



## wwPDB EM Validation Summary Report ⓘ

Mar 6, 2026 – 09:53 PM UTC

PDB ID : 8KDE / pdb\_00008kde  
EMDB ID : EMD-37133  
Title : Cryo-EM structure of an intermediate-state complex during the process of photosystem II repair  
Authors : Li, A.; Wang, Y.; Liu, Z.  
Deposited on : 2023-08-09  
Resolution : 2.60 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](mailto: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>.

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

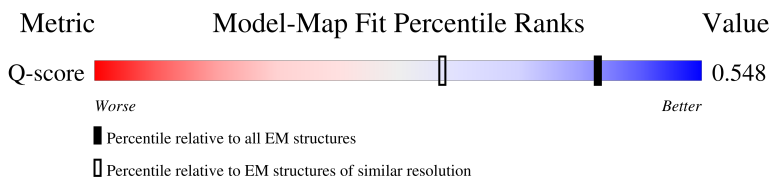
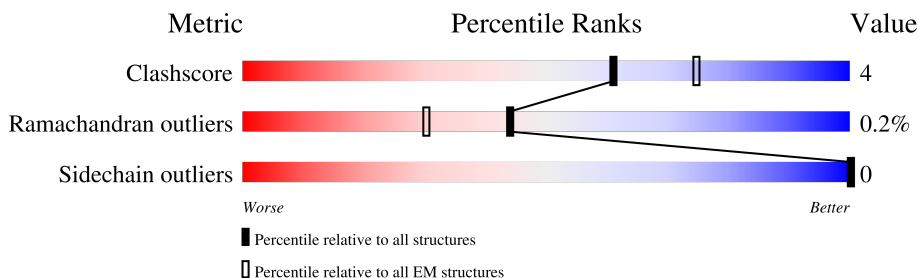
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (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 i

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

The reported resolution of this entry is 2.60 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	8728 ( 2.10 - 3.10 )

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  $\geq 3$ , 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	B	508	87% 8% 5%
2	D	352	89% 10%
3	E	82	83% 12% 5%
4	F	44	61% 16% 23%

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Mol	Chain	Length	Quality of chain
5	H	88	
6	I	37	
7	K	46	
8	L	38	
9	M	34	
10	T	31	
11	V	33	
12	X	101	
13	Z	62	
14	G	196	
15	3	131	
16	C	461	
17	A	352	
18	1	117	

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
19	CLA	A	403	X	-	-	-
19	CLA	A	404	X	-	-	-
19	CLA	A	405	X	-	-	-
19	CLA	B	601	X	-	-	-
19	CLA	B	602	X	-	-	-
19	CLA	B	603	X	-	-	-
19	CLA	B	604	X	-	-	-
19	CLA	B	605	X	-	-	-
19	CLA	B	606	X	-	-	-
19	CLA	B	607	X	-	-	-
19	CLA	B	608	X	-	-	-
19	CLA	B	609	X	-	-	-
19	CLA	B	610	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	B	611	X	-	-	-
19	CLA	B	612	X	-	-	-
19	CLA	B	613	X	-	-	-
19	CLA	B	614	X	-	-	-
19	CLA	B	615	X	-	-	-
19	CLA	B	616	X	-	-	-
19	CLA	C	602	X	-	-	-
19	CLA	C	603	X	-	-	-
19	CLA	C	604	X	-	-	-
19	CLA	C	605	X	-	-	-
19	CLA	C	606	X	-	-	-
19	CLA	C	607	X	-	-	-
19	CLA	C	608	X	-	-	-
19	CLA	C	609	X	-	-	-
19	CLA	C	610	X	-	-	-
19	CLA	C	611	X	-	-	-
19	CLA	C	612	X	-	-	-
19	CLA	C	613	X	-	-	-
19	CLA	C	614	X	-	-	-
19	CLA	D	401	X	-	-	-
19	CLA	D	402	X	-	-	-
19	CLA	D	409	X	-	-	-

## 2 Entry composition i

There are 30 unique types of molecules in this entry. The entry contains 22087 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 CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	B	482	3766	2469	629	656	12	0	0

- Molecule 2 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	D	351	2791	1841	459	479	12	0	0

- Molecule 3 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	E	78	633	414	104	115	0	0

- Molecule 4 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	F	34	277	190	45	41	1	0	0

- Molecule 5 is a protein called Photosystem II reaction center protein H.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	H	73	561	372	84	103	2	0	0

- Molecule 6 is a protein called Photosystem II reaction center protein I.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	I	35	283	193	43	45	2	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
7	K	37	297	209	43	45	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	L	38	314	210	51	52	1	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
9	M	31	239	163	33	43	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	T	31	256	177	38	39	2	0	0

- Molecule 11 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
11	V	32	224	147	37	40	0	0

- Molecule 12 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
12	X	35	242	159	39	44	0	0

- Molecule 13 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	Z	61	458	314	68	75	1	0	0

- Molecule 14 is a protein called Thylakoid enriched factor 14 (TEF14).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	G	145	1070	656	191	222	1	0	0

- Molecule 15 is a protein called Photosystem II repair factor 1 (PRF1).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	3	97	694	429	121	144		0	0

- Molecule 16 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	C	430	3368	2209	561	581	17	0	0

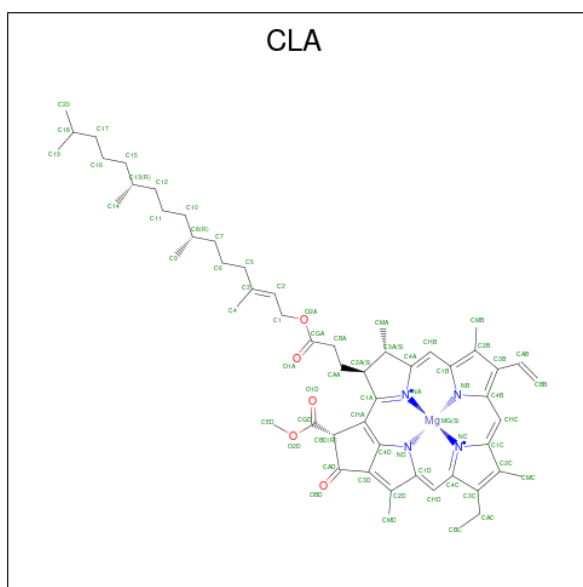
- Molecule 17 is a protein called Photosystem II protein D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	A	309	2418	1587	401	415	15	0	0

- Molecule 18 is a protein called Photosystem II repair factor 2 (PRF2).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	1	45	320	201	59	58	2	0	0

- Molecule 19 is CHLOROPHYLL A (CCD ID: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>) (labeled as "Ligand of Interest" by depositor).



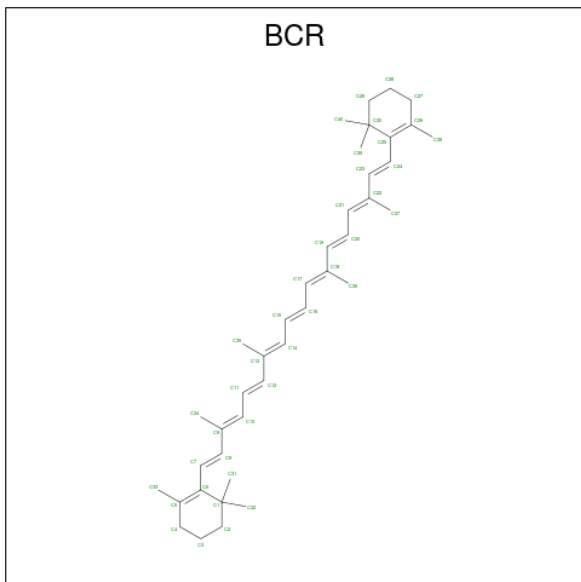
Mol	Chain	Residues	Atoms				AltConf	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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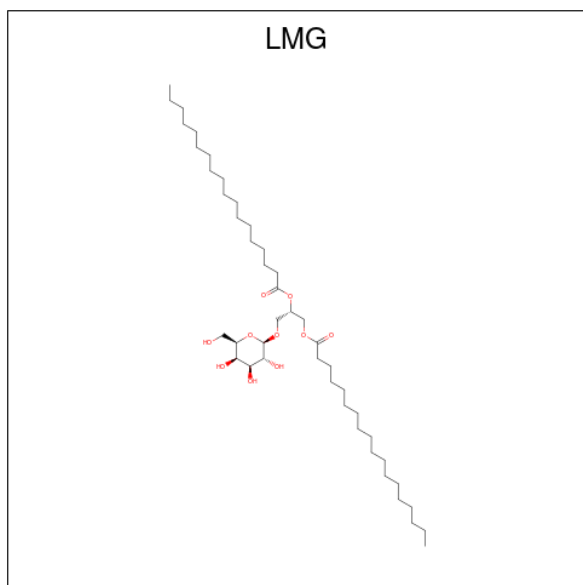
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
19	B	1	65	55	1	4	5	0
19	B	1	65	55	1	4	5	0
19	D	1	65	55	1	4	5	0
19	D	1	65	55	1	4	5	0
19	D	1	65	55	1	4	5	0
19	C	1	65	55	1	4	5	0
19	C	1	65	55	1	4	5	0
19	C	1	65	55	1	4	5	0
19	C	1	65	55	1	4	5	0
19	C	1	65	55	1	4	5	0
19	C	1	65	55	1	4	5	0
19	C	1	65	55	1	4	5	0
19	C	1	65	55	1	4	5	0
19	C	1	65	55	1	4	5	0
19	C	1	65	55	1	4	5	0
19	C	1	65	55	1	4	5	0
19	C	1	65	55	1	4	5	0
19	C	1	65	55	1	4	5	0
19	A	1	65	55	1	4	5	0
19	A	1	49	39	1	4	5	0
19	A	1	60	50	1	4	5	0

- Molecule 20 is BETA-CAROTENE (CCD ID: BCR) (formula:  $C_{40}H_{56}$ ) (labeled as "Ligand of Interest" by depositor).



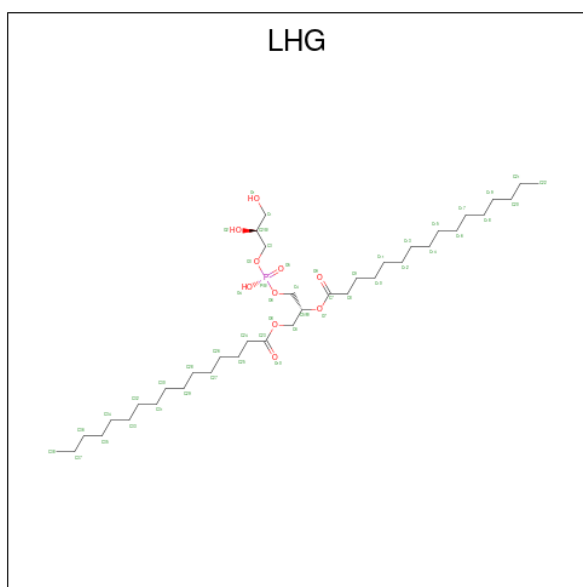
Mol	Chain	Residues	Atoms	AltConf
20	B	1	Total C 40 40	0
20	B	1	Total C 40 40	0
20	B	1	Total C 40 40	0
20	D	1	Total C 40 40	0
20	H	1	Total C 40 40	0
20	K	1	Total C 40 40	0
20	Z	1	Total C 40 40	0
20	C	1	Total C 40 40	0
20	C	1	Total C 40 40	0
20	A	1	Total C 40 40	0

- Molecule 21 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula:  $C_{45}H_{86}O_{10}$ ) (labeled as "Ligand of Interest" by depositor).



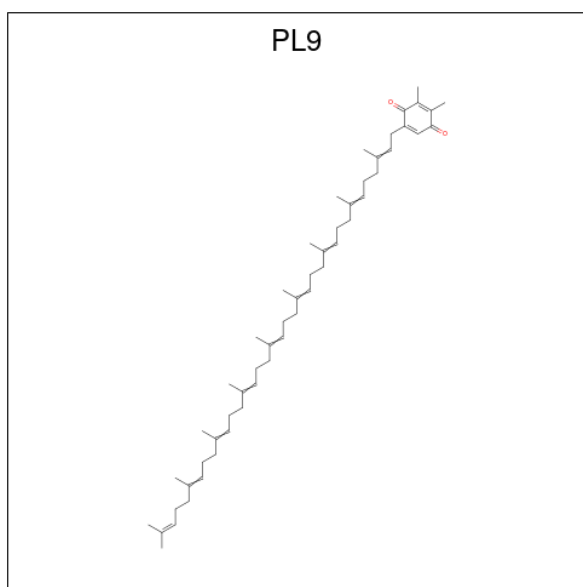
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
21	B	1	46	36	10	0
21	B	1	48	38	10	0
21	D	1	46	36	10	0
21	K	1	51	41	10	0
21	C	1	49	39	10	0
21	A	1	48	38	10	0

- Molecule 22 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula:  $C_{38}H_{75}O_{10}P$ ) (labeled as "Ligand of Interest" by depositor).



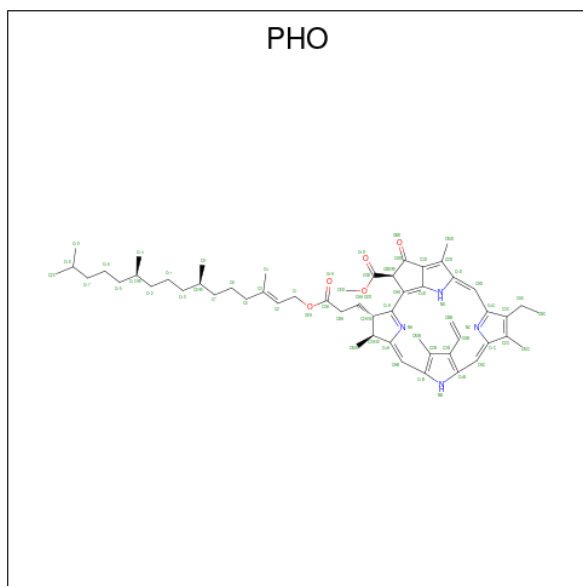
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
22	B	1	47	36	10	1	0
22	B	1	49	38	10	1	0
22	B	1	49	38	10	1	0
22	D	1	44	33	10	1	0
22	D	1	49	38	10	1	0
22	D	1	43	32	10	1	0
22	K	1	41	30	10	1	0
22	L	1	49	38	10	1	0
22	X	1	49	38	10	1	0
22	A	1	49	38	10	1	0

- Molecule 23 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: C<sub>53</sub>H<sub>80</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



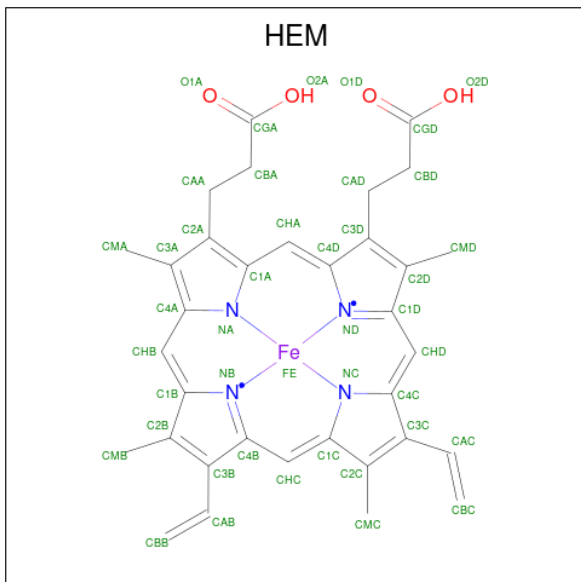
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
23	D	1	55	53	2	0

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



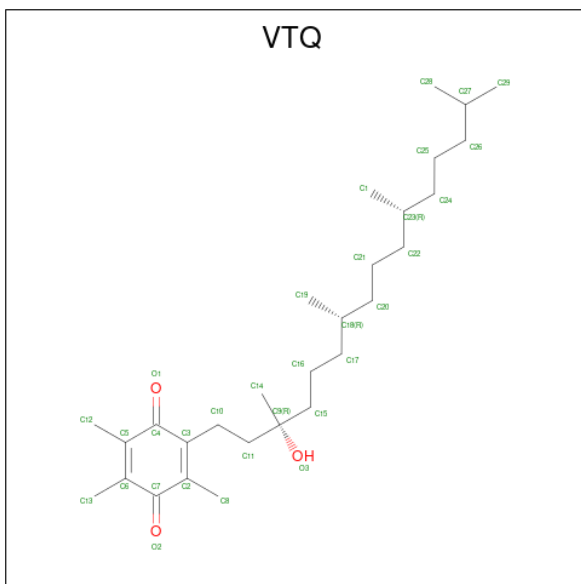
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
24	D	1	64	55	4	5	0
24	D	1	64	55	4	5	0

- Molecule 25 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ) (labeled as "Ligand of Interest" by depositor).



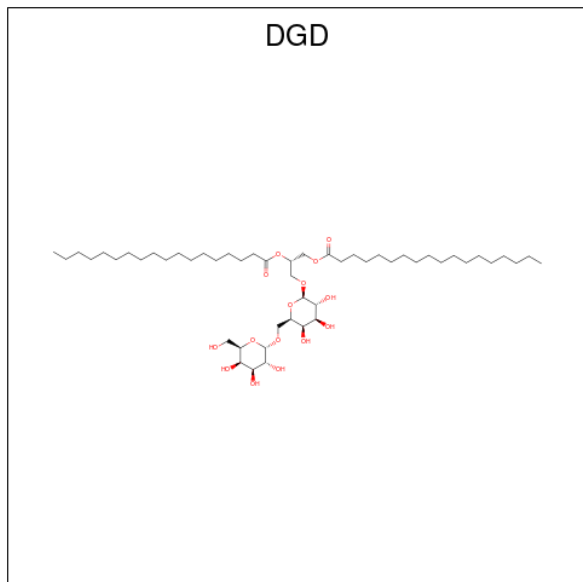
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Fe	N	O	
25	E	1	43	34	1	4	4	0

- Molecule 26 is RRR-ALPHA-TOCOPHERYLQUINONE (CCD ID: VTQ) (formula:  $C_{29}H_{50}O_3$ ) (labeled as "Ligand of Interest" by depositor).



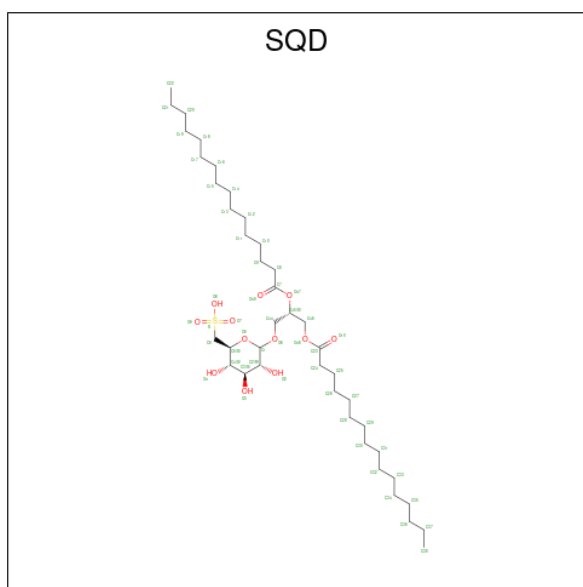
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
26	X	1	32	29	3	0

- Molecule 27 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula:  $C_{51}H_{96}O_{15}$ ) (labeled as "Ligand of Interest" by depositor).



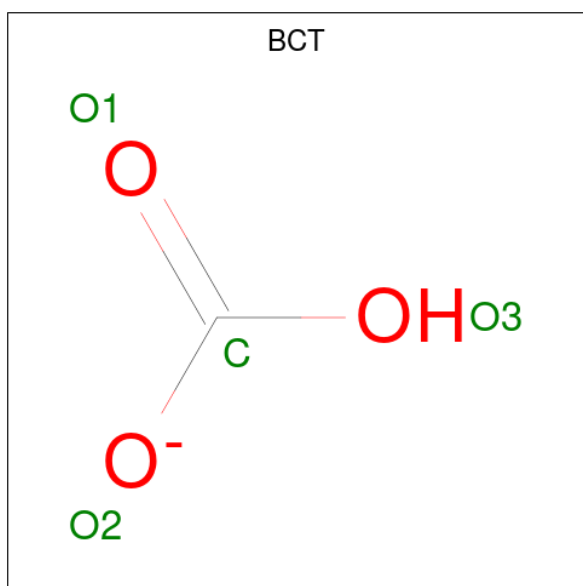
Mol	Chain	Residues	Atoms			AltConf
27	C	1	Total	C	O	0
			55	40	15	
27	C	1	Total	C	O	0
			57	42	15	
27	C	1	Total	C	O	0
			59	44	15	

- 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	
			Total	C	O		S
28	C	1	51	38	12	1	0

- Molecule 29 is BICARBONATE ION (CCD ID: BCT) (formula:  $\text{CHO}_3$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
29	A	1	4	1	3	0


- Molecule 30 is FE (II) ION (CCD ID: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

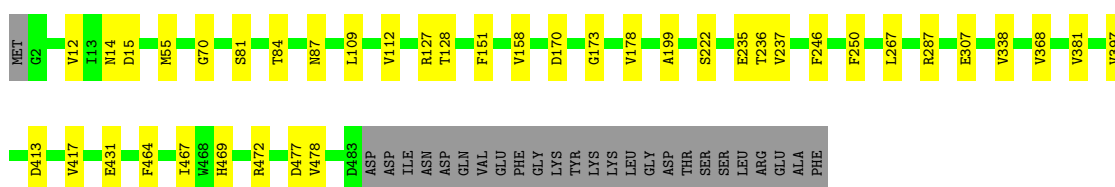
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>AltConf</b>
30	A	1	Total 1	Fe 1	0

### 3 Residue-property plots [i](#)


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

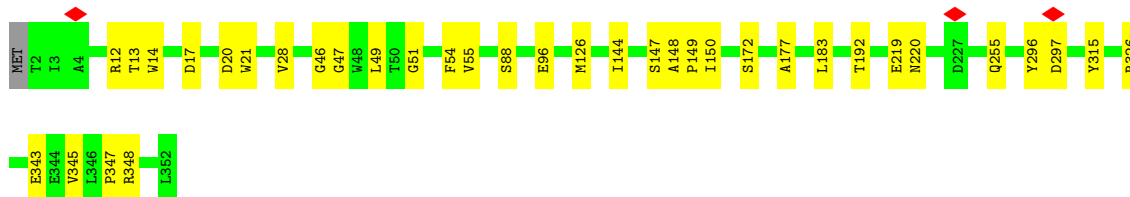
- Molecule 1: Photosystem II CP47 reaction center protein

Chain B: 




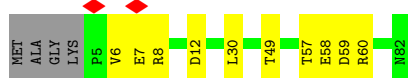
- Molecule 2: Photosystem II D2 protein

Chain D: 



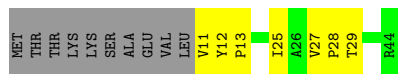
- Molecule 3: Cytochrome b559 subunit alpha

Chain E: 

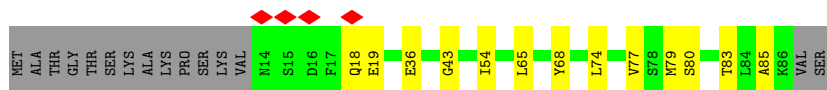


- Molecule 4: Cytochrome b559 subunit beta

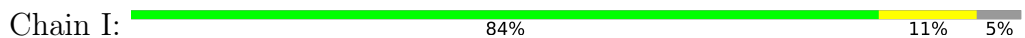
Chain F: 



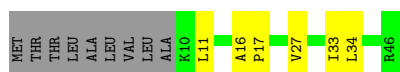
- Molecule 5: Photosystem II reaction center protein H



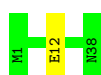
• Molecule 6: Photosystem II reaction center protein I



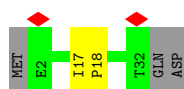
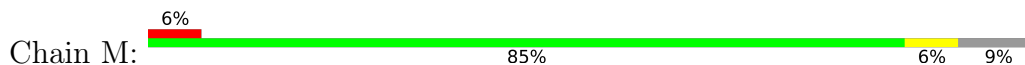
• Molecule 7: Photosystem II reaction center protein K



• Molecule 8: Photosystem II reaction center protein L



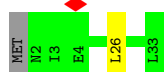
• Molecule 9: Photosystem II reaction center protein M



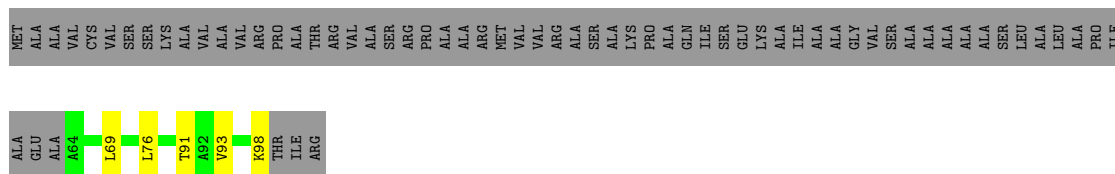
• Molecule 10: Photosystem II reaction center protein T



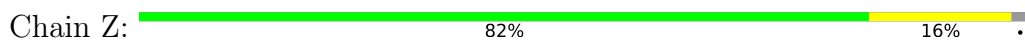
• Molecule 11: Photosystem II reaction center protein Ycf12



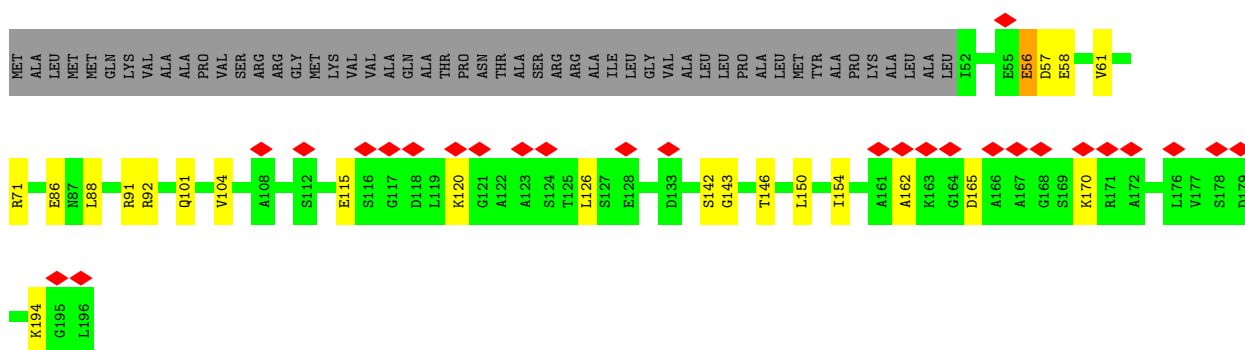
• Molecule 12: Uncharacterized protein



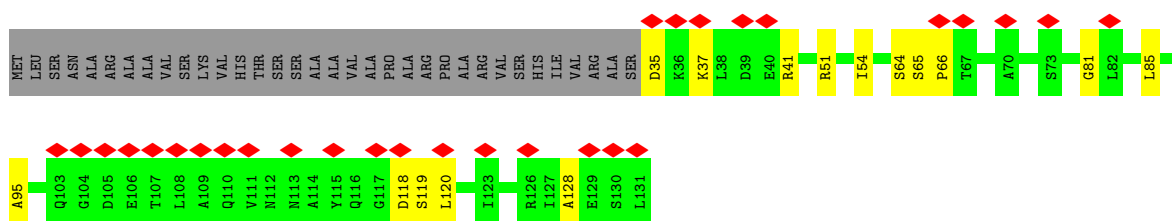
- Molecule 13: Photosystem II reaction center protein Z



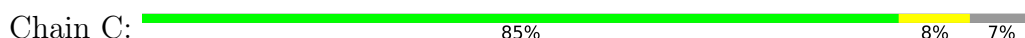
- Molecule 14: Thylakoid enriched factor 14 (TEF14)



- Molecule 15: Photosystem II repair factor 1 (PRF1)



- Molecule 16: Photosystem II CP43 reaction center protein





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	510932	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	61.421	Depositor
Minimum map value	-0.960	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.995	Depositor
Recommended contour level	3.9	Depositor
Map size (Å)	332.8, 332.8, 332.8	wwPDB
Map dimensions	320, 320, 320	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: FE2, VTQ, PHO, SQD, LHG, BCT, CLA, BCR, LMG, HEM, PL9, DGD

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	B	0.15	0/3894	0.26	0/5302
2	D	0.15	0/2886	0.27	0/3937
3	E	0.13	0/652	0.31	0/890
4	F	0.13	0/286	0.27	0/389
5	H	0.12	0/573	0.25	0/783
6	I	0.19	0/291	0.37	0/394
7	K	0.11	0/309	0.29	0/425
8	L	0.16	0/322	0.22	0/437
9	M	0.09	0/243	0.21	0/333
10	T	0.15	0/263	0.23	0/354
11	V	0.06	0/224	0.17	0/307
12	X	0.12	0/244	0.23	0/330
13	Z	0.14	0/469	0.24	0/644
14	G	0.11	0/1079	0.28	0/1454
15	3	0.11	0/700	0.29	0/947
16	C	0.13	0/3486	0.26	0/4743
17	A	0.15	0/2495	0.31	0/3402
18	1	0.16	0/323	0.28	0/435
All	All	0.14	0/18739	0.27	0/25506

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [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	B	3766	0	3649	30	0
2	D	2791	0	2678	26	0
3	E	633	0	622	9	0
4	F	277	0	288	4	0
5	H	561	0	581	10	0
6	I	283	0	293	3	0
7	K	297	0	308	3	0
8	L	314	0	327	1	0
9	M	239	0	258	1	0
10	T	256	0	273	4	0
11	V	224	0	256	1	0
12	X	242	0	266	7	0
13	Z	458	0	490	8	0
14	G	1070	0	1077	19	0
15	3	694	0	698	14	0
16	C	3368	0	3240	28	0
17	A	2418	0	2349	32	0
18	1	320	0	340	4	0
19	A	174	0	170	2	0
19	B	1020	0	1113	4	0
19	C	845	0	936	5	0
19	D	195	0	216	4	0
20	A	40	0	56	3	0
20	B	120	0	168	2	0
20	C	80	0	112	6	0
20	D	40	0	56	1	0
20	H	40	0	56	6	0
20	K	40	0	56	1	0
20	Z	40	0	56	7	0
21	A	48	0	66	0	0
21	B	94	0	128	1	0
21	C	49	0	68	0	0
21	D	46	0	62	0	0
21	K	51	0	72	0	0
22	A	49	0	74	0	0
22	B	145	0	215	0	0
22	D	136	0	191	2	0
22	K	41	0	52	0	0
22	L	49	0	74	0	0
22	X	49	0	74	0	0
23	D	55	0	80	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	D	128	0	148	1	0
25	E	43	0	30	4	0
26	X	32	0	50	0	0
27	C	171	0	216	2	0
28	C	51	0	69	0	0
29	A	4	0	0	0	0
30	A	1	0	0	0	0
All	All	22087	0	22657	198	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 4.

