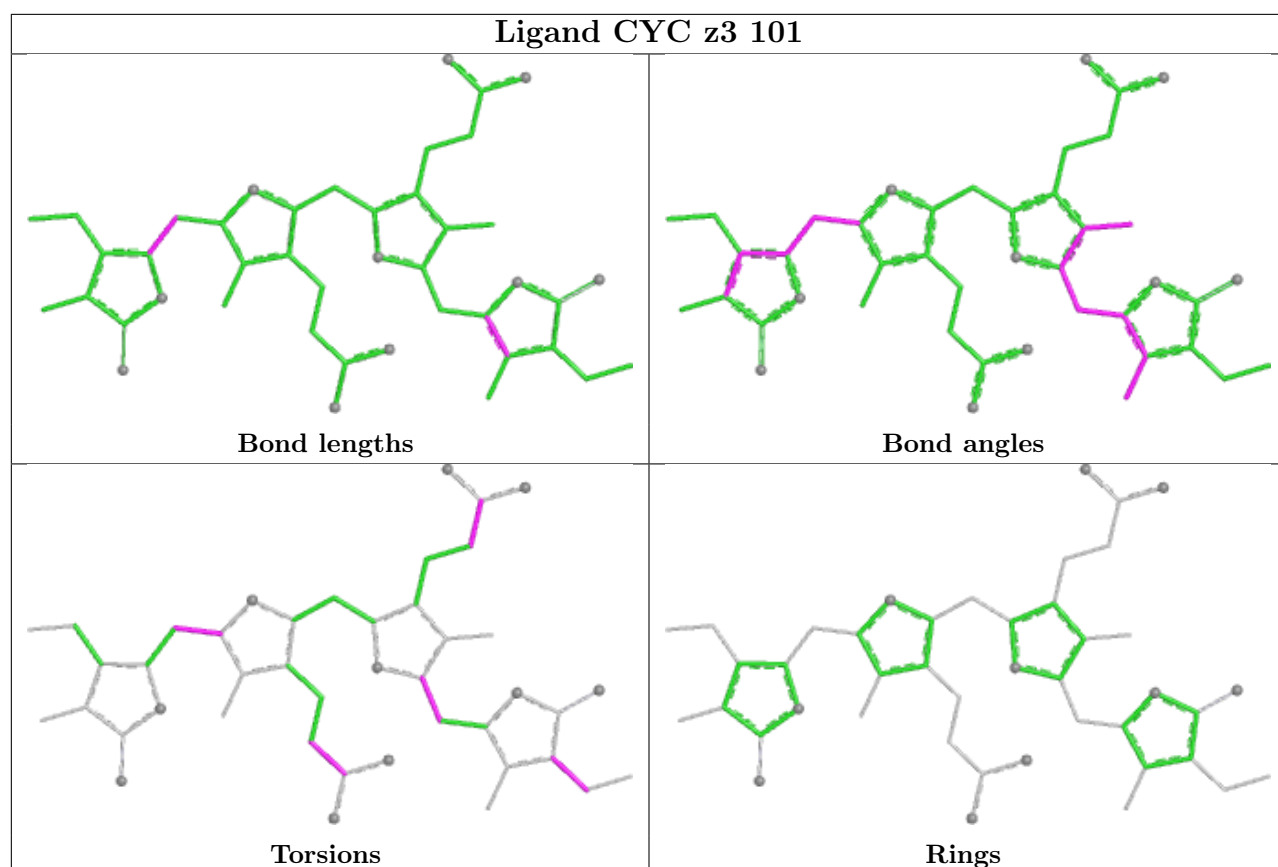
Ligand CYC K3 201

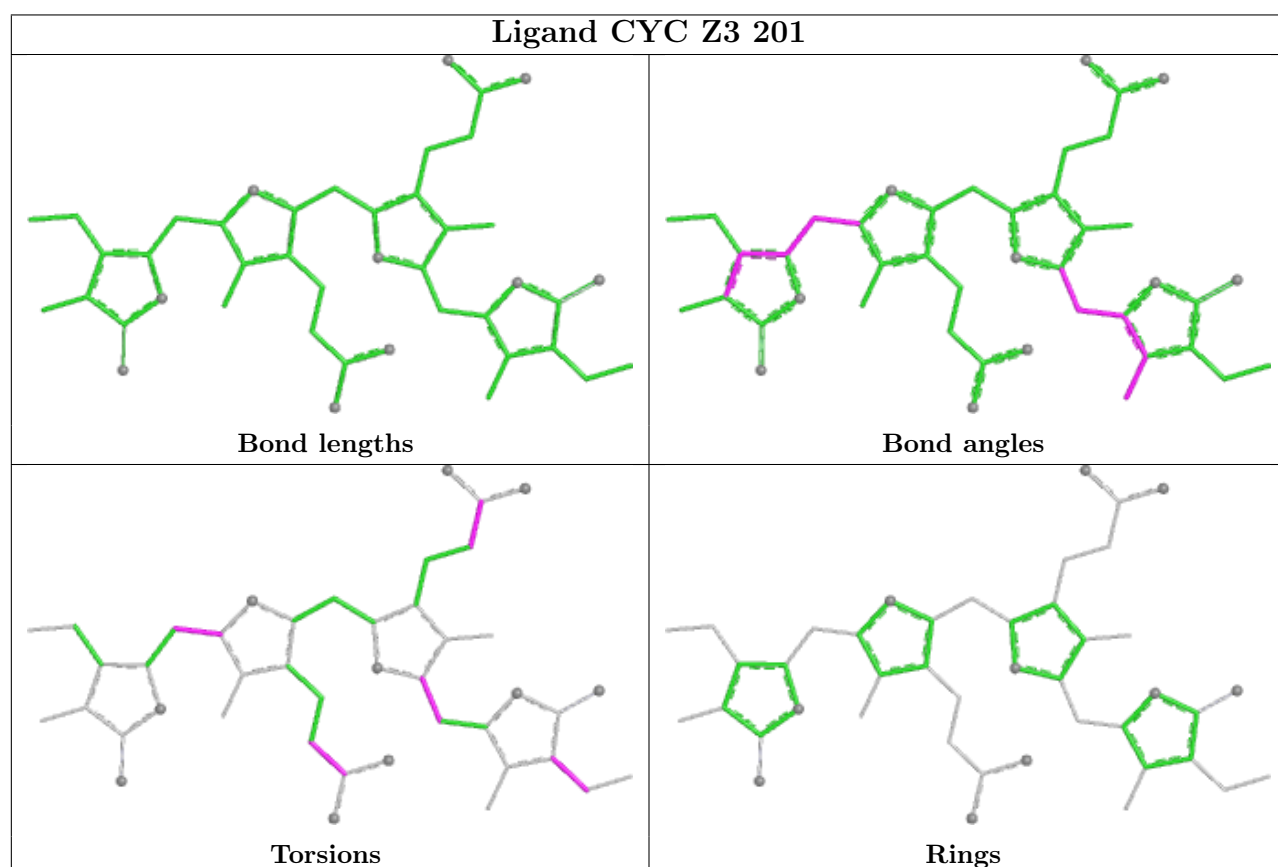
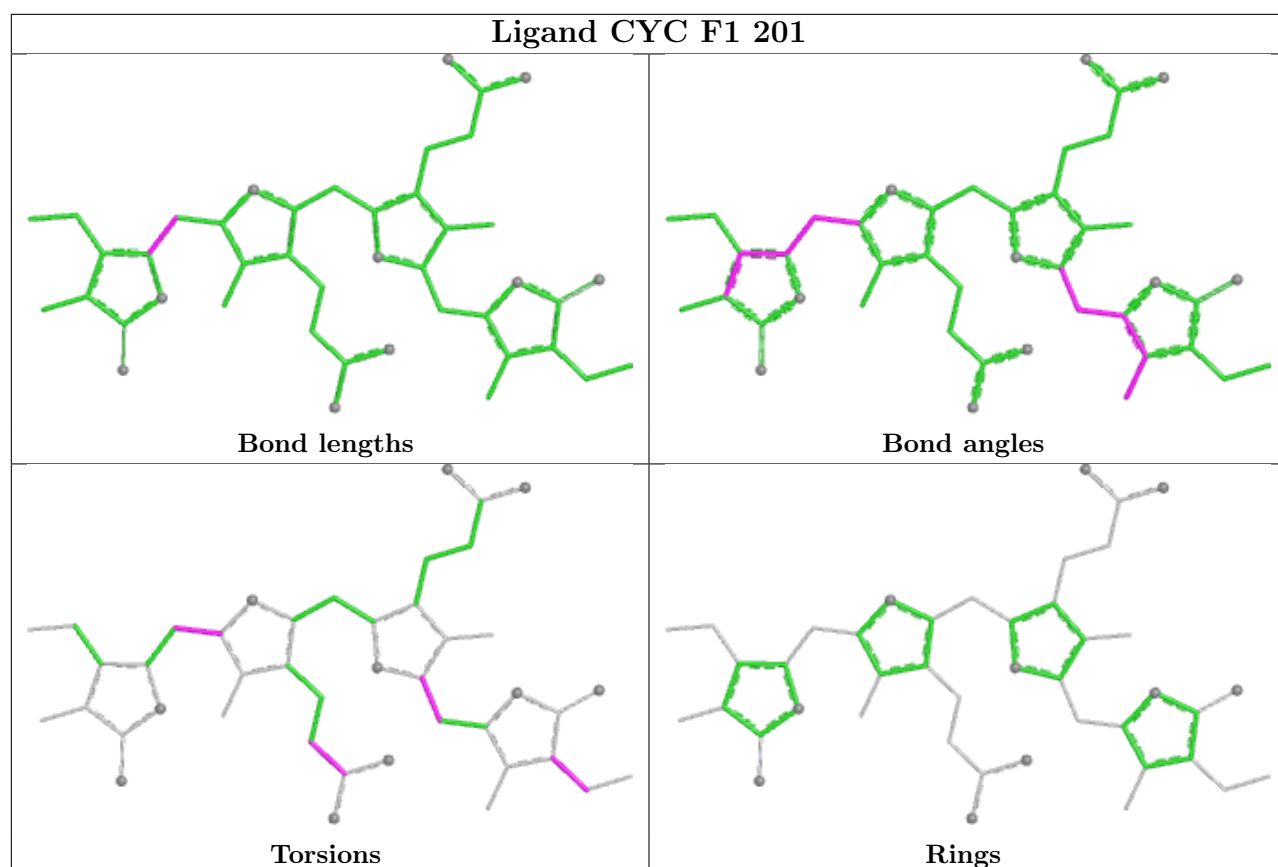


