



wwPDB EM Validation Summary Report ⓘ

Aug 6, 2026 – 09:40 AM JST

PDB ID : 7VB9 / pdb_00007vb9
EMDB ID : EMD-31875
Title : Rba sphaeroides PufY-KO RC-LH1 dimer type-2
Authors : Bracun, L.; Yamagata, A.; Liu, L.N.; Shirouzu, M.
Deposited on : 2021-08-30
Resolution : 3.45 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.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
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) : 2.50

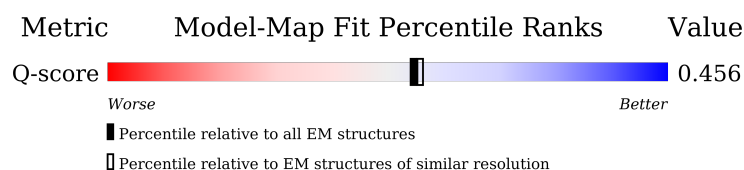
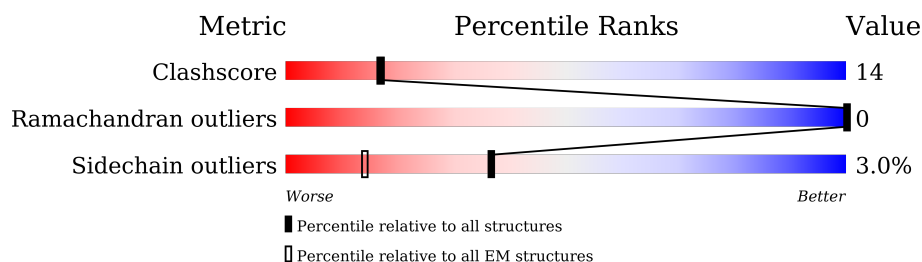
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.45 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	13836 (2.95 - 3.95)

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	13% 68% 26% • 5%
1	l	282	89% 11%
2	M	308	33% 83% 16% •
2	m	308	82% 16% •

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Mol	Chain	Length	Quality of chain
3	H	260	
3	h	260	
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	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	y	58	
5	0	49	

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Mol	Chain	Length	Quality of chain
5	4	49	
5	8	49	
5	B	49	
5	E	49	
5	G	49	
5	J	49	
5	N	49	
5	aa	49	
5	ab	49	
5	b	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	x	49	
5	z	49	
6	C	82	
6	c	82	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	SPO	0	101	-	X	-	-
11	SPO	0	103	-	X	-	-
11	SPO	9	101	-	X	-	-
11	SPO	9	103	-	X	-	-
11	SPO	C	1203	-	X	-	-
11	SPO	D	102	-	X	-	-
11	SPO	E	102	-	X	-	-
11	SPO	F	102	-	X	-	-
11	SPO	F	103	-	X	-	-
11	SPO	G	102	-	X	-	-
11	SPO	G	103	-	X	-	-
11	SPO	J	102	-	X	-	-
11	SPO	M	404	-	X	-	-
11	SPO	Q	603	-	X	-	-
11	SPO	aa	101	-	X	-	-
11	SPO	ab	102	-	X	-	-
11	SPO	b	101	-	X	-	-
11	SPO	b	103	-	X	-	-
11	SPO	d	102	-	X	-	-
11	SPO	d	103	-	X	-	-
11	SPO	e	102	-	X	-	-
11	SPO	f	102	-	X	-	-
11	SPO	g	101	-	X	-	-
11	SPO	i	103	-	X	-	-
11	SPO	j	101	-	X	-	-
11	SPO	m	405	-	X	-	-
11	SPO	n	102	-	X	-	-
11	SPO	o	102	-	X	-	-
11	SPO	p	102	-	X	-	-
11	SPO	p	103	-	X	-	-
11	SPO	q	102	-	X	-	-
11	SPO	s	101	-	X	-	-
11	SPO	t	102	-	X	-	-
11	SPO	u	101	-	X	-	-
11	SPO	v	102	-	X	-	-
11	SPO	w	102	-	X	-	-

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 36474 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	268	Total	C	N	O	S	0	0
			2132	1440	338	346	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	305	Total	C	N	O	S	0	0
			2431	1623	397	400	11		
2	m	305	Total	C	N	O	S	0	0
			2431	1623	397	400	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	260	Total	C	N	O	S	0	0
			1972	1264	335	362	11		
3	h	260	Total	C	N	O	S	0	0
			1972	1264	335	362	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	54	Total	C	N	O	S	0	0
			455	310	73	69	3		
4	D	54	Total	C	N	O	S	0	0
			455	310	73	69	3		
4	F	54	Total	C	N	O	S	0	0
			455	310	73	69	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	44	Total	C	N	O	S	0	0
			362	244	60	57	1		
4	O	43	Total	C	N	O	S	0	0
			351	235	59	56	1		
4	7	46	Total	C	N	O	S	0	0
			392	271	60	58	3		
4	9	54	Total	C	N	O	S	0	0
			455	310	73	69	3		
4	a	54	Total	C	N	O	S	0	0
			455	310	73	69	3		
4	d	54	Total	C	N	O	S	0	0
			455	310	73	69	3		
4	f	54	Total	C	N	O	S	0	0
			455	310	73	69	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
			455	310	73	69	3		
4	o	54	Total	C	N	O	S	0	0
			455	310	73	69	3		
4	q	54	Total	C	N	O	S	0	0
			455	310	73	69	3		
4	s	54	Total	C	N	O	S	0	0
			455	310	73	69	3		
4	u	54	Total	C	N	O	S	0	0
			455	310	73	69	3		
4	w	43	Total	C	N	O	S	0	0
			351	235	59	56	1		
4	y	42	Total	C	N	O	S	0	0
			343	231	58	53	1		
4	5	42	Total	C	N	O	S	0	0
			343	231	58	53	1		
4	6	46	Total	C	N	O	S	0	0
			392	271	60	58	3		
4	Q	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
			359	240	56	62	1		

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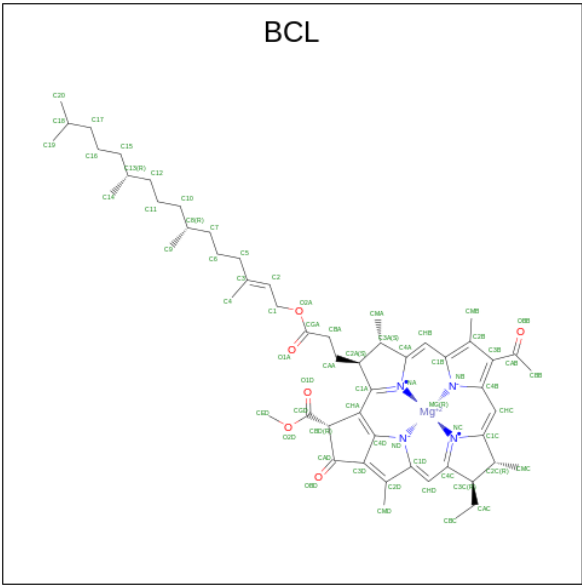
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Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	43	Total	C	N	O	S	0	0
			351	236	55	59	1		
5	G	44	Total	C	N	O	S	0	0
			359	240	56	62	1		
5	J	43	Total	C	N	O	S	0	0
			351	236	55	59	1		
5	N	41	Total	C	N	O	S	0	0
			339	228	53	57	1		
5	8	44	Total	C	N	O	S	0	0
			359	240	56	62	1		
5	0	44	Total	C	N	O	S	0	0
			359	240	56	62	1		
5	b	44	Total	C	N	O	S	0	0
			359	240	56	62	1		
5	e	43	Total	C	N	O	S	0	0
			351	236	55	59	1		
5	g	44	Total	C	N	O	S	0	0
			359	240	56	62	1		
5	j	43	Total	C	N	O	S	0	0
			351	236	55	59	1		
5	n	38	Total	C	N	O	S	0	0
			316	213	50	52	1		
5	p	39	Total	C	N	O	S	0	0
			320	215	51	53	1		
5	r	43	Total	C	N	O	S	0	0
			351	236	55	59	1		
5	t	42	Total	C	N	O	S	0	0
			343	230	54	58	1		
5	v	37	Total	C	N	O	S	0	0
			308	207	49	51	1		
5	x	42	Total	C	N	O	S	0	0
			343	230	54	58	1		
5	z	38	Total	C	N	O	S	0	0
			312	209	50	52	1		
5	4	36	Total	C	N	O	S	0	0
			297	198	48	50	1		
5	aa	44	Total	C	N	O	S	0	0
			359	240	56	62	1		
5	ab	44	Total	C	N	O	S	0	0
			359	240	56	62	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	64	Total	C	N	O	S	0	0
			500	328	88	81	3		
6	c	68	Total	C	N	O	S	0	0
			529	345	93	88	3		

- Molecule 7 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: C₅₅H₇₄MgN₄O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
7	L	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	L	1	Total	C	Mg	N	O	0
			62	51	1	4	6	
7	L	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
7	M	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	A	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	B	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	D	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	E	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	F	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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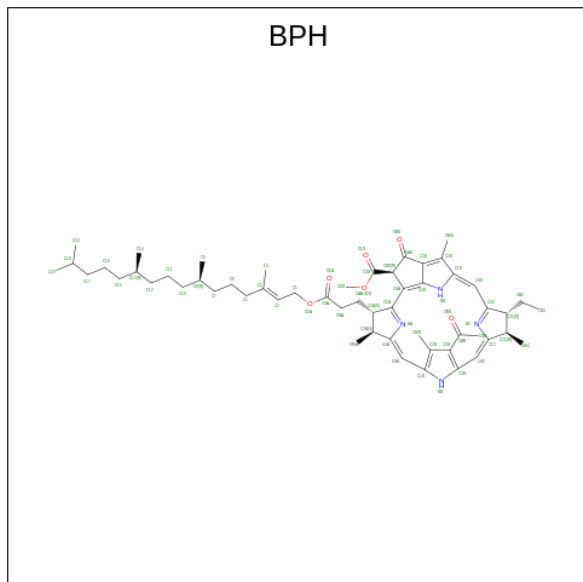
Mol	Chain	Residues	Atoms					AltConf
7	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	I	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	J	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	K	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	O	1	Total 46	C 35	Mg 1	N 4	O 6	0
7	8	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	9	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	0	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	C	1	Total 61	C 50	Mg 1	N 4	O 6	0
7	l	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	l	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	m	1	Total 62	C 51	Mg 1	N 4	O 6	0
7	m	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	a	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	b	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	d	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	e	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	f	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	g	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	i	1	Total 66	C 55	Mg 1	N 4	O 6	0

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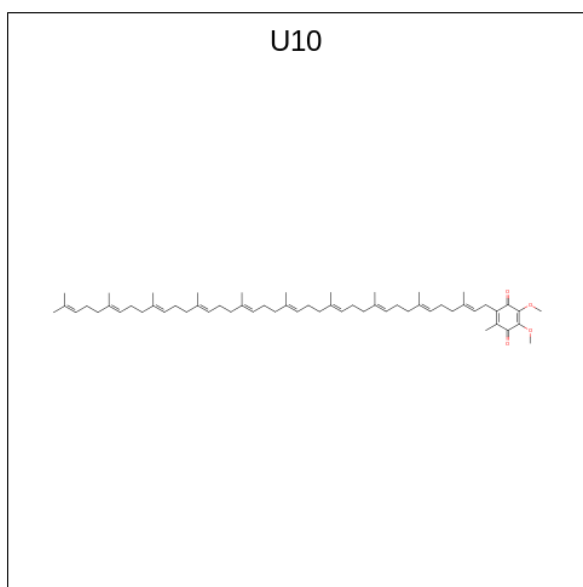
Mol	Chain	Residues	Atoms					AltConf
7	i	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	k	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	n	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	o	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	p	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	q	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	q	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	r	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	s	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	t	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	v	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	w	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	x	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	y	1	Total 46	C 35	Mg 1	N 4	O 6	0
7	z	1	Total 46	C 35	Mg 1	N 4	O 6	0
7	5	1	Total 46	C 35	Mg 1	N 4	O 6	0
7	4	1	Total 46	C 35	Mg 1	N 4	O 6	0
7	aa	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	Q	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	ab	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	c	1	Total 61	C 50	Mg 1	N 4	O 6	0

- Molecule 8 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: $C_{55}H_{76}N_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
8	L	1	Total	C	N	O	0
			62	52	4	6	
8	L	1	Total	C	N	O	0
			55	45	4	6	
8	1	1	Total	C	N	O	0
			62	52	4	6	
8	1	1	Total	C	N	O	0
			55	45	4	6	

- Molecule 9 is UBIQUINONE-10 (CCD ID: U10) (formula: $C_{59}H_{90}O_4$) (labeled as "Ligand of Interest" by depositor).

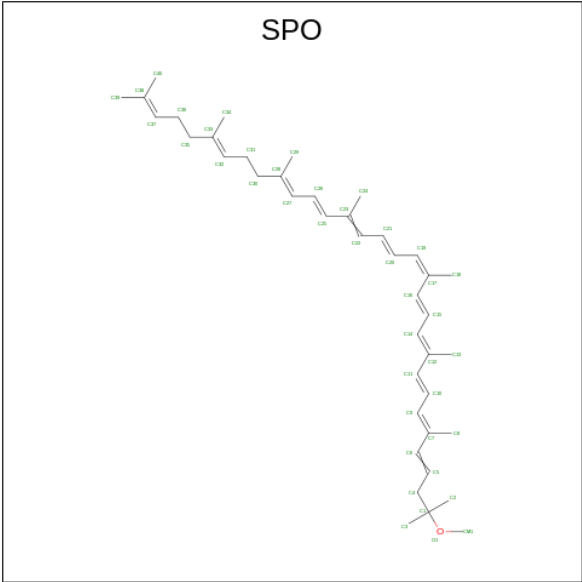


Mol	Chain	Residues	Atoms			AltConf
9	L	1	Total	C	O	0
			43	39	4	
9	M	1	Total	C	O	0
			48	44	4	
9	l	1	Total	C	O	0
			63	59	4	
9	m	1	Total	C	O	0
			48	44	4	

- Molecule 10 is FE (II) ION (CCD ID: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 11 is SPHEROIDENE (CCD ID: SPO) (formula: C₄₁H₆₀O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
11	M	1	Total	C	O	0
			42	41	1	
11	D	1	Total	C	O	0
			42	41	1	
11	E	1	Total	C	O	0
			42	41	1	
11	F	1	Total	C	O	0
			42	41	1	
11	F	1	Total	C	O	0
			42	41	1	
11	G	1	Total	C	O	0
			42	41	1	
11	G	1	Total	C	O	0
			42	41	1	
11	J	1	Total	C	O	0
			42	41	1	
11	9	1	Total	C	O	0
			42	41	1	
11	9	1	Total	C	O	0
			42	41	1	
11	0	1	Total	C	O	0
			42	41	1	
11	0	1	Total	C	O	0
			42	41	1	
11	C	1	Total	C	O	0
			42	41	1	
11	m	1	Total	C	O	0
			42	41	1	

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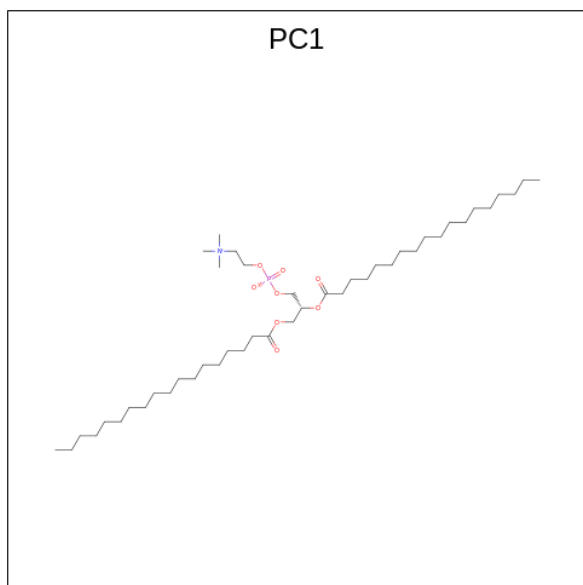
Mol	Chain	Residues	Atoms			AltConf
11	b	1	Total 42	C 41	O 1	0
11	b	1	Total 42	C 41	O 1	0
11	d	1	Total 42	C 41	O 1	0
11	d	1	Total 42	C 41	O 1	0
11	e	1	Total 42	C 41	O 1	0
11	f	1	Total 42	C 41	O 1	0
11	g	1	Total 42	C 41	O 1	0
11	i	1	Total 42	C 41	O 1	0
11	j	1	Total 42	C 41	O 1	0
11	n	1	Total 42	C 41	O 1	0
11	o	1	Total 42	C 41	O 1	0
11	p	1	Total 42	C 41	O 1	0
11	p	1	Total 42	C 41	O 1	0
11	q	1	Total 42	C 41	O 1	0
11	s	1	Total 42	C 41	O 1	0
11	t	1	Total 42	C 41	O 1	0
11	u	1	Total 42	C 41	O 1	0
11	v	1	Total 42	C 41	O 1	0
11	w	1	Total 42	C 41	O 1	0
11	aa	1	Total 42	C 41	O 1	0
11	Q	1	Total 42	C 41	O 1	0

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Mol	Chain	Residues	Atoms			AltConf
11	ab	1	Total	C	O	0
			42	41	1	

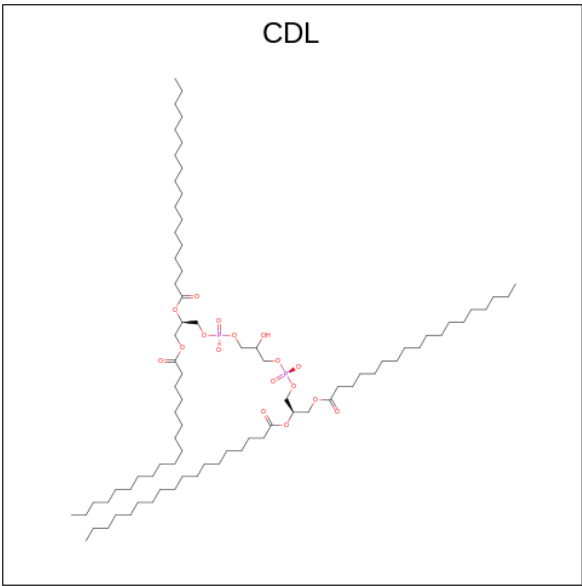
- Molecule 12 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
12	H	1	Total	C	N	O	P		0
			44	34	1	8	1		
12	H	1	Total	C	N	O	P		0
			54	44	1	8	1		
12	A	1	Total	C	N	O	P		0
			43	33	1	8	1		
12	A	1	Total	C	N	O	P		0
			46	36	1	8	1		
12	C	1	Total	C	N	O	P		0
			54	44	1	8	1		
12	h	1	Total	C	N	O	P		0
			48	38	1	8	1		
12	a	1	Total	C	N	O	P		0
			40	30	1	8	1		
12	Q	1	Total	C	N	O	P		0
			54	44	1	8	1		
12	c	1	Total	C	N	O	P		0
			48	38	1	8	1		

- Molecule 13 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand

of Interest" by depositor).

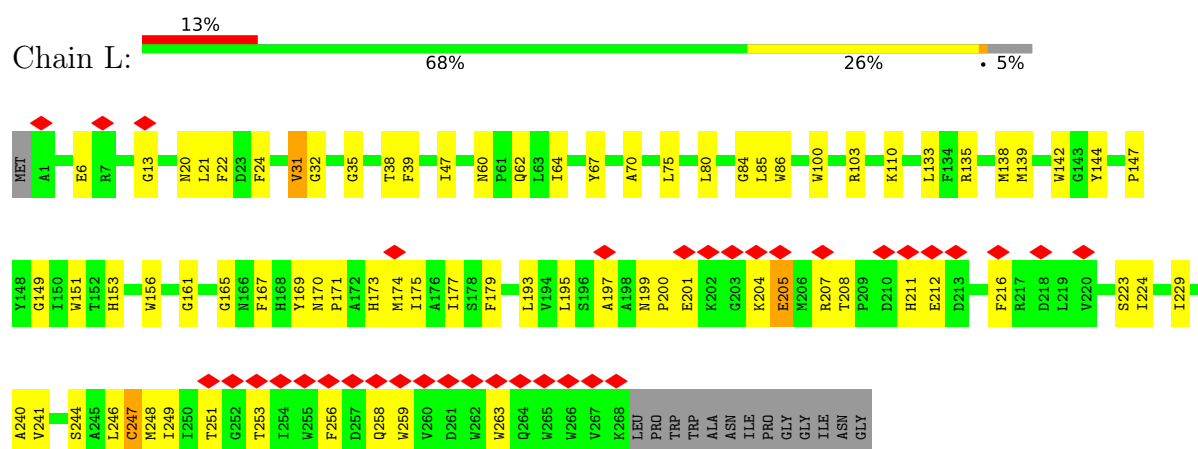


Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
13	m	1	100	81	17	2	0

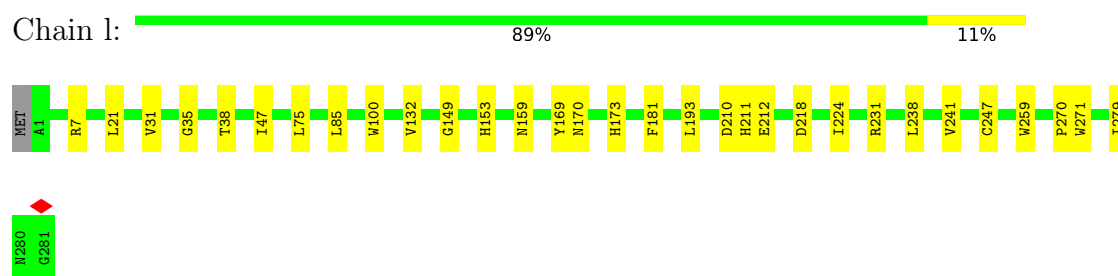
3 Residue-property plots

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

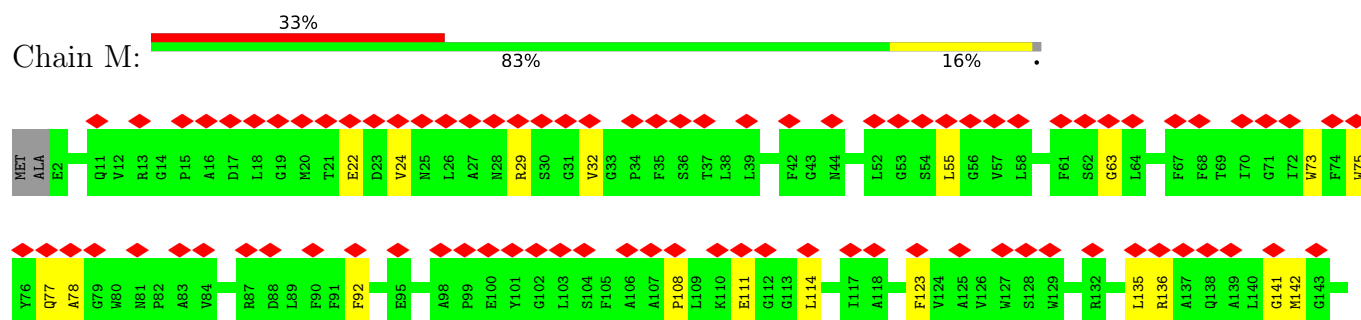
• Molecule 1: Reaction center protein L chain

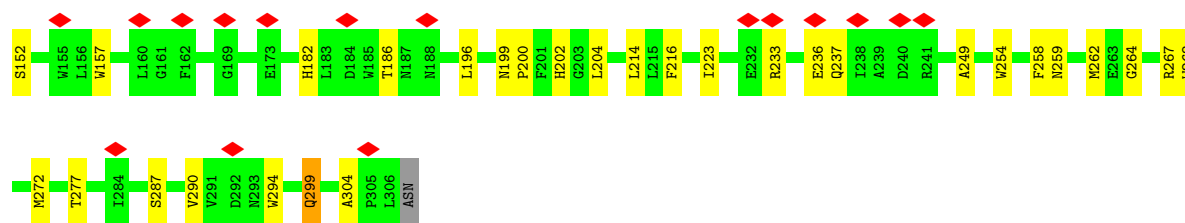


• Molecule 1: Reaction center protein L chain



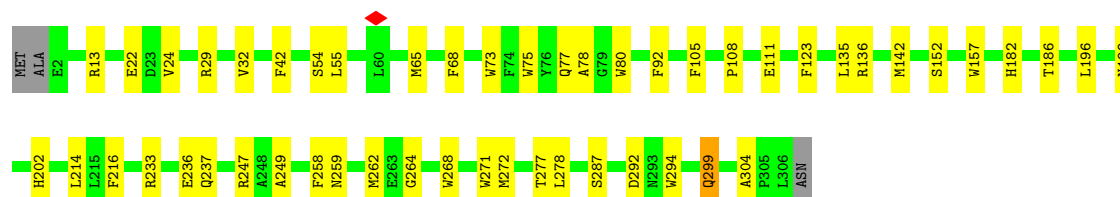
• Molecule 2: Reaction center protein M chain





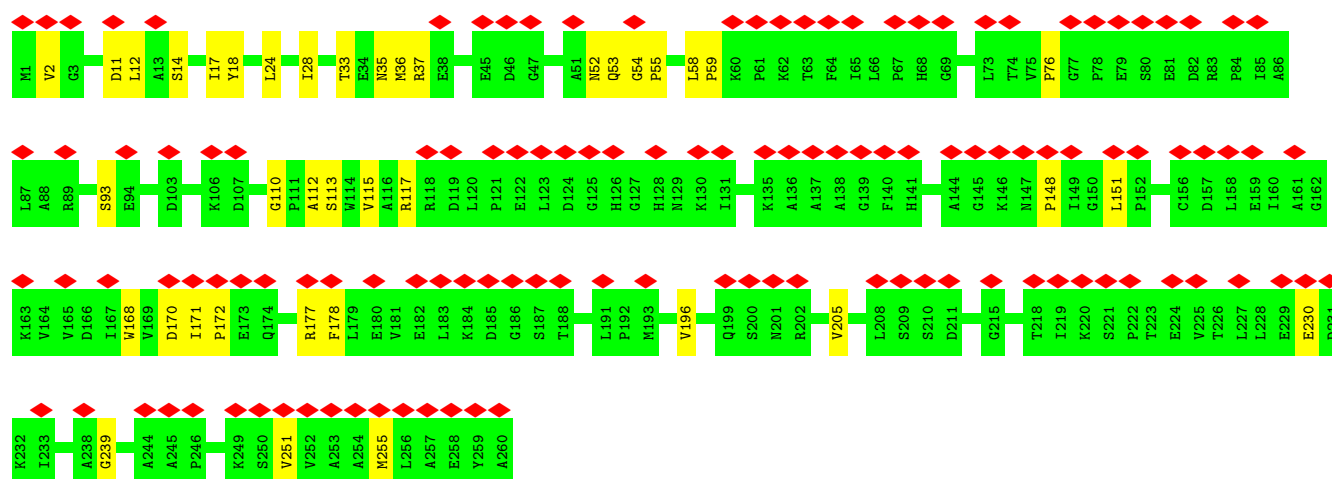
• Molecule 2: Reaction center protein M chain

Chain m: 82% 16% .



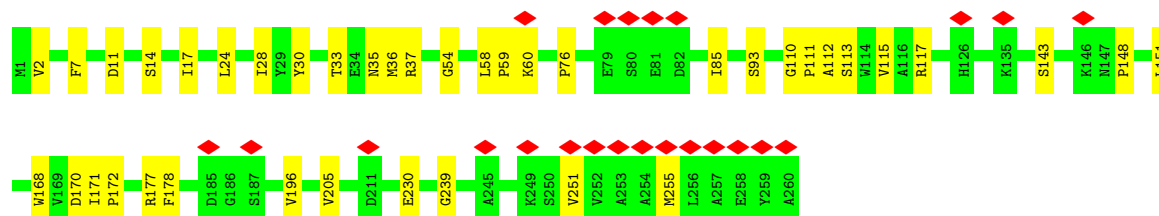
• Molecule 3: Reaction center protein H chain

Chain H: 48% 85% 15%



• Molecule 3: Reaction center protein H chain

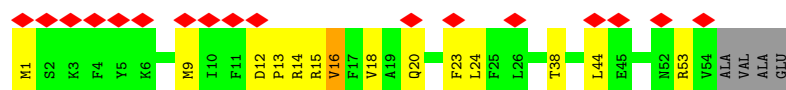
Chain h: 9% 85% 15%



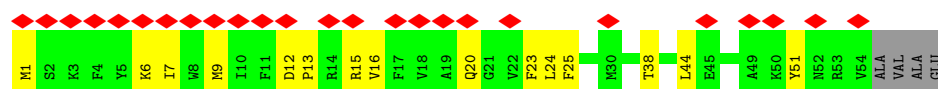
• Molecule 4: Light-harvesting protein B-875 alpha chain



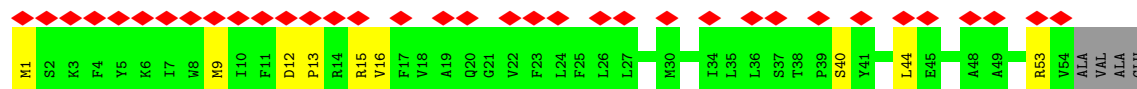
- Molecule 4: Light-harvesting protein B-875 alpha chain



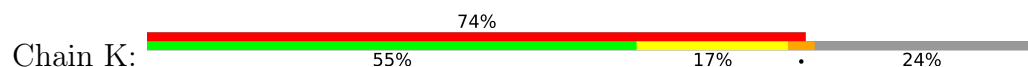
- Molecule 4: Light-harvesting protein B-875 alpha chain



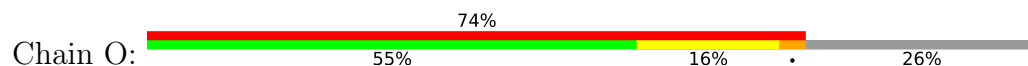
- Molecule 4: Light-harvesting protein B-875 alpha chain



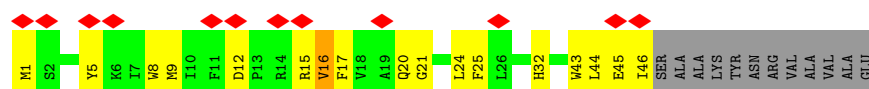
- Molecule 4: Light-harvesting protein B-875 alpha chain



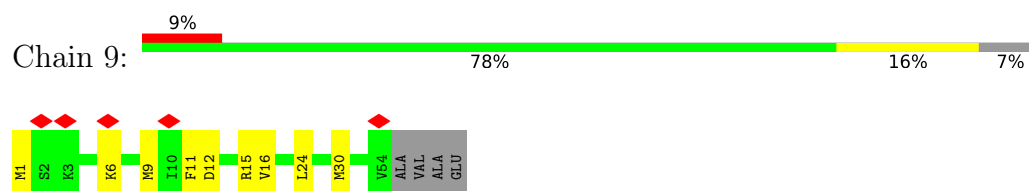
- Molecule 4: Light-harvesting protein B-875 alpha chain



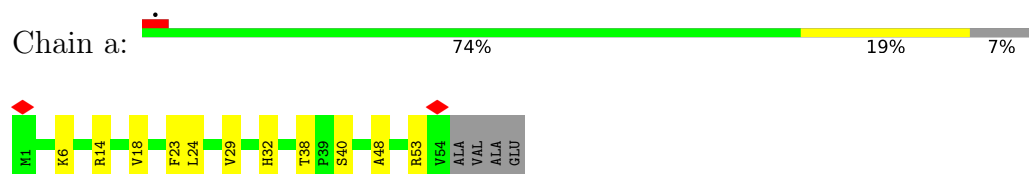
- Molecule 4: Light-harvesting protein B-875 alpha chain



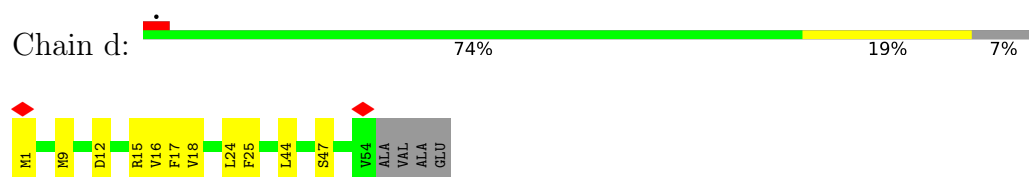
- Molecule 4: Light-harvesting protein B-875 alpha chain



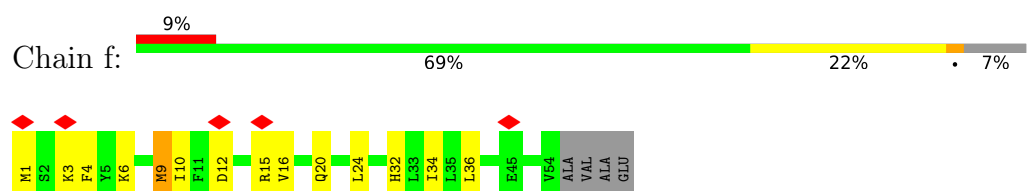
- Molecule 4: Light-harvesting protein B-875 alpha chain



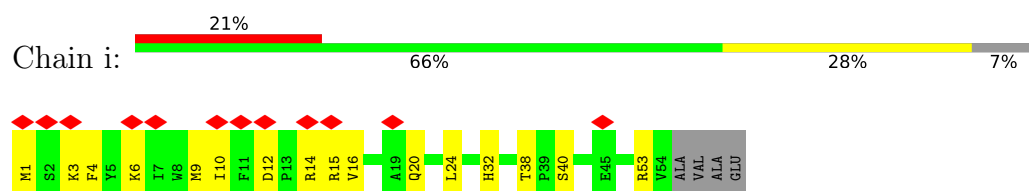
- Molecule 4: Light-harvesting protein B-875 alpha chain



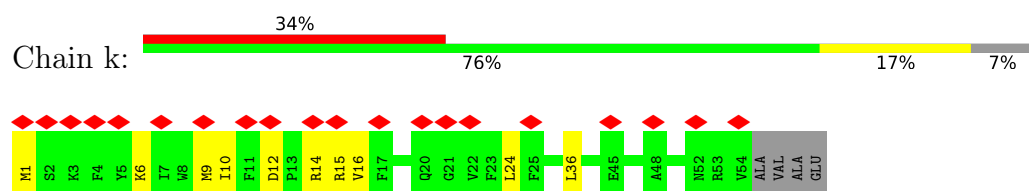
- Molecule 4: Light-harvesting protein B-875 alpha chain



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

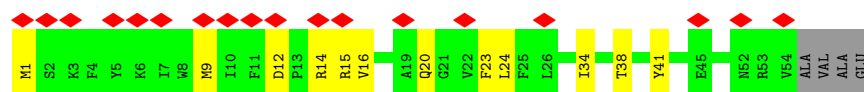


- Molecule 4: Light-harvesting protein B-875 alpha chain



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

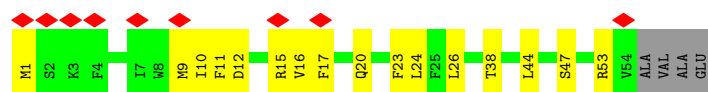




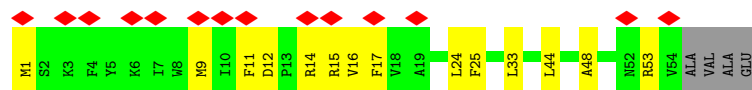
- Molecule 4: Light-harvesting protein B-875 alpha chain



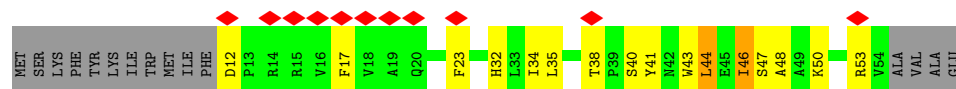
- Molecule 4: Light-harvesting protein B-875 alpha chain



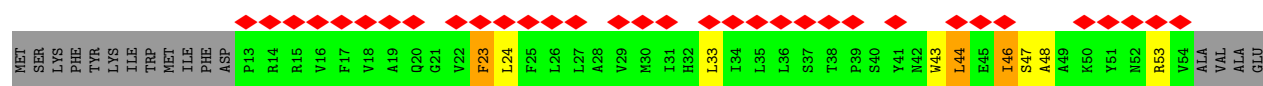
- Molecule 4: Light-harvesting protein B-875 alpha chain



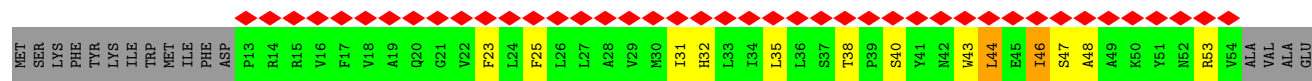
- Molecule 4: Light-harvesting protein B-875 alpha chain



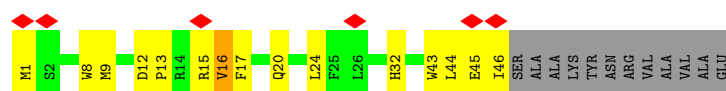
- Molecule 4: Light-harvesting protein B-875 alpha chain



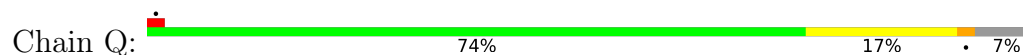
- Molecule 4: Light-harvesting protein B-875 alpha chain



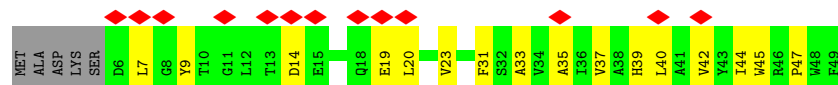
- Molecule 4: Light-harvesting protein B-875 alpha chain



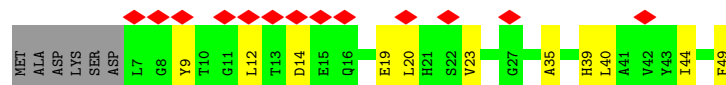
- Molecule 4: Light-harvesting protein B-875 alpha chain



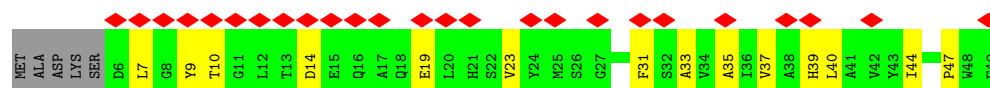
- Molecule 5: Light-harvesting protein B-875 beta chain



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



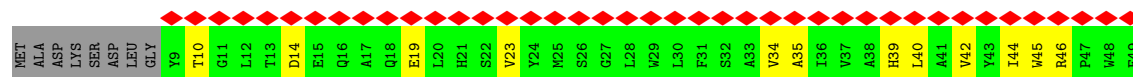
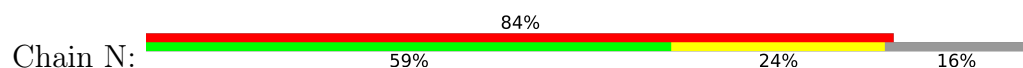
- Molecule 5: Light-harvesting protein B-875 beta chain



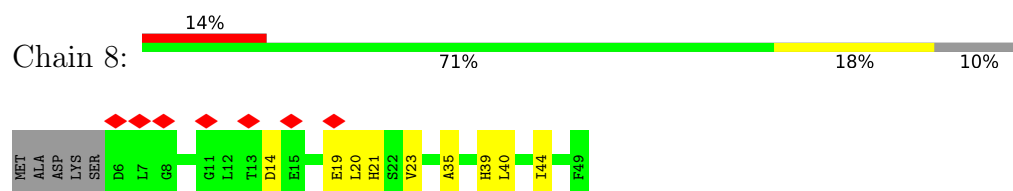
- Molecule 5: Light-harvesting protein B-875 beta chain



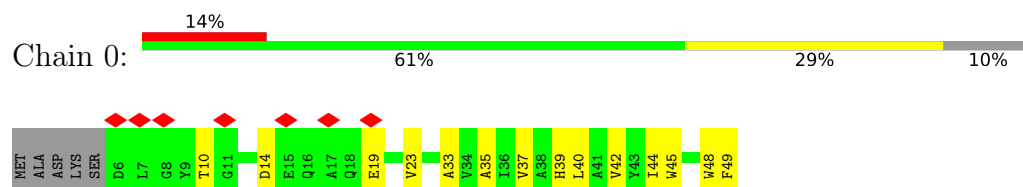
- Molecule 5: Light-harvesting protein B-875 beta chain



