



wwPDB EM Validation Summary Report ⓘ

Aug 6, 2026 – 12:18 AM JST

PDB ID : 8YGD / pdb_00008ygd
EMDB ID : EMD-39244
Title : Rhodobacter blasticus RC-LH1 dimer
Authors : Liu, L.N.; Zhang, Y.Z.; Wang, P.; Christianson, B.M.; Ugurlar, D.
Deposited on : 2024-02-26
Resolution : 2.84 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:

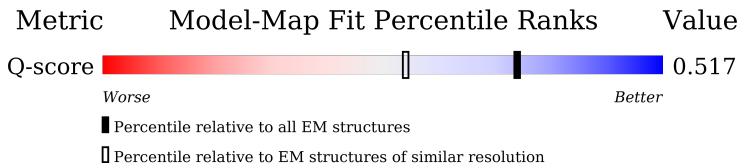
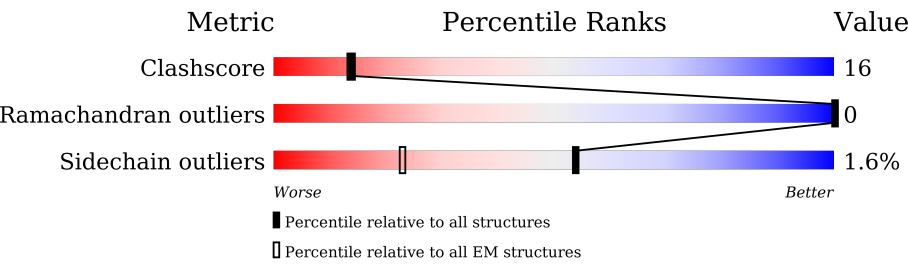
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using 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 i

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

The reported resolution of this entry is 2.84 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	11884 (2.34 - 3.34)

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	0	49	67%22%10%
1	2	49	14% 57%22%20%
1	8	49	61%24%•12%
1	B	49	71%16%12%

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Mol	Chain	Length	Quality of chain
1	C	49	
1	E	49	
1	G	49	
1	J	49	
1	N	49	
1	P	49	
1	R	49	
1	T	49	
1	V	49	
1	Z	49	
1	b	49	
2	1	62	
2	3	62	
2	7	62	
2	9	62	
2	A	62	
2	D	62	
2	F	62	
2	I	62	
2	K	62	
2	O	62	
2	Q	62	
2	S	62	
2	U	62	
2	W	62	

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Mol	Chain	Length	Quality of chain
2	a	62	
3	H	256	
4	L	282	
5	M	307	
6	X	75	

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
7	BCL	N	102	-	-	X	-
7	BCL	a	101	-	-	X	-

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 23255 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 Antenna pigment protein beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	44	Total	C	N	O	S	0	0
			360	241	56	62	1		
1	2	39	Total	C	N	O	S	0	0
			319	213	51	54	1		
1	8	43	Total	C	N	O	S	0	0
			352	237	55	59	1		
1	B	43	Total	C	N	O	S	0	0
			352	237	55	59	1		
1	C	43	Total	C	N	O	S	0	0
			352	237	55	59	1		
1	E	43	Total	C	N	O	S	0	0
			352	237	55	59	1		
1	G	43	Total	C	N	O	S	0	0
			352	237	55	59	1		
1	J	43	Total	C	N	O	S	0	0
			352	237	55	59	1		
1	N	43	Total	C	N	O	S	0	0
			352	237	55	59	1		
1	P	43	Total	C	N	O	S	0	0
			352	237	55	59	1		
1	R	43	Total	C	N	O	S	0	0
			352	237	55	59	1		
1	T	43	Total	C	N	O	S	0	0
			352	237	55	59	1		
1	V	43	Total	C	N	O	S	0	0
			352	237	55	59	1		
1	Z	41	Total	C	N	O	S	0	0
			338	228	53	56	1		
1	b	36	Total	C	N	O	S	0	0
			300	201	48	50	1		

- Molecule 2 is a protein called Antenna pigment protein alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	49	Total	C	N	O	S	0	0
			412	283	65	63	1		
2	3	52	Total	C	N	O	S	0	0
			438	298	72	67	1		
2	7	44	Total	C	N	O	S	0	0
			379	262	60	55	2		
2	9	53	Total	C	N	O	S	0	0
			446	303	73	68	2		
2	A	53	Total	C	N	O	S	0	0
			446	303	73	68	2		
2	D	53	Total	C	N	O	S	0	0
			446	303	73	68	2		
2	F	53	Total	C	N	O	S	0	0
			446	303	73	68	2		
2	I	53	Total	C	N	O	S	0	0
			446	303	73	68	2		
2	K	52	Total	C	N	O	S	0	0
			438	298	72	67	1		
2	O	52	Total	C	N	O	S	0	0
			438	298	72	67	1		
2	Q	52	Total	C	N	O	S	0	0
			438	298	72	67	1		
2	S	52	Total	C	N	O	S	0	0
			438	298	72	67	1		
2	U	52	Total	C	N	O	S	0	0
			438	298	72	67	1		
2	W	51	Total	C	N	O	S	0	0
			432	295	71	65	1		
2	a	48	Total	C	N	O	S	0	0
			401	274	64	62	1		

- Molecule 3 is a protein called Photosynthetic reaction center subunit H.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	254	Total	C	N	O	S	0	0
			1980	1259	347	366	8		

- Molecule 4 is a protein called Reaction center protein L chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	281	Total	C	N	O	S	0	0
			2231	1503	349	370	9		

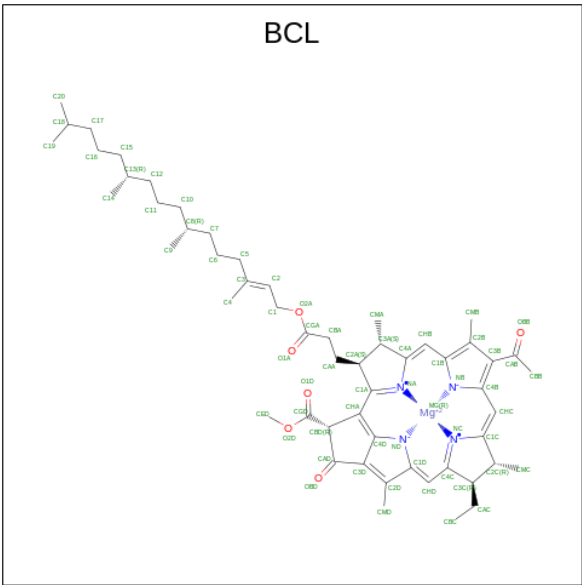
- Molecule 5 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	M	304	Total	C	N	O	S	0	0
			2432	1622	394	405	11		

- Molecule 6 is a protein called 1-deoxy-D-xylulose-5-phosphate synthase.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	X	60	Total	C	N	O	S	0	0
			451	298	74	77	2		

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



Mol	Chain	Residues	Atoms					AltConf
7	0	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
7	1	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
7	1	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
7	3	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	3	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	7	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
7	8	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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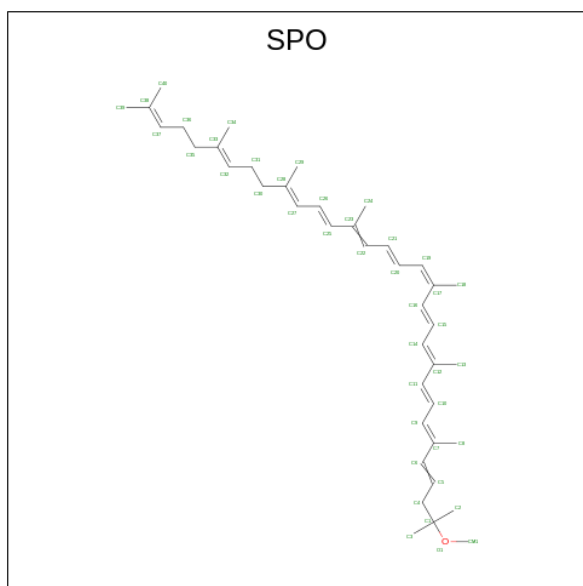
Mol	Chain	Residues	Atoms					AltConf
7	9	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	A	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	B	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	C	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	D	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	E	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	F	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	F	1	Total 66	C 55	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	L	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	L	1	Total 63	C 52	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 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	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

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Mol	Chain	Residues	Atoms					AltConf
7	T	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	U	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	V	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	W	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	a	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
7	b	1	Total	C	Mg	N	O	0
			61	50	1	4	6	

- Molecule 8 is SPHEROIDENE (CCD ID: SPO) (formula: $C_{41}H_{60}O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
8	0	1	Total	C	O	0
			42	41	1	
8	0	1	Total	C	O	0
			42	41	1	
8	2	1	Total	C	O	0
			42	41	1	
8	2	1	Total	C	O	0
			42	41	1	
8	2	1	Total	C	O	0
			42	41	1	

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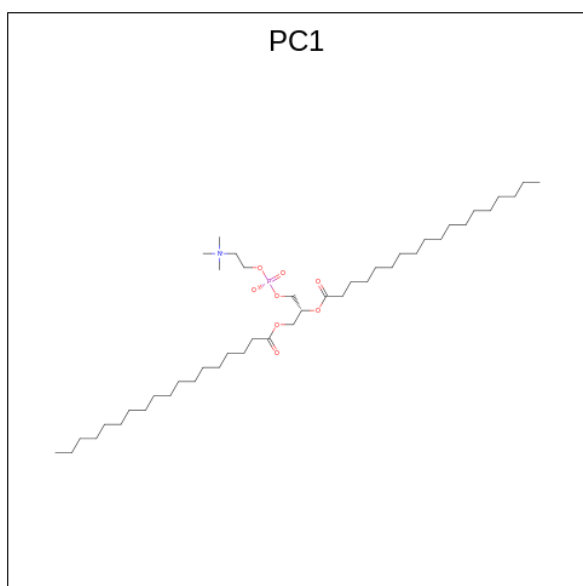
Mol	Chain	Residues	Atoms			AltConf
8	3	1	Total	C	O	0
			42	41	1	
8	8	1	Total	C	O	0
			39	38	1	
8	9	1	Total	C	O	0
			42	41	1	
8	A	1	Total	C	O	0
			42	41	1	
8	D	1	Total	C	O	0
			42	41	1	
8	D	1	Total	C	O	0
			42	41	1	
8	E	1	Total	C	O	0
			42	41	1	
8	F	1	Total	C	O	0
			42	41	1	
8	I	1	Total	C	O	0
			42	41	1	
8	J	1	Total	C	O	0
			42	41	1	
8	K	1	Total	C	O	0
			42	41	1	
8	M	1	Total	C	O	0
			42	41	1	
8	N	1	Total	C	O	0
			42	41	1	
8	O	1	Total	C	O	0
			42	41	1	
8	P	1	Total	C	O	0
			42	41	1	
8	R	1	Total	C	O	0
			42	41	1	
8	R	1	Total	C	O	0
			42	41	1	
8	S	1	Total	C	O	0
			42	41	1	
8	S	1	Total	C	O	0
			42	41	1	
8	T	1	Total	C	O	0
			42	41	1	
8	U	1	Total	C	O	0
			42	41	1	

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Mol	Chain	Residues	Atoms			AltConf
8	U	1	Total	C	O	0
			42	41	1	
8	W	1	Total	C	O	0
			42	41	1	
8	Z	1	Total	C	O	0
			42	41	1	

- Molecule 9 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).



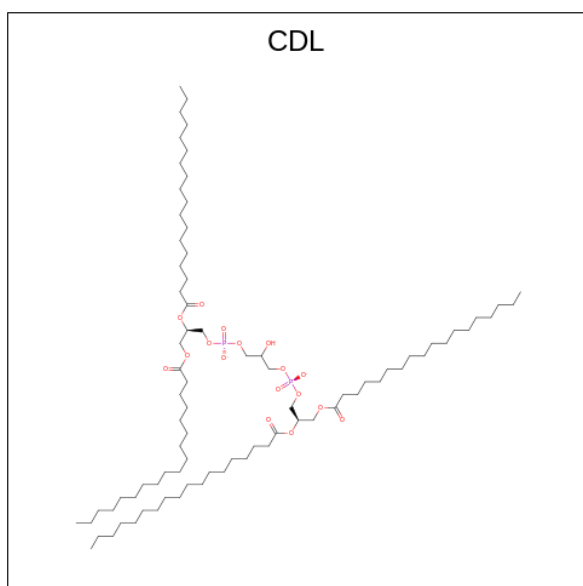
Mol	Chain	Residues	Atoms					AltConf
9	9	1	Total	C	N	O	P	0
			45	35	1	8	1	
9	A	1	Total	C	N	O	P	0
			32	22	1	8	1	
9	A	1	Total	C	N	O	P	0
			32	22	1	8	1	
9	F	1	Total	C	N	O	P	0
			37	27	1	8	1	
9	H	1	Total	C	N	O	P	0
			47	37	1	8	1	
9	L	1	Total	C	N	O	P	0
			36	26	1	8	1	
9	M	1	Total	C	N	O	P	0
			40	30	1	8	1	
9	M	1	Total	C	N	O	P	0
			35	25	1	8	1	

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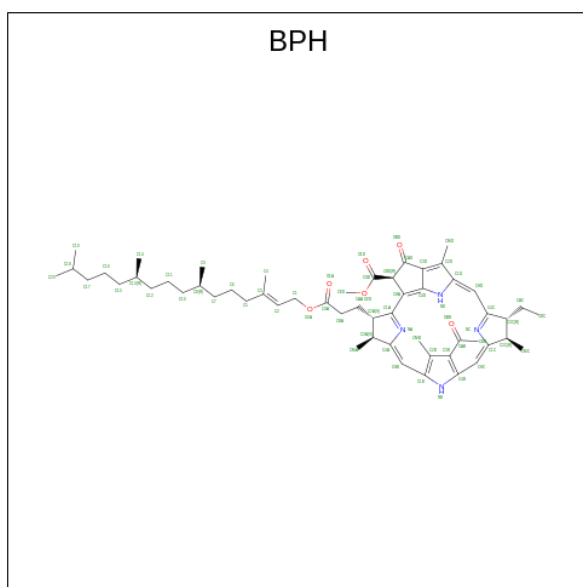
Mol	Chain	Residues	Atoms					AltConf
9	M	1	Total	C	N	O	P	0
			45	35	1	8	1	
9	M	1	Total	C	N	O	P	0
			32	22	1	8	1	
9	W	1	Total	C	N	O	P	0
			32	22	1	8	1	

- Molecule 10 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



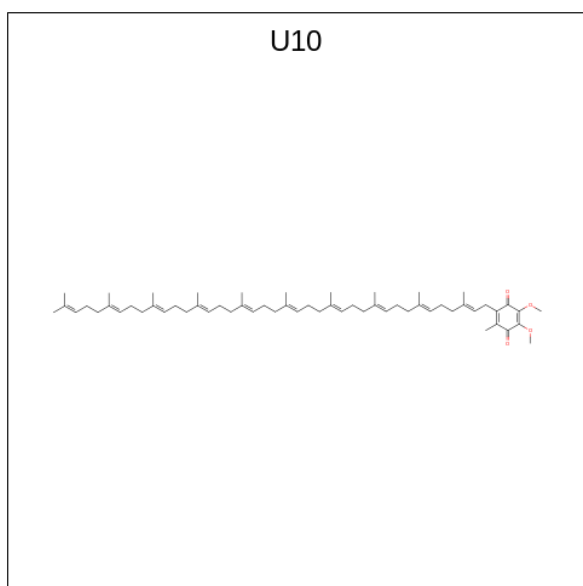
Mol	Chain	Residues	Atoms				AltConf
10	F	1	Total	C	O	P	0
			78	59	17	2	
10	M	1	Total	C	O	P	0
			100	81	17	2	
10	M	1	Total	C	O	P	0
			78	59	17	2	

- Molecule 11 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
11	L	1	Total	C	N	O	0
			62	52	4	6	
11	L	1	Total	C	N	O	0
			55	45	4	6	

- Molecule 12 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
12	L	1	Total	C	O	0
			43	39	4	

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Mol	Chain	Residues	Atoms			AltConf
12	L	1	Total	C	O	0
			43	39	4	
12	L	1	Total	C	O	0
			48	44	4	
12	L	1	Total	C	O	0
			19	15	4	
12	L	1	Total	C	O	0
			38	34	4	
12	M	1	Total	C	O	0
			48	44	4	
12	X	1	Total	C	O	0
			48	44	4	

- Molecule 13 is FE (II) ION (CCD ID: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

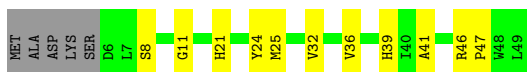
Mol	Chain	Residues	Atoms		AltConf
13	M	1	Total	Fe	0
			1	1	

3 Residue-property plots [i](#)

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

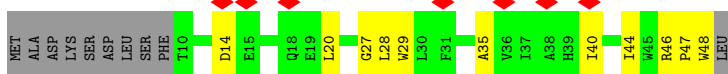
- Molecule 1: Antenna pigment protein beta chain

Chain 0: 



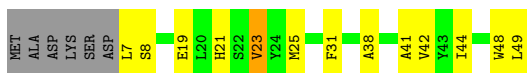
- Molecule 1: Antenna pigment protein beta chain

Chain 2: 



- Molecule 1: Antenna pigment protein beta chain

Chain 8: 



- Molecule 1: Antenna pigment protein beta chain

Chain B: 



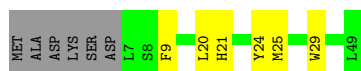
- Molecule 1: Antenna pigment protein beta chain

Chain C: 



- Molecule 1: Antenna pigment protein beta chain

Chain E:  76% 12% 12%



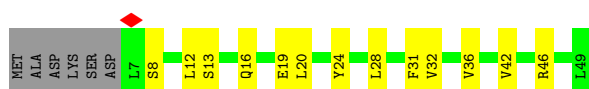
- Molecule 1: Antenna pigment protein beta chain

Chain G:  76% 12% 12%



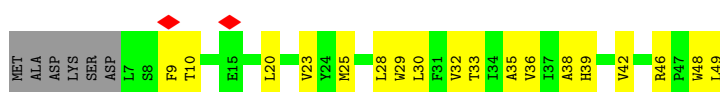
- Molecule 1: Antenna pigment protein beta chain

Chain J:  61% 27% 12%



- Molecule 1: Antenna pigment protein beta chain

Chain N:  51% 37% 12%



- Molecule 1: Antenna pigment protein beta chain

Chain P:  59% 29% 12%



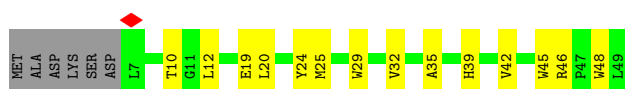
- Molecule 1: Antenna pigment protein beta chain

Chain R:  6% 59% 29% 12%

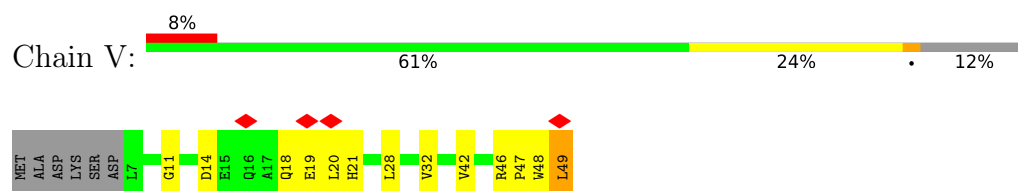


- Molecule 1: Antenna pigment protein beta chain

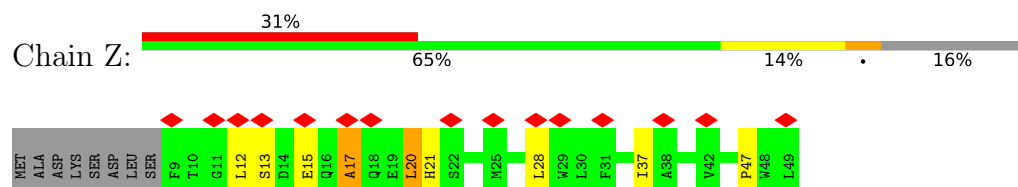
Chain T:  59% 29% 12%



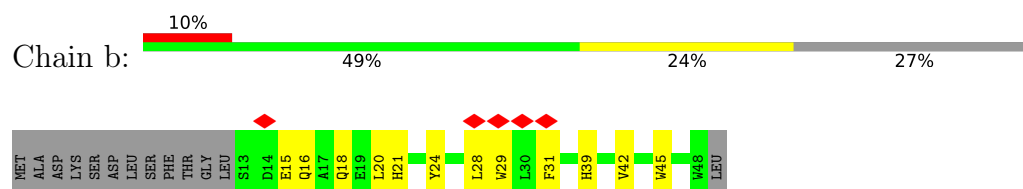
- Molecule 1: Antenna pigment protein beta chain



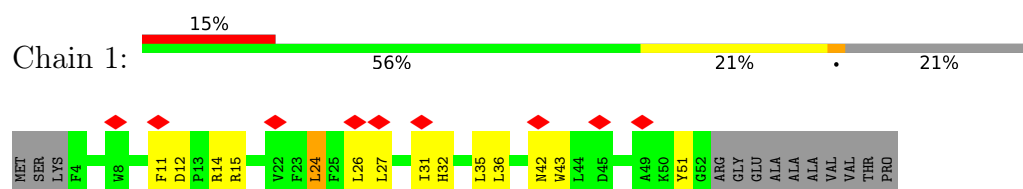
- Molecule 1: Antenna pigment protein beta chain



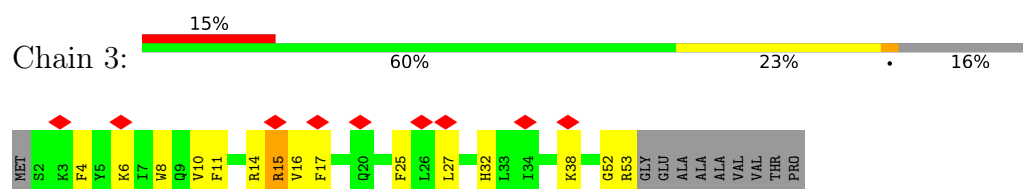
- Molecule 1: Antenna pigment protein beta chain



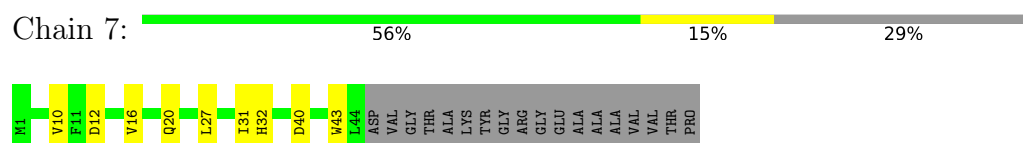
- Molecule 2: Antenna pigment protein alpha chain



- Molecule 2: Antenna pigment protein alpha chain

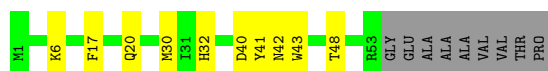


- Molecule 2: Antenna pigment protein alpha chain

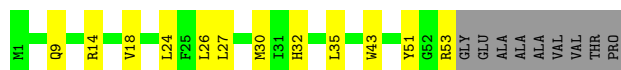


- Molecule 2: Antenna pigment protein alpha chain





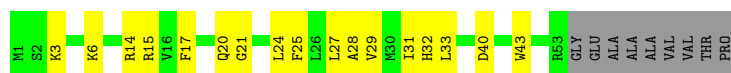
- Molecule 2: Antenna pigment protein alpha chain



- Molecule 2: Antenna pigment protein alpha chain



- Molecule 2: Antenna pigment protein alpha chain



- Molecule 2: Antenna pigment protein alpha chain



- Molecule 2: Antenna pigment protein alpha chain

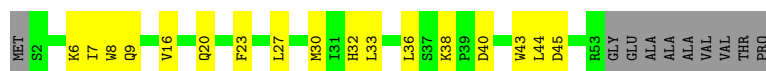


- Molecule 2: Antenna pigment protein alpha chain



- Molecule 2: Antenna pigment protein alpha chain





- Molecule 2: Antenna pigment protein alpha chain



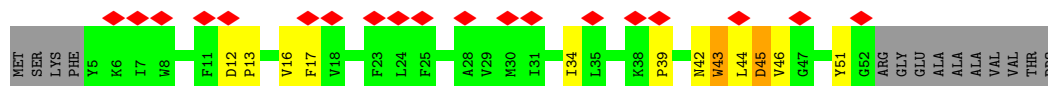
- Molecule 2: Antenna pigment protein alpha chain



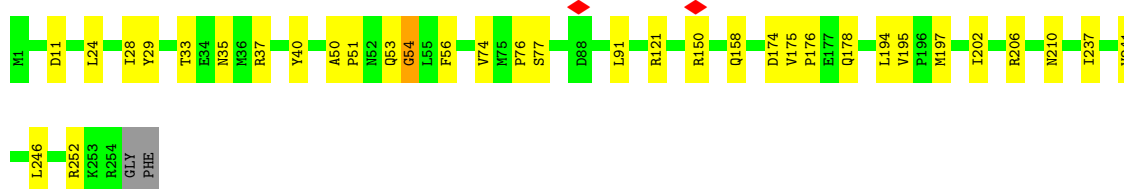
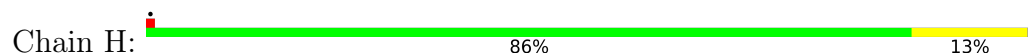
- Molecule 2: Antenna pigment protein alpha chain



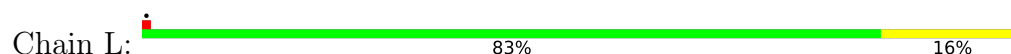
- Molecule 2: Antenna pigment protein alpha chain



- Molecule 3: Photosynthetic reaction center subunit H

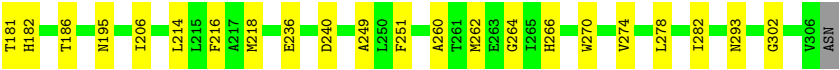
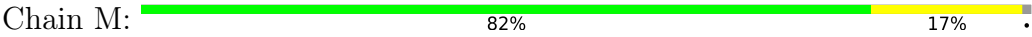


- Molecule 4: Reaction center protein L chain





• Molecule 5: Reaction center protein M chain



• Molecule 6: 1-deoxy-D-xylulose-5-phosphate synthase



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	9149	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.177	Depositor
Minimum map value	-0.768	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.082	Depositor
Recommended contour level	0.16	Depositor
Map size (Å)	237.824, 237.824, 237.824	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.929, 0.929, 0.929	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0	0.55	0/372	0.40	0/510
1	2	0.79	0/330	1.16	2/453 (0.4%)
1	8	0.58	0/364	0.65	1/499 (0.2%)
1	B	0.57	0/364	0.52	0/499
1	C	0.79	0/364	1.04	0/499
1	E	0.73	0/364	0.59	0/499
1	G	0.65	0/364	0.56	0/499
1	J	0.54	0/364	0.56	0/499
1	N	0.44	0/364	0.70	2/499 (0.4%)
1	P	0.48	0/364	0.58	0/499
1	R	0.37	0/364	0.39	0/499
1	T	0.45	0/364	0.61	0/499
1	V	0.89	1/364 (0.3%)	1.20	1/499 (0.2%)
1	Z	0.83	0/350	1.21	2/480 (0.4%)
1	b	0.78	0/311	1.12	1/427 (0.2%)
2	1	0.64	0/426	0.77	0/579
2	3	0.72	0/452	1.05	1/612 (0.2%)
2	7	0.69	0/392	0.51	0/531
2	9	0.64	0/460	0.46	0/622
2	A	0.69	0/460	0.53	0/622
2	D	0.69	0/460	0.61	0/622
2	F	0.68	0/460	0.54	0/622
2	I	0.75	0/460	0.66	0/622
2	K	0.53	0/452	0.51	0/612
2	O	0.49	0/452	0.48	0/612
2	Q	0.46	0/452	0.45	0/612
2	S	0.56	0/452	0.71	0/612
2	U	0.55	0/452	0.68	0/612
2	W	0.83	0/446	1.04	1/604 (0.2%)
2	a	0.88	1/414 (0.2%)	1.15	2/563 (0.4%)
3	H	0.66	1/2030 (0.0%)	0.66	1/2757 (0.0%)
4	L	0.81	0/2317	0.75	3/3172 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
5	M	0.82	0/2525	0.77	7/3453 (0.2%)
6	X	0.67	0/463	0.80	2/636 (0.3%)
All	All	0.70	3/19392 (0.0%)	0.74	26/26436 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	H	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	a	43	TRP	C-N	6.79	1.43	1.33
1	V	19	GLU	C-N	-5.50	1.26	1.33
3	H	54	GLY	C-O	-5.19	1.17	1.23

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	175	VAL	N-CA-C	12.19	119.12	108.63
1	Z	17	ALA	N-CA-C	-8.16	102.38	111.28
4	L	30	PHE	N-CA-C	7.76	121.76	110.28
2	a	43	TRP	O-C-N	7.70	130.28	122.12
1	N	9	PHE	N-CA-C	-7.65	102.94	111.28

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	H	40	TYR	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	360	0	350	10	0
1	2	319	0	310	9	0
1	8	352	0	346	8	0
1	B	352	0	346	7	0
1	C	352	0	346	9	0
1	E	352	0	346	5	0
1	G	352	0	346	8	0
1	J	352	0	346	15	0
1	N	352	0	346	17	0
1	P	352	0	346	15	0
1	R	352	0	346	13	0
1	T	352	0	346	15	0
1	V	352	0	346	20	0
1	Z	338	0	330	7	0
1	b	300	0	289	7	0
2	1	412	0	420	16	0
2	3	438	0	451	16	0
2	7	379	0	397	8	0
2	9	446	0	463	14	0
2	A	446	0	463	11	0
2	D	446	0	463	12	0
2	F	446	0	463	20	0
2	I	446	0	463	13	0
2	K	438	0	451	15	0
2	O	438	0	451	10	0
2	Q	438	0	451	17	0
2	S	438	0	451	17	0
2	U	438	0	451	24	0
2	W	432	0	446	20	0
2	a	401	0	411	10	0
3	H	1980	0	1952	23	0
4	L	2231	0	2169	33	0
5	M	2432	0	2331	42	0
6	X	451	0	461	11	0
7	0	61	0	61	11	0
7	1	117	0	112	28	0
7	3	132	0	148	32	0
7	7	61	0	61	7	0
7	8	66	0	74	5	0
7	9	66	0	74	12	0
7	A	66	0	74	11	0
7	B	66	0	74	8	0
7	C	66	0	74	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	D	66	0	74	4	0
7	E	66	0	74	14	0
7	F	132	0	148	28	0
7	I	66	0	74	8	0
7	J	66	0	74	14	0
7	K	66	0	74	13	0
7	L	195	0	213	21	0
7	M	66	0	74	9	0
7	N	66	0	74	22	0
7	O	66	0	74	12	0
7	P	66	0	74	8	0
7	Q	66	0	74	14	0
7	R	66	0	74	7	0
7	S	66	0	74	8	0
7	T	66	0	74	13	0
7	U	66	0	74	12	0
7	V	66	0	74	7	0
7	W	66	0	74	13	0
7	a	56	0	51	21	0
7	b	61	0	61	4	0
8	0	84	0	120	10	0
8	2	126	0	180	24	0
8	3	42	0	60	1	0
8	8	39	0	53	0	0
8	9	42	0	60	9	0
8	A	42	0	60	8	0
8	D	84	0	120	5	0
8	E	42	0	60	4	0
8	F	42	0	60	3	0
8	I	42	0	60	5	0
8	J	42	0	60	11	0
8	K	42	0	60	5	0
8	M	42	0	60	8	0
8	N	42	0	60	9	0
8	O	42	0	60	1	0
8	P	42	0	60	8	0
8	R	84	0	120	9	0
8	S	84	0	120	10	0
8	T	42	0	60	4	0
8	U	84	0	120	12	0
8	W	42	0	60	3	0
8	Z	42	0	60	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	9	45	0	67	3	0
9	A	64	0	76	4	0
9	F	37	0	48	5	0
9	H	47	0	71	0	0
9	L	36	0	46	0	0
9	M	152	0	203	5	0
9	W	32	0	38	2	0
10	F	78	0	106	1	0
10	M	178	0	262	5	0
11	L	117	0	120	11	0
12	L	191	0	237	19	0
12	M	48	0	63	4	0
12	X	48	0	63	12	0
13	M	1	0	0	0	0
All	All	23255	0	24235	747	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 16.