Ligand CYC M3 201

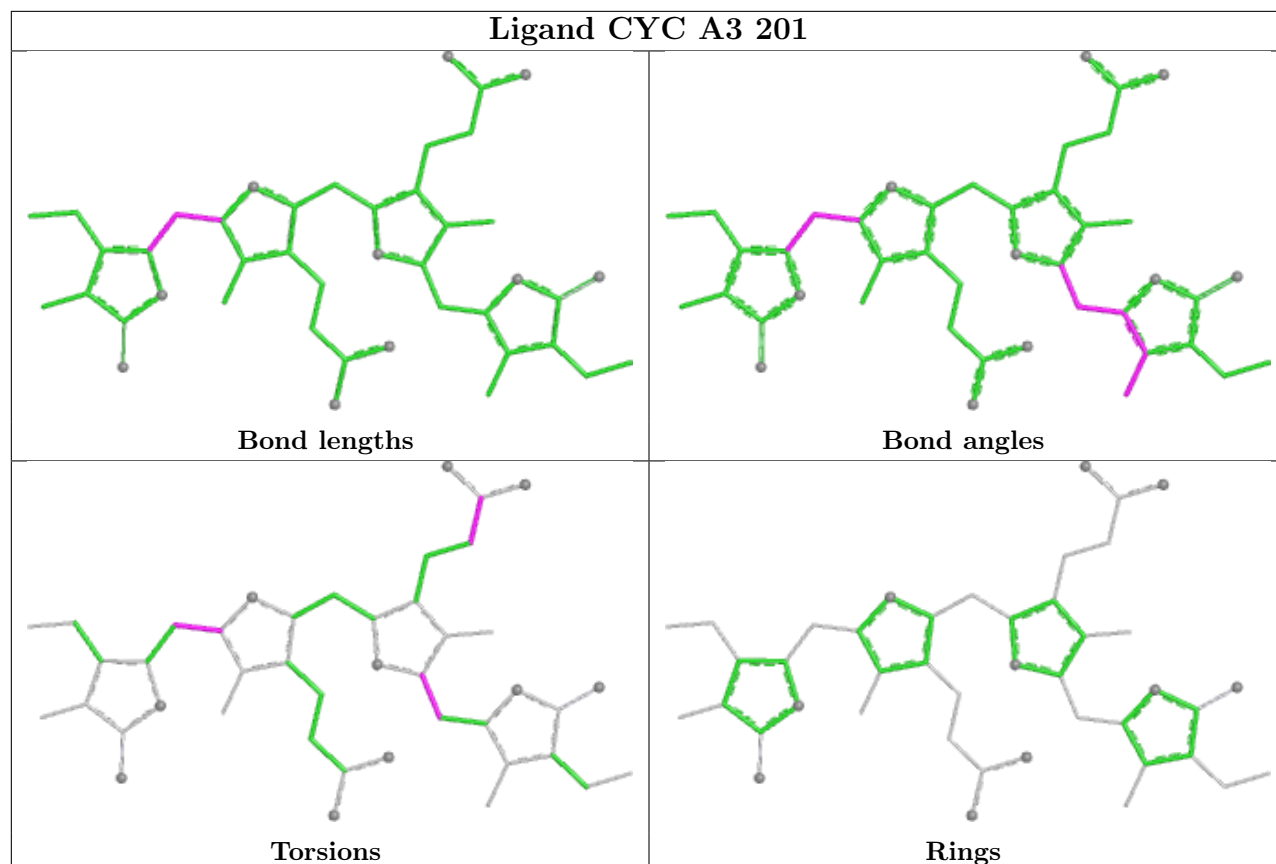




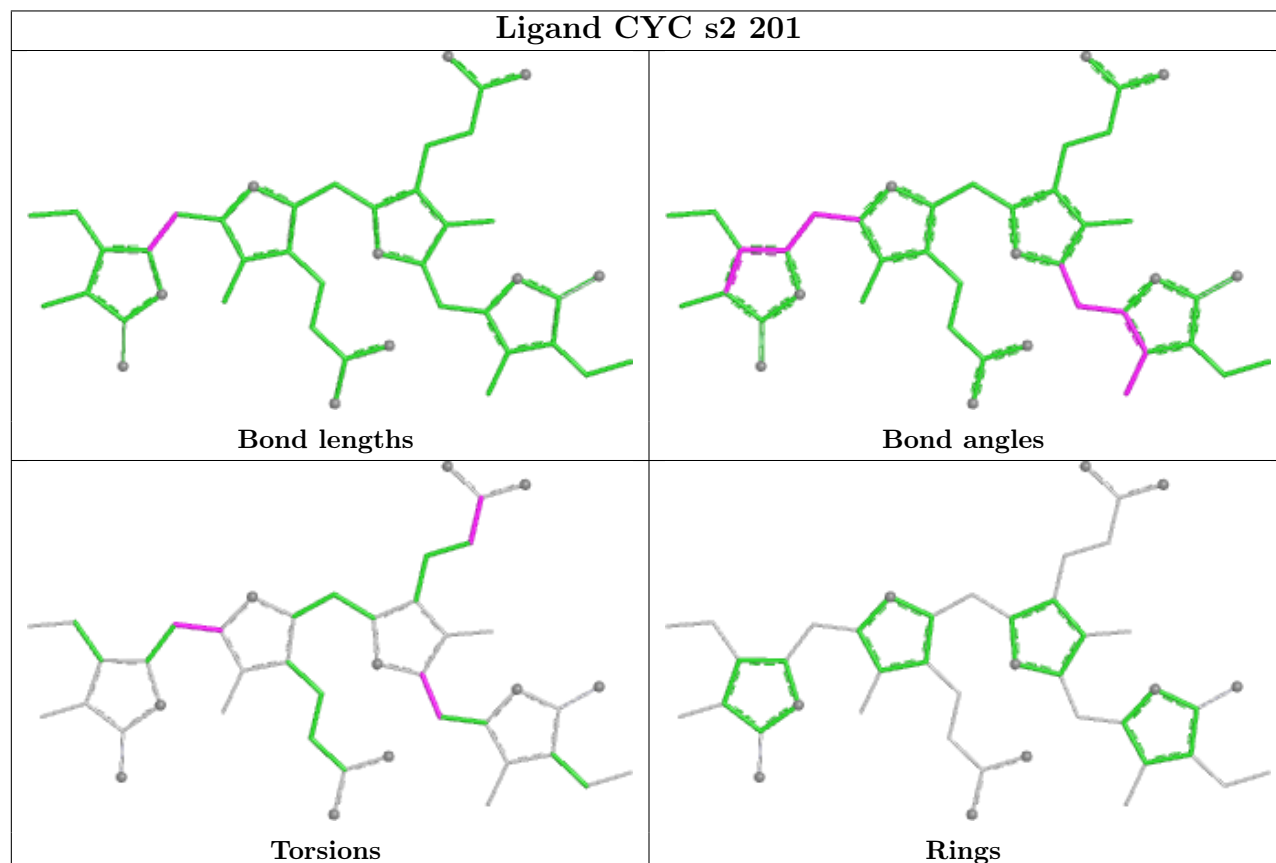


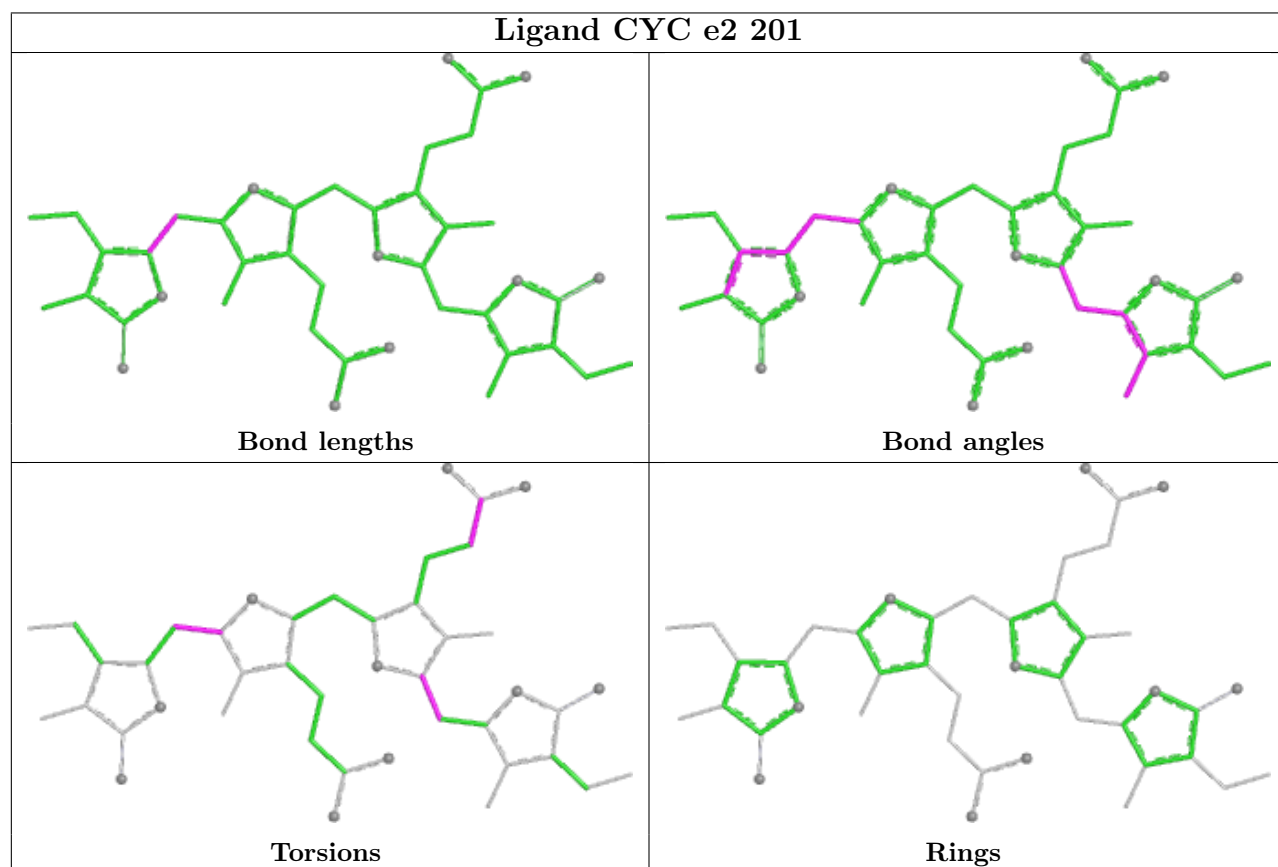
