



wwPDB EM Validation Summary Report ⓘ

Mar 20, 2026 – 12:58 PM UTC

PDB ID : 7VOT / pdb_00007vot
EMDB ID : EMD-32059
Title : The structure of dimeric photosynthetic RC-LH1 supercomplex in Class-2
Authors : Cao, P.; Li, M.; Liu, L.N.
Deposited on : 2021-10-14
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

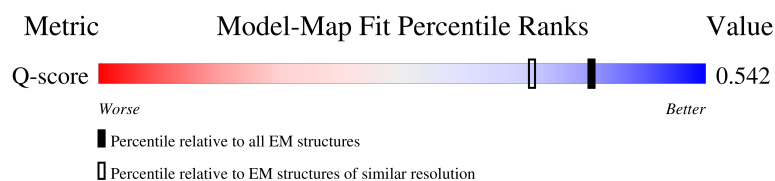
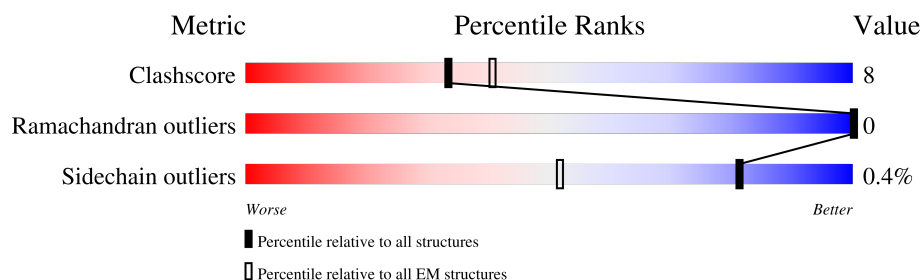
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

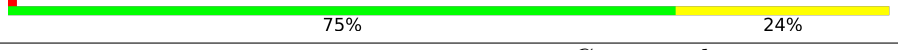
The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13054 (2.40 - 3.40)

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

Mol	Chain	Length	Quality of chain
1	L	282	
1	l	282	
2	M	308	
2	m	308	

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Mol	Chain	Length	Quality of chain
3	H	260	
3	h	260	
4	1	58	
4	3	58	
4	5	58	
4	6	58	
4	7	58	
4	9	58	
4	A	58	
4	D	58	
4	F	58	
4	I	58	
4	K	58	
4	O	58	
4	Q	58	
4	S	58	
4	U	58	
4	W	58	
4	a	58	
4	b1	58	
4	b9	58	
4	d	58	
4	f	58	
4	i	58	
4	k	58	

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Mol	Chain	Length	Quality of chain
4	o	58	
4	q	58	
4	s	58	
4	u	58	
4	w	58	
5	0	49	
5	2	49	
5	4	49	
5	8	49	
5	B	49	
5	C	49	
5	E	49	
5	G	49	
5	J	49	
5	N	49	
5	P	49	
5	R	49	
5	T	49	
5	V	49	
5	Z	49	
5	b	49	
5	b0	49	
5	b8	49	
5	c	49	
5	e	49	

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Mol	Chain	Length	Quality of chain
5	g	49	
5	j	49	
5	n	49	
5	p	49	
5	r	49	
5	t	49	
5	v	49	
5	z	49	
6	X	82	
6	x	82	
7	Y	53	
7	y	53	

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 44984 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 Reaction center protein L chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	L	281	Total	C	N	O	S	0	0
			2232	1507	355	362	8		
1	l	281	Total	C	N	O	S	0	0
			2232	1507	355	362	8		

- Molecule 2 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	M	307	Total	C	N	O	S	0	0
			2445	1630	400	404	11		
2	m	307	Total	C	N	O	S	0	0
			2445	1630	400	404	11		

- Molecule 3 is a protein called Reaction center protein H chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	258	Total	C	N	O	S	0	0
			1955	1252	333	359	11		
3	h	258	Total	C	N	O	S	0	0
			1955	1252	333	359	11		

- Molecule 4 is a protein called Light-harvesting protein B-875 alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	55	Total	C	N	O	S	0	0
			460	313	74	70	3		
4	D	55	Total	C	N	O	S	0	0
			460	313	74	70	3		
4	F	55	Total	C	N	O	S	0	0
			460	313	74	70	3		
4	I	54	Total	C	N	O	S	0	0
			455	310	73	69	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	K	54	Total	C	N	O	S	0	0
			452	308	73	69	2		
4	O	54	Total	C	N	O	S	0	0
			455	310	73	69	3		
4	Q	55	Total	C	N	O	S	0	0
			460	313	74	70	3		
4	S	55	Total	C	N	O	S	0	0
			460	313	74	70	3		
4	U	53	Total	C	N	O	S	0	0
			447	305	72	68	2		
4	W	53	Total	C	N	O	S	0	0
			447	305	72	68	2		
4	3	54	Total	C	N	O	S	0	0
			455	310	73	69	3		
4	1	53	Total	C	N	O	S	0	0
			447	305	72	68	2		
4	7	48	Total	C	N	O	S	0	0
			403	277	62	61	3		
4	9	54	Total	C	N	O	S	0	0
			455	310	73	69	3		
4	a	55	Total	C	N	O	S	0	0
			460	313	74	70	3		
4	d	55	Total	C	N	O	S	0	0
			460	313	74	70	3		
4	f	55	Total	C	N	O	S	0	0
			460	313	74	70	3		
4	i	54	Total	C	N	O	S	0	0
			455	310	73	69	3		
4	k	54	Total	C	N	O	S	0	0
			452	308	73	69	2		
4	o	54	Total	C	N	O	S	0	0
			455	310	73	69	3		
4	q	55	Total	C	N	O	S	0	0
			460	313	74	70	3		
4	s	55	Total	C	N	O	S	0	0
			460	313	74	70	3		
4	u	53	Total	C	N	O	S	0	0
			447	305	72	68	2		
4	w	53	Total	C	N	O	S	0	0
			447	305	72	68	2		
4	5	54	Total	C	N	O	S	0	0
			455	310	73	69	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	b1	53	Total	C	N	O	S	0	0
			447	305	72	68	2		
4	6	48	Total	C	N	O	S	0	0
			403	277	62	61	3		
4	b9	54	Total	C	N	O	S	0	0
			455	310	73	69	3		

- Molecule 5 is a protein called Light-harvesting protein B-875 beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	44	Total	C	N	O	S	0	0
			360	240	56	63	1		
5	E	43	Total	C	N	O	S	0	0
			352	236	55	60	1		
5	G	43	Total	C	N	O	S	0	0
			352	236	55	60	1		
5	J	42	Total	C	N	O	S	0	0
			344	230	54	59	1		
5	N	42	Total	C	N	O	S	0	0
			344	230	54	59	1		
5	P	43	Total	C	N	O	S	0	0
			352	236	55	60	1		
5	R	43	Total	C	N	O	S	0	0
			352	236	55	60	1		
5	T	42	Total	C	N	O	S	0	0
			344	230	54	59	1		
5	V	42	Total	C	N	O	S	0	0
			344	230	54	59	1		
5	C	43	Total	C	N	O	S	0	0
			352	236	55	60	1		
5	Z	42	Total	C	N	O	S	0	0
			344	230	54	59	1		
5	2	40	Total	C	N	O	S	0	0
			328	219	52	56	1		
5	8	44	Total	C	N	O	S	0	0
			360	240	56	63	1		
5	0	43	Total	C	N	O	S	0	0
			352	236	55	60	1		
5	b	44	Total	C	N	O	S	0	0
			360	240	56	63	1		
5	e	43	Total	C	N	O	S	0	0
			352	236	55	60	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	g	43	Total	C	N	O	S	0	0
			352	236	55	60	1		
5	j	42	Total	C	N	O	S	0	0
			344	230	54	59	1		
5	n	42	Total	C	N	O	S	0	0
			344	230	54	59	1		
5	p	43	Total	C	N	O	S	0	0
			352	236	55	60	1		
5	r	43	Total	C	N	O	S	0	0
			352	236	55	60	1		
5	t	42	Total	C	N	O	S	0	0
			344	230	54	59	1		
5	v	42	Total	C	N	O	S	0	0
			344	230	54	59	1		
5	c	43	Total	C	N	O	S	0	0
			352	236	55	60	1		
5	z	42	Total	C	N	O	S	0	0
			344	230	54	59	1		
5	4	40	Total	C	N	O	S	0	0
			328	219	52	56	1		
5	b8	44	Total	C	N	O	S	0	0
			360	240	56	63	1		
5	b0	43	Total	C	N	O	S	0	0
			352	236	55	60	1		

- Molecule 6 is a protein called Intrinsic membrane protein PufX.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	X	52	Total	C	N	O	S	0	0
			404	268	70	63	3		
6	x	52	Total	C	N	O	S	0	0
			404	268	70	63	3		

- Molecule 7 is a protein called Rsp_7571 Protein-Y PufY.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	Y	51	Total	C	N	O	S	0	0
			375	255	58	59	3		
7	y	51	Total	C	N	O	S	0	0
			375	255	58	59	3		

- Molecule 8 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: $C_{55}H_{74}MgN_4O_6$).



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Mol	Chain	Residues	Atoms					AltConf
8	O	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	P	1	Total 61	C 50	Mg 1	N 4	O 6	0
8	Q	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	R	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	S	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	T	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	U	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	V	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	W	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	C	1	Total 61	C 50	Mg 1	N 4	O 6	0
8	3	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	Z	1	Total 57	C 46	Mg 1	N 4	O 6	0
8	1	1	Total 51	C 40	Mg 1	N 4	O 6	0
8	2	1	Total 56	C 45	Mg 1	N 4	O 6	0
8	7	1	Total 61	C 50	Mg 1	N 4	O 6	0
8	8	1	Total 61	C 50	Mg 1	N 4	O 6	0
8	9	1	Total 56	C 45	Mg 1	N 4	O 6	0
8	0	1	Total 61	C 50	Mg 1	N 4	O 6	0
8	1	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	1	1	Total 63	C 52	Mg 1	N 4	O 6	0
8	1	1	Total 66	C 55	Mg 1	N 4	O 6	0

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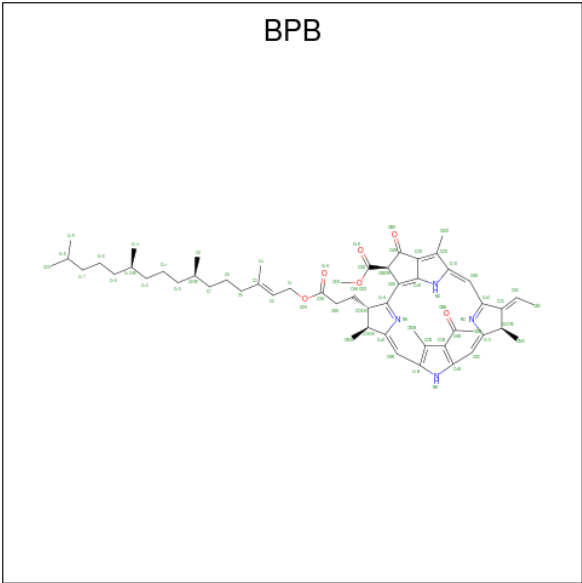
Mol	Chain	Residues	Atoms					AltConf
8	m	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	a	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	b	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	d	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	e	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	f	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	g	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	i	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	j	1	Total 61	C 50	Mg 1	N 4	O 6	0
8	k	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	n	1	Total 61	C 50	Mg 1	N 4	O 6	0
8	o	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	p	1	Total 61	C 50	Mg 1	N 4	O 6	0
8	q	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	r	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	s	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	t	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	u	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	v	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	w	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	c	1	Total 61	C 50	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
8	5	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	z	1	Total	C	Mg	N	O	0
			57	46	1	4	6	
8	b1	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
8	4	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
8	6	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
8	b8	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
8	b9	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
8	b0	1	Total	C	Mg	N	O	0
			61	50	1	4	6	

- Molecule 9 is BACTERIOPHEOPHYTIN B (CCD ID: BPB) (formula: C₅₅H₇₄N₄O₆).



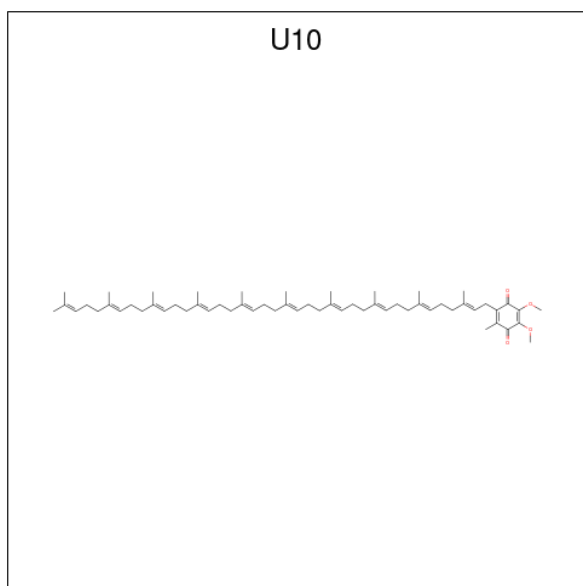
Mol	Chain	Residues	Atoms				AltConf
9	L	1	Total	C	N	O	0
			65	55	4	6	
9	M	1	Total	C	N	O	0
			55	45	4	6	
9	l	1	Total	C	N	O	0
			65	55	4	6	

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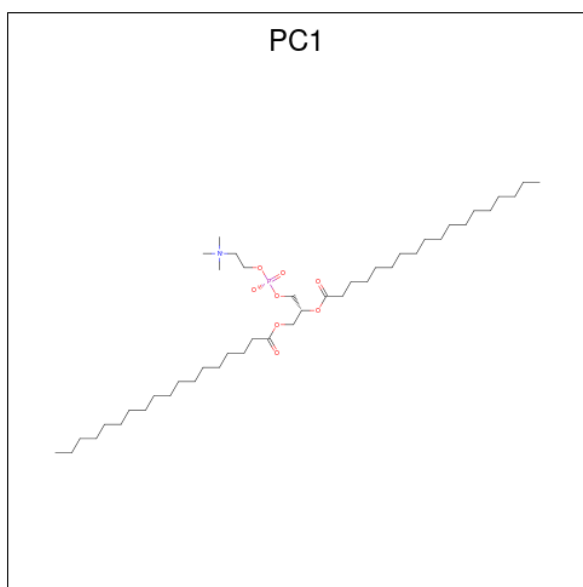
Mol	Chain	Residues	Atoms				AltConf
9	m	1	Total	C	N	O	0
			55	45	4	6	

- Molecule 10 is UBIQUINONE-10 (CCD ID: U10) (formula: $C_{59}H_{90}O_4$).



Mol	Chain	Residues	Atoms				AltConf
10	L	1	Total	C	O		0
			38	34	4		
10	L	1	Total	C	O		0
			43	39	4		
10	M	1	Total	C	O		0
			48	44	4		
10	M	1	Total	C	O		0
			38	34	4		
10	l	1	Total	C	O		0
			38	34	4		
10	l	1	Total	C	O		0
			43	39	4		
10	m	1	Total	C	O		0
			48	44	4		
10	m	1	Total	C	O		0
			38	34	4		

- Molecule 11 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
11	L	1	Total	C	N	O	P	0
			39	29	1	8	1	
11	L	1	Total	C	N	O	P	0
			32	22	1	8	1	
11	H	1	Total	C	N	O	P	0
			42	32	1	8	1	
11	H	1	Total	C	N	O	P	0
			34	24	1	8	1	
11	A	1	Total	C	N	O	P	0
			45	35	1	8	1	
11	A	1	Total	C	N	O	P	0
			31	21	1	8	1	
11	A	1	Total	C	N	O	P	0
			36	26	1	8	1	
11	D	1	Total	C	N	O	P	0
			40	30	1	8	1	
11	D	1	Total	C	N	O	P	0
			37	27	1	8	1	
11	l	1	Total	C	N	O	P	0
			39	29	1	8	1	
11	l	1	Total	C	N	O	P	0
			32	22	1	8	1	
11	h	1	Total	C	N	O	P	0
			42	32	1	8	1	
11	h	1	Total	C	N	O	P	0
			34	24	1	8	1	
11	a	1	Total	C	N	O	P	0
			45	35	1	8	1	

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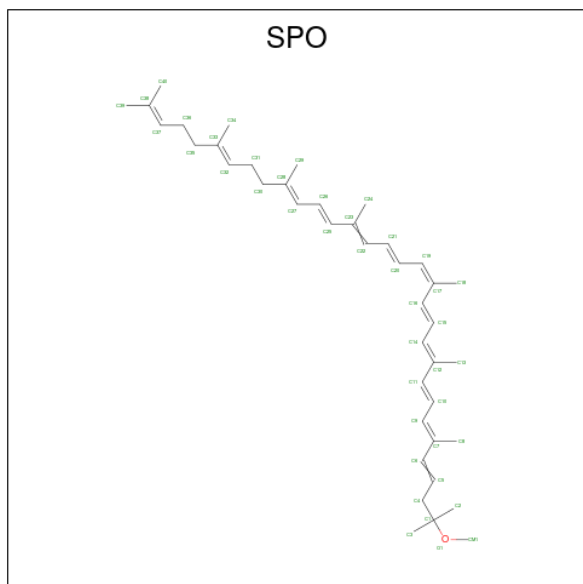
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Mol	Chain	Residues	Atoms					AltConf
11	a	1	Total	C	N	O	P	0
			31	21	1	8	1	
11	a	1	Total	C	N	O	P	0
			36	26	1	8	1	
11	d	1	Total	C	N	O	P	0
			40	30	1	8	1	
11	d	1	Total	C	N	O	P	0
			37	27	1	8	1	

- Molecule 12 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		AltConf
12	M	1	Total	Fe	0
			1	1	
12	m	1	Total	Fe	0
			1	1	

- Molecule 13 is SPHEROIDENE (CCD ID: SPO) (formula: C₄₁H₆₀O).



Mol	Chain	Residues	Atoms			AltConf
13	M	1	Total	C	O	0
			42	41	1	
13	A	1	Total	C	O	0
			42	41	1	
13	B	1	Total	C	O	0
			42	41	1	

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Mol	Chain	Residues	Atoms			AltConf
13	D	1	Total 42	C 41	O 1	0
13	E	1	Total 42	C 41	O 1	0
13	F	1	Total 42	C 41	O 1	0
13	F	1	Total 42	C 41	O 1	0
13	I	1	Total 42	C 41	O 1	0
13	I	1	Total 42	C 41	O 1	0
13	J	1	Total 42	C 41	O 1	0
13	N	1	Total 42	C 41	O 1	0
13	N	1	Total 42	C 41	O 1	0
13	O	1	Total 42	C 41	O 1	0
13	R	1	Total 42	C 41	O 1	0
13	R	1	Total 42	C 41	O 1	0
13	R	1	Total 42	C 41	O 1	0
13	S	1	Total 42	C 41	O 1	0
13	U	1	Total 42	C 41	O 1	0
13	V	1	Total 42	C 41	O 1	0
13	V	1	Total 42	C 41	O 1	0
13	C	1	Total 42	C 41	O 1	0
13	3	1	Total 42	C 41	O 1	0
13	3	1	Total 42	C 41	O 1	0
13	7	1	Total 42	C 41	O 1	0

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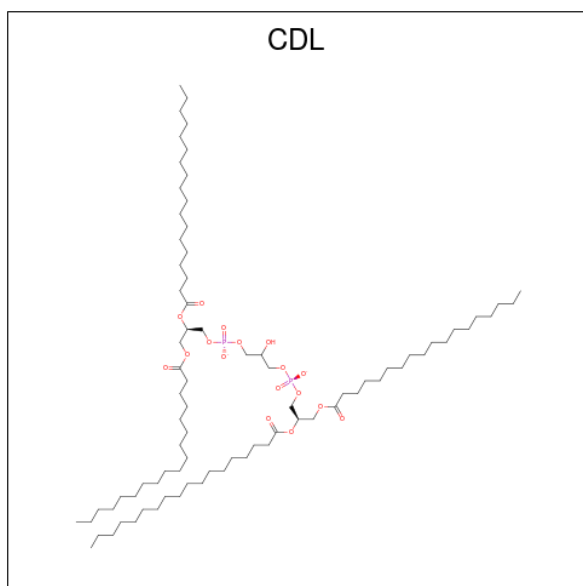
Mol	Chain	Residues	Atoms			AltConf
13	9	1	Total	C	O	0
			42	41	1	
13	0	1	Total	C	O	0
			42	41	1	
13	m	1	Total	C	O	0
			42	41	1	
13	a	1	Total	C	O	0
			42	41	1	
13	b	1	Total	C	O	0
			42	41	1	
13	d	1	Total	C	O	0
			42	41	1	
13	e	1	Total	C	O	0
			42	41	1	
13	f	1	Total	C	O	0
			42	41	1	
13	f	1	Total	C	O	0
			42	41	1	
13	i	1	Total	C	O	0
			42	41	1	
13	i	1	Total	C	O	0
			42	41	1	
13	j	1	Total	C	O	0
			42	41	1	
13	n	1	Total	C	O	0
			42	41	1	
13	n	1	Total	C	O	0
			42	41	1	
13	o	1	Total	C	O	0
			42	41	1	
13	r	1	Total	C	O	0
			42	41	1	
13	r	1	Total	C	O	0
			42	41	1	
13	r	1	Total	C	O	0
			42	41	1	
13	s	1	Total	C	O	0
			42	41	1	
13	u	1	Total	C	O	0
			42	41	1	
13	v	1	Total	C	O	0
			42	41	1	

Continued on next page...

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Mol	Chain	Residues	Atoms			AltConf
13	v	1	Total	C	O	0
			42	41	1	
13	c	1	Total	C	O	0
			42	41	1	
13	5	1	Total	C	O	0
			42	41	1	
13	5	1	Total	C	O	0
			42	41	1	
13	6	1	Total	C	O	0
			42	41	1	
13	b9	1	Total	C	O	0
			42	41	1	
13	b0	1	Total	C	O	0
			42	41	1	

- Molecule 14 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).

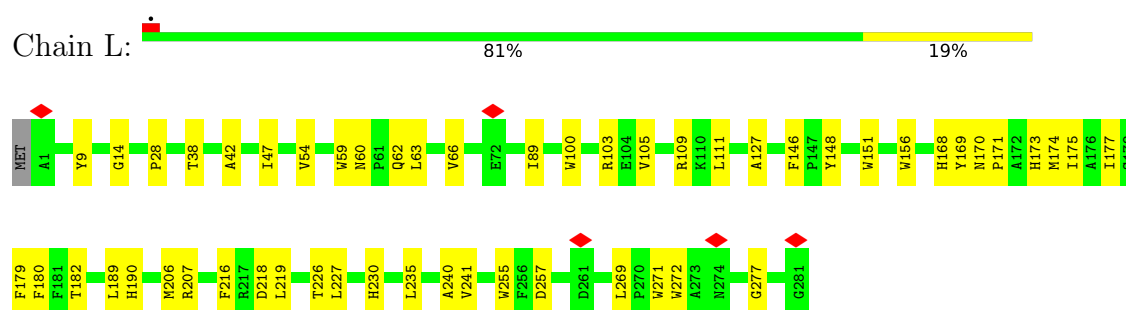


Mol	Chain	Residues	Atoms				AltConf
14	M	1	Total	C	O	P	0
			76	57	17	2	
14	H	1	Total	C	O	P	0
			63	44	17	2	
14	m	1	Total	C	O	P	0
			76	57	17	2	
14	h	1	Total	C	O	P	0
			63	44	17	2	

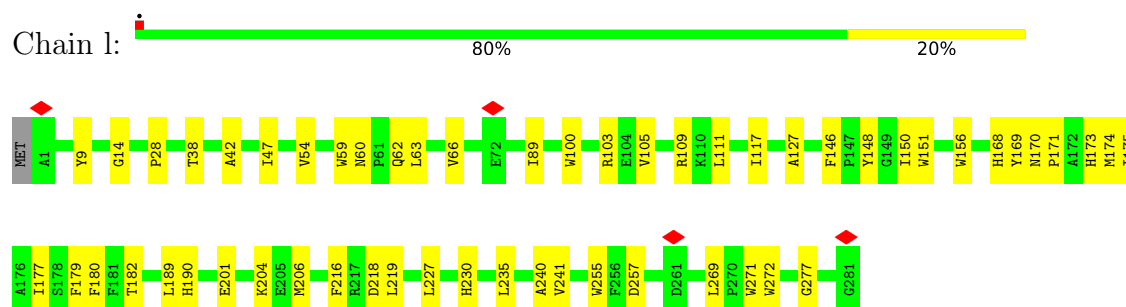
3 Residue-property plots [i](#)

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

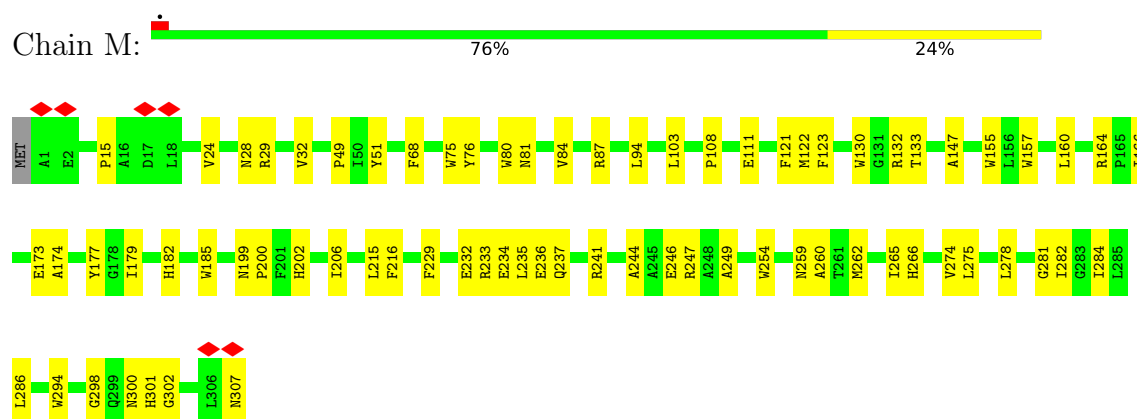
- Molecule 1: Reaction center protein L chain



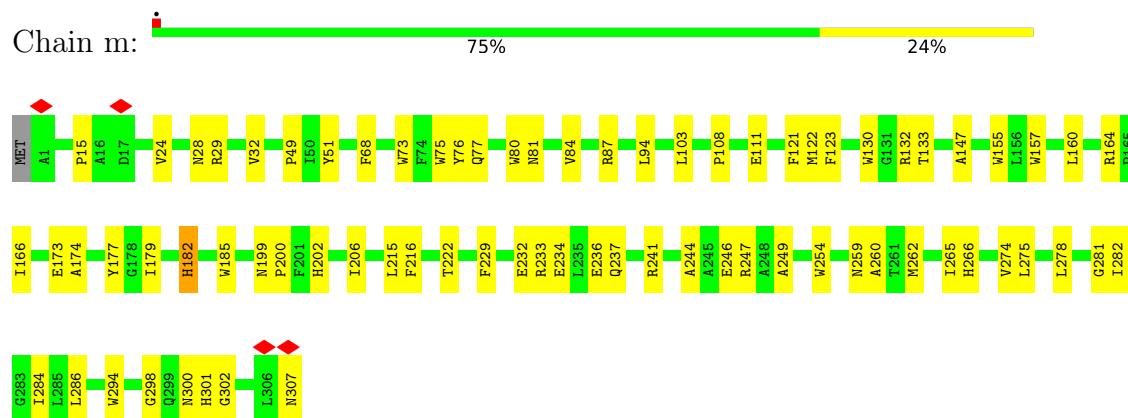
- Molecule 1: Reaction center protein L chain



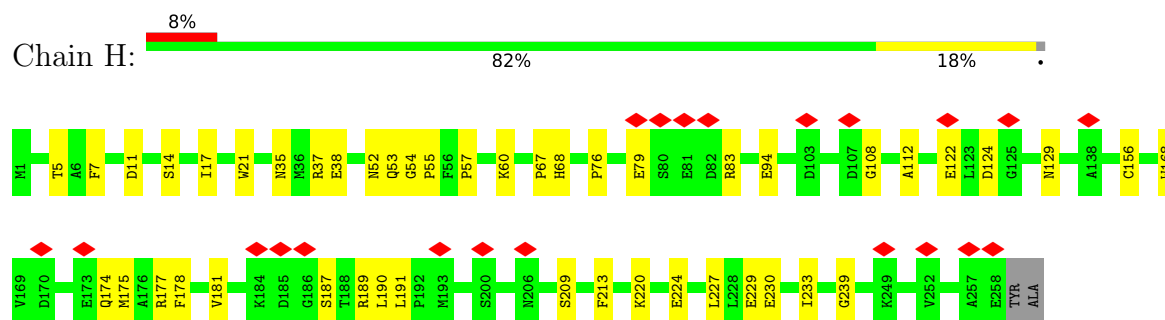
- Molecule 2: Reaction center protein M chain



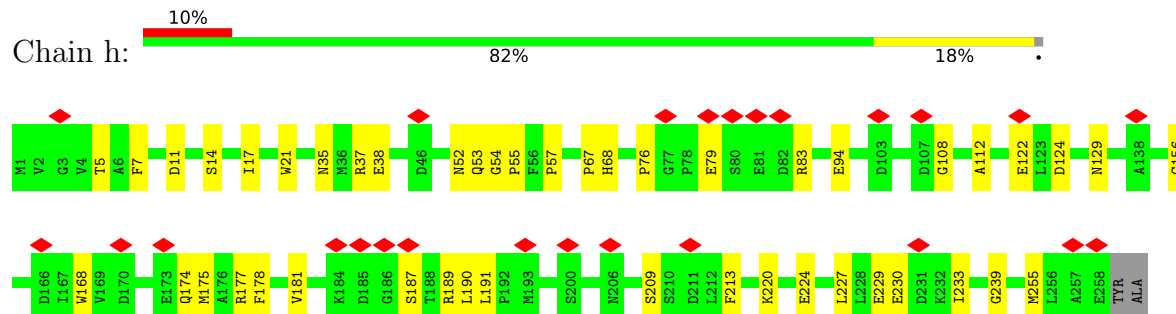
- Molecule 2: Reaction center protein M chain



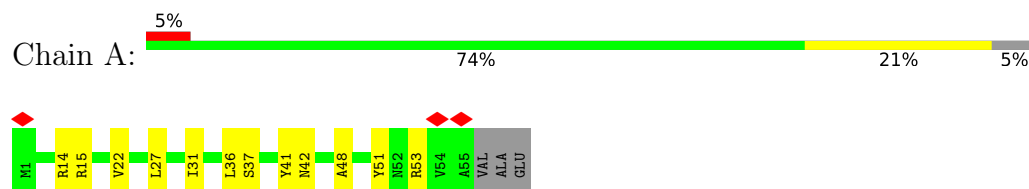
- Molecule 3: Reaction center protein H chain



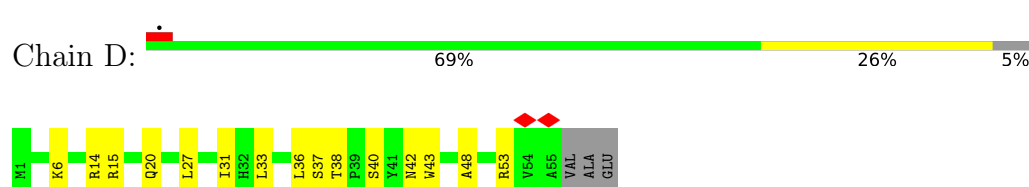
- Molecule 3: Reaction center protein H chain



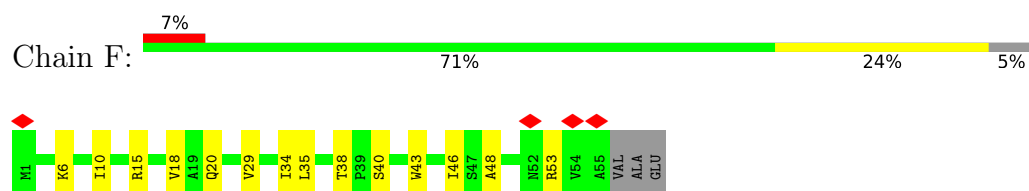
- Molecule 4: Light-harvesting protein B-875 alpha chain



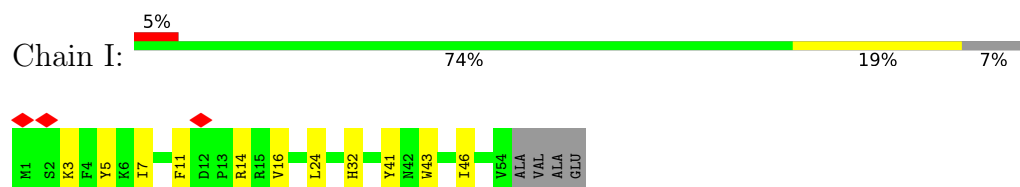
- Molecule 4: Light-harvesting protein B-875 alpha chain



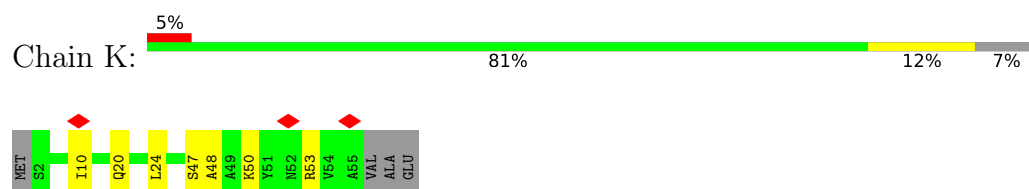
- Molecule 4: Light-harvesting protein B-875 alpha chain



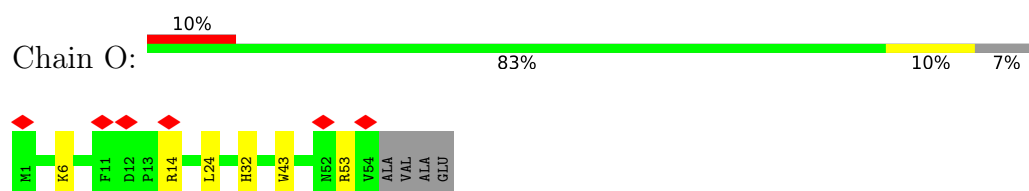
- Molecule 4: Light-harvesting protein B-875 alpha chain



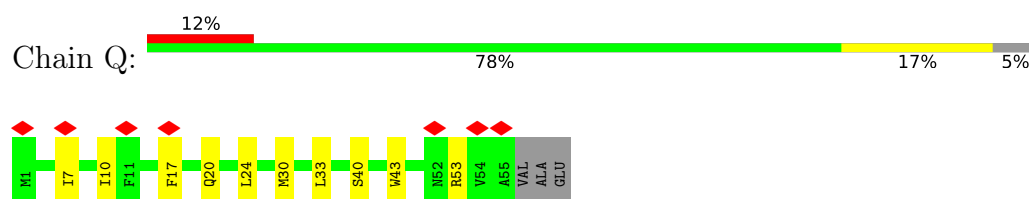
- Molecule 4: Light-harvesting protein B-875 alpha chain



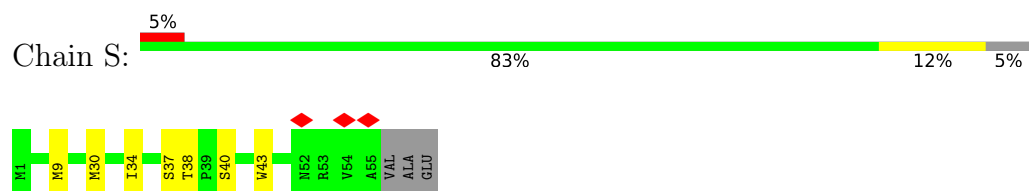
- Molecule 4: Light-harvesting protein B-875 alpha chain



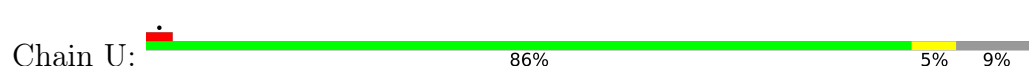
- Molecule 4: Light-harvesting protein B-875 alpha chain

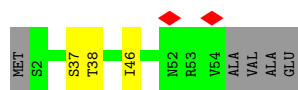


- Molecule 4: Light-harvesting protein B-875 alpha chain

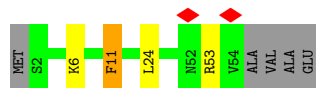
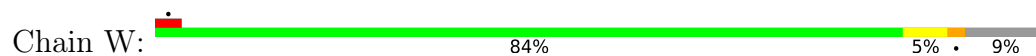


- Molecule 4: Light-harvesting protein B-875 alpha chain

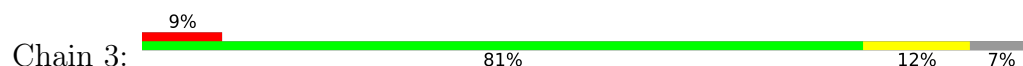




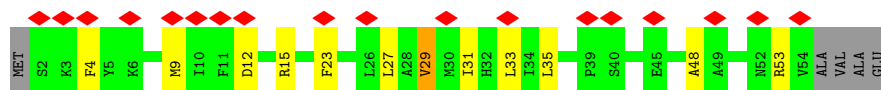
- Molecule 4: Light-harvesting protein B-875 alpha chain



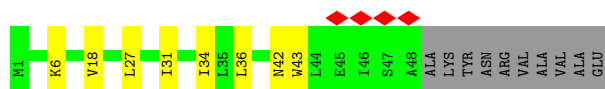
- Molecule 4: Light-harvesting protein B-875 alpha chain



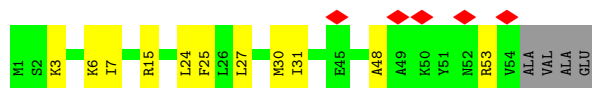
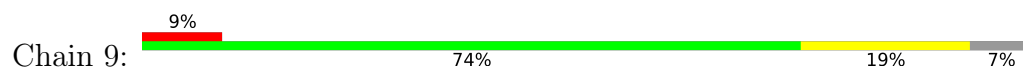
- Molecule 4: Light-harvesting protein B-875 alpha chain



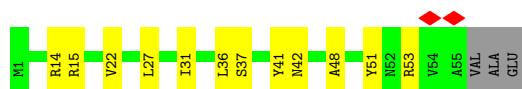
- Molecule 4: Light-harvesting protein B-875 alpha chain



- Molecule 4: Light-harvesting protein B-875 alpha chain



- Molecule 4: Light-harvesting protein B-875 alpha chain



- Molecule 4: Light-harvesting protein B-875 alpha chain

Chain d:  74% 21% 5%



- Molecule 4: Light-harvesting protein B-875 alpha chain

Chain f:  71% 24% 5%



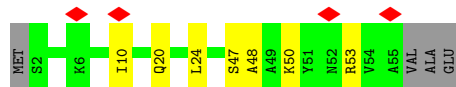
- Molecule 4: Light-harvesting protein B-875 alpha chain

Chain i:  74% 19% 7%



- Molecule 4: Light-harvesting protein B-875 alpha chain

Chain k:  81% 12% 7%



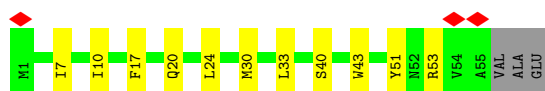
- Molecule 4: Light-harvesting protein B-875 alpha chain

Chain o:  79% 14% 7%



- Molecule 4: Light-harvesting protein B-875 alpha chain

Chain q:  76% 19% 5%



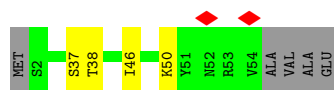
- Molecule 4: Light-harvesting protein B-875 alpha chain

Chain s:  83% 12% 5%



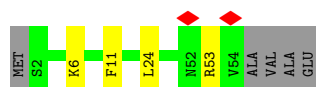
- Molecule 4: Light-harvesting protein B-875 alpha chain

Chain u:  84% 7% 9%



- Molecule 4: Light-harvesting protein B-875 alpha chain

Chain w:  84% 7% 9%



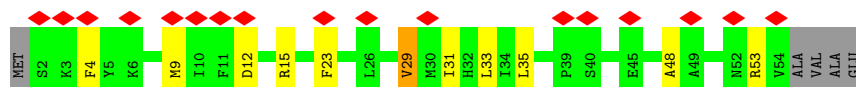
- Molecule 4: Light-harvesting protein B-875 alpha chain

Chain 5:  9% 81% 12% 7%



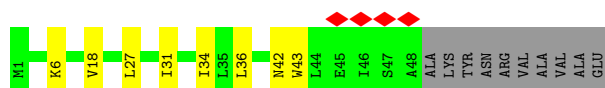
- Molecule 4: Light-harvesting protein B-875 alpha chain

Chain b1:  29% 72% 17% 9%



- Molecule 4: Light-harvesting protein B-875 alpha chain

Chain 6:  7% 69% 14% 17%



- Molecule 4: Light-harvesting protein B-875 alpha chain

Chain b9:  7% 76% 17% 7%

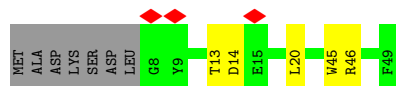
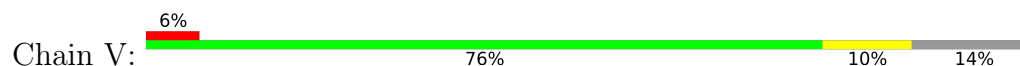


- Molecule 5: Light-harvesting protein B-875 beta chain

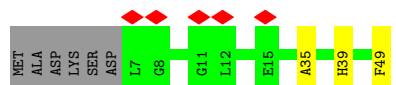
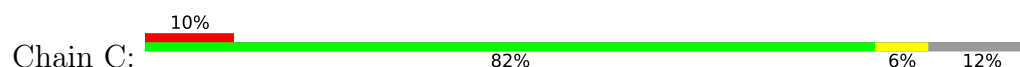
Chain B:  78% 12% 10%



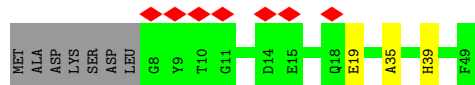
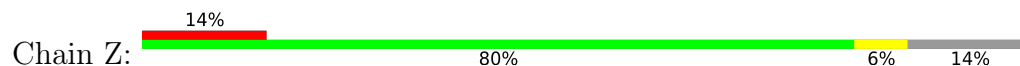
- Molecule 5: Light-harvesting protein B-875 beta chain



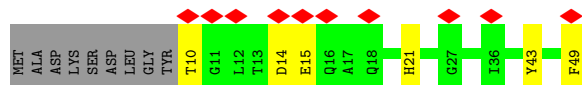
- Molecule 5: Light-harvesting protein B-875 beta chain



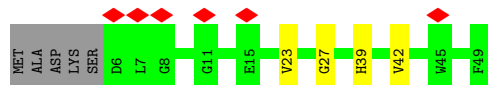
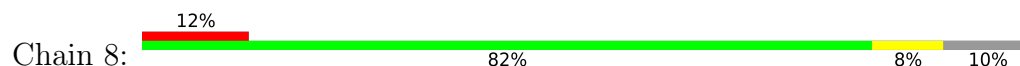
- Molecule 5: Light-harvesting protein B-875 beta chain



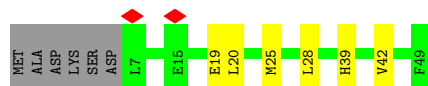
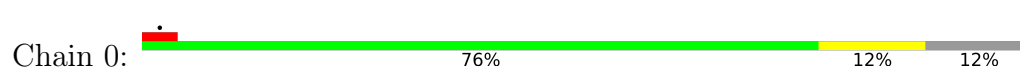
- Molecule 5: Light-harvesting protein B-875 beta chain



- Molecule 5: Light-harvesting protein B-875 beta chain



- Molecule 5: Light-harvesting protein B-875 beta chain



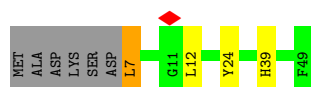
- Molecule 5: Light-harvesting protein B-875 beta chain

Chain b: 



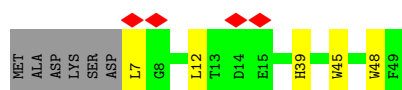
- Molecule 5: Light-harvesting protein B-875 beta chain

Chain e: 



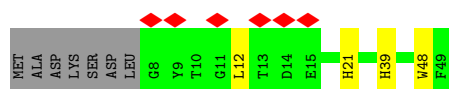
- Molecule 5: Light-harvesting protein B-875 beta chain

Chain g: 



- Molecule 5: Light-harvesting protein B-875 beta chain

Chain j: 



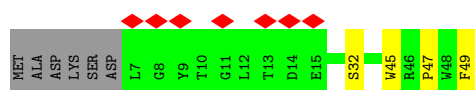
- Molecule 5: Light-harvesting protein B-875 beta chain

Chain n: 



- Molecule 5: Light-harvesting protein B-875 beta chain

Chain p: 

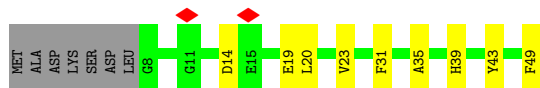


- Molecule 5: Light-harvesting protein B-875 beta chain

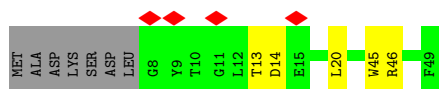
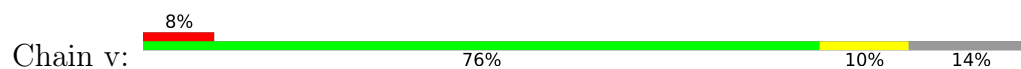
Chain r: 



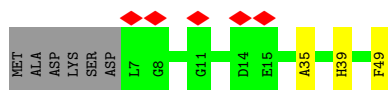
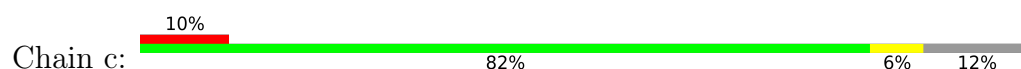
- Molecule 5: Light-harvesting protein B-875 beta chain



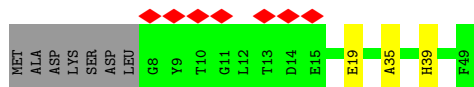
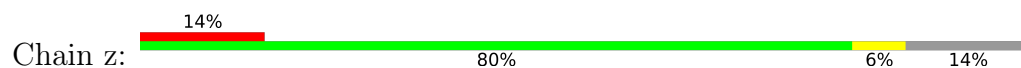
- Molecule 5: Light-harvesting protein B-875 beta chain



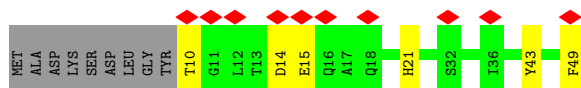
- Molecule 5: Light-harvesting protein B-875 beta chain



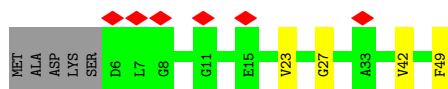
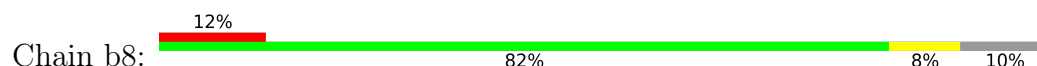
- Molecule 5: Light-harvesting protein B-875 beta chain



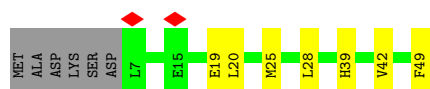
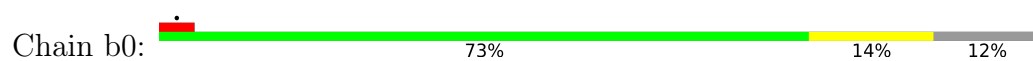
- Molecule 5: Light-harvesting protein B-875 beta chain



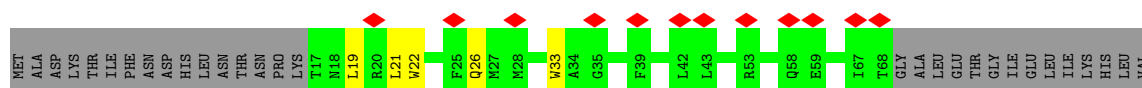
- Molecule 5: Light-harvesting protein B-875 beta chain



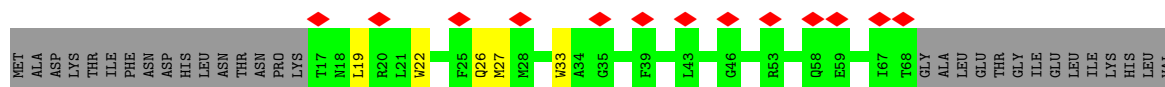
- Molecule 5: Light-harvesting protein B-875 beta chain



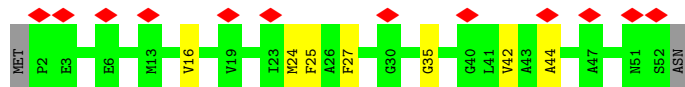
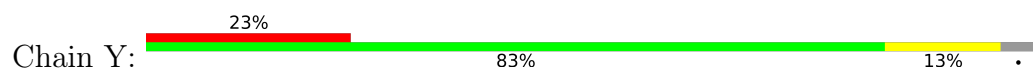
• Molecule 6: Intrinsic membrane protein PufX



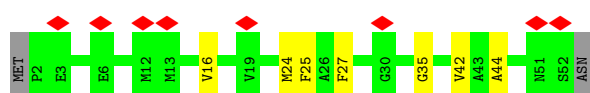
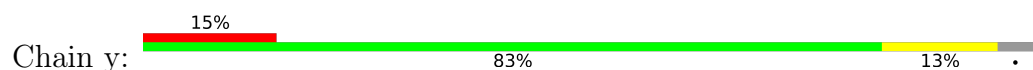
• Molecule 6: Intrinsic membrane protein PufX



• Molecule 7: Rsp_7571 Protein-Y PufY



• Molecule 7: Rsp_7571 Protein-Y PufY



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	147085	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.126	Depositor
Minimum map value	-0.076	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	432.63998, 432.63998, 432.63998	wwPDB
Map dimensions	416, 416, 416	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FE2, BPB, BCL, U10, PC1, CDL, SPO

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	L	0.20	0/2320	0.26	0/3175
1	l	0.21	0/2320	0.26	0/3175
2	M	0.23	0/2538	0.28	0/3464
2	m	0.23	0/2538	0.28	0/3464
3	H	0.15	0/2005	0.25	0/2727
3	h	0.15	0/2005	0.25	0/2727
4	1	0.10	0/461	0.21	0/625
4	3	0.13	0/469	0.21	0/635
4	5	0.13	0/469	0.21	0/635
4	6	0.14	0/416	0.24	0/564
4	7	0.14	0/416	0.24	0/564
4	9	0.17	0/469	0.26	0/635
4	A	0.18	0/474	0.25	0/642
4	D	0.19	0/474	0.25	0/642
4	F	0.17	0/474	0.24	0/642
4	I	0.14	0/469	0.23	0/635
4	K	0.14	0/466	0.23	0/632
4	O	0.14	0/469	0.24	0/635
4	Q	0.16	0/474	0.31	0/642
4	S	0.18	0/474	0.24	0/642
4	U	0.17	0/461	0.29	0/625
4	W	0.16	0/461	0.25	0/625
4	a	0.19	0/474	0.25	0/642
4	b1	0.11	0/461	0.21	0/625
4	b9	0.17	0/469	0.26	0/635
4	d	0.19	0/474	0.25	0/642
4	f	0.17	0/474	0.24	0/642
4	i	0.14	0/469	0.23	0/635
4	k	0.14	0/466	0.23	0/632
4	o	0.15	0/469	0.25	0/635
4	q	0.17	0/474	0.31	0/642
4	s	0.18	0/474	0.24	0/642

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
4	u	0.17	0/461	0.29	0/625
4	w	0.16	0/461	0.25	0/625
5	0	0.14	0/365	0.20	0/499
5	2	0.10	0/340	0.21	0/465
5	4	0.10	0/340	0.21	0/465
5	8	0.11	0/373	0.16	0/510
5	B	0.15	0/373	0.20	0/510
5	C	0.12	0/365	0.19	0/499
5	E	0.16	0/365	0.23	0/499
5	G	0.14	0/365	0.20	0/499
5	J	0.12	0/357	0.19	0/488
5	N	0.11	0/357	0.18	0/488
5	P	0.11	0/365	0.19	0/499
5	R	0.13	0/365	0.22	0/499
5	T	0.14	0/357	0.20	0/488
5	V	0.15	0/357	0.19	0/488
5	Z	0.10	0/357	0.19	0/488
5	b	0.16	0/373	0.20	0/510
5	b0	0.14	0/365	0.20	0/499
5	b8	0.12	0/373	0.17	0/510
5	c	0.12	0/365	0.19	0/499
5	e	0.16	0/365	0.23	0/499
5	g	0.14	0/365	0.20	0/499
5	j	0.12	0/357	0.19	0/488
5	n	0.11	0/357	0.18	0/488
5	p	0.11	0/365	0.19	0/499
5	r	0.13	0/365	0.22	0/499
5	t	0.14	0/357	0.20	0/488
5	v	0.15	0/357	0.19	0/488
5	z	0.11	0/357	0.19	0/488
6	X	0.13	0/415	0.21	0/562
6	x	0.13	0/415	0.21	0/562
7	Y	0.12	0/387	0.21	0/524
7	y	0.13	0/387	0.21	0/524
All	All	0.17	0/38474	0.24	0/52384

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	L	2232	0	2187	49	0
1	l	2232	0	2187	52	0
2	M	2445	0	2359	59	0
2	m	2445	0	2359	59	0
3	H	1955	0	1967	40	0
3	h	1955	0	1967	41	0
4	1	447	0	465	10	0
4	3	455	0	477	6	0
4	5	455	0	477	6	0
4	6	403	0	422	6	0
4	7	403	0	422	6	0
4	9	455	0	477	8	0
4	A	460	0	482	9	0
4	D	460	0	482	16	0
4	F	460	0	482	13	0
4	I	455	0	477	11	0
4	K	452	0	470	6	0
4	O	455	0	477	8	0
4	Q	460	0	482	12	0
4	S	460	0	482	6	0
4	U	447	0	465	3	0
4	W	447	0	465	4	0
4	a	460	0	482	11	0
4	b1	447	0	465	11	0
4	b9	455	0	477	8	0
4	d	460	0	482	14	0
4	f	460	0	482	13	0
4	i	455	0	477	11	0
4	k	452	0	470	6	0
4	o	455	0	477	9	0
4	q	460	0	482	13	0
4	s	460	0	482	6	0
4	u	447	0	465	4	0
4	w	447	0	465	3	0
5	0	352	0	336	6	0
5	2	328	0	313	4	0
5	4	328	0	313	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	8	360	0	340	4	0
5	B	360	0	340	7	0
5	C	352	0	336	2	0
5	E	352	0	336	4	0
5	G	352	0	336	6	0
5	J	344	0	325	5	0
5	N	344	0	325	5	0
5	P	352	0	336	3	0
5	R	352	0	336	7	0
5	T	344	0	325	7	0
5	V	344	0	325	4	0
5	Z	344	0	325	2	0
5	b	360	0	340	8	0
5	b0	352	0	336	7	0
5	b8	360	0	340	4	0
5	c	352	0	336	2	0
5	e	352	0	336	4	0
5	g	352	0	336	6	0
5	j	344	0	325	5	0
5	n	344	0	325	5	0
5	p	352	0	336	4	0
5	r	352	0	336	7	0
5	t	344	0	325	8	0
5	v	344	0	325	4	0
5	z	344	0	325	2	0
6	X	404	0	414	4	0
6	x	404	0	414	4	0
7	Y	375	0	371	6	0
7	y	375	0	371	7	0
8	0	61	0	61	2	0
8	1	51	0	41	0	0
8	2	56	0	51	1	0
8	3	66	0	74	4	0
8	4	56	0	51	2	0
8	5	66	0	74	4	0
8	6	61	0	61	2	0
8	7	61	0	61	2	0
8	8	61	0	61	2	0
8	9	56	0	51	4	0
8	A	66	0	74	4	0
8	B	66	0	74	3	0
8	C	61	0	61	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	D	66	0	74	5	0
8	E	66	0	74	2	0
8	F	66	0	74	4	0
8	G	66	0	74	5	0
8	I	66	0	74	5	0
8	J	61	0	61	5	0
8	K	66	0	74	4	0
8	L	195	0	213	10	0
8	M	66	0	74	1	0
8	N	61	0	61	5	0
8	O	66	0	74	10	0
8	P	61	0	61	4	0
8	Q	66	0	74	6	0
8	R	66	0	74	3	0
8	S	66	0	74	5	0
8	T	66	0	74	3	0
8	U	66	0	74	1	0
8	V	66	0	74	2	0
8	W	66	0	74	2	0
8	Z	57	0	53	0	0
8	a	66	0	74	3	0
8	b	66	0	74	5	0
8	b0	61	0	61	2	0
8	b1	51	0	41	0	0
8	b8	61	0	61	0	0
8	b9	56	0	51	4	0
8	c	61	0	61	2	0
8	d	66	0	74	6	0
8	e	66	0	74	2	0
8	f	66	0	74	5	0
8	g	66	0	74	5	0
8	i	66	0	74	6	0
8	j	61	0	61	5	0
8	k	66	0	74	4	0
8	l	195	0	213	11	0
8	m	66	0	74	1	0
8	n	61	0	61	5	0
8	o	66	0	74	10	0
8	p	61	0	61	4	0
8	q	66	0	74	6	0
8	r	66	0	74	3	0
8	s	66	0	74	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	t	66	0	74	4	0
8	u	66	0	74	2	0
8	v	66	0	74	1	0
8	w	66	0	74	1	0
8	z	57	0	53	0	0
9	L	65	0	74	5	0
9	M	55	0	51	2	0
9	l	65	0	74	4	0
9	m	55	0	51	2	0
10	L	81	0	102	8	0
10	M	86	0	110	3	0
10	l	81	0	102	9	0
10	m	86	0	110	3	0
11	A	112	0	146	13	0
11	D	77	0	102	7	0
11	H	76	0	100	8	0
11	L	71	0	90	5	0
11	a	112	0	146	12	0
11	d	77	0	102	7	0
11	h	76	0	100	10	0
11	l	71	0	90	5	0
12	M	1	0	0	0	0
12	m	1	0	0	0	0
13	0	42	0	60	0	0
13	3	84	0	120	7	0
13	5	84	0	120	6	0
13	6	42	0	60	5	0
13	7	42	0	60	5	0
13	9	42	0	60	3	0
13	A	42	0	60	4	0
13	B	42	0	60	2	0
13	C	42	0	60	2	0
13	D	42	0	60	2	0
13	E	42	0	60	0	0
13	F	84	0	120	6	0
13	I	84	0	120	4	0
13	J	42	0	60	4	0
13	M	42	0	60	5	0
13	N	84	0	120	7	0
13	O	42	0	60	3	0
13	R	126	0	180	13	0
13	S	42	0	60	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	U	42	0	60	3	0
13	V	84	0	120	1	0
13	a	42	0	60	4	0
13	b	42	0	60	2	0
13	b0	42	0	60	1	0
13	b9	42	0	60	2	0
13	c	42	0	60	2	0
13	d	42	0	60	2	0
13	e	42	0	60	0	0
13	f	84	0	120	7	0
13	i	84	0	120	3	0
13	j	42	0	60	4	0
13	m	42	0	60	5	0
13	n	84	0	120	6	0
13	o	42	0	60	2	0
13	r	126	0	180	12	0
13	s	42	0	60	4	0
13	u	42	0	60	2	0
13	v	84	0	120	1	0
14	H	63	0	70	2	0
14	M	76	0	96	4	0
14	h	63	0	70	2	0
14	m	76	0	96	1	0
All	All	44984	0	46412	754	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 8.