The worst 5 of 747 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:N:102:BCL:H91	7:N:102:BCL:H142	1.41	1.02
7:L:309:BCL:H91	12:L:310:U10:H3M1	1.44	1.00
7:3:102:BCL:H101	7:3:102:BCL:H143	1.43	0.98
8:Z:101:SPO:H27	8:Z:101:SPO:H241	1.53	0.91
1:2:27:GLY:HA3	8:2:101:SPO:H26	1.54	0.90

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	0	42/49 (86%)	40 (95%)	2 (5%)	0	100	100
1	2	37/49 (76%)	35 (95%)	2 (5%)	0	100	100
1	8	41/49 (84%)	40 (98%)	1 (2%)	0	100	100
1	B	41/49 (84%)	40 (98%)	1 (2%)	0	100	100
1	C	41/49 (84%)	38 (93%)	3 (7%)	0	100	100
1	E	41/49 (84%)	41 (100%)	0	0	100	100
1	G	41/49 (84%)	41 (100%)	0	0	100	100
1	J	41/49 (84%)	40 (98%)	1 (2%)	0	100	100
1	N	41/49 (84%)	40 (98%)	1 (2%)	0	100	100
1	P	41/49 (84%)	40 (98%)	1 (2%)	0	100	100
1	R	41/49 (84%)	41 (100%)	0	0	100	100
1	T	41/49 (84%)	40 (98%)	1 (2%)	0	100	100
1	V	41/49 (84%)	40 (98%)	1 (2%)	0	100	100
1	Z	39/49 (80%)	37 (95%)	2 (5%)	0	100	100
1	b	34/49 (69%)	34 (100%)	0	0	100	100
2	1	47/62 (76%)	46 (98%)	1 (2%)	0	100	100
2	3	50/62 (81%)	49 (98%)	1 (2%)	0	100	100
2	7	42/62 (68%)	41 (98%)	1 (2%)	0	100	100
2	9	51/62 (82%)	50 (98%)	1 (2%)	0	100	100
2	A	51/62 (82%)	49 (96%)	2 (4%)	0	100	100
2	D	51/62 (82%)	49 (96%)	2 (4%)	0	100	100
2	F	51/62 (82%)	49 (96%)	2 (4%)	0	100	100
2	I	51/62 (82%)	50 (98%)	1 (2%)	0	100	100
2	K	50/62 (81%)	48 (96%)	2 (4%)	0	100	100
2	O	50/62 (81%)	47 (94%)	3 (6%)	0	100	100
2	Q	50/62 (81%)	46 (92%)	4 (8%)	0	100	100
2	S	50/62 (81%)	46 (92%)	4 (8%)	0	100	100
2	U	50/62 (81%)	49 (98%)	1 (2%)	0	100	100
2	W	49/62 (79%)	48 (98%)	1 (2%)	0	100	100
2	a	46/62 (74%)	46 (100%)	0	0	100	100
3	H	252/256 (98%)	235 (93%)	17 (7%)	0	100	100
4	L	279/282 (99%)	262 (94%)	17 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	M	302/307 (98%)	291 (96%)	11 (4%)	0	100	100
6	X	58/75 (77%)	55 (95%)	3 (5%)	0	100	100
All	All	2233/2585 (86%)	2143 (96%)	90 (4%)	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	0	38/42 (90%)	38 (100%)	0	100	100
1	2	33/42 (79%)	31 (94%)	2 (6%)	17	35
1	8	37/42 (88%)	35 (95%)	2 (5%)	20	42
1	B	37/42 (88%)	37 (100%)	0	100	100
1	C	37/42 (88%)	34 (92%)	3 (8%)	11	24
1	E	37/42 (88%)	36 (97%)	1 (3%)	39	63
1	G	37/42 (88%)	36 (97%)	1 (3%)	39	63
1	J	37/42 (88%)	37 (100%)	0	100	100
1	N	37/42 (88%)	37 (100%)	0	100	100
1	P	37/42 (88%)	36 (97%)	1 (3%)	39	63
1	R	37/42 (88%)	37 (100%)	0	100	100
1	T	37/42 (88%)	37 (100%)	0	100	100
1	V	37/42 (88%)	36 (97%)	1 (3%)	39	63
1	Z	35/42 (83%)	33 (94%)	2 (6%)	18	39
1	b	31/42 (74%)	27 (87%)	4 (13%)	4	8
2	1	43/52 (83%)	41 (95%)	2 (5%)	23	47
2	3	46/52 (88%)	44 (96%)	2 (4%)	26	50
2	7	41/52 (79%)	41 (100%)	0	100	100
2	9	47/52 (90%)	47 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	47/52 (90%)	47 (100%)	0	100	100
2	D	47/52 (90%)	47 (100%)	0	100	100
2	F	47/52 (90%)	47 (100%)	0	100	100
2	I	47/52 (90%)	46 (98%)	1 (2%)	47	70
2	K	46/52 (88%)	46 (100%)	0	100	100
2	O	46/52 (88%)	46 (100%)	0	100	100
2	Q	46/52 (88%)	46 (100%)	0	100	100
2	S	46/52 (88%)	44 (96%)	2 (4%)	26	50
2	U	46/52 (88%)	46 (100%)	0	100	100
2	W	45/52 (86%)	45 (100%)	0	100	100
2	a	42/52 (81%)	40 (95%)	2 (5%)	23	46
3	H	207/208 (100%)	207 (100%)	0	100	100
4	L	223/224 (100%)	220 (99%)	3 (1%)	61	79
5	M	237/239 (99%)	235 (99%)	2 (1%)	73	86
6	X	47/59 (80%)	47 (100%)	0	100	100
All	All	1940/2140 (91%)	1909 (98%)	31 (2%)	54	76

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	L	224	SER
1	b	18	GLN
5	M	175	VAL
1	b	28	LEU
1	Z	20	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	V	21	HIS
1	b	39	HIS
2	F	32	HIS
3	H	32	GLN
3	H	132	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 87 ligands modelled in this entry, 1 is monoatomic - leaving 86 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	SPO	2	103	-	40,41,41	0.92	1 (2%)	47,50,50	2.08	15 (31%)
7	BCL	I	101	2	69,74,74	0.97	2 (2%)	83,115,115	1.30	11 (13%)
7	BCL	S	102	-	69,74,74	0.84	2 (2%)	83,115,115	1.34	13 (15%)
7	BCL	Q	101	-	69,74,74	0.96	2 (2%)	83,115,115	1.28	11 (13%)
7	BCL	b	101	-	64,69,74	0.97	1 (1%)	77,109,115	1.65	18 (23%)
8	SPO	D	101	-	40,41,41	0.28	0	47,50,50	0.63	1 (2%)
11	BPH	L	303	-	56,67,70	1.39	6 (10%)	57,97,101	1.12	5 (8%)
7	BCL	O	101	-	69,74,74	0.95	2 (2%)	83,115,115	1.25	13 (15%)
7	BCL	8	102	1	69,74,74	1.00	3 (4%)	83,115,115	1.27	13 (15%)
7	BCL	L	309	-	69,74,74	1.05	3 (4%)	83,115,115	1.29	12 (14%)
10	CDL	M	407	-	99,99,99	0.32	0	105,111,111	0.44	0
7	BCL	D	102	-	69,74,74	0.98	2 (2%)	83,115,115	1.28	13 (15%)
7	BCL	N	102	1	69,74,74	0.96	1 (1%)	83,115,115	1.32	14 (16%)
8	SPO	9	102	-	40,41,41	0.40	0	47,50,50	0.69	2 (4%)
9	PC1	L	305	-	35,35,53	0.35	0	41,43,61	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	SPO	K	102	-	40,41,41	1.10	2 (5%)	47,50,50	2.60	16 (34%)
7	BCL	T	101	1	69,74,74	0.94	3 (4%)	83,115,115	1.37	13 (15%)
7	BCL	0	101	1	64,69,74	1.14	4 (6%)	77,109,115	1.43	14 (18%)
8	SPO	J	101	-	40,41,41	0.28	0	47,50,50	0.63	2 (4%)
8	SPO	U	103	-	40,41,41	0.19	0	47,50,50	0.50	0
12	U10	X	101	-	48,48,63	0.28	0	58,61,79	0.78	2 (3%)
7	BCL	K	101	2	69,74,74	1.01	2 (2%)	83,115,115	1.32	15 (18%)
7	BCL	M	403	-	69,74,74	1.06	2 (2%)	83,115,115	1.29	12 (14%)
7	BCL	R	103	1	69,74,74	0.99	3 (4%)	83,115,115	1.30	13 (15%)
9	PC1	M	402	-	34,34,53	1.15	2 (5%)	40,42,61	0.99	2 (5%)
8	SPO	R	101	-	40,41,41	0.22	0	47,50,50	0.50	1 (2%)
7	BCL	L	301	-	69,74,74	0.98	3 (4%)	83,115,115	1.35	13 (15%)
7	BCL	1	102	-	64,69,74	0.94	2 (3%)	77,109,115	1.31	12 (15%)
7	BCL	F	102	-	69,74,74	0.93	2 (2%)	83,115,115	1.26	12 (14%)
8	SPO	S	101	-	40,41,41	1.09	2 (5%)	47,50,50	2.13	15 (31%)
9	PC1	A	103	-	31,31,53	1.24	2 (6%)	37,39,61	1.32	5 (13%)
8	SPO	2	101	-	40,41,41	0.25	0	47,50,50	0.91	3 (6%)
8	SPO	M	406	-	40,41,41	0.40	0	47,50,50	0.59	1 (2%)
8	SPO	F	105	-	40,41,41	0.85	1 (2%)	47,50,50	1.53	6 (12%)
9	PC1	H	301	-	46,46,53	1.00	2 (4%)	52,54,61	1.00	2 (3%)
9	PC1	M	410	-	31,31,53	0.36	0	37,39,61	0.35	0
8	SPO	8	101	-	37,38,41	0.40	0	43,46,50	0.88	2 (4%)
7	BCL	F	104	-	69,74,74	1.07	4 (5%)	83,115,115	1.35	13 (15%)
7	BCL	3	101	-	69,74,74	0.82	2 (2%)	83,115,115	1.37	15 (18%)
8	SPO	P	101	-	40,41,41	0.25	0	47,50,50	0.66	1 (2%)
8	SPO	0	103	-	40,41,41	0.83	2 (5%)	47,50,50	2.63	17 (36%)
12	U10	M	405	-	48,48,63	0.32	0	58,61,79	0.56	1 (1%)
12	U10	L	307	-	48,48,63	0.24	0	58,61,79	0.60	1 (1%)
7	BCL	L	302	-	66,71,74	1.00	4 (6%)	79,111,115	1.36	13 (16%)
8	SPO	N	101	-	40,41,41	0.30	0	47,50,50	0.66	2 (4%)
8	SPO	3	103	-	40,41,41	1.03	2 (5%)	47,50,50	1.91	15 (31%)
8	SPO	U	102	-	40,41,41	0.19	0	47,50,50	0.48	0
8	SPO	2	102	-	40,41,41	0.97	2 (5%)	47,50,50	2.04	15 (31%)
8	SPO	D	103	-	40,41,41	0.23	0	47,50,50	0.64	1 (2%)
7	BCL	1	101	-	59,64,74	1.01	2 (3%)	71,103,115	1.37	14 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	SPO	S	103	-	40,41,41	0.30	0	47,50,50	0.78	2 (4%)
7	BCL	9	101	-	69,74,74	0.97	2 (2%)	83,115,115	1.32	12 (14%)
8	SPO	R	102	-	40,41,41	0.88	0	47,50,50	1.84	12 (25%)
9	PC1	F	103	-	36,36,53	0.35	0	42,44,61	0.35	0
12	U10	L	306	-	43,43,63	0.21	0	52,55,79	0.55	1 (1%)
7	BCL	P	102	1	69,74,74	1.03	3 (4%)	83,115,115	1.29	14 (16%)
9	PC1	9	103	-	44,44,53	0.32	0	50,52,61	0.50	0
9	PC1	A	104	-	31,31,53	0.38	0	37,39,61	0.40	0
7	BCL	V	101	1	69,74,74	0.92	2 (2%)	83,115,115	1.31	14 (16%)
10	CDL	F	101	-	77,77,99	1.06	4 (5%)	83,89,111	1.05	7 (8%)
12	U10	L	310	-	38,38,63	0.21	0	46,49,79	0.50	1 (2%)
12	U10	L	308	-	19,19,63	0.33	0	23,26,79	0.73	1 (4%)
7	BCL	E	101	1	69,74,74	1.02	3 (4%)	83,115,115	1.29	12 (14%)
7	BCL	U	101	-	69,74,74	0.90	2 (2%)	83,115,115	1.27	12 (14%)
8	SPO	Z	101	-	40,41,41	0.22	0	47,50,50	0.71	1 (2%)
8	SPO	W	101	-	40,41,41	1.03	3 (7%)	47,50,50	1.63	10 (21%)
7	BCL	A	101	-	69,74,74	1.04	2 (2%)	83,115,115	1.25	11 (13%)
7	BCL	3	102	-	69,74,74	0.90	3 (4%)	83,115,115	1.34	14 (16%)
8	SPO	E	102	-	40,41,41	1.13	4 (10%)	47,50,50	2.13	15 (31%)
9	PC1	M	401	-	39,39,53	0.34	0	45,47,61	0.33	0
7	BCL	C	101	1	69,74,74	0.92	4 (5%)	83,115,115	1.31	12 (14%)
9	PC1	W	103	-	31,31,53	0.36	0	37,39,61	0.49	0
7	BCL	J	102	-	69,74,74	1.07	5 (7%)	83,115,115	1.35	14 (16%)
9	PC1	M	409	-	44,44,53	0.30	0	50,52,61	0.39	0
8	SPO	A	102	-	40,41,41	0.38	0	47,50,50	0.57	1 (2%)
10	CDL	M	408	-	77,77,99	0.34	0	83,89,111	0.41	0
7	BCL	B	101	1	69,74,74	1.09	3 (4%)	83,115,115	1.33	14 (16%)
7	BCL	W	102	-	69,74,74	0.89	1 (1%)	83,115,115	1.28	13 (15%)
8	SPO	O	102	-	40,41,41	0.97	2 (5%)	47,50,50	1.67	11 (23%)
7	BCL	a	101	-	59,64,74	0.96	2 (3%)	71,103,115	1.44	11 (15%)
12	U10	L	304	-	43,43,63	0.24	0	52,55,79	0.52	1 (1%)
7	BCL	7	101	-	64,69,74	1.02	3 (4%)	77,109,115	1.38	13 (16%)
8	SPO	0	102	-	40,41,41	1.02	3 (7%)	47,50,50	2.40	13 (27%)
8	SPO	I	102	-	40,41,41	1.22	3 (7%)	47,50,50	2.37	14 (29%)
8	SPO	T	102	-	40,41,41	0.84	0	47,50,50	1.64	10 (21%)
11	BPH	L	311	-	49,60,70	1.45	6 (12%)	49,89,101	1.22	7 (14%)

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	SPO	2	103	-	-	11/47/47/47	-
7	BCL	I	101	2	-	11/41/137/137	-
7	BCL	S	102	-	-	13/41/137/137	-
7	BCL	Q	101	-	-	16/41/137/137	-
7	BCL	b	101	-	-	24/35/131/137	-
8	SPO	D	101	-	-	6/47/47/47	-
11	BPH	L	303	-	-	7/34/102/105	0/5/6/6
7	BCL	O	101	-	-	14/41/137/137	-
7	BCL	8	102	1	-	20/41/137/137	-
7	BCL	L	309	-	-	19/41/137/137	-
10	CDL	M	407	-	-	39/110/110/110	-
7	BCL	D	102	-	-	15/41/137/137	-
7	BCL	N	102	1	-	16/41/137/137	-
8	SPO	9	102	-	-	6/47/47/47	-
9	PC1	L	305	-	-	13/39/39/57	-
8	SPO	K	102	-	-	11/47/47/47	-
7	BCL	T	101	1	-	15/41/137/137	-
7	BCL	0	101	1	-	15/35/131/137	-
8	SPO	J	101	-	-	6/47/47/47	-
8	SPO	U	103	-	-	10/47/47/47	-
12	U10	X	101	-	-	18/45/69/87	0/1/1/1
7	BCL	K	101	2	-	13/41/137/137	-
7	BCL	M	403	-	-	17/41/137/137	-
7	BCL	R	103	1	-	27/41/137/137	-
9	PC1	M	402	-	-	14/38/38/57	-
8	SPO	R	101	-	-	4/47/47/47	-
7	BCL	L	301	-	-	4/41/137/137	-
7	BCL	1	102	-	-	19/35/131/137	-
7	BCL	F	102	-	-	23/41/137/137	-
8	SPO	S	101	-	-	6/47/47/47	-
9	PC1	A	103	-	-	8/35/35/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	SPO	2	101	-	-	13/47/47/47	-
8	SPO	M	406	-	-	8/47/47/47	-
8	SPO	F	105	-	-	3/47/47/47	-
9	PC1	H	301	-	-	20/50/50/57	-
9	PC1	M	410	-	-	8/35/35/57	-
8	SPO	8	101	-	-	6/44/44/47	-
7	BCL	F	104	-	-	24/41/137/137	-
7	BCL	3	101	-	-	18/41/137/137	-
8	SPO	P	101	-	-	4/47/47/47	-
8	SPO	0	103	-	-	15/47/47/47	-
12	U10	M	405	-	-	5/45/69/87	0/1/1/1
12	U10	L	307	-	-	12/45/69/87	0/1/1/1
7	BCL	L	302	-	-	10/38/134/137	-
8	SPO	N	101	-	-	4/47/47/47	-
8	SPO	3	103	-	-	11/47/47/47	-
8	SPO	U	102	-	-	5/47/47/47	-
8	SPO	2	102	-	-	7/47/47/47	-
8	SPO	D	103	-	-	13/47/47/47	-
7	BCL	1	101	-	-	11/29/125/137	-
8	SPO	S	103	-	-	17/47/47/47	-
7	BCL	9	101	-	-	19/41/137/137	-
8	SPO	R	102	-	-	11/47/47/47	-
9	PC1	F	103	-	-	13/40/40/57	-
12	U10	L	306	-	-	14/39/63/87	0/1/1/1
7	BCL	P	102	1	-	21/41/137/137	-
9	PC1	9	103	-	-	21/48/48/57	-
9	PC1	A	104	-	-	10/35/35/57	-
7	BCL	V	101	1	-	20/41/137/137	-
10	CDL	F	101	-	-	34/88/88/110	-
12	U10	L	310	-	-	10/33/57/87	0/1/1/1
12	U10	L	308	-	-	1/11/35/87	0/1/1/1
7	BCL	E	101	1	-	25/41/137/137	-
7	BCL	U	101	-	-	18/41/137/137	-
8	SPO	Z	101	-	-	12/47/47/47	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	SPO	W	101	-	-	7/47/47/47	-
7	BCL	A	101	-	-	11/41/137/137	-
7	BCL	3	102	-	-	16/41/137/137	-
8	SPO	E	102	-	-	10/47/47/47	-
9	PC1	M	401	-	-	11/43/43/57	-
7	BCL	C	101	1	-	25/41/137/137	-
9	PC1	W	103	-	-	16/35/35/57	-
7	BCL	J	102	-	-	21/41/137/137	-
9	PC1	M	409	-	-	12/48/48/57	-
8	SPO	A	102	-	-	8/47/47/47	-
10	CDL	M	408	-	-	20/88/88/110	-
7	BCL	B	101	1	-	19/41/137/137	-
7	BCL	W	102	-	-	16/41/137/137	-
8	SPO	O	102	-	-	4/47/47/47	-
7	BCL	a	101	-	-	15/29/125/137	-
12	U10	L	304	-	-	10/39/63/87	0/1/1/1
7	BCL	7	101	-	-	8/35/131/137	-
8	SPO	0	102	-	-	14/47/47/47	-
8	SPO	I	102	-	-	5/47/47/47	-
8	SPO	T	102	-	-	3/47/47/47	-
11	BPH	L	311	-	-	7/25/93/105	0/5/6/6

The worst 5 of 135 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	0	101	BCL	C4D-ND	-7.13	1.27	1.37
7	M	403	BCL	C4D-ND	-7.02	1.28	1.37
7	A	101	BCL	C4D-ND	-6.93	1.28	1.37
7	P	102	BCL	C4D-ND	-6.83	1.28	1.37
7	B	101	BCL	C4D-ND	-6.67	1.28	1.37

The worst 5 of 683 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	K	102	SPO	C8-C7-C9	-9.27	109.93	122.92
8	0	103	SPO	C20-C19-C17	-8.78	114.78	127.31
8	0	103	SPO	C20-C21-C22	-6.88	109.38	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	I	102	SPO	C29-C28-C30	6.57	126.32	115.27
8	K	102	SPO	C10-C9-C7	6.50	136.58	127.31

There are no chirality outliers.

5 of 1141 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	0	101	BCL	C1-C2-C3-C4
7	0	101	BCL	C1-C2-C3-C5
7	1	101	BCL	C4C-C3C-CAC-CBC
7	1	101	BCL	CHA-CBD-CGD-O1D
7	1	101	BCL	CHA-CBD-CGD-O2D

There are no ring outliers.

81 monomers are involved in 500 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	2	103	SPO	1	0
7	I	101	BCL	8	0
7	S	102	BCL	8	0
7	Q	101	BCL	14	0
7	b	101	BCL	4	0
8	D	101	SPO	2	0
11	L	303	BPH	5	0
7	O	101	BCL	12	0
7	8	102	BCL	5	0
7	L	309	BCL	12	0
10	M	407	CDL	3	0
7	D	102	BCL	4	0
7	N	102	BCL	22	0
8	9	102	SPO	9	0
8	K	102	SPO	5	0
7	T	101	BCL	13	0
7	0	101	BCL	11	0
8	J	101	SPO	11	0
8	U	103	SPO	8	0
12	X	101	U10	12	0
7	K	101	BCL	13	0
7	M	403	BCL	9	0
7	R	103	BCL	7	0
8	R	101	SPO	5	0

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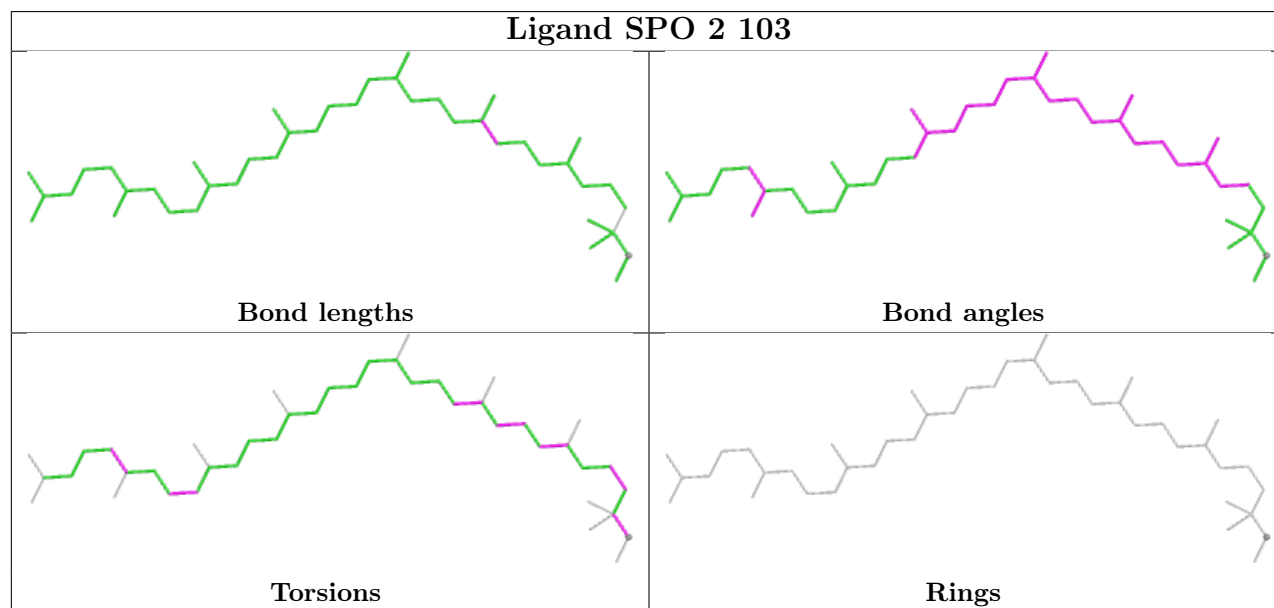
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	L	301	BCL	7	0
7	1	102	BCL	14	0
7	F	102	BCL	18	0
8	S	101	SPO	3	0
9	A	103	PC1	3	0
8	2	101	SPO	18	0
8	M	406	SPO	8	0
8	F	105	SPO	3	0
7	F	104	BCL	10	0
7	3	101	BCL	19	0
8	P	101	SPO	8	0
8	0	103	SPO	2	0
12	M	405	U10	4	0
12	L	307	U10	3	0
7	L	302	BCL	5	0
8	N	101	SPO	9	0
8	3	103	SPO	1	0
8	U	102	SPO	4	0
8	2	102	SPO	5	0
8	D	103	SPO	3	0
7	1	101	BCL	14	0
8	S	103	SPO	7	0
7	9	101	BCL	12	0
8	R	102	SPO	4	0
9	F	103	PC1	5	0
12	L	306	U10	6	0
7	P	102	BCL	8	0
9	9	103	PC1	3	0
9	A	104	PC1	1	0
7	V	101	BCL	7	0
10	F	101	CDL	1	0
12	L	310	U10	5	0
12	L	308	U10	1	0
7	E	101	BCL	14	0
7	U	101	BCL	12	0
8	Z	101	SPO	8	0
8	W	101	SPO	3	0
7	A	101	BCL	11	0
7	3	102	BCL	13	0
8	E	102	SPO	4	0
9	M	401	PC1	2	0
7	C	101	BCL	16	0