The worst 5 of 198 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)
16:C:185:ARG:NH2	16:C:219:GLU:OE2	2.13	0.81
8:L:12:GLU:OE2	15:3:51:ARG:NH2	2.14	0.80
19:D:409:CLA:HMD3	17:A:183:MET:HE1	1.66	0.77
1:B:235:GLU:OE2	1:B:469:HIS:ND1	2.20	0.73
20:C:616:BCR:H383	20:C:616:BCR:H23C	1.71	0.72

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	B	480/508 (94%)	465 (97%)	15 (3%)	0	100	100
2	D	349/352 (99%)	331 (95%)	18 (5%)	0	100	100
3	E	76/82 (93%)	71 (93%)	5 (7%)	0	100	100
4	F	32/44 (73%)	29 (91%)	3 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	H	71/88 (81%)	68 (96%)	3 (4%)	0	100	100
6	I	33/37 (89%)	33 (100%)	0	0	100	100
7	K	35/46 (76%)	34 (97%)	0	1 (3%)	3	6
8	L	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
9	M	29/34 (85%)	28 (97%)	1 (3%)	0	100	100
10	T	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
11	V	30/33 (91%)	29 (97%)	1 (3%)	0	100	100
12	X	33/101 (33%)	33 (100%)	0	0	100	100
13	Z	59/62 (95%)	59 (100%)	0	0	100	100
14	G	143/196 (73%)	134 (94%)	8 (6%)	1 (1%)	18	38
15	3	95/131 (72%)	84 (88%)	11 (12%)	0	100	100
16	C	424/461 (92%)	415 (98%)	9 (2%)	0	100	100
17	A	305/352 (87%)	294 (96%)	9 (3%)	2 (1%)	18	38
18	1	43/117 (37%)	40 (93%)	3 (7%)	0	100	100
All	All	2302/2713 (85%)	2210 (96%)	88 (4%)	4 (0%)	44	66

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
17	A	335	ASN
17	A	298	ASN
14	G	56	GLU
7	K	11	LEU

### 5.3.2 Protein sidechains [i](#)

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	B	384/407 (94%)	384 (100%)	0	100	100
2	D	280/281 (100%)	280 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	E	69/71 (97%)	69 (100%)	0	100	100
4	F	28/37 (76%)	28 (100%)	0	100	100
5	H	63/75 (84%)	63 (100%)	0	100	100
6	I	32/34 (94%)	32 (100%)	0	100	100
7	K	31/38 (82%)	31 (100%)	0	100	100
8	L	35/35 (100%)	35 (100%)	0	100	100
9	M	27/30 (90%)	27 (100%)	0	100	100
10	T	28/28 (100%)	28 (100%)	0	100	100
11	V	26/27 (96%)	26 (100%)	0	100	100
12	X	25/67 (37%)	25 (100%)	0	100	100
13	Z	51/52 (98%)	51 (100%)	0	100	100
14	G	112/149 (75%)	112 (100%)	0	100	100
15	3	73/98 (74%)	73 (100%)	0	100	100
16	C	338/362 (93%)	338 (100%)	0	100	100
17	A	251/289 (87%)	251 (100%)	0	100	100
18	1	31/87 (36%)	31 (100%)	0	100	100
All	All	1884/2167 (87%)	1884 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
17	A	75	ASN
14	G	95	GLN
3	E	53	ASN
2	D	220	ASN
7	K	40	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 72 ligands modelled in this entry, 1 is monoatomic - leaving 71 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
26	VTQ	X	202	-	30,32,32	1.51	5 (16%)	39,44,44	0.95	1 (2%)
19	CLA	B	608	-	69,73,73	1.15	6 (8%)	82,113,113	1.09	4 (4%)
19	CLA	C	602	-	69,73,73	1.17	7 (10%)	82,113,113	1.09	4 (4%)
20	BCR	B	619	-	41,41,41	0.79	1 (2%)	56,56,56	2.05	20 (35%)
20	BCR	A	406	-	41,41,41	0.80	1 (2%)	56,56,56	1.92	18 (32%)
22	LHG	B	621	-	46,46,48	0.97	2 (4%)	49,52,54	0.96	2 (4%)
22	LHG	A	408	-	48,48,48	0.95	2 (4%)	51,54,54	0.95	2 (3%)
27	DGD	C	617	-	56,56,67	0.94	2 (3%)	70,70,81	0.98	4 (5%)
20	BCR	B	618	-	41,41,41	0.76	1 (2%)	56,56,56	2.01	20 (35%)
19	CLA	B	601	-	69,73,73	1.18	8 (11%)	82,113,113	1.10	6 (7%)
19	CLA	B	607	-	69,73,73	1.17	7 (10%)	82,113,113	1.08	5 (6%)
22	LHG	D	406	-	48,48,48	0.92	2 (4%)	51,54,54	0.98	2 (3%)
22	LHG	D	407	-	42,42,48	0.99	2 (4%)	45,48,54	1.07	3 (6%)
27	DGD	C	619	-	60,60,67	0.90	2 (3%)	74,74,81	0.88	2 (2%)
19	CLA	C	614	-	69,73,73	1.16	6 (8%)	82,113,113	1.12	5 (6%)
22	LHG	B	624	-	48,48,48	0.93	2 (4%)	51,54,54	0.99	3 (5%)
20	BCR	D	403	-	41,41,41	0.78	1 (2%)	56,56,56	2.17	22 (39%)
23	PL9	D	404	-	55,55,55	1.19	4 (7%)	68,69,69	1.51	12 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	BCR	B	617	-	41,41,41	0.79	1 (2%)	56,56,56	1.98	20 (35%)
19	CLA	C	611	-	69,73,73	1.18	8 (11%)	82,113,113	1.09	3 (3%)
19	CLA	C	608	-	69,73,73	1.17	7 (10%)	82,113,113	1.20	5 (6%)
19	CLA	B	610	-	69,73,73	1.15	7 (10%)	82,113,113	1.16	5 (6%)
19	CLA	C	604	-	69,73,73	1.17	6 (8%)	82,113,113	1.14	7 (8%)
22	LHG	X	201	-	48,48,48	0.94	2 (4%)	51,54,54	1.04	3 (5%)
28	SQD	C	620	-	49,51,54	1.16	3 (6%)	59,62,65	1.11	6 (10%)
24	PHO	D	410	-	58,69,69	2.12	11 (18%)	55,99,99	1.47	7 (12%)
19	CLA	C	610	-	69,73,73	1.16	7 (10%)	82,113,113	1.14	3 (3%)
19	CLA	B	614	-	49,53,73	1.37	7 (14%)	58,89,113	1.26	4 (6%)
19	CLA	D	402	-	69,73,73	1.17	7 (10%)	82,113,113	1.10	4 (4%)
19	CLA	C	609	-	69,73,73	1.17	8 (11%)	82,113,113	1.05	5 (6%)
22	LHG	K	103	-	40,40,48	1.03	2 (5%)	43,46,54	1.01	3 (6%)
20	BCR	H	101	-	41,41,41	0.68	0	56,56,56	2.26	21 (37%)
29	BCT	A	401	30	3,3,3	1.12	0	2,3,3	4.18	1 (50%)
19	CLA	B	611	-	69,73,73	1.16	6 (8%)	82,113,113	1.10	5 (6%)
19	CLA	D	409	-	69,73,73	1.16	8 (11%)	82,113,113	1.07	6 (7%)
20	BCR	K	101	-	41,41,41	0.74	0	56,56,56	2.22	20 (35%)
27	DGD	C	618	-	58,58,67	0.92	2 (3%)	72,72,81	1.00	4 (5%)
19	CLA	A	403	-	69,73,73	1.17	8 (11%)	82,113,113	1.10	5 (6%)
19	CLA	C	606	-	69,73,73	1.15	8 (11%)	82,113,113	1.04	4 (4%)
19	CLA	B	605	-	69,73,73	1.16	7 (10%)	82,113,113	1.08	4 (4%)
24	PHO	D	411	-	58,69,69	2.13	11 (18%)	55,99,99	1.42	6 (10%)
21	LMG	C	601	-	49,49,55	0.97	2 (4%)	57,57,63	0.95	2 (3%)
19	CLA	B	616	-	69,73,73	1.15	8 (11%)	82,113,113	1.12	5 (6%)
19	CLA	C	605	-	69,73,73	1.17	7 (10%)	82,113,113	1.09	4 (4%)
21	LMG	D	408	-	46,46,55	1.00	2 (4%)	54,54,63	0.91	2 (3%)
19	CLA	B	615	-	69,73,73	1.16	7 (10%)	82,113,113	1.15	4 (4%)
19	CLA	B	609	-	69,73,73	1.16	6 (8%)	82,113,113	1.13	7 (8%)
19	CLA	B	603	-	69,73,73	1.16	7 (10%)	82,113,113	1.11	6 (7%)
21	LMG	B	623	-	48,48,55	0.98	2 (4%)	56,56,63	0.98	2 (3%)
22	LHG	L	101	-	48,48,48	0.95	2 (4%)	51,54,54	0.94	2 (3%)
19	CLA	B	612	-	69,73,73	1.17	8 (11%)	82,113,113	1.18	5 (6%)
19	CLA	B	613	-	69,73,73	1.17	7 (10%)	82,113,113	1.15	6 (7%)
19	CLA	C	613	-	69,73,73	1.16	6 (8%)	82,113,113	1.11	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
19	CLA	A	404	-	53,57,73	1.31	7 (13%)	61,93,113	1.20	4 (6%)
20	BCR	C	616	-	41,41,41	0.80	1 (2%)	56,56,56	2.00	17 (30%)
19	CLA	B	604	-	69,73,73	1.16	7 (10%)	82,113,113	1.14	5 (6%)
21	LMG	B	620	-	46,46,55	1.00	2 (4%)	54,54,63	0.93	2 (3%)
21	LMG	K	102	-	51,51,55	0.96	3 (5%)	59,59,63	0.93	3 (5%)
19	CLA	A	405	-	64,68,73	1.21	7 (10%)	76,107,113	1.15	5 (6%)
22	LHG	D	405	-	43,43,48	1.00	2 (4%)	46,49,54	1.00	2 (4%)
19	CLA	C	603	-	69,73,73	1.16	8 (11%)	82,113,113	1.19	6 (7%)
19	CLA	C	612	16	69,73,73	1.18	7 (10%)	82,113,113	1.08	4 (4%)
19	CLA	B	606	-	69,73,73	1.17	7 (10%)	82,113,113	1.06	6 (7%)
19	CLA	C	607	-	69,73,73	1.18	7 (10%)	82,113,113	1.11	6 (7%)
20	BCR	C	615	-	41,41,41	0.80	1 (2%)	56,56,56	2.31	23 (41%)
22	LHG	B	622	-	48,48,48	0.92	2 (4%)	51,54,54	0.94	2 (3%)
20	BCR	Z	101	-	41,41,41	0.83	1 (2%)	56,56,56	1.94	18 (32%)
21	LMG	A	407	-	48,48,55	1.00	3 (6%)	56,56,63	1.13	5 (8%)
19	CLA	D	401	-	69,73,73	1.17	7 (10%)	82,113,113	1.21	6 (7%)
19	CLA	B	602	-	69,73,73	1.16	8 (11%)	82,113,113	1.11	6 (7%)
25	HEM	E	101	3,4	50,50,50	1.45	8 (16%)	67,82,82	1.14	4 (5%)

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
26	VTQ	X	202	-	-	7/25/49/49	0/1/1/1
19	CLA	B	608	-	1/1/15/20	14/39/115/115	-
19	CLA	C	602	-	1/1/15/20	13/39/115/115	-
20	BCR	B	619	-	-	4/29/63/63	0/2/2/2
20	BCR	A	406	-	-	4/29/63/63	0/2/2/2
22	LHG	B	621	-	-	8/51/51/53	-
22	LHG	A	408	-	-	8/53/53/53	-
27	DGD	C	617	-	-	10/44/84/95	0/2/2/2
20	BCR	B	618	-	-	4/29/63/63	0/2/2/2
19	CLA	B	601	-	1/1/15/20	10/39/115/115	-
19	CLA	B	607	-	1/1/15/20	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	LHG	D	406	-	-	11/53/53/53	-
22	LHG	D	407	-	-	17/47/47/53	-
27	DGD	C	619	-	-	6/48/88/95	0/2/2/2
19	CLA	C	614	-	1/1/15/20	15/39/115/115	-
22	LHG	B	624	-	-	12/53/53/53	-
20	BCR	D	403	-	-	4/29/63/63	0/2/2/2
23	PL9	D	404	-	-	8/53/73/73	0/1/1/1
20	BCR	B	617	-	-	4/29/63/63	0/2/2/2
19	CLA	C	611	-	1/1/15/20	14/39/115/115	-
19	CLA	C	608	-	1/1/15/20	6/39/115/115	-
19	CLA	B	610	-	1/1/15/20	17/39/115/115	-
19	CLA	C	604	-	1/1/15/20	16/39/115/115	-
22	LHG	X	201	-	-	11/53/53/53	-
28	SQD	C	620	-	-	12/46/66/69	0/1/1/1
24	PHO	D	410	-	-	10/37/103/103	0/5/6/6
19	CLA	C	610	-	1/1/15/20	16/39/115/115	-
19	CLA	B	614	-	1/1/11/20	3/15/91/115	-
19	CLA	D	402	-	1/1/15/20	15/39/115/115	-
19	CLA	C	609	-	1/1/15/20	17/39/115/115	-
22	LHG	K	103	-	-	8/45/45/53	-
20	BCR	H	101	-	-	5/29/63/63	0/2/2/2
19	CLA	B	611	-	1/1/15/20	14/39/115/115	-
19	CLA	D	409	-	1/1/15/20	8/39/115/115	-
20	BCR	K	101	-	-	4/29/63/63	0/2/2/2
27	DGD	C	618	-	-	8/46/86/95	0/2/2/2
19	CLA	A	403	-	1/1/15/20	10/39/115/115	-
19	CLA	C	606	-	1/1/15/20	16/39/115/115	-
19	CLA	B	605	-	1/1/15/20	16/39/115/115	-
24	PHO	D	411	-	-	10/37/103/103	0/5/6/6
21	LMG	C	601	-	-	3/44/64/70	0/1/1/1
19	CLA	B	616	-	1/1/15/20	10/39/115/115	-
19	CLA	C	605	-	1/1/15/20	8/39/115/115	-
21	LMG	D	408	-	-	6/41/61/70	0/1/1/1
19	CLA	B	615	-	1/1/15/20	3/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	B	609	-	1/1/15/20	15/39/115/115	-
19	CLA	B	603	-	1/1/15/20	11/39/115/115	-
21	LMG	B	623	-	-	9/43/63/70	0/1/1/1
22	LHG	L	101	-	-	8/53/53/53	-
19	CLA	B	612	-	1/1/15/20	11/39/115/115	-
19	CLA	B	613	-	1/1/15/20	11/39/115/115	-
19	CLA	C	613	-	1/1/15/20	16/39/115/115	-
19	CLA	A	404	-	1/1/11/20	3/20/96/115	-
20	BCR	C	616	-	-	4/29/63/63	0/2/2/2
19	CLA	B	604	-	1/1/15/20	16/39/115/115	-
21	LMG	B	620	-	-	5/41/61/70	0/1/1/1
21	LMG	K	102	-	-	7/46/66/70	0/1/1/1
19	CLA	A	405	-	1/1/14/20	6/33/109/115	-
22	LHG	D	405	-	-	10/48/48/53	-
19	CLA	C	603	-	1/1/15/20	14/39/115/115	-
19	CLA	C	612	16	1/1/15/20	14/39/115/115	-
19	CLA	B	606	-	1/1/15/20	11/39/115/115	-
19	CLA	C	607	-	1/1/15/20	18/39/115/115	-
20	BCR	C	615	-	-	3/29/63/63	0/2/2/2
22	LHG	B	622	-	-	11/53/53/53	-
20	BCR	Z	101	-	-	4/29/63/63	0/2/2/2
21	LMG	A	407	-	-	10/43/63/70	0/1/1/1
19	CLA	D	401	-	1/1/15/20	16/39/115/115	-
19	CLA	B	602	-	1/1/15/20	7/39/115/115	-
25	HEM	E	101	3,4	-	3/14/54/54	-

The worst 5 of 339 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	D	411	PHO	C1B-C2B	9.53	1.50	1.39
24	D	410	PHO	C1B-C2B	9.29	1.49	1.39
24	D	411	PHO	C3B-C4B	8.29	1.49	1.41
24	D	410	PHO	C3B-C4B	8.28	1.49	1.41
28	C	620	SQD	O8-S	4.51	1.64	1.47

The worst 5 of 460 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	C	615	BCR	C30-C25-C26	-6.12	114.27	122.64
20	C	615	BCR	C3-C4-C5	-5.86	103.60	114.06
19	B	612	CLA	C4A-NA-C1A	5.86	109.35	106.68
19	C	608	CLA	C4A-NA-C1A	5.63	109.25	106.68
29	A	401	BCT	O2-C-O1	5.58	133.94	119.68

5 of 35 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
19	B	601	CLA	ND
19	B	602	CLA	ND
19	B	603	CLA	ND
19	B	604	CLA	ND
19	B	605	CLA	ND

5 of 680 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	B	603	CLA	C1A-C2A-CAA-CBA
19	B	603	CLA	C3A-C2A-CAA-CBA
19	B	603	CLA	CAD-CBD-CGD-O1D
19	B	603	CLA	CAD-CBD-CGD-O2D
19	B	606	CLA	C1A-C2A-CAA-CBA

There are no ring outliers.

27 monomers are involved in 50 short contacts:

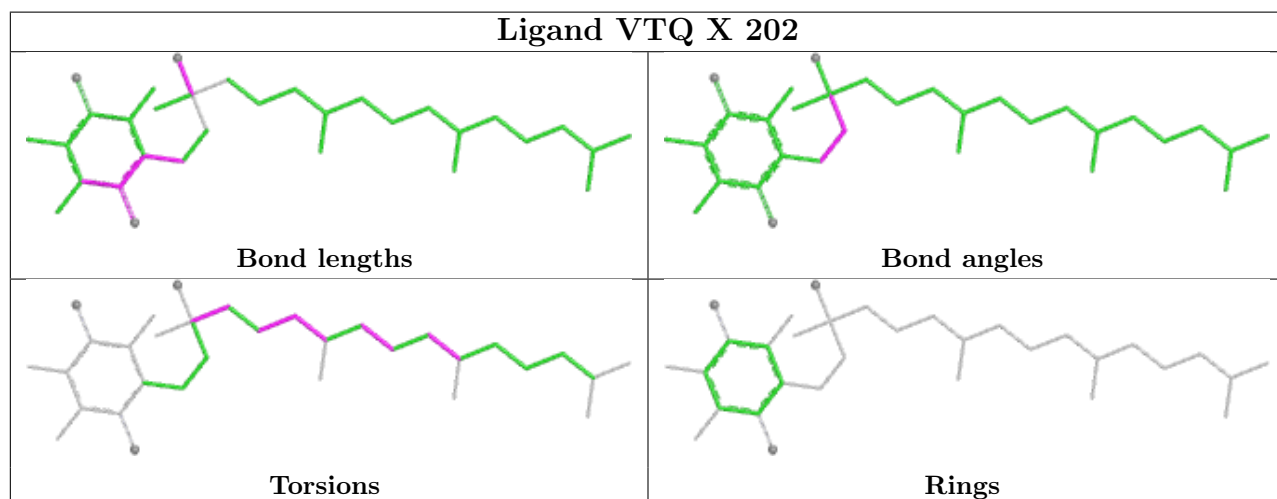
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	C	602	CLA	1	0
20	A	406	BCR	3	0
20	B	618	BCR	1	0
22	D	407	LHG	2	0
27	C	619	DGD	2	0
20	D	403	BCR	1	0
20	B	617	BCR	1	0
19	C	604	CLA	1	0
19	C	610	CLA	1	0
19	B	614	CLA	1	0
19	D	402	CLA	2	0
20	H	101	BCR	6	0
19	D	409	CLA	1	0
20	K	101	BCR	1	0
19	A	403	CLA	1	0