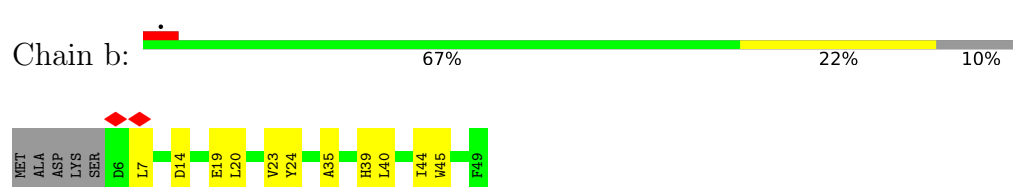
- Molecule 5: Light-harvesting protein B-875 beta chain



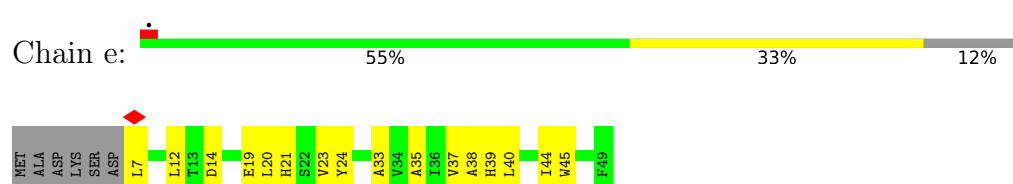
- Molecule 5: Light-harvesting protein B-875 beta chain



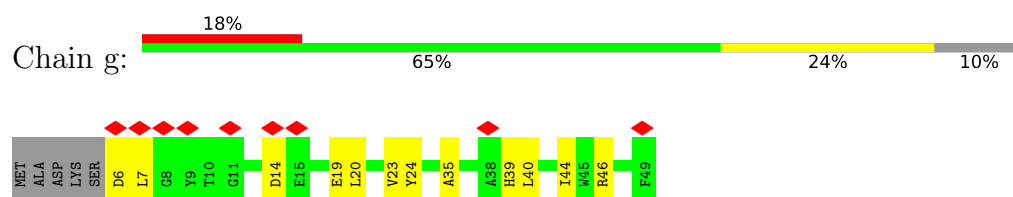
- Molecule 5: Light-harvesting protein B-875 beta chain



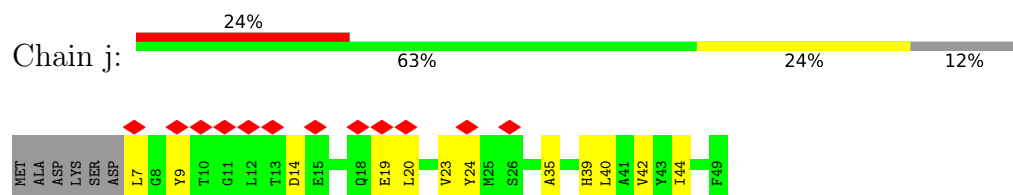
- Molecule 5: Light-harvesting protein B-875 beta chain



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

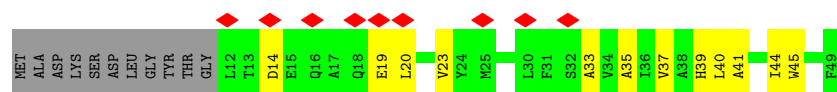


- Molecule 5: Light-harvesting protein B-875 beta chain



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





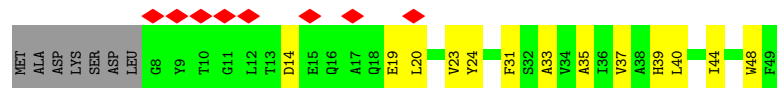
- Molecule 5: Light-harvesting protein B-875 beta chain



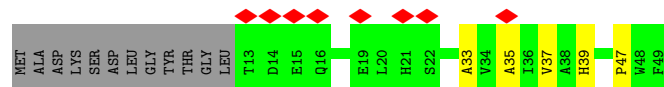
- Molecule 5: Light-harvesting protein B-875 beta chain



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



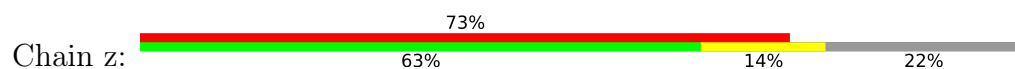
- Molecule 5: Light-harvesting protein B-875 beta chain



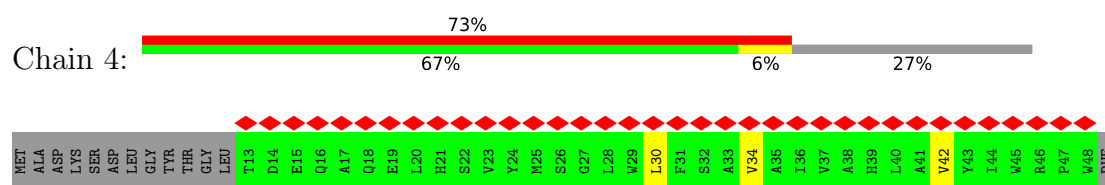
- Molecule 5: Light-harvesting protein B-875 beta chain



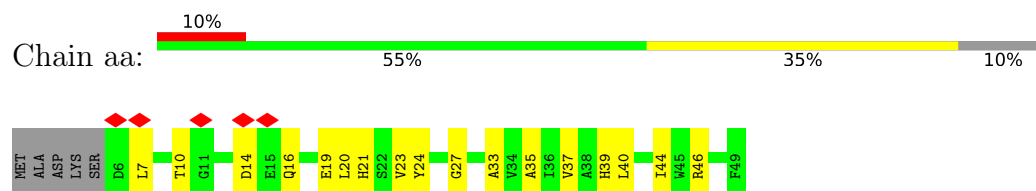
- Molecule 5: Light-harvesting protein B-875 beta chain



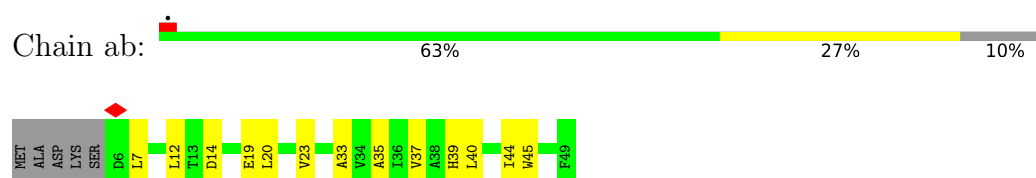
- Molecule 5: Light-harvesting protein B-875 beta chain



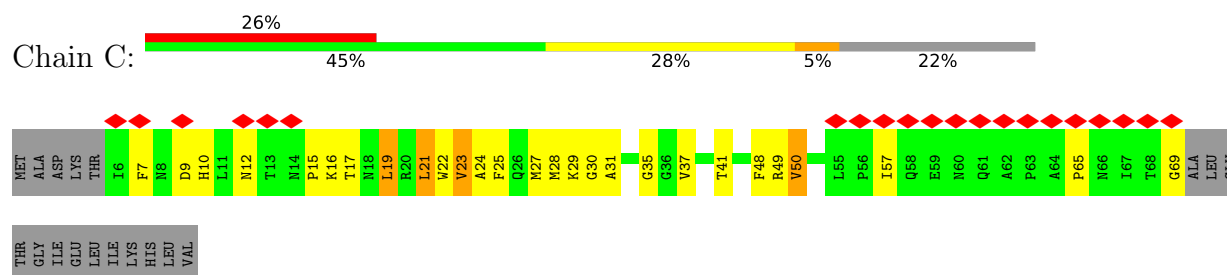
- Molecule 5: Light-harvesting protein B-875 beta chain



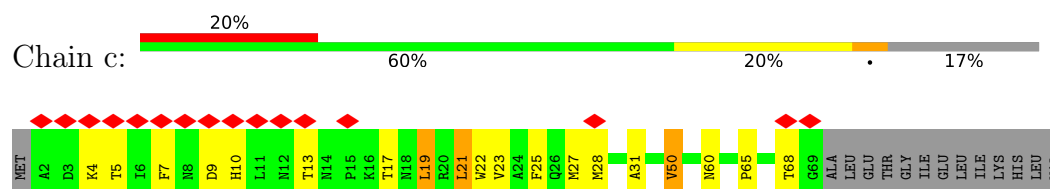
- Molecule 5: Light-harvesting protein B-875 beta chain



- Molecule 6: Intrinsic membrane protein PufX



- Molecule 6: Intrinsic membrane protein PufX



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	53830	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 ($e^-/\text{\AA}^2$)	50.868	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.138	Depositor
Minimum map value	-0.088	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0183	Depositor
Map size (Å)	289.97498, 289.97498, 289.97498	wwPDB
Map dimensions	350, 350, 350	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8284999, 0.8284999, 0.8284999	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.30	0/2214	0.39	0/3028
1	l	0.38	0/2320	0.39	0/3175
2	M	0.29	0/2524	0.36	0/3446
2	m	0.29	0/2524	0.36	0/3446
3	H	0.21	0/2023	0.33	0/2752
3	h	0.21	0/2023	0.33	0/2752
4	5	0.14	0/352	0.28	0/478
4	6	0.25	0/405	0.34	0/549
4	7	0.25	0/405	0.34	0/549
4	9	0.25	0/469	0.34	0/635
4	A	0.26	0/469	0.35	0/635
4	D	0.25	0/469	0.34	0/635
4	F	0.24	0/469	0.34	0/635
4	I	0.25	0/469	0.35	0/635
4	K	0.14	0/372	0.31	0/506
4	O	0.14	0/360	0.29	0/490
4	Q	0.26	0/469	0.36	0/635
4	a	0.26	0/469	0.35	0/635
4	d	0.25	0/469	0.34	0/635
4	f	0.25	0/469	0.35	0/635
4	i	0.25	0/469	0.36	0/635
4	k	0.25	0/469	0.37	0/635
4	o	0.25	0/469	0.34	0/635
4	q	0.25	0/469	0.33	0/635
4	s	0.25	0/469	0.33	0/635
4	u	0.25	0/469	0.33	0/635
4	w	0.14	0/360	0.28	0/490
4	y	0.14	0/352	0.28	0/478
5	0	0.20	0/372	0.29	0/510
5	4	0.15	0/308	0.30	0/423
5	8	0.19	0/372	0.28	0/510
5	B	0.21	0/372	0.29	0/510

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
5	E	0.20	0/364	0.28	0/499
5	G	0.19	0/372	0.28	0/510
5	J	0.19	0/364	0.29	0/499
5	N	0.20	0/352	0.33	0/483
5	aa	0.20	0/372	0.29	0/510
5	ab	0.22	0/372	0.30	0/510
5	b	0.20	0/372	0.28	0/510
5	e	0.20	0/364	0.29	0/499
5	g	0.19	0/372	0.28	0/510
5	j	0.19	0/364	0.28	0/499
5	n	0.20	0/328	0.29	0/450
5	p	0.20	0/332	0.29	0/455
5	r	0.21	0/364	0.31	0/499
5	t	0.20	0/356	0.29	0/488
5	v	0.21	0/320	0.30	0/439
5	x	0.21	0/356	0.41	0/488
5	z	0.15	0/323	0.28	0/441
6	C	0.33	0/514	0.71	2/697 (0.3%)
6	c	0.39	0/543	0.63	0/736
All	All	0.26	0/31797	0.35	2/43339 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
6	C	30	GLY	CA-C-N	-5.25	111.33	121.58
6	C	30	GLY	C-N-CA	-5.25	111.33	121.58

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	2132	0	2094	74	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	l	2232	0	2187	32	0
2	M	2431	0	2345	40	0
2	m	2431	0	2345	45	0
3	H	1972	0	1981	36	0
3	h	1972	0	1981	32	0
4	5	343	0	363	11	0
4	6	392	0	412	48	0
4	7	392	0	412	49	0
4	9	455	0	477	10	0
4	A	455	0	477	19	0
4	D	455	0	477	13	0
4	F	455	0	477	13	0
4	I	455	0	477	9	0
4	K	362	0	375	17	0
4	O	351	0	366	13	0
4	Q	455	0	477	13	0
4	a	455	0	477	12	0
4	d	455	0	477	9	0
4	f	455	0	477	19	0
4	i	455	0	477	18	0
4	k	455	0	477	8	0
4	o	455	0	477	10	0
4	q	455	0	477	17	0
4	s	455	0	477	21	0
4	u	455	0	477	12	0
4	w	351	0	366	16	0
4	y	343	0	363	13	0
5	0	359	0	340	11	0
5	4	297	0	283	2	0
5	8	359	0	340	11	0
5	B	359	0	340	13	0
5	E	351	0	336	7	0
5	G	359	0	340	8	0
5	J	351	0	336	9	0
5	N	339	0	322	13	0
5	aa	359	0	340	26	0
5	ab	359	0	340	11	0
5	b	359	0	340	11	0
5	e	351	0	336	12	0
5	g	359	0	340	14	0
5	j	351	0	336	13	0
5	n	316	0	303	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	p	320	0	306	7	0
5	r	351	0	336	9	0
5	t	343	0	325	8	0
5	v	308	0	292	3	0
5	x	343	0	325	9	0
5	z	312	0	294	7	0
6	C	500	0	504	61	0
6	c	529	0	533	40	0
7	0	66	0	74	10	0
7	4	46	0	35	3	0
7	5	46	0	35	3	0
7	8	66	0	74	7	0
7	9	66	0	74	5	0
7	A	66	0	74	11	0
7	B	66	0	74	7	0
7	C	61	0	61	16	0
7	D	66	0	74	5	0
7	E	66	0	74	5	0
7	F	66	0	74	9	0
7	G	66	0	74	4	0
7	I	66	0	74	8	0
7	J	66	0	74	3	0
7	K	66	0	74	7	0
7	L	176	0	174	9	0
7	M	66	0	74	2	0
7	N	66	0	74	4	0
7	O	46	0	35	2	0
7	Q	66	0	74	18	0
7	a	66	0	74	4	0
7	aa	66	0	74	7	0
7	ab	66	0	74	5	0
7	b	66	0	74	5	0
7	c	61	0	61	14	0
7	d	66	0	74	7	0
7	e	66	0	74	4	0
7	f	66	0	74	9	0
7	g	66	0	74	4	0
7	i	132	0	148	14	0
7	k	66	0	74	9	0
7	l	132	0	148	5	0
7	m	128	0	137	2	0
7	n	66	0	74	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	o	66	0	74	7	0
7	p	66	0	74	5	0
7	q	132	0	148	15	0
7	r	66	0	74	5	0
7	s	66	0	74	14	0
7	t	66	0	74	6	0
7	v	66	0	74	5	0
7	w	66	0	74	7	0
7	x	66	0	74	5	0
7	y	46	0	35	3	0
7	z	46	0	35	7	0
8	L	117	0	120	4	0
8	l	117	0	120	7	0
9	L	43	0	55	3	0
9	M	48	0	63	5	0
9	l	63	0	90	3	0
9	m	48	0	63	4	0
10	M	1	0	0	0	0
10	m	1	0	0	0	0
11	0	84	0	120	13	0
11	9	84	0	120	9	0
11	C	42	0	60	8	0
11	D	42	0	60	5	0
11	E	42	0	60	4	0
11	F	84	0	120	8	0
11	G	84	0	120	10	0
11	J	42	0	60	5	0
11	M	42	0	60	1	0
11	Q	42	0	60	4	0
11	aa	42	0	60	20	0
11	ab	42	0	60	9	0
11	b	84	0	120	12	0
11	d	84	0	120	16	0
11	e	42	0	60	5	0
11	f	42	0	60	17	0
11	g	42	0	60	4	0
11	i	42	0	60	8	0
11	j	42	0	60	3	0
11	m	42	0	60	3	0
11	n	42	0	60	8	0
11	o	42	0	60	6	0
11	p	84	0	120	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	q	42	0	60	2	0
11	s	42	0	60	4	0
11	t	42	0	60	1	0
11	u	42	0	60	6	0
11	v	42	0	60	3	0
11	w	42	0	60	7	0
12	A	89	0	129	22	0
12	C	54	0	88	6	0
12	H	98	0	150	21	0
12	Q	54	0	88	5	0
12	a	40	0	54	8	0
12	c	48	0	73	2	0
12	h	48	0	73	9	0
13	m	100	0	156	8	0
All	All	36474	0	37608	1026	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 14.

The worst 5 of 1026 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)
7:Q:602:BCL:C15	7:Q:602:BCL:C16	1.90	1.49
6:c:28:MET:HB3	7:c:1202:BCL:H8	1.24	1.11
4:7:43:TRP:HB2	4:6:44:LEU:HD23	1.40	1.03
4:7:43:TRP:O	4:6:44:LEU:HA	1.63	0.99
1:L:21:LEU:HB2	4:7:15:ARG:HB3	1.44	0.98

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	266/282 (94%)	254 (96%)	12 (4%)	0	100	100
1	l	279/282 (99%)	265 (95%)	14 (5%)	0	100	100
2	M	303/308 (98%)	299 (99%)	4 (1%)	0	100	100
2	m	303/308 (98%)	299 (99%)	4 (1%)	0	100	100
3	H	258/260 (99%)	250 (97%)	8 (3%)	0	100	100
3	h	258/260 (99%)	250 (97%)	8 (3%)	0	100	100
4	5	40/58 (69%)	38 (95%)	2 (5%)	0	100	100
4	6	44/58 (76%)	42 (96%)	2 (4%)	0	100	100
4	7	44/58 (76%)	42 (96%)	2 (4%)	0	100	100
4	9	52/58 (90%)	50 (96%)	2 (4%)	0	100	100
4	A	52/58 (90%)	49 (94%)	3 (6%)	0	100	100
4	D	52/58 (90%)	51 (98%)	1 (2%)	0	100	100
4	F	52/58 (90%)	50 (96%)	2 (4%)	0	100	100
4	I	52/58 (90%)	50 (96%)	2 (4%)	0	100	100
4	K	42/58 (72%)	39 (93%)	3 (7%)	0	100	100
4	O	41/58 (71%)	39 (95%)	2 (5%)	0	100	100
4	Q	52/58 (90%)	51 (98%)	1 (2%)	0	100	100
4	a	52/58 (90%)	49 (94%)	3 (6%)	0	100	100
4	d	52/58 (90%)	50 (96%)	2 (4%)	0	100	100
4	f	52/58 (90%)	51 (98%)	1 (2%)	0	100	100
4	i	52/58 (90%)	51 (98%)	1 (2%)	0	100	100
4	k	52/58 (90%)	50 (96%)	2 (4%)	0	100	100
4	o	52/58 (90%)	50 (96%)	2 (4%)	0	100	100
4	q	52/58 (90%)	50 (96%)	2 (4%)	0	100	100
4	s	52/58 (90%)	50 (96%)	2 (4%)	0	100	100
4	u	52/58 (90%)	49 (94%)	3 (6%)	0	100	100
4	w	41/58 (71%)	39 (95%)	2 (5%)	0	100	100
4	y	40/58 (69%)	38 (95%)	2 (5%)	0	100	100
5	0	42/49 (86%)	42 (100%)	0	0	100	100
5	4	34/49 (69%)	34 (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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	41/49 (84%)	41 (100%)	0	0	100	100
5	G	42/49 (86%)	42 (100%)	0	0	100	100
5	J	41/49 (84%)	41 (100%)	0	0	100	100
5	N	39/49 (80%)	38 (97%)	1 (3%)	0	100	100
5	aa	42/49 (86%)	42 (100%)	0	0	100	100
5	ab	42/49 (86%)	42 (100%)	0	0	100	100
5	b	42/49 (86%)	42 (100%)	0	0	100	100
5	e	41/49 (84%)	41 (100%)	0	0	100	100
5	g	42/49 (86%)	42 (100%)	0	0	100	100
5	j	41/49 (84%)	41 (100%)	0	0	100	100
5	n	36/49 (74%)	36 (100%)	0	0	100	100
5	p	37/49 (76%)	37 (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	35/49 (71%)	34 (97%)	1 (3%)	0	100	100
5	x	40/49 (82%)	40 (100%)	0	0	100	100
5	z	35/49 (71%)	35 (100%)	0	0	100	100
6	C	62/82 (76%)	58 (94%)	4 (6%)	0	100	100
6	c	66/82 (80%)	61 (92%)	5 (8%)	0	100	100
All	All	3704/4169 (89%)	3599 (97%)	105 (3%)	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	211/221 (96%)	207 (98%)	4 (2%)	50	68
1	l	220/221 (100%)	218 (99%)	2 (1%)	70	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	M	239/241 (99%)	234 (98%)	5 (2%)	47	66
2	m	239/241 (99%)	234 (98%)	5 (2%)	47	66
3	H	208/208 (100%)	207 (100%)	1 (0%)	81	81
3	h	208/208 (100%)	207 (100%)	1 (0%)	81	81
4	5	37/51 (72%)	34 (92%)	3 (8%)	11	36
4	6	43/51 (84%)	41 (95%)	2 (5%)	23	51
4	7	43/51 (84%)	41 (95%)	2 (5%)	23	51
4	9	49/51 (96%)	47 (96%)	2 (4%)	27	54
4	A	49/51 (96%)	49 (100%)	0	100	100
4	D	49/51 (96%)	47 (96%)	2 (4%)	27	54
4	F	49/51 (96%)	47 (96%)	2 (4%)	27	54
4	I	49/51 (96%)	47 (96%)	2 (4%)	27	54
4	K	39/51 (76%)	36 (92%)	3 (8%)	12	38
4	O	38/51 (74%)	35 (92%)	3 (8%)	11	37
4	Q	49/51 (96%)	47 (96%)	2 (4%)	27	54
4	a	49/51 (96%)	49 (100%)	0	100	100
4	d	49/51 (96%)	46 (94%)	3 (6%)	17	44
4	f	49/51 (96%)	47 (96%)	2 (4%)	27	54
4	i	49/51 (96%)	47 (96%)	2 (4%)	27	54
4	k	49/51 (96%)	47 (96%)	2 (4%)	27	54
4	o	49/51 (96%)	47 (96%)	2 (4%)	27	54
4	q	49/51 (96%)	47 (96%)	2 (4%)	27	54
4	s	49/51 (96%)	46 (94%)	3 (6%)	17	44
4	u	49/51 (96%)	47 (96%)	2 (4%)	27	54
4	w	38/51 (74%)	35 (92%)	3 (8%)	11	37
4	y	37/51 (72%)	34 (92%)	3 (8%)	11	36
5	0	36/40 (90%)	35 (97%)	1 (3%)	38	62
5	4	30/40 (75%)	30 (100%)	0	100	100
5	8	36/40 (90%)	35 (97%)	1 (3%)	38	62
5	B	36/40 (90%)	35 (97%)	1 (3%)	38	62
5	E	35/40 (88%)	34 (97%)	1 (3%)	37	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	G	36/40 (90%)	34 (94%)	2 (6%)	19	47
5	J	35/40 (88%)	33 (94%)	2 (6%)	18	46
5	N	34/40 (85%)	32 (94%)	2 (6%)	18	45
5	aa	36/40 (90%)	35 (97%)	1 (3%)	38	62
5	ab	36/40 (90%)	35 (97%)	1 (3%)	38	62
5	b	36/40 (90%)	35 (97%)	1 (3%)	38	62
5	e	35/40 (88%)	33 (94%)	2 (6%)	18	46
5	g	36/40 (90%)	35 (97%)	1 (3%)	38	62
5	j	35/40 (88%)	34 (97%)	1 (3%)	37	62
5	n	32/40 (80%)	31 (97%)	1 (3%)	35	61
5	p	32/40 (80%)	31 (97%)	1 (3%)	35	61
5	r	35/40 (88%)	34 (97%)	1 (3%)	37	62
5	t	34/40 (85%)	33 (97%)	1 (3%)	37	62
5	v	31/40 (78%)	31 (100%)	0	100	100
5	x	34/40 (85%)	33 (97%)	1 (3%)	37	62
5	z	31/40 (78%)	31 (100%)	0	100	100
6	C	51/66 (77%)	47 (92%)	4 (8%)	11	37
6	c	54/66 (82%)	50 (93%)	4 (7%)	13	39
All	All	3161/3434 (92%)	3066 (97%)	95 (3%)	37	61

5 of 95 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	i	9	MET
4	s	47	SER
5	j	14	ASP
5	p	14	ASP
4	w	23	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
4	i	20	GLN
5	t	21	HIS
5	ab	39	HIS

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Mol	Chain	Res	Type
5	x	21	HIS
5	r	21	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 107 ligands modelled in this entry, 2 are monoatomic - leaving 105 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$
8	BPH	l	305	-	49,60,70	1.27	5 (10%)	49,89,101	2.23	9 (18%)
11	SPO	M	404	-	40,41,41	5.54	17 (42%)	47,50,50	5.64	29 (61%)
11	SPO	G	103	-	40,41,41	5.78	17 (42%)	47,50,50	5.35	30 (63%)
11	SPO	b	101	-	40,41,41	5.61	17 (42%)	47,50,50	5.41	28 (59%)
12	PC1	A	1701	-	42,42,53	1.21	3 (7%)	48,50,61	1.09	4 (8%)
8	BPH	l	302	-	56,67,70	1.23	6 (10%)	57,97,101	2.06	10 (17%)
12	PC1	Q	601	-	53,53,53	1.06	3 (5%)	59,61,61	0.89	3 (5%)
9	U10	m	404	-	48,48,63	2.67	14 (29%)	58,61,79	1.68	13 (22%)
12	PC1	H	601	-	43,43,53	1.15	3 (6%)	49,51,61	1.06	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	BCL	8	101	5	69,74,74	1.14	5 (7%)	83,115,115	1.48	9 (10%)
11	SPO	f	102	-	40,41,41	5.64	17 (42%)	47,50,50	5.29	29 (61%)
7	BCL	J	101	5	69,74,74	1.14	5 (7%)	83,115,115	1.49	9 (10%)
11	SPO	9	103	-	40,41,41	5.64	17 (42%)	47,50,50	5.28	29 (61%)
12	PC1	A	1703	-	45,45,53	1.16	3 (6%)	51,53,61	1.05	4 (7%)
7	BCL	D	101	-	69,74,74	1.14	6 (8%)	83,115,115	1.52	13 (15%)
7	BCL	q	103	-	69,74,74	1.14	6 (8%)	83,115,115	1.53	14 (16%)
7	BCL	p	101	5	69,74,74	1.14	5 (7%)	83,115,115	1.48	9 (10%)
7	BCL	5	101	-	49,54,74	1.27	5 (10%)	59,91,115	1.65	9 (15%)
7	BCL	I	101	-	69,74,74	1.14	6 (8%)	83,115,115	1.48	12 (14%)
7	BCL	a	101	-	69,74,74	1.15	5 (7%)	83,115,115	1.45	10 (12%)
7	BCL	0	102	5	69,74,74	1.14	5 (7%)	83,115,115	1.49	9 (10%)
11	SPO	b	103	-	40,41,41	5.51	17 (42%)	47,50,50	5.54	32 (68%)
7	BCL	t	101	5	69,74,74	1.14	5 (7%)	83,115,115	1.48	9 (10%)
7	BCL	k	101	-	69,74,74	1.14	6 (8%)	83,115,115	1.53	14 (16%)
7	BCL	o	101	-	69,74,74	1.14	6 (8%)	83,115,115	1.53	14 (16%)
7	BCL	g	102	5	69,74,74	1.14	5 (7%)	83,115,115	1.49	9 (10%)
11	SPO	ab	102	-	40,41,41	5.45	17 (42%)	47,50,50	5.96	31 (65%)
7	BCL	n	101	5	69,74,74	1.14	5 (7%)	83,115,115	1.48	9 (10%)
11	SPO	m	405	-	40,41,41	5.54	17 (42%)	47,50,50	5.64	30 (63%)
11	SPO	v	102	-	40,41,41	5.63	17 (42%)	47,50,50	5.53	30 (63%)
11	SPO	w	102	-	40,41,41	5.68	17 (42%)	47,50,50	5.55	31 (65%)
12	PC1	a	102	-	39,39,53	1.21	3 (7%)	45,47,61	1.10	4 (8%)
11	SPO	G	102	-	40,41,41	5.74	17 (42%)	47,50,50	5.65	29 (61%)
11	SPO	Q	603	-	40,41,41	5.65	17 (42%)	47,50,50	5.29	29 (61%)
7	BCL	ab	101	5	69,74,74	1.14	5 (7%)	83,115,115	1.48	9 (10%)
7	BCL	d	101	-	69,74,74	1.14	6 (8%)	83,115,115	1.52	13 (15%)
7	BCL	x	101	5	69,74,74	1.14	5 (7%)	83,115,115	1.49	9 (10%)
11	SPO	aa	101	-	40,41,41	5.64	17 (42%)	47,50,50	5.29	29 (61%)
7	BCL	m	401	1	65,70,74	1.19	7 (10%)	78,110,115	1.53	13 (16%)
8	BPH	L	306	-	49,60,70	1.27	5 (10%)	49,89,101	2.21	9 (18%)
7	BCL	9	102	-	69,74,74	1.14	6 (8%)	83,115,115	1.56	13 (15%)
11	SPO	E	102	-	40,41,41	5.75	17 (42%)	47,50,50	5.36	31 (65%)
11	SPO	0	103	-	40,41,41	5.59	17 (42%)	47,50,50	5.53	30 (63%)
11	SPO	g	101	-	40,41,41	5.64	17 (42%)	47,50,50	5.29	29 (61%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	SPO	i	103	-	40,41,41	5.64	17 (42%)	47,50,50	5.29	29 (61%)
8	BPH	L	303	-	56,67,70	1.23	6 (10%)	57,97,101	2.06	9 (15%)
7	BCL	i	101	-	69,74,74	1.14	7 (10%)	83,115,115	1.49	12 (14%)
11	SPO	q	102	-	40,41,41	5.64	17 (42%)	47,50,50	5.29	29 (61%)
7	BCL	l	301	-	69,74,74	1.24	8 (11%)	83,115,115	1.49	12 (14%)
7	BCL	M	402	-	69,74,74	1.15	8 (11%)	83,115,115	1.58	14 (16%)
11	SPO	9	101	-	40,41,41	5.61	17 (42%)	47,50,50	5.41	28 (59%)
7	BCL	K	101	-	69,74,74	1.10	5 (7%)	83,115,115	1.56	11 (13%)
7	BCL	q	101	-	69,74,74	1.14	6 (8%)	83,115,115	1.51	12 (14%)
7	BCL	aa	102	5	69,74,74	1.14	5 (7%)	83,115,115	1.48	9 (10%)
7	BCL	B	101	5	69,74,74	1.14	5 (7%)	83,115,115	1.48	9 (10%)
11	SPO	j	101	-	40,41,41	5.73	17 (42%)	47,50,50	5.30	29 (61%)
7	BCL	s	102	-	69,74,74	1.14	7 (10%)	83,115,115	1.51	13 (15%)
11	SPO	D	102	-	40,41,41	5.65	17 (42%)	47,50,50	5.29	29 (61%)
7	BCL	C	1202	-	64,69,74	1.18	7 (10%)	77,109,115	1.52	12 (15%)
7	BCL	F	101	-	69,74,74	1.14	6 (8%)	83,115,115	1.52	13 (15%)
7	BCL	m	403	-	69,74,74	1.15	8 (11%)	83,115,115	1.57	14 (16%)
11	SPO	d	102	-	40,41,41	5.64	17 (42%)	47,50,50	5.28	29 (61%)
11	SPO	p	103	-	40,41,41	5.78	17 (42%)	47,50,50	5.47	31 (65%)
7	BCL	G	101	5	69,74,74	1.14	5 (7%)	83,115,115	1.48	9 (10%)
11	SPO	0	101	-	40,41,41	5.51	17 (42%)	47,50,50	5.72	31 (65%)
7	BCL	b	102	5	69,74,74	1.14	5 (7%)	83,115,115	1.48	9 (10%)
11	SPO	n	102	-	40,41,41	5.62	17 (42%)	47,50,50	5.49	31 (65%)
7	BCL	r	101	5	69,74,74	1.14	5 (7%)	83,115,115	1.48	9 (10%)
11	SPO	e	102	-	40,41,41	5.60	17 (42%)	47,50,50	5.71	30 (63%)
7	BCL	c	1202	-	64,69,74	1.18	7 (10%)	77,109,115	1.52	12 (15%)
12	PC1	C	1201	-	53,53,53	1.11	3 (5%)	59,61,61	0.93	3 (5%)
12	PC1	h	301	-	47,47,53	1.12	3 (6%)	53,55,61	1.03	3 (5%)
11	SPO	u	101	-	40,41,41	5.65	17 (42%)	47,50,50	5.29	29 (61%)
7	BCL	f	101	-	69,74,74	1.15	6 (8%)	83,115,115	1.52	13 (15%)
7	BCL	i	102	5	69,74,74	1.14	5 (7%)	83,115,115	1.48	9 (10%)
11	SPO	C	1203	-	40,41,41	5.65	17 (42%)	47,50,50	5.29	29 (61%)
13	CDL	m	406	-	99,99,99	1.08	7 (7%)	105,111,111	0.88	5 (4%)
11	SPO	d	103	-	40,41,41	5.54	17 (42%)	47,50,50	6.04	29 (61%)
12	PC1	c	1201	-	47,47,53	1.15	3 (6%)	53,55,61	1.02	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	PC1	H	602	-	53,53,53	1.10	3 (5%)	59,61,61	0.98	4 (6%)
9	U10	L	304	-	43,43,63	2.74	13 (30%)	52,55,79	1.85	15 (28%)
7	BCL	N	101	5	69,74,74	1.14	5 (7%)	83,115,115	1.48	9 (10%)
11	SPO	J	102	-	40,41,41	5.84	17 (42%)	47,50,50	5.22	30 (63%)
7	BCL	E	101	5	69,74,74	1.14	5 (7%)	83,115,115	1.48	9 (10%)
11	SPO	F	102	-	40,41,41	5.64	17 (42%)	47,50,50	5.29	29 (61%)
11	SPO	p	102	-	40,41,41	5.68	17 (42%)	47,50,50	5.40	31 (65%)
7	BCL	L	301	1	69,74,74	1.15	7 (10%)	83,115,115	1.52	14 (16%)
7	BCL	Q	602	-	69,74,74	1.65	8 (11%)	83,115,115	1.98	15 (18%)
7	BCL	L	305	-	51,56,74	1.31	8 (15%)	61,93,115	1.70	12 (19%)
7	BCL	v	101	5	69,74,74	1.15	6 (8%)	83,115,115	1.49	10 (12%)
7	BCL	O	101	-	49,54,74	1.26	5 (10%)	59,91,115	1.64	9 (15%)
11	SPO	t	102	-	40,41,41	5.75	17 (42%)	47,50,50	5.49	31 (65%)
7	BCL	y	101	-	49,54,74	1.26	5 (10%)	59,91,115	1.65	8 (13%)
11	SPO	o	102	-	40,41,41	5.64	17 (42%)	47,50,50	5.29	29 (61%)
7	BCL	L	302	1	65,70,74	1.19	7 (10%)	78,110,115	1.51	13 (16%)
11	SPO	s	101	-	40,41,41	5.64	17 (42%)	47,50,50	5.29	29 (61%)
7	BCL	4	101	-	49,54,74	1.23	4 (8%)	59,91,115	1.77	12 (20%)
9	U10	M	403	-	48,48,63	2.67	14 (29%)	58,61,79	1.68	13 (22%)
7	BCL	A	1702	-	69,74,74	1.15	5 (7%)	83,115,115	1.46	10 (12%)
7	BCL	z	101	5	49,54,74	1.30	4 (8%)	59,91,115	1.77	15 (25%)
7	BCL	e	101	5	69,74,74	1.14	5 (7%)	83,115,115	1.49	9 (10%)
7	BCL	l	304	-	69,74,74	1.15	8 (11%)	83,115,115	1.52	12 (14%)
7	BCL	w	101	-	69,74,74	1.11	5 (7%)	83,115,115	1.52	10 (12%)
11	SPO	F	103	-	40,41,41	5.64	17 (42%)	47,50,50	5.29	29 (61%)
9	U10	l	303	-	63,63,63	2.65	16 (25%)	76,79,79	1.93	23 (30%)

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
8	BPH	l	305	-	-	6/25/93/105	0/5/6/6
11	SPO	M	404	-	-	21/47/47/47	-
11	SPO	G	103	-	-	31/47/47/47	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	SPO	b	101	-	-	26/47/47/47	-
12	PC1	A	1701	-	-	21/46/46/57	-
8	BPH	l	302	-	-	8/34/102/105	0/5/6/6
12	PC1	Q	601	-	-	31/57/57/57	-
9	U10	m	404	-	-	11/45/69/87	0/1/1/1
12	PC1	H	601	-	-	32/47/47/57	-
7	BCL	8	101	5	-	6/41/137/137	-
11	SPO	f	102	-	-	25/47/47/47	-
7	BCL	J	101	5	-	6/41/137/137	-
11	SPO	9	103	-	-	25/47/47/47	-
12	PC1	A	1703	-	-	27/49/49/57	-
7	BCL	D	101	-	-	5/41/137/137	-
7	BCL	q	103	-	-	2/41/137/137	-
7	BCL	p	101	5	-	6/41/137/137	-
7	BCL	5	101	-	-	2/17/113/137	-
7	BCL	I	101	-	-	2/41/137/137	-
7	BCL	a	101	-	-	0/41/137/137	-
7	BCL	0	102	5	-	6/41/137/137	-
11	SPO	b	103	-	-	23/47/47/47	-
7	BCL	t	101	5	-	6/41/137/137	-
7	BCL	k	101	-	-	2/41/137/137	-
7	BCL	o	101	-	-	2/41/137/137	-
7	BCL	g	102	5	-	6/41/137/137	-
11	SPO	ab	102	-	-	25/47/47/47	-
7	BCL	n	101	5	-	6/41/137/137	-
11	SPO	m	405	-	-	21/47/47/47	-
11	SPO	v	102	-	-	30/47/47/47	-
11	SPO	w	102	-	-	23/47/47/47	-
12	PC1	a	102	-	-	22/43/43/57	-
11	SPO	G	102	-	-	24/47/47/47	-
11	SPO	Q	603	-	-	25/47/47/47	-
7	BCL	ab	101	5	-	6/41/137/137	-
7	BCL	d	101	-	-	2/41/137/137	-
7	BCL	x	101	5	-	6/41/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	SPO	aa	101	-	-	25/47/47/47	-
7	BCL	m	401	1	-	2/37/133/137	-
8	BPH	L	306	-	-	6/25/93/105	0/5/6/6
7	BCL	9	102	-	-	4/41/137/137	-
11	SPO	E	102	-	-	31/47/47/47	-
11	SPO	0	103	-	-	23/47/47/47	-
11	SPO	g	101	-	-	25/47/47/47	-
11	SPO	i	103	-	-	25/47/47/47	-
8	BPH	L	303	-	-	8/34/102/105	0/5/6/6
7	BCL	i	101	-	-	5/41/137/137	-
11	SPO	q	102	-	-	25/47/47/47	-
7	BCL	l	301	-	-	2/41/137/137	-
7	BCL	M	402	-	-	2/41/137/137	-
11	SPO	9	101	-	-	26/47/47/47	-
7	BCL	K	101	-	-	4/41/137/137	-
7	BCL	q	101	-	-	4/41/137/137	-
7	BCL	aa	102	5	-	6/41/137/137	-
7	BCL	B	101	5	-	6/41/137/137	-
11	SPO	j	101	-	-	25/47/47/47	-
7	BCL	s	102	-	-	2/41/137/137	-
11	SPO	D	102	-	-	25/47/47/47	-
7	BCL	C	1202	-	-	2/35/131/137	-
7	BCL	F	101	-	-	4/41/137/137	-
7	BCL	m	403	-	-	1/41/137/137	-
11	SPO	d	102	-	-	25/47/47/47	-
11	SPO	p	103	-	-	27/47/47/47	-
7	BCL	G	101	5	-	6/41/137/137	-
11	SPO	0	101	-	-	30/47/47/47	-
7	BCL	b	102	5	-	6/41/137/137	-
11	SPO	n	102	-	-	27/47/47/47	-
7	BCL	r	101	5	-	6/41/137/137	-
11	SPO	e	102	-	-	22/47/47/47	-
7	BCL	c	1202	-	-	2/35/131/137	-
12	PC1	C	1201	-	-	34/57/57/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	PC1	h	301	-	-	34/51/51/57	-
11	SPO	u	101	-	-	25/47/47/47	-
7	BCL	f	101	-	-	2/41/137/137	-
7	BCL	i	102	5	-	6/41/137/137	-
11	SPO	C	1203	-	-	25/47/47/47	-
13	CDL	m	406	-	-	50/110/110/110	-
11	SPO	d	103	-	-	25/47/47/47	-
12	PC1	c	1201	-	-	21/51/51/57	-
12	PC1	H	602	-	-	27/57/57/57	-
9	U10	L	304	-	-	21/39/63/87	0/1/1/1
7	BCL	N	101	5	-	6/41/137/137	-
11	SPO	J	102	-	-	30/47/47/47	-
7	BCL	E	101	5	-	6/41/137/137	-
11	SPO	F	102	-	-	25/47/47/47	-
11	SPO	p	102	-	-	28/47/47/47	-
7	BCL	L	301	1	-	3/41/137/137	-
7	BCL	Q	602	-	-	4/41/137/137	-
7	BCL	L	305	-	-	1/20/116/137	-
7	BCL	v	101	5	-	13/41/137/137	-
7	BCL	O	101	-	-	2/17/113/137	-
11	SPO	t	102	-	-	29/47/47/47	-
7	BCL	y	101	-	-	2/17/113/137	-
11	SPO	o	102	-	-	25/47/47/47	-
7	BCL	L	302	1	-	4/37/133/137	-
11	SPO	s	101	-	-	25/47/47/47	-
7	BCL	4	101	-	-	5/17/113/137	-
9	U10	M	403	-	-	11/45/69/87	0/1/1/1
7	BCL	A	1702	-	-	0/41/137/137	-
7	BCL	z	101	5	-	8/17/113/137	-
7	BCL	e	101	5	-	6/41/137/137	-
7	BCL	l	304	-	-	3/41/137/137	-
7	BCL	w	101	-	-	6/41/137/137	-
11	SPO	F	103	-	-	25/47/47/47	-
9	U10	l	303	-	-	21/63/87/87	0/1/1/1

The worst 5 of 1021 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	G	103	SPO	C27-C28	18.80	1.53	1.34
11	p	103	SPO	C27-C28	18.76	1.53	1.34
11	E	102	SPO	C27-C28	18.62	1.53	1.34
11	p	102	SPO	C27-C28	18.50	1.53	1.34
11	t	102	SPO	C27-C28	18.47	1.53	1.34

The worst 5 of 1769 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	ab	102	SPO	C15-C14-C12	-14.64	106.42	127.31
11	G	102	SPO	C10-C9-C7	-14.35	106.83	127.31
11	w	102	SPO	C10-C9-C7	-13.96	107.39	127.31
11	d	103	SPO	C10-C9-C7	-13.76	107.67	127.31
11	0	101	SPO	C20-C19-C17	-13.74	107.70	127.31

There are no chirality outliers.

