



wwPDB EM Validation Summary Report ⓘ

Mar 12, 2026 – 04:32 PM UTC

PDB ID : 7UEB / pdb_00007ueb
EMDB ID : EMD-26471
Title : Photosynthetic assembly of Chlorobaculum tepidum (RC-FMO2)
Authors : Puskar, R.; Truong, C.D.; Swain, K.; Li, S.; Cheng, K.-W.; Wang, T.Y.; Poh, Y.-P.; Liu, H.; Chou, T.-F.; Nannenga, B.; Chiu, P.-L.
Deposited on : 2022-03-21
Resolution : 3.08 Å(reported)
Based on initial model : 6M32

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

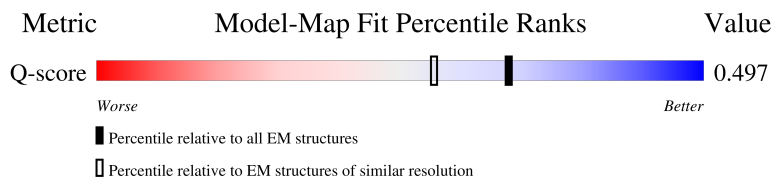
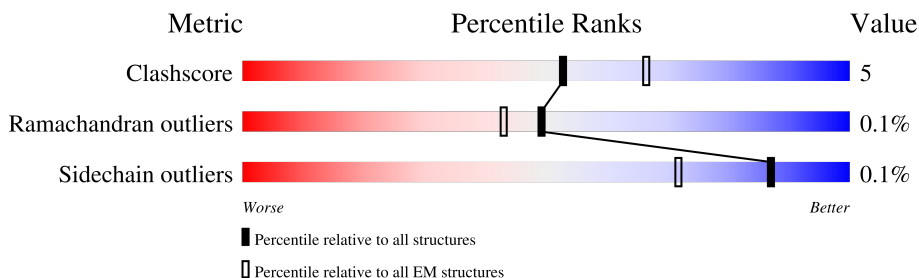
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.08 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	14000 (2.58 - 3.58)

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	A	731	
1	a	731	
2	B	231	
3	C	206	

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Mol	Chain	Length	Quality of chain
3	c	206	
4	D	143	
5	E	59	
6	F	58	
7	U	366	
7	V	366	
7	W	366	
7	X	366	
7	Y	366	
7	Z	366	

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
8	GS0	A	801	X	-	-	-
8	GS0	a	802	X	-	-	-
9	G2O	A	802	X	-	-	-
9	G2O	A	826	X	-	-	-
9	G2O	A	827	X	-	-	-
9	G2O	a	801	X	-	-	-

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 37570 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 Photosystem P840 reaction center, large subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	650	Total	C	N	O	S	0	0
			5197	3469	827	875	26		
1	a	652	Total	C	N	O	S	0	0
			5214	3478	832	878	26		

- Molecule 2 is a protein called Photosystem P840 reaction center iron-sulfur protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	114	Total	C	N	O	S	0	0
			887	564	148	166	9		

- Molecule 3 is a protein called Cytochrome c.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	122	Total	C	N	O	S	0	0
			950	637	149	157	7		
3	c	105	Total	C	N	O	S	0	0
			839	565	130	138	6		

- Molecule 4 is a protein called P840 reaction center 17 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	101	Total	C	N	O	S	0	0
			823	523	145	151	4		

- Molecule 5 is a protein called PscE.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	56	Total	C	N	O	S	0	0
			441	280	75	83	3		

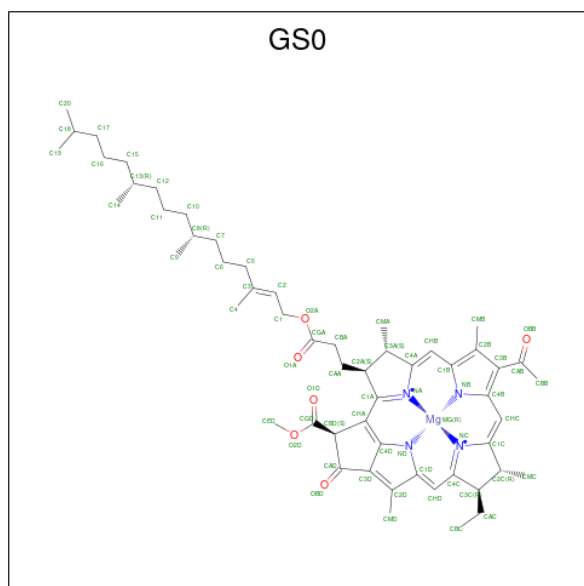
- Molecule 6 is a protein called PscF.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	50	Total	C	N	O	S	0	0
			379	253	62	61	3		

- Molecule 7 is a protein called Bacteriochlorophyll a protein.

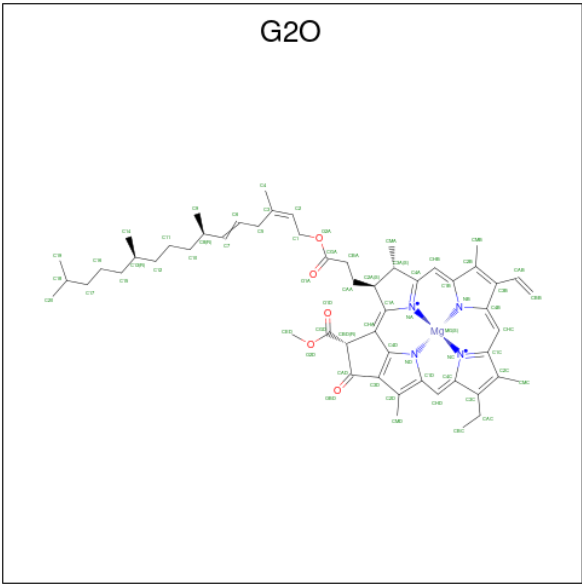
Mol	Chain	Residues	Atoms					AltConf	Trace
7	U	363	Total	C	N	O	S	0	0
			2826	1792	502	525	7		
7	V	360	Total	C	N	O	S	0	0
			2805	1778	499	521	7		
7	W	358	Total	C	N	O	S	0	0
			2789	1770	496	516	7		
7	X	357	Total	C	N	O	S	0	0
			2782	1765	495	515	7		
7	Y	360	Total	C	N	O	S	0	0
			2805	1778	499	521	7		
7	Z	358	Total	C	N	O	S	0	0
			2789	1770	496	516	7		

- Molecule 8 is Bacteriochlorophyll A isomer (CCD ID: GS0) (formula: $C_{55}H_{74}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



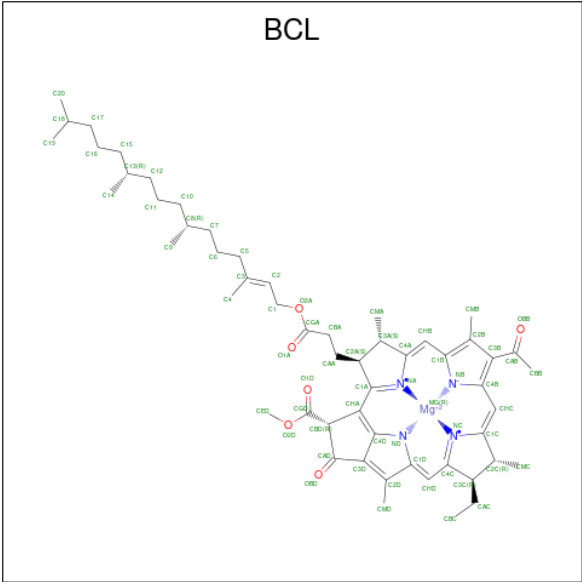
Mol	Chain	Residues	Atoms					AltConf
8	A	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	a	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 9 is Chlorophyll A ester (CCD ID: G2O) (formula: $C_{55}H_{70}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
9	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 10 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: $C_{55}H_{74}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
10	A	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	A	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	A	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	A	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	A	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	A	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	A	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	A	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	A	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	A	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	A	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	A	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	A	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	A	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	A	1	Total 65	C 54	Mg 1	N 4	O 6	0
10	a	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	a	1	Total 66	C 55	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
10	a	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	a	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	a	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	a	1	Total 46	C 35	Mg 1	N 4	O 6	0
10	a	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	a	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	a	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	a	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	a	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	a	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	a	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	B	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	U	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	U	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	U	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	U	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	U	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	U	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	U	1	Total 46	C 35	Mg 1	N 4	O 6	1
10	V	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	V	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	V	1	Total 66	C 55	Mg 1	N 4	O 6	0

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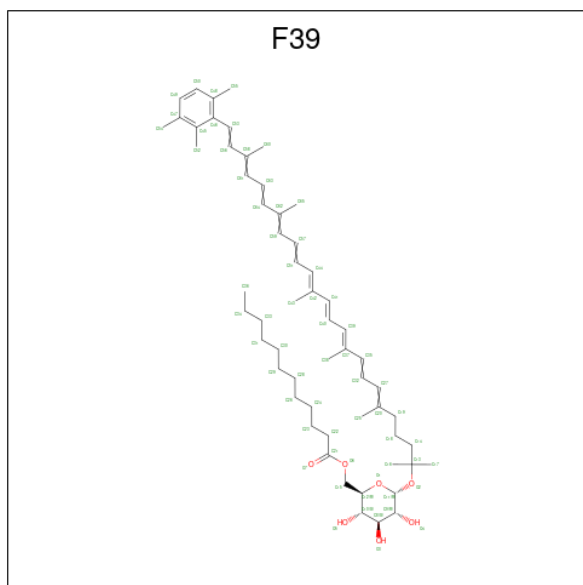
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10	V	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	V	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	V	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	V	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	V	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	V	1	Total 46	C 35	Mg 1	N 4	O 6	1
10	W	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	W	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	W	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	W	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	W	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	W	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	W	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	W	1	Total 46	C 35	Mg 1	N 4	O 6	1
10	X	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	X	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	X	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	X	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	X	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	X	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	X	1	Total 46	C 35	Mg 1	N 4	O 6	1

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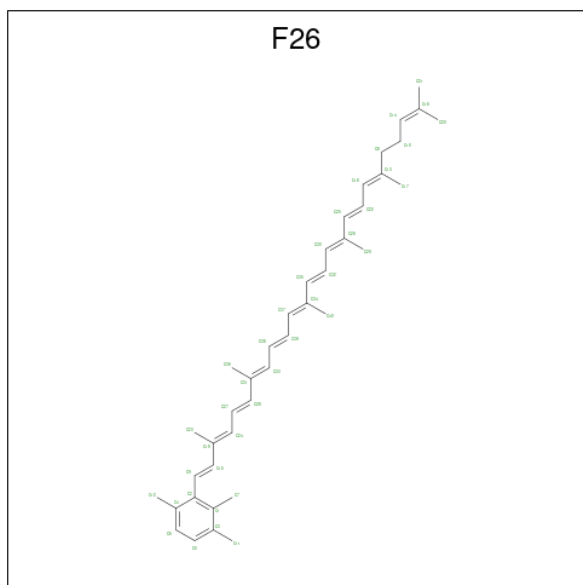
Mol	Chain	Residues	Atoms					AltConf
10	X	1	Total	C	Mg	N	O	1
			46	35	1	4	6	
10	X	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
10	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
10	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
10	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
10	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
10	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
10	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
10	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
10	Z	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
10	Z	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
10	Z	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
10	Z	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
10	Z	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
10	Z	1	Total	C	Mg	N	O	1
			46	35	1	4	6	

- Molecule 11 is [(2R,3S,4S,5R,6R)-6-[(10E,12E,14E)-2,6,10,14,19,23-hexamethyl-25-(2,3,6-trimethylphenyl)pentacos-6,8,10,12,14,16,18,20,22,24-decaen-2-yl]oxy-3,4,5-tris(oxidanyl)oxan-2-yl]methyl dodecanoate (CCD ID: F39) (formula: C₅₈H₈₆O₇) (labeled as "Ligand of Interest" by depositor).



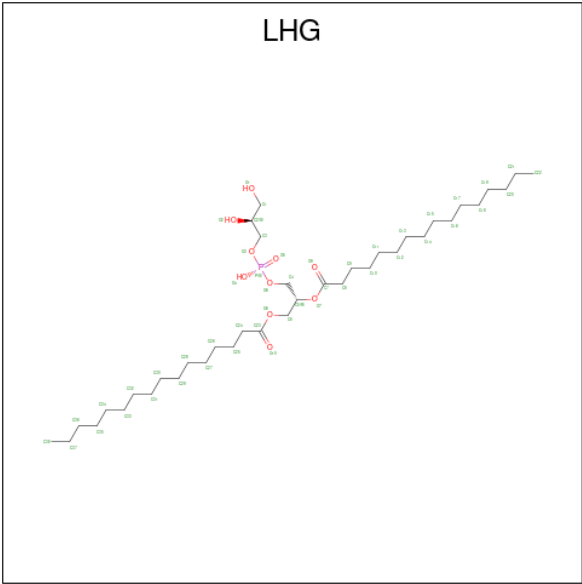
Mol	Chain	Residues	Atoms			AltConf
11	A	1	Total	C	O	0
			65	58	7	
11	a	1	Total	C	O	0
			65	58	7	
11	C	1	Total	C	O	0
			65	58	7	

- Molecule 12 is 2-[(1E,3E,5E,7E,9E,11E,13E,15E,17E,19E)-3,7,12,16,20,24-hexamethylpentacos-1,3,5,7,9,11,13,15,17,19,23-undecaenyl]-1,3,4-trimethyl-benzene (CCD ID: F26) (formula: C₄₀H₅₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		AltConf
12	A	1	Total	C	0
			40	40	
12	a	1	Total	C	0
			40	40	
12	a	1	Total	C	0
			40	40	

- Molecule 13 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P) (labeled as "Ligand of Interest" by depositor).



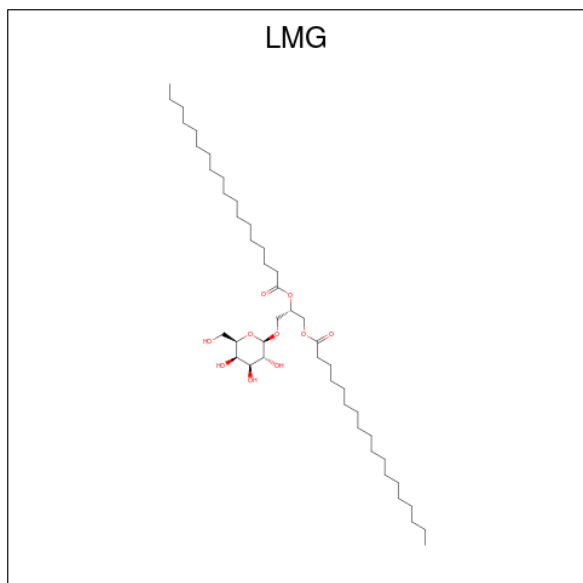
Mol	Chain	Residues	Atoms				AltConf
13	A	1	Total	C	O	P	0
			37	26	10	1	
13	A	1	Total	C	O	P	0
			40	29	10	1	
13	A	1	Total	C	O	P	0
			34	23	10	1	
13	a	1	Total	C	O	P	0
			45	34	10	1	
13	a	1	Total	C	O	P	0
			34	23	10	1	
13	a	1	Total	C	O	P	0
			38	27	10	1	
13	a	1	Total	C	O	P	0
			38	27	10	1	
13	E	1	Total	C	O	P	0
			39	28	10	1	

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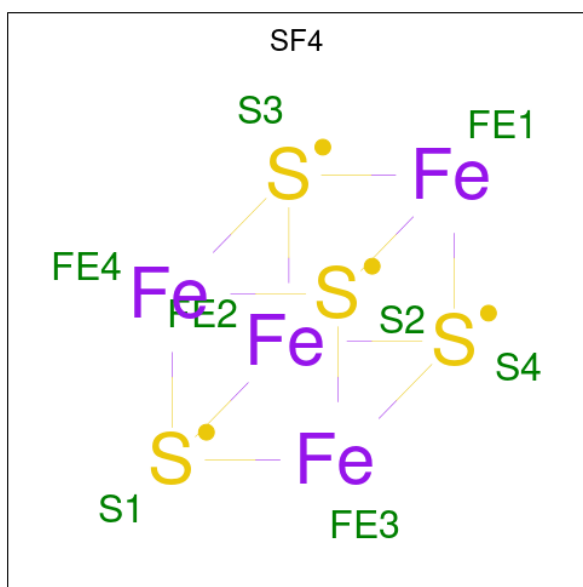
Mol	Chain	Residues	Atoms				AltConf
13	E	1	Total	C	O	P	0
			43	32	10	1	
13	Z	1	Total	C	O	P	0
			43	32	10	1	

- Molecule 14 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
14	A	1	Total	C	O		0
			42	32	10		
14	A	1	Total	C	O		0
			41	31	10		
14	A	1	Total	C	O		0
			42	32	10		
14	A	1	Total	C	O		0
			31	21	10		
14	a	1	Total	C	O		0
			45	35	10		
14	C	1	Total	C	O		0
			42	32	10		

- Molecule 15 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
15	A	1	Total	Fe	S	0
			8	4	4	
15	B	1	Total	Fe	S	0
			8	4	4	
15	B	1	Total	Fe	S	0
			8	4	4	

- Molecule 16 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

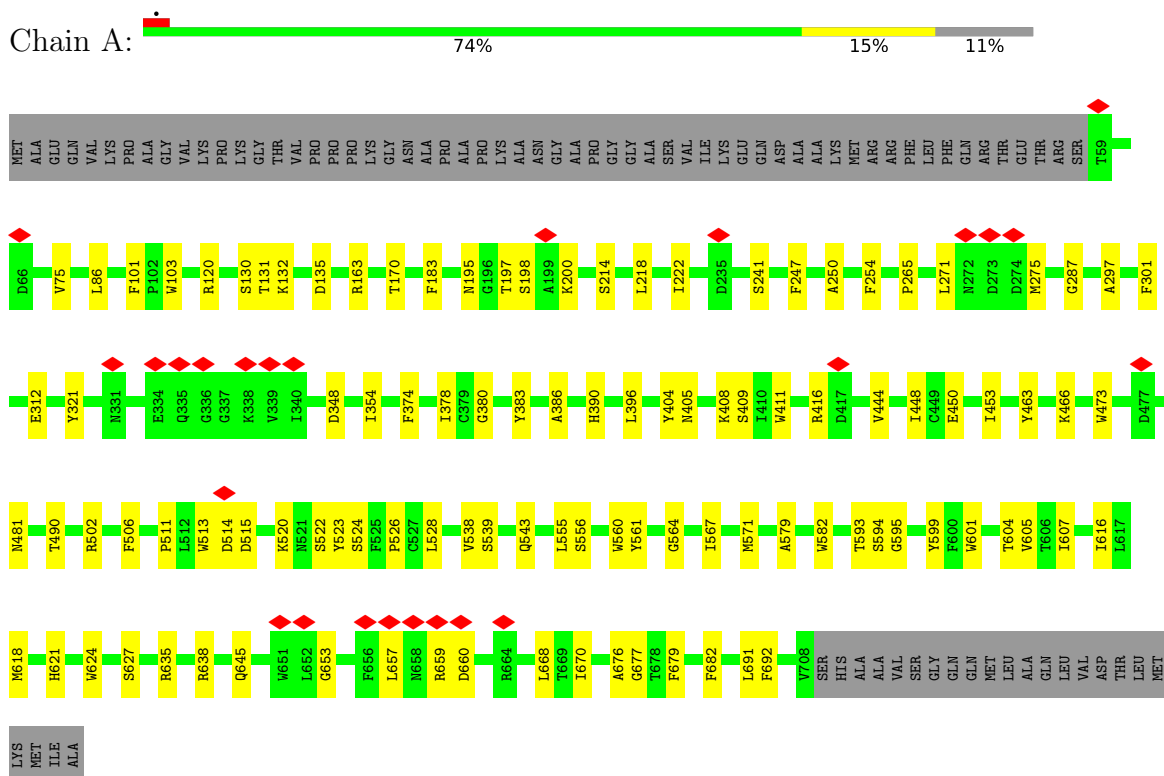
Mol	Chain	Residues	Atoms		AltConf
16	A	1	Total	Ca	0
			1	1	
16	a	1	Total	Ca	0
			1	1	

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.

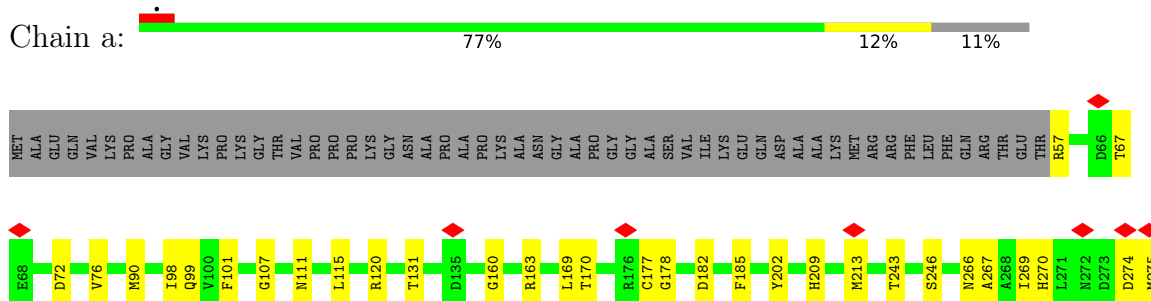
- Molecule 1: Photosystem P840 reaction center, large subunit

Chain A:

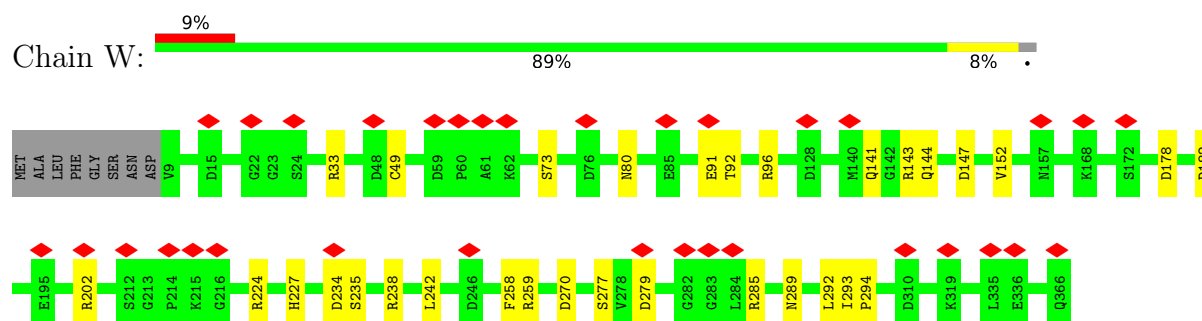


- Molecule 1: Photosystem P840 reaction center, large subunit

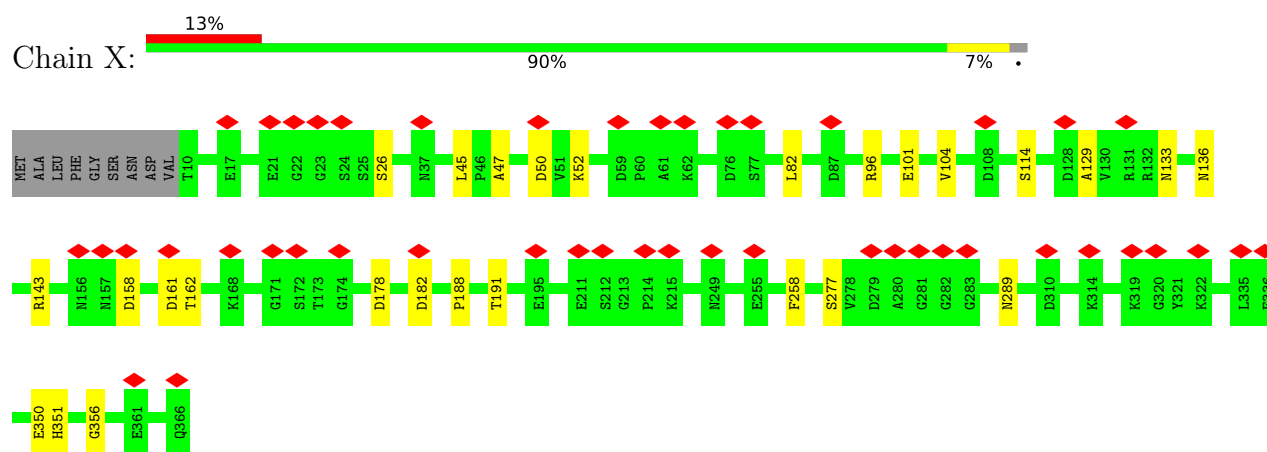
Chain a:



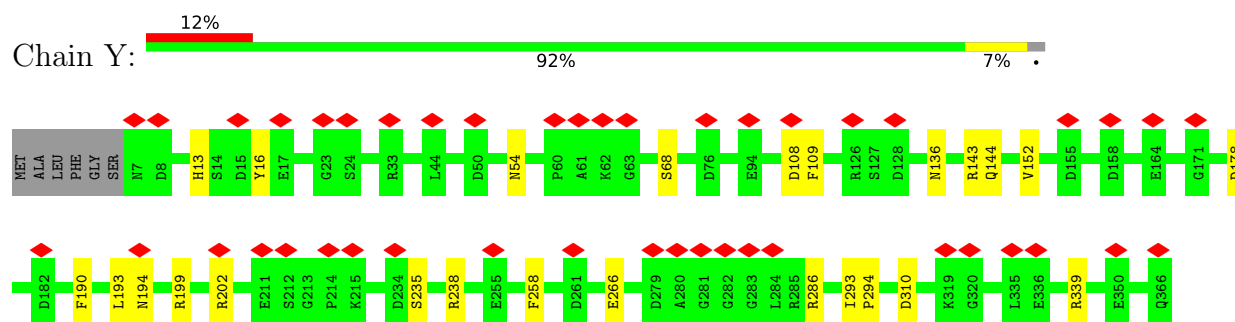
- Molecule 7: Bacteriochlorophyll a protein



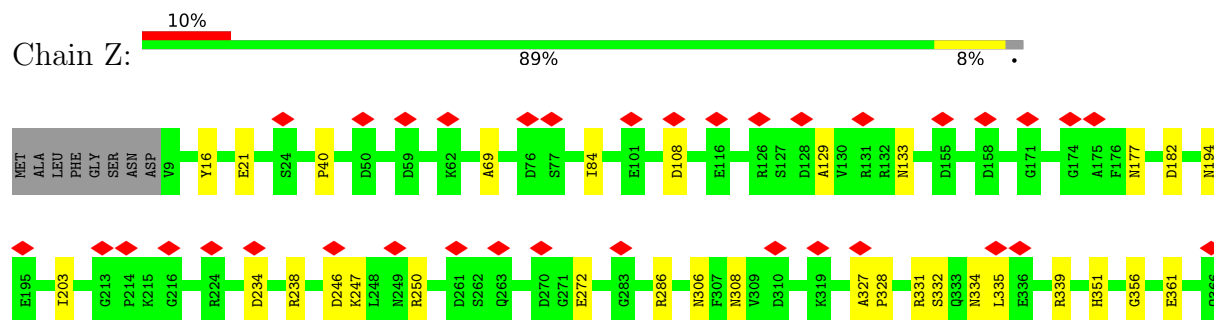
- Molecule 7: Bacteriochlorophyll a protein



- Molecule 7: Bacteriochlorophyll a protein



- Molecule 7: Bacteriochlorophyll a protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	157486	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 ($e^-/\text{\AA}^2$)	45.4	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	47259	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	4.835	Depositor
Minimum map value	-2.409	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.112	Depositor
Recommended contour level	0.428	Depositor
Map size (Å)	374.4, 374.4, 374.4	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, BCL, F39, G2O, GS0, SF4, F26, LMG, LHG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.21	0/5379	0.32	0/7330
1	a	0.19	0/5396	0.32	0/7352
2	B	0.19	0/910	0.39	1/1230 (0.1%)
3	C	0.17	0/975	0.35	0/1319
3	c	0.17	0/863	0.39	0/1167
4	D	0.14	0/839	0.34	0/1130
5	E	0.23	0/446	0.52	0/593
6	F	0.22	0/386	0.47	0/525
7	U	0.18	0/2897	0.33	0/3926
7	V	0.18	0/2875	0.31	0/3897
7	W	0.17	0/2859	0.30	0/3875
7	X	0.16	0/2852	0.28	0/3865
7	Y	0.17	0/2875	0.31	0/3897
7	Z	0.18	0/2859	0.32	0/3875
All	All	0.18	0/32411	0.33	1/43981 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	172	CYS	CA-CB-SG	5.20	126.36	114.40

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	A	5197	0	5090	81	0
1	a	5214	0	5107	75	0
2	B	887	0	833	19	0
3	C	950	0	996	15	0
3	c	839	0	870	16	0
4	D	823	0	839	12	0
5	E	441	0	476	11	0
6	F	379	0	419	21	0
7	U	2826	0	2759	24	0
7	V	2805	0	2742	15	0
7	W	2789	0	2732	22	0
7	X	2782	0	2723	20	0
7	Y	2805	0	2742	19	0
7	Z	2789	0	2732	23	0
8	A	66	0	0	3	0
8	a	66	0	0	0	0
9	A	195	0	0	1	0
9	a	65	0	0	3	0
10	A	791	0	884	30	0
10	B	66	0	74	3	0
10	U	442	0	479	7	0
10	V	574	0	627	4	0
10	W	508	0	553	13	0
10	X	554	0	588	10	0
10	Y	528	0	592	5	0
10	Z	442	0	479	10	0
10	a	772	0	849	24	0
11	A	65	0	0	0	0
11	C	65	0	0	0	0
11	a	65	0	0	0	0
12	A	40	0	0	0	0
12	a	80	0	0	0	0
13	A	111	0	135	7	0
13	E	82	0	104	6	0
13	Z	43	0	59	5	0
13	a	155	0	193	6	0
14	A	156	0	192	8	0
14	C	42	0	54	4	0
14	a	45	0	60	3	0
15	A	8	0	0	0	0
15	B	16	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	A	1	0	0	0	0
16	a	1	0	0	0	0
All	All	37570	0	36982	397	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 5.

The worst 5 of 397 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:W:73:SER:OG	7:W:80:ASN:OD1	1.98	0.82
2:B:225:ARG:NH1	7:U:15:ASP:OD1	2.14	0.81
1:A:659:ARG:NH2	1:A:660:ASP:O	2.14	0.81
7:X:50:ASP:OD2	7:X:52:LYS:NZ	2.14	0.80
3:C:99:TYR:OH	5:E:31:ARG:NH2	2.16	0.77

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	648/731 (89%)	619 (96%)	29 (4%)	0	100	100
1	a	650/731 (89%)	616 (95%)	34 (5%)	0	100	100
2	B	110/231 (48%)	99 (90%)	10 (9%)	1 (1%)	14	41
3	C	120/206 (58%)	108 (90%)	12 (10%)	0	100	100
3	c	103/206 (50%)	91 (88%)	11 (11%)	1 (1%)	12	39
4	D	99/143 (69%)	88 (89%)	11 (11%)	0	100	100
5	E	54/59 (92%)	42 (78%)	12 (22%)	0	100	100
6	F	48/58 (83%)	46 (96%)	1 (2%)	1 (2%)	5	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	U	361/366 (99%)	340 (94%)	21 (6%)	0	100	100
7	V	358/366 (98%)	345 (96%)	13 (4%)	0	100	100
7	W	356/366 (97%)	338 (95%)	18 (5%)	0	100	100
7	X	355/366 (97%)	343 (97%)	12 (3%)	0	100	100
7	Y	358/366 (98%)	344 (96%)	14 (4%)	0	100	100
7	Z	356/366 (97%)	343 (96%)	13 (4%)	0	100	100
All	All	3976/4561 (87%)	3762 (95%)	211 (5%)	3 (0%)	49	76

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	8	LYS
6	F	37	ILE
3	c	106	THR

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	538/599 (90%)	536 (100%)	2 (0%)	84	84
1	a	540/599 (90%)	540 (100%)	0	100	100
2	B	96/162 (59%)	96 (100%)	0	100	100
3	C	103/173 (60%)	103 (100%)	0	100	100
3	c	92/173 (53%)	92 (100%)	0	100	100
4	D	90/128 (70%)	90 (100%)	0	100	100
5	E	49/52 (94%)	48 (98%)	1 (2%)	48	69
6	F	40/45 (89%)	40 (100%)	0	100	100
7	U	300/302 (99%)	300 (100%)	0	100	100
7	V	298/302 (99%)	298 (100%)	0	100	100
7	W	296/302 (98%)	296 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	X	295/302 (98%)	295 (100%)	0	100	100
7	Y	298/302 (99%)	298 (100%)	0	100	100
7	Z	296/302 (98%)	296 (100%)	0	100	100
All	All	3331/3743 (89%)	3328 (100%)	3 (0%)	87	89

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	103	TRP
1	A	214	SER
5	E	6	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	a	699	GLN
7	Z	198	GLN
7	W	133	ASN
7	Z	209	ASN
7	Z	141	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 106 ligands modelled in this entry, 2 are monoatomic - leaving 104 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$
10	BCL	a	809	-	69,74,74	1.16	6 (8%)	79,115,115	1.34	7 (8%)
10	BCL	A	803	-	69,74,74	1.13	5 (7%)	79,115,115	1.51	14 (17%)
11	F39	a	815	-	66,66,66	2.80	19 (28%)	83,85,85	2.20	21 (25%)
10	BCL	X	406	-	69,74,74	1.07	5 (7%)	79,115,115	1.44	12 (15%)
9	G2O	a	801	-	68,73,73	4.25	41 (60%)	81,113,113	2.82	18 (22%)
10	BCL	a	805	-	69,74,74	1.11	6 (8%)	79,115,115	1.38	11 (13%)
10	BCL	W	405	-	69,74,74	1.11	5 (7%)	79,115,115	1.33	8 (10%)
9	G2O	A	802	-	68,73,73	4.12	39 (57%)	81,113,113	2.85	18 (22%)
10	BCL	V	402	-	69,74,74	1.10	6 (8%)	79,115,115	1.54	14 (17%)
10	BCL	Z	406	-	69,74,74	1.08	4 (5%)	79,115,115	1.43	9 (11%)
10	BCL	X	405	-	69,74,74	1.10	5 (7%)	79,115,115	1.45	9 (11%)
14	LMG	A	821	-	41,41,55	0.82	0	49,49,63	1.16	4 (8%)
10	BCL	Z	402	-	69,74,74	1.09	4 (5%)	79,115,115	1.63	15 (18%)
10	BCL	W	407	-	69,74,74	1.07	4 (5%)	79,115,115	1.37	11 (13%)
10	BCL	Y	407	-	69,74,74	1.10	5 (7%)	79,115,115	1.46	10 (12%)
10	BCL	a	806	10	69,74,74	1.09	4 (5%)	79,115,115	1.57	12 (15%)
10	BCL	U	402	-	69,74,74	1.07	4 (5%)	79,115,115	1.39	10 (12%)
13	LHG	a	820	-	37,37,48	0.65	0	40,43,54	0.97	2 (5%)
10	BCL	Z	405	7	69,74,74	1.06	4 (5%)	79,115,115	1.40	10 (12%)
8	GS0	a	802	8	69,74,74	2.38	15 (21%)	79,115,115	2.83	28 (35%)
10	BCL	V	404	-	69,74,74	1.10	4 (5%)	79,115,115	1.45	9 (11%)
10	BCL	W	406	-	69,74,74	1.10	4 (5%)	79,115,115	1.37	7 (8%)
10	BCL	A	814	-	68,73,74	1.12	4 (5%)	77,113,115	1.39	13 (16%)
10	BCL	a	807	10	69,74,74	1.07	5 (7%)	79,115,115	1.47	10 (12%)
10	BCL	V	408	-	69,74,74	1.08	4 (5%)	79,115,115	1.36	10 (12%)
10	BCL	W	402	-	69,74,74	1.08	4 (5%)	79,115,115	1.38	9 (11%)
10	BCL	B	301	14	69,74,74	1.14	6 (8%)	79,115,115	1.52	14 (17%)
10	BCL	a	813	-	69,74,74	1.12	4 (5%)	79,115,115	1.38	11 (13%)
15	SF4	A	824	1	0,12,12	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	BCL	a	812	-	69,74,74	1.14	5 (7%)	79,115,115	1.42	12 (15%)
10	BCL	Y	402	-	69,74,74	1.08	4 (5%)	79,115,115	1.48	10 (12%)
10	BCL	A	804	-	69,74,74	1.14	4 (5%)	79,115,115	1.43	12 (15%)
14	LMG	A	820	-	42,42,55	0.84	1 (2%)	50,50,63	1.17	4 (8%)
10	BCL	X	402	-	69,74,74	1.10	5 (7%)	79,115,115	1.44	11 (13%)
13	LHG	E	102	-	42,42,48	0.64	0	45,48,54	1.00	2 (4%)
10	BCL	a	804	-	69,74,74	1.12	5 (7%)	79,115,115	1.37	10 (12%)
14	LMG	A	822	-	42,42,55	0.80	1 (2%)	50,50,63	1.12	4 (8%)
10	BCL	A	813	-	69,74,74	1.13	6 (8%)	79,115,115	1.38	10 (12%)
10	BCL	A	809	-	69,74,74	1.10	6 (8%)	79,115,115	1.45	11 (13%)
11	F39	C	301	-	66,66,66	2.87	20 (30%)	83,85,85	2.12	24 (28%)
9	G2O	A	826	-	68,73,73	4.31	40 (58%)	81,113,113	2.93	19 (23%)
14	LMG	C	302	-	42,42,55	0.80	0	50,50,63	1.16	4 (8%)
10	BCL	W	401	-	69,74,74	1.10	5 (7%)	79,115,115	1.62	14 (17%)
10	BCL	A	810	-	69,74,74	1.11	5 (7%)	79,115,115	1.57	10 (12%)
10	BCL	V	401	-	69,74,74	1.09	5 (7%)	79,115,115	1.42	10 (12%)
8	GS0	A	801	8	69,74,74	2.23	15 (21%)	79,115,115	2.96	30 (37%)
10	BCL	A	812	-	69,74,74	1.12	5 (7%)	79,115,115	1.76	14 (17%)
13	LHG	a	819	-	33,33,48	0.71	0	36,39,54	0.99	2 (5%)
10	BCL	Y	406	7	69,74,74	1.06	4 (5%)	79,115,115	1.37	11 (13%)
10	BCL	U	401	-	69,74,74	1.09	4 (5%)	79,115,115	1.55	11 (13%)
10	BCL	A	807	-	69,74,74	1.09	6 (8%)	79,115,115	1.43	9 (11%)
14	LMG	a	822	-	45,45,55	0.77	0	53,53,63	1.16	4 (7%)
10	BCL	Z	408[B]	7	49,54,74	1.25	5 (10%)	55,91,115	1.50	9 (16%)
10	BCL	a	808	1	49,54,74	1.21	4 (8%)	55,91,115	1.61	11 (20%)
10	BCL	A	808	1	69,74,74	1.12	5 (7%)	79,115,115	1.38	10 (12%)
10	BCL	Y	408	-	69,74,74	1.09	4 (5%)	79,115,115	1.38	12 (15%)
10	BCL	A	805	-	69,74,74	1.15	6 (8%)	79,115,115	1.48	12 (15%)
10	BCL	U	405	-	69,74,74	1.11	4 (5%)	79,115,115	1.33	8 (10%)
10	BCL	Z	407	-	69,74,74	1.07	6 (8%)	79,115,115	1.43	11 (13%)
12	F26	a	817	-	40,40,40	1.74	10 (25%)	49,50,50	2.27	15 (30%)
10	BCL	X	403	-	69,74,74	1.07	5 (7%)	79,115,115	1.45	13 (16%)
10	BCL	W	403	-	69,74,74	1.10	4 (5%)	79,115,115	1.44	10 (12%)
10	BCL	X	409	-	69,74,74	1.09	6 (8%)	79,115,115	1.46	11 (13%)
10	BCL	a	810	-	69,74,74	1.09	4 (5%)	79,115,115	1.51	13 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	BCL	V	405	-	69,74,74	1.06	4 (5%)	79,115,115	1.40	10 (12%)
13	LHG	E	101	-	38,38,48	0.67	0	41,44,54	0.97	2 (4%)
10	BCL	X	407[B]	7	49,54,74	1.24	4 (8%)	55,91,115	1.36	7 (12%)
10	BCL	A	806	-	69,74,74	1.15	4 (5%)	79,115,115	1.63	12 (15%)
10	BCL	Z	403	-	69,74,74	1.09	5 (7%)	79,115,115	1.40	9 (11%)
10	BCL	U	403	-	69,74,74	1.05	5 (7%)	79,115,115	1.46	15 (18%)
13	LHG	A	818	-	39,39,48	0.71	1 (2%)	42,45,54	1.02	3 (7%)
10	BCL	U	406	-	69,74,74	1.10	5 (7%)	79,115,115	1.39	11 (13%)
10	BCL	a	811	-	69,74,74	1.11	6 (8%)	79,115,115	1.39	12 (15%)
13	LHG	a	818	-	44,44,48	0.64	1 (2%)	47,50,54	0.96	2 (4%)
12	F26	A	816	-	40,40,40	1.78	10 (25%)	49,50,50	2.31	15 (30%)
10	BCL	Y	403	-	69,74,74	1.08	5 (7%)	79,115,115	1.40	12 (15%)
13	LHG	A	819	-	33,33,48	0.74	1 (3%)	36,39,54	1.02	3 (8%)
11	F39	A	815	-	66,66,66	2.74	19 (28%)	83,85,85	2.17	21 (25%)
10	BCL	W	404	-	69,74,74	1.05	4 (5%)	79,115,115	1.37	11 (13%)
10	BCL	Y	405	-	69,74,74	1.04	5 (7%)	79,115,115	1.40	11 (13%)
10	BCL	V	406	7	69,74,74	1.08	4 (5%)	79,115,115	1.45	8 (10%)
10	BCL	W	408[B]	7	49,54,74	1.23	6 (12%)	55,91,115	1.44	7 (12%)
10	BCL	X	401	-	69,74,74	1.09	4 (5%)	79,115,115	1.46	12 (15%)
15	SF4	B	302	2	0,12,12	-	-	-	-	-
10	BCL	a	814	-	69,74,74	1.12	5 (7%)	79,115,115	1.53	11 (13%)
13	LHG	A	817	-	36,36,48	0.73	1 (2%)	39,42,54	0.99	2 (5%)
10	BCL	Y	404	-	69,74,74	1.08	5 (7%)	79,115,115	1.51	9 (11%)
10	BCL	V	407	-	69,74,74	1.12	6 (8%)	79,115,115	1.51	12 (15%)
15	SF4	B	303	2	0,12,12	-	-	-	-	-
10	BCL	X	404	7	69,74,74	1.06	4 (5%)	79,115,115	1.33	10 (12%)
13	LHG	Z	401	-	42,42,48	0.62	0	45,48,54	0.98	2 (4%)
10	BCL	V	409[B]	7	49,54,74	1.24	6 (12%)	55,91,115	1.41	6 (10%)
14	LMG	A	823	10	31,31,55	0.90	1 (3%)	39,39,63	1.20	4 (10%)
10	BCL	Y	401	-	69,74,74	1.11	5 (7%)	79,115,115	1.48	11 (13%)
10	BCL	U	407[B]	7	49,54,74	1.29	6 (12%)	55,91,115	1.43	7 (12%)
10	BCL	X	408[B]	7	49,54,74	1.25	6 (12%)	55,91,115	1.40	7 (12%)
13	LHG	a	821	-	37,37,48	0.69	1 (2%)	40,43,54	0.99	2 (5%)
10	BCL	A	811	-	69,74,74	1.12	6 (8%)	79,115,115	1.44	11 (13%)
10	BCL	U	404	7	69,74,74	1.09	4 (5%)	79,115,115	1.44	10 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	F26	a	816	-	40,40,40	1.66	10 (25%)	49,50,50	2.22	13 (26%)
10	BCL	V	403	-	69,74,74	1.09	5 (7%)	79,115,115	1.33	10 (12%)
10	BCL	Z	404	-	69,74,74	1.04	5 (7%)	79,115,115	1.46	12 (15%)
9	G2O	A	827	-	68,73,73	4.16	40 (58%)	81,113,113	2.80	20 (24%)
10	BCL	a	803	-	69,74,74	1.10	5 (7%)	79,115,115	1.38	11 (13%)

