



wwPDB EM Validation Summary Report ⓘ

Sep 28, 2026 – 12:38 PM JST

PDB ID : 9XK3 / pdb_00009xk3
EMDB ID : EMD-66946
Title : In situ C2S2M2L4-type PSII-LHCII supercomplex, core, protomer 1
Authors : Li, J.; Elias, E.; Zhang, K.; Croce, R.; Zhu, J.
Deposited on : 2025-11-05
Resolution : 2.70 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 Phenix2.2
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) : 2.51

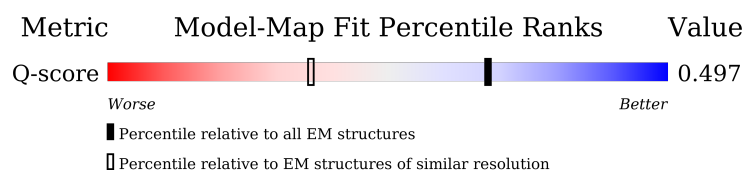
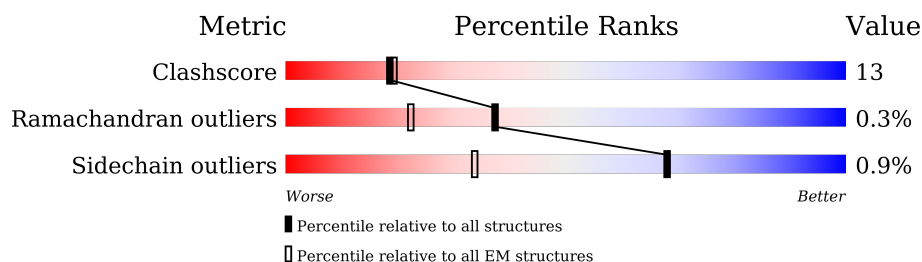
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.70 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	10327 (2.20 - 3.20)

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	1A	334	
2	1B	503	
3	1C	450	
4	1D	341	

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Mol	Chain	Length	Quality of chain
5	1E	75	
6	1F	36	
7	1H	60	
8	1I	34	
9	1J	35	
10	1K	37	
11	1L	37	
12	1M	33	
13	1O	248	
14	1P	186	
15	1T	32	
16	1U	27	
17	1V	105	
18	1W	54	
19	1X	39	
20	1Y	34	
21	1Z	62	

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
23	CLA	1A	402	X	-	-	-
23	CLA	1B	601	X	-	-	-
23	CLA	1B	602	X	-	-	-
23	CLA	1B	603	X	-	-	-
23	CLA	1B	604	X	-	-	-
23	CLA	1B	605	X	-	-	-
23	CLA	1B	606	X	-	-	-
23	CLA	1B	607	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	1B	608	X	-	-	-
23	CLA	1B	609	X	-	-	-
23	CLA	1B	610	X	-	-	-
23	CLA	1B	611	X	-	-	-
23	CLA	1B	612	X	-	-	-
23	CLA	1B	613	X	-	-	-
23	CLA	1B	616	X	-	-	-
23	CLA	1C	501	X	-	-	-
23	CLA	1C	502	X	-	-	-
23	CLA	1C	503	X	-	-	-
23	CLA	1C	504	X	-	-	-
23	CLA	1C	505	X	-	-	-
23	CLA	1C	507	X	-	-	-
23	CLA	1C	508	X	-	-	-
23	CLA	1C	509	X	-	-	-
23	CLA	1C	510	X	-	-	-
23	CLA	1C	512	X	-	-	-
23	CLA	1D	401	X	-	-	-
23	CLA	1D	404	X	-	-	-
27	PL9	1E	102	-	-	X	-

2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 26005 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 II protein D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1A	334	Total	C	N	O	S	0	0
			2612	1706	430	463	13		

- Molecule 2 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1B	503	Total	C	N	O	S	0	0
			3945	2577	663	693	12		

- Molecule 3 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	1C	450	Total	C	N	O	S	0	0
			3486	2296	582	599	9		

- Molecule 4 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	1D	340	Total	C	N	O	S	0	0
			2708	1790	442	464	12		

- Molecule 5 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	1E	75	Total	C	N	O	0	0
			614	400	100	114		

- Molecule 6 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	1F	35	Total	C	N	O	S	0	0
			286	192	49	44	1		

- Molecule 7 is a protein called Photosystem II reaction center protein H.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	1H	60	Total	C	N	O	S	0	0
			454	299	73	79	3		

- Molecule 8 is a protein called Photosystem II reaction center protein I.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	1I	34	Total	C	N	O	S	0	0
			277	190	43	43	1		

- Molecule 9 is a protein called Photosystem II reaction center protein J.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	1J	35	Total	C	N	O	S	0	0
			255	172	39	44			

- Molecule 10 is a protein called Photosystem II reaction center protein K.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	1K	37	Total	C	N	O	S	0	0
			305	214	44	46	1		

- Molecule 11 is a protein called Photosystem II reaction center protein L.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	1L	36	Total	C	N	O	S	0	0
			304	201	48	55			

- Molecule 12 is a protein called Photosystem II reaction center protein M.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	1M	32	Total	C	N	O	S	0	0
			247	171	35	41			

- Molecule 13 is a protein called 33 kDa subunit of oxygen evolving system of photosystem II.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	1O	247	Total	C	N	O	S	0	0
			1861	1177	306	373	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1O	248	SER	-	insertion	UNP Q943W1

- Molecule 14 is a protein called 23 kDa subunit of oxygen evolving system of photosystem II.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	1P	186	Total	C	N	O	S	0	0
			1422	901	236	284	1		

- Molecule 15 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	1T	32	Total	C	N	O	S	0	0
			261	182	37	41	1		

- Molecule 16 is a protein called Os02g0581100 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	1U	27	Total	C	N	O	S	0	0
			208	130	39	36	3		

- Molecule 17 is a protein called Photosystem II 10 kDa polypeptide, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	1V	98	Total	C	N	O		0	0
			715	464	117	134			

- Molecule 18 is a protein called Photosystem II reaction center W protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	1W	54	Total	C	N	O	S	0	0
			413	263	61	88	1		

- Molecule 19 is a protein called Os07g0673550 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	1X	39	Total	C	N	O		0	0
			276	181	46	49			

- Molecule 20 is a protein called Os08g0119800 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	1Y	34	Total	C	N	O	S	0	0
			270	176	50	43	1		

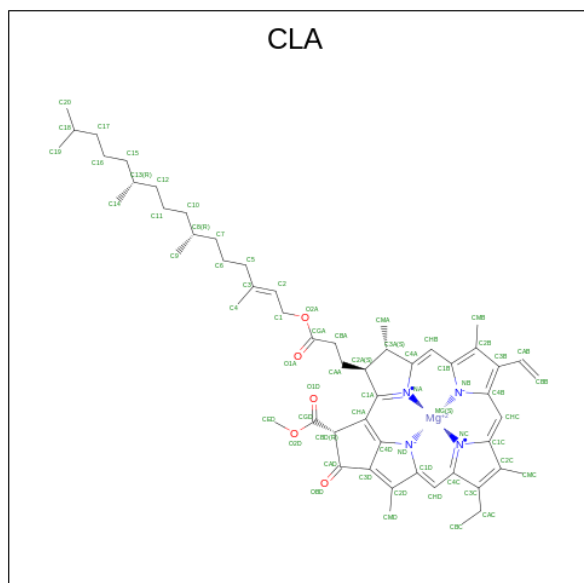
- Molecule 21 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	1Z	62	Total	C	N	O	S	0	0
			466	313	70	82	1		

- Molecule 22 is FE (II) ION (CCD ID: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
22	1A	1	Total	Fe	0
			1	1	

- Molecule 23 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
23	1A	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
23	1A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
23	1B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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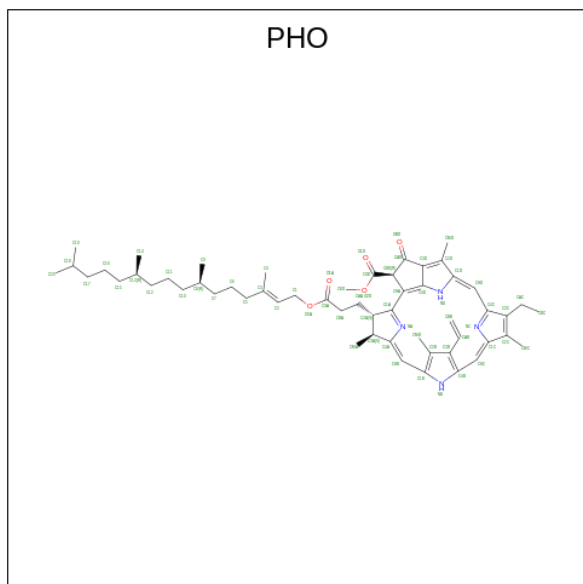
Mol	Chain	Residues	Atoms					AltConf
23	1B	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
23	1B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	1B	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
23	1B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	1B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	1B	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
23	1B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	1B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	1B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	1B	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
23	1B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	1B	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
23	1B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
23	1B	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
23	1B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
23	1C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	1C	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
23	1C	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
23	1C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	1C	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
23	1C	1	Total	C	Mg	N	O	0
			49	39	1	4	5	

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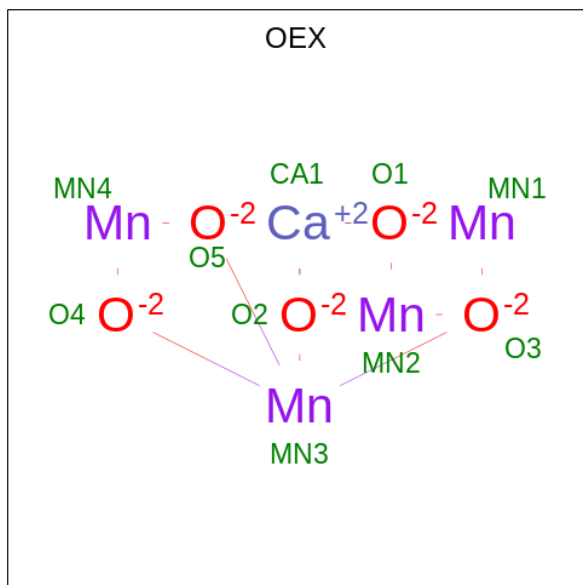
Mol	Chain	Residues	Atoms					AltConf
23	1C	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
23	1C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	1C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	1C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	1C	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
23	1C	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
23	1C	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
23	1D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	1D	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
23	1D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	1D	1	Total	C	Mg	N	O	0
			42	34	1	4	3	

- Molecule 24 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$) (labeled as "Ligand of Interest" by depositor).



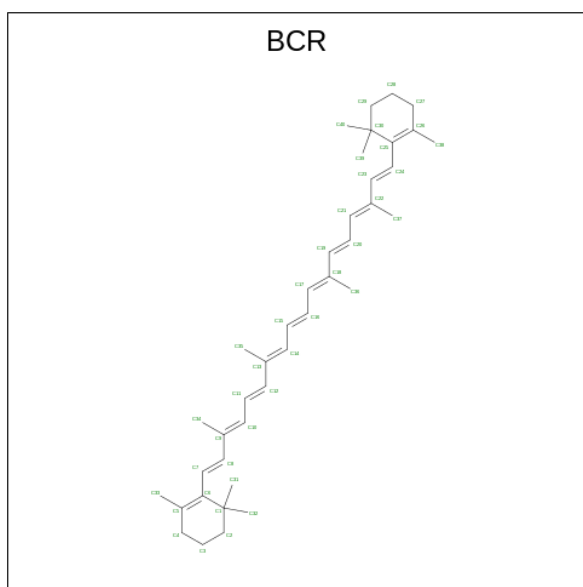
Mol	Chain	Residues	Atoms				AltConf
24	1A	1	Total	C	N	O	0
			64	55	4	5	
24	1A	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 25 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5).



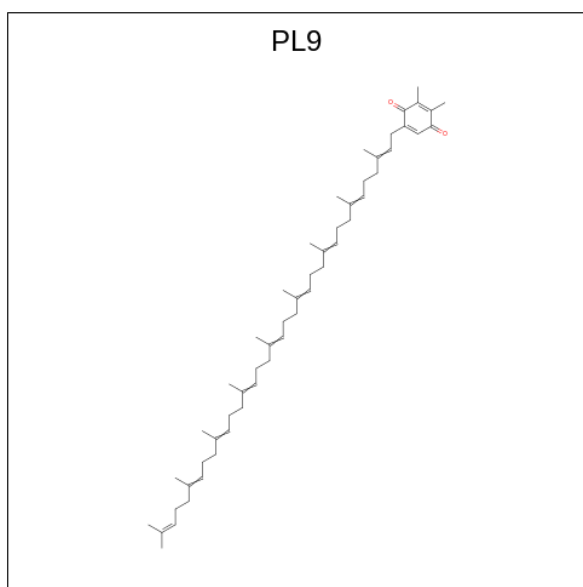
Mol	Chain	Residues	Atoms				AltConf
25	1A	1	Total	Ca	Mn	O	0
			10	1	4	5	

- Molecule 26 is BETA-CAROTENE (CCD ID: BCR) (formula: $\text{C}_{40}\text{H}_{56}$) (labeled as "Ligand of Interest" by depositor).



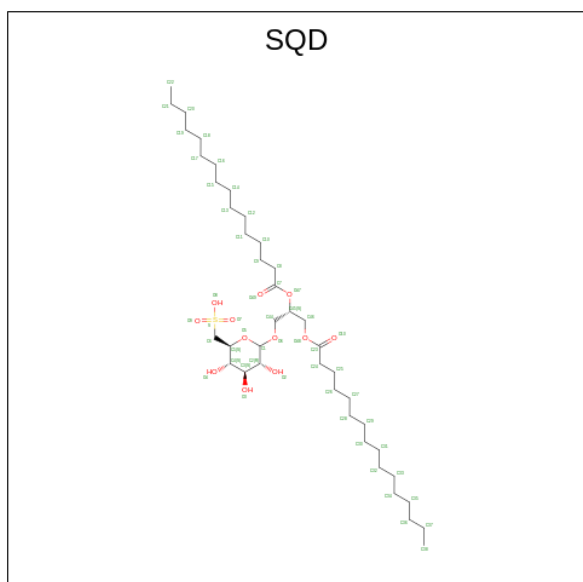
Mol	Chain	Residues	Atoms	AltConf
26	1A	1	Total C 40 40	0
26	1B	1	Total C 40 40	0
26	1B	1	Total C 40 40	0
26	1B	1	Total C 40 40	0
26	1D	1	Total C 40 40	0
26	1H	1	Total C 40 40	0
26	1I	1	Total C 40 40	0
26	1J	1	Total C 40 40	0
26	1T	1	Total C 40 40	0
26	1Z	1	Total C 40 40	0
26	1Z	1	Total C 40 40	0

- Molecule 27 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: C₅₃H₈₀O₂) (labeled as "Ligand of Interest" by depositor).



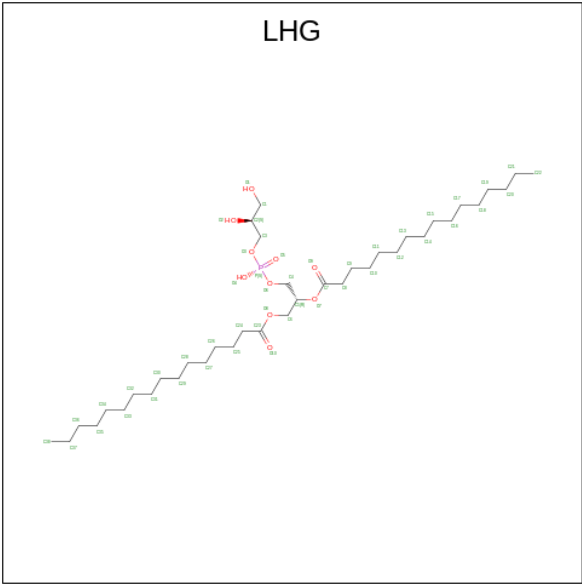
Mol	Chain	Residues	Atoms			AltConf
27	1A	1	Total	C	O	0
			55	53	2	
27	1D	1	Total	C	O	0
			55	53	2	
27	1E	1	Total	C	O	0
			55	53	2	
27	1H	1	Total	C	O	0
			55	53	2	

- Molecule 28 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
28	1A	1	Total	C	O	S	0
			48	35	12	1	
28	1A	1	Total	C	O	S	0
			42	29	12	1	
28	1A	1	Total	C	O	S	0
			45	32	12	1	
28	1B	1	Total	C	O	S	0
			45	32	12	1	
28	1B	1	Total	C	O	S	0
			50	37	12	1	
28	1C	1	Total	C	O	S	0
			51	38	12	1	
28	1C	1	Total	C	O	S	0
			46	33	12	1	
28	1D	1	Total	C	O	S	0
			46	33	12	1	
28	1D	1	Total	C	O	S	0
			43	30	12	1	
28	1M	1	Total	C	O	S	0
			42	29	12	1	

- Molecule 29 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



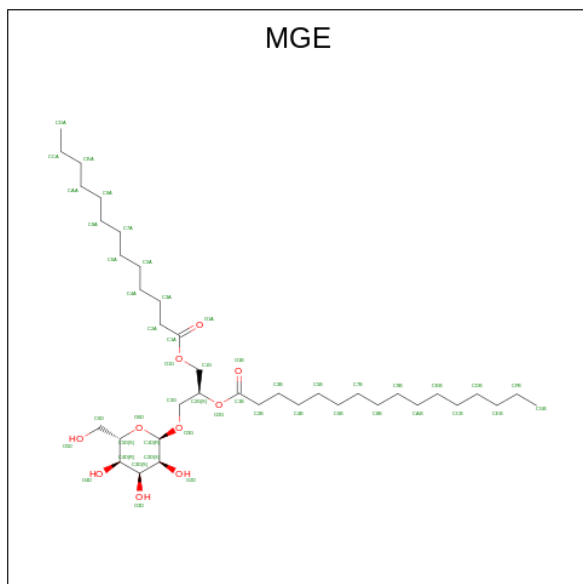
Mol	Chain	Residues	Atoms				AltConf
29	1B	1	Total	C	O	P	0
			38	27	10	1	

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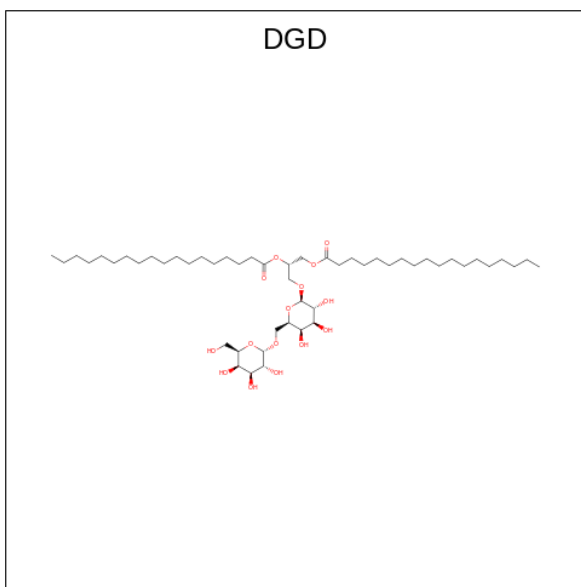
Mol	Chain	Residues	Atoms				AltConf
29	1B	1	Total	C	O	P	0
			39	31	7	1	
29	1C	1	Total	C	O	P	0
			34	23	10	1	
29	1C	1	Total	C	O	P	0
			29	18	10	1	
29	1C	1	Total	C	O	P	0
			32	22	9	1	
29	1C	1	Total	C	O	P	0
			34	23	10	1	
29	1C	1	Total	C	O	P	0
			37	26	10	1	
29	1D	1	Total	C	O	P	0
			31	20	10	1	
29	1D	1	Total	C	O	P	0
			43	32	10	1	
29	1D	1	Total	C	O	P	0
			32	21	10	1	
29	1D	1	Total	C	O	P	0
			41	32	8	1	
29	1E	1	Total	C	O	P	0
			30	19	10	1	
29	1F	1	Total	C	O	P	0
			30	21	8	1	
29	1I	1	Total	C	O	P	0
			32	23	8	1	
29	1I	1	Total	C	O	P	0
			39	28	10	1	
29	1J	1	Total	C	O	P	0
			43	34	8	1	
29	1K	1	Total	C	O	P	0
			43	34	8	1	
29	1L	1	Total	C	O	P	0
			49	38	10	1	
29	1P	1	Total	C	O	P	0
			45	36	8	1	
29	1V	1	Total	C	O	P	0
			49	38	10	1	
29	1W	1	Total	C	O	P	0
			44	33	10	1	
29	1W	1	Total	C	O	P	0
			44	33	10	1	

- Molecule 30 is (1S)-2-(ALPHA-L-ALLOPYRANOSYLOXY)-1-[(TRIDECANOYLOXY)METHYL]ETHYL PALMITATE (CCD ID: MGE) (formula: $C_{38}H_{72}O_{10}$) (labeled as "Ligand of Interest" by depositor).



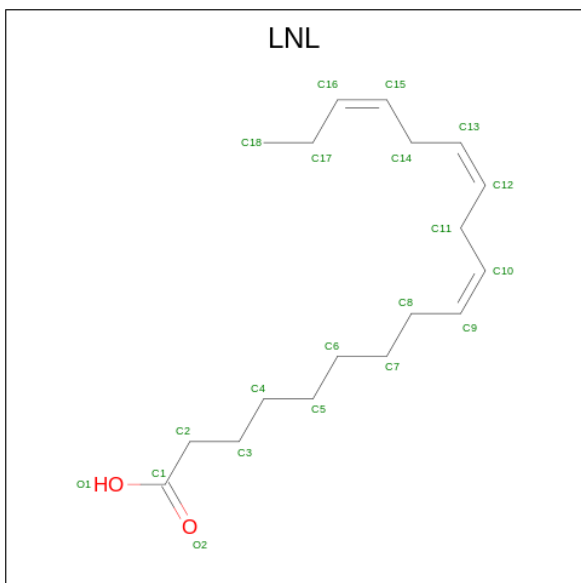
Mol	Chain	Residues	Atoms			AltConf
30	1B	1	Total	C	O	0
			44	34	10	
30	1B	1	Total	C	O	0
			43	33	10	
30	1C	1	Total	C	O	0
			45	35	10	

- Molecule 31 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



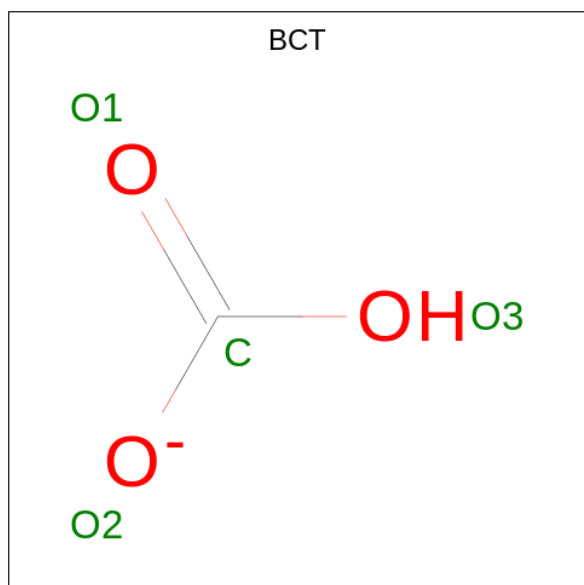
Mol	Chain	Residues	Atoms			AltConf
31	1B	1	Total	C	O	0
			62	47	15	
31	1C	1	Total	C	O	0
			55	40	15	
31	1C	1	Total	C	O	0
			58	43	15	
31	1C	1	Total	C	O	0
			60	45	15	

- Molecule 32 is ALPHA-LINOLENIC ACID (CCD ID: LNL) (formula: $C_{18}H_{30}O_2$) (labeled as "Ligand of Interest" by depositor).



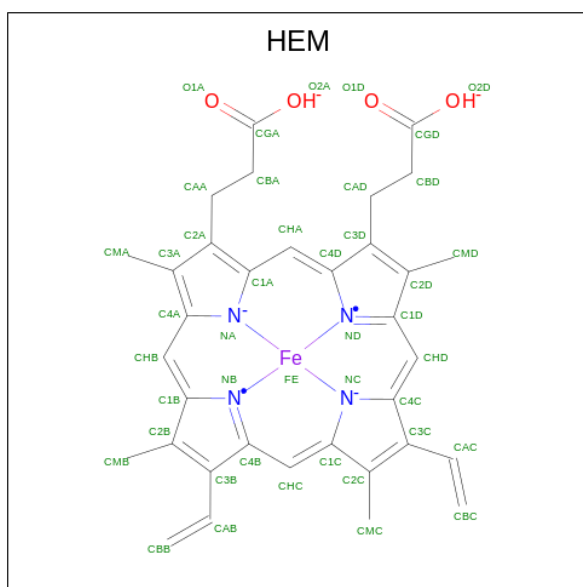
Mol	Chain	Residues	Atoms			AltConf
32	1C	1	Total	C	O	0
			18	16	2	
32	1C	1	Total	C	O	0
			17	15	2	

- Molecule 33 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3) (labeled as "Ligand of Interest" by depositor).



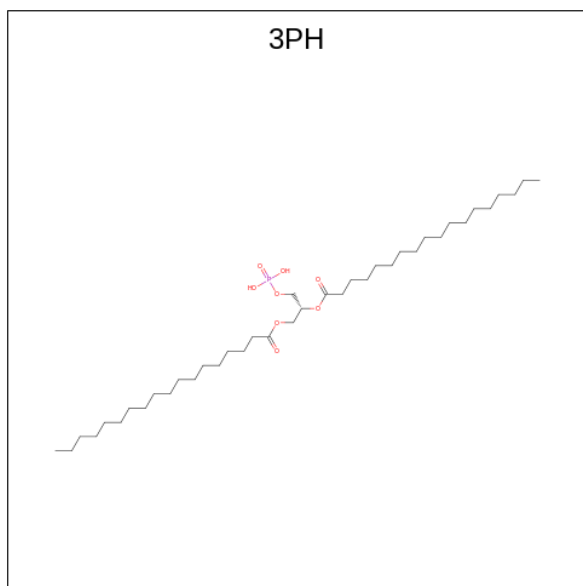
Mol	Chain	Residues	Atoms			AltConf
33	1D	1	Total	C	O	0
			4	1	3	

- Molecule 34 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
34	1E	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 35 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (CCD ID: 3PH) (formula: $C_{39}H_{77}O_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
35	1X	1	Total	C	O	P	0
			39	30	8	1	

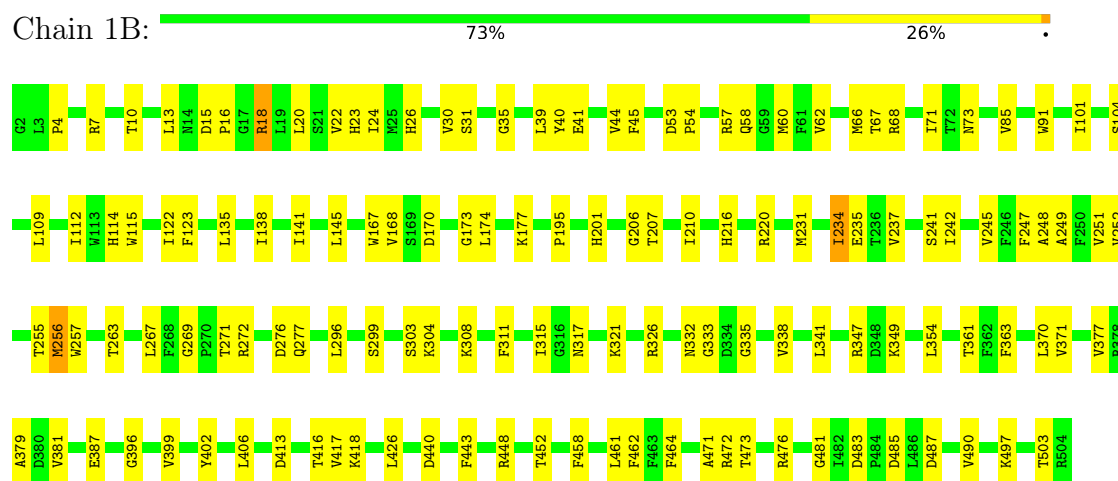
3 Residue-property plots

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.

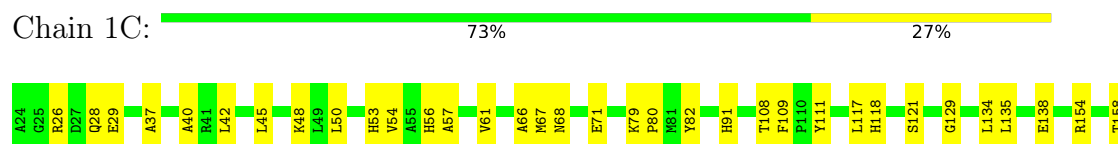
• Molecule 1: Photosystem II protein D1

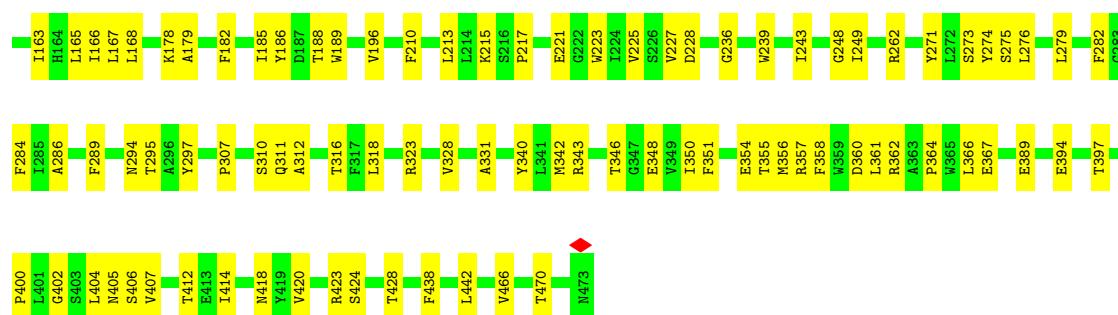


• Molecule 2: Photosystem II CP47 reaction center protein



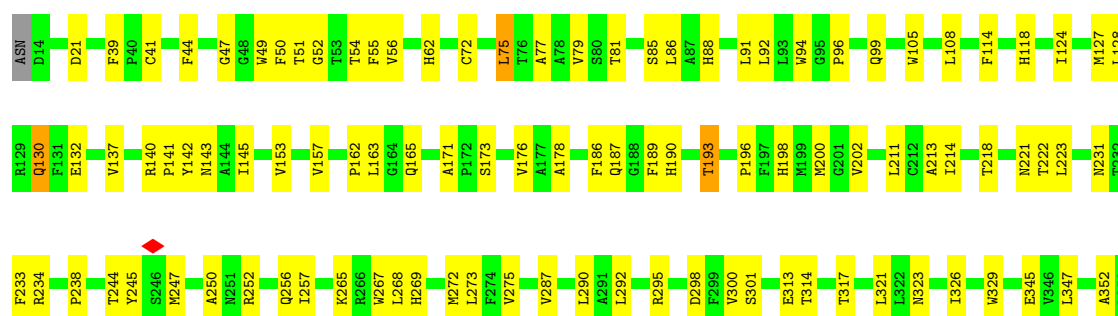
• Molecule 3: Photosystem II CP43 reaction center protein





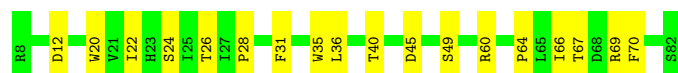
• Molecule 4: Photosystem II D2 protein

Chain 1D: 70% 29% .



• Molecule 5: Cytochrome b559 subunit alpha

Chain 1E: 76% 24% .



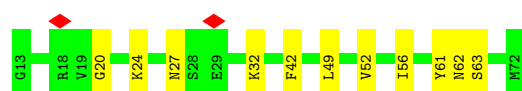
• Molecule 6: Cytochrome b559 subunit beta

Chain 1F: 47% 50% .



• Molecule 7: Photosystem II reaction center protein H

Chain 1H: 82% 18% .



• Molecule 8: Photosystem II reaction center protein I

Chain 1I: 32% 56% 12% .



- Molecule 9: Photosystem II reaction center protein J

Chain 1J: 74% 26%



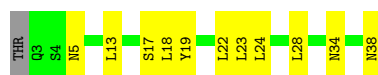
- Molecule 10: Photosystem II reaction center protein K

Chain 1K: 73% 27%



- Molecule 11: Photosystem II reaction center protein L

Chain 1L: 68% 30% .



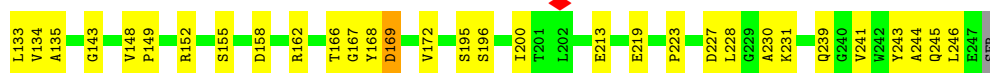
- Molecule 12: Photosystem II reaction center protein M

Chain 1M: 73% 21% . .



- Molecule 13: 33 kDa subunit of oxygen evolving system of photosystem II

Chain 1O: 74% 25%



- Molecule 14: 23 kDa subunit of oxygen evolving system of photosystem II

Chain 1P: 86% 14%



- Molecule 15: Photosystem II reaction center protein T

Chain 1T:  66% 34%



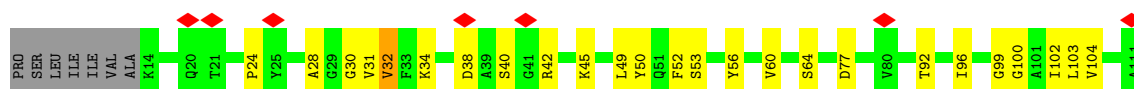
- Molecule 16: Os02g0581100 protein

Chain 1U:  93% 7%



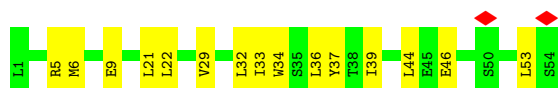
- Molecule 17: Photosystem II 10 kDa polypeptide, chloroplastic

Chain 1V:  70% 23% 7%



- Molecule 18: Photosystem II reaction center W protein, chloroplastic

Chain 1W:  72% 28%



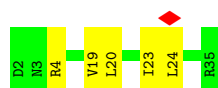
- Molecule 19: Os07g0673550 protein

Chain 1X:  77% 21%



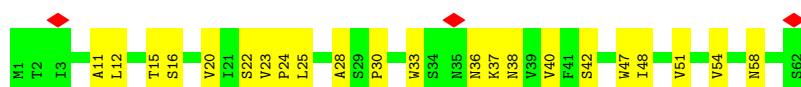
- Molecule 20: Os08g0119800 protein

Chain 1Y:  85% 15%



- Molecule 21: Photosystem II reaction center protein Z

Chain 1Z:  65% 35% 5%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	173752	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.375	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.401	Depositor
Minimum map value	-0.269	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	419.84, 419.84, 419.84	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82, 0.82, 0.82	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 3PH, LHG, BCR, PHO, SQD, CLA, DGD, MGE, BCT, OEX, LNL, HEM, PL9, FE2

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1A	0.31	0/2693	0.62	3/3672 (0.1%)
2	1B	0.27	0/4077	0.52	1/5551 (0.0%)
3	1C	0.24	0/3603	0.49	0/4910
4	1D	0.30	1/2801 (0.0%)	0.59	2/3818 (0.1%)
5	1E	0.26	0/632	0.53	0/860
6	1F	0.43	0/295	0.62	0/400
7	1H	0.25	0/464	0.56	0/630
8	1I	0.51	0/285	0.62	0/385
9	1J	0.24	0/261	0.63	0/353
10	1K	0.28	0/317	0.57	0/433
11	1L	0.26	0/312	0.51	0/424
12	1M	0.34	0/251	0.89	0/344
13	1O	0.25	0/1898	0.59	1/2567 (0.0%)
14	1P	0.19	0/1452	0.48	0/1961
15	1T	0.19	0/269	0.40	0/365
16	1U	0.12	0/211	0.32	0/281
17	1V	0.22	0/731	0.51	0/991
18	1W	0.27	0/419	0.62	0/567
19	1X	0.23	0/279	0.47	0/380
20	1Y	0.29	0/275	0.57	0/376
21	1Z	0.33	0/476	0.70	0/652
All	All	0.28	1/22001 (0.0%)	0.56	7/29920 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	1D	39	PHE	C-N	5.22	1.38	1.33

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	284	TRP	CA-CB-CG	6.19	125.36	113.60
13	1O	49	LYS	N-CA-C	5.71	115.82	108.34
1	1A	168	PHE	N-CA-C	-5.67	106.20	113.01
4	1D	267	TRP	CA-C-N	5.54	132.11	121.54
4	1D	267	TRP	C-N-CA	5.54	132.11	121.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	2612	0	2522	86	0
2	1B	3945	0	3810	104	0
3	1C	3486	0	3396	95	0
4	1D	2708	0	2598	89	0
5	1E	614	0	592	19	0
6	1F	286	0	293	21	0
7	1H	454	0	473	12	0
8	1I	277	0	289	27	0
9	1J	255	0	265	8	0
10	1K	305	0	311	11	0
11	1L	304	0	292	13	0
12	1M	247	0	272	8	0
13	1O	1861	0	1847	42	0
14	1P	1422	0	1384	15	0
15	1T	261	0	280	9	0
16	1U	208	0	221	2	0
17	1V	715	0	721	18	0
18	1W	413	0	401	13	0
19	1X	276	0	303	8	0
20	1Y	270	0	289	5	0
21	1Z	466	0	494	15	0
22	1A	1	0	0	0	0
23	1A	106	0	94	3	0
23	1B	958	0	977	68	0
23	1C	751	0	736	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	1D	222	0	214	17	0
24	1A	128	0	148	7	0
25	1A	10	0	0	0	0
26	1A	40	0	56	4	0
26	1B	120	0	168	15	0
26	1D	40	0	56	4	0
26	1H	40	0	56	2	0
26	1I	40	0	56	6	0
26	1J	40	0	56	4	0
26	1T	40	0	56	1	0
26	1Z	80	0	112	9	0
27	1A	55	0	80	6	0
27	1D	55	0	80	6	0
27	1E	55	0	80	29	0
27	1H	55	0	80	6	0
28	1A	135	0	162	9	0
28	1B	95	0	121	10	0
28	1C	97	0	125	7	0
28	1D	89	0	106	7	0
28	1M	42	0	48	6	0
29	1B	77	0	102	3	0
29	1C	166	0	181	6	0
29	1D	147	0	181	5	0
29	1E	30	0	30	0	0
29	1F	30	0	31	1	0
29	1I	71	0	88	4	0
29	1J	43	0	60	4	0
29	1K	43	0	60	1	0
29	1L	49	0	74	2	0
29	1P	45	0	67	8	0
29	1V	49	0	74	2	0
29	1W	88	0	122	2	0
30	1B	87	0	120	4	0
30	1C	45	0	63	4	0
31	1B	62	0	82	5	0
31	1C	173	0	220	15	0
32	1C	35	0	45	1	0
33	1D	4	0	0	1	0
34	1E	43	0	30	4	0
35	1X	39	0	51	1	0
All	All	26005	0	26401	681	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 13.