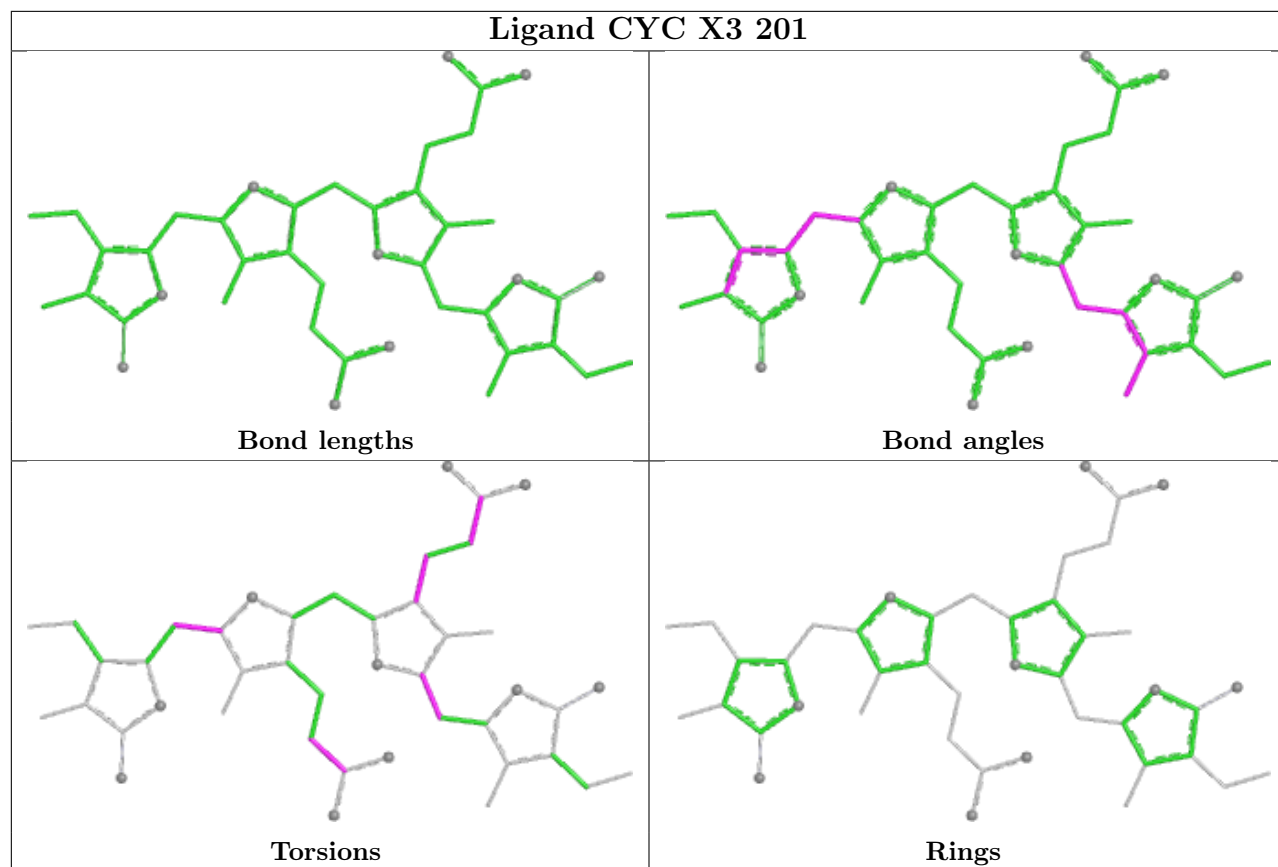


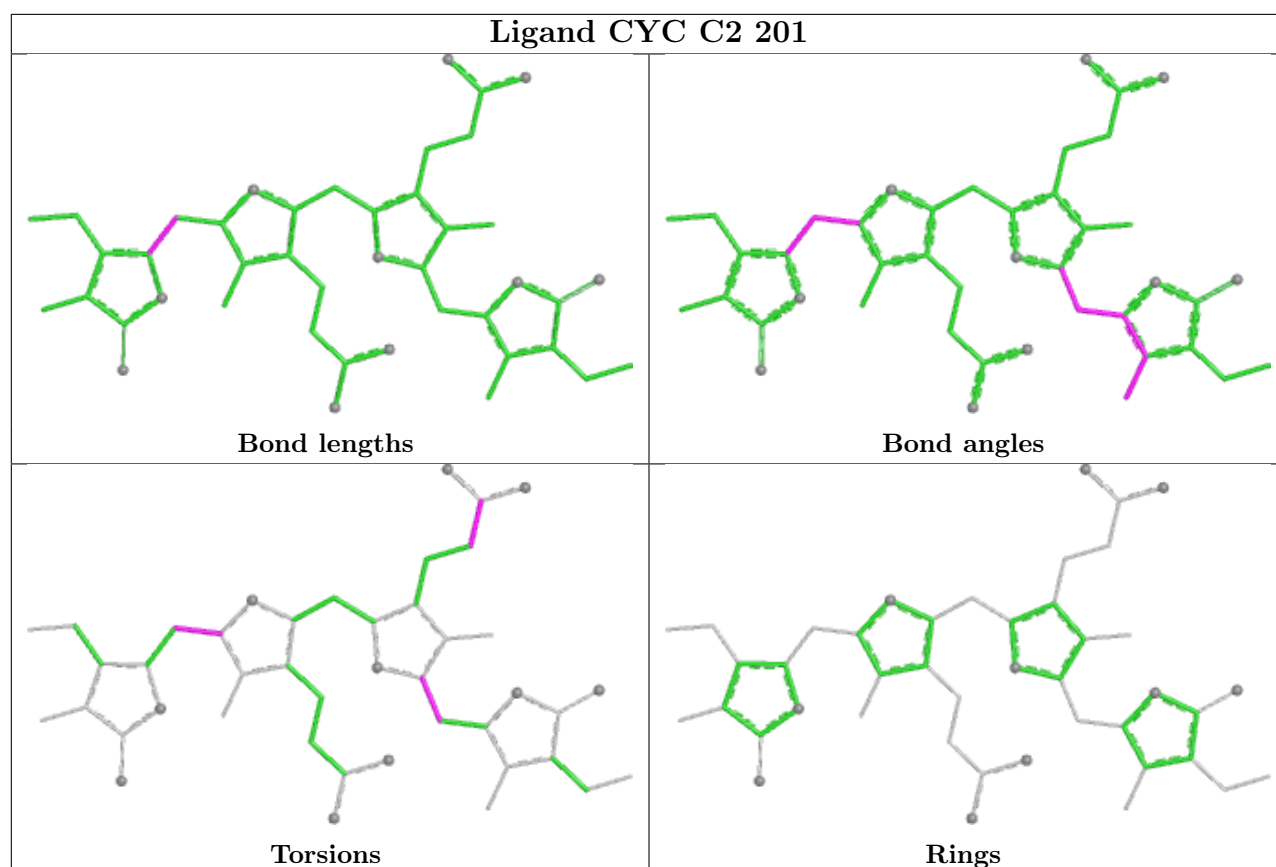
Ligand CYC A3 201



Ligand CYC s2 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.