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
10	BCL	a	809	-	-	17/41/137/137	-
10	BCL	A	803	-	-	14/41/137/137	-
11	F39	a	815	-	-	39/58/78/78	0/2/2/2
10	BCL	X	406	-	-	5/41/137/137	-
9	G2O	a	801	-	3/3/15/22	21/39/115/115	-
10	BCL	a	805	-	-	5/41/137/137	-
10	BCL	W	405	-	-	15/41/137/137	-
9	G2O	A	802	-	3/3/15/22	17/39/115/115	-
10	BCL	V	402	-	-	8/41/137/137	-
10	BCL	Z	406	-	-	9/41/137/137	-
10	BCL	X	405	-	-	3/41/137/137	-
14	LMG	A	821	-	-	23/36/56/70	0/1/1/1
10	BCL	Z	402	-	-	6/41/137/137	-
10	BCL	W	407	-	-	7/41/137/137	-
10	BCL	Y	407	-	-	11/41/137/137	-
10	BCL	a	806	10	-	21/41/137/137	-
10	BCL	U	402	-	-	16/41/137/137	-
13	LHG	a	820	-	-	25/42/42/53	-
10	BCL	Z	405	7	-	12/41/137/137	-
8	GS0	a	802	8	2/2/21/25	17/41/137/137	-
10	BCL	V	404	-	-	12/41/137/137	-
10	BCL	W	406	-	-	5/41/137/137	-
10	BCL	A	814	-	-	16/40/136/137	-
10	BCL	a	807	10	-	14/41/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	BCL	V	408	-	-	9/41/137/137	-
10	BCL	W	402	-	-	9/41/137/137	-
10	BCL	B	301	14	-	17/41/137/137	-
10	BCL	a	813	-	-	19/41/137/137	-
15	SF4	A	824	1	-	-	0/6/5/5
10	BCL	a	812	-	-	18/41/137/137	-
10	BCL	Y	402	-	-	7/41/137/137	-
10	BCL	A	804	-	-	15/41/137/137	-
14	LMG	A	820	-	-	19/37/57/70	0/1/1/1
10	BCL	X	402	-	-	13/41/137/137	-
13	LHG	E	102	-	-	24/47/47/53	-
10	BCL	a	804	-	-	12/41/137/137	-
14	LMG	A	822	-	-	25/37/57/70	0/1/1/1
10	BCL	A	813	-	-	26/41/137/137	-
10	BCL	A	809	-	-	15/41/137/137	-
11	F39	C	301	-	-	33/58/78/78	0/2/2/2
9	G2O	A	826	-	3/3/15/22	22/39/115/115	-
14	LMG	C	302	-	-	19/37/57/70	0/1/1/1
10	BCL	W	401	-	-	6/41/137/137	-
10	BCL	A	810	-	-	7/41/137/137	-
10	BCL	V	401	-	-	12/41/137/137	-
8	GS0	A	801	8	2/2/21/25	21/41/137/137	-
10	BCL	A	812	-	-	15/41/137/137	-
13	LHG	a	819	-	-	19/38/38/53	-
10	BCL	Y	406	7	-	8/41/137/137	-
10	BCL	U	401	-	-	7/41/137/137	-
10	BCL	A	807	-	-	13/41/137/137	-
14	LMG	a	822	-	-	20/40/60/70	0/1/1/1
10	BCL	Z	408[B]	7	-	9/17/113/137	-
10	BCL	a	808	1	-	6/17/113/137	-
10	BCL	A	808	1	-	7/41/137/137	-
10	BCL	Y	408	-	-	5/41/137/137	-
10	BCL	A	805	-	-	13/41/137/137	-
10	BCL	U	405	-	-	6/41/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	BCL	Z	407	-	-	7/41/137/137	-
12	F26	a	817	-	-	22/36/36/36	0/1/1/1
10	BCL	X	403	-	-	9/41/137/137	-
10	BCL	W	403	-	-	14/41/137/137	-
10	BCL	X	409	-	-	5/41/137/137	-
10	BCL	a	810	-	-	13/41/137/137	-
10	BCL	V	405	-	-	9/41/137/137	-
13	LHG	E	101	-	-	20/43/43/53	-
10	BCL	X	407[B]	7	-	8/17/113/137	-
10	BCL	A	806	-	-	16/41/137/137	-
10	BCL	Z	403	-	-	15/41/137/137	-
10	BCL	U	403	-	-	10/41/137/137	-
13	LHG	A	818	-	-	22/44/44/53	-
10	BCL	U	406	-	-	5/41/137/137	-
10	BCL	a	811	-	-	7/41/137/137	-
13	LHG	a	818	-	-	23/49/49/53	-
12	F26	A	816	-	-	19/36/36/36	0/1/1/1
10	BCL	Y	403	-	-	10/41/137/137	-
13	LHG	A	819	-	-	19/38/38/53	-
11	F39	A	815	-	-	33/58/78/78	0/2/2/2
10	BCL	W	404	-	-	6/41/137/137	-
10	BCL	Y	405	-	-	6/41/137/137	-
10	BCL	V	406	7	-	7/41/137/137	-
10	BCL	W	408[B]	7	-	11/17/113/137	-
10	BCL	X	401	-	-	5/41/137/137	-
15	SF4	B	302	2	-	-	0/6/5/5
10	BCL	a	814	-	-	13/41/137/137	-
13	LHG	A	817	-	-	17/41/41/53	-
10	BCL	Y	404	-	-	16/41/137/137	-
10	BCL	V	407	-	-	7/41/137/137	-
15	SF4	B	303	2	-	-	0/6/5/5
10	BCL	X	404	7	-	7/41/137/137	-
13	LHG	Z	401	-	-	26/47/47/53	-
10	BCL	V	409[B]	7	-	11/17/113/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	LMG	A	823	10	-	4/26/46/70	0/1/1/1
10	BCL	Y	401	-	-	10/41/137/137	-
10	BCL	U	407[B]	7	-	9/17/113/137	-
10	BCL	X	408[B]	7	-	8/17/113/137	-
13	LHG	a	821	-	-	20/42/42/53	-
10	BCL	A	811	-	-	6/41/137/137	-
10	BCL	U	404	7	-	10/41/137/137	-
12	F26	a	816	-	-	19/36/36/36	0/1/1/1
10	BCL	V	403	-	-	7/41/137/137	-
10	BCL	Z	404	-	-	8/41/137/137	-
9	G2O	A	827	-	3/3/15/22	12/39/115/115	-
10	BCL	a	803	-	-	11/41/137/137	-

The worst 5 of 639 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	826	G2O	MG-ND	17.12	2.39	2.05
9	a	801	G2O	MG-ND	15.45	2.36	2.05
9	A	827	G2O	MG-ND	14.66	2.34	2.05
9	A	802	G2O	MG-ND	14.27	2.34	2.05
9	A	826	G2O	MG-NA	12.95	2.37	2.06

The worst 5 of 1062 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	826	G2O	C1A-NA-C4A	19.27	115.47	106.68
9	A	802	G2O	C1A-NA-C4A	18.67	115.20	106.68
9	a	801	G2O	C1A-NA-C4A	18.38	115.06	106.68
9	A	827	G2O	C1A-NA-C4A	17.72	114.76	106.68
8	A	801	GS0	C4A-NA-C1A	13.32	112.76	106.68

5 of 16 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	A	801	GS0	CBD
8	A	801	GS0	C13
8	a	802	GS0	C3C
8	a	802	GS0	CBD
9	A	802	G2O	C2A

5 of 1356 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	801	GS0	C1-C2-C3-C4
8	A	801	GS0	C1-C2-C3-C5
8	A	801	GS0	C3A-C2A-CAA-CBA
8	A	801	GS0	CBD-CGD-O2D-CED
8	A	801	GS0	O1D-CGD-O2D-CED

There are no ring outliers.

71 monomers are involved in 146 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	a	809	BCL	5	0
10	A	803	BCL	5	0
10	X	406	BCL	1	0
9	a	801	G2O	3	0
10	a	805	BCL	3	0
10	W	405	BCL	1	0
10	V	402	BCL	1	0
10	Z	406	BCL	2	0
10	X	405	BCL	1	0
14	A	821	LMG	2	0
10	Z	402	BCL	1	0
10	a	806	BCL	5	0
10	U	402	BCL	1	0
13	a	820	LHG	3	0
10	Z	405	BCL	1	0
10	W	406	BCL	4	0
10	A	814	BCL	2	0
10	a	807	BCL	1	0
10	W	402	BCL	2	0
10	B	301	BCL	3	0
10	a	813	BCL	3	0
10	Y	402	BCL	1	0
10	A	804	BCL	2	0
14	A	820	LMG	2	0
10	X	402	BCL	3	0
13	E	102	LHG	3	0
10	a	804	BCL	2	0
10	A	813	BCL	2	0
10	A	809	BCL	4	0
14	C	302	LMG	4	0
10	W	401	BCL	3	0

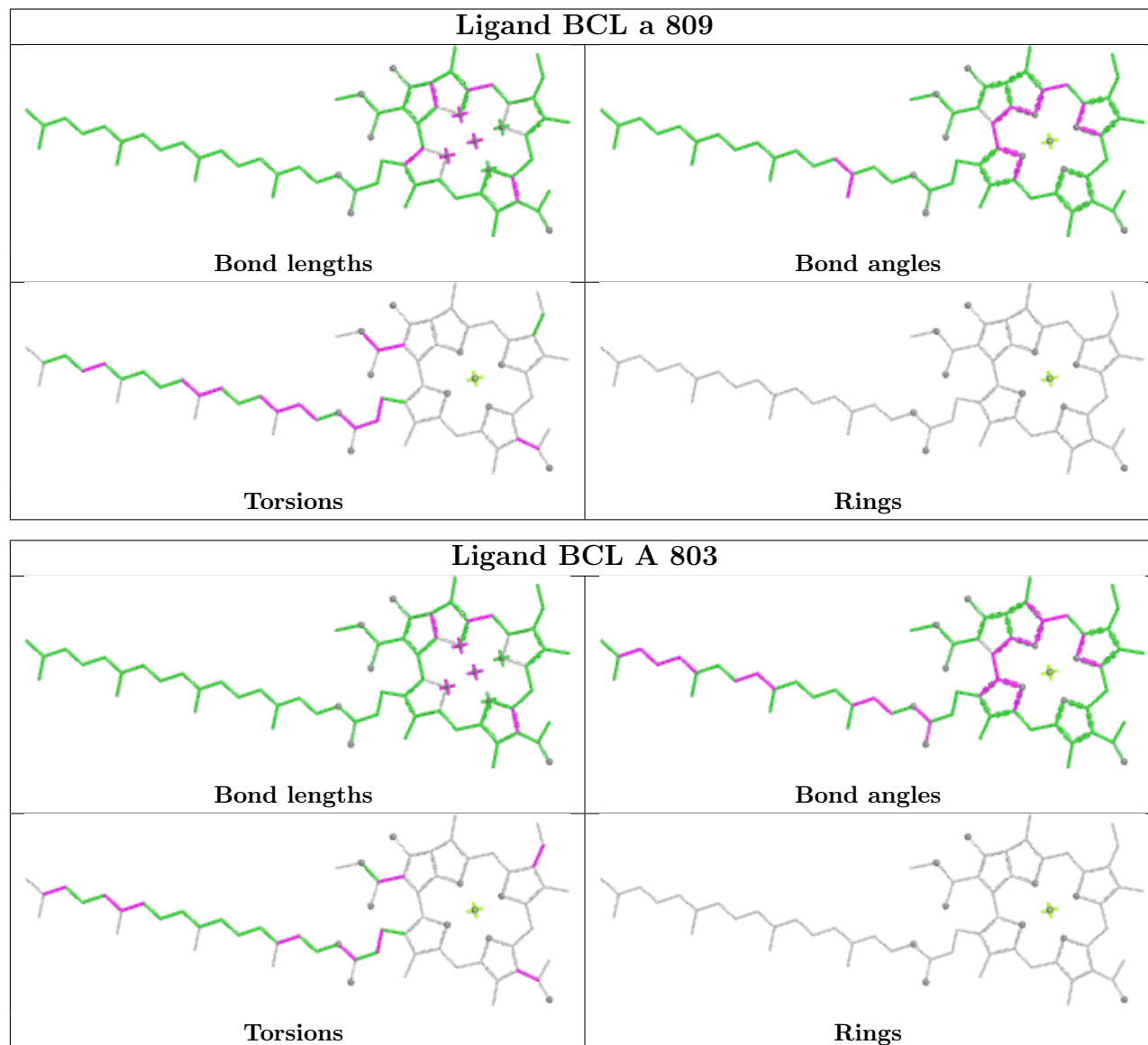
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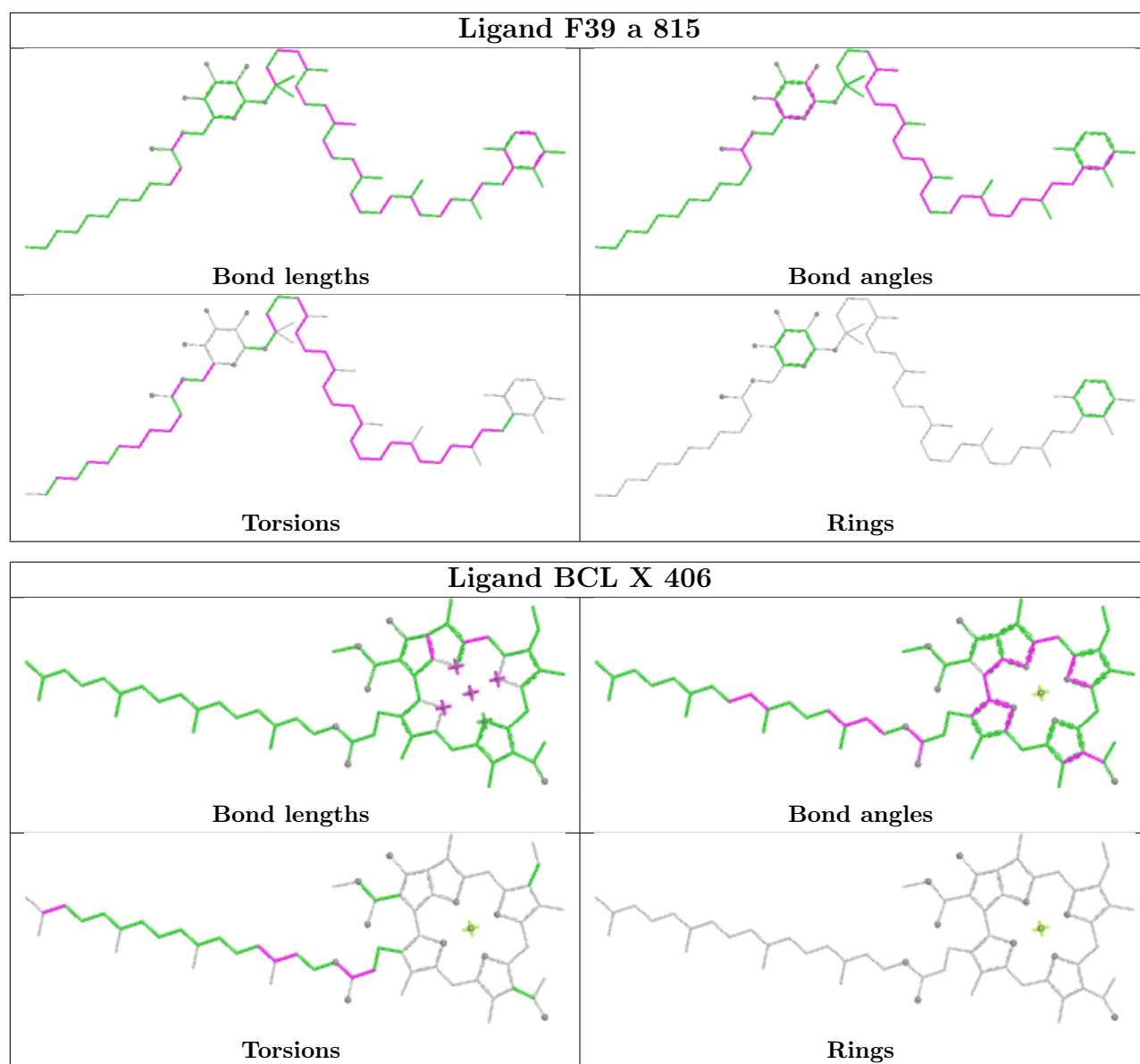
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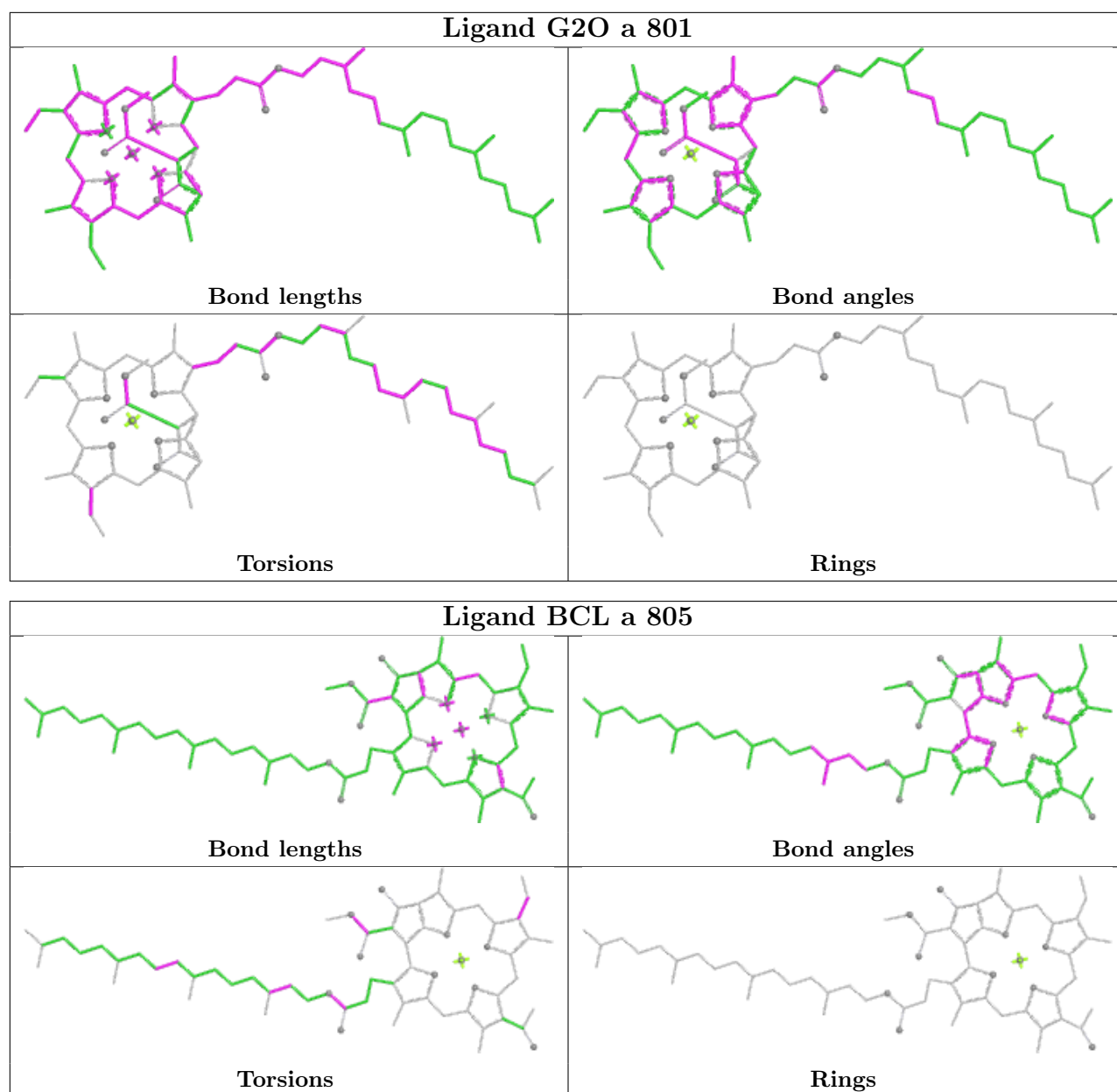
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	810	BCL	2	0
8	A	801	GS0	3	0
10	A	812	BCL	3	0
13	a	819	LHG	2	0
10	Y	406	BCL	1	0
10	U	401	BCL	1	0
10	A	807	BCL	1	0
14	a	822	LMG	3	0
10	a	808	BCL	1	0
10	A	808	BCL	3	0
10	Y	408	BCL	1	0
10	A	805	BCL	6	0
10	Z	407	BCL	2	0
10	X	403	BCL	2	0
10	W	403	BCL	2	0
10	X	409	BCL	2	0
10	a	810	BCL	3	0
10	V	405	BCL	1	0
13	E	101	LHG	3	0
10	A	806	BCL	1	0
10	Z	403	BCL	5	0
10	U	403	BCL	4	0
13	A	818	LHG	3	0
13	A	819	LHG	3	0
10	W	404	BCL	3	0
10	X	401	BCL	1	0
10	a	814	BCL	3	0
13	A	817	LHG	1	0
10	Y	404	BCL	2	0
10	V	407	BCL	1	0
13	Z	401	LHG	5	0
10	V	409[B]	BCL	1	0
14	A	823	LMG	4	0
10	X	408[B]	BCL	1	0
13	a	821	LHG	1	0
10	A	811	BCL	4	0
10	U	404	BCL	2	0
10	Z	404	BCL	2	0
9	A	827	G2O	1	0
10	a	803	BCL	1	0

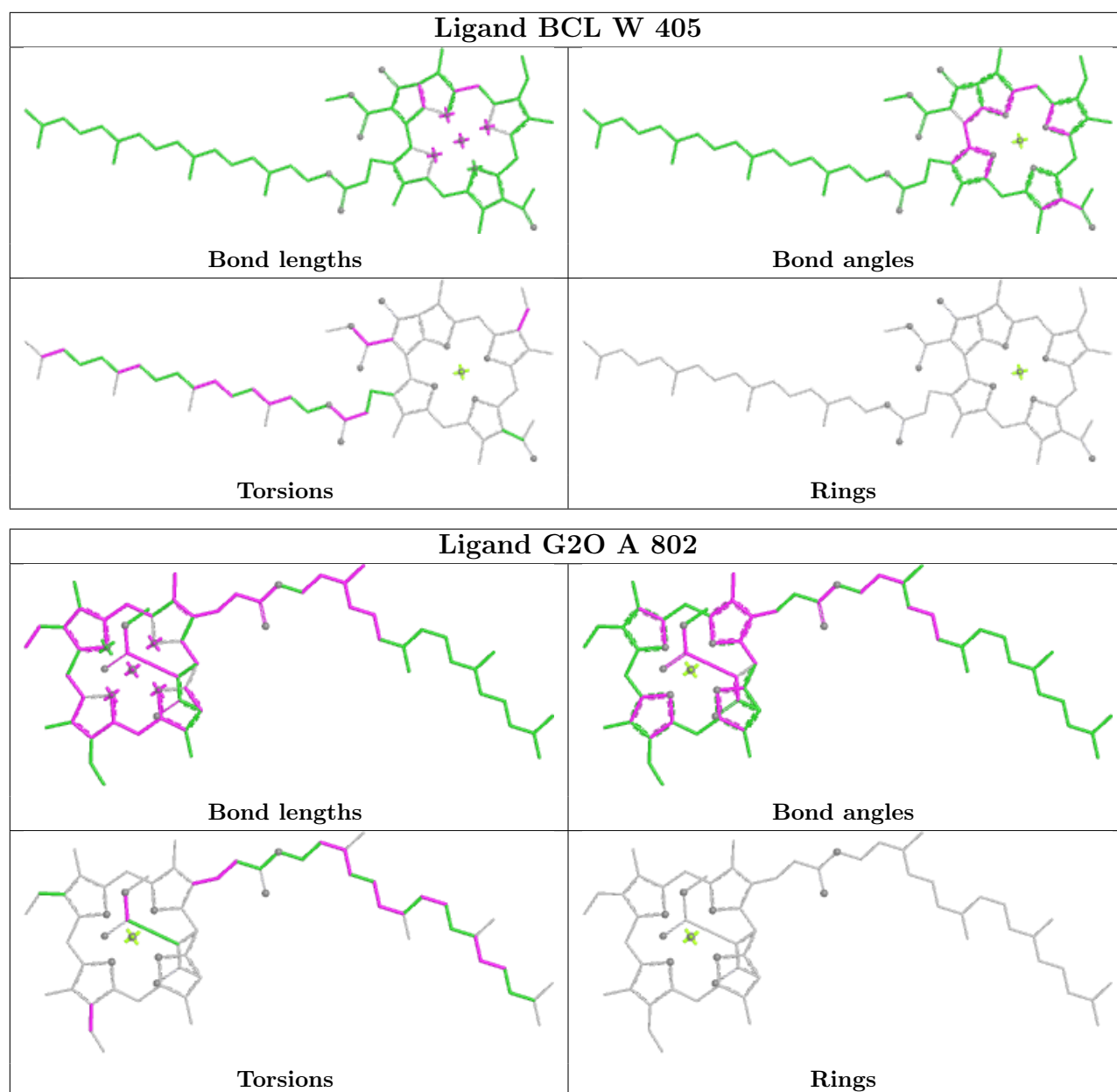
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

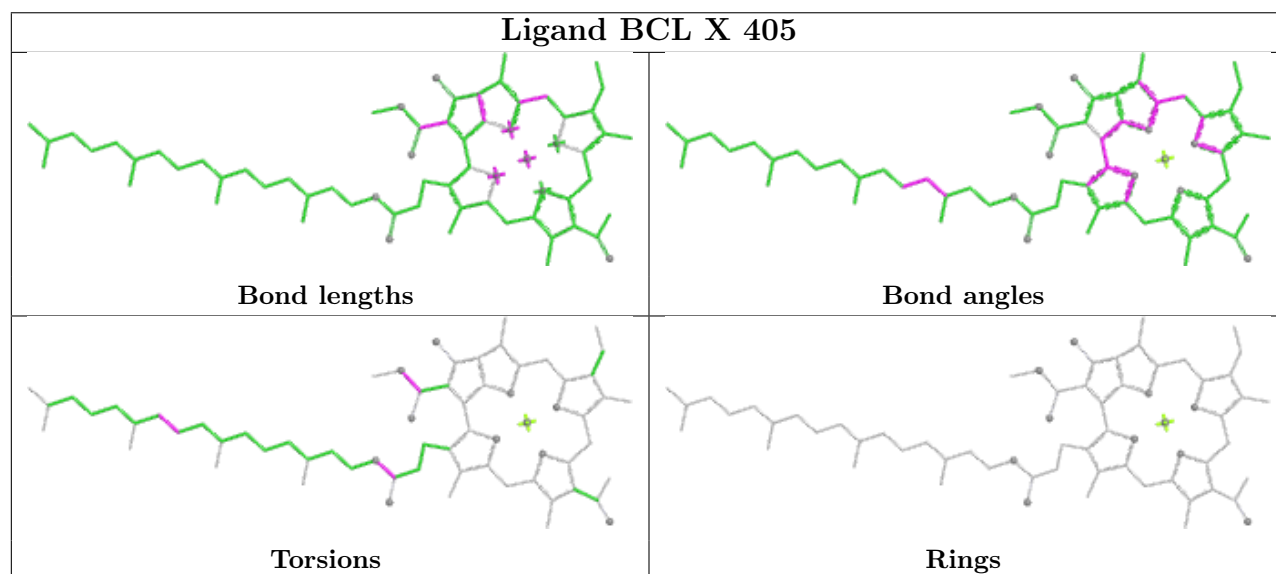
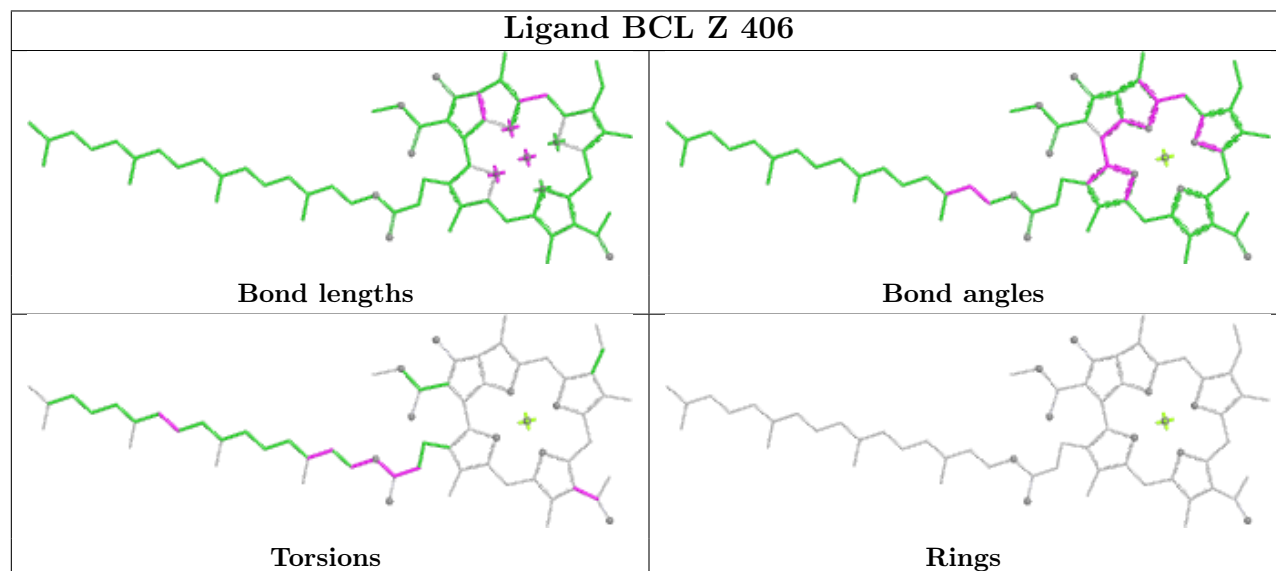
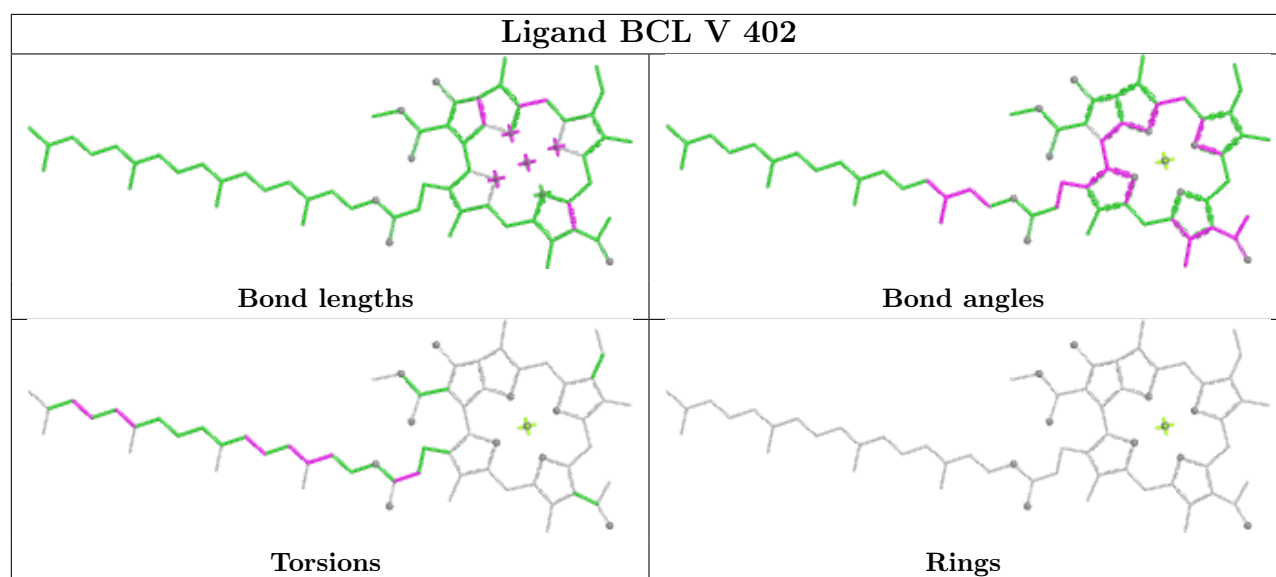
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.

