



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 24, 2022 – 12:54 pm GMT

PDB ID : 5E7C
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.27
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

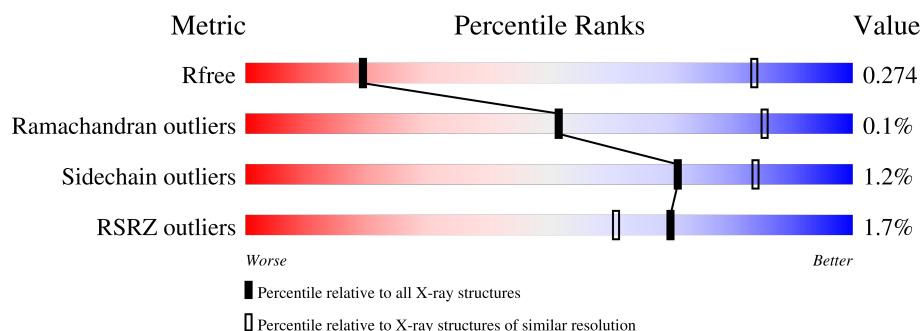
1 Overall quality at a glance

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.



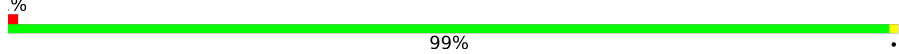

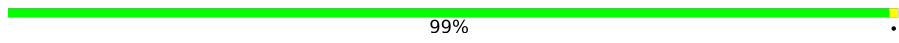
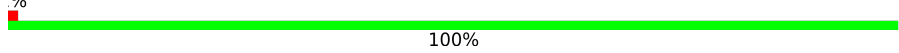
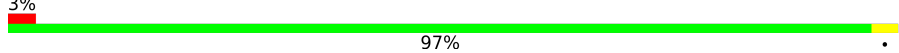

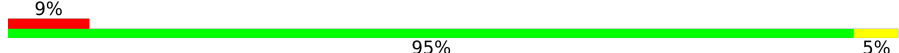
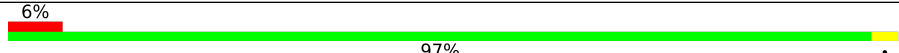
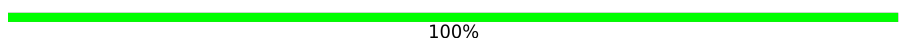

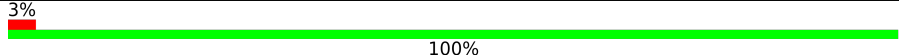
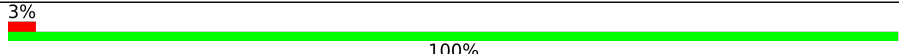
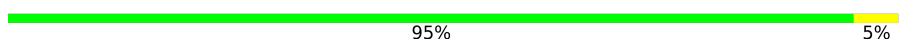
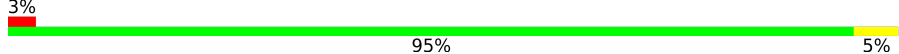
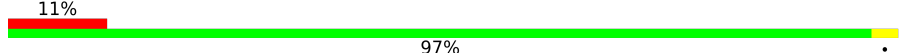
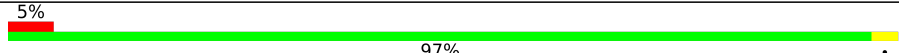
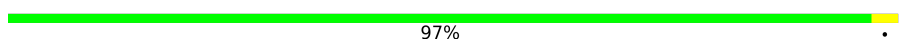
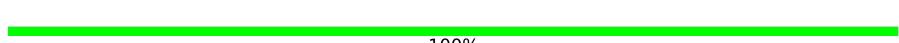
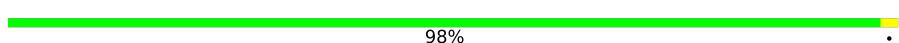
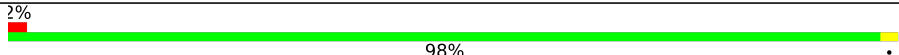
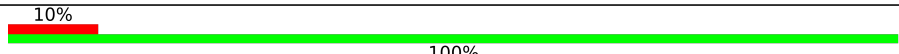

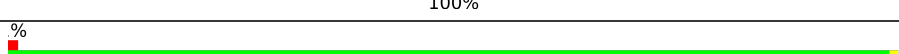
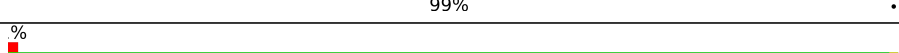
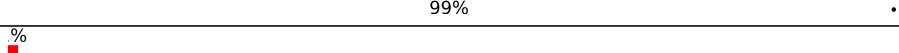
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1055 (5.20-3.80)
Ramachandran outliers	138981	1069 (5.20-3.80)
Sidechain outliers	138945	1050 (5.20-3.80)
RSRZ outliers	127900	1101 (5.30-3.70)

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	
1	a	334	
2	B	504	
2	b	504	
3	C	451	
3	c	451	

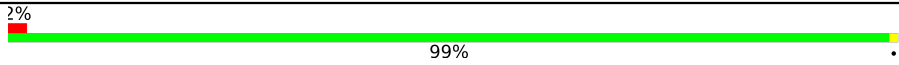
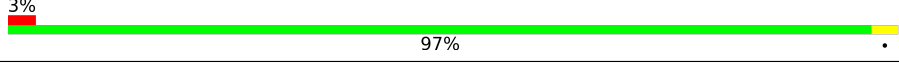
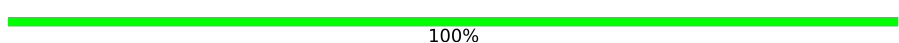
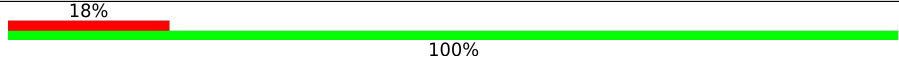
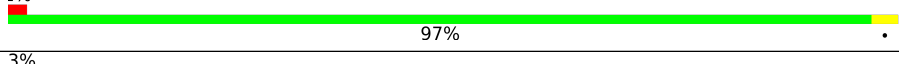
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Mol	Chain	Length	Quality of chain
4	D	342	%  99% .
4	d	342	%  100%
5	E	81	 99% .
5	e	81	%  100%
6	F	34	3%  97% .
6	f	34	3%  100%
7	H	65	9%  95% 5%
7	h	65	6%  97% .
8	I	38	 100%
8	i	38	3%  100%
9	J	38	3%  100%
9	j	38	3%  100%
10	K	37	 95% 5%
10	k	37	3%  95% 5%
11	L	37	11%  97% .
11	l	37	5%  97% .
12	M	34	 97% .
12	m	34	 100%
13	O	243	 98% .
13	o	243	2%  98% .
14	T	30	10%  100%
14	t	30	 100%
15	U	97	%  99% .
15	u	97	%  99% .
16	V	137	%  99% .

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Mol	Chain	Length	Quality of chain
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
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	-	-	-
23	CLA	B	615	X	-	-	-
23	CLA	B	616	X	-	-	-
23	CLA	B	617	X	-	-	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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	C	506	X	-	-	-
23	CLA	C	507	X	-	-	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	-	-	X
23	CLA	C	513	X	-	-	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	-	-	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	-	-	X
23	CLA	b	609[B]	X	-	-	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	-	-	-
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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	c	512	X	-	-	-
23	CLA	c	513	X	-	-	X
23	CLA	c	514	X	-	-	-
23	CLA	d	402	X	-	-	-
23	CLA	d	403	X	-	-	-
25	BCR	A	609	-	X	-	X
25	BCR	B	618	-	X	-	-
25	BCR	B	619	-	X	-	-
25	BCR	B	620	-	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	-	X
25	BCR	K	101	-	X	-	-
25	BCR	T	101	-	X	-	X
25	BCR	a	608	-	X	-	X
25	BCR	b	620	-	X	-	X
25	BCR	b	621	-	X	-	-
25	BCR	b	622	-	X	-	X
25	BCR	c	515	-	X	-	X
25	BCR	c	516	-	X	-	-
25	BCR	c	522	-	X	-	-
25	BCR	f	101	-	X	-	-
25	BCR	h	101	-	X	-	X
25	BCR	k	101	-	X	-	-
25	BCR	t	101	-	X	-	-
26	PL9	A	610	-	X	-	-
26	PL9	a	609	-	X	-	X
26	PL9	d	404	-	X	-	-
27	SQD	A	611	-	-	-	X
27	SQD	a	610	-	-	-	X
27	SQD	b	602	-	-	-	X
27	SQD	x	101	-	-	-	X
28	LMG	C	519	-	-	-	X
28	LMG	C	520	-	-	-	X
28	LMG	c	521	-	-	-	X
28	LMG	z	101	-	-	-	X
30	CA	B	601	-	-	-	X
30	CA	b	603	-	-	-	X
32	DGD	D	406	-	-	-	X
32	DGD	d	405	-	-	-	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			

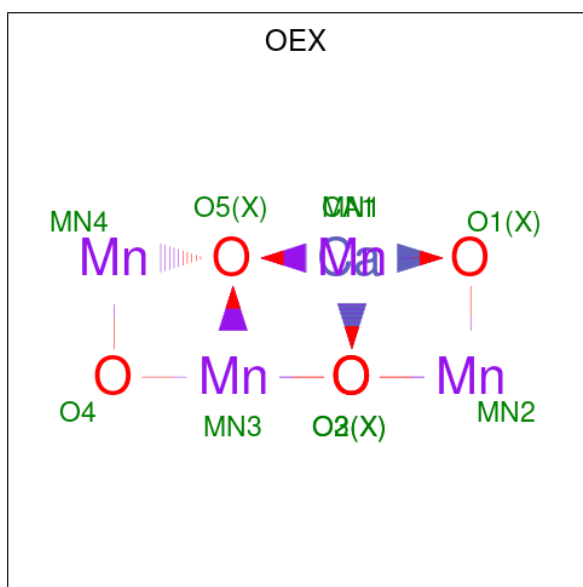
- Molecule 18 is a protein called Photosystem II reaction center X protein.

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 (three-letter code: OEX) (formula: CaMn_4O_5).

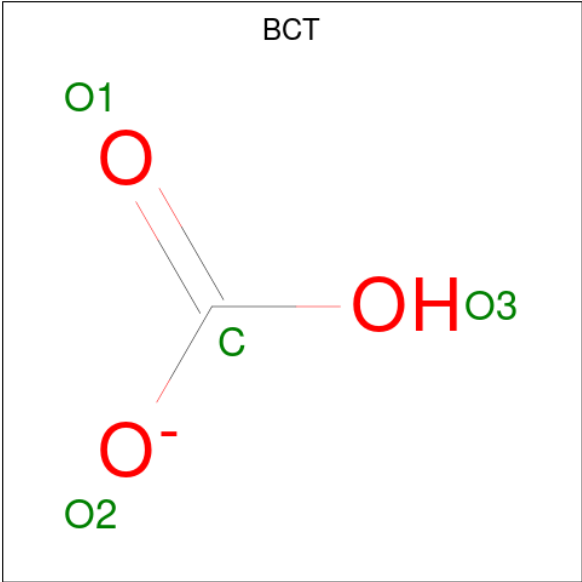


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	A	1	Total	Ca	Mn	O	0	0
			10	1	4	5		
20	a	1	Total	Ca	Mn	O	0	0
			10	1	4	5		

- Molecule 21 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

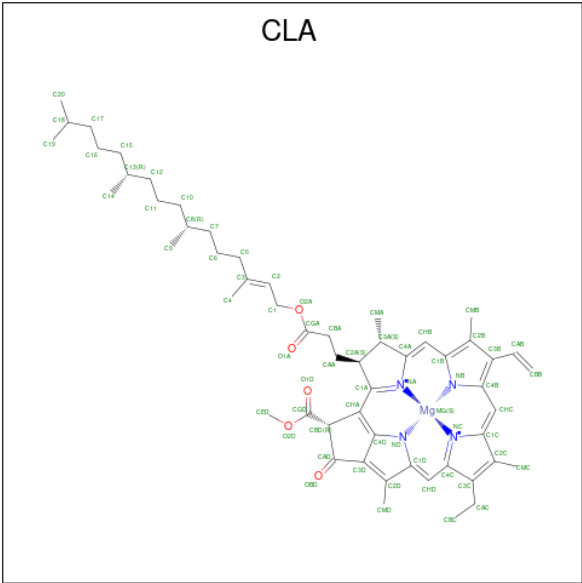
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	A	2	Total	Cl	0	0
			2	2		
21	V	1	Total	Cl	0	0
			1	1		
21	a	1	Total	Cl	0	0
			1	1		
21	c	1	Total	Cl	0	0
			1	1		
21	u	1	Total	Cl	0	0
			1	1		

- Molecule 22 is BICARBONATE ION (three-letter code: BCT) (formula: CHO₃).



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 (three-letter code: 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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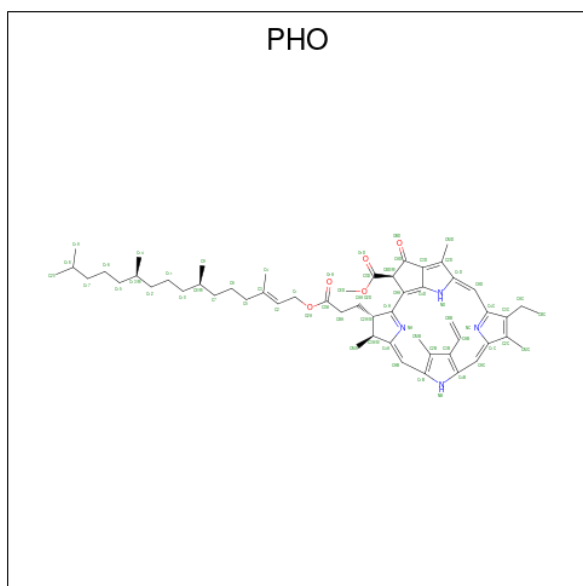
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	b	1	Total	C	Mg	N	O	0	1
			130	110	2	8	10		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	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	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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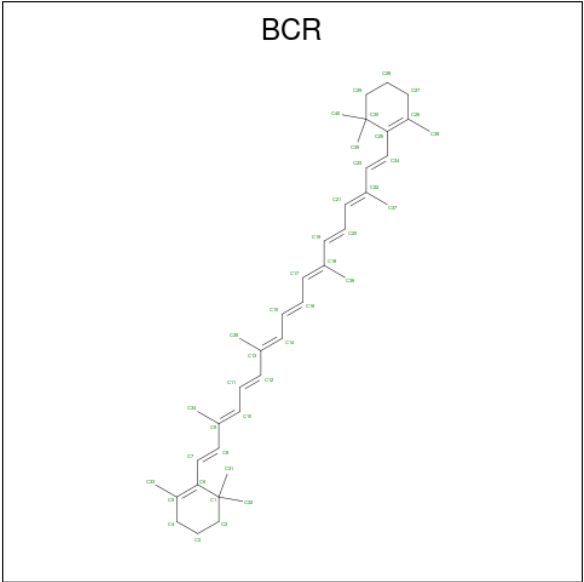
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 24 is PHEOPHYTIN A (three-letter code: 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 (three-letter code: BCR) (formula: $C_{40}H_{56}$).



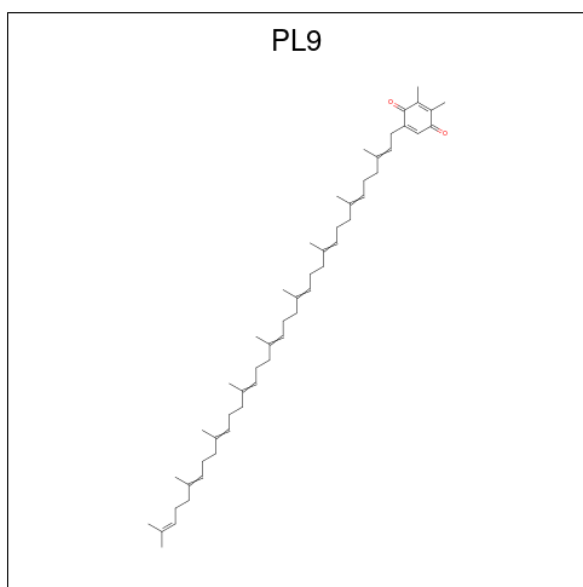
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	F	1	Total C 40 40	0	0
25	H	1	Total C 40 40	0	0
25	K	1	Total C 40 40	0	0
25	T	1	Total 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 (three-letter code: PL9) (formula: $C_{53}H_{80}O_2$).



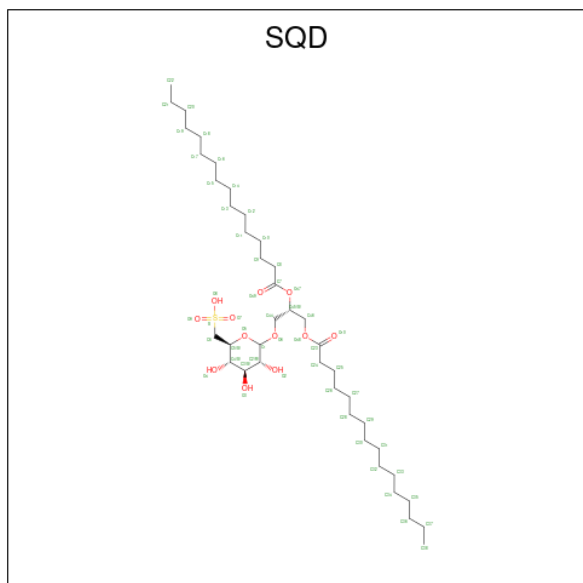
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C O 55 53 2	0	0
26	D	1	Total C O 55 53 2	0	0

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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		

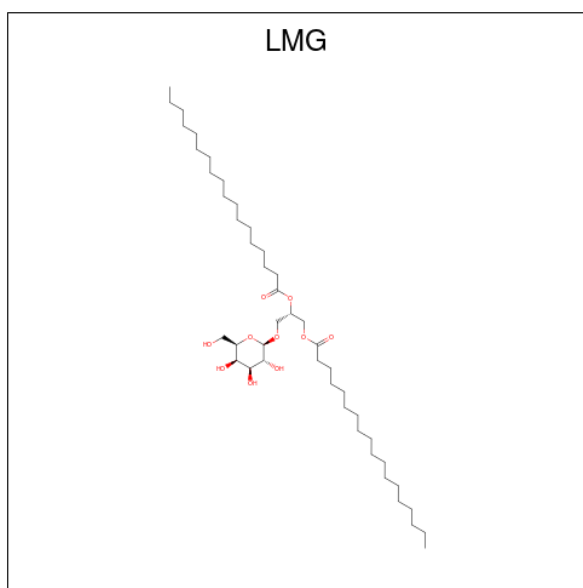
- Molecule 27 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



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 (three-letter

code: 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		

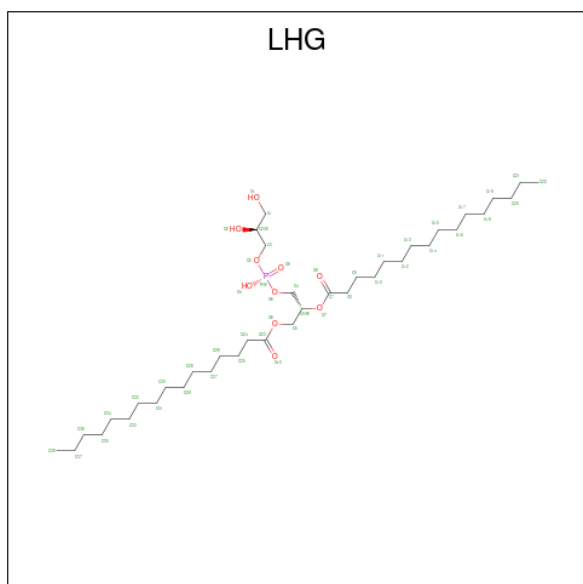
- Molecule 29 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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 (three-letter code: 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 (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



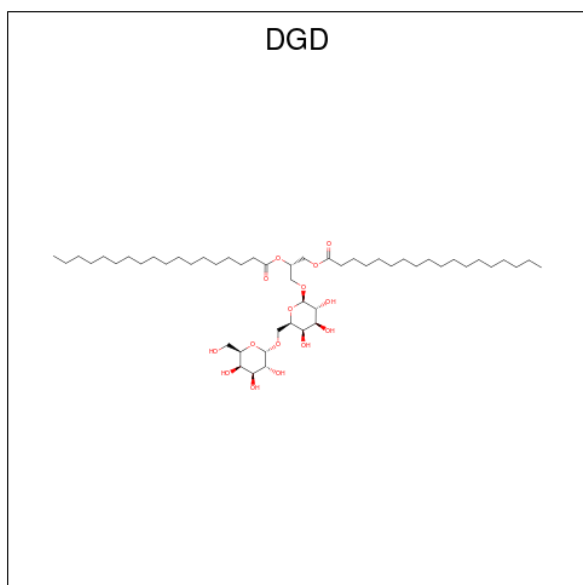
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	B	1	Total	C	O	P	0	0
			49	38	10	1		

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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) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



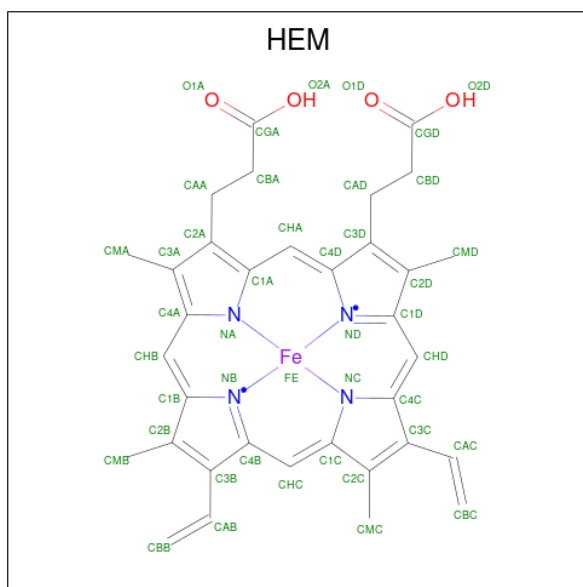
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	C	1	Total	C	O	0	0
			62	47	15		
32	C	1	Total	C	O	0	0
			62	47	15		

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

- Molecule 33 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

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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		

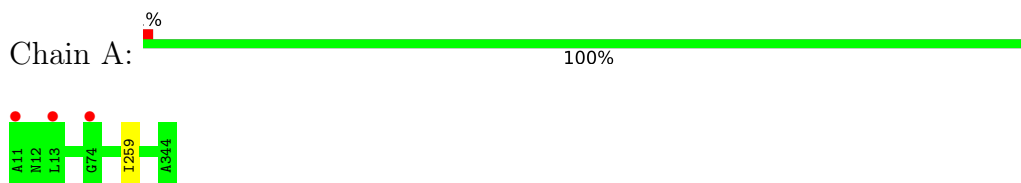
- Molecule 34 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

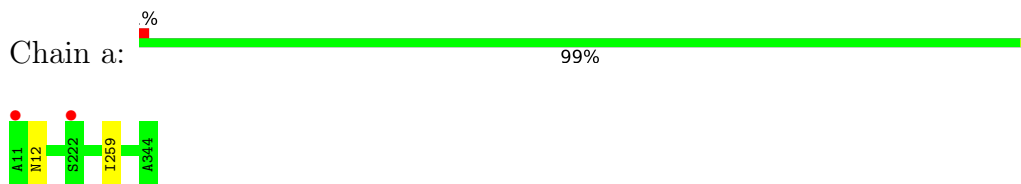
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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.

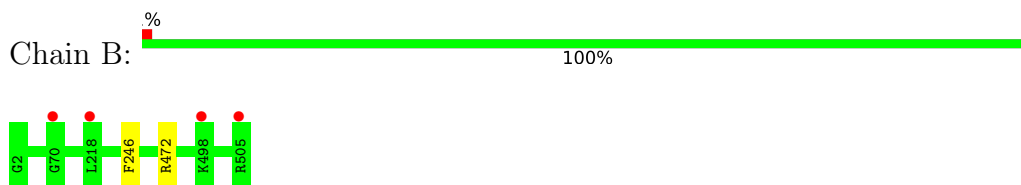
- Molecule 1: Photosystem II protein D1 1



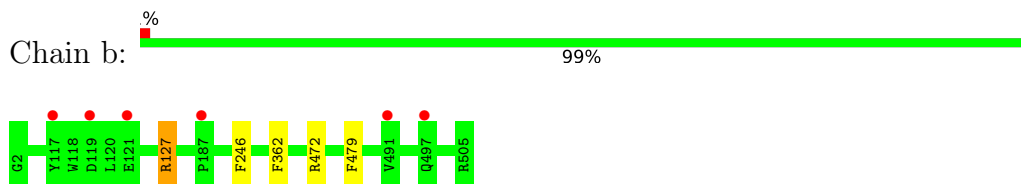
- Molecule 1: Photosystem II protein D1 1



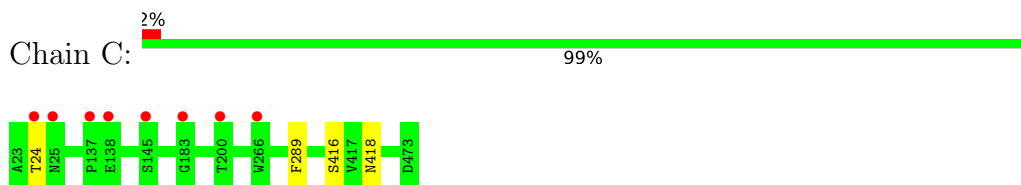
- Molecule 2: Photosystem II CP47 reaction center protein



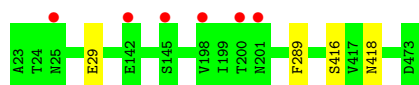
- Molecule 2: Photosystem II CP47 reaction center protein



- Molecule 3: Photosystem II CP43 reaction center protein



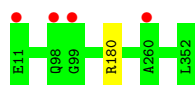
- Molecule 3: Photosystem II CP43 reaction center protein



- 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



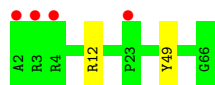
- Molecule 6: Cytochrome b559 subunit beta



- Molecule 7: Photosystem II reaction center protein H



- Molecule 7: Photosystem II reaction center protein H



- Molecule 8: Photosystem II reaction center protein I



There are no outlier residues recorded for this chain.

- Molecule 8: Photosystem II reaction center protein I



- Molecule 9: Photosystem II reaction center protein J



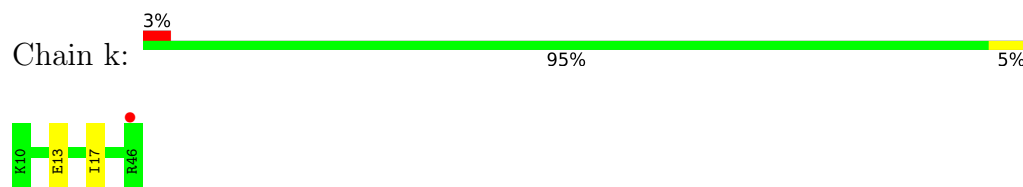
- Molecule 9: Photosystem II reaction center protein J



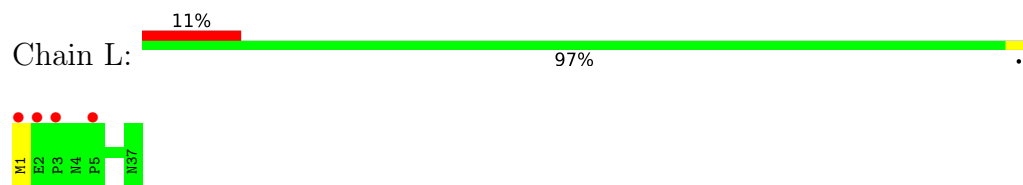
- Molecule 10: Photosystem II reaction center protein K



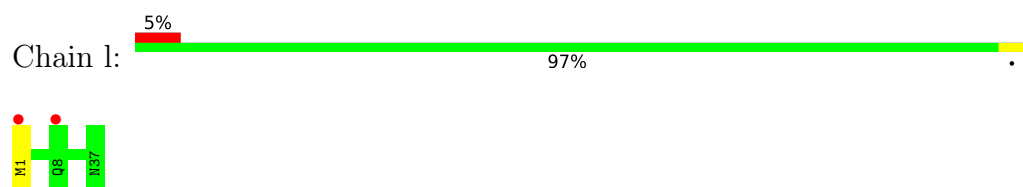
- Molecule 10: Photosystem II reaction center protein K



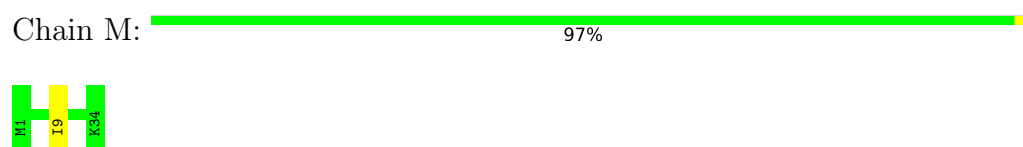
- Molecule 11: Photosystem II reaction center protein L



- Molecule 11: Photosystem II reaction center protein L



- Molecule 12: Photosystem II reaction center protein M

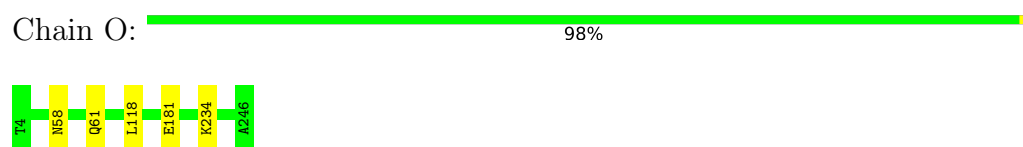


- Molecule 12: Photosystem II reaction center protein M

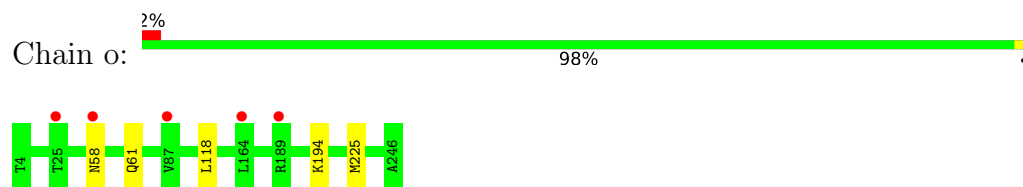


There are no outlier residues recorded for this chain.

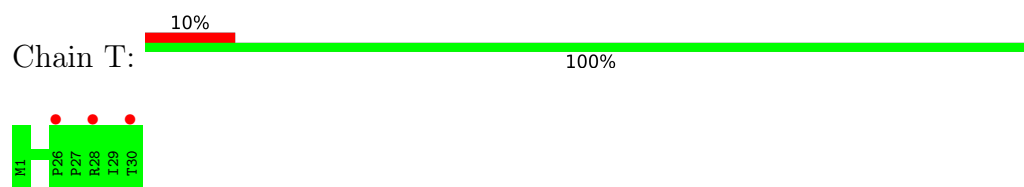
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



- Molecule 13: Photosystem II manganese-stabilizing polypeptide



- Molecule 14: Photosystem II reaction center protein T

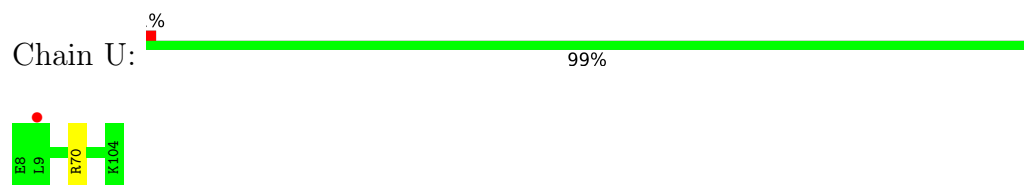


- Molecule 14: Photosystem II reaction center protein T

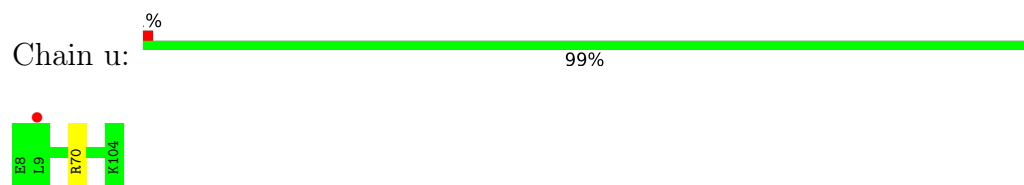


There are no outlier residues recorded for this chain.

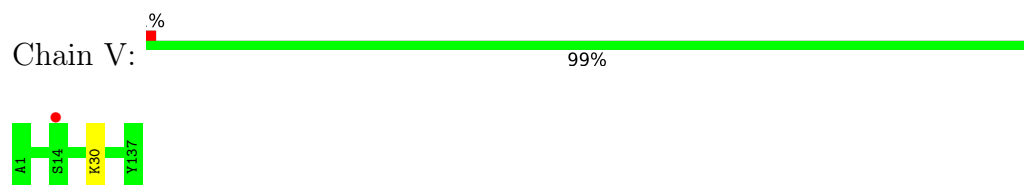
- Molecule 15: Photosystem II 12 kDa extrinsic protein



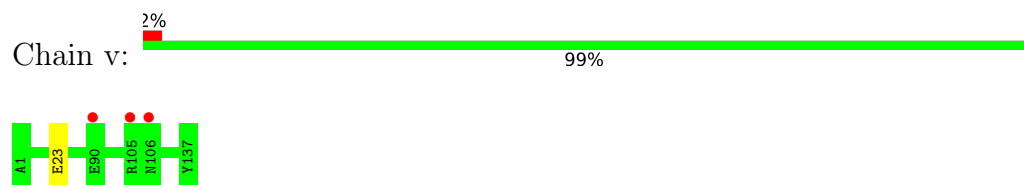
- Molecule 15: Photosystem II 12 kDa extrinsic protein



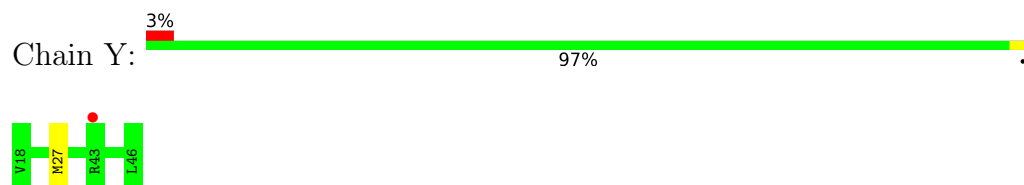
- Molecule 16: Cytochrome c-550



- Molecule 16: Cytochrome c-550



- Molecule 17: Photosystem II reaction center protein Ycf12



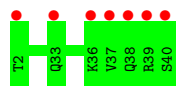
- Molecule 17: Photosystem II reaction center protein Ycf12

Chain y:  100%

There are no outlier residues recorded for this chain.