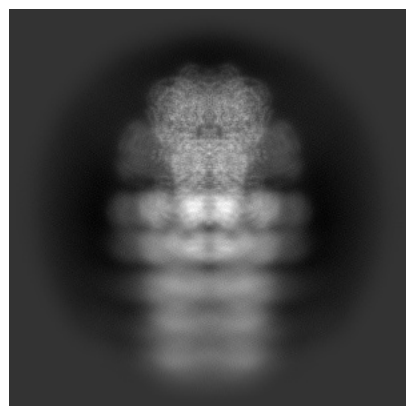
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-63604. These allow visual inspection of the internal detail of the map and identification of artifacts.

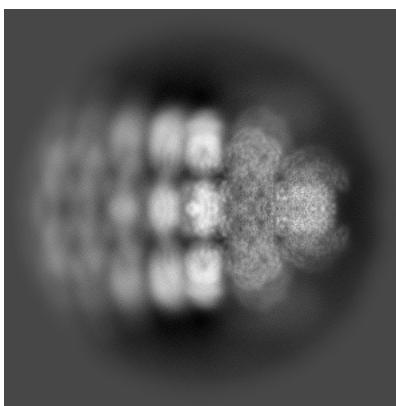
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

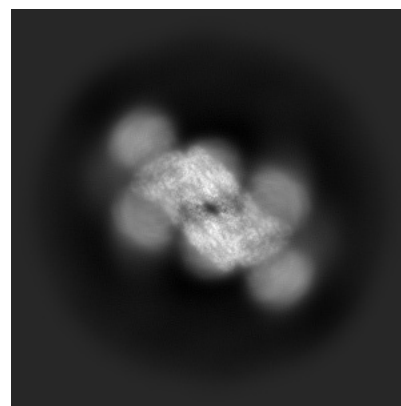
6.1.1 Primary map



X

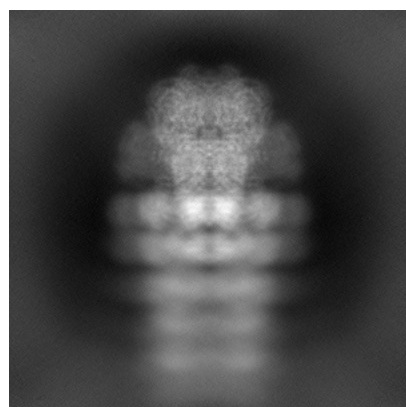


Y

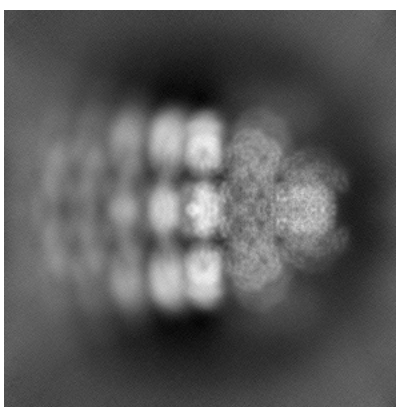


Z

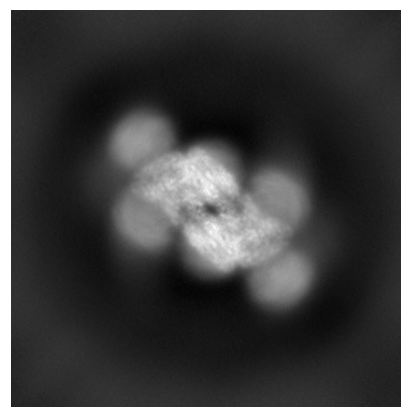
6.1.2 Raw map



X



Y

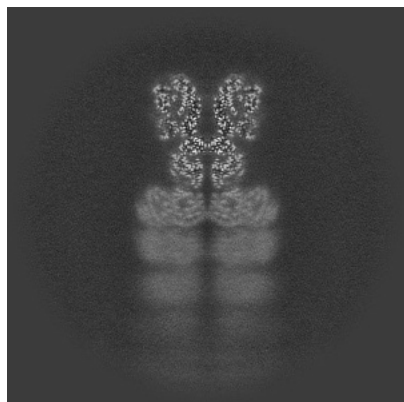


Z

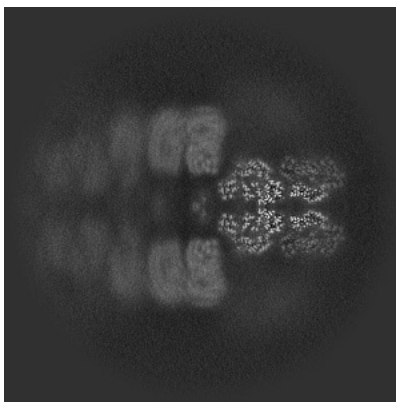
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

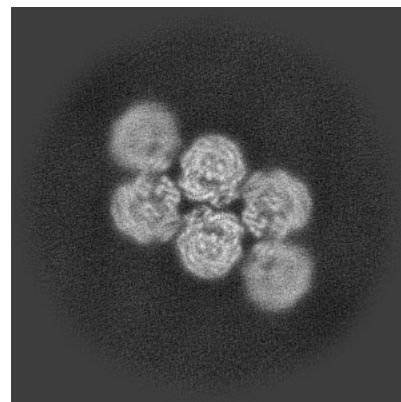
6.2.1 Primary map



X Index: 290

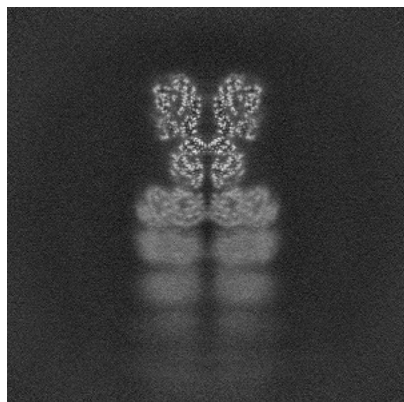


Y Index: 290

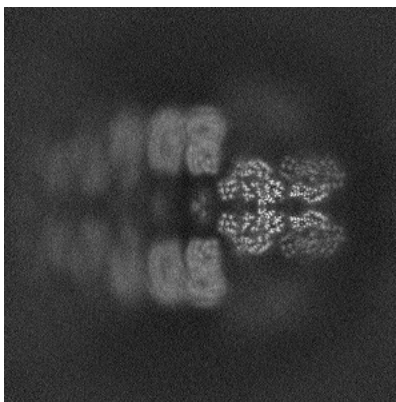


Z Index: 290

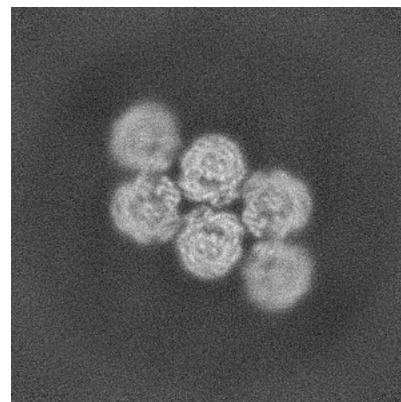
6.2.2 Raw map



X Index: 290



Y Index: 290

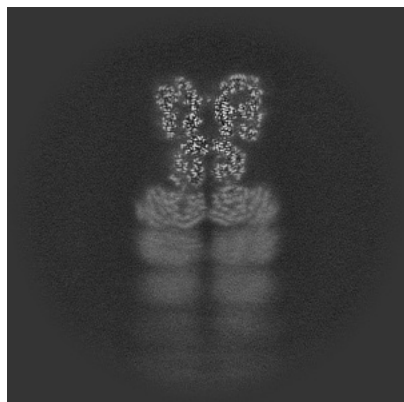


Z Index: 290

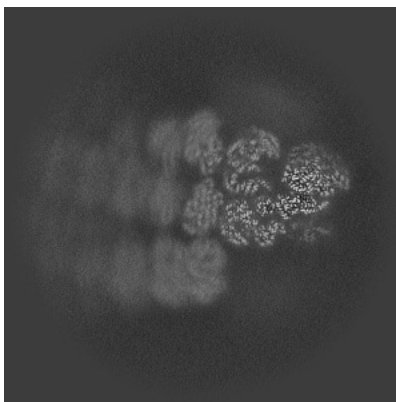
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

