



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 24, 2026 – 04:36 PM UTC

PDB ID : 5E7C / pdb_00005e7c
Title : Macromolecular diffractive imaging using imperfect crystals - Bragg data
Authors : Ayer, K.; Yefanov, O.; Oberthuer, D.; Roy-Chowdhury, S.; Galli, L.; Mariani, V.; Basu, S.; Coe, J.; Conrad, C.E.; Fromme, R.; Schaffner, A.; Doerner, K.; James, D.; Kupitz, C.; Metz, M.; Nelson, G.; Xavier, P.L.; Beyerlein, K.R.; Schmidt, M.; Sarrou, I.; Spence, J.C.H.; Weierstall, U.; White, T.A.; Yang, J.-H.; Zhao, Y.; Liang, M.; Aquila, A.; Hunter, M.S.; Robinson, J.S.; Koglin, J.E.; Boutet, S.; Fromme, P.; Barty, A.; Chapman, H.N.
Deposited on : 2015-10-12
Resolution : 4.50 Å(reported)

This is a wwPDB X-ray Structure 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/XrayValidationReportHelp>
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:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12

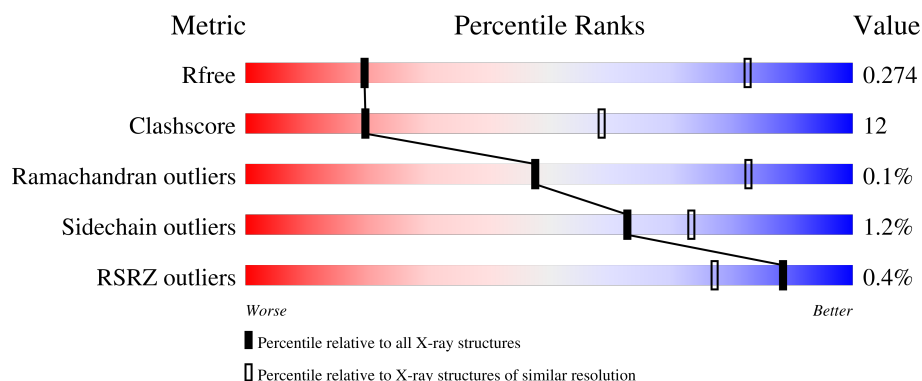
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.50 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1127 (5.10-3.90)
Clashscore	190562	1002 (5.06-3.94)
Ramachandran outliers	187476	1060 (5.10-3.90)
Sidechain outliers	187428	1043 (5.10-3.90)
RSRZ outliers	180081	1122 (5.10-3.90)

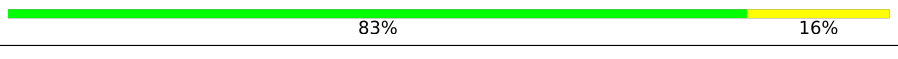
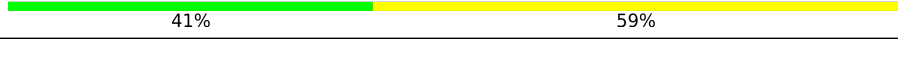
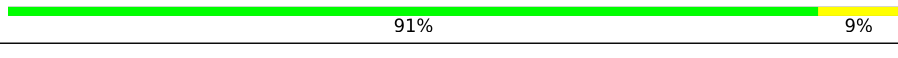
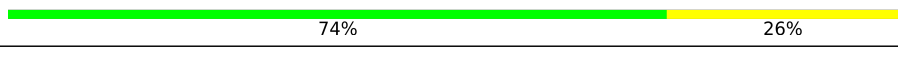
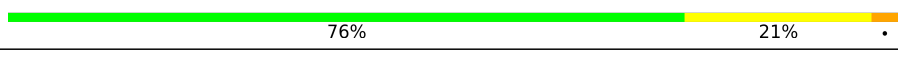
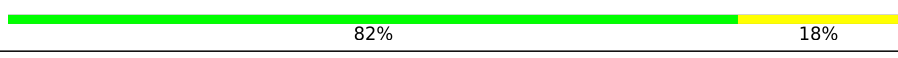
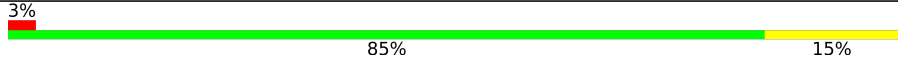
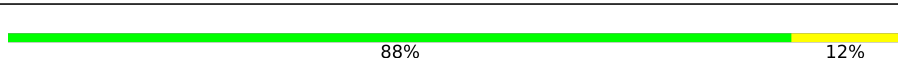
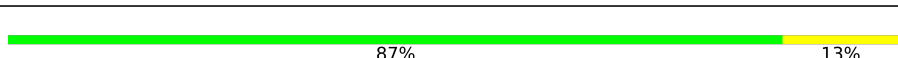
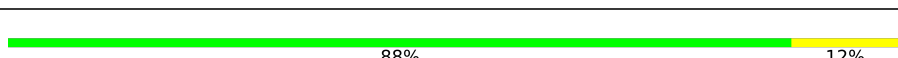
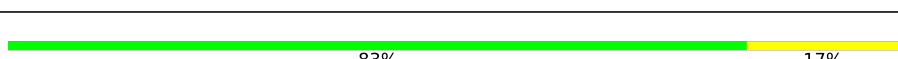
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	334	78% 22%
1	a	334	79% 21%
2	B	504	81% 18% .

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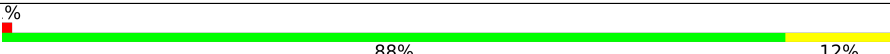
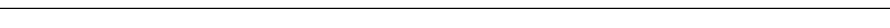
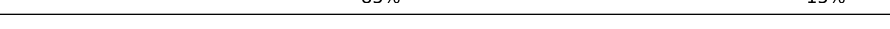
Ideal geometry (proteins) : Engh & Huber (2001)
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Chain	Length	Quality of chain	
2	b	504		%
3	C	451		
3	c	451		
4	D	342		%
4	d	342		2%
5	E	81		
5	e	81		
6	F	34		
6	f	34		
7	H	65		
7	h	65		
8	I	38		
8	i	38		
9	J	38		
9	j	38		
10	K	37		
10	k	37		
11	L	37		
11	l	37		
12	M	34		3%
12	m	34		
13	O	243		
13	o	243		
14	T	30		
14	t	30		

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Mol	Chain	Length	Quality of chain
15	U	97	
15	u	97	
16	V	137	
16	v	137	
17	Y	29	
17	y	29	
18	X	39	
18	x	39	
19	Z	62	
19	z	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
21	CL	u	201	-	-	-	X
22	BCT	A	604	-	X	-	-
22	BCT	a	603	-	X	-	-
23	CLA	A	605	X	-	-	-
23	CLA	A	606	X	-	-	-
23	CLA	A	608	X	-	-	-
23	CLA	B	602	X	-	-	-
23	CLA	B	603	X	-	-	-
23	CLA	B	604	X	-	-	-
23	CLA	B	605	X	-	-	-
23	CLA	B	606	X	-	-	-
23	CLA	B	607[A]	X	-	-	-
23	CLA	B	607[B]	X	-	-	-
23	CLA	B	608	X	-	-	-
23	CLA	B	609	X	-	-	-
23	CLA	B	610	X	-	-	-
23	CLA	B	611	X	-	-	-
23	CLA	B	612	X	-	-	-
23	CLA	B	613	X	-	-	-
23	CLA	B	614	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	B	615	X	-	-	-
23	CLA	B	616	X	-	-	-
23	CLA	B	617	X	-	-	-
23	CLA	C	501	X	-	-	-
23	CLA	C	502	X	-	-	-
23	CLA	C	503	X	-	-	-
23	CLA	C	504	X	-	-	-
23	CLA	C	505	X	-	-	-
23	CLA	C	506	X	-	-	-
23	CLA	C	507	X	-	-	-
23	CLA	C	508	X	-	-	-
23	CLA	C	509	X	-	-	-
23	CLA	C	510	X	-	-	-
23	CLA	C	511	X	-	-	-
23	CLA	C	512	X	-	-	-
23	CLA	C	513	X	-	-	-
23	CLA	D	402	X	-	-	-
23	CLA	D	403	X	-	-	-
23	CLA	D	404	X	-	-	-
23	CLA	a	604	X	-	-	-
23	CLA	a	605	X	-	-	-
23	CLA	a	607	X	-	-	-
23	CLA	a	613	X	-	-	-
23	CLA	b	604	X	-	-	-
23	CLA	b	605	X	-	-	-
23	CLA	b	606	X	-	-	-
23	CLA	b	607	X	-	-	-
23	CLA	b	608	X	-	-	-
23	CLA	b	609[A]	X	-	-	-
23	CLA	b	609[B]	X	-	-	-
23	CLA	b	610	X	-	-	-
23	CLA	b	611	X	-	-	-
23	CLA	b	612	X	-	-	-
23	CLA	b	613	X	-	-	-
23	CLA	b	614	X	-	-	-
23	CLA	b	615	X	-	-	-
23	CLA	b	616	X	-	-	-
23	CLA	b	617	X	-	-	-
23	CLA	b	618	X	-	-	-
23	CLA	b	619	X	-	-	-
23	CLA	c	502	X	-	-	-
23	CLA	c	503	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	c	504	X	-	-	-
23	CLA	c	505	X	-	-	-
23	CLA	c	506	X	-	-	-
23	CLA	c	507	X	-	-	-
23	CLA	c	508	X	-	-	-
23	CLA	c	509	X	-	-	-
23	CLA	c	510	X	-	-	-
23	CLA	c	511	X	-	-	-
23	CLA	c	512	X	-	-	-
23	CLA	c	513	X	-	-	-
23	CLA	c	514	X	-	-	-
23	CLA	d	402	X	-	-	-
23	CLA	d	403	X	-	-	-
25	BCR	A	609	-	X	-	-
25	BCR	B	618	-	X	X	-
25	BCR	B	619	-	X	X	-
25	BCR	B	620	-	X	X	-
25	BCR	C	514	-	X	-	-
25	BCR	C	515	-	X	-	-
25	BCR	C	521	-	X	-	-
25	BCR	F	101	-	X	-	-
25	BCR	H	101	-	X	-	-
25	BCR	K	101	-	X	X	-
25	BCR	T	101	-	X	X	-
25	BCR	a	608	-	X	-	-
25	BCR	b	620	-	X	X	-
25	BCR	b	621	-	X	X	-
25	BCR	b	622	-	X	-	-
25	BCR	c	515	-	X	-	-
25	BCR	c	516	-	X	-	-
25	BCR	c	522	-	X	-	-
25	BCR	f	101	-	X	X	-
25	BCR	h	101	-	X	-	-
25	BCR	k	101	-	X	X	-
25	BCR	t	101	-	X	X	-
26	PL9	A	610	-	X	-	-
26	PL9	D	405	-	X	-	-
26	PL9	a	609	-	X	-	-
26	PL9	d	404	-	X	-	-

2 Entry composition [i](#)

There are 34 unique types of molecules in this entry. The entry contains 49966 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	4	0
			2637	1730	432	460	15			
1	a	334	Total	C	N	O	S	0	4	0
			2637	1730	432	460	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	286	ALA	THR	conflict	UNP P0A444
a	286	ALA	THR	conflict	UNP P0A444

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	504	Total	C	N	O	S	0	10	0
			4024	2641	668	702	13			
2	b	504	Total	C	N	O	S	6	10	0
			4024	2641	668	702	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	451	Total	C	N	O	S	0	5	0
			3506	2296	584	613	13			
3	c	451	Total	C	N	O	S	0	5	0
			3506	2296	584	613	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	342	Total	C	N	O	S	0	0	0
			2726	1805	445	464	12			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	d	342	Total	C	N	O	S	0	0	0
			2726	1805	445	464	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	81	Total	C	N	O		0	2	0
			668	436	107	125				
5	e	81	Total	C	N	O		0	2	0
			668	436	107	125				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	34	Total	C	N	O	S	0	0	0
			275	187	45	42	1			
6	f	34	Total	C	N	O	S	0	0	0
			275	187	45	42	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	65	Total	C	N	O	S	0	2	0
			525	351	86	86	2			
7	h	65	Total	C	N	O	S	0	2	0
			525	351	86	86	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	38	Total	C	N	O	S	0	1	0
			320	215	49	54	2			
8	i	38	Total	C	N	O	S	0	1	0
			320	215	49	54	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	38	Total	C	N	O	S	0	0	0
			272	182	42	47	1			
9	j	38	Total	C	N	O	S	0	0	0
			272	182	42	47	1			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	K	37	Total	C	N	O	0	0	0
			293	204	43	46			
10	k	37	Total	C	N	O	0	0	0
			293	204	43	46			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	L	37	Total	C	N	O	S	0	1	0
			309	207	48	53	1			
11	l	37	Total	C	N	O	S	0	1	0
			309	207	48	53	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	34	Total	C	N	O	S	0	1	0
			272	183	40	48	1			
12	m	34	Total	C	N	O	S	0	1	0
			272	183	40	48	1			

- Molecule 13 is a protein called Photosystem II manganese-stabilizing polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	243	Total	C	N	O	S	0	4	0
			1883	1178	315	385	5			
13	o	243	Total	C	N	O	S	0	4	0
			1883	1178	315	385	5			

- Molecule 14 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	30	Total	C	N	O	S	0	2	0
			270	189	37	41	3			
14	t	30	Total	C	N	O	S	0	2	0
			270	189	37	41	3			

- Molecule 15 is a protein called Photosystem II 12 kDa extrinsic protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	U	97	Total	C	N	O	0	0	0
			774	491	129	154			
15	u	97	Total	C	N	O	0	0	0
			774	491	129	154			

- Molecule 16 is a protein called Cytochrome c-550.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total	C	N	O	S	0	1	0
			1072	680	180	208	4			
16	v	137	Total	C	N	O	S	0	1	0
			1072	680	180	208	4			

- Molecule 17 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Y	29	Total	C	N	O	S	0	0	0
			215	142	37	33	3			
17	y	29	Total	C	N	O	S	0	0	0
			215	142	37	33	3			

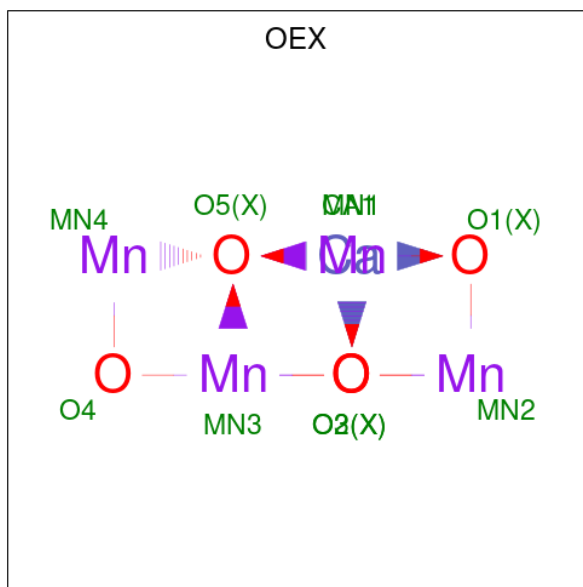
- Molecule 18 is a protein called Photosystem II reaction center X protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	X	39	Total	C	N	O	0	1	0
			292	196	46	50			
18	x	39	Total	C	N	O	0	1	0
			292	196	46	50			

- Molecule 19 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Z	62	Total	C	N	O	S	0	0	0
			479	328	72	77	2			
19	z	62	Total	C	N	O	S	0	0	0
			479	328	72	77	2			

- Molecule 20 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5).

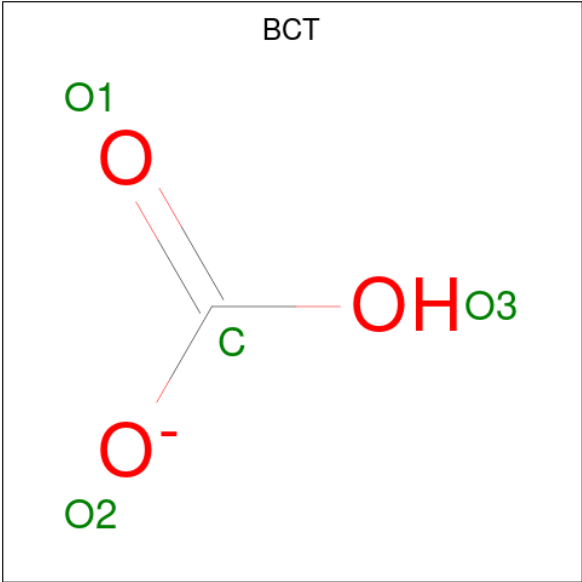


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	A	1	Total	Ca	Mn	O	0	0
			10	1	4	5		
20	a	1	Total	Ca	Mn	O	0	0
			10	1	4	5		

- Molecule 21 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

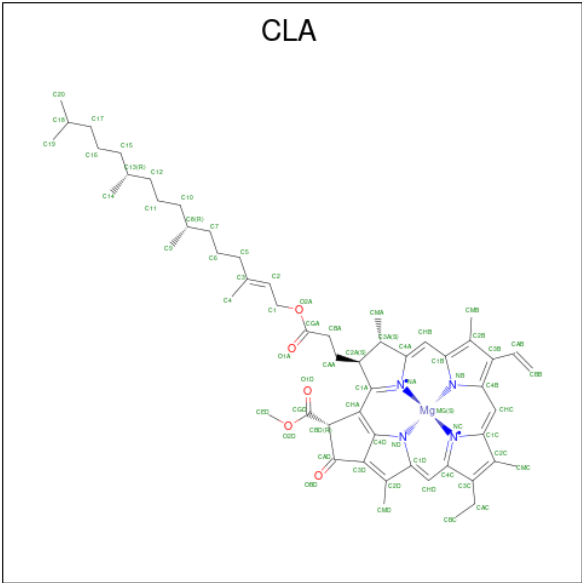
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	A	2	Total	Cl	0	0
			2	2		
21	V	1	Total	Cl	0	0
			1	1		
21	a	1	Total	Cl	0	0
			1	1		
21	c	1	Total	Cl	0	0
			1	1		
21	u	1	Total	Cl	0	0
			1	1		

- Molecule 22 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	A	1	Total 4	C 1	O 3	0	0
22	a	1	Total 4	C 1	O 3	0	0

- Molecule 23 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 130	C 110	Mg 2	N 8	O 10	0	1
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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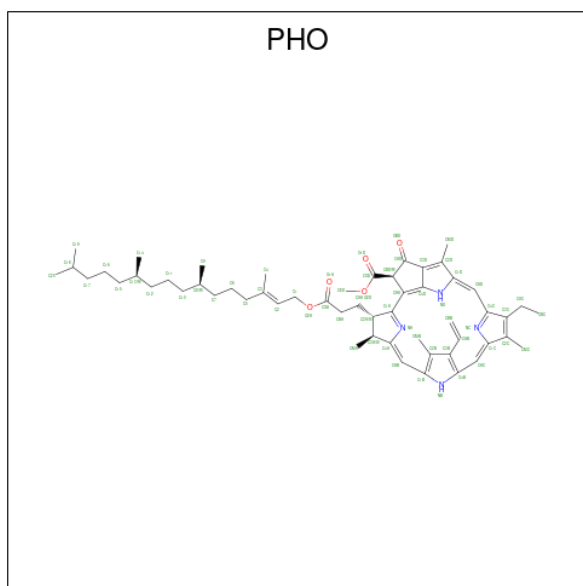
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	b	1	Total	C	Mg	N	O	0	1
			130	110	2	8	10		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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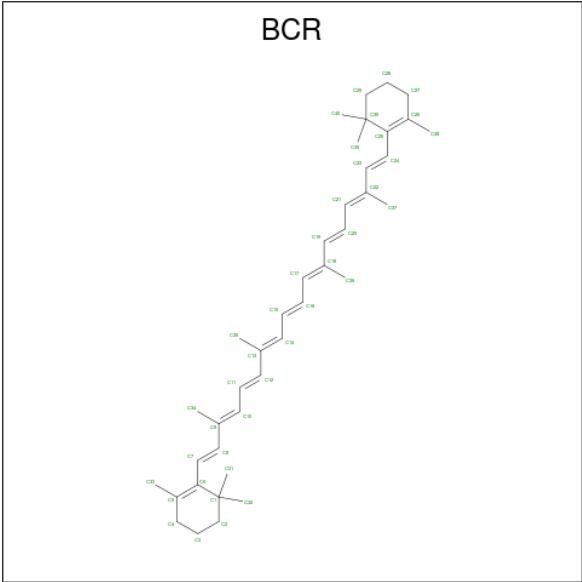
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 24 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



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

- Molecule 25 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



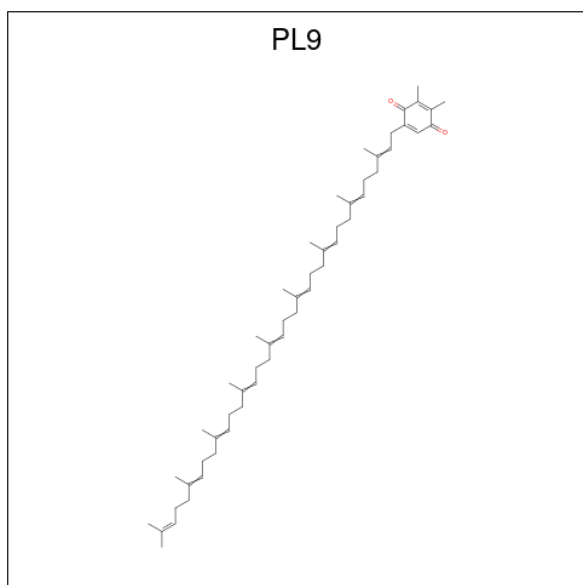
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	F	1	Total C 40 40	0	0
25	H	1	Total C 40 40	0	0
25	K	1	Total C 40 40	0	0
25	T	1	Total C 40 40	0	0
25	a	1	Total C 40 40	0	0
25	b	1	Total C 40 40	0	0
25	b	1	Total C 40 40	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	b	1	Total C 40 40	0	0
25	c	1	Total C 40 40	0	0
25	c	1	Total C 40 40	0	0
25	c	1	Total C 40 40	0	0
25	f	1	Total C 40 40	0	0
25	h	1	Total C 40 40	0	0
25	k	1	Total C 40 40	0	0
25	t	1	Total C 40 40	0	0

- Molecule 26 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).



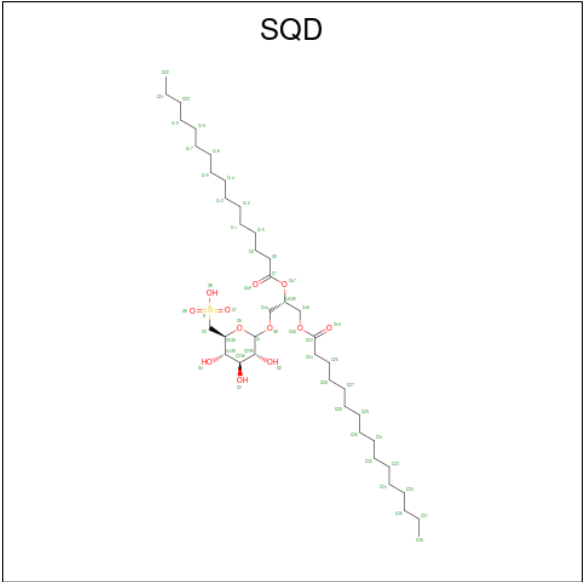
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C O 55 53 2	0	0
26	D	1	Total C O 55 53 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	a	1	Total	C	O	0	0
			55	53	2		
26	d	1	Total	C	O	0	0
			55	53	2		

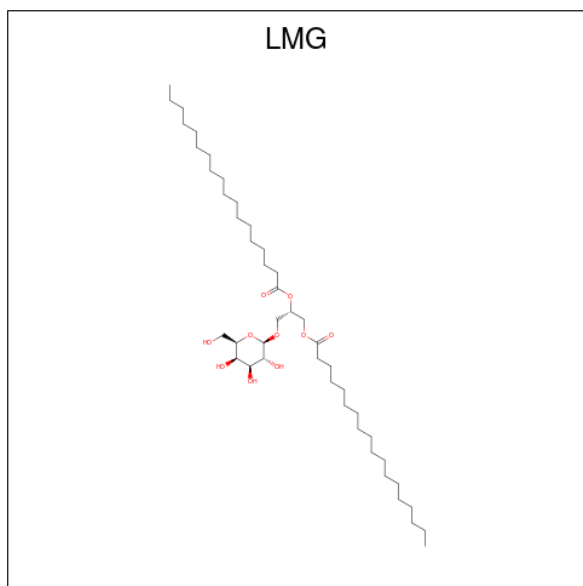
- Molecule 27 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	A	1	Total	C	O	S	0	0
			54	41	12	1		
27	B	1	Total	C	O	S	0	0
			54	41	12	1		
27	X	1	Total	C	O	S	0	0
			43	30	12	1		
27	a	1	Total	C	O	S	0	0
			54	41	12	1		
27	a	1	Total	C	O	S	0	0
			54	41	12	1		
27	b	1	Total	C	O	S	0	0
			54	41	12	1		
27	b	1	Total	C	O	S	0	0
			54	41	12	1		
27	x	1	Total	C	O	S	0	0
			43	30	12	1		

- Molecule 28 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID:

LMG) (formula: C₄₅H₈₆O₁₀).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	A	1	Total	C	O	0	0
			51	41	10		
28	B	1	Total	C	O	0	0
			51	41	10		
28	C	1	Total	C	O	0	0
			51	41	10		
28	C	1	Total	C	O	0	0
			51	41	10		
28	J	1	Total	C	O	0	0
			51	41	10		
28	Z	1	Total	C	O	0	0
			37	27	10		
28	a	1	Total	C	O	0	0
			51	41	10		
28	b	1	Total	C	O	0	0
			51	41	10		
28	c	1	Total	C	O	0	0
			51	41	10		
28	c	1	Total	C	O	0	0
			51	41	10		
28	j	1	Total	C	O	0	0
			51	41	10		
28	z	1	Total	C	O	0	0
			37	27	10		

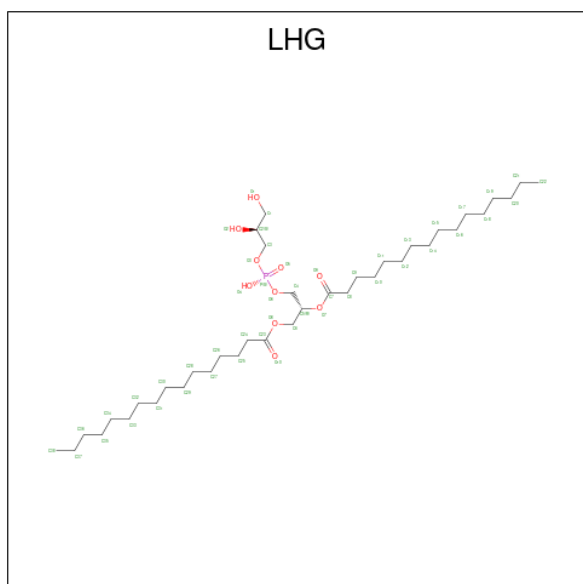
- Molecule 29 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	A	1	Total	Fe	0	0
			1	1		
29	a	1	Total	Fe	0	0
			1	1		

- Molecule 30 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	B	1	Total	Ca	0	0
			1	1		
30	F	1	Total	Ca	0	0
			1	1		
30	O	1	Total	Ca	0	0
			1	1		
30	b	1	Total	Ca	0	0
			1	1		
30	f	1	Total	Ca	0	0
			1	1		
30	o	1	Total	Ca	0	0
			1	1		

- Molecule 31 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



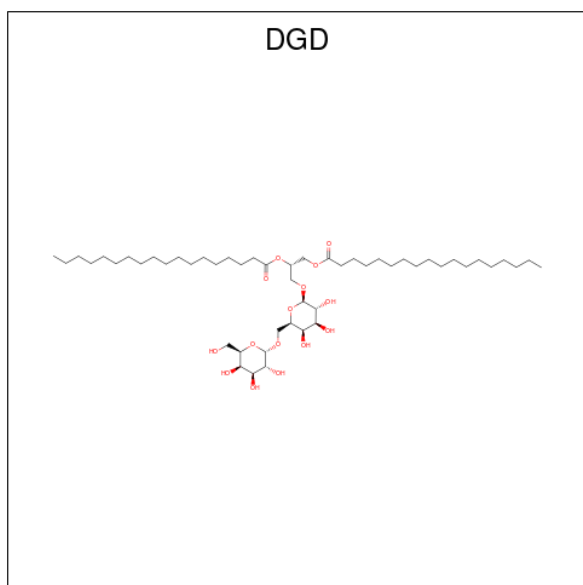
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	B	1	Total	C	O	P	0	0
			49	38	10	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	D	1	Total	C	O	P	0	0
			49	38	10	1		
31	D	1	Total	C	O	P	0	0
			49	38	10	1		
31	E	1	Total	C	O	P	0	0
			42	31	10	1		
31	L	1	Total	C	O	P	0	0
			49	38	10	1		
31	a	1	Total	C	O	P	0	0
			49	38	10	1		
31	b	1	Total	C	O	P	0	0
			49	38	10	1		
31	d	1	Total	C	O	P	0	0
			49	38	10	1		
31	e	1	Total	C	O	P	0	0
			42	31	10	1		
31	l	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 32 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	C	1	Total	C	O	0	0
			62	47	15		
32	C	1	Total	C	O	0	0
			62	47	15		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	C	1	Total 62	C 47	O 15	0	0
32	D	1	Total 62	C 47	O 15	0	0
32	H	1	Total 62	C 47	O 15	0	0
32	c	1	Total 62	C 47	O 15	0	0
32	c	1	Total 62	C 47	O 15	0	0
32	c	1	Total 62	C 47	O 15	0	0
32	d	1	Total 62	C 47	O 15	0	0
32	h	1	Total 62	C 47	O 15	0	0

- # HEM

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



WORLD WIDE
PDB
PROTEIN DATA BANK

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
33	v	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

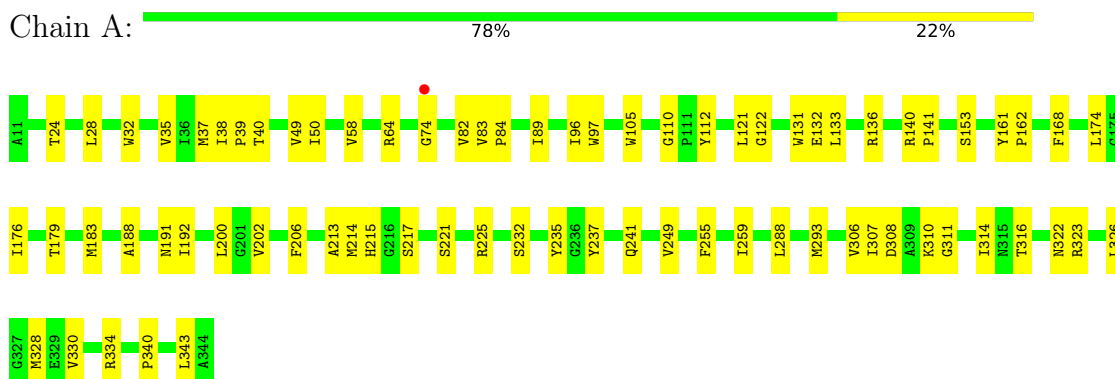
- Molecule 34 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	J	1	Total	Mg	0	0
			1	1		
34	j	1	Total	Mg	0	0
			1	1		

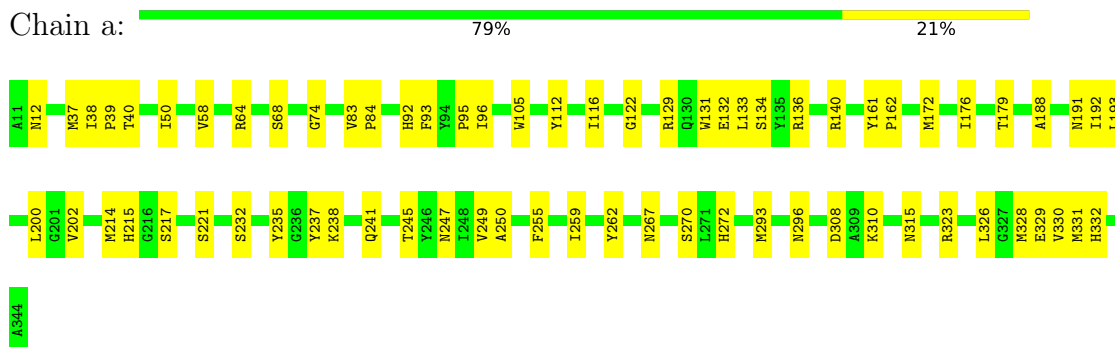
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

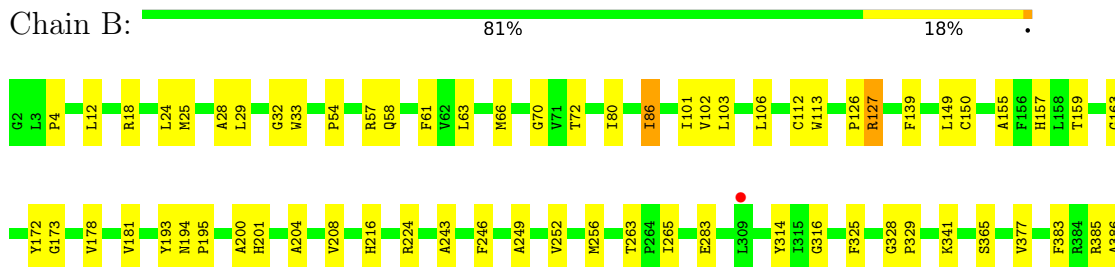
- Molecule 1: Photosystem II protein D1 1



- Molecule 1: Photosystem II protein D1 1

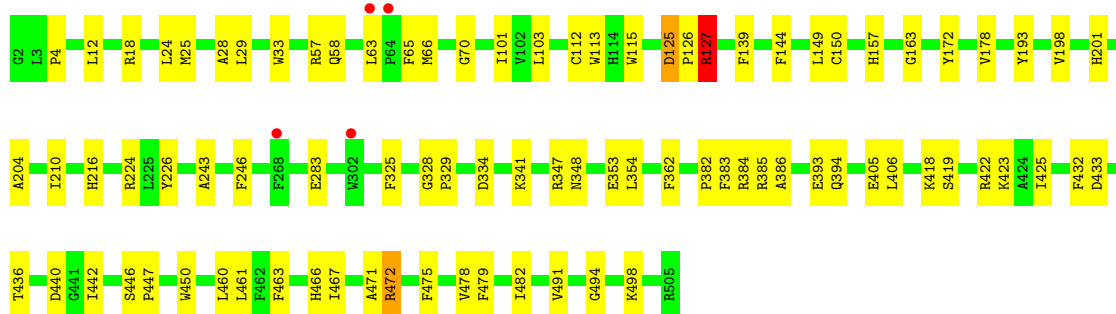
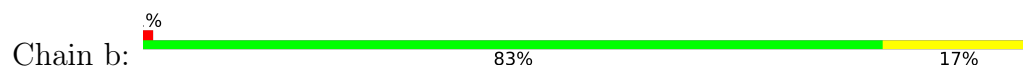


- Molecule 2: Photosystem II CP47 reaction center protein

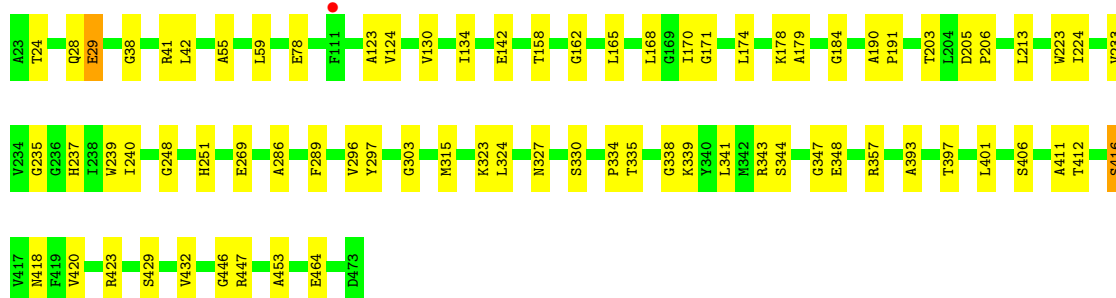
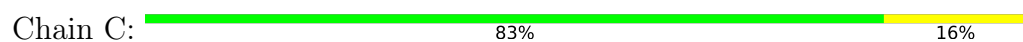




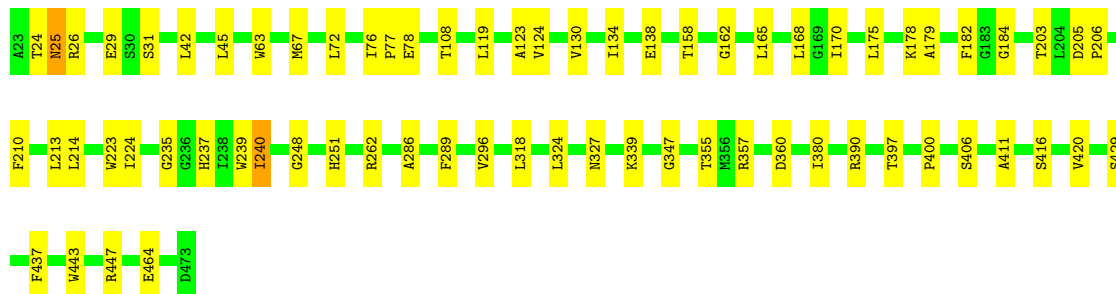
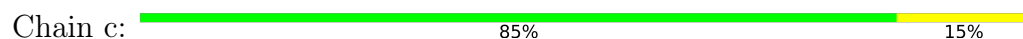
• Molecule 2: Photosystem II CP47 reaction center protein



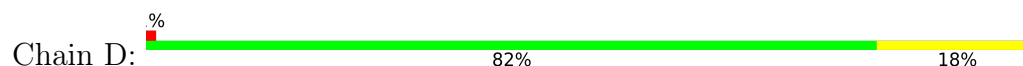
• Molecule 3: Photosystem II CP43 reaction center protein

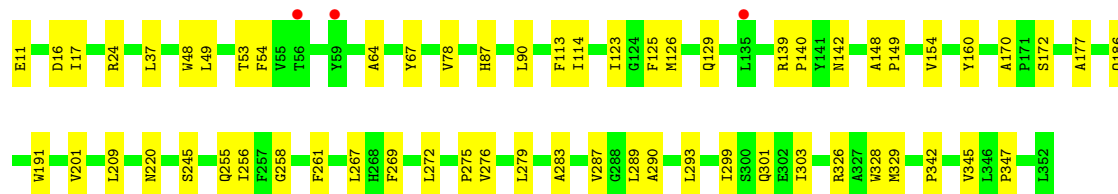


• Molecule 3: Photosystem II CP43 reaction center protein

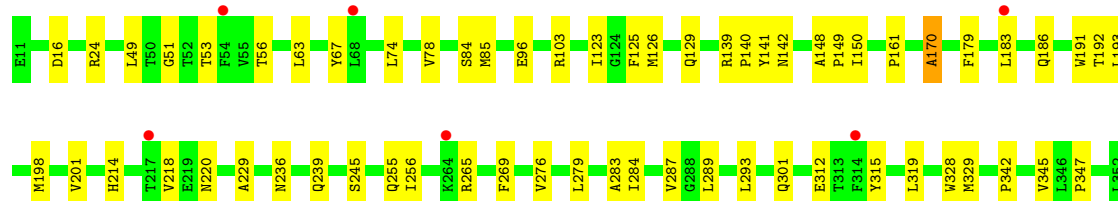
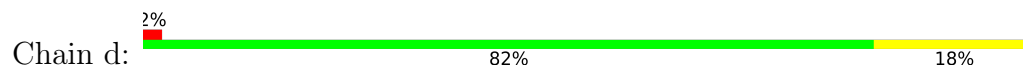


• Molecule 4: Photosystem II D2 protein

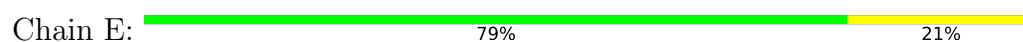




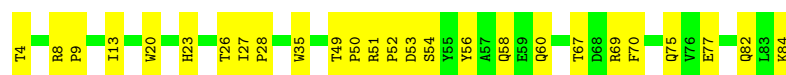
• Molecule 4: Photosystem II D2 protein



• Molecule 5: Cytochrome b559 subunit alpha



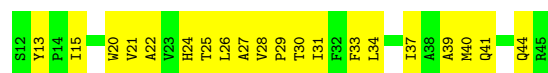
• Molecule 5: Cytochrome b559 subunit alpha



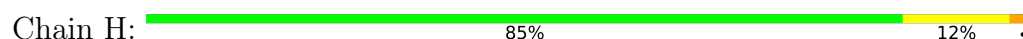
• Molecule 6: Cytochrome b559 subunit beta



• Molecule 6: Cytochrome b559 subunit beta



• Molecule 7: Photosystem II reaction center protein H





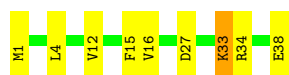
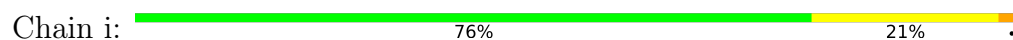
- Molecule 7: Photosystem II reaction center protein H



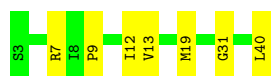
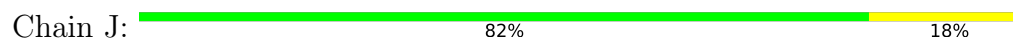
- Molecule 8: Photosystem II reaction center protein I



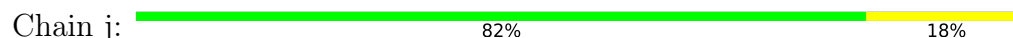
- Molecule 8: Photosystem II reaction center protein I



- Molecule 9: Photosystem II reaction center protein J



- Molecule 9: Photosystem II reaction center protein J

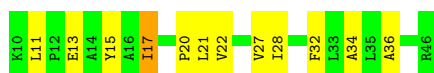


- Molecule 10: Photosystem II reaction center protein K



- Molecule 10: Photosystem II reaction center protein K





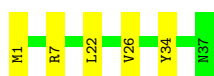
- Molecule 11: Photosystem II reaction center protein L

Chain L: 84% 16%



- Molecule 11: Photosystem II reaction center protein L

Chain l: 86% 14%



- Molecule 12: Photosystem II reaction center protein M

Chain M: 3% 85% 15%



- Molecule 12: Photosystem II reaction center protein M

Chain m: 88% 12%



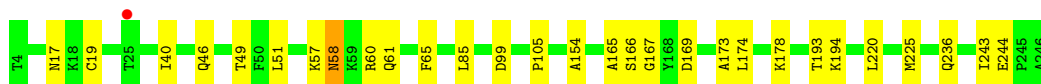
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O: 87% 13%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o: 88% 12%

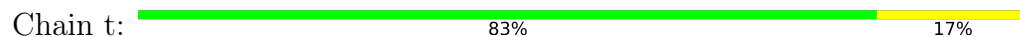


- Molecule 14: Photosystem II reaction center protein T

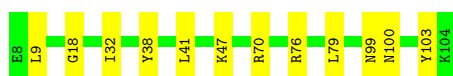
Chain T: 83% 17%



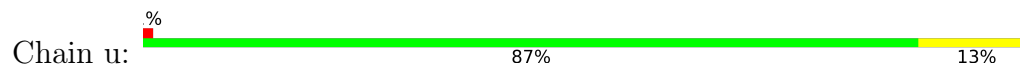
- Molecule 14: Photosystem II reaction center protein T



- Molecule 15: Photosystem II 12 kDa extrinsic protein



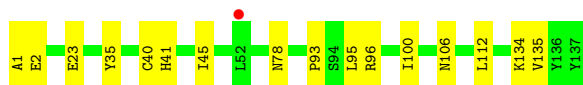
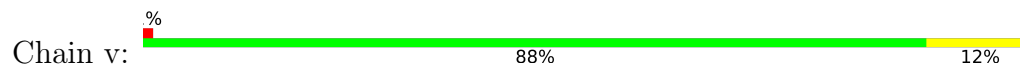
- Molecule 15: Photosystem II 12 kDa extrinsic protein



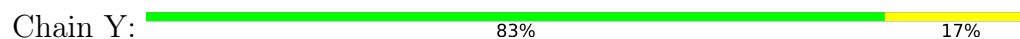
- Molecule 16: Cytochrome c-550



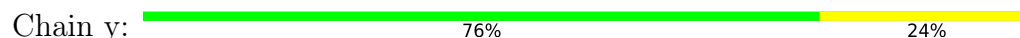
- Molecule 16: Cytochrome c-550



- Molecule 17: Photosystem II reaction center protein Ycf12



- Molecule 17: Photosystem II reaction center protein Ycf12





- Molecule 18: Photosystem II reaction center X protein

Chain X: 85% 15%



- Molecule 18: Photosystem II reaction center X protein

Chain x: 77% 23%



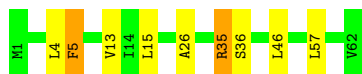
- Molecule 19: Photosystem II reaction center protein Z

Chain Z: 92% 8%



- Molecule 19: Photosystem II reaction center protein Z

Chain z: 85% 11% .



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	133.25Å 226.26Å 307.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.93 – 4.50 29.93 – 4.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.93-4.50) 99.5 (29.93-4.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 4.44Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.246 , 0.275 0.254 , 0.274	Depositor DCC
R_{free} test set	2721 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	211.4	Xtriage
Anisotropy	0.314	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 11.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	49966	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.74% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CLA, PL9, DGD, CL, FE2, LMG, LHG, BCT, HEM, SQD, PHO, CA, MG, OEX, BCR

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.43	0/2734	0.84	0/3727
1	a	0.44	0/2734	0.84	0/3727
2	B	0.38	0/4194	0.80	5/5713 (0.1%)
2	b	0.40	0/4194	0.83	6/5713 (0.1%)
3	C	0.39	0/3634	0.82	0/4947
3	c	0.41	0/3634	0.84	3/4947 (0.1%)
4	D	0.37	0/2821	0.79	3/3844 (0.1%)
4	d	0.38	0/2821	0.79	2/3844 (0.1%)
5	E	0.42	0/693	0.79	0/944
5	e	0.42	0/693	0.86	0/944
6	F	0.54	0/284	0.82	0/387
6	f	0.61	0/284	1.39	4/387 (1.0%)
7	H	0.38	0/544	0.80	1/739 (0.1%)
7	h	0.39	0/544	0.81	0/739
8	I	0.38	0/327	0.82	0/439
8	i	0.39	0/327	0.91	1/439 (0.2%)
9	J	0.36	0/278	0.84	0/376
9	j	0.39	0/278	0.84	0/376
10	K	0.44	0/303	0.86	0/416
10	k	0.44	0/303	0.82	0/416
11	L	0.36	0/319	0.76	0/433
11	l	0.36	0/319	0.74	0/433
12	M	0.46	0/278	0.90	0/378
12	m	0.45	0/278	0.88	0/378
13	O	0.36	0/1926	0.77	0/2611
13	o	0.39	0/1926	0.84	2/2611 (0.1%)
14	T	0.36	0/282	0.76	0/382
14	t	0.39	0/282	0.77	0/382
15	U	0.35	0/785	0.74	0/1064
15	u	0.39	0/785	0.84	0/1064
16	V	0.39	0/1096	0.78	0/1487
16	v	0.38	0/1096	0.87	1/1487 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	Y	0.44	0/216	0.85	0/289
17	y	0.50	0/216	1.01	0/289
18	X	0.38	0/298	0.79	0/403
18	x	0.45	0/298	0.89	0/403
19	Z	0.44	0/490	0.89	0/669
19	z	0.56	0/490	1.10	2/669 (0.3%)
All	All	0.40	0/43004	0.83	30/58496 (0.1%)

There are no bond length outliers.

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	f	15	ILE	CA-C-N	-9.18	110.91	122.84
6	f	15	ILE	C-N-CA	-9.18	110.91	122.84
19	z	35	ARG	CB-CG-CD	7.49	128.53	111.30
19	z	5	PHE	N-CA-C	6.30	117.81	111.07
16	v	35	TYR	N-CA-C	5.99	117.48	111.07

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	A	2637	0	2551	69	0
1	a	2637	0	2551	60	0
2	B	4024	0	3901	91	0
2	b	4024	0	3901	83	0
3	C	3506	0	3439	70	0
3	c	3506	0	3439	60	0
4	D	2726	0	2627	52	0
4	d	2726	0	2627	61	0
5	E	668	0	658	14	0
5	e	668	0	658	24	0
6	F	275	0	282	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	f	275	0	282	19	0
7	H	525	0	558	9	0
7	h	525	0	558	6	0
8	I	320	0	339	10	0
8	i	320	0	339	8	0
9	J	272	0	279	7	0
9	j	272	0	279	6	0
10	K	293	0	305	11	0
10	k	293	0	305	12	0
11	L	309	0	327	6	0
11	l	309	0	327	6	0
12	M	272	0	300	5	0
12	m	272	0	300	6	0
13	O	1883	0	1865	26	0
13	o	1883	0	1865	22	0
14	T	270	0	278	8	0
14	t	270	0	278	9	0
15	U	774	0	773	11	0
15	u	774	0	773	11	0
16	V	1072	0	1088	13	0
16	v	1072	0	1088	12	0
17	Y	215	0	246	9	0
17	y	215	0	246	9	0
18	X	292	0	328	8	0
18	x	292	0	328	9	0
19	Z	479	0	516	3	0
19	z	479	0	516	4	0
20	A	10	0	0	1	0
20	a	10	0	0	1	0
21	A	2	0	0	0	0
21	V	1	0	0	0	0
21	a	1	0	0	0	0
21	c	1	0	0	0	0
21	u	1	0	0	0	0
22	A	4	0	1	0	0
22	a	4	0	1	0	0
23	A	195	0	216	15	0
23	B	1105	0	1224	53	0
23	C	845	0	936	46	0
23	D	195	0	216	7	0
23	a	260	0	288	13	0
23	b	1105	0	1224	49	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	c	845	0	936	40	0
23	d	130	0	144	7	0
24	A	64	0	74	1	0
24	D	64	0	74	8	0
24	a	64	0	74	0	0
24	d	64	0	74	6	0
25	A	40	0	55	16	0
25	B	120	0	165	74	0
25	C	120	0	164	44	0
25	F	40	0	54	16	0
25	H	40	0	55	10	0
25	K	40	0	55	25	0
25	T	40	0	55	28	0
25	a	40	0	55	14	0
25	b	120	0	165	71	0
25	c	120	0	165	48	0
25	f	40	0	55	24	0
25	h	40	0	55	15	0
25	k	40	0	55	22	0
25	t	40	0	55	30	0
26	A	55	0	80	16	0
26	D	55	0	80	6	0
26	a	55	0	80	10	0
26	d	55	0	80	3	0
27	A	54	0	78	4	0
27	B	54	0	78	9	0
27	X	43	0	53	3	0
27	a	108	0	156	3	0
27	b	108	0	156	15	0
27	x	43	0	53	4	0
28	A	51	0	72	2	0
28	B	51	0	72	4	0
28	C	102	0	144	1	0
28	J	51	0	72	3	0
28	Z	37	0	44	1	0
28	a	51	0	72	2	0
28	b	51	0	72	3	0
28	c	102	0	144	1	0
28	j	51	0	72	3	0
28	z	37	0	44	2	0
29	A	1	0	0	0	0
29	a	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	B	1	0	0	0	0
30	F	1	0	0	0	0
30	O	1	0	0	0	0
30	b	1	0	0	0	0
30	f	1	0	0	0	0
30	o	1	0	0	0	0
31	B	49	0	74	3	0
31	D	98	0	148	11	0
31	E	42	0	57	0	0
31	L	49	0	74	2	0
31	a	49	0	74	8	0
31	b	49	0	74	4	0
31	d	49	0	74	1	0
31	e	42	0	57	4	0
31	l	49	0	74	4	0
32	C	186	0	246	8	0
32	D	62	0	82	1	0
32	H	62	0	82	5	0
32	c	186	0	246	8	0
32	d	62	0	82	2	0
32	h	62	0	82	3	0
33	E	43	0	30	3	0
33	V	43	0	30	4	0
33	e	43	0	30	3	0
33	v	43	0	30	1	0
34	J	1	0	0	0	0
34	j	1	0	0	0	0
All	All	49966	0	51358	1169	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 12.

The worst 5 of 1169 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)
25:b:620:BCR:C19	25:b:620:BCR:C20	1.74	1.66
25:b:622:BCR:C19	25:b:622:BCR:C20	1.75	1.64
25:c:516:BCR:C20	25:c:516:BCR:C19	1.74	1.64
25:T:101:BCR:C16	25:T:101:BCR:C17	1.75	1.64
25:k:101:BCR:C19	25:k:101:BCR:C20	1.75	1.64

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	336/334 (101%)	332 (99%)	3 (1%)	1 (0%)	36	71
1	a	336/334 (101%)	330 (98%)	5 (2%)	1 (0%)	36	71
2	B	512/504 (102%)	507 (99%)	5 (1%)	0	100	100
2	b	512/504 (102%)	503 (98%)	9 (2%)	0	100	100
3	C	454/451 (101%)	443 (98%)	9 (2%)	2 (0%)	30	67
3	c	454/451 (101%)	441 (97%)	11 (2%)	2 (0%)	30	67
4	D	340/342 (99%)	332 (98%)	8 (2%)	0	100	100
4	d	340/342 (99%)	333 (98%)	7 (2%)	0	100	100
5	E	81/81 (100%)	80 (99%)	1 (1%)	0	100	100
5	e	81/81 (100%)	80 (99%)	1 (1%)	0	100	100
6	F	32/34 (94%)	32 (100%)	0	0	100	100
6	f	32/34 (94%)	32 (100%)	0	0	100	100
7	H	65/65 (100%)	60 (92%)	5 (8%)	0	100	100
7	h	65/65 (100%)	57 (88%)	8 (12%)	0	100	100
8	I	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
8	i	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
9	J	36/38 (95%)	36 (100%)	0	0	100	100
9	j	36/38 (95%)	36 (100%)	0	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100
10	k	35/37 (95%)	35 (100%)	0	0	100	100
11	L	36/37 (97%)	36 (100%)	0	0	100	100
11	l	36/37 (97%)	36 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	M	33/34 (97%)	33 (100%)	0	0	100	100
12	m	33/34 (97%)	33 (100%)	0	0	100	100
13	O	245/243 (101%)	237 (97%)	7 (3%)	1 (0%)	30	67
13	o	245/243 (101%)	235 (96%)	9 (4%)	1 (0%)	30	67
14	T	29/30 (97%)	28 (97%)	1 (3%)	0	100	100
14	t	29/30 (97%)	29 (100%)	0	0	100	100
15	U	95/97 (98%)	93 (98%)	2 (2%)	0	100	100
15	u	95/97 (98%)	93 (98%)	2 (2%)	0	100	100
16	V	136/137 (99%)	132 (97%)	4 (3%)	0	100	100
16	v	136/137 (99%)	131 (96%)	5 (4%)	0	100	100
17	Y	27/29 (93%)	27 (100%)	0	0	100	100
17	y	27/29 (93%)	27 (100%)	0	0	100	100
18	X	38/39 (97%)	37 (97%)	1 (3%)	0	100	100
18	x	38/39 (97%)	37 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
19	z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
All	All	5252/5264 (100%)	5134 (98%)	110 (2%)	8 (0%)	48	77

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	O	58	ASN
13	o	58	ASN
3	C	416[A]	SER
3	C	416[B]	SER
3	c	416[A]	SER

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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	273/269 (102%)	273 (100%)	0	100	100
1	a	273/269 (102%)	272 (100%)	1 (0%)	84	82
2	B	412/402 (102%)	408 (99%)	4 (1%)	68	76
2	b	412/402 (102%)	409 (99%)	3 (1%)	76	79
3	C	357/352 (101%)	352 (99%)	5 (1%)	59	71
3	c	357/352 (101%)	353 (99%)	4 (1%)	65	74
4	D	277/277 (100%)	275 (99%)	2 (1%)	76	79
4	d	277/277 (100%)	276 (100%)	1 (0%)	84	82
5	E	74/72 (103%)	73 (99%)	1 (1%)	59	71
5	e	74/72 (103%)	74 (100%)	0	100	100
6	F	28/28 (100%)	27 (96%)	1 (4%)	31	52
6	f	28/28 (100%)	27 (96%)	1 (4%)	31	52
7	H	56/54 (104%)	53 (95%)	3 (5%)	20	42
7	h	56/54 (104%)	54 (96%)	2 (4%)	31	52
8	I	36/35 (103%)	36 (100%)	0	100	100
8	i	36/35 (103%)	36 (100%)	0	100	100
9	J	26/26 (100%)	26 (100%)	0	100	100
9	j	26/26 (100%)	26 (100%)	0	100	100
10	K	30/30 (100%)	28 (93%)	2 (7%)	15	37
10	k	30/30 (100%)	28 (93%)	2 (7%)	15	37
11	L	36/35 (103%)	35 (97%)	1 (3%)	38	59
11	l	36/35 (103%)	35 (97%)	1 (3%)	38	59
12	M	32/31 (103%)	31 (97%)	1 (3%)	35	56
12	m	32/31 (103%)	32 (100%)	0	100	100
13	O	210/206 (102%)	206 (98%)	4 (2%)	50	66
13	o	210/206 (102%)	207 (99%)	3 (1%)	59	71
14	T	29/27 (107%)	29 (100%)	0	100	100
14	t	29/27 (107%)	29 (100%)	0	100	100
15	U	84/84 (100%)	83 (99%)	1 (1%)	63	73
15	u	84/84 (100%)	83 (99%)	1 (1%)	63	73
16	V	118/117 (101%)	117 (99%)	1 (1%)	73	77
16	v	118/117 (101%)	117 (99%)	1 (1%)	73	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	Y	22/22 (100%)	21 (96%)	1 (4%)	24	46
17	y	22/22 (100%)	22 (100%)	0	100	100
18	X	33/32 (103%)	33 (100%)	0	100	100
18	x	33/32 (103%)	32 (97%)	1 (3%)	36	57
19	Z	52/52 (100%)	50 (96%)	2 (4%)	29	51
19	z	52/52 (100%)	50 (96%)	2 (4%)	29	51
All	All	4370/4302 (102%)	4318 (99%)	52 (1%)	63	73

5 of 52 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
19	Z	6	GLN
3	c	289	PHE
18	x	2	THR
1	a	12	ASN
2	b	472	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
3	c	25	ASN
4	d	197	HIS
15	u	78	ASN
3	c	44	ASN
4	d	255	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 166 ligands modelled in this entry, 16 are monoatomic - leaving 150 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
33	HEM	E	102	5,6	50,50,50	2.01	10 (20%)	67,82,82	1.19	4 (5%)
25	BCR	B	618	-	41,41,41	7.66	29 (70%)	56,56,56	6.20	32 (57%)
23	CLA	C	512	-	69,73,73	3.04	34 (49%)	82,113,113	1.75	18 (21%)
28	LMG	Z	101	-	37,37,55	1.45	4 (10%)	45,45,63	1.25	3 (6%)
23	CLA	b	612	-	69,73,73	3.04	32 (46%)	82,113,113	1.67	17 (20%)
31	LHG	L	101	-	48,48,48	1.12	3 (6%)	51,54,54	0.88	3 (5%)
23	CLA	C	509	-	69,73,73	3.05	33 (47%)	82,113,113	1.74	18 (21%)
28	LMG	C	519	-	51,51,55	1.34	4 (7%)	59,59,63	1.06	2 (3%)
28	LMG	j	101	34	51,51,55	1.33	4 (7%)	59,59,63	0.93	4 (6%)
23	CLA	C	508	-	69,73,73	3.06	33 (47%)	82,113,113	1.76	16 (19%)
23	CLA	B	613	-	69,73,73	3.09	32 (46%)	82,113,113	1.74	17 (20%)
31	LHG	d	406	-	48,48,48	1.13	3 (6%)	51,54,54	0.91	3 (5%)
23	CLA	B	603	-	69,73,73	3.03	33 (47%)	82,113,113	1.77	19 (23%)
20	OEX	a	601	1,3	0,15,15	-	-	-	-	-
25	BCR	b	621	-	41,41,41	7.71	29 (70%)	56,56,56	5.78	30 (53%)
23	CLA	B	612	-	69,73,73	3.07	33 (47%)	82,113,113	1.82	15 (18%)
23	CLA	b	605	-	69,73,73	3.06	32 (46%)	82,113,113	1.75	16 (19%)
23	CLA	b	607	-	69,73,73	3.06	33 (47%)	82,113,113	1.77	17 (20%)
31	LHG	D	408	-	48,48,48	1.12	3 (6%)	51,54,54	0.98	3 (5%)
25	BCR	c	516	-	41,41,41	7.72	30 (73%)	56,56,56	5.96	27 (48%)
23	CLA	C	501	-	69,73,73	3.04	32 (46%)	82,113,113	1.78	19 (23%)
23	CLA	C	505	-	69,73,73	3.09	31 (44%)	82,113,113	1.68	11 (13%)
23	CLA	C	506	-	69,73,73	3.04	33 (47%)	82,113,113	1.73	18 (21%)
23	CLA	C	504	-	69,73,73	3.06	33 (47%)	82,113,113	1.79	17 (20%)
23	CLA	C	510	-	69,73,73	3.07	32 (46%)	82,113,113	1.67	17 (20%)
23	CLA	B	602	-	69,73,73	3.03	33 (47%)	82,113,113	1.75	16 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	a	607	-	69,73,73	3.08	33 (47%)	82,113,113	1.71	17 (20%)
25	BCR	T	101	-	41,41,41	7.69	30 (73%)	56,56,56	6.14	28 (50%)
23	CLA	a	613	-	69,73,73	3.07	34 (49%)	82,113,113	1.76	17 (20%)
24	PHO	d	401	-	58,69,69	2.22	10 (17%)	55,99,99	1.41	7 (12%)
25	BCR	c	515	-	41,41,41	7.59	31 (75%)	56,56,56	6.41	32 (57%)
23	CLA	b	616	-	69,73,73	3.05	33 (47%)	82,113,113	1.73	18 (21%)
25	BCR	k	101	-	41,41,41	7.73	30 (73%)	56,56,56	5.81	26 (46%)
32	DGD	C	518	-	63,63,67	1.69	16 (25%)	77,77,81	1.03	5 (6%)
27	SQD	X	101	-	41,43,54	1.16	3 (7%)	51,54,65	1.42	7 (13%)
23	CLA	d	402	-	69,73,73	3.08	32 (46%)	82,113,113	1.62	13 (15%)
22	BCT	A	604	29	3,3,3	2.87	1 (33%)	2,3,3	3.85	2 (100%)
23	CLA	A	605	-	69,73,73	3.07	32 (46%)	82,113,113	1.72	15 (18%)
23	CLA	c	506	-	69,73,73	3.08	31 (44%)	82,113,113	1.66	12 (14%)
23	CLA	c	513	-	69,73,73	3.04	33 (47%)	82,113,113	1.72	19 (23%)
25	BCR	K	101	-	41,41,41	7.69	29 (70%)	56,56,56	6.01	27 (48%)
32	DGD	d	405	-	63,63,67	1.72	15 (23%)	77,77,81	1.04	7 (9%)
23	CLA	b	617	-	69,73,73	3.05	32 (46%)	82,113,113	1.73	17 (20%)
25	BCR	B	619	-	41,41,41	8.02	30 (73%)	56,56,56	5.44	28 (50%)
23	CLA	b	614	-	69,73,73	3.10	33 (47%)	82,113,113	1.80	16 (19%)
25	BCR	a	608	-	41,41,41	7.74	30 (73%)	56,56,56	5.81	25 (44%)
33	HEM	v	201	16	50,50,50	1.93	9 (18%)	67,82,82	1.27	6 (8%)
25	BCR	H	101	-	41,41,41	7.59	30 (73%)	56,56,56	5.98	36 (64%)
23	CLA	c	505	-	69,73,73	3.04	34 (49%)	82,113,113	1.79	17 (20%)
28	LMG	b	623	-	51,51,55	1.31	4 (7%)	59,59,63	0.95	2 (3%)
28	LMG	J	101	34	51,51,55	1.33	4 (7%)	59,59,63	0.99	4 (6%)
23	CLA	B	616	-	69,73,73	3.02	33 (47%)	82,113,113	1.75	18 (21%)
23	CLA	b	609[B]	-	69,73,73	3.06	32 (46%)	82,113,113	1.84	19 (23%)
31	LHG	e	101	-	41,41,48	1.22	3 (7%)	44,47,54	0.97	2 (4%)
23	CLA	C	502	-	69,73,73	3.05	33 (47%)	82,113,113	1.76	18 (21%)
23	CLA	b	609[A]	-	69,73,73	3.03	32 (46%)	82,113,113	1.85	18 (21%)
23	CLA	c	509	-	69,73,73	3.03	33 (47%)	82,113,113	1.81	16 (19%)
23	CLA	B	606	-	69,73,73	3.04	32 (46%)	82,113,113	1.73	17 (20%)
25	BCR	C	521	-	41,41,41	7.67	29 (70%)	56,56,56	6.02	27 (48%)
23	CLA	c	512	3	69,73,73	3.05	33 (47%)	82,113,113	1.71	14 (17%)
28	LMG	a	611	-	51,51,55	1.32	4 (7%)	59,59,63	1.00	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	SQD	a	610	-	52,54,54	0.92	2 (3%)	62,65,65	1.49	11 (17%)
23	CLA	B	617	-	69,73,73	3.05	33 (47%)	82,113,113	1.74	15 (18%)
32	DGD	C	517	-	63,63,67	1.66	17 (26%)	77,77,81	1.03	5 (6%)
32	DGD	c	518	-	63,63,67	1.67	16 (25%)	77,77,81	1.00	6 (7%)
23	CLA	B	604	-	69,73,73	3.08	32 (46%)	82,113,113	1.69	17 (20%)
23	CLA	B	615	-	69,73,73	3.04	32 (46%)	82,113,113	1.74	18 (21%)
23	CLA	c	507	-	69,73,73	3.06	33 (47%)	82,113,113	1.74	17 (20%)
26	PL9	D	405	-	55,55,55	4.35	21 (38%)	68,69,69	3.68	35 (51%)
23	CLA	b	610	-	69,73,73	3.06	32 (46%)	82,113,113	1.76	19 (23%)
23	CLA	C	511	3	69,73,73	3.06	33 (47%)	82,113,113	1.76	16 (19%)
28	LMG	c	520	-	51,51,55	1.34	4 (7%)	59,59,63	1.03	2 (3%)
32	DGD	h	102	-	63,63,67	1.70	15 (23%)	77,77,81	0.98	4 (5%)
31	LHG	E	101	-	41,41,48	1.22	3 (7%)	44,47,54	0.92	3 (6%)
23	CLA	A	606	-	69,73,73	3.08	32 (46%)	82,113,113	1.76	16 (19%)
28	LMG	c	521	-	51,51,55	1.33	4 (7%)	59,59,63	1.01	3 (5%)
23	CLA	c	508	-	69,73,73	3.03	31 (44%)	82,113,113	1.88	17 (20%)
23	CLA	b	618	-	69,73,73	3.02	33 (47%)	82,113,113	1.76	19 (23%)
20	OEX	A	601	1,3	0,15,15	-	-	-	-	-
27	SQD	A	611	-	52,54,54	0.92	2 (3%)	62,65,65	1.49	11 (17%)
27	SQD	b	602	-	52,54,54	1.03	3 (5%)	62,65,65	1.41	9 (14%)
23	CLA	a	604	-	69,73,73	3.07	33 (47%)	82,113,113	1.73	15 (18%)
23	CLA	b	615	-	69,73,73	3.08	33 (47%)	82,113,113	1.76	17 (20%)
23	CLA	b	611	-	69,73,73	3.03	31 (44%)	82,113,113	1.79	17 (20%)
23	CLA	B	608	-	69,73,73	3.05	33 (47%)	82,113,113	1.76	19 (23%)
23	CLA	B	605	-	69,73,73	3.06	33 (47%)	82,113,113	1.73	16 (19%)
23	CLA	B	609	-	69,73,73	3.03	31 (44%)	82,113,113	1.77	20 (24%)
23	CLA	D	403	-	69,73,73	3.08	32 (46%)	82,113,113	1.63	16 (19%)
26	PL9	a	609	-	55,55,55	4.32	22 (40%)	68,69,69	3.75	37 (54%)
27	SQD	x	101	-	41,43,54	1.15	3 (7%)	51,54,65	1.42	7 (13%)
23	CLA	B	610	-	69,73,73	3.04	32 (46%)	82,113,113	1.69	15 (18%)
23	CLA	c	510	-	69,73,73	3.05	33 (47%)	82,113,113	1.76	17 (20%)
25	BCR	A	609	-	41,41,41	7.78	30 (73%)	56,56,56	5.79	26 (46%)
23	CLA	B	607[B]	-	69,73,73	3.06	32 (46%)	82,113,113	1.84	18 (21%)
24	PHO	A	607	-	58,69,69	2.21	10 (17%)	55,99,99	1.38	5 (9%)
25	BCR	h	101	-	41,41,41	7.66	30 (73%)	56,56,56	5.99	37 (66%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	PL9	A	610	-	55,55,55	4.35	22 (40%)	68,69,69	3.70	38 (55%)
25	BCR	c	522	-	41,41,41	7.64	30 (73%)	56,56,56	5.98	27 (48%)
23	CLA	B	607[A]	-	69,73,73	3.05	32 (46%)	82,113,113	1.85	19 (23%)
28	LMG	C	520	-	51,51,55	1.32	4 (7%)	59,59,63	1.02	4 (6%)
33	HEM	V	202	16	50,50,50	1.87	8 (16%)	67,82,82	1.26	5 (7%)
32	DGD	D	406	-	63,63,67	1.74	14 (22%)	77,77,81	1.13	7 (9%)
23	CLA	C	513	-	69,73,73	3.03	32 (46%)	82,113,113	1.73	17 (20%)
28	LMG	z	101	-	37,37,55	1.45	4 (10%)	45,45,63	1.21	4 (8%)
31	LHG	l	101	-	48,48,48	1.14	2 (4%)	51,54,54	0.90	2 (3%)
32	DGD	C	516	-	63,63,67	1.72	16 (25%)	77,77,81	0.93	3 (3%)
23	CLA	b	619	-	69,73,73	3.07	31 (44%)	82,113,113	1.72	16 (19%)
27	SQD	a	612	-	52,54,54	0.99	2 (3%)	62,65,65	1.19	6 (9%)
23	CLA	B	611	-	69,73,73	3.05	34 (49%)	82,113,113	1.71	16 (19%)
23	CLA	C	507	-	69,73,73	3.00	32 (46%)	82,113,113	1.86	19 (23%)
25	BCR	B	620	-	41,41,41	7.63	31 (75%)	56,56,56	6.22	31 (55%)
23	CLA	b	608	-	69,73,73	3.06	32 (46%)	82,113,113	1.75	17 (20%)
25	BCR	C	514	-	41,41,41	7.60	31 (75%)	56,56,56	6.31	31 (55%)
31	LHG	b	624	-	48,48,48	1.12	3 (6%)	51,54,54	0.97	3 (5%)
23	CLA	D	402	-	69,73,73	3.06	32 (46%)	82,113,113	1.74	18 (21%)
33	HEM	e	102	5,6	50,50,50	1.99	9 (18%)	67,82,82	1.21	3 (4%)
32	DGD	c	517	-	63,63,67	1.72	16 (25%)	77,77,81	0.93	5 (6%)
23	CLA	b	604	-	69,73,73	3.04	34 (49%)	82,113,113	1.73	17 (20%)
25	BCR	b	620	-	41,41,41	7.56	30 (73%)	56,56,56	6.01	28 (50%)
31	LHG	B	622	-	48,48,48	1.15	3 (6%)	51,54,54	0.98	5 (9%)
23	CLA	B	614	-	69,73,73	3.08	32 (46%)	82,113,113	1.69	17 (20%)
25	BCR	C	515	-	41,41,41	7.66	30 (73%)	56,56,56	6.11	29 (51%)
28	LMG	A	612	-	51,51,55	1.32	4 (7%)	59,59,63	0.98	3 (5%)
23	CLA	c	511	-	69,73,73	3.07	34 (49%)	82,113,113	1.66	16 (19%)
23	CLA	c	503	-	69,73,73	3.06	32 (46%)	82,113,113	1.79	18 (21%)
22	BCT	a	603	29	3,3,3	2.81	1 (33%)	2,3,3	3.31	2 (100%)
23	CLA	c	514	-	69,73,73	3.02	33 (47%)	82,113,113	1.73	14 (17%)
23	CLA	c	502	-	69,73,73	3.05	32 (46%)	82,113,113	1.75	16 (19%)
27	SQD	b	601	-	52,54,54	0.99	2 (3%)	62,65,65	1.19	6 (9%)
32	DGD	c	519	-	63,63,67	1.68	16 (25%)	77,77,81	1.07	4 (5%)
25	BCR	b	622	-	41,41,41	7.74	31 (75%)	56,56,56	5.97	31 (55%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	d	403	-	69,73,73	3.03	33 (47%)	82,113,113	1.77	17 (20%)
24	PHO	a	606	-	58,69,69	2.18	10 (17%)	55,99,99	1.38	6 (10%)
31	LHG	D	407	-	48,48,48	1.13	3 (6%)	51,54,54	0.91	3 (5%)
25	BCR	t	101	-	41,41,41	7.71	29 (70%)	56,56,56	5.91	28 (50%)
23	CLA	D	404	-	69,73,73	3.04	32 (46%)	82,113,113	1.80	17 (20%)
23	CLA	a	605	-	69,73,73	3.06	33 (47%)	82,113,113	1.73	17 (20%)
24	PHO	D	401	-	58,69,69	2.20	10 (17%)	55,99,99	1.41	7 (12%)
23	CLA	b	613	-	69,73,73	3.07	33 (47%)	82,113,113	1.73	16 (19%)
25	BCR	F	101	-	41,41,41	7.64	29 (70%)	56,56,56	6.19	28 (50%)
23	CLA	C	503	-	69,73,73	3.05	33 (47%)	82,113,113	1.72	17 (20%)
23	CLA	c	504	-	69,73,73	3.03	33 (47%)	82,113,113	1.67	17 (20%)
23	CLA	b	606	-	69,73,73	3.12	33 (47%)	82,113,113	1.70	16 (19%)
27	SQD	B	623	-	52,54,54	1.03	3 (5%)	62,65,65	1.41	9 (14%)
23	CLA	A	608	-	69,73,73	3.07	32 (46%)	82,113,113	1.73	17 (20%)
32	DGD	H	102	-	63,63,67	1.71	15 (23%)	77,77,81	0.92	3 (3%)
26	PL9	d	404	-	55,55,55	4.37	21 (38%)	68,69,69	3.67	35 (51%)
25	BCR	f	101	-	41,41,41	7.72	30 (73%)	56,56,56	5.93	27 (48%)
31	LHG	a	614	-	48,48,48	1.11	2 (4%)	51,54,54	1.04	3 (5%)
28	LMG	B	621	-	51,51,55	1.29	4 (7%)	59,59,63	0.91	2 (3%)

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
33	HEM	E	102	5,6	-	4/14/54/54	-
25	BCR	B	618	-	-	24/29/63/63	0/2/2/2
23	CLA	C	512	-	1/1/15/20	9/39/115/115	-
28	LMG	Z	101	-	-	15/31/51/70	0/1/1/1
23	CLA	b	612	-	1/1/15/20	5/39/115/115	-
31	LHG	L	101	-	-	17/53/53/53	-
23	CLA	C	509	-	1/1/15/20	6/39/115/115	-
28	LMG	C	519	-	-	20/46/66/70	0/1/1/1
28	LMG	j	101	34	-	19/46/66/70	0/1/1/1
23	CLA	C	508	-	1/1/15/20	3/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	B	613	-	1/1/15/20	4/39/115/115	-
31	LHG	d	406	-	-	13/53/53/53	-
23	CLA	B	603	-	1/1/15/20	4/39/115/115	-
25	BCR	b	621	-	-	21/29/63/63	0/2/2/2
23	CLA	B	612	-	1/1/15/20	5/39/115/115	-
23	CLA	b	605	-	1/1/15/20	4/39/115/115	-
23	CLA	b	607	-	1/1/15/20	7/39/115/115	-
31	LHG	D	408	-	-	16/53/53/53	-
25	BCR	c	516	-	-	21/29/63/63	0/2/2/2
23	CLA	C	501	-	1/1/15/20	9/39/115/115	-
23	CLA	C	505	-	1/1/15/20	8/39/115/115	-
23	CLA	C	506	-	1/1/15/20	15/39/115/115	-
23	CLA	C	504	-	1/1/15/20	10/39/115/115	-
23	CLA	C	510	-	1/1/15/20	8/39/115/115	-
23	CLA	B	602	-	1/1/15/20	17/39/115/115	-
23	CLA	a	607	-	1/1/15/20	11/39/115/115	-
25	BCR	T	101	-	-	24/29/63/63	0/2/2/2
23	CLA	a	613	-	1/1/15/20	3/39/115/115	-
24	PHO	d	401	-	-	0/37/103/103	0/5/6/6
25	BCR	c	515	-	-	24/29/63/63	0/2/2/2
23	CLA	b	616	-	1/1/15/20	5/39/115/115	-
25	BCR	k	101	-	-	19/29/63/63	0/2/2/2
32	DGD	C	518	-	-	16/51/91/95	0/2/2/2
27	SQD	X	101	-	-	17/38/58/69	0/1/1/1
23	CLA	d	402	-	1/1/15/20	2/39/115/115	-
23	CLA	c	506	-	1/1/15/20	6/39/115/115	-
23	CLA	A	605	-	1/1/15/20	0/39/115/115	-
23	CLA	c	513	-	1/1/15/20	7/39/115/115	-
25	BCR	K	101	-	-	21/29/63/63	0/2/2/2
32	DGD	d	405	-	-	33/51/91/95	0/2/2/2
23	CLA	b	617	-	1/1/15/20	12/39/115/115	-
25	BCR	B	619	-	-	24/29/63/63	0/2/2/2
23	CLA	b	614	-	1/1/15/20	5/39/115/115	-
25	BCR	a	608	-	-	19/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	HEM	v	201	16	-	2/14/54/54	-
25	BCR	H	101	-	-	23/29/63/63	0/2/2/2
23	CLA	c	505	-	1/1/15/20	11/39/115/115	-
28	LMG	b	623	-	-	21/46/66/70	0/1/1/1
28	LMG	J	101	34	-	19/46/66/70	0/1/1/1
23	CLA	B	616	-	1/1/15/20	13/39/115/115	-
23	CLA	b	609[B]	-	1/1/15/20	9/39/115/115	-
31	LHG	e	101	-	-	20/46/46/53	-
23	CLA	C	502	-	1/1/15/20	8/39/115/115	-
23	CLA	b	609[A]	-	1/1/15/20	8/39/115/115	-
23	CLA	c	509	-	1/1/15/20	3/39/115/115	-
23	CLA	B	606	-	1/1/15/20	5/39/115/115	-
25	BCR	C	521	-	-	17/29/63/63	0/2/2/2
23	CLA	c	512	3	1/1/15/20	2/39/115/115	-
28	LMG	a	611	-	-	31/46/66/70	0/1/1/1
27	SQD	a	610	-	-	17/49/69/69	0/1/1/1
23	CLA	B	617	-	1/1/15/20	16/39/115/115	-
32	DGD	C	517	-	-	28/51/91/95	0/2/2/2
32	DGD	c	518	-	-	30/51/91/95	0/2/2/2
23	CLA	B	604	-	1/1/15/20	8/39/115/115	-
23	CLA	B	615	-	1/1/15/20	13/39/115/115	-
23	CLA	c	507	-	1/1/15/20	14/39/115/115	-
26	PL9	D	405	-	-	25/53/73/73	0/1/1/1
23	CLA	b	610	-	1/1/15/20	3/39/115/115	-
23	CLA	C	511	3	1/1/15/20	3/39/115/115	-
28	LMG	c	520	-	-	22/46/66/70	0/1/1/1
32	DGD	h	102	-	-	19/51/91/95	0/2/2/2
31	LHG	E	101	-	-	22/46/46/53	-
23	CLA	A	606	-	1/1/15/20	7/39/115/115	-
28	LMG	c	521	-	-	19/46/66/70	0/1/1/1
23	CLA	c	508	-	1/1/15/20	12/39/115/115	-
23	CLA	b	618	-	1/1/15/20	13/39/115/115	-
27	SQD	A	611	-	-	17/49/69/69	0/1/1/1
27	SQD	b	602	-	-	29/49/69/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	a	604	-	1/1/15/20	1/39/115/115	-
23	CLA	b	615	-	1/1/15/20	4/39/115/115	-
23	CLA	b	611	-	1/1/15/20	2/39/115/115	-
23	CLA	B	608	-	1/1/15/20	3/39/115/115	-
23	CLA	B	605	-	1/1/15/20	7/39/115/115	-
23	CLA	B	609	-	1/1/15/20	3/39/115/115	-
23	CLA	D	403	-	1/1/15/20	2/39/115/115	-
26	PL9	a	609	-	-	26/53/73/73	0/1/1/1
27	SQD	x	101	-	-	17/38/58/69	0/1/1/1
23	CLA	B	610	-	1/1/15/20	1/39/115/115	-
23	CLA	c	510	-	1/1/15/20	7/39/115/115	-
25	BCR	A	609	-	-	21/29/63/63	0/2/2/2
23	CLA	B	607[B]	-	1/1/15/20	9/39/115/115	-
24	PHO	A	607	-	-	2/37/103/103	0/5/6/6
25	BCR	h	101	-	-	25/29/63/63	0/2/2/2
26	PL9	A	610	-	-	25/53/73/73	0/1/1/1
25	BCR	c	522	-	-	20/29/63/63	0/2/2/2
23	CLA	B	607[A]	-	1/1/15/20	9/39/115/115	-
28	LMG	C	520	-	-	19/46/66/70	0/1/1/1
33	HEM	V	202	16	-	2/14/54/54	-
32	DGD	D	406	-	-	35/51/91/95	0/2/2/2
23	CLA	C	513	-	1/1/15/20	9/39/115/115	-
28	LMG	z	101	-	-	18/31/51/70	0/1/1/1
31	LHG	l	101	-	-	22/53/53/53	-
32	DGD	C	516	-	-	25/51/91/95	0/2/2/2
23	CLA	b	619	-	1/1/15/20	16/39/115/115	-
27	SQD	a	612	-	-	23/49/69/69	0/1/1/1
23	CLA	B	611	-	1/1/15/20	8/39/115/115	-
23	CLA	C	507	-	1/1/15/20	12/39/115/115	-
25	BCR	B	620	-	-	17/29/63/63	0/2/2/2
23	CLA	b	608	-	1/1/15/20	6/39/115/115	-
25	BCR	C	514	-	-	22/29/63/63	0/2/2/2
31	LHG	b	624	-	-	13/53/53/53	-
23	CLA	D	402	-	1/1/15/20	2/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	HEM	e	102	5,6	-	2/14/54/54	-
32	DGD	c	517	-	-	25/51/91/95	0/2/2/2
23	CLA	b	604	-	1/1/15/20	18/39/115/115	-
25	BCR	b	620	-	-	18/29/63/63	0/2/2/2
31	LHG	B	622	-	-	13/53/53/53	-
23	CLA	B	614	-	1/1/15/20	5/39/115/115	-
25	BCR	C	515	-	-	19/29/63/63	0/2/2/2
28	LMG	A	612	-	-	31/46/66/70	0/1/1/1
23	CLA	c	511	-	1/1/15/20	9/39/115/115	-
23	CLA	c	503	-	1/1/15/20	9/39/115/115	-
23	CLA	c	514	-	1/1/15/20	9/39/115/115	-
23	CLA	c	502	-	1/1/15/20	9/39/115/115	-
27	SQD	b	601	-	-	23/49/69/69	0/1/1/1
32	DGD	c	519	-	-	18/51/91/95	0/2/2/2
25	BCR	b	622	-	-	21/29/63/63	0/2/2/2
23	CLA	d	403	-	1/1/15/20	13/39/115/115	-
24	PHO	a	606	-	-	0/37/103/103	0/5/6/6
31	LHG	D	407	-	-	13/53/53/53	-
25	BCR	t	101	-	-	23/29/63/63	0/2/2/2
23	CLA	D	404	-	1/1/15/20	13/39/115/115	-
23	CLA	a	605	-	1/1/15/20	7/39/115/115	-
24	PHO	D	401	-	-	1/37/103/103	0/5/6/6
23	CLA	b	613	-	1/1/15/20	8/39/115/115	-
25	BCR	F	101	-	-	22/29/63/63	0/2/2/2
23	CLA	C	503	-	1/1/15/20	5/39/115/115	-
23	CLA	c	504	-	1/1/15/20	3/39/115/115	-
23	CLA	b	606	-	1/1/15/20	7/39/115/115	-
27	SQD	B	623	-	-	29/49/69/69	0/1/1/1
23	CLA	A	608	-	1/1/15/20	11/39/115/115	-
32	DGD	H	102	-	-	24/51/91/95	0/2/2/2
26	PL9	d	404	-	-	26/53/73/73	0/1/1/1
25	BCR	f	101	-	-	23/29/63/63	0/2/2/2
31	LHG	a	614	-	-	16/53/53/53	-
28	LMG	B	621	-	-	22/46/66/70	0/1/1/1

The worst 5 of 3416 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	609	BCR	C14-C13	15.92	1.72	1.35
25	B	618	BCR	C20-C19	15.90	1.76	1.34
25	a	608	BCR	C14-C13	15.84	1.72	1.35
25	C	521	BCR	C14-C13	15.77	1.72	1.35
25	t	101	BCR	C14-C13	15.74	1.72	1.35

The worst 5 of 2223 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	621	BCR	C15-C16-C17	26.28	177.29	123.52
25	c	515	BCR	C15-C16-C17	25.42	175.54	123.52
25	T	101	BCR	C15-C16-C17	25.33	175.34	123.52
25	A	609	BCR	C15-C16-C17	25.25	175.18	123.52
25	a	608	BCR	C15-C16-C17	25.24	175.17	123.52

5 of 72 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	A	605	CLA	ND
23	A	606	CLA	ND
23	A	608	CLA	ND
23	B	602	CLA	ND
23	B	603	CLA	ND

5 of 1969 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	B	602	CLA	CAD-CBD-CGD-O2D
23	B	608	CLA	C1A-C2A-CAA-CBA
23	B	615	CLA	CAD-CBD-CGD-O1D
23	B	615	CLA	CAD-CBD-CGD-O2D
23	B	616	CLA	C2B-C3B-CAB-CBB

There are no ring outliers.