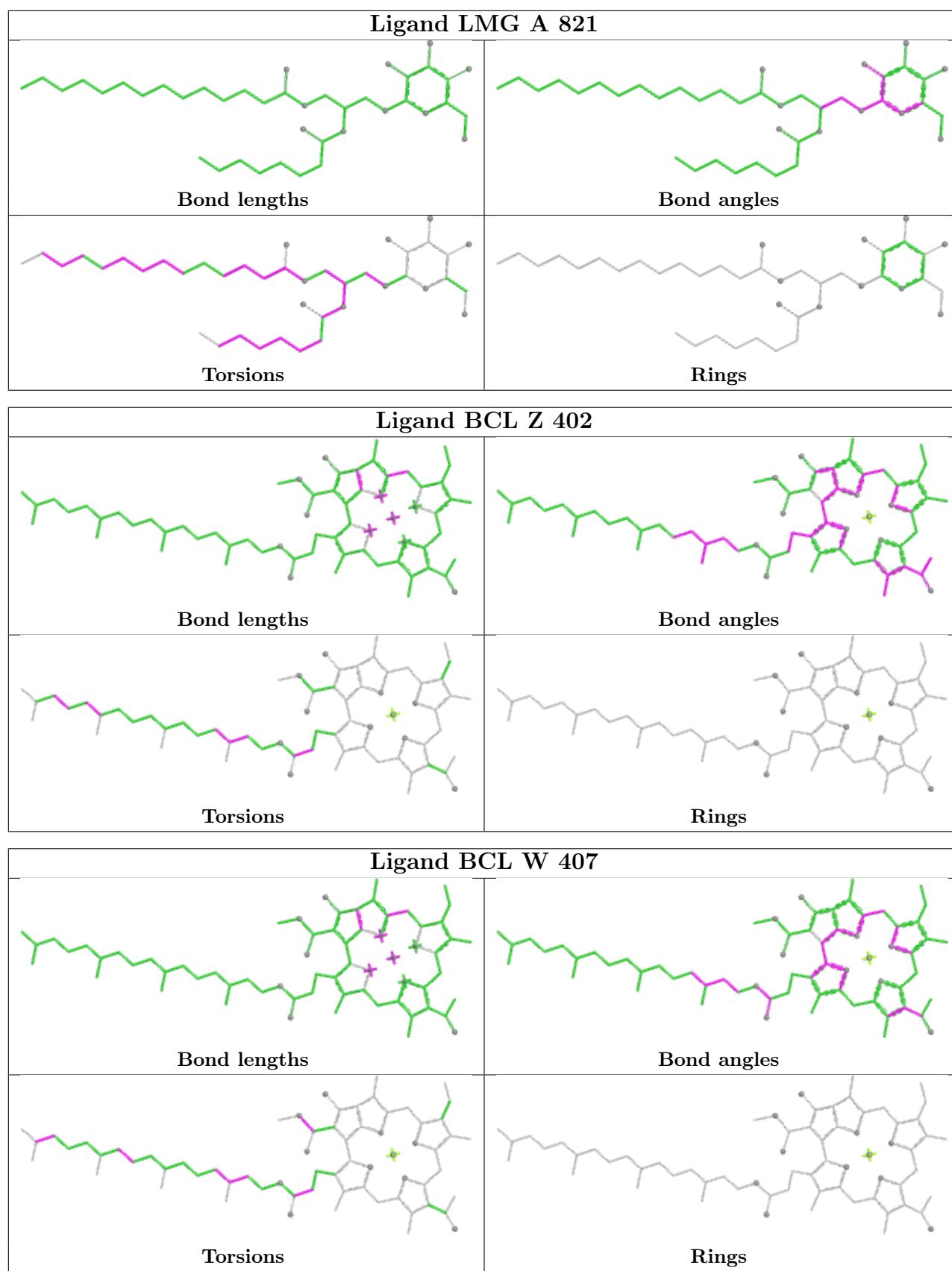


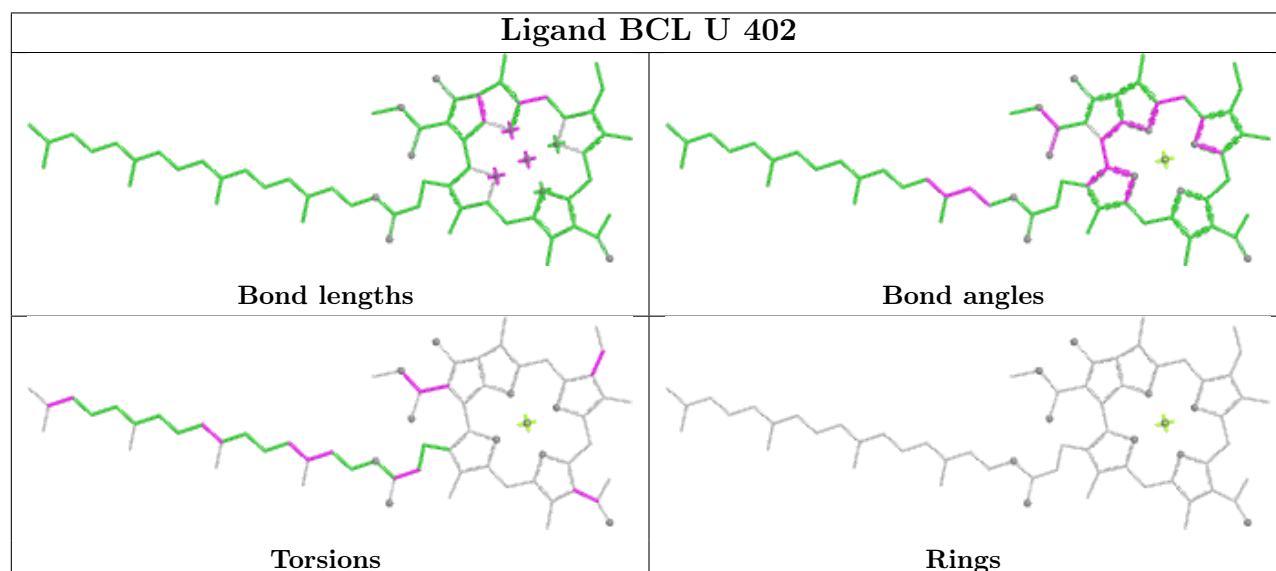
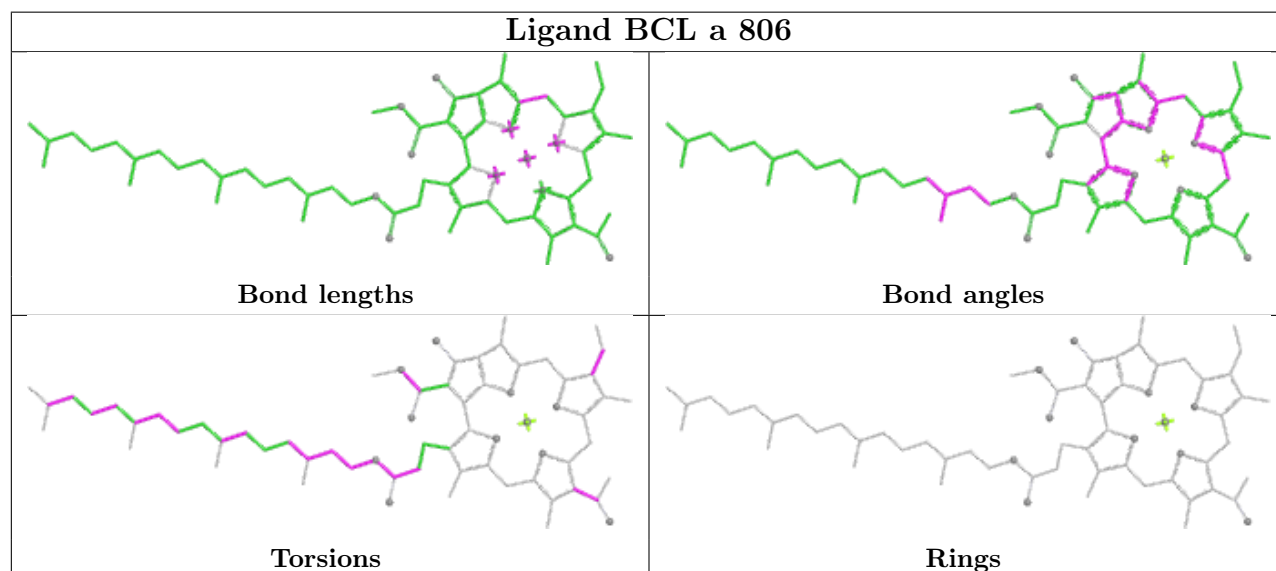
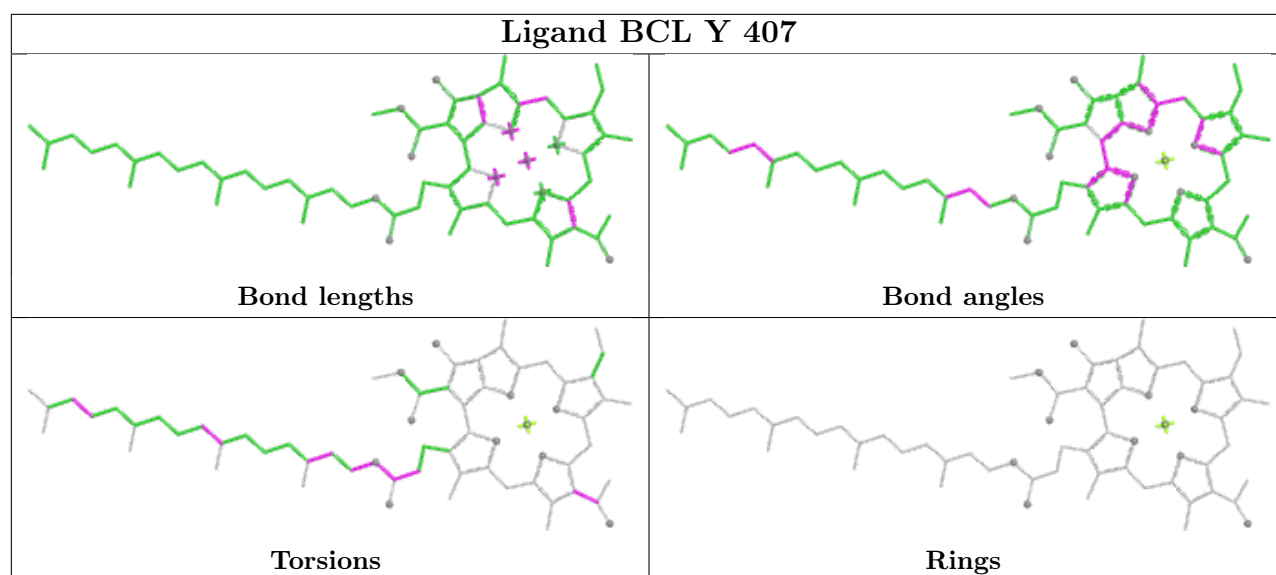


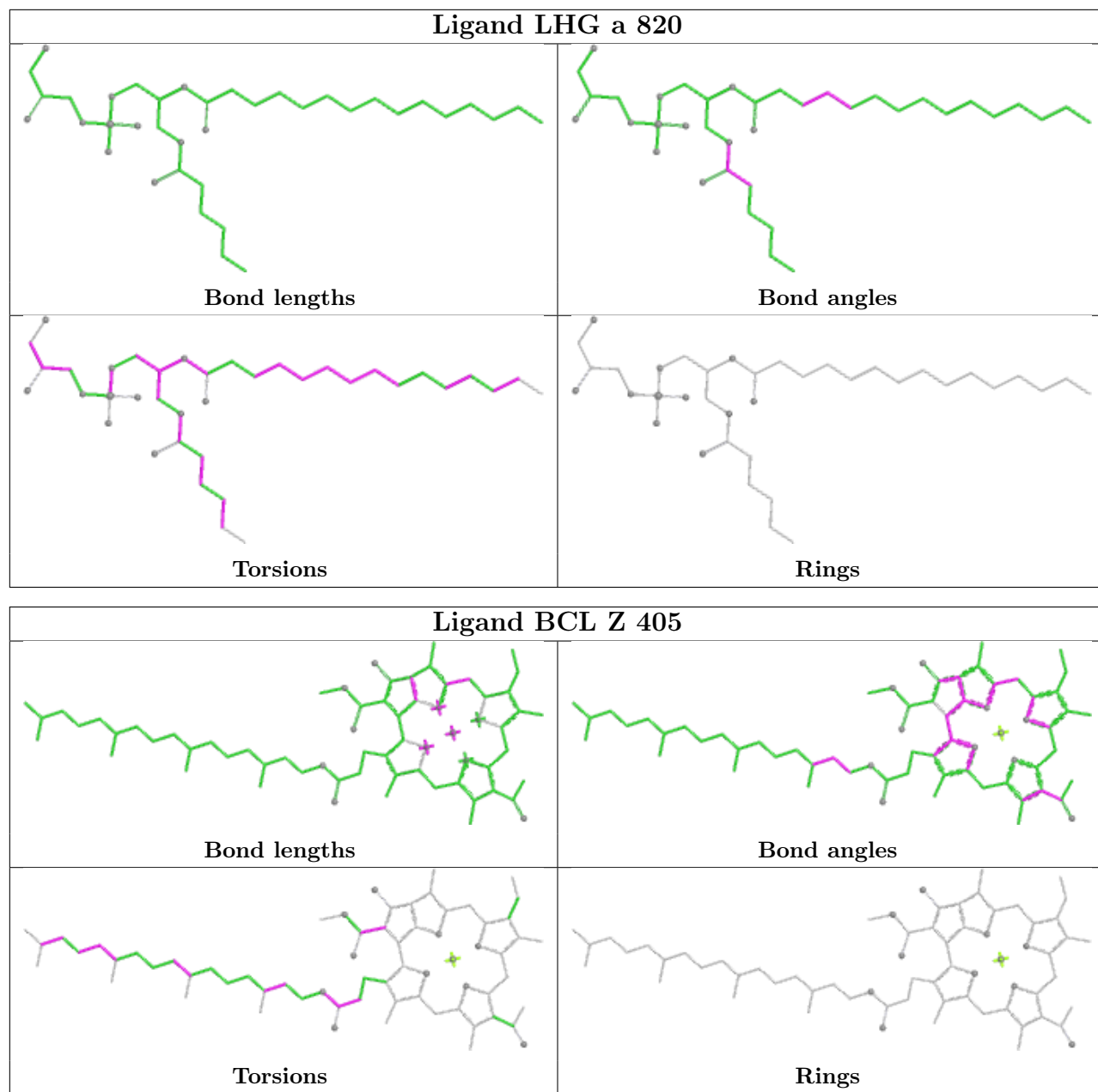


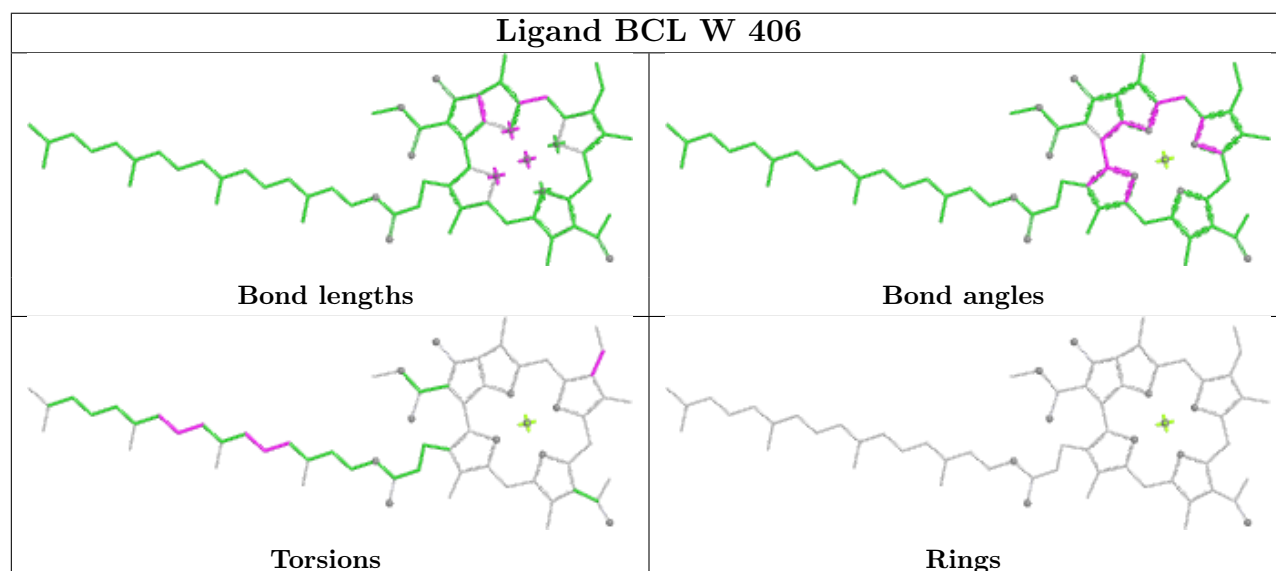
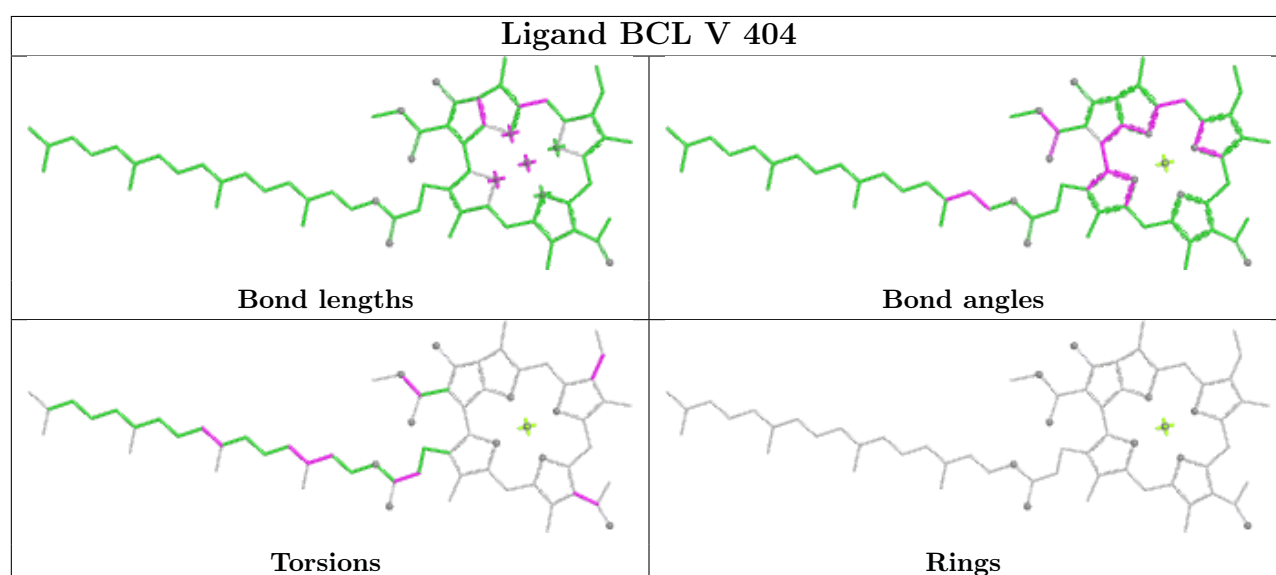
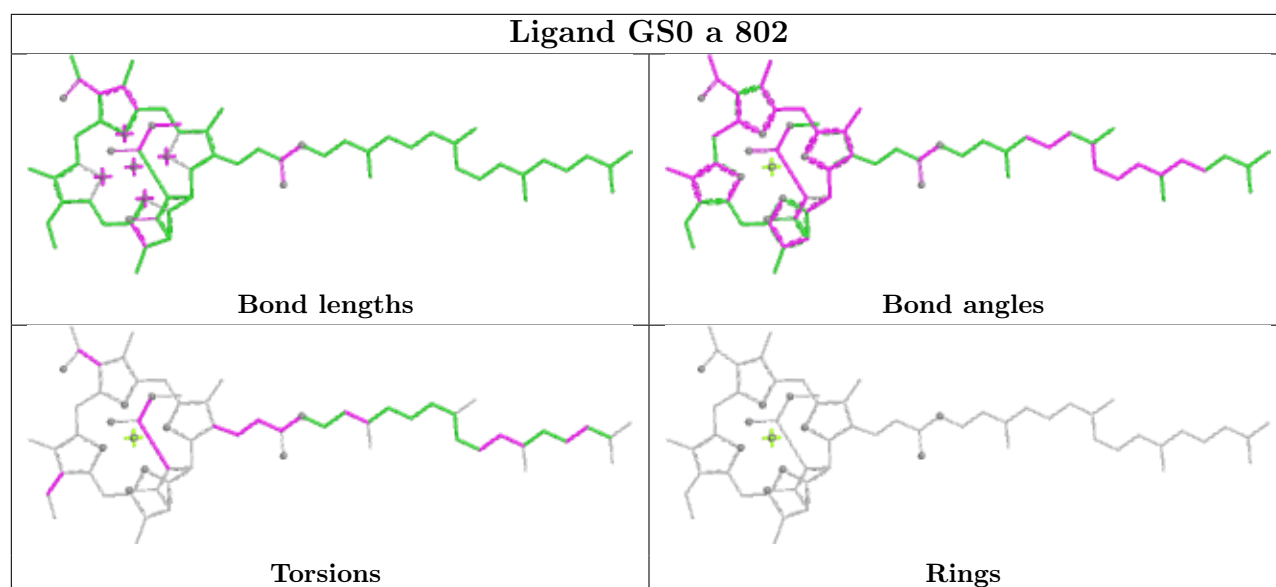


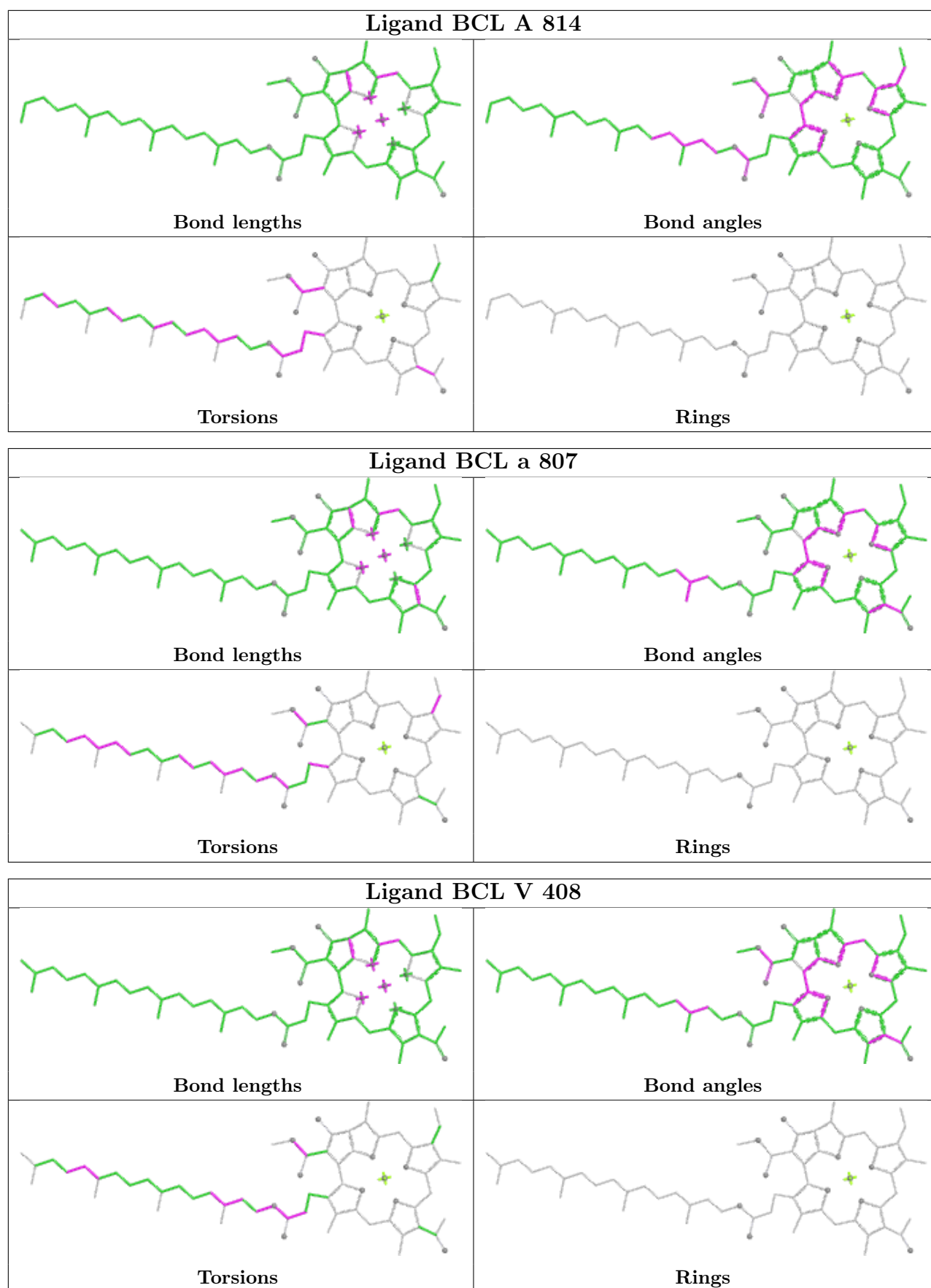


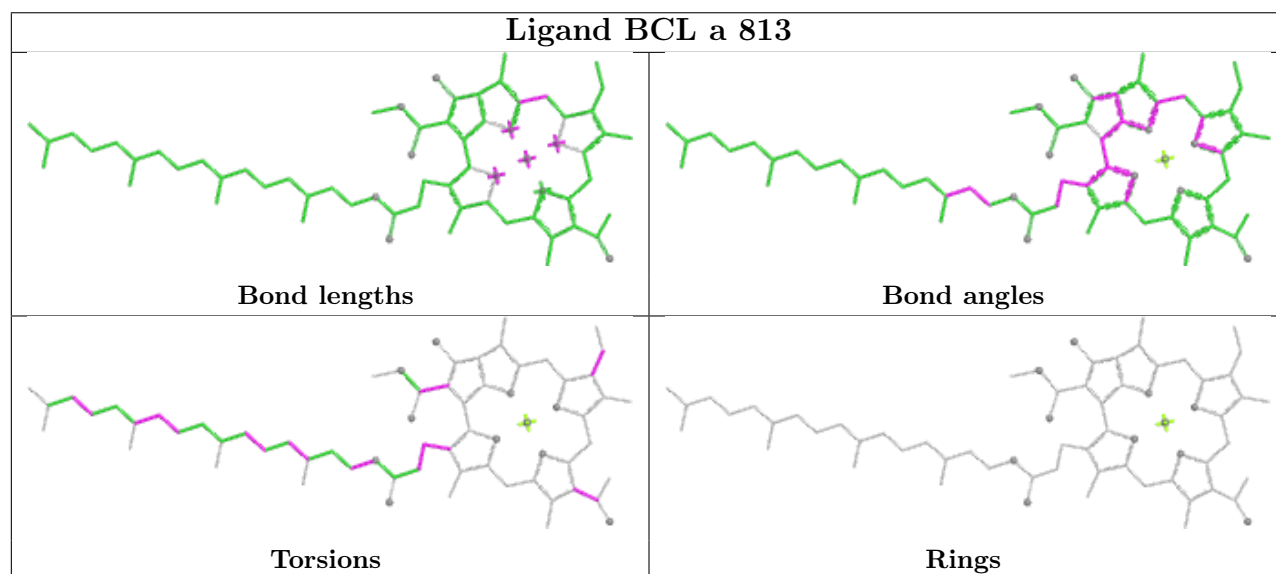
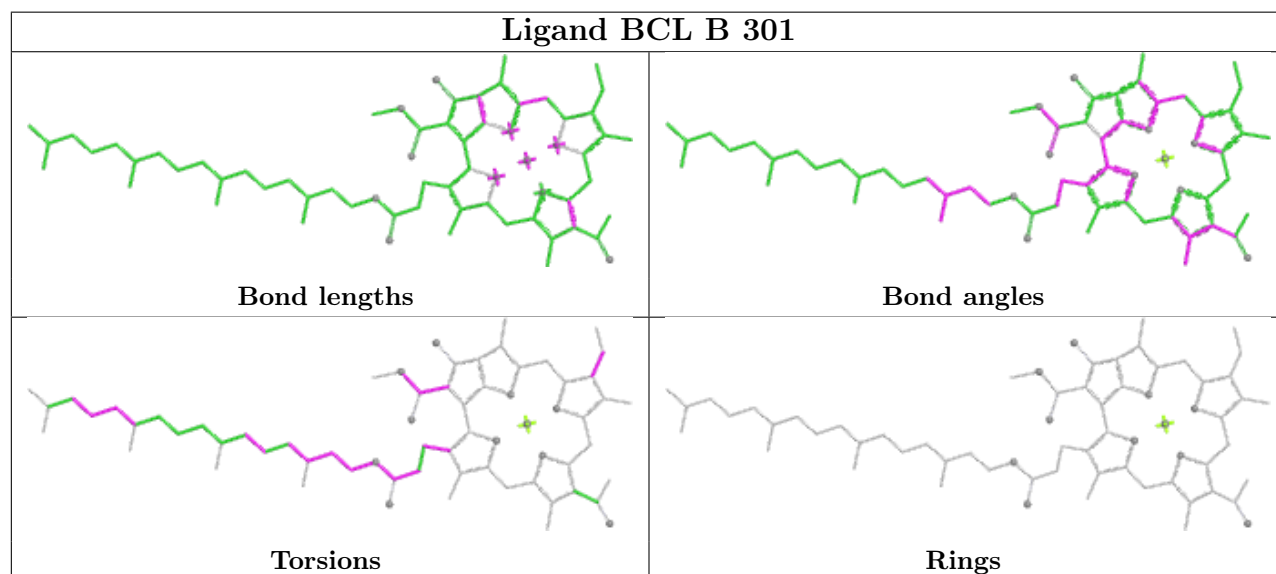
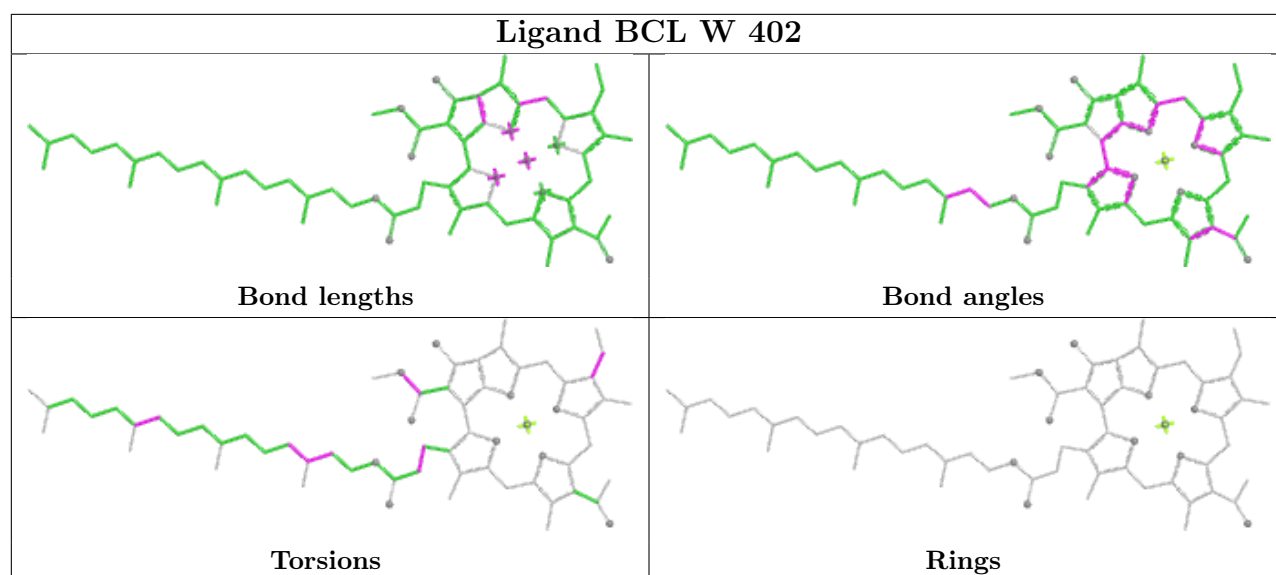


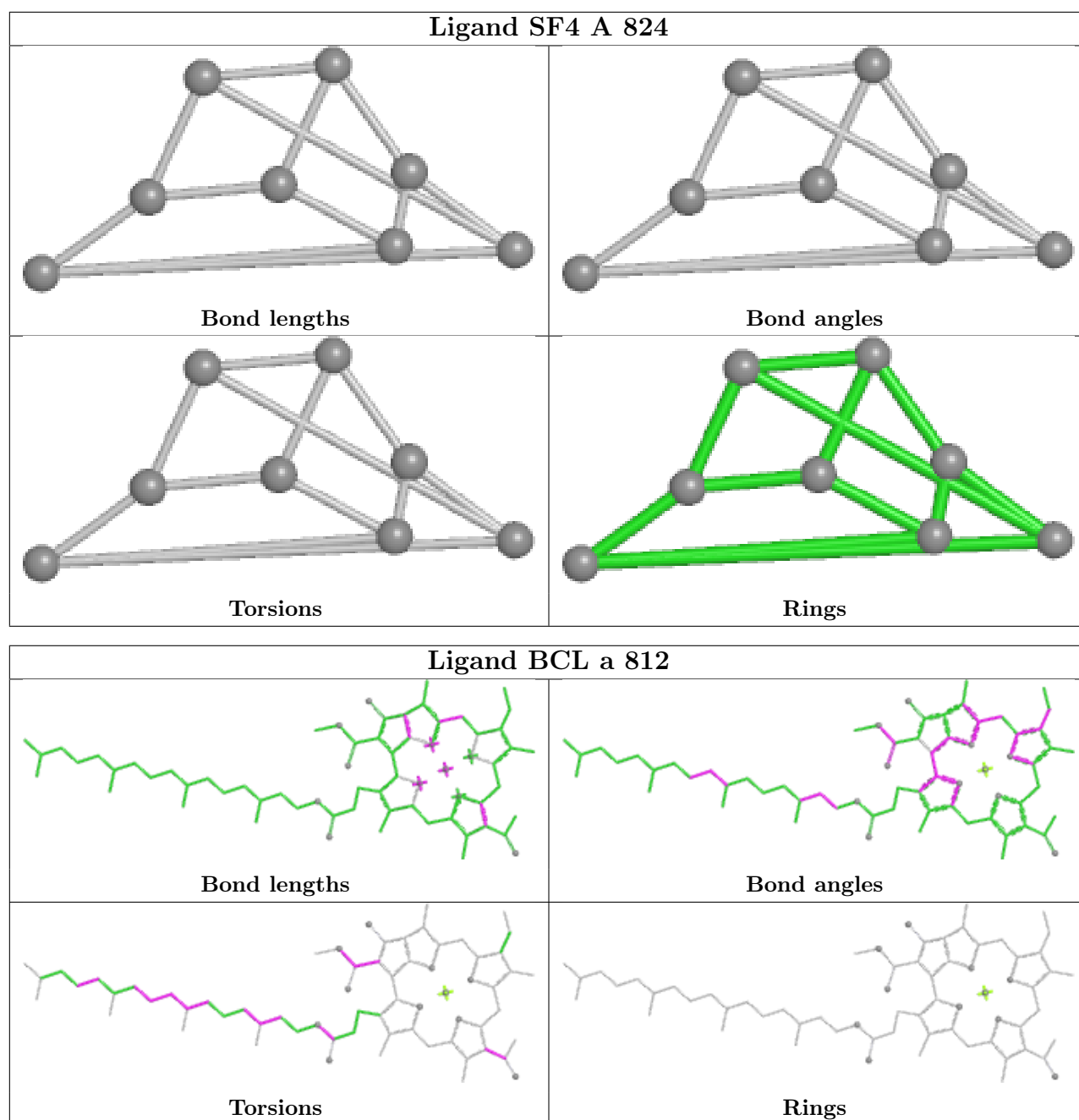


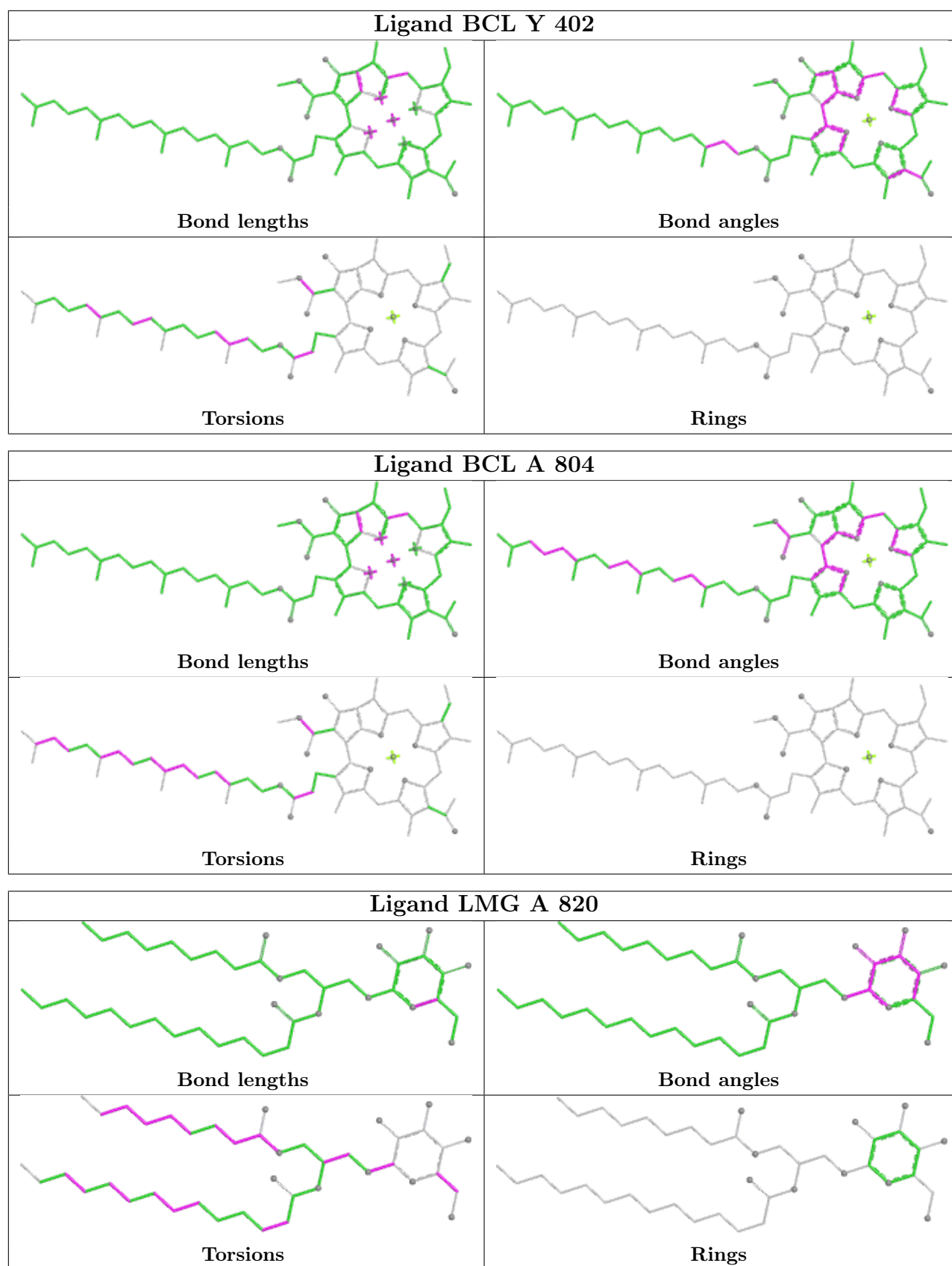


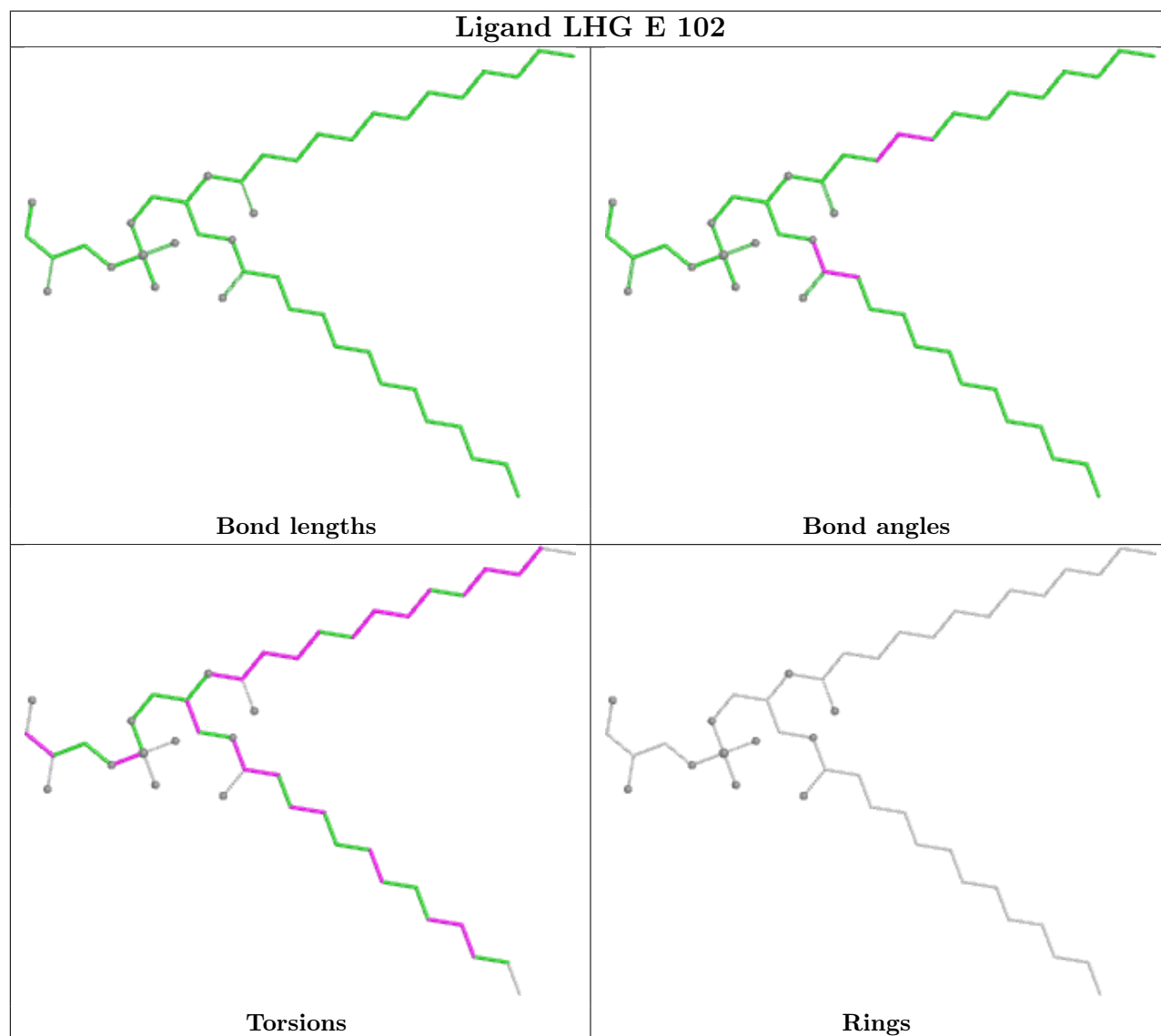
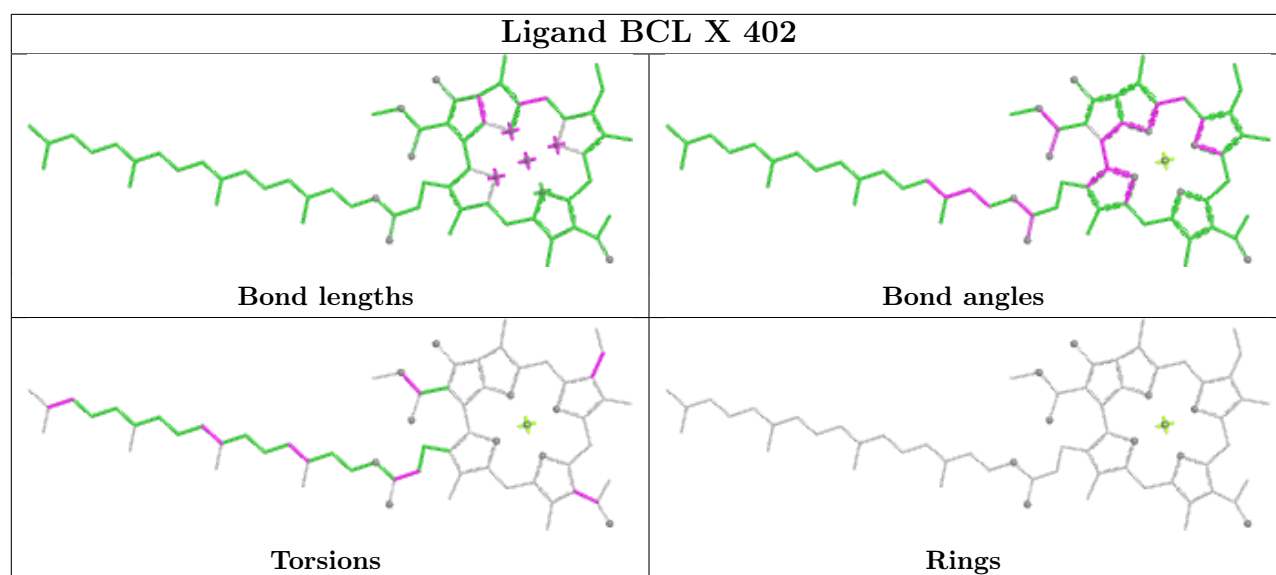