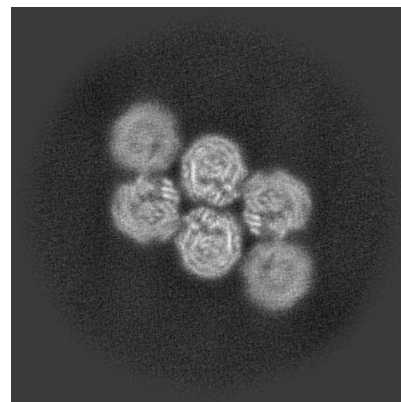
6.3.1 Primary map



X Index: 285

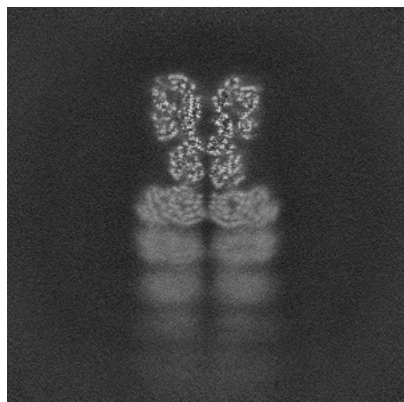


Y Index: 269

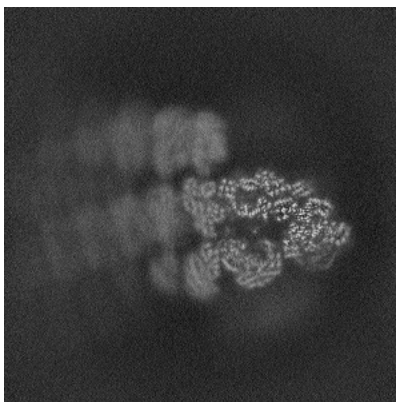


Z Index: 287

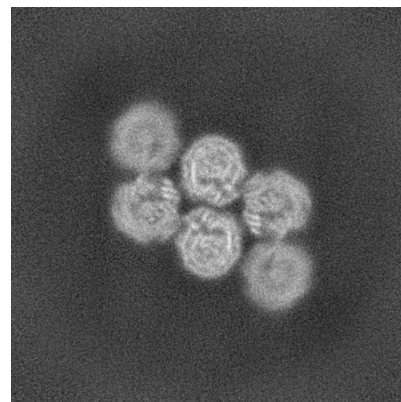
6.3.2 Raw map



X Index: 293



Y Index: 318

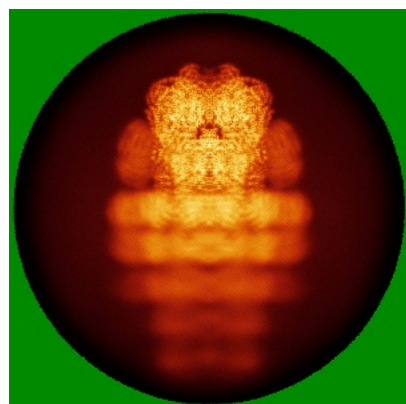


Z Index: 287

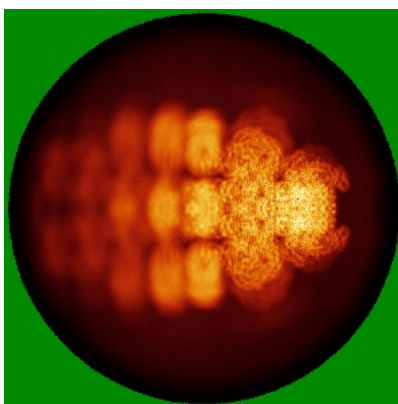
The images above show the largest variance slices of the map in three orthogonal directions.

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

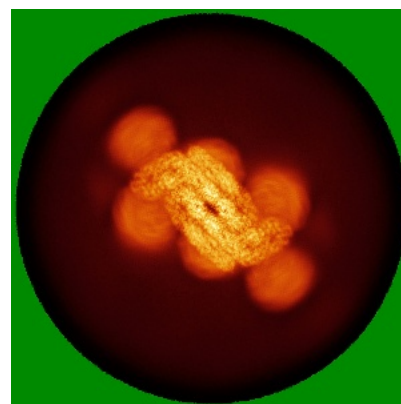
6.4.1 Primary map



X

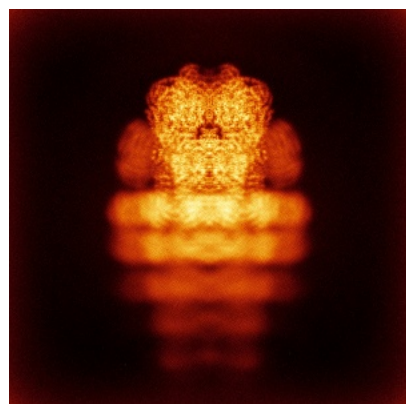


Y

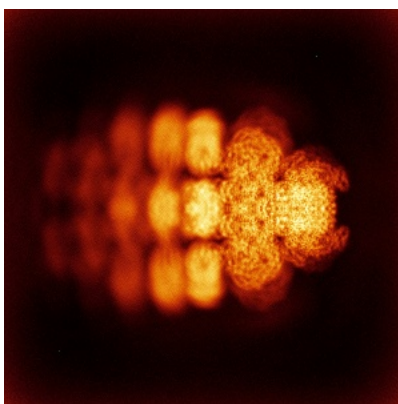


Z

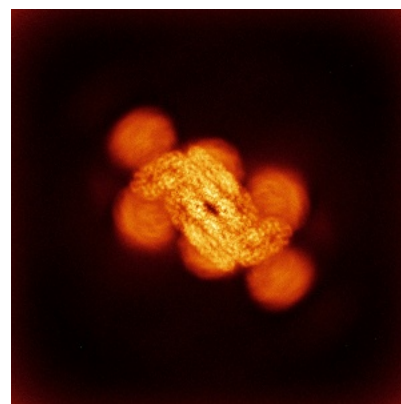
6.4.2 Raw map



X



Y

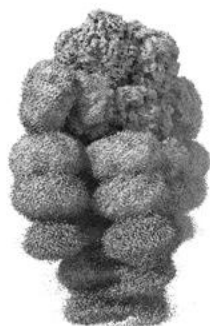


Z

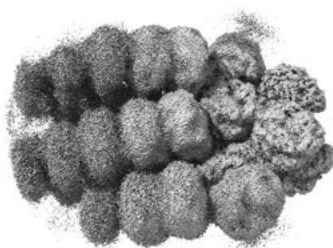
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

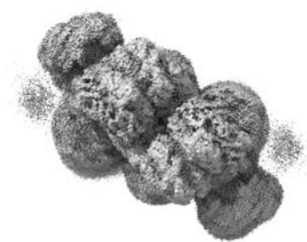
6.5.1 Primary map



X



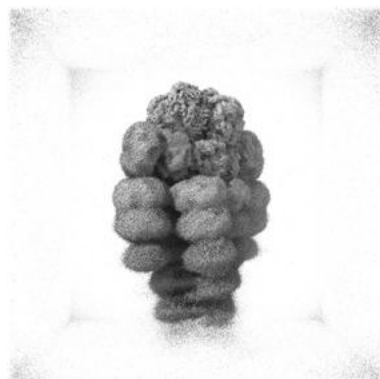
Y



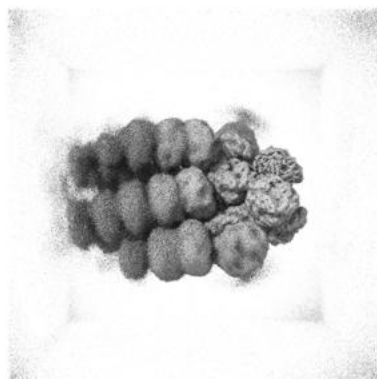
Z

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.