The worst 5 of 681 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)
27:1E:102:PL9:H371	29:1P:201:LHG:H202	1.59	0.85
4:1D:130:GLN:NE2	4:1D:143:ASN:OD1	2.09	0.84
2:1B:114:HIS:HE1	23:1B:614:CLA:ND	1.75	0.81
23:1B:613:CLA:HHC	23:1B:613:CLA:HBB1	1.65	0.75
4:1D:252:ARG:HD2	4:1D:256:GLN:HE21	1.52	0.75

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	1A	332/334 (99%)	314 (95%)	18 (5%)	0	100	100
2	1B	501/503 (100%)	476 (95%)	24 (5%)	1 (0%)	43	68
3	1C	448/450 (100%)	427 (95%)	20 (4%)	1 (0%)	43	68
4	1D	338/341 (99%)	319 (94%)	17 (5%)	2 (1%)	21	44
5	1E	73/75 (97%)	68 (93%)	5 (7%)	0	100	100
6	1F	33/36 (92%)	33 (100%)	0	0	100	100
7	1H	58/60 (97%)	53 (91%)	5 (9%)	0	100	100
8	1I	32/34 (94%)	23 (72%)	8 (25%)	1 (3%)	3	8
9	1J	33/35 (94%)	33 (100%)	0	0	100	100
10	1K	35/37 (95%)	32 (91%)	3 (9%)	0	100	100
11	1L	34/37 (92%)	33 (97%)	1 (3%)	0	100	100
12	1M	30/33 (91%)	24 (80%)	5 (17%)	1 (3%)	3	7
13	1O	245/248 (99%)	210 (86%)	35 (14%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	1P	184/186 (99%)	164 (89%)	19 (10%)	1 (0%)	24	48
15	1T	30/32 (94%)	30 (100%)	0	0	100	100
16	1U	25/27 (93%)	23 (92%)	2 (8%)	0	100	100
17	1V	96/105 (91%)	79 (82%)	16 (17%)	1 (1%)	12	32
18	1W	52/54 (96%)	47 (90%)	5 (10%)	0	100	100
19	1X	37/39 (95%)	36 (97%)	1 (3%)	0	100	100
20	1Y	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
21	1Z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
All	All	2708/2762 (98%)	2513 (93%)	187 (7%)	8 (0%)	37	60

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	1B	18	ARG
4	1D	268	LEU
12	1M	3	VAL
14	1P	53	PHE
3	1C	355	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	1A	270/270 (100%)	268 (99%)	2 (1%)	76	90
2	1B	402/402 (100%)	399 (99%)	3 (1%)	76	90
3	1C	346/350 (99%)	344 (99%)	2 (1%)	78	91
4	1D	274/275 (100%)	271 (99%)	3 (1%)	65	85
5	1E	68/68 (100%)	68 (100%)	0	100	100
6	1F	30/31 (97%)	30 (100%)	0	100	100
7	1H	49/49 (100%)	49 (100%)	0	100	100
8	1I	31/31 (100%)	28 (90%)	3 (10%)	8	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	1J	26/26 (100%)	26 (100%)	0	100	100
10	1K	32/32 (100%)	32 (100%)	0	100	100
11	1L	34/35 (97%)	34 (100%)	0	100	100
12	1M	27/29 (93%)	27 (100%)	0	100	100
13	1O	202/204 (99%)	200 (99%)	2 (1%)	68	86
14	1P	149/149 (100%)	149 (100%)	0	100	100
15	1T	29/29 (100%)	28 (97%)	1 (3%)	32	62
16	1U	23/23 (100%)	23 (100%)	0	100	100
17	1V	70/77 (91%)	70 (100%)	0	100	100
18	1W	46/46 (100%)	44 (96%)	2 (4%)	26	54
19	1X	32/32 (100%)	31 (97%)	1 (3%)	35	65
20	1Y	28/28 (100%)	28 (100%)	0	100	100
21	1Z	54/54 (100%)	54 (100%)	0	100	100
All	All	2222/2240 (99%)	2203 (99%)	19 (1%)	68	87

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	1O	169	ASP
18	1W	53	LEU
19	1X	57	SER
18	1W	9	GLU
4	1D	130	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
11	1L	34	ASN
20	1Y	22	ASN
13	1O	27	ASN
20	1Y	29	ASN
16	1U	133	ASN

5.3.3 RNA ⓘ

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 98 ligands modelled in this entry, 1 is monoatomic - leaving 97 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
29	LHG	1F	101	-	29,29,48	0.36	0	32,34,54	0.46	0
28	SQD	1D	412	-	42,43,54	0.44	1 (2%)	51,54,65	0.66	2 (3%)
26	BCR	1A	407	-	41,41,41	1.72	8 (19%)	56,56,56	1.71	12 (21%)
32	LNL	1C	514	-	17,17,19	0.63	0	17,17,19	0.59	0
34	HEM	1E	103	5	50,50,50	1.63	9 (18%)	66,82,82	1.74	12 (18%)
29	LHG	1P	201	-	44,44,48	0.28	0	47,49,54	0.35	0
26	BCR	1H	102	-	41,41,41	1.76	8 (19%)	56,56,56	1.74	14 (25%)
23	CLA	1D	402	-	54,58,73	2.38	18 (33%)	65,95,113	3.20	30 (46%)
23	CLA	1D	405	4	46,50,73	2.51	19 (41%)	55,85,113	3.44	27 (49%)
29	LHG	1L	101	-	48,48,48	0.28	0	51,54,54	0.39	0
27	PL9	1D	407	-	55,55,55	0.81	1 (1%)	68,69,69	0.59	2 (2%)
31	DGD	1C	516	-	56,56,67	0.89	2 (3%)	70,70,81	0.95	3 (4%)
28	SQD	1C	522	-	50,51,54	0.40	1 (2%)	59,62,65	0.44	1 (1%)
23	CLA	1C	509	3	69,73,73	2.12	19 (27%)	83,113,113	2.89	30 (36%)
26	BCR	1B	617	-	41,41,41	1.69	9 (21%)	56,56,56	1.79	13 (23%)
23	CLA	1A	402	1	65,69,73	2.13	19 (29%)	78,108,113	3.03	27 (34%)
24	PHO	1A	403	-	58,69,69	0.80	3 (5%)	56,99,99	1.07	4 (7%)
28	SQD	1A	411	-	44,45,54	0.42	1 (2%)	53,56,65	1.12	5 (9%)
27	PL9	1E	102	-	55,55,55	0.57	1 (1%)	68,69,69	1.92	21 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	MGE	1C	525	-	45,45,48	0.24	0	53,53,56	0.52	0
32	LNL	1C	515	-	16,16,19	0.61	0	15,16,19	0.64	0
26	BCR	1B	618	-	41,41,41	1.71	8 (19%)	56,56,56	1.76	14 (25%)
29	LHG	1B	621	-	37,37,48	0.30	0	40,43,54	0.37	0
35	3PH	1X	101	-	38,38,47	0.70	1 (2%)	42,43,52	0.65	1 (2%)
23	CLA	1C	501	3	69,73,73	2.15	20 (28%)	83,113,113	2.85	29 (34%)
23	CLA	1B	602	2	65,69,73	2.13	19 (29%)	78,108,113	2.74	27 (34%)
26	BCR	1D	406	-	41,41,41	1.76	8 (19%)	56,56,56	1.78	14 (25%)
29	LHG	1V	201	-	48,48,48	0.27	0	51,54,54	0.34	0
30	MGE	1B	624	-	44,44,48	0.25	0	52,52,56	0.65	1 (1%)
30	MGE	1B	625	-	43,43,48	0.33	0	51,51,56	0.53	0
29	LHG	1D	408	-	30,30,48	0.34	0	33,36,54	0.38	0
29	LHG	1D	409	-	42,42,48	0.30	0	45,48,54	0.36	0
29	LHG	1C	520	-	28,28,48	0.38	0	31,34,54	0.45	0
29	LHG	1C	524	-	33,33,48	0.35	0	36,39,54	0.93	1 (2%)
29	LHG	1C	526	-	36,36,48	0.34	0	39,42,54	0.53	1 (2%)
23	CLA	1B	613	-	62,66,73	2.37	19 (30%)	74,104,113	3.19	32 (43%)
28	SQD	1B	620	-	44,45,54	0.43	1 (2%)	53,56,65	0.55	1 (1%)
26	BCR	1I	102	-	41,41,41	1.69	8 (19%)	56,56,56	1.64	12 (21%)
27	PL9	1A	408	-	55,55,55	0.68	1 (1%)	68,69,69	0.72	1 (1%)
31	DGD	1B	626	-	63,63,67	0.86	2 (3%)	77,77,81	0.88	2 (2%)
23	CLA	1B	614	2	49,53,73	2.57	19 (38%)	59,89,113	3.61	27 (45%)
26	BCR	1B	619	-	41,41,41	1.68	9 (21%)	56,56,56	1.98	17 (30%)
23	CLA	1B	605	-	69,73,73	2.07	19 (27%)	83,113,113	2.78	29 (34%)
28	SQD	1A	410	-	41,42,54	0.46	1 (2%)	50,53,65	0.63	1 (2%)
29	LHG	1I	101	-	31,31,48	0.43	0	35,36,54	0.56	1 (2%)
26	BCR	1J	101	-	41,41,41	1.71	9 (21%)	56,56,56	1.95	15 (26%)
29	LHG	1E	101	-	29,29,48	0.31	0	32,35,54	0.40	0
23	CLA	1B	615	-	45,49,73	2.62	19 (42%)	54,84,113	3.50	28 (51%)
23	CLA	1C	513	3	45,49,73	2.58	19 (42%)	54,84,113	3.53	27 (50%)
29	LHG	1K	101	-	42,42,48	0.30	0	45,47,54	0.36	0
23	CLA	1D	404	4	69,73,73	2.01	19 (27%)	83,113,113	2.77	30 (36%)
25	OEX	1A	406	1,3	0,14,14	-	-	-	-	-
23	CLA	1A	405	1	49,53,73	2.44	19 (38%)	59,89,113	3.35	27 (45%)
29	LHG	1I	103	-	38,38,48	0.30	0	41,44,54	0.38	0
23	CLA	1C	510	3	69,73,73	2.10	20 (28%)	83,113,113	2.88	30 (36%)
23	CLA	1D	401	-	69,73,73	2.11	18 (26%)	83,113,113	2.97	32 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	1B	611	2	60,64,73	2.27	18 (30%)	72,102,113	3.14	29 (40%)
23	CLA	1B	607	2	66,70,73	2.16	19 (28%)	79,109,113	3.00	32 (40%)
24	PHO	1A	404	-	58,69,69	0.76	1 (1%)	56,99,99	1.07	4 (7%)
33	BCT	1D	403	22	2,3,3	0.96	0	2,3,3	0.36	0
23	CLA	1C	504	-	69,73,73	2.09	19 (27%)	83,113,113	2.86	29 (34%)
29	LHG	1D	413	-	40,40,48	0.30	0	43,45,54	0.36	0
29	LHG	1B	623	-	35,38,48	0.26	0	36,41,54	0.34	0
26	BCR	1Z	101	-	41,41,41	1.72	8 (19%)	56,56,56	1.68	12 (21%)
23	CLA	1B	604	2	60,64,73	2.25	18 (30%)	72,102,113	3.05	31 (43%)
23	CLA	1B	603	2	69,73,73	2.07	18 (26%)	83,113,113	2.92	30 (36%)
28	SQD	1A	409	-	47,48,54	0.39	1 (2%)	56,59,65	0.45	0
28	SQD	1B	622	-	49,50,54	0.42	1 (2%)	58,61,65	0.64	1 (1%)
23	CLA	1B	601	2	69,73,73	2.05	19 (27%)	83,113,113	2.89	31 (37%)
23	CLA	1B	612	2	69,73,73	2.09	19 (27%)	83,113,113	2.83	30 (36%)
28	SQD	1M	101	-	41,42,54	0.45	1 (2%)	50,53,65	0.46	0
29	LHG	1C	519	-	33,33,48	0.32	0	36,39,54	0.37	0
29	LHG	1W	101	-	43,43,48	0.30	0	46,49,54	0.37	0
23	CLA	1C	505	3	64,68,73	2.17	19 (29%)	77,107,113	2.97	30 (38%)
23	CLA	1C	507	3	62,66,73	2.18	19 (30%)	74,104,113	2.95	28 (37%)
23	CLA	1B	606	2	69,73,73	2.05	18 (26%)	83,113,113	2.67	29 (34%)
23	CLA	1C	511	-	50,54,73	2.41	19 (38%)	60,90,113	3.37	28 (46%)
26	BCR	1T	101	-	41,41,41	1.87	9 (21%)	56,56,56	2.15	19 (33%)
23	CLA	1C	508	3	69,73,73	2.12	19 (27%)	83,113,113	2.95	31 (37%)
29	LHG	1C	521	-	30,31,48	0.34	0	33,37,54	0.41	0
31	DGD	1C	517	-	59,59,67	0.88	2 (3%)	73,73,81	1.03	5 (6%)
31	DGD	1C	518	-	61,61,67	0.86	2 (3%)	75,75,81	0.96	4 (5%)
23	CLA	1B	610	-	69,73,73	2.03	17 (24%)	83,113,113	2.77	31 (37%)
23	CLA	1C	506	-	53,57,73	2.38	19 (35%)	62,93,113	3.32	28 (45%)
23	CLA	1C	512	3	59,63,73	2.31	18 (30%)	71,101,113	3.11	33 (46%)
26	BCR	1Z	102	-	41,41,41	1.68	8 (19%)	56,56,56	1.83	17 (30%)
28	SQD	1C	523	-	45,46,54	0.44	1 (2%)	54,57,65	0.40	0
23	CLA	1B	608	-	69,73,73	2.13	18 (26%)	83,113,113	2.90	28 (33%)
23	CLA	1C	503	3	60,64,73	2.23	20 (33%)	72,102,113	3.11	30 (41%)
27	PL9	1H	101	-	55,55,55	0.69	1 (1%)	68,69,69	0.76	1 (1%)
28	SQD	1D	411	-	45,46,54	0.44	0	54,57,65	1.05	6 (11%)
29	LHG	1J	102	-	42,42,48	0.30	0	45,47,54	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	1B	609	2	69,73,73	2.05	19 (27%)	83,113,113	2.71	28 (33%)
29	LHG	1D	410	-	31,31,48	0.34	0	34,37,54	0.47	0
29	LHG	1W	102	-	43,43,48	0.31	0	46,49,54	0.73	1 (2%)
23	CLA	1B	616	2	63,67,73	2.17	19 (30%)	75,105,113	3.11	33 (44%)
23	CLA	1C	502	3	65,69,73	2.11	18 (27%)	78,108,113	2.93	29 (37%)

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
29	LHG	1F	101	-	-	10/33/33/53	-
28	SQD	1D	412	-	-	4/38/58/69	0/1/1/1
26	BCR	1A	407	-	-	3/29/63/63	0/2/2/2
32	LNL	1C	514	-	-	7/15/15/17	-
34	HEM	1E	103	5	-	6/14/54/54	-
29	LHG	1P	201	-	-	6/48/48/53	-
26	BCR	1H	102	-	-	5/29/63/63	0/2/2/2
23	CLA	1D	402	-	-	8/21/97/115	-
23	CLA	1D	405	4	-	4/12/88/115	-
29	LHG	1L	101	-	-	10/53/53/53	-
27	PL9	1D	407	-	-	6/53/73/73	0/1/1/1
31	DGD	1C	516	-	-	6/44/84/95	0/2/2/2
28	SQD	1C	522	-	-	5/46/66/69	0/1/1/1
23	CLA	1C	509	3	1/1/15/20	11/39/115/115	-
26	BCR	1B	617	-	-	4/29/63/63	0/2/2/2
23	CLA	1A	402	1	1/1/14/20	8/35/111/115	-
24	PHO	1A	403	-	-	7/37/103/103	0/5/6/6
28	SQD	1A	411	-	-	9/40/60/69	0/1/1/1
27	PL9	1E	102	-	-	10/53/73/73	0/1/1/1
30	MGE	1C	525	-	-	6/40/60/63	0/1/1/1
32	LNL	1C	515	-	-	3/14/14/17	-
26	BCR	1B	618	-	-	3/29/63/63	0/2/2/2
29	LHG	1B	621	-	-	6/42/42/53	-
35	3PH	1X	101	-	-	18/40/40/49	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	1C	501	3	1/1/15/20	9/39/115/115	-
23	CLA	1B	602	2	1/1/14/20	14/35/111/115	-
26	BCR	1D	406	-	-	4/29/63/63	0/2/2/2
29	LHG	1V	201	-	-	9/53/53/53	-
30	MGE	1B	624	-	-	8/39/59/63	0/1/1/1
30	MGE	1B	625	-	-	4/38/58/63	0/1/1/1
29	LHG	1D	408	-	-	2/35/35/53	-
29	LHG	1D	409	-	-	7/47/47/53	-
29	LHG	1C	520	-	-	4/33/33/53	-
29	LHG	1C	524	-	-	11/38/38/53	-
29	LHG	1C	526	-	-	12/41/41/53	-
23	CLA	1B	613	-	1/1/13/20	6/31/107/115	-
28	SQD	1B	620	-	-	7/40/60/69	0/1/1/1
26	BCR	1I	102	-	-	3/29/63/63	0/2/2/2
27	PL9	1A	408	-	-	11/53/73/73	0/1/1/1
31	DGD	1B	626	-	-	10/51/91/95	0/2/2/2
23	CLA	1B	614	2	-	6/15/91/115	-
26	BCR	1B	619	-	-	4/29/63/63	0/2/2/2
23	CLA	1B	605	-	1/1/15/20	11/39/115/115	-
28	SQD	1A	410	-	-	4/37/57/69	0/1/1/1
29	LHG	1I	101	-	-	3/33/33/53	-
26	BCR	1J	101	-	-	5/29/63/63	0/2/2/2
29	LHG	1E	101	-	-	8/34/34/53	-
23	CLA	1B	615	-	-	4/10/86/115	-
23	CLA	1C	513	3	-	5/10/86/115	-
29	LHG	1K	101	-	-	12/46/46/53	-
23	CLA	1D	404	4	1/1/15/20	15/39/115/115	-
23	CLA	1A	405	1	-	3/15/91/115	-
29	LHG	1I	103	-	-	4/43/43/53	-
23	CLA	1C	510	3	1/1/15/20	5/39/115/115	-
23	CLA	1D	401	-	1/1/15/20	7/39/115/115	-
23	CLA	1B	611	2	1/1/13/20	8/29/105/115	-
23	CLA	1B	607	2	1/1/14/20	10/36/112/115	-
24	PHO	1A	404	-	-	10/37/103/103	0/5/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	1C	504	-	1/1/15/20	7/39/115/115	-
29	LHG	1D	413	-	-	2/44/44/53	-
29	LHG	1B	623	-	-	7/38/40/53	-
26	BCR	1Z	101	-	-	2/29/63/63	0/2/2/2
23	CLA	1B	604	2	1/1/13/20	6/29/105/115	-
23	CLA	1B	603	2	1/1/15/20	10/39/115/115	-
28	SQD	1A	409	-	-	2/43/63/69	0/1/1/1
28	SQD	1B	622	-	-	6/45/65/69	0/1/1/1
23	CLA	1B	601	2	1/1/15/20	15/39/115/115	-
23	CLA	1B	612	2	1/1/15/20	16/39/115/115	-
28	SQD	1M	101	-	-	5/37/57/69	0/1/1/1
29	LHG	1C	519	-	-	9/38/38/53	-
29	LHG	1W	101	-	-	13/48/48/53	-
23	CLA	1C	505	3	1/1/14/20	16/33/109/115	-
23	CLA	1C	507	3	1/1/13/20	6/31/107/115	-
23	CLA	1B	606	2	1/1/15/20	8/39/115/115	-
23	CLA	1C	511	-	-	7/17/93/115	-
26	BCR	1T	101	-	-	7/29/63/63	0/2/2/2
23	CLA	1C	508	3	1/1/15/20	14/39/115/115	-
29	LHG	1C	521	-	-	4/35/35/53	-
31	DGD	1C	517	-	-	11/47/87/95	0/2/2/2
31	DGD	1C	518	-	-	7/49/89/95	0/2/2/2
23	CLA	1B	610	-	1/1/15/20	17/39/115/115	-
23	CLA	1C	512	3	1/1/13/20	10/27/103/115	-
23	CLA	1C	506	-	-	7/20/96/115	-
26	BCR	1Z	102	-	-	4/29/63/63	0/2/2/2
28	SQD	1C	523	-	-	6/41/61/69	0/1/1/1
23	CLA	1C	503	3	1/1/13/20	6/29/105/115	-
23	CLA	1B	608	-	1/1/15/20	17/39/115/115	-
27	PL9	1H	101	-	-	18/53/73/73	0/1/1/1
28	SQD	1D	411	-	-	9/41/61/69	0/1/1/1
29	LHG	1J	102	-	-	12/46/46/53	-
23	CLA	1B	609	2	1/1/15/20	11/39/115/115	-
29	LHG	1D	410	-	-	3/36/36/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	LHG	1W	102	-	-	21/48/48/53	-
23	CLA	1B	616	2	1/1/13/20	5/32/108/115	-
23	CLA	1C	502	3	1/1/14/20	10/35/111/115	-

The worst 5 of 784 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	1B	613	CLA	C1D-ND	10.60	1.50	1.37
23	1B	614	CLA	C1D-ND	8.78	1.48	1.37
23	1C	508	CLA	C1D-ND	8.73	1.48	1.37
23	1B	607	CLA	C1D-ND	8.73	1.48	1.37
23	1B	608	CLA	C1D-ND	8.64	1.48	1.37

The worst 5 of 1271 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	1B	613	CLA	C1D-ND-C4D	-11.20	98.38	106.33
23	1B	614	CLA	C1D-ND-C4D	-10.35	98.99	106.33
23	1C	513	CLA	C1D-ND-C4D	-10.26	99.05	106.33
23	1C	508	CLA	C2C-C1C-NC	10.21	119.54	109.97
23	1D	401	CLA	C1D-ND-C4D	-10.08	99.18	106.33

5 of 27 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	1A	402	CLA	C8
23	1B	601	CLA	C8
23	1B	602	CLA	C8
23	1B	603	CLA	C8
23	1B	604	CLA	C8

5 of 746 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	1B	601	CLA	C2B-C3B-CAB-CBB
23	1B	601	CLA	C4B-C3B-CAB-CBB
23	1B	602	CLA	C4B-C3B-CAB-CBB
23	1B	602	CLA	C6-C7-C8-C9
23	1B	610	CLA	C1A-C2A-CAA-CBA

There are no ring outliers.

89 monomers are involved in 286 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	1F	101	LHG	1	0
28	1D	412	SQD	4	0
26	1A	407	BCR	4	0
32	1C	514	LNL	1	0
34	1E	103	HEM	4	0
29	1P	201	LHG	8	0
26	1H	102	BCR	2	0
23	1D	402	CLA	1	0
23	1D	405	CLA	2	0
29	1L	101	LHG	2	0
27	1D	407	PL9	6	0
31	1C	516	DGD	9	0
28	1C	522	SQD	4	0
23	1C	509	CLA	2	0
26	1B	617	BCR	6	0
23	1A	402	CLA	3	0
24	1A	403	PHO	6	0
28	1A	411	SQD	2	0
27	1E	102	PL9	29	0
30	1C	525	MGE	4	0
26	1B	618	BCR	3	0
29	1B	621	LHG	2	0
35	1X	101	3PH	1	0
23	1C	501	CLA	2	0
23	1B	602	CLA	3	0
26	1D	406	BCR	4	0
29	1V	201	LHG	2	0
30	1B	624	MGE	2	0
30	1B	625	MGE	2	0
29	1D	408	LHG	1	0
29	1D	409	LHG	2	0
29	1C	526	LHG	3	0
23	1B	613	CLA	10	0
28	1B	620	SQD	8	0
26	1I	102	BCR	6	0
27	1A	408	PL9	6	0
31	1B	626	DGD	5	0
23	1B	614	CLA	6	0
26	1B	619	BCR	6	0
23	1B	605	CLA	2	0
28	1A	410	SQD	2	0
29	1I	101	LHG	1	0

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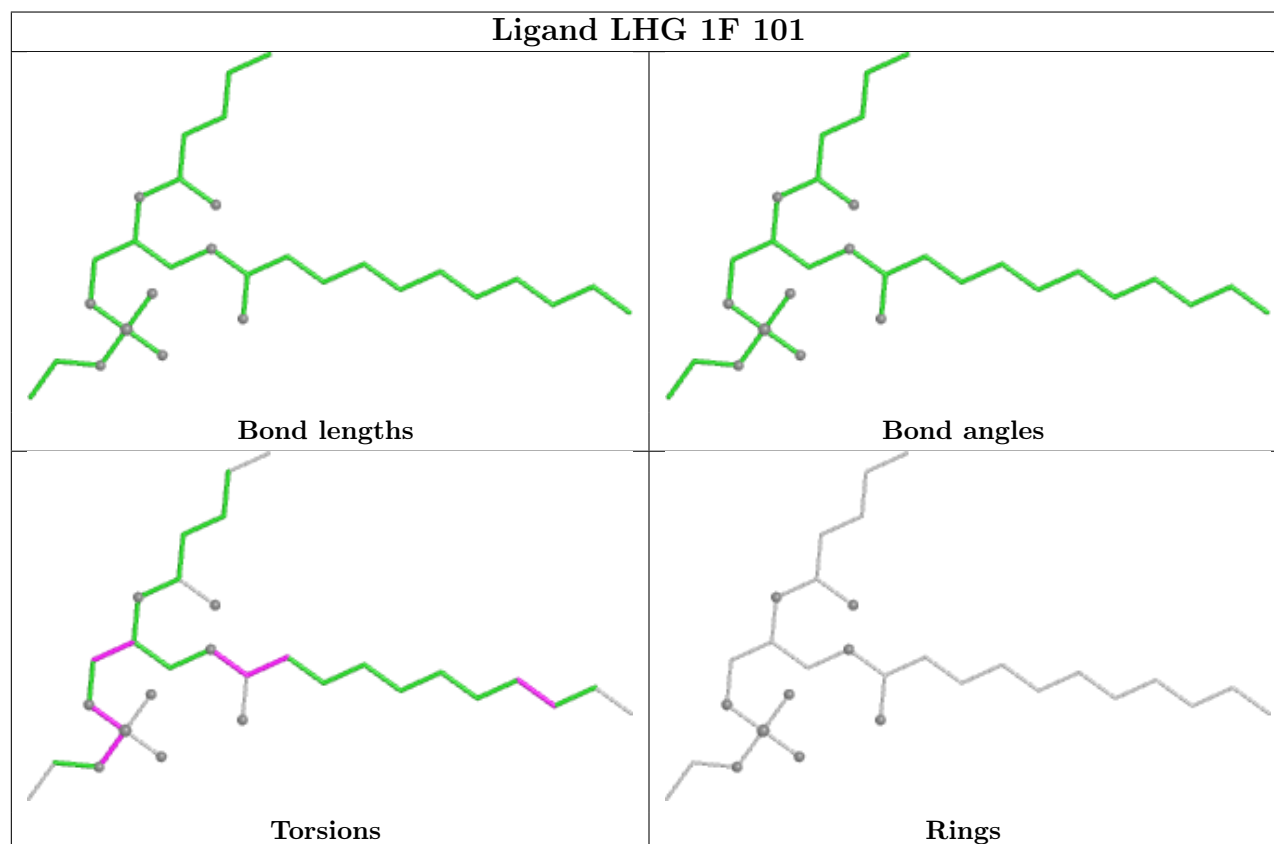
Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	1J	101	BCR	4	0
23	1C	513	CLA	2	0
29	1K	101	LHG	1	0
23	1D	404	CLA	7	0
29	1I	103	LHG	3	0
23	1C	510	CLA	5	0
23	1D	401	CLA	8	0
23	1B	611	CLA	8	0
23	1B	607	CLA	7	0
24	1A	404	PHO	1	0
33	1D	403	BCT	1	0
23	1C	504	CLA	2	0
29	1B	623	LHG	1	0
26	1Z	101	BCR	4	0
23	1B	604	CLA	2	0
23	1B	603	CLA	4	0
28	1A	409	SQD	5	0
28	1B	622	SQD	2	0
23	1B	601	CLA	5	0
23	1B	612	CLA	6	0
28	1M	101	SQD	6	0
29	1C	519	LHG	1	0
29	1W	101	LHG	1	0
23	1C	505	CLA	4	0
23	1C	507	CLA	5	0
23	1B	606	CLA	5	0
23	1C	511	CLA	1	0
26	1T	101	BCR	1	0
23	1C	508	CLA	8	0
29	1C	521	LHG	2	0
31	1C	517	DGD	5	0
31	1C	518	DGD	1	0
23	1B	610	CLA	8	0
23	1C	506	CLA	2	0
23	1C	512	CLA	3	0
26	1Z	102	BCR	5	0
28	1C	523	SQD	3	0
23	1B	608	CLA	7	0
23	1C	503	CLA	1	0
27	1H	101	PL9	6	0
28	1D	411	SQD	3	0
29	1J	102	LHG	4	0

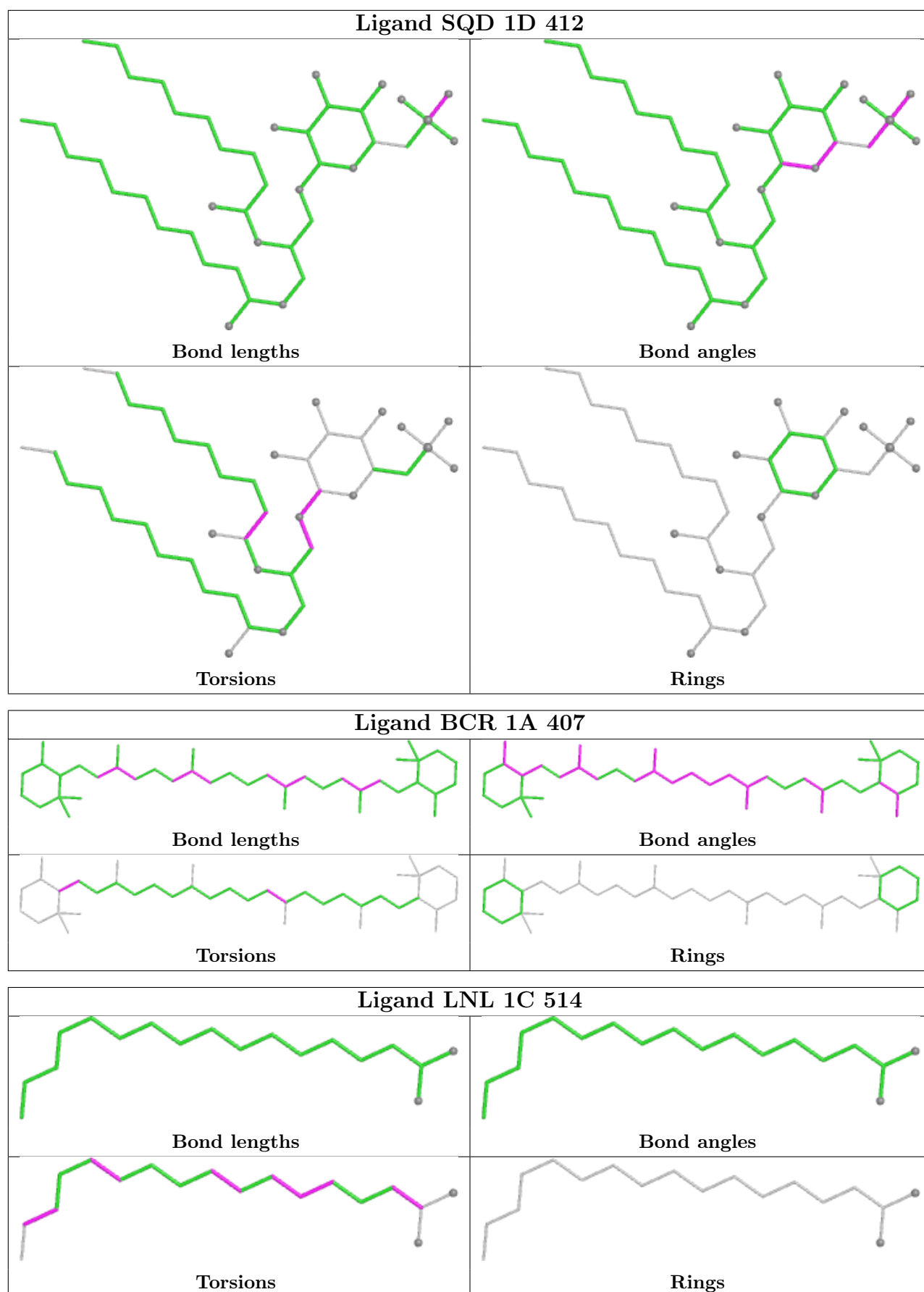
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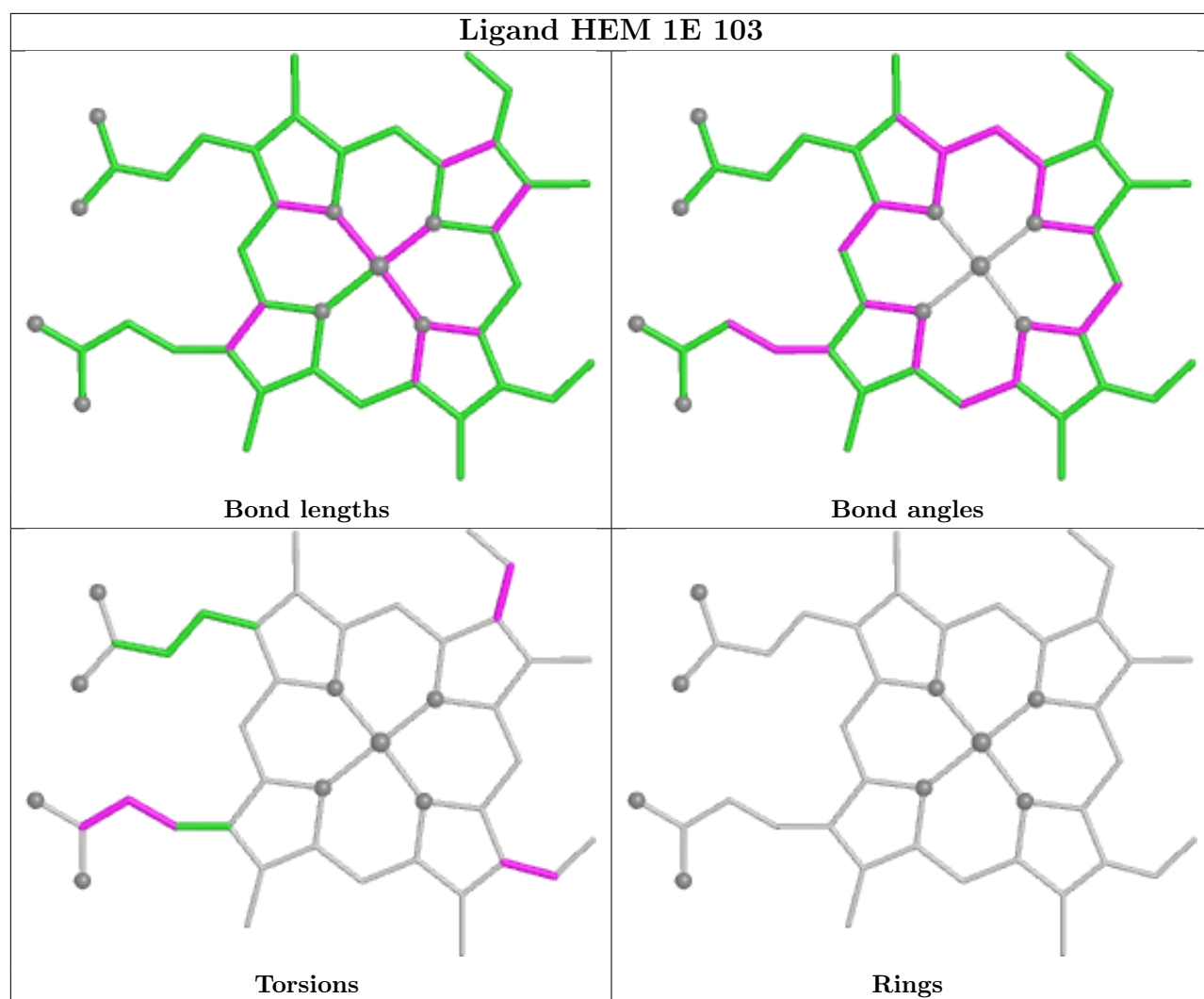
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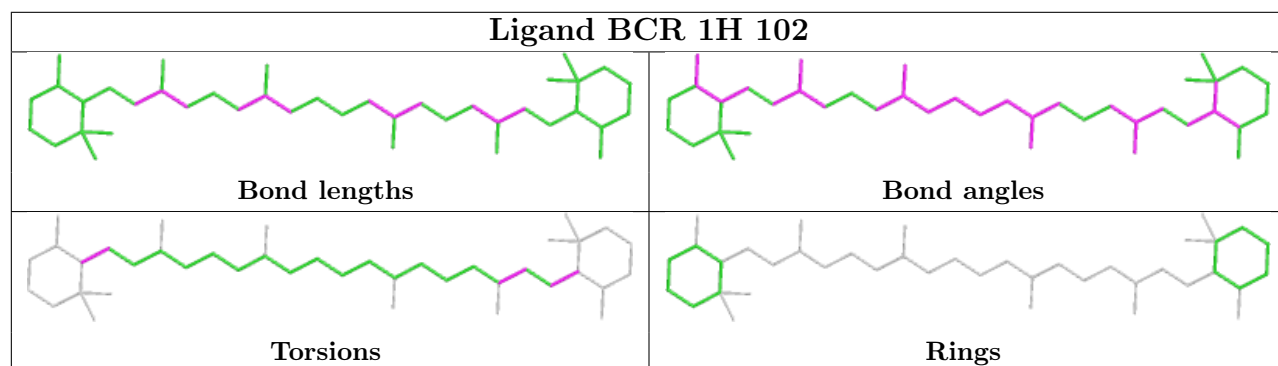
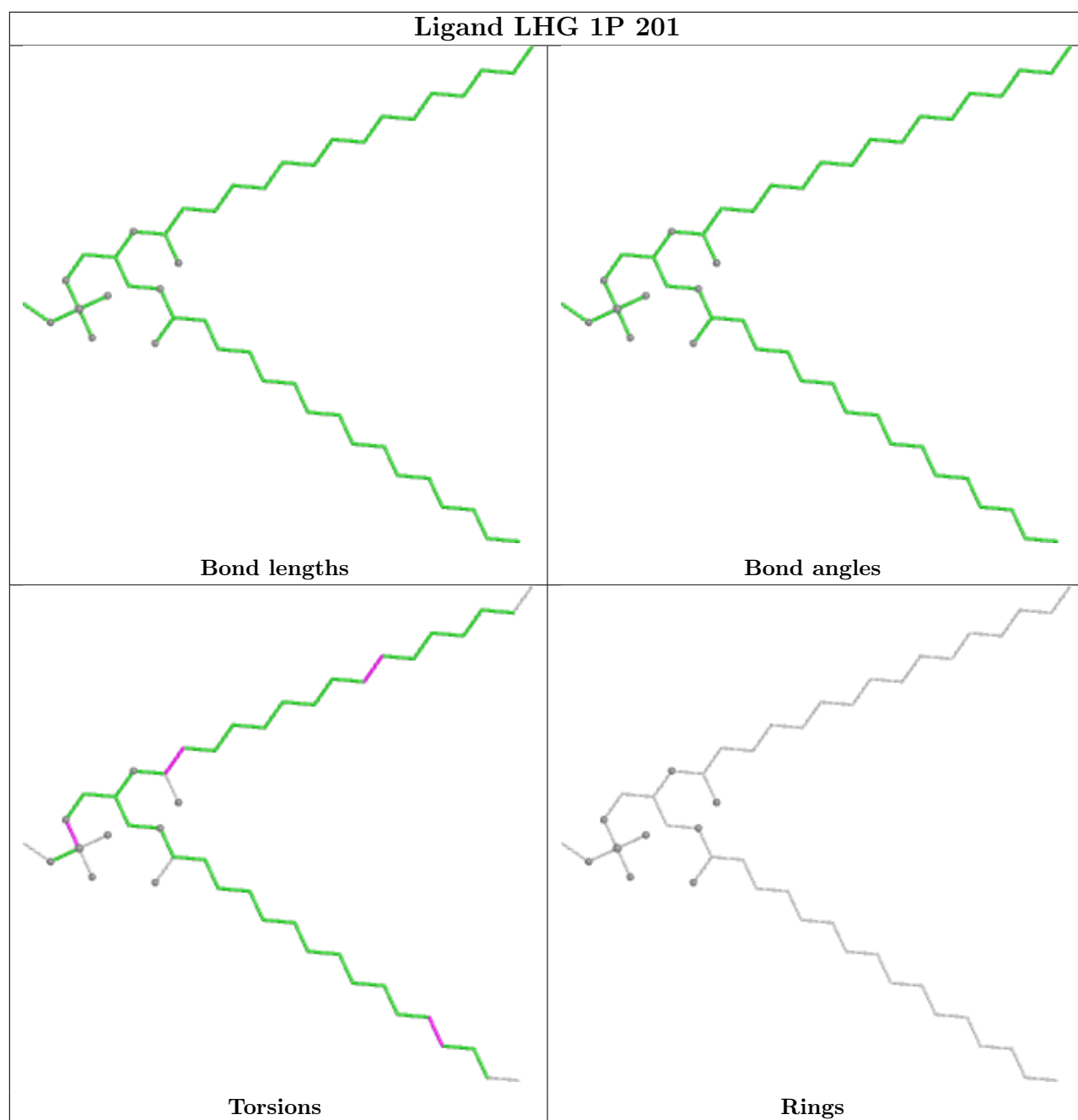
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	1B	609	CLA	8	0
29	1D	410	LHG	2	0
29	1W	102	LHG	2	0
23	1B	616	CLA	4	0
23	1C	502	CLA	2	0

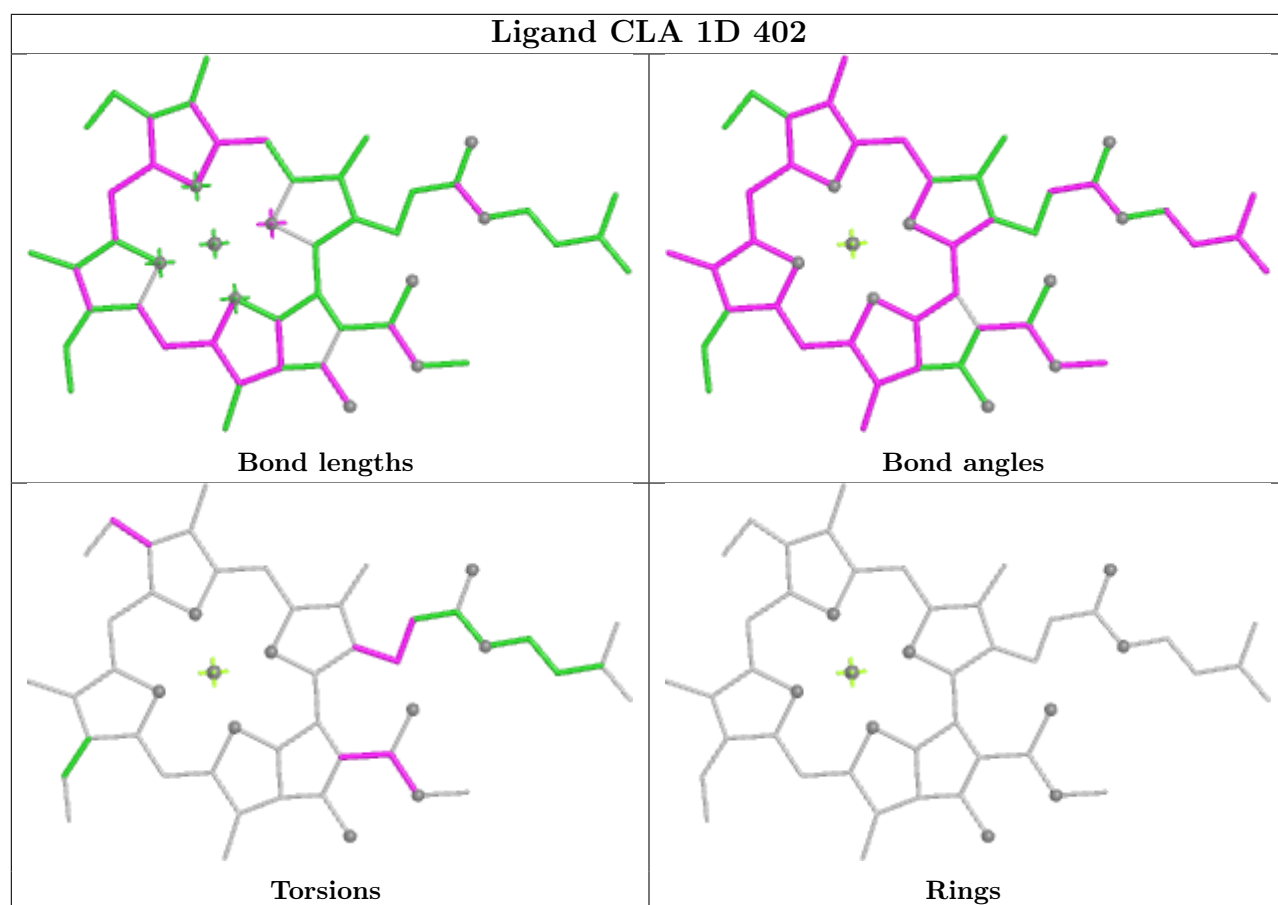
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