The worst 5 of 754 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:M:234:GLU:OE1	2:M:266:HIS:CE1	2.27	0.88
2:m:234:GLU:OE1	2:m:266:HIS:CE1	2.27	0.86
1:l:230:HIS:CE1	2:m:234:GLU:OE2	2.30	0.84
1:L:230:HIS:CE1	2:M:234:GLU:OE2	2.30	0.83
13:N:103:SPO:H10	5:P:45:TRP:HB2	1.69	0.75

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	L	279/282 (99%)	273 (98%)	6 (2%)	0	100	100
1	l	279/282 (99%)	273 (98%)	6 (2%)	0	100	100
2	M	305/308 (99%)	297 (97%)	8 (3%)	0	100	100
2	m	305/308 (99%)	297 (97%)	8 (3%)	0	100	100
3	H	256/260 (98%)	252 (98%)	4 (2%)	0	100	100
3	h	256/260 (98%)	252 (98%)	4 (2%)	0	100	100
4	1	51/58 (88%)	49 (96%)	2 (4%)	0	100	100
4	3	52/58 (90%)	52 (100%)	0	0	100	100
4	5	52/58 (90%)	52 (100%)	0	0	100	100
4	6	46/58 (79%)	45 (98%)	1 (2%)	0	100	100
4	7	46/58 (79%)	45 (98%)	1 (2%)	0	100	100
4	9	52/58 (90%)	51 (98%)	1 (2%)	0	100	100
4	A	53/58 (91%)	53 (100%)	0	0	100	100
4	D	53/58 (91%)	52 (98%)	1 (2%)	0	100	100
4	F	53/58 (91%)	51 (96%)	2 (4%)	0	100	100
4	I	52/58 (90%)	52 (100%)	0	0	100	100
4	K	52/58 (90%)	51 (98%)	1 (2%)	0	100	100
4	O	52/58 (90%)	51 (98%)	1 (2%)	0	100	100
4	Q	53/58 (91%)	51 (96%)	2 (4%)	0	100	100
4	S	53/58 (91%)	52 (98%)	1 (2%)	0	100	100
4	U	51/58 (88%)	50 (98%)	1 (2%)	0	100	100
4	W	51/58 (88%)	50 (98%)	1 (2%)	0	100	100
4	a	53/58 (91%)	53 (100%)	0	0	100	100
4	b1	51/58 (88%)	49 (96%)	2 (4%)	0	100	100
4	b9	52/58 (90%)	51 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	d	53/58 (91%)	52 (98%)	1 (2%)	0	100	100
4	f	53/58 (91%)	51 (96%)	2 (4%)	0	100	100
4	i	52/58 (90%)	52 (100%)	0	0	100	100
4	k	52/58 (90%)	51 (98%)	1 (2%)	0	100	100
4	o	52/58 (90%)	51 (98%)	1 (2%)	0	100	100
4	q	53/58 (91%)	51 (96%)	2 (4%)	0	100	100
4	s	53/58 (91%)	52 (98%)	1 (2%)	0	100	100
4	u	51/58 (88%)	50 (98%)	1 (2%)	0	100	100
4	w	51/58 (88%)	50 (98%)	1 (2%)	0	100	100
5	0	41/49 (84%)	40 (98%)	1 (2%)	0	100	100
5	2	38/49 (78%)	38 (100%)	0	0	100	100
5	4	38/49 (78%)	38 (100%)	0	0	100	100
5	8	42/49 (86%)	42 (100%)	0	0	100	100
5	B	42/49 (86%)	42 (100%)	0	0	100	100
5	C	41/49 (84%)	41 (100%)	0	0	100	100
5	E	41/49 (84%)	40 (98%)	1 (2%)	0	100	100
5	G	41/49 (84%)	41 (100%)	0	0	100	100
5	J	40/49 (82%)	40 (100%)	0	0	100	100
5	N	40/49 (82%)	40 (100%)	0	0	100	100
5	P	41/49 (84%)	41 (100%)	0	0	100	100
5	R	41/49 (84%)	41 (100%)	0	0	100	100
5	T	40/49 (82%)	40 (100%)	0	0	100	100
5	V	40/49 (82%)	40 (100%)	0	0	100	100
5	Z	40/49 (82%)	40 (100%)	0	0	100	100
5	b	42/49 (86%)	42 (100%)	0	0	100	100
5	b0	41/49 (84%)	40 (98%)	1 (2%)	0	100	100
5	b8	42/49 (86%)	42 (100%)	0	0	100	100
5	c	41/49 (84%)	41 (100%)	0	0	100	100
5	e	41/49 (84%)	40 (98%)	1 (2%)	0	100	100
5	g	41/49 (84%)	41 (100%)	0	0	100	100
5	j	40/49 (82%)	40 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	n	40/49 (82%)	40 (100%)	0	0	100	100
5	p	41/49 (84%)	41 (100%)	0	0	100	100
5	r	41/49 (84%)	41 (100%)	0	0	100	100
5	t	40/49 (82%)	40 (100%)	0	0	100	100
5	v	40/49 (82%)	40 (100%)	0	0	100	100
5	z	40/49 (82%)	40 (100%)	0	0	100	100
6	X	50/82 (61%)	50 (100%)	0	0	100	100
6	x	50/82 (61%)	50 (100%)	0	0	100	100
7	Y	49/53 (92%)	49 (100%)	0	0	100	100
7	y	49/53 (92%)	49 (100%)	0	0	100	100
All	All	4462/4966 (90%)	4394 (98%)	68 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	L	220/221 (100%)	219 (100%)	1 (0%)	81	93
1	l	220/221 (100%)	219 (100%)	1 (0%)	81	93
2	M	240/241 (100%)	237 (99%)	3 (1%)	61	86
2	m	240/241 (100%)	237 (99%)	3 (1%)	61	86
3	H	207/208 (100%)	207 (100%)	0	100	100
3	h	207/208 (100%)	207 (100%)	0	100	100
4	1	48/51 (94%)	47 (98%)	1 (2%)	47	77
4	3	49/51 (96%)	49 (100%)	0	100	100
4	5	49/51 (96%)	49 (100%)	0	100	100
4	6	44/51 (86%)	44 (100%)	0	100	100
4	7	44/51 (86%)	44 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	9	49/51 (96%)	49 (100%)	0	100	100
4	A	49/51 (96%)	49 (100%)	0	100	100
4	D	49/51 (96%)	49 (100%)	0	100	100
4	F	49/51 (96%)	49 (100%)	0	100	100
4	I	49/51 (96%)	49 (100%)	0	100	100
4	K	48/51 (94%)	48 (100%)	0	100	100
4	O	49/51 (96%)	49 (100%)	0	100	100
4	Q	49/51 (96%)	49 (100%)	0	100	100
4	S	49/51 (96%)	49 (100%)	0	100	100
4	U	48/51 (94%)	48 (100%)	0	100	100
4	W	48/51 (94%)	47 (98%)	1 (2%)	47	77
4	a	49/51 (96%)	49 (100%)	0	100	100
4	b1	48/51 (94%)	47 (98%)	1 (2%)	47	77
4	b9	49/51 (96%)	49 (100%)	0	100	100
4	d	49/51 (96%)	49 (100%)	0	100	100
4	f	49/51 (96%)	49 (100%)	0	100	100
4	i	49/51 (96%)	49 (100%)	0	100	100
4	k	48/51 (94%)	48 (100%)	0	100	100
4	o	49/51 (96%)	49 (100%)	0	100	100
4	q	49/51 (96%)	49 (100%)	0	100	100
4	s	49/51 (96%)	49 (100%)	0	100	100
4	u	48/51 (94%)	48 (100%)	0	100	100
4	w	48/51 (94%)	47 (98%)	1 (2%)	47	77
5	0	35/40 (88%)	35 (100%)	0	100	100
5	2	33/40 (82%)	33 (100%)	0	100	100
5	4	33/40 (82%)	33 (100%)	0	100	100
5	8	36/40 (90%)	36 (100%)	0	100	100
5	B	36/40 (90%)	36 (100%)	0	100	100
5	C	35/40 (88%)	35 (100%)	0	100	100
5	E	35/40 (88%)	34 (97%)	1 (3%)	37	71
5	G	35/40 (88%)	35 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	J	34/40 (85%)	34 (100%)	0	100	100
5	N	34/40 (85%)	34 (100%)	0	100	100
5	P	35/40 (88%)	35 (100%)	0	100	100
5	R	35/40 (88%)	35 (100%)	0	100	100
5	T	34/40 (85%)	34 (100%)	0	100	100
5	V	34/40 (85%)	34 (100%)	0	100	100
5	Z	34/40 (85%)	34 (100%)	0	100	100
5	b	36/40 (90%)	36 (100%)	0	100	100
5	b0	35/40 (88%)	35 (100%)	0	100	100
5	b8	36/40 (90%)	36 (100%)	0	100	100
5	c	35/40 (88%)	35 (100%)	0	100	100
5	e	35/40 (88%)	34 (97%)	1 (3%)	37	71
5	g	35/40 (88%)	35 (100%)	0	100	100
5	j	34/40 (85%)	34 (100%)	0	100	100
5	n	34/40 (85%)	34 (100%)	0	100	100
5	p	35/40 (88%)	35 (100%)	0	100	100
5	r	35/40 (88%)	35 (100%)	0	100	100
5	t	34/40 (85%)	34 (100%)	0	100	100
5	v	34/40 (85%)	34 (100%)	0	100	100
5	z	34/40 (85%)	34 (100%)	0	100	100
6	X	40/66 (61%)	40 (100%)	0	100	100
6	x	40/66 (61%)	40 (100%)	0	100	100
7	Y	35/37 (95%)	35 (100%)	0	100	100
7	y	35/37 (95%)	35 (100%)	0	100	100
All	All	3808/4094 (93%)	3794 (100%)	14 (0%)	81	94

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	l	235	LEU
2	m	182	HIS
4	b1	29	VAL
5	e	7	LEU
4	w	11	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
5	p	18	GLN
4	6	20	GLN
5	b8	16	GLN
4	6	42	ASN
4	3	52	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 152 ligands modelled in this entry, 2 are monoatomic - leaving 150 for Mogul analysis.

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	$\# Z > 2$
11	PC1	l	308	-	31,31,53	0.61	0	37,39,61	0.77	1 (2%)
10	U10	m	404	-	48,48,63	2.73	14 (29%)	60,61,79	1.70	15 (25%)
13	SPO	I	103	-	41,41,41	0.20	0	47,50,50	0.28	0
10	U10	M	407	-	38,38,63	2.74	12 (31%)	48,49,79	1.66	12 (25%)
11	PC1	a	104	-	30,30,53	0.61	0	36,38,61	0.71	1 (2%)
8	BCL	b8	101	-	64,69,74	1.13	5 (7%)	73,109,115	1.51	9 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	BCL	b9	101	-	59,64,74	1.17	5 (8%)	67,103,115	1.48	8 (11%)
8	BCL	j	101	-	64,69,74	1.12	5 (7%)	73,109,115	1.36	7 (9%)
8	BCL	P	101	-	64,69,74	1.13	4 (6%)	73,109,115	1.35	6 (8%)
8	BCL	1	101	-	54,59,74	1.22	5 (9%)	61,97,115	1.51	8 (13%)
8	BCL	Q	101	-	69,74,74	1.09	5 (7%)	79,115,115	1.43	10 (12%)
8	BCL	T	101	-	69,74,74	1.10	5 (7%)	79,115,115	1.40	7 (8%)
11	PC1	A	104	-	30,30,53	0.61	0	36,38,61	0.71	1 (2%)
13	SPO	5	103	-	41,41,41	0.18	0	47,50,50	0.33	0
13	SPO	b9	102	-	41,41,41	0.25	0	47,50,50	0.23	0
8	BCL	l	302	-	66,71,74	1.12	7 (10%)	75,111,115	1.33	6 (8%)
8	BCL	b1	101	-	54,59,74	1.22	5 (9%)	61,97,115	1.51	8 (13%)
8	BCL	R	102	-	69,74,74	1.10	5 (7%)	79,115,115	1.31	7 (8%)
13	SPO	s	102	-	41,41,41	0.22	0	47,50,50	0.30	0
13	SPO	6	102	-	41,41,41	0.20	0	47,50,50	0.29	0
13	SPO	F	102	-	41,41,41	0.17	0	47,50,50	0.25	0
13	SPO	v	103	-	41,41,41	0.23	0	47,50,50	0.36	0
11	PC1	d	102	-	36,36,53	0.59	0	42,44,61	0.70	1 (2%)
13	SPO	V	102	-	41,41,41	0.25	0	47,50,50	0.45	0
13	SPO	r	101	-	41,41,41	0.22	0	47,50,50	0.24	0
11	PC1	a	105	-	35,35,53	0.55	0	41,43,61	0.65	1 (2%)
8	BCL	J	101	-	64,69,74	1.12	5 (7%)	73,109,115	1.36	7 (9%)
9	BPB	l	303	-	57,70,70	1.07	3 (5%)	55,101,101	1.99	10 (18%)
11	PC1	d	101	-	39,39,53	0.56	0	45,47,61	0.68	2 (4%)
13	SPO	V	103	-	41,41,41	0.23	0	47,50,50	0.37	0
8	BCL	6	101	-	64,69,74	1.12	4 (6%)	73,109,115	1.40	7 (9%)
8	BCL	q	101	-	69,74,74	1.09	5 (7%)	79,115,115	1.43	10 (12%)
11	PC1	D	101	-	39,39,53	0.56	0	45,47,61	0.68	2 (4%)
8	BCL	k	101	-	69,74,74	1.09	6 (8%)	79,115,115	1.40	9 (11%)
13	SPO	D	104	-	41,41,41	0.22	0	47,50,50	0.25	0
14	CDL	m	406	-	75,75,99	1.06	8 (10%)	81,87,111	1.28	7 (8%)
8	BCL	Z	101	-	60,65,74	1.17	5 (8%)	68,104,115	1.37	7 (10%)
13	SPO	5	102	-	41,41,41	0.19	0	47,50,50	0.23	0
8	BCL	s	101	-	69,74,74	1.11	5 (7%)	79,115,115	1.46	10 (12%)
11	PC1	a	103	-	44,44,53	0.55	0	50,52,61	0.67	1 (2%)
13	SPO	r	103	-	41,41,41	0.30	0	47,50,50	0.41	0
9	BPB	m	403	-	47,60,70	1.21	2 (4%)	43,89,101	2.15	9 (20%)
8	BCL	0	101	-	64,69,74	1.12	5 (7%)	73,109,115	1.47	9 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CDL	h	303	-	62,62,99	1.17	8 (12%)	68,74,111	1.27	6 (8%)
13	SPO	N	103	-	41,41,41	0.18	0	47,50,50	0.31	0
13	SPO	c	101	-	41,41,41	0.19	0	47,50,50	0.20	0
8	BCL	a	101	-	69,74,74	1.10	6 (8%)	79,115,115	1.40	11 (13%)
8	BCL	5	101	-	69,74,74	1.10	6 (8%)	79,115,115	1.37	8 (10%)
8	BCL	2	101	-	59,64,74	1.17	4 (6%)	67,103,115	1.41	6 (8%)
13	SPO	U	102	-	41,41,41	0.20	0	47,50,50	0.31	0
13	SPO	b	102	-	41,41,41	0.22	0	47,50,50	0.24	0
11	PC1	L	308	-	31,31,53	0.61	0	37,39,61	0.77	1 (2%)
8	BCL	d	103	-	69,74,74	1.11	7 (10%)	79,115,115	1.42	11 (13%)
13	SPO	n	103	-	41,41,41	0.18	0	47,50,50	0.31	0
8	BCL	M	402	-	69,74,74	1.12	7 (10%)	79,115,115	1.41	9 (11%)
8	BCL	K	101	-	69,74,74	1.09	6 (8%)	79,115,115	1.40	9 (11%)
13	SPO	B	102	-	41,41,41	0.22	0	47,50,50	0.24	0
8	BCL	W	101	-	69,74,74	1.11	5 (7%)	79,115,115	1.35	7 (8%)
14	CDL	M	406	-	75,75,99	1.07	8 (10%)	81,87,111	1.27	7 (8%)
11	PC1	A	103	-	44,44,53	0.55	0	50,52,61	0.67	1 (2%)
10	U10	M	404	-	48,48,63	2.73	14 (29%)	60,61,79	1.70	15 (25%)
13	SPO	S	102	-	41,41,41	0.21	0	47,50,50	0.30	0
8	BCL	n	102	-	64,69,74	1.13	4 (6%)	73,109,115	1.35	6 (8%)
13	SPO	0	102	-	41,41,41	0.19	0	47,50,50	0.44	0
11	PC1	l	306	-	38,38,53	0.57	0	44,46,61	0.61	1 (2%)
8	BCL	U	101	-	69,74,74	1.11	7 (10%)	79,115,115	1.39	9 (11%)
8	BCL	9	101	-	59,64,74	1.17	5 (8%)	67,103,115	1.48	8 (11%)
8	BCL	D	103	-	69,74,74	1.11	7 (10%)	79,115,115	1.42	11 (13%)
8	BCL	L	307	-	69,74,74	1.09	6 (8%)	79,115,115	1.38	7 (8%)
11	PC1	h	302	-	33,33,53	0.56	0	39,41,61	0.73	1 (2%)
11	PC1	A	105	-	35,35,53	0.55	0	41,43,61	0.65	1 (2%)
8	BCL	B	101	-	69,74,74	1.09	5 (7%)	79,115,115	1.35	9 (11%)
11	PC1	D	102	-	36,36,53	0.59	0	42,44,61	0.70	1 (2%)
13	SPO	R	103	-	41,41,41	0.30	0	47,50,50	0.41	0
9	BPB	M	403	-	47,60,70	1.22	2 (4%)	43,89,101	2.16	9 (20%)
8	BCL	V	101	-	69,74,74	1.11	5 (7%)	79,115,115	1.34	8 (10%)
11	PC1	H	301	-	41,41,53	0.55	0	47,49,61	0.66	0
13	SPO	F	103	-	41,41,41	0.28	0	47,50,50	0.37	0
13	SPO	e	102	-	41,41,41	0.23	0	47,50,50	0.18	0
8	BCL	l	301	-	69,74,74	1.12	6 (8%)	79,115,115	1.34	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	BCL	O	101	-	69,74,74	1.08	6 (8%)	79,115,115	1.44	8 (10%)
8	BCL	A	101	-	69,74,74	1.10	6 (8%)	79,115,115	1.40	11 (13%)
10	U10	m	407	-	38,38,63	2.74	12 (31%)	48,49,79	1.66	12 (25%)
8	BCL	l	307	-	69,74,74	1.09	6 (8%)	79,115,115	1.39	7 (8%)
13	SPO	7	102	-	41,41,41	0.20	0	47,50,50	0.29	0
13	SPO	M	405	-	41,41,41	0.26	0	47,50,50	0.30	0
8	BCL	e	101	-	69,74,74	1.09	5 (7%)	79,115,115	1.30	6 (7%)
13	SPO	9	102	-	41,41,41	0.26	0	47,50,50	0.23	0
8	BCL	C	102	-	64,69,74	1.13	5 (7%)	73,109,115	1.36	8 (10%)
11	PC1	h	301	-	41,41,53	0.55	0	47,49,61	0.66	0
10	U10	l	305	-	43,43,63	2.74	13 (30%)	54,55,79	1.72	14 (25%)
8	BCL	7	101	-	64,69,74	1.13	5 (7%)	73,109,115	1.40	7 (9%)
13	SPO	N	101	-	41,41,41	0.16	0	47,50,50	0.24	0
13	SPO	C	101	-	41,41,41	0.19	0	47,50,50	0.20	0
11	PC1	L	306	-	38,38,53	0.57	0	44,46,61	0.61	1 (2%)
13	SPO	m	405	-	41,41,41	0.26	0	47,50,50	0.30	0
8	BCL	L	301	-	69,74,74	1.12	6 (8%)	79,115,115	1.34	9 (11%)
8	BCL	F	101	-	69,74,74	1.10	5 (7%)	79,115,115	1.40	8 (10%)
10	U10	L	304	-	38,38,63	2.74	12 (31%)	48,49,79	1.72	13 (27%)
9	BPB	L	303	-	57,70,70	1.07	3 (5%)	55,101,101	2.00	10 (18%)
13	SPO	I	102	-	41,41,41	0.16	0	47,50,50	0.22	0
8	BCL	p	101	-	64,69,74	1.13	4 (6%)	73,109,115	1.35	6 (8%)
13	SPO	R	101	-	41,41,41	0.22	0	47,50,50	0.25	0
8	BCL	L	302	-	66,71,74	1.12	7 (10%)	75,111,115	1.33	6 (8%)
8	BCL	S	101	-	69,74,74	1.10	5 (7%)	79,115,115	1.46	10 (12%)
8	BCL	b	101	-	69,74,74	1.09	5 (7%)	79,115,115	1.35	9 (11%)
13	SPO	o	102	-	41,41,41	0.19	0	47,50,50	0.28	0
8	BCL	3	101	-	69,74,74	1.10	6 (8%)	79,115,115	1.37	8 (10%)
8	BCL	8	101	-	64,69,74	1.13	5 (7%)	73,109,115	1.52	9 (12%)
8	BCL	g	101	-	69,74,74	1.09	5 (7%)	79,115,115	1.33	7 (8%)
8	BCL	4	101	-	59,64,74	1.17	4 (6%)	67,103,115	1.42	6 (8%)
13	SPO	O	102	-	41,41,41	0.19	0	47,50,50	0.28	0
13	SPO	f	103	-	41,41,41	0.28	0	47,50,50	0.37	0
13	SPO	i	103	-	41,41,41	0.20	0	47,50,50	0.27	0
8	BCL	I	101	-	69,74,74	1.06	5 (7%)	79,115,115	1.41	8 (10%)
13	SPO	d	104	-	41,41,41	0.21	0	47,50,50	0.25	0
13	SPO	r	104	-	41,41,41	0.21	0	47,50,50	0.25	0
13	SPO	b0	102	-	41,41,41	0.20	0	47,50,50	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	PC1	H	302	-	33,33,53	0.56	0	39,41,61	0.73	1 (2%)
13	SPO	u	102	-	41,41,41	0.20	0	47,50,50	0.31	0
8	BCL	t	101	-	69,74,74	1.10	5 (7%)	79,115,115	1.40	7 (8%)
8	BCL	c	102	-	64,69,74	1.14	5 (7%)	73,109,115	1.36	8 (10%)
10	U10	l	304	-	38,38,63	2.74	12 (31%)	48,49,79	1.72	13 (27%)
8	BCL	w	101	-	69,74,74	1.11	5 (7%)	79,115,115	1.35	7 (8%)
8	BCL	v	101	-	69,74,74	1.11	5 (7%)	79,115,115	1.34	8 (10%)
10	U10	L	305	-	43,43,63	2.74	13 (30%)	54,55,79	1.71	14 (25%)
13	SPO	3	102	-	41,41,41	0.20	0	47,50,50	0.23	0
13	SPO	i	102	-	41,41,41	0.16	0	47,50,50	0.22	0
8	BCL	m	402	-	69,74,74	1.12	7 (10%)	79,115,115	1.41	9 (11%)
8	BCL	b0	101	-	64,69,74	1.13	5 (7%)	73,109,115	1.47	8 (10%)
8	BCL	u	101	-	69,74,74	1.11	7 (10%)	79,115,115	1.39	9 (11%)
13	SPO	f	102	-	41,41,41	0.17	0	47,50,50	0.25	0
13	SPO	J	102	-	41,41,41	0.17	0	47,50,50	0.26	0
13	SPO	A	102	-	41,41,41	0.18	0	47,50,50	0.29	0
13	SPO	R	104	-	41,41,41	0.21	0	47,50,50	0.25	0
8	BCL	z	101	-	60,65,74	1.17	4 (6%)	68,104,115	1.37	7 (10%)
13	SPO	3	103	-	41,41,41	0.18	0	47,50,50	0.33	0
13	SPO	a	102	-	41,41,41	0.18	0	47,50,50	0.29	0
8	BCL	i	101	-	69,74,74	1.07	5 (7%)	79,115,115	1.41	8 (10%)
13	SPO	n	101	-	41,41,41	0.16	0	47,50,50	0.24	0
8	BCL	o	101	-	69,74,74	1.08	6 (8%)	79,115,115	1.44	8 (10%)
8	BCL	N	102	-	64,69,74	1.13	4 (6%)	73,109,115	1.35	6 (8%)
8	BCL	f	101	-	69,74,74	1.10	5 (7%)	79,115,115	1.40	9 (11%)
8	BCL	G	101	-	69,74,74	1.10	5 (7%)	79,115,115	1.33	7 (8%)
8	BCL	r	102	-	69,74,74	1.10	5 (7%)	79,115,115	1.31	7 (8%)
8	BCL	E	101	-	69,74,74	1.09	5 (7%)	79,115,115	1.30	6 (7%)
14	CDL	H	303	-	62,62,99	1.17	8 (12%)	68,74,111	1.27	6 (8%)
13	SPO	E	102	-	41,41,41	0.23	0	47,50,50	0.18	0
13	SPO	v	102	-	41,41,41	0.26	0	47,50,50	0.46	0
13	SPO	j	102	-	41,41,41	0.17	0	47,50,50	0.26	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
11	PC1	l	308	-	-	17/35/35/57	-
10	U10	m	404	-	-	11/45/69/87	0/1/1/1
13	SPO	I	103	-	-	12/47/47/47	-
10	U10	M	407	-	-	11/33/57/87	0/1/1/1
11	PC1	a	104	-	-	18/34/34/57	-
8	BCL	b8	101	-	-	5/35/131/137	-
8	BCL	b9	101	-	-	1/29/125/137	-
8	BCL	j	101	-	-	4/35/131/137	-
8	BCL	P	101	-	-	7/35/131/137	-
8	BCL	l	101	-	-	1/23/119/137	-
8	BCL	Q	101	-	-	2/41/137/137	-
8	BCL	T	101	-	-	4/41/137/137	-
11	PC1	A	104	-	-	18/34/34/57	-
13	SPO	5	103	-	-	13/47/47/47	-
13	SPO	b9	102	-	-	14/47/47/47	-
8	BCL	l	302	-	-	0/38/134/137	-
8	BCL	b1	101	-	-	1/23/119/137	-
8	BCL	R	102	-	-	4/41/137/137	-
13	SPO	s	102	-	-	8/47/47/47	-
13	SPO	6	102	-	-	10/47/47/47	-
13	SPO	F	102	-	-	9/47/47/47	-
13	SPO	v	103	-	-	10/47/47/47	-
11	PC1	d	102	-	-	19/40/40/57	-
13	SPO	V	102	-	-	9/47/47/47	-
13	SPO	r	101	-	-	12/47/47/47	-
11	PC1	a	105	-	-	18/39/39/57	-
8	BCL	J	101	-	-	4/35/131/137	-
9	BPB	l	303	-	-	4/37/105/105	0/5/6/6
11	PC1	d	101	-	-	18/43/43/57	-
13	SPO	V	103	-	-	10/47/47/47	-
8	BCL	6	101	-	-	3/35/131/137	-
8	BCL	q	101	-	-	2/41/137/137	-
11	PC1	D	101	-	-	18/43/43/57	-
8	BCL	k	101	-	-	2/41/137/137	-
13	SPO	D	104	-	-	7/47/47/47	-
14	CDL	m	406	-	-	35/86/86/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	BCL	Z	101	-	-	2/31/127/137	-
13	SPO	5	102	-	-	10/47/47/47	-
8	BCL	s	101	-	-	4/41/137/137	-
11	PC1	a	103	-	-	19/48/48/57	-
13	SPO	r	103	-	-	20/47/47/47	-
9	BPB	m	403	-	-	4/25/93/105	0/5/6/6
8	BCL	0	101	-	-	1/35/131/137	-
14	CDL	h	303	-	-	27/73/73/110	-
13	SPO	N	103	-	-	10/47/47/47	-
13	SPO	c	101	-	-	11/47/47/47	-
8	BCL	a	101	-	-	3/41/137/137	-
8	BCL	5	101	-	-	1/41/137/137	-
8	BCL	2	101	-	-	3/29/125/137	-
13	SPO	U	102	-	-	9/47/47/47	-
13	SPO	b	102	-	-	14/47/47/47	-
11	PC1	L	308	-	-	17/35/35/57	-
8	BCL	d	103	-	-	2/41/137/137	-
13	SPO	n	103	-	-	10/47/47/47	-
8	BCL	M	402	-	-	2/41/137/137	-
8	BCL	K	101	-	-	2/41/137/137	-
13	SPO	B	102	-	-	14/47/47/47	-
8	BCL	W	101	-	-	1/41/137/137	-
14	CDL	M	406	-	-	35/86/86/110	-
11	PC1	A	103	-	-	19/48/48/57	-
10	U10	M	404	-	-	11/45/69/87	0/1/1/1
13	SPO	S	102	-	-	8/47/47/47	-
8	BCL	n	102	-	-	5/35/131/137	-
13	SPO	0	102	-	-	9/47/47/47	-
11	PC1	l	306	-	-	13/42/42/57	-
8	BCL	U	101	-	-	1/41/137/137	-
8	BCL	9	101	-	-	1/29/125/137	-
8	BCL	D	103	-	-	2/41/137/137	-
8	BCL	L	307	-	-	4/41/137/137	-
11	PC1	h	302	-	-	11/37/37/57	-
11	PC1	A	105	-	-	18/39/39/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	BCL	B	101	-	-	4/41/137/137	-
11	PC1	D	102	-	-	19/40/40/57	-
13	SPO	R	103	-	-	20/47/47/47	-
9	BPB	M	403	-	-	4/25/93/105	0/5/6/6
8	BCL	V	101	-	-	5/41/137/137	-
11	PC1	H	301	-	-	7/45/45/57	-
13	SPO	F	103	-	-	13/47/47/47	-
13	SPO	e	102	-	-	15/47/47/47	-
8	BCL	l	301	-	-	1/41/137/137	-
8	BCL	O	101	-	-	0/41/137/137	-
8	BCL	A	101	-	-	3/41/137/137	-
10	U10	m	407	-	-	11/33/57/87	0/1/1/1
8	BCL	l	307	-	-	4/41/137/137	-
13	SPO	7	102	-	-	10/47/47/47	-
13	SPO	M	405	-	-	8/47/47/47	-
8	BCL	e	101	-	-	2/41/137/137	-
13	SPO	9	102	-	-	14/47/47/47	-
8	BCL	C	102	-	-	6/35/131/137	-
11	PC1	h	301	-	-	7/45/45/57	-
10	U10	l	305	-	-	10/39/63/87	0/1/1/1
8	BCL	7	101	-	-	3/35/131/137	-
13	SPO	N	101	-	-	9/47/47/47	-
13	SPO	C	101	-	-	11/47/47/47	-
11	PC1	L	306	-	-	13/42/42/57	-
13	SPO	m	405	-	-	8/47/47/47	-
8	BCL	L	301	-	-	1/41/137/137	-
8	BCL	F	101	-	-	3/41/137/137	-
10	U10	L	304	-	-	10/33/57/87	0/1/1/1
9	BPB	L	303	-	-	4/37/105/105	0/5/6/6
13	SPO	I	102	-	-	11/47/47/47	-
8	BCL	p	101	-	-	7/35/131/137	-
13	SPO	R	101	-	-	11/47/47/47	-
8	BCL	L	302	-	-	0/38/134/137	-
8	BCL	S	101	-	-	4/41/137/137	-
8	BCL	b	101	-	-	4/41/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	SPO	o	102	-	-	8/47/47/47	-
8	BCL	3	101	-	-	1/41/137/137	-
8	BCL	8	101	-	-	5/35/131/137	-
8	BCL	g	101	-	-	6/41/137/137	-
8	BCL	4	101	-	-	3/29/125/137	-
13	SPO	O	102	-	-	8/47/47/47	-
13	SPO	f	103	-	-	13/47/47/47	-
13	SPO	i	103	-	-	12/47/47/47	-
8	BCL	I	101	-	-	1/41/137/137	-
13	SPO	d	104	-	-	7/47/47/47	-
13	SPO	r	104	-	-	11/47/47/47	-
13	SPO	b0	102	-	-	9/47/47/47	-
11	PC1	H	302	-	-	11/37/37/57	-
13	SPO	u	102	-	-	9/47/47/47	-
8	BCL	t	101	-	-	4/41/137/137	-
8	BCL	c	102	-	-	6/35/131/137	-
10	U10	l	304	-	-	10/33/57/87	0/1/1/1
8	BCL	w	101	-	-	1/41/137/137	-
8	BCL	v	101	-	-	5/41/137/137	-
10	U10	L	305	-	-	10/39/63/87	0/1/1/1
13	SPO	3	102	-	-	10/47/47/47	-
13	SPO	i	102	-	-	11/47/47/47	-
8	BCL	m	402	-	-	2/41/137/137	-
8	BCL	b0	101	-	-	1/35/131/137	-
8	BCL	u	101	-	-	1/41/137/137	-
13	SPO	f	102	-	-	9/47/47/47	-
13	SPO	J	102	-	-	10/47/47/47	-
13	SPO	A	102	-	-	9/47/47/47	-
13	SPO	R	104	-	-	11/47/47/47	-
8	BCL	z	101	-	-	2/31/127/137	-
13	SPO	3	103	-	-	13/47/47/47	-
13	SPO	a	102	-	-	9/47/47/47	-
8	BCL	i	101	-	-	1/41/137/137	-
13	SPO	n	101	-	-	9/47/47/47	-
8	BCL	o	101	-	-	0/41/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	BCL	N	102	-	-	5/35/131/137	-
8	BCL	f	101	-	-	3/41/137/137	-
8	BCL	G	101	-	-	6/41/137/137	-
8	BCL	r	102	-	-	4/41/137/137	-
8	BCL	E	101	-	-	2/41/137/137	-
14	CDL	H	303	-	-	27/73/73/110	-
13	SPO	E	102	-	-	15/47/47/47	-
13	SPO	v	102	-	-	9/47/47/47	-
13	SPO	j	102	-	-	10/47/47/47	-

The worst 5 of 484 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	L	305	U10	C13-C14	6.30	1.47	1.33
10	l	305	U10	C13-C14	6.30	1.47	1.33
10	l	304	U10	C23-C24	6.26	1.47	1.33
10	l	305	U10	C8-C9	6.25	1.47	1.33
10	L	304	U10	C23-C24	6.24	1.47	1.33

The worst 5 of 700 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	L	303	BPB	C4D-CHA-CBD	-10.09	103.61	108.45
9	l	303	BPB	C4D-CHA-CBD	-10.08	103.62	108.45
9	M	403	BPB	C4D-CHA-CBD	-9.99	103.66	108.45
9	m	403	BPB	C4D-CHA-CBD	-9.97	103.67	108.45
8	b9	101	BCL	C4D-CHA-C1A	5.50	127.81	121.24

There are no chirality outliers.

5 of 1245 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	N	102	BCL	C4C-C3C-CAC-CBC
8	P	101	BCL	C2C-C3C-CAC-CBC
8	P	101	BCL	C4C-C3C-CAC-CBC
8	S	101	BCL	C4C-C3C-CAC-CBC
8	2	101	BCL	C2-C3-C5-C6

There are no ring outliers.

140 monomers are involved in 426 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	l	308	PC1	3	0
10	m	404	U10	1	0
13	I	103	SPO	1	0
10	M	407	U10	2	0
11	a	104	PC1	4	0
8	b9	101	BCL	4	0
8	j	101	BCL	5	0
8	P	101	BCL	4	0
8	Q	101	BCL	6	0
8	T	101	BCL	3	0
11	A	104	PC1	4	0
13	5	103	SPO	5	0
13	b9	102	SPO	2	0
8	l	302	BCL	4	0
8	R	102	BCL	3	0
13	s	102	SPO	4	0
13	6	102	SPO	5	0
13	F	102	SPO	2	0
11	d	102	PC1	5	0
13	V	102	SPO	1	0
13	r	101	SPO	1	0
11	a	105	PC1	6	0
8	J	101	BCL	5	0
9	l	303	BPB	4	0
11	d	101	PC1	2	0
8	6	101	BCL	2	0
8	q	101	BCL	6	0
11	D	101	PC1	2	0
8	k	101	BCL	4	0
13	D	104	SPO	2	0
14	m	406	CDL	1	0
13	5	102	SPO	1	0
8	s	101	BCL	5	0
11	a	103	PC1	2	0
13	r	103	SPO	9	0
9	m	403	BPB	2	0
8	0	101	BCL	2	0
14	h	303	CDL	2	0
13	N	103	SPO	5	0
13	c	101	SPO	2	0
8	a	101	BCL	3	0
8	5	101	BCL	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	2	101	BCL	1	0
13	U	102	SPO	3	0
13	b	102	SPO	2	0
11	L	308	PC1	3	0
8	d	103	BCL	6	0
13	n	103	SPO	5	0
8	M	402	BCL	1	0
8	K	101	BCL	4	0
13	B	102	SPO	2	0
8	W	101	BCL	2	0
14	M	406	CDL	4	0
11	A	103	PC1	2	0
10	M	404	U10	1	0
13	S	102	SPO	4	0
8	n	102	BCL	5	0
11	l	306	PC1	2	0
8	U	101	BCL	1	0
8	9	101	BCL	4	0
8	D	103	BCL	5	0
8	L	307	BCL	3	0
11	h	302	PC1	1	0
11	A	105	PC1	7	0
8	B	101	BCL	3	0
11	D	102	PC1	5	0
13	R	103	SPO	9	0
9	M	403	BPB	2	0
8	V	101	BCL	2	0
11	H	301	PC1	7	0
13	F	103	SPO	4	0
8	l	301	BCL	4	0
8	O	101	BCL	10	0
8	A	101	BCL	4	0
10	m	407	U10	2	0
8	l	307	BCL	4	0
13	7	102	SPO	5	0
13	M	405	SPO	5	0
8	e	101	BCL	2	0
13	9	102	SPO	3	0
8	C	102	BCL	2	0
11	h	301	PC1	9	0
10	l	305	U10	6	0
8	7	101	BCL	2	0

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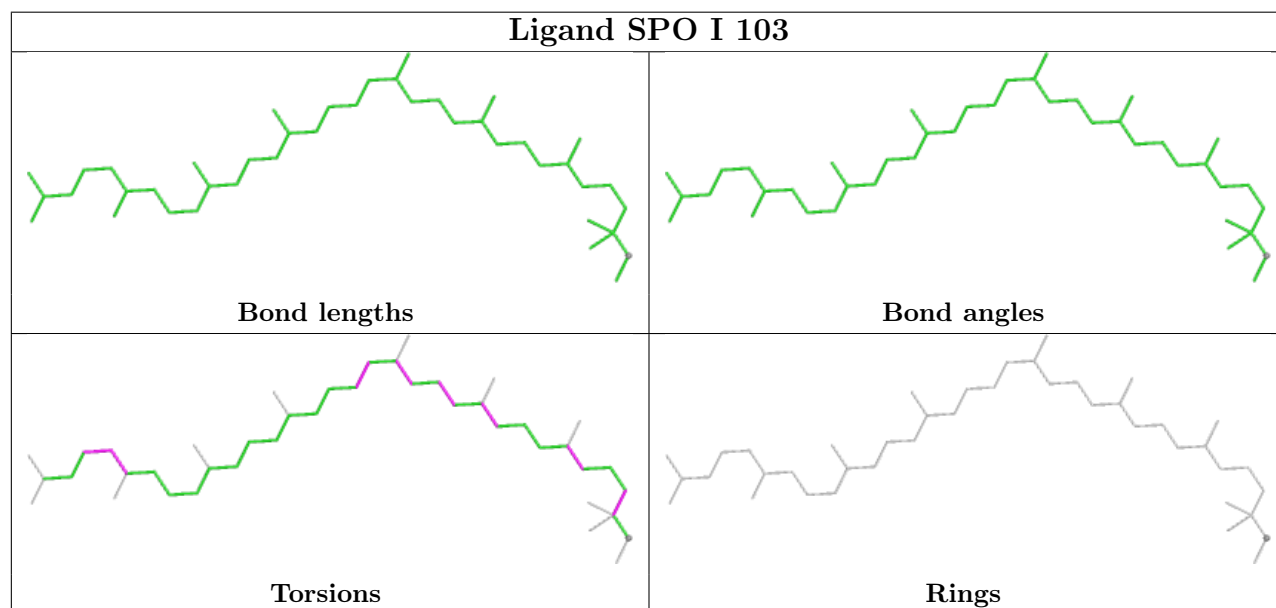
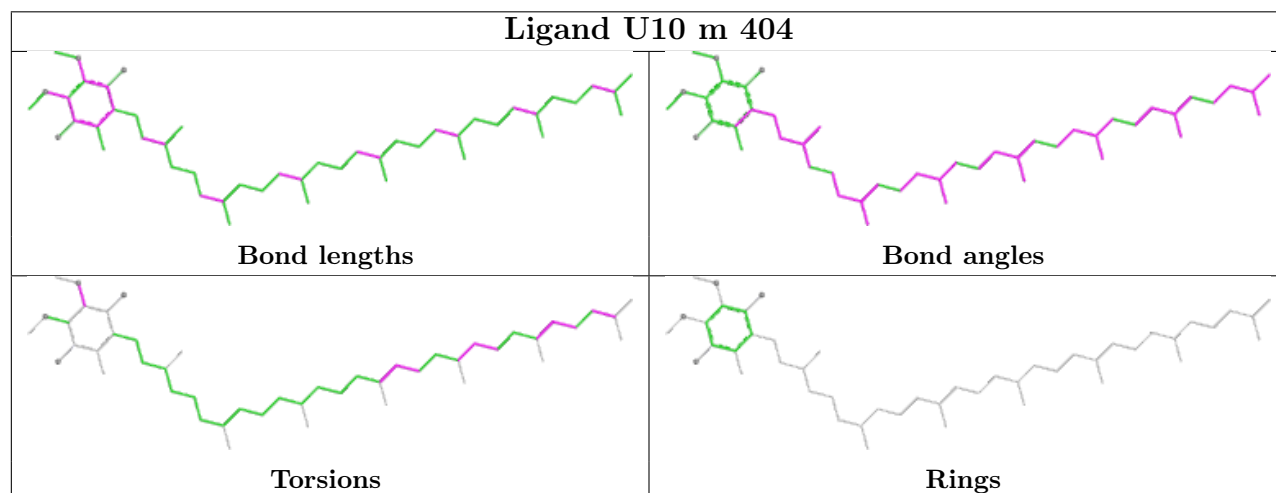
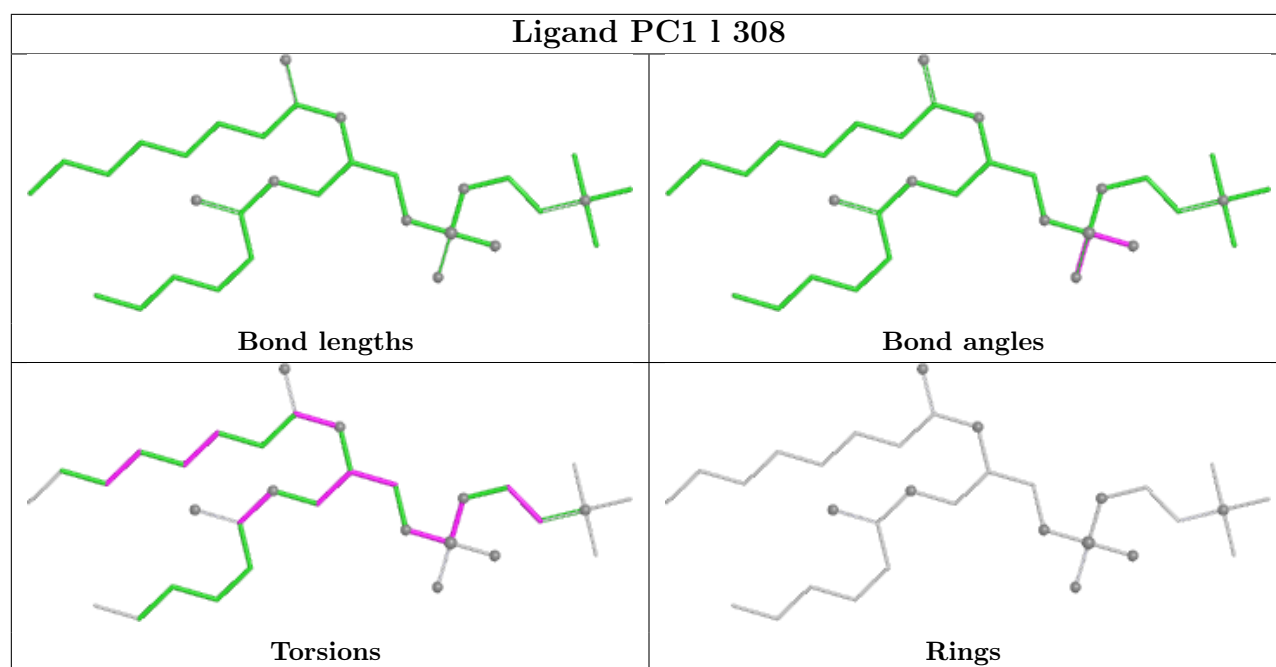
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	N	101	SPO	2	0
13	C	101	SPO	2	0
11	L	306	PC1	2	0
13	m	405	SPO	5	0
8	L	301	BCL	4	0
8	F	101	BCL	4	0
10	L	304	U10	3	0
9	L	303	BPB	5	0
13	I	102	SPO	3	0
8	p	101	BCL	4	0
13	R	101	SPO	1	0
8	L	302	BCL	4	0
8	S	101	BCL	5	0
8	b	101	BCL	5	0
13	o	102	SPO	2	0
8	3	101	BCL	4	0
8	8	101	BCL	2	0
8	g	101	BCL	5	0
8	4	101	BCL	2	0
13	O	102	SPO	3	0
13	f	103	SPO	4	0
13	i	103	SPO	1	0
8	I	101	BCL	5	0
13	d	104	SPO	2	0
13	r	104	SPO	2	0
13	b0	102	SPO	1	0
11	H	302	PC1	1	0
13	u	102	SPO	2	0
8	t	101	BCL	4	0
8	c	102	BCL	2	0
10	l	304	U10	3	0
8	w	101	BCL	1	0
8	v	101	BCL	1	0
10	L	305	U10	5	0
13	3	102	SPO	2	0
13	i	102	SPO	2	0
8	m	402	BCL	1	0
8	b0	101	BCL	2	0
8	u	101	BCL	2	0
13	f	102	SPO	3	0
13	J	102	SPO	4	0
13	A	102	SPO	4	0