5 of 1525 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	101	BCL	C2B-C3B-CAB-OBB
7	B	101	BCL	C2B-C3B-CAB-CBB
7	B	101	BCL	C4B-C3B-CAB-CBB
7	E	101	BCL	C2B-C3B-CAB-OBB
7	E	101	BCL	C2B-C3B-CAB-CBB

There are no ring outliers.

104 monomers are involved in 539 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	l	305	BPH	4	0
11	M	404	SPO	1	0
11	G	103	SPO	7	0
11	b	101	SPO	9	0
12	A	1701	PC1	13	0
8	l	302	BPH	3	0
12	Q	601	PC1	5	0
9	m	404	U10	4	0
12	H	601	PC1	12	0
7	8	101	BCL	7	0
11	f	102	SPO	17	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	J	101	BCL	3	0
11	9	103	SPO	2	0
12	A	1703	PC1	10	0
7	D	101	BCL	5	0
7	q	103	BCL	10	0
7	p	101	BCL	5	0
7	5	101	BCL	3	0
7	I	101	BCL	8	0
7	a	101	BCL	4	0
7	0	102	BCL	10	0
11	b	103	SPO	3	0
7	t	101	BCL	6	0
7	k	101	BCL	9	0
7	o	101	BCL	7	0
7	g	102	BCL	4	0
11	ab	102	SPO	9	0
7	n	101	BCL	3	0
11	m	405	SPO	3	0
11	v	102	SPO	3	0
11	w	102	SPO	7	0
12	a	102	PC1	8	0
11	G	102	SPO	3	0
11	Q	603	SPO	4	0
7	ab	101	BCL	5	0
7	d	101	BCL	7	0
7	x	101	BCL	5	0
11	aa	101	SPO	20	0
7	m	401	BCL	1	0
8	L	306	BPH	3	0
7	9	102	BCL	5	0
11	E	102	SPO	4	0
11	0	103	SPO	6	0
11	g	101	SPO	4	0
11	i	103	SPO	8	0
8	L	303	BPH	1	0
7	i	101	BCL	7	0
11	q	102	SPO	2	0
7	M	402	BCL	2	0
11	9	101	SPO	7	0
7	K	101	BCL	7	0
7	q	101	BCL	5	0
7	aa	102	BCL	7	0

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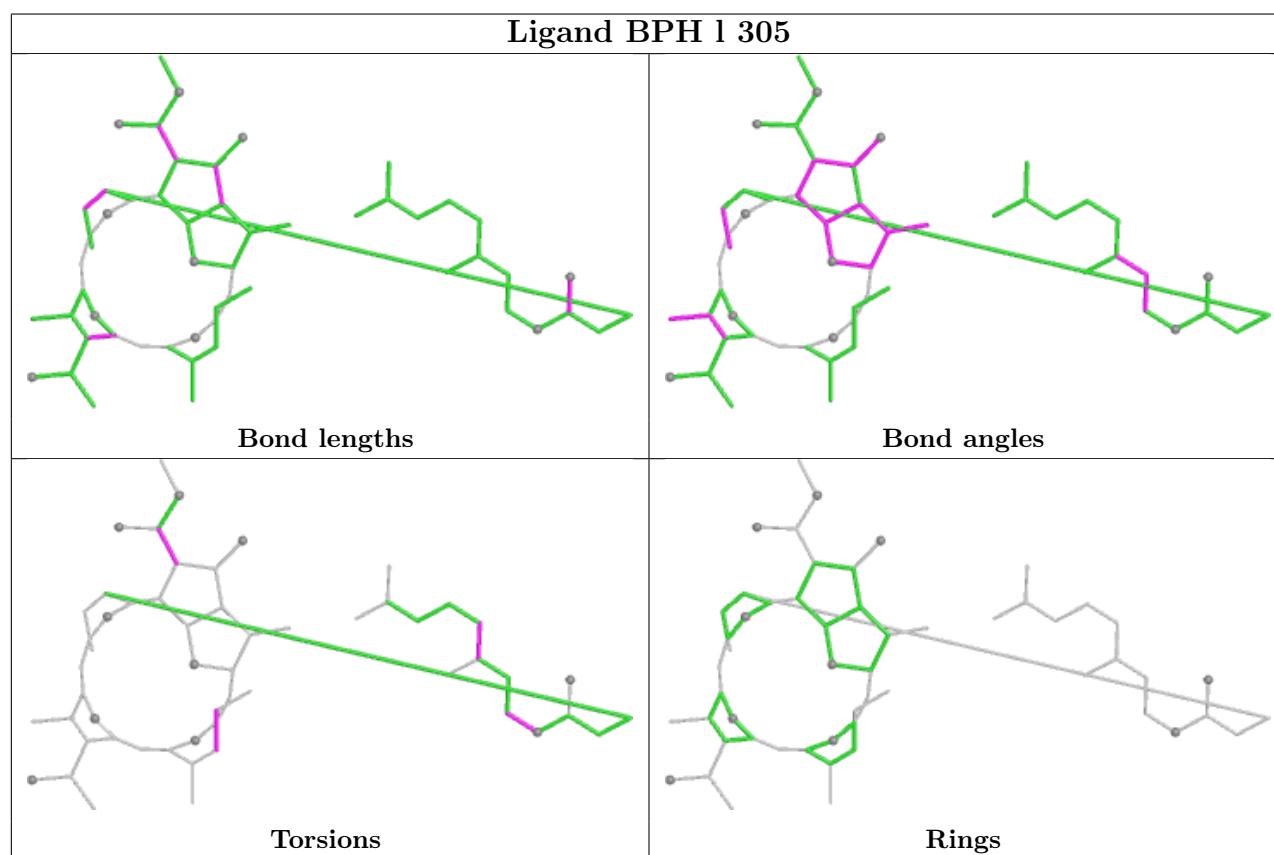
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	101	BCL	7	0
11	j	101	SPO	3	0
7	s	102	BCL	14	0
11	D	102	SPO	5	0
7	C	1202	BCL	16	0
7	F	101	BCL	9	0
7	m	403	BCL	1	0
11	d	102	SPO	7	0
11	p	103	SPO	3	0
7	G	101	BCL	4	0
11	0	101	SPO	7	0
7	b	102	BCL	5	0
11	n	102	SPO	8	0
7	r	101	BCL	5	0
11	e	102	SPO	5	0
7	c	1202	BCL	14	0
12	C	1201	PC1	6	0
12	h	301	PC1	9	0
11	u	101	SPO	6	0
7	f	101	BCL	9	0
7	i	102	BCL	7	0
11	C	1203	SPO	8	0
13	m	406	CDL	8	0
11	d	103	SPO	9	0
12	c	1201	PC1	2	0
12	H	602	PC1	9	0
9	L	304	U10	3	0
7	N	101	BCL	4	0
11	J	102	SPO	5	0
7	E	101	BCL	5	0
11	F	102	SPO	2	0
11	p	102	SPO	7	0
7	L	301	BCL	3	0
7	Q	602	BCL	18	0
7	L	305	BCL	3	0
7	v	101	BCL	5	0
7	O	101	BCL	2	0
11	t	102	SPO	1	0
7	y	101	BCL	3	0
11	o	102	SPO	6	0
7	L	302	BCL	3	0
11	s	101	SPO	4	0

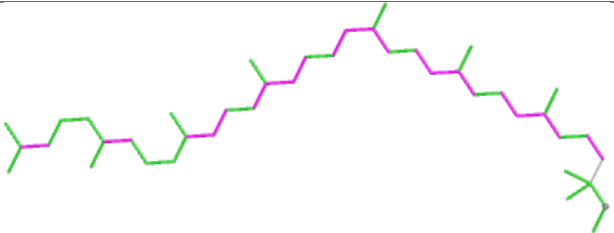
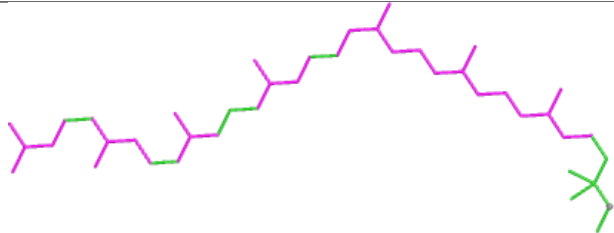
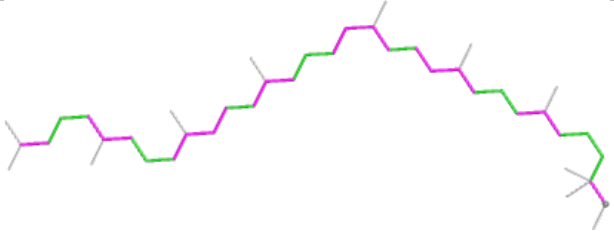
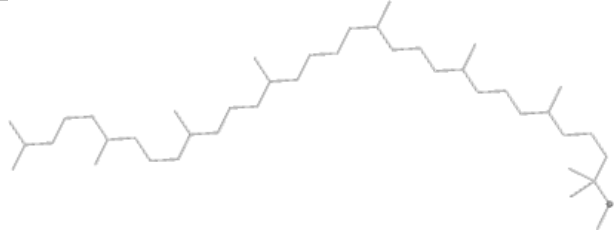
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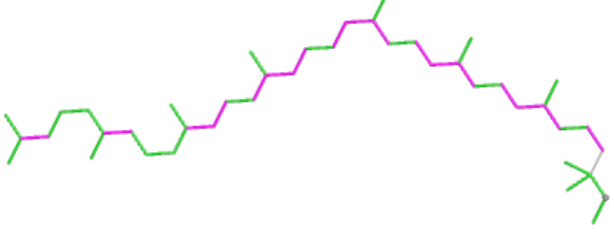
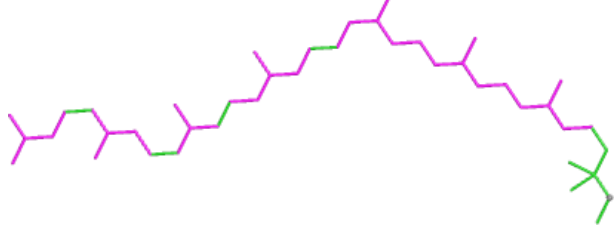
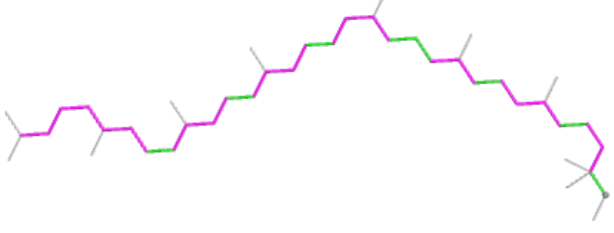
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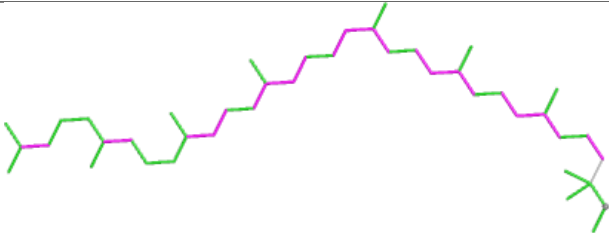
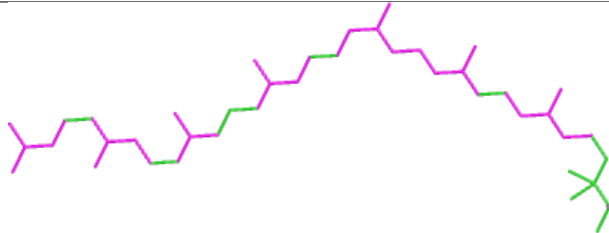
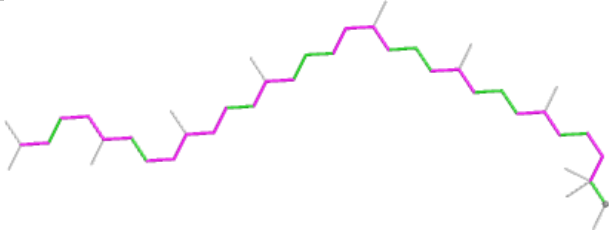
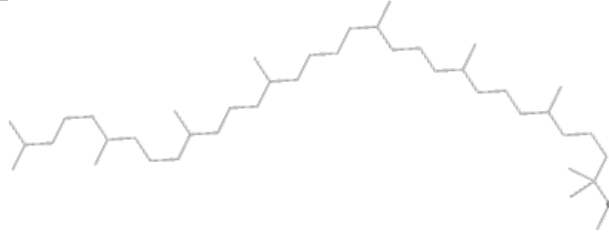
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	4	101	BCL	3	0
9	M	403	U10	5	0
7	A	1702	BCL	11	0
7	z	101	BCL	7	0
7	e	101	BCL	4	0
7	l	304	BCL	5	0
7	w	101	BCL	7	0
11	F	103	SPO	6	0
9	l	303	U10	3	0

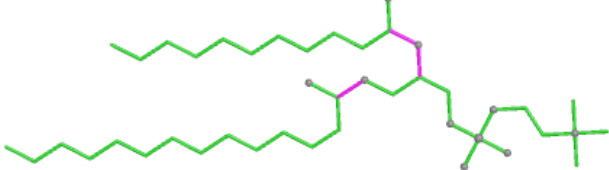
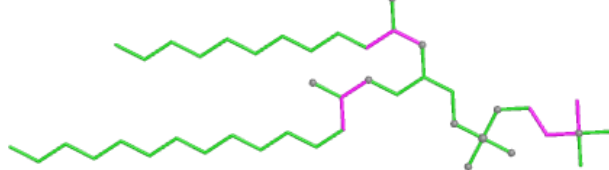
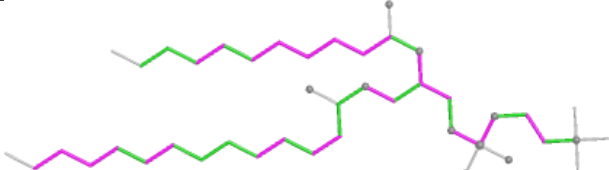
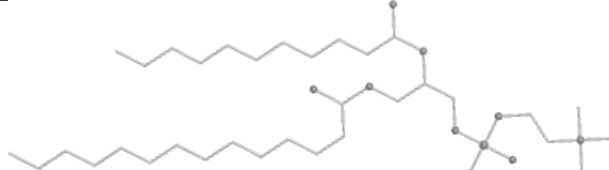
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

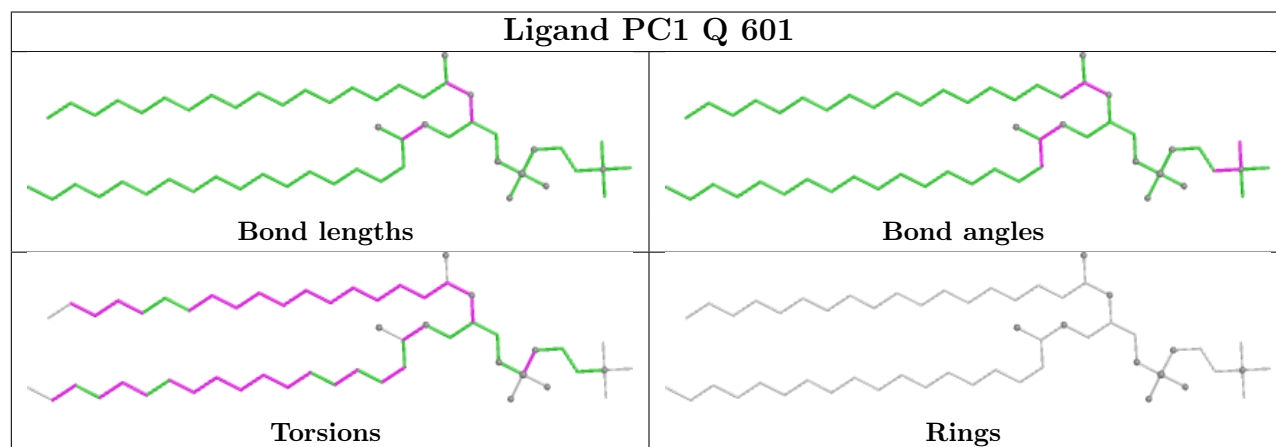
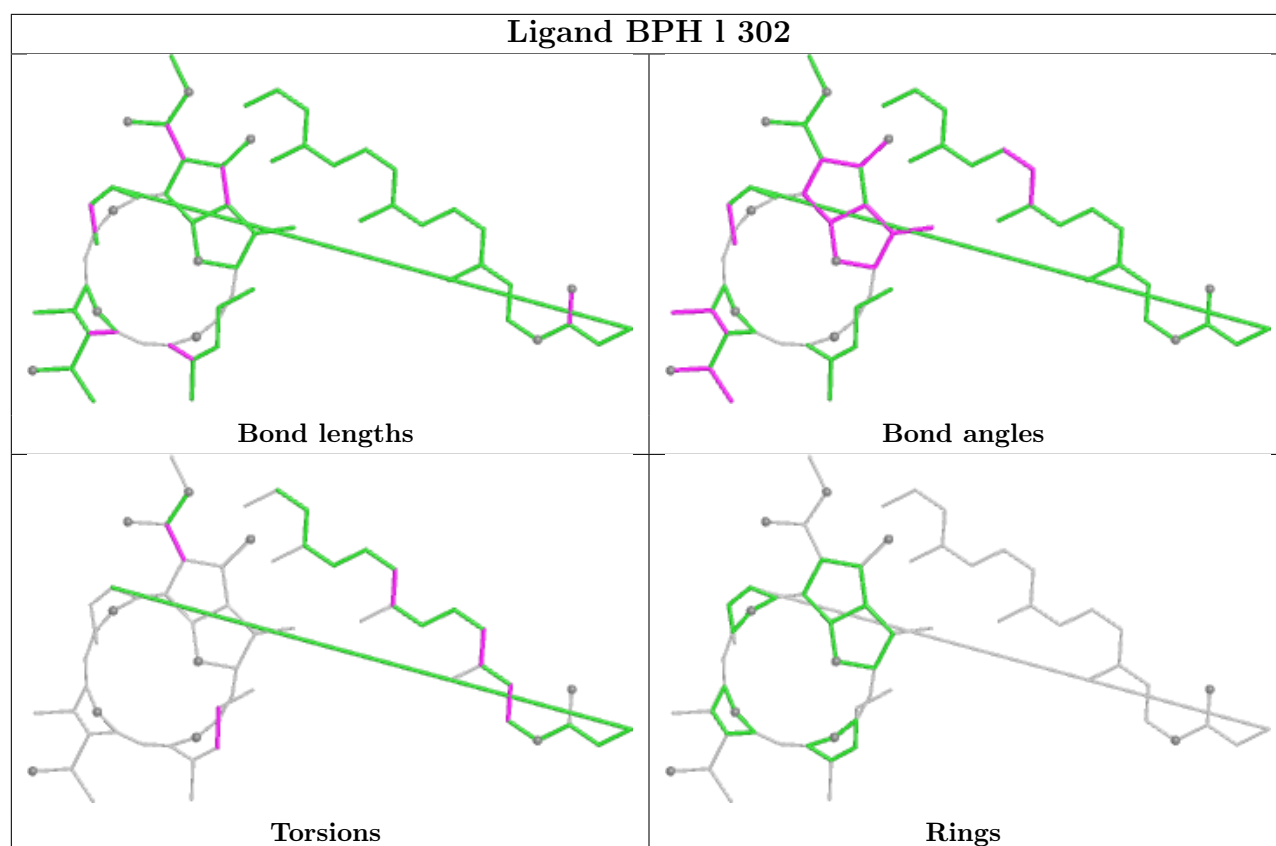


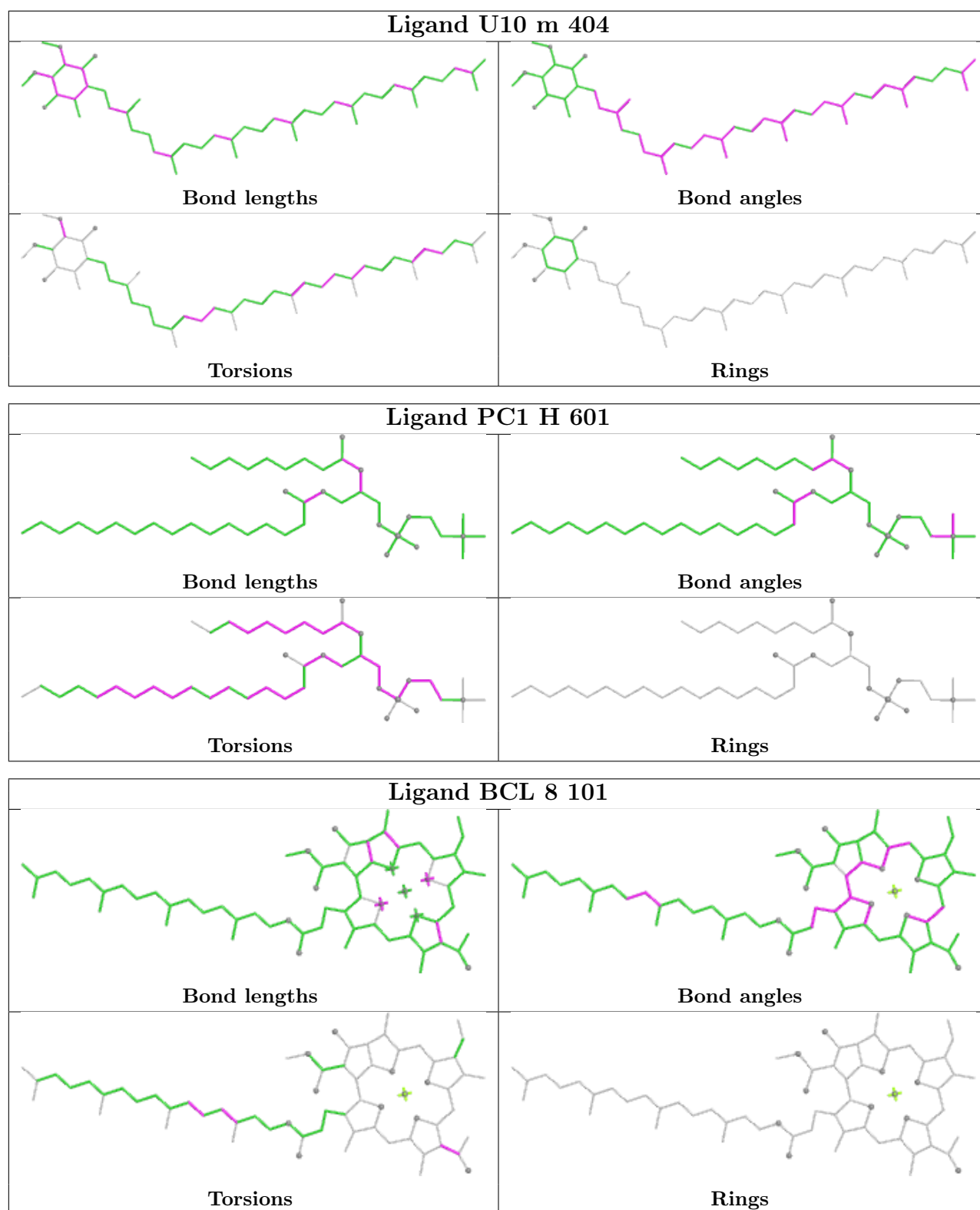
Ligand SPO M 404	
	
Bond lengths	Bond angles
	
Torsions	Rings

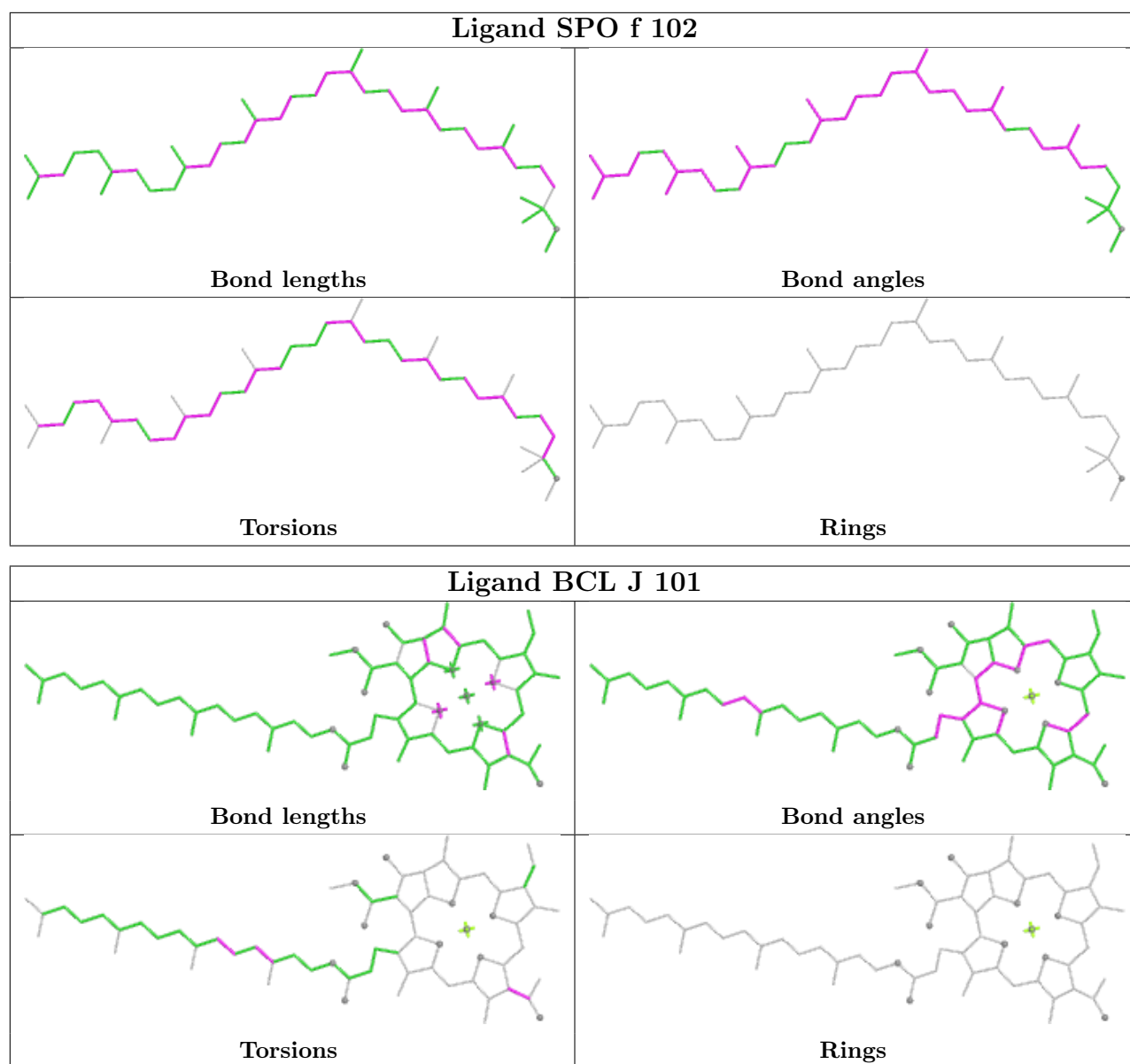
Ligand SPO G 103	
	
Bond lengths	Bond angles
	
Torsions	Rings

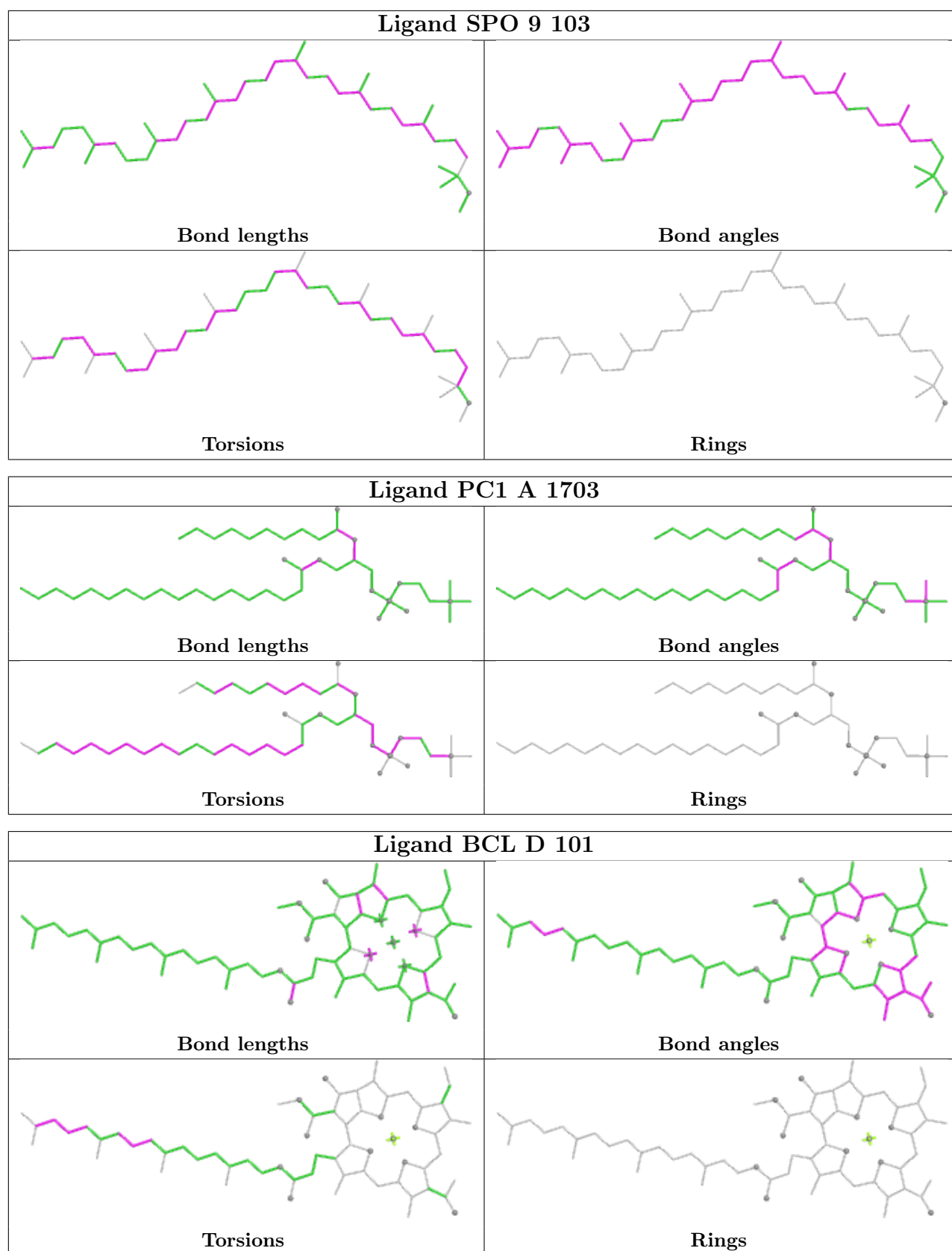
Ligand SPO b 101	
	Bond lengths
	Bond angles
	Torsions
	Rings

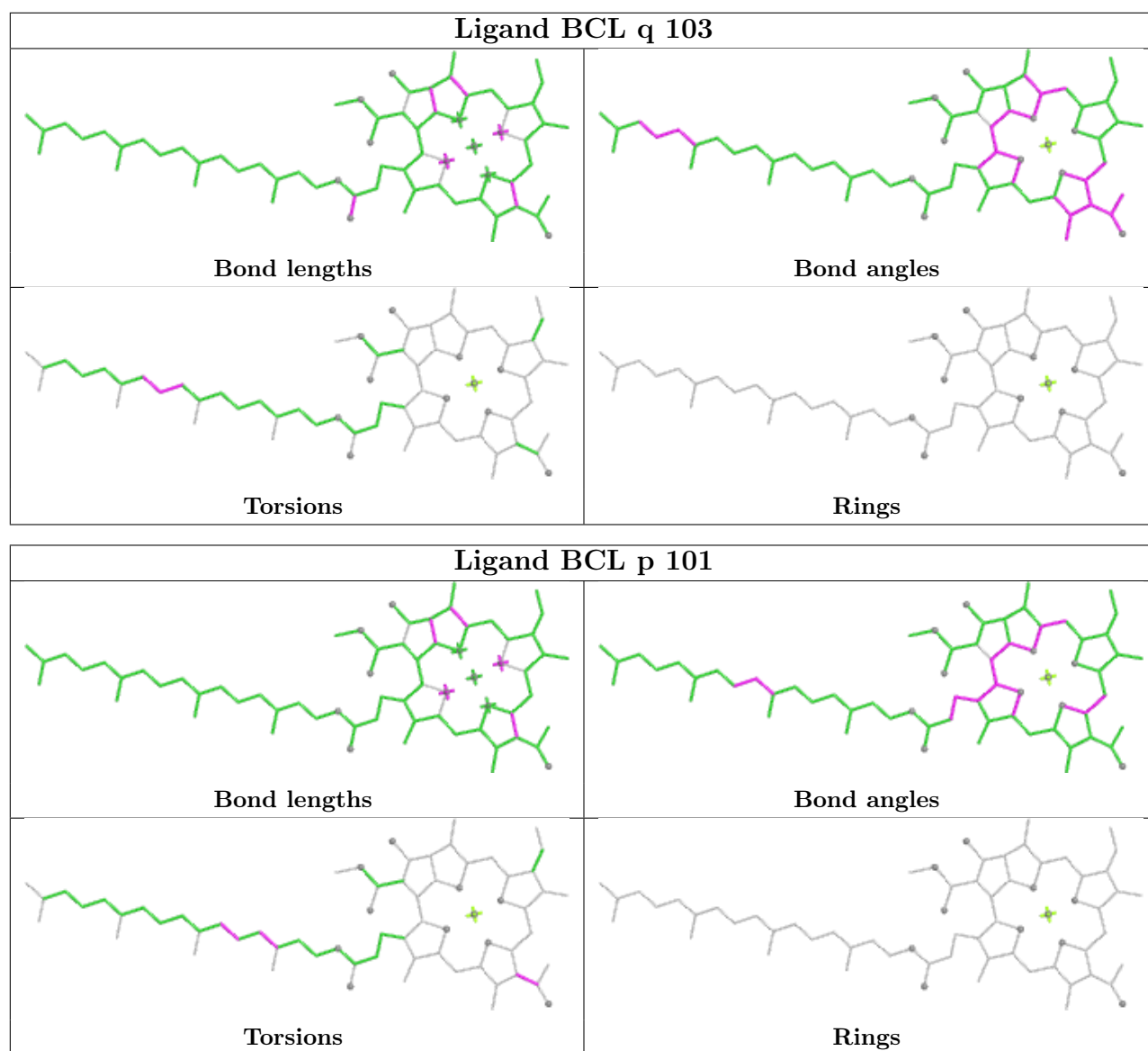
Ligand PC1 A 1701	
	Bond lengths
	Bond angles
	Torsions
	Rings