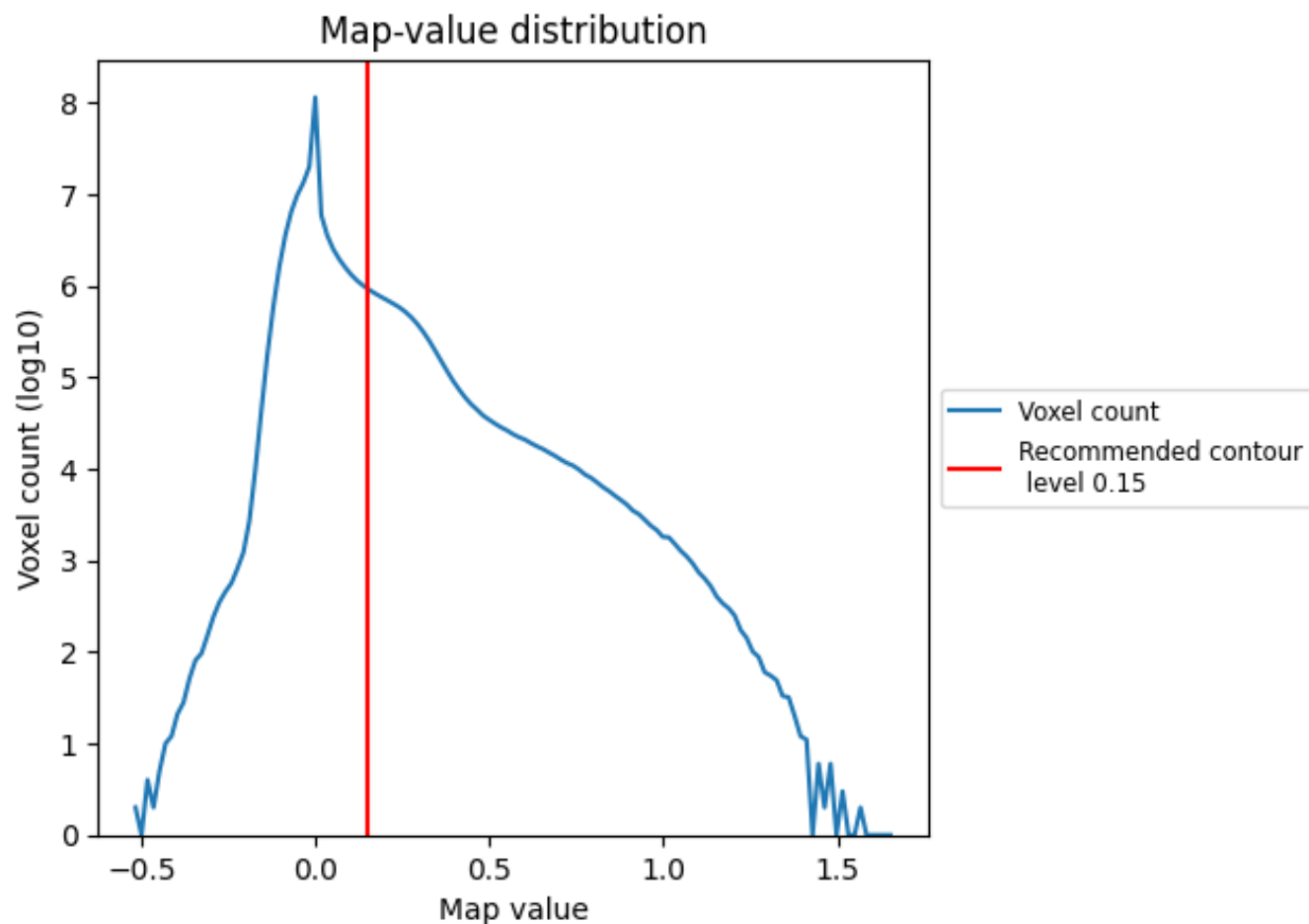
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

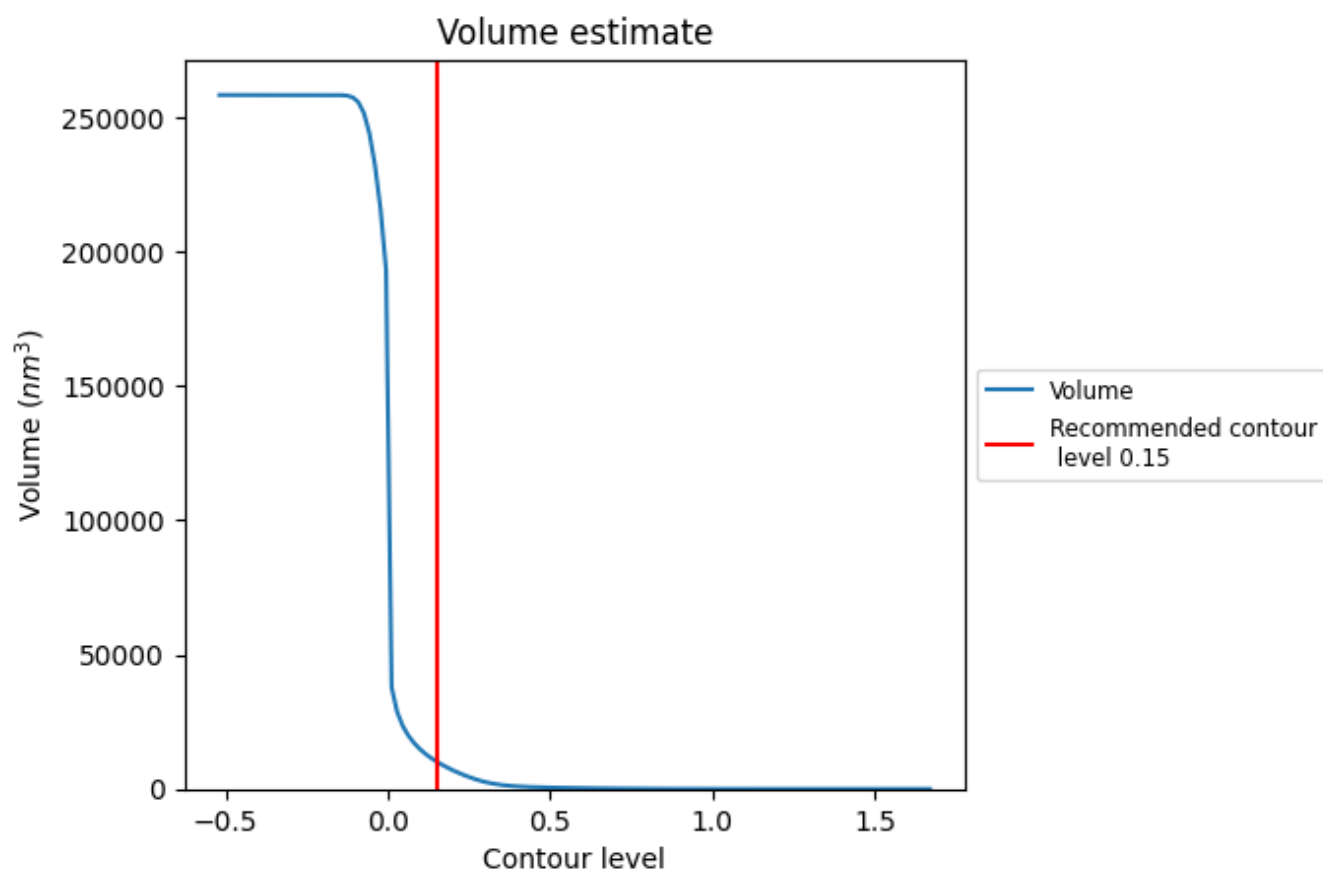
This section contains the results of statistical analysis of the map.

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.

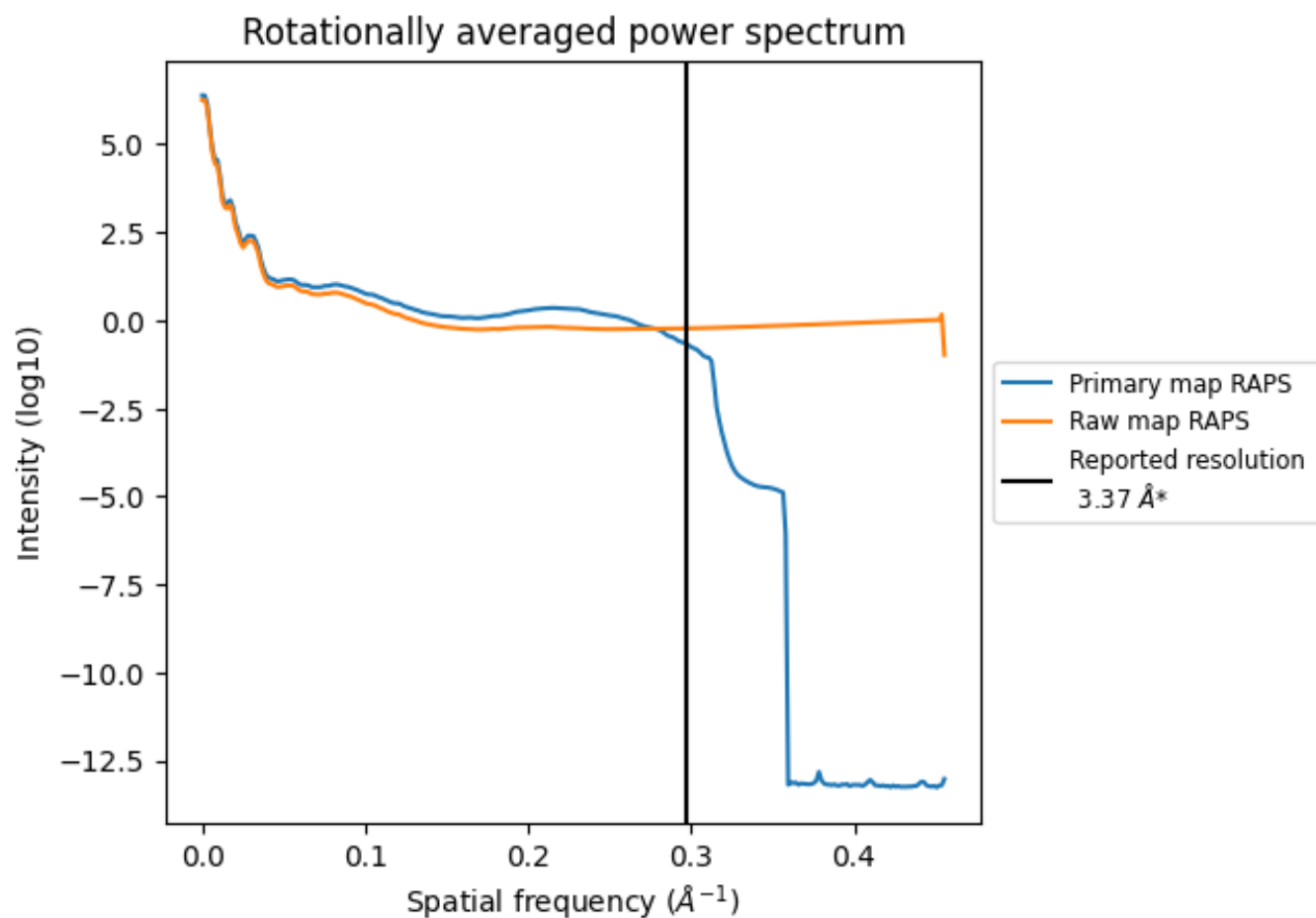
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 10190 nm^3 ; this corresponds to an approximate mass of 9205 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 ⓘ