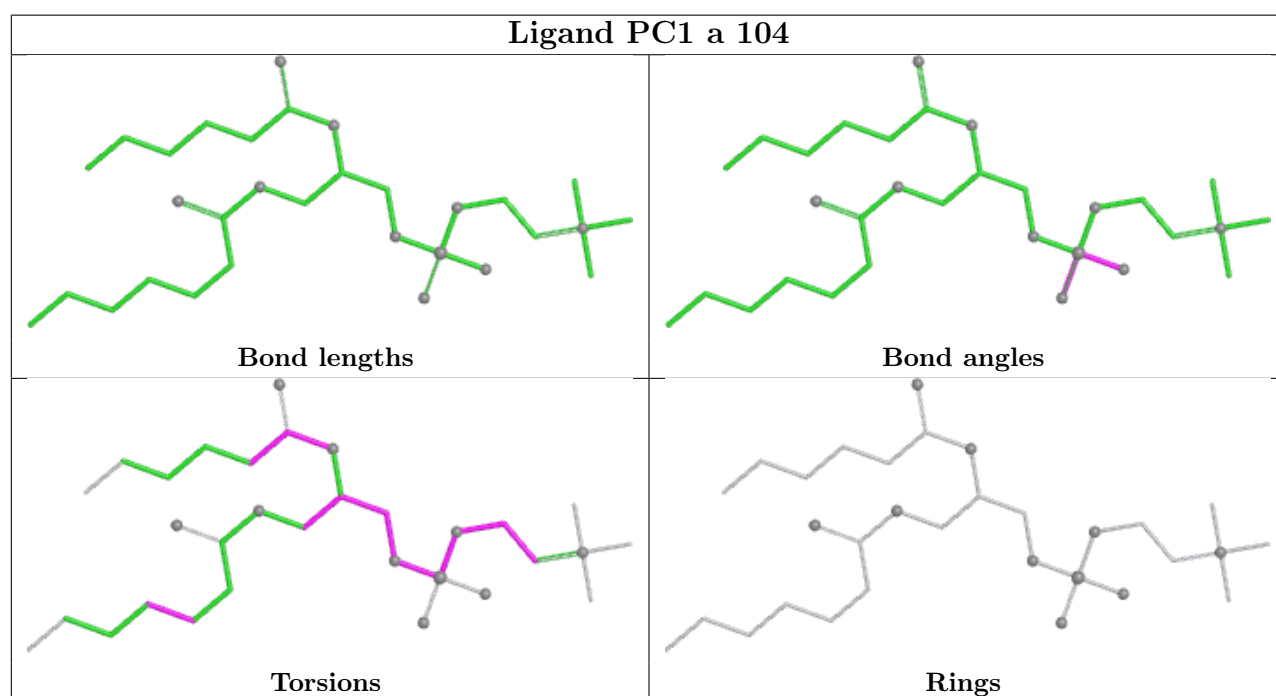
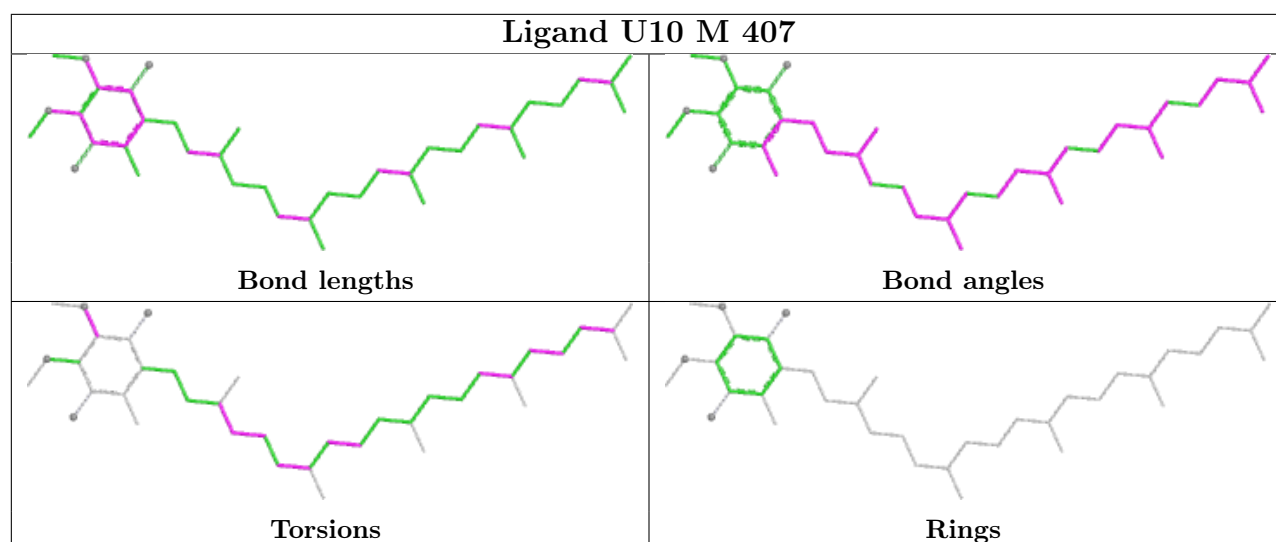
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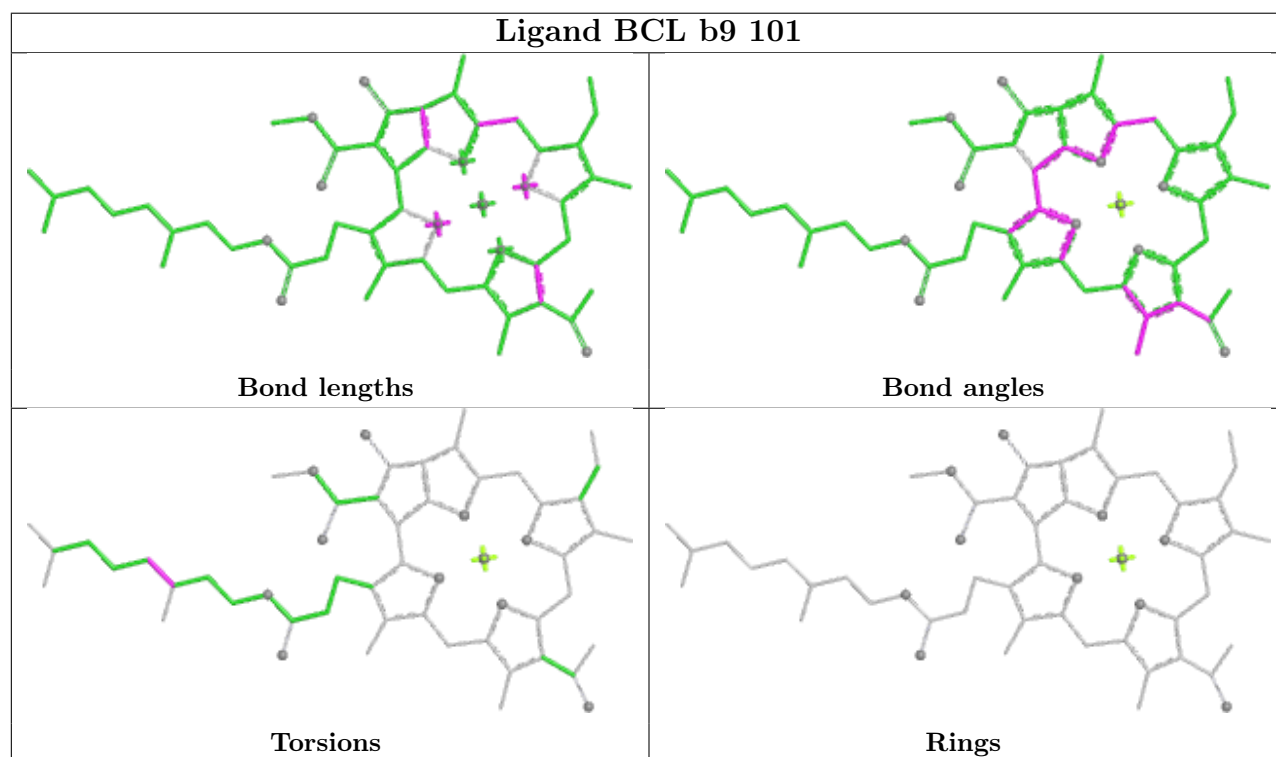
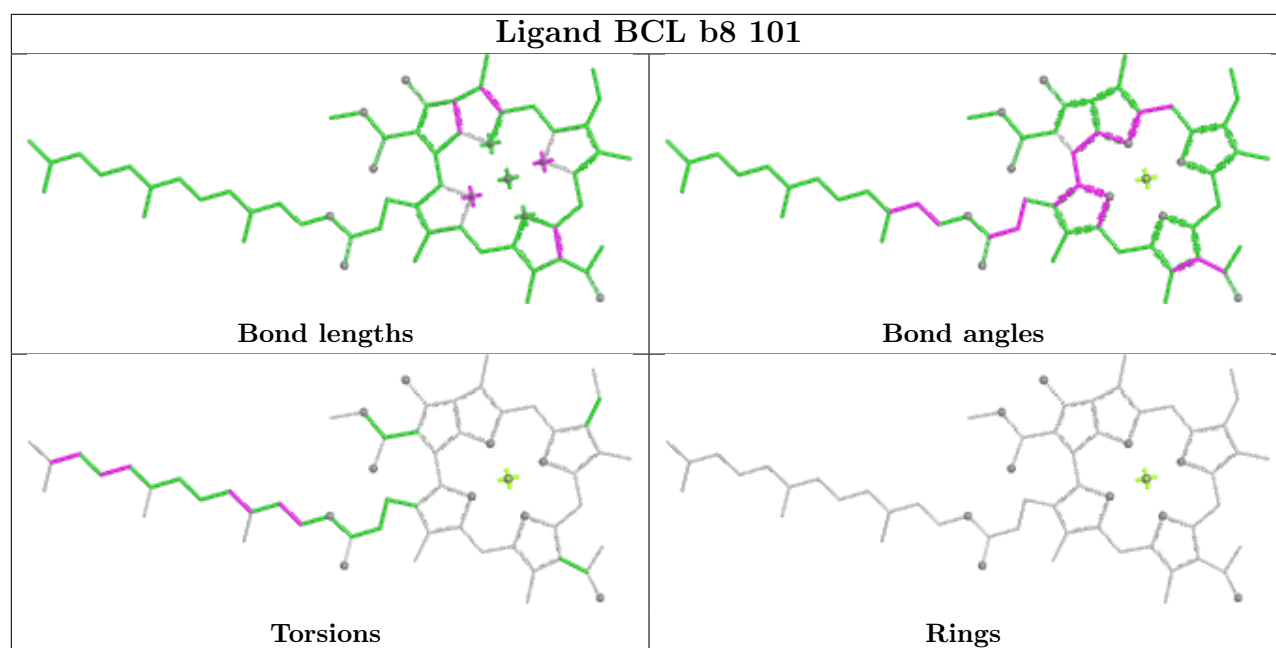
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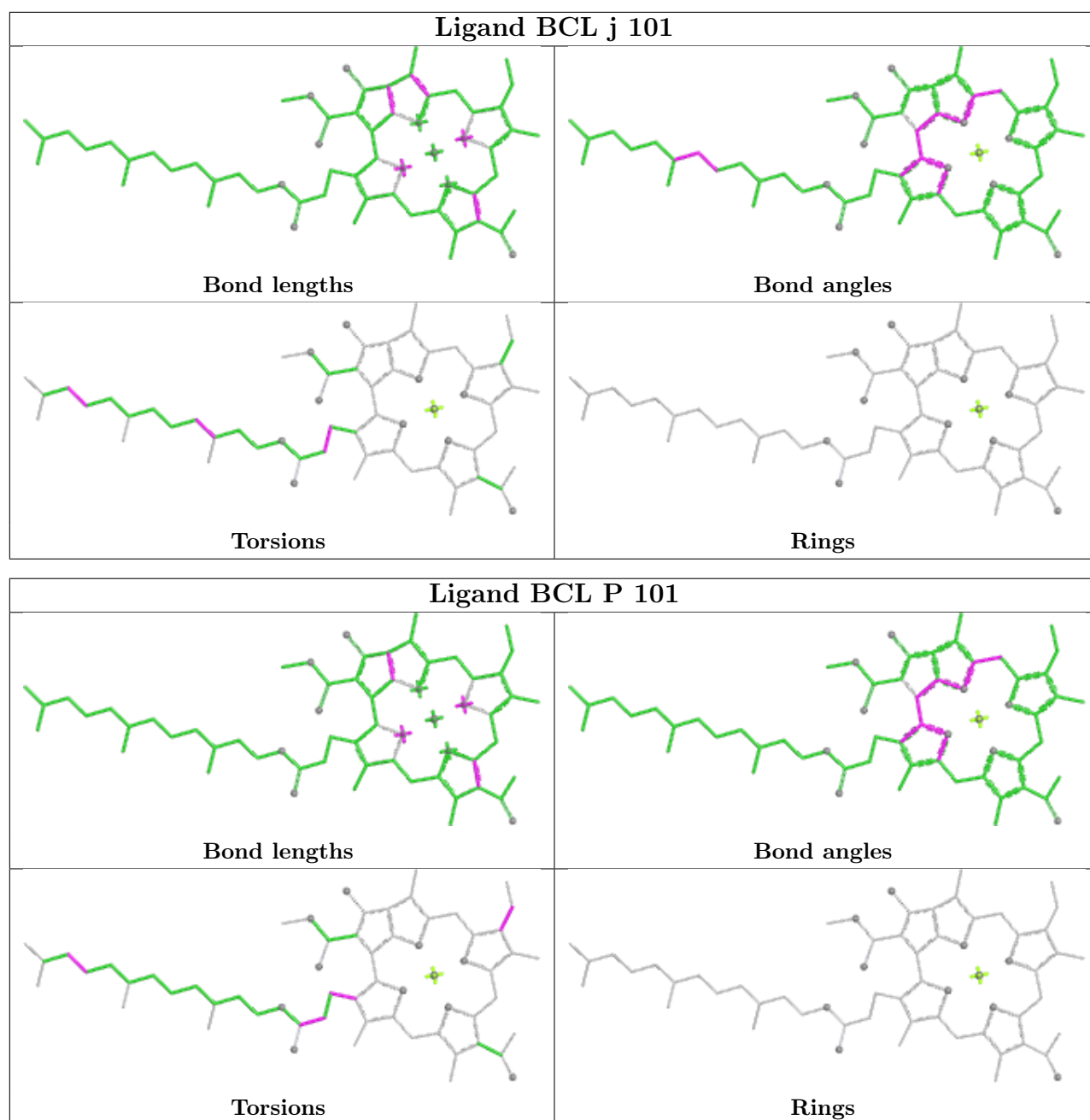
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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13	3	103	SPO	5	0
13	a	102	SPO	4	0
8	i	101	BCL	6	0
13	n	101	SPO	1	0
8	o	101	BCL	10	0
8	N	102	BCL	5	0
8	f	101	BCL	5	0
8	G	101	BCL	5	0
8	r	102	BCL	3	0
8	E	101	BCL	2	0
14	H	303	CDL	2	0
13	v	102	SPO	1	0
13	j	102	SPO	4	0

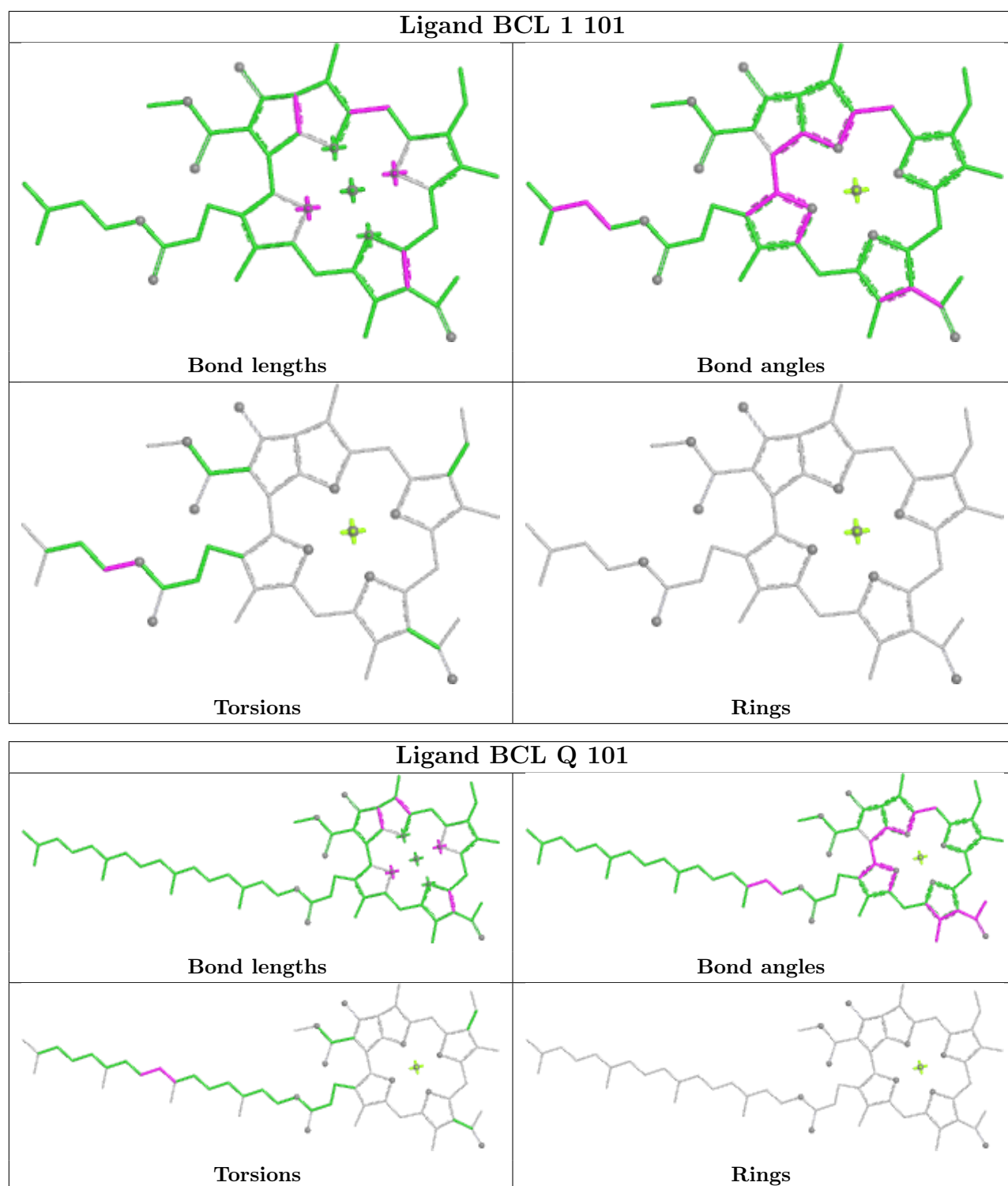
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

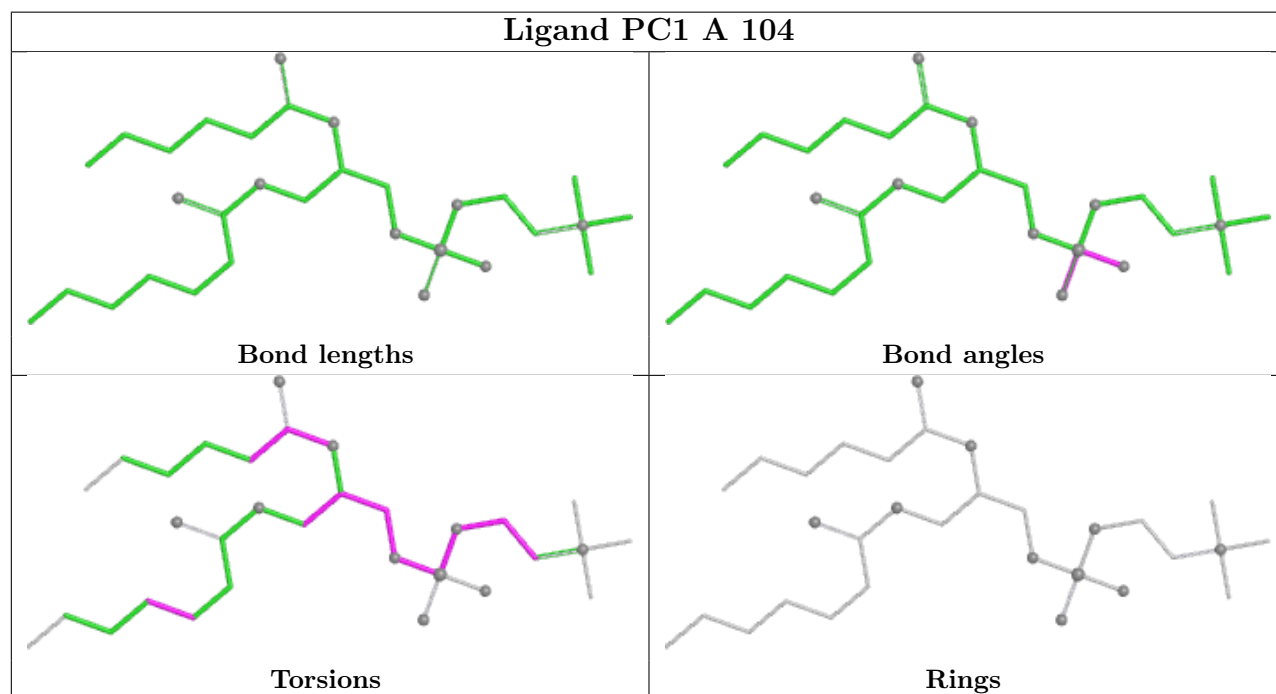
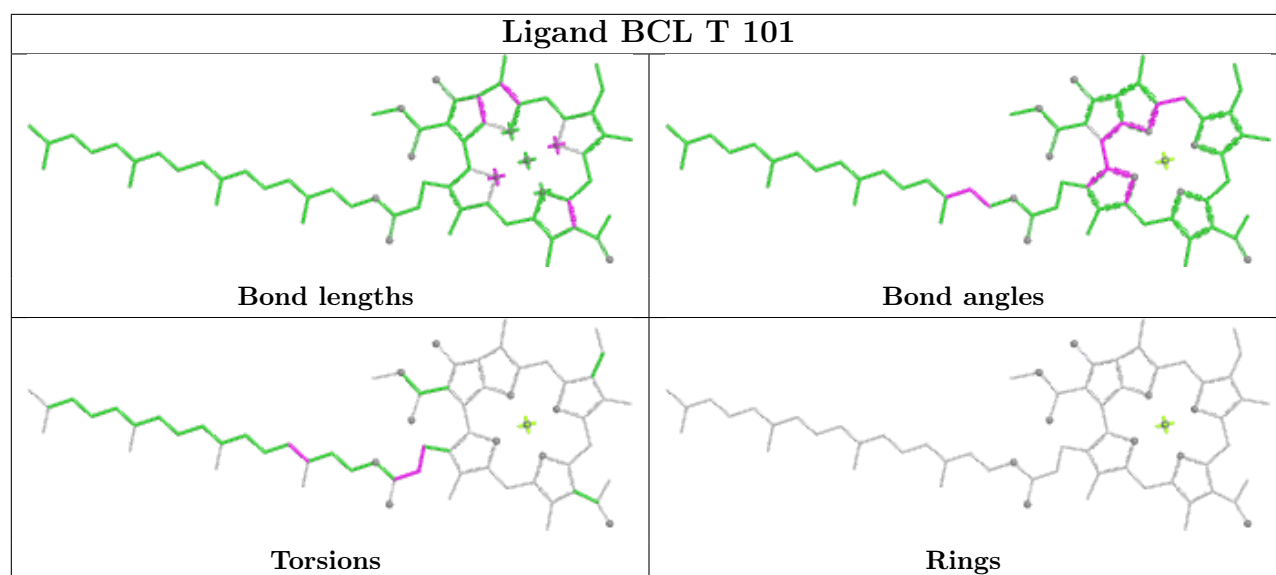


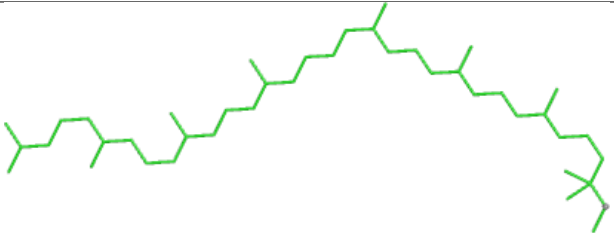
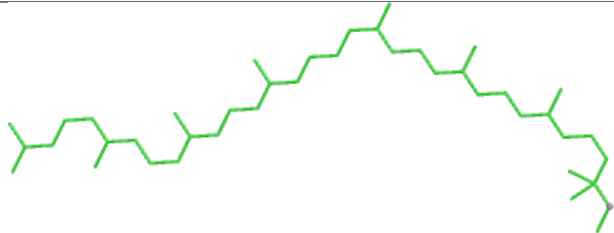
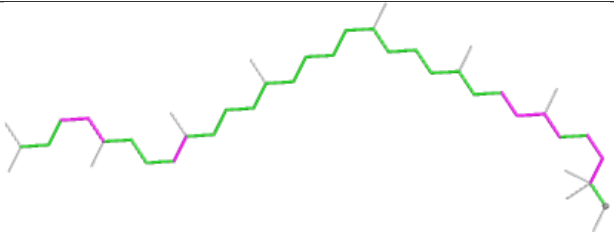
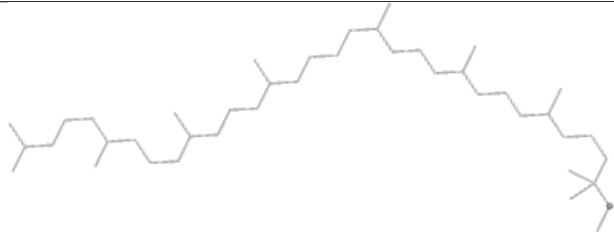


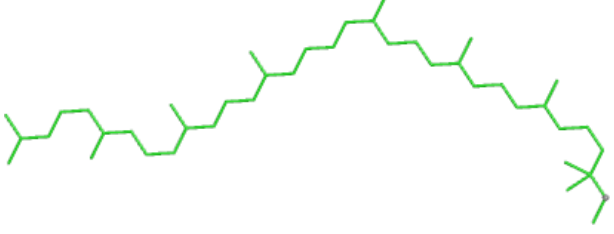
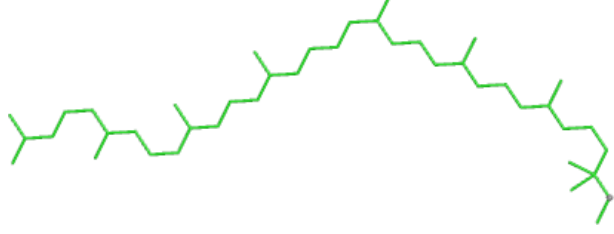
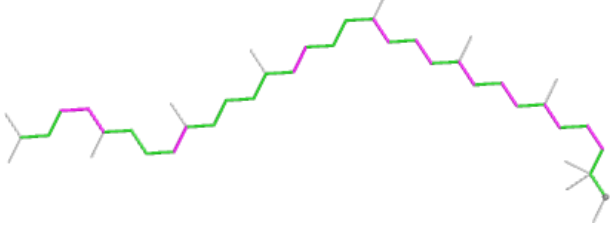
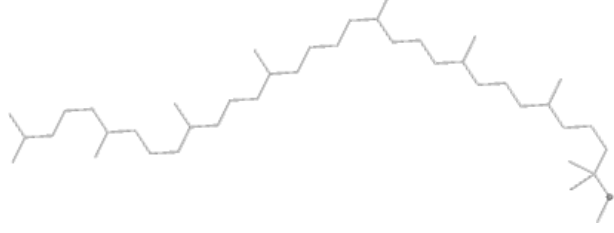


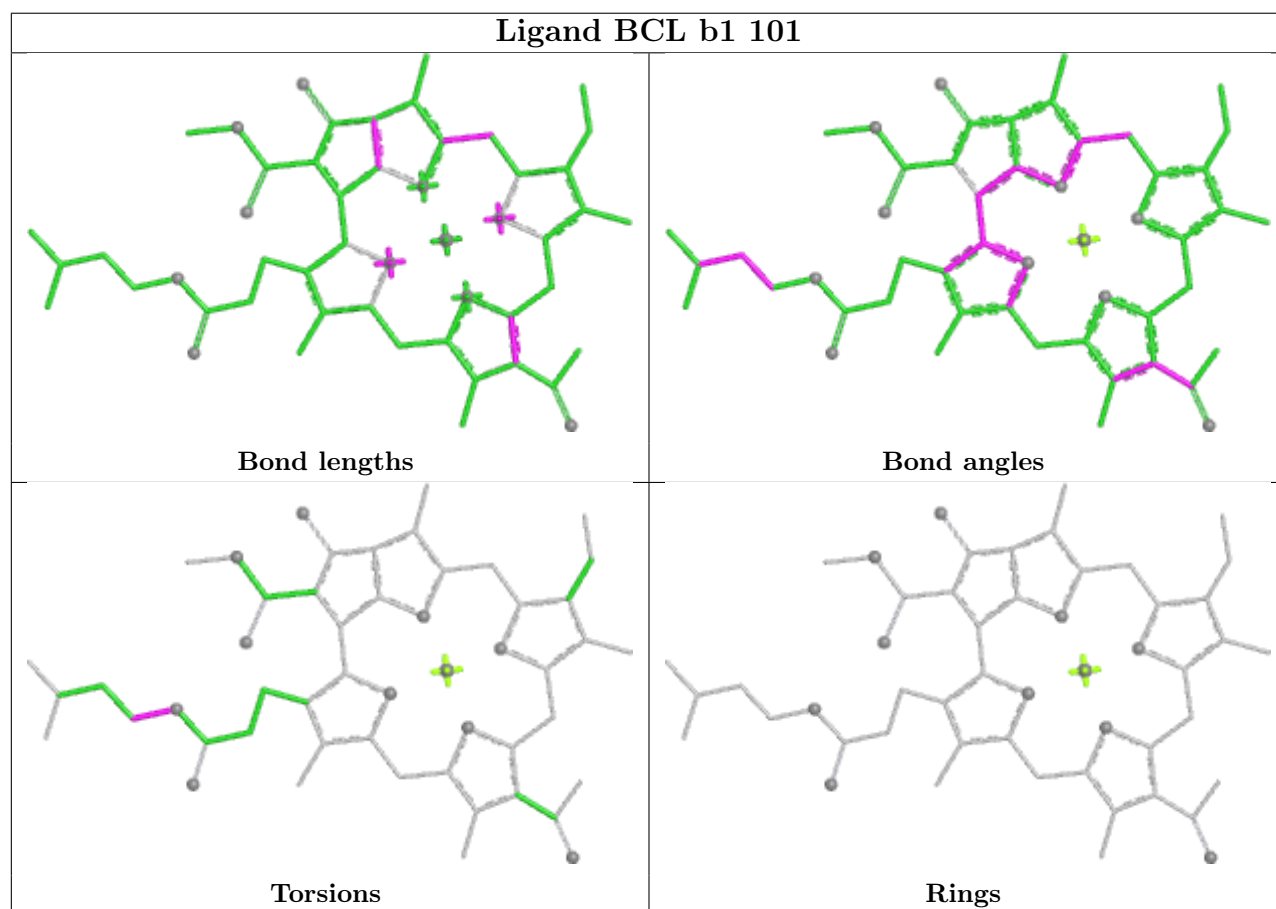
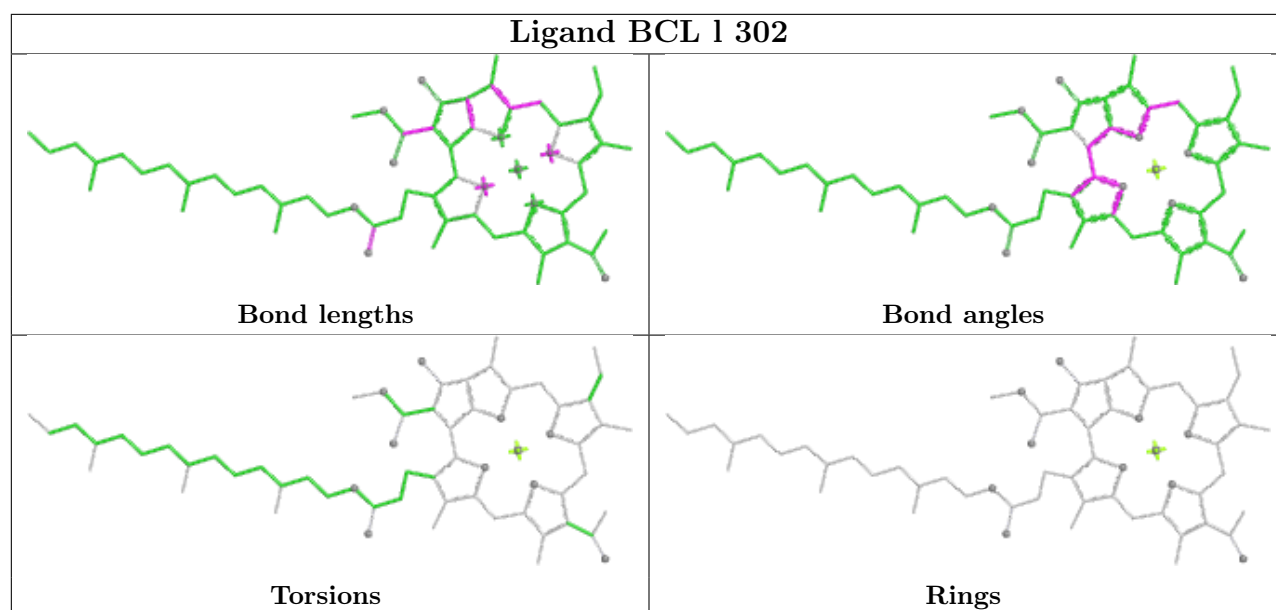


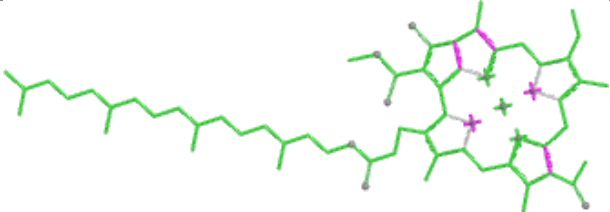
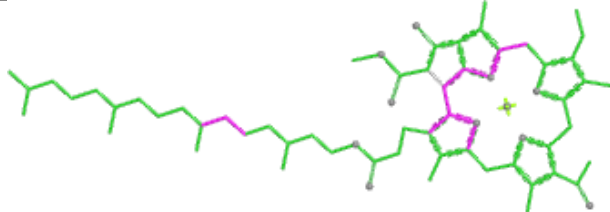
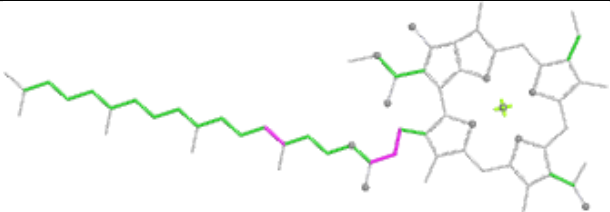
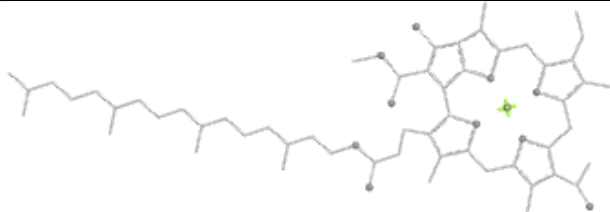
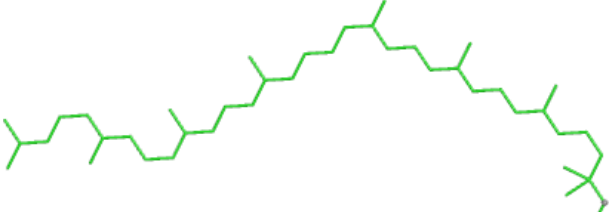
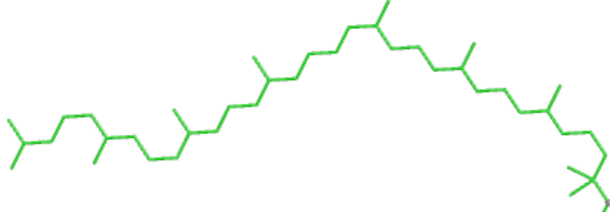
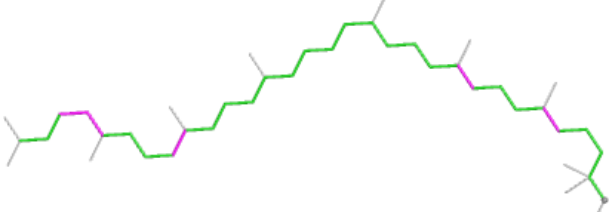
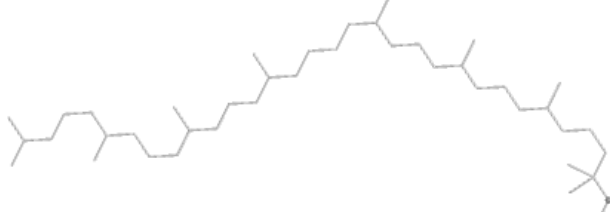


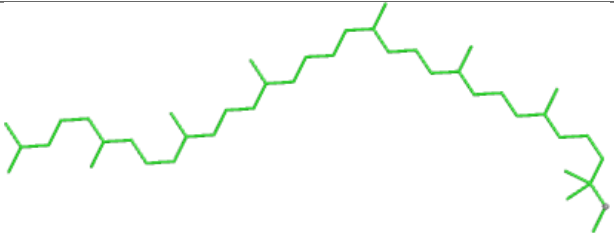
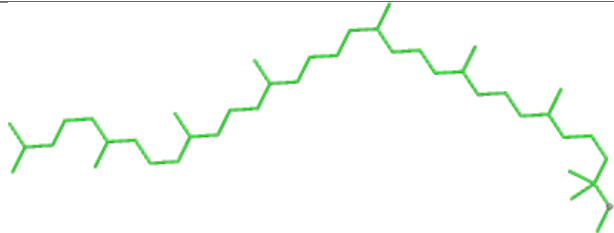
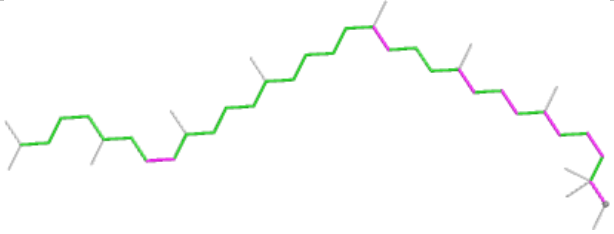
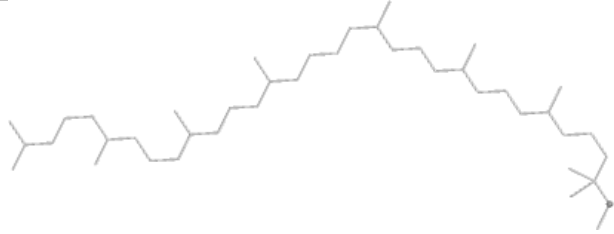


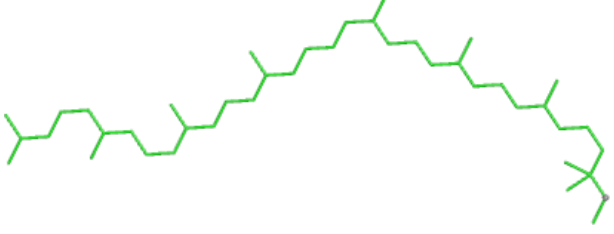
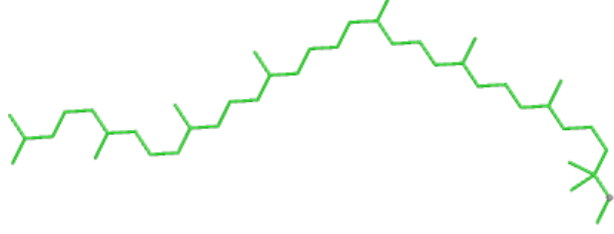
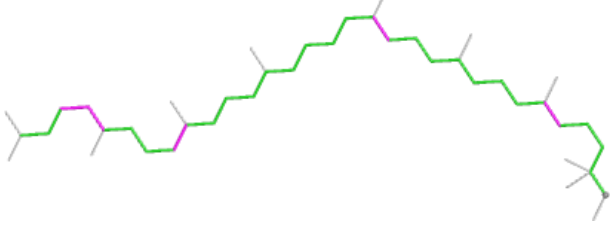
Ligand SPO 5 103	
 Bond lengths	 Bond angles
 Torsions	 Rings

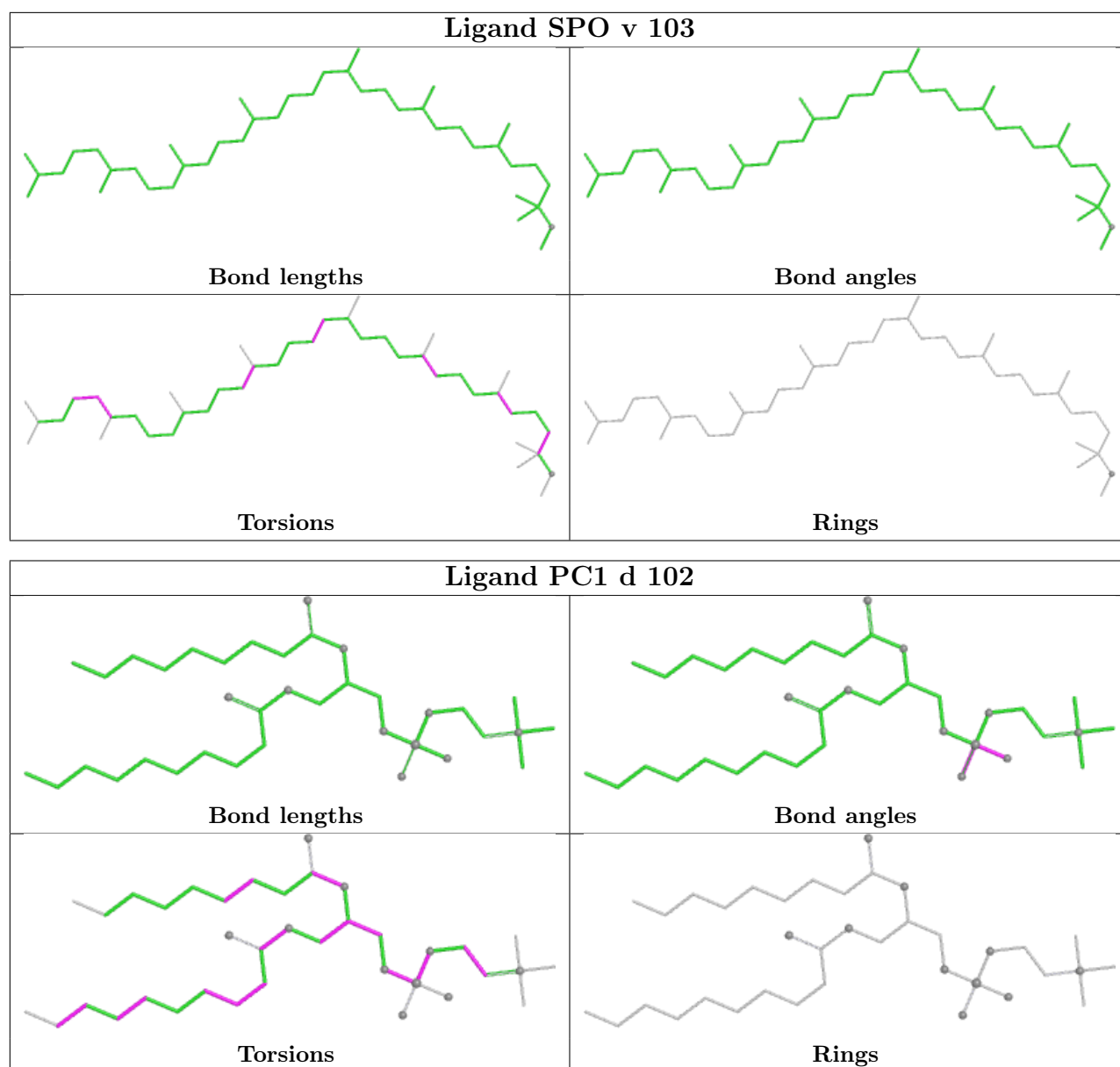
Ligand SPO b9 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

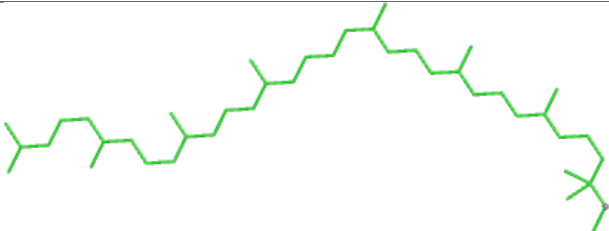
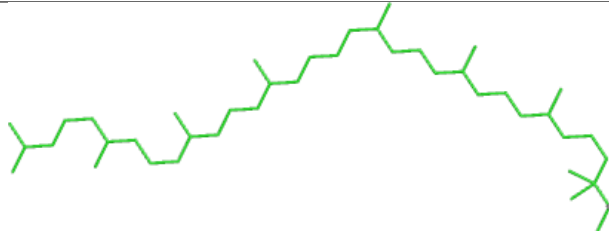
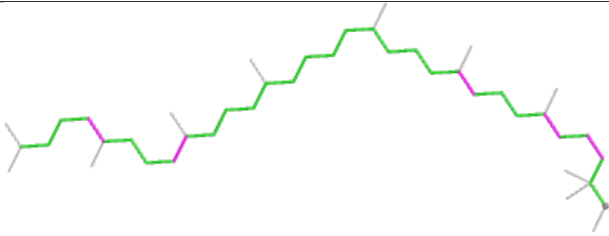
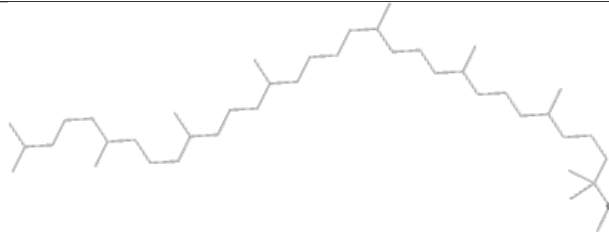


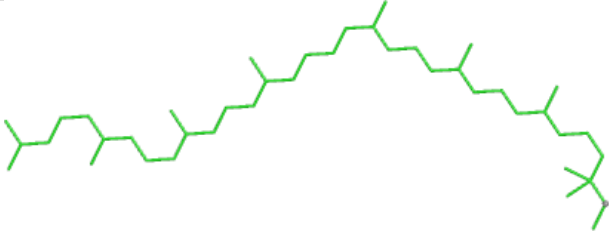
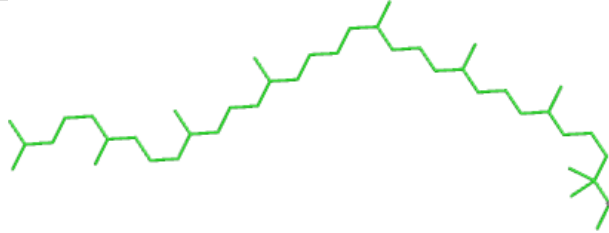
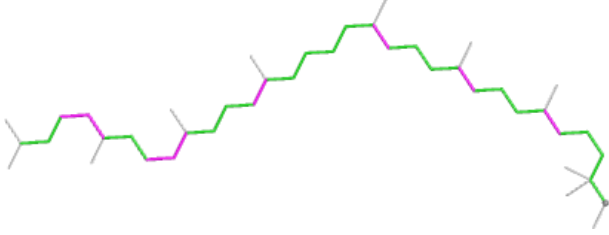
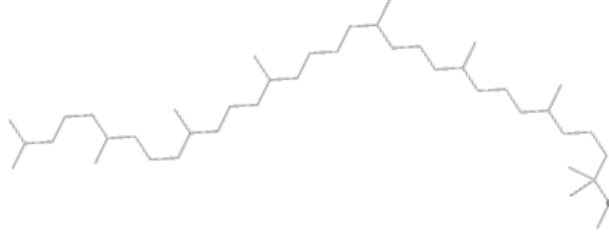
Ligand BCL R 102	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand SPO s 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

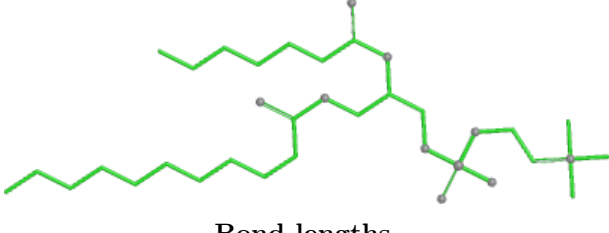
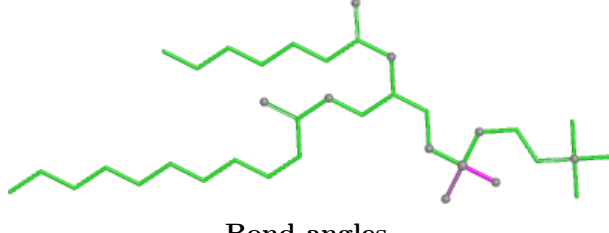
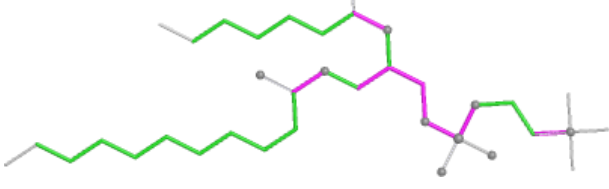
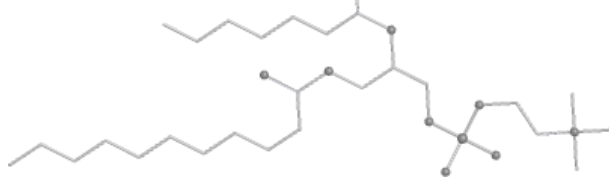
Ligand SPO 6 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