- Molecule 18: Photosystem II reaction center X protein

Chain X:  100%



- Molecule 18: Photosystem II reaction center X protein

Chain x:  97%



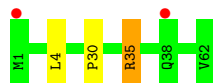
- Molecule 19: Photosystem II reaction center protein Z

Chain Z:  97%



- Molecule 19: Photosystem II reaction center protein Z

Chain z:  95%



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 36.50 – 4.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.93-4.50) 99.9 (36.50-4.50)	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 0.250 , 0.274	Depositor DCC
R_{free} test set	2721 reflections (4.88%)	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)	(Not available) , (Not available)	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: OEX, PHO, BCT, DGD, CLA, FE2, HEM, SQD, LMG, CA, LHG, MG, BCR, PL9, CL

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	0.33	0/2734	0.53	0/3727
1	a	0.33	0/2734	0.53	0/3727
2	B	0.30	0/4194	0.51	0/5713
2	b	0.31	0/4194	0.52	1/5713 (0.0%)
3	C	0.31	0/3634	0.49	0/4947
3	c	0.32	0/3634	0.52	0/4947
4	D	0.31	0/2821	0.50	0/3844
4	d	0.30	0/2821	0.50	0/3844
5	E	0.30	0/693	0.49	0/944
5	e	0.31	0/693	0.55	0/944
6	F	0.34	0/284	0.49	0/387
6	f	0.40	0/284	0.74	0/387
7	H	0.29	0/544	0.52	0/739
7	h	0.28	0/544	0.52	0/739
8	I	0.31	0/327	0.54	0/439
8	i	0.31	0/327	0.60	0/439
9	J	0.27	0/278	0.44	0/376
9	j	0.31	0/278	0.50	0/376
10	K	0.31	0/303	0.57	0/416
10	k	0.34	0/303	0.55	0/416
11	L	0.28	0/319	0.44	0/433
11	l	0.28	0/319	0.45	0/433
12	M	0.33	0/278	0.56	0/378
12	m	0.34	0/278	0.57	0/378
13	O	0.29	0/1926	0.53	0/2611
13	o	0.32	0/1926	0.58	0/2611
14	T	0.34	0/282	0.52	0/382
14	t	0.34	0/282	0.51	0/382
15	U	0.28	0/785	0.51	0/1064
15	u	0.31	0/785	0.56	0/1064
16	V	0.29	0/1096	0.50	0/1487
16	v	0.29	0/1096	0.56	0/1487

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	Y	0.33	0/216	0.49	0/289
17	y	0.36	0/216	0.59	0/289
18	X	0.29	0/298	0.42	0/403
18	x	0.32	0/298	0.54	0/403
19	Z	0.32	0/490	0.46	0/669
19	z	0.41	0/490	0.68	1/669 (0.1%)
All	All	0.31	0/43004	0.52	2/58496 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	z	35	ARG	CB-CG-CD	6.51	128.53	111.60
2	b	127	ARG	CG-CD-NE	5.53	123.42	111.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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%)	41	76
1	a	336/334 (101%)	330 (98%)	5 (2%)	1 (0%)	41	76
2	B	512/504 (102%)	507 (99%)	5 (1%)	0	100	100
2	b	512/504 (102%)	503 (98%)	9 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	454/451 (101%)	443 (98%)	9 (2%)	2 (0%)	34	72
3	c	454/451 (101%)	441 (97%)	11 (2%)	2 (0%)	34	72
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
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%)	34	72
13	o	245/243 (101%)	235 (96%)	9 (4%)	1 (0%)	34	72
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	51	81

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%)	91	94
2	B	412/402 (102%)	410 (100%)	2 (0%)	88	93
2	b	412/402 (102%)	407 (99%)	5 (1%)	71	84
3	C	357/352 (101%)	354 (99%)	3 (1%)	81	89
3	c	357/352 (101%)	354 (99%)	3 (1%)	81	89
4	D	277/277 (100%)	274 (99%)	3 (1%)	73	85
4	d	277/277 (100%)	276 (100%)	1 (0%)	91	94
5	E	74/72 (103%)	73 (99%)	1 (1%)	67	81
5	e	74/72 (103%)	74 (100%)	0	100	100
6	F	28/28 (100%)	27 (96%)	1 (4%)	35	60
6	f	28/28 (100%)	28 (100%)	0	100	100
7	H	56/54 (104%)	52 (93%)	4 (7%)	14	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	h	56/54 (104%)	53 (95%)	3 (5%)	22	49
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%)	16	43
10	k	30/30 (100%)	28 (93%)	2 (7%)	16	43
11	L	36/35 (103%)	35 (97%)	1 (3%)	43	65
11	l	36/35 (103%)	35 (97%)	1 (3%)	43	65
12	M	32/31 (103%)	31 (97%)	1 (3%)	40	63
12	m	32/31 (103%)	32 (100%)	0	100	100
13	O	210/206 (102%)	206 (98%)	4 (2%)	57	75
13	o	210/206 (102%)	206 (98%)	4 (2%)	57	75
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%)	71	84
15	u	84/84 (100%)	83 (99%)	1 (1%)	71	84
16	V	118/117 (101%)	117 (99%)	1 (1%)	81	89
16	v	118/117 (101%)	117 (99%)	1 (1%)	81	89
17	Y	22/22 (100%)	21 (96%)	1 (4%)	27	54
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%)	41	63
19	Z	52/52 (100%)	50 (96%)	2 (4%)	33	58
19	z	52/52 (100%)	49 (94%)	3 (6%)	20	47
All	All	4370/4302 (102%)	4317 (99%)	53 (1%)	71	84

5 of 53 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	b	127	ARG
3	c	418	ASN
18	x	2	THR

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Mol	Chain	Res	Type
2	b	246	PHE
2	b	479	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
12	M	33	GLN
1	a	198	HIS
3	c	25	ASN
12	m	33	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 monosaccharides 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	$\# Z > 2$
23	CLA	C	508	-	56,73,73	3.86	21 (37%)	55,113,113	2.13	13 (23%)
23	CLA	b	604	-	56,73,73	3.88	21 (37%)	55,113,113	2.00	12 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	B	606	-	56,73,73	3.83	21 (37%)	55,113,113	2.00	11 (20%)
23	CLA	b	615	-	56,73,73	3.84	21 (37%)	55,113,113	2.06	13 (23%)
25	BCR	F	101	-	41,41,41	9.25	29 (70%)	56,56,56	6.08	28 (50%)
23	CLA	b	610	-	56,73,73	3.83	21 (37%)	55,113,113	2.02	16 (29%)
23	CLA	C	510	-	56,73,73	3.84	21 (37%)	55,113,113	2.00	12 (21%)
32	DGD	c	519	-	63,63,67	1.67	16 (25%)	77,77,81	1.06	4 (5%)
28	LMG	Z	101	-	37,37,55	1.42	4 (10%)	45,45,63	1.25	3 (6%)
24	PHO	d	401	-	67,69,69	1.28	7 (10%)	85,99,99	1.04	4 (4%)
27	SQD	X	101	-	42,43,54	1.21	3 (7%)	51,54,65	1.45	7 (13%)
27	SQD	a	612	-	53,54,54	1.05	3 (5%)	62,65,65	1.22	6 (9%)
27	SQD	A	611	-	53,54,54	0.98	3 (5%)	62,65,65	1.53	11 (17%)
23	CLA	B	605	-	56,73,73	3.86	21 (37%)	55,113,113	2.10	14 (25%)
25	BCR	c	515	-	41,41,41	9.14	30 (73%)	56,56,56	6.26	33 (58%)
23	CLA	c	512	3	56,73,73	3.82	21 (37%)	55,113,113	2.05	12 (21%)
31	LHG	a	614	-	48,48,48	1.09	2 (4%)	51,54,54	1.02	3 (5%)
23	CLA	C	503	-	56,73,73	3.85	21 (37%)	55,113,113	2.01	11 (20%)
33	HEM	E	102	6,5	27,50,50	2.11	6 (22%)	17,82,82	1.77	3 (17%)
25	BCR	k	101	-	41,41,41	9.29	30 (73%)	56,56,56	5.70	26 (46%)
23	CLA	a	613	-	56,73,73	3.83	21 (37%)	55,113,113	2.08	14 (25%)
23	CLA	b	606	-	56,73,73	3.85	21 (37%)	55,113,113	2.06	14 (25%)
25	BCR	C	514	-	41,41,41	9.14	31 (75%)	56,56,56	6.17	31 (55%)
23	CLA	d	402	-	56,73,73	3.82	21 (37%)	55,113,113	1.94	11 (20%)
32	DGD	C	517	-	63,63,67	1.65	17 (26%)	77,77,81	1.02	5 (6%)
28	LMG	B	621	-	51,51,55	1.27	4 (7%)	59,59,63	0.90	2 (3%)
23	CLA	B	609	-	56,73,73	3.88	21 (37%)	55,113,113	2.10	16 (29%)
23	CLA	B	603	-	56,73,73	3.85	21 (37%)	55,113,113	2.12	16 (29%)
32	DGD	c	518	-	63,63,67	1.66	17 (26%)	77,77,81	1.00	5 (6%)
25	BCR	A	609	-	41,41,41	9.39	30 (73%)	56,56,56	5.67	28 (50%)
28	LMG	c	520	-	51,51,55	1.32	4 (7%)	59,59,63	1.02	2 (3%)
23	CLA	c	506	-	56,73,73	3.86	21 (37%)	55,113,113	2.04	12 (21%)
25	BCR	f	101	-	41,41,41	9.23	30 (73%)	56,56,56	5.80	28 (50%)
24	PHO	A	607	-	67,69,69	1.27	10 (14%)	85,99,99	1.03	4 (4%)
23	CLA	C	513	-	56,73,73	3.79	21 (37%)	55,113,113	2.06	15 (27%)
23	CLA	b	614	-	56,73,73	3.85	21 (37%)	55,113,113	2.13	13 (23%)
32	DGD	C	518	-	63,63,67	1.68	16 (25%)	77,77,81	1.03	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	C	506	-	56,73,73	3.81	21 (37%)	55,113,113	2.11	13 (23%)
32	DGD	c	517	-	63,63,67	1.71	16 (25%)	77,77,81	0.92	3 (3%)
23	CLA	B	602	-	56,73,73	3.94	21 (37%)	55,113,113	1.98	11 (20%)
23	CLA	B	613	-	56,73,73	3.86	21 (37%)	55,113,113	2.05	14 (25%)
25	BCR	b	621	-	41,41,41	9.18	30 (73%)	56,56,56	5.68	31 (55%)
26	PL9	d	404	-	55,55,55	4.26	19 (34%)	68,69,69	3.70	35 (51%)
25	BCR	B	618	-	41,41,41	9.17	30 (73%)	56,56,56	6.07	30 (53%)
23	CLA	c	513	-	56,73,73	3.84	21 (37%)	55,113,113	2.05	16 (29%)
25	BCR	H	101	-	41,41,41	9.23	30 (73%)	56,56,56	5.84	36 (64%)
31	LHG	e	101	-	41,41,48	1.20	3 (7%)	44,47,54	0.95	2 (4%)
24	PHO	a	606	-	67,69,69	1.26	10 (14%)	85,99,99	1.02	4 (4%)
23	CLA	c	505	-	56,73,73	3.85	21 (37%)	55,113,113	2.09	13 (23%)
25	BCR	C	515	-	41,41,41	9.29	30 (73%)	56,56,56	5.97	30 (53%)
23	CLA	b	618	-	56,73,73	3.85	21 (37%)	55,113,113	2.02	13 (23%)
22	BCT	A	604	29	0,3,3	-	-	0,3,3	-	-
23	CLA	a	605	-	56,73,73	3.84	21 (37%)	55,113,113	2.06	13 (23%)
23	CLA	C	512	-	56,73,73	3.85	21 (37%)	55,113,113	2.13	16 (29%)
23	CLA	c	504	-	56,73,73	3.86	21 (37%)	55,113,113	1.96	13 (23%)
23	CLA	B	612	-	56,73,73	3.86	21 (37%)	55,113,113	2.16	13 (23%)
31	LHG	E	101	-	41,41,48	1.20	3 (7%)	44,47,54	0.91	3 (6%)
23	CLA	b	608	-	56,73,73	3.82	21 (37%)	55,113,113	2.01	12 (21%)
23	CLA	A	605	-	56,73,73	3.86	21 (37%)	55,113,113	2.08	12 (21%)
23	CLA	B	607[B]	-	56,73,73	3.84	21 (37%)	55,113,113	2.16	15 (27%)
23	CLA	c	503	-	56,73,73	3.84	21 (37%)	55,113,113	2.10	13 (23%)
28	LMG	z	101	-	37,37,55	1.43	4 (10%)	45,45,63	1.21	4 (8%)
28	LMG	a	611	-	51,51,55	1.30	4 (7%)	59,59,63	1.00	2 (3%)
32	DGD	C	516	-	63,63,67	1.71	16 (25%)	77,77,81	0.92	2 (2%)
31	LHG	D	407	-	48,48,48	1.11	3 (6%)	51,54,54	0.90	3 (5%)
25	BCR	t	101	-	41,41,41	9.30	29 (70%)	56,56,56	5.77	28 (50%)
23	CLA	a	604	-	56,73,73	3.84	21 (37%)	55,113,113	2.09	13 (23%)
27	SQD	b	602	-	53,54,54	1.08	4 (7%)	62,65,65	1.44	9 (14%)
23	CLA	D	404	-	56,73,73	3.85	21 (37%)	55,113,113	2.14	15 (27%)
22	BCT	a	603	29	0,3,3	-	-	0,3,3	-	-
23	CLA	b	609[A]	-	56,73,73	3.84	21 (37%)	55,113,113	2.17	15 (27%)
23	CLA	C	502	-	56,73,73	3.83	21 (37%)	55,113,113	2.10	11 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	BCR	B	620	-	41,41,41	9.20	30 (73%)	56,56,56	6.08	32 (57%)
28	LMG	C	520	-	51,51,55	1.30	5 (9%)	59,59,63	1.01	4 (6%)
23	CLA	b	607	-	56,73,73	3.88	21 (37%)	55,113,113	2.15	14 (25%)
28	LMG	C	519	-	51,51,55	1.32	4 (7%)	59,59,63	1.06	2 (3%)
23	CLA	B	614	-	56,73,73	3.86	21 (37%)	55,113,113	2.01	13 (23%)
26	PL9	A	610	-	55,55,55	4.25	22 (40%)	68,69,69	3.74	39 (57%)
23	CLA	B	611	-	56,73,73	3.90	21 (37%)	55,113,113	2.05	11 (20%)
23	CLA	b	605	-	56,73,73	3.84	21 (37%)	55,113,113	2.12	14 (25%)
26	PL9	D	405	-	55,55,55	4.25	19 (34%)	68,69,69	3.72	35 (51%)
25	BCR	T	101	-	41,41,41	9.24	29 (70%)	56,56,56	6.00	30 (53%)
25	BCR	h	101	-	41,41,41	9.22	30 (73%)	56,56,56	5.85	37 (66%)
23	CLA	d	403	-	56,73,73	3.84	21 (37%)	55,113,113	2.11	13 (23%)
23	CLA	A	608	-	56,73,73	3.79	21 (37%)	55,113,113	2.05	14 (25%)
23	CLA	b	617	-	56,73,73	3.82	21 (37%)	55,113,113	2.06	13 (23%)
33	HEM	V	202	16	27,50,50	2.07	5 (18%)	17,82,82	1.83	6 (35%)
23	CLA	a	607	-	56,73,73	3.83	21 (37%)	55,113,113	2.03	14 (25%)
25	BCR	c	516	-	41,41,41	9.34	30 (73%)	56,56,56	5.82	27 (48%)
28	LMG	b	623	-	51,51,55	1.29	4 (7%)	59,59,63	0.94	2 (3%)
23	CLA	b	616	-	56,73,73	3.85	21 (37%)	55,113,113	2.07	14 (25%)
23	CLA	B	604	-	56,73,73	3.81	21 (37%)	55,113,113	2.08	14 (25%)
23	CLA	A	606	-	56,73,73	3.83	21 (37%)	55,113,113	2.08	13 (23%)
23	CLA	C	505	-	56,73,73	3.89	21 (37%)	55,113,113	2.08	12 (21%)
23	CLA	C	507	-	56,73,73	3.77	20 (35%)	55,113,113	2.19	14 (25%)
31	LHG	l	101	-	48,48,48	1.12	2 (4%)	51,54,54	0.89	2 (3%)
27	SQD	b	601	-	53,54,54	1.05	3 (5%)	62,65,65	1.22	6 (9%)
23	CLA	c	514	-	56,73,73	3.79	21 (37%)	55,113,113	2.05	11 (20%)
20	OEX	a	601	1,3	0,15,15	-	-	-	-	-
23	CLA	b	613	-	56,73,73	3.91	21 (37%)	55,113,113	2.07	11 (20%)
25	BCR	C	521	-	41,41,41	9.29	30 (73%)	56,56,56	5.89	26 (46%)
25	BCR	c	522	-	41,41,41	9.22	30 (73%)	56,56,56	5.86	28 (50%)
23	CLA	C	504	-	56,73,73	3.83	21 (37%)	55,113,113	2.09	13 (23%)
25	BCR	a	608	-	41,41,41	9.29	30 (73%)	56,56,56	5.68	26 (46%)
24	PHO	D	401	-	67,69,69	1.27	7 (10%)	85,99,99	1.06	4 (4%)
25	BCR	B	619	-	41,41,41	9.63	30 (73%)	56,56,56	5.36	29 (51%)
31	LHG	B	622	-	48,48,48	1.14	3 (6%)	51,54,54	0.96	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	c	510	-	56,73,73	3.84	21 (37%)	55,113,113	2.10	14 (25%)
23	CLA	D	403	-	56,73,73	3.85	21 (37%)	55,113,113	1.99	13 (23%)
23	CLA	b	611	-	56,73,73	3.87	21 (37%)	55,113,113	2.17	16 (29%)
28	LMG	j	101	34	51,51,55	1.30	4 (7%)	59,59,63	0.92	4 (6%)
23	CLA	b	619	-	56,73,73	3.85	21 (37%)	55,113,113	2.04	12 (21%)
31	LHG	d	406	-	48,48,48	1.11	3 (6%)	51,54,54	0.90	3 (5%)
23	CLA	B	615	-	56,73,73	3.83	21 (37%)	55,113,113	2.06	14 (25%)
23	CLA	b	609[B]	-	56,73,73	3.84	21 (37%)	55,113,113	2.14	15 (27%)
31	LHG	b	624	-	48,48,48	1.10	3 (6%)	51,54,54	0.96	3 (5%)
32	DGD	H	102	-	63,63,67	1.70	15 (23%)	77,77,81	0.92	3 (3%)
28	LMG	A	612	-	51,51,55	1.30	4 (7%)	59,59,63	0.97	3 (5%)
33	HEM	e	102	6,5	27,50,50	2.07	6 (22%)	17,82,82	1.81	4 (23%)
26	PL9	a	609	-	55,55,55	4.23	21 (38%)	68,69,69	3.79	35 (51%)
23	CLA	c	509	-	56,73,73	3.84	21 (37%)	55,113,113	2.19	12 (21%)
32	DGD	d	405	-	63,63,67	1.71	15 (23%)	77,77,81	1.03	6 (7%)
25	BCR	b	622	-	41,41,41	9.32	31 (75%)	56,56,56	5.84	32 (57%)
23	CLA	D	402	-	56,73,73	3.83	21 (37%)	55,113,113	2.08	14 (25%)
33	HEM	v	201	16	27,50,50	2.13	5 (18%)	17,82,82	1.83	4 (23%)
32	DGD	h	102	-	63,63,67	1.69	15 (23%)	77,77,81	0.97	4 (5%)
32	DGD	D	406	-	63,63,67	1.73	14 (22%)	77,77,81	1.13	7 (9%)
23	CLA	B	607[A]	-	56,73,73	3.81	21 (37%)	55,113,113	2.16	15 (27%)
23	CLA	c	502	-	56,73,73	3.81	21 (37%)	55,113,113	2.12	13 (23%)
23	CLA	C	509	-	56,73,73	3.80	20 (35%)	55,113,113	2.08	14 (25%)
28	LMG	c	521	-	51,51,55	1.31	4 (7%)	59,59,63	1.01	3 (5%)
27	SQD	a	610	-	53,54,54	0.99	3 (5%)	62,65,65	1.53	11 (17%)
23	CLA	B	616	-	56,73,73	3.84	21 (37%)	55,113,113	2.01	13 (23%)
23	CLA	B	610	-	56,73,73	3.84	21 (37%)	55,113,113	2.08	12 (21%)
23	CLA	c	511	-	56,73,73	3.86	21 (37%)	55,113,113	1.96	12 (21%)
31	LHG	D	408	-	48,48,48	1.11	3 (6%)	51,54,54	0.97	3 (5%)
31	LHG	L	101	-	48,48,48	1.10	3 (6%)	51,54,54	0.87	2 (3%)
28	LMG	J	101	34	51,51,55	1.31	4 (7%)	59,59,63	0.99	4 (6%)
23	CLA	B	617	-	56,73,73	3.86	21 (37%)	55,113,113	2.03	11 (20%)
25	BCR	b	620	-	41,41,41	9.09	30 (73%)	56,56,56	5.87	29 (51%)
20	OEX	A	601	1,3	0,15,15	-	-	-	-	-
23	CLA	c	508	-	56,73,73	3.80	20 (35%)	55,113,113	2.21	14 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	C	501	-	56,73,73	3.79	21 (37%)	55,113,113	2.16	15 (27%)
23	CLA	B	608	-	56,73,73	3.84	21 (37%)	55,113,113	2.07	15 (27%)
23	CLA	c	507	-	56,73,73	3.85	21 (37%)	55,113,113	2.15	15 (27%)
27	SQD	x	101	-	42,43,54	1.21	3 (7%)	51,54,65	1.46	7 (13%)
23	CLA	b	612	-	56,73,73	3.81	21 (37%)	55,113,113	2.04	13 (23%)
23	CLA	C	511	3	56,73,73	3.85	21 (37%)	55,113,113	2.05	12 (21%)
25	BCR	K	101	-	41,41,41	9.19	30 (73%)	56,56,56	5.89	26 (46%)
27	SQD	B	623	-	53,54,54	1.07	4 (7%)	62,65,65	1.44	9 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	C	508	-	1/1/15/20	5/37/115/115	-
23	CLA	b	604	-	1/1/15/20	19/37/115/115	-
23	CLA	B	606	-	1/1/15/20	6/37/115/115	-
23	CLA	b	615	-	1/1/15/20	5/37/115/115	-
25	BCR	F	101	-	-	23/29/63/63	0/2/2/2
23	CLA	b	610	-	1/1/15/20	3/37/115/115	-
23	CLA	C	510	-	1/1/15/20	10/37/115/115	-
32	DGD	c	519	-	-	18/51/91/95	0/2/2/2
28	LMG	Z	101	-	-	15/31/51/70	0/1/1/1
24	PHO	d	401	-	-	1/53/103/103	0/5/6/6
27	SQD	X	101	-	-	16/38/58/69	0/1/1/1
27	SQD	a	612	-	-	23/49/69/69	0/1/1/1
27	SQD	A	611	-	-	16/49/69/69	0/1/1/1
23	CLA	B	605	-	1/1/15/20	8/37/115/115	-
25	BCR	c	515	-	-	25/29/63/63	0/2/2/2
23	CLA	c	512	3	1/1/15/20	5/37/115/115	-
31	LHG	a	614	-	-	16/53/53/53	-
23	CLA	C	503	-	1/1/15/20	3/37/115/115	-
33	HEM	E	102	6,5	-	0/6/54/54	-
25	BCR	k	101	-	-	19/29/63/63	0/2/2/2
23	CLA	a	613	-	1/1/15/20	5/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	b	606	-	1/1/15/20	7/37/115/115	-
25	BCR	C	514	-	-	23/29/63/63	0/2/2/2
23	CLA	d	402	-	1/1/15/20	2/37/115/115	-
32	DGD	C	517	-	-	29/51/91/95	0/2/2/2
28	LMG	B	621	-	-	22/46/66/70	0/1/1/1
23	CLA	B	609	-	1/1/15/20	4/37/115/115	-
23	CLA	B	603	-	1/1/15/20	3/37/115/115	-
32	DGD	c	518	-	-	30/51/91/95	0/2/2/2
25	BCR	A	609	-	-	21/29/63/63	0/2/2/2
28	LMG	c	520	-	-	22/46/66/70	0/1/1/1
23	CLA	c	506	-	1/1/15/20	7/37/115/115	-
25	BCR	f	101	-	-	24/29/63/63	0/2/2/2
24	PHO	A	607	-	-	4/53/103/103	0/5/6/6
23	CLA	C	513	-	1/1/15/20	11/37/115/115	-
23	CLA	b	614	-	1/1/15/20	5/37/115/115	-
32	DGD	C	518	-	-	16/51/91/95	0/2/2/2
23	CLA	C	506	-	1/1/15/20	16/37/115/115	-
32	DGD	c	517	-	-	25/51/91/95	0/2/2/2
23	CLA	B	602	-	1/1/15/20	17/37/115/115	-
23	CLA	B	613	-	1/1/15/20	5/37/115/115	-
25	BCR	b	621	-	-	21/29/63/63	0/2/2/2
26	PL9	d	404	-	-	27/53/73/73	0/1/1/1
25	BCR	B	618	-	-	24/29/63/63	0/2/2/2
23	CLA	c	513	-	1/1/15/20	7/37/115/115	-
25	BCR	H	101	-	-	23/29/63/63	0/2/2/2
31	LHG	e	101	-	-	23/46/46/53	-
24	PHO	a	606	-	-	3/53/103/103	0/5/6/6
23	CLA	c	505	-	1/1/15/20	11/37/115/115	-
25	BCR	C	515	-	-	21/29/63/63	0/2/2/2
23	CLA	b	618	-	1/1/15/20	11/37/115/115	-
23	CLA	a	605	-	1/1/15/20	8/37/115/115	-
23	CLA	C	512	-	1/1/15/20	9/37/115/115	-
23	CLA	c	504	-	1/1/15/20	3/37/115/115	-
23	CLA	B	612	-	1/1/15/20	5/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LHG	E	101	-	-	24/46/46/53	-
23	CLA	b	608	-	1/1/15/20	6/37/115/115	-
23	CLA	A	605	-	1/1/15/20	0/37/115/115	-
23	CLA	B	607[B]	-	1/1/15/20	10/37/115/115	-
23	CLA	c	503	-	1/1/15/20	8/37/115/115	-
28	LMG	z	101	-	-	18/31/51/70	0/1/1/1
28	LMG	a	611	-	-	31/46/66/70	0/1/1/1
32	DGD	C	516	-	-	25/51/91/95	0/2/2/2
31	LHG	D	407	-	-	14/53/53/53	-
25	BCR	t	101	-	-	23/29/63/63	0/2/2/2
23	CLA	a	604	-	1/1/15/20	1/37/115/115	-
27	SQD	b	602	-	-	29/49/69/69	0/1/1/1
23	CLA	D	404	-	1/1/15/20	14/37/115/115	-
25	BCR	B	620	-	-	17/29/63/63	0/2/2/2
23	CLA	b	609[A]	-	1/1/15/20	8/37/115/115	-
23	CLA	C	502	-	1/1/15/20	8/37/115/115	-
28	LMG	C	520	-	-	19/46/66/70	0/1/1/1
23	CLA	b	607	-	1/1/15/20	9/37/115/115	-
28	LMG	C	519	-	-	21/46/66/70	0/1/1/1
23	CLA	B	614	-	1/1/15/20	5/37/115/115	-
26	PL9	A	610	-	-	25/53/73/73	0/1/1/1
23	CLA	B	611	-	1/1/15/20	9/37/115/115	-
23	CLA	b	605	-	1/1/15/20	5/37/115/115	-
26	PL9	D	405	-	-	25/53/73/73	0/1/1/1
25	BCR	T	101	-	-	24/29/63/63	0/2/2/2
25	BCR	h	101	-	-	25/29/63/63	0/2/2/2
23	CLA	d	403	-	1/1/15/20	13/37/115/115	-
23	CLA	A	608	-	1/1/15/20	13/37/115/115	-
23	CLA	b	617	-	1/1/15/20	13/37/115/115	-
33	HEM	V	202	16	-	0/6/54/54	-
23	CLA	a	607	-	1/1/15/20	14/37/115/115	-
25	BCR	c	516	-	-	21/29/63/63	0/2/2/2
28	LMG	b	623	-	-	21/46/66/70	0/1/1/1
23	CLA	b	616	-	1/1/15/20	4/37/115/115	-
23	CLA	B	604	-	1/1/15/20	8/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	A	606	-	1/1/15/20	9/37/115/115	-
23	CLA	C	505	-	1/1/15/20	7/37/115/115	-
23	CLA	C	507	-	1/1/15/20	8/37/115/115	-
31	LHG	l	101	-	-	22/53/53/53	-
27	SQD	b	601	-	-	23/49/69/69	0/1/1/1
23	CLA	c	514	-	1/1/15/20	11/37/115/115	-
23	CLA	b	613	-	1/1/15/20	8/37/115/115	-
25	BCR	C	521	-	-	17/29/63/63	0/2/2/2
25	BCR	c	522	-	-	20/29/63/63	0/2/2/2
23	CLA	C	504	-	1/1/15/20	8/37/115/115	-
25	BCR	a	608	-	-	19/29/63/63	0/2/2/2
24	PHO	D	401	-	-	2/53/103/103	0/5/6/6
25	BCR	B	619	-	-	24/29/63/63	0/2/2/2
31	LHG	B	622	-	-	13/53/53/53	-
23	CLA	c	510	-	1/1/15/20	8/37/115/115	-
23	CLA	D	403	-	1/1/15/20	2/37/115/115	-
23	CLA	b	611	-	1/1/15/20	3/37/115/115	-
28	LMG	j	101	34	-	18/46/66/70	0/1/1/1
23	CLA	b	619	-	1/1/15/20	14/37/115/115	-
31	LHG	d	406	-	-	14/53/53/53	-
23	CLA	B	615	-	1/1/15/20	14/37/115/115	-
23	CLA	b	609[B]	-	1/1/15/20	10/37/115/115	-
31	LHG	b	624	-	-	13/53/53/53	-
32	DGD	H	102	-	-	23/51/91/95	0/2/2/2
28	LMG	A	612	-	-	31/46/66/70	0/1/1/1
33	HEM	e	102	6,5	-	0/6/54/54	-
26	PL9	a	609	-	-	26/53/73/73	0/1/1/1
23	CLA	c	509	-	1/1/15/20	5/37/115/115	-
32	DGD	d	405	-	-	33/51/91/95	0/2/2/2
25	BCR	b	622	-	-	21/29/63/63	0/2/2/2
23	CLA	D	402	-	1/1/15/20	3/37/115/115	-
33	HEM	v	201	16	-	2/6/54/54	-
32	DGD	h	102	-	-	19/51/91/95	0/2/2/2
32	DGD	D	406	-	-	34/51/91/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	B	607[A]	-	1/1/15/20	9/37/115/115	-
23	CLA	c	502	-	1/1/15/20	11/37/115/115	-
23	CLA	C	509	-	1/1/15/20	7/37/115/115	-
28	LMG	c	521	-	-	19/46/66/70	0/1/1/1
27	SQD	a	610	-	-	16/49/69/69	0/1/1/1
23	CLA	B	616	-	1/1/15/20	11/37/115/115	-
23	CLA	B	610	-	1/1/15/20	6/37/115/115	-
23	CLA	c	511	-	1/1/15/20	11/37/115/115	-
31	LHG	D	408	-	-	17/53/53/53	-
31	LHG	L	101	-	-	18/53/53/53	-
28	LMG	J	101	34	-	19/46/66/70	0/1/1/1
23	CLA	B	617	-	1/1/15/20	14/37/115/115	-
25	BCR	b	620	-	-	18/29/63/63	0/2/2/2
23	CLA	c	508	-	1/1/15/20	9/37/115/115	-
23	CLA	C	501	-	1/1/15/20	11/37/115/115	-
23	CLA	B	608	-	1/1/15/20	3/37/115/115	-
23	CLA	c	507	-	1/1/15/20	14/37/115/115	-
27	SQD	x	101	-	-	16/38/58/69	0/1/1/1
23	CLA	b	612	-	1/1/15/20	6/37/115/115	-
23	CLA	C	511	3	1/1/15/20	6/37/115/115	-
25	BCR	K	101	-	-	21/29/63/63	0/2/2/2
27	SQD	B	623	-	-	29/49/69/69	0/1/1/1

The worst 5 of 2565 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	609	BCR	C14-C13	27.78	1.72	1.35
25	a	608	BCR	C14-C13	27.64	1.72	1.35
25	C	521	BCR	C14-C13	27.51	1.72	1.35
25	t	101	BCR	C14-C13	27.47	1.72	1.35
25	C	515	BCR	C14-C13	27.41	1.72	1.35

The worst 5 of 1959 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	621	BCR	C15-C16-C17	26.27	177.29	123.47
25	c	515	BCR	C15-C16-C17	25.42	175.54	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	T	101	BCR	C15-C16-C17	25.32	175.34	123.47
25	A	609	BCR	C15-C16-C17	25.24	175.18	123.47
25	a	608	BCR	C15-C16-C17	25.24	175.17	123.47

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

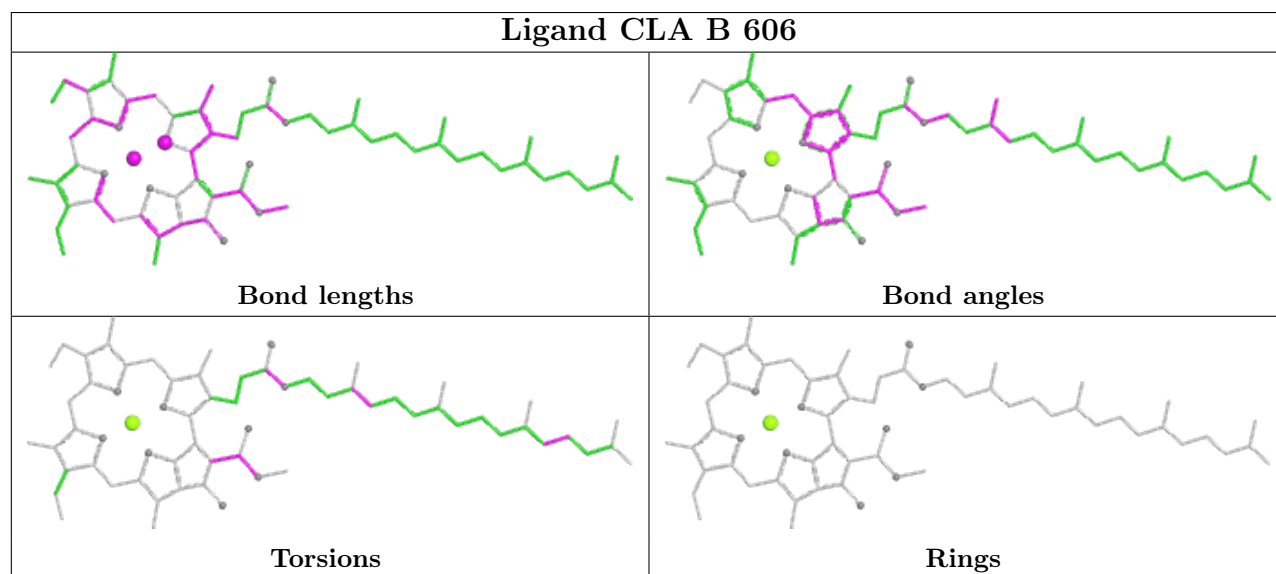
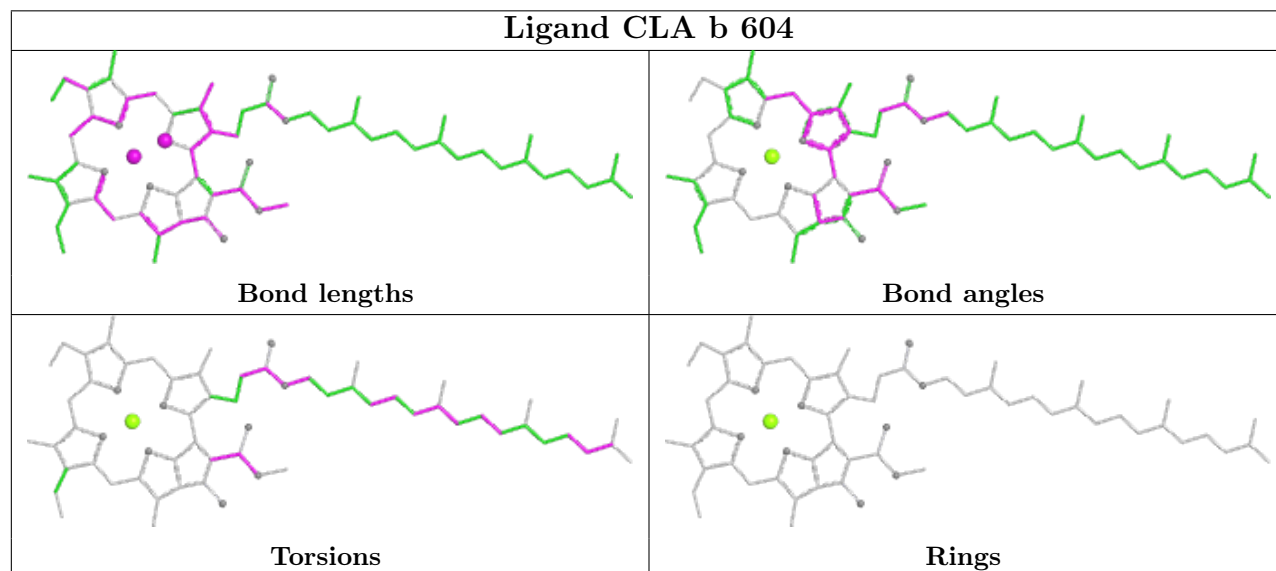
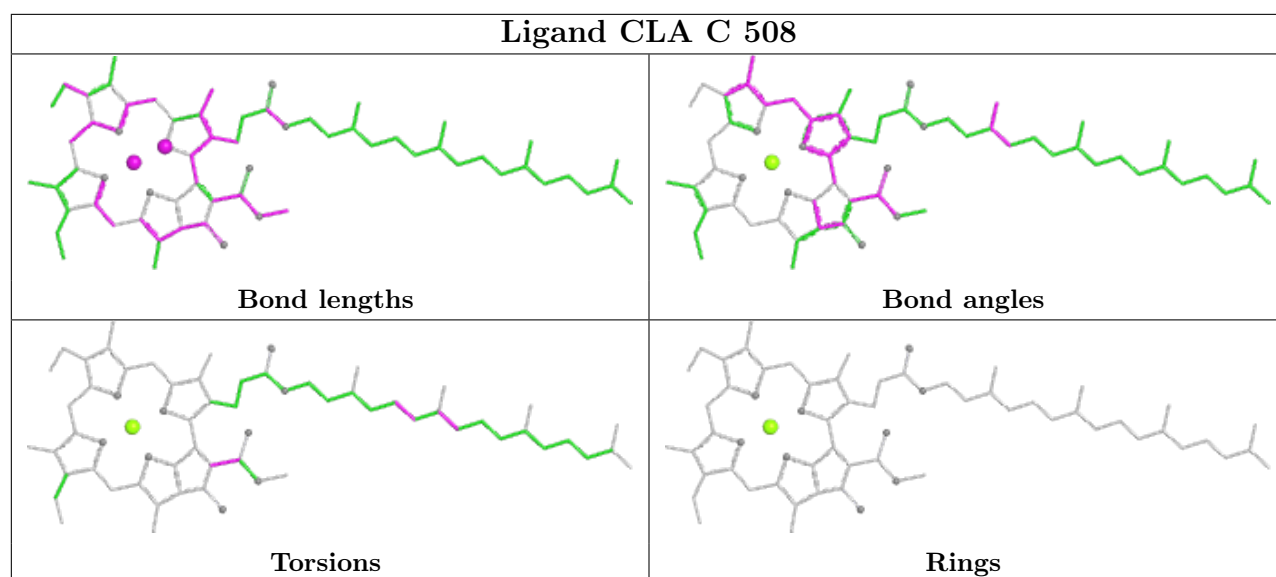
5 of 2015 torsion outliers are listed below:

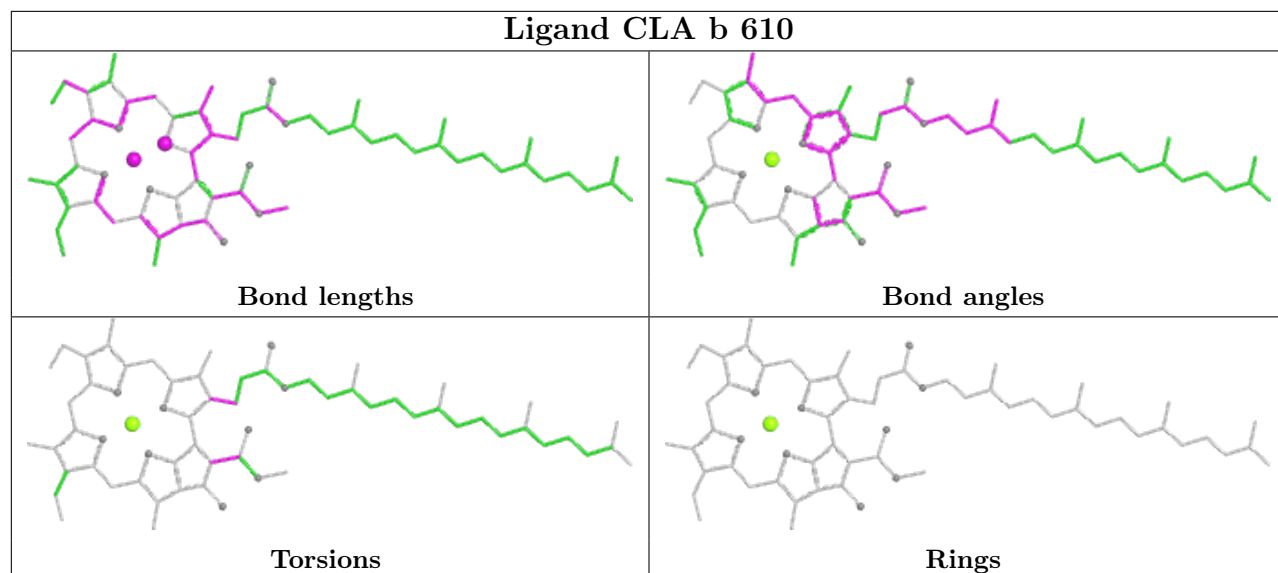
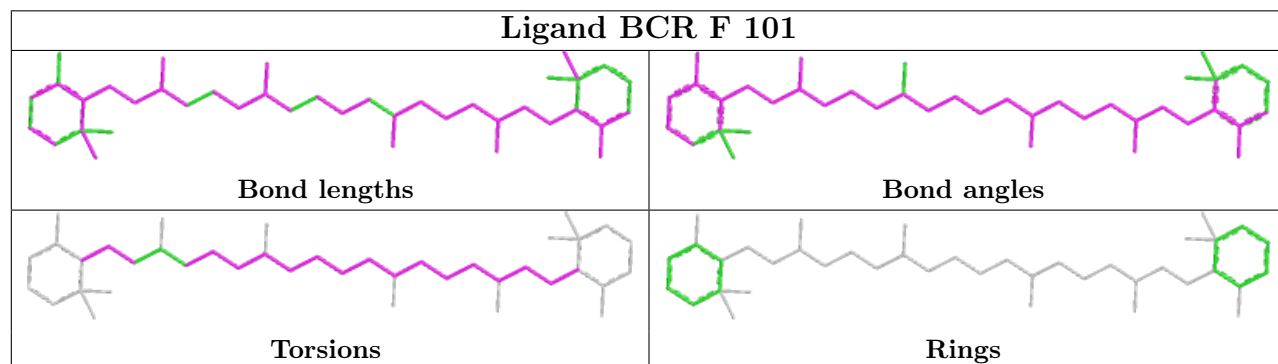
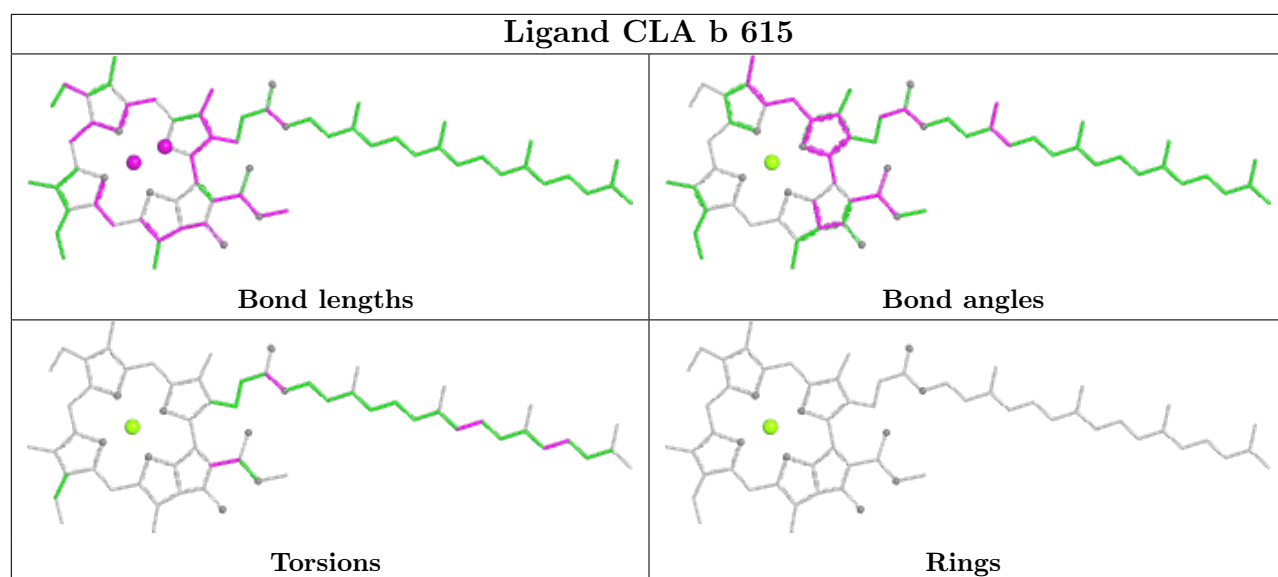
Mol	Chain	Res	Type	Atoms
23	A	606	CLA	CHA-CBD-CGD-O1D
23	A	606	CLA	CHA-CBD-CGD-O2D
23	B	602	CLA	CHA-CBD-CGD-O1D
23	B	602	CLA	CHA-CBD-CGD-O2D
23	B	603	CLA	CHA-CBD-CGD-O1D

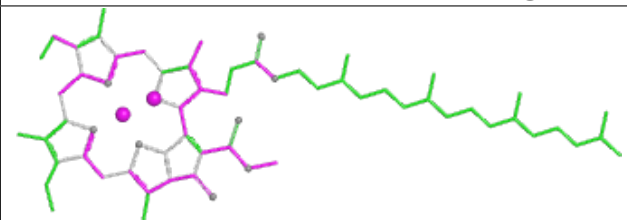
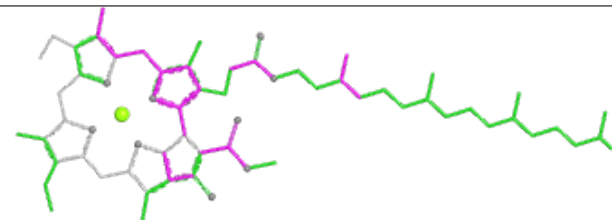
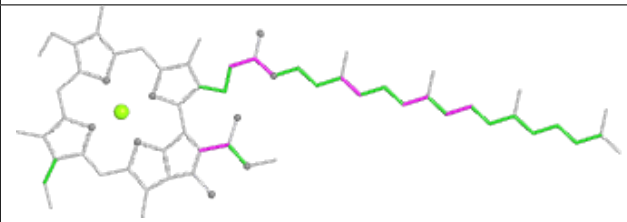
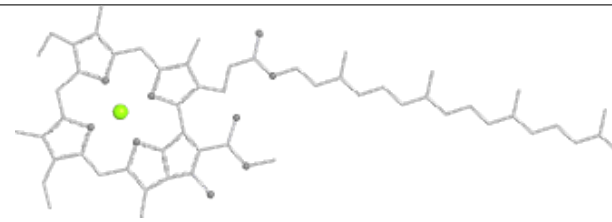
There are no ring outliers.

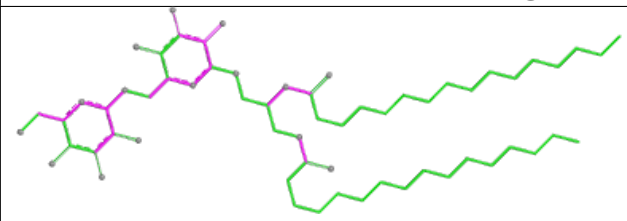
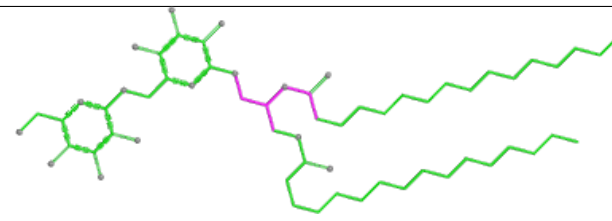
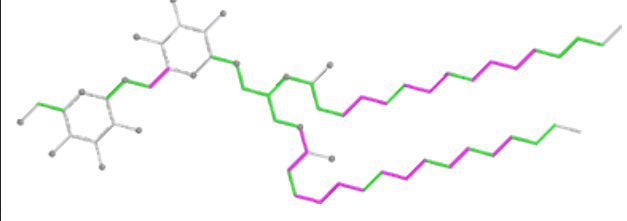
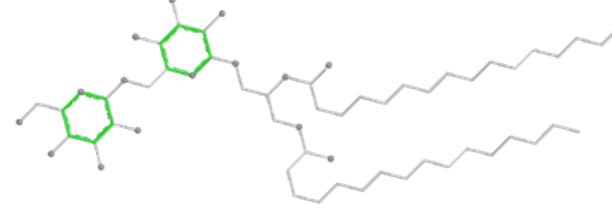
No monomer is involved in short contacts.

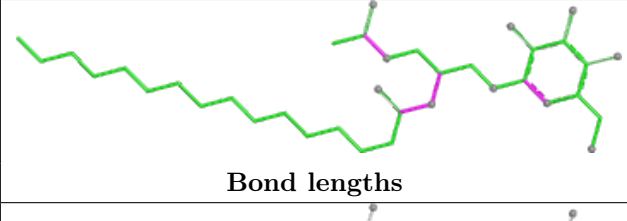
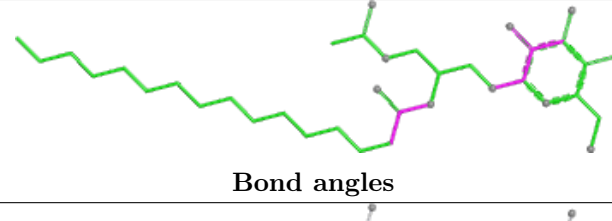
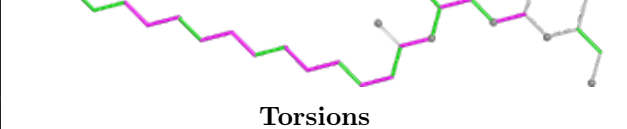

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

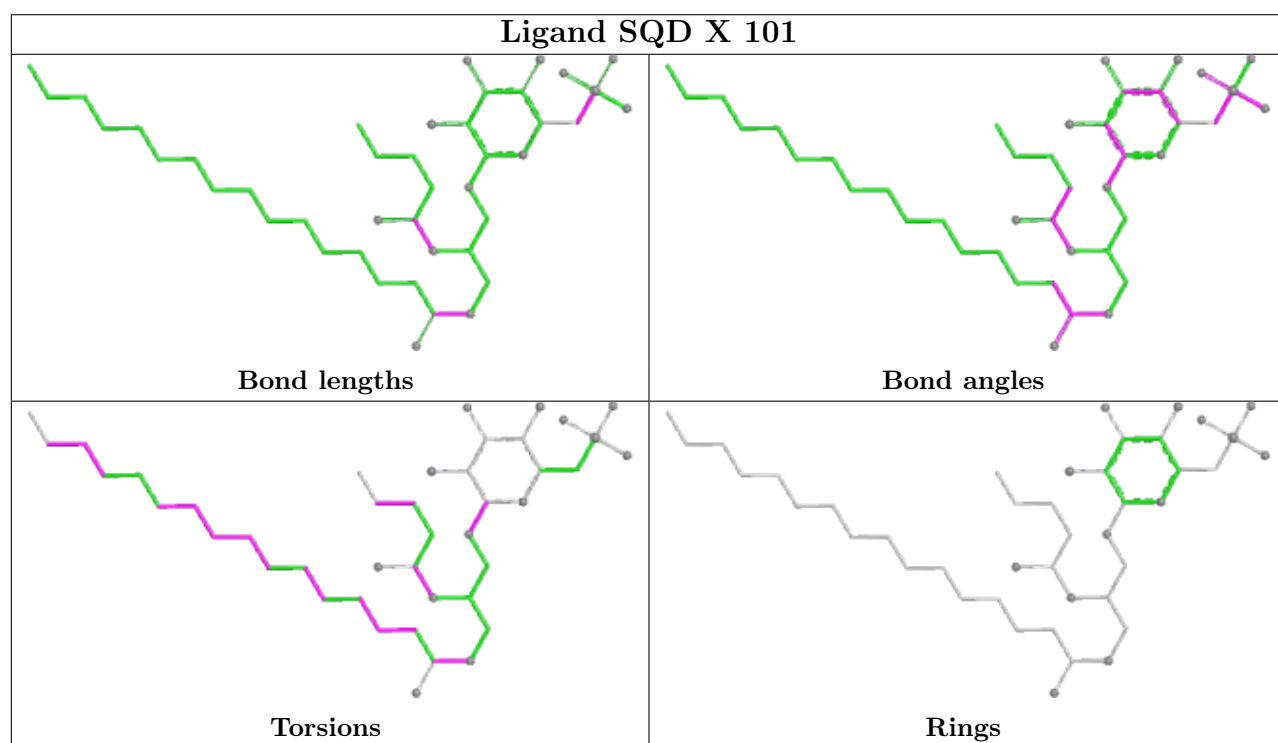
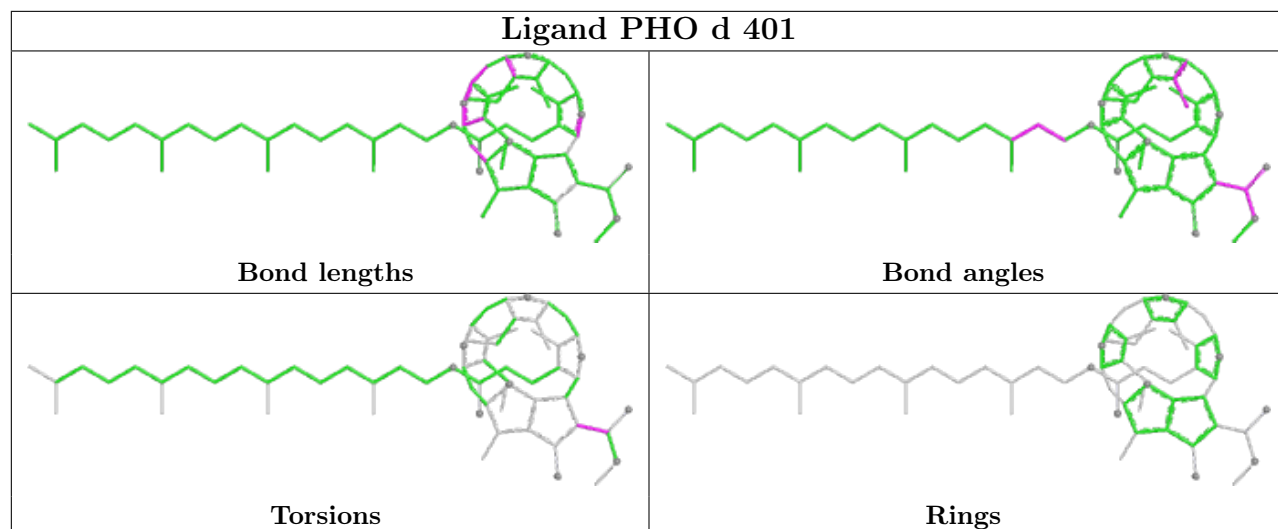


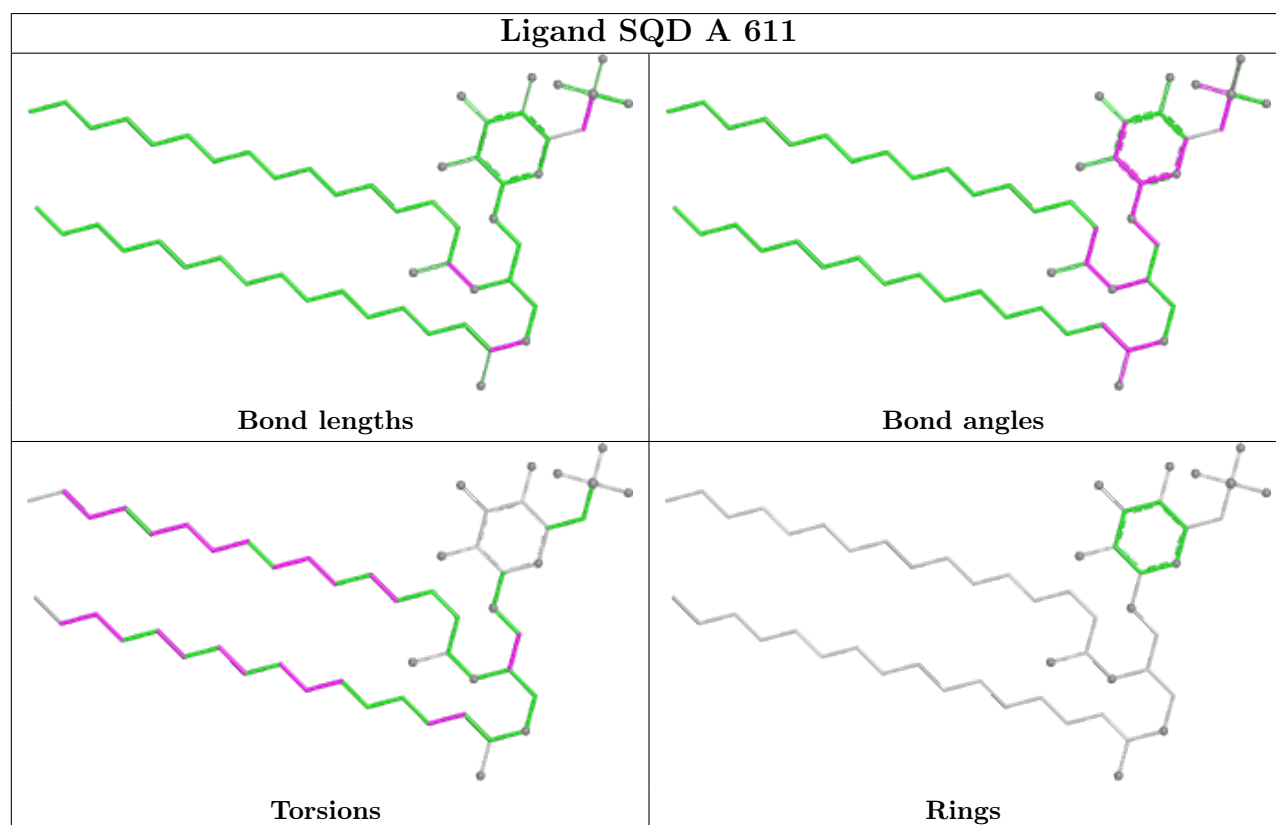
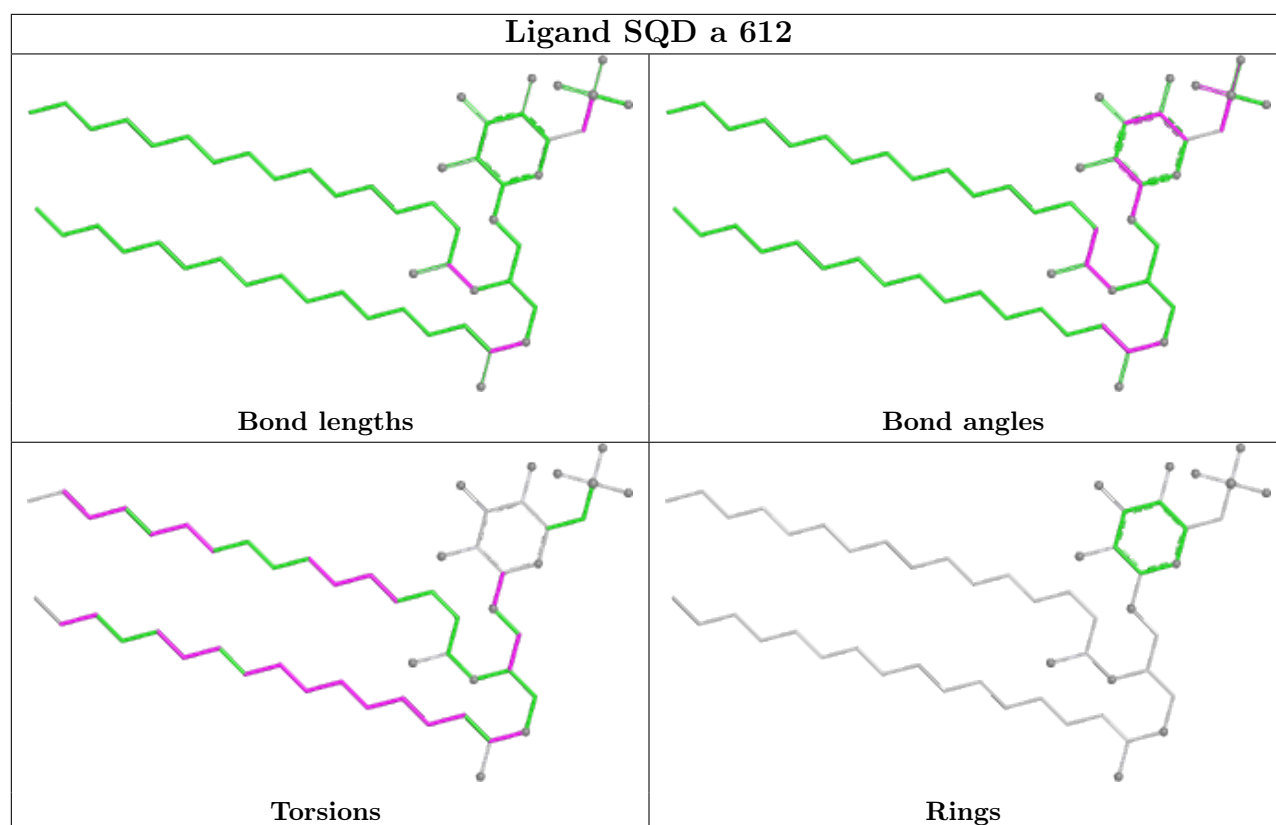


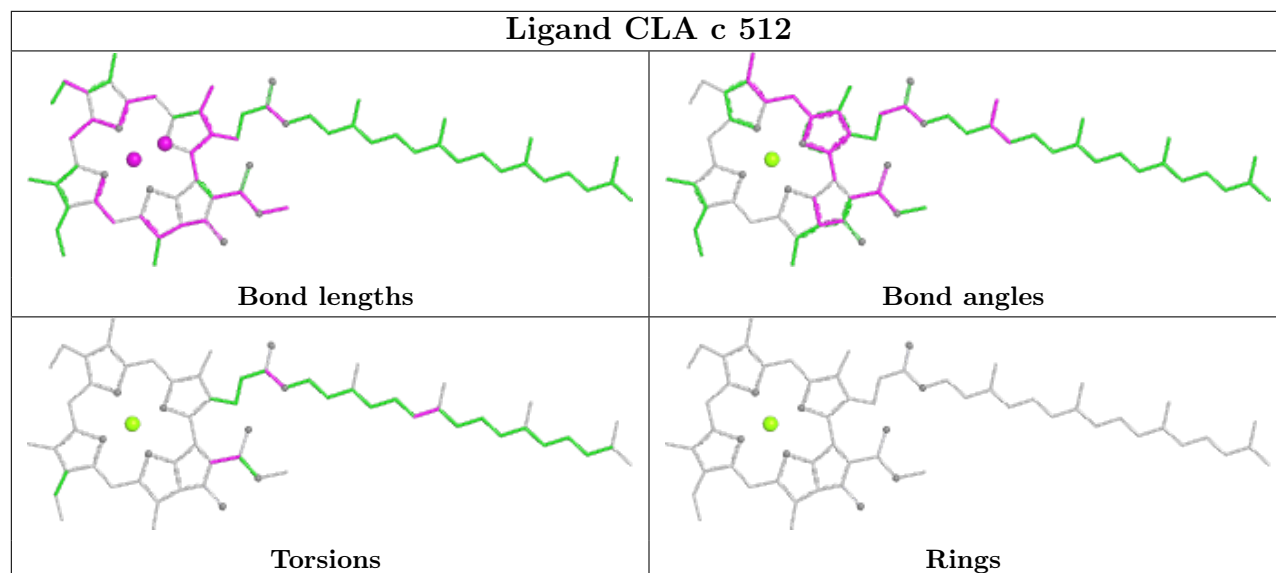
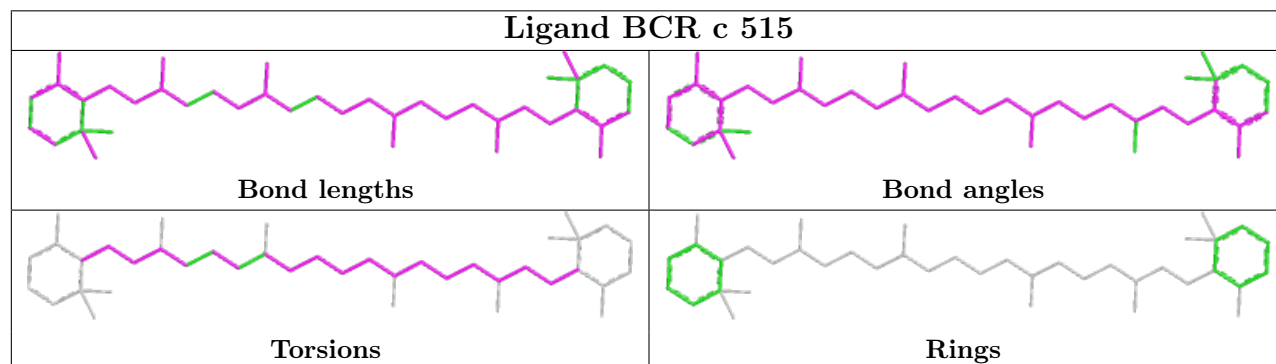
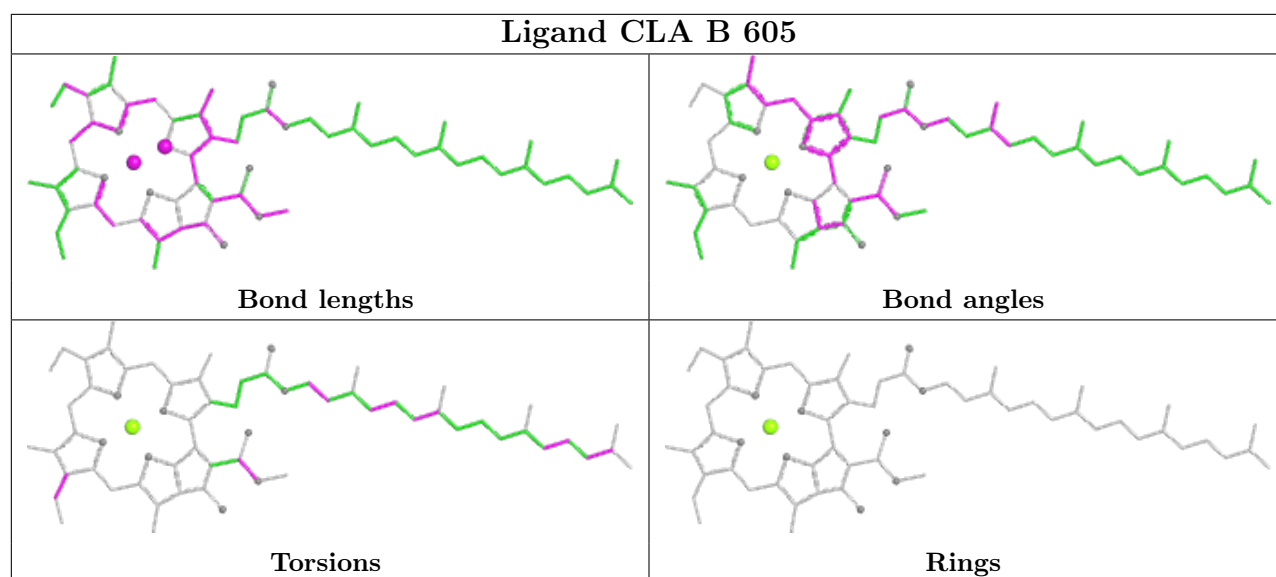
Ligand CLA C 510	
	
Bond lengths	Bond angles
	
Torsions	Rings

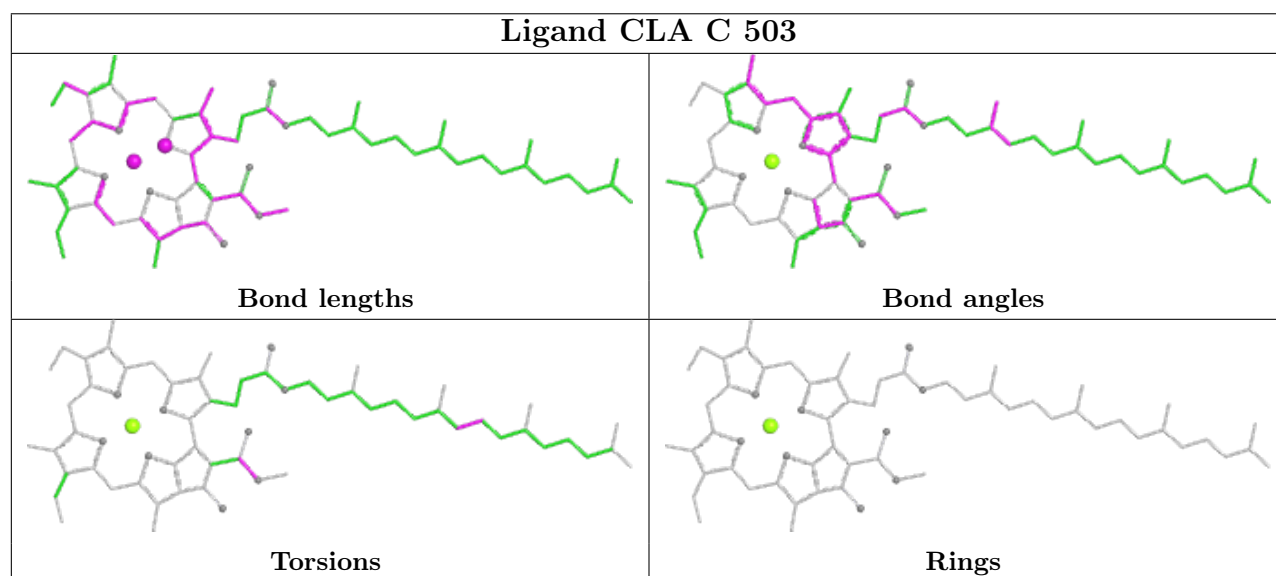
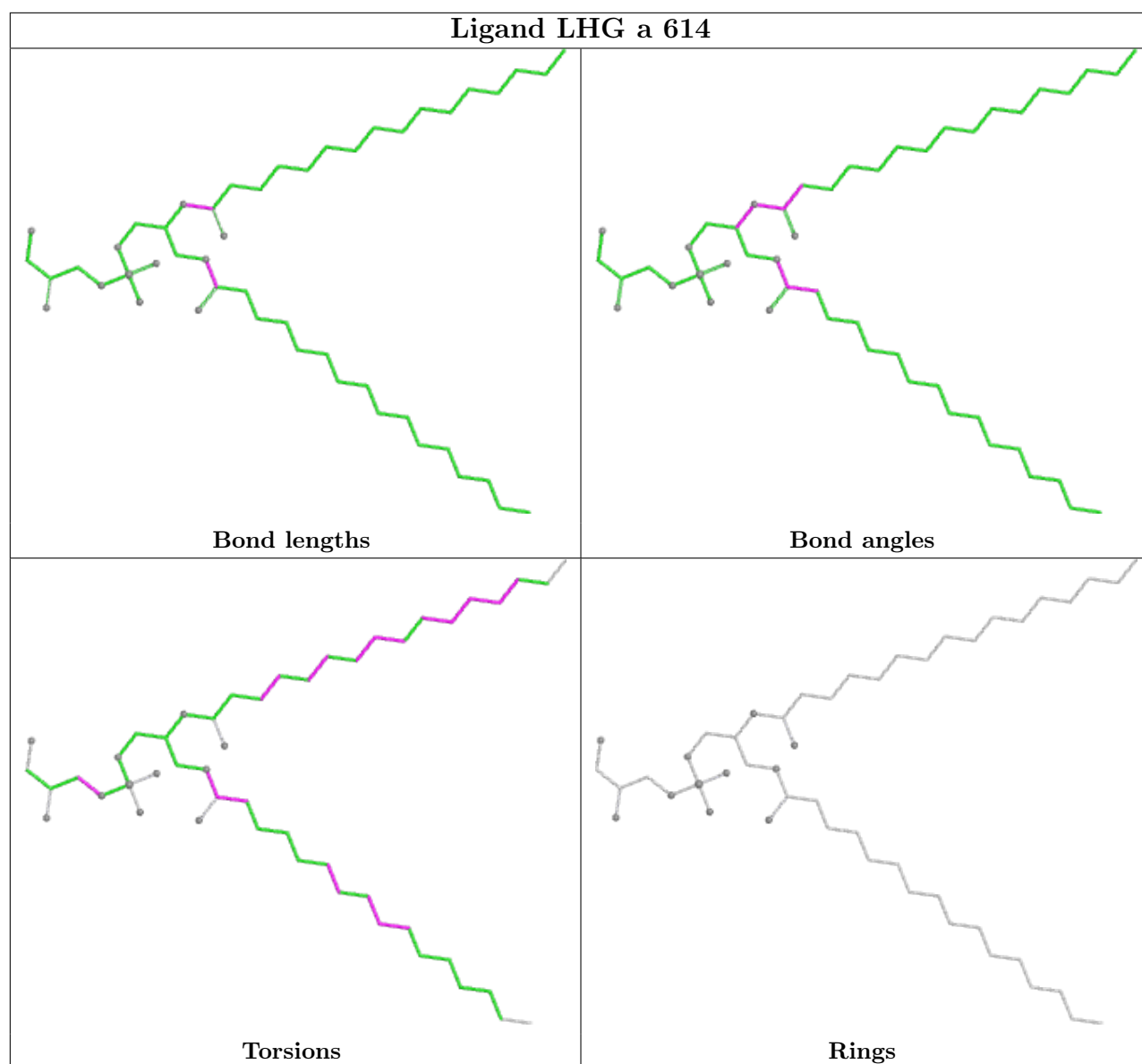
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Bond lengths	Bond angles
	