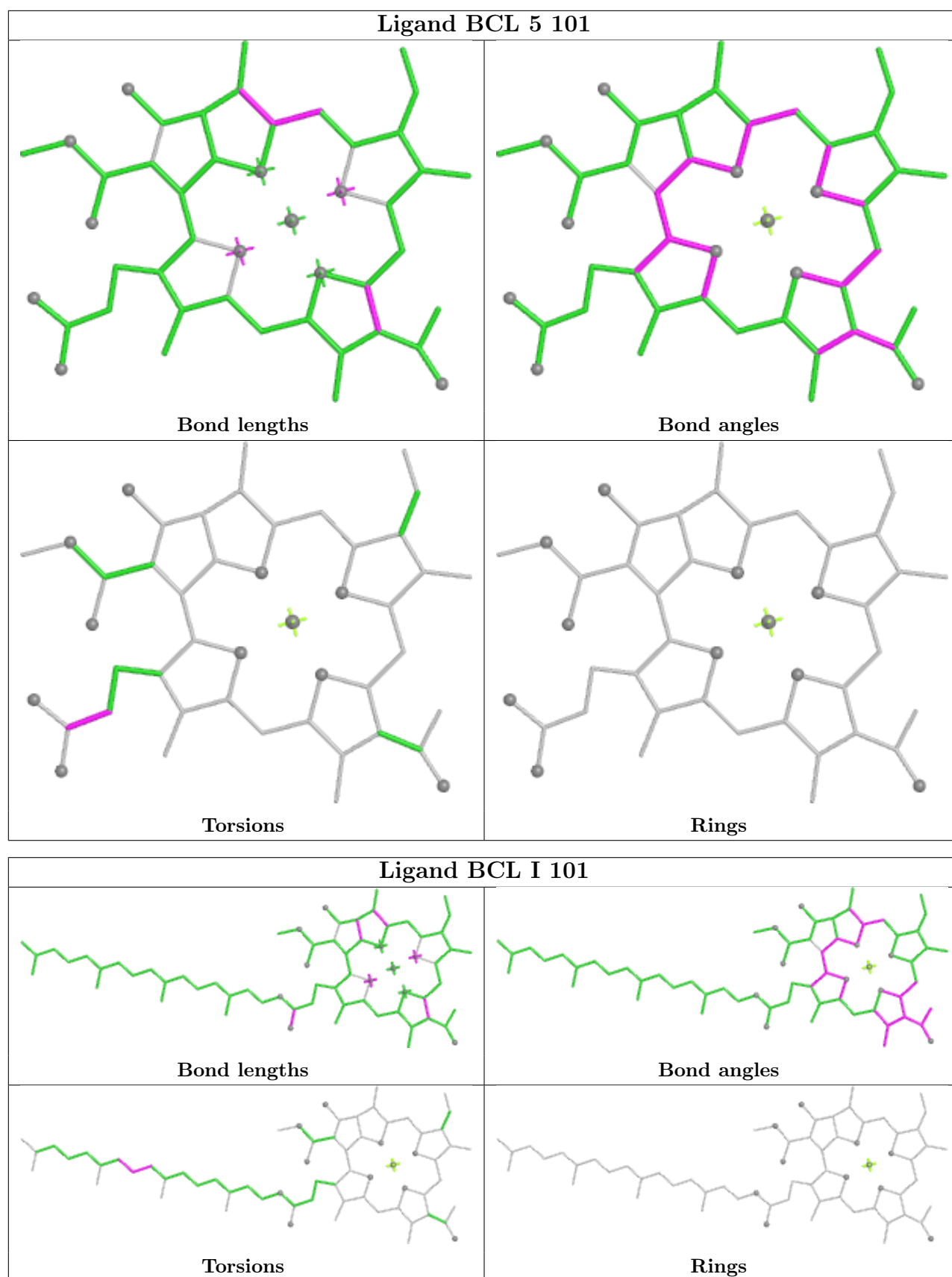


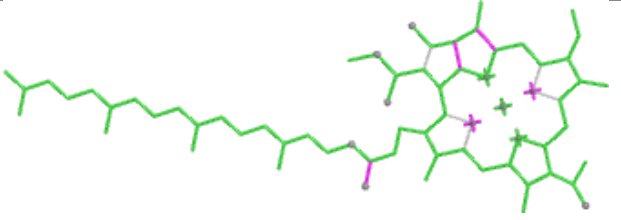
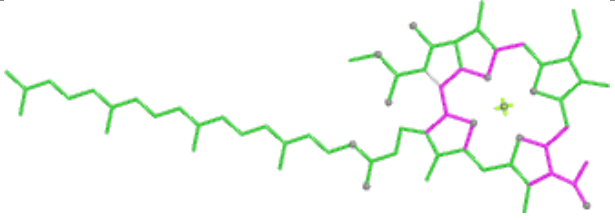
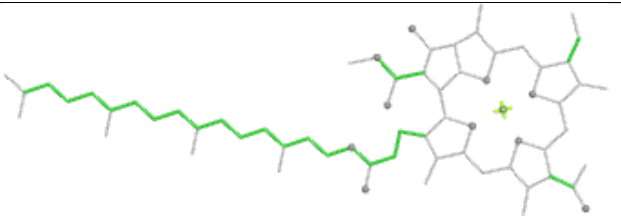
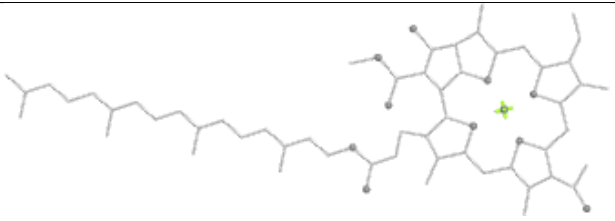
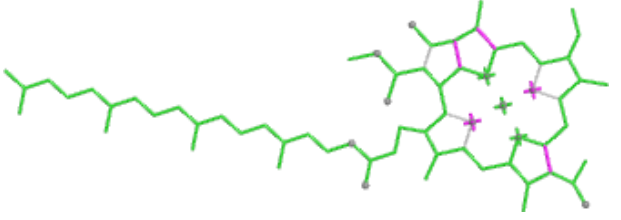
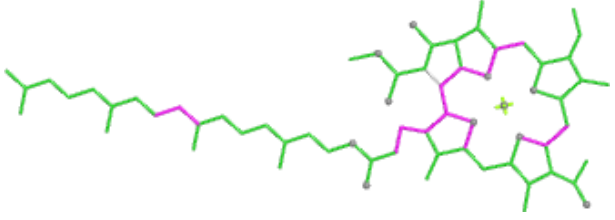
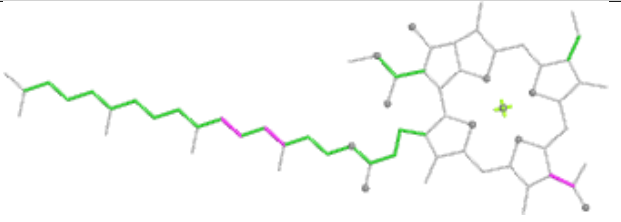
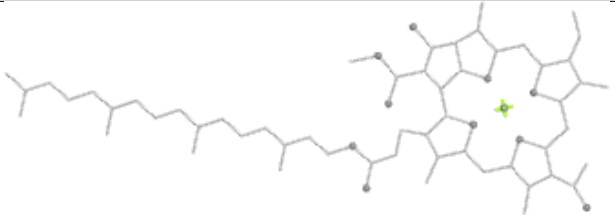
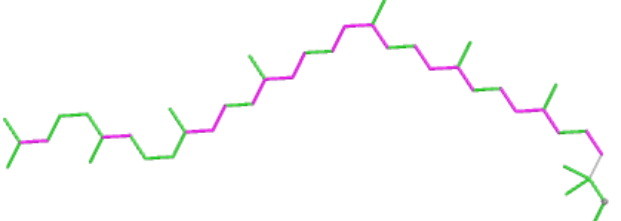
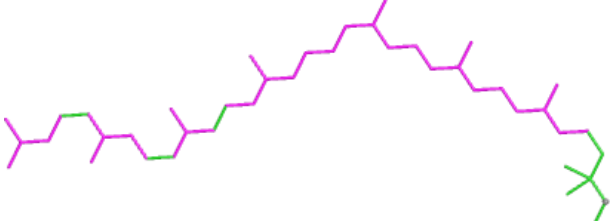
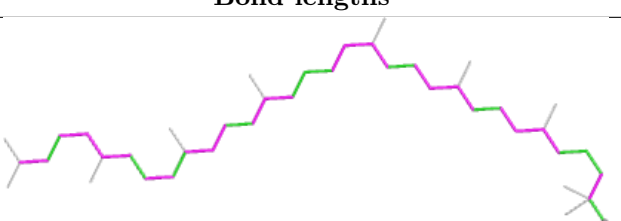


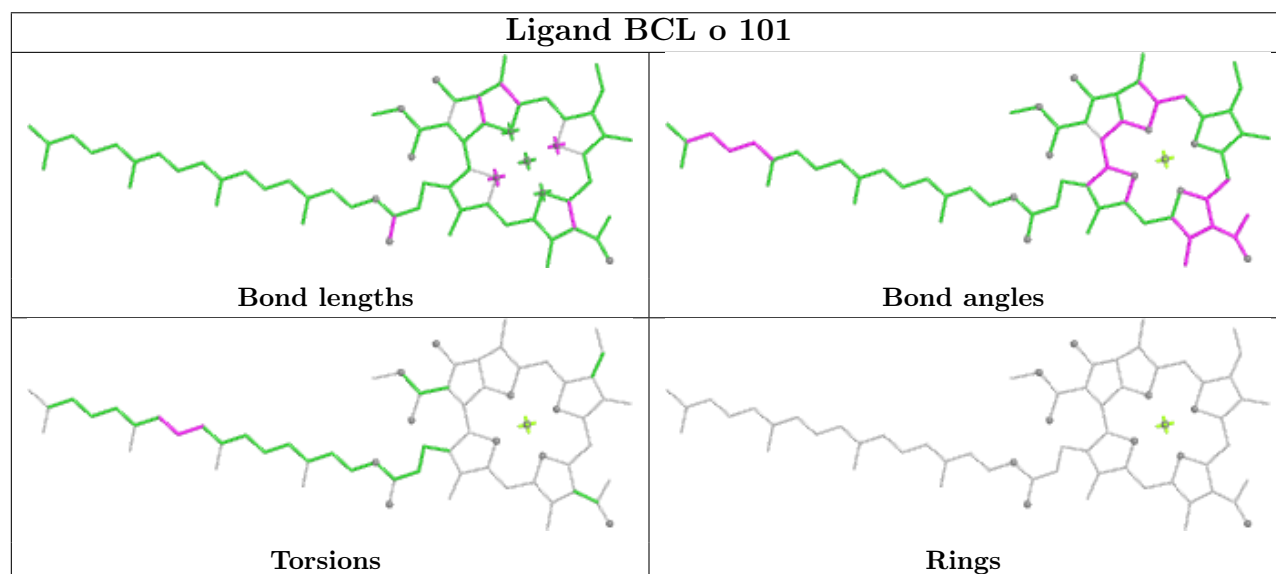
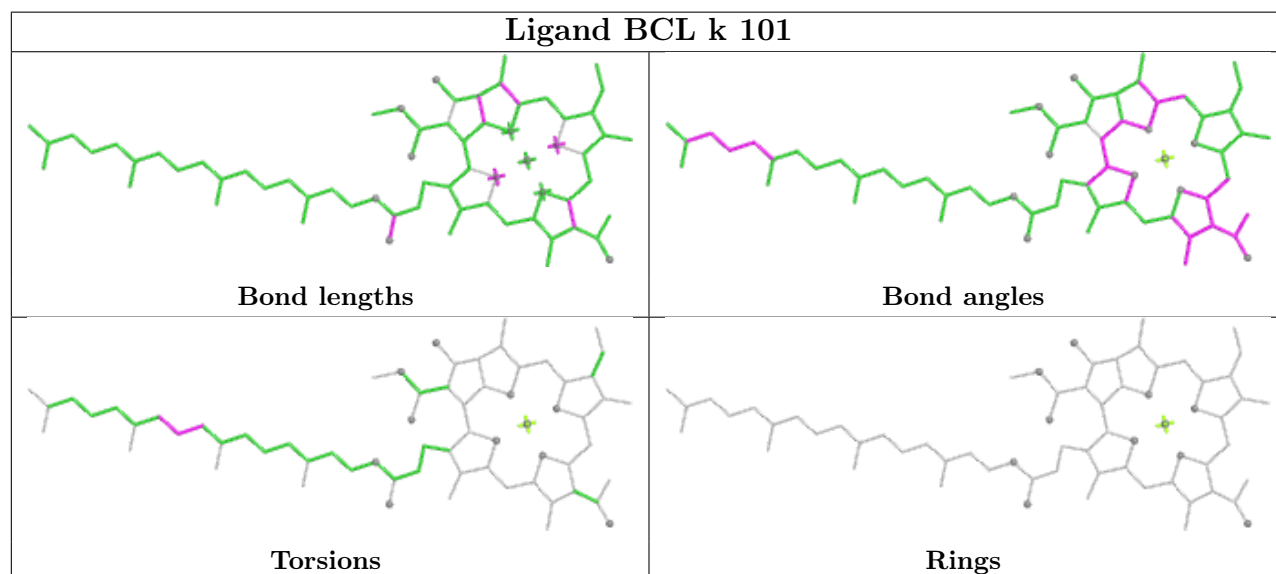
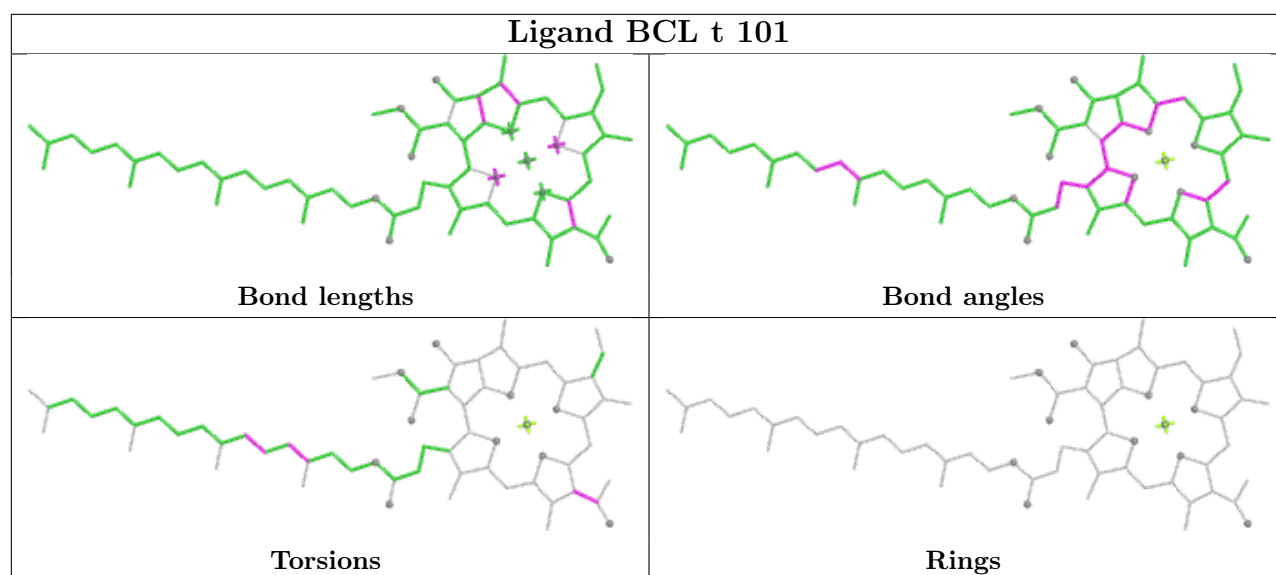


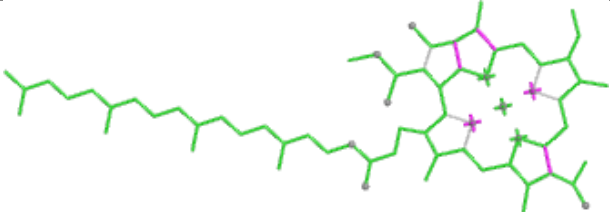
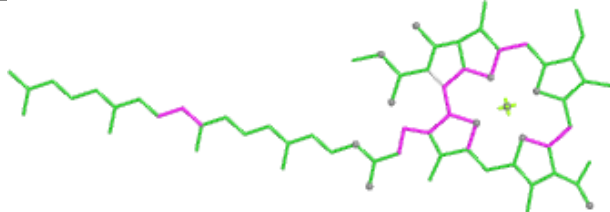
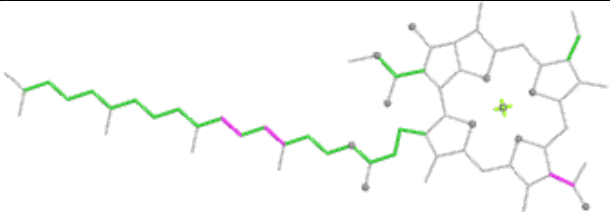
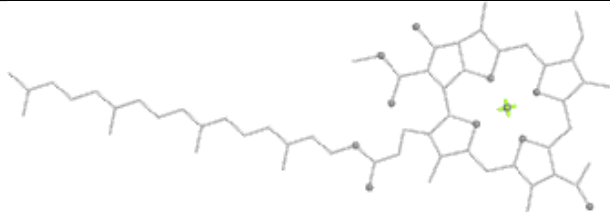
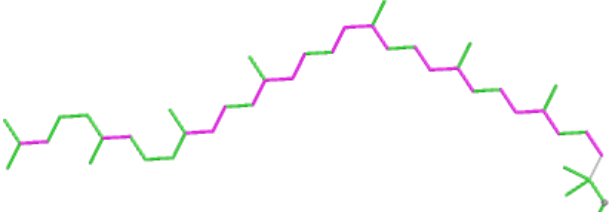
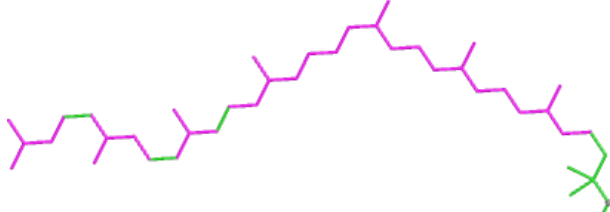
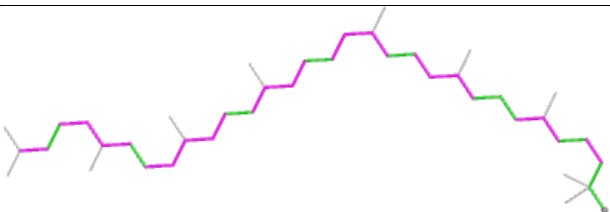
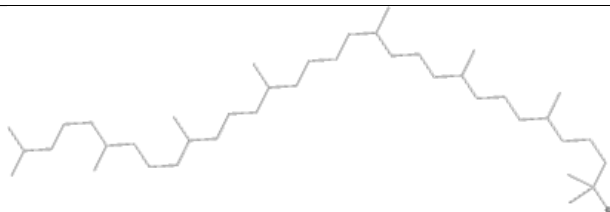
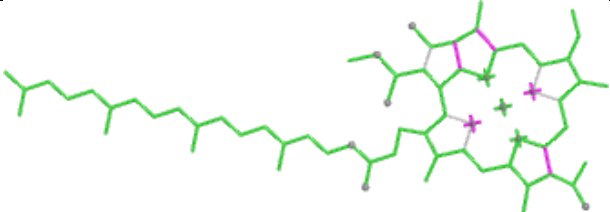
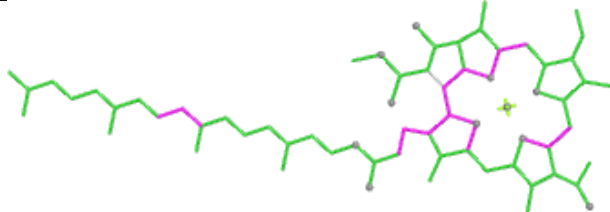
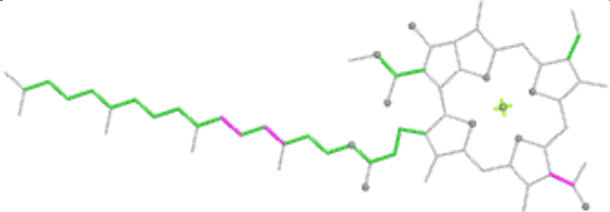
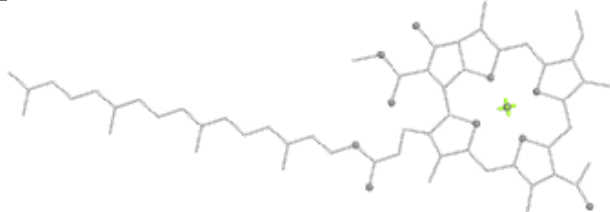


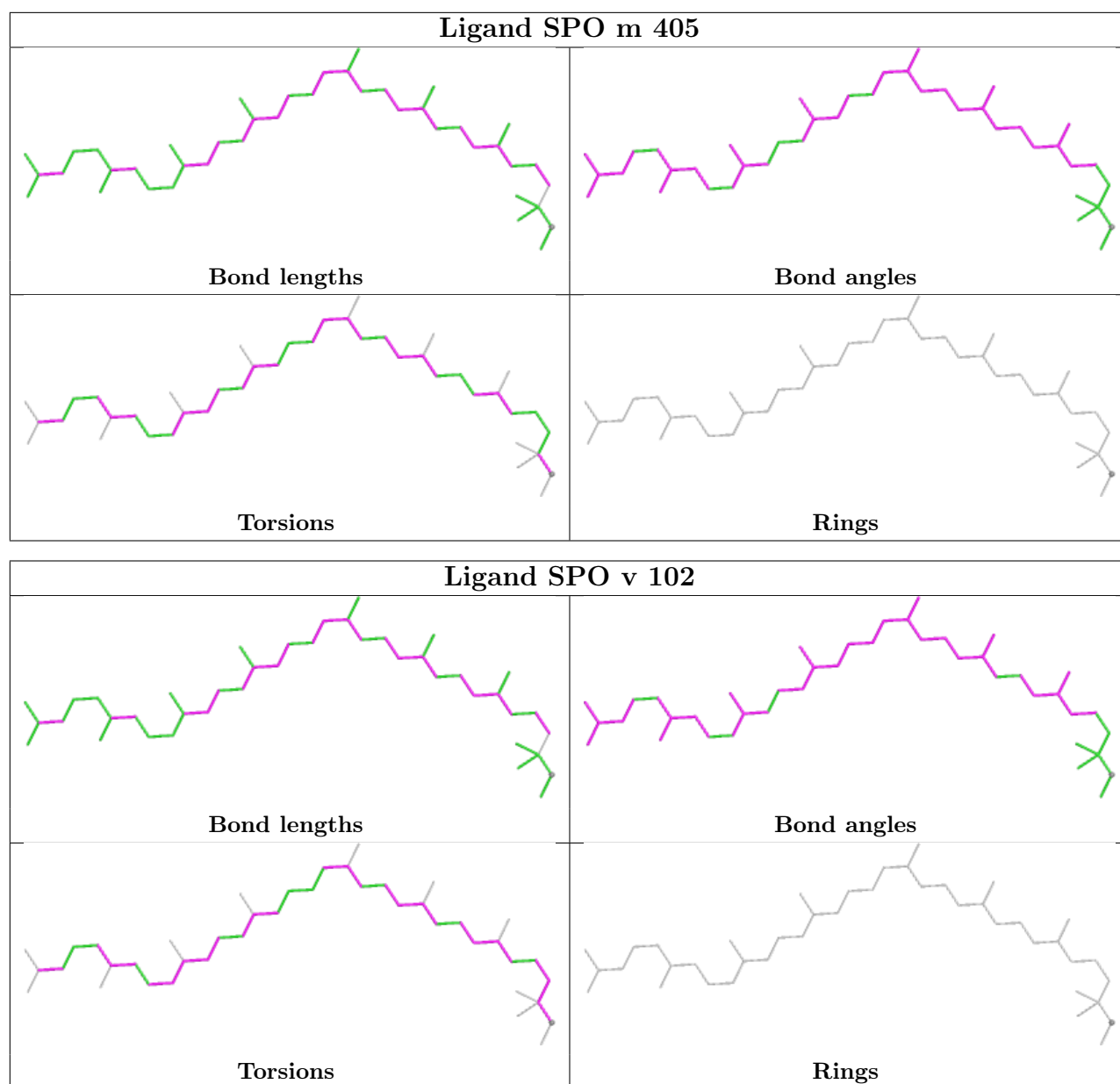


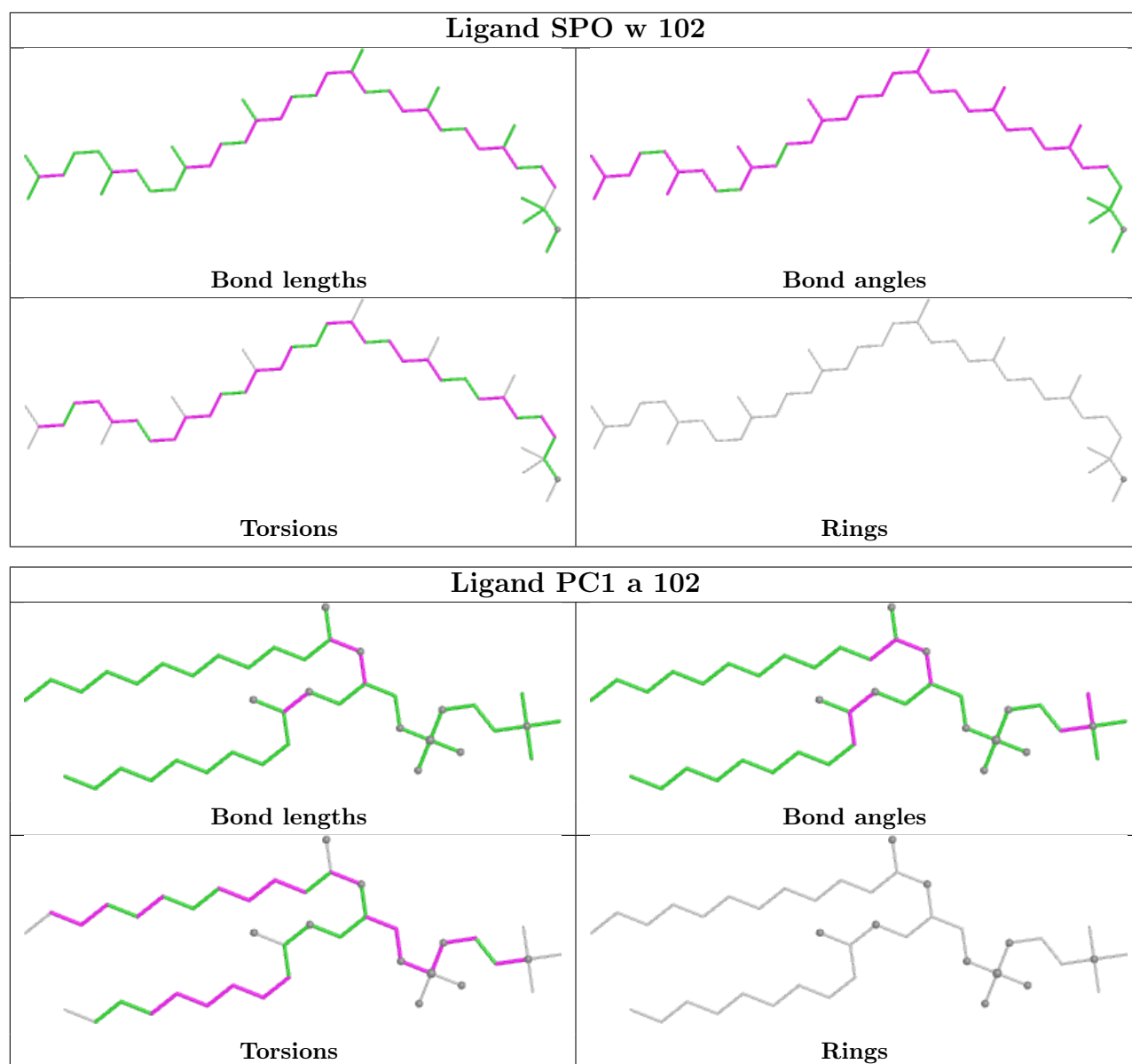


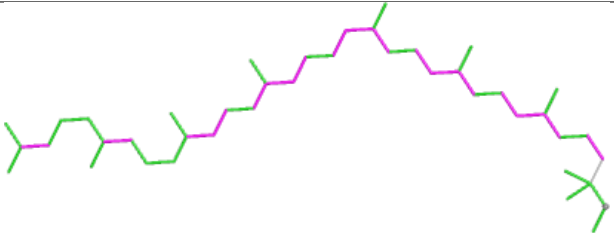
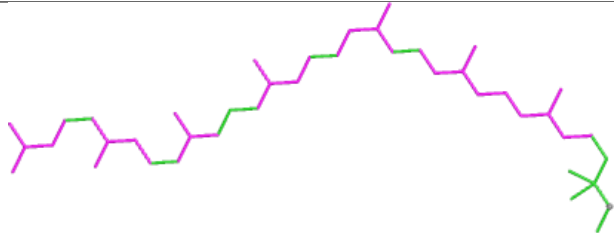
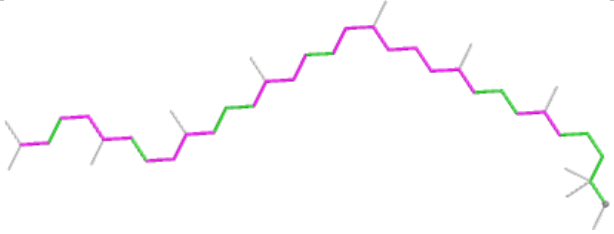
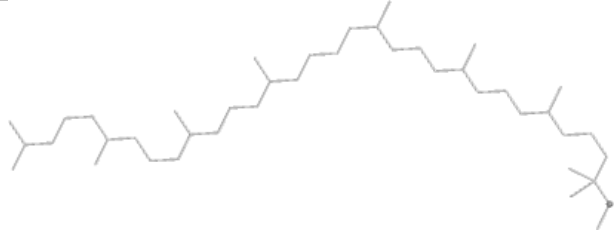
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 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCL 0 102	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand SPO b 103	
 Bond lengths	 Bond angles
 Torsions	 Rings

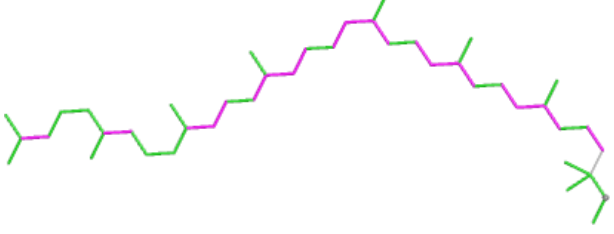
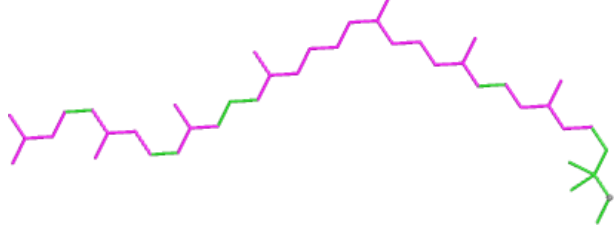
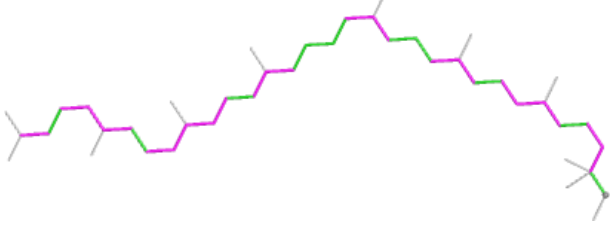


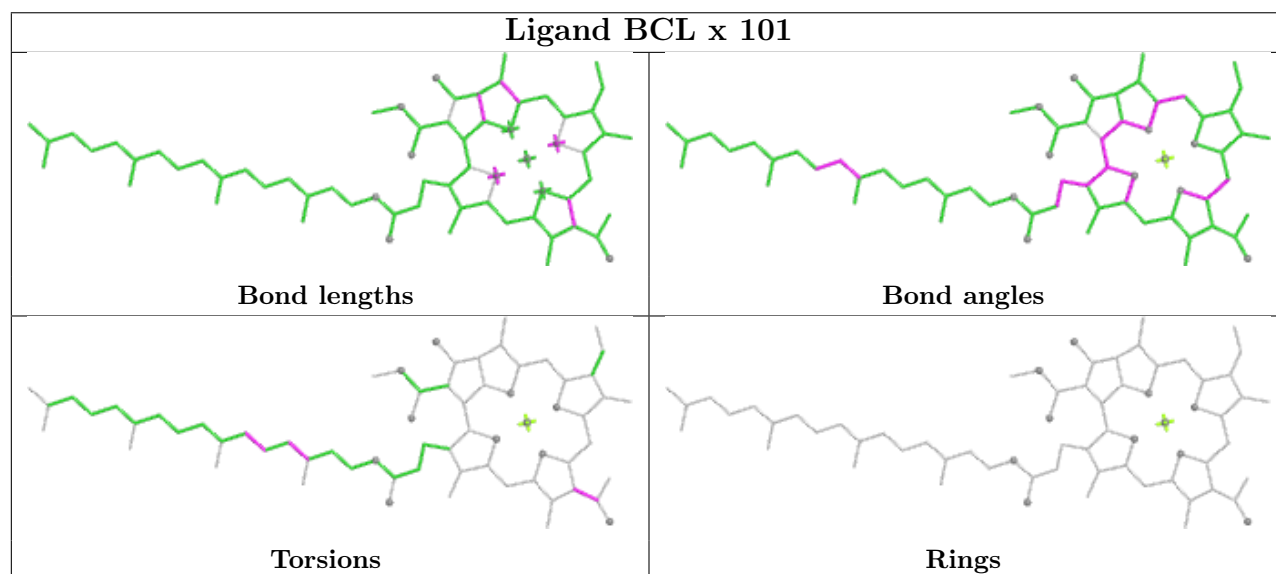
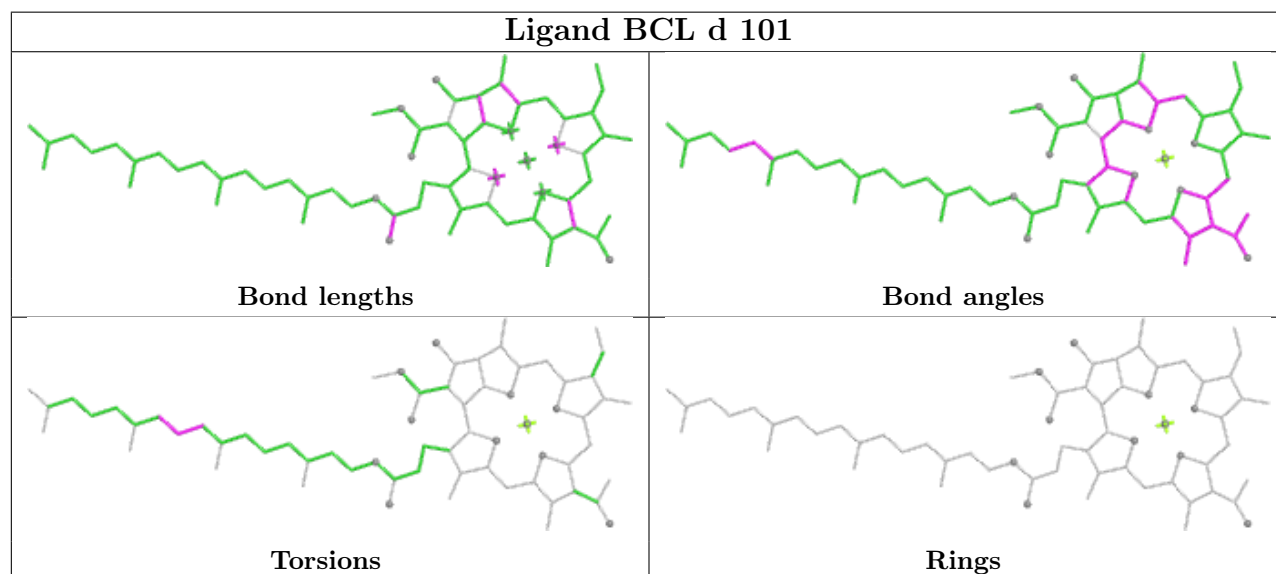
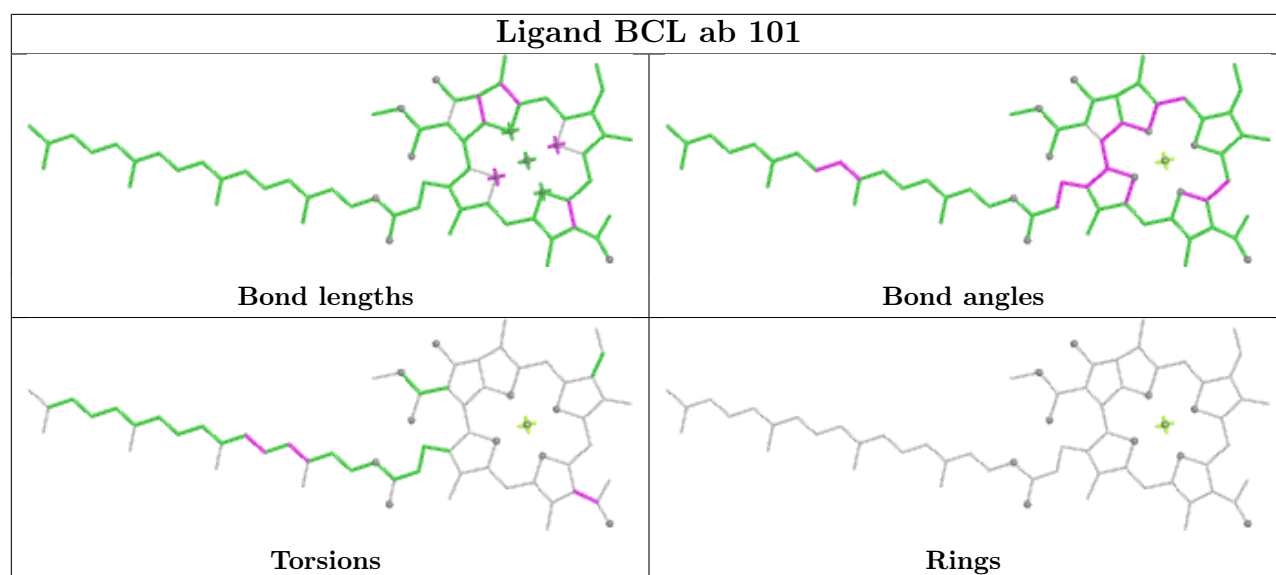
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 Bond lengths	 Bond angles
 Torsions	 Rings
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 Bond lengths	 Bond angles
 Torsions	 Rings

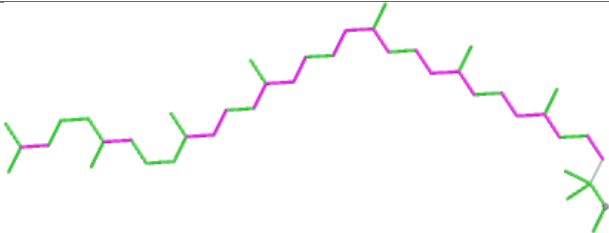
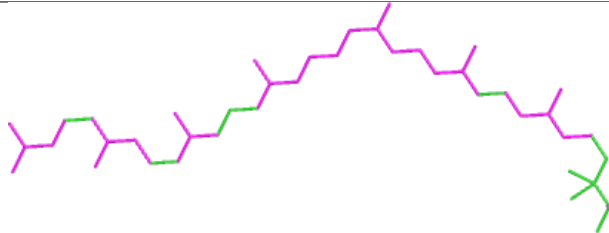
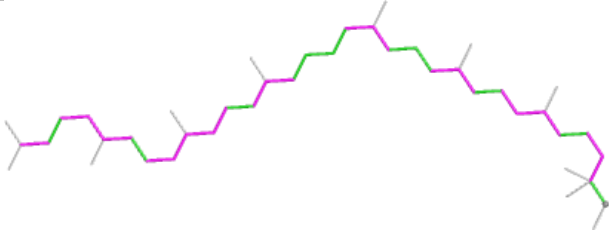
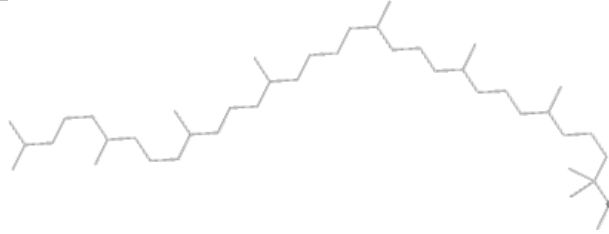


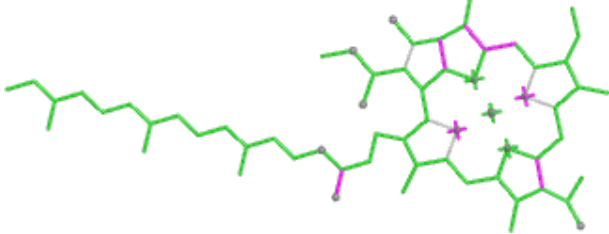
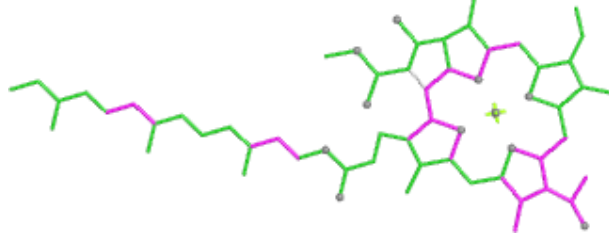
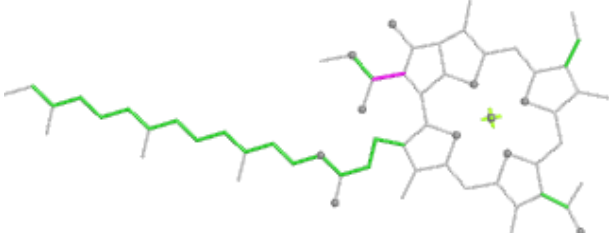
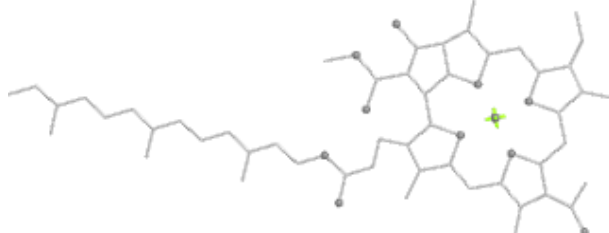


