



## wwPDB EM Validation Summary Report ⓘ

Oct 20, 2025 – 01:58 AM JST

PDB ID : 9V7J / pdb\_00009v7j  
EMDB ID : EMD-64815  
Title : Phycobilisome core from *Gloeobacter violaceus* PCC 7421  
Authors : Burtseva, A.D.; Baymukhametov, T.N.; Slonimskiy, Y.B.; Popov, V.O.;  
Sluchanko, N.N.; Boyko, K.M.  
Deposited on : 2025-05-28  
Resolution : 2.85 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev129  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
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) : 2.46

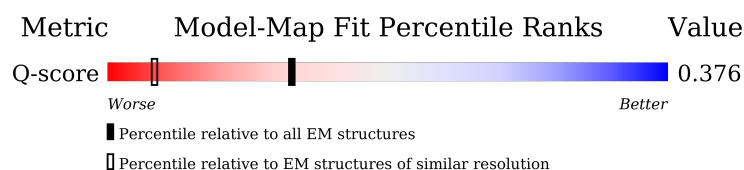
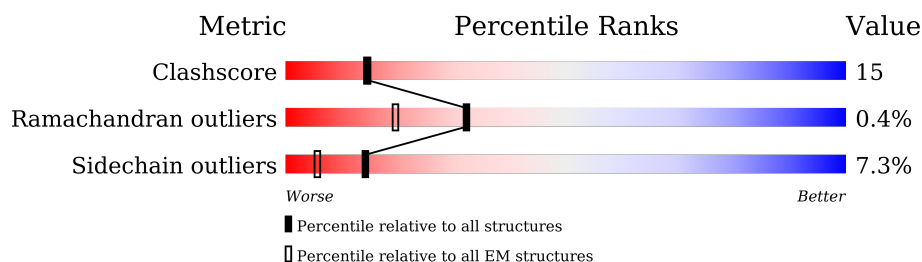
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.85 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	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	11965 ( 2.35 - 3.35 )

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1155	<div> <div>59%</div> <div>28%</div> <div>6%</div> <div>6%</div> </div>
1	C	1155	<div> <div>58%</div> <div>29%</div> <div>6%</div> <div>6%</div> </div>
2	1	161	<div> <div>65%</div> <div>27%</div> <div>.</div> <div>.</div> </div>
2	3	161	<div> <div>63%</div> <div>29%</div> <div>6%</div> <div>.</div> </div>


























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Mol	Chain	Length	Quality of chain
2	5	161	 67% 27% 5% ..
2	7	161	 68% 23% 7% ..
2	9	161	 63% 26% 8% ..
2	AA	161	 70% 23% 5% ..
2	AC	161	 66% 26% 7% ..
2	AE	161	 63% 29% 5% ..
2	AG	161	 61% 29% 7% ..
2	AI	161	 64% 26% 8% ..
2	AK	161	 63% 29% 6% ..
2	AM	161	 70% 24% . ..
2	AO	161	 66% 26% 7% ..
2	AQ	161	 63% 30% 5% ..
2	AS	161	 62% 29% 7% ..
2	AU	161	 63% 27% 8% ..
2	AW	161	 63% 29% 7% ..
2	E	161	 66% 24% 8% ..
2	G	161	 68% 24% 6% ..
2	I	161	 66% 25% 7% ..
2	K	161	 66% 26% 6% ..
2	M	161	 68% 23% 7% ..
2	O	161	 71% 21% 7% .
2	Q	161	 68% 24% 7% ..
2	S	161	 70% 22% 7% .
2	U	161	 66% 24% 9% ..
2	W	161	 68% 24% 6% ..











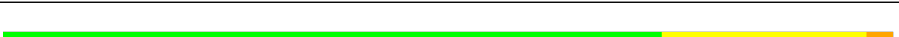


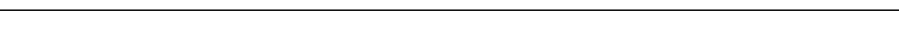
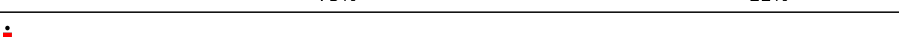
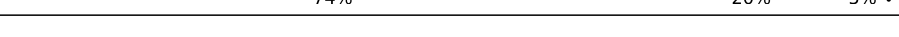



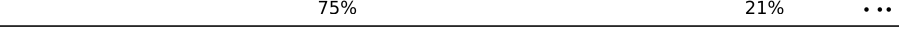





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Mol	Chain	Length	Quality of chain
2	Y	161	 66% 24% 7% ..
2	a	161	 67% 25% 6% ..
2	c	161	 55% 35% 7% ..
2	e	161	 68% 25% 5% .
2	g	161	 61% 28% 9% .
2	i	161	 67% 22% 6% ..
2	k	161	 57% 29% 11% ..
2	m	161	 66% 26% 6% ..
2	o	161	 65% 27% 6% ..
2	r	161	 68% 25% 5% ..
2	t	161	 68% 25% 6% ..
2	w	161	 61% 30% 7% .
2	y	161	 66% 26% 6% ..
3	0	161	 73% 21% 5% .
3	2	161	 68% 21% 6% ..
3	4	161	 73% 20% . .
3	6	161	 73% 25% ..
3	8	161	 80% 16% ..
3	AB	161	 76% 20% ..
3	AD	161	 70% 21% 7% ..
3	AF	161	 69% 24% . ..
3	AH	161	 75% 22% .
3	AJ	161	 75% 19% . .
3	AL	161	 73% 22% . .
3	AN	161	 74% 22% ..

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Mol	Chain	Length	Quality of chain
3	AP	161	 70%20%6% ..
3	AR	161	 69%25%.. ..
3	AT	161	 74%22%. .
3	AV	161	 73%22%.. .
3	AX	161	 73%23%.. .
3	F	161	 75%22%.. .
3	H	161	 76%20%.. .
3	J	161	 74%20%6% .
3	L	161	 74%20%5% .
3	N	161	 73%22%.. .
3	P	161	 74%23% .
3	R	161	 71%24%.. .
3	T	161	 73%24% .
3	V	161	 75%22%.. .
3	X	161	 74%20%5% .
3	Z	161	 75%19%6% .
3	b	161	 74%20%6% .
3	d	161	 74%20%.. ..
3	f	161	 75%21%.. ..
3	h	161	 75%23%.. .
3	j	161	 71%19%6% ..
3	l	161	 71%21%6% ..
3	n	161	 78%19% .
3	p	161	 76%20% .
3	q	161	 75%19%6% .

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Mol	Chain	Length	Quality of chain
3	v	161	
3	x	161	
3	z	161	
4	s	161	
4	u	161	
5	AY	69	
5	AZ	69	
5	Aa	69	
5	Ab	69	
5	Ac	69	
5	Ad	69	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	CYC	C	2101	-	-	X	-

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 123484 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Phycobiliprotein ApcE.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1089	Total	C	N	O	S	0	0
			8678	5505	1533	1621	19		
1	C	1089	Total	C	N	O	S	0	0
			8678	5505	1533	1621	19		

- Molecule 2 is a protein called Allophycocyanin alpha subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	M	160	Total	C	N	O	S	0	0
			1223	771	210	237	5		
2	O	159	Total	C	N	O	S	0	0
			1213	766	208	234	5		
2	E	160	Total	C	N	O	S	0	0
			1223	771	210	237	5		
2	G	160	Total	C	N	O	S	0	0
			1223	771	210	237	5		
2	I	160	Total	C	N	O	S	0	0
			1223	771	210	237	5		
2	K	160	Total	C	N	O	S	0	0
			1223	771	210	237	5		
2	Q	160	Total	C	N	O	S	0	0
			1223	771	210	237	5		
2	S	159	Total	C	N	O	S	0	0
			1213	766	208	234	5		
2	U	160	Total	C	N	O	S	0	0
			1223	771	210	237	5		
2	W	160	Total	C	N	O	S	0	0
			1223	771	210	237	5		
2	Y	160	Total	C	N	O	S	0	0
			1223	771	210	237	5		
2	a	160	Total	C	N	O	S	0	0
			1223	771	210	237	5		
2	c	159	Total	C	N	O	S	0	0
			1213	766	208	234	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	e	159	Total 1213	C 766	N 208	O 234	S 5	0	0
2	g	159	Total 1213	C 766	N 208	O 234	S 5	0	0
2	i	158	Total 1207	C 763	N 207	O 232	S 5	0	0
2	k	158	Total 1207	C 763	N 207	O 232	S 5	0	0
2	m	160	Total 1223	C 771	N 210	O 237	S 5	0	0
2	o	159	Total 1213	C 766	N 208	O 234	S 5	0	0
2	r	160	Total 1223	C 771	N 210	O 237	S 5	0	0
2	t	159	Total 1213	C 766	N 208	O 234	S 5	0	0
2	w	159	Total 1213	C 766	N 208	O 234	S 5	0	0
2	y	159	Total 1213	C 766	N 208	O 234	S 5	0	0
2	1	158	Total 1207	C 763	N 207	O 232	S 5	0	0
2	3	159	Total 1213	C 766	N 208	O 234	S 5	0	0
2	5	159	Total 1213	C 766	N 208	O 234	S 5	0	0
2	7	160	Total 1223	C 771	N 210	O 237	S 5	0	0
2	9	158	Total 1207	C 763	N 207	O 232	S 5	0	0
2	AA	160	Total 1223	C 771	N 210	O 237	S 5	0	0
2	AC	160	Total 1223	C 771	N 210	O 237	S 5	0	0
2	AE	160	Total 1223	C 771	N 210	O 237	S 5	0	0
2	AG	160	Total 1223	C 771	N 210	O 237	S 5	0	0
2	AI	159	Total 1213	C 766	N 208	O 234	S 5	0	0
2	AK	159	Total 1213	C 766	N 208	O 234	S 5	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	AM	160	Total	C	N	O	S	0	0
			1223	771	210	237	5		
2	AO	160	Total	C	N	O	S	0	0
			1223	771	210	237	5		
2	AQ	160	Total	C	N	O	S	0	0
			1223	771	210	237	5		
2	AS	160	Total	C	N	O	S	0	0
			1223	771	210	237	5		
2	AU	159	Total	C	N	O	S	0	0
			1213	766	208	234	5		
2	AW	159	Total	C	N	O	S	0	0
			1213	766	208	234	5		

- Molecule 3 is a protein called Allophycocyanin beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	N	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
3	P	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
3	F	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
3	H	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
3	J	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
3	L	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
3	R	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
3	T	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
3	V	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
3	X	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
3	Z	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
3	b	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
3	d	158	Total	C	N	O	S	0	0
			1187	753	199	230	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	f	160	Total	C	N	O	S	0	0
			1202	762	201	234	5		
3	h	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
3	j	158	Total	C	N	O	S	0	0
			1187	753	199	230	5		
3	l	159	Total	C	N	O	S	0	0
			1195	759	200	231	5		
3	n	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
3	p	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
3	q	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
3	v	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
3	x	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
3	z	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
3	2	158	Total	C	N	O	S	0	0
			1187	753	199	230	5		
3	4	158	Total	C	N	O	S	0	0
			1187	753	199	230	5		
3	6	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
3	8	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
3	0	159	Total	C	N	O	S	0	0
			1195	759	200	231	5		
3	AB	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
3	AD	159	Total	C	N	O	S	0	0
			1195	759	200	231	5		
3	AF	160	Total	C	N	O	S	0	0
			1202	762	201	234	5		
3	AH	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
3	AJ	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
3	AL	160	Total	C	N	O	S	0	0
			1203	764	201	232	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	AN	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
3	AP	159	Total	C	N	O	S	0	0
			1195	759	200	231	5		
3	AR	160	Total	C	N	O	S	0	0
			1202	762	201	234	5		
3	AT	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
3	AV	161	Total	C	N	O	S	0	0
			1210	767	202	235	6		
3	AX	160	Total	C	N	O	S	0	0
			1203	764	201	232	6		

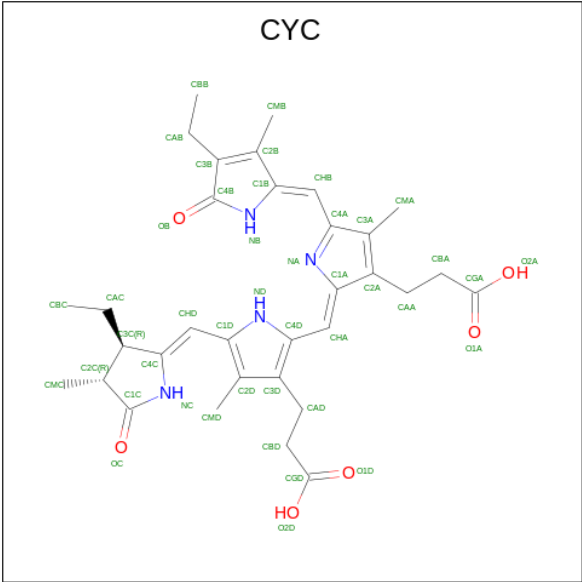
- Molecule 4 is a protein called Phycobilisome core component.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	s	161	Total	C	N	O	S	0	0
			1227	779	206	237	5		
4	u	160	Total	C	N	O	S	0	0
			1217	774	204	234	5		

- Molecule 5 is a protein called Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AY	66	Total	C	N	O	S	0	0
			529	340	96	92	1		
5	AZ	66	Total	C	N	O	S	0	0
			529	340	96	92	1		
5	Aa	66	Total	C	N	O	S	0	0
			529	340	96	92	1		
5	Ab	65	Total	C	N	O	S	0	0
			522	335	95	91	1		
5	Ac	64	Total	C	N	O	S	0	0
			518	333	94	90	1		
5	Ad	66	Total	C	N	O	S	0	0
			529	340	96	92	1		

- Molecule 6 is PHYCOCYANOBILIN (CCD ID: CYC) (formula:  $C_{33}H_{40}N_4O_6$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			43	33	4	6	
6	C	1	Total	C	N	O	0
			43	33	4	6	
6	M	1	Total	C	N	O	0
			43	33	4	6	
6	N	1	Total	C	N	O	0
			43	33	4	6	
6	O	1	Total	C	N	O	0
			43	33	4	6	
6	P	1	Total	C	N	O	0
			43	33	4	6	
6	E	1	Total	C	N	O	0
			43	33	4	6	
6	F	1	Total	C	N	O	0
			43	33	4	6	
6	G	1	Total	C	N	O	0
			43	33	4	6	
6	H	1	Total	C	N	O	0
			43	33	4	6	
6	I	1	Total	C	N	O	0
			43	33	4	6	
6	J	1	Total	C	N	O	0
			43	33	4	6	
6	K	1	Total	C	N	O	0
			43	33	4	6	
6	L	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
6	Q	1	Total 43	C 33	N 4	O 6	0
6	R	1	Total 43	C 33	N 4	O 6	0
6	S	1	Total 43	C 33	N 4	O 6	0
6	T	1	Total 43	C 33	N 4	O 6	0
6	U	1	Total 43	C 33	N 4	O 6	0
6	V	1	Total 43	C 33	N 4	O 6	0
6	W	1	Total 43	C 33	N 4	O 6	0
6	X	1	Total 43	C 33	N 4	O 6	0
6	Y	1	Total 43	C 33	N 4	O 6	0
6	Z	1	Total 43	C 33	N 4	O 6	0
6	a	1	Total 43	C 33	N 4	O 6	0
6	b	1	Total 43	C 33	N 4	O 6	0
6	c	1	Total 43	C 33	N 4	O 6	0
6	d	1	Total 43	C 33	N 4	O 6	0
6	e	1	Total 43	C 33	N 4	O 6	0
6	f	1	Total 43	C 33	N 4	O 6	0
6	g	1	Total 43	C 33	N 4	O 6	0
6	h	1	Total 43	C 33	N 4	O 6	0
6	i	1	Total 43	C 33	N 4	O 6	0
6	j	1	Total 43	C 33	N 4	O 6	0
6	k	1	Total 43	C 33	N 4	O 6	0

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Mol	Chain	Residues	Atoms				AltConf
6	l	1	Total 43	C 33	N 4	O 6	0
6	m	1	Total 43	C 33	N 4	O 6	0
6	n	1	Total 43	C 33	N 4	O 6	0
6	o	1	Total 43	C 33	N 4	O 6	0
6	p	1	Total 43	C 33	N 4	O 6	0
6	q	1	Total 43	C 33	N 4	O 6	0
6	r	1	Total 43	C 33	N 4	O 6	0
6	s	1	Total 43	C 33	N 4	O 6	0
6	t	1	Total 43	C 33	N 4	O 6	0
6	u	1	Total 43	C 33	N 4	O 6	0
6	v	1	Total 43	C 33	N 4	O 6	0
6	w	1	Total 43	C 33	N 4	O 6	0
6	x	1	Total 43	C 33	N 4	O 6	0
6	y	1	Total 43	C 33	N 4	O 6	0
6	z	1	Total 43	C 33	N 4	O 6	0
6	1	1	Total 43	C 33	N 4	O 6	0
6	2	1	Total 43	C 33	N 4	O 6	0
6	3	1	Total 43	C 33	N 4	O 6	0
6	4	1	Total 43	C 33	N 4	O 6	0
6	5	1	Total 43	C 33	N 4	O 6	0
6	6	1	Total 43	C 33	N 4	O 6	0

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Mol	Chain	Residues	Atoms				AltConf
6	7	1	Total	C	N	O	0
			43	33	4	6	
6	8	1	Total	C	N	O	0
			43	33	4	6	
6	9	1	Total	C	N	O	0
			43	33	4	6	
6	0	1	Total	C	N	O	0
			43	33	4	6	
6	AA	1	Total	C	N	O	0
			43	33	4	6	
6	AB	1	Total	C	N	O	0
			43	33	4	6	
6	AC	1	Total	C	N	O	0
			43	33	4	6	
6	AD	1	Total	C	N	O	0
			43	33	4	6	
6	AE	1	Total	C	N	O	0
			43	33	4	6	
6	AF	1	Total	C	N	O	0
			43	33	4	6	
6	AG	1	Total	C	N	O	0
			43	33	4	6	
6	AH	1	Total	C	N	O	0
			43	33	4	6	
6	AI	1	Total	C	N	O	0
			43	33	4	6	
6	AJ	1	Total	C	N	O	0
			43	33	4	6	
6	AK	1	Total	C	N	O	0
			43	33	4	6	
6	AL	1	Total	C	N	O	0
			43	33	4	6	
6	AM	1	Total	C	N	O	0
			43	33	4	6	
6	AN	1	Total	C	N	O	0
			43	33	4	6	
6	AO	1	Total	C	N	O	0
			43	33	4	6	
6	AP	1	Total	C	N	O	0
			43	33	4	6	
6	AQ	1	Total	C	N	O	0
			43	33	4	6	

*Continued on next page...*

*Continued from previous page...*

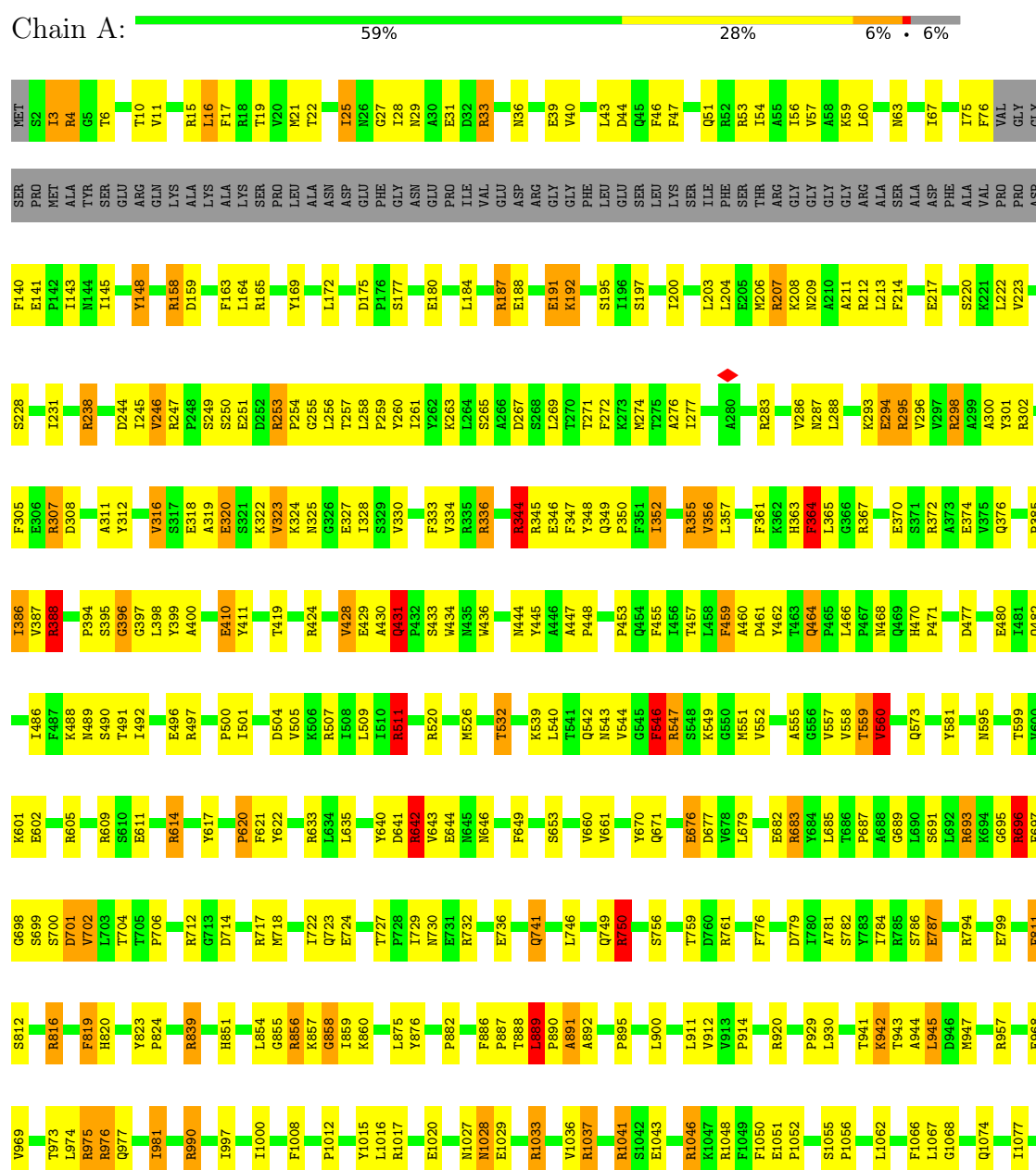
Mol	Chain	Residues	Atoms				AltConf
6	AR	1	Total 43	C 33	N 4	O 6	0
6	AS	1	Total 43	C 33	N 4	O 6	0
6	AT	1	Total 43	C 33	N 4	O 6	0
6	AU	1	Total 43	C 33	N 4	O 6	0
6	AV	1	Total 43	C 33	N 4	O 6	0
6	AW	1	Total 43	C 33	N 4	O 6	0
6	AX	1	Total 43	C 33	N 4	O 6	0

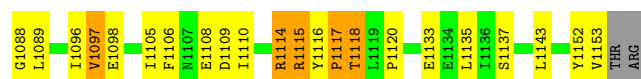


### 3 Residue-property plots

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

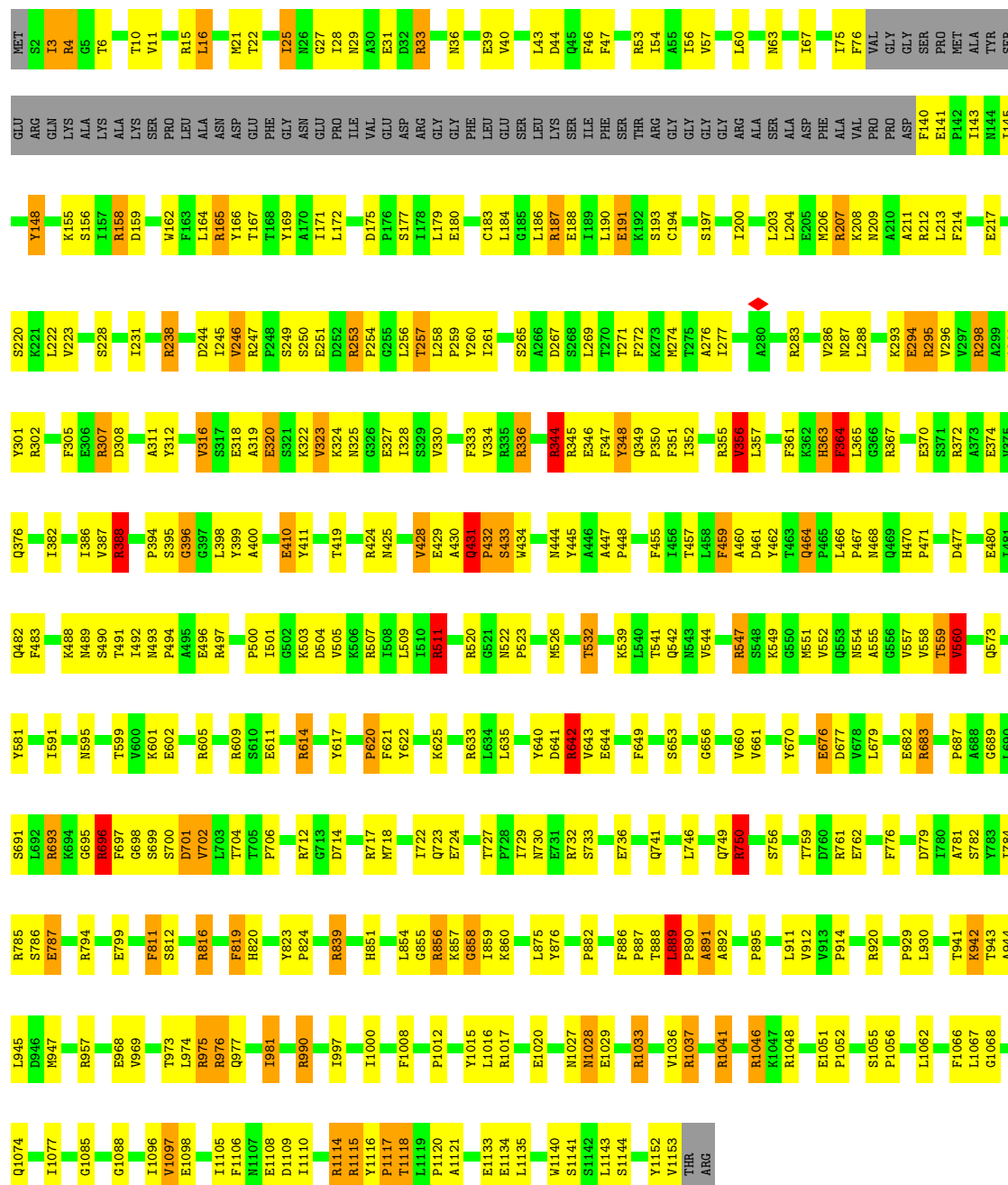
#### • Molecule 1: Phycobiliprotein ApcE





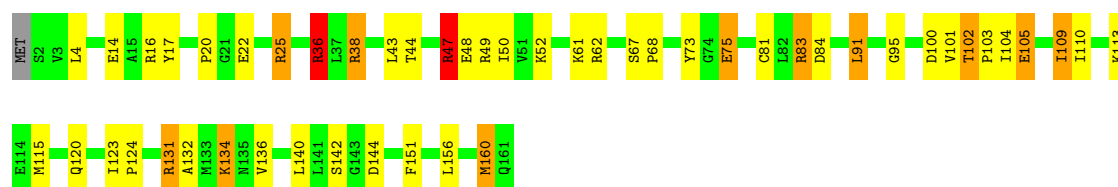
### • Molecule 1: Phycobiliprotein ApcE

Chain C: 58% 29% 6% 6%



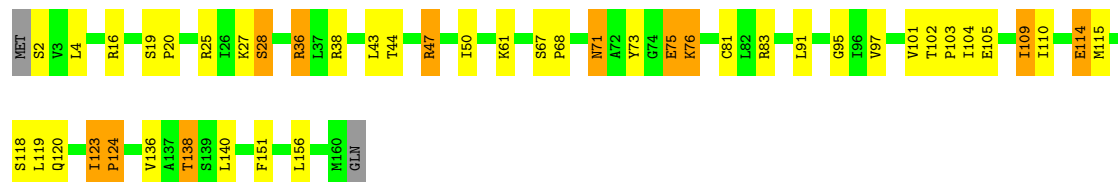
### • Molecule 2: Allophycocyanin alpha subunit

Chain M: 68% 23% 7% 2%



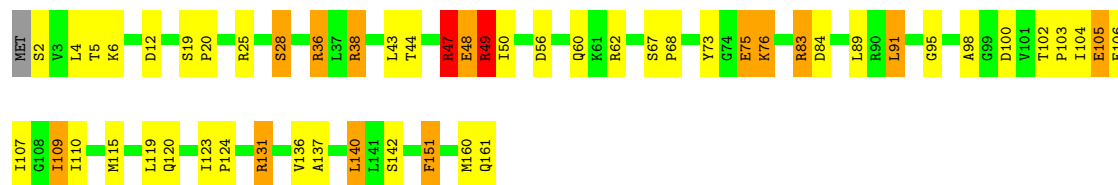
• Molecule 2: Allophycocyanin alpha subunit

Chain O: 71% 21% 7% •



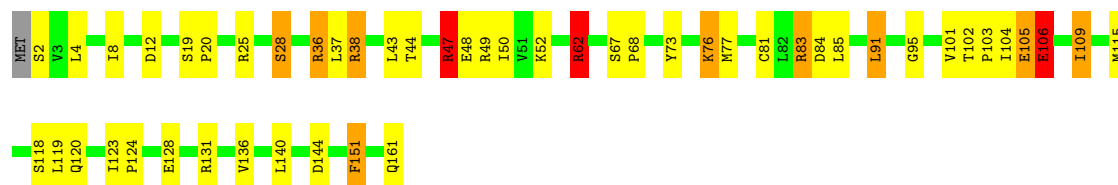
• Molecule 2: Allophycocyanin alpha subunit

Chain E: 66% 24% 8% ••



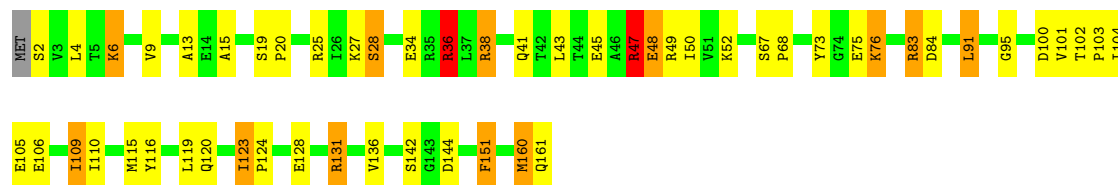
• Molecule 2: Allophycocyanin alpha subunit

Chain G: 68% 24% 6% ••



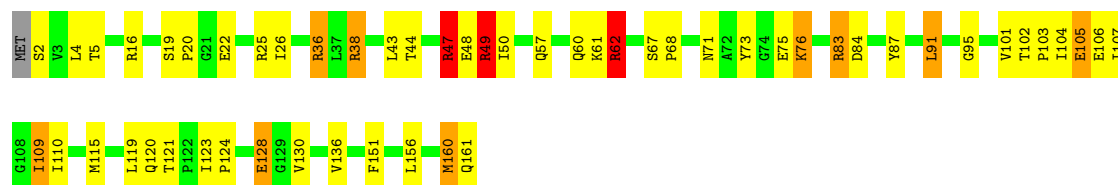
• Molecule 2: Allophycocyanin alpha subunit

Chain I: 66% 25% 7% ••



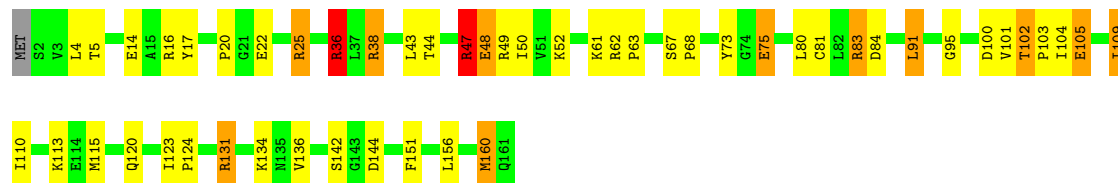
• Molecule 2: Allophycocyanin alpha subunit

Chain K: 66% 26% 6% ••



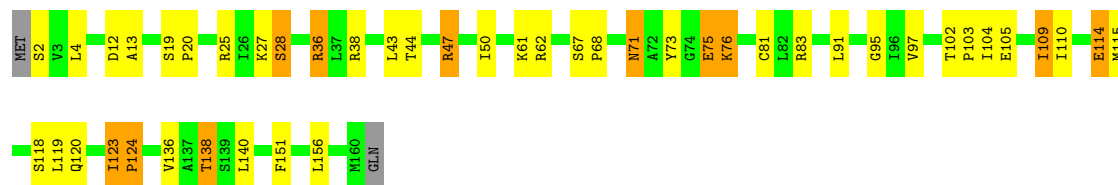
- Molecule 2: Allophycocyanin alpha subunit

Chain Q: 68% 24% 7% ..



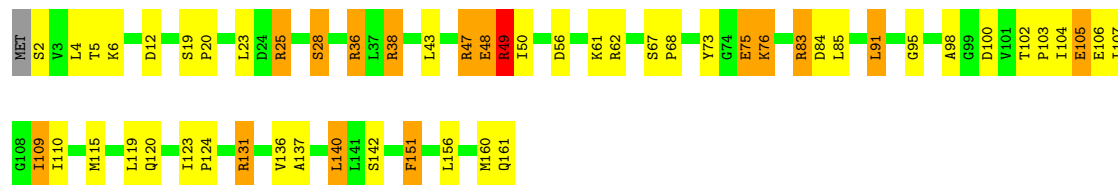
- Molecule 2: Allophycocyanin alpha subunit

Chain S: 70% 22% 7% .



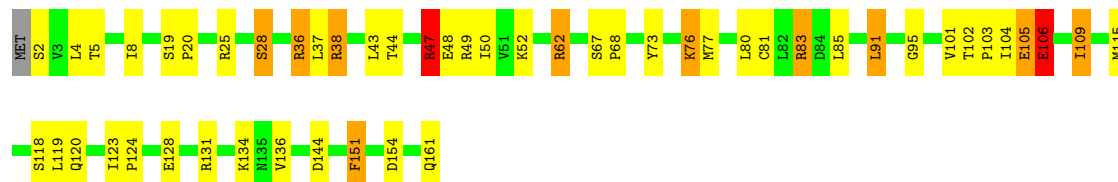
- Molecule 2: Allophycocyanin alpha subunit

Chain U: 66% 24% 9% ..



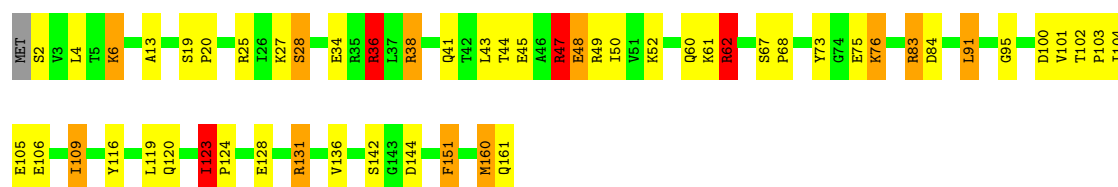
- Molecule 2: Allophycocyanin alpha subunit

Chain W: 68% 24% 6% ..



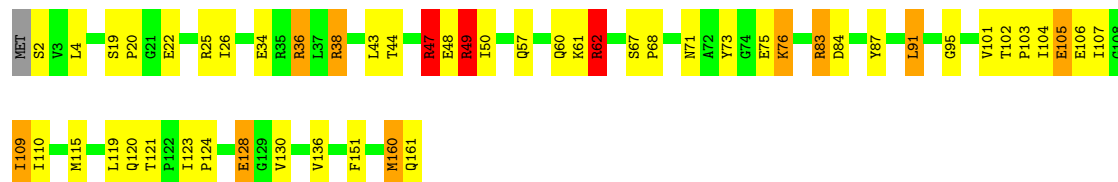
- Molecule 2: Allophycocyanin alpha subunit

Chain Y: 66% 24% 7% ..



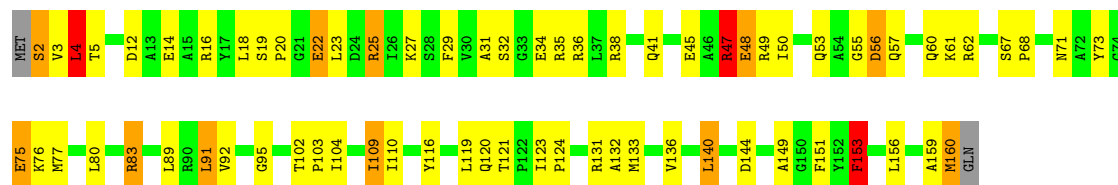
• Molecule 2: Allophycocyanin alpha subunit

Chain a: 67% 25% 6% ..



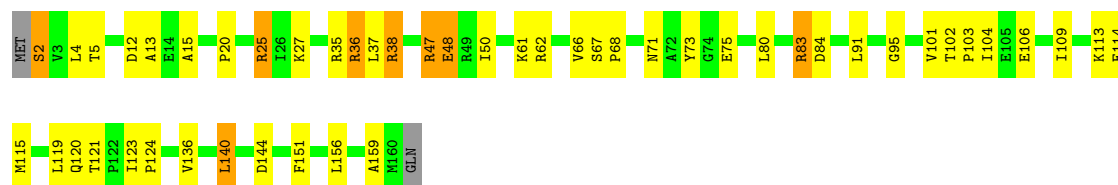
• Molecule 2: Allophycocyanin alpha subunit

Chain c: 55% 35% 7% ..



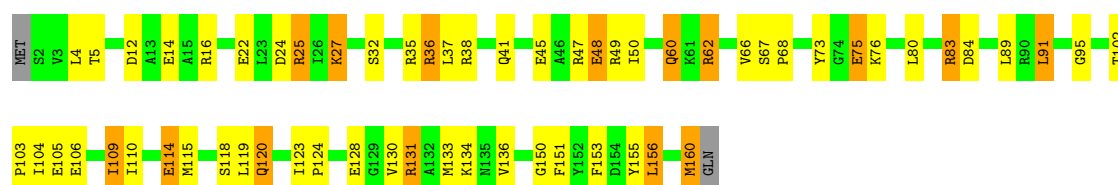
• Molecule 2: Allophycocyanin alpha subunit

Chain e: 68% 25% 5% •



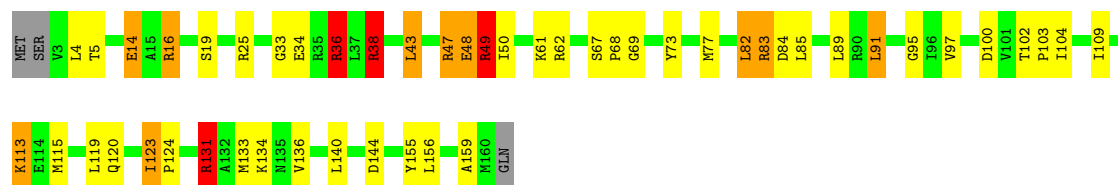
• Molecule 2: Allophycocyanin alpha subunit

Chain g: 61% 28% 9% •

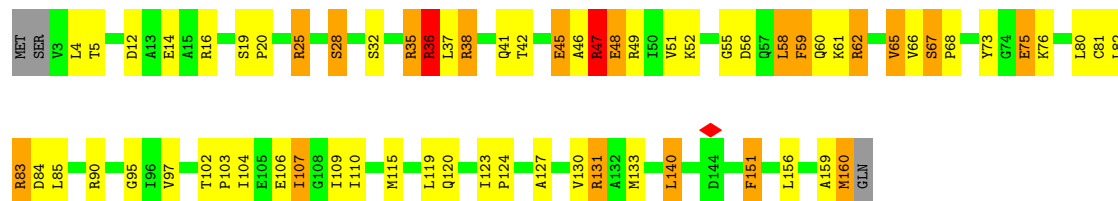


• Molecule 2: Allophycocyanin alpha subunit

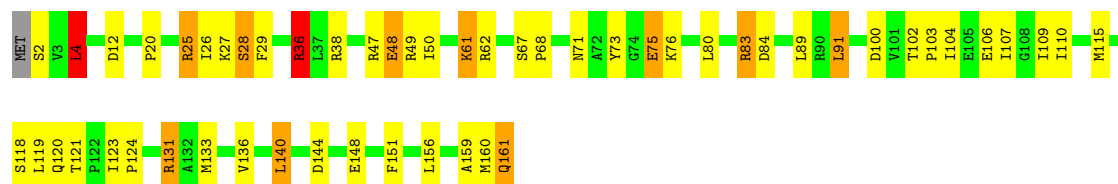
Chain i: 67% 22% 6% ..



- Molecule 2: Allophycocyanin alpha subunit



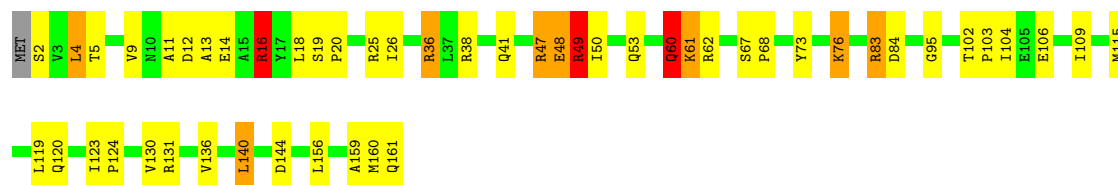
- Molecule 2: Allophycocyanin alpha subunit



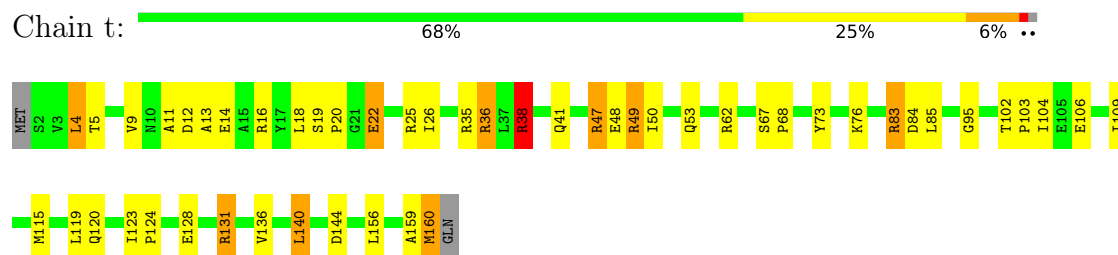
- Molecule 2: Allophycocyanin alpha subunit



- Molecule 2: Allophycocyanin alpha subunit



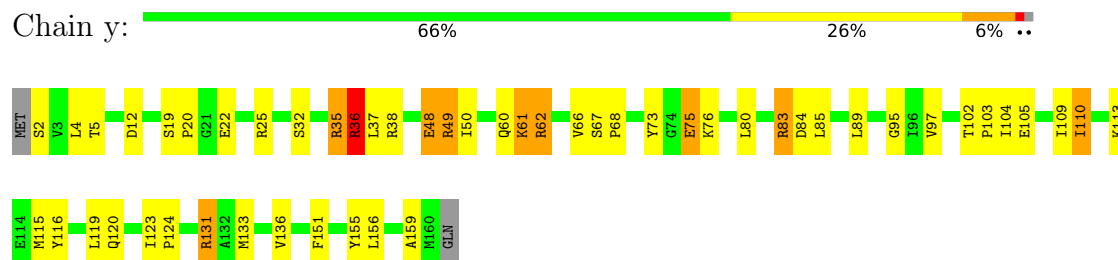
- Molecule 2: Allophycocyanin alpha subunit



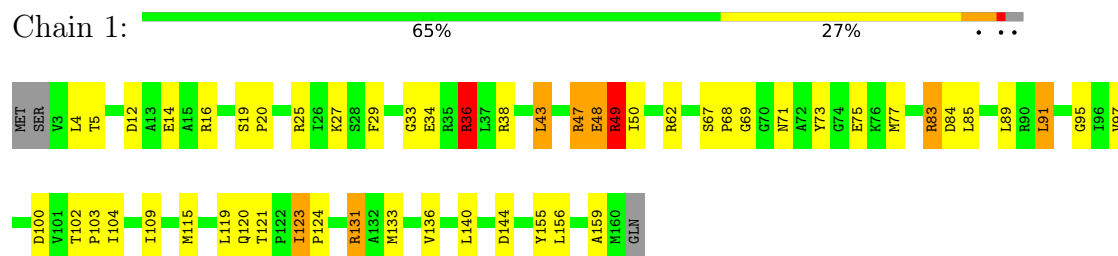
- Molecule 2: Allophycocyanin alpha subunit



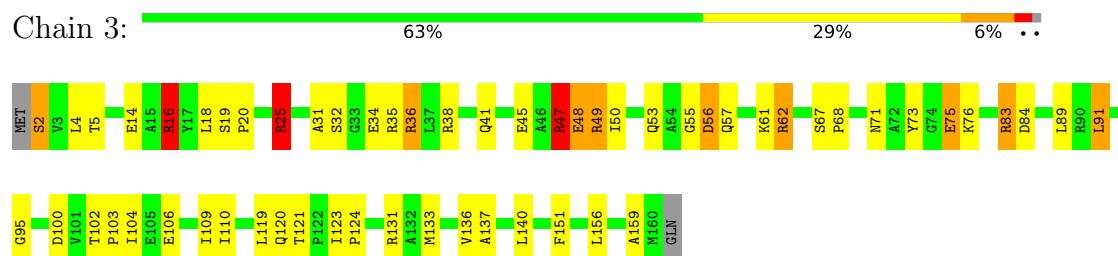
- Molecule 2: Allophycocyanin alpha subunit



- Molecule 2: Allophycocyanin alpha subunit

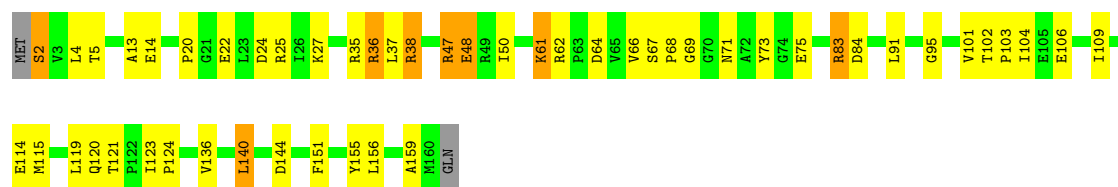


- Molecule 2: Allophycocyanin alpha subunit



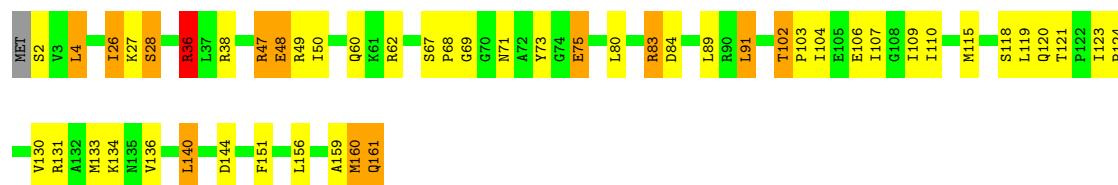
- Molecule 2: Allophycocyanin alpha subunit

Chain 5: 



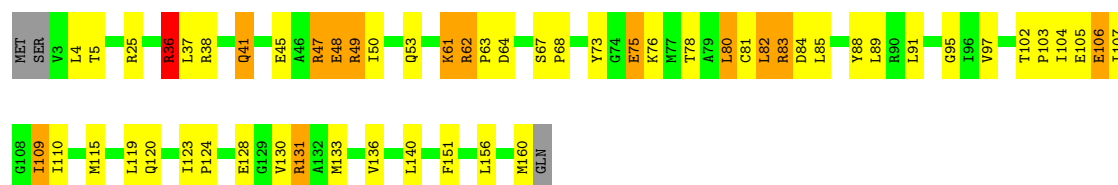
• Molecule 2: Allophycocyanin alpha subunit

Chain 7: 



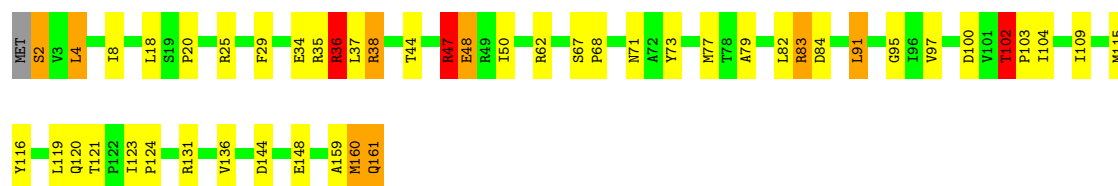
• Molecule 2: Allophycocyanin alpha subunit

Chain 9: 



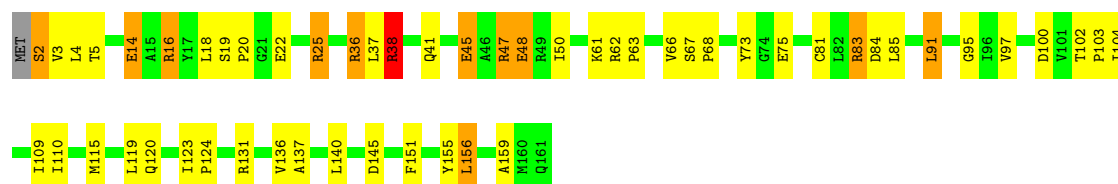
• Molecule 2: Allophycocyanin alpha subunit

Chain AA: 



• Molecule 2: Allophycocyanin alpha subunit

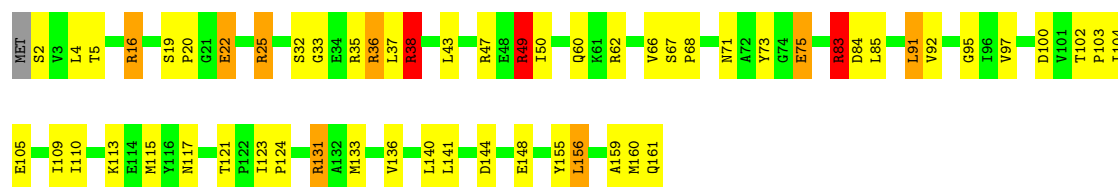
Chain AC: 



• Molecule 2: Allophycocyanin alpha subunit

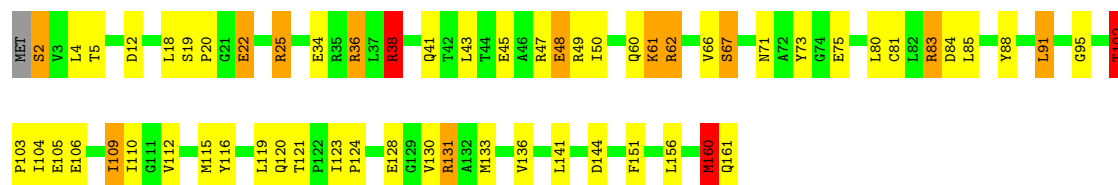


Chain AE:  63% 29% 5% ..



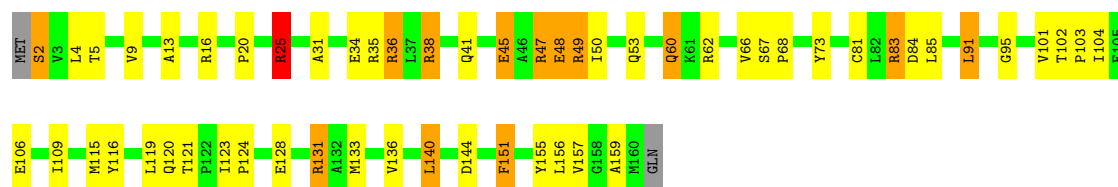
- Molecule 2: Allophycocyanin alpha subunit

Chain AG:  61% 29% 7% ..



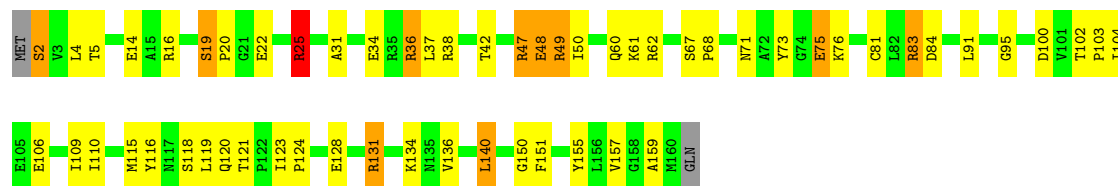
- Molecule 2: Allophycocyanin alpha subunit

Chain AI:  64% 26% 8% ..



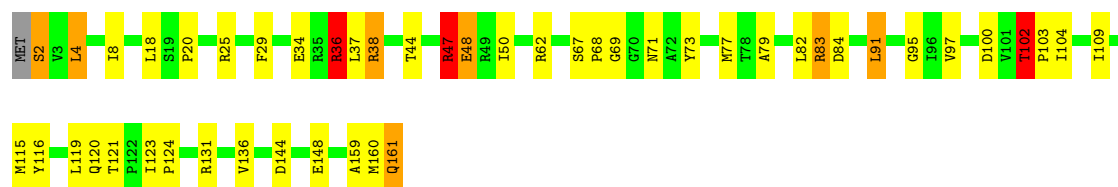
- Molecule 2: Allophycocyanin alpha subunit

Chain AK:  63% 29% 6% ..



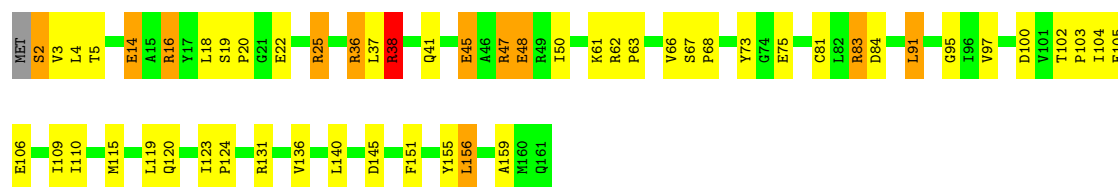
- Molecule 2: Allophycocyanin alpha subunit

Chain AM:  70% 24% ..



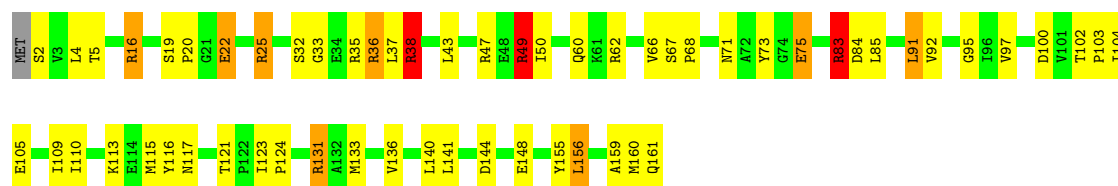
- Molecule 2: Allophycocyanin alpha subunit

Chain AO:  66% 26% 7% ..



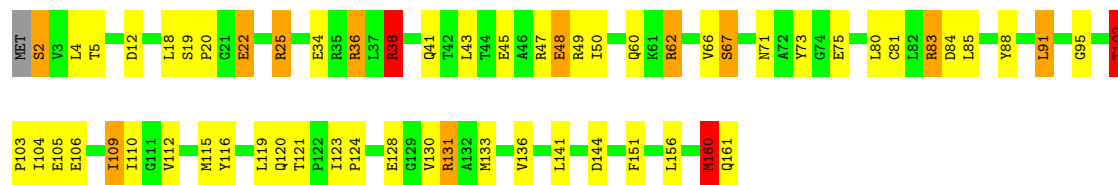
- Molecule 2: Allophycocyanin alpha subunit

Chain AQ:  63% 30% 5% ..



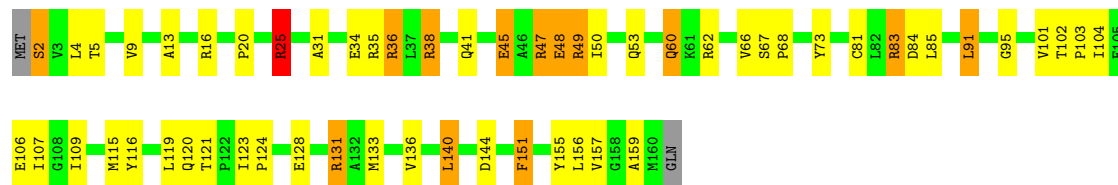
- Molecule 2: Allophycocyanin alpha subunit

Chain AS:  62% 29% 7% ..



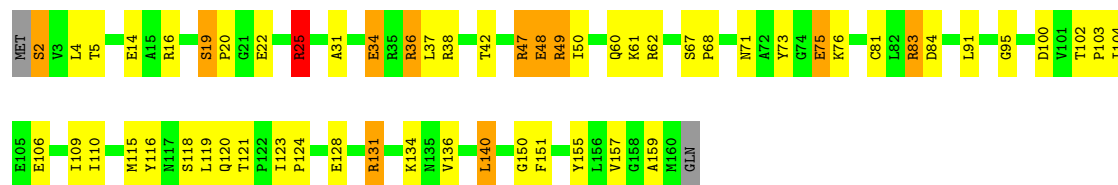
- Molecule 2: Allophycocyanin alpha subunit

Chain AU:  63% 27% 8% ..



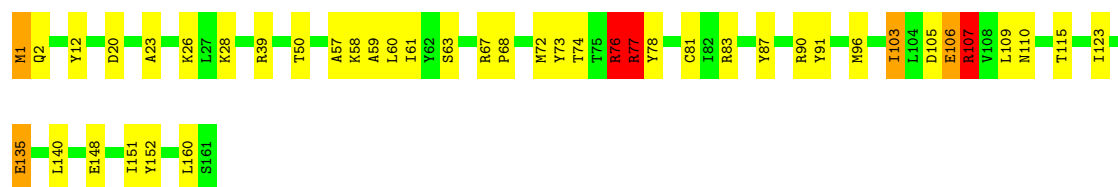
- Molecule 2: Allophycocyanin alpha subunit

Chain AW:  63% 29% 7% ..



- Molecule 3: Allophycocyanin beta subunit

Chain N:  73% 22% ..



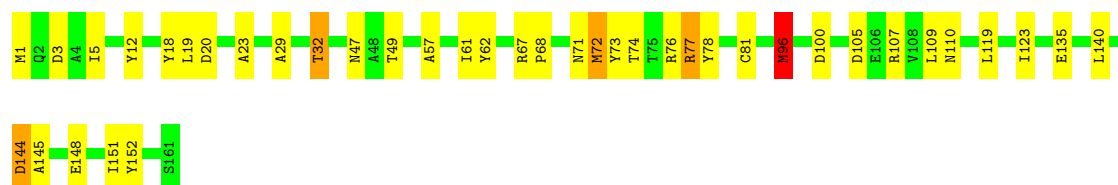
- Molecule 3: Allophycocyanin beta subunit

Chain P:  74% 23% .




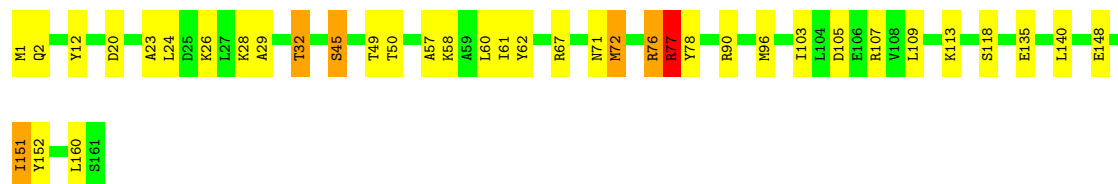
- Molecule 3: Allophycocyanin beta subunit

Chain F:  75% 22% ..