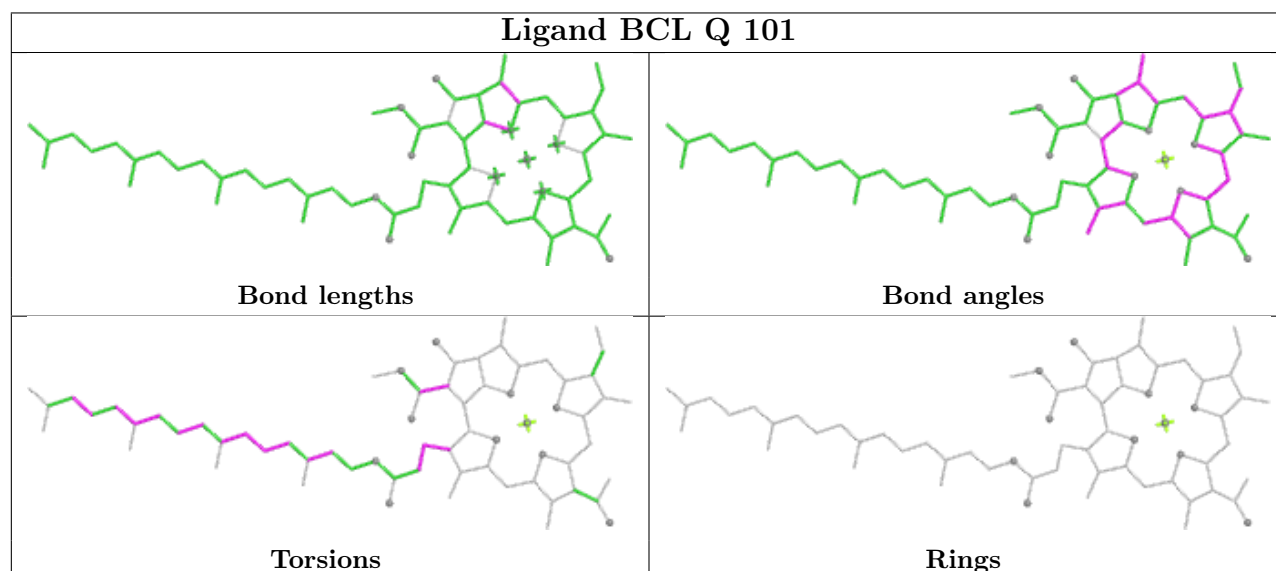
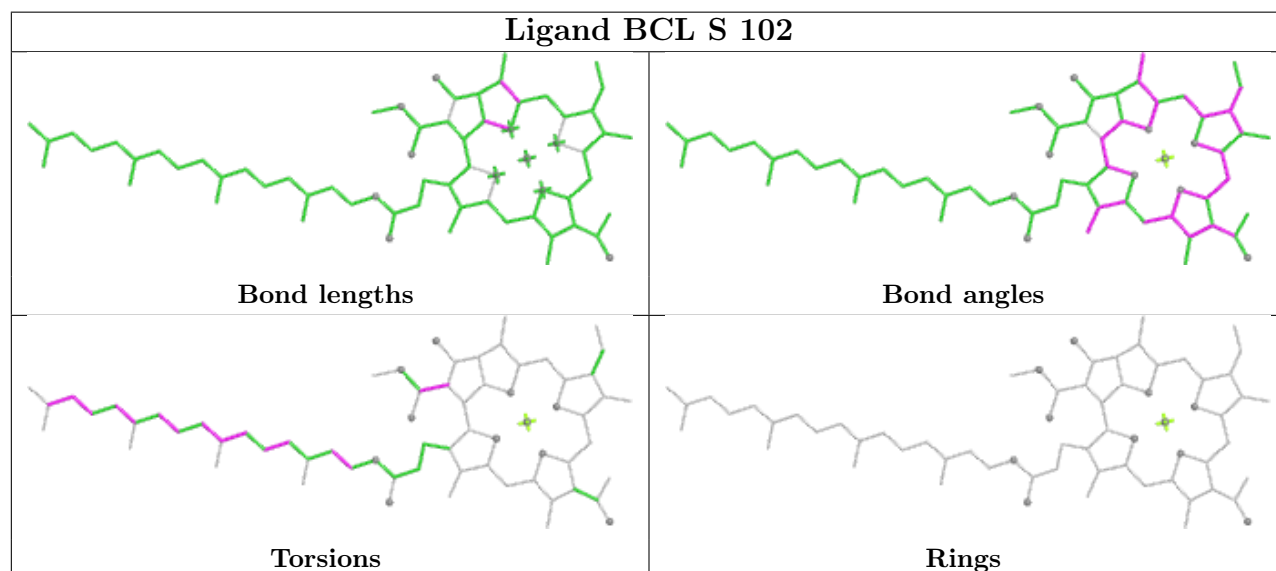
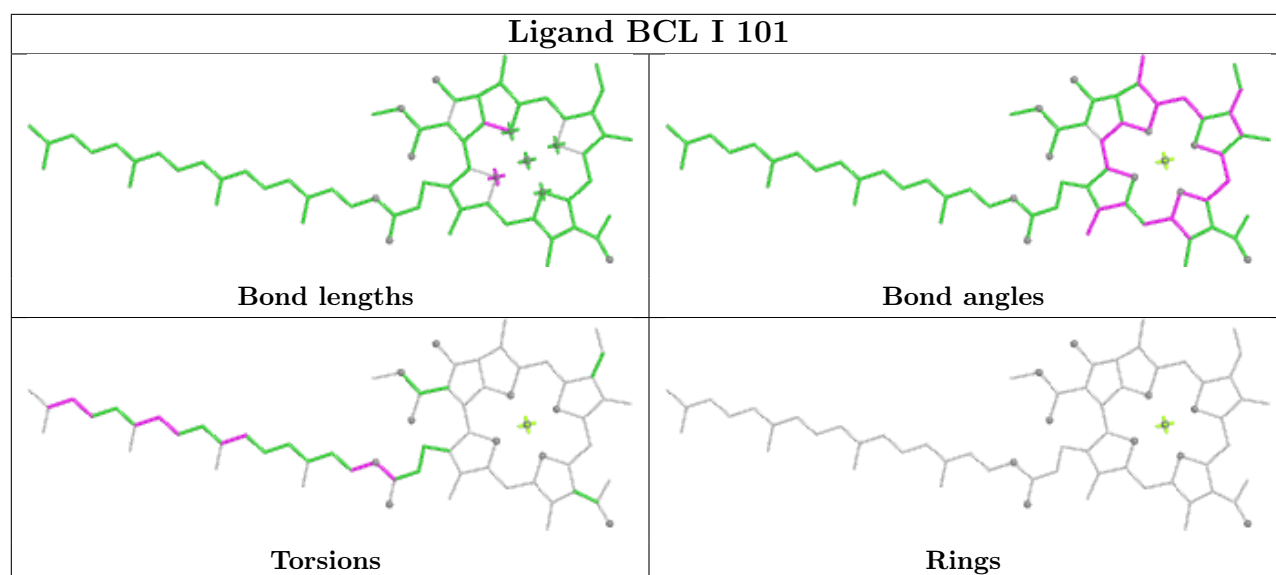
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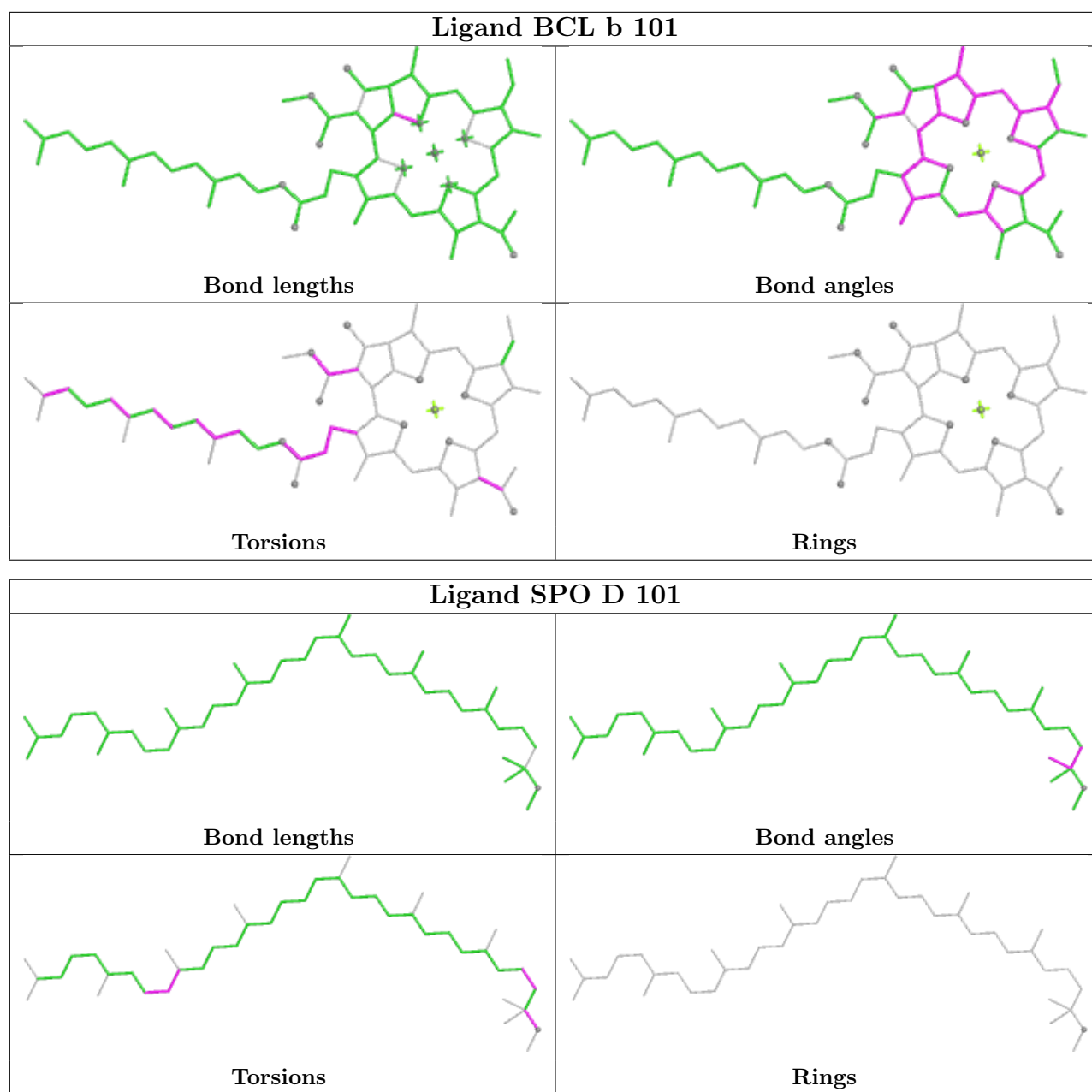
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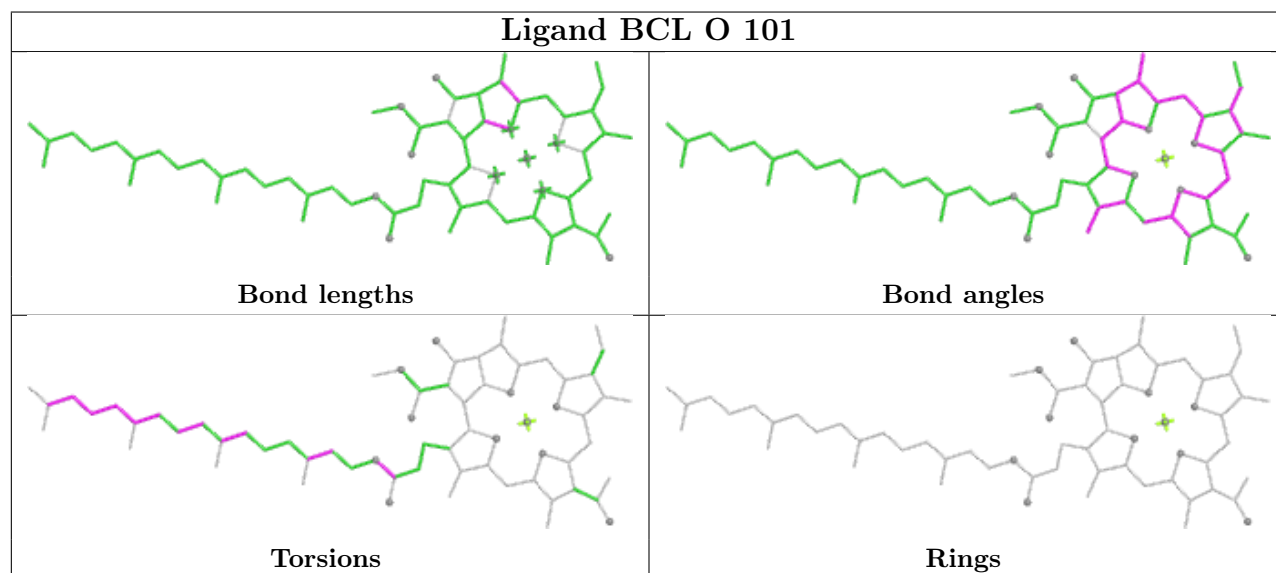
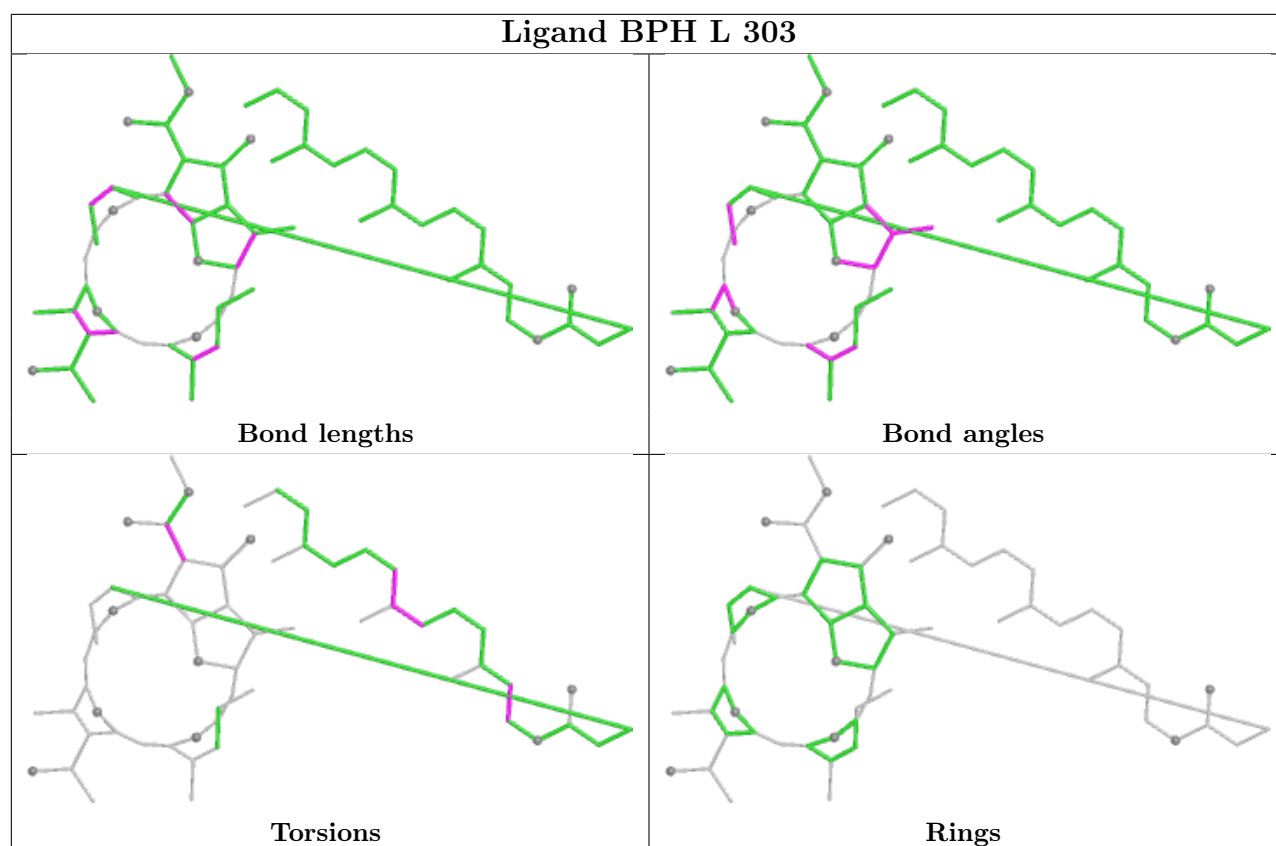
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	W	103	PC1	2	0
7	J	102	BCL	14	0
9	M	409	PC1	3	0
8	A	102	SPO	8	0
10	M	408	CDL	2	0
7	B	101	BCL	8	0
7	W	102	BCL	13	0
8	O	102	SPO	1	0
7	a	101	BCL	21	0
12	L	304	U10	4	0
7	7	101	BCL	7	0
8	0	102	SPO	8	0
8	I	102	SPO	5	0
8	T	102	SPO	4	0
11	L	311	BPH	6	0

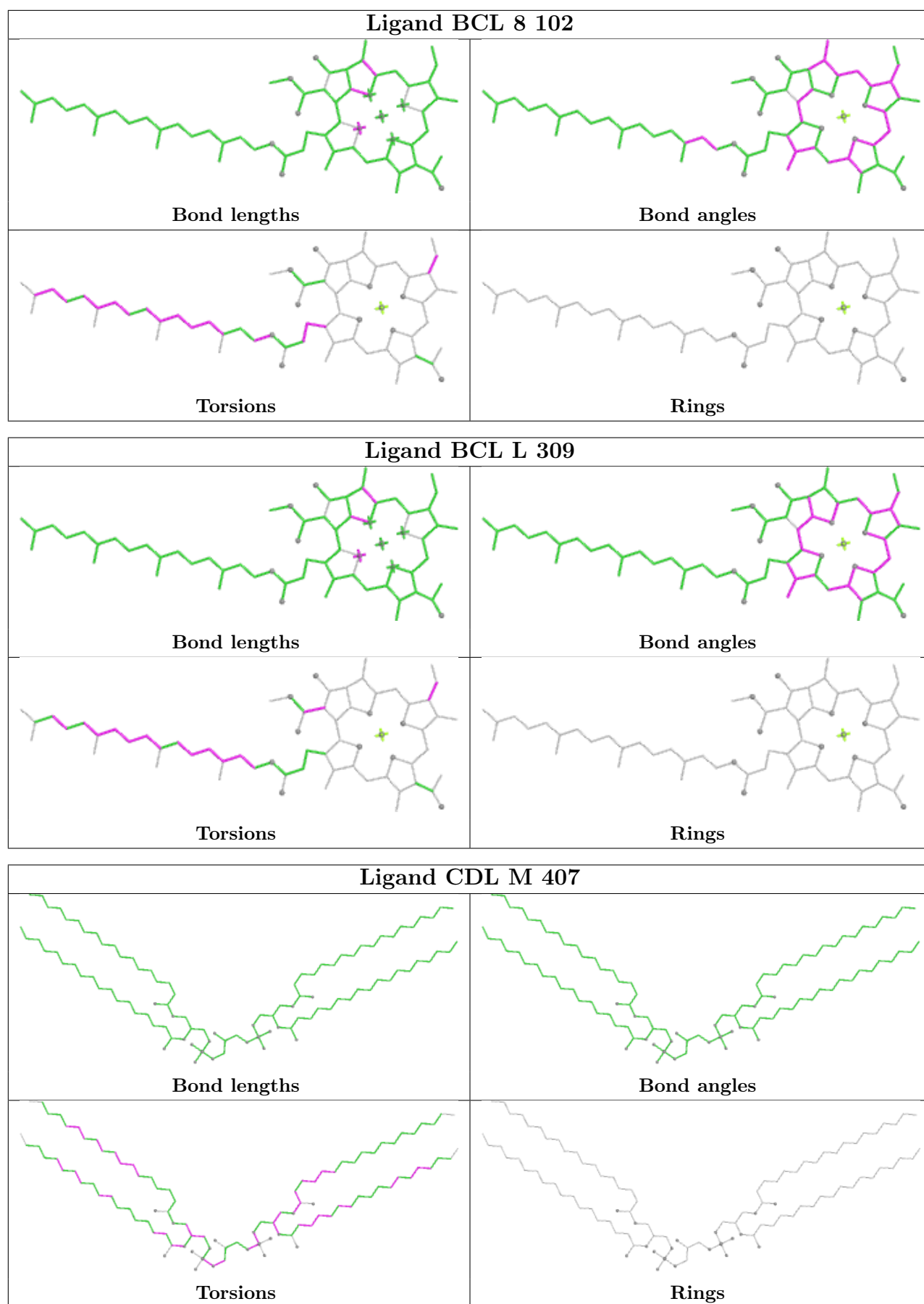
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

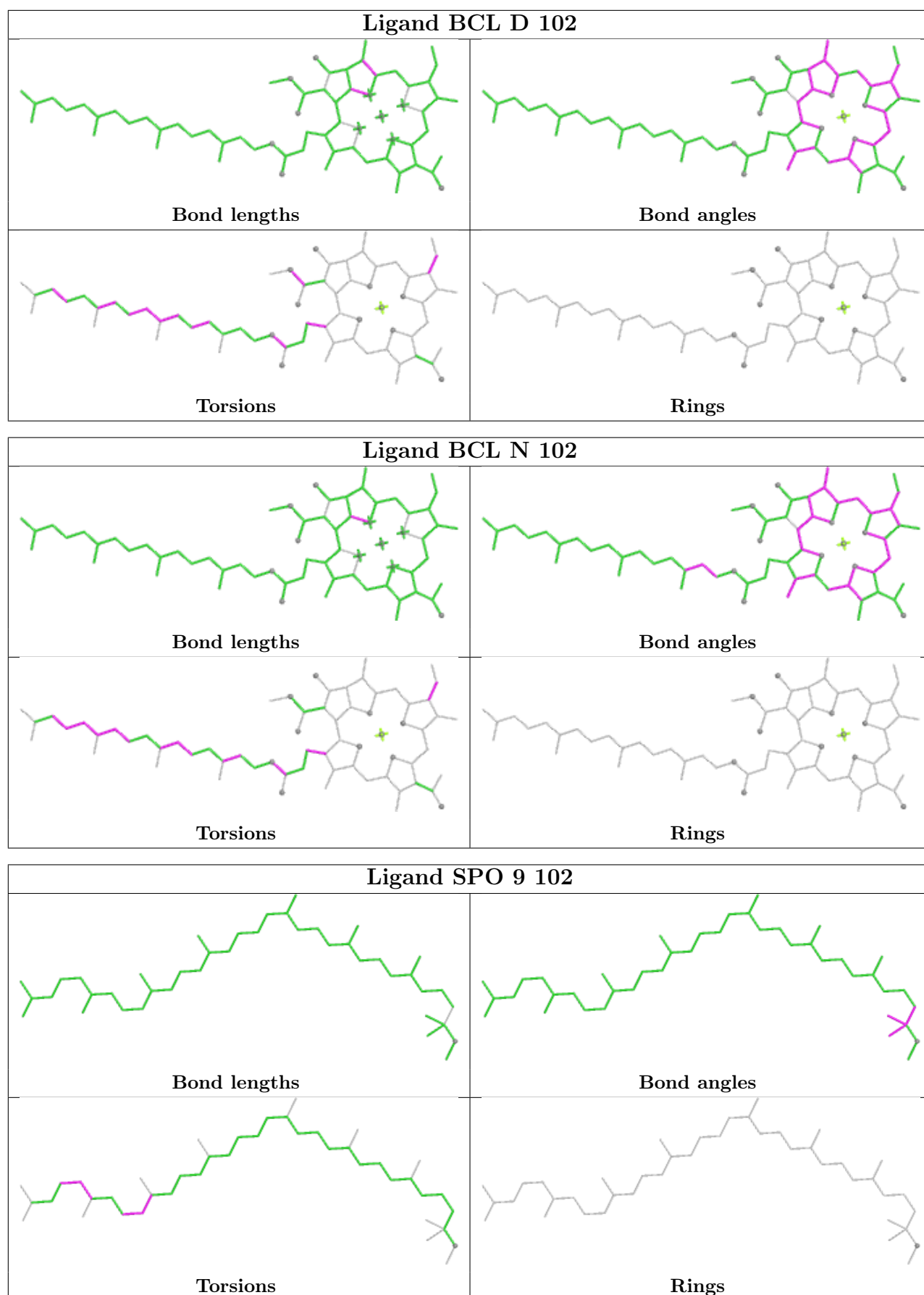


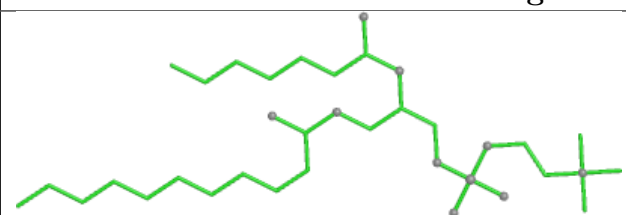
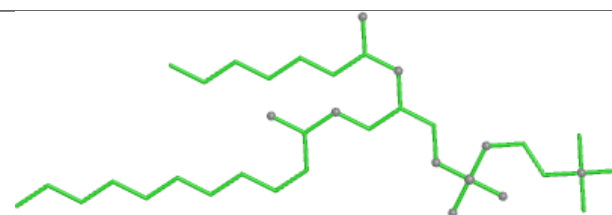
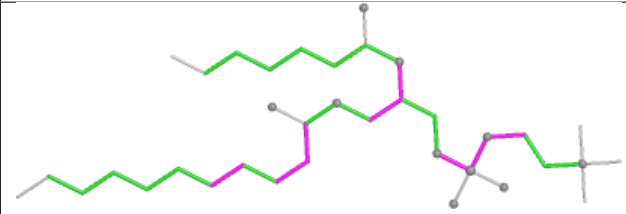
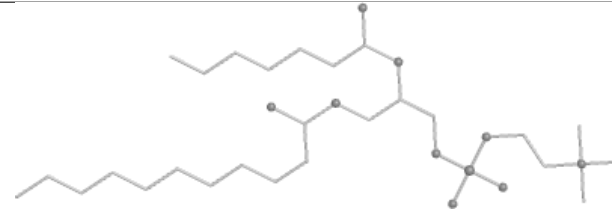


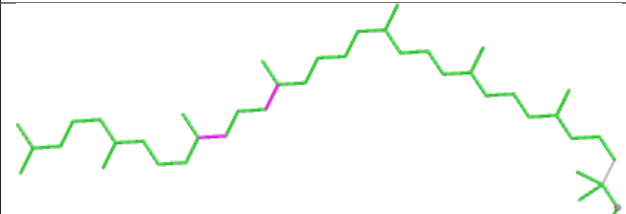
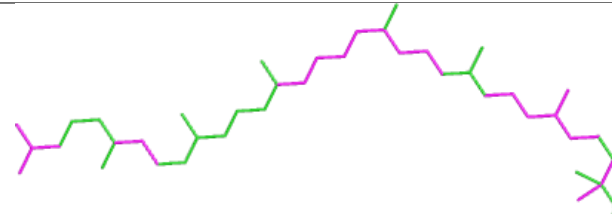
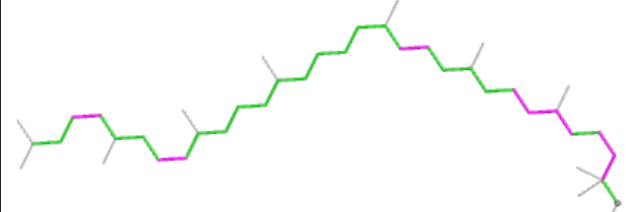
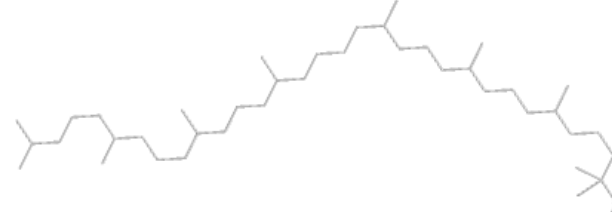


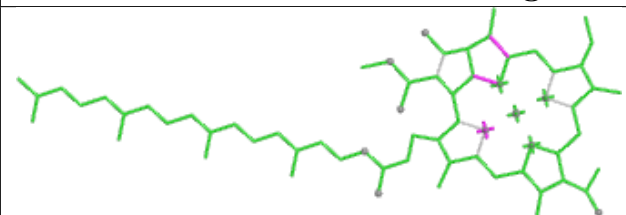
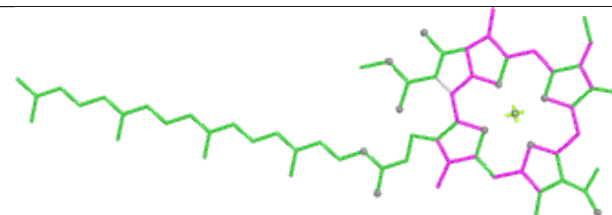
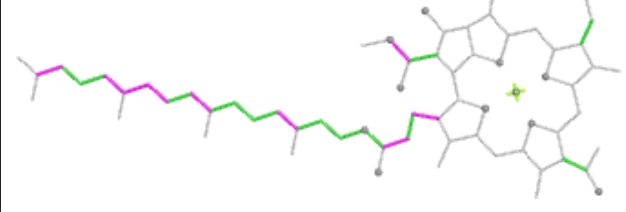
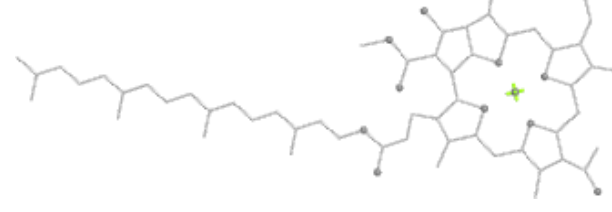


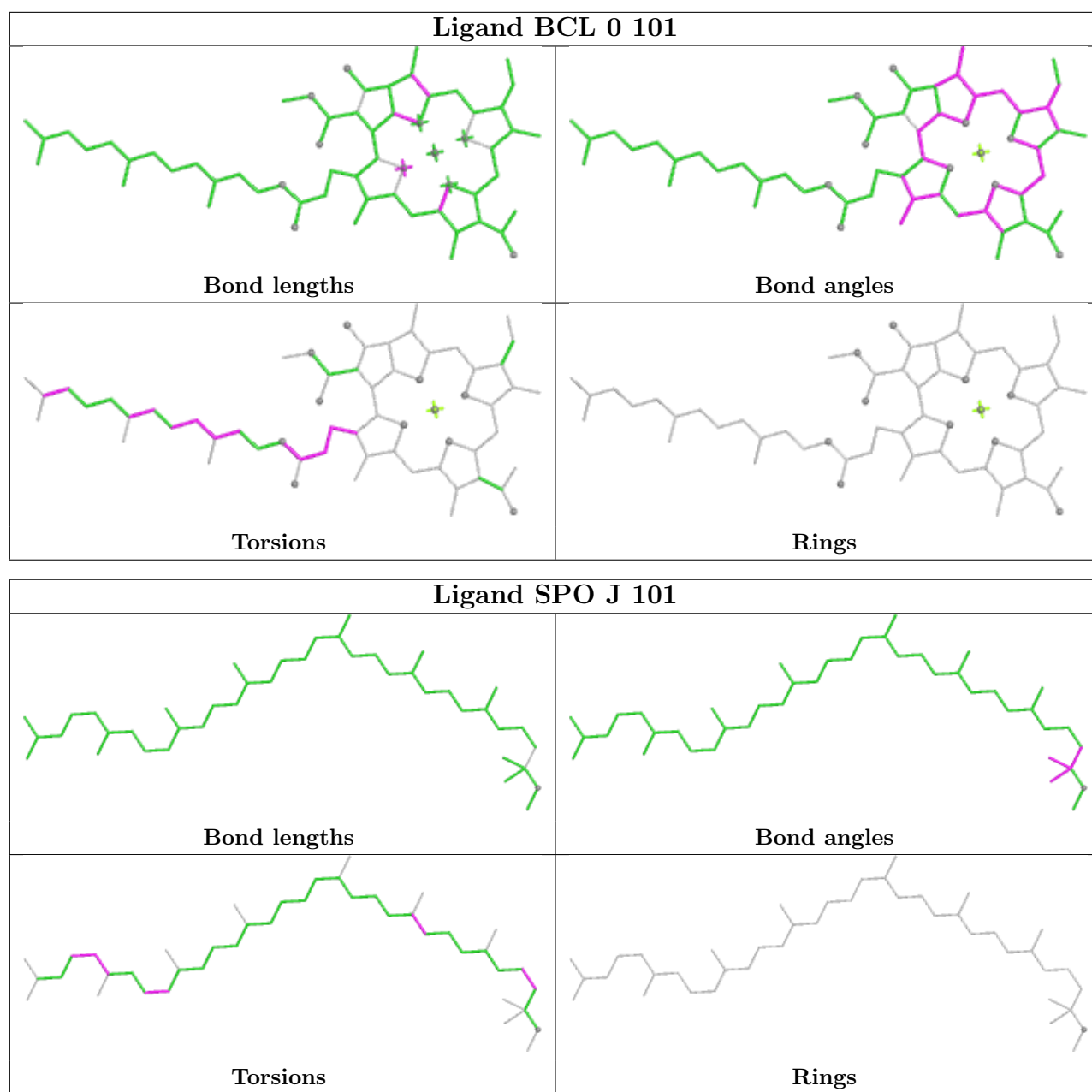


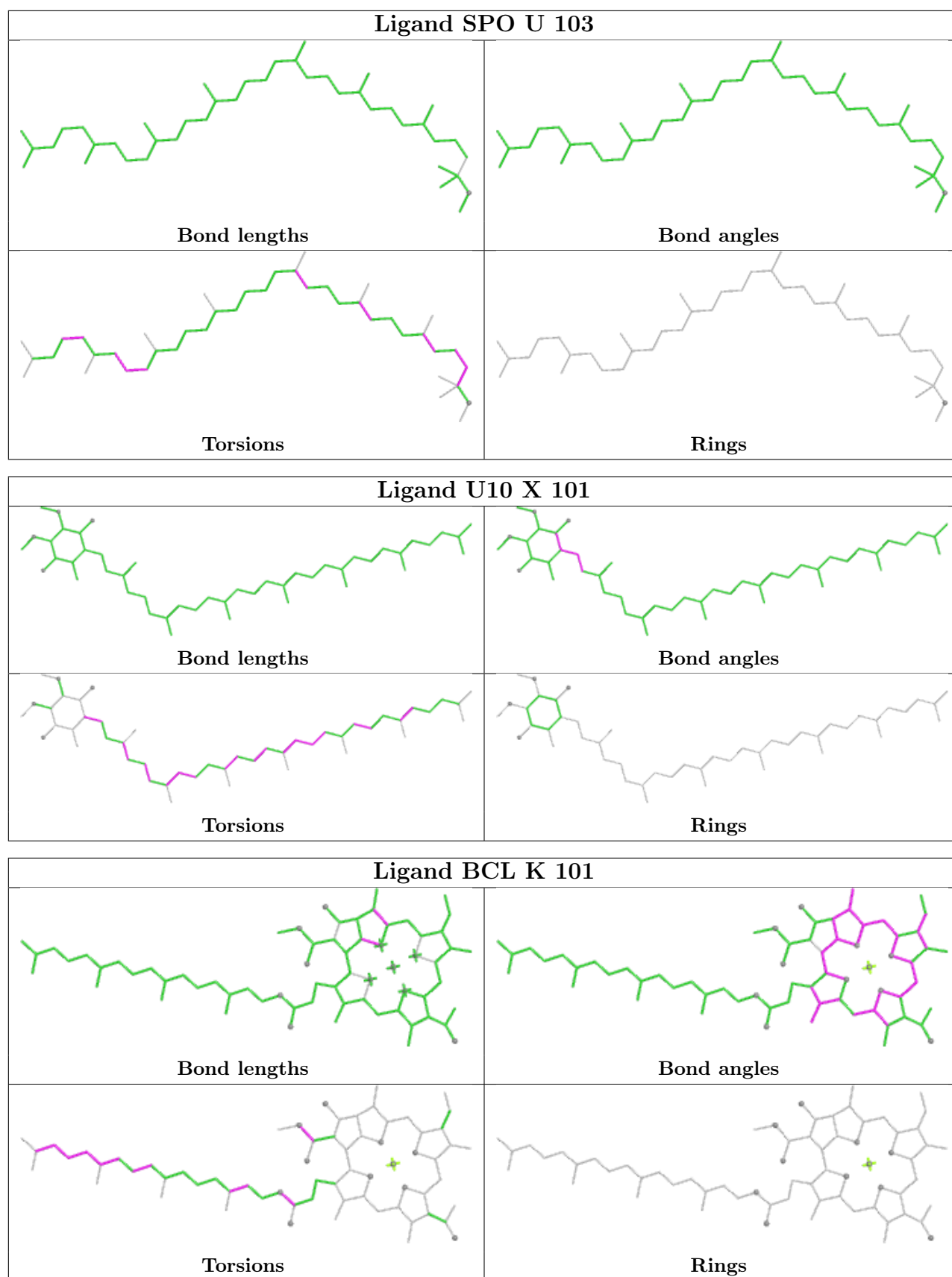


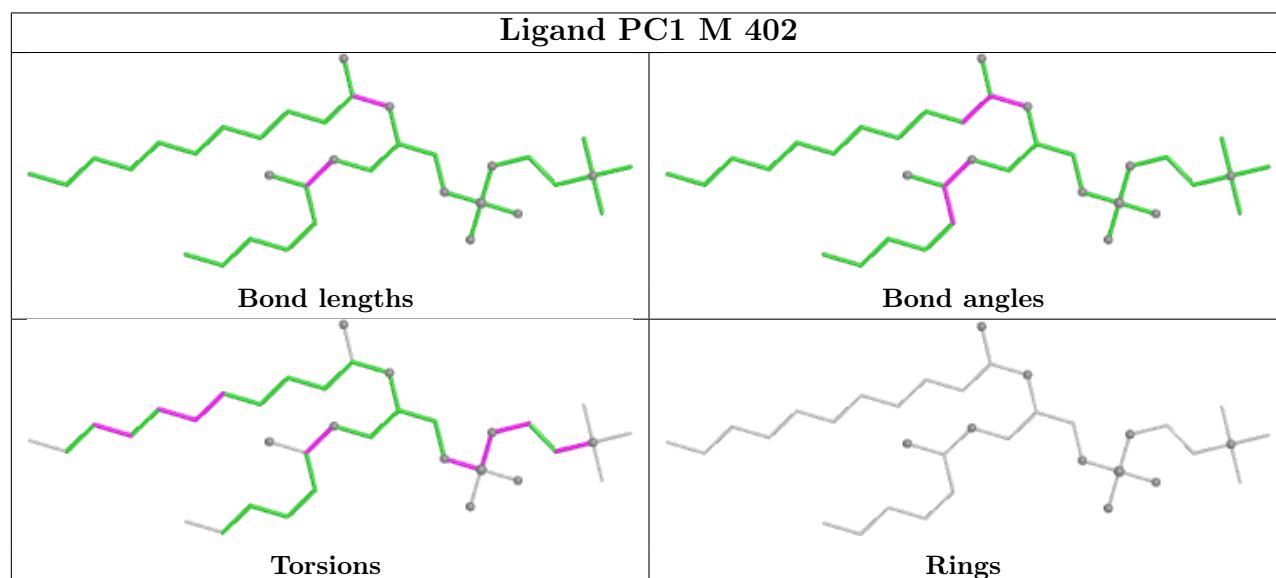
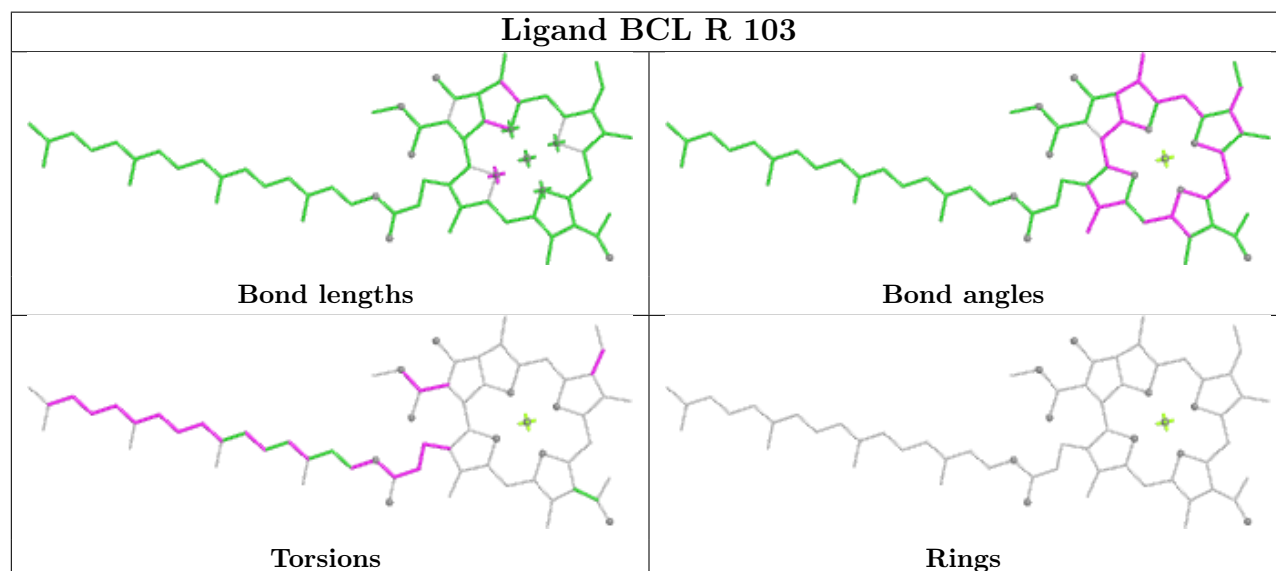
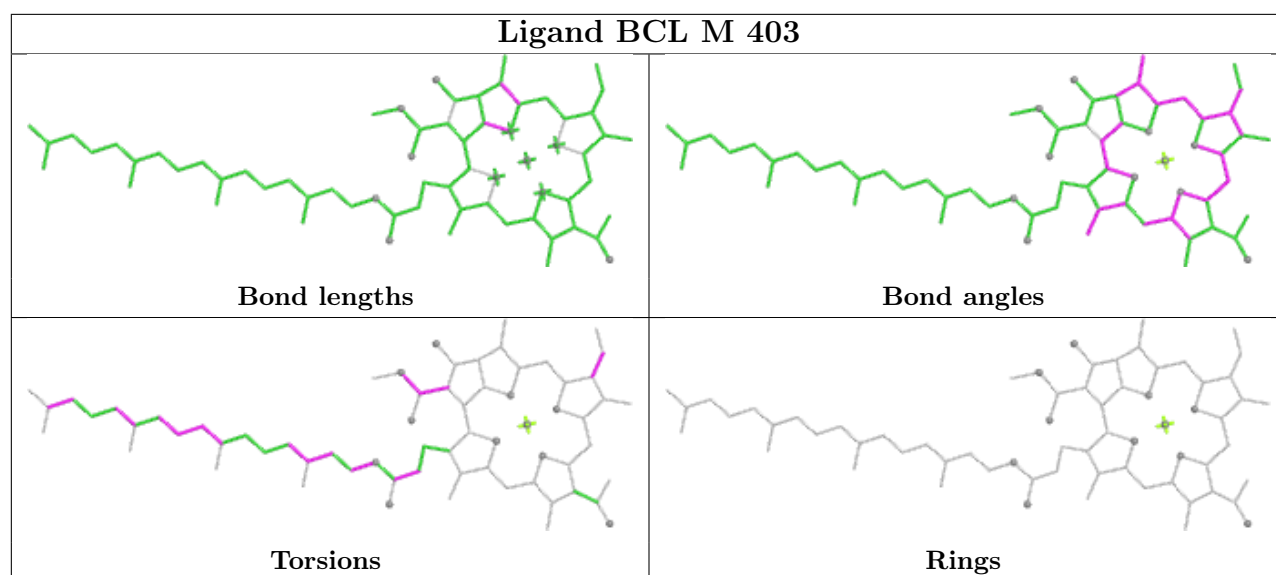
Ligand PC1 L 305	
	