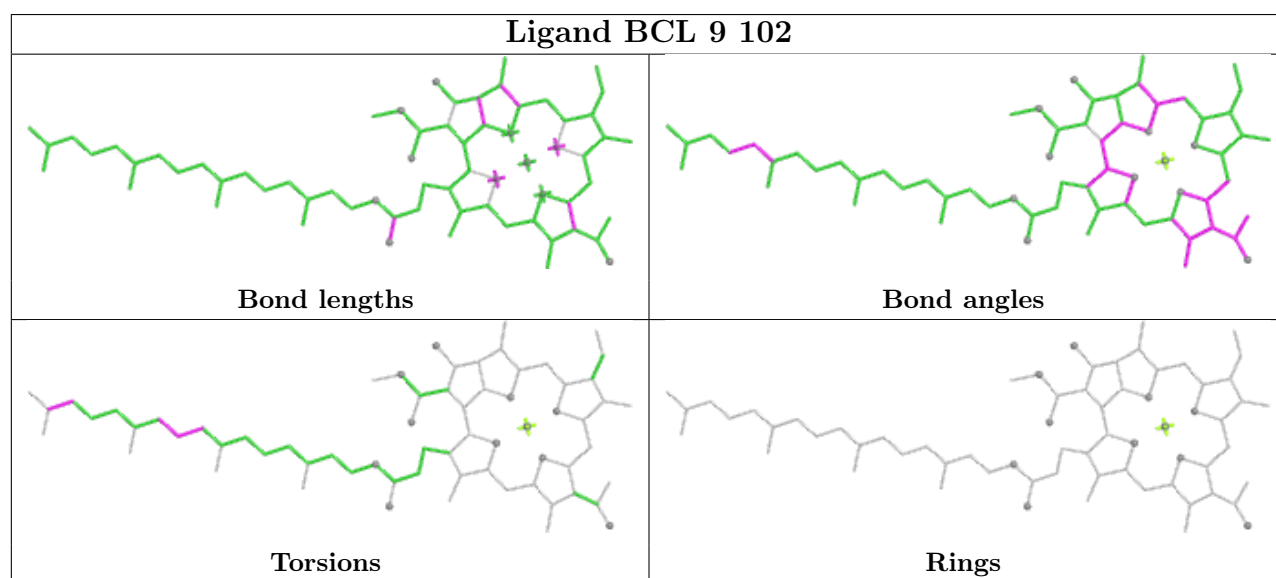
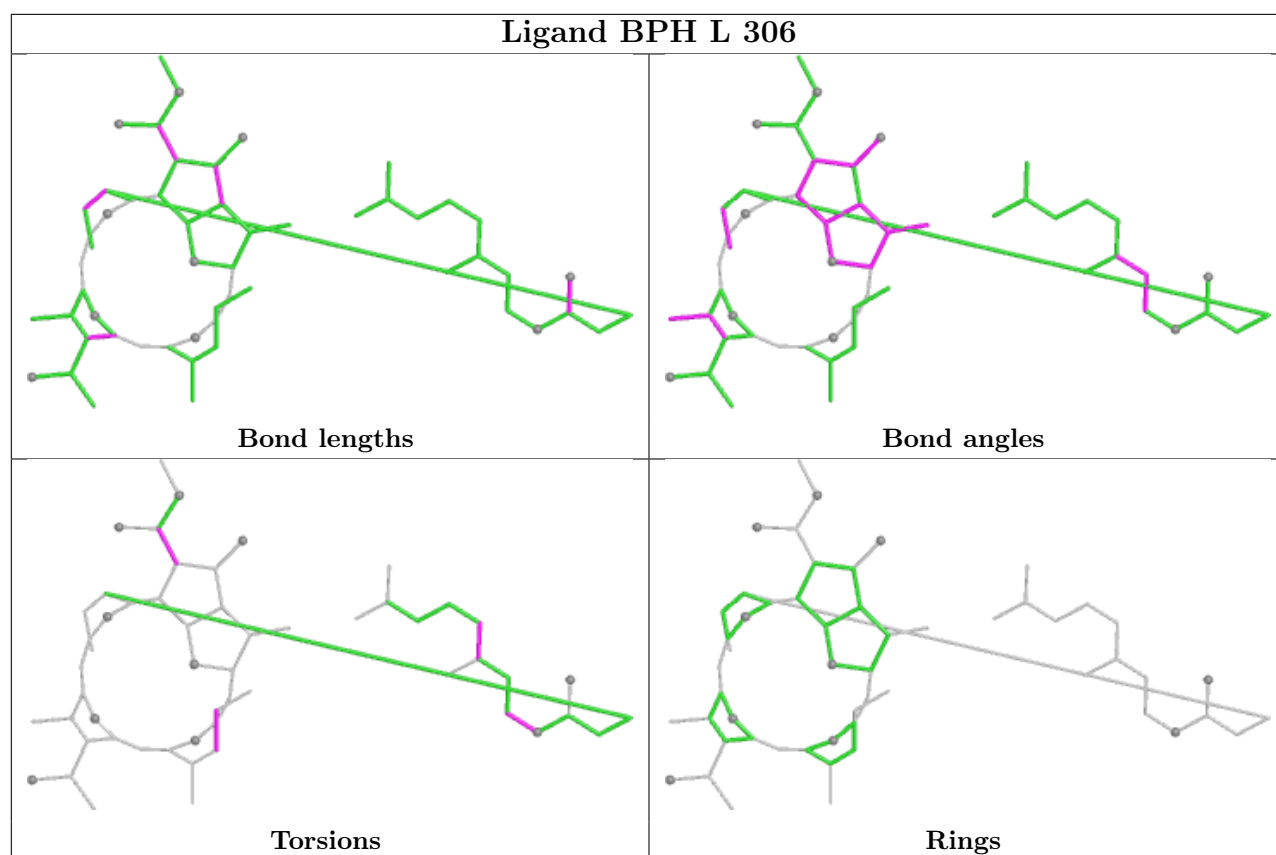
Ligand SPO G 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

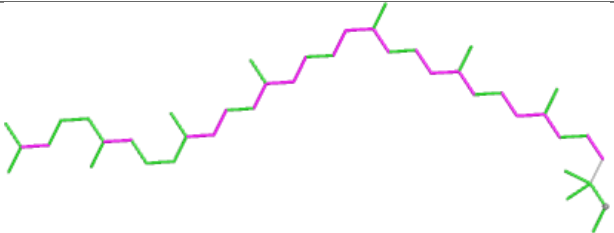
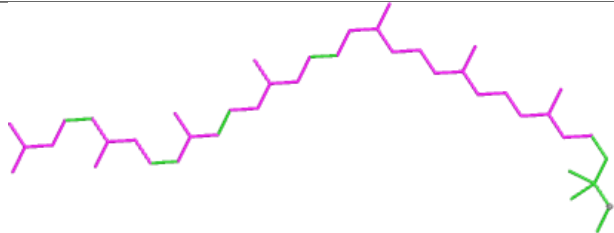
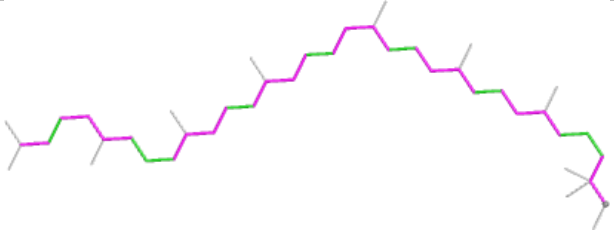
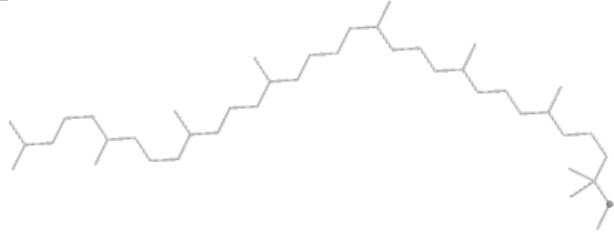
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Bond lengths	Bond angles
	
Torsions	Rings

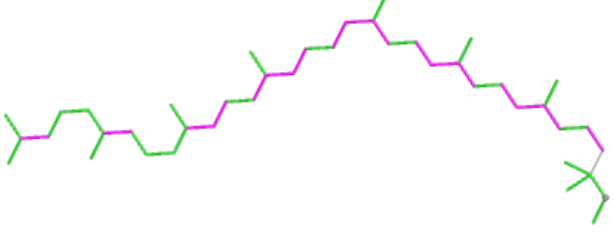
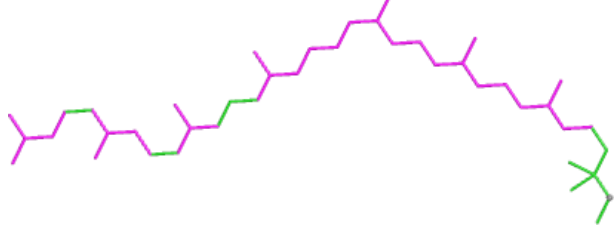
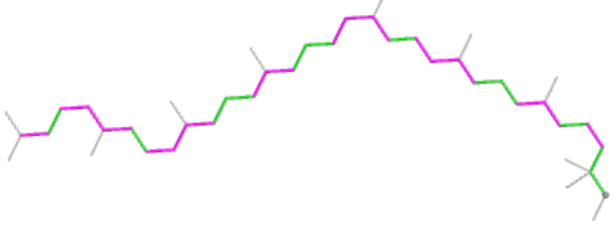


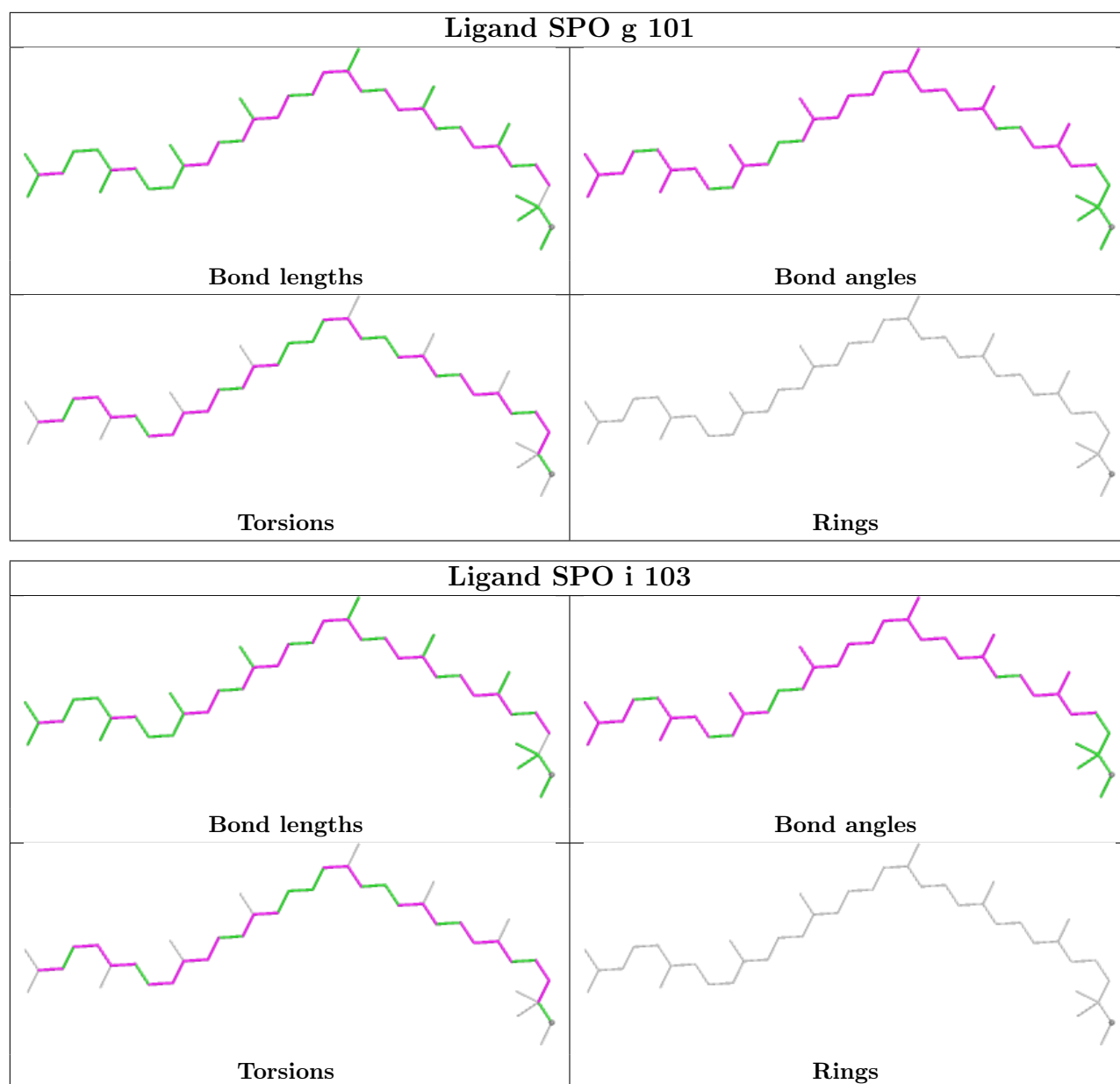
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Bond lengths	Bond angles
	
Torsions	Rings

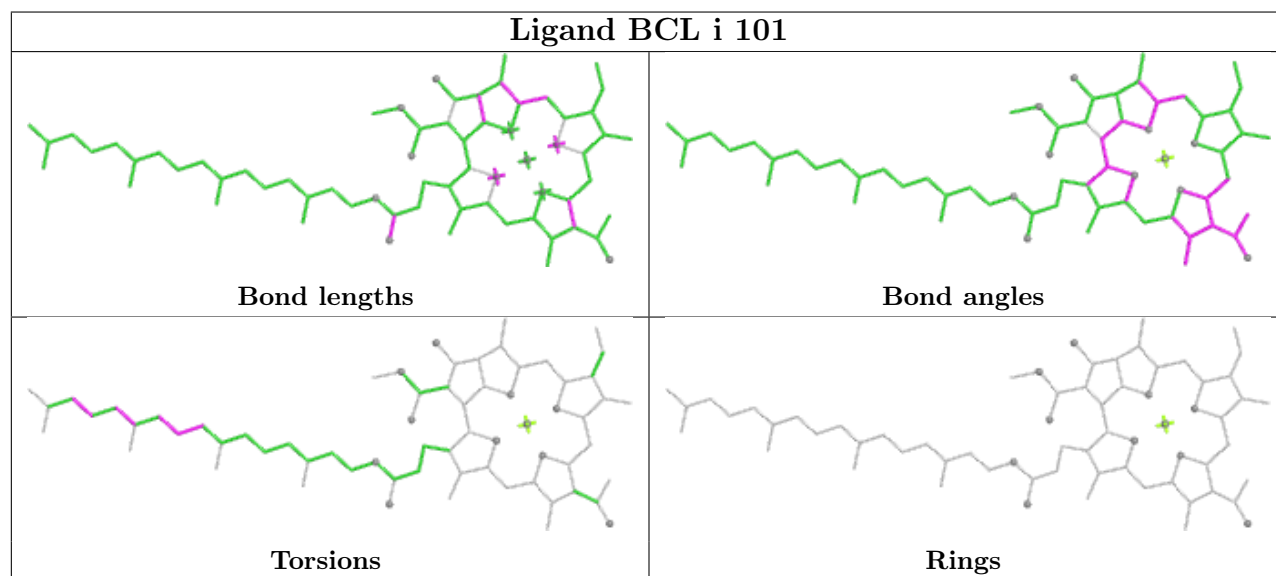
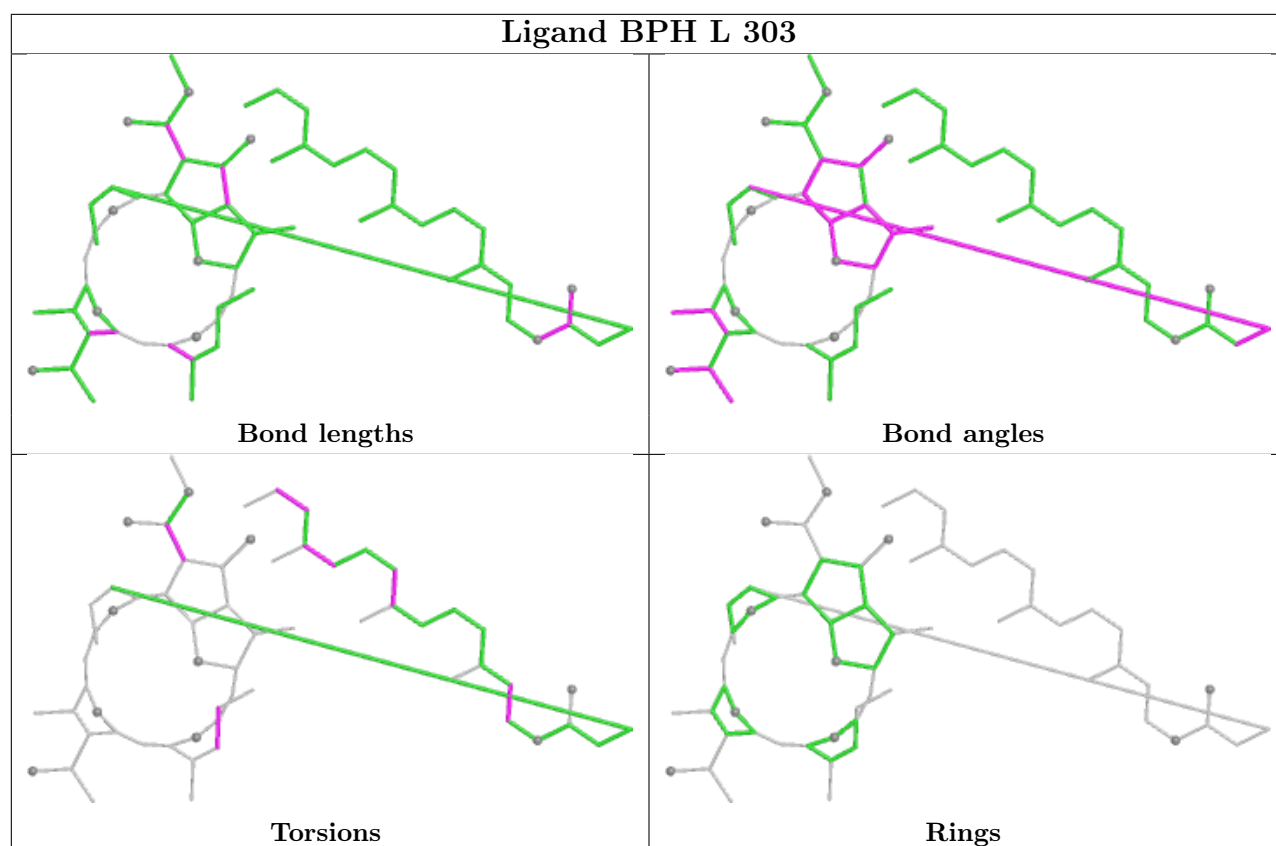
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Bond lengths	Bond angles
	
Torsions	Rings

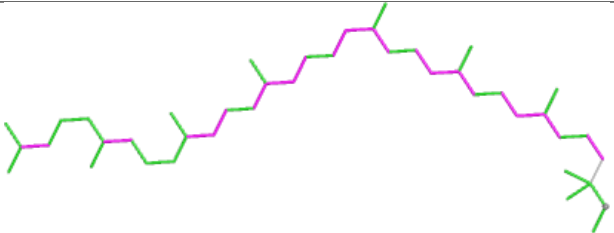
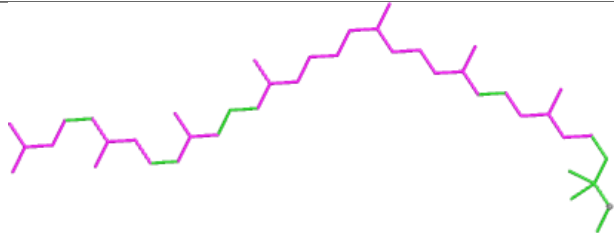
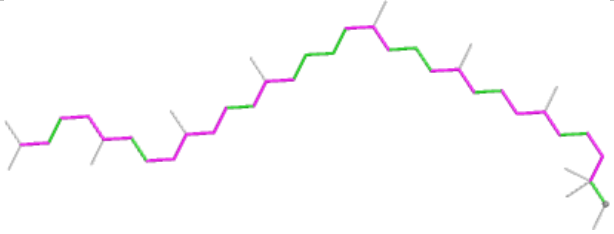
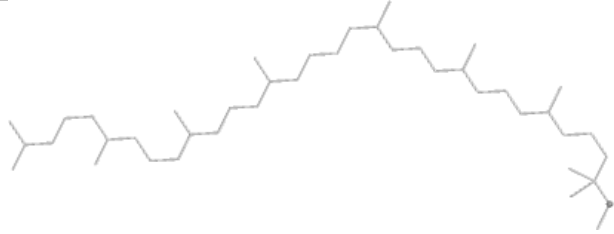


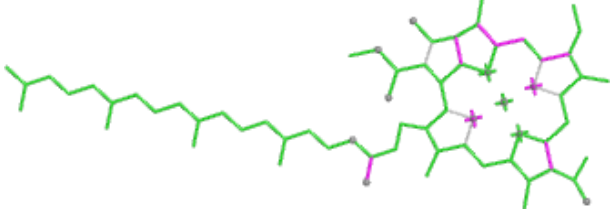
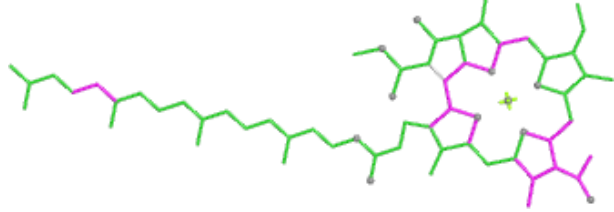
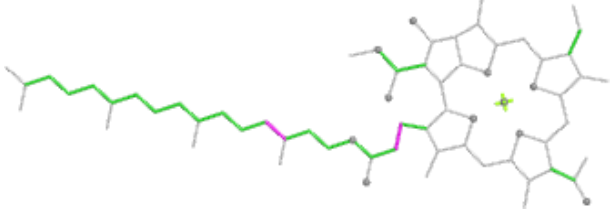
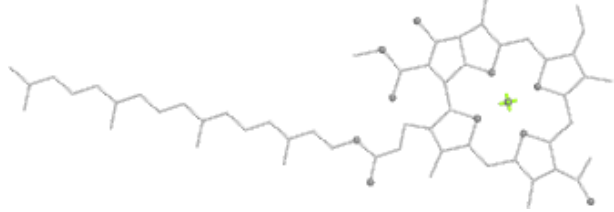
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Bond lengths	Bond angles
	
Torsions	Rings

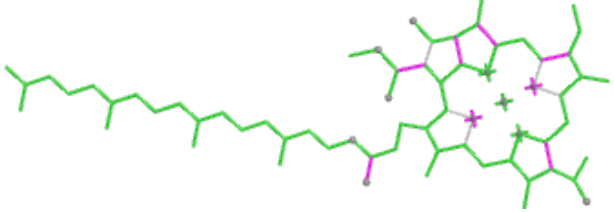
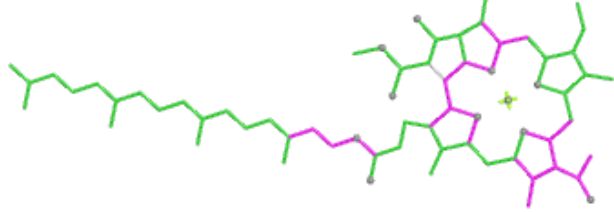
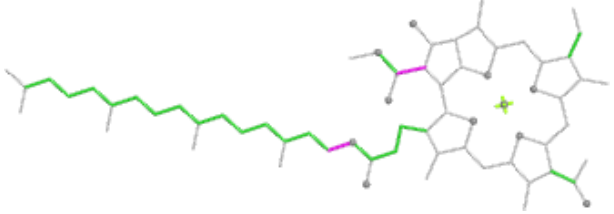
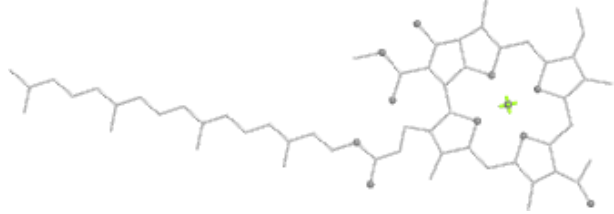
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Bond lengths	Bond angles
	
Torsions	Rings

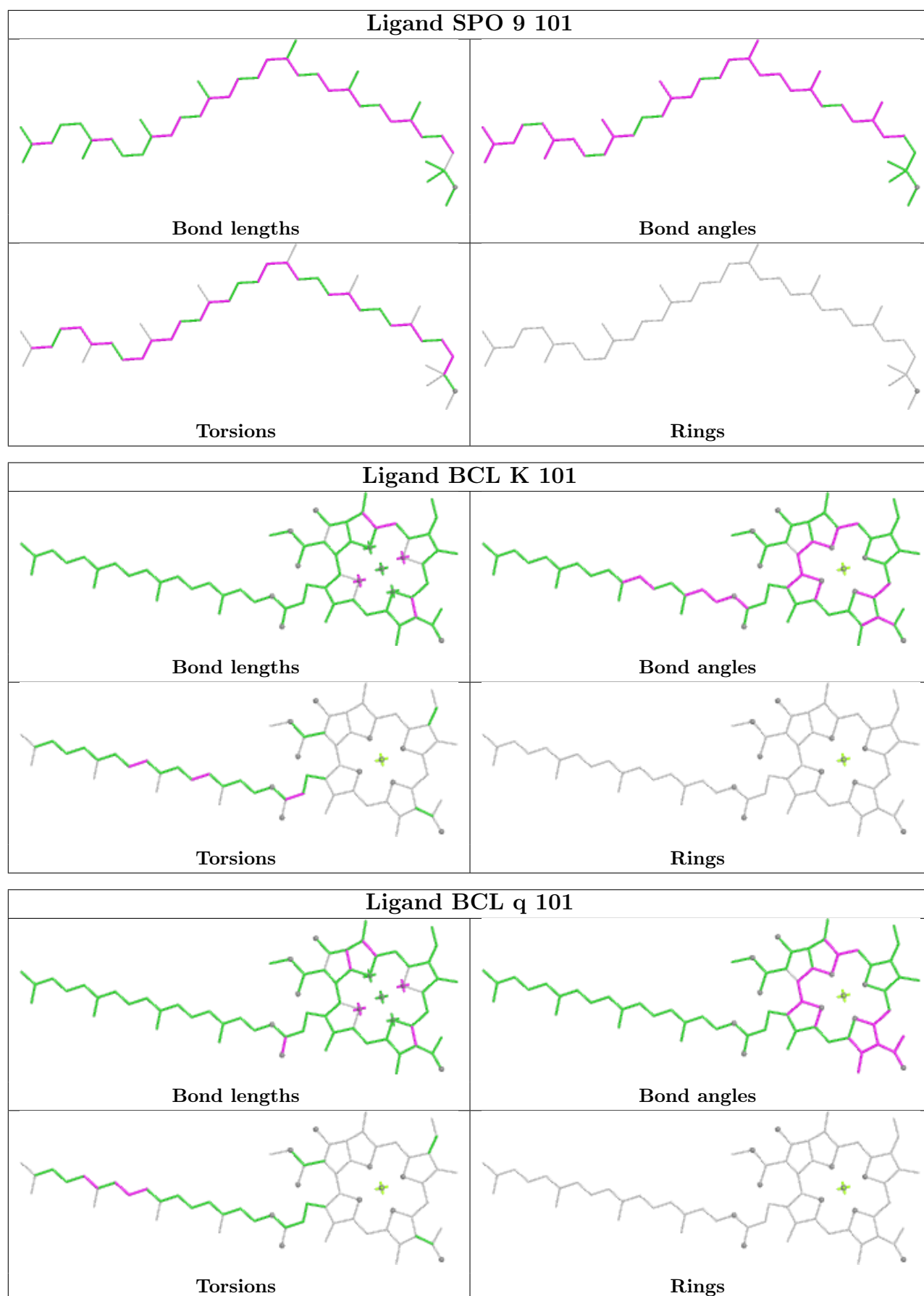


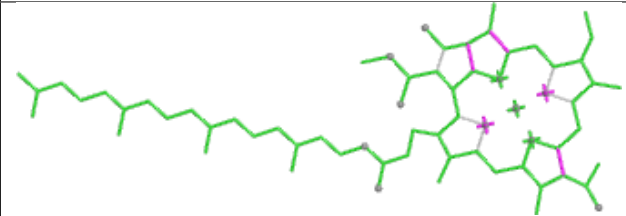
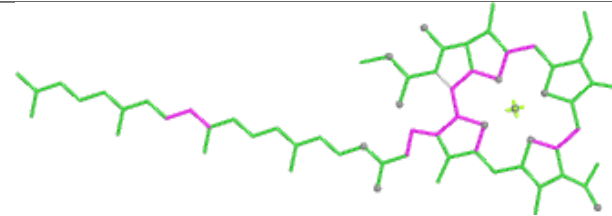
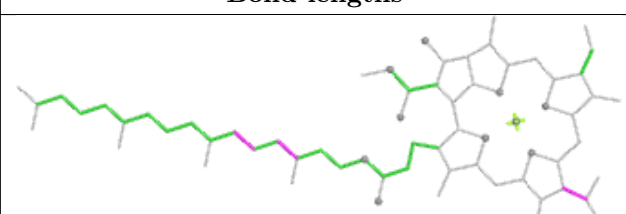
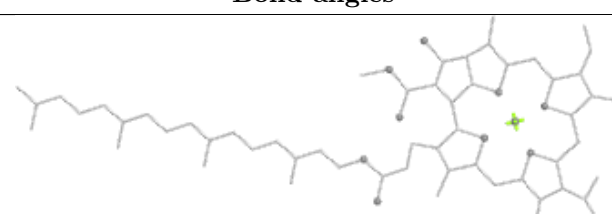


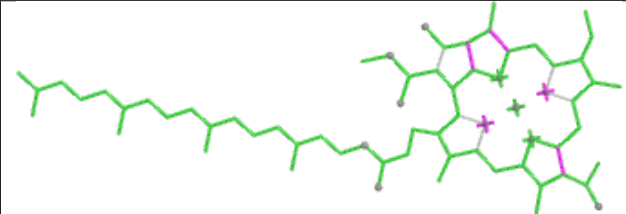
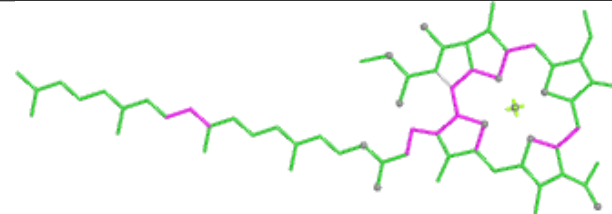
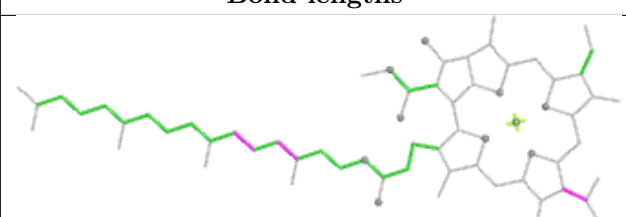
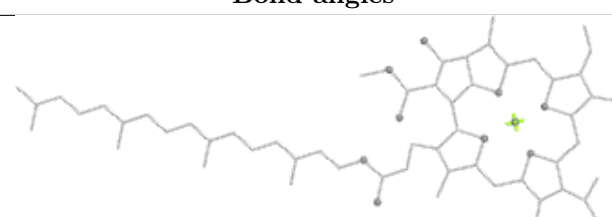
Ligand SPO q 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

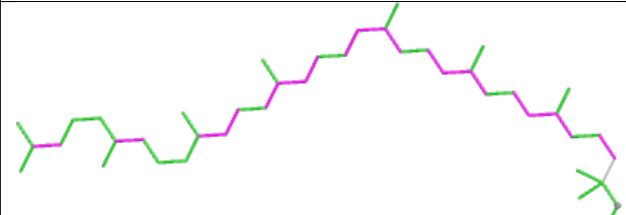
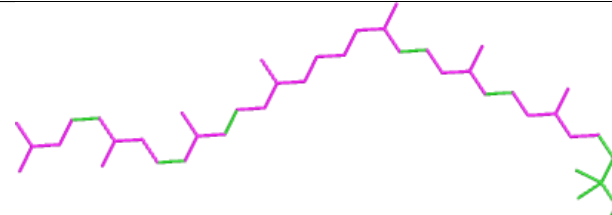
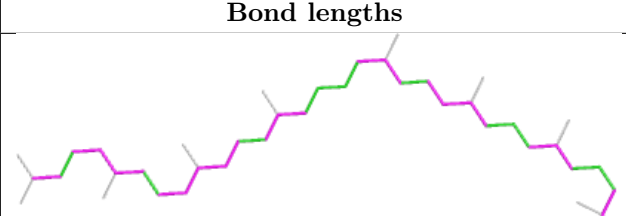
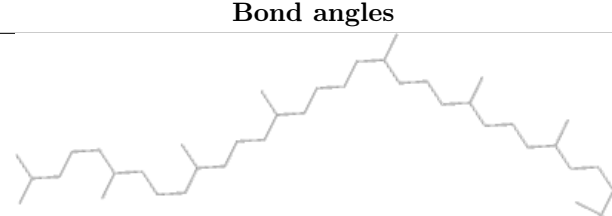
Ligand BCL l 301	
	
Bond lengths	Bond angles
	
Torsions	Rings

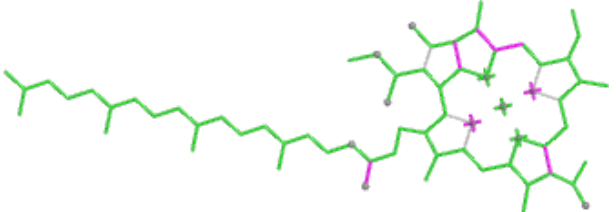
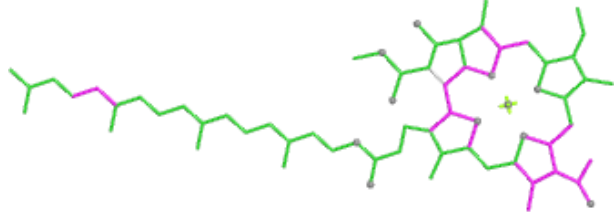
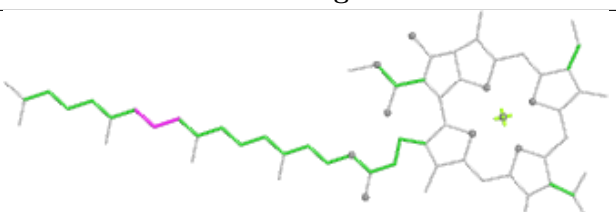
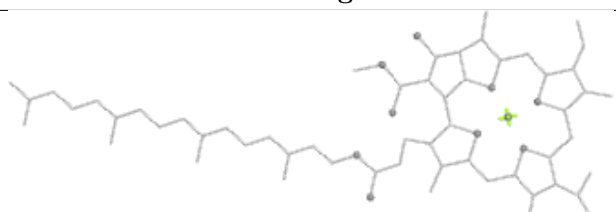
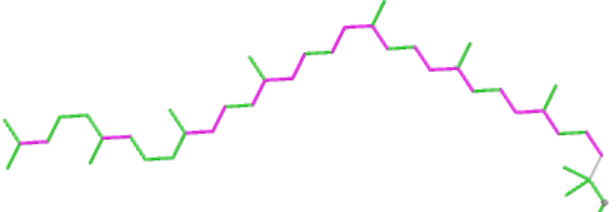
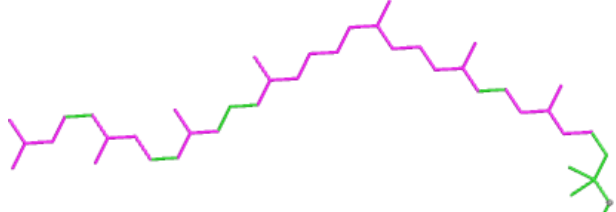
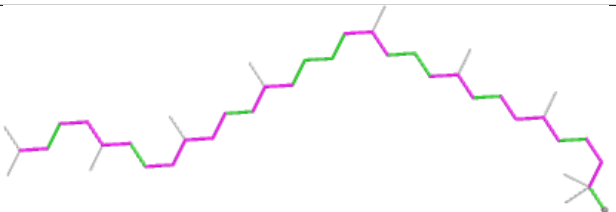
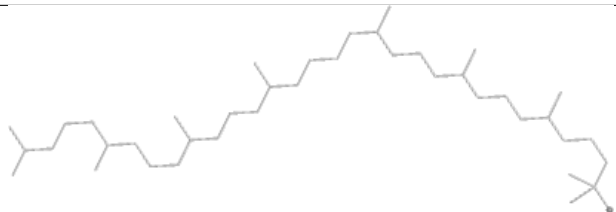
Ligand BCL M 402	
	
Bond lengths	Bond angles
	
Torsions	Rings

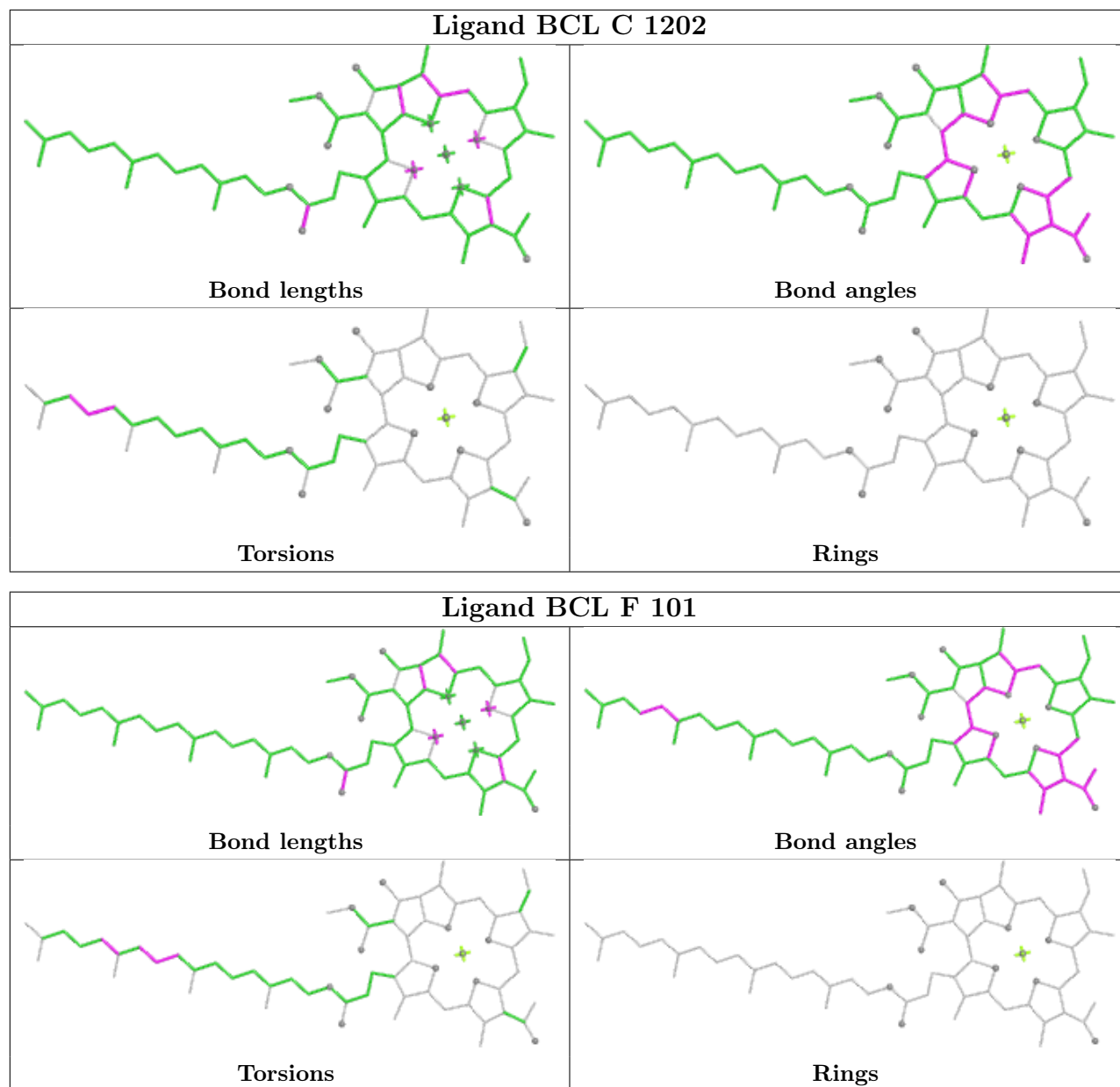


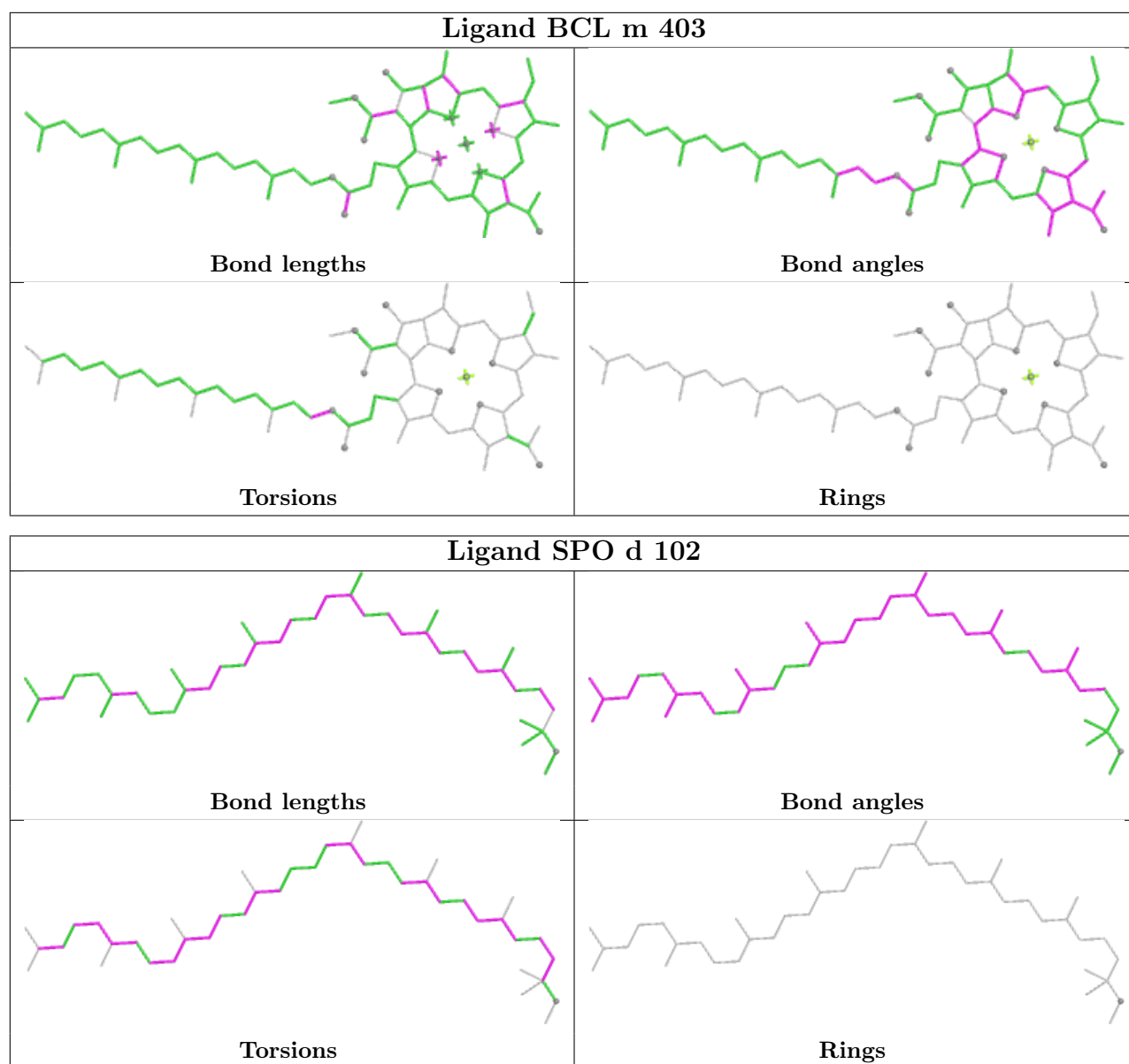
Ligand BCL aa 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