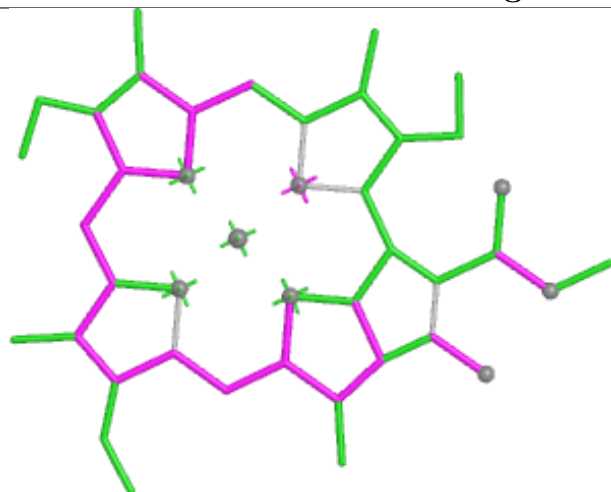




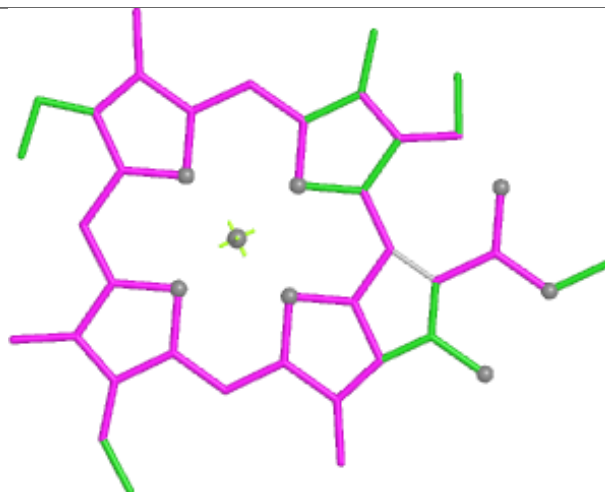




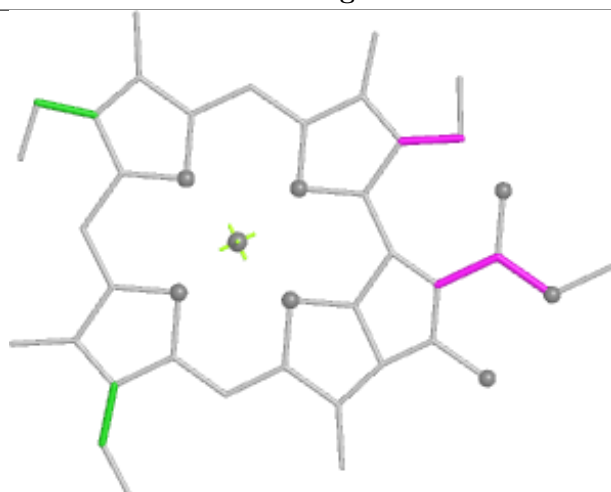
Ligand CLA 1D 405



Bond lengths



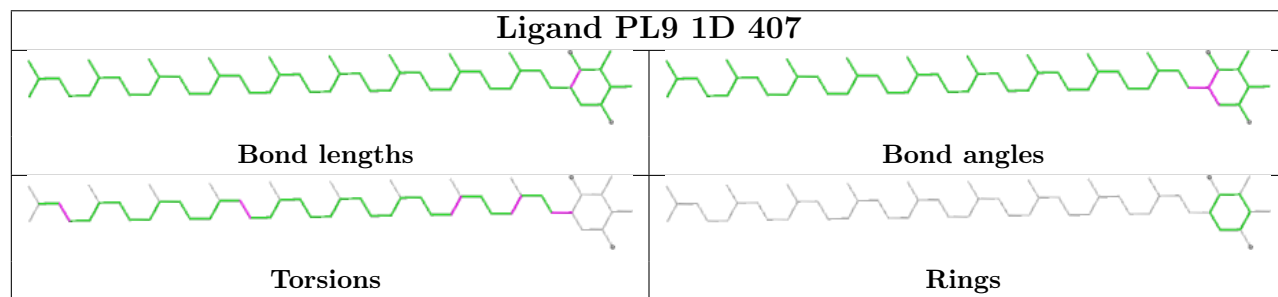
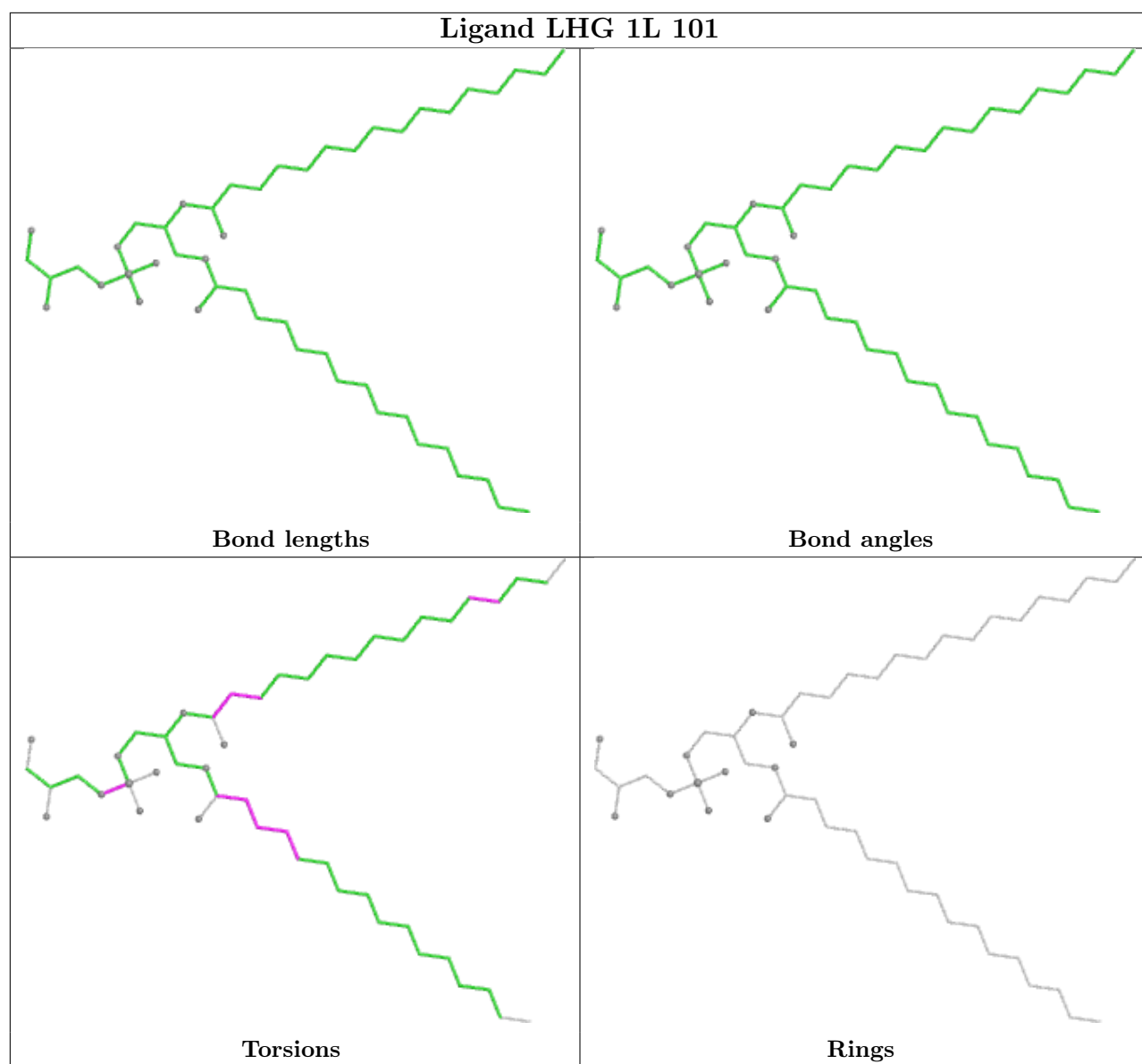
Bond angles

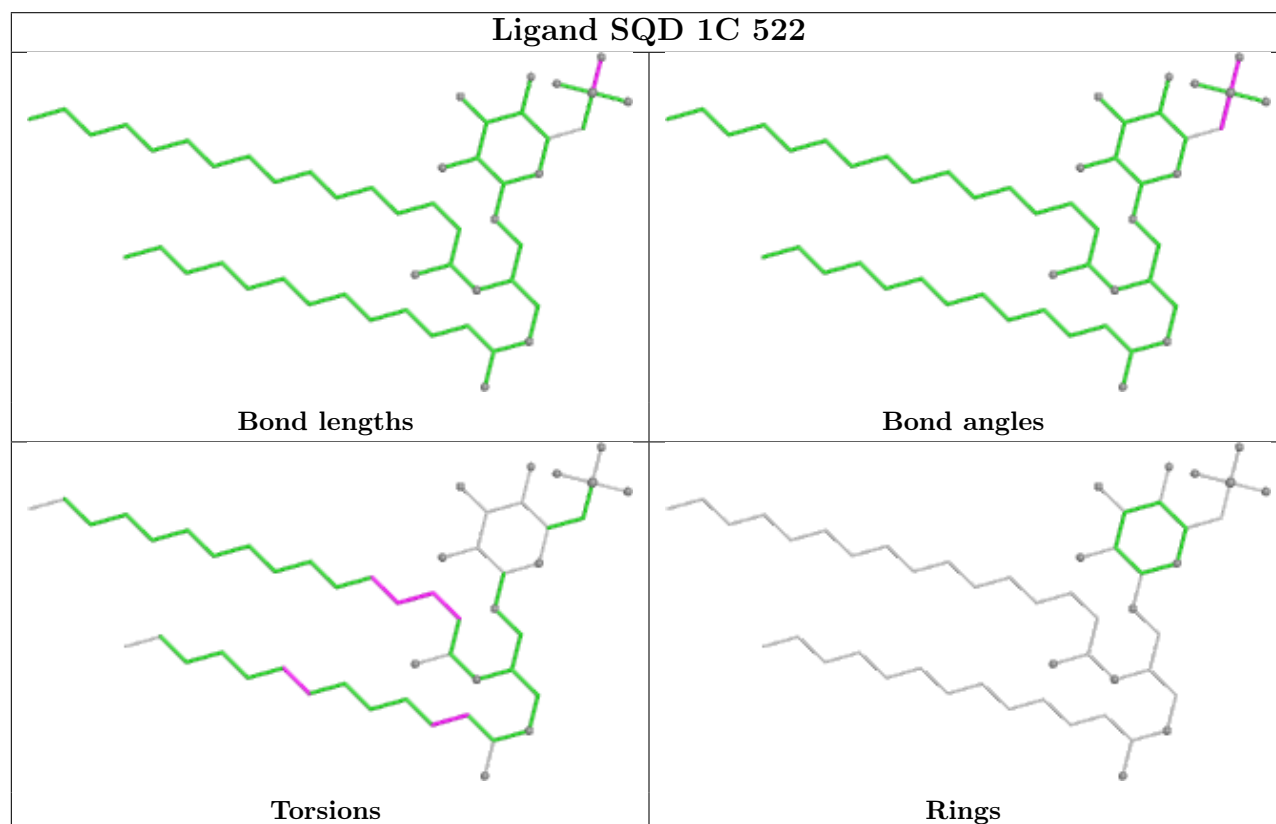
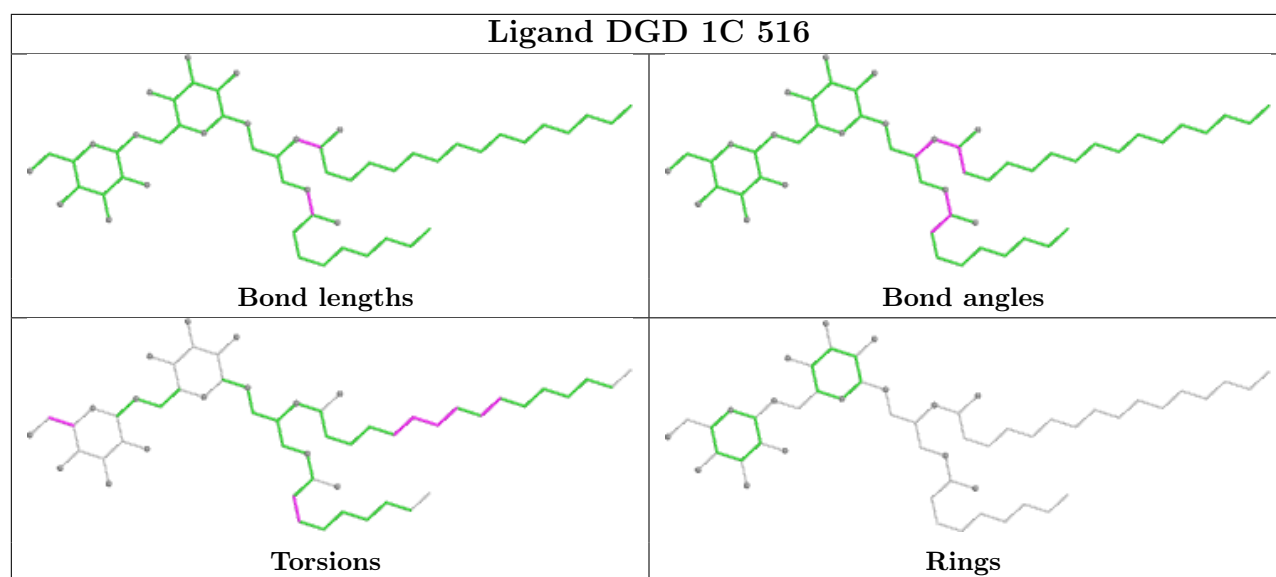


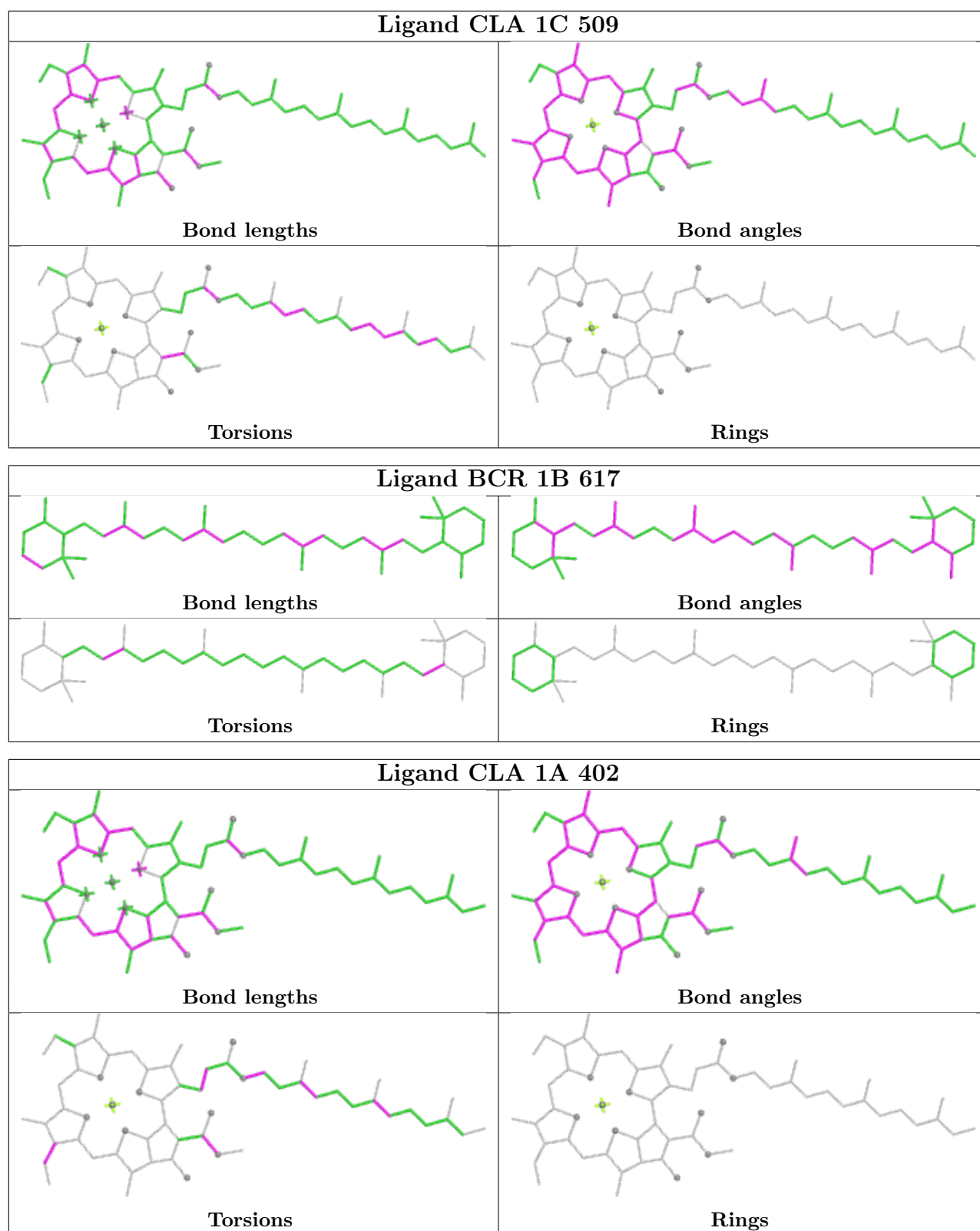
Torsions

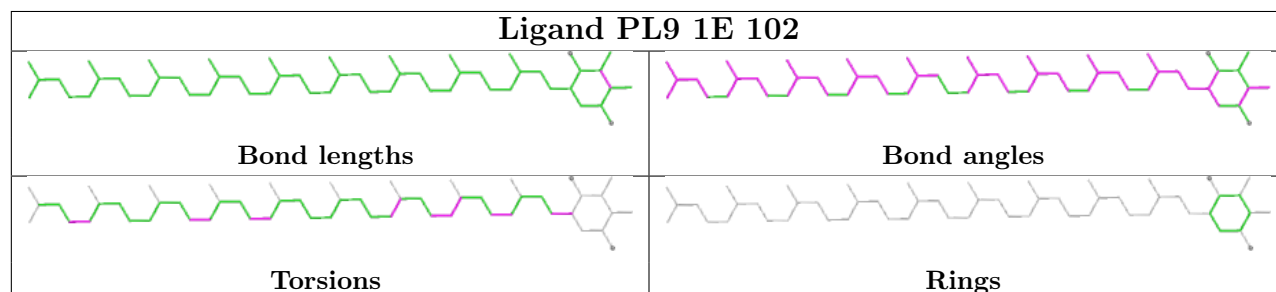
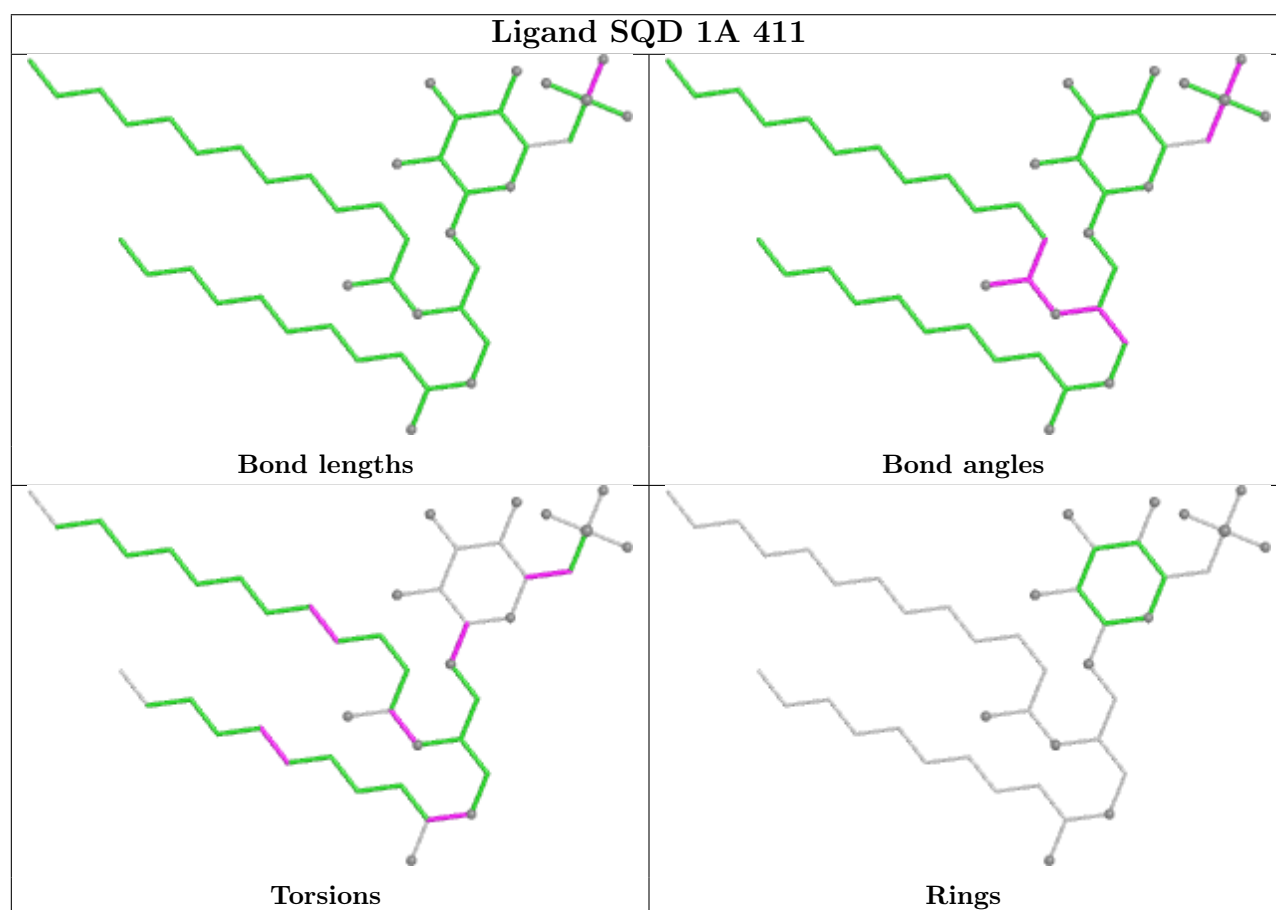
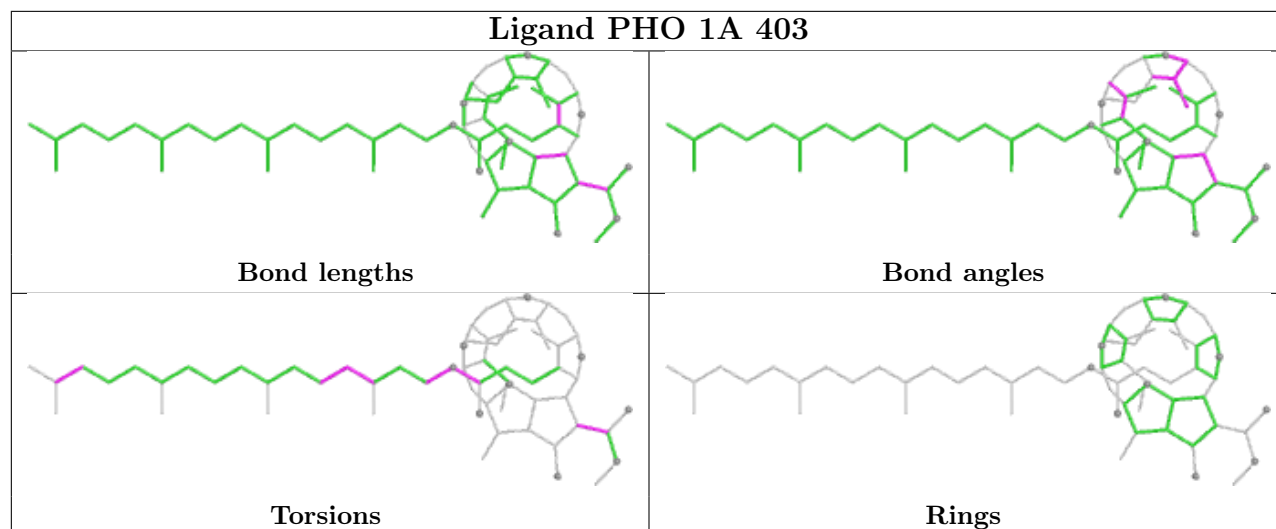


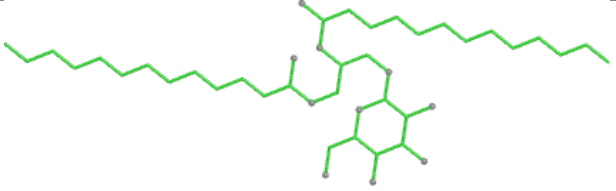
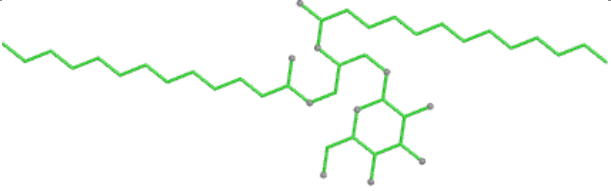
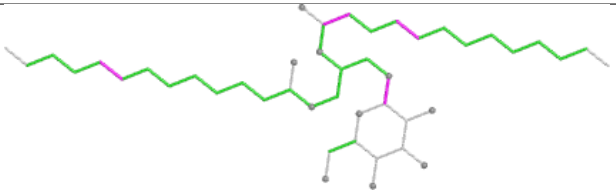
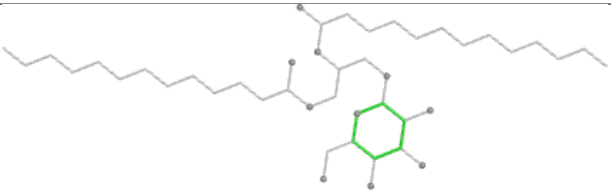
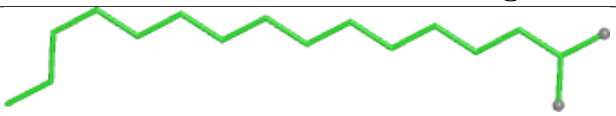
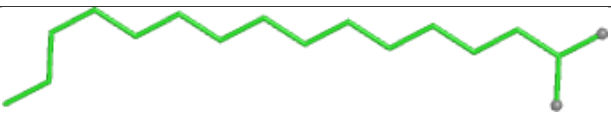
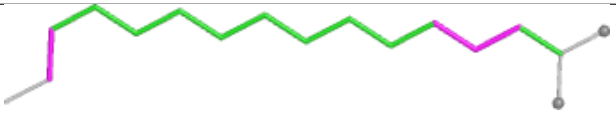
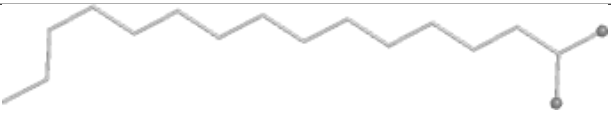
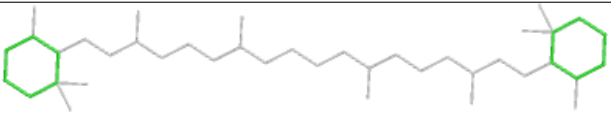
Rings

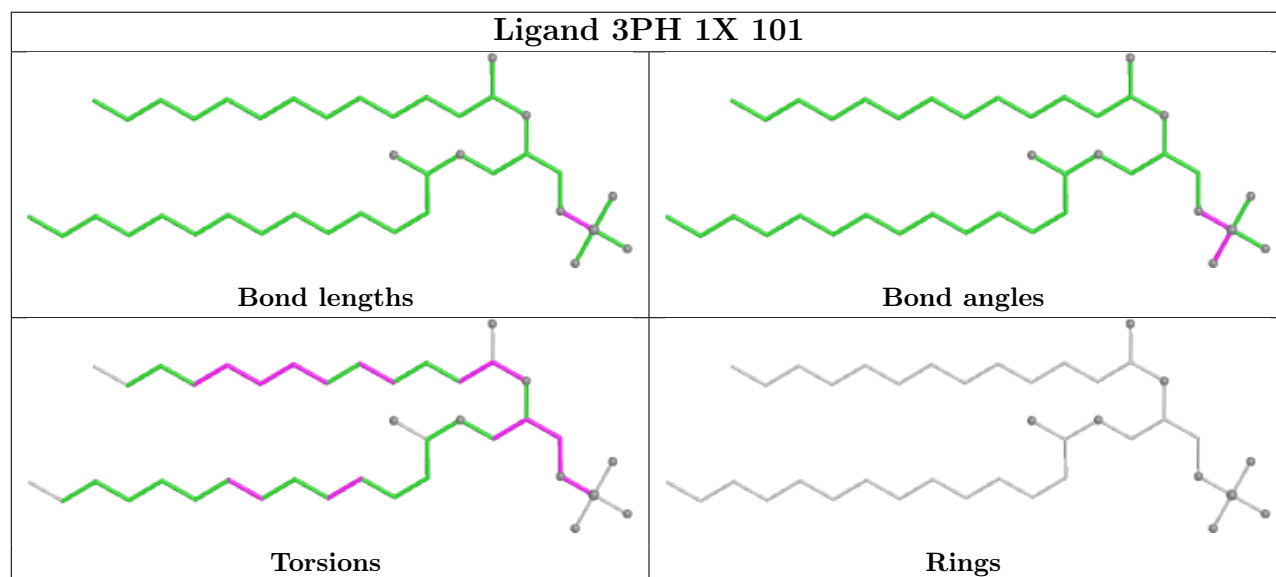
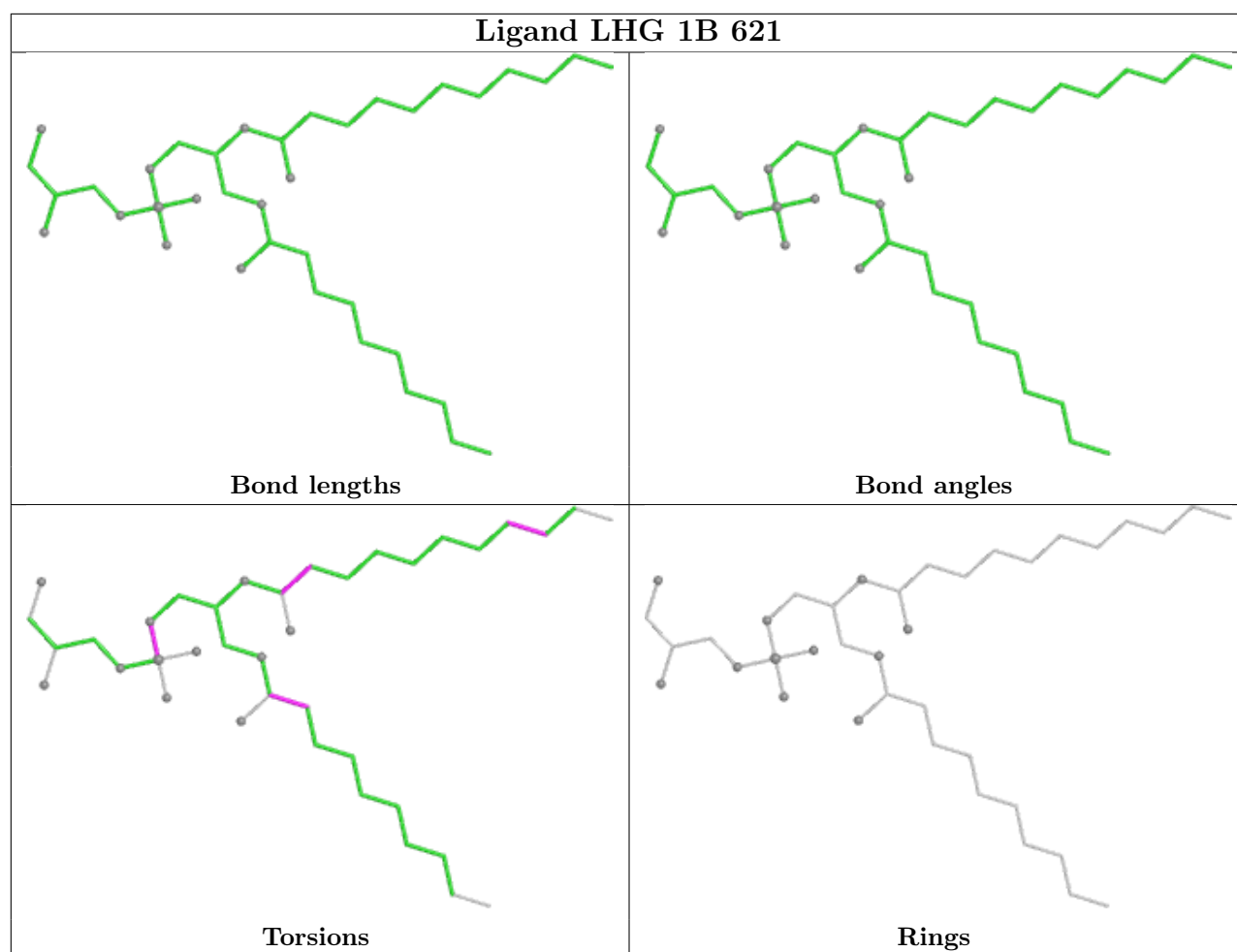


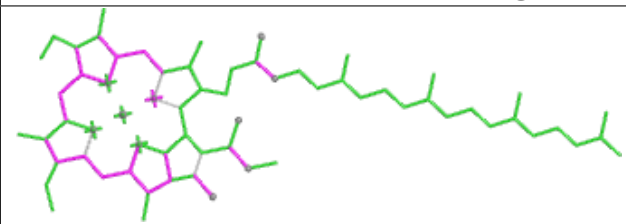
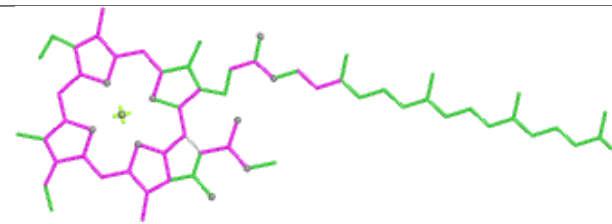
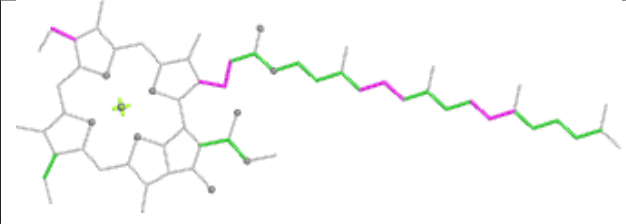
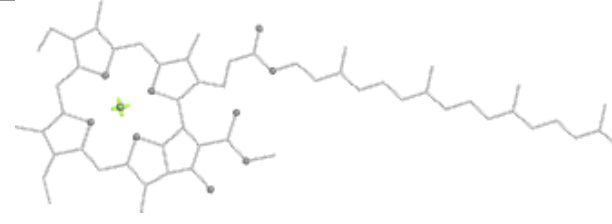


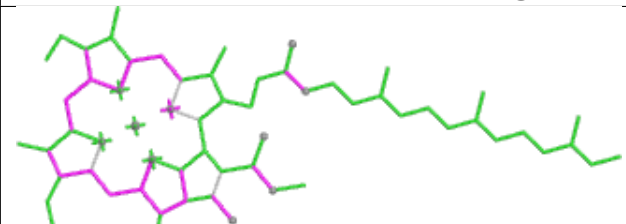
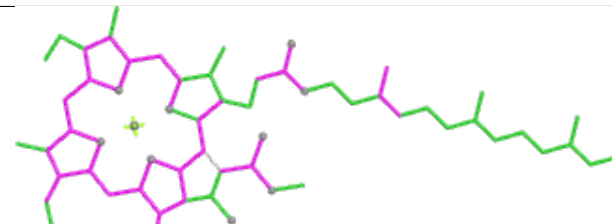
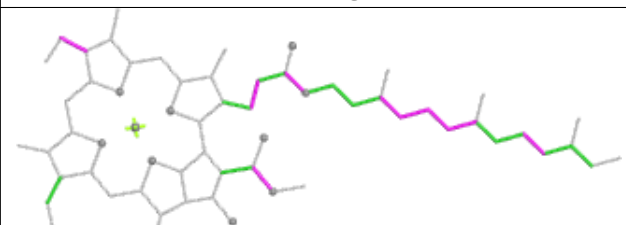
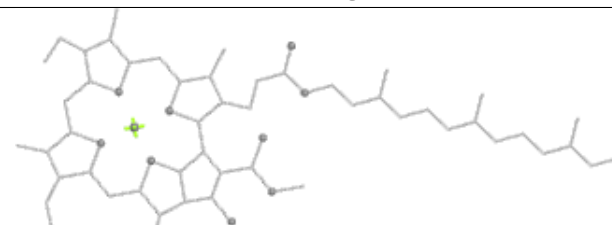


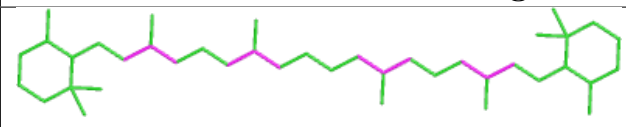
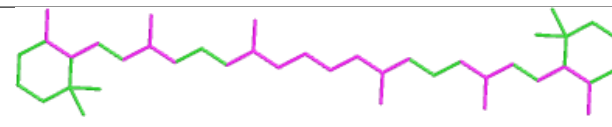
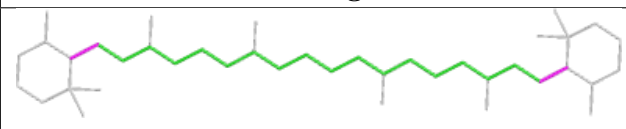
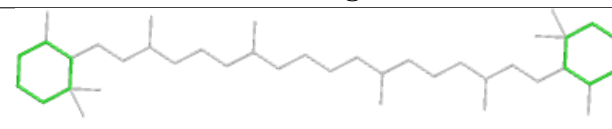


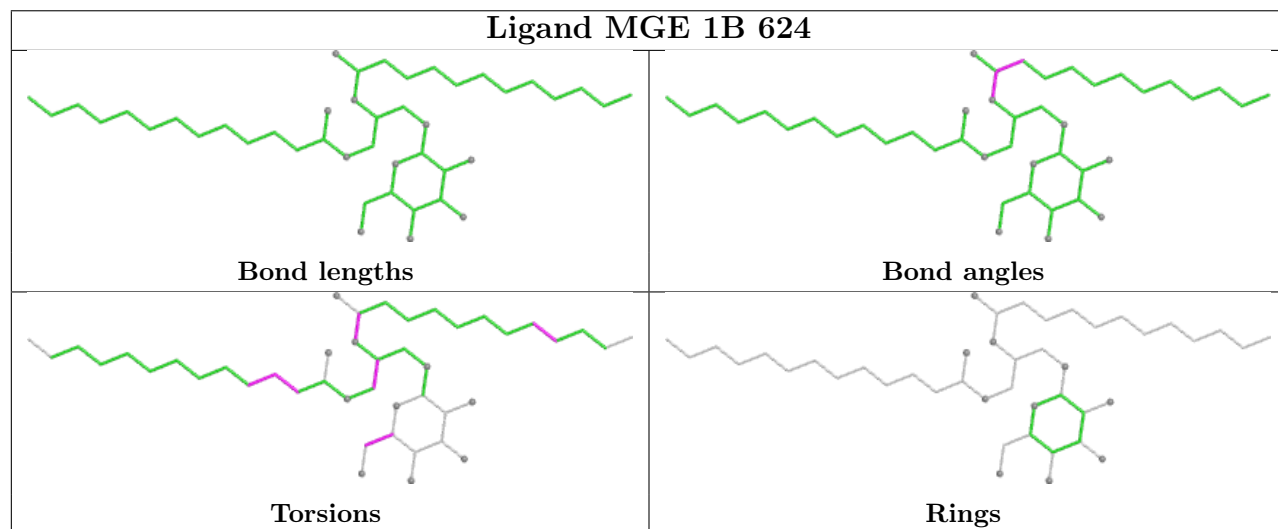
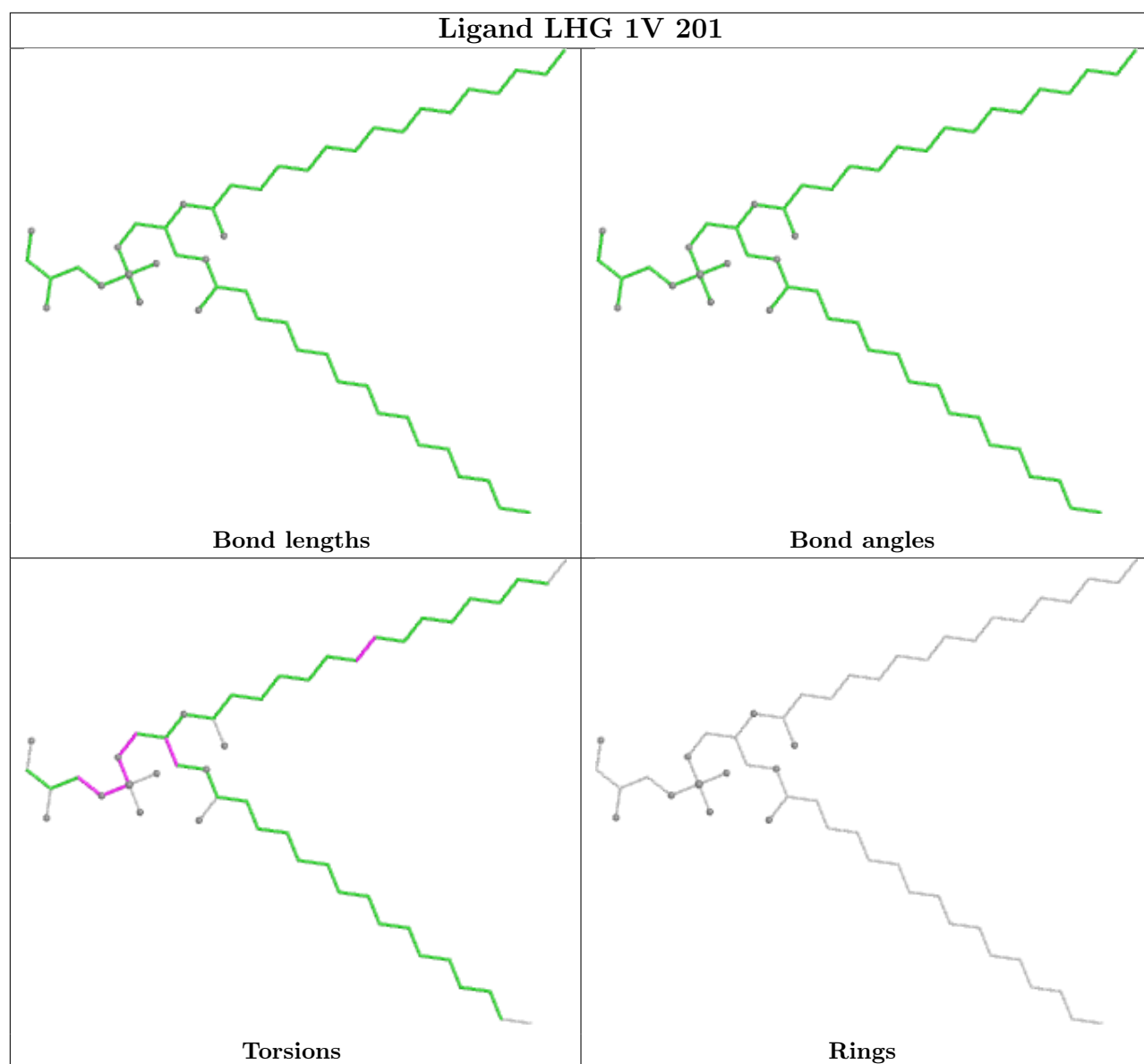
Ligand MGE 1C 525			
 Bond lengths		 Bond angles	
 Torsions		 Rings	
Ligand LNL 1C 515			
 Bond lengths		 Bond angles	
 Torsions		 Rings	
Ligand BCR 1B 618			
 Bond lengths		 Bond angles	
 Torsions		 Rings	