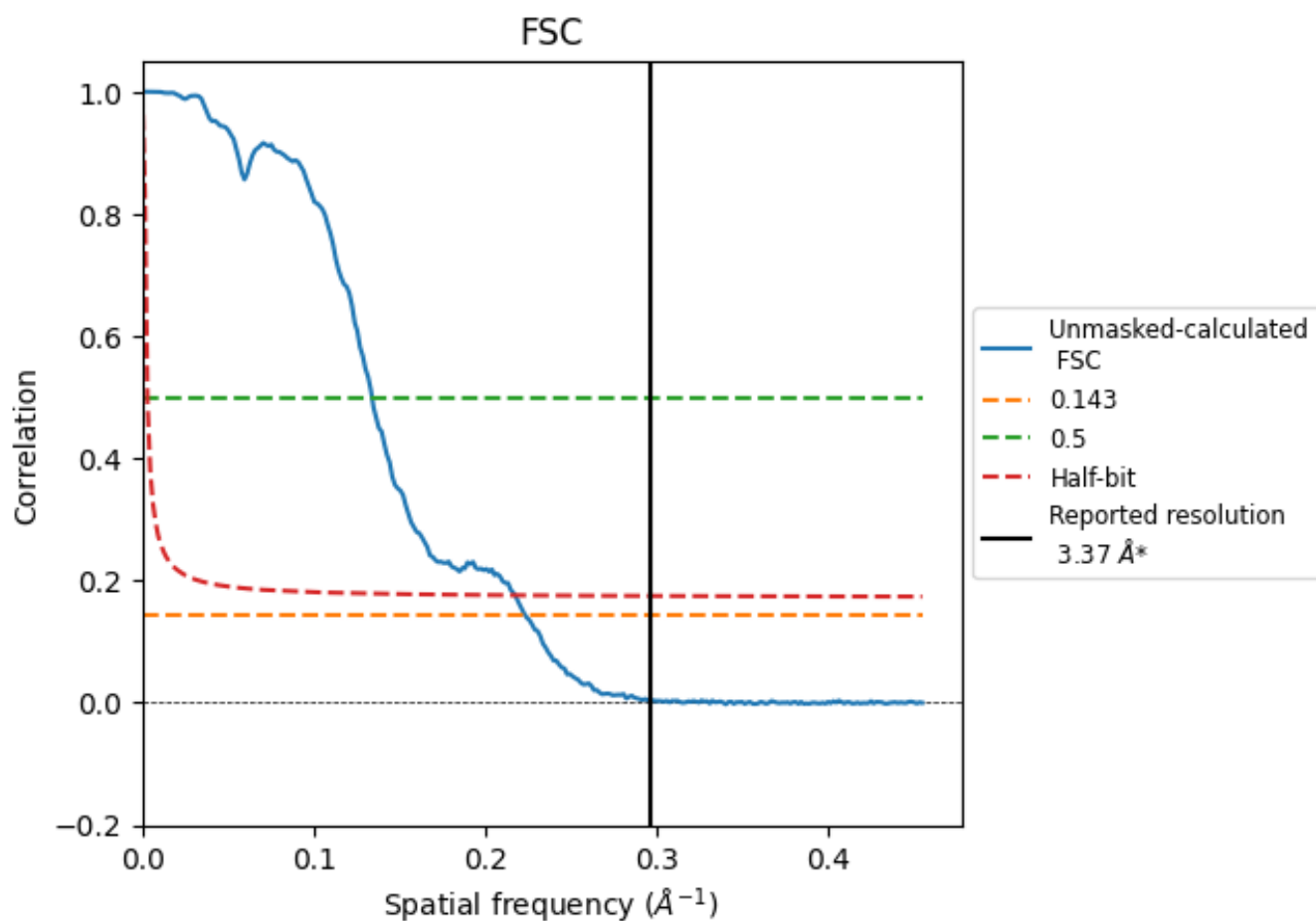


*Reported resolution corresponds to spatial frequency of 0.297 Å⁻¹

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 0.297 Å⁻¹

8.2 Resolution estimates [i](#)

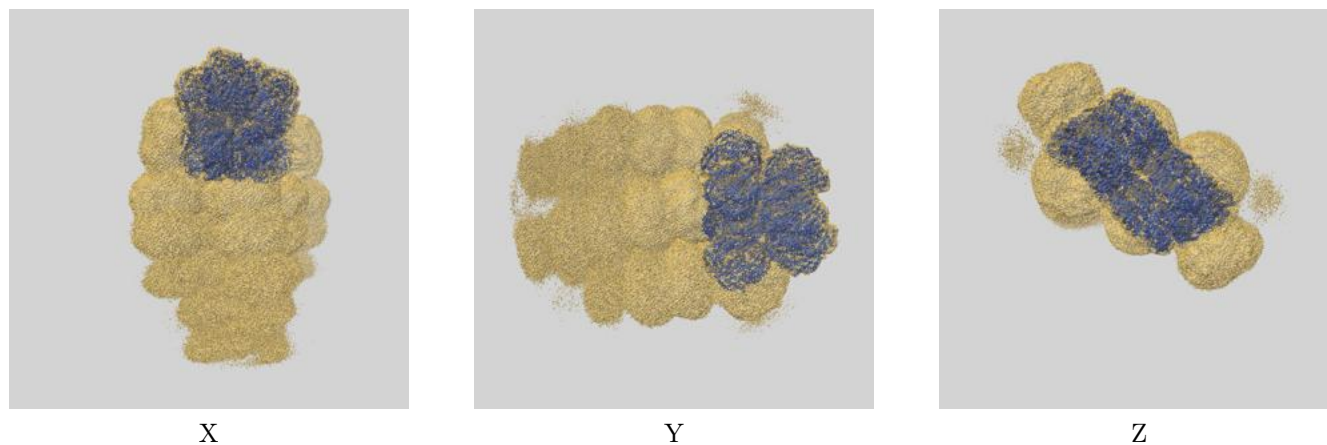
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.37	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.47	7.46	4.60

*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 4.47 differs from the reported value 3.37 by more than 10 %

9 Map-model fit [i](#)

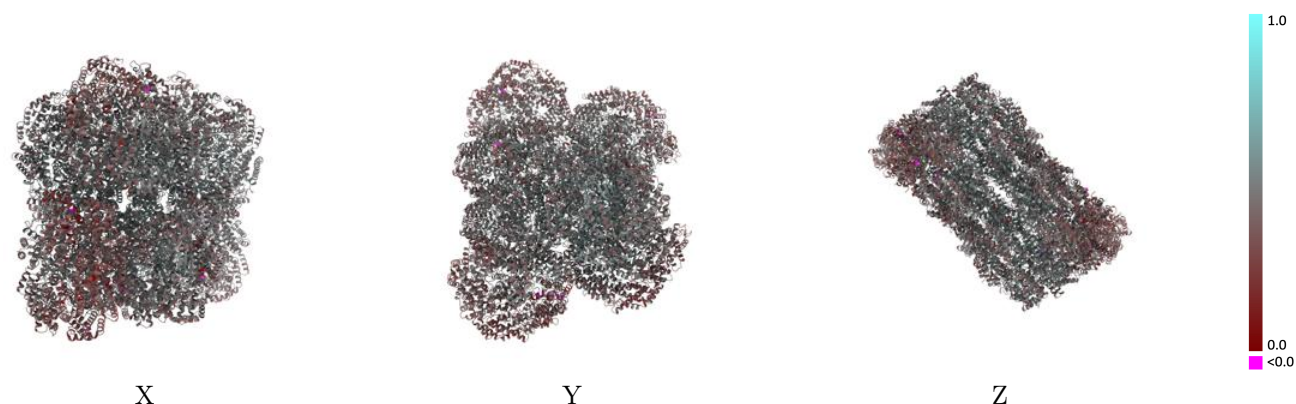
This section contains information regarding the fit between EMDB map EMD-63604 and PDB model 9M3J. Per-residue inclusion information can be found in section [3](#) on page [18](#).