Bond lengths	Bond angles
	
Torsions	Rings

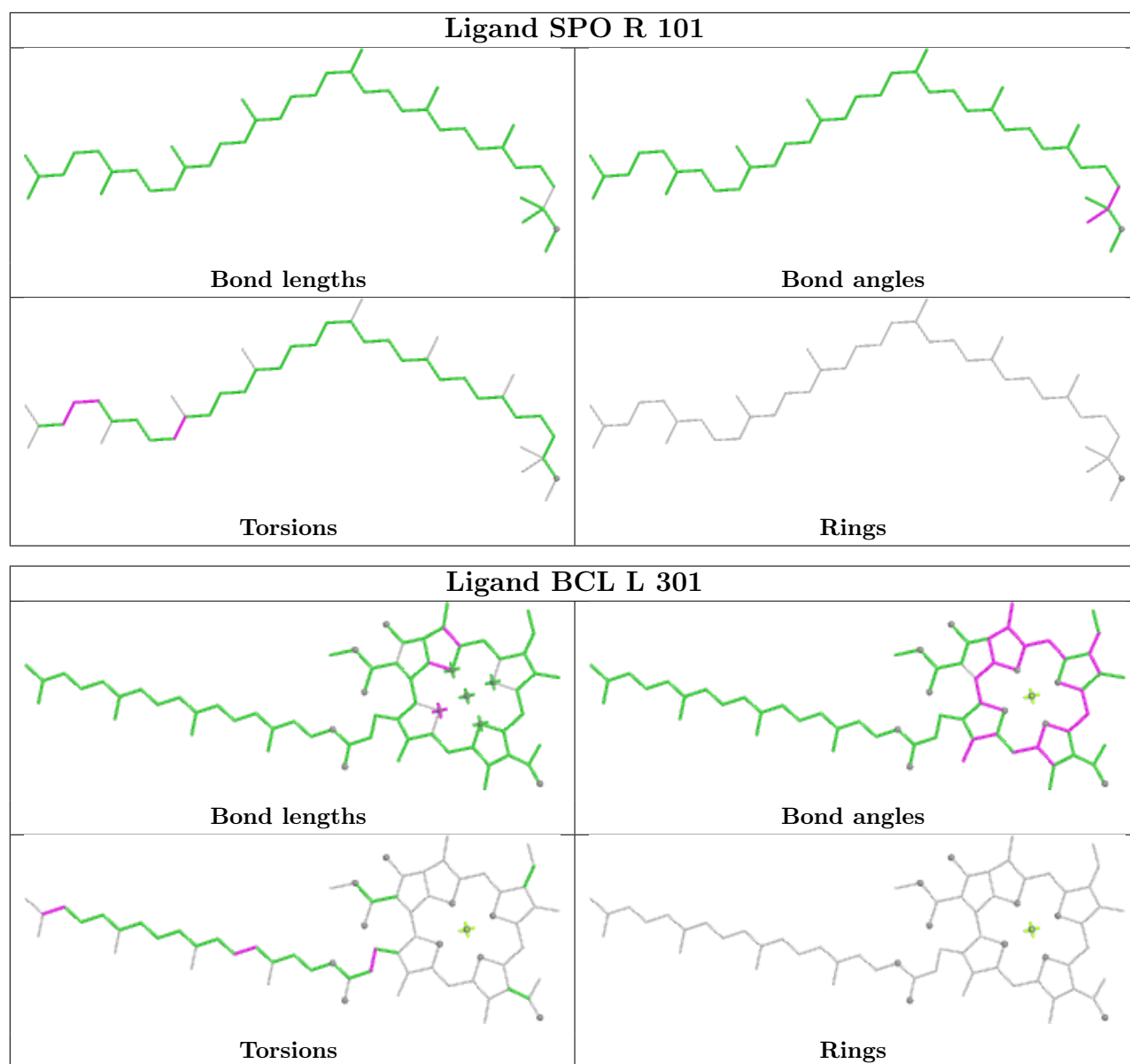
Ligand SPO K 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

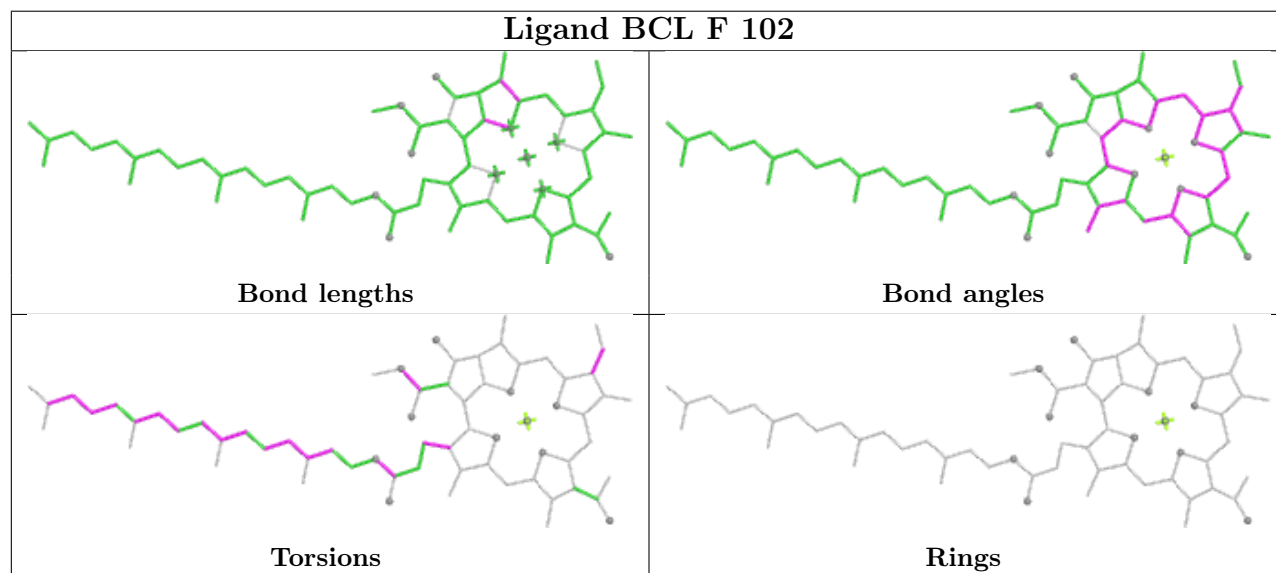
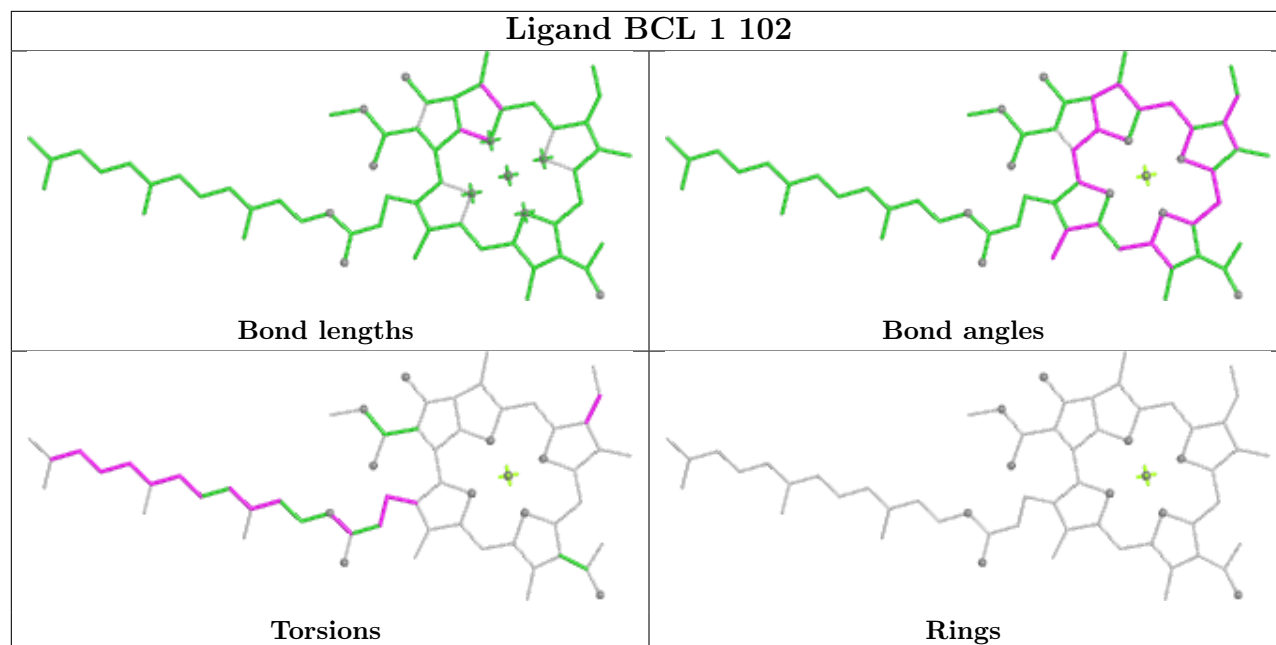
Ligand BCL T 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

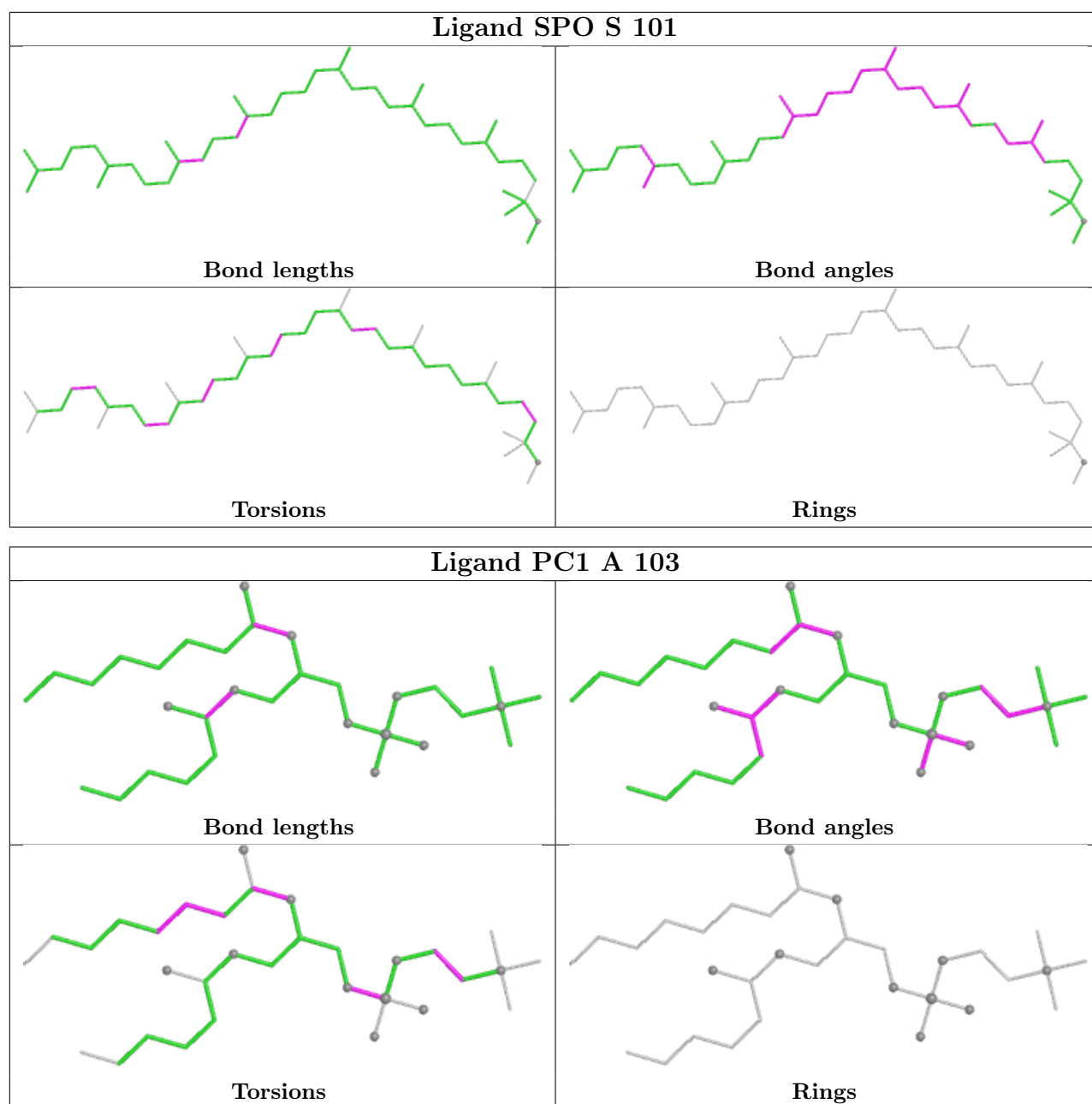


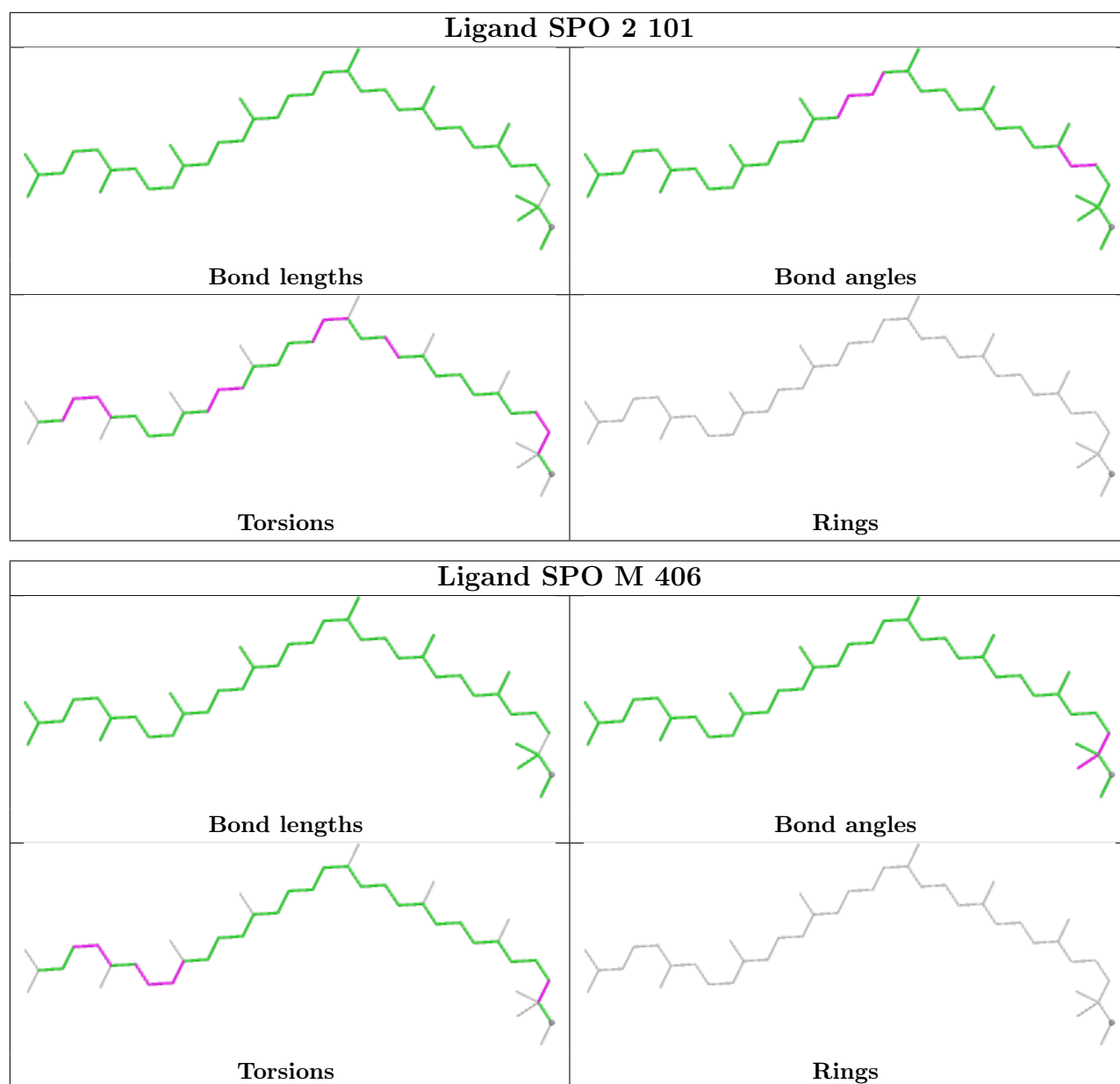


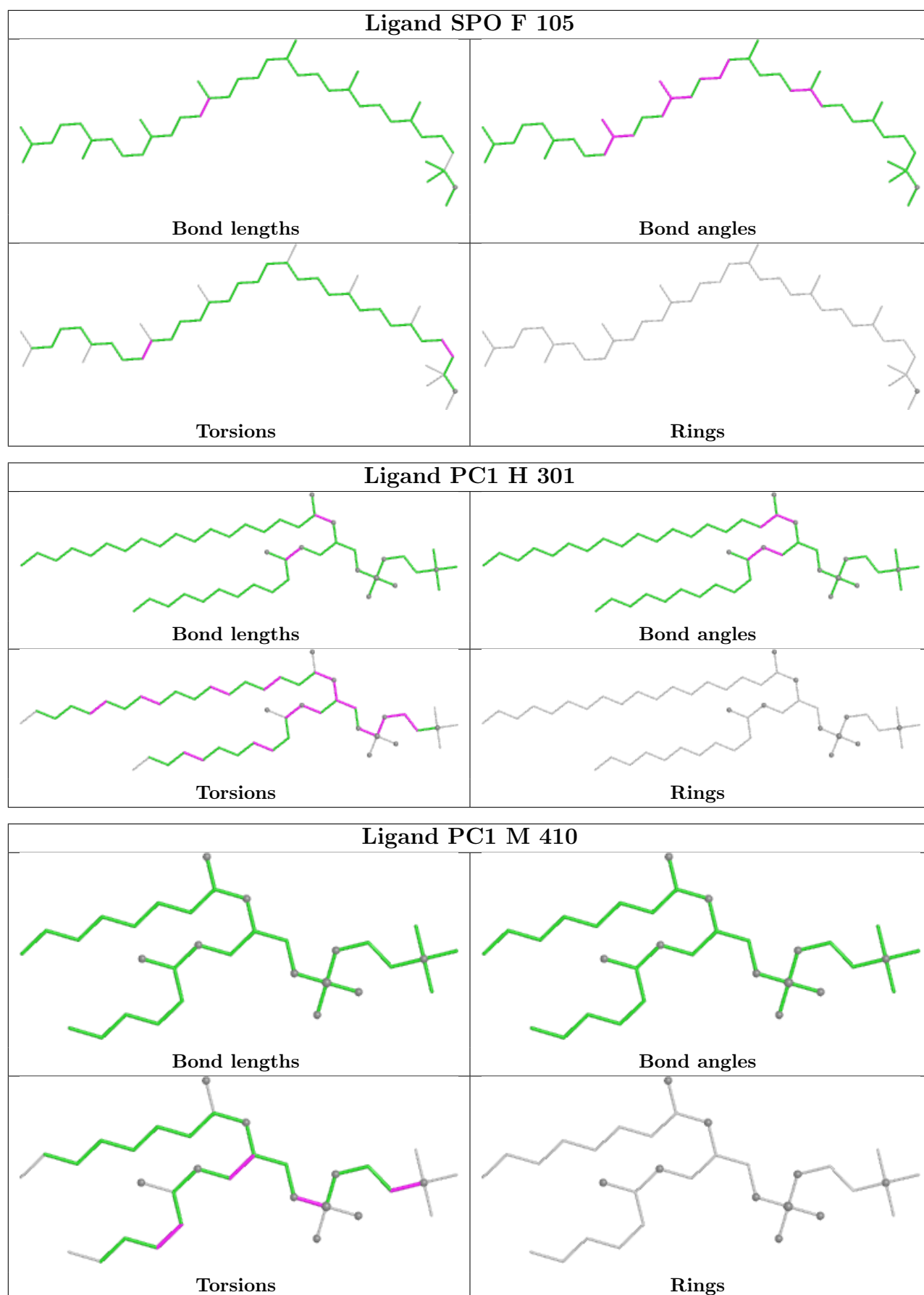


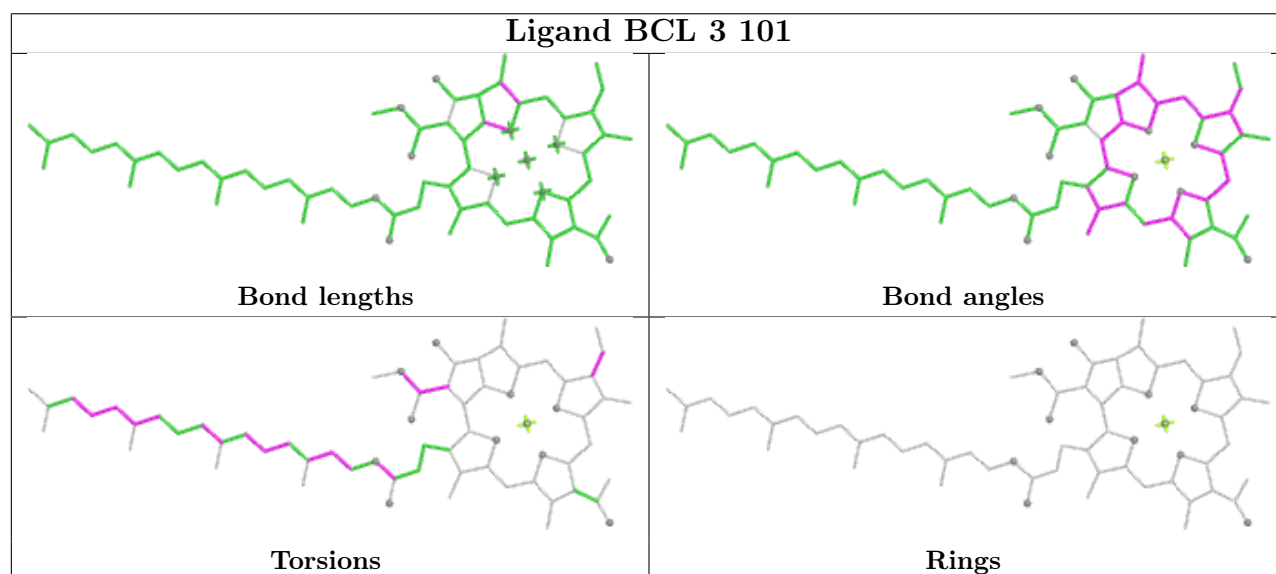
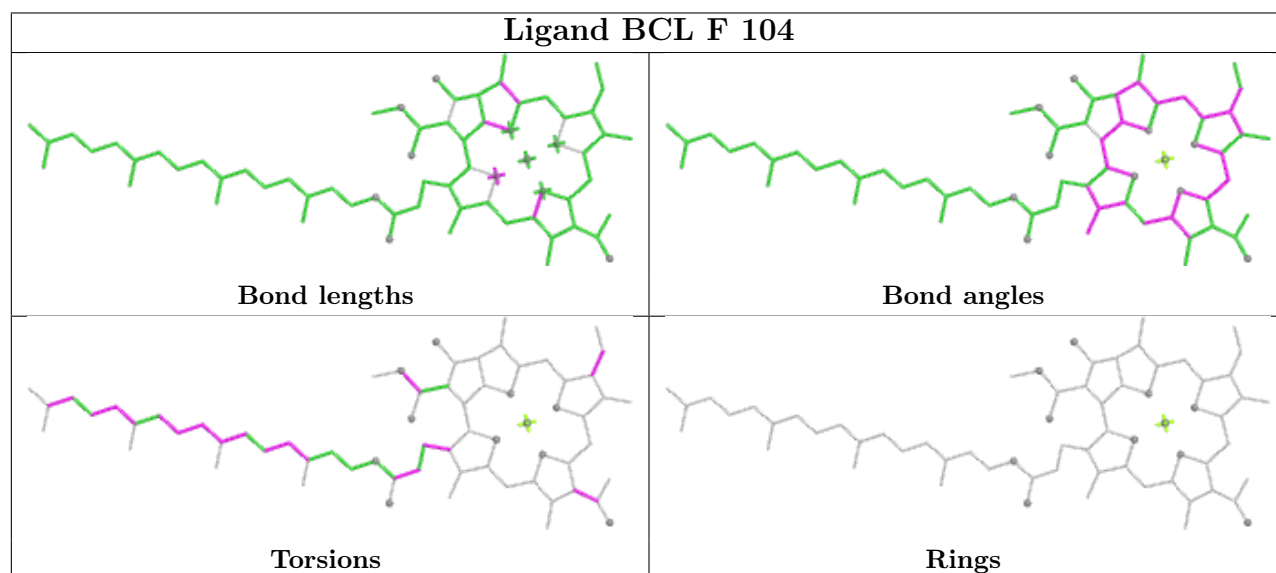
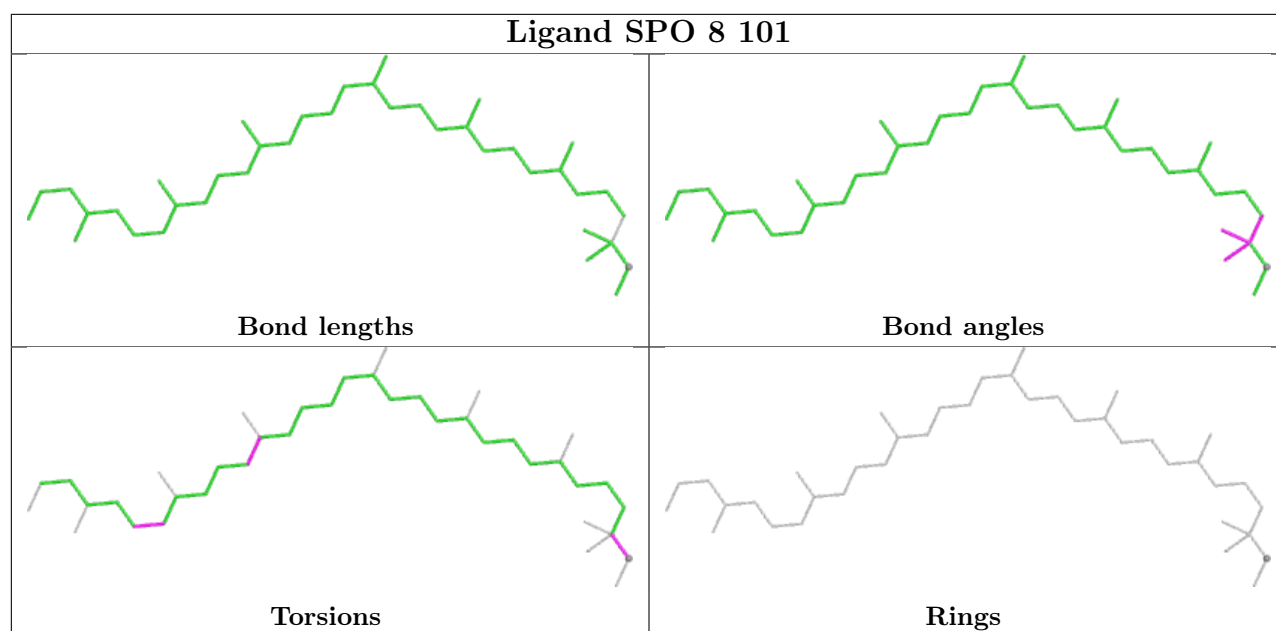