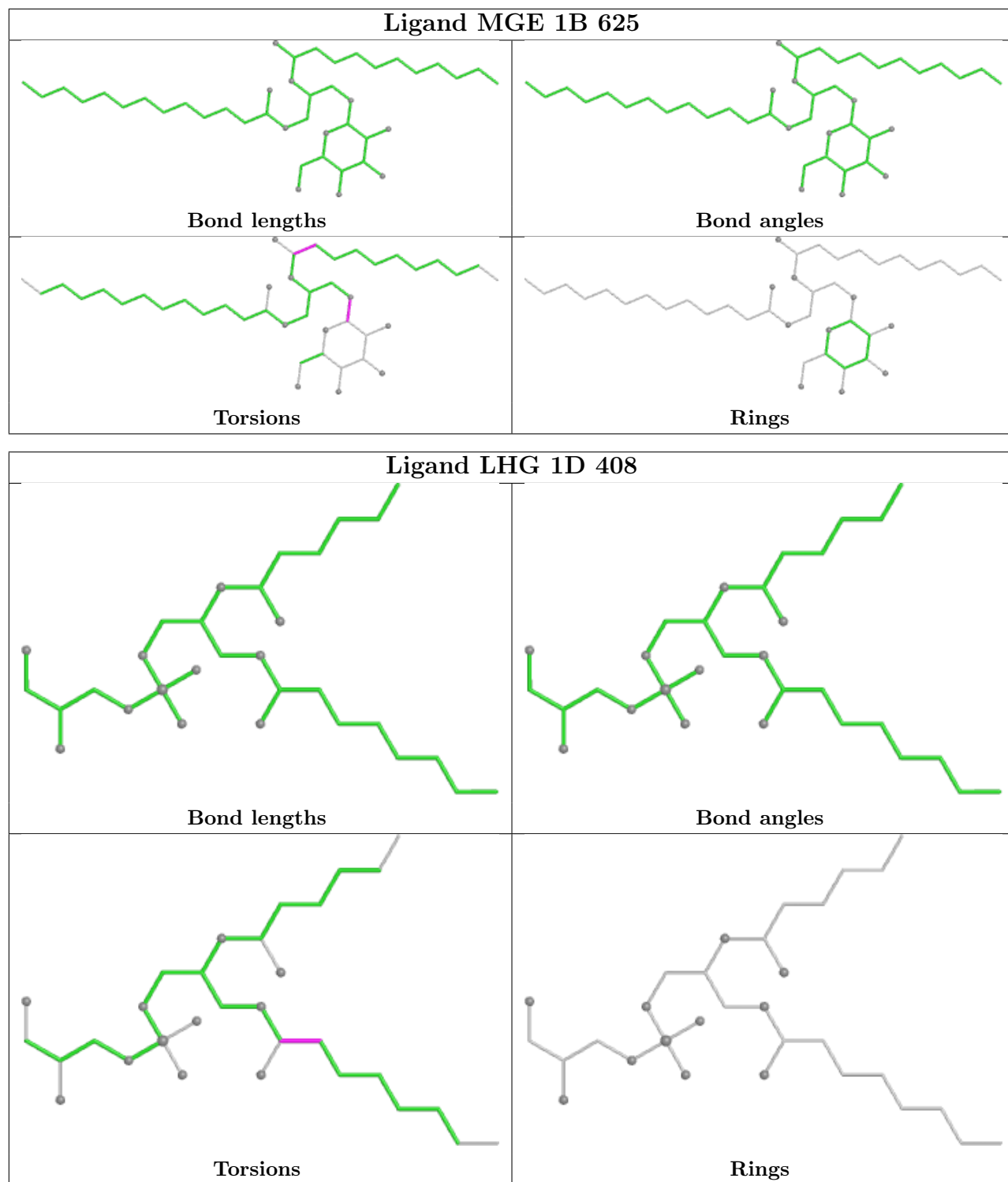


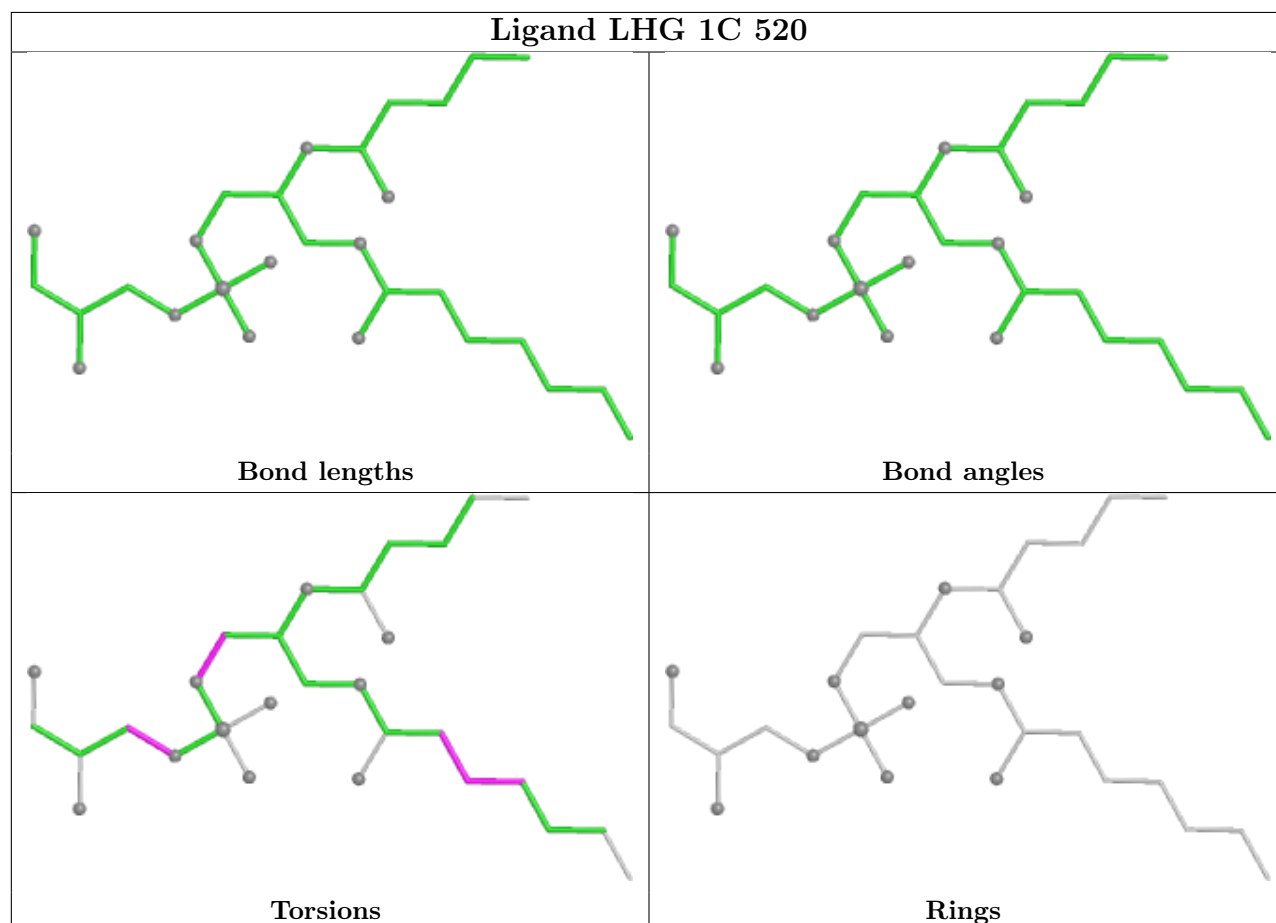
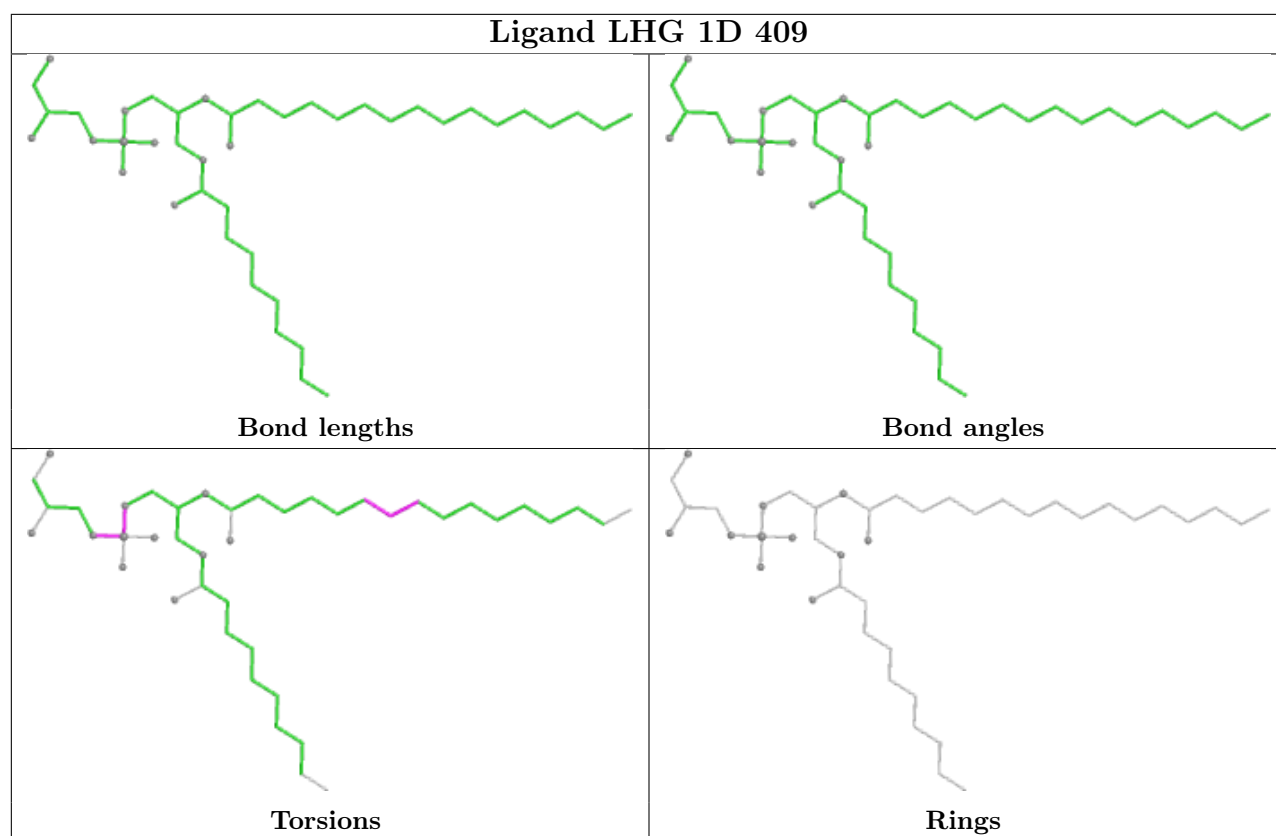
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Bond lengths	Bond angles
	
Torsions	Rings

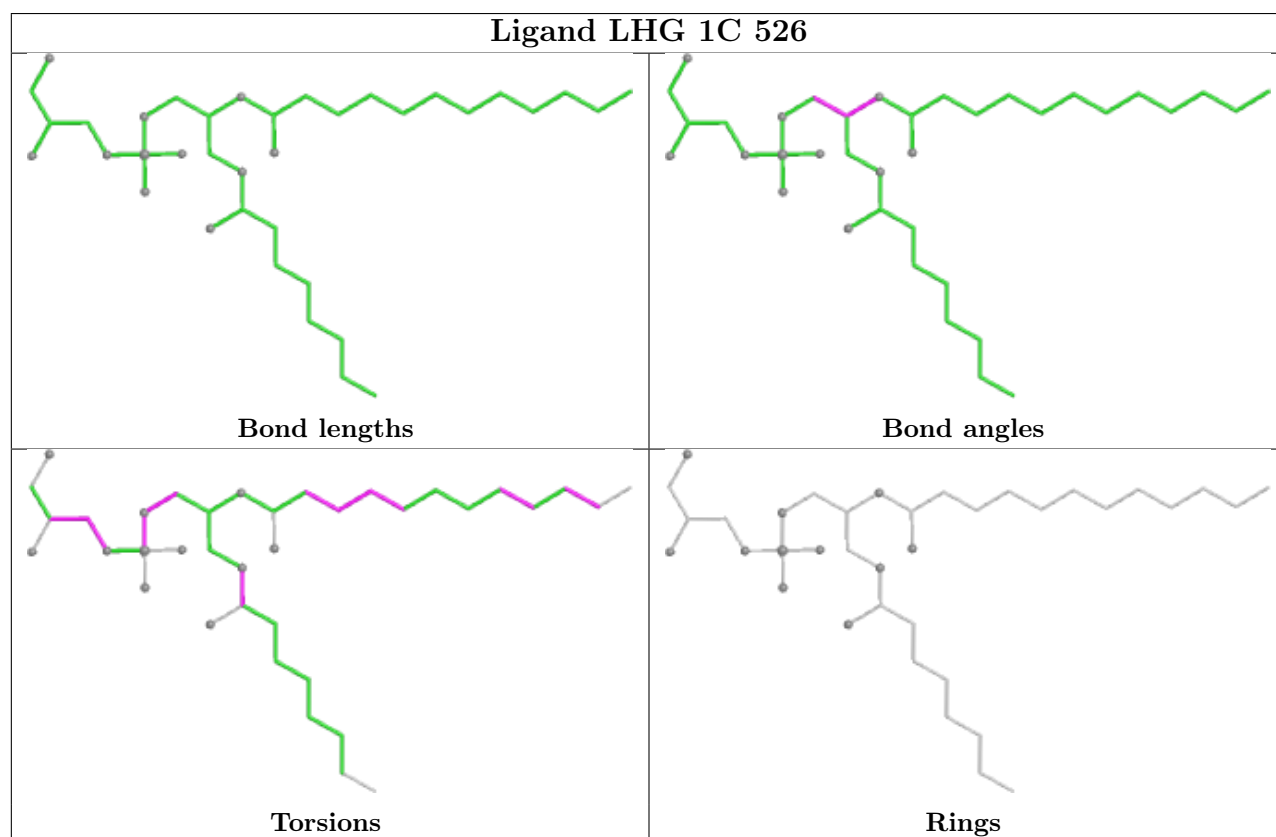
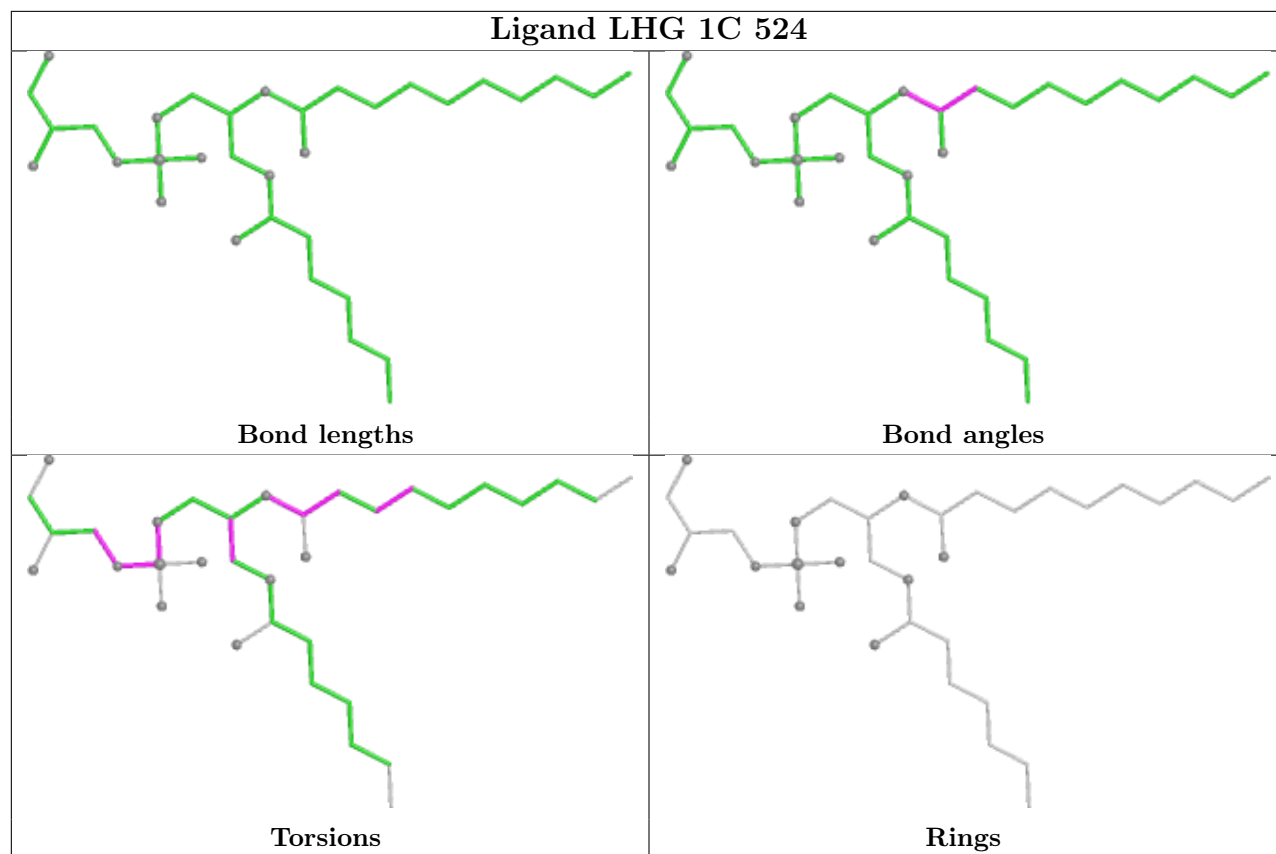
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Bond lengths	Bond angles
	
Torsions	Rings

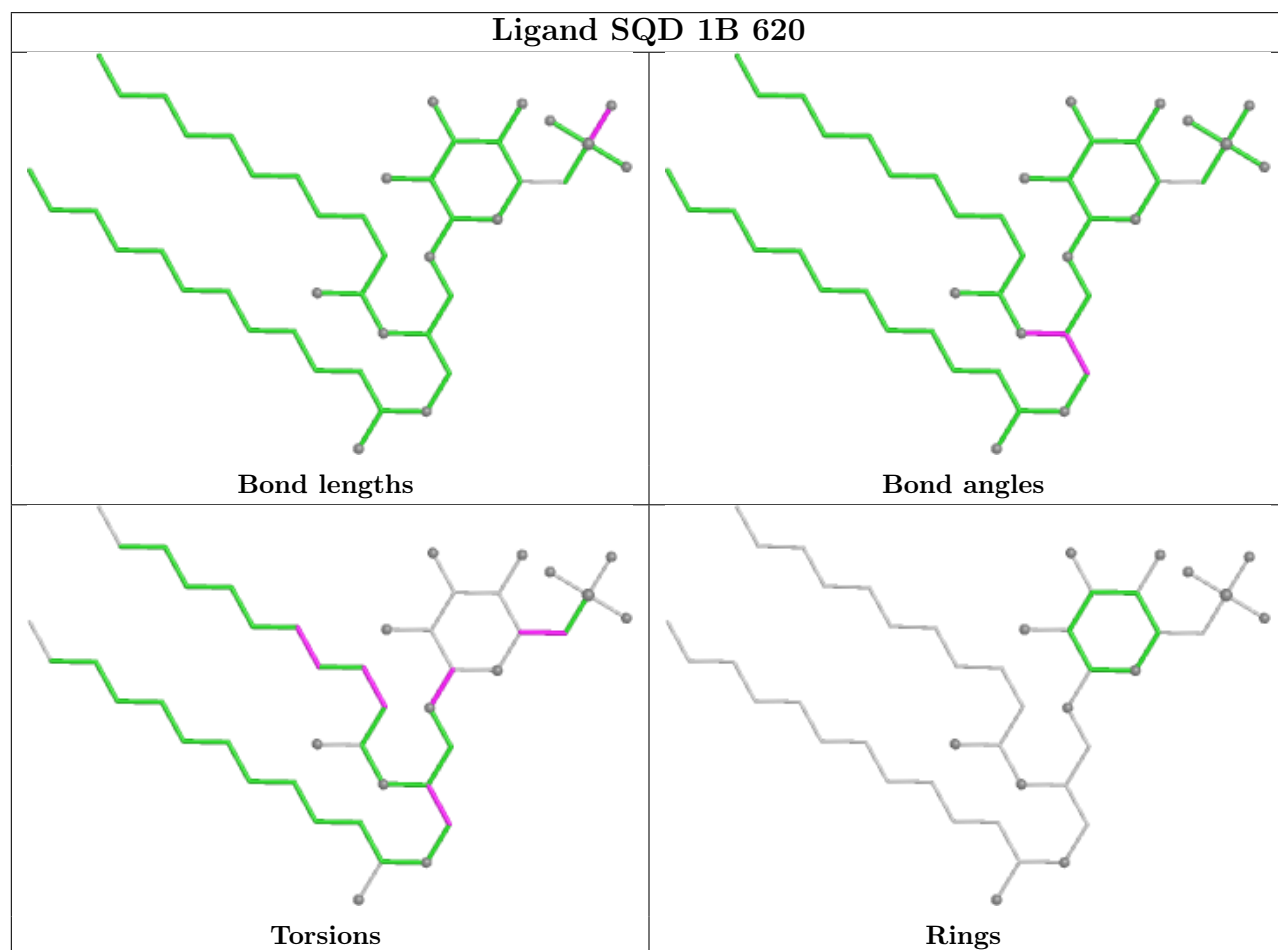
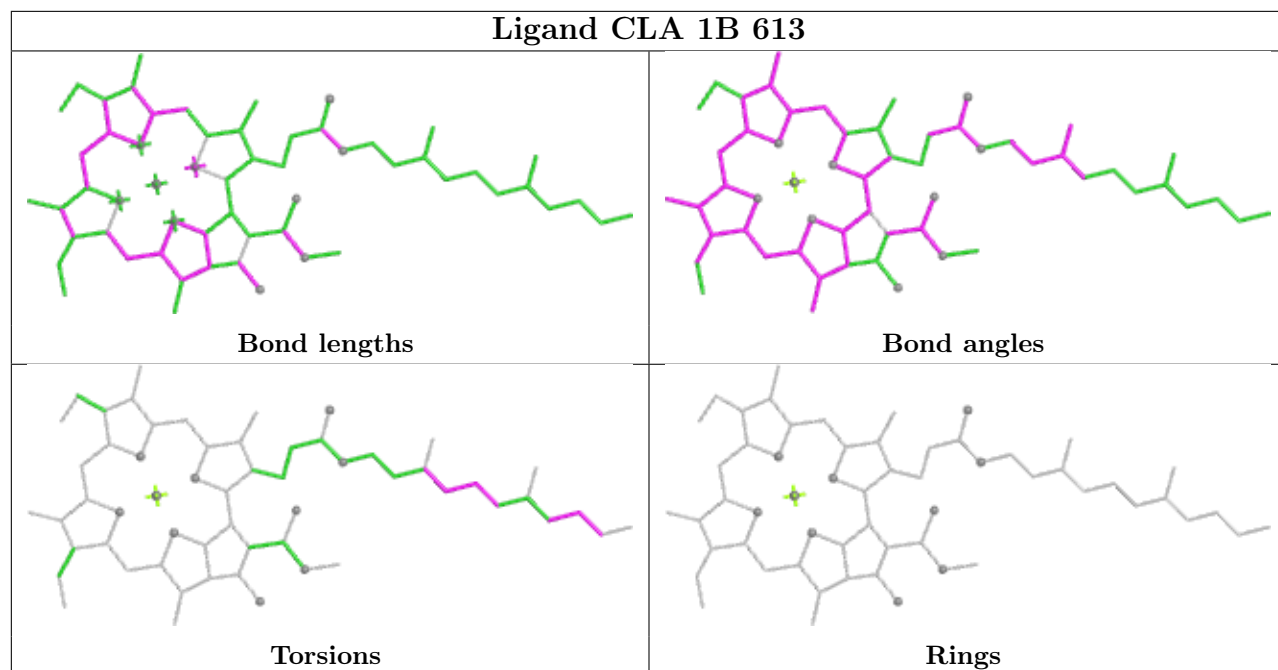
Ligand BCR 1D 406	
	
Bond lengths	Bond angles
	
Torsions	Rings

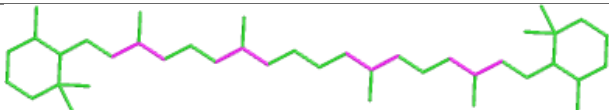
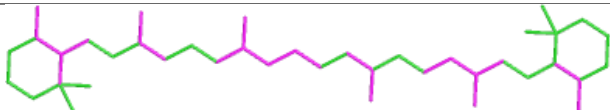
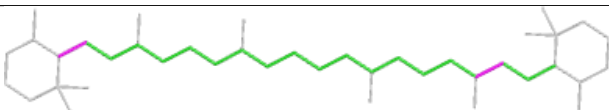
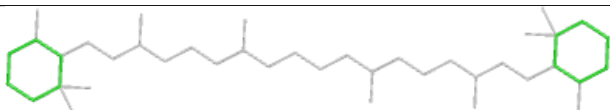


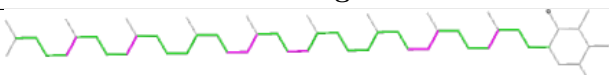
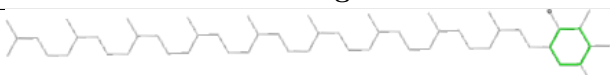


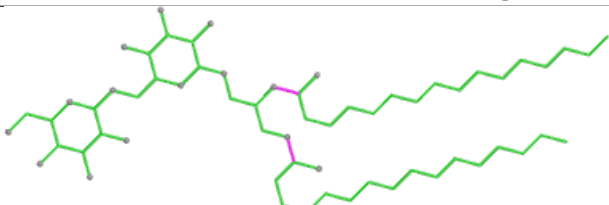
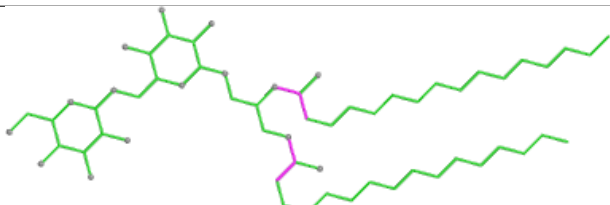
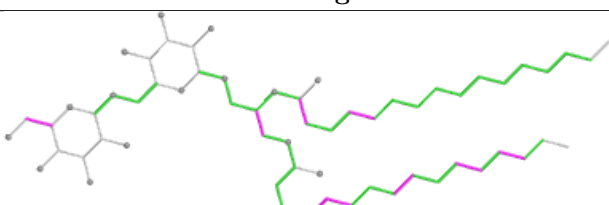
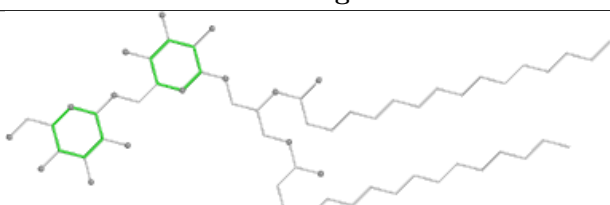


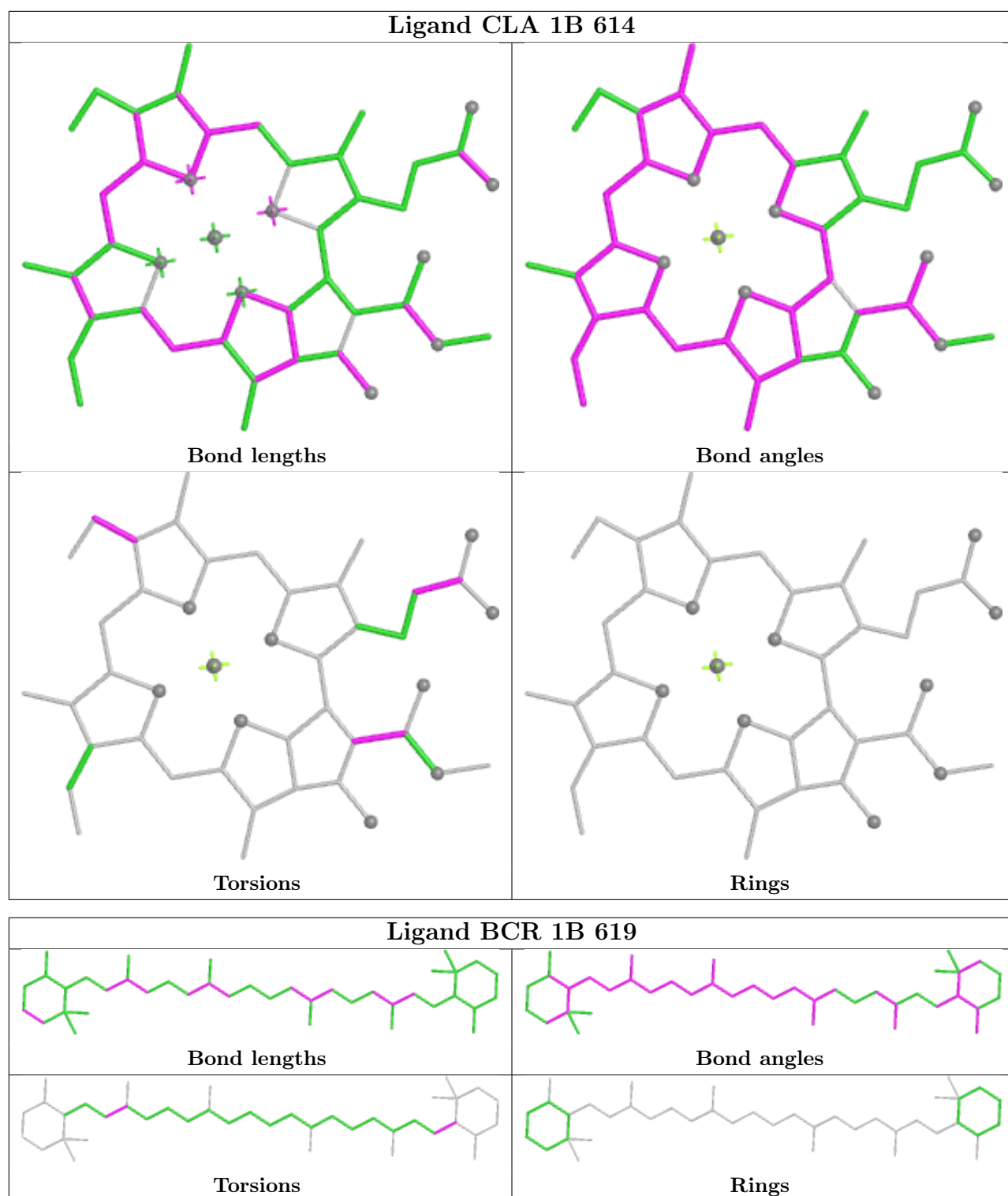


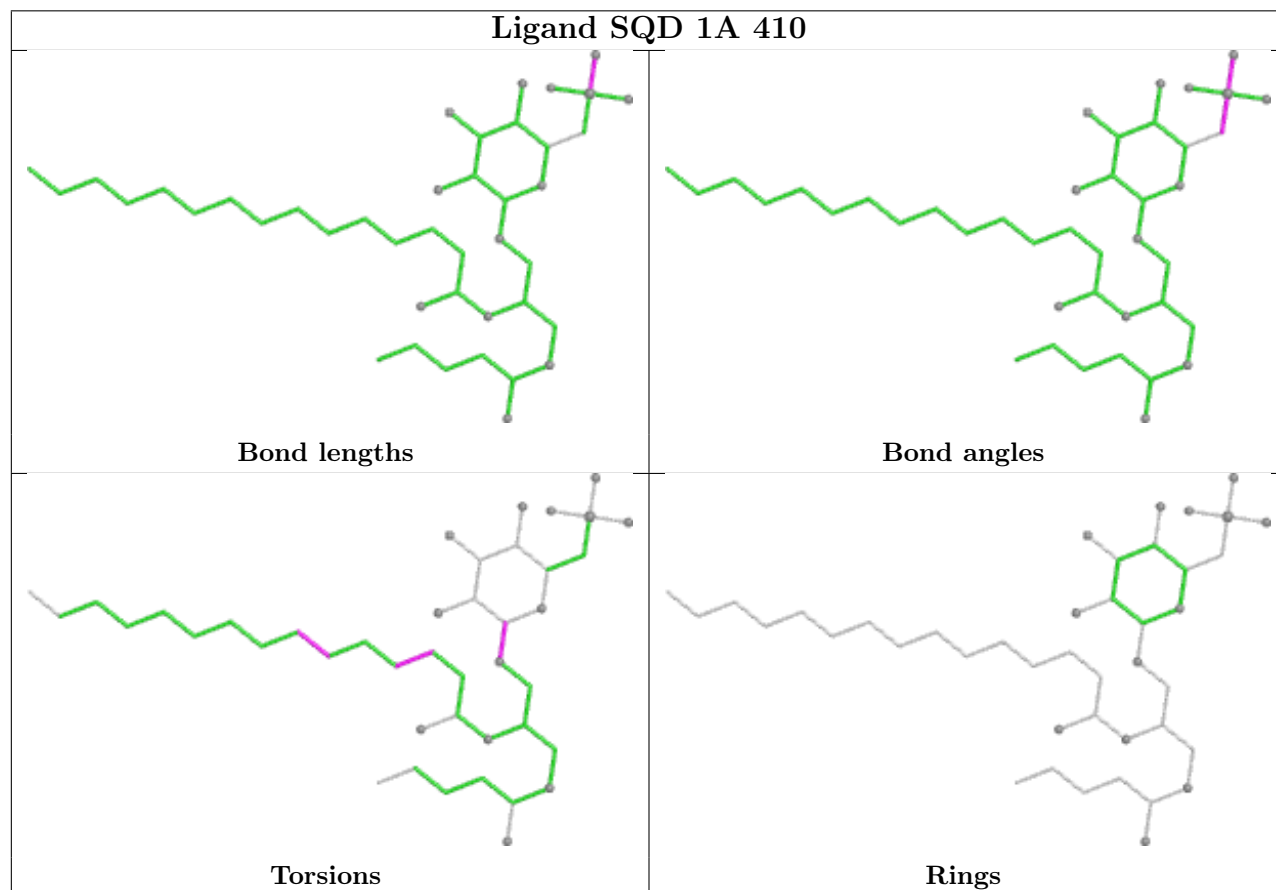
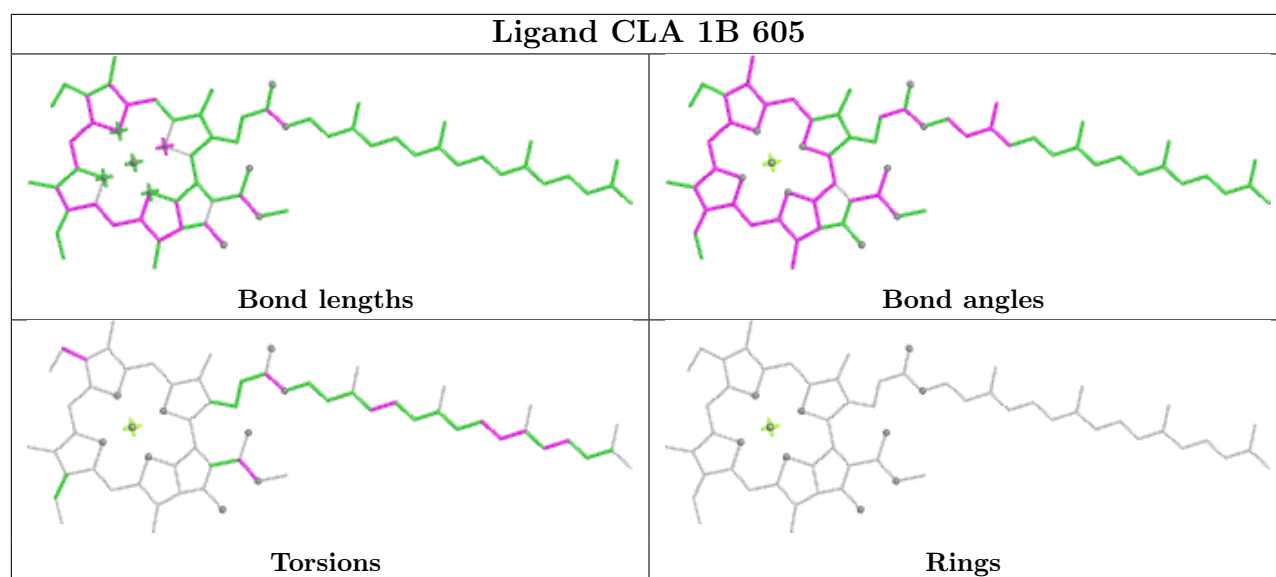


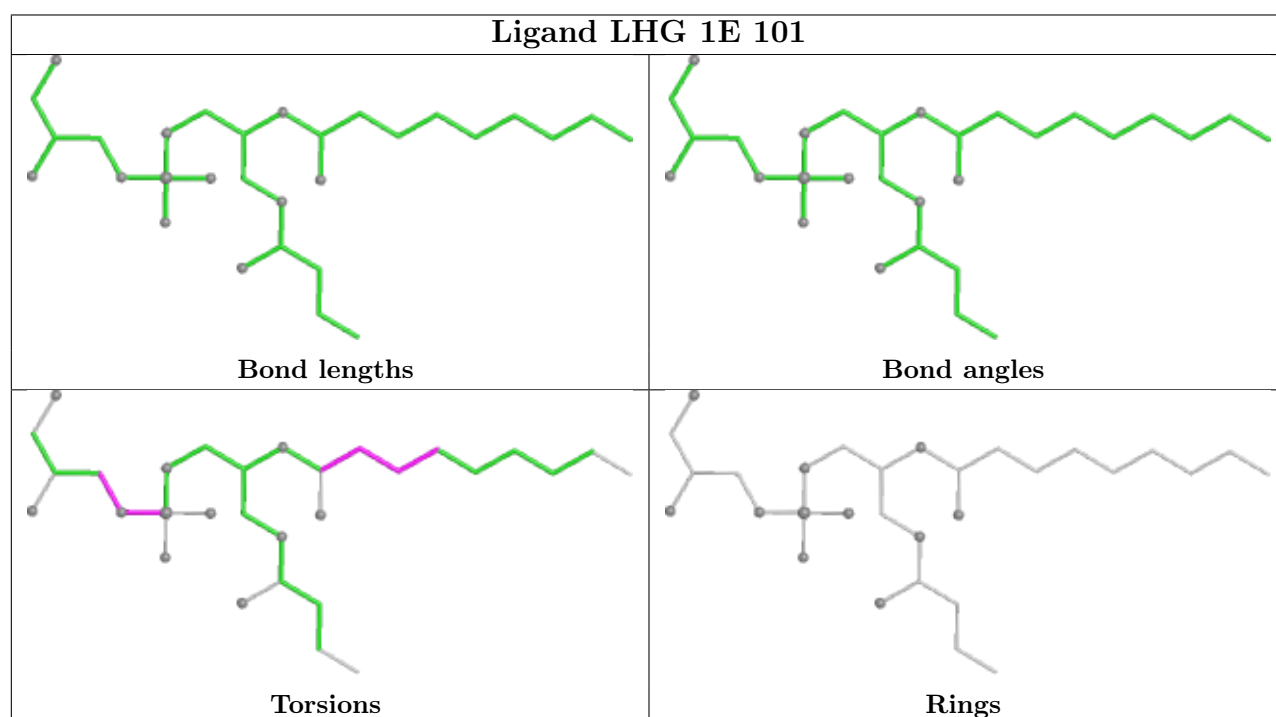
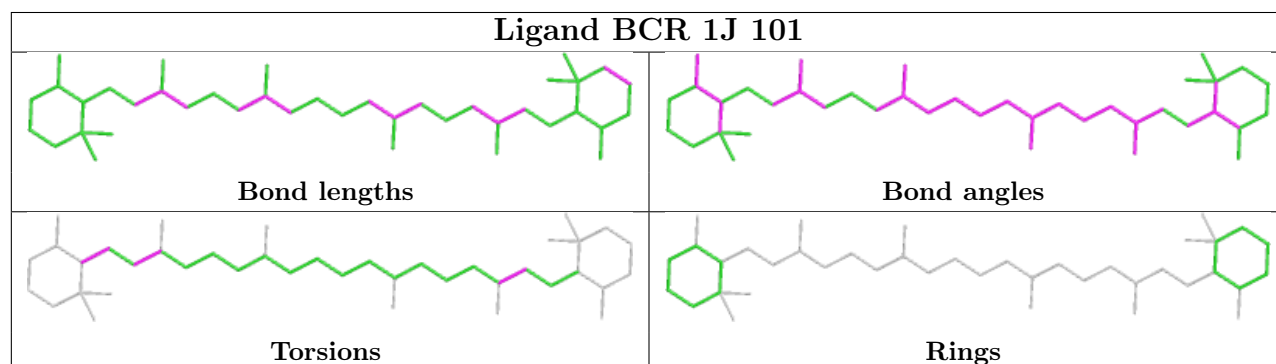
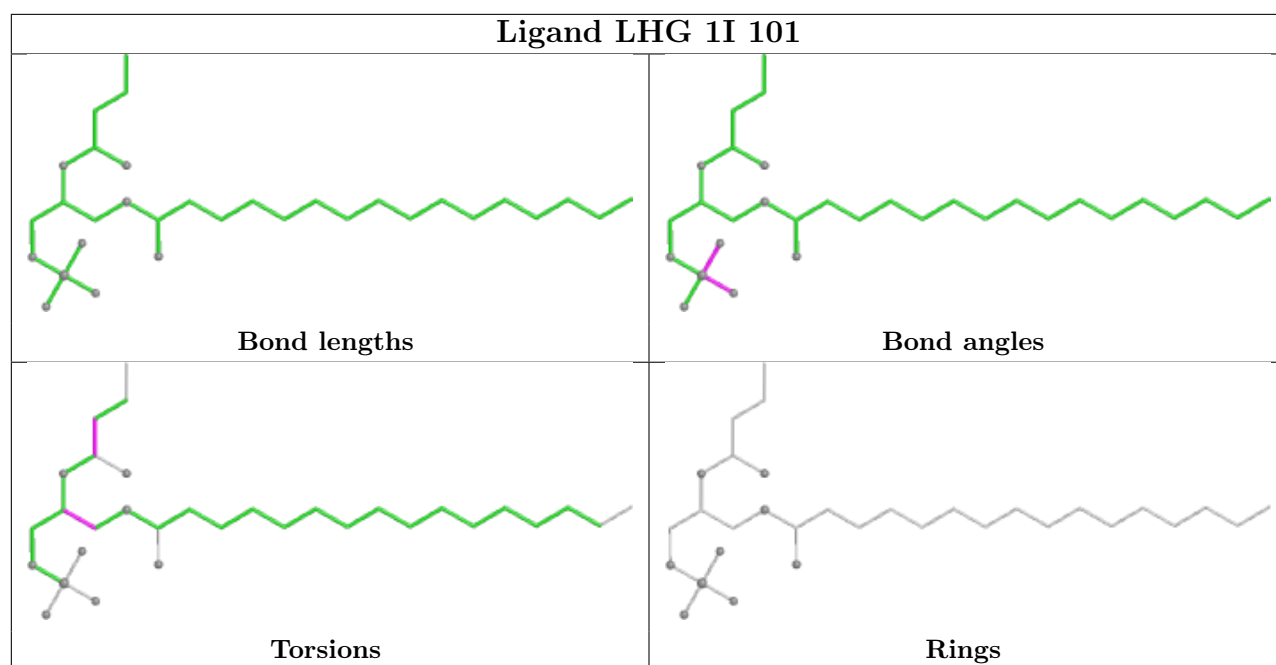
Ligand BCR 1I 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