9.1 Map-model overlay [i](#)



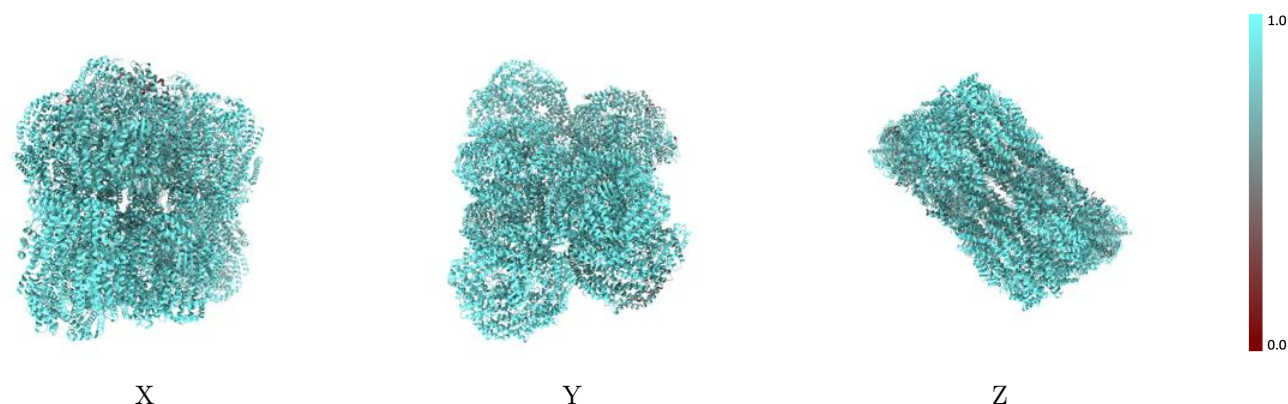
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



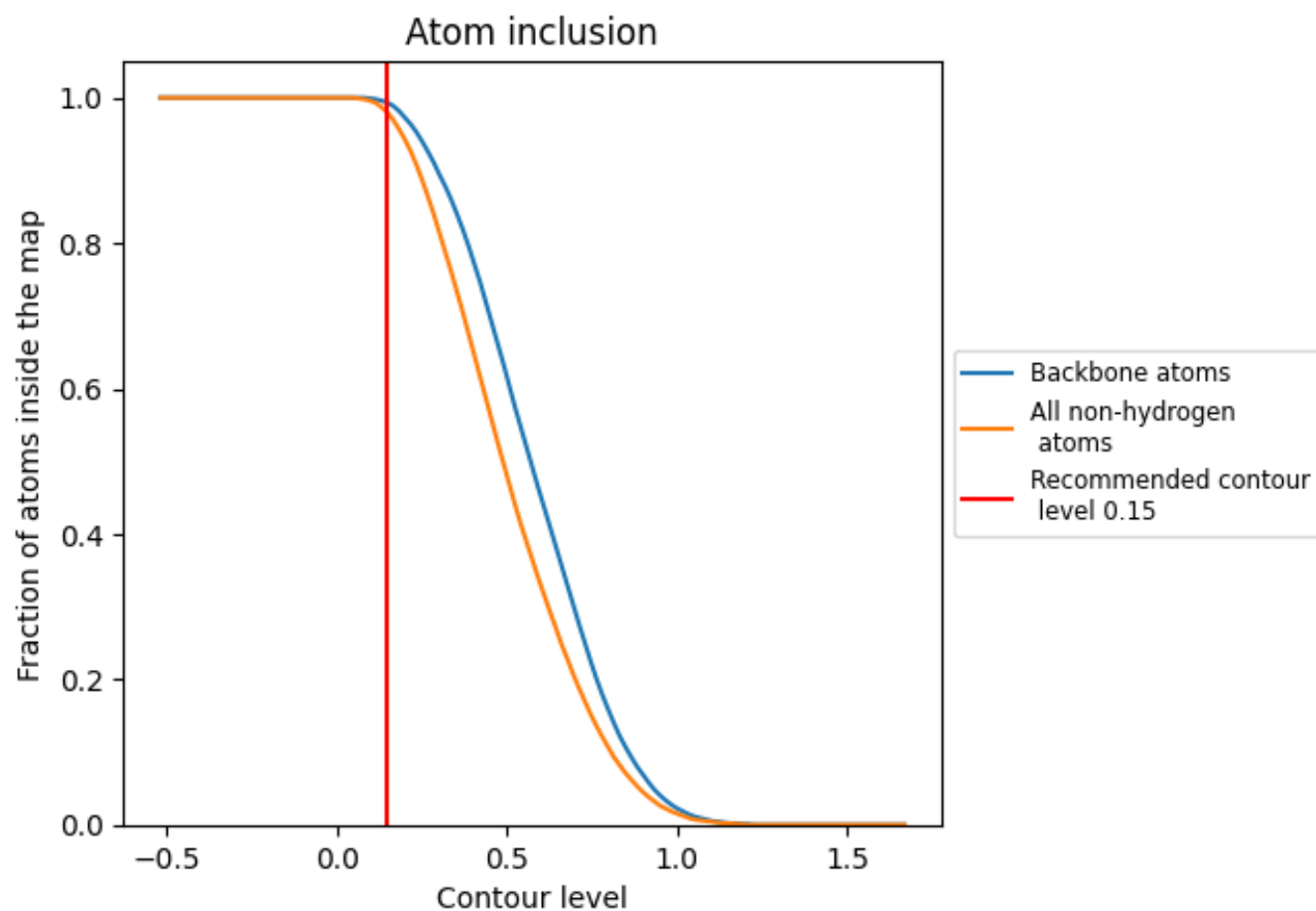
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.15).

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 98% 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	 0.9790	 0.4460
A1	 0.8970	 0.4600
A2	 0.9900	 0.4460
A3	 0.9970	 0.4750
B1	 0.8710	 0.4130
B2	 0.9960	 0.4640
B3	 0.9990	 0.4720
C1	 0.8360	 0.3640
C2	 0.9950	 0.4550
C3	 0.9980	 0.4520
D1	 0.7600	 0.3450
D2	 0.9990	 0.5280
D3	 0.9980	 0.4510
E1	 0.8860	 0.4620
E2	 0.9990	 0.5100
E3	 0.9980	 0.4530
F1	 0.8490	 0.4450
F2	 0.9970	 0.5010
F3	 0.9920	 0.4680
G1	 0.8710	 0.4140
G2	 0.9920	 0.4470
G3	 0.9940	 0.4600
H1	 0.8170	 0.3600
H2	 0.9940	 0.4630
H3	 0.9980	 0.4670
I1	 0.7590	 0.3510
I2	 0.9940	 0.4580
I3	 0.9940	 0.4500
J1	 0.8360	 0.4350
J2	 1.0000	 0.5220
J3	 0.9970	 0.4510
K1	 0.8350	 0.4230
K2	 0.9980	 0.5130
K3	 0.9980	 0.4510
L1	 0.8320	 0.4160



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Chain	Atom inclusion	Q-score
L2	 0.9960	 0.4990
L3	 0.9970	 0.4710
M1	 0.9420	 0.4670
M2	 0.9980	 0.4200
M3	 0.9970	 0.5030
N2	 0.9940	 0.4370
N3	 0.9980	 0.5290
O2	 0.9980	 0.4150
O3	 0.9990	 0.4820
P2	 0.9980	 0.4210
P3	 0.9990	 0.4960
Q2	 0.9900	 0.4200
Q3	 0.9980	 0.4520
R2	 0.9970	 0.4090
R3	 0.9960	 0.5100
S2	 0.9980	 0.4090
S3	 0.9950	 0.5040
T2	 0.9970	 0.4260
T3	 0.9960	 0.5310
U2	 0.9910	 0.3970
U3	 0.9980	 0.4880
V2	 0.9970	 0.4180
V3	 0.9980	 0.5020
W2	 0.9900	 0.4240
W3	 0.9960	 0.4520
X2	 0.9960	 0.4060
X3	 0.9980	 0.5150
Y2	 0.9950	 0.3260
Y3	 0.9970	 0.4410
Z2	 0.9970	 0.3640
Z3	 0.9950	 0.5240
a2	 0.9980	 0.3960
a3	 0.9990	 0.5050
b2	 1.0000	 0.4400
b3	 0.9940	 0.4480
c2	 0.9900	 0.3530
c3	 0.9960	 0.4450
d2	 0.9980	 0.3690
d3	 0.9950	 0.5230
e2	 0.9970	 0.3220
e3	 0.9990	 0.5070
f2	 0.9980	 0.3570

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Chain	Atom inclusion	Q-score
f3	 0.9960	 0.4540
g2	 0.9970	 0.4010
g3	 0.9980	 0.4960
h2	 0.9980	 0.4370
h3	 0.9950	 0.4940
i2	 0.9920	 0.3570
i3	 0.9980	 0.5120
j2	 0.9970	 0.3640
j3	 0.9950	 0.4800
k2	 0.9970	 0.3790
k3	 0.9950	 0.4810
l2	 0.9970	 0.3560
m2	 0.9980	 0.3520
n2	 0.9950	 0.4210
o2	 0.9970	 0.4670
p2	 0.9910	 0.4070
q2	 0.9940	 0.3440
r2	 0.9920	 0.3560
s2	 0.9970	 0.3580
t2	 0.9950	 0.4220
u2	 0.9980	 0.4730
v2	 0.9920	 0.3970
w2	 1.0000	 0.4980
x2	 1.0000	 0.4430
y2	 0.9980	 0.4450
z1	 0.9340	 0.4710
z2	 1.0000	 0.5010
z3	 0.9980	 0.5060