Torsions	Rings

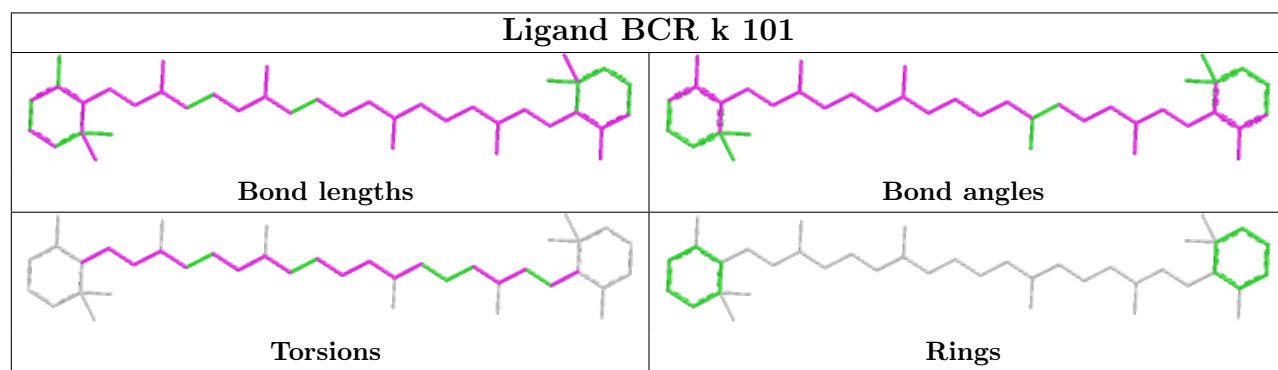
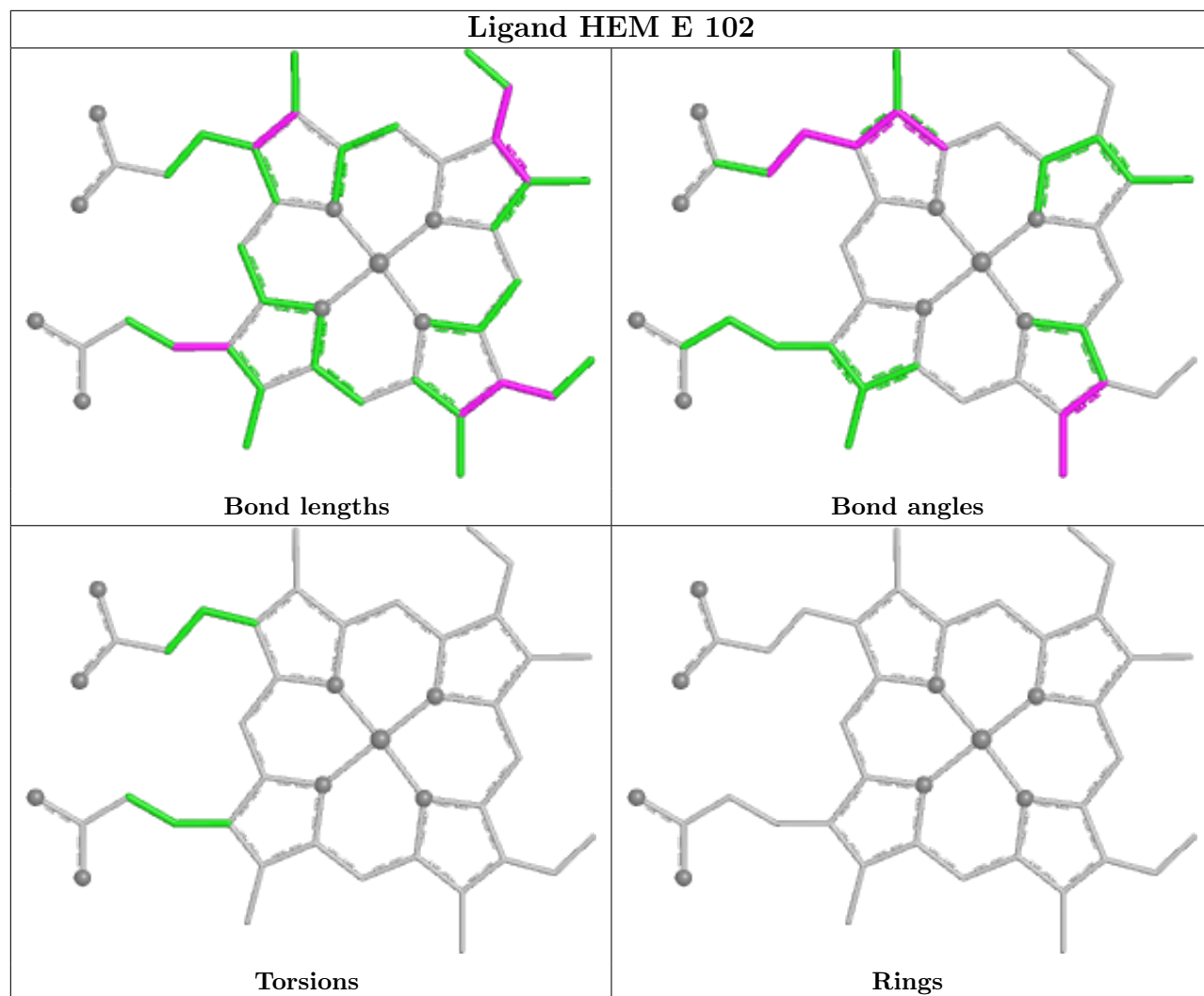
Ligand LMG Z 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

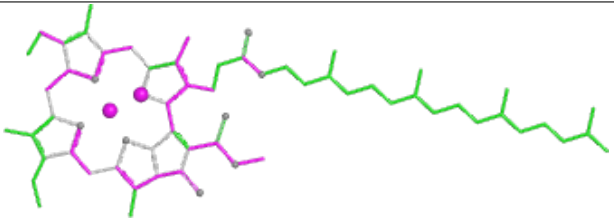
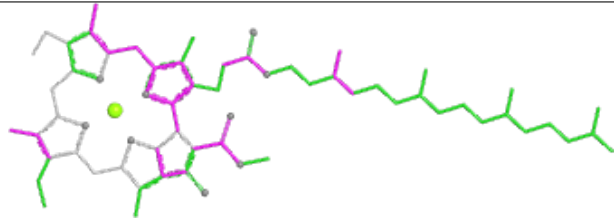
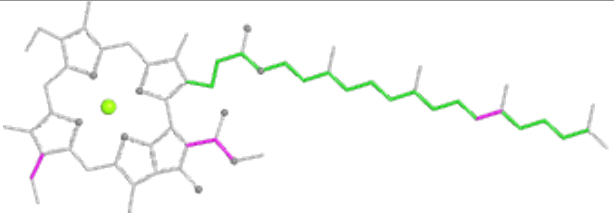
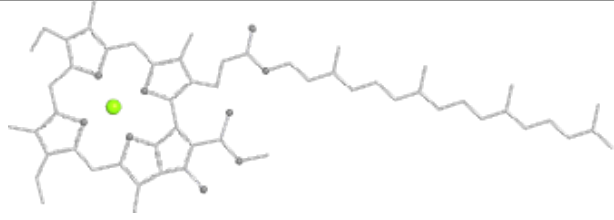


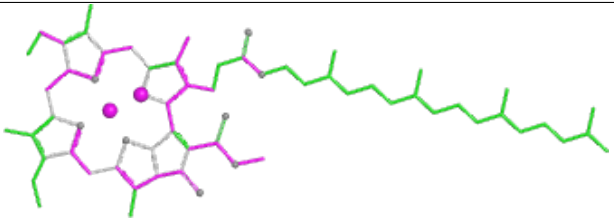
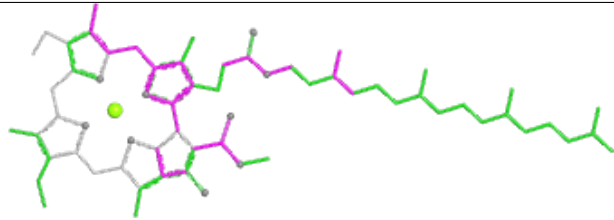
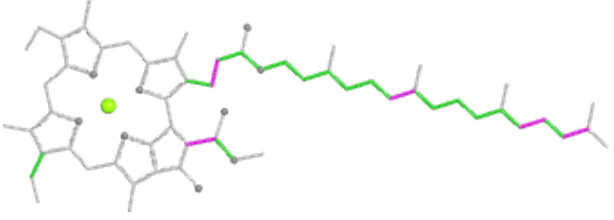
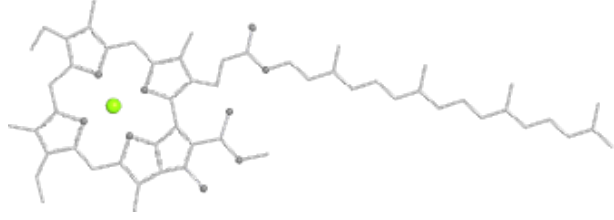


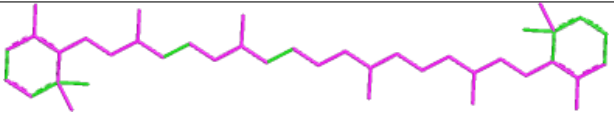
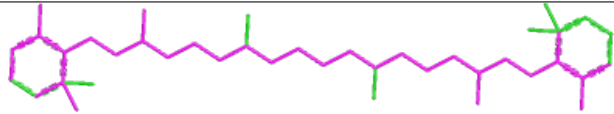
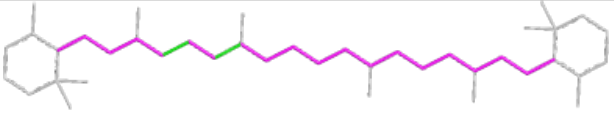





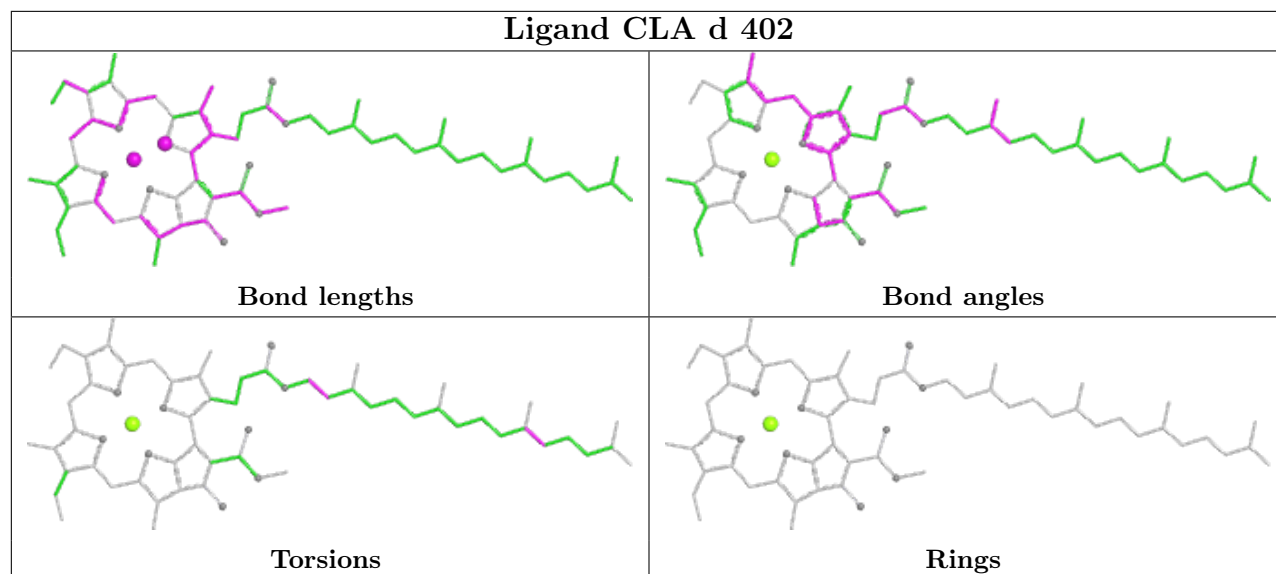


Ligand CLA a 613	
	
Bond lengths	Bond angles
	
Torsions	Rings

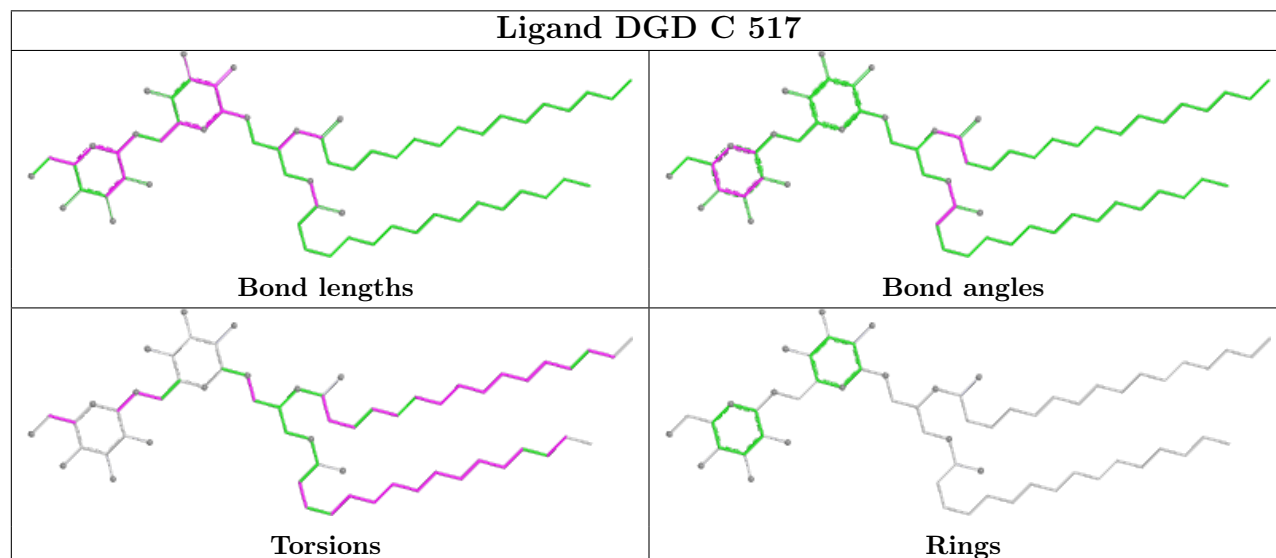
Ligand CLA b 606	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR C 514	
	
Bond lengths	Bond angles
	
Torsions	Rings

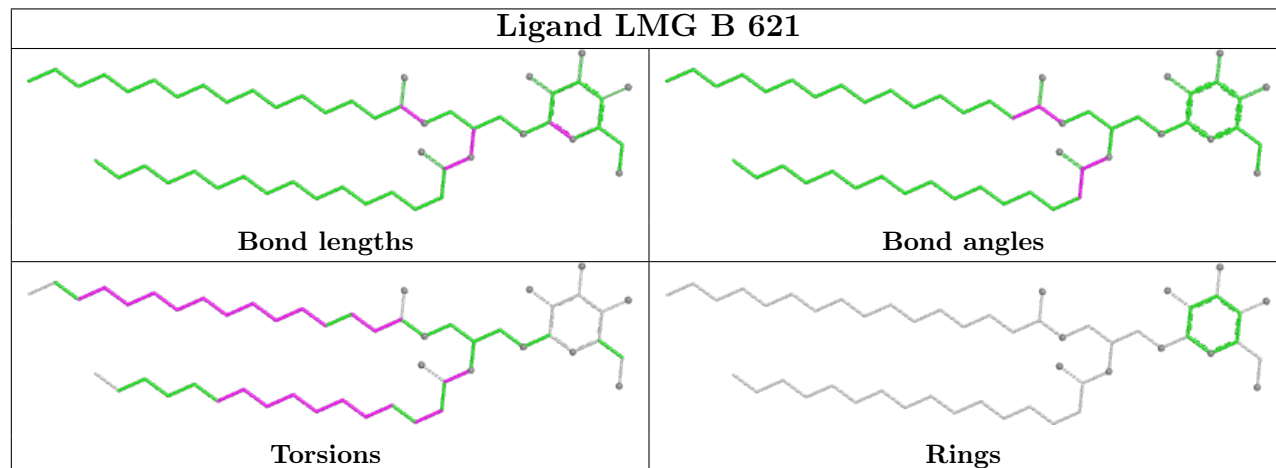
Ligand CLA d 402

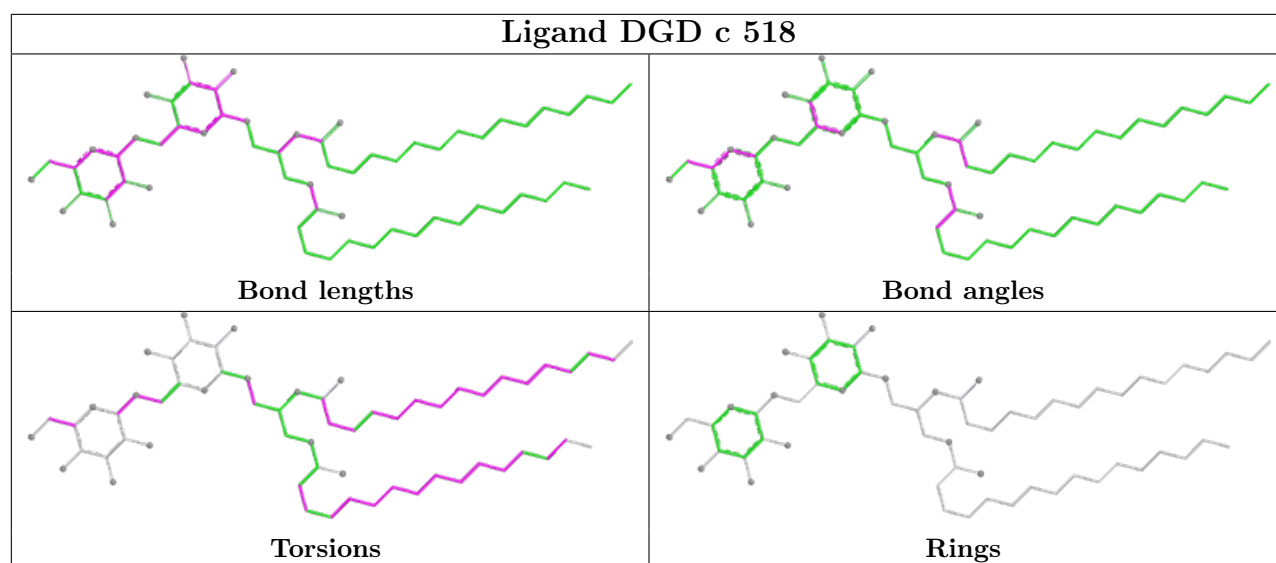
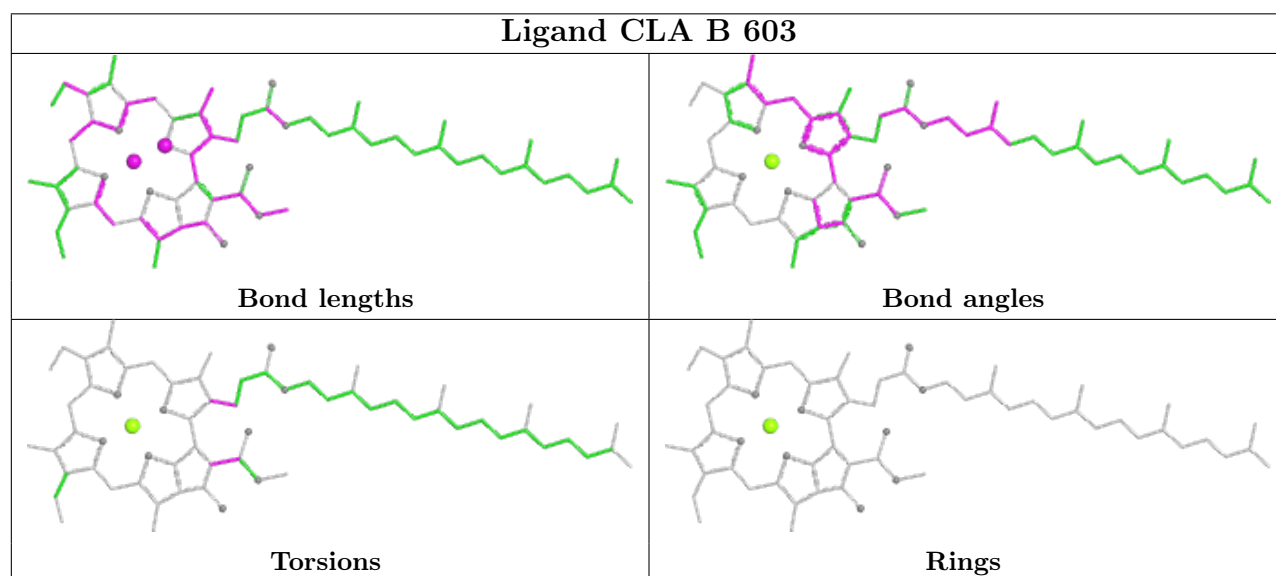
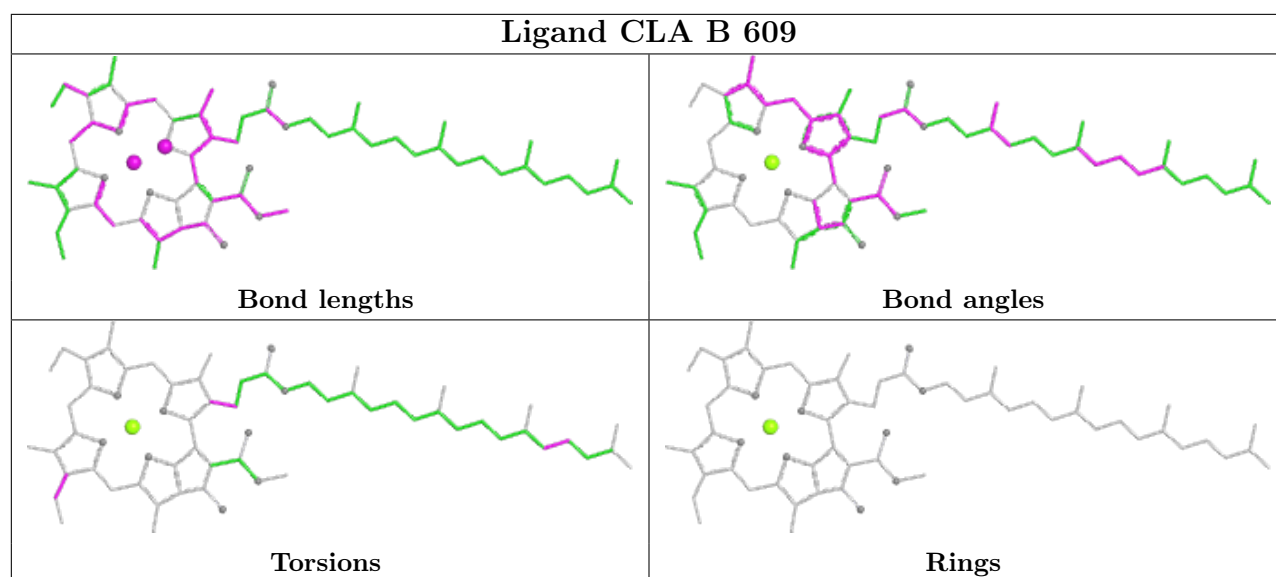


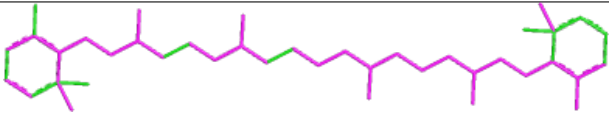
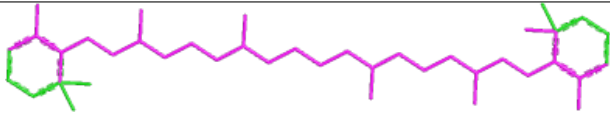
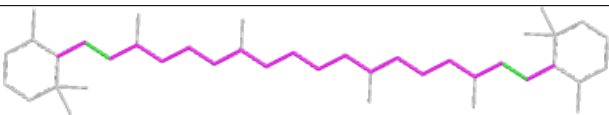
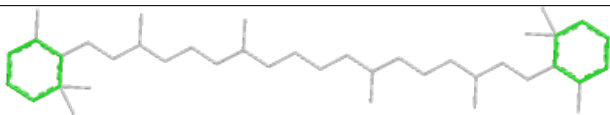
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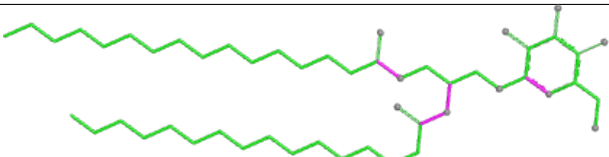
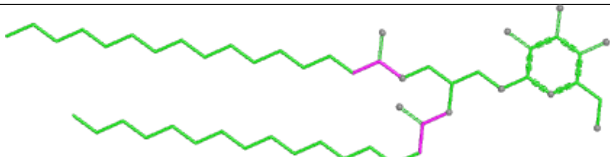
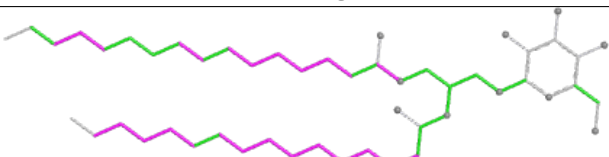
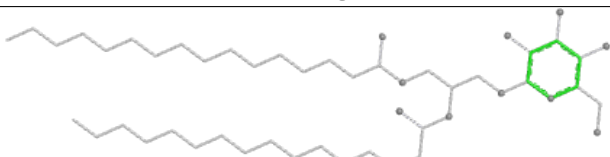


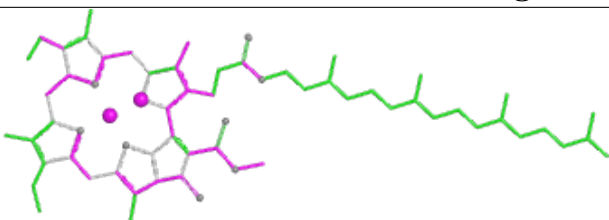
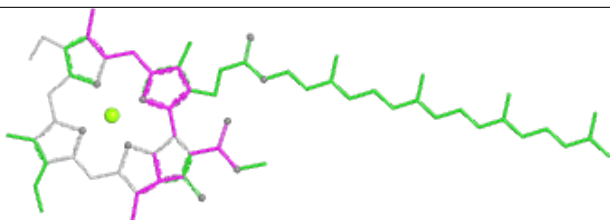
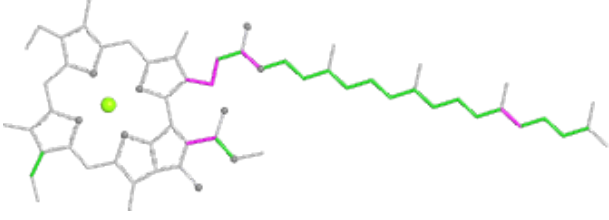
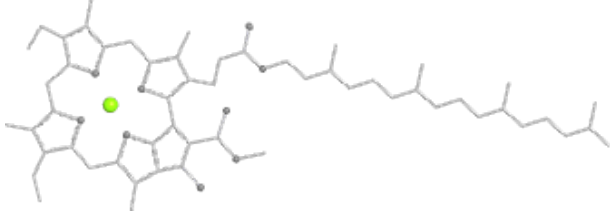
Ligand LMG B 621

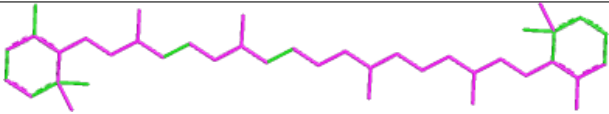
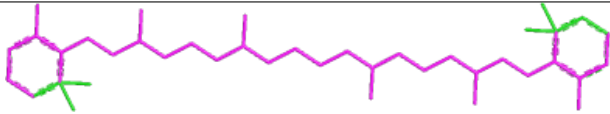
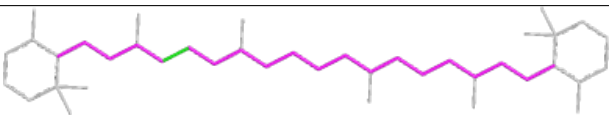
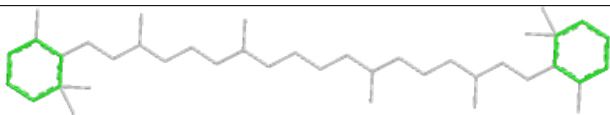


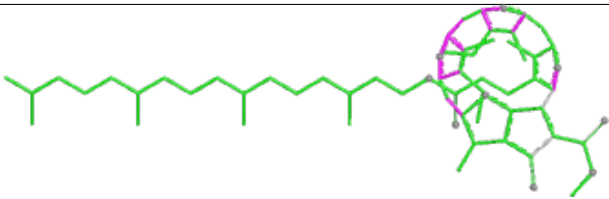
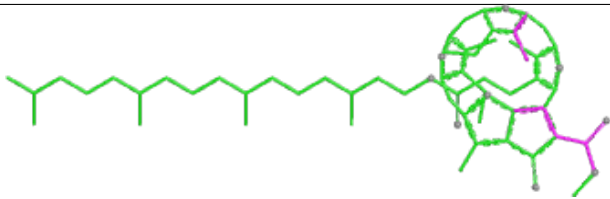
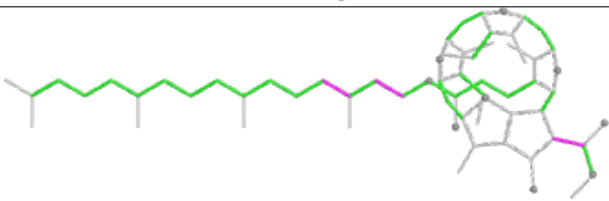
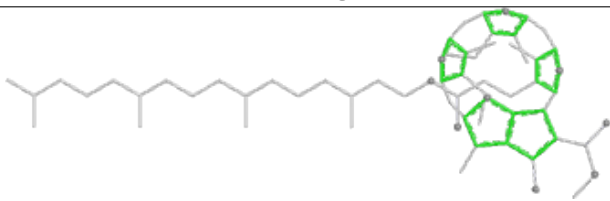


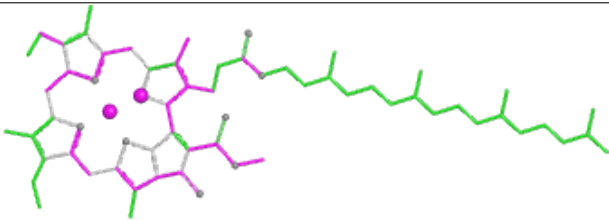
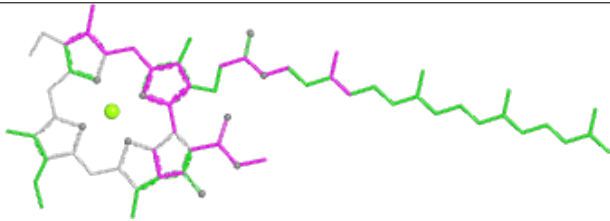
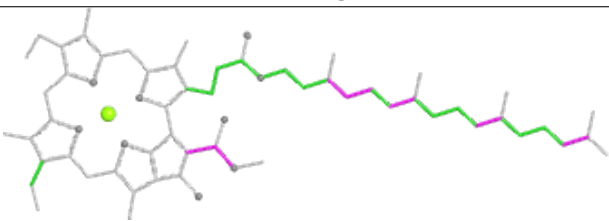
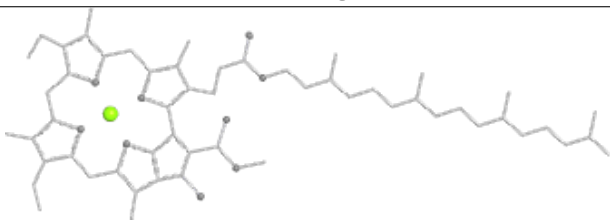
Ligand BCR A 609	
	