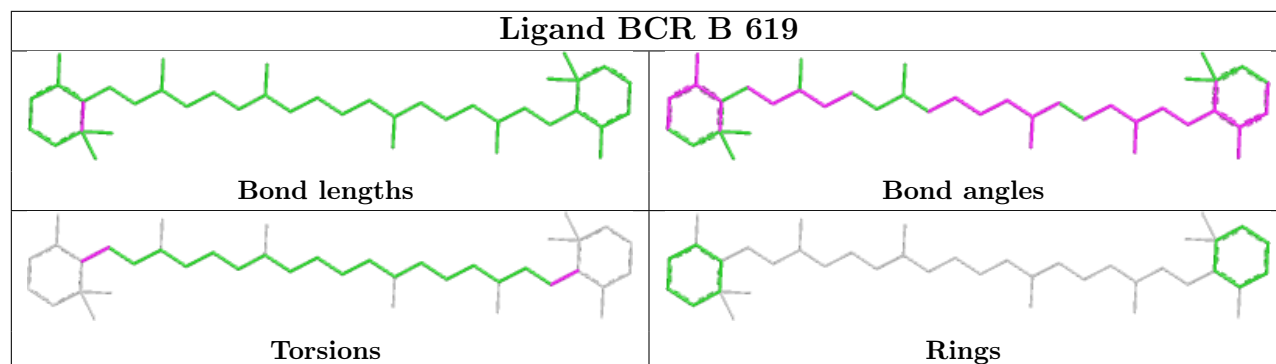
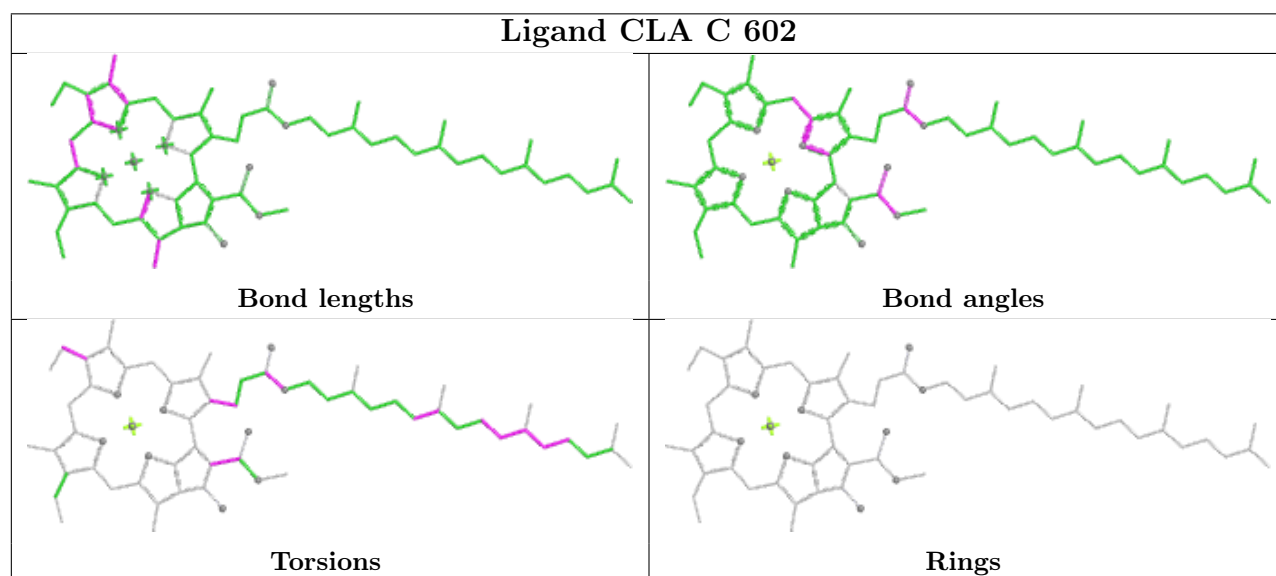
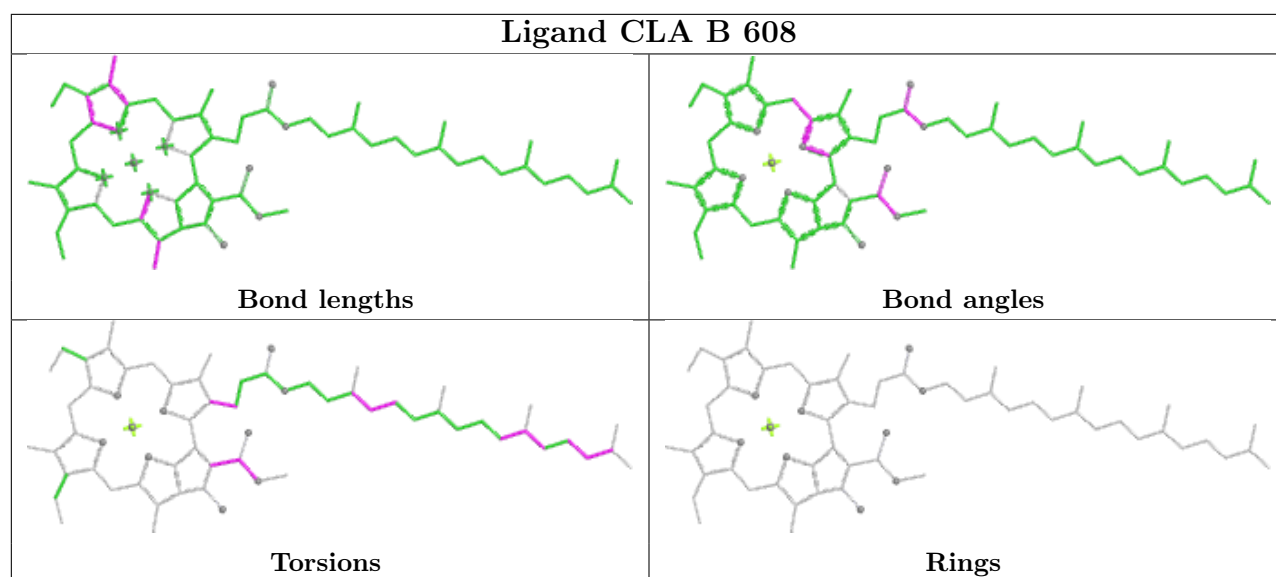
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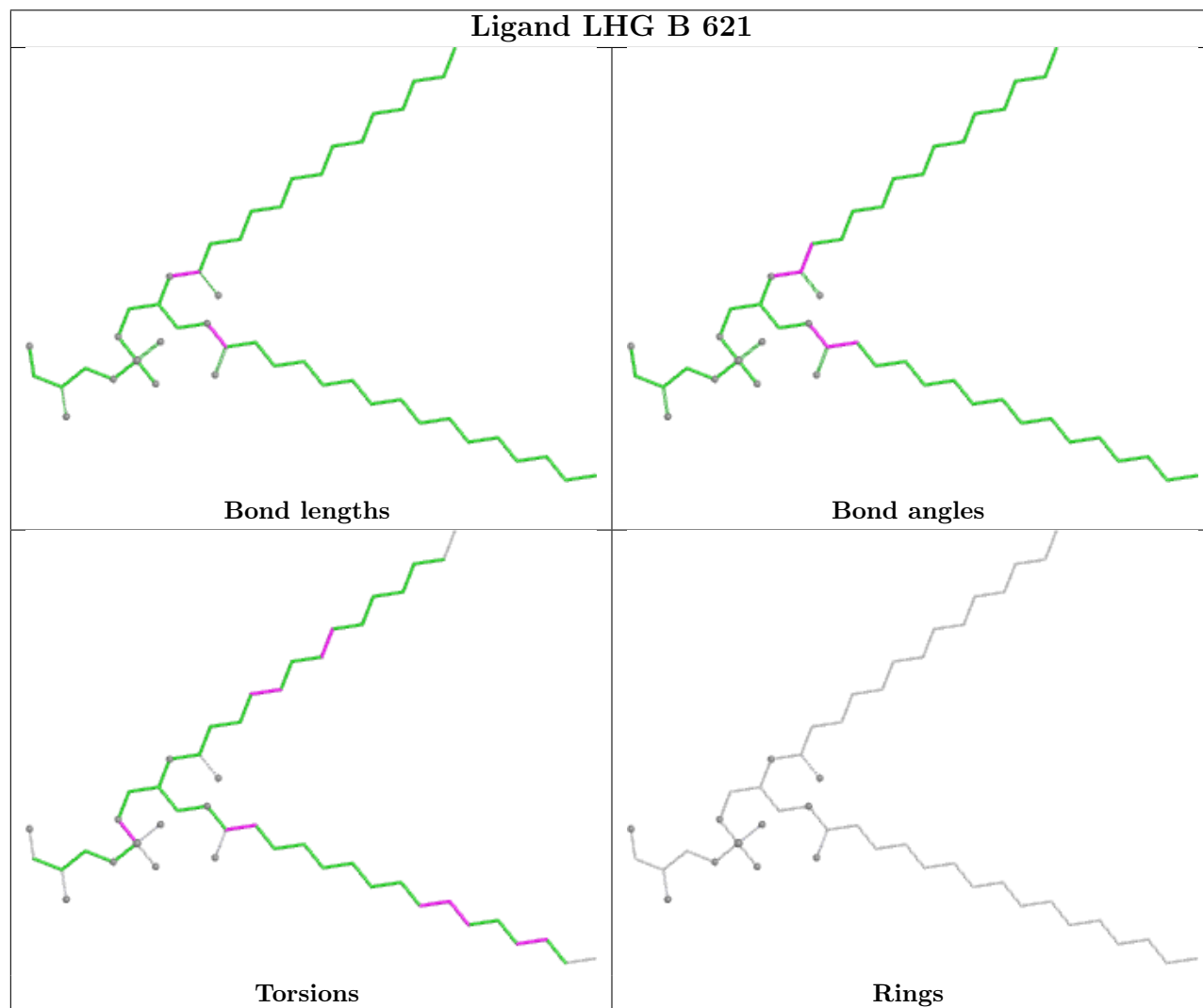
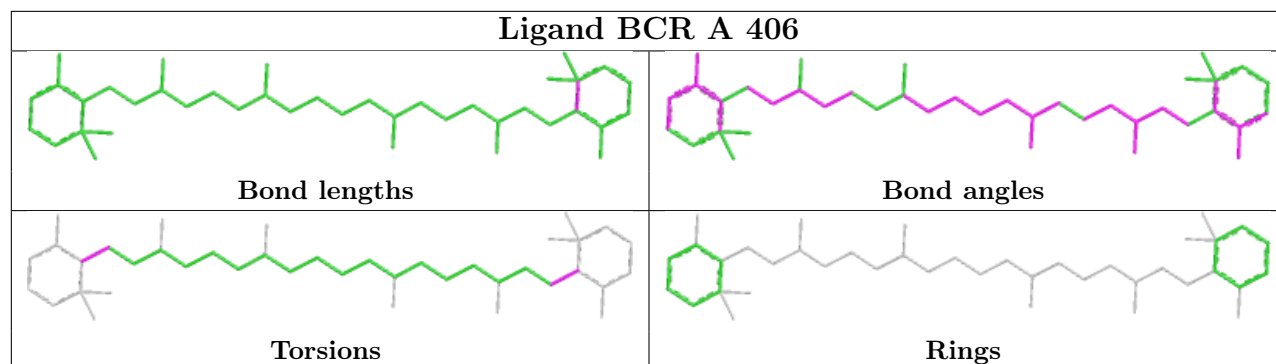
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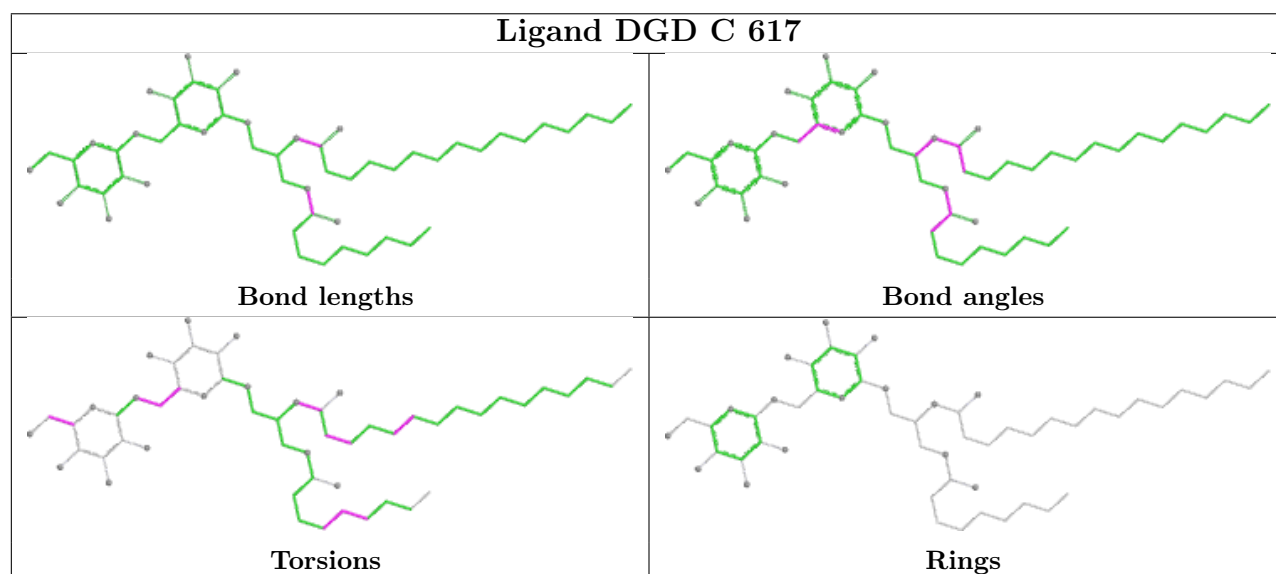
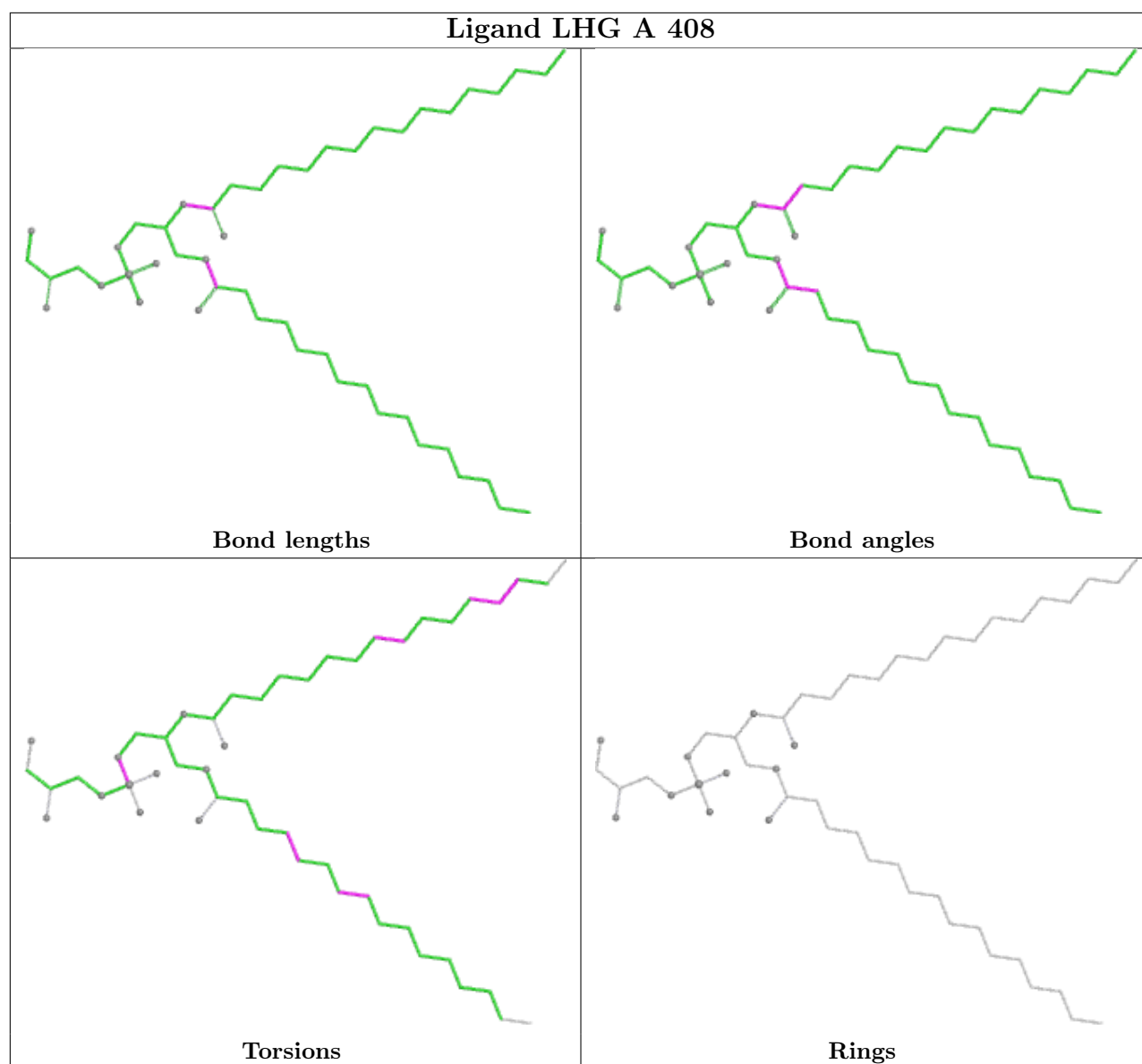
Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	D	411	PHO	1	0
21	B	623	LMG	1	0
19	B	612	CLA	2	0
19	A	404	CLA	1	0
20	C	616	BCR	2	0
19	B	604	CLA	1	0
19	C	603	CLA	3	0
20	C	615	BCR	4	0
20	Z	101	BCR	7	0
19	D	401	CLA	1	0
19	B	602	CLA	1	0
25	E	101	HEM	4	0

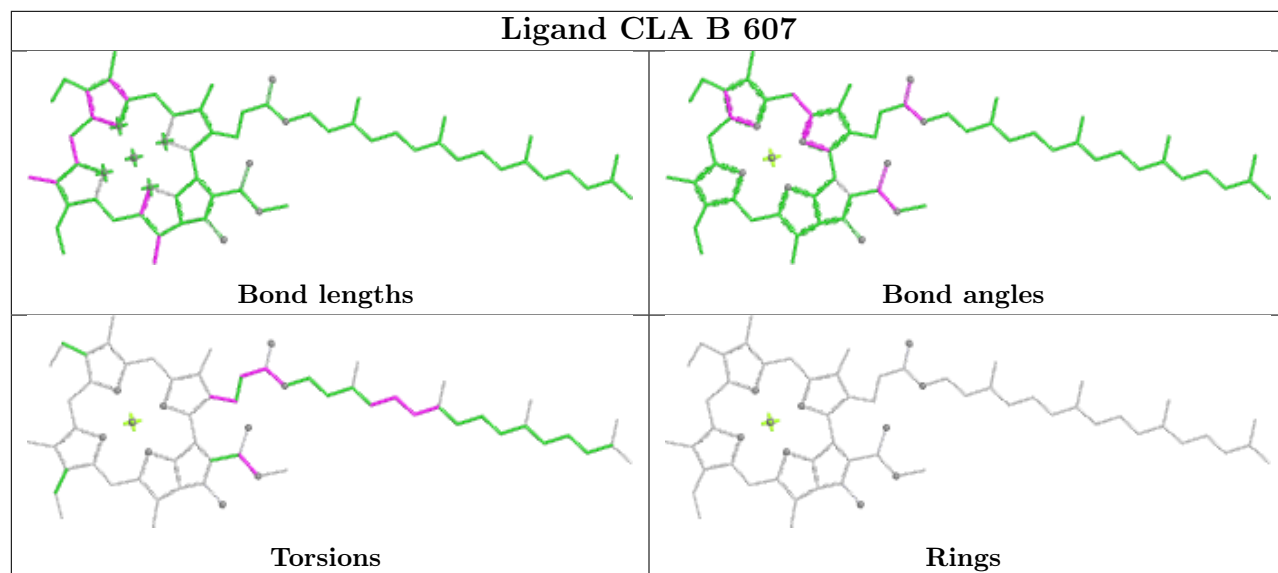
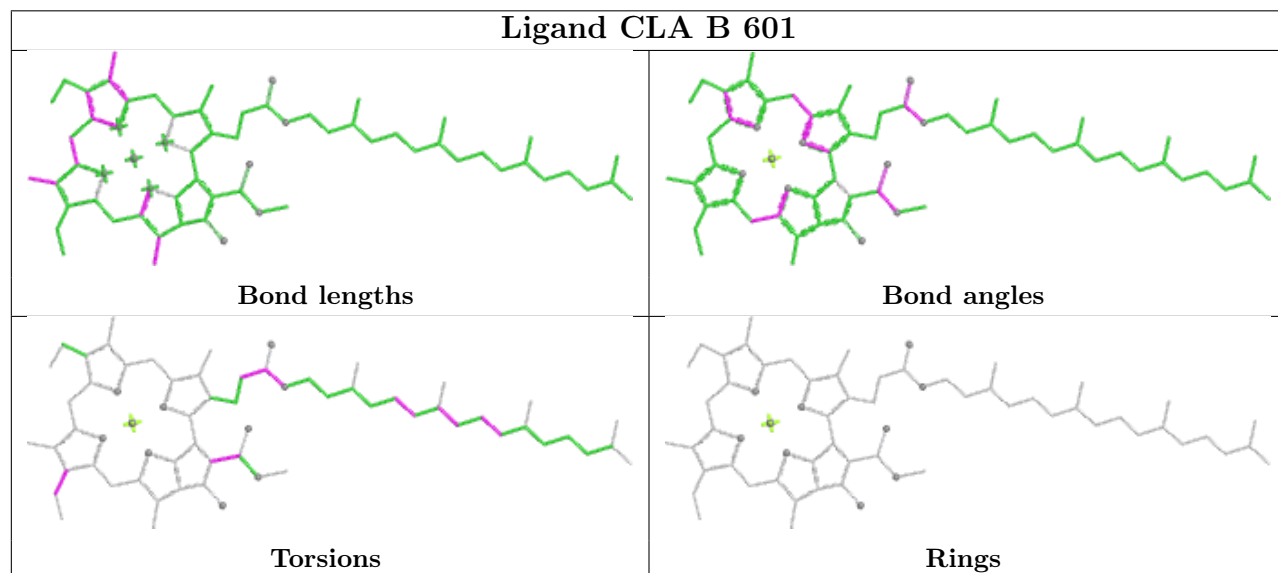
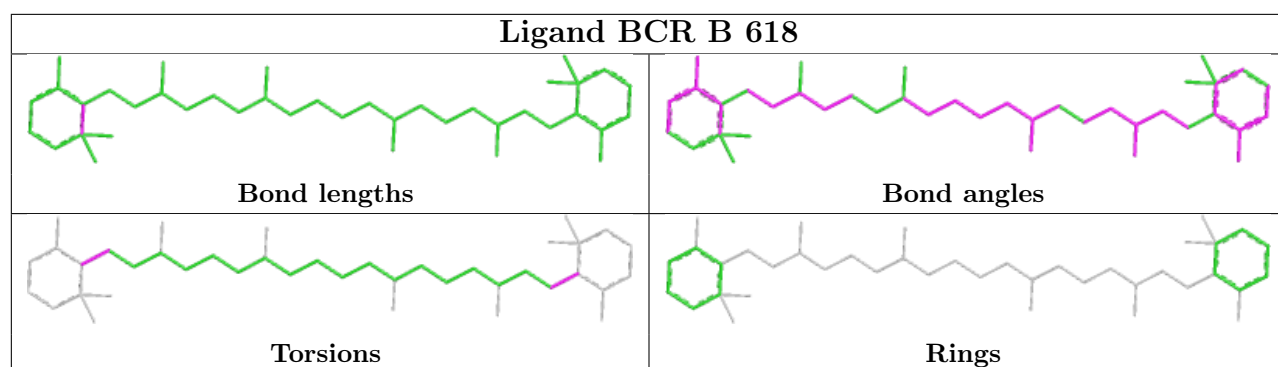
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

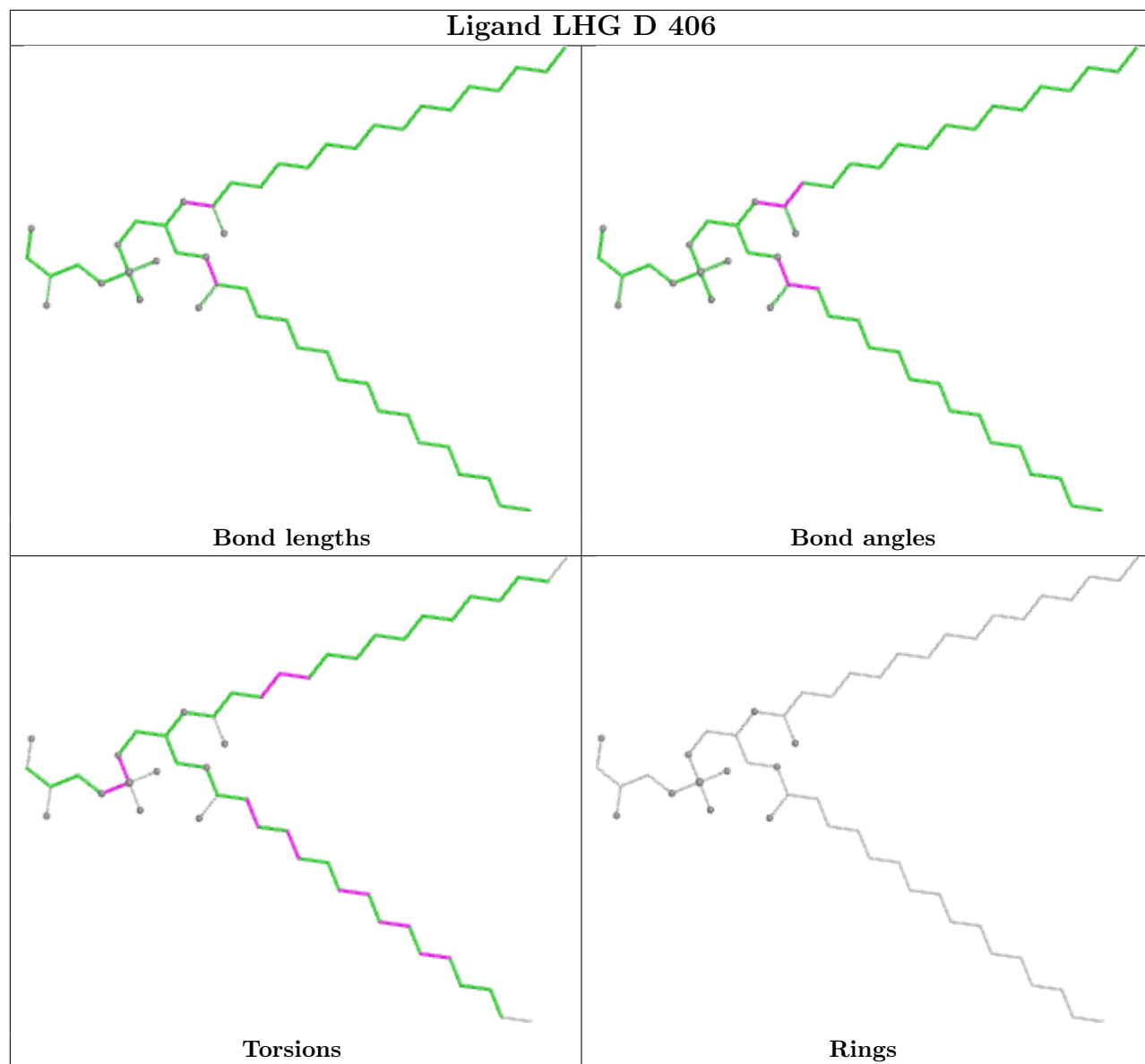


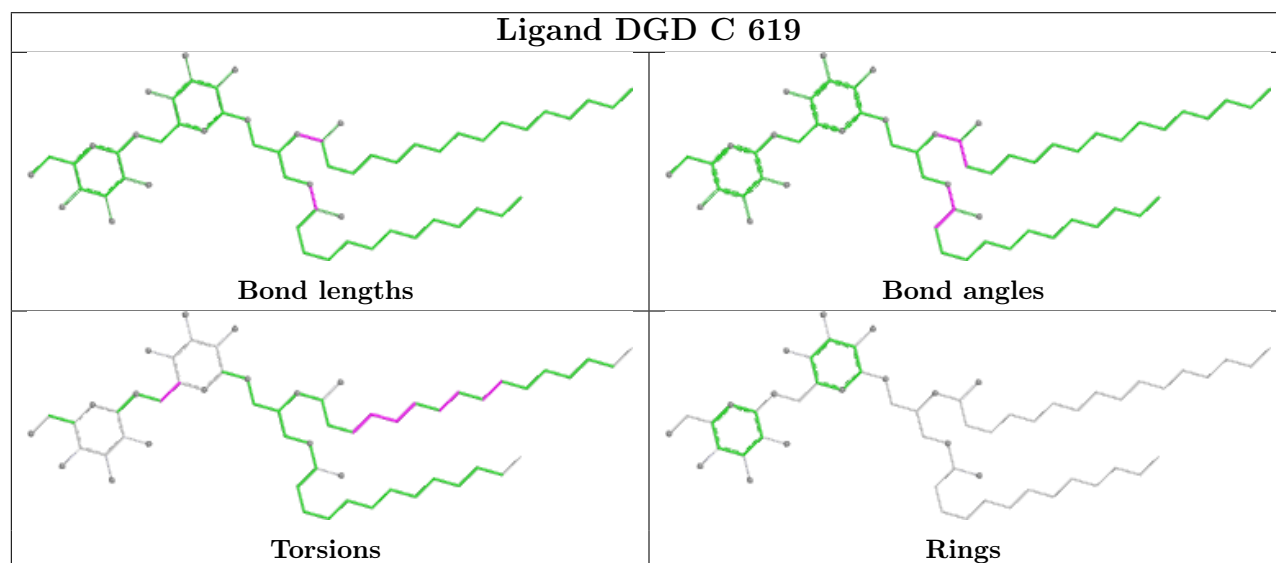
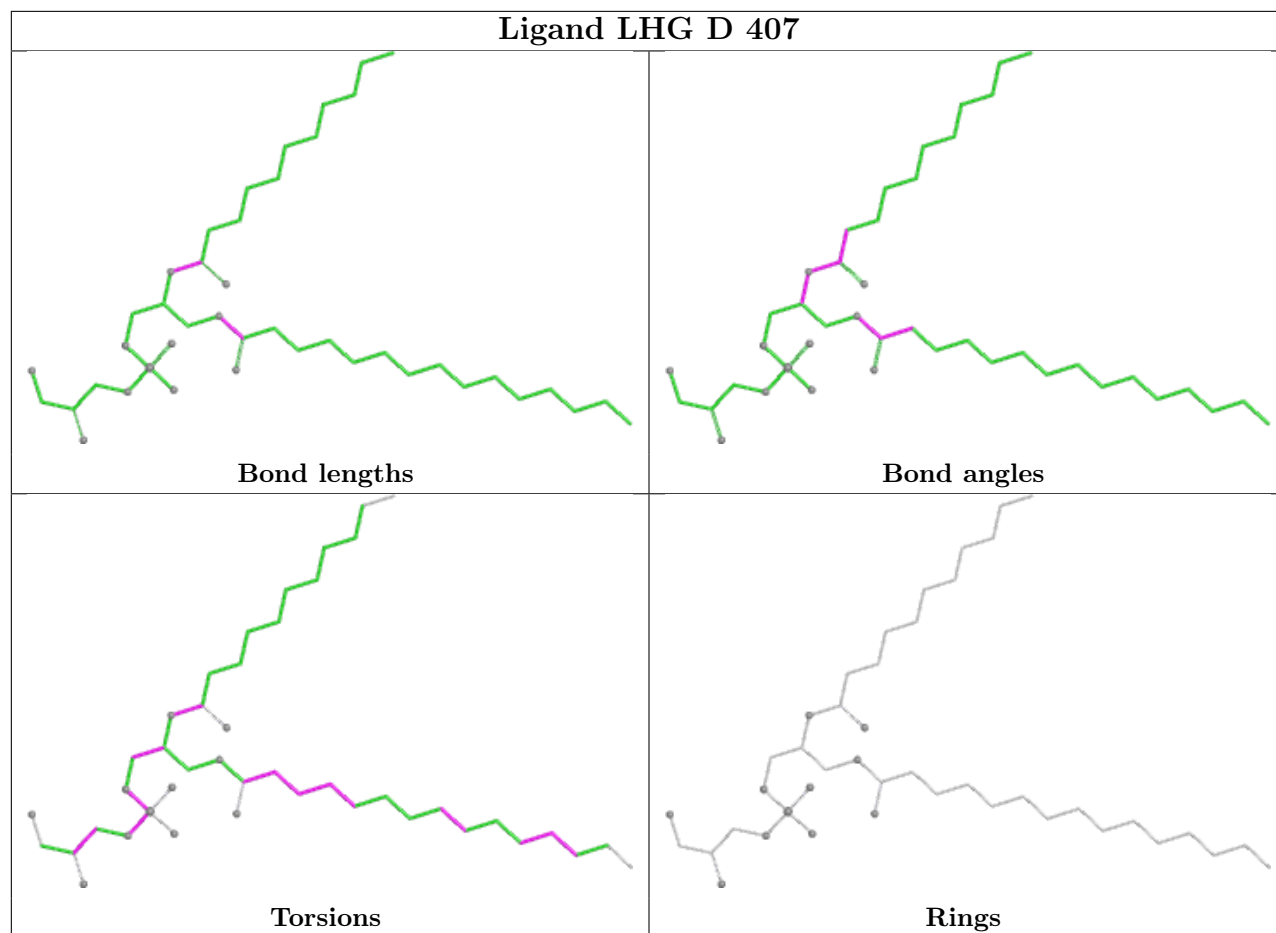


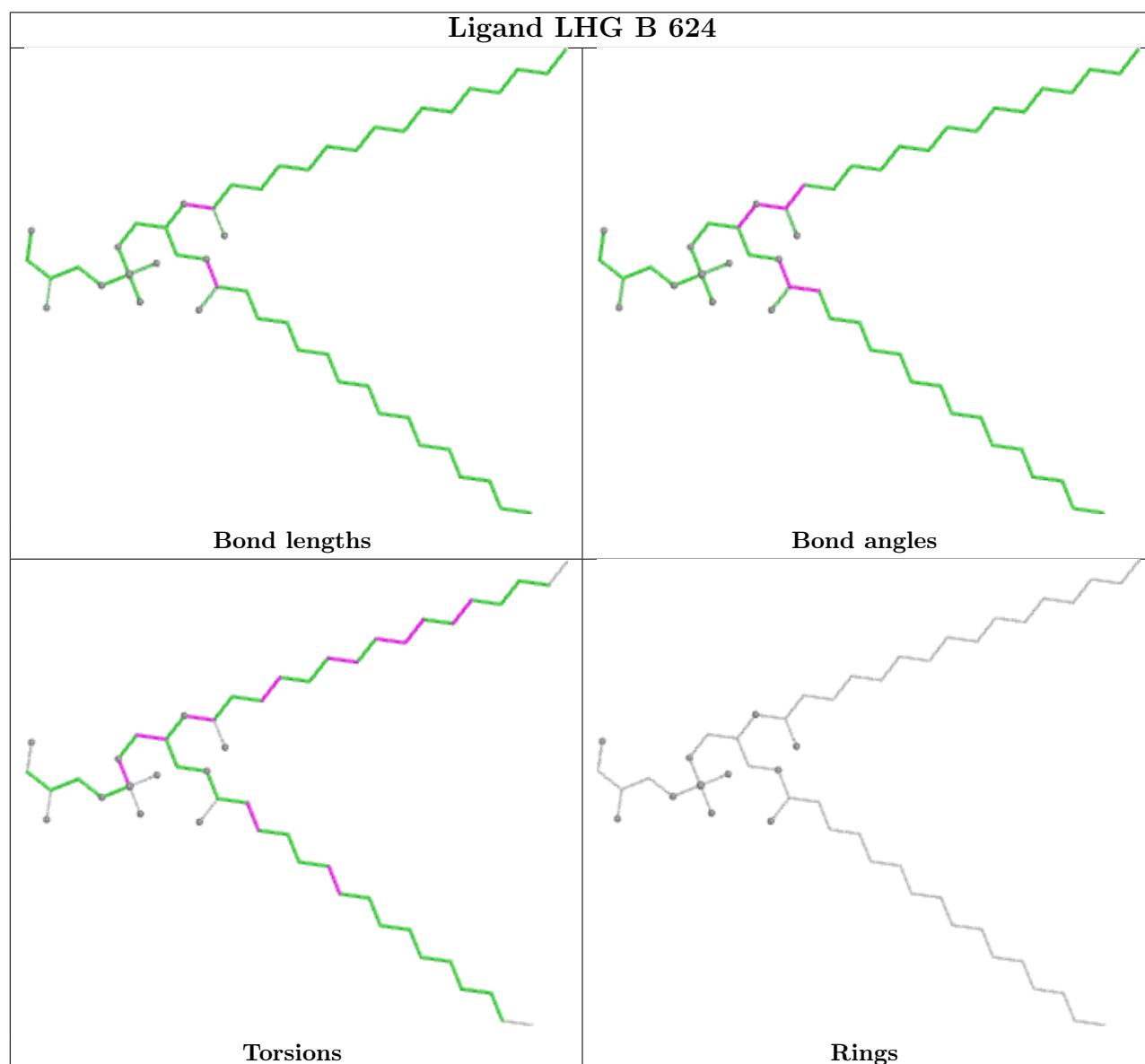
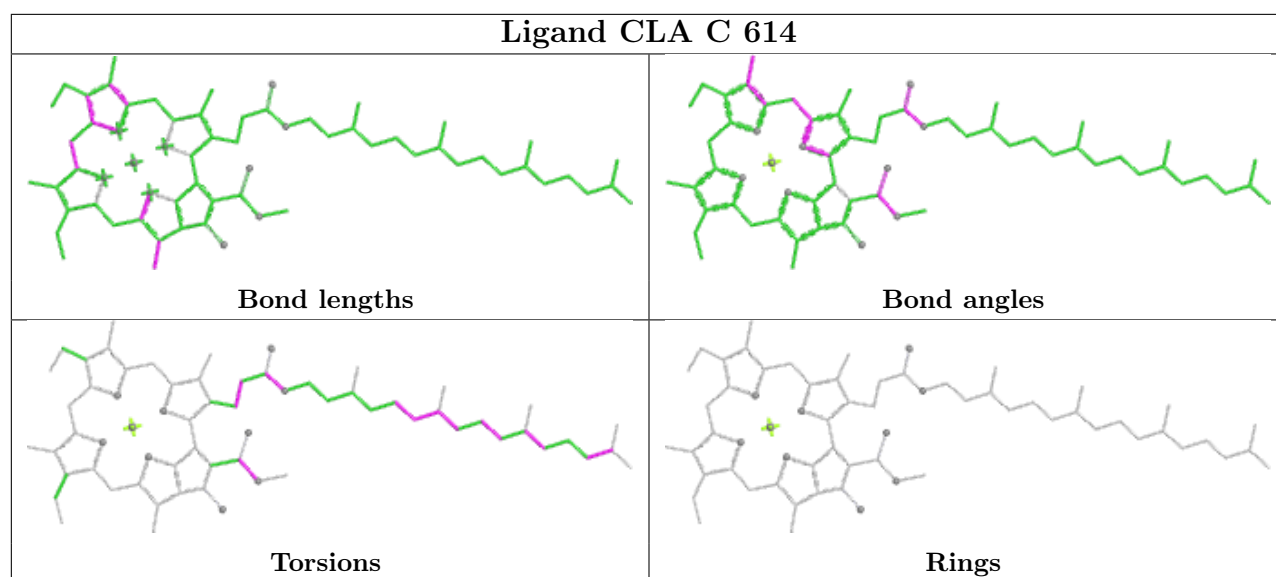