141 monomers are involved in 751 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	E	102	HEM	3	0
25	B	618	BCR	28	0
23	C	512	CLA	4	0
28	Z	101	LMG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	b	612	CLA	2	0
31	L	101	LHG	2	0
23	C	509	CLA	3	0
28	C	519	LMG	1	0
28	j	101	LMG	3	0
23	C	508	CLA	3	0
23	B	613	CLA	3	0
31	d	406	LHG	1	0
23	B	603	CLA	3	0
20	a	601	OEX	1	0
25	b	621	BCR	28	0
23	B	612	CLA	2	0
23	b	605	CLA	2	0
23	b	607	CLA	6	0
31	D	408	LHG	10	0
25	c	516	BCR	17	0
23	C	501	CLA	7	0
23	C	505	CLA	8	0
23	C	506	CLA	7	0
23	C	504	CLA	2	0
23	C	510	CLA	3	0
23	B	602	CLA	3	0
23	a	607	CLA	5	0
25	T	101	BCR	28	0
23	a	613	CLA	3	0
24	d	401	PHO	6	0
25	c	515	BCR	13	0
23	b	616	CLA	2	0
25	k	101	BCR	22	0
32	C	518	DGD	4	0
27	X	101	SQD	3	0
23	d	402	CLA	5	0
23	A	605	CLA	4	0
23	c	506	CLA	5	0
23	c	513	CLA	2	0
25	K	101	BCR	25	0
32	d	405	DGD	2	0
23	b	617	CLA	9	0
25	B	619	BCR	29	0
25	a	608	BCR	14	0
33	v	201	HEM	1	0
25	H	101	BCR	10	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	c	505	CLA	2	0
28	b	623	LMG	3	0
28	J	101	LMG	3	0
23	B	616	CLA	3	0
23	b	609[B]	CLA	2	0
31	e	101	LHG	4	0
23	C	502	CLA	4	0
23	b	609[A]	CLA	2	0
23	c	509	CLA	5	0
23	B	606	CLA	9	0
25	C	521	BCR	15	0
23	c	512	CLA	2	0
28	a	611	LMG	2	0
27	a	610	SQD	1	0
23	B	617	CLA	7	0
32	C	517	DGD	2	0
32	c	518	DGD	4	0
23	B	604	CLA	7	0
23	B	615	CLA	4	0
23	c	507	CLA	6	0
26	D	405	PL9	6	0
23	b	610	CLA	2	0
23	C	511	CLA	3	0
28	c	520	LMG	1	0
32	h	102	DGD	3	0
23	A	606	CLA	4	0
23	c	508	CLA	5	0
23	b	618	CLA	1	0
20	A	601	OEX	1	0
27	A	611	SQD	4	0
27	b	602	SQD	11	0
23	a	604	CLA	2	0
23	b	615	CLA	3	0
23	B	608	CLA	5	0
23	B	605	CLA	5	0
23	B	609	CLA	1	0
23	D	403	CLA	3	0
26	a	609	PL9	10	0
27	x	101	SQD	4	0
23	B	610	CLA	2	0
23	c	510	CLA	3	0
25	A	609	BCR	16	0

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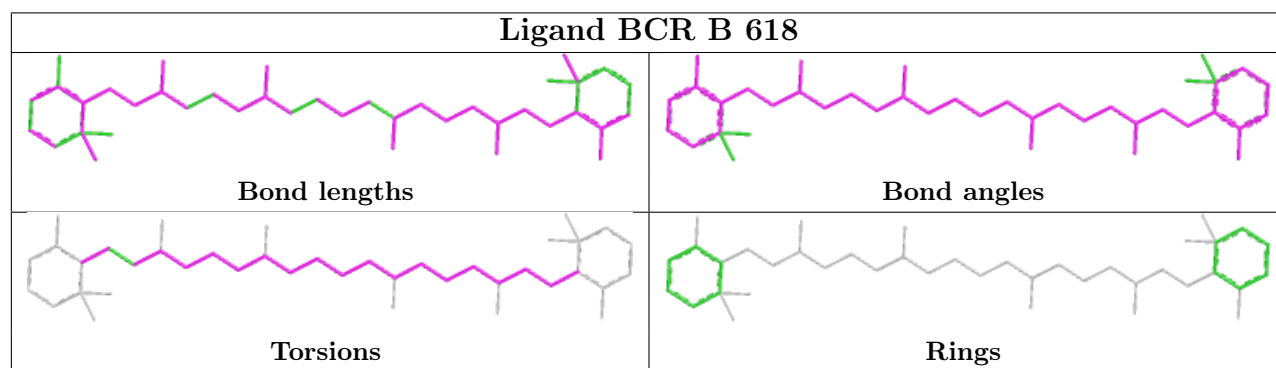
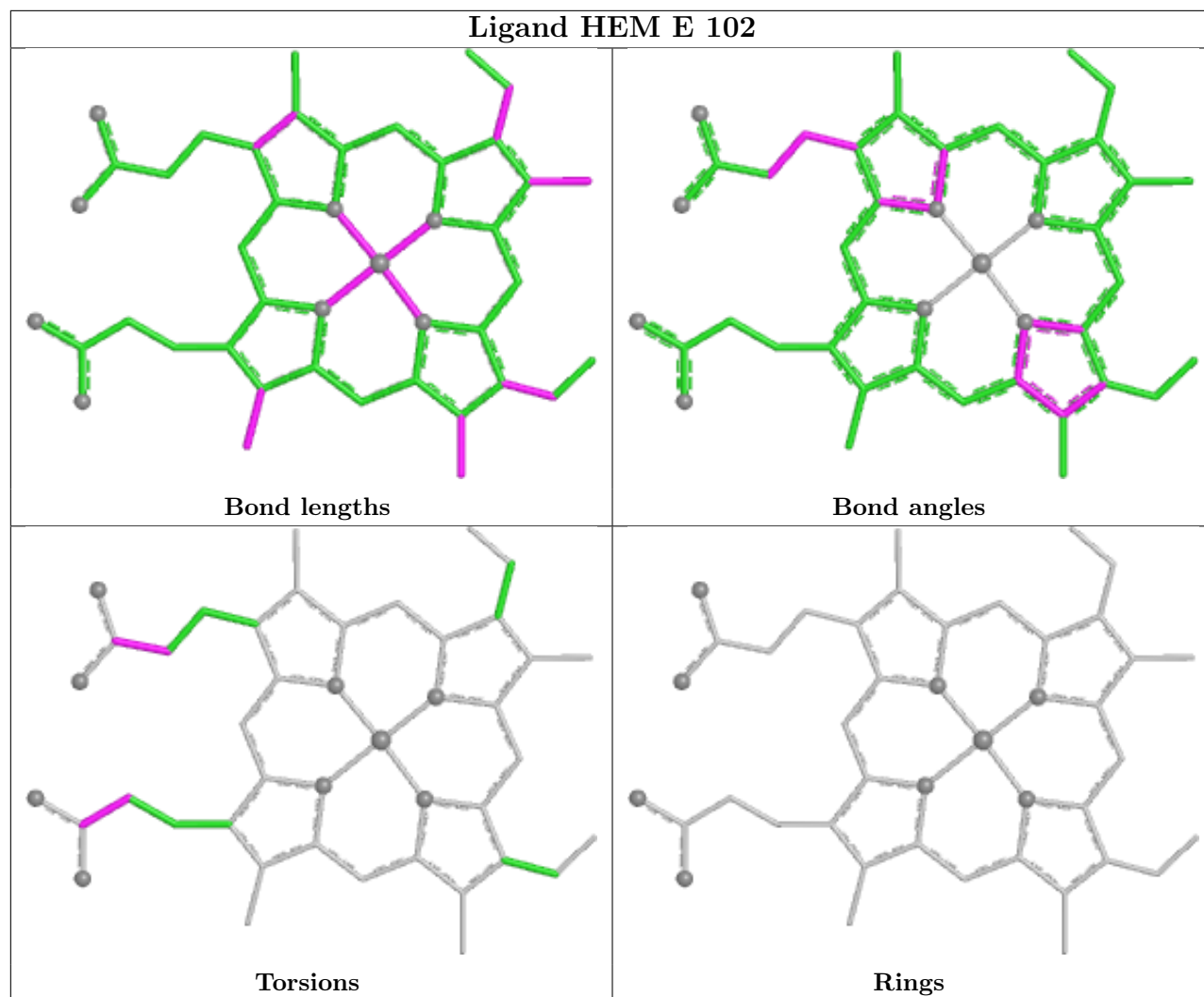
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	B	607[B]	CLA	3	0
24	A	607	PHO	1	0
25	h	101	BCR	15	0
26	A	610	PL9	16	0
25	c	522	BCR	18	0
33	V	202	HEM	4	0
32	D	406	DGD	1	0
23	C	513	CLA	2	0
28	z	101	LMG	2	0
31	l	101	LHG	4	0
32	C	516	DGD	2	0
23	b	619	CLA	1	0
27	a	612	SQD	2	0
23	B	611	CLA	2	0
23	C	507	CLA	7	0
25	B	620	BCR	22	0
23	b	608	CLA	12	0
25	C	514	BCR	11	0
31	b	624	LHG	4	0
23	D	402	CLA	2	0
33	e	102	HEM	3	0
32	c	517	DGD	1	0
23	b	604	CLA	6	0
25	b	620	BCR	31	0
31	B	622	LHG	3	0
23	B	614	CLA	4	0
25	C	515	BCR	18	0
28	A	612	LMG	2	0
23	c	511	CLA	3	0
23	c	503	CLA	6	0
23	c	514	CLA	1	0
23	c	502	CLA	8	0
27	b	601	SQD	4	0
32	c	519	DGD	4	0
25	b	622	BCR	15	0
23	d	403	CLA	2	0
31	D	407	LHG	1	0
25	t	101	BCR	30	0
23	D	404	CLA	2	0
23	a	605	CLA	4	0
24	D	401	PHO	8	0
23	b	613	CLA	5	0

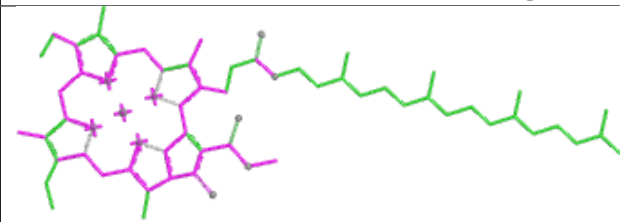
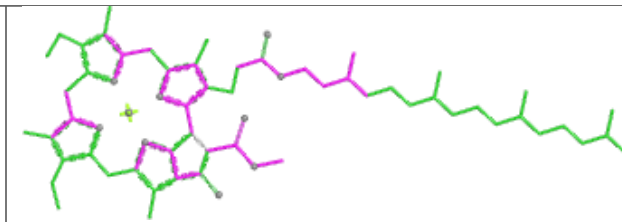
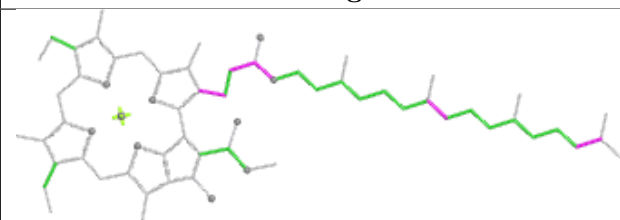
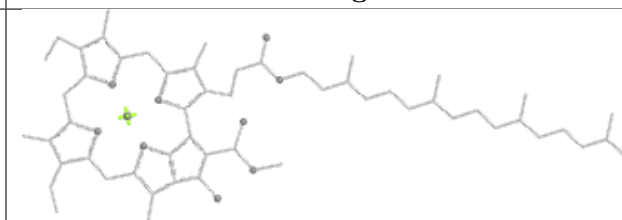
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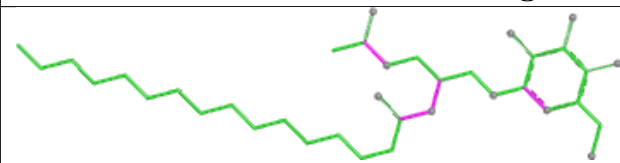
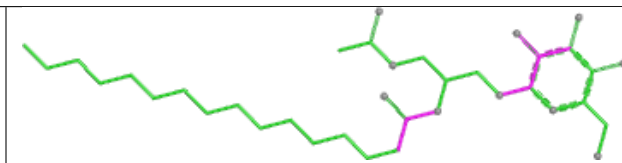
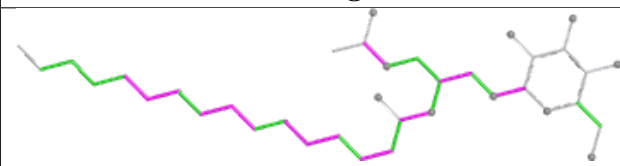
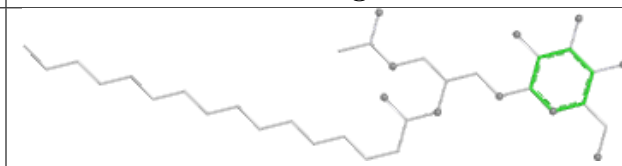
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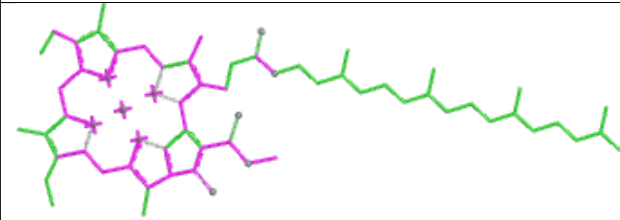
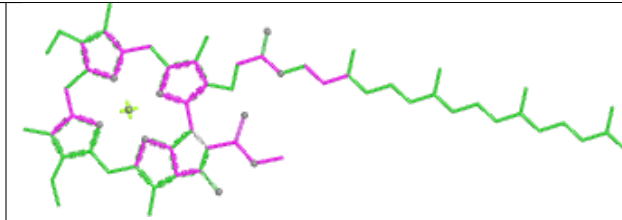
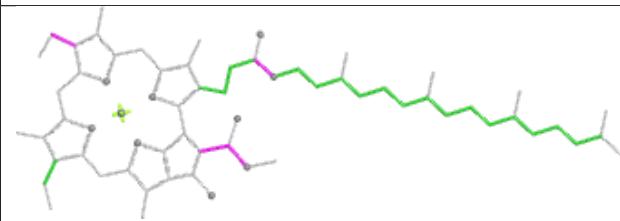
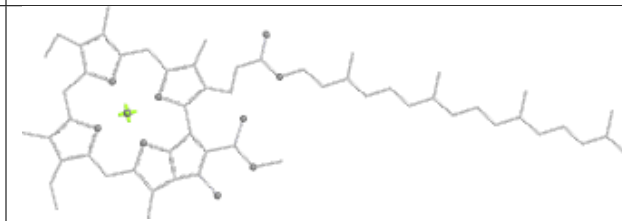
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	F	101	BCR	16	0
23	C	503	CLA	6	0
23	c	504	CLA	7	0
23	b	606	CLA	6	0
27	B	623	SQD	9	0
23	A	608	CLA	7	0
32	H	102	DGD	5	0
26	d	404	PL9	3	0
25	f	101	BCR	24	0
31	a	614	LHG	8	0
28	B	621	LMG	4	0

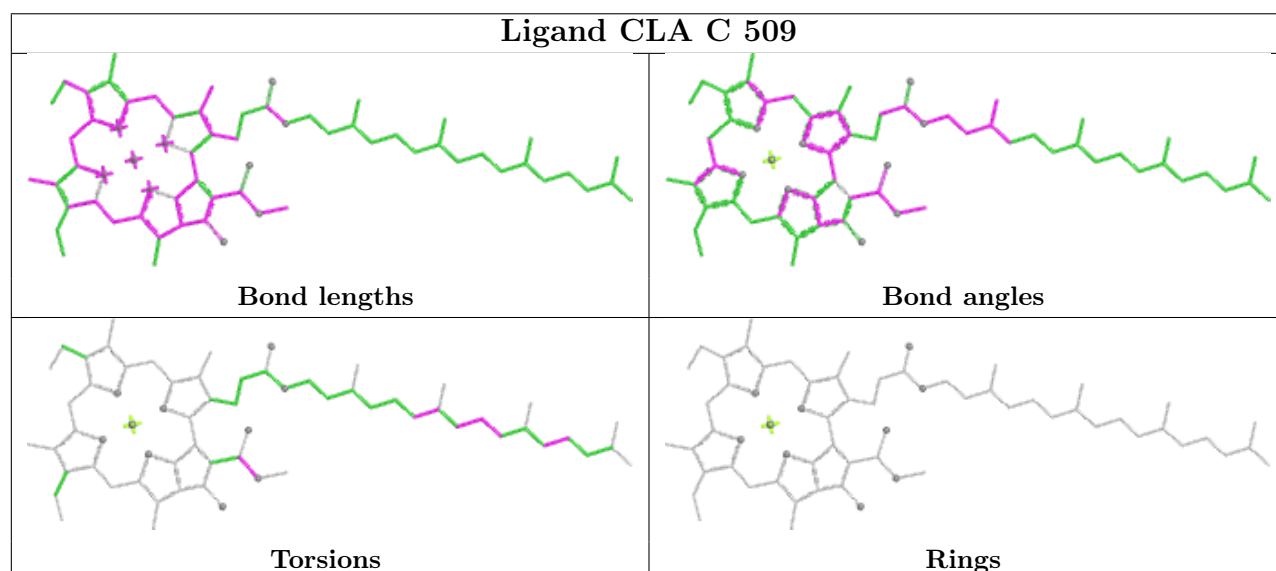
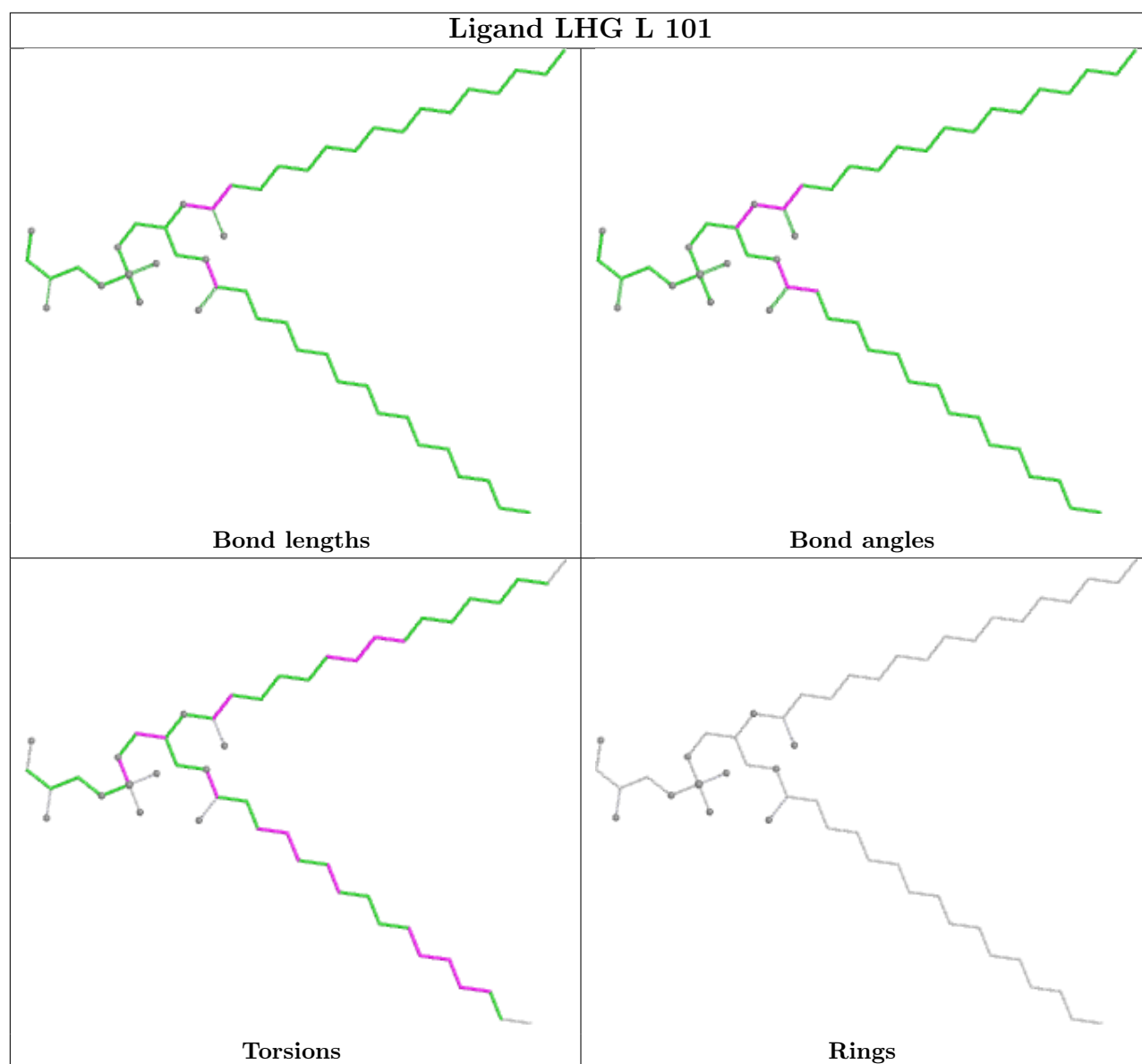
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

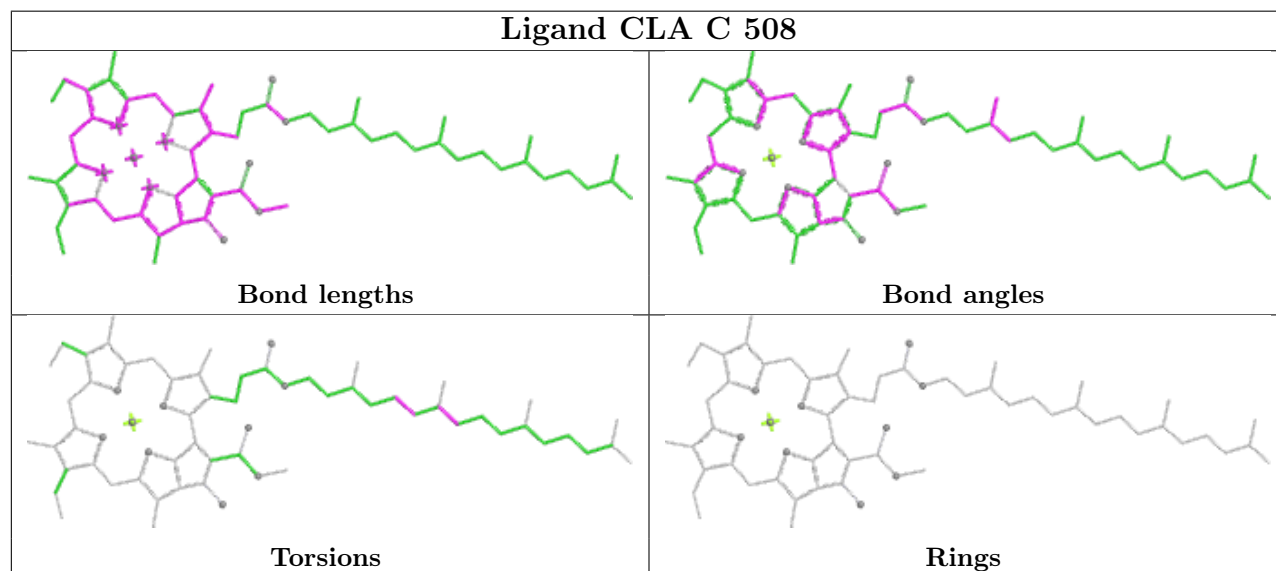
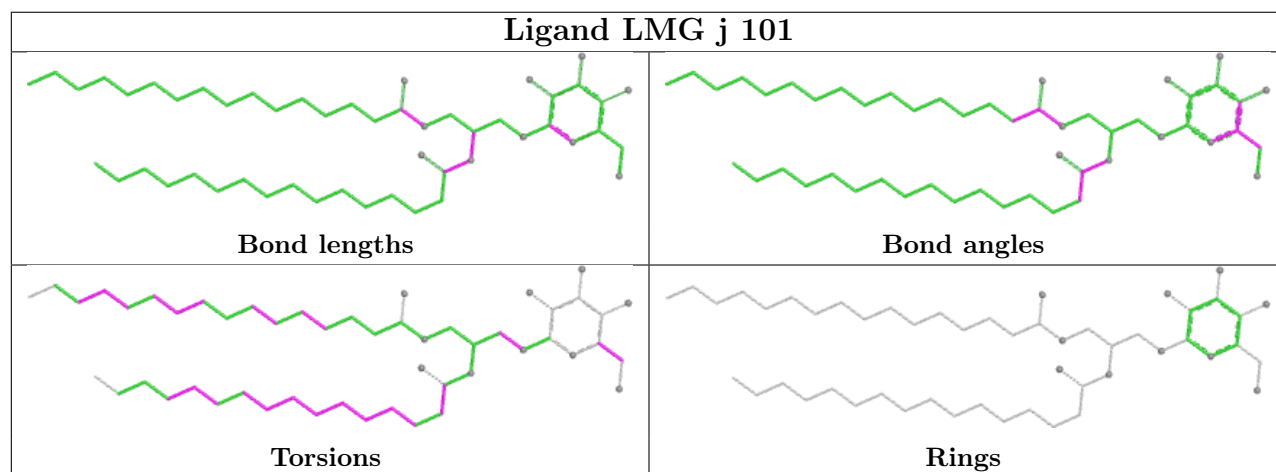
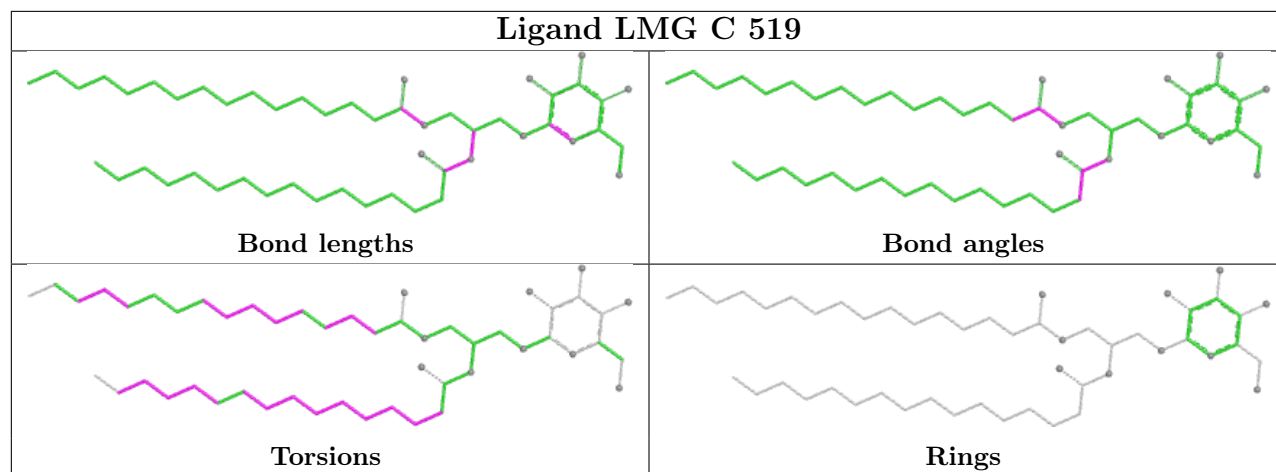


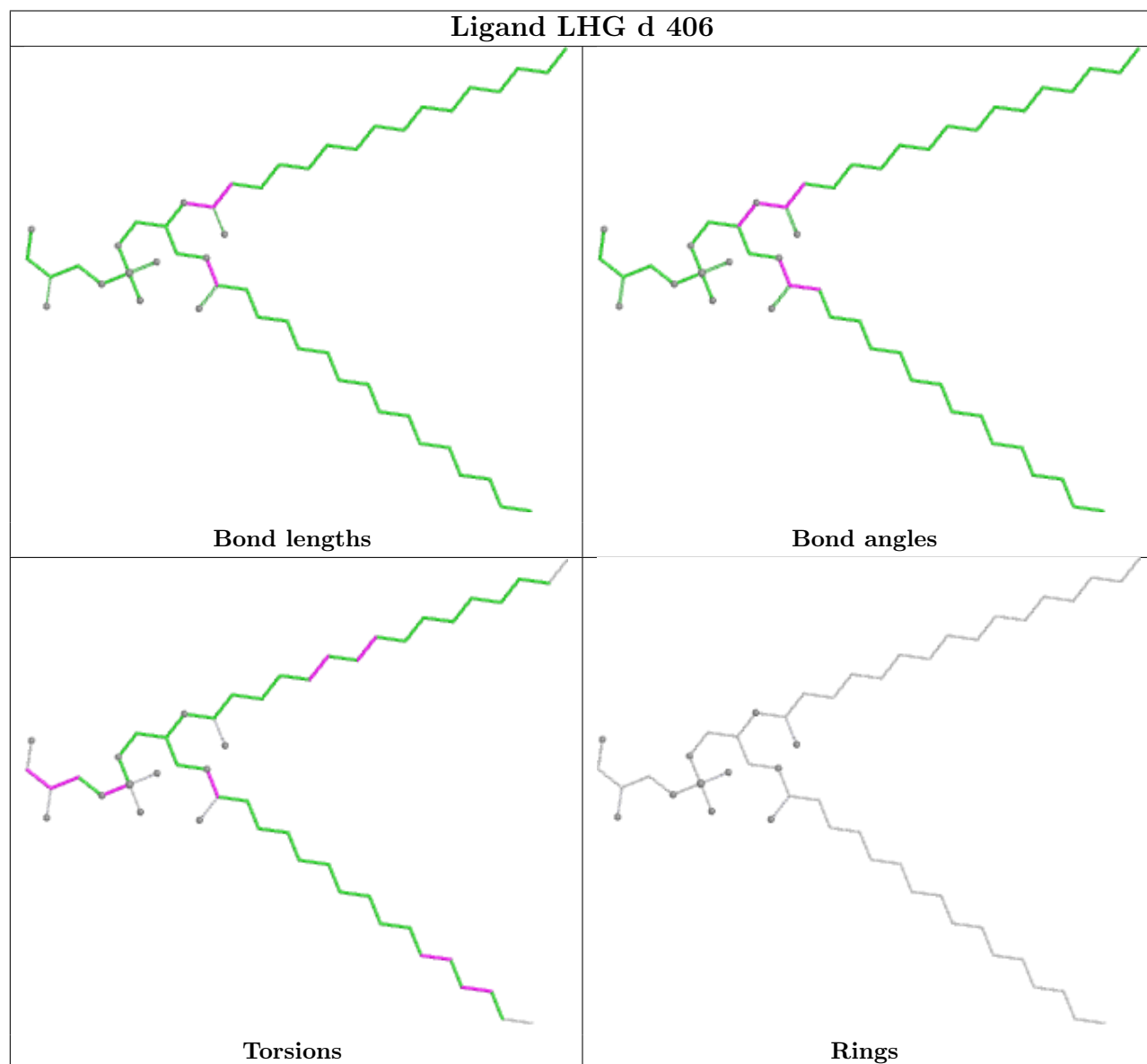
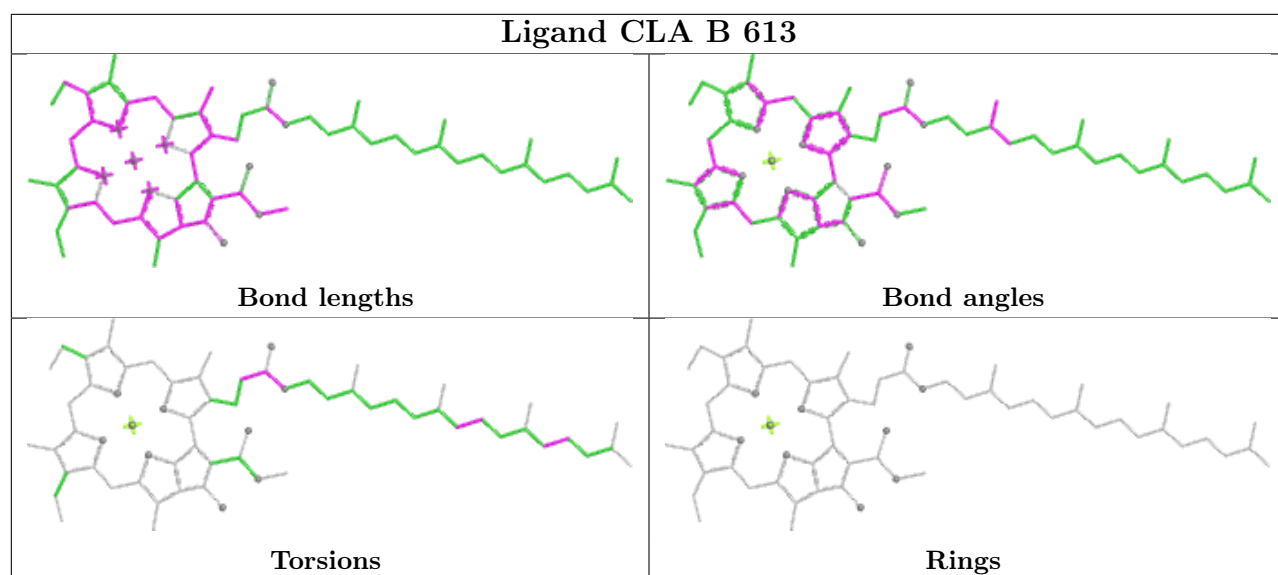
Ligand CLA C 512	
	
Bond lengths	Bond angles
	
Torsions	Rings

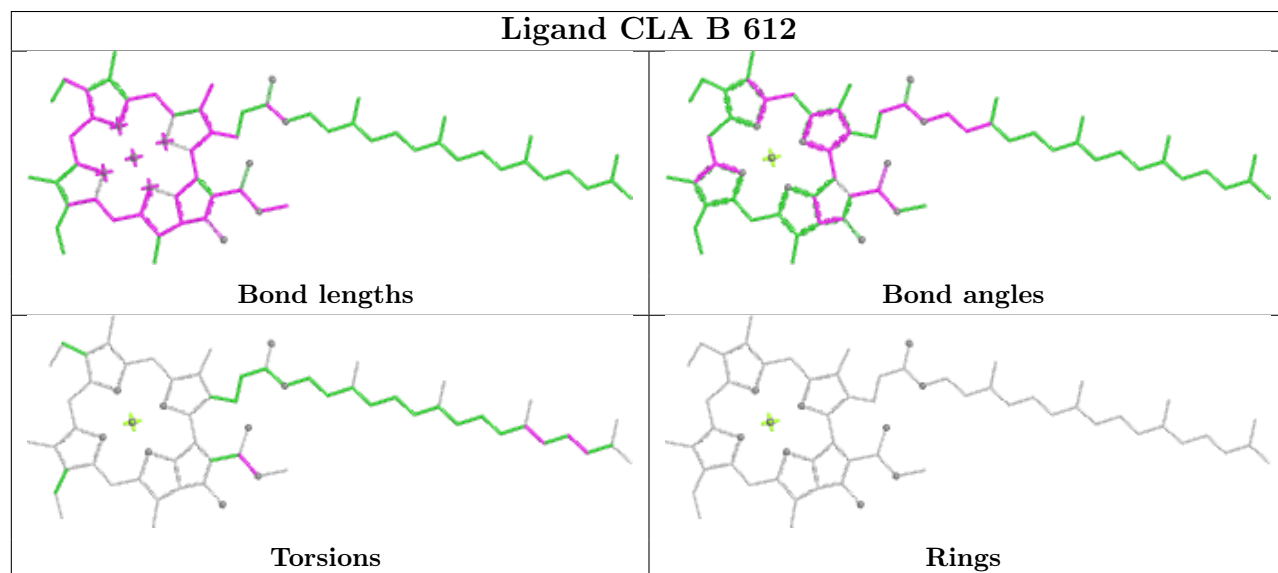
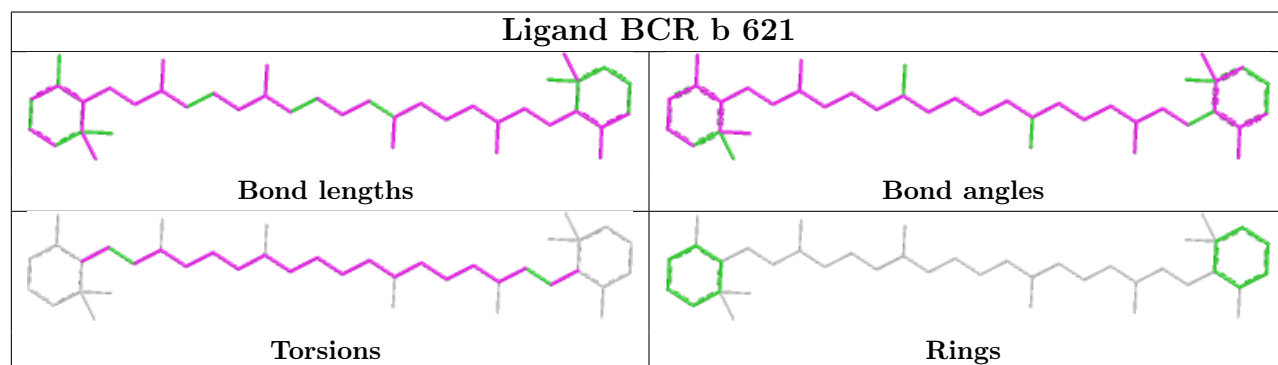
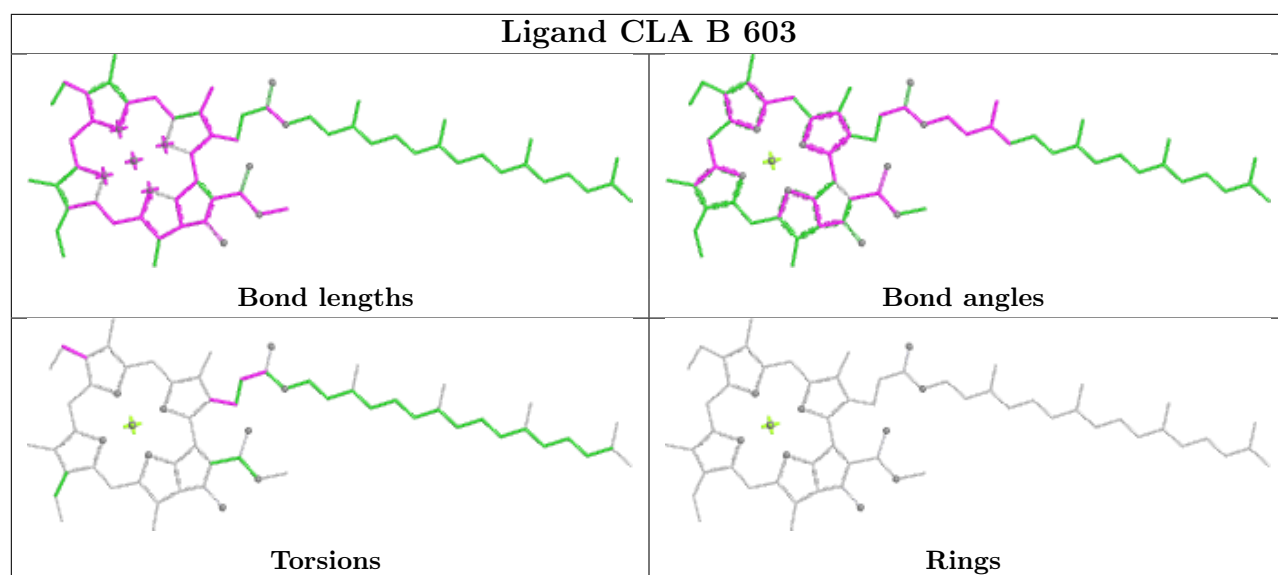
Ligand LMG Z 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

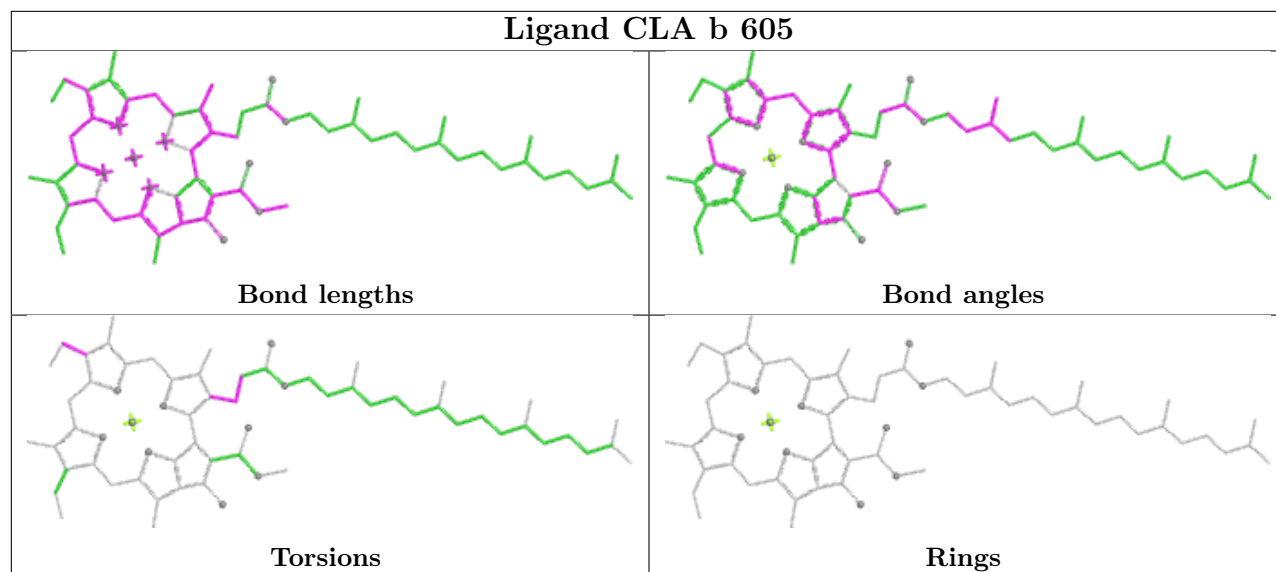
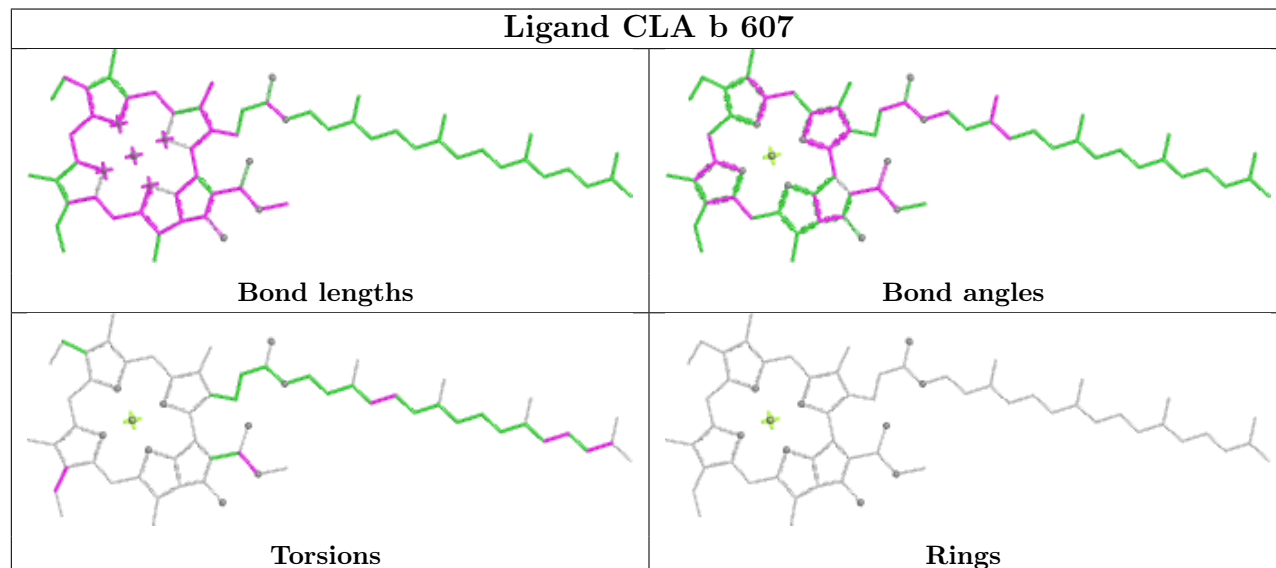
Ligand CLA b 612	
	
Bond lengths	Bond angles
	
Torsions	Rings

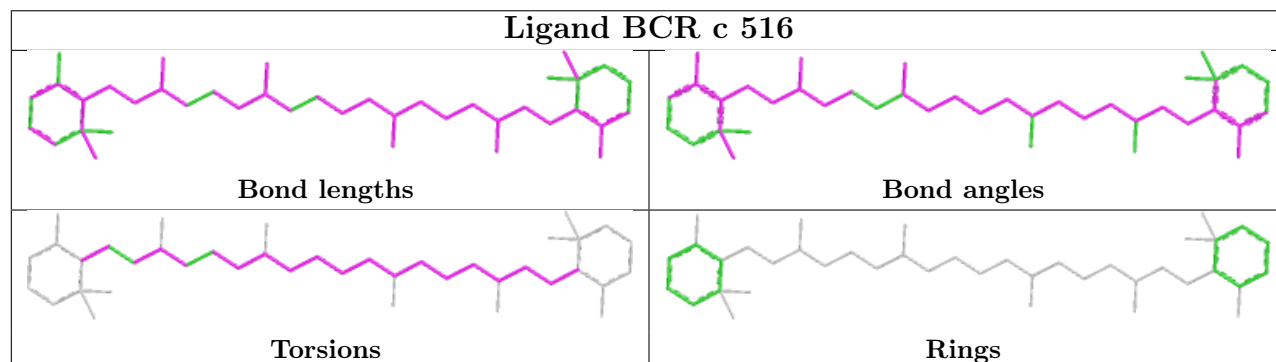
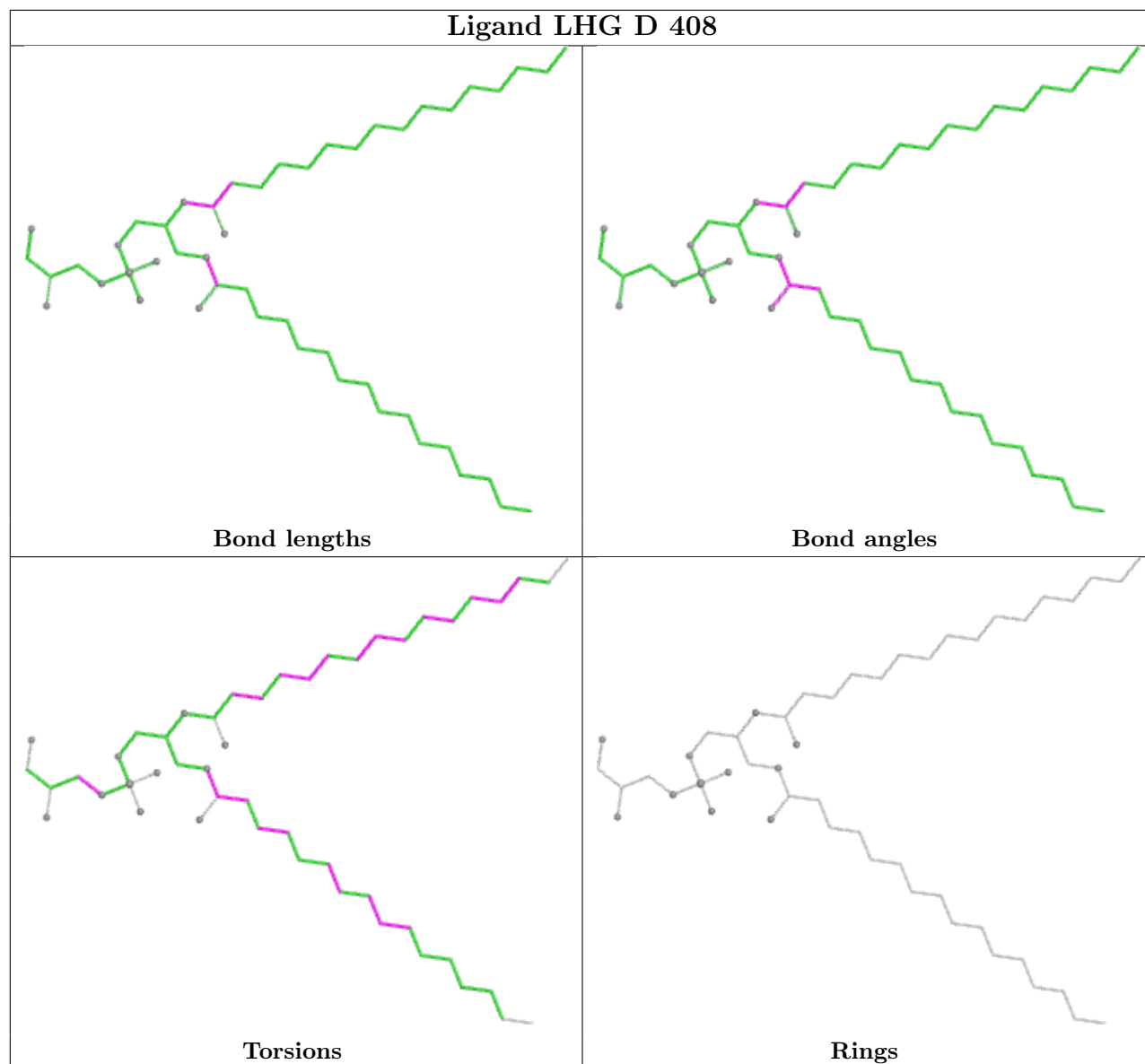


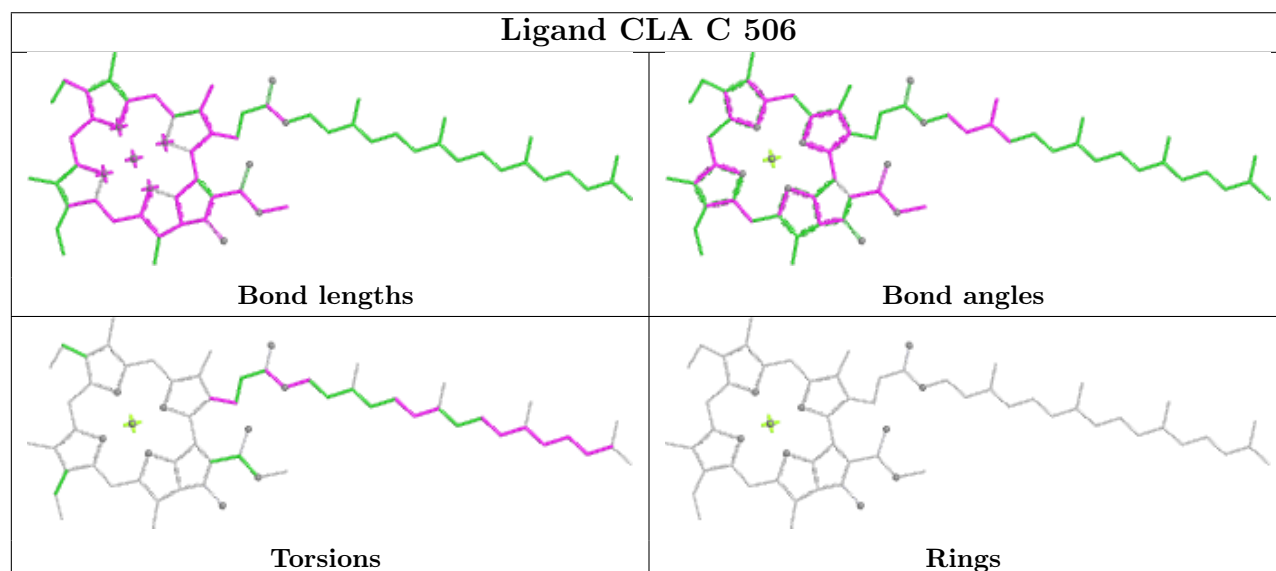
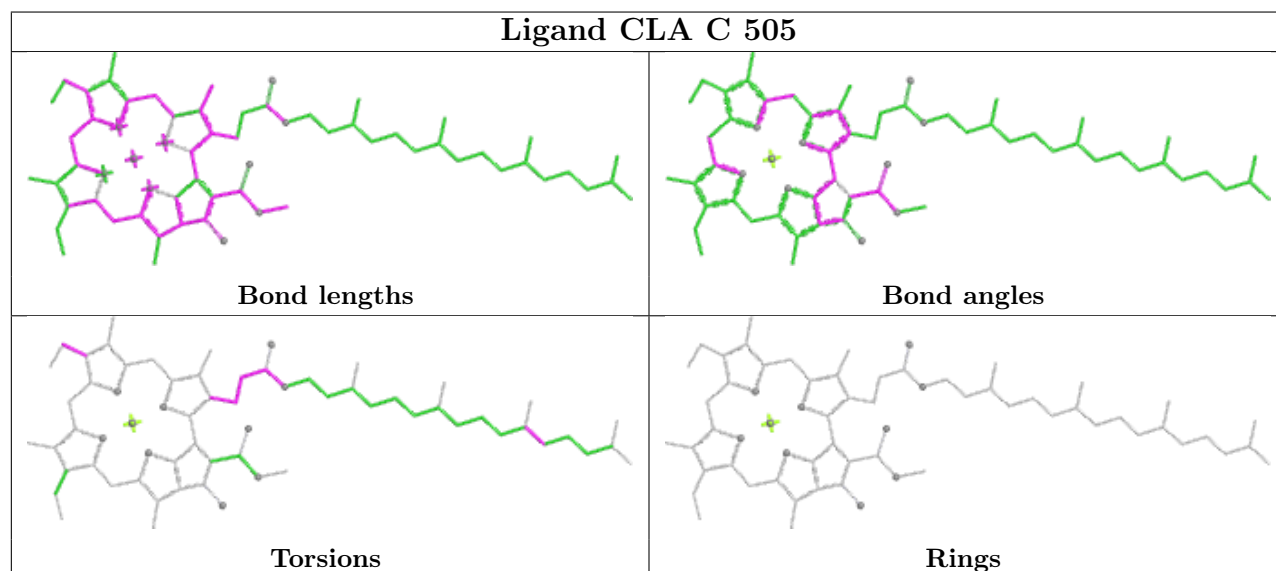
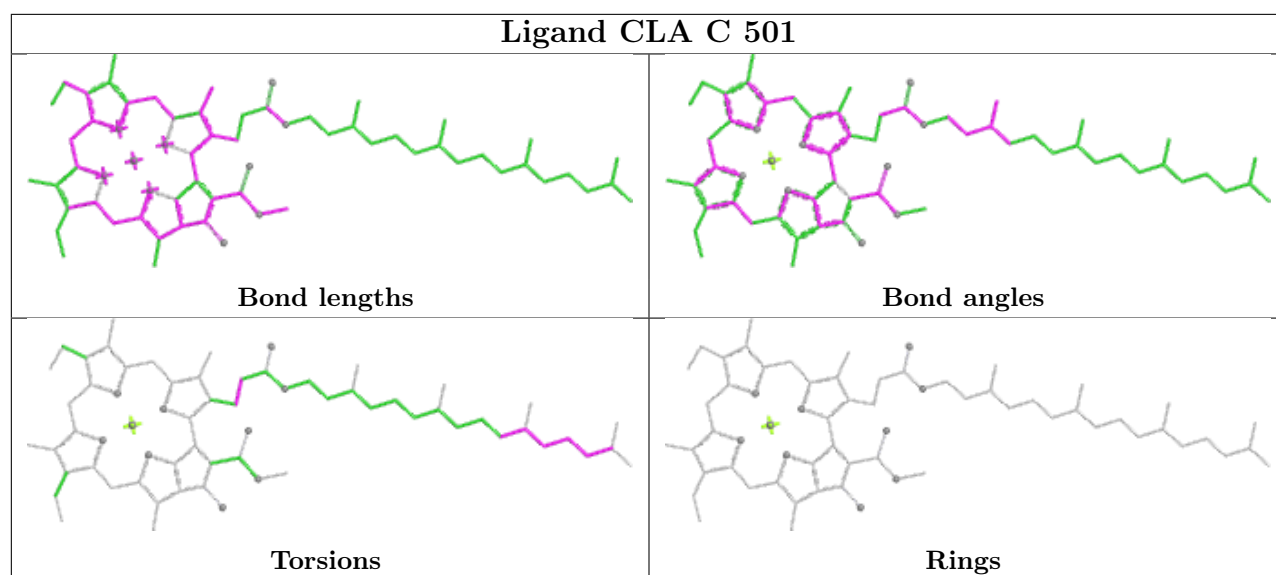


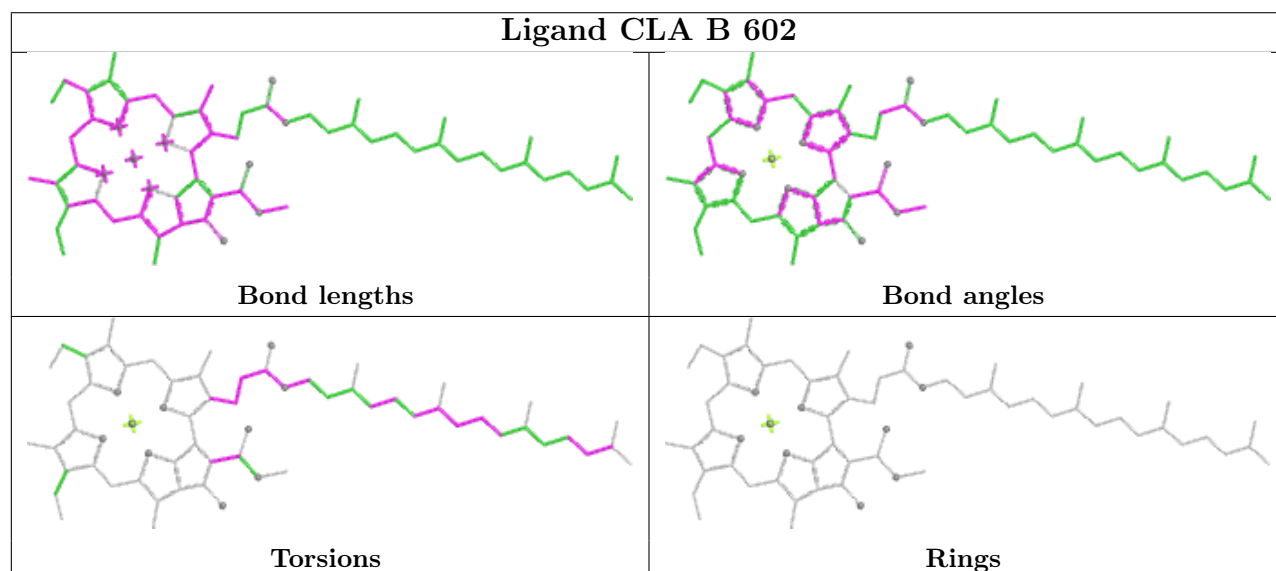
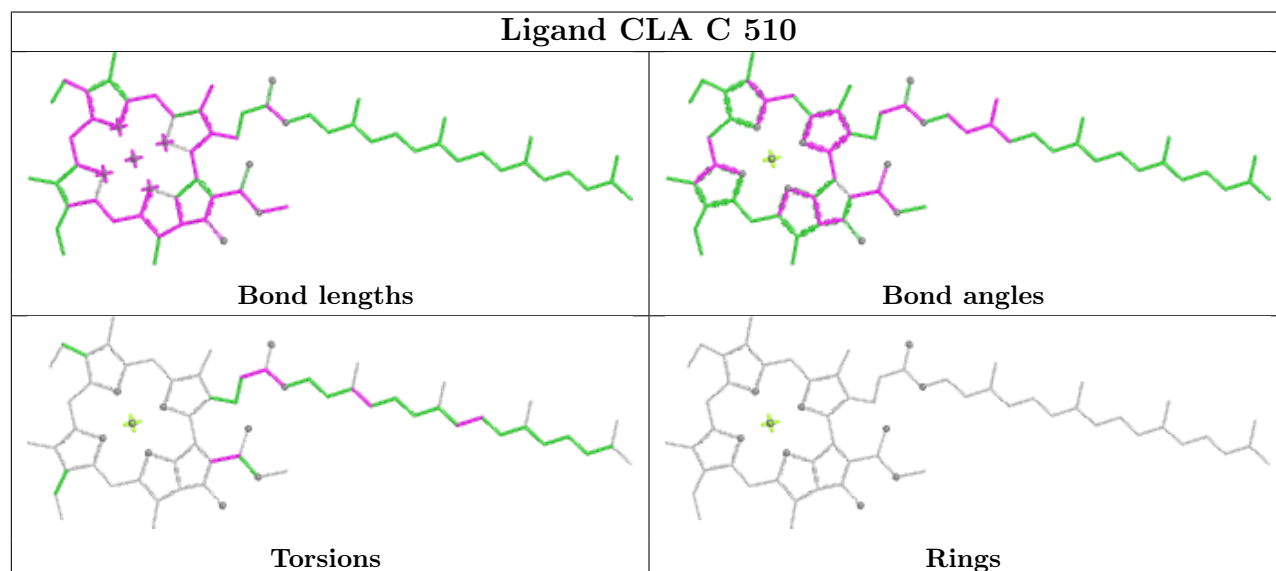
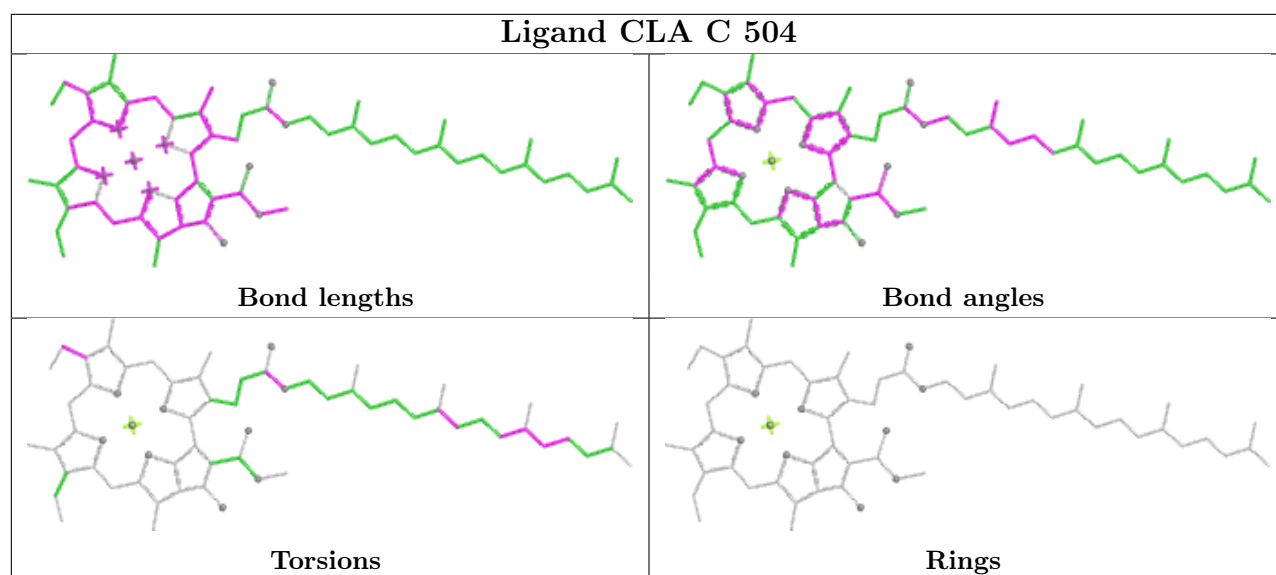