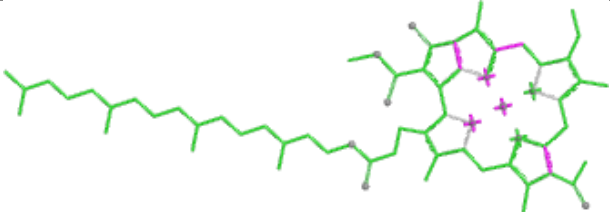
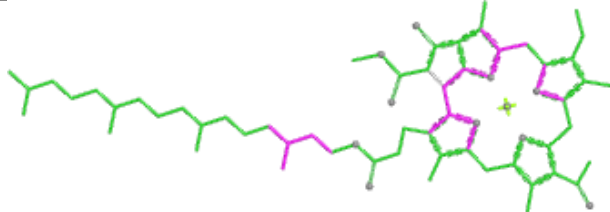
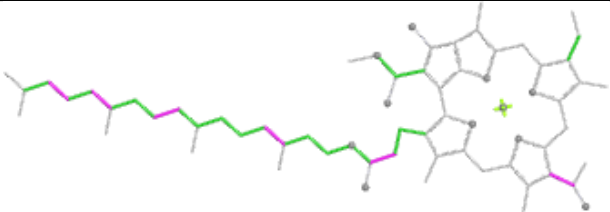
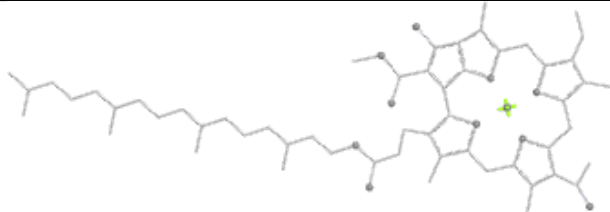
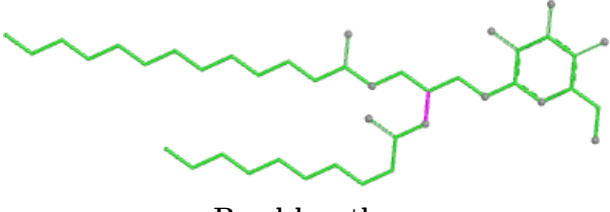
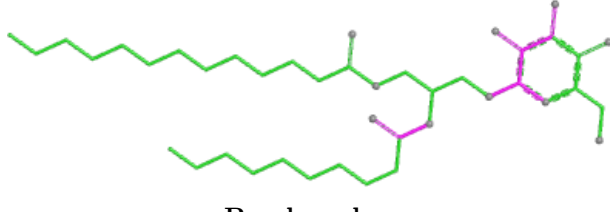
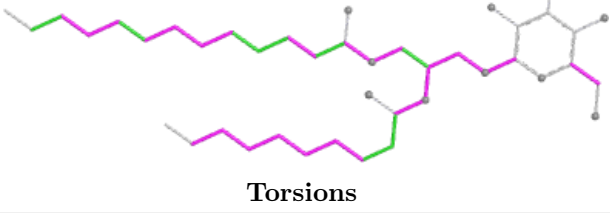
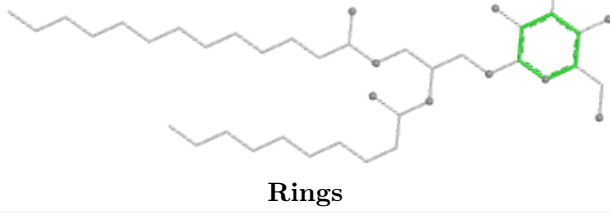
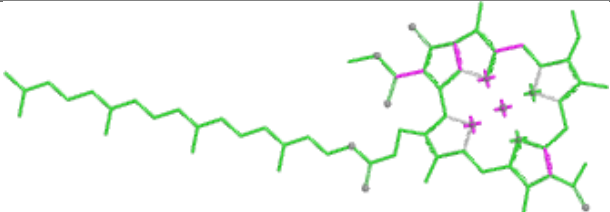
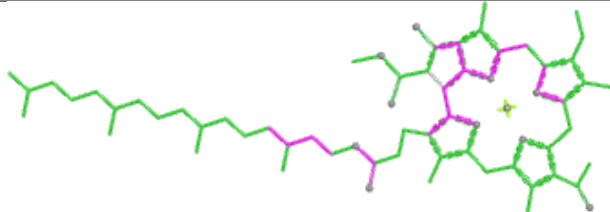
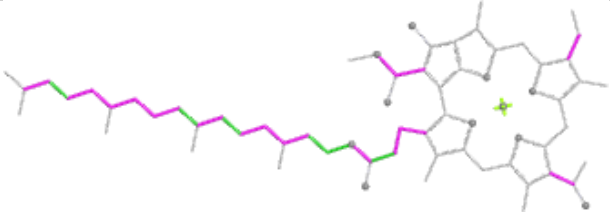
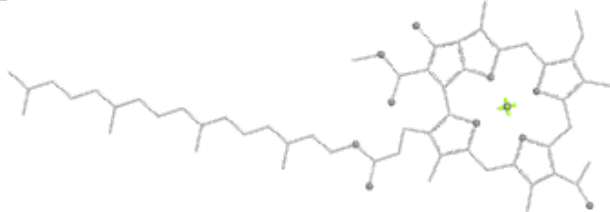


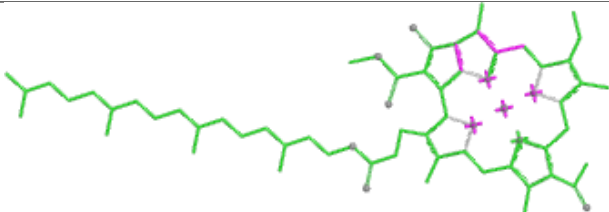
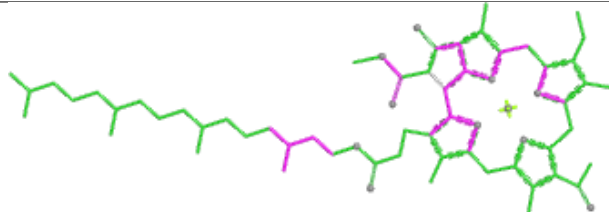
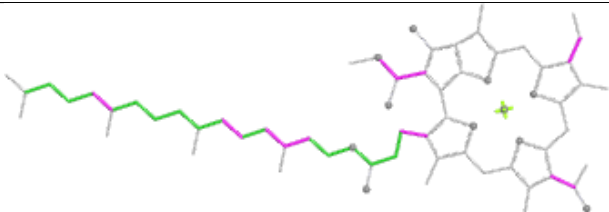
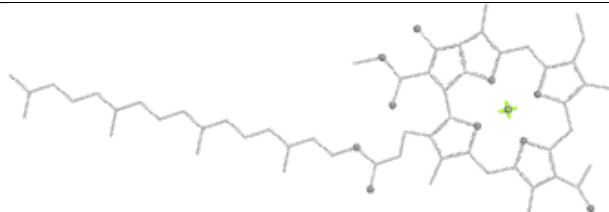


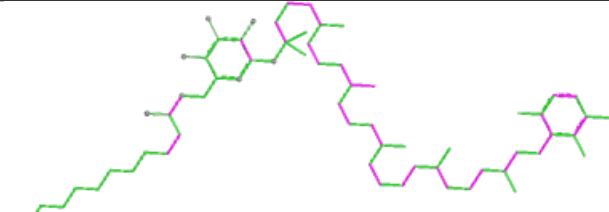
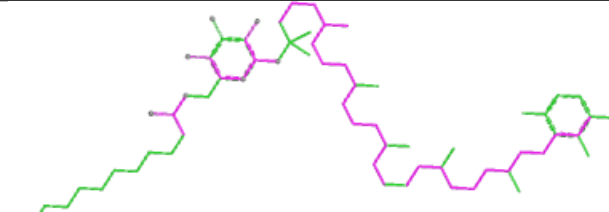
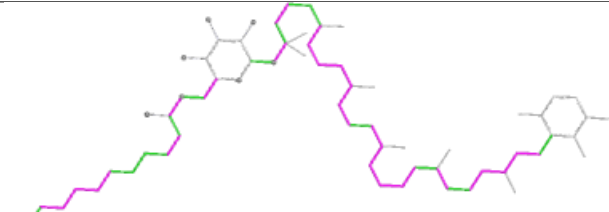
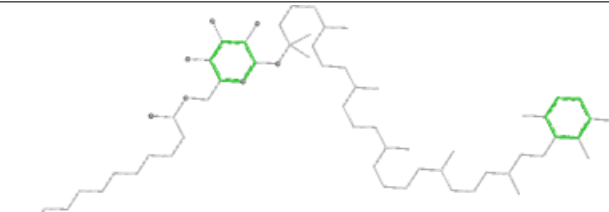


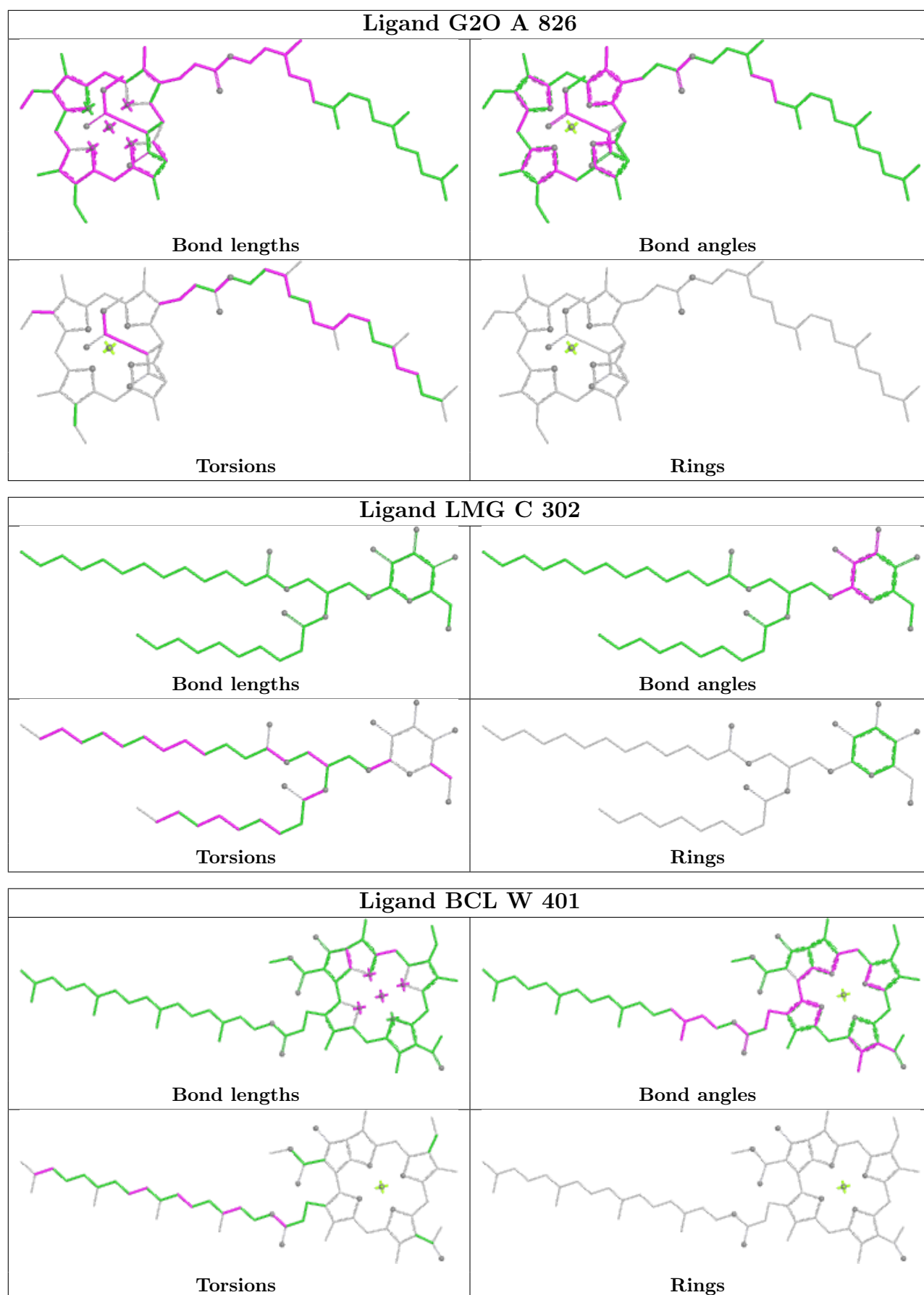


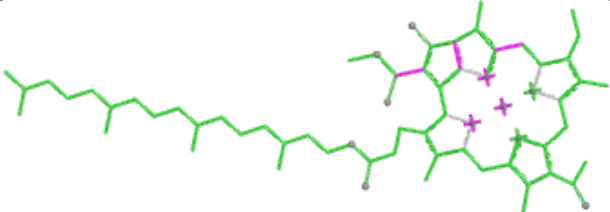
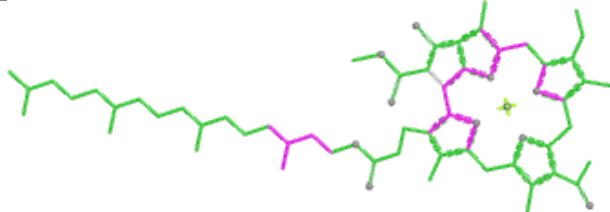
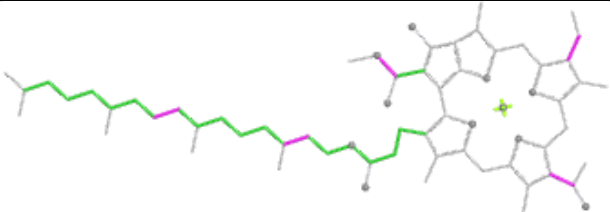
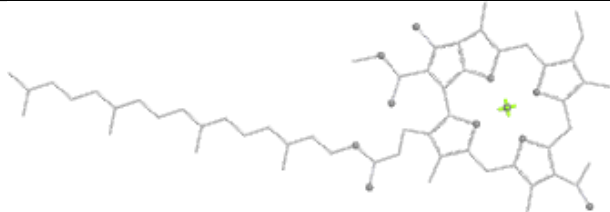
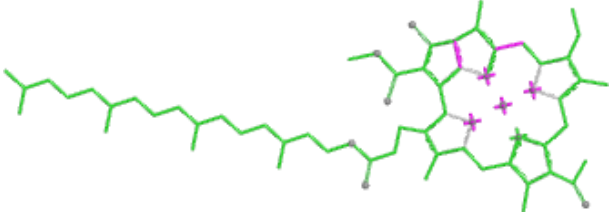
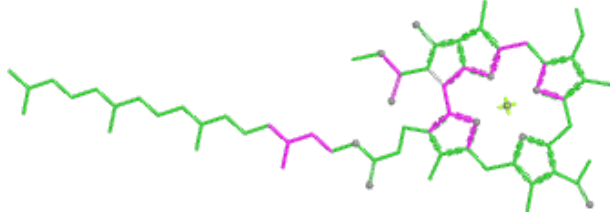
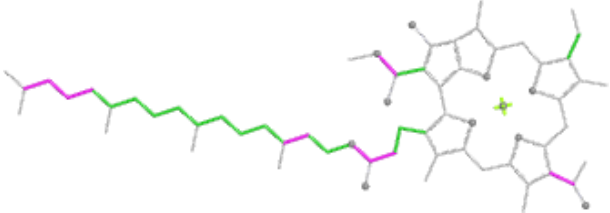
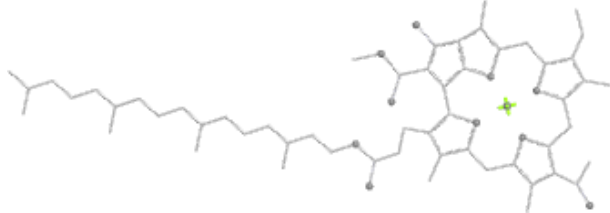
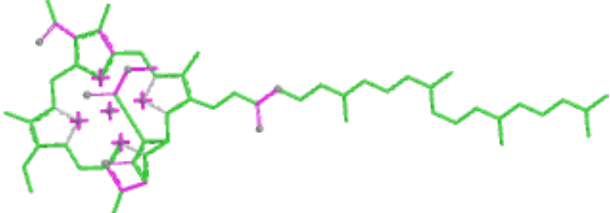
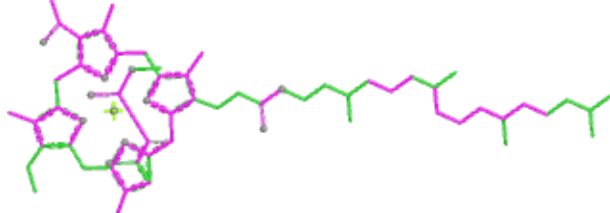
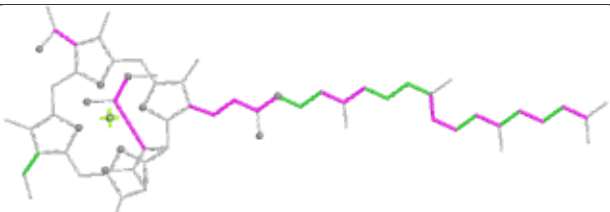
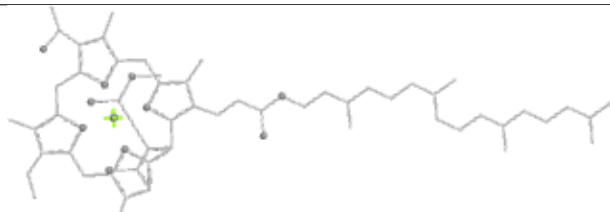


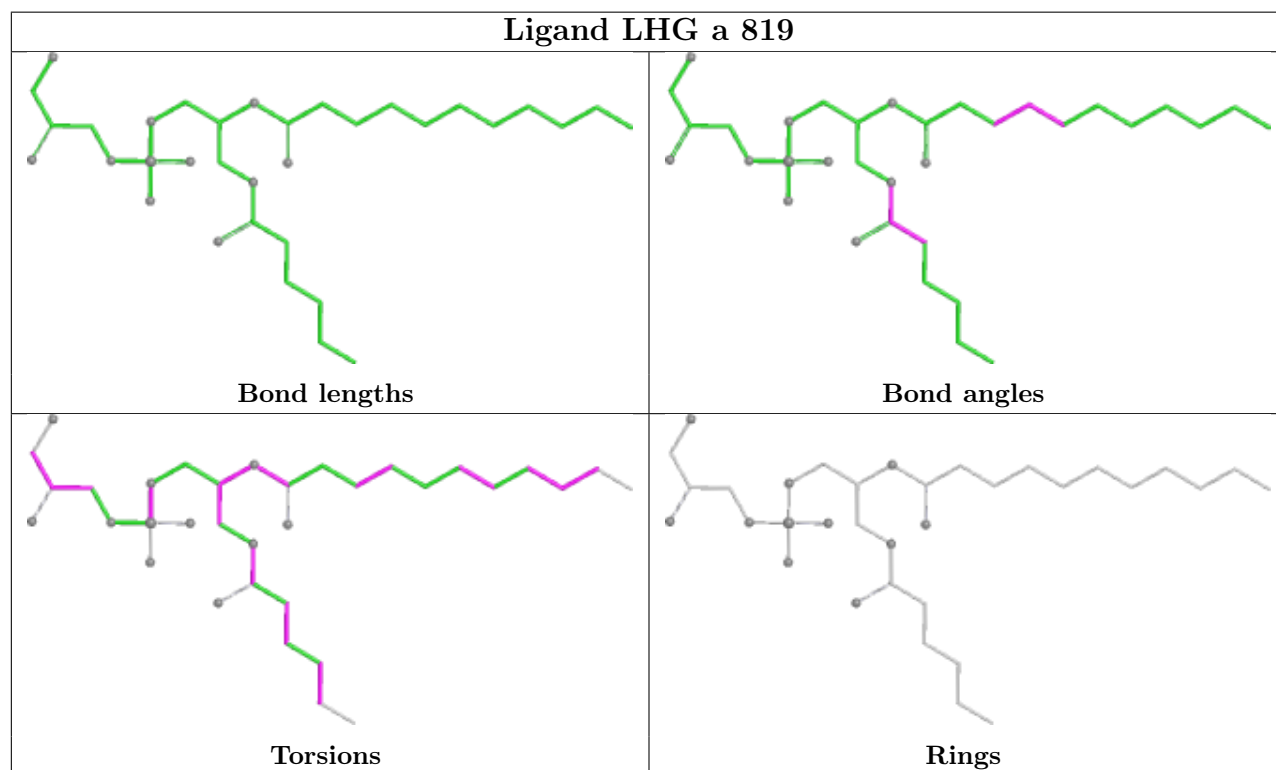
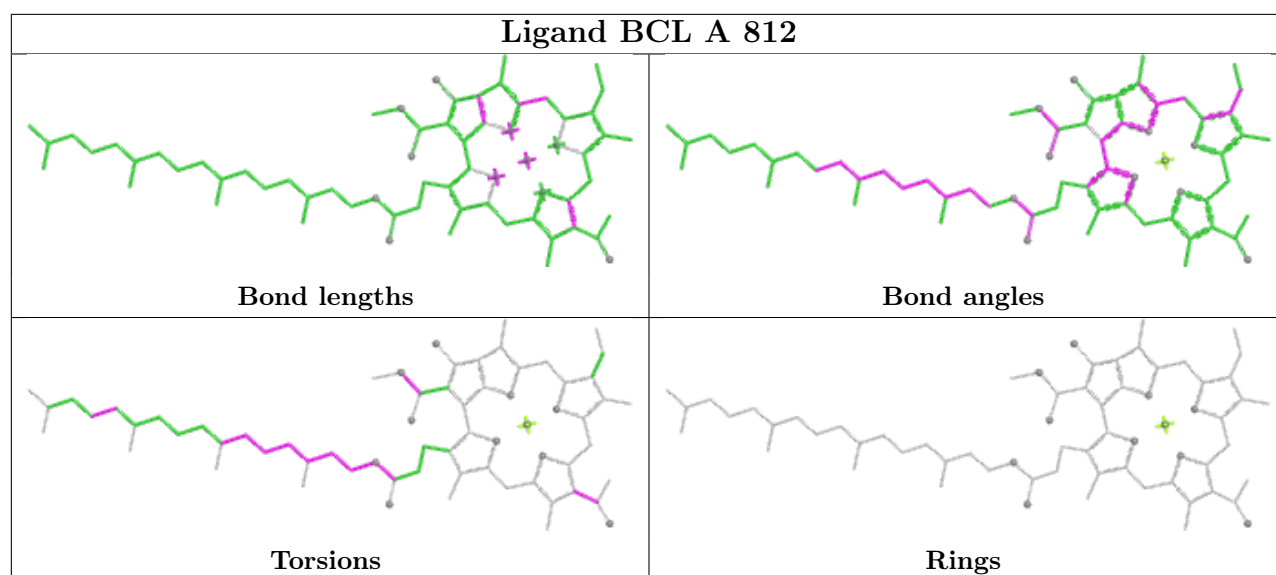
Ligand BCL a 804	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG A 822	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCL A 813	
 Bond lengths	 Bond angles
 Torsions	 Rings

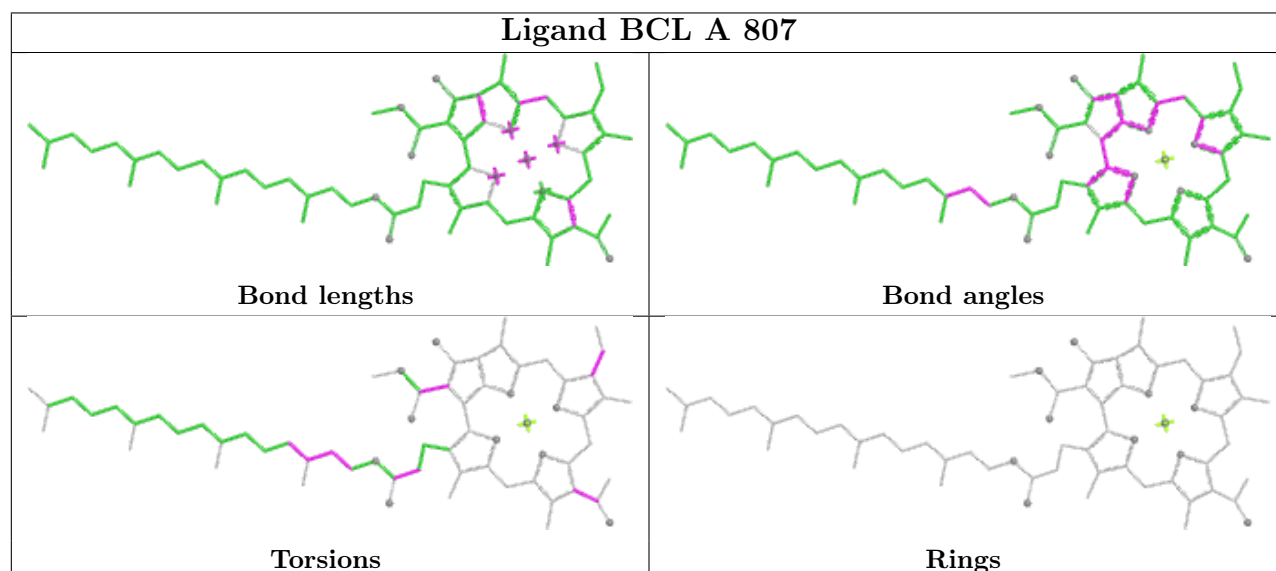
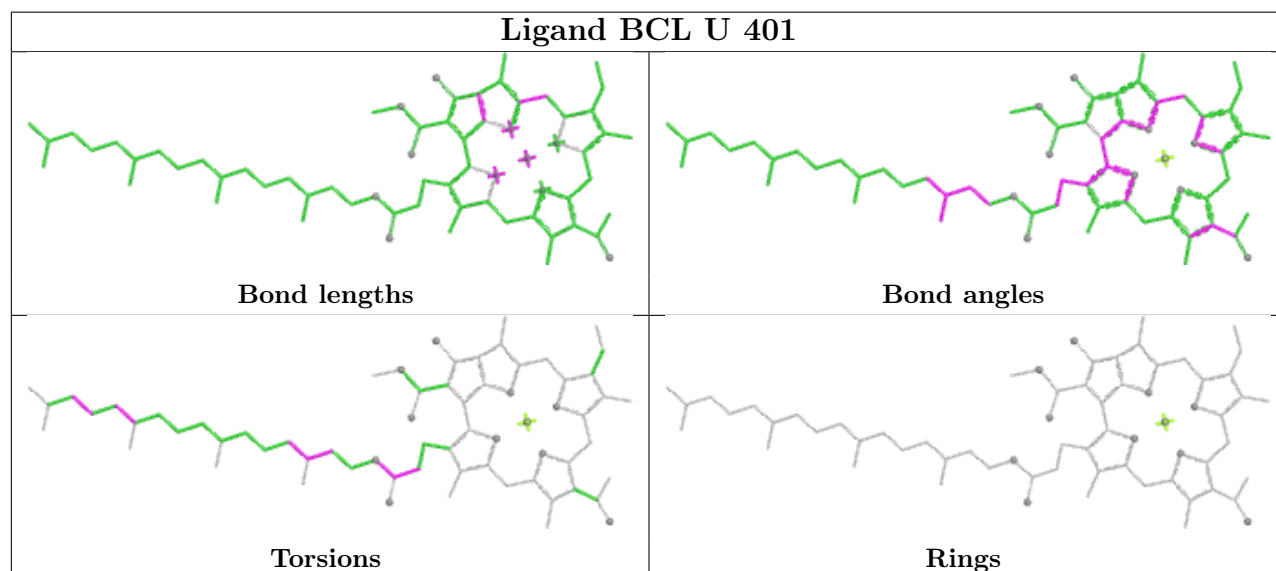
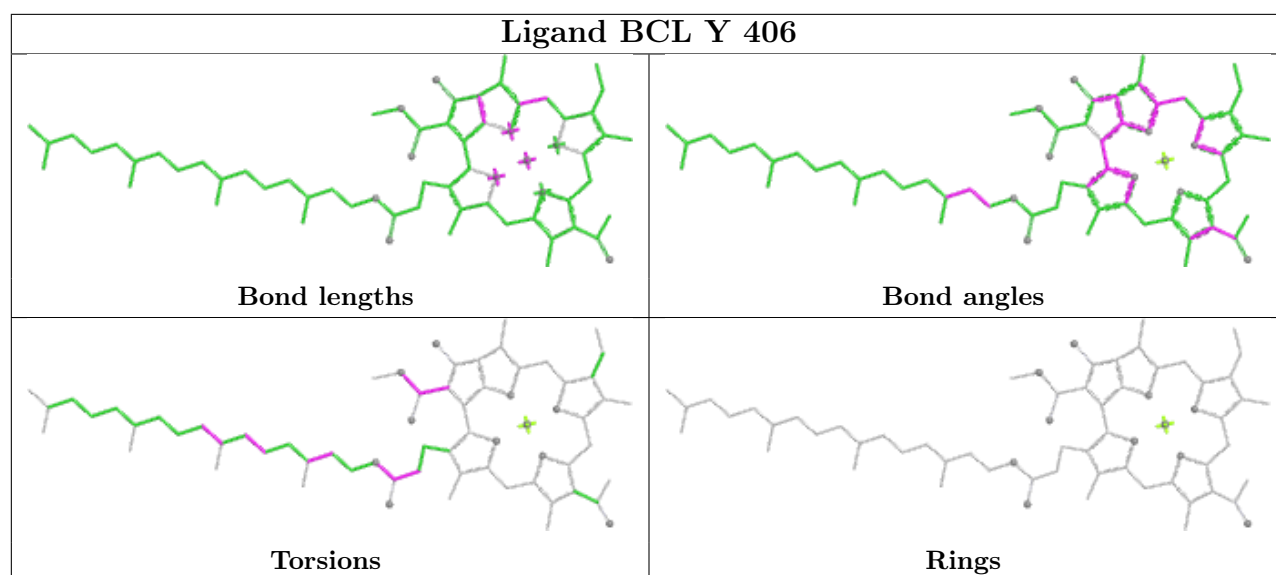
Ligand BCL A 809	
	
Bond lengths	Bond angles
	
Torsions	Rings

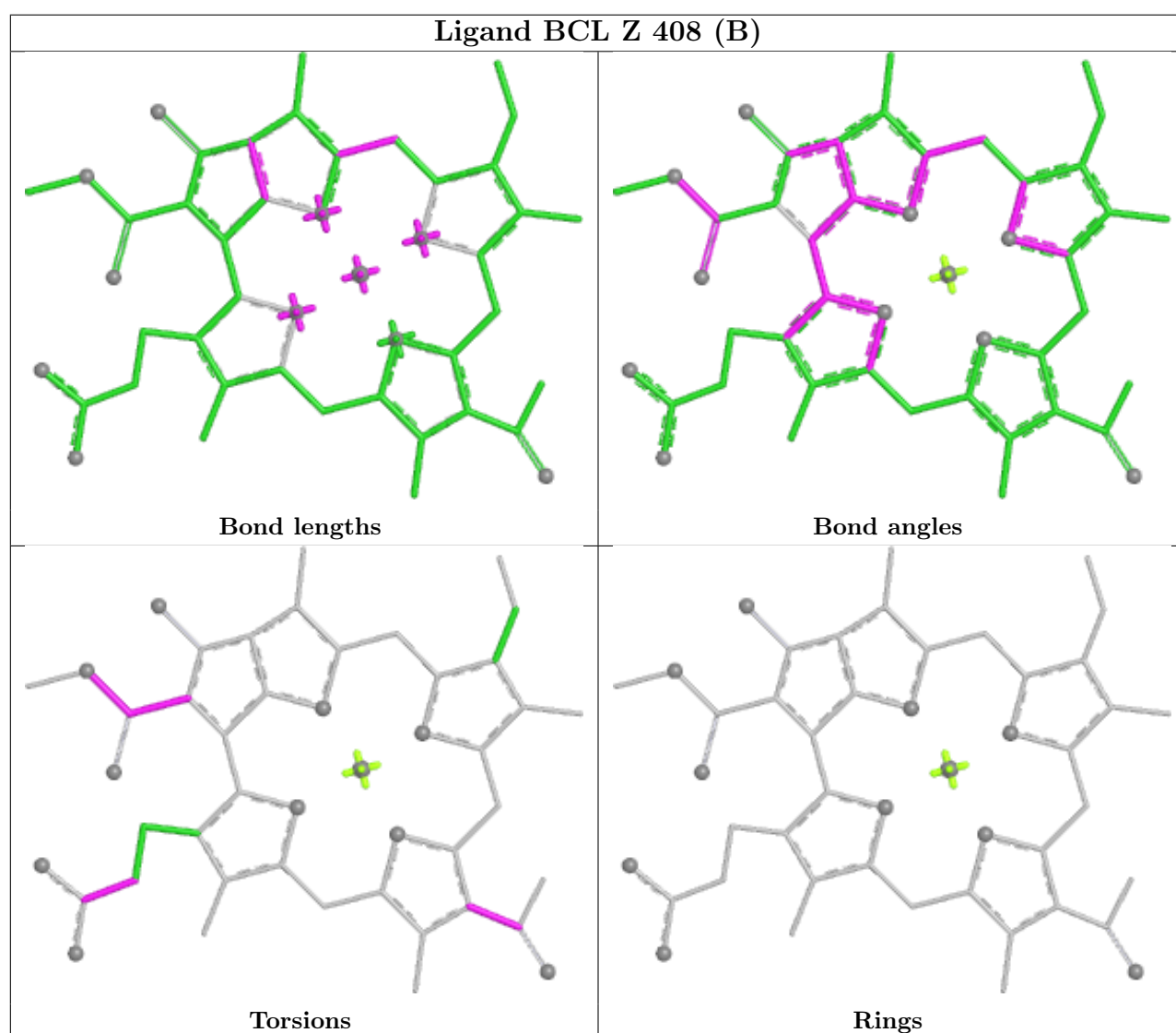
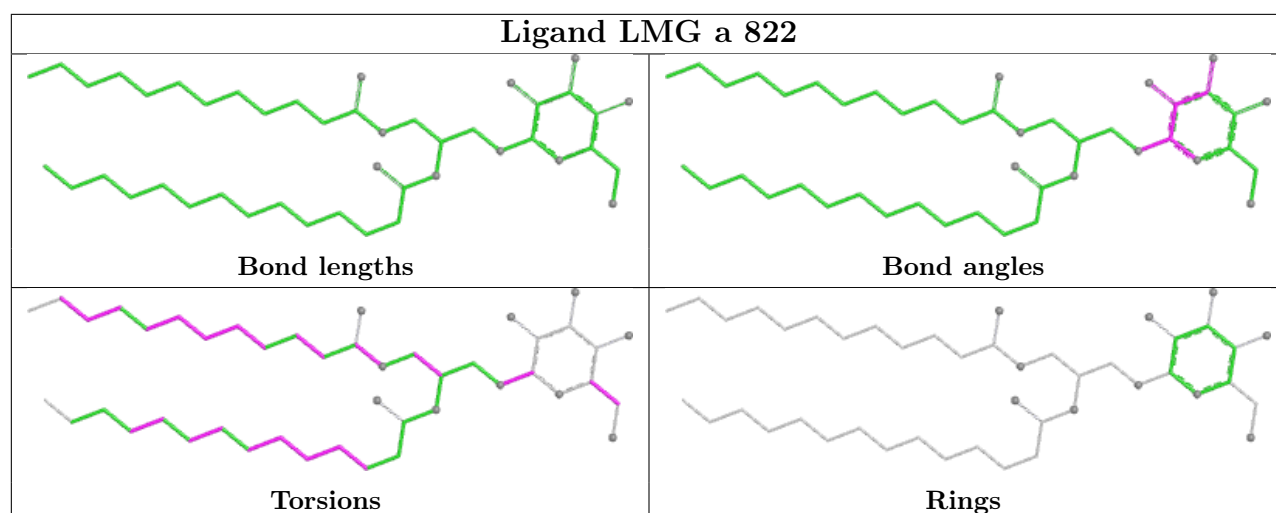
Ligand F39 C 301	
	