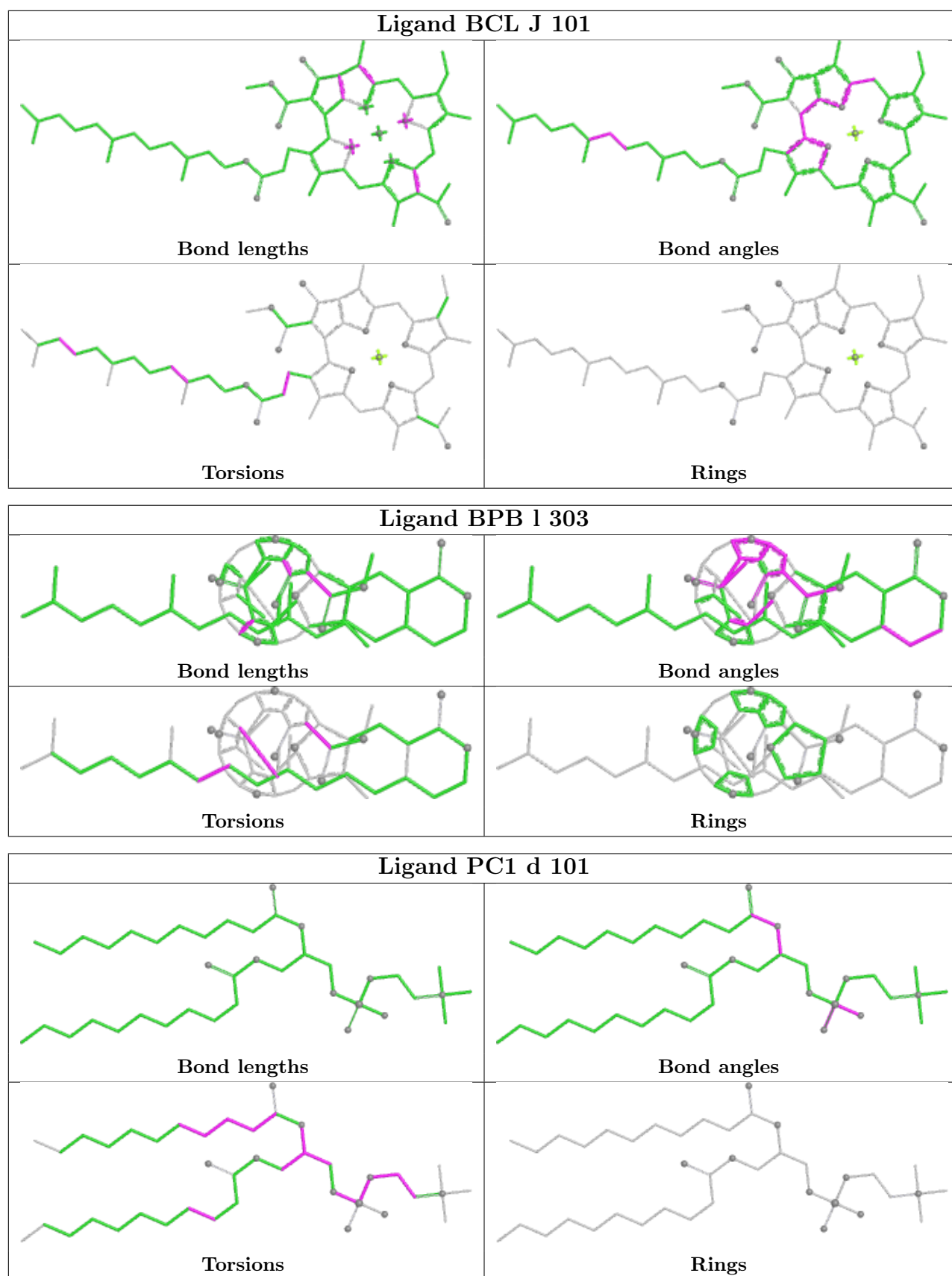
Ligand SPO F 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

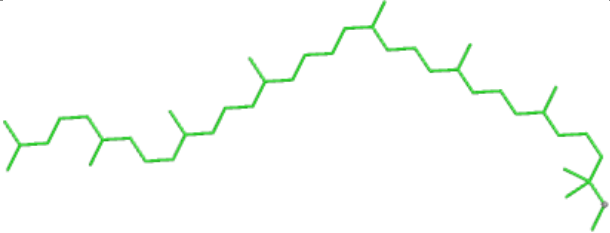
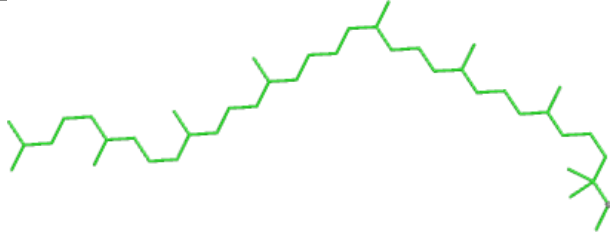
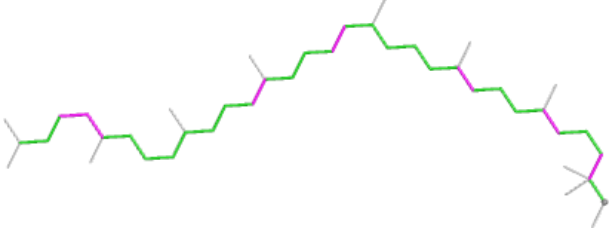
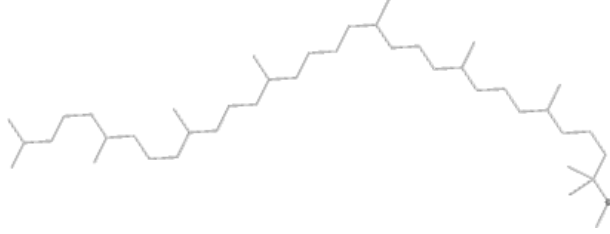
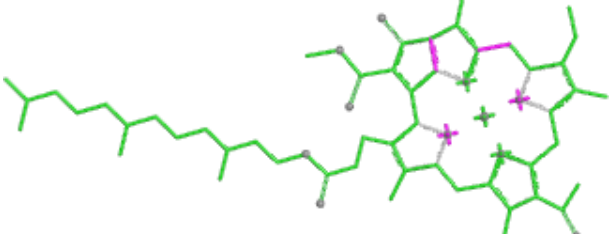
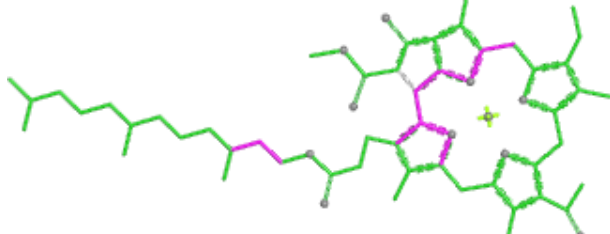
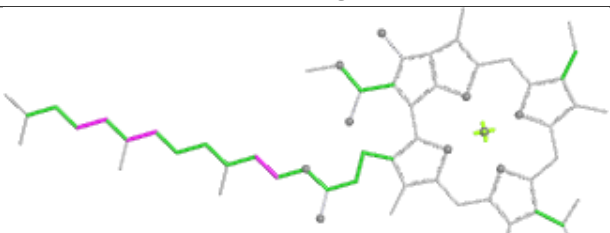
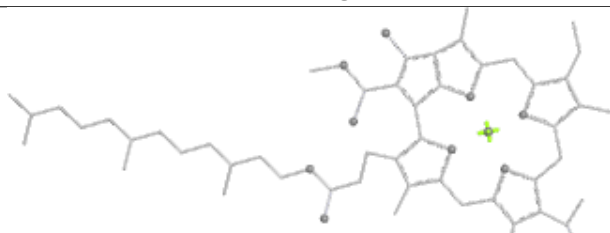


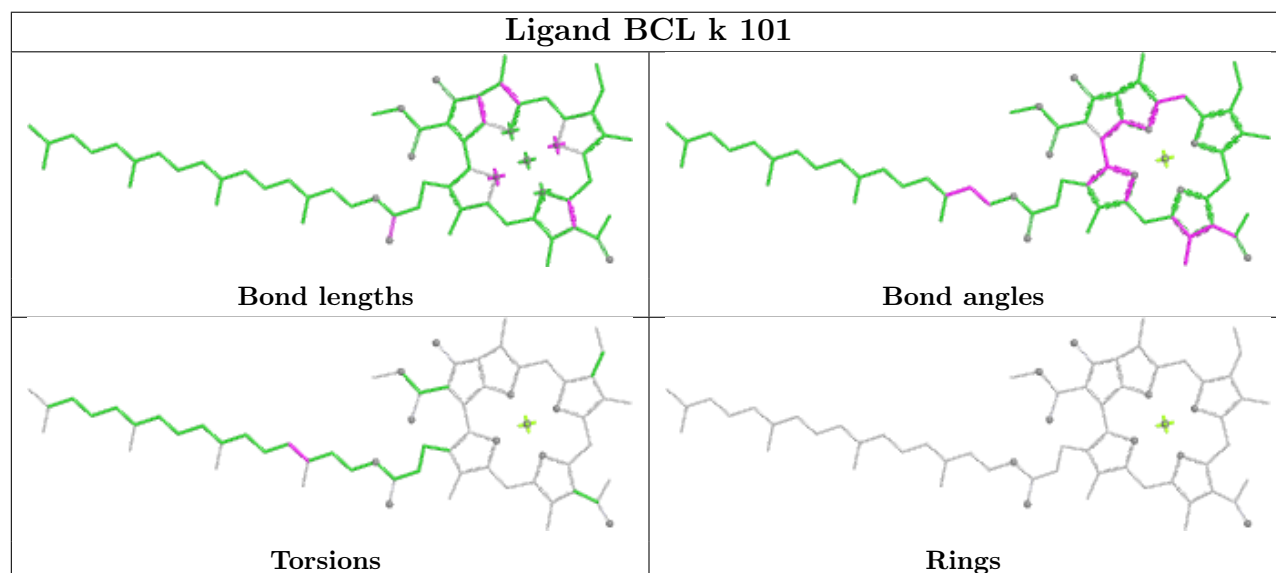
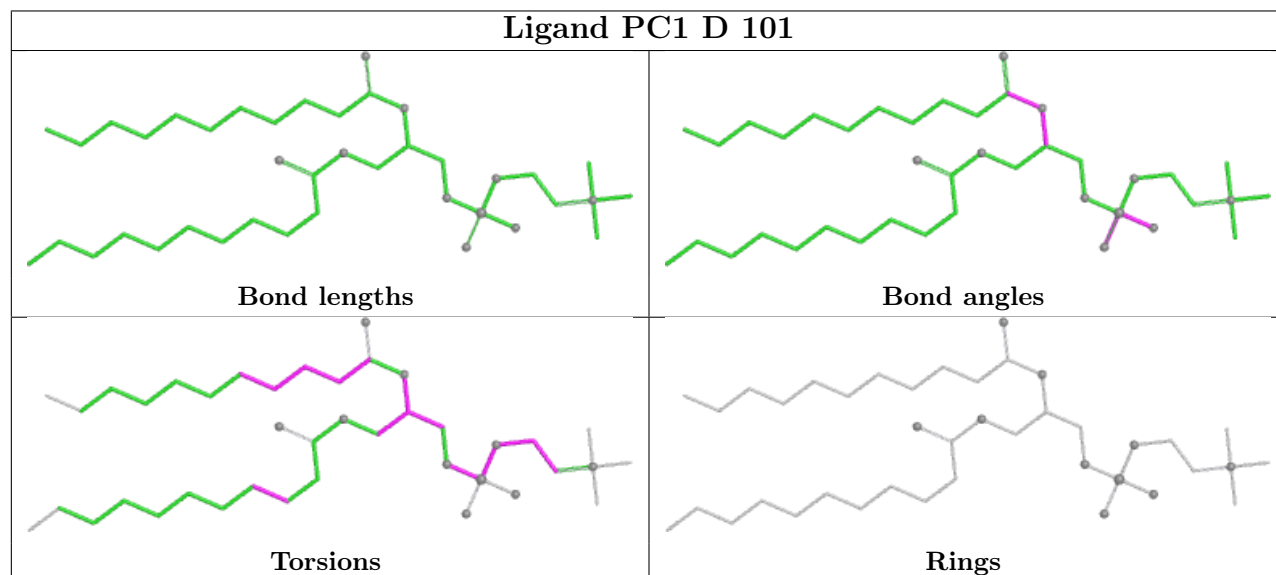
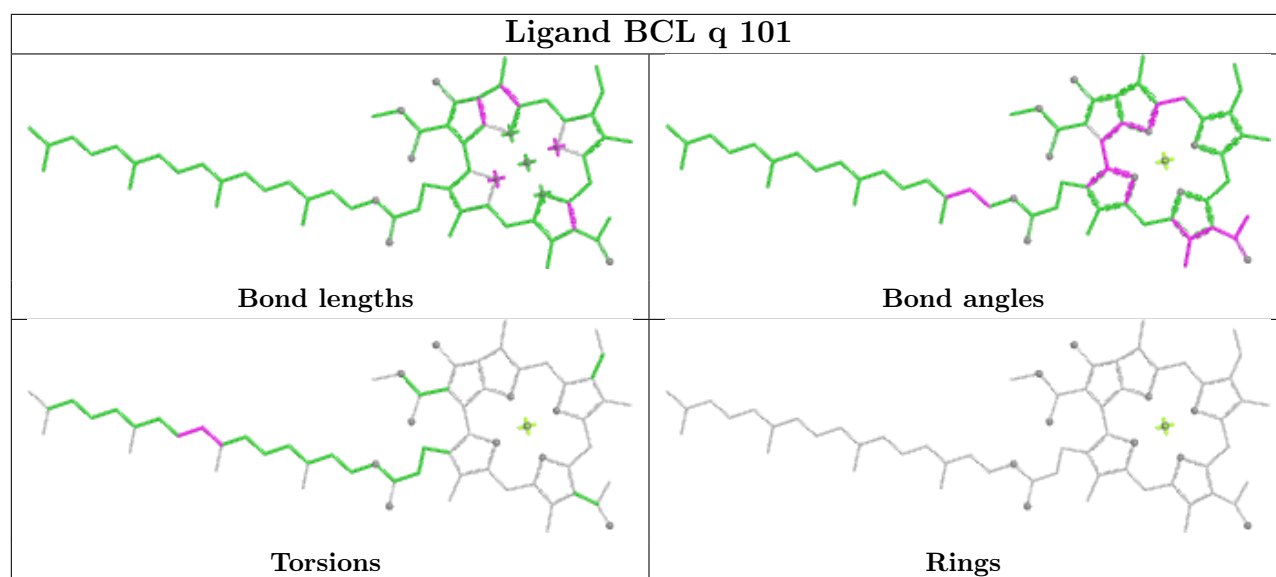
Ligand SPO V 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

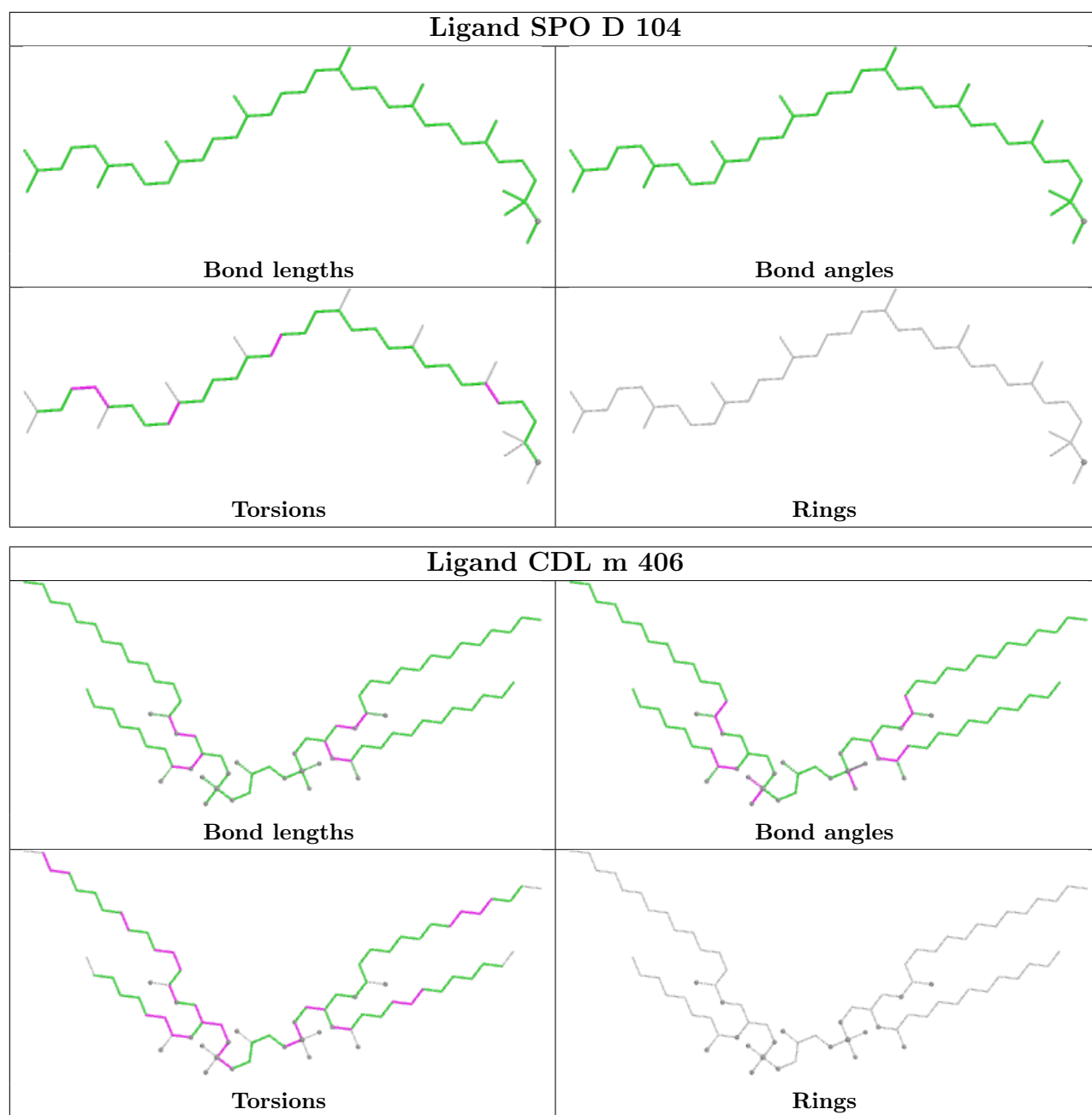
Ligand SPO r 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

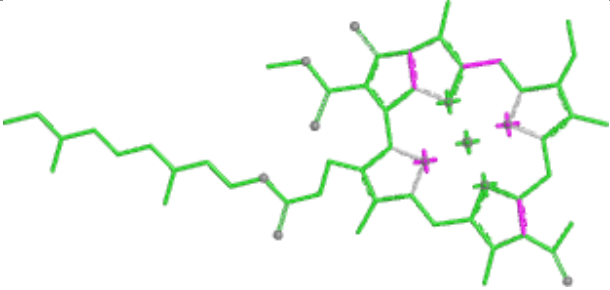
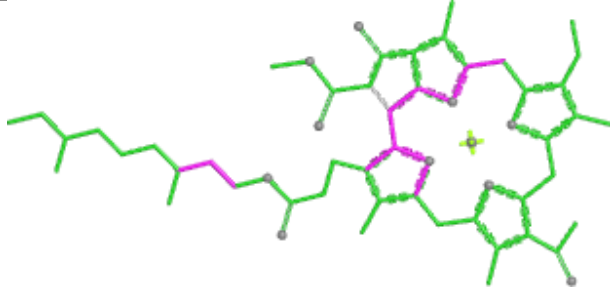
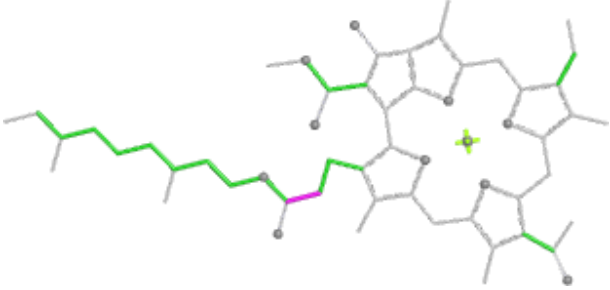
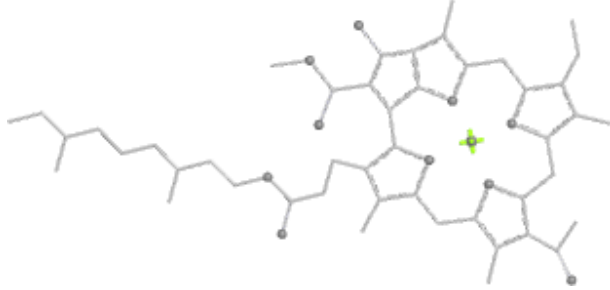
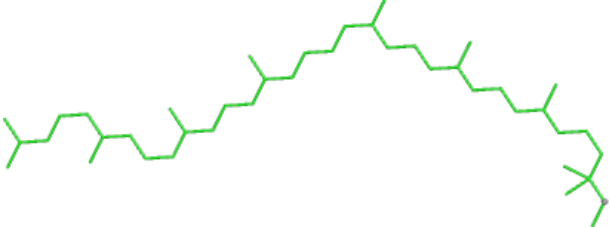
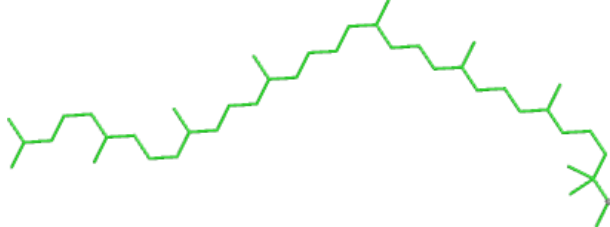
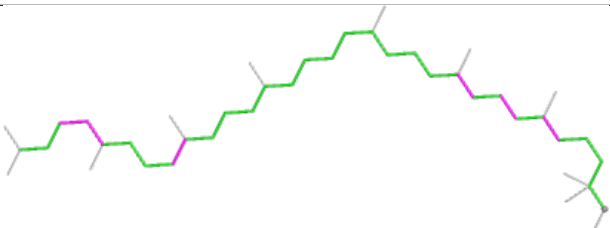
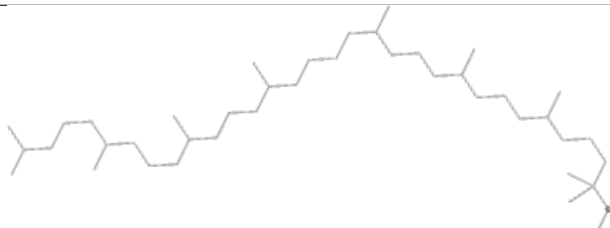
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Bond lengths	Bond angles
	
Torsions	Rings

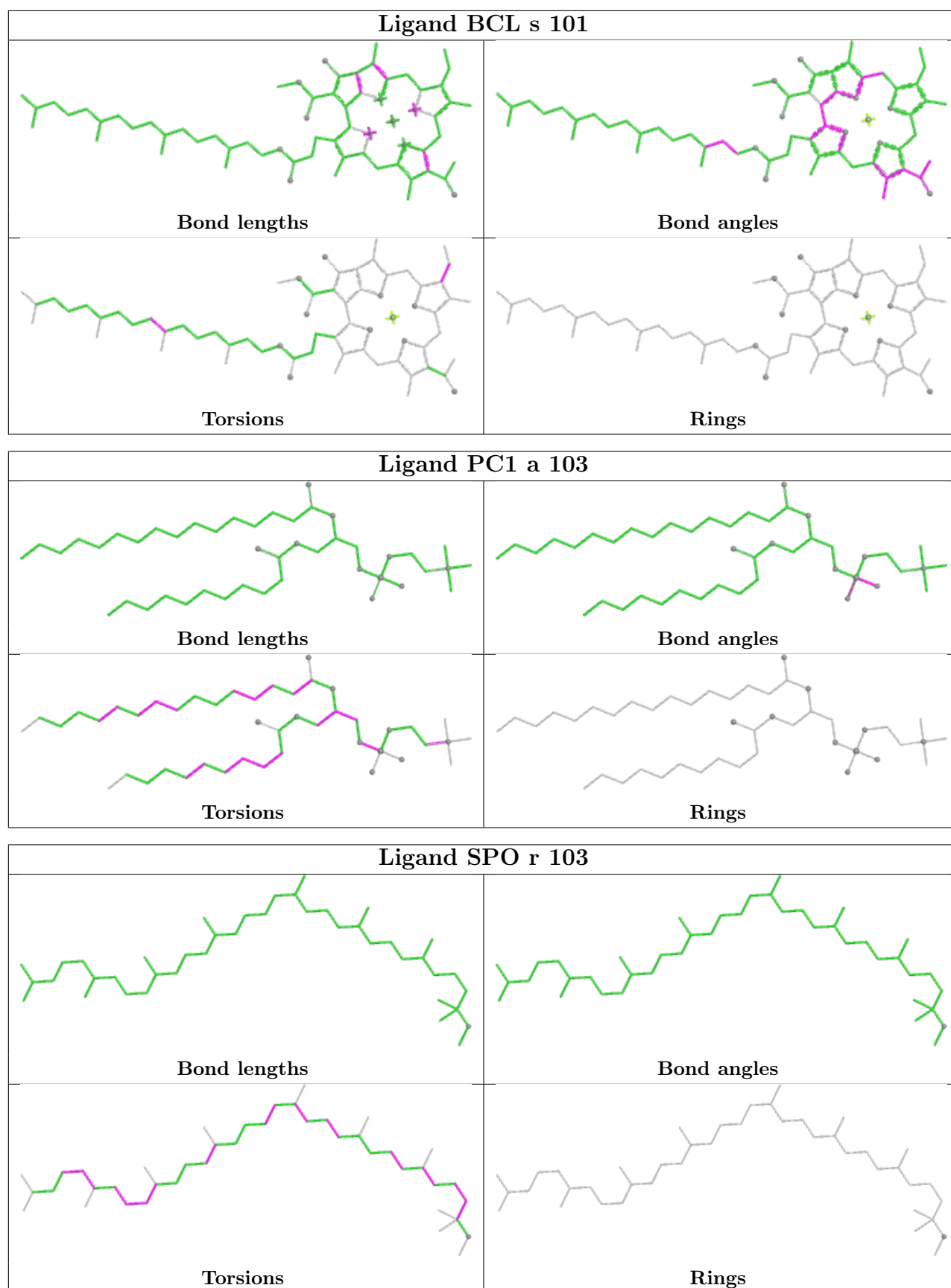


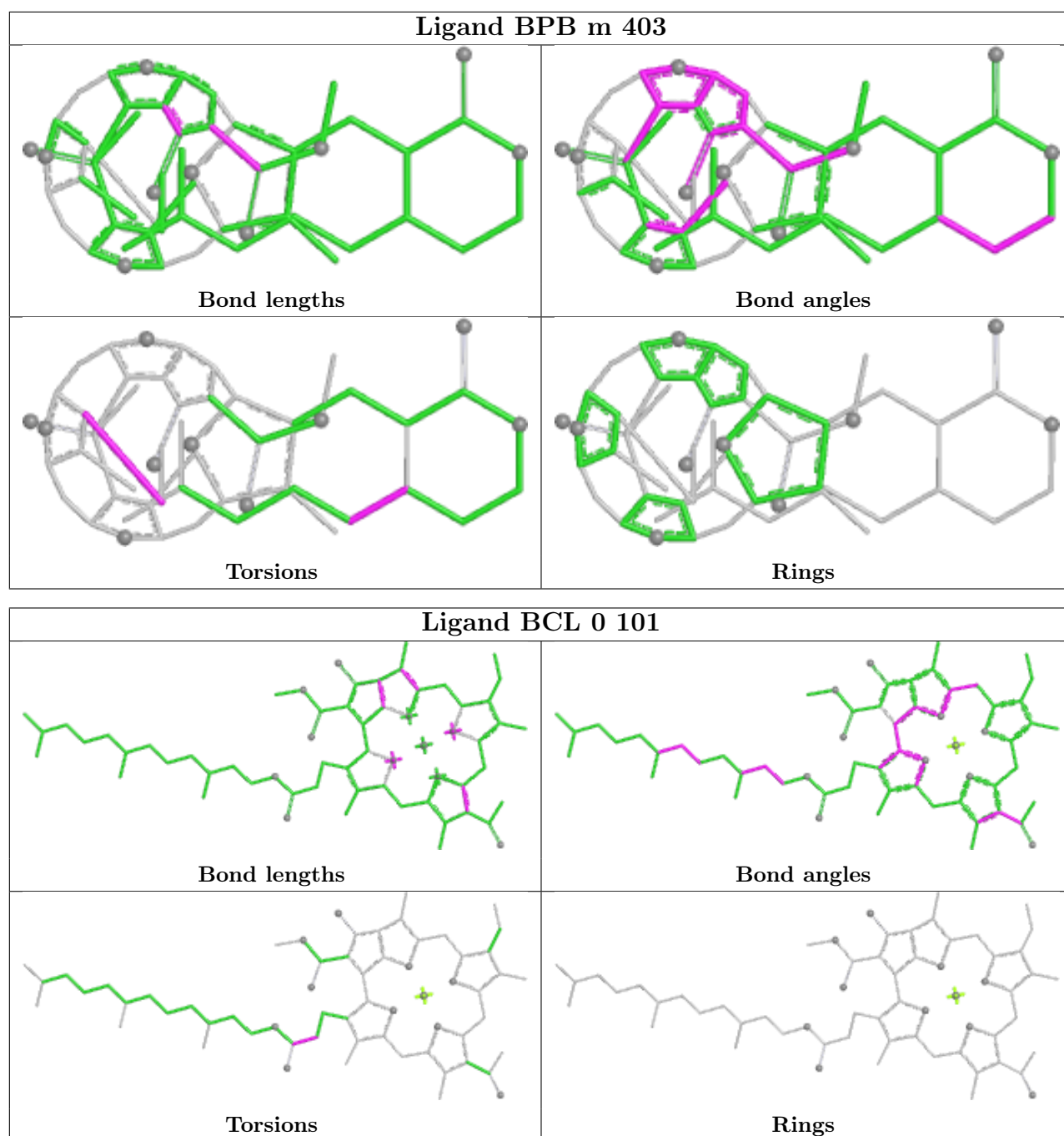
Ligand SPO V 103	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCL 6 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

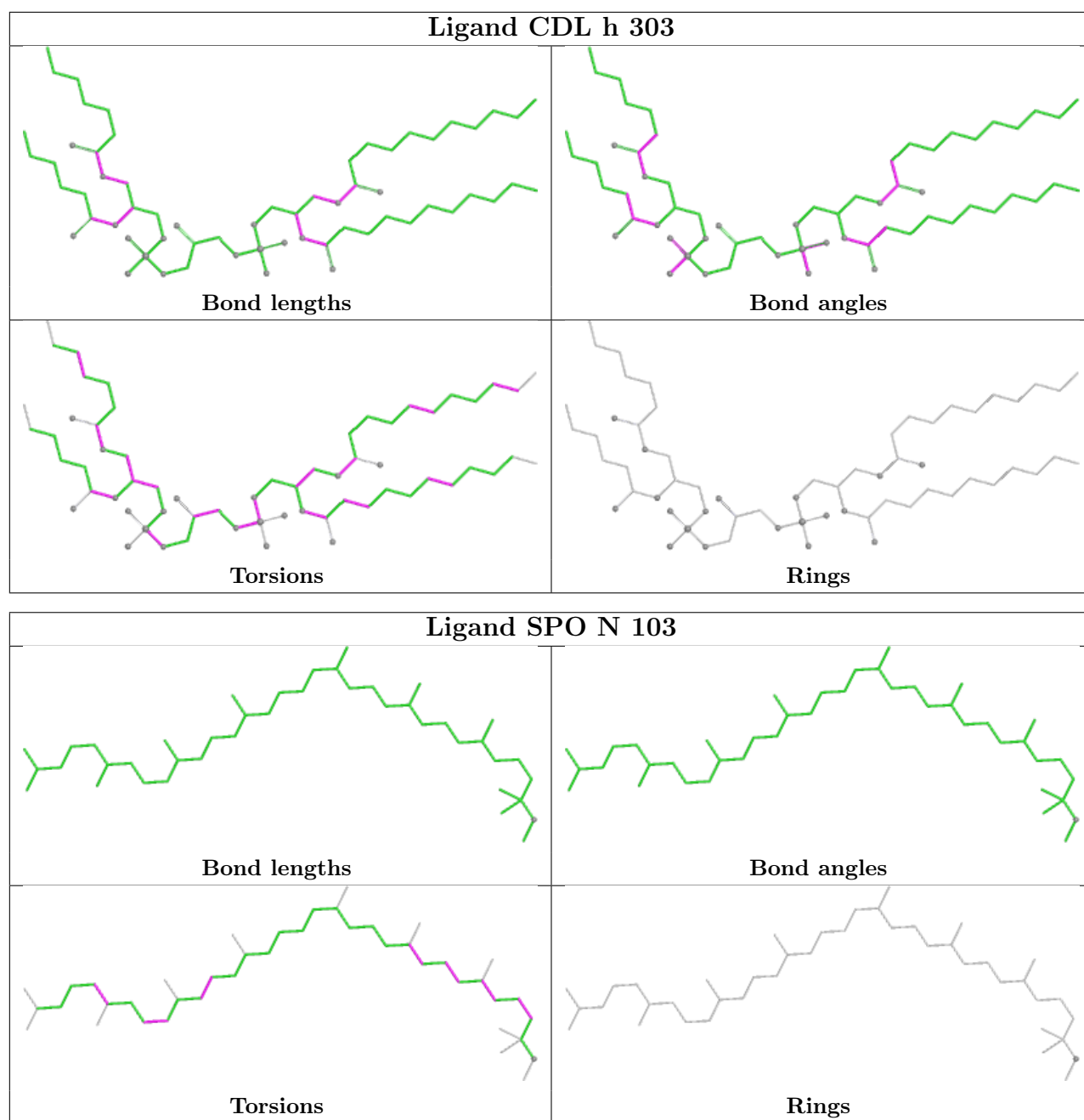


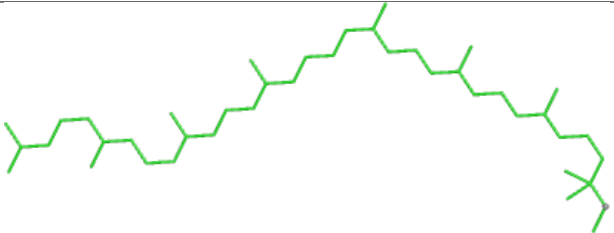
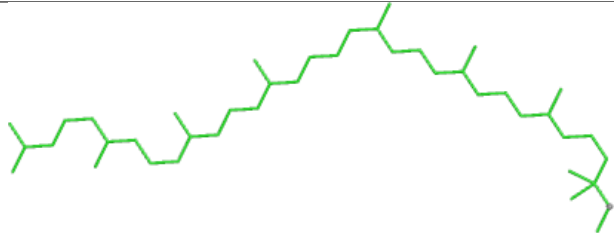
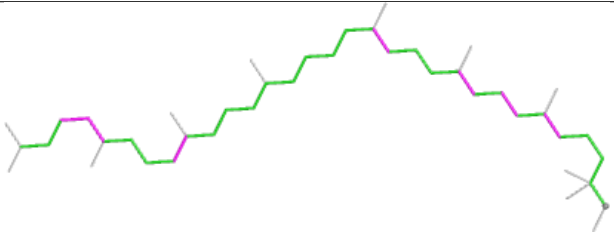
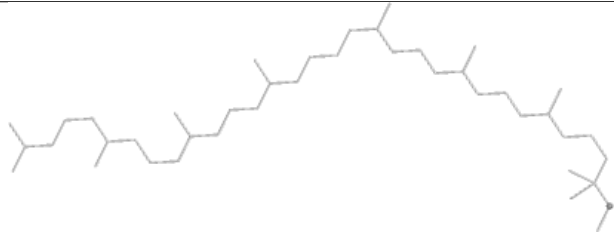
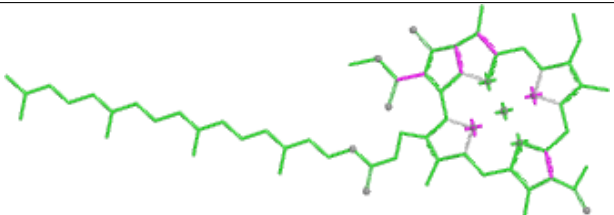
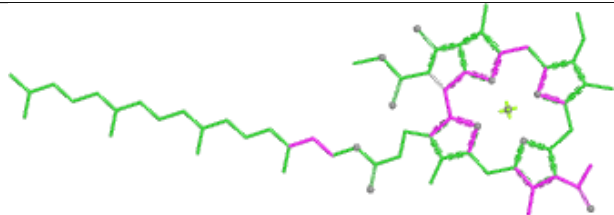
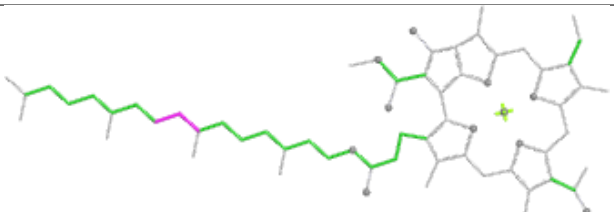
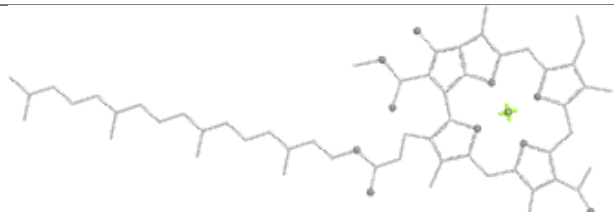
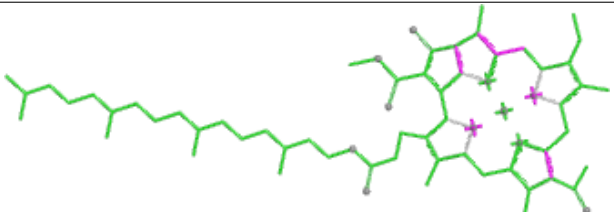
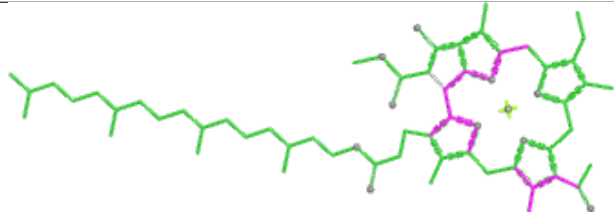
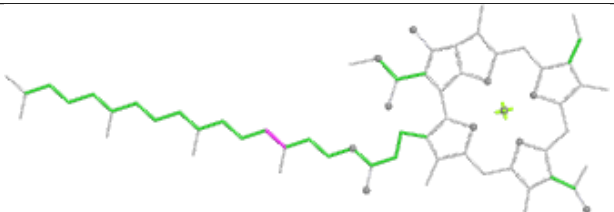
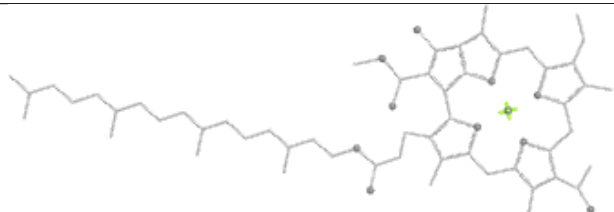


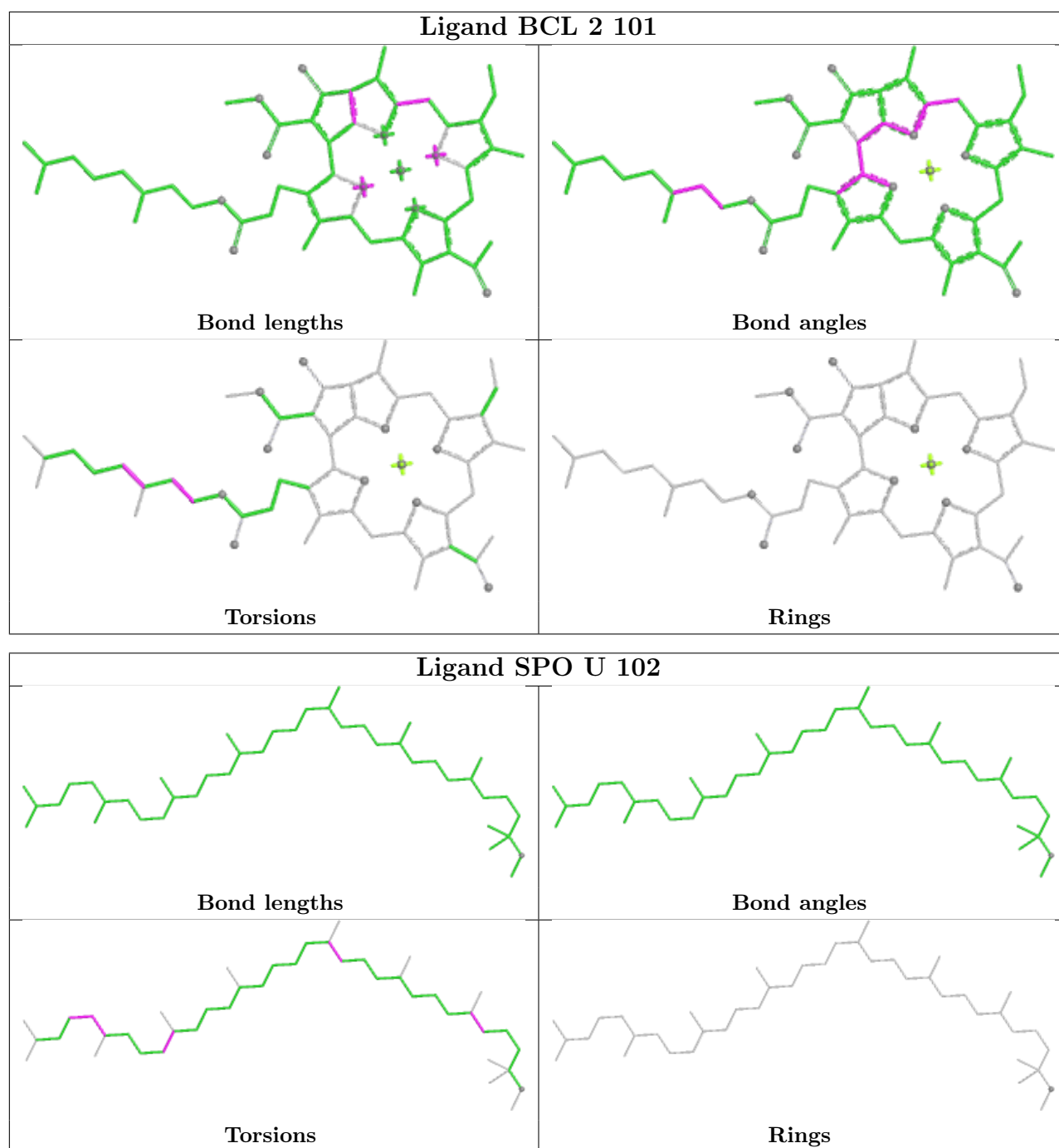
Ligand BCL Z 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand SPO 5 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

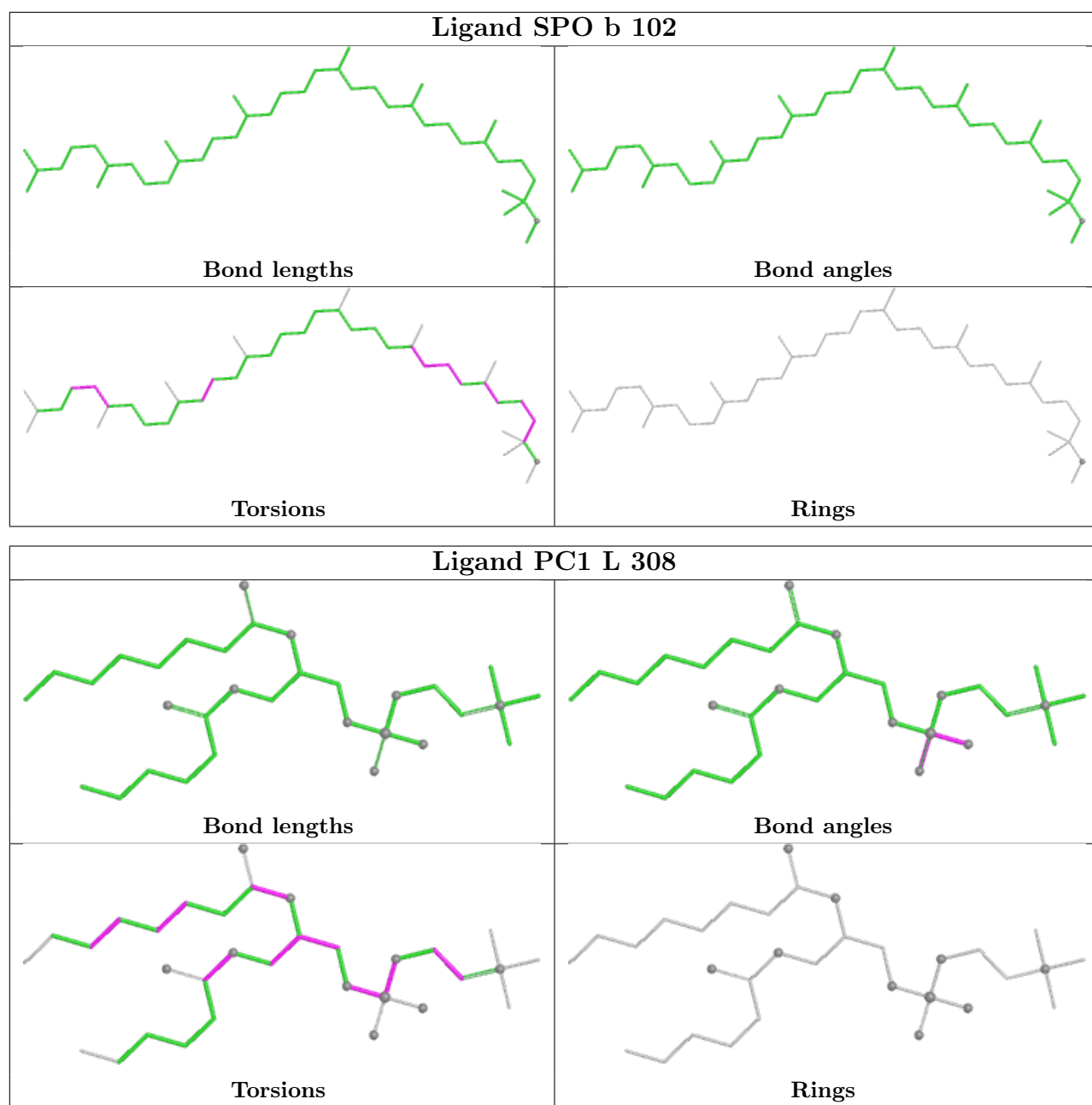


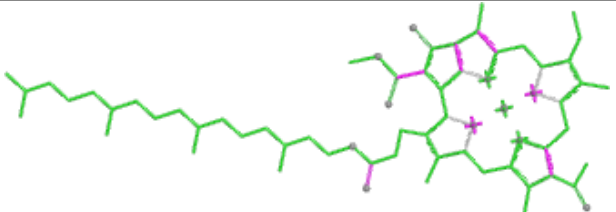
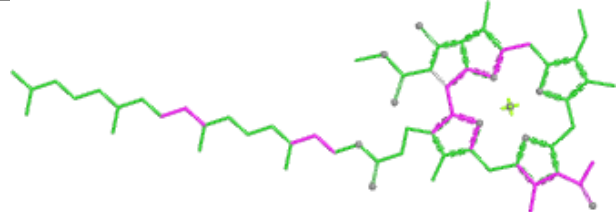
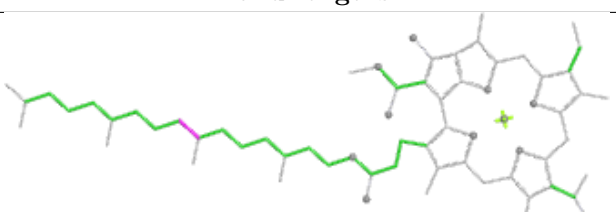
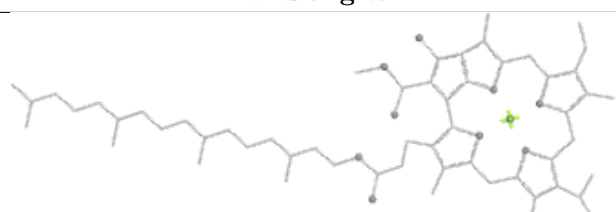


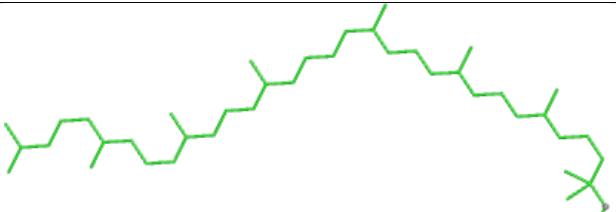
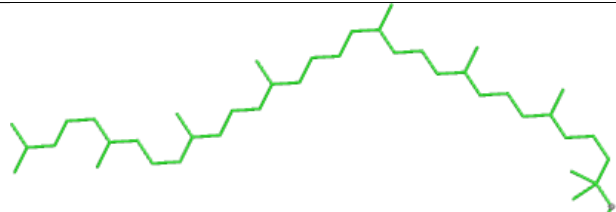
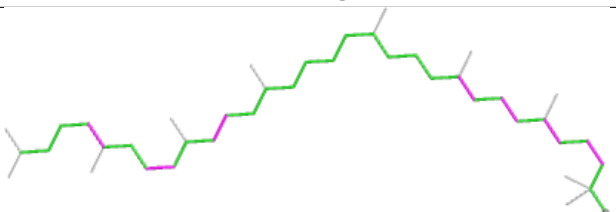


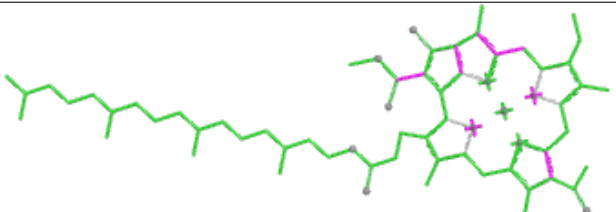
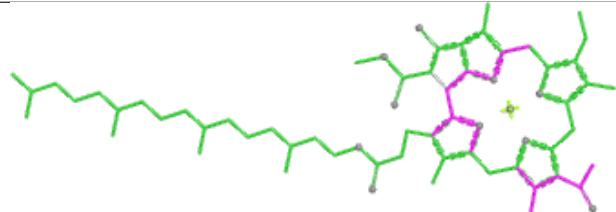
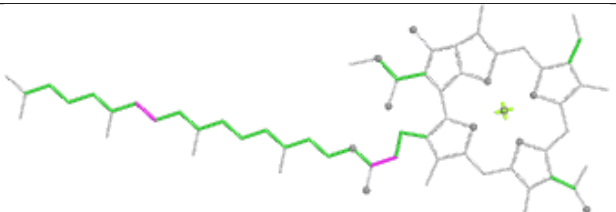
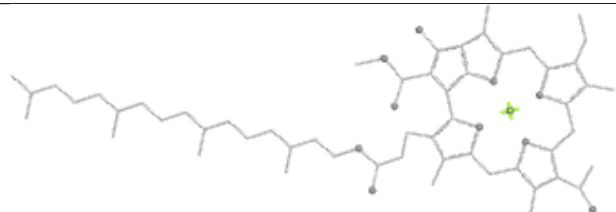
Ligand SPO c 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCL a 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCL 5 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

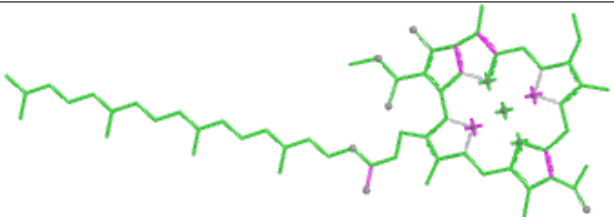
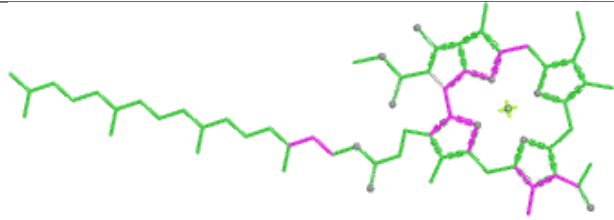
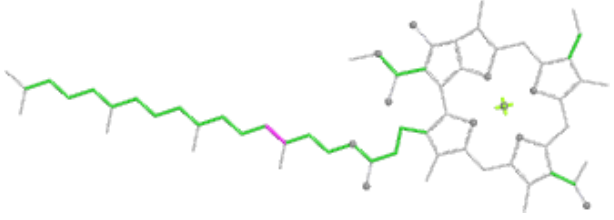
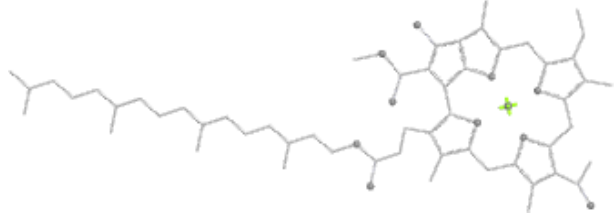