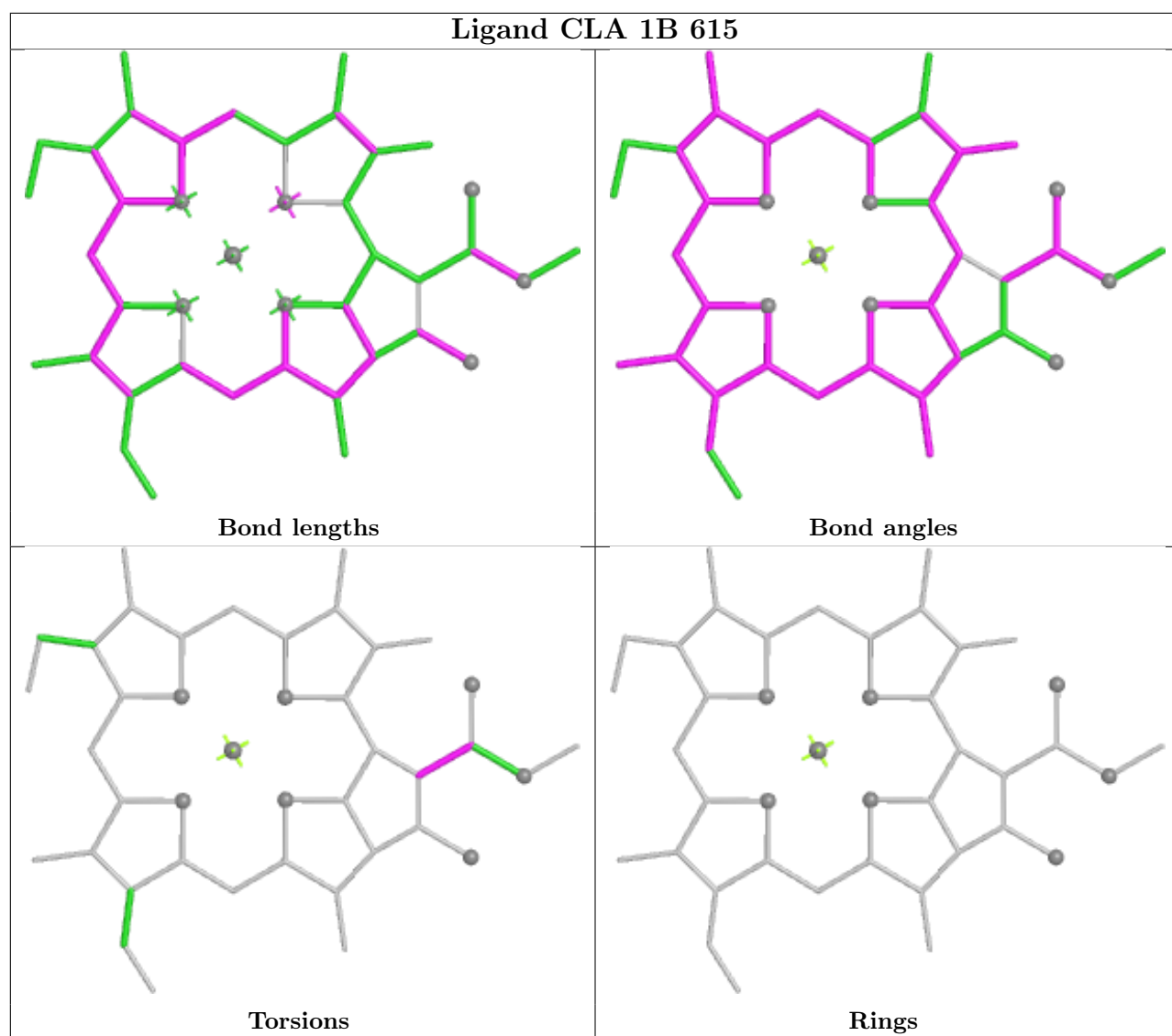
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Bond lengths	Bond angles
	
Torsions	Rings

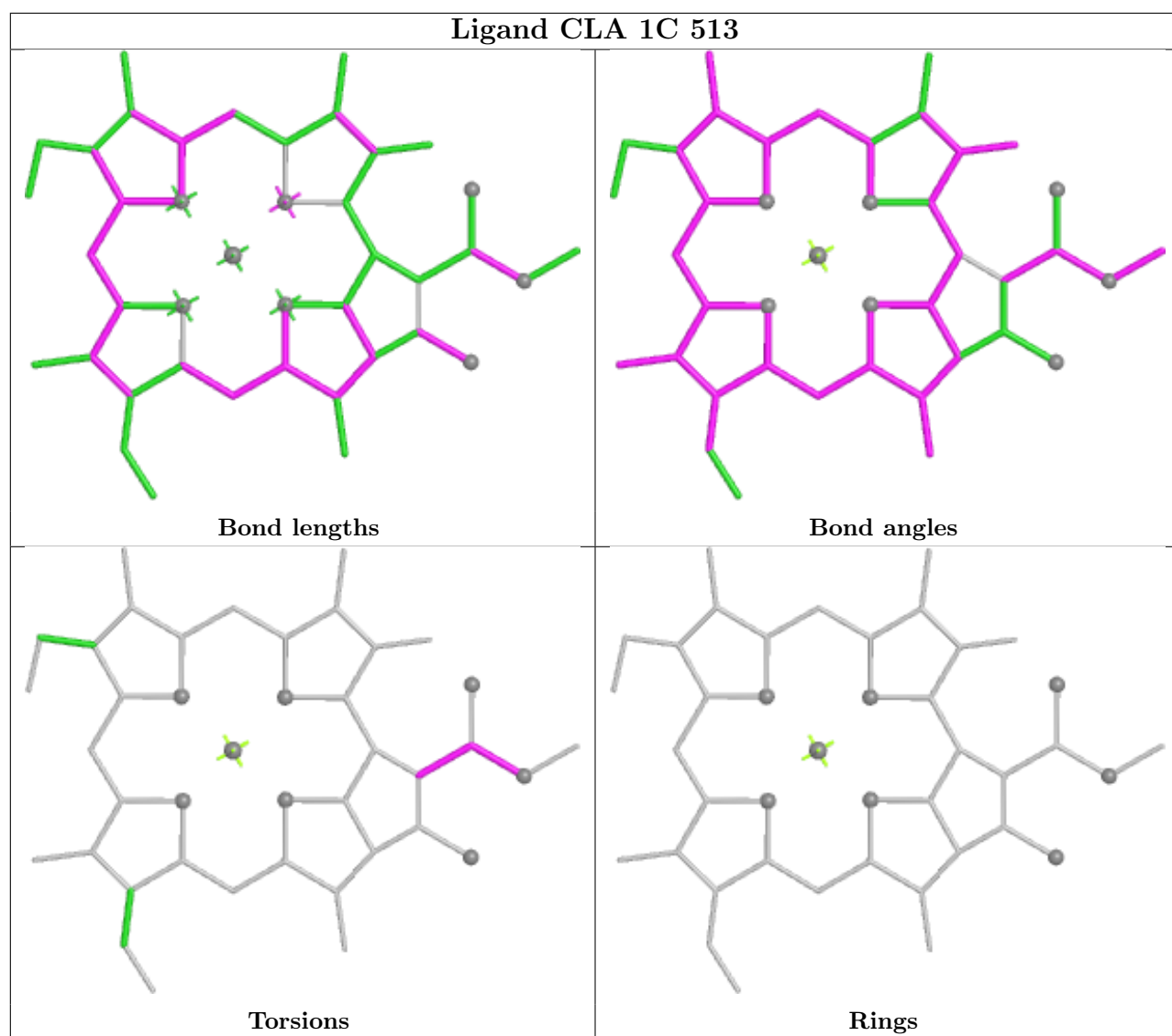
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Bond lengths	Bond angles
	
Torsions	Rings

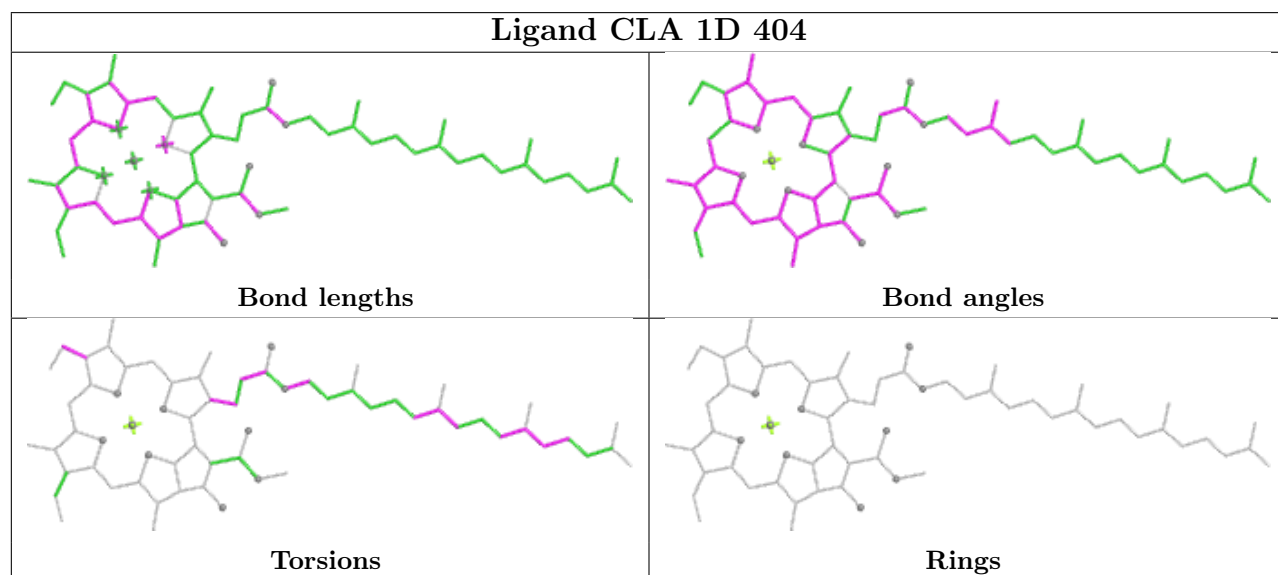
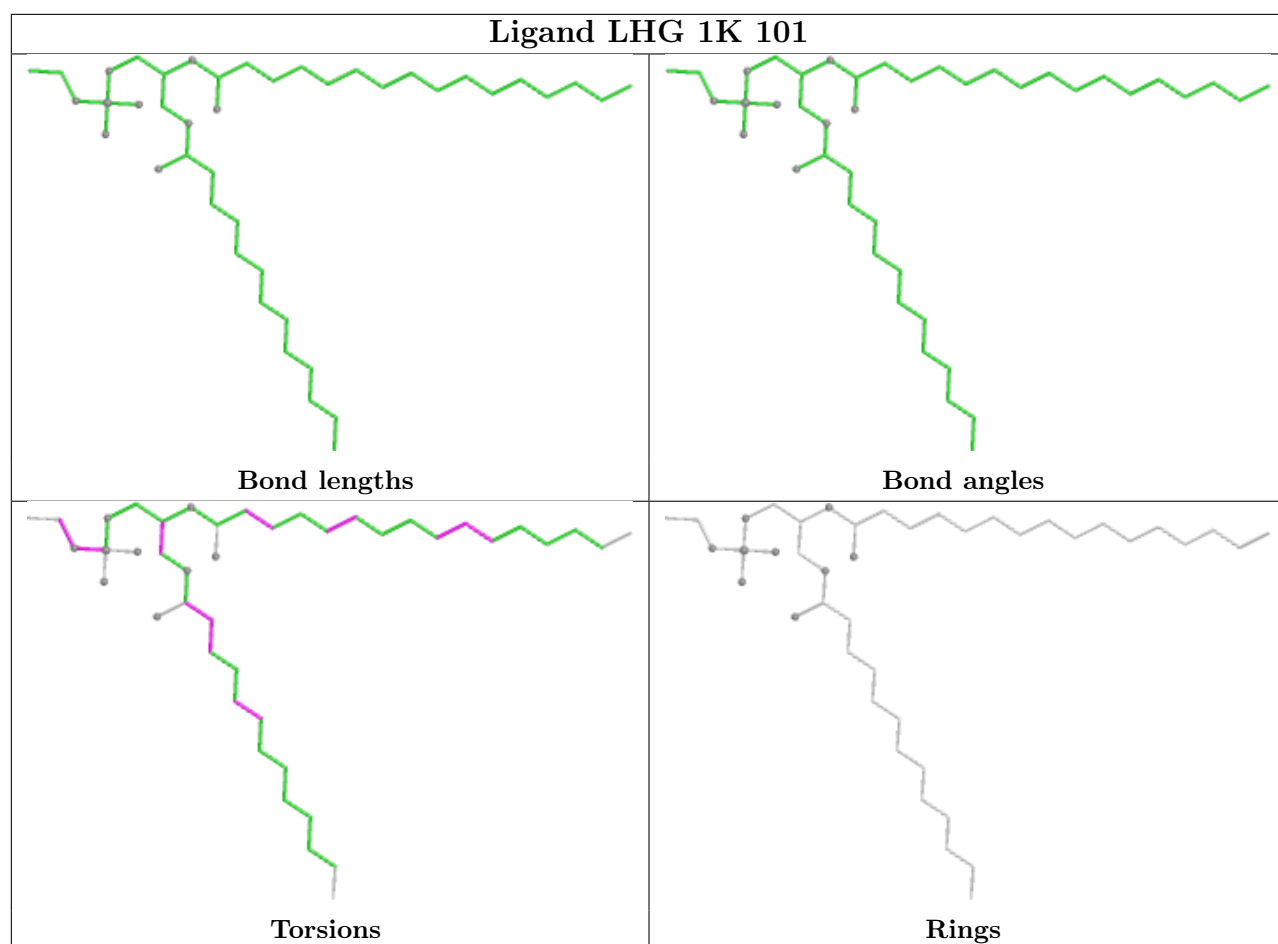


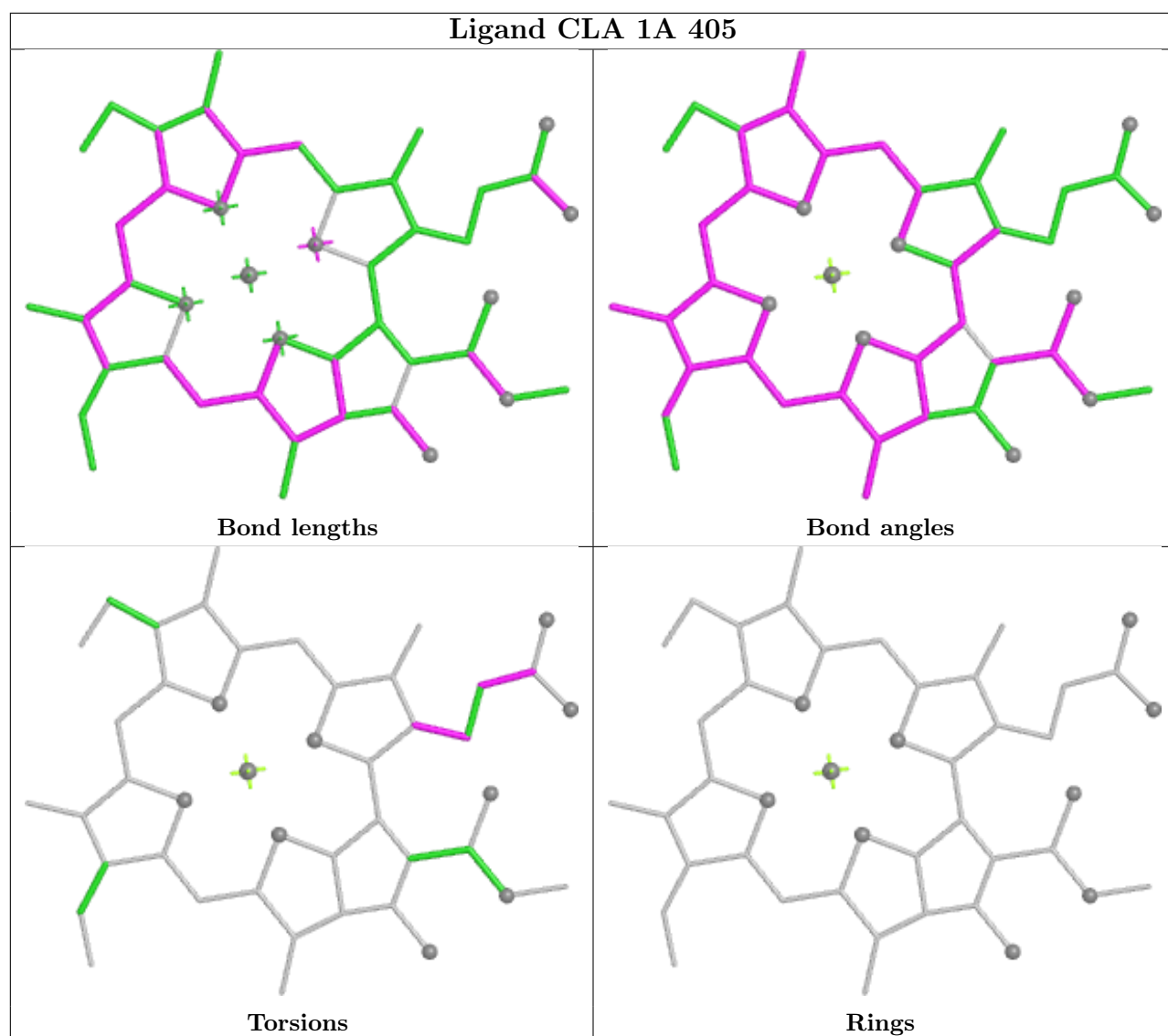


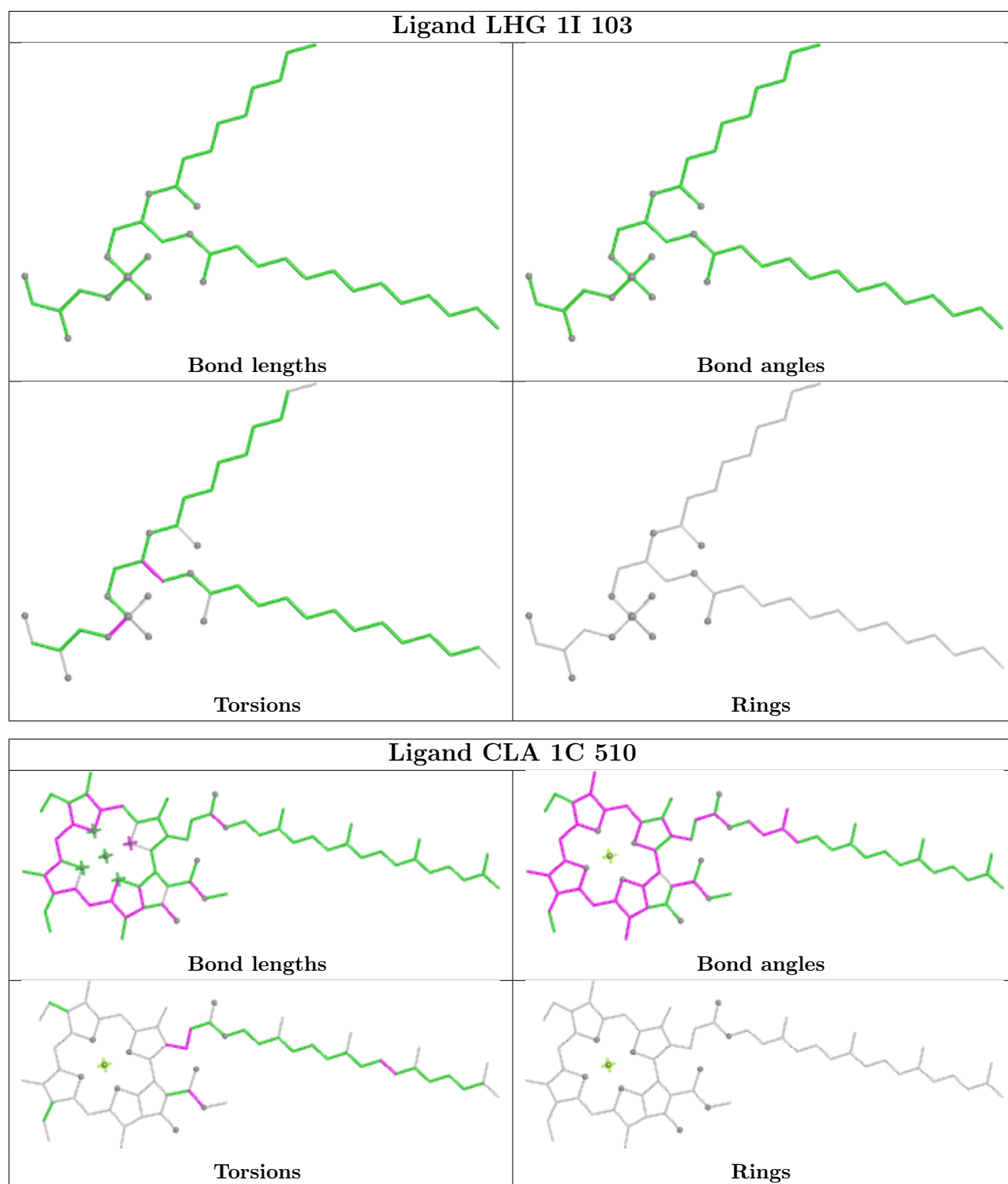


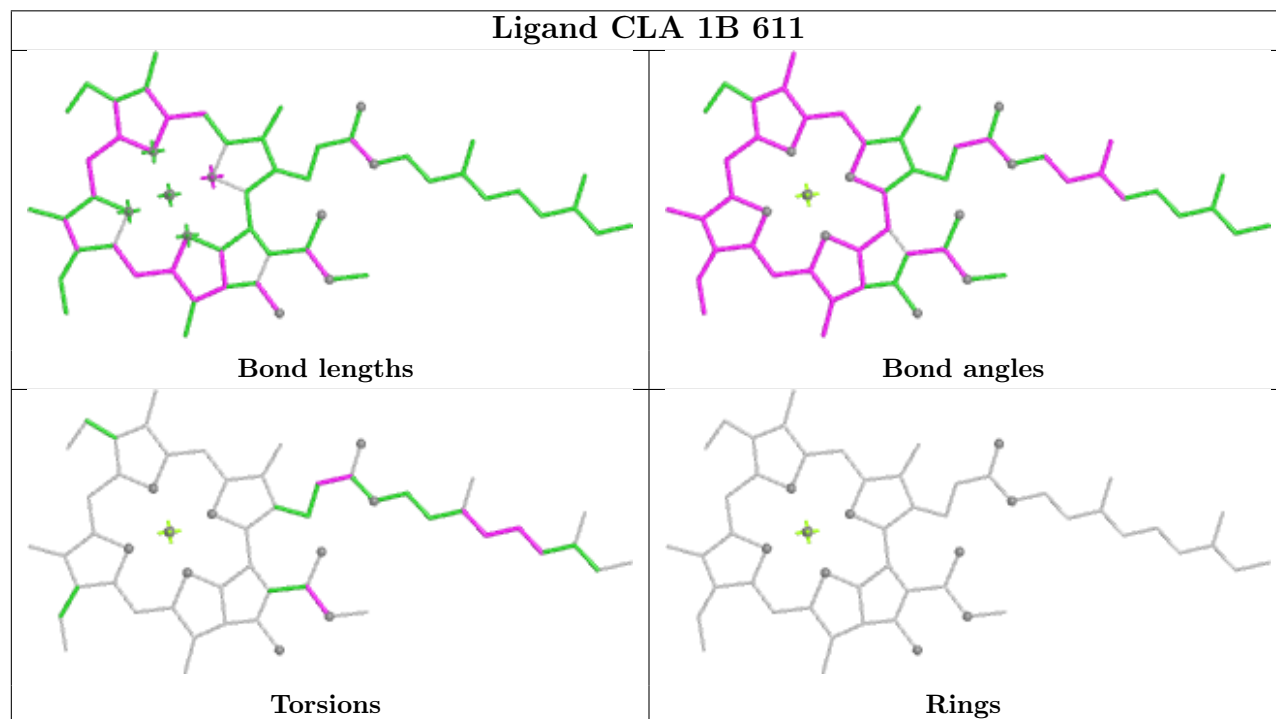
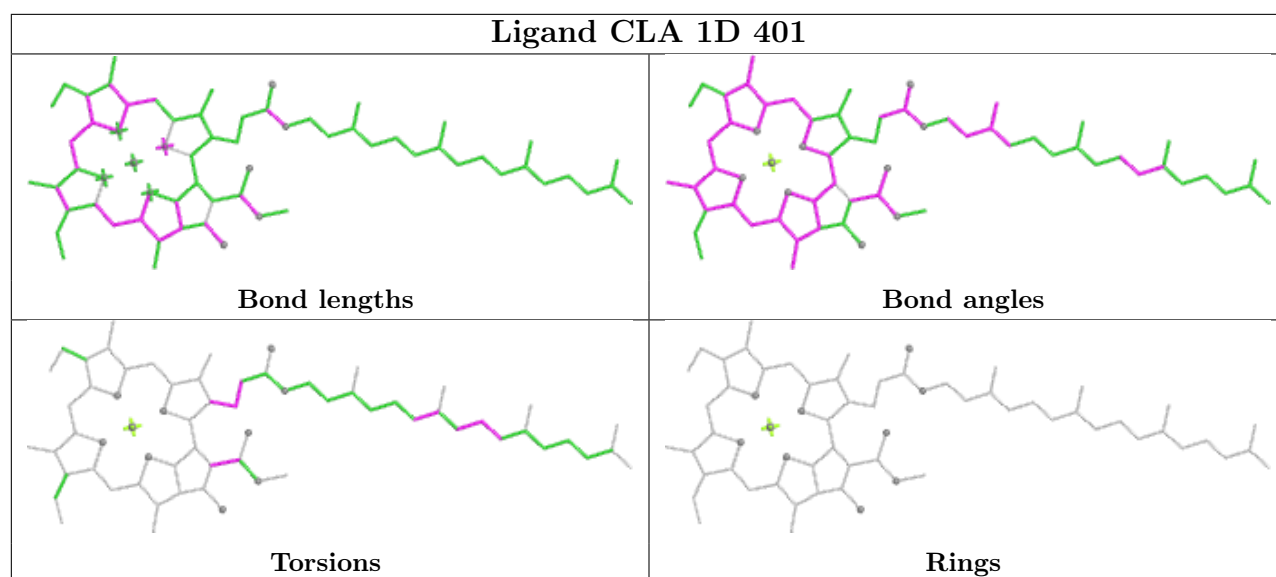


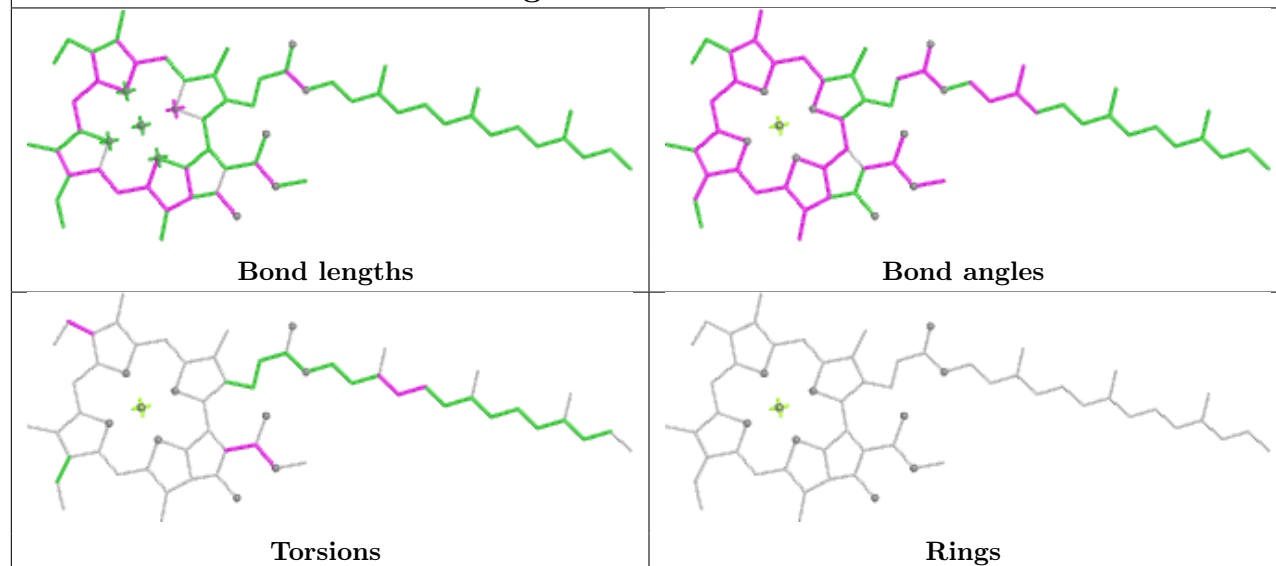
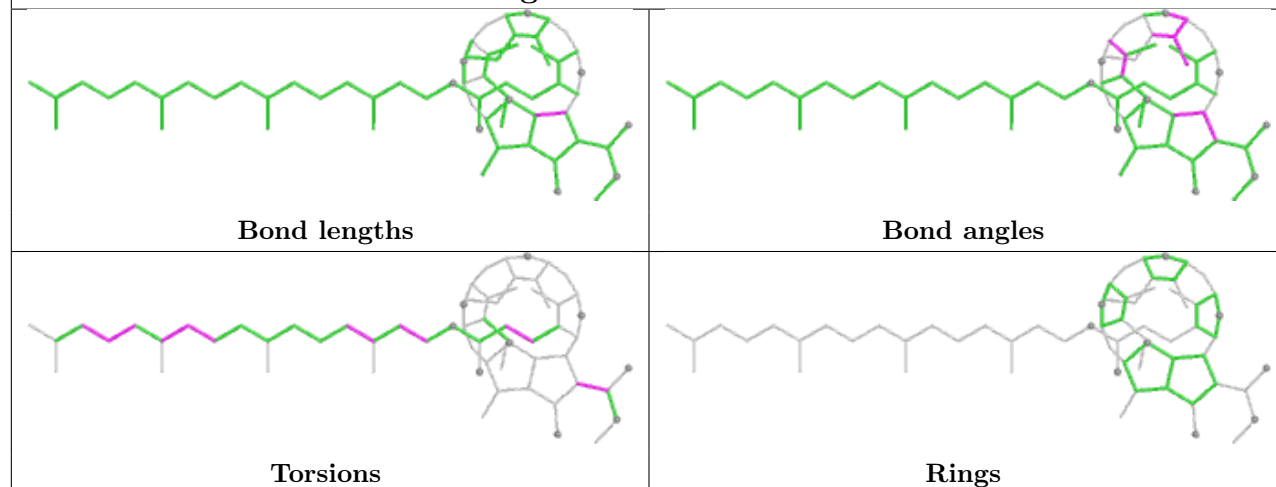


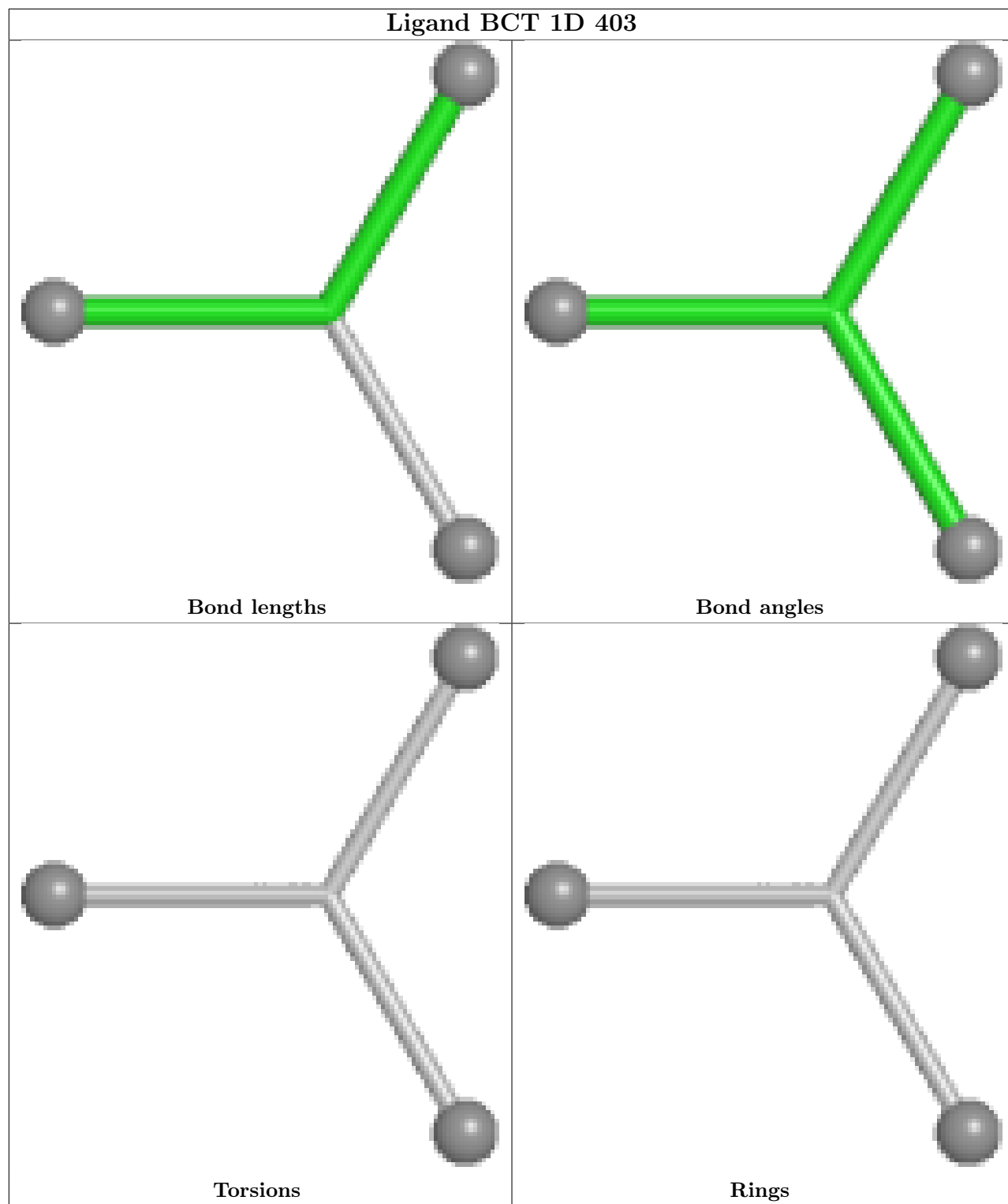


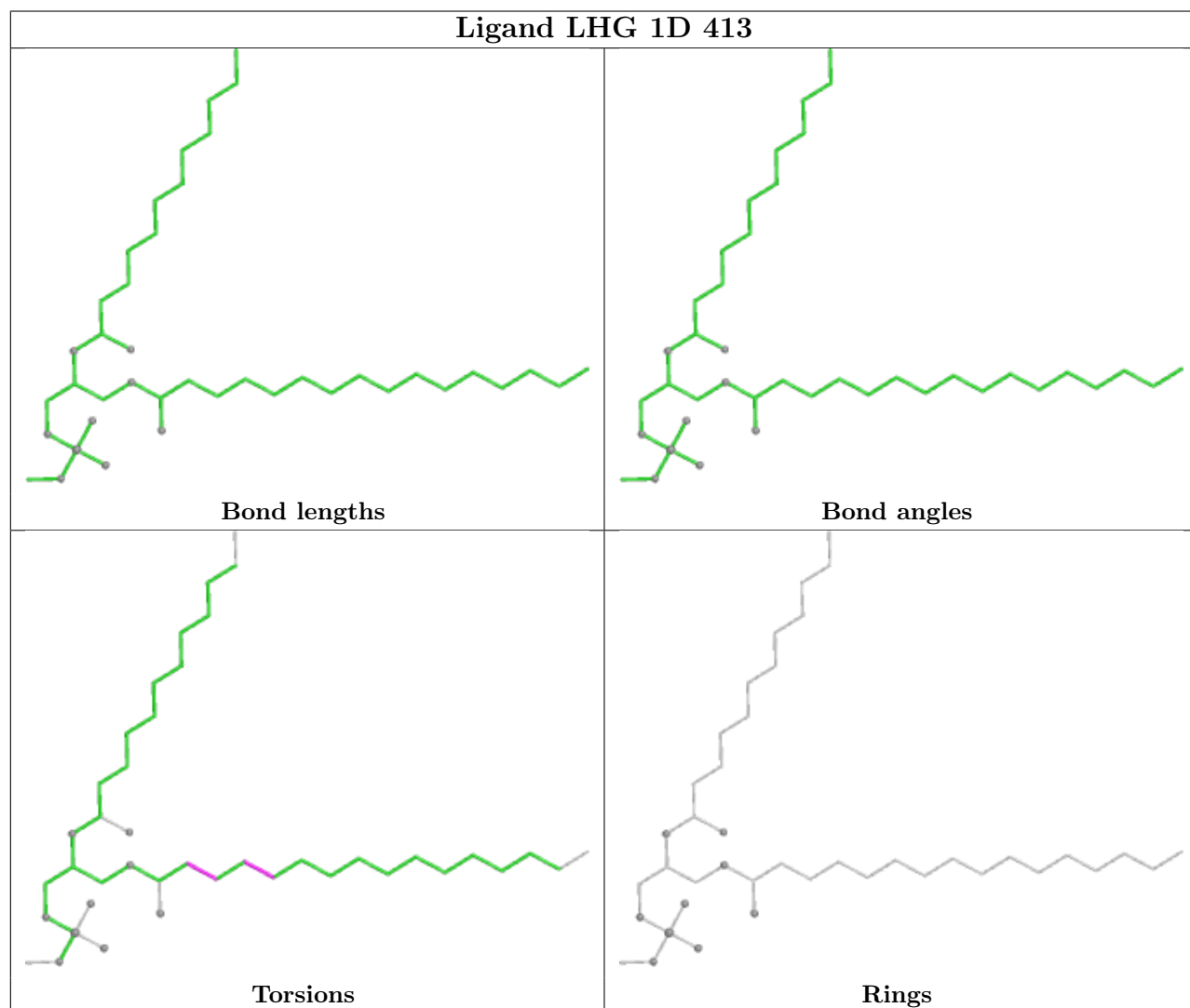
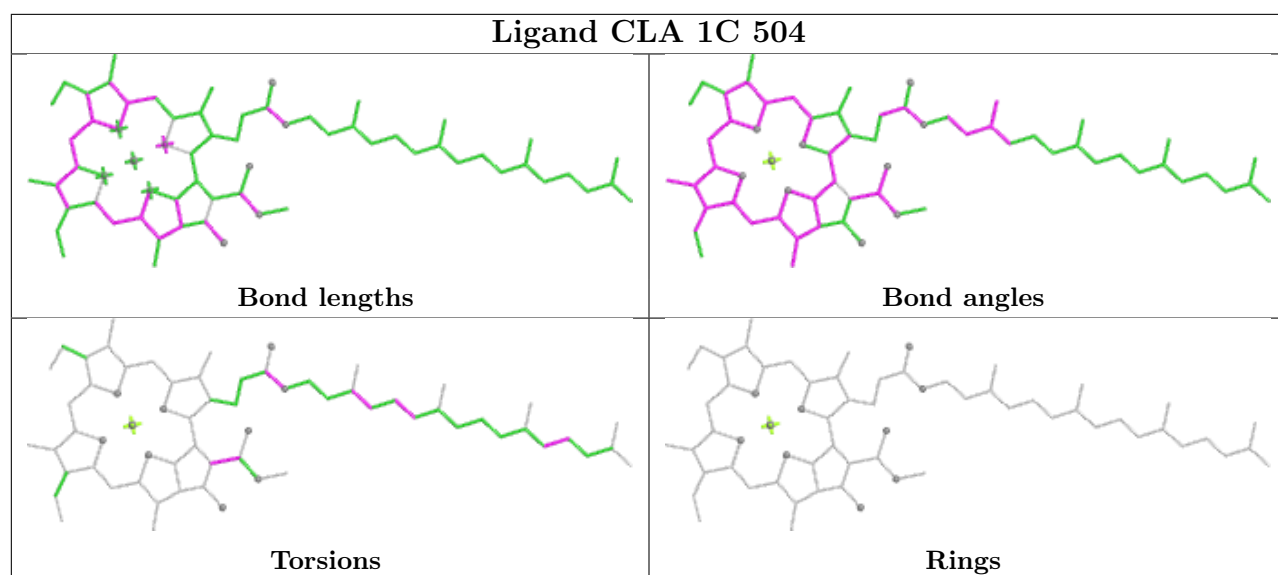