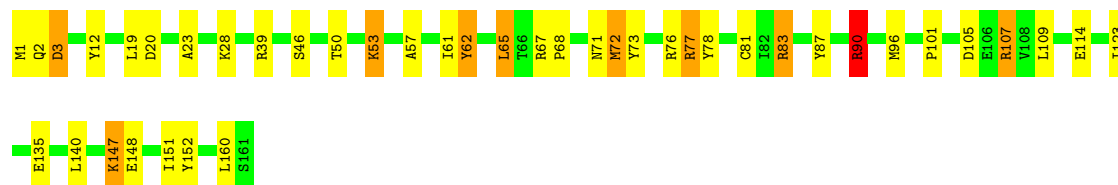
- Molecule 3: Allophycocyanin beta subunit

Chain H:  76% 20% ..



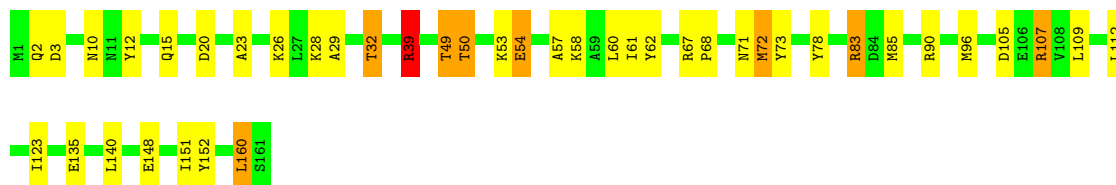
- Molecule 3: Allophycocyanin beta subunit

Chain J:  74% 20% 6% .



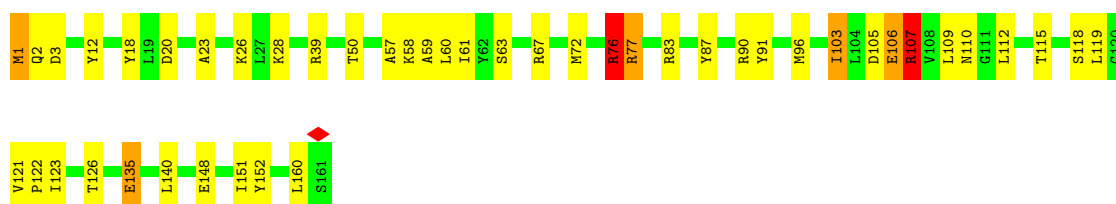
- Molecule 3: Allophycocyanin beta subunit

Chain L:  74% 20% 5% •



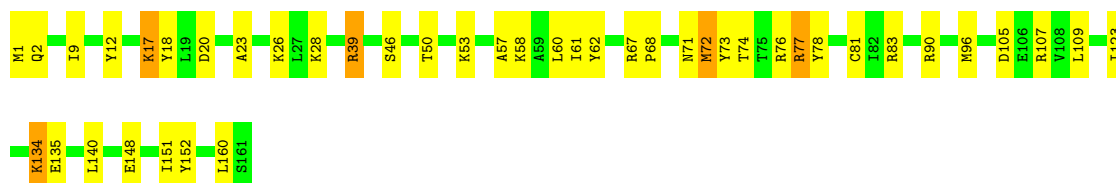
- Molecule 3: Allophycocyanin beta subunit

Chain R:  71% 24% • •




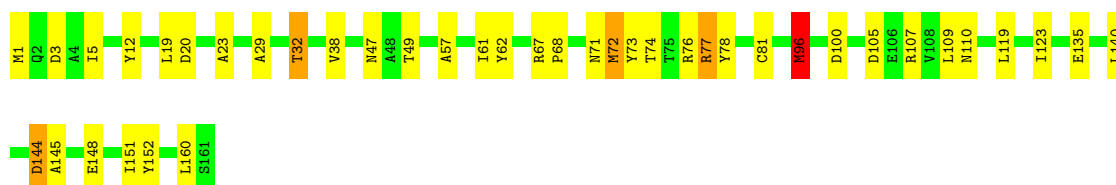
- Molecule 3: Allophycocyanin beta subunit

Chain T:  73% 24% •



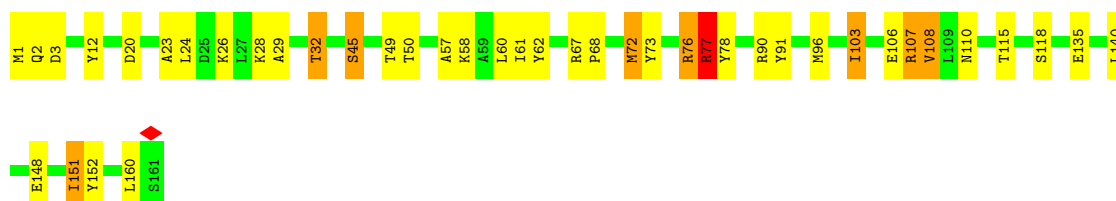
- Molecule 3: Allophycocyanin beta subunit

Chain V:  75% 22% • •



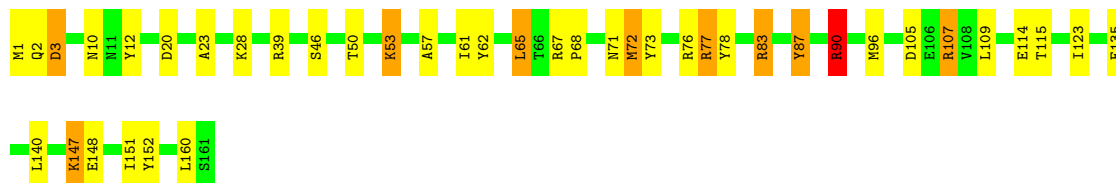
- Molecule 3: Allophycocyanin beta subunit

Chain X:  74% 20% 5% •




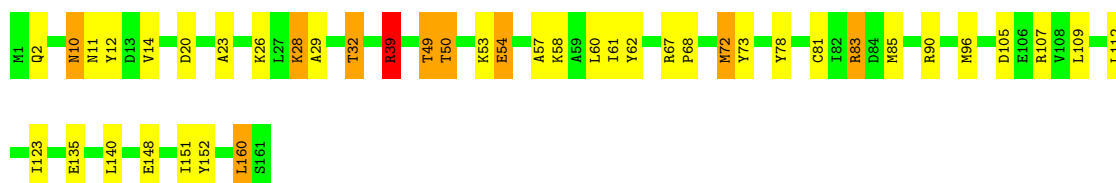
- Molecule 3: Allophycocyanin beta subunit

Chain Z:  75% 19% 6% .



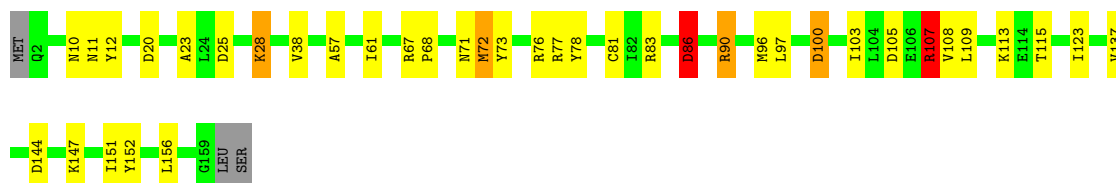
- Molecule 3: Allophycocyanin beta subunit

Chain b:  74% 20% 6% .



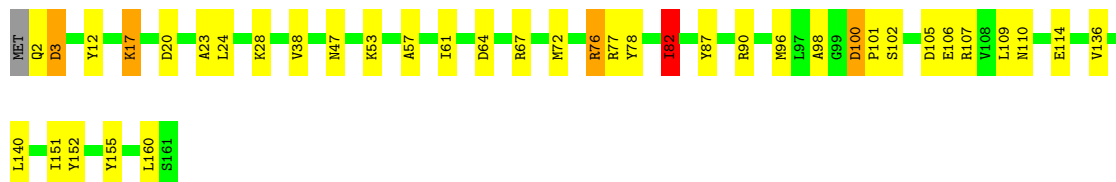
- Molecule 3: Allophycocyanin beta subunit

Chain d:  74% 20% . . .



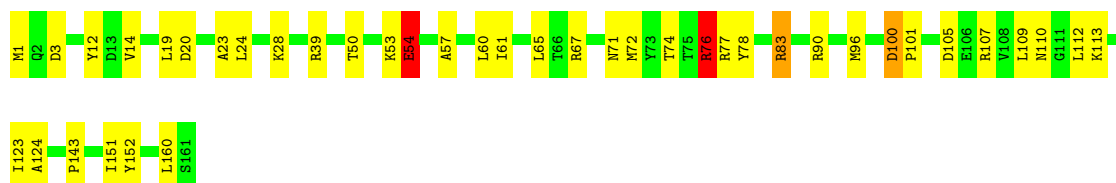
- Molecule 3: Allophycocyanin beta subunit

Chain f:  75% 21% . . .



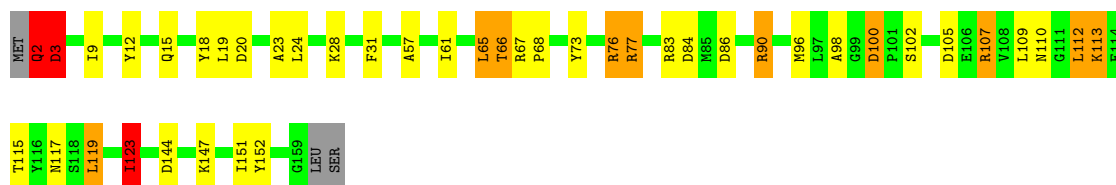
- Molecule 3: Allophycocyanin beta subunit

Chain h:  75% 23% . .



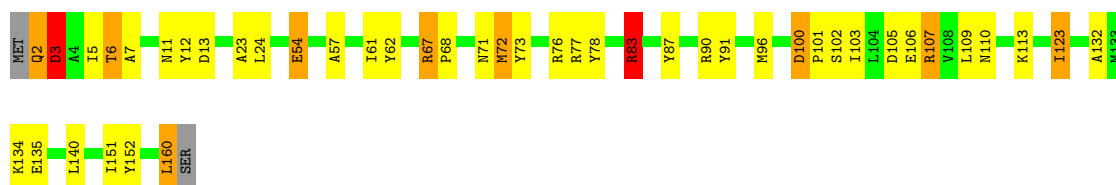
- Molecule 3: Allophycocyanin beta subunit

Chain j:  71% 19% 6% ..




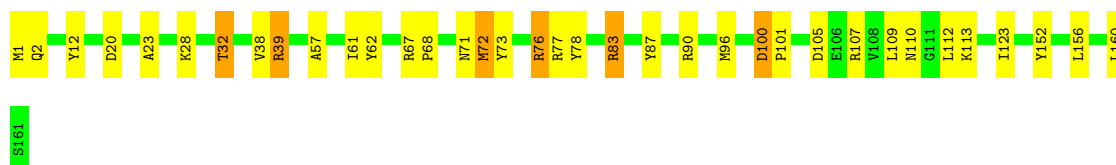
- Molecule 3: Allophycocyanin beta subunit

Chain l:  71% 21% 6% ..




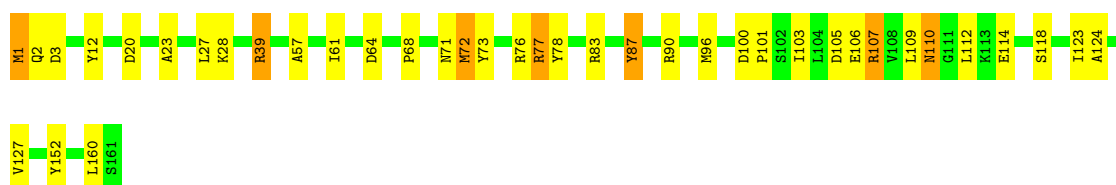
- Molecule 3: Allophycocyanin beta subunit

Chain n:  78% 19% .




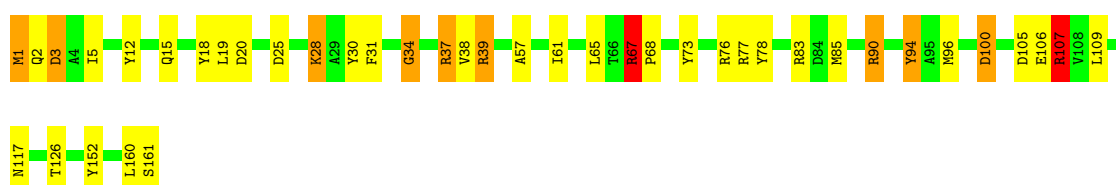
- Molecule 3: Allophycocyanin beta subunit

Chain p:  76% 20% .



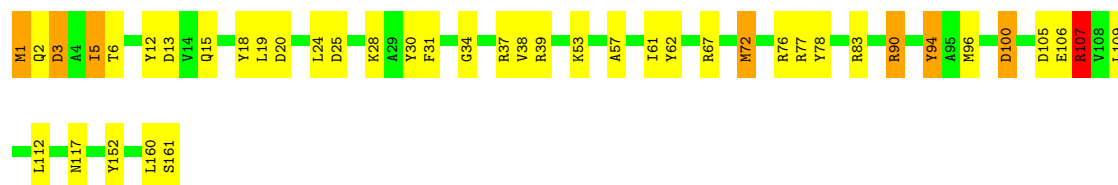
- Molecule 3: Allophycocyanin beta subunit

Chain q:  75% 19% 6% .




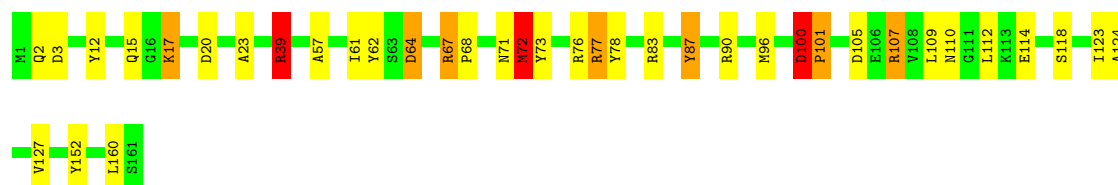
- Molecule 3: Allophycocyanin beta subunit

Chain v:  73% 22% . .



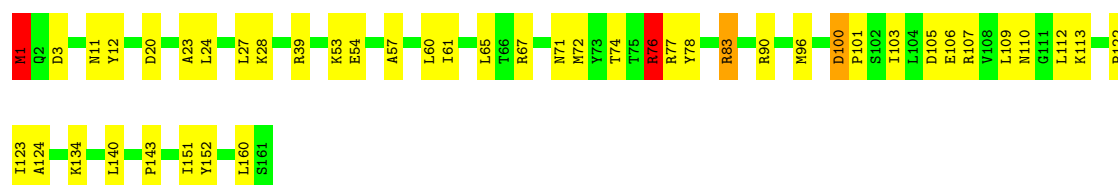
- Molecule 3: Allophycocyanin beta subunit

Chain x:  76% 17% . .



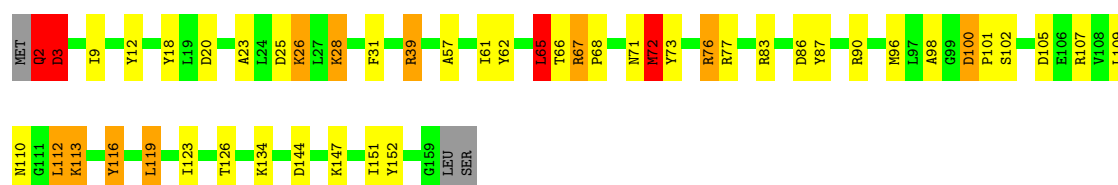
- Molecule 3: Allophycocyanin beta subunit

Chain z:  72% 25% . .



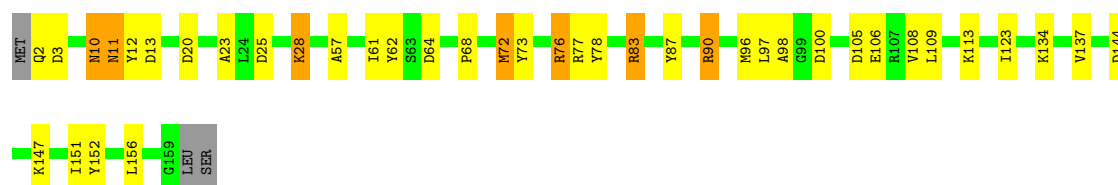
- Molecule 3: Allophycocyanin beta subunit

Chain 2:  68% 21% 6% . .

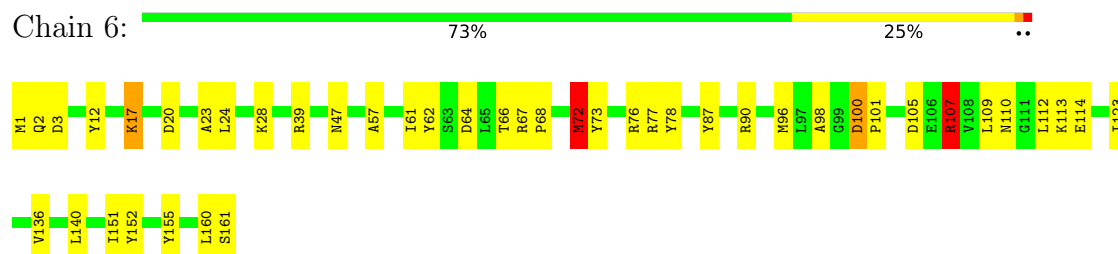


- Molecule 3: Allophycocyanin beta subunit

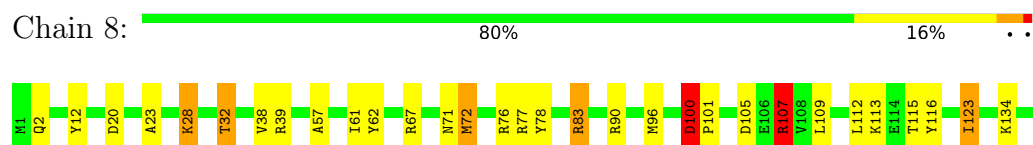
Chain 4:  73% 20% . .



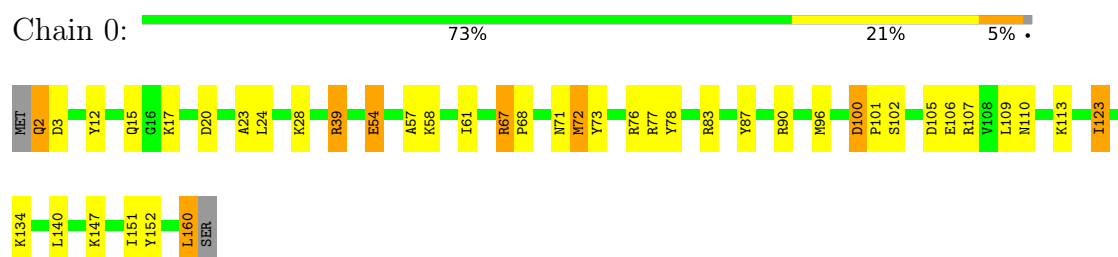
- Molecule 3: Allophycocyanin beta subunit



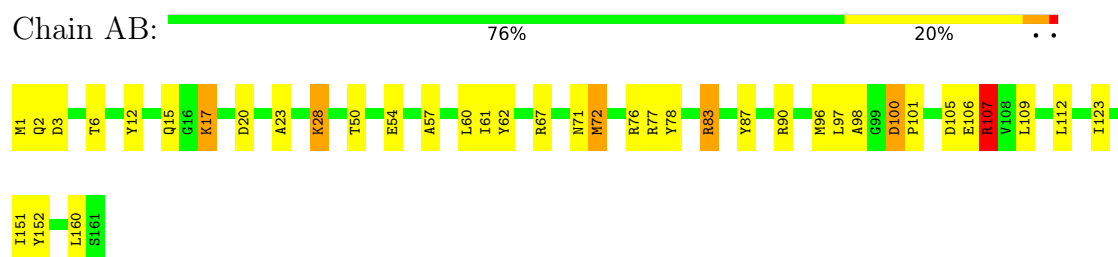
- Molecule 3: Allophycocyanin beta subunit



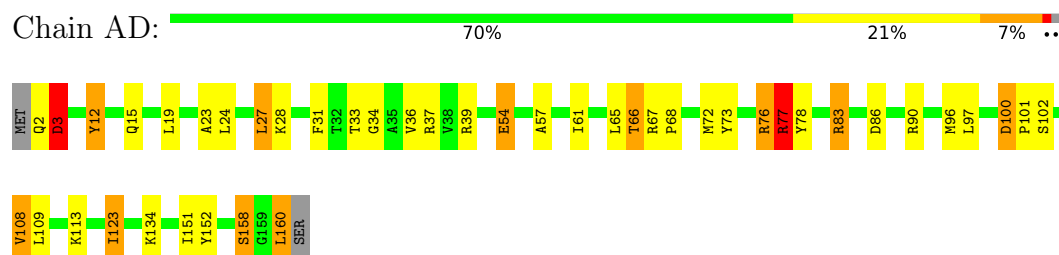
- Molecule 3: Allophycocyanin beta subunit



- Molecule 3: Allophycocyanin beta subunit



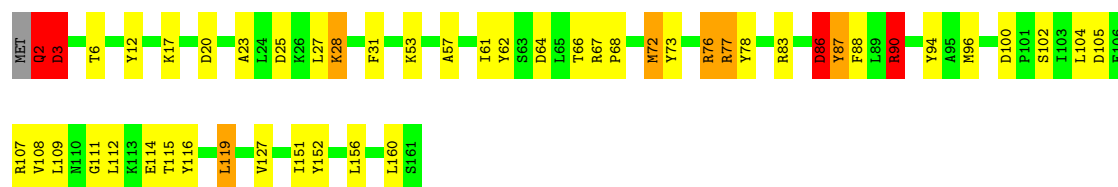
- Molecule 3: Allophycocyanin beta subunit




- Molecule 3: Allophycocyanin beta subunit

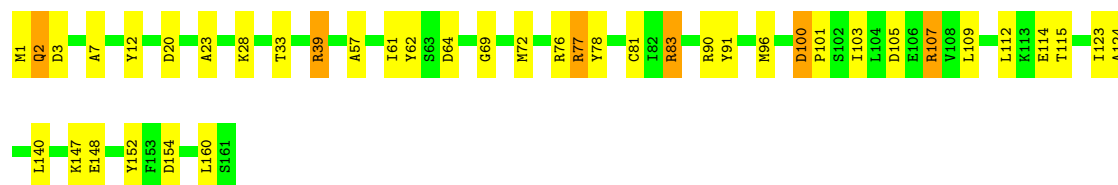


Chain AF:  69% 24% . .



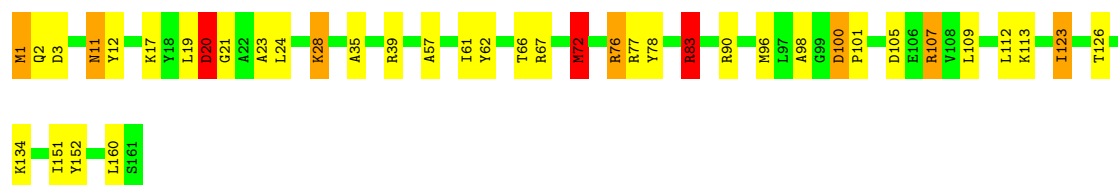
- Molecule 3: Allophycocyanin beta subunit

Chain AH:  75% 22% .



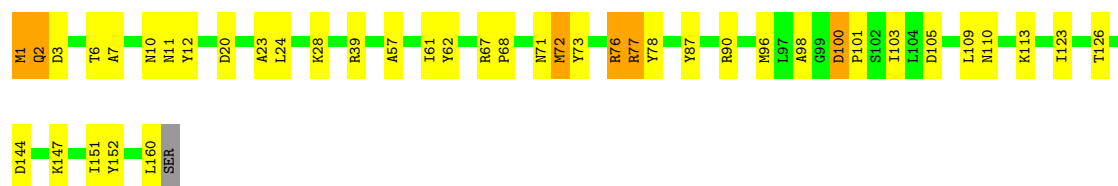
- Molecule 3: Allophycocyanin beta subunit

Chain AJ:  75% 19% . .



- Molecule 3: Allophycocyanin beta subunit

Chain AL:  73% 22% . .



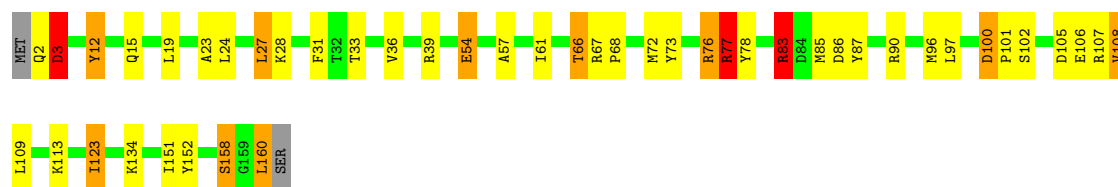
- Molecule 3: Allophycocyanin beta subunit

Chain AN:  74% 22% . .



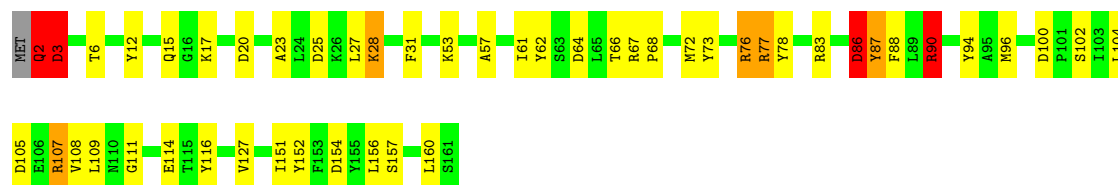
- Molecule 3: Allophycocyanin beta subunit

Chain AP:  70% 20% 6% ..




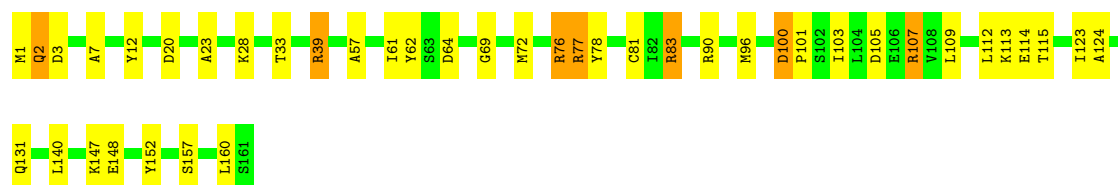
- Molecule 3: Allophycocyanin beta subunit

Chain AR:  69% 25% ..




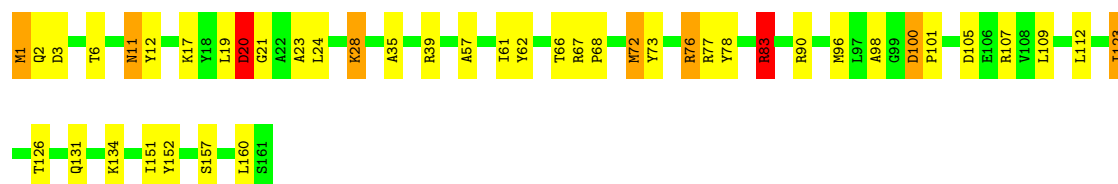
- Molecule 3: Allophycocyanin beta subunit

Chain AT:  74% 22% .



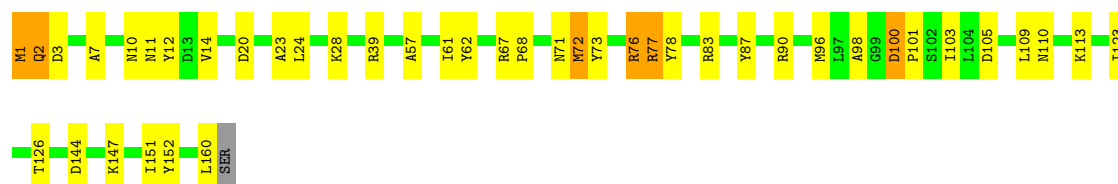
- Molecule 3: Allophycocyanin beta subunit

Chain AV:  73% 22% ..



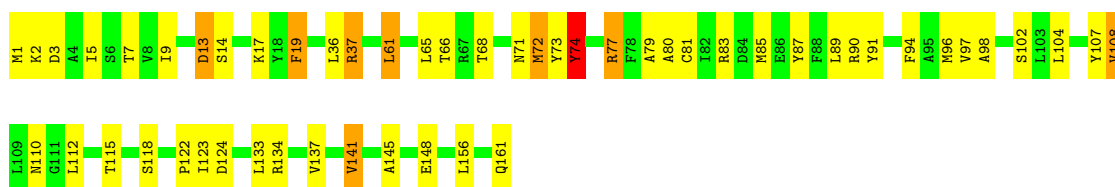
- Molecule 3: Allophycocyanin beta subunit

Chain AX:  73% 23% ..



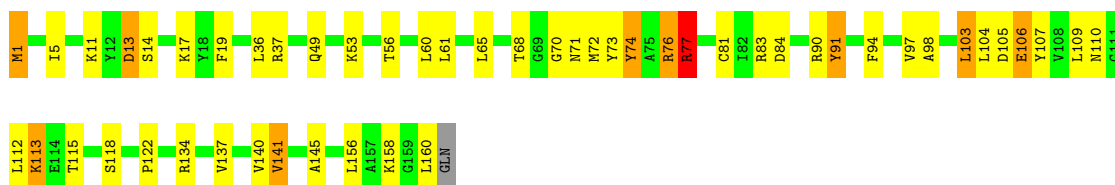
- Molecule 4: Phycobilisome core component

Chain s: 



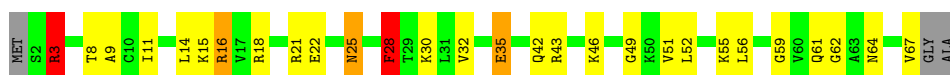
- Molecule 4: Phycobilisome core component

Chain u: 



- Molecule 5: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core

Chain AY: 



- Molecule 5: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core

Chain AZ: 



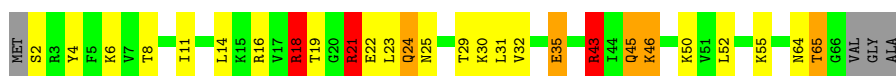
- Molecule 5: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core

Chain Aa: 



- Molecule 5: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core

Chain Ab: 

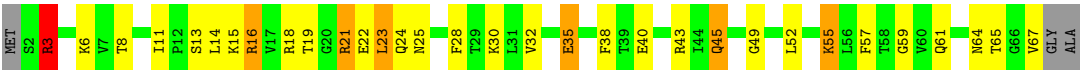


- Molecule 5: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core

Chain Ac: 



- Molecule 5: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	746972	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	66	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	85000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.556	Depositor
Minimum map value	-0.381	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.040	Depositor
Recommended contour level	0.2	Depositor
Map size ( $\text{\AA}$ )	840.0, 840.0, 840.0	wwPDB
Map dimensions	672, 672, 672	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.25, 1.25, 1.25	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	A	0.62	0/8858	1.21	41/11976 (0.3%)
1	C	0.62	0/8858	1.20	38/11976 (0.3%)
2	1	0.69	0/1224	1.30	11/1656 (0.7%)
2	3	0.79	1/1230 (0.1%)	1.38	21/1664 (1.3%)
2	5	0.65	0/1230	1.21	7/1664 (0.4%)
2	7	0.74	0/1240	1.30	12/1676 (0.7%)
2	9	0.75	1/1224 (0.1%)	1.41	15/1656 (0.9%)
2	AA	0.72	2/1240 (0.2%)	1.31	11/1676 (0.7%)
2	AC	0.76	1/1240 (0.1%)	1.45	14/1676 (0.8%)
2	AE	0.83	4/1240 (0.3%)	1.65	25/1676 (1.5%)
2	AG	0.75	2/1240 (0.2%)	1.57	21/1676 (1.3%)
2	AI	0.65	0/1230	1.20	9/1664 (0.5%)
2	AK	0.63	0/1230	1.25	13/1664 (0.8%)
2	AM	0.72	2/1240 (0.2%)	1.31	11/1676 (0.7%)
2	AO	0.76	1/1240 (0.1%)	1.46	15/1676 (0.9%)
2	AQ	0.83	4/1240 (0.3%)	1.65	24/1676 (1.4%)
2	AS	0.75	2/1240 (0.2%)	1.56	21/1676 (1.3%)
2	AU	0.65	0/1230	1.20	8/1664 (0.5%)
2	AW	0.63	0/1230	1.25	14/1664 (0.8%)
2	E	0.69	0/1240	1.29	13/1676 (0.8%)
2	G	0.65	0/1240	1.29	15/1676 (0.9%)
2	I	0.69	0/1240	1.38	14/1676 (0.8%)
2	K	0.65	0/1240	1.30	12/1676 (0.7%)
2	M	0.69	1/1240 (0.1%)	1.41	13/1676 (0.8%)
2	O	0.75	1/1230 (0.1%)	1.39	13/1664 (0.8%)
2	Q	0.69	1/1240 (0.1%)	1.41	13/1676 (0.8%)
2	S	0.76	1/1230 (0.1%)	1.40	14/1664 (0.8%)
2	U	0.68	1/1240 (0.1%)	1.28	13/1676 (0.8%)
2	W	0.65	0/1240	1.29	15/1676 (0.9%)
2	Y	0.69	1/1240 (0.1%)	1.38	14/1676 (0.8%)
2	a	0.64	0/1240	1.30	12/1676 (0.7%)
2	c	0.78	1/1230 (0.1%)	1.40	17/1664 (1.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
2	e	0.66	0/1230	1.17	4/1664 (0.2%)
2	g	0.78	1/1230 (0.1%)	1.38	19/1664 (1.1%)
2	i	0.67	1/1224 (0.1%)	1.36	13/1656 (0.8%)
2	k	0.85	2/1224 (0.2%)	1.56	20/1656 (1.2%)
2	m	0.72	0/1240	1.39	19/1676 (1.1%)
2	o	0.66	0/1230	1.28	8/1664 (0.5%)
2	r	0.73	0/1240	1.30	10/1676 (0.6%)
2	t	0.70	0/1230	1.46	15/1664 (0.9%)
2	w	0.65	0/1230	1.27	10/1664 (0.6%)
2	y	0.71	1/1230 (0.1%)	1.32	10/1664 (0.6%)
3	0	0.75	0/1203	1.26	7/1630 (0.4%)
3	2	0.90	1/1195 (0.1%)	1.43	19/1619 (1.2%)
3	4	0.70	0/1195	1.28	13/1619 (0.8%)
3	6	0.68	0/1218	1.21	10/1648 (0.6%)
3	8	0.71	1/1218 (0.1%)	1.42	14/1648 (0.8%)
3	AB	0.83	4/1218 (0.3%)	1.30	7/1648 (0.4%)
3	AD	0.74	0/1203	1.32	14/1630 (0.9%)
3	AF	0.79	1/1210 (0.1%)	1.59	19/1638 (1.2%)
3	AH	0.89	1/1218 (0.1%)	1.26	9/1648 (0.5%)
3	AJ	0.66	0/1218	1.22	10/1648 (0.6%)
3	AL	0.63	0/1211	1.15	5/1640 (0.3%)
3	AN	0.83	4/1218 (0.3%)	1.30	7/1648 (0.4%)
3	AP	0.76	0/1203	1.32	14/1630 (0.9%)
3	AR	0.78	1/1210 (0.1%)	1.58	17/1638 (1.0%)
3	AT	0.90	1/1218 (0.1%)	1.26	9/1648 (0.5%)
3	AV	0.67	0/1218	1.22	10/1648 (0.6%)
3	AX	0.63	0/1211	1.14	5/1640 (0.3%)
3	F	0.79	3/1218 (0.2%)	1.25	8/1648 (0.5%)
3	H	0.66	1/1218 (0.1%)	1.16	5/1648 (0.3%)
3	J	0.69	2/1218 (0.2%)	1.41	17/1648 (1.0%)
3	L	0.69	1/1218 (0.1%)	1.27	14/1648 (0.8%)
3	N	0.68	0/1218	1.29	7/1648 (0.4%)
3	P	0.64	1/1218 (0.1%)	1.43	13/1648 (0.8%)
3	R	0.67	0/1218	1.28	7/1648 (0.4%)
3	T	0.64	1/1218 (0.1%)	1.43	14/1648 (0.8%)
3	V	0.79	3/1218 (0.2%)	1.25	8/1648 (0.5%)
3	X	0.69	1/1218 (0.1%)	1.18	8/1648 (0.5%)
3	Z	0.70	2/1218 (0.2%)	1.41	15/1648 (0.9%)
3	b	0.70	1/1218 (0.1%)	1.27	13/1648 (0.8%)
3	d	0.70	1/1195 (0.1%)	1.25	9/1619 (0.6%)
3	f	0.66	0/1210	1.20	4/1638 (0.2%)
3	h	0.82	0/1218	1.48	14/1648 (0.8%)
3	j	0.87	1/1195 (0.1%)	1.35	12/1619 (0.7%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
3	l	0.80	1/1203 (0.1%)	1.32	12/1630 (0.7%)
3	n	0.74	0/1218	1.40	10/1648 (0.6%)
3	p	0.81	3/1218 (0.2%)	1.29	13/1648 (0.8%)
3	q	0.89	3/1218 (0.2%)	1.42	15/1648 (0.9%)
3	v	0.89	4/1218 (0.3%)	1.37	11/1648 (0.7%)
3	x	0.73	0/1218	1.30	14/1648 (0.8%)
3	z	0.82	0/1218	1.46	16/1648 (1.0%)
4	s	0.55	0/1246	1.15	1/1682 (0.1%)
4	u	0.55	0/1236	1.25	7/1670 (0.4%)
5	AY	0.51	0/539	1.05	3/725 (0.4%)
5	AZ	0.51	0/539	1.05	3/725 (0.4%)
5	Aa	0.52	0/539	1.07	2/725 (0.3%)
5	Ab	0.51	0/532	1.08	3/715 (0.4%)
5	Ac	0.52	0/528	1.04	0/710
5	Ad	0.52	0/539	1.07	2/725 (0.3%)
All	All	0.71	75/121330 (0.1%)	1.32	1106/164095 (0.7%)

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	A	0	40
1	C	0	40
2	1	0	8
2	3	0	8
2	5	0	5
2	7	0	7
2	9	0	7
2	AA	0	7
2	AC	0	6
2	AE	0	5
2	AG	0	7
2	AI	0	9
2	AK	0	9
2	AM	0	6
2	AO	0	6
2	AQ	0	5
2	AS	0	7
2	AU	0	9
2	AW	0	9

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	E	0	6
2	G	0	6
2	I	0	4
2	K	0	6
2	M	0	5
2	O	0	4
2	Q	0	5
2	S	0	4
2	U	0	6
2	W	0	6
2	Y	0	5
2	a	0	5
2	c	0	8
2	e	0	6
2	g	0	9
2	i	0	9
2	k	0	11
2	m	0	7
2	o	0	7
2	r	0	9
2	t	0	8
2	w	0	5
2	y	0	6
3	0	0	6
3	2	0	8
3	4	0	4
3	6	0	5
3	8	0	5
3	AB	0	6
3	AD	0	7
3	AF	0	7
3	AH	0	5
3	AJ	0	6
3	AL	0	6
3	AN	0	6
3	AP	0	7
3	AR	0	7
3	AT	0	6
3	AV	0	5
3	AX	0	6
3	F	0	1
3	H	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	J	0	7
3	L	0	4
3	N	0	3
3	P	0	2
3	R	0	3
3	T	0	2
3	V	0	1
3	X	0	4
3	Z	0	6
3	b	0	4
3	d	0	5
3	f	0	5
3	h	0	4
3	j	0	7
3	l	0	5
3	n	0	5
3	p	0	6
3	q	0	10
3	v	0	9
3	x	0	8
3	z	0	4
4	s	0	4
4	u	0	3
5	AY	0	3
5	AZ	0	3
5	Aa	0	3
5	Ab	0	3
5	Ac	0	5
5	Ad	0	3
All	All	0	584

The worst 5 of 75 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	l	83	ARG	NE-CZ	-12.99	1.18	1.33
2	g	62	ARG	CG-CD	-10.83	1.20	1.52
3	2	83	ARG	NE-CZ	-9.64	1.22	1.33
3	j	100	ASP	CG-OD1	-8.95	1.08	1.25
3	p	39	ARG	NE-CZ	-8.51	1.23	1.33

The worst 5 of 1106 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AQ	38	ARG	NE-CZ-NH2	25.43	142.09	119.20
2	AE	38	ARG	NE-CZ-NH2	25.25	141.93	119.20
2	AS	62	ARG	NE-CZ-NH1	-23.54	97.96	121.50
2	AG	62	ARG	NE-CZ-NH1	-23.50	98.00	121.50
3	AR	90	ARG	NE-CZ-NH2	21.94	138.94	119.20

There are no chirality outliers.

5 of 584 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	165	ARG	Sidechain
1	A	187	ARG	Sidechain
1	A	207	ARG	Sidechain
1	A	33	ARG	Sidechain
1	A	4	ARG	Sidechain

## 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	A	8678	0	8690	439	0
1	C	8678	0	8691	474	0
2	1	1207	0	1222	44	0
2	3	1213	0	1227	60	0
2	5	1213	0	1227	59	0
2	7	1223	0	1235	54	0
2	9	1207	0	1222	53	0
2	AA	1223	0	1235	45	0
2	AC	1223	0	1235	55	0
2	AE	1223	0	1235	54	0
2	AG	1223	0	1235	48	0
2	AI	1213	0	1227	65	0
2	AK	1213	0	1227	55	0
2	AM	1223	0	1235	44	0
2	AO	1223	0	1235	55	0
2	AQ	1223	0	1235	53	0
2	AS	1223	0	1235	47	0
2	AU	1213	0	1227	69	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	AW	1213	0	1227	55	0
2	E	1223	0	1235	34	0
2	G	1223	0	1235	35	0
2	I	1223	0	1235	40	0
2	K	1223	0	1235	35	0
2	M	1223	0	1235	34	0
2	O	1213	0	1227	25	0
2	Q	1223	0	1235	37	0
2	S	1213	0	1227	25	0
2	U	1223	0	1235	32	0
2	W	1223	0	1235	34	0
2	Y	1223	0	1235	26	0
2	a	1223	0	1235	32	0
2	c	1213	0	1227	63	0
2	e	1213	0	1227	52	0
2	g	1213	0	1227	51	0
2	i	1207	0	1222	48	0
2	k	1207	0	1222	62	0
2	m	1223	0	1235	51	0
2	o	1213	0	1227	60	0
2	r	1223	0	1235	44	0
2	t	1213	0	1227	33	0
2	w	1213	0	1227	58	0
2	y	1213	0	1227	55	0
3	0	1195	0	1203	40	0
3	2	1187	0	1192	33	0
3	4	1187	0	1192	30	0
3	6	1210	0	1220	48	0
3	8	1210	0	1220	21	0
3	AB	1210	0	1220	32	0
3	AD	1195	0	1203	41	0
3	AF	1202	0	1208	44	0
3	AH	1210	0	1220	44	0
3	AJ	1210	0	1220	42	0
3	AL	1203	0	1215	41	0
3	AN	1210	0	1220	33	0
3	AP	1195	0	1203	44	0
3	AR	1202	0	1208	41	0
3	AT	1210	0	1220	41	0
3	AV	1210	0	1220	45	0
3	AX	1203	0	1215	47	0
3	F	1210	0	1220	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	1210	0	1220	21	0
3	J	1210	0	1220	17	0
3	L	1210	0	1220	17	0
3	N	1210	0	1220	29	0
3	P	1210	0	1220	21	0
3	R	1210	0	1220	33	0
3	T	1210	0	1220	24	0
3	V	1210	0	1220	32	0
3	X	1210	0	1220	21	0
3	Z	1210	0	1220	24	0
3	b	1210	0	1220	18	0
3	d	1187	0	1192	29	0
3	f	1202	0	1208	51	0
3	h	1210	0	1220	38	0
3	j	1187	0	1192	36	0
3	l	1195	0	1203	54	0
3	n	1210	0	1220	29	0
3	p	1210	0	1220	29	0
3	q	1210	0	1220	47	0
3	v	1210	0	1220	51	0
3	x	1210	0	1220	29	0
3	z	1210	0	1220	44	0
4	s	1227	0	1231	51	0
4	u	1217	0	1223	55	0
5	AY	529	0	547	13	0
5	AZ	529	0	547	13	0
5	Aa	529	0	547	22	0
5	Ab	522	0	538	19	0
5	Ac	518	0	535	18	0
5	Ad	529	0	547	24	0
6	0	43	0	37	2	0
6	1	43	0	37	2	0
6	2	43	0	37	1	0
6	3	43	0	37	5	0
6	4	43	0	37	6	0
6	5	43	0	37	8	0
6	6	43	0	37	5	0
6	7	43	0	37	8	0
6	8	43	0	37	1	0
6	9	43	0	37	7	0
6	A	43	0	37	3	0
6	AA	43	0	37	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	AB	43	0	37	3	0
6	AC	43	0	37	2	0
6	AD	43	0	37	2	0
6	AE	43	0	37	1	0
6	AF	43	0	37	4	0
6	AG	43	0	37	12	0
6	AH	43	0	37	4	0
6	AI	43	0	37	1	0
6	AJ	43	0	37	3	0
6	AK	43	0	37	11	0
6	AL	43	0	37	3	0
6	AM	43	0	37	7	0
6	AN	43	0	37	3	0
6	AO	43	0	37	2	0
6	AP	43	0	37	4	0
6	AQ	43	0	37	1	0
6	AR	43	0	37	1	0
6	AS	43	0	37	13	0
6	AT	43	0	37	4	0
6	AU	43	0	37	1	0
6	AV	43	0	37	3	0
6	AW	43	0	37	11	0
6	AX	43	0	37	4	0
6	C	43	0	38	33	0
6	E	43	0	37	8	0
6	F	43	0	37	9	0
6	G	43	0	37	5	0
6	H	43	0	37	5	0
6	I	43	0	37	3	0
6	J	43	0	37	2	0
6	K	43	0	37	3	0
6	L	43	0	37	2	0
6	M	43	0	37	6	0
6	N	43	0	37	7	0
6	O	43	0	37	3	0
6	P	43	0	37	3	0
6	Q	43	0	37	10	0
6	R	43	0	37	13	0
6	S	43	0	37	3	0
6	T	43	0	37	5	0
6	U	43	0	37	7	0
6	V	43	0	37	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	W	43	0	37	5	0
6	X	43	0	37	8	0
6	Y	43	0	37	3	0
6	Z	43	0	37	3	0
6	a	43	0	37	4	0
6	b	43	0	37	2	0
6	c	43	0	37	6	0
6	d	43	0	37	5	0
6	e	43	0	37	10	0
6	f	43	0	37	3	0
6	g	43	0	37	6	0
6	h	43	0	37	1	0
6	i	43	0	37	4	0
6	j	43	0	37	2	0
6	k	43	0	37	5	0
6	l	43	0	37	1	0
6	m	43	0	37	9	0
6	n	43	0	37	4	0
6	o	43	0	37	3	0
6	p	43	0	37	3	0
6	q	43	0	37	2	0
6	r	43	0	37	4	0
6	s	43	0	38	12	0
6	t	43	0	37	4	0
6	u	43	0	38	14	0
6	v	43	0	37	1	0
6	w	43	0	37	1	0
6	x	43	0	37	3	0
6	y	43	0	37	9	0
6	z	43	0	37	2	0
All	All	123484	0	124009	3743	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 15.

The worst 5 of 3743 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)
2:AU:116:TYR:CD1	2:AU:121:THR:HG21	1.66	1.30
2:AI:116:TYR:CD1	2:AI:121:THR:HG21	1.67	1.29
3:v:161:SER:OXT	3:6:101:PRO:HG3	1.31	1.28

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:f:101:PRO:HG3	3:q:161:SER:OXT	1.33	1.24
3:l:103:ILE:HD11	3:l:107:ARG:NH2	1.55	1.21

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1085/1155 (94%)	1016 (94%)	46 (4%)	23 (2%)	5	13
1	C	1085/1155 (94%)	1017 (94%)	42 (4%)	26 (2%)	5	11
2	1	156/161 (97%)	153 (98%)	3 (2%)	0	100	100
2	3	157/161 (98%)	154 (98%)	3 (2%)	0	100	100
2	5	157/161 (98%)	154 (98%)	3 (2%)	0	100	100
2	7	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
2	9	156/161 (97%)	153 (98%)	3 (2%)	0	100	100
2	AA	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
2	AC	158/161 (98%)	154 (98%)	3 (2%)	1 (1%)	22	40
2	AE	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
2	AG	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
2	AI	157/161 (98%)	154 (98%)	3 (2%)	0	100	100
2	AK	157/161 (98%)	154 (98%)	3 (2%)	0	100	100
2	AM	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
2	AO	158/161 (98%)	154 (98%)	3 (2%)	1 (1%)	22	40
2	AQ	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
2	AS	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
2	AU	157/161 (98%)	154 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AW	157/161 (98%)	154 (98%)	3 (2%)	0	100	100
2	E	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
2	G	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
2	I	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
2	K	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
2	M	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
2	O	157/161 (98%)	154 (98%)	3 (2%)	0	100	100
2	Q	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
2	S	157/161 (98%)	154 (98%)	3 (2%)	0	100	100
2	U	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
2	W	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
2	Y	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
2	a	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
2	c	157/161 (98%)	154 (98%)	3 (2%)	0	100	100
2	e	157/161 (98%)	154 (98%)	3 (2%)	0	100	100
2	g	157/161 (98%)	154 (98%)	3 (2%)	0	100	100
2	i	156/161 (97%)	153 (98%)	3 (2%)	0	100	100
2	k	156/161 (97%)	153 (98%)	3 (2%)	0	100	100
2	m	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
2	o	157/161 (98%)	154 (98%)	3 (2%)	0	100	100
2	r	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
2	t	157/161 (98%)	154 (98%)	3 (2%)	0	100	100
2	w	157/161 (98%)	154 (98%)	3 (2%)	0	100	100
2	y	157/161 (98%)	154 (98%)	3 (2%)	0	100	100
3	0	156/161 (97%)	153 (98%)	3 (2%)	0	100	100
3	2	155/161 (96%)	151 (97%)	4 (3%)	0	100	100
3	4	155/161 (96%)	152 (98%)	3 (2%)	0	100	100
3	6	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
3	8	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
3	AB	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
3	AD	156/161 (97%)	152 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	AF	157/161 (98%)	153 (98%)	4 (2%)	0	100	100
3	AH	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
3	AJ	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
3	AL	157/161 (98%)	153 (98%)	4 (2%)	0	100	100
3	AN	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
3	AP	156/161 (97%)	152 (97%)	4 (3%)	0	100	100
3	AR	157/161 (98%)	153 (98%)	4 (2%)	0	100	100
3	AT	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
3	AV	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
3	AX	157/161 (98%)	153 (98%)	4 (2%)	0	100	100
3	F	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
3	H	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
3	J	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
3	L	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
3	N	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
3	P	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
3	R	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
3	T	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
3	V	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
3	X	158/161 (98%)	155 (98%)	2 (1%)	1 (1%)	22	40
3	Z	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
3	b	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
3	d	155/161 (96%)	152 (98%)	3 (2%)	0	100	100
3	f	157/161 (98%)	153 (98%)	4 (2%)	0	100	100
3	h	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
3	j	155/161 (96%)	151 (97%)	4 (3%)	0	100	100
3	l	156/161 (97%)	153 (98%)	3 (2%)	0	100	100
3	n	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
3	p	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
3	q	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
3	v	158/161 (98%)	154 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	x	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
3	z	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
4	s	159/161 (99%)	153 (96%)	4 (2%)	2 (1%)	10	22
4	u	158/161 (98%)	153 (97%)	4 (2%)	1 (1%)	22	40
5	AY	64/69 (93%)	63 (98%)	1 (2%)	0	100	100
5	AZ	64/69 (93%)	63 (98%)	1 (2%)	0	100	100
5	Aa	64/69 (93%)	63 (98%)	1 (2%)	0	100	100
5	Ab	63/69 (91%)	62 (98%)	1 (2%)	0	100	100
5	Ac	62/69 (90%)	62 (100%)	0	0	100	100
5	Ad	64/69 (93%)	64 (100%)	0	0	100	100
All	All	15460/15926 (97%)	15054 (97%)	351 (2%)	55 (0%)	32	49

5 of 55 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	191	GLU
1	A	364	PHE
1	A	560	VAL
1	A	701	ASP
1	A	750	ARG

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	927/977 (95%)	866 (93%)	61 (7%)	14	28
1	C	927/977 (95%)	868 (94%)	59 (6%)	14	29
2	1	125/128 (98%)	120 (96%)	5 (4%)	27	51
2	3	126/128 (98%)	122 (97%)	4 (3%)	34	60
2	5	126/128 (98%)	122 (97%)	4 (3%)	34	60
2	7	127/128 (99%)	119 (94%)	8 (6%)	15	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	9	125/128 (98%)	118 (94%)	7 (6%)	17	35
2	AA	127/128 (99%)	120 (94%)	7 (6%)	18	37
2	AC	127/128 (99%)	121 (95%)	6 (5%)	22	44
2	AE	127/128 (99%)	120 (94%)	7 (6%)	18	37
2	AG	127/128 (99%)	117 (92%)	10 (8%)	10	21
2	AI	126/128 (98%)	121 (96%)	5 (4%)	27	51
2	AK	126/128 (98%)	120 (95%)	6 (5%)	21	42
2	AM	127/128 (99%)	120 (94%)	7 (6%)	18	37
2	AO	127/128 (99%)	121 (95%)	6 (5%)	22	44
2	AQ	127/128 (99%)	120 (94%)	7 (6%)	18	37
2	AS	127/128 (99%)	118 (93%)	9 (7%)	12	26
2	AU	126/128 (98%)	121 (96%)	5 (4%)	27	51
2	AW	126/128 (98%)	120 (95%)	6 (5%)	21	42
2	E	127/128 (99%)	109 (86%)	18 (14%)	2	4
2	G	127/128 (99%)	112 (88%)	15 (12%)	4	8
2	I	127/128 (99%)	106 (84%)	21 (16%)	2	3
2	K	127/128 (99%)	112 (88%)	15 (12%)	4	8
2	M	127/128 (99%)	109 (86%)	18 (14%)	2	4
2	O	126/128 (98%)	110 (87%)	16 (13%)	3	6
2	Q	127/128 (99%)	109 (86%)	18 (14%)	2	4
2	S	126/128 (98%)	110 (87%)	16 (13%)	3	6
2	U	127/128 (99%)	109 (86%)	18 (14%)	2	4
2	W	127/128 (99%)	113 (89%)	14 (11%)	5	9
2	Y	127/128 (99%)	103 (81%)	24 (19%)	1	1
2	a	127/128 (99%)	112 (88%)	15 (12%)	4	8
2	c	126/128 (98%)	119 (94%)	7 (6%)	17	35
2	e	126/128 (98%)	122 (97%)	4 (3%)	34	60
2	g	126/128 (98%)	121 (96%)	5 (4%)	27	51
2	i	125/128 (98%)	119 (95%)	6 (5%)	21	42
2	k	125/128 (98%)	115 (92%)	10 (8%)	10	20
2	m	127/128 (99%)	119 (94%)	8 (6%)	15	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	o	126/128 (98%)	120 (95%)	6 (5%)	21	42
2	r	127/128 (99%)	119 (94%)	8 (6%)	15	30
2	t	126/128 (98%)	121 (96%)	5 (4%)	27	51
2	w	126/128 (98%)	120 (95%)	6 (5%)	21	42
2	y	126/128 (98%)	120 (95%)	6 (5%)	21	42
3	0	119/121 (98%)	113 (95%)	6 (5%)	20	40
3	2	118/121 (98%)	109 (92%)	9 (8%)	11	23
3	4	118/121 (98%)	115 (98%)	3 (2%)	42	68
3	6	121/121 (100%)	117 (97%)	4 (3%)	33	59
3	8	121/121 (100%)	119 (98%)	2 (2%)	56	78
3	AB	121/121 (100%)	118 (98%)	3 (2%)	42	68
3	AD	119/121 (98%)	109 (92%)	10 (8%)	9	19
3	AF	120/121 (99%)	115 (96%)	5 (4%)	25	48
3	AH	121/121 (100%)	120 (99%)	1 (1%)	79	90
3	AJ	121/121 (100%)	117 (97%)	4 (3%)	33	59
3	AL	120/121 (99%)	117 (98%)	3 (2%)	42	68
3	AN	121/121 (100%)	118 (98%)	3 (2%)	42	68
3	AP	119/121 (98%)	109 (92%)	10 (8%)	9	19
3	AR	120/121 (99%)	115 (96%)	5 (4%)	25	48
3	AT	121/121 (100%)	119 (98%)	2 (2%)	56	78
3	AV	121/121 (100%)	117 (97%)	4 (3%)	33	59
3	AX	120/121 (99%)	117 (98%)	3 (2%)	42	68
3	F	121/121 (100%)	114 (94%)	7 (6%)	17	34
3	H	121/121 (100%)	107 (88%)	14 (12%)	4	8
3	J	121/121 (100%)	107 (88%)	14 (12%)	4	8
3	L	121/121 (100%)	108 (89%)	13 (11%)	5	10
3	N	121/121 (100%)	107 (88%)	14 (12%)	4	8
3	P	121/121 (100%)	111 (92%)	10 (8%)	9	19
3	R	121/121 (100%)	107 (88%)	14 (12%)	4	8
3	T	121/121 (100%)	111 (92%)	10 (8%)	9	19
3	V	121/121 (100%)	114 (94%)	7 (6%)	17	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	X	121/121 (100%)	106 (88%)	15 (12%)	4	7
3	Z	121/121 (100%)	107 (88%)	14 (12%)	4	8
3	b	121/121 (100%)	109 (90%)	12 (10%)	6	12
3	d	118/121 (98%)	113 (96%)	5 (4%)	25	48
3	f	120/121 (99%)	115 (96%)	5 (4%)	25	48
3	h	121/121 (100%)	118 (98%)	3 (2%)	42	68
3	j	118/121 (98%)	108 (92%)	10 (8%)	8	18
3	l	119/121 (98%)	114 (96%)	5 (4%)	25	48
3	n	121/121 (100%)	117 (97%)	4 (3%)	33	59
3	p	121/121 (100%)	118 (98%)	3 (2%)	42	68
3	q	121/121 (100%)	120 (99%)	1 (1%)	79	90
3	v	121/121 (100%)	119 (98%)	2 (2%)	56	78
3	x	121/121 (100%)	117 (97%)	4 (3%)	33	59
3	z	121/121 (100%)	118 (98%)	3 (2%)	42	68
4	s	123/123 (100%)	111 (90%)	12 (10%)	6	13
4	u	122/123 (99%)	110 (90%)	12 (10%)	6	13
5	AY	57/58 (98%)	41 (72%)	16 (28%)	0	0
5	AZ	57/58 (98%)	41 (72%)	16 (28%)	0	0
5	Aa	57/58 (98%)	41 (72%)	16 (28%)	0	0
5	Ab	56/58 (97%)	36 (64%)	20 (36%)	0	0
5	Ac	56/58 (97%)	39 (70%)	17 (30%)	0	0
5	Ad	57/58 (98%)	41 (72%)	16 (28%)	0	0
All	All	12311/12508 (98%)	11412 (93%)	899 (7%)	14	24

5 of 899 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	b	39	ARG
5	Ad	16	ARG
4	s	141	VAL
5	Ac	30	LYS
5	AY	14	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 223 such sidechains are listed below:

Mol	Chain	Res	Type
3	q	47	ASN
5	Ad	45	GLN
3	4	15	GLN
5	Ab	45	GLN
3	AT	11	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

40 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	$\# Z  > 2$
3	MEN	l	71	3	7,8,9	0.55	0	6,9,11	0.50	0
3	MEN	o	71	3	7,8,9	0.57	0	6,9,11	0.46	0
3	MEN	H	71	3	7,8,9	0.47	0	6,9,11	0.79	0
3	MEN	p	71	3	7,8,9	0.68	0	6,9,11	0.77	0
3	MEN	V	71	3	7,8,9	0.60	0	6,9,11	0.42	0
3	MEN	AT	71	3	7,8,9	0.52	0	6,9,11	0.74	0
3	MEN	h	71	3	7,8,9	0.75	0	6,9,11	0.90	0
3	MEN	J	71	3	7,8,9	0.50	0	6,9,11	0.49	0
3	MEN	AN	71	3	7,8,9	0.53	0	6,9,11	0.58	0
3	MEN	X	71	3	7,8,9	0.48	0	6,9,11	0.75	0
3	MEN	N	71	3	7,8,9	0.48	0	6,9,11	0.59	0
3	MEN	6	71	3	7,8,9	0.69	0	6,9,11	0.78	0
3	MEN	d	71	3	7,8,9	0.65	0	6,9,11	0.58	0
3	MEN	AX	71	3	7,8,9	0.48	0	6,9,11	0.52	0
3	MEN	n	71	3	7,8,9	0.52	0	6,9,11	0.66	0
3	MEN	b	71	3	7,8,9	0.47	0	6,9,11	0.52	0
3	MEN	AV	71	3	7,8,9	0.55	0	6,9,11	0.72	0
3	MEN	4	71	3	7,8,9	0.51	0	6,9,11	0.63	0
3	MEN	T	71	3	7,8,9	0.49	0	6,9,11	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	MEN	v	71	3	7,8,9	0.76	0	6,9,11	0.72	0
3	MEN	8	71	3	7,8,9	0.54	0	6,9,11	0.68	0
3	MEN	x	71	3	7,8,9	0.68	0	6,9,11	0.79	0
3	MEN	q	71	3	7,8,9	0.75	0	6,9,11	0.85	0
3	MEN	AH	71	3	7,8,9	0.54	0	6,9,11	0.75	0
3	MEN	j	71	3	7,8,9	0.95	0	6,9,11	0.79	0
3	MEN	AB	71	3	7,8,9	0.52	0	6,9,11	0.57	0
3	MEN	F	71	3	7,8,9	0.61	0	6,9,11	0.41	0
3	MEN	AD	71	3	7,8,9	0.56	0	6,9,11	0.58	0
3	MEN	f	71	3	7,8,9	0.48	0	6,9,11	0.32	0
3	MEN	2	71	3	7,8,9	1.02	0	6,9,11	1.82	1 (16%)
3	MEN	R	71	3	7,8,9	0.49	0	6,9,11	0.71	0
3	MEN	AR	71	3	7,8,9	0.46	0	6,9,11	0.59	0
3	MEN	AP	71	3	7,8,9	0.52	0	6,9,11	0.52	0
3	MEN	L	71	3	7,8,9	0.48	0	6,9,11	0.53	0
3	MEN	z	71	3	7,8,9	0.75	0	6,9,11	0.87	0
3	MEN	AF	71	3	7,8,9	0.48	0	6,9,11	0.58	0
3	MEN	P	71	3	7,8,9	0.49	0	6,9,11	0.53	0
3	MEN	Z	71	3	7,8,9	0.51	0	6,9,11	0.44	0
3	MEN	AJ	71	3	7,8,9	0.56	0	6,9,11	0.72	0
3	MEN	AL	71	3	7,8,9	0.48	0	6,9,11	0.52	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
3	MEN	l	71	3	-	5/7/8/10	-
3	MEN	0	71	3	-	5/7/8/10	-
3	MEN	H	71	3	-	6/7/8/10	-
3	MEN	p	71	3	-	4/7/8/10	-
3	MEN	V	71	3	-	3/7/8/10	-
3	MEN	AT	71	3	-	3/7/8/10	-
3	MEN	h	71	3	-	3/7/8/10	-
3	MEN	J	71	3	-	5/7/8/10	-
3	MEN	AN	71	3	-	5/7/8/10	-
3	MEN	X	71	3	-	6/7/8/10	-
3	MEN	N	71	3	-	5/7/8/10	-
3	MEN	6	71	3	-	4/7/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MEN	d	71	3	-	5/7/8/10	-
3	MEN	AX	71	3	-	4/7/8/10	-
3	MEN	n	71	3	-	5/7/8/10	-
3	MEN	b	71	3	-	5/7/8/10	-
3	MEN	AV	71	3	-	4/7/8/10	-
3	MEN	4	71	3	-	5/7/8/10	-
3	MEN	T	71	3	-	5/7/8/10	-
3	MEN	v	71	3	-	5/7/8/10	-
3	MEN	8	71	3	-	5/7/8/10	-
3	MEN	x	71	3	-	4/7/8/10	-
3	MEN	q	71	3	-	5/7/8/10	-
3	MEN	AH	71	3	-	3/7/8/10	-
3	MEN	j	71	3	-	4/7/8/10	-
3	MEN	AB	71	3	-	5/7/8/10	-
3	MEN	F	71	3	-	3/7/8/10	-
3	MEN	AD	71	3	-	5/7/8/10	-
3	MEN	f	71	3	-	5/7/8/10	-
3	MEN	2	71	3	-	4/7/8/10	-
3	MEN	R	71	3	-	5/7/8/10	-
3	MEN	AR	71	3	-	4/7/8/10	-
3	MEN	AP	71	3	-	5/7/8/10	-
3	MEN	L	71	3	-	4/7/8/10	-
3	MEN	z	71	3	-	3/7/8/10	-
3	MEN	AF	71	3	-	4/7/8/10	-
3	MEN	P	71	3	-	4/7/8/10	-
3	MEN	Z	71	3	-	5/7/8/10	-
3	MEN	AJ	71	3	-	4/7/8/10	-
3	MEN	AL	71	3	-	4/7/8/10	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
3	2	71	MEN	OD1-CG-CB	4.04	127.41	121.50

There are no chirality outliers.