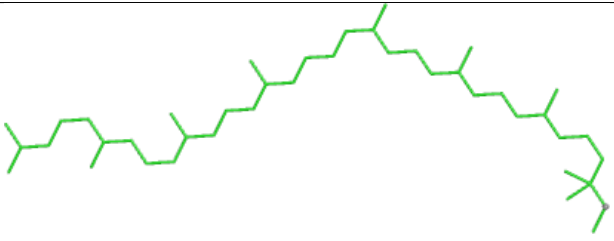
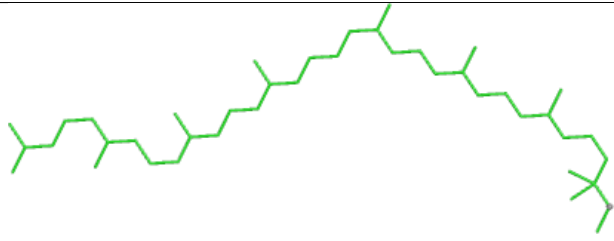
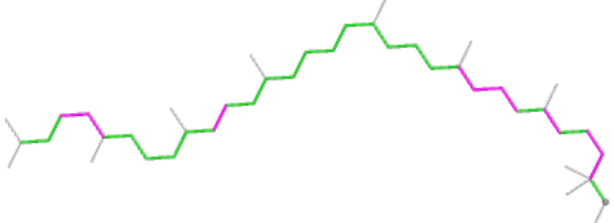
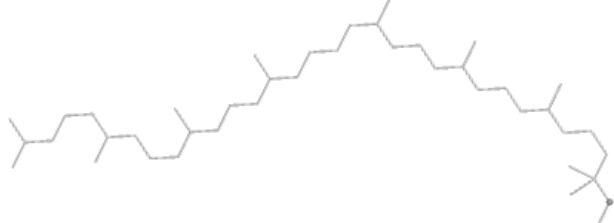


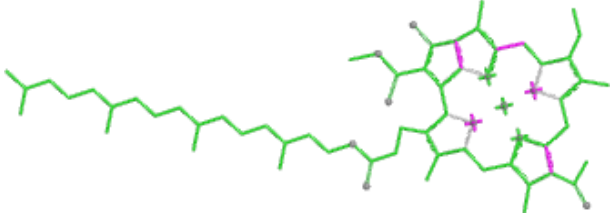
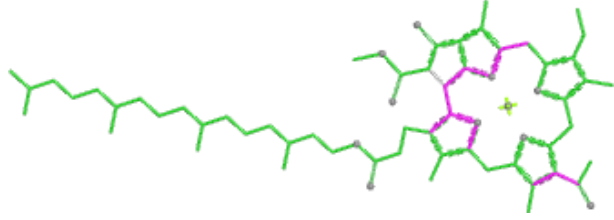
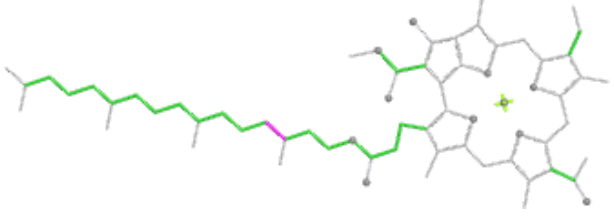
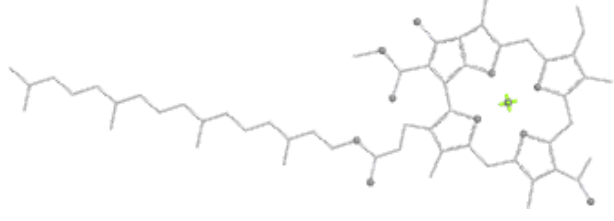
Ligand BCL d 103	
	
Bond lengths	Bond angles
	
Torsions	Rings

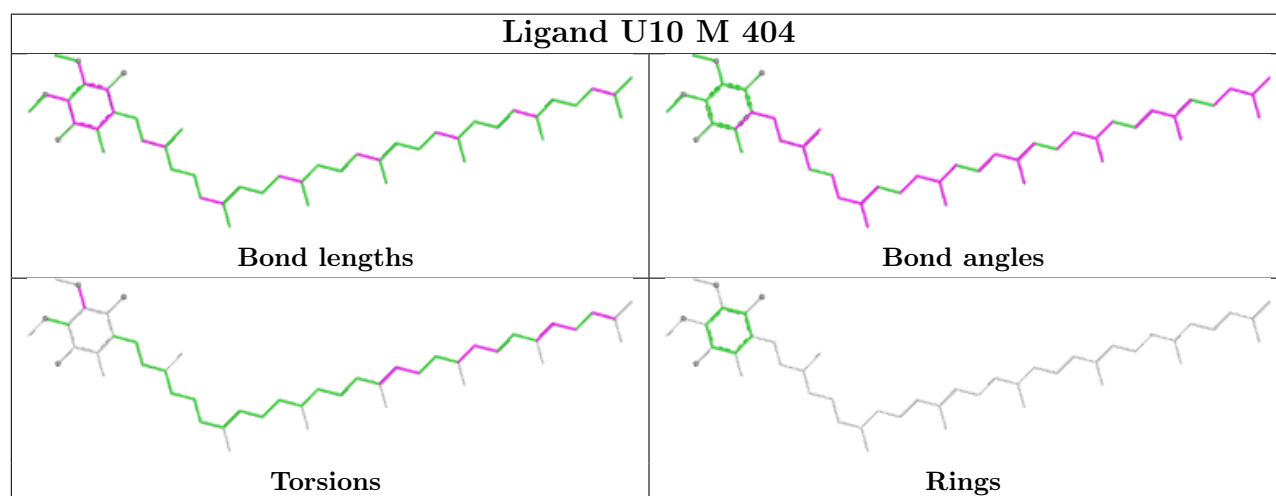
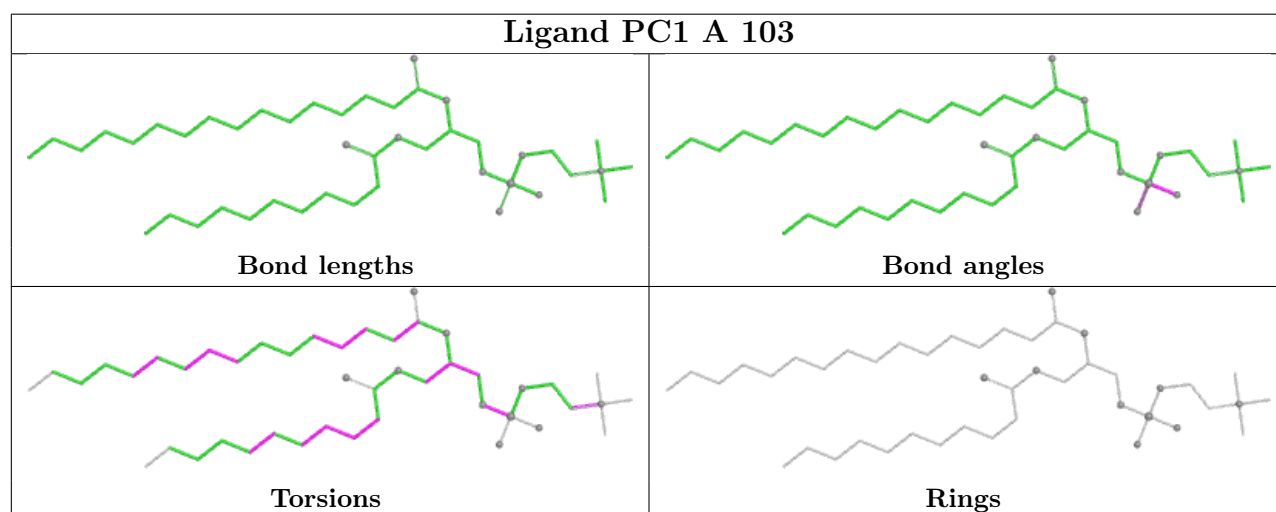
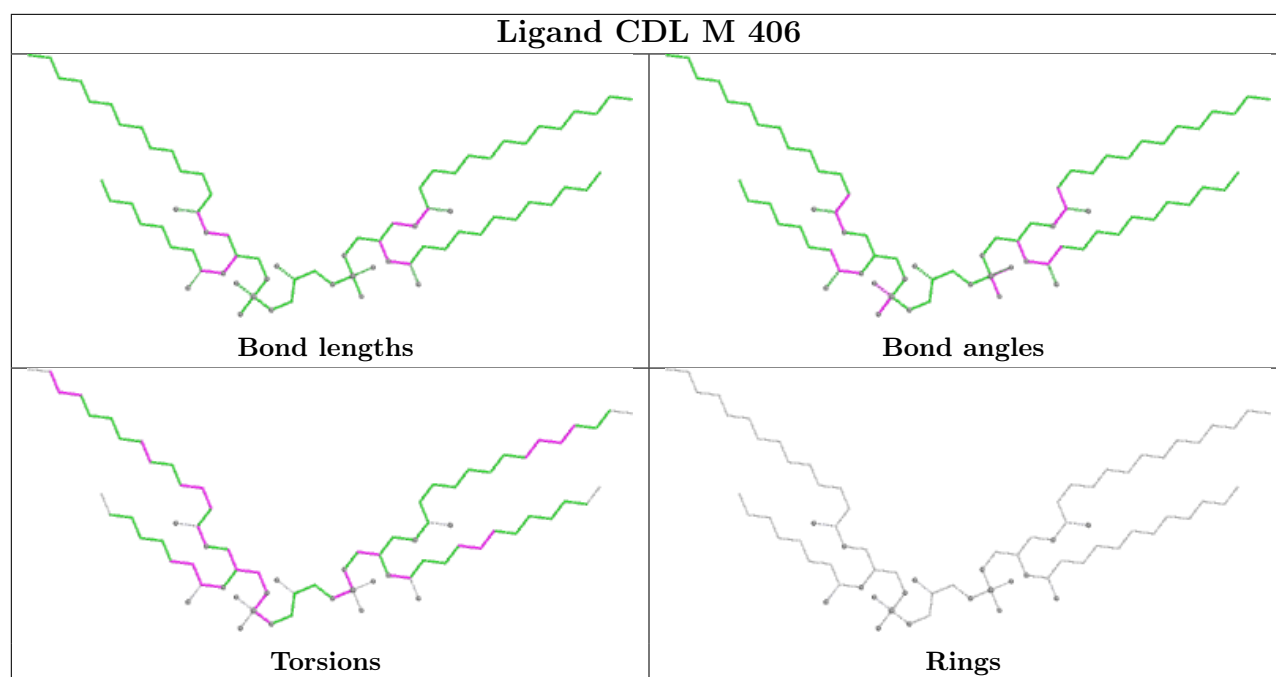
Ligand SPO n 103	
	
Bond lengths	Bond angles
	
Torsions	Rings

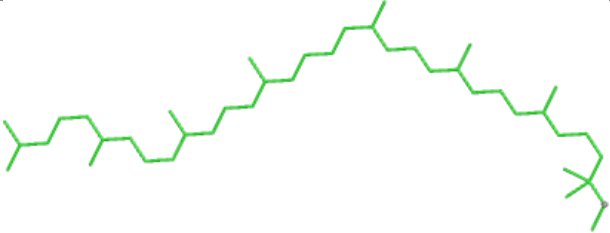
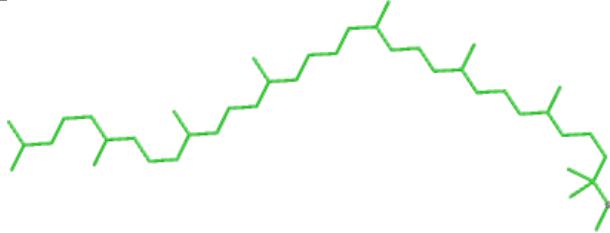
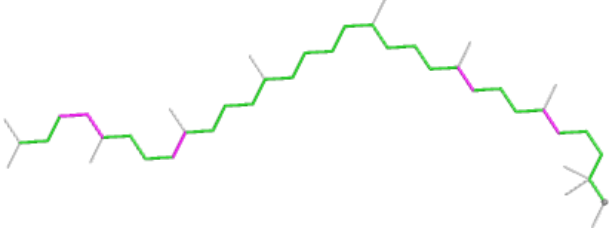
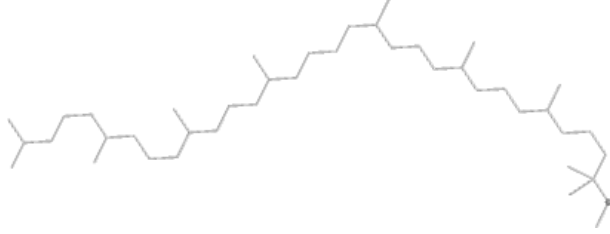
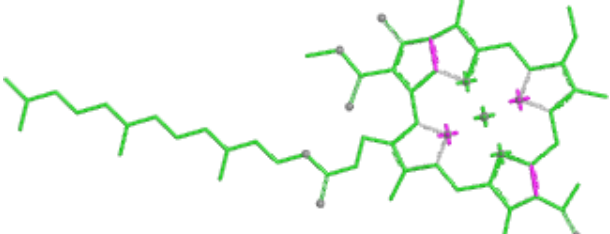
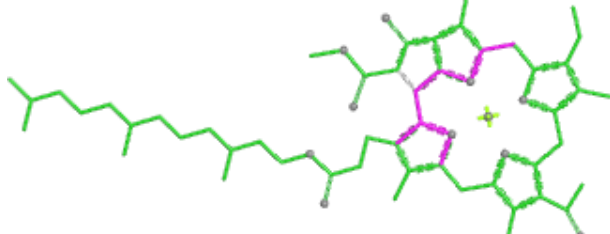
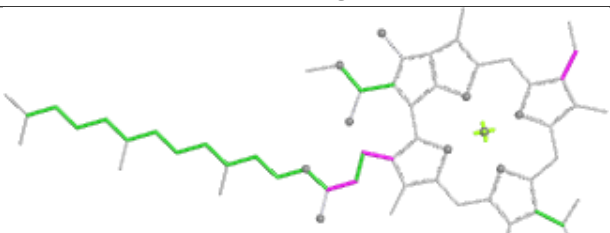
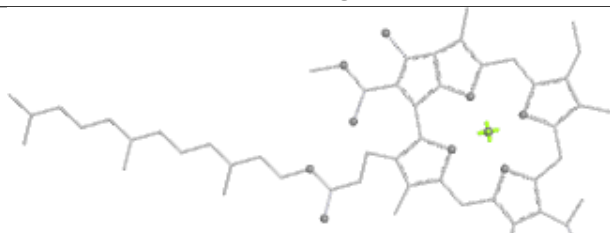
Ligand BCL M 402	
	
Bond lengths	Bond angles
	
Torsions	Rings

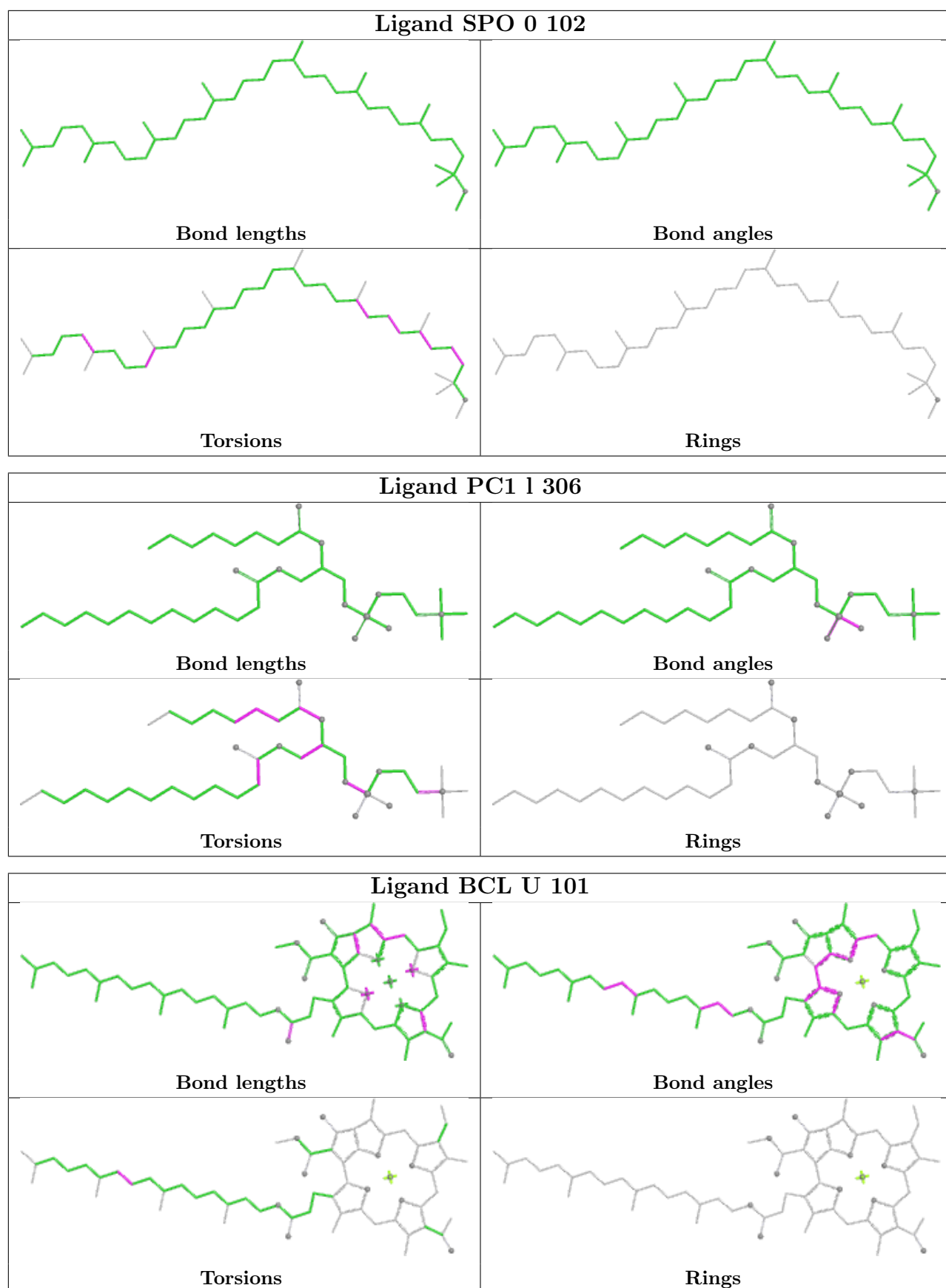
Ligand BCL K 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

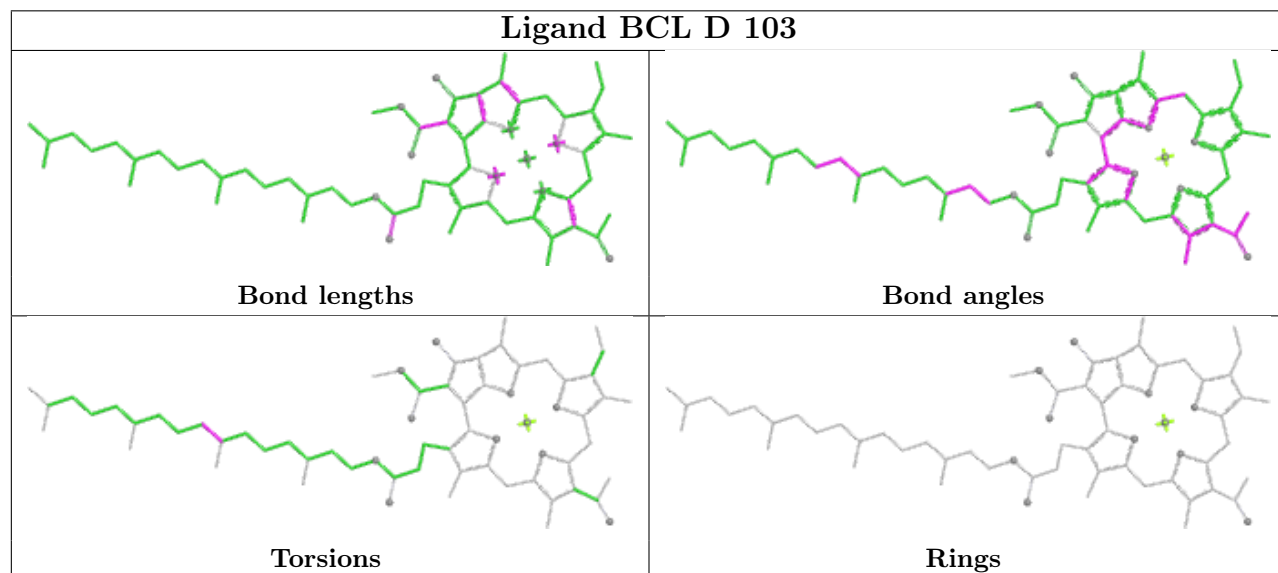
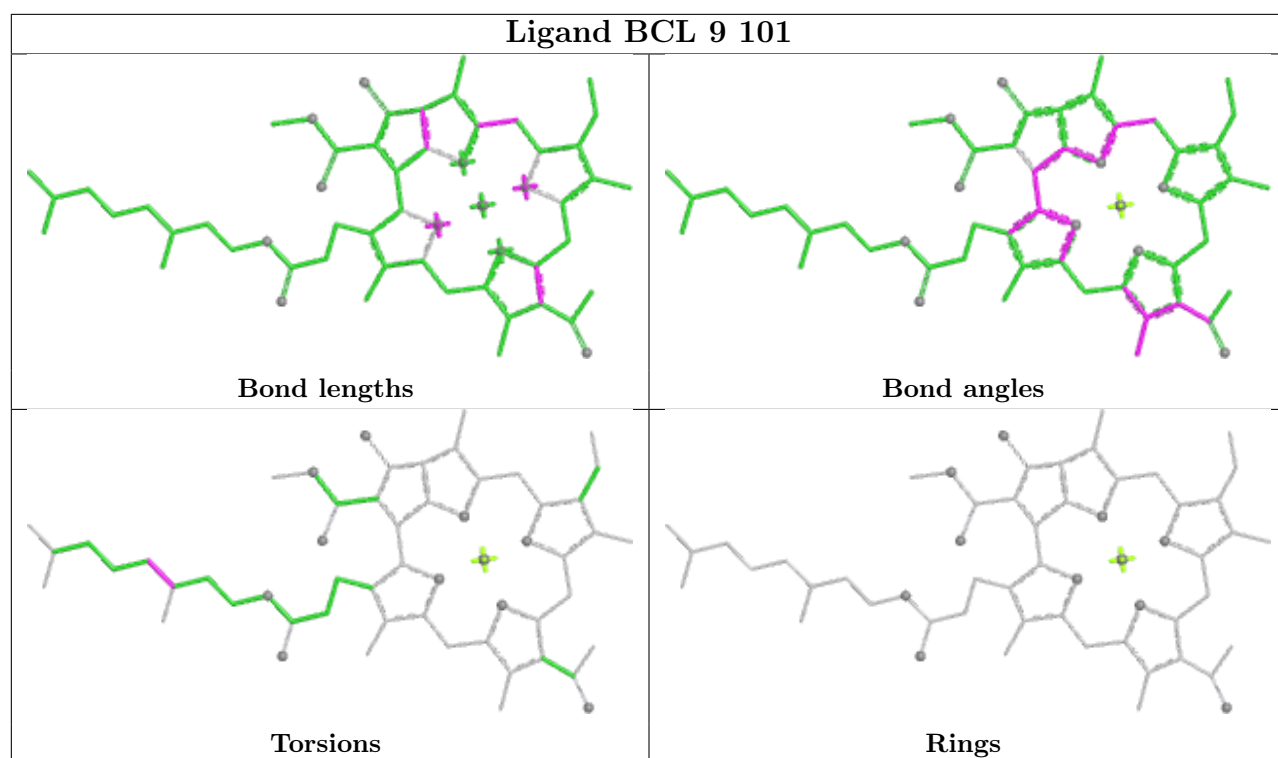
Ligand SPO B 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

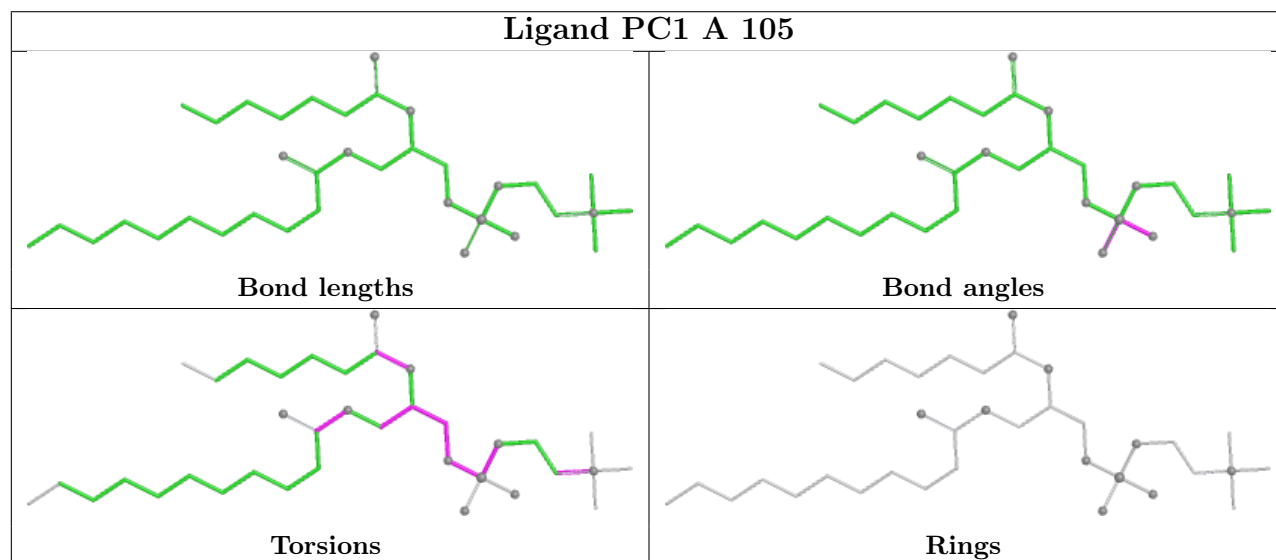
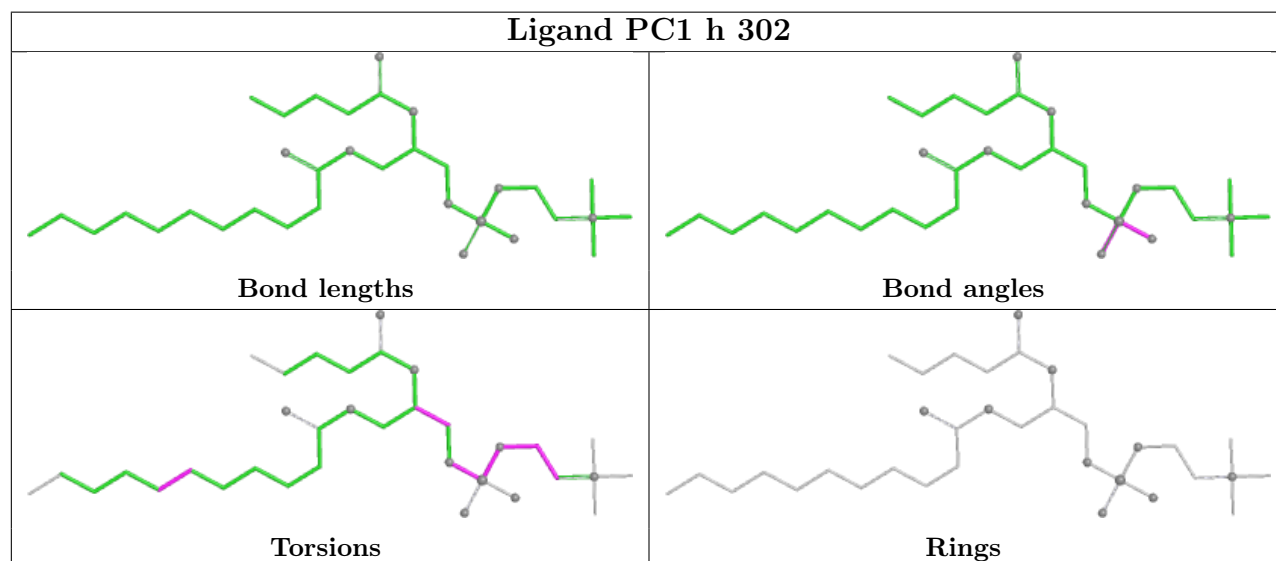
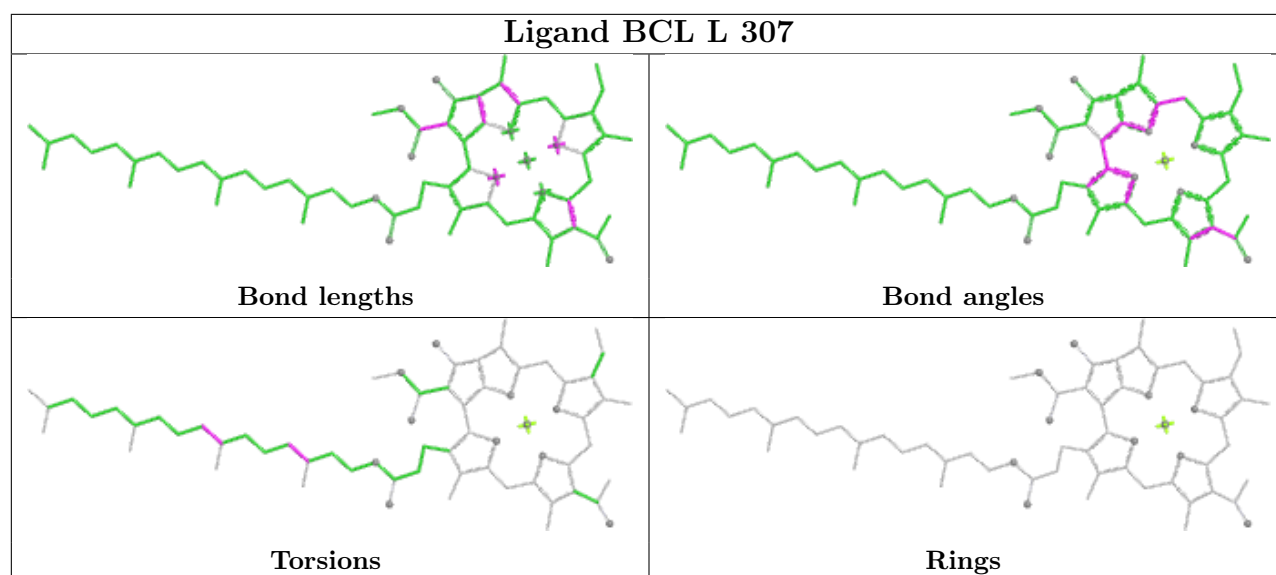
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Bond lengths	Bond angles
	
Torsions	Rings

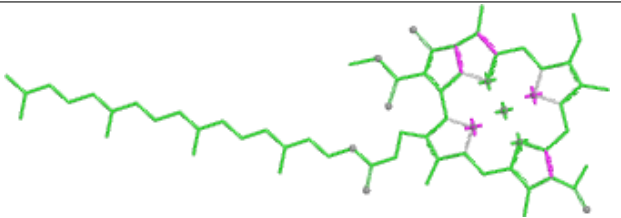
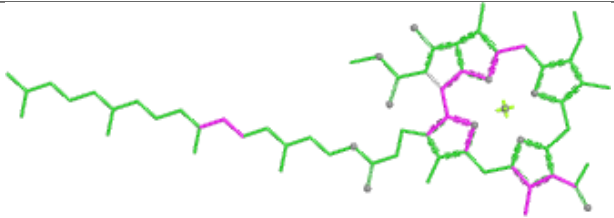
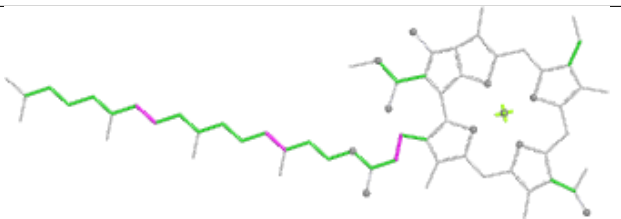
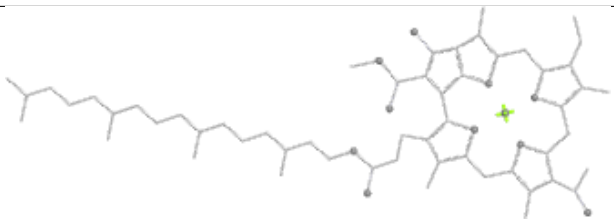


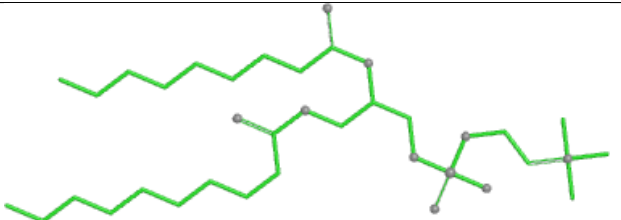
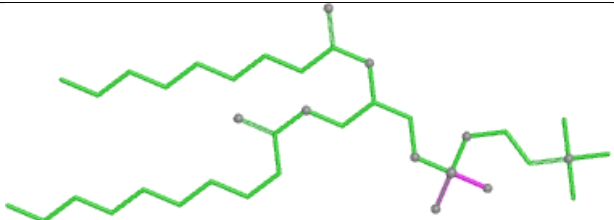
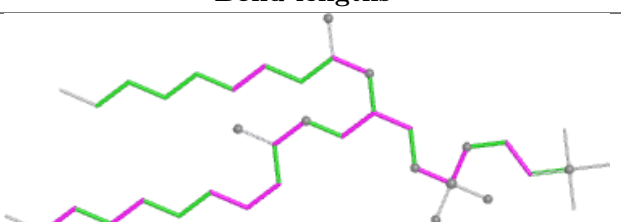
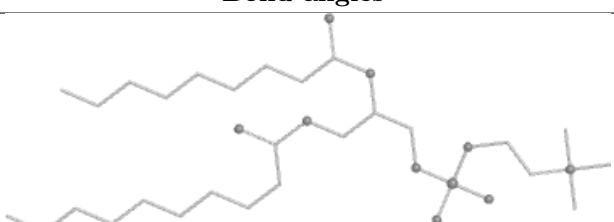
Ligand SPO S 102	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCL n 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

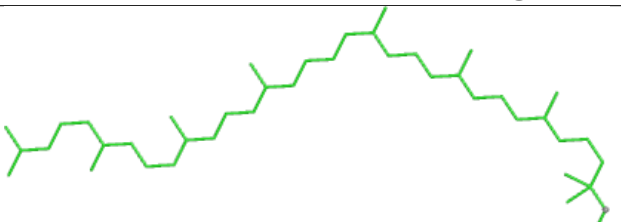
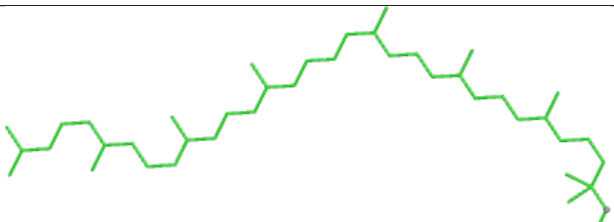
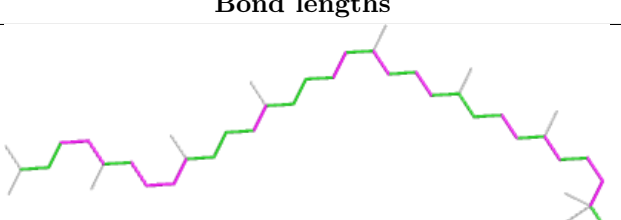
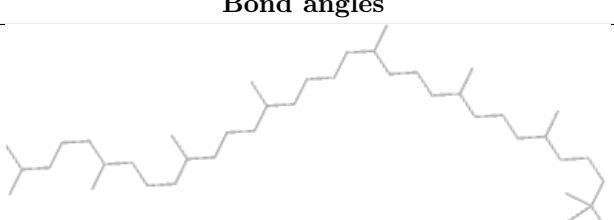


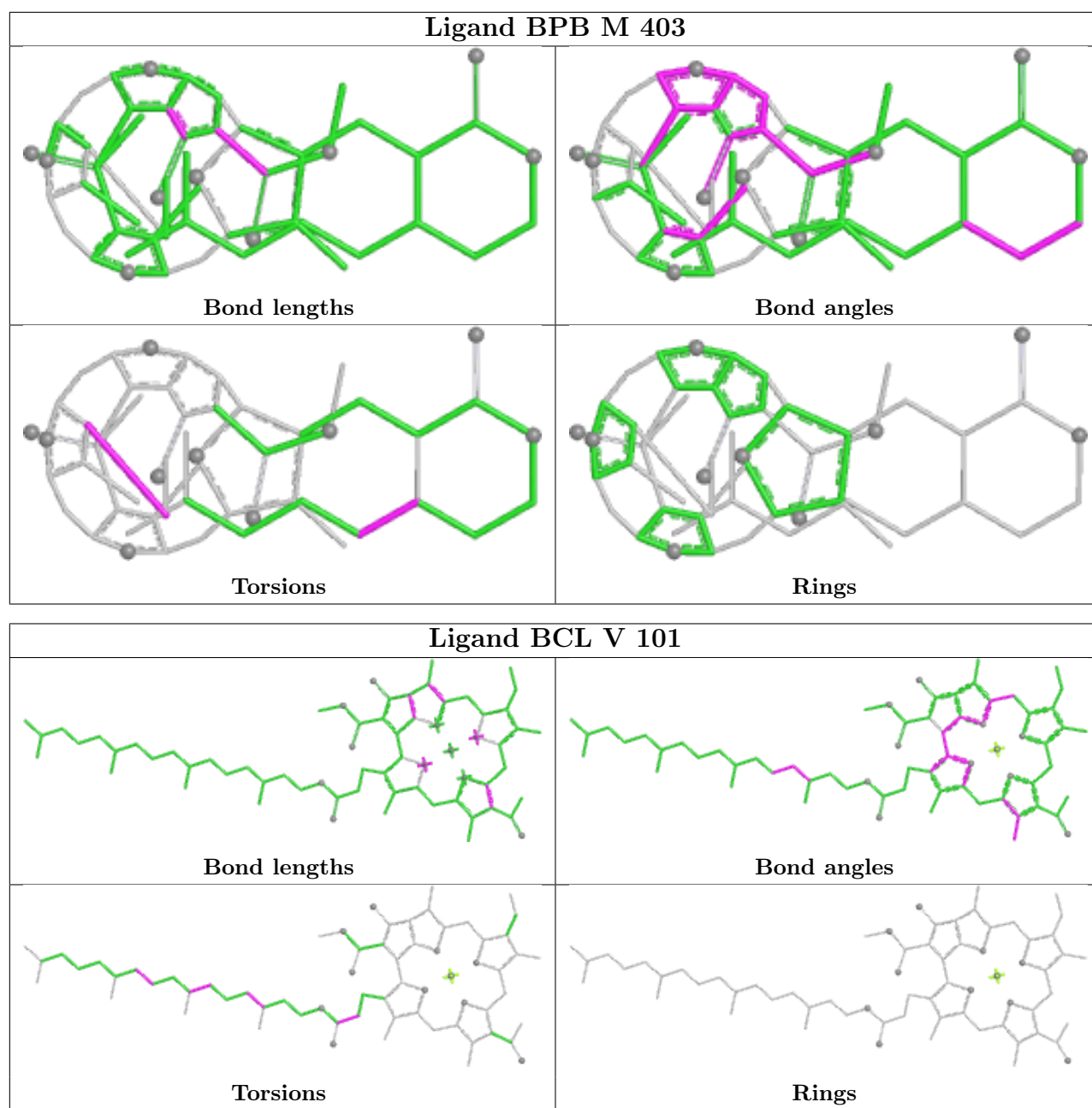


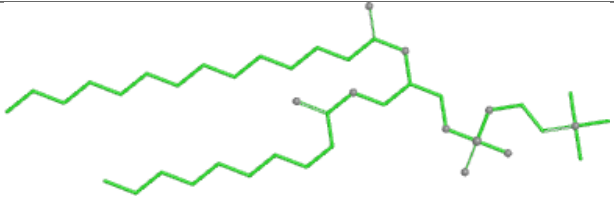
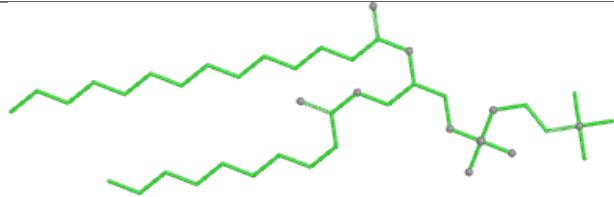
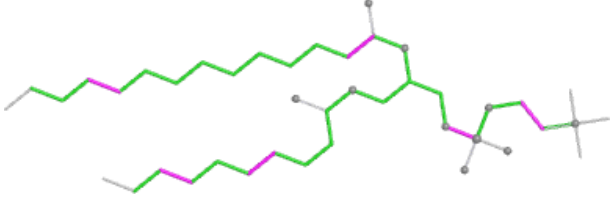
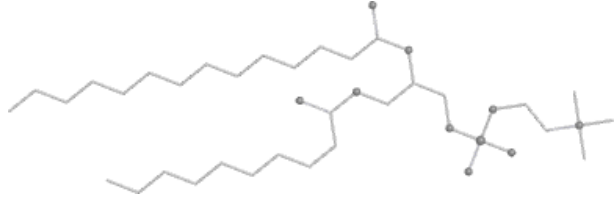
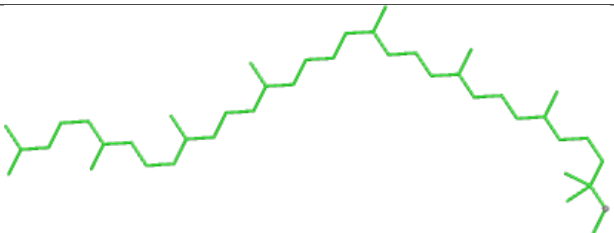
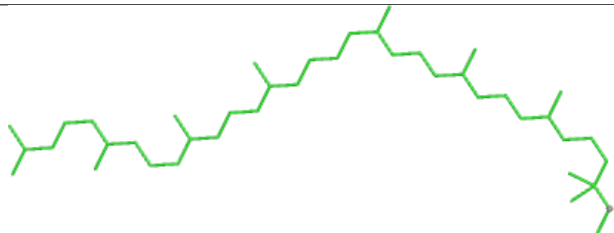
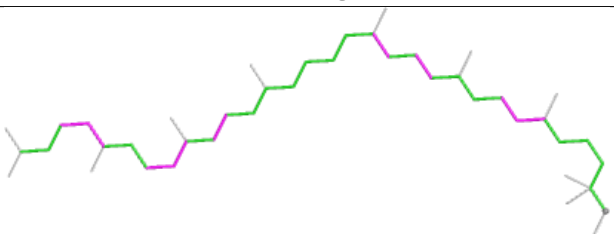
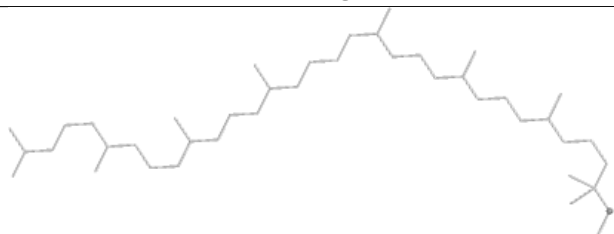
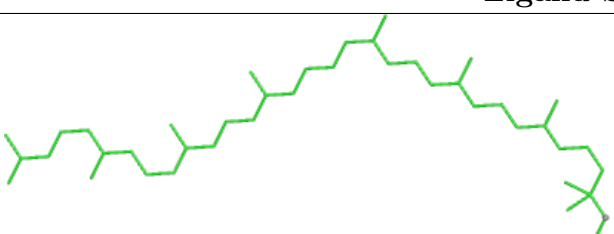
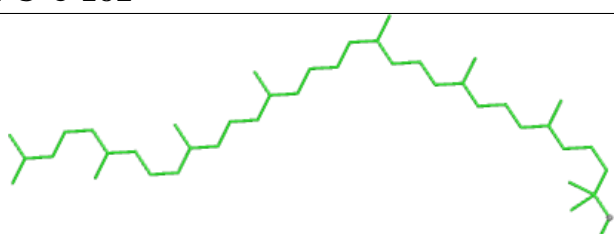
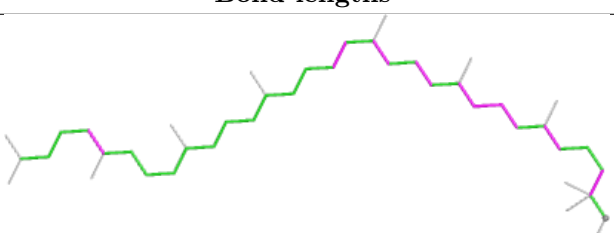
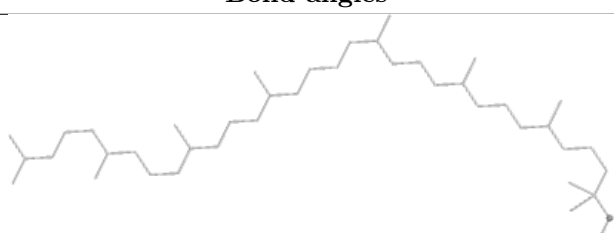


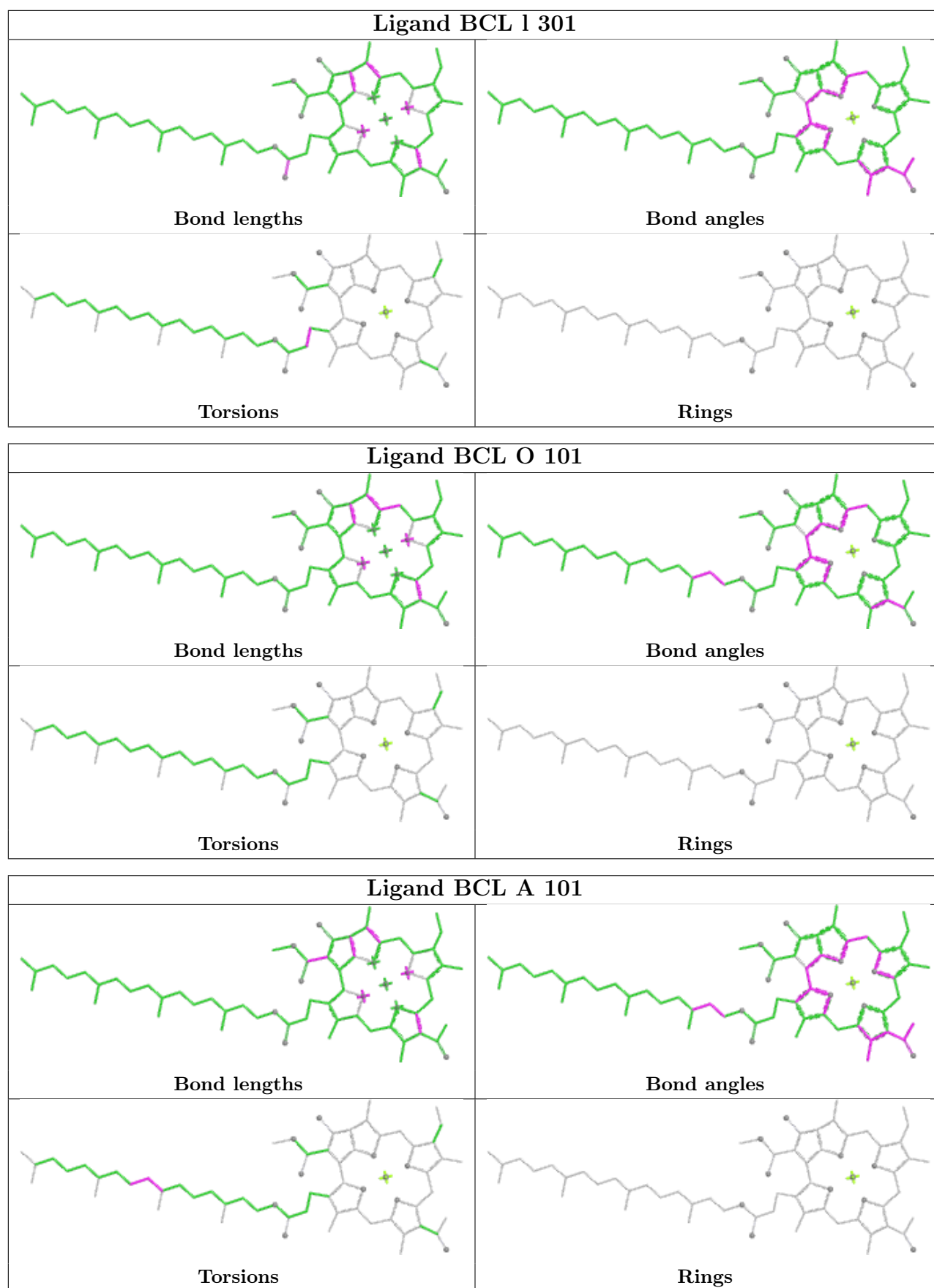
Ligand BCL B 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