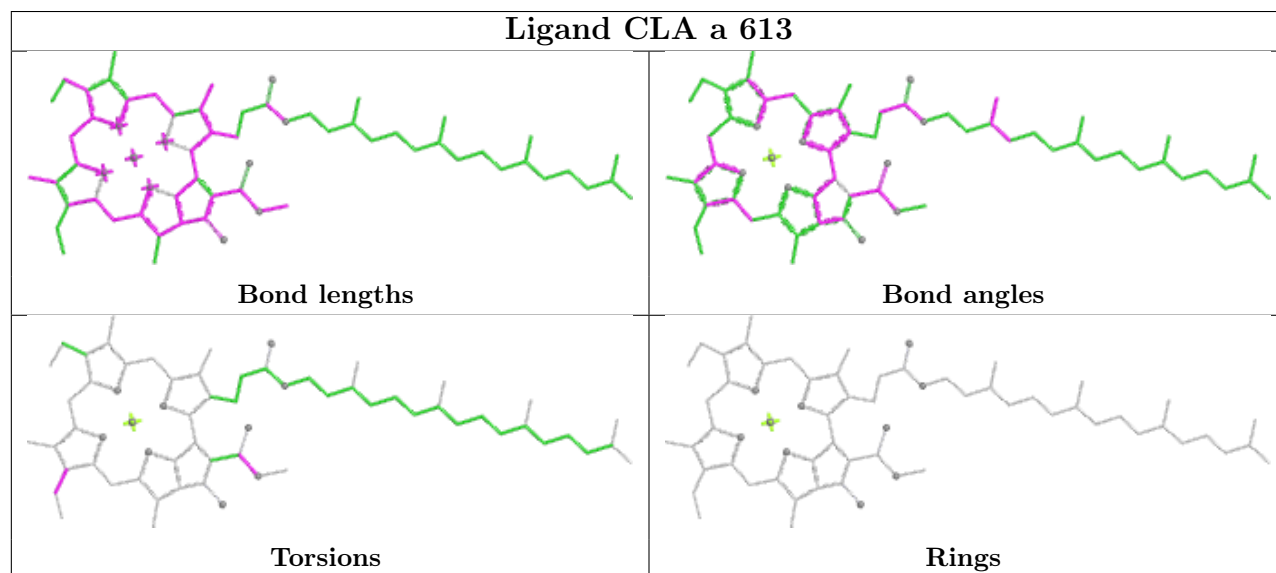
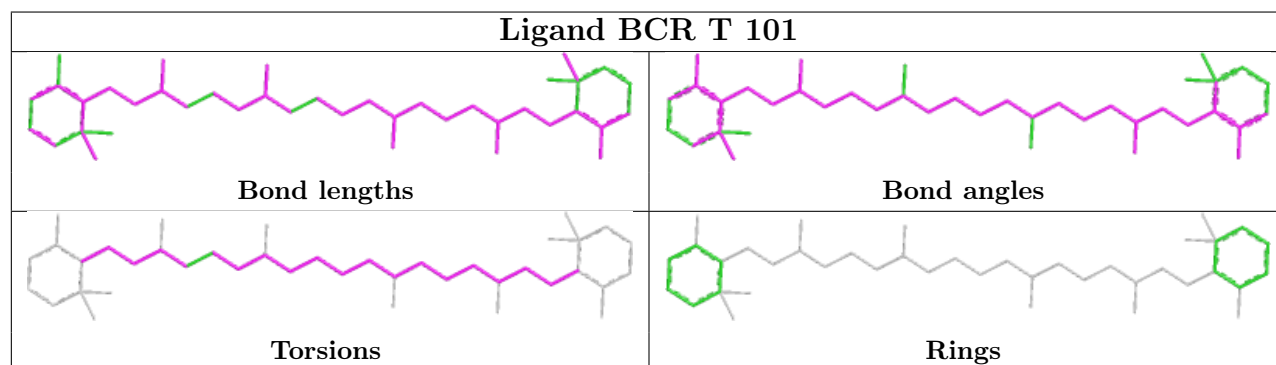
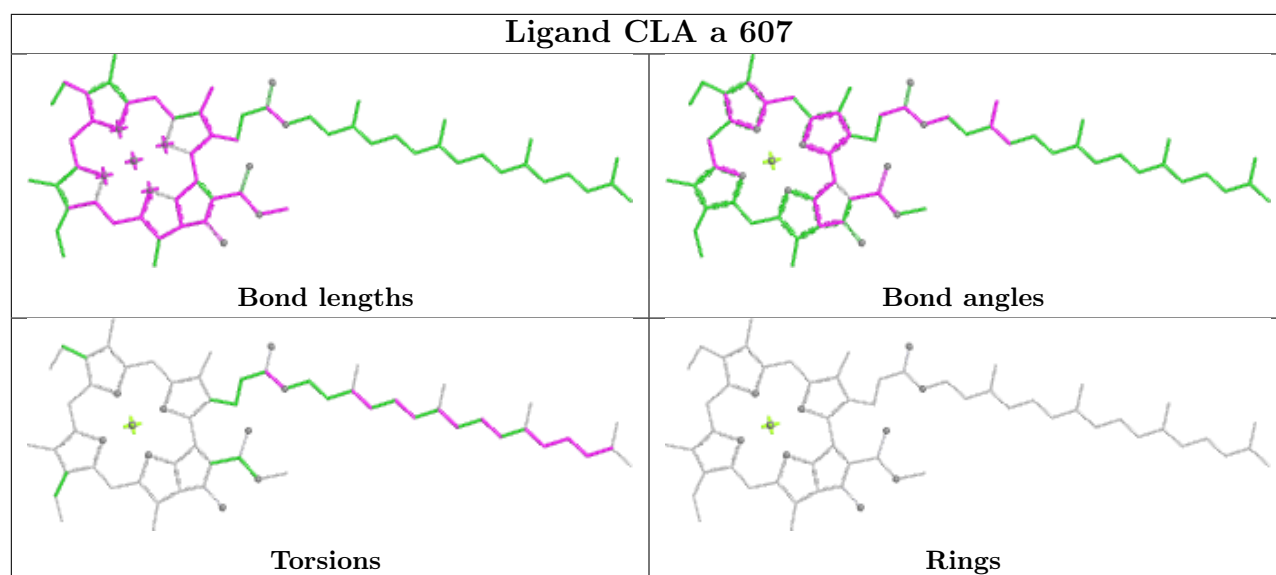


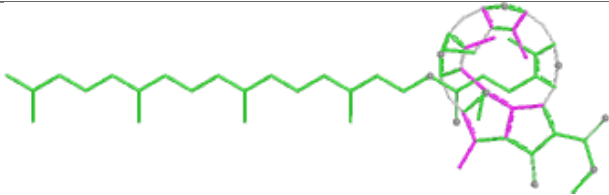
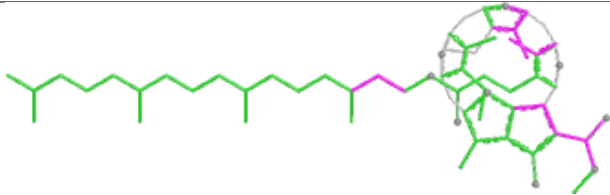
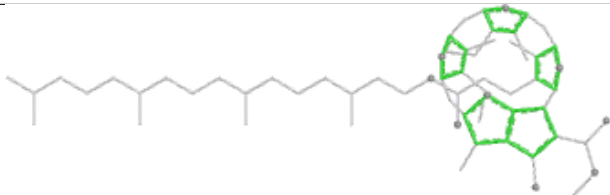
Ligand CLA b 605**Ligand CLA b 607**

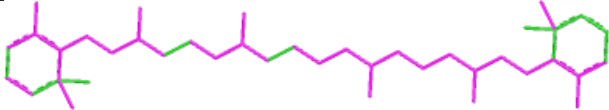
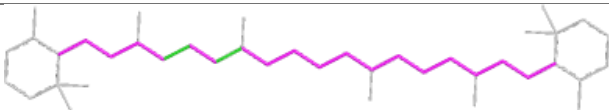
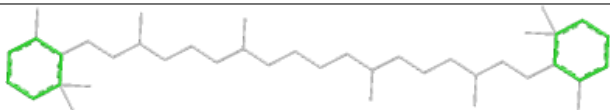


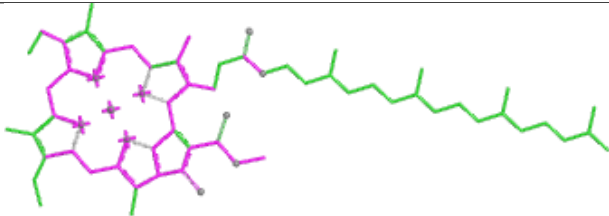
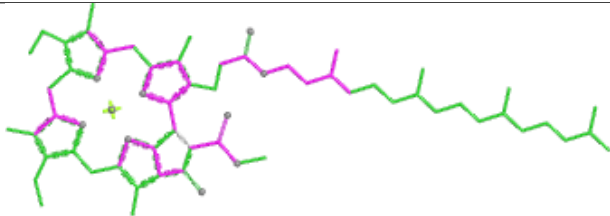
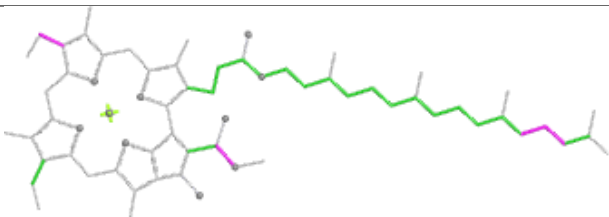
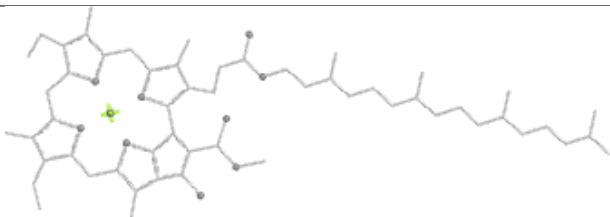


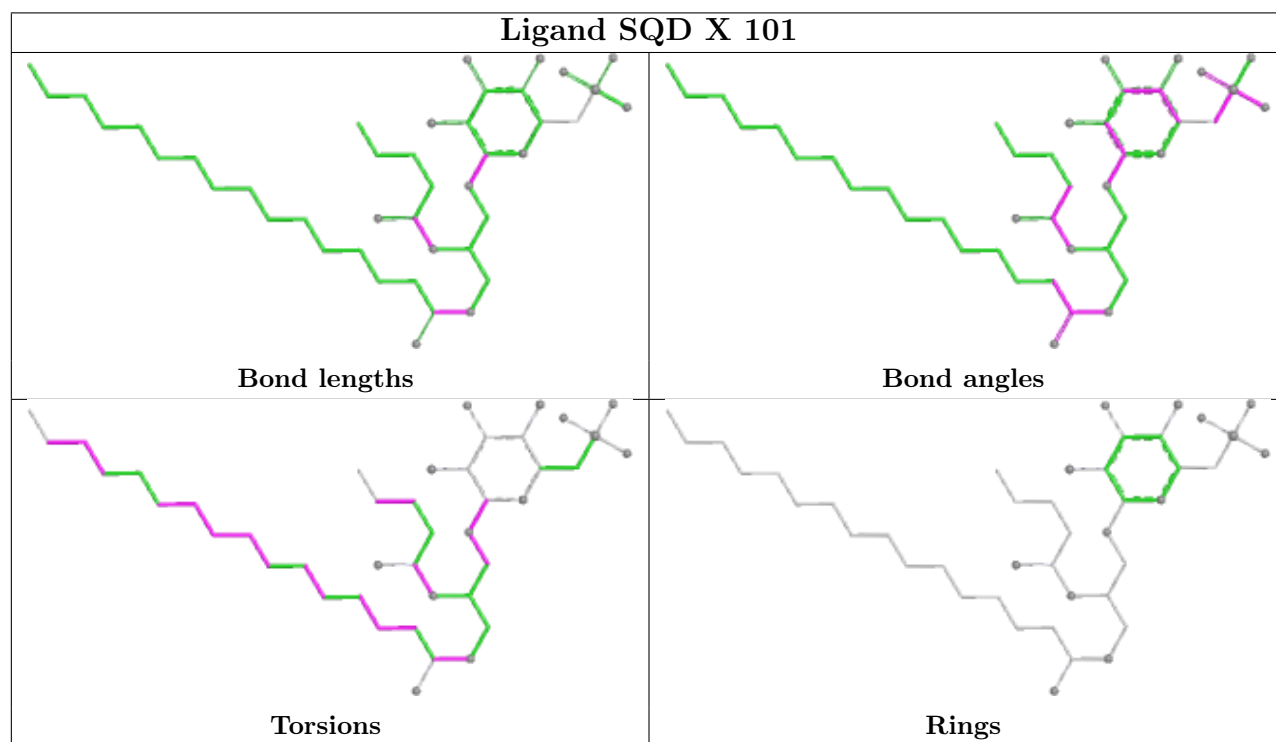
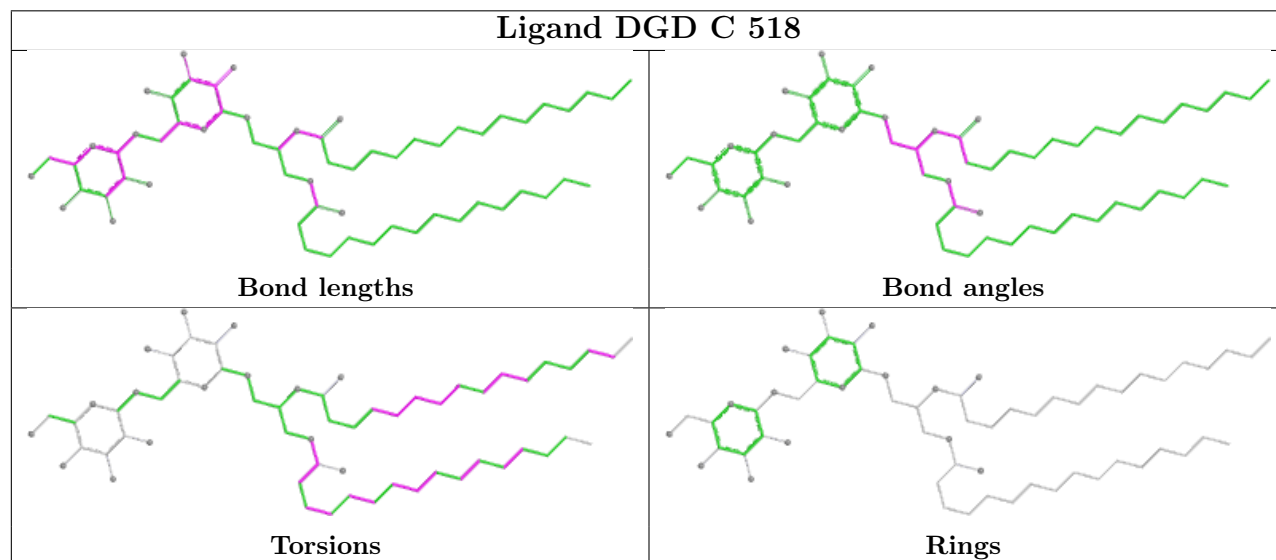
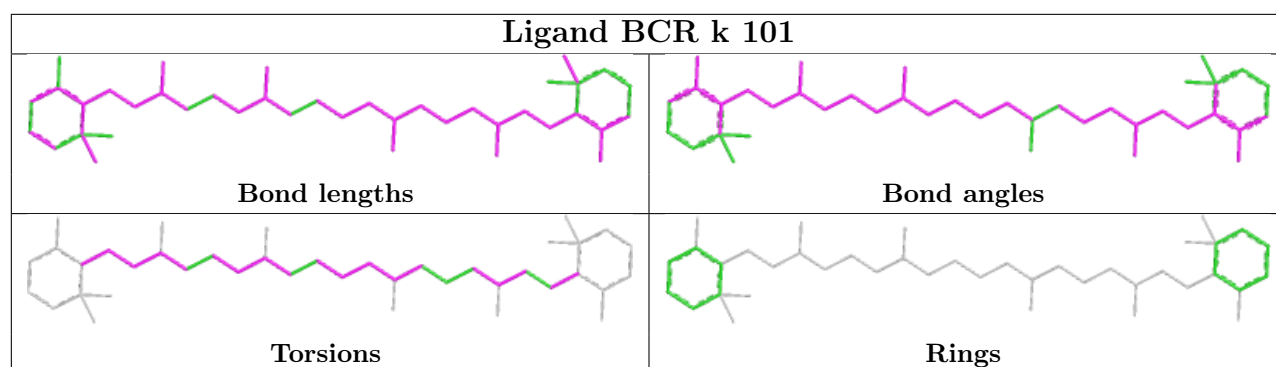




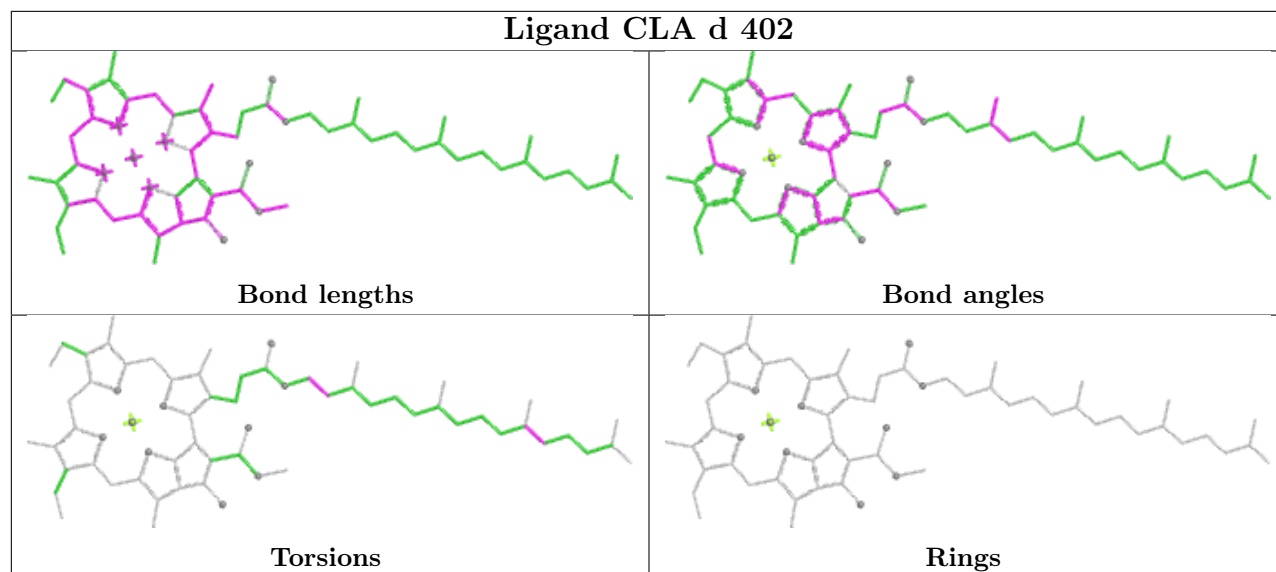
Ligand PHO d 401	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR c 515	
	
Bond lengths	Bond angles
	
Torsions	Rings

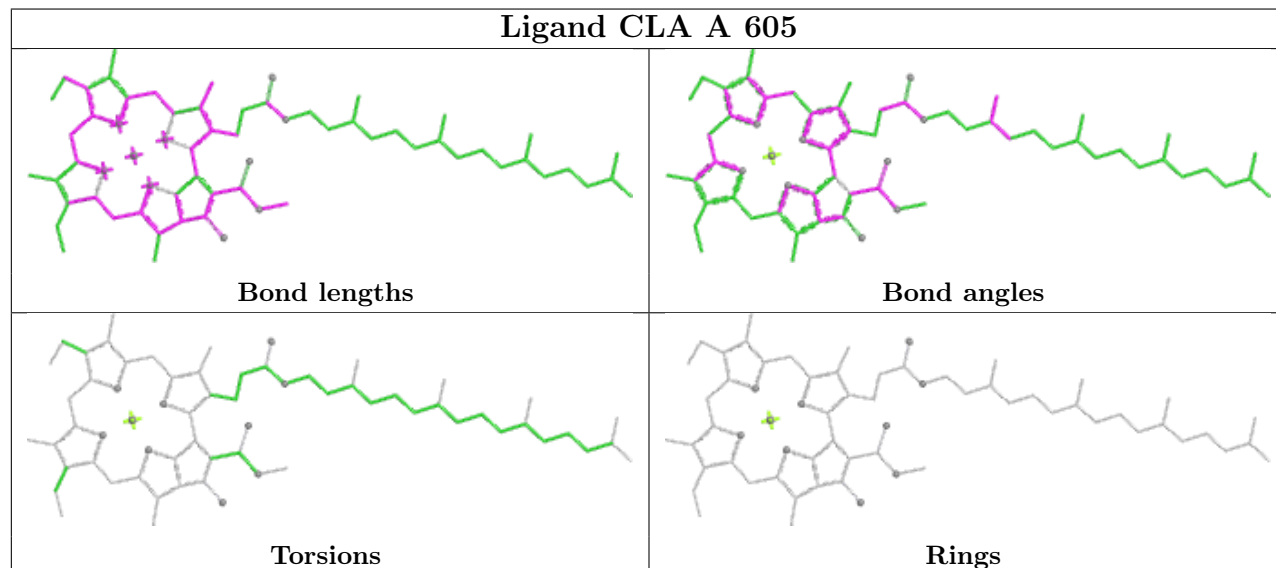
Ligand CLA b 616	
	
Bond lengths	Bond angles
	
Torsions	Rings



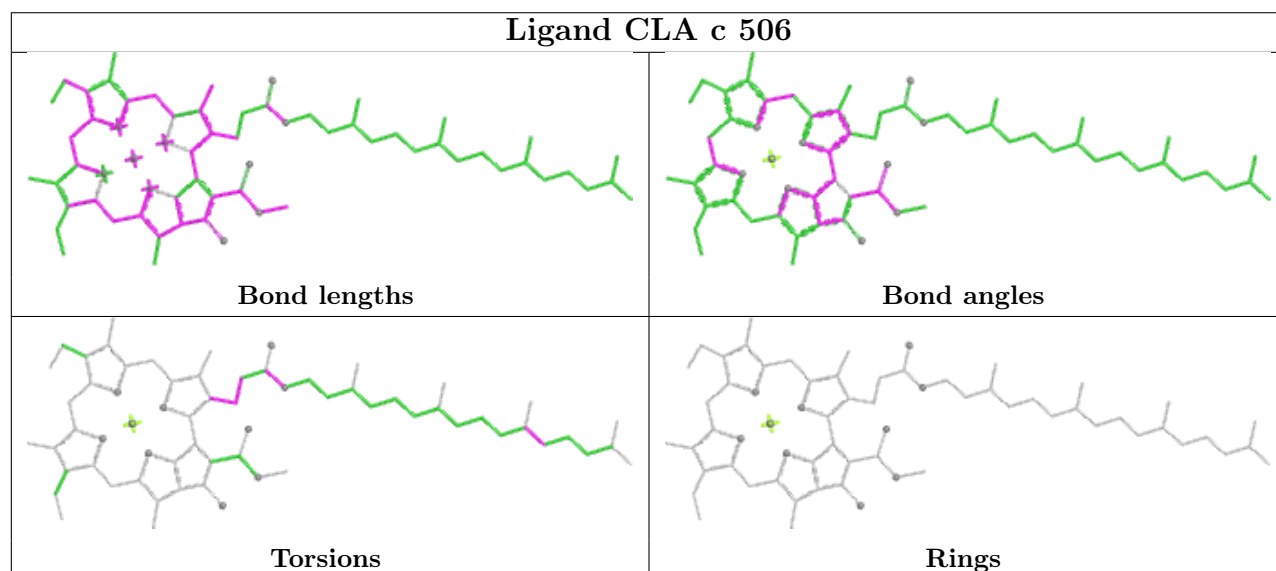
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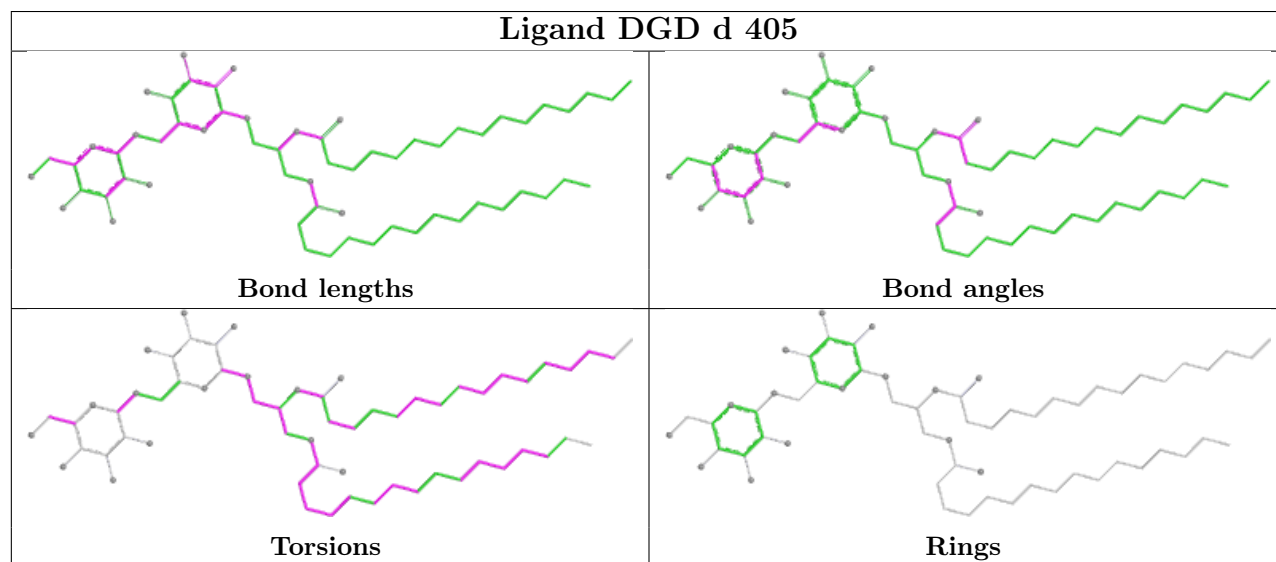
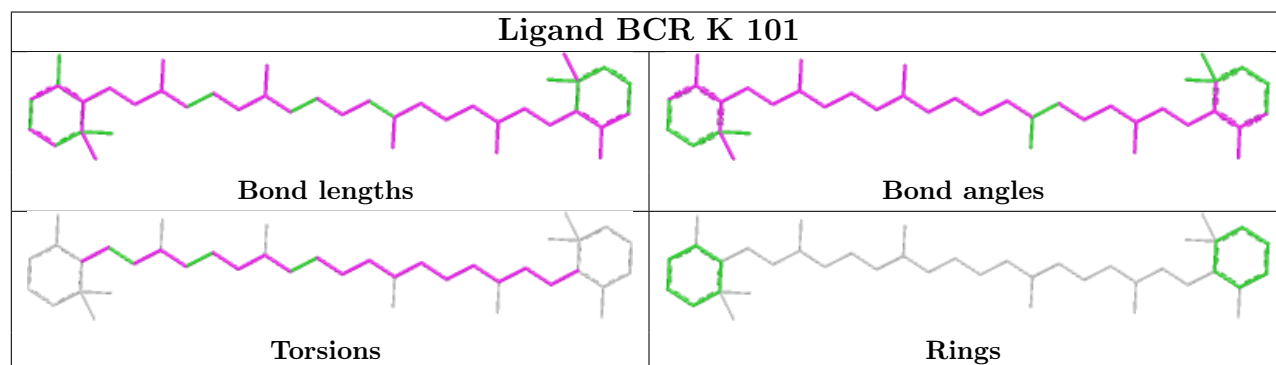
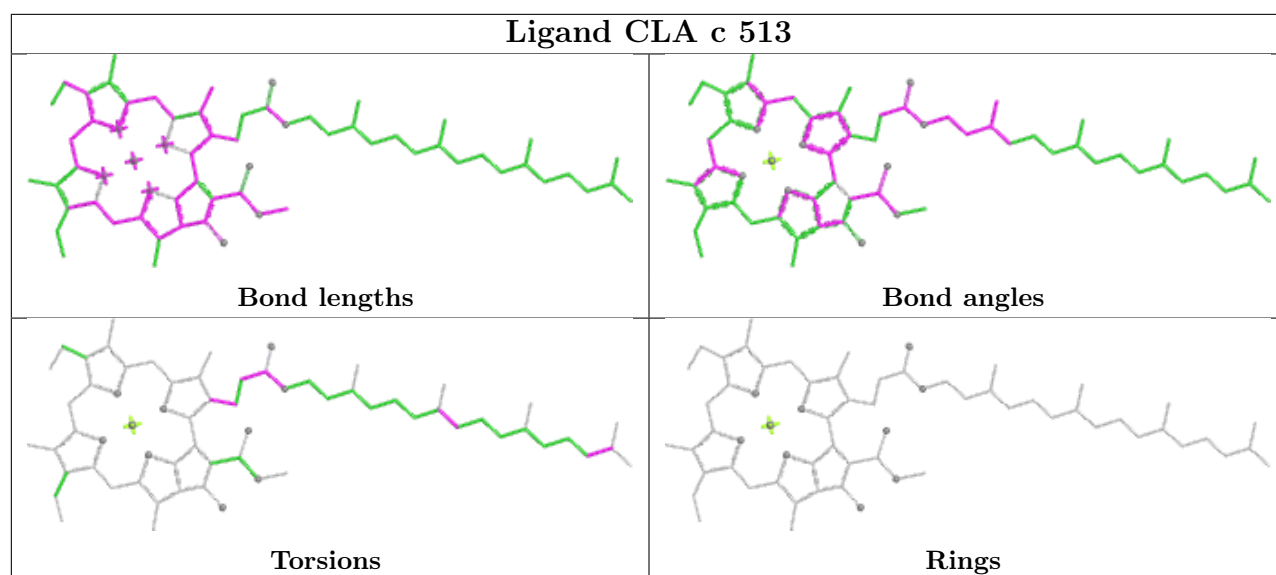


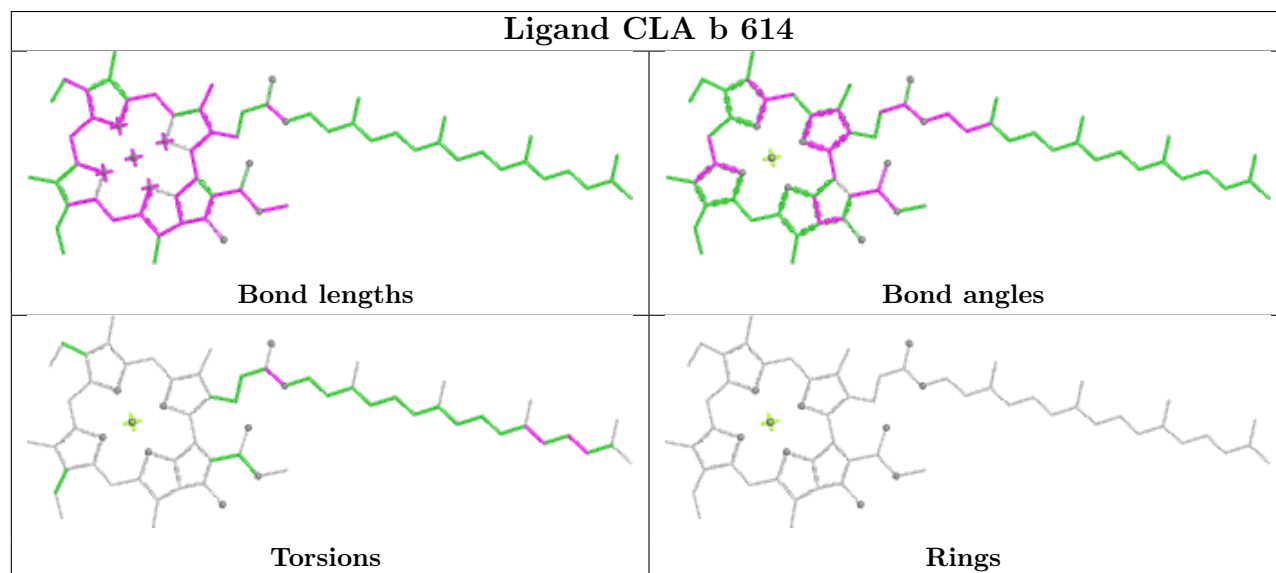
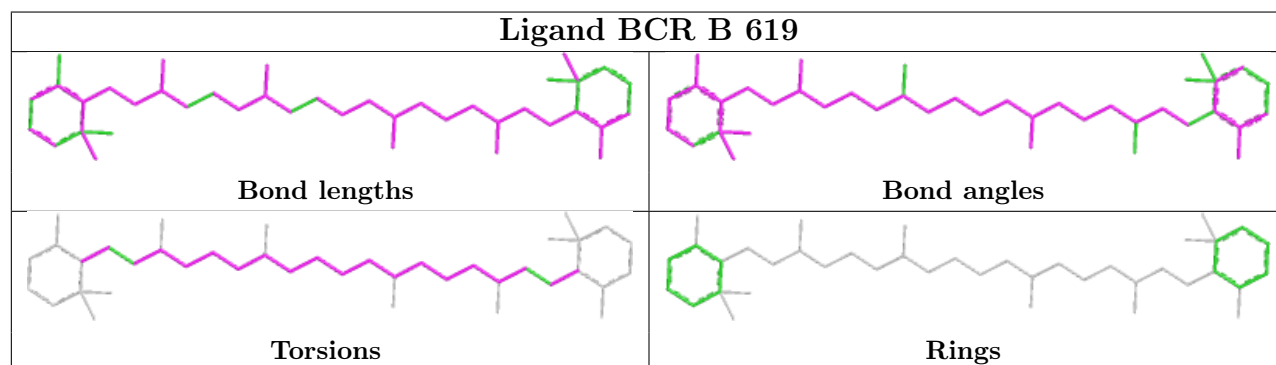
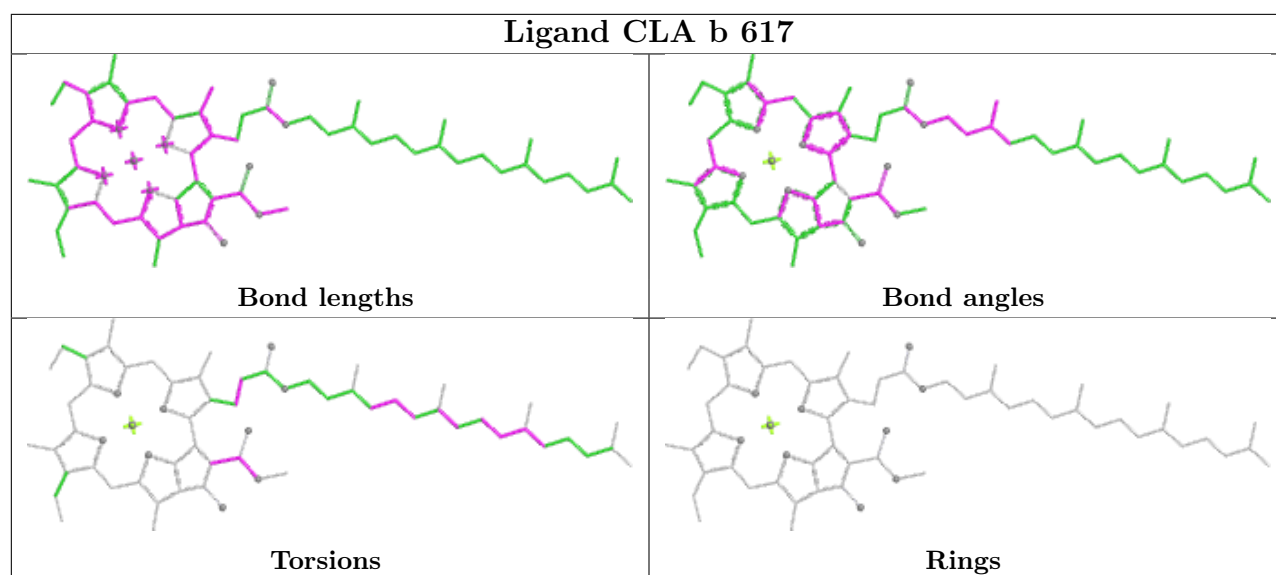
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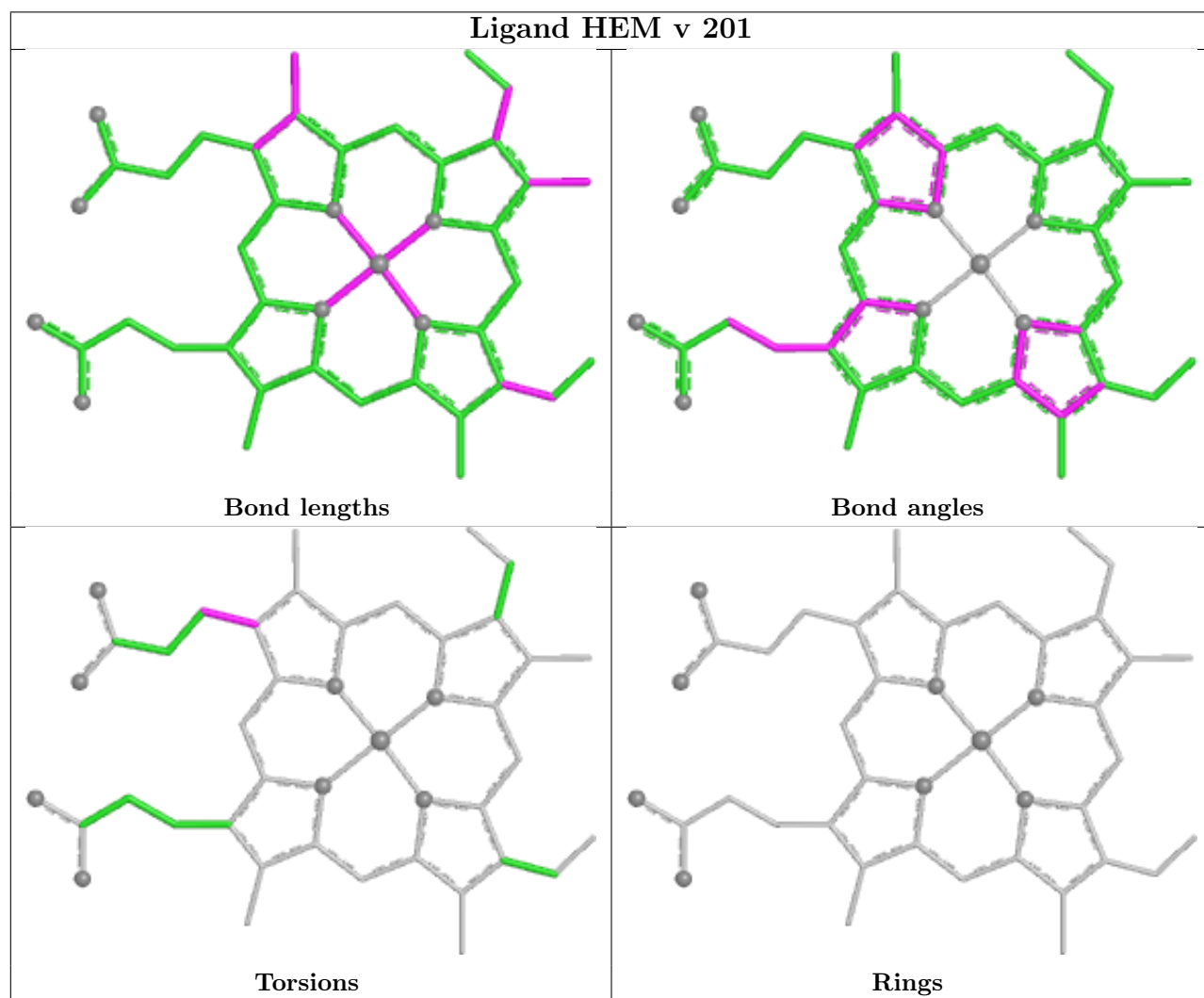
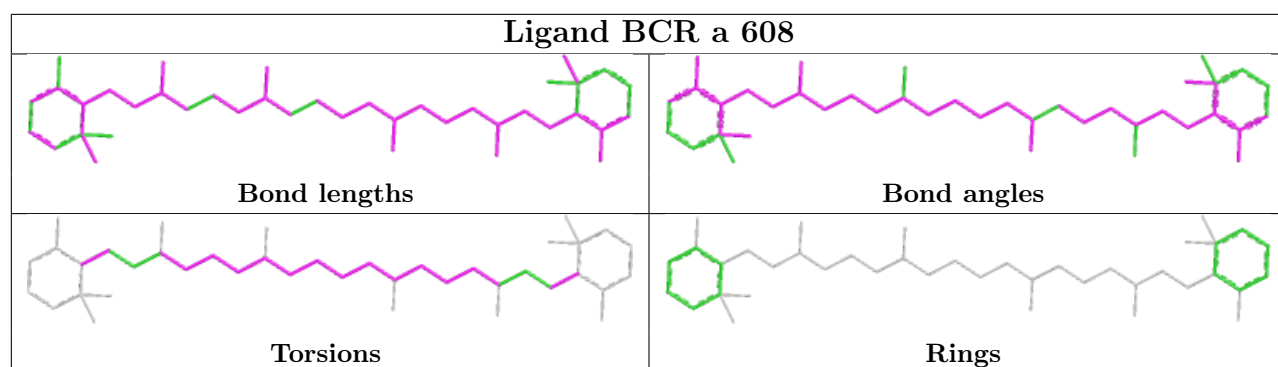


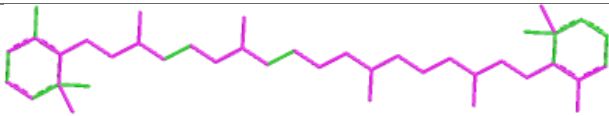
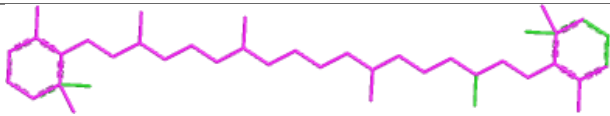
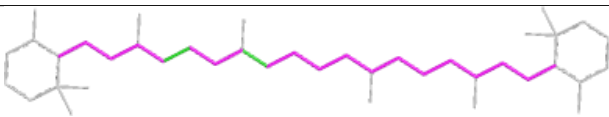
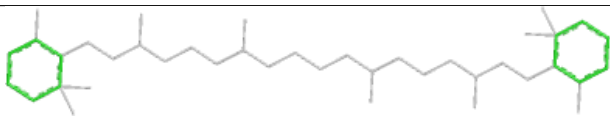
Ligand CLA c 506

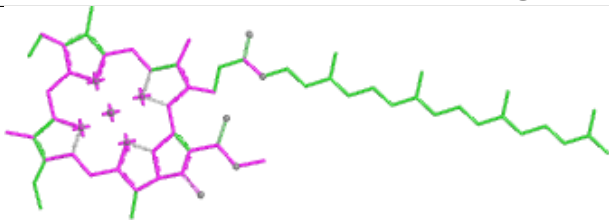
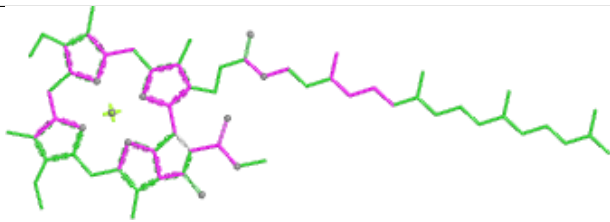
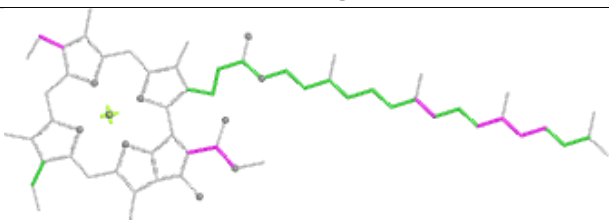
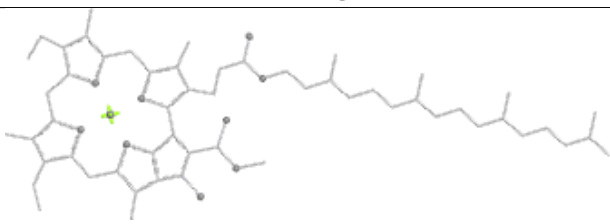


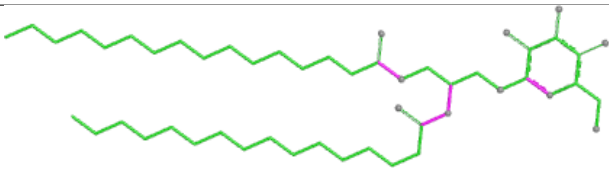
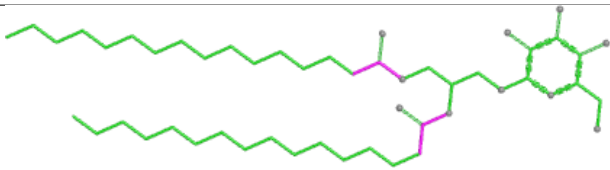
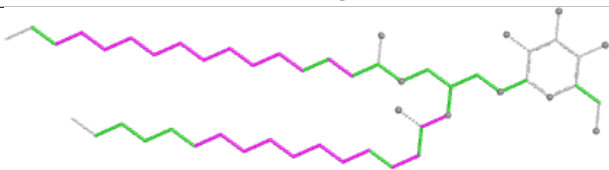
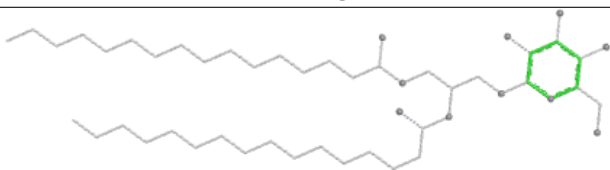


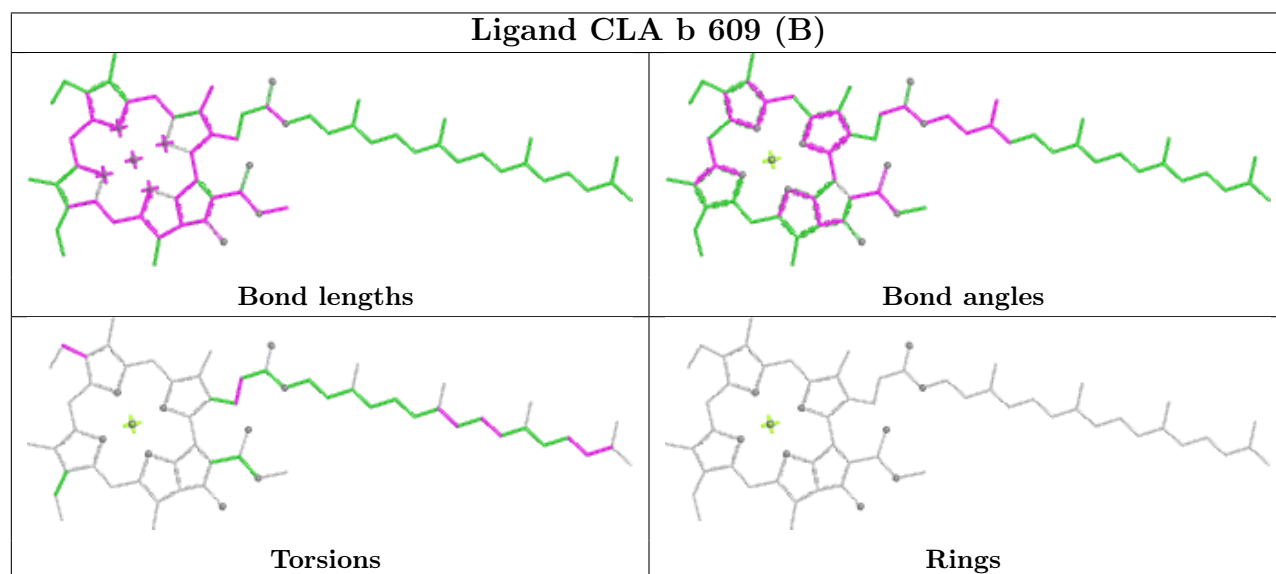
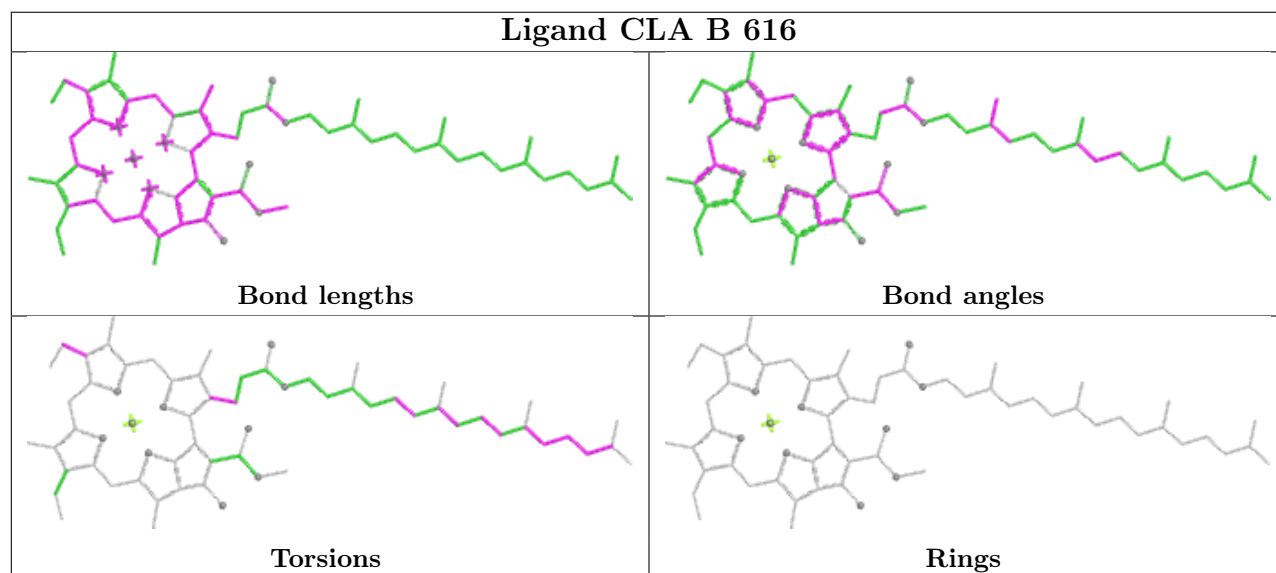
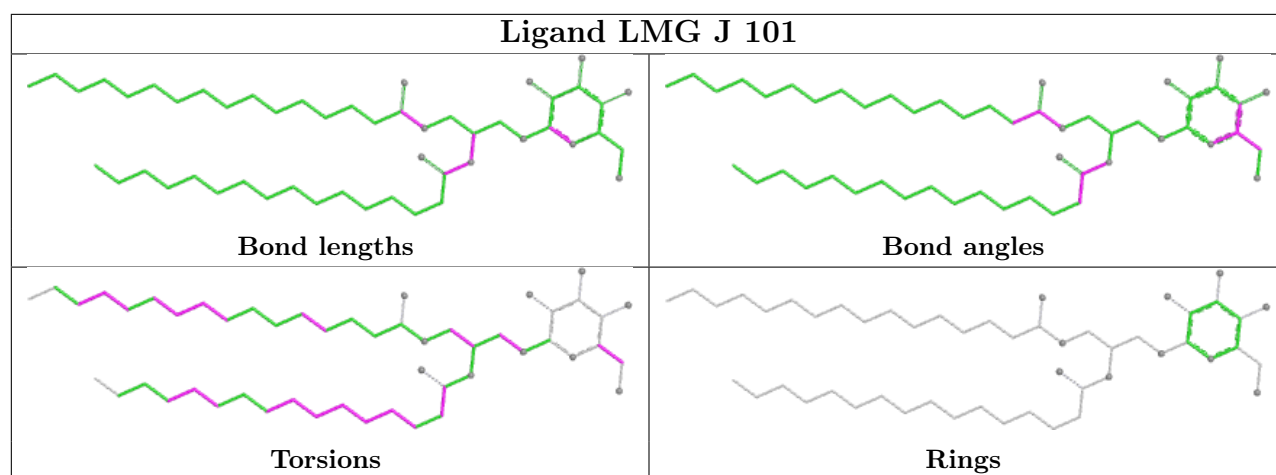




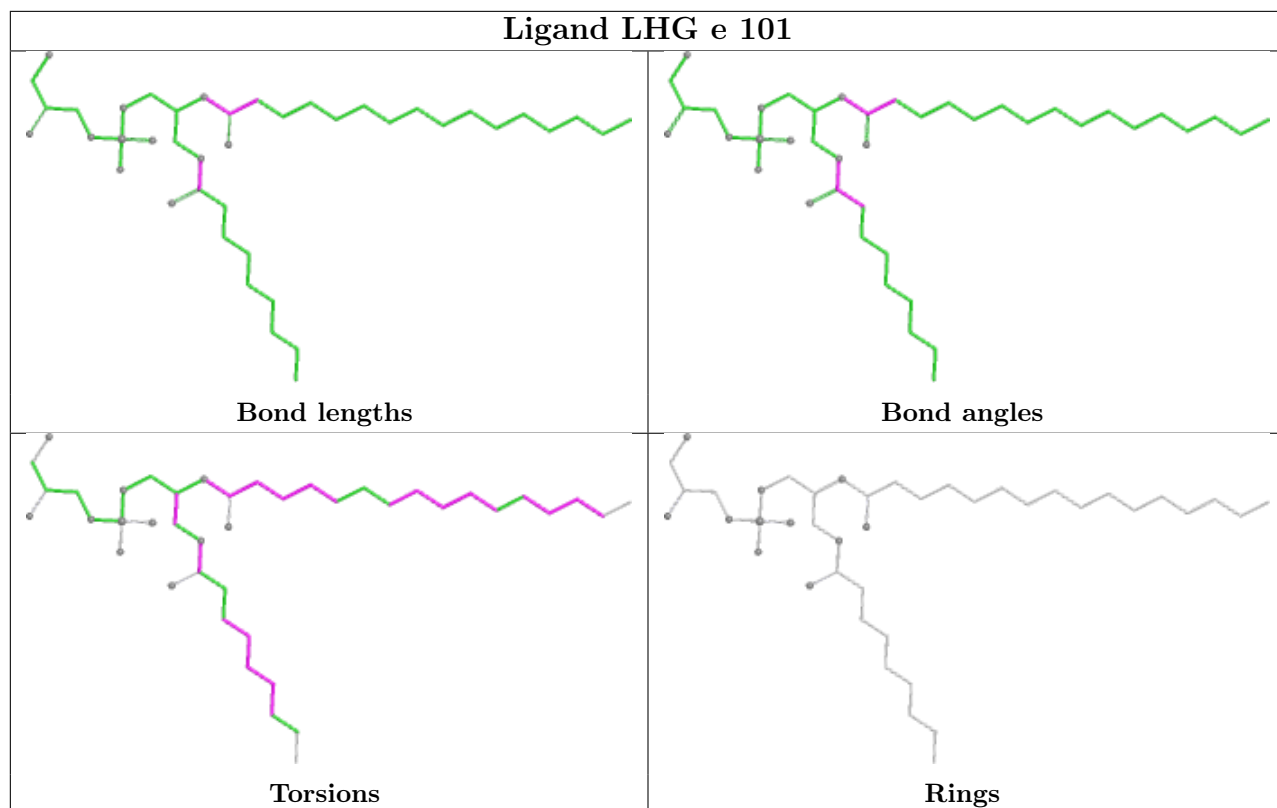
Ligand BCR H 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA c 505	
	
Bond lengths	Bond angles
	
Torsions	Rings

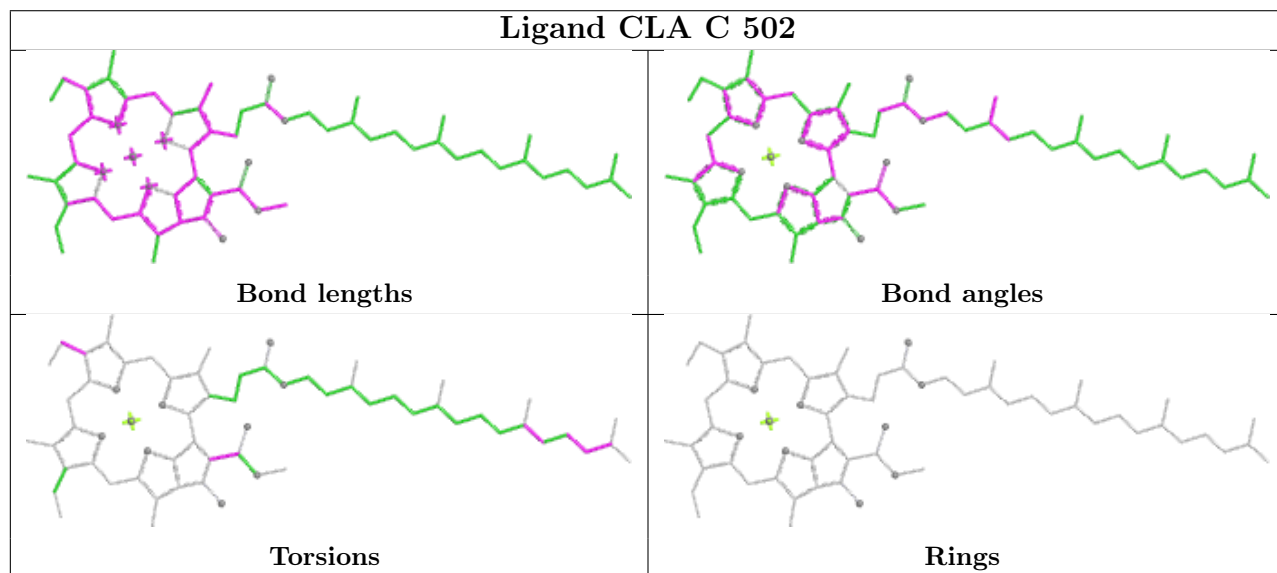
Ligand LMG b 623	
	
Bond lengths	Bond angles
	
Torsions	Rings

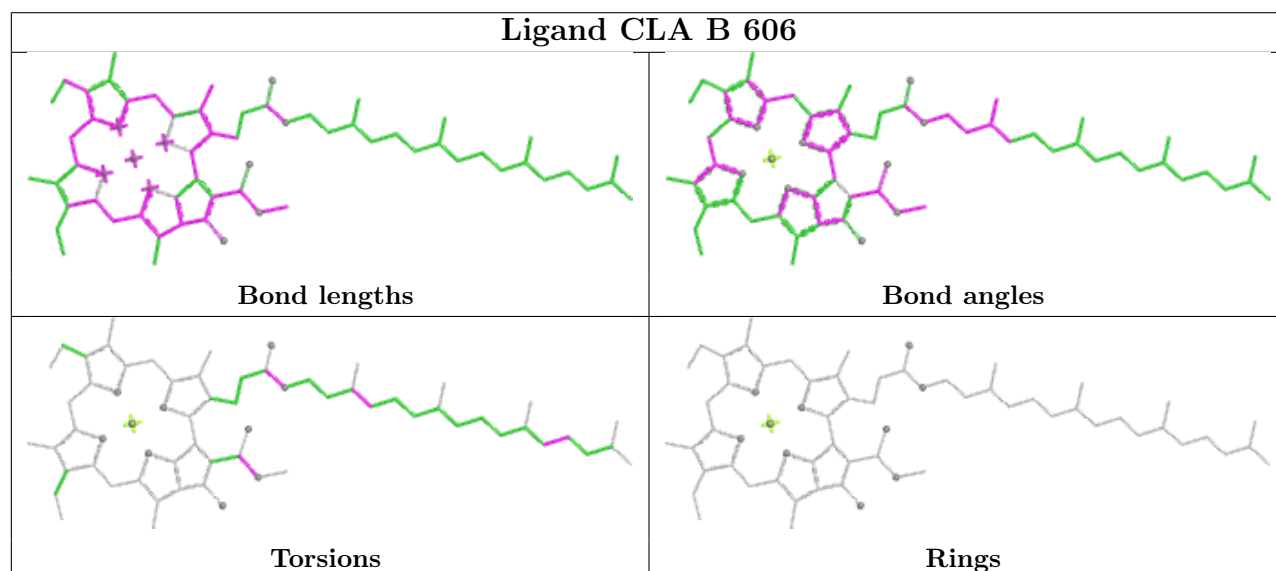
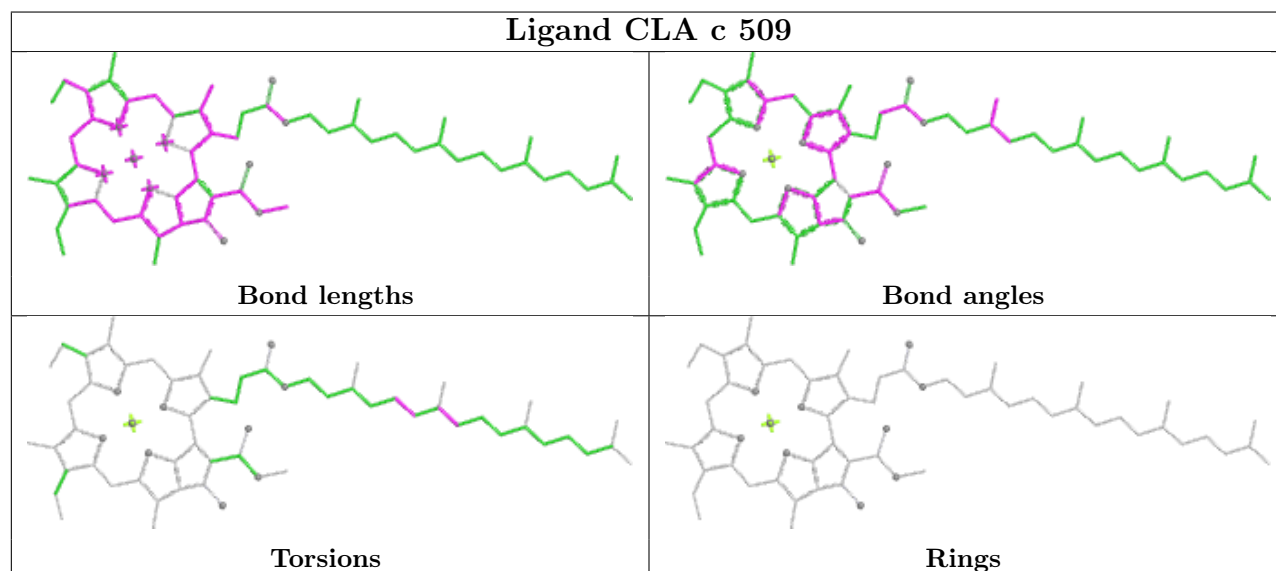
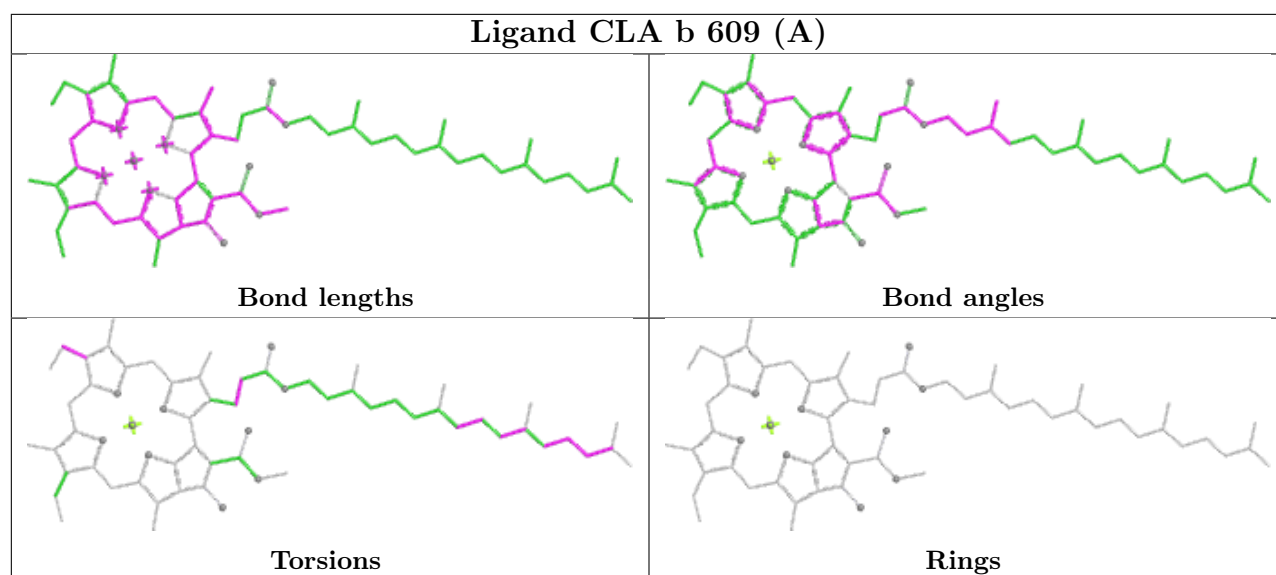


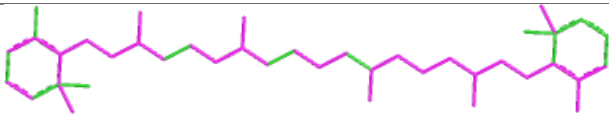
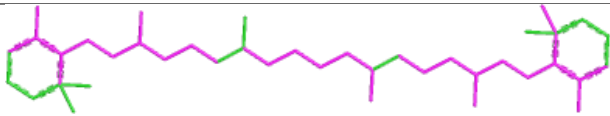
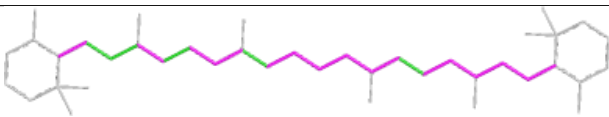
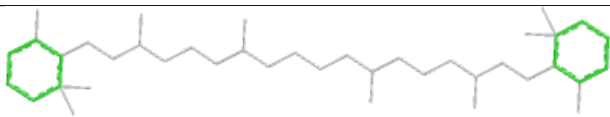
Ligand LHG e 101

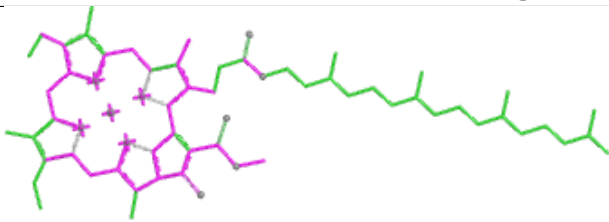
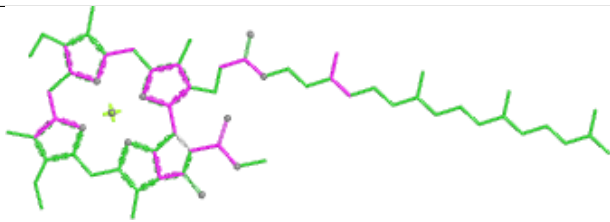
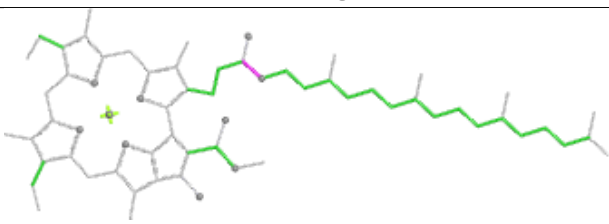
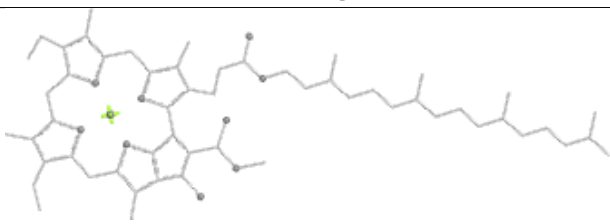


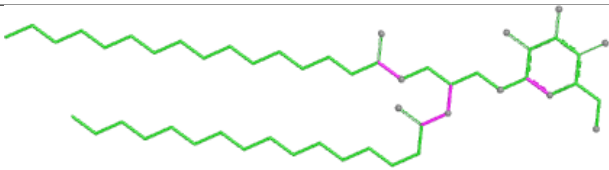
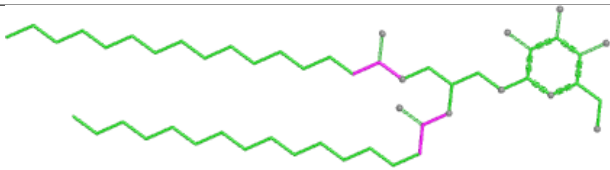
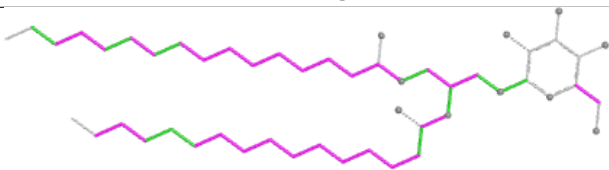
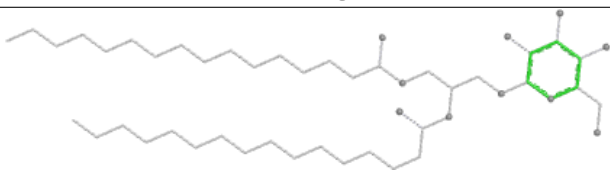
Ligand CLA C 502

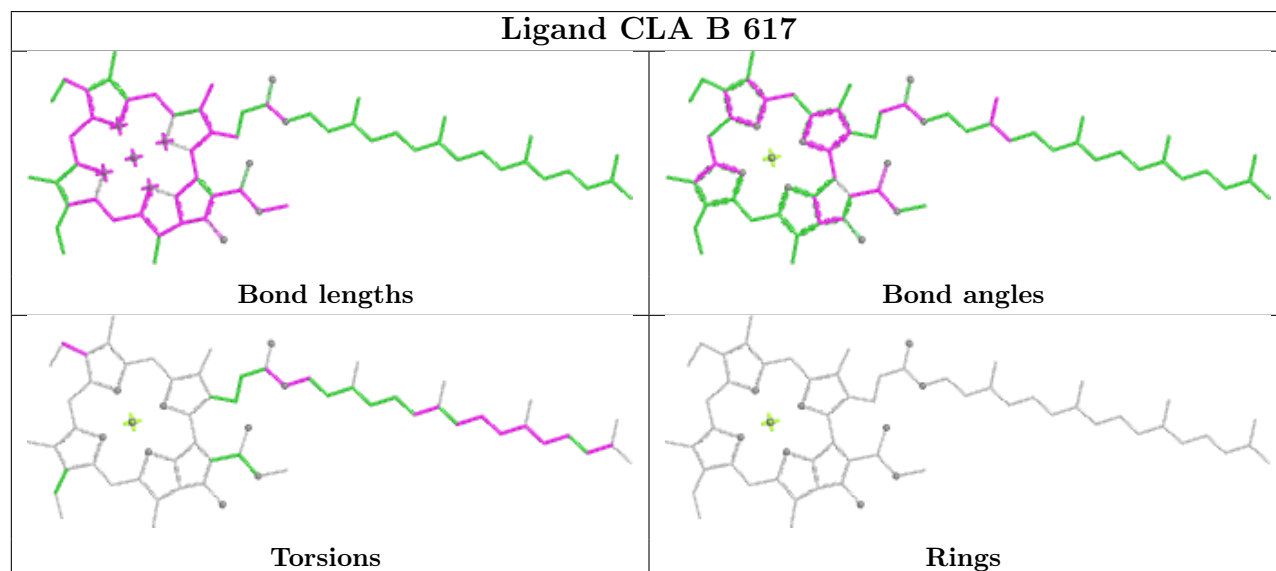
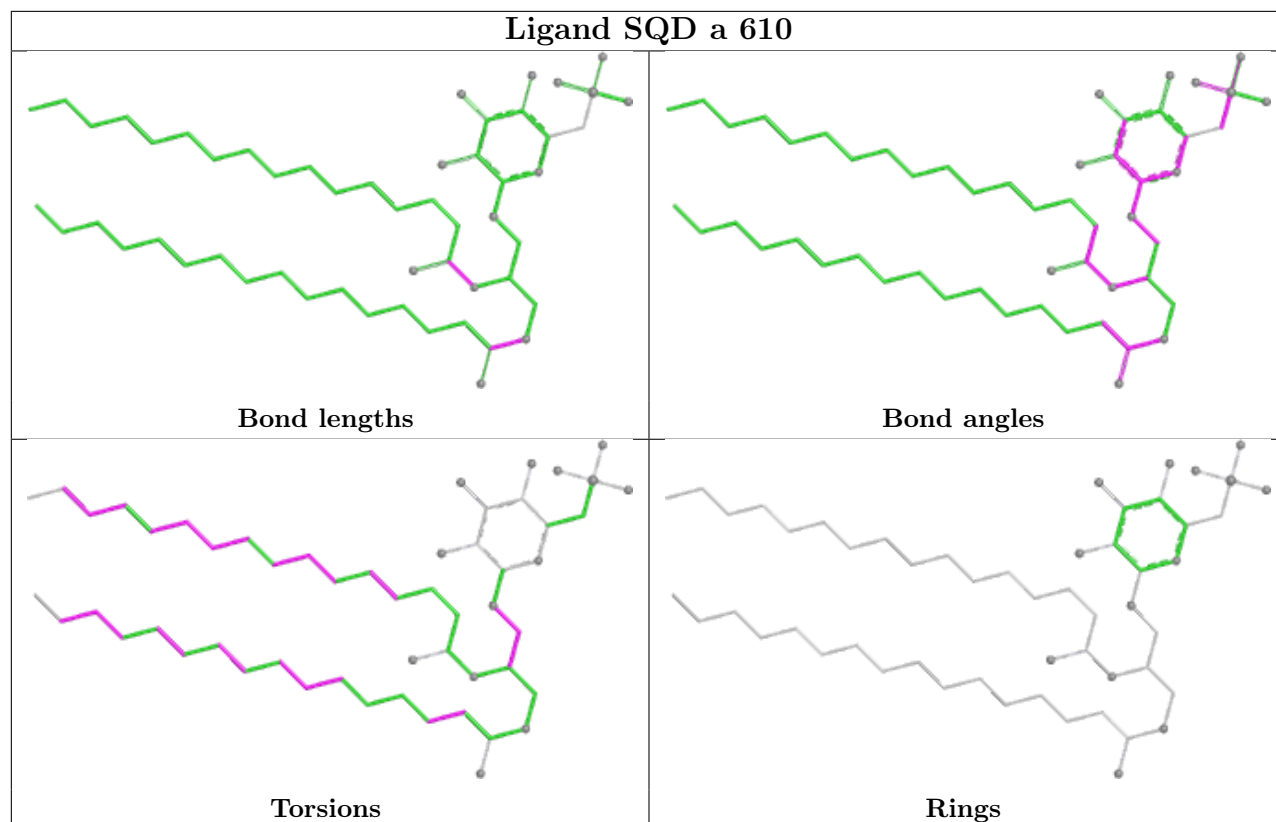