5 of 177 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	N	71	MEN	C-CA-CB-CG
3	N	71	MEN	CB-CG-ND2-CE2
3	P	71	MEN	C-CA-CB-CG
3	P	71	MEN	CB-CG-ND2-CE2
3	F	71	MEN	O-C-CA-CB

There are no ring outliers.

21 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	l	71	MEN	1	0
3	o	71	MEN	1	0
3	H	71	MEN	1	0
3	p	71	MEN	1	0
3	V	71	MEN	1	0
3	h	71	MEN	1	0
3	J	71	MEN	1	0
3	AN	71	MEN	1	0
3	d	71	MEN	1	0
3	AX	71	MEN	1	0
3	n	71	MEN	1	0
3	T	71	MEN	1	0
3	8	71	MEN	1	0
3	x	71	MEN	1	0
3	AB	71	MEN	1	0
3	F	71	MEN	1	0
3	L	71	MEN	1	0
3	z	71	MEN	1	0
3	P	71	MEN	1	0
3	Z	71	MEN	1	0
3	AL	71	MEN	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

84 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	A	2101	1	42,46,46	1.21	2 (4%)	50,67,67	1.21	4 (8%)
6	CYC	4	201	3	42,46,46	0.97	1 (2%)	50,67,67	1.07	2 (4%)
6	CYC	1	201	3	42,46,46	0.93	1 (2%)	50,67,67	1.31	3 (6%)
6	CYC	0	201	3	42,46,46	0.94	1 (2%)	50,67,67	1.26	3 (6%)
6	CYC	M	201	2	42,46,46	0.96	1 (2%)	50,67,67	1.36	6 (12%)
6	CYC	a	201	2	42,46,46	1.14	1 (2%)	50,67,67	1.21	3 (6%)
6	CYC	h	201	3	42,46,46	1.34	5 (11%)	50,67,67	1.46	8 (16%)
6	CYC	5	201	2	42,46,46	0.96	2 (4%)	50,67,67	1.32	3 (6%)
6	CYC	AD	201	3	42,46,46	0.92	1 (2%)	50,67,67	1.14	3 (6%)
6	CYC	AS	201	2	42,46,46	1.14	1 (2%)	50,67,67	1.24	4 (8%)
6	CYC	AX	201	3	42,46,46	1.06	2 (4%)	50,67,67	1.03	2 (4%)
6	CYC	z	201	3	42,46,46	1.35	4 (9%)	50,67,67	1.47	9 (18%)
6	CYC	6	201	3	42,46,46	0.94	1 (2%)	50,67,67	1.49	9 (18%)
6	CYC	AN	201	3	42,46,46	1.12	4 (9%)	50,67,67	1.34	7 (14%)
6	CYC	8	201	3	42,46,46	1.14	5 (11%)	50,67,67	1.48	8 (16%)
6	CYC	R	201	3	42,46,46	0.92	1 (2%)	50,67,67	1.36	2 (4%)
6	CYC	e	201	2	42,46,46	1.10	2 (4%)	50,67,67	1.30	5 (10%)
6	CYC	AC	201	2	42,46,46	0.99	1 (2%)	50,67,67	1.25	6 (12%)
6	CYC	C	2101	-	42,46,46	1.26	2 (4%)	50,67,67	1.45	9 (18%)
6	CYC	L	201	3	42,46,46	0.93	1 (2%)	50,67,67	1.25	5 (10%)
6	CYC	c	201	2	42,46,46	0.88	1 (2%)	50,67,67	1.32	5 (10%)
6	CYC	AP	201	3	42,46,46	0.94	1 (2%)	50,67,67	1.17	4 (8%)
6	CYC	Y	201	2	42,46,46	1.04	1 (2%)	50,67,67	1.31	5 (10%)
6	CYC	AL	201	3	42,46,46	1.05	2 (4%)	50,67,67	1.06	2 (4%)
6	CYC	Z	201	3	42,46,46	1.03	2 (4%)	50,67,67	1.11	3 (6%)
6	CYC	AO	201	2	42,46,46	1.00	1 (2%)	50,67,67	1.24	6 (12%)
6	CYC	t	201	2	42,46,46	1.14	4 (9%)	50,67,67	1.44	8 (16%)
6	CYC	G	201	2	42,46,46	1.16	2 (4%)	50,67,67	1.28	6 (12%)
6	CYC	b	201	3	42,46,46	0.93	1 (2%)	50,67,67	1.27	5 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	CYC	2	201	3	42,46,46	1.17	2 (4%)	50,67,67	1.26	6 (12%)
6	CYC	S	201	2	42,46,46	0.95	1 (2%)	50,67,67	1.23	5 (10%)
6	CYC	w	201	2	42,46,46	1.05	1 (2%)	50,67,67	1.14	4 (8%)
6	CYC	J	201	3	42,46,46	0.99	1 (2%)	50,67,67	1.11	3 (6%)
6	CYC	AJ	201	3	42,46,46	1.04	2 (4%)	50,67,67	1.39	6 (12%)
6	CYC	k	201	2	42,46,46	0.97	1 (2%)	50,67,67	1.27	5 (10%)
6	CYC	u	201	-	42,46,46	1.04	2 (4%)	50,67,67	1.14	6 (12%)
6	CYC	g	201	2	42,46,46	1.20	1 (2%)	50,67,67	1.13	5 (10%)
6	CYC	W	201	2	42,46,46	1.16	2 (4%)	50,67,67	1.28	6 (12%)
6	CYC	U	201	2	42,46,46	1.06	1 (2%)	50,67,67	1.32	6 (12%)
6	CYC	j	201	3	42,46,46	1.29	2 (4%)	50,67,67	1.05	2 (4%)
6	CYC	AR	201	3	42,46,46	0.96	1 (2%)	50,67,67	1.21	3 (6%)
6	CYC	o	201	2	42,46,46	0.94	1 (2%)	50,67,67	1.22	2 (4%)
6	CYC	O	201	2	42,46,46	0.98	1 (2%)	50,67,67	1.25	5 (10%)
6	CYC	AU	201	2	42,46,46	0.98	1 (2%)	50,67,67	1.16	4 (8%)
6	CYC	K	201	2	42,46,46	1.12	1 (2%)	50,67,67	1.21	3 (6%)
6	CYC	9	201	2	42,46,46	0.92	1 (2%)	50,67,67	1.29	6 (12%)
6	CYC	AW	201	2	42,46,46	1.00	1 (2%)	50,67,67	1.22	4 (8%)
6	CYC	1	201	2	42,46,46	0.86	1 (2%)	50,67,67	1.25	4 (8%)
6	CYC	d	201	3	42,46,46	1.05	1 (2%)	50,67,67	1.05	2 (4%)
6	CYC	AF	201	3	42,46,46	0.97	1 (2%)	50,67,67	1.21	3 (6%)
6	CYC	n	201	3	42,46,46	1.15	4 (9%)	50,67,67	1.38	7 (14%)
6	CYC	x	201	3	42,46,46	1.09	2 (4%)	50,67,67	1.13	4 (8%)
6	CYC	AI	201	2	42,46,46	0.99	1 (2%)	50,67,67	1.17	5 (10%)
6	CYC	AB	201	3	42,46,46	1.11	4 (9%)	50,67,67	1.34	7 (14%)
6	CYC	y	201	2	42,46,46	1.09	1 (2%)	50,67,67	1.13	4 (8%)
6	CYC	AM	201	2	42,46,46	1.15	4 (9%)	50,67,67	1.50	9 (18%)
6	CYC	AQ	201	2	42,46,46	0.88	1 (2%)	50,67,67	1.16	3 (6%)
6	CYC	i	201	2	42,46,46	0.79	0	50,67,67	1.32	4 (8%)
6	CYC	s	201	-	42,46,46	1.11	1 (2%)	50,67,67	1.30	5 (10%)
6	CYC	AE	201	2	42,46,46	0.87	1 (2%)	50,67,67	1.16	3 (6%)
6	CYC	N	201	3	42,46,46	0.93	1 (2%)	50,67,67	1.31	2 (4%)
6	CYC	P	201	3	42,46,46	0.92	1 (2%)	50,67,67	1.28	4 (8%)
6	CYC	I	201	2	42,46,46	1.00	1 (2%)	50,67,67	1.32	4 (8%)
6	CYC	AT	201	3	42,46,46	1.11	6 (14%)	50,67,67	1.48	8 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	CYC	T	201	3	42,46,46	0.93	1 (2%)	50,67,67	1.28	5 (10%)
6	CYC	AV	201	3	42,46,46	1.05	2 (4%)	50,67,67	1.38	5 (10%)
6	CYC	3	201	2	42,46,46	0.88	1 (2%)	50,67,67	1.22	5 (10%)
6	CYC	Q	201	2	42,46,46	1.08	1 (2%)	50,67,67	1.34	4 (8%)
6	CYC	q	201	3	42,46,46	1.09	2 (4%)	50,67,67	1.11	3 (6%)
6	CYC	AG	201	2	42,46,46	1.14	1 (2%)	50,67,67	1.23	4 (8%)
6	CYC	r	201	2	42,46,46	1.13	4 (9%)	50,67,67	1.46	10 (20%)
6	CYC	p	201	3	42,46,46	1.09	2 (4%)	50,67,67	1.13	4 (8%)
6	CYC	f	201	3	42,46,46	0.88	1 (2%)	50,67,67	1.51	7 (14%)
6	CYC	E	201	2	42,46,46	1.12	1 (2%)	50,67,67	1.32	6 (12%)
6	CYC	H	201	3	42,46,46	1.04	2 (4%)	50,67,67	1.35	6 (12%)
6	CYC	F	201	3	42,46,46	1.18	1 (2%)	50,67,67	1.21	4 (8%)
6	CYC	X	201	3	42,46,46	1.03	2 (4%)	50,67,67	1.40	7 (14%)
6	CYC	7	201	2	42,46,46	1.38	6 (14%)	50,67,67	1.55	12 (24%)
6	CYC	V	201	3	42,46,46	1.17	1 (2%)	50,67,67	1.20	4 (8%)
6	CYC	AK	201	2	42,46,46	0.99	1 (2%)	50,67,67	1.21	4 (8%)
6	CYC	m	201	2	42,46,46	1.35	6 (14%)	50,67,67	1.55	12 (24%)
6	CYC	v	201	3	42,46,46	1.08	2 (4%)	50,67,67	1.10	3 (6%)
6	CYC	AH	201	3	42,46,46	1.12	5 (11%)	50,67,67	1.47	8 (16%)
6	CYC	AA	201	2	42,46,46	1.15	4 (9%)	50,67,67	1.50	9 (18%)

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	A	2101	1	-	16/25/74/74	0/4/4/4
6	CYC	4	201	3	-	5/25/74/74	0/4/4/4
6	CYC	l	201	3	-	9/25/74/74	0/4/4/4
6	CYC	0	201	3	-	8/25/74/74	0/4/4/4
6	CYC	M	201	2	-	8/25/74/74	0/4/4/4
6	CYC	a	201	2	-	6/25/74/74	0/4/4/4
6	CYC	h	201	3	-	9/25/74/74	0/4/4/4
6	CYC	5	201	2	-	11/25/74/74	0/4/4/4
6	CYC	AD	201	3	-	7/25/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	CYC	AS	201	2	-	7/25/74/74	0/4/4/4
6	CYC	AX	201	3	-	7/25/74/74	0/4/4/4
6	CYC	z	201	3	-	9/25/74/74	0/4/4/4
6	CYC	6	201	3	-	7/25/74/74	0/4/4/4
6	CYC	AN	201	3	-	8/25/74/74	0/4/4/4
6	CYC	8	201	3	-	7/25/74/74	0/4/4/4
6	CYC	R	201	3	-	7/25/74/74	0/4/4/4
6	CYC	e	201	2	-	13/25/74/74	0/4/4/4
6	CYC	AC	201	2	-	8/25/74/74	0/4/4/4
6	CYC	C	2101	-	-	11/25/74/74	0/4/4/4
6	CYC	L	201	3	-	11/25/74/74	0/4/4/4
6	CYC	c	201	2	-	8/25/74/74	0/4/4/4
6	CYC	AP	201	3	-	11/25/74/74	0/4/4/4
6	CYC	Y	201	2	-	10/25/74/74	0/4/4/4
6	CYC	AL	201	3	-	6/25/74/74	0/4/4/4
6	CYC	Z	201	3	-	8/25/74/74	0/4/4/4
6	CYC	AO	201	2	-	8/25/74/74	0/4/4/4
6	CYC	t	201	2	-	12/25/74/74	0/4/4/4
6	CYC	G	201	2	-	7/25/74/74	0/4/4/4
6	CYC	b	201	3	-	11/25/74/74	0/4/4/4
6	CYC	2	201	3	-	5/25/74/74	0/4/4/4
6	CYC	S	201	2	-	8/25/74/74	0/4/4/4
6	CYC	w	201	2	-	8/25/74/74	0/4/4/4
6	CYC	J	201	3	-	8/25/74/74	0/4/4/4
6	CYC	AJ	201	3	-	6/25/74/74	0/4/4/4
6	CYC	k	201	2	-	8/25/74/74	0/4/4/4
6	CYC	u	201	-	-	14/25/74/74	0/4/4/4
6	CYC	g	201	2	-	9/25/74/74	0/4/4/4
6	CYC	W	201	2	-	6/25/74/74	0/4/4/4
6	CYC	U	201	2	-	5/25/74/74	0/4/4/4
6	CYC	j	201	3	-	7/25/74/74	0/4/4/4
6	CYC	AR	201	3	-	7/25/74/74	0/4/4/4
6	CYC	o	201	2	-	4/25/74/74	0/4/4/4
6	CYC	O	201	2	-	8/25/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	CYC	AU	201	2	-	8/25/74/74	0/4/4/4
6	CYC	K	201	2	-	6/25/74/74	0/4/4/4
6	CYC	9	201	2	-	7/25/74/74	0/4/4/4
6	CYC	AW	201	2	-	7/25/74/74	0/4/4/4
6	CYC	1	201	2	-	11/25/74/74	0/4/4/4
6	CYC	d	201	3	-	8/25/74/74	0/4/4/4
6	CYC	AF	201	3	-	7/25/74/74	0/4/4/4
6	CYC	n	201	3	-	9/25/74/74	0/4/4/4
6	CYC	x	201	3	-	8/25/74/74	0/4/4/4
6	CYC	AI	201	2	-	8/25/74/74	0/4/4/4
6	CYC	AB	201	3	-	8/25/74/74	0/4/4/4
6	CYC	y	201	2	-	10/25/74/74	0/4/4/4
6	CYC	AM	201	2	-	11/25/74/74	0/4/4/4
6	CYC	AQ	201	2	-	4/25/74/74	0/4/4/4
6	CYC	i	201	2	-	10/25/74/74	0/4/4/4
6	CYC	s	201	-	-	13/25/74/74	0/4/4/4
6	CYC	AE	201	2	-	4/25/74/74	0/4/4/4
6	CYC	N	201	3	-	9/25/74/74	0/4/4/4
6	CYC	P	201	3	-	10/25/74/74	0/4/4/4
6	CYC	I	201	2	-	10/25/74/74	0/4/4/4
6	CYC	AT	201	3	-	6/25/74/74	0/4/4/4
6	CYC	T	201	3	-	10/25/74/74	0/4/4/4
6	CYC	AV	201	3	-	6/25/74/74	0/4/4/4
6	CYC	3	201	2	-	7/25/74/74	0/4/4/4
6	CYC	Q	201	2	-	9/25/74/74	0/4/4/4
6	CYC	q	201	3	-	11/25/74/74	0/4/4/4
6	CYC	AG	201	2	-	7/25/74/74	0/4/4/4
6	CYC	r	201	2	-	12/25/74/74	0/4/4/4
6	CYC	p	201	3	-	8/25/74/74	0/4/4/4
6	CYC	f	201	3	-	9/25/74/74	0/4/4/4
6	CYC	E	201	2	-	5/25/74/74	0/4/4/4
6	CYC	H	201	3	-	9/25/74/74	0/4/4/4
6	CYC	F	201	3	-	7/25/74/74	0/4/4/4
6	CYC	X	201	3	-	6/25/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	CYC	7	201	2	-	11/25/74/74	0/4/4/4
6	CYC	V	201	3	-	7/25/74/74	0/4/4/4
6	CYC	AK	201	2	-	7/25/74/74	0/4/4/4
6	CYC	m	201	2	-	11/25/74/74	0/4/4/4
6	CYC	v	201	3	-	11/25/74/74	0/4/4/4
6	CYC	AH	201	3	-	6/25/74/74	0/4/4/4
6	CYC	AA	201	2	-	11/25/74/74	0/4/4/4

The worst 5 of 154 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	j	201	CYC	CHA-C1A	6.35	1.40	1.35
6	F	201	CYC	CHA-C1A	6.29	1.40	1.35
6	V	201	CYC	CHA-C1A	6.18	1.40	1.35
6	g	201	CYC	CHA-C1A	6.09	1.40	1.35
6	C	2101	CYC	CHA-C1A	6.06	1.40	1.35

The worst 5 of 426 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	f	201	CYC	CMB-C2B-C1B	6.17	131.87	124.17
6	6	201	CYC	CMB-C2B-C1B	5.58	131.13	124.17
6	AT	201	CYC	CMB-C2B-C1B	5.09	130.52	124.17
6	AH	201	CYC	CMB-C2B-C1B	5.08	130.51	124.17
6	Q	201	CYC	CMB-C2B-C1B	4.88	130.26	124.17

There are no chirality outliers.

5 of 702 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	2101	CYC	NA-C4A-CHB-C1B
6	A	2101	CYC	C3A-C4A-CHB-C1B
6	A	2101	CYC	C2B-C1B-CHB-C4A
6	A	2101	CYC	C2C-C3C-CAC-CBC
6	A	2101	CYC	NC-C4C-CHD-C1D

There are no ring outliers.

84 monomers are involved in 429 short contacts:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	2101	CYC	3	0
6	4	201	CYC	6	0
6	l	201	CYC	1	0
6	0	201	CYC	2	0
6	M	201	CYC	6	0
6	a	201	CYC	4	0
6	h	201	CYC	1	0
6	5	201	CYC	8	0
6	AD	201	CYC	2	0
6	AS	201	CYC	13	0
6	AX	201	CYC	4	0
6	z	201	CYC	2	0
6	6	201	CYC	5	0
6	AN	201	CYC	3	0
6	8	201	CYC	1	0
6	R	201	CYC	13	0
6	e	201	CYC	10	0
6	AC	201	CYC	2	0
6	C	2101	CYC	33	0
6	L	201	CYC	2	0
6	c	201	CYC	6	0
6	AP	201	CYC	4	0
6	Y	201	CYC	3	0
6	AL	201	CYC	3	0
6	Z	201	CYC	3	0
6	AO	201	CYC	2	0
6	t	201	CYC	4	0
6	G	201	CYC	5	0
6	b	201	CYC	2	0
6	2	201	CYC	1	0
6	S	201	CYC	3	0
6	w	201	CYC	1	0
6	J	201	CYC	2	0
6	AJ	201	CYC	3	0
6	k	201	CYC	5	0
6	u	201	CYC	14	0
6	g	201	CYC	6	0
6	W	201	CYC	5	0
6	U	201	CYC	7	0
6	j	201	CYC	2	0
6	AR	201	CYC	1	0
6	o	201	CYC	3	0
6	O	201	CYC	3	0

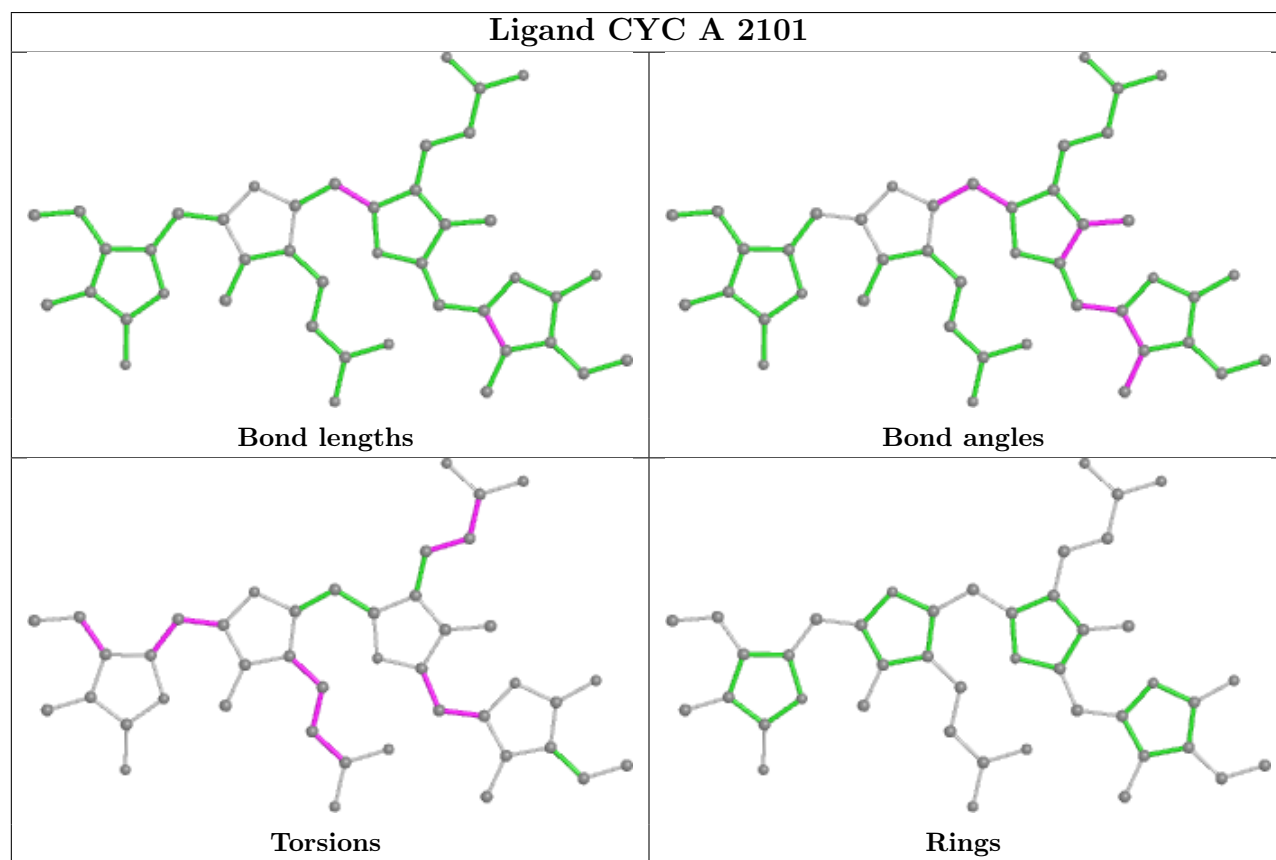
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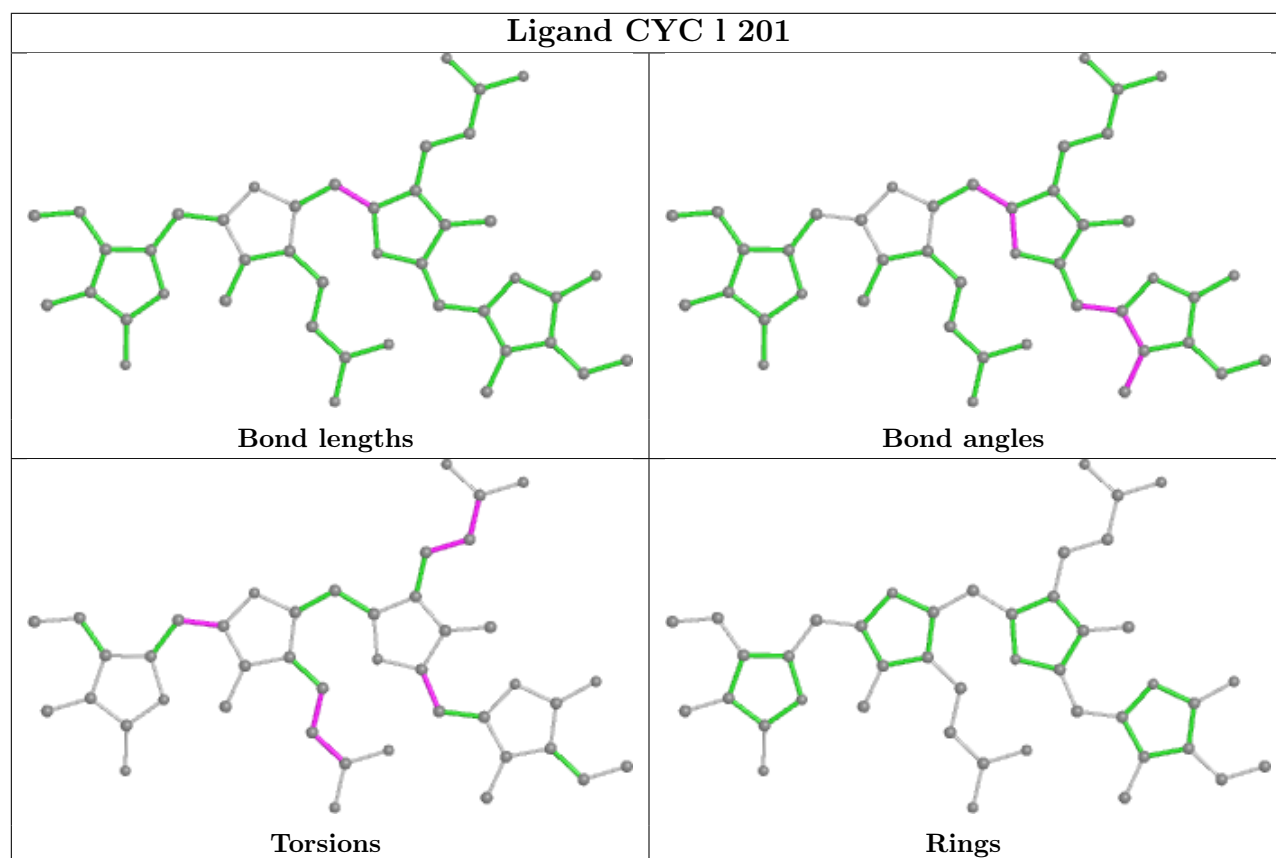
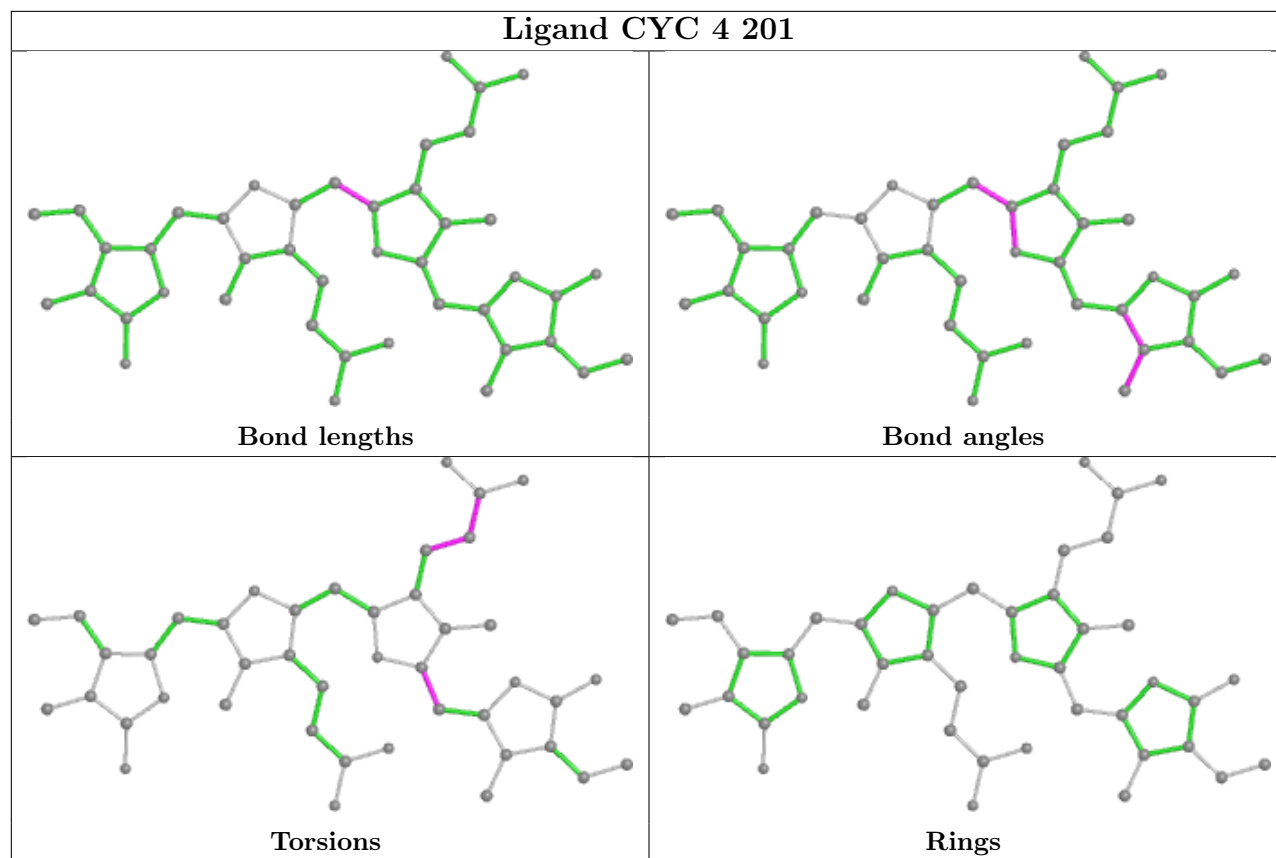
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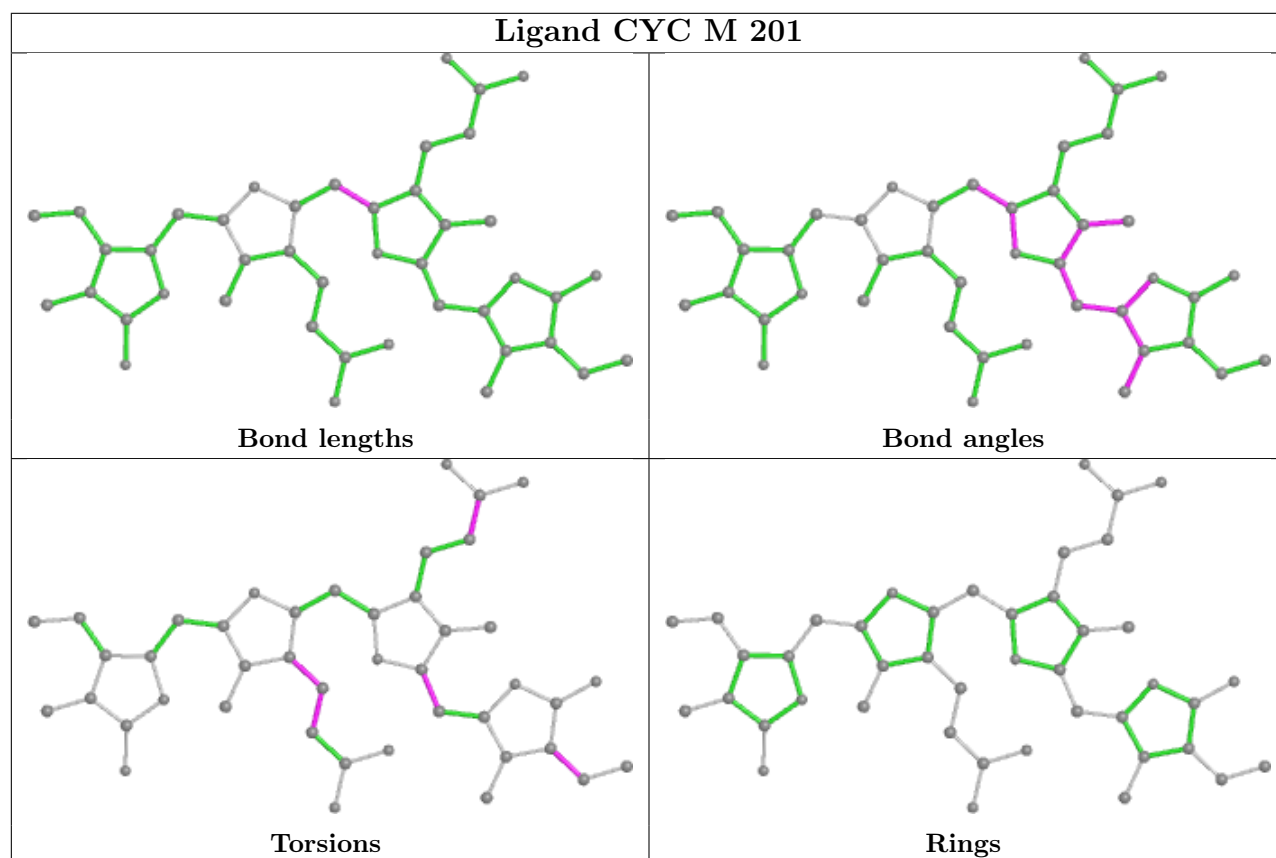
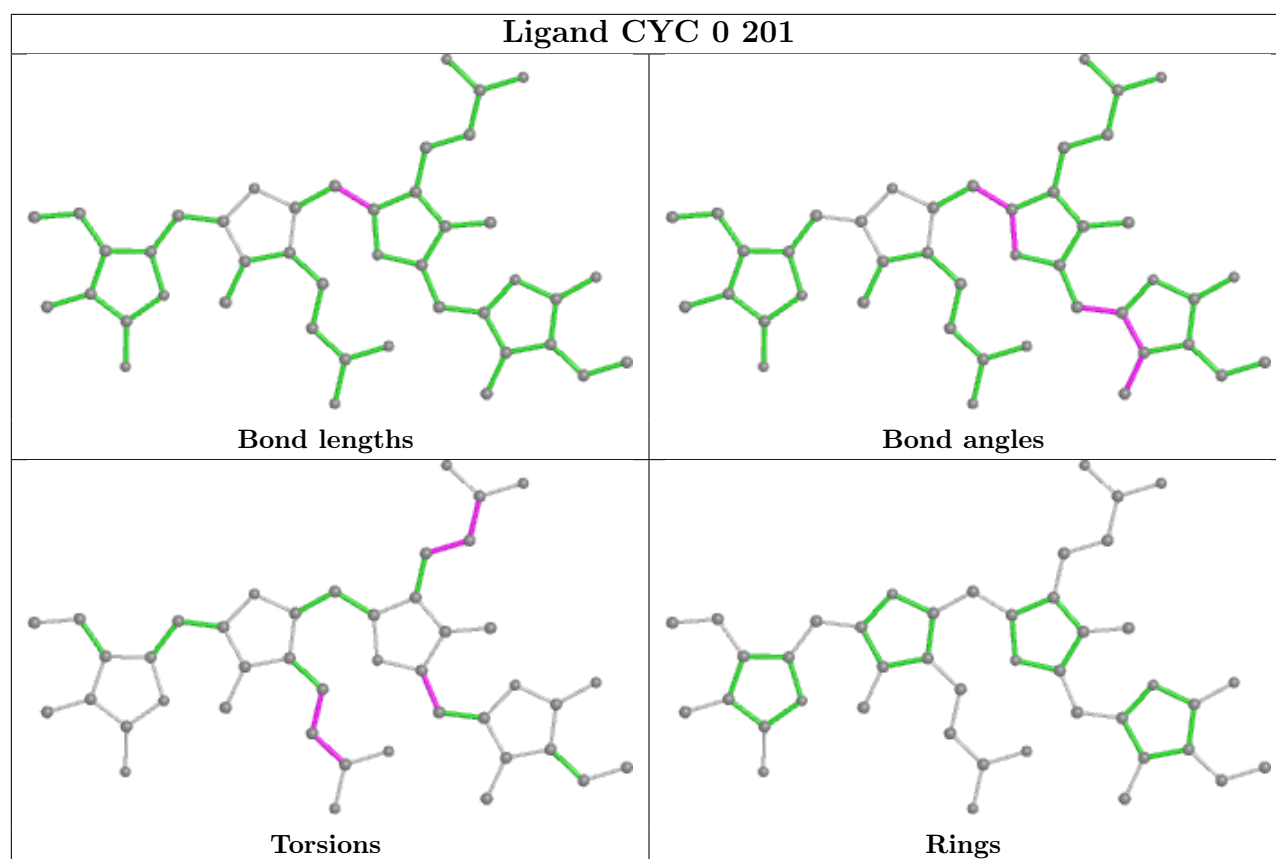
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	AU	201	CYC	1	0
6	K	201	CYC	3	0
6	9	201	CYC	7	0
6	AW	201	CYC	11	0
6	1	201	CYC	2	0
6	d	201	CYC	5	0
6	AF	201	CYC	4	0
6	n	201	CYC	4	0
6	x	201	CYC	3	0
6	AI	201	CYC	1	0
6	AB	201	CYC	3	0
6	y	201	CYC	9	0
6	AM	201	CYC	7	0
6	AQ	201	CYC	1	0
6	i	201	CYC	4	0
6	s	201	CYC	12	0
6	AE	201	CYC	1	0
6	N	201	CYC	7	0
6	P	201	CYC	3	0
6	I	201	CYC	3	0
6	AT	201	CYC	4	0
6	T	201	CYC	5	0
6	AV	201	CYC	3	0
6	3	201	CYC	5	0
6	Q	201	CYC	10	0
6	q	201	CYC	2	0
6	AG	201	CYC	12	0
6	r	201	CYC	4	0
6	p	201	CYC	3	0
6	f	201	CYC	3	0
6	E	201	CYC	8	0
6	H	201	CYC	5	0
6	F	201	CYC	9	0
6	X	201	CYC	8	0
6	7	201	CYC	8	0
6	V	201	CYC	8	0
6	AK	201	CYC	11	0
6	m	201	CYC	9	0
6	v	201	CYC	1	0
6	AH	201	CYC	4	0
6	AA	201	CYC	7	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

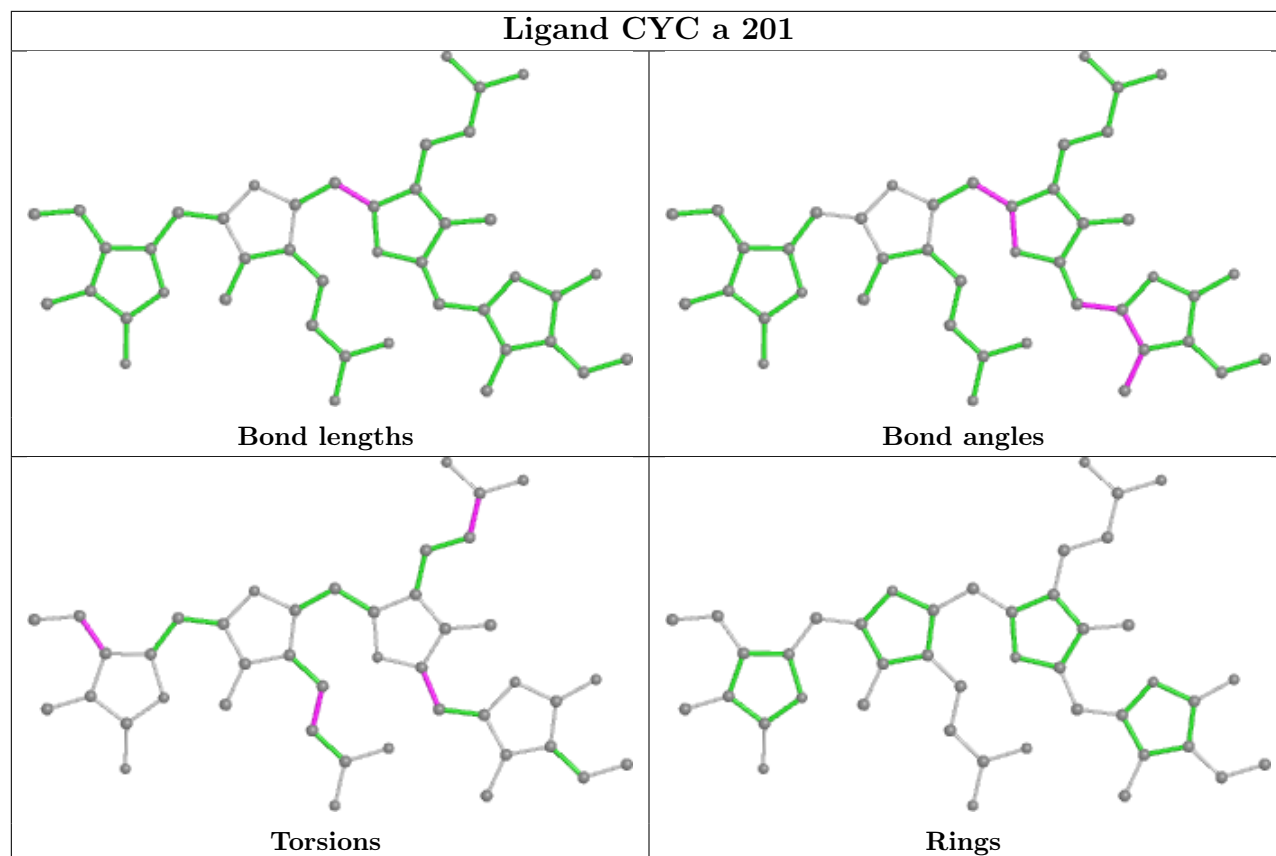
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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.



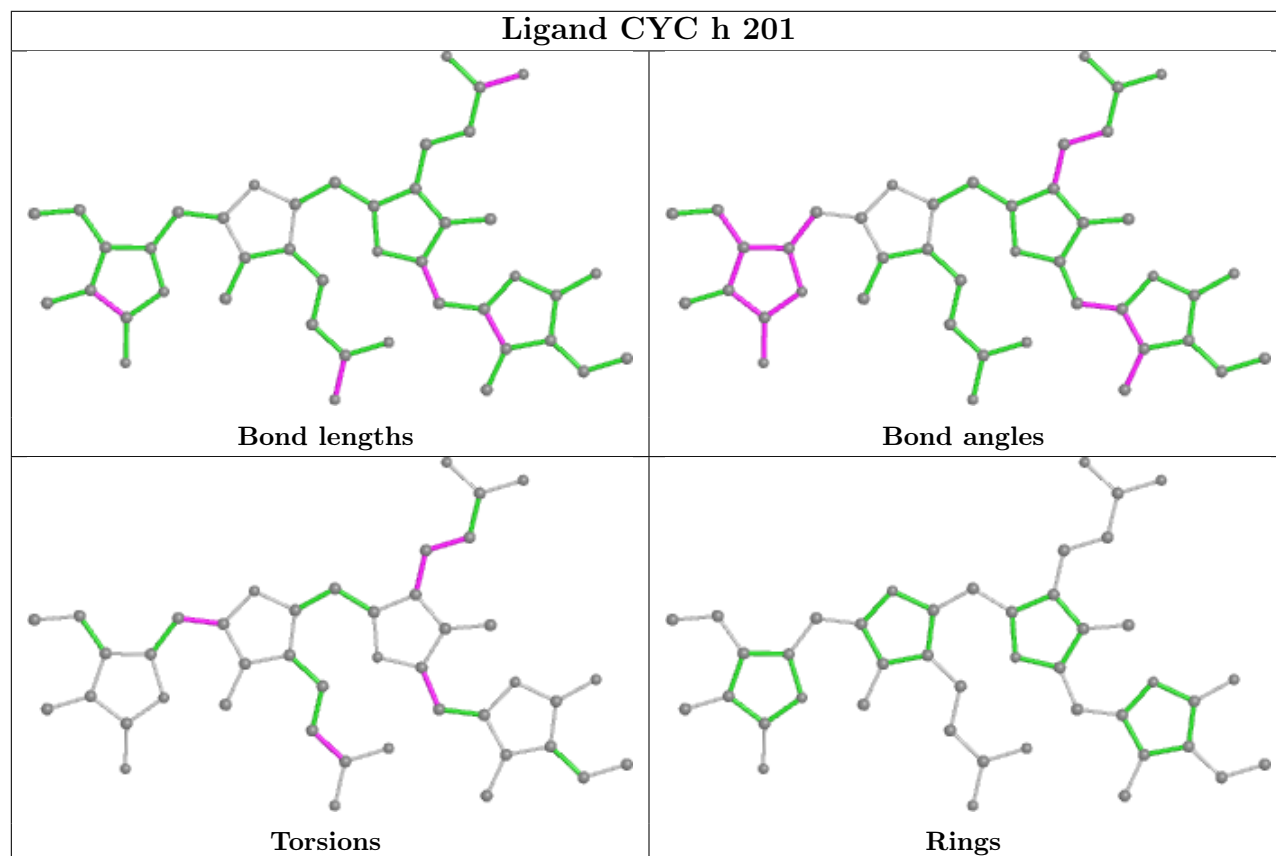


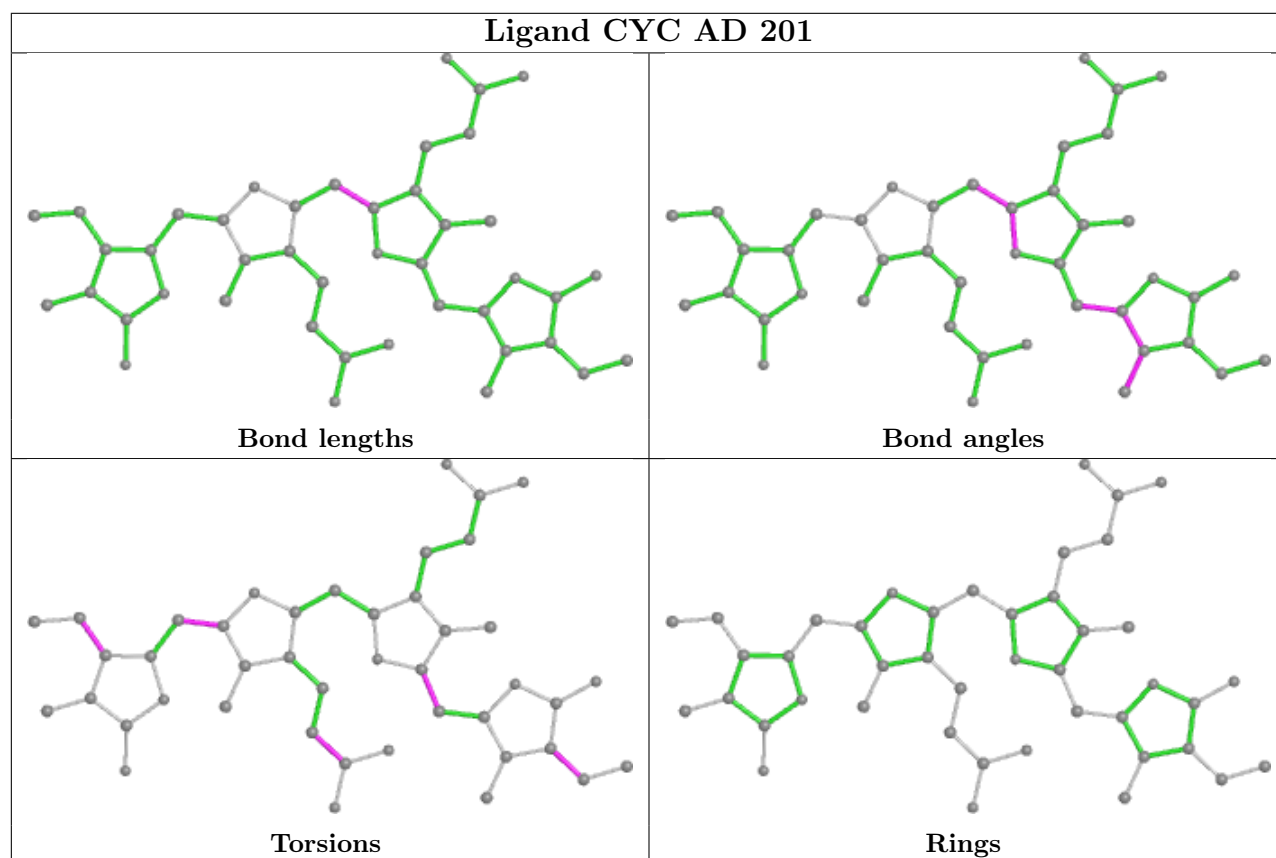
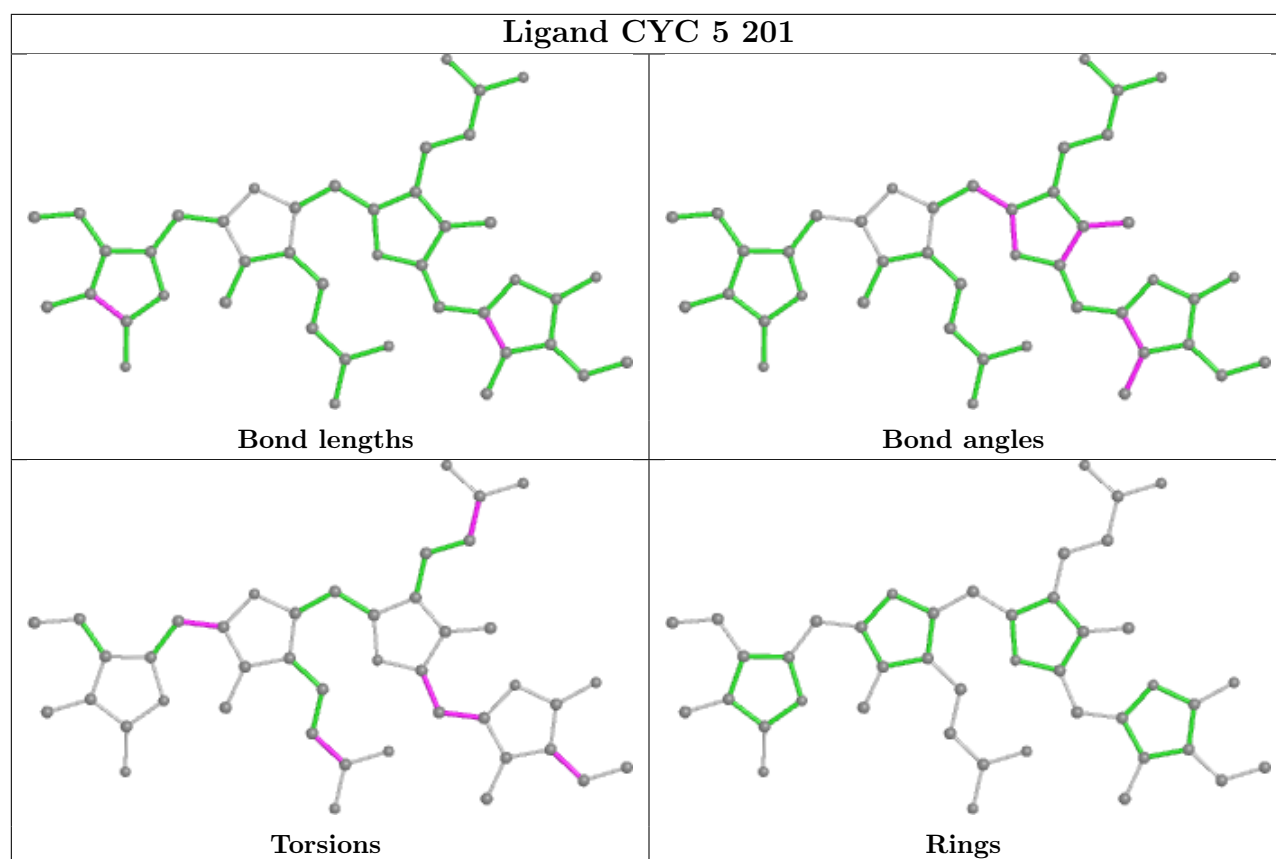