Bond lengths	Bond angles
	
Torsions	Rings

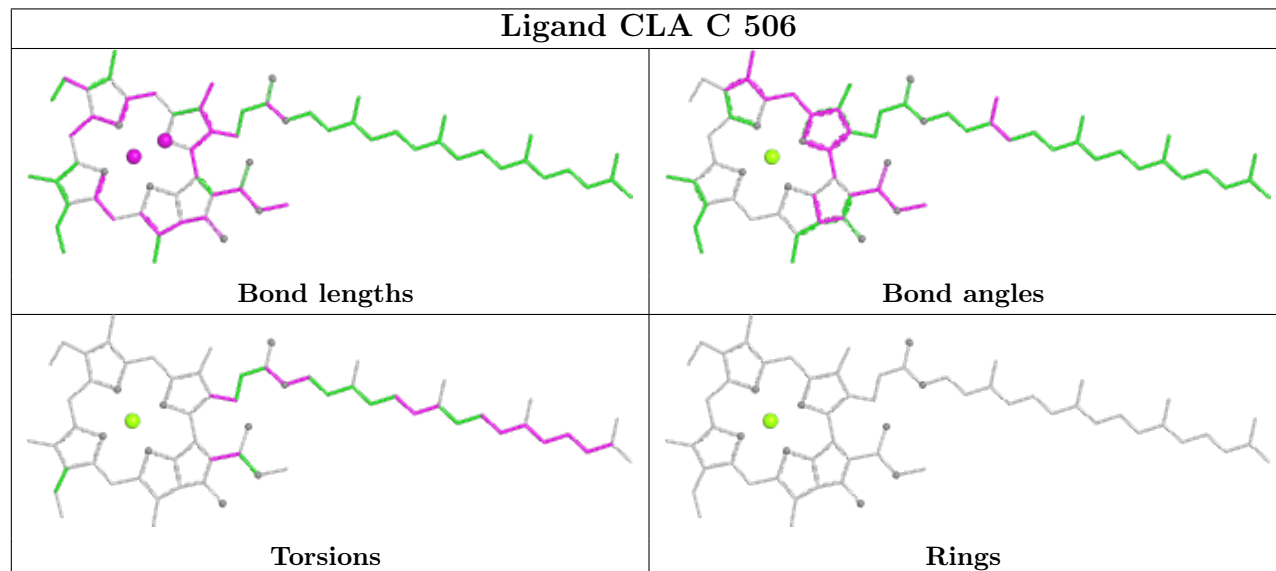
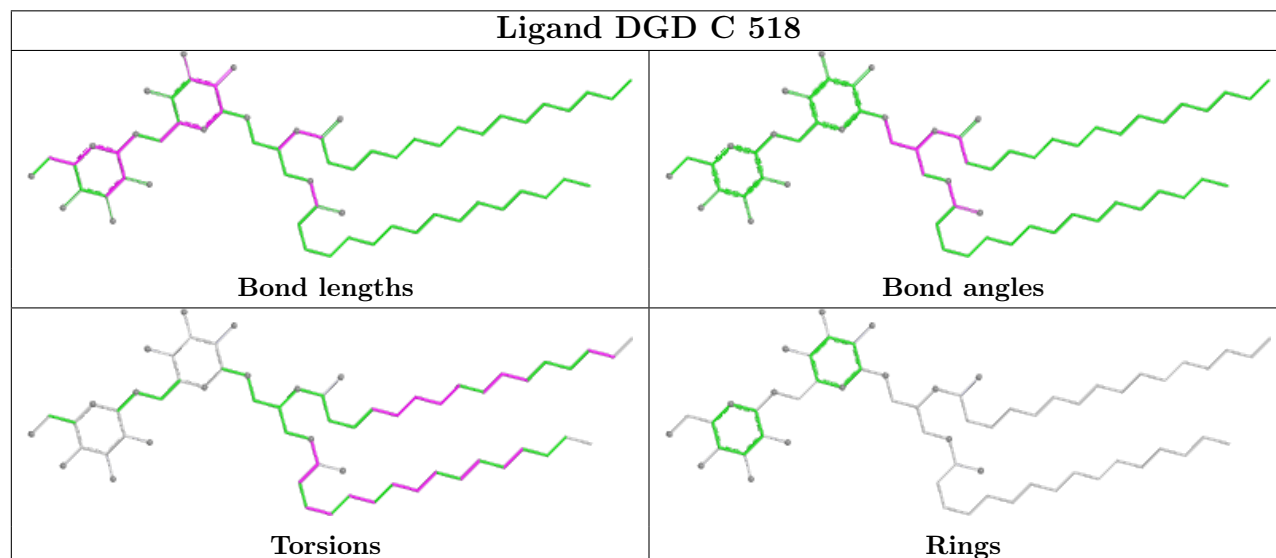
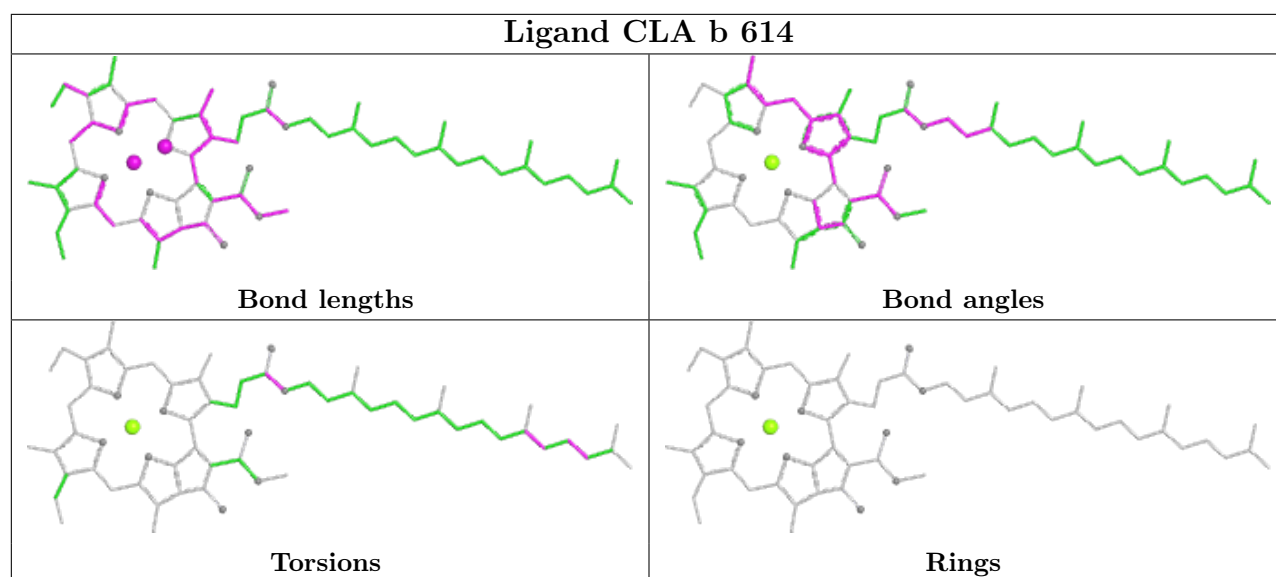
Ligand LMG c 520	
	
Bond lengths	Bond angles
	
Torsions	Rings

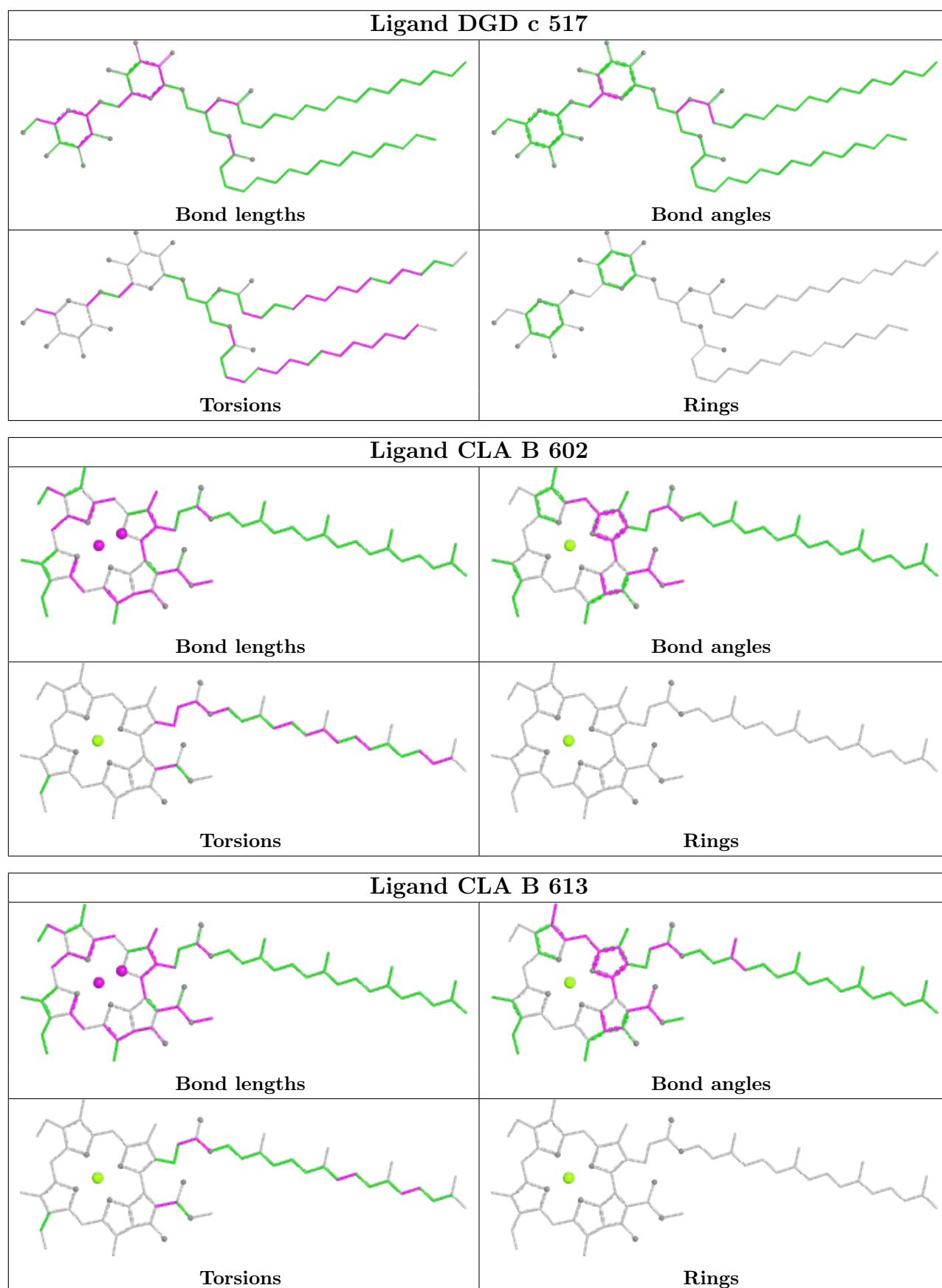
Ligand CLA c 506	
	
Bond lengths	Bond angles
	
Torsions	Rings

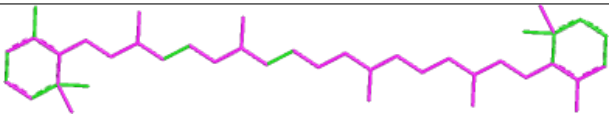
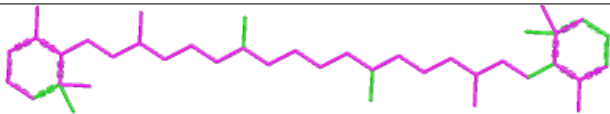
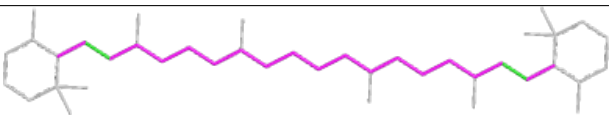
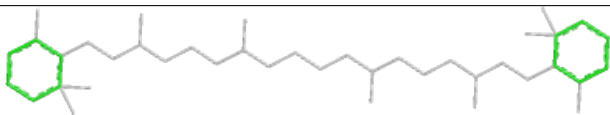
Ligand BCR f 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

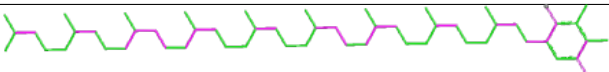
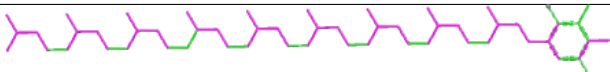
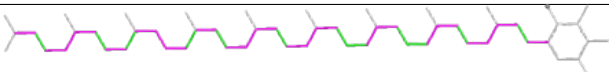
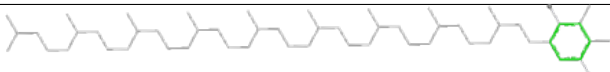
Ligand PHO A 607	
	
Bond lengths	Bond angles
	
Torsions	Rings

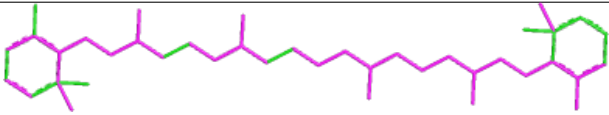
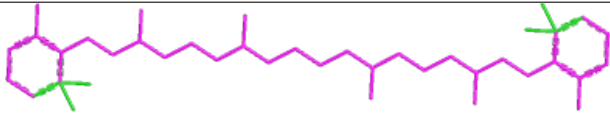
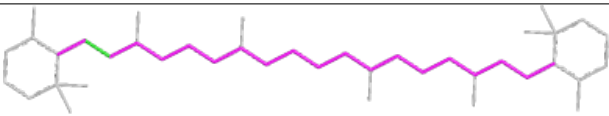
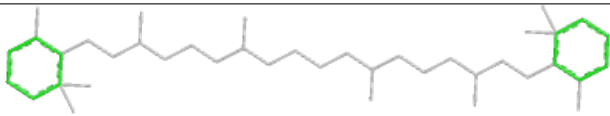
Ligand CLA C 513	
	
Bond lengths	Bond angles
	
Torsions	Rings

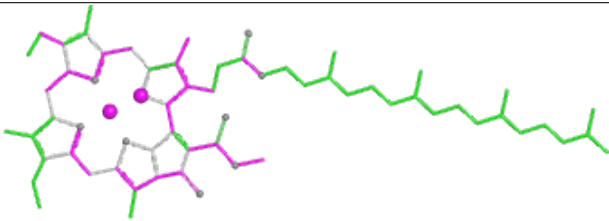
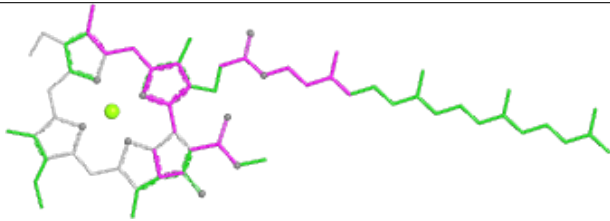
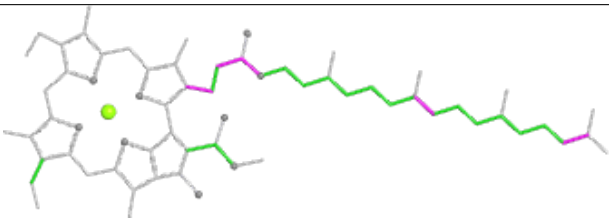
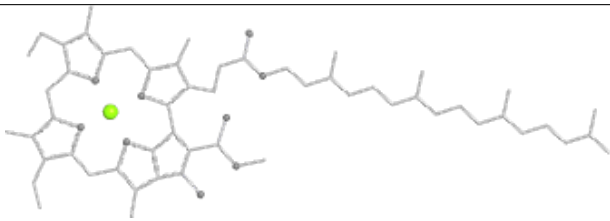


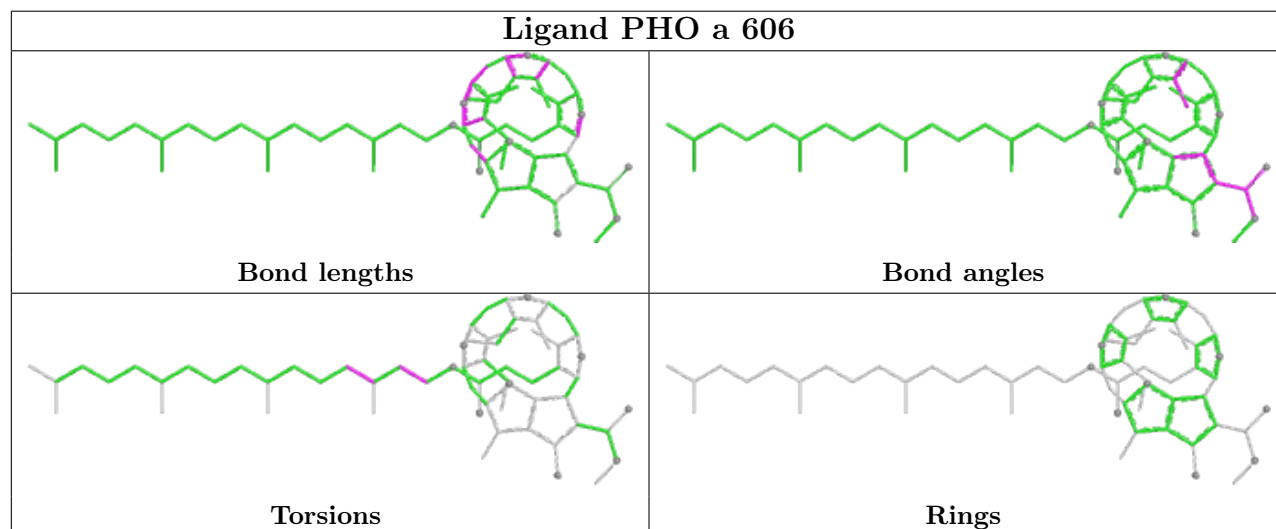
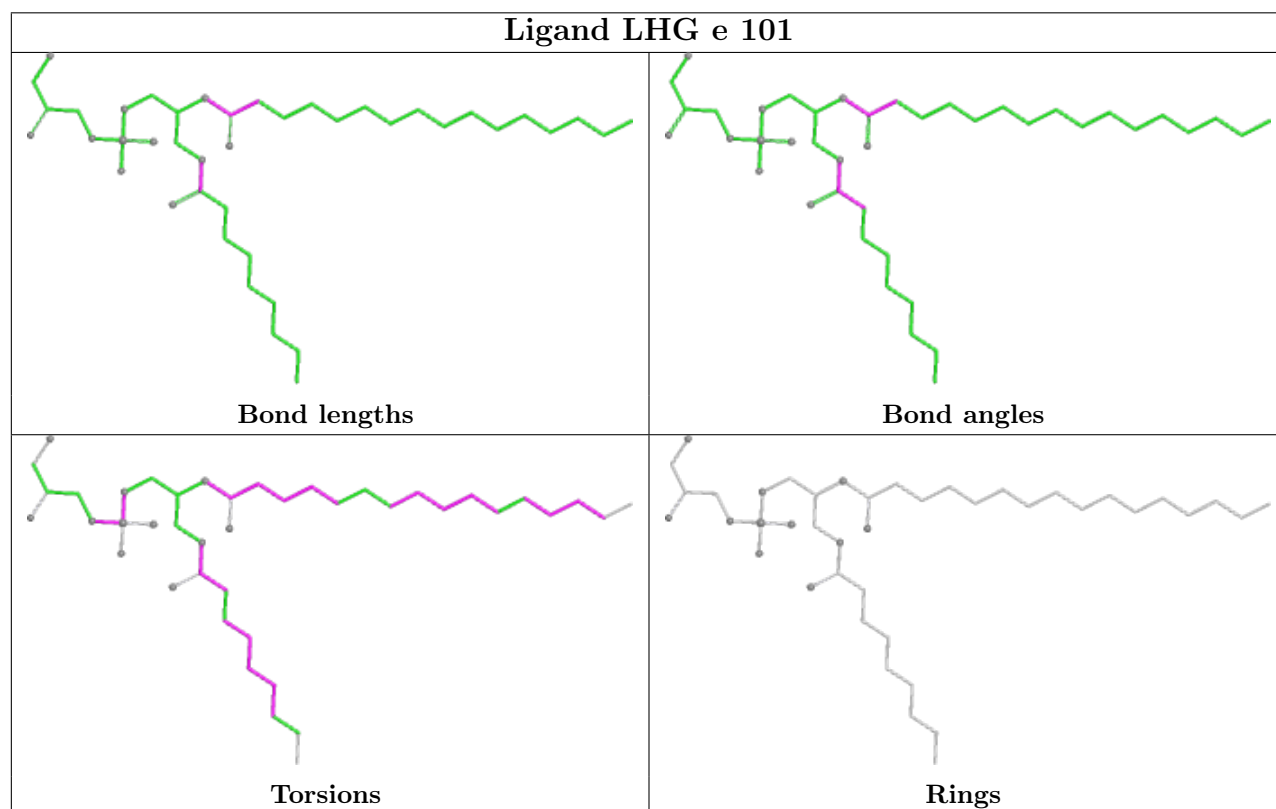
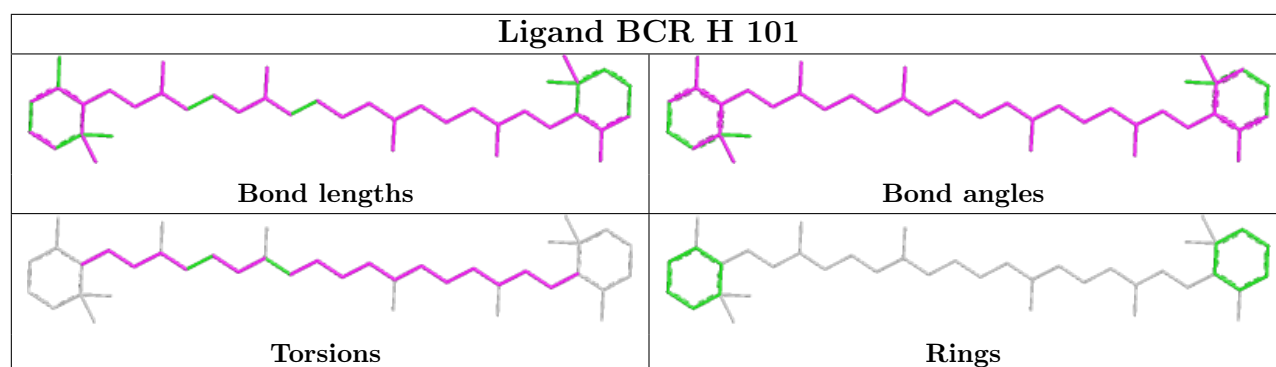


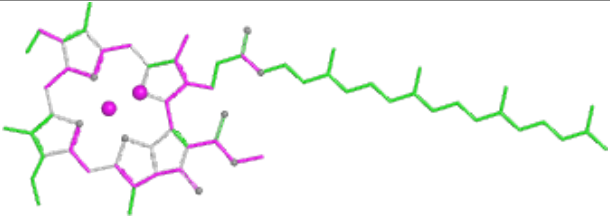
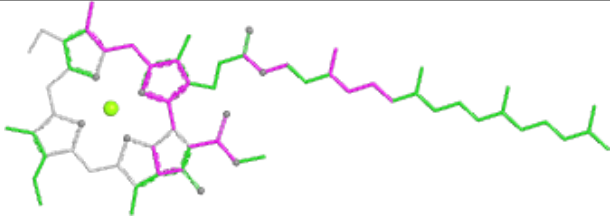
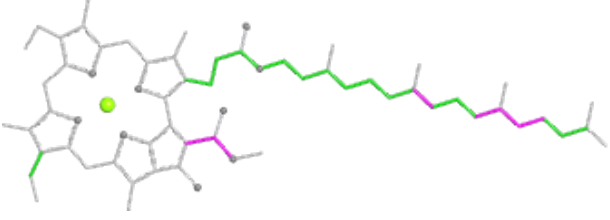
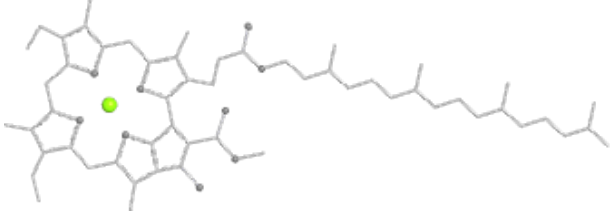
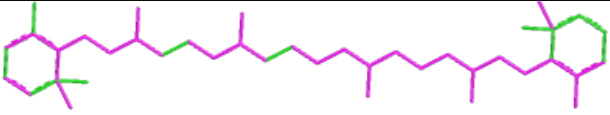
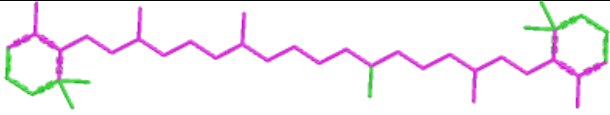
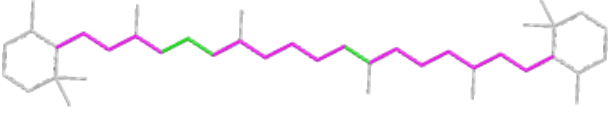
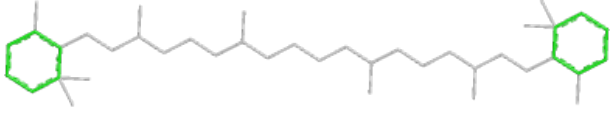
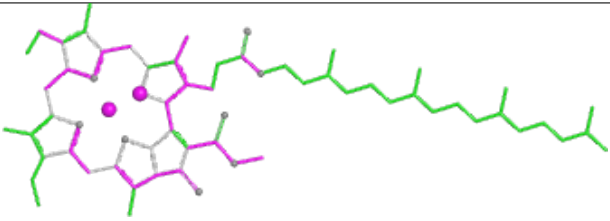
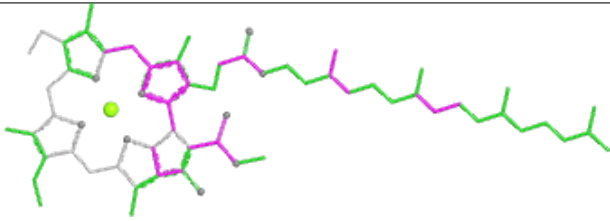
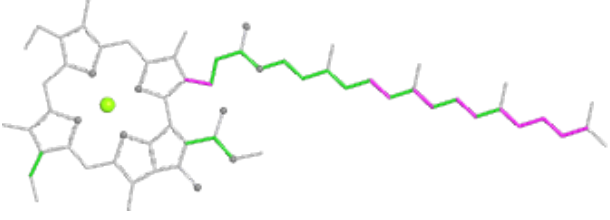
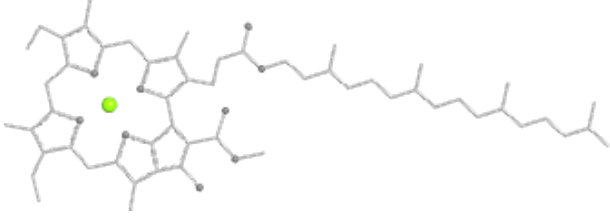
Ligand BCR b 621	
	
Bond lengths	Bond angles
	
Torsions	Rings

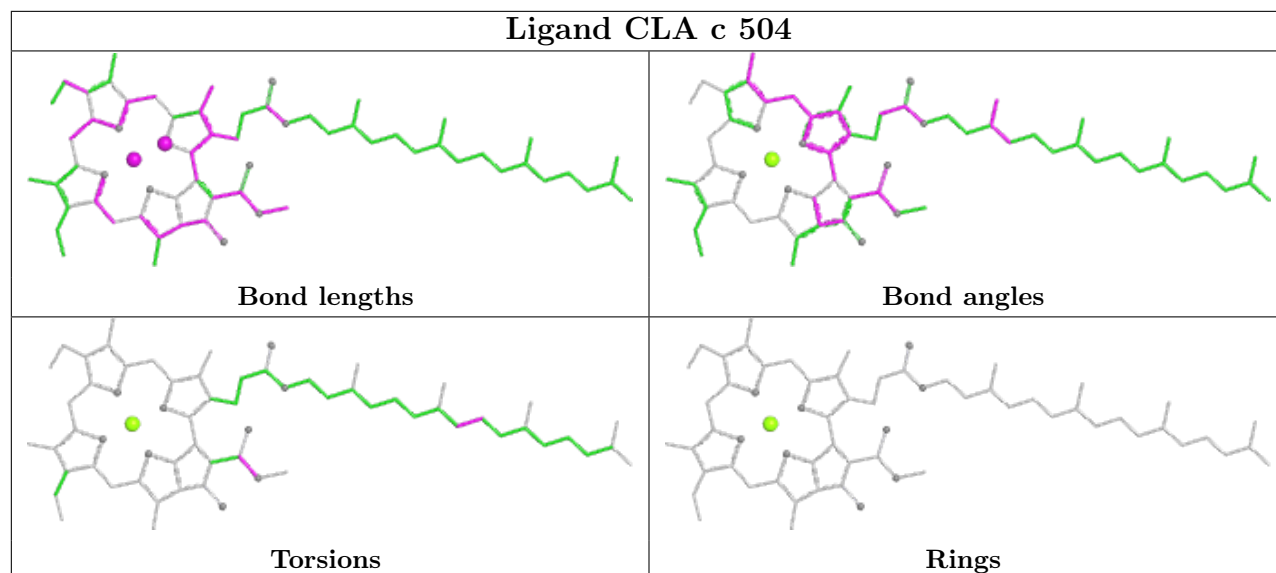
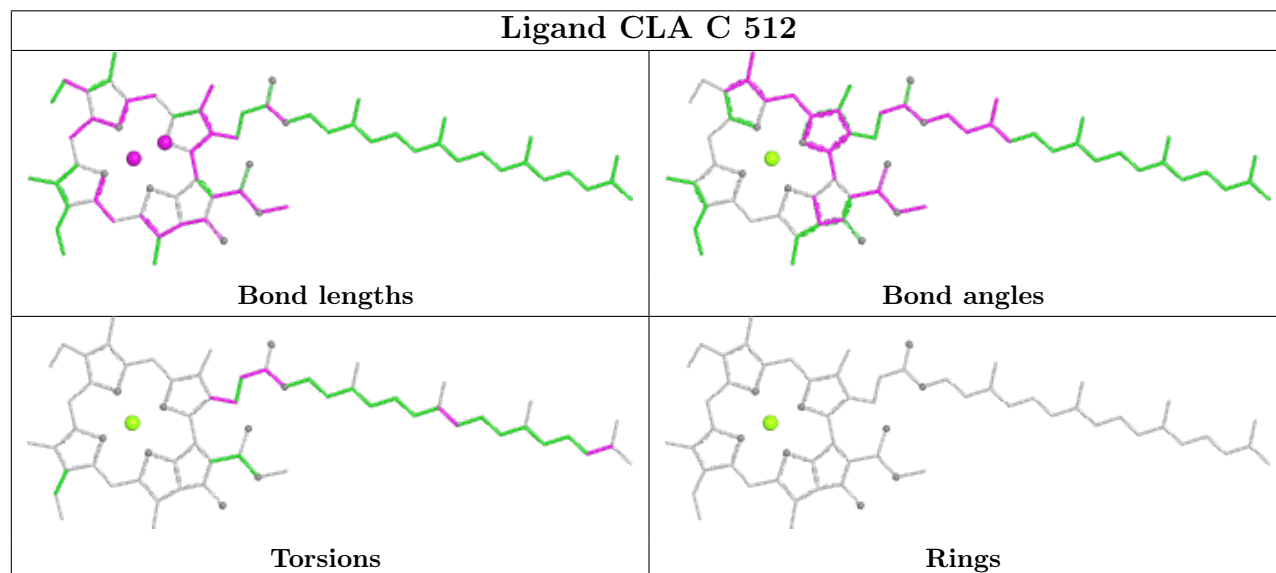
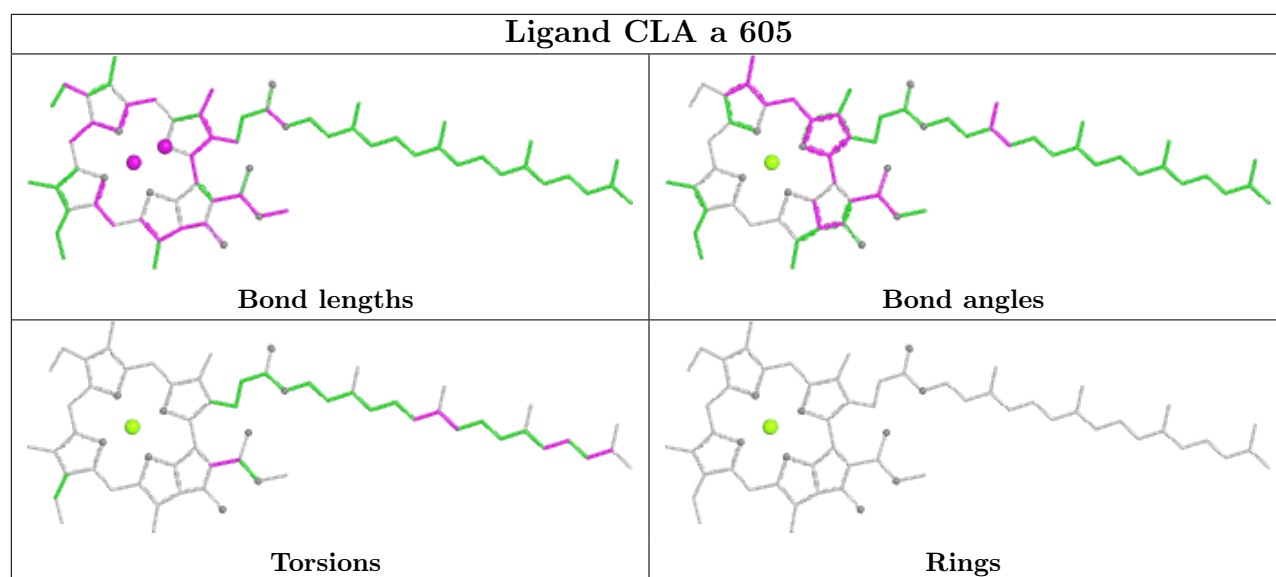
Ligand PL9 d 404	
	
Bond lengths	Bond angles
	
Torsions	Rings

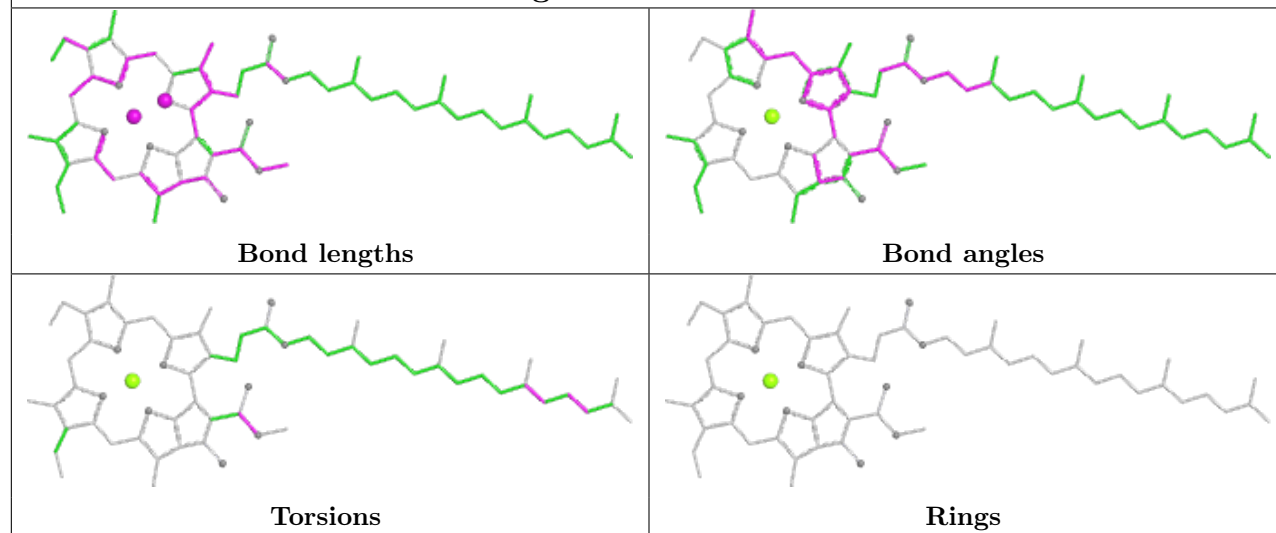
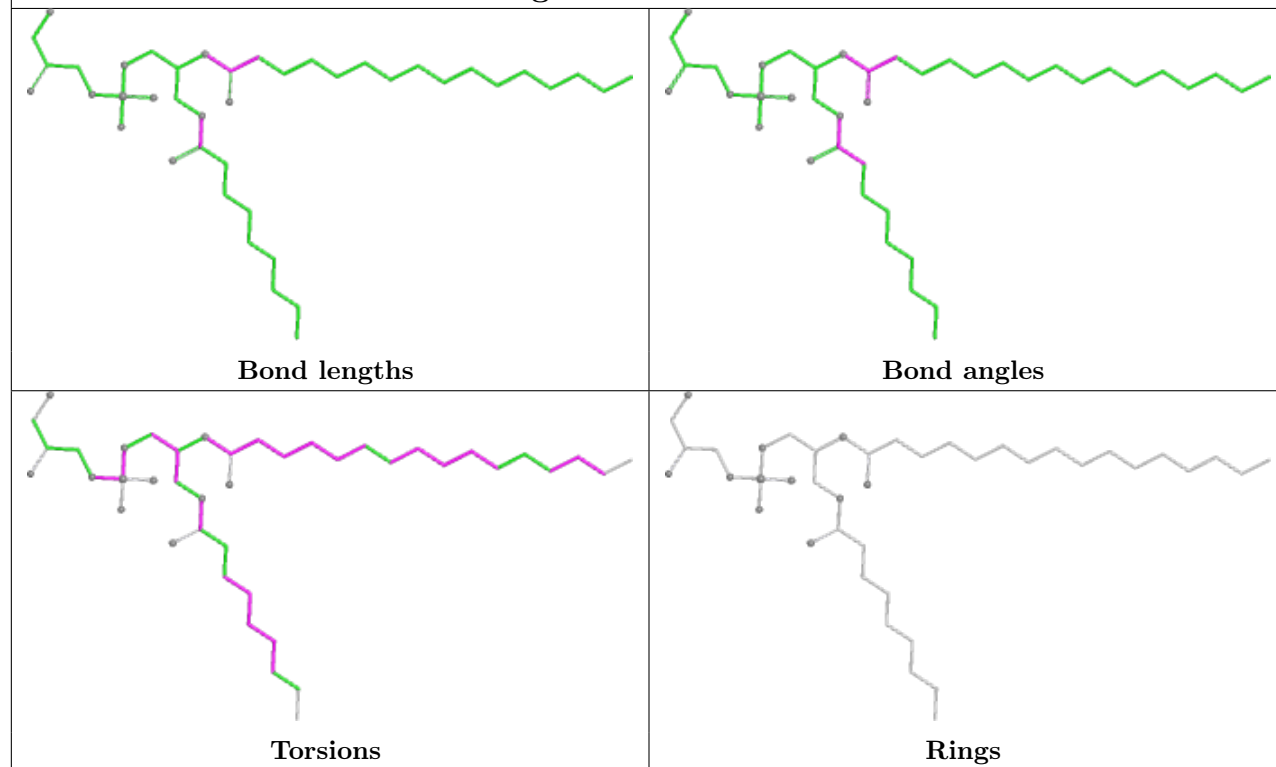
Ligand BCR B 618	
	