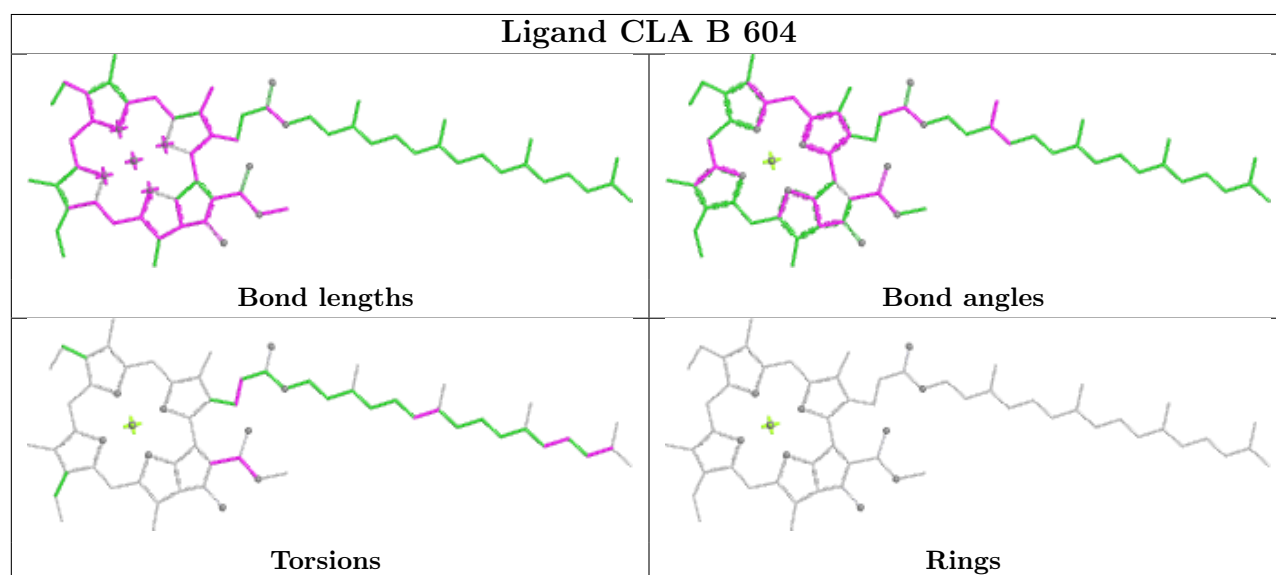
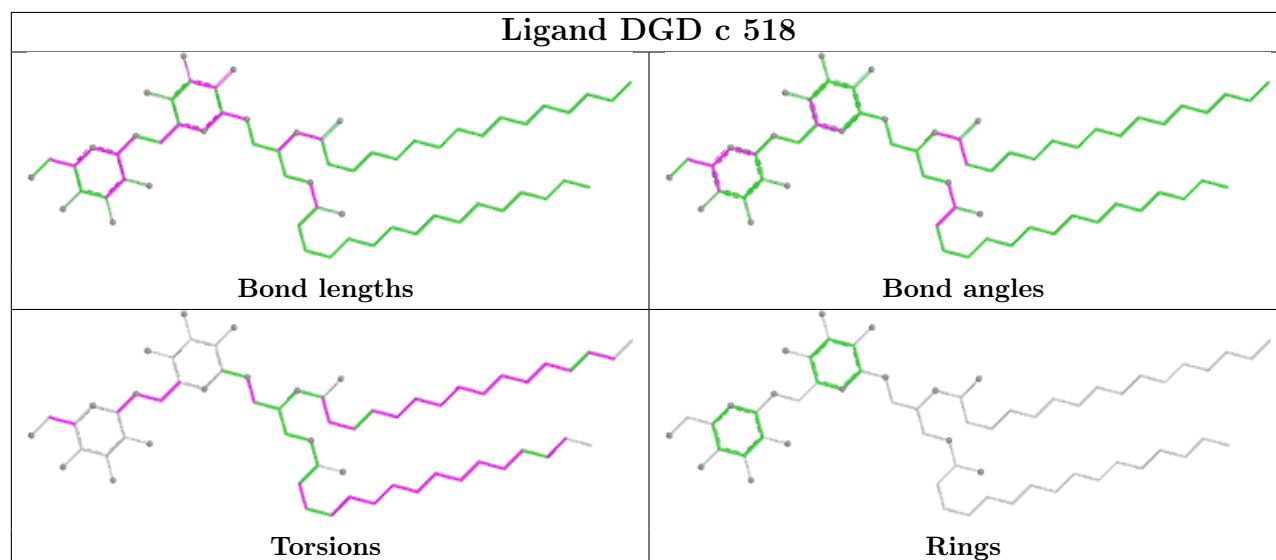
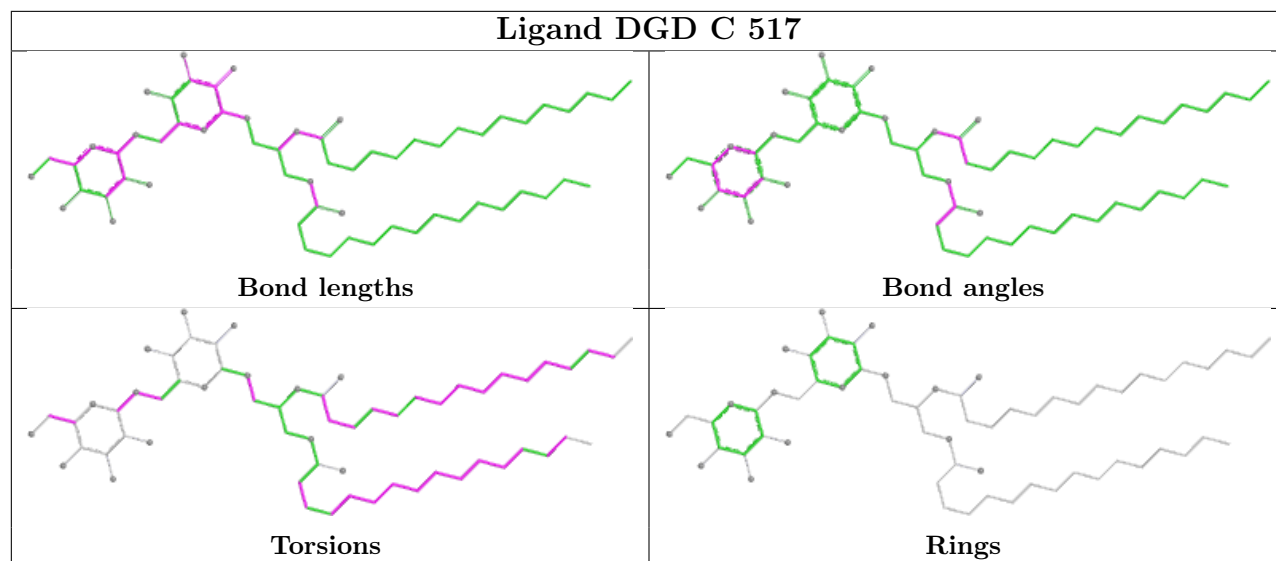


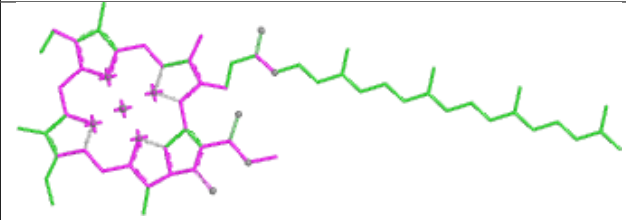
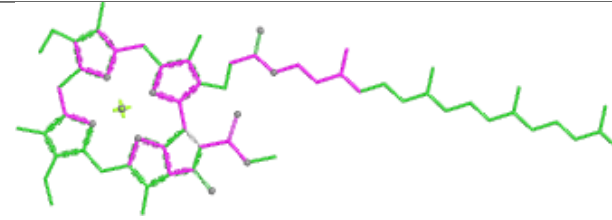
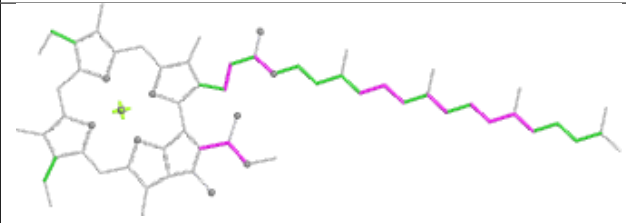
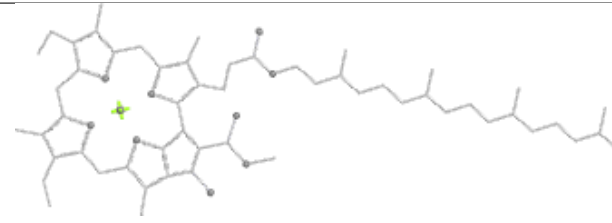
Ligand BCR C 521	
	
Bond lengths	Bond angles
	
Torsions	Rings

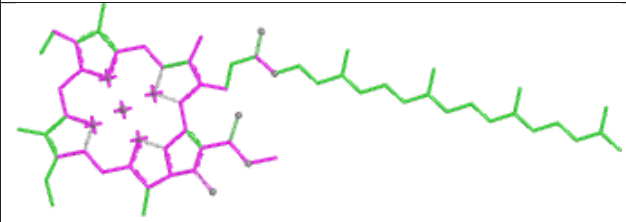
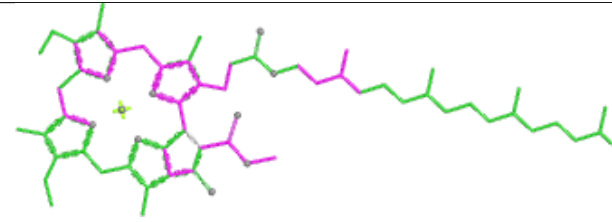
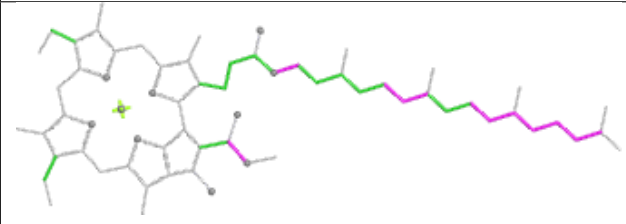
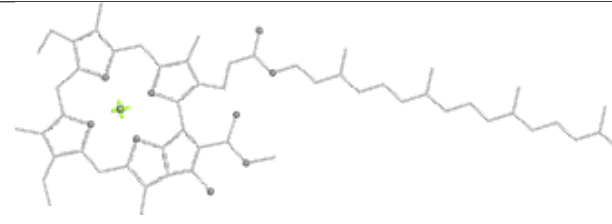
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Bond lengths	Bond angles
	
Torsions	Rings

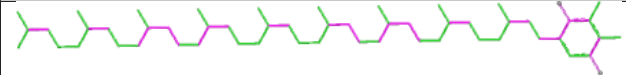
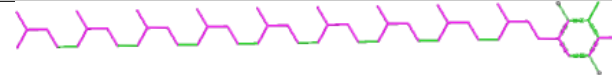
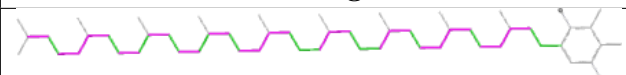
Ligand LMG a 611	
	
Bond lengths	Bond angles
	
Torsions	Rings

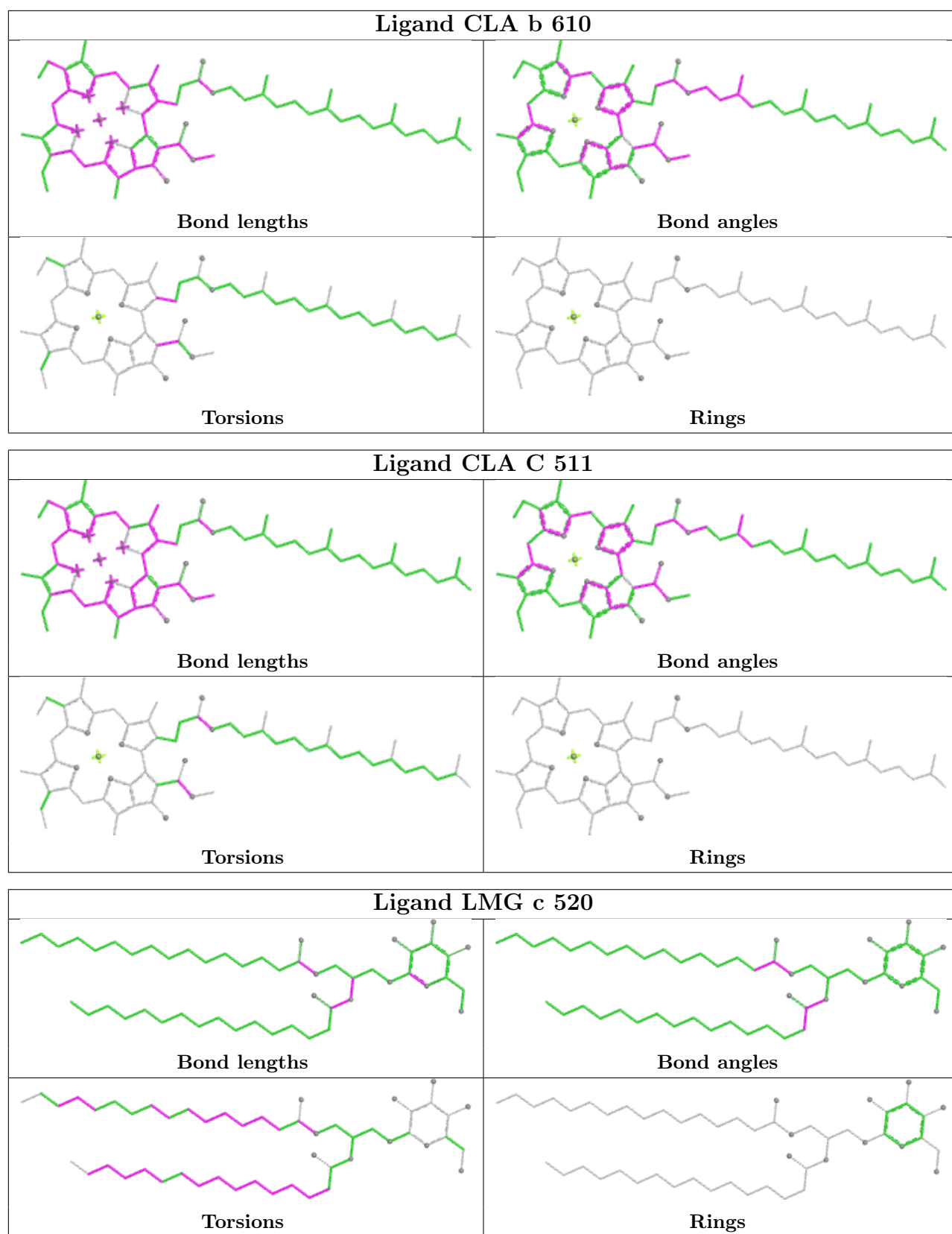


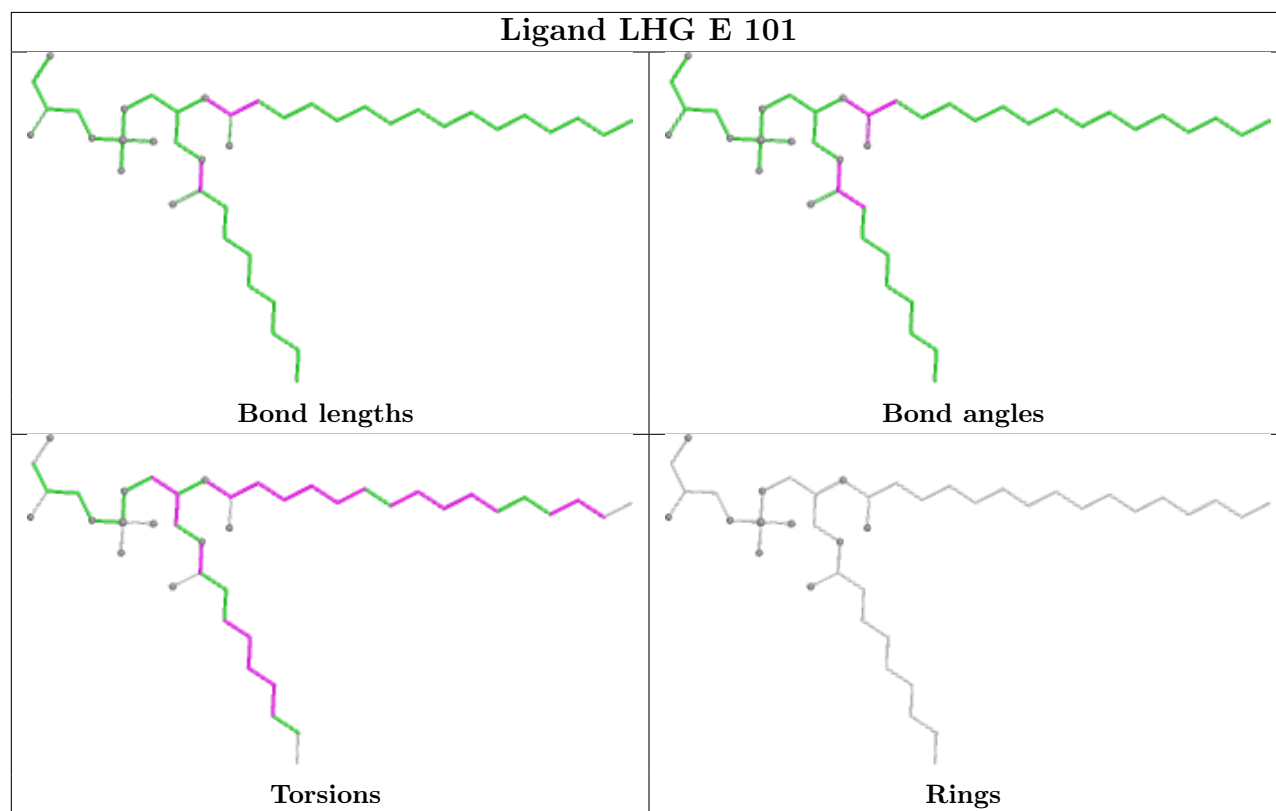
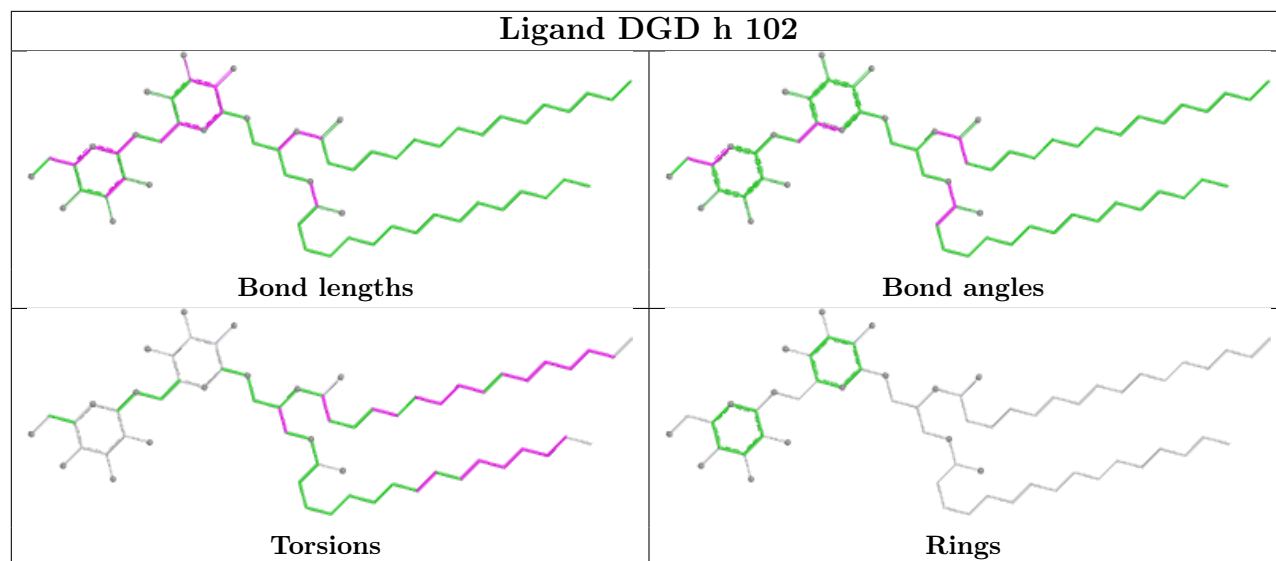


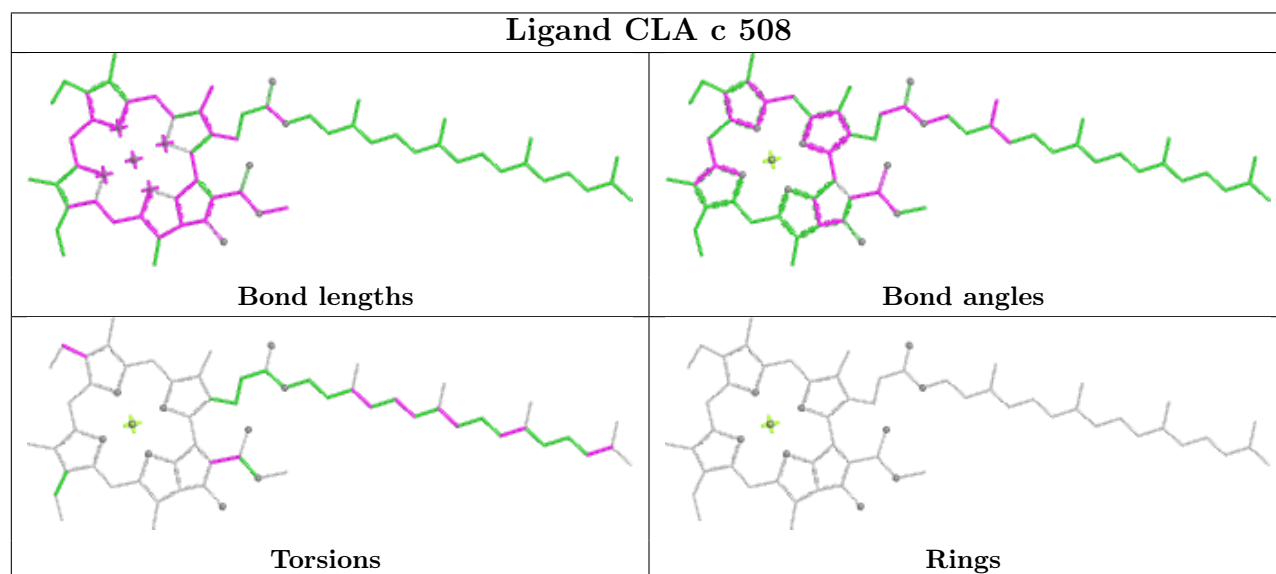
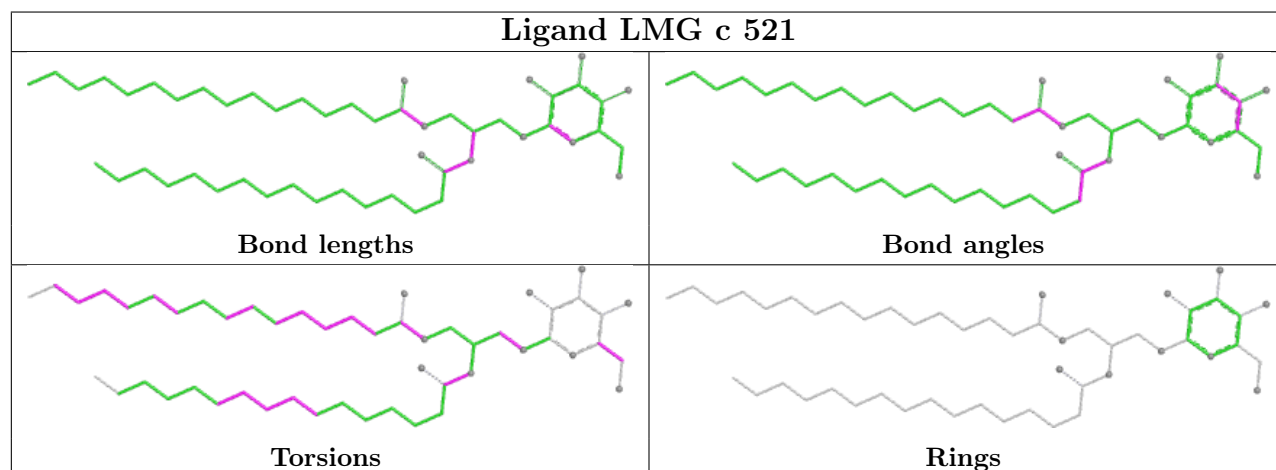
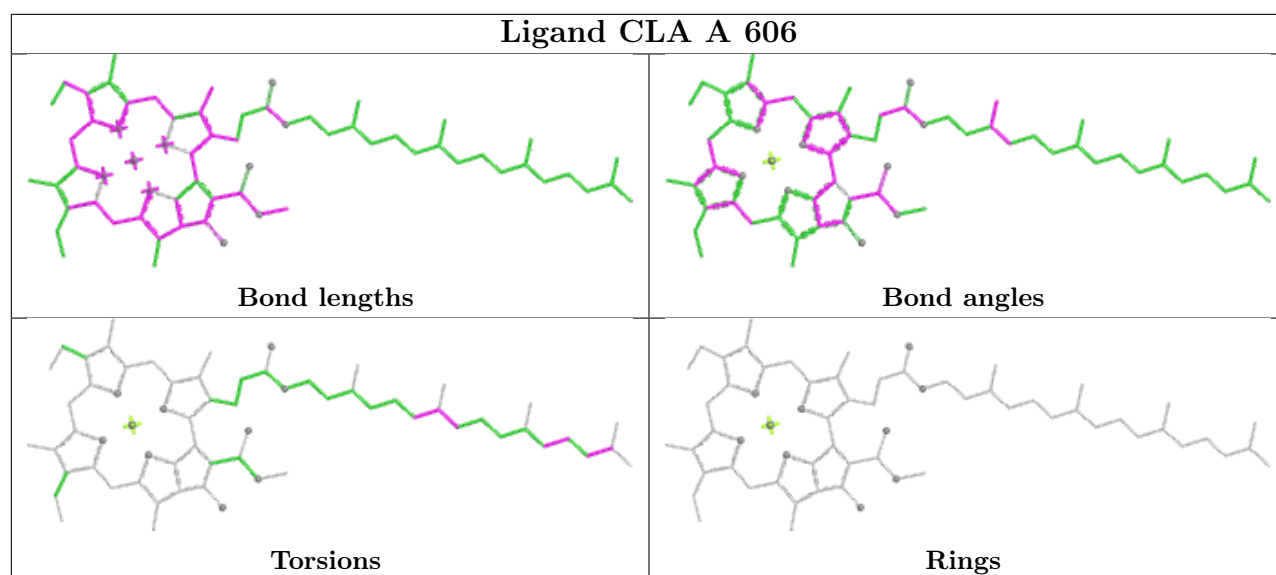
Ligand CLA B 615	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA c 507	
	
Bond lengths	Bond angles
	
Torsions	Rings

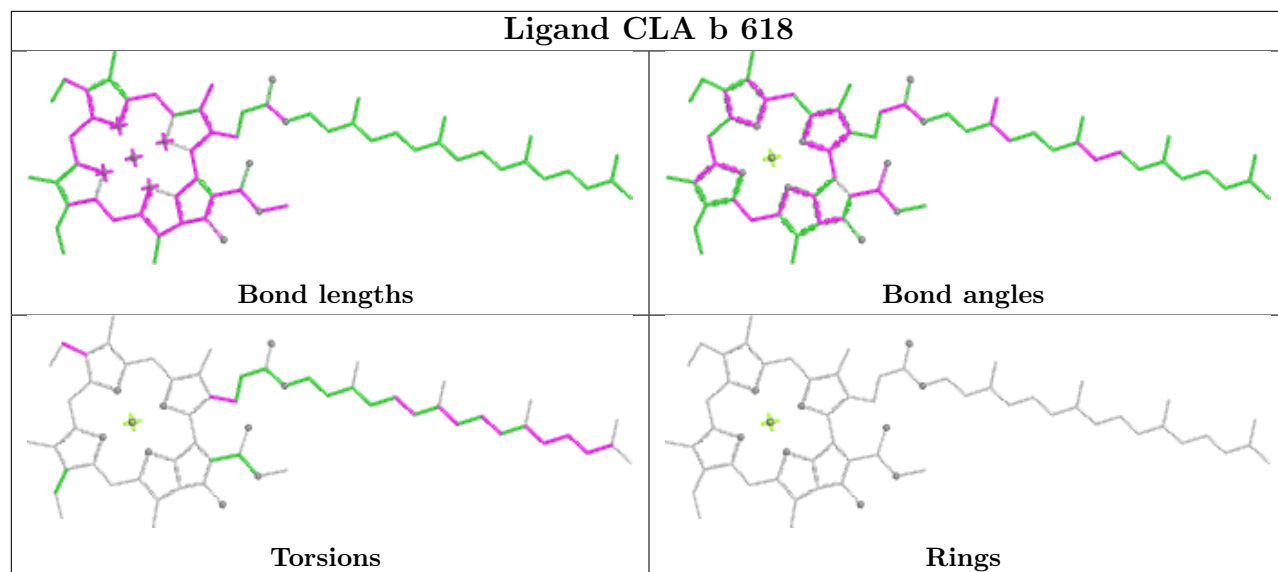
Ligand PL9 D 405	
	
Bond lengths	Bond angles
	
Torsions	Rings



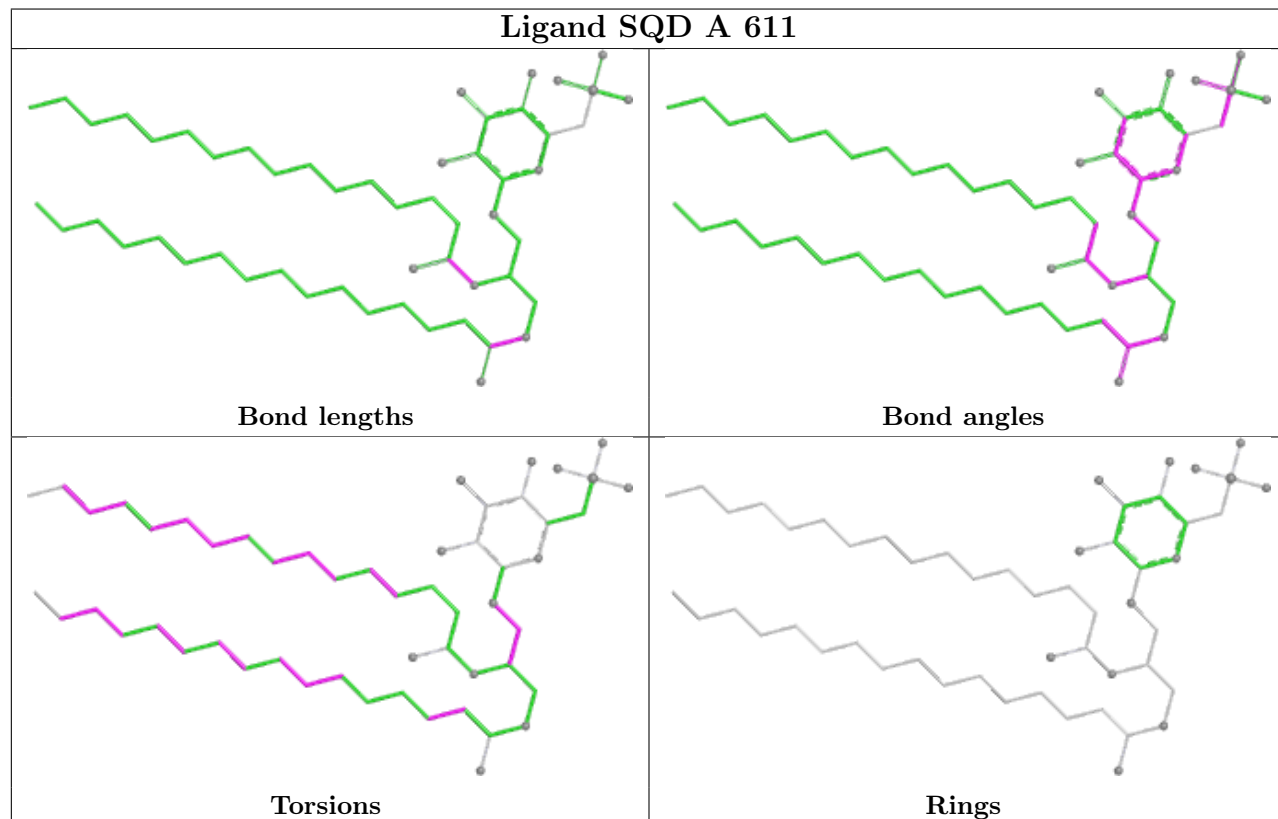


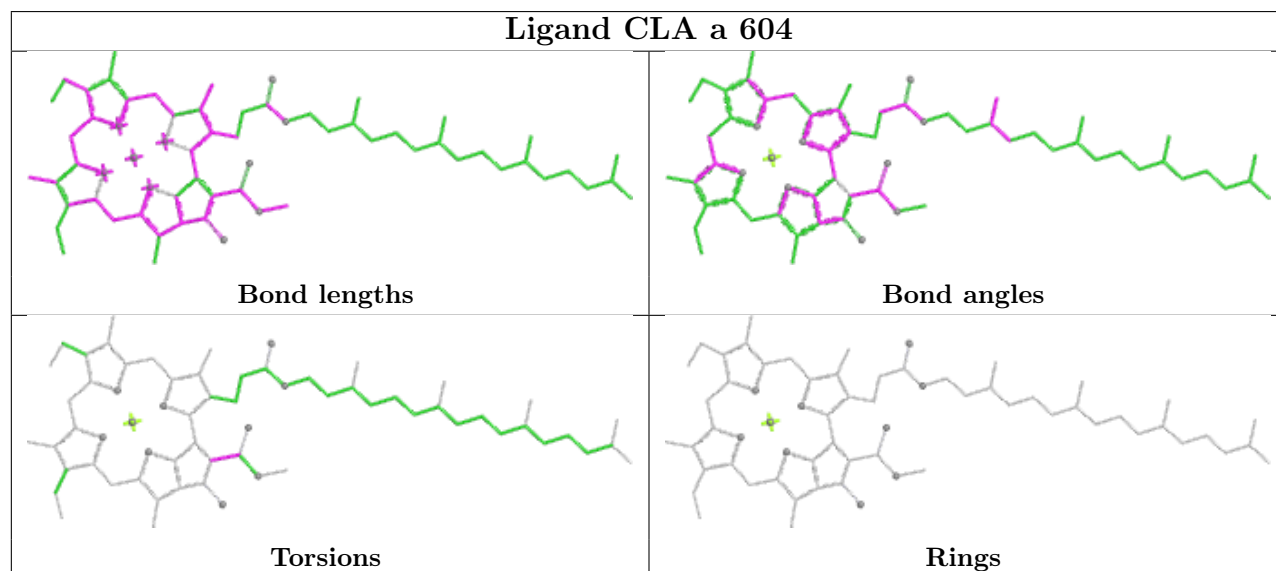
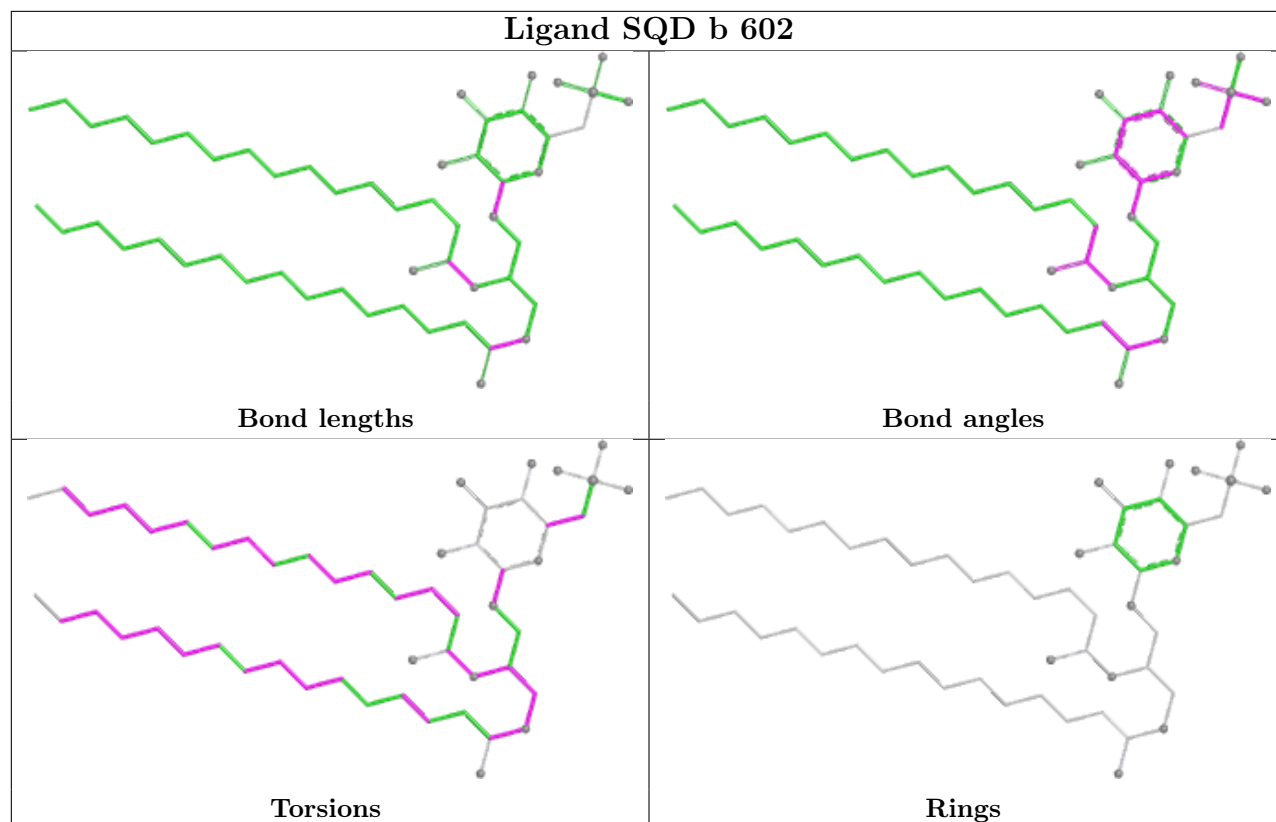


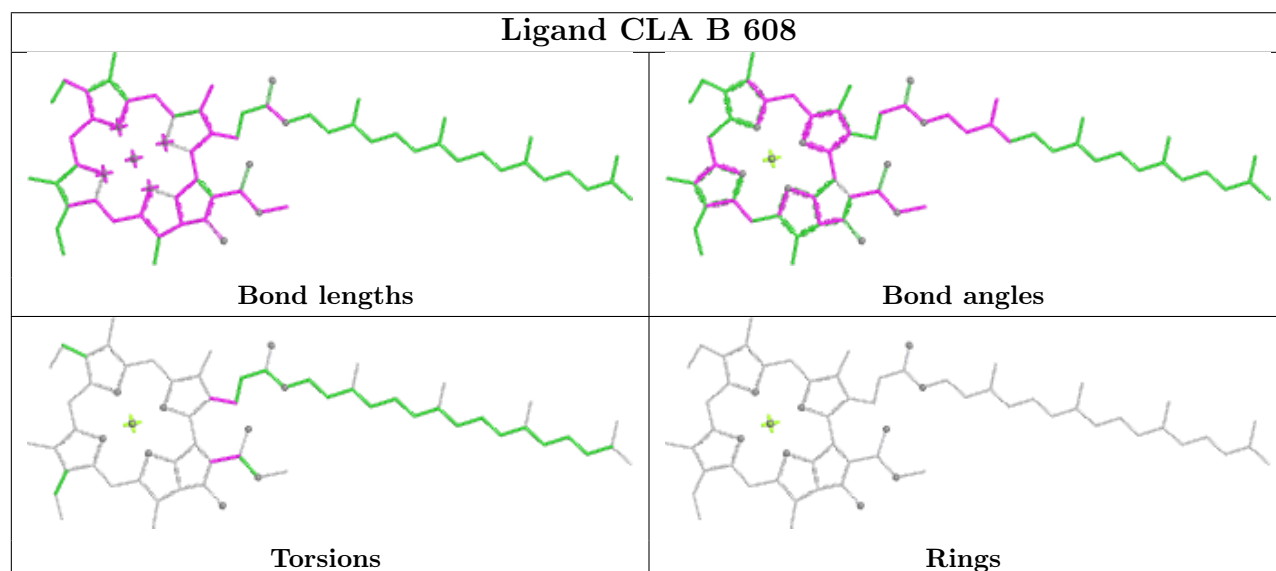
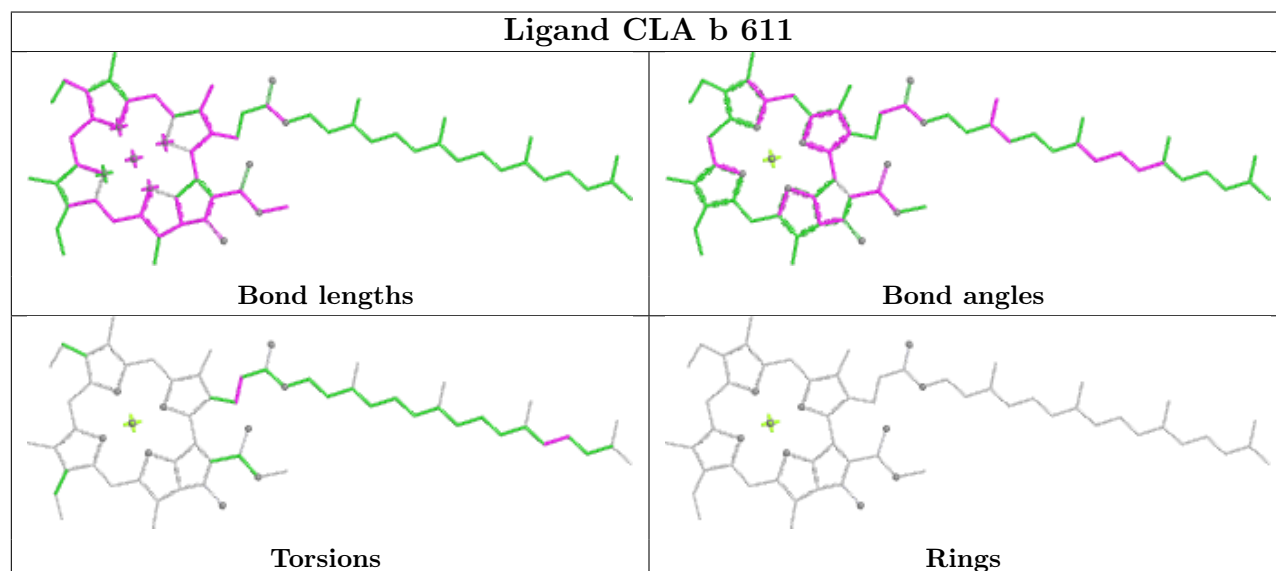
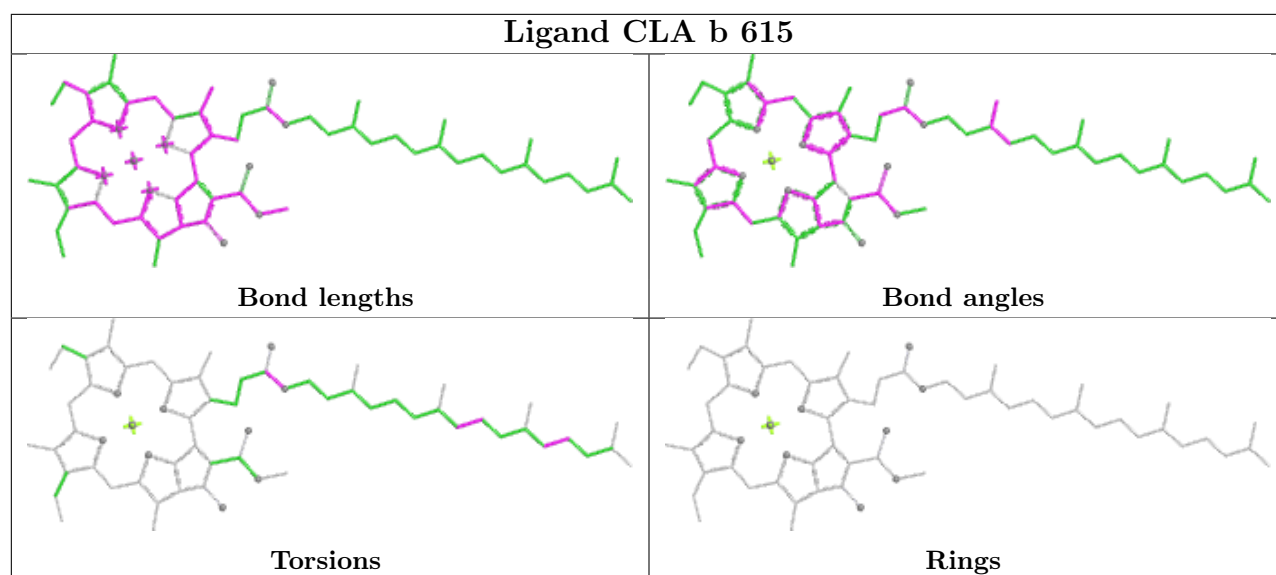
Ligand CLA b 618

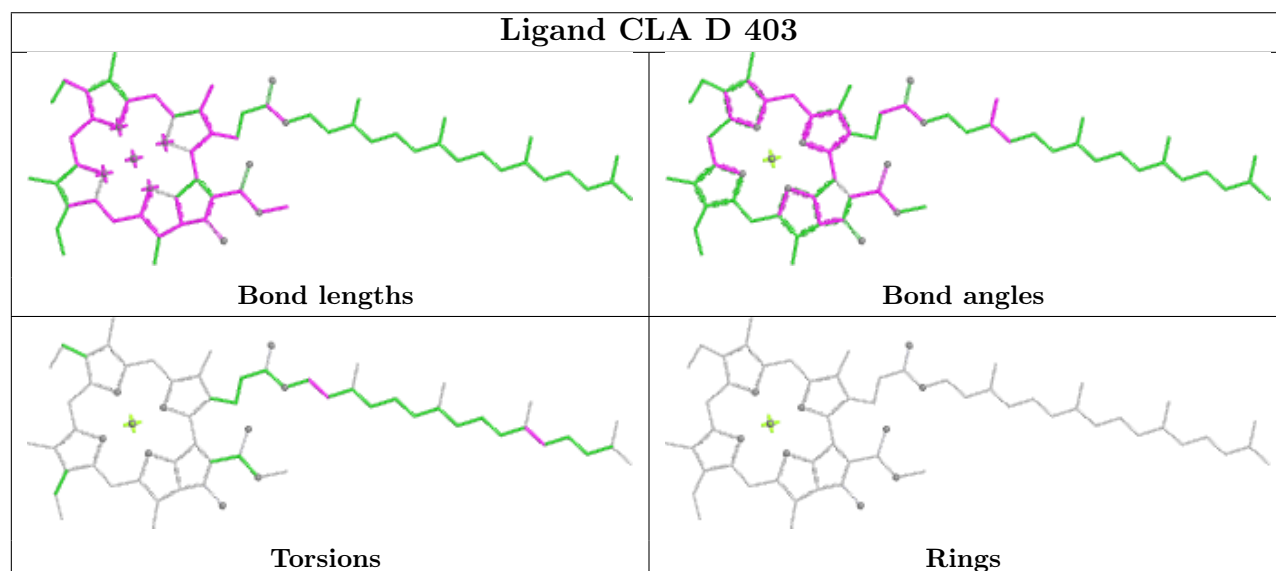
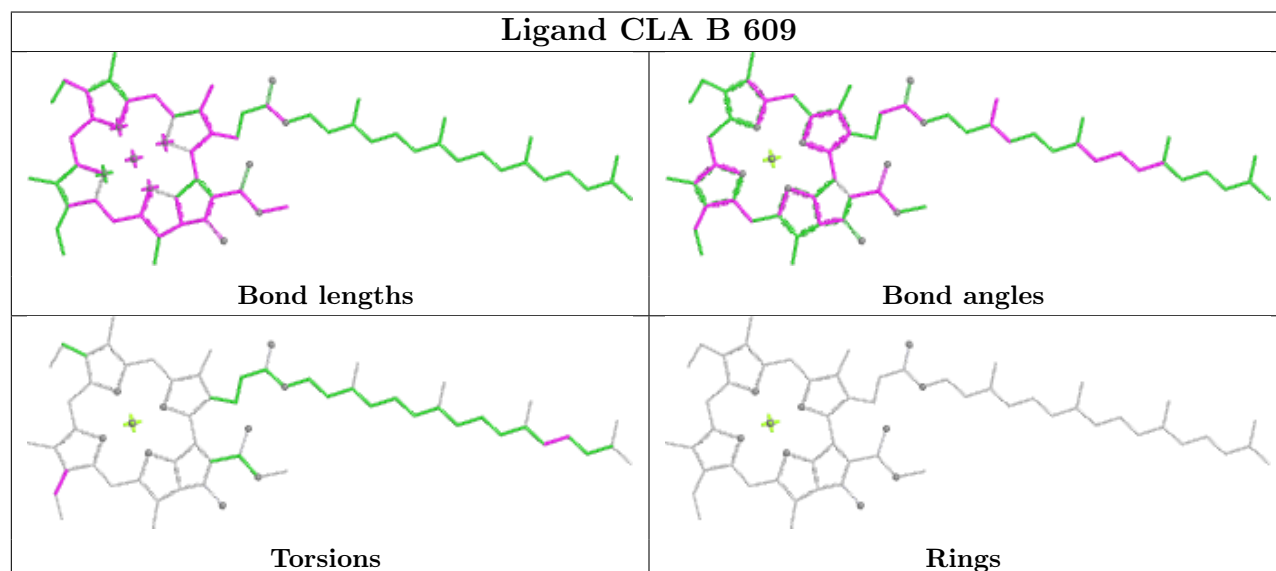
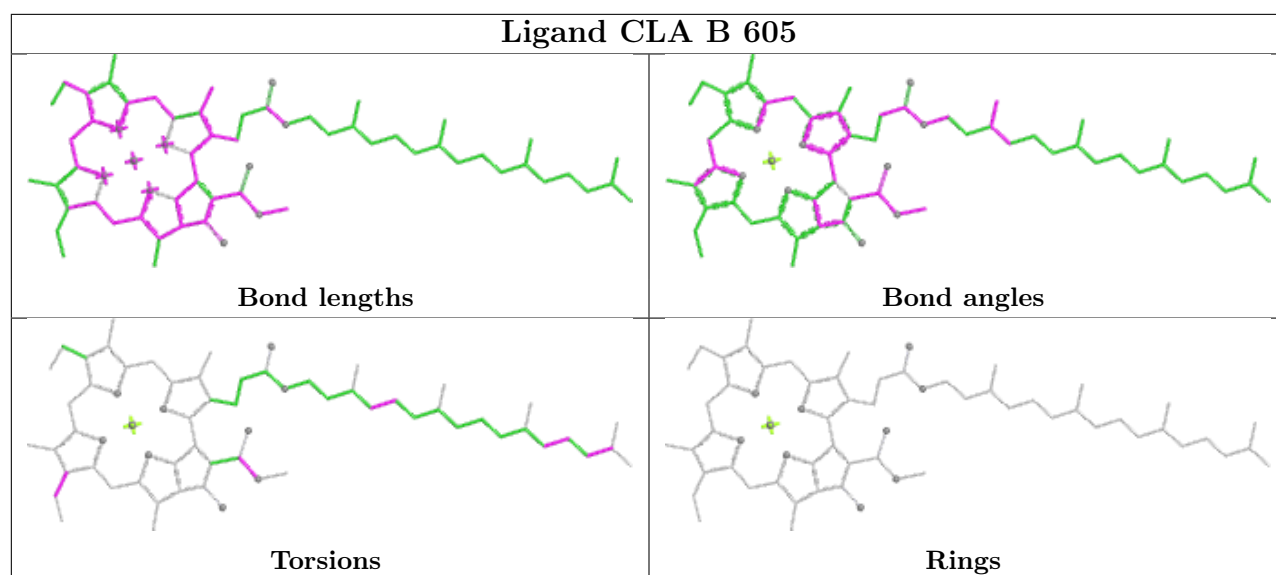


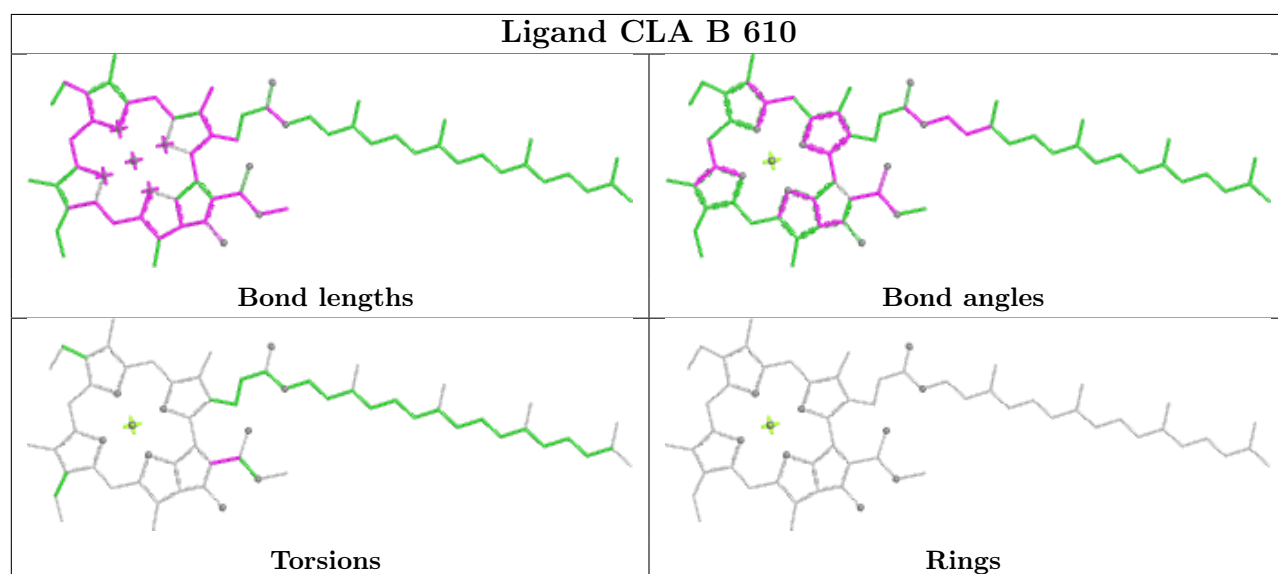
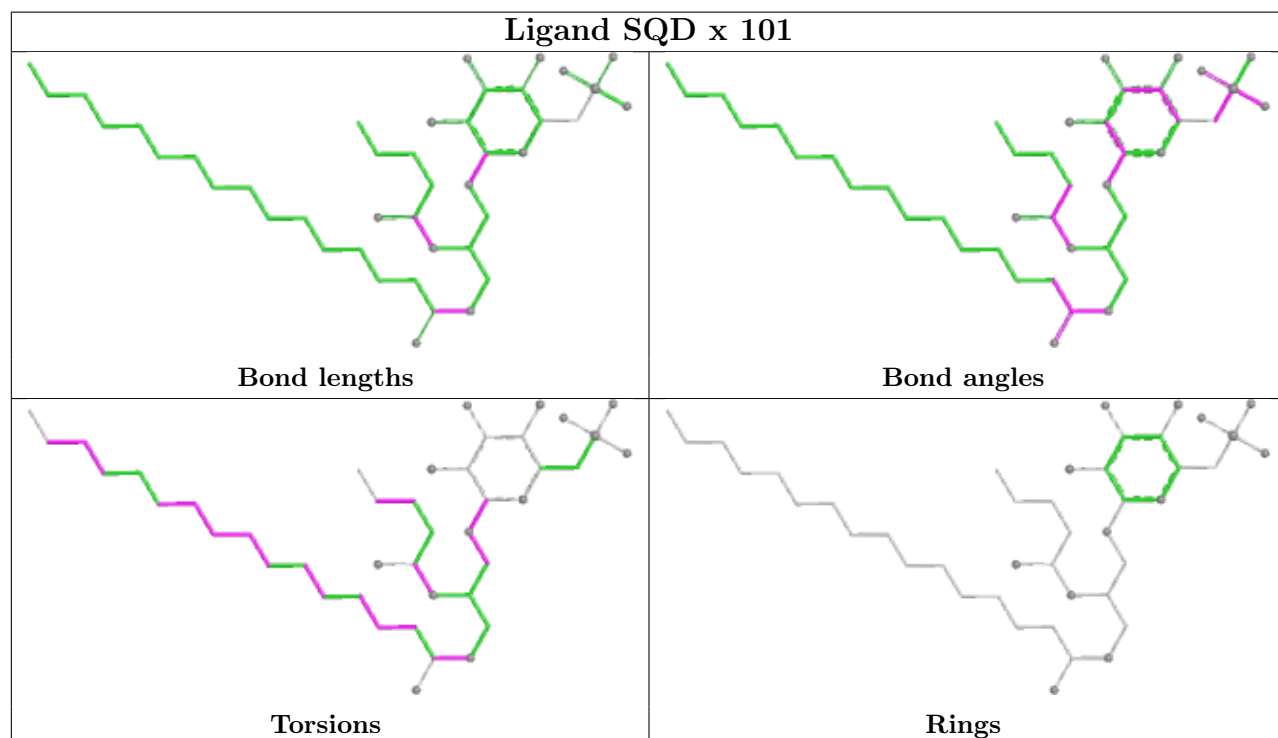
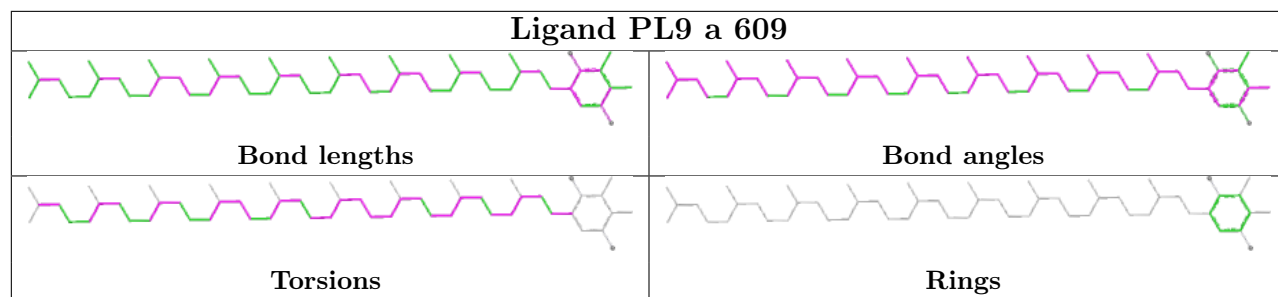
Ligand SQD A 611

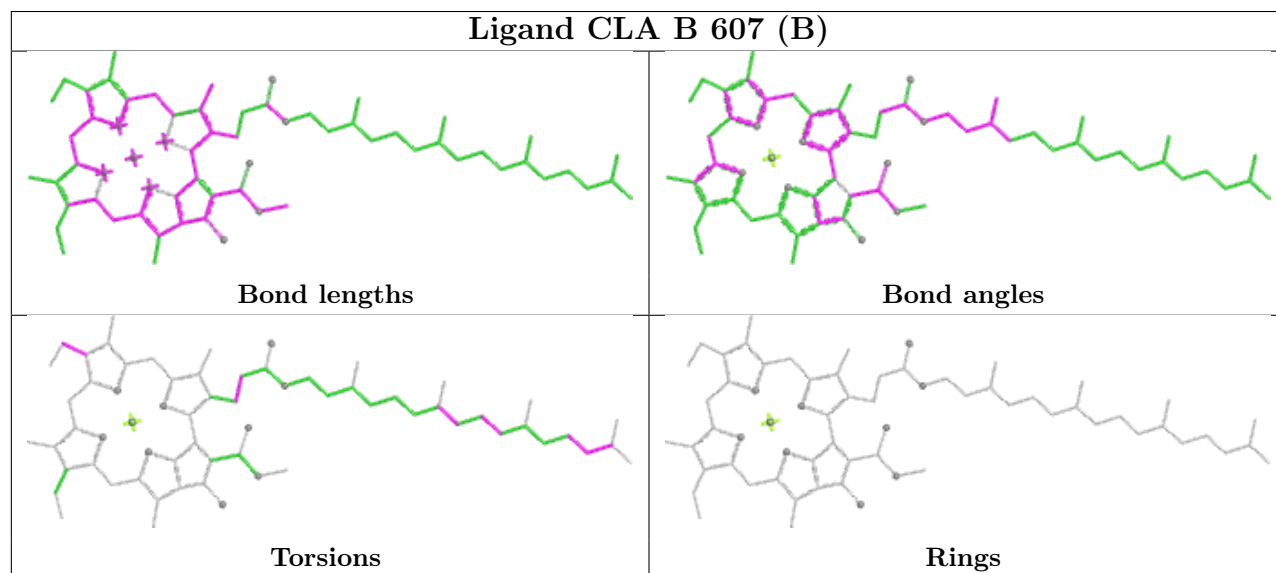
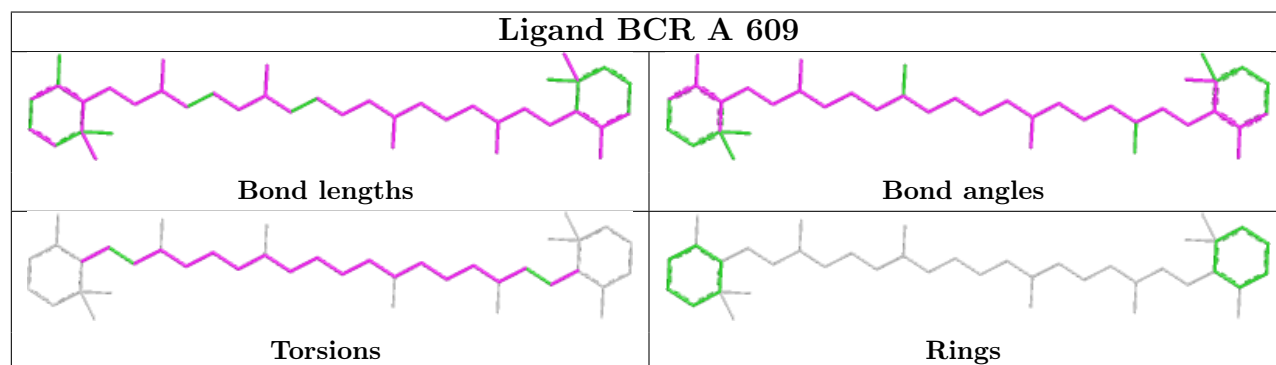
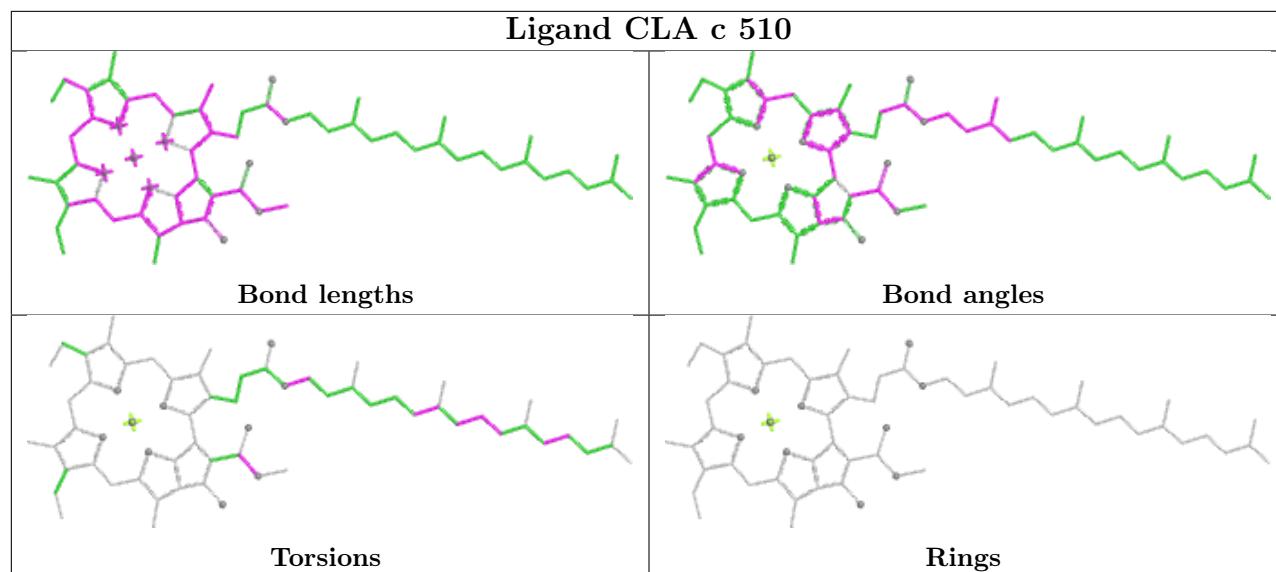


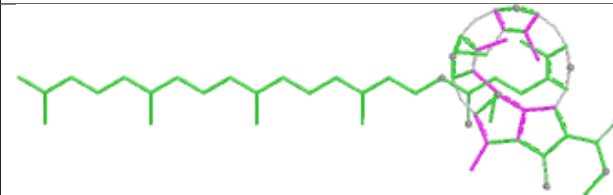
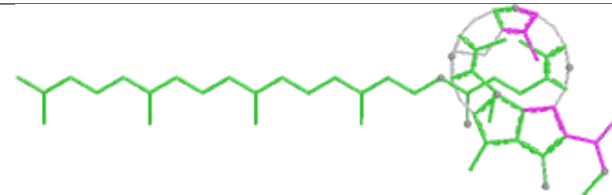
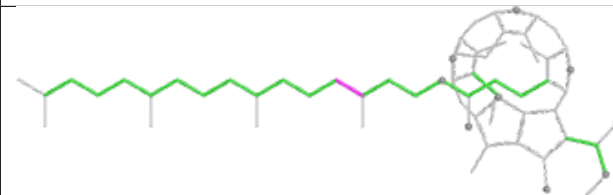
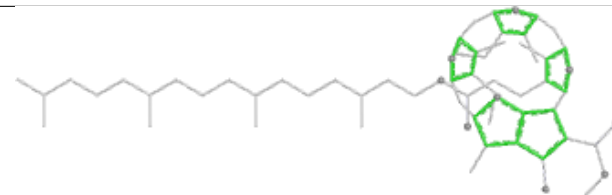


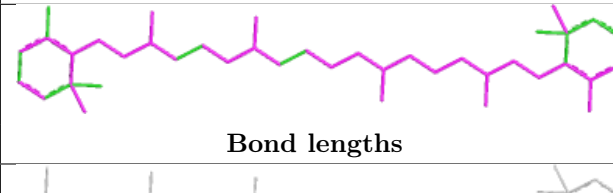
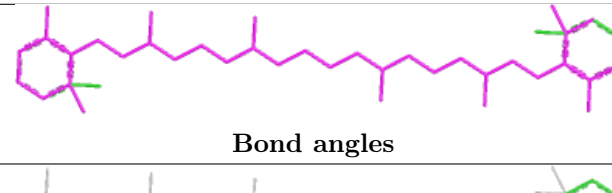
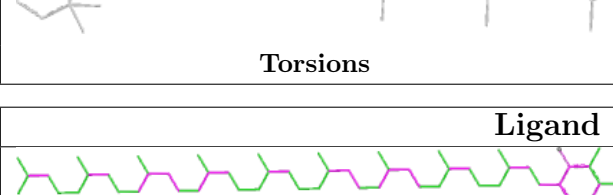
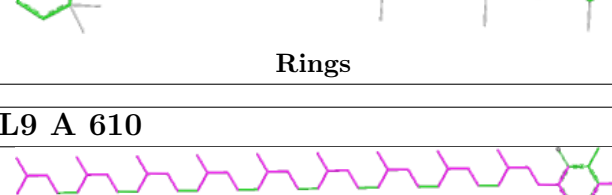


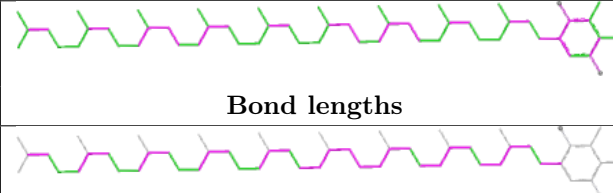
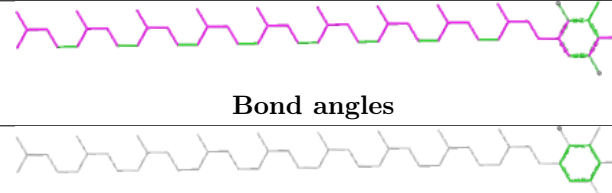
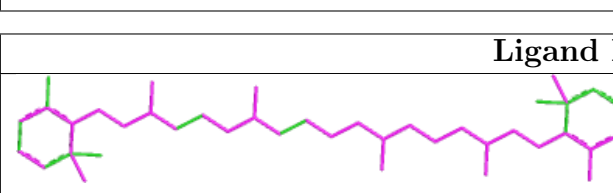
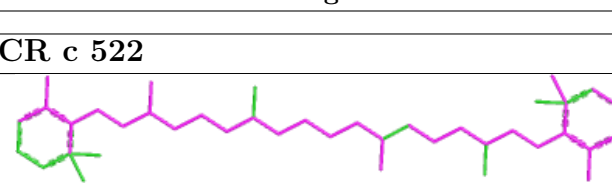


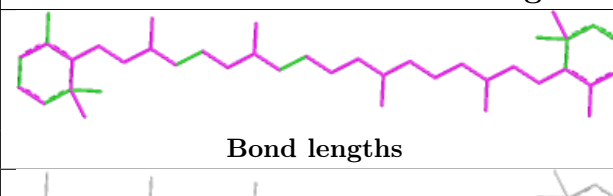
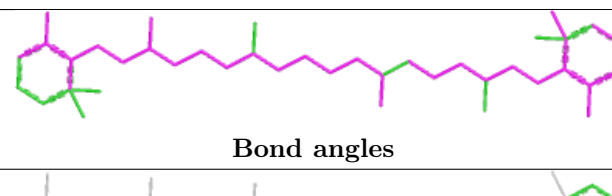


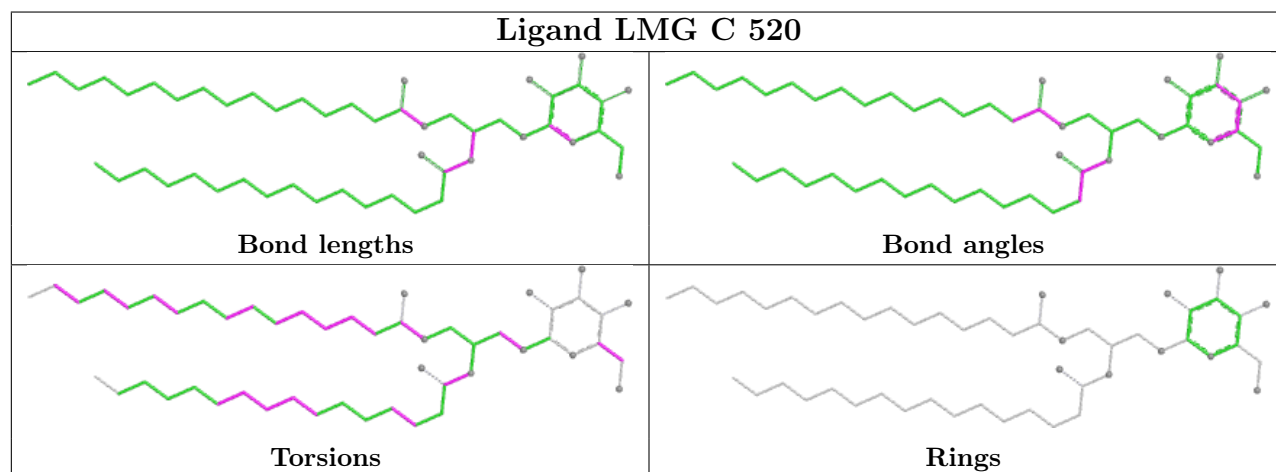
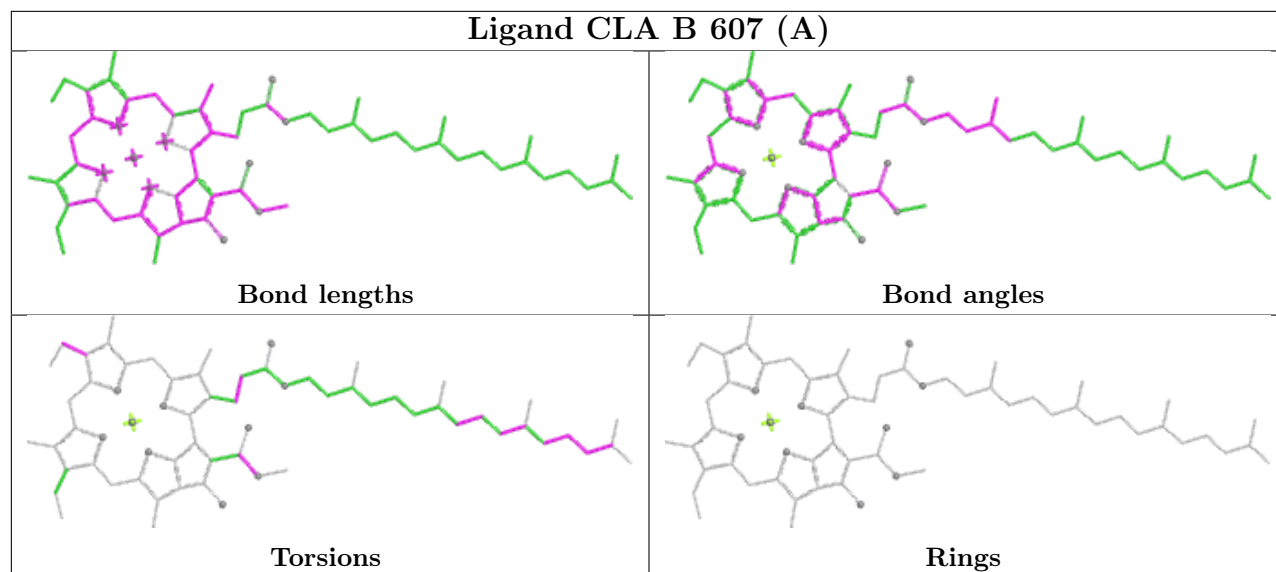