## Ligand CYC a 201

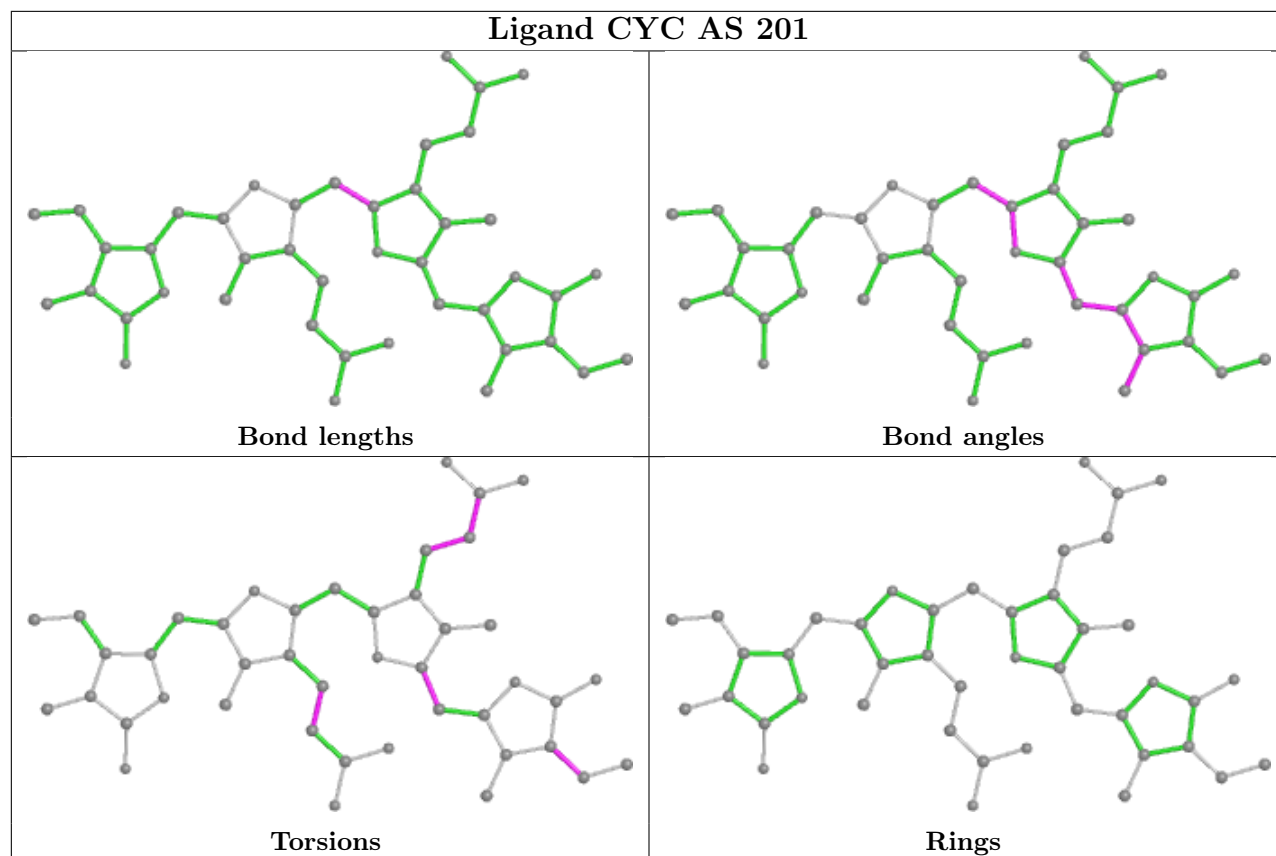


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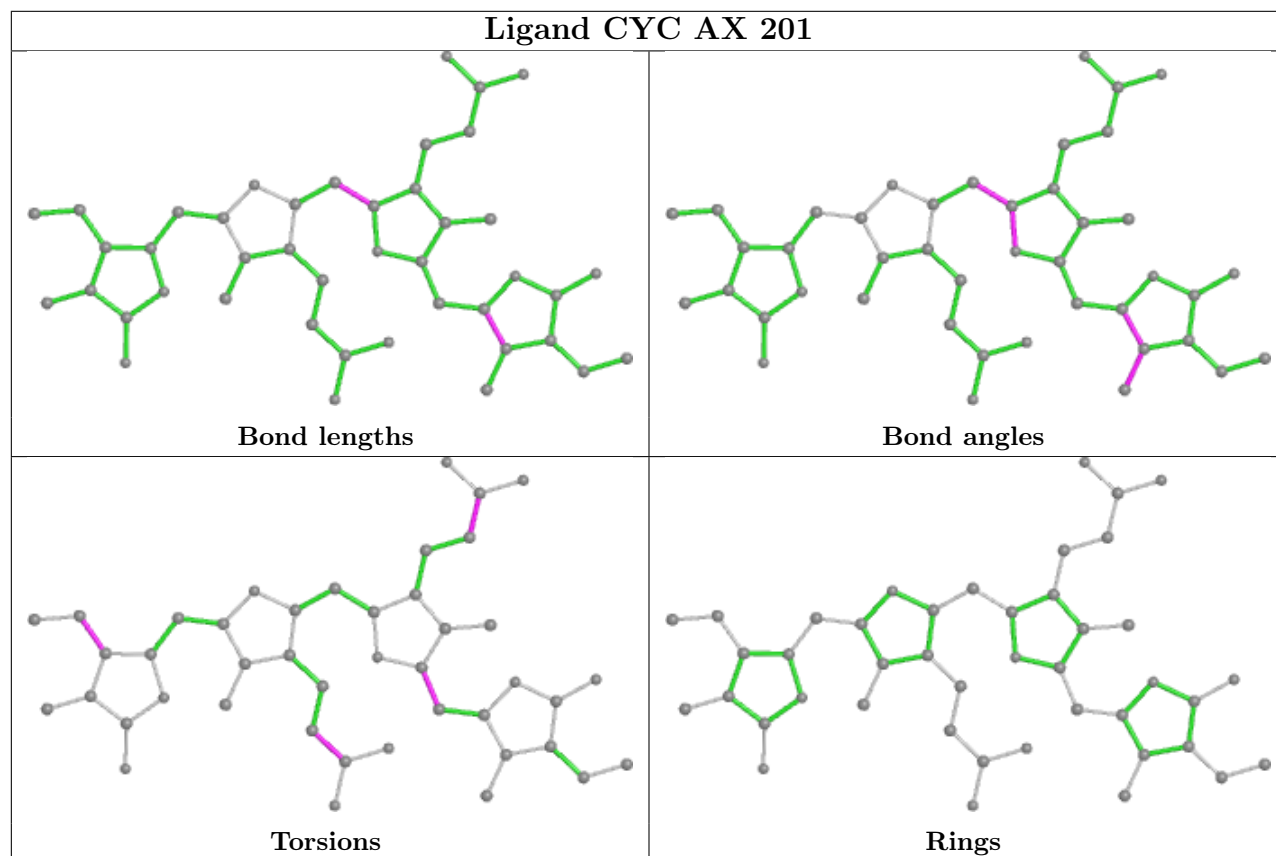




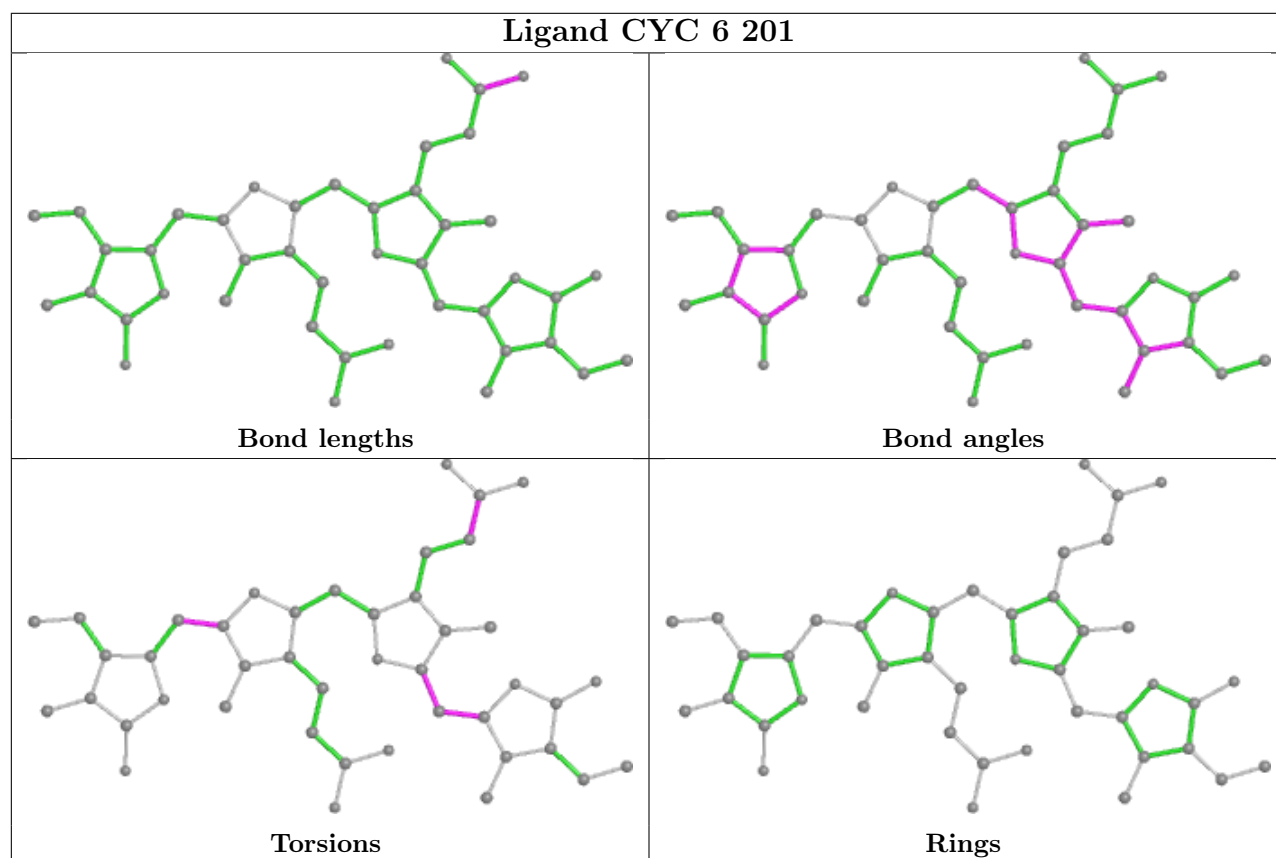
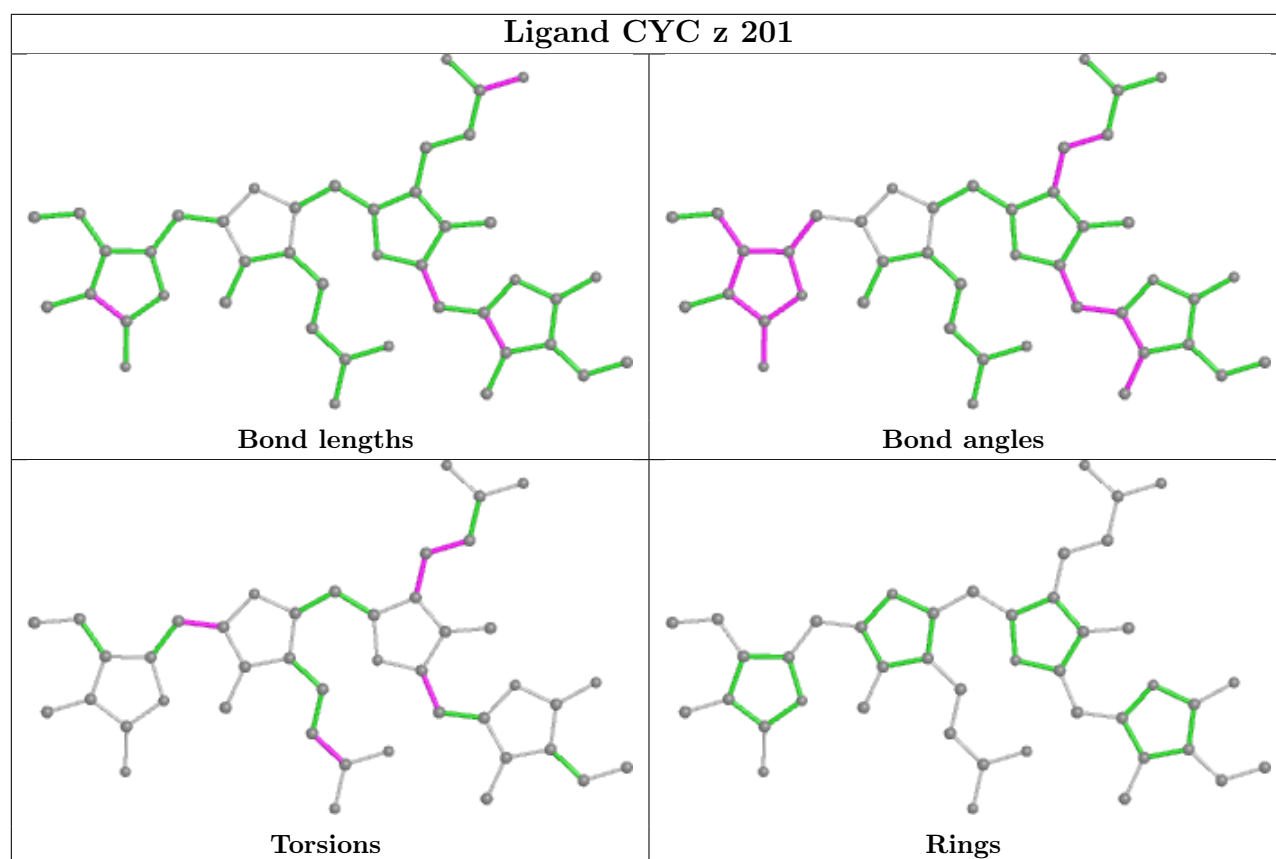
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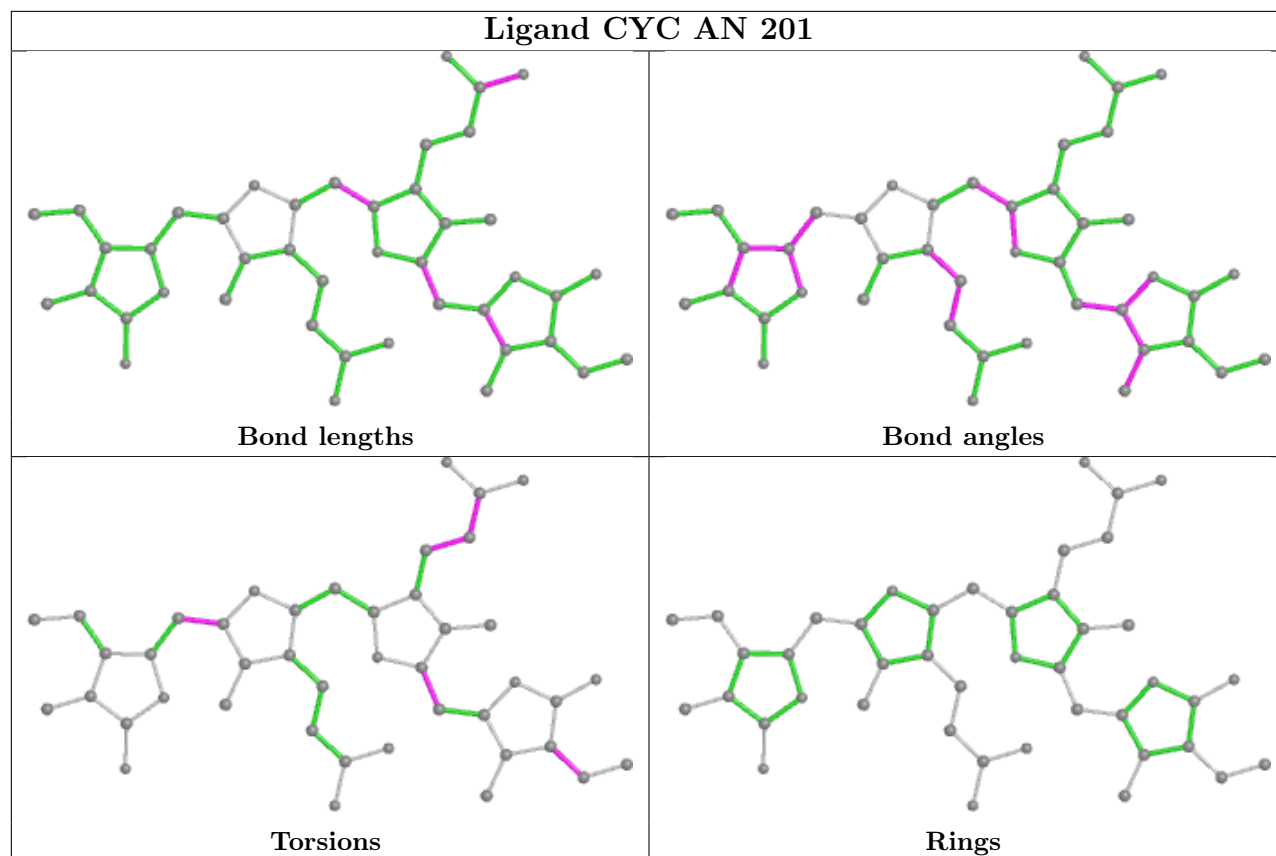
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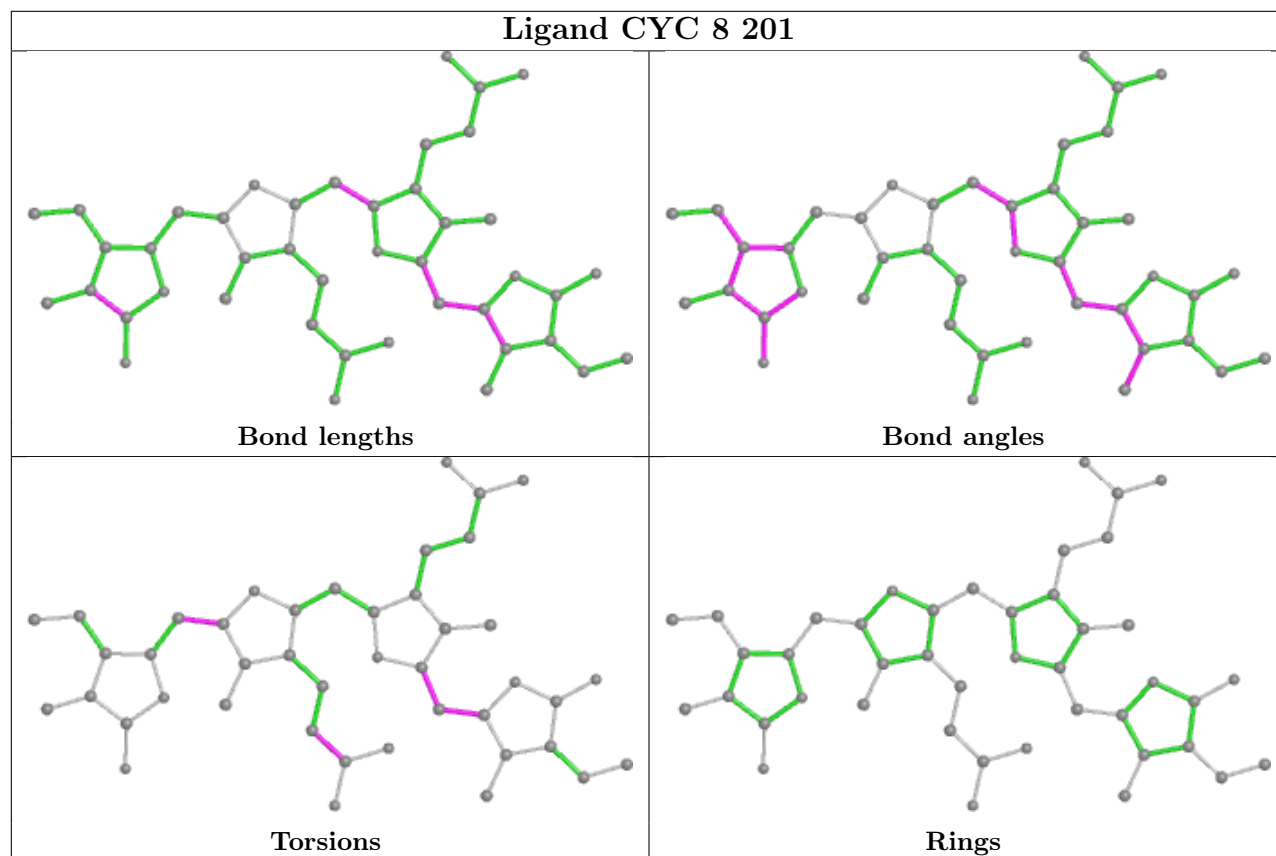


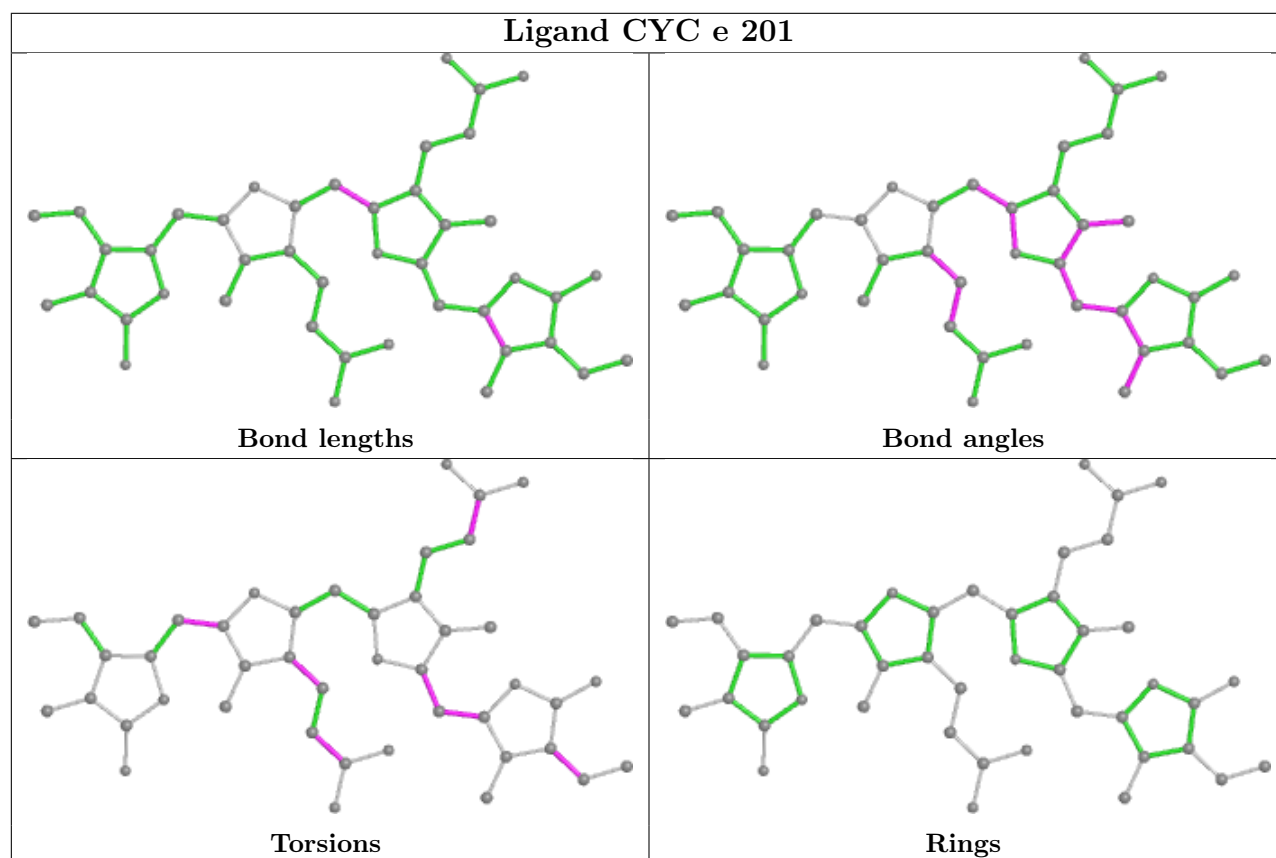
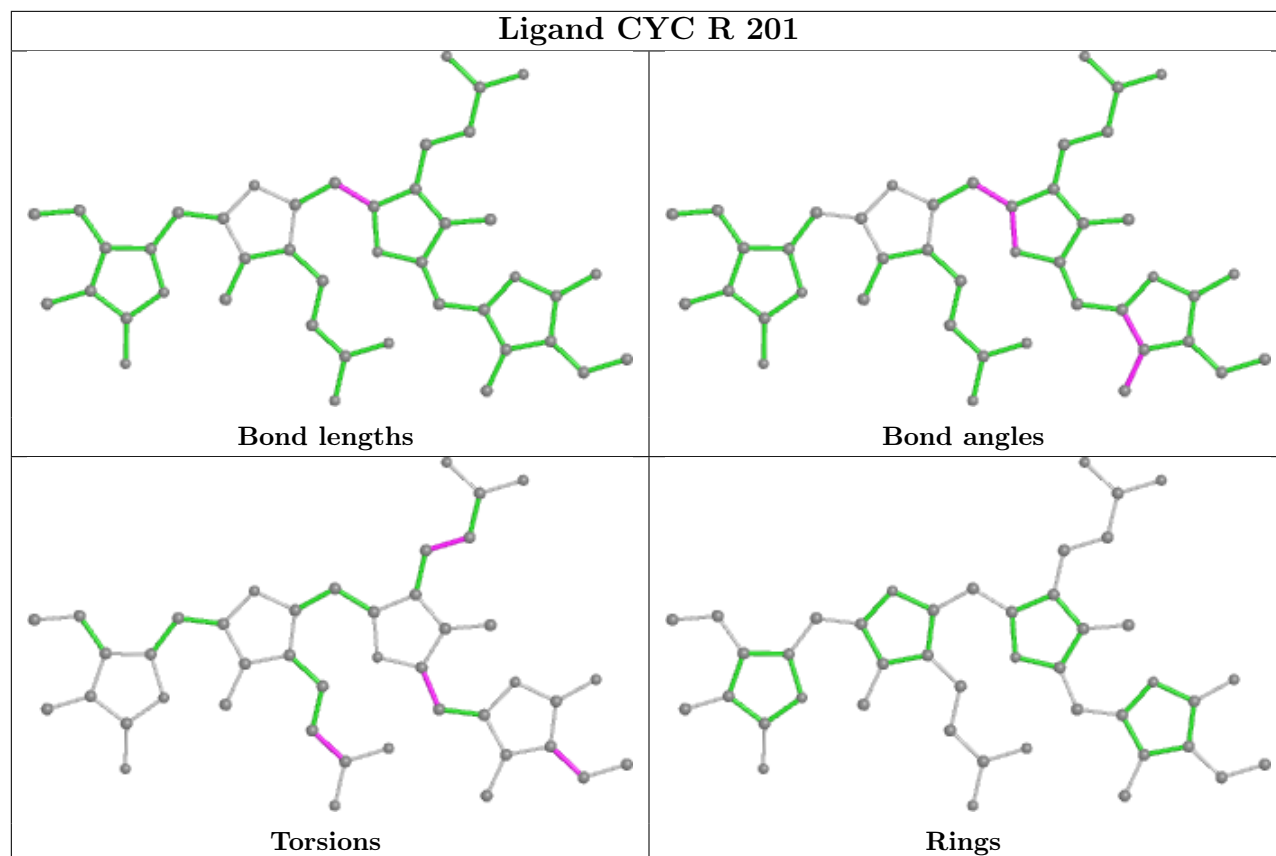


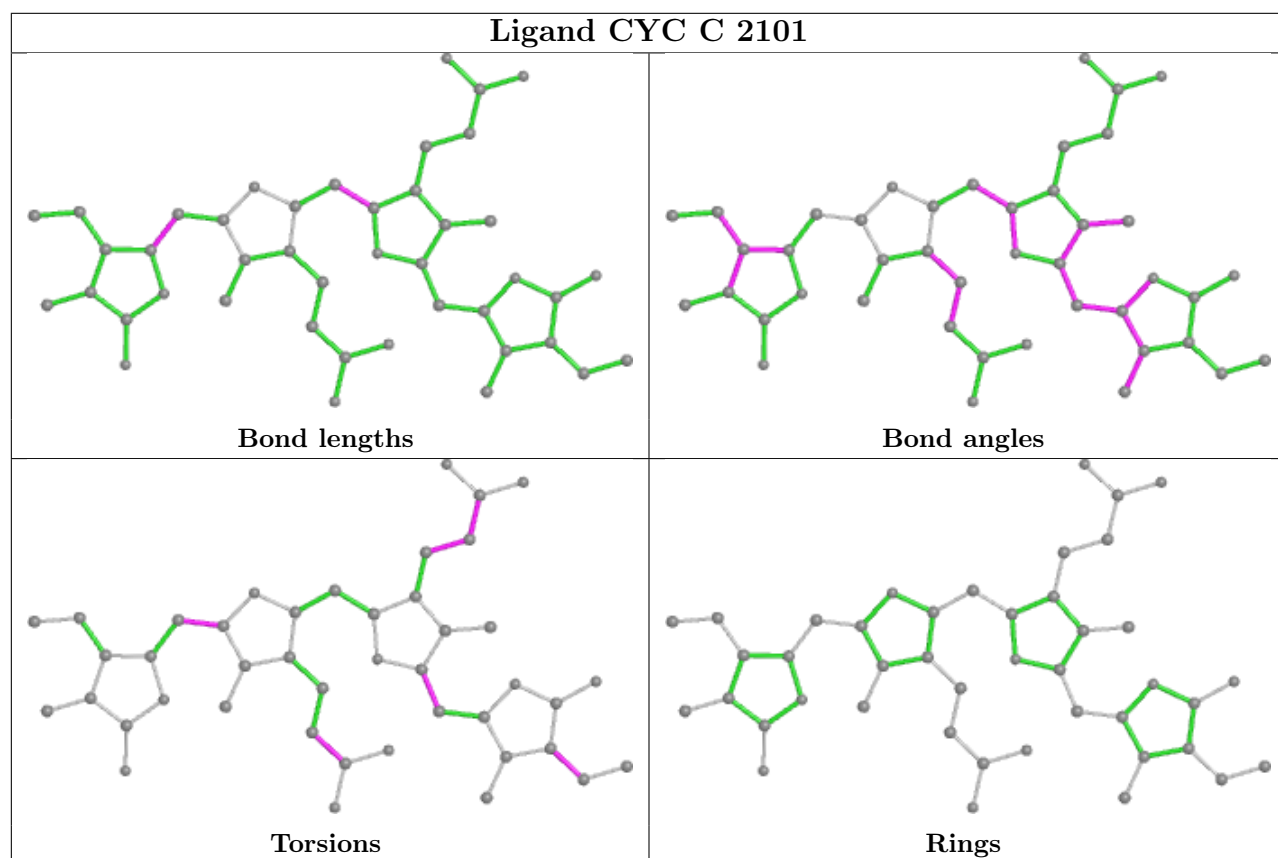
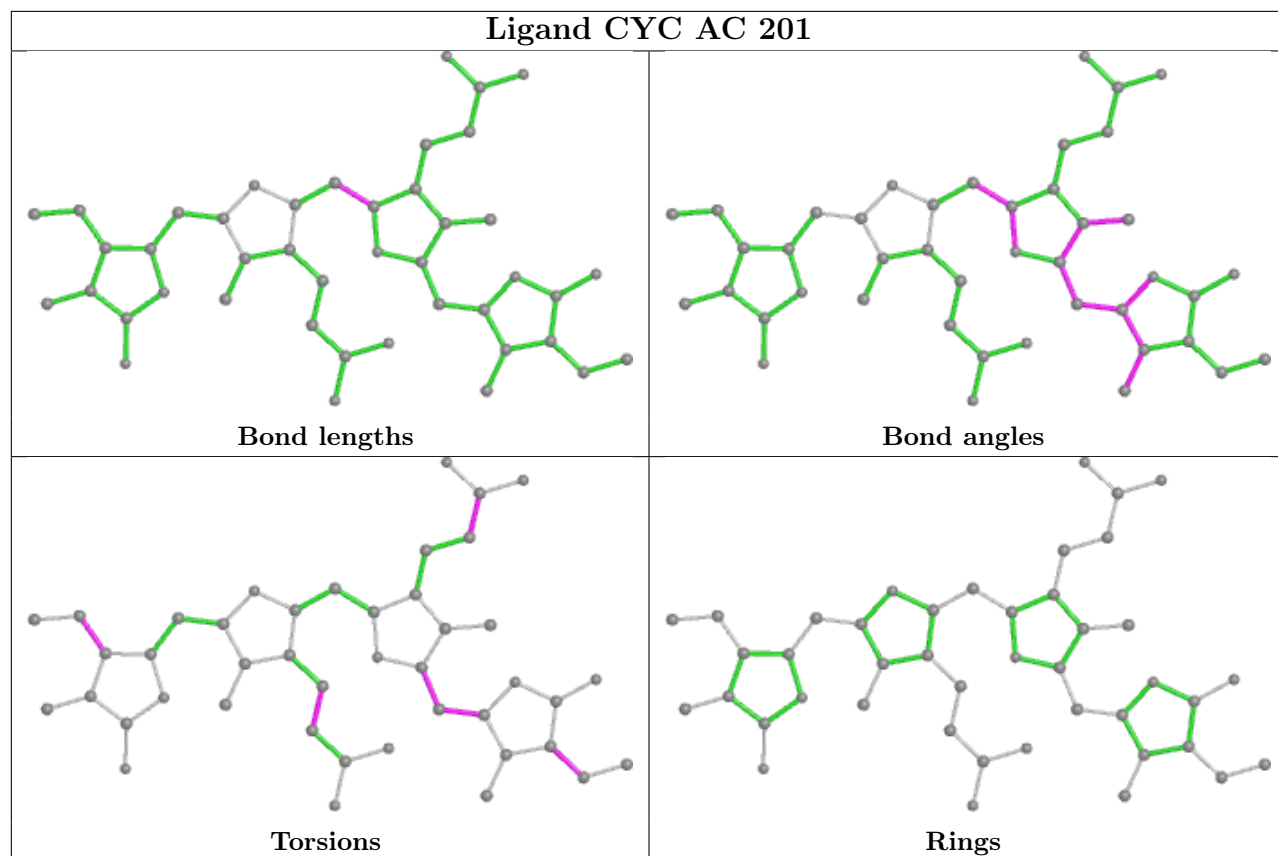
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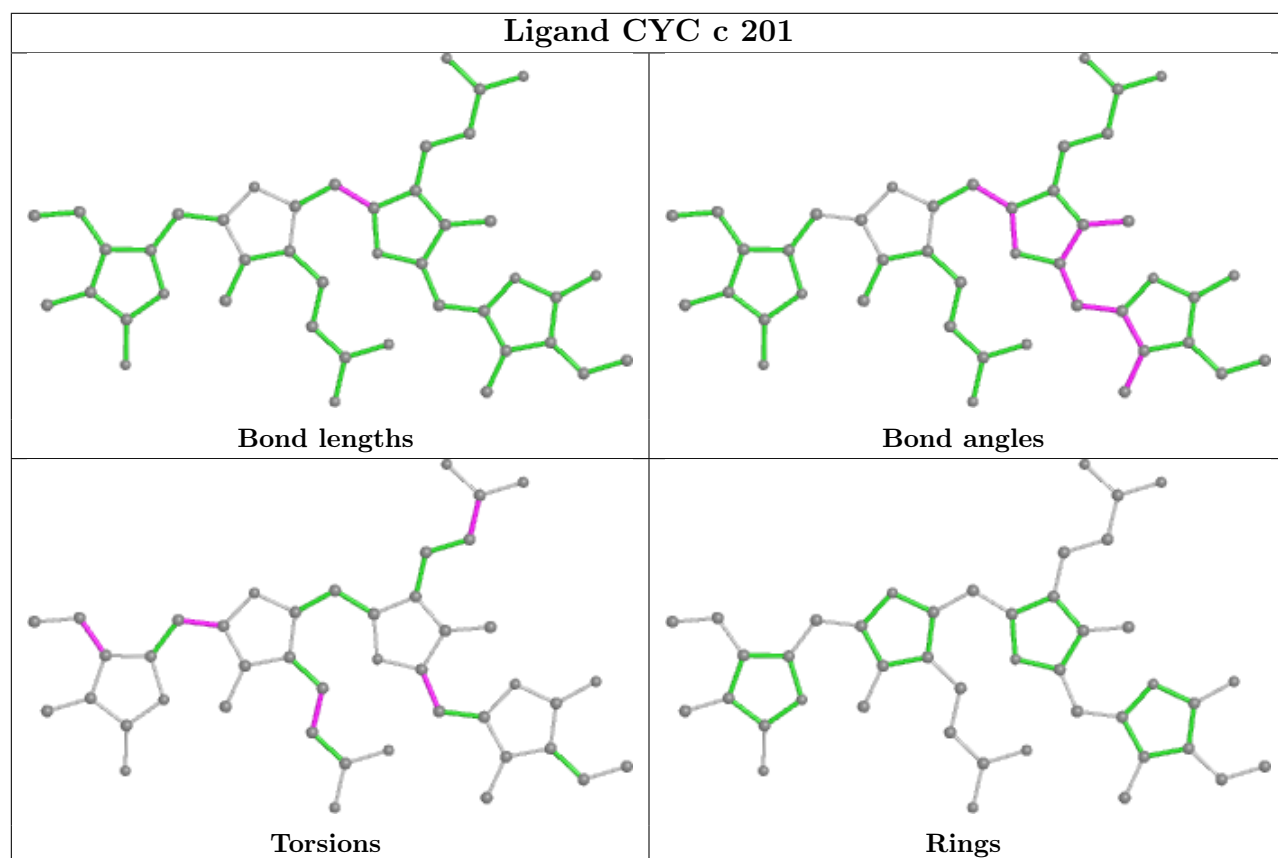
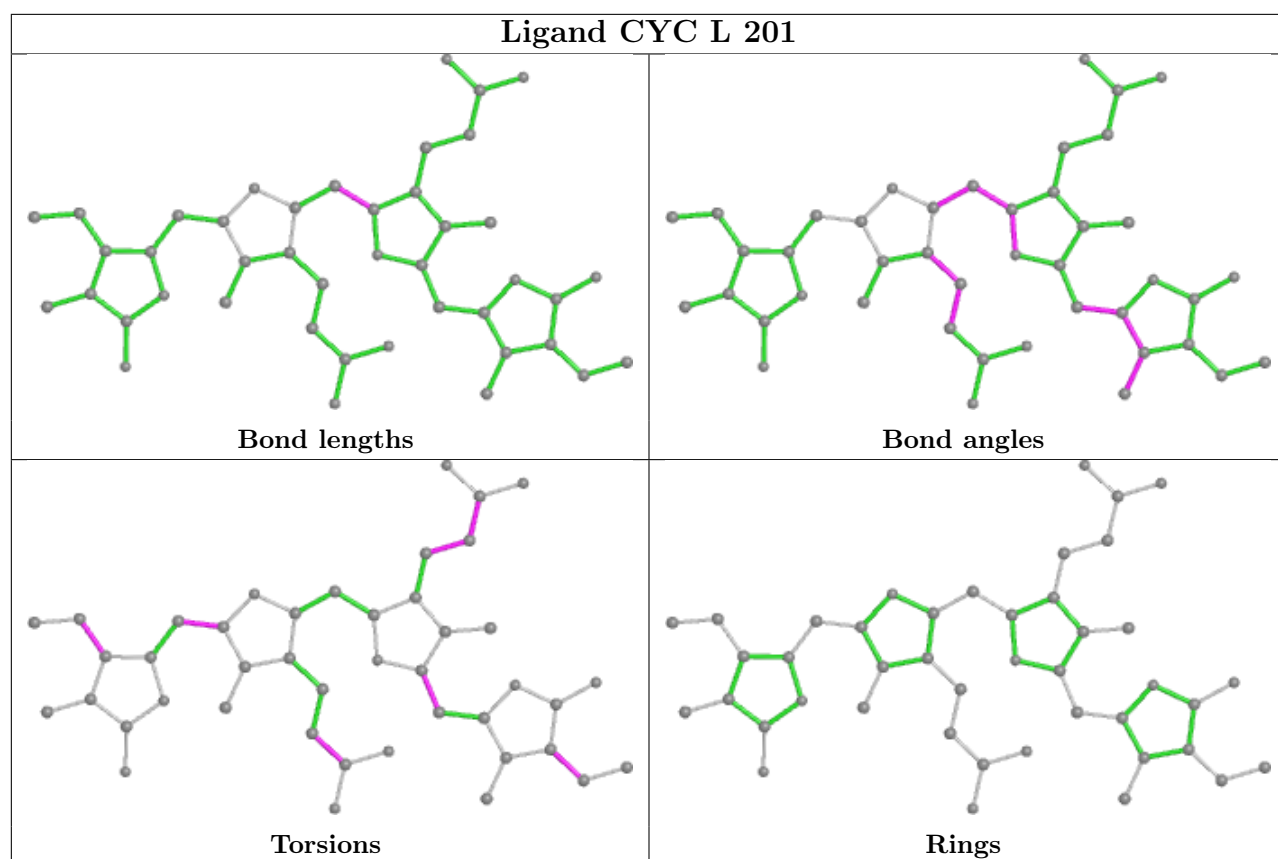


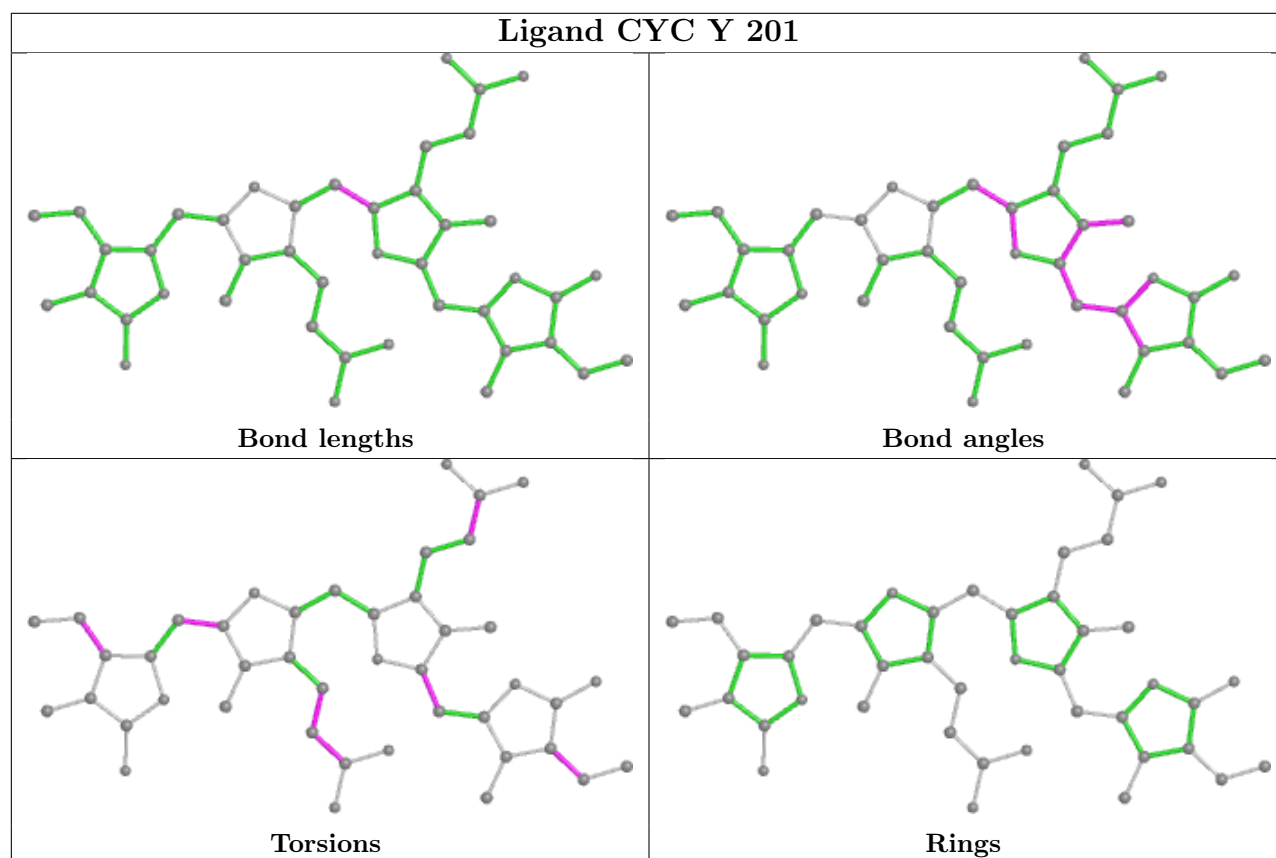
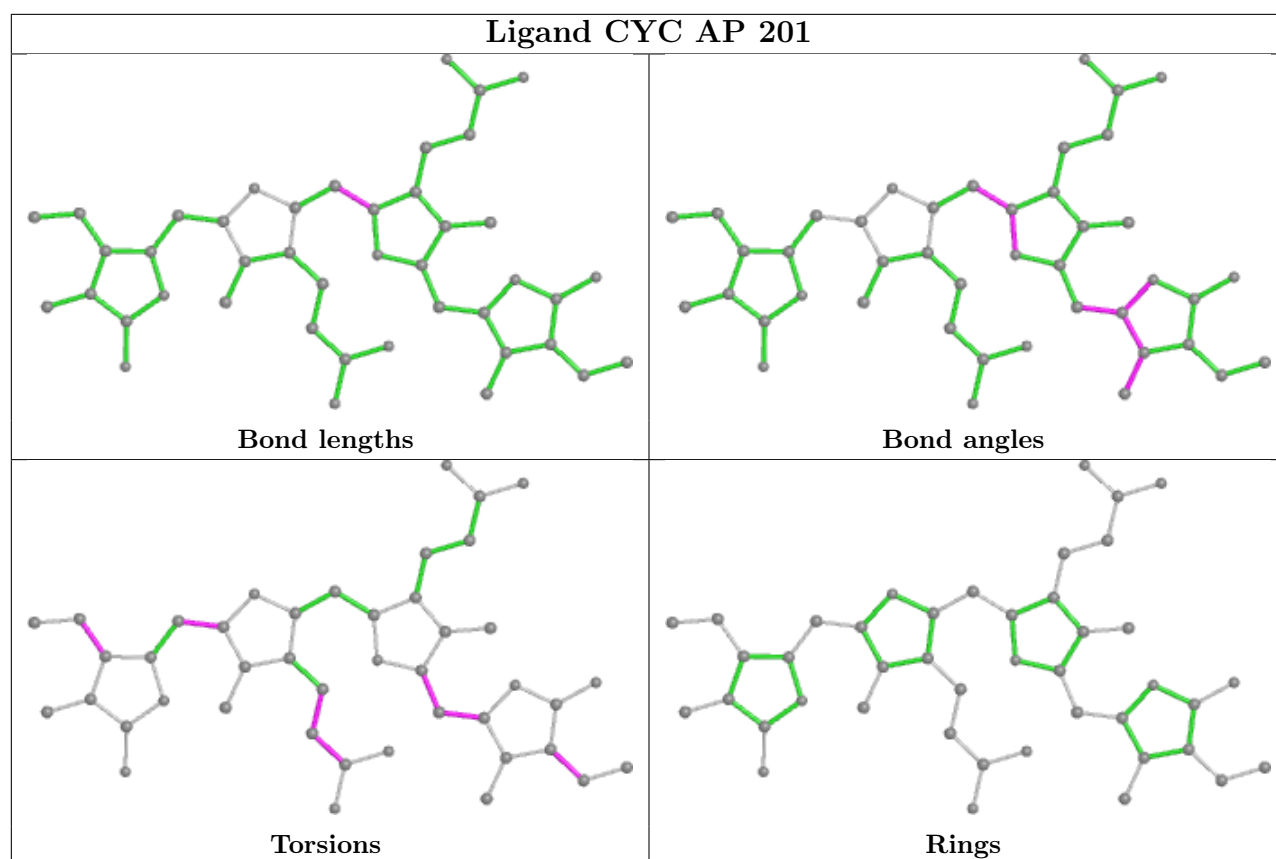
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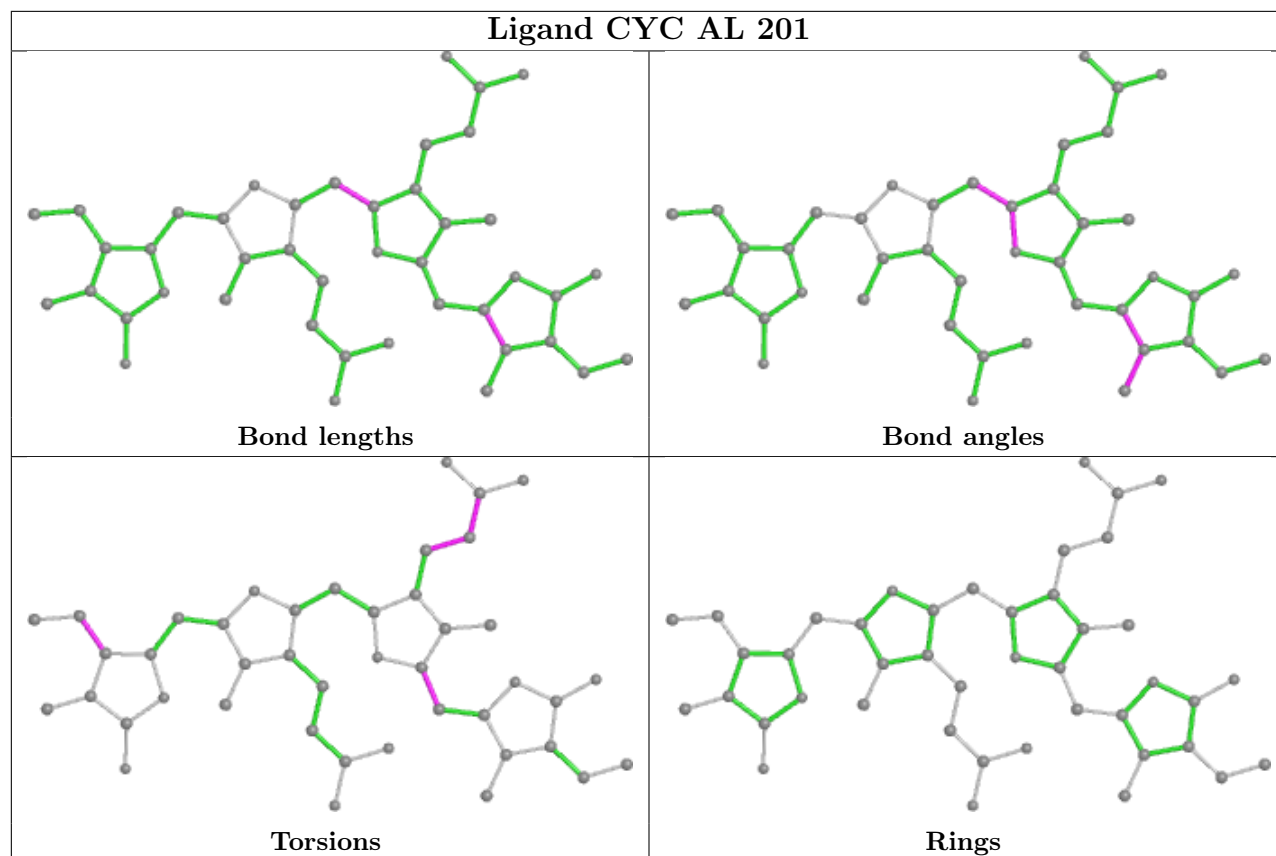




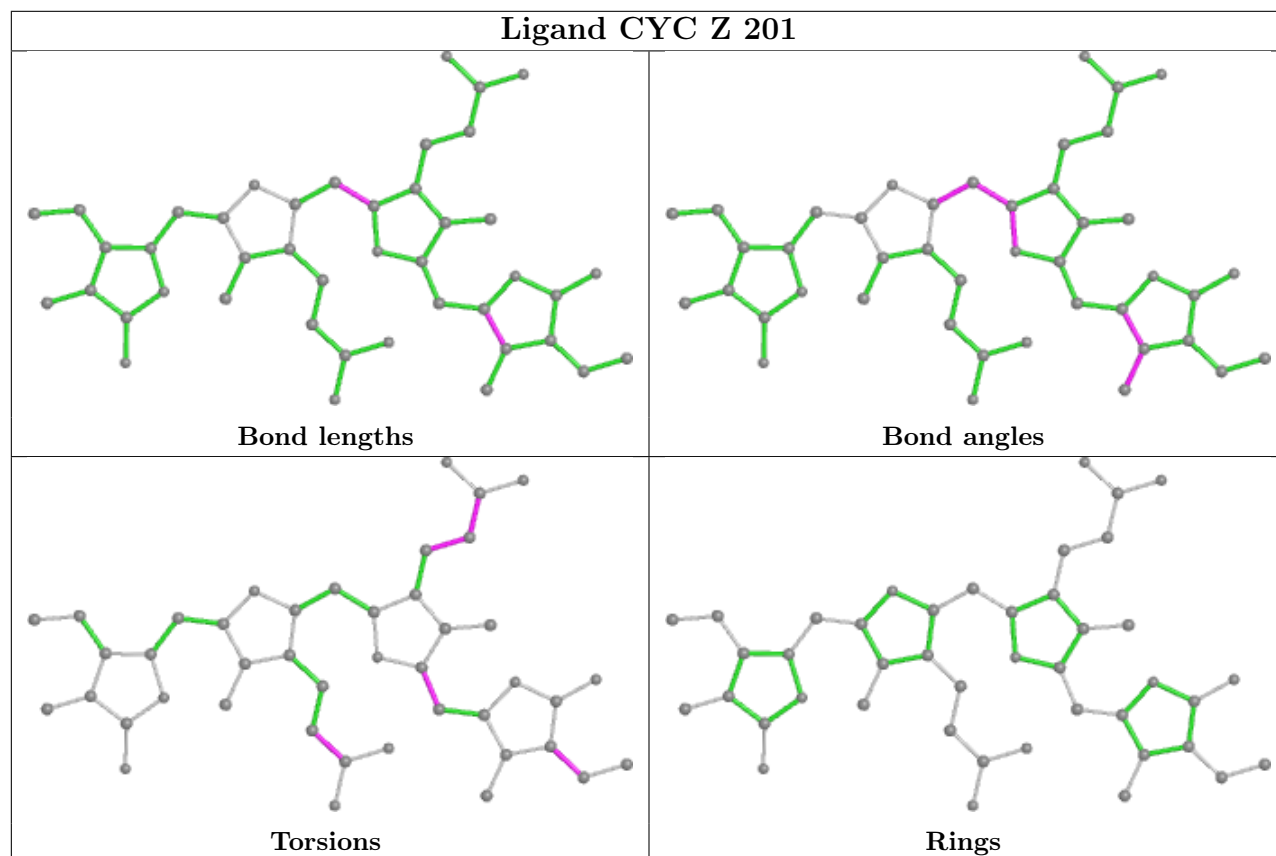


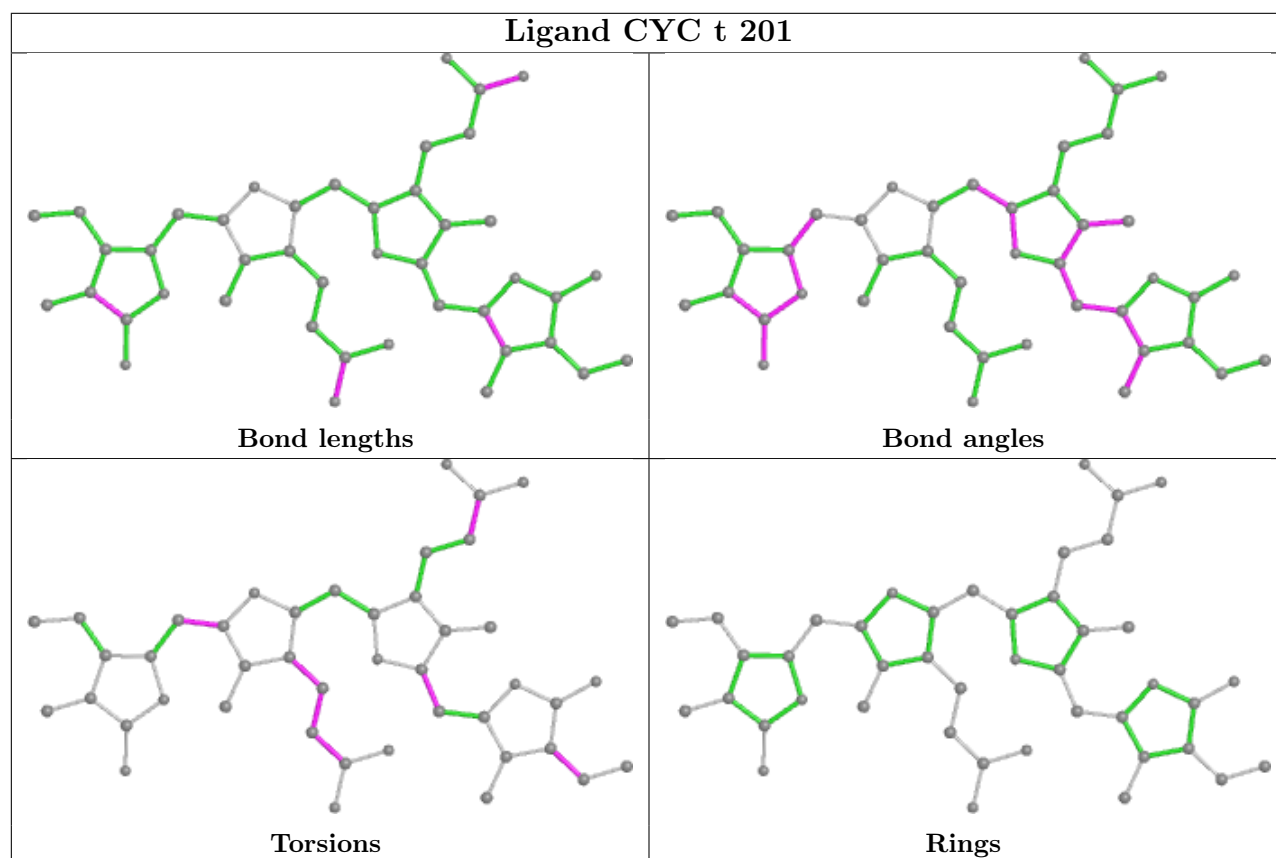
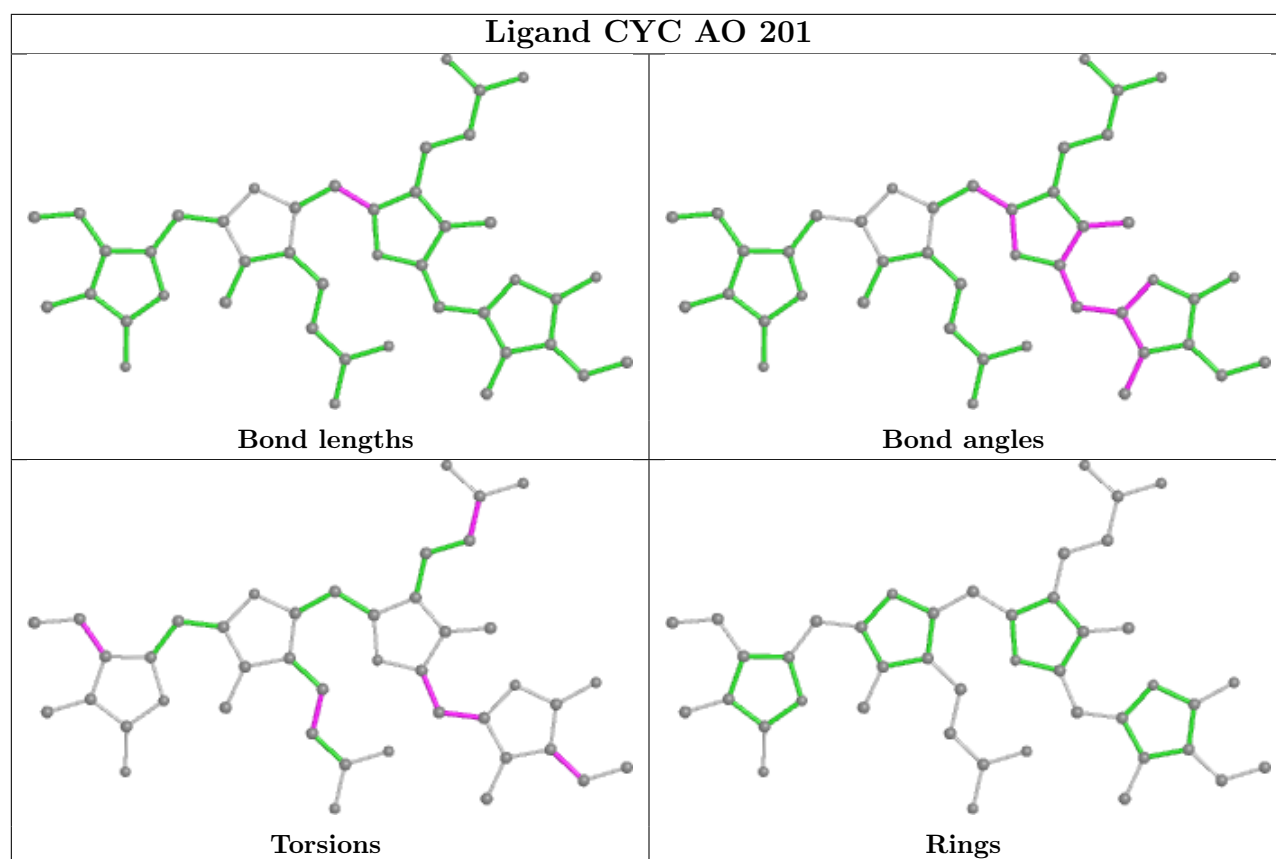