Bond lengths	Bond angles
	
Torsions	Rings

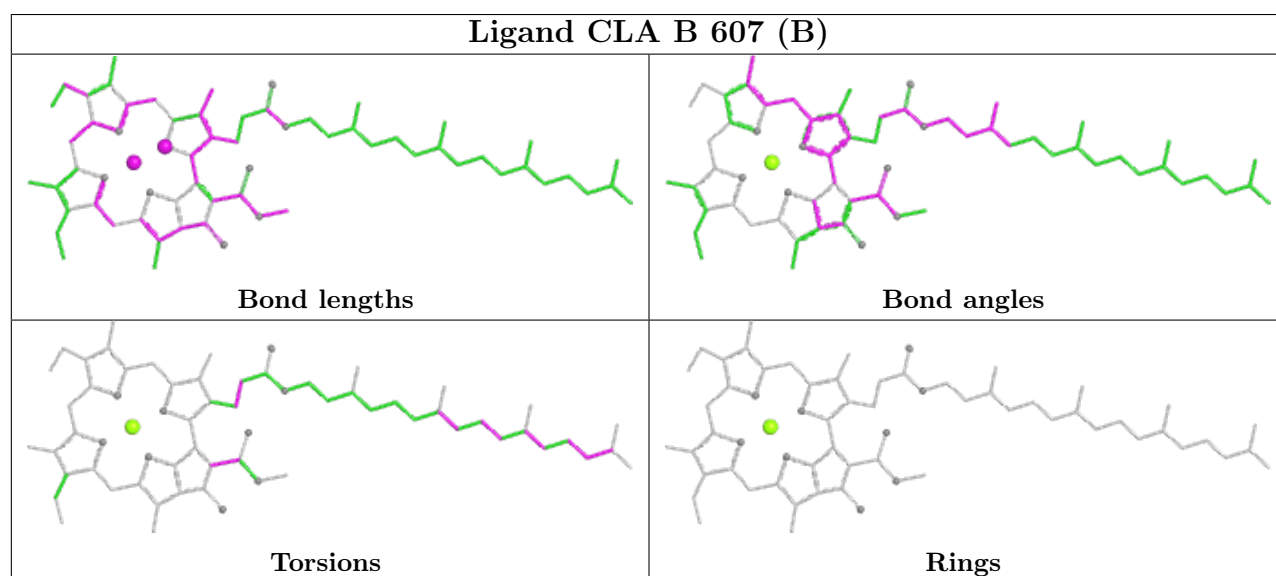
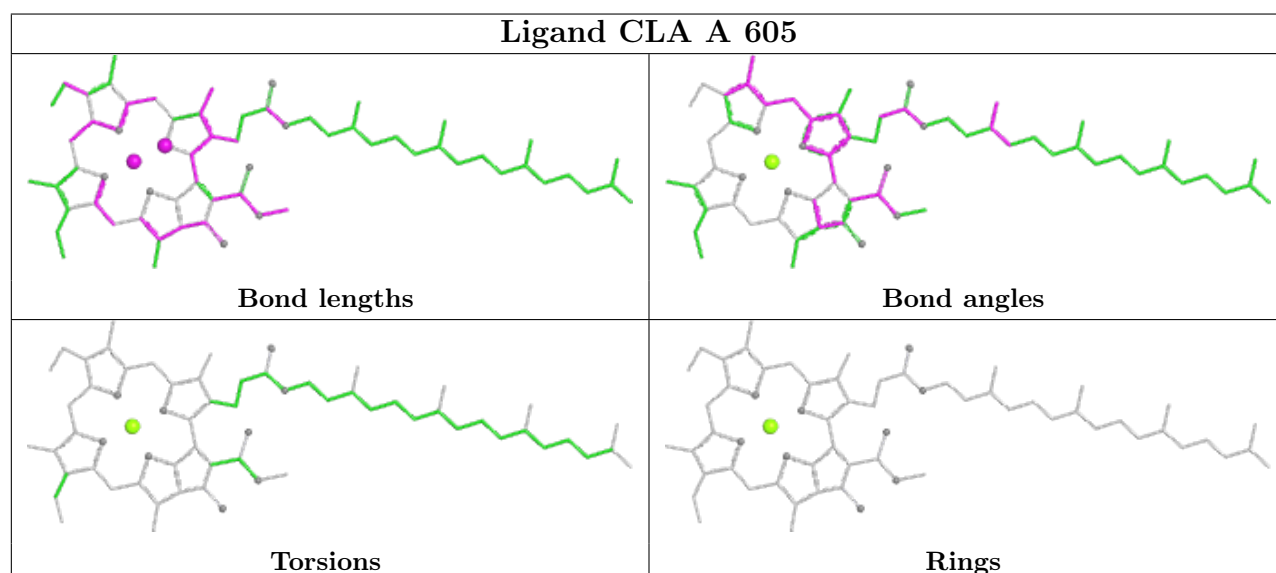
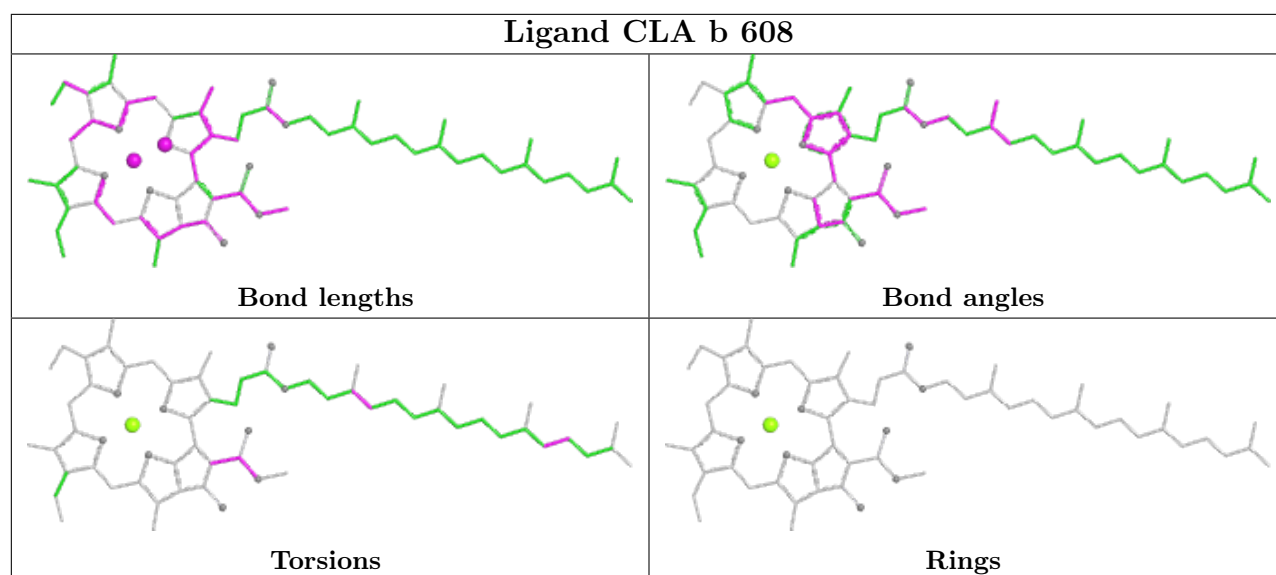
Ligand CLA c 513	
	
Bond lengths	Bond angles
	
Torsions	Rings

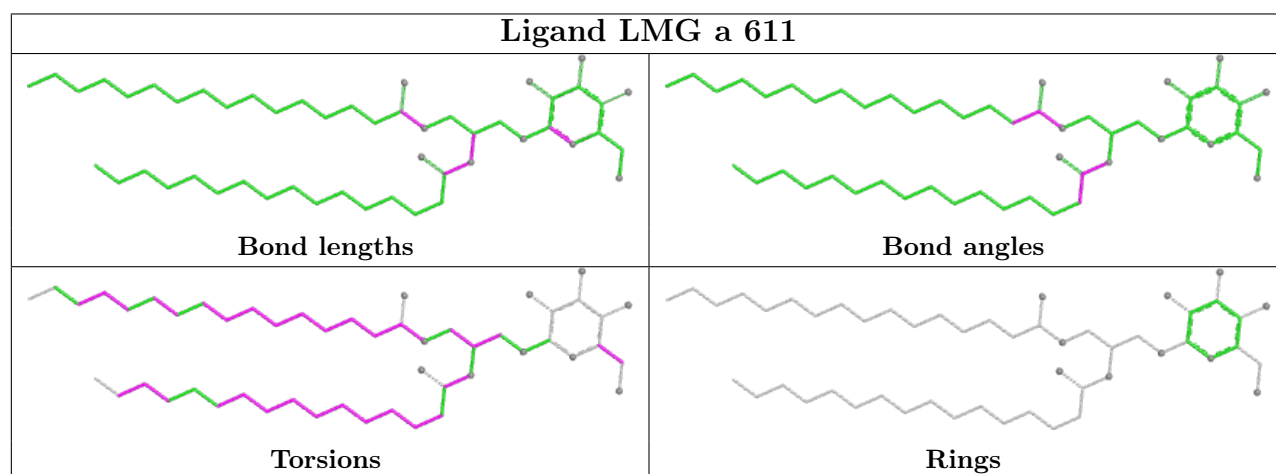
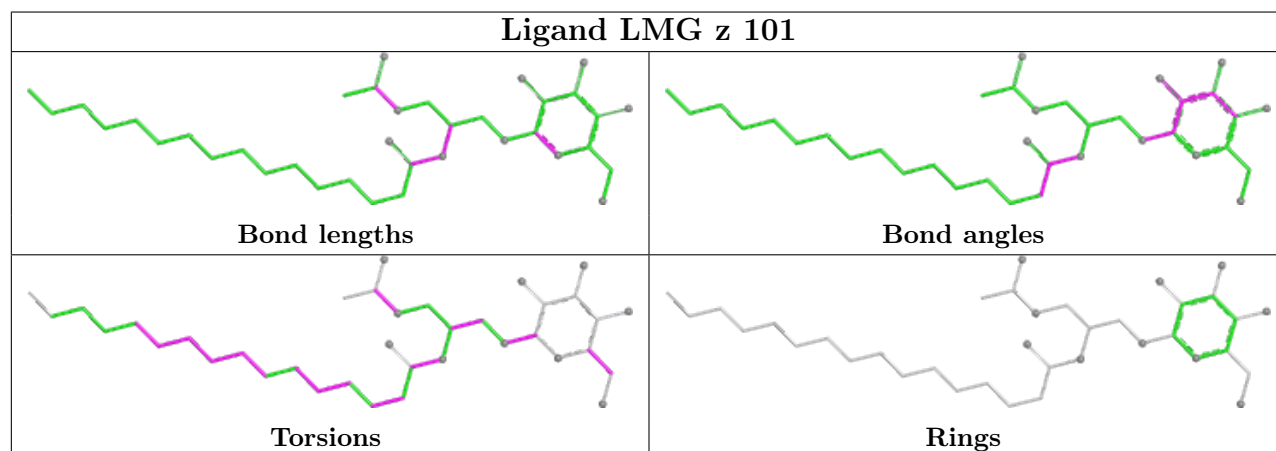
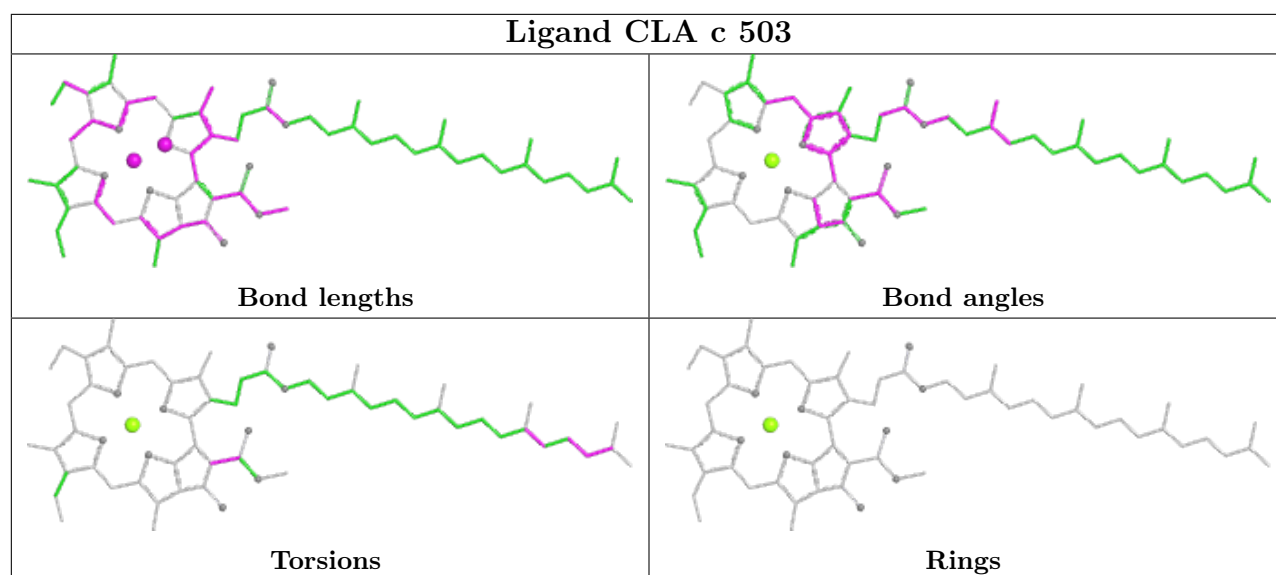


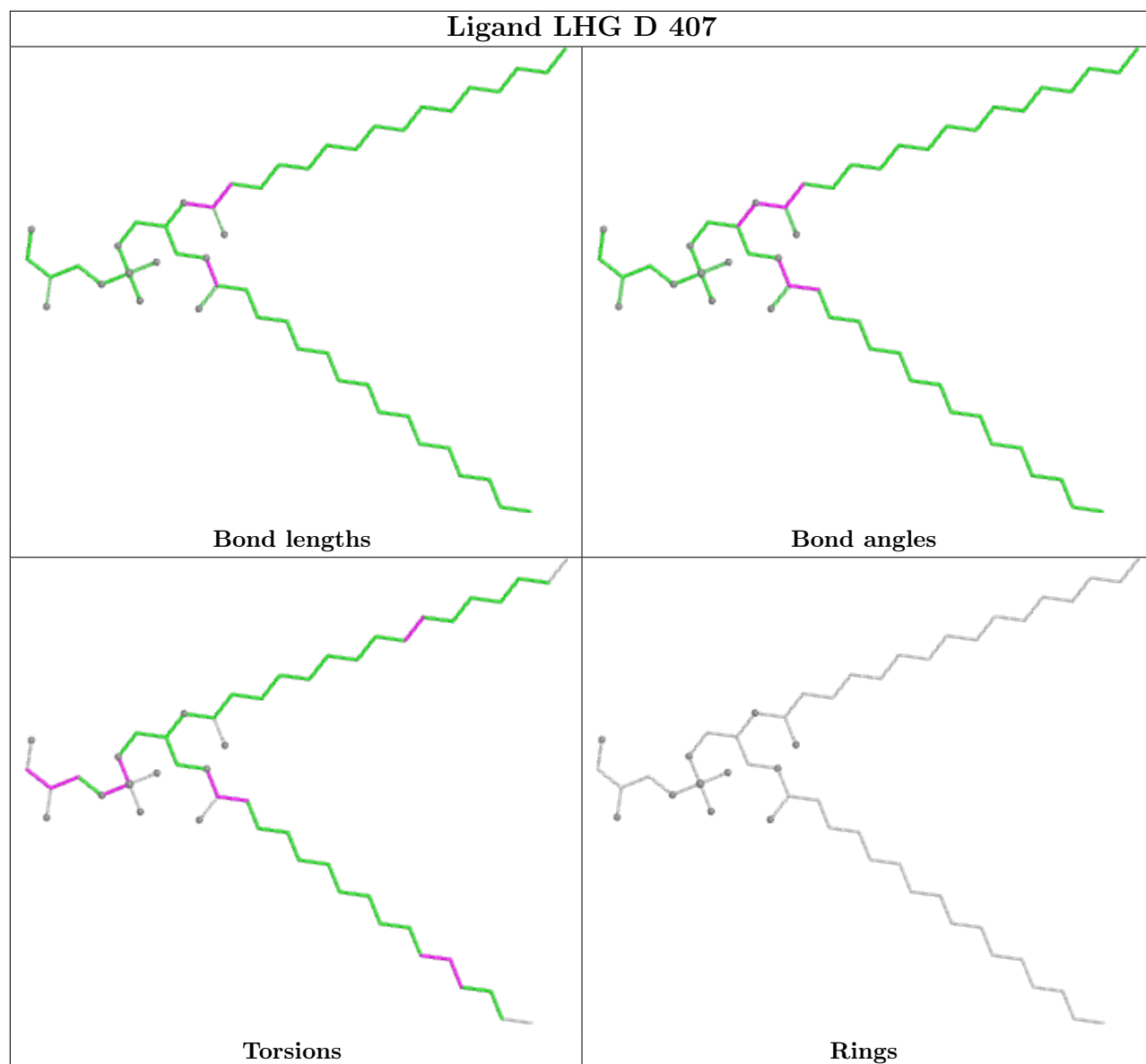
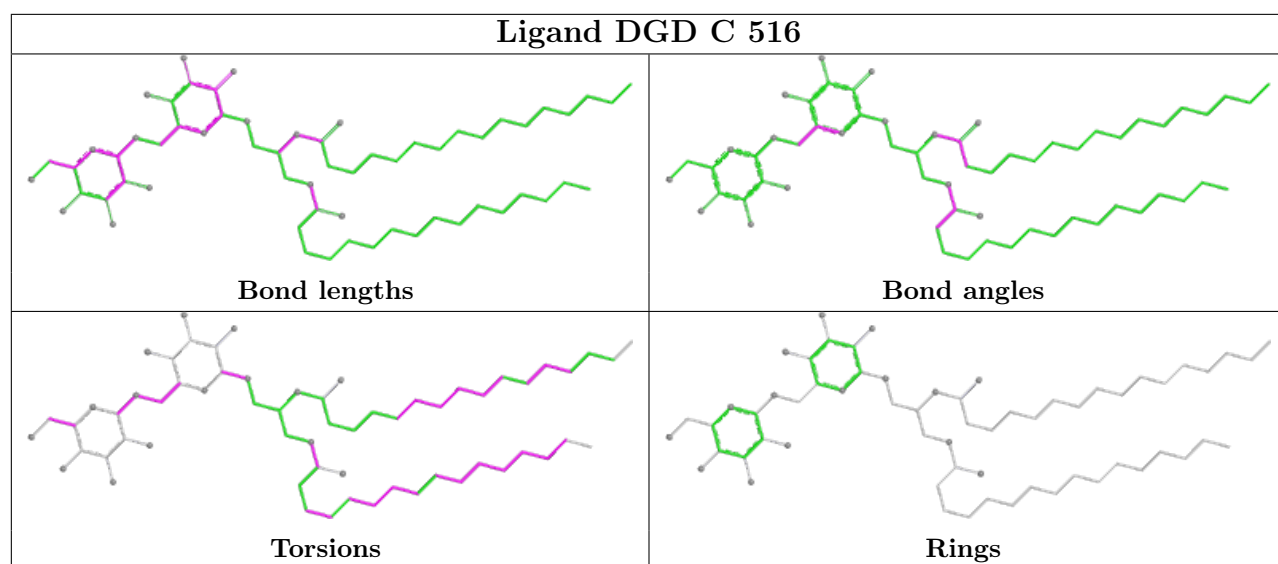
Ligand CLA c 505	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR C 515	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand CLA b 618	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

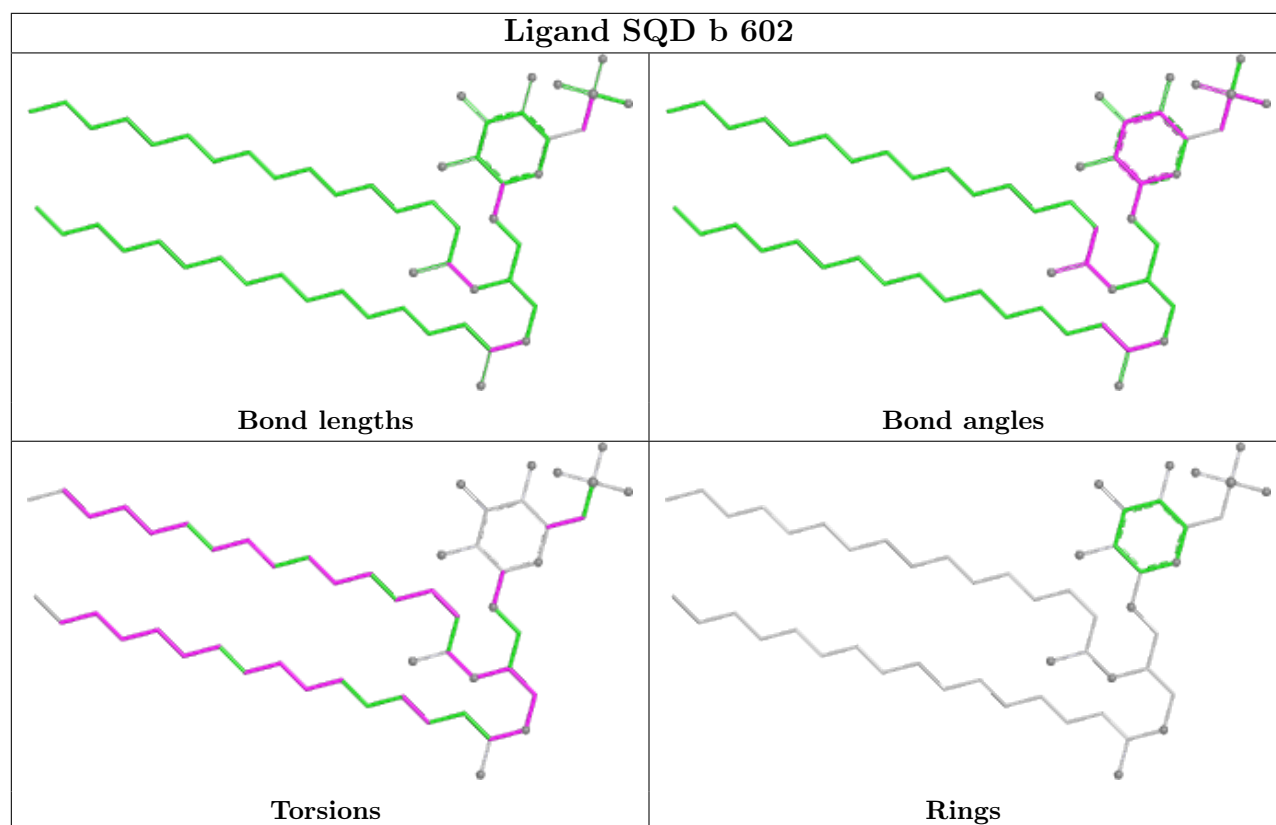
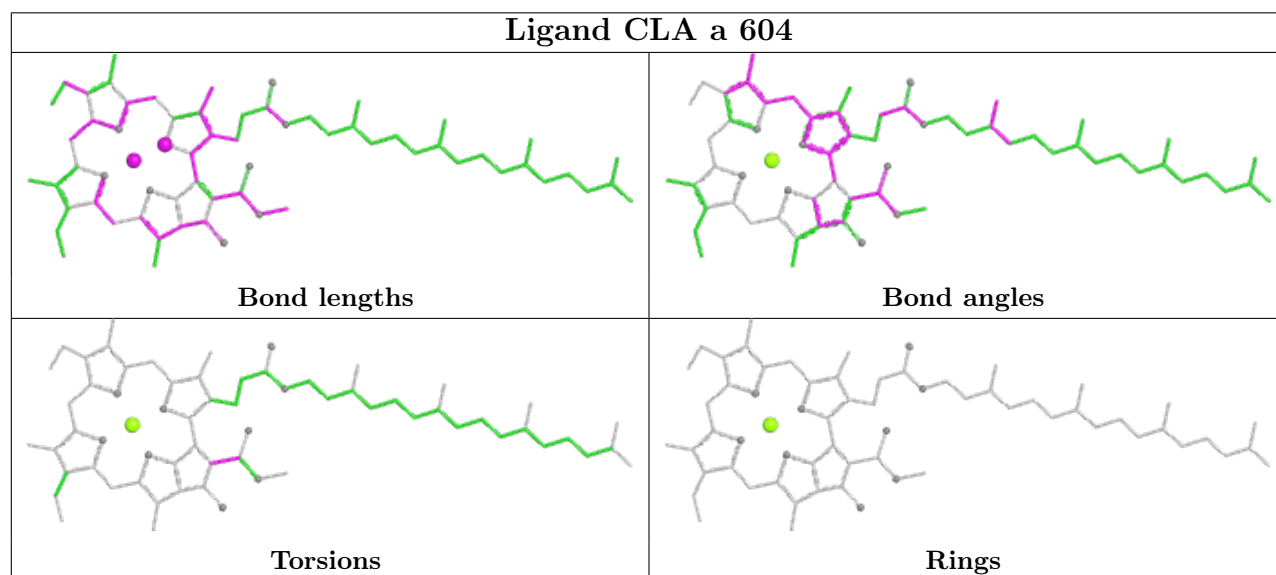
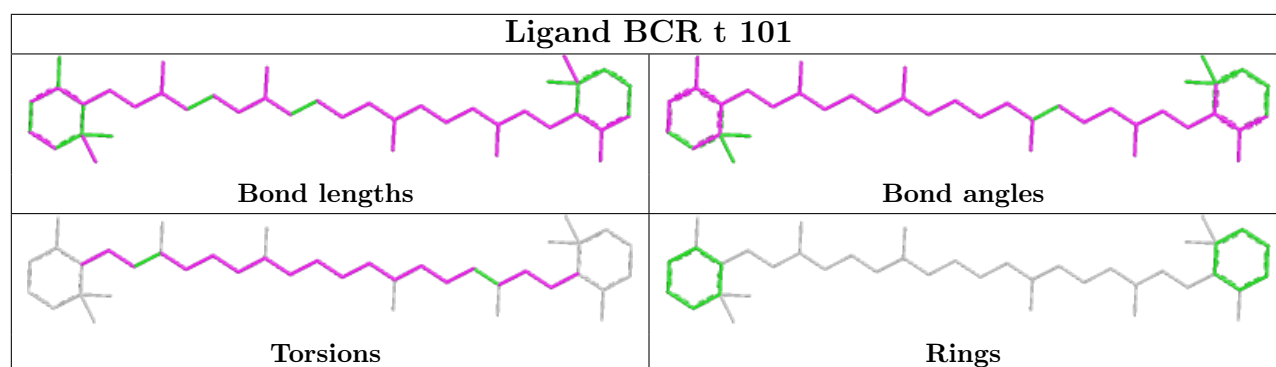


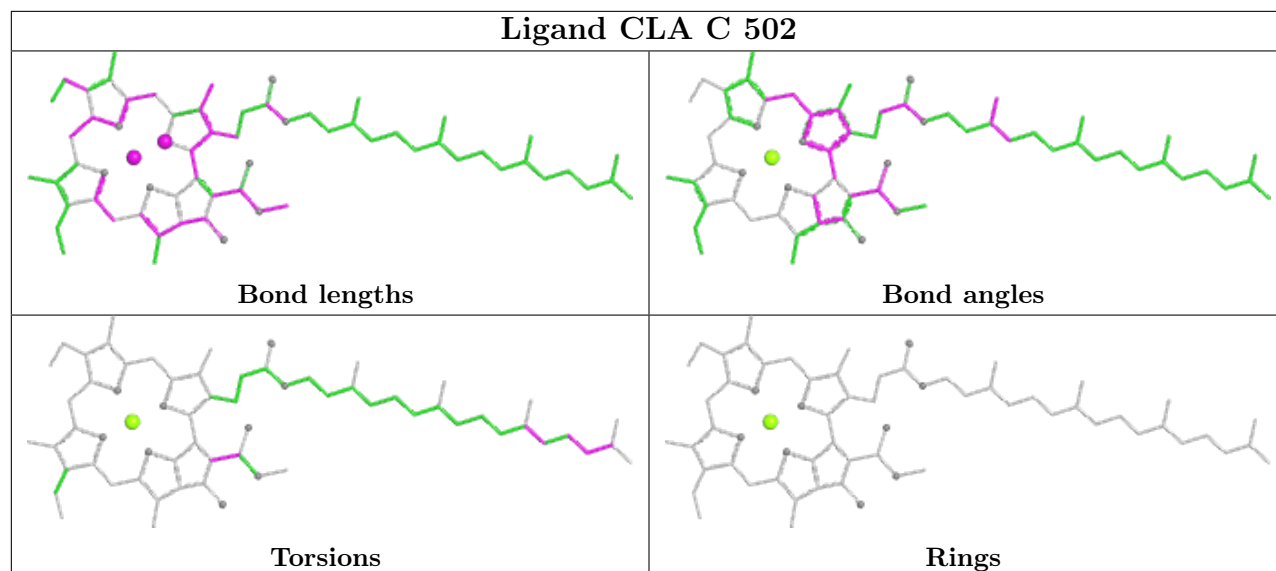
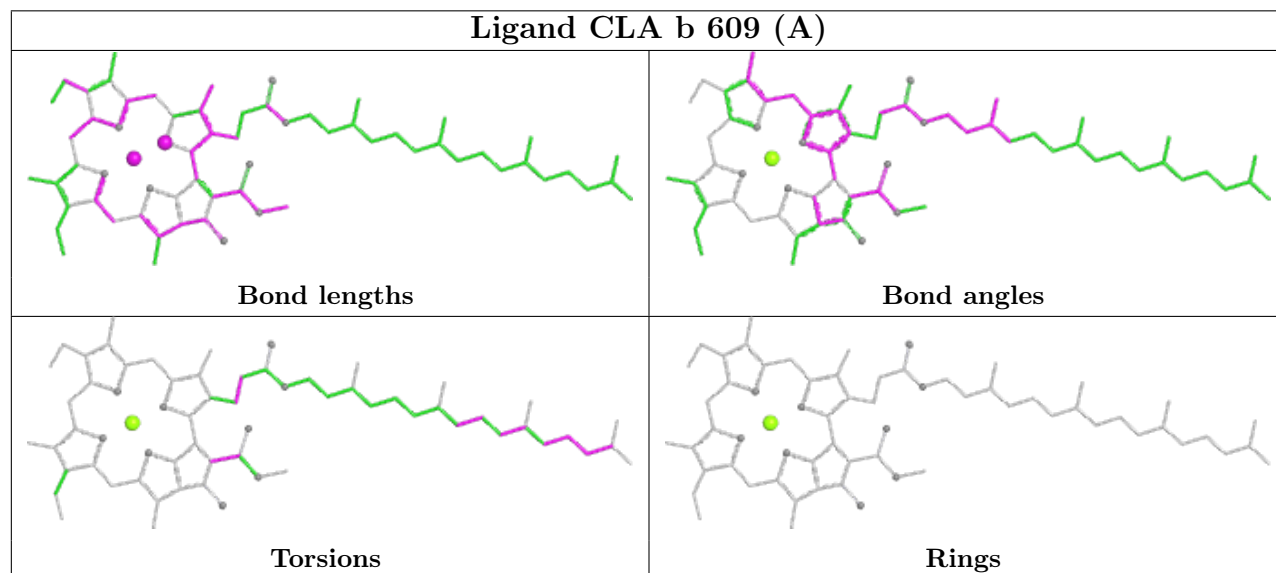
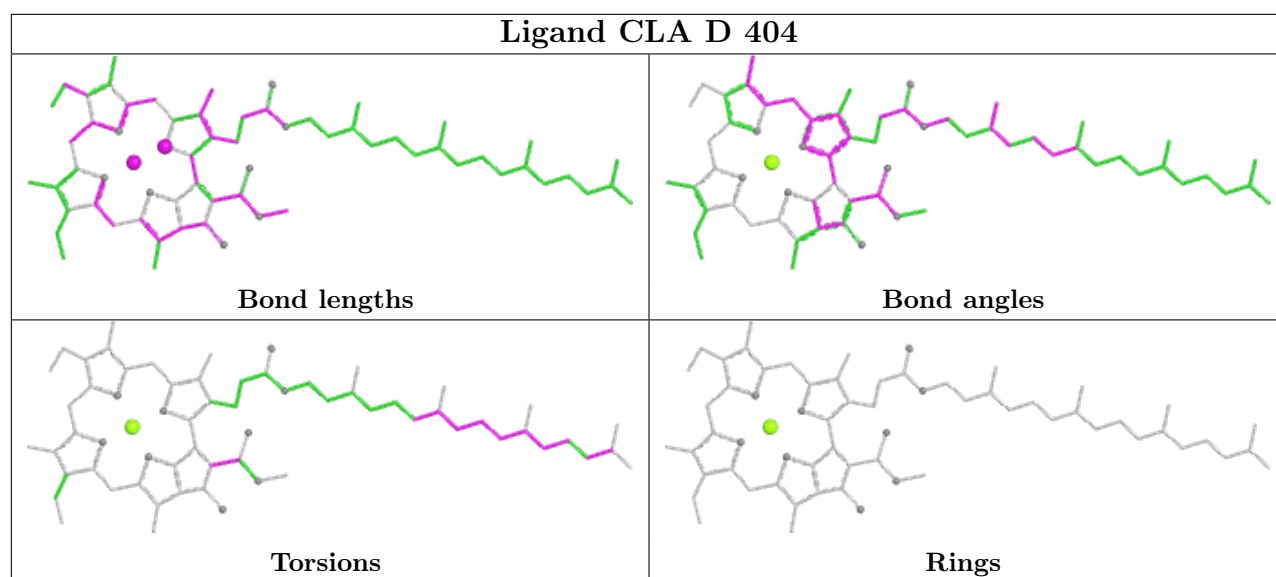
Ligand CLA B 612**Ligand LHG E 101**