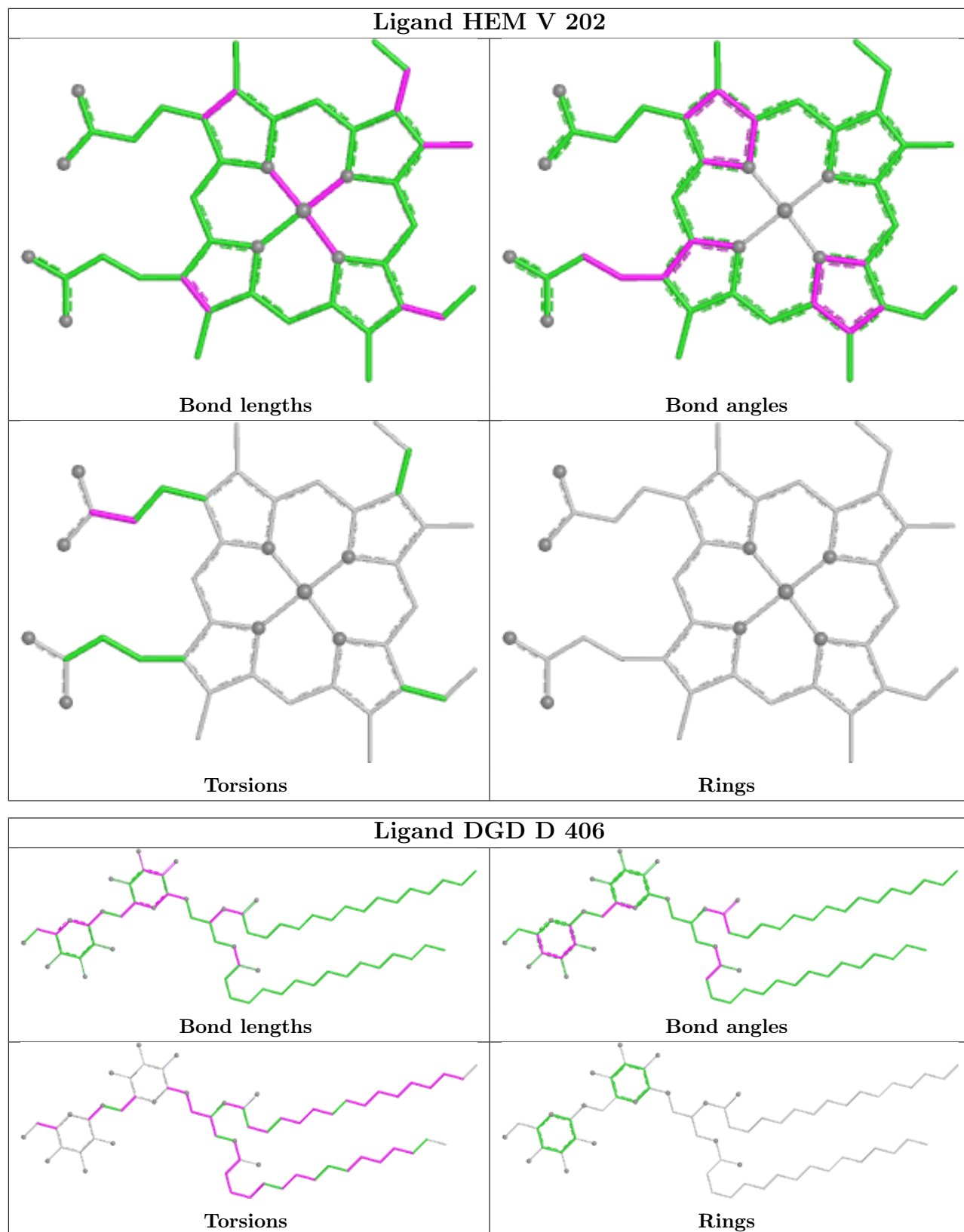
Ligand PHO A 607	
	
Bond lengths	Bond angles
	
Torsions	Rings

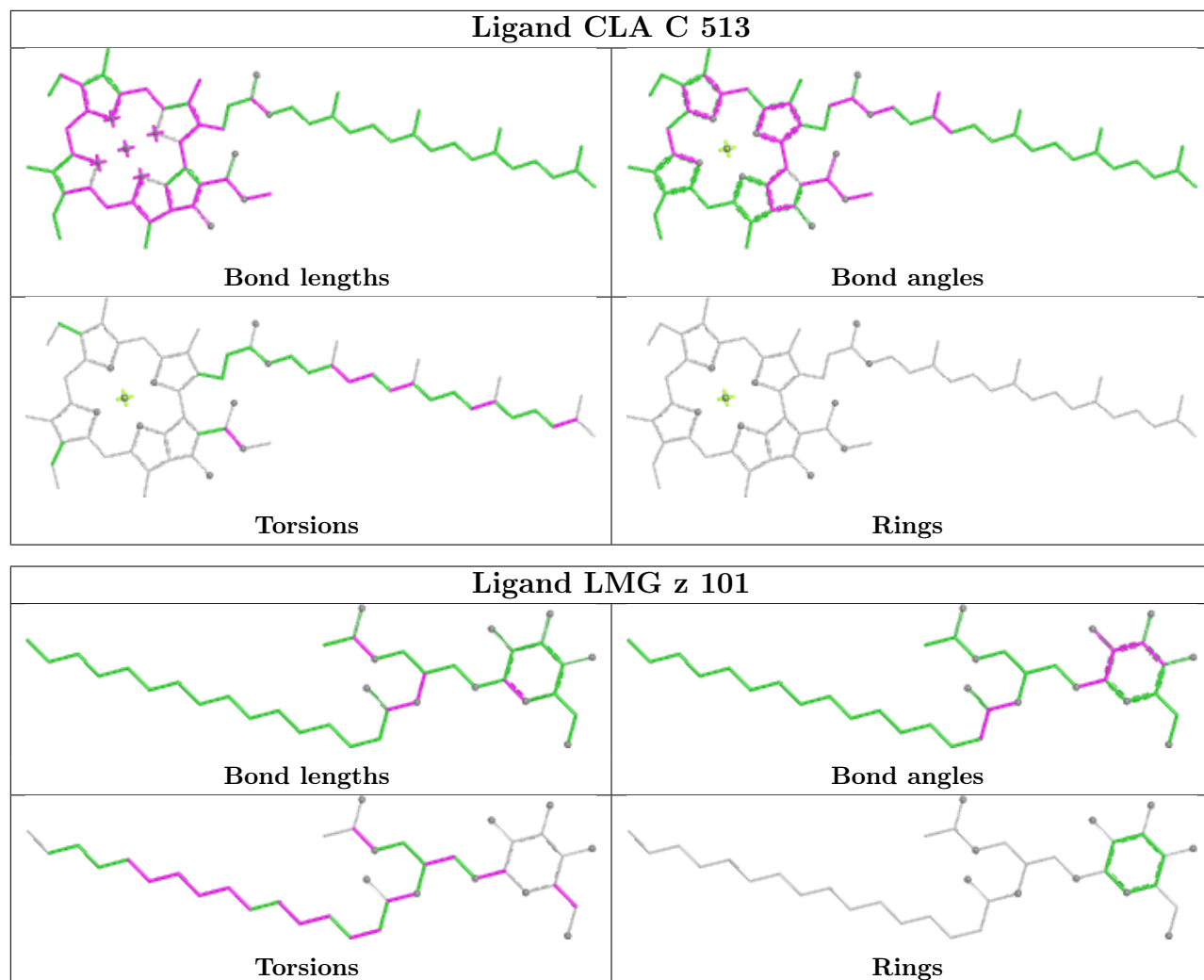
Ligand BCR h 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PL9 A 610	
	
Bond lengths	Bond angles
	
Torsions	Rings

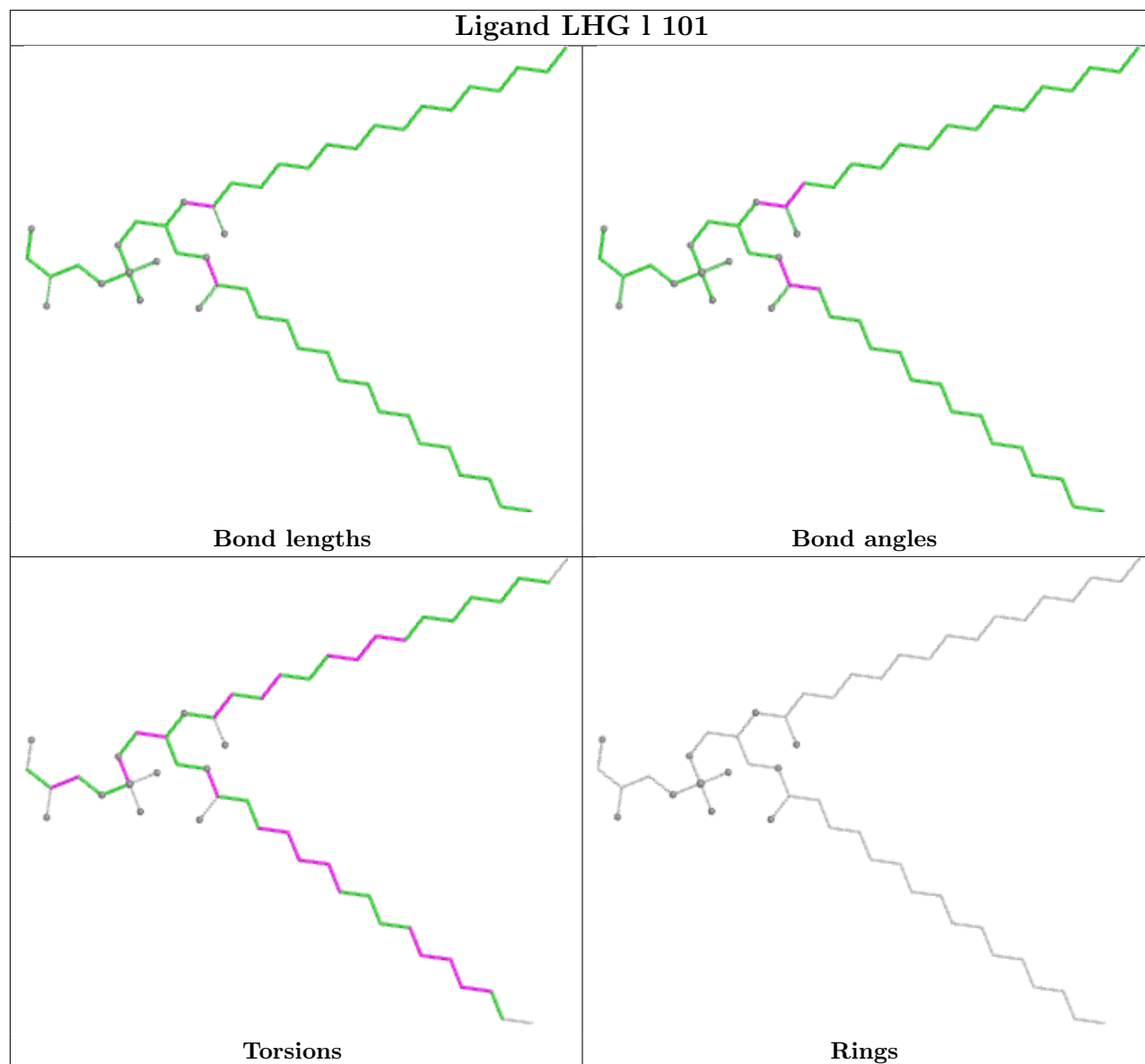
Ligand BCR c 522	
	
Bond lengths	Bond angles
	
Torsions	Rings



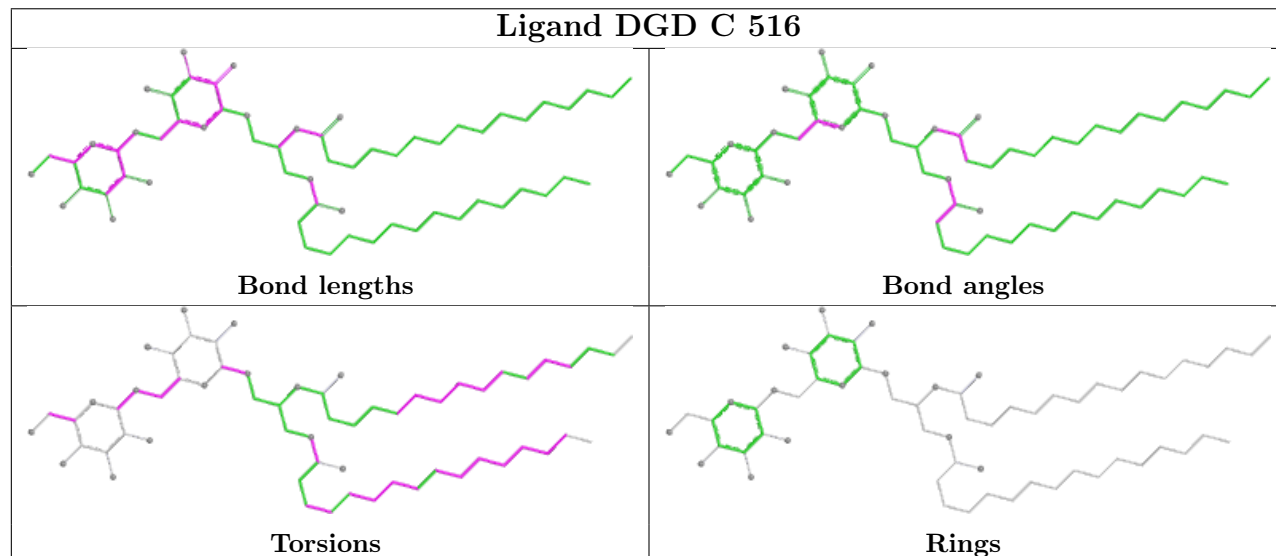


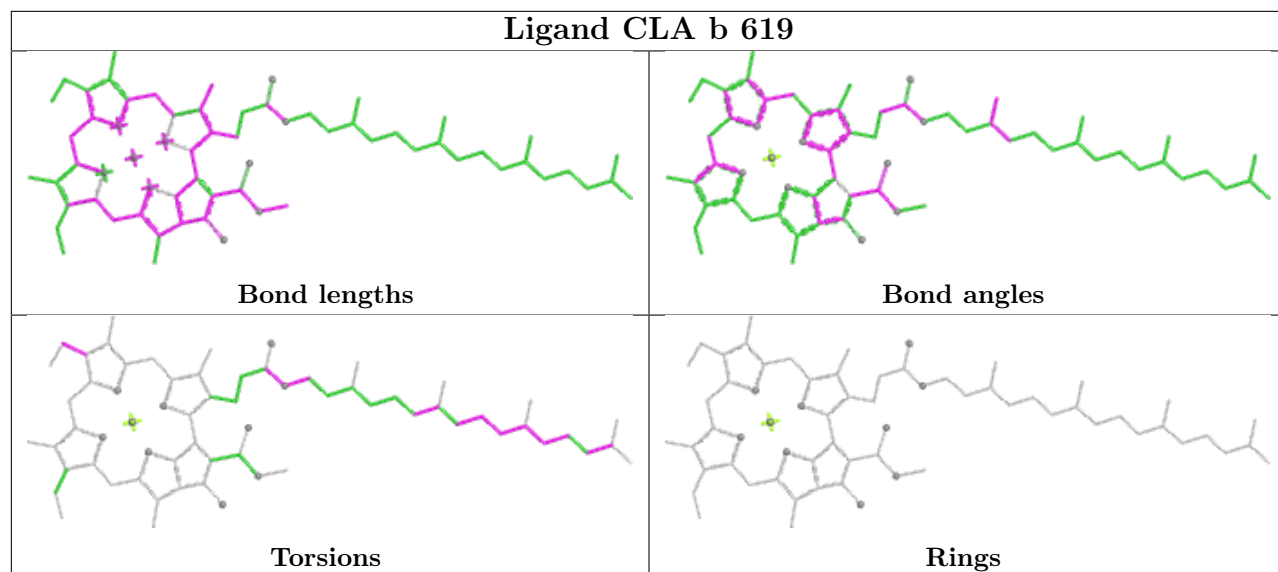
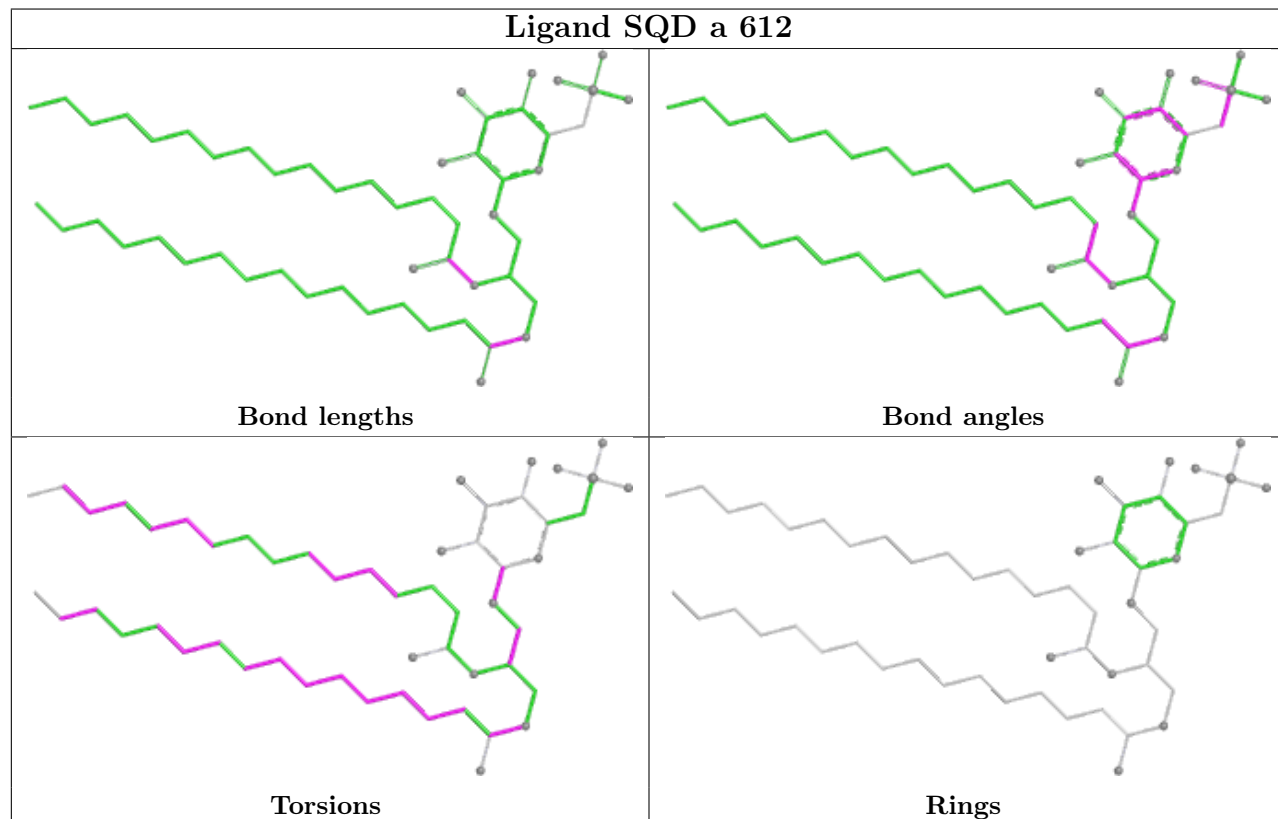


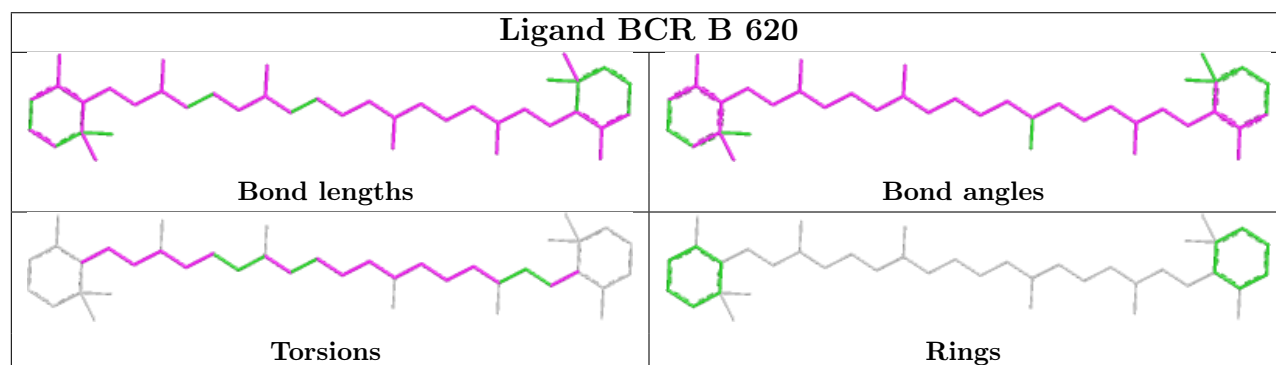
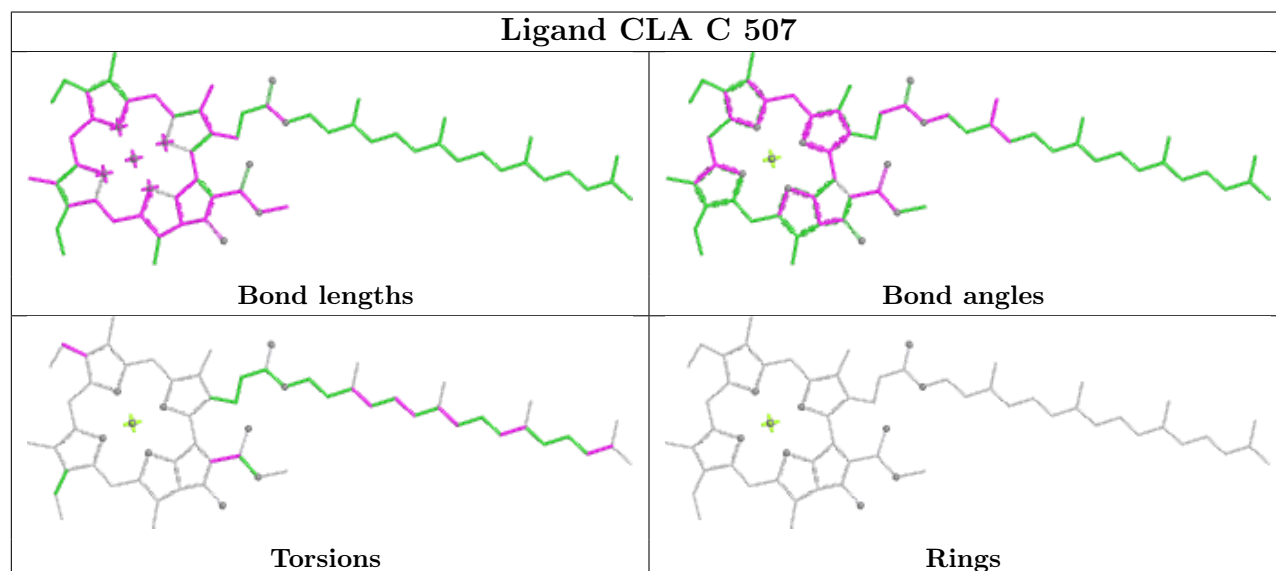
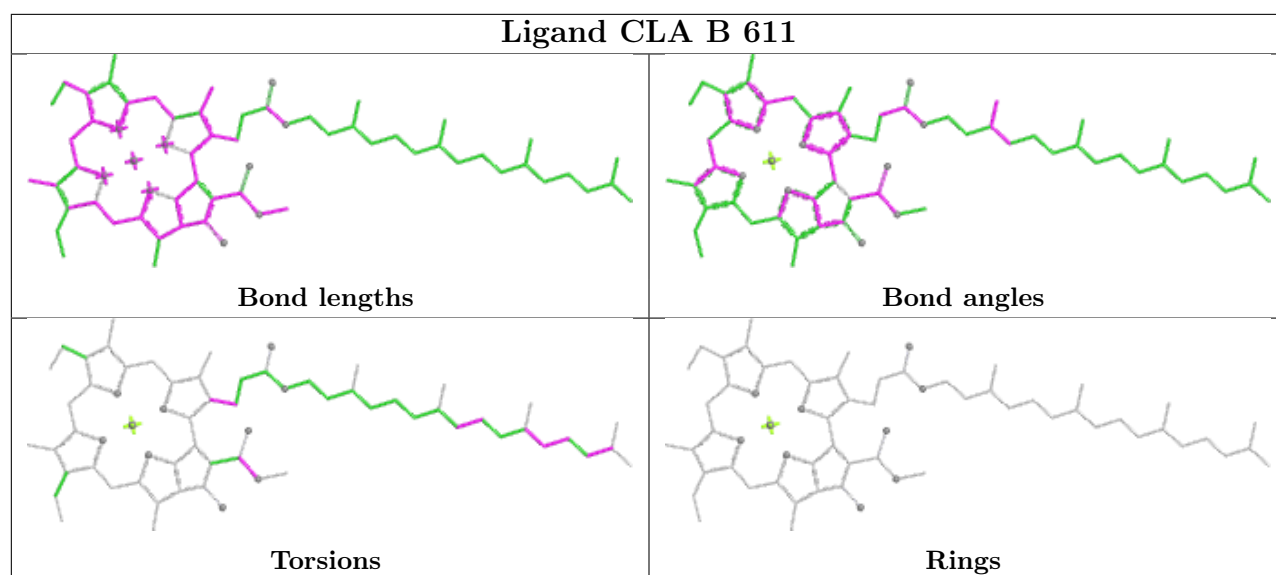
Ligand LHG 1 101

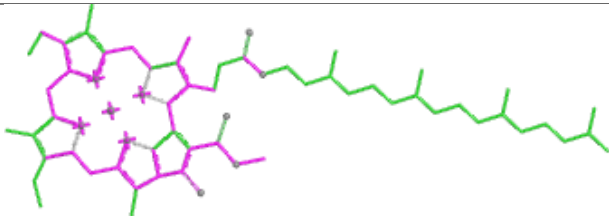
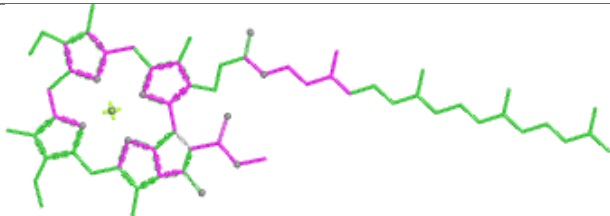
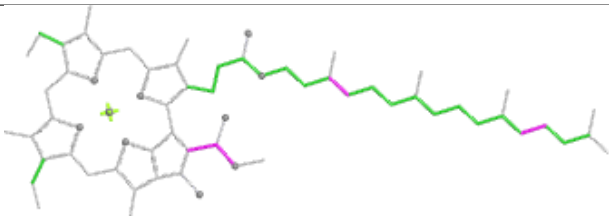
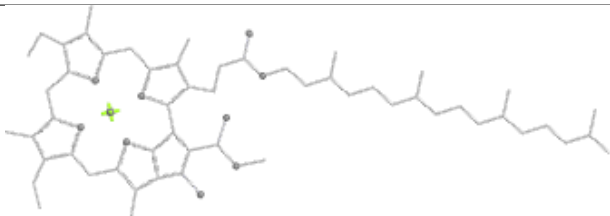


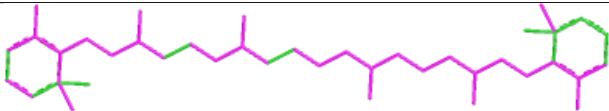
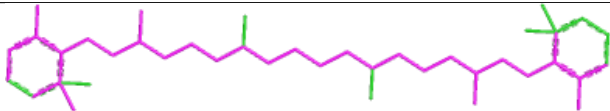
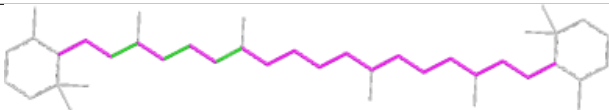
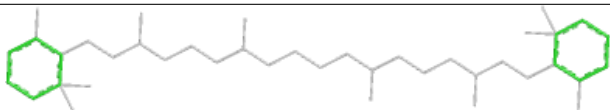
Ligand DGD C 516

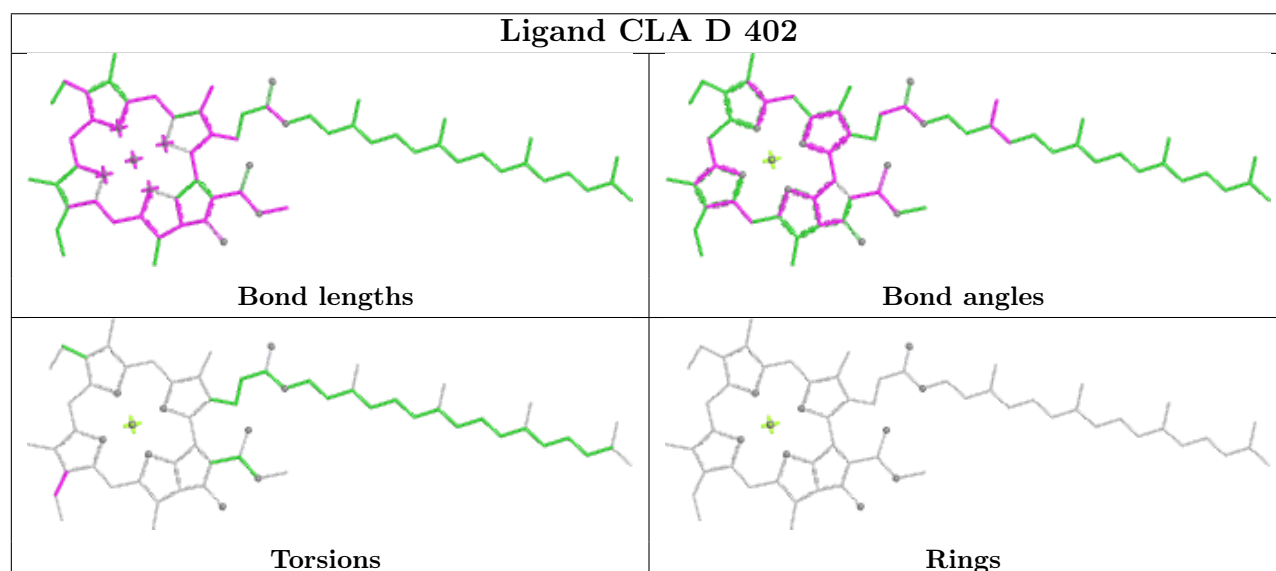
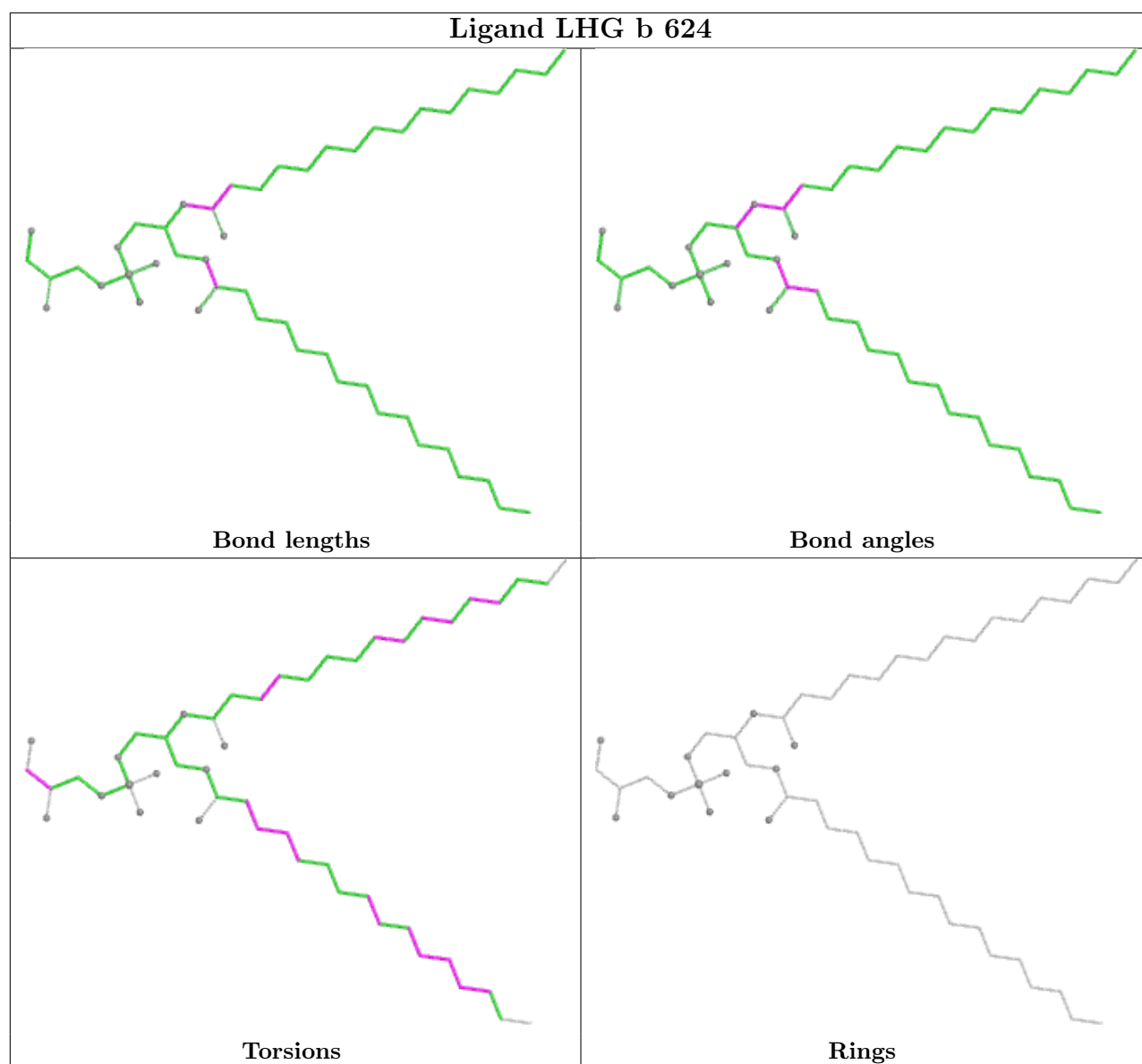


Ligand CLA b 619**Ligand SQD a 612**

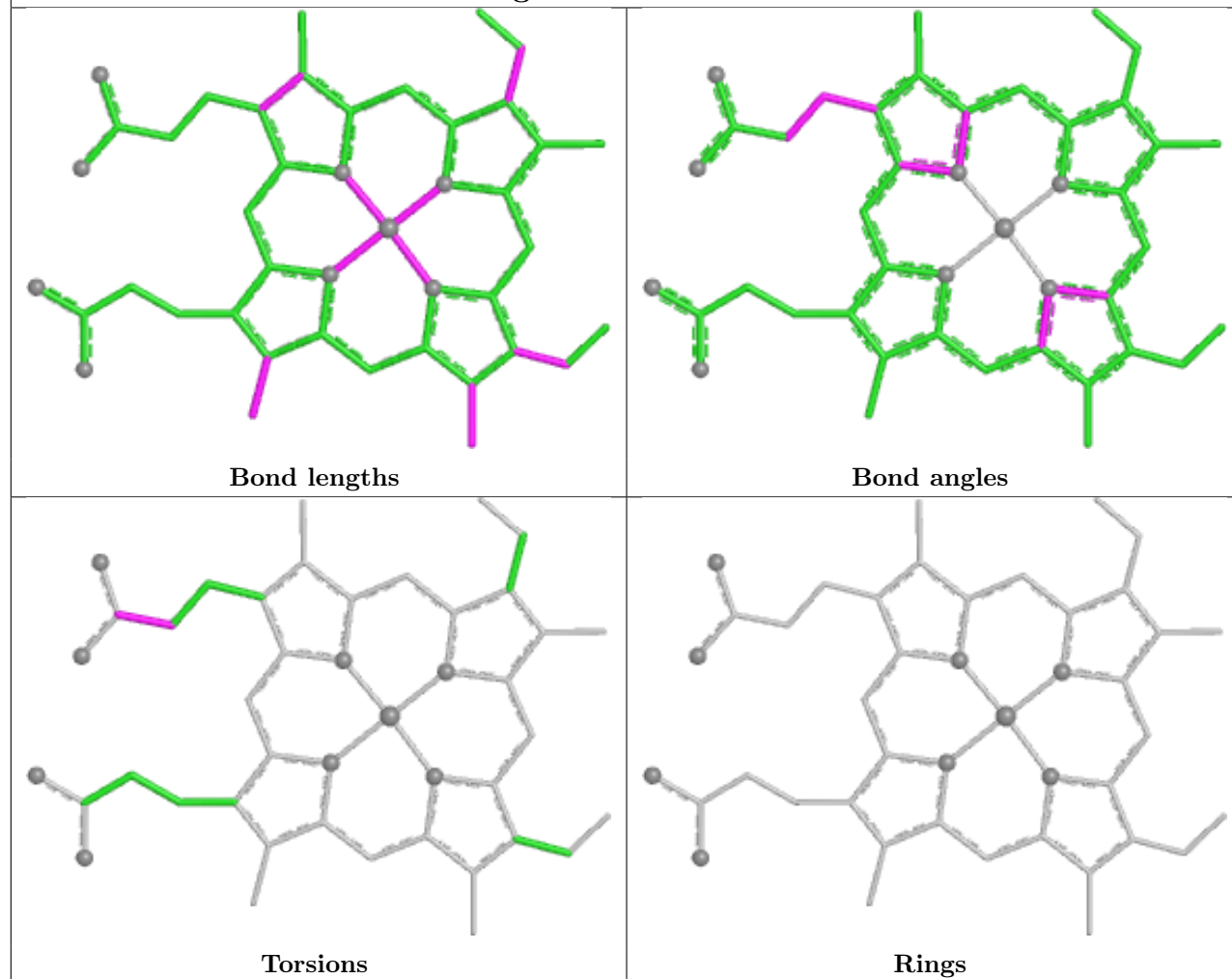


Ligand CLA b 608	
	
Bond lengths	Bond angles
	
Torsions	Rings

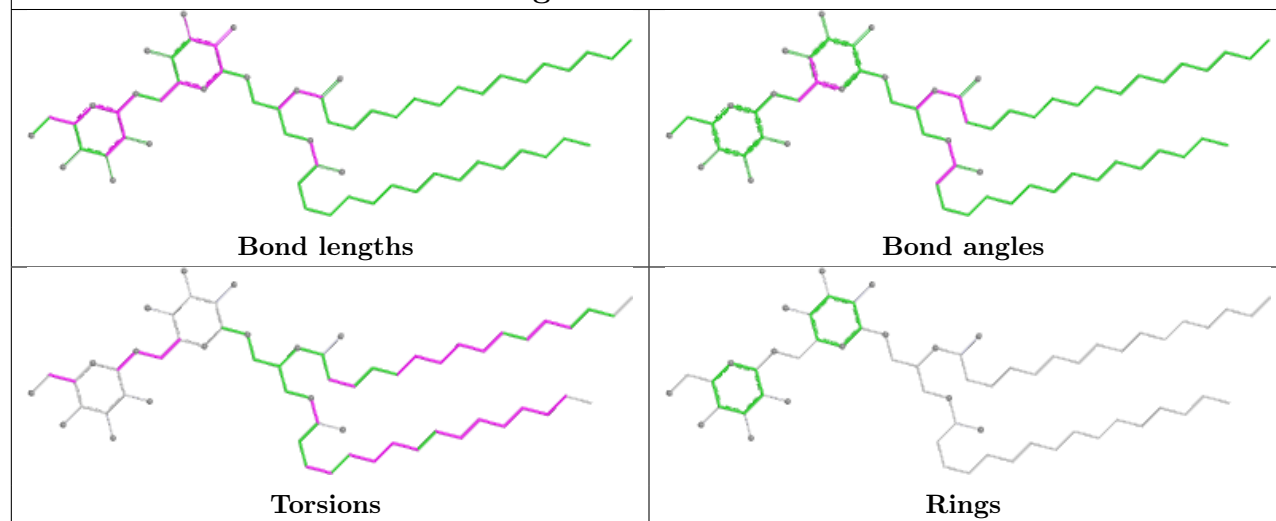
Ligand BCR C 514	
	
Bond lengths	Bond angles
	
Torsions	Rings

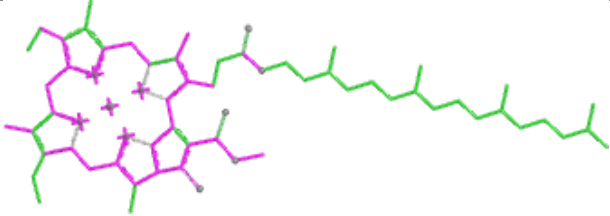
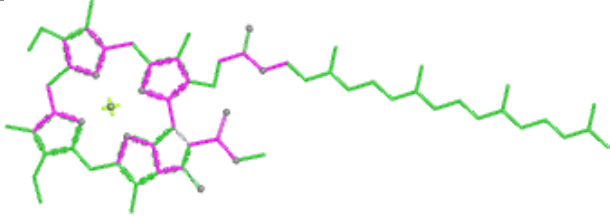
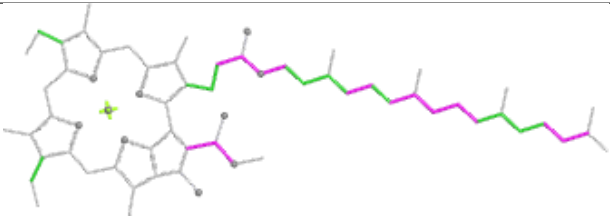
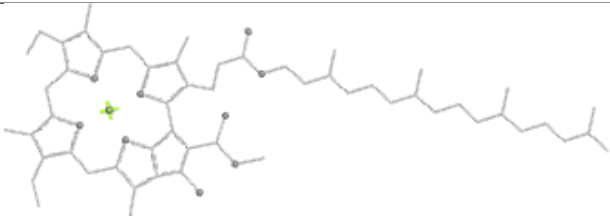
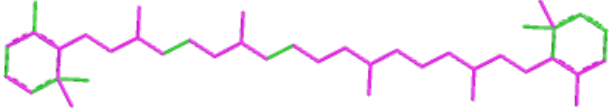
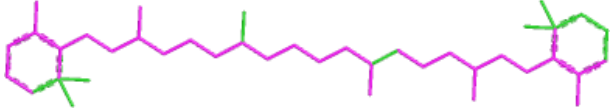
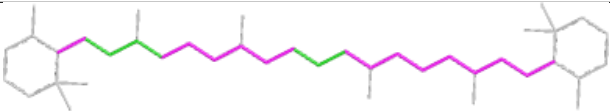
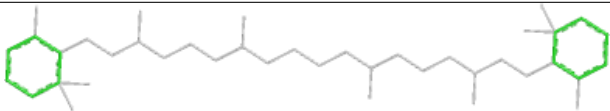


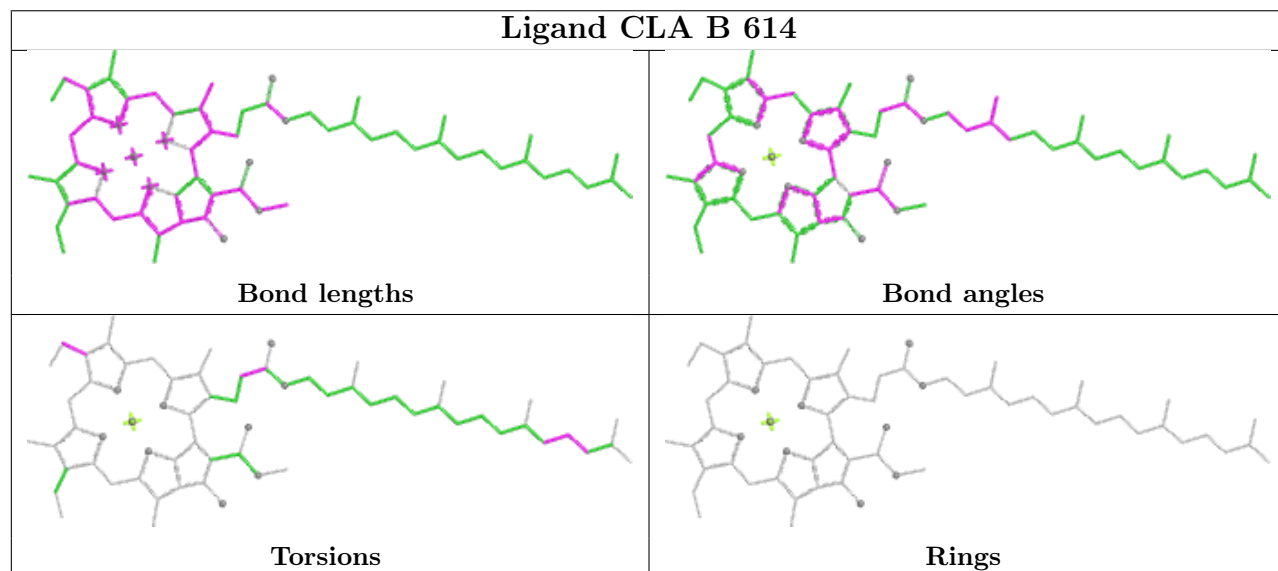
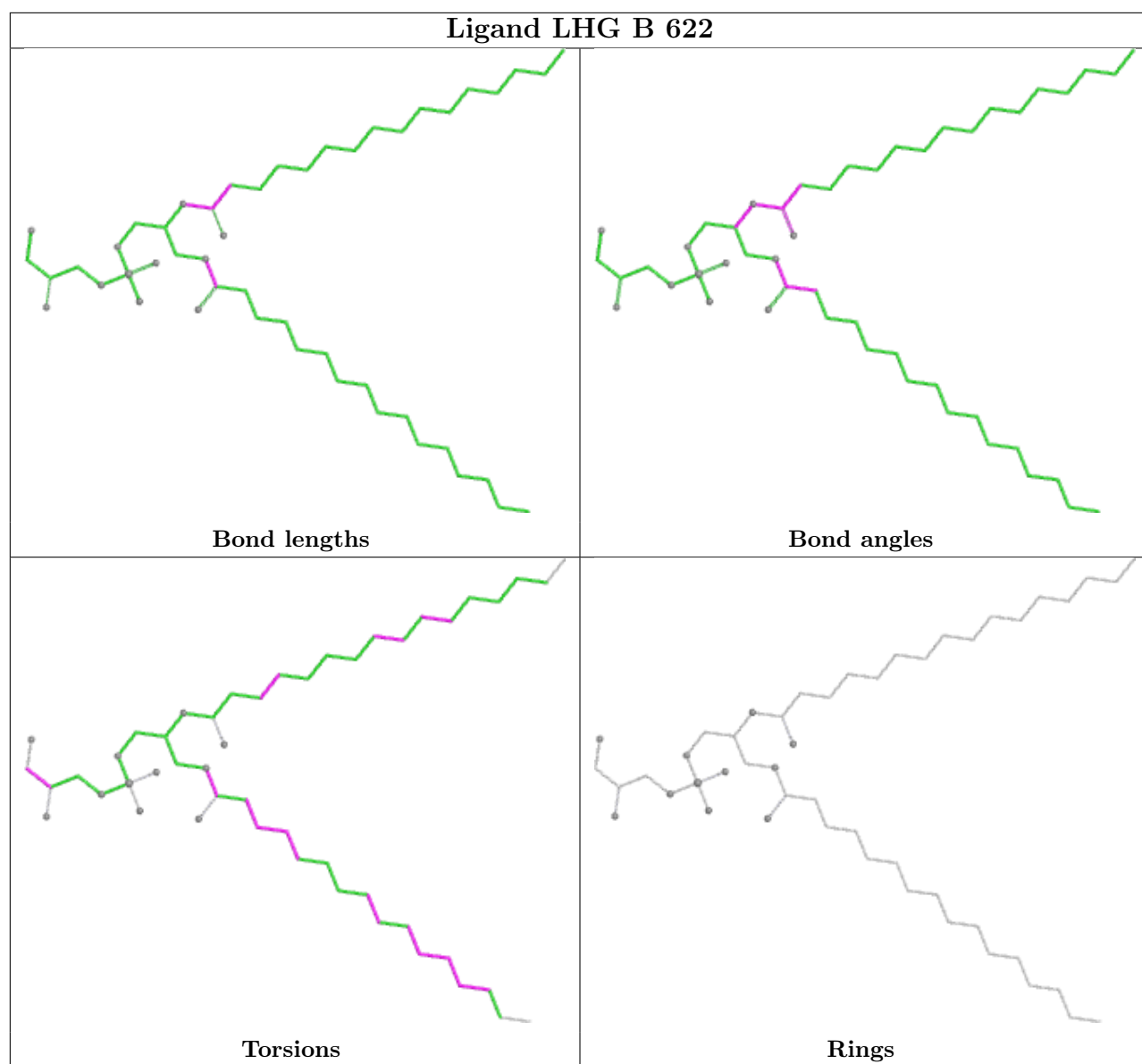
Ligand HEM e 102

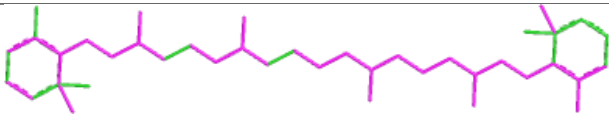
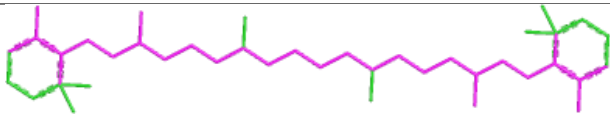
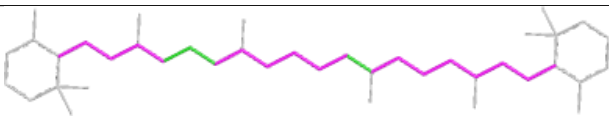
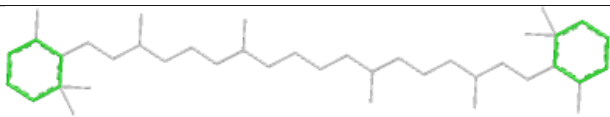


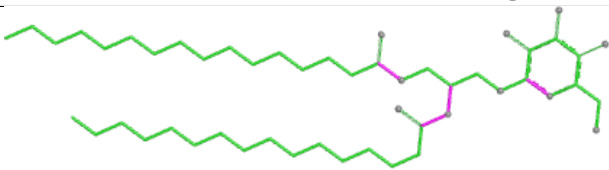
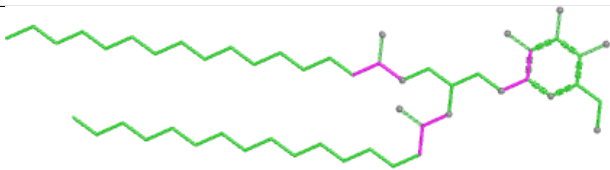
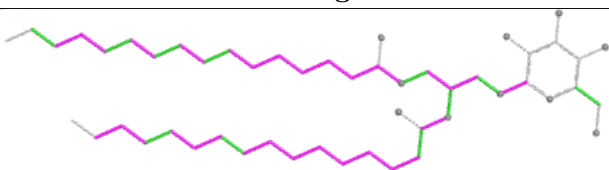
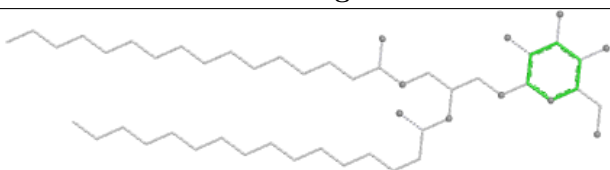
Ligand DGD c 517

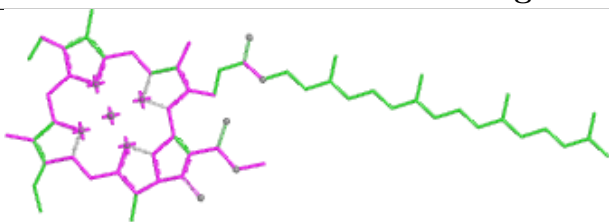
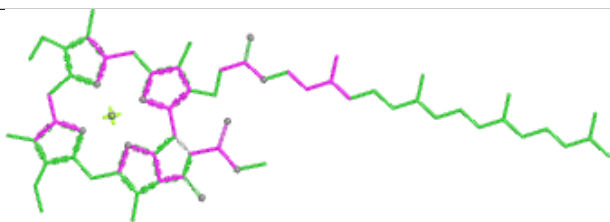
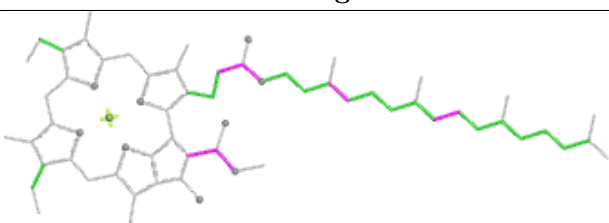
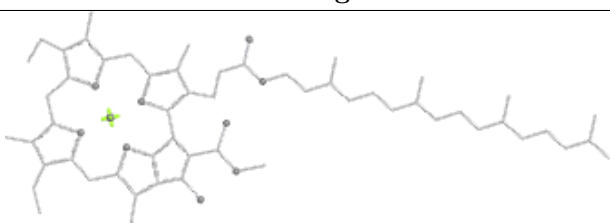


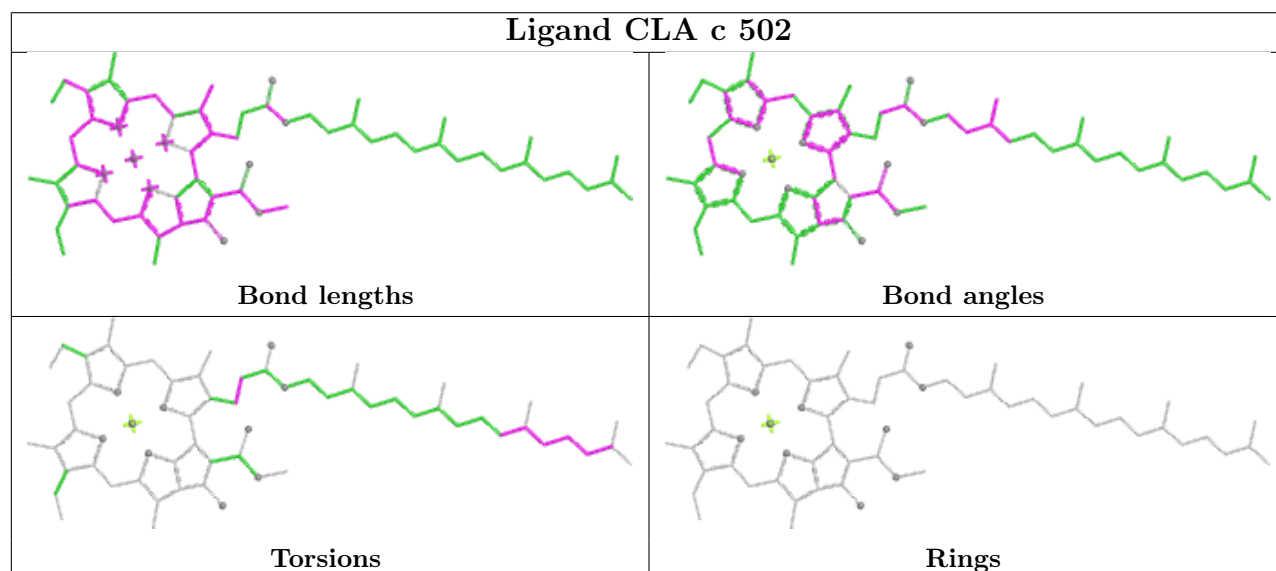
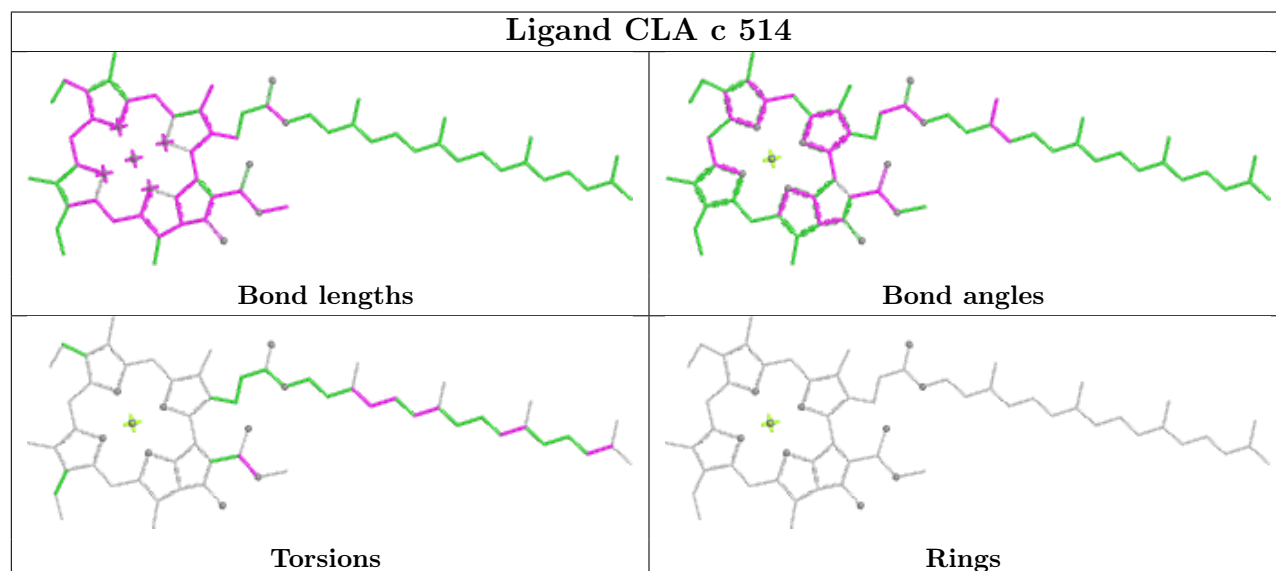
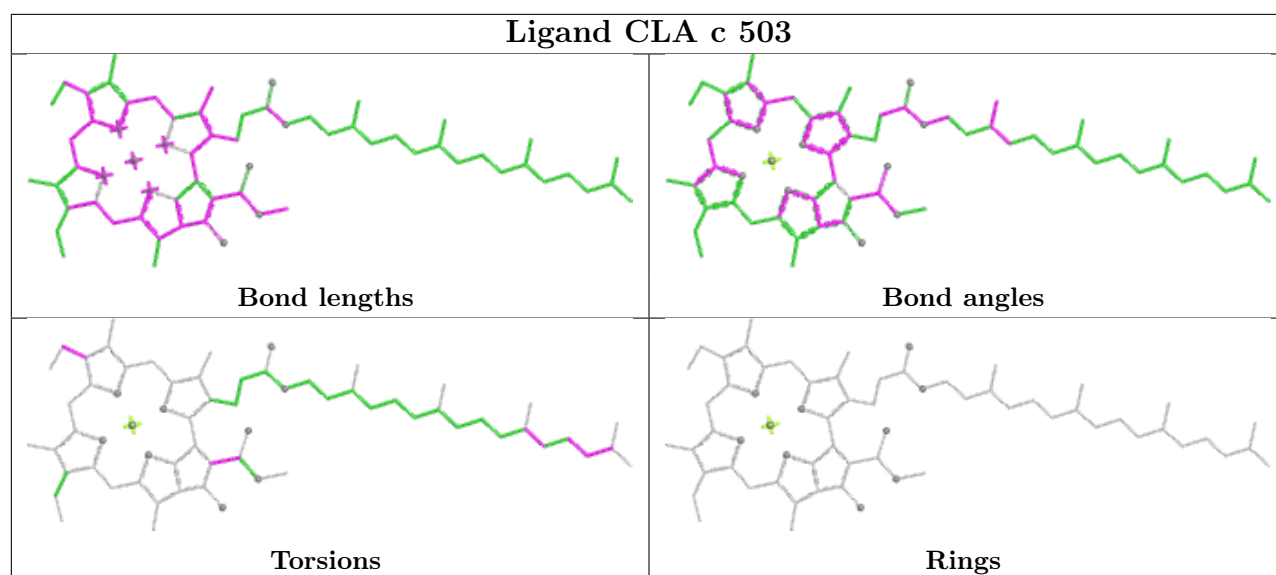
Ligand CLA b 604	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR b 620	
 Bond lengths	 Bond angles
 Torsions	 Rings

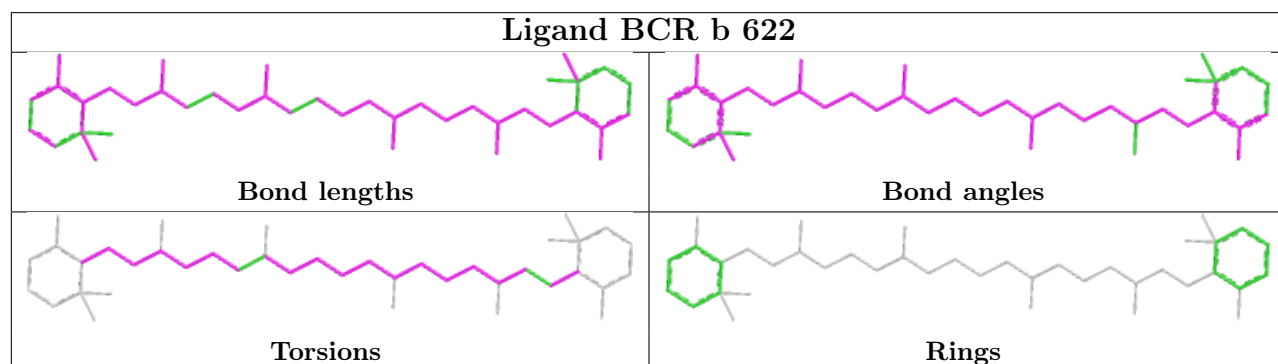
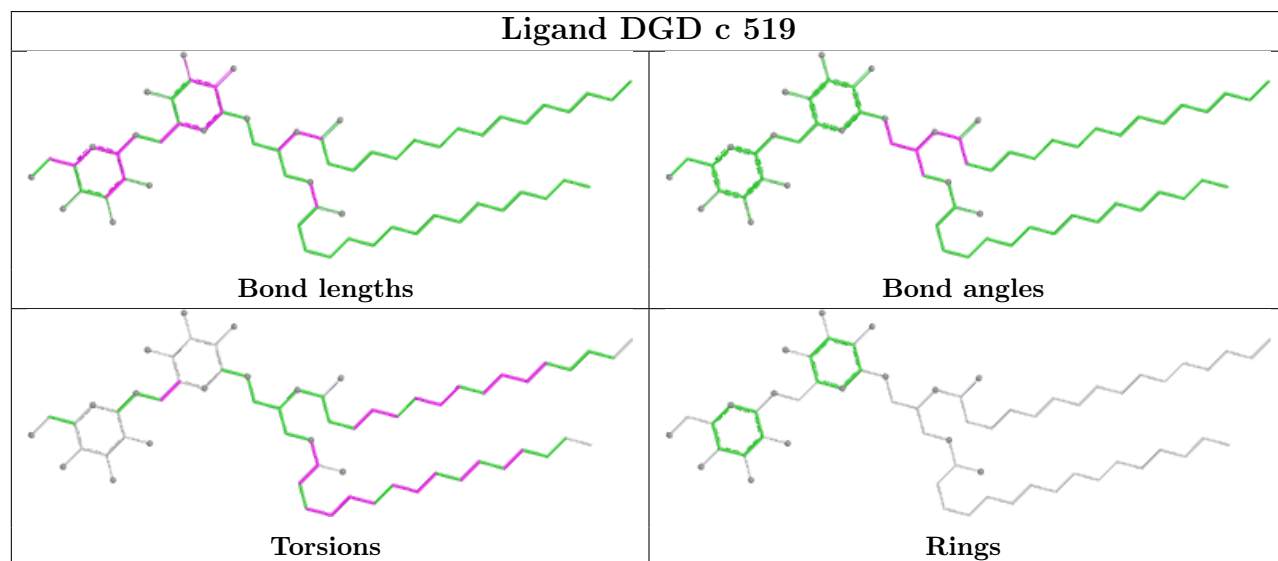
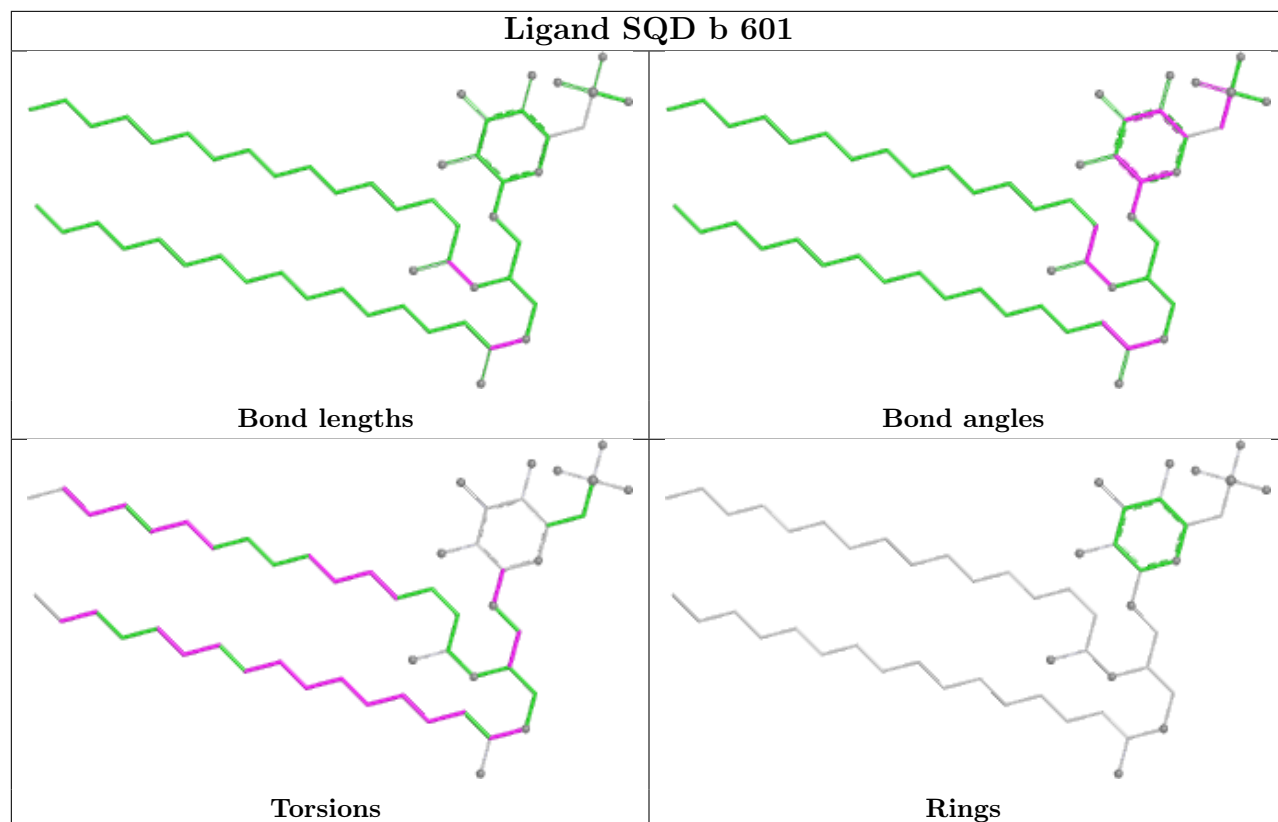


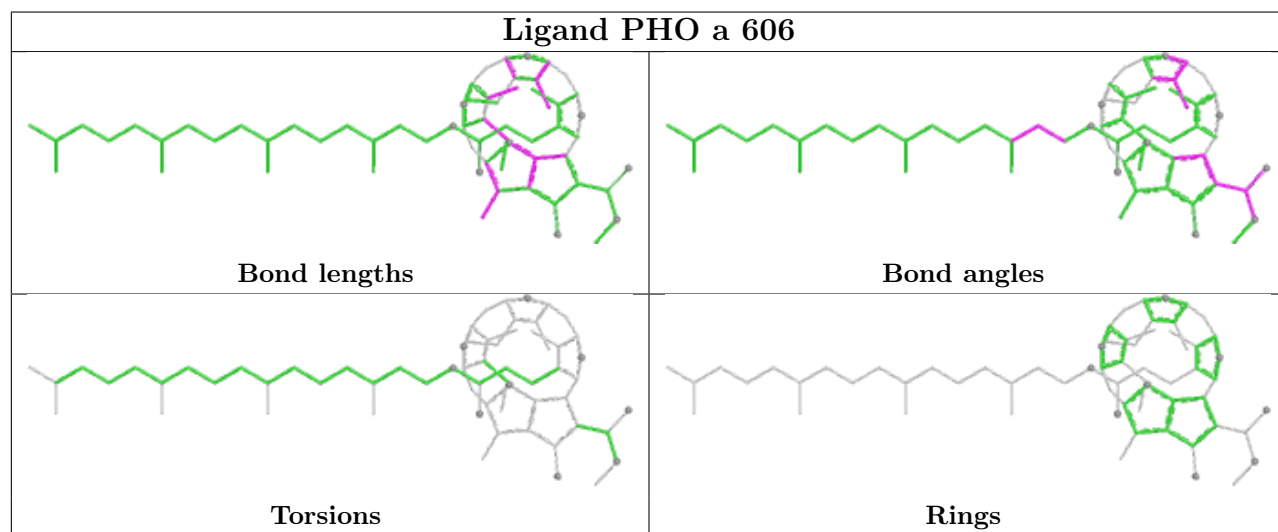
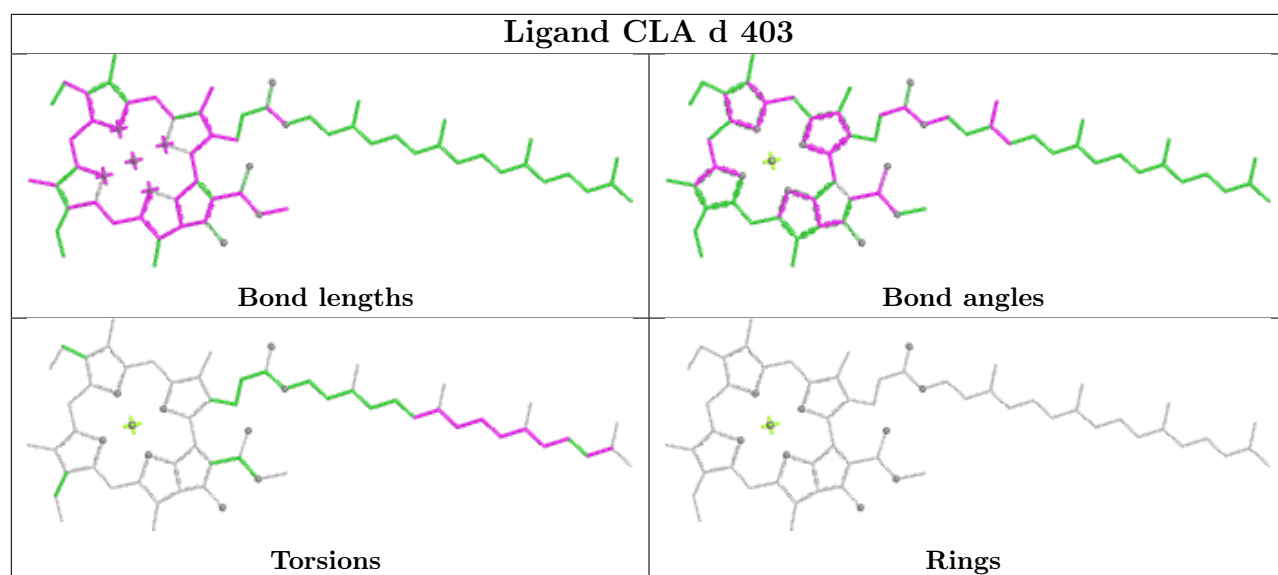
Ligand BCR C 515	
	
Bond lengths	Bond angles
	
Torsions	Rings

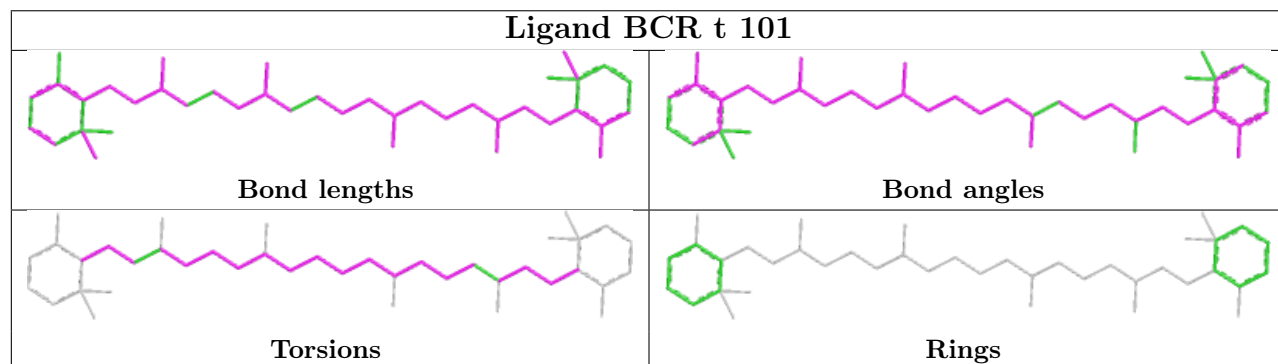
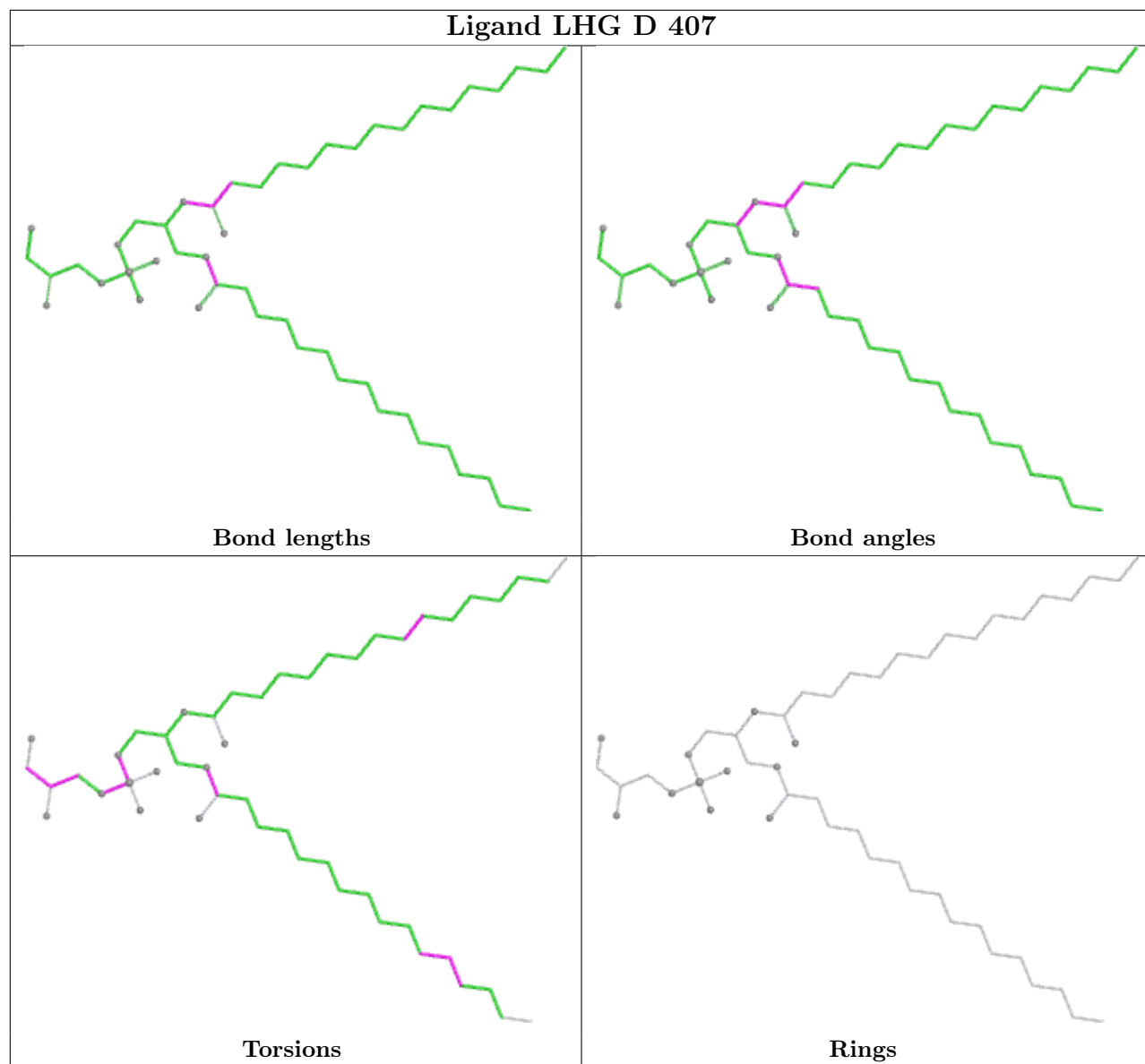
Ligand LMG A 612	
	