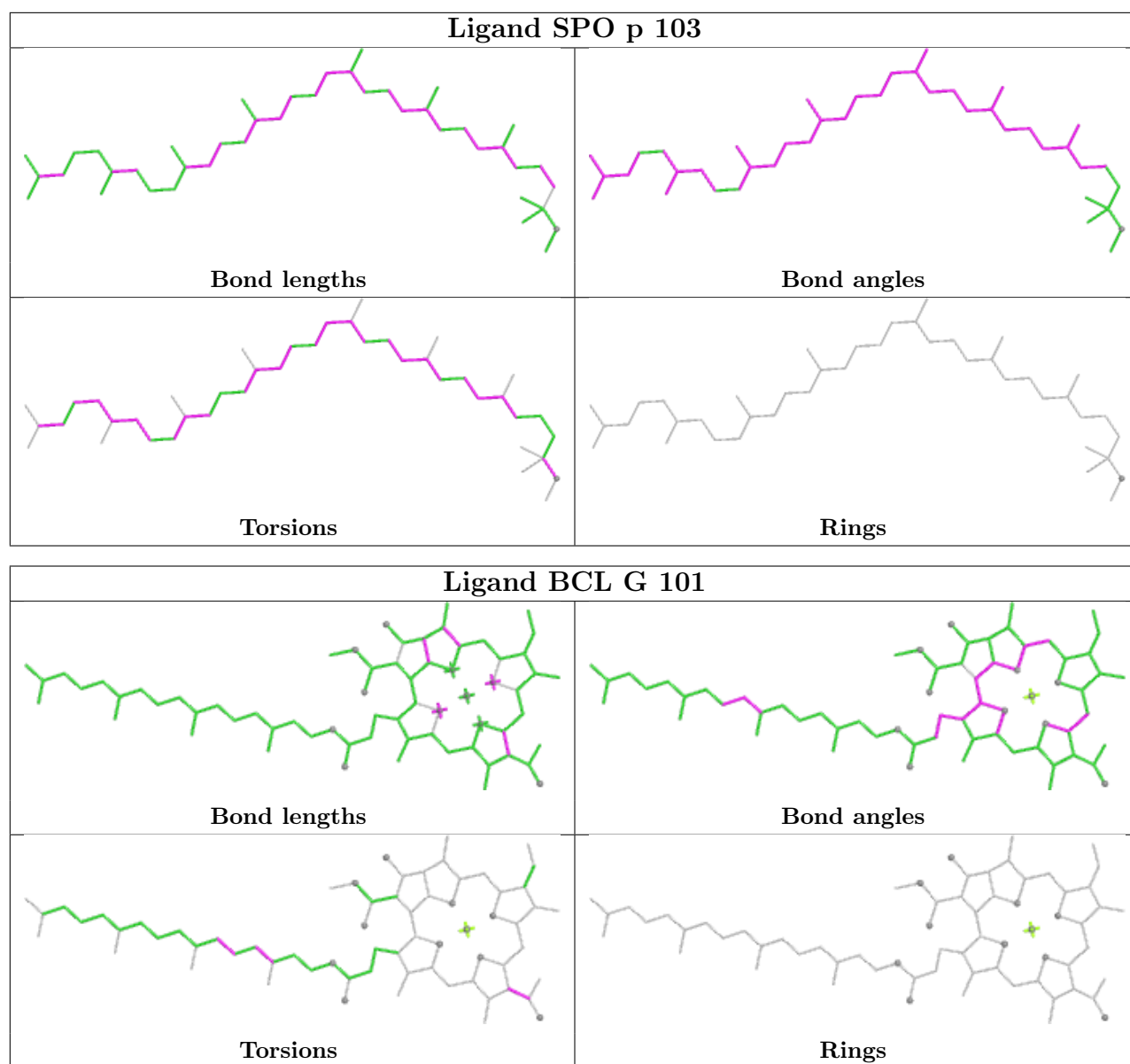
Ligand BCL B 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

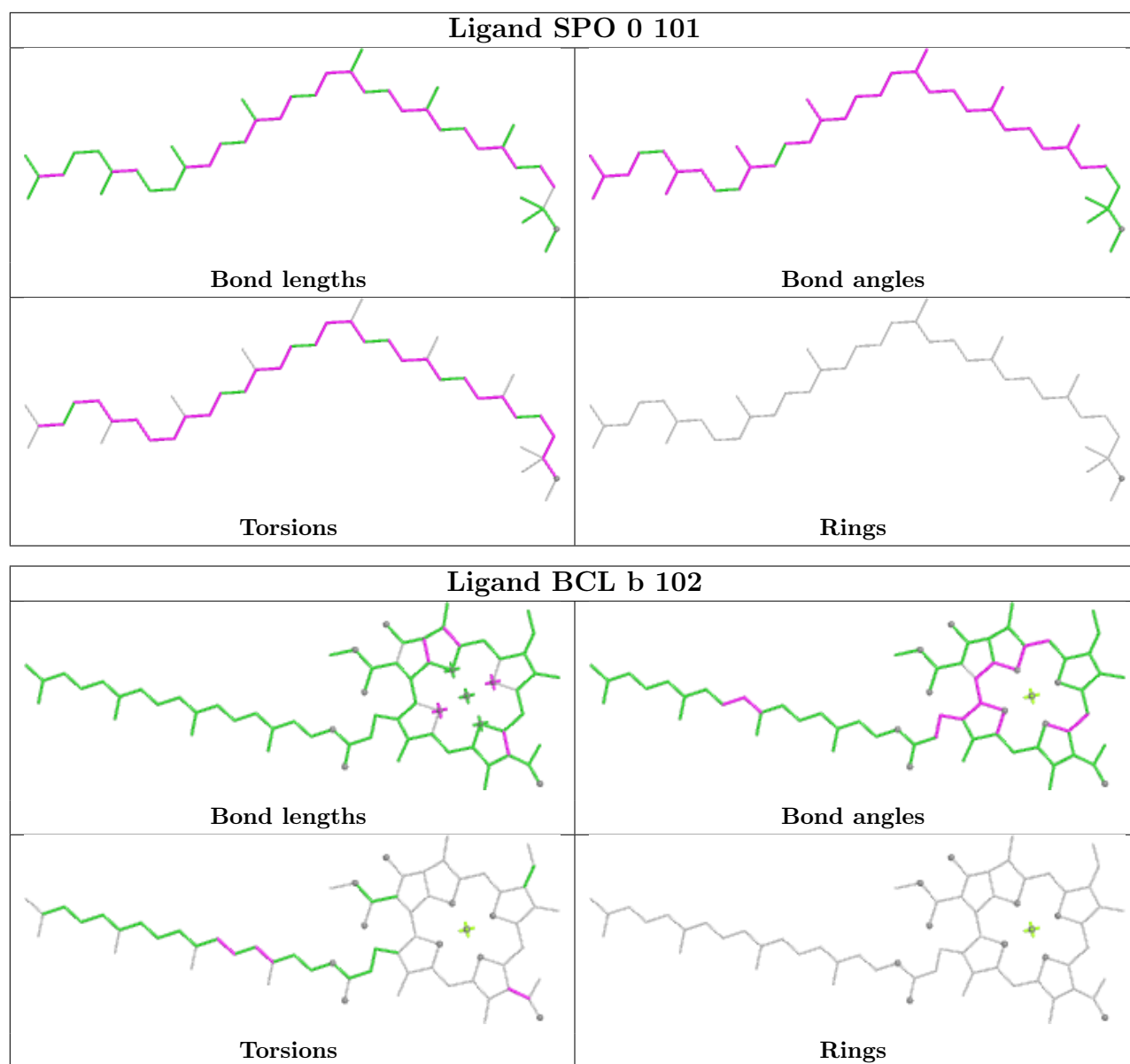
Ligand SPO j 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

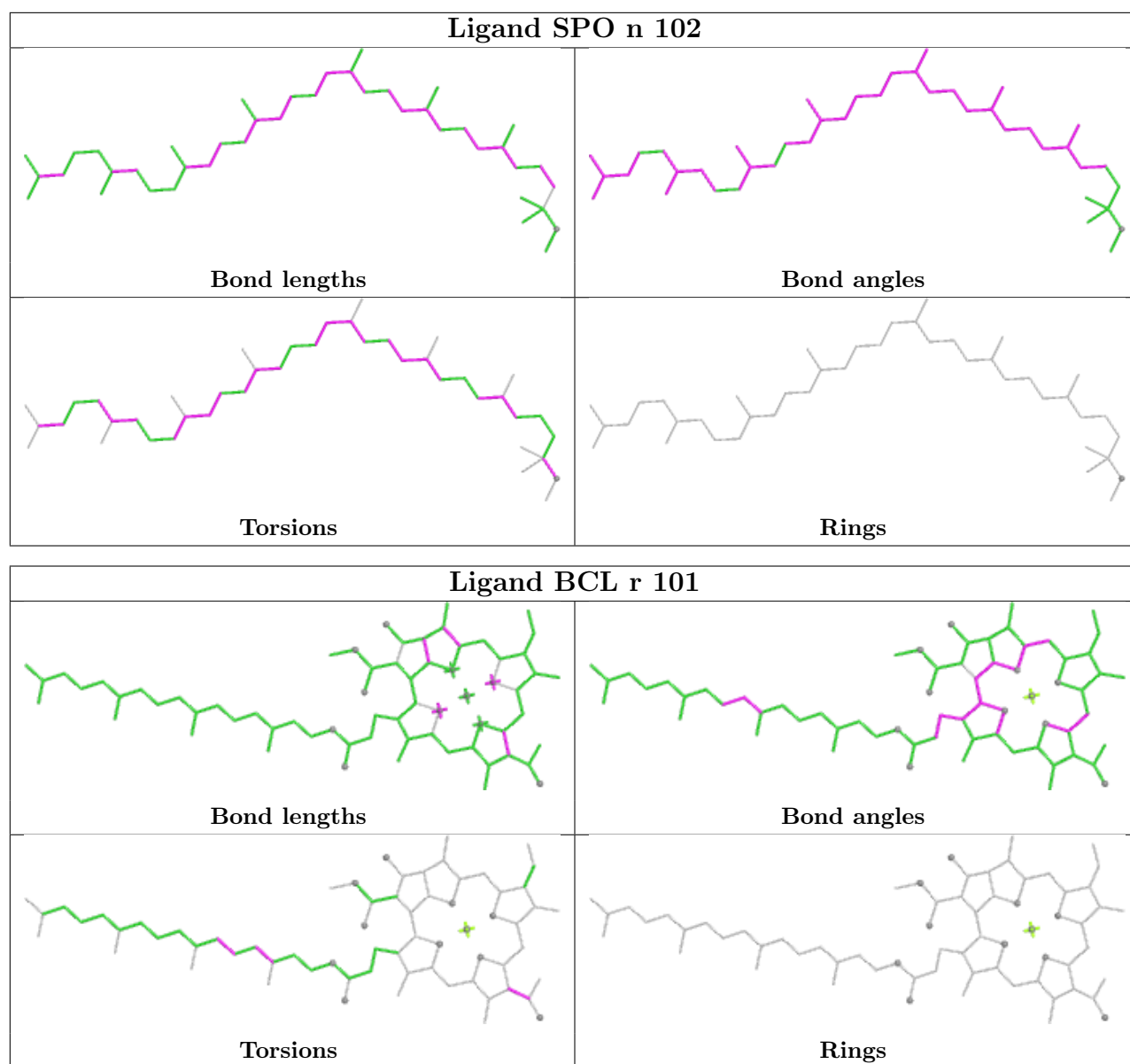
Ligand BCL s 102	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand SPO D 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

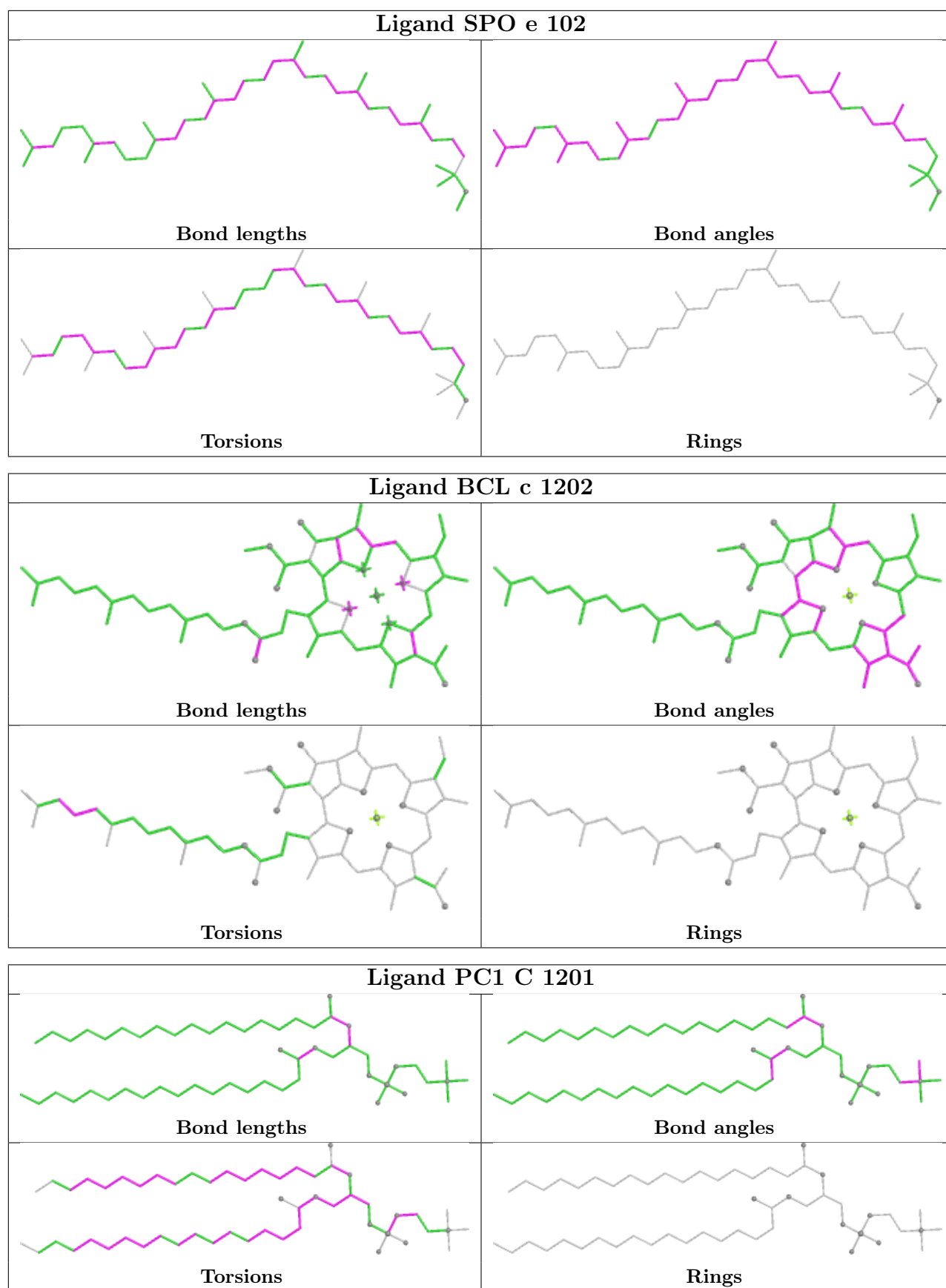


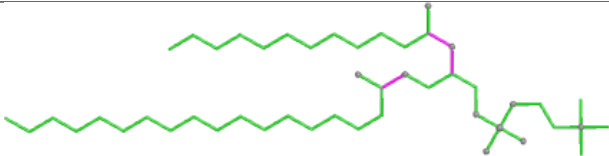
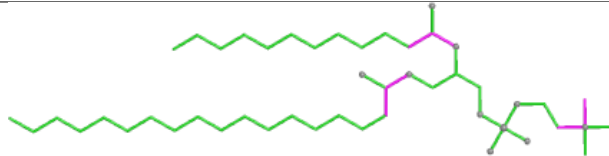
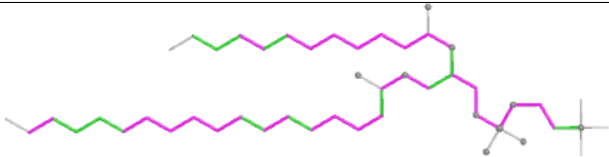
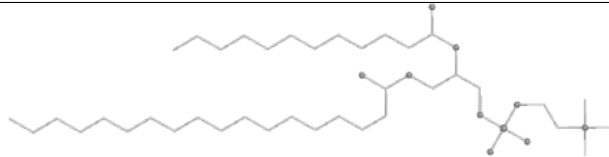


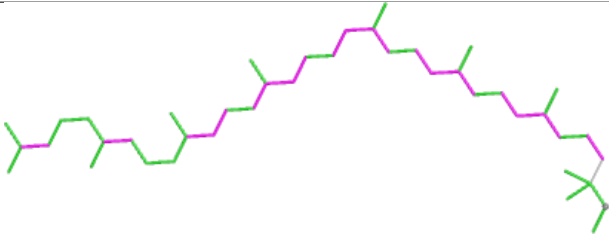
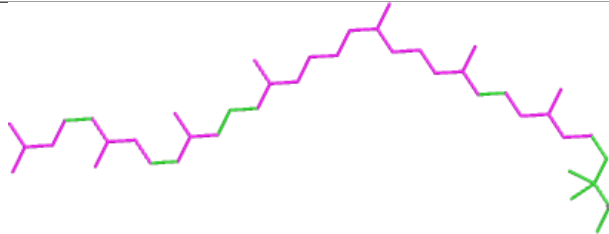
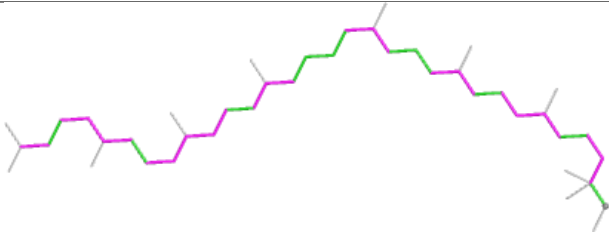
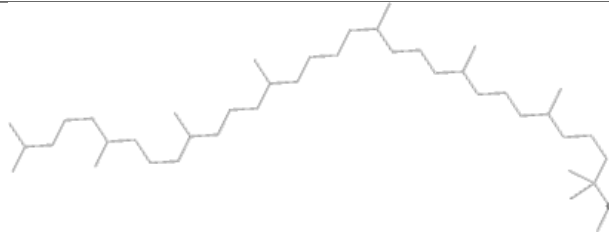


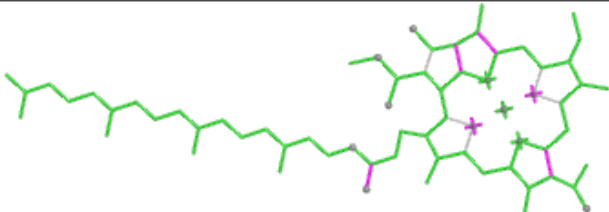
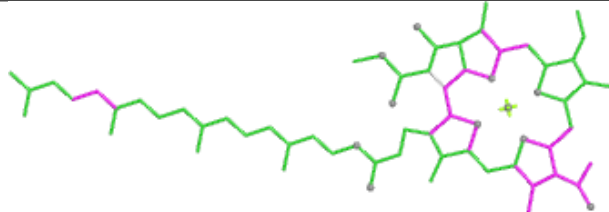
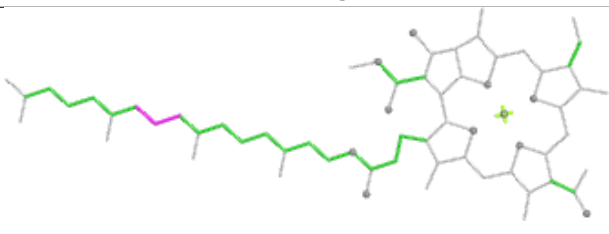
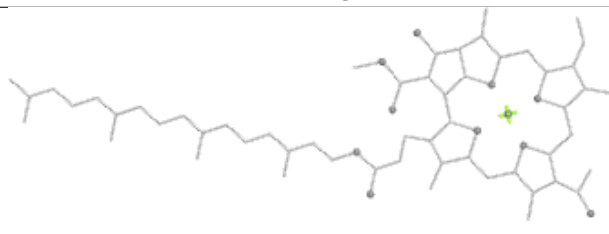


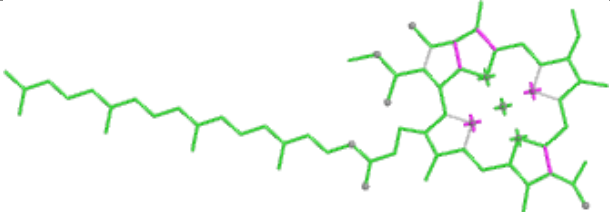
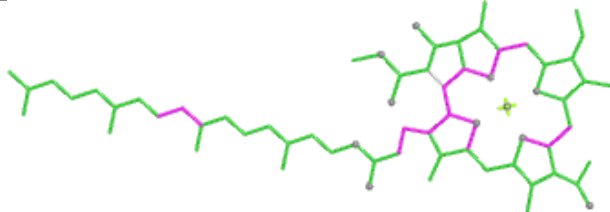
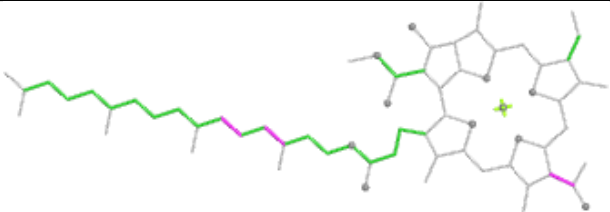
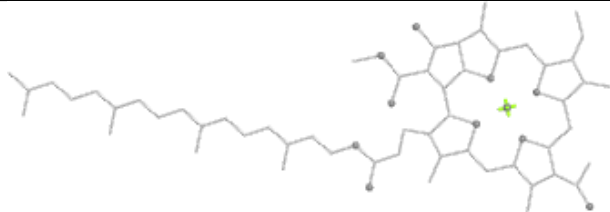
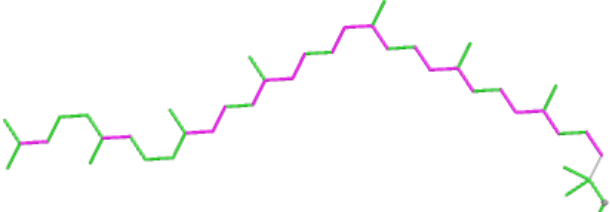
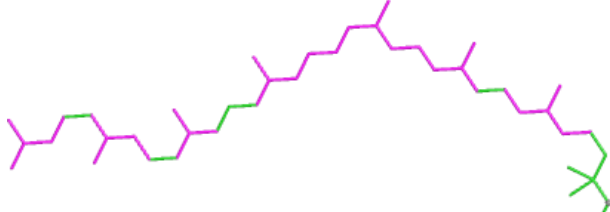
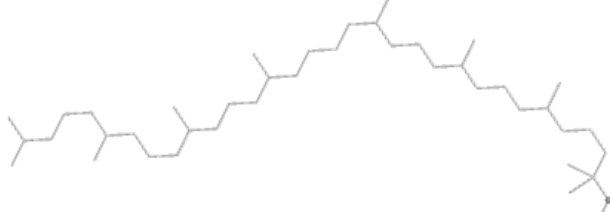


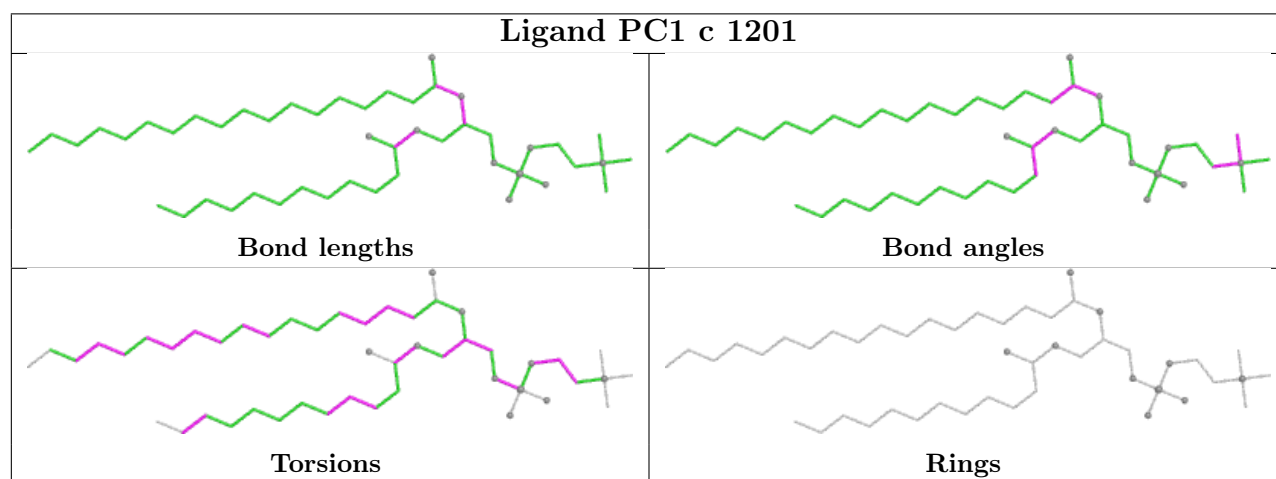
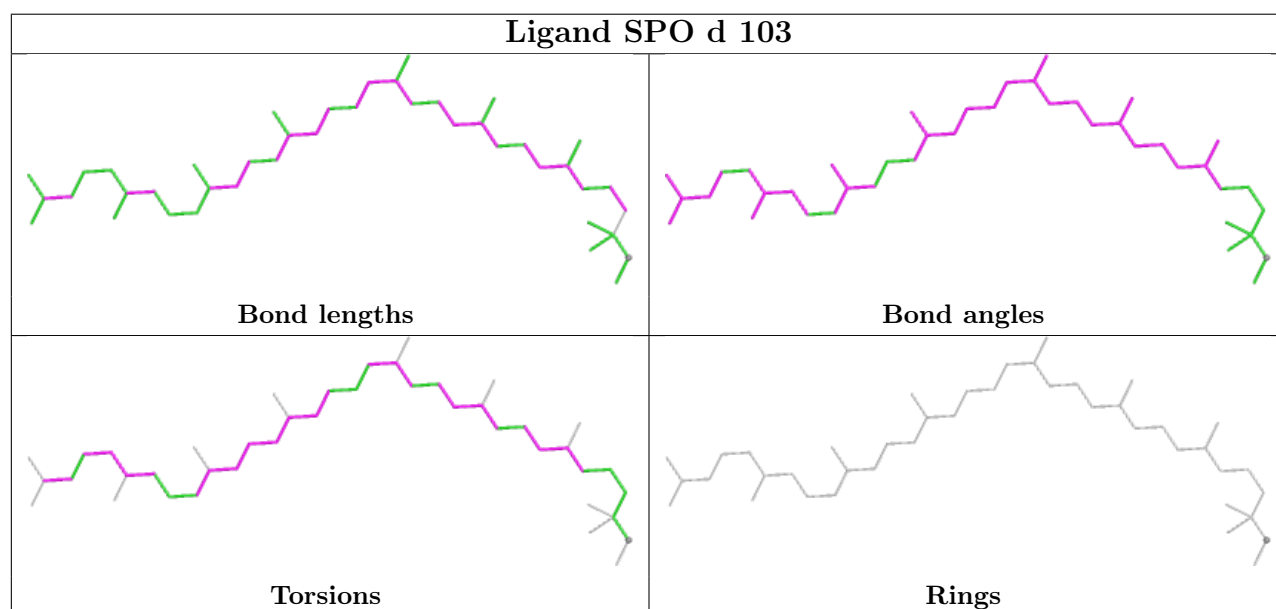
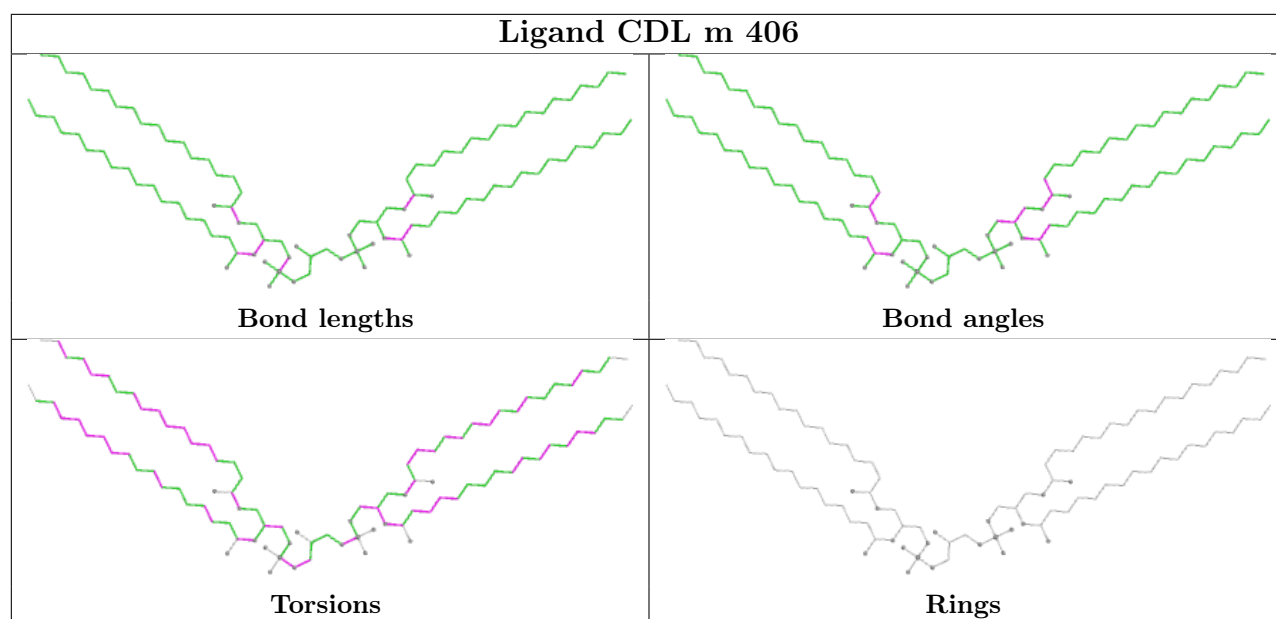


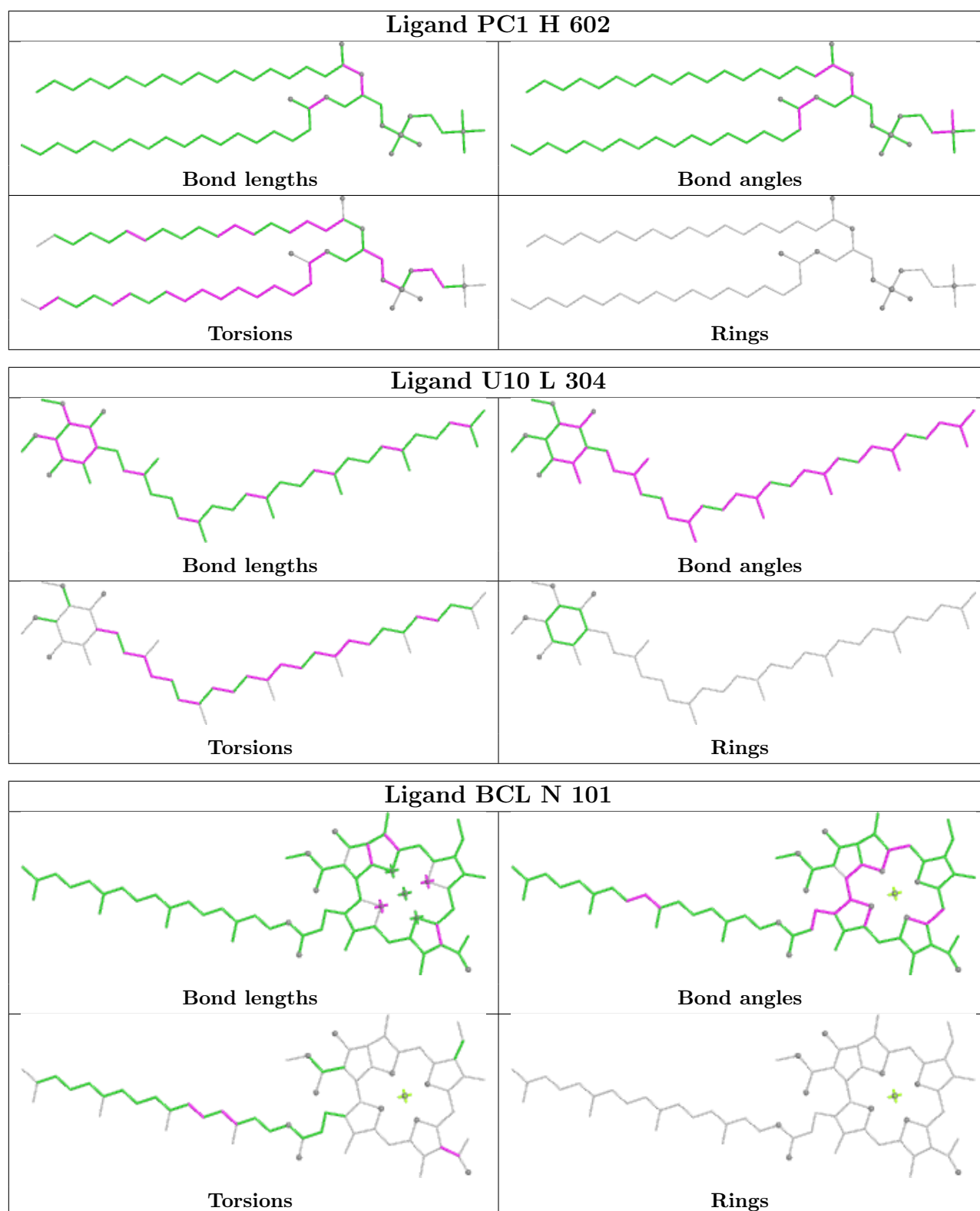
Ligand PC1 h 301	
	
Bond lengths	Bond angles
	
Torsions	Rings

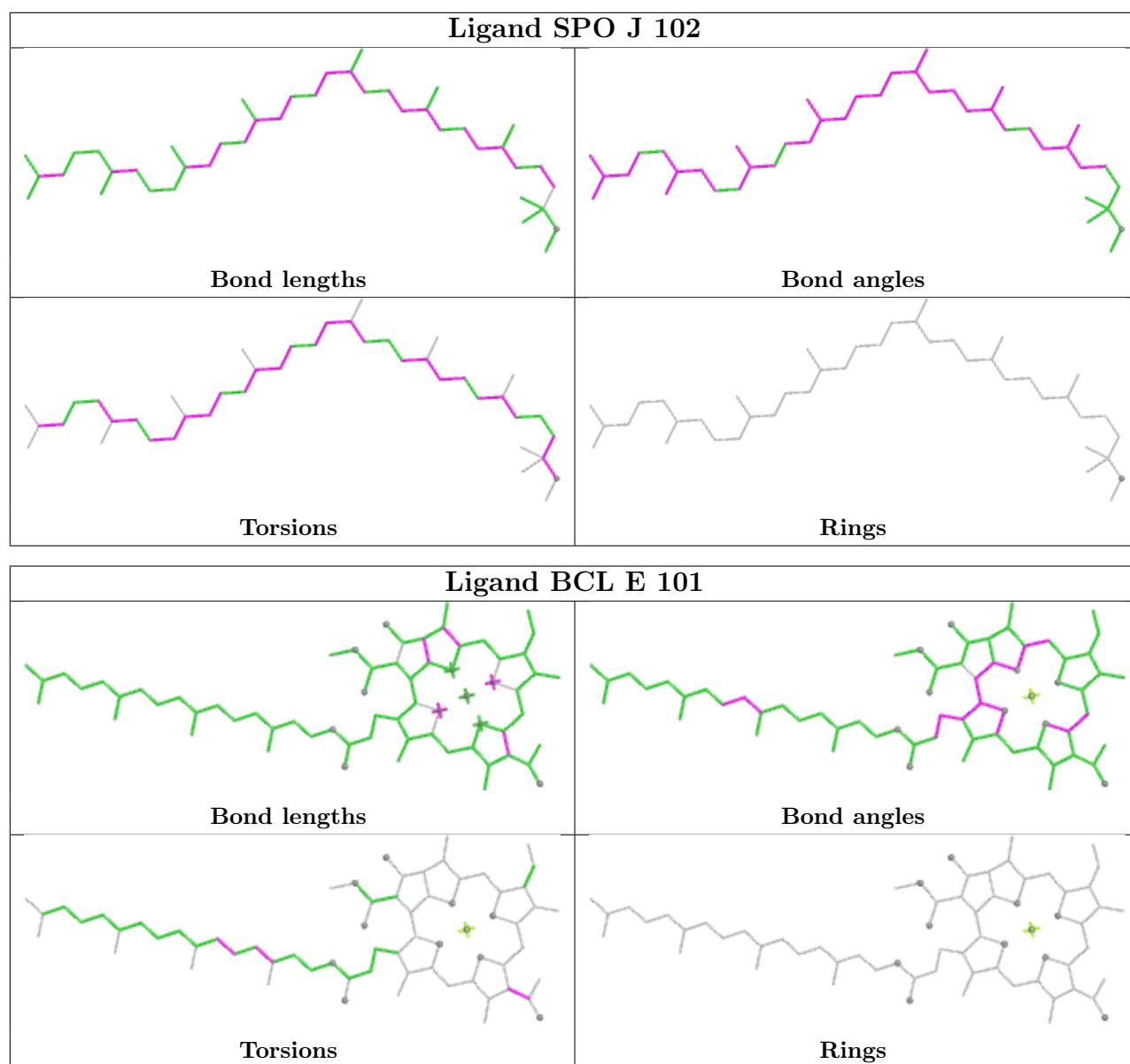
Ligand SPO u 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