Bond lengths	Bond angles
	
Torsions	Rings

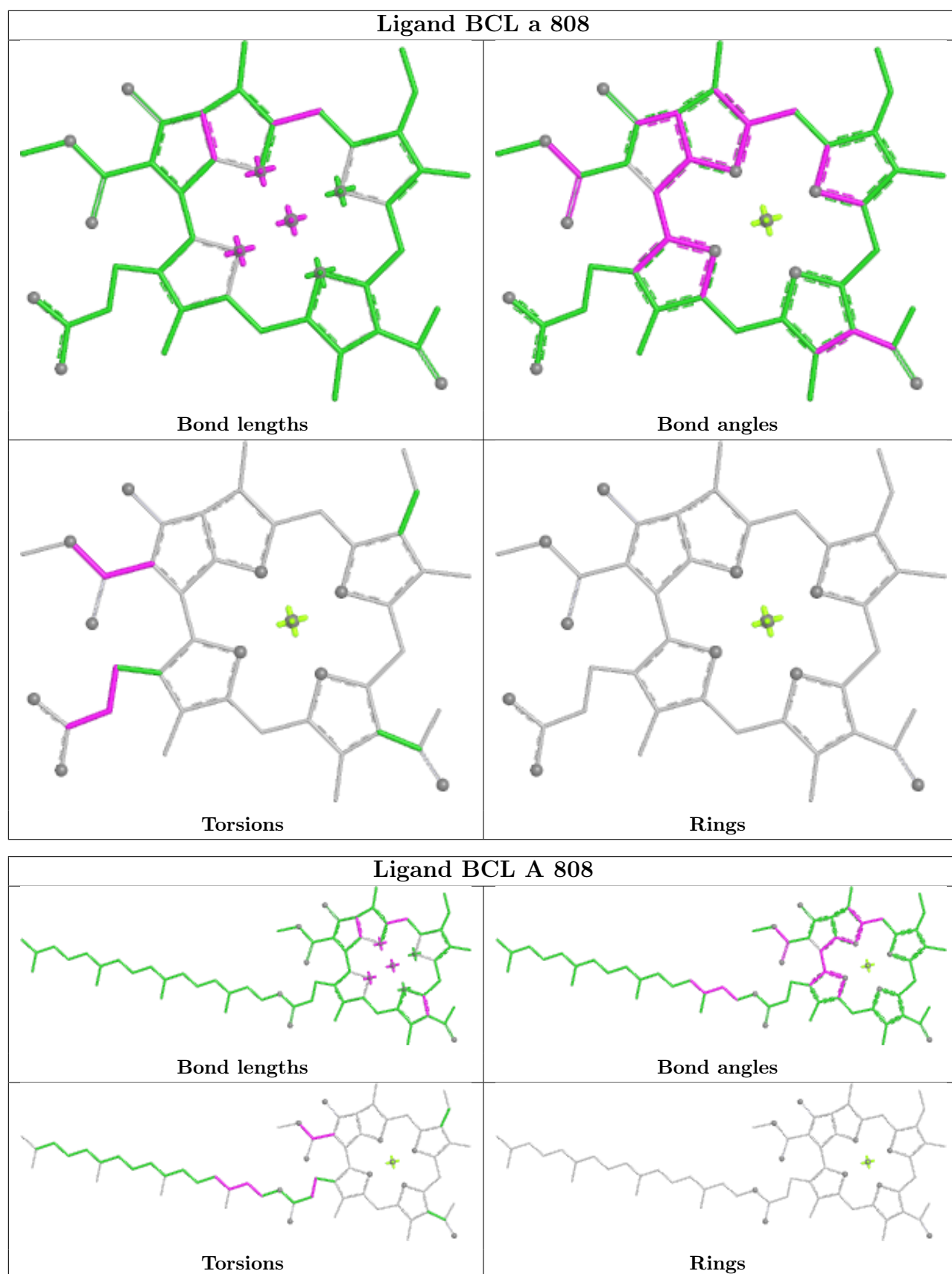


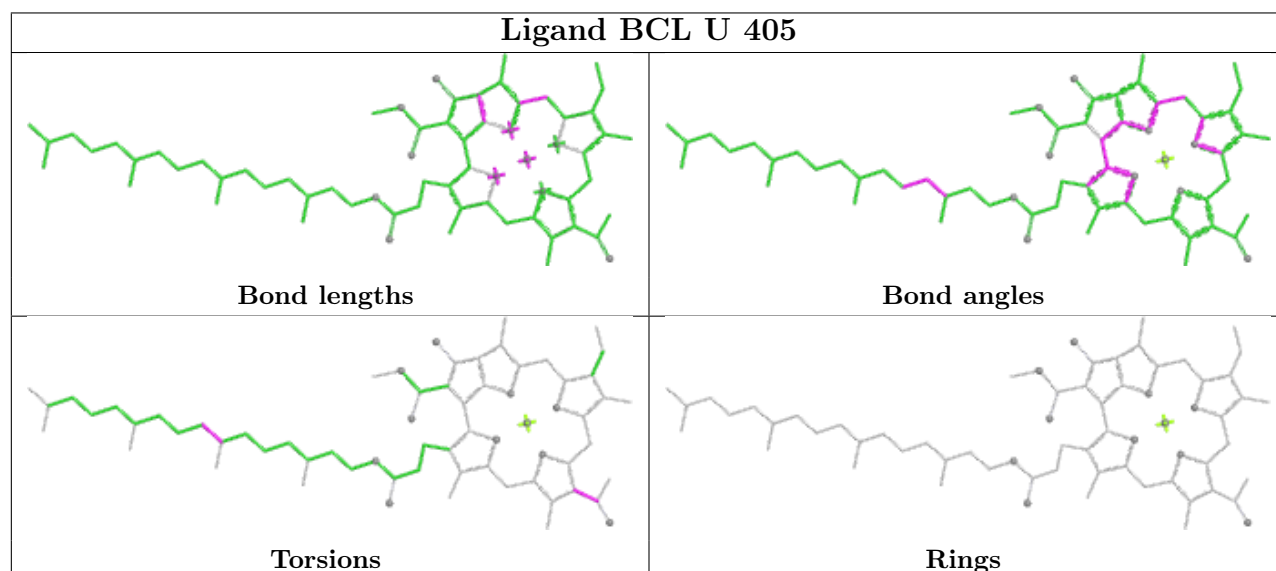
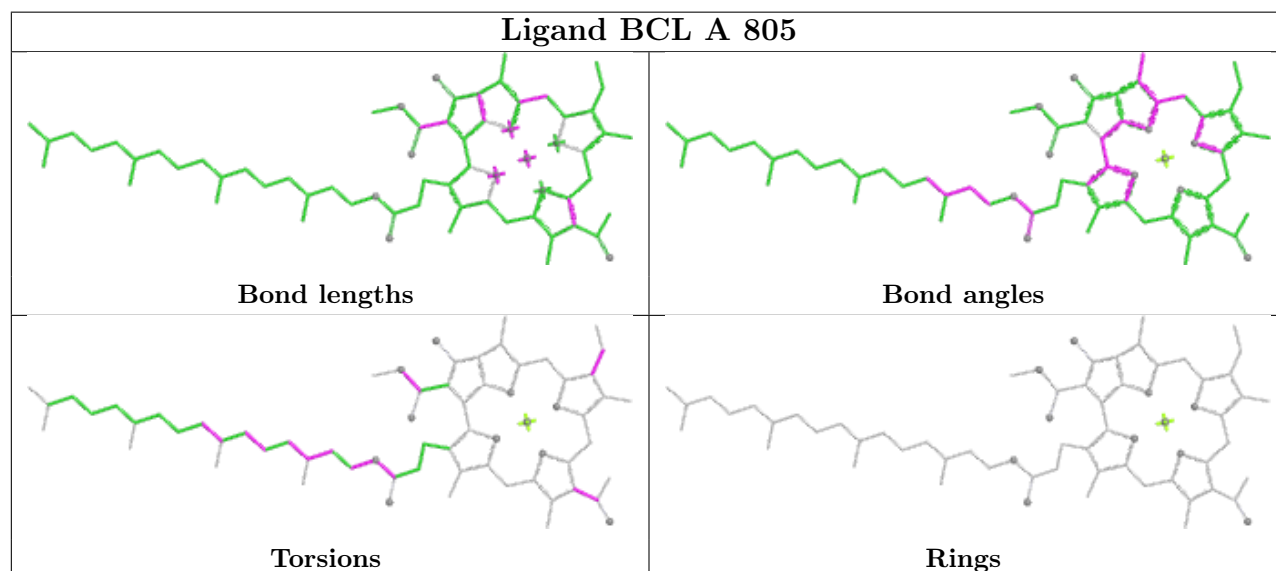
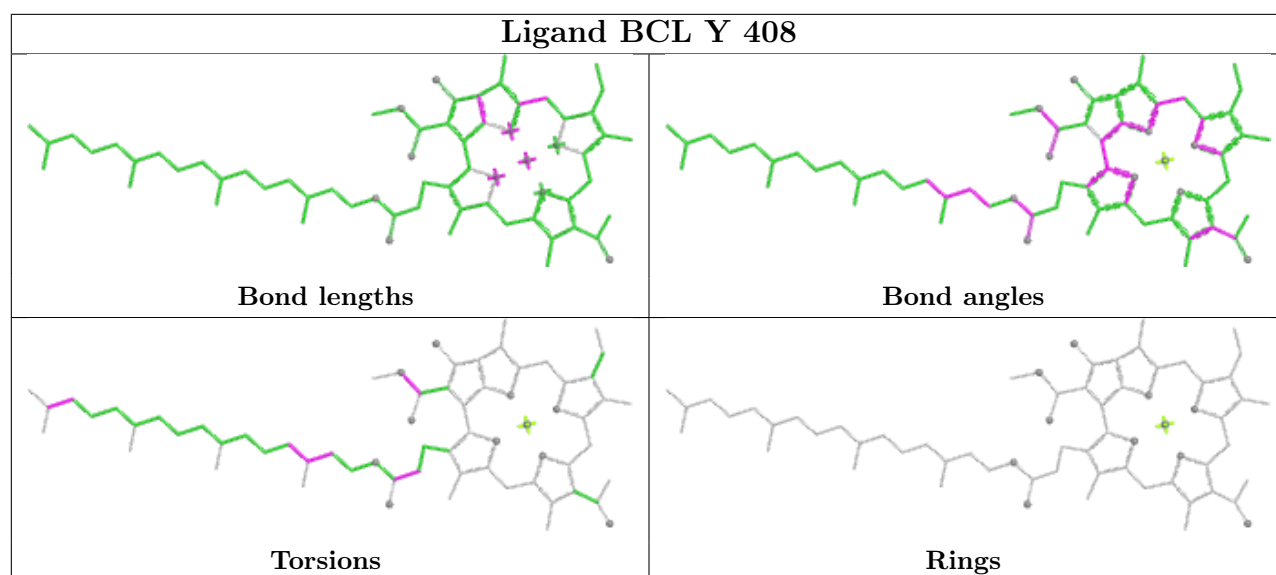
Ligand BCL A 810	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCL V 401	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand GS0 A 801	
 Bond lengths	 Bond angles
 Torsions	 Rings

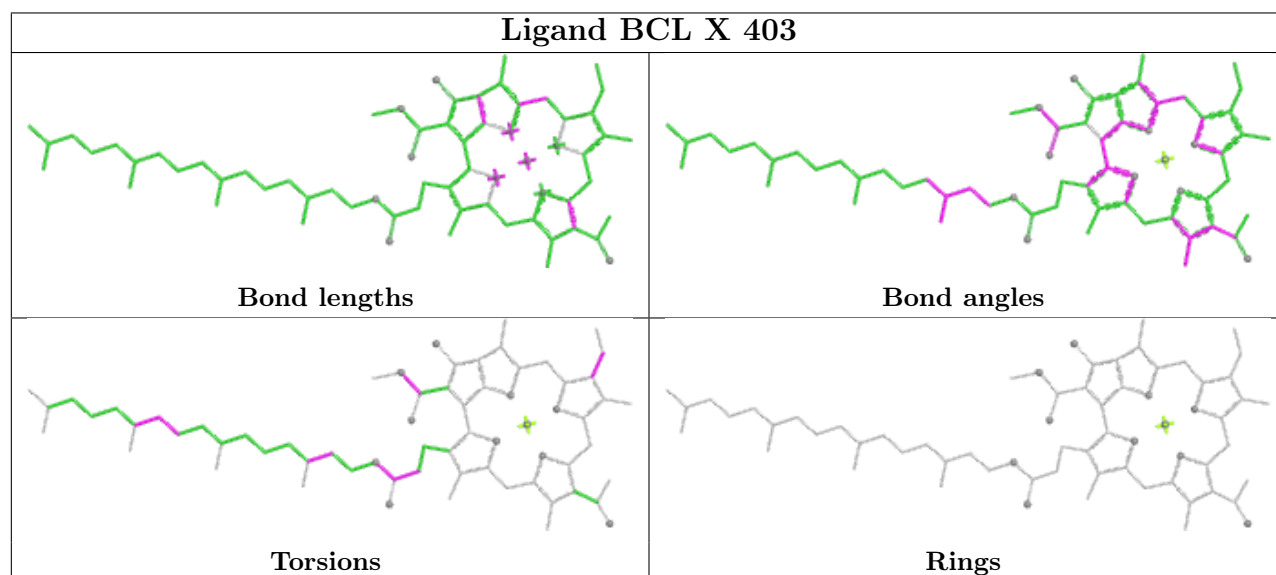
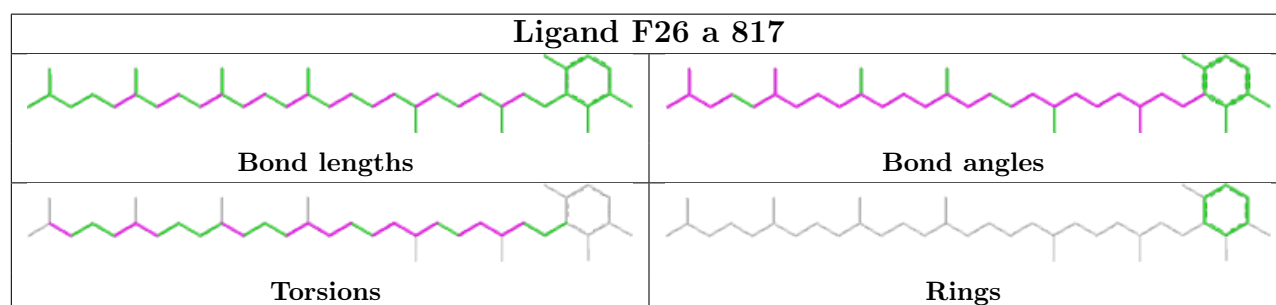
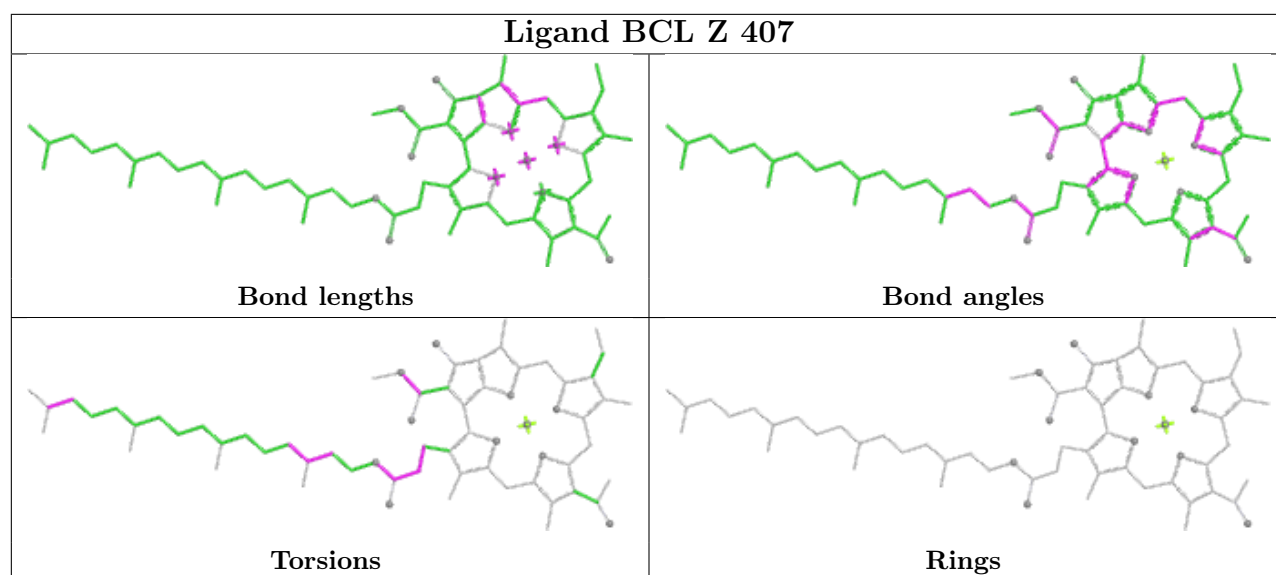


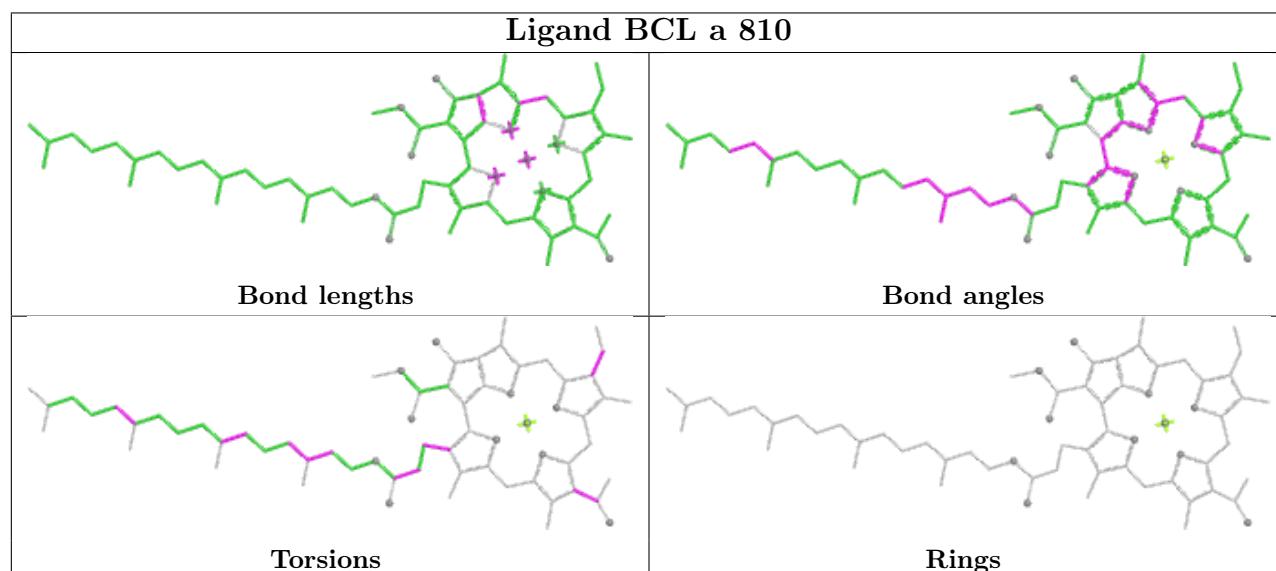
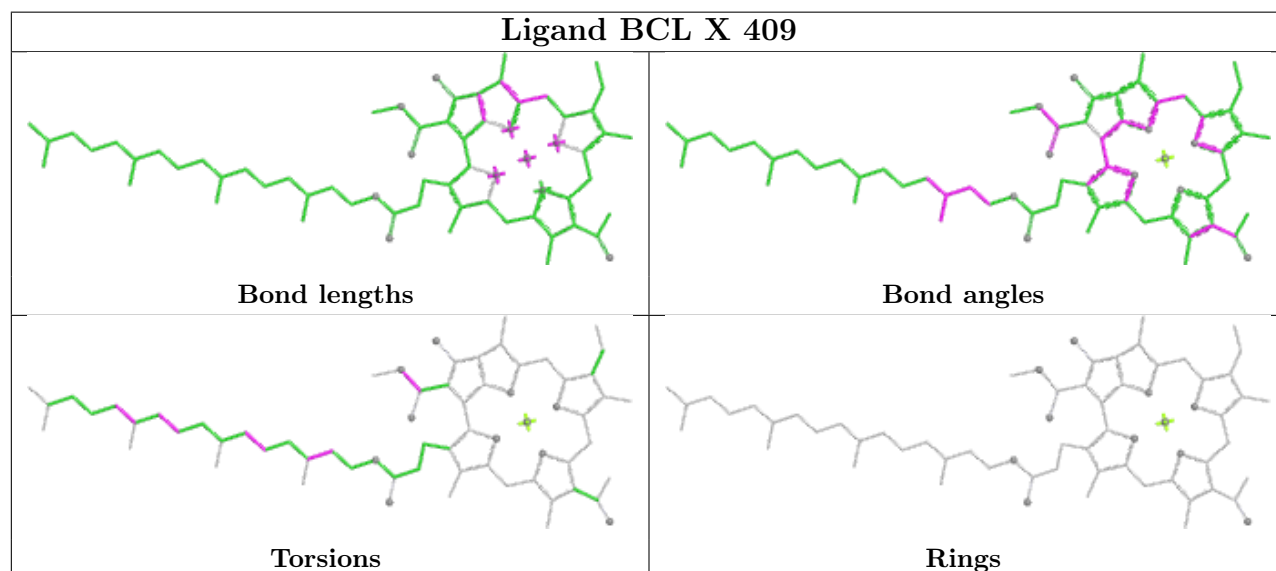
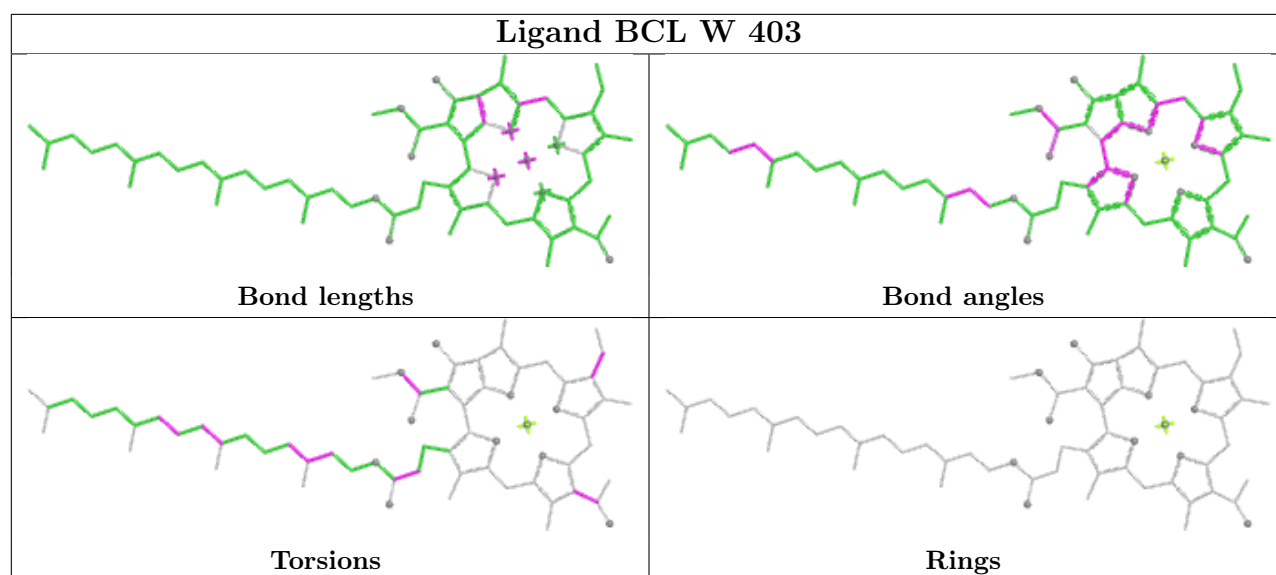


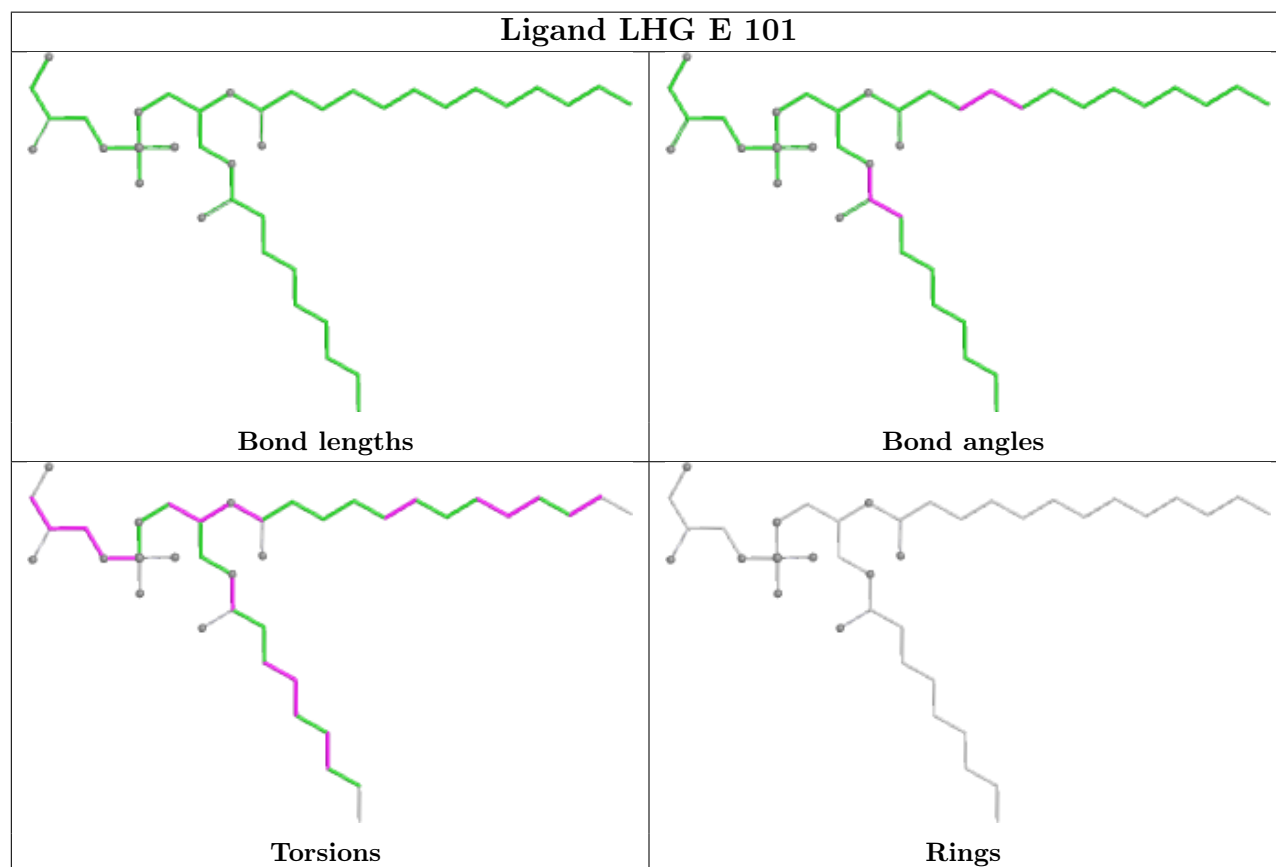
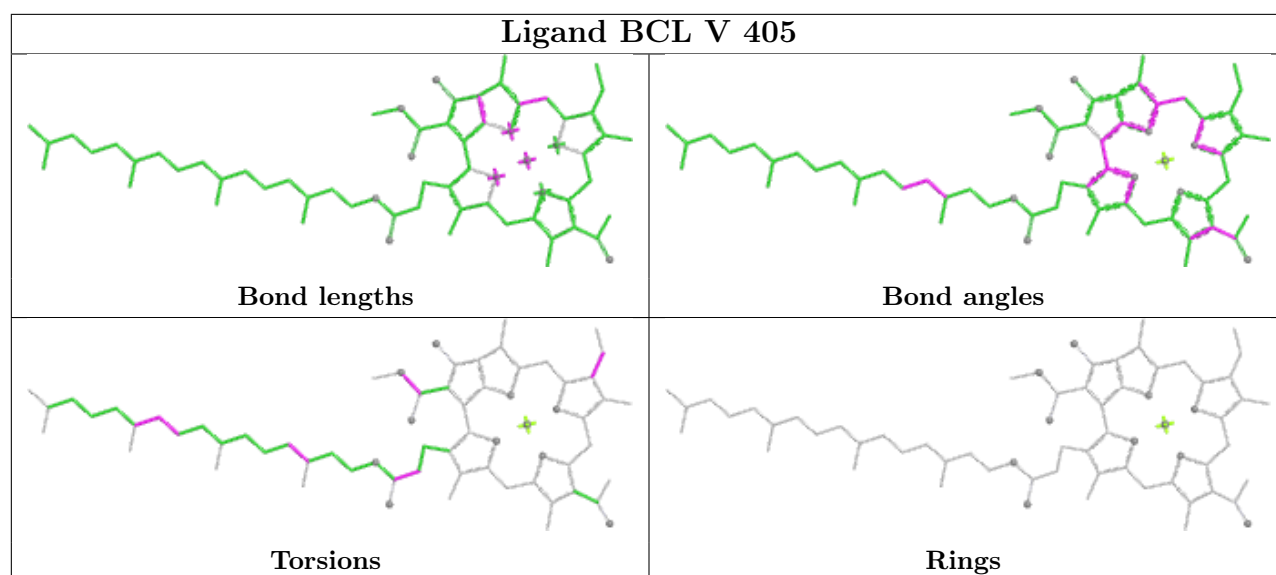


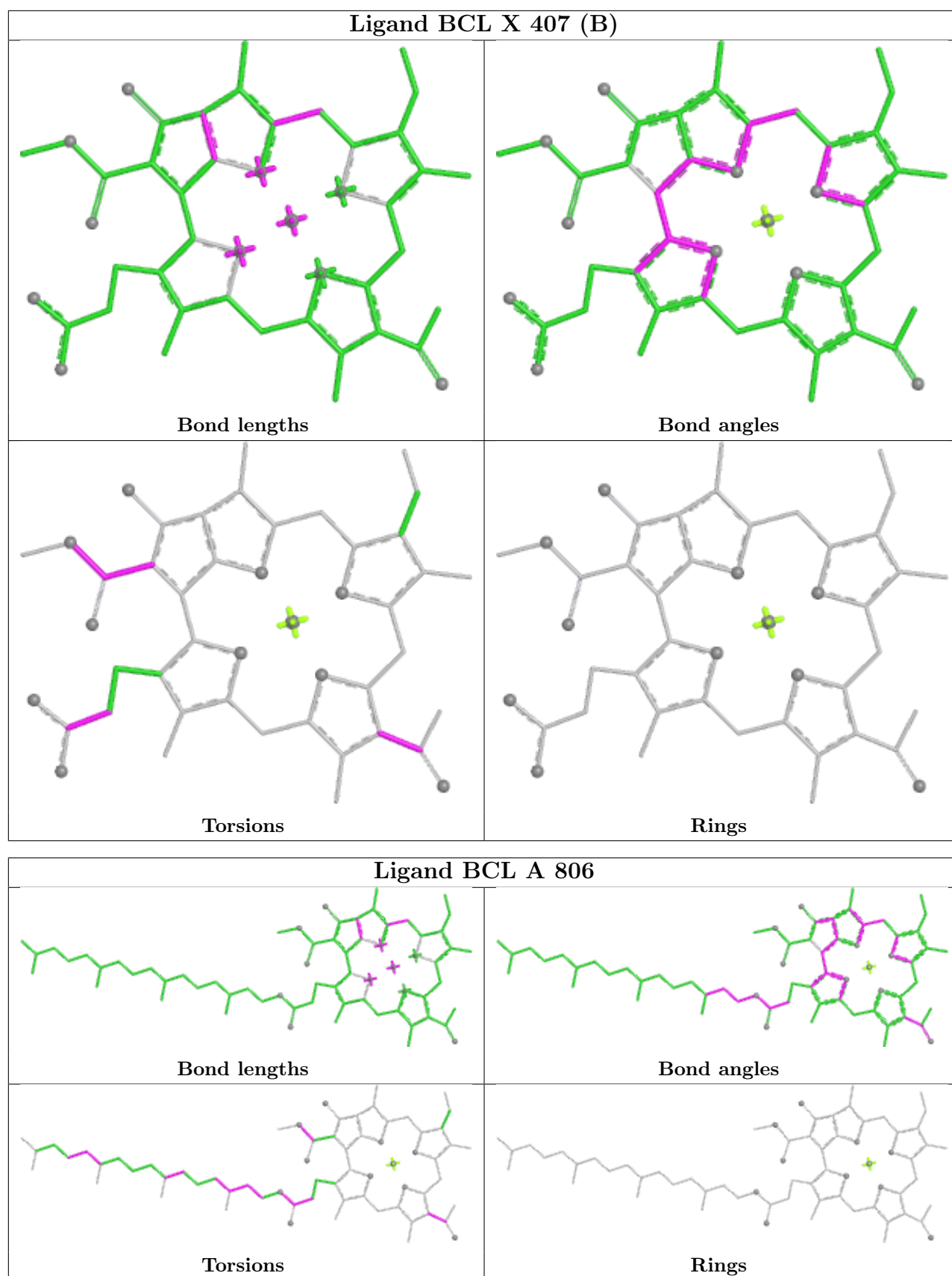


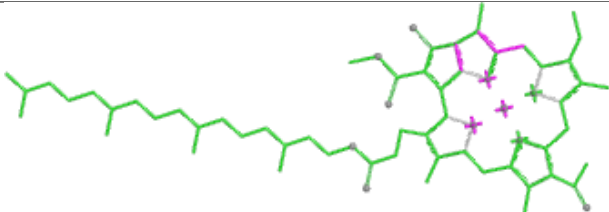
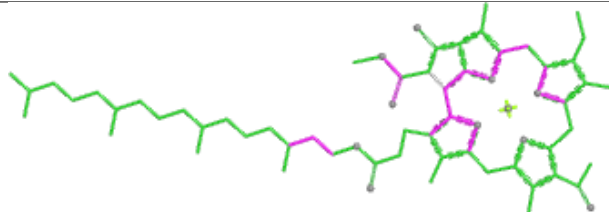
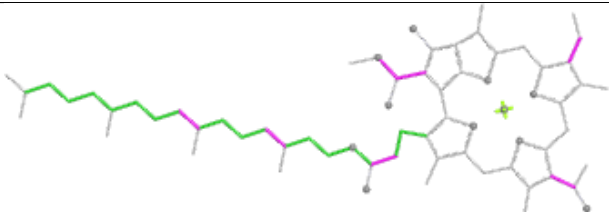
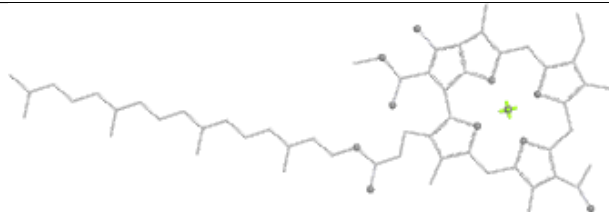


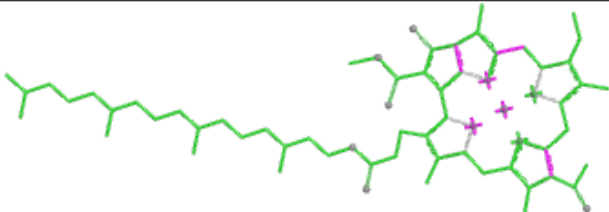
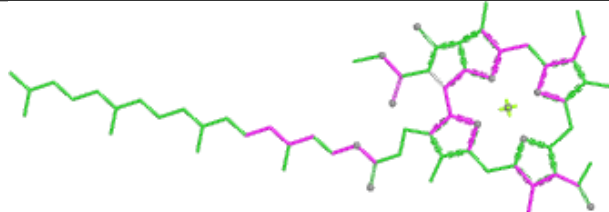
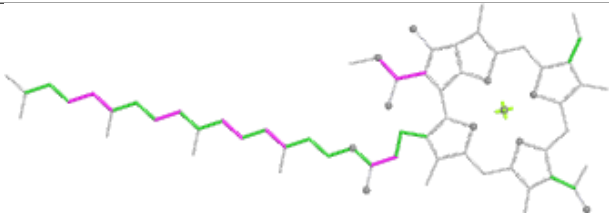
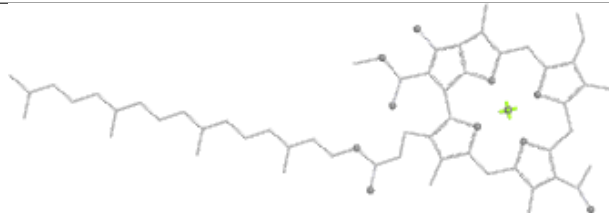


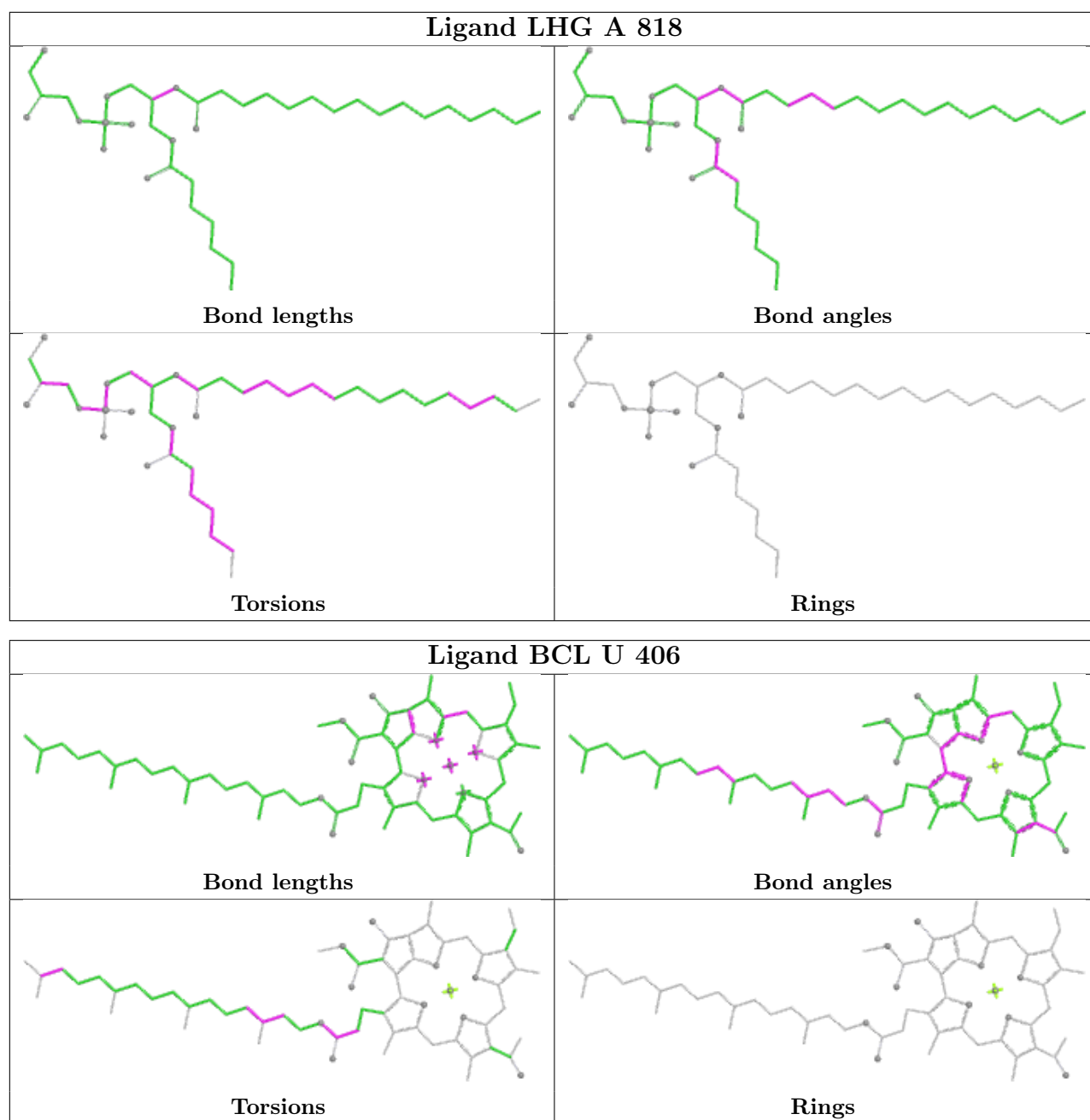


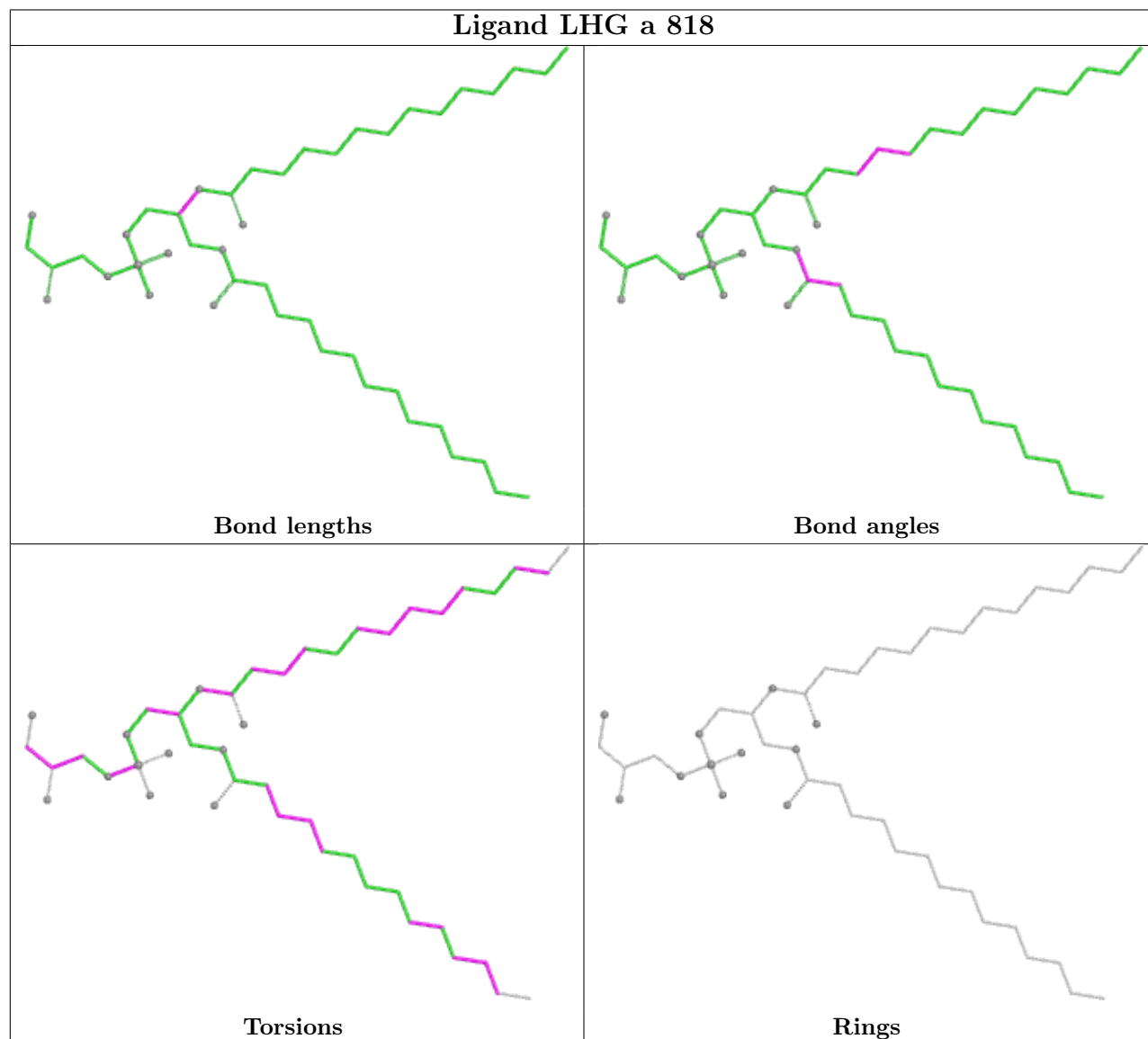
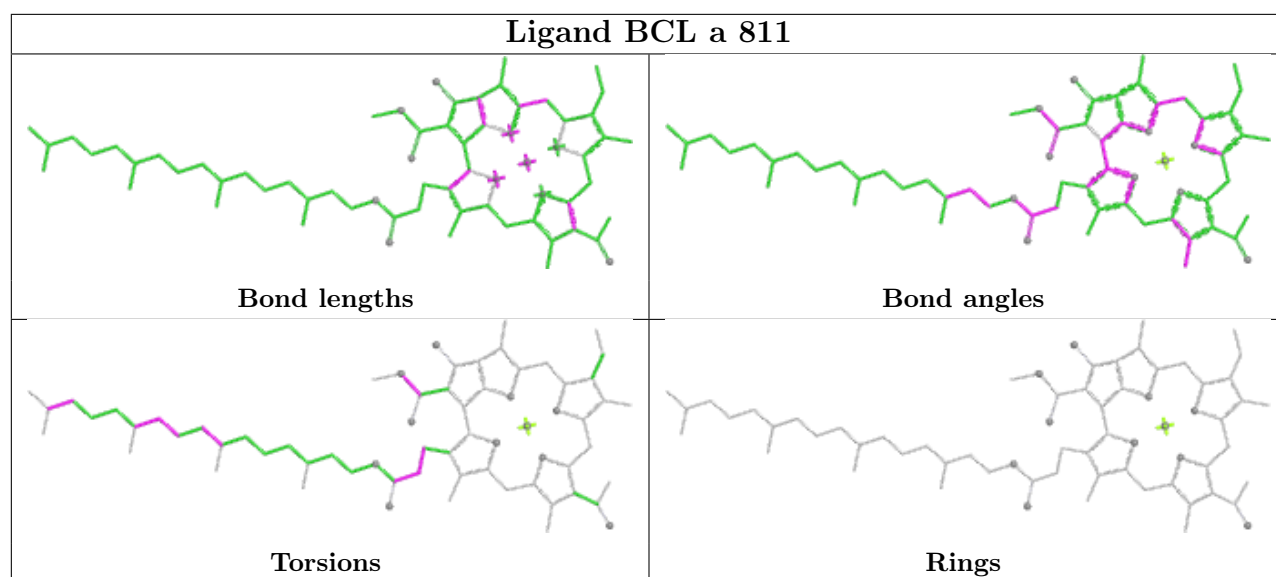