Bond lengths	Bond angles
	
Torsions	Rings

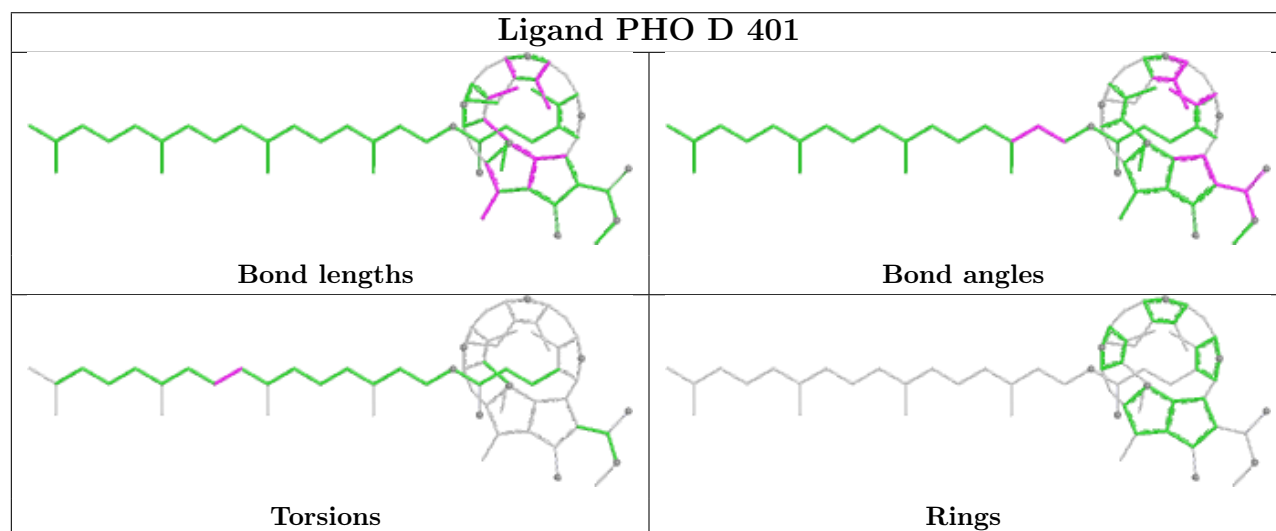
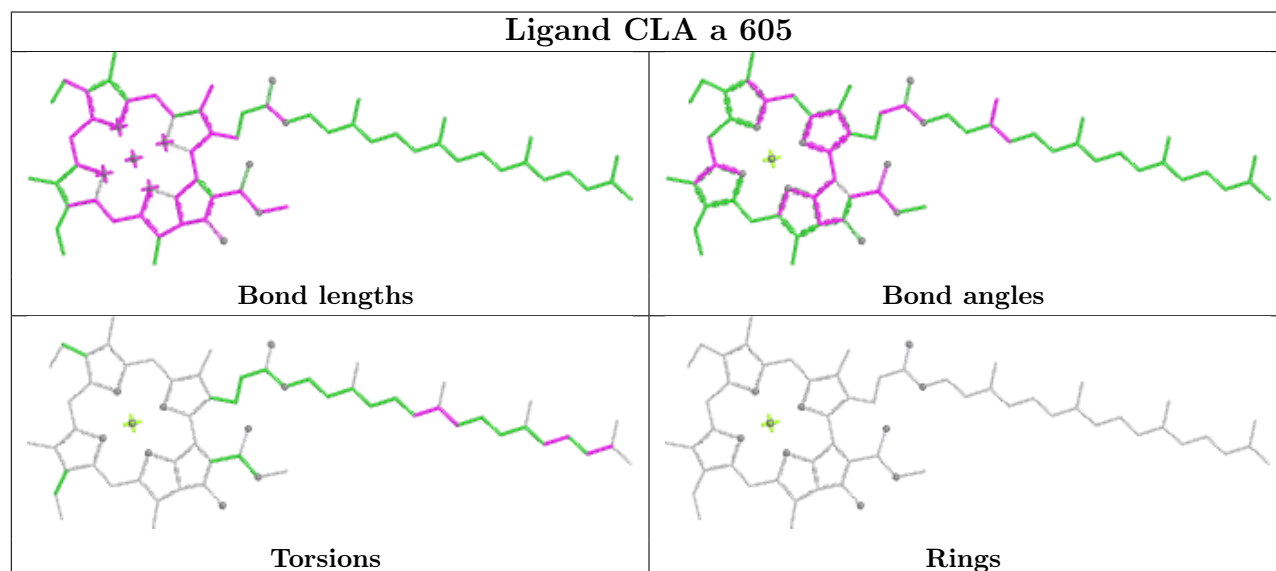
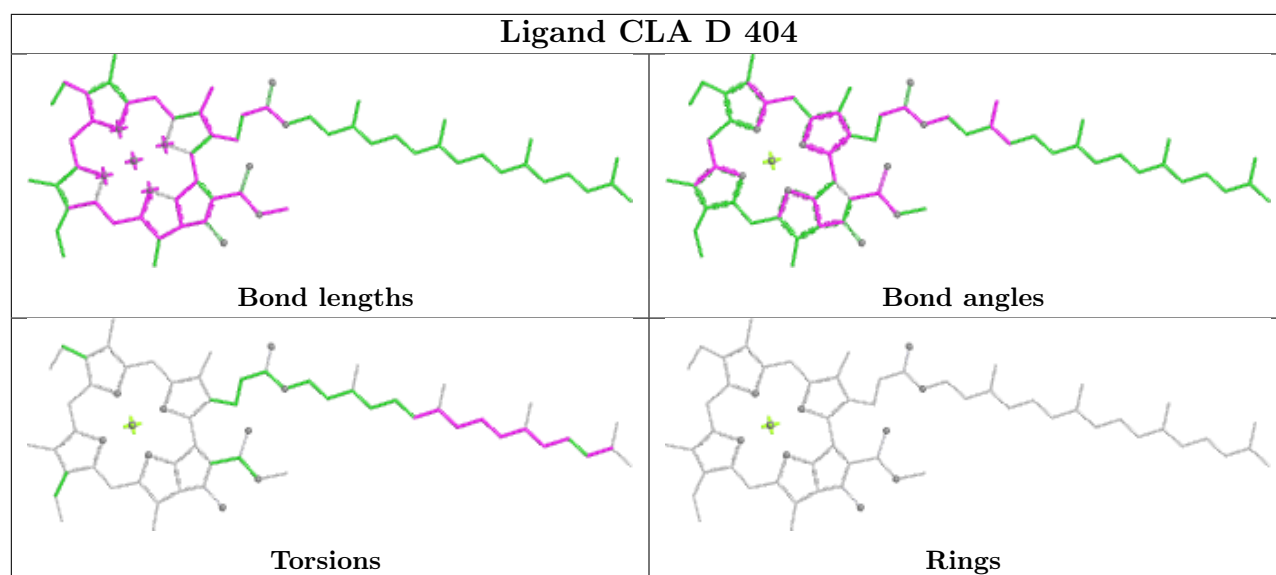
Ligand CLA c 511	
	
Bond lengths	Bond angles
	
Torsions	Rings

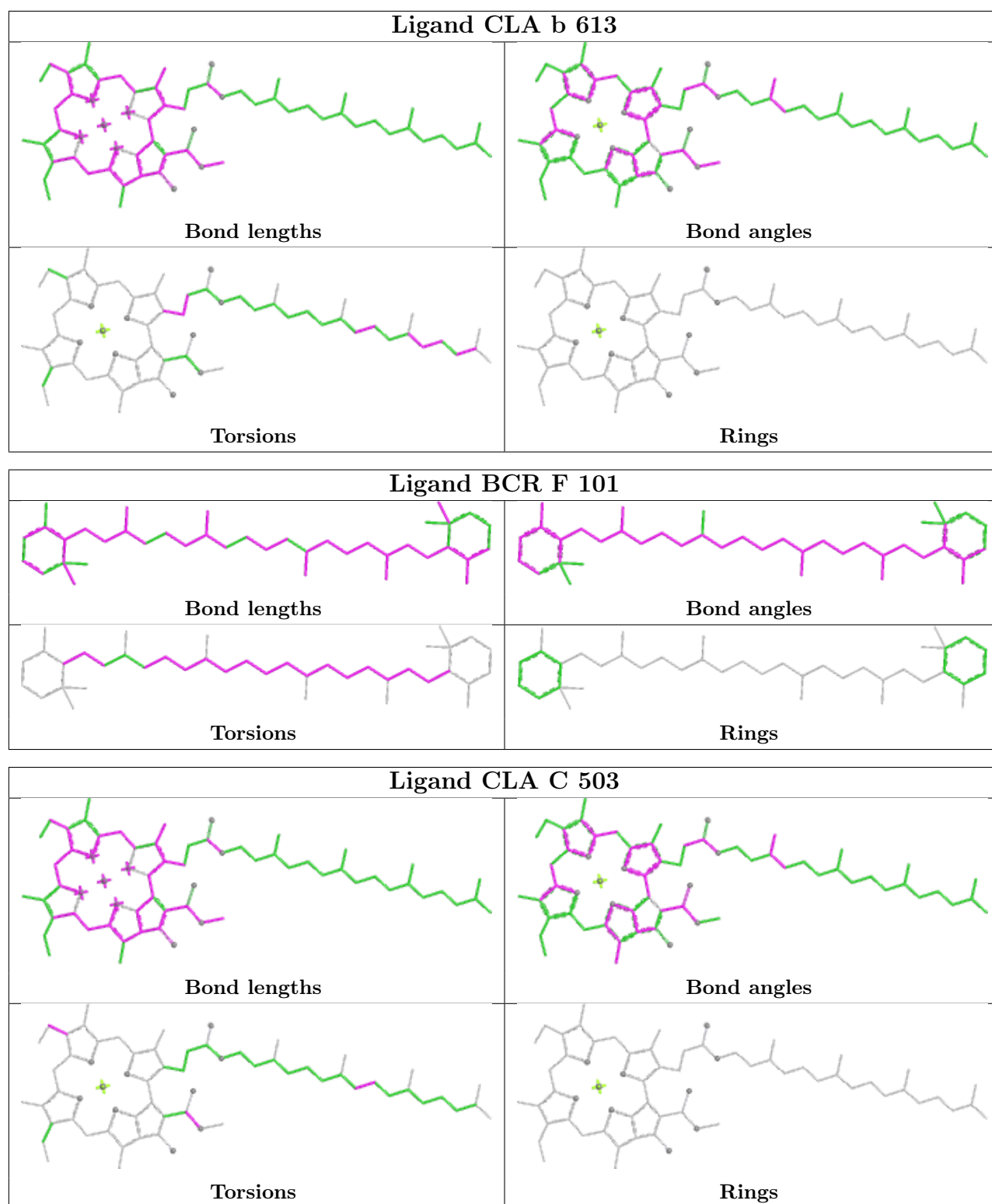


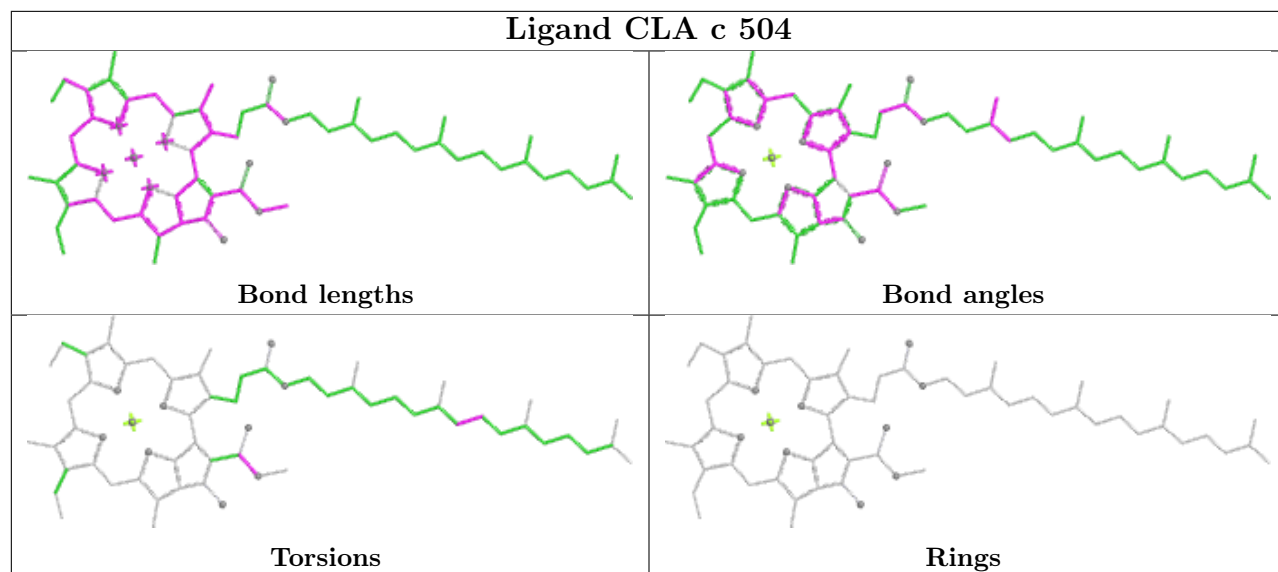
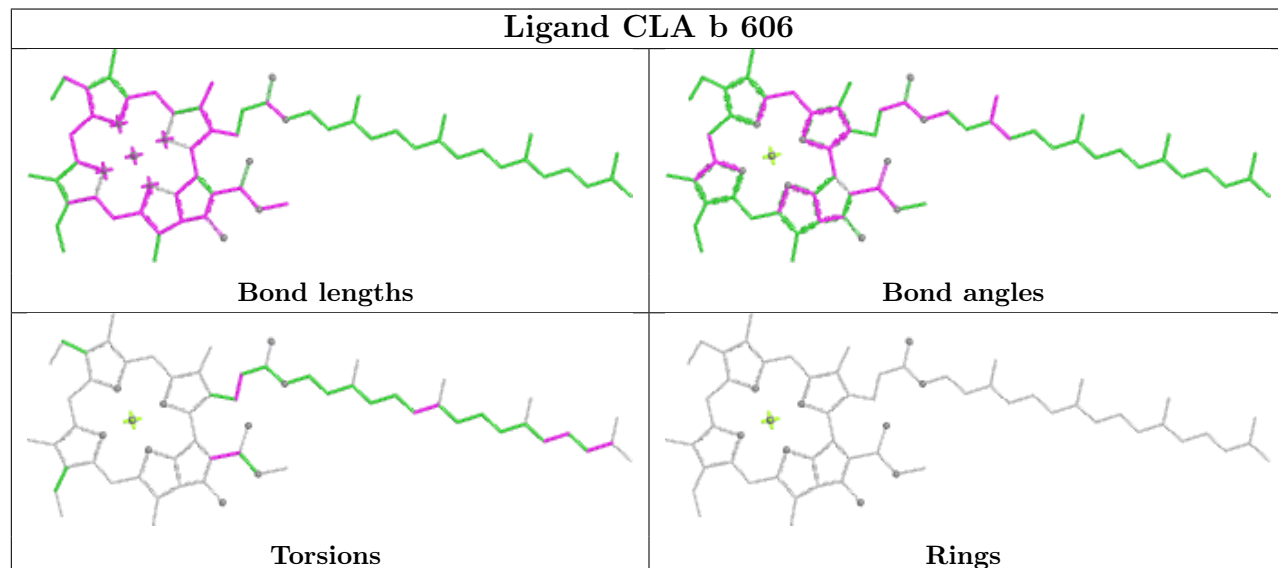


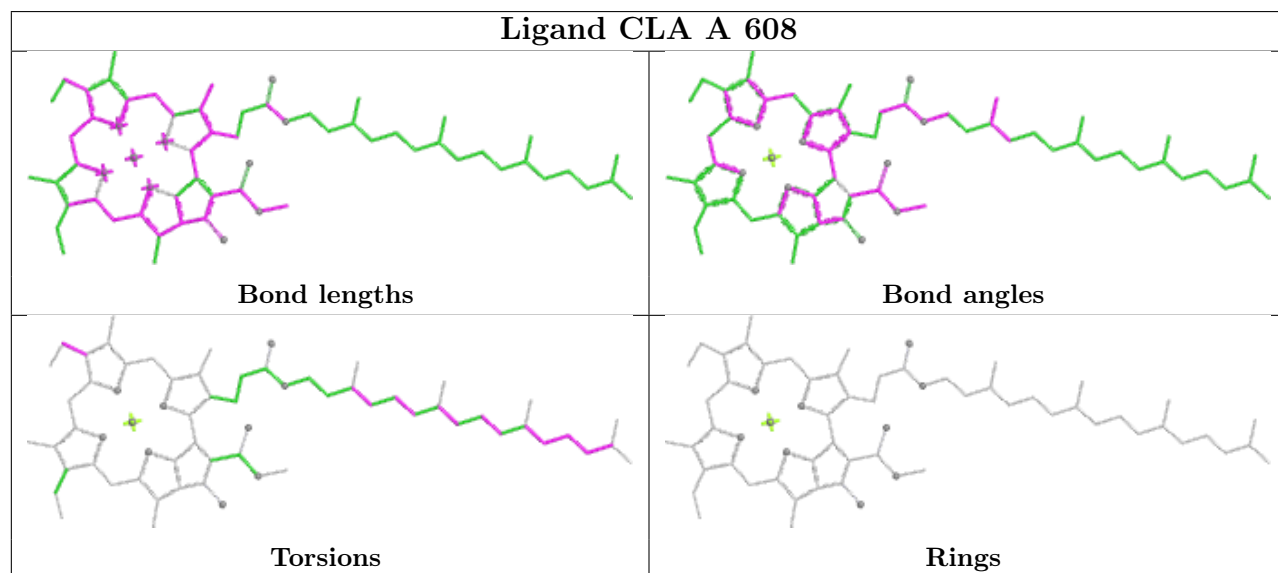
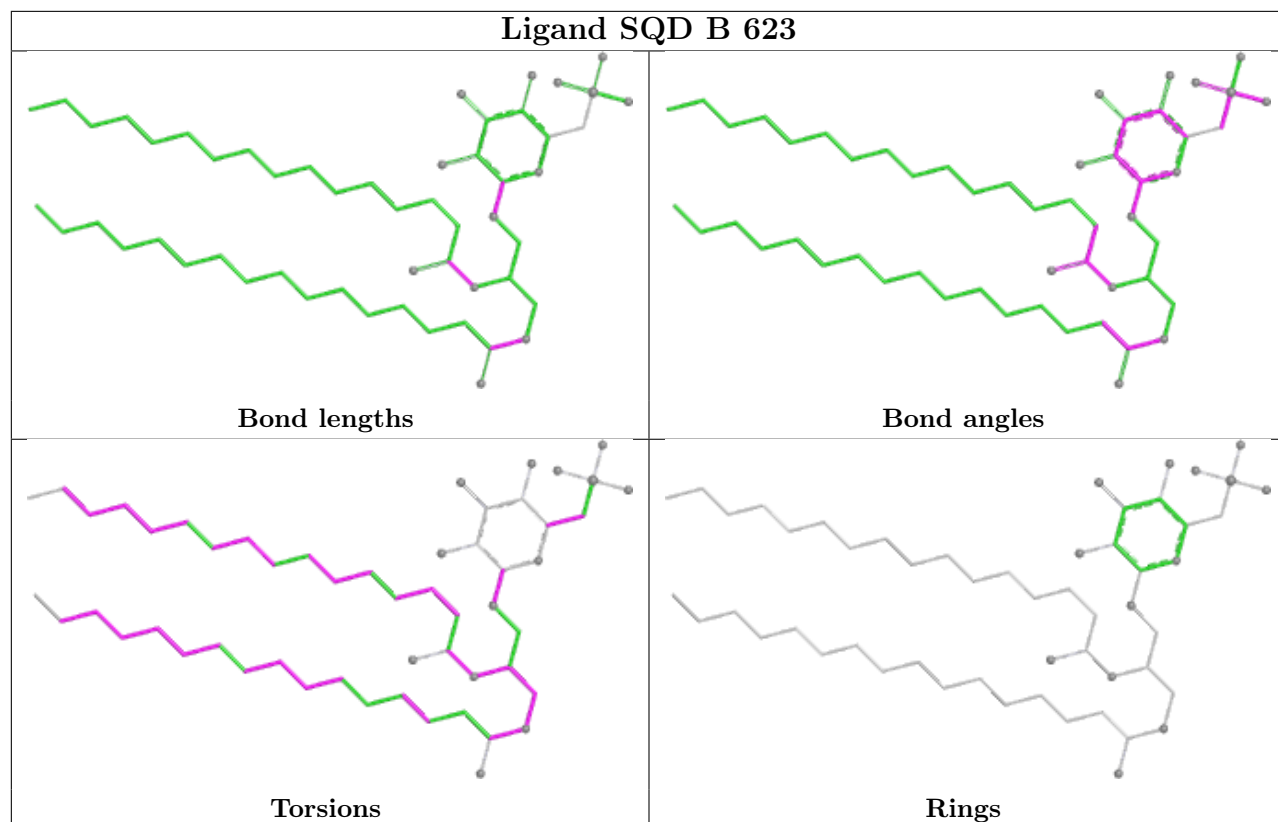


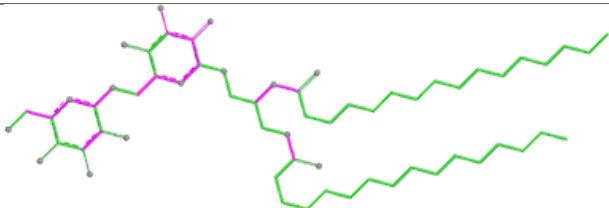
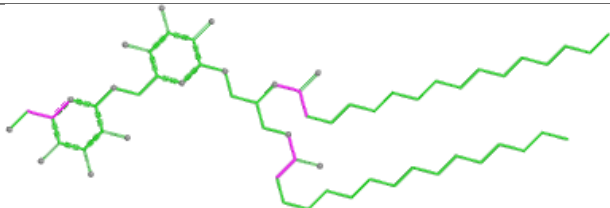
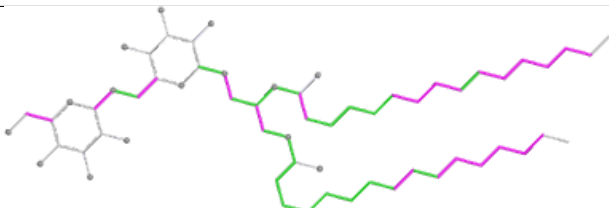
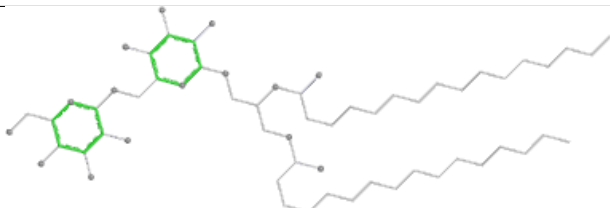


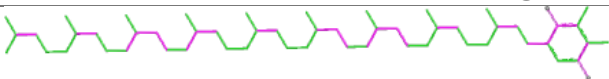
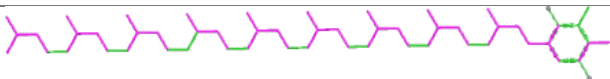
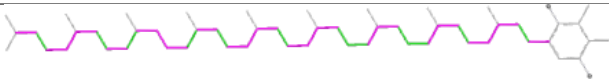
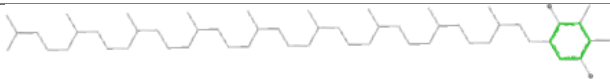


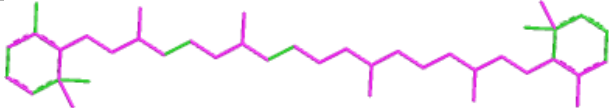
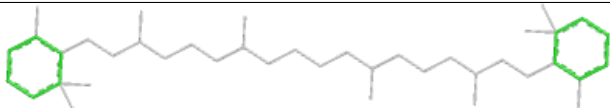


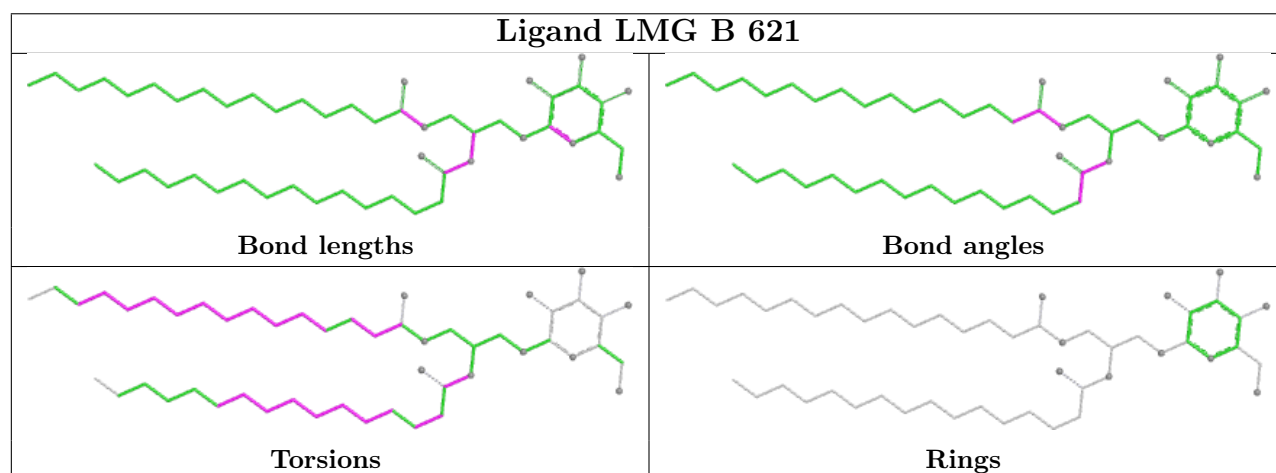
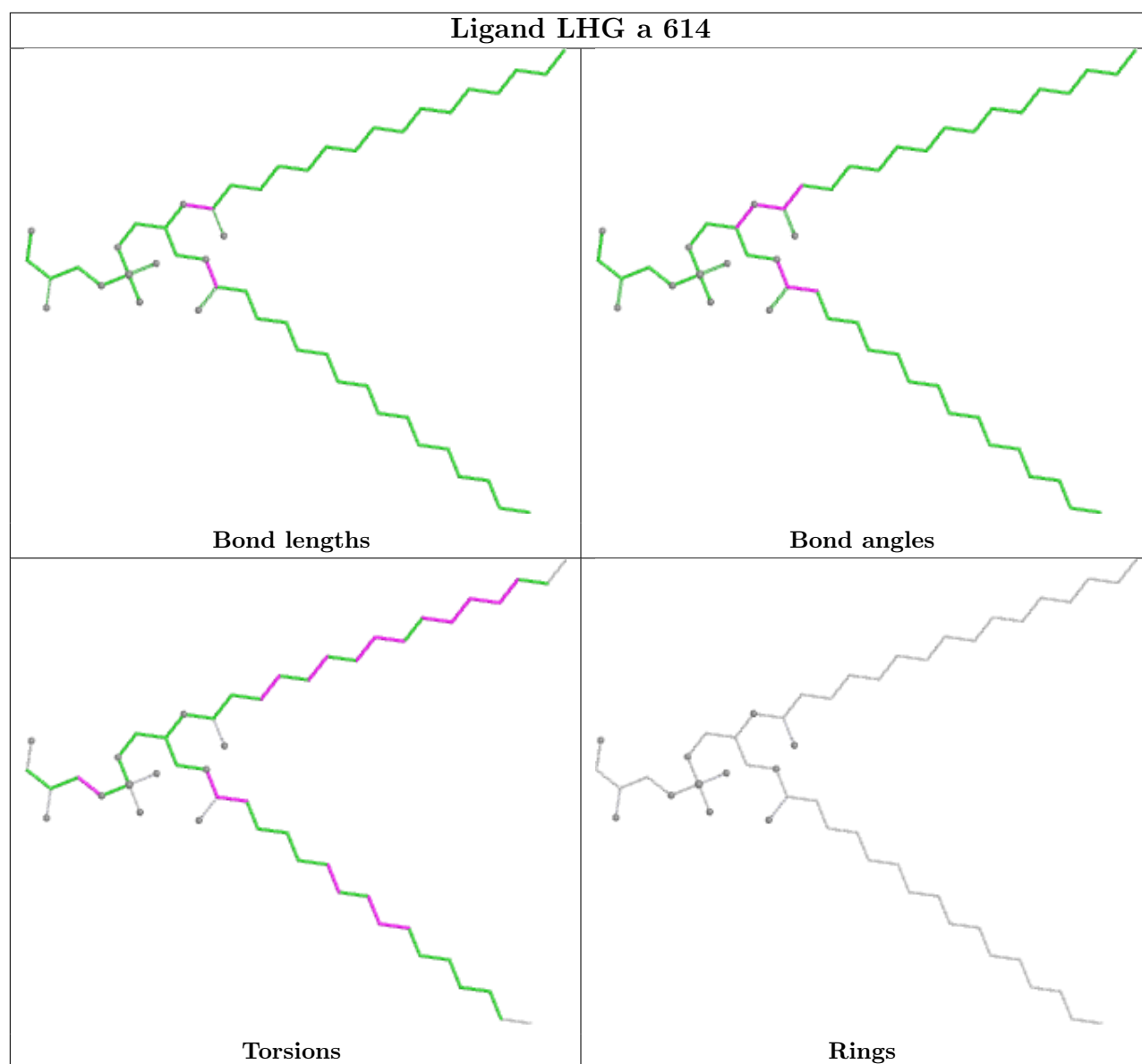
Ligand CLA c 504**Ligand CLA b 606**



Ligand DGD H 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PL9 d 404	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR f 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 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	334/334 (100%)	-0.26	1 (0%) 90 80	39, 63, 84, 93	4 (1%)
1	a	334/334 (100%)	-0.33	0 100 100	52, 84, 104, 114	4 (1%)
2	B	504/504 (100%)	-0.42	1 (0%) 91 83	41, 68, 89, 111	10 (1%)
2	b	504/504 (100%)	-0.33	4 (0%) 82 69	53, 88, 110, 131	10 (1%)
3	C	451/451 (100%)	-0.42	1 (0%) 91 83	43, 72, 84, 97	5 (1%)
3	c	451/451 (100%)	-0.43	0 100 100	57, 92, 105, 118	5 (1%)
4	D	342/342 (100%)	-0.28	3 (0%) 81 67	57, 64, 80, 102	0
4	d	342/342 (100%)	-0.18	6 (1%) 67 53	78, 85, 101, 123	0
5	E	81/81 (100%)	-0.47	0 100 100	47, 80, 98, 104	2 (2%)
5	e	81/81 (100%)	-0.42	0 100 100	61, 101, 119, 125	2 (2%)
6	F	34/34 (100%)	-0.47	0 100 100	68, 74, 99, 102	0
6	f	34/34 (100%)	-0.49	0 100 100	89, 95, 120, 122	0
7	H	65/65 (100%)	-0.40	0 100 100	43, 74, 81, 99	2 (3%)
7	h	65/65 (100%)	-0.27	0 100 100	55, 95, 101, 120	2 (3%)
8	I	38/38 (100%)	-0.40	0 100 100	36, 74, 105, 109	1 (2%)
8	i	38/38 (100%)	-0.49	0 100 100	45, 95, 126, 130	1 (2%)
9	J	38/38 (100%)	-0.69	0 100 100	66, 78, 109, 112	0
9	j	38/38 (100%)	-0.50	0 100 100	87, 99, 129, 133	0
10	K	37/37 (100%)	-0.43	0 100 100	74, 79, 86, 88	0
10	k	37/37 (100%)	-0.35	0 100 100	94, 100, 107, 108	0
11	L	37/37 (100%)	-0.41	0 100 100	37, 62, 90, 99	1 (2%)
11	l	37/37 (100%)	-0.40	0 100 100	49, 83, 111, 120	1 (2%)
12	M	34/34 (100%)	-0.40	1 (2%) 53 42	39, 64, 77, 93	1 (2%)
12	m	34/34 (100%)	-0.42	0 100 100	51, 84, 98, 114	1 (2%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/243 (100%)	-0.45	0 100 100	40, 73, 95, 111	4 (1%)
13	o	243/243 (100%)	-0.39	1 (0%) 88 77	53, 94, 116, 132	4 (1%)
14	T	30/30 (100%)	-0.47	0 100 100	32, 64, 85, 93	2 (6%)
14	t	30/30 (100%)	-0.44	0 100 100	43, 84, 105, 114	2 (6%)
15	U	97/97 (100%)	-0.45	0 100 100	64, 71, 89, 90	0
15	u	97/97 (100%)	-0.28	1 (1%) 79 64	84, 92, 110, 111	0
16	V	137/137 (100%)	-0.49	0 100 100	39, 69, 80, 88	1 (0%)
16	v	137/137 (100%)	-0.47	1 (0%) 84 71	51, 89, 101, 109	1 (0%)
17	Y	29/29 (100%)	-0.40	0 100 100	82, 89, 115, 118	0
17	y	29/29 (100%)	-0.52	0 100 100	103, 110, 136, 138	0
18	X	39/39 (100%)	-0.37	0 100 100	48, 80, 107, 108	1 (2%)
18	x	39/39 (100%)	-0.57	0 100 100	61, 101, 127, 129	1 (2%)
19	Z	62/62 (100%)	-0.39	0 100 100	80, 89, 109, 112	0
19	z	62/62 (100%)	-0.27	0 100 100	101, 110, 129, 133	0
All	All	5264/5264 (100%)	-0.37	20 (0%) 88 77	32, 83, 107, 138	68 (1%)

The worst 5 of 20 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	d	54	PHE	3.8
2	b	63	LEU	3.7
4	D	56	THR	3.1
4	d	217	THR	3.0
2	b	268	PHE	2.9

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
21	CL	V	201	1/1	0.18	0.11	91,91,91,91	0
30	CA	F	102	1/1	0.49	0.19	97,97,97,97	0
30	CA	b	603	1/1	0.49	0.11	137,137,137,137	0
21	CL	u	201	1/1	0.51	0.41	112,112,112,112	0
21	CL	A	602	1/1	0.64	0.16	65,65,65,65	0
30	CA	f	102	1/1	0.64	0.10	118,118,118,118	0
28	LMG	Z	101	37/55	0.66	0.12	96,124,129,129	0
28	LMG	c	521	51/55	0.68	0.15	104,137,142,143	0
28	LMG	C	520	51/55	0.68	0.13	83,117,122,123	0
27	SQD	a	610	54/54	0.69	0.11	110,119,128,128	0
30	CA	B	601	1/1	0.71	0.12	117,117,117,117	0
23	CLA	b	604	65/65	0.72	0.14	94,102,127,128	0
31	LHG	E	101	42/49	0.73	0.16	110,124,127,127	0
32	DGD	D	406	62/66	0.73	0.17	118,130,143,144	0
23	CLA	C	513	65/65	0.75	0.14	80,85,105,105	0
23	CLA	B	602	65/65	0.75	0.12	73,82,107,107	0
25	BCR	C	514	40/40	0.76	0.13	78,84,87,88	0
25	BCR	b	622	40/40	0.76	0.12	89,94,100,101	0
23	CLA	b	609[A]	65/65	0.77	0.14	85,90,102,103	65
23	CLA	b	609[B]	65/65	0.77	0.14	83,87,93,95	65
27	SQD	A	611	54/54	0.77	0.11	90,98,107,108	0
30	CA	O	301	1/1	0.77	0.08	90,90,90,90	0
31	LHG	e	101	42/49	0.78	0.12	131,145,147,148	0
27	SQD	x	101	43/54	0.78	0.15	128,136,140,140	0
25	BCR	T	101	40/40	0.79	0.12	65,78,85,86	0
32	DGD	d	405	62/66	0.79	0.16	138,151,164,165	0
28	LMG	z	101	37/55	0.80	0.10	117,145,149,150	0
25	BCR	B	620	40/40	0.80	0.10	68,74,80,80	0
32	DGD	c	519	62/66	0.81	0.10	83,93,113,117	0
27	SQD	b	602	54/54	0.81	0.15	99,107,121,121	0
34	MG	j	102	1/1	0.81	0.07	89,89,89,89	0
31	LHG	a	614	49/49	0.82	0.12	87,94,124,125	0
25	BCR	F	101	40/40	0.82	0.13	66,71,88,90	0
28	LMG	b	623	51/55	0.82	0.12	91,100,112,116	0
25	BCR	A	609	40/40	0.83	0.12	63,68,73,73	0
25	BCR	a	608	40/40	0.83	0.13	83,89,93,94	0
28	LMG	C	519	51/55	0.83	0.13	72,98,113,114	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	BCR	b	620	40/40	0.83	0.13	84,88,90,90	0
27	SQD	b	601	54/54	0.84	0.12	91,103,109,109	0
23	CLA	b	619	65/65	0.84	0.11	83,90,139,139	0
26	PL9	A	610	55/55	0.84	0.17	93,109,118,119	0
26	PL9	a	609	55/55	0.84	0.16	113,130,139,140	0
23	CLA	C	507	65/65	0.84	0.14	70,74,92,94	0
25	BCR	B	618	40/40	0.84	0.12	63,68,69,70	0
27	SQD	a	612	54/54	0.84	0.11	111,124,129,130	0
25	BCR	k	101	40/40	0.85	0.09	95,99,100,100	0
25	BCR	t	101	40/40	0.85	0.12	86,99,106,106	0
23	CLA	a	605	65/65	0.85	0.12	80,83,124,126	0
25	BCR	b	621	40/40	0.85	0.12	83,89,101,101	0
25	BCR	H	101	40/40	0.85	0.17	67,74,83,83	0
25	BCR	c	516	40/40	0.85	0.14	92,98,102,102	0
25	BCR	f	101	40/40	0.85	0.11	87,91,109,110	0
27	SQD	X	101	43/54	0.86	0.11	108,115,119,119	0
23	CLA	D	404	65/65	0.86	0.12	65,68,106,107	0
28	LMG	c	520	51/55	0.86	0.12	92,118,134,135	0
26	PL9	d	404	55/55	0.86	0.18	80,84,91,93	0
28	LMG	j	101	51/55	0.86	0.11	87,96,126,129	0
23	CLA	c	514	65/65	0.86	0.10	101,106,125,126	0
23	CLA	B	607[B]	65/65	0.87	0.14	63,67,72,75	65
23	CLA	B	617	65/65	0.87	0.10	63,69,118,119	0
23	CLA	B	607[A]	65/65	0.87	0.14	65,69,81,82	65
28	LMG	A	612	51/55	0.87	0.12	94,100,105,105	0
28	LMG	B	621	51/55	0.87	0.11	70,80,92,95	0
23	CLA	c	508	65/65	0.87	0.12	91,94,113,115	0
31	LHG	D	407	49/49	0.87	0.15	64,69,78,81	0
23	CLA	c	513	65/65	0.87	0.12	99,102,124,124	0
25	BCR	c	515	40/40	0.87	0.10	99,105,108,108	0
28	LMG	a	611	51/55	0.87	0.13	114,121,126,126	0
32	DGD	C	518	62/66	0.87	0.10	62,72,93,97	0
27	SQD	B	623	54/54	0.87	0.13	119,127,141,142	0
23	CLA	C	512	65/65	0.87	0.12	78,82,103,104	0
25	BCR	K	101	40/40	0.87	0.10	75,78,79,80	0
25	BCR	h	101	40/40	0.87	0.13	87,94,103,104	0
23	CLA	C	506	65/65	0.88	0.11	72,79,115,115	0
23	CLA	c	502	65/65	0.88	0.14	90,93,106,108	0
32	DGD	C	517	62/66	0.88	0.10	63,75,103,104	0
23	CLA	c	504	65/65	0.88	0.14	89,93,96,97	0
23	CLA	c	507	65/65	0.88	0.10	93,100,136,136	0
23	CLA	B	616	65/65	0.88	0.11	65,68,86,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	BCR	C	515	40/40	0.88	0.11	71,78,81,82	0
22	BCT	a	603	4/4	0.88	0.30	100,101,101,103	0
25	BCR	B	619	40/40	0.89	0.09	62,69,81,81	0
23	CLA	C	504	65/65	0.89	0.12	66,68,95,95	0
24	PHO	d	401	64/64	0.89	0.10	80,84,90,94	0
28	LMG	J	101	51/55	0.89	0.11	66,76,106,108	0
30	CA	o	301	1/1	0.89	0.04	110,110,110,110	0
23	CLA	b	618	65/65	0.90	0.11	86,89,107,108	0
32	DGD	c	517	62/66	0.90	0.13	84,94,122,124	0
23	CLA	B	608	65/65	0.90	0.11	58,61,73,74	0
31	LHG	D	408	49/49	0.90	0.10	67,74,103,104	0
34	MG	J	102	1/1	0.90	0.11	68,68,68,68	0
23	CLA	b	616	65/65	0.90	0.10	80,84,106,108	0
23	CLA	B	615	65/65	0.91	0.10	61,65,101,102	0
23	CLA	d	403	65/65	0.91	0.09	86,89,126,128	0
23	CLA	C	505	65/65	0.91	0.12	69,71,85,85	0
31	LHG	l	101	49/49	0.91	0.12	84,92,104,106	0
23	CLA	B	606	65/65	0.91	0.12	59,64,75,76	0
23	CLA	a	607	65/65	0.91	0.09	83,85,133,133	0
23	CLA	c	503	65/65	0.91	0.12	85,87,101,103	0
23	CLA	B	610	65/65	0.91	0.10	64,69,72,73	0
23	CLA	C	508	65/65	0.91	0.09	66,70,95,99	0
23	CLA	C	501	65/65	0.91	0.12	69,73,85,87	0
32	DGD	h	102	62/66	0.91	0.17	87,93,99,101	0
25	BCR	C	521	40/40	0.91	0.15	70,74,78,78	0
23	CLA	b	611	65/65	0.91	0.11	82,86,92,93	0
23	CLA	b	617	65/65	0.92	0.11	82,86,121,122	0
21	CL	A	603	1/1	0.92	0.15	62,62,62,62	0
31	LHG	b	624	49/49	0.92	0.14	91,96,102,102	0
31	LHG	d	406	49/49	0.92	0.15	85,89,98,102	0
23	CLA	C	511	65/65	0.92	0.12	70,75,78,79	0
23	CLA	B	603	65/65	0.92	0.12	64,67,72,73	0
32	DGD	C	516	62/66	0.92	0.11	64,73,102,103	0
23	CLA	b	605	65/65	0.92	0.13	85,88,93,94	0
23	CLA	b	608	65/65	0.92	0.12	80,84,95,97	0
23	CLA	B	605	65/65	0.92	0.12	60,63,91,91	0
32	DGD	H	102	62/66	0.92	0.13	66,72,79,81	0
23	CLA	D	403	65/65	0.92	0.12	54,59,75,76	0
32	DGD	c	518	62/66	0.92	0.08	84,96,124,124	0
23	CLA	b	610	65/65	0.92	0.12	79,82,94,95	0
23	CLA	A	608	65/65	0.92	0.10	62,65,112,113	0
23	CLA	b	612	65/65	0.92	0.10	85,90,92,93	0

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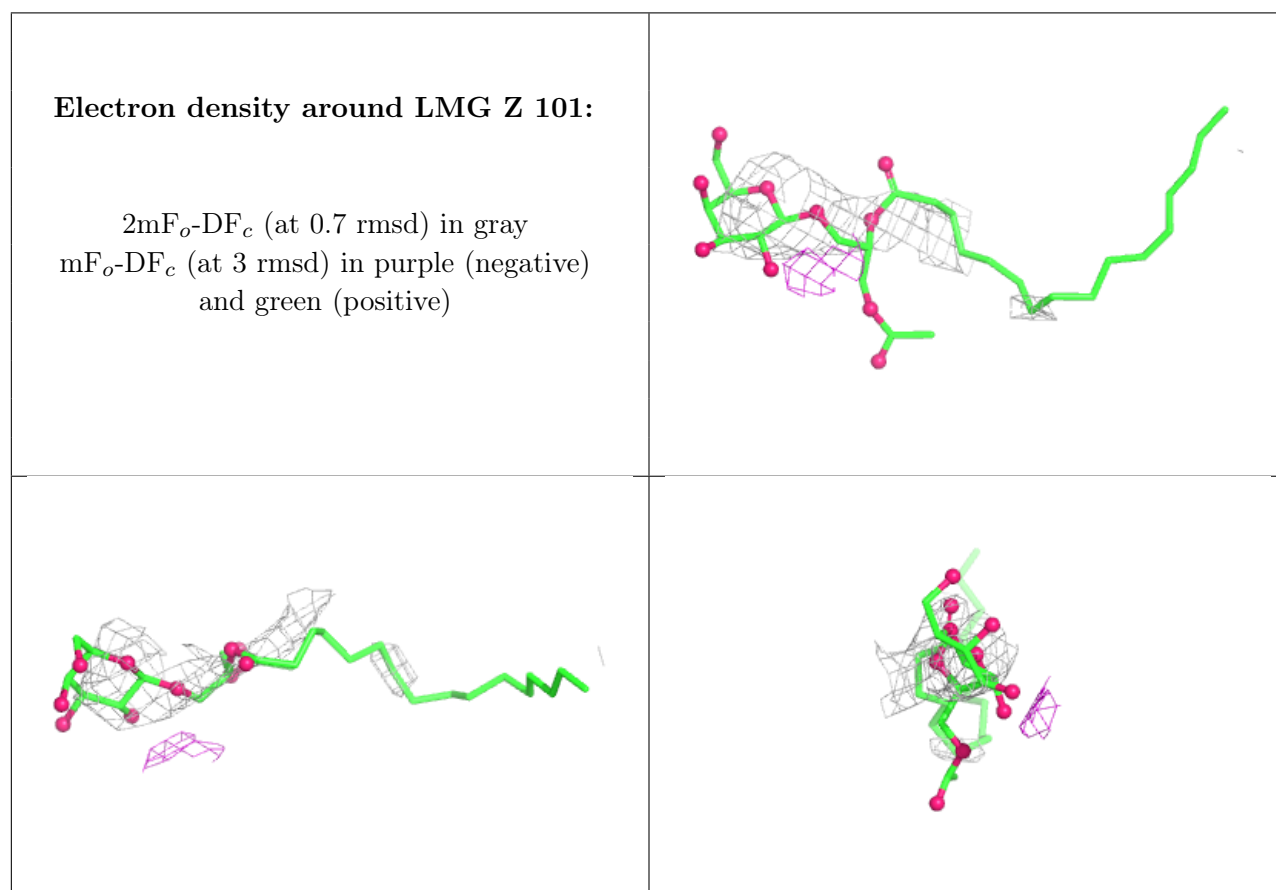
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	PHO	D	401	64/64	0.92	0.10	59,63,69,73	0
23	CLA	a	604	65/65	0.92	0.12	77,80,87,95	0
23	CLA	C	509	65/65	0.93	0.14	70,72,87,88	0
23	CLA	b	606	65/65	0.93	0.14	79,84,92,96	0
23	CLA	c	506	65/65	0.93	0.10	89,92,106,106	0
23	CLA	b	614	65/65	0.93	0.10	80,83,94,96	0
25	BCR	c	522	40/40	0.93	0.13	91,95,98,99	0
22	BCT	A	604	4/4	0.93	0.10	79,80,81,82	0
31	LHG	L	101	49/49	0.93	0.12	63,72,83,85	0
23	CLA	c	510	65/65	0.93	0.12	91,93,108,108	0
23	CLA	B	614	65/65	0.94	0.08	60,63,85,87	0
23	CLA	B	609	65/65	0.94	0.09	61,65,71,72	0
23	CLA	b	613	65/65	0.94	0.12	82,86,94,98	0
21	CL	a	602	1/1	0.94	0.08	86,86,86,86	0
23	CLA	b	615	65/65	0.94	0.17	81,85,91,92	0
23	CLA	B	611	65/65	0.94	0.13	62,65,73,77	0
31	LHG	B	622	49/49	0.94	0.12	70,75,81,82	0
23	CLA	c	509	65/65	0.94	0.08	87,90,115,119	0
23	CLA	B	613	65/65	0.94	0.14	61,64,71,72	0
23	CLA	c	511	65/65	0.94	0.08	86,90,96,99	0
23	CLA	c	512	65/65	0.94	0.09	90,95,99,99	0
23	CLA	C	502	65/65	0.94	0.09	65,67,80,83	0
33	HEM	e	102	43/43	0.94	0.11	101,103,107,108	0
23	CLA	C	503	65/65	0.94	0.12	68,72,76,77	0
29	FE2	a	615	1/1	0.94	0.06	88,88,88,88	0
24	PHO	a	606	64/64	0.95	0.10	78,83,86,87	0
26	PL9	D	405	55/55	0.95	0.14	60,64,70,72	0
23	CLA	A	606	65/65	0.95	0.13	60,62,104,106	0
23	CLA	B	604	65/65	0.95	0.11	58,63,72,76	0
23	CLA	c	505	65/65	0.95	0.09	86,89,115,116	0
23	CLA	B	612	65/65	0.95	0.08	60,62,73,75	0
23	CLA	b	607	65/65	0.95	0.10	81,84,111,112	0
21	CL	c	501	1/1	0.95	0.08	83,83,83,83	0
20	OEX	A	601	10/10	0.95	0.15	63,64,67,67	0
20	OEX	a	601	10/10	0.96	0.15	83,84,87,88	0
23	CLA	a	613	65/65	0.96	0.13	75,79,91,96	0
23	CLA	d	402	65/65	0.96	0.12	75,80,95,96	0
23	CLA	A	605	65/65	0.96	0.12	56,59,66,75	0
33	HEM	E	102	43/43	0.96	0.08	80,82,86,87	0
24	PHO	A	607	64/64	0.96	0.07	57,62,65,67	0
33	HEM	v	201	43/43	0.96	0.15	84,86,88,90	0
23	CLA	C	510	65/65	0.96	0.09	65,69,76,78	0

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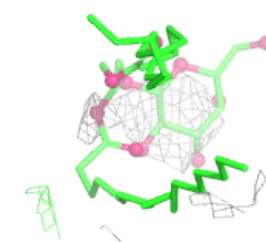
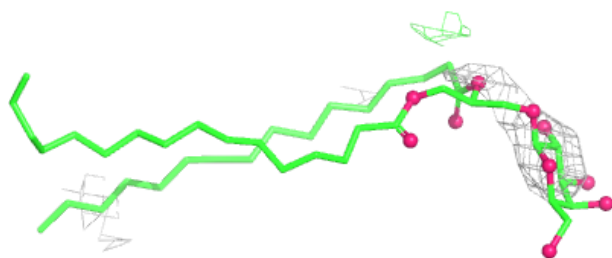
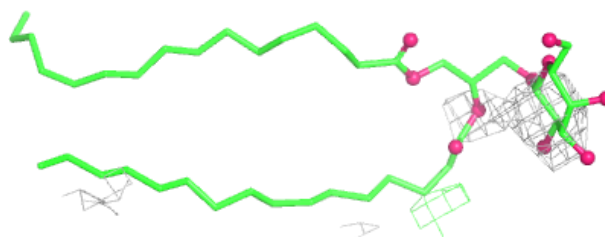
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	CLA	D	402	65/65	0.96	0.11	54,59,70,76	0
29	FE2	A	613	1/1	0.97	0.08	67,67,67,67	0
33	HEM	V	202	43/43	0.97	0.10	63,65,68,69	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

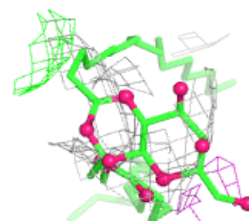
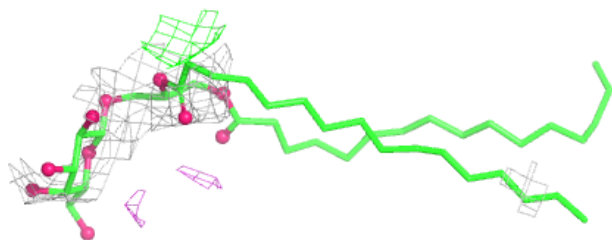
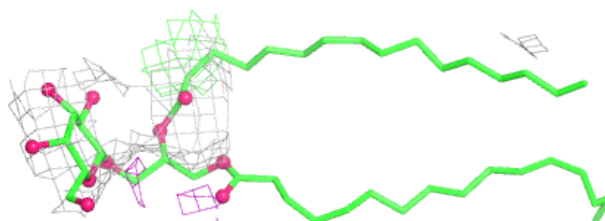


Electron density around LMG c 521:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

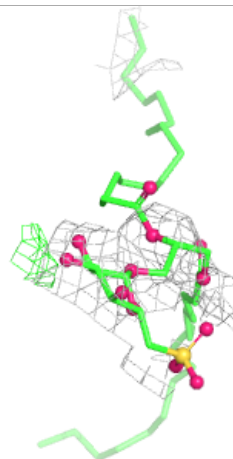
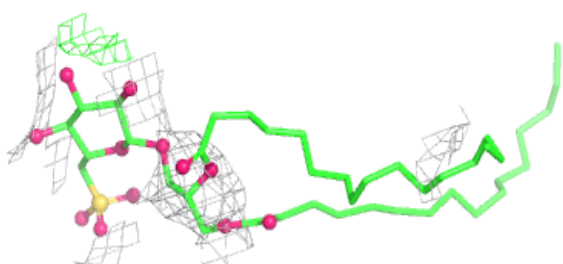
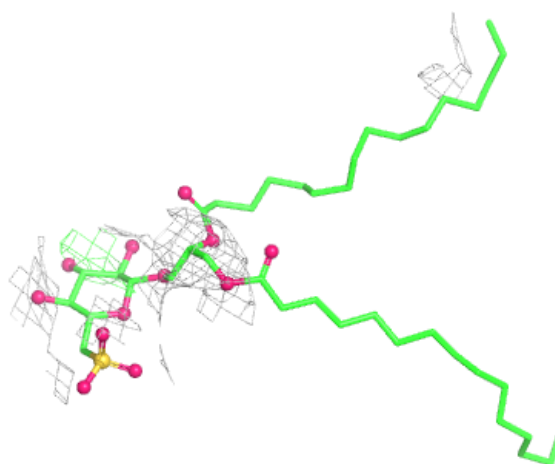
**Electron density around LMG C 520:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



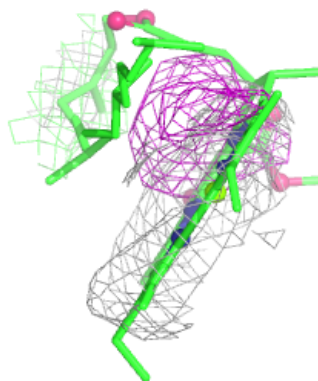
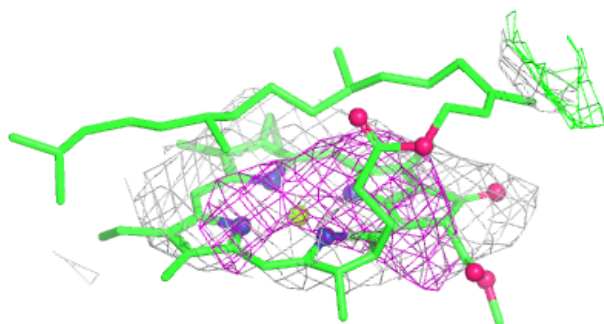
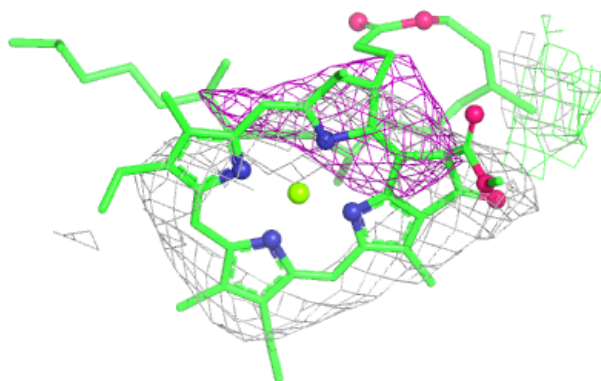
Electron density around SQD a 610:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

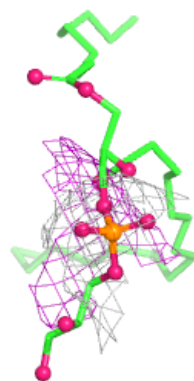
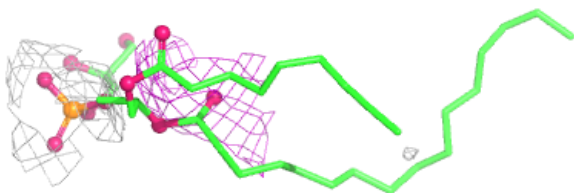
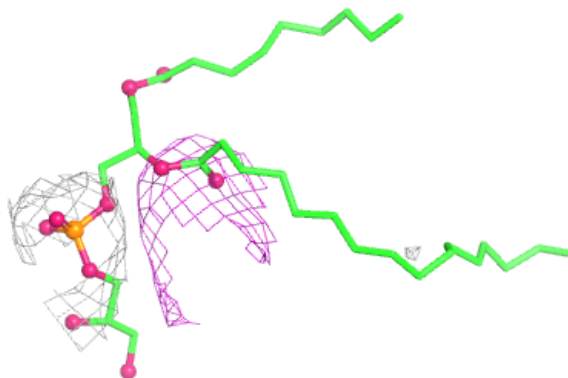


Electron density around CLA b 604:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

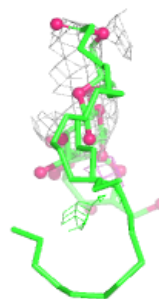
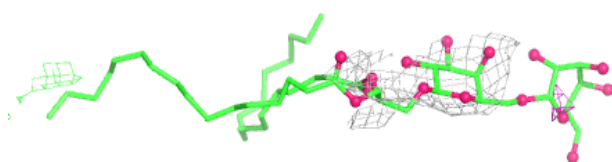
**Electron density around LHG E 101:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

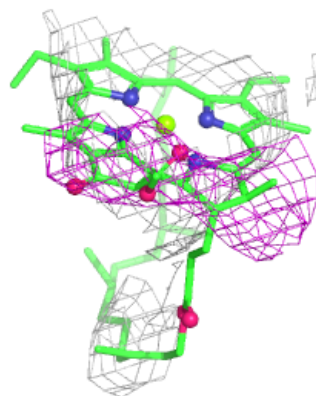
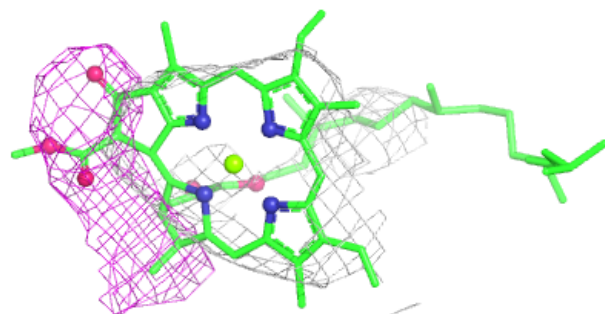
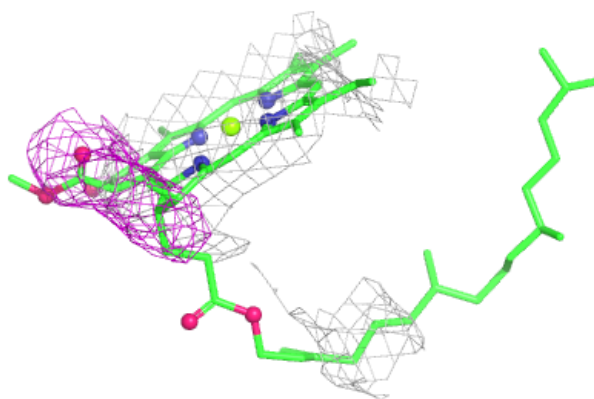


Electron density around DGD D 406:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

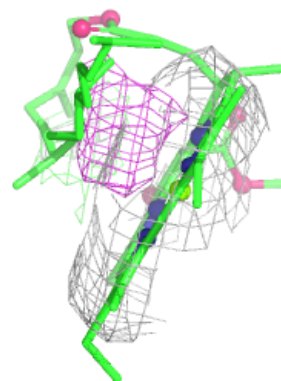
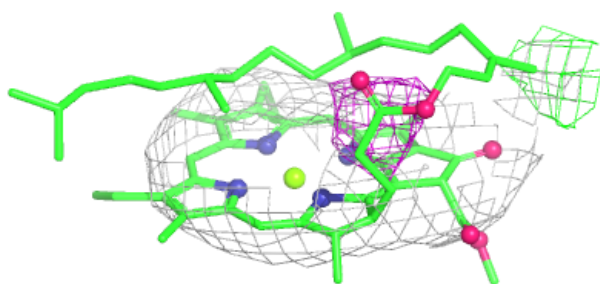
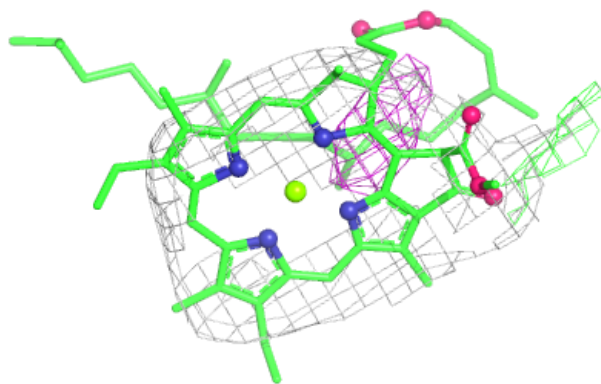
**Electron density around CLA C 513:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

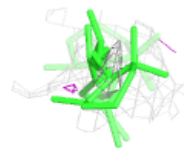
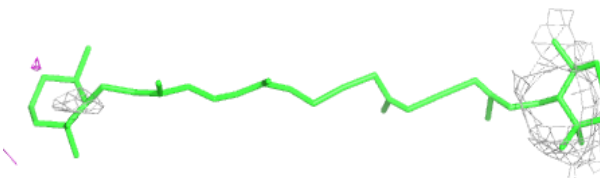
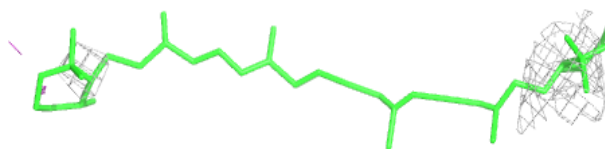


Electron density around CLA B 602:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

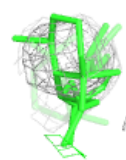
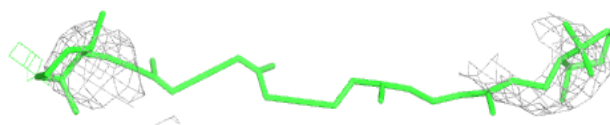
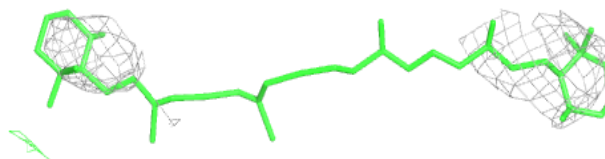
**Electron density around BCR C 514:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

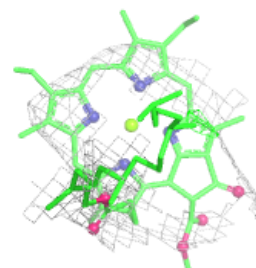
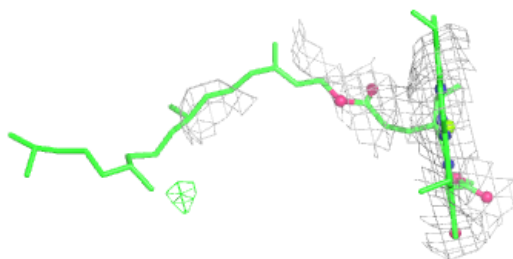
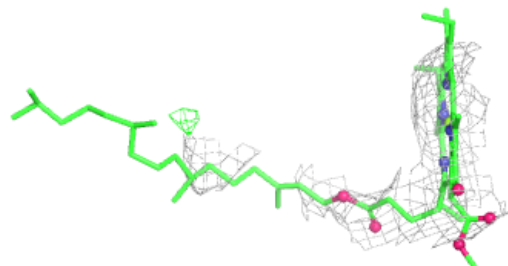


Electron density around BCR b 622:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

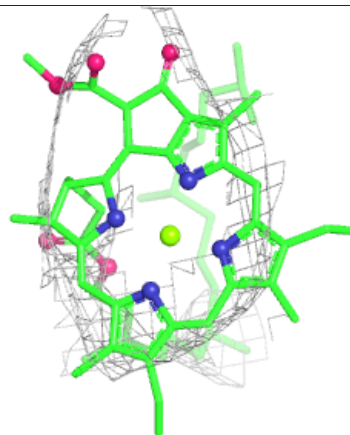
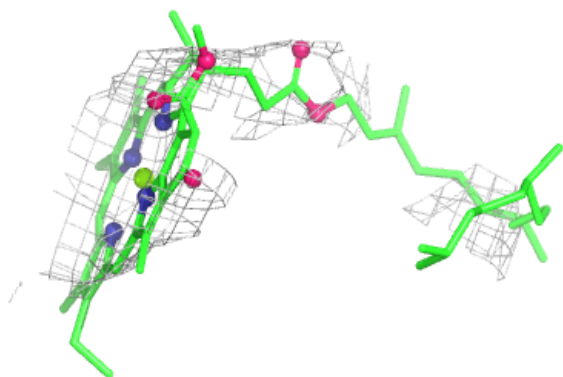
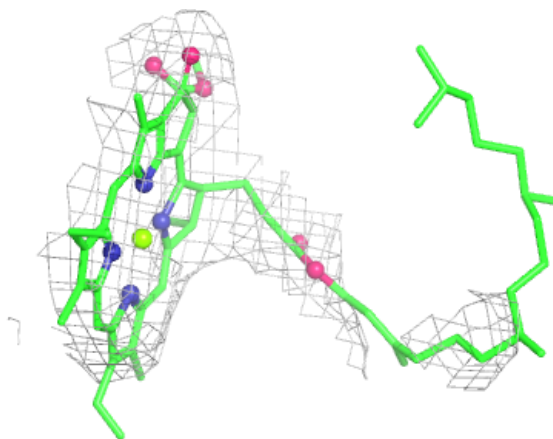
**Electron density around CLA b 609 (A):**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA b 609 (B):

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



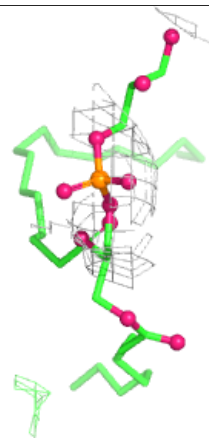
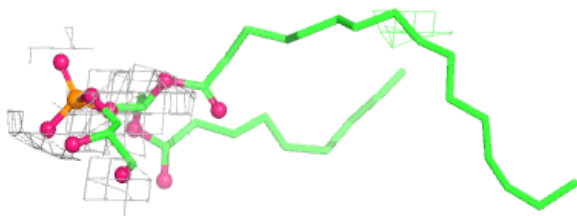
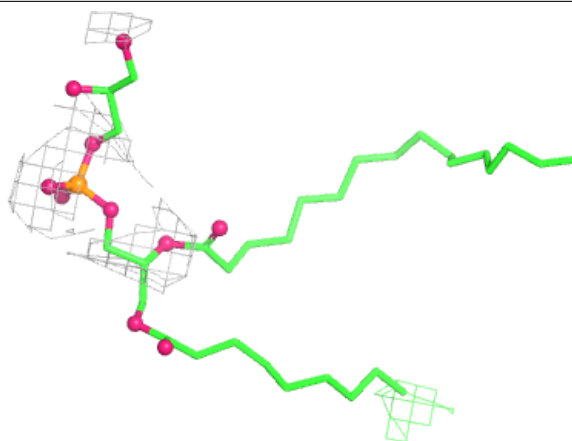
Electron density around SQD A 611:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



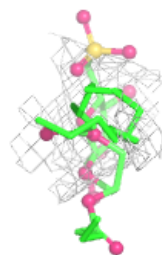
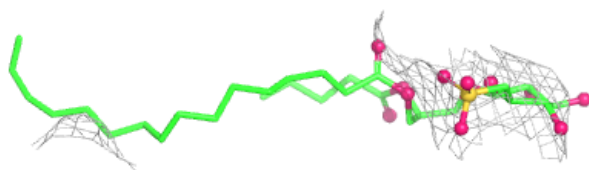
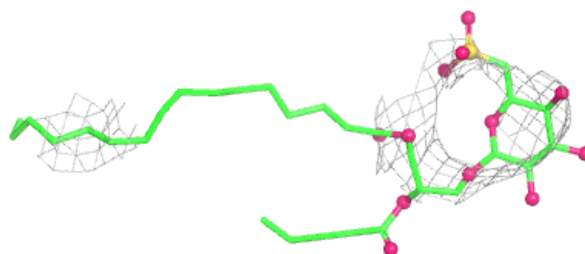
Electron density around LHG e 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

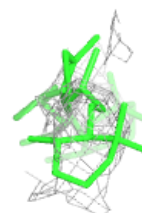
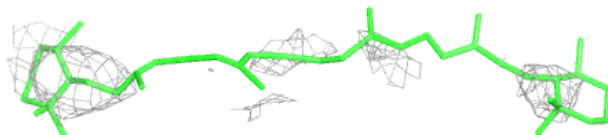
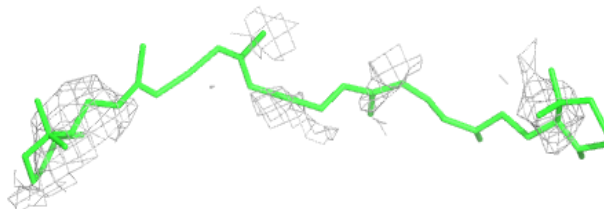


Electron density around SQD x 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

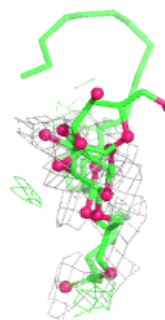
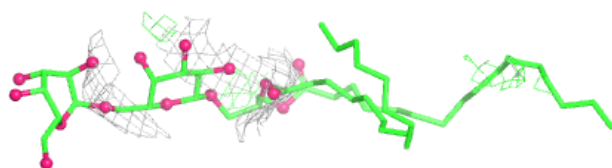
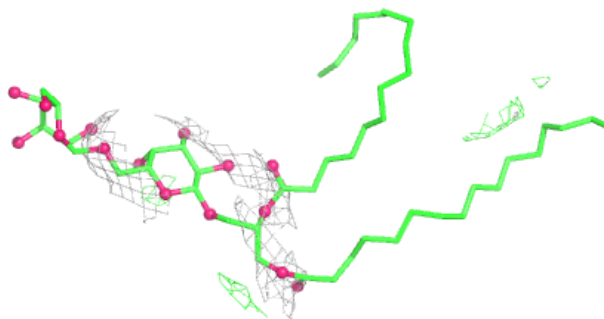
**Electron density around BCR T 101:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

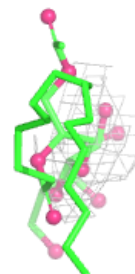
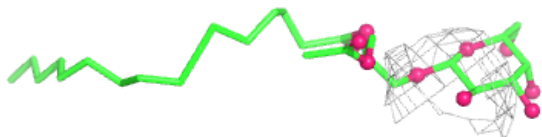
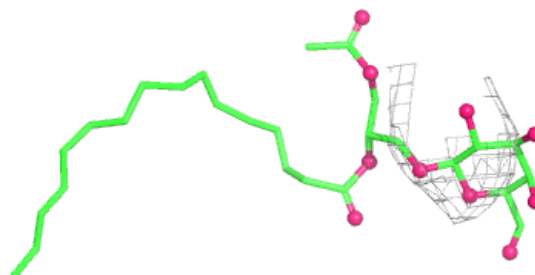


Electron density around DGD d 405:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

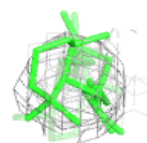
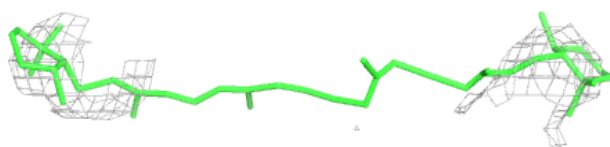
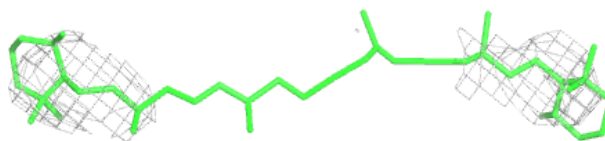
**Electron density around LMG z 101:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

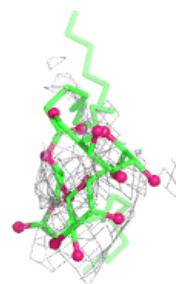
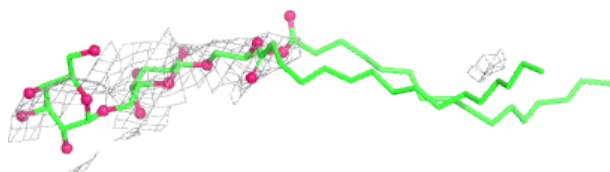
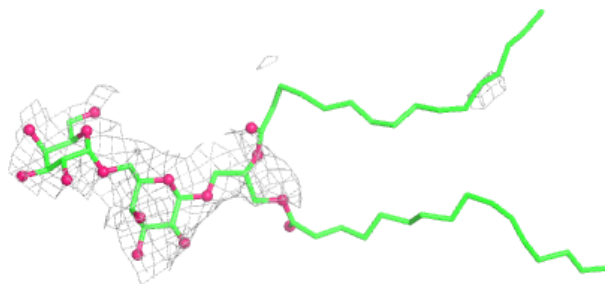


Electron density around BCR B 620:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

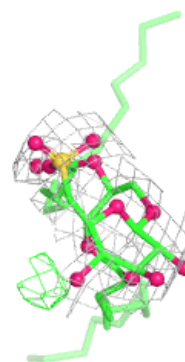
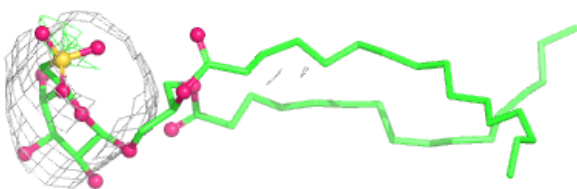
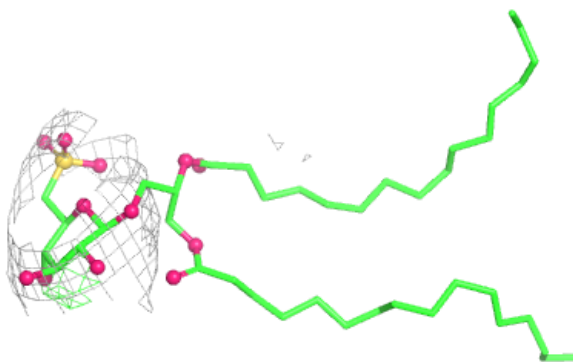
**Electron density around DGD c 519:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

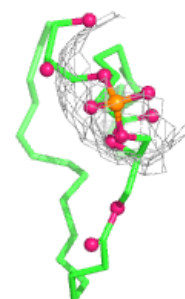


Electron density around SQD b 602:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

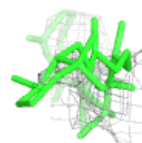
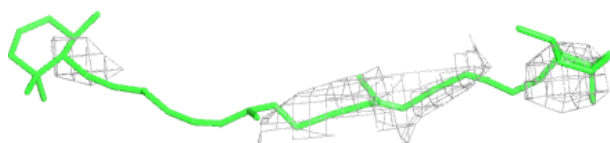
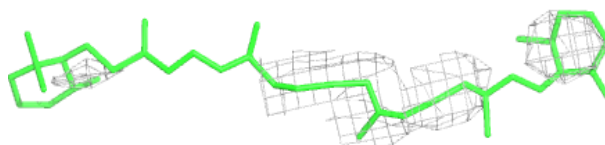
**Electron density around LHG a 614:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

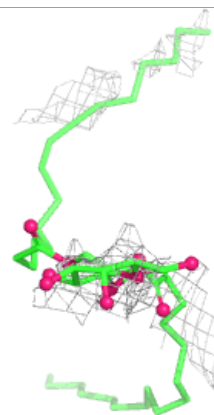
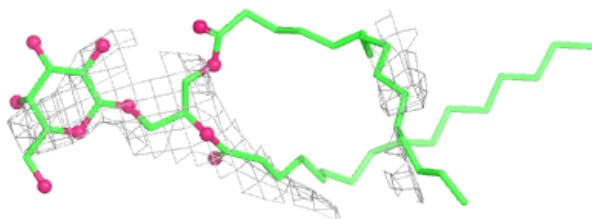
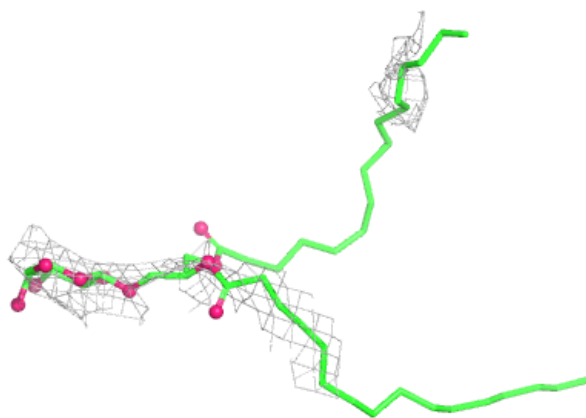


Electron density around BCR F 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

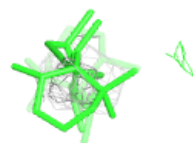
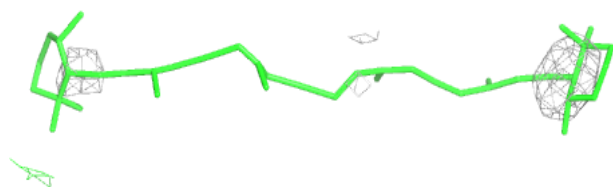
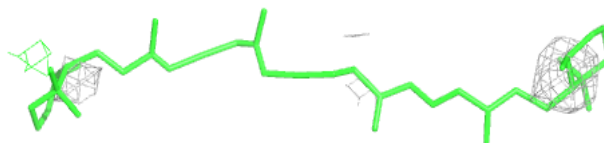
**Electron density around LMG b 623:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