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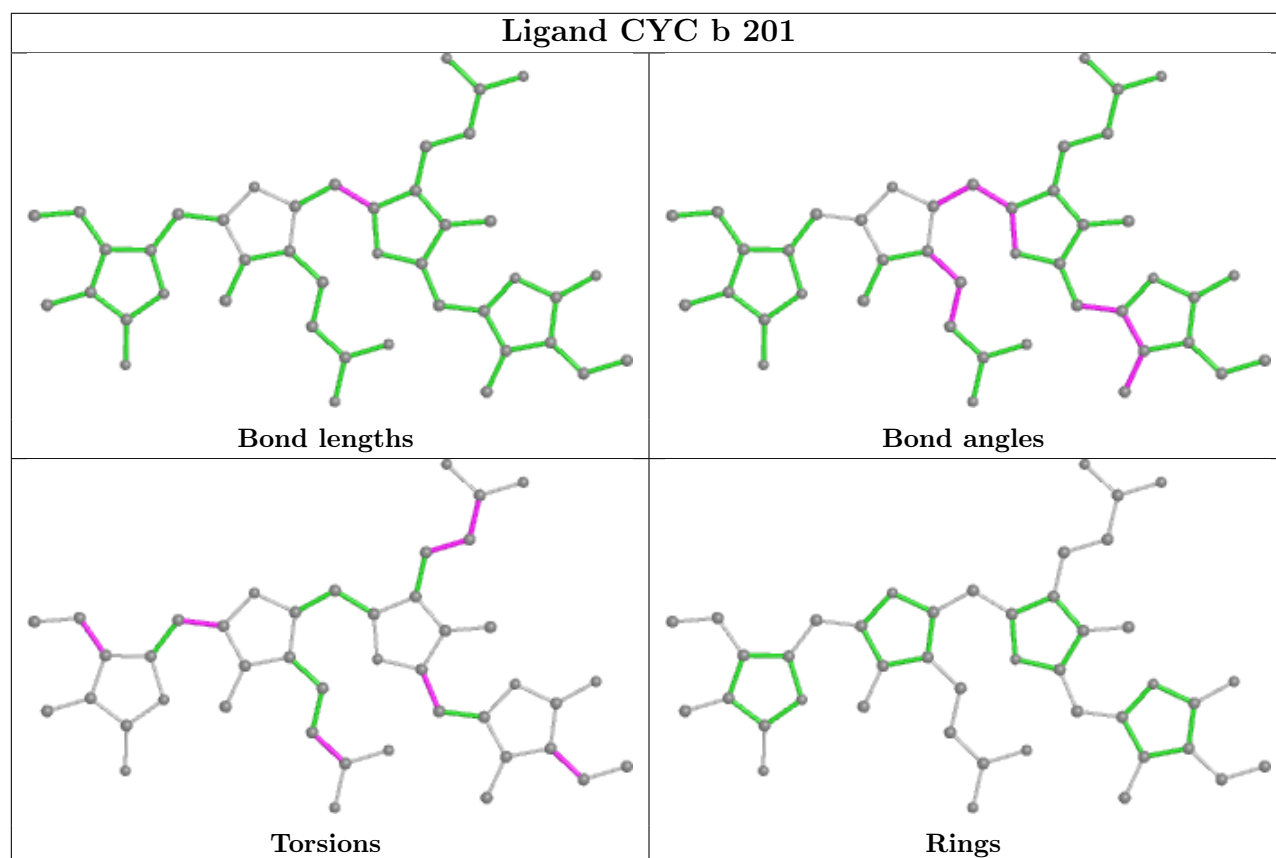
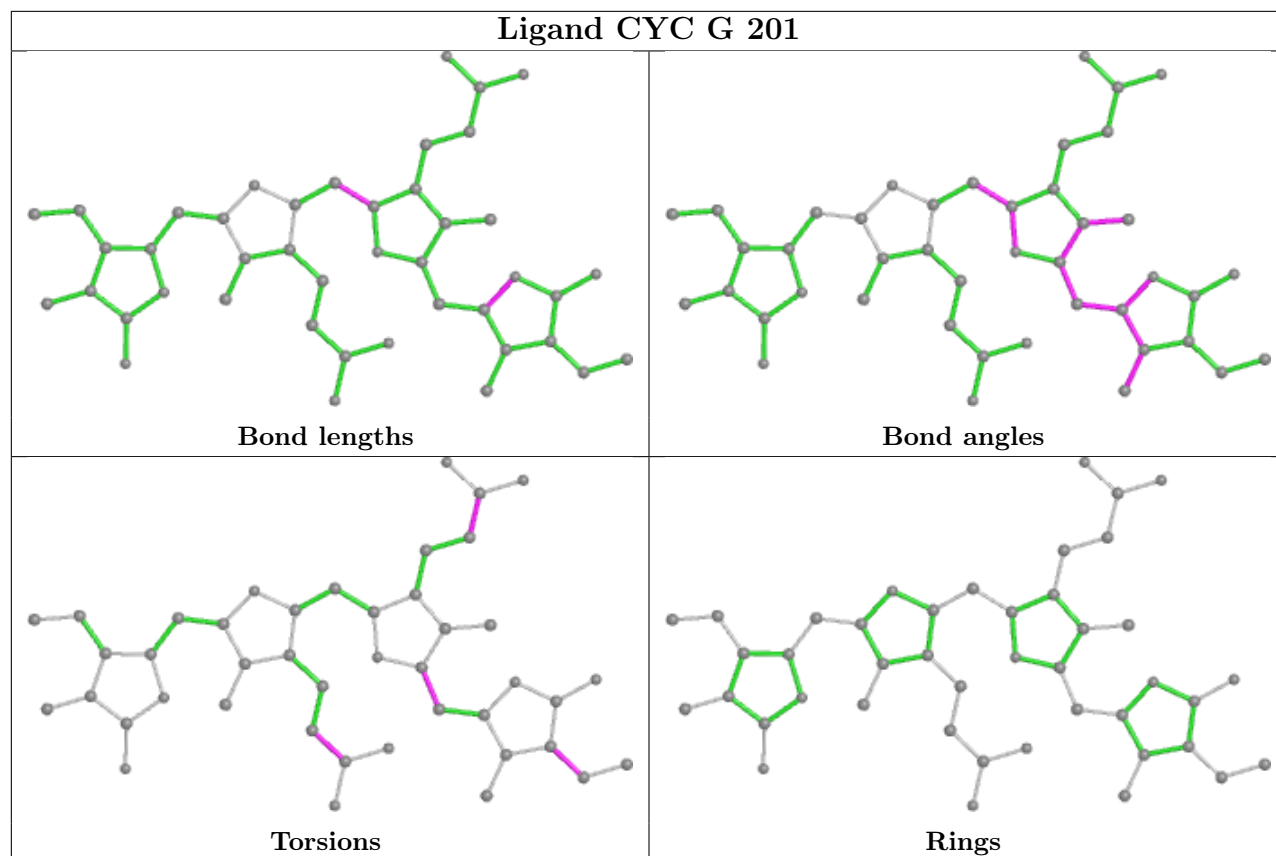


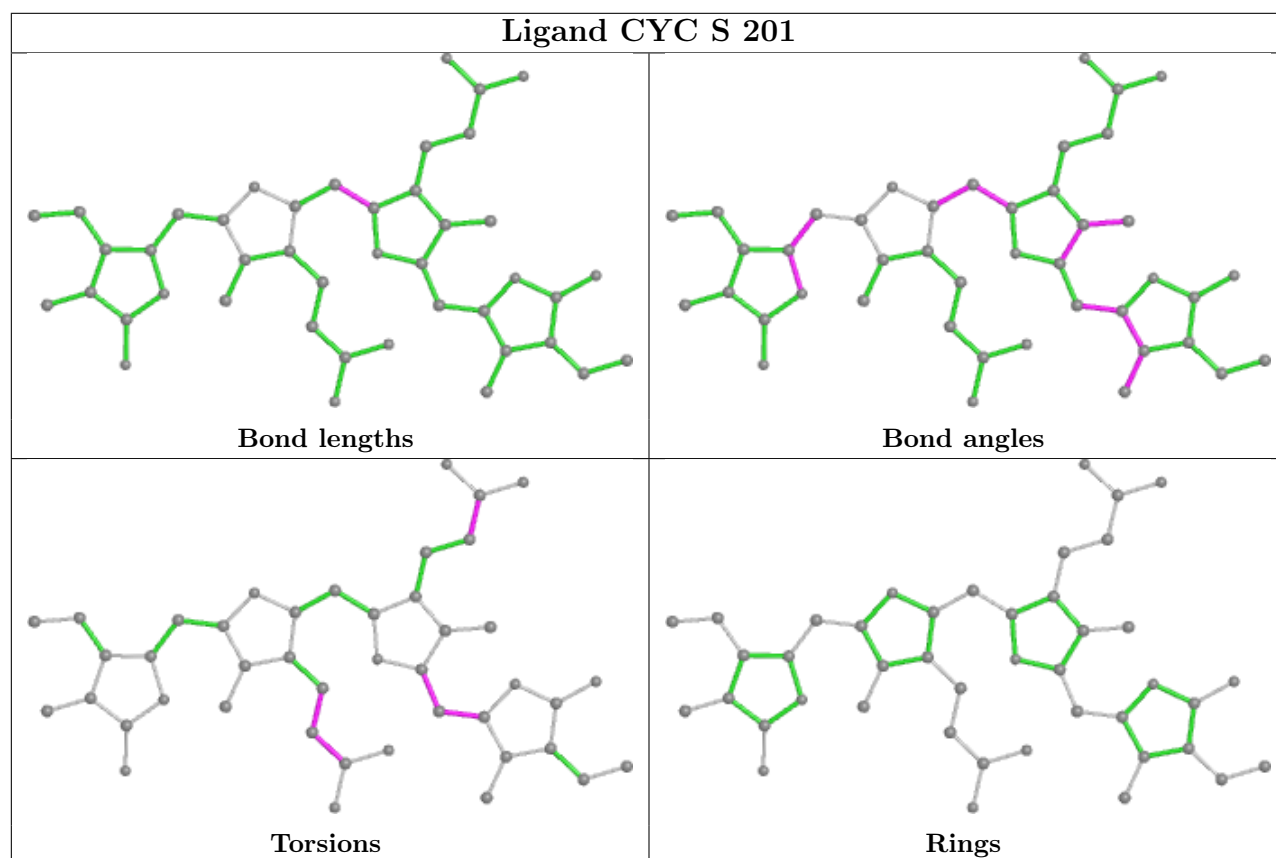
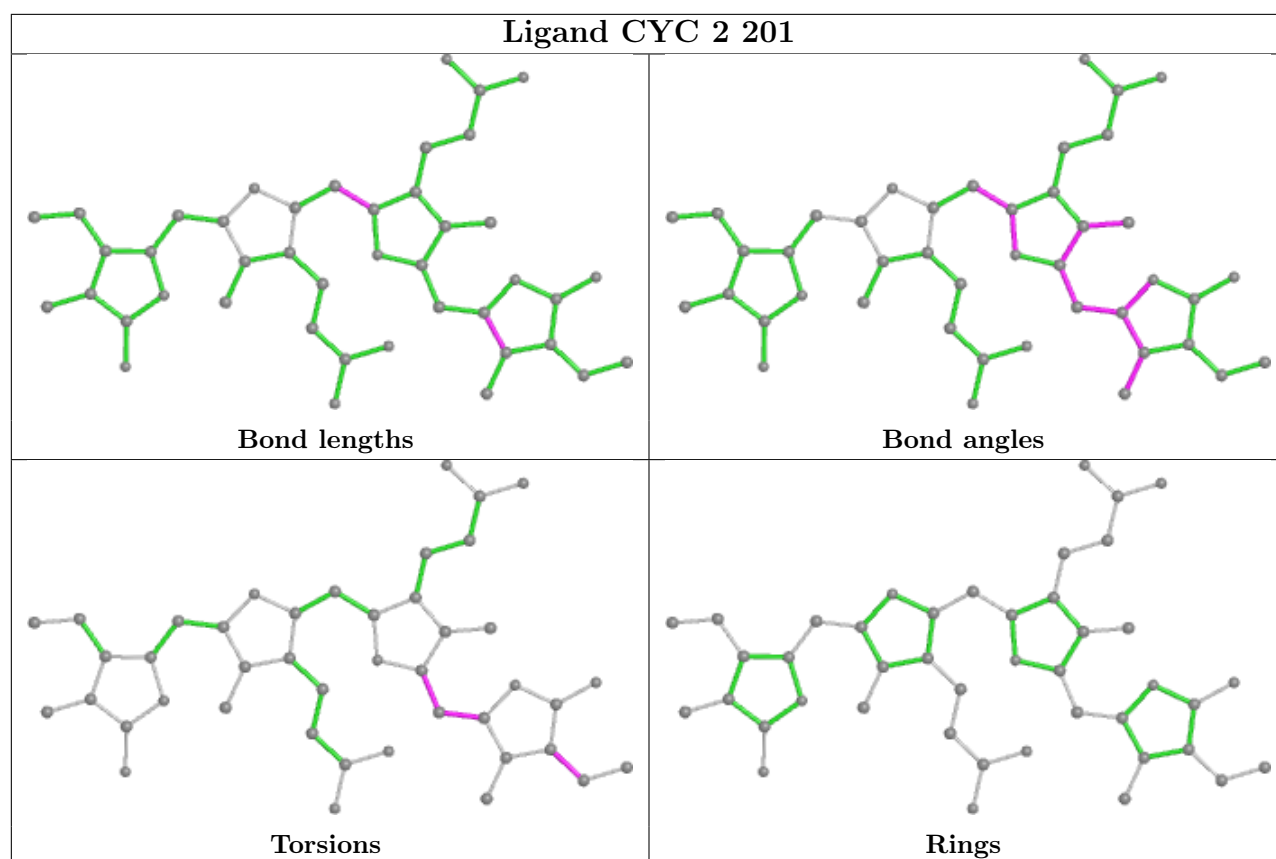
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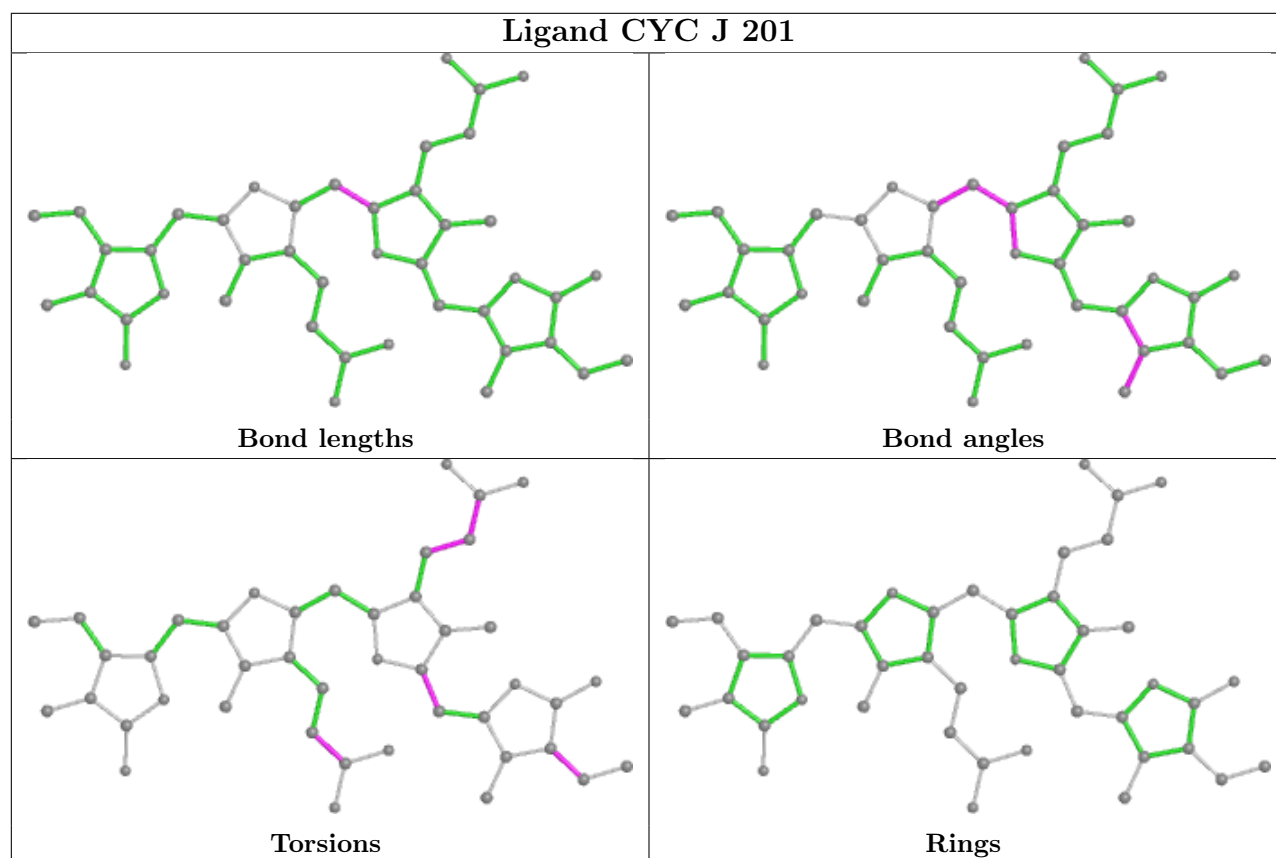
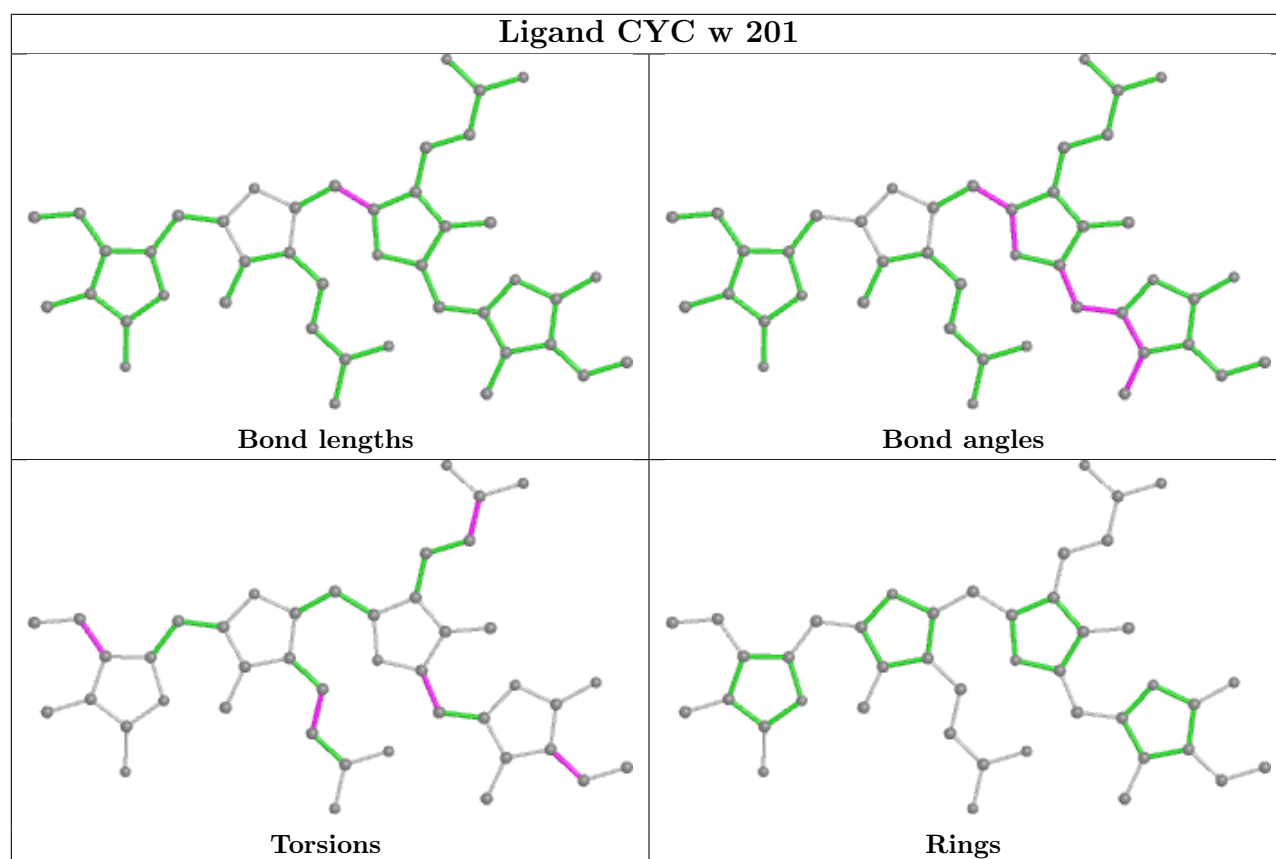


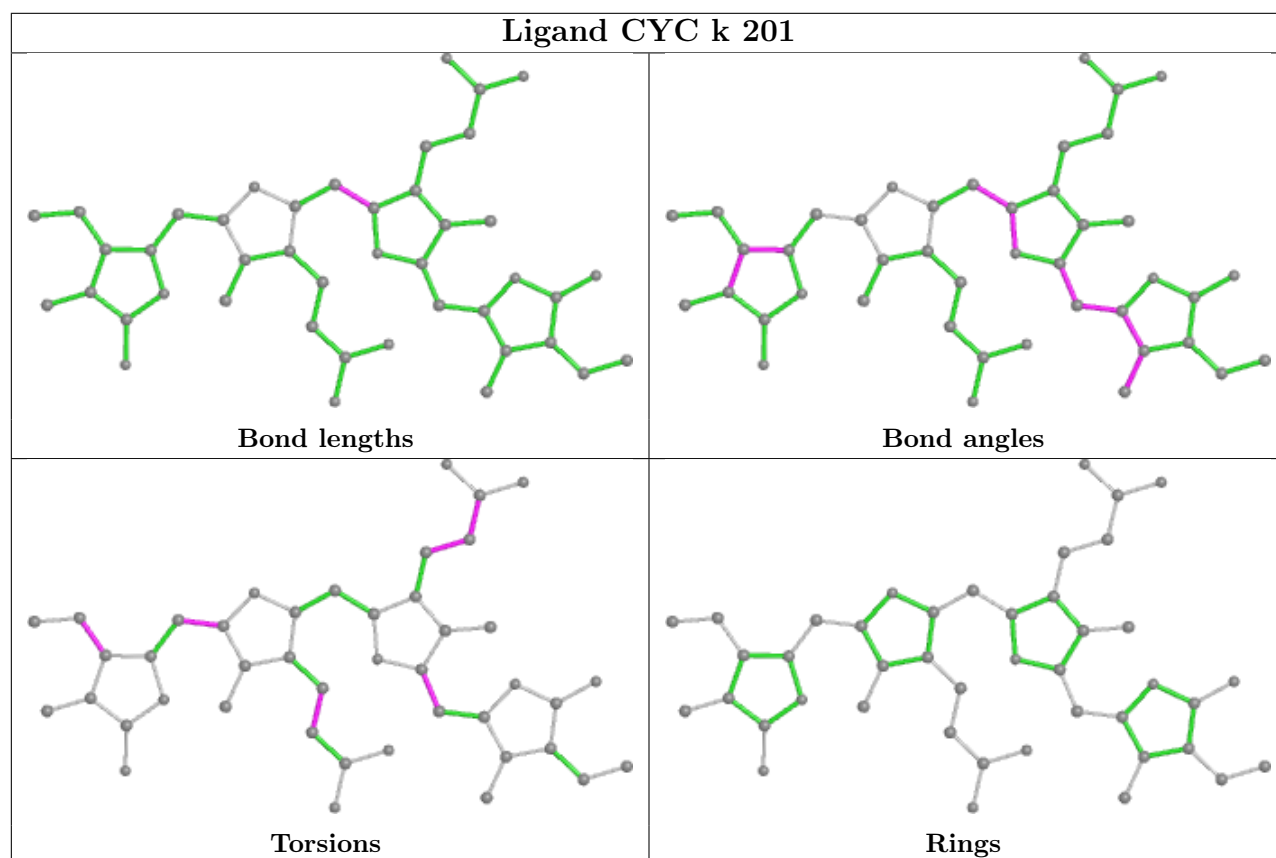
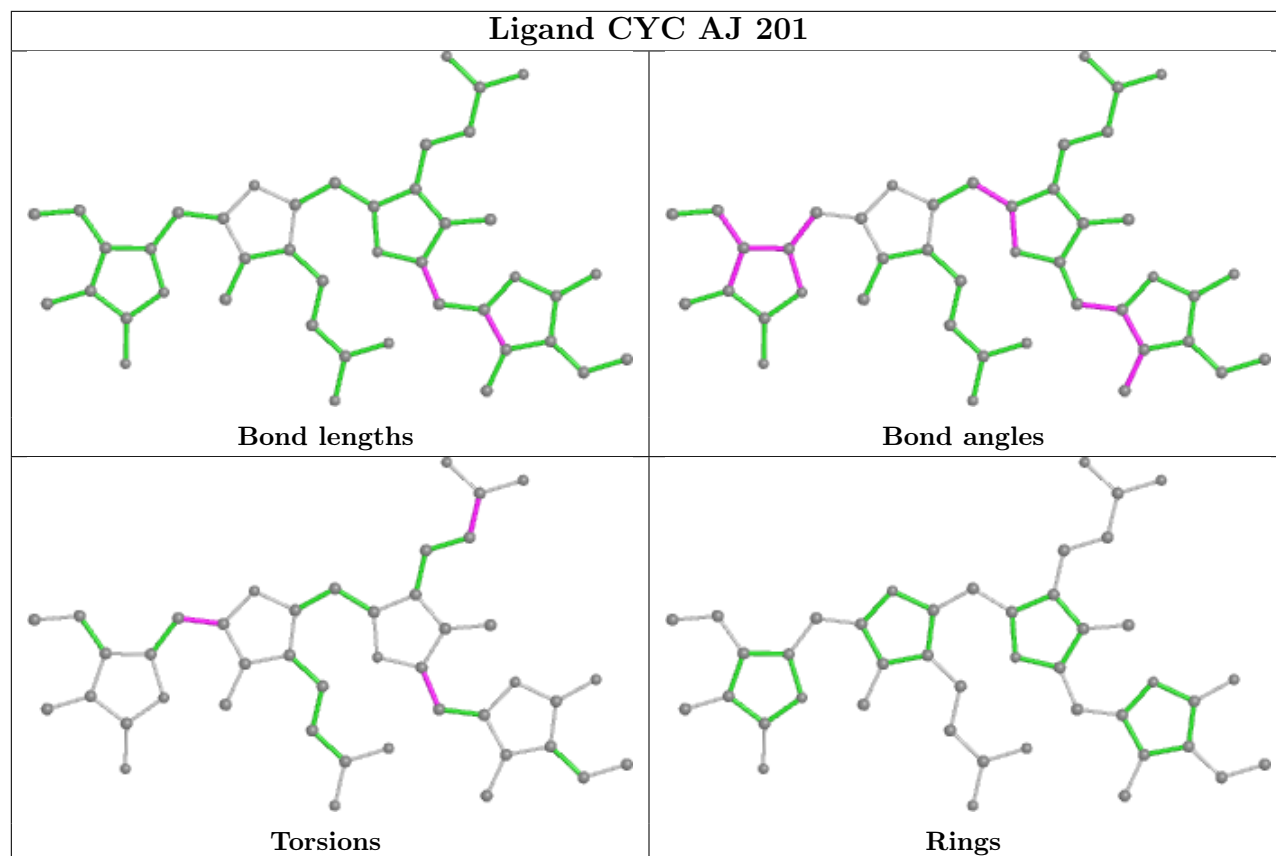




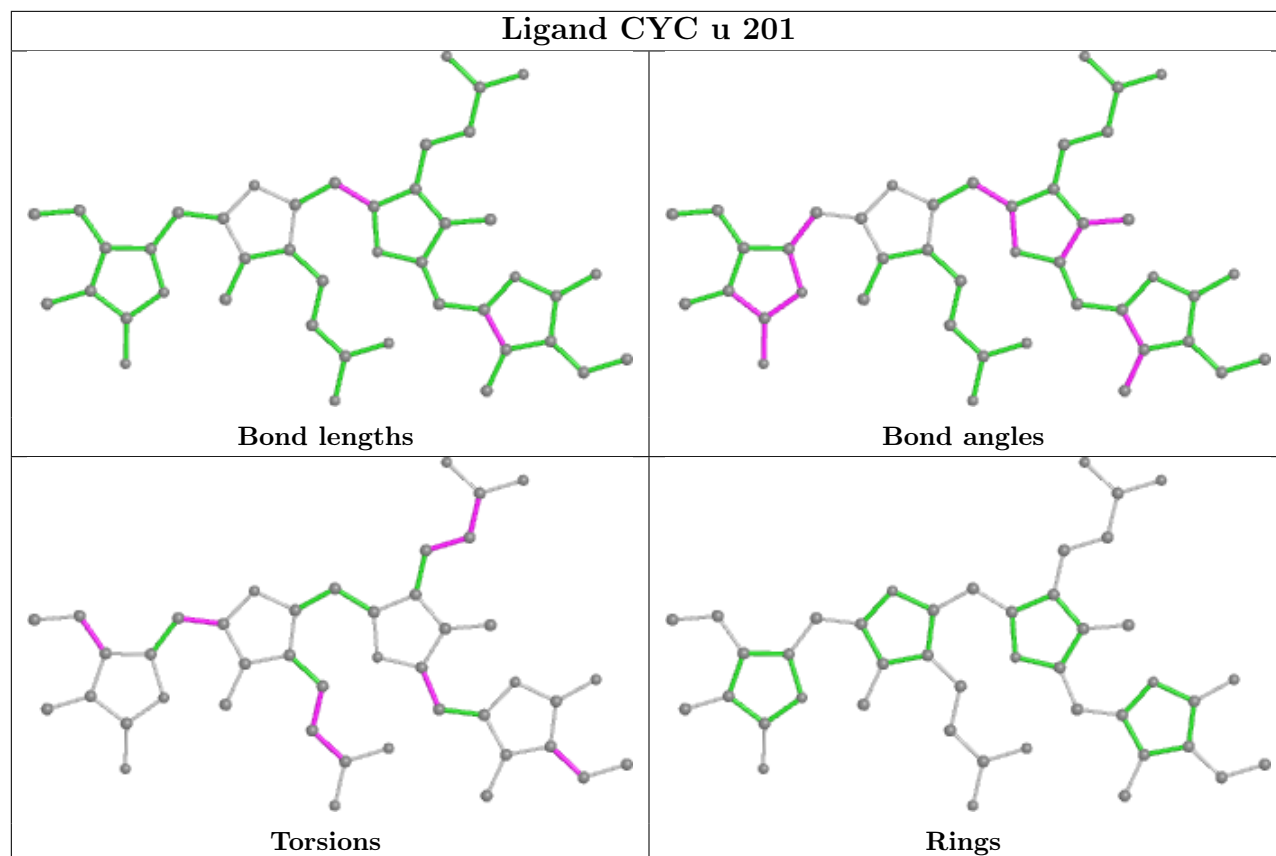




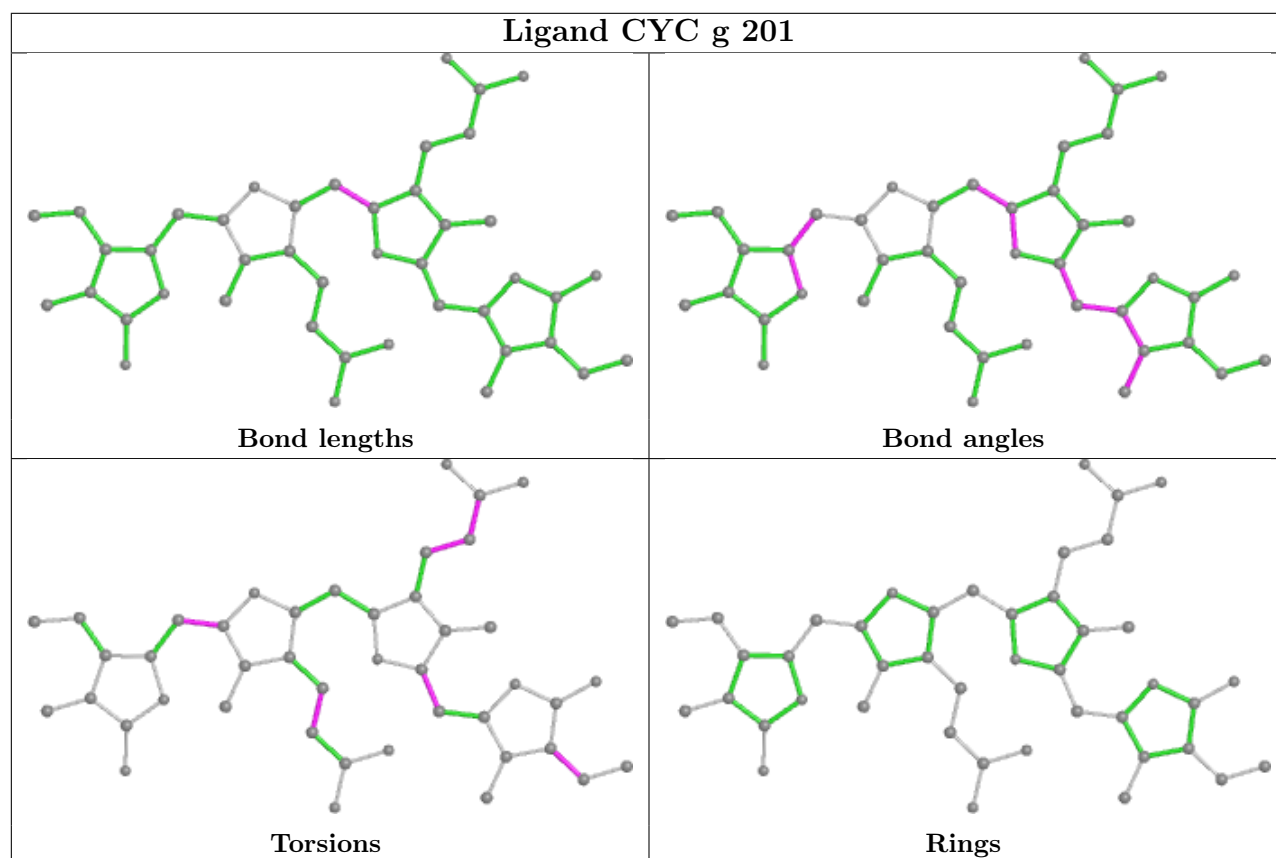


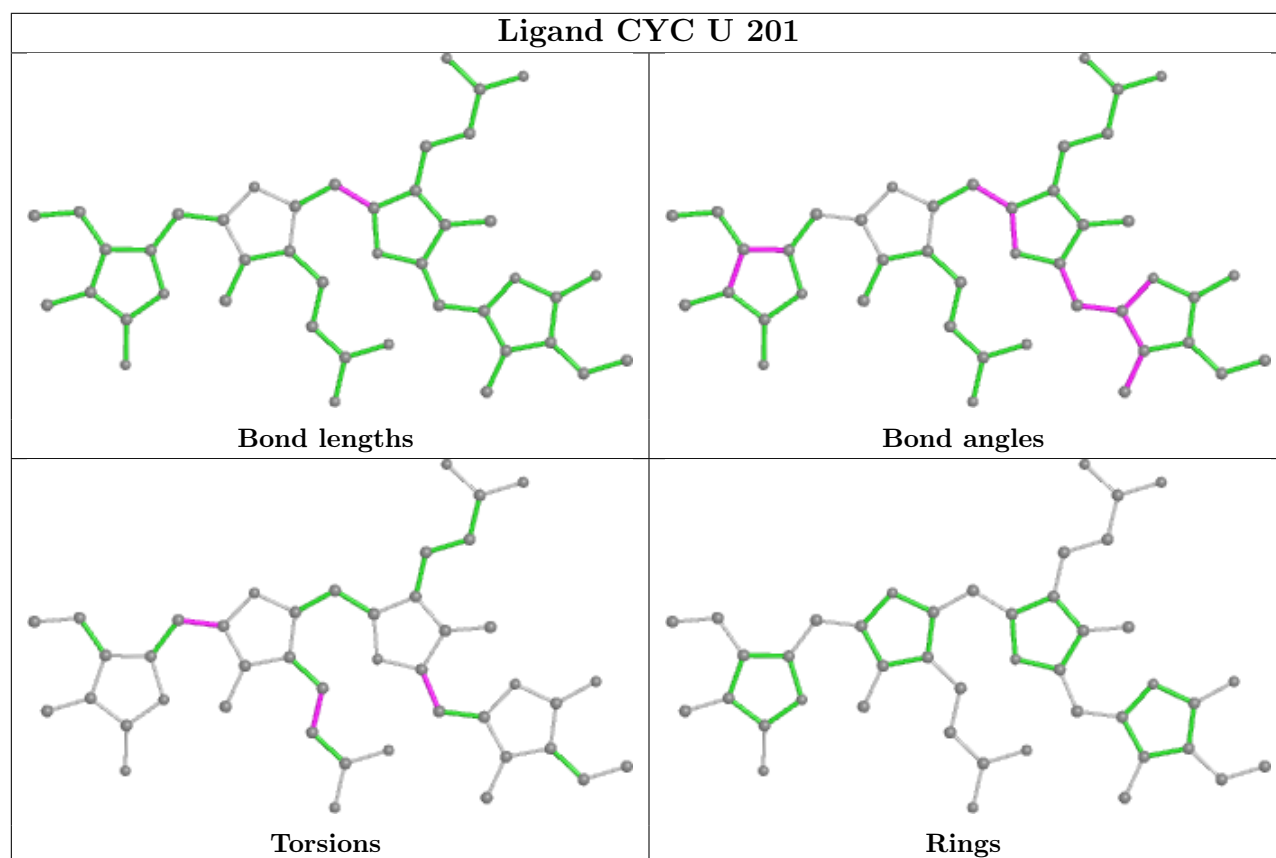
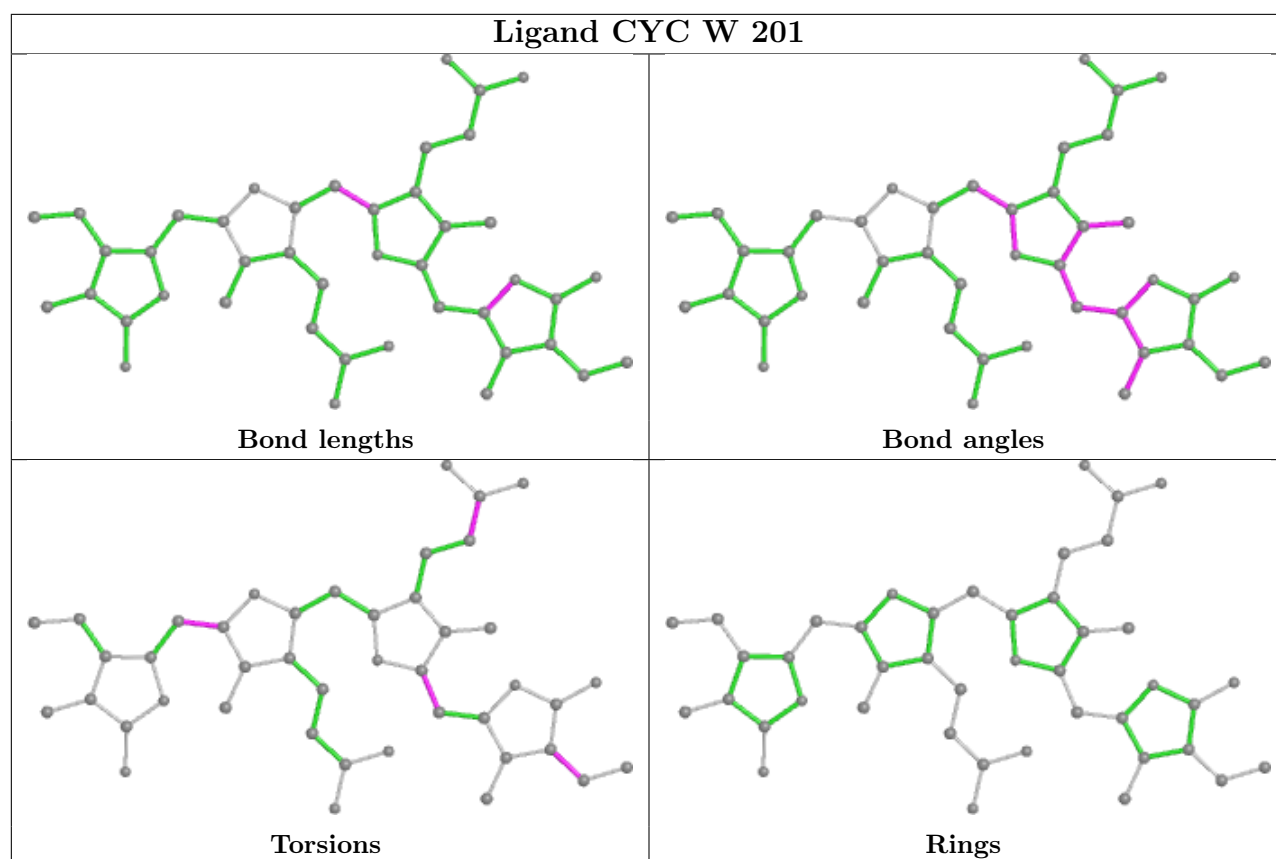


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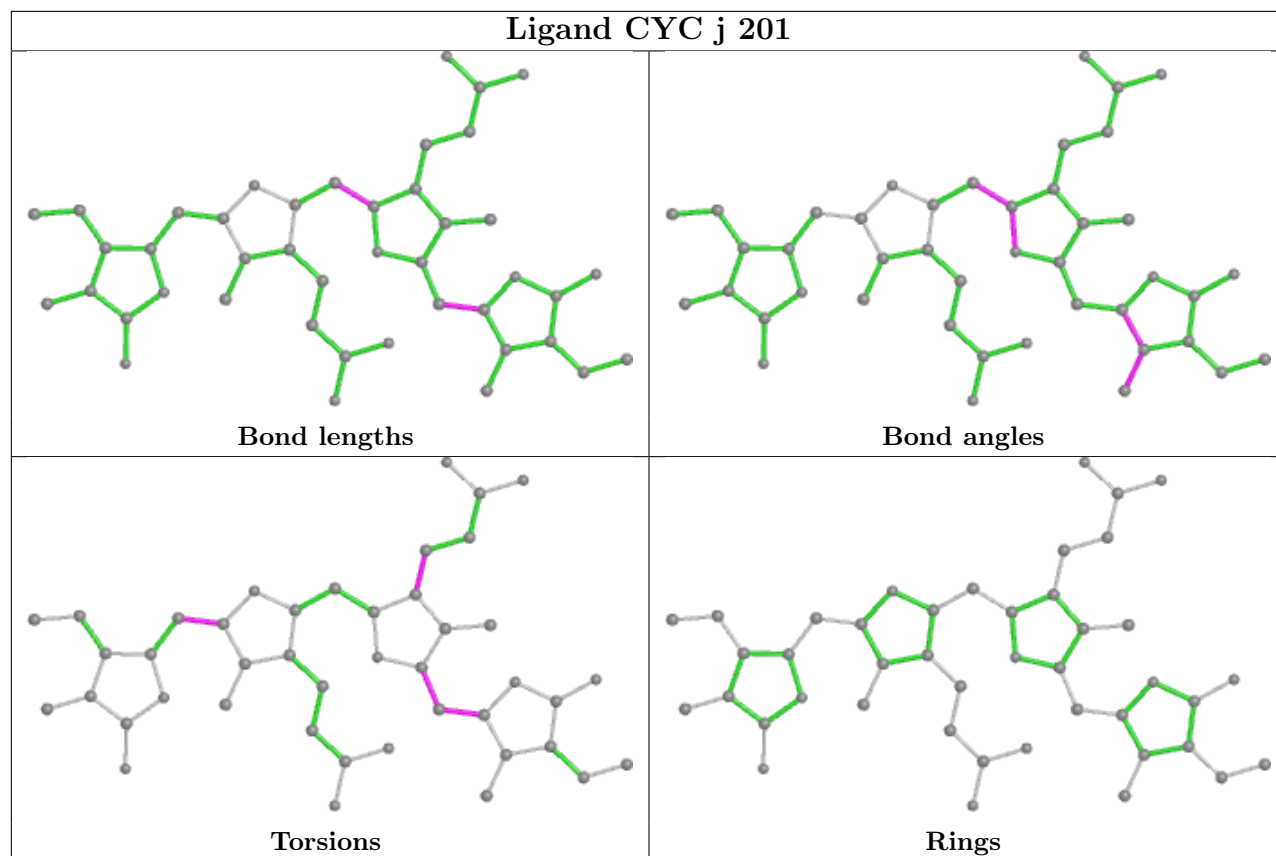


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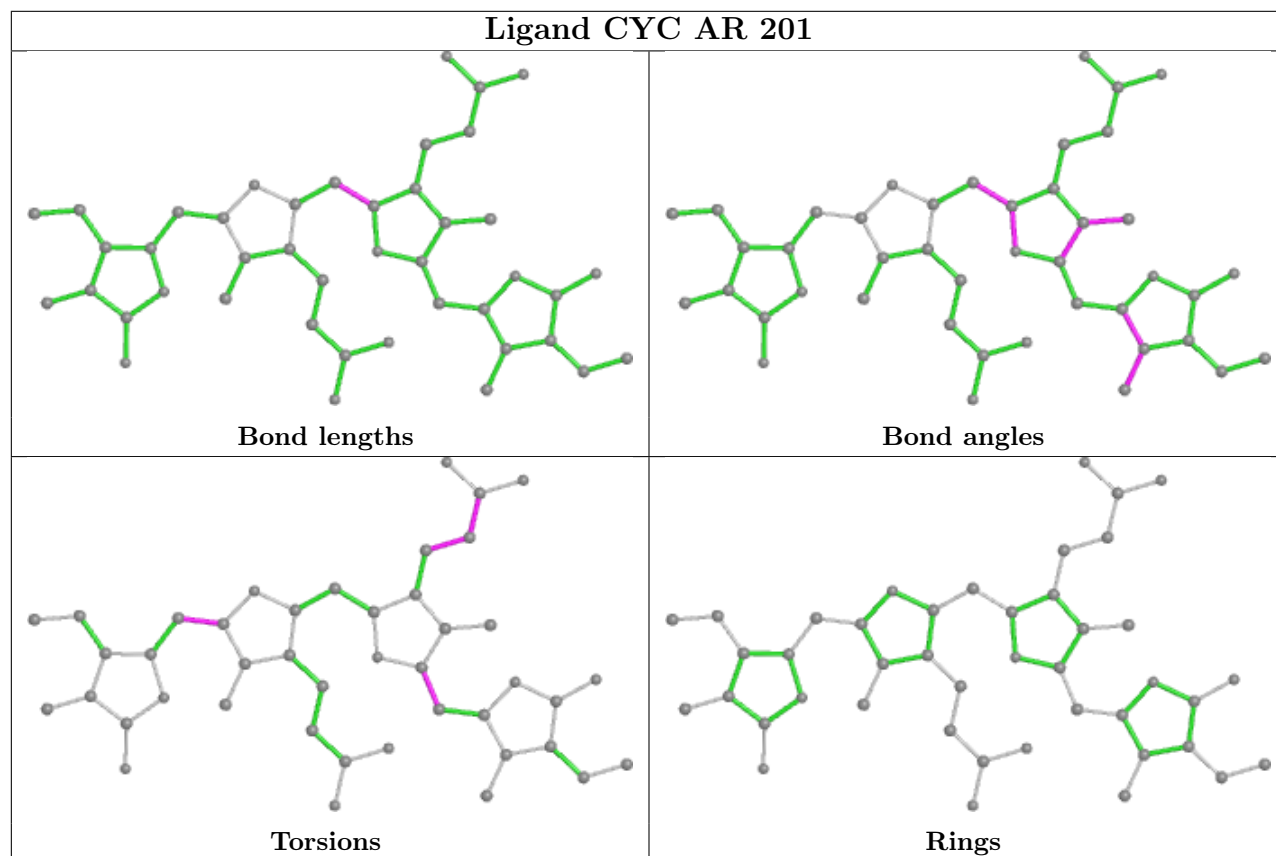


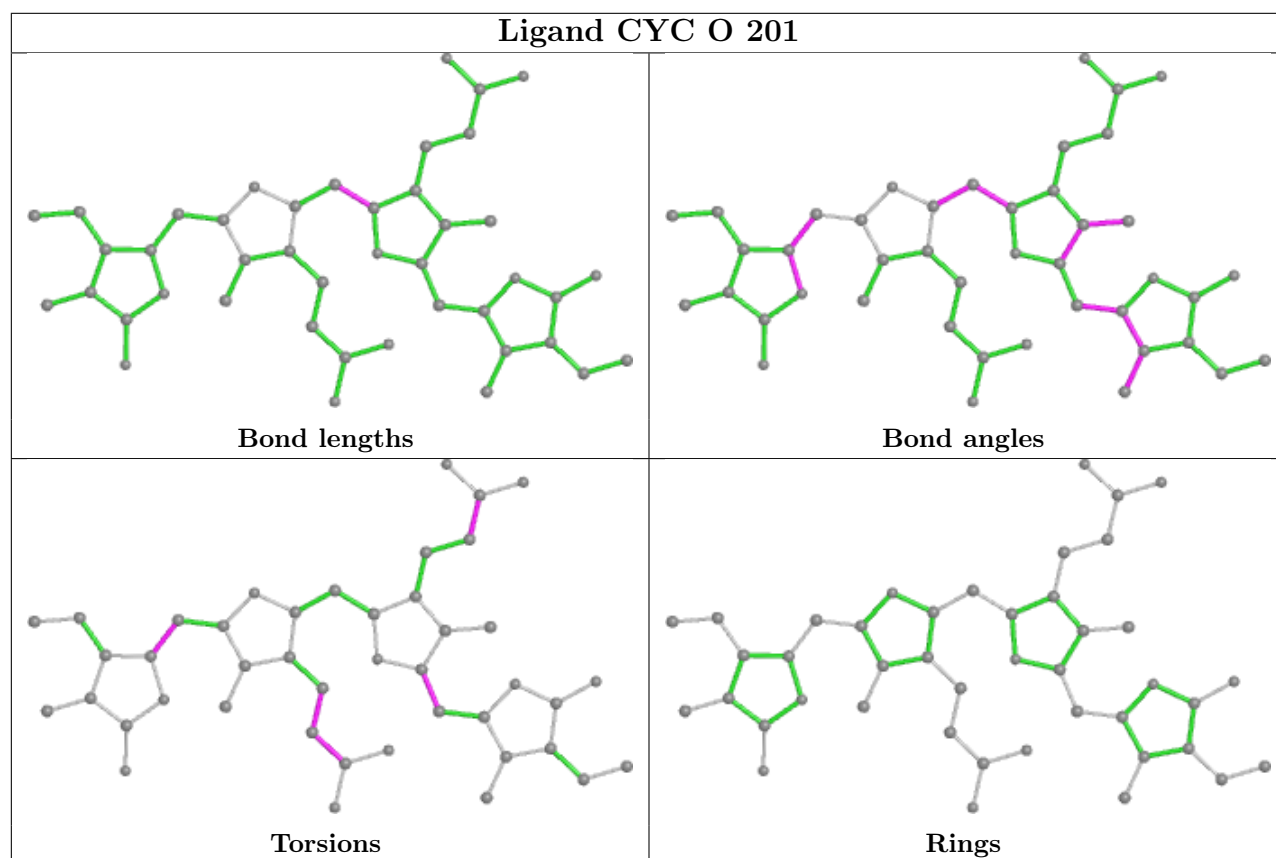
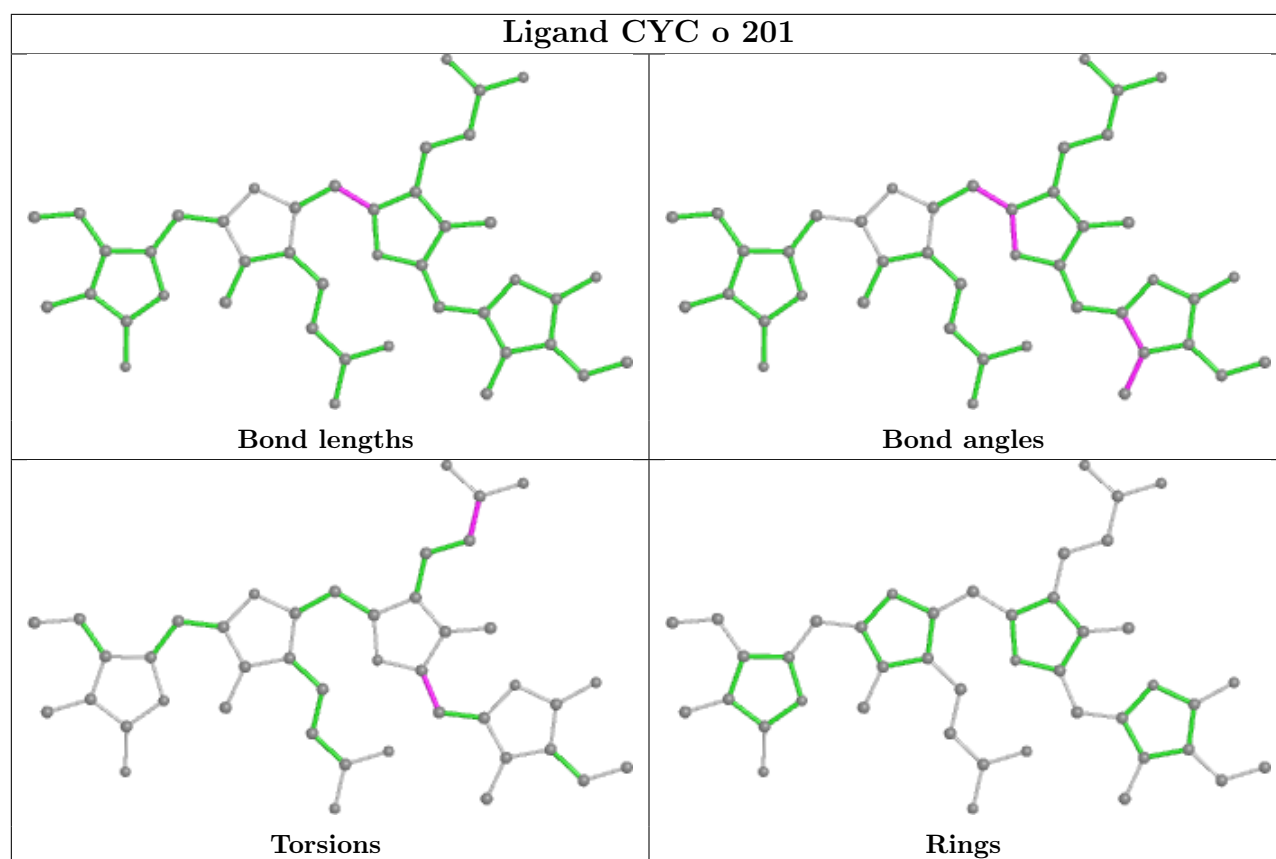


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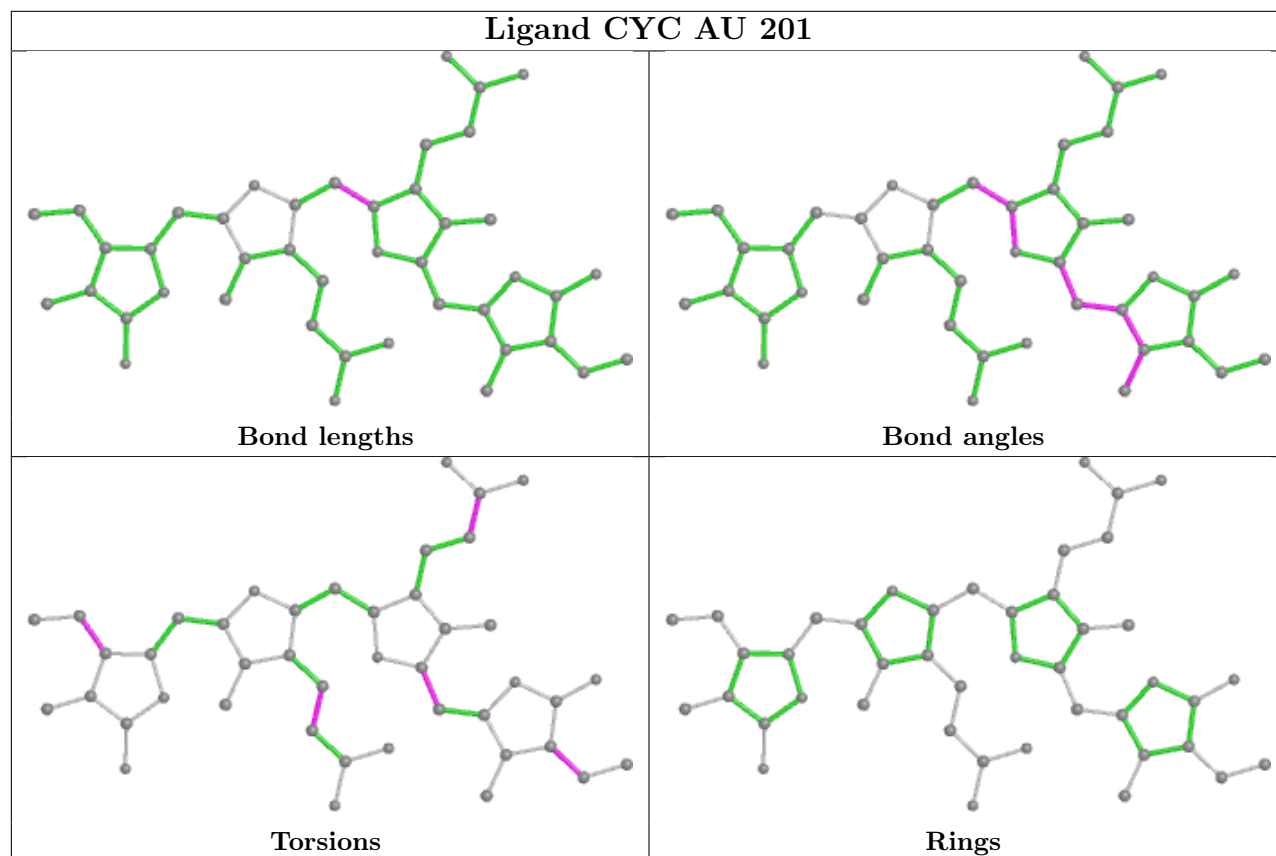
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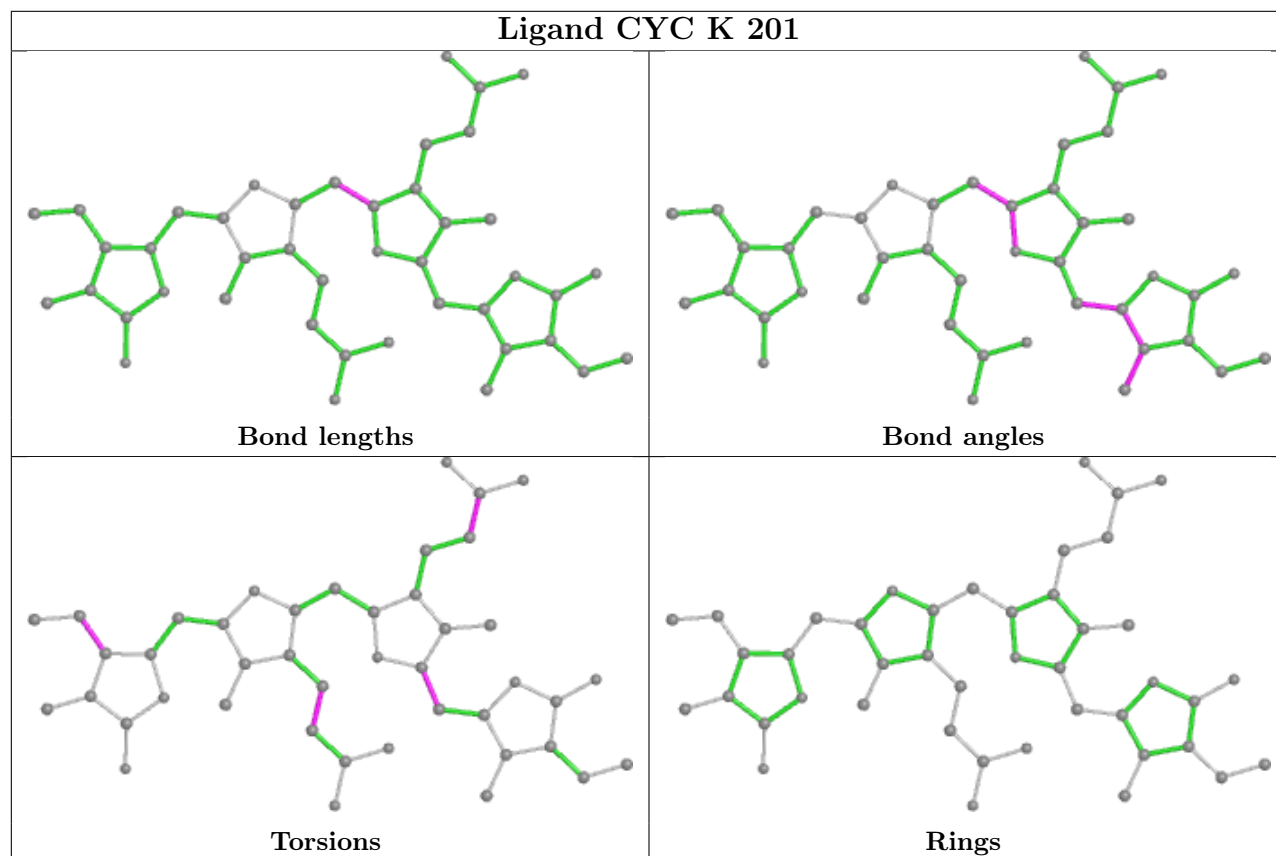