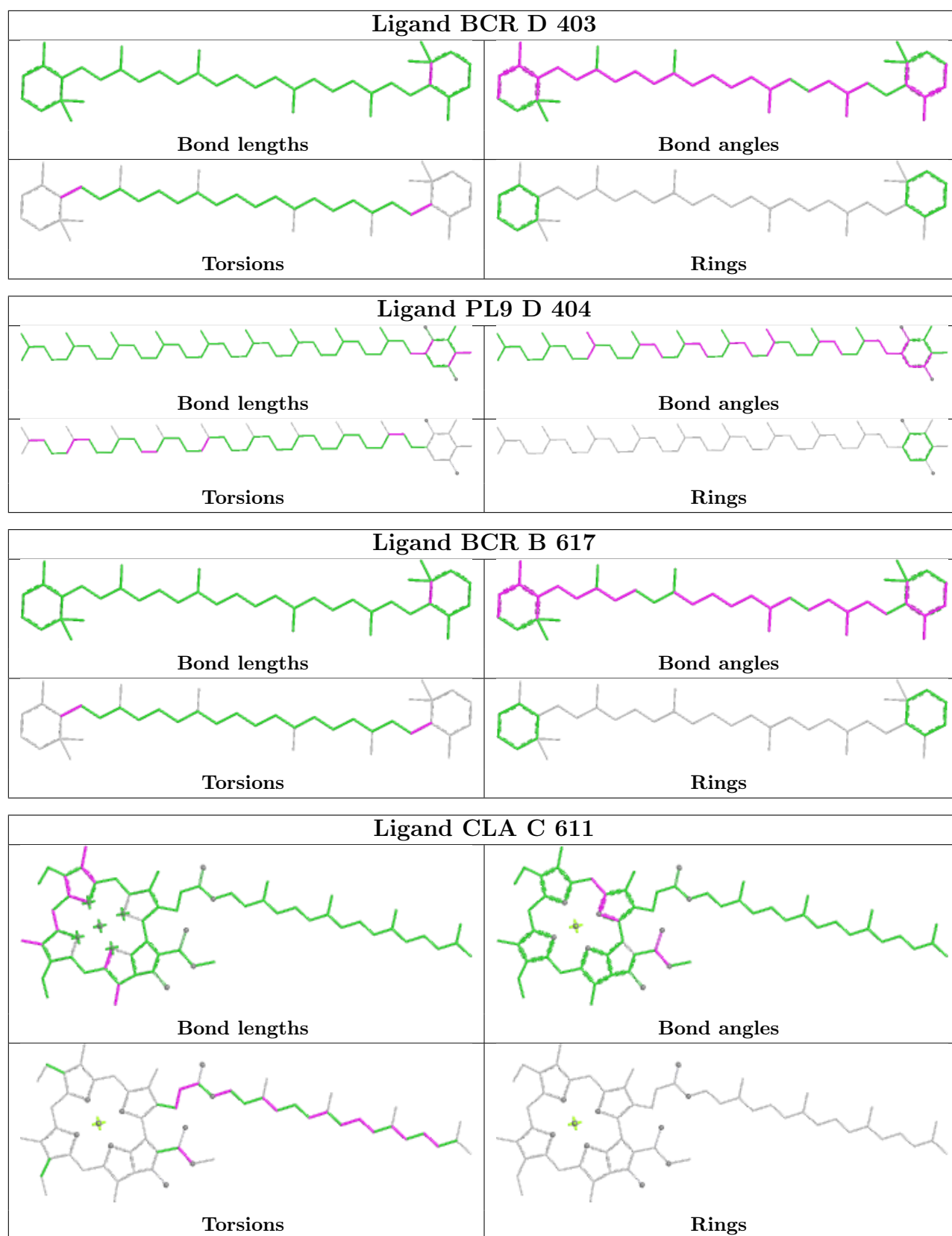


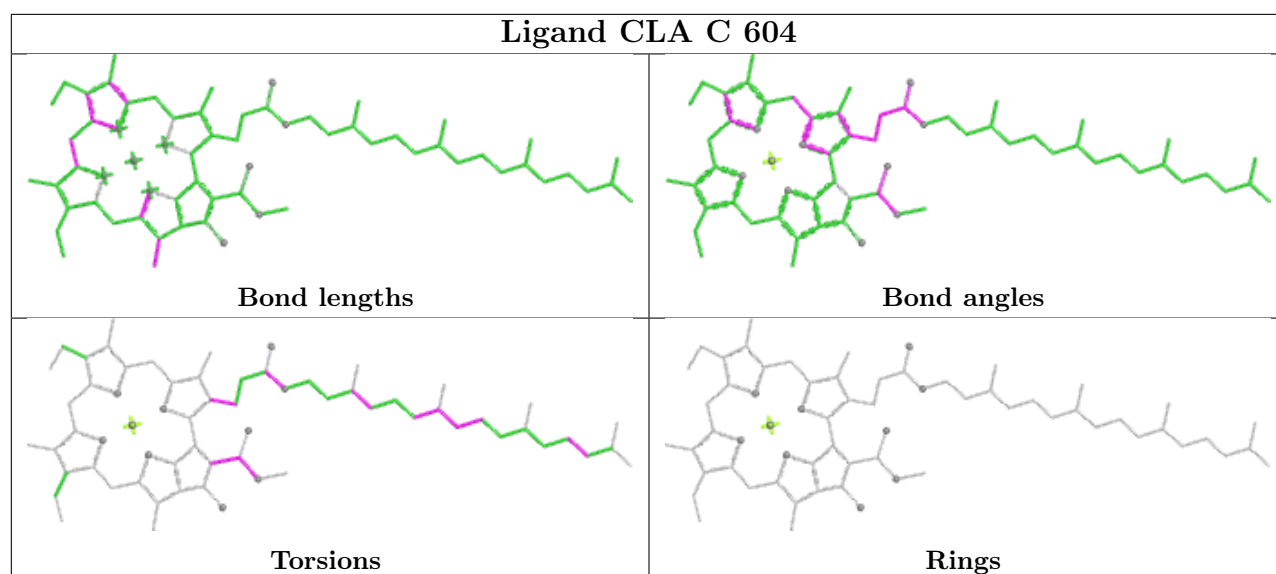
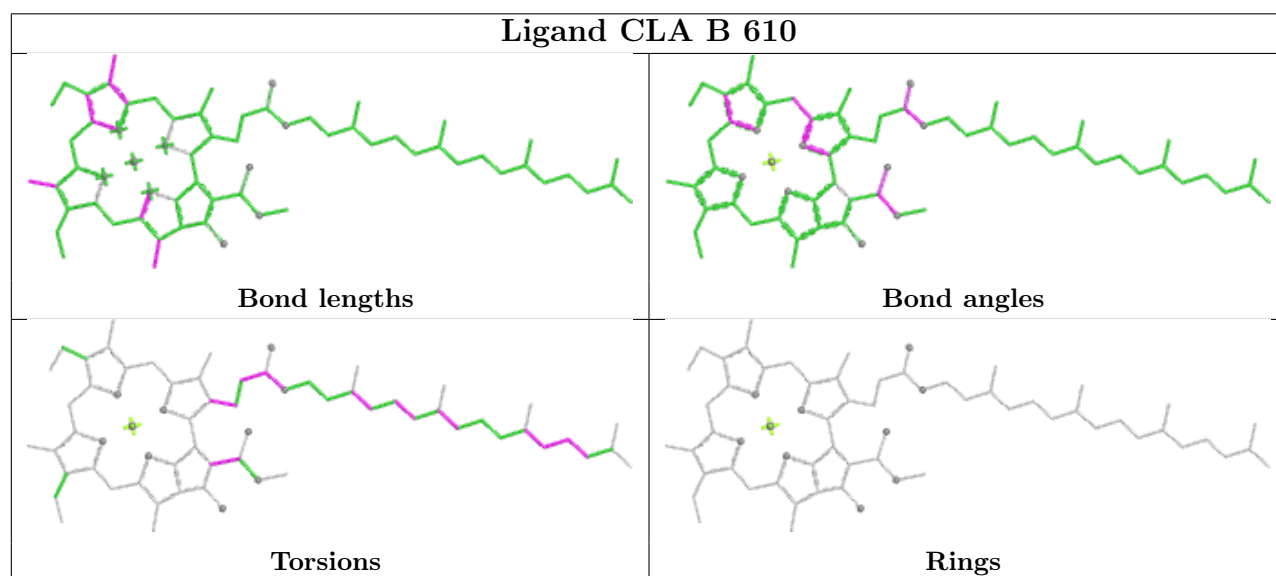
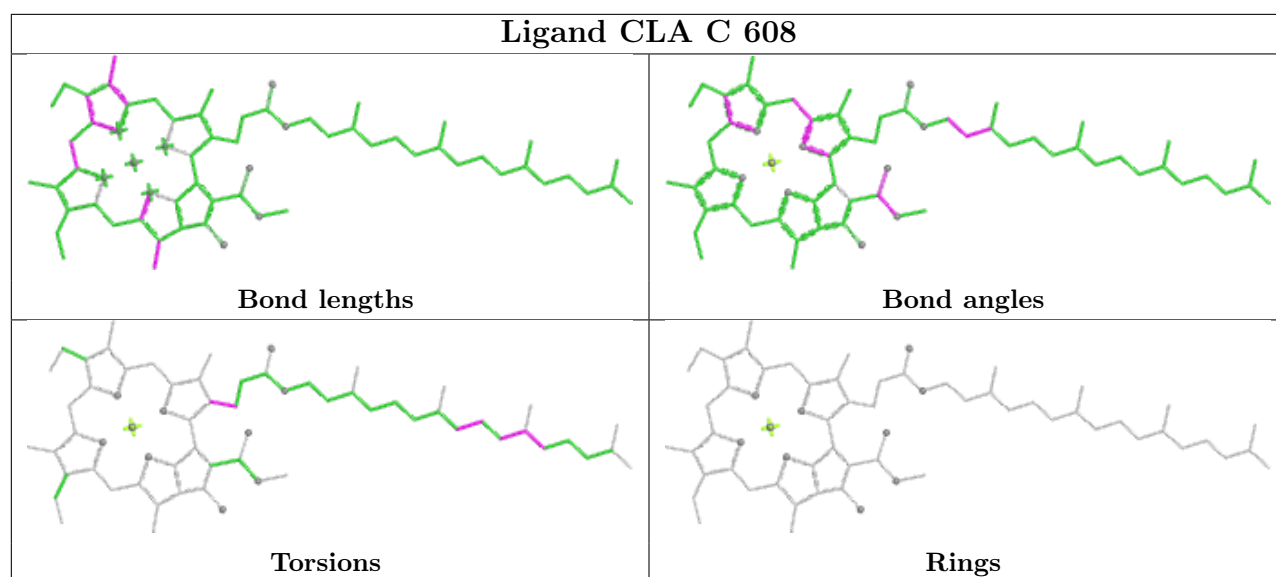


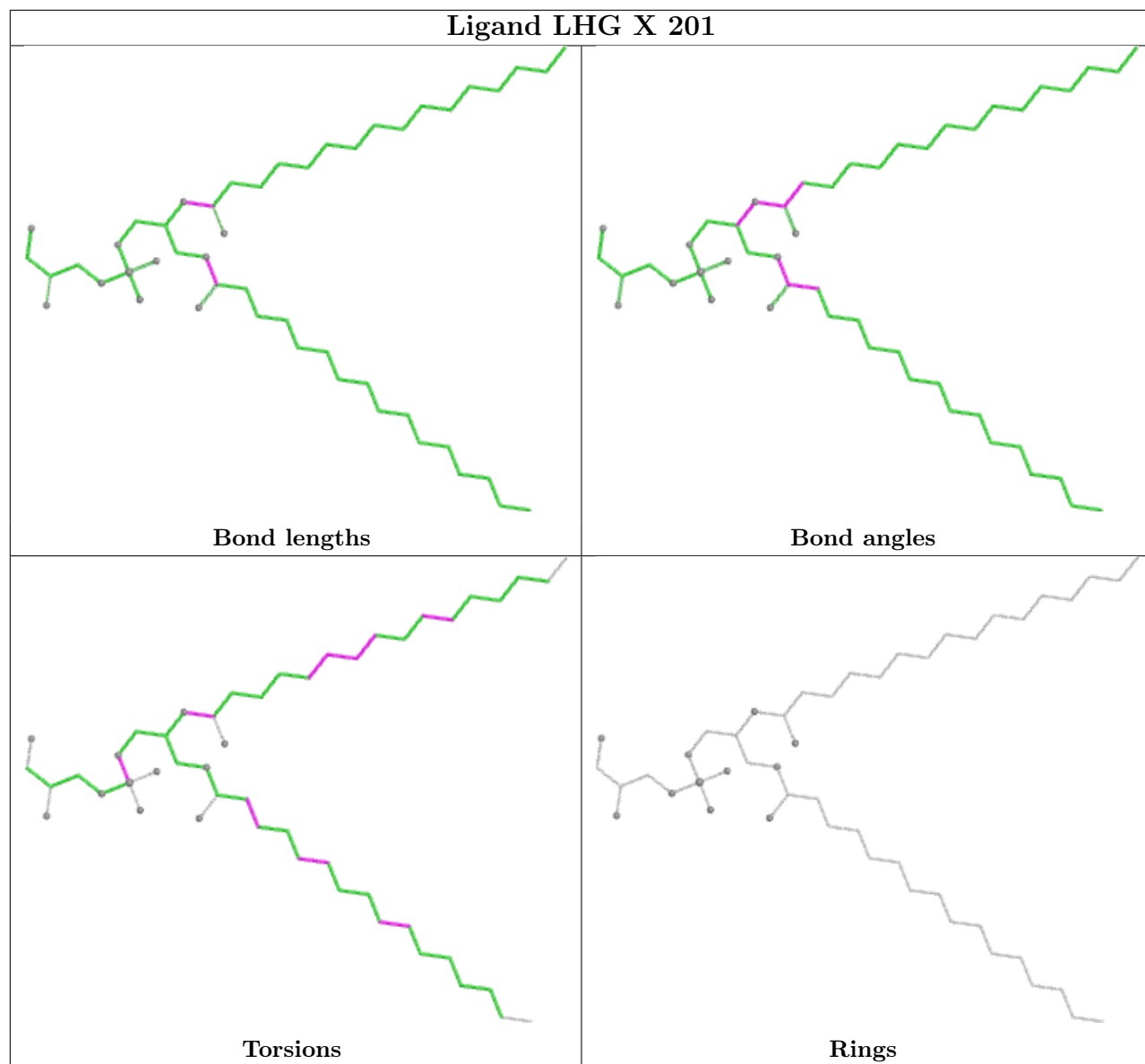


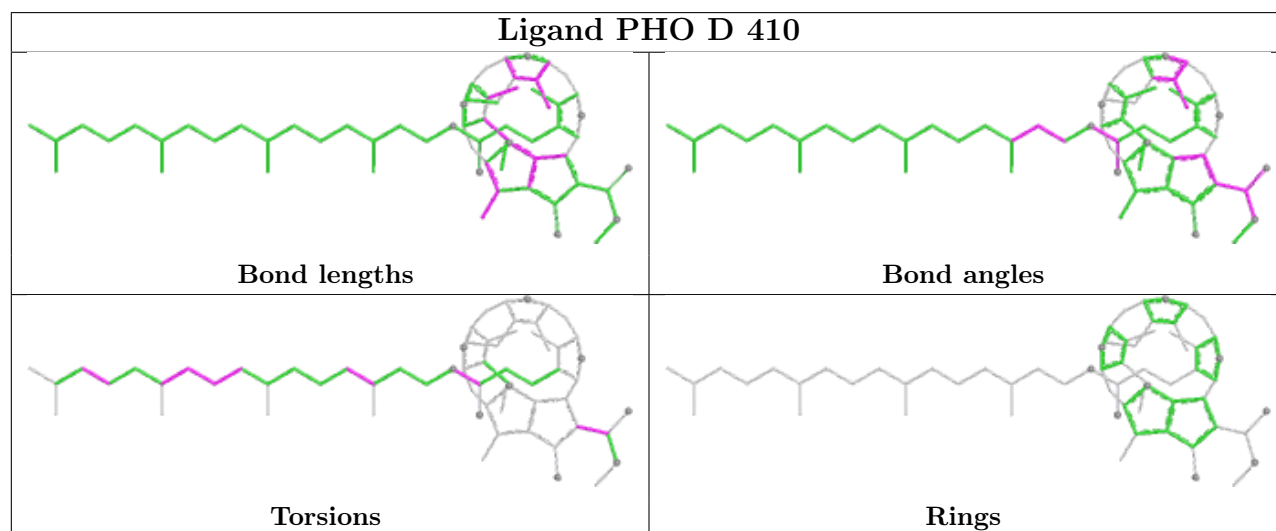
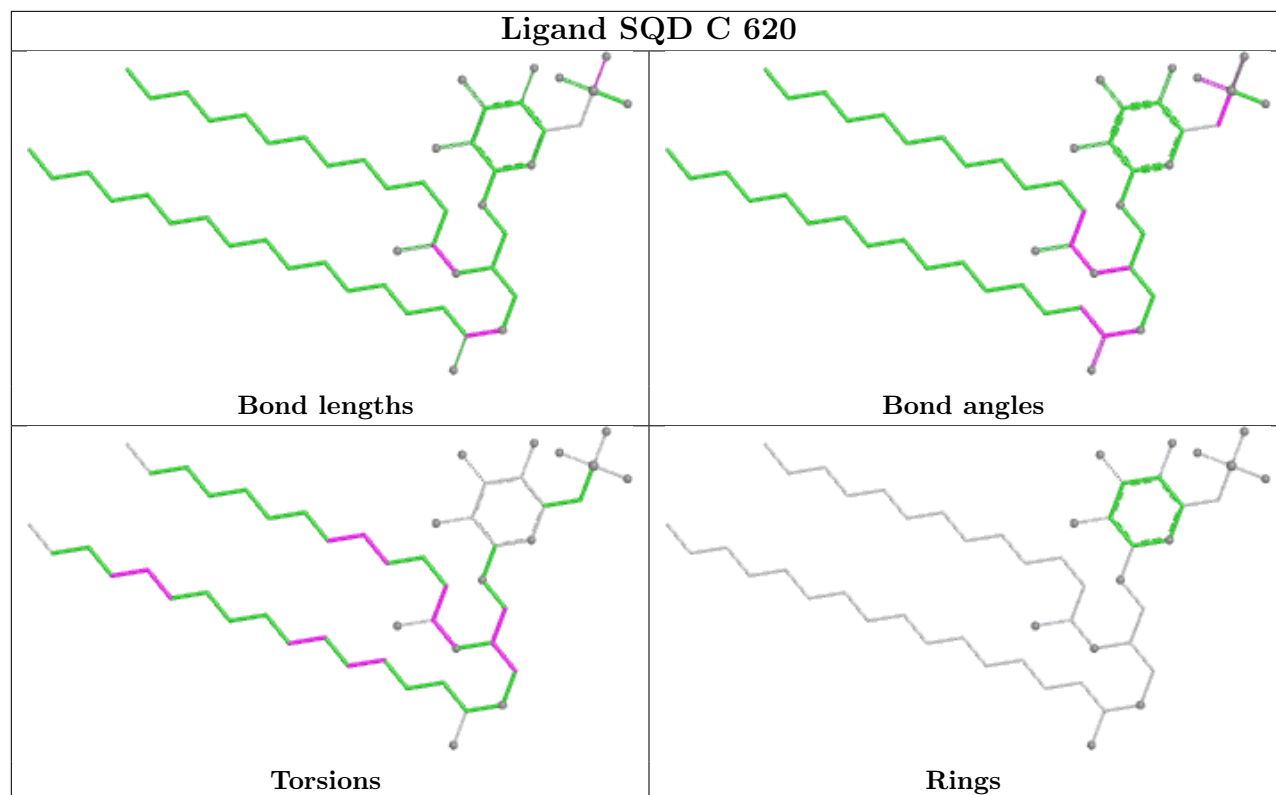


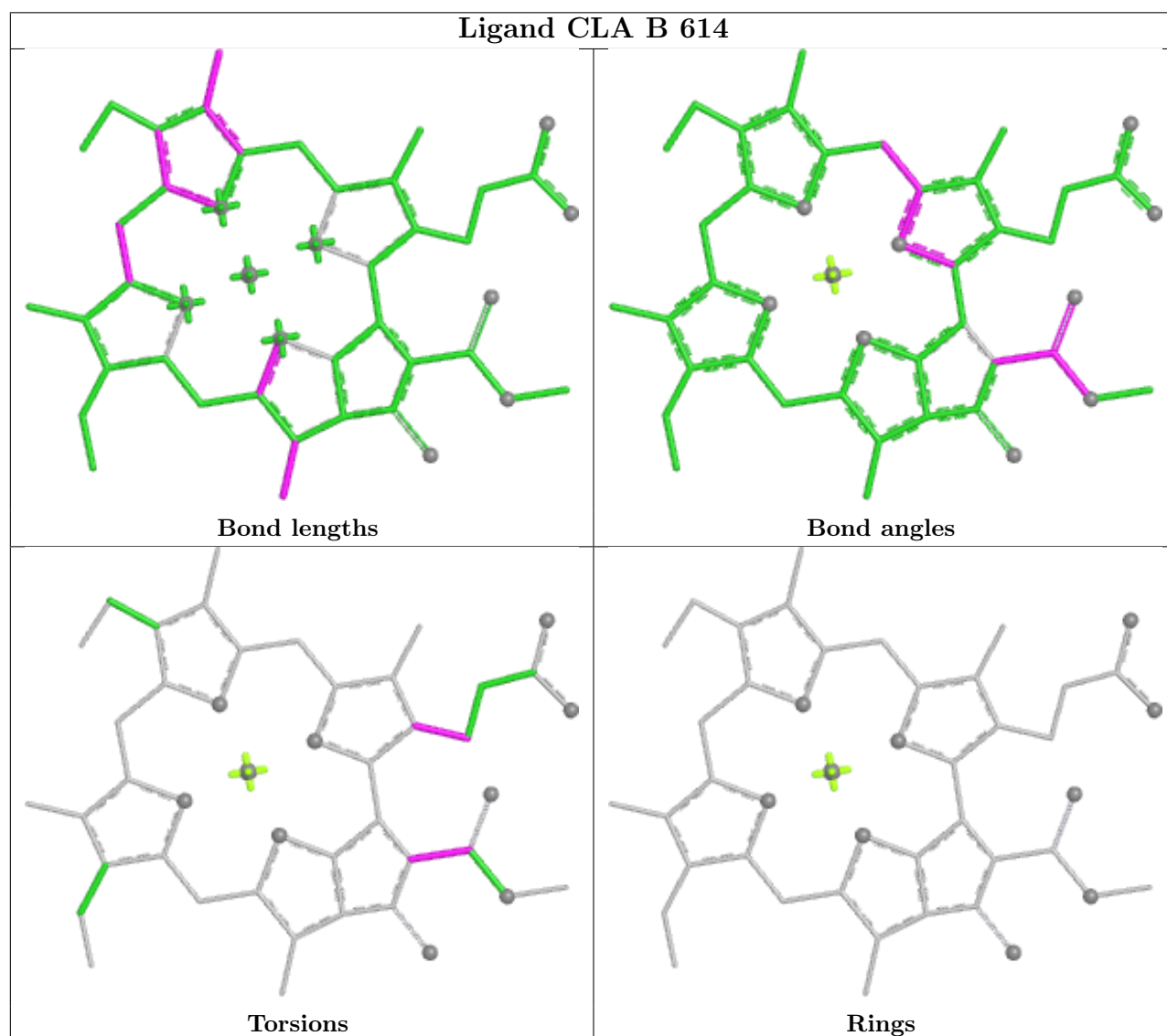
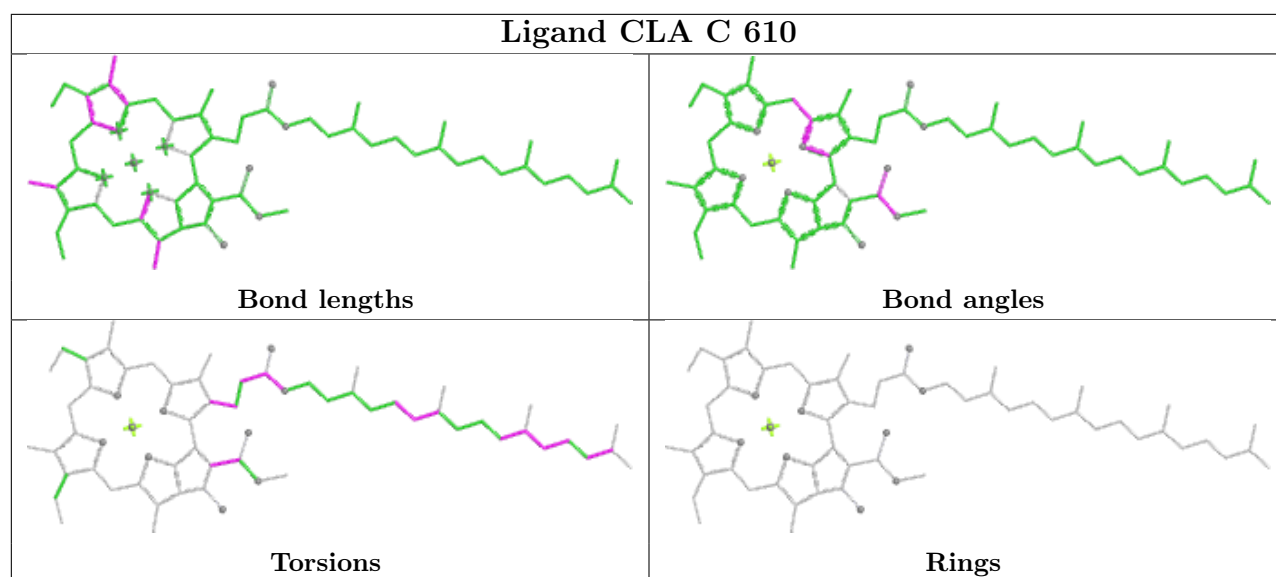