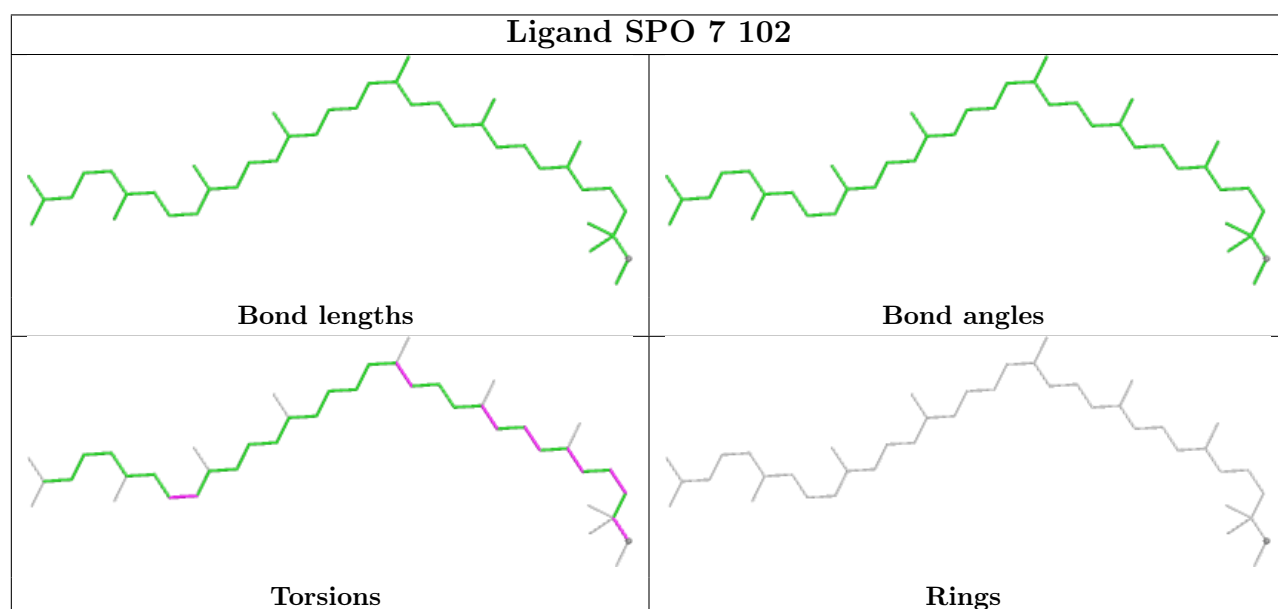
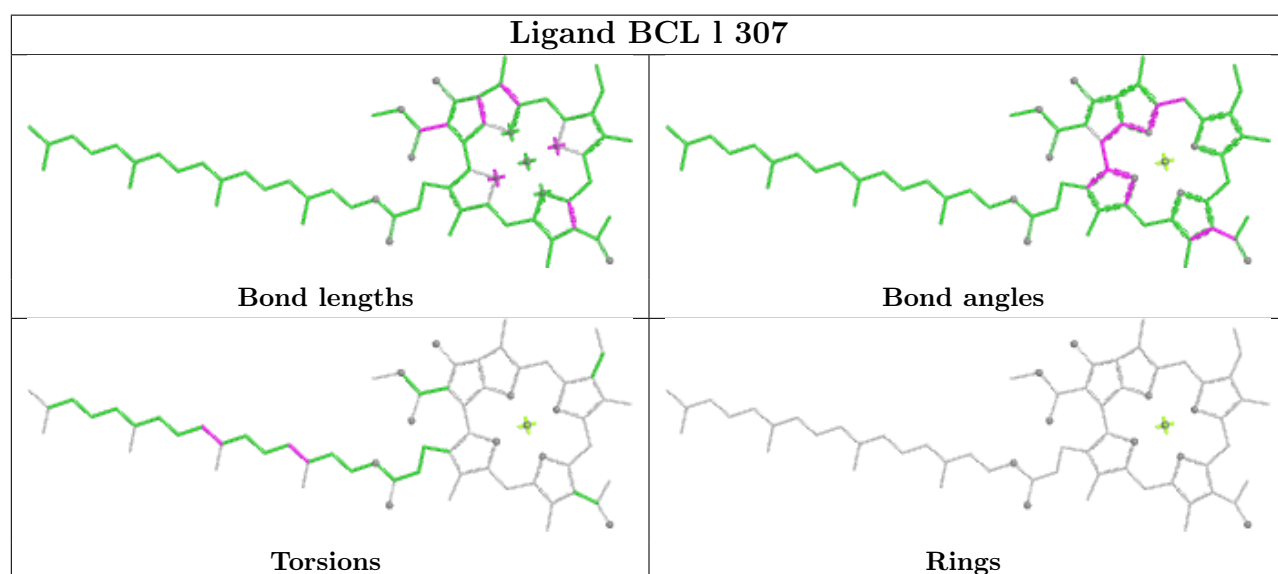
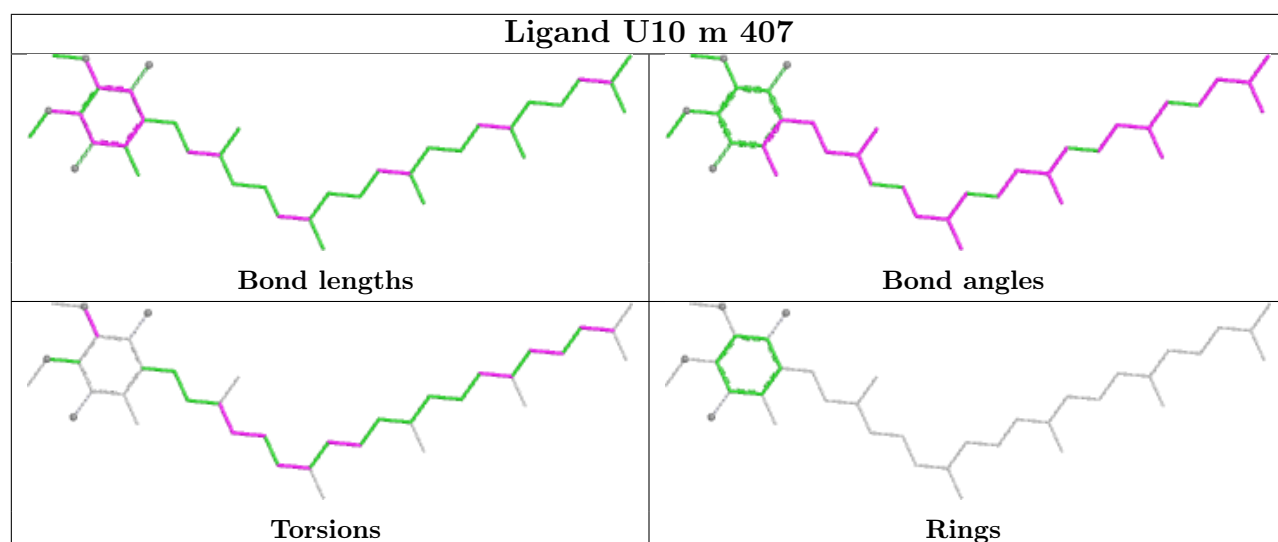
Ligand PC1 D 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

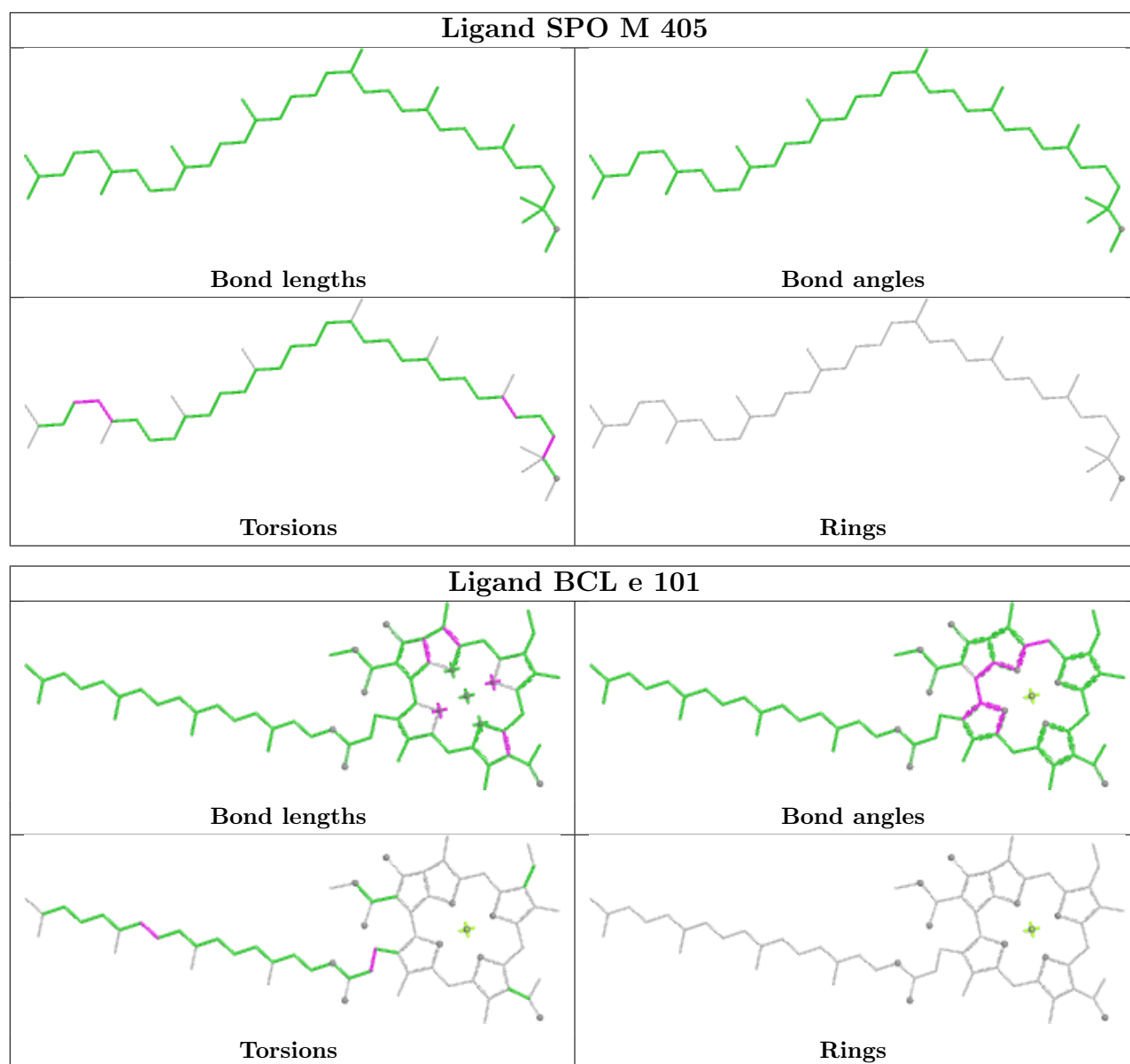
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Bond lengths	Bond angles
	
Torsions	Rings

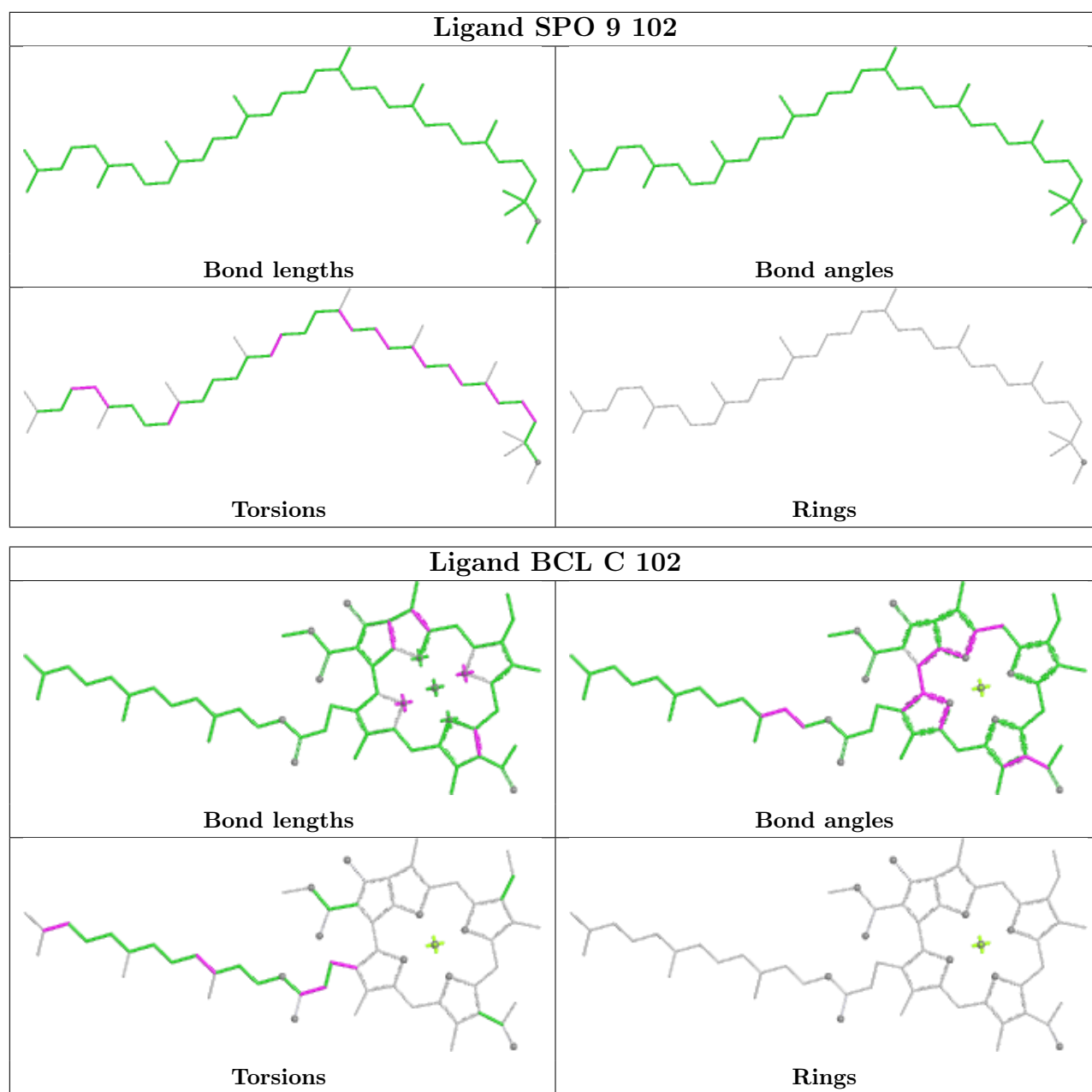


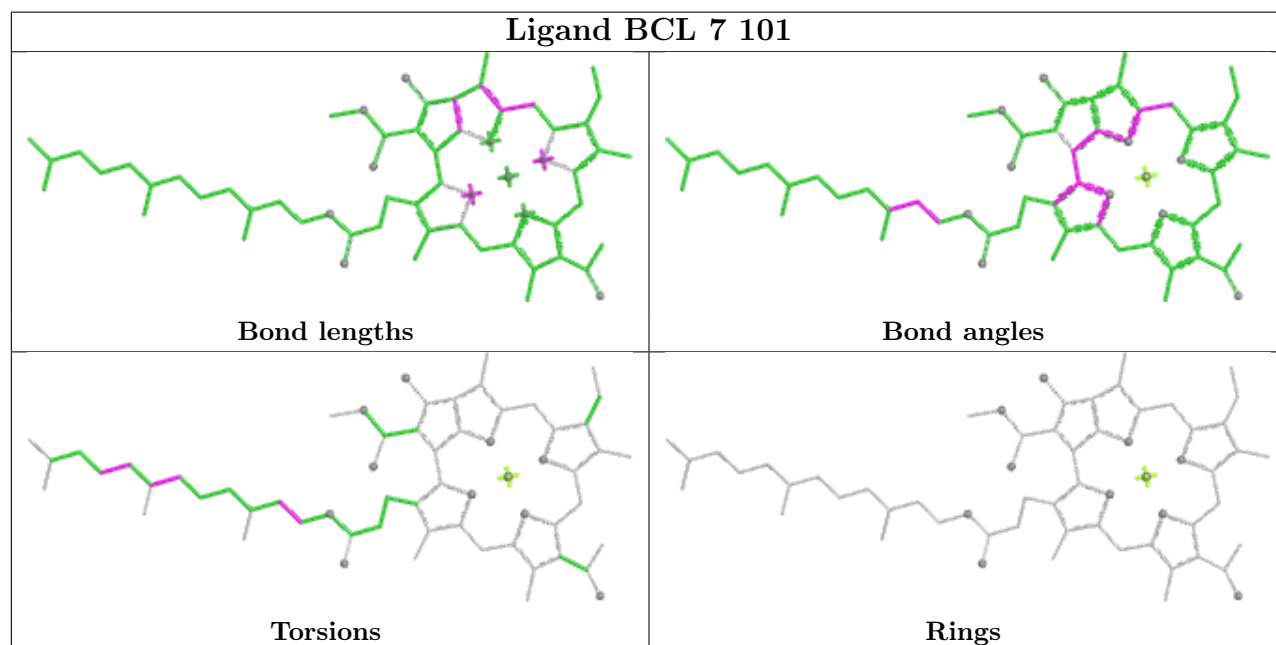
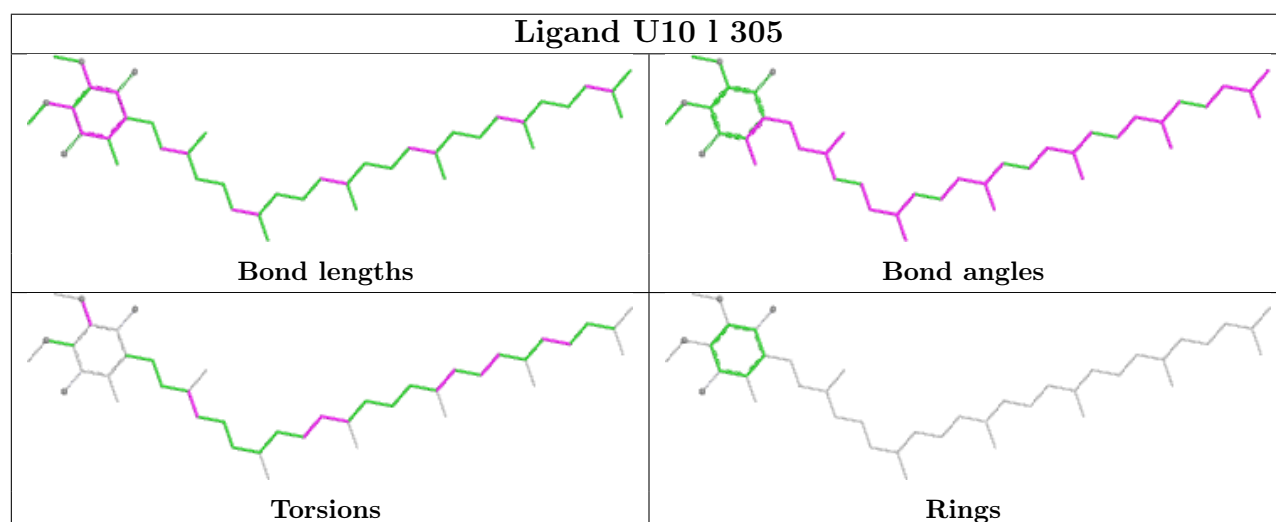
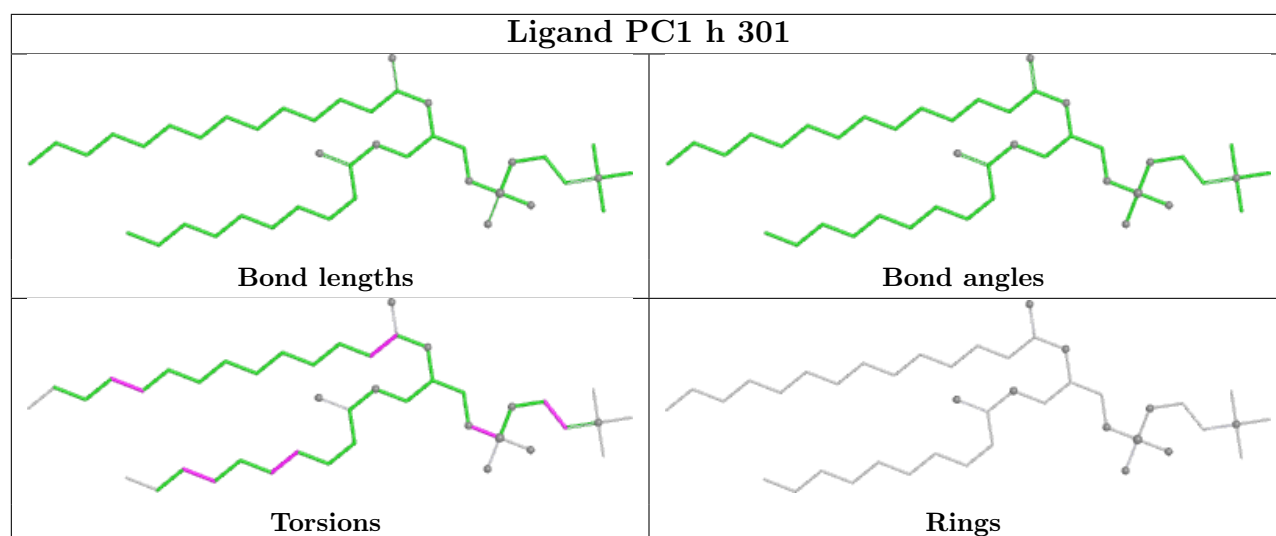
Ligand PC1 H 301	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand SPO F 103	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand SPO e 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

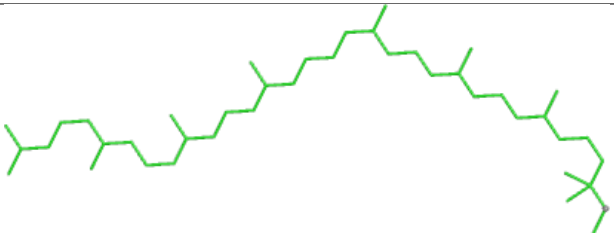
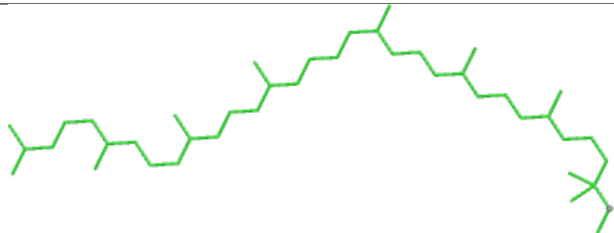
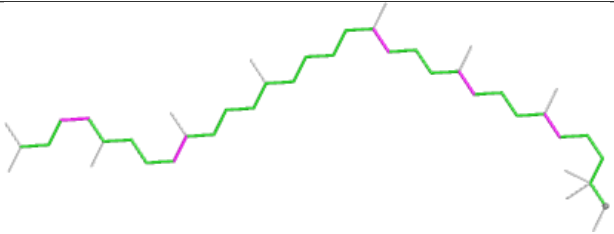
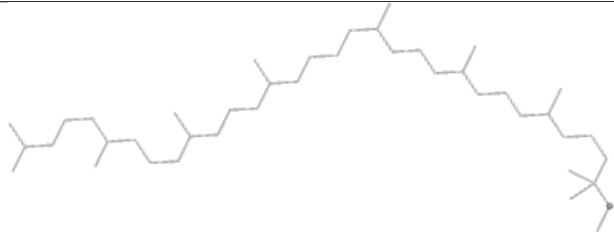


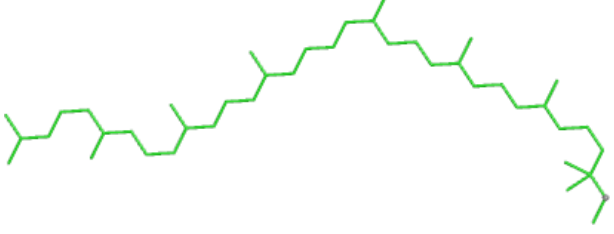
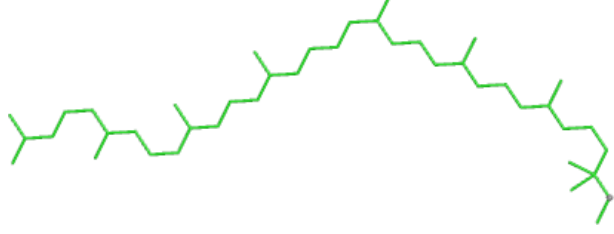
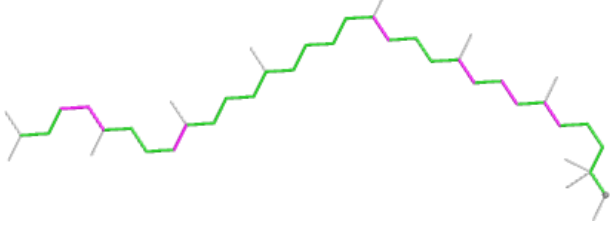


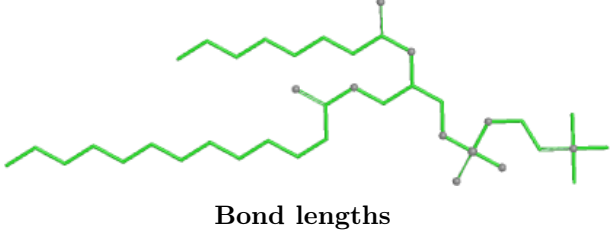
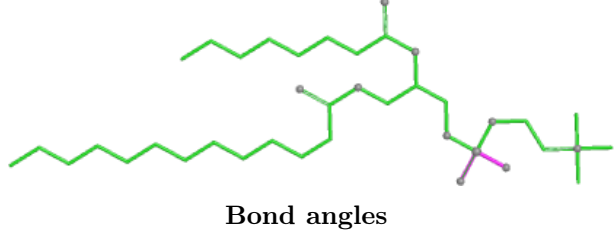
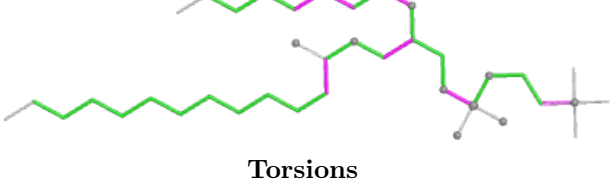
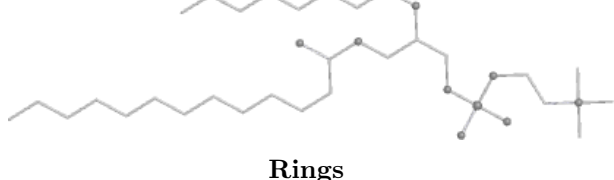


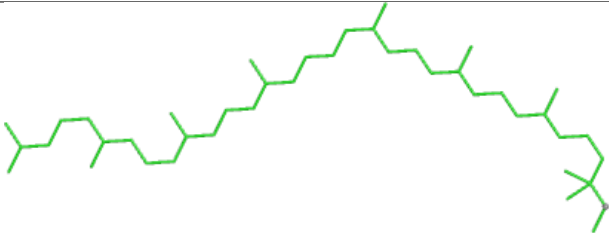
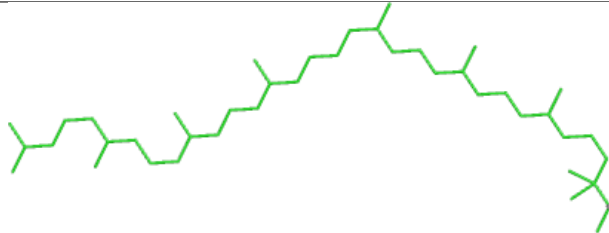
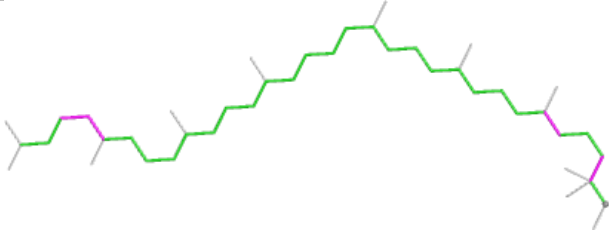
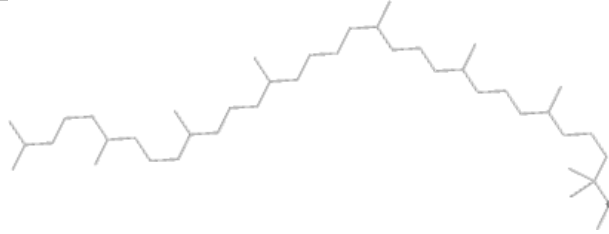


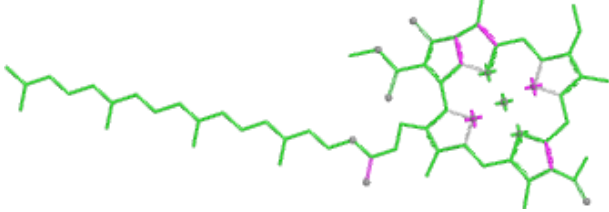
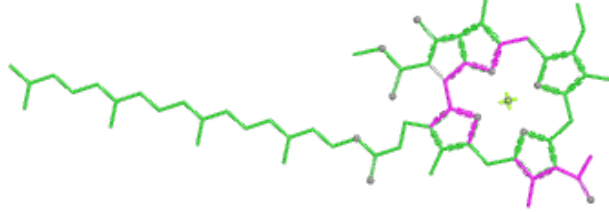
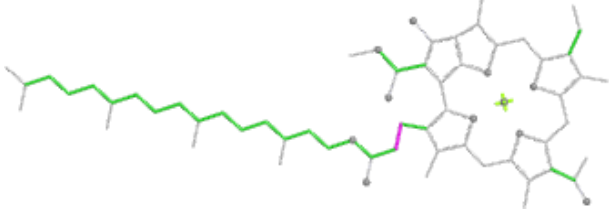
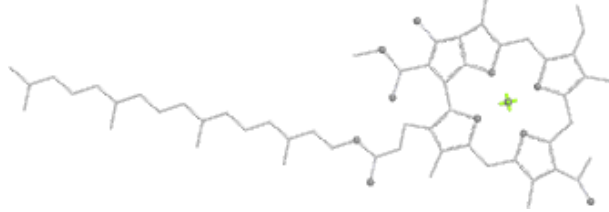


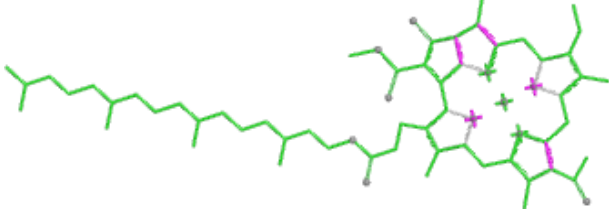
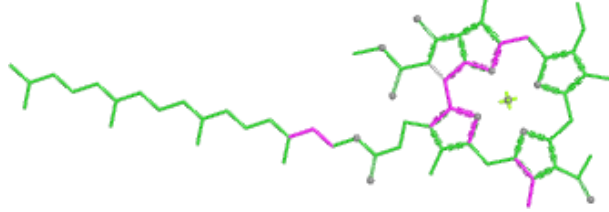
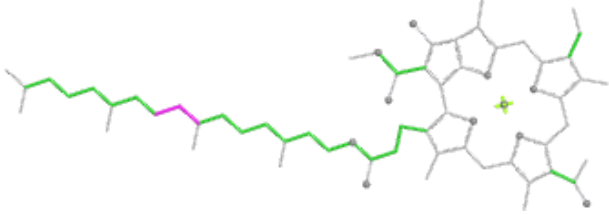
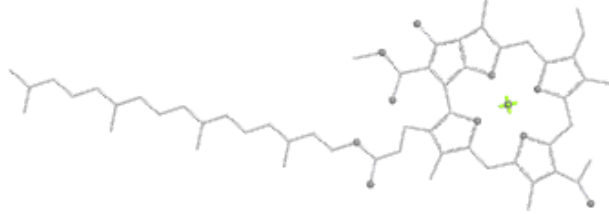
Ligand SPO N 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

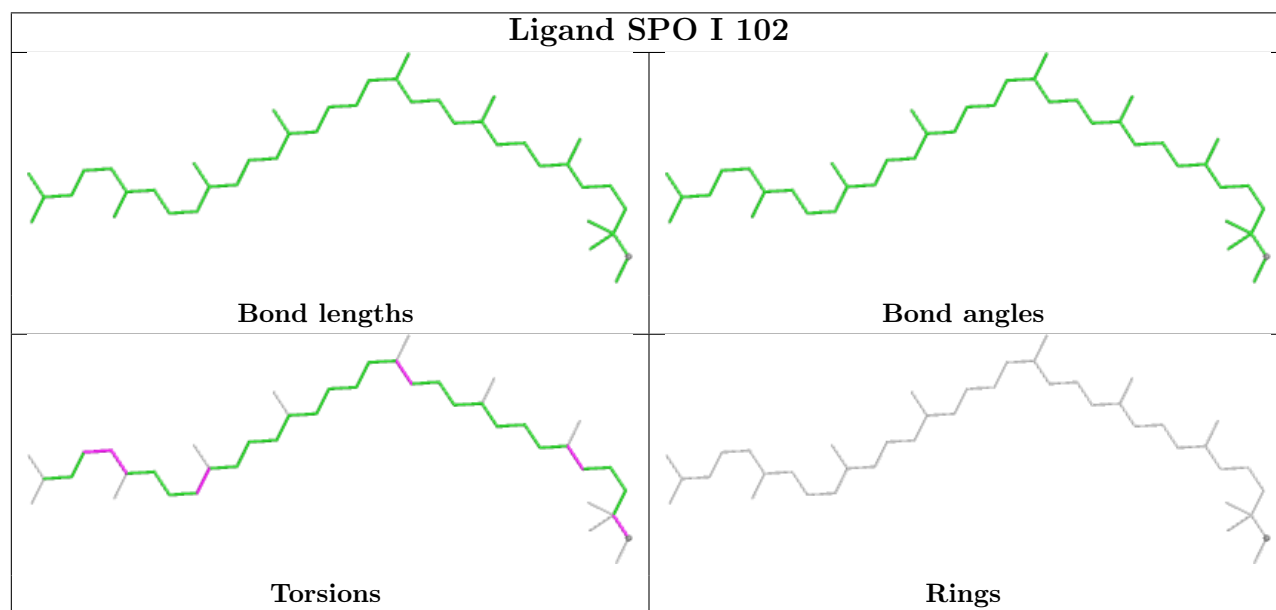
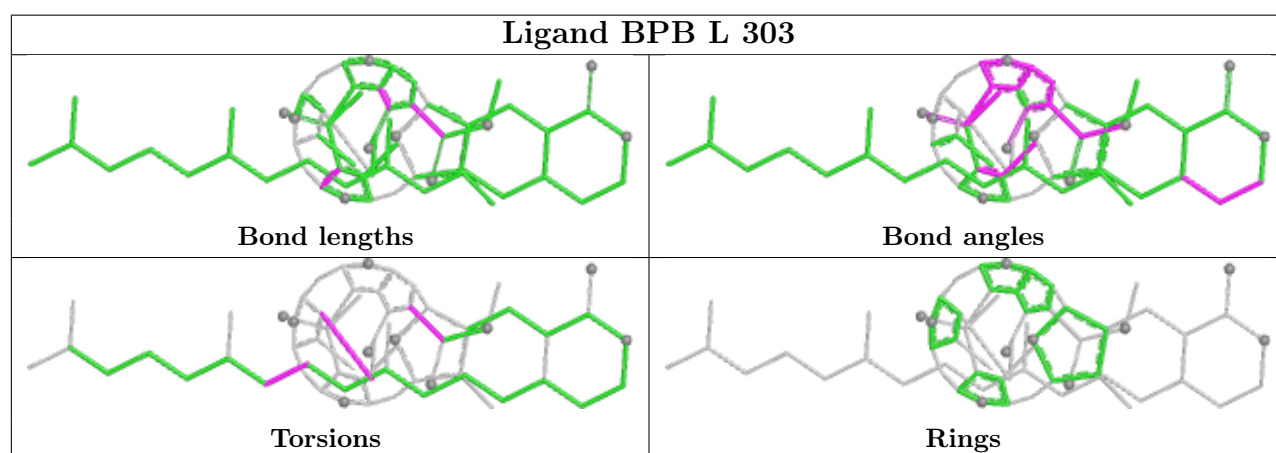
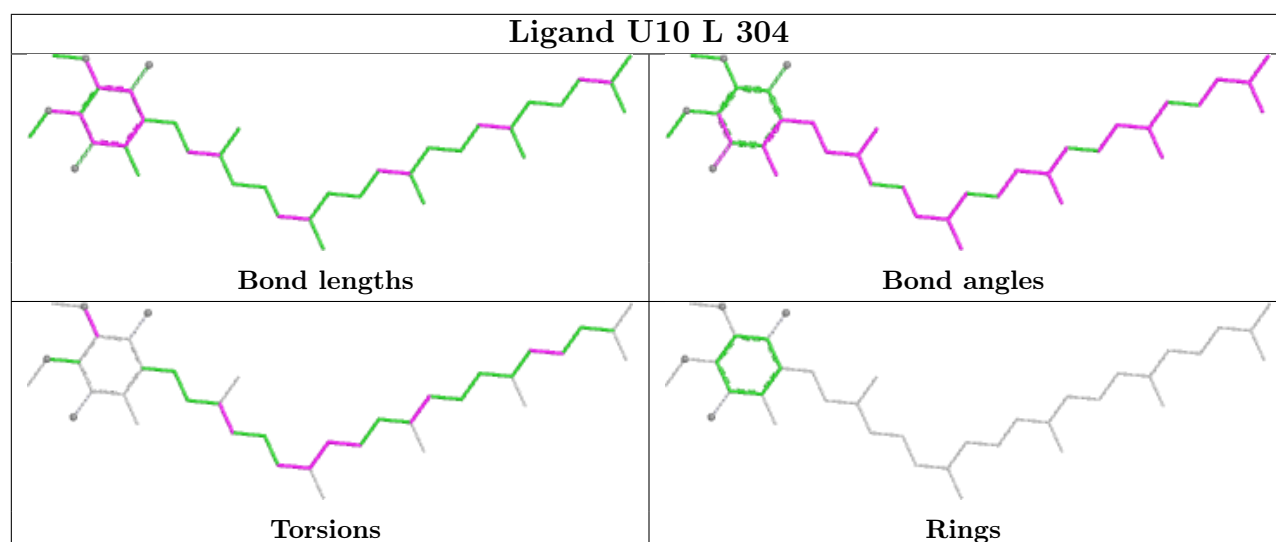
Ligand SPO C 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

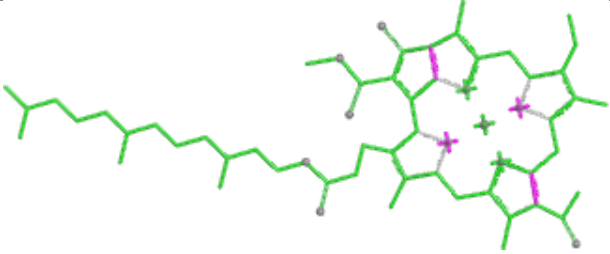
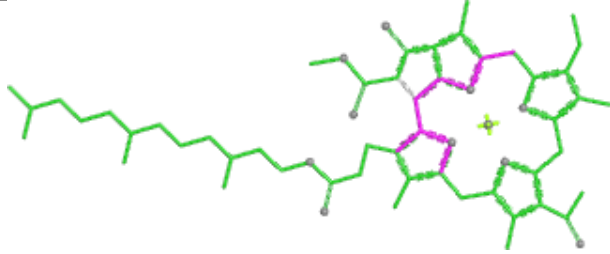
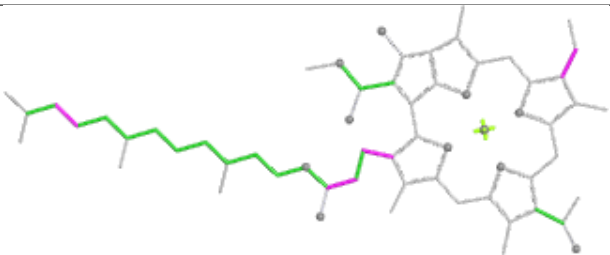
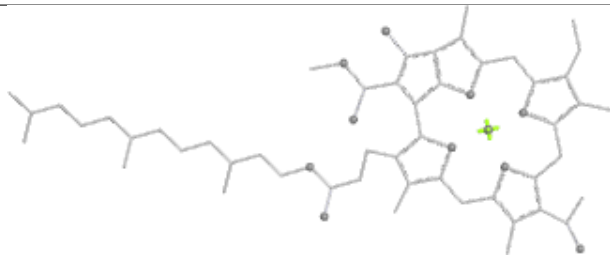
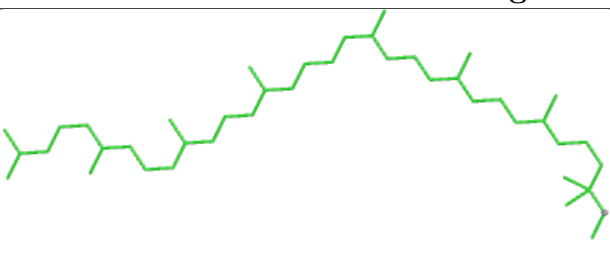
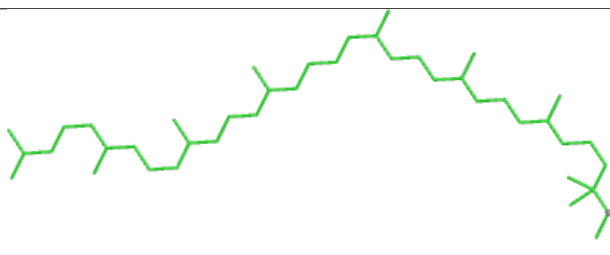
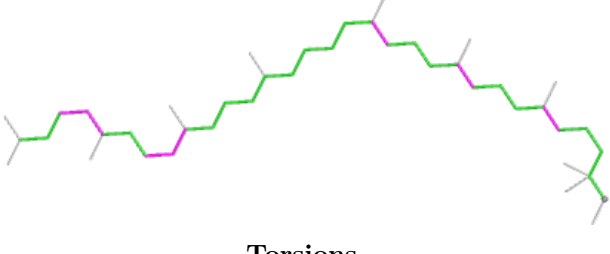
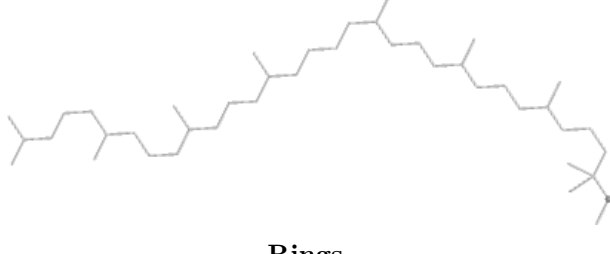
Ligand PC1 L 306	
	
Bond lengths	Bond angles
	
Torsions	Rings

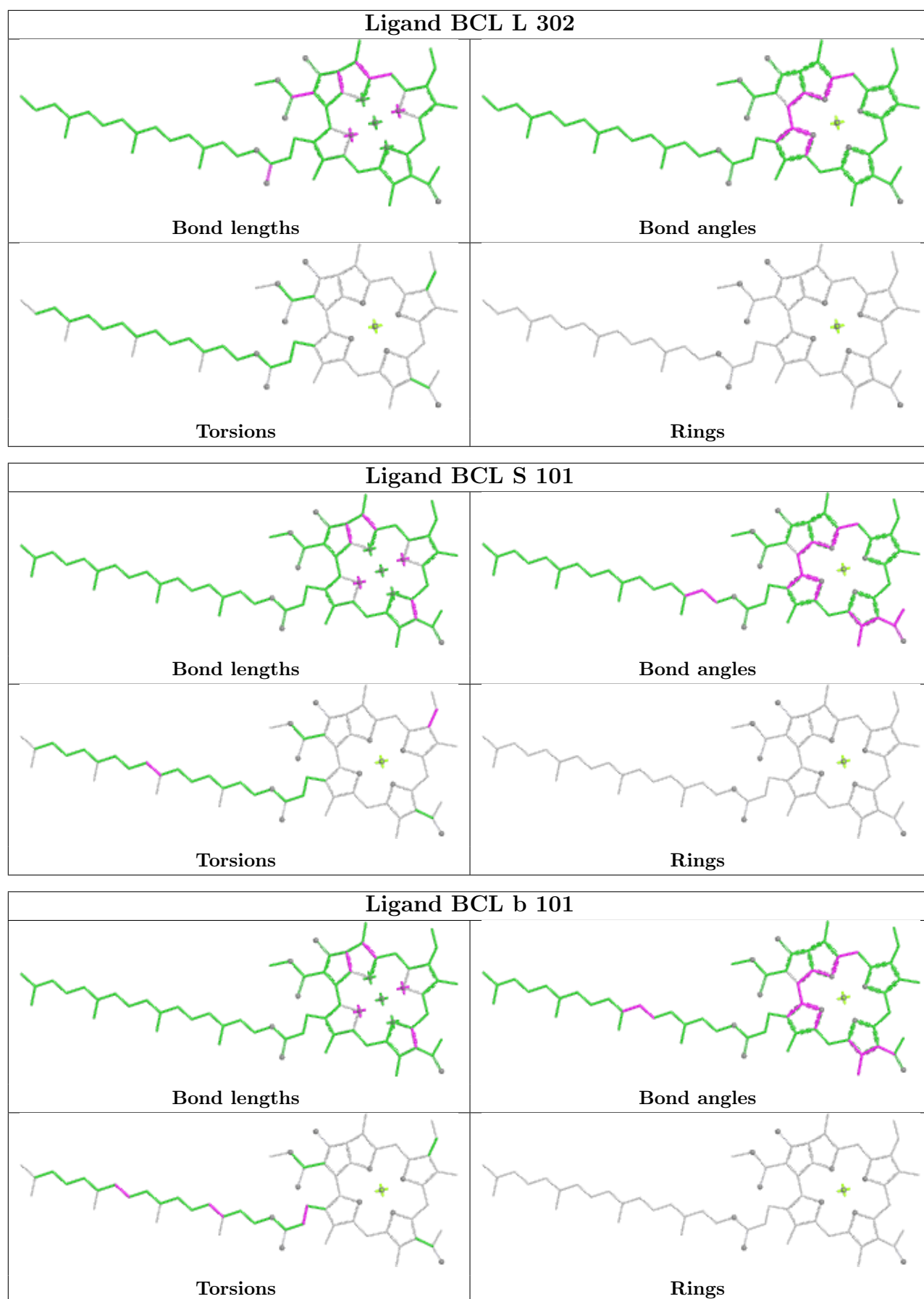
Ligand SPO m 405	
	
Bond lengths	Bond angles
	
Torsions	Rings

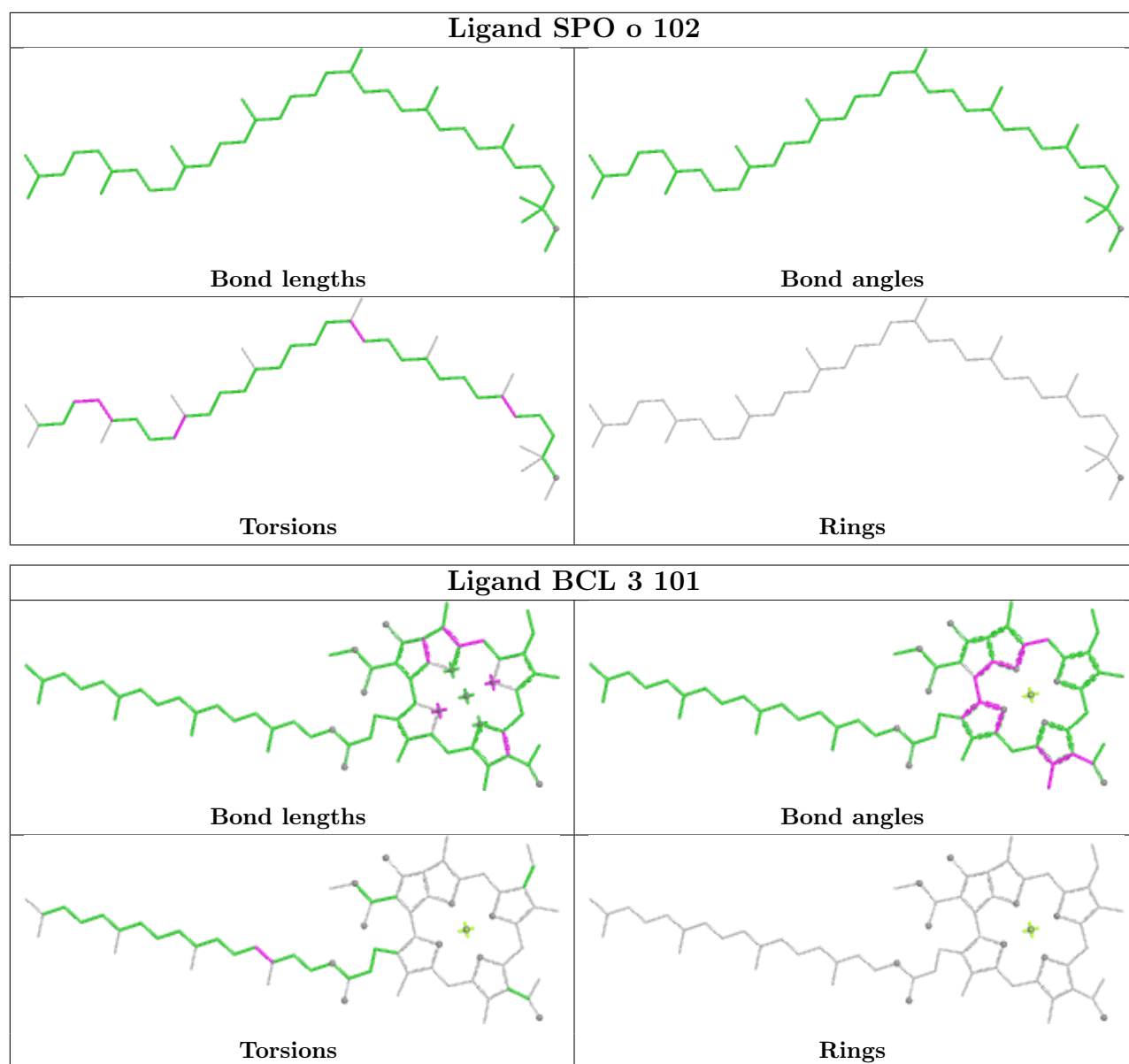
Ligand BCL L 301	
	
Bond lengths	Bond angles
	
Torsions	Rings

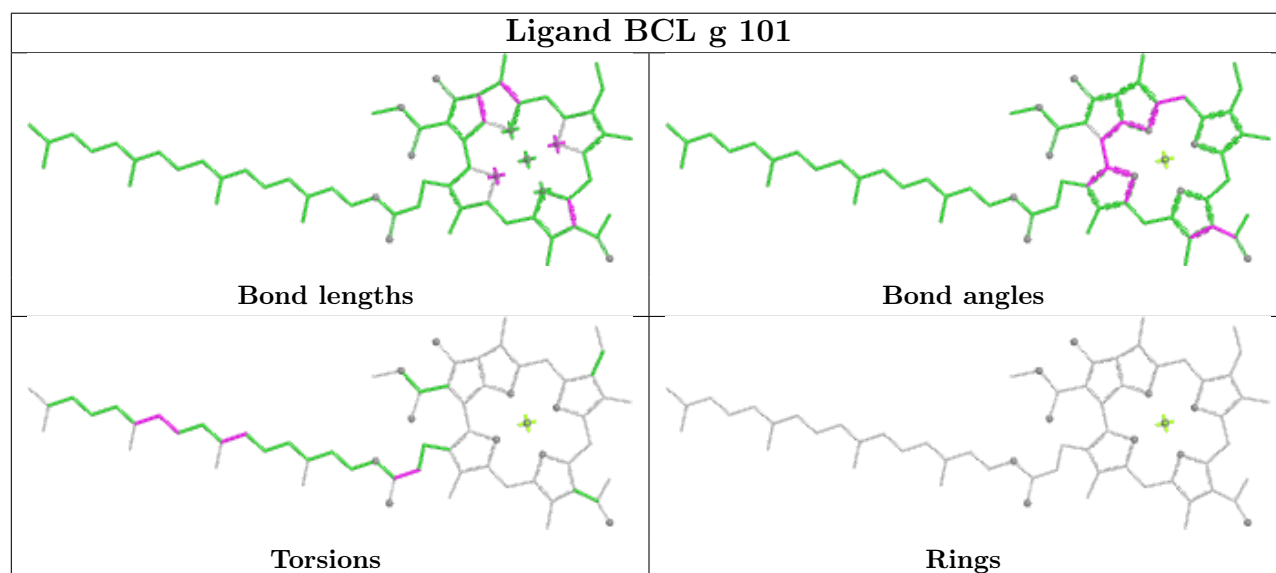
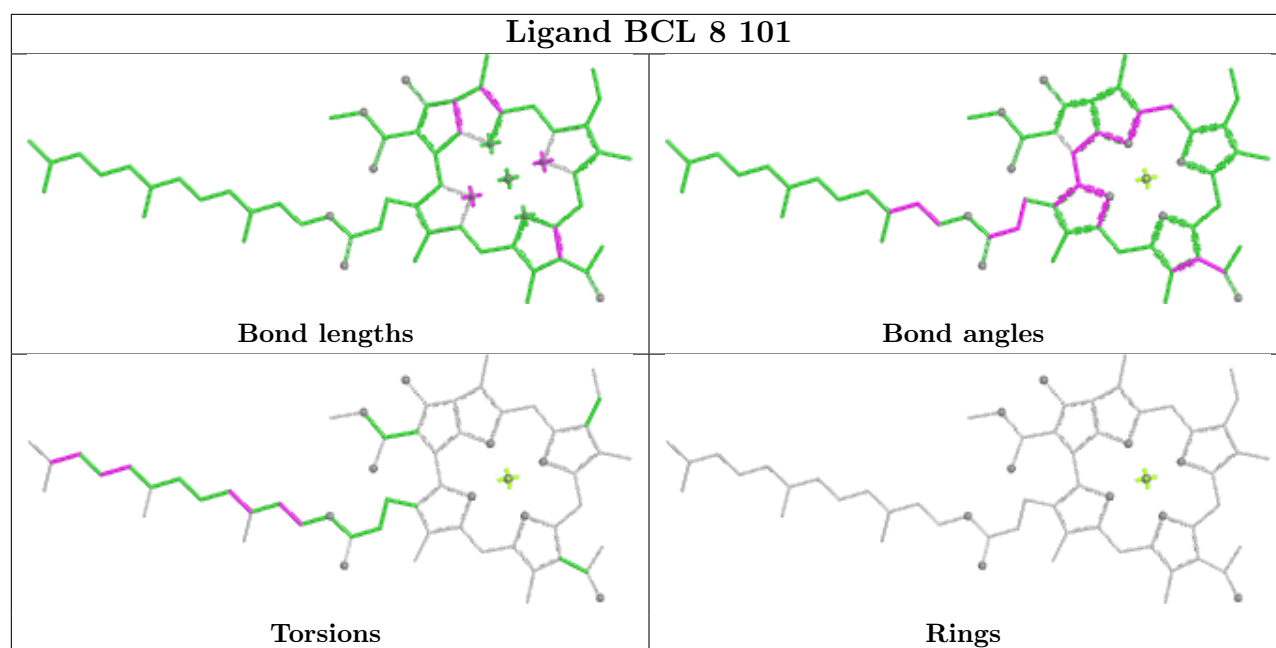
Ligand BCL F 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