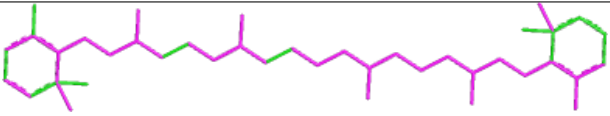
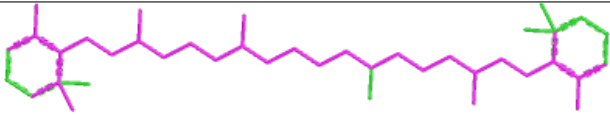
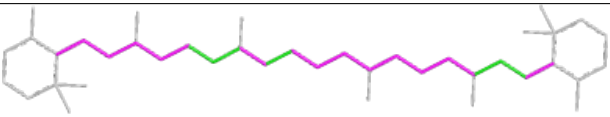
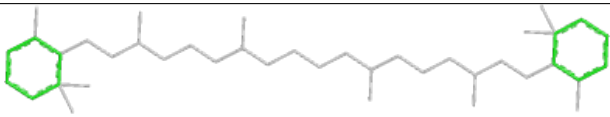
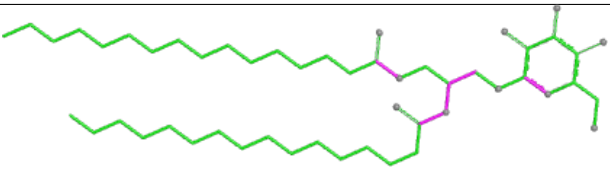
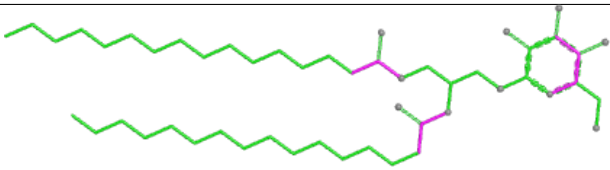
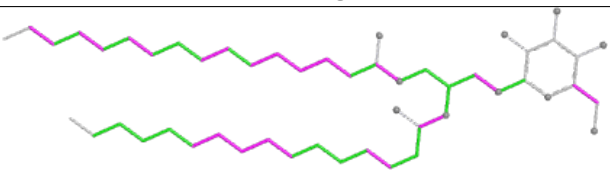
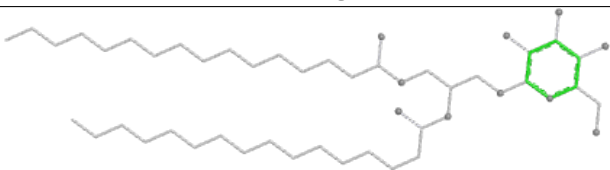
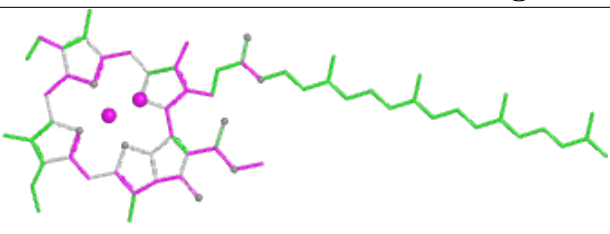
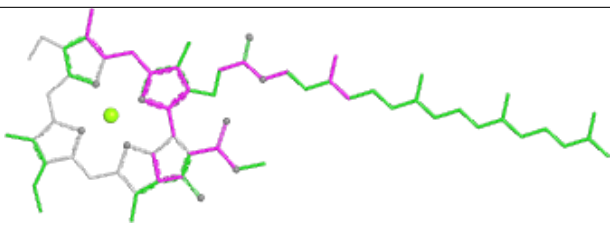
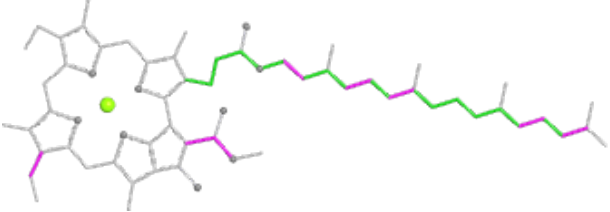
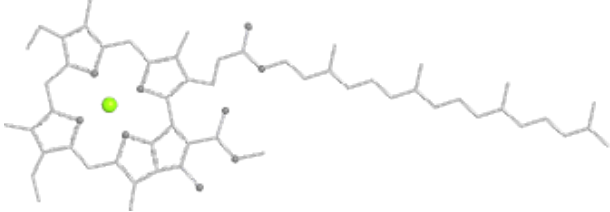


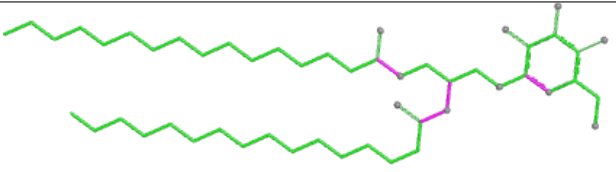
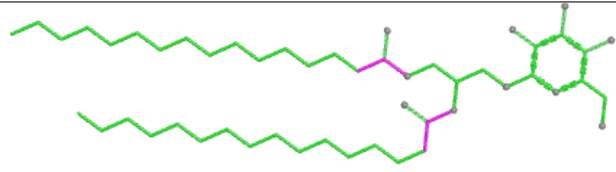
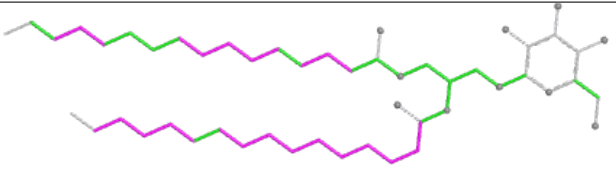
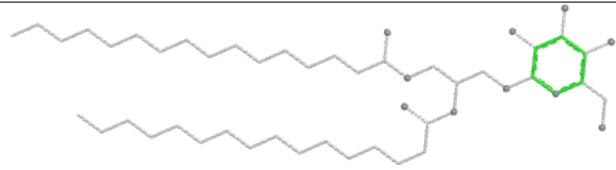


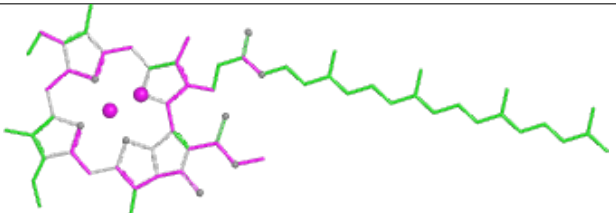
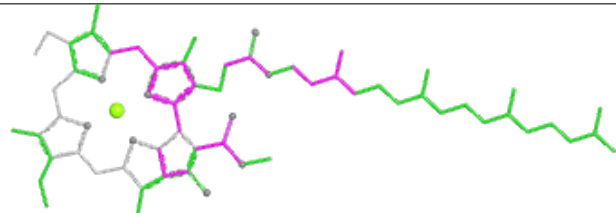
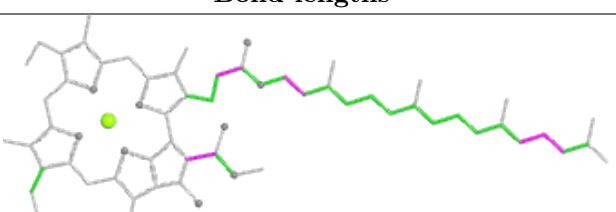
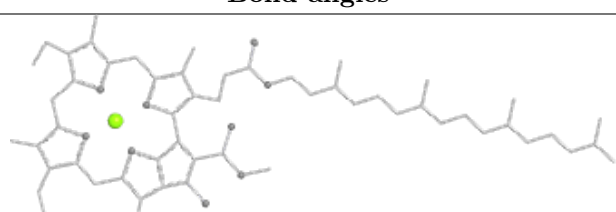


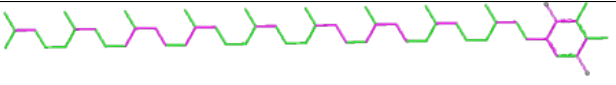
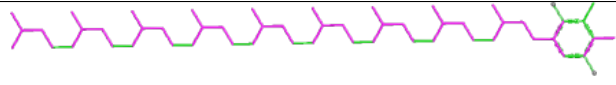
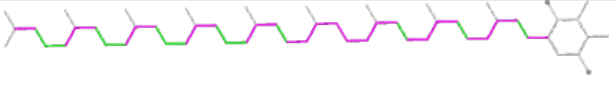



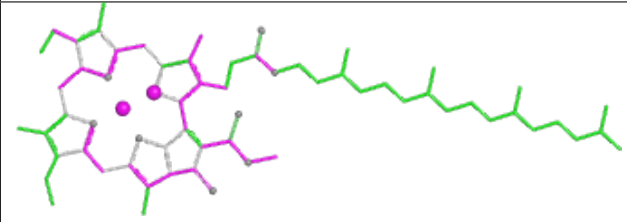
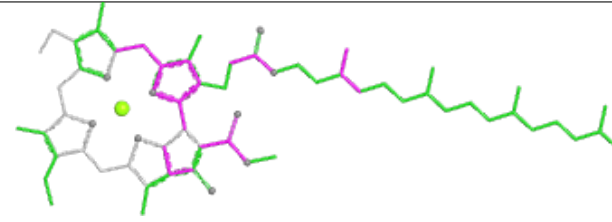
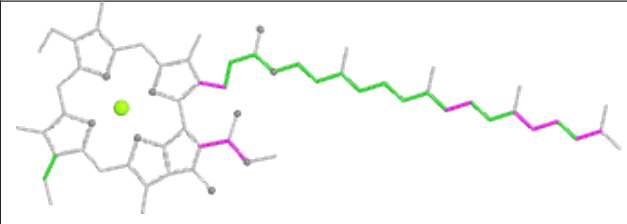
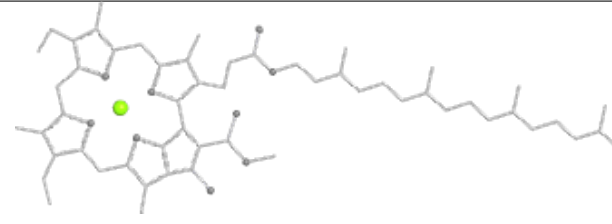


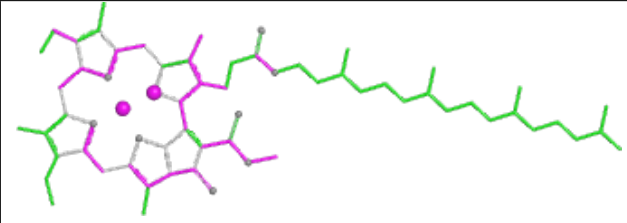
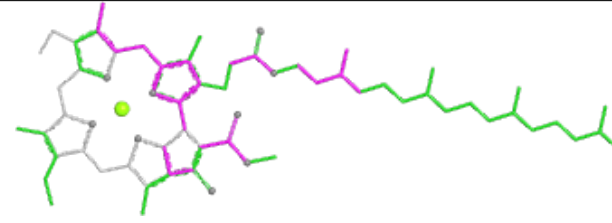
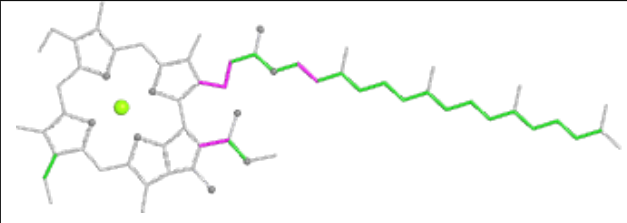
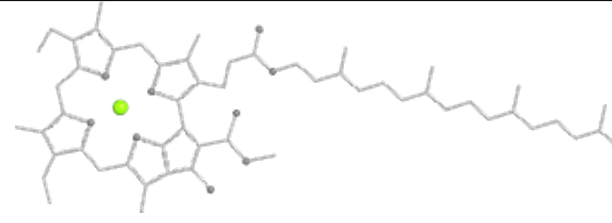
Ligand BCR B 620	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand LMG C 520	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand CLA b 607	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

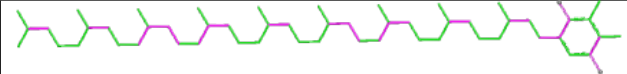
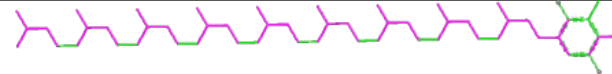
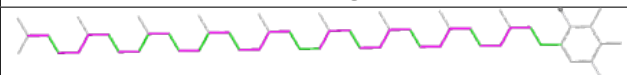

Ligand LMG C 519	
	
Bond lengths	Bond angles
	
Torsions	Rings

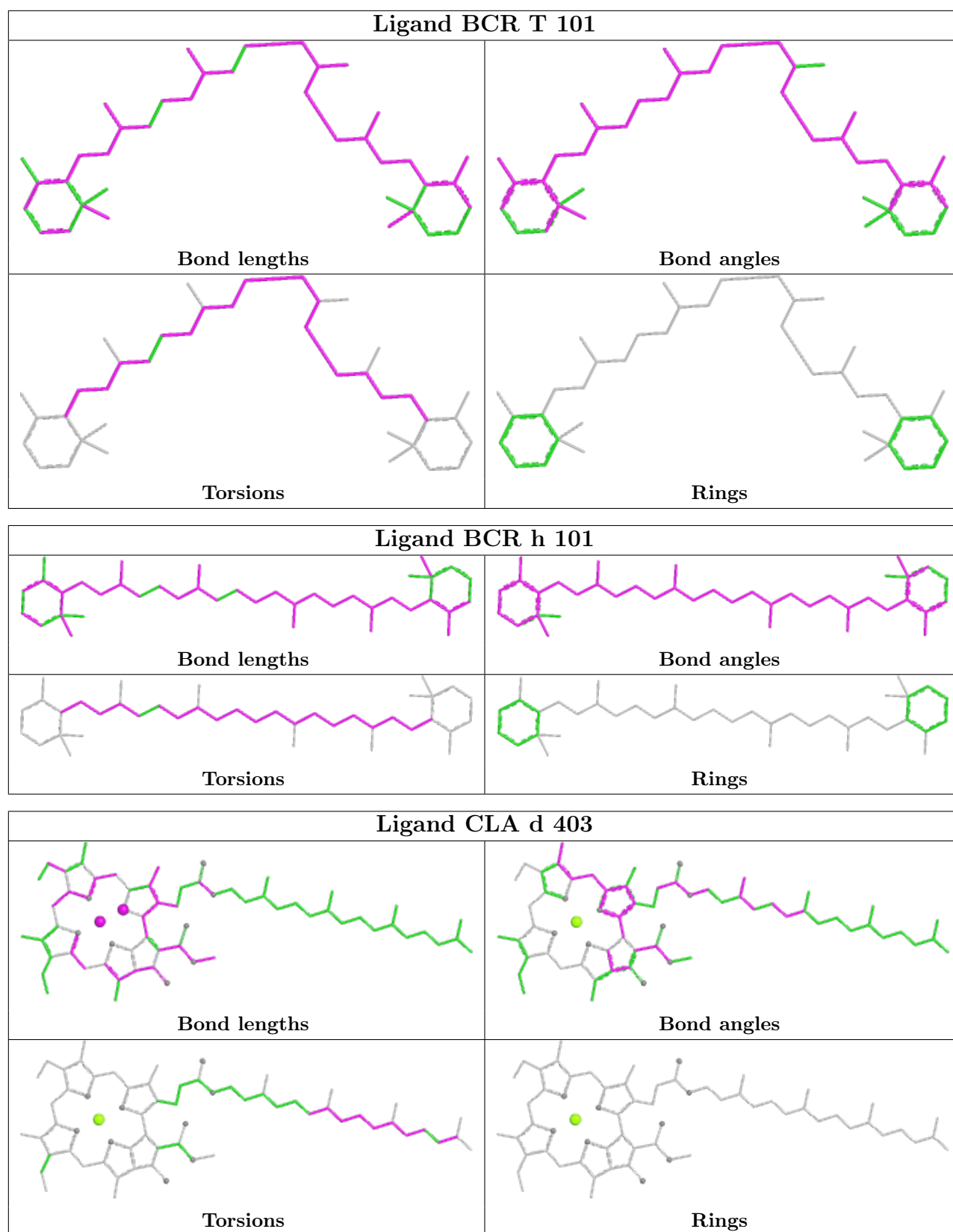
Ligand CLA B 614	
	
Bond lengths	Bond angles
	
Torsions	Rings

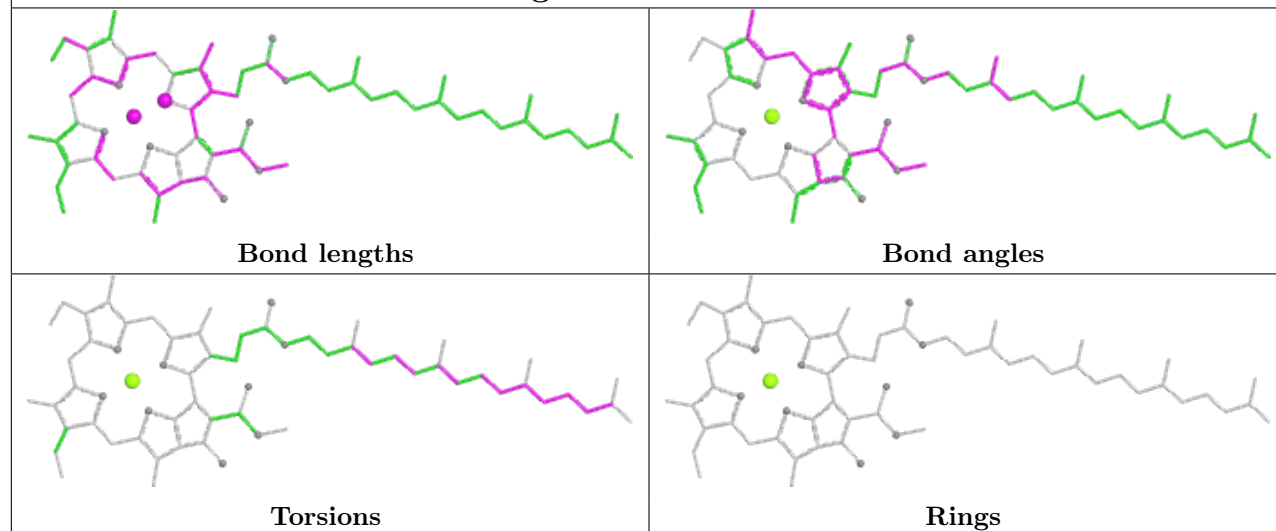
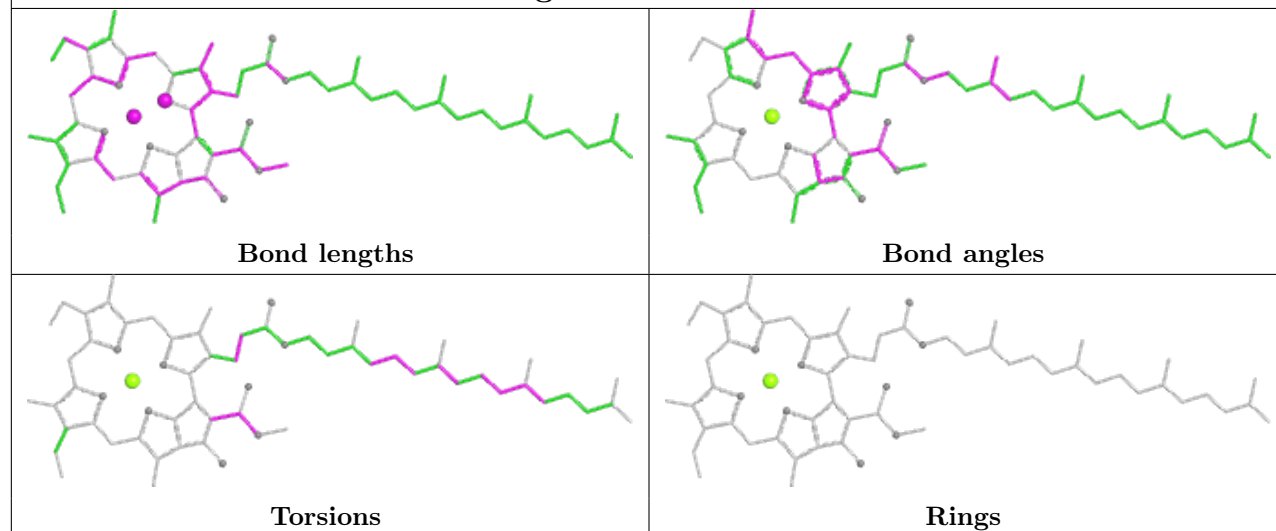
Ligand PL9 A 610	
	
Bond lengths	Bond angles
	
Torsions	Rings

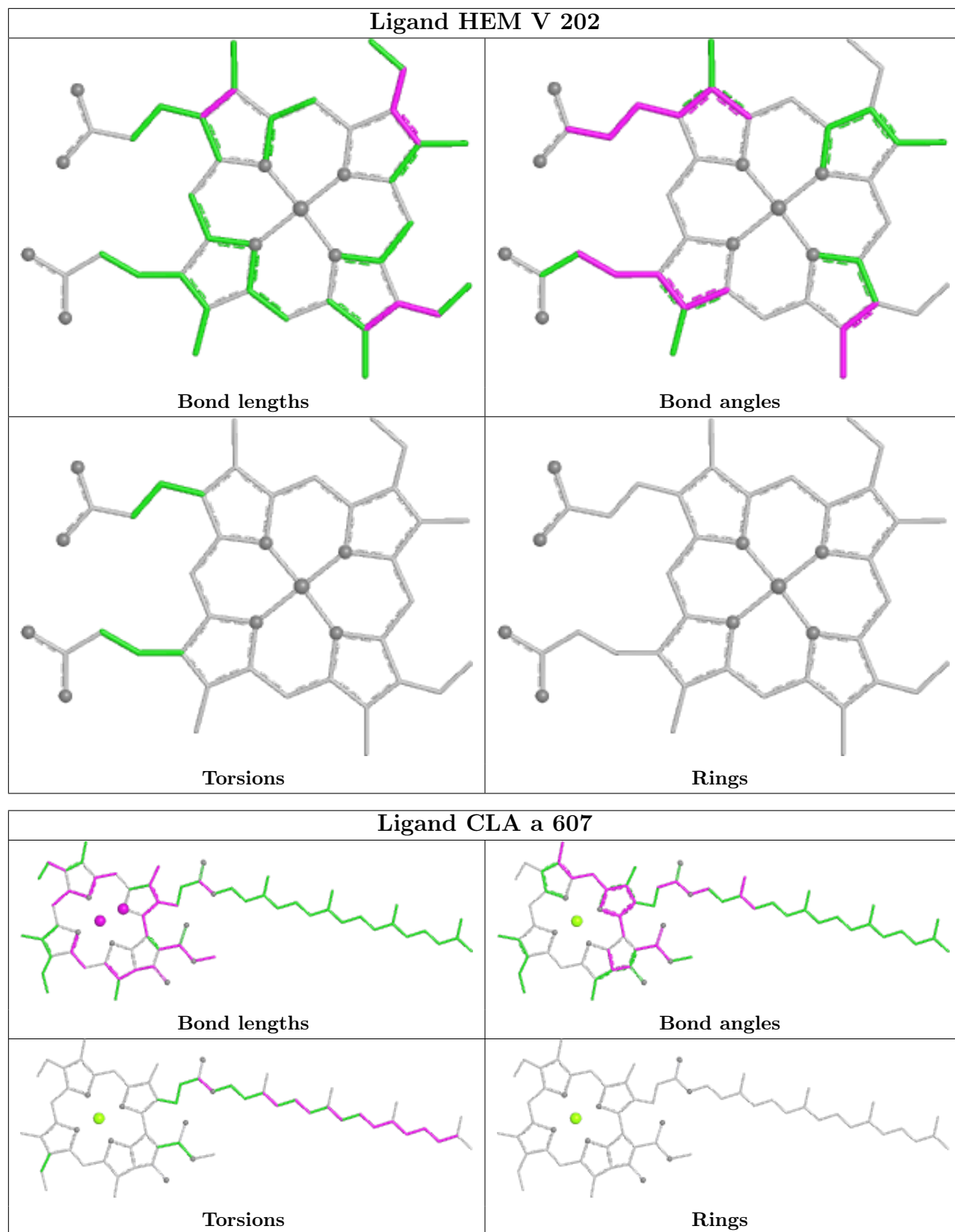
Ligand CLA B 611	
	
Bond lengths	Bond angles
	
Torsions	Rings

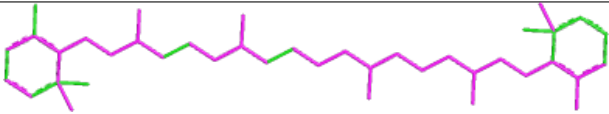
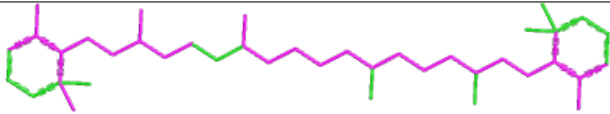
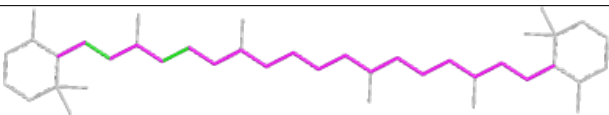
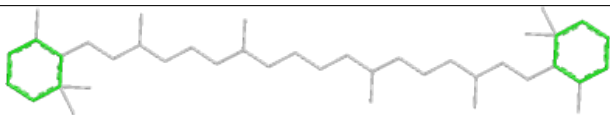
Ligand CLA b 605	
	
Bond lengths	Bond angles
	
Torsions	Rings

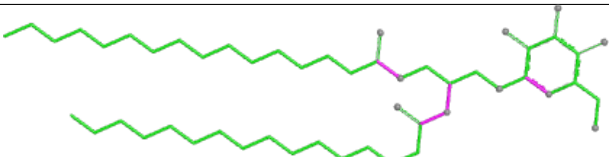
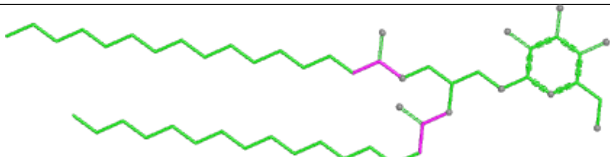
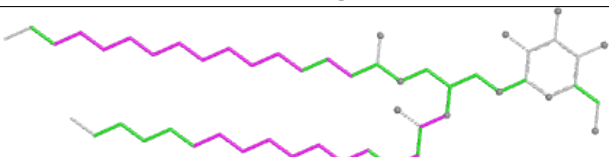
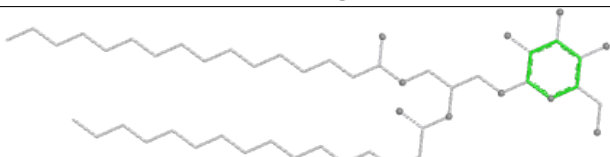
Ligand PL9 D 405	
	
Bond lengths	Bond angles
	
Torsions	Rings

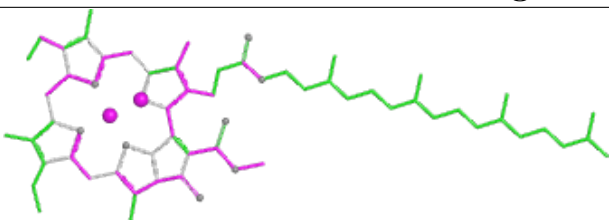
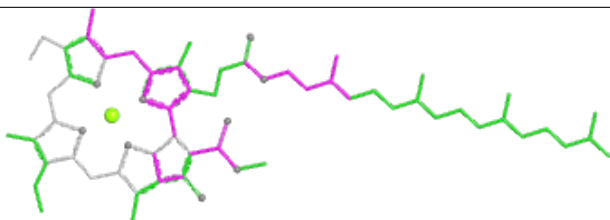
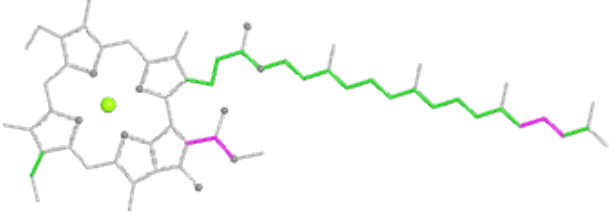
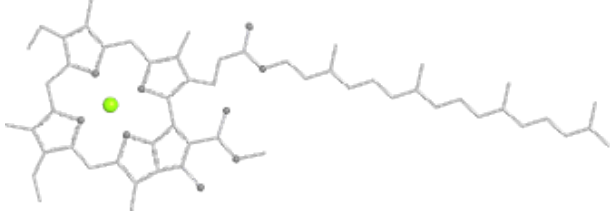


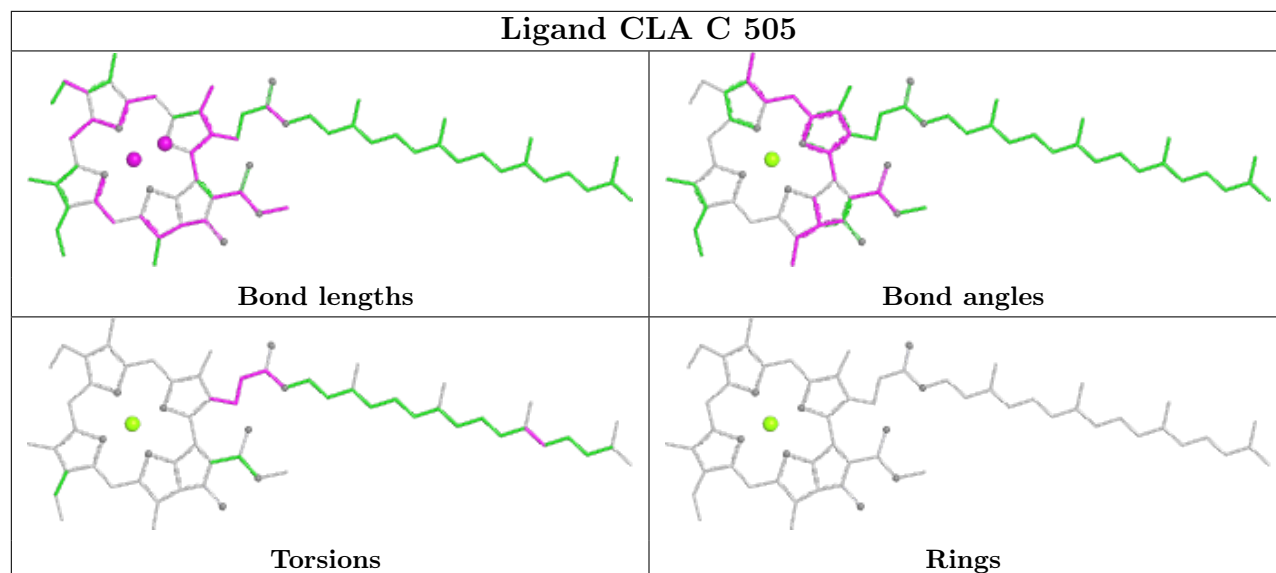
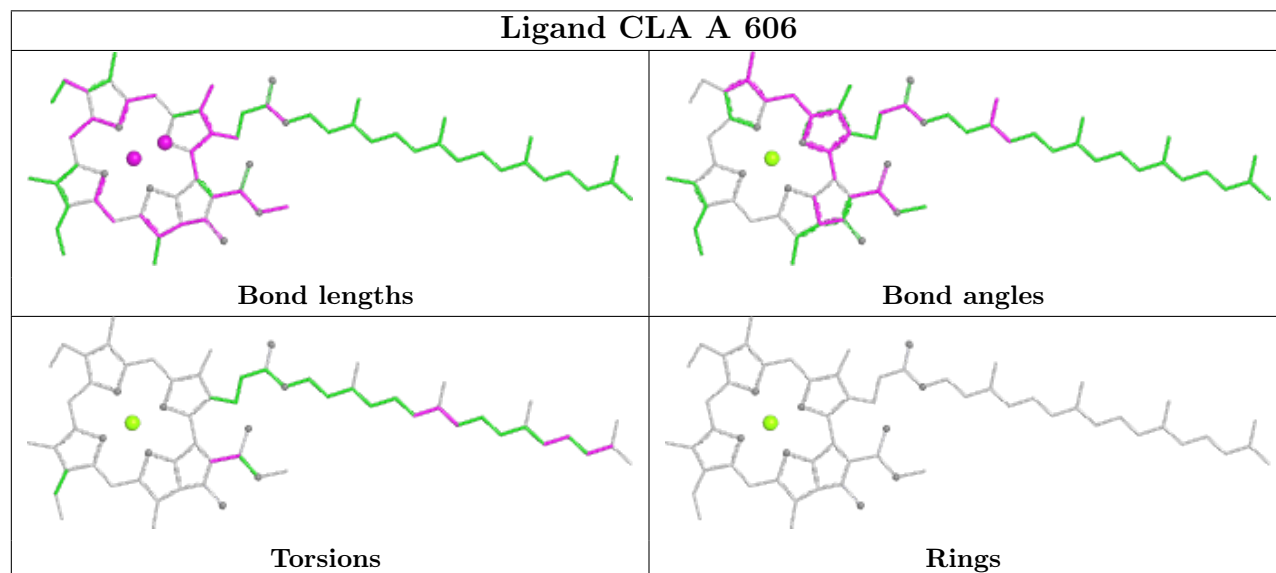
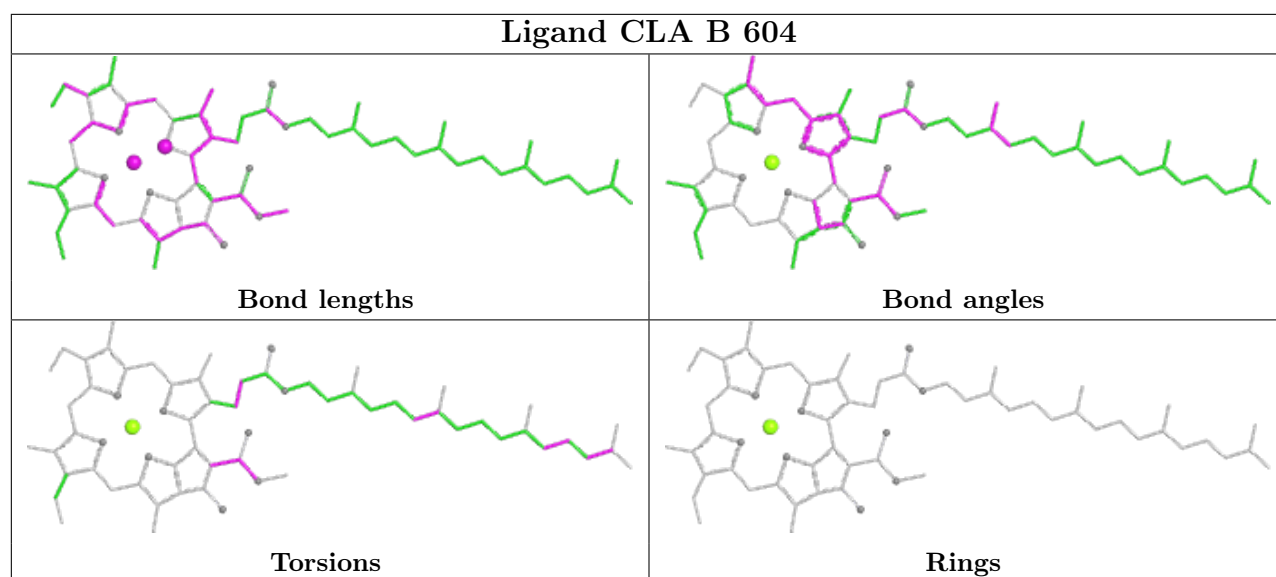
Ligand CLA A 608**Ligand CLA b 617**