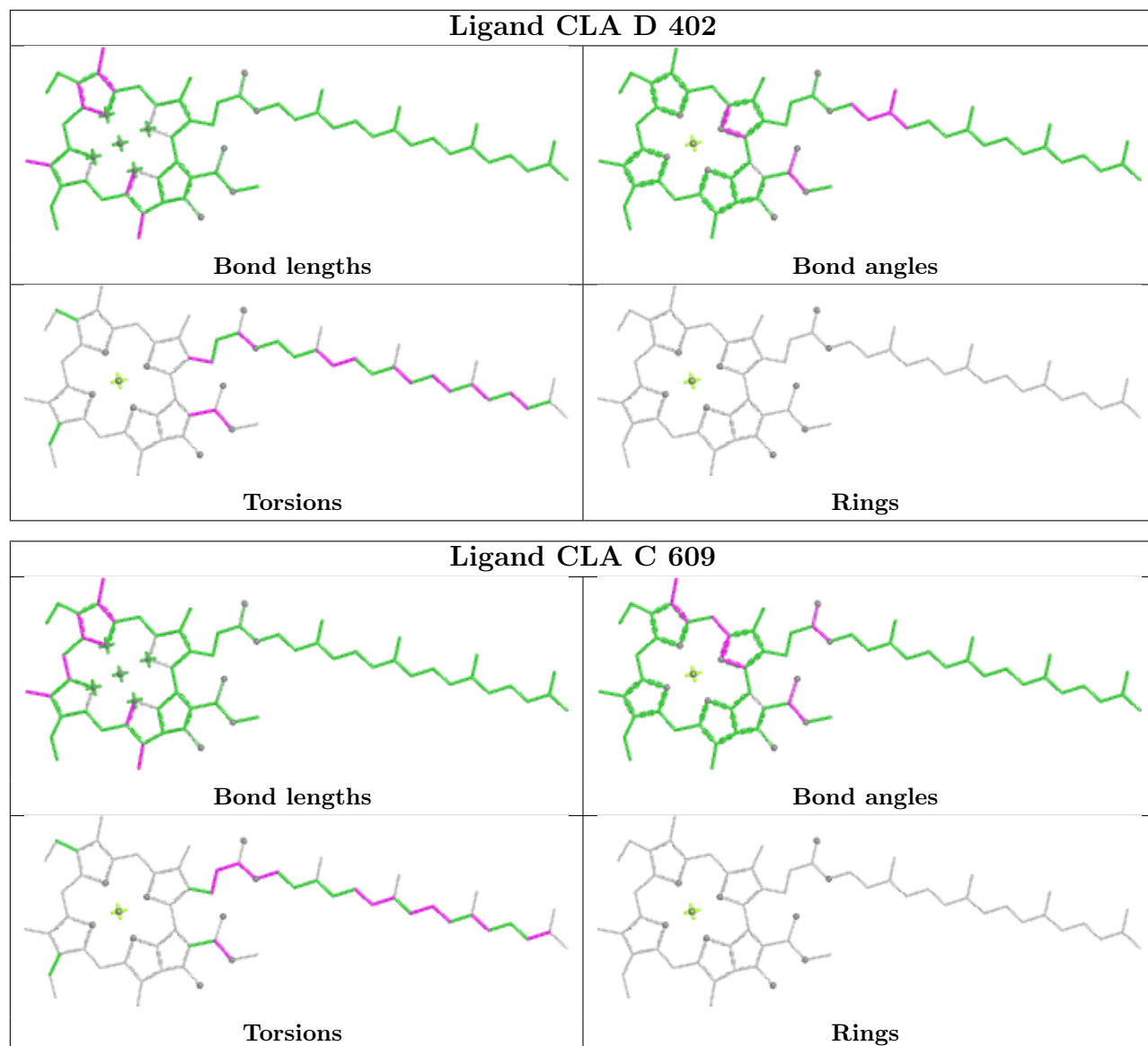


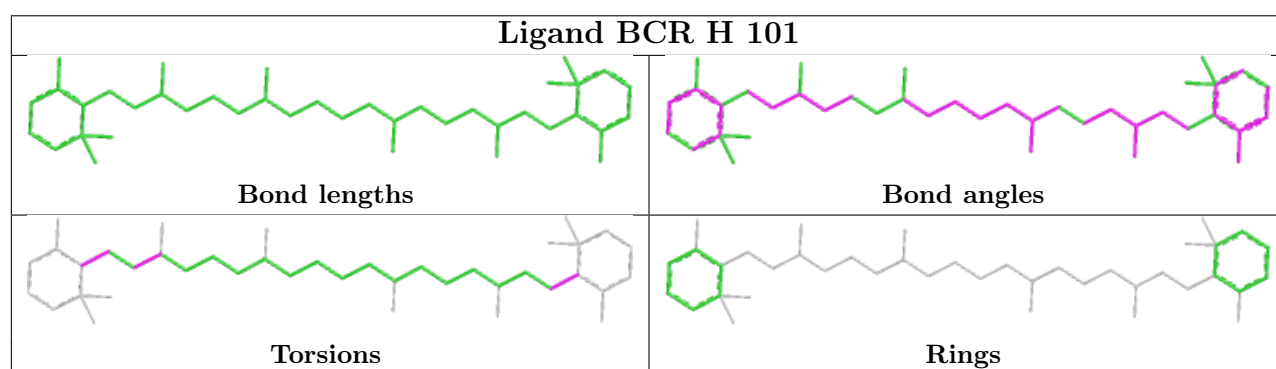
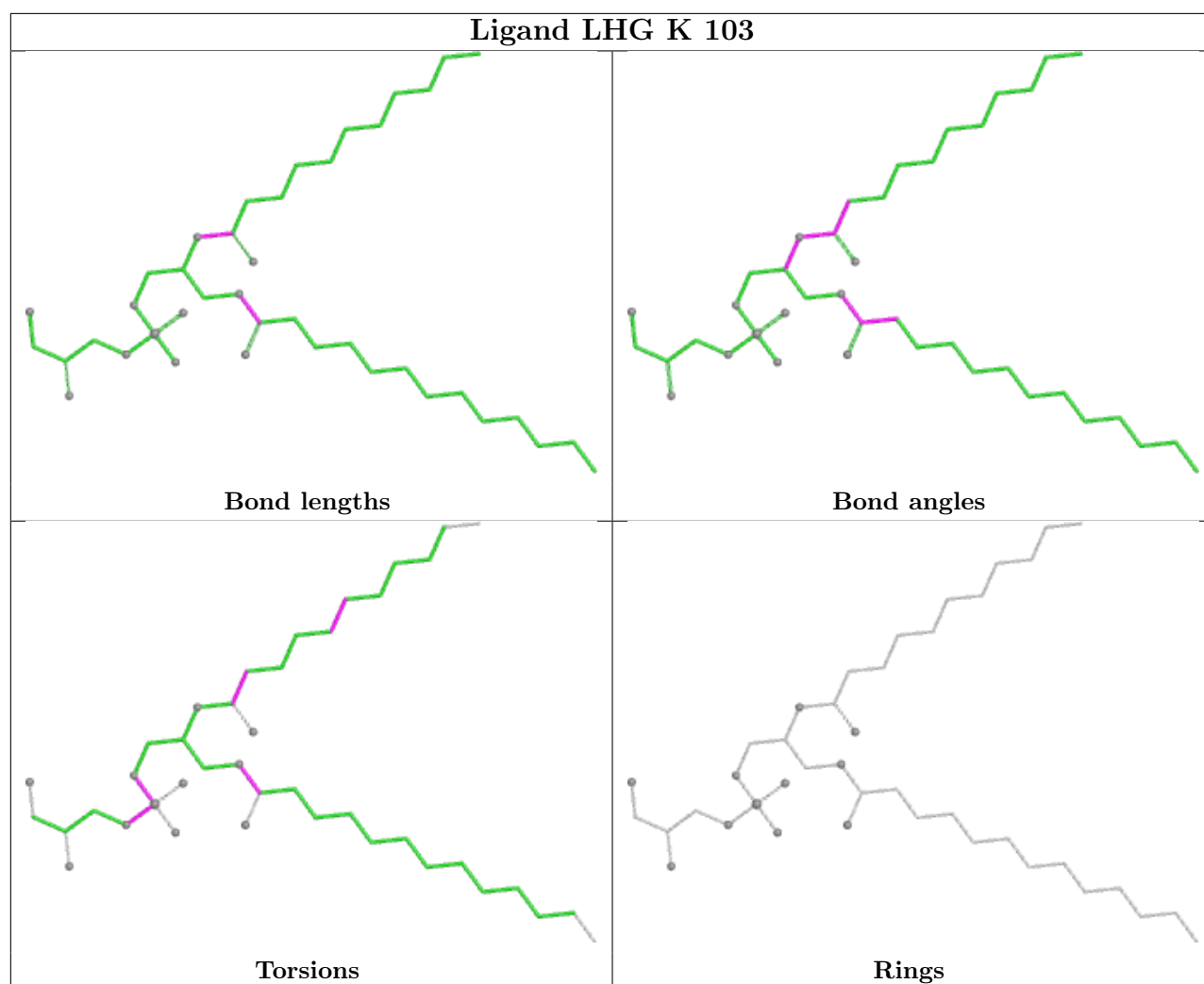


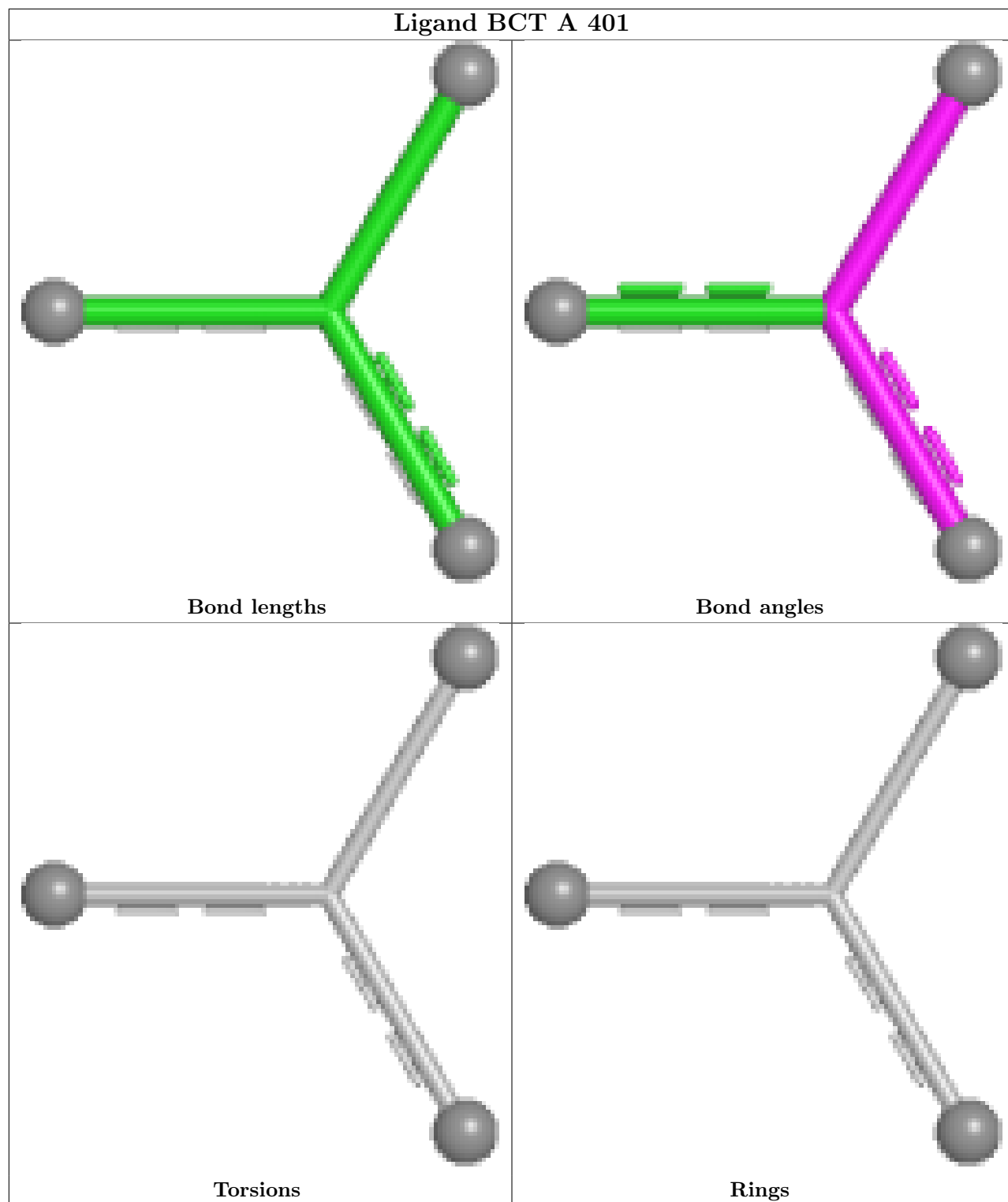


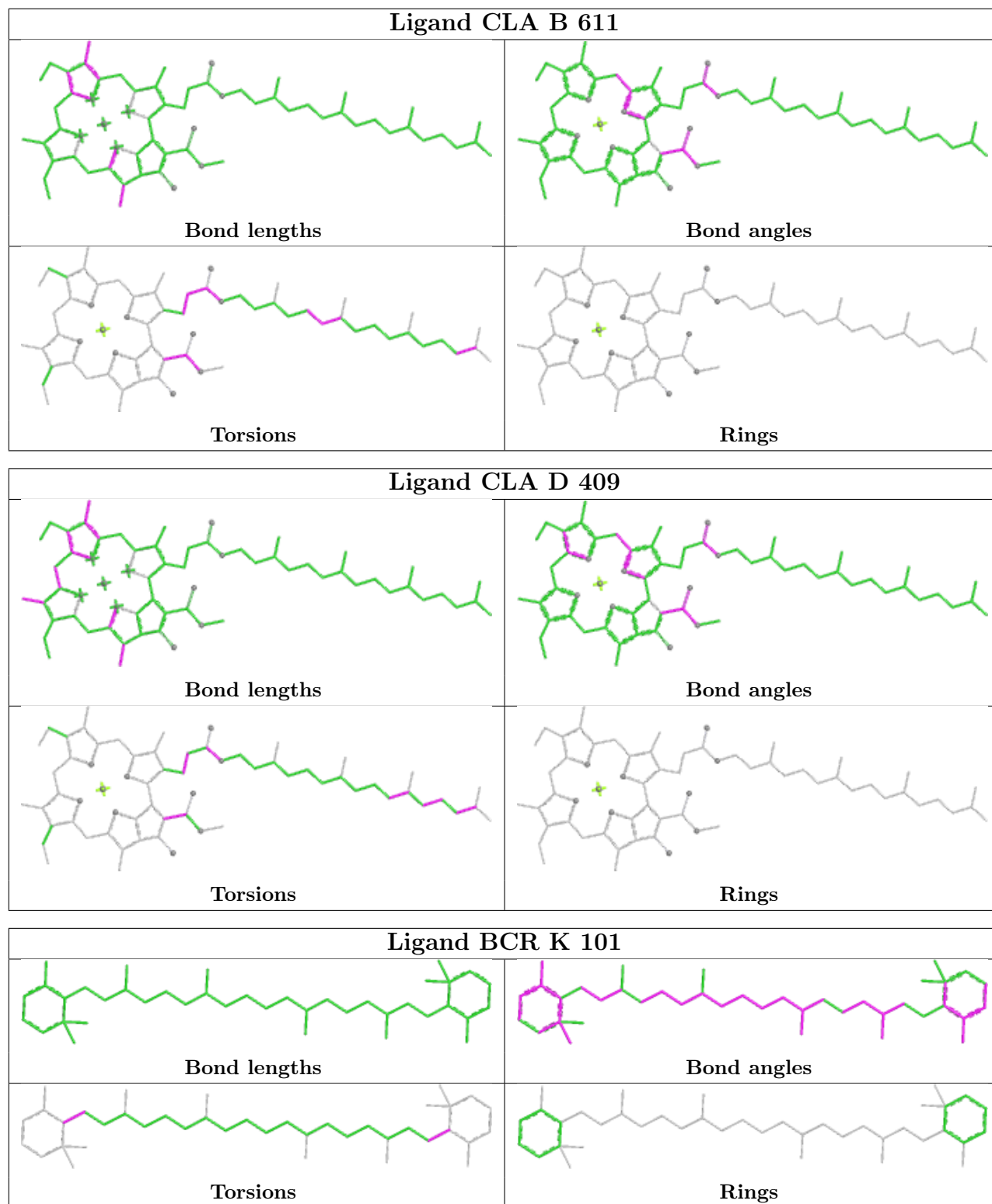


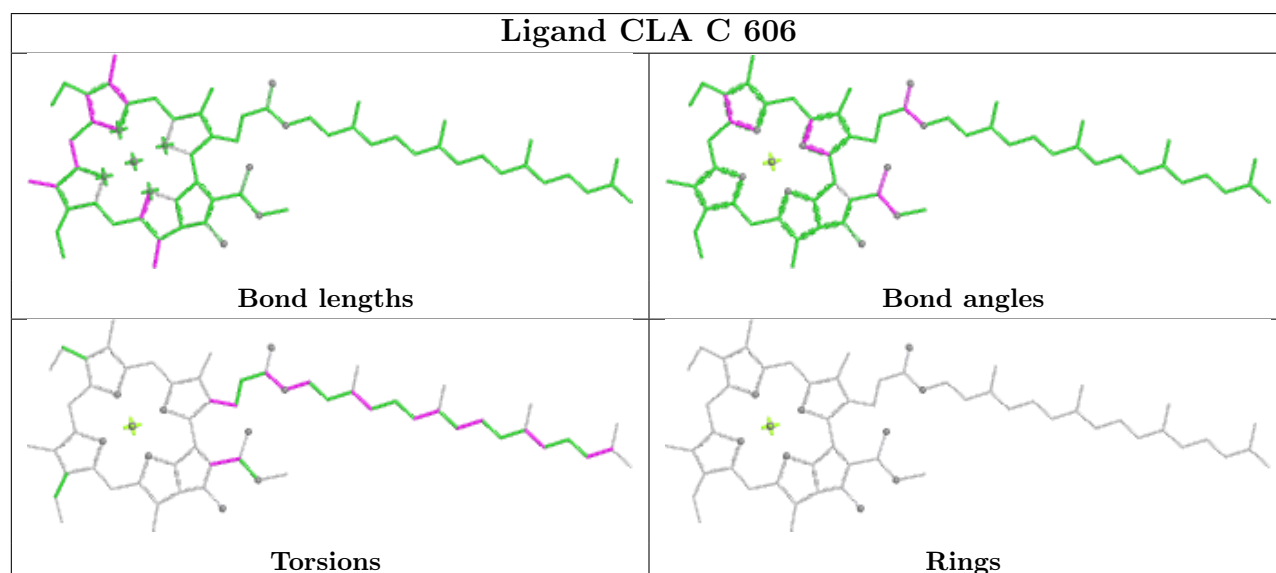
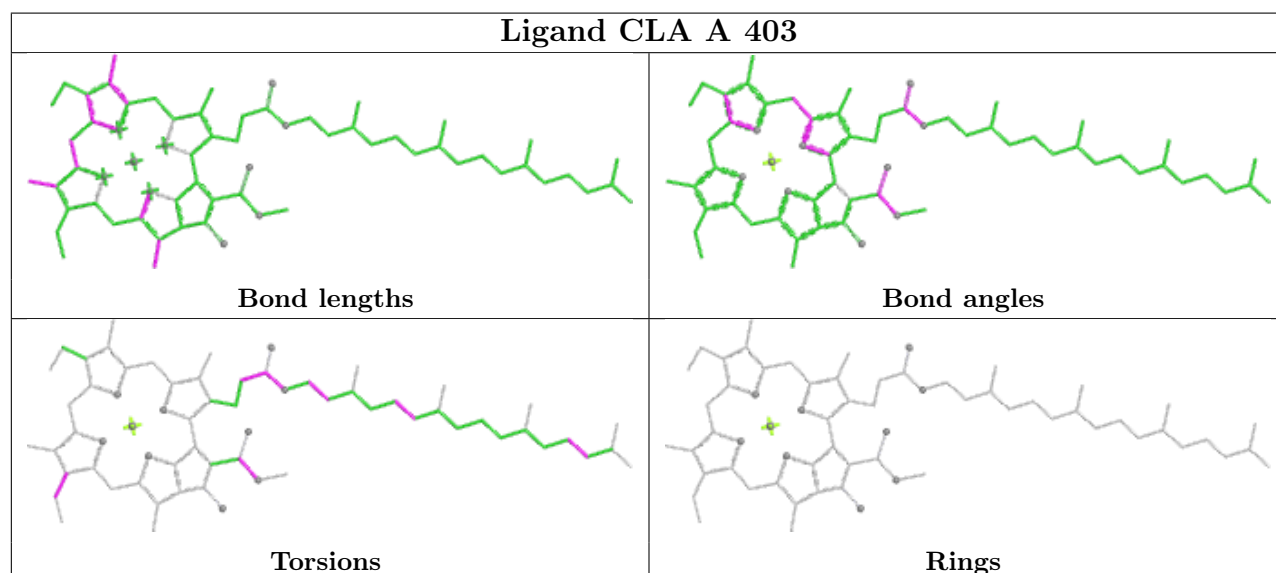
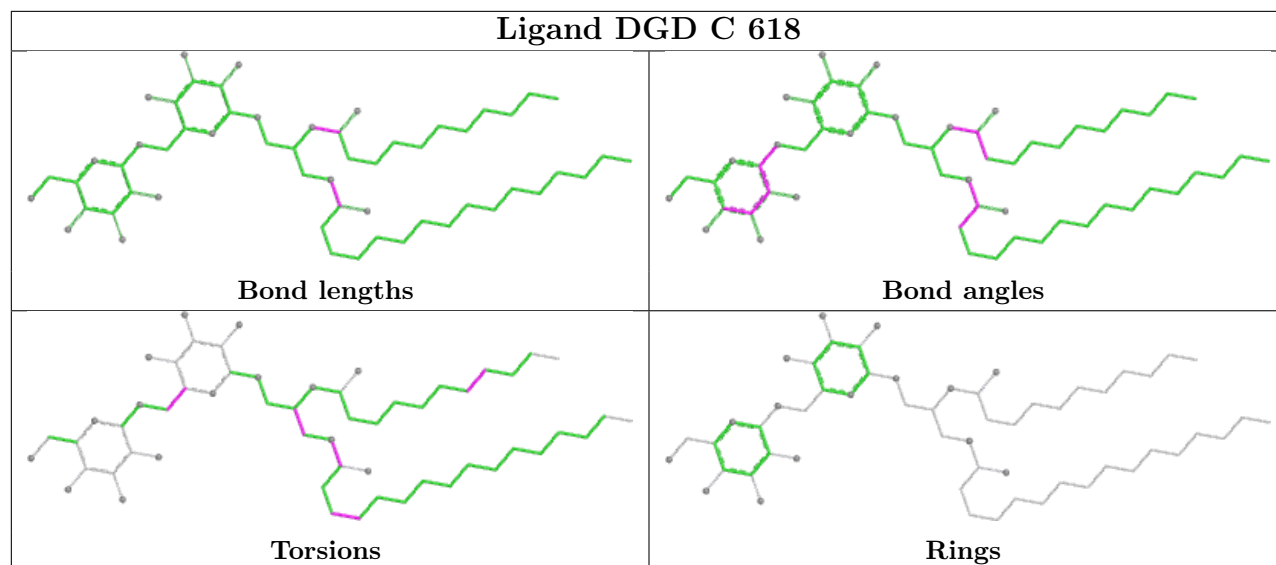