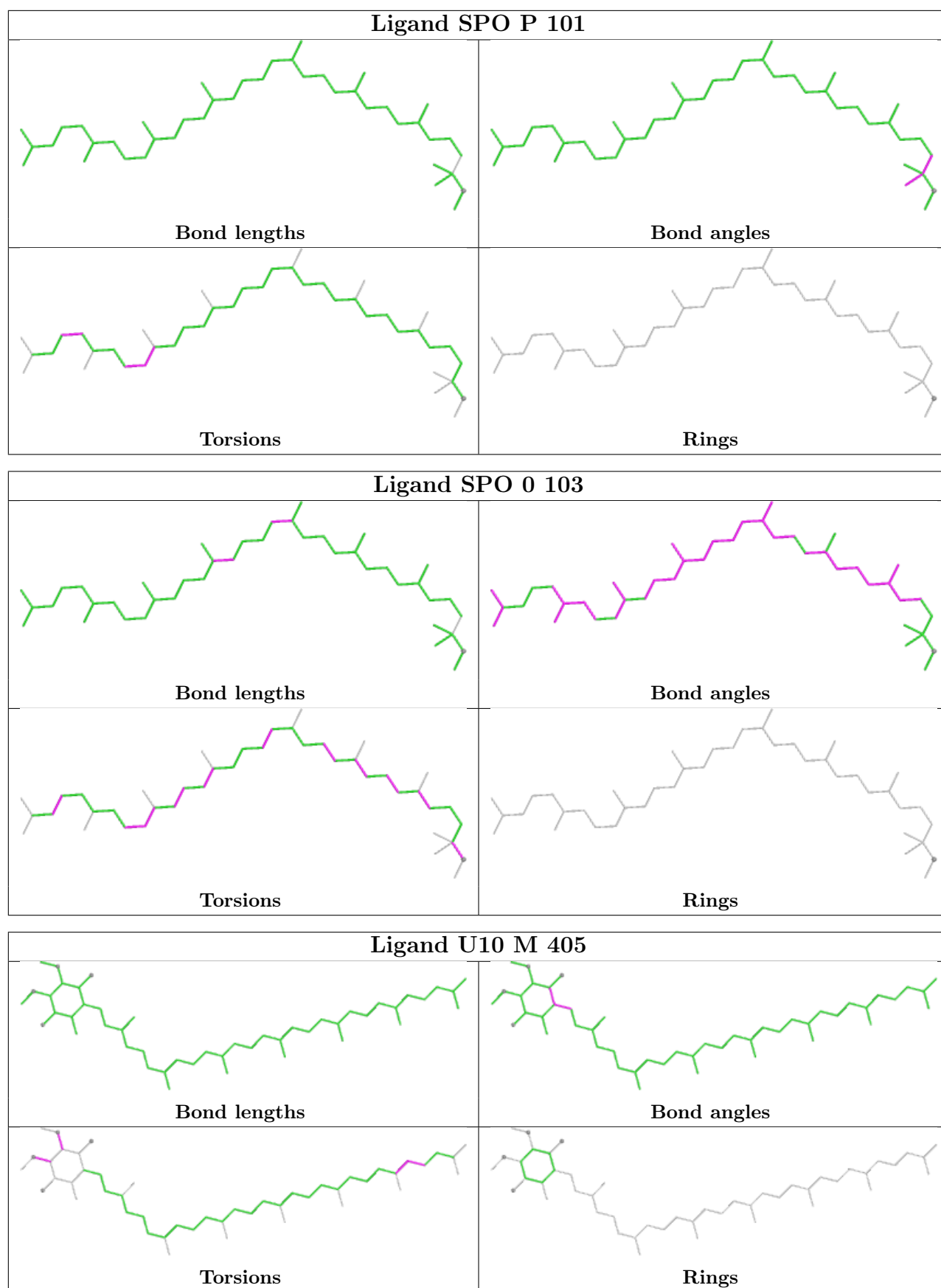


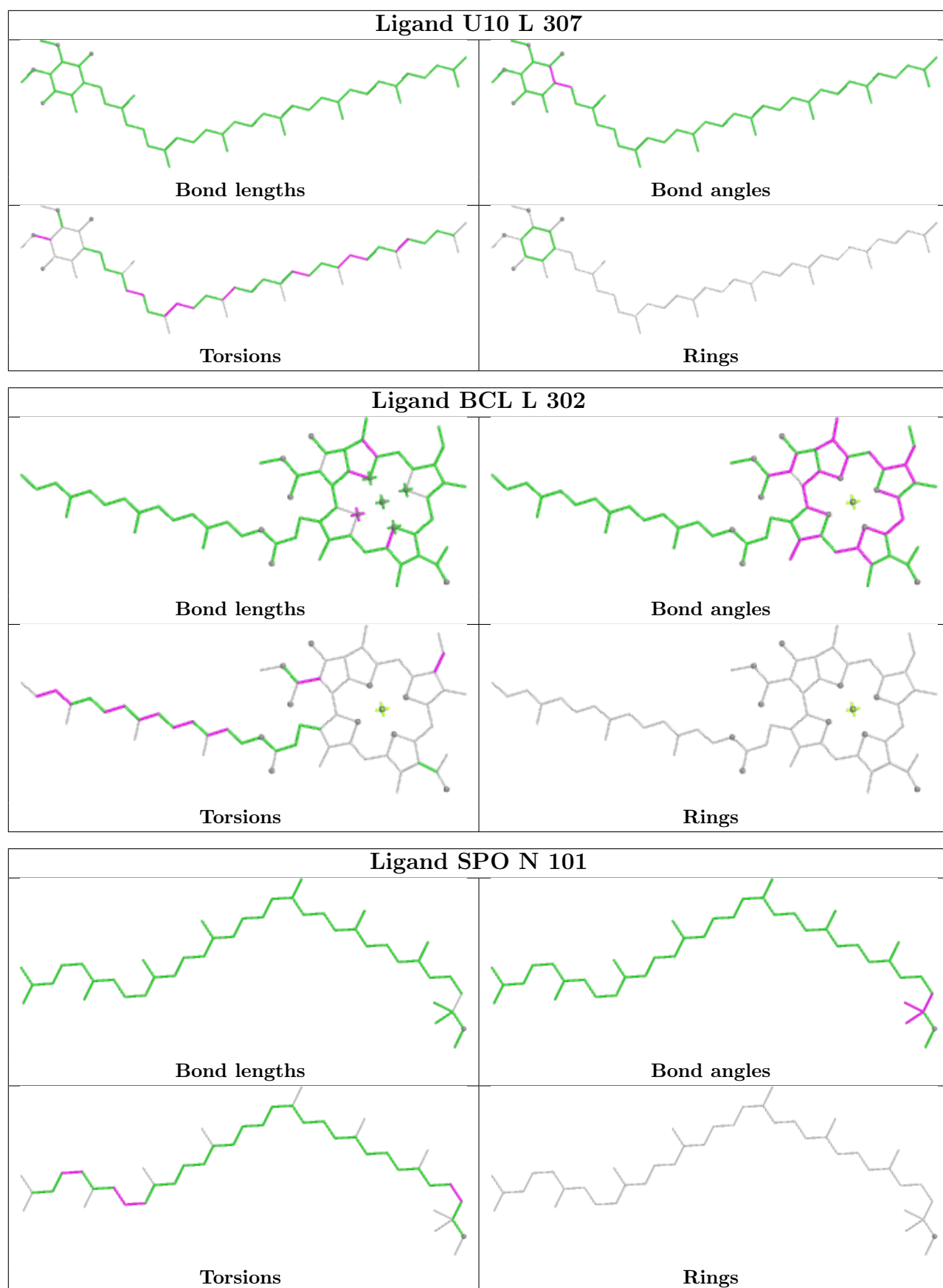


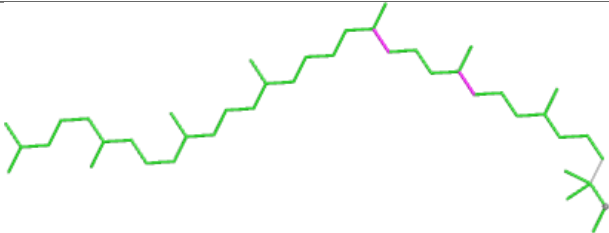
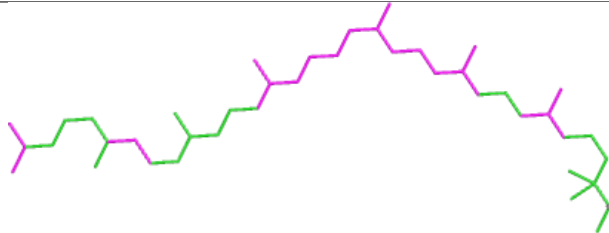
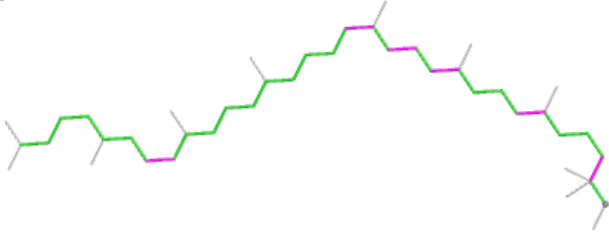
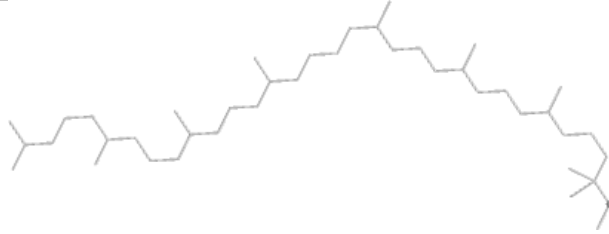


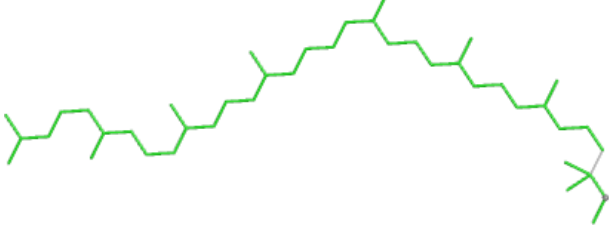
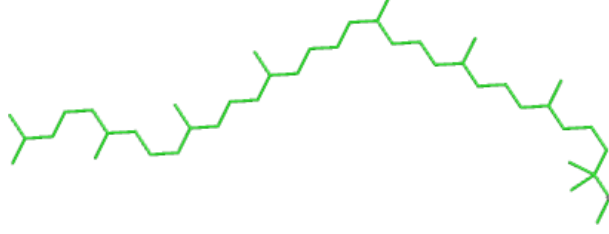
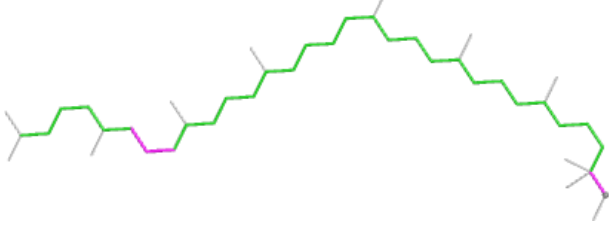
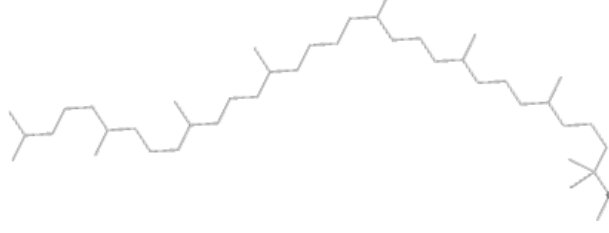


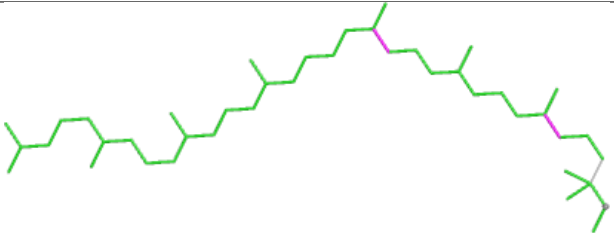
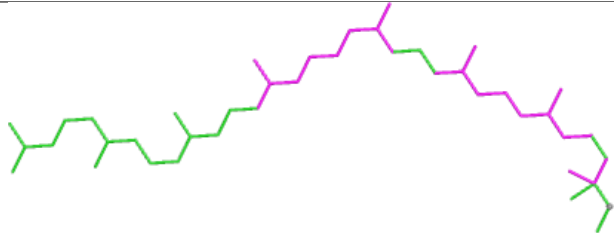
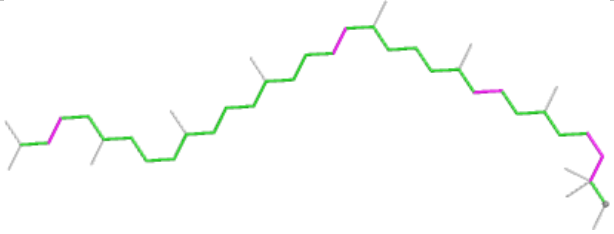
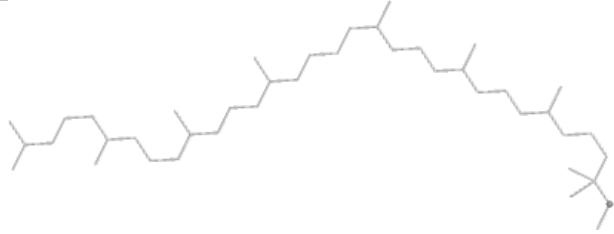


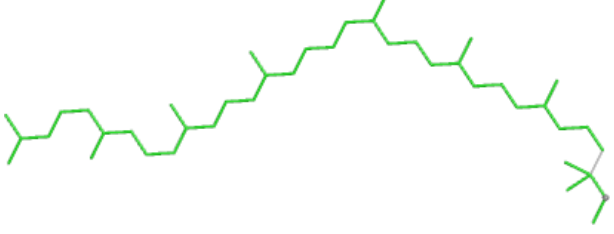
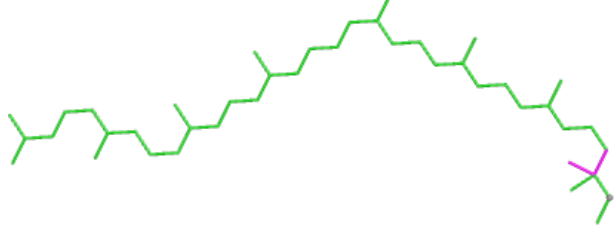
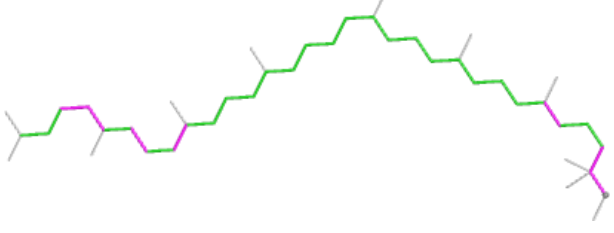


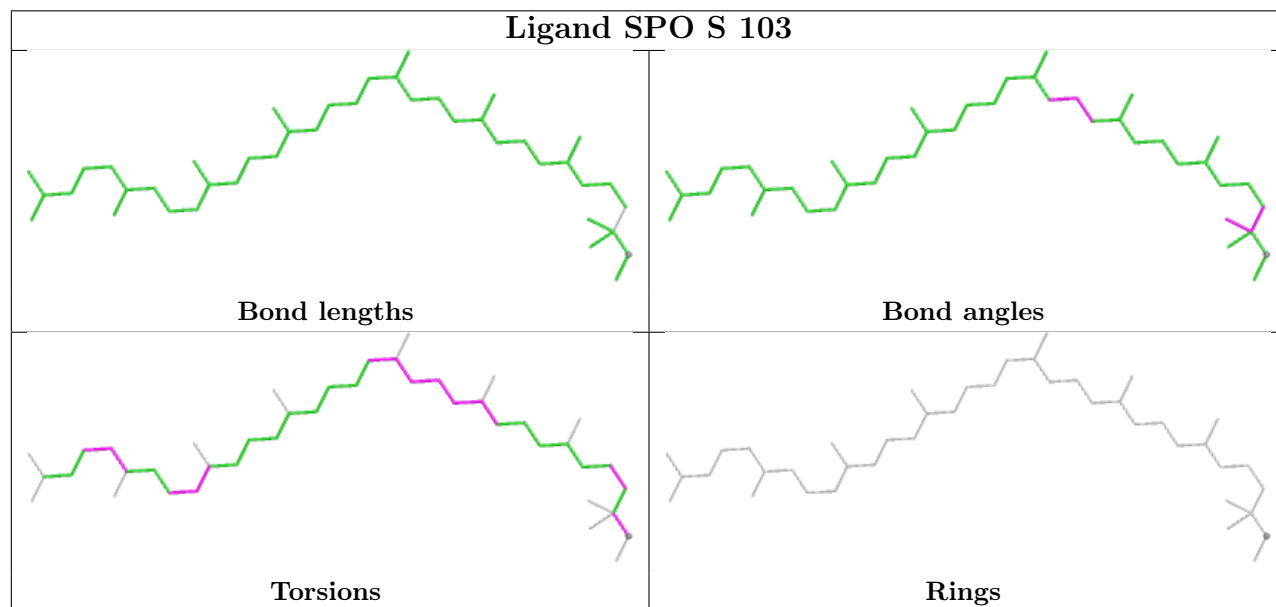
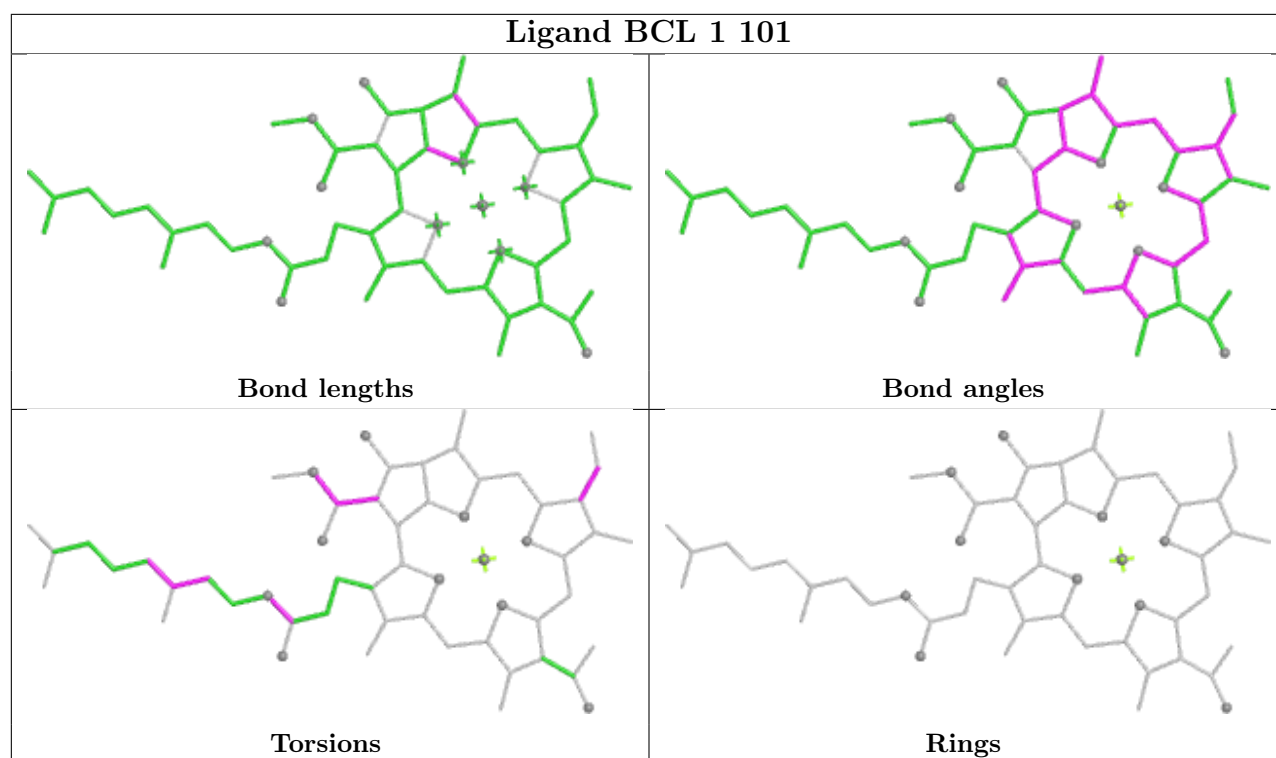


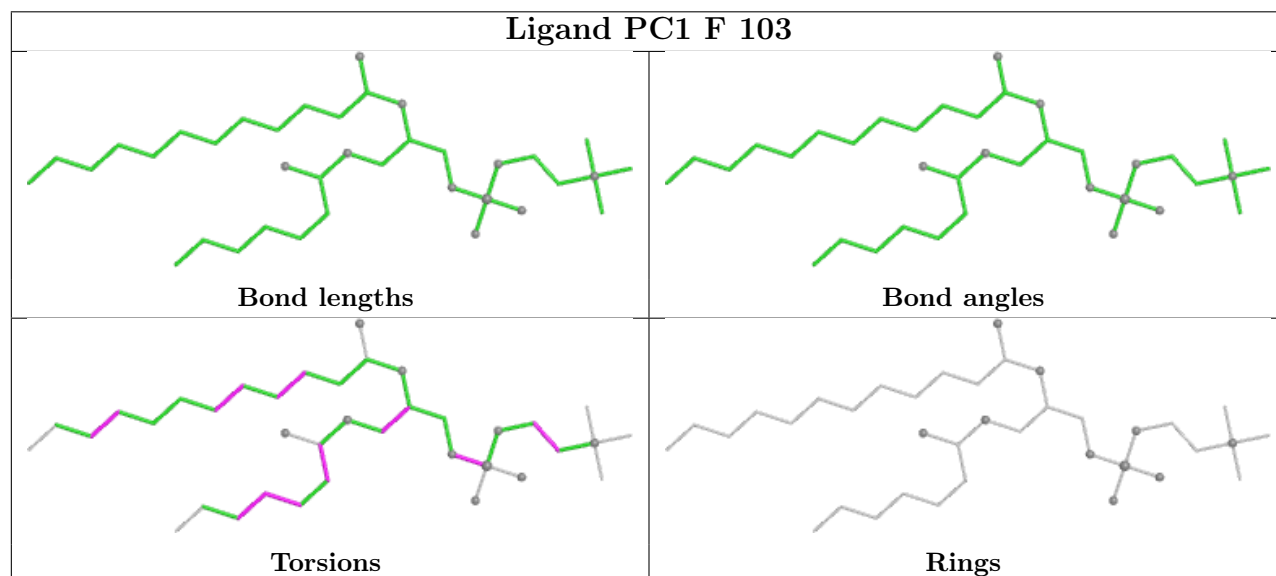
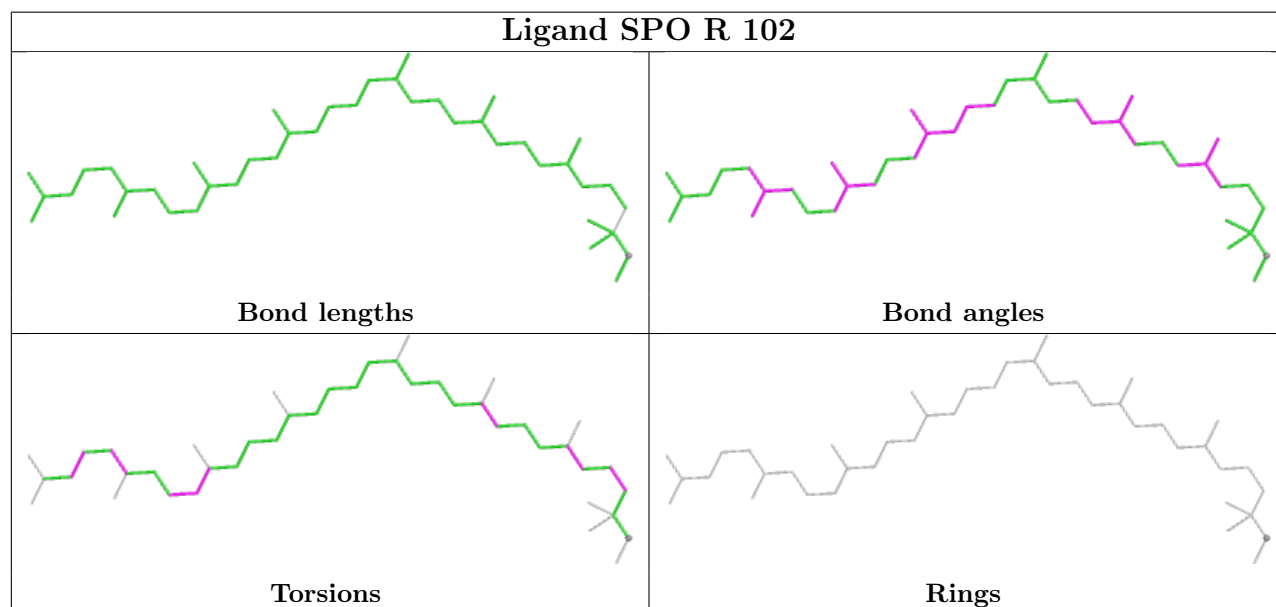
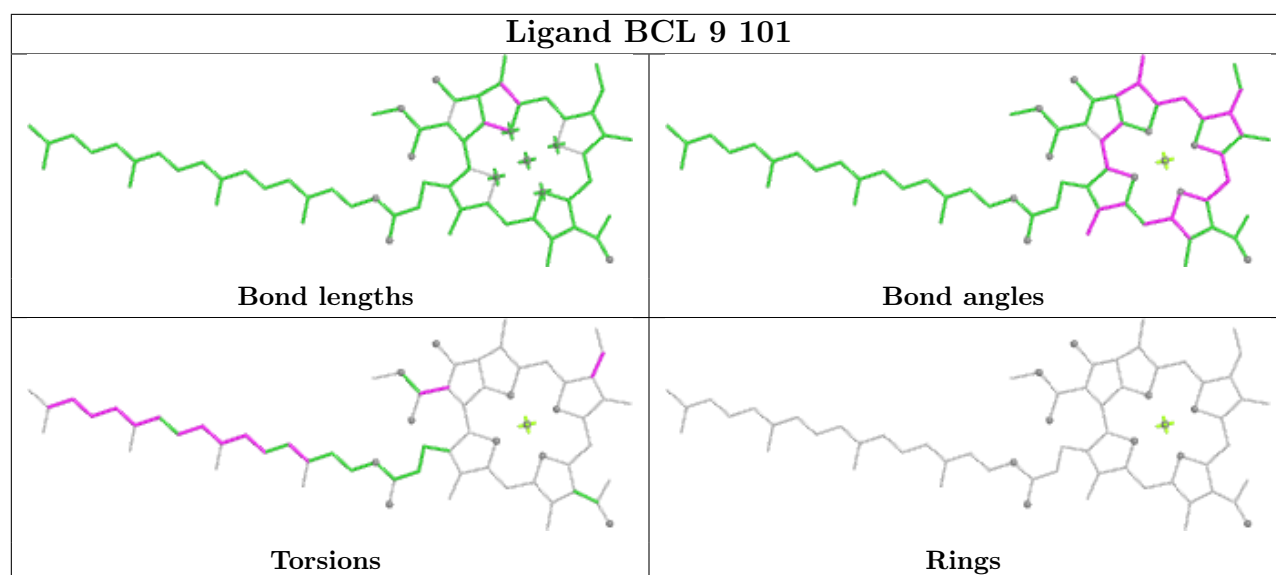
Ligand SPO 3 103	
	
Bond lengths	Bond angles
	
Torsions	Rings

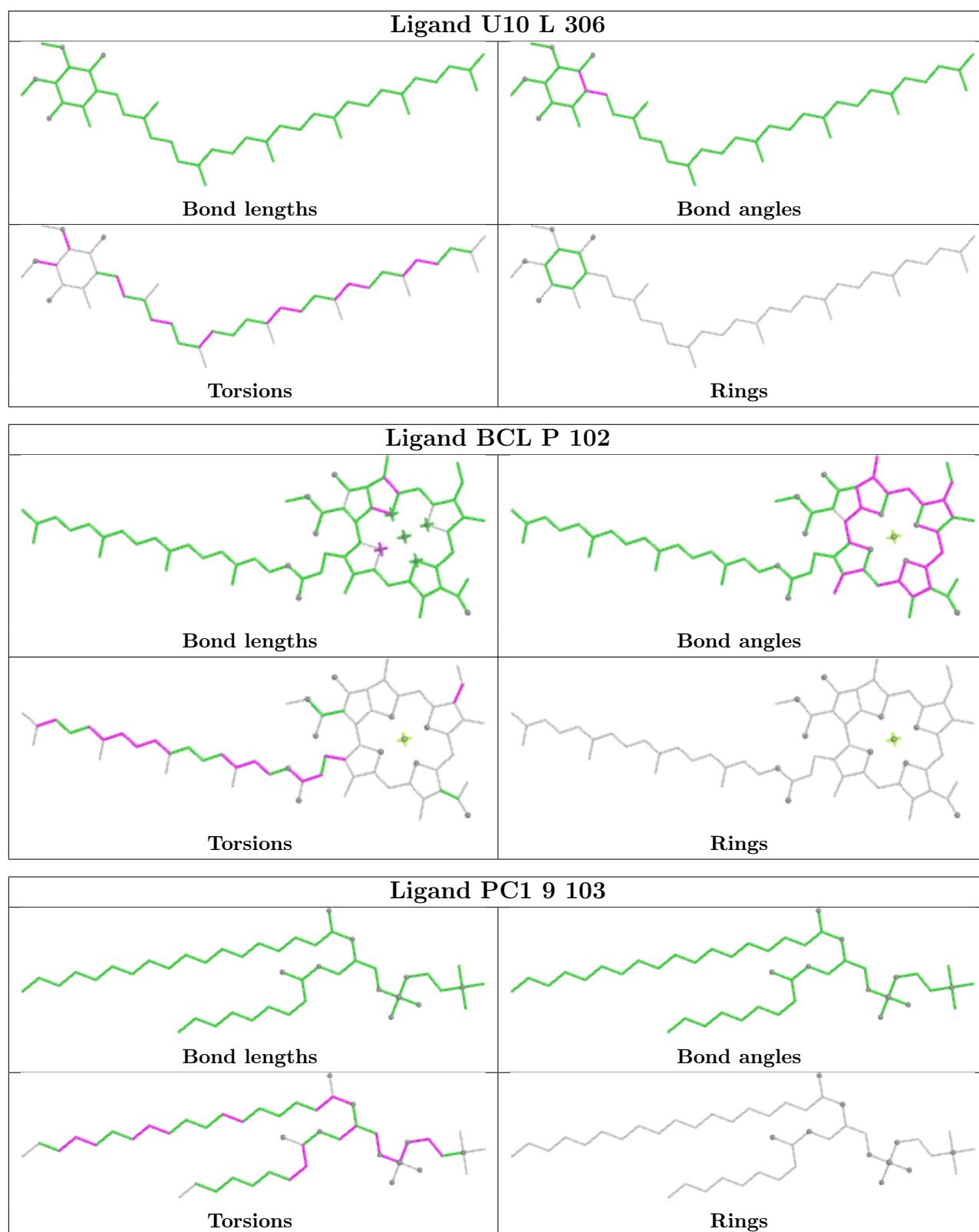
Ligand SPO U 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