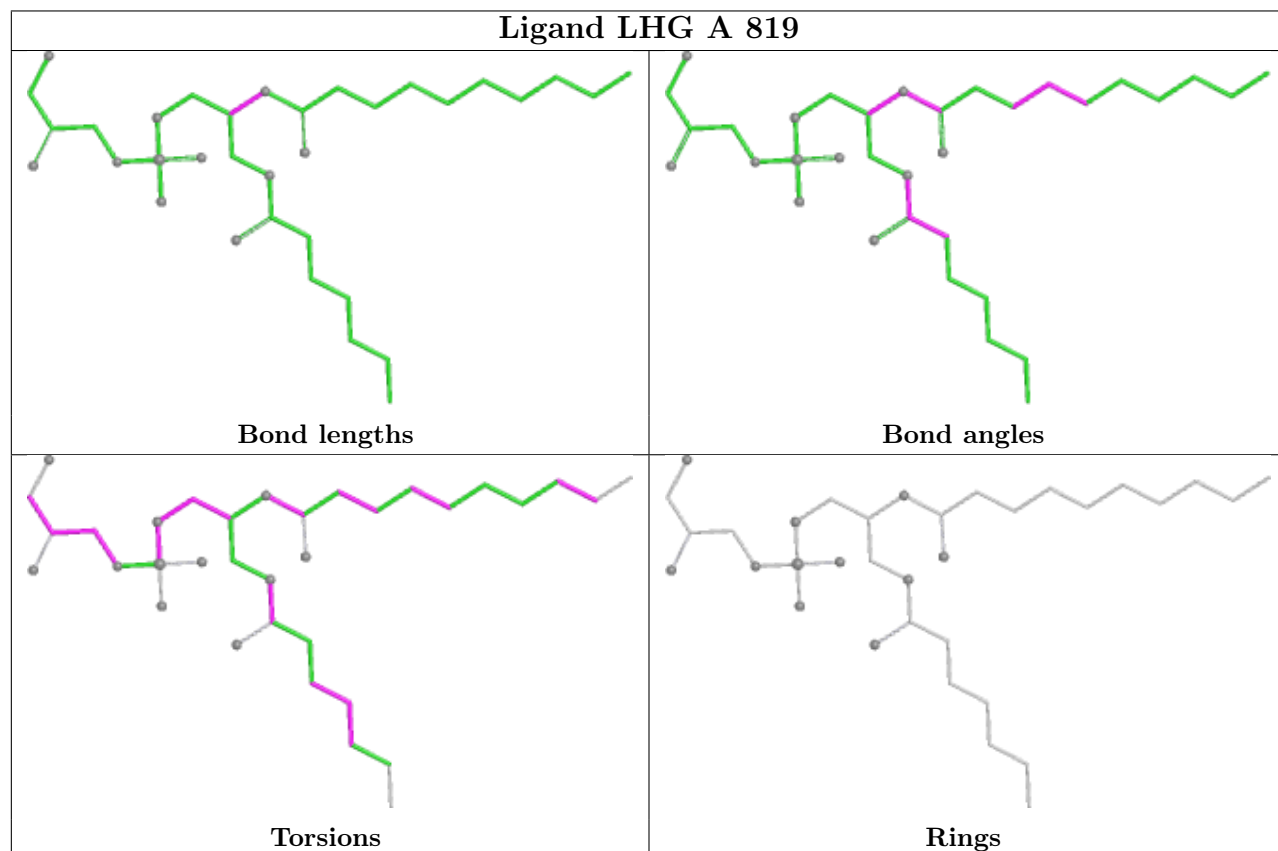
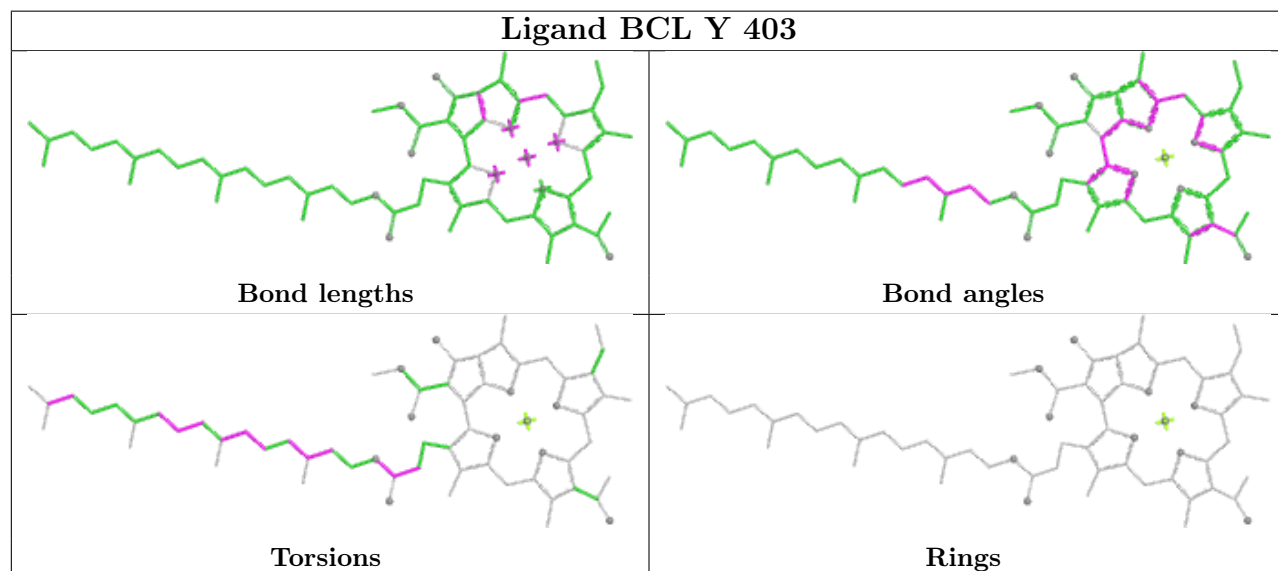
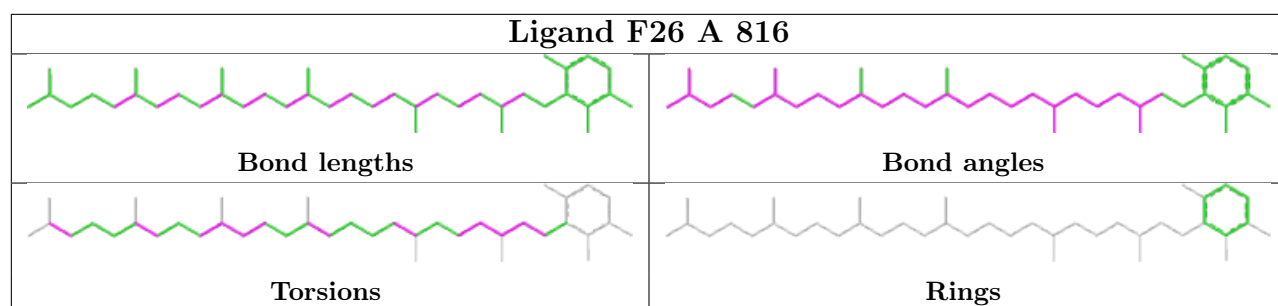


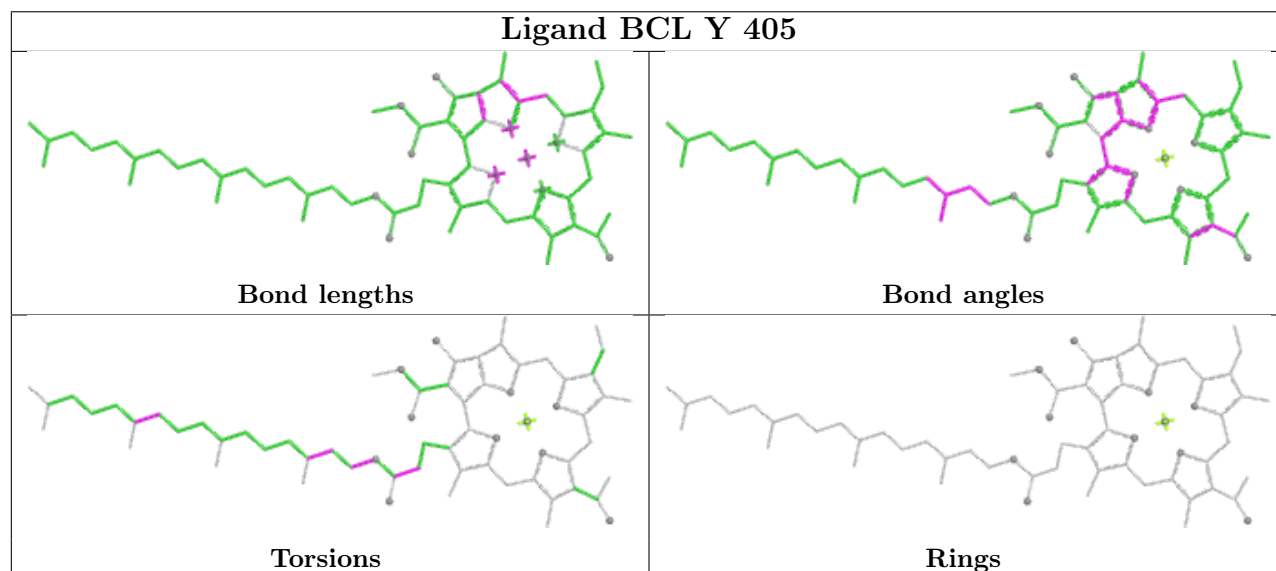
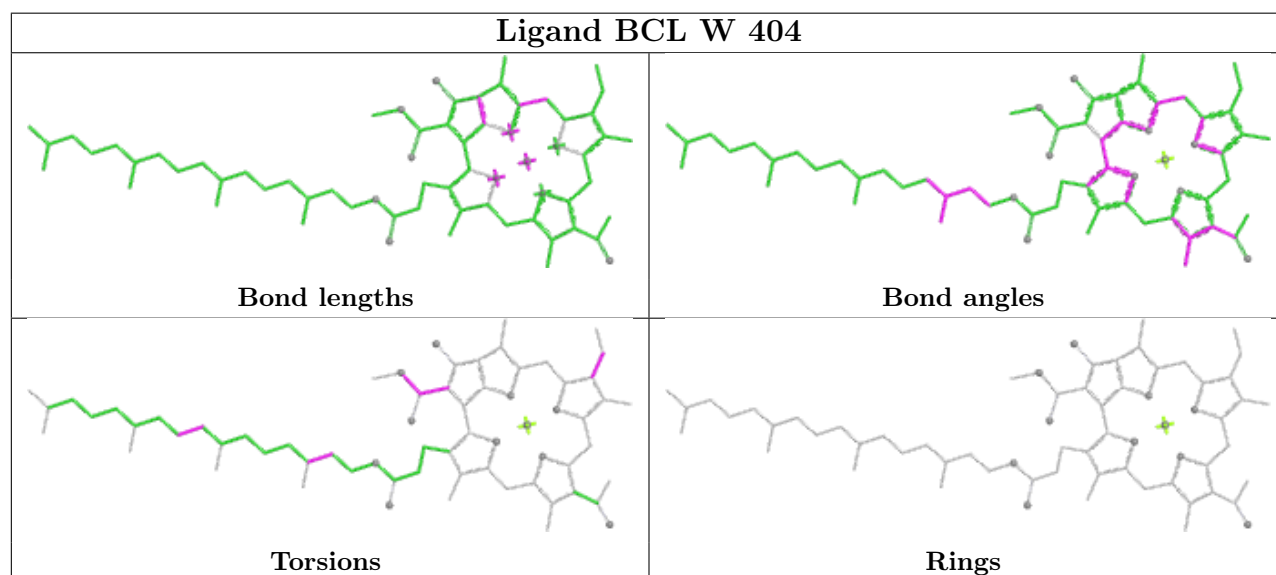
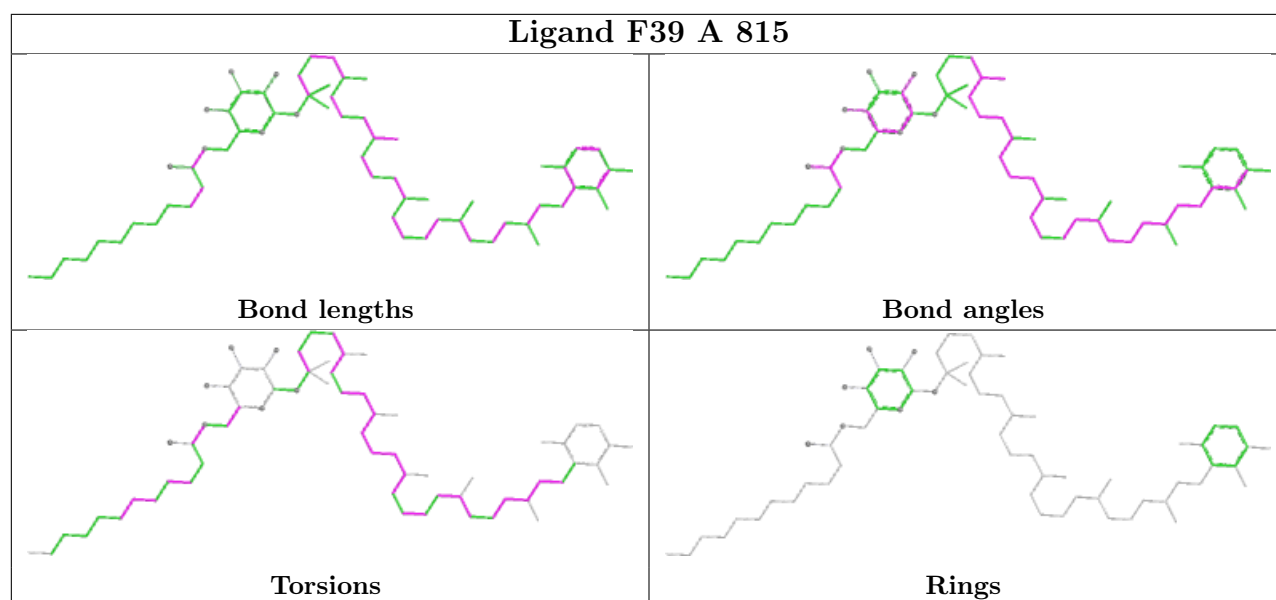
Ligand BCL Z 403	
	
Bond lengths	Bond angles
	
Torsions	Rings

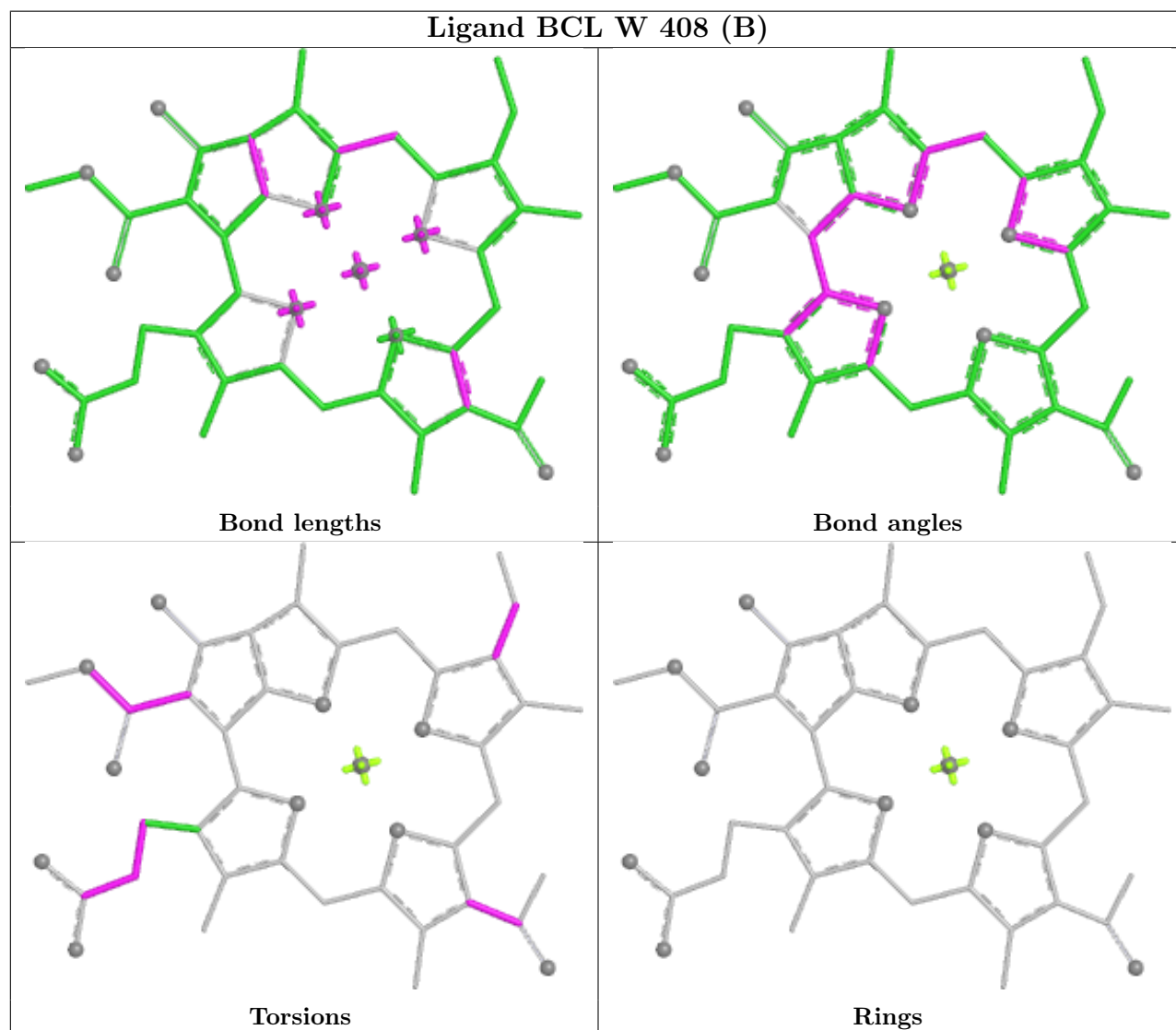
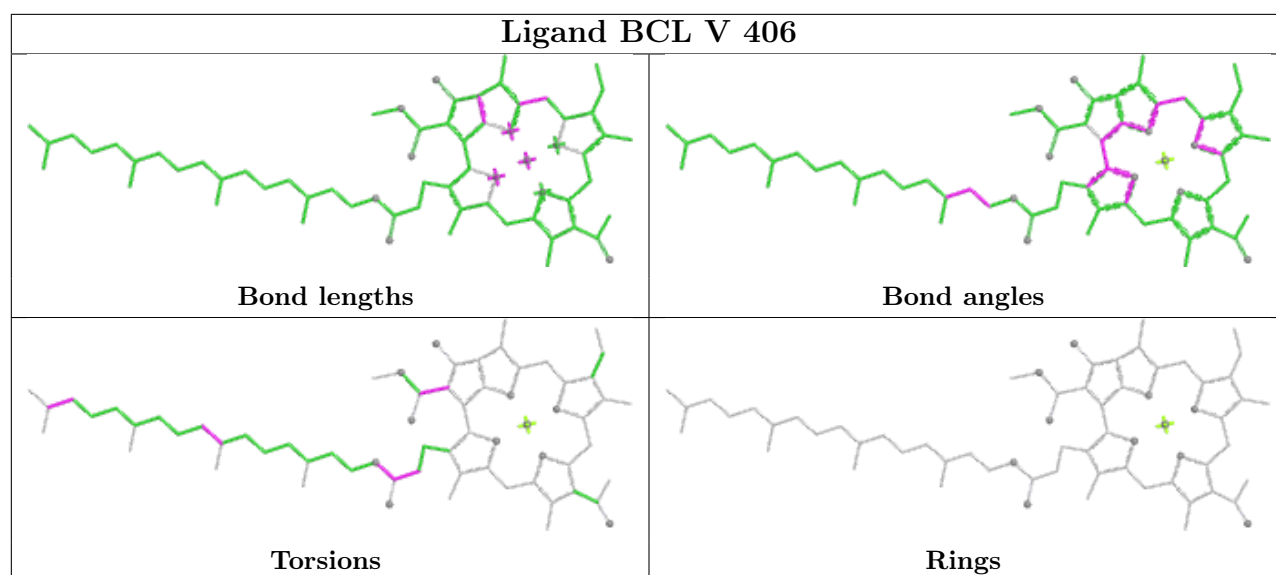
Ligand BCL U 403	
	
Bond lengths	Bond angles
	
Torsions	Rings

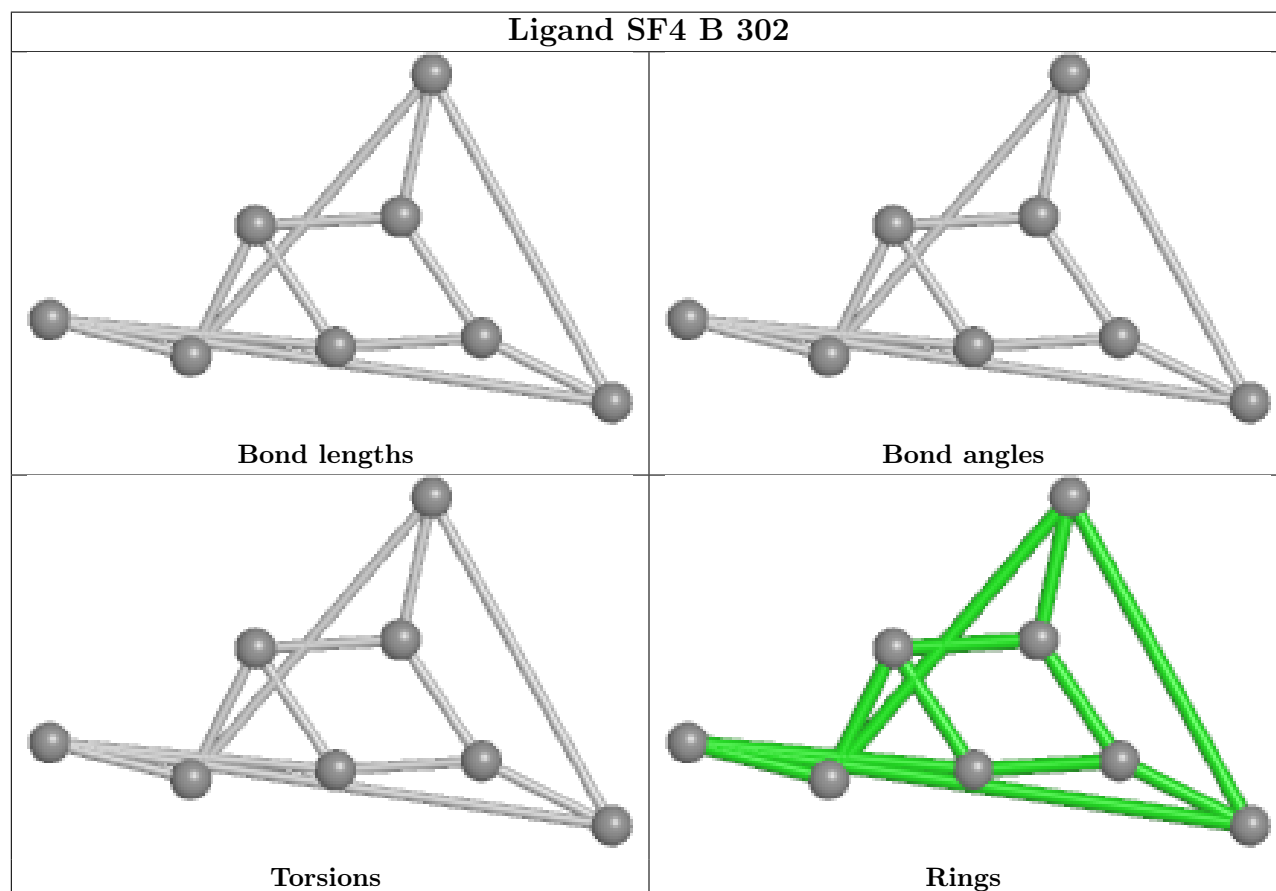
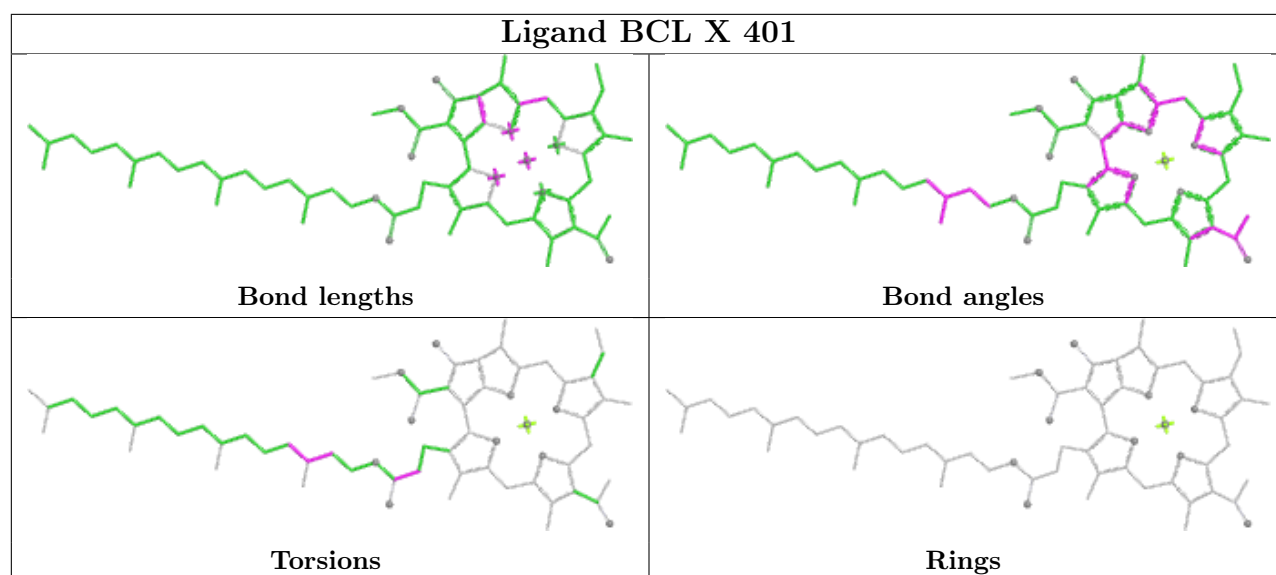


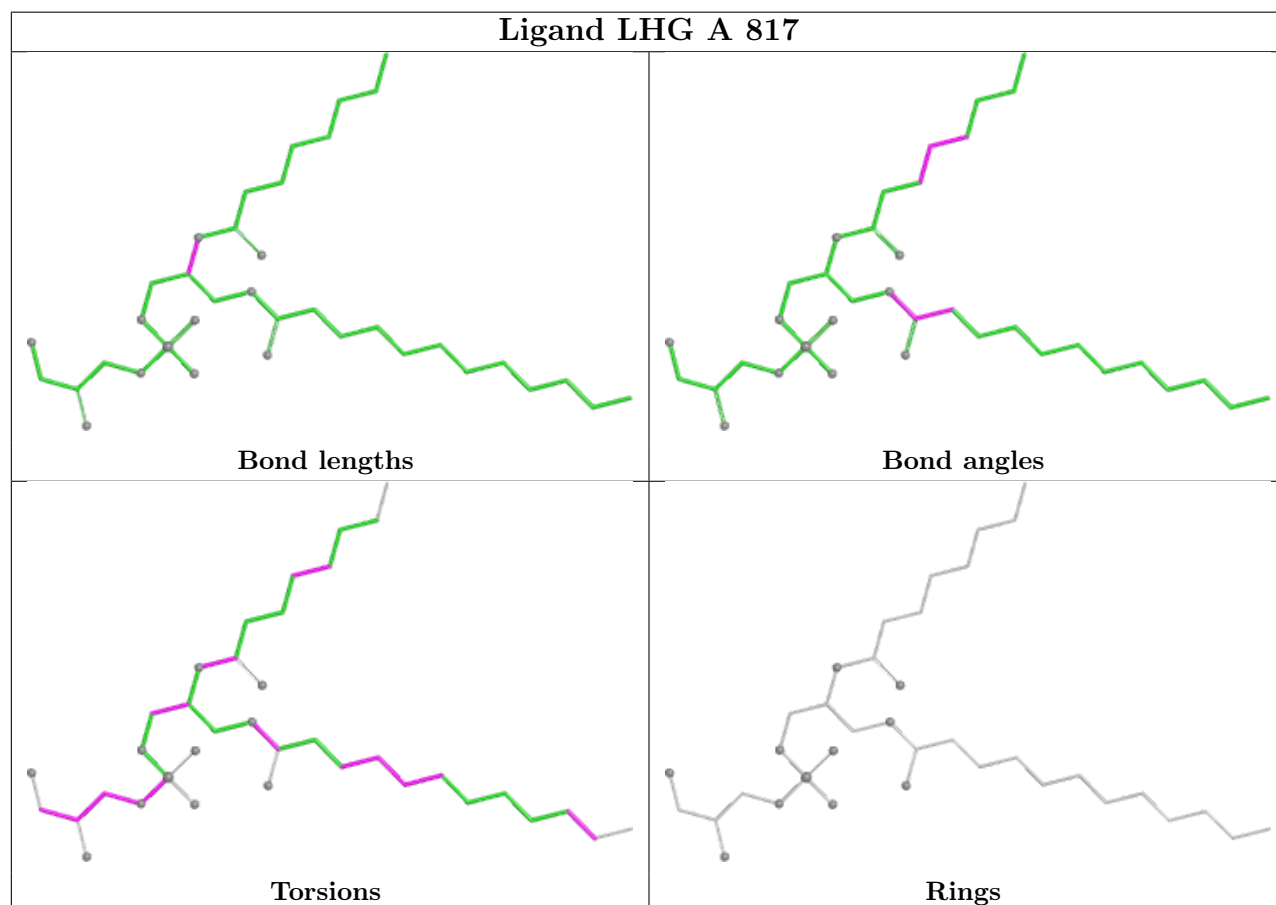
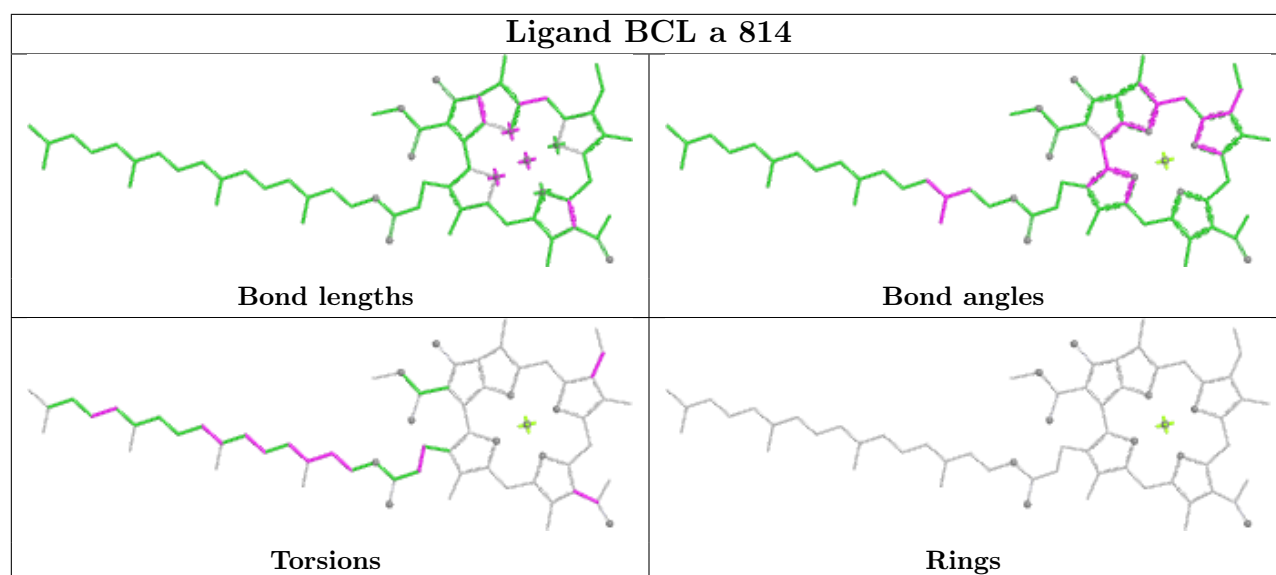