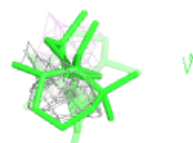
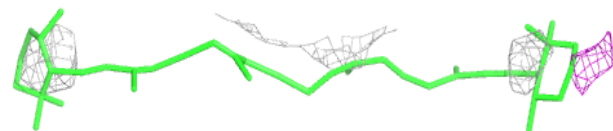
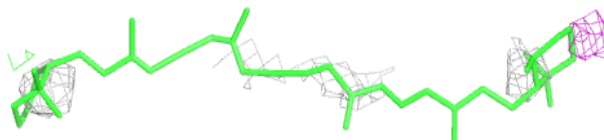


Electron density around BCR A 609:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

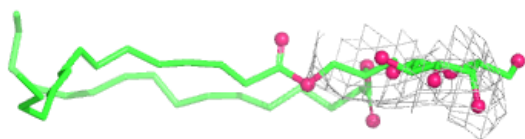
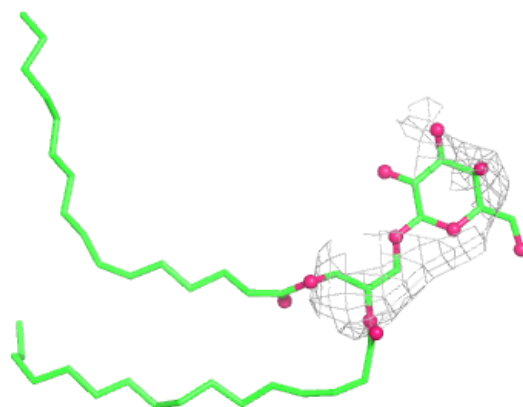
**Electron density around BCR a 608:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

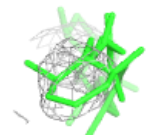
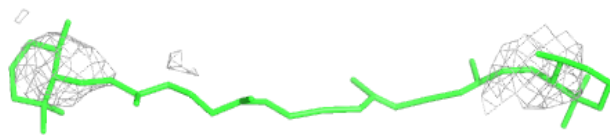
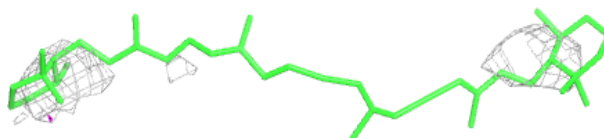


Electron density around LMG C 519:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

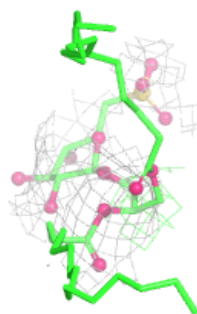
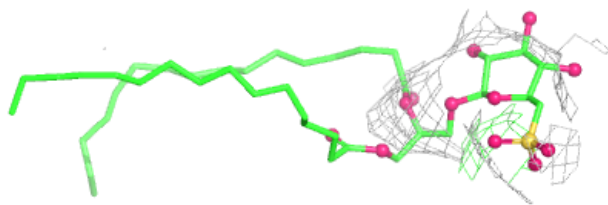
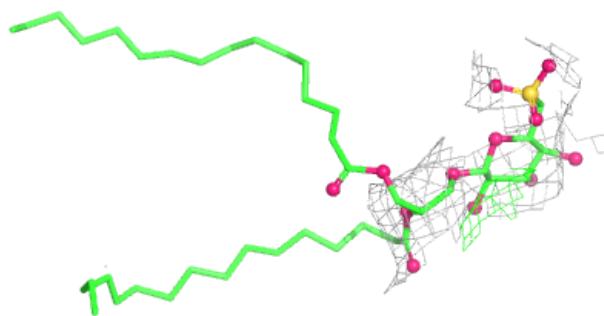
**Electron density around BCR b 620:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



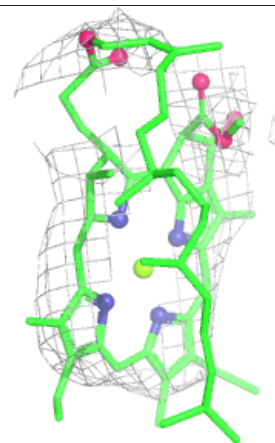
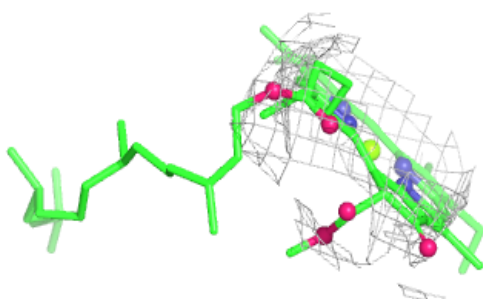
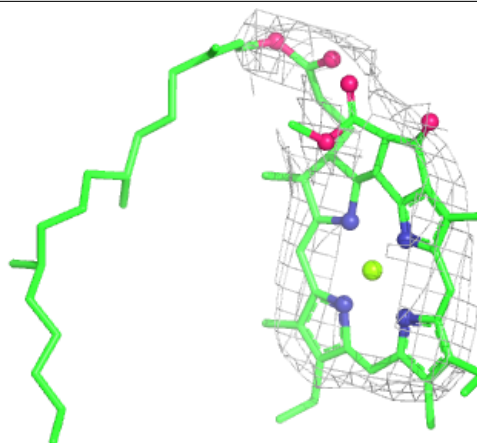
Electron density around SQD b 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

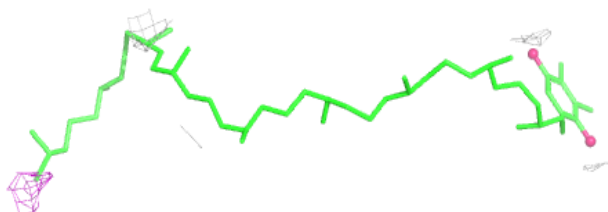


Electron density around CLA b 619:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

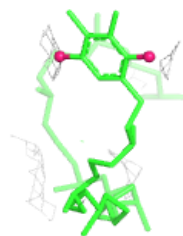
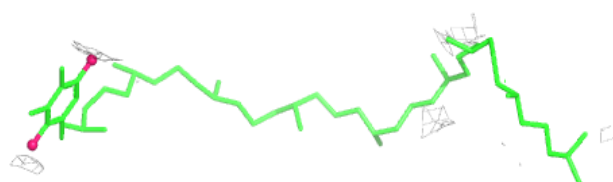
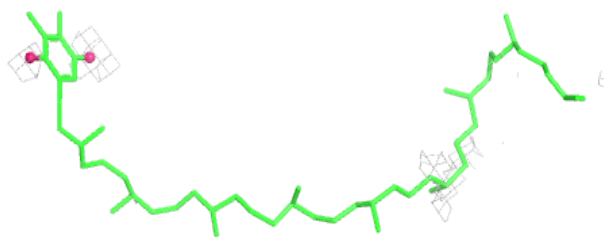
**Electron density around PL9 A 610:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

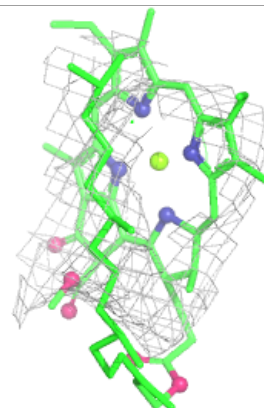
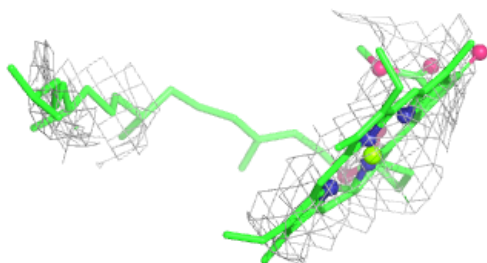
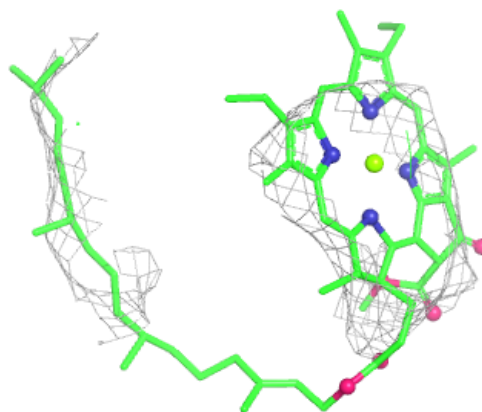


Electron density around PL9 a 609:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

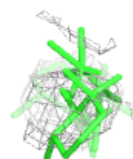
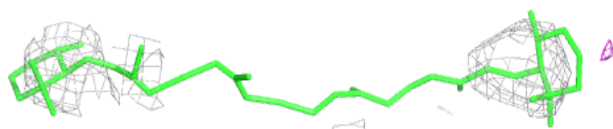
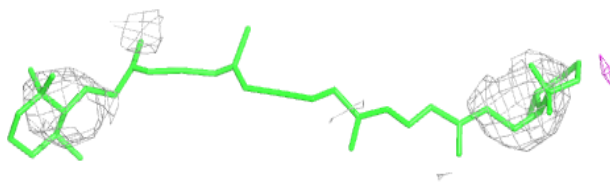
**Electron density around CLA C 507:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

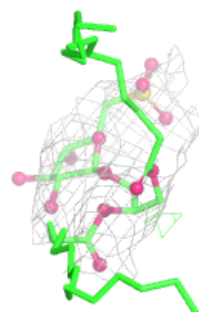
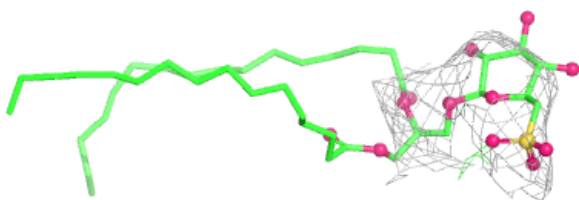
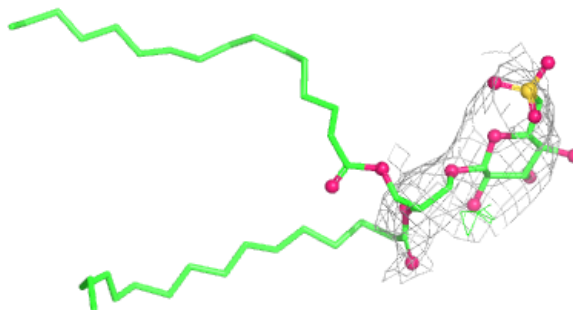


Electron density around BCR B 618:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

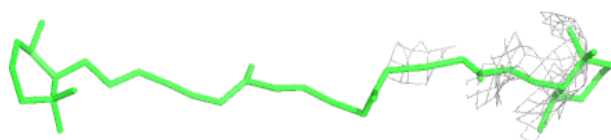
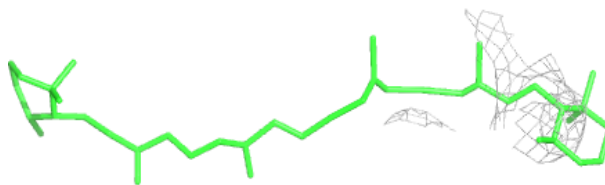
**Electron density around SQD a 612:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

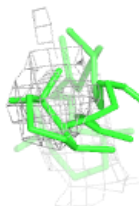
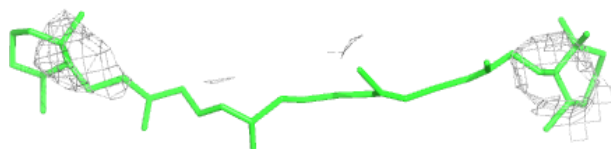
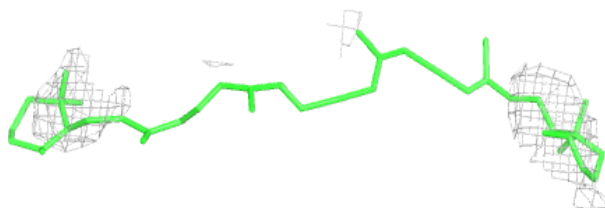


Electron density around BCR k 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

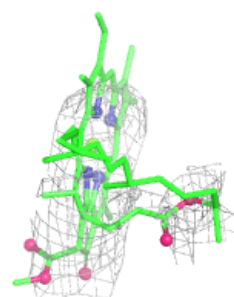
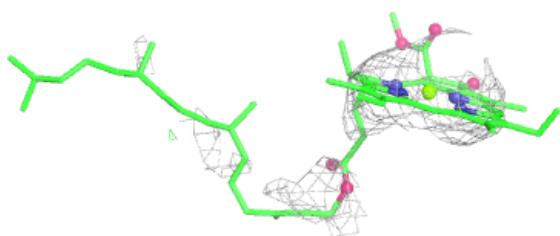
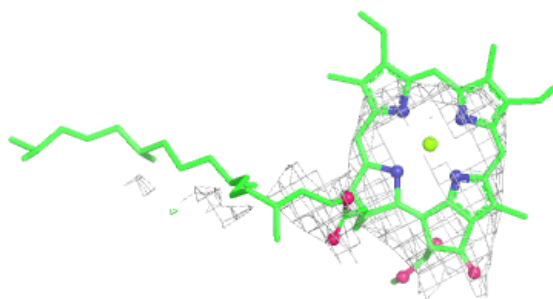
**Electron density around BCR t 101:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

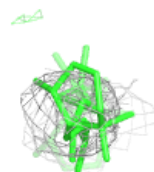
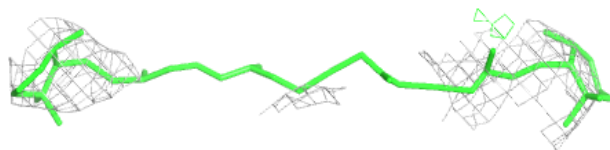
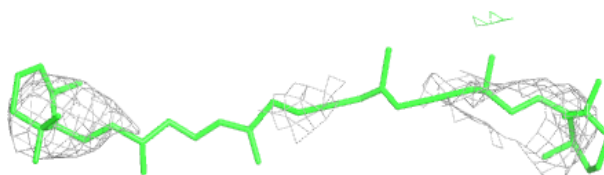


Electron density around CLA a 605:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

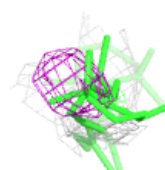
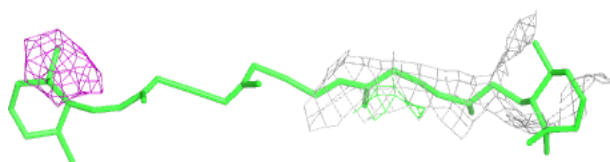
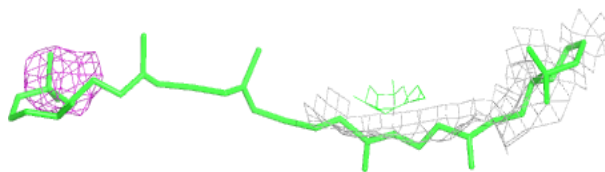
**Electron density around BCR b 621:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

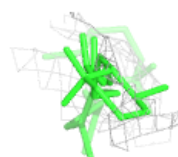
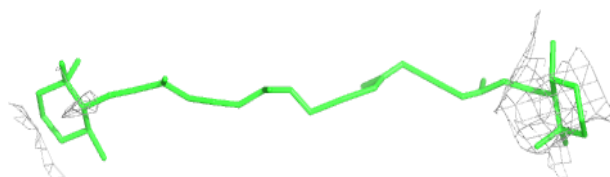
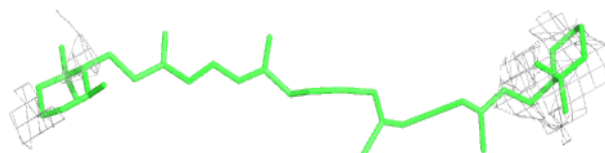


Electron density around BCR H 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

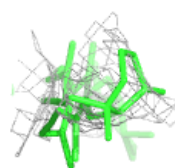
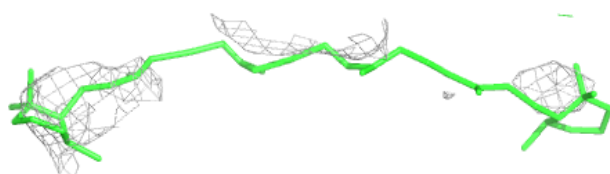
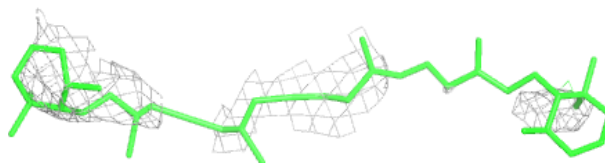
**Electron density around BCR c 516:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

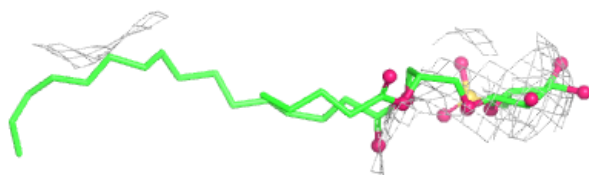
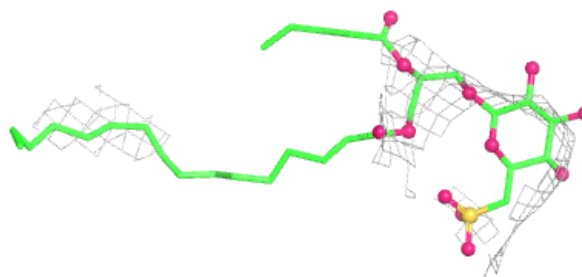


Electron density around BCR f 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

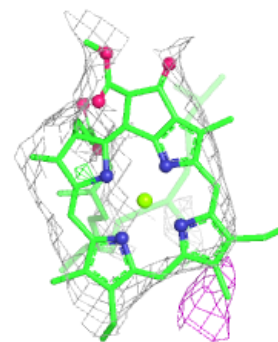
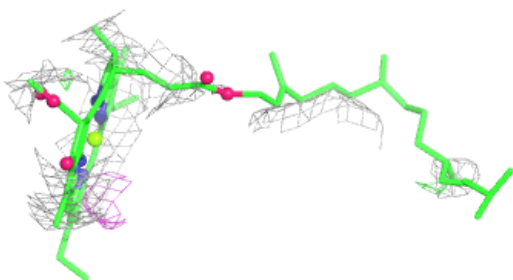
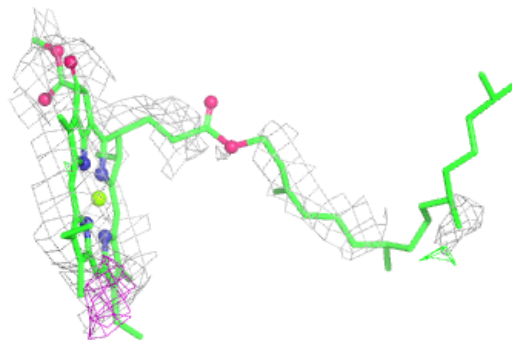
**Electron density around SQD X 101:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

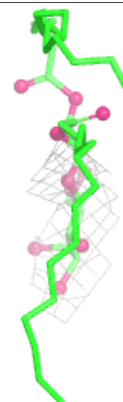
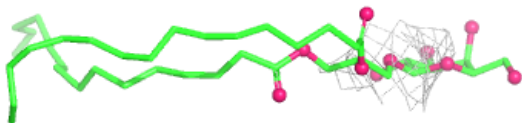
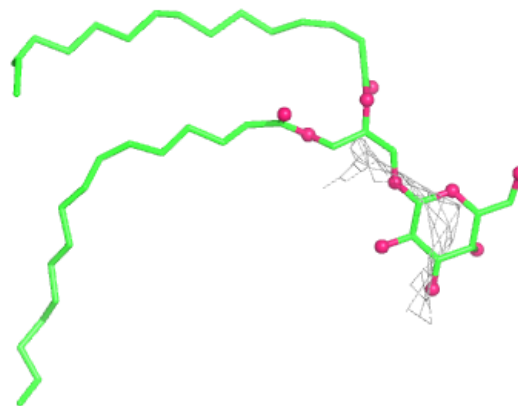


Electron density around CLA D 404:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

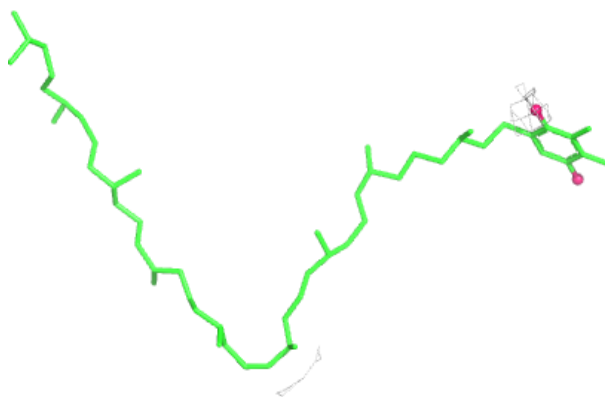
**Electron density around LMG c 520:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

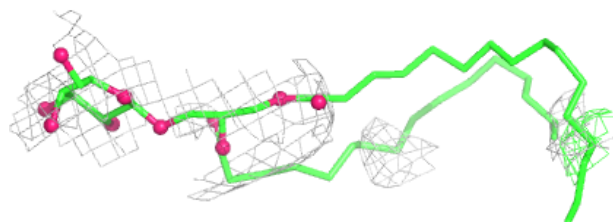
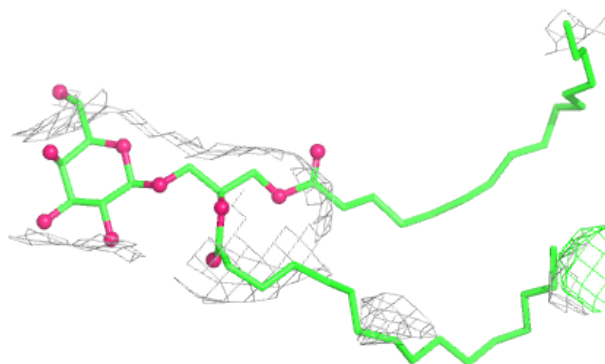


Electron density around PL9 d 404:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

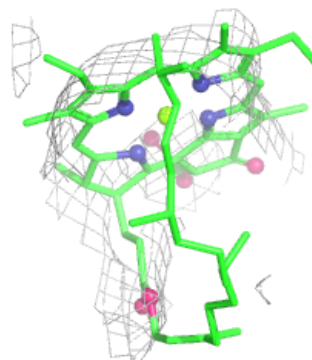
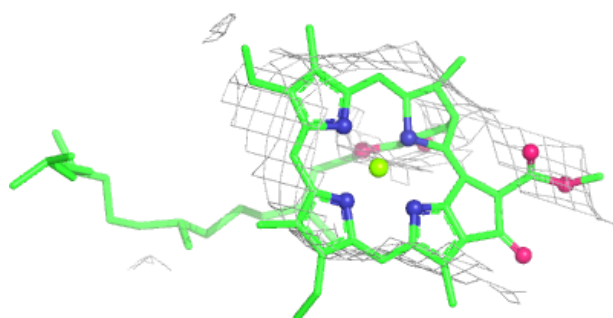
**Electron density around LMG j 101:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

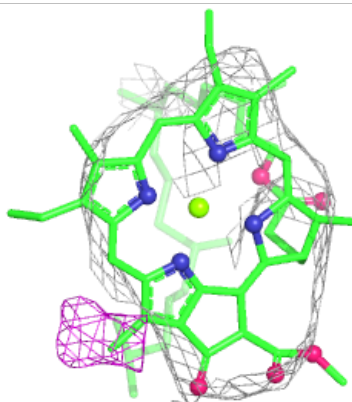
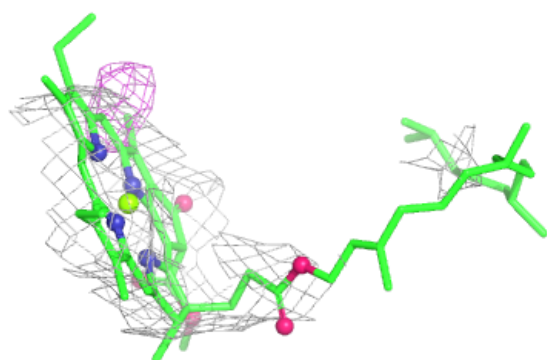
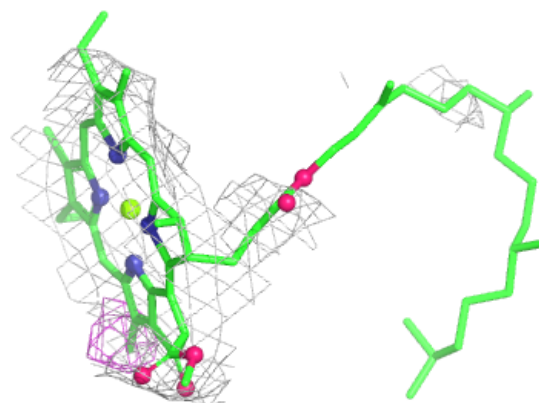


Electron density around CLA c 514:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

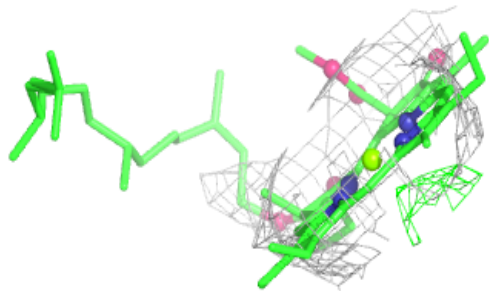
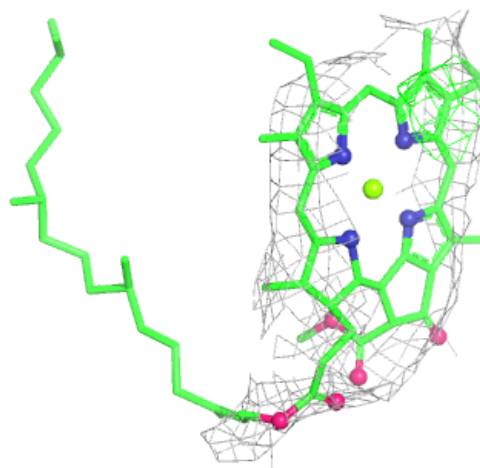
**Electron density around CLA B 607 (B):**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



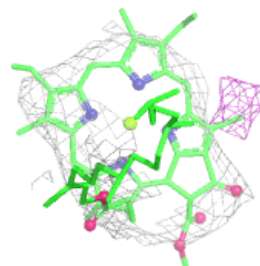
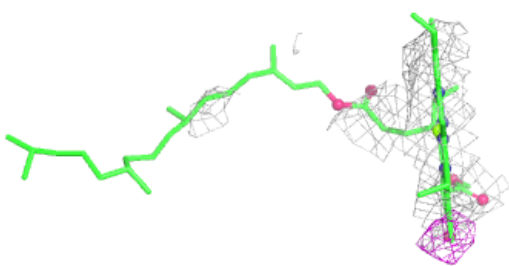
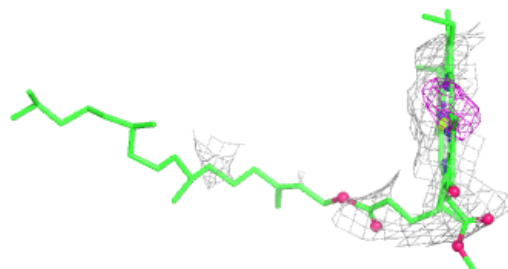
Electron density around CLA B 617:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

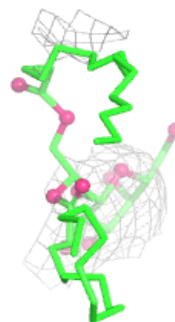
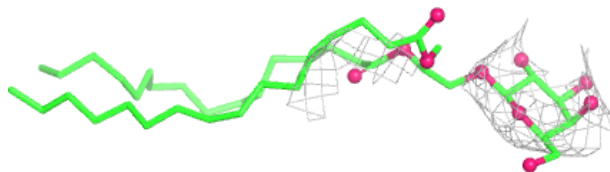


Electron density around CLA B 607 (A):

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

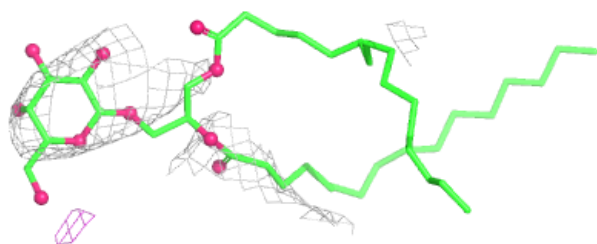
**Electron density around LMG A 612:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

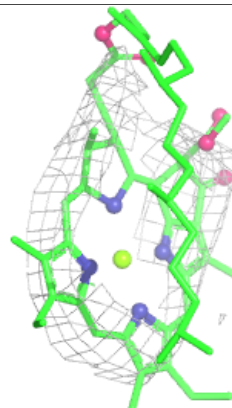
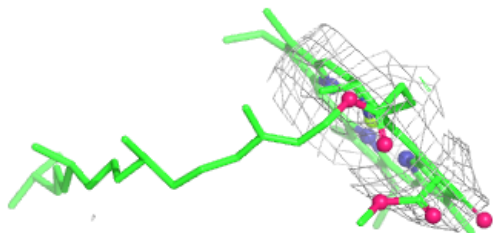
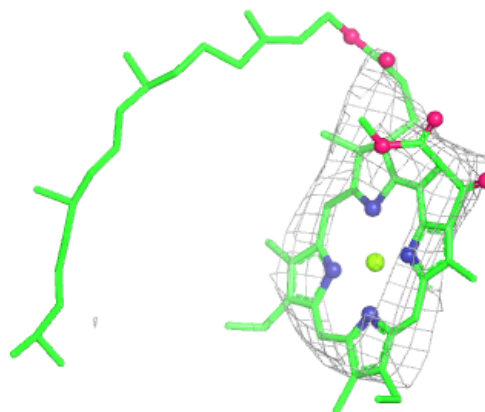


Electron density around LMG B 621:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

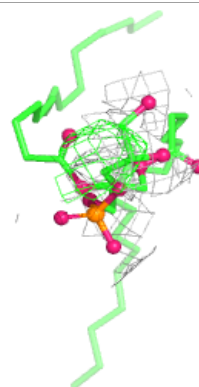
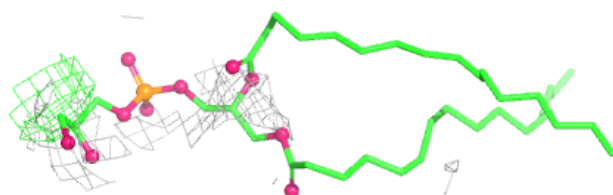
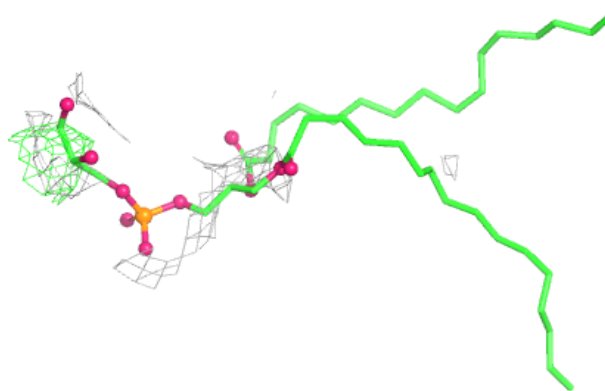
**Electron density around CLA c 508:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



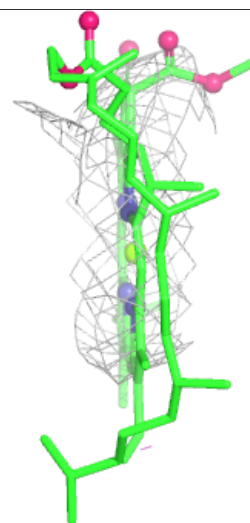
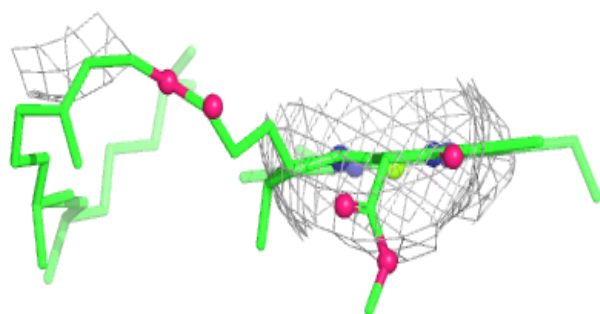
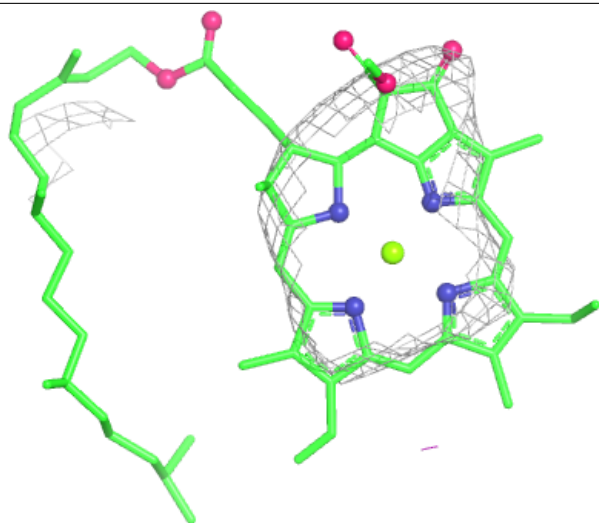
Electron density around LHG D 407:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



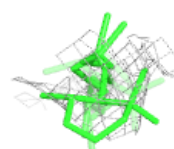
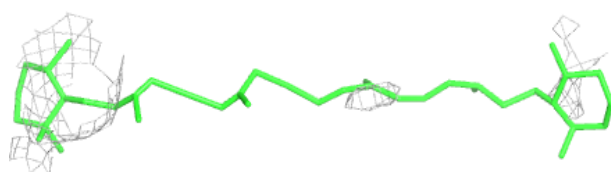
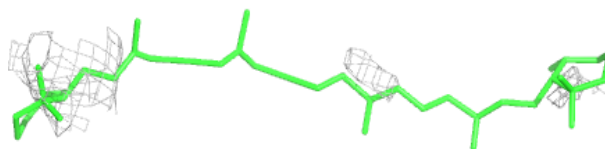
Electron density around CLA c 513:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

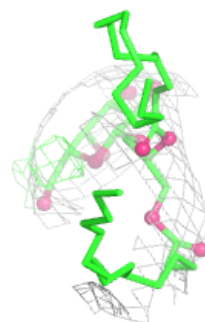
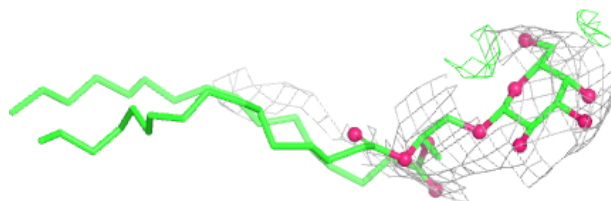
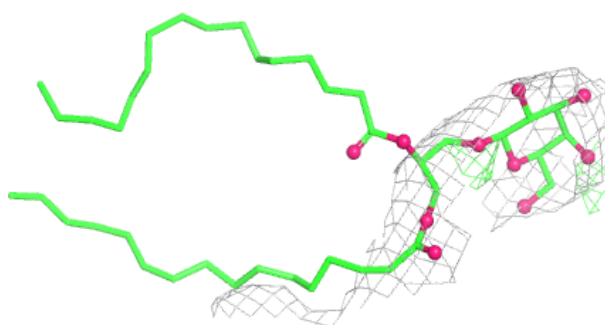


Electron density around BCR c 515:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

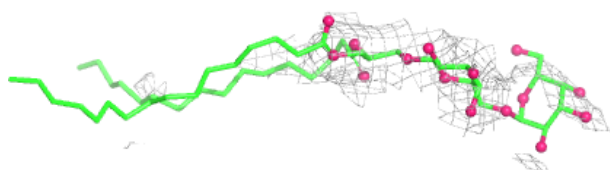
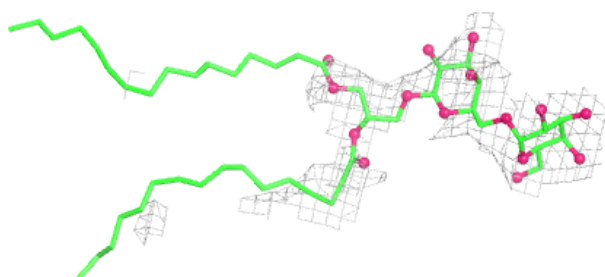
**Electron density around LMG a 611:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

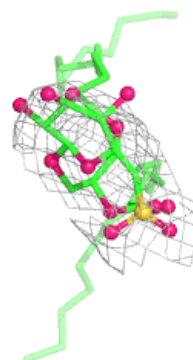
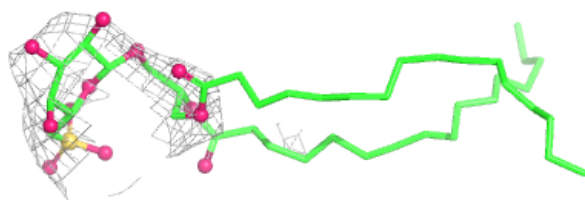
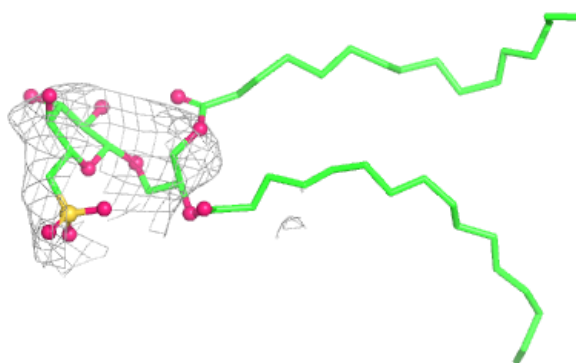


Electron density around DGD C 518:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

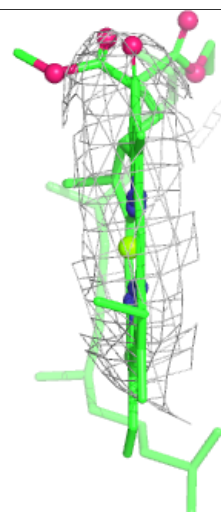
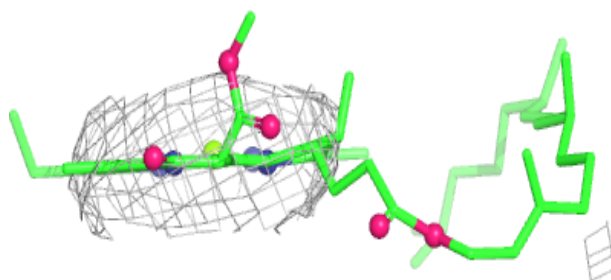
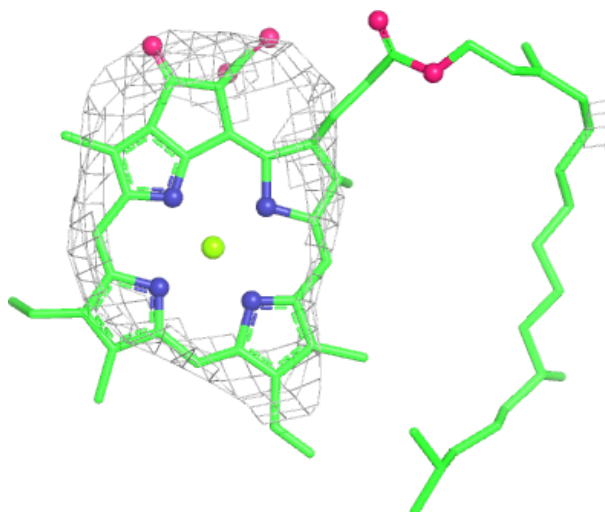
**Electron density around SQD B 623:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



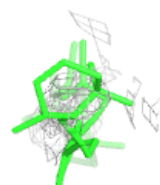
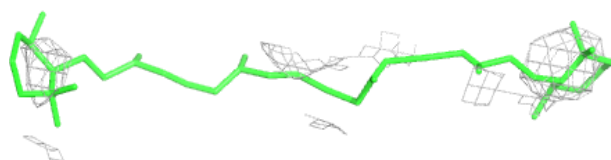
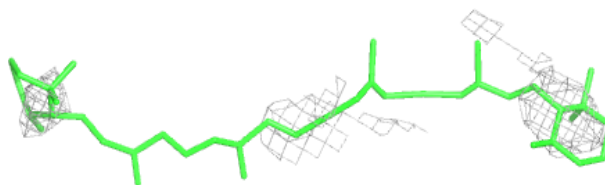
Electron density around CLA C 512:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

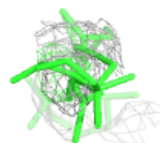
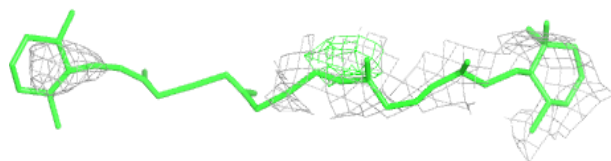
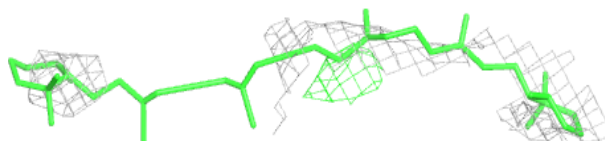


Electron density around BCR K 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

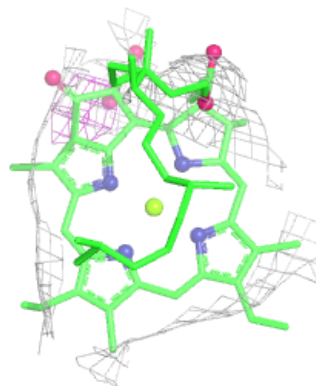
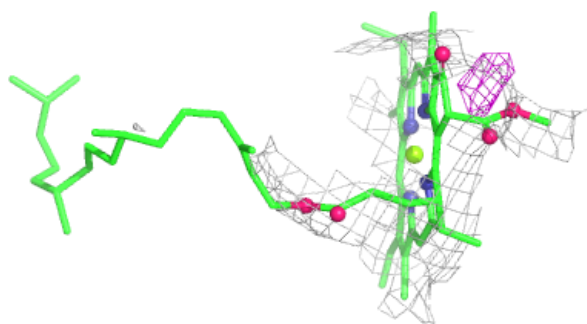
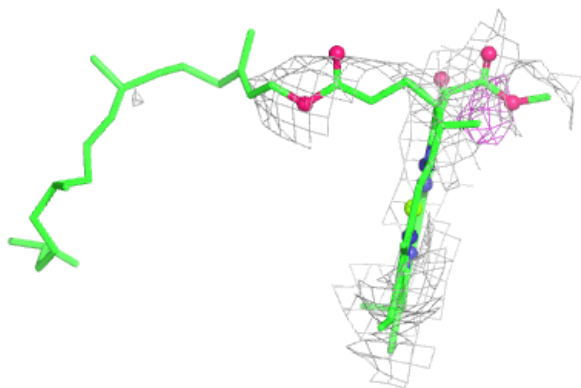
**Electron density around BCR h 101:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

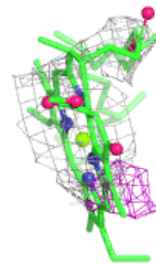
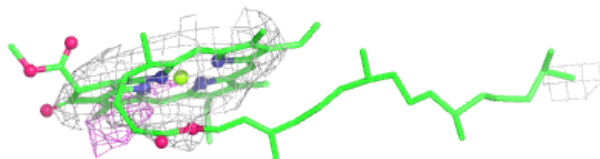
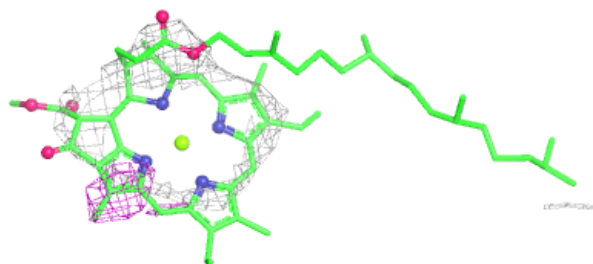


Electron density around CLA C 506:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

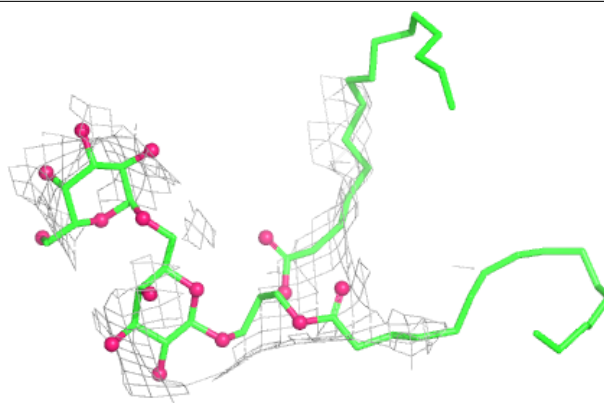
**Electron density around CLA c 502:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

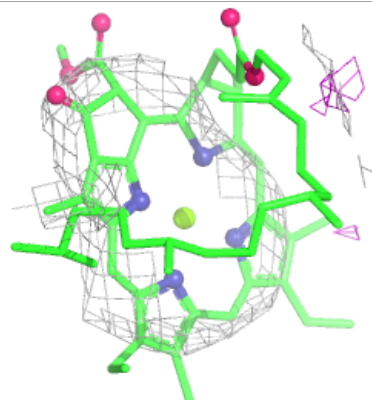
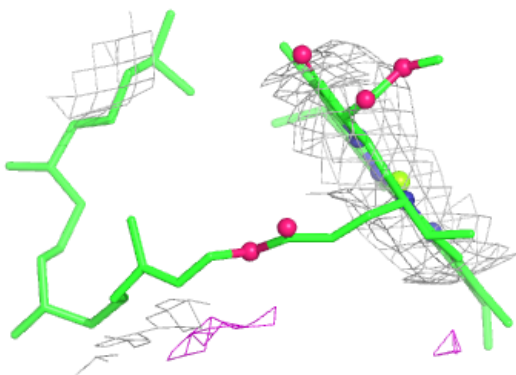
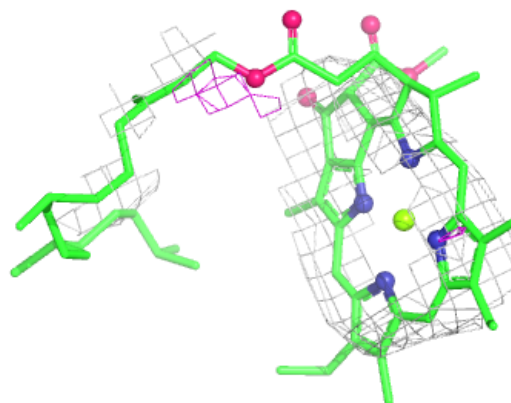


Electron density around DGD C 517:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

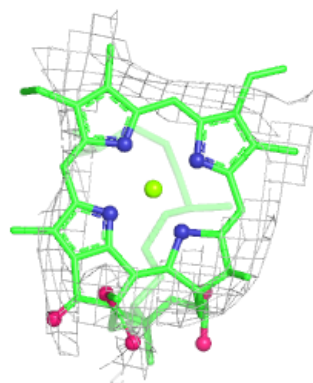
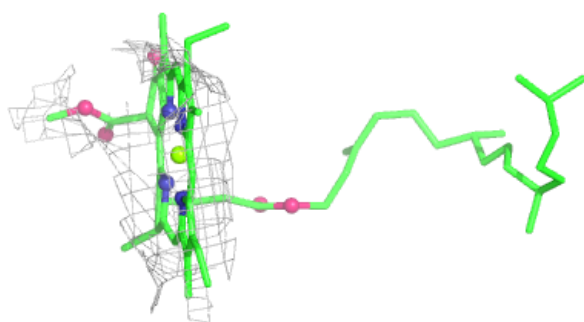
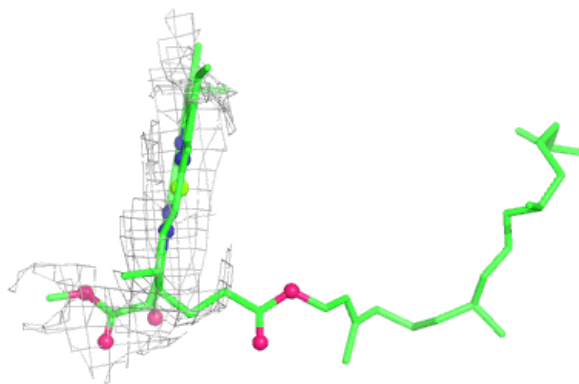
**Electron density around CLA c 504:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



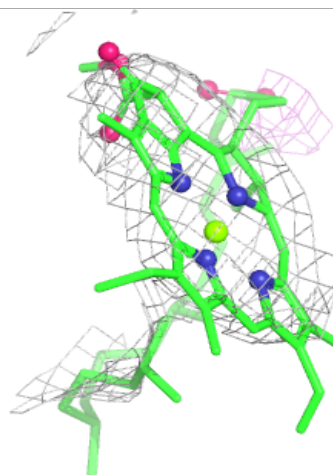
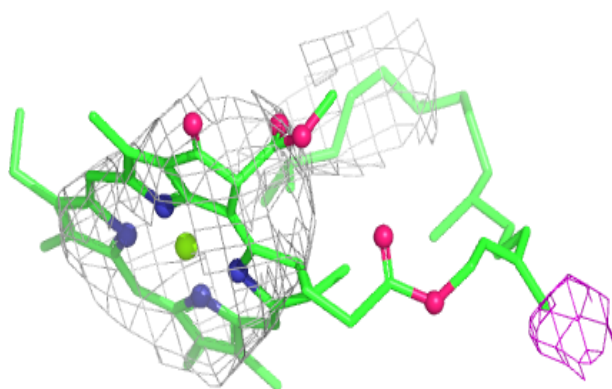
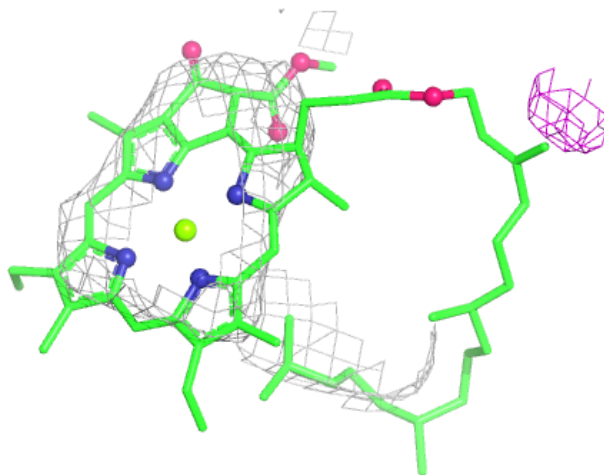
Electron density around CLA c 507:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



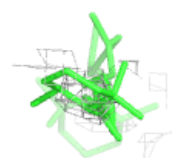
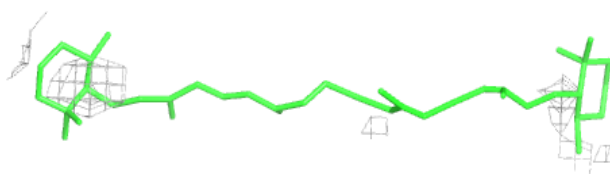
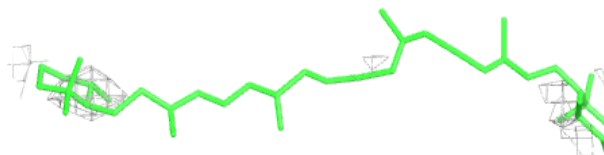
Electron density around CLA B 616:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

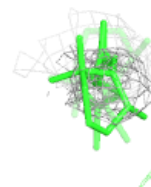
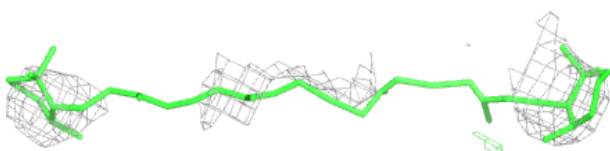
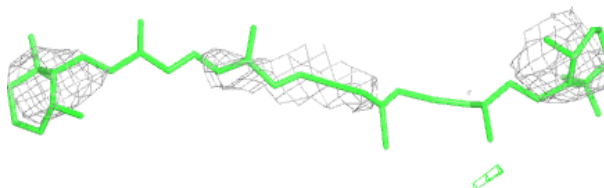


Electron density around BCR C 515:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

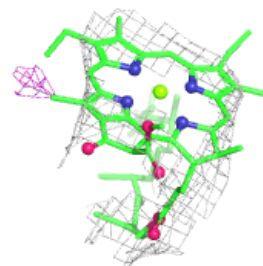
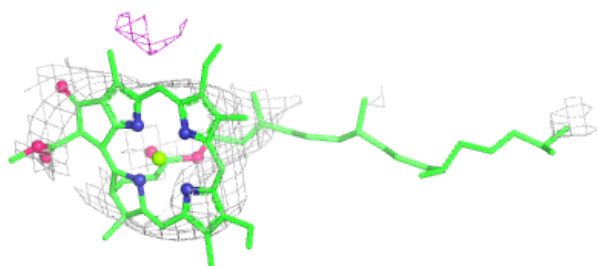
**Electron density around BCR B 619:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



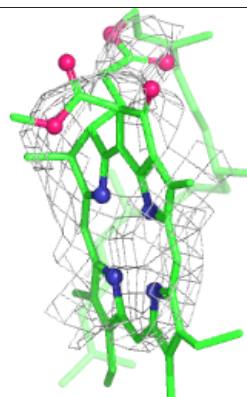
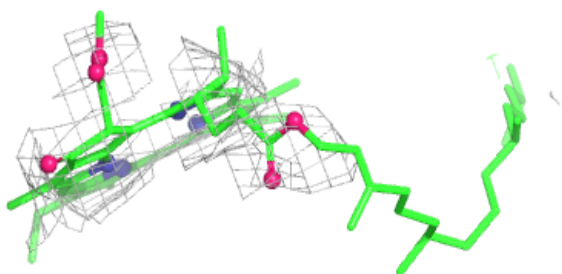
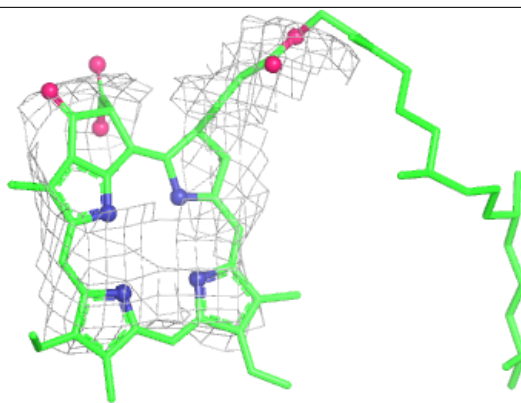
Electron density around CLA C 504:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

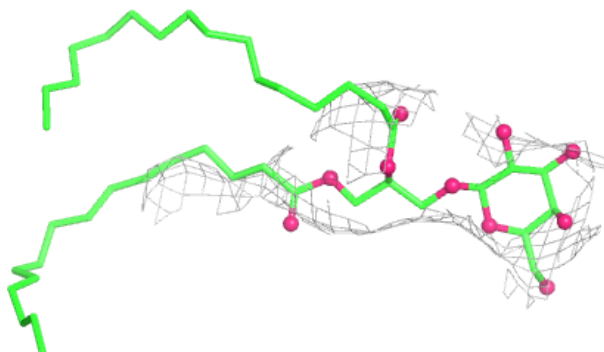


Electron density around PHO d 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

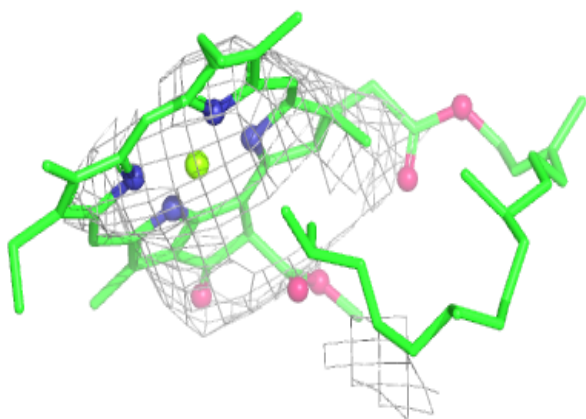
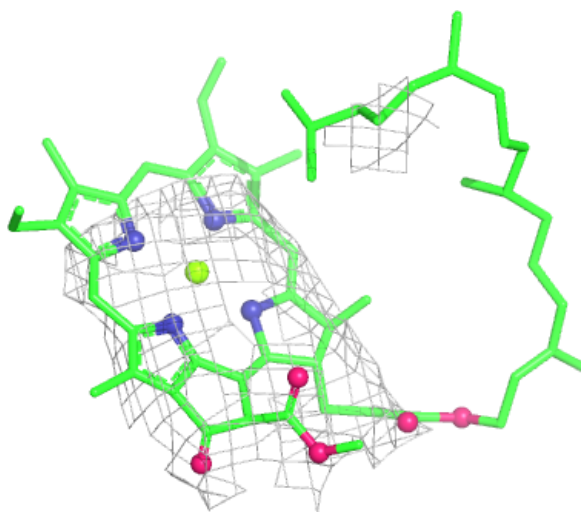
**Electron density around LMG J 101:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



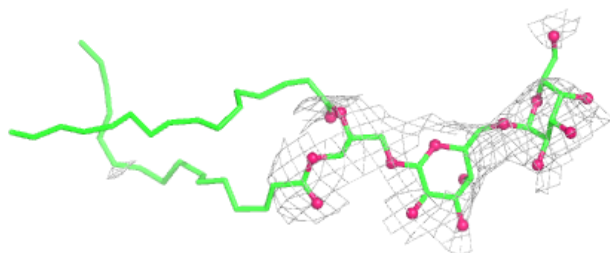
Electron density around CLA b 618:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

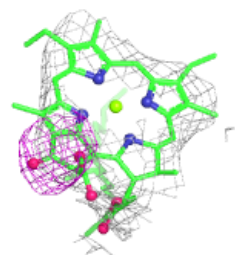
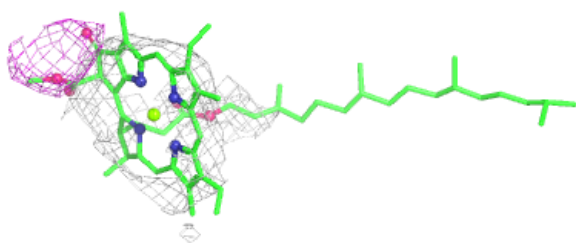
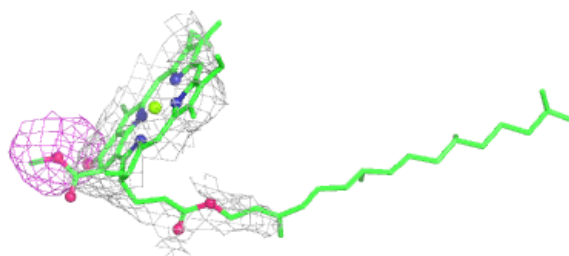


Electron density around DGD c 517:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

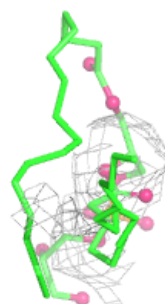
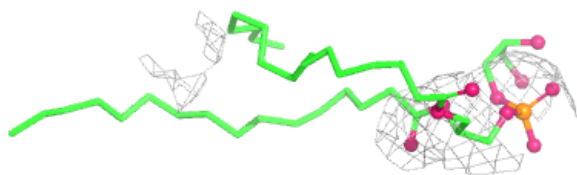
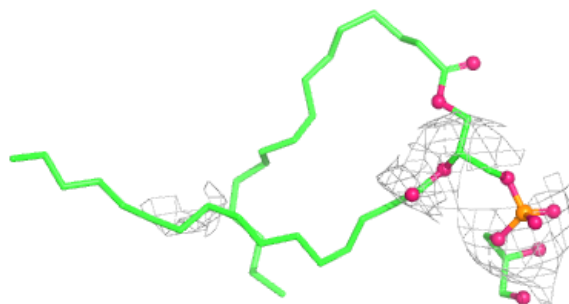
**Electron density around CLA B 608:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



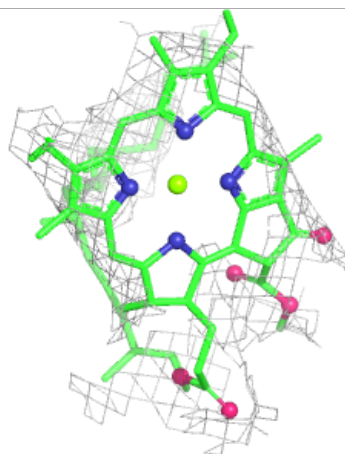
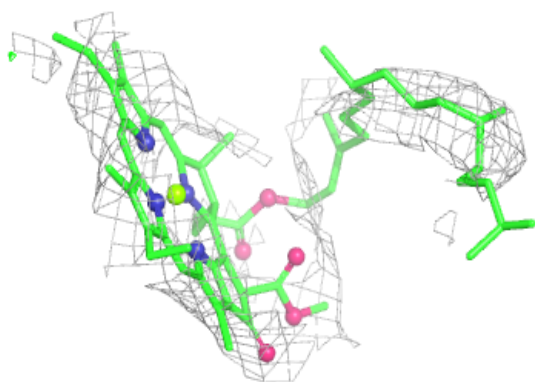
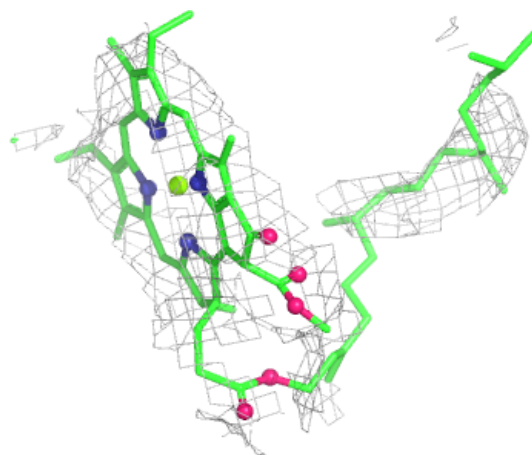
Electron density around LHG D 408:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



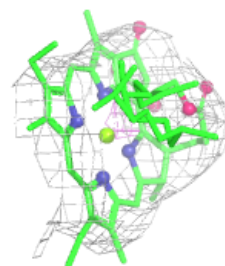
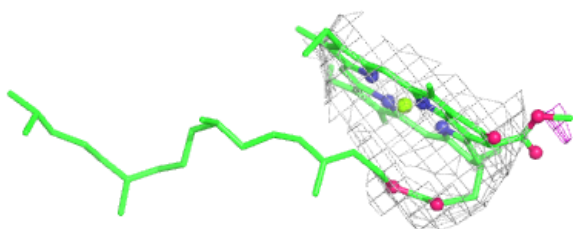
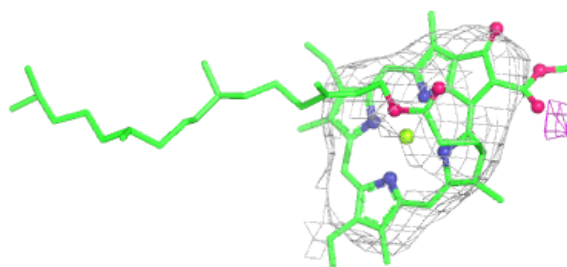
Electron density around CLA b 616:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

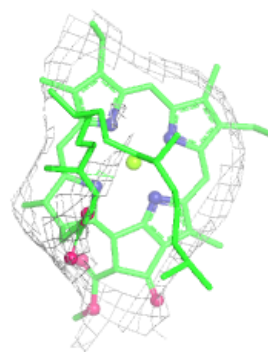
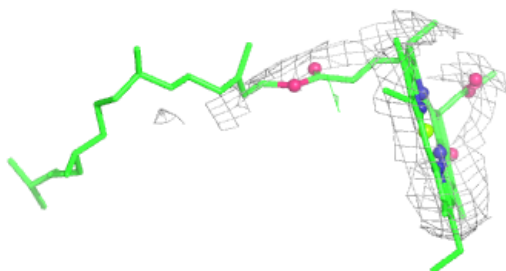
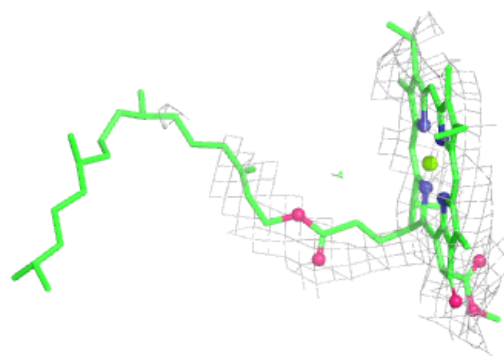


Electron density around CLA B 615:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

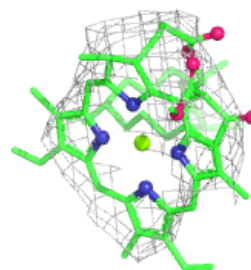
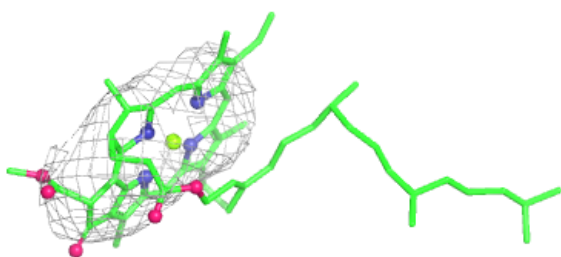
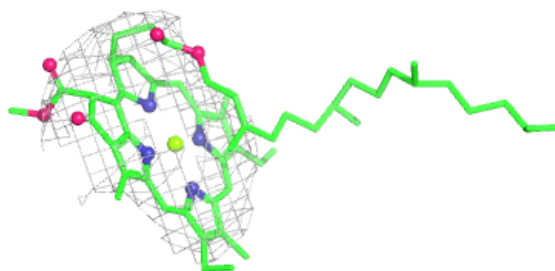
**Electron density around CLA d 403:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



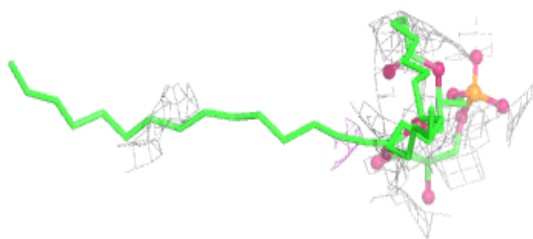
Electron density around CLA C 505:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



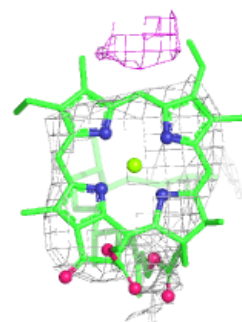
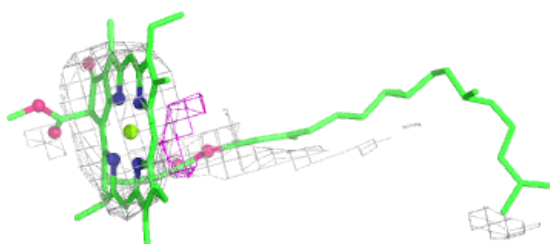
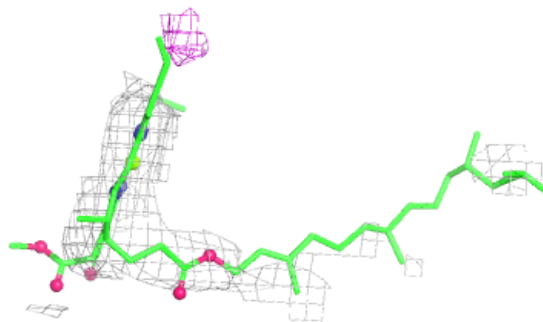
Electron density around LHG 1 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

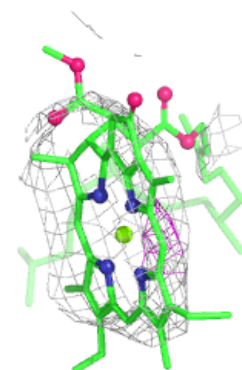
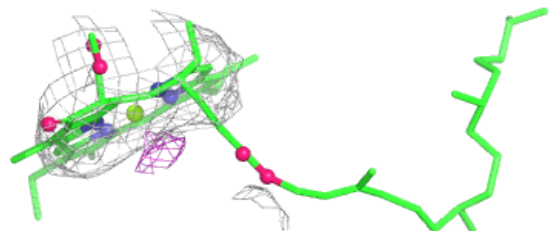
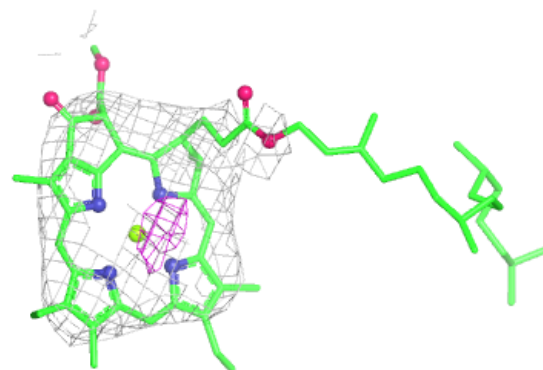


Electron density around CLA B 606:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

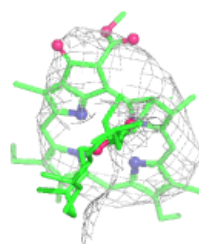
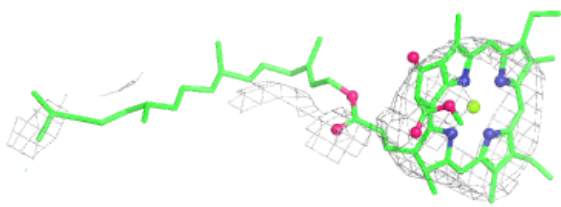
**Electron density around CLA a 607:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

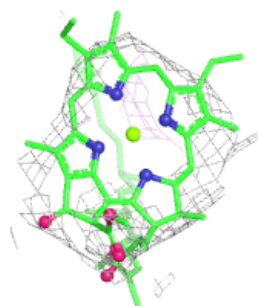
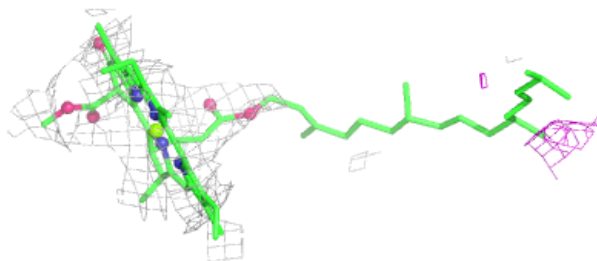
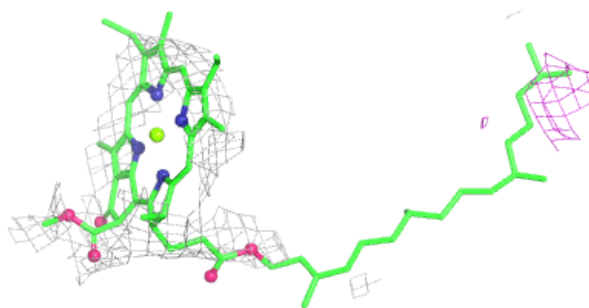


Electron density around CLA c 503:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

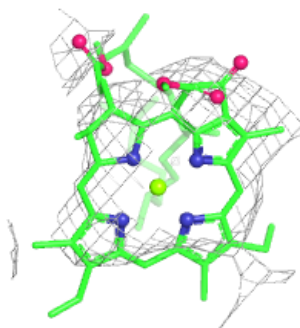
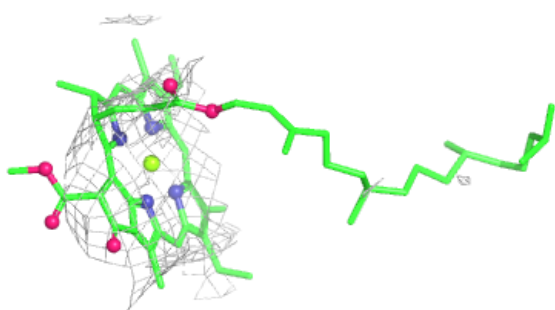
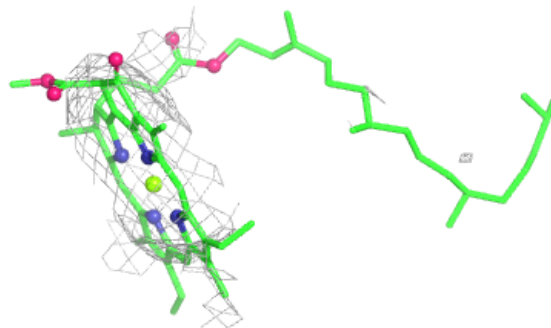
**Electron density around CLA B 610:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

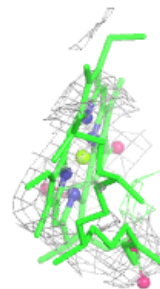
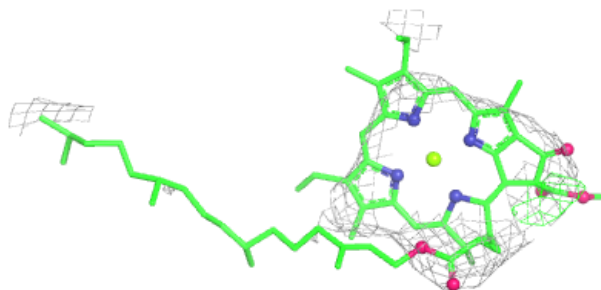


Electron density around CLA C 508:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

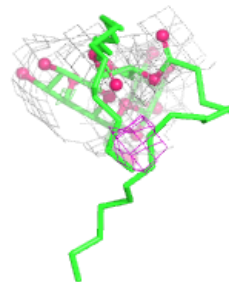
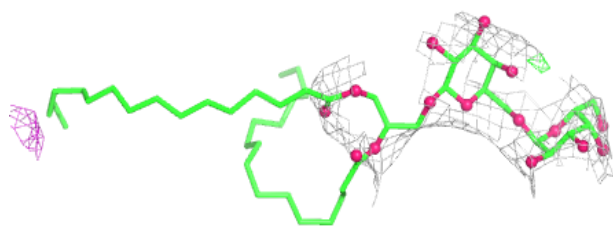
**Electron density around CLA C 501:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

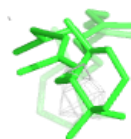
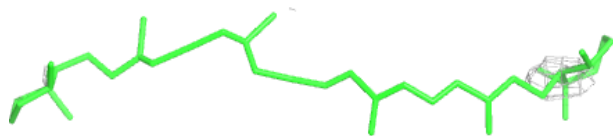
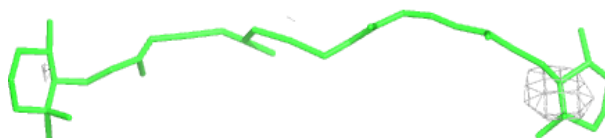


Electron density around DGD h 102:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