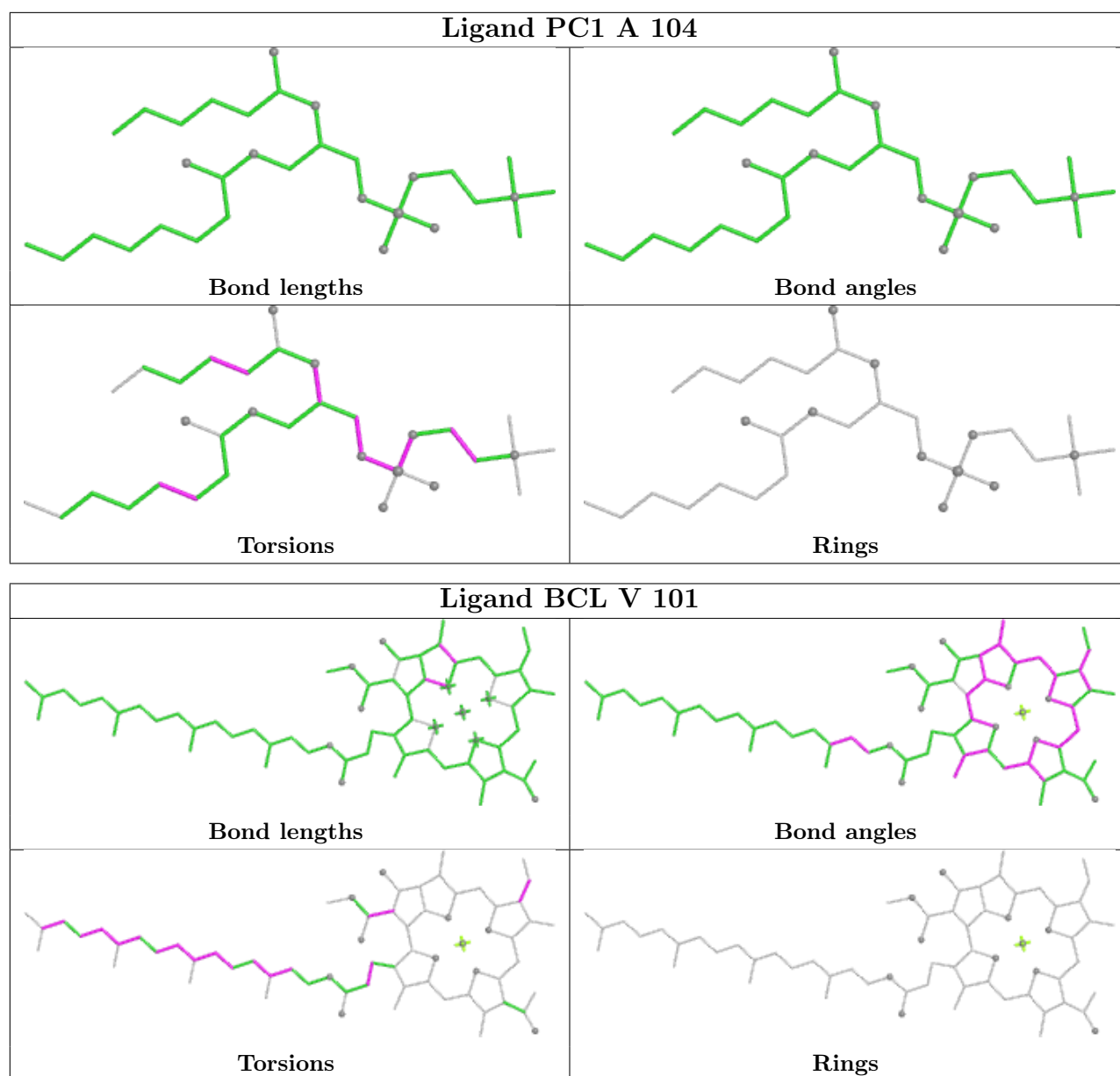
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Bond lengths	Bond angles
	
Torsions	Rings

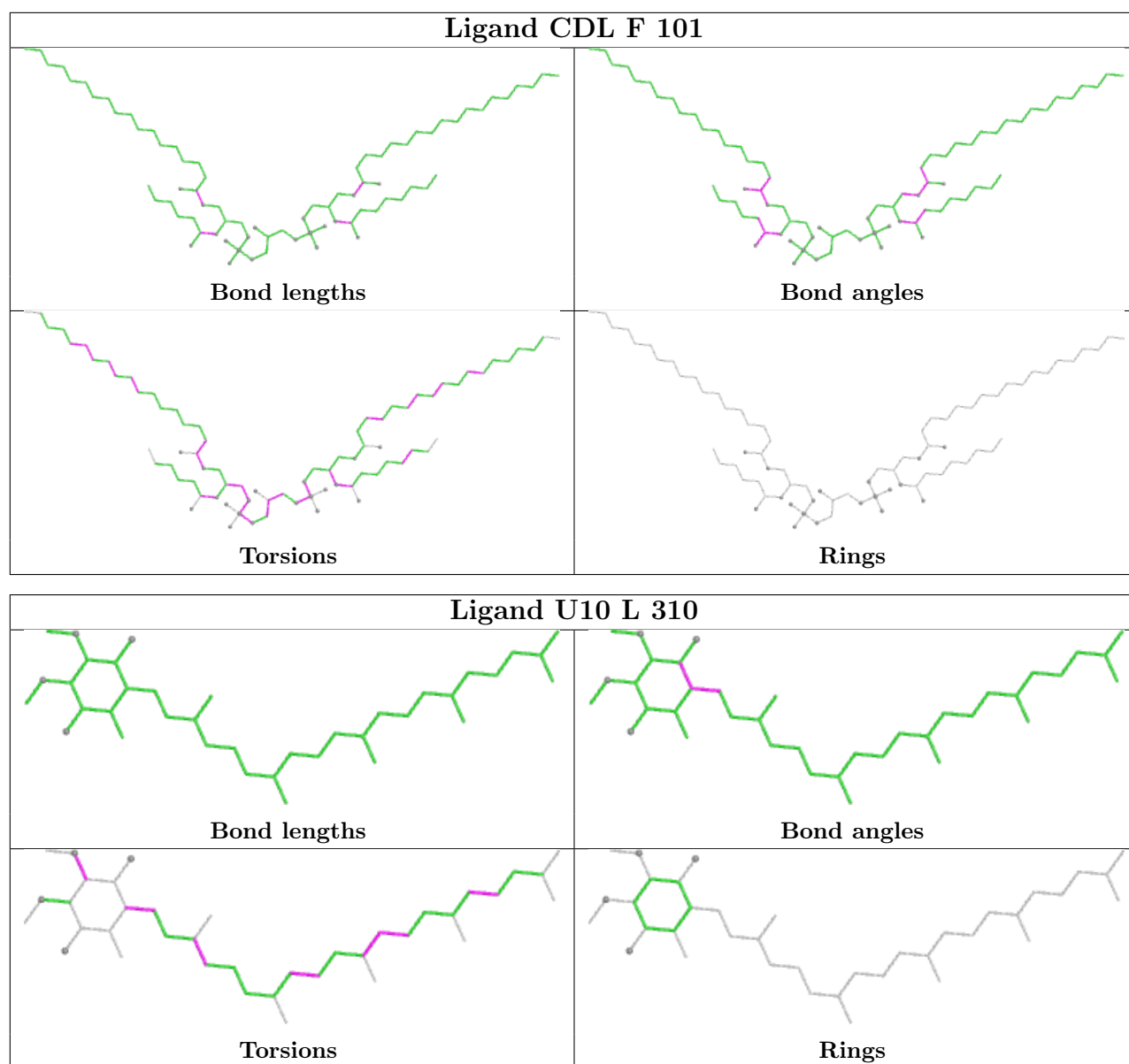
Ligand SPO D 103	
	
Bond lengths	Bond angles
	
Torsions	Rings

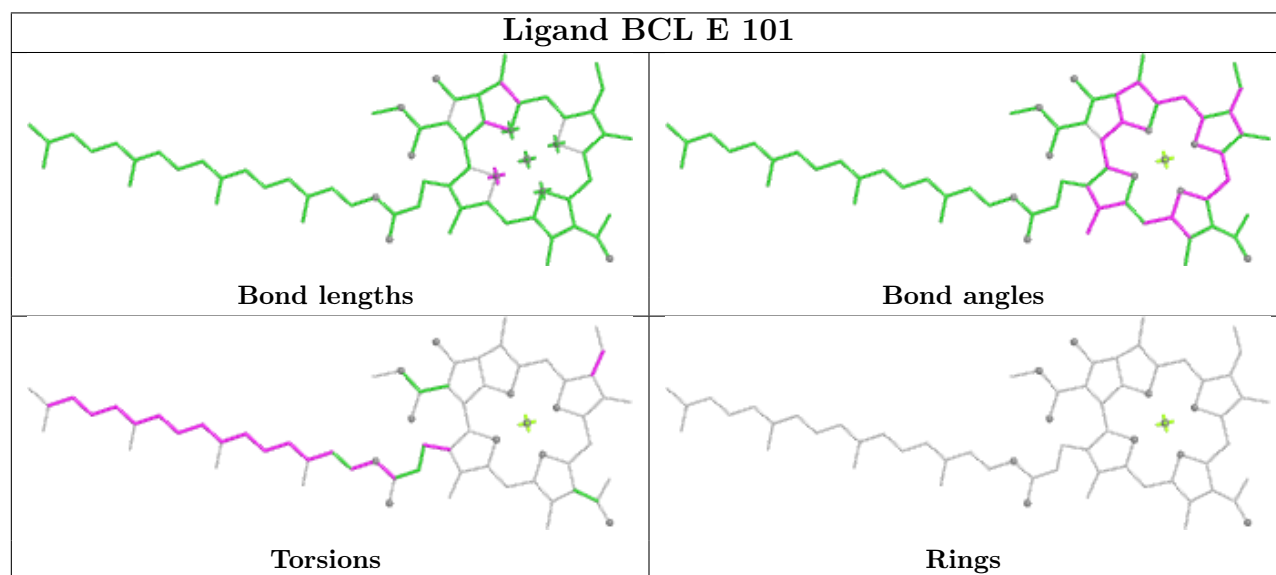
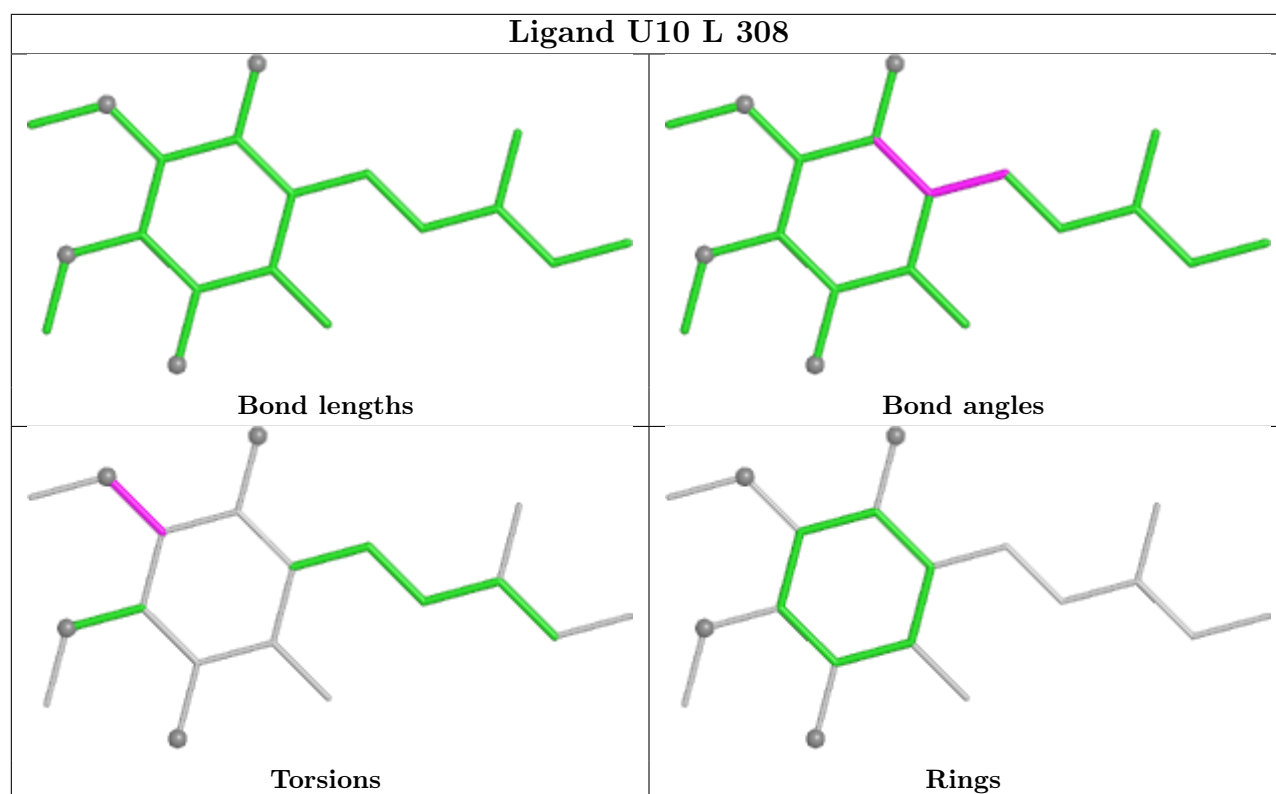


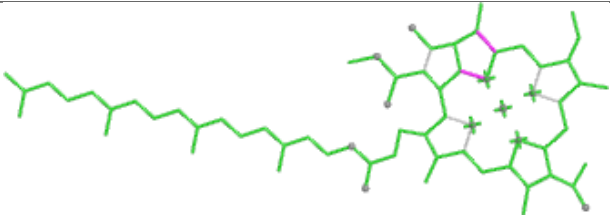
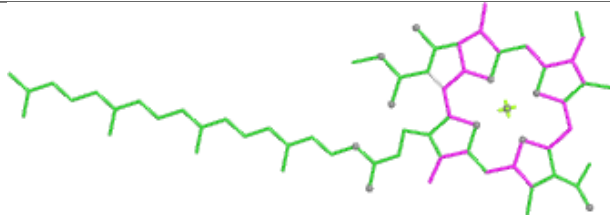
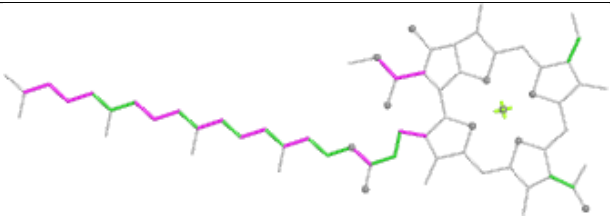
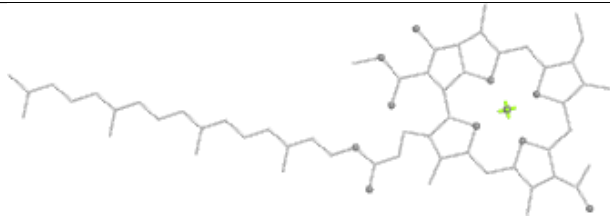
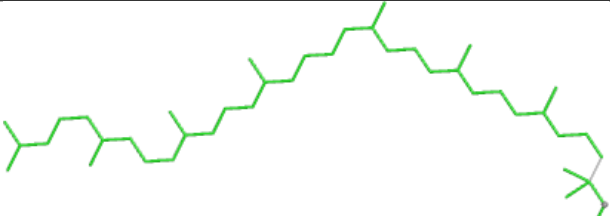
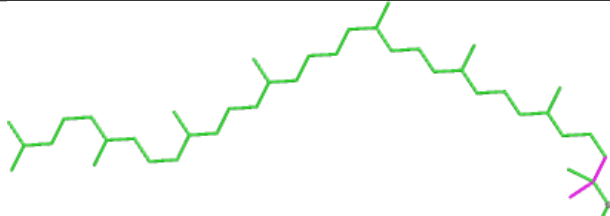
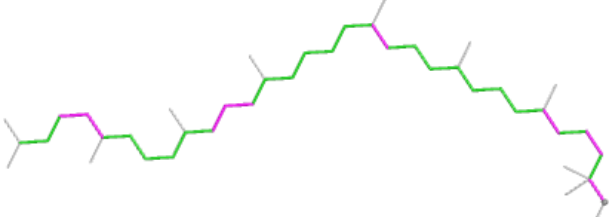
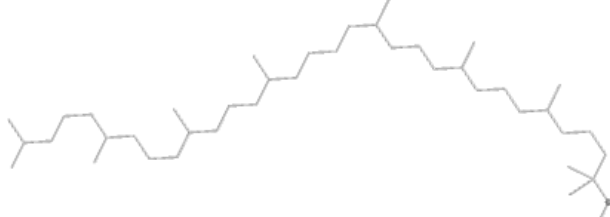


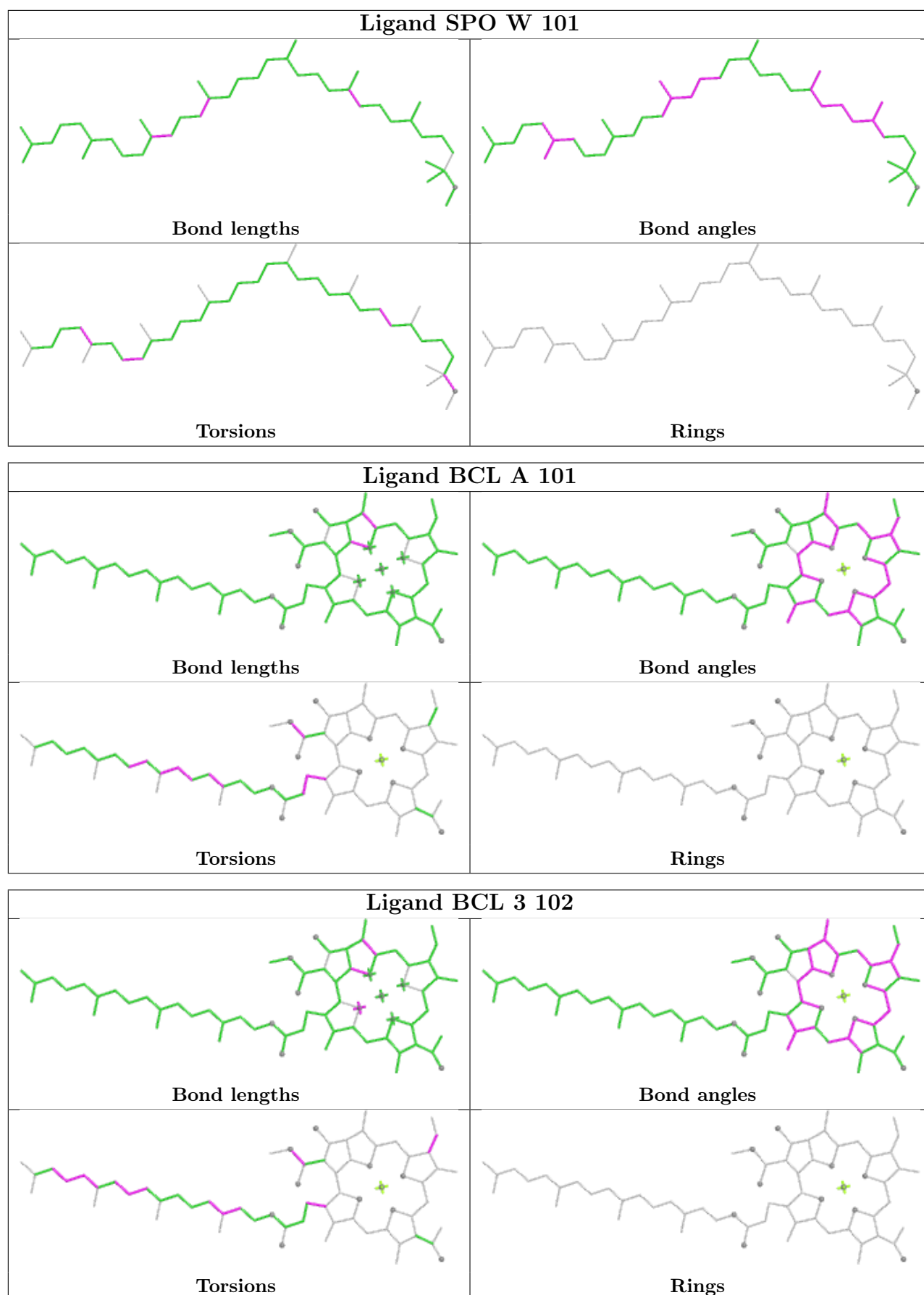


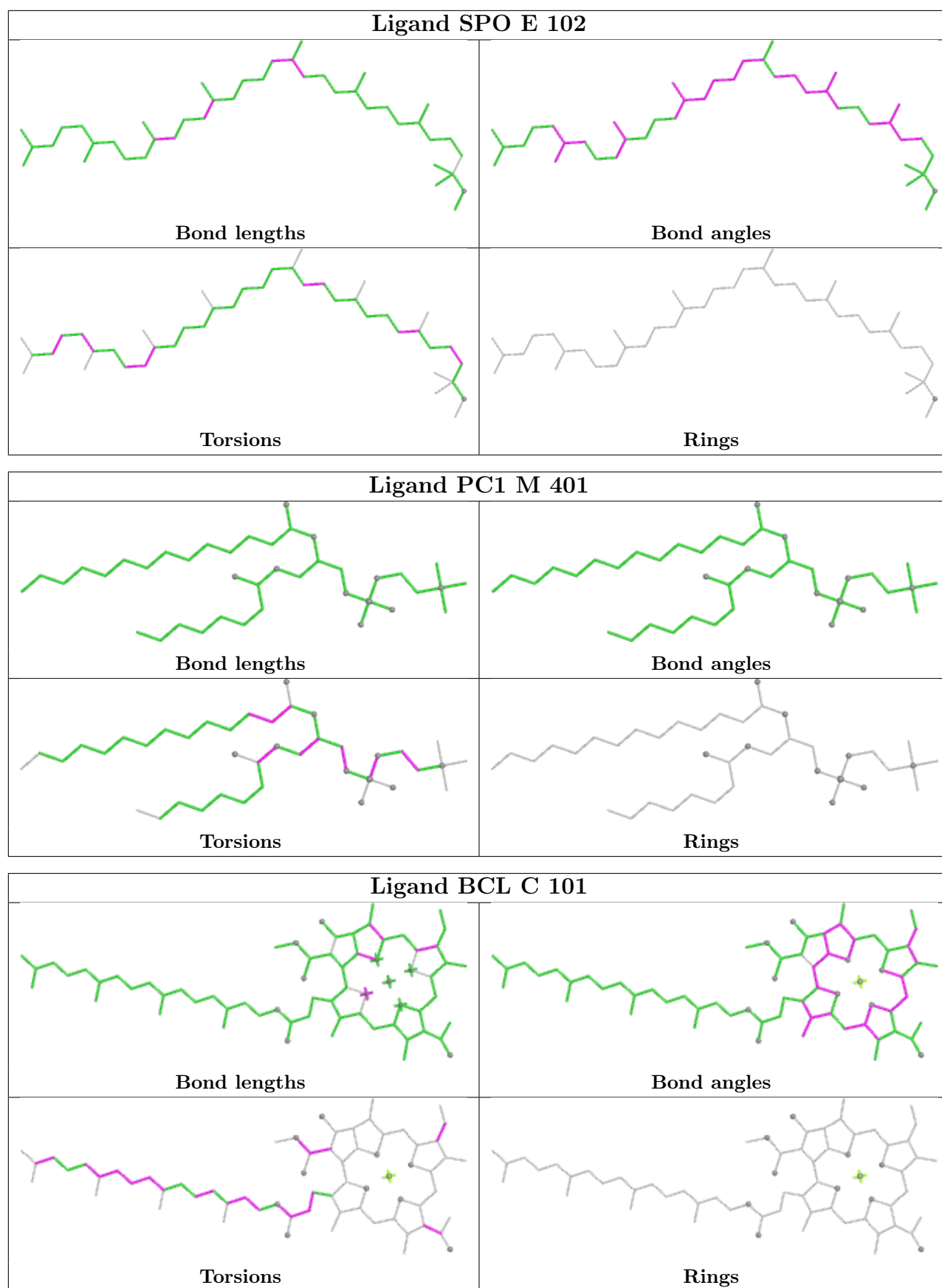


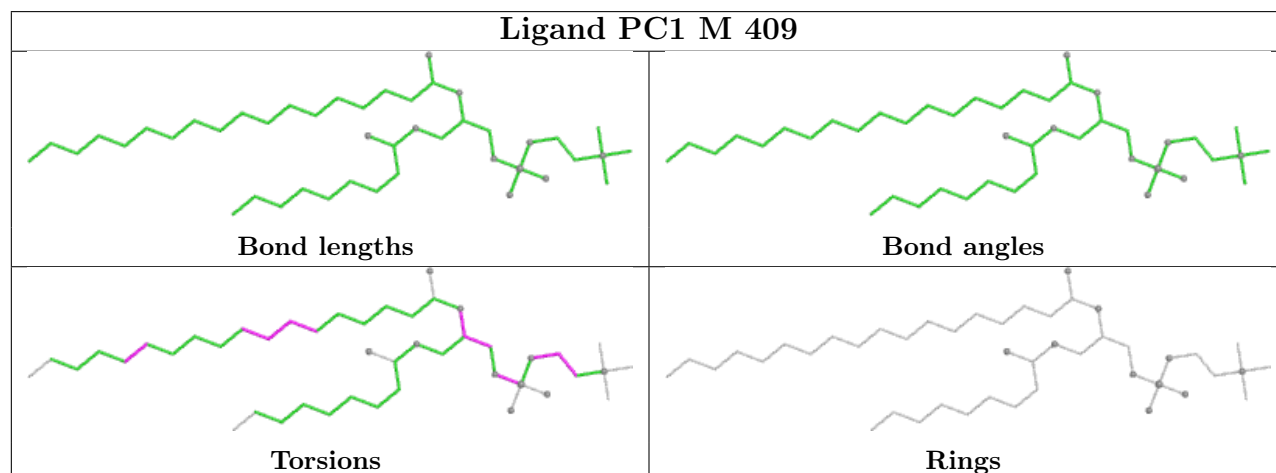
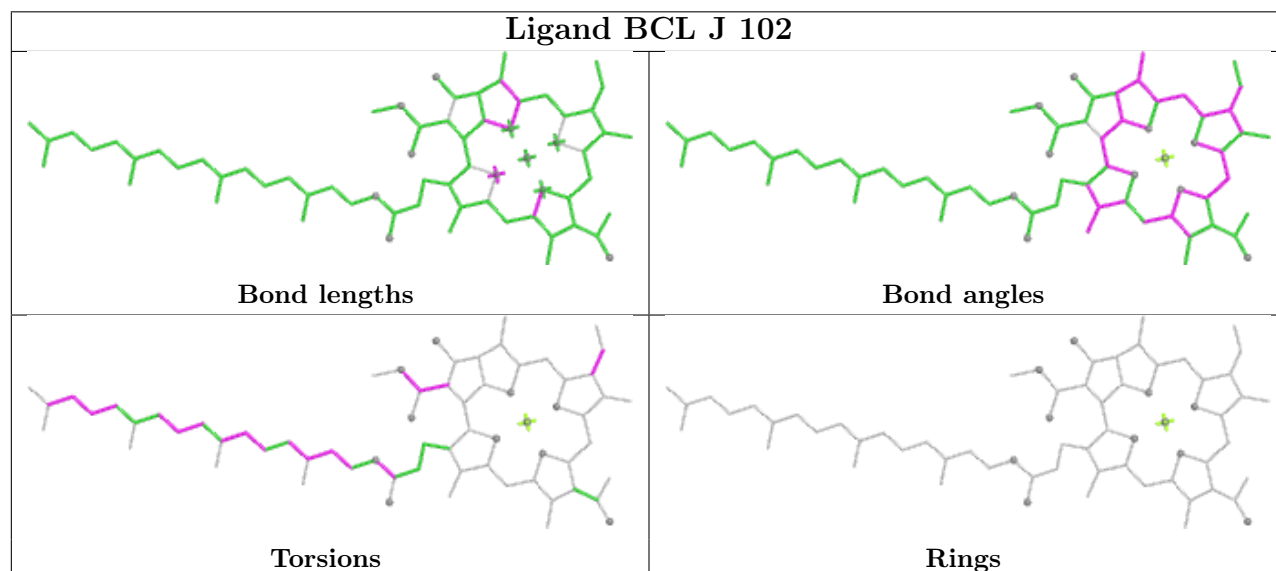
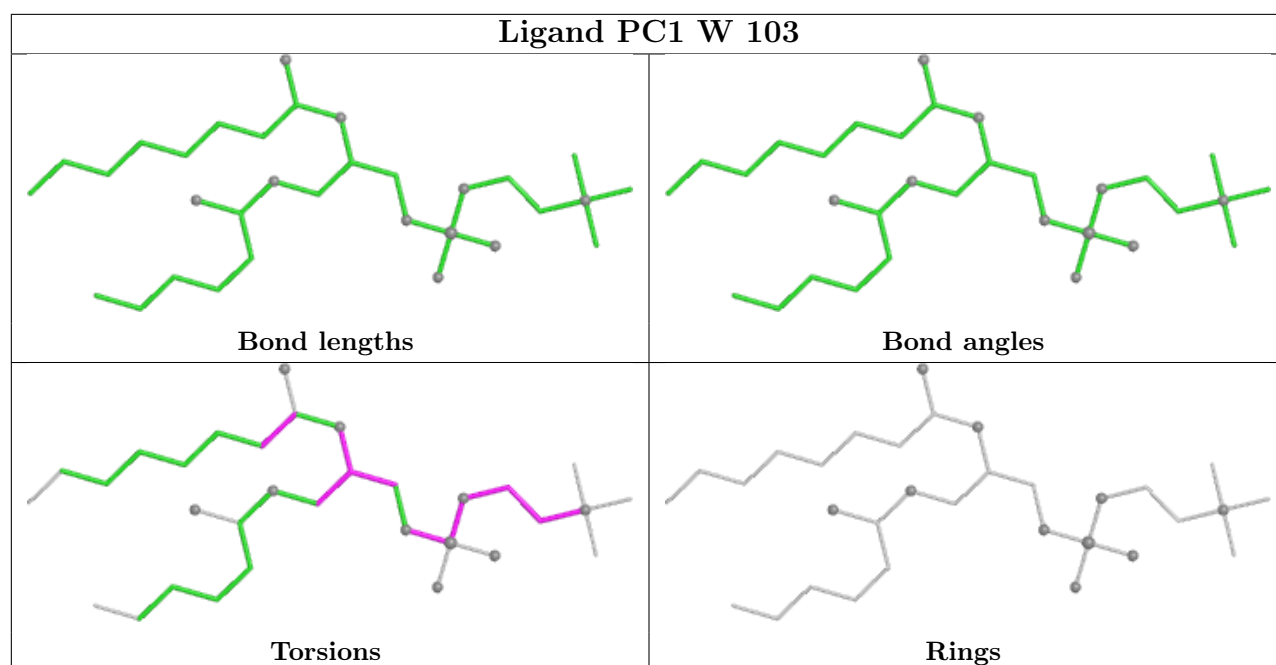