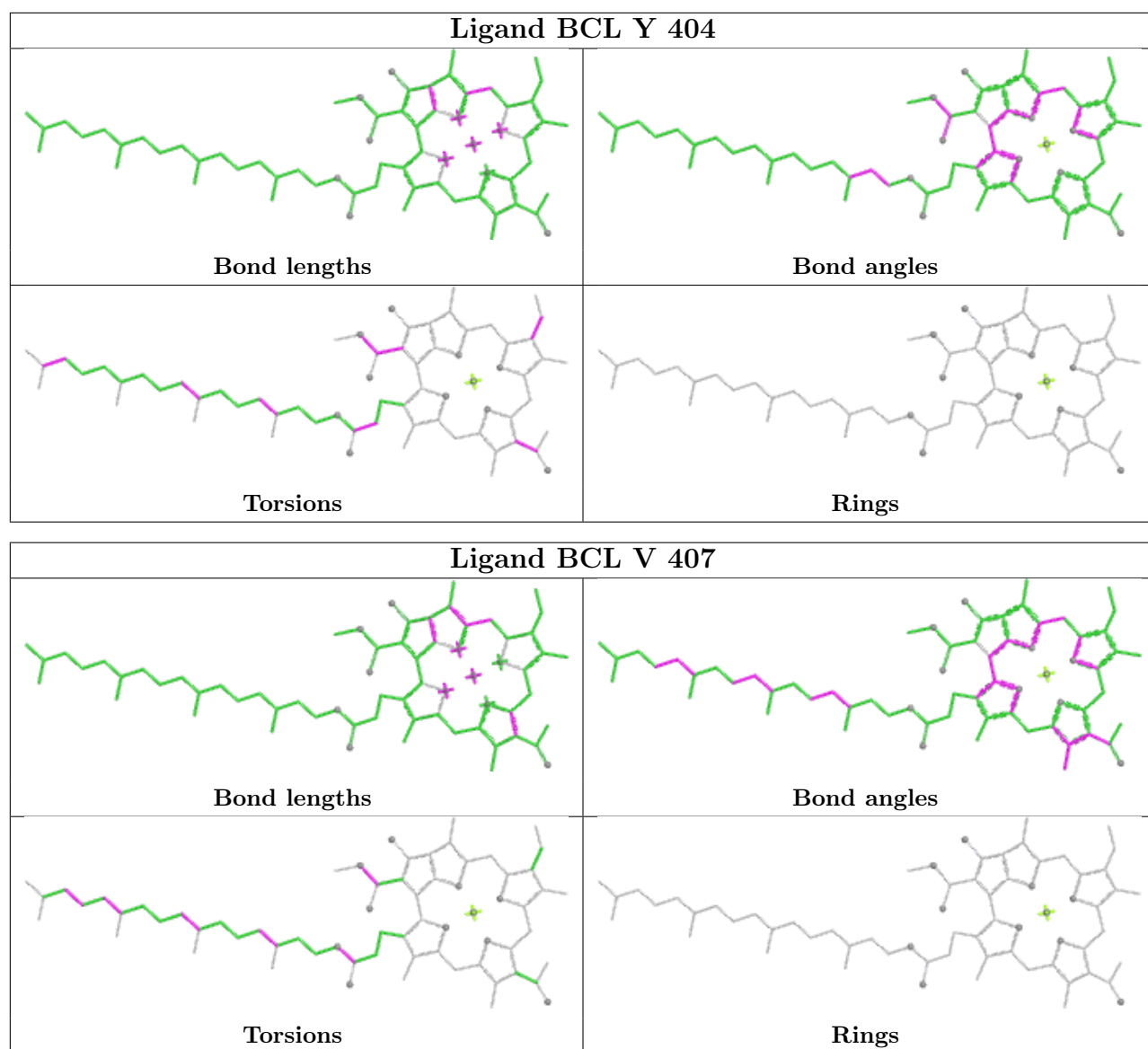


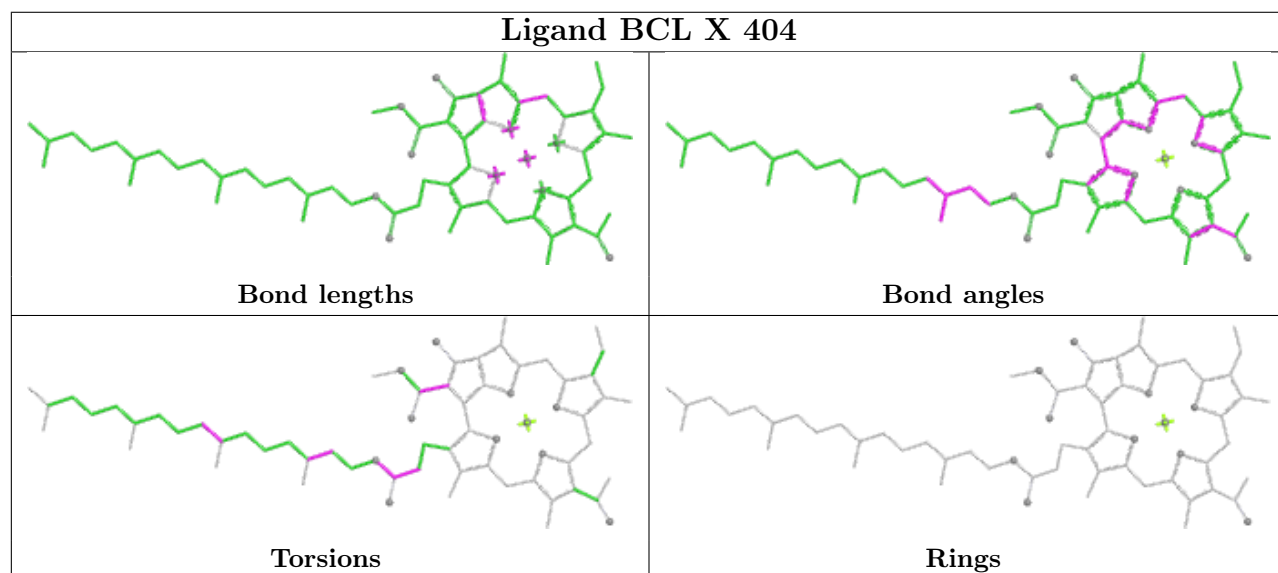
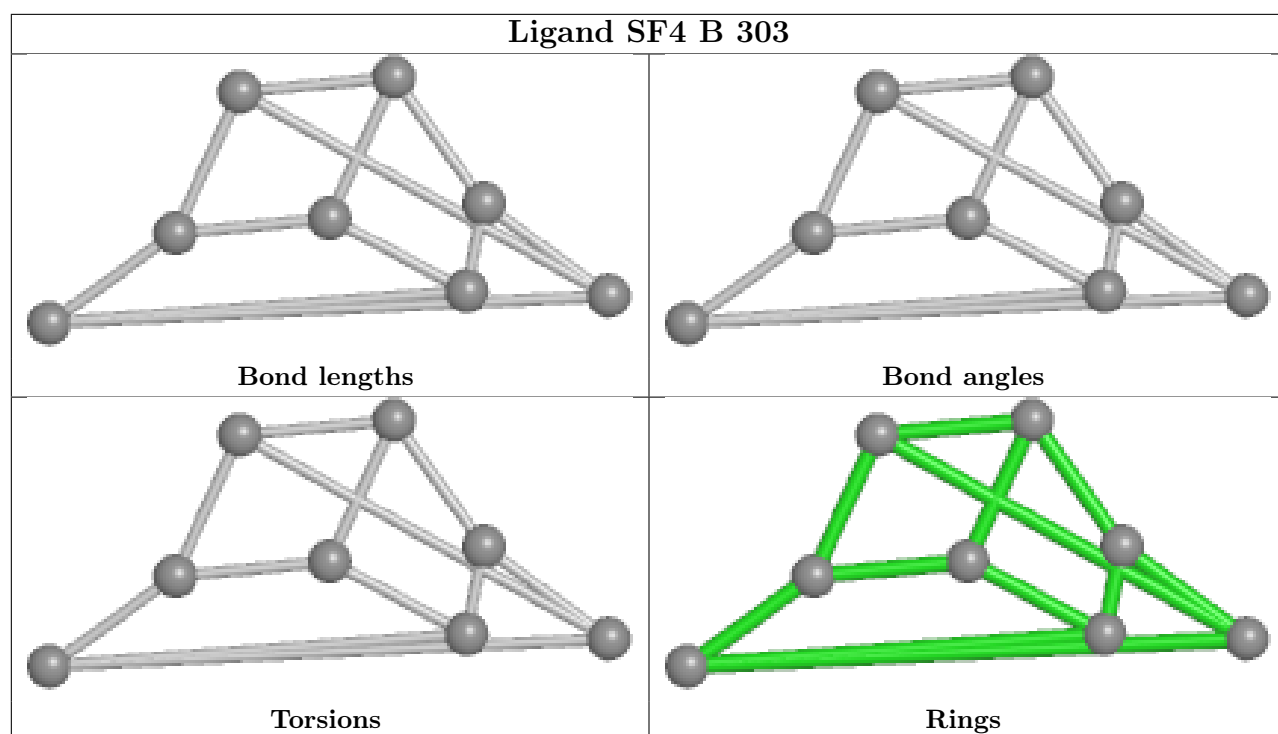


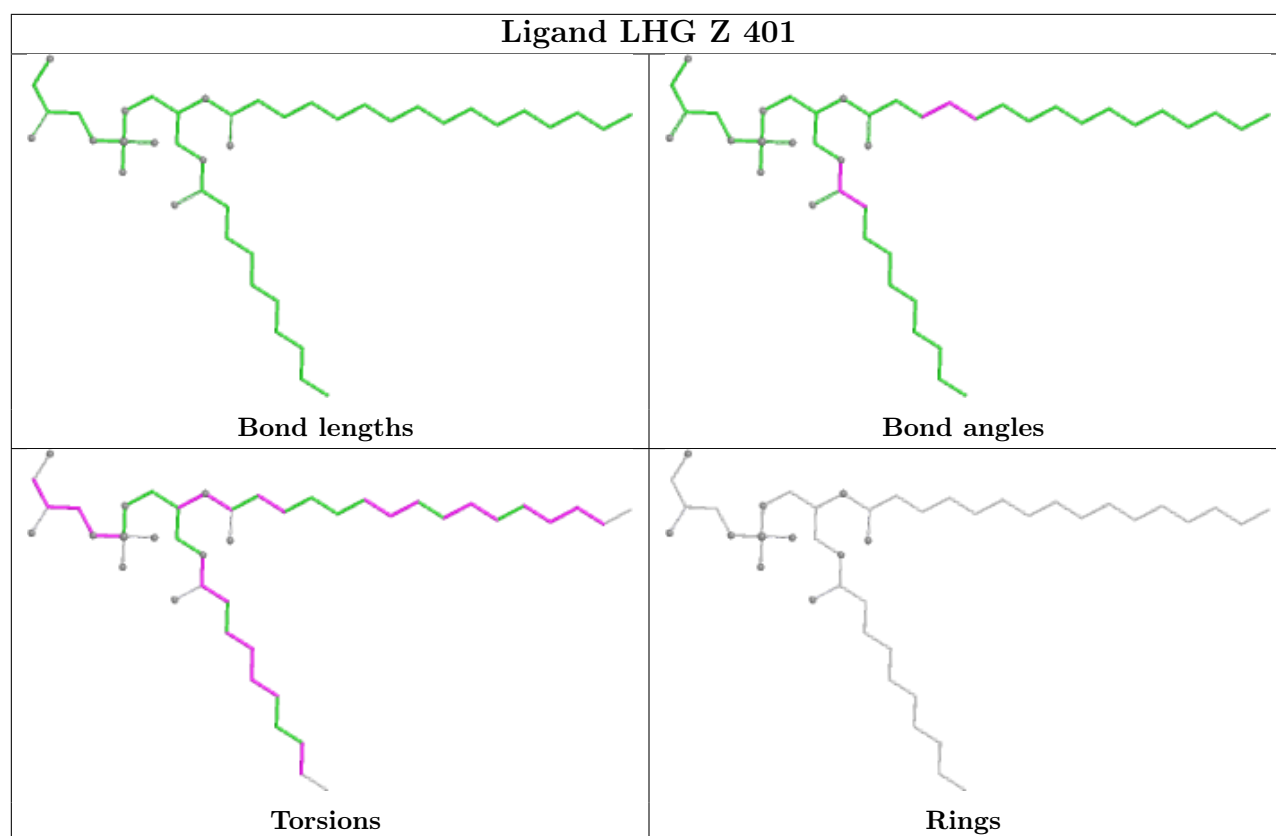




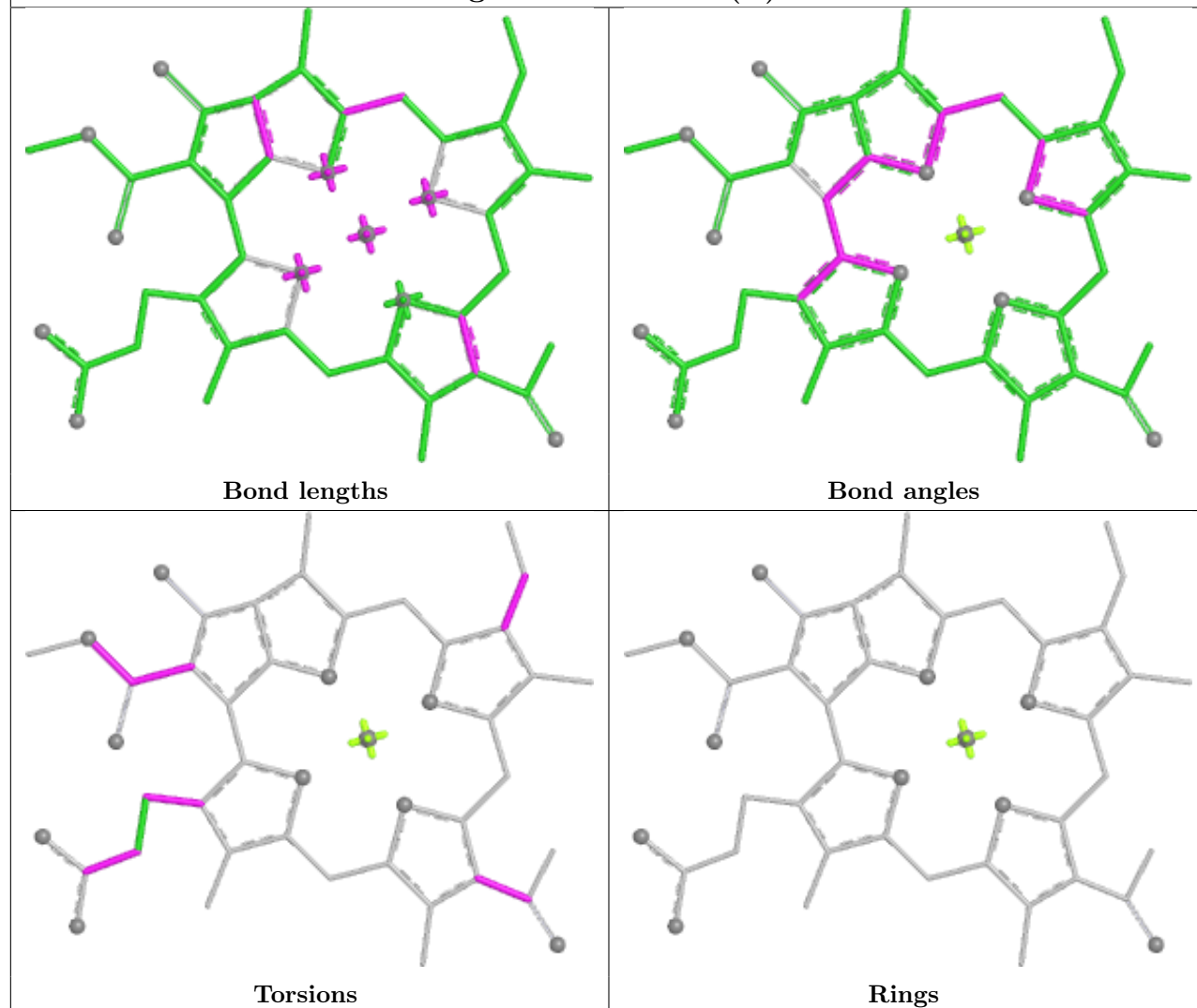




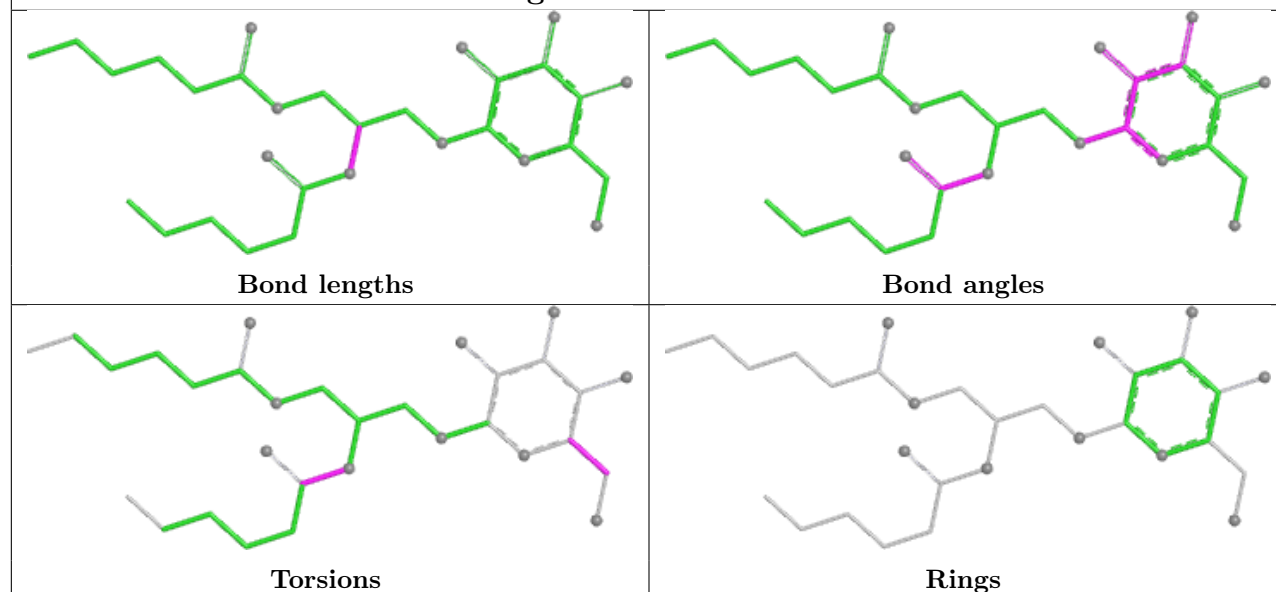


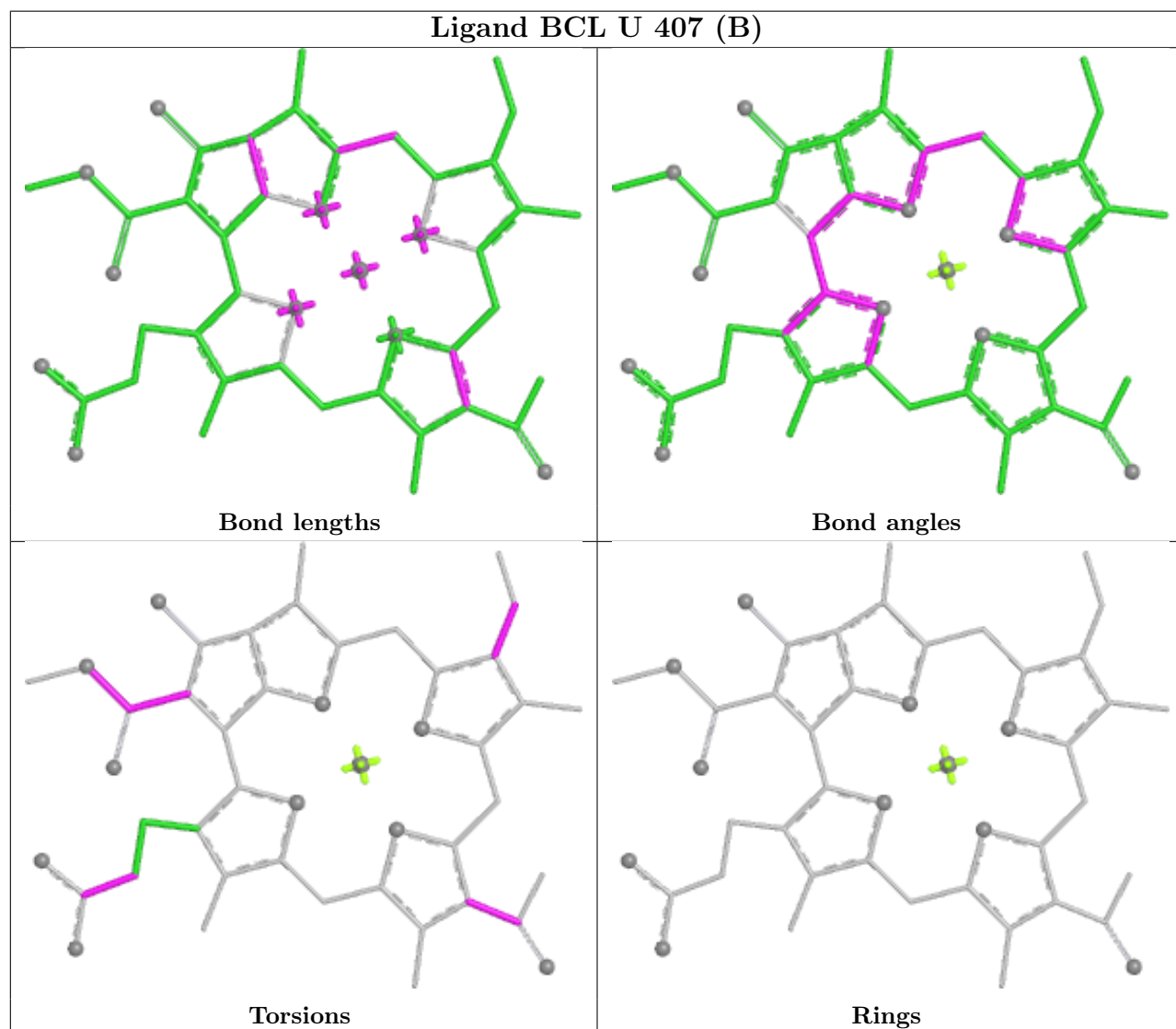
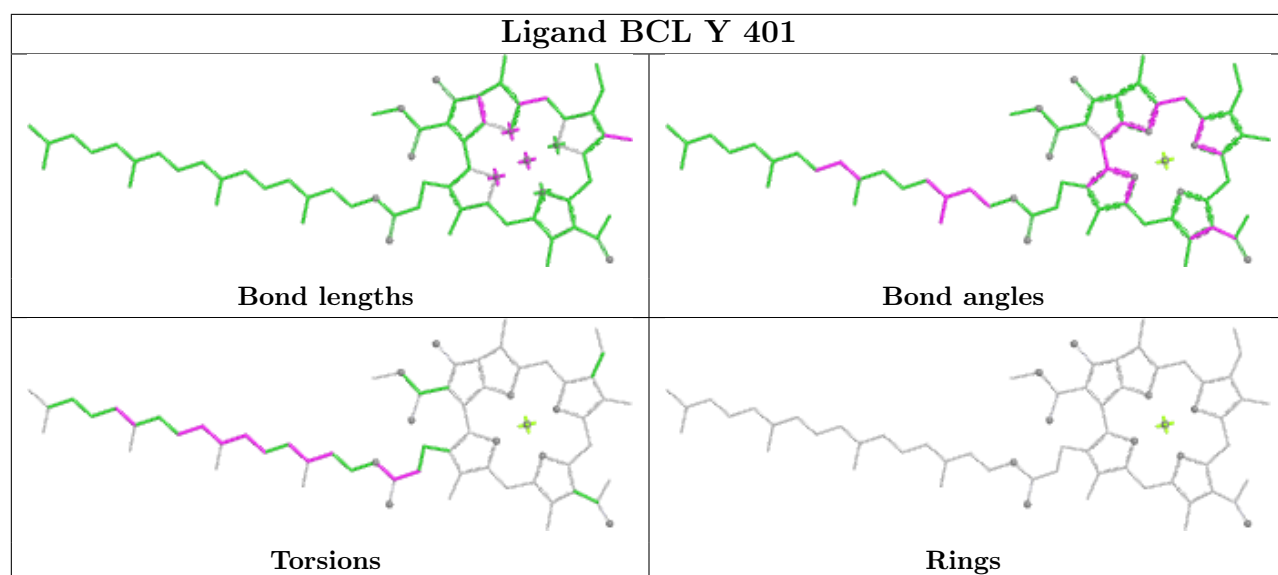


Ligand BCL V 409 (B)

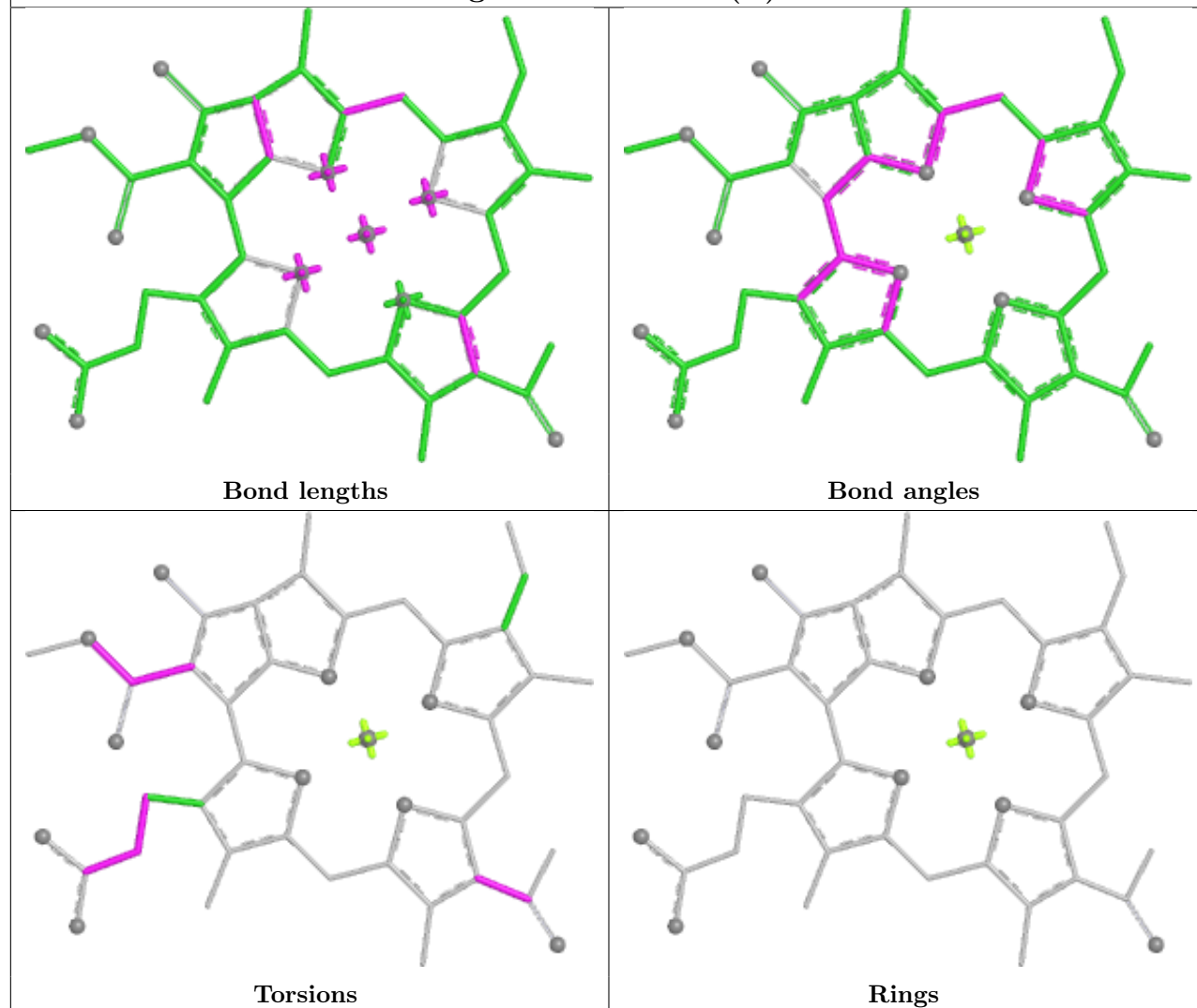


Ligand LMG A 823

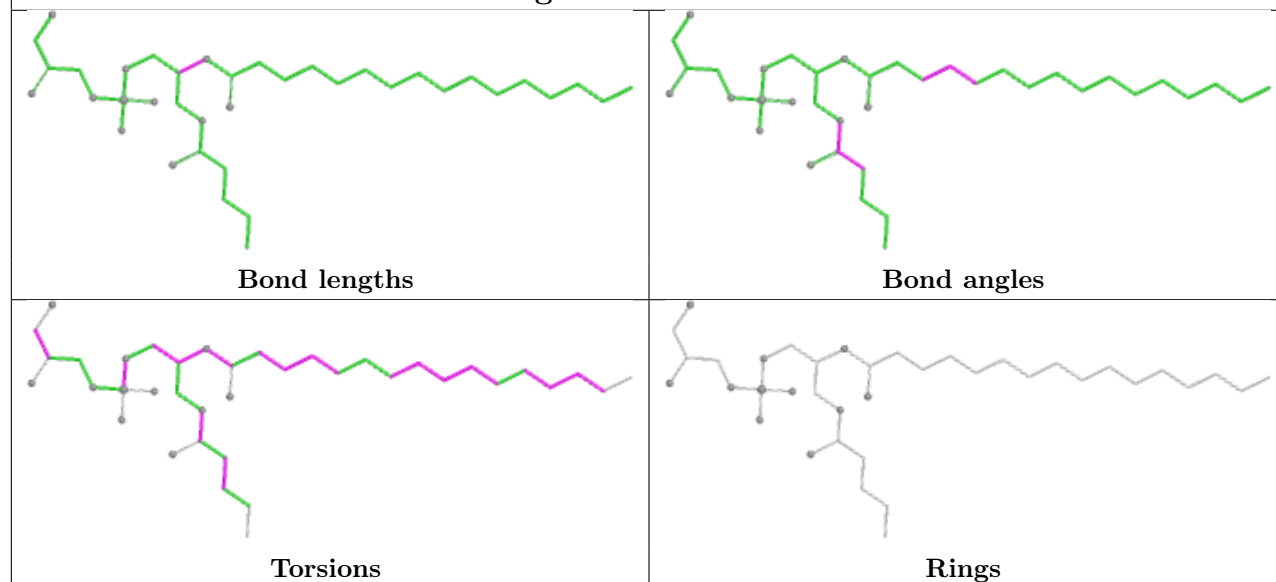


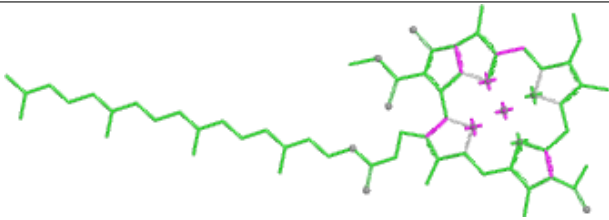
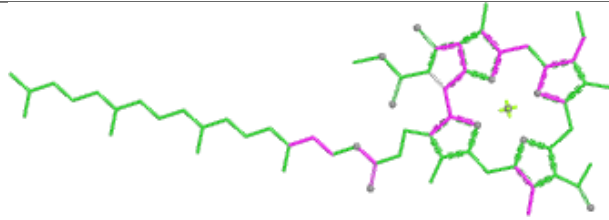
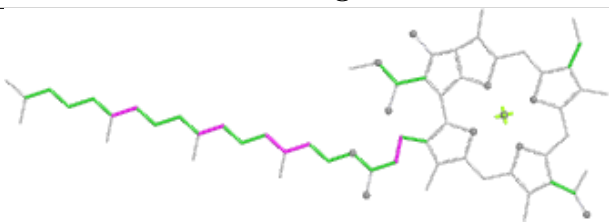
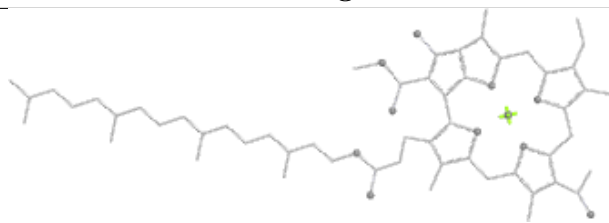


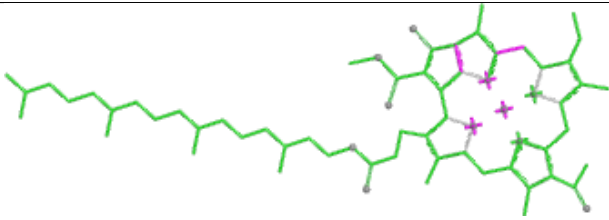
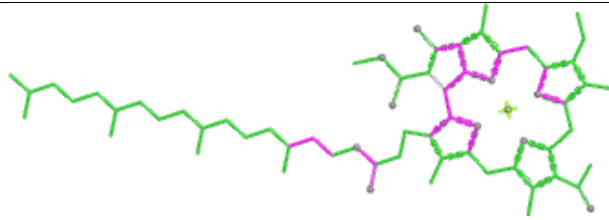
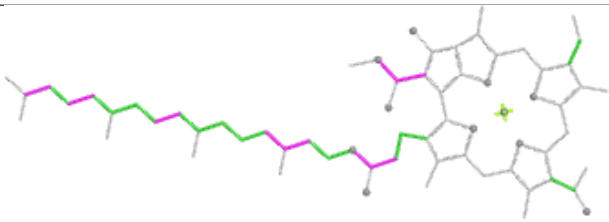
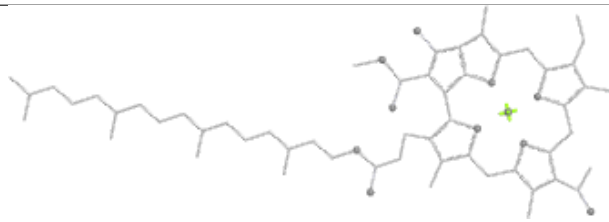
Ligand BCL X 408 (B)

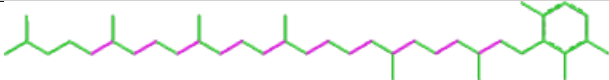
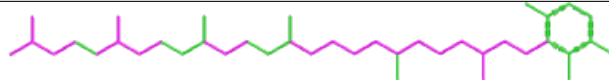
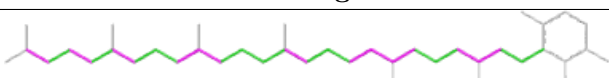
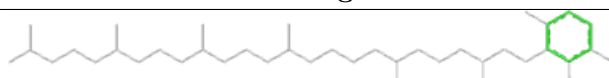


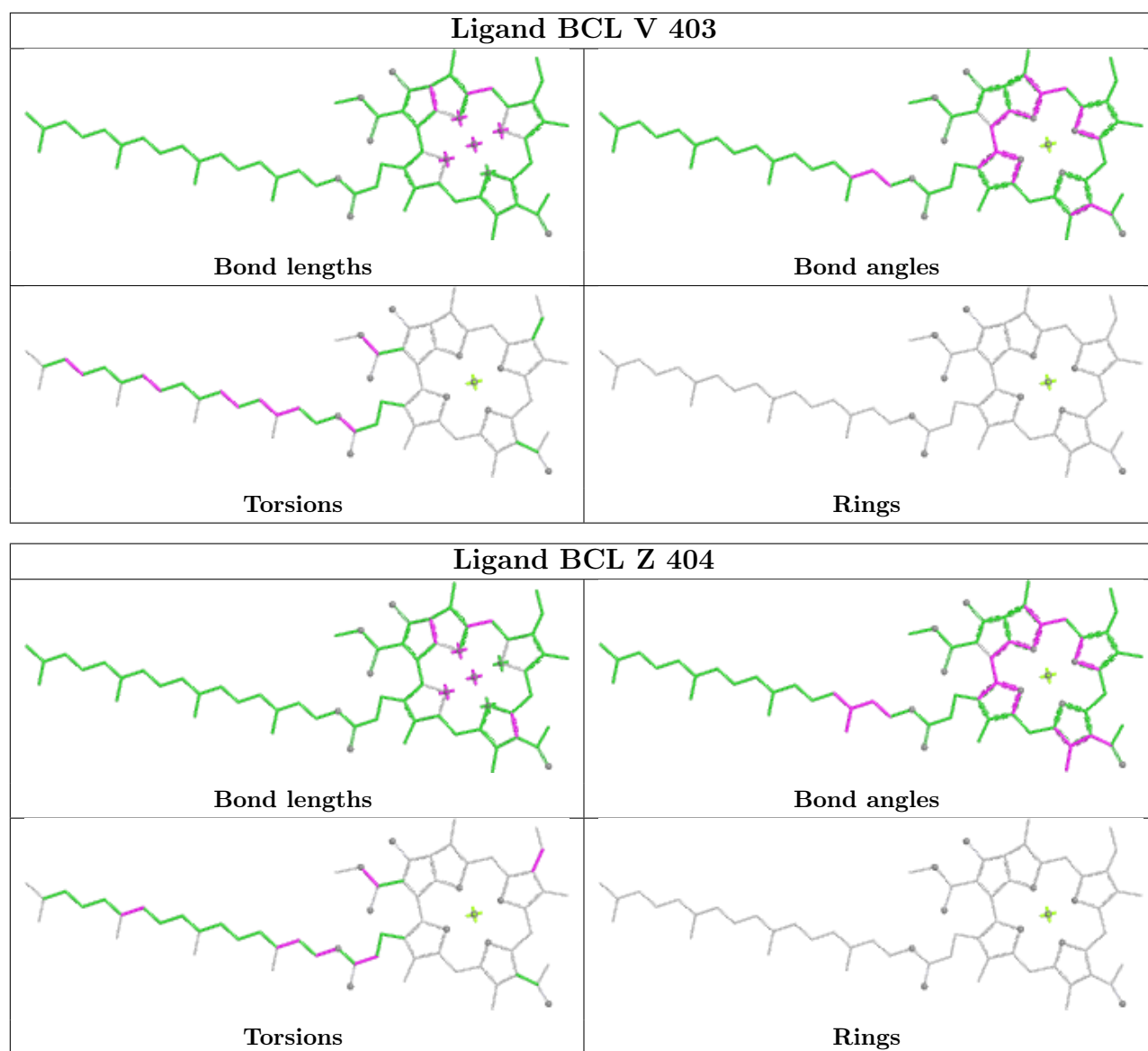
Ligand LHG a 821

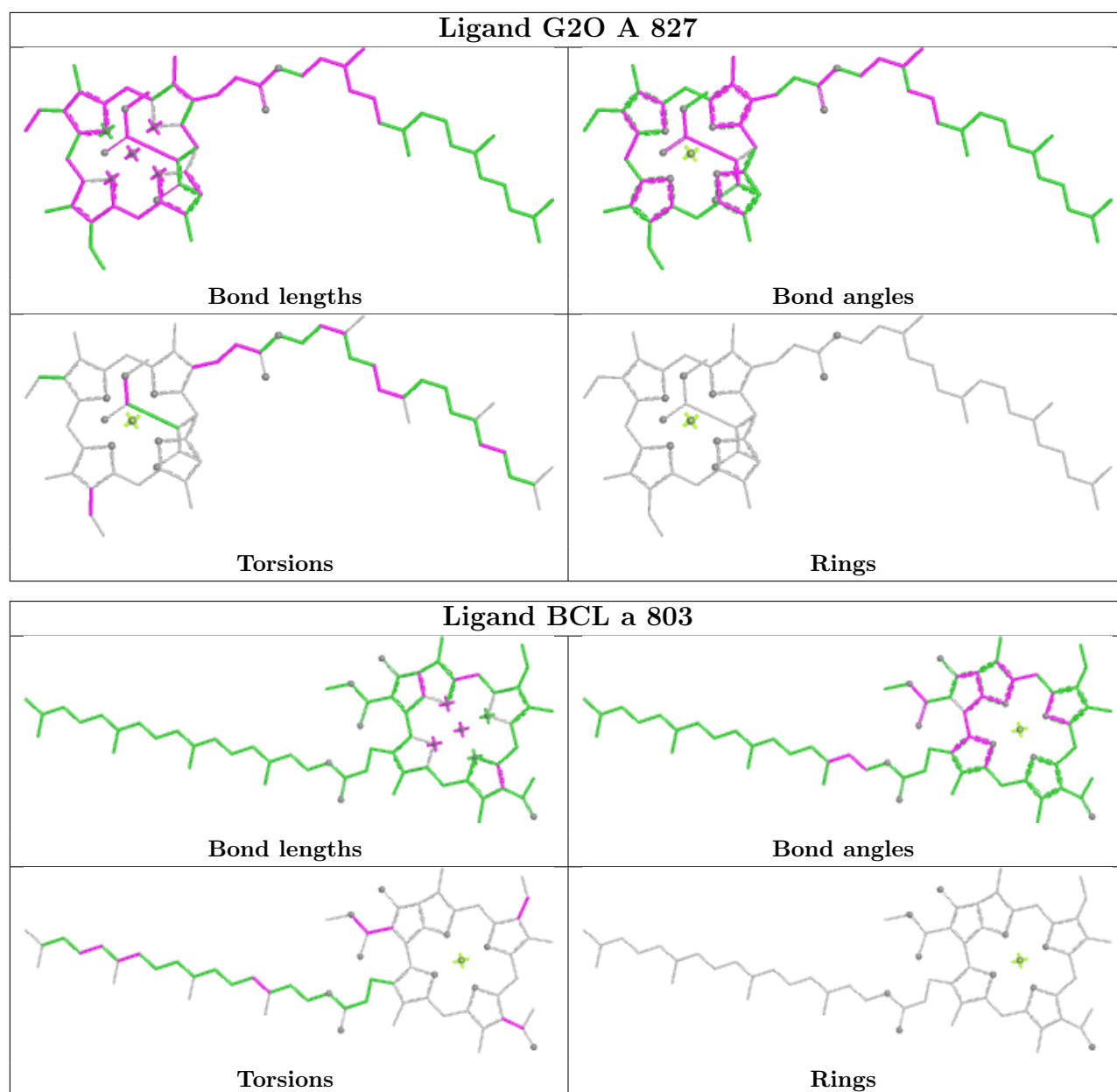


Ligand BCL A 811	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCL U 404	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand F26 a 816	
	
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.

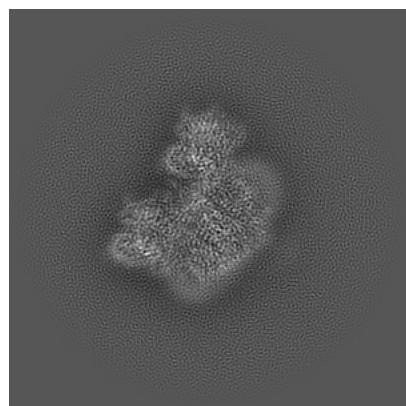
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26471. These allow visual inspection of the internal detail of the map and identification of artifacts.