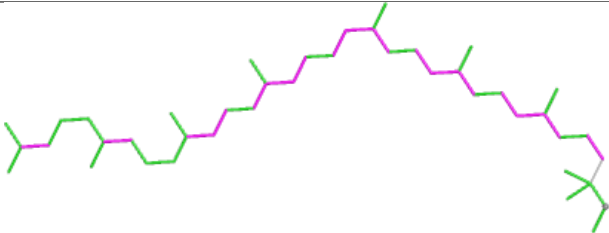
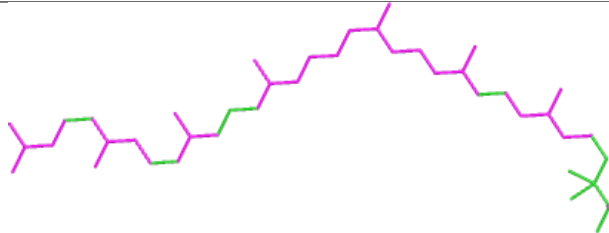
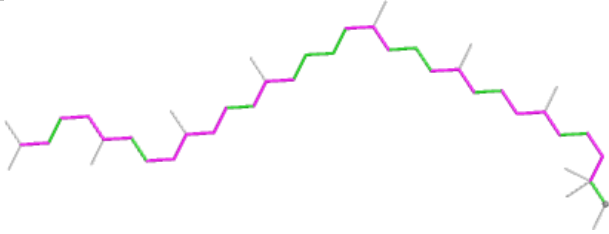
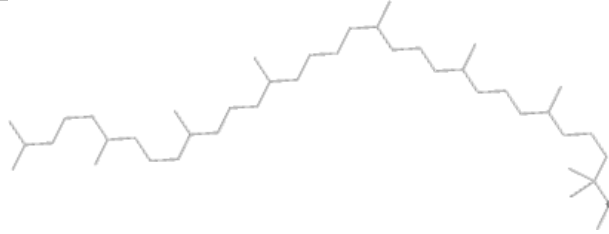
Ligand BCL f 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

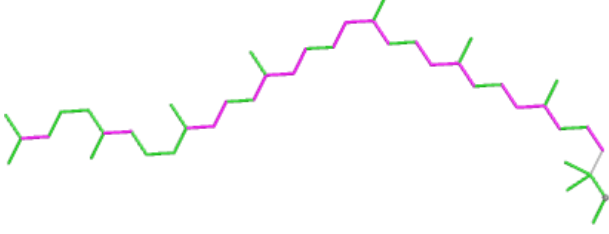
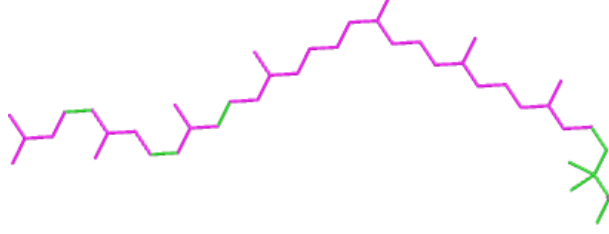
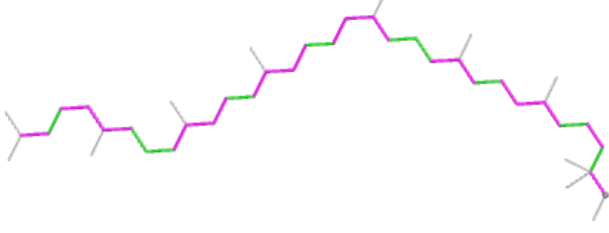
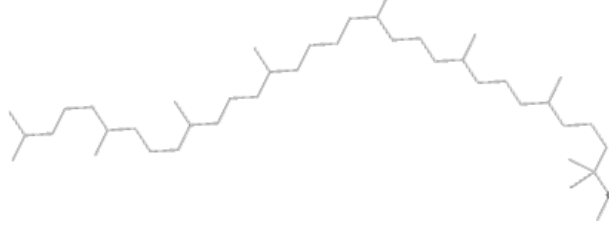
Ligand BCL i 102	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand SPO C 1203	
 Bond lengths	 Bond angles
 Torsions	 Rings

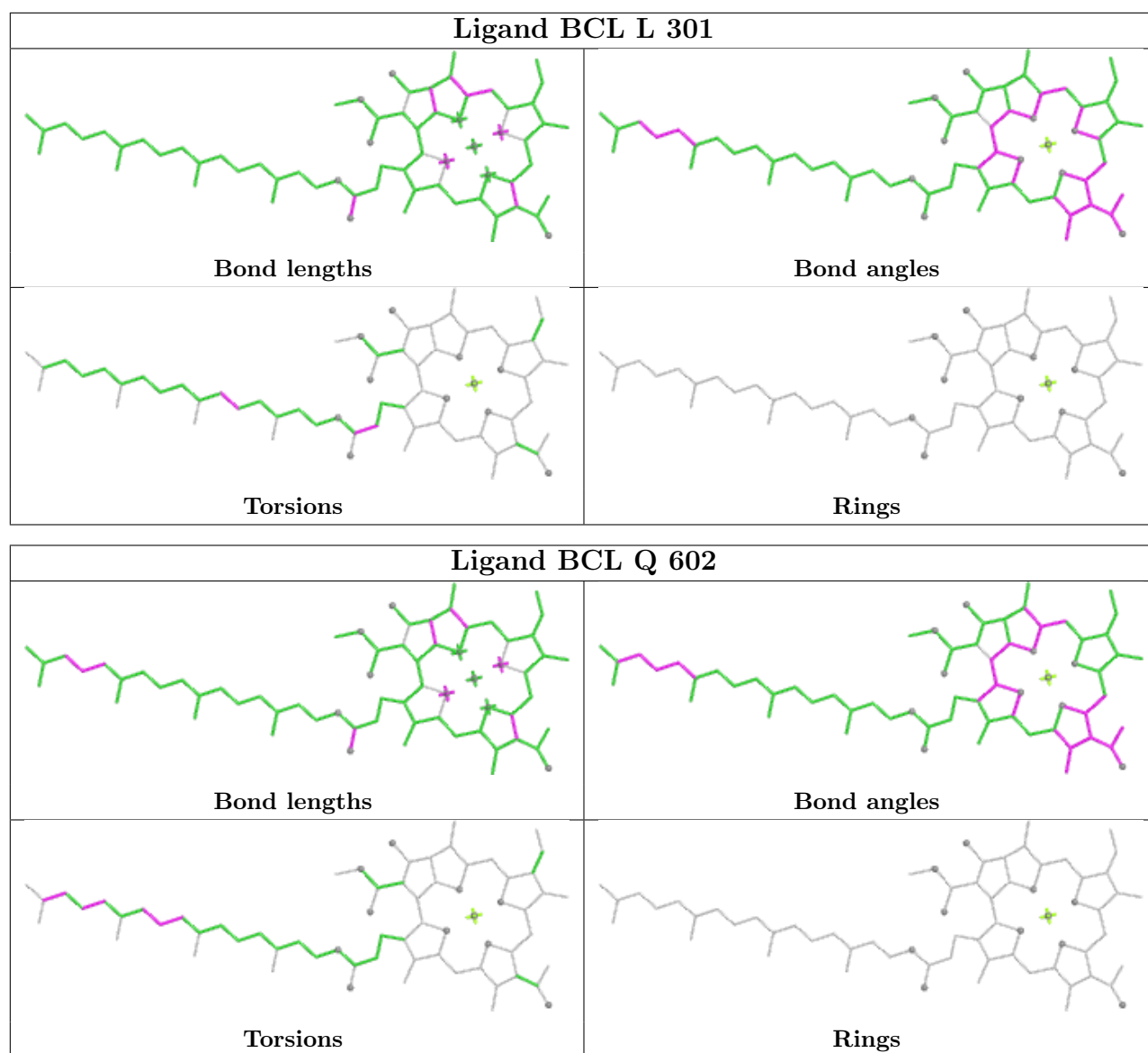




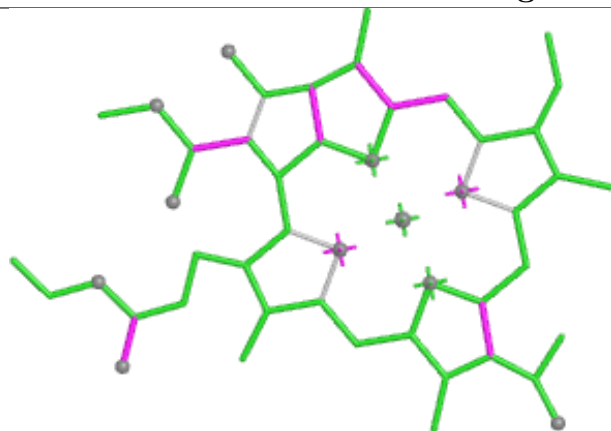


Ligand SPO F 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

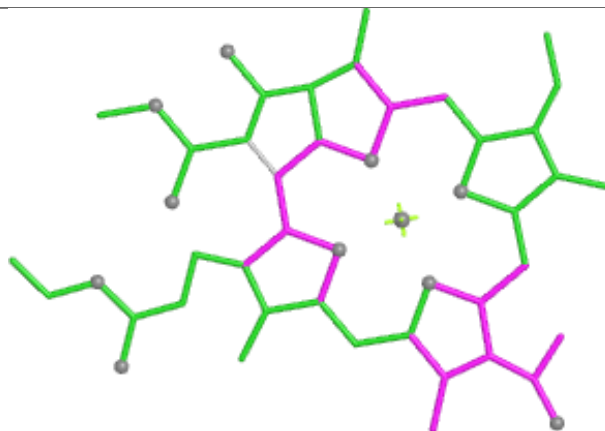
Ligand SPO p 102	
	
Bond lengths	Bond angles
	
Torsions	Rings



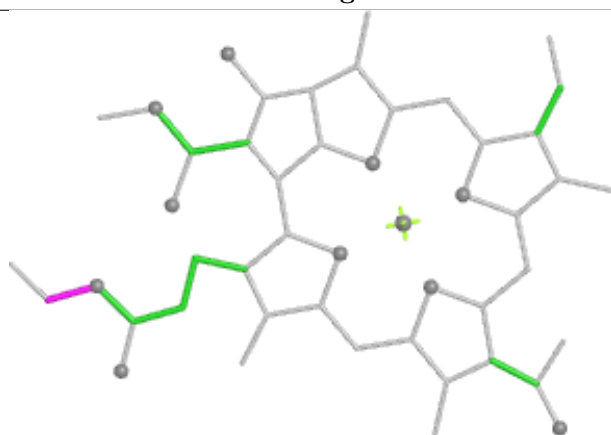
Ligand BCL L 305



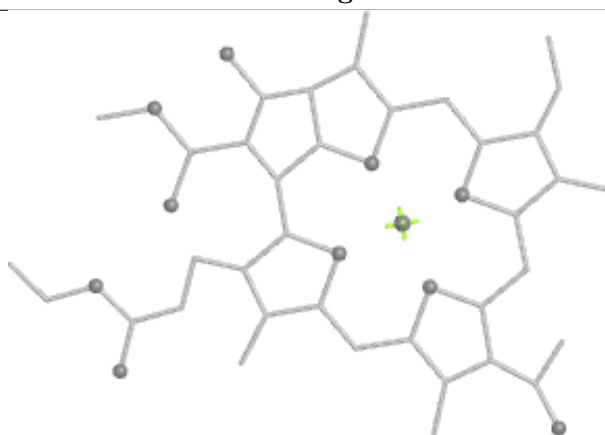
Bond lengths



Bond angles

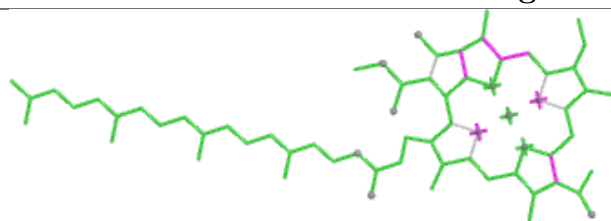


Torsions

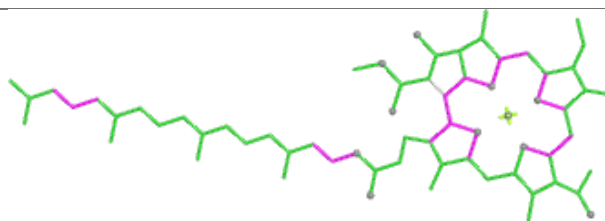


Rings

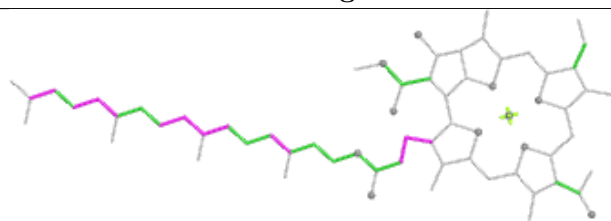
Ligand BCL v 101



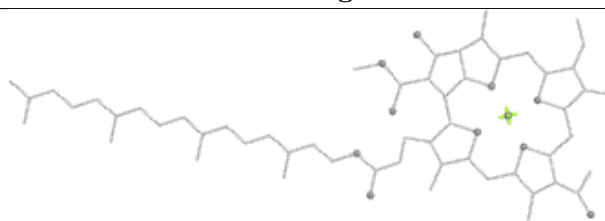
Bond lengths



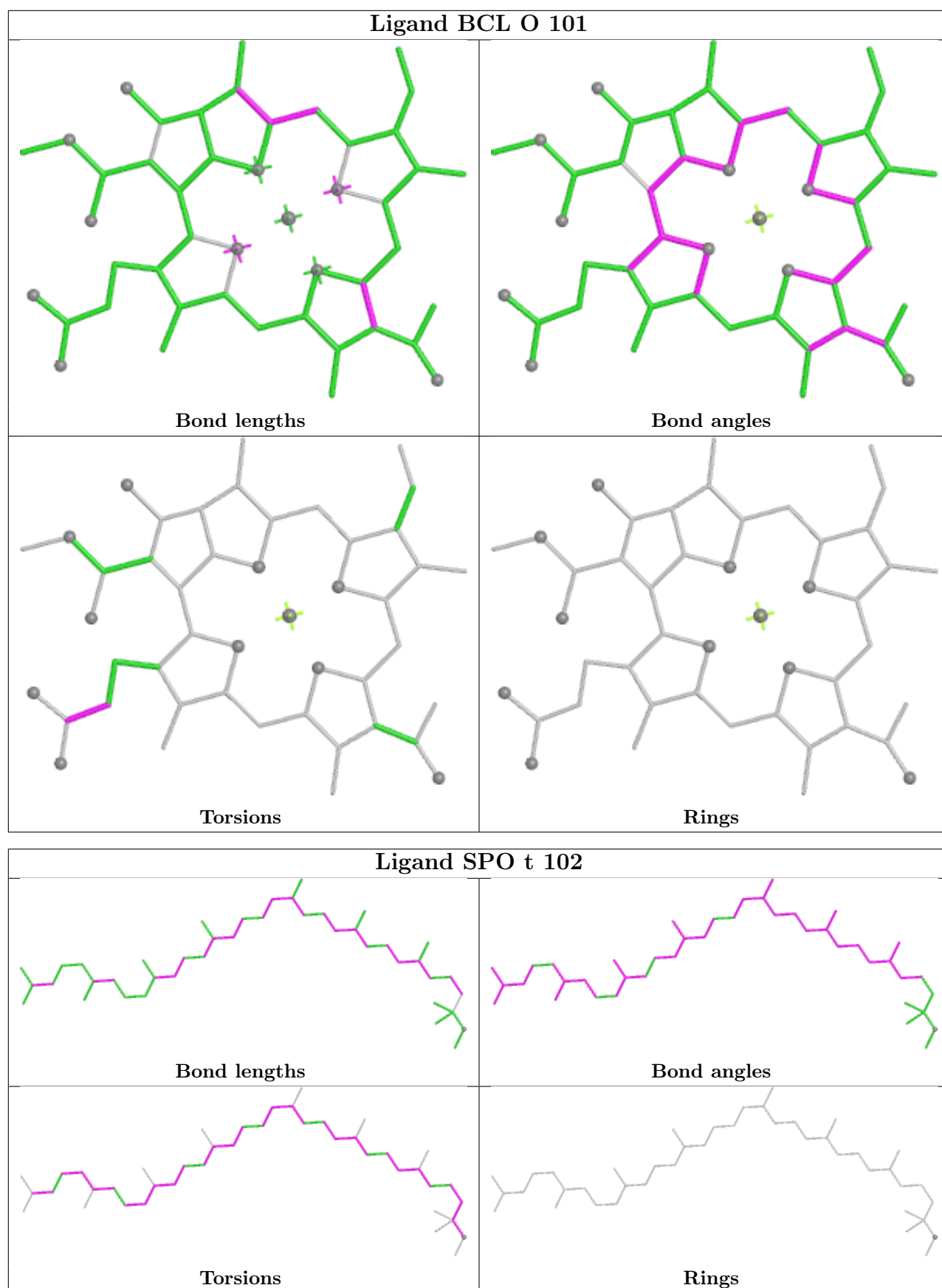
Bond angles

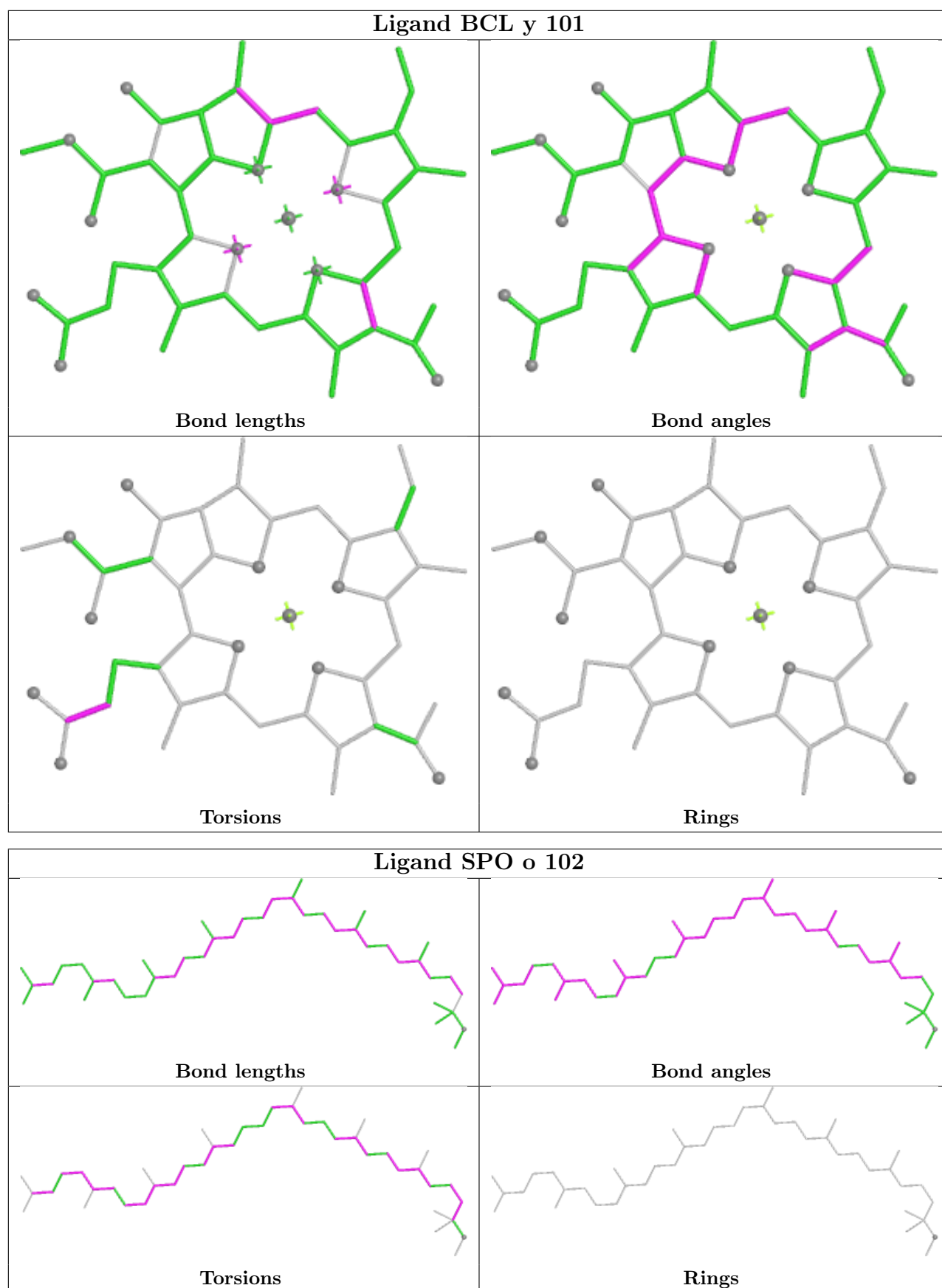


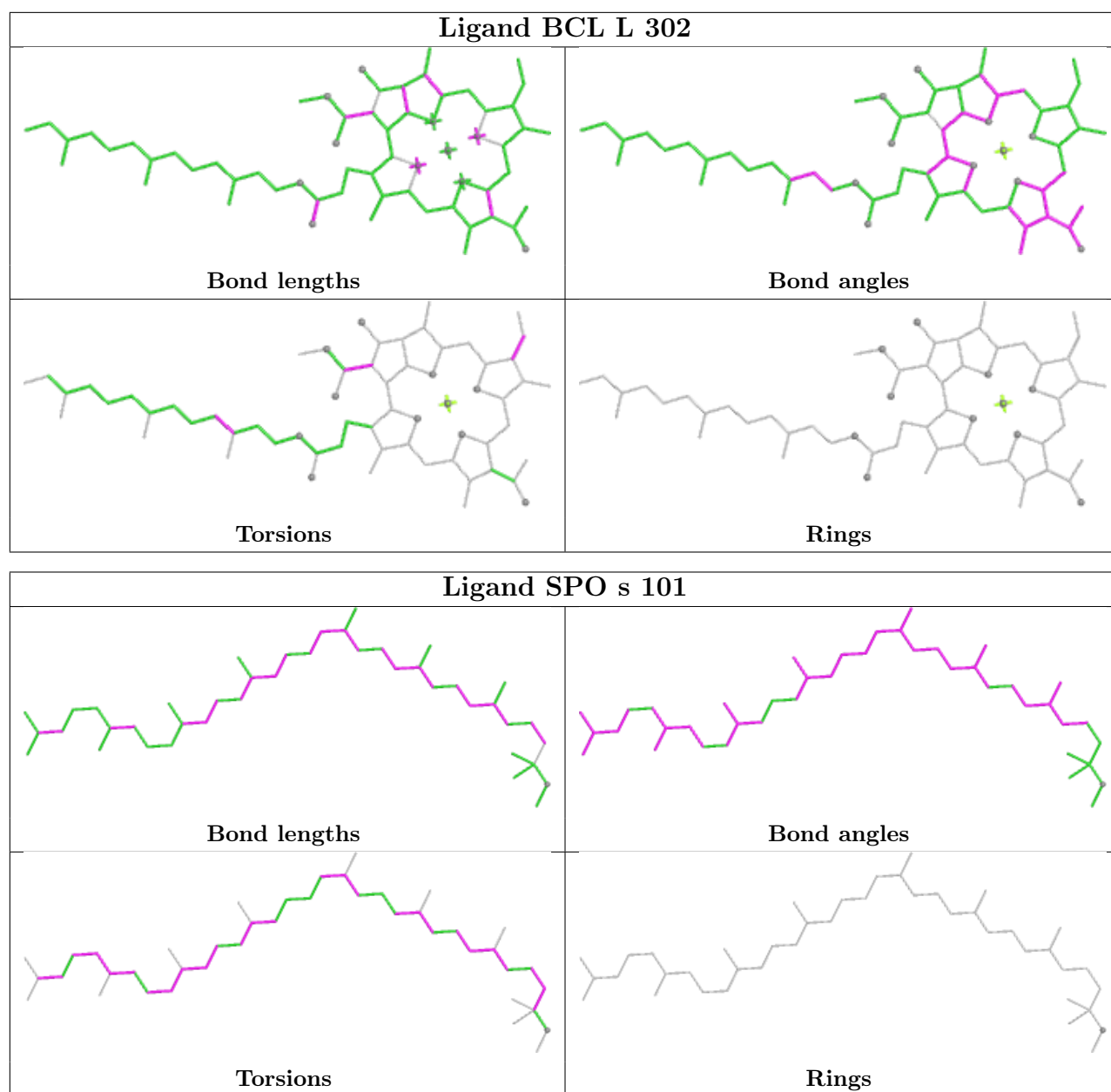
Torsions



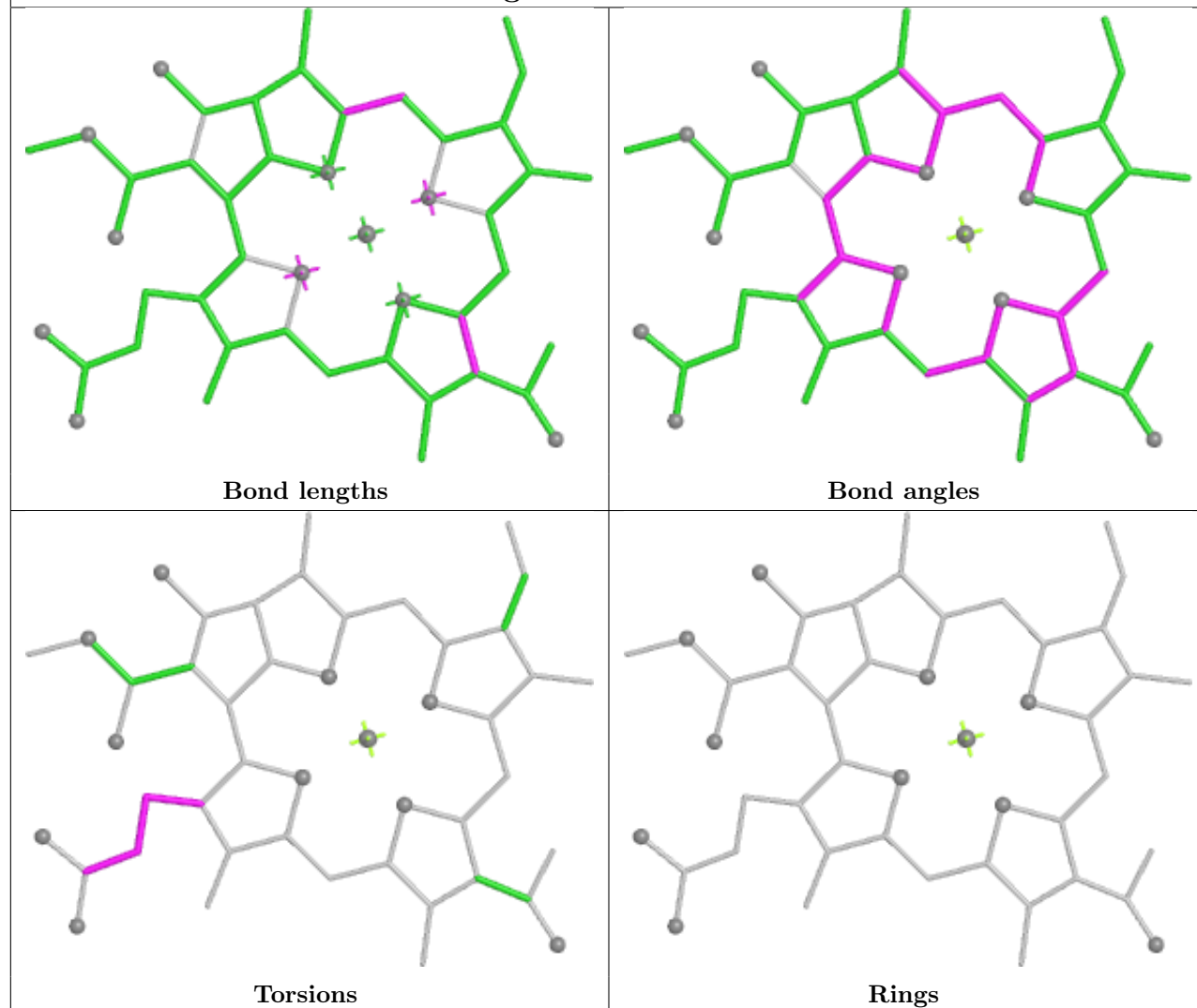
Rings



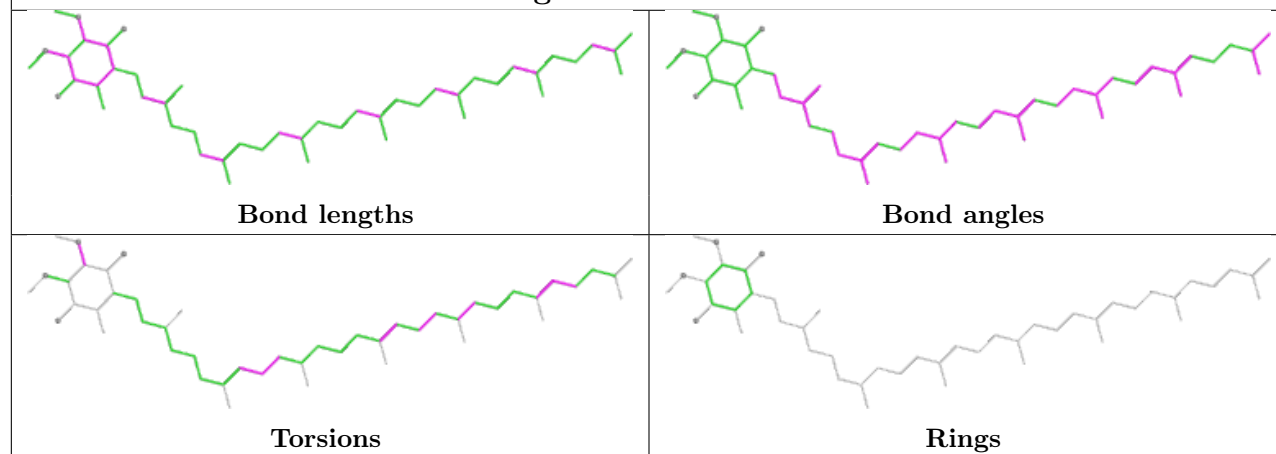


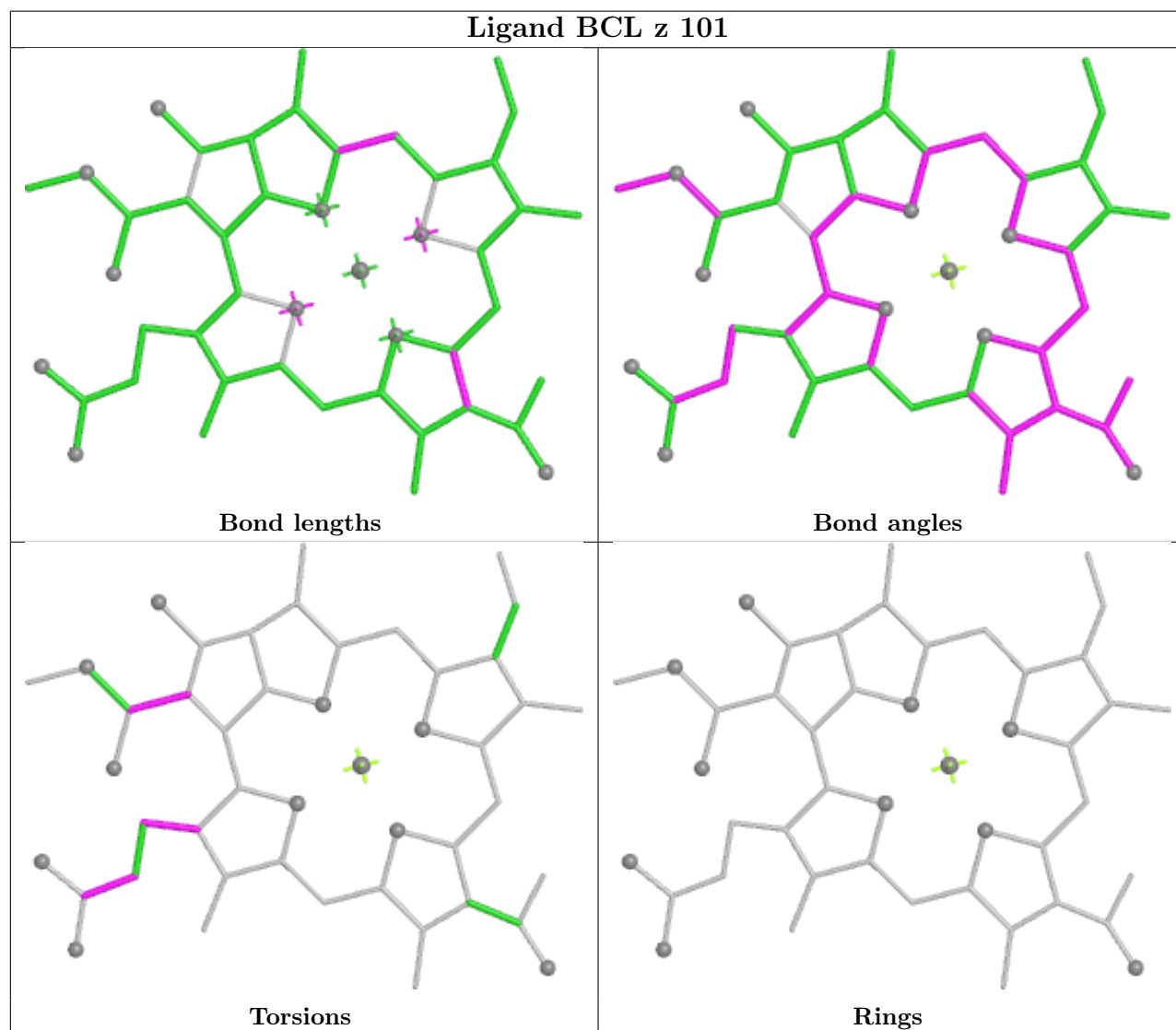
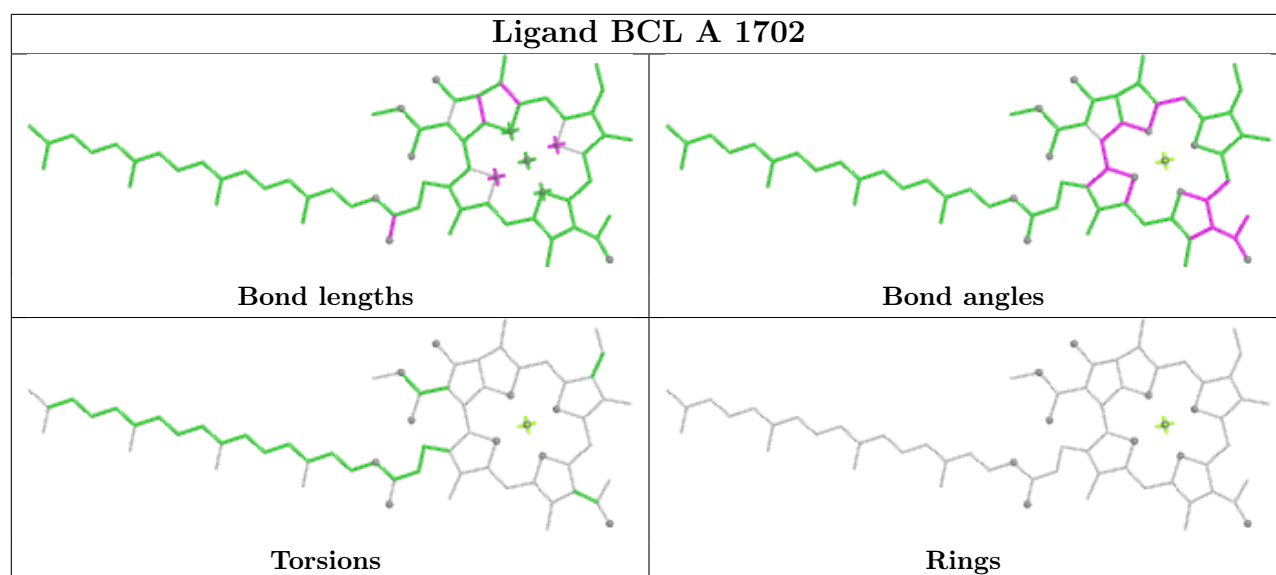


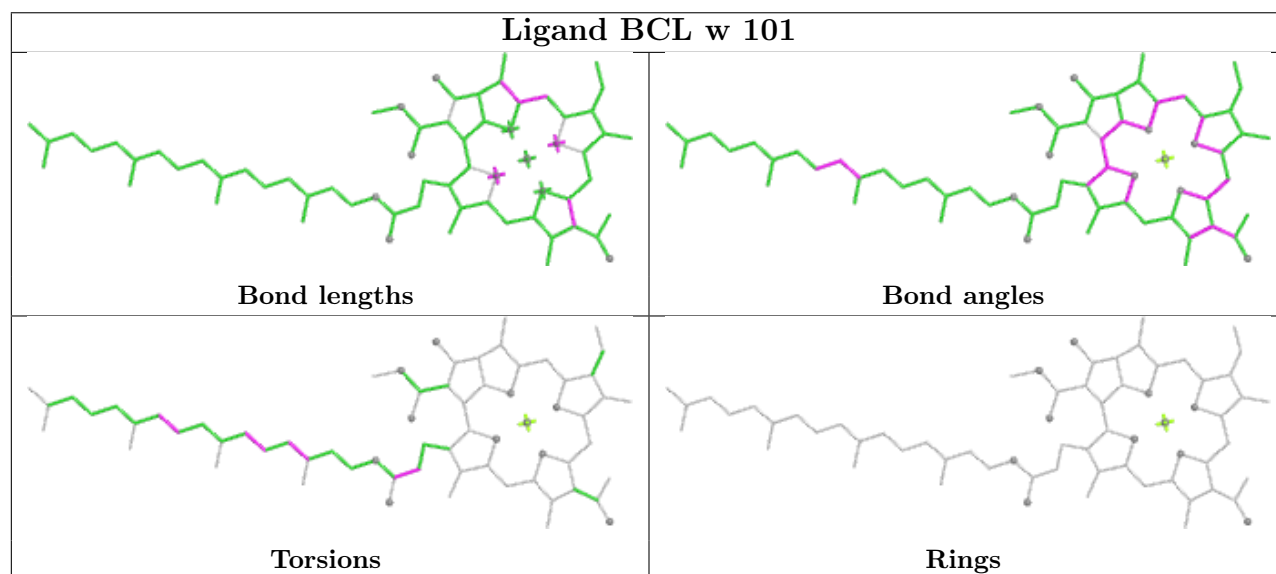
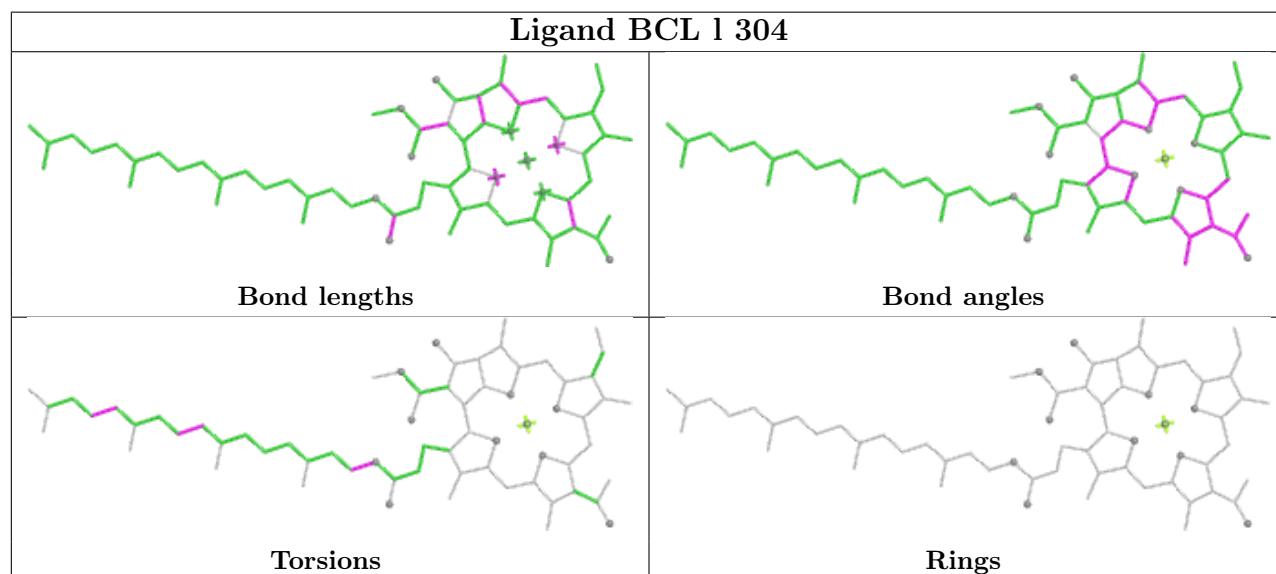
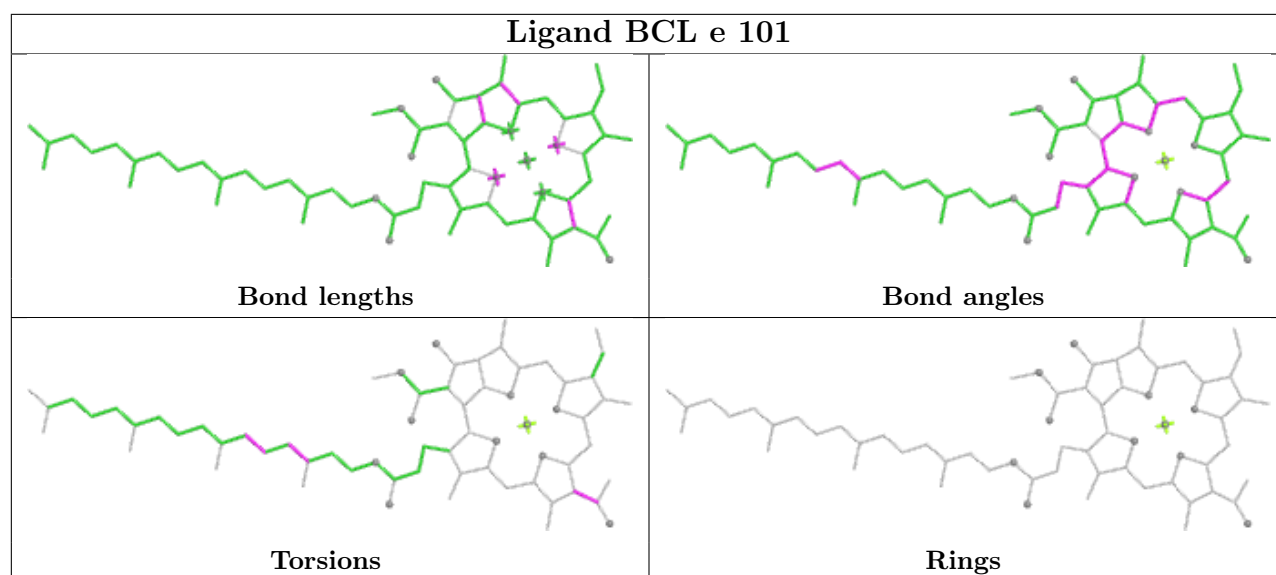
Ligand BCL 4 101