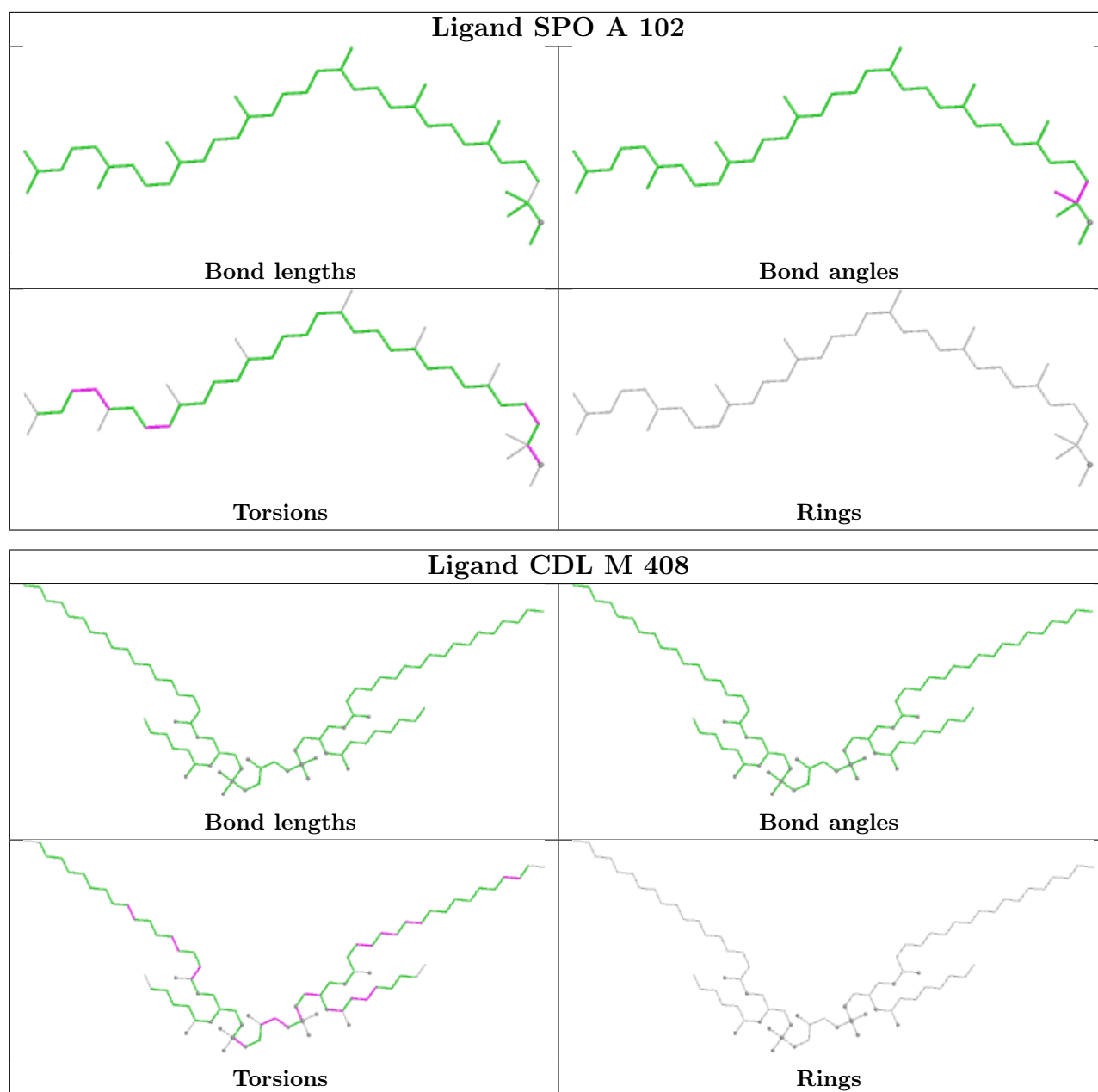


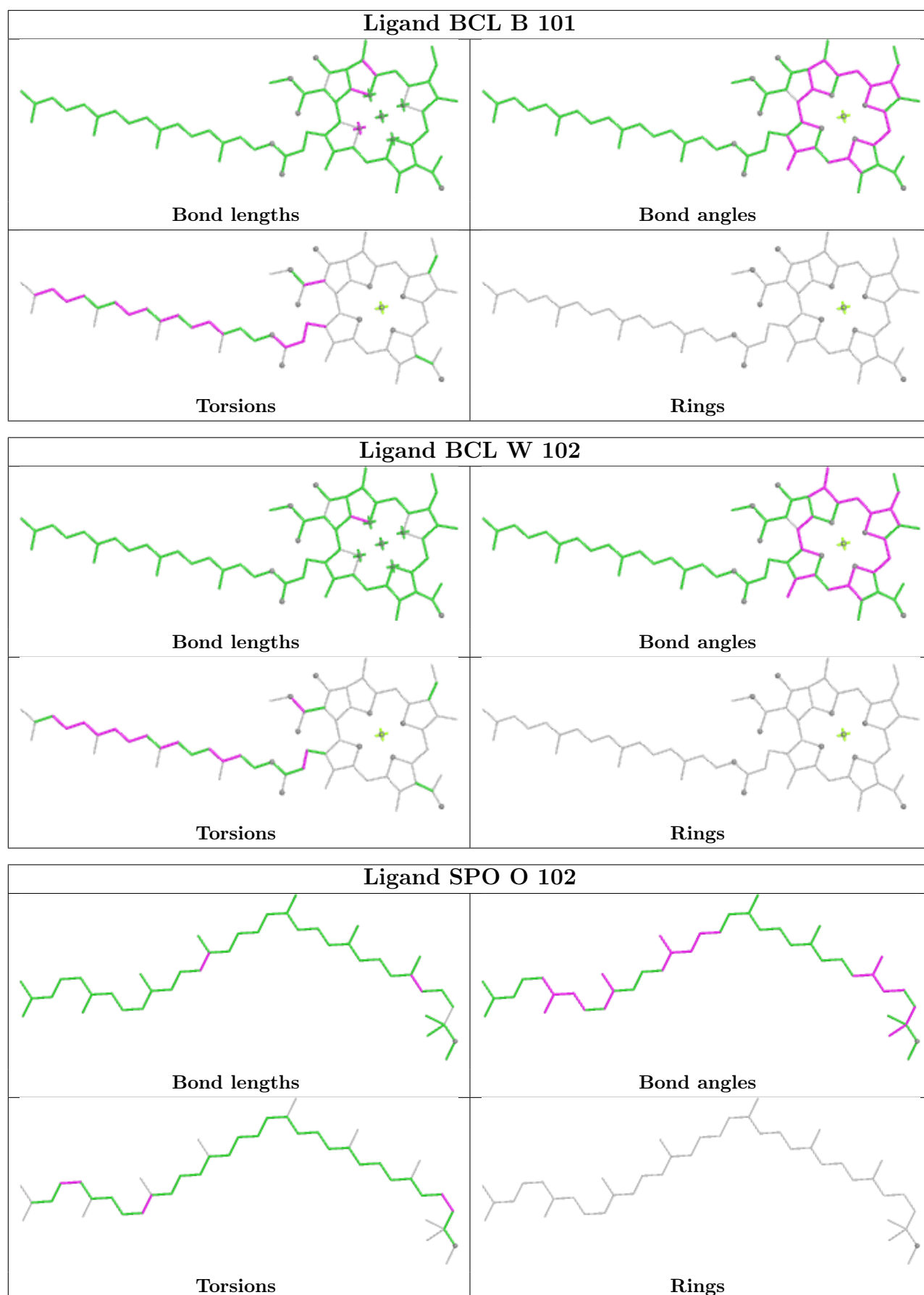
Ligand BCL U 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand SPO Z 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

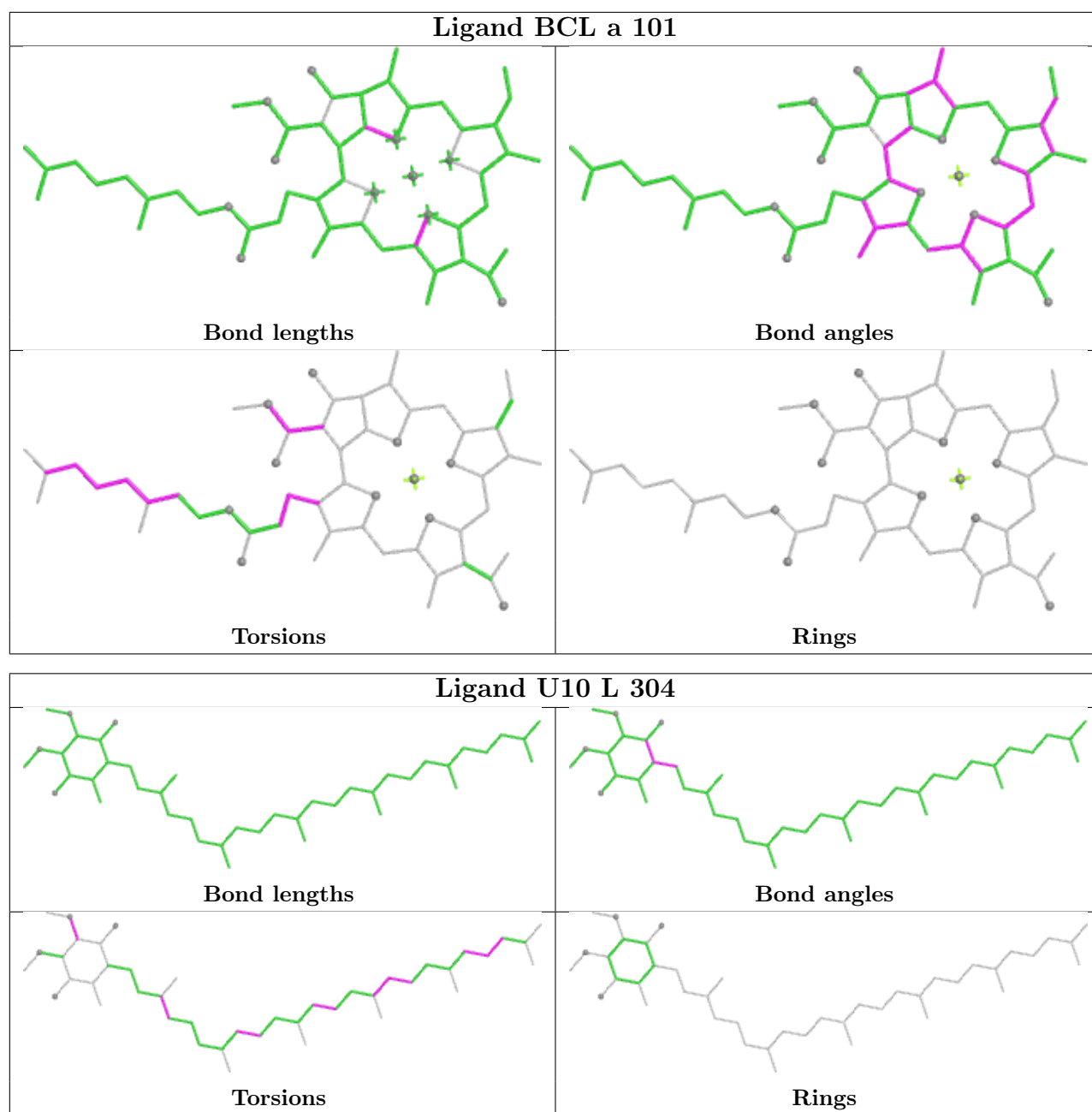


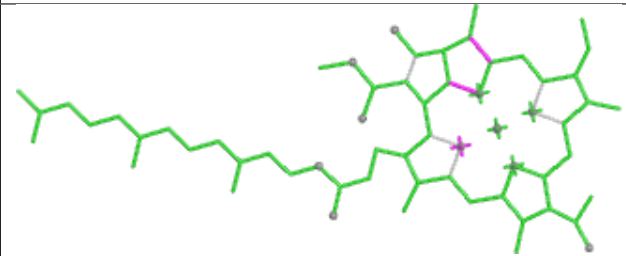
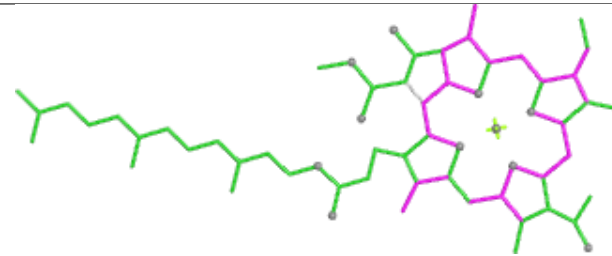
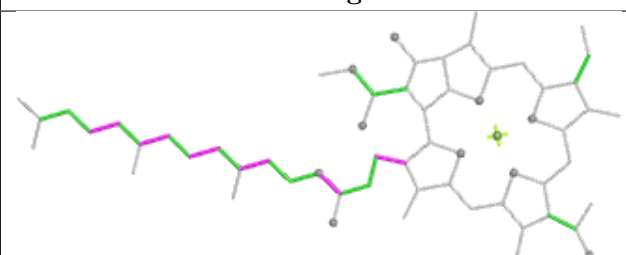
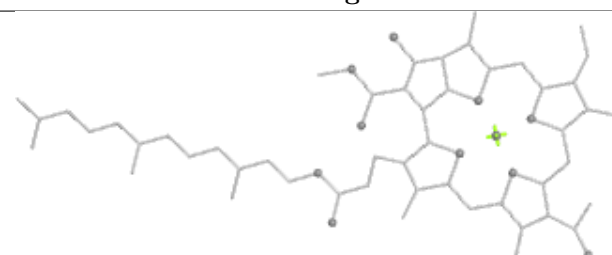


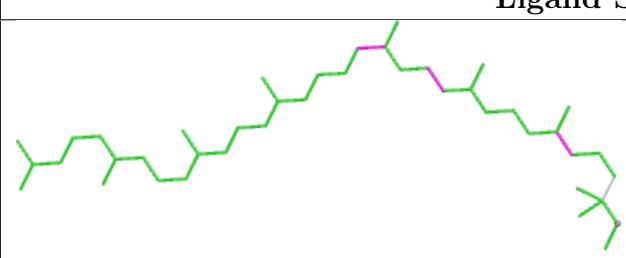
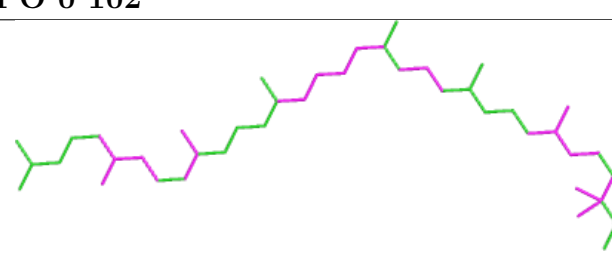
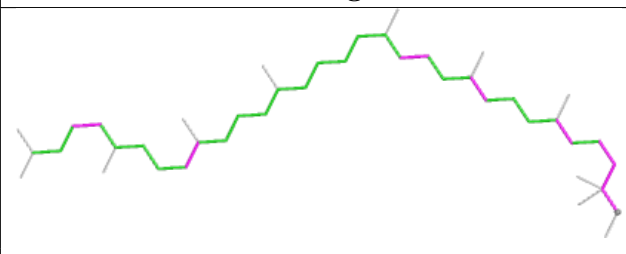
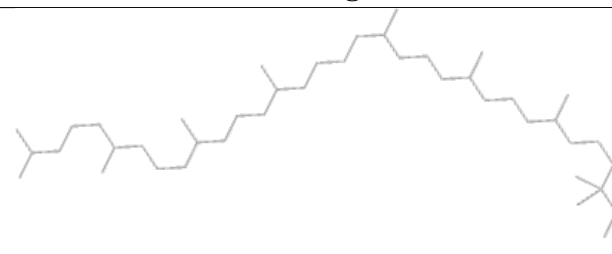


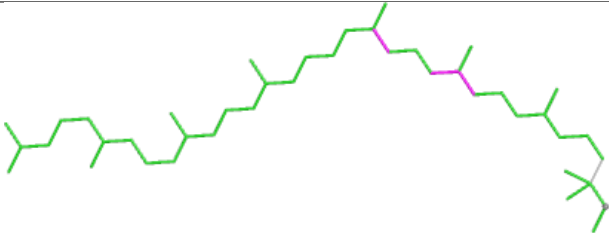
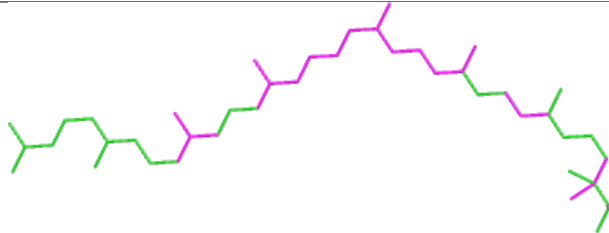
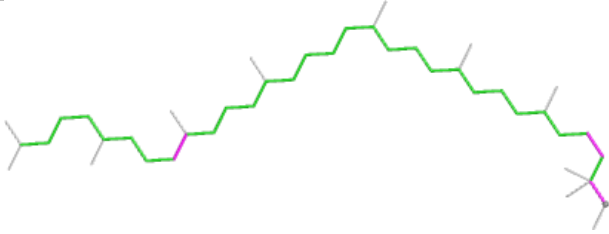
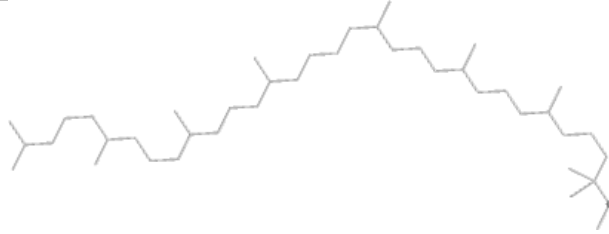


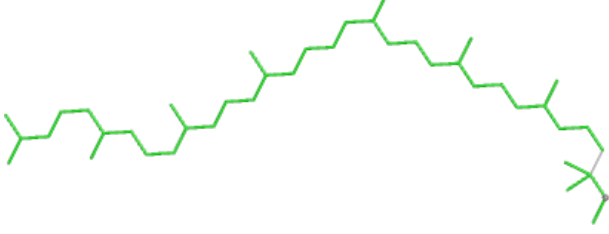
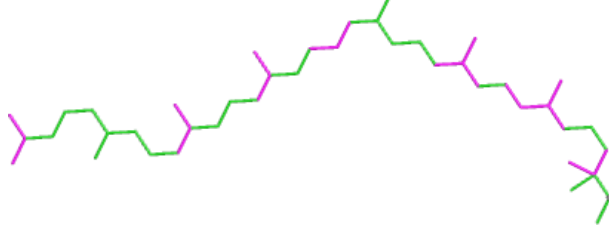
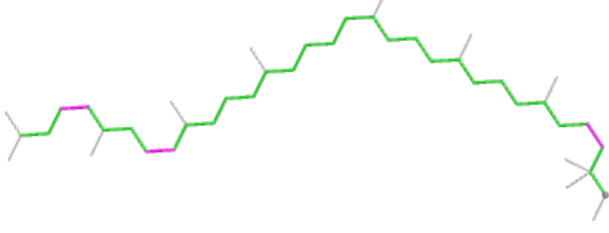
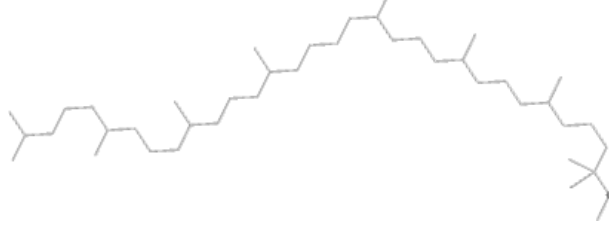


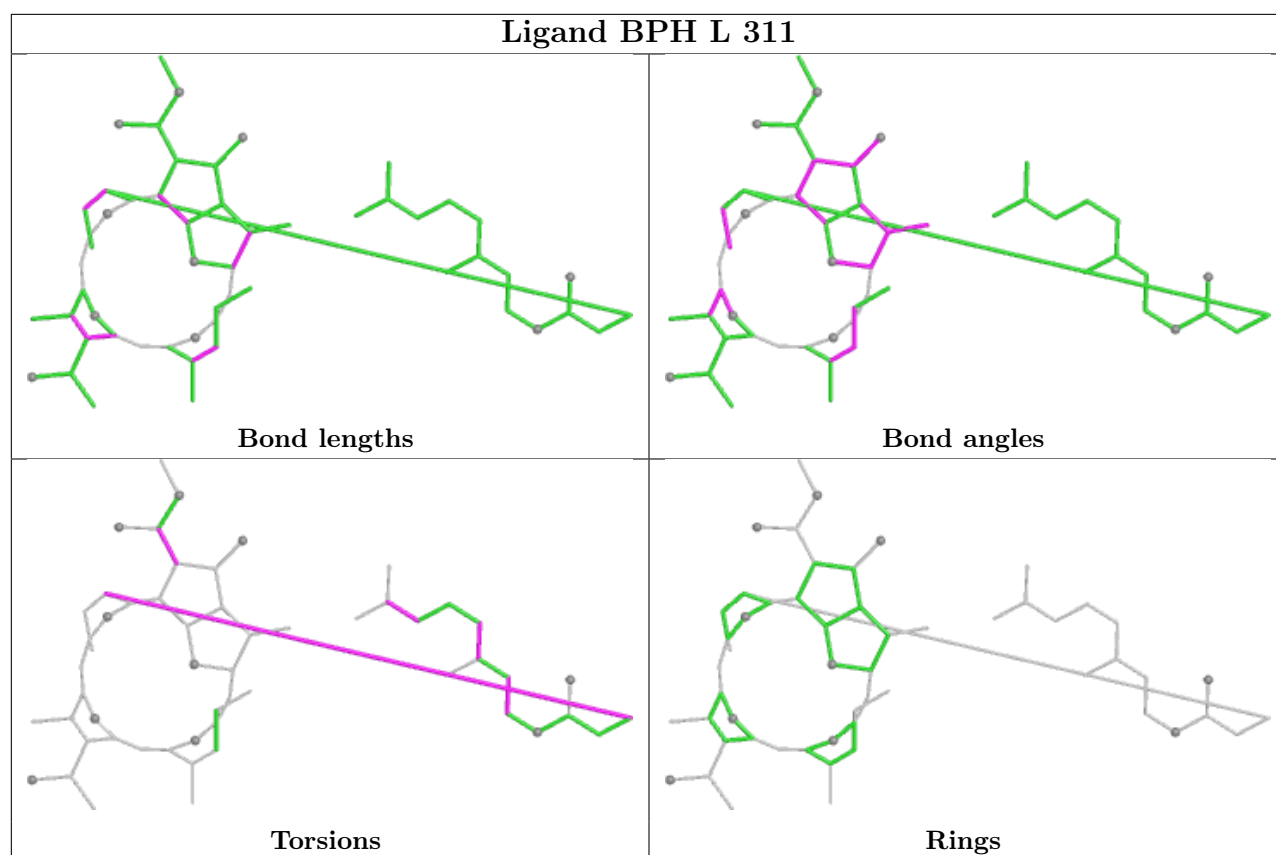


Ligand BCL 7 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand SPO 0 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand SPO I 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand SPO T 102	
	
Bond lengths	Bond angles
	
Torsions	Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

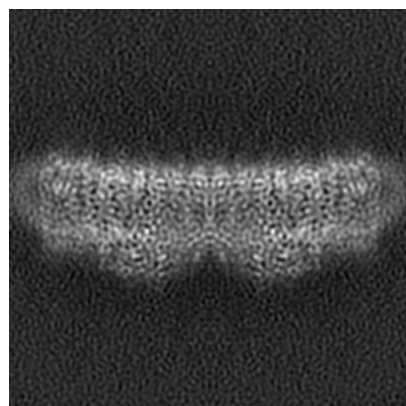
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39244. These allow visual inspection of the internal detail of the map and identification of artifacts.

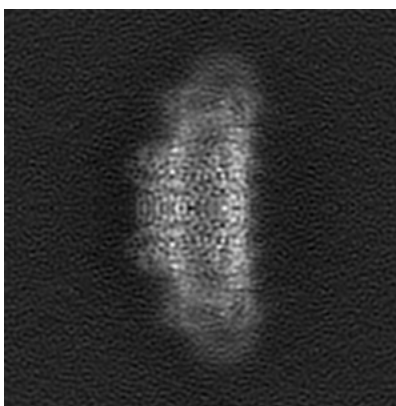
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

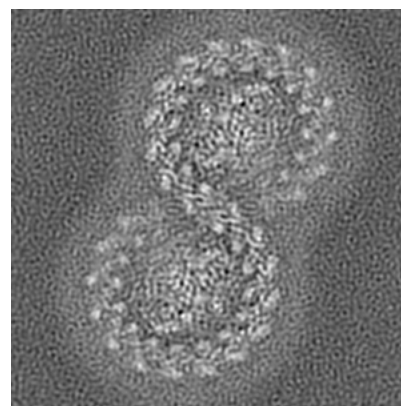
6.1.1 Primary map



X

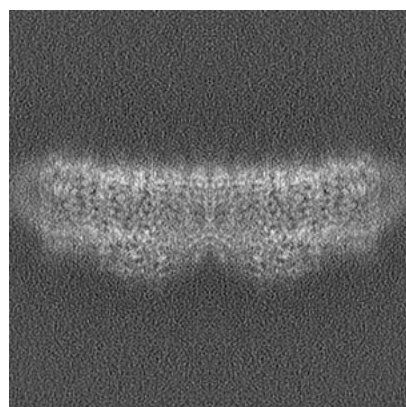


Y

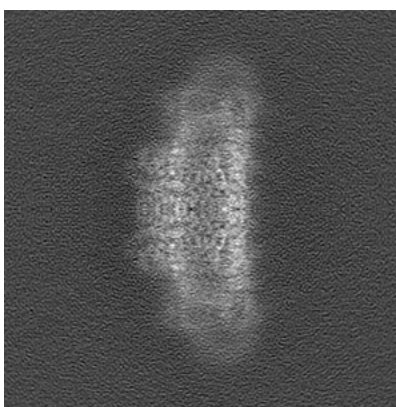


Z

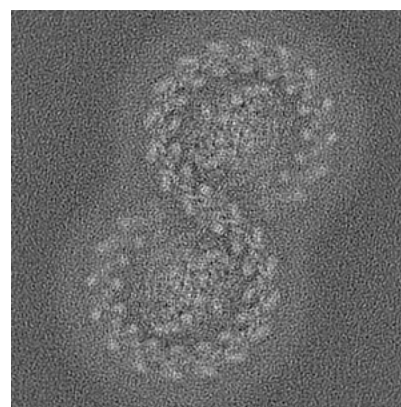
6.1.2 Raw map



X



Y

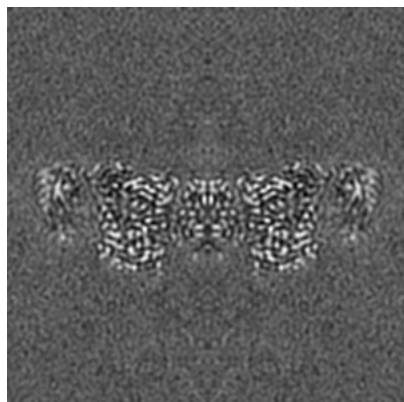


Z

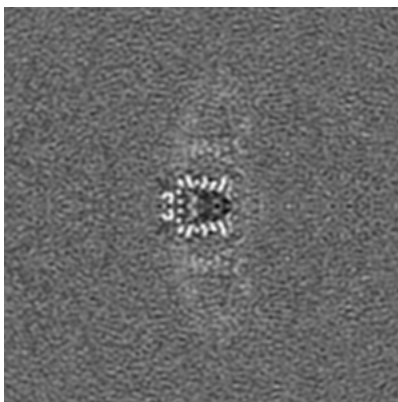
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

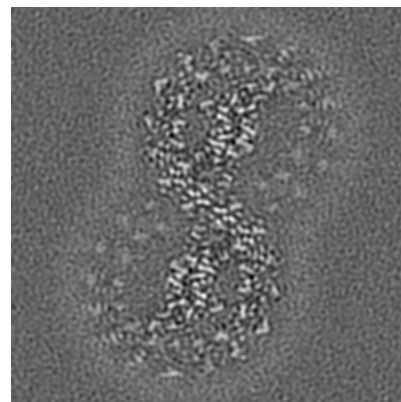
6.2.1 Primary map



X Index: 128

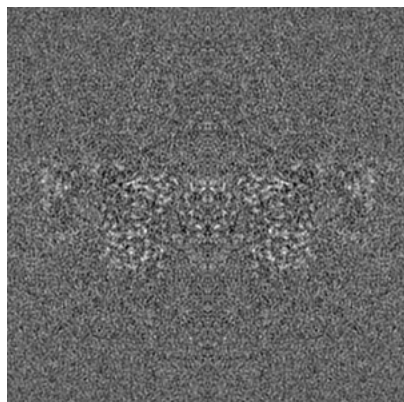


Y Index: 128

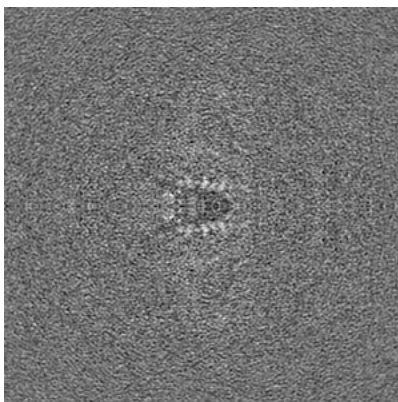


Z Index: 128

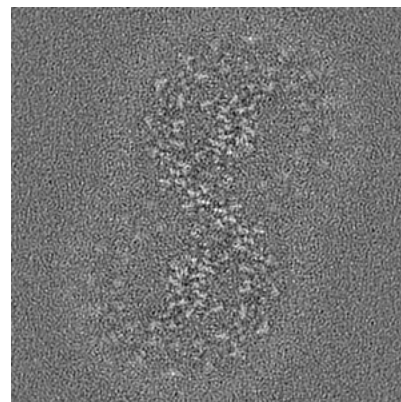
6.2.2 Raw map



X Index: 128



Y Index: 128

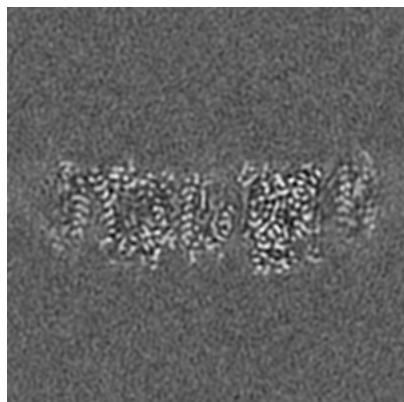


Z Index: 128

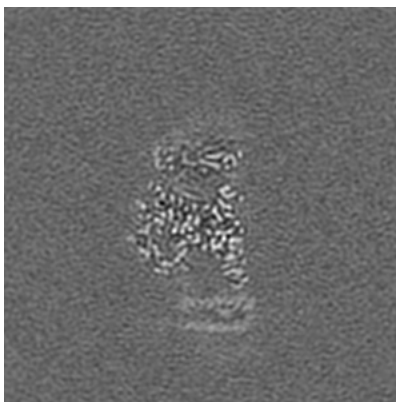
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

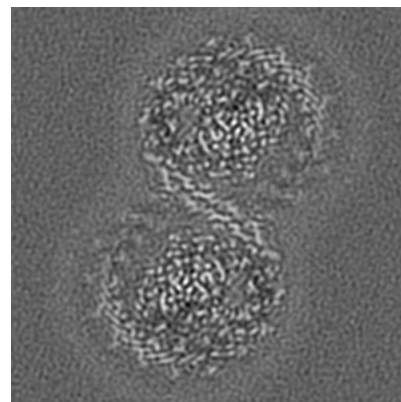
6.3.1 Primary map



X Index: 134

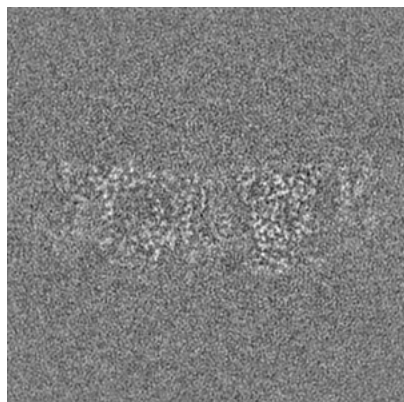


Y Index: 81

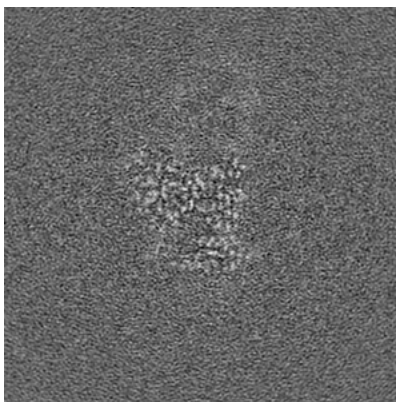


Z Index: 144

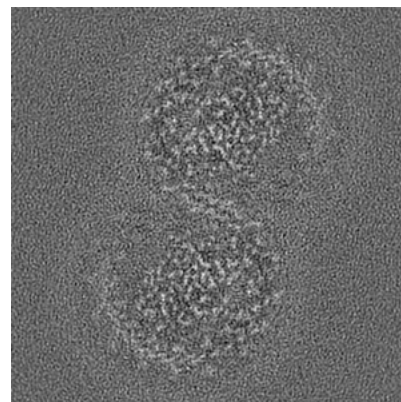
6.3.2 Raw map



X Index: 134



Y Index: 165

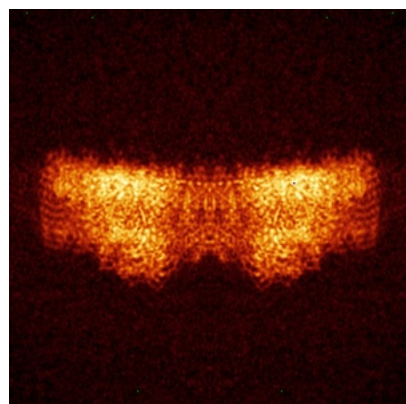


Z Index: 143

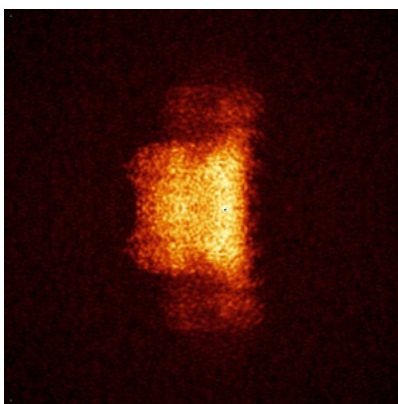
The images above show the largest variance slices of the map in three orthogonal directions.