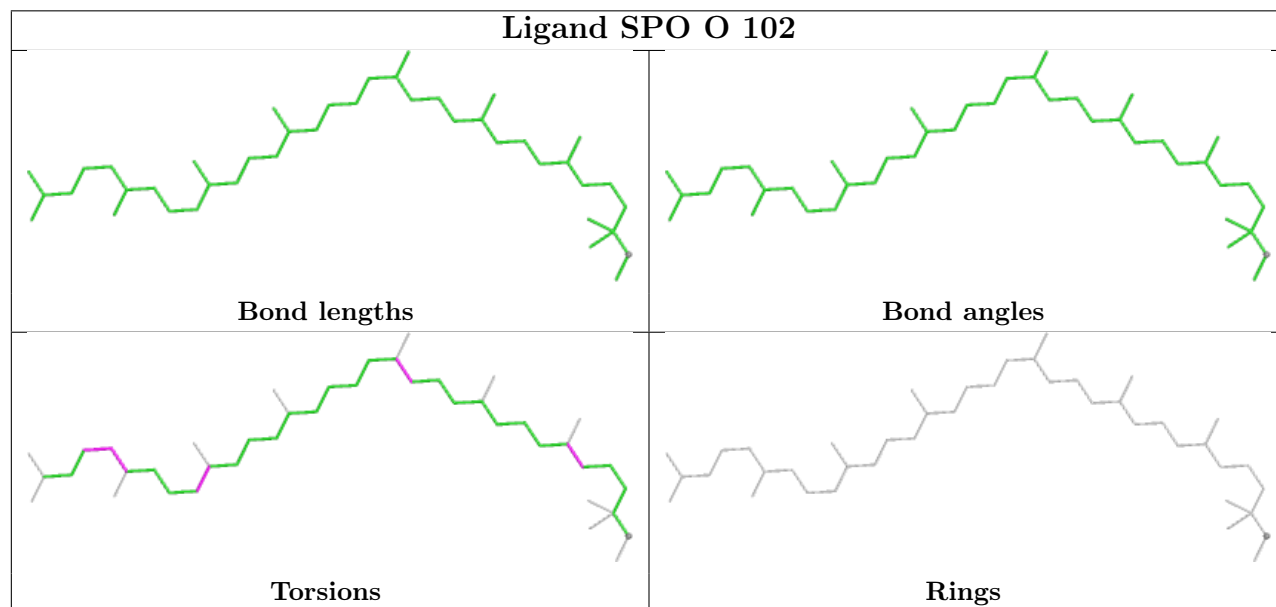
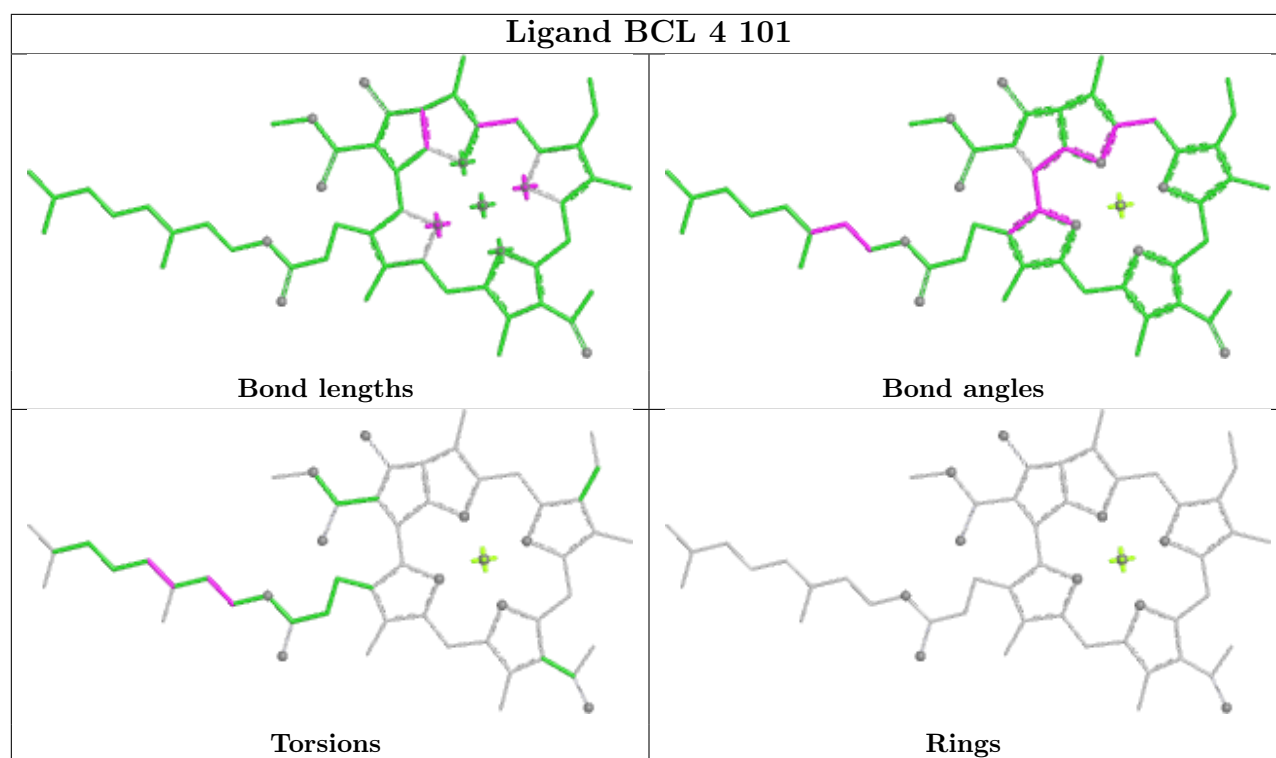


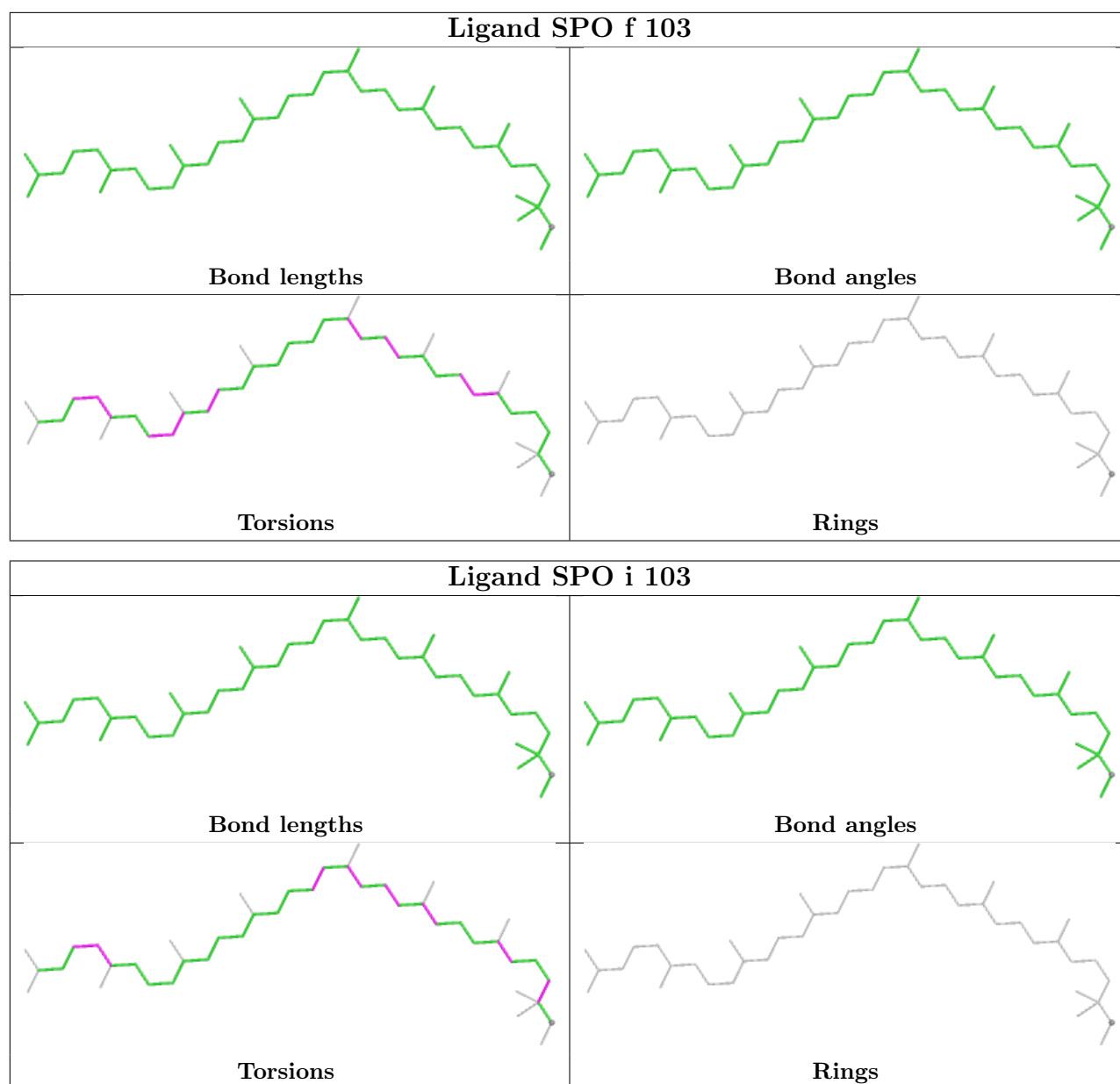
Ligand BCL p 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand SPO R 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

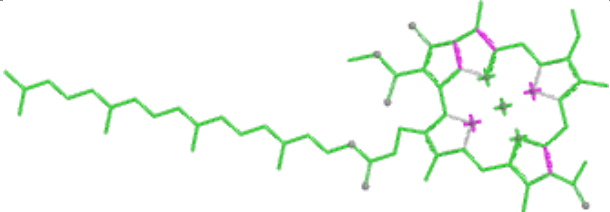
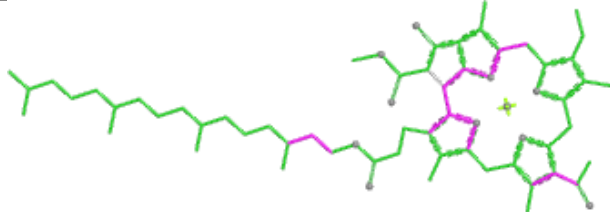
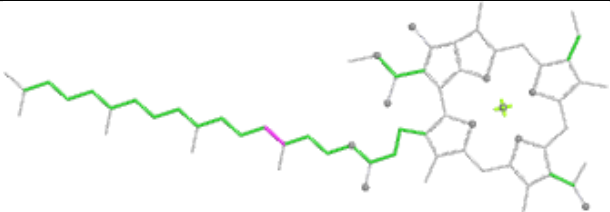
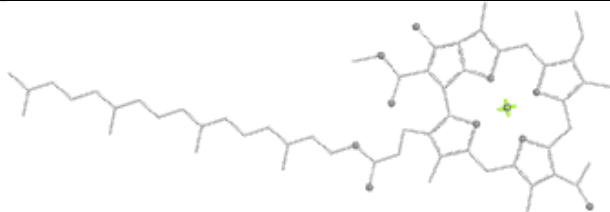
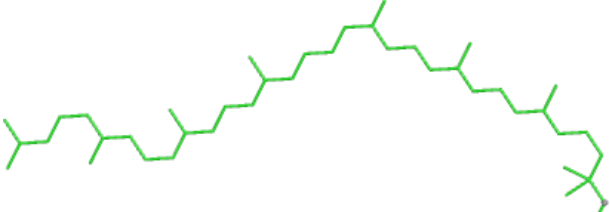
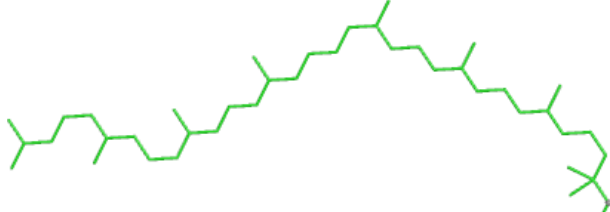
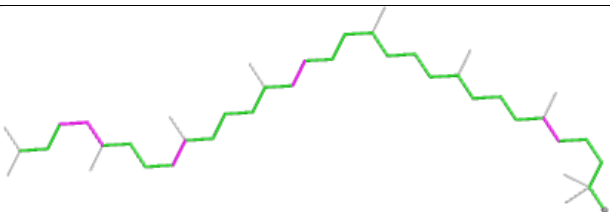
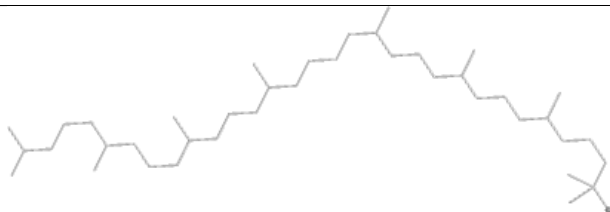


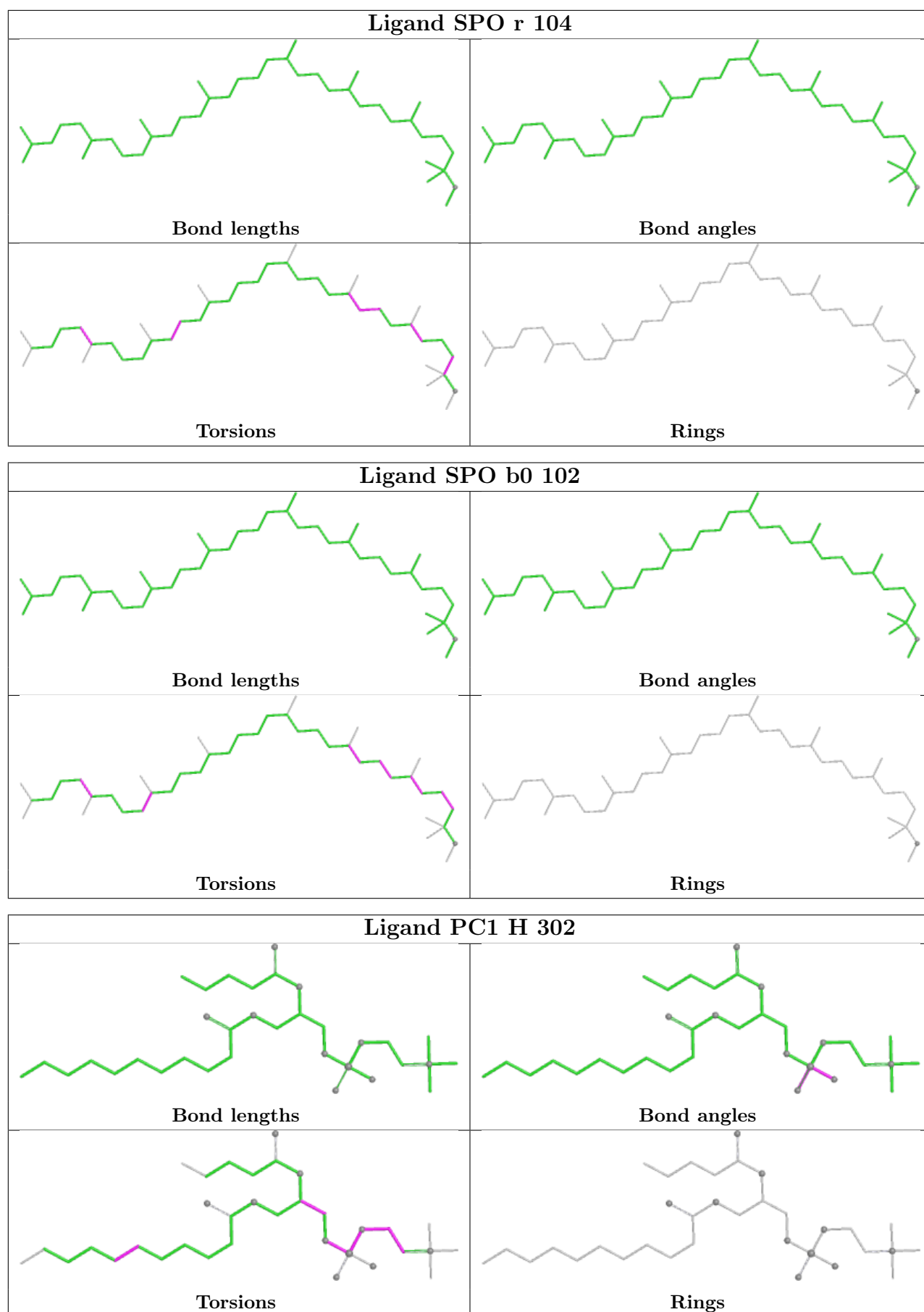


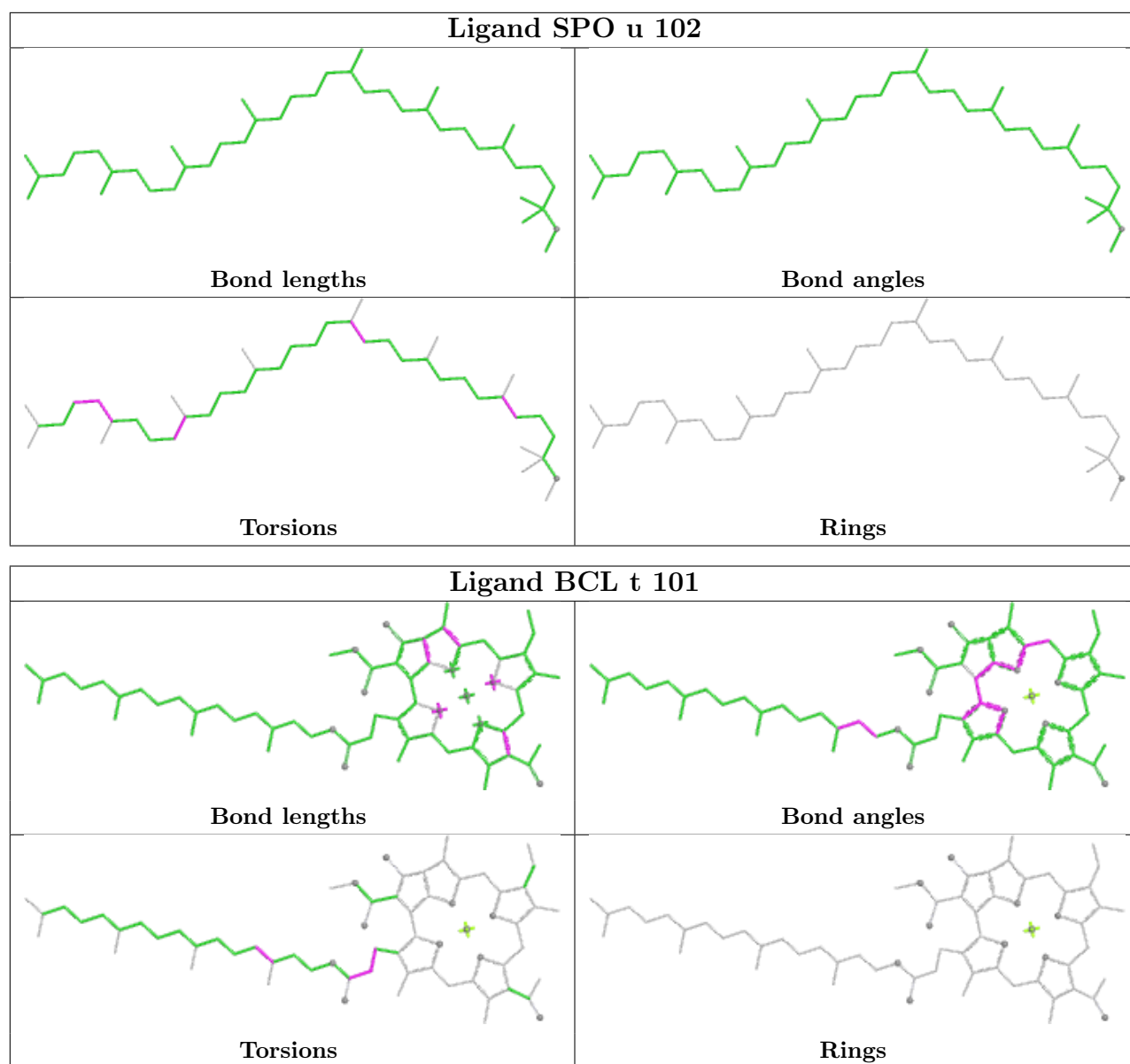


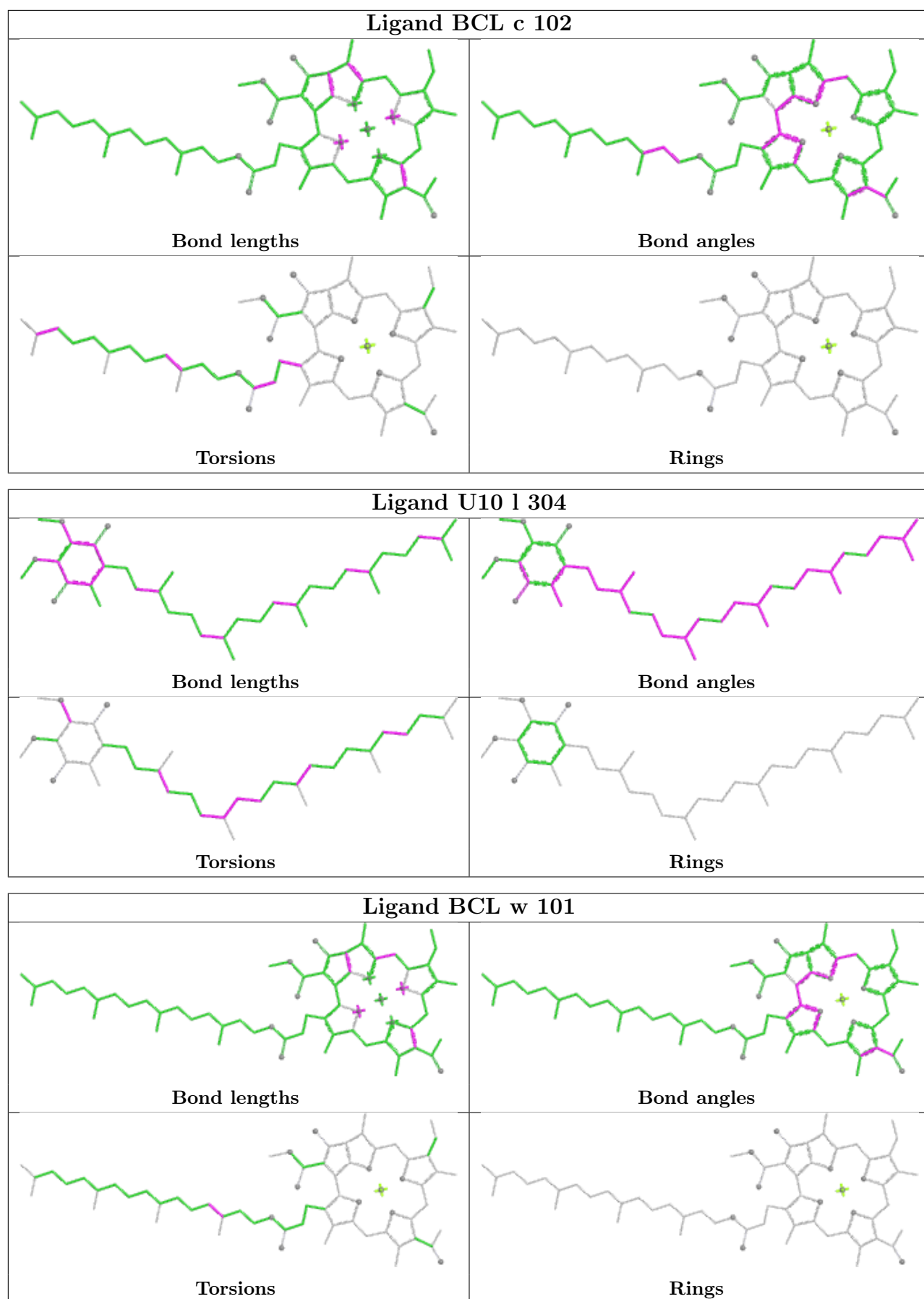


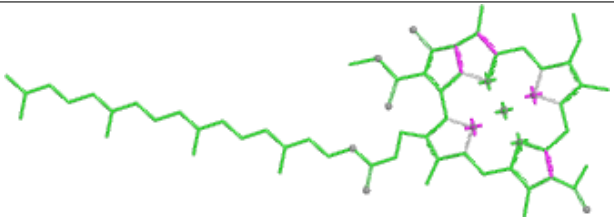
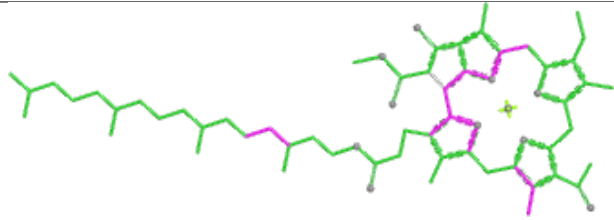
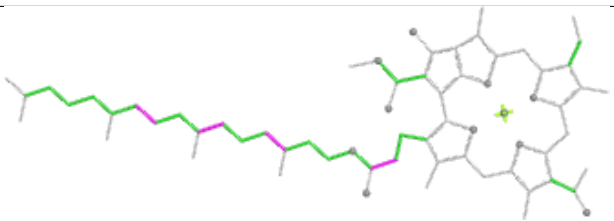
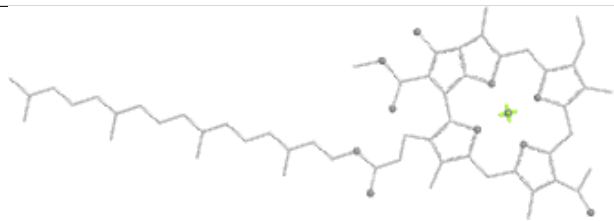


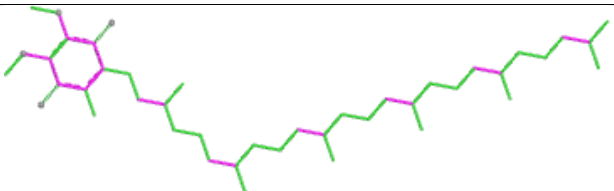
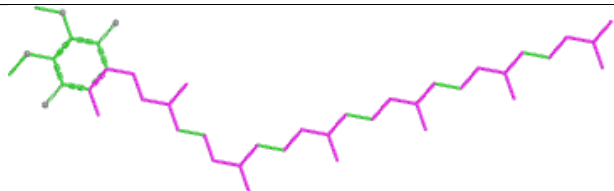
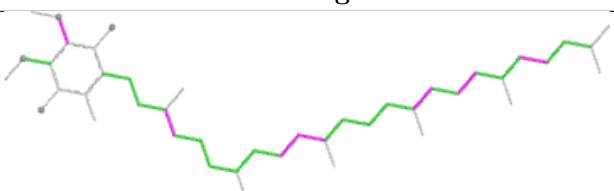
Ligand BCL I 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand SPO d 104	
 Bond lengths	 Bond angles
 Torsions	 Rings

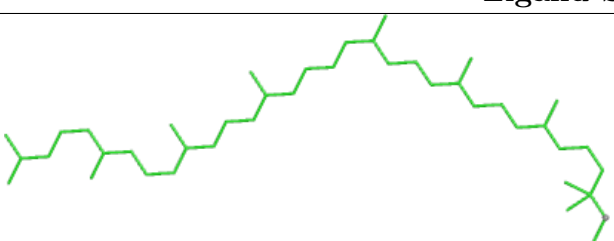
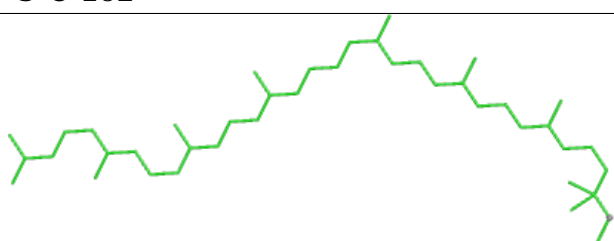
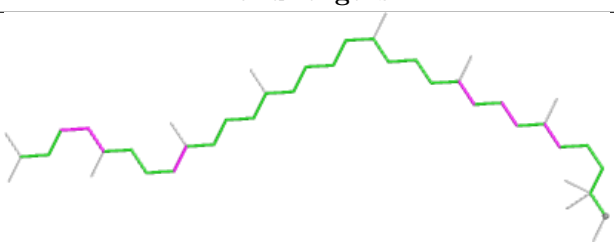
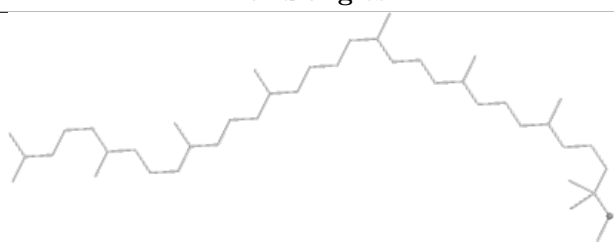


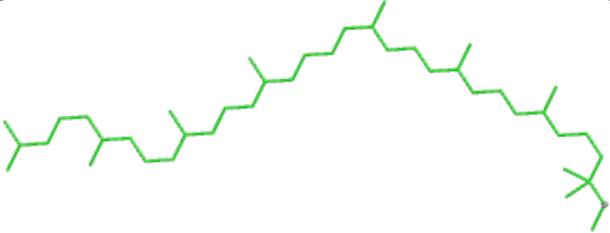
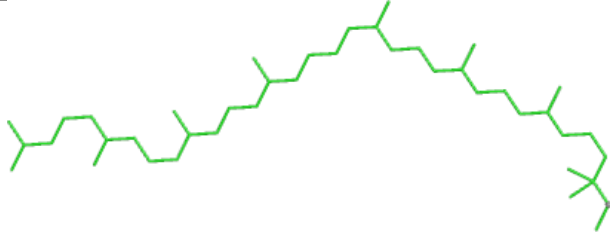
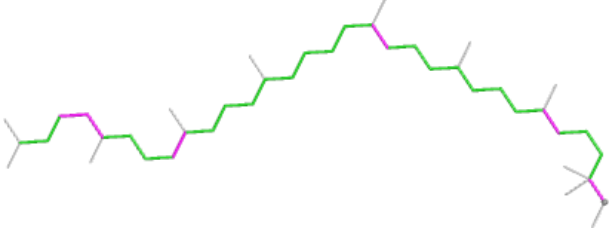
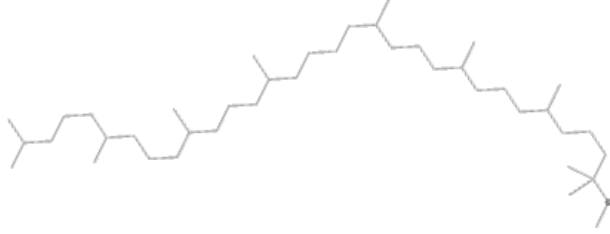
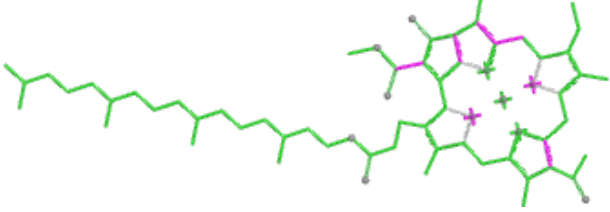
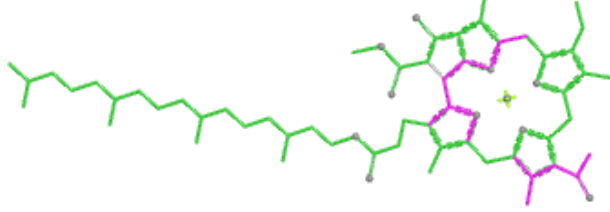
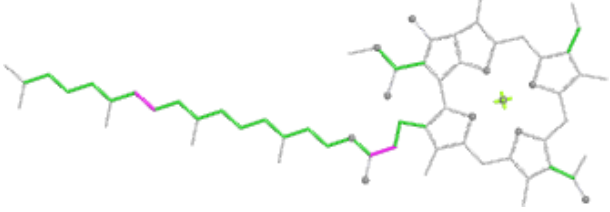
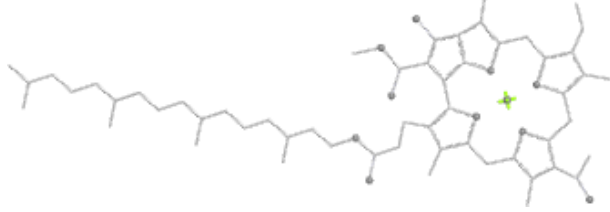


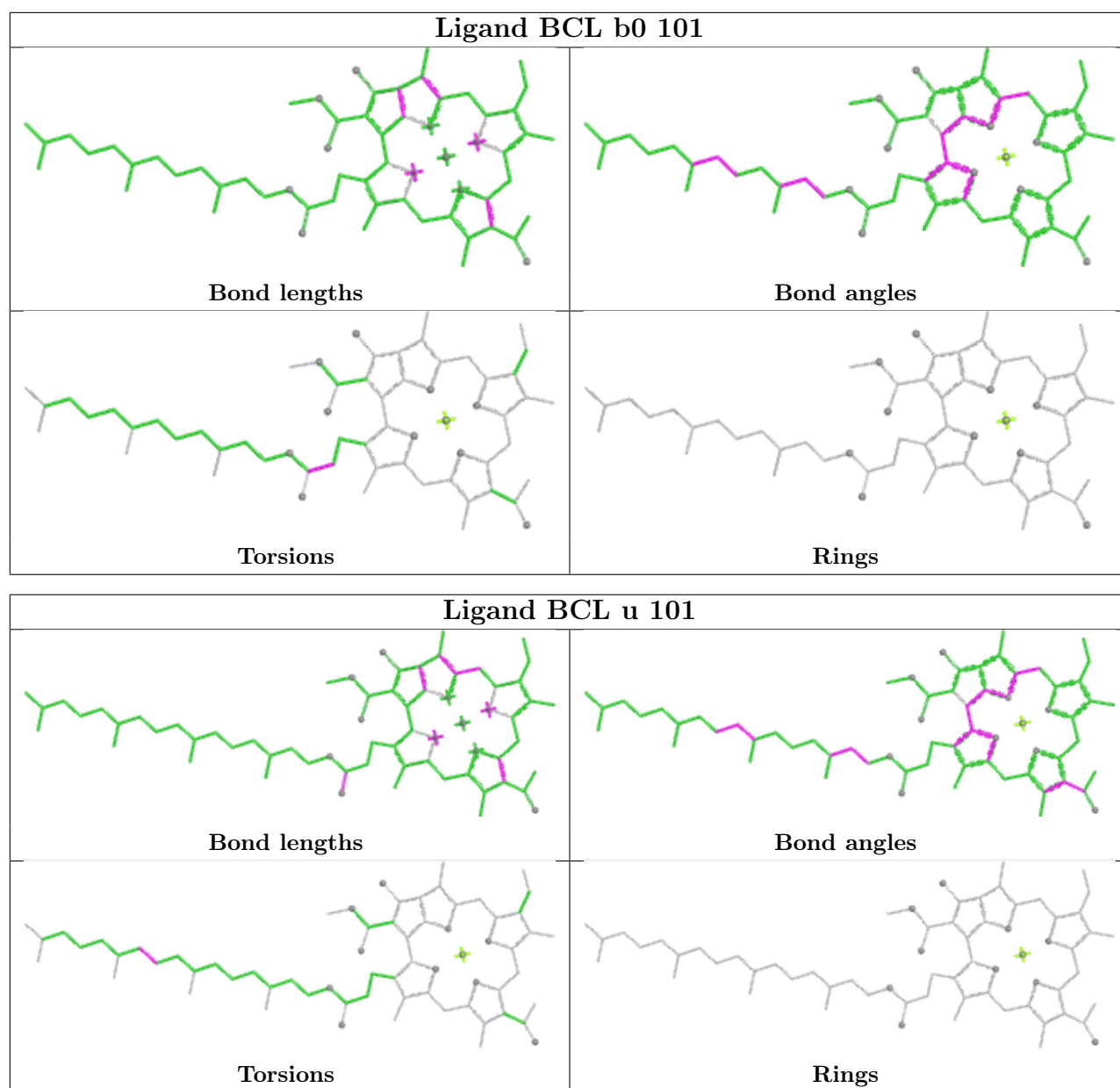


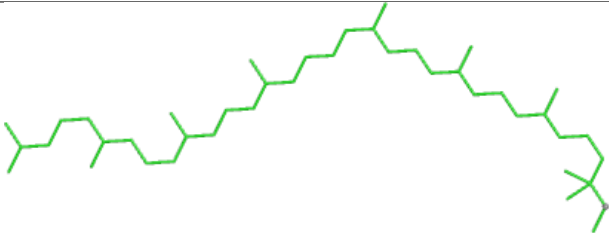
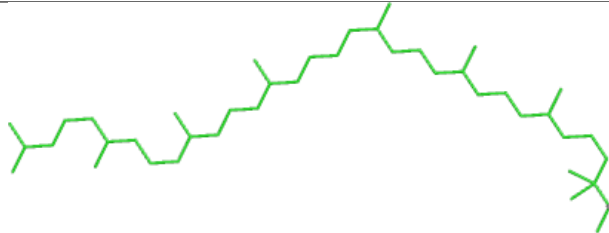
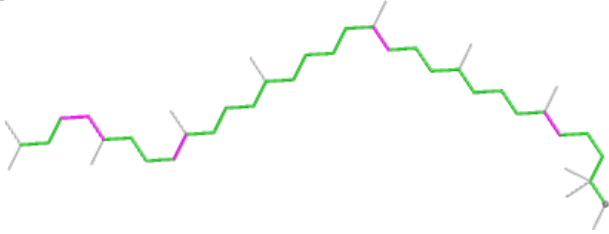
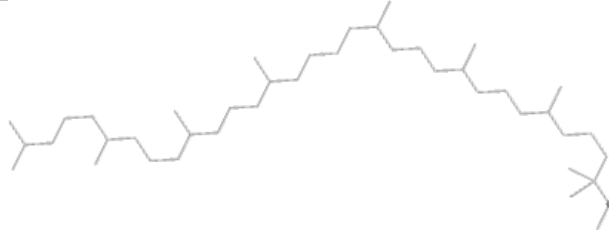
Ligand BCL v 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

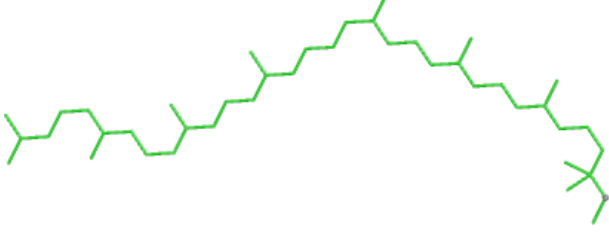
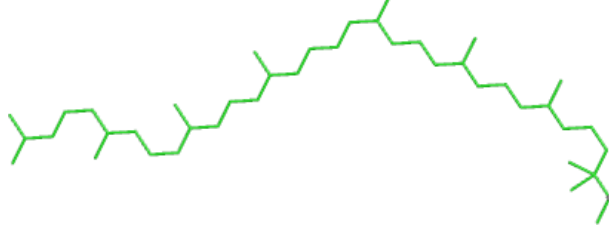
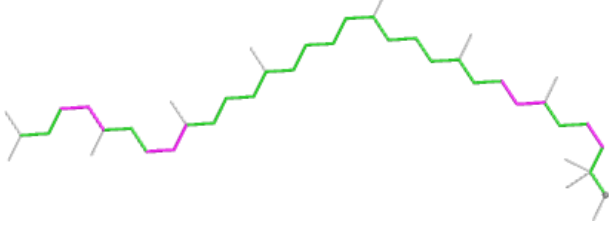
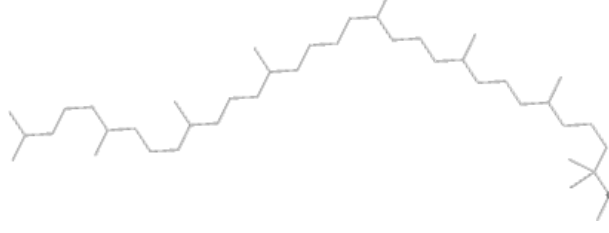
Ligand U10 L 305	
	
Bond lengths	Bond angles
	
Torsions	Rings

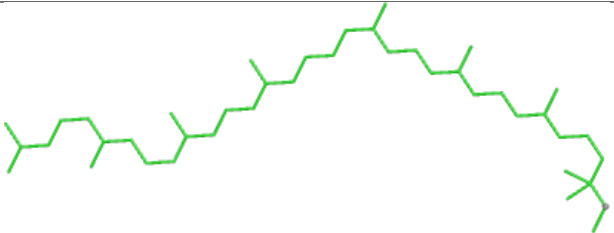
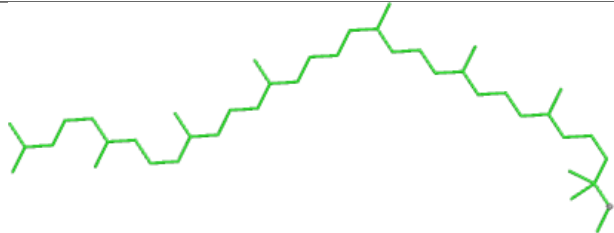
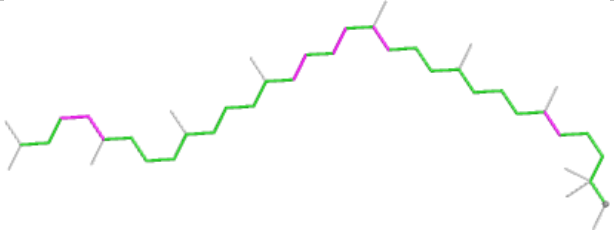
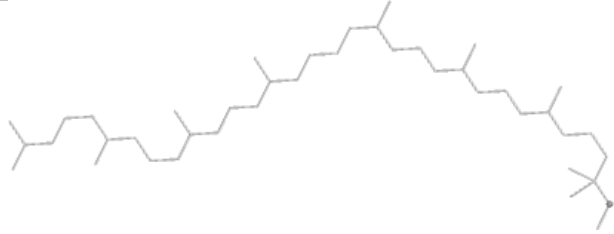
Ligand SPO 3 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

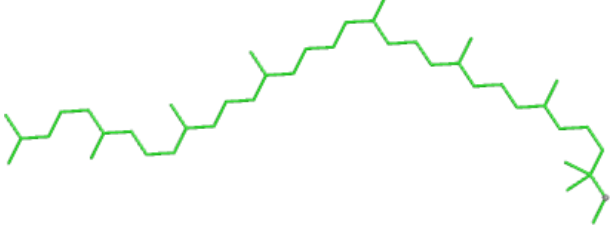
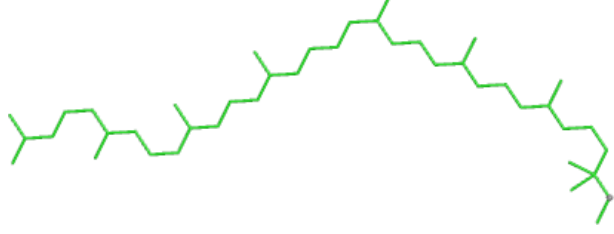
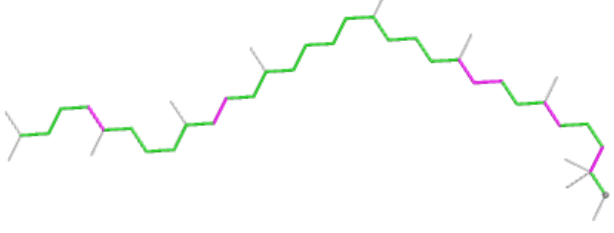
Ligand SPO i 102	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCL m 402	
 Bond lengths	 Bond angles
 Torsions	 Rings

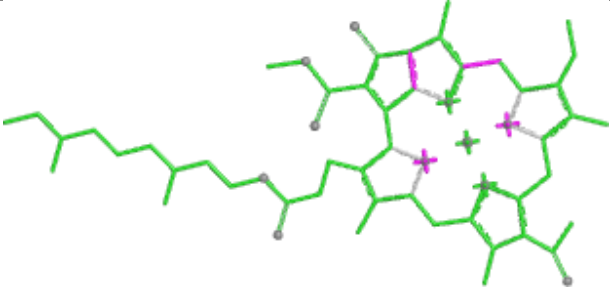
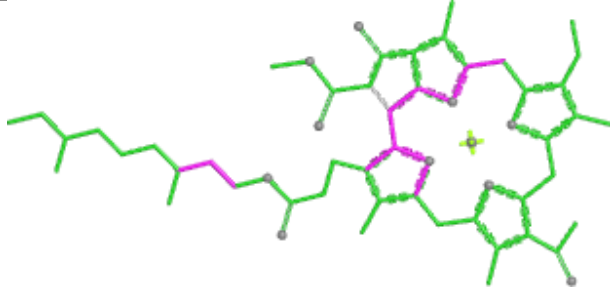
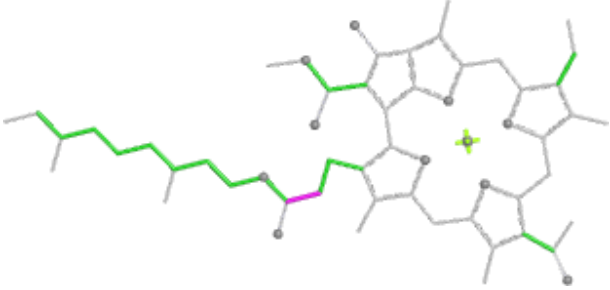
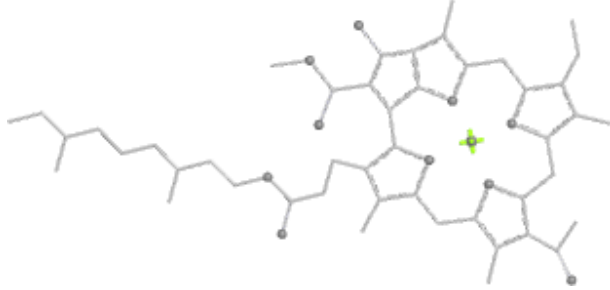
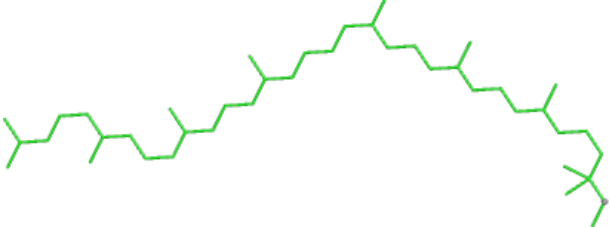
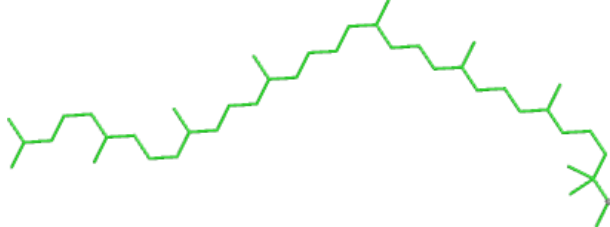
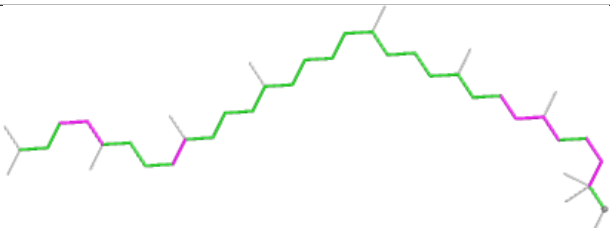
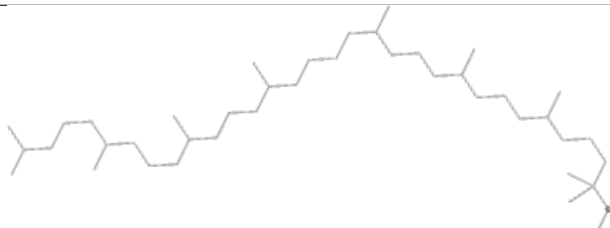


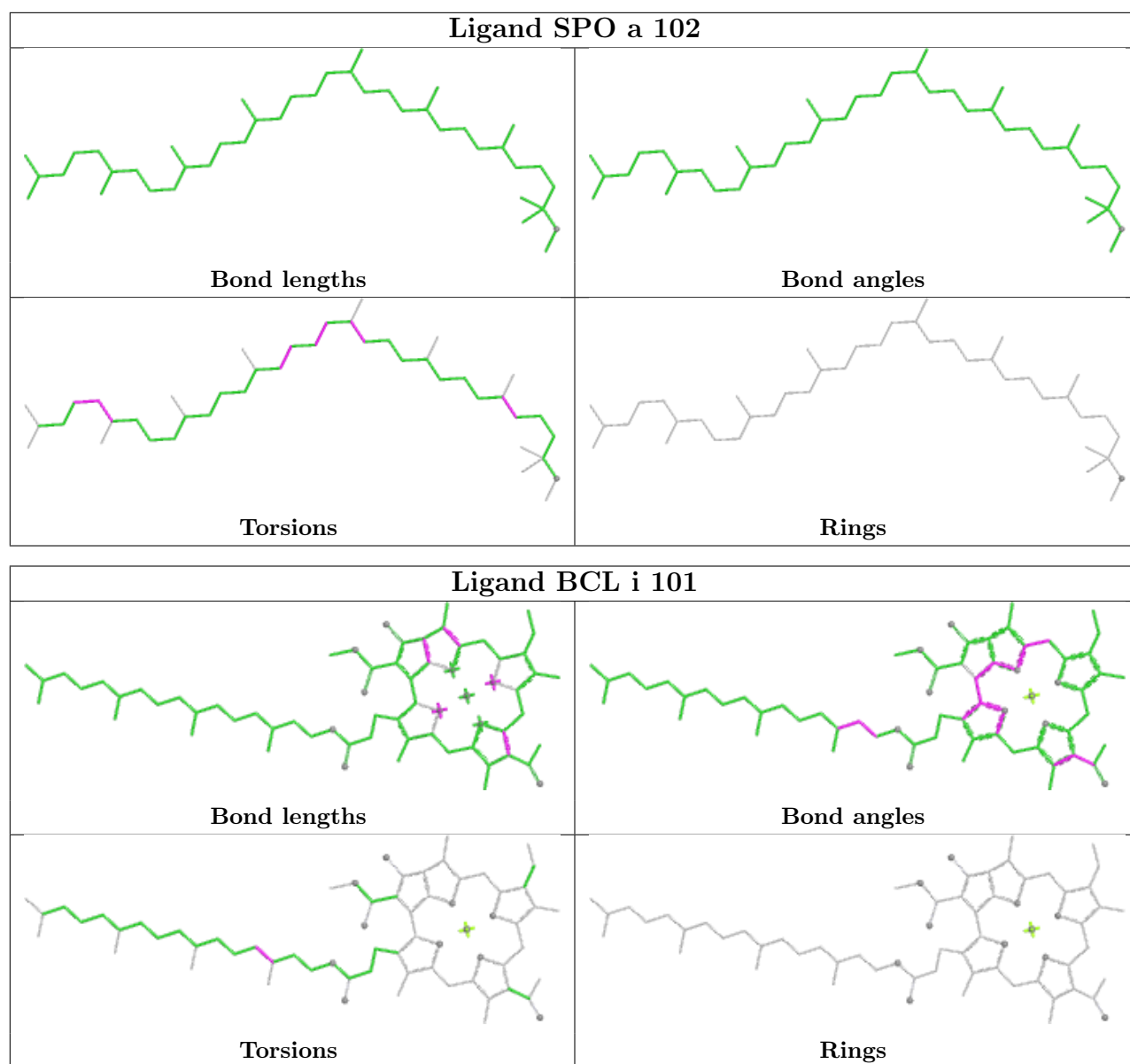
Ligand SPO f 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