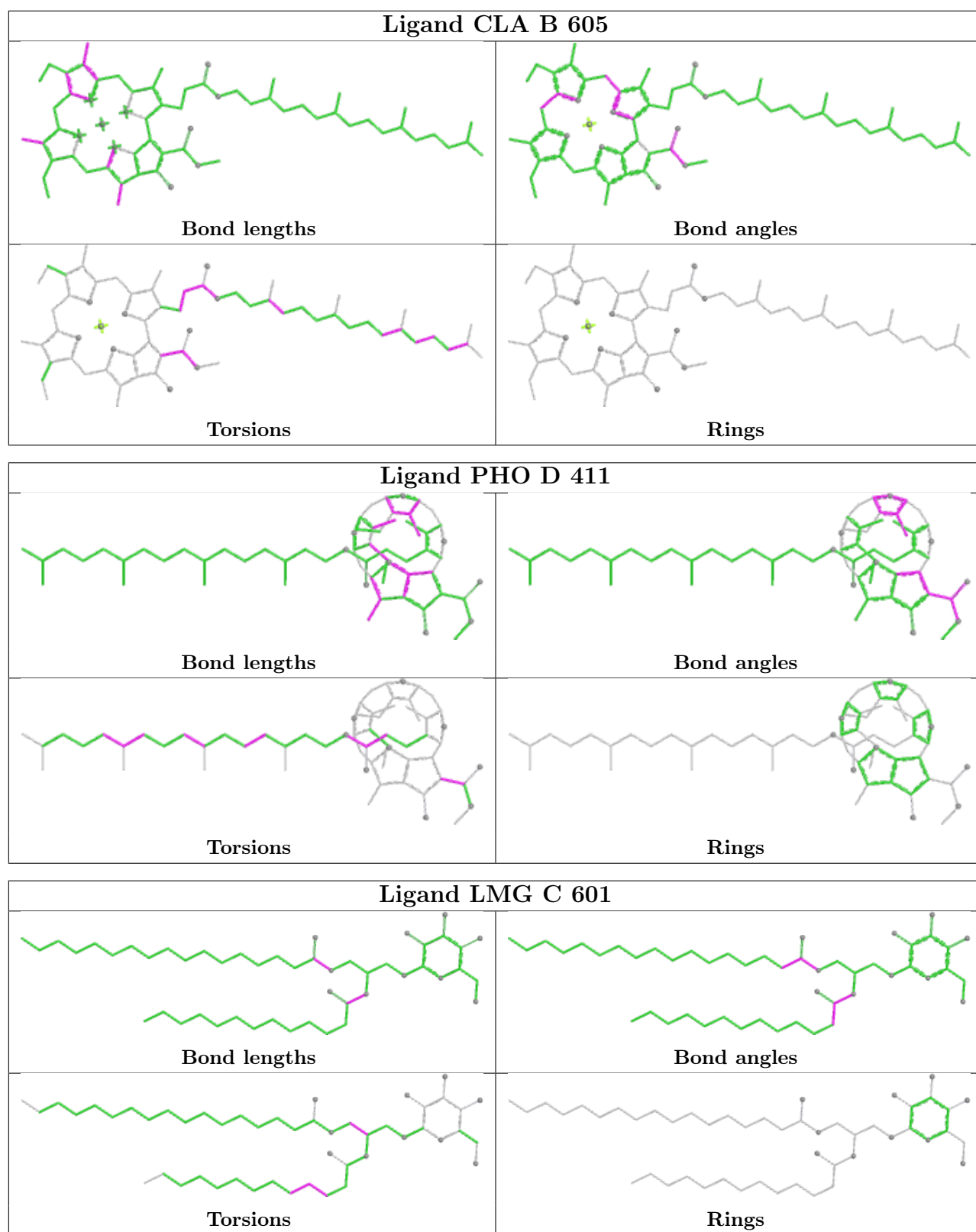


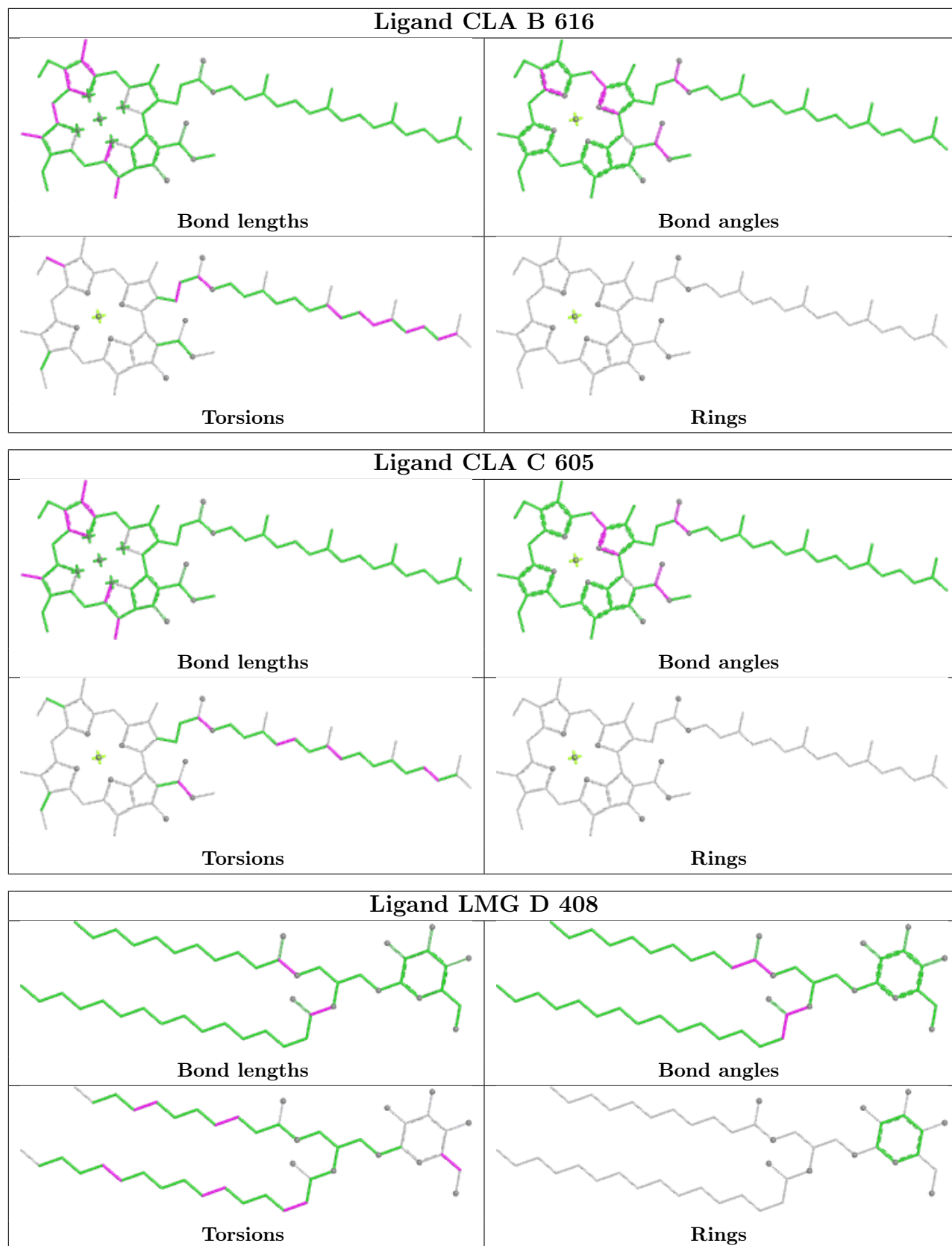


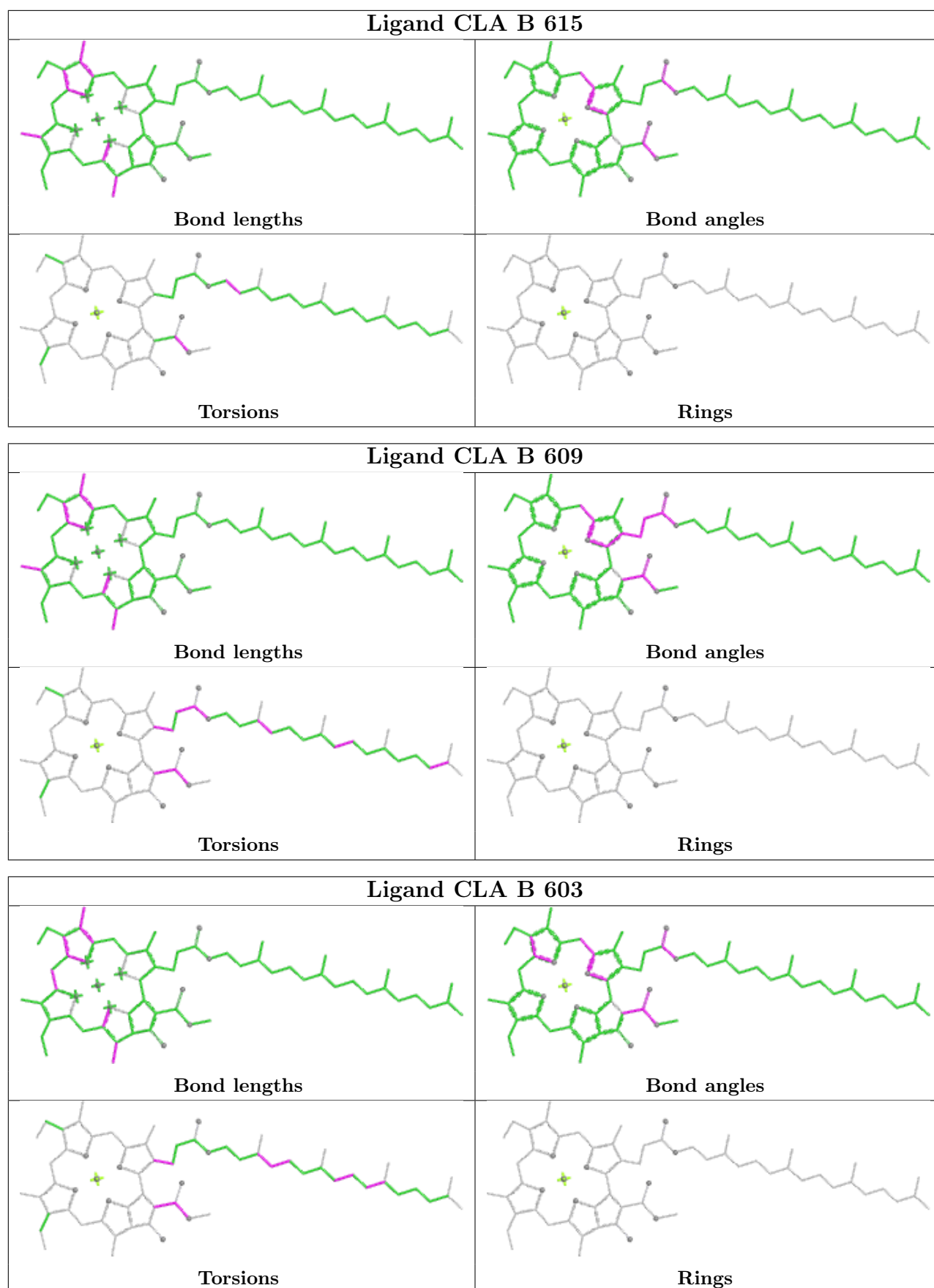


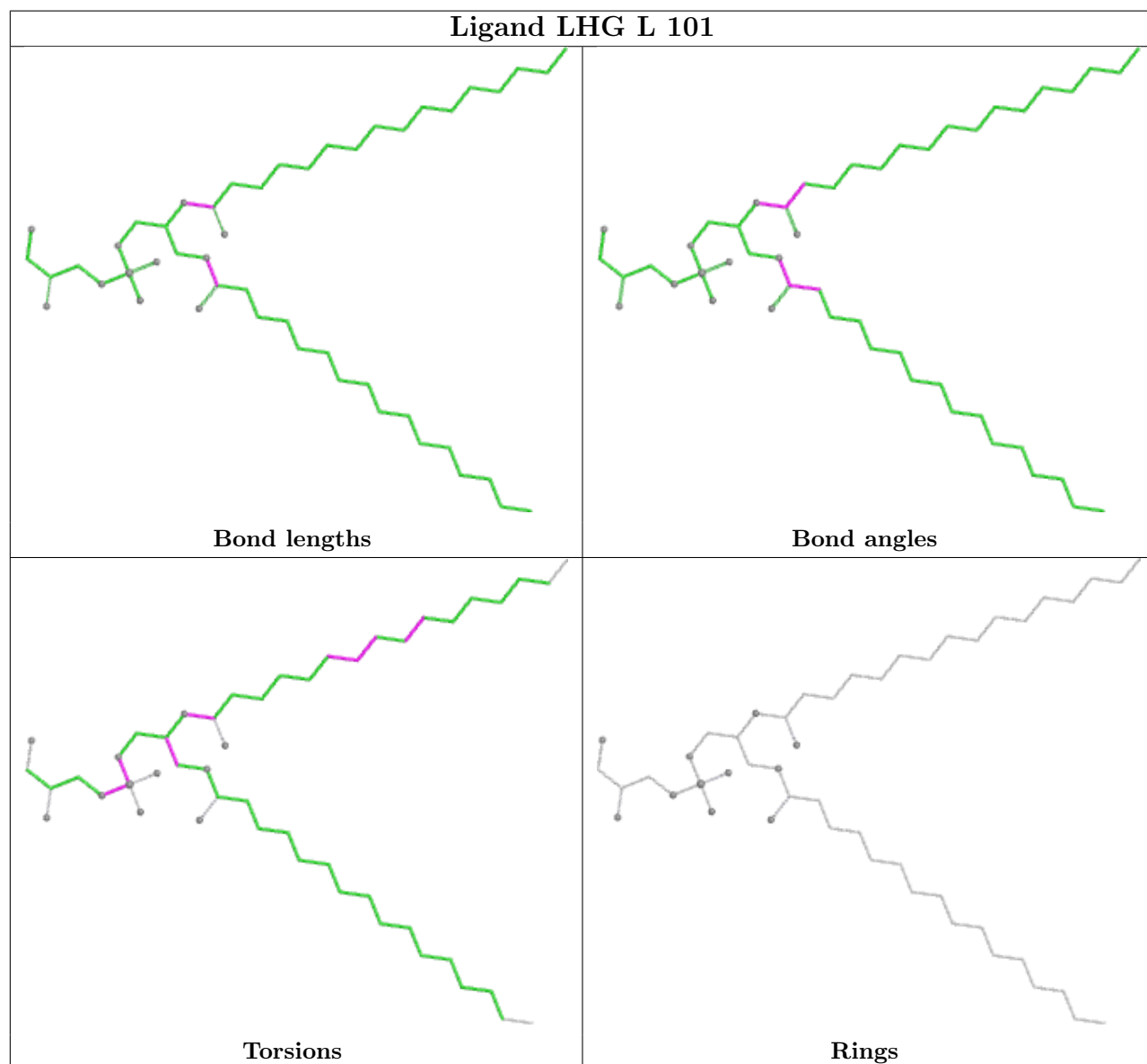
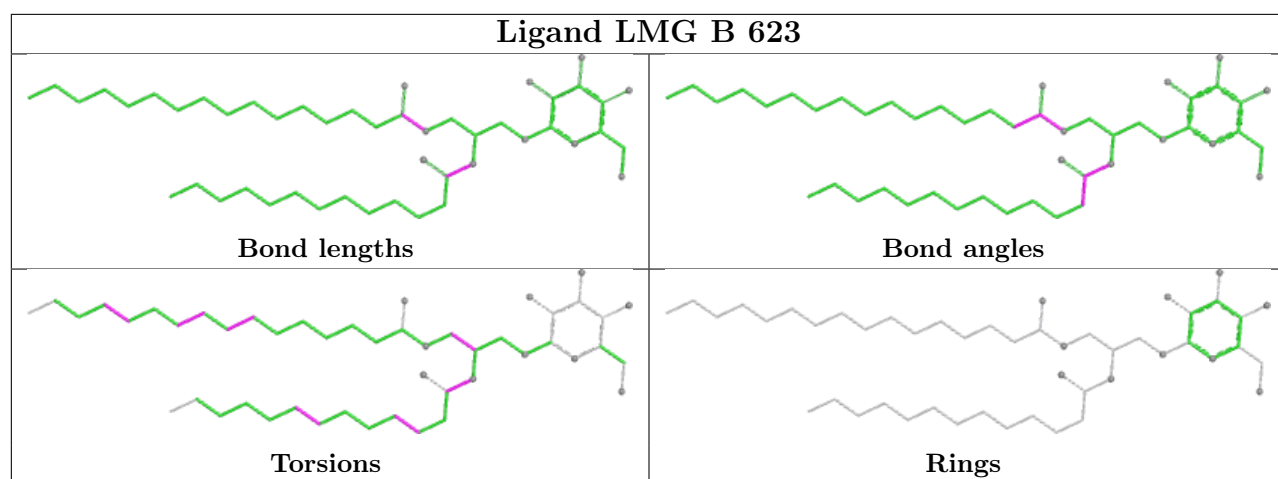


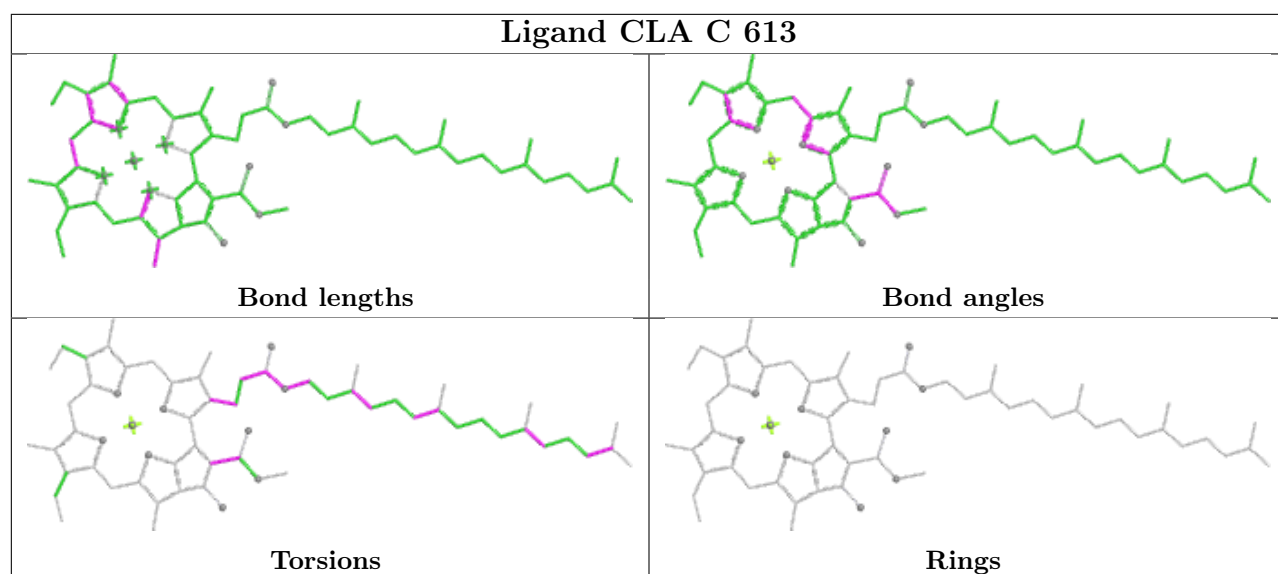
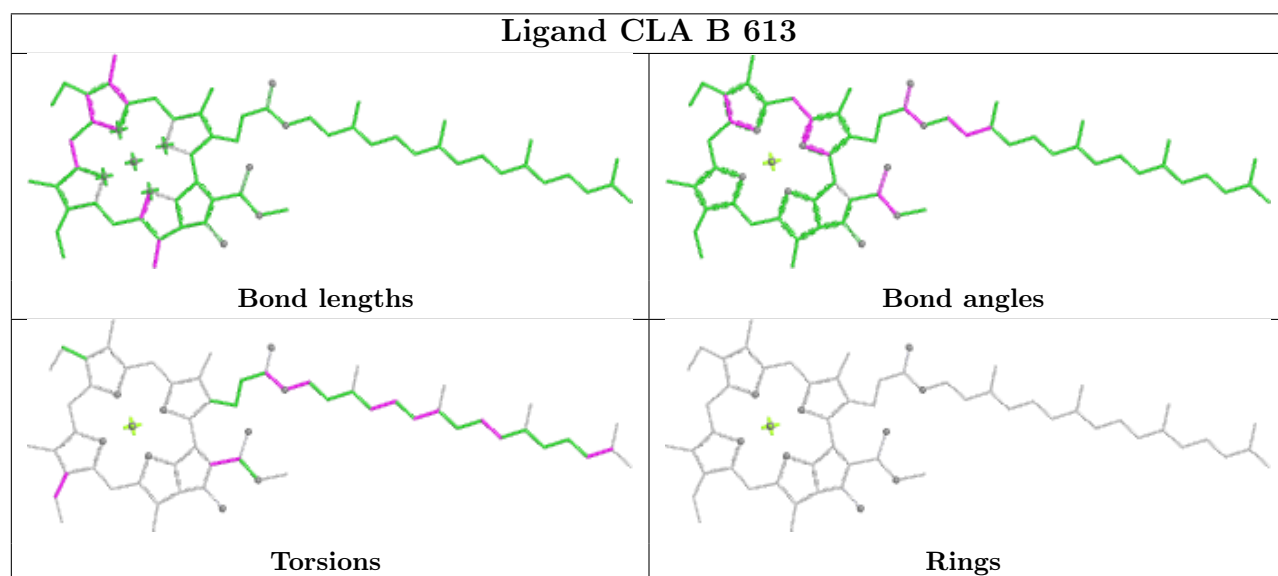
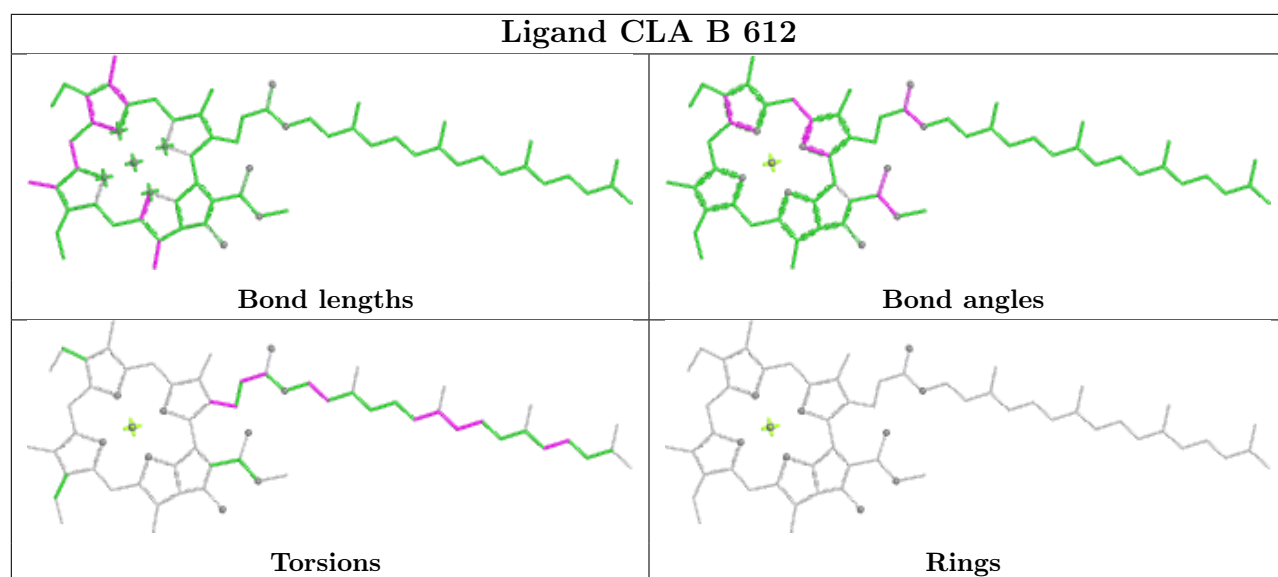


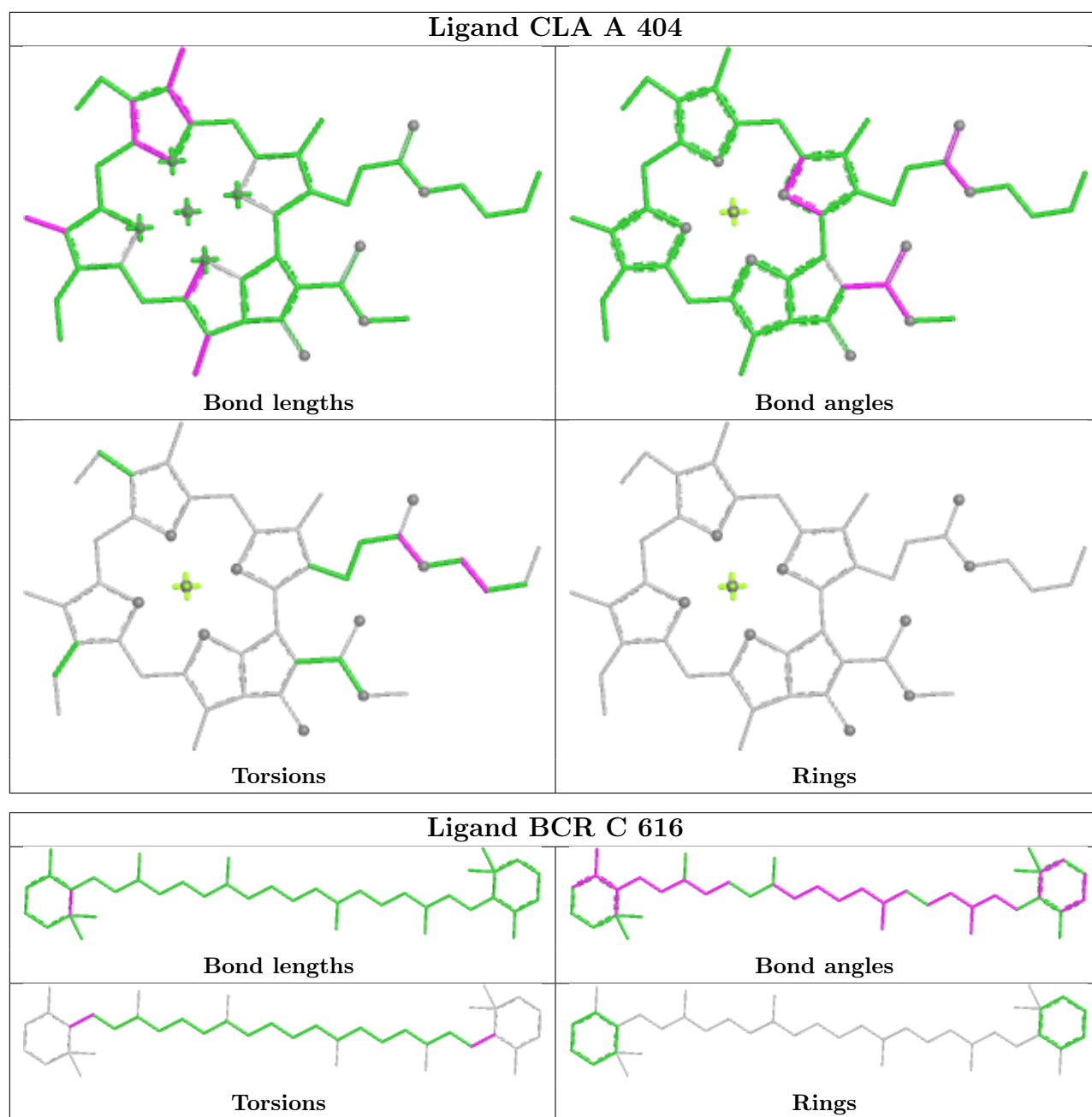


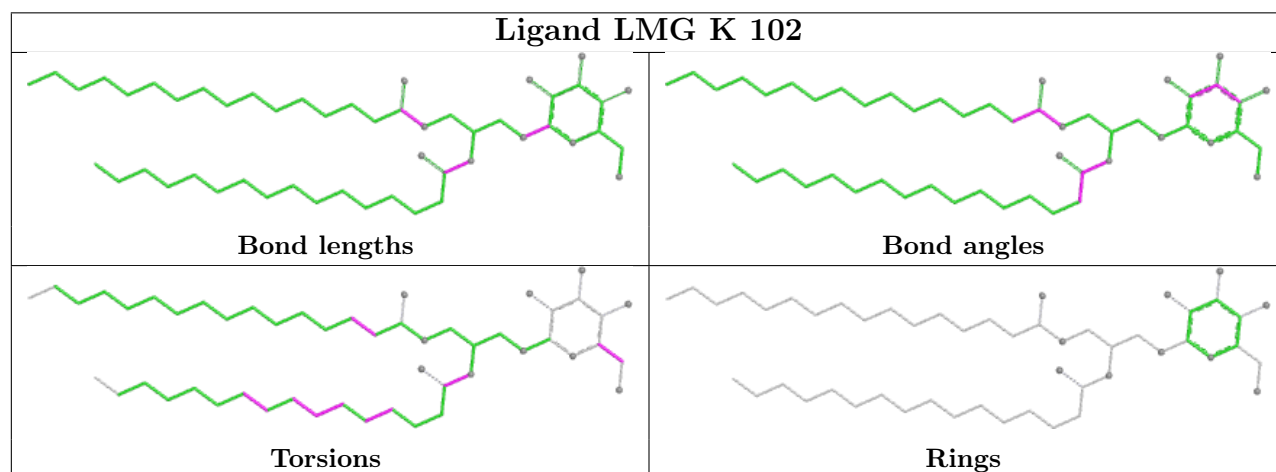
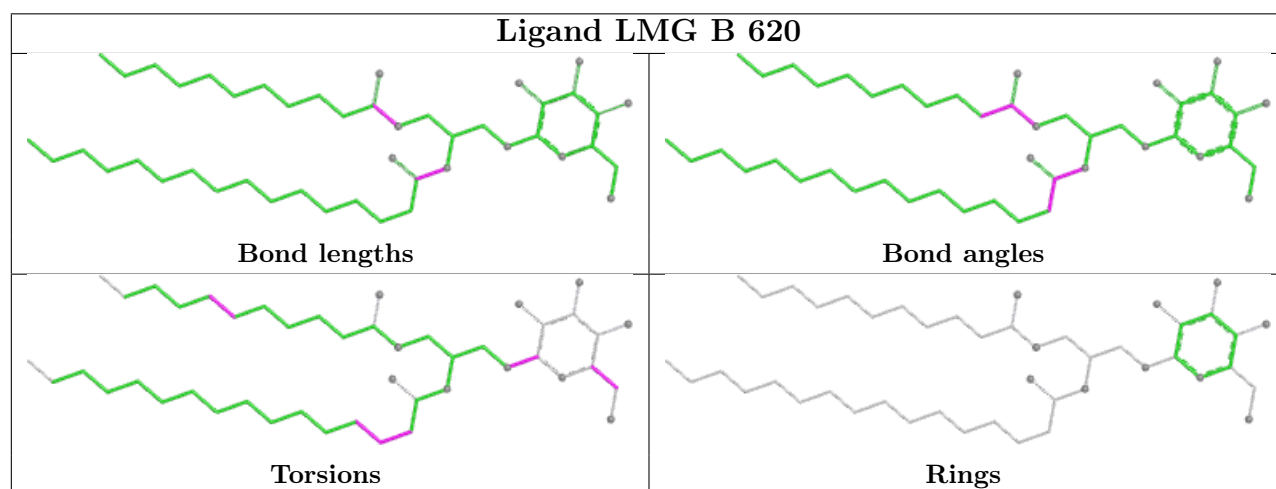
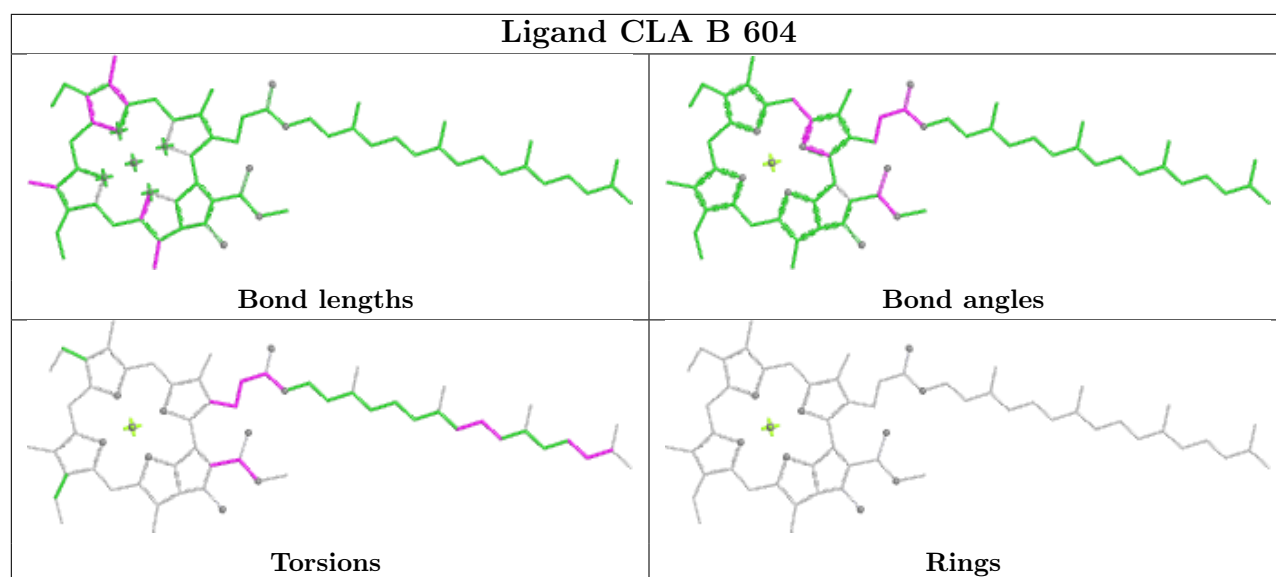


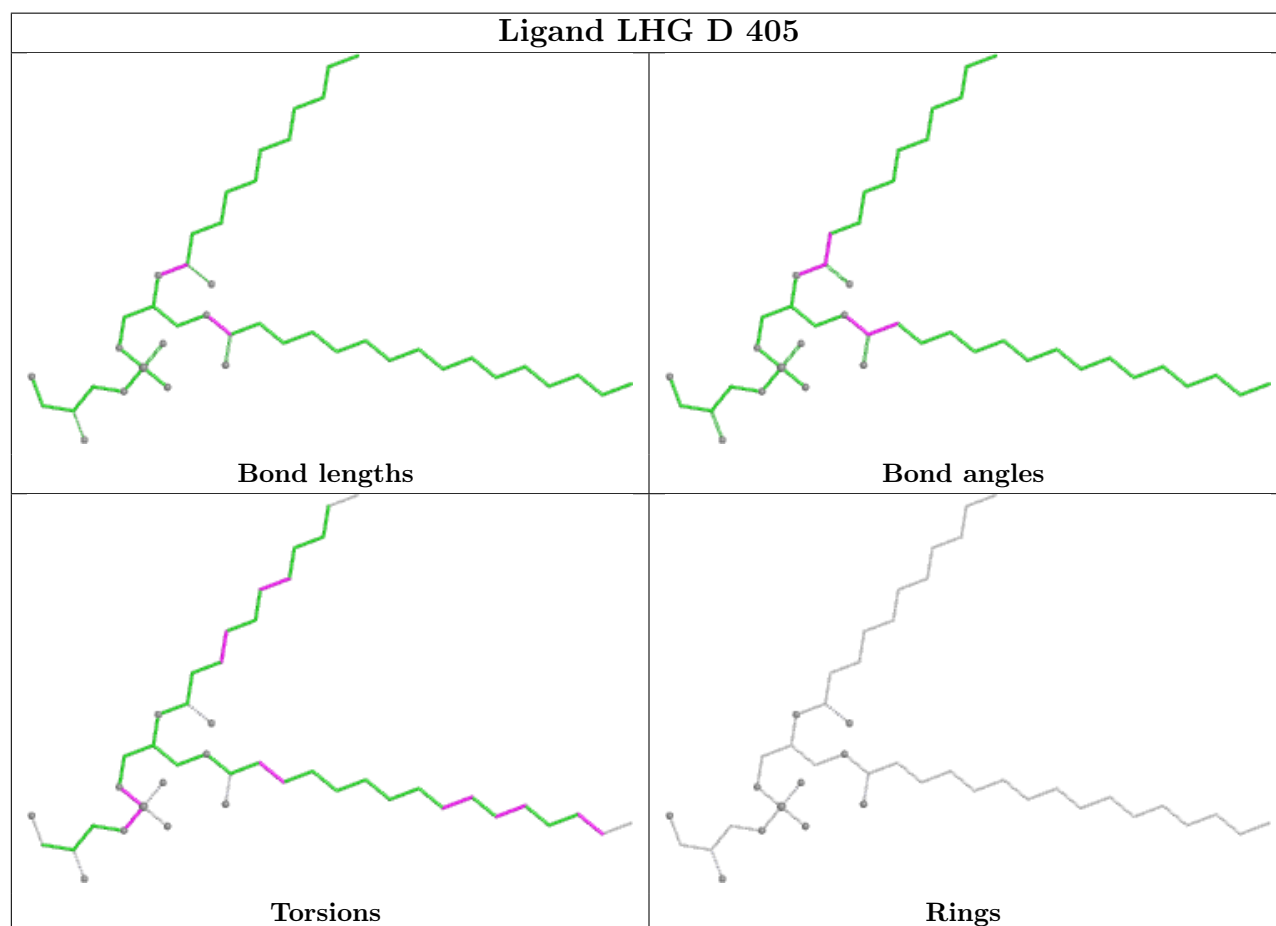
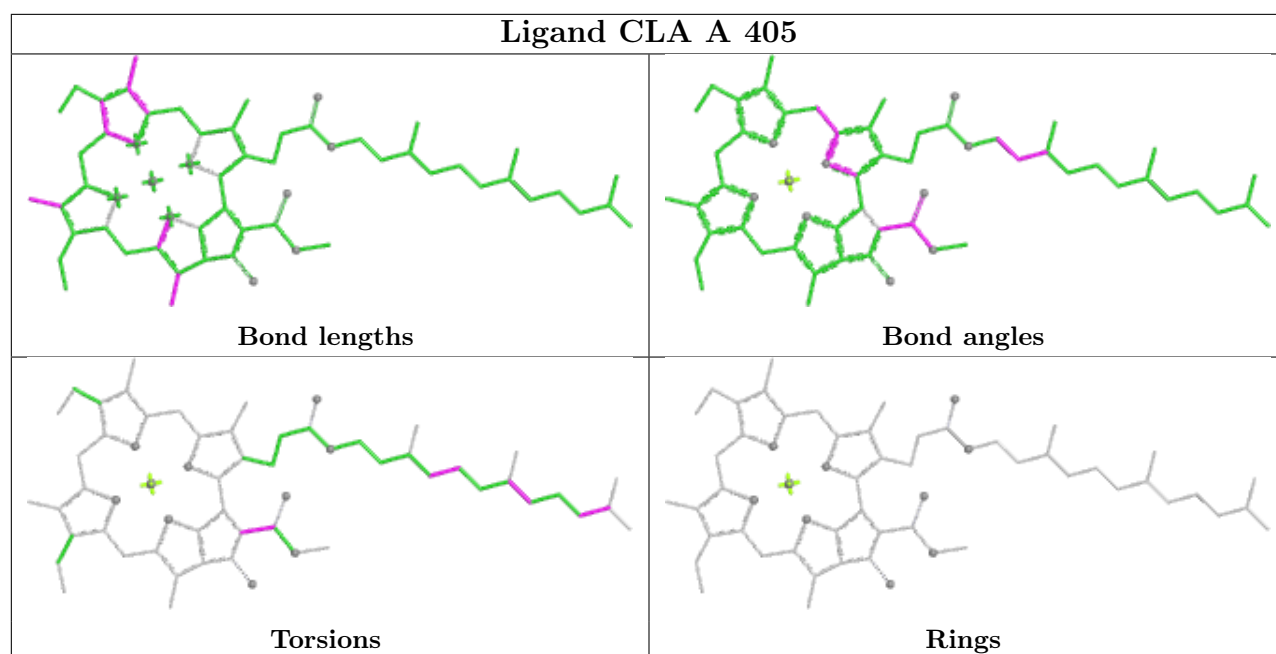