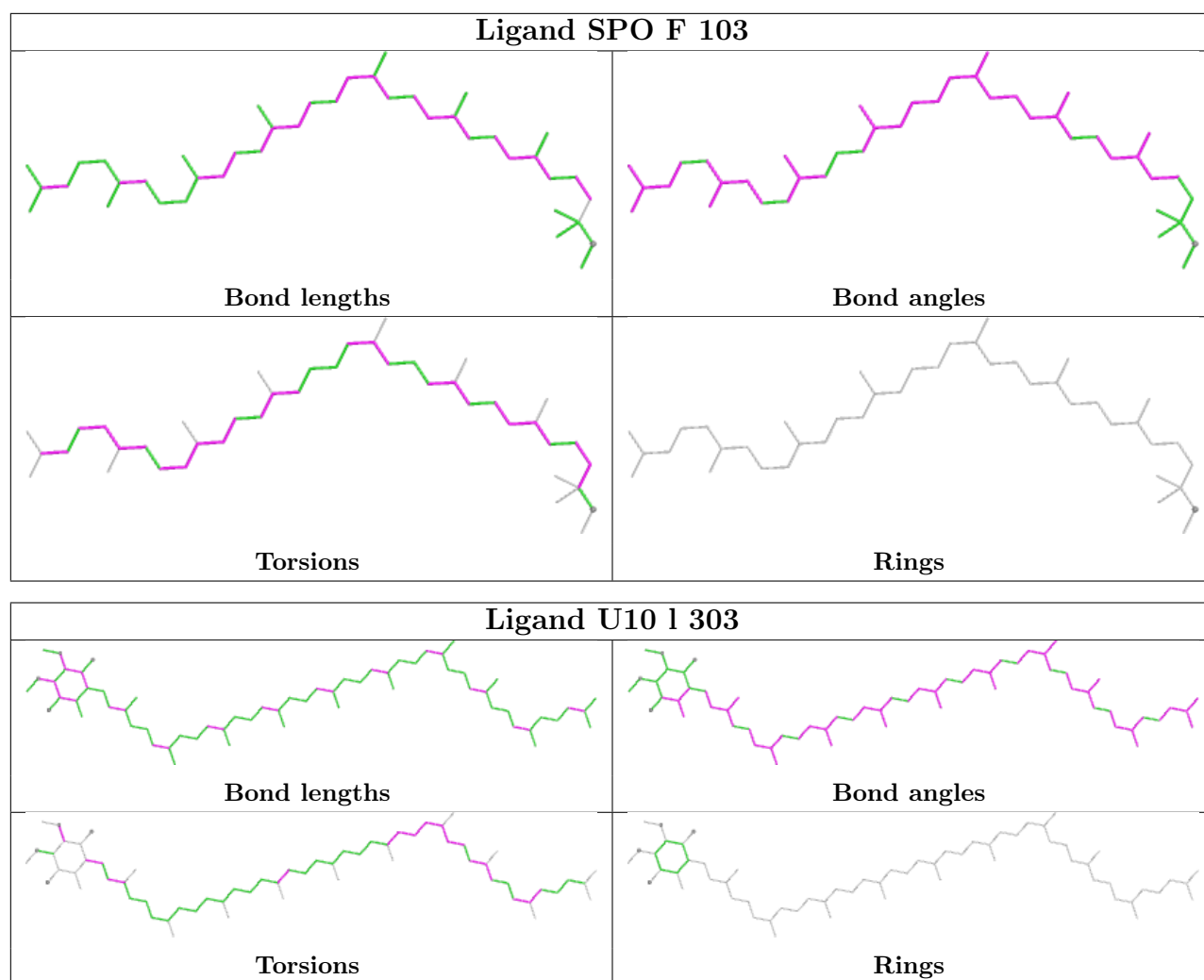


Ligand U10 M 403









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.

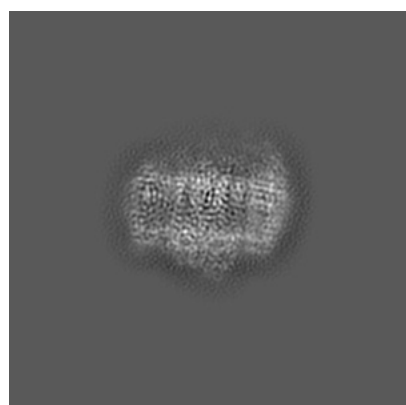
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31875. 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](#)

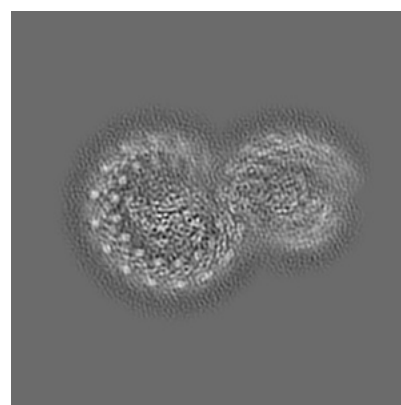
6.1.1 Primary map



X



Y

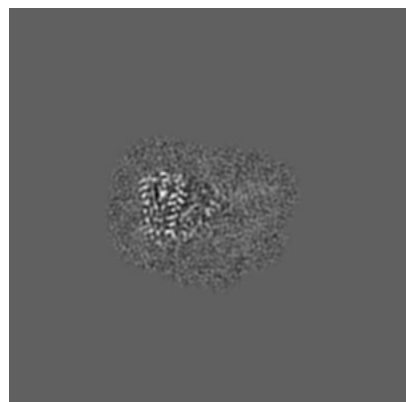


Z

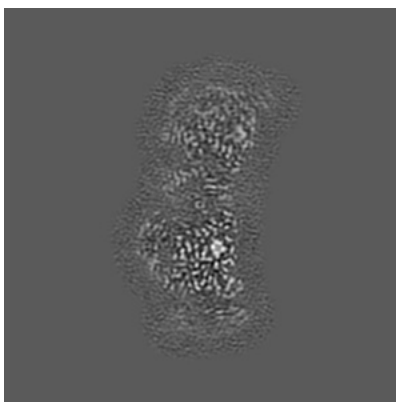
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

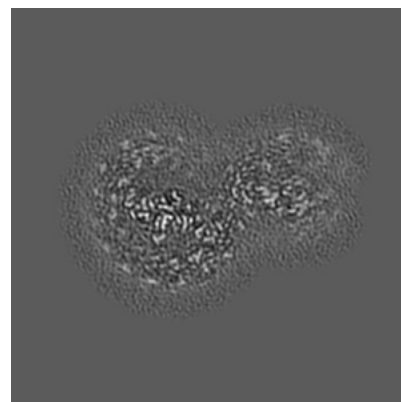
6.2.1 Primary map



X Index: 175



Y Index: 175

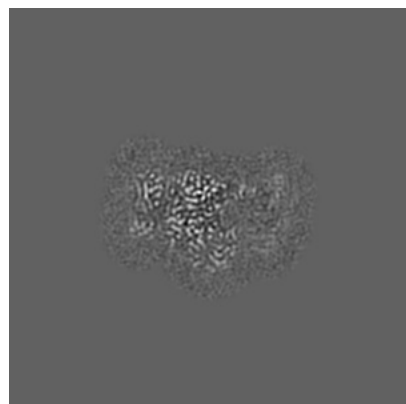


Z Index: 175

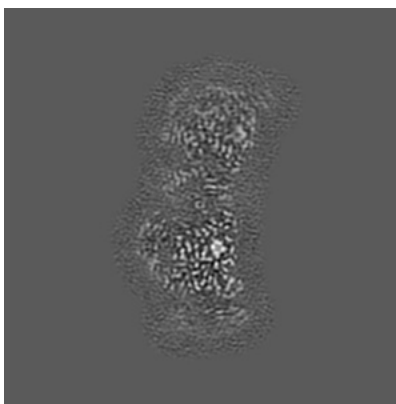
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

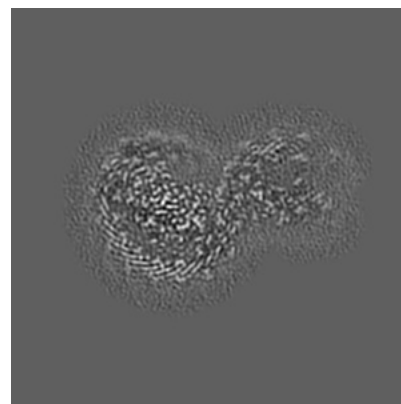
6.3.1 Primary map



X Index: 132



Y Index: 175

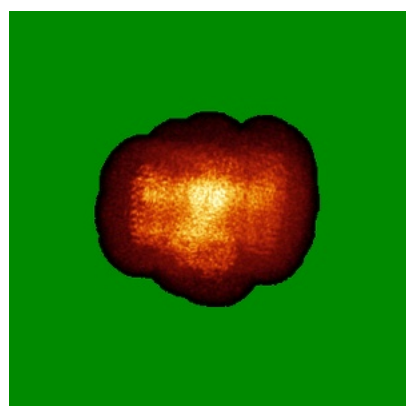


Z Index: 190

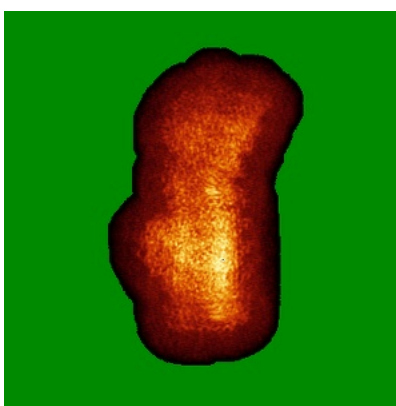
The images above show the largest variance slices of the map in three orthogonal directions.

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

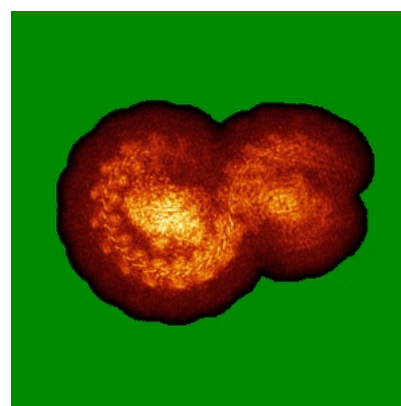
6.4.1 Primary map



X



Y

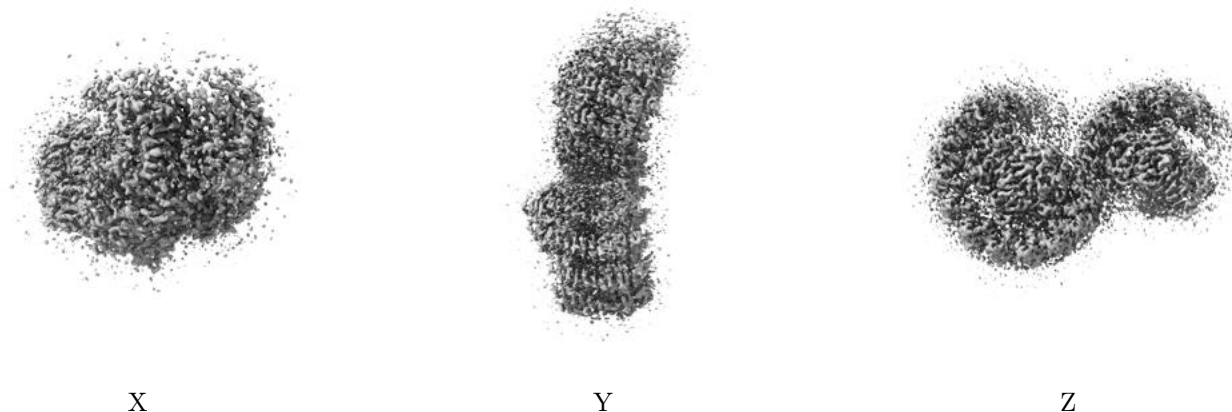


Z

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 0.0183. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

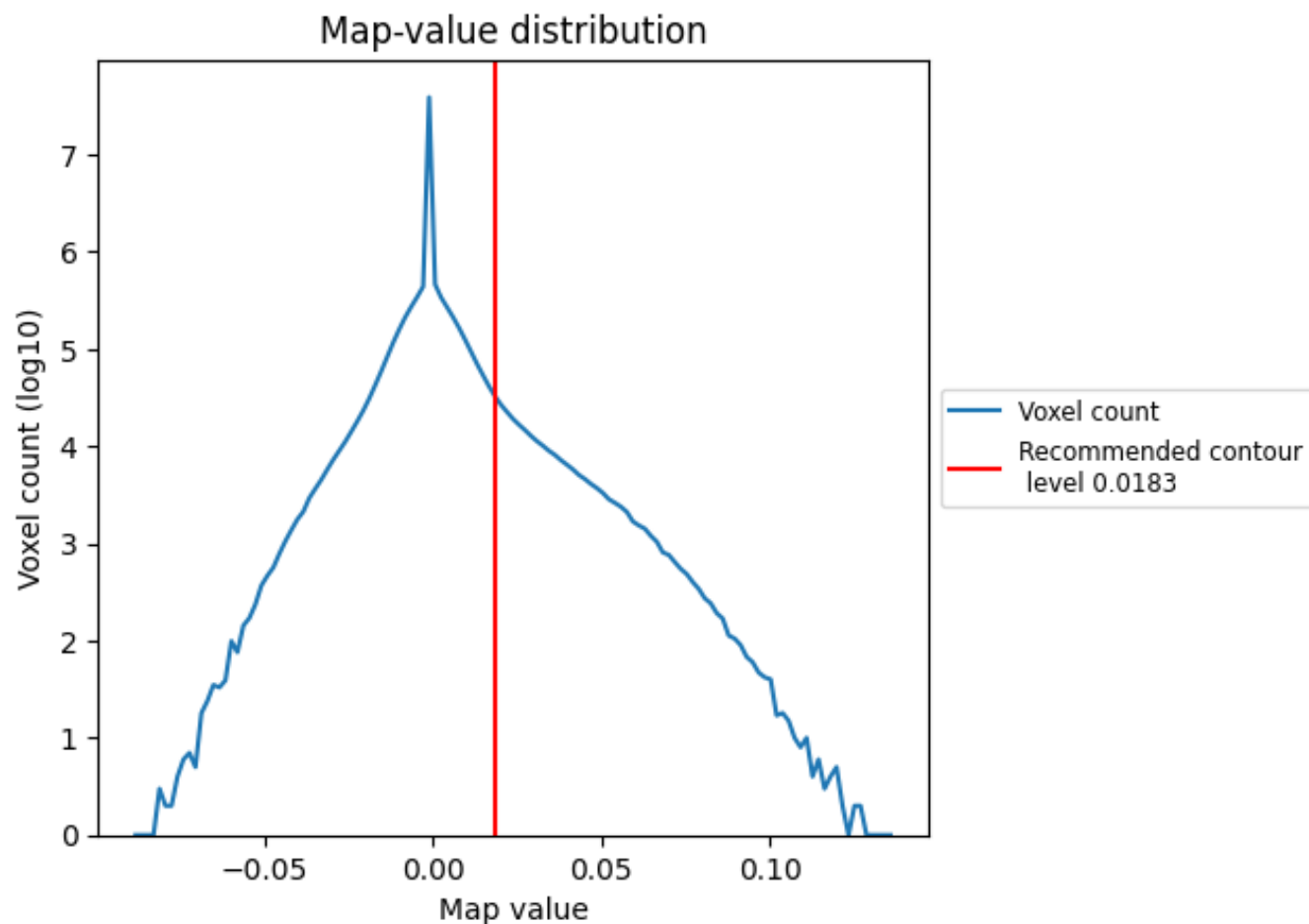
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

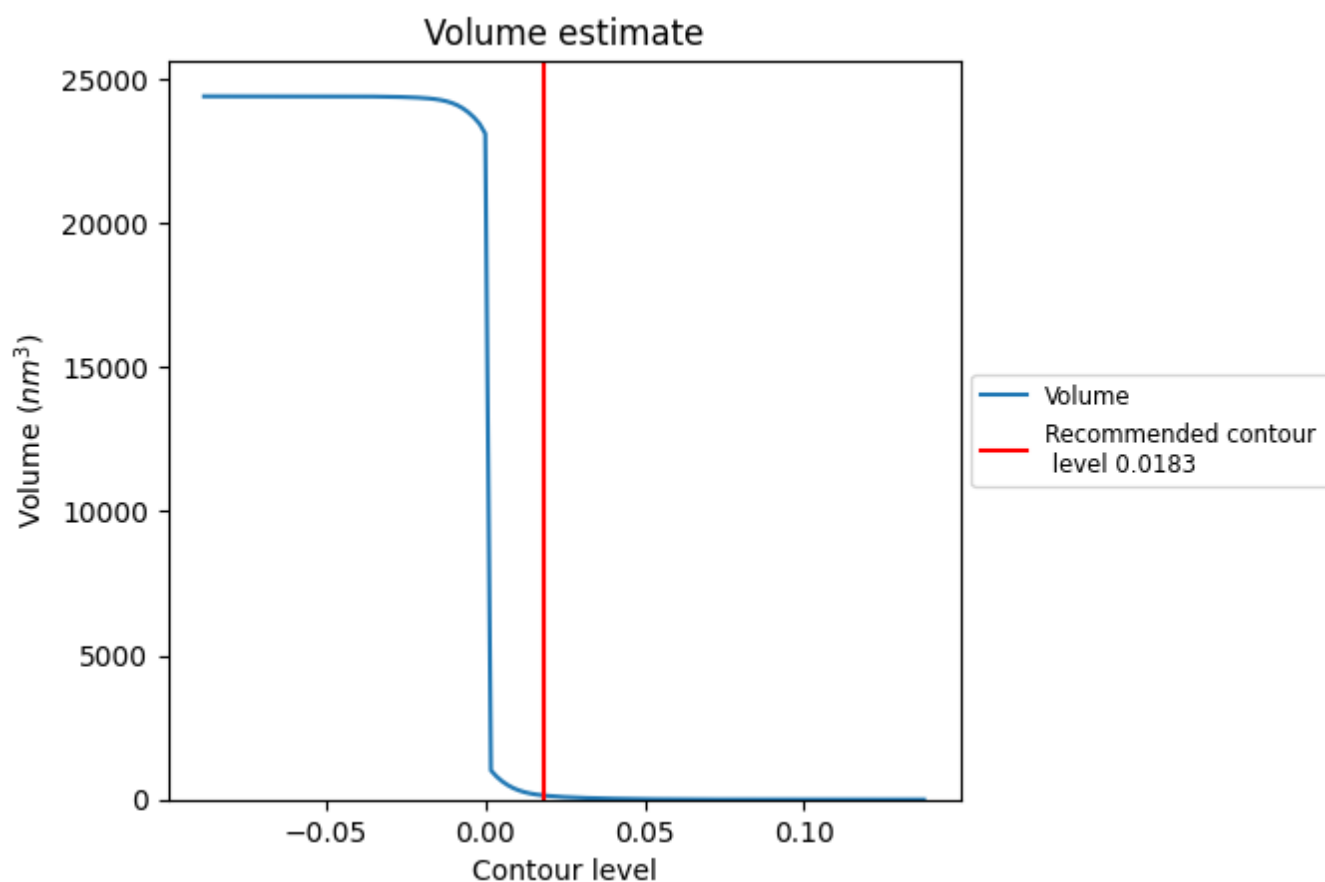
This section contains the results of statistical analysis of the map.

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.

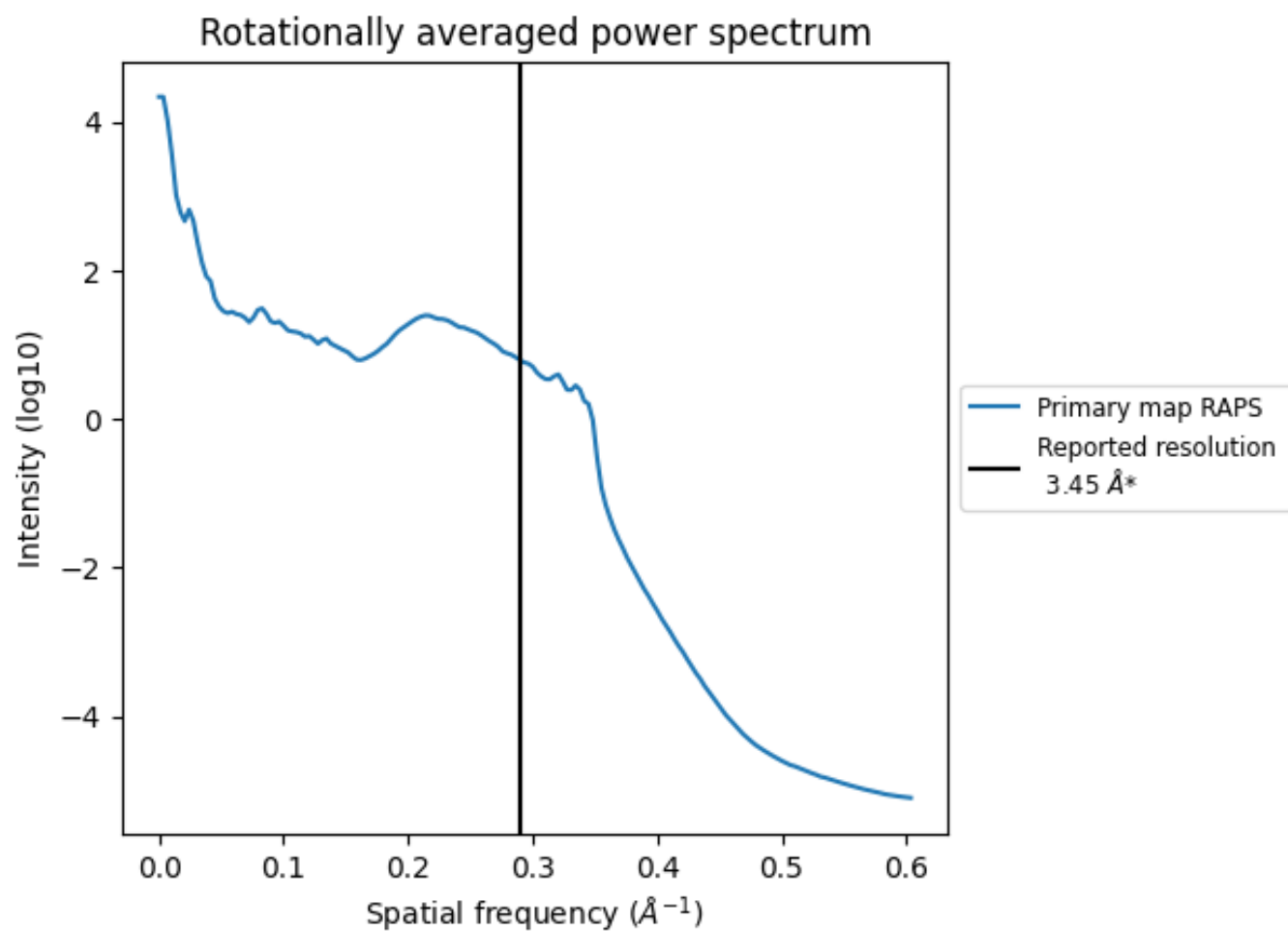
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 142 nm³; this corresponds to an approximate mass of 128 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 ⓘ

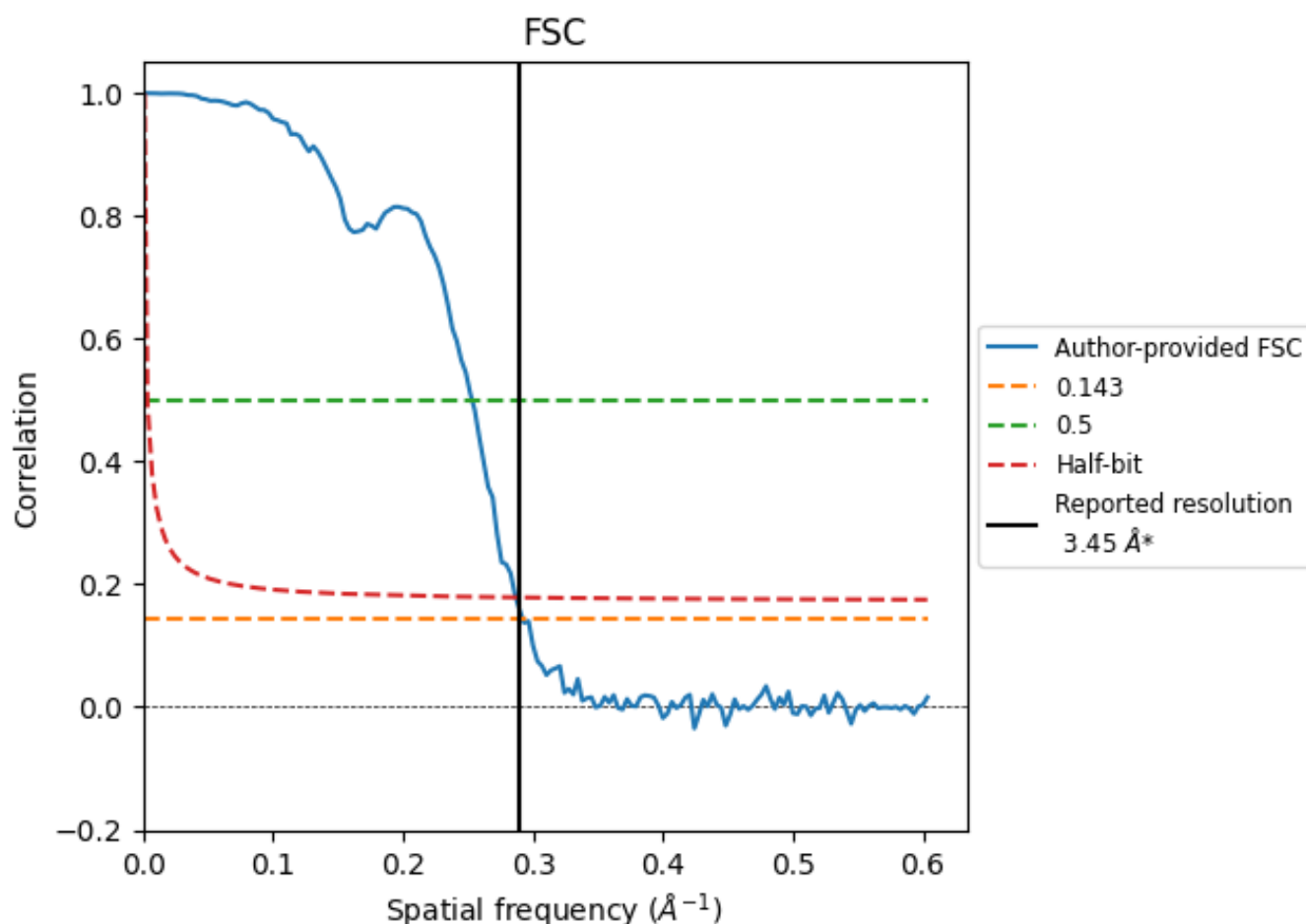


*Reported resolution corresponds to spatial frequency of 0.290 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.290 Å⁻¹

8.2 Resolution estimates [i](#)

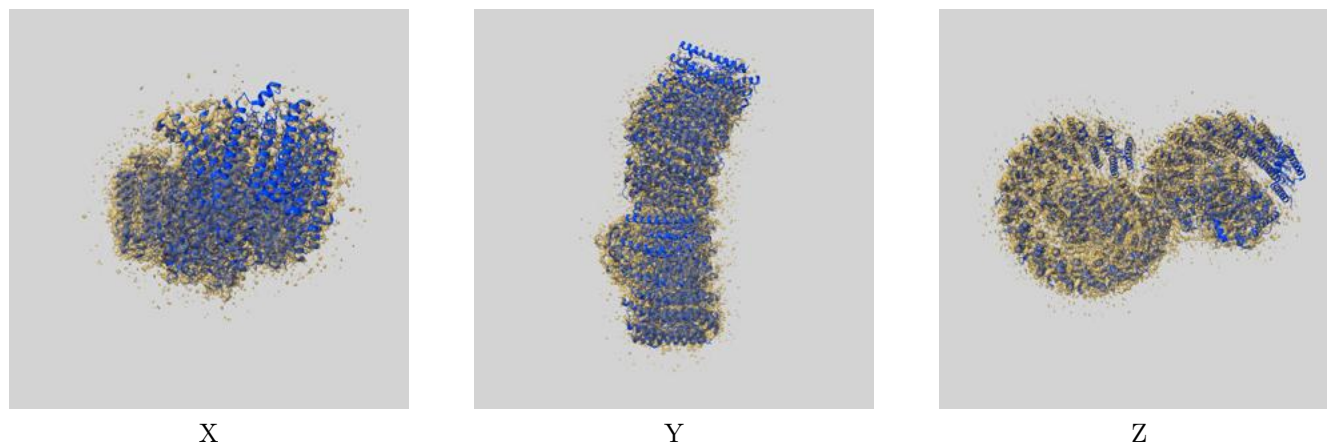
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.45	-	-
Author-provided FSC curve	3.42	3.95	3.49
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

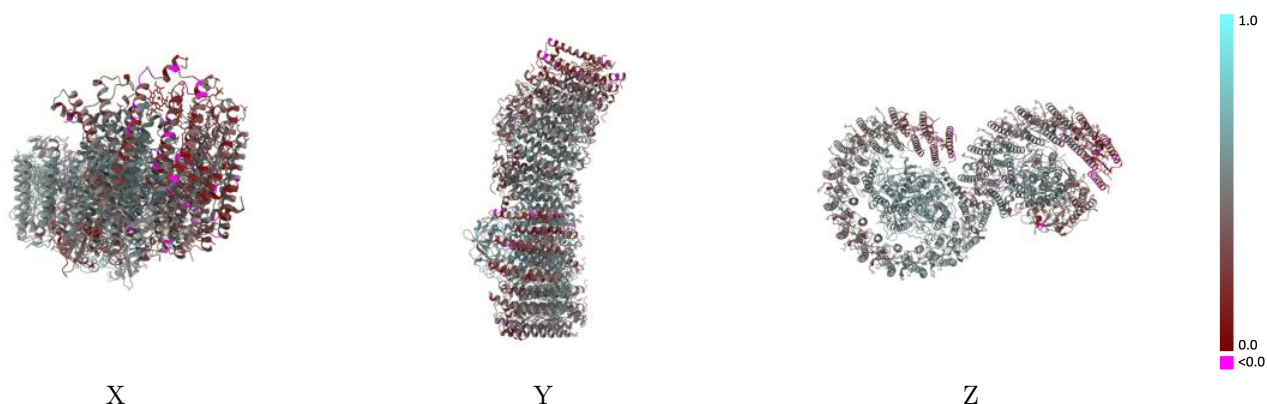
This section contains information regarding the fit between EMDB map EMD-31875 and PDB model 7VB9. Per-residue inclusion information can be found in [section 3](#) on [page 18](#).

9.1 Map-model overlay [i](#)



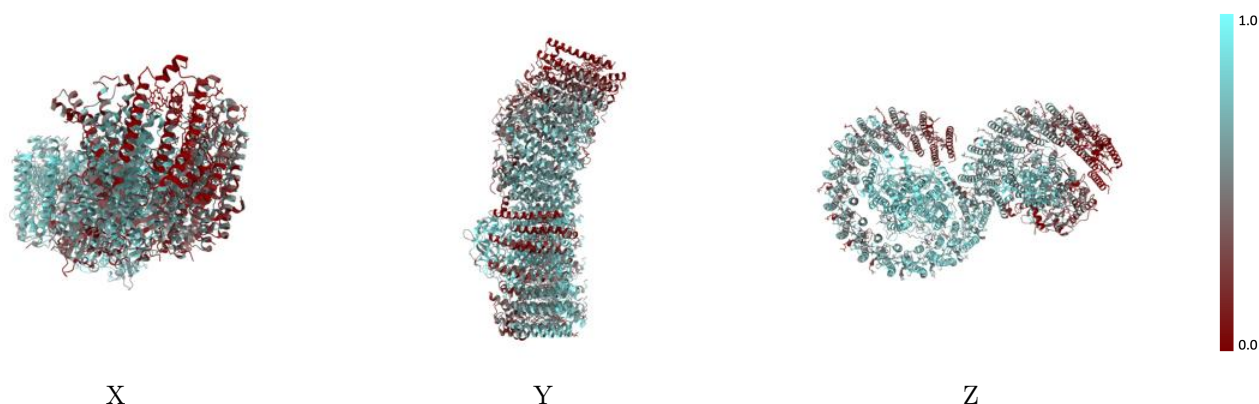
The images above show the 3D surface view of the map at the recommended contour level 0.0183 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



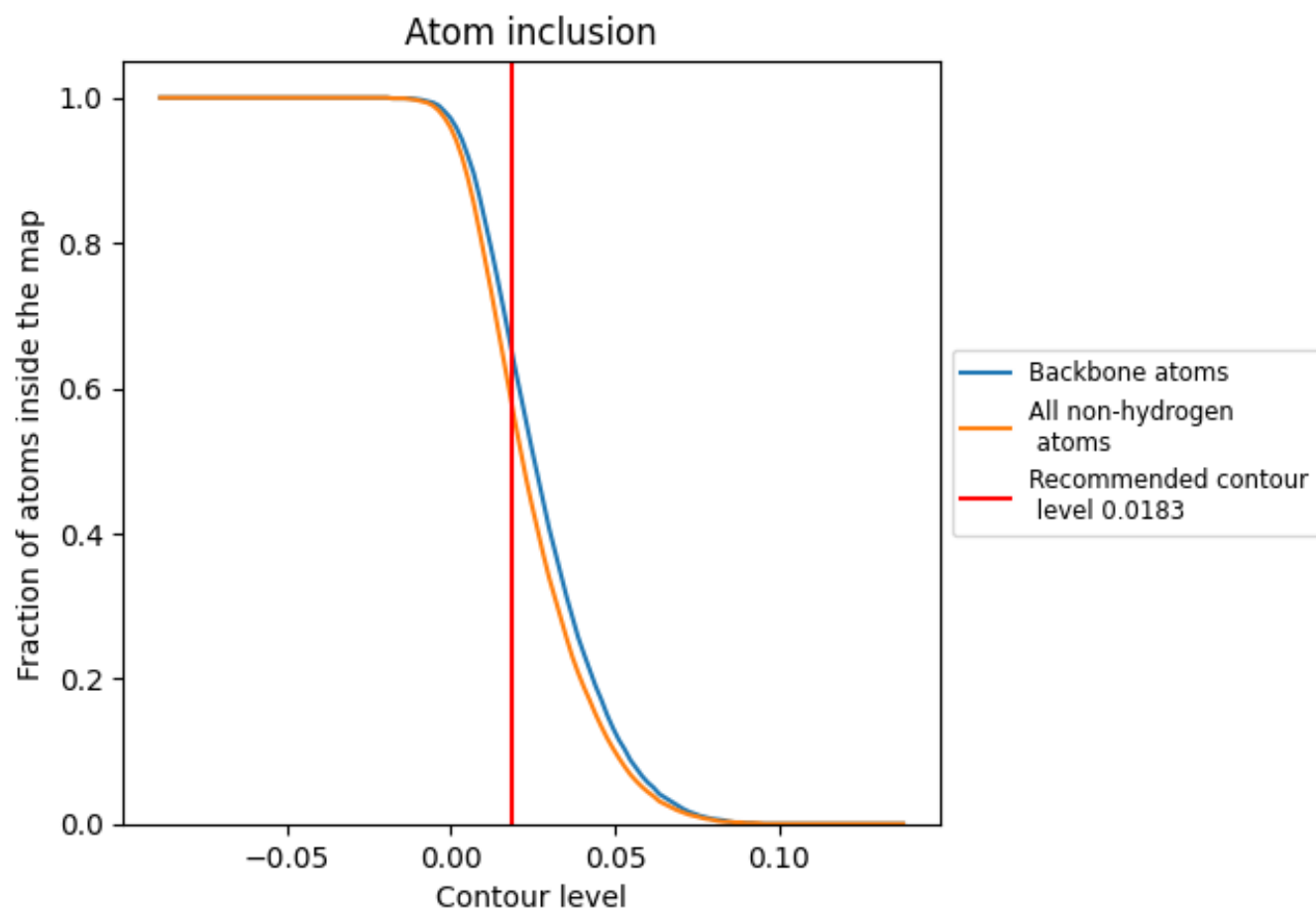
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0183).

9.4 Atom inclusion [i](#)



At the recommended contour level, 66% of all backbone atoms, 58% 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 (0.0183) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5820	 0.4560
0	 0.5960	 0.4550
4	 0.0750	 0.1650
5	 0.0980	 0.2140
6	 0.6430	 0.3960
7	 0.5960	 0.4010
8	 0.6170	 0.4820
9	 0.6760	 0.4980
A	 0.5500	 0.4550
B	 0.5690	 0.4450
C	 0.5150	 0.4220
D	 0.5420	 0.4370
E	 0.4920	 0.4190
F	 0.3880	 0.3730
G	 0.3480	 0.3640
H	 0.4320	 0.4160
I	 0.3020	 0.3300
J	 0.2190	 0.2690
K	 0.1130	 0.2440
L	 0.6680	 0.5110
M	 0.5240	 0.4540
N	 0.0280	 0.1940
O	 0.0210	 0.1590
Q	 0.7630	 0.5250
a	 0.7820	 0.5420
aa	 0.7280	 0.4960
ab	 0.7690	 0.5280
b	 0.7540	 0.5280
c	 0.5920	 0.4700
d	 0.7510	 0.5110
e	 0.7160	 0.5220
f	 0.6810	 0.4880
g	 0.6590	 0.4670
h	 0.7220	 0.5370
i	 0.5750	 0.4520



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Chain	Atom inclusion	Q-score
j	 0.5400	 0.4230
k	 0.5450	 0.4220
l	 0.8530	 0.5950
m	 0.8450	 0.5820
n	 0.5230	 0.4120
o	 0.5470	 0.4540
p	 0.4810	 0.4110
q	 0.5790	 0.4560
r	 0.5800	 0.4210
s	 0.5970	 0.4470
t	 0.5580	 0.4390
u	 0.5230	 0.3980
v	 0.5330	 0.4340
w	 0.5090	 0.4180
x	 0.3400	 0.3060
y	 0.2820	 0.2910
z	 0.1610	 0.2340