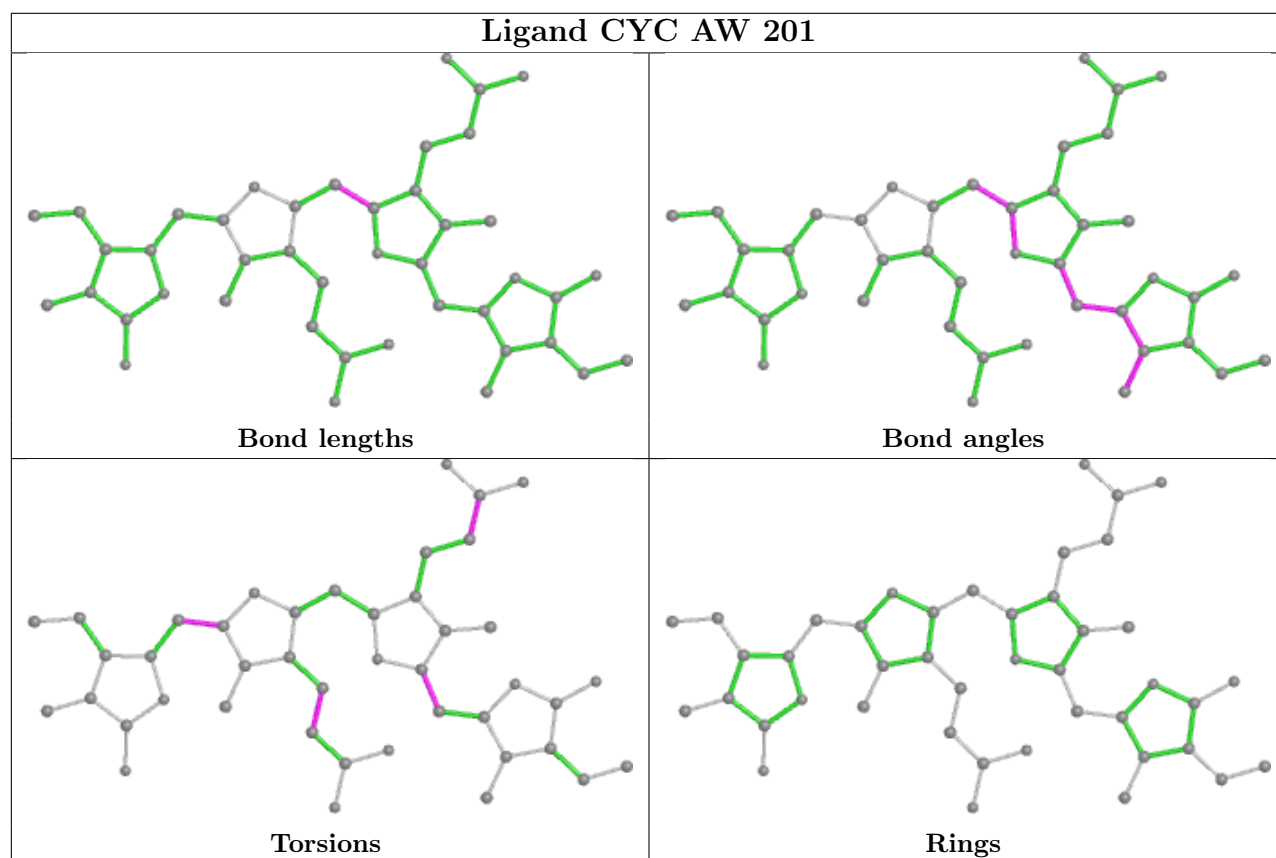
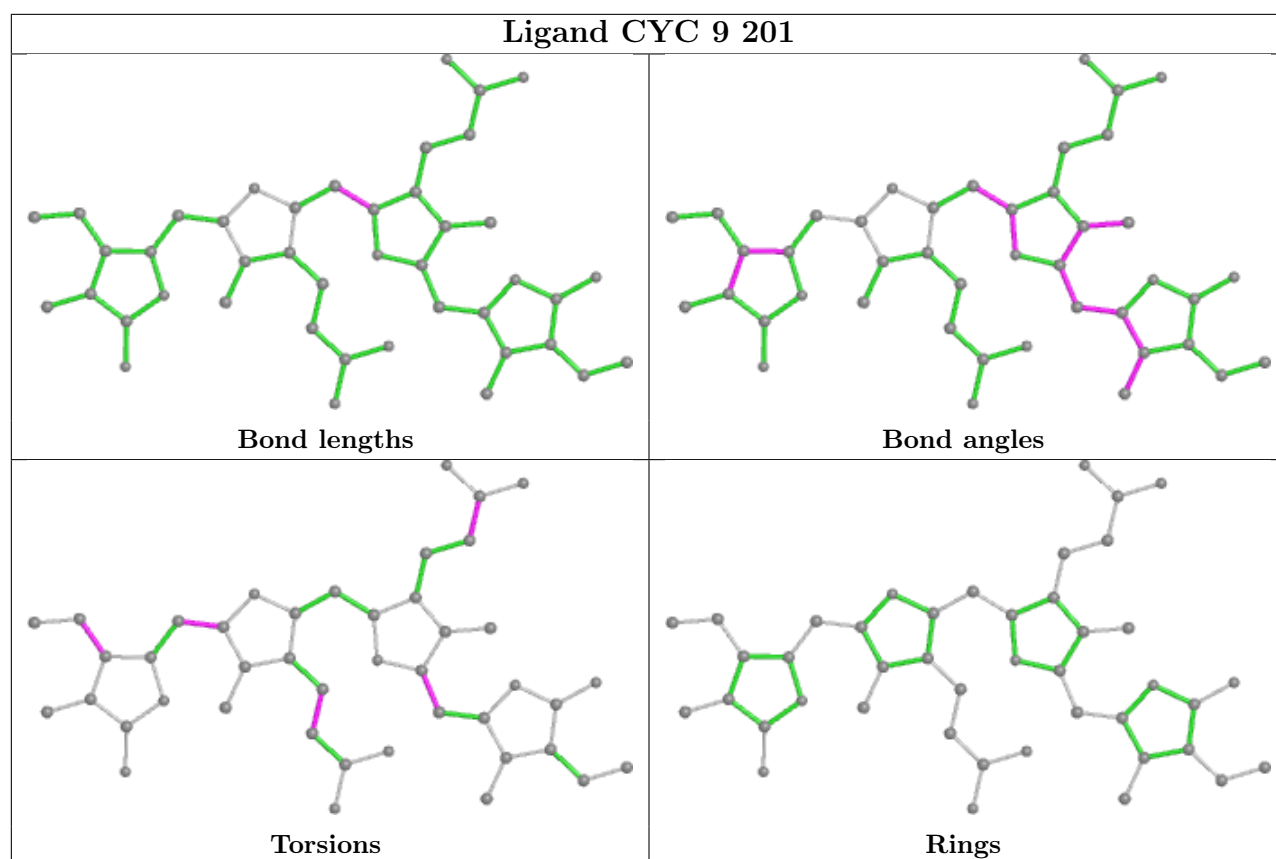


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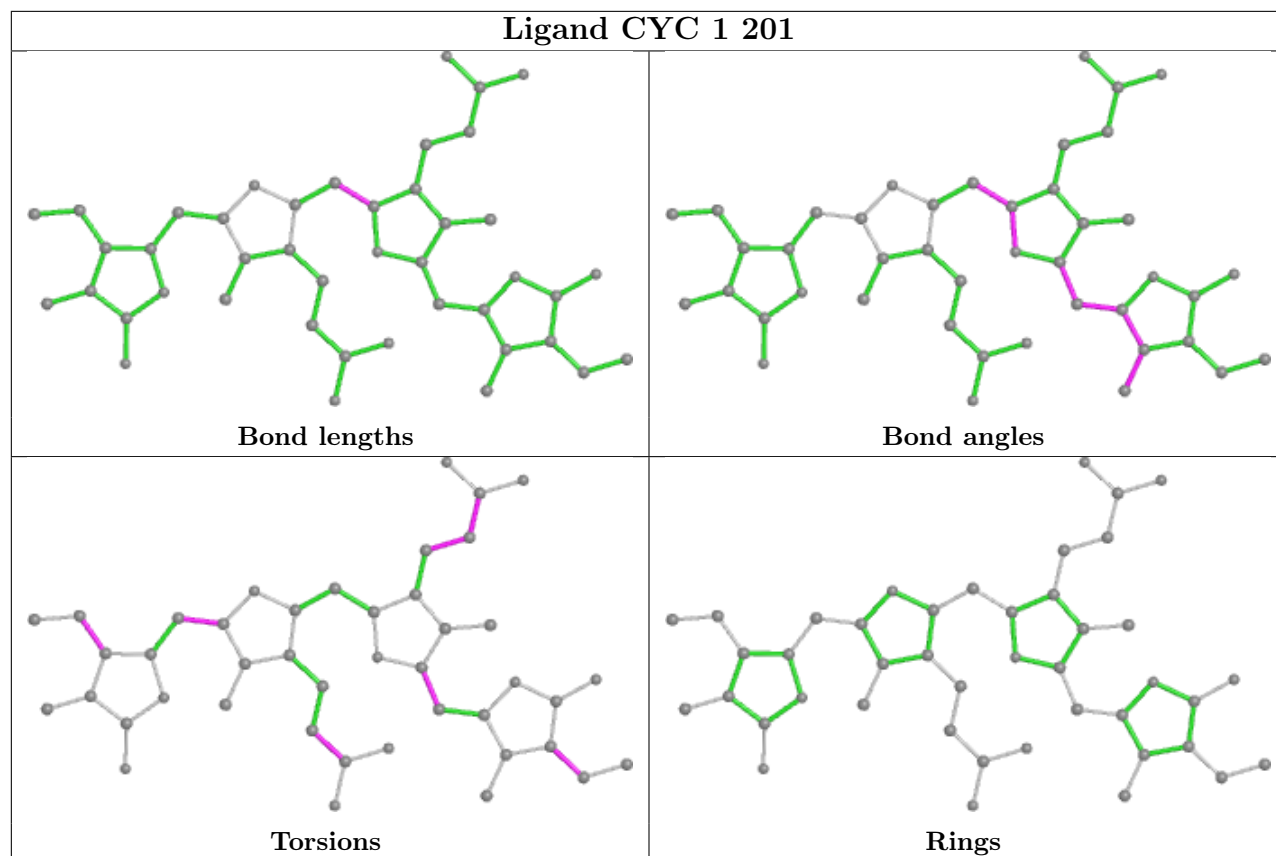


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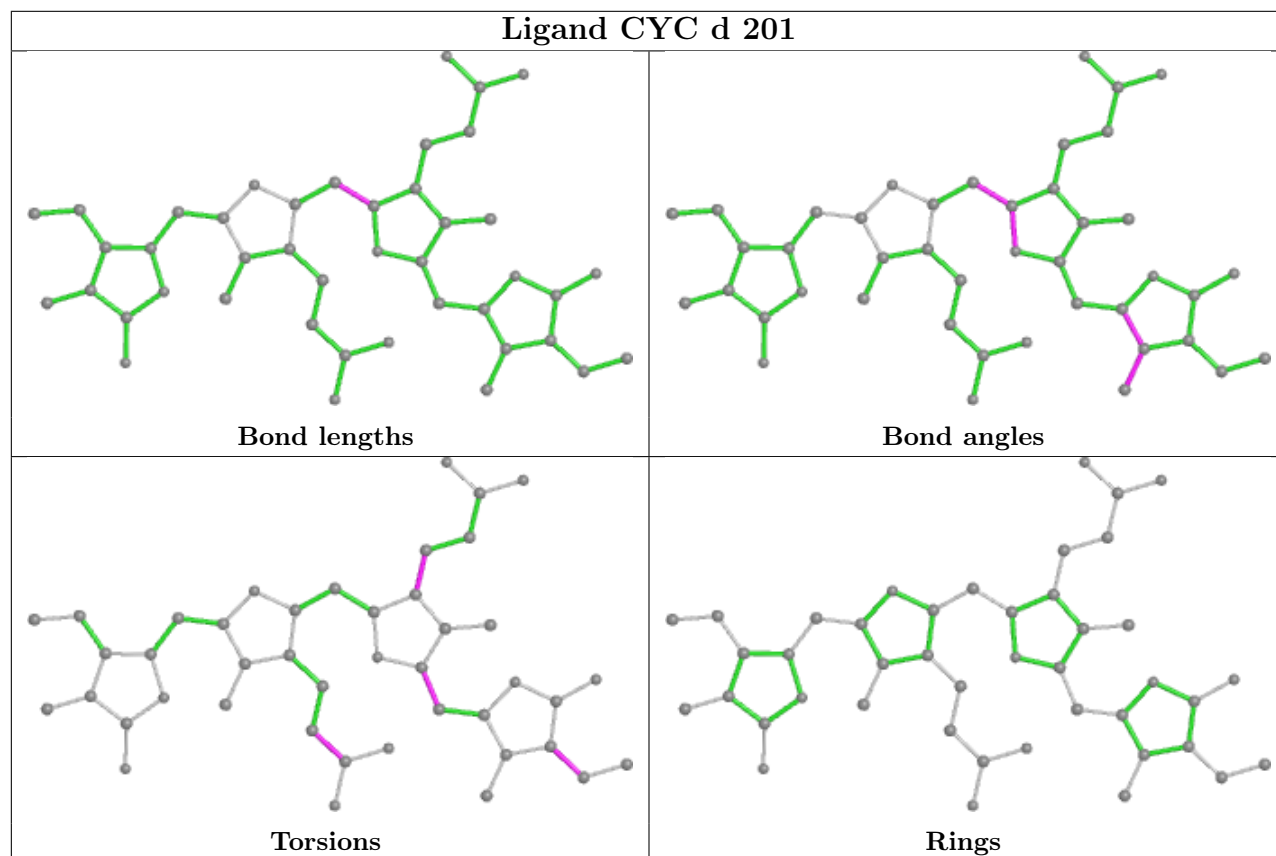


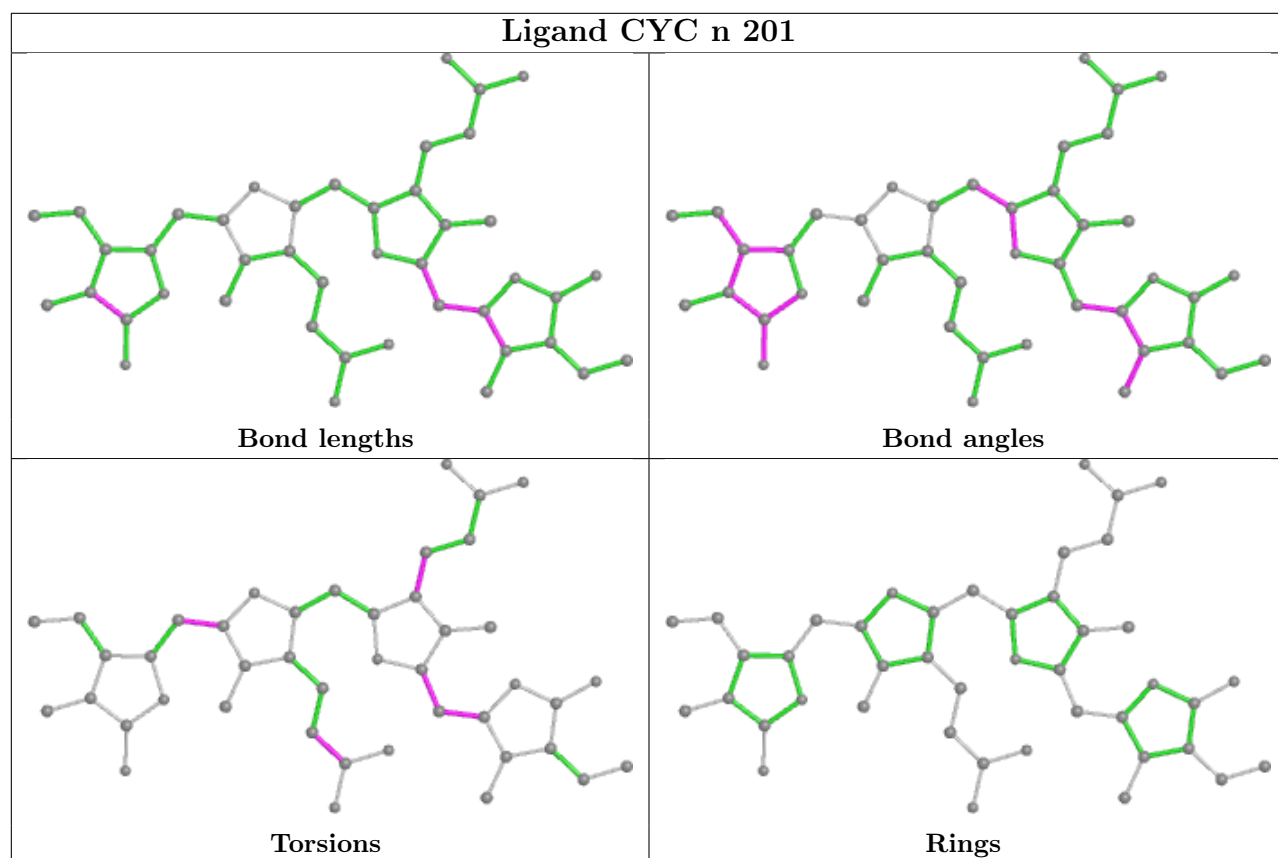
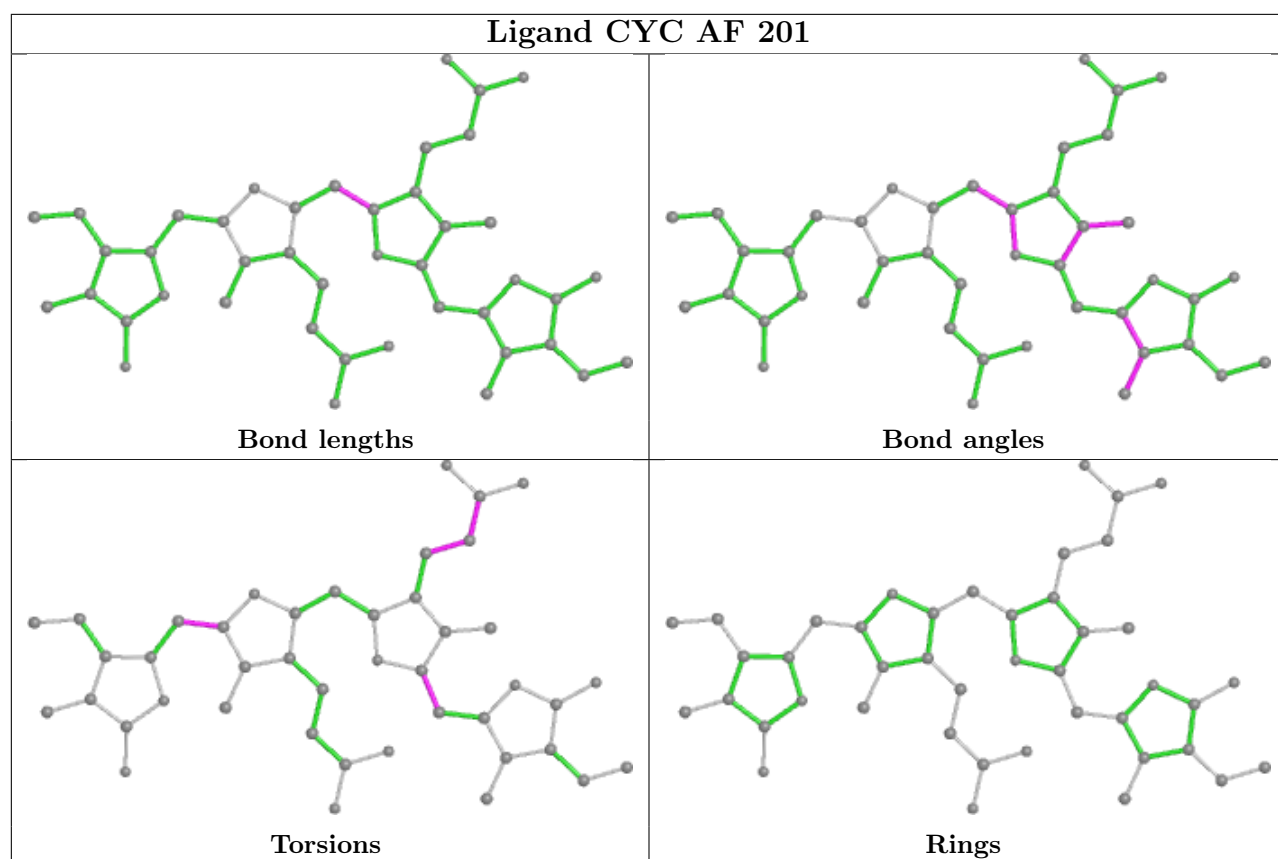


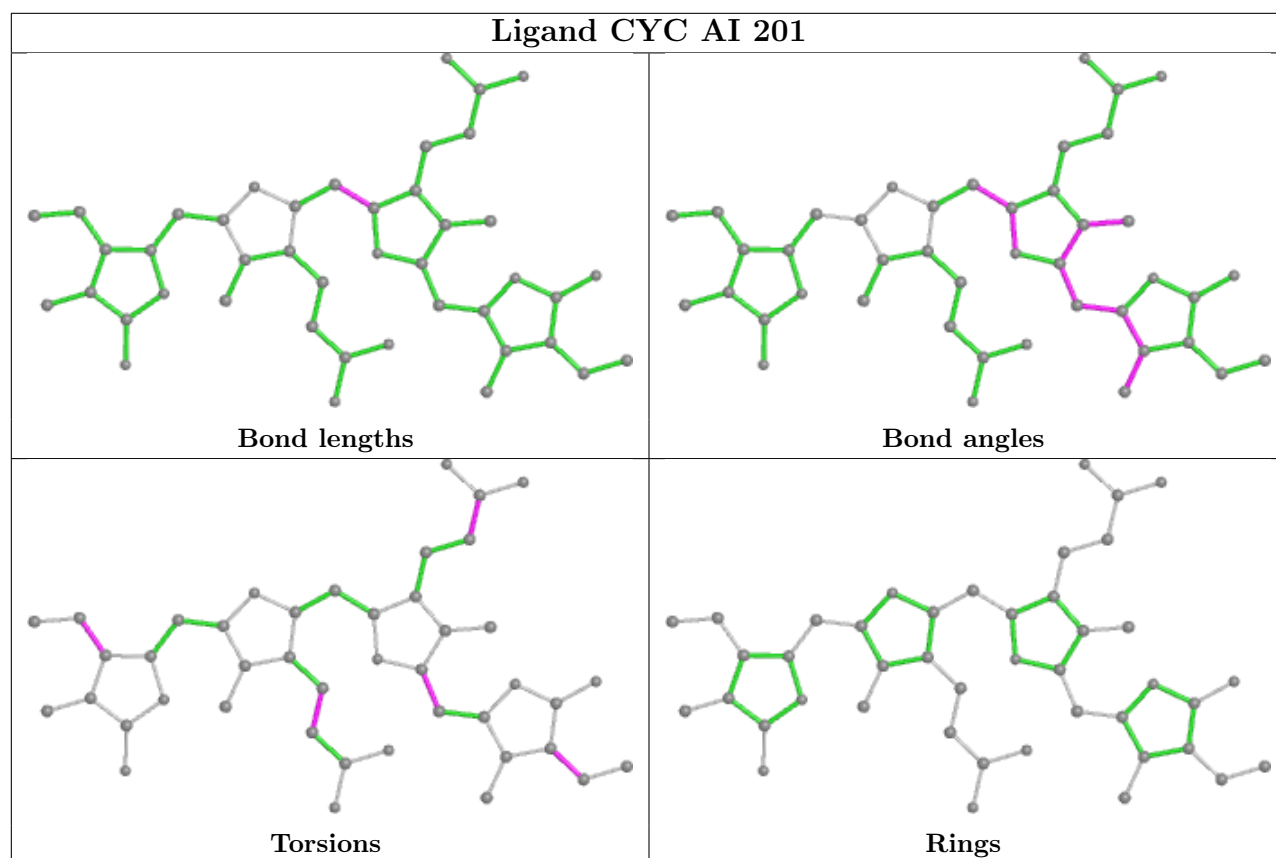
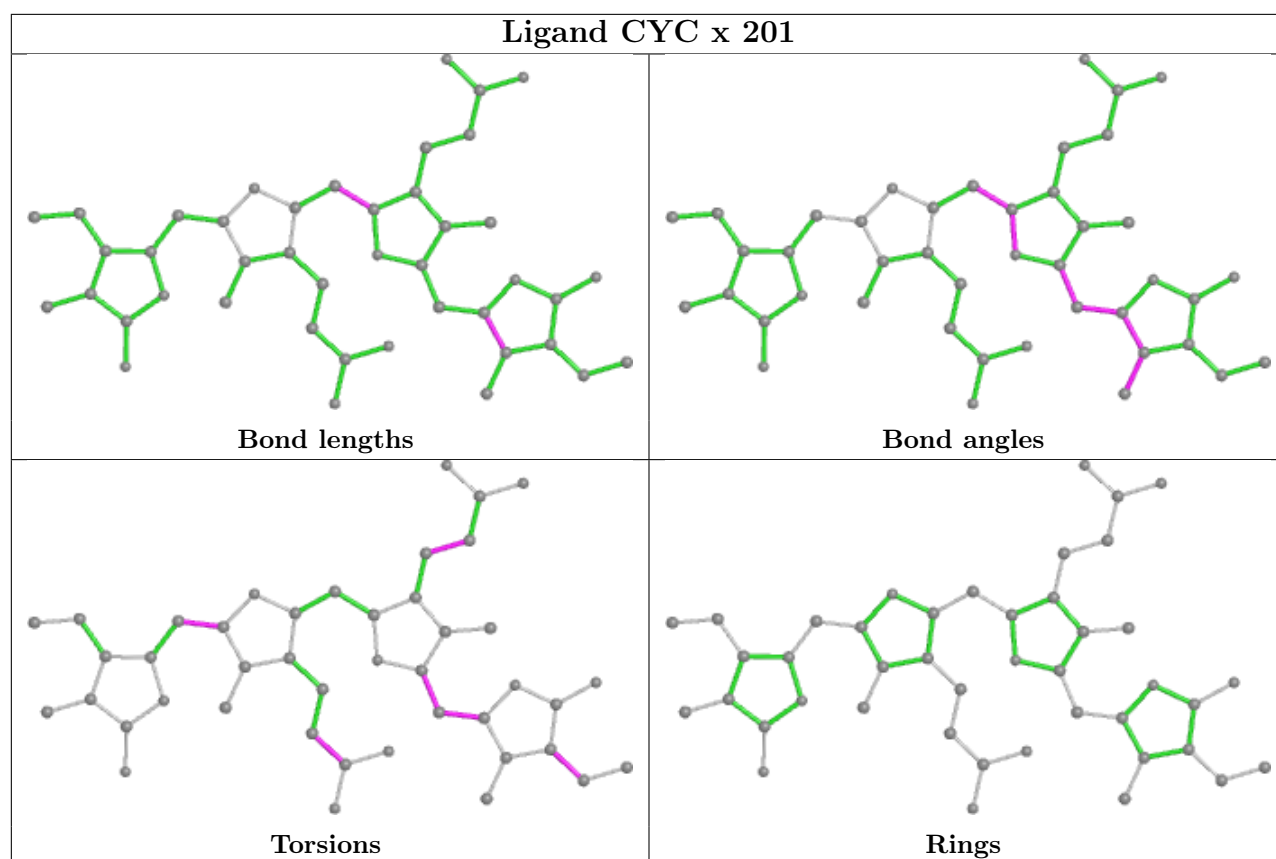
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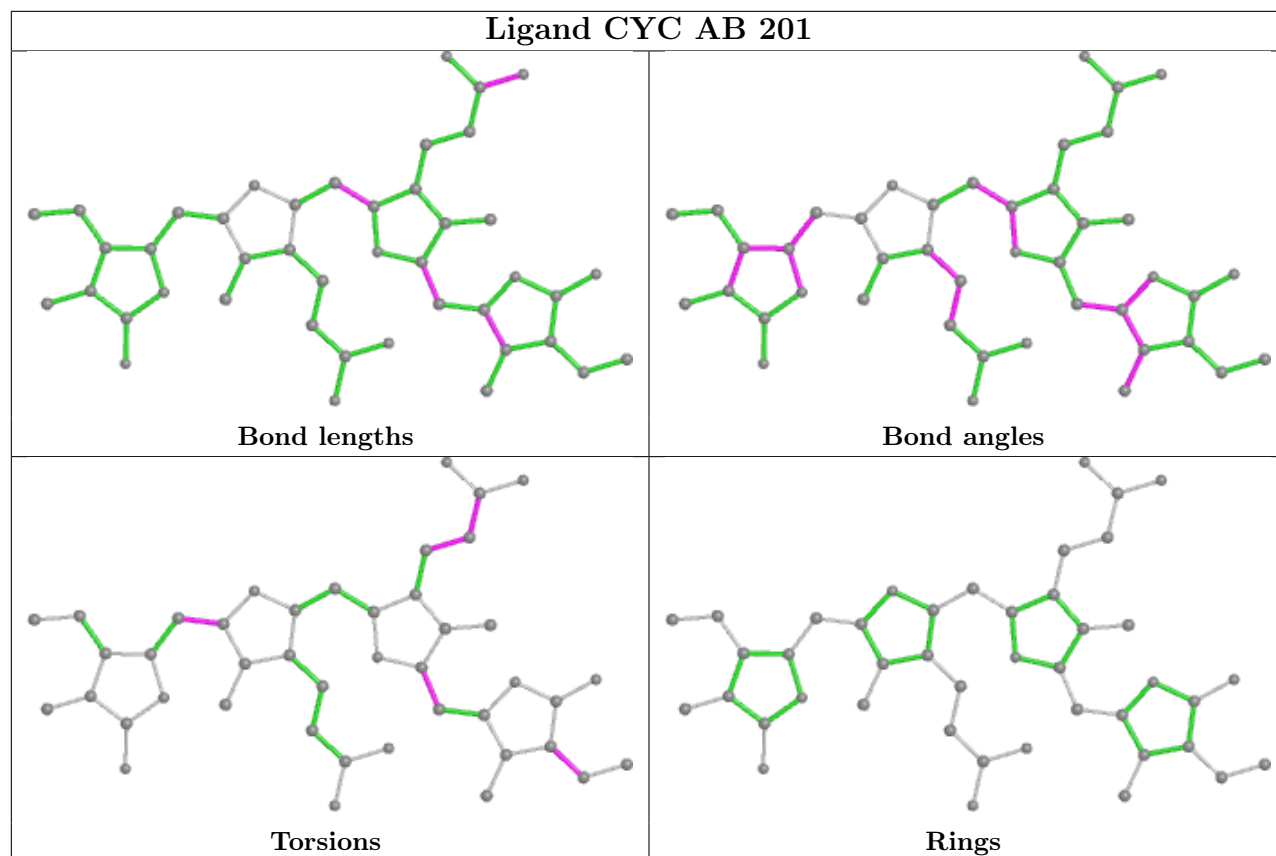
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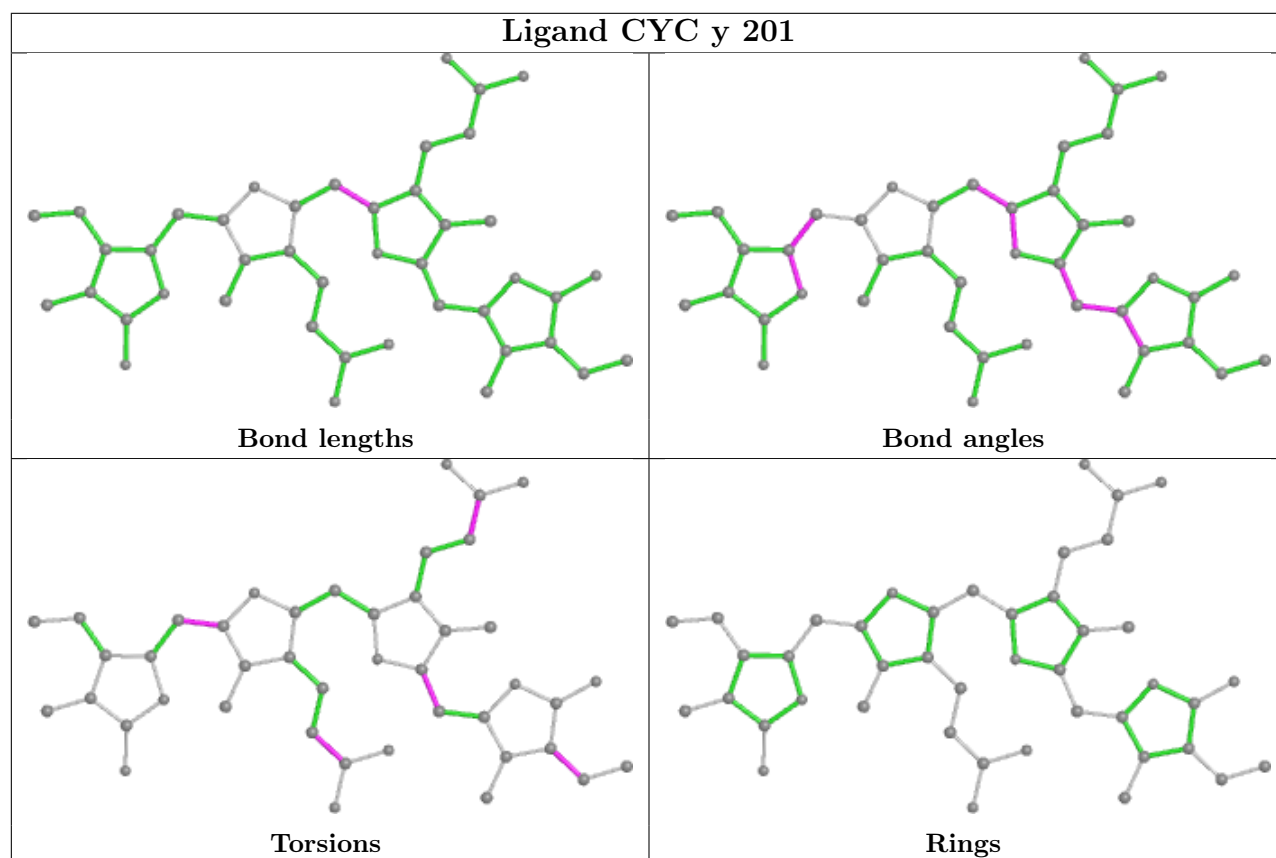


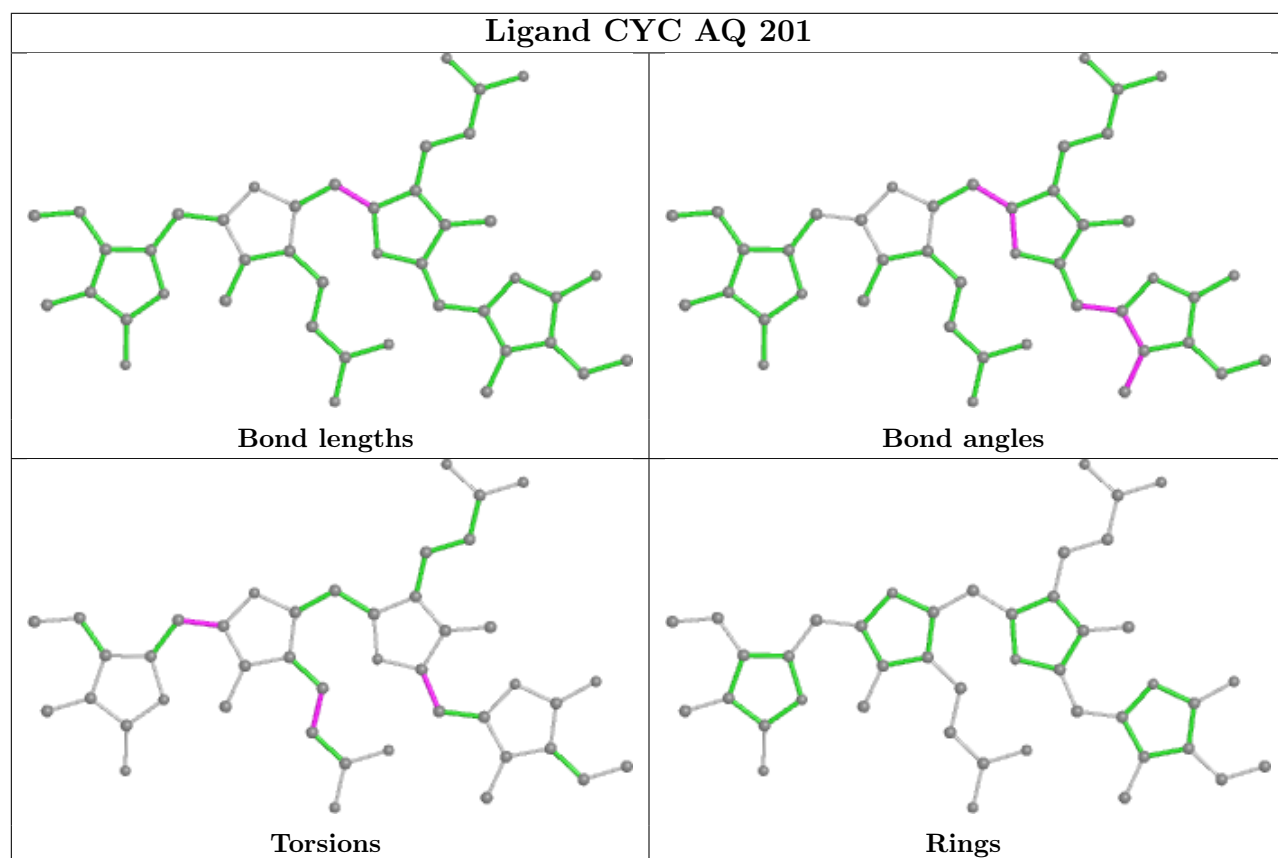
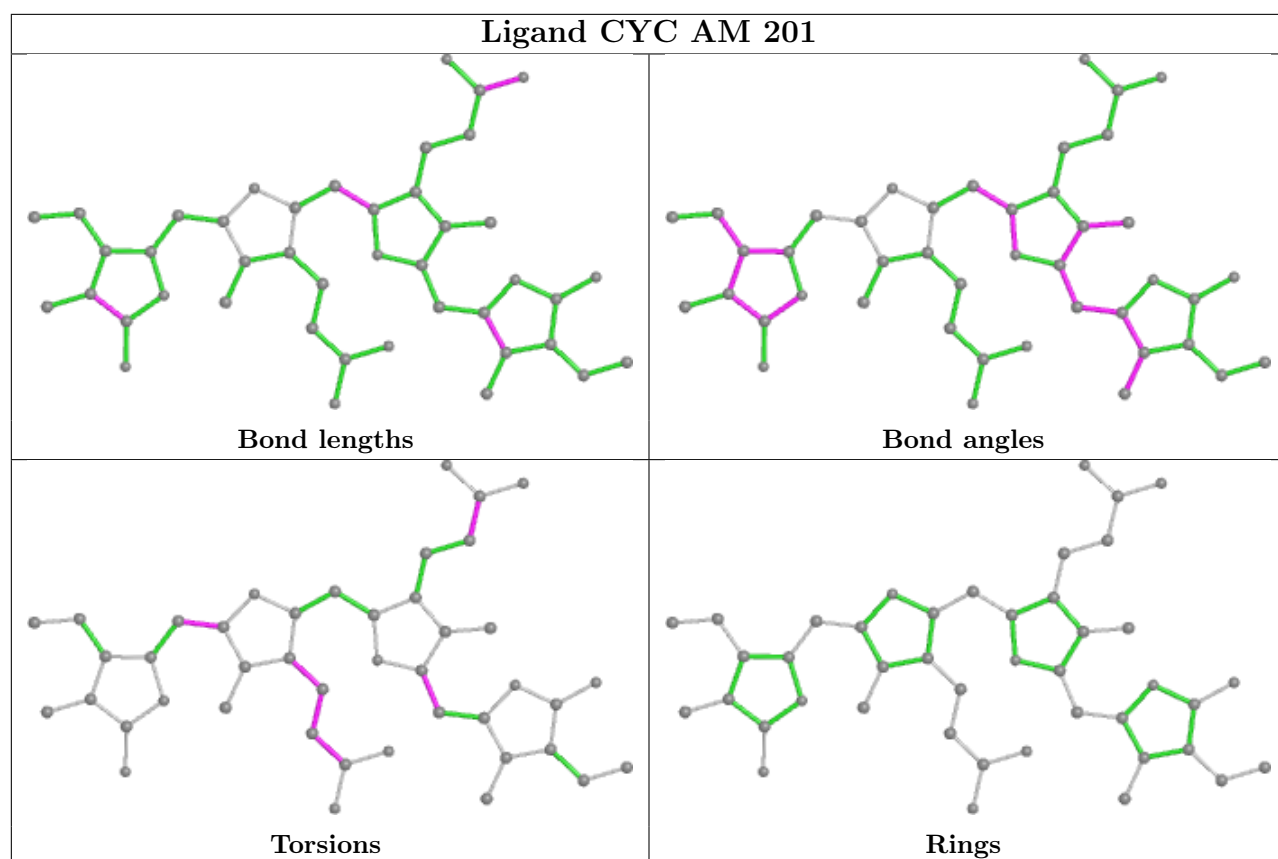


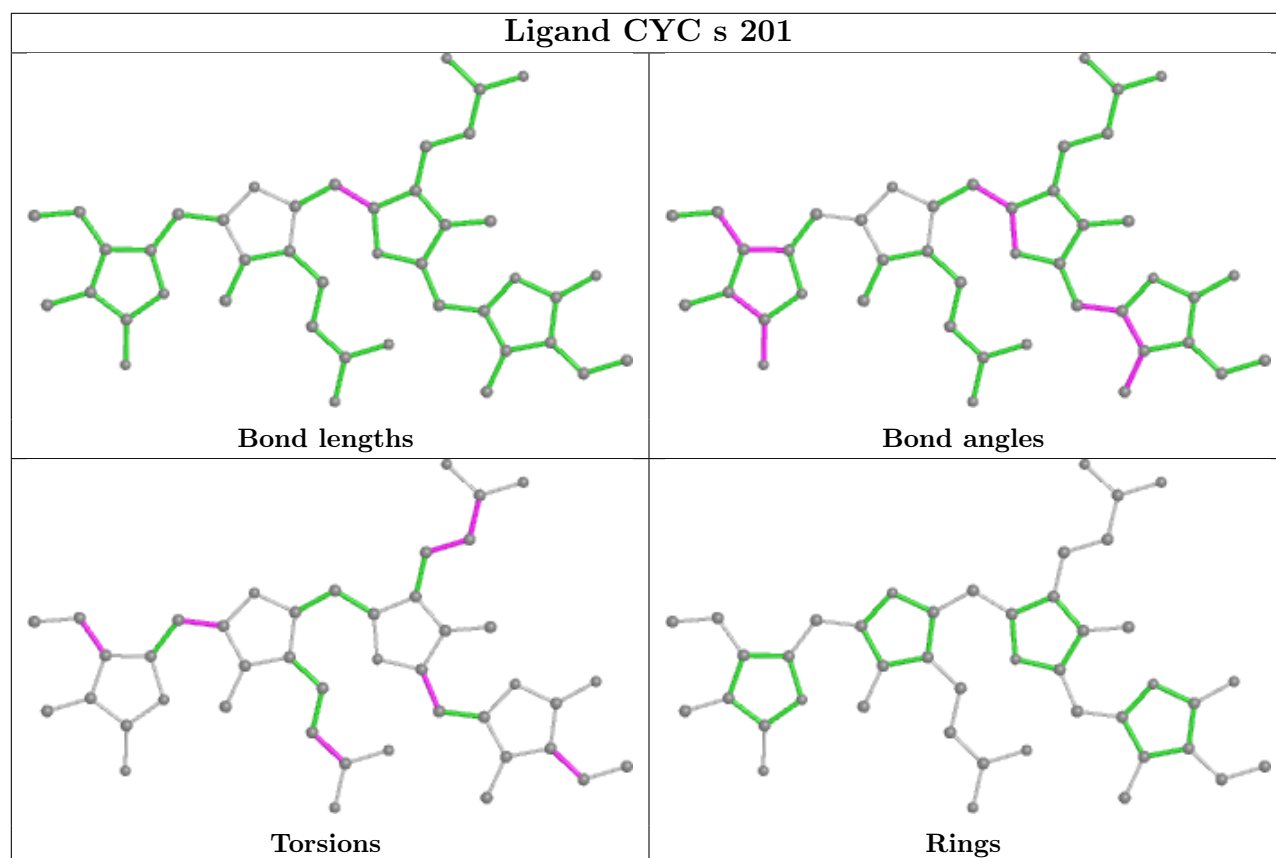
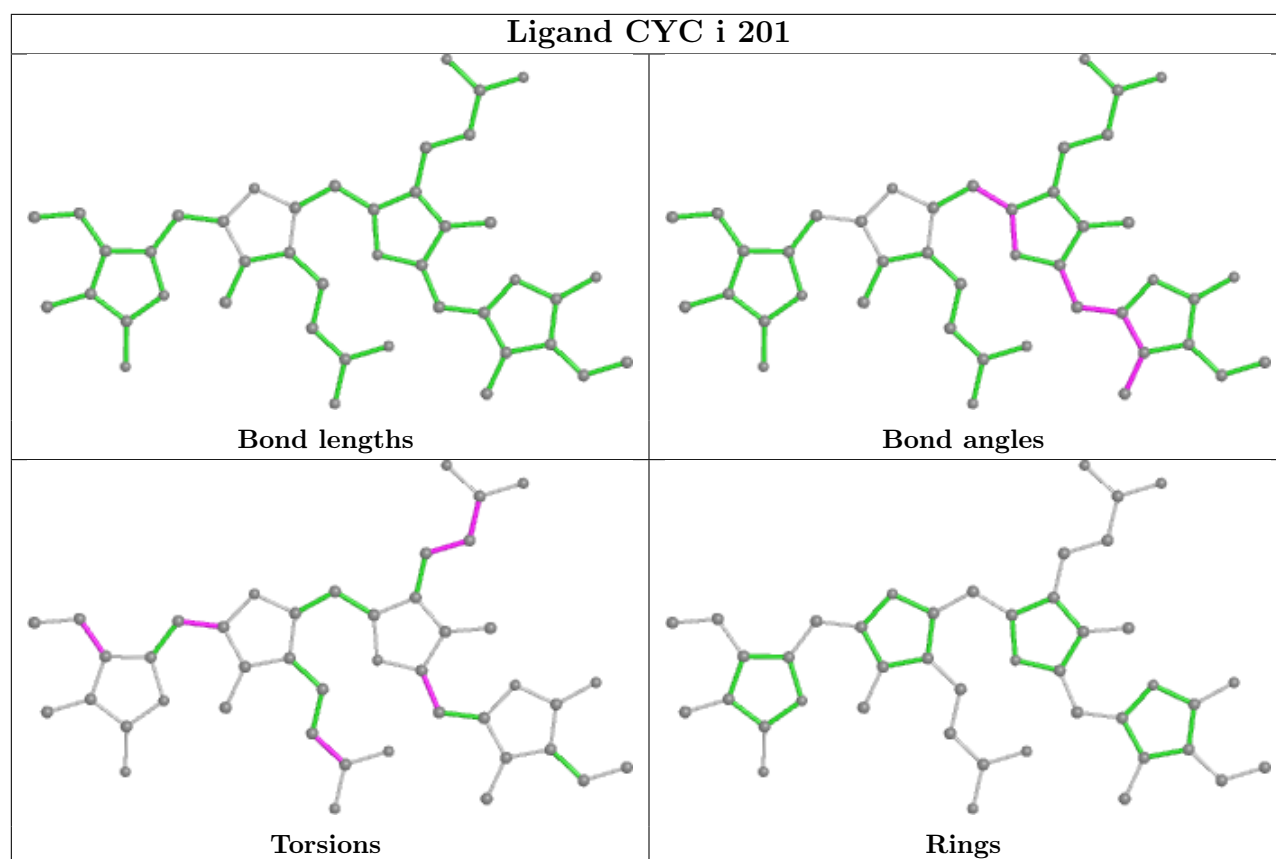
## Ligand CYC AB 201



## Ligand CYC y 201

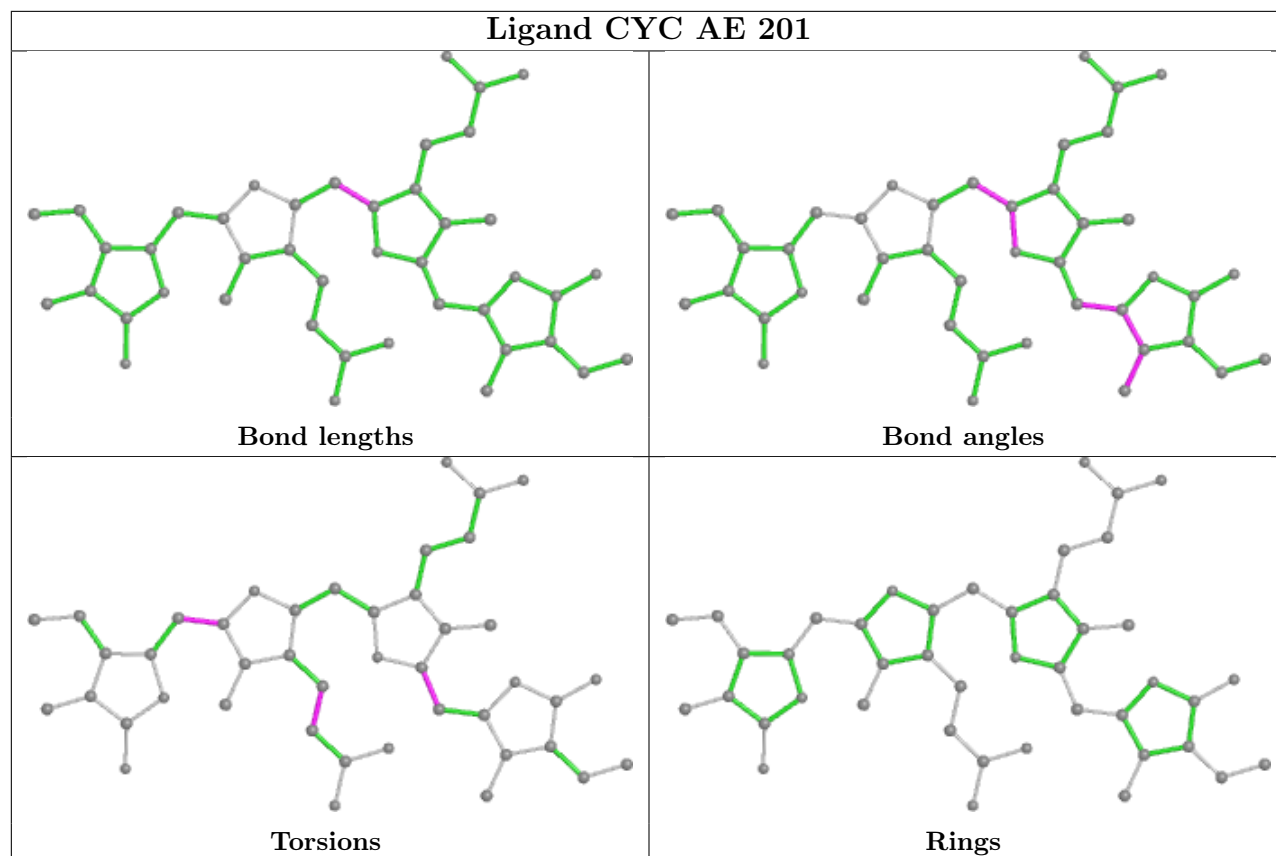




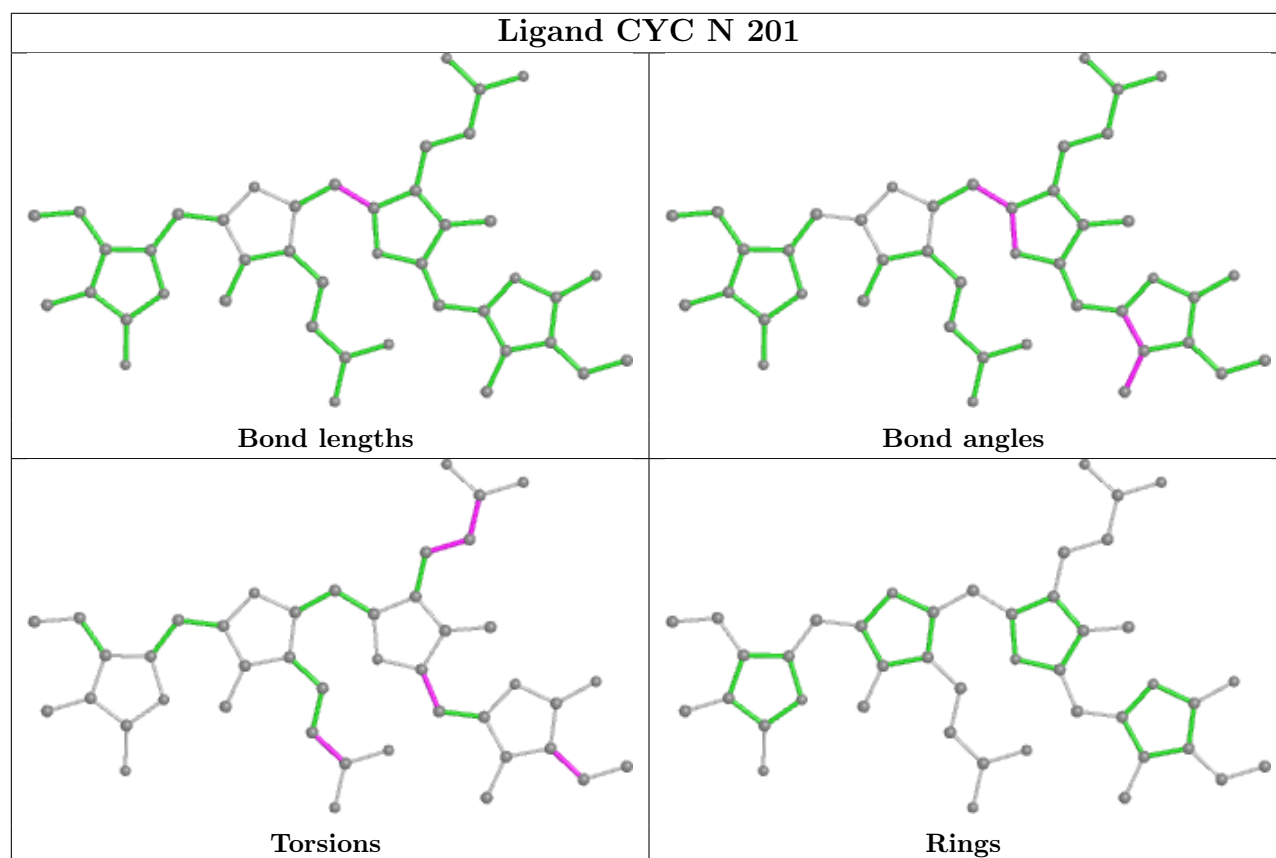


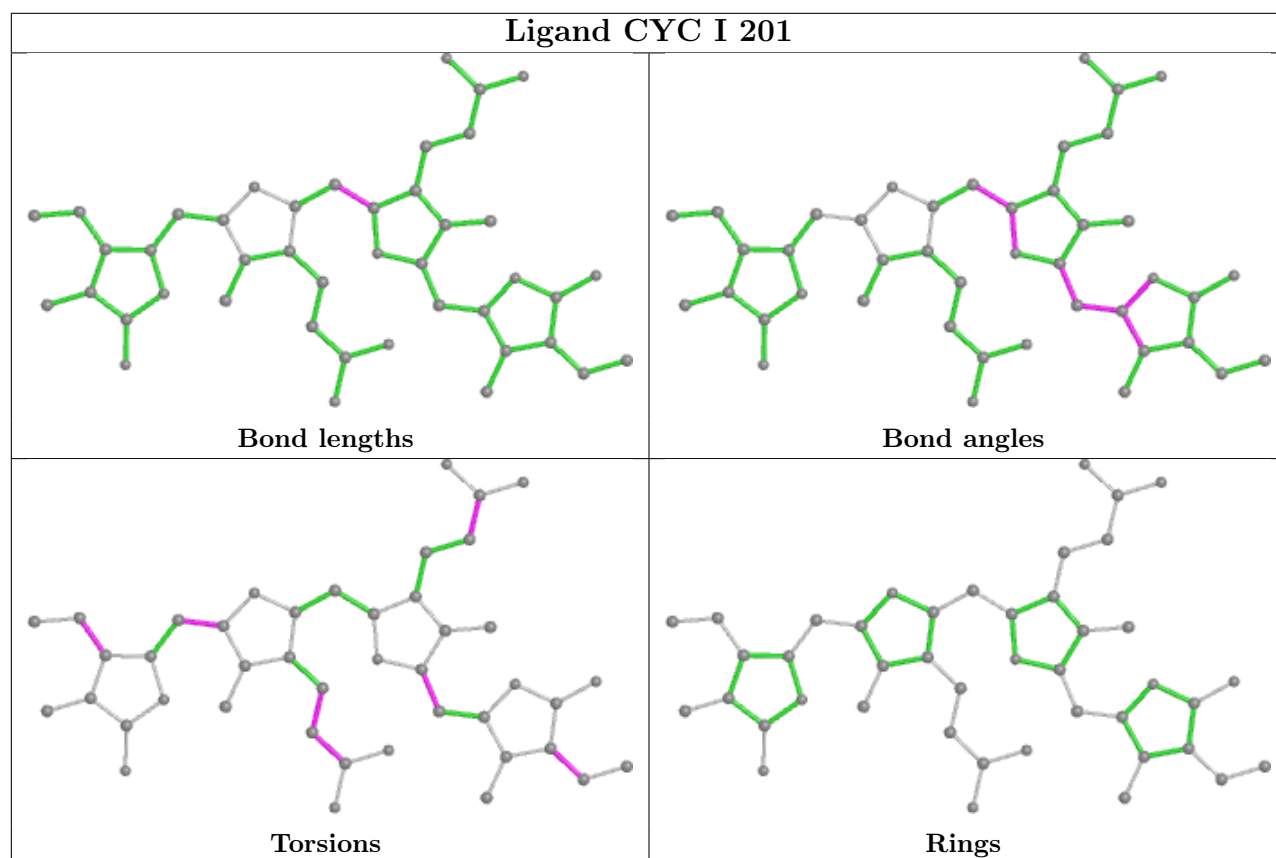
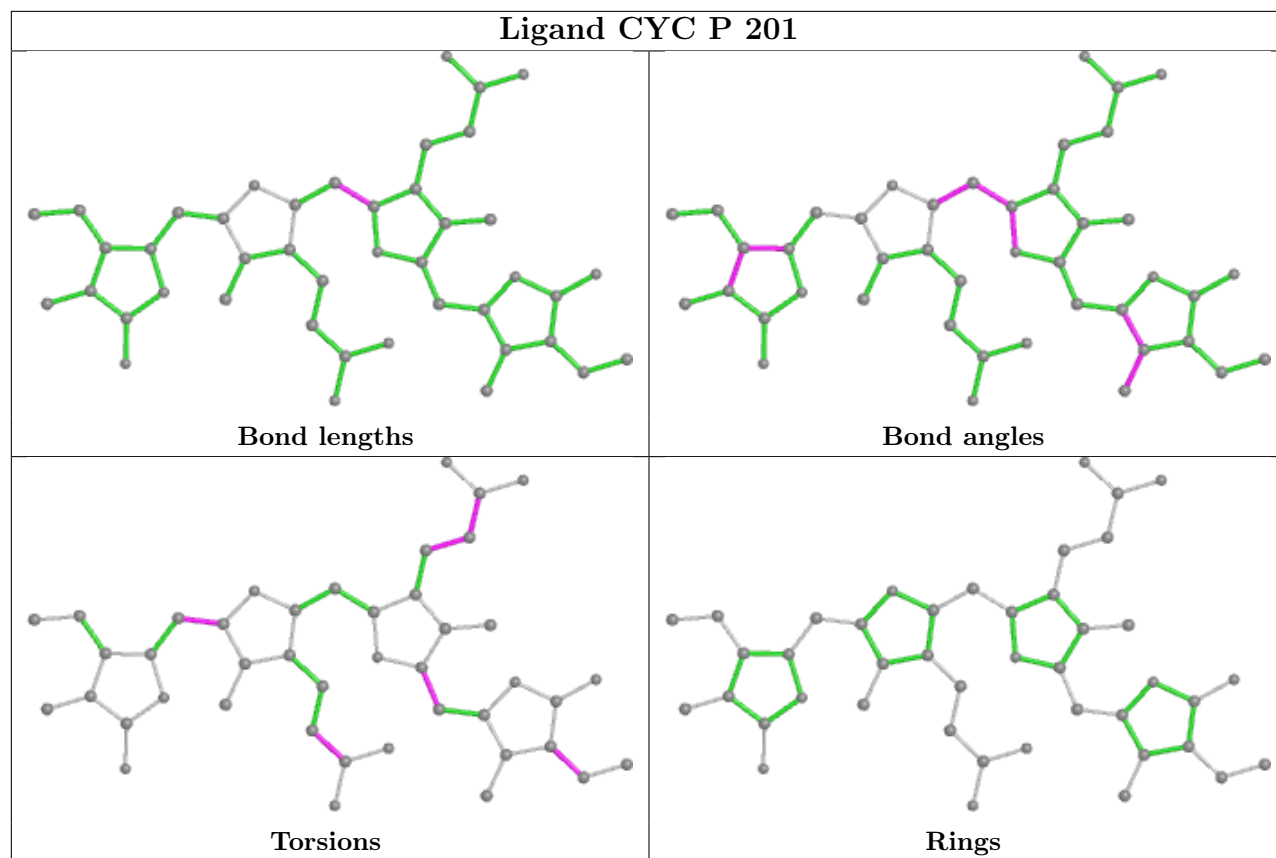