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

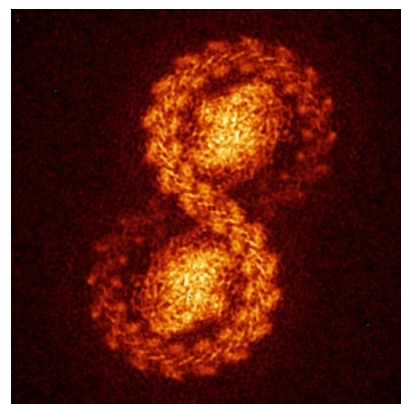
6.4.1 Primary map



X

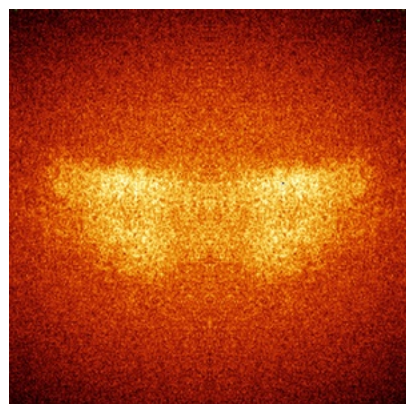


Y

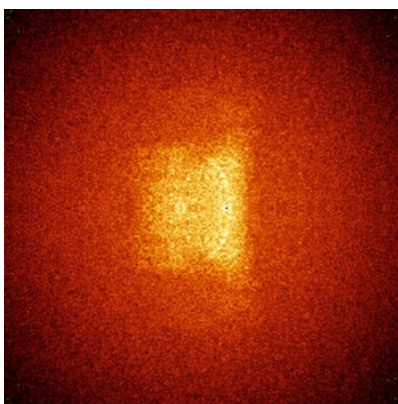


Z

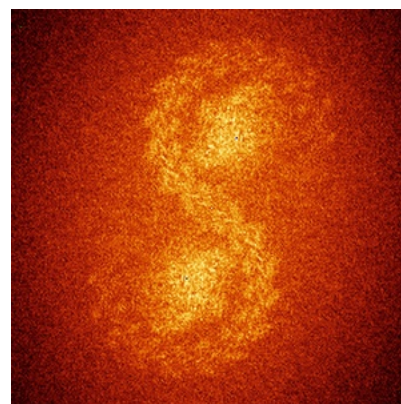
6.4.2 Raw map



X



Y

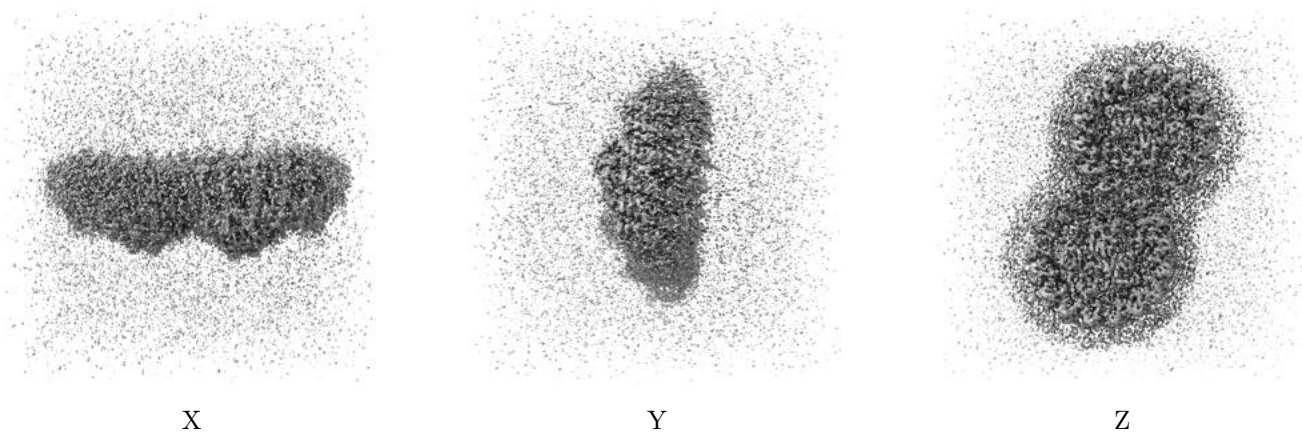


Z

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

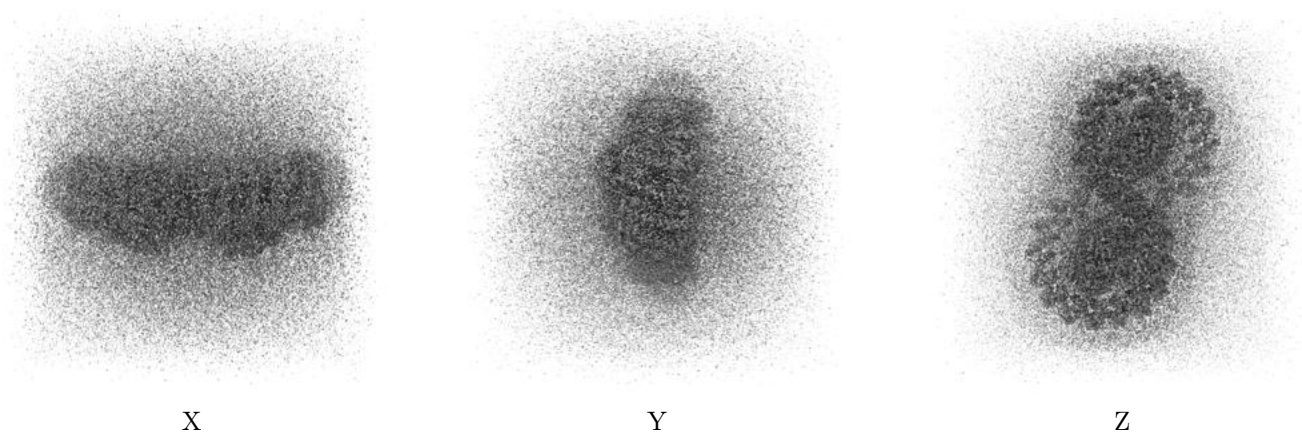
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.16. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

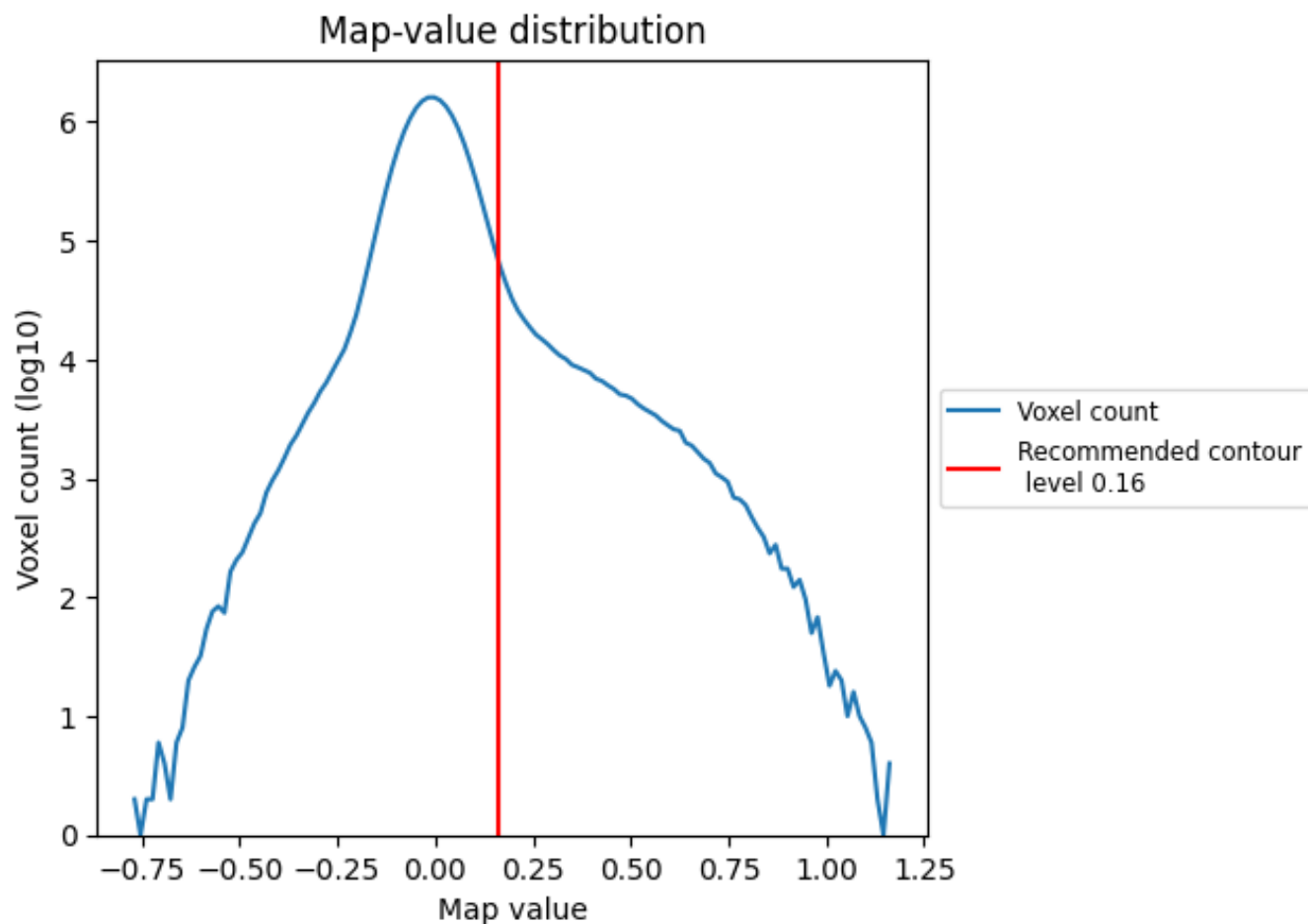
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

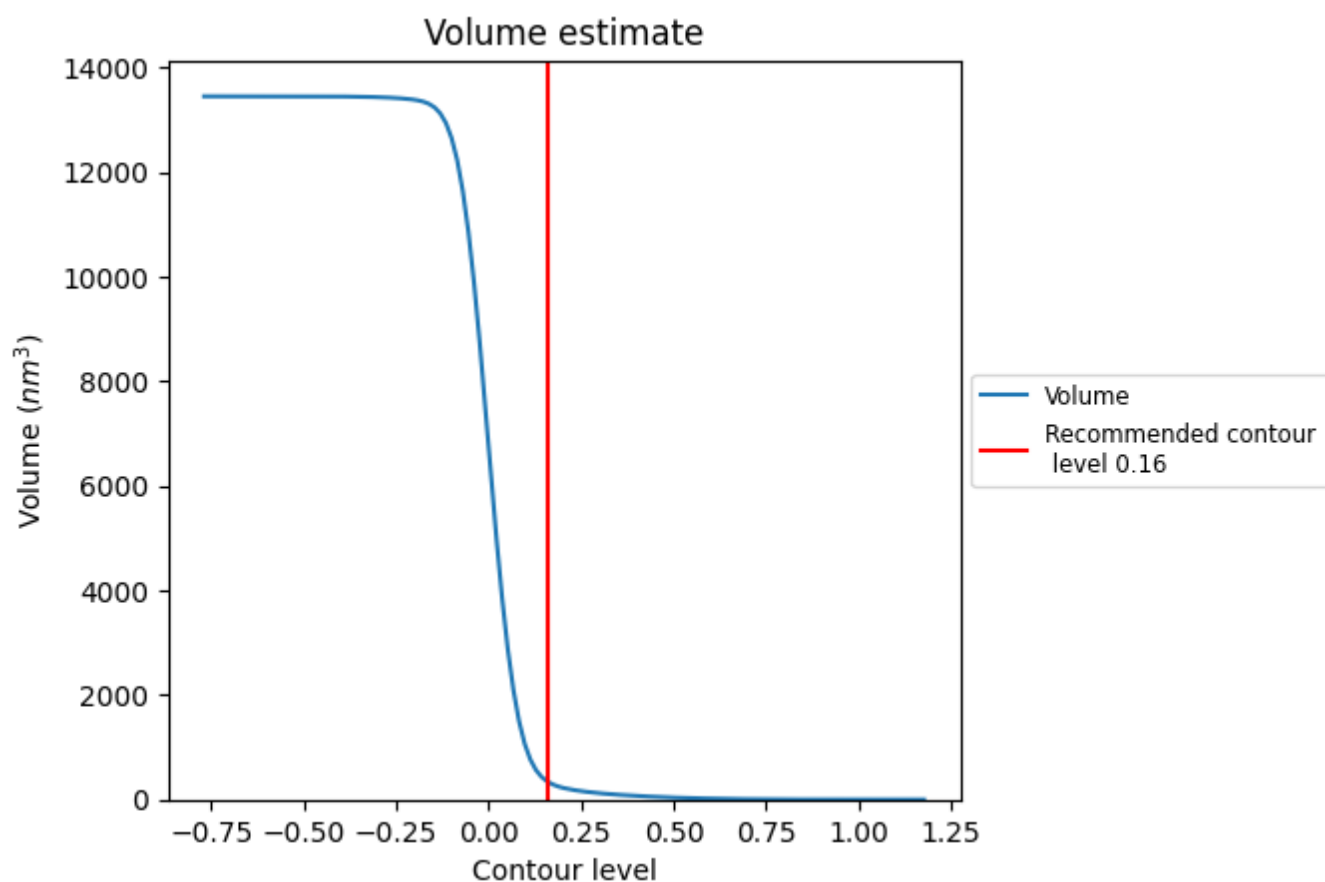
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

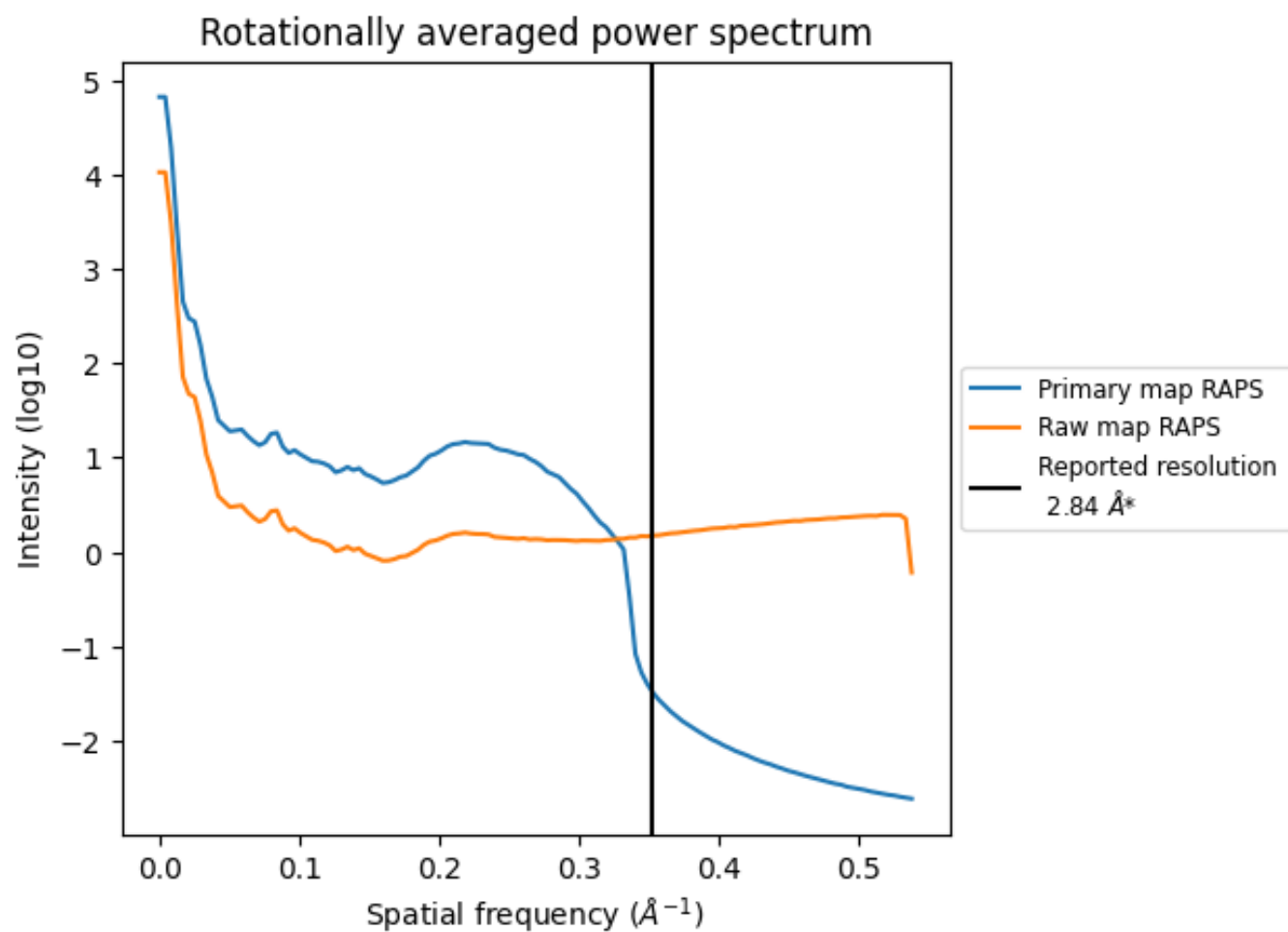
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 342 nm³; this corresponds to an approximate mass of 309 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 ⓘ

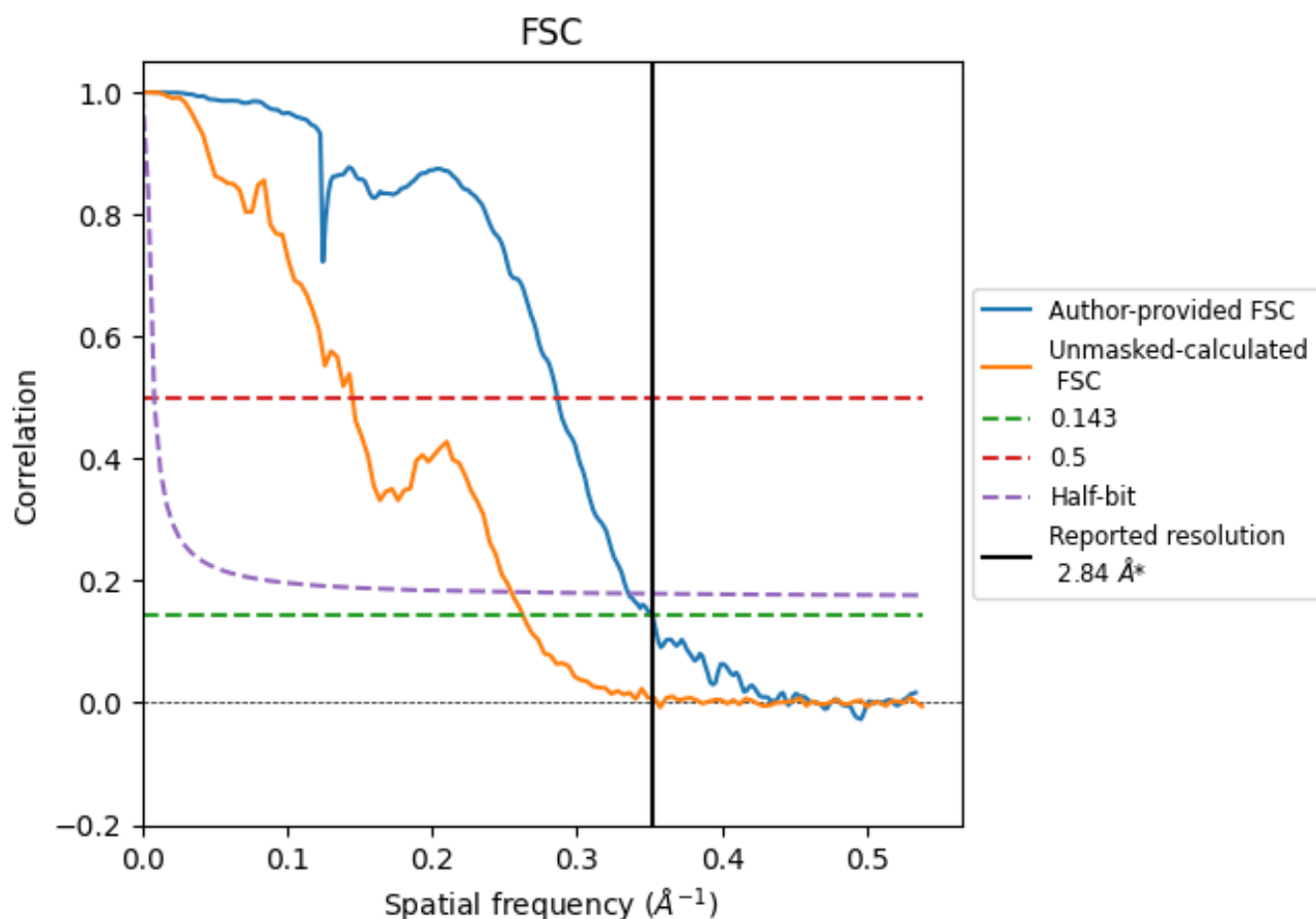


*Reported resolution corresponds to spatial frequency of 0.352 Å⁻¹

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 $0.352 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.84	-	-
Author-provided FSC curve	2.84	3.49	2.97
Unmasked-calculated*	3.81	6.89	3.93

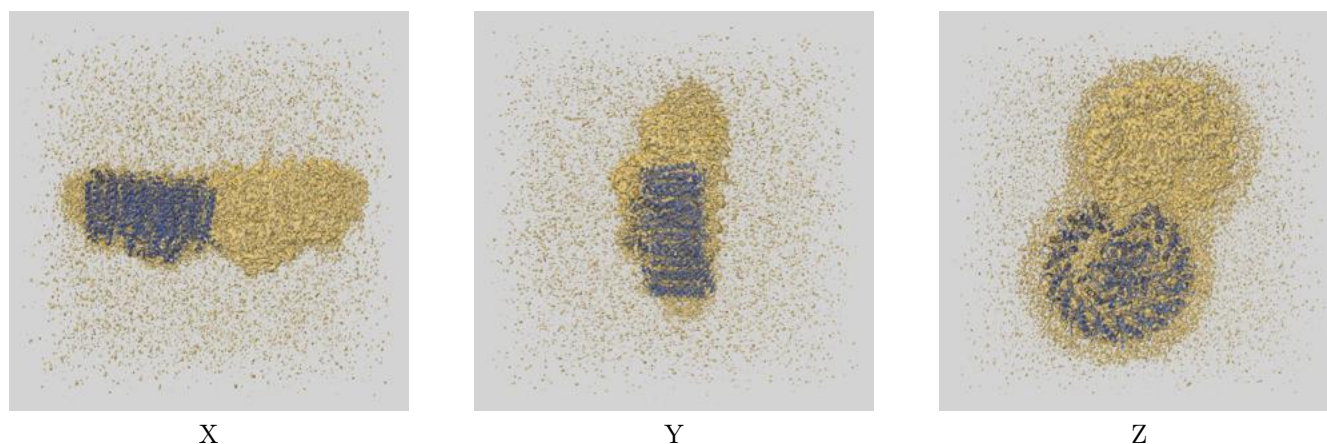
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.81 differs from the reported value 2.84 by more than 10 %

9 Map-model fit [i](#)

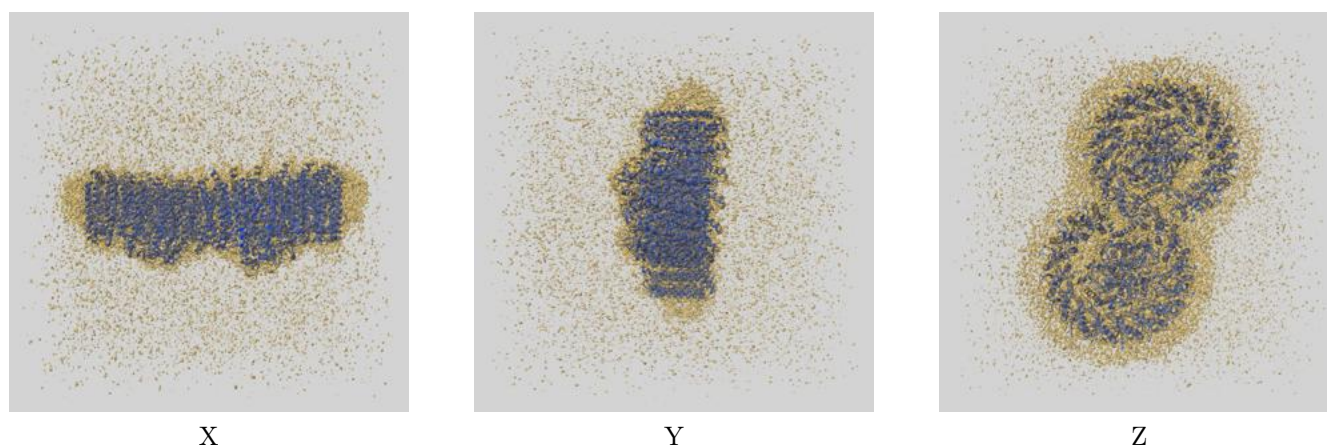
This section contains information regarding the fit between EMDB map EMD-39244 and PDB model 8YGD. Per-residue inclusion information can be found in section [3](#) on page [15](#).

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

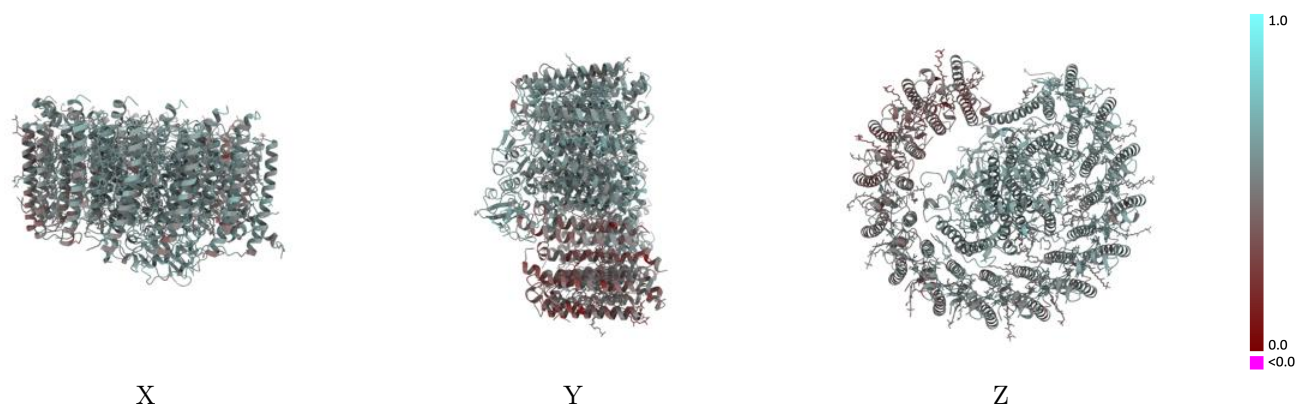


9.1.2 Map-model assembly overlay [i](#)



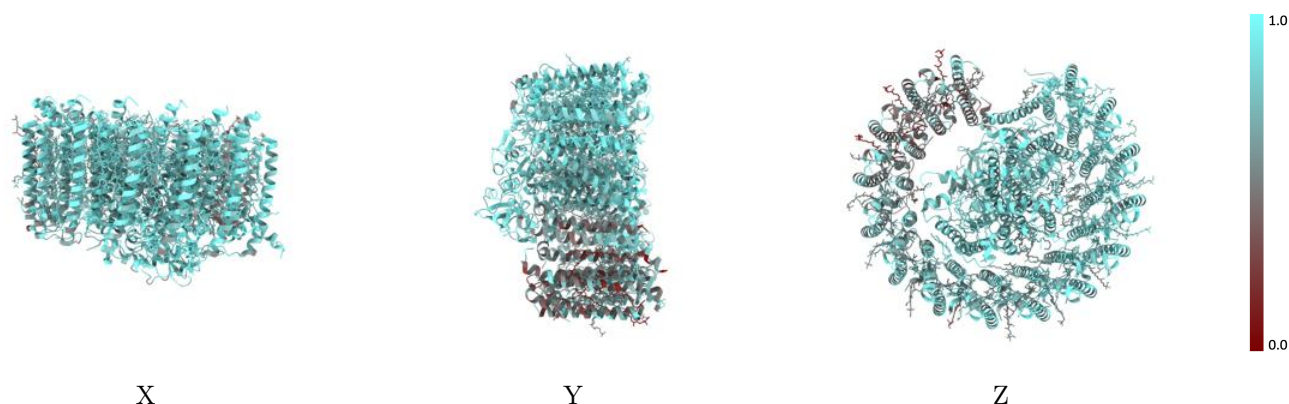
The images above show the 3D surface view of the map at the recommended contour level 0.16 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



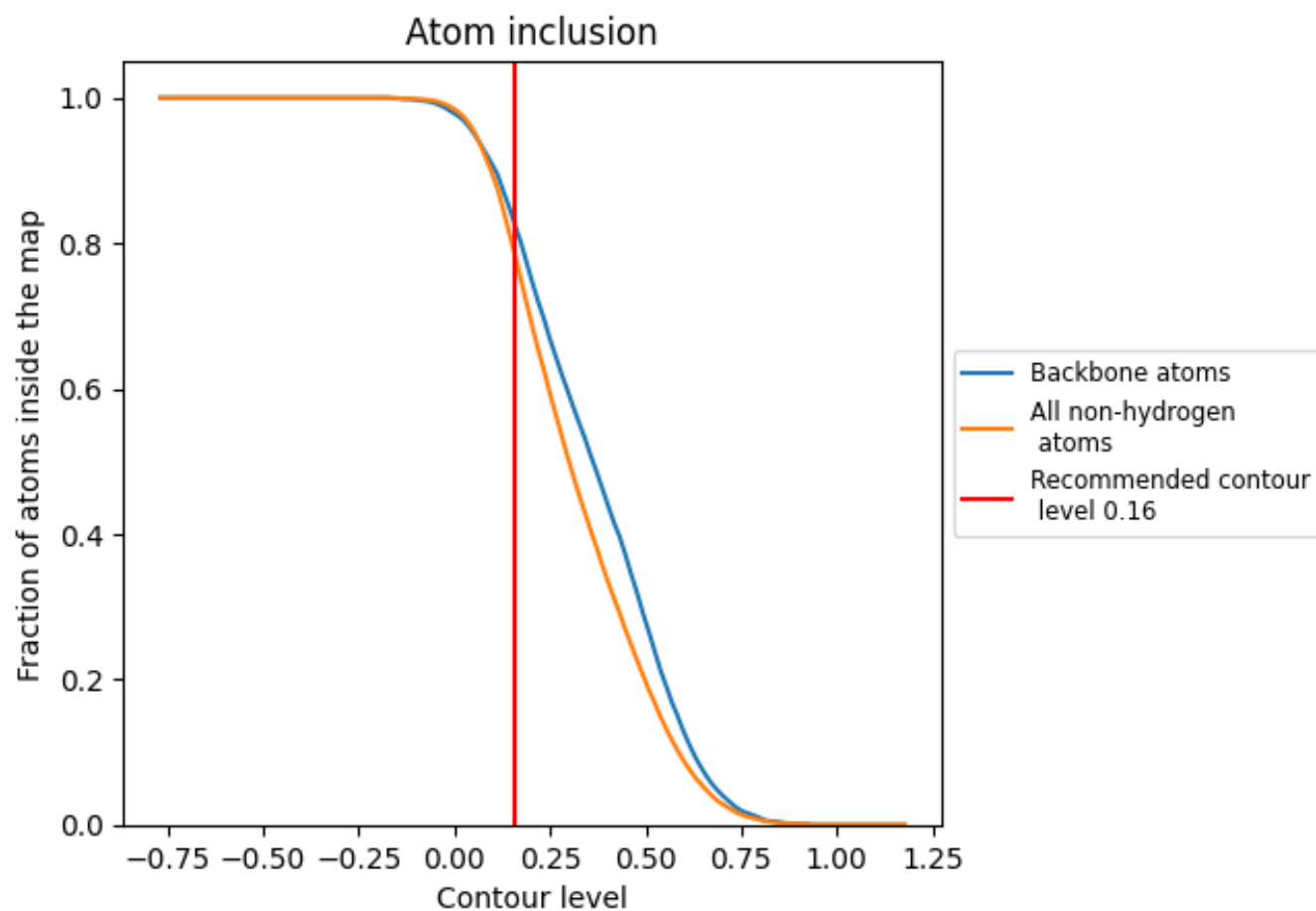
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.16).

9.4 Atom inclusion ⓘ



At the recommended contour level, 82% of all backbone atoms, 78% 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 (0.16) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7800	 0.5170
0	 0.8460	 0.5400
1	 0.5350	 0.3930
2	 0.4540	 0.3430
3	 0.5160	 0.4100
7	 0.9210	 0.5730
8	 0.8390	 0.5570
9	 0.8780	 0.5730
A	 0.8660	 0.5660
B	 0.8350	 0.5370
C	 0.5550	 0.3730
D	 0.9040	 0.5680
E	 0.8150	 0.5290
F	 0.8280	 0.5400
G	 0.8440	 0.5220
H	 0.8740	 0.5680
I	 0.8130	 0.5190
J	 0.8060	 0.5160
K	 0.7980	 0.5050
L	 0.8700	 0.5770
M	 0.8580	 0.5640
N	 0.7330	 0.4690
O	 0.7700	 0.5130
P	 0.7480	 0.4960
Q	 0.8080	 0.5140
R	 0.7010	 0.4760
S	 0.7440	 0.4890
T	 0.7060	 0.4610
U	 0.6980	 0.4760
V	 0.6810	 0.4420
W	 0.6350	 0.4590
X	 0.7870	 0.5370
Z	 0.4910	 0.3700
a	 0.5070	 0.3920
b	 0.6090	 0.4210