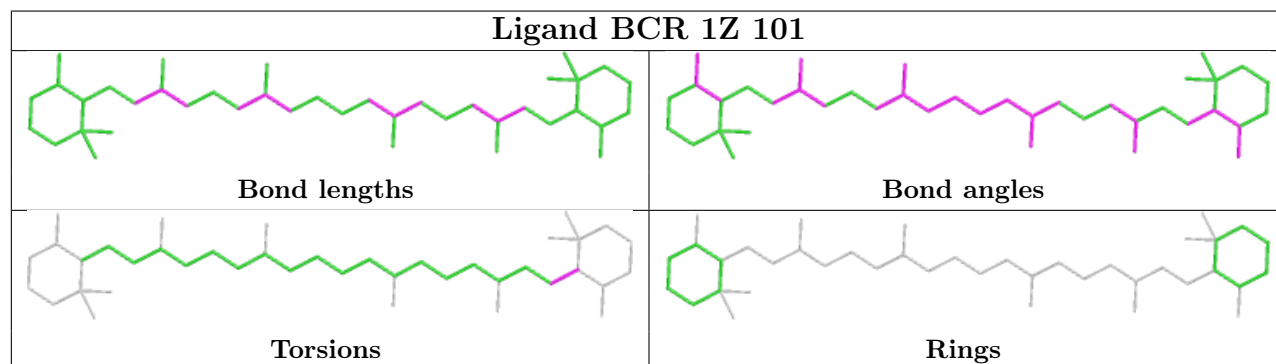
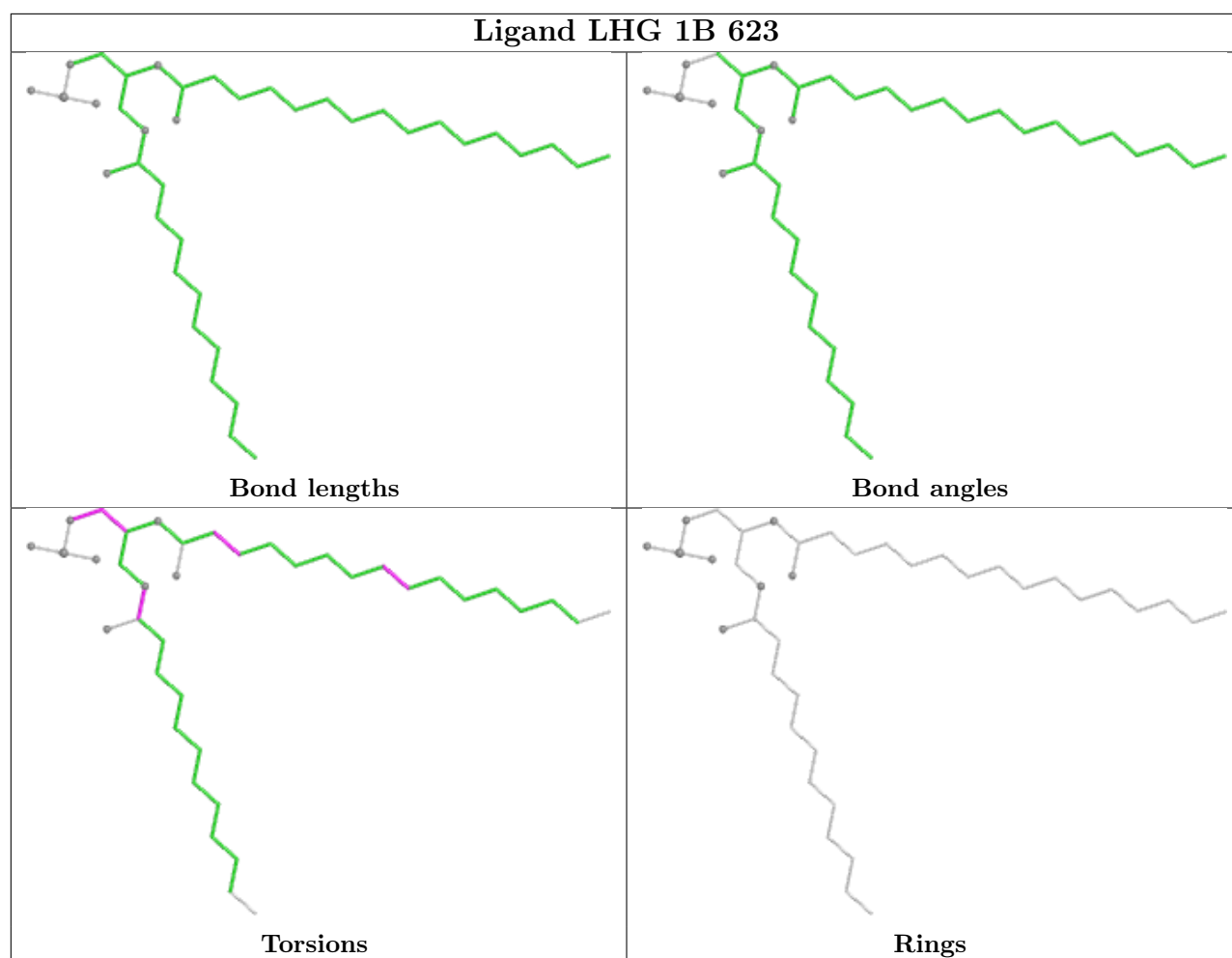


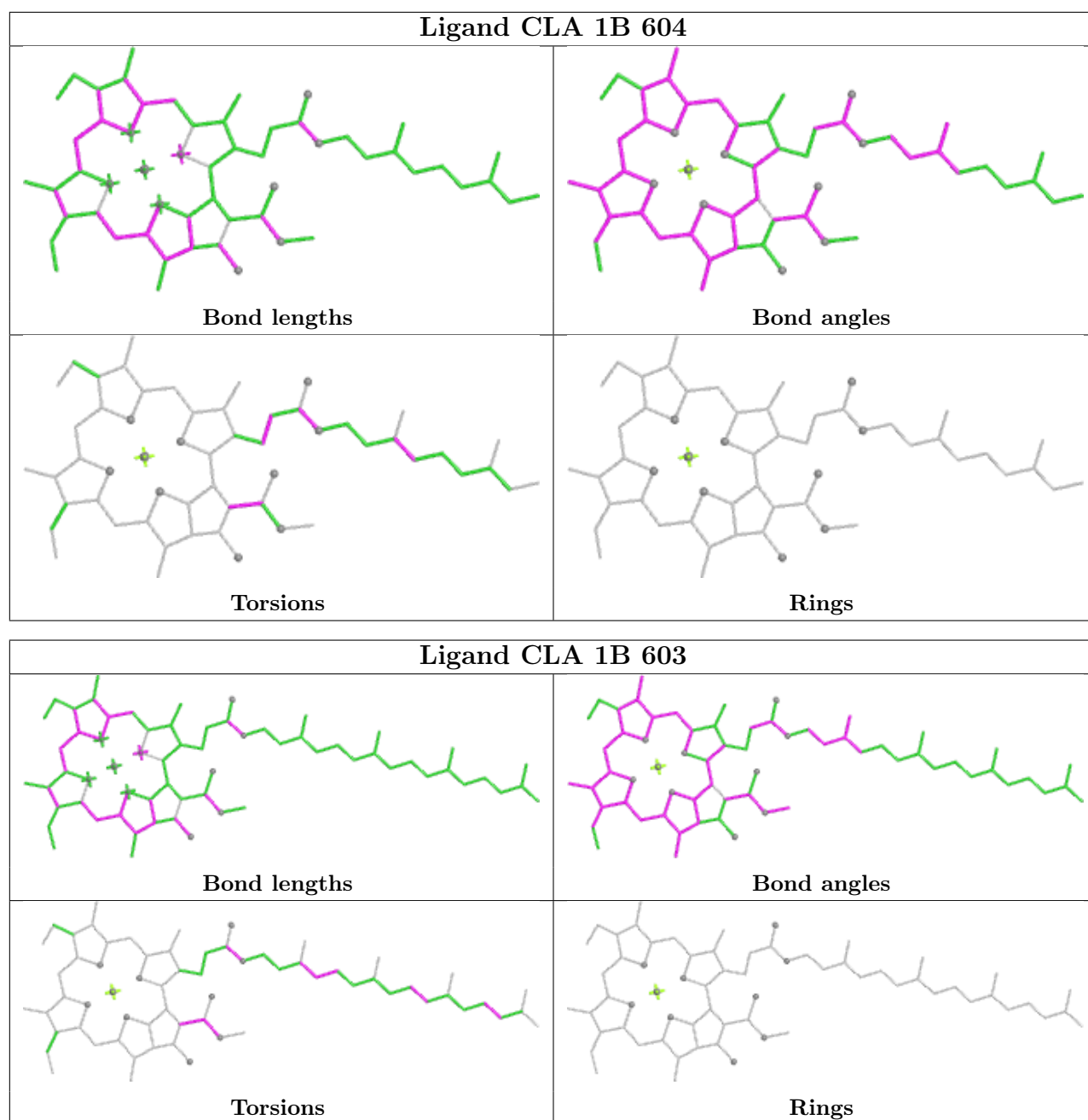


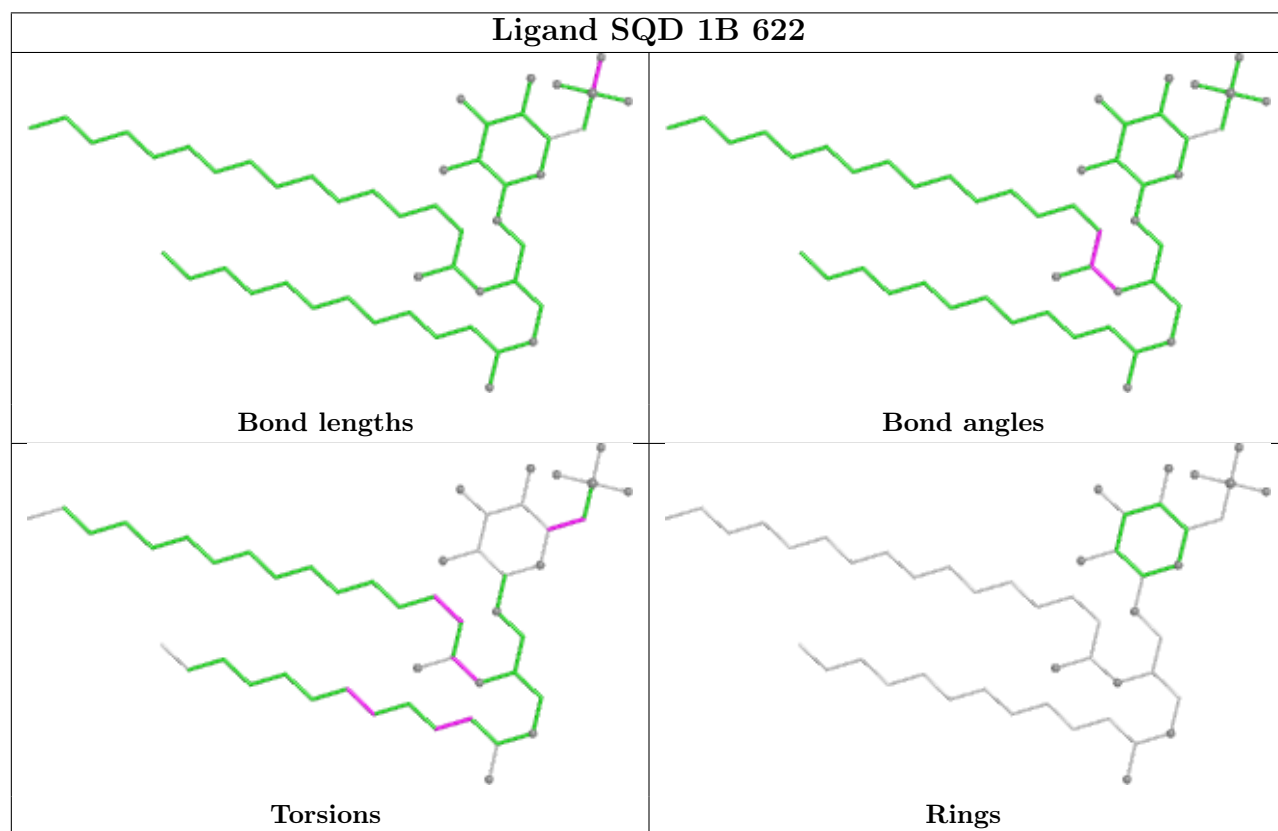
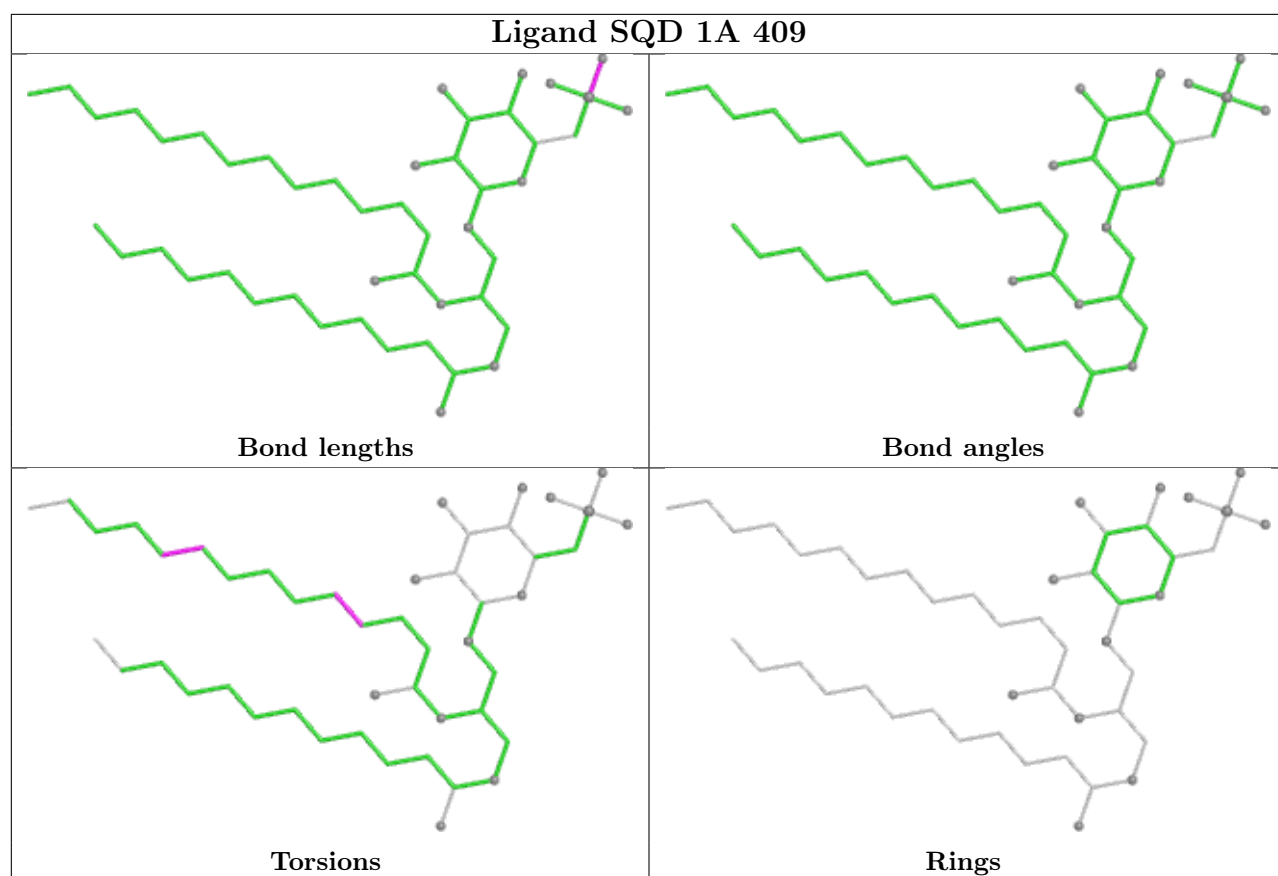
Ligand CLA 1B 607**Ligand PHO 1A 404**

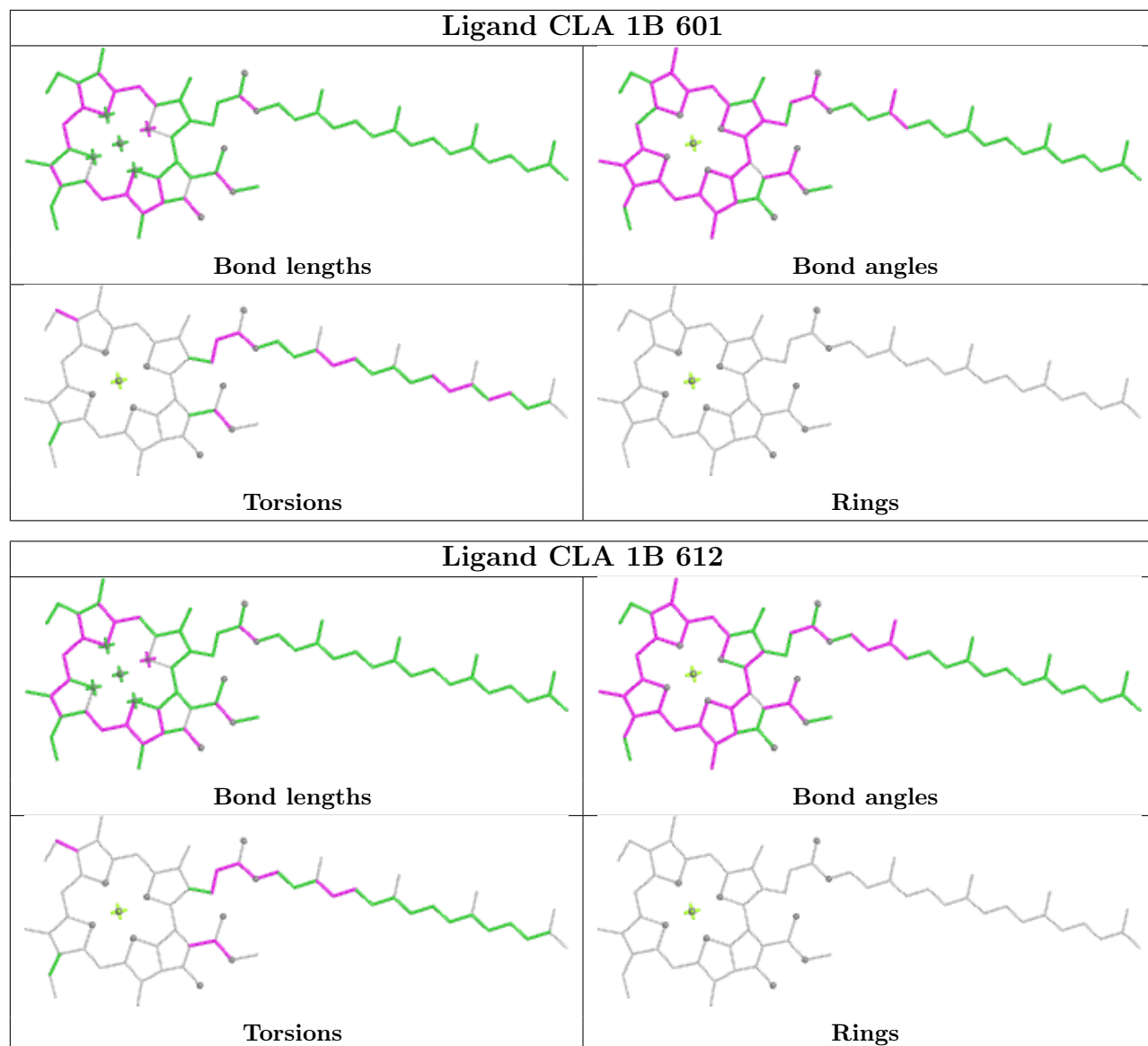


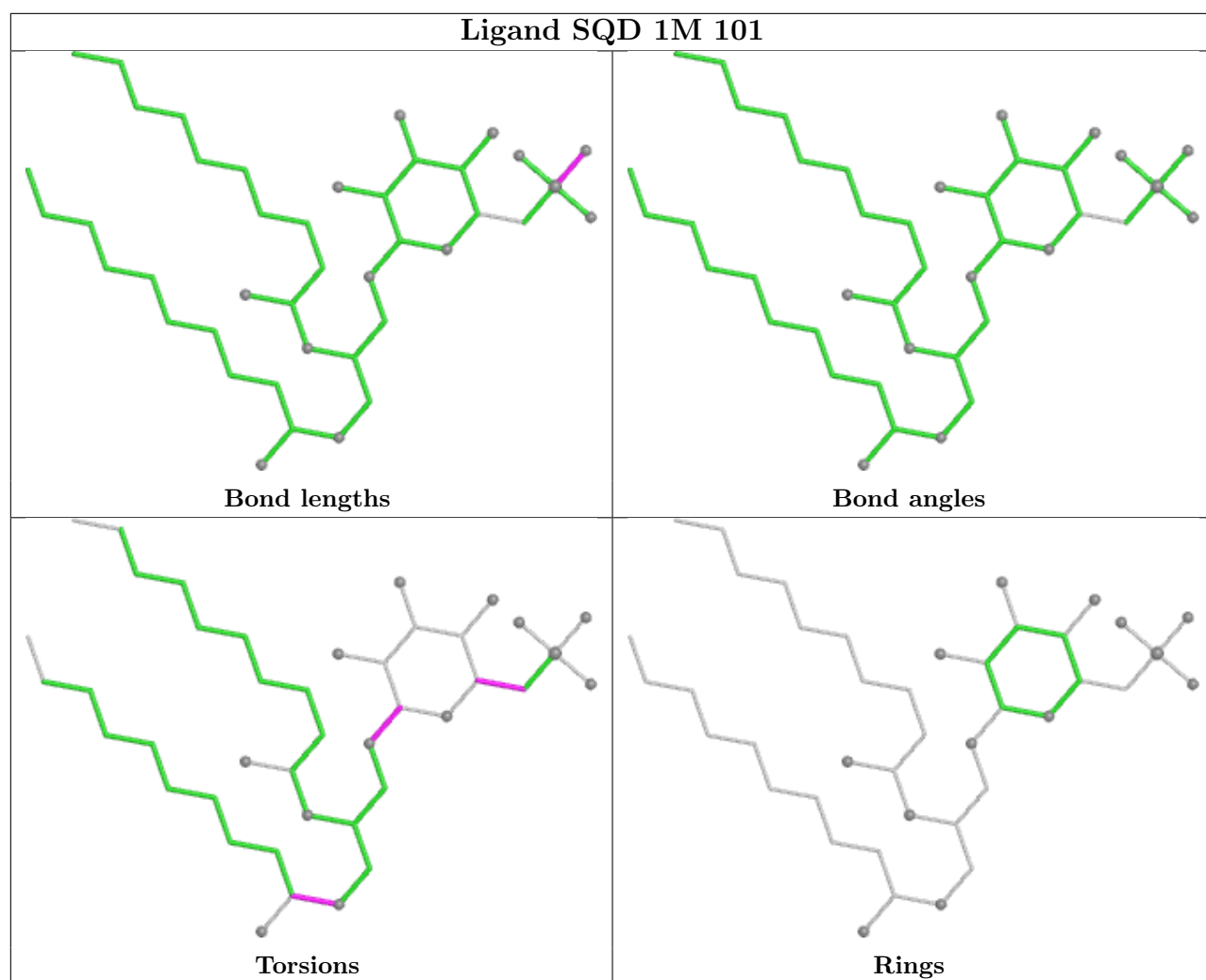


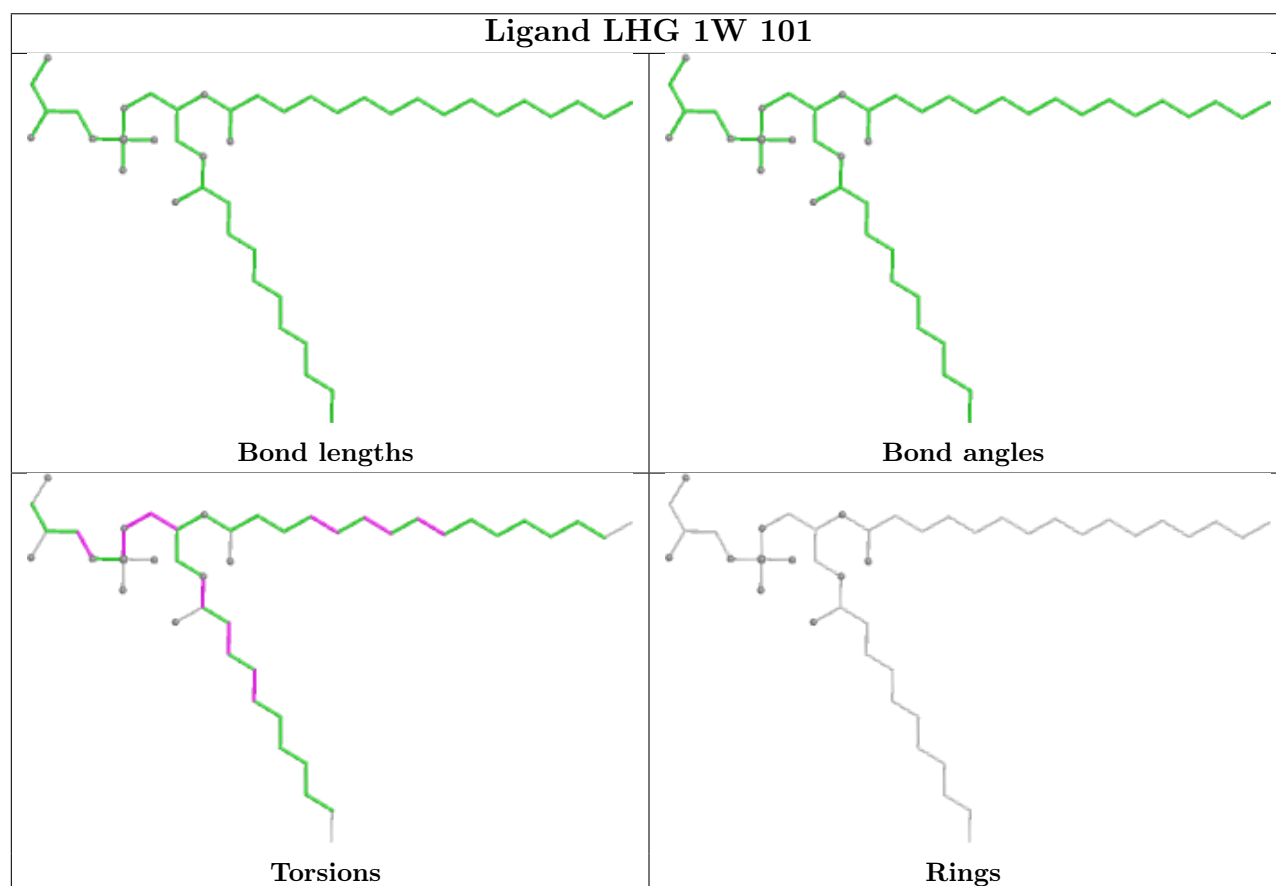
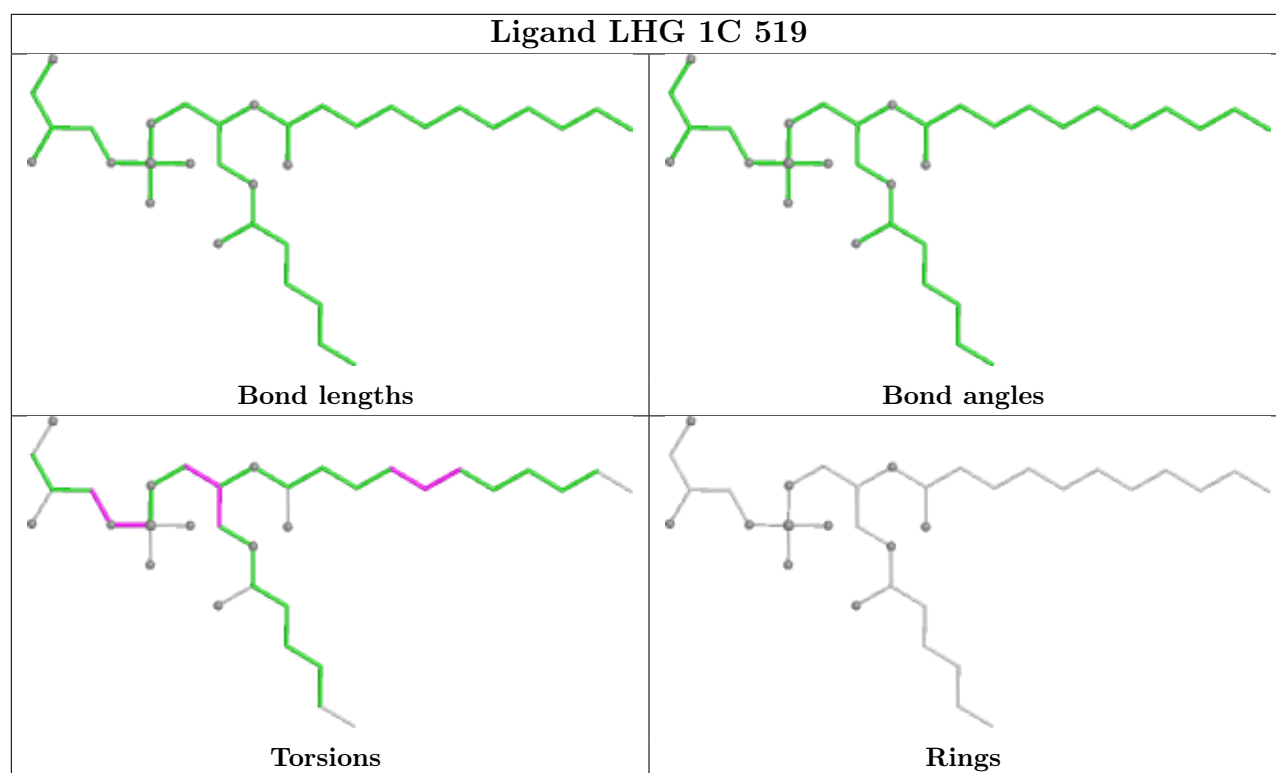


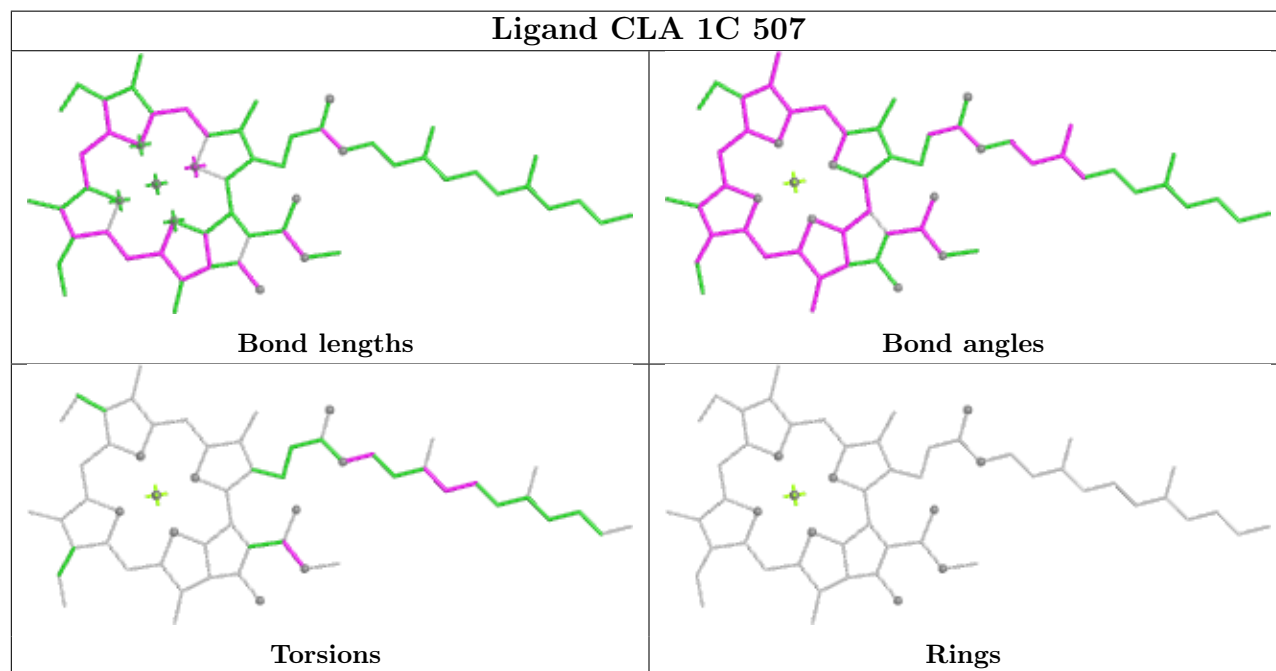
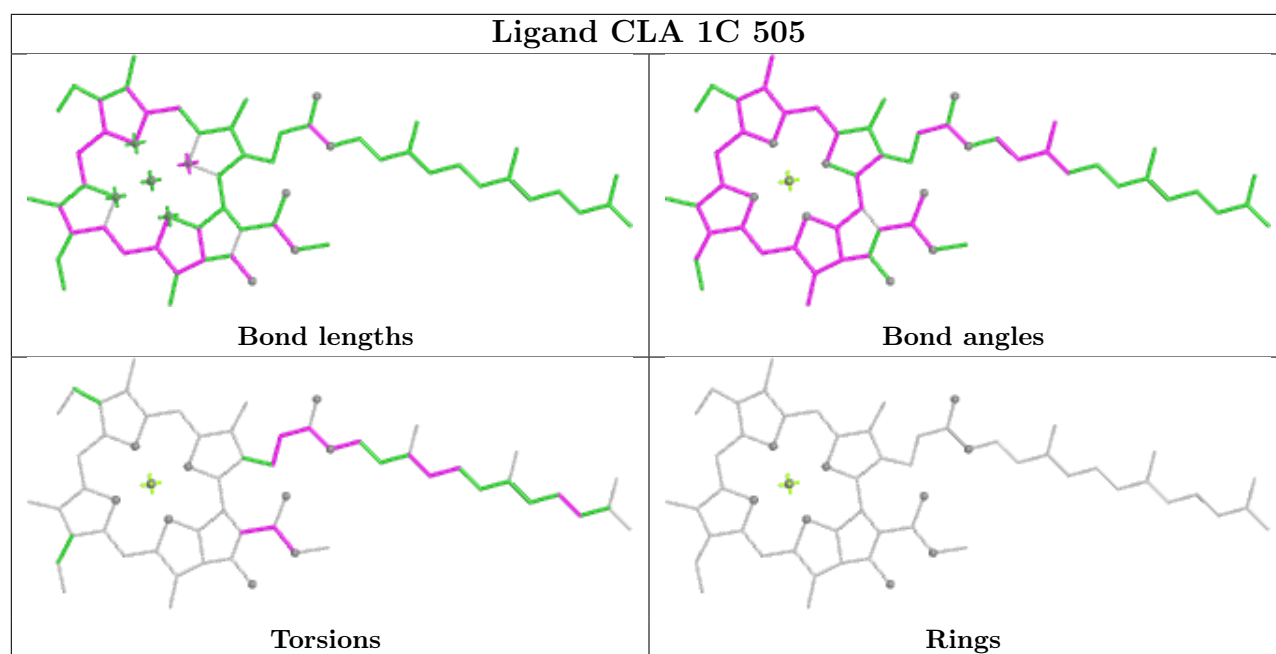




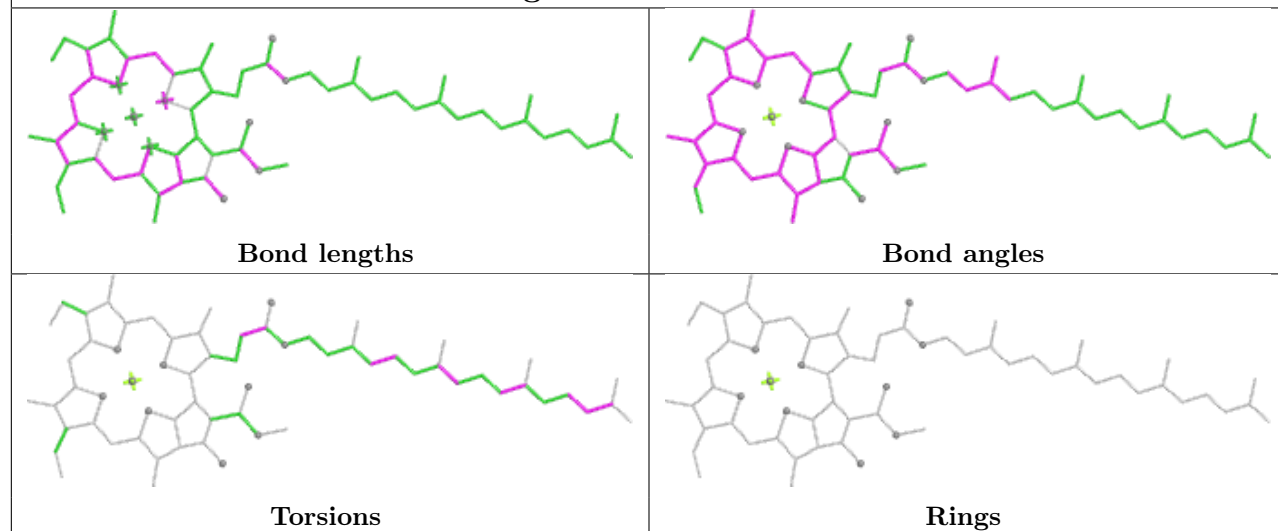




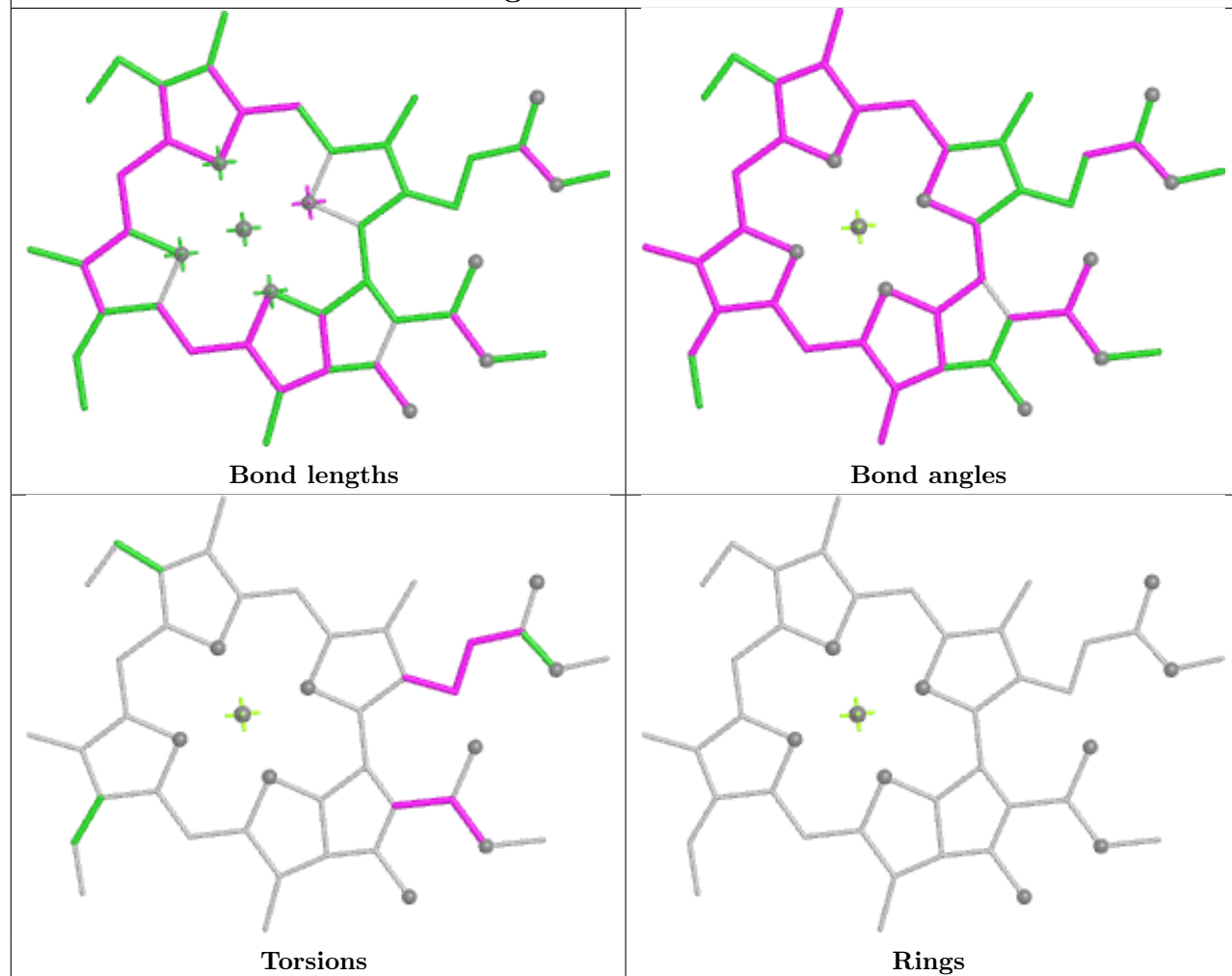


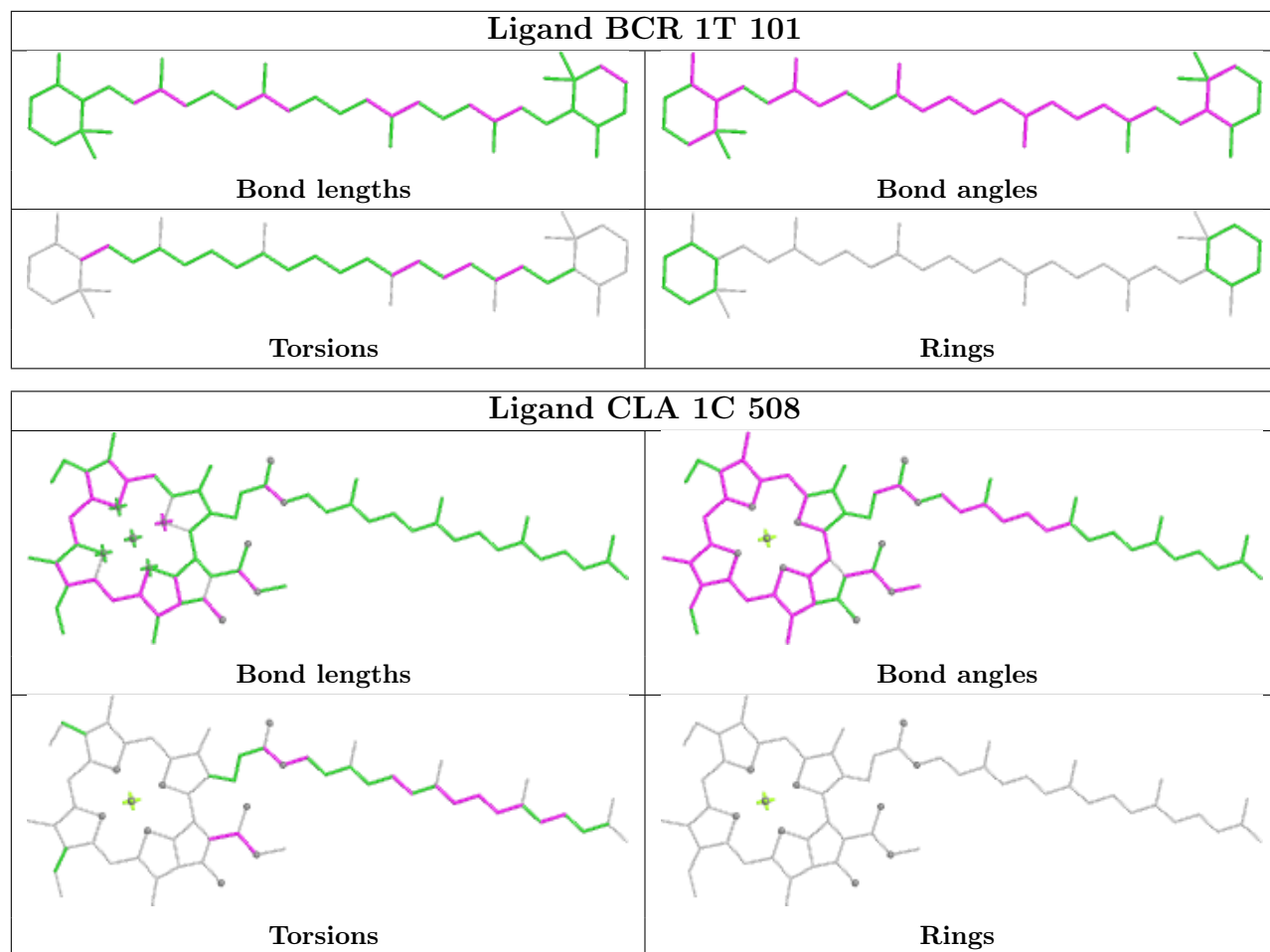


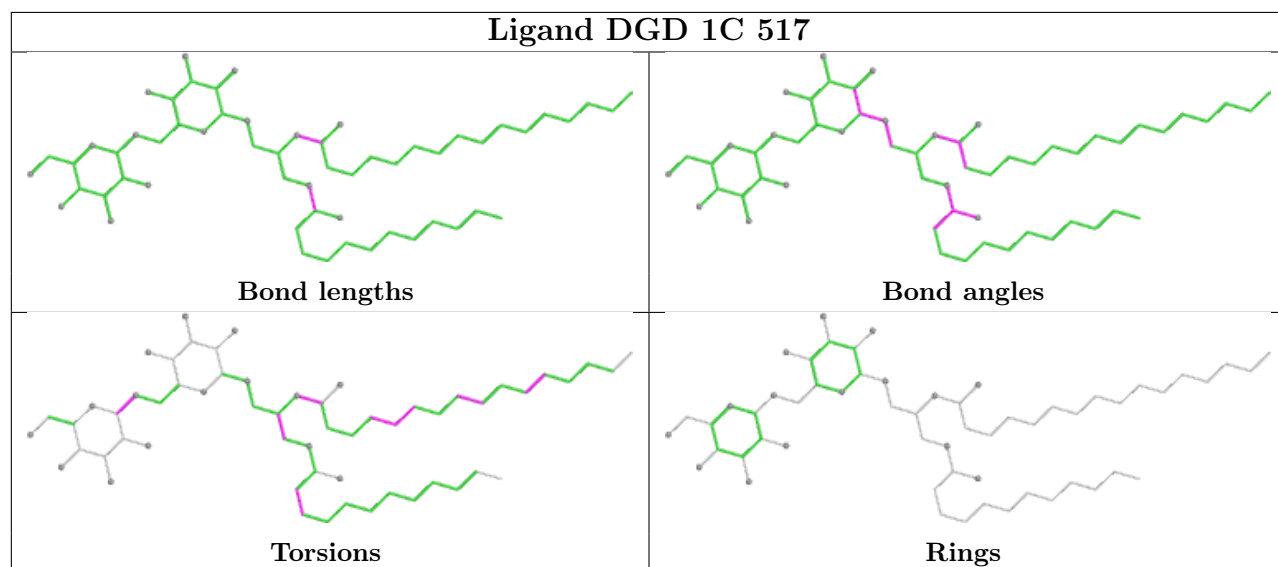
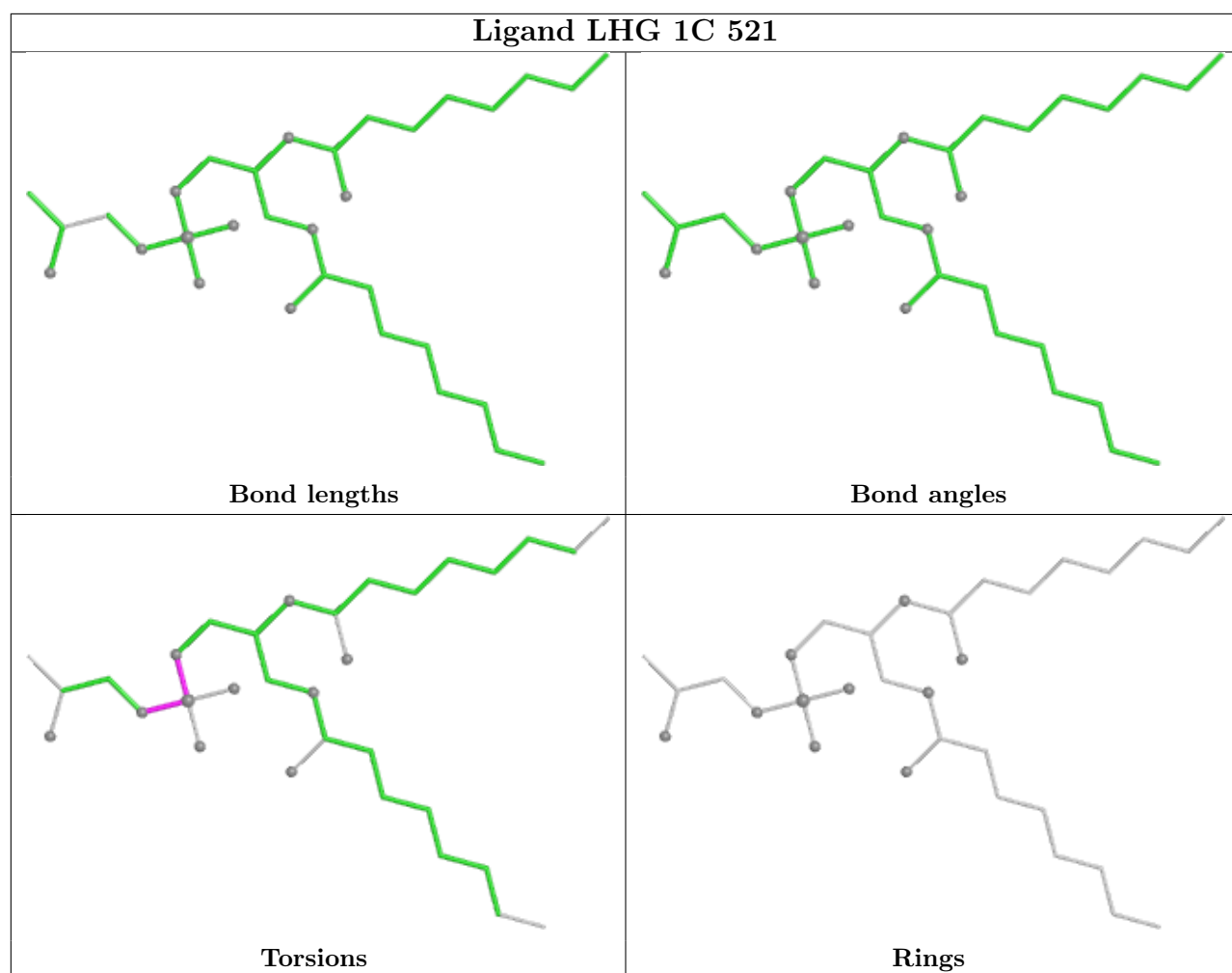
Ligand CLA 1B 606