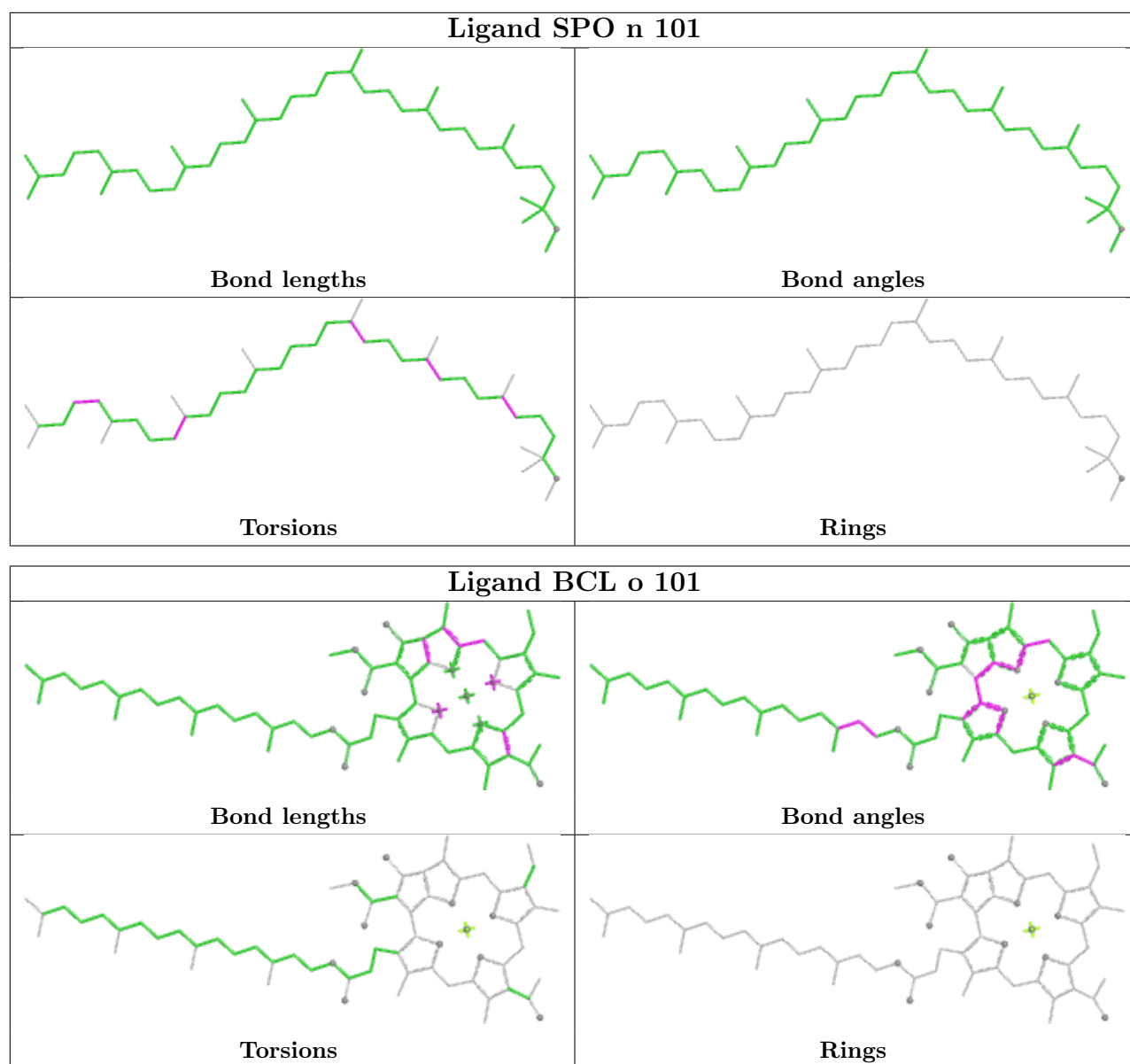
Ligand SPO J 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

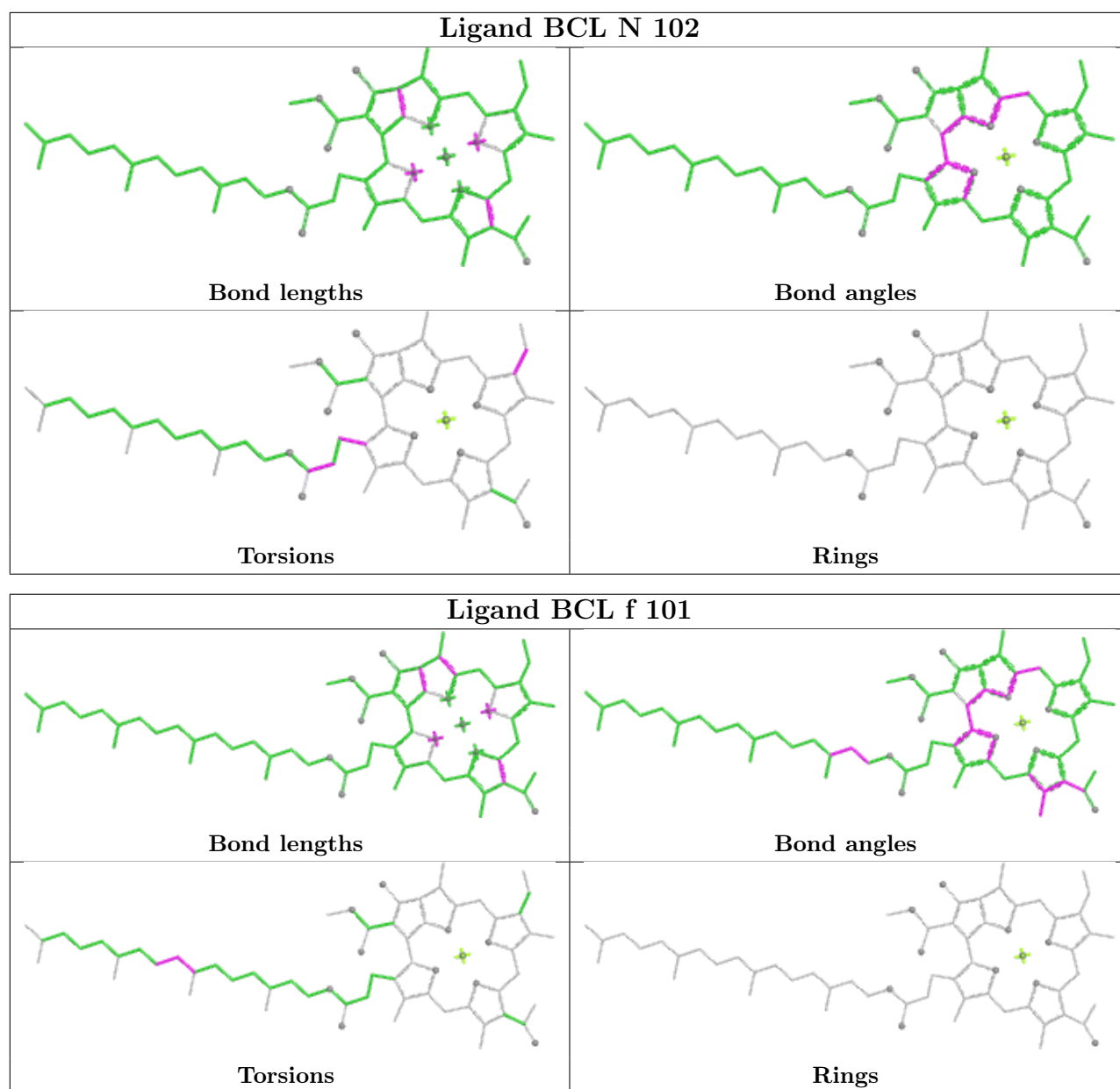
Ligand SPO A 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

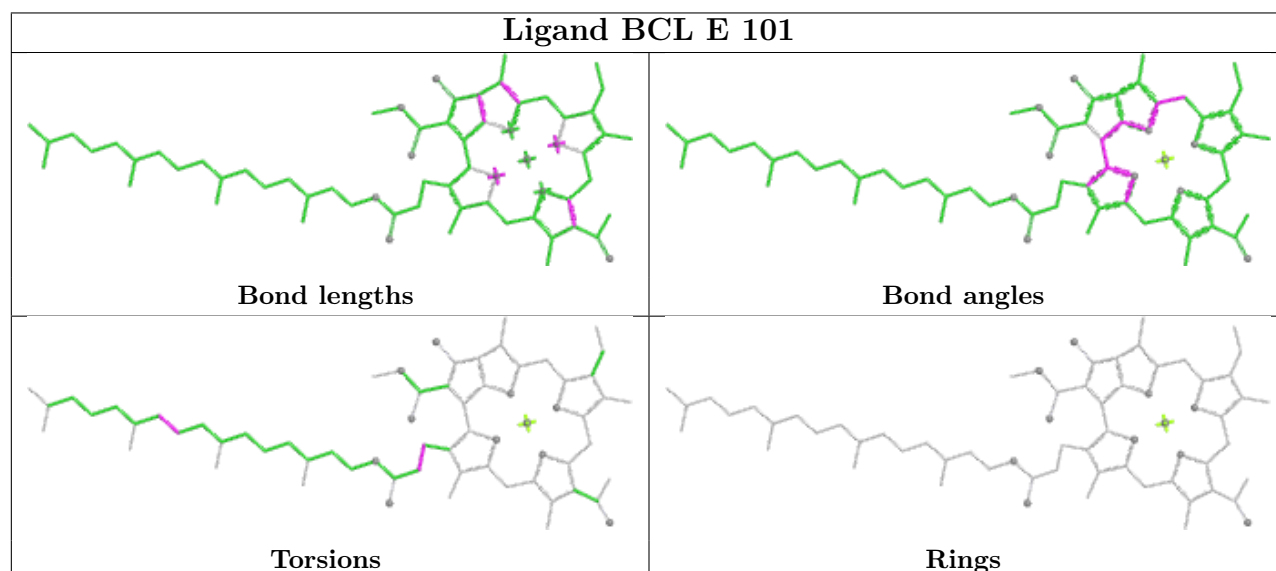
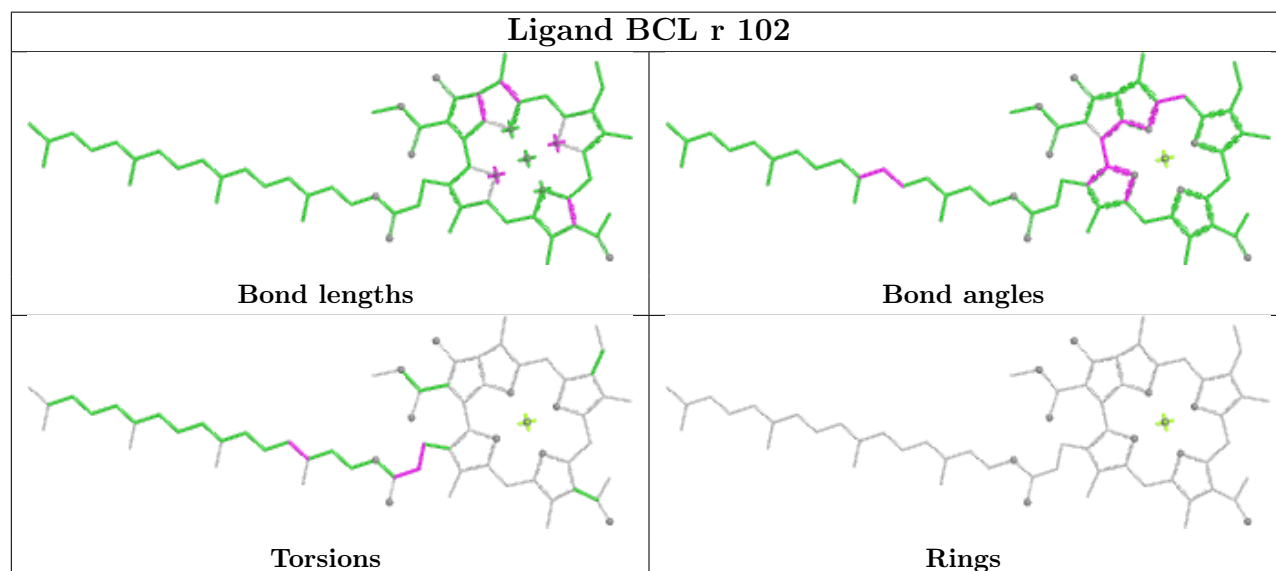
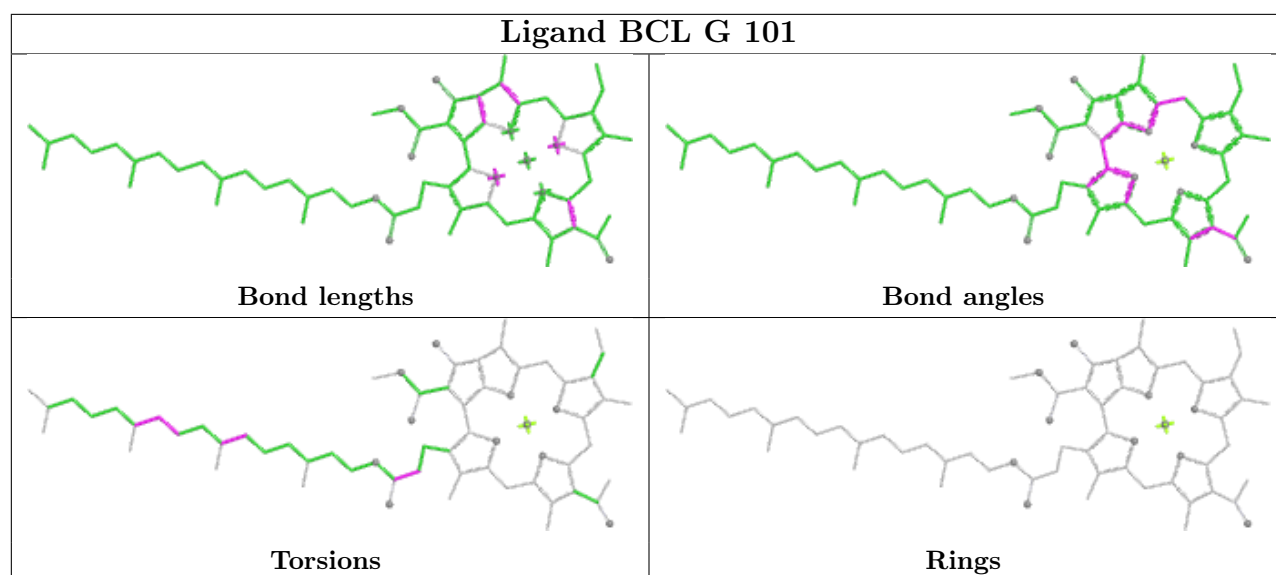
Ligand SPO R 104	
 Bond lengths	 Bond angles
 Torsions	 Rings

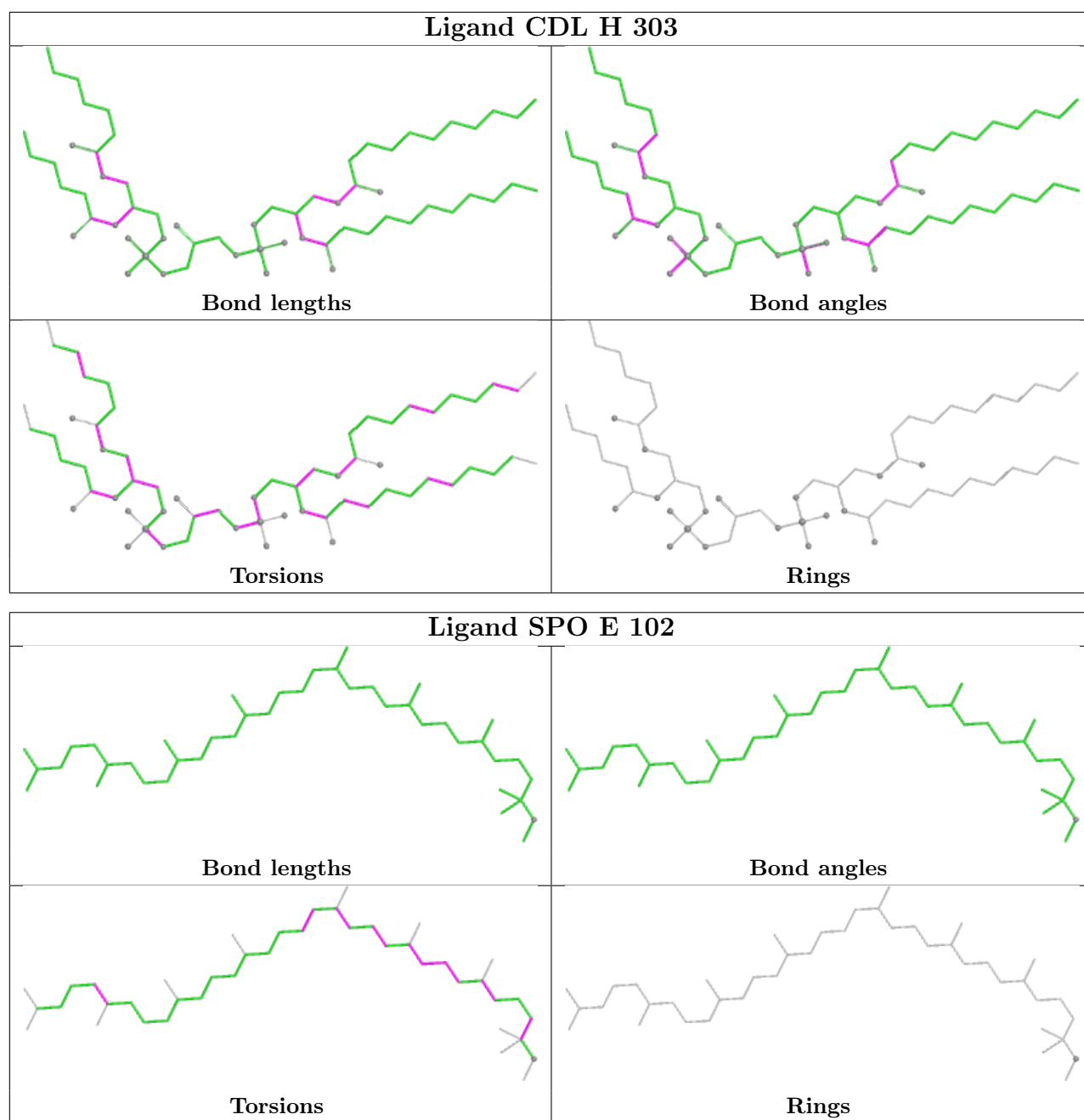
Ligand BCL z 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand SPO 3 103	
 Bond lengths	 Bond angles
 Torsions	 Rings

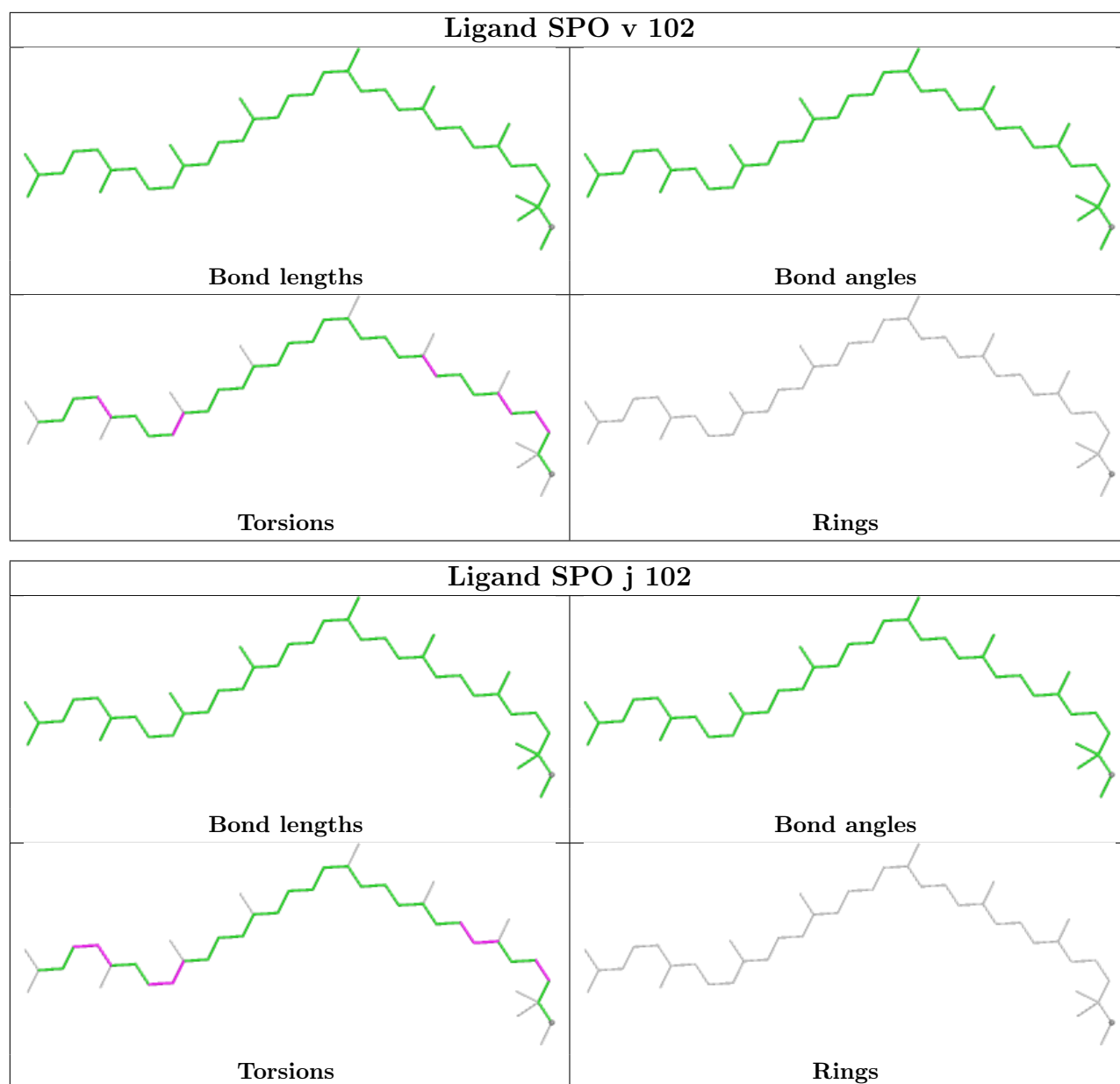












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

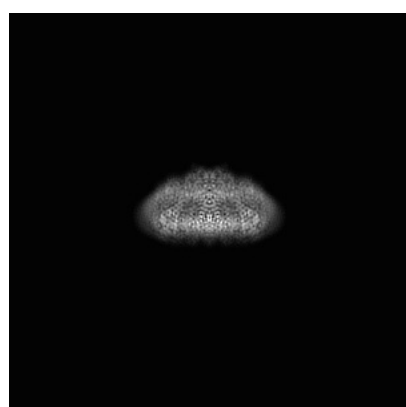
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32059. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections [i](#)

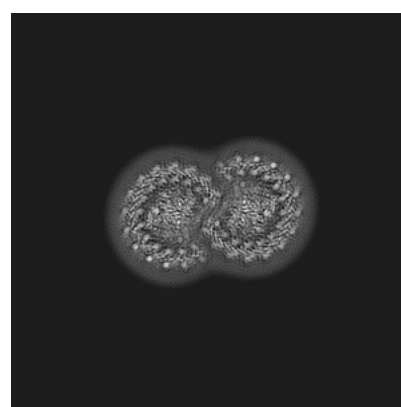
6.1.1 Primary map



X



Y

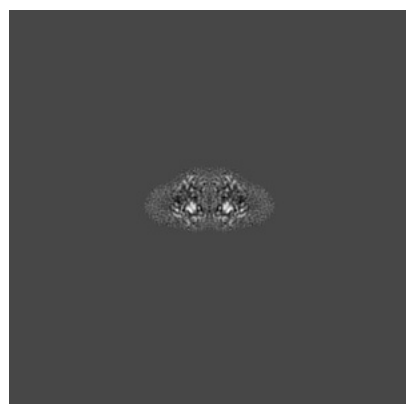


Z

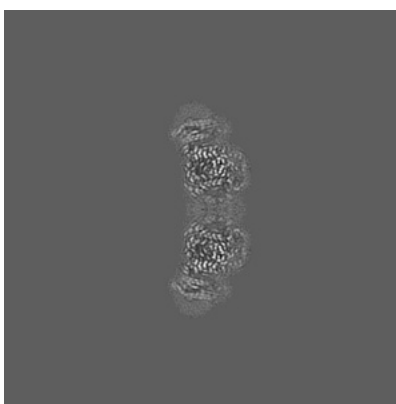
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

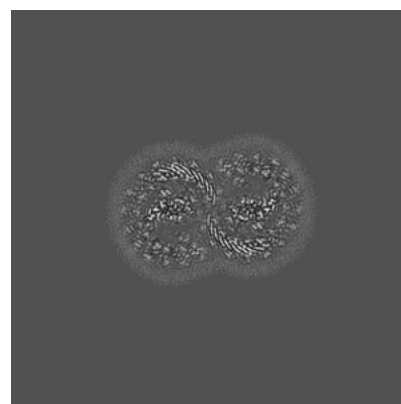
6.2.1 Primary map



X Index: 208



Y Index: 208



Z Index: 208

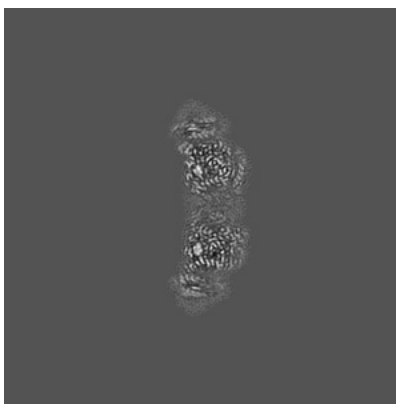
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

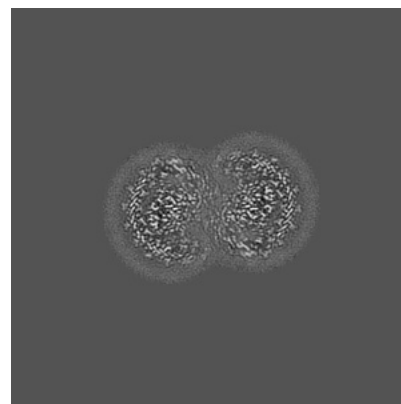
6.3.1 Primary map



X Index: 255



Y Index: 210

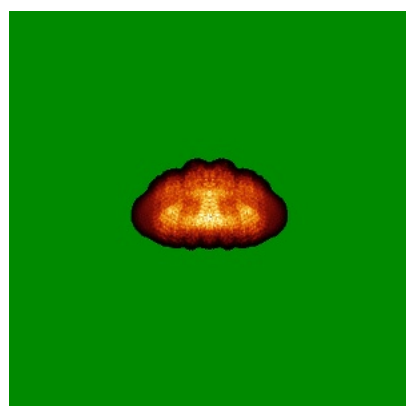


Z Index: 198

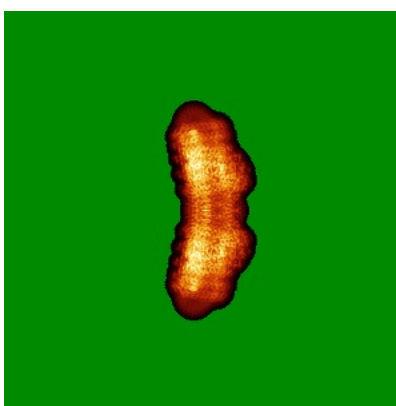
The images above show the largest variance slices of the map in three orthogonal directions.

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

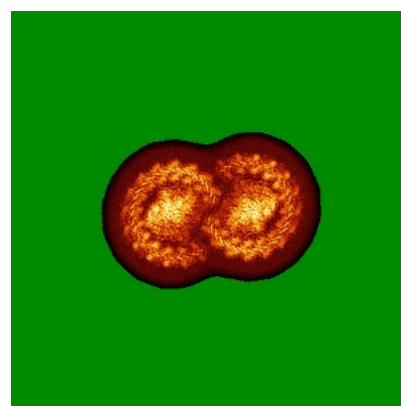
6.4.1 Primary map



X



Y

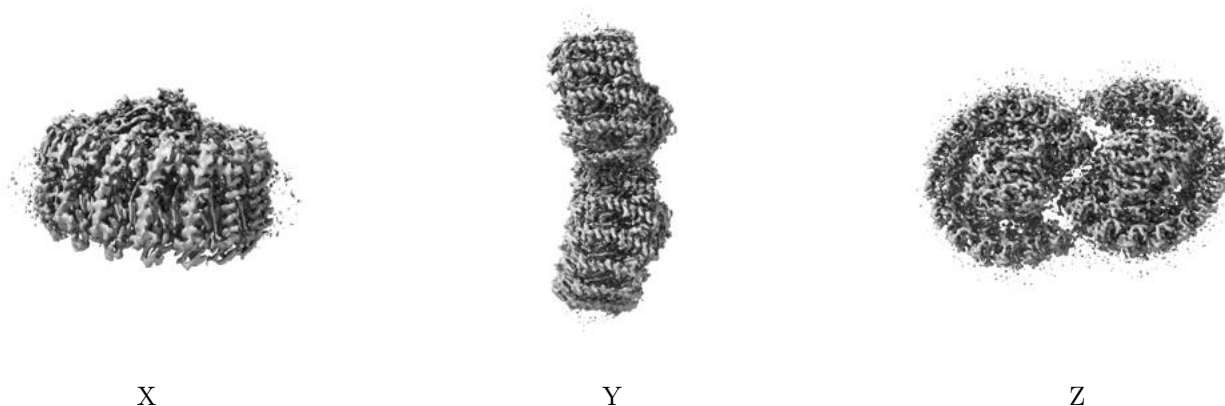


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

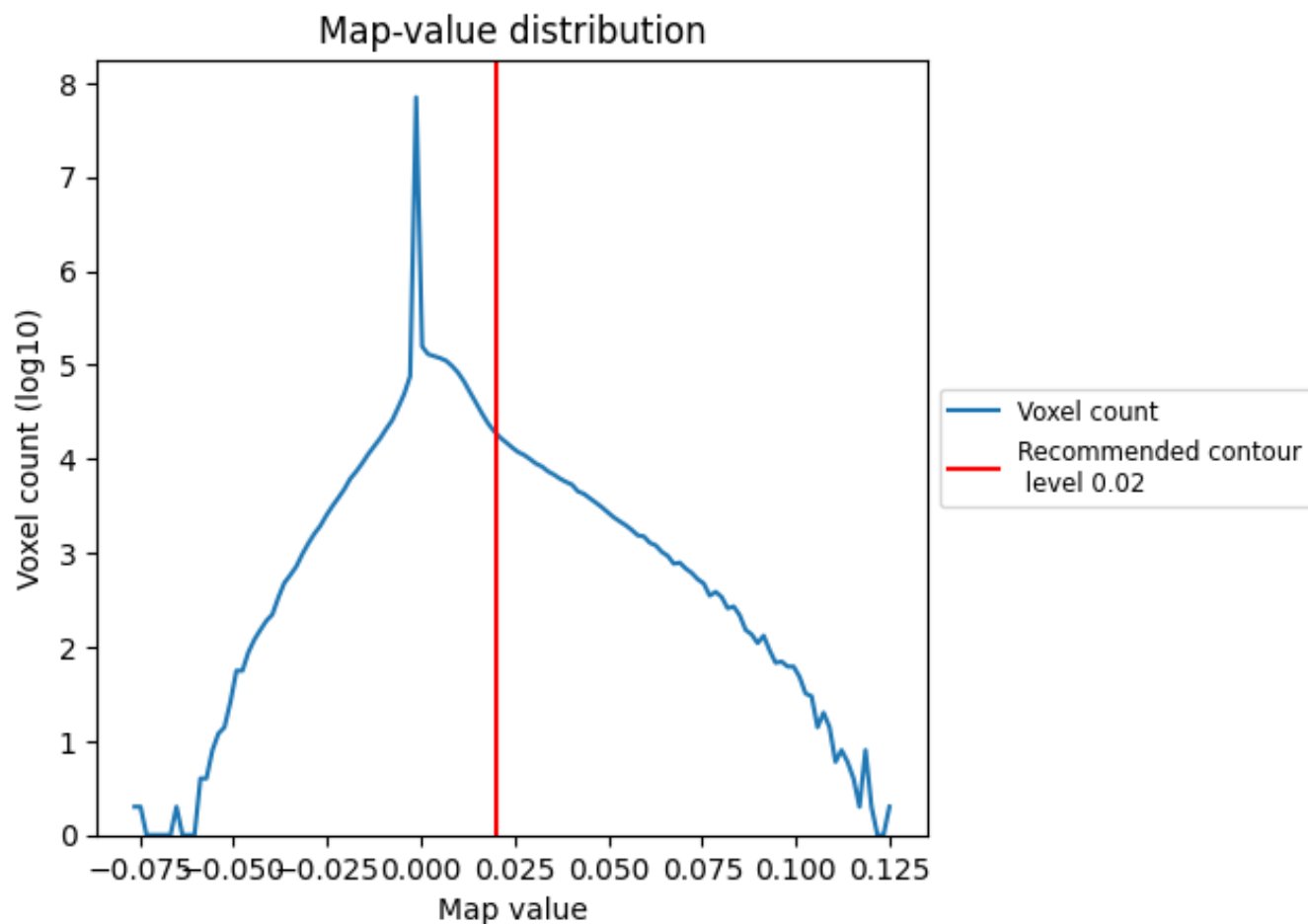
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

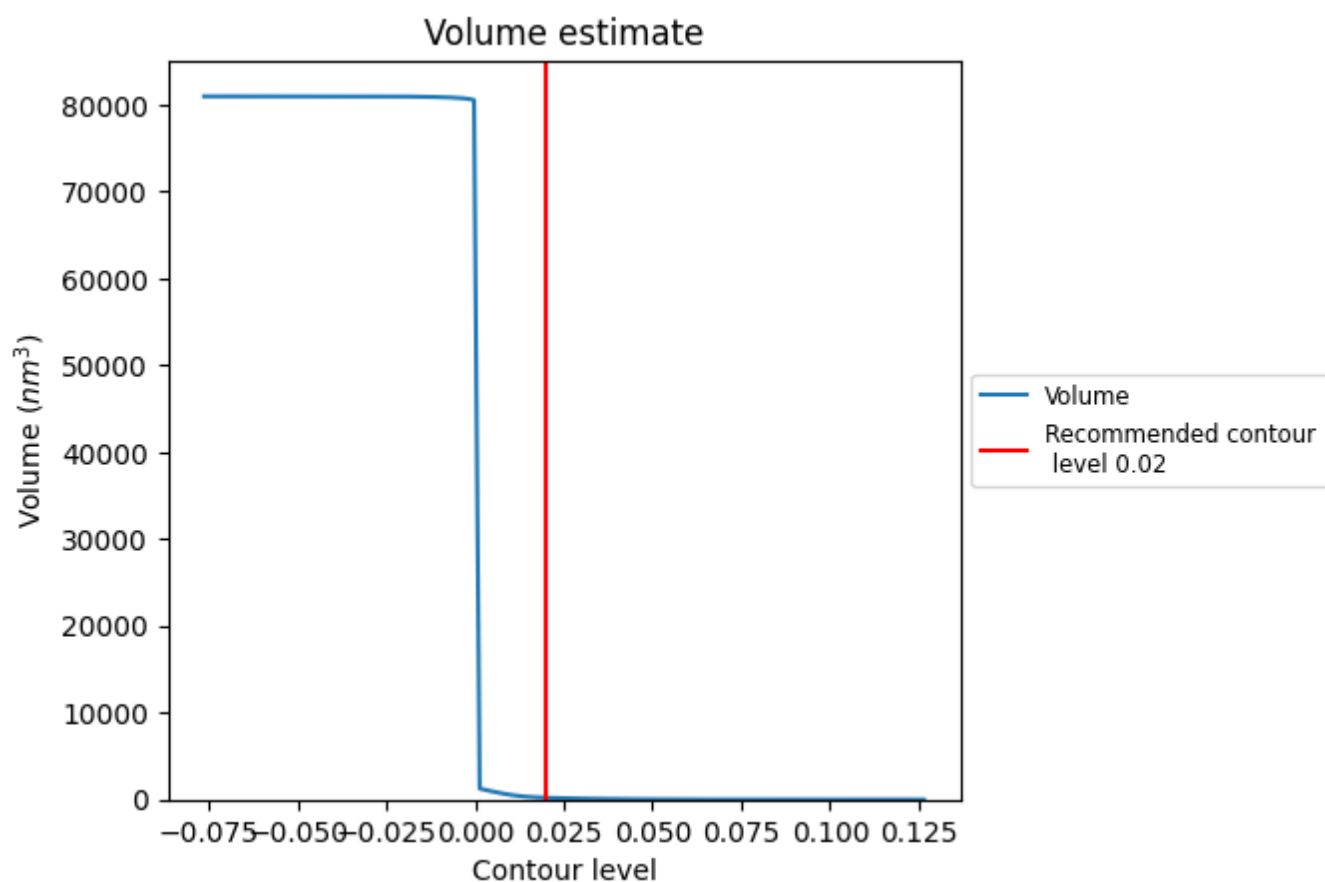
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

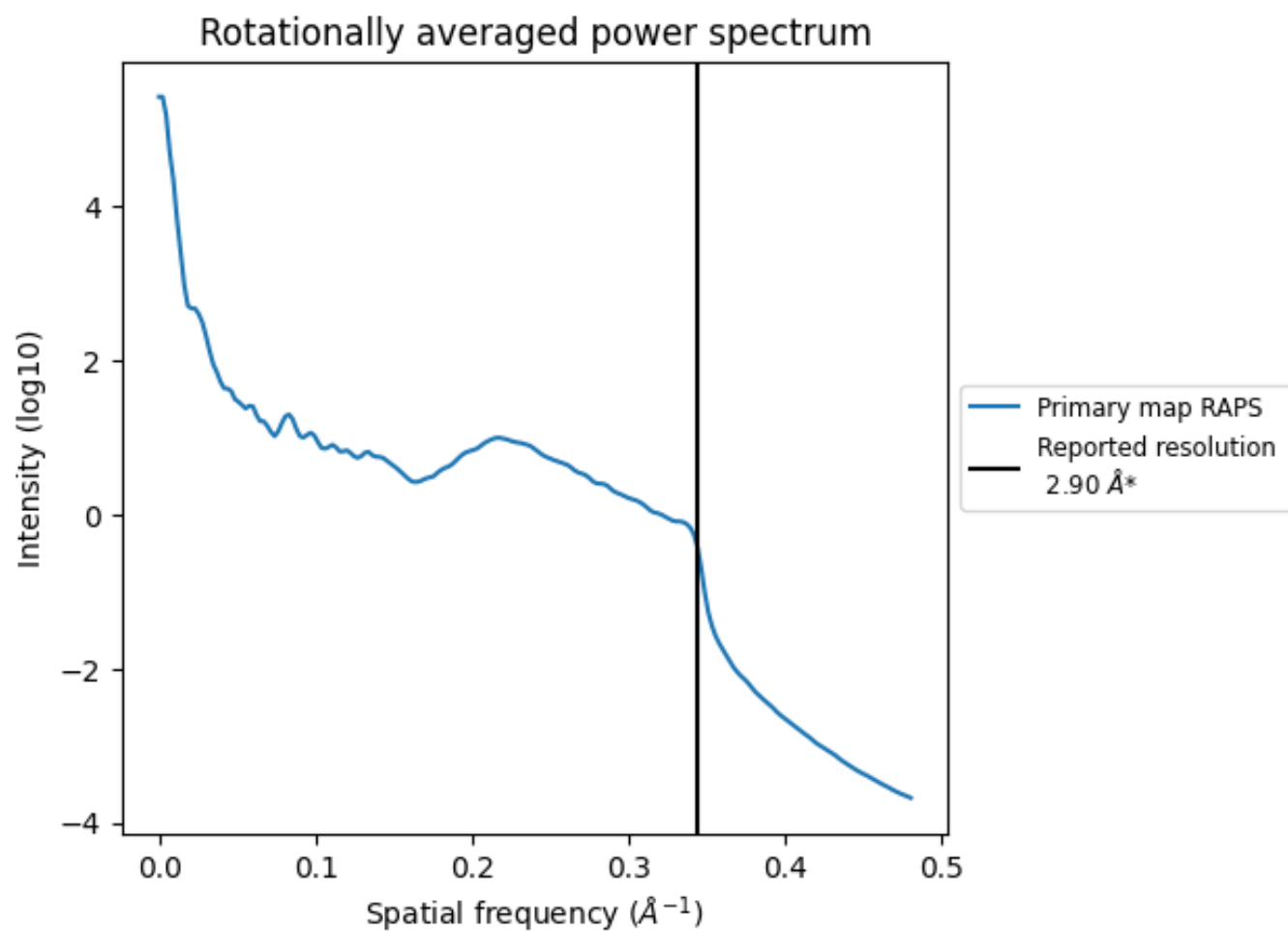
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 208 nm^3 ; this corresponds to an approximate mass of 188 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 0.345 Å⁻¹

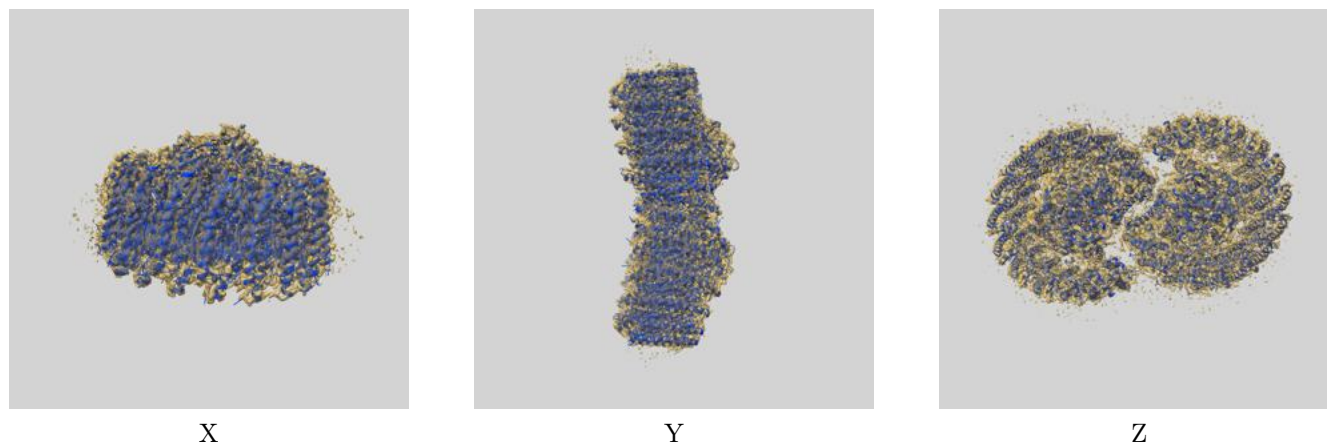
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

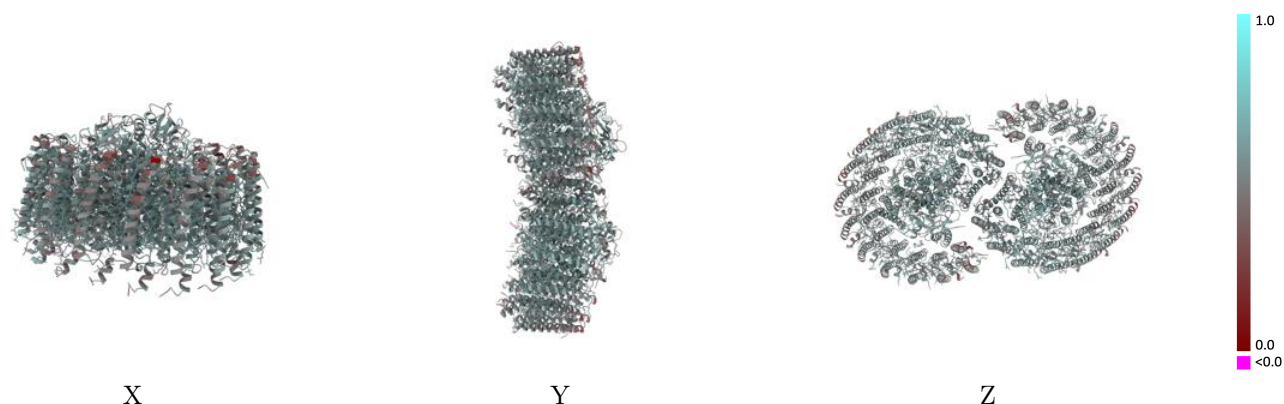
This section contains information regarding the fit between EMDB map EMD-32059 and PDB model 7VOT. Per-residue inclusion information can be found in [section 3](#) on [page 20](#).

9.1 Map-model overlay [i](#)



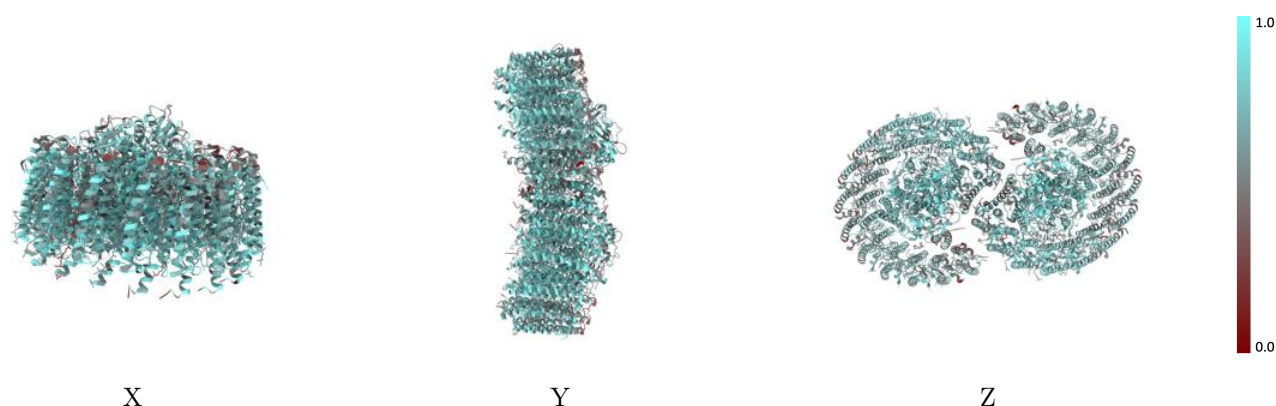
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



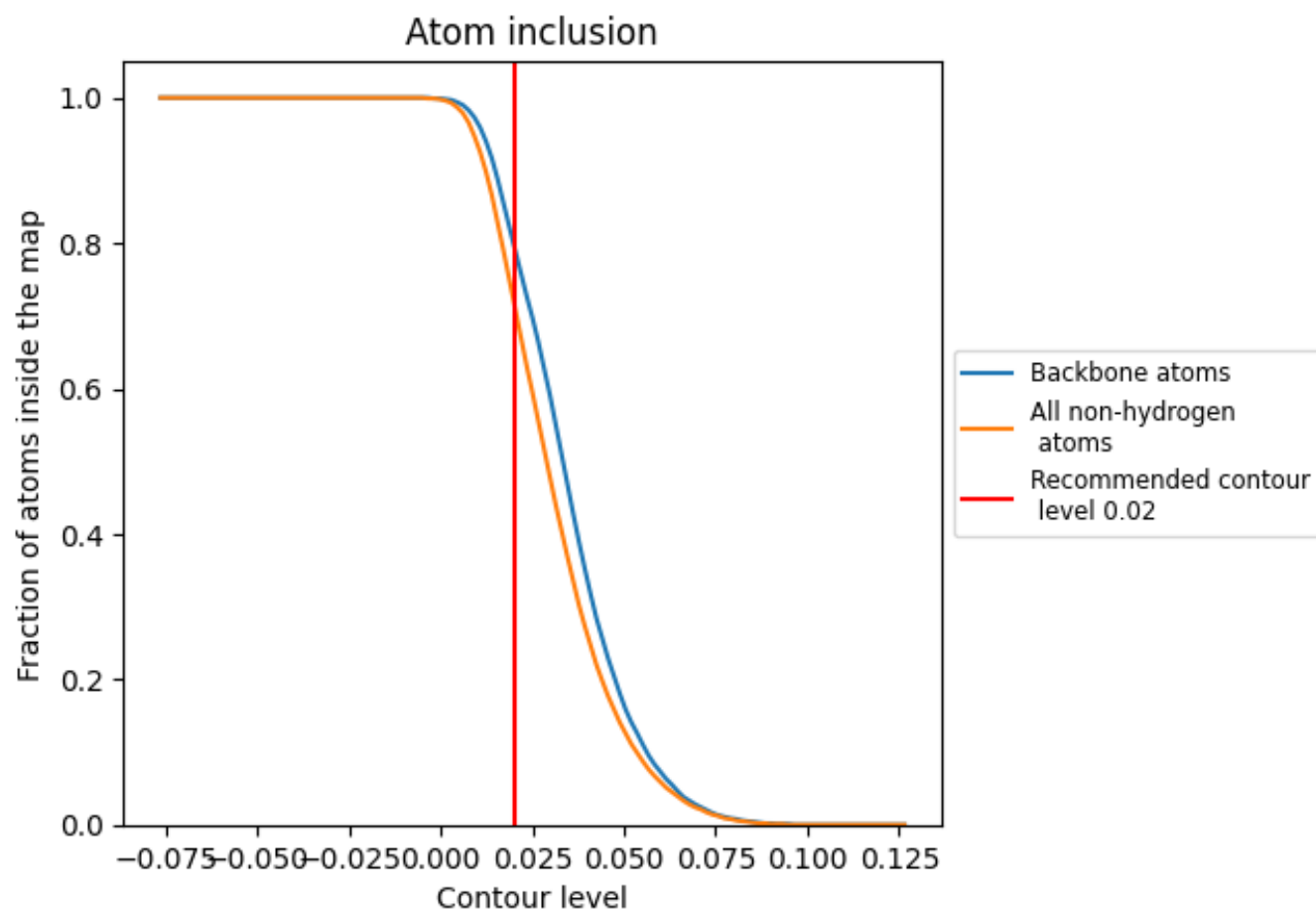
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 72% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7190	 0.5420
0	 0.7520	 0.5420
1	 0.5400	 0.4860
2	 0.5740	 0.4560
3	 0.6340	 0.5180
4	 0.5870	 0.4580
5	 0.6490	 0.5250
6	 0.6960	 0.5410
7	 0.6740	 0.5300
8	 0.6580	 0.5080
9	 0.7490	 0.5570
A	 0.7460	 0.5650
B	 0.7260	 0.5520
C	 0.6750	 0.5260
D	 0.7400	 0.5580
E	 0.7390	 0.5450
F	 0.7430	 0.5490
G	 0.6850	 0.5230
H	 0.6870	 0.5400
I	 0.6680	 0.5250
J	 0.6300	 0.5050
K	 0.6660	 0.5000
L	 0.8120	 0.5840
M	 0.8380	 0.5840
N	 0.6290	 0.4710
O	 0.6390	 0.5040
P	 0.6560	 0.4620
Q	 0.6790	 0.5150
R	 0.6320	 0.5030
S	 0.7140	 0.5400
T	 0.6990	 0.5120
U	 0.7440	 0.5440
V	 0.6930	 0.5230
W	 0.7290	 0.5370
X	 0.6090	 0.5230



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Y	 0.5750	 0.5260
Z	 0.6200	 0.5010
a	 0.7520	 0.5700
b	 0.7350	 0.5580
b0	 0.7670	 0.5540
b1	 0.5510	 0.4870
b8	 0.6600	 0.5110
b9	 0.7770	 0.5660
c	 0.7110	 0.5360
d	 0.7560	 0.5660
e	 0.7460	 0.5540
f	 0.7460	 0.5550
g	 0.6970	 0.5260
h	 0.6920	 0.5460
i	 0.6810	 0.5300
j	 0.6390	 0.5110
k	 0.6680	 0.5090
l	 0.8170	 0.5840
m	 0.8450	 0.5840
n	 0.6270	 0.4770
o	 0.6300	 0.5120
p	 0.6560	 0.4750
q	 0.6890	 0.5250
r	 0.6410	 0.5170
s	 0.7250	 0.5460
t	 0.7140	 0.5230
u	 0.7650	 0.5520
v	 0.7120	 0.5310
w	 0.7410	 0.5430
x	 0.6160	 0.5280
y	 0.5620	 0.5410
z	 0.6350	 0.5070