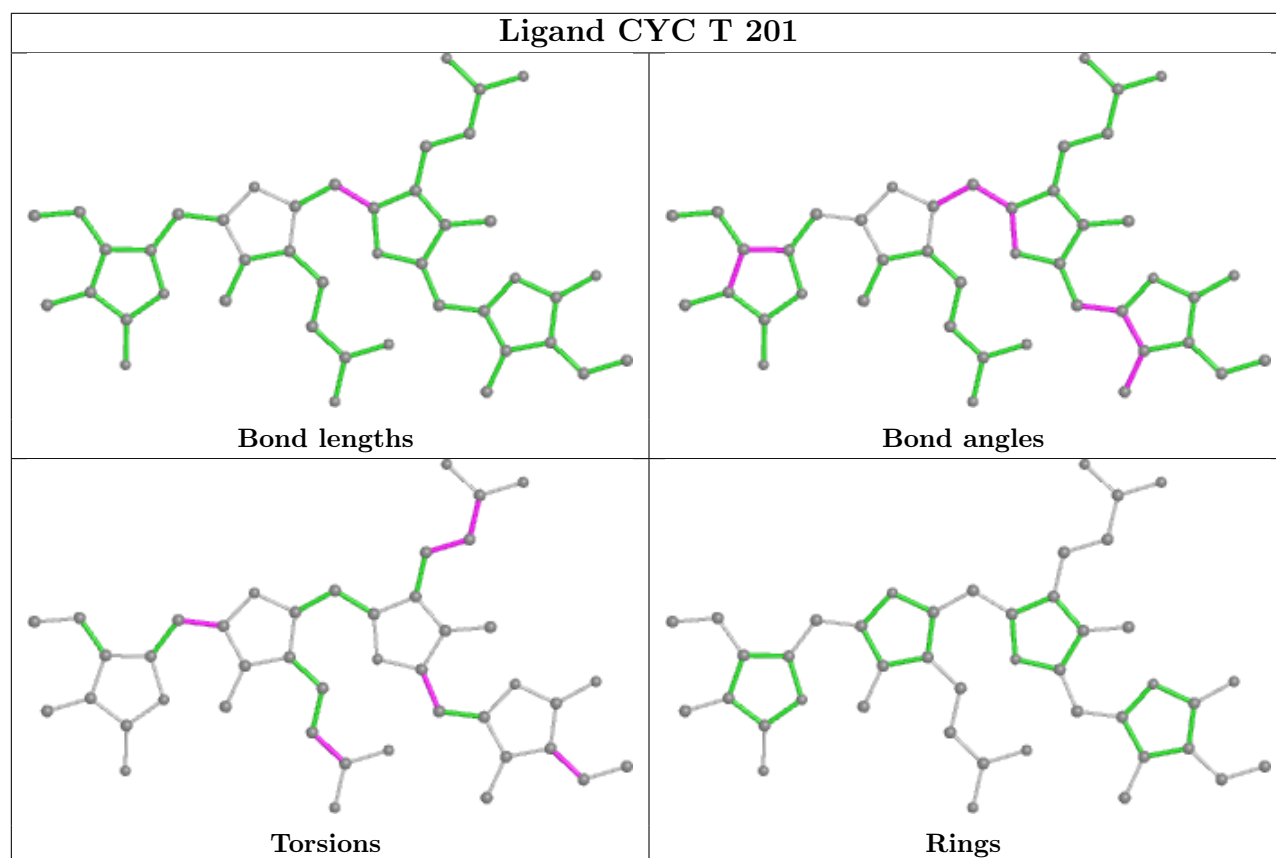
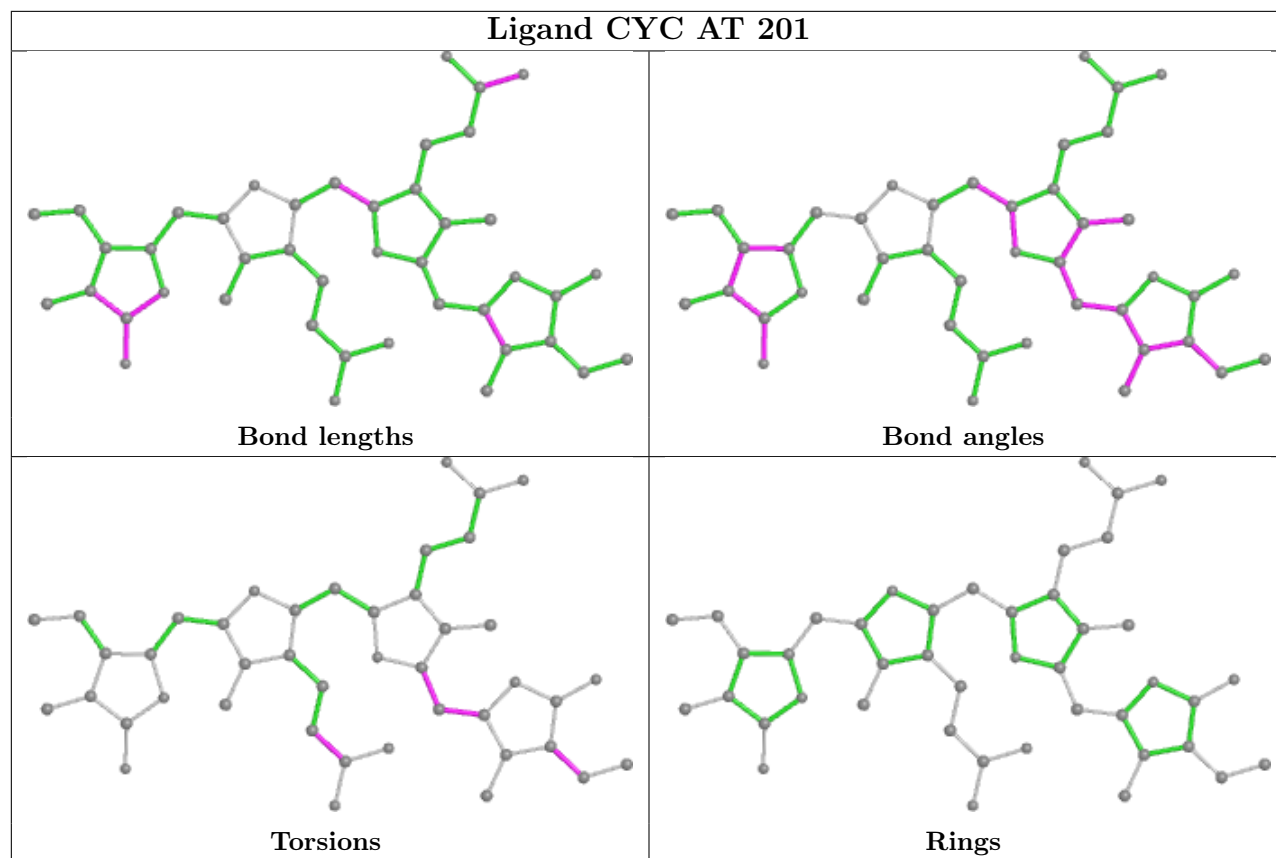
## Ligand CYC AE 201



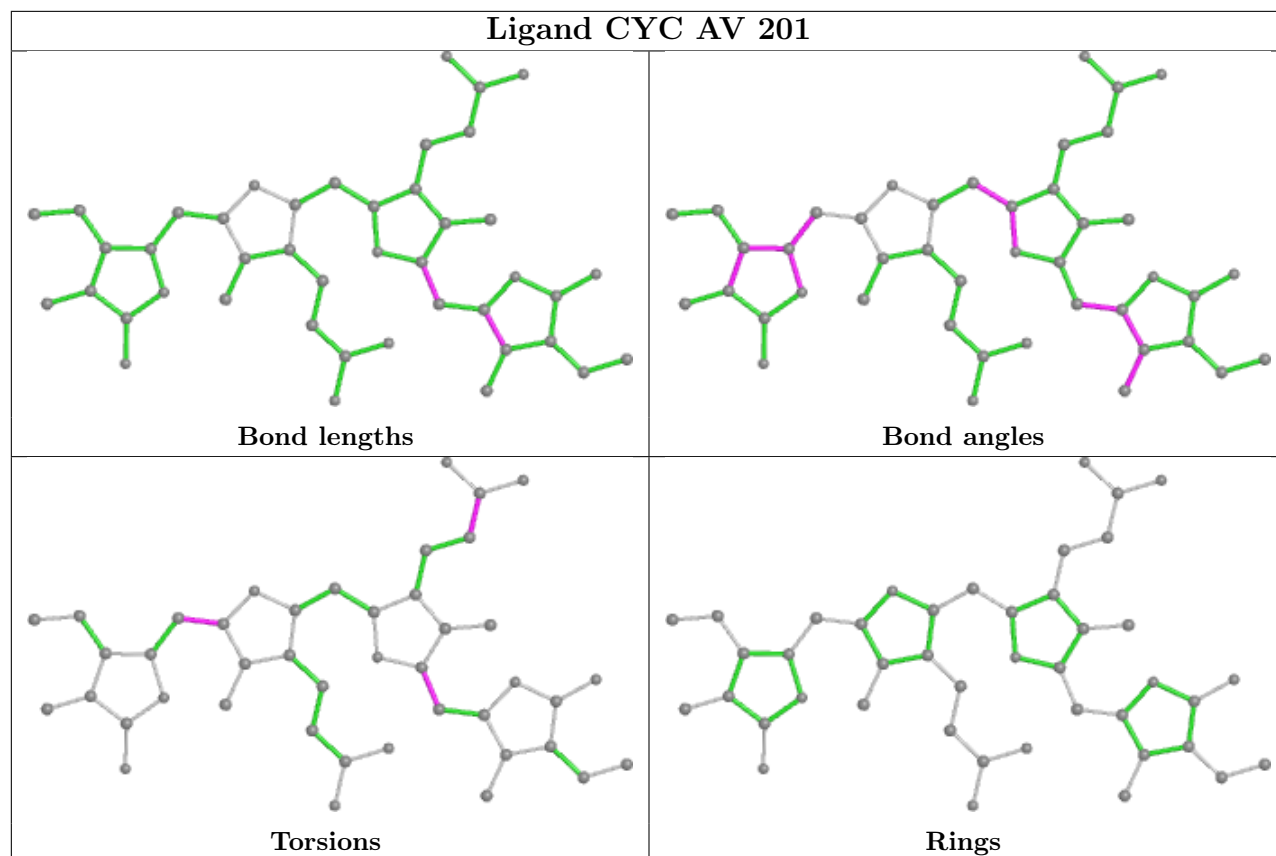
## Ligand CYC N 201



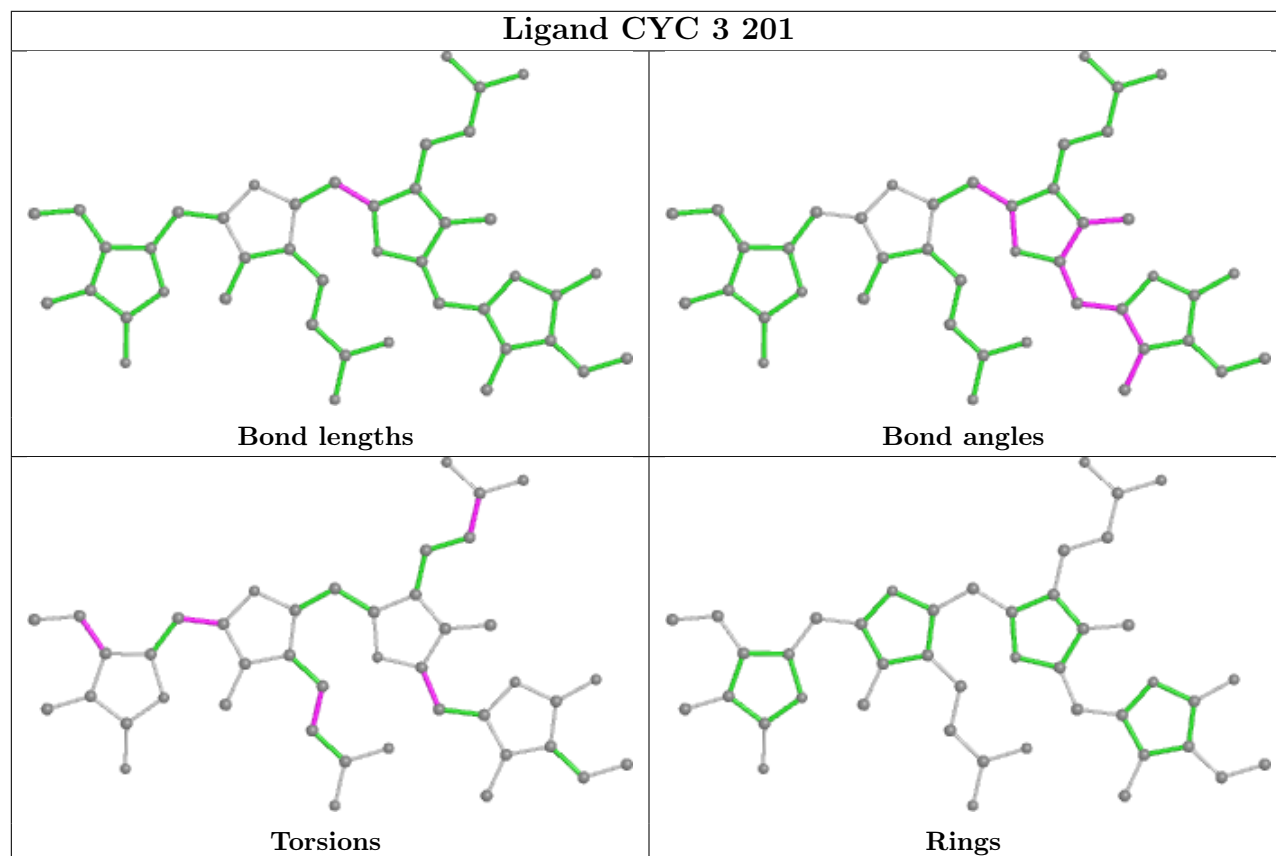


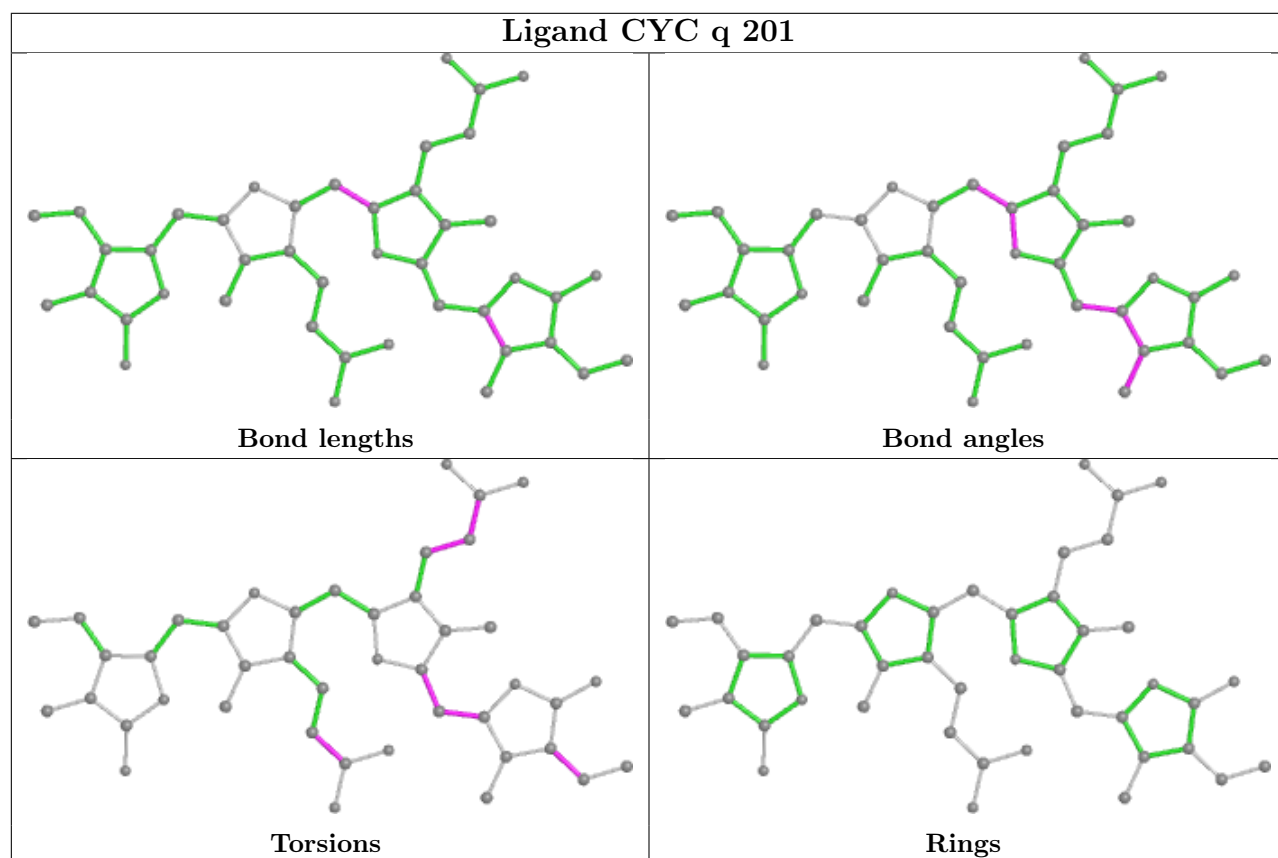
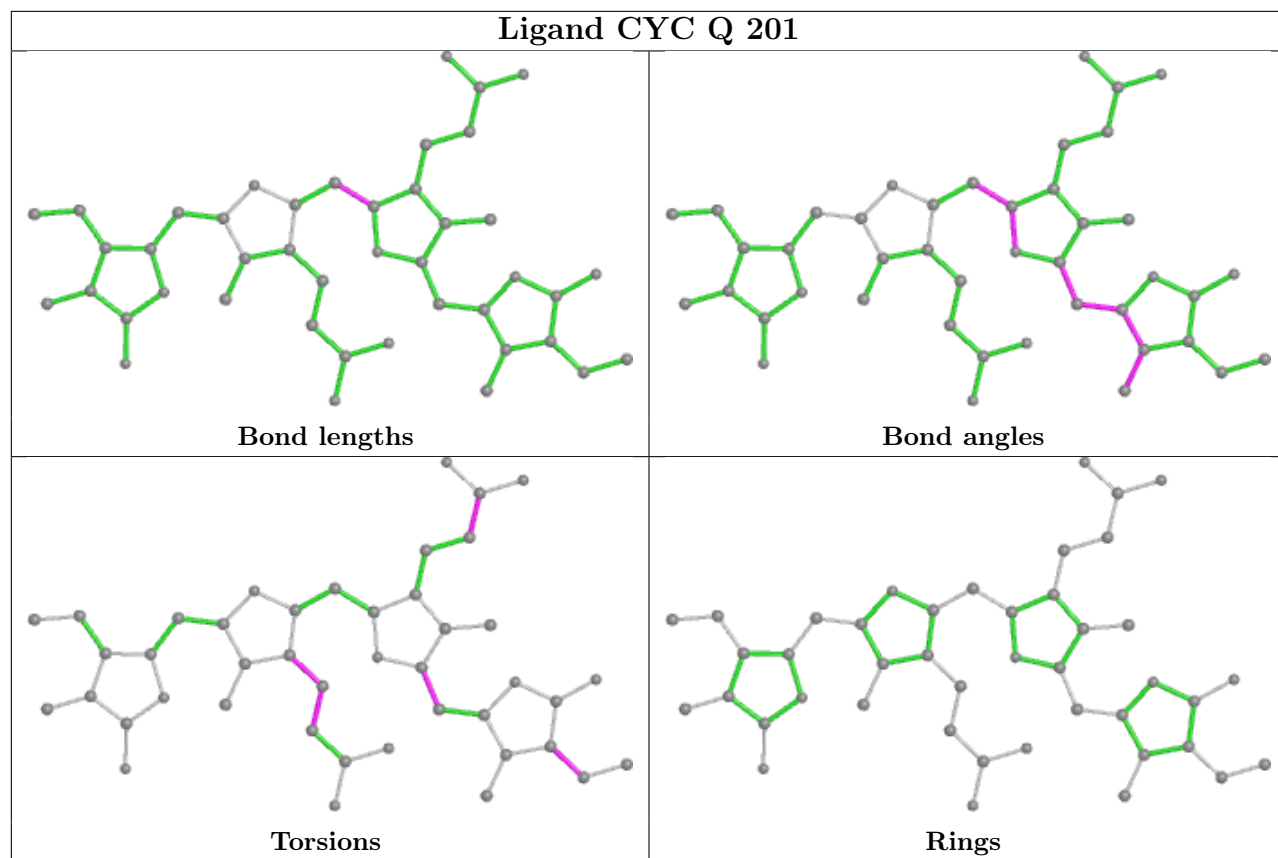


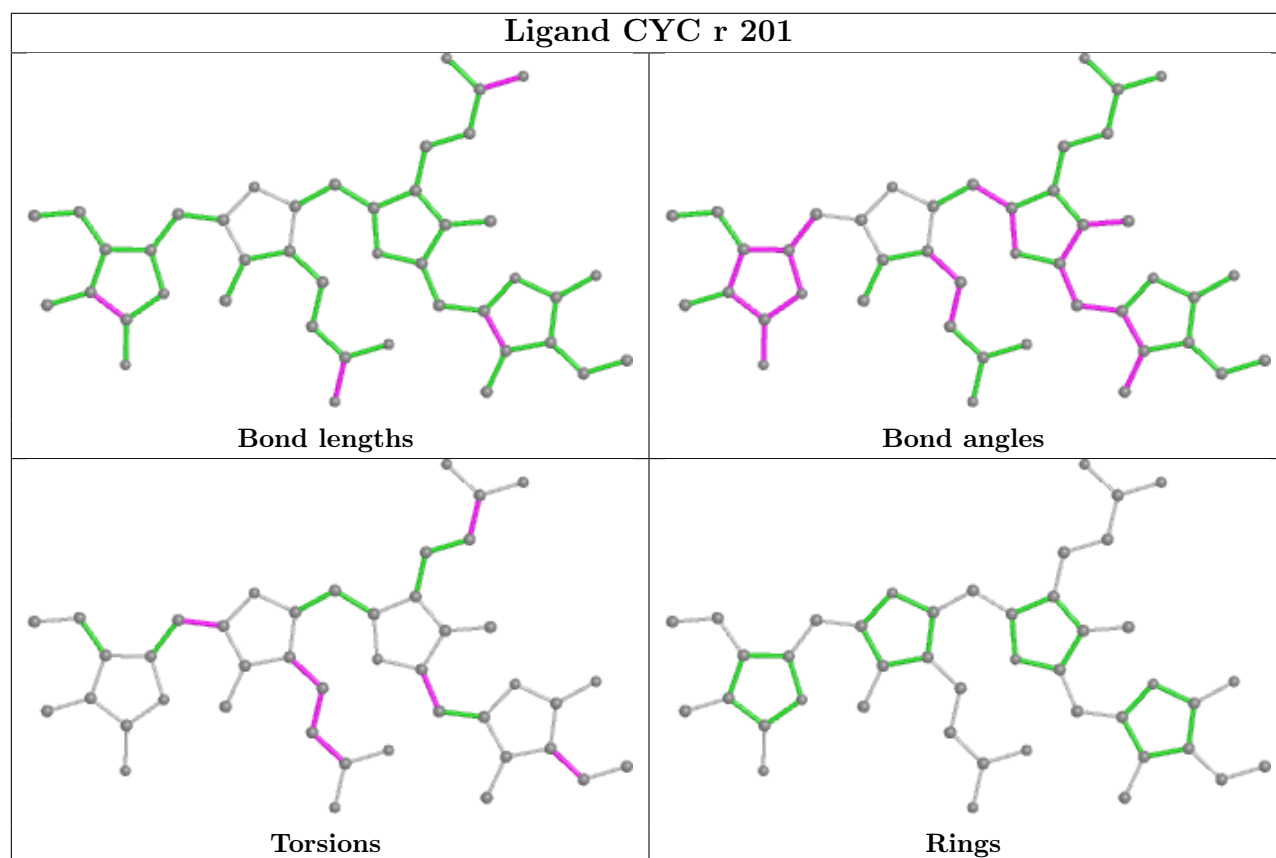
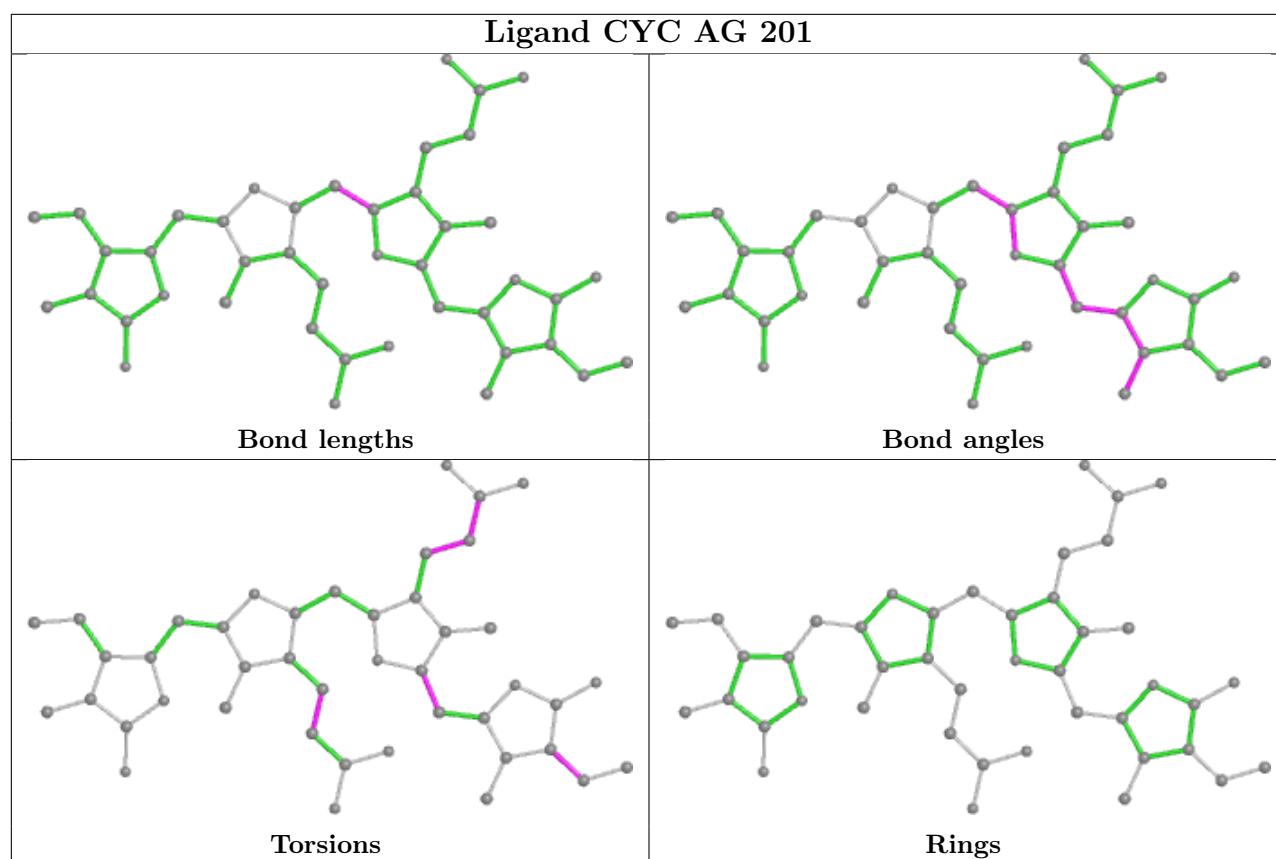
## Ligand CYC AV 201

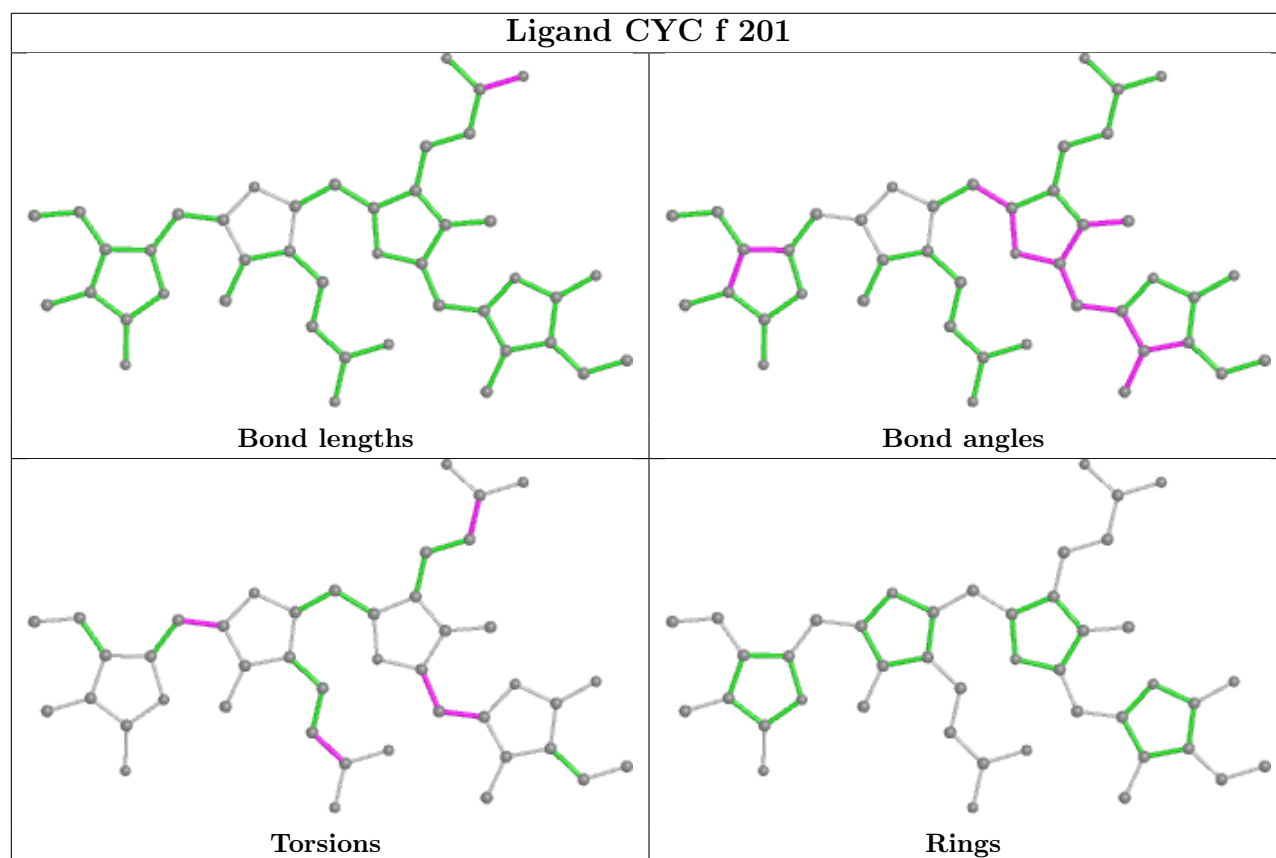
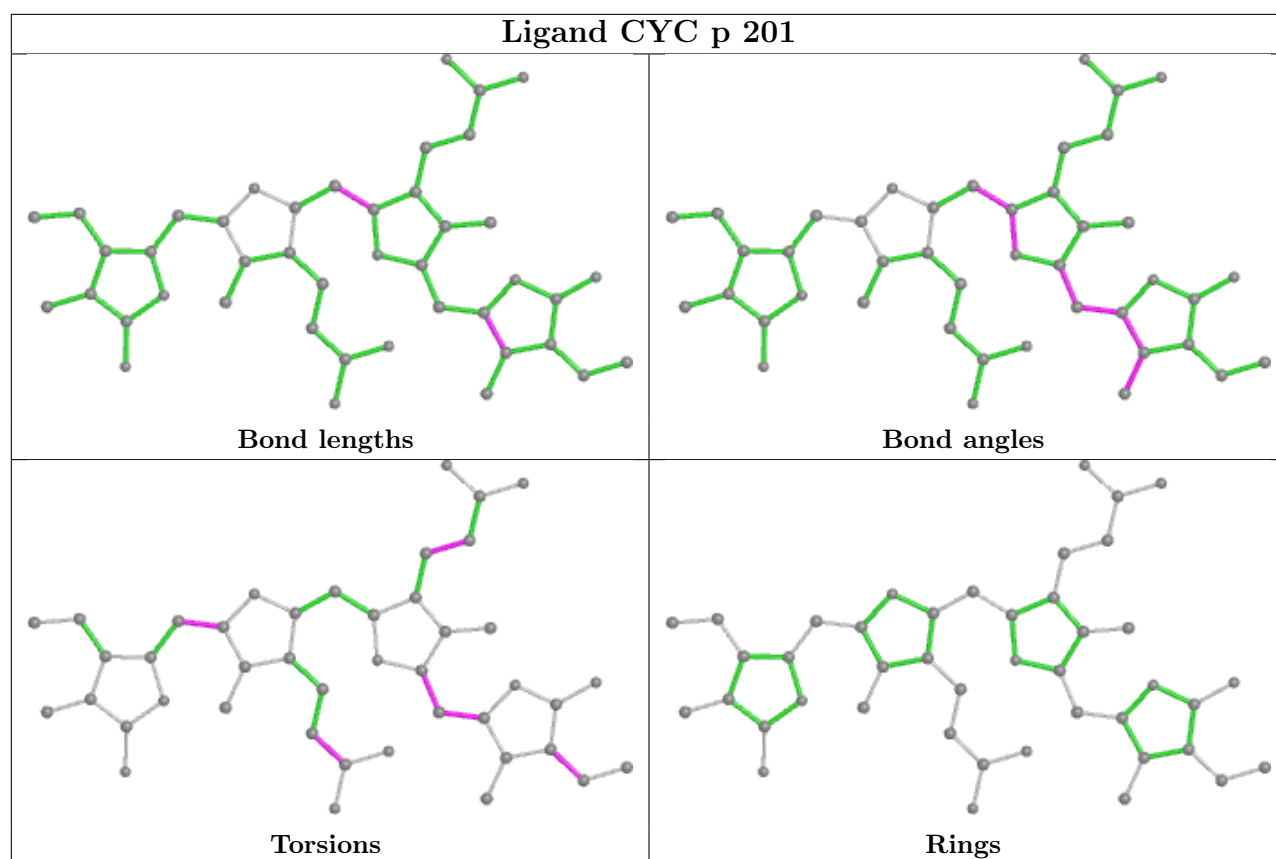


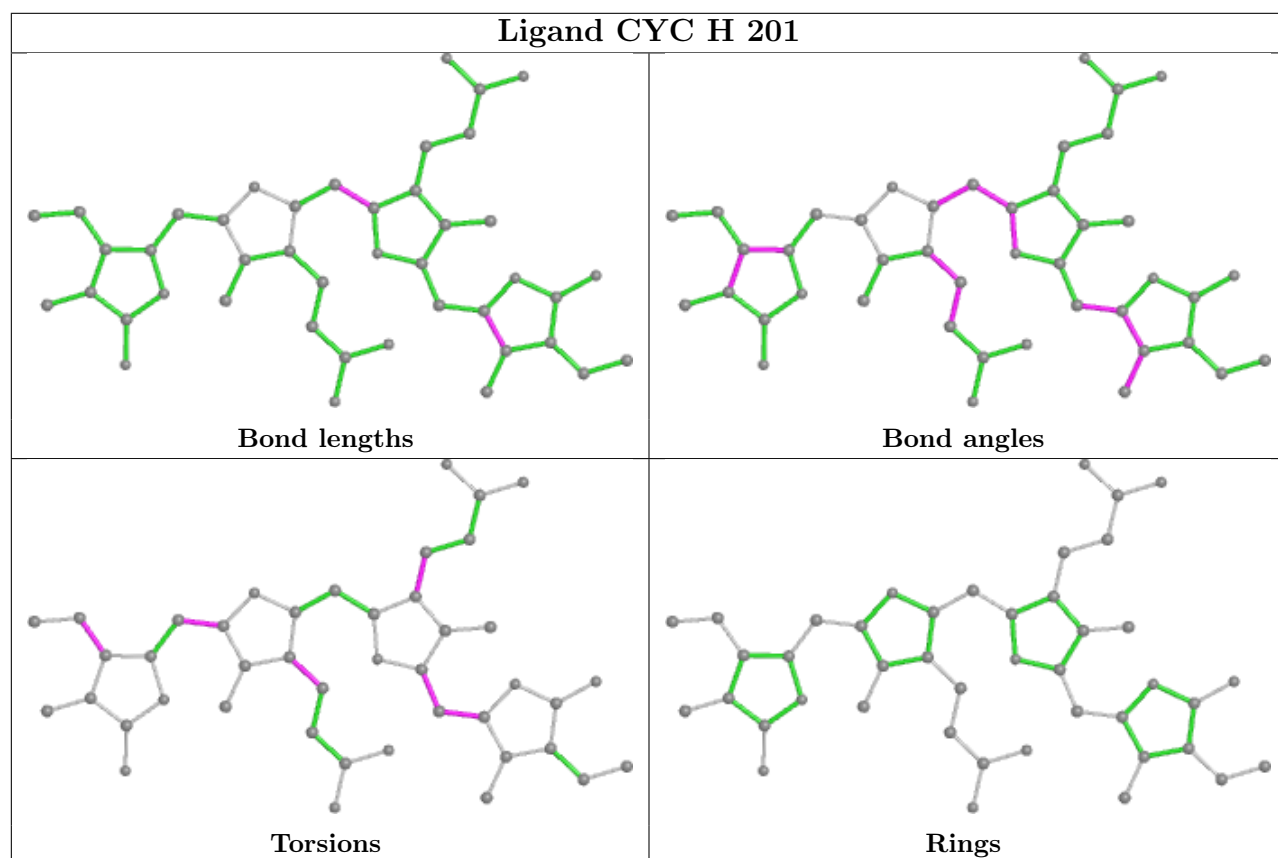
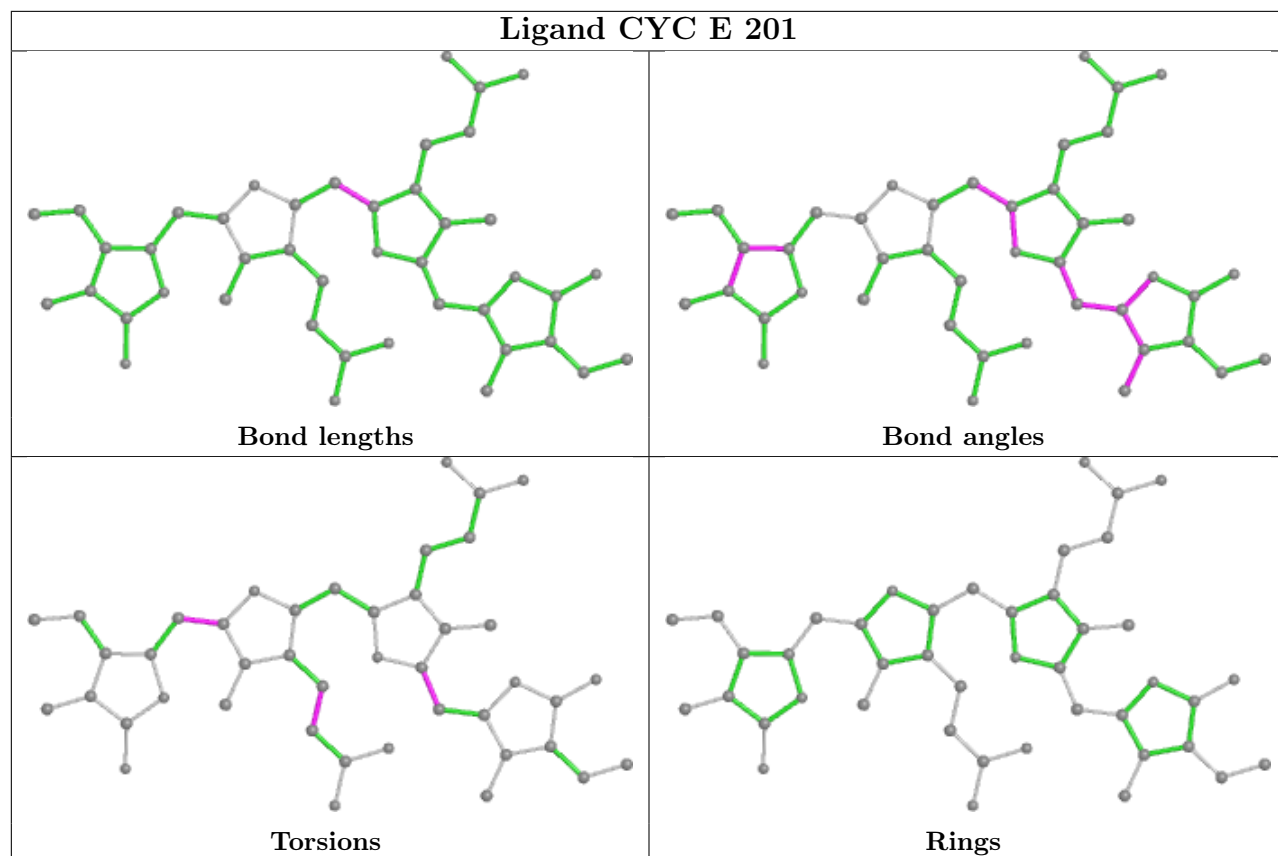
## Ligand CYC 3 201



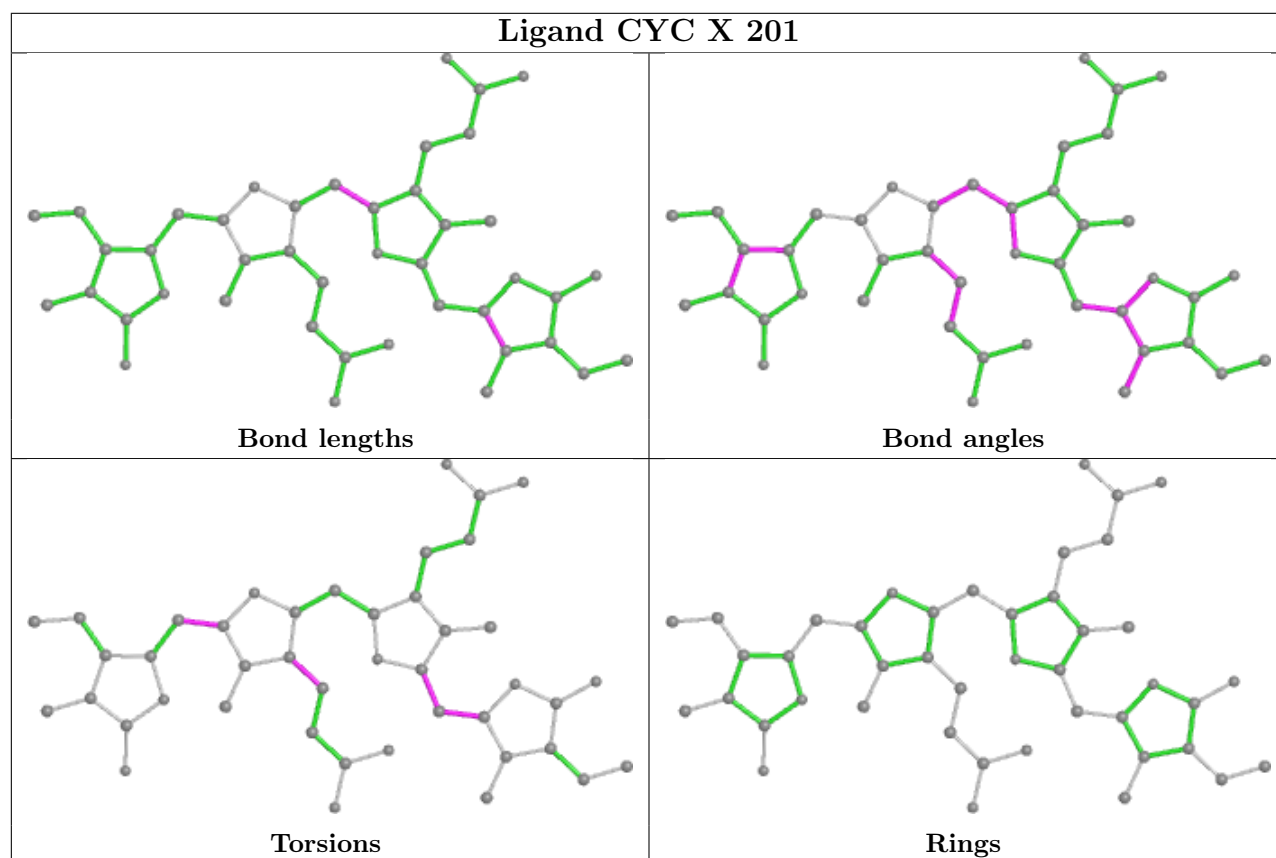
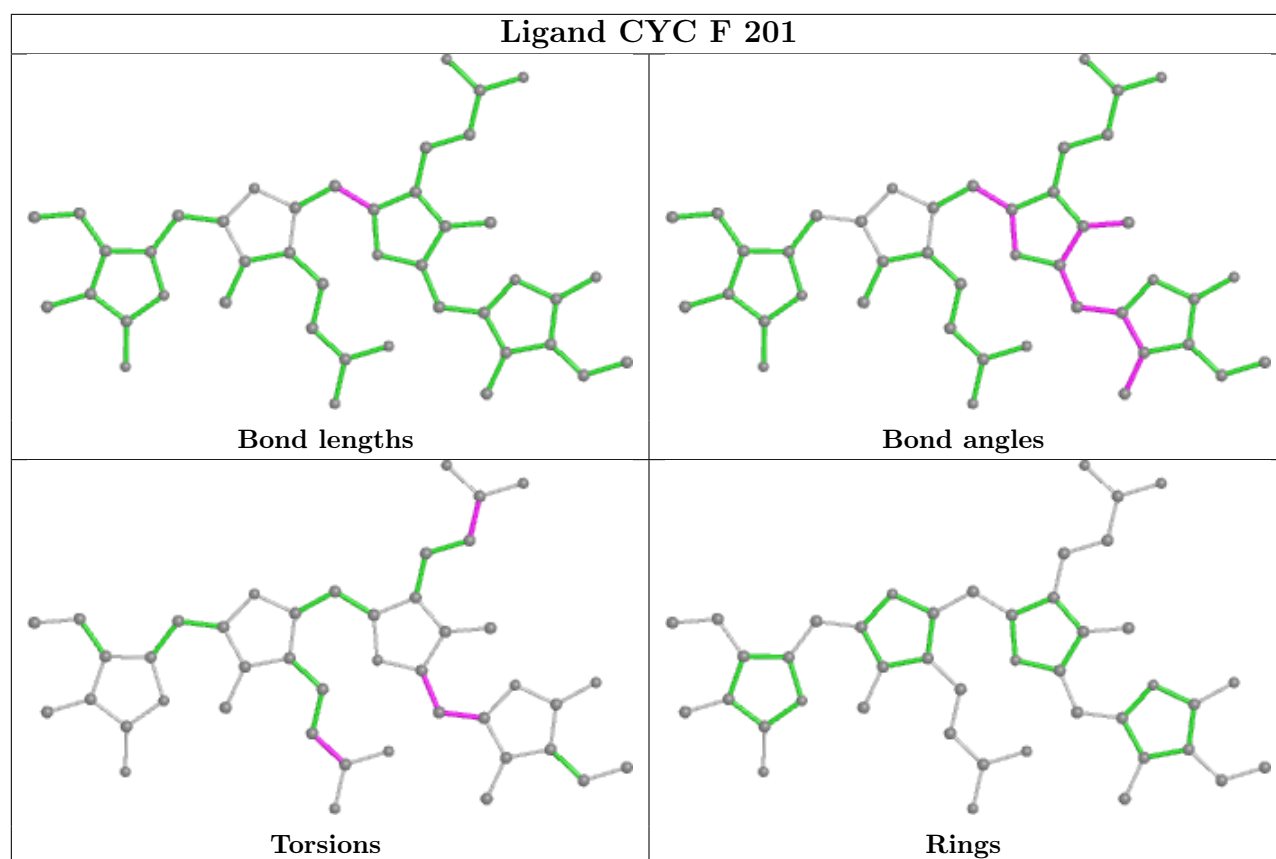