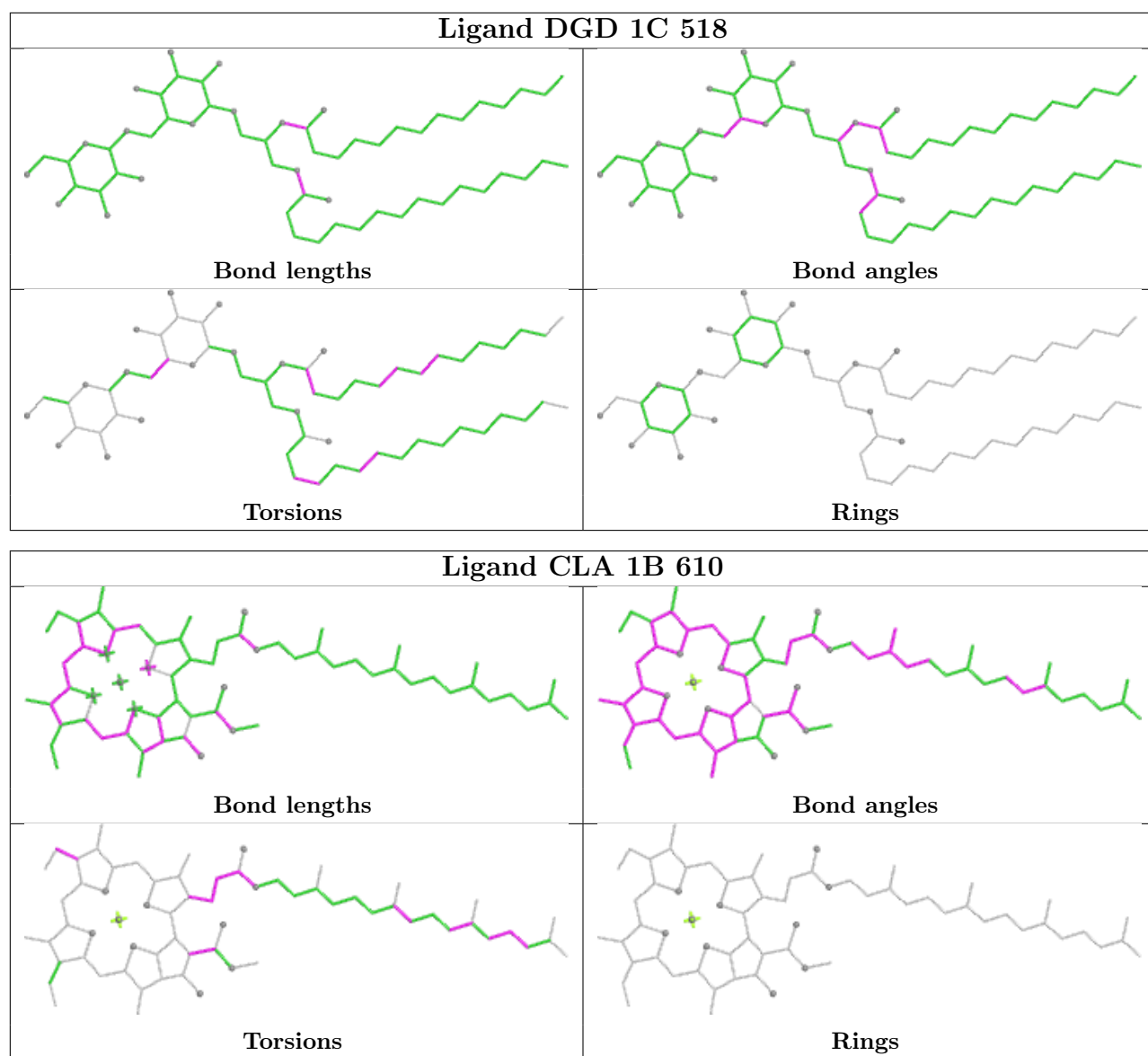


Ligand CLA 1C 511

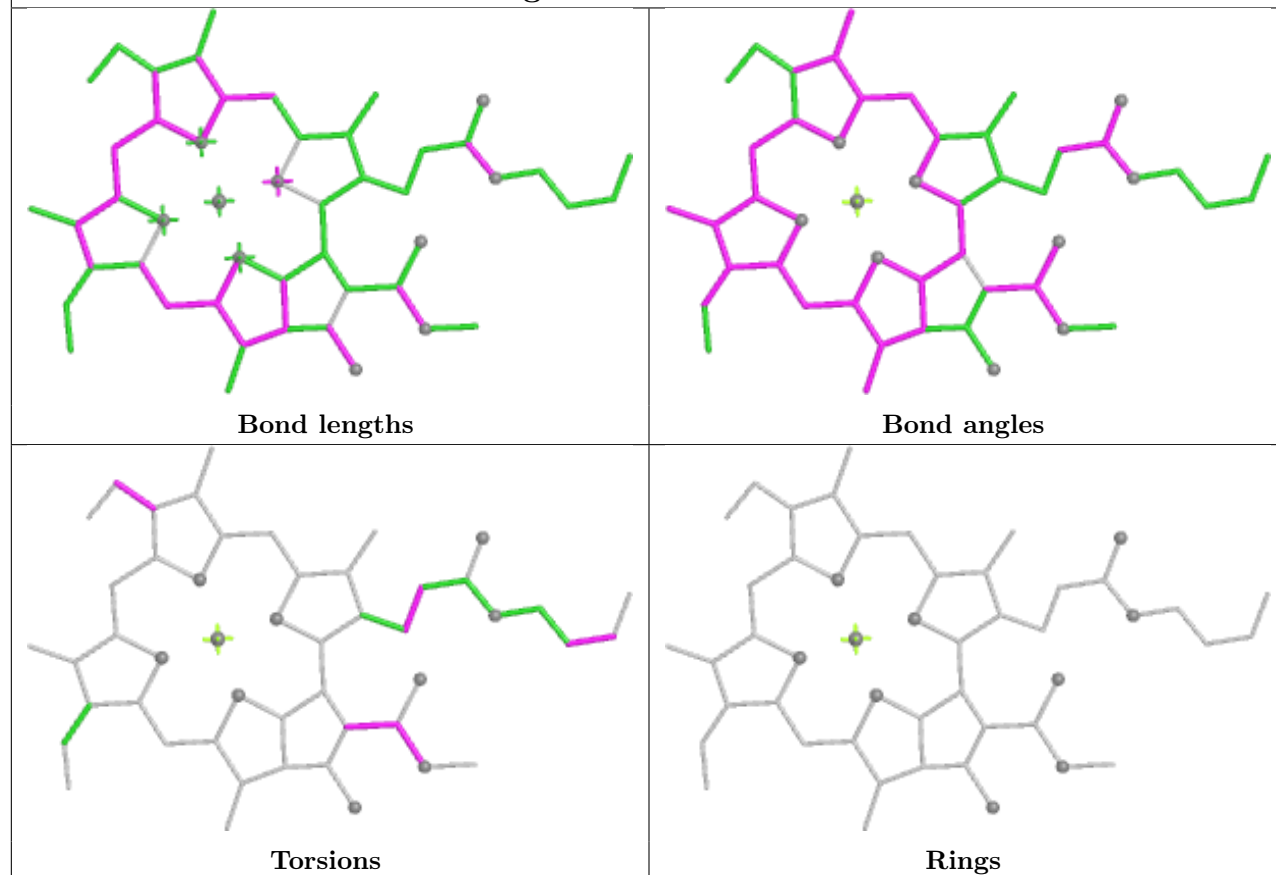




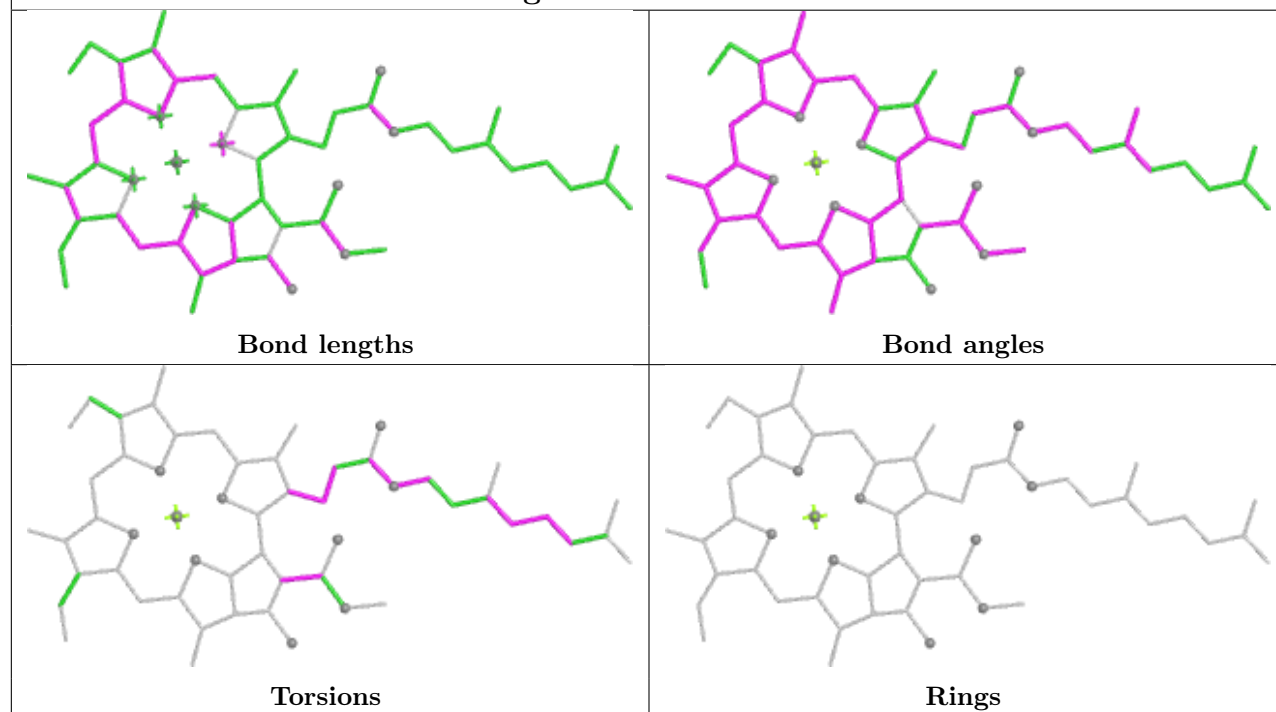


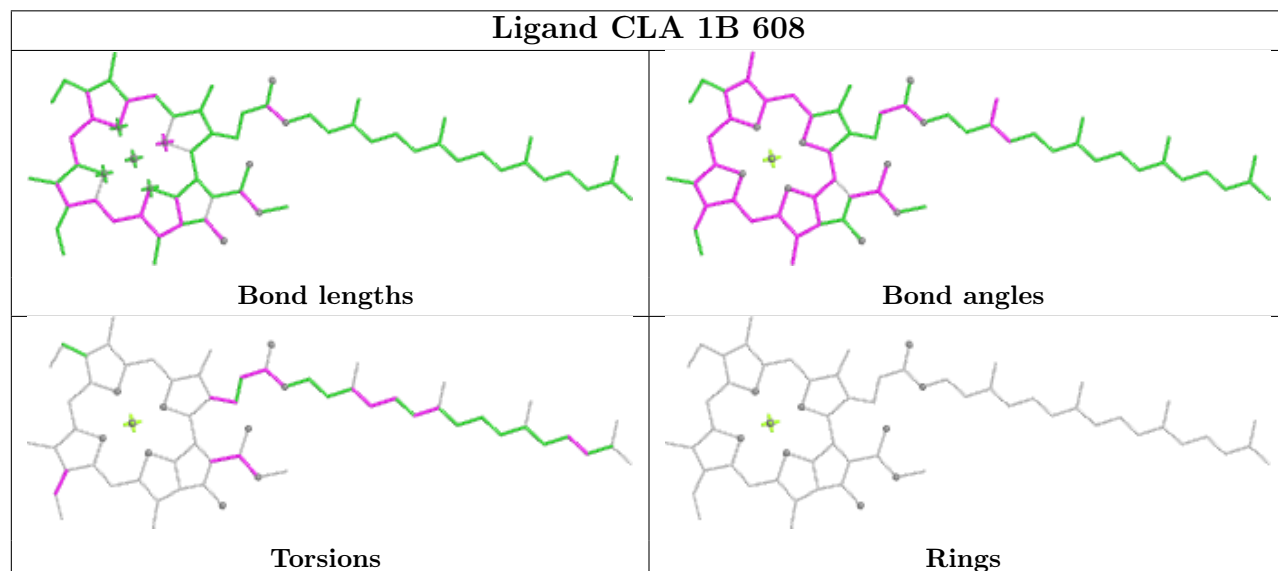
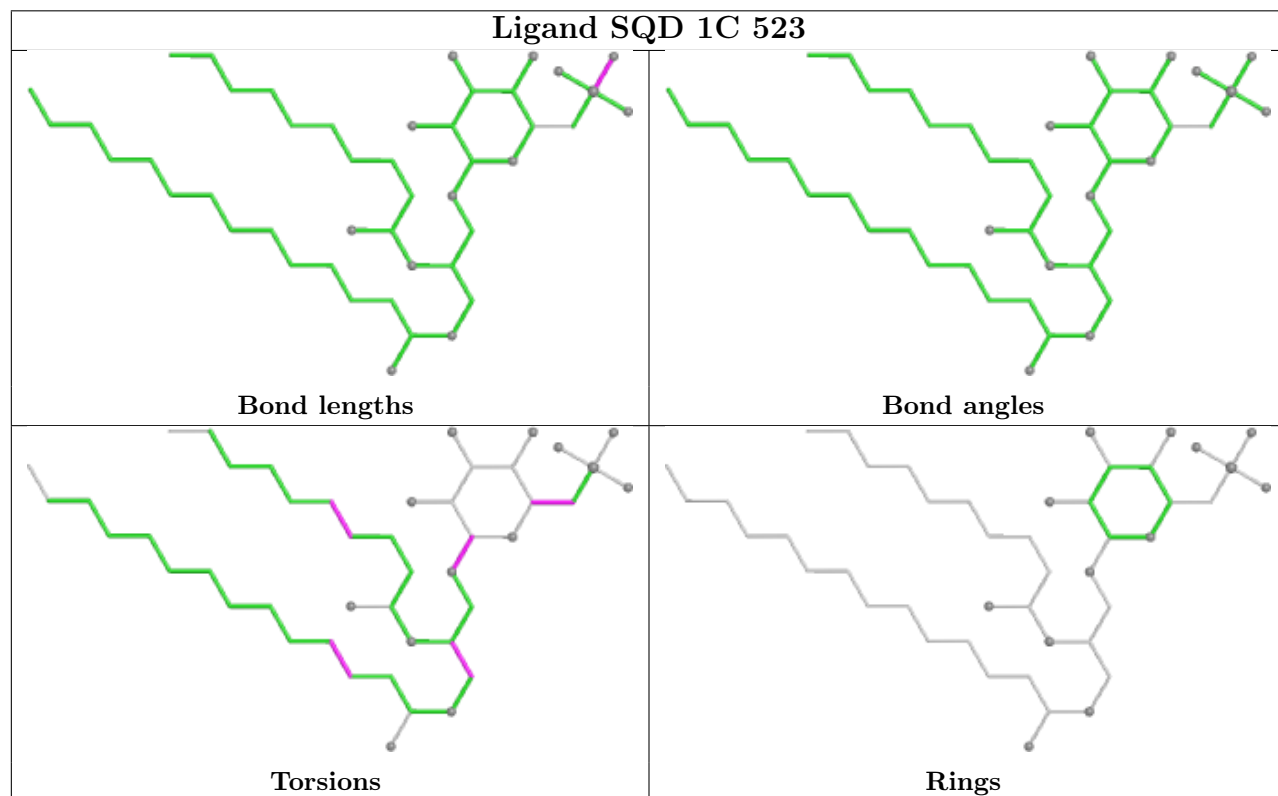
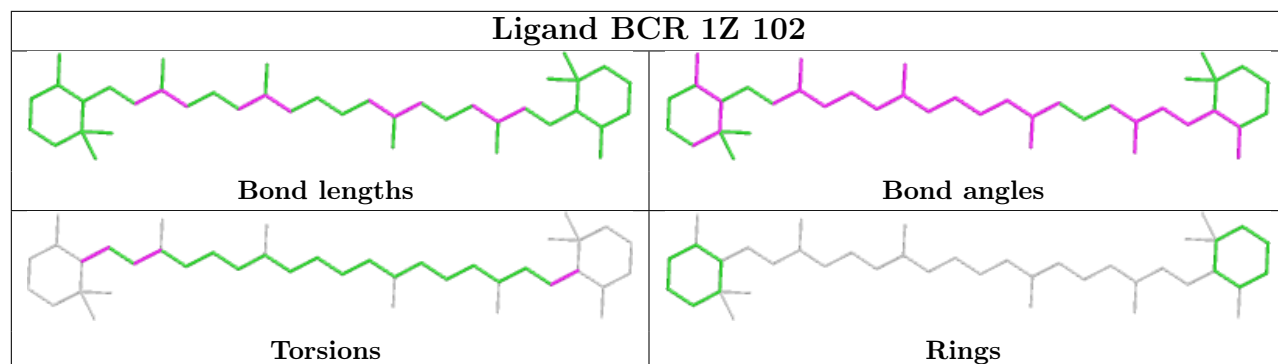


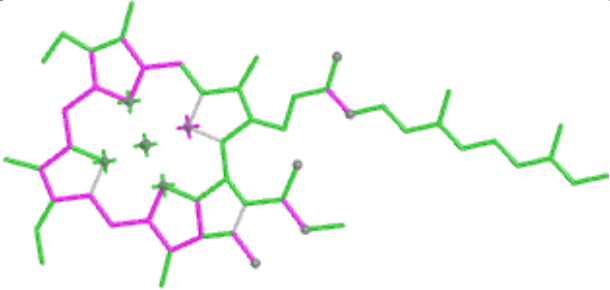
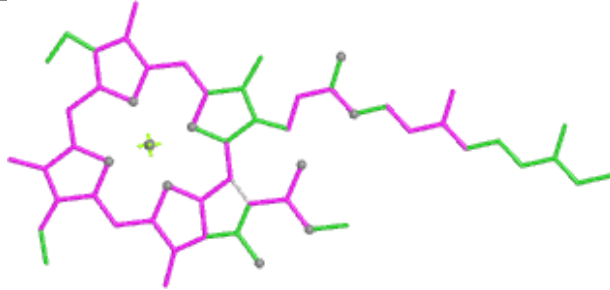
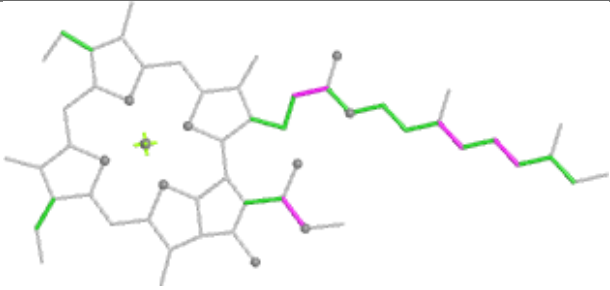
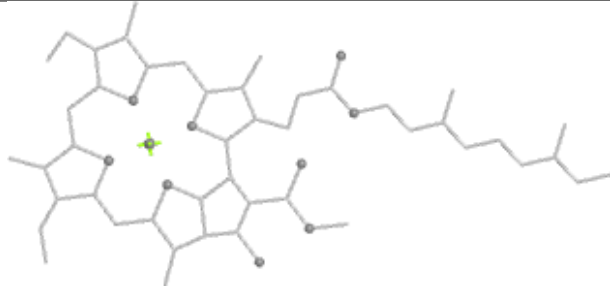
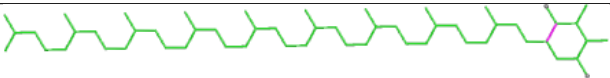
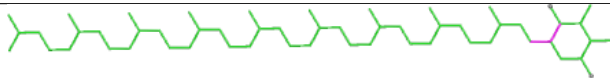
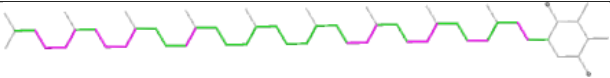
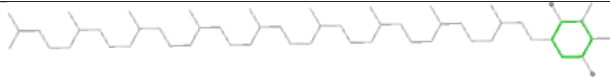
Ligand CLA 1C 506

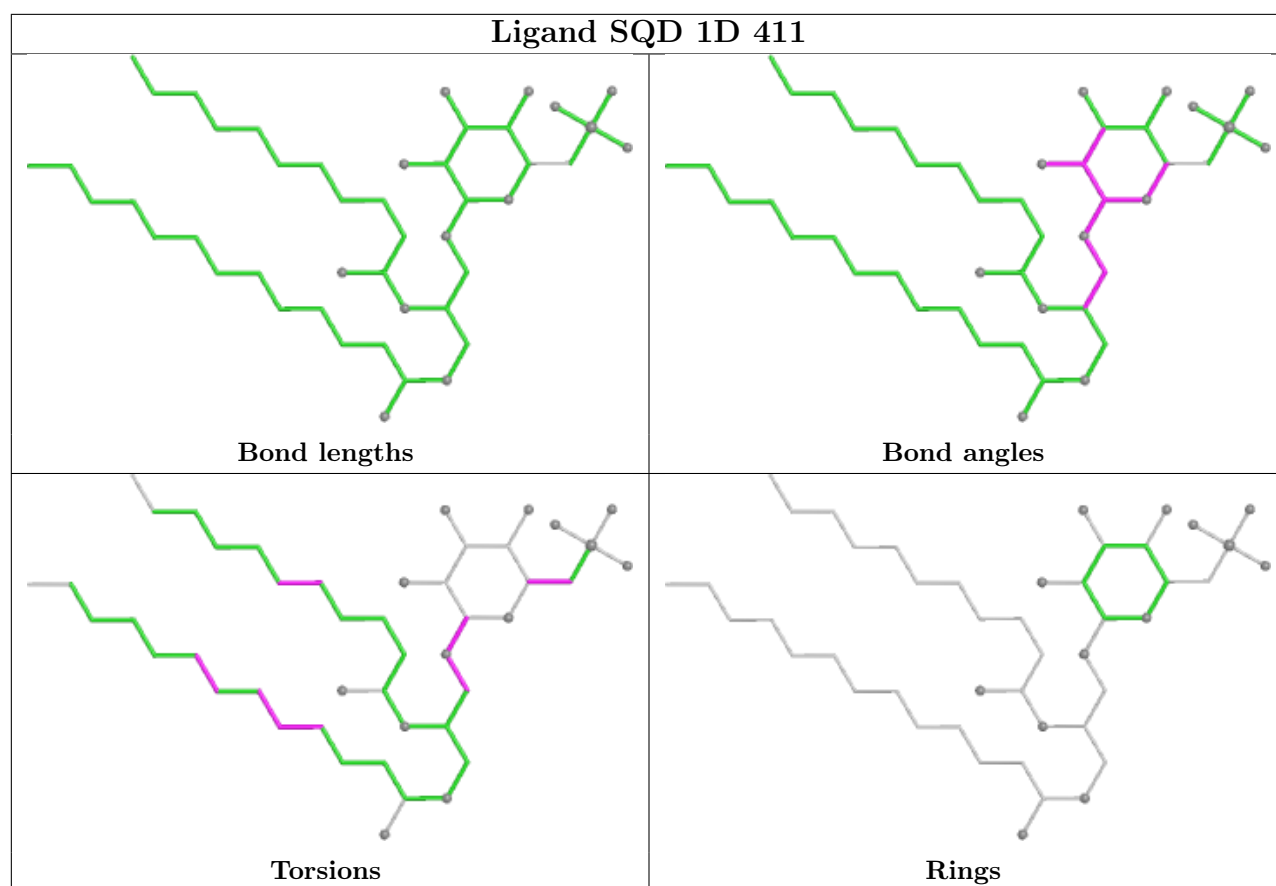


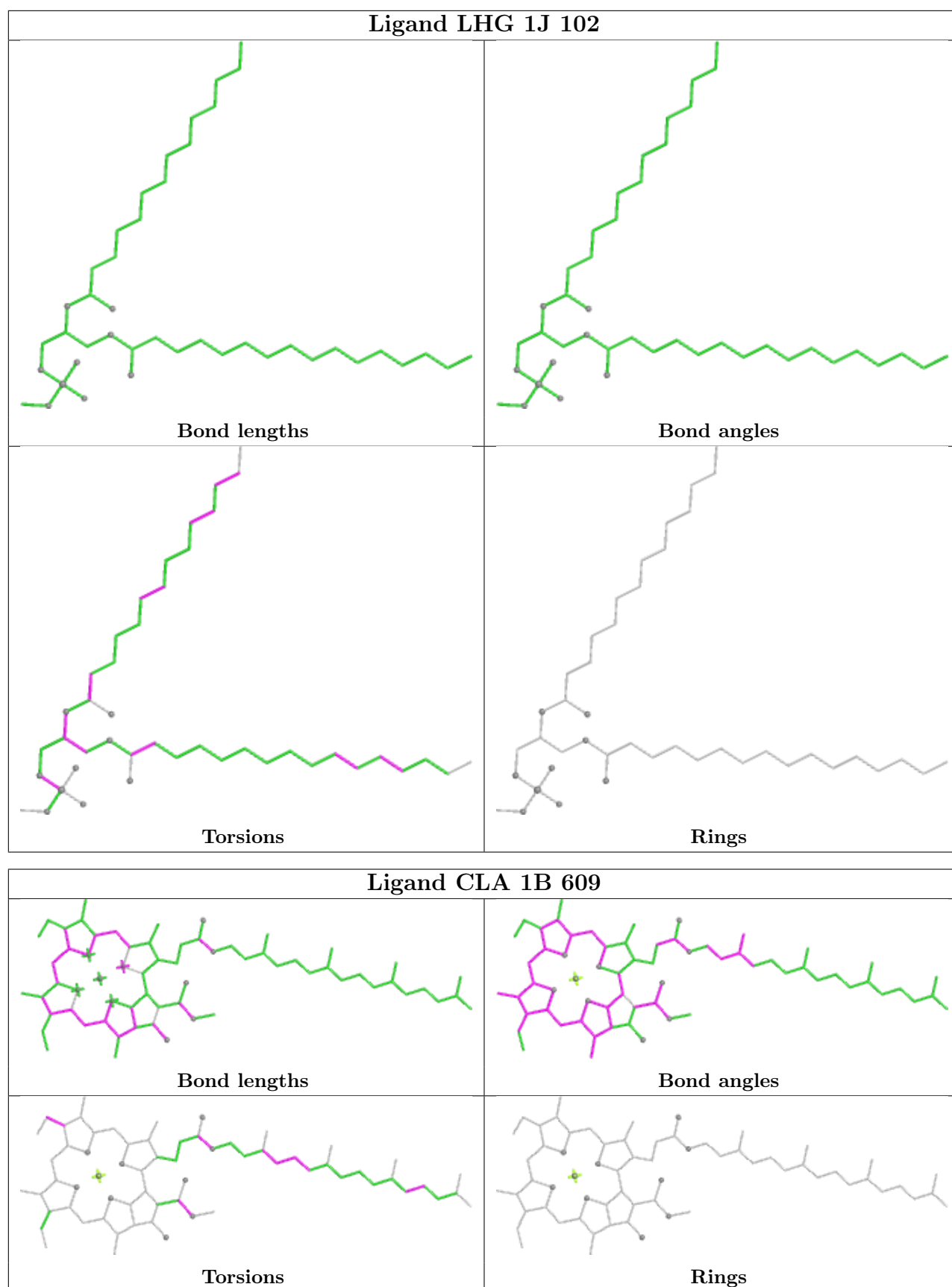
Ligand CLA 1C 512

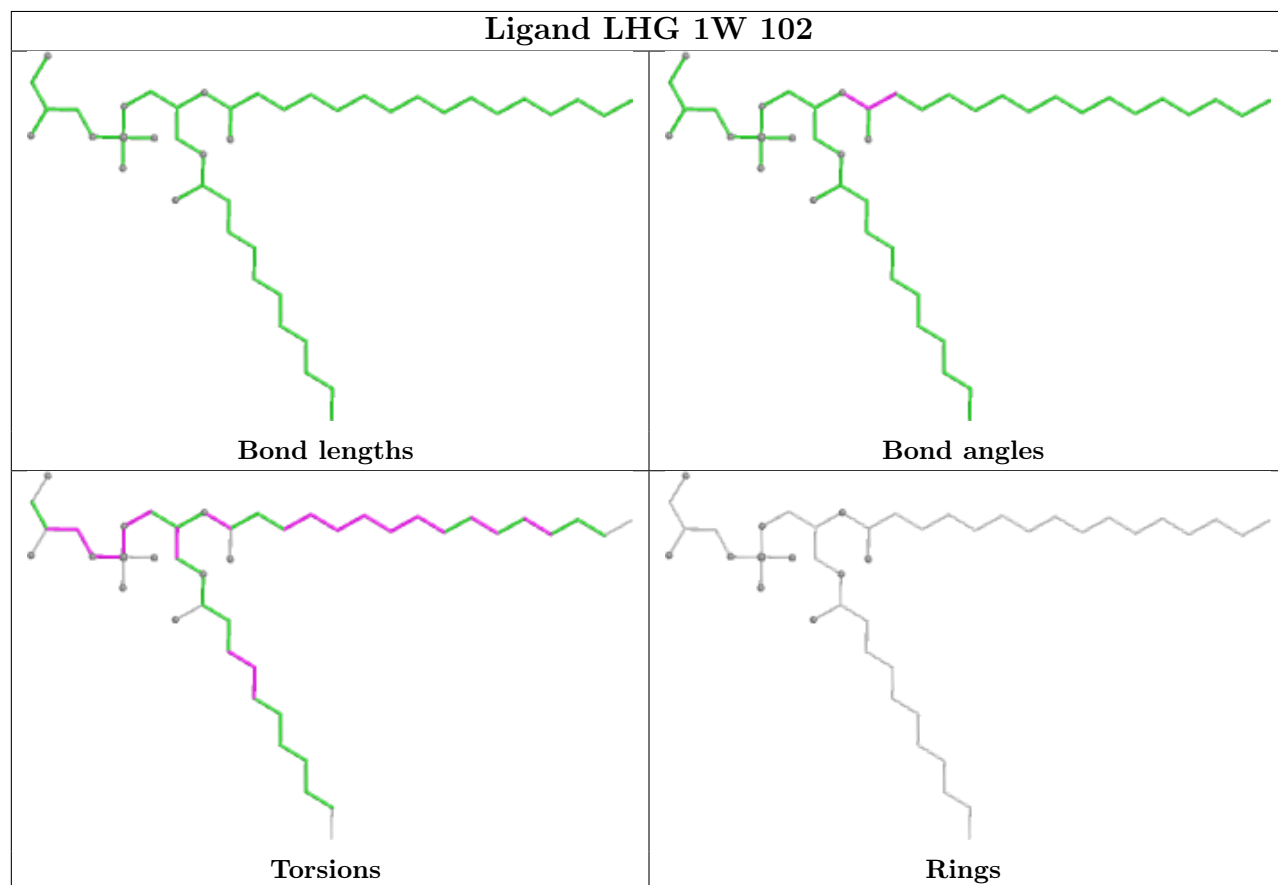
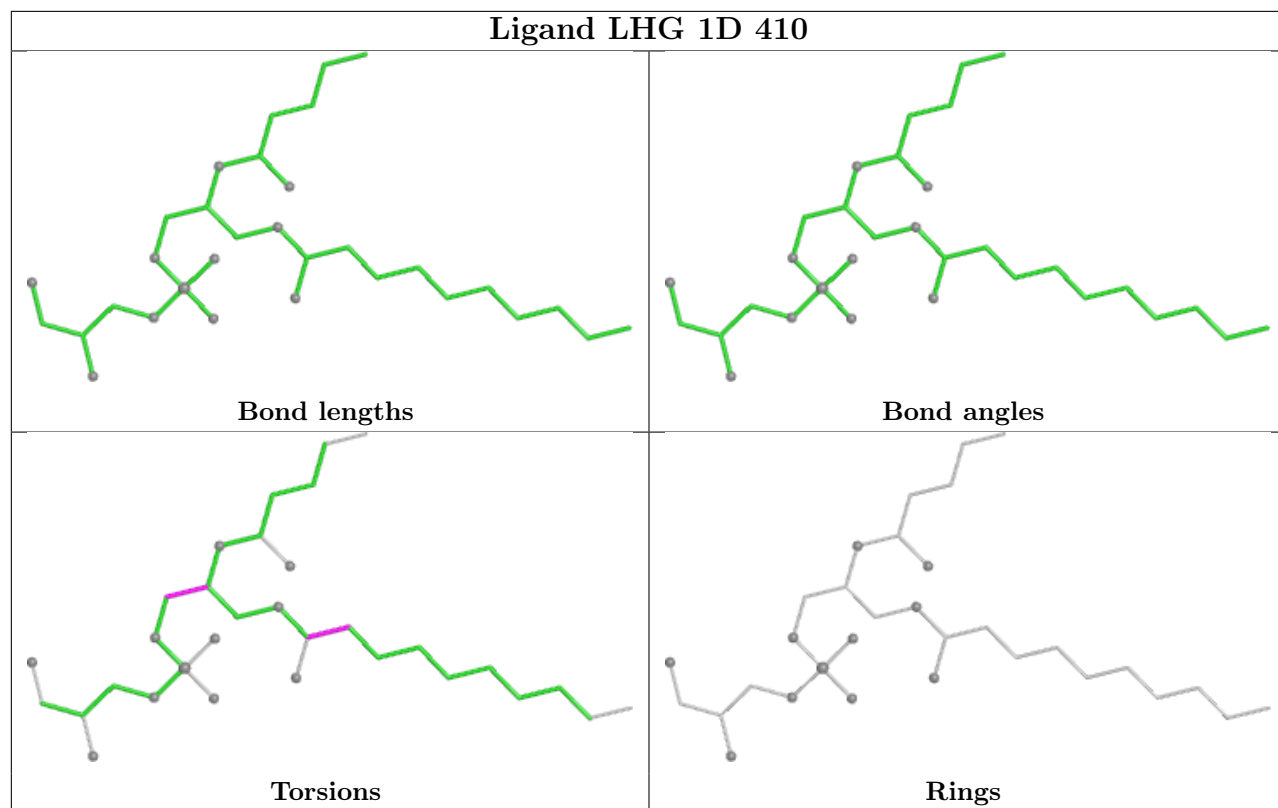


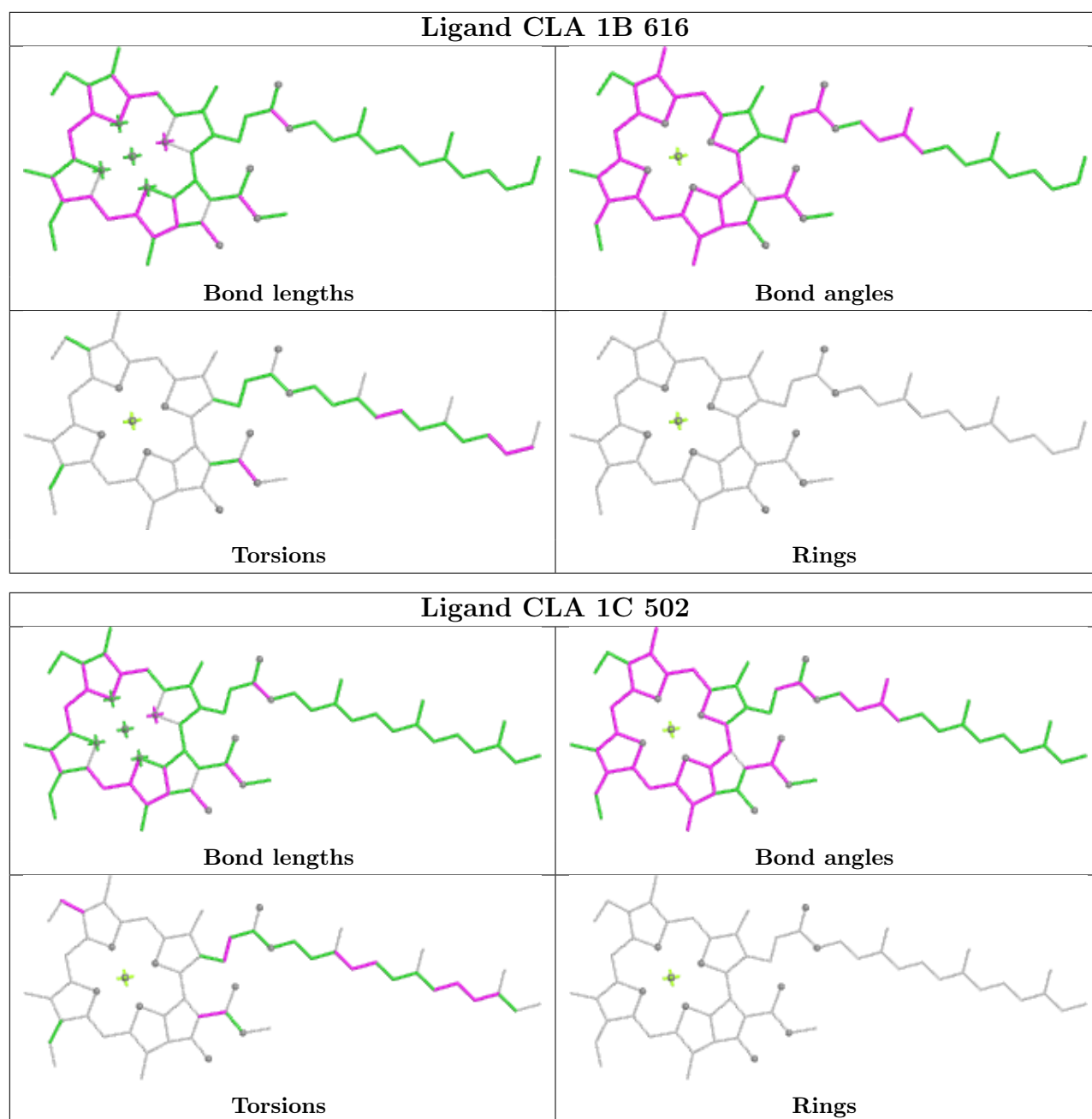


Ligand CLA 1C 503	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PL9 1H 101	
 Bond lengths	 Bond angles
 Torsions	 Rings









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.