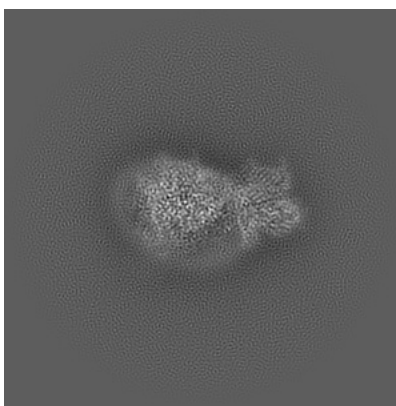
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

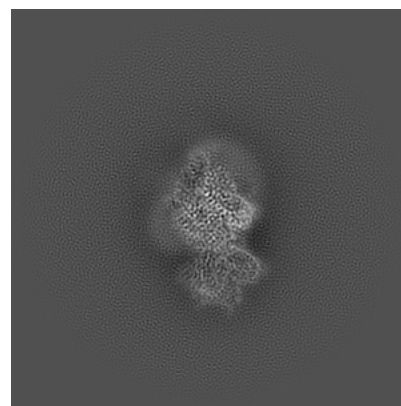
6.1.1 Primary map



X

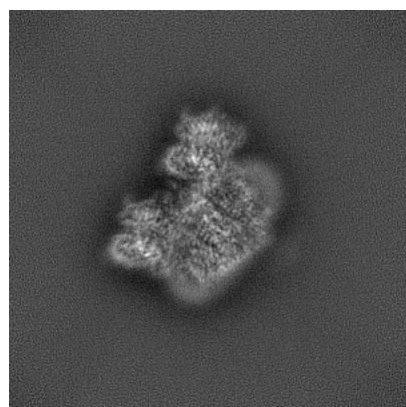


Y

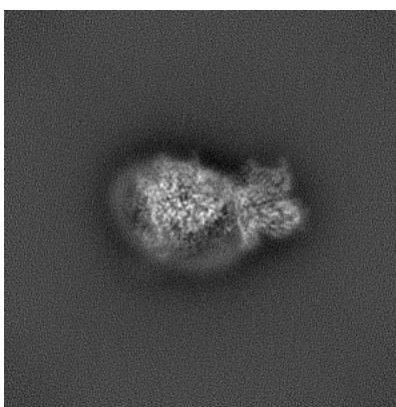


Z

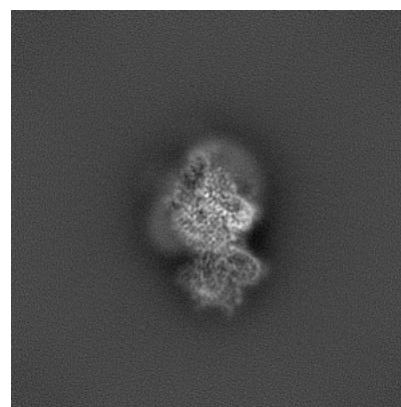
6.1.2 Raw map



X



Y

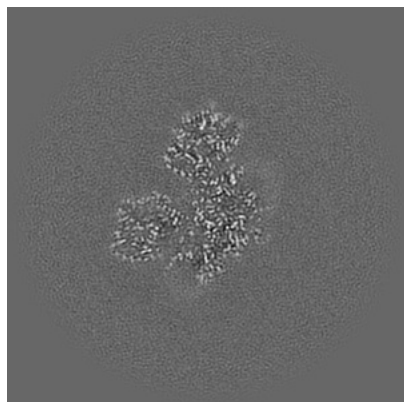


Z

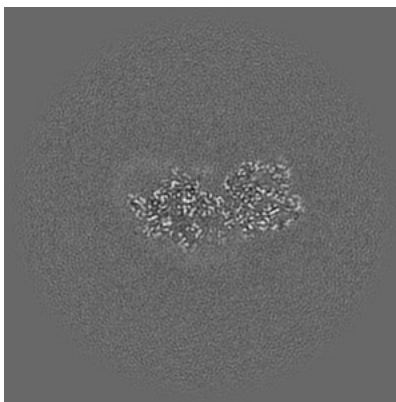
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

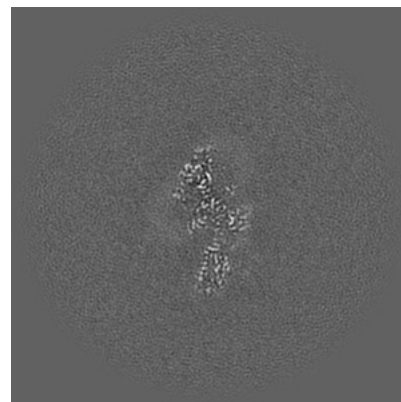
6.2.1 Primary map



X Index: 180

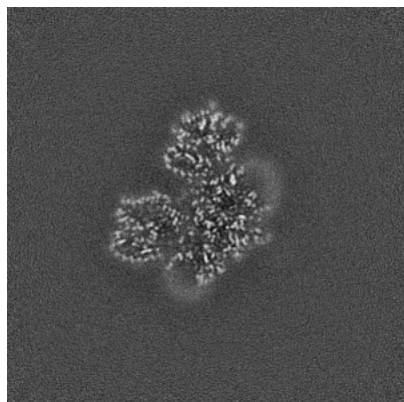


Y Index: 180

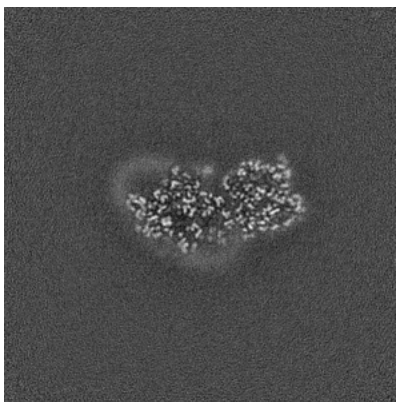


Z Index: 180

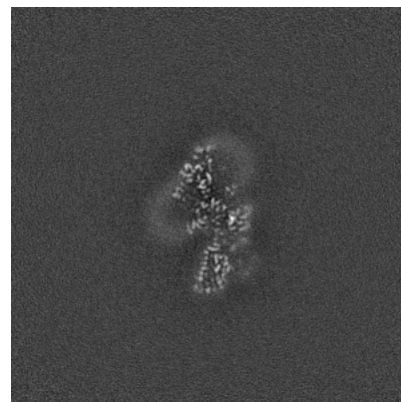
6.2.2 Raw map



X Index: 180



Y Index: 180

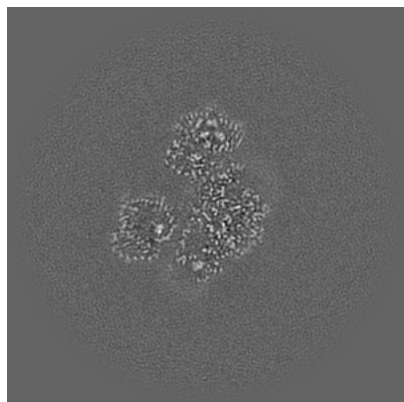


Z Index: 180

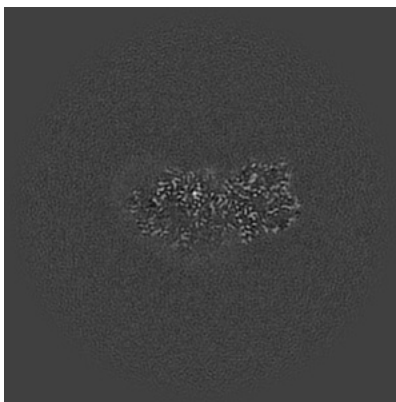
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

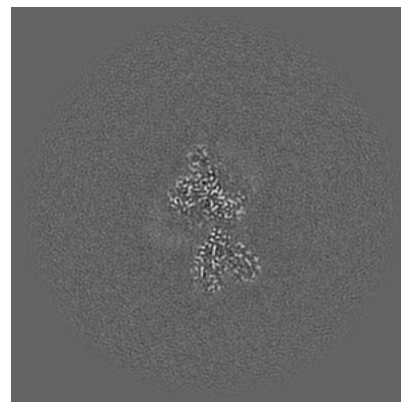
6.3.1 Primary map



X Index: 177

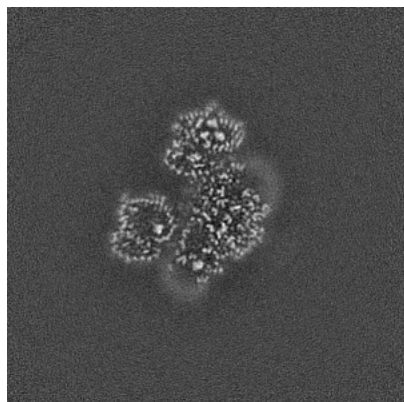


Y Index: 176

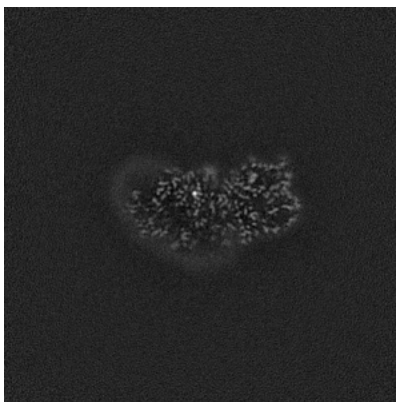


Z Index: 165

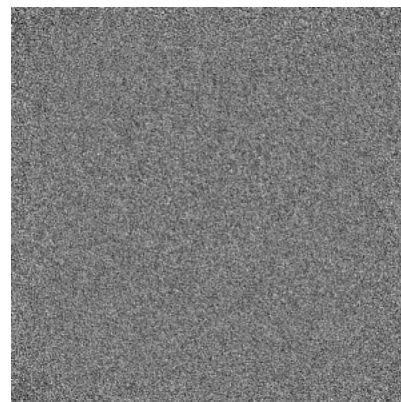
6.3.2 Raw map



X Index: 177



Y Index: 176

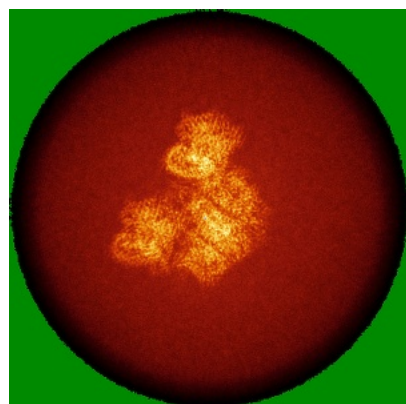


Z Index: 359

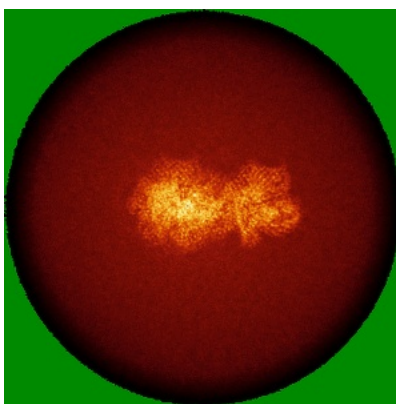
The images above show the largest variance slices of the map in three orthogonal directions.

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

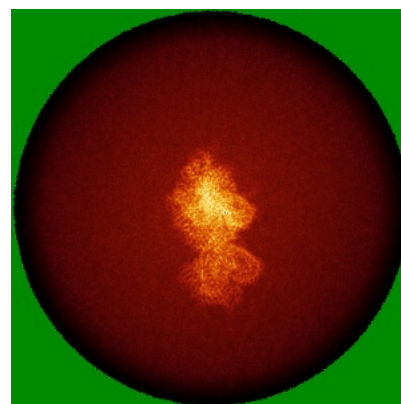
6.4.1 Primary map



X

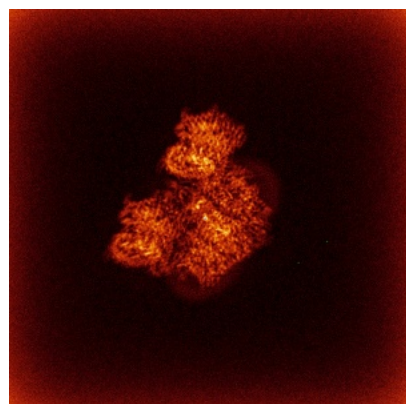


Y

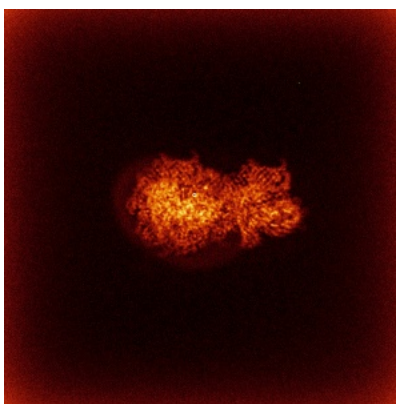


Z

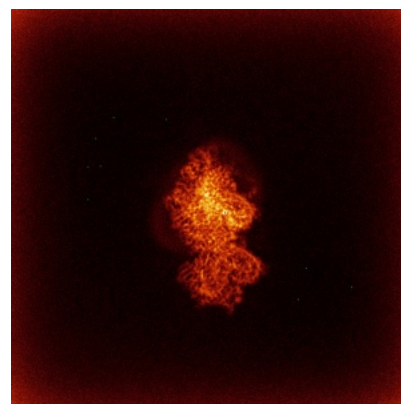
6.4.2 Raw map



X



Y

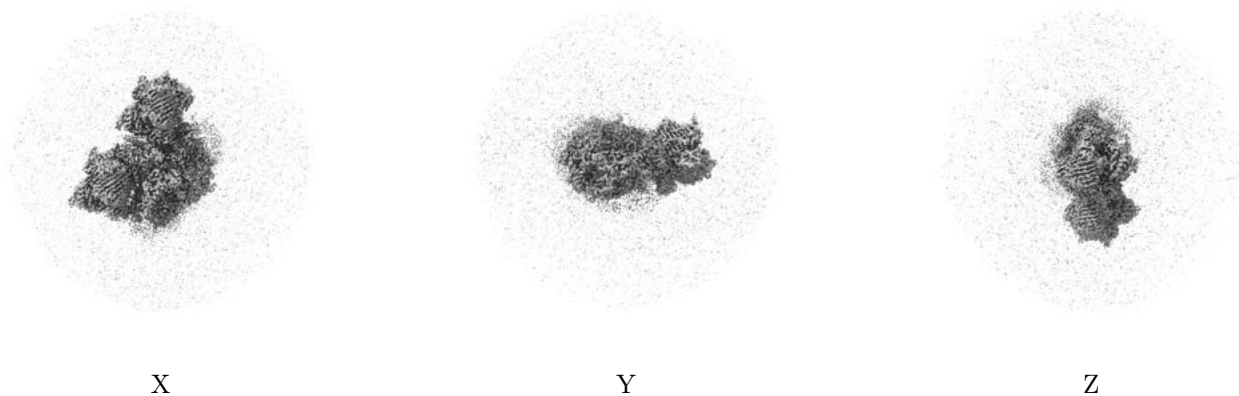


Z

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.

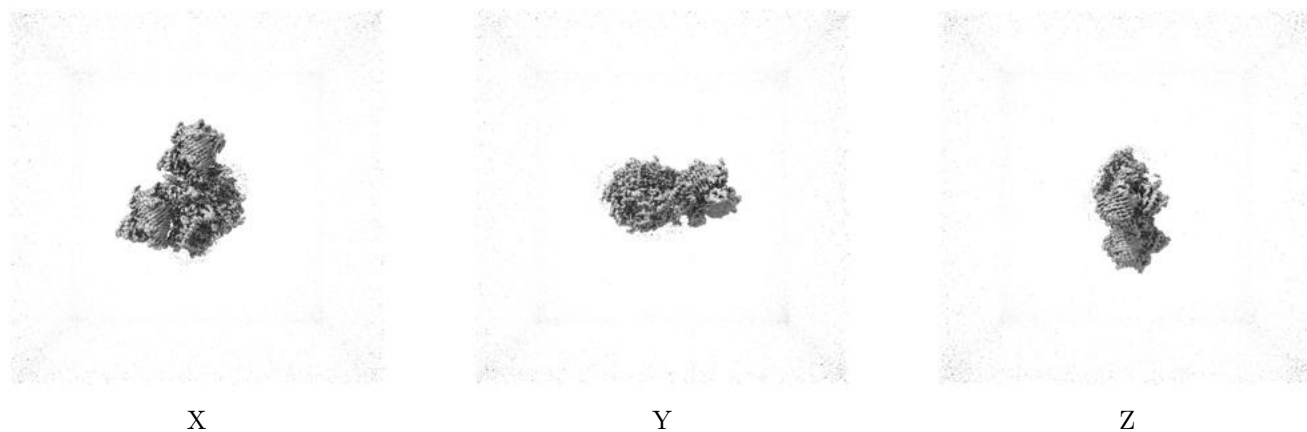
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.428. 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.

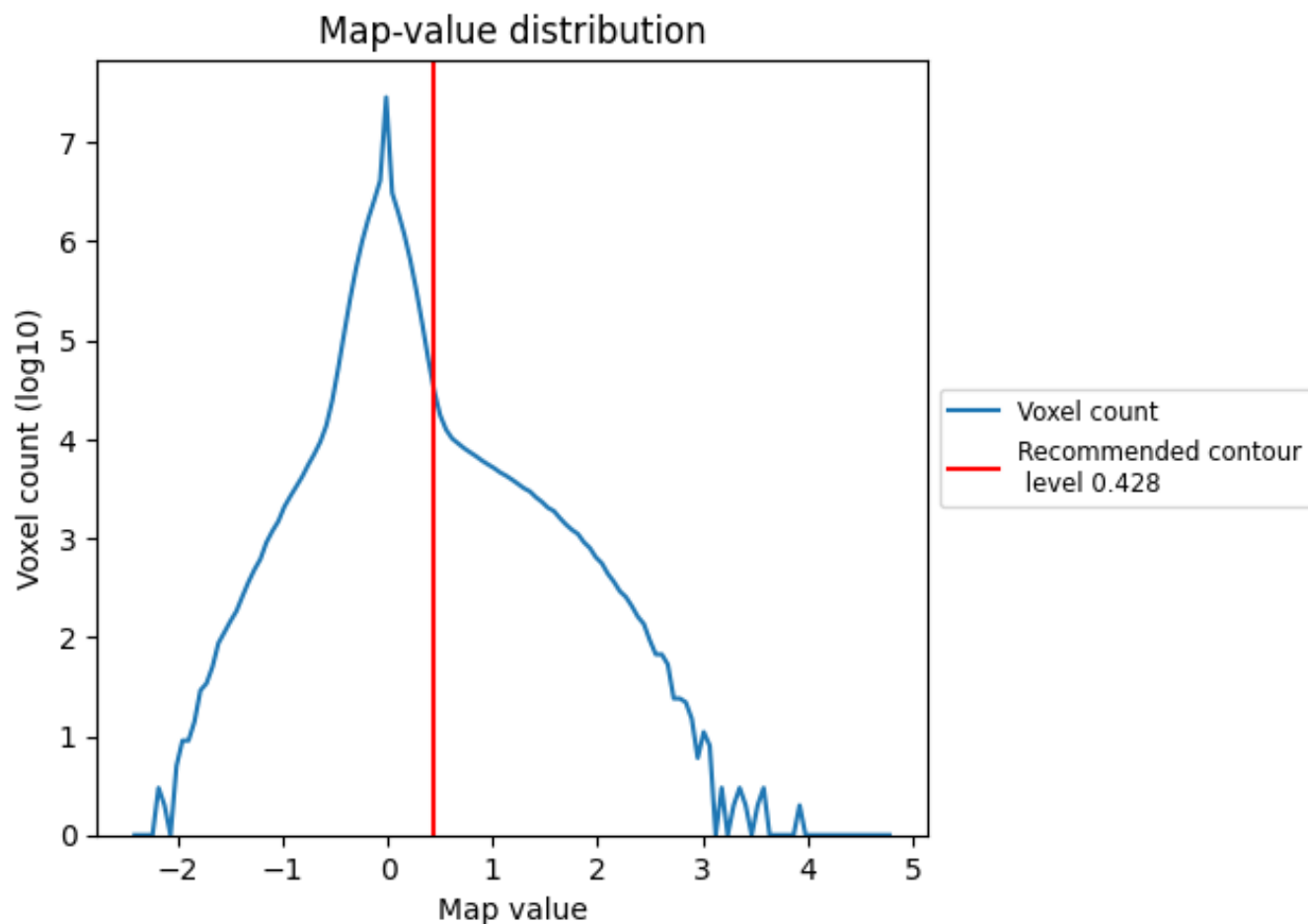
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

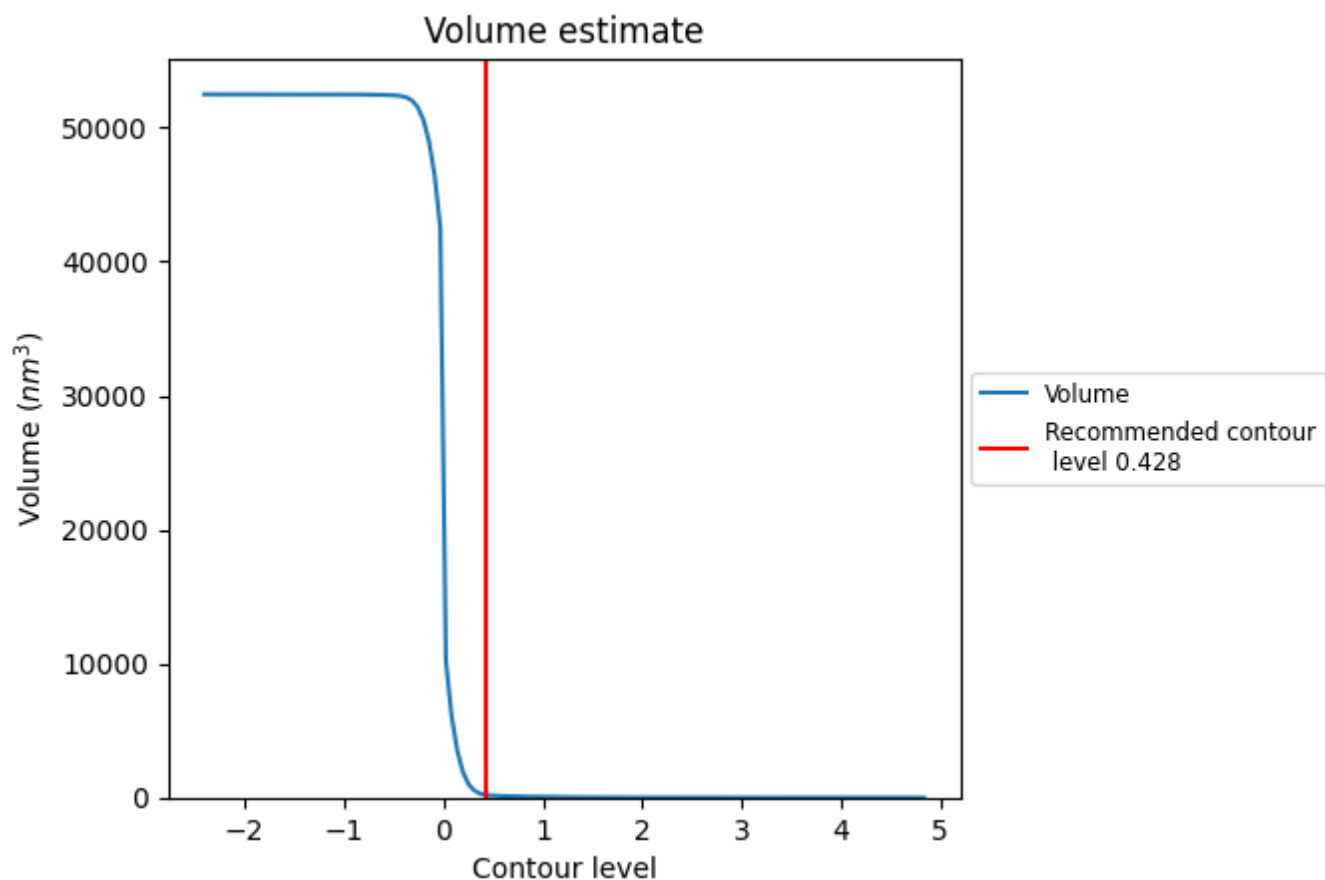
This section contains the results of statistical analysis of the map.

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.

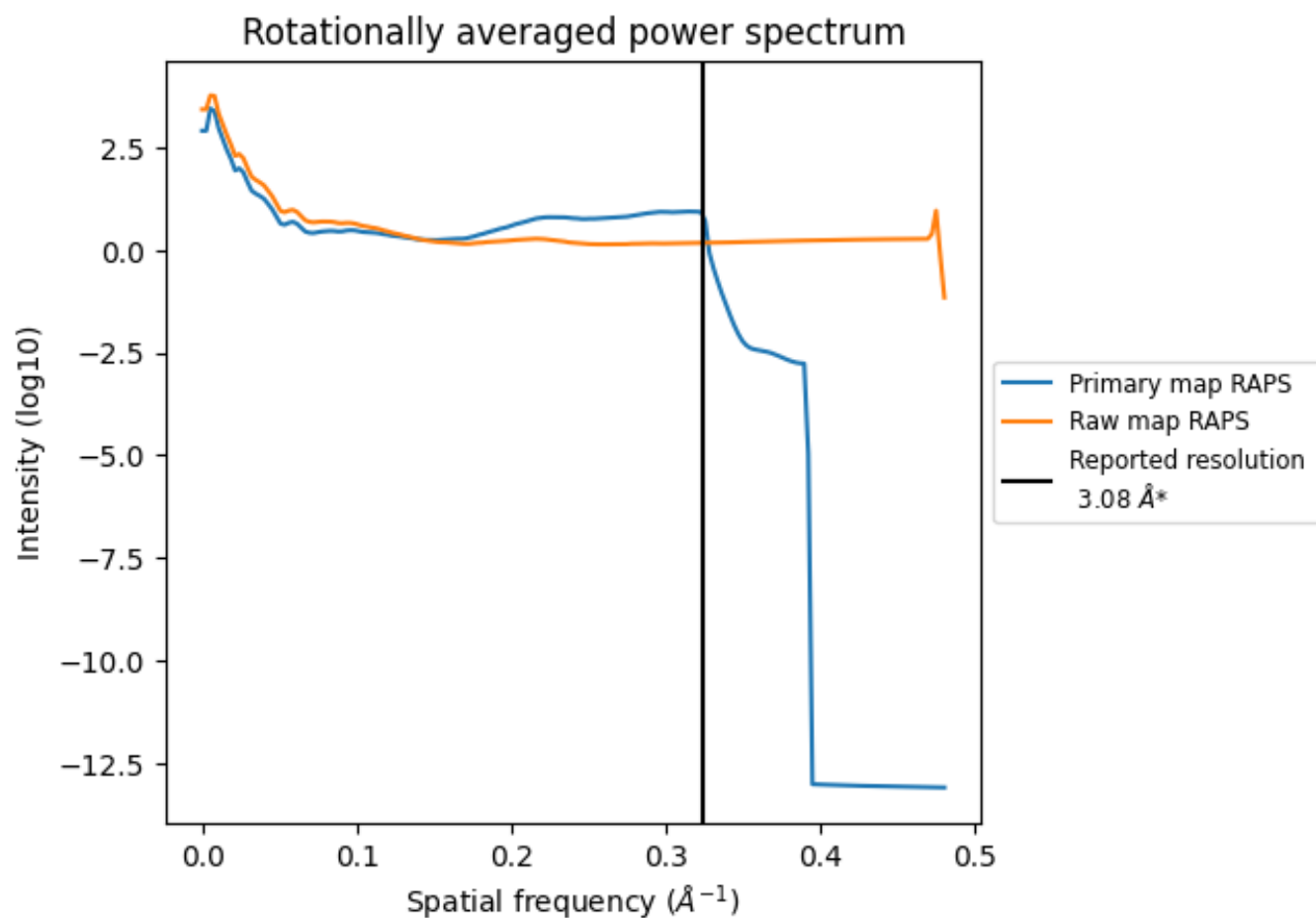
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 198 nm³; this corresponds to an approximate mass of 179 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 ⓘ

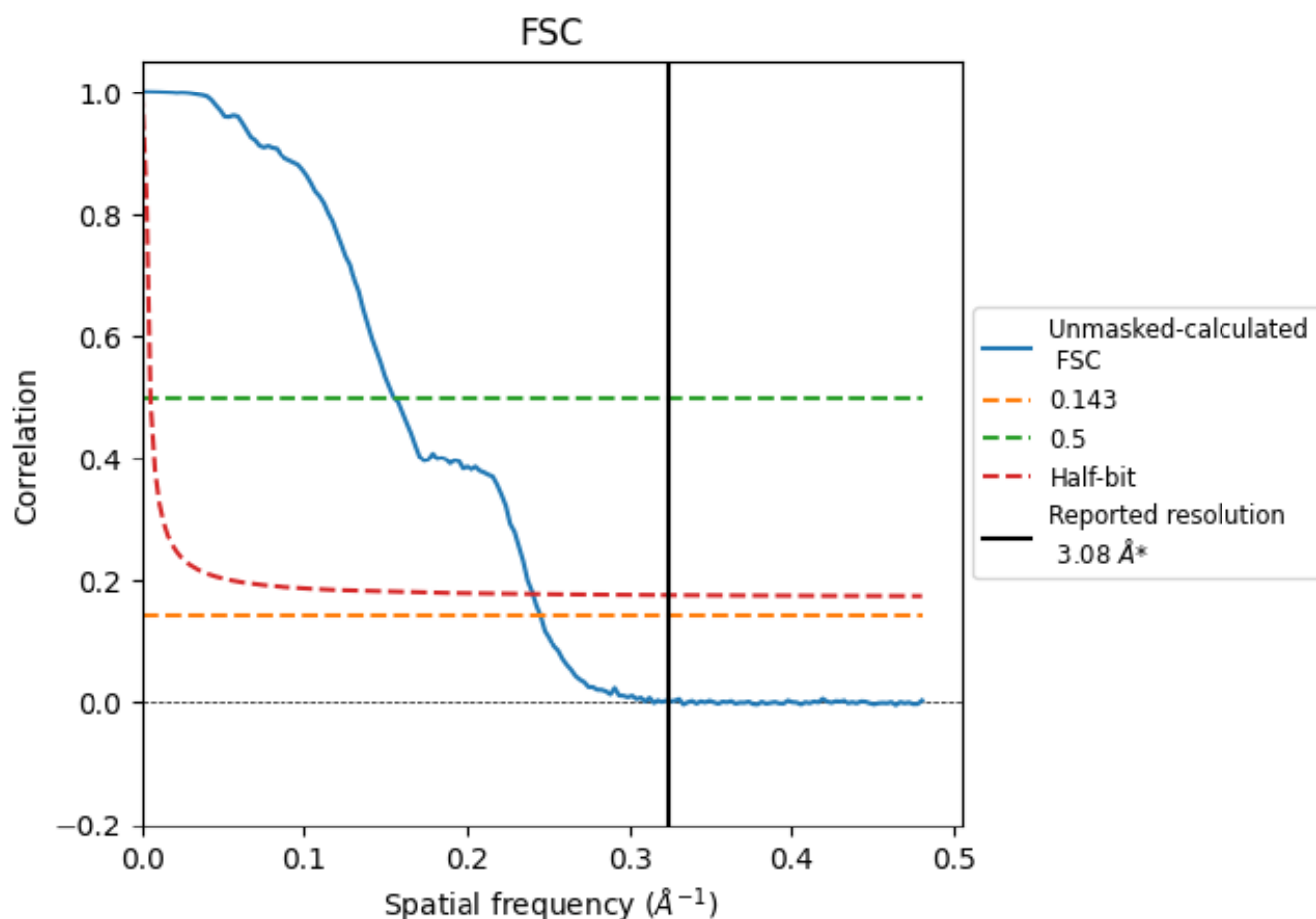


*Reported resolution corresponds to spatial frequency of 0.325 Å⁻¹

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 0.325 Å⁻¹

8.2 Resolution estimates [i](#)

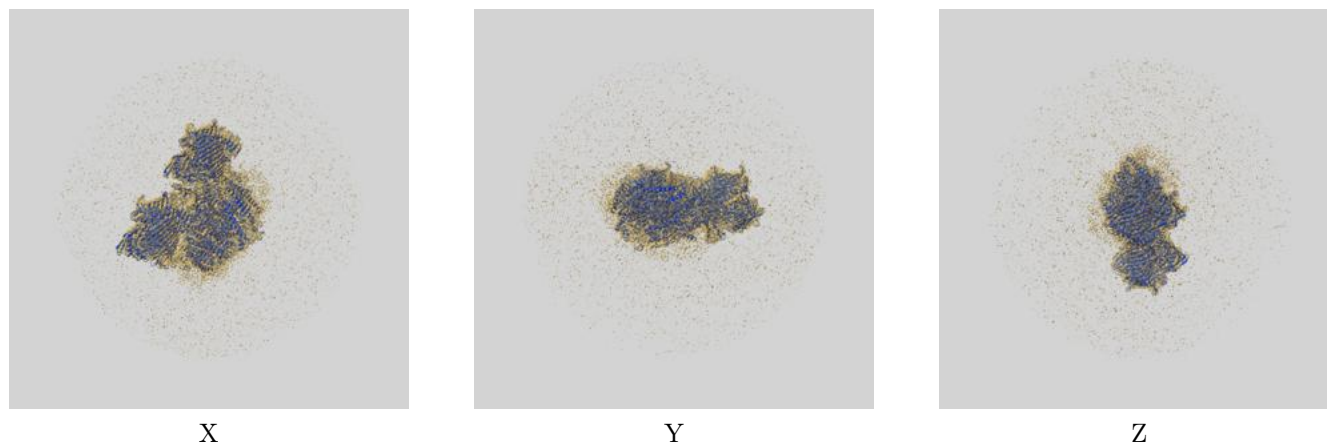
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.08	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.07	6.46	4.15

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.07 differs from the reported value 3.08 by more than 10 %

9 Map-model fit [i](#)

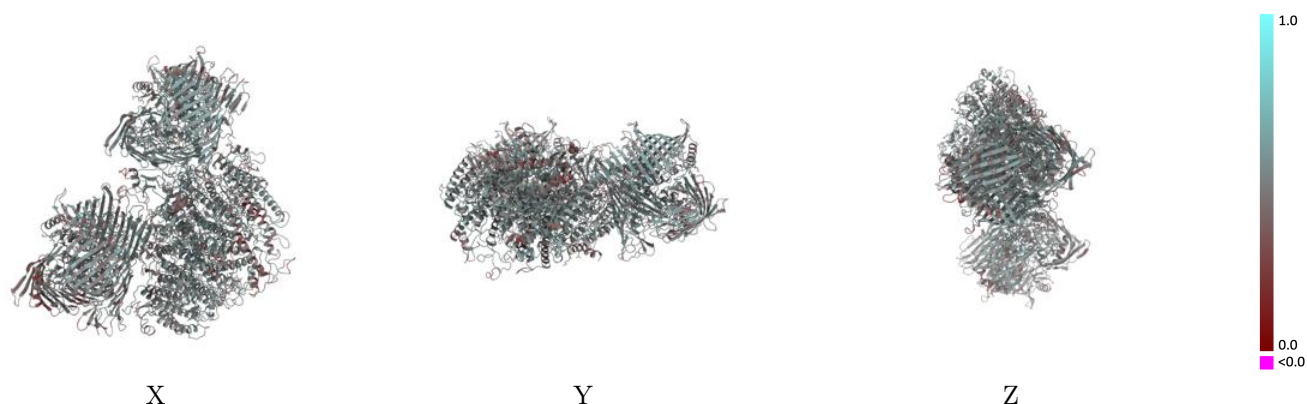
This section contains information regarding the fit between EMDB map EMD-26471 and PDB model 7UEB. Per-residue inclusion information can be found in section 3 on page 15.

9.1 Map-model overlay [i](#)



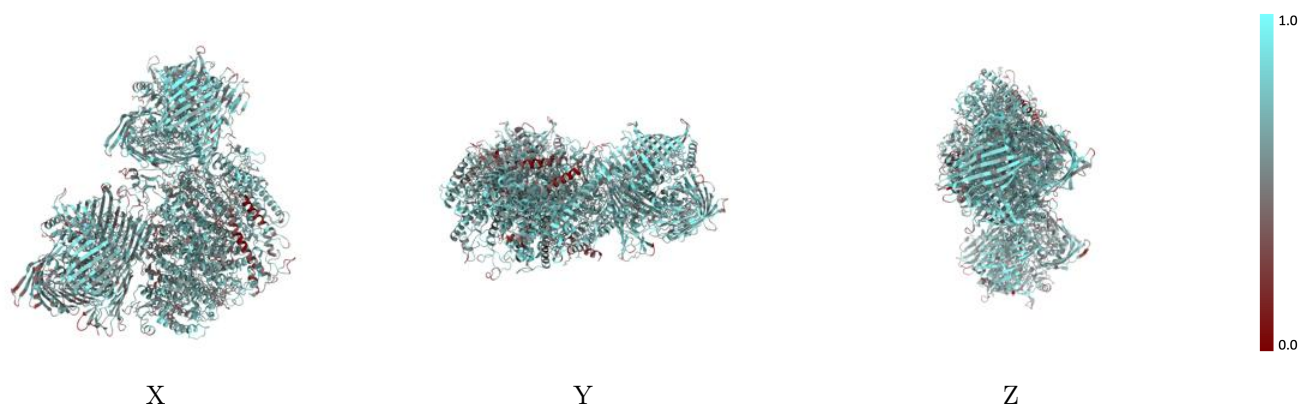
The images above show the 3D surface view of the map at the recommended contour level 0.428 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



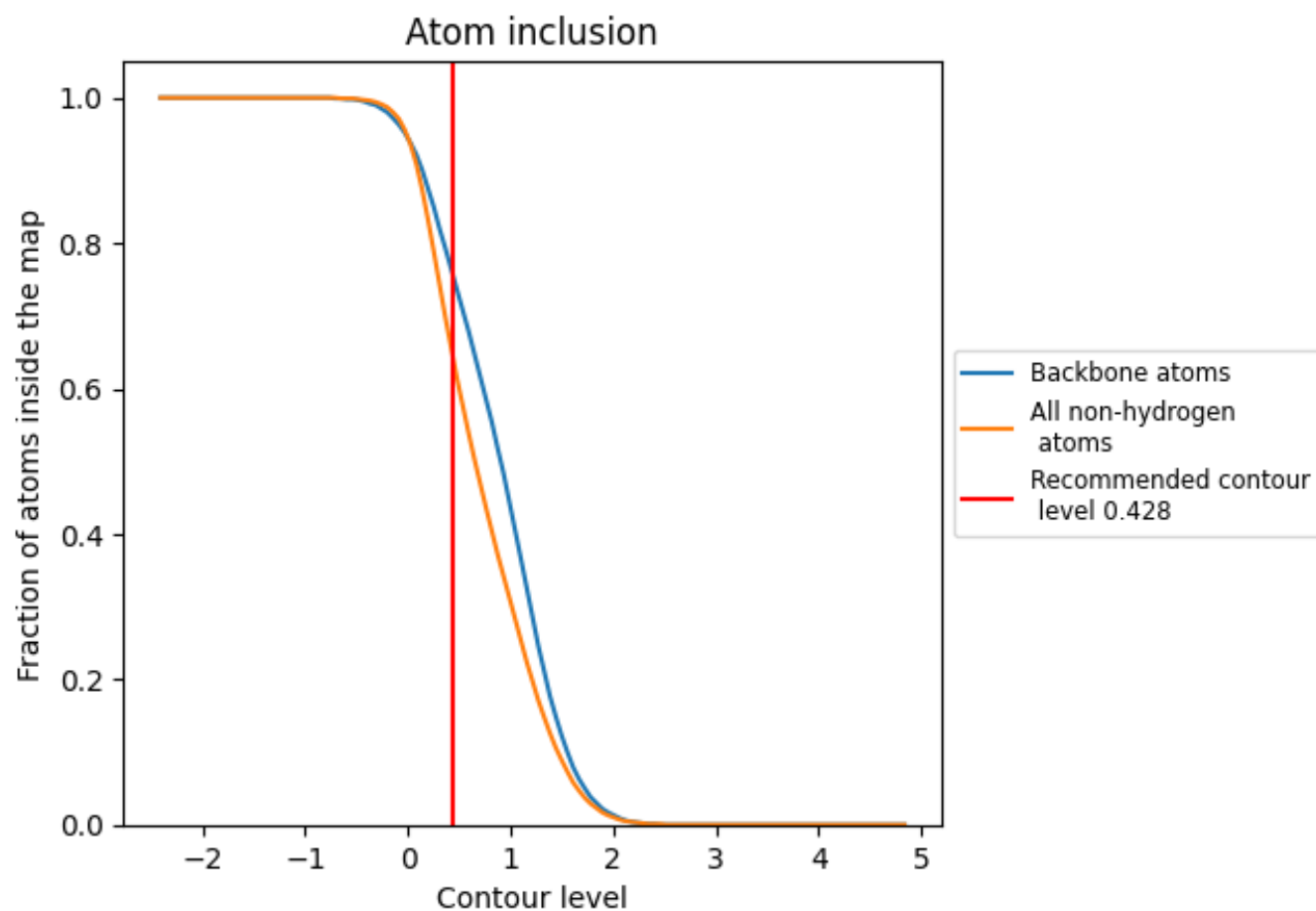
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.428).

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 65% 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 (0.428) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6500	0.4970
A	0.6790	0.5170
B	0.6410	0.4920
C	0.5490	0.4680
D	0.5260	0.4370
E	0.4120	0.3720
F	0.3410	0.3920
U	0.7040	0.5110
V	0.7100	0.5230
W	0.6780	0.4930
X	0.6250	0.4710
Y	0.6320	0.4870
Z	0.6690	0.5120
a	0.6680	0.5140
c	0.3480	0.3940

1.0

0.0

<0.0