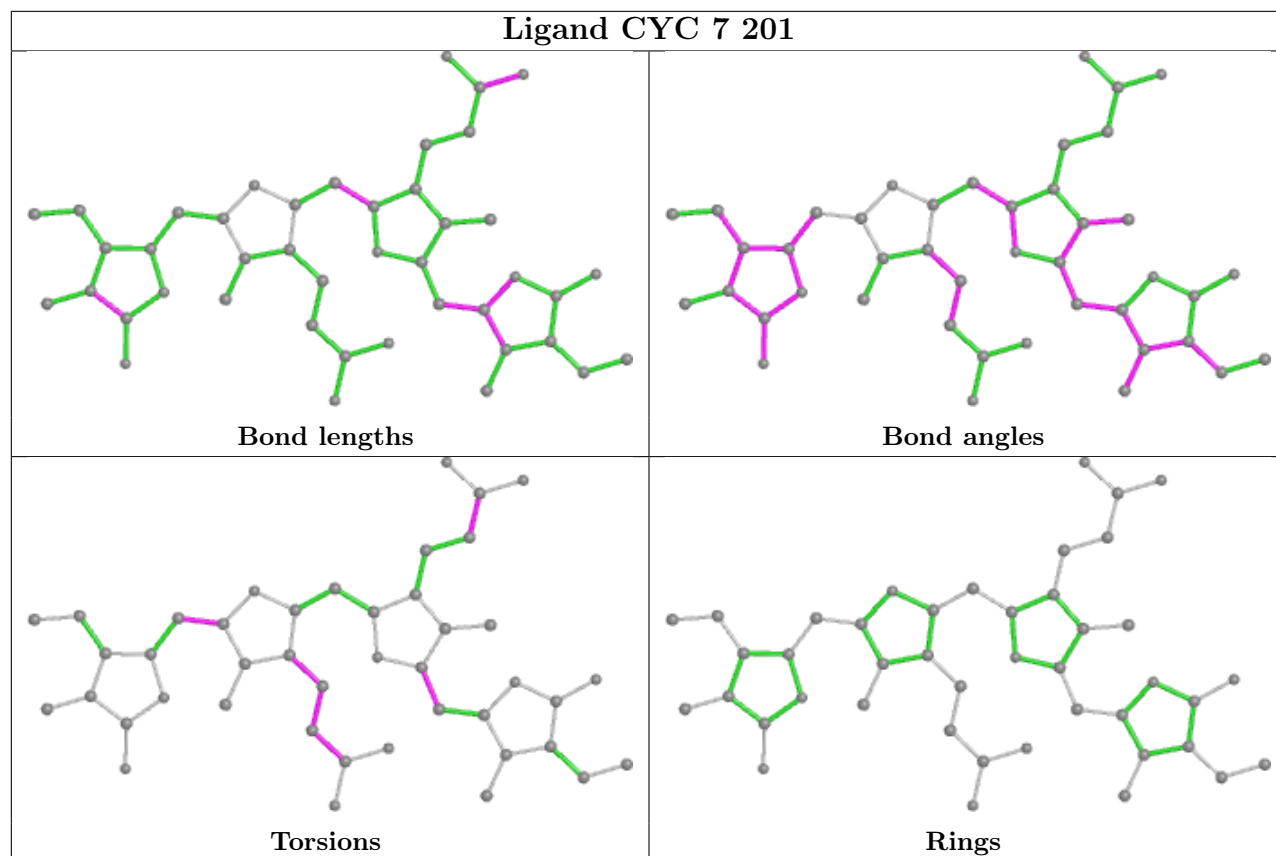




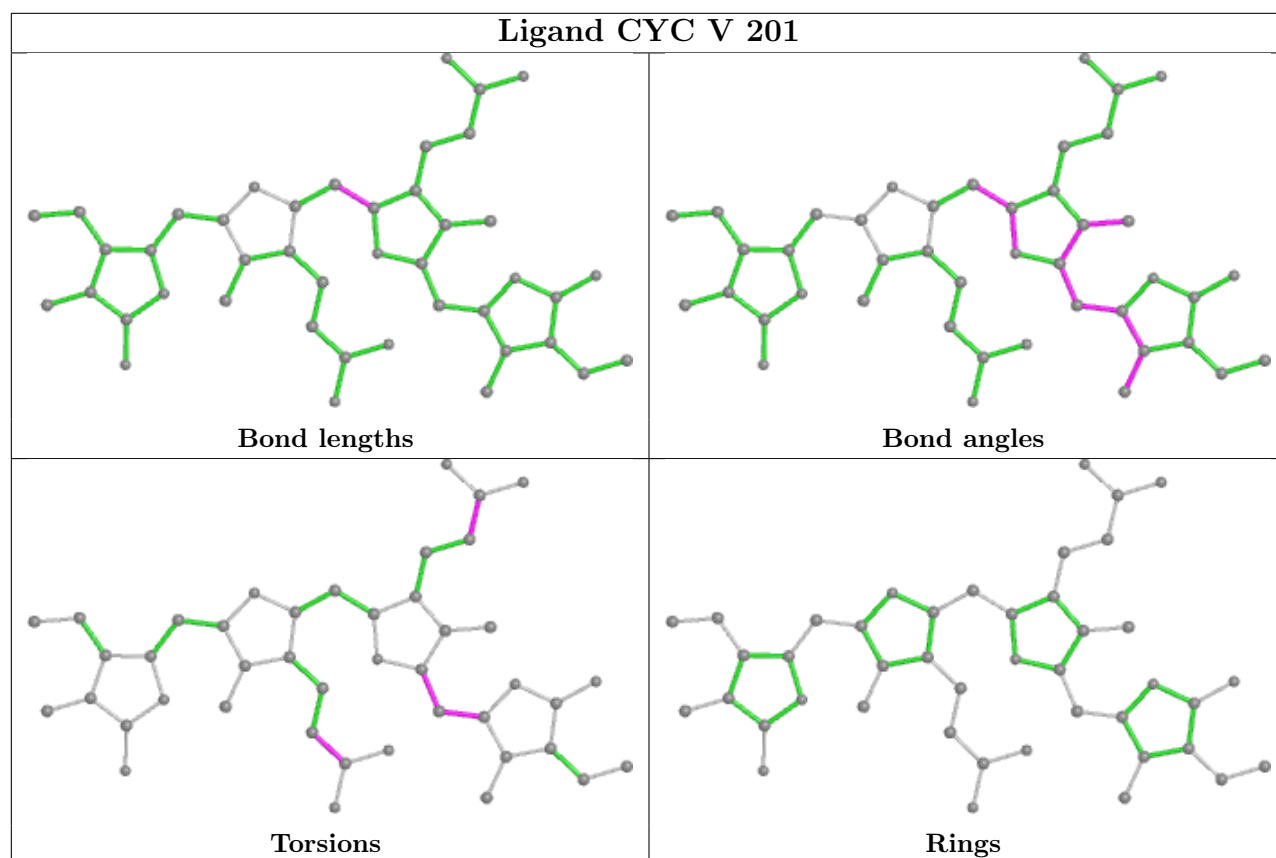




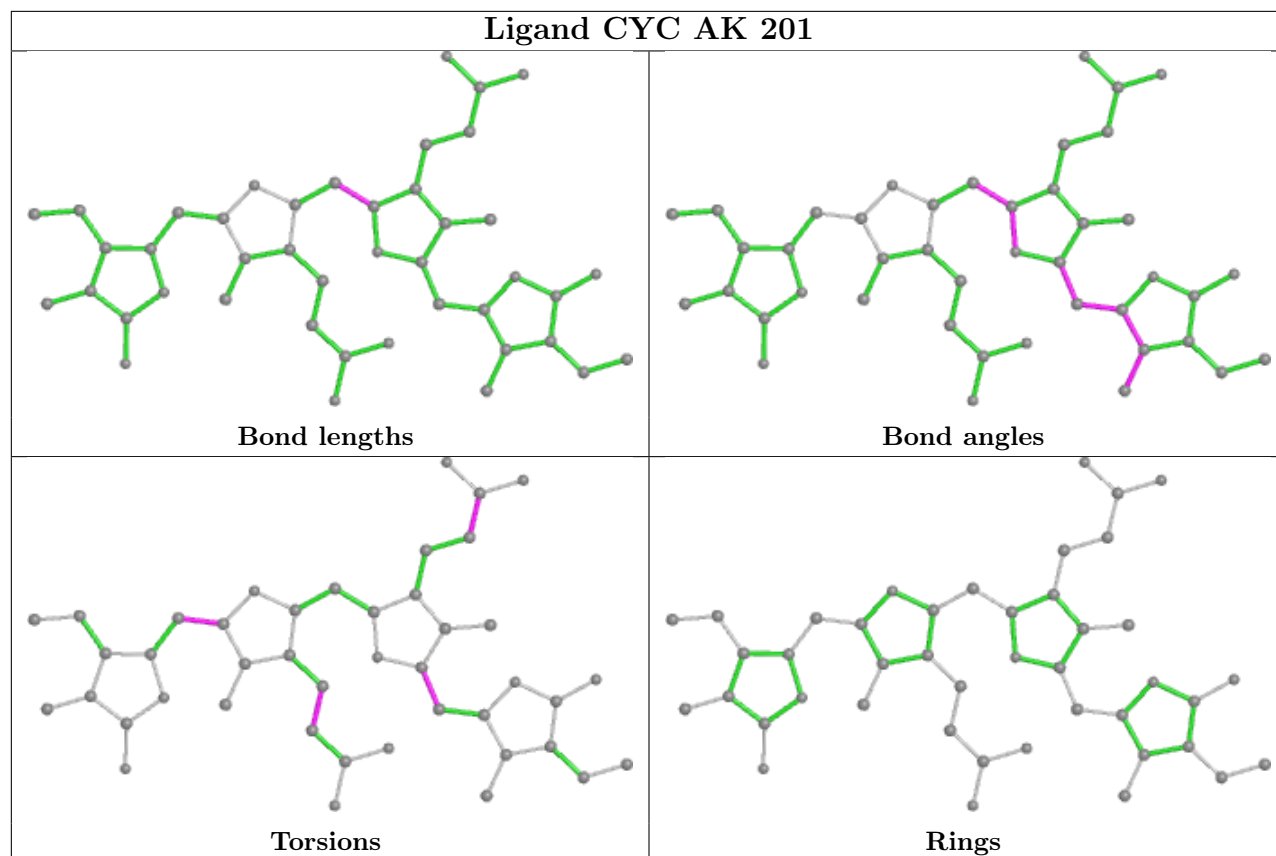
## Ligand CYC 7 201



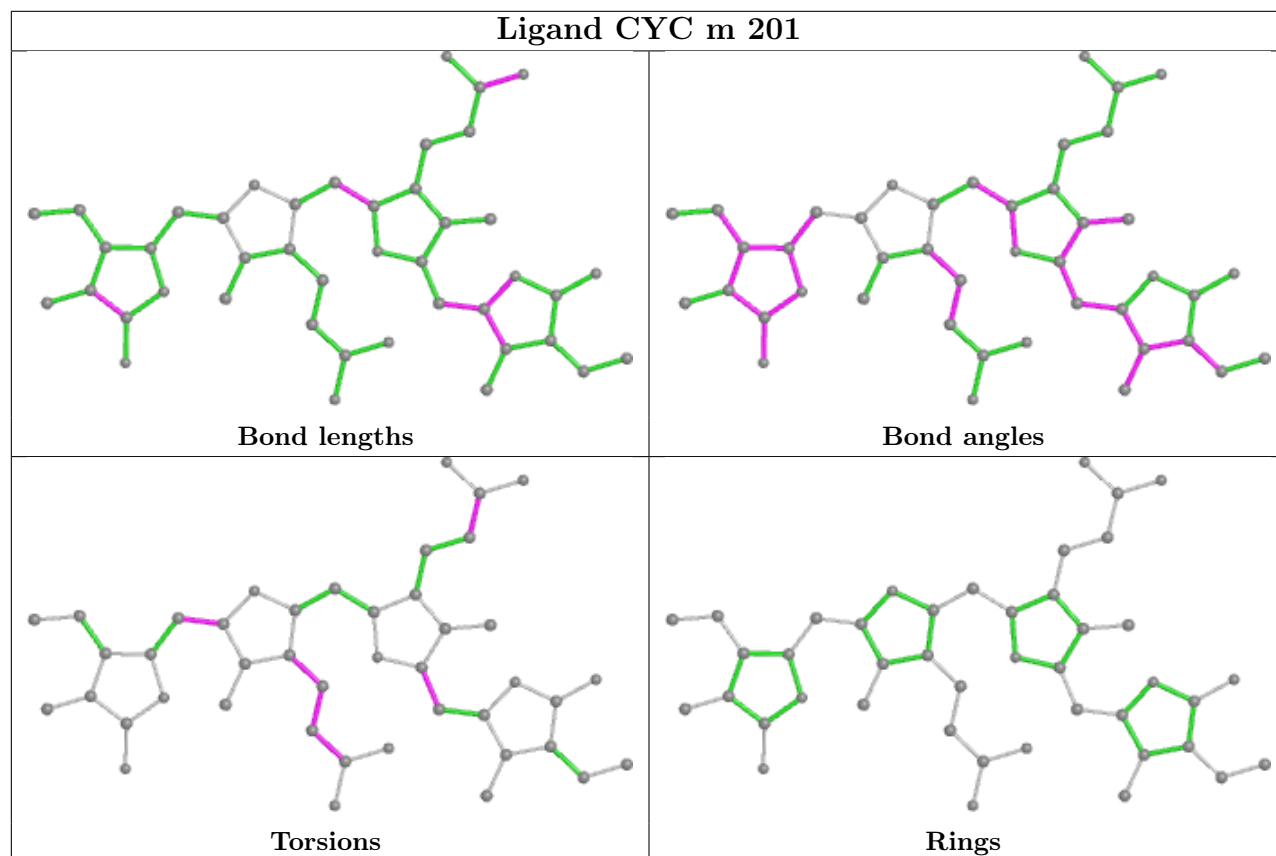
## Ligand CYC V 201

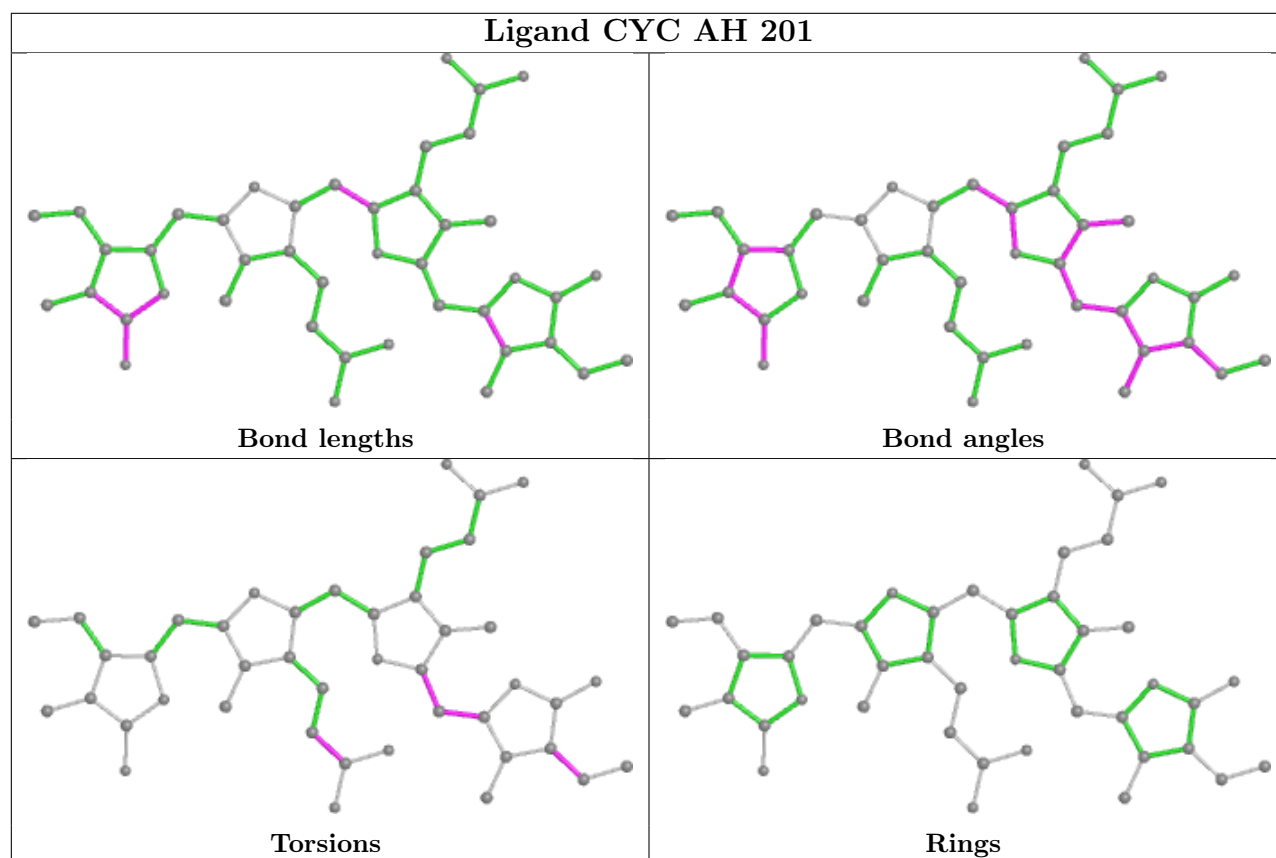
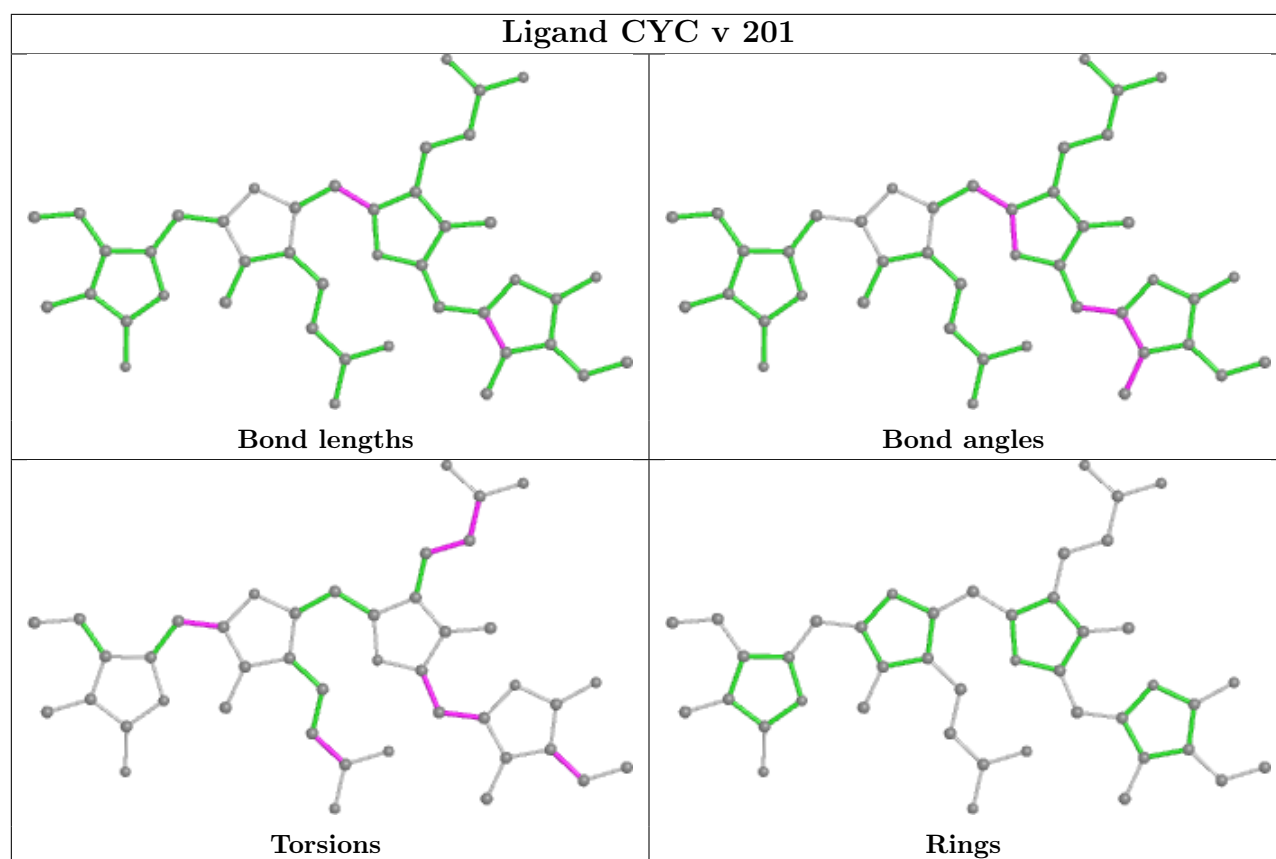


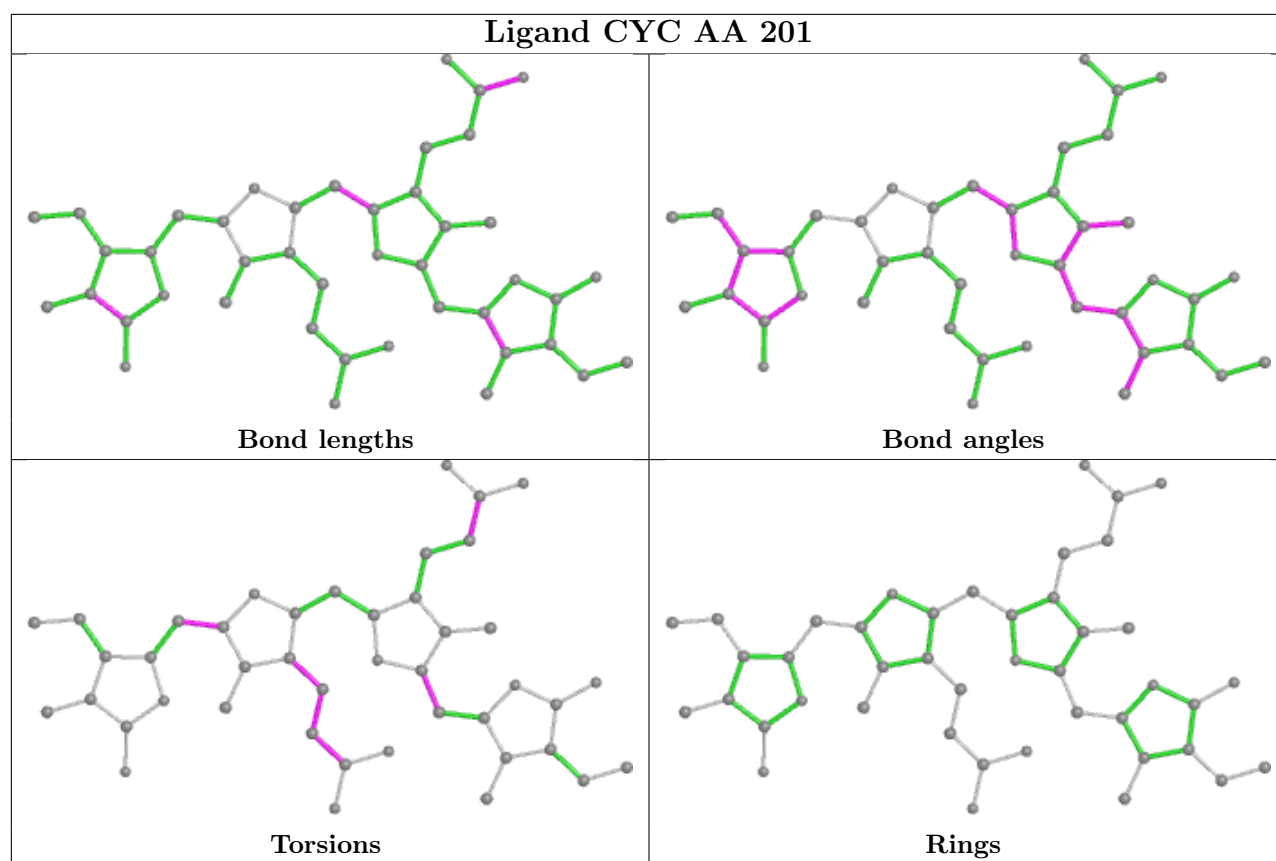
## Ligand CYC AK 201



## Ligand CYC m 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.

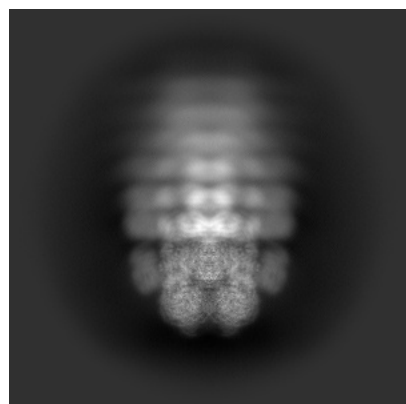
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-64815. These allow visual inspection of the internal detail of the map and identification of artifacts.

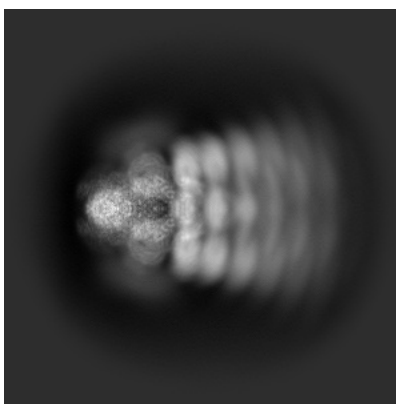
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

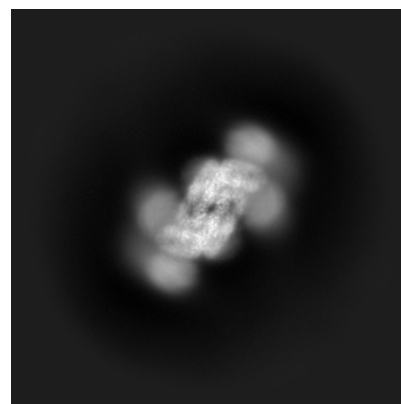
#### 6.1.1 Primary map



X

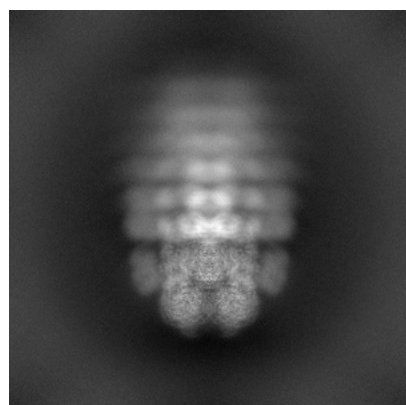


Y

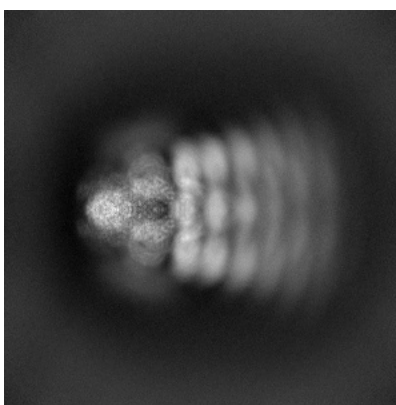


Z

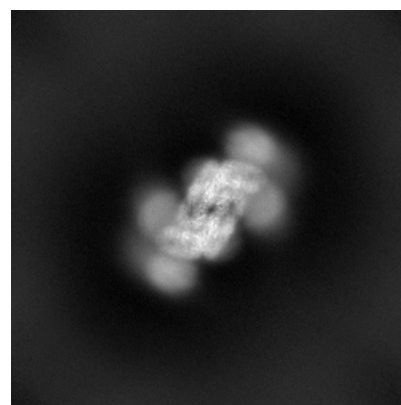
#### 6.1.2 Raw map



X



Y

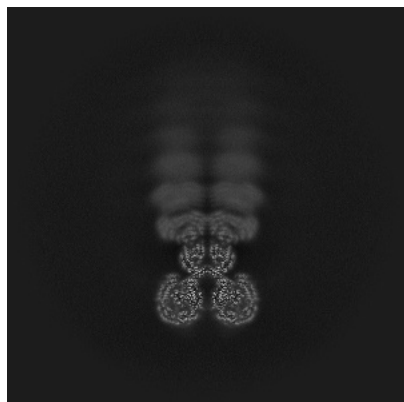


Z

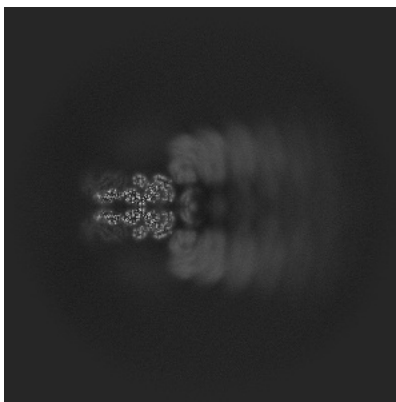
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

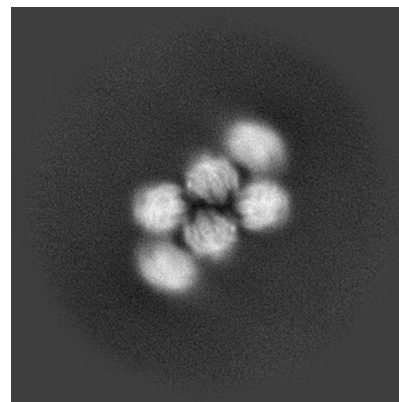
### 6.2.1 Primary map



X Index: 336

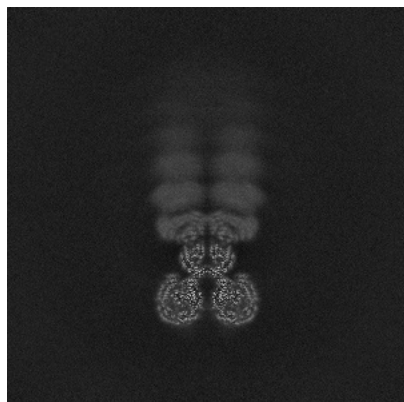


Y Index: 336

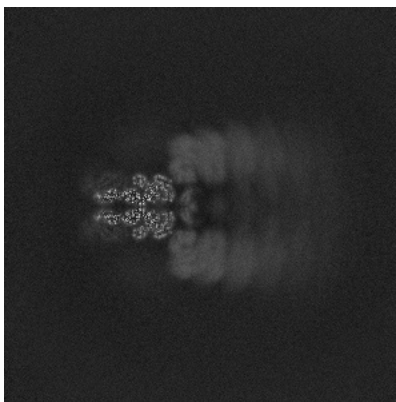


Z Index: 336

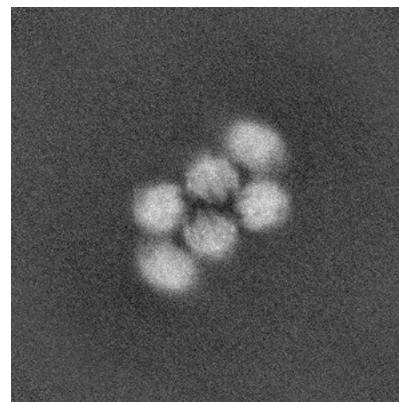
### 6.2.2 Raw map



X Index: 336



Y Index: 336



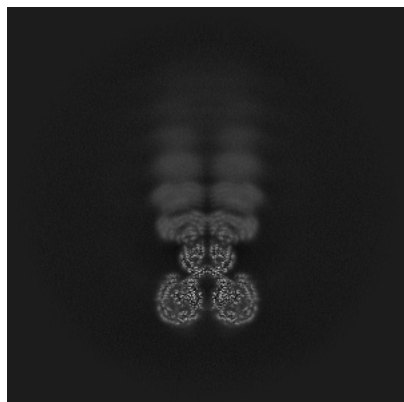
Z Index: 336

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

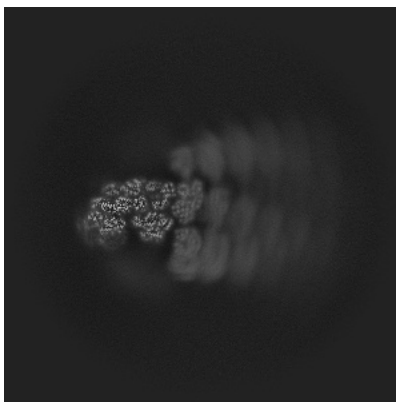


## 6.3 Largest variance slices [i](#)

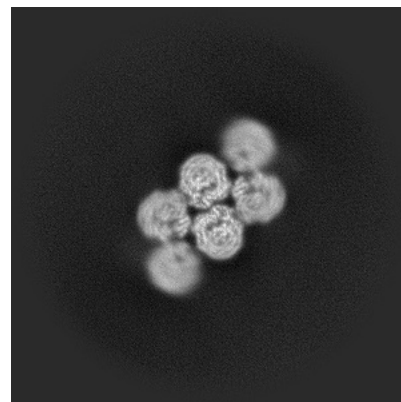
### 6.3.1 Primary map



X Index: 336

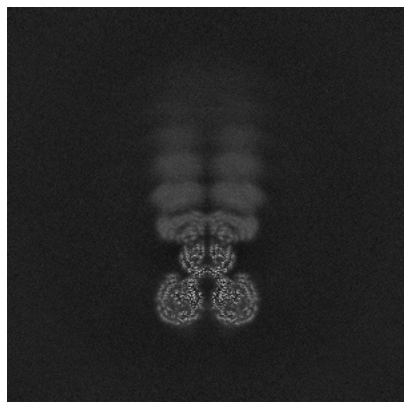


Y Index: 316

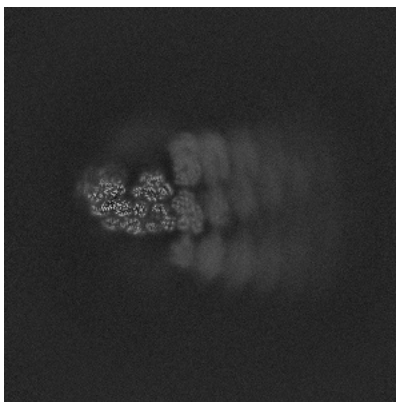


Z Index: 307

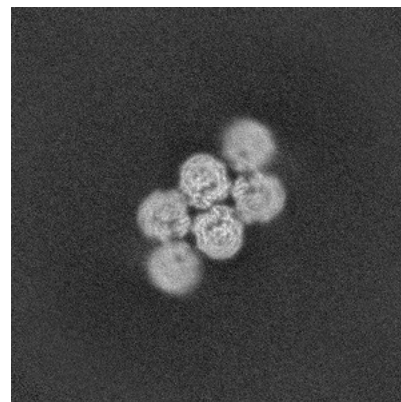
### 6.3.2 Raw map



X Index: 336



Y Index: 356



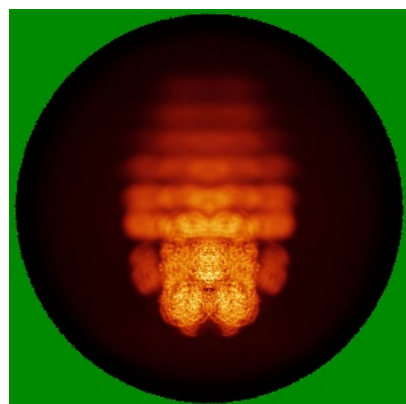
Z Index: 307

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

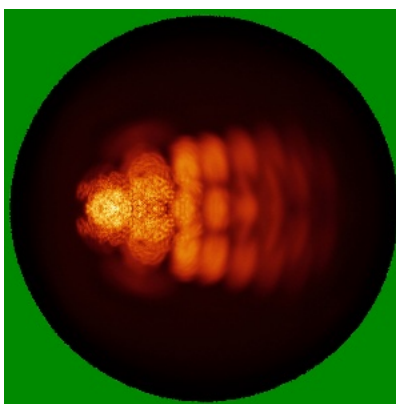


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

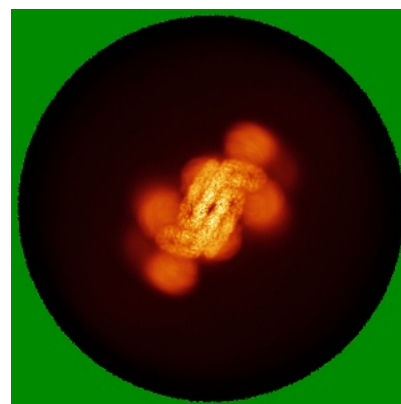
### 6.4.1 Primary map



X

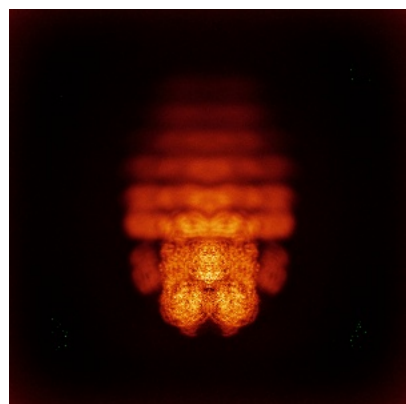


Y

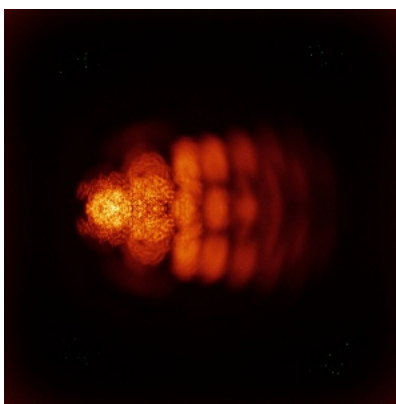


Z

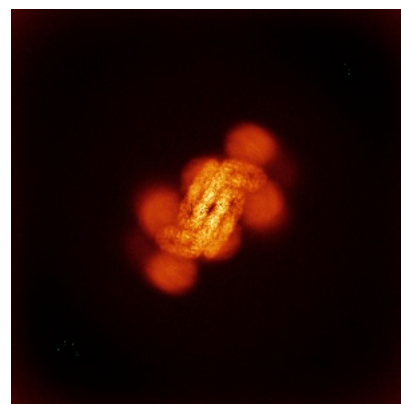
### 6.4.2 Raw map



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.

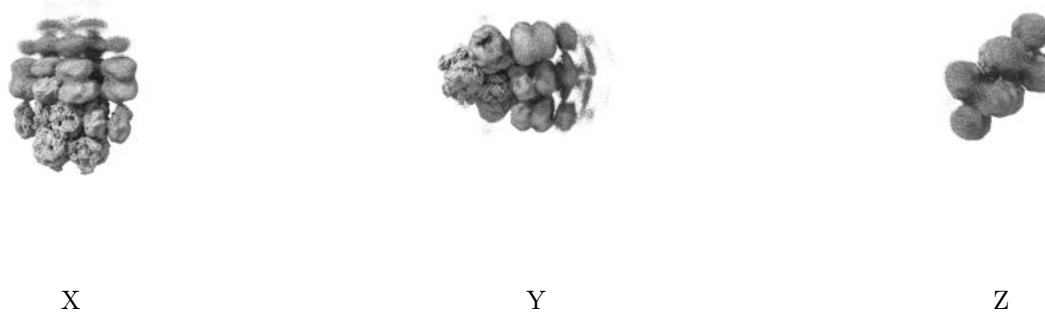
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. 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



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.

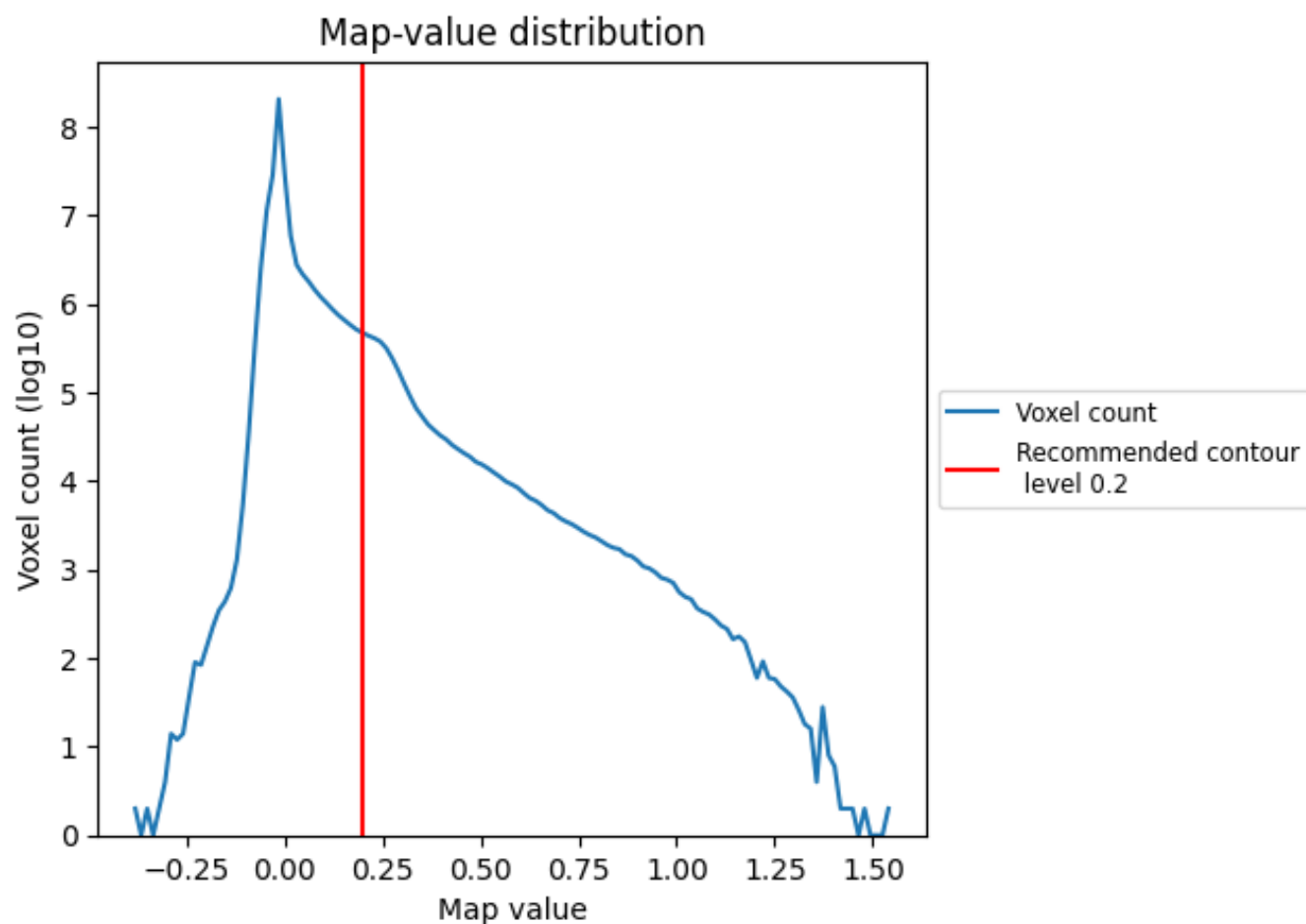
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

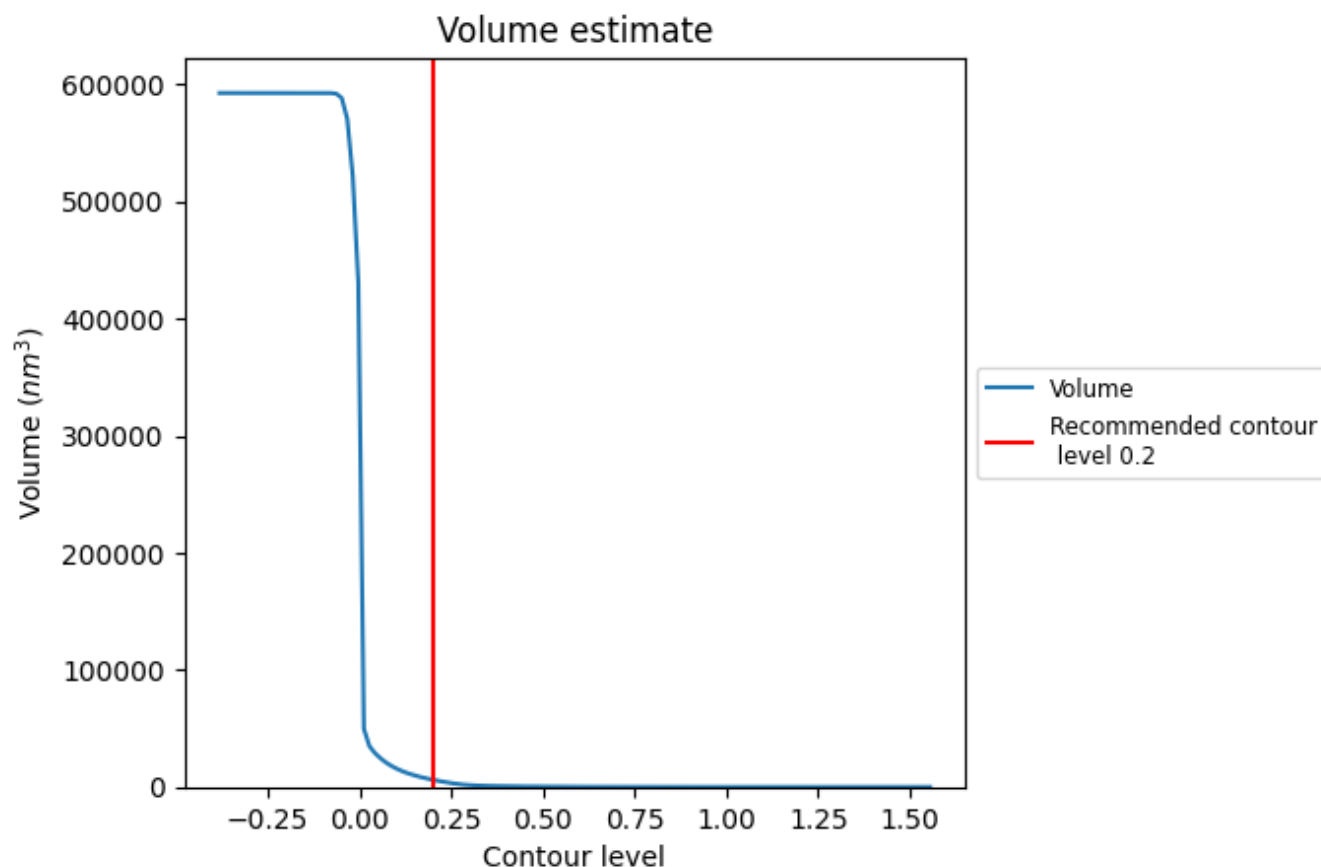
This section contains the results of statistical analysis of the map.

### 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.

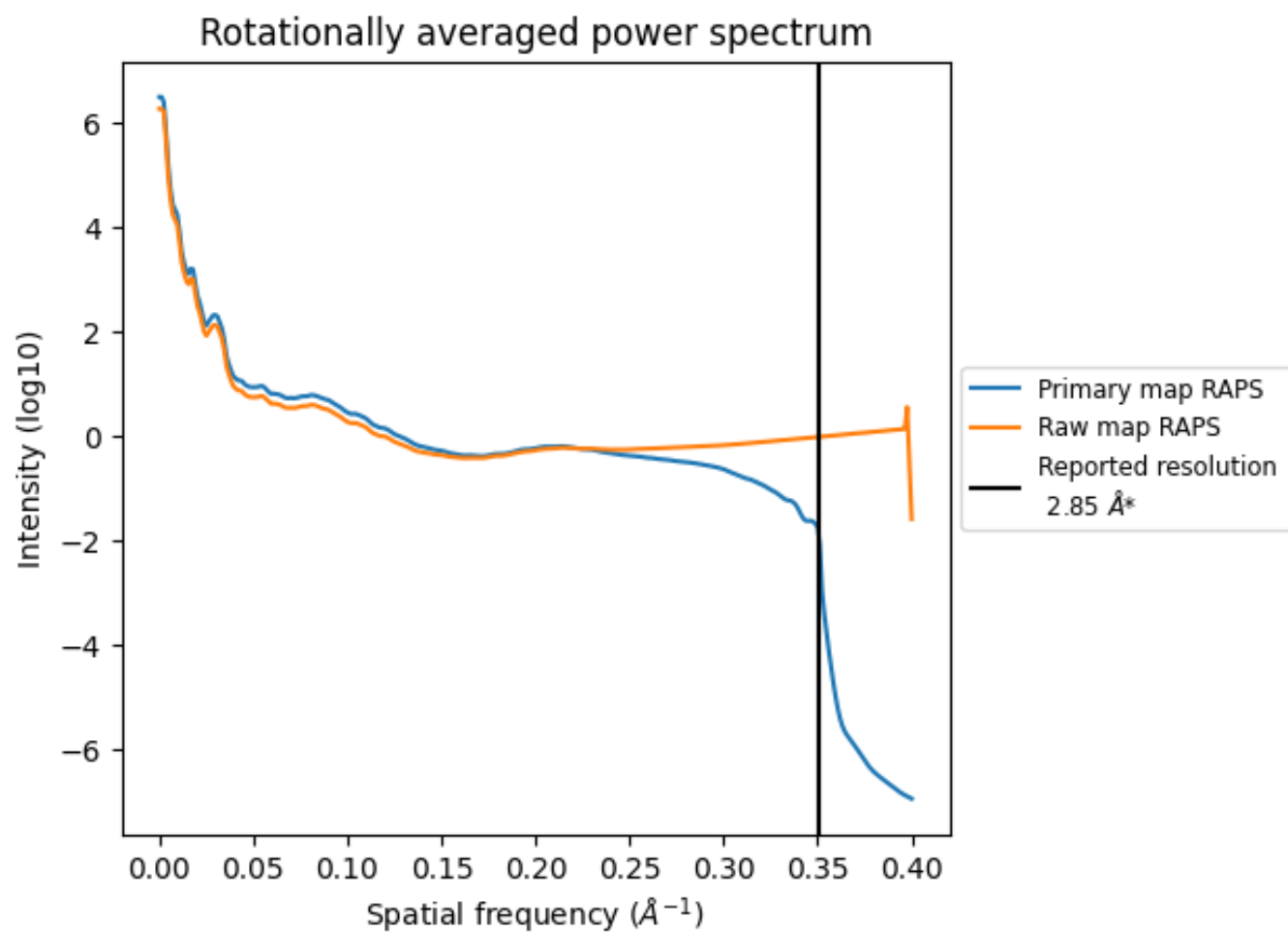
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 6137  $\text{nm}^3$ ; this corresponds to an approximate mass of 5544 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 ⓘ

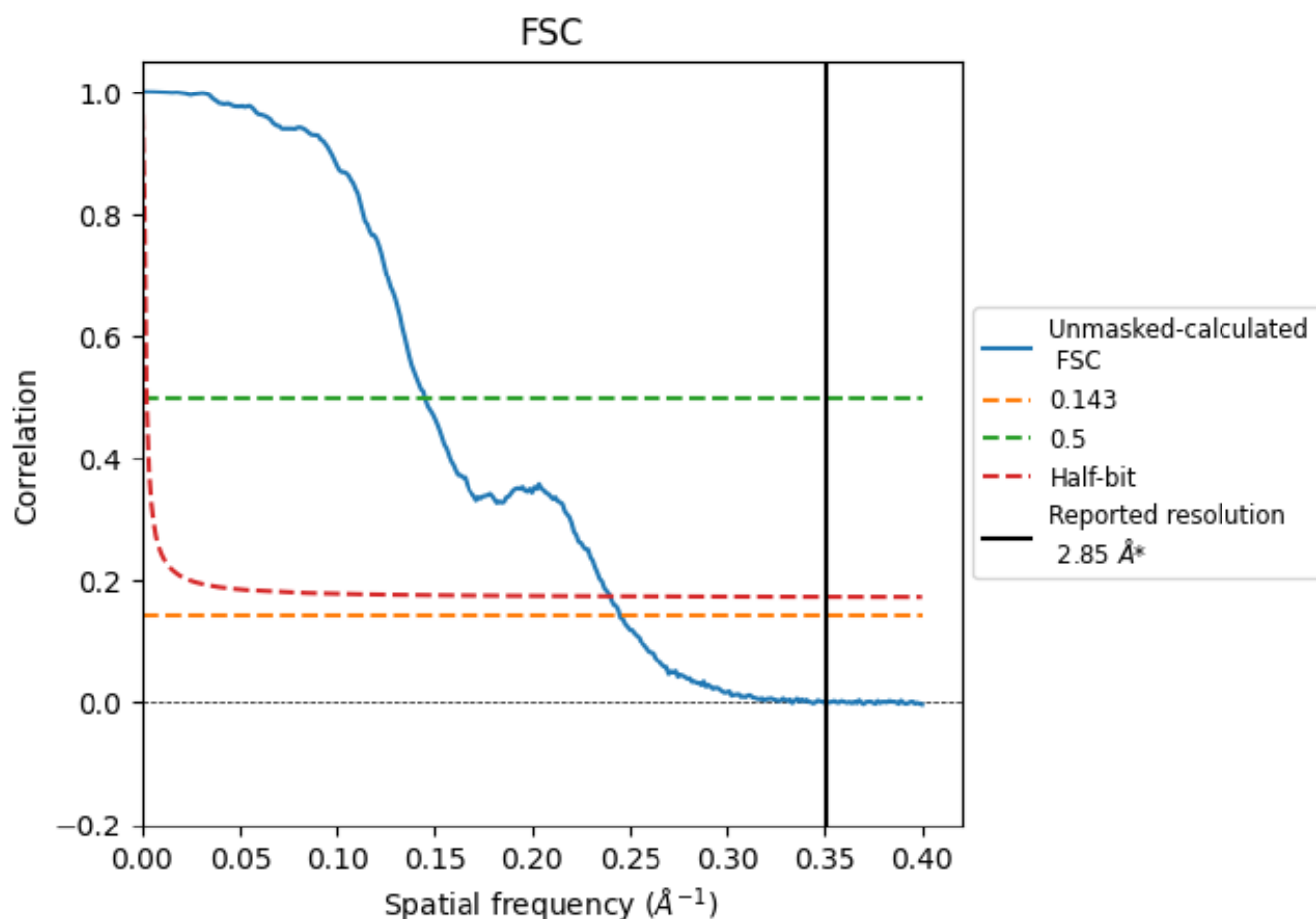


\*Reported resolution corresponds to spatial frequency of 0.351  $\text{\AA}^{-1}$

## 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 0.351 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

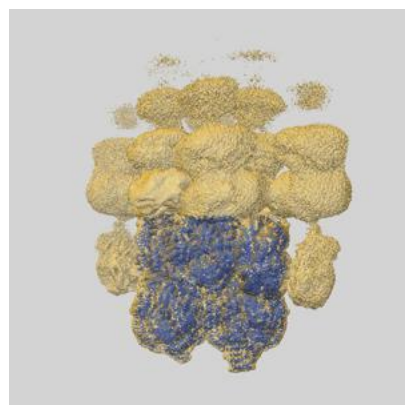
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.85	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.08	6.90	4.17

\*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 4.08 differs from the reported value 2.85 by more than 10 %

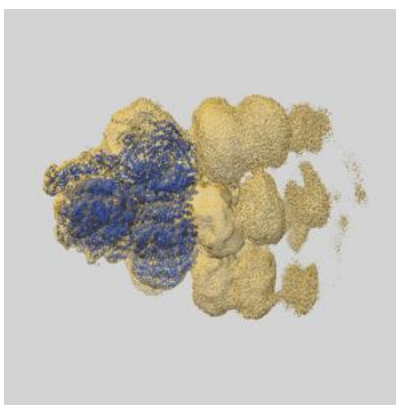
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-64815 and PDB model 9V7J. Per-residue inclusion information can be found in [section 3](#) on [page 17](#).

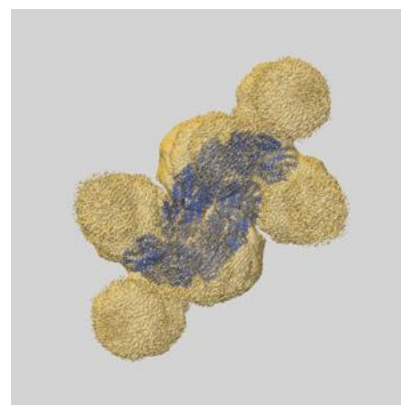
### 9.1 Map-model overlay [i](#)



X



Y

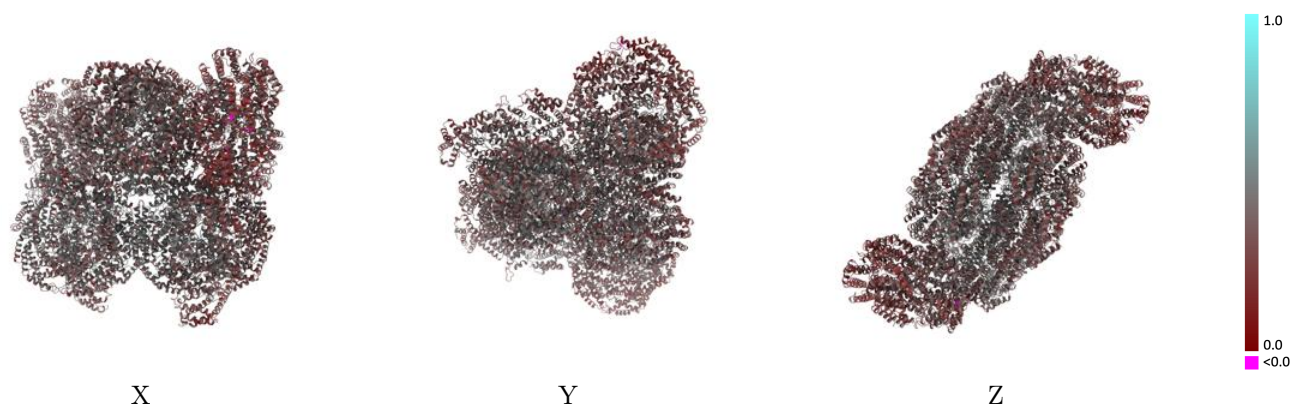


Z

The images above show the 3D surface view of the map at the recommended contour level 0.2 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.

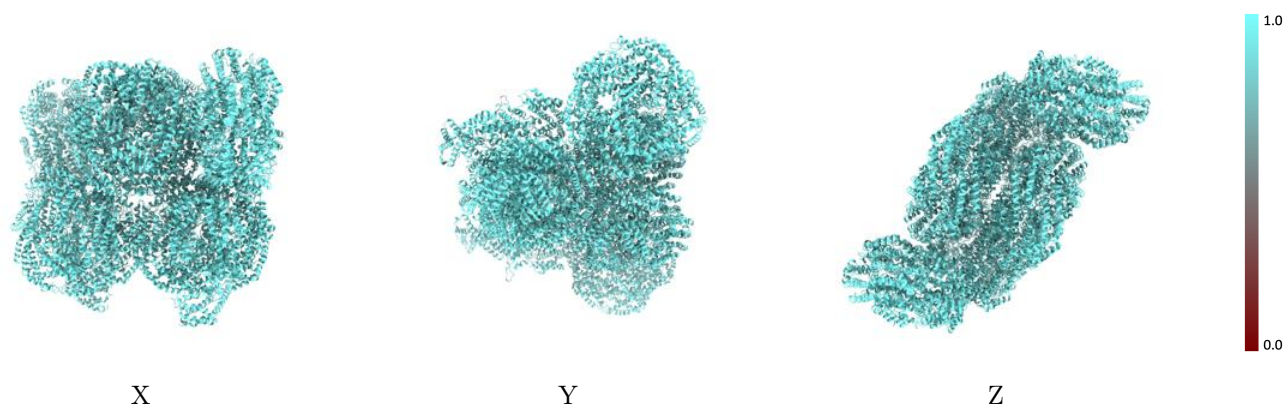


## 9.2 Q-score mapped to coordinate model [i](#)



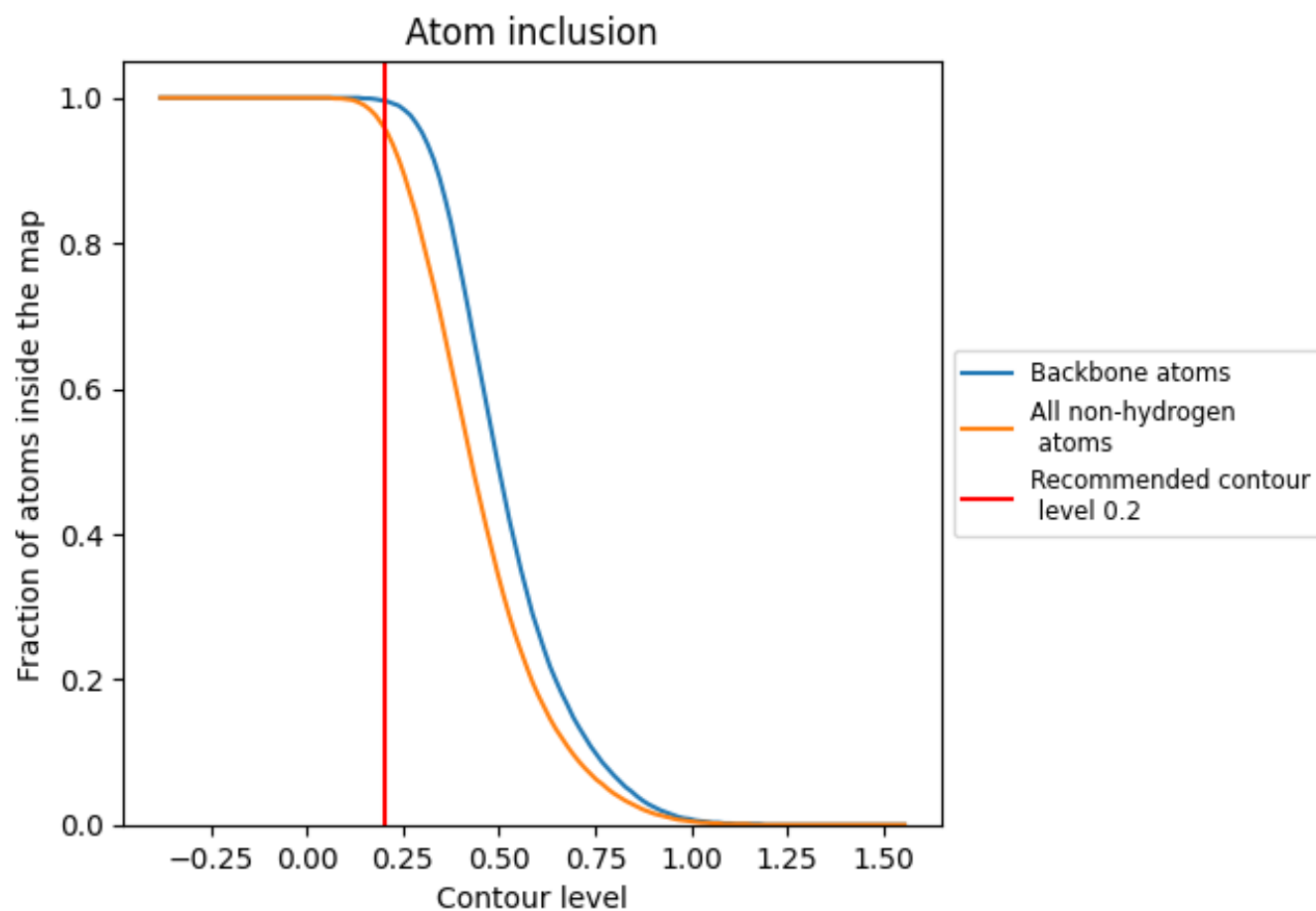
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 96% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9600	 0.3760
0	 0.9740	 0.3860
1	 0.9550	 0.3720
2	 0.9810	 0.3800
3	 0.9780	 0.4030
4	 0.9800	 0.3880
5	 0.9880	 0.4310
6	 0.9940	 0.4490
7	 0.9530	 0.4270
8	 0.9660	 0.4680
9	 0.9280	 0.4050
A	 0.9620	 0.4140
AA	 0.9590	 0.4480
AB	 0.9520	 0.4410
AC	 0.9380	 0.3750
AD	 0.9720	 0.3660
AE	 0.9560	 0.3680
AF	 0.9630	 0.3560
AG	 0.9280	 0.3580
AH	 0.9620	 0.4350
AI	 0.9470	 0.3900
AJ	 0.9330	 0.3880
AK	 0.9170	 0.3340
AL	 0.9540	 0.3880
AM	 0.9600	 0.4220
AN	 0.9390	 0.4140
AO	 0.9290	 0.3440
AP	 0.9630	 0.3450
AQ	 0.9450	 0.3740
AR	 0.9560	 0.3650
AS	 0.9310	 0.3680
AT	 0.9620	 0.4600
AU	 0.9190	 0.3490
AV	 0.9380	 0.4000
AW	 0.9340	 0.3640































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*Continued from previous page...*

Chain	Atom inclusion	Q-score
AX	 0.9390	 0.3580
AY	 0.9850	 0.3500
AZ	 0.9830	 0.3190
Aa	 0.9590	 0.4100
Ab	 0.9750	 0.3750
Ac	 0.8910	 0.3650
Ad	 0.8800	 0.3390
C	 0.9610	 0.3940
E	 0.9890	 0.3420
F	 0.9860	 0.2820
G	 0.9730	 0.2440
H	 0.9540	 0.3200
I	 0.9600	 0.2930
J	 0.9480	 0.2580
K	 0.9710	 0.2310
L	 0.9760	 0.2740
M	 0.9530	 0.3620
N	 0.9250	 0.3500
O	 0.9490	 0.3010
P	 0.9800	 0.3520
Q	 0.9480	 0.3800
R	 0.9240	 0.4000
S	 0.9360	 0.3100
T	 0.9710	 0.3730
U	 0.9800	 0.3720
V	 0.9910	 0.2960
W	 0.9810	 0.2550
X	 0.9530	 0.3520
Y	 0.9660	 0.3250
Z	 0.9460	 0.2900
a	 0.9720	 0.2440
b	 0.9800	 0.3000
c	 0.9800	 0.3640
d	 0.9780	 0.3660
e	 0.9780	 0.3730
f	 0.9860	 0.4090
g	 0.9830	 0.3930
h	 0.9800	 0.4500
i	 0.9620	 0.3810
j	 0.9770	 0.3810
k	 0.9150	 0.3740
l	 0.9640	 0.3770

*Continued on next page...*

*Continued from previous page...*

Chain	Atom inclusion	Q-score
m	 0.9650	 0.4410
n	 0.9430	 0.4230
o	 0.9610	 0.3260
p	 0.9560	 0.4240
q	 0.9670	 0.3880
r	 0.9660	 0.4330
s	 0.9690	 0.4130
t	 0.9710	 0.4310
u	 0.9680	 0.4100
v	 0.9660	 0.4010
w	 0.9830	 0.3940
x	 0.9590	 0.4550
y	 0.9860	 0.3990
z	 0.9810	 0.4540