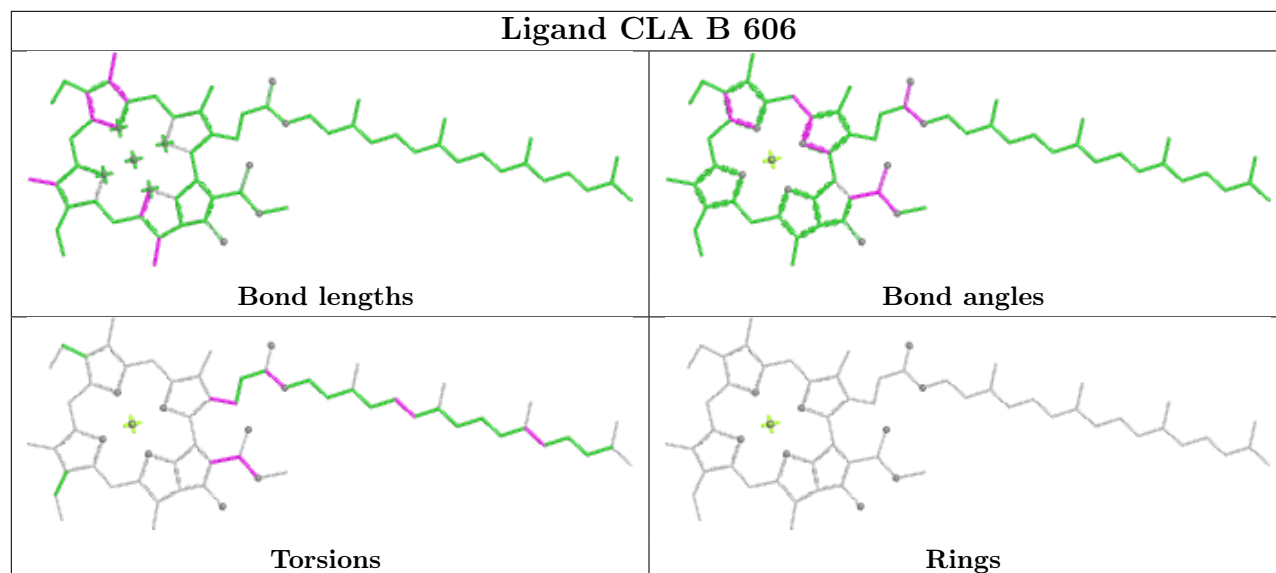
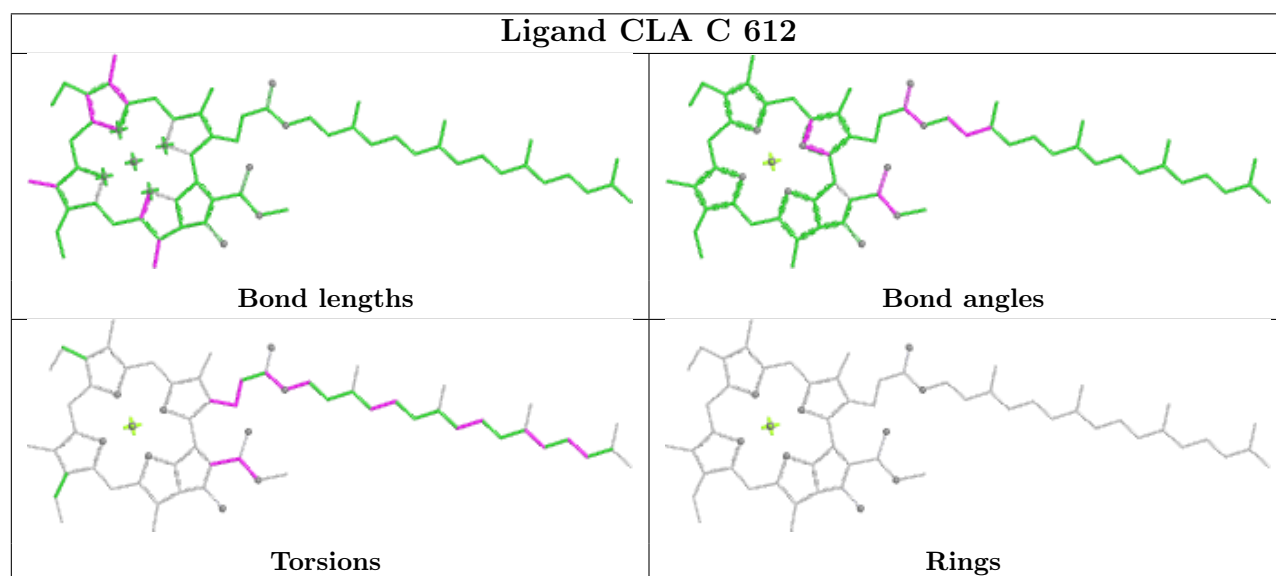
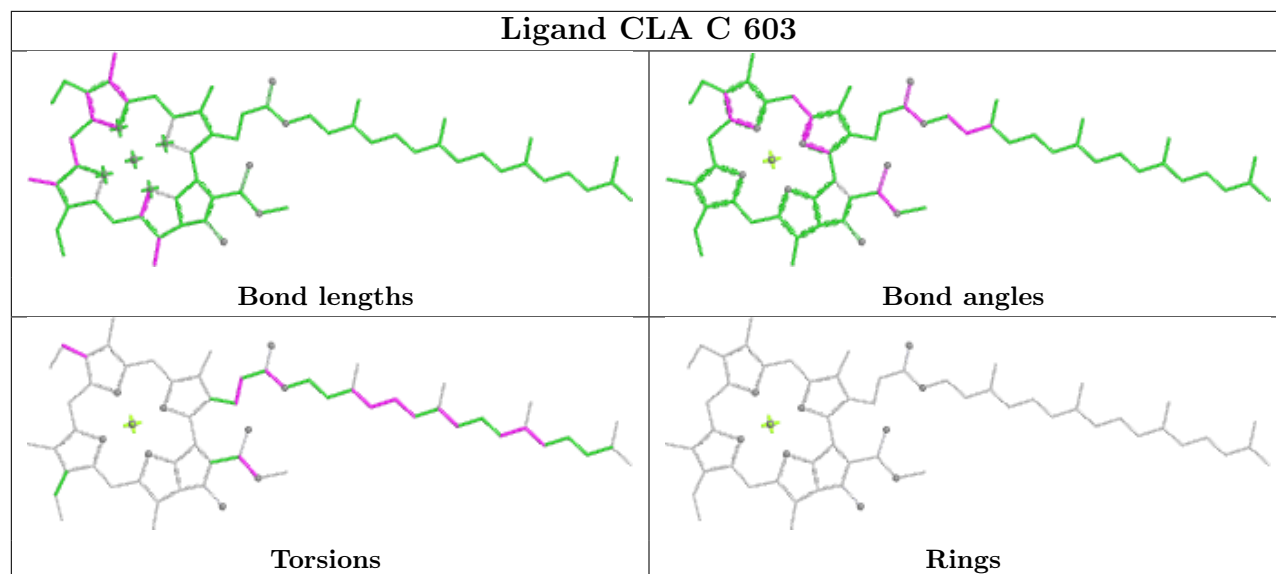


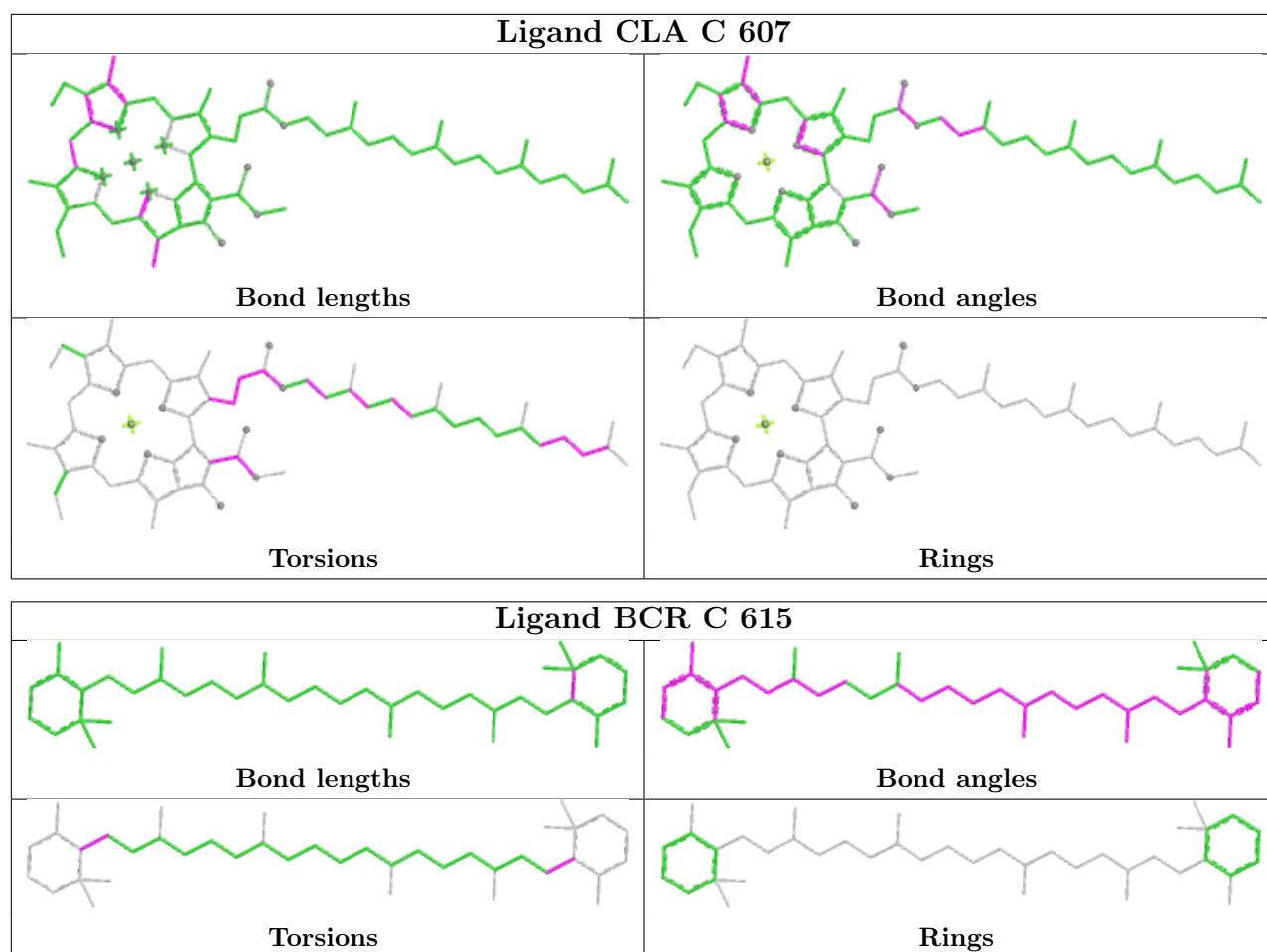


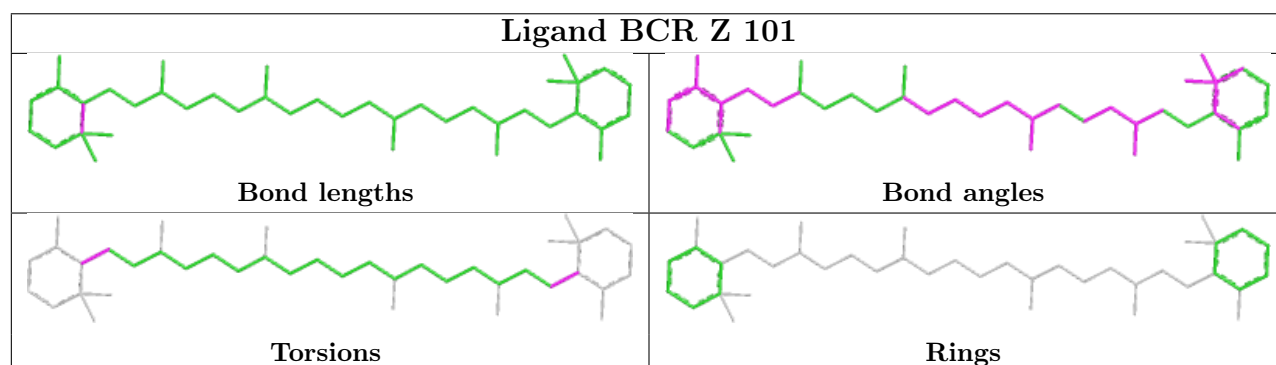
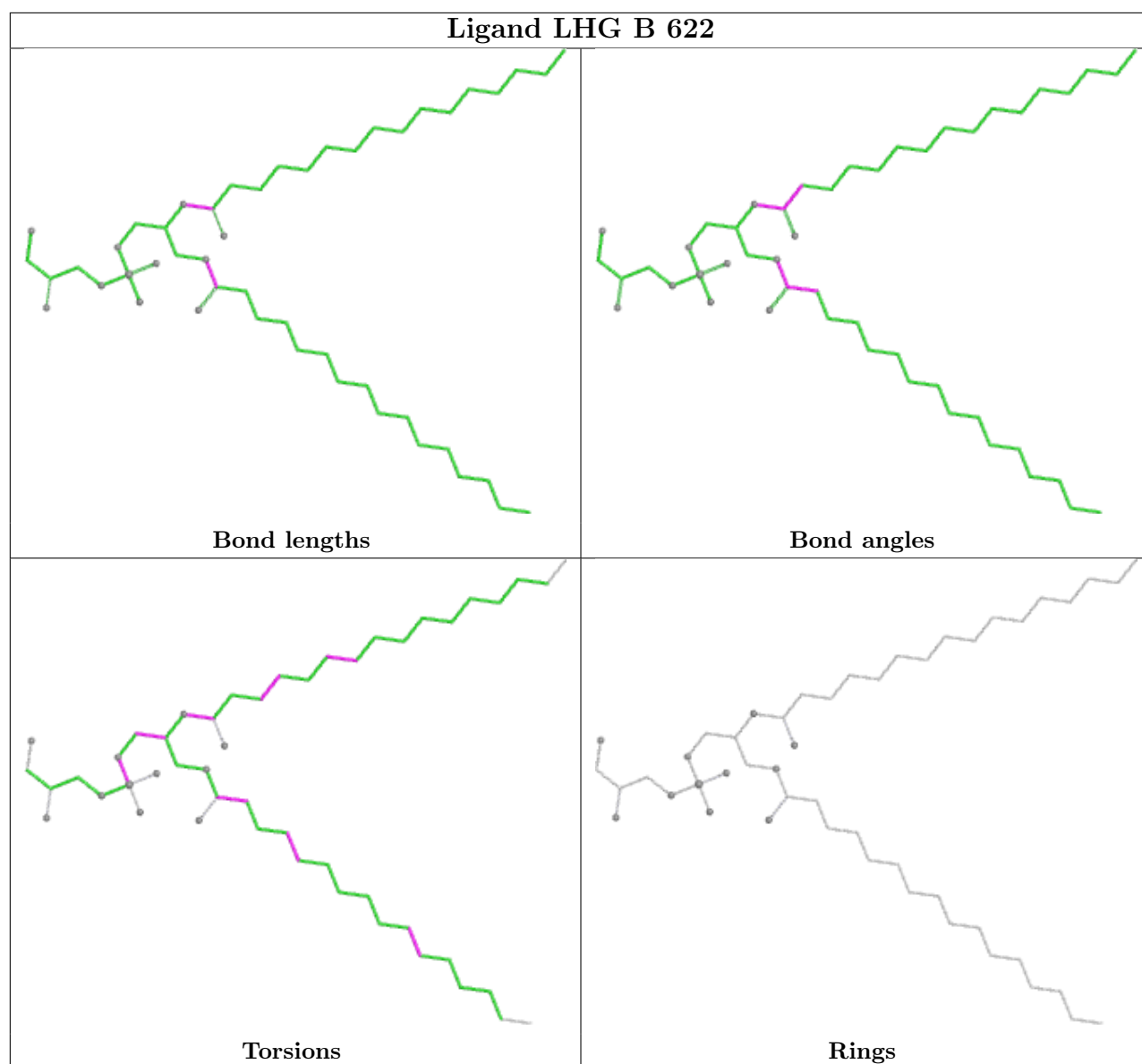


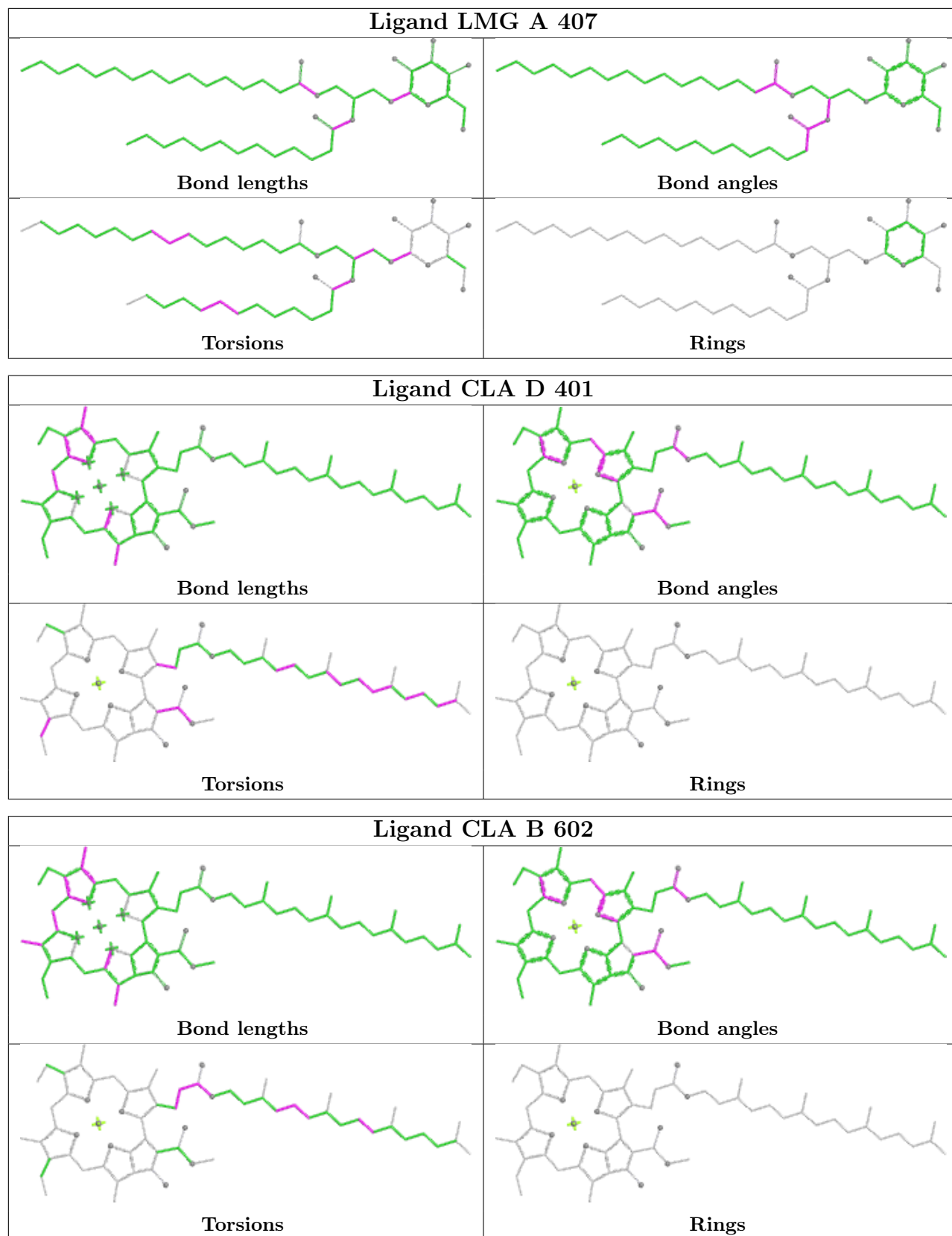


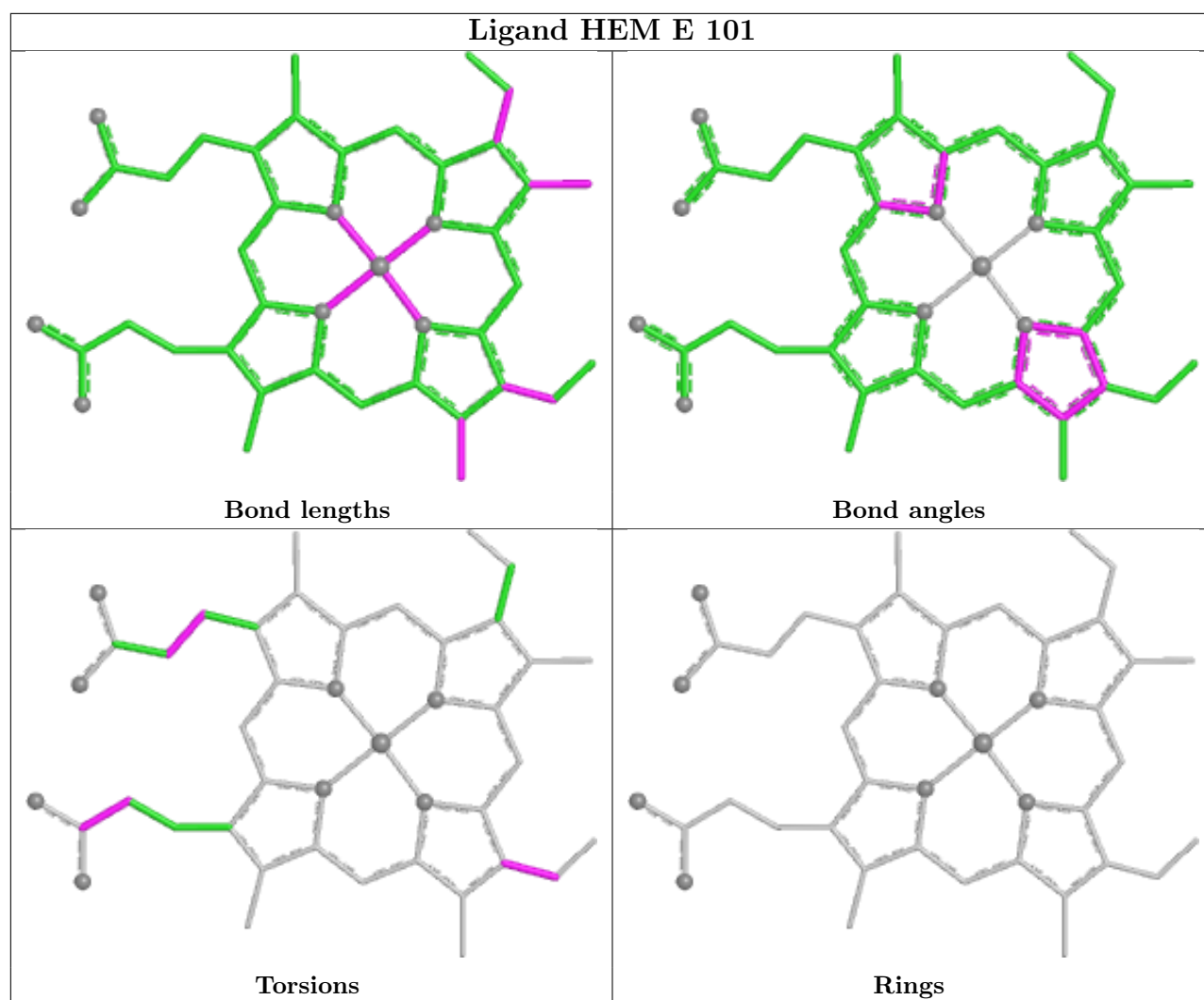












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

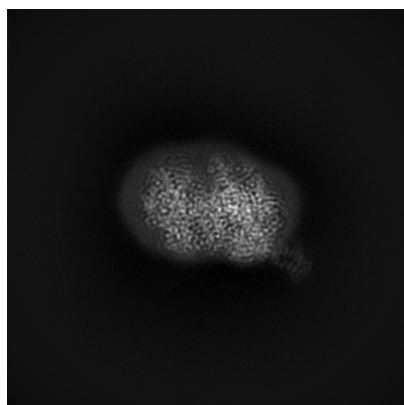
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37133. These allow visual inspection of the internal detail of the map and identification of artifacts.

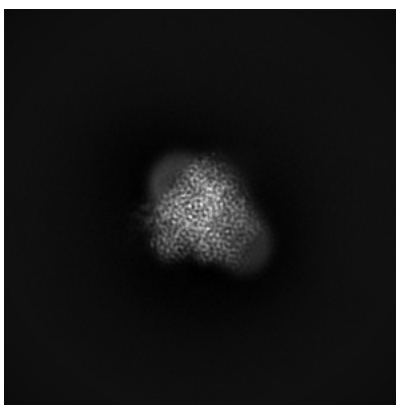
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

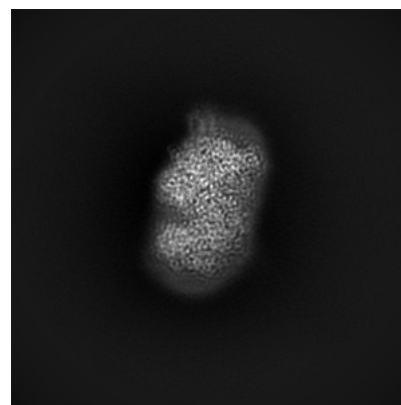
#### 6.1.1 Primary map



X



Y

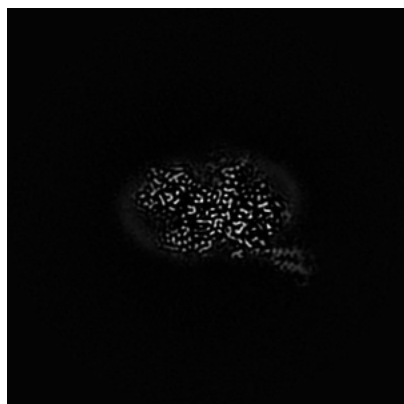


Z

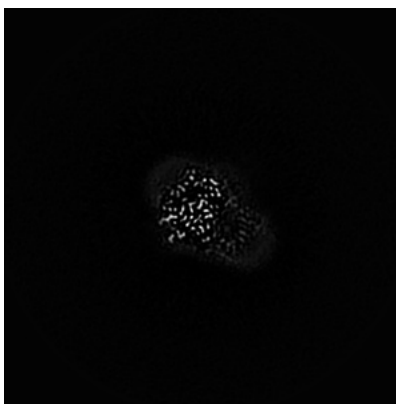
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

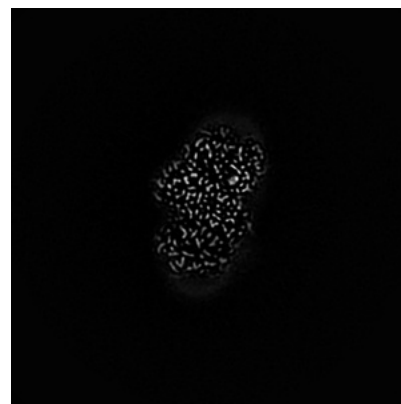
#### 6.2.1 Primary map



X Index: 160



Y Index: 160

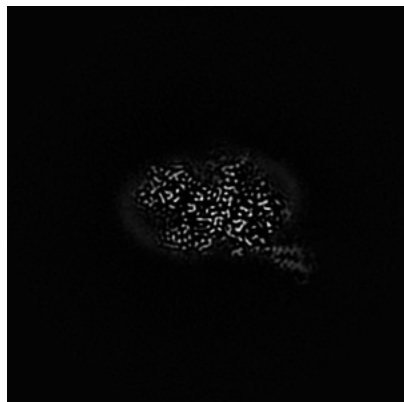


Z Index: 160

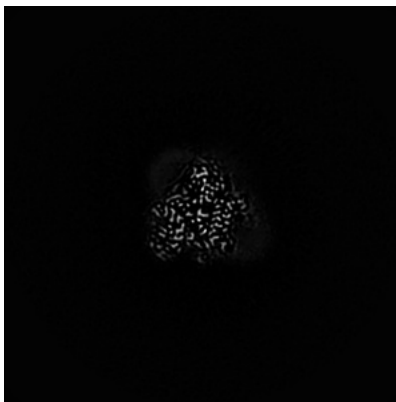
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

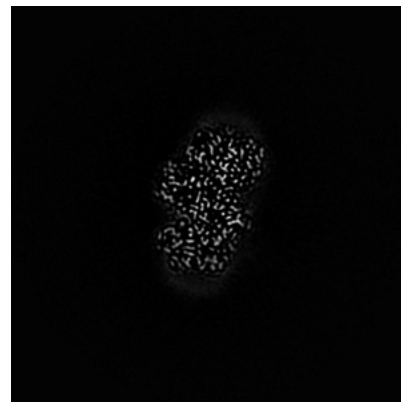
### 6.3.1 Primary map



X Index: 160



Y Index: 183

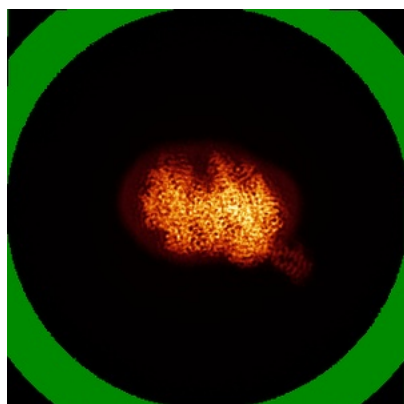


Z Index: 162

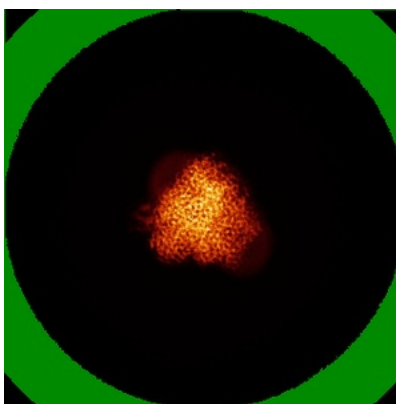
The images above show the largest variance slices of the map in three orthogonal directions.