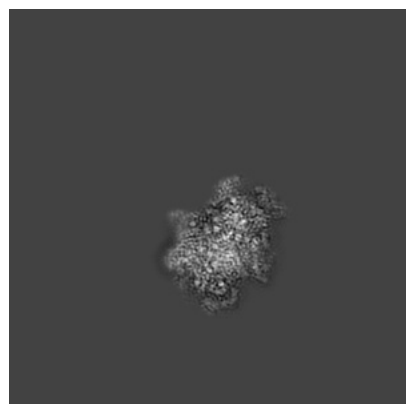
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-66946. These allow visual inspection of the internal detail of the map and identification of artifacts.

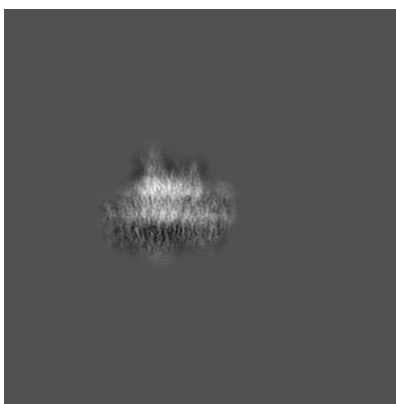
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

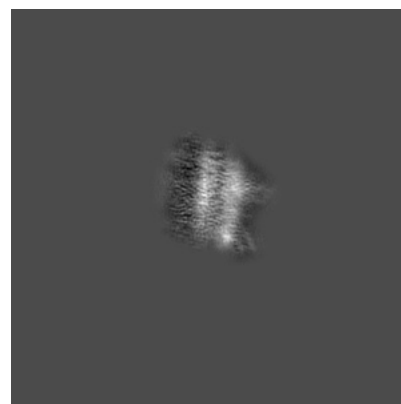
6.1.1 Primary map



X

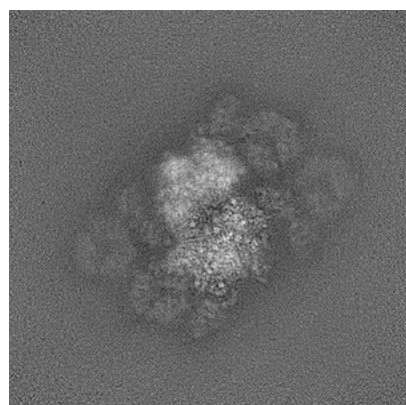


Y

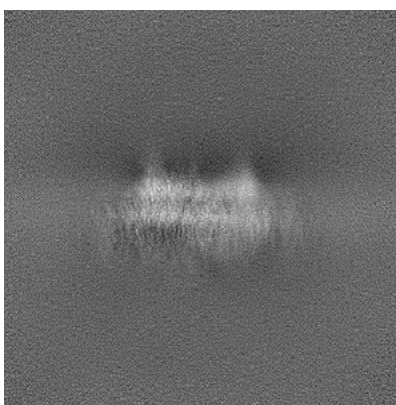


Z

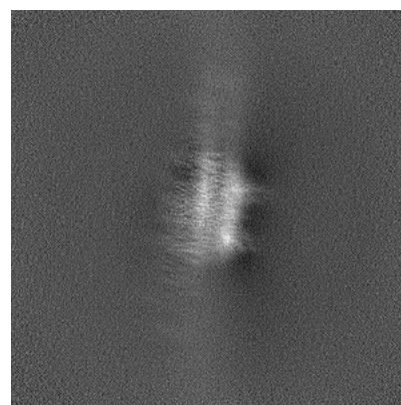
6.1.2 Raw map



X



Y

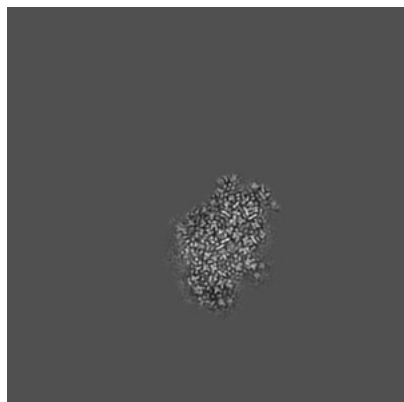


Z

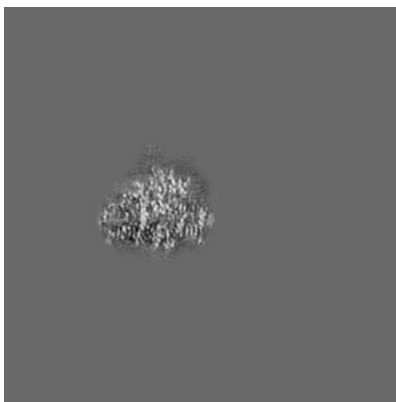
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

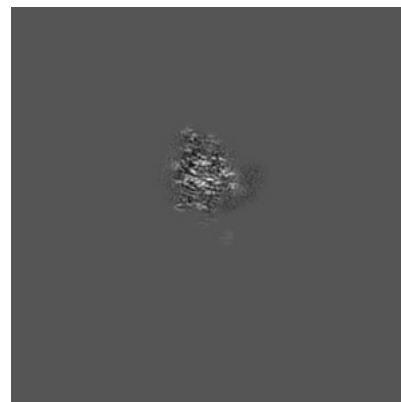
6.2.1 Primary map



X Index: 256

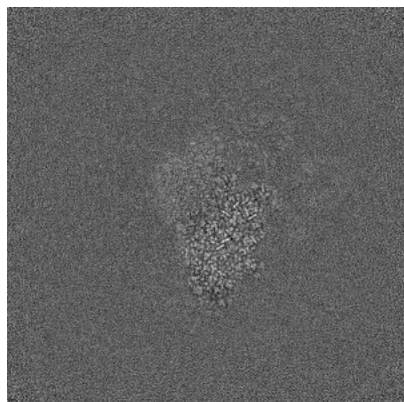


Y Index: 256

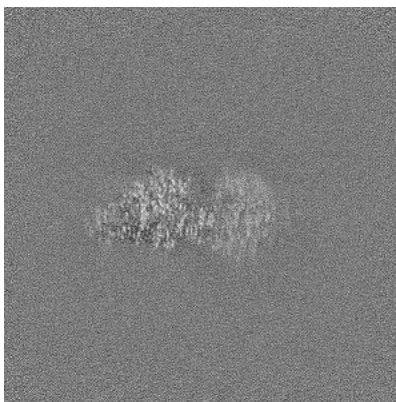


Z Index: 256

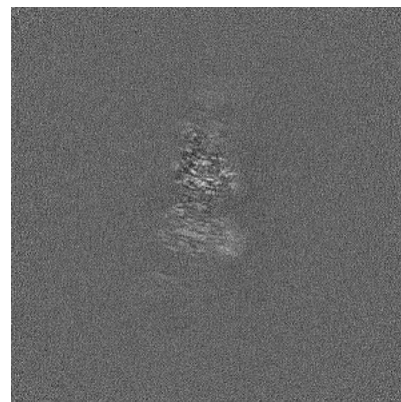
6.2.2 Raw map



X Index: 256



Y Index: 256

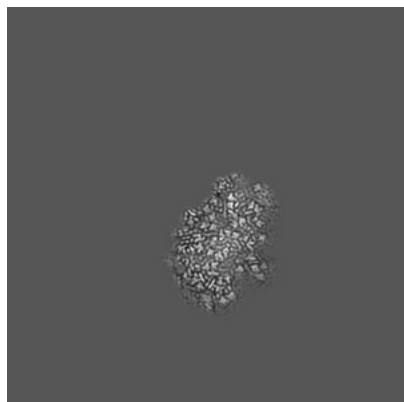


Z Index: 256

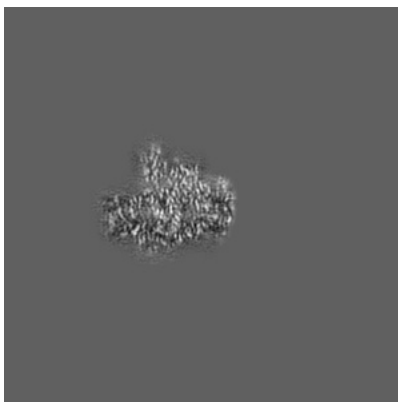
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

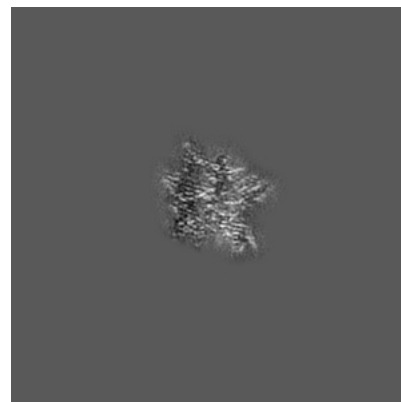
6.3.1 Primary map



X Index: 247

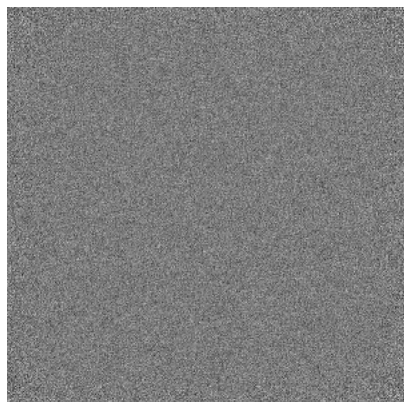


Y Index: 280

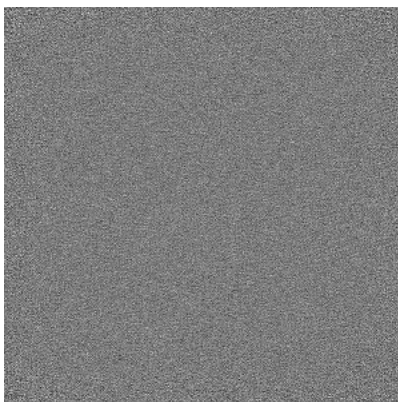


Z Index: 193

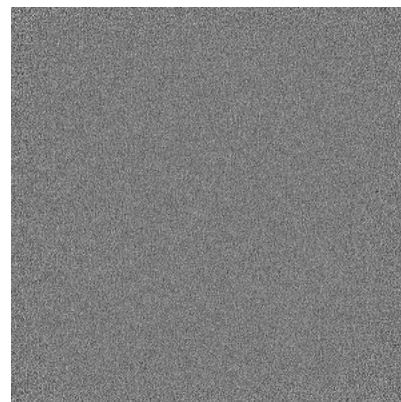
6.3.2 Raw map



X Index: 0



Y Index: 0

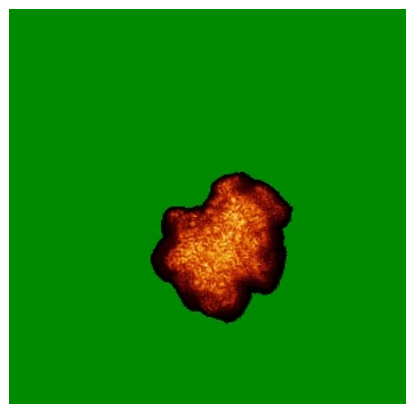


Z Index: 0

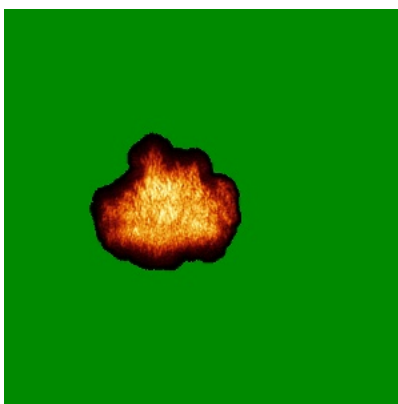
The images above show the largest variance slices of the map in three orthogonal directions.

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

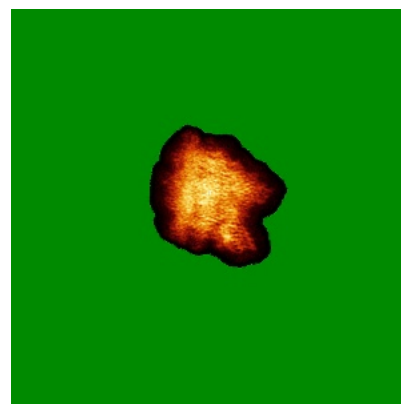
6.4.1 Primary map



X

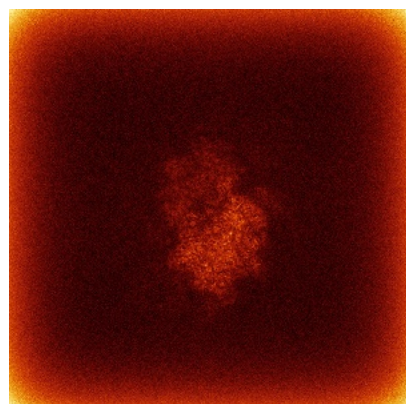


Y

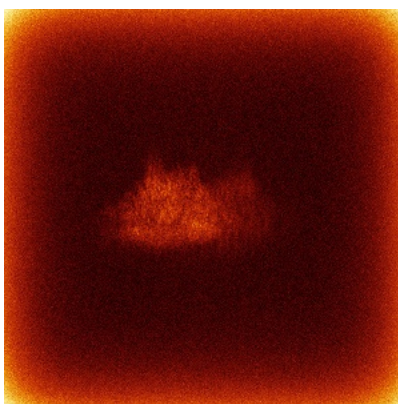


Z

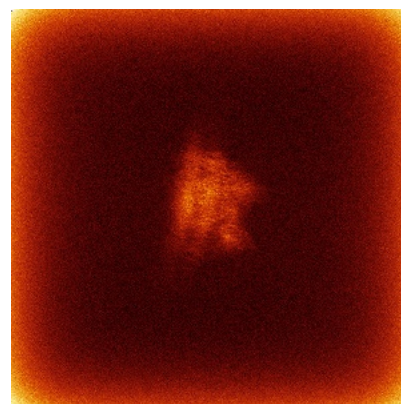
6.4.2 Raw map



X



Y

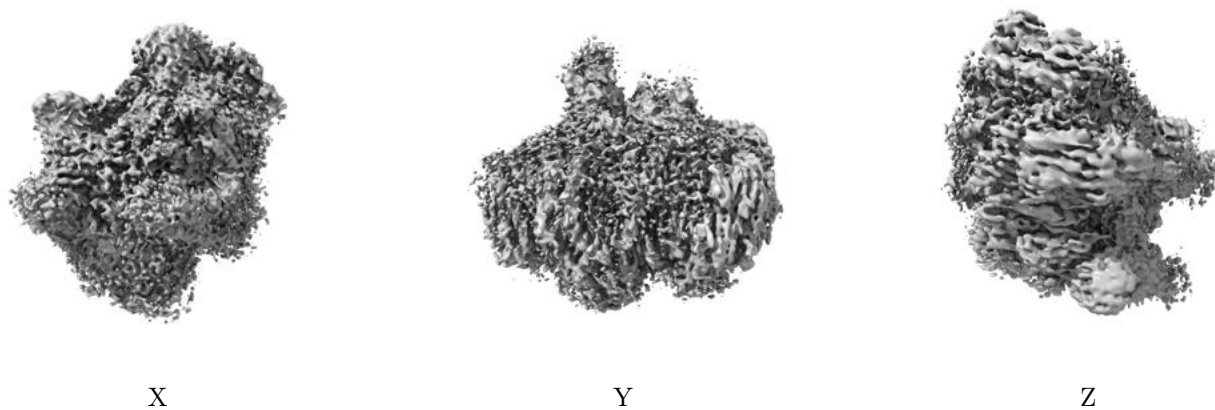


Z

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.

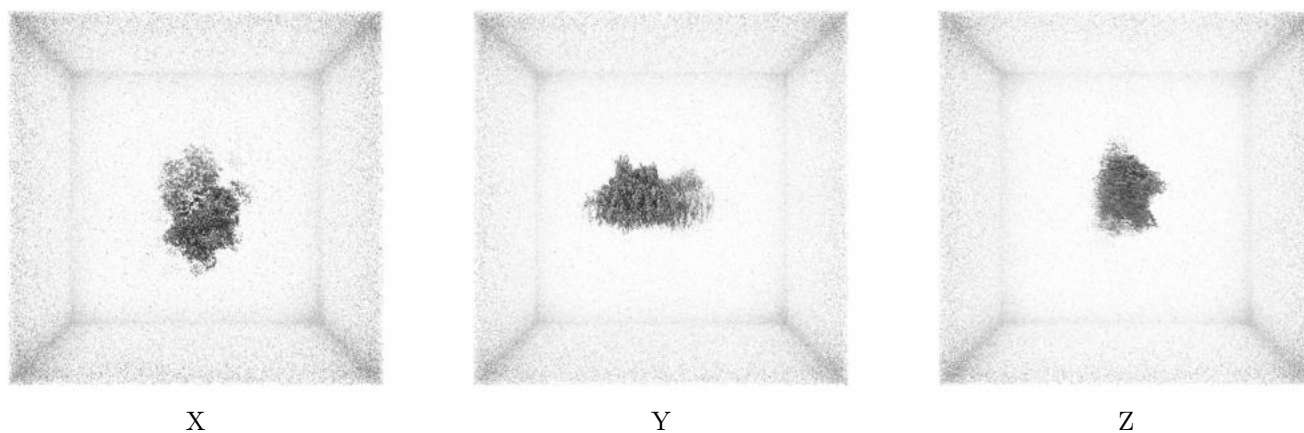
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. 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.

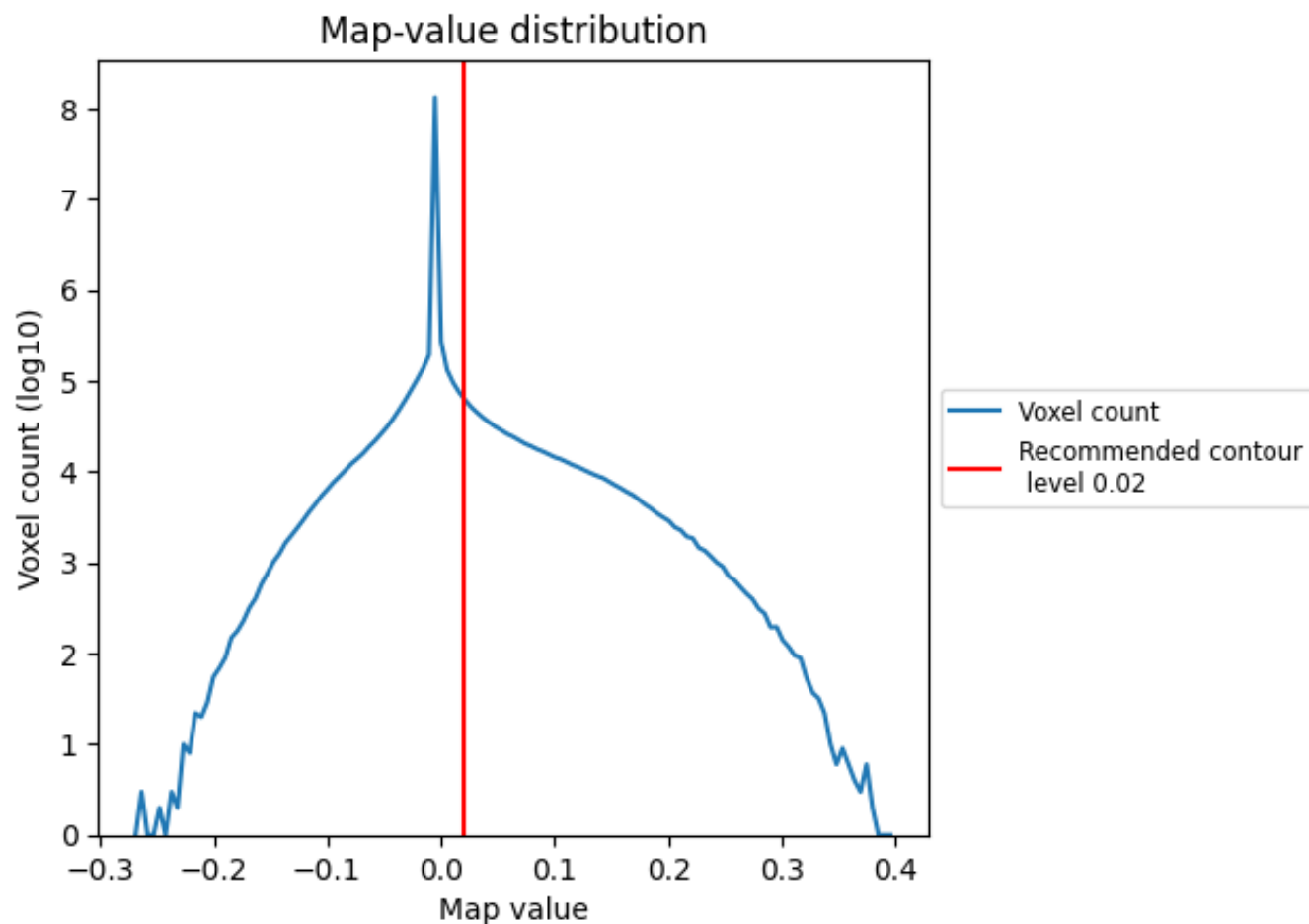
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

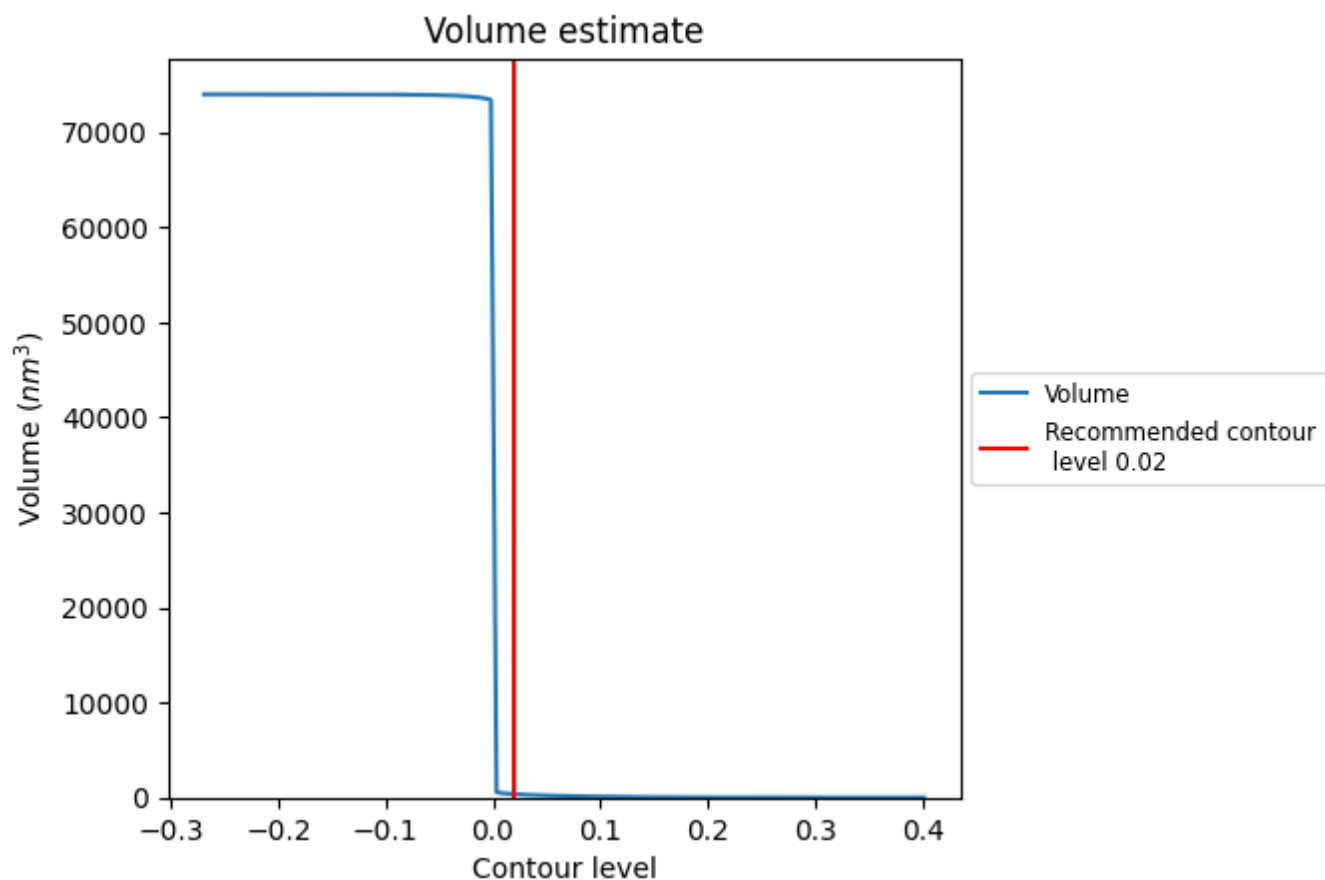
This section contains the results of statistical analysis of the map.

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.

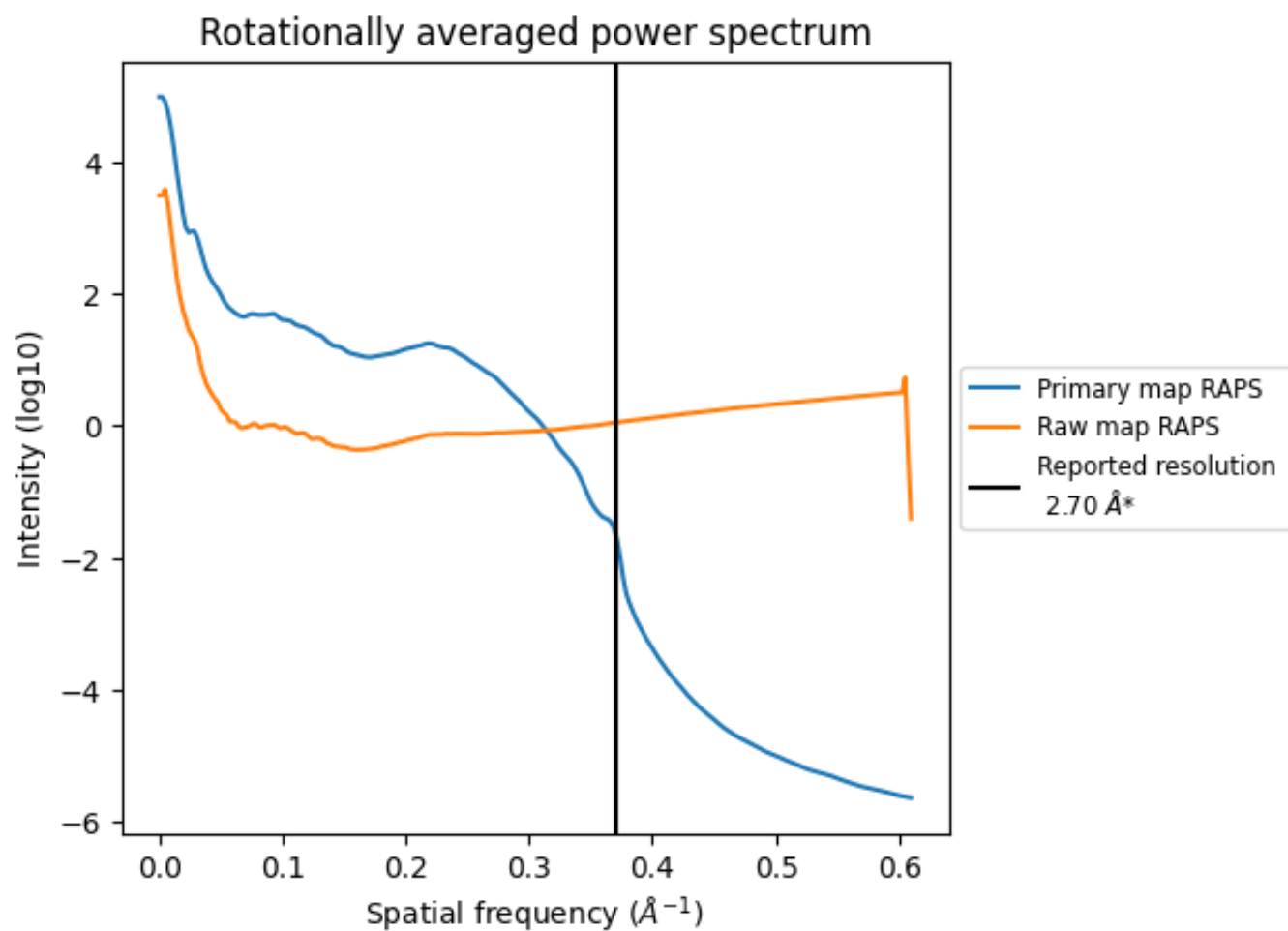
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 358 nm^3 ; this corresponds to an approximate mass of 323 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 ⓘ

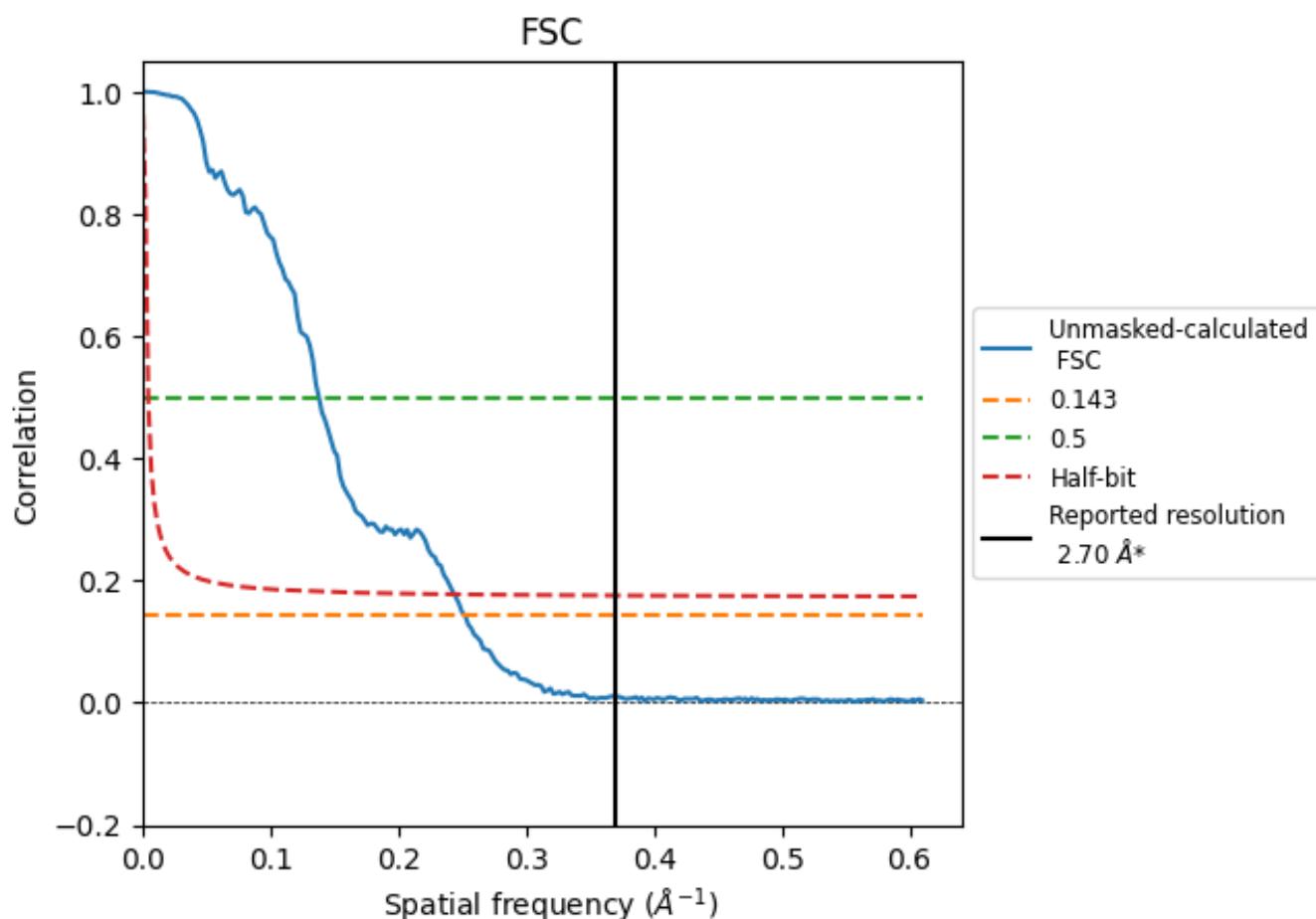


*Reported resolution corresponds to spatial frequency of 0.370 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

8.2 Resolution estimates [i](#)

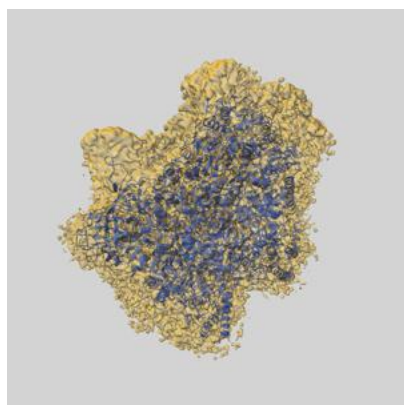
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.96	7.24	4.10

*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 3.96 differs from the reported value 2.7 by more than 10 %

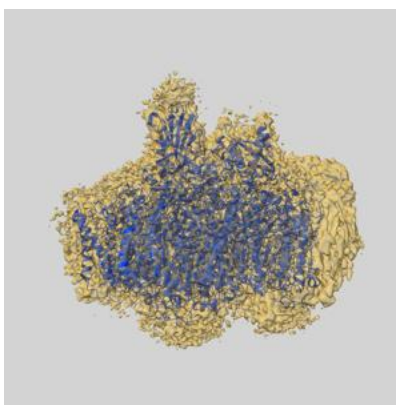
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-66946 and PDB model 9XK3. Per-residue inclusion information can be found in [section 3](#) on [page 20](#).

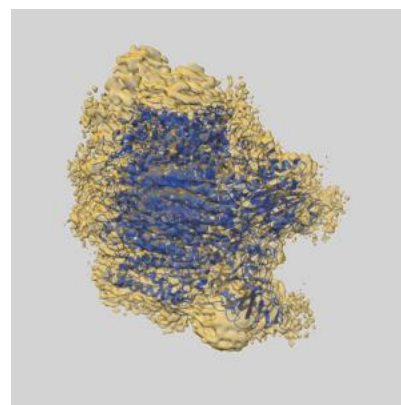
9.1 Map-model overlay [i](#)



X



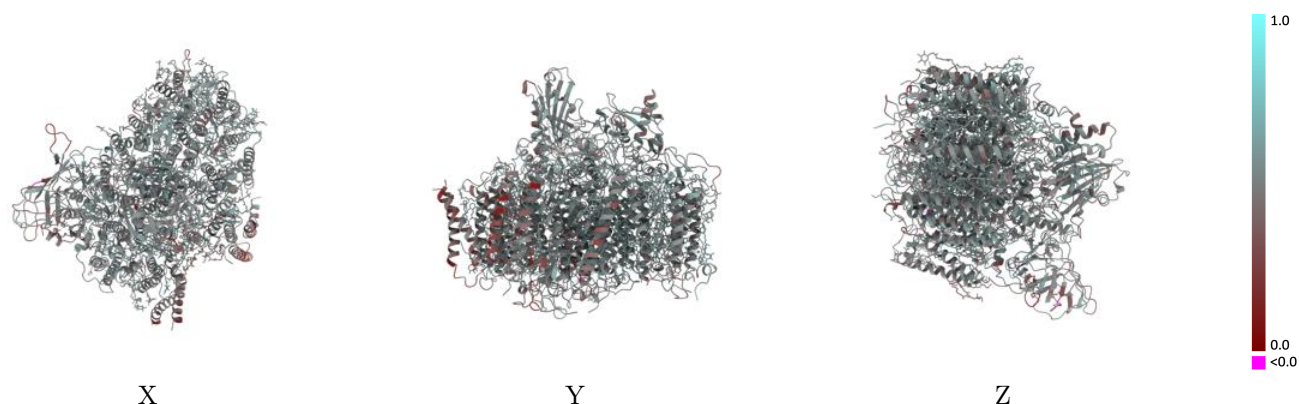
Y



Z

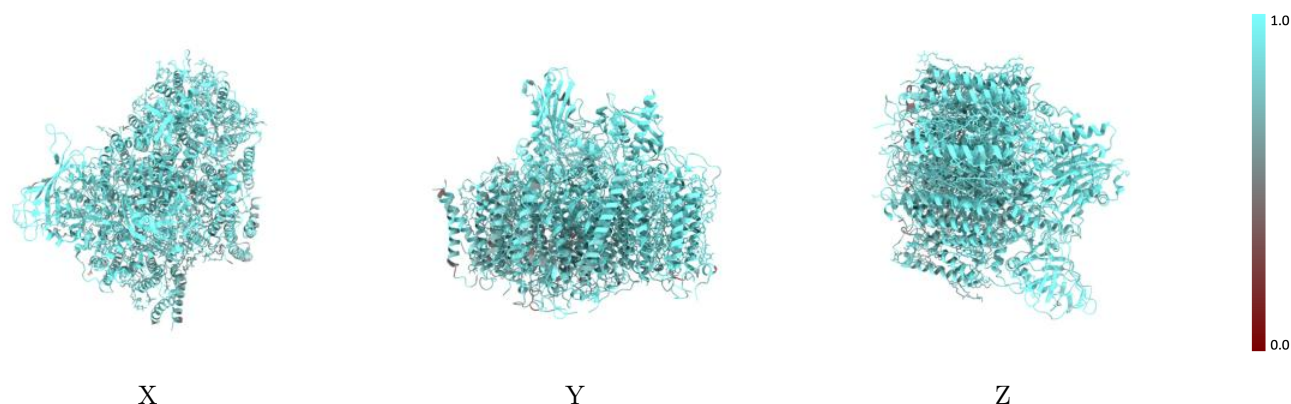
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



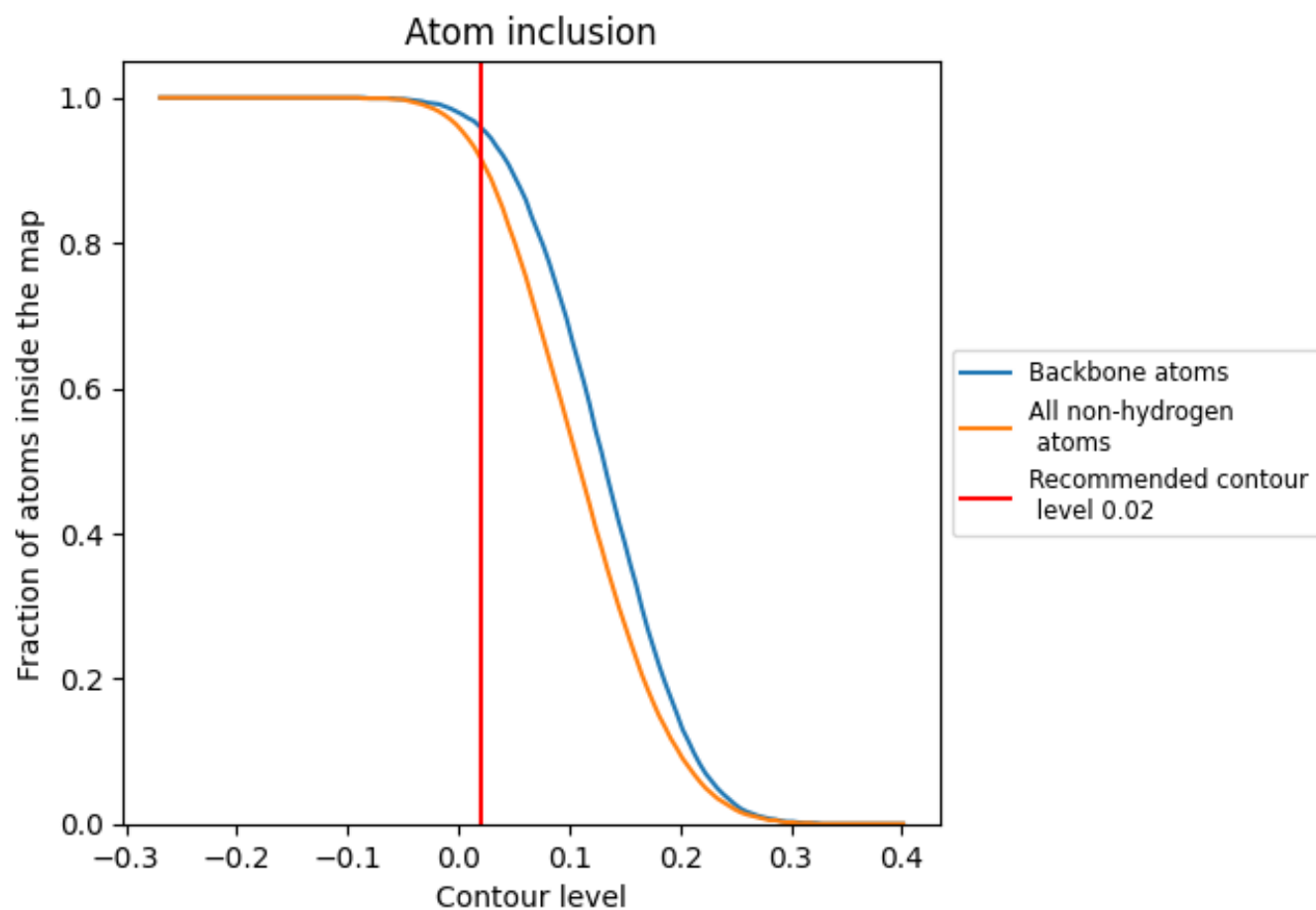
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 92% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9170	 0.4970
1A	 0.9110	 0.5080
1B	 0.9440	 0.5120
1C	 0.9270	 0.5150
1D	 0.9370	 0.5230
1E	 0.9070	 0.4910
1F	 0.9250	 0.4940
1H	 0.8840	 0.4850
1I	 0.8620	 0.4930
1J	 0.8980	 0.4760
1K	 0.8630	 0.4850
1L	 0.9110	 0.5160
1M	 0.8260	 0.4680
1O	 0.9610	 0.4620
1P	 0.9520	 0.4930
1T	 0.9160	 0.5110
1U	 0.9660	 0.4840
1V	 0.7400	 0.4040
1W	 0.8360	 0.4320
1X	 0.8910	 0.4780
1Y	 0.8010	 0.4060
1Z	 0.7940	 0.3970