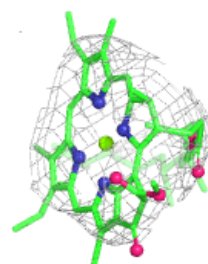
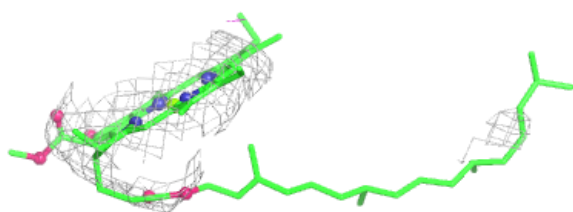
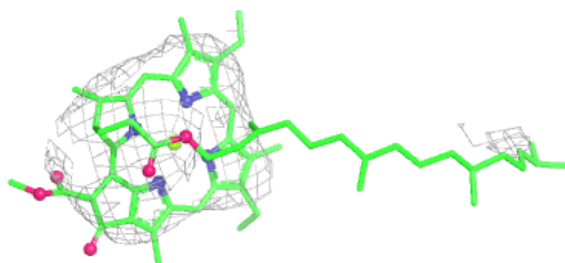
**Electron density around BCR C 521:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

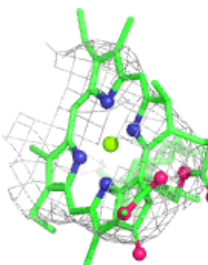
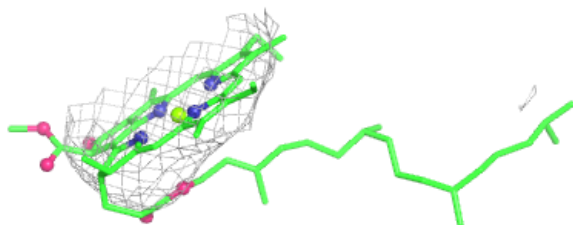
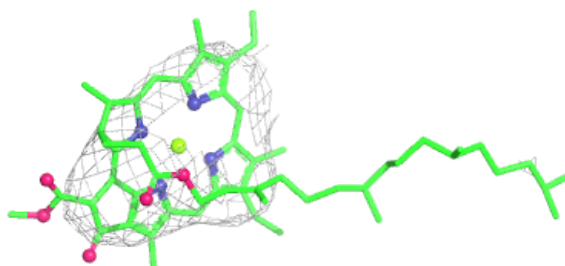


Electron density around CLA b 611:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

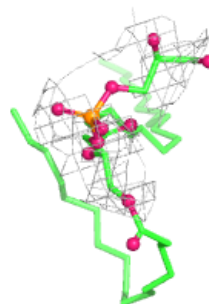
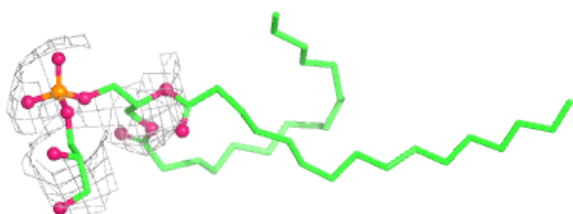
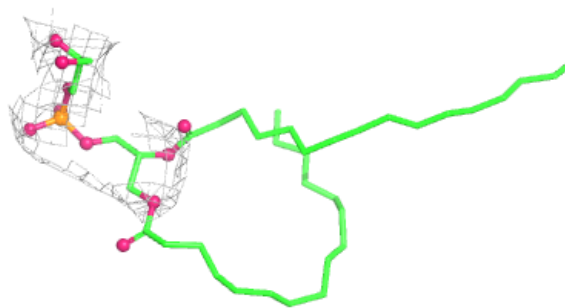
**Electron density around CLA b 617:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

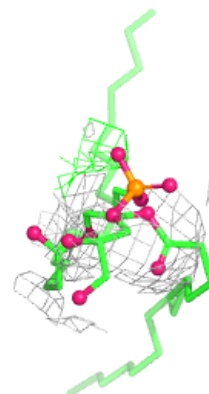
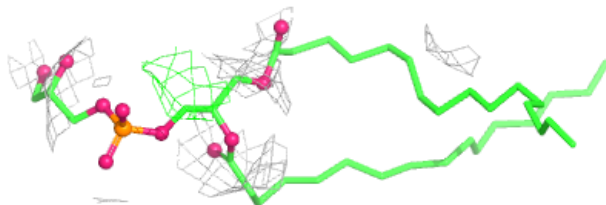
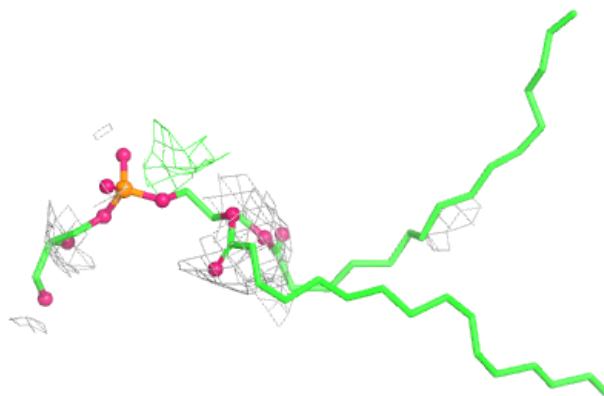


Electron density around LHG b 624:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

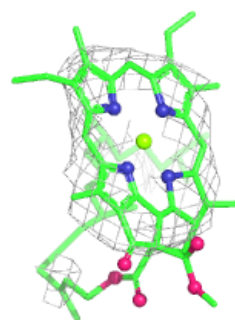
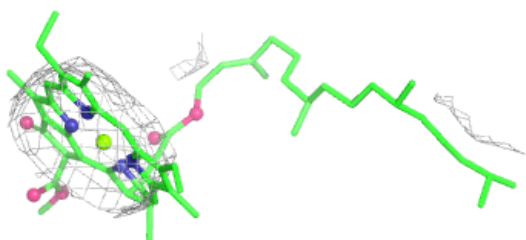
**Electron density around LHG d 406:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

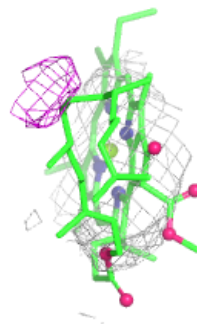
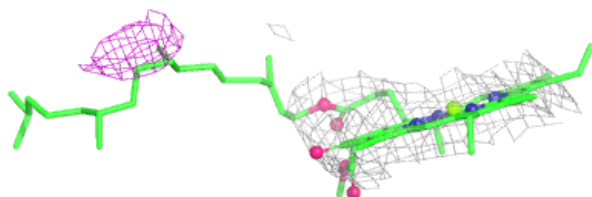
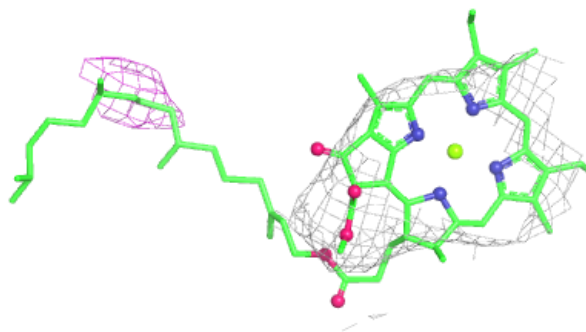


Electron density around CLA C 511:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

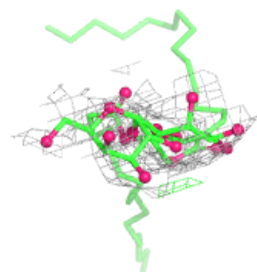
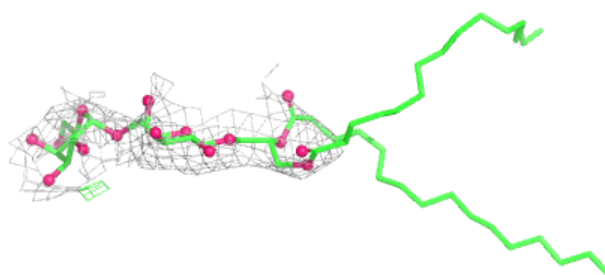
**Electron density around CLA B 603:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

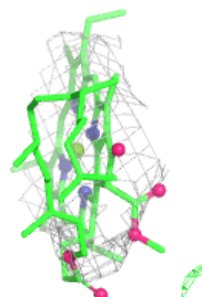
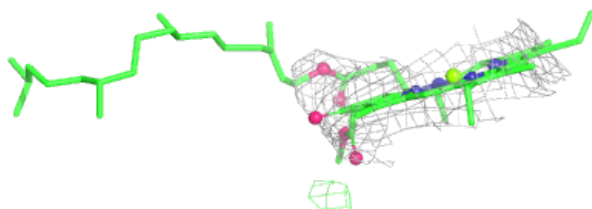
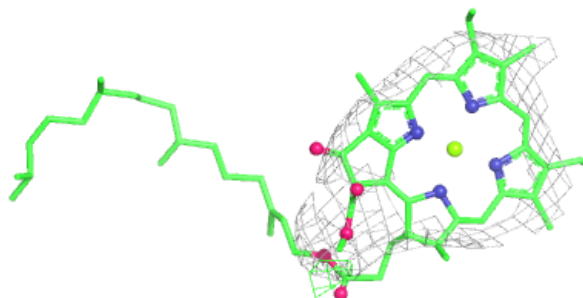


Electron density around DGD C 516:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

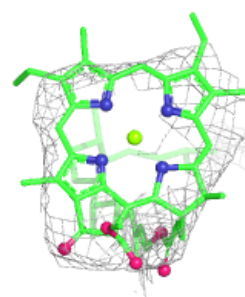
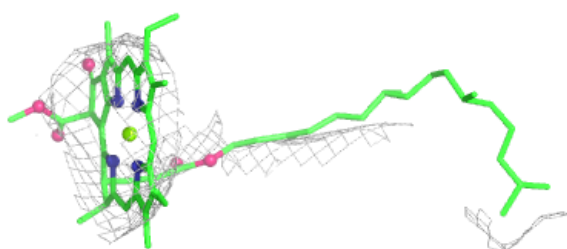
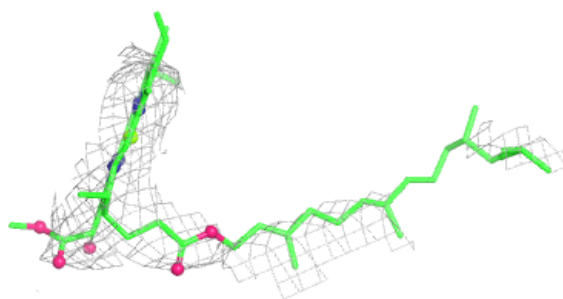
**Electron density around CLA b 605:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

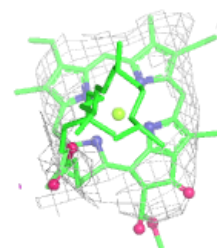
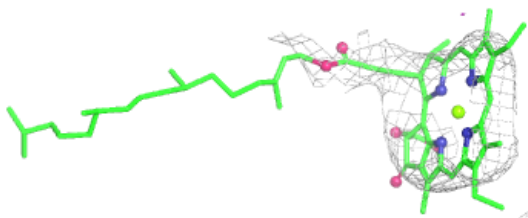
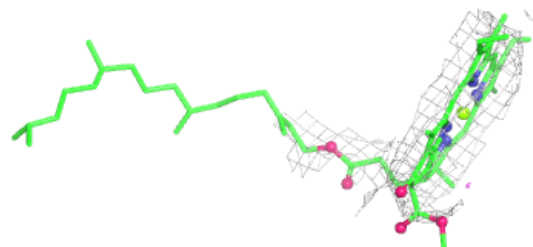


Electron density around CLA b 608:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

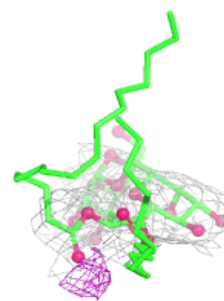
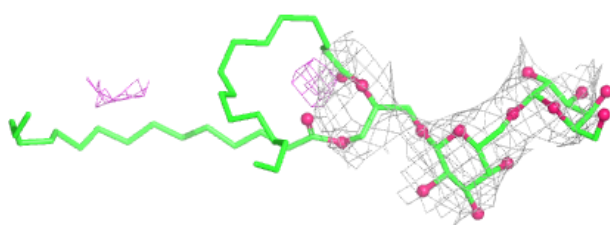
**Electron density around CLA B 605:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

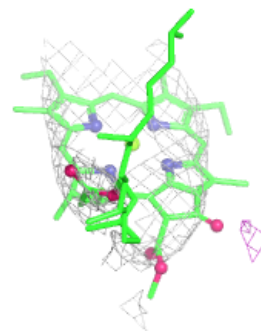
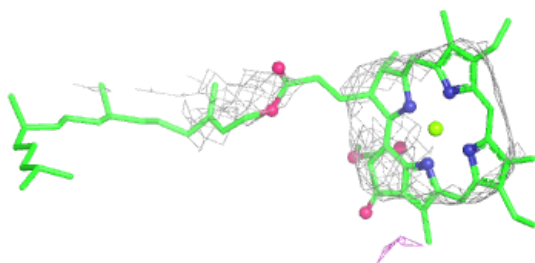
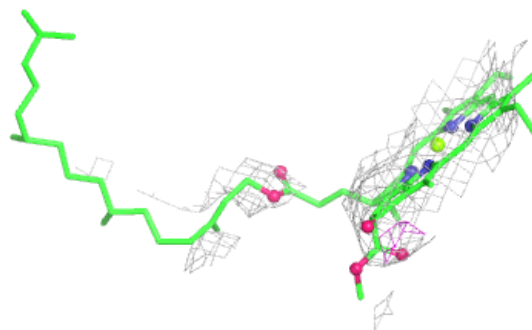


Electron density around DGD H 102:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

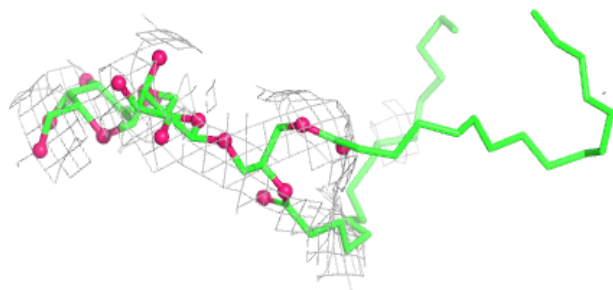
**Electron density around CLA D 403:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

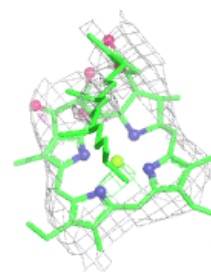
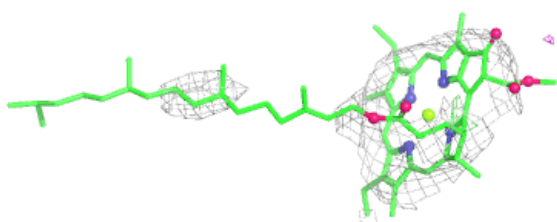
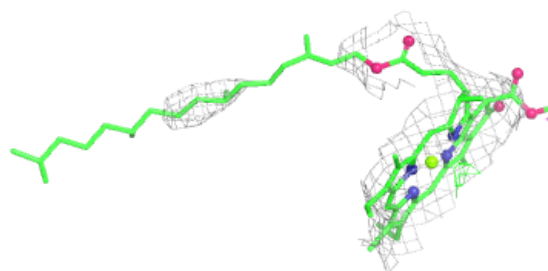


Electron density around DGD c 518:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

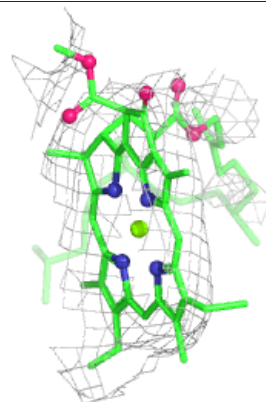
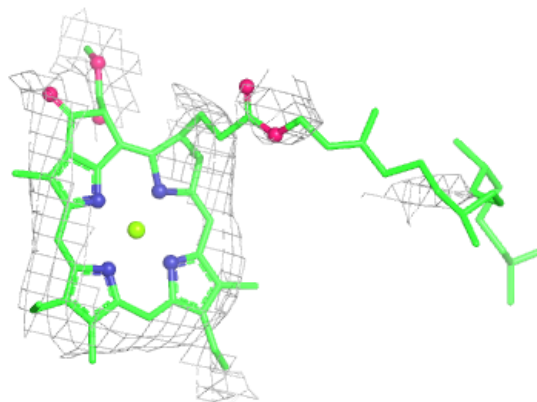
**Electron density around CLA b 610:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

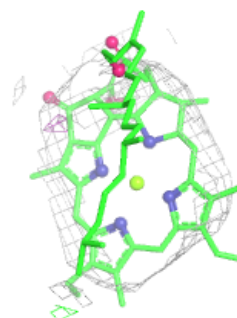
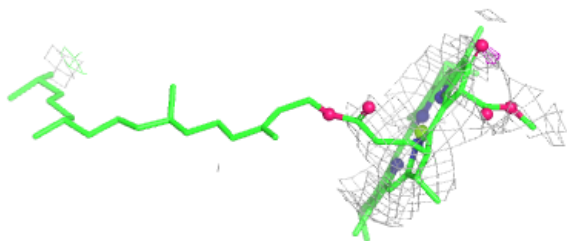
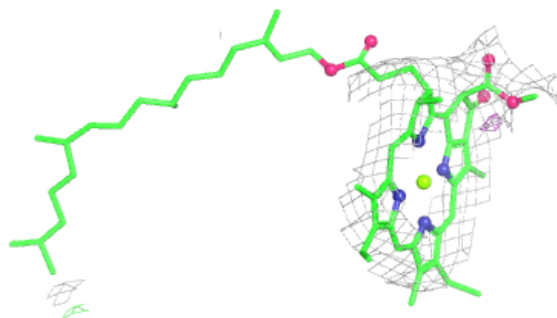


Electron density around CLA A 608:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

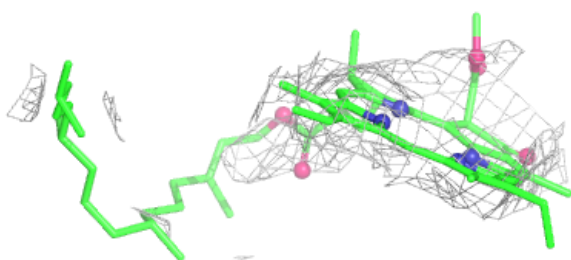
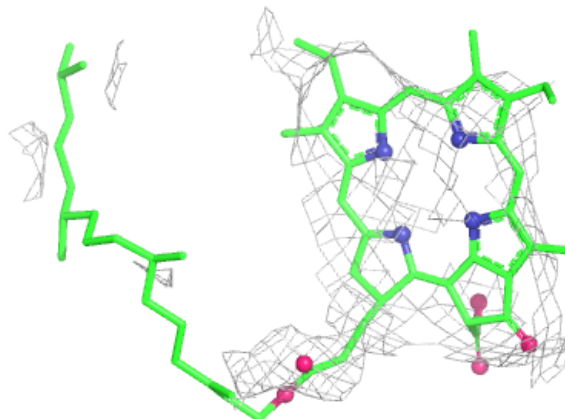
**Electron density around CLA b 612:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

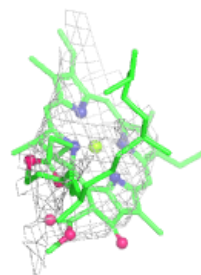
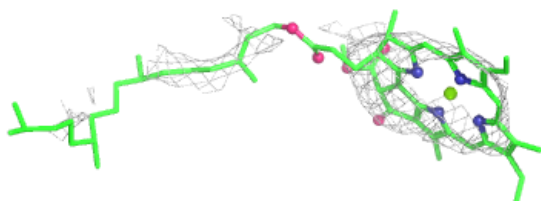
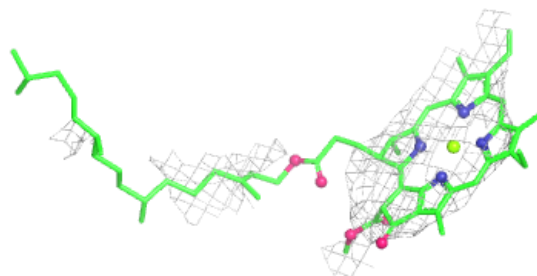


Electron density around PHO D 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

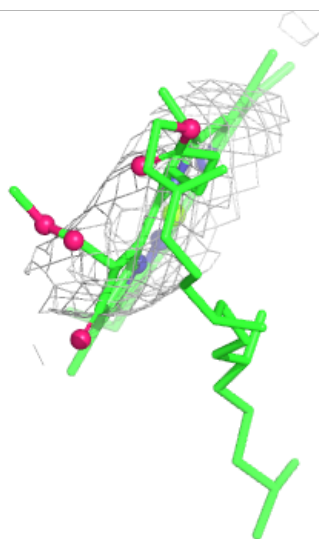
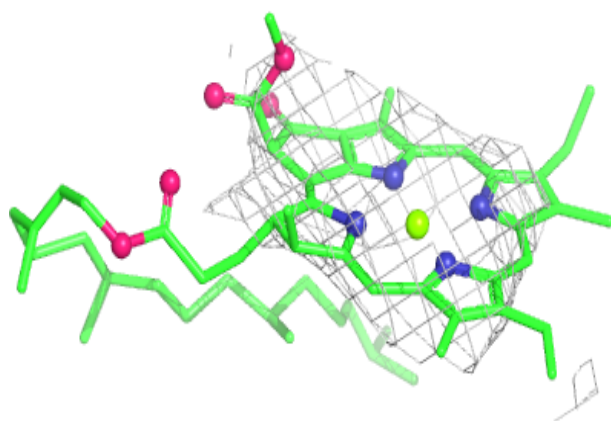
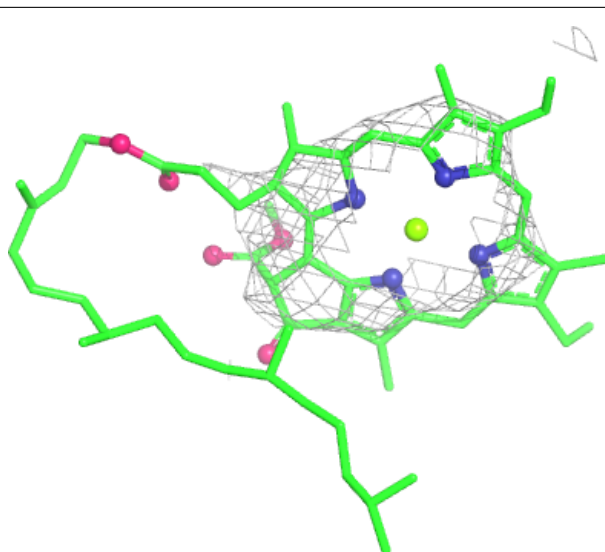
**Electron density around CLA a 604:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



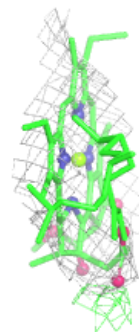
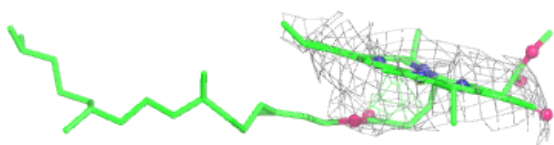
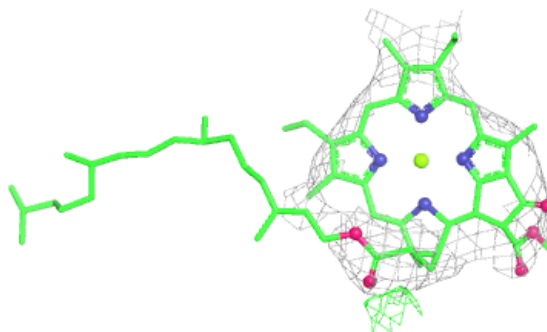
Electron density around CLA C 509:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

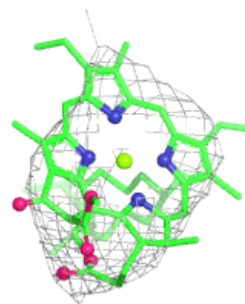
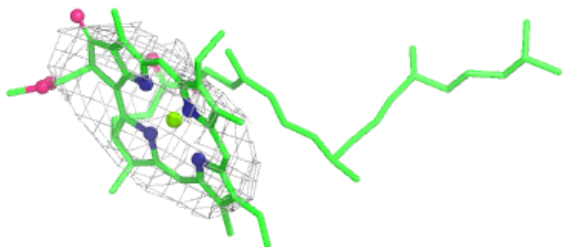
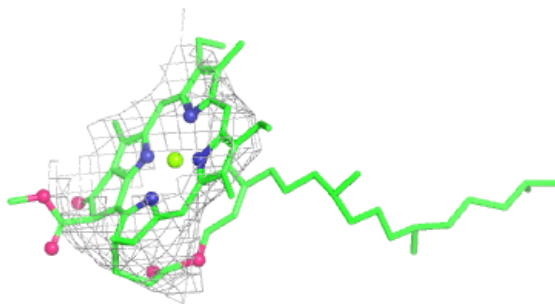


Electron density around CLA b 606:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

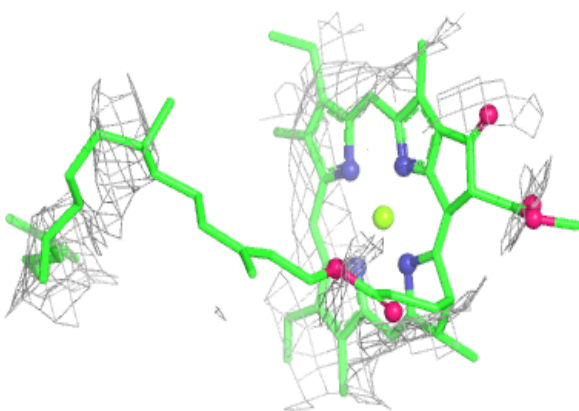
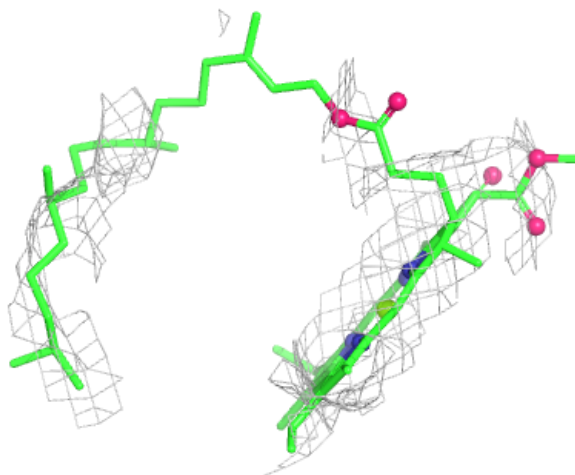
**Electron density around CLA c 506:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



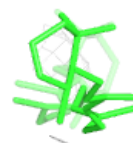
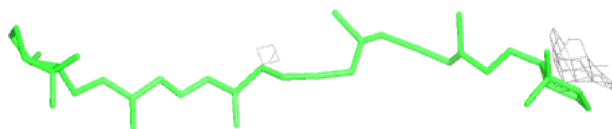
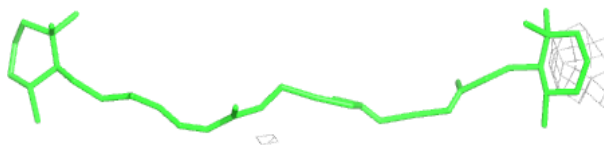
Electron density around CLA b 614:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



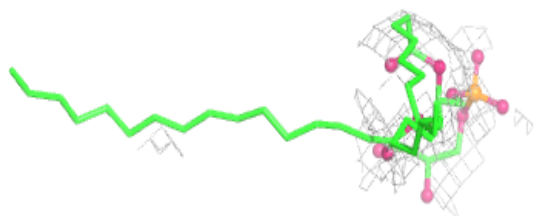
Electron density around BCR c 522:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



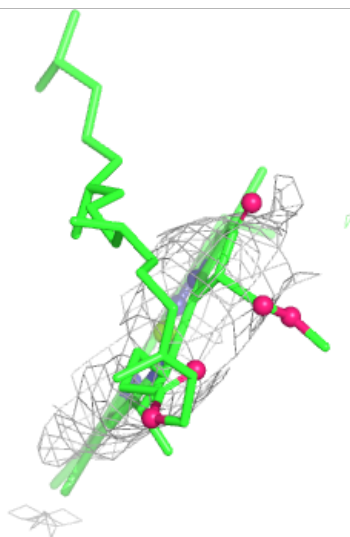
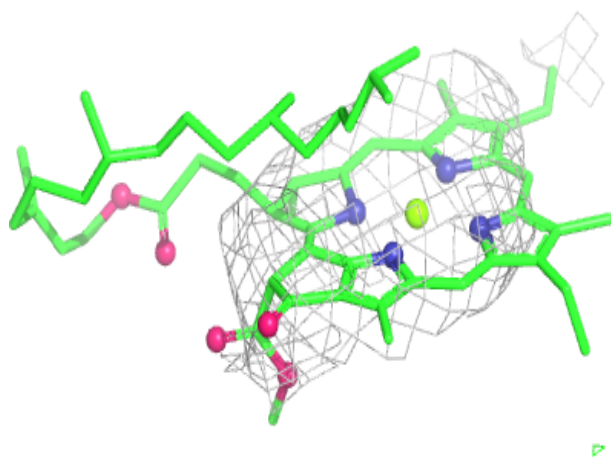
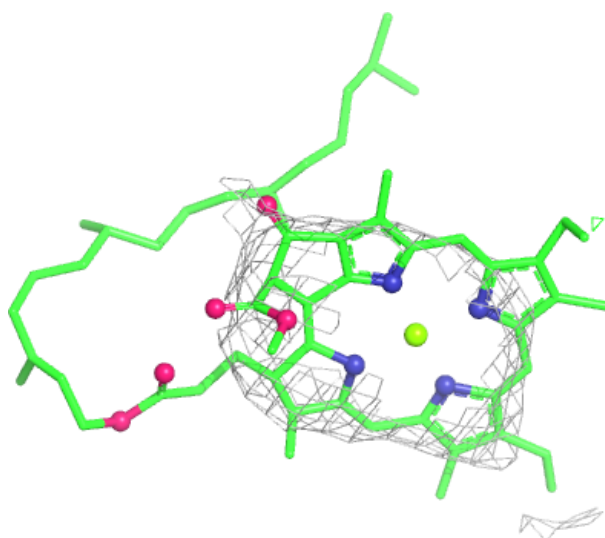
Electron density around LHG L 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



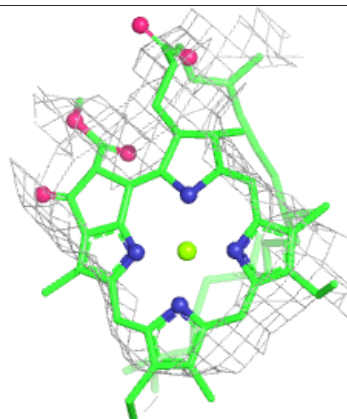
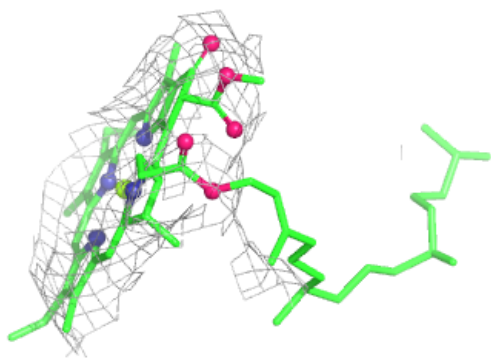
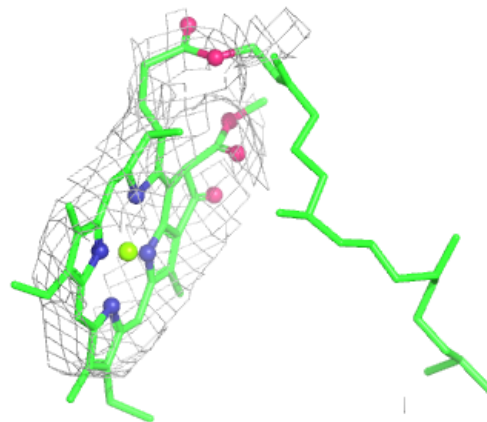
Electron density around CLA c 510:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

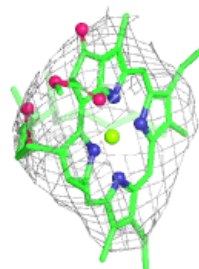
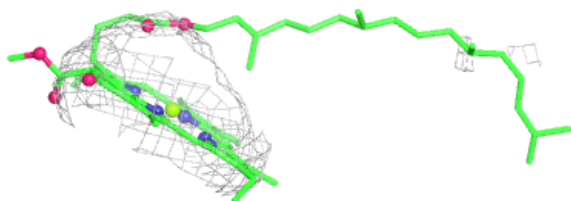
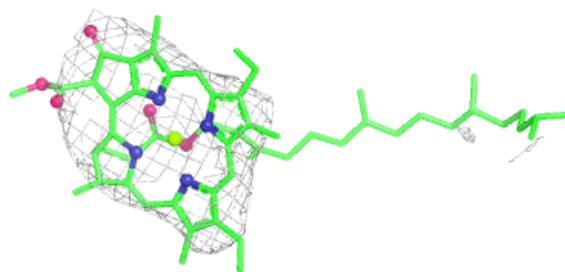


Electron density around CLA B 614:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

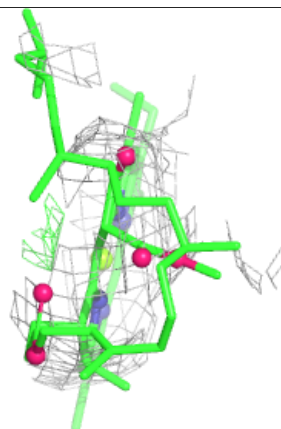
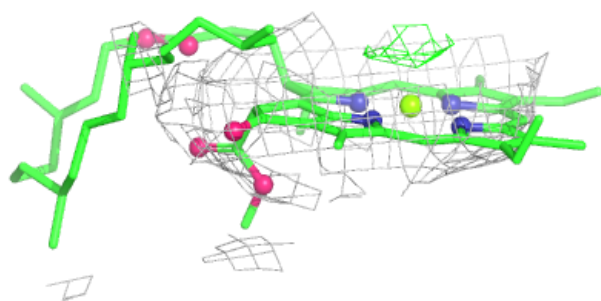
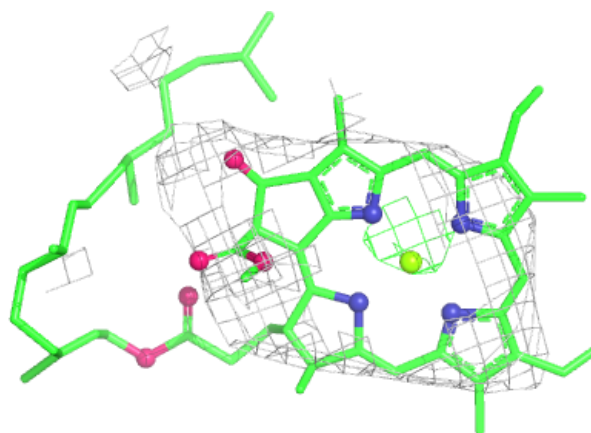
**Electron density around CLA B 609:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

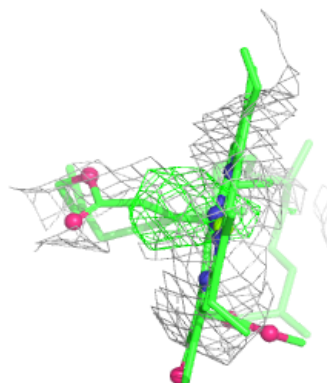
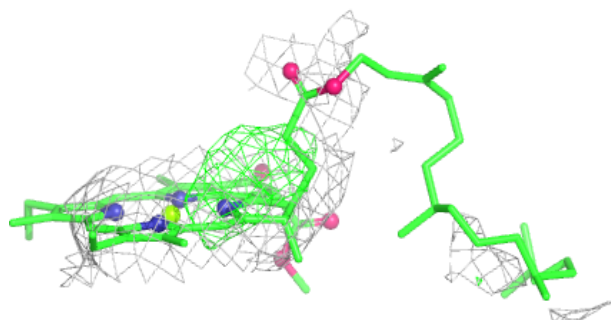
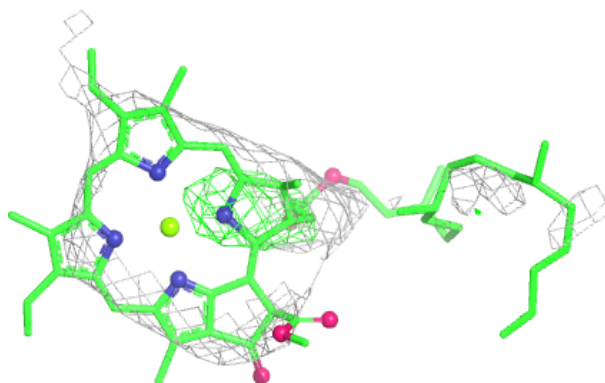


Electron density around CLA b 613:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

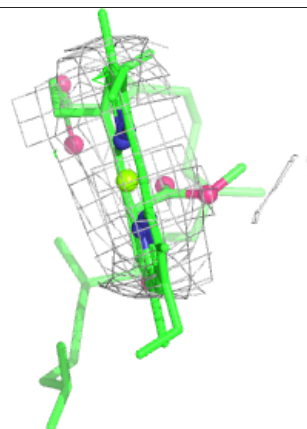
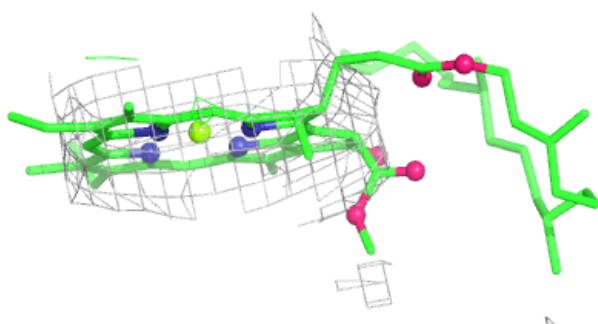
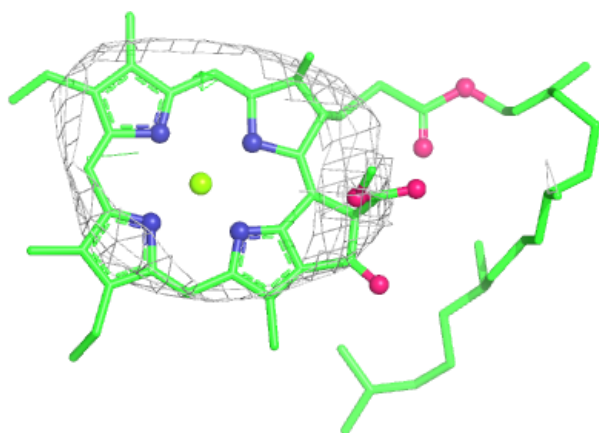
**Electron density around CLA b 615:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

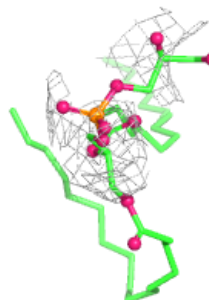
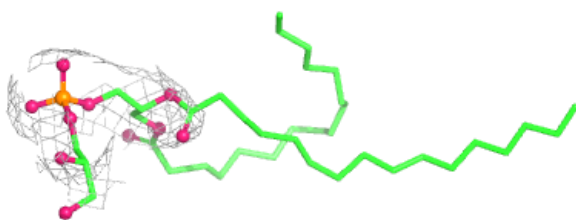
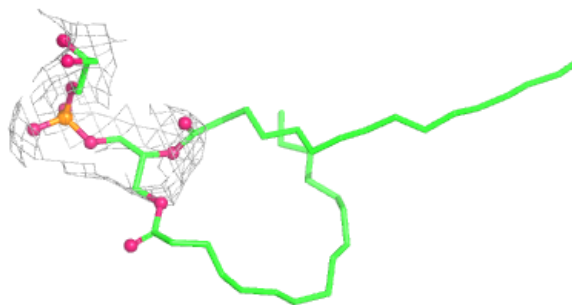


Electron density around CLA B 611:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

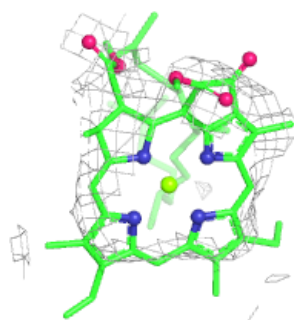
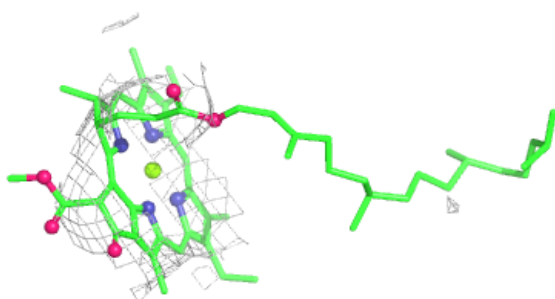
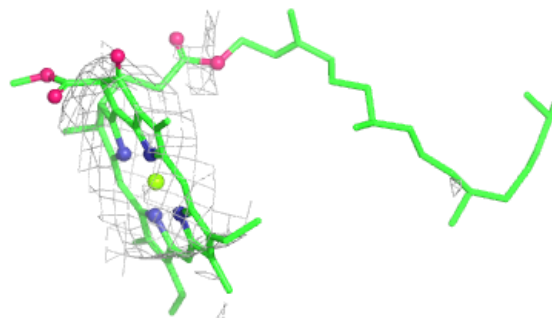
**Electron density around LHG B 622:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

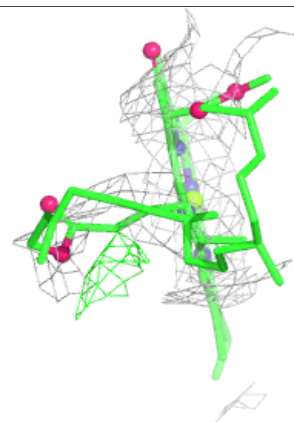
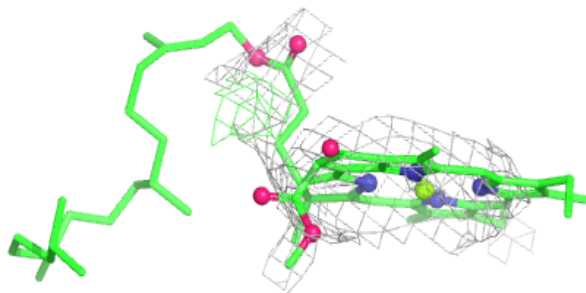
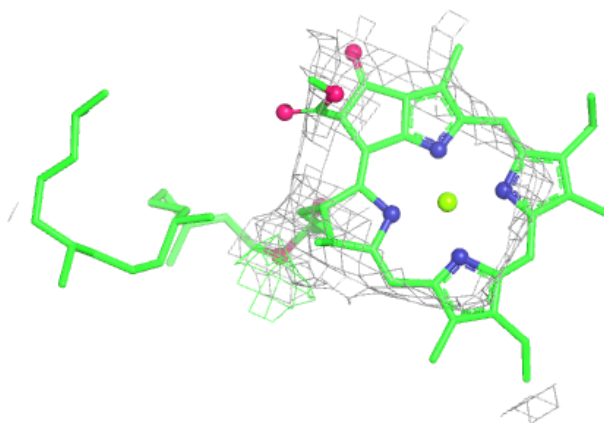


Electron density around CLA c 509:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

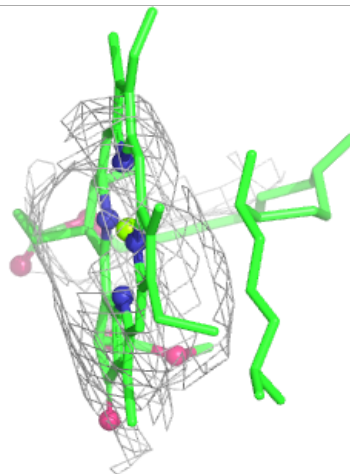
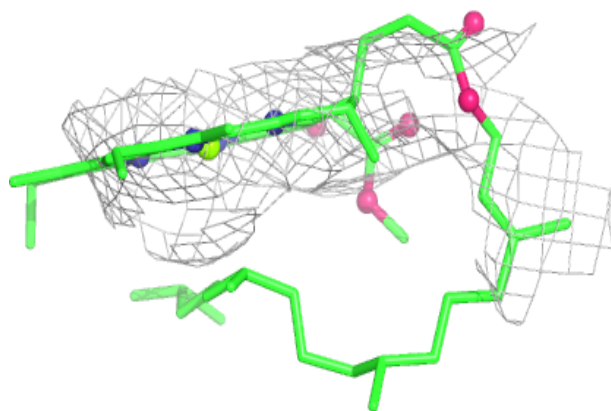
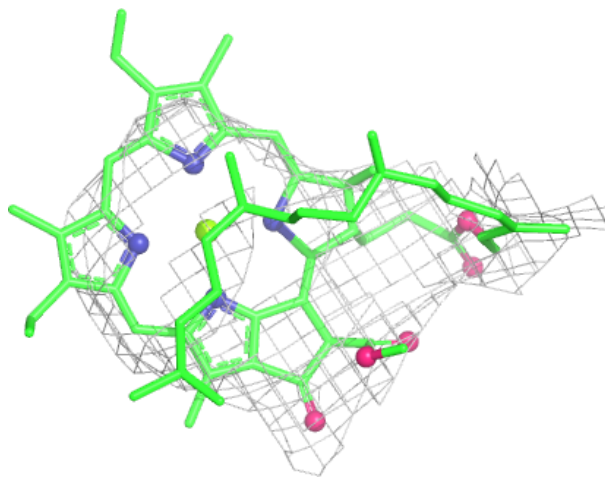
**Electron density around CLA B 613:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



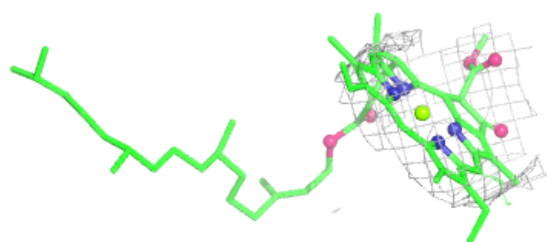
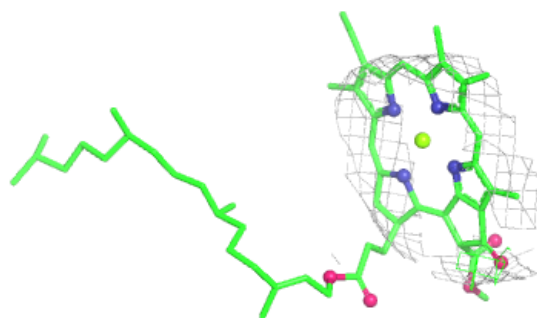
Electron density around CLA c 511:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

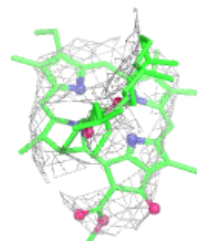
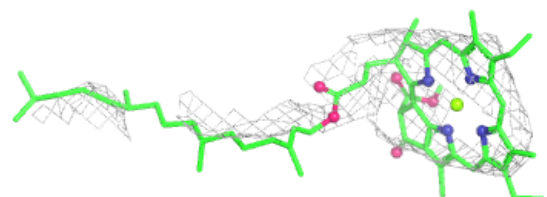
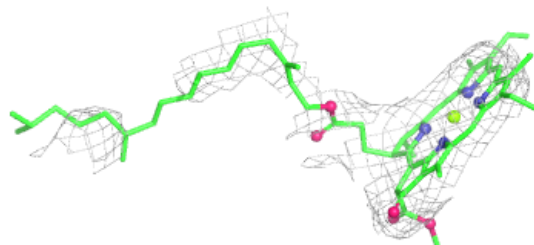


Electron density around CLA c 512:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

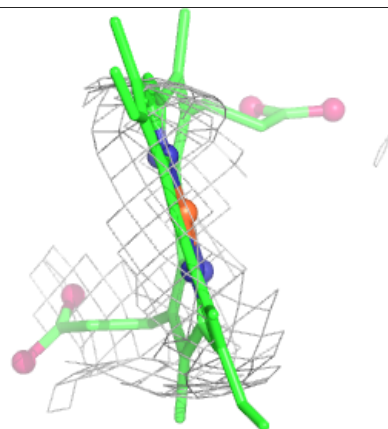
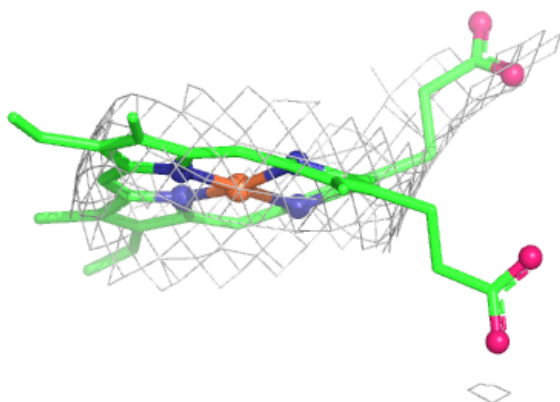
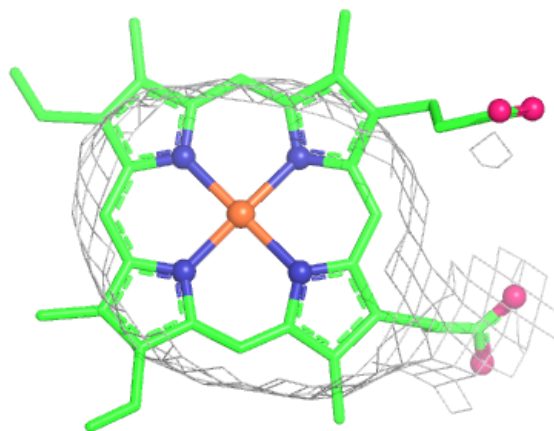
**Electron density around CLA C 502:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



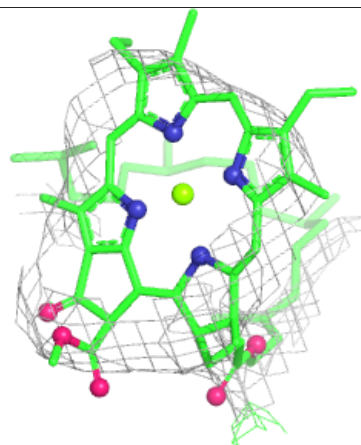
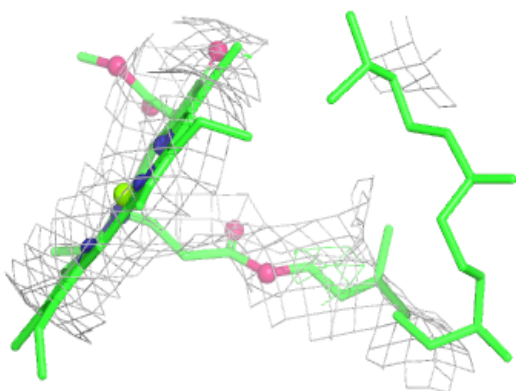
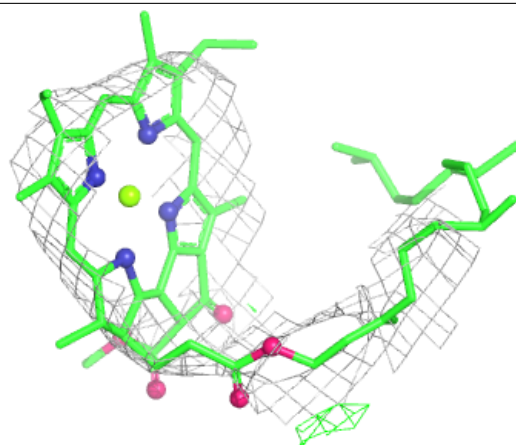
Electron density around HEM e 102:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



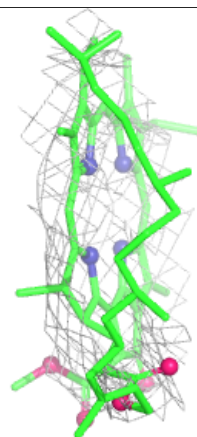
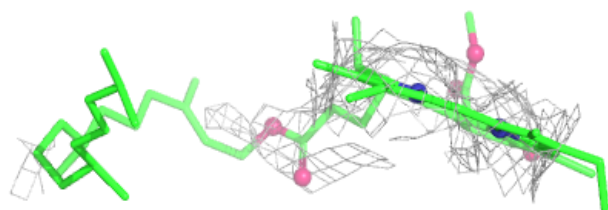
Electron density around CLA C 503:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

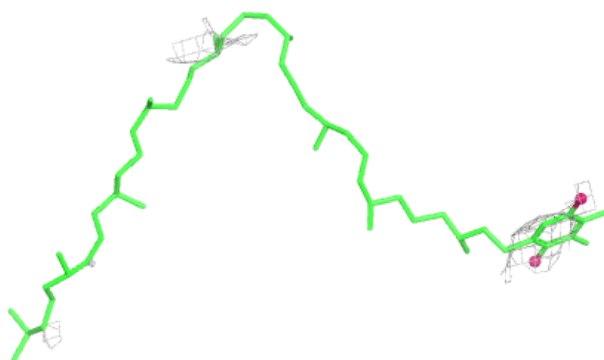


Electron density around PHO a 606:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

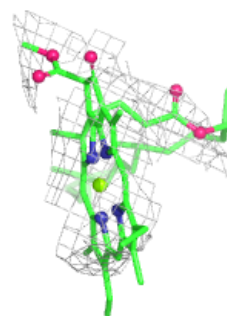
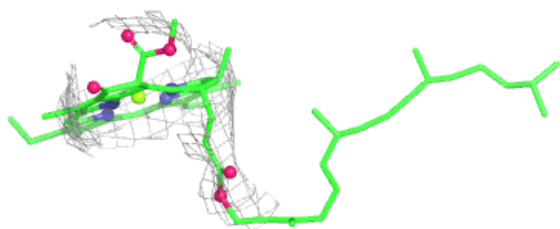
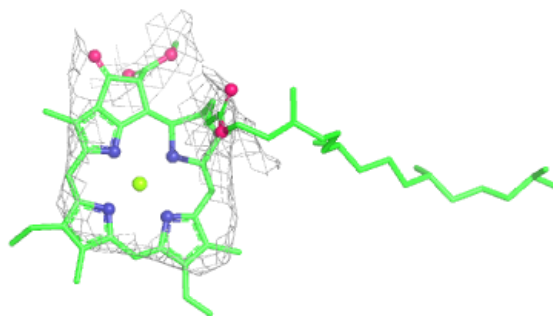
**Electron density around PL9 D 405:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

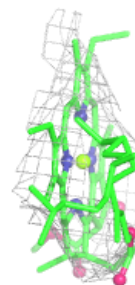
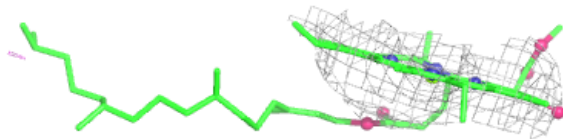
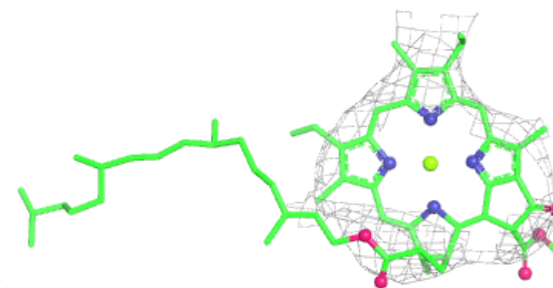


Electron density around CLA A 606:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

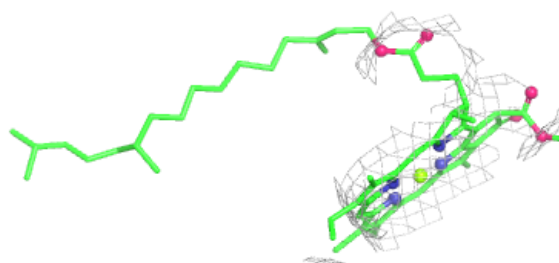
**Electron density around CLA B 604:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



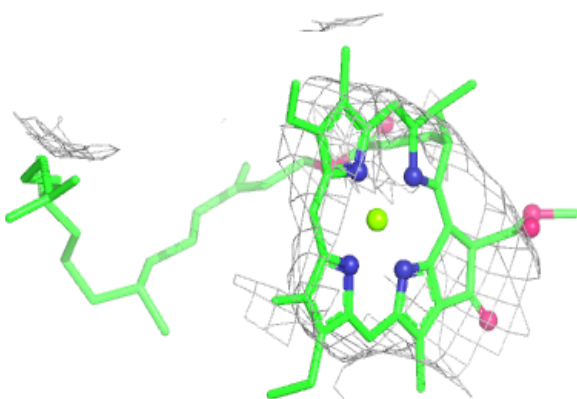
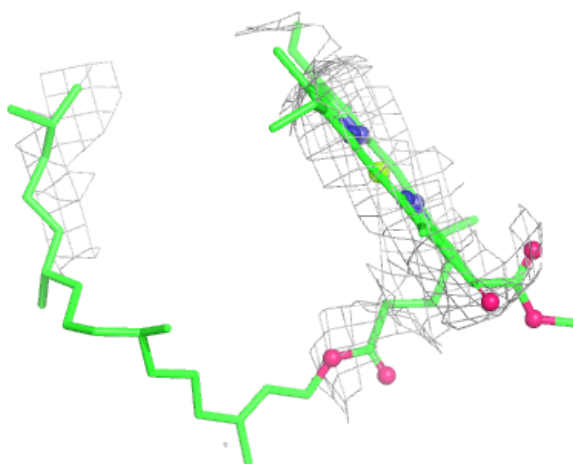
Electron density around CLA c 505:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



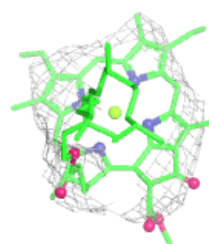
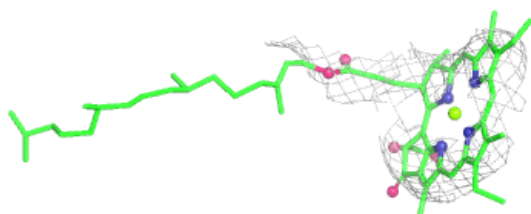
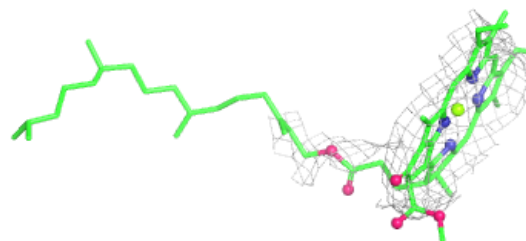
Electron density around CLA B 612:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

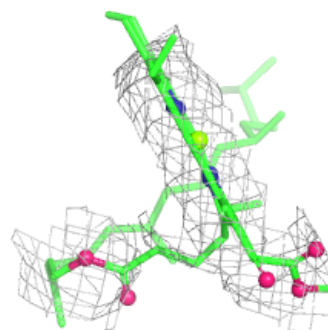
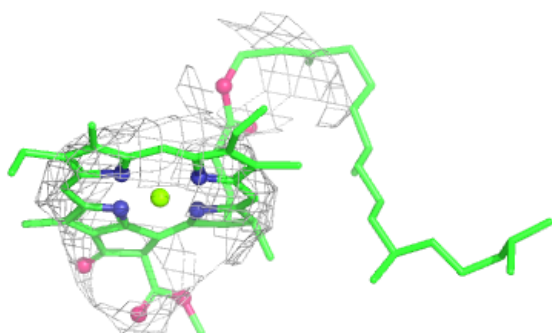
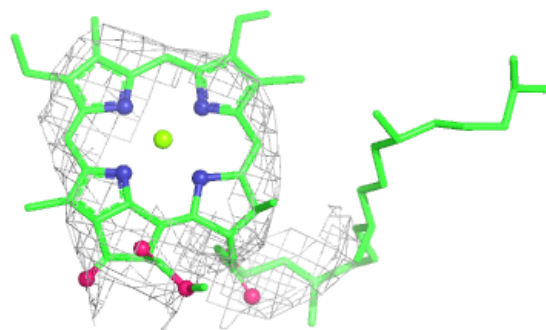


Electron density around CLA b 607:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

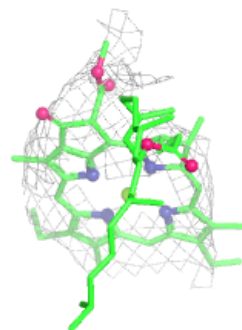
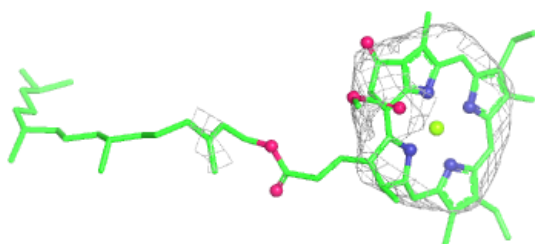
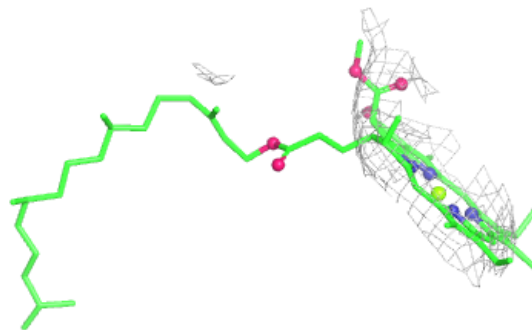
**Electron density around CLA a 613:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

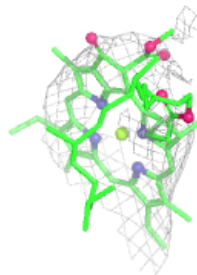
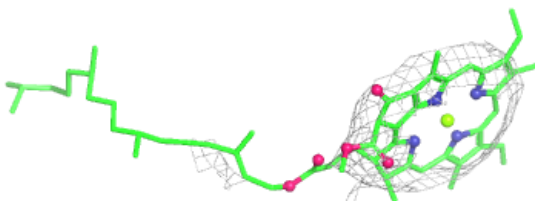
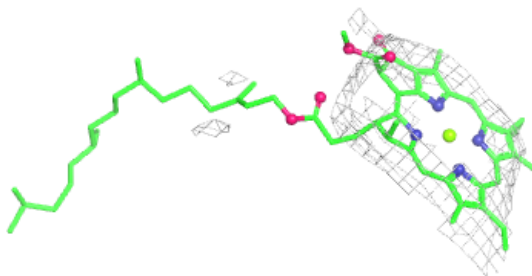


Electron density around CLA d 402:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

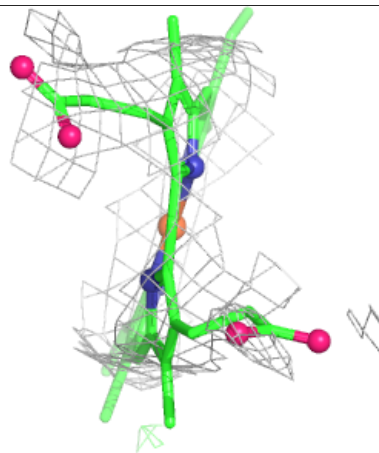
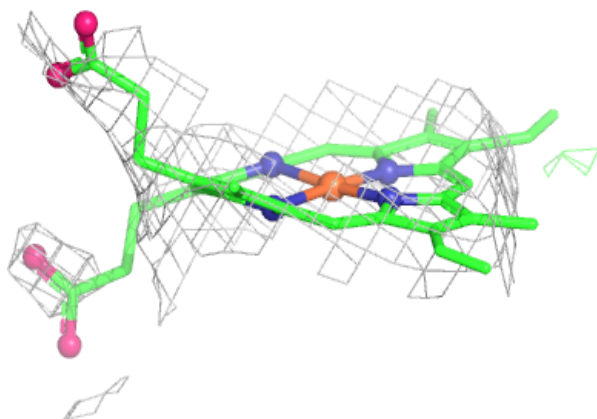
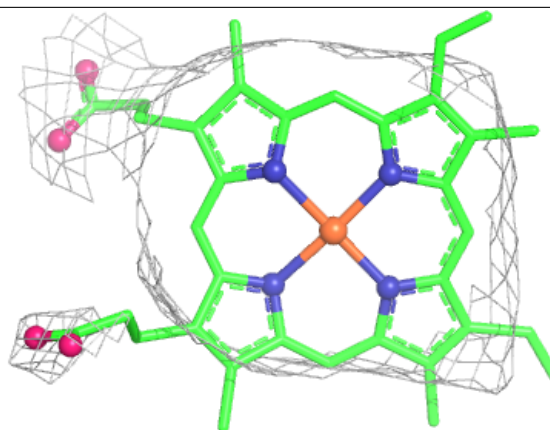
**Electron density around CLA A 605:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



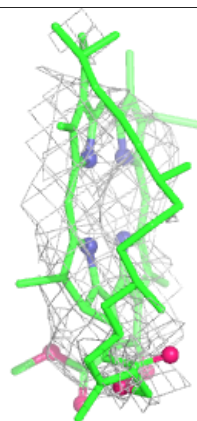
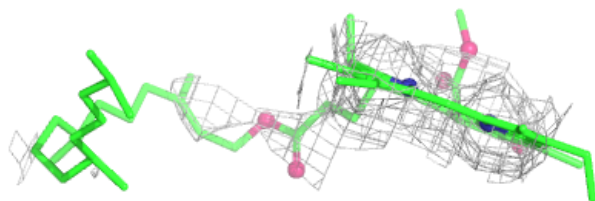
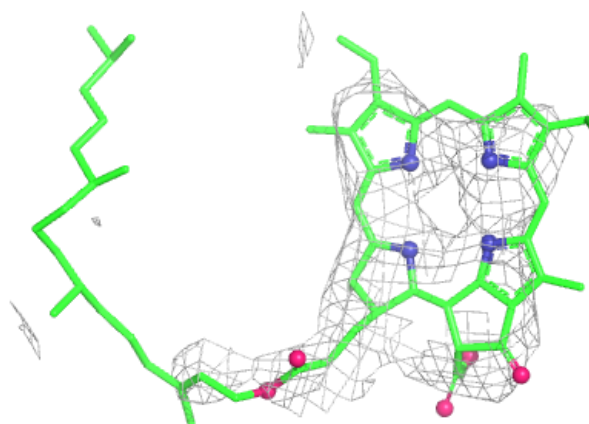
Electron density around HEM E 102:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



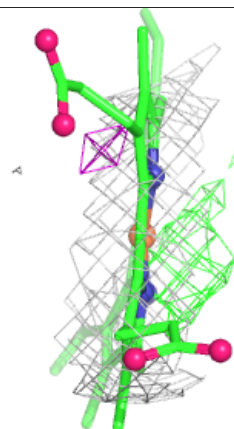
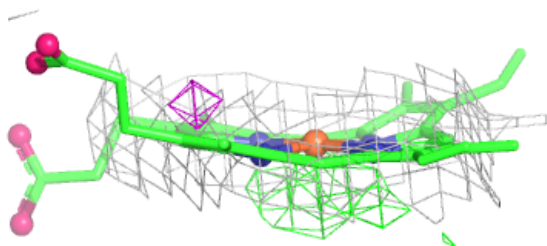
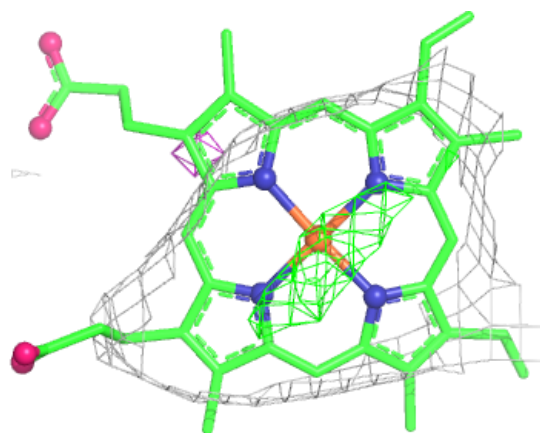
Electron density around PHO A 607:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



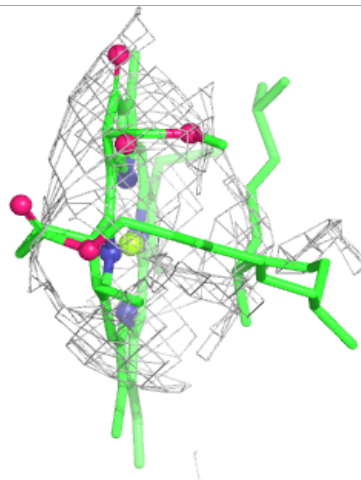
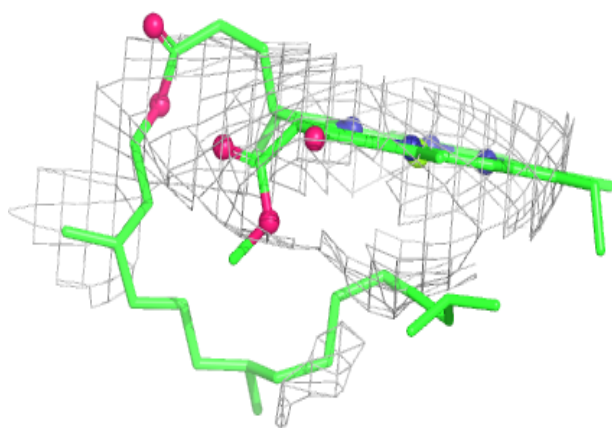
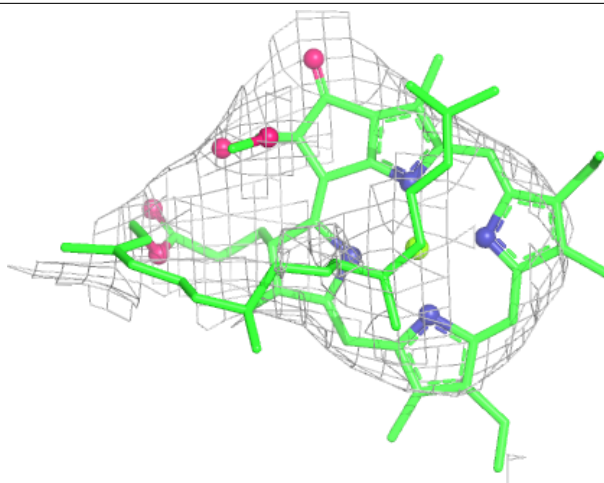
Electron density around HEM v 201:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



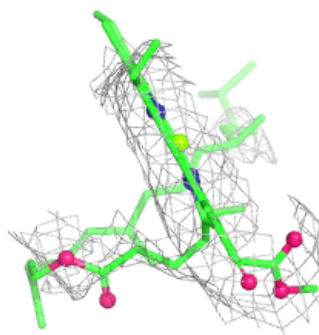
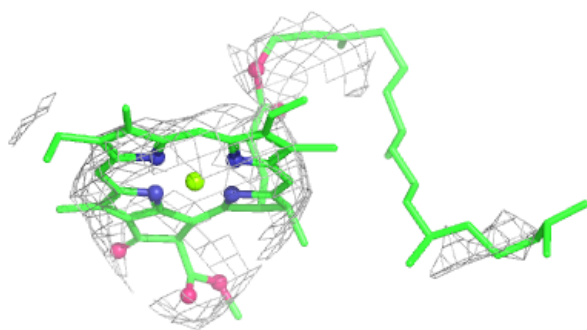
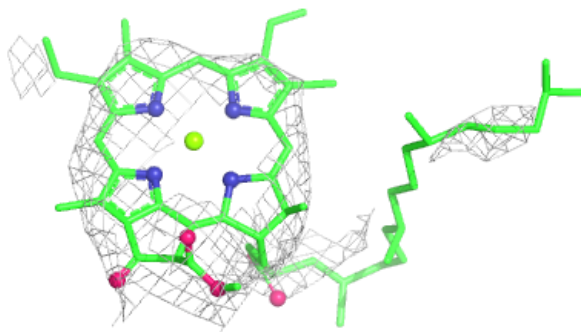
Electron density around CLA C 510:

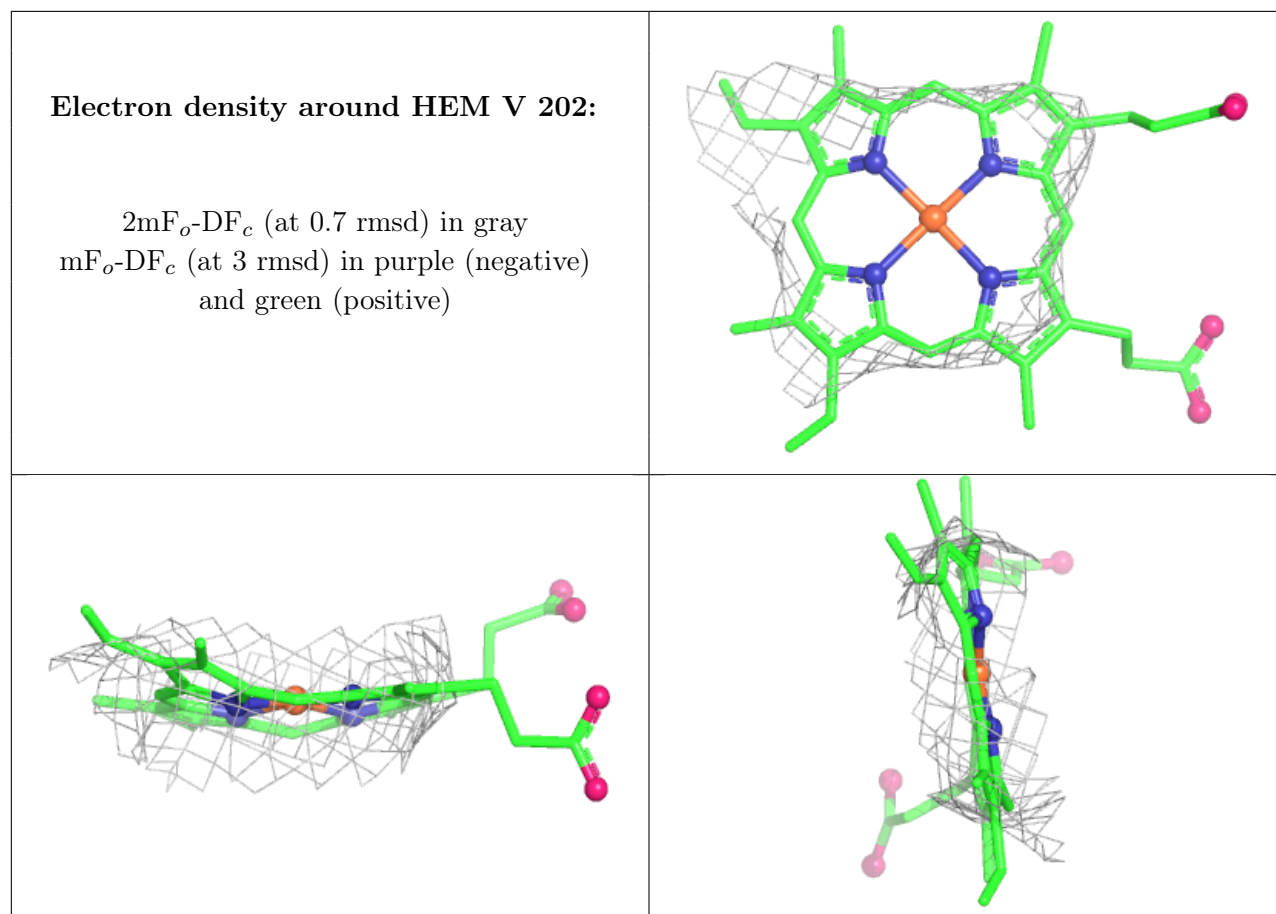
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA D 402:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.