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

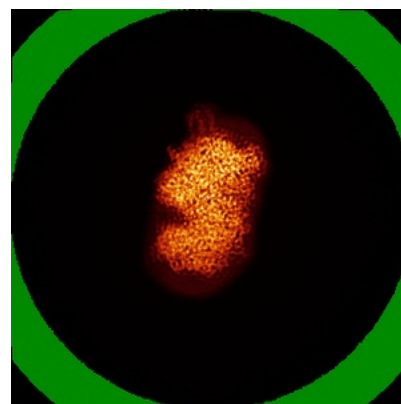
### 6.4.1 Primary map



X



Y

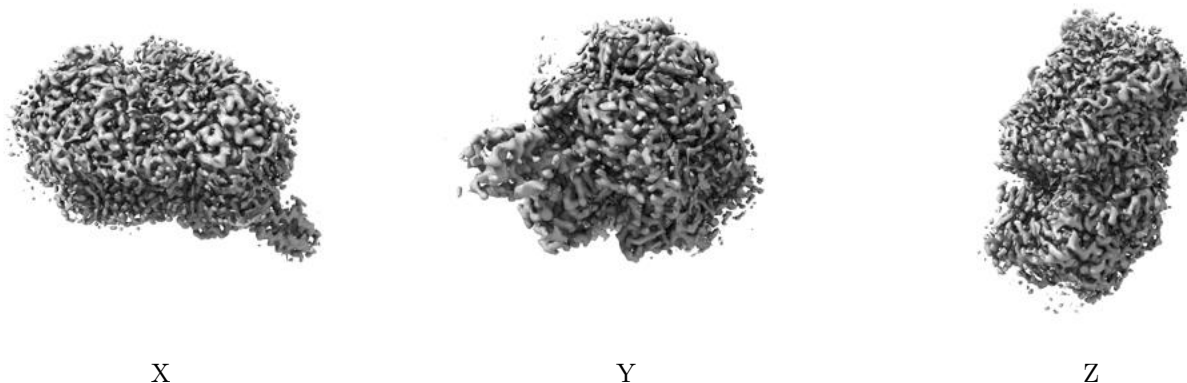


Z

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

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 3.9. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

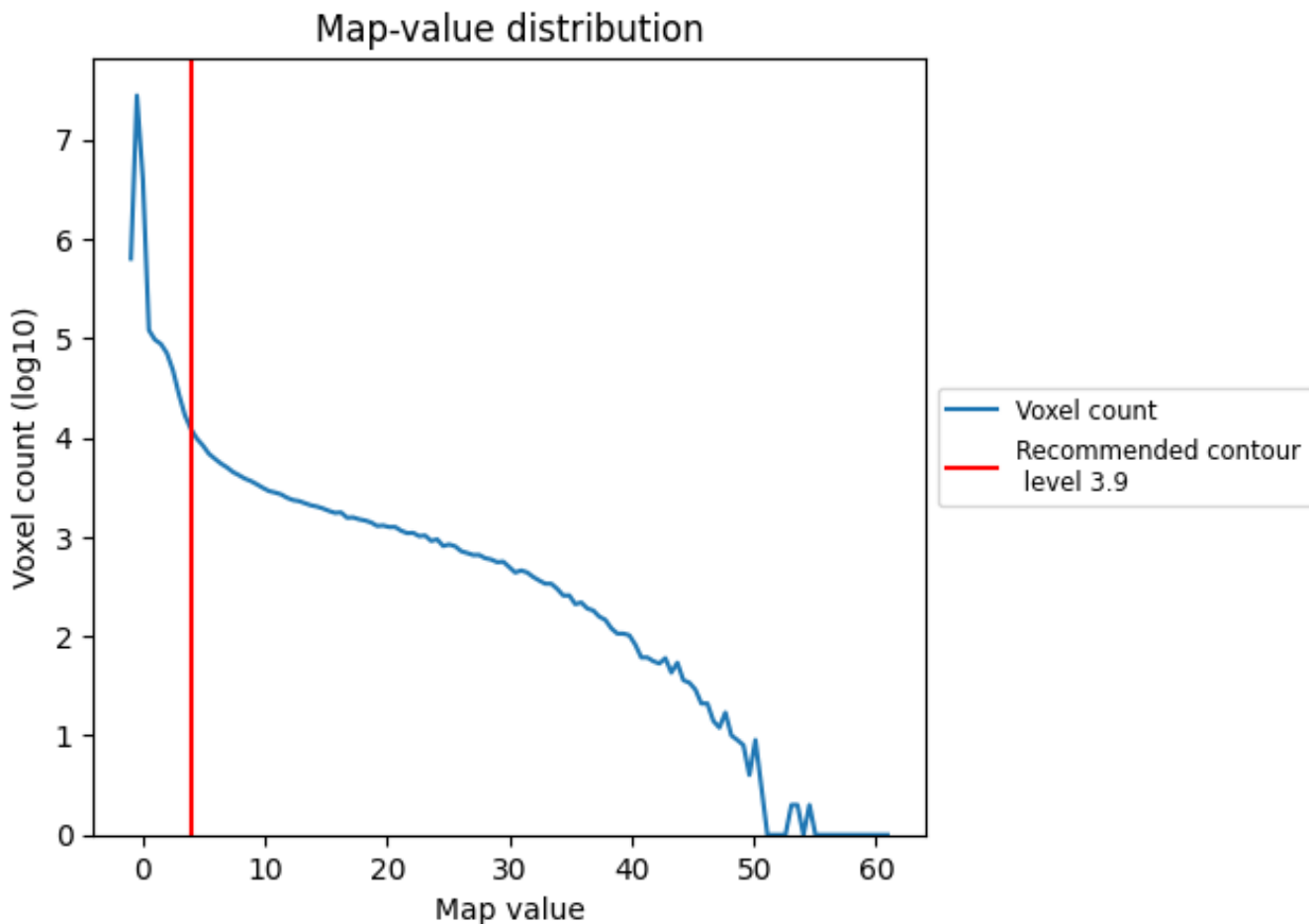
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

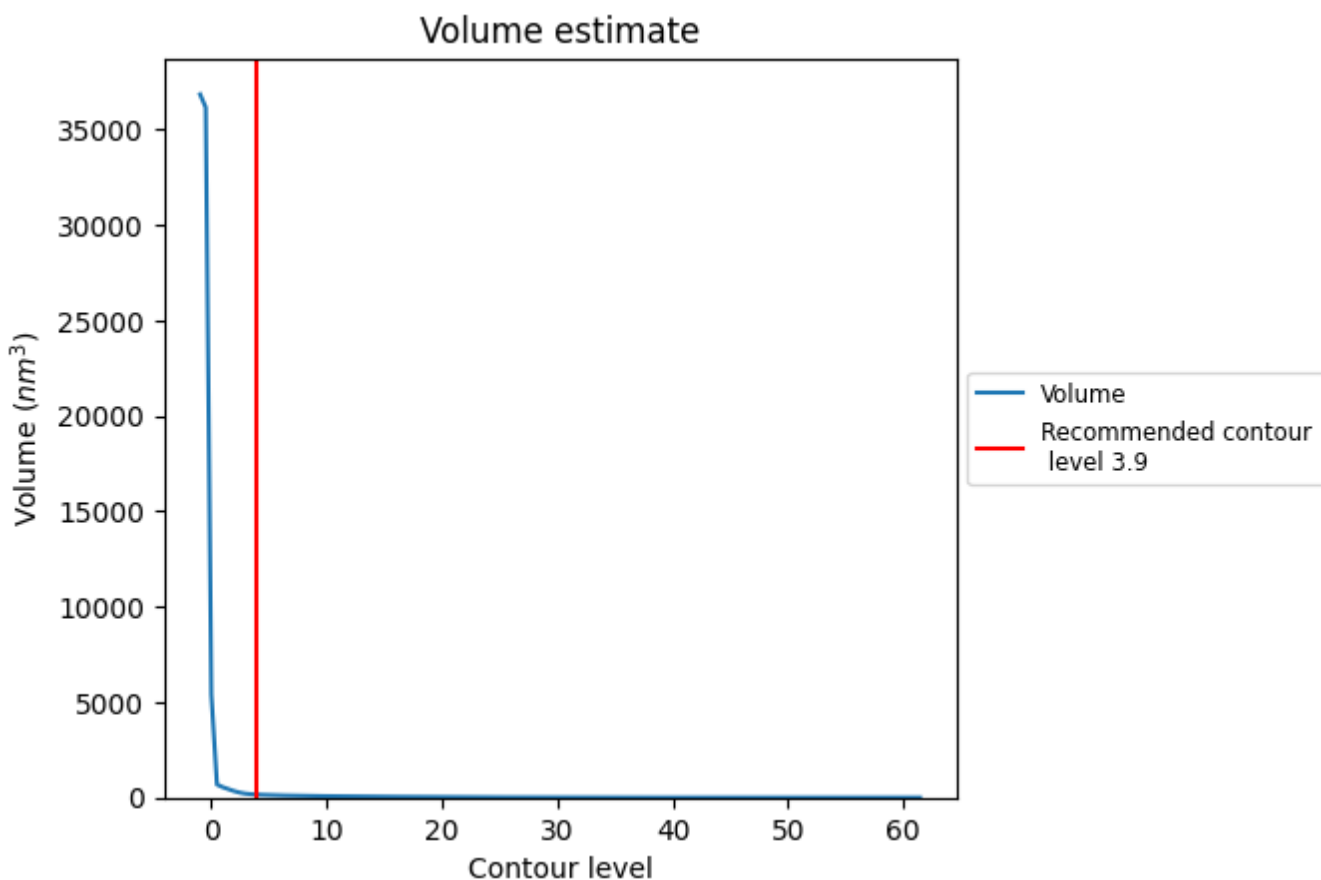
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

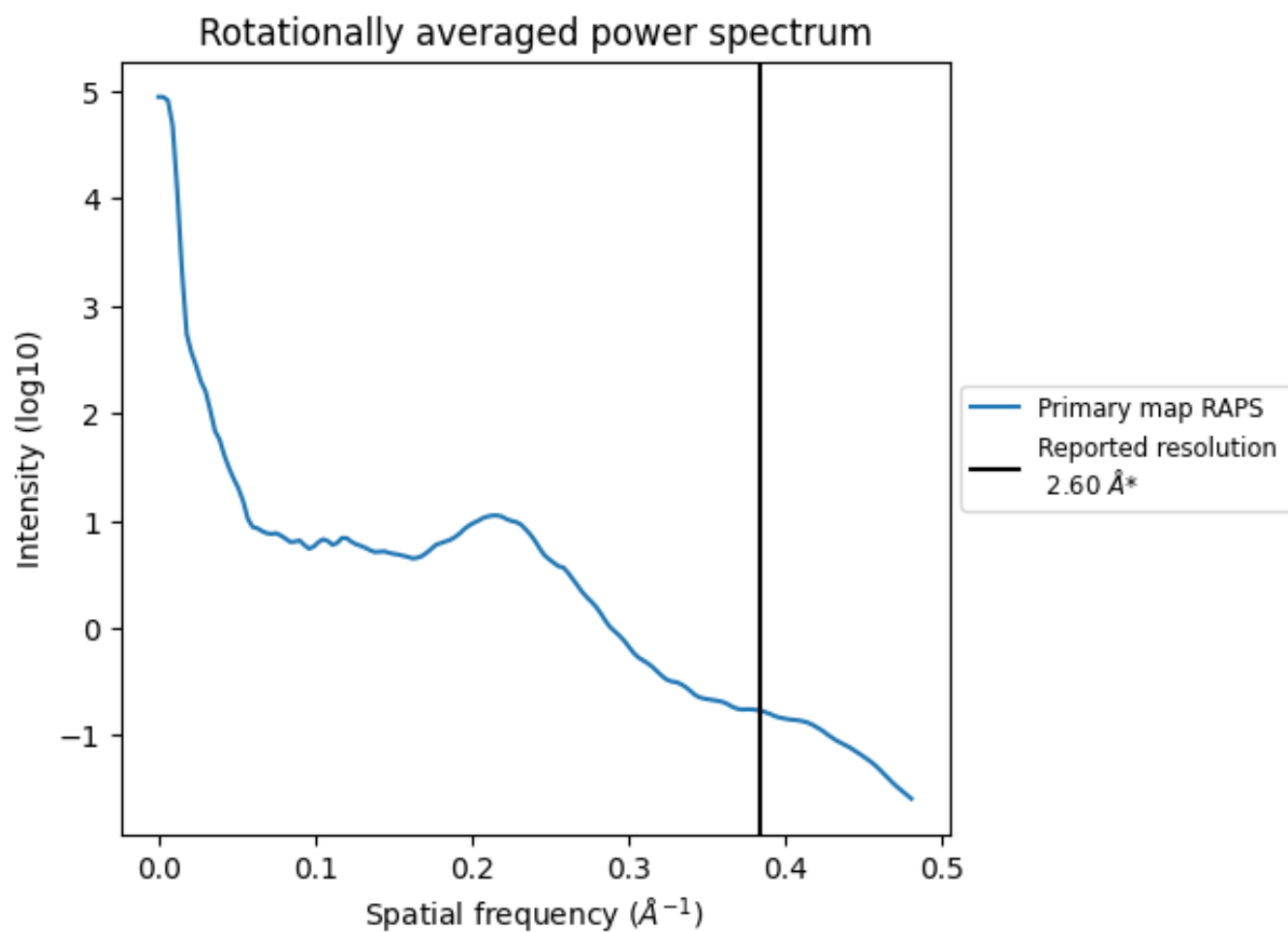
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 158  $\text{nm}^3$ ; this corresponds to an approximate mass of 142 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 [i](#)

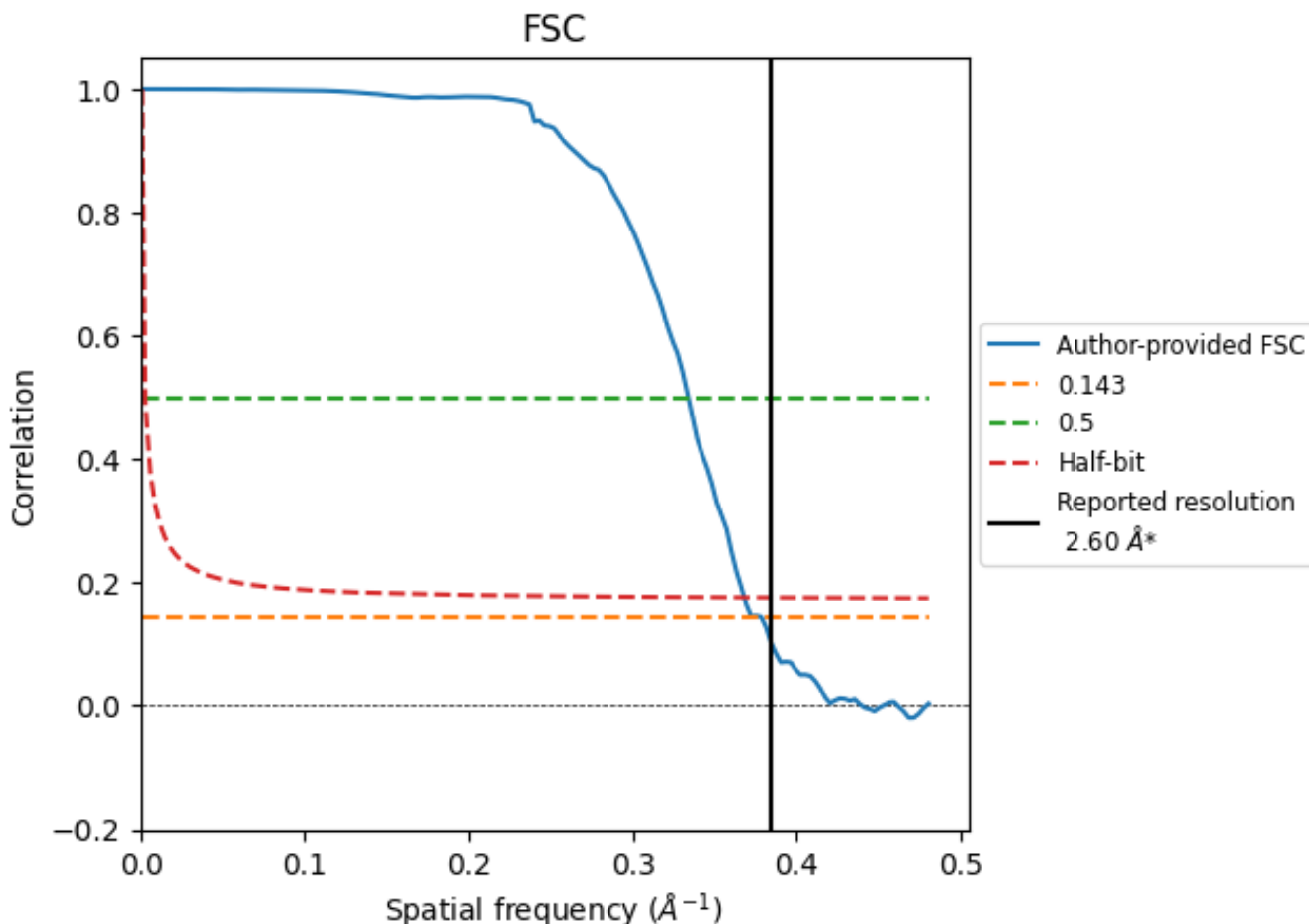


\*Reported resolution corresponds to spatial frequency of 0.385 Å<sup>-1</sup>

## 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 0.385  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

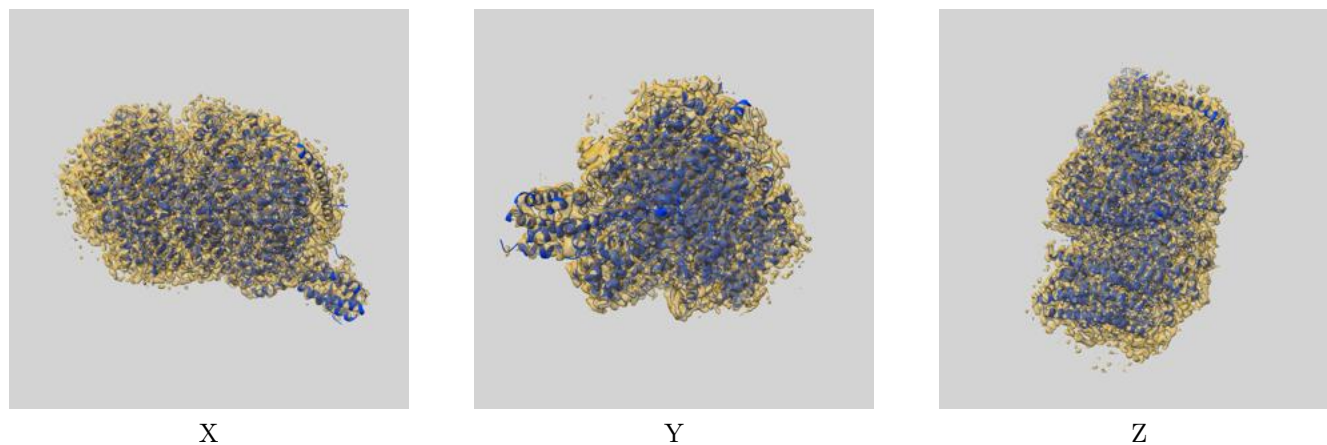
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	2.64	2.99	2.72
Unmasked-calculated*	-	-	-

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

## 9 Map-model fit [i](#)

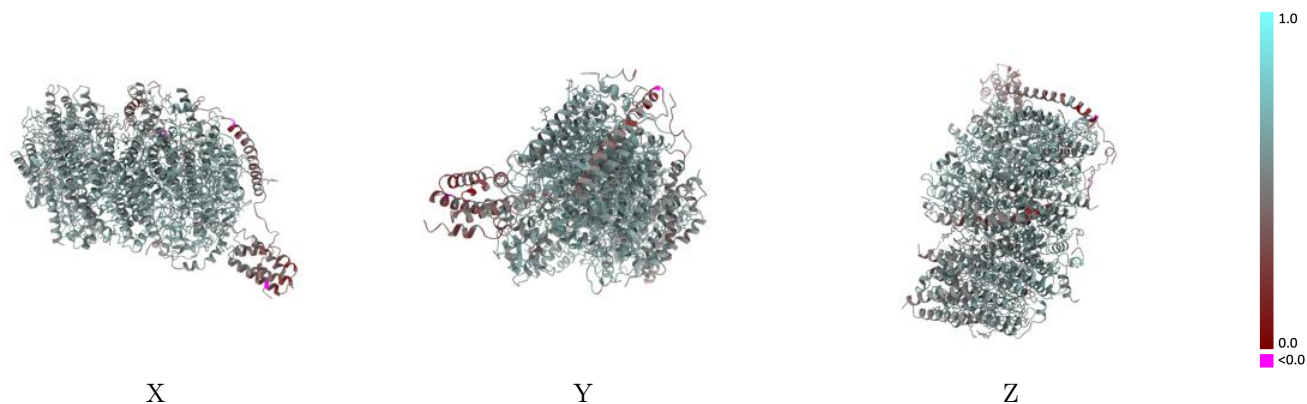
This section contains information regarding the fit between EMDB map EMD-37133 and PDB model 8KDE. Per-residue inclusion information can be found in section 3 on page 18.

### 9.1 Map-model overlay [i](#)



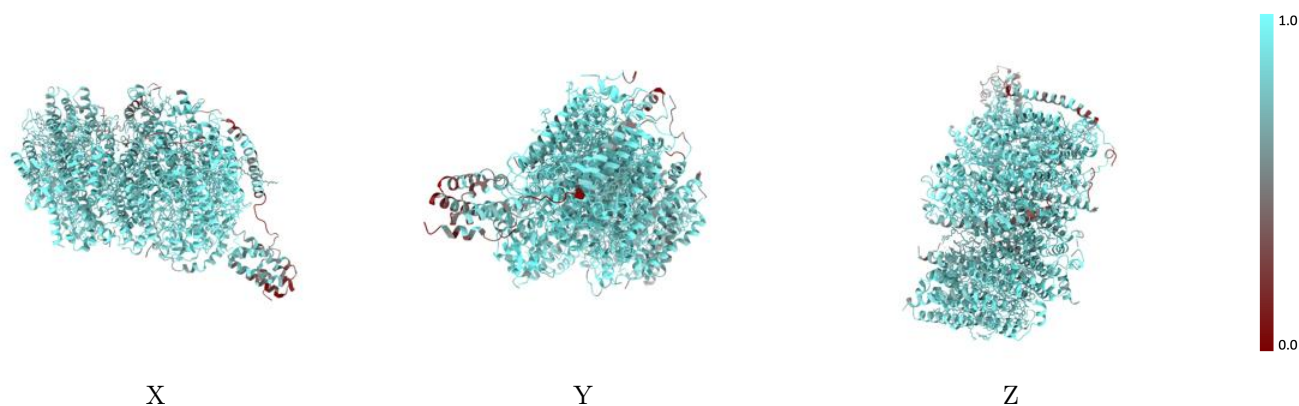
The images above show the 3D surface view of the map at the recommended contour level 3.9 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



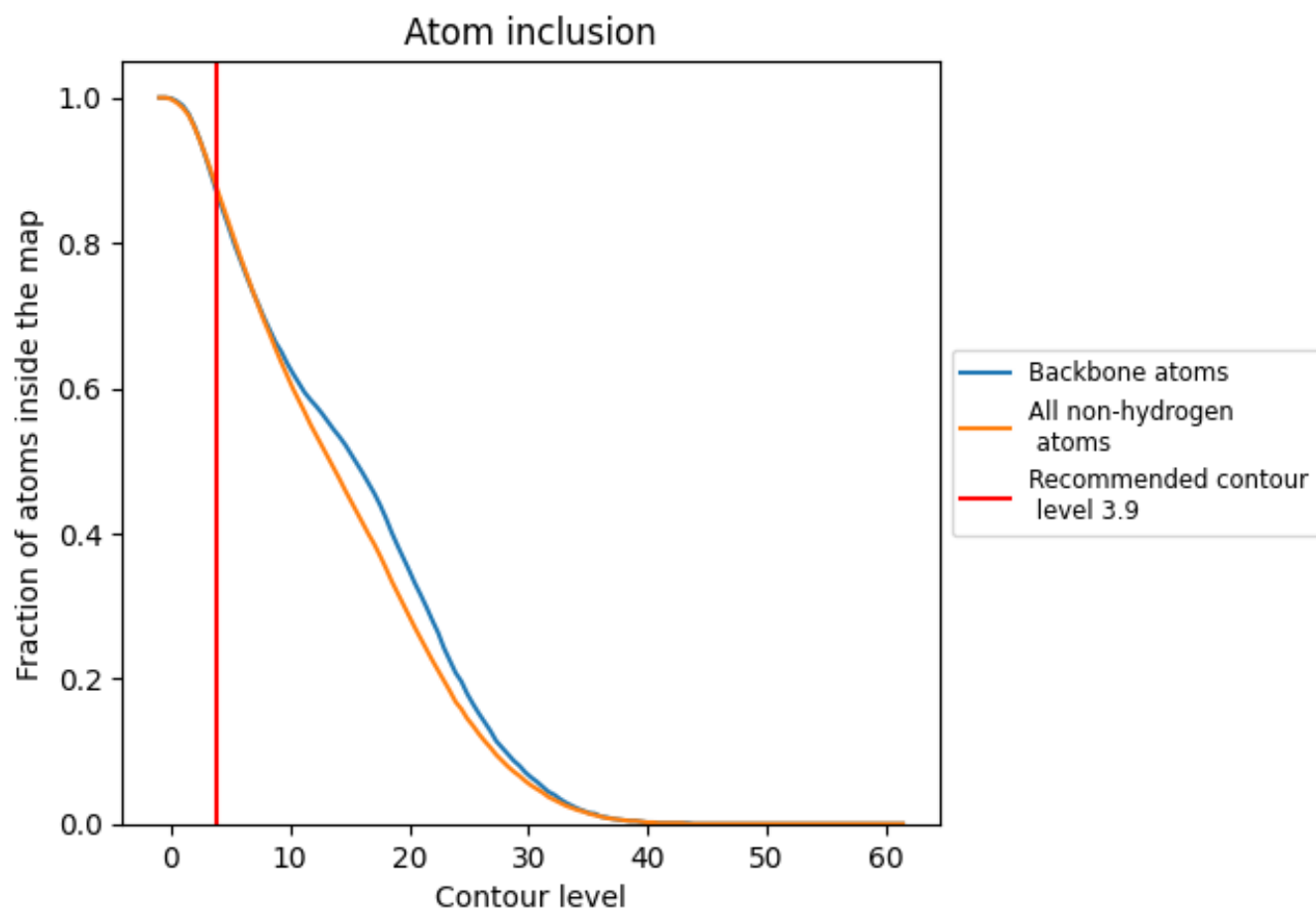
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (3.9).







































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 87% 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 (3.9) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8730	 0.5480
1	 0.6020	 0.3960
3	 0.5530	 0.3920
A	 0.9080	 0.5660
B	 0.9380	 0.5830
C	 0.8950	 0.5590
D	 0.9260	 0.5830
E	 0.8750	 0.5390
F	 0.8670	 0.5110
G	 0.6420	 0.4010
H	 0.8730	 0.5470
I	 0.8820	 0.5470
K	 0.7930	 0.5090
L	 0.8960	 0.5600
M	 0.7760	 0.5220
T	 0.8370	 0.5440
V	 0.7160	 0.4850
X	 0.8510	 0.5440
Z	 0.7860	 0.4900