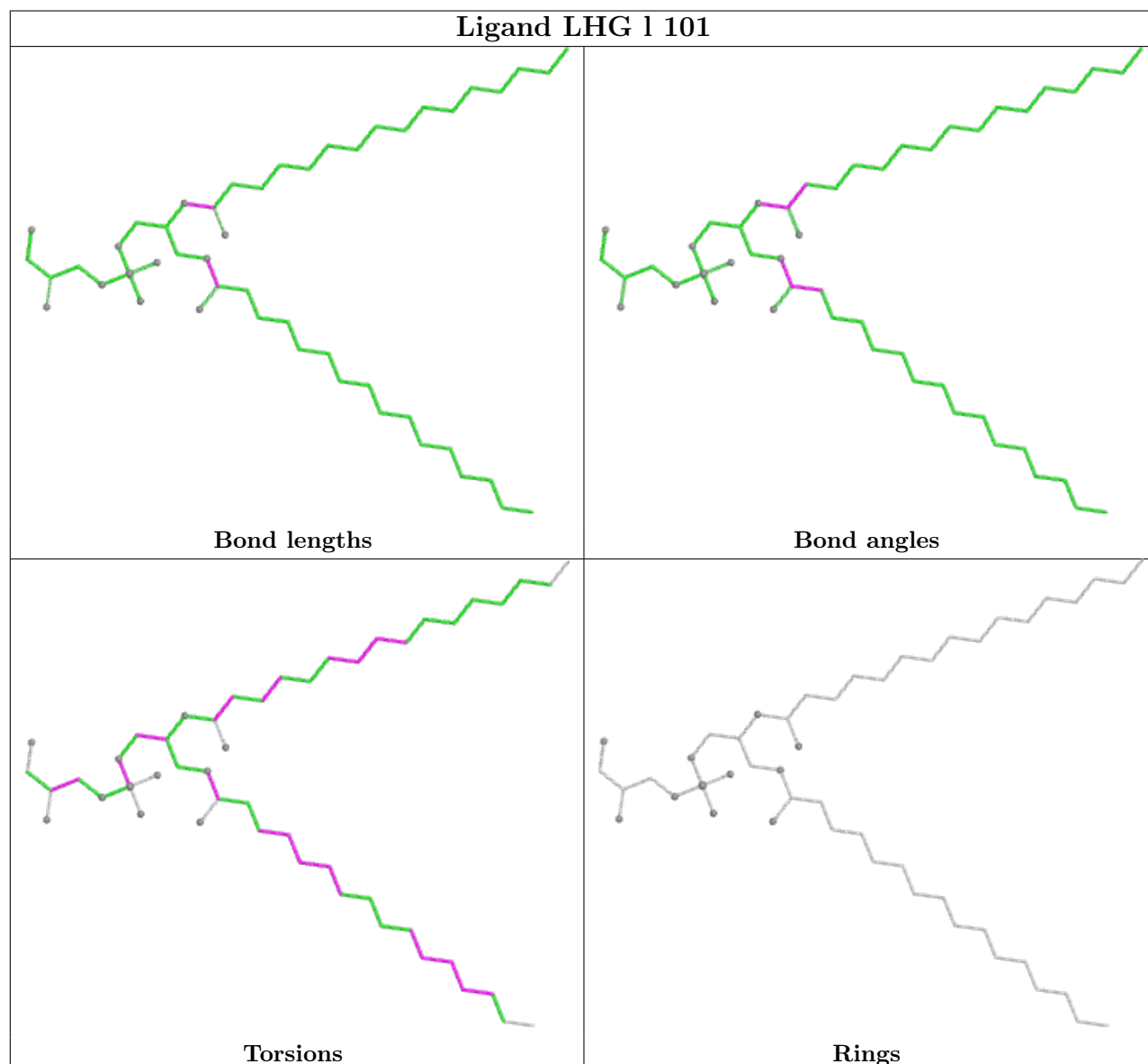
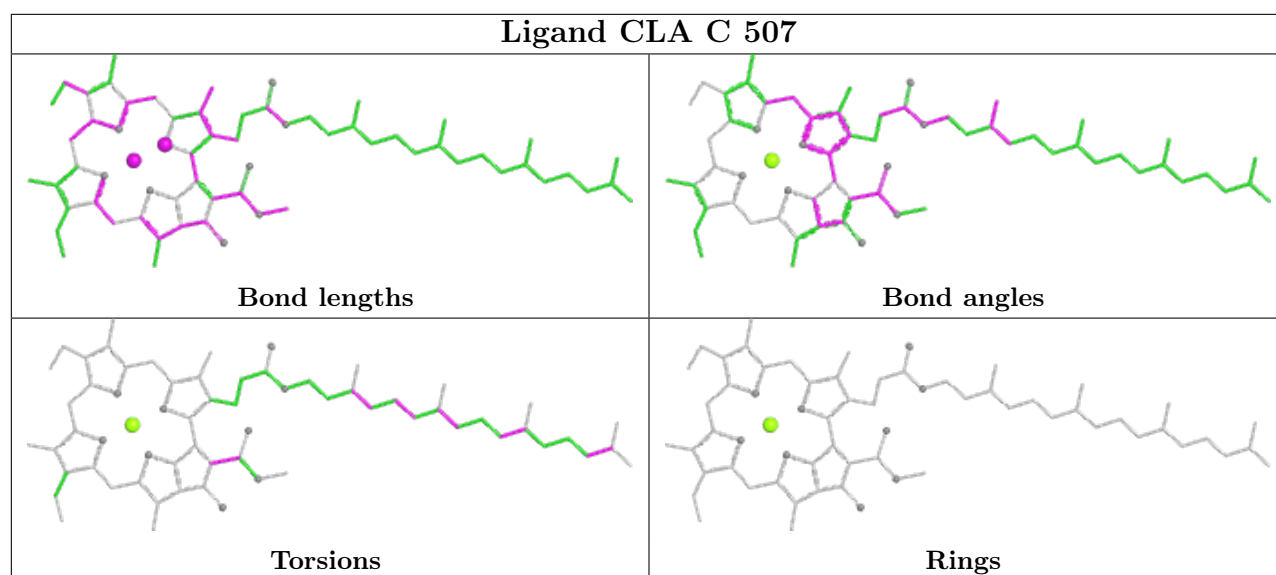


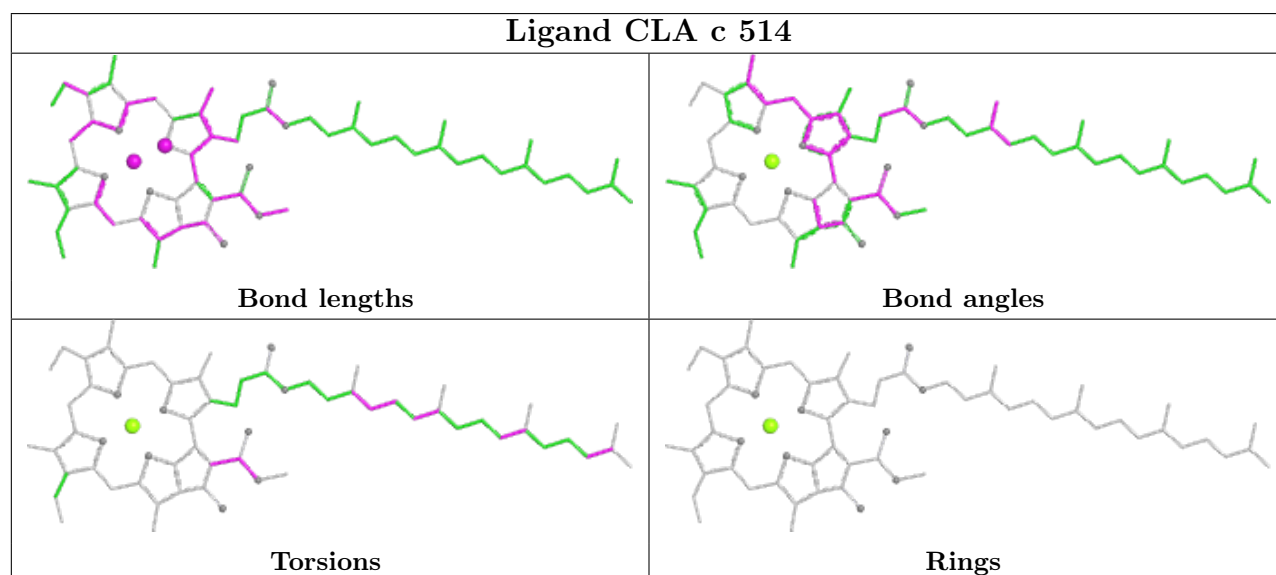
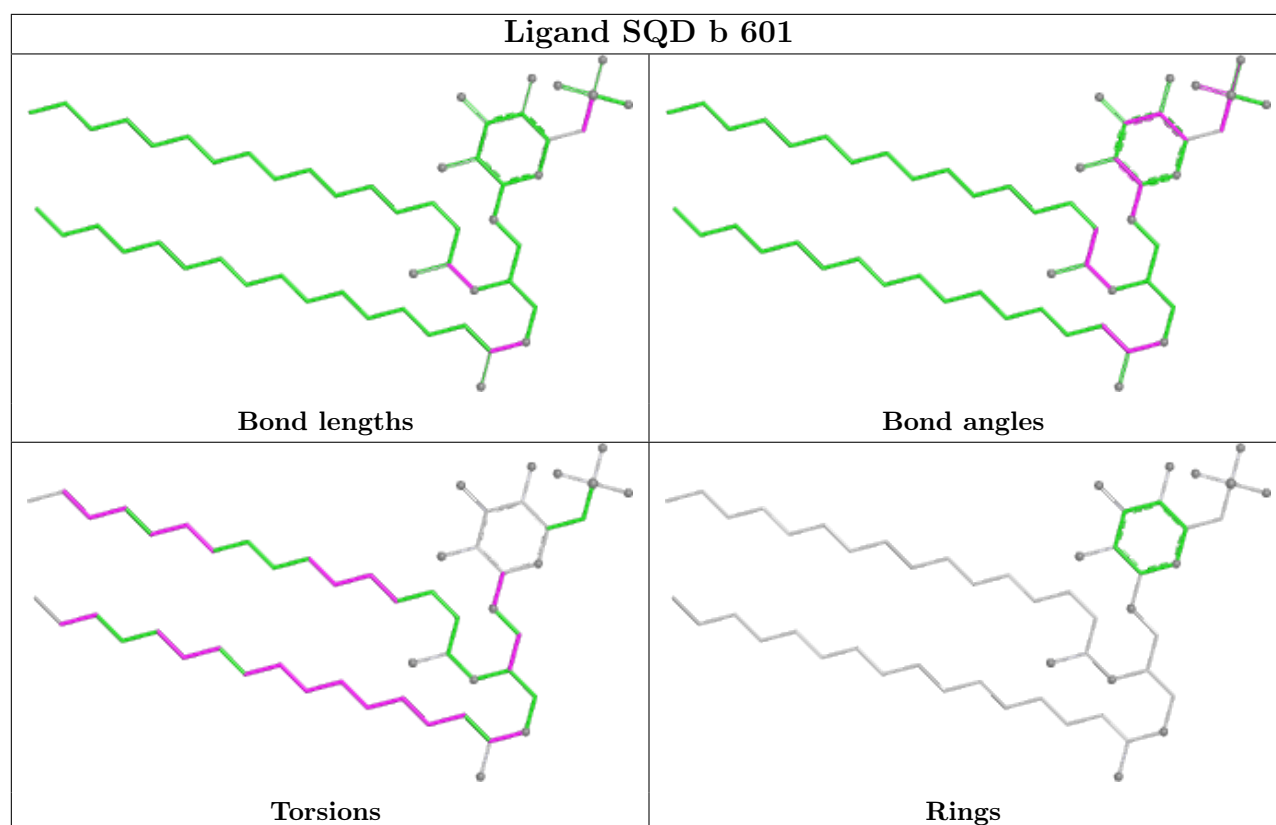
Ligand BCR c 516	
	
Bond lengths	Bond angles
	
Torsions	Rings

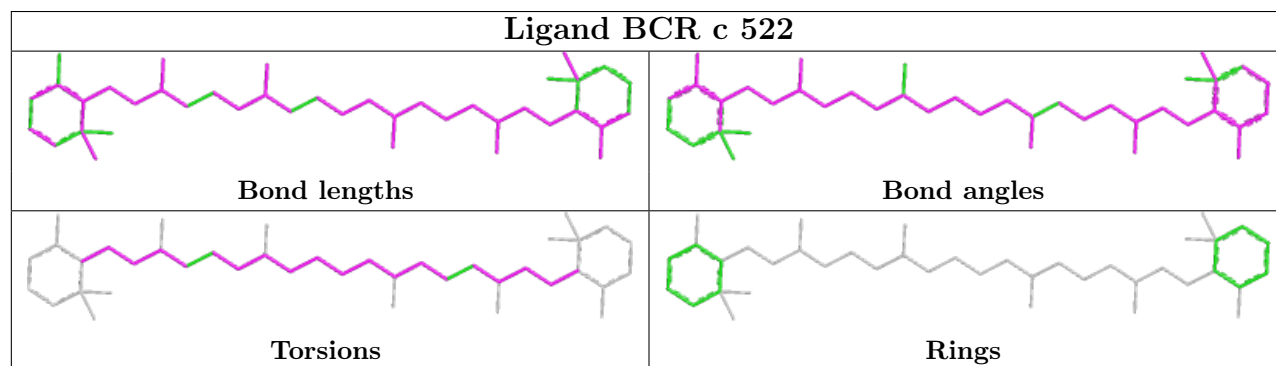
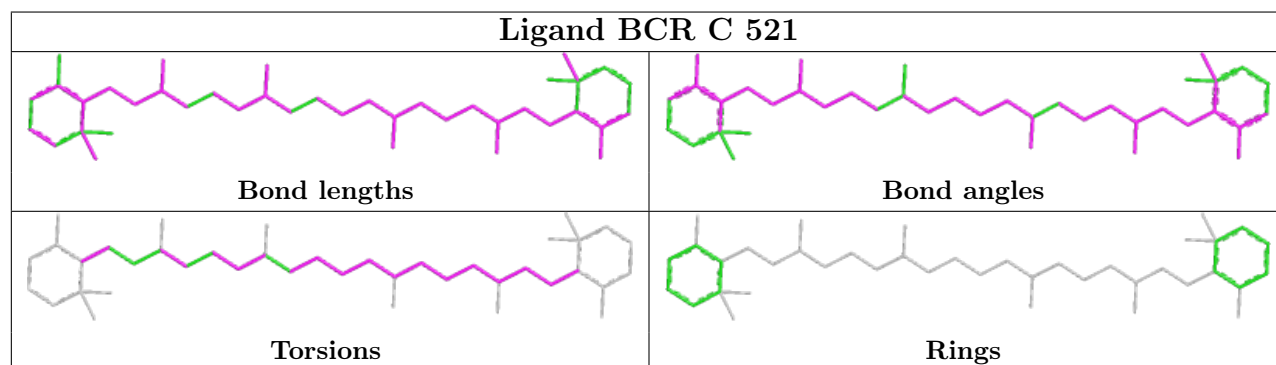
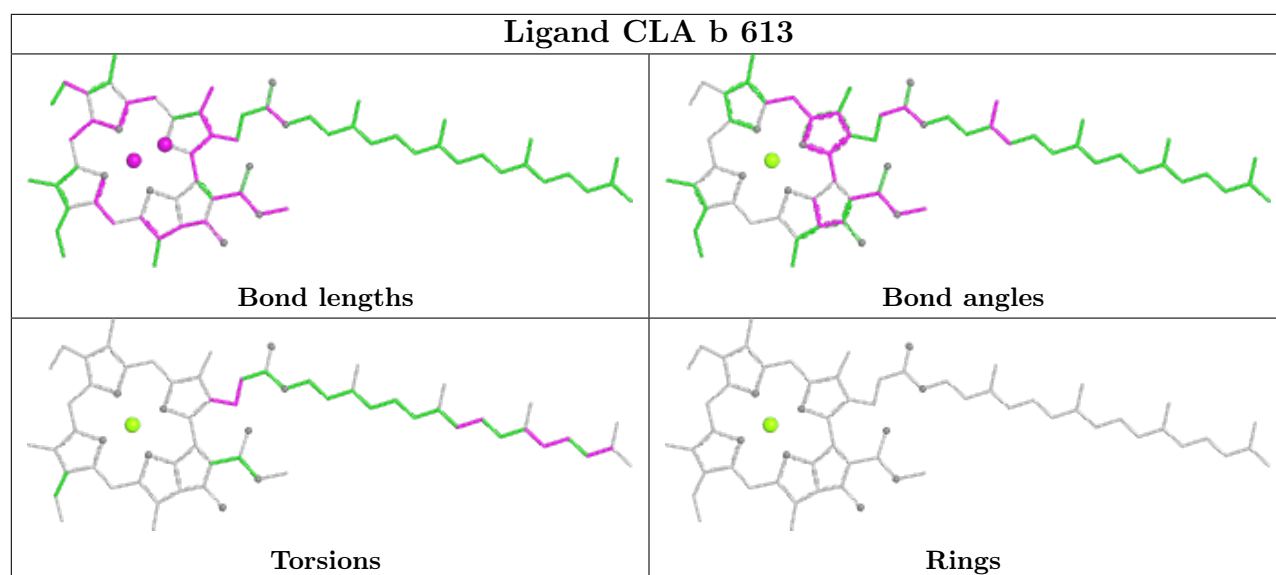
Ligand LMG b 623	
	
Bond lengths	Bond angles
	
Torsions	Rings

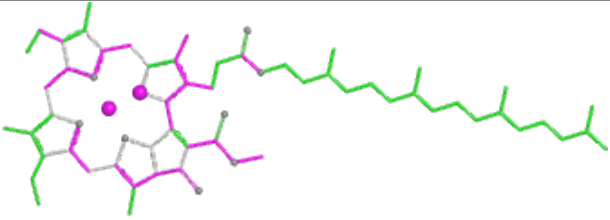
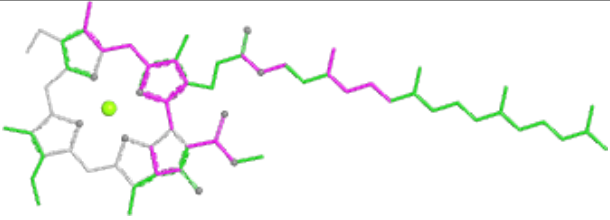
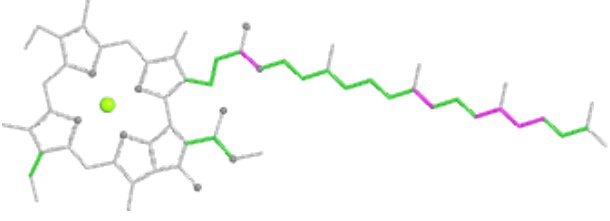
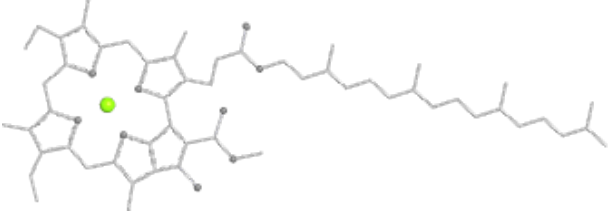
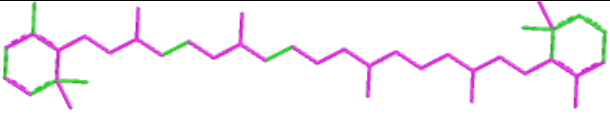
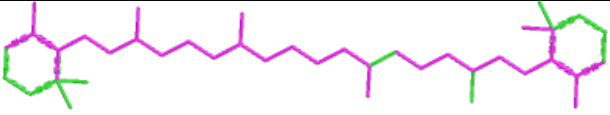

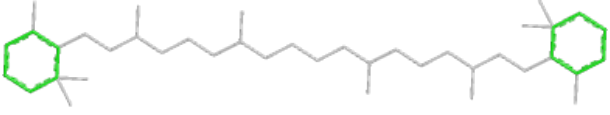
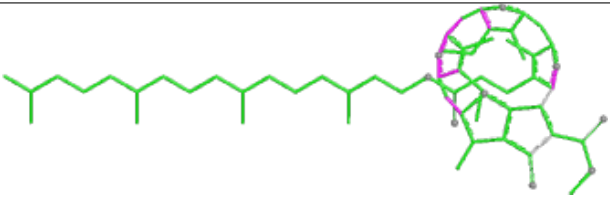
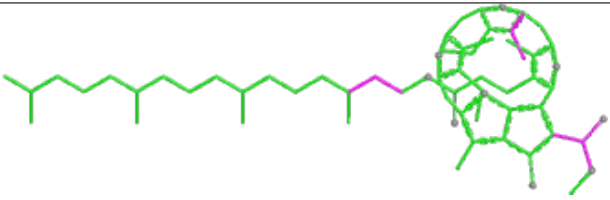
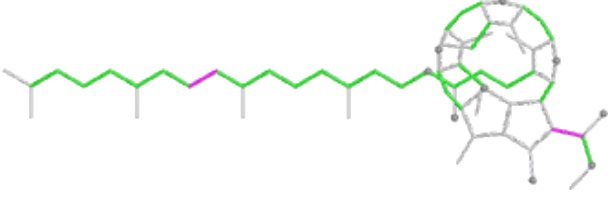
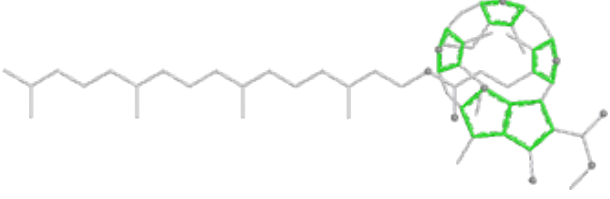
Ligand CLA b 616	
	
Bond lengths	Bond angles
	
Torsions	Rings

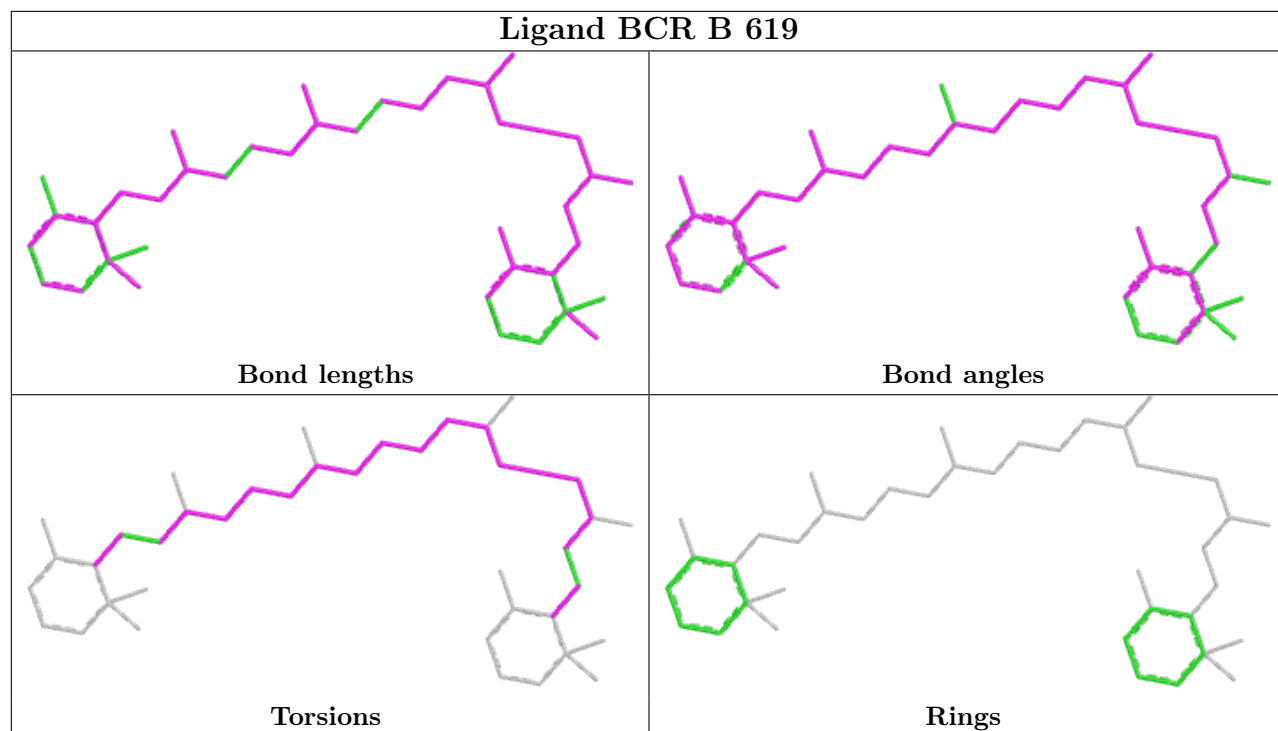


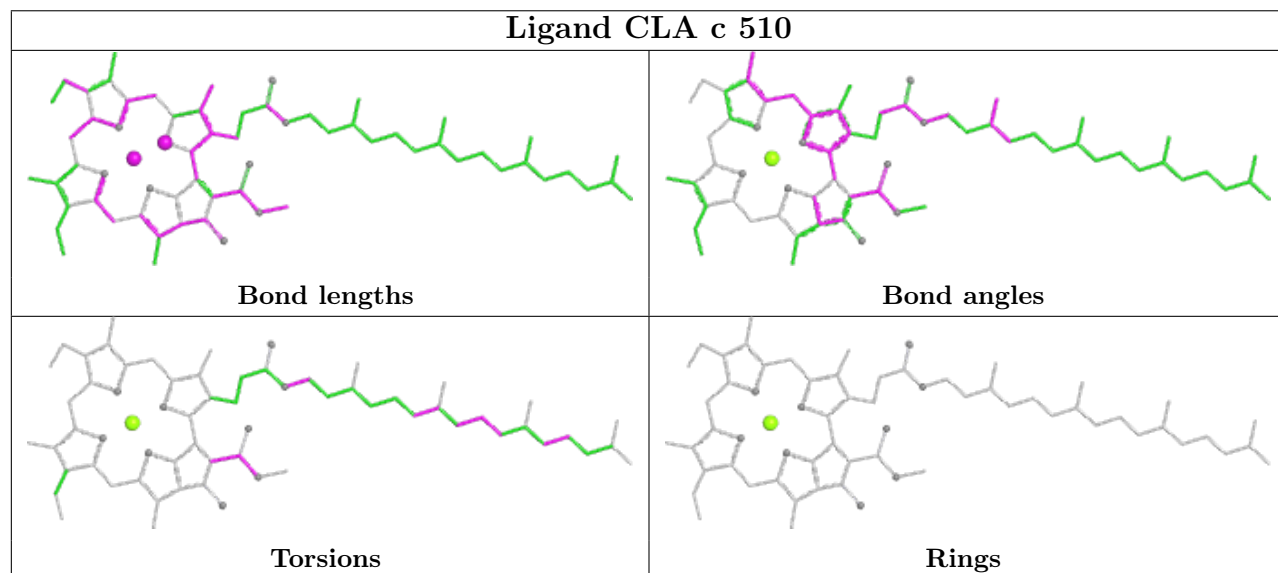
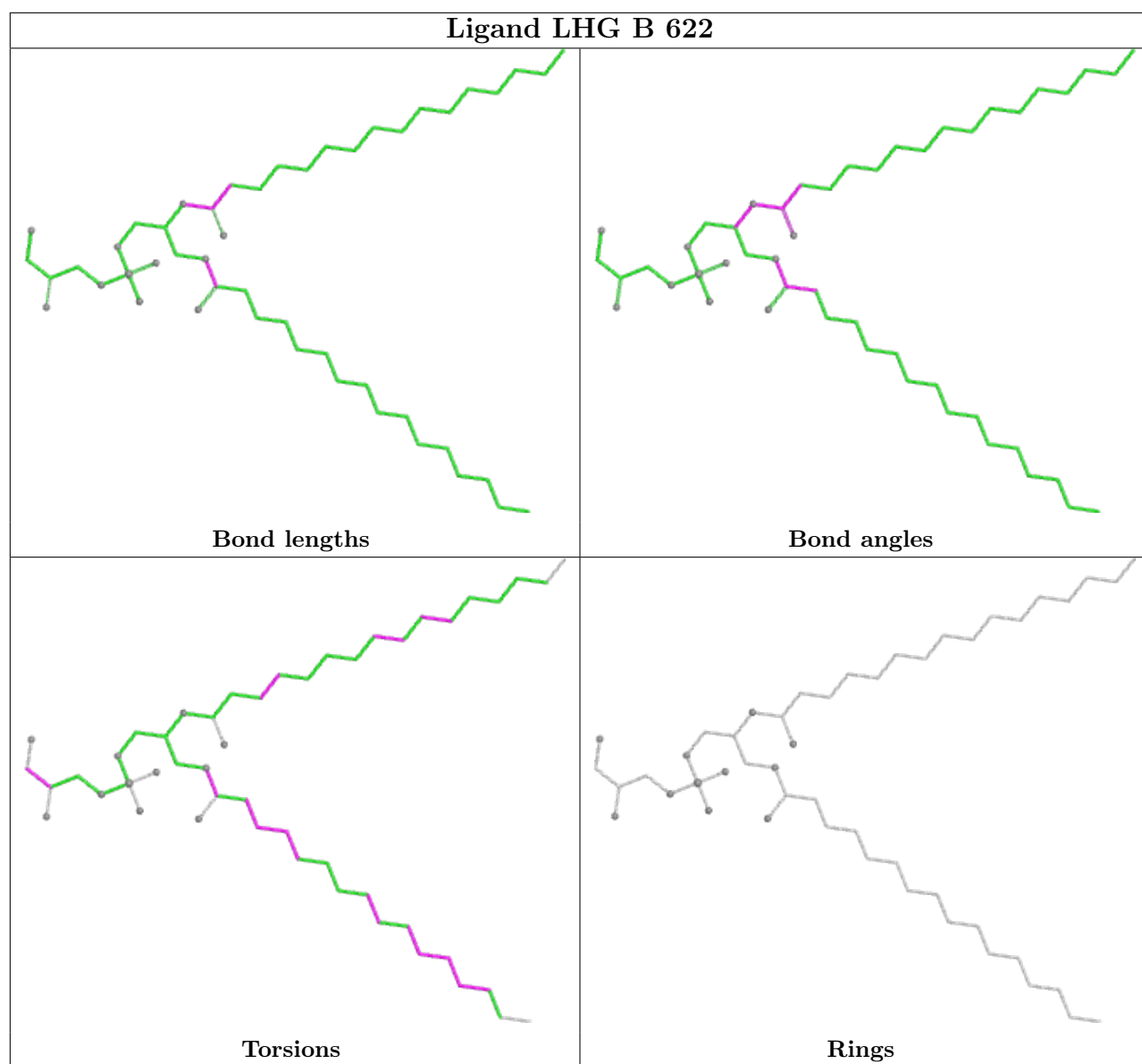


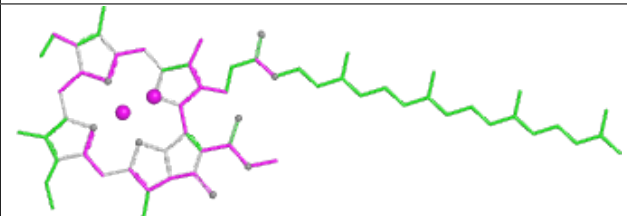
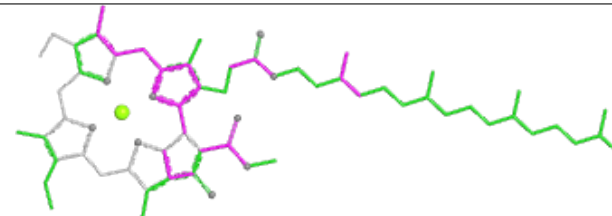
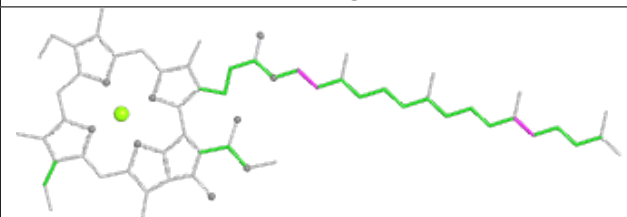
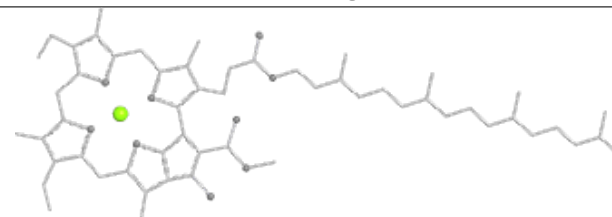


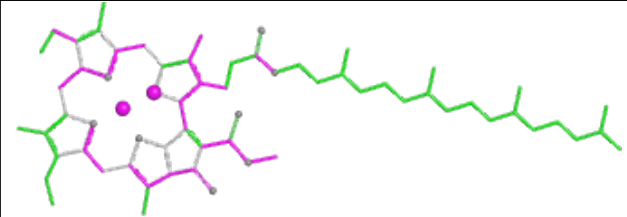
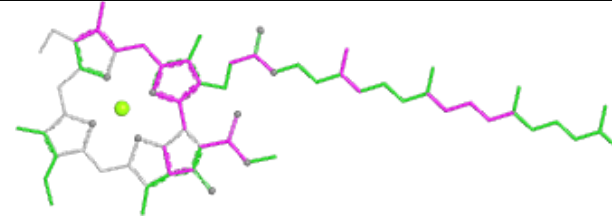
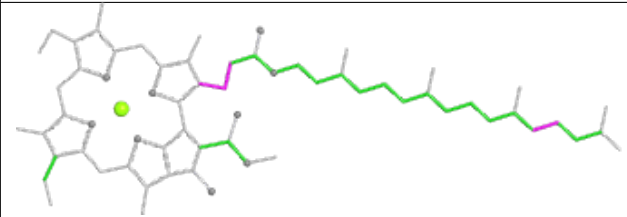
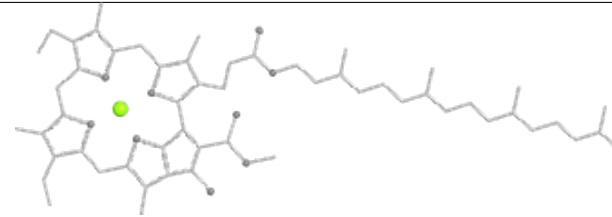


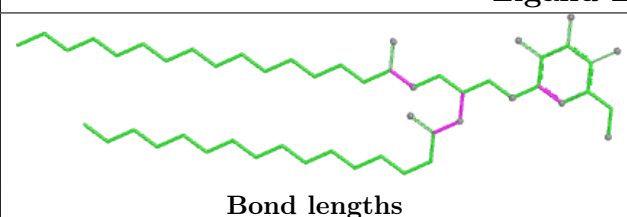
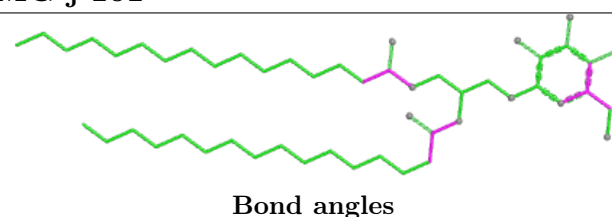
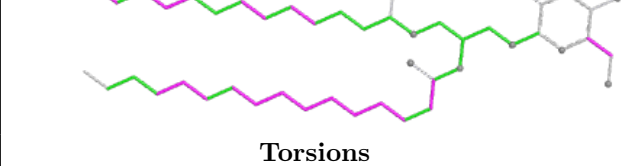

Ligand CLA C 504	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR a 608	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand PHO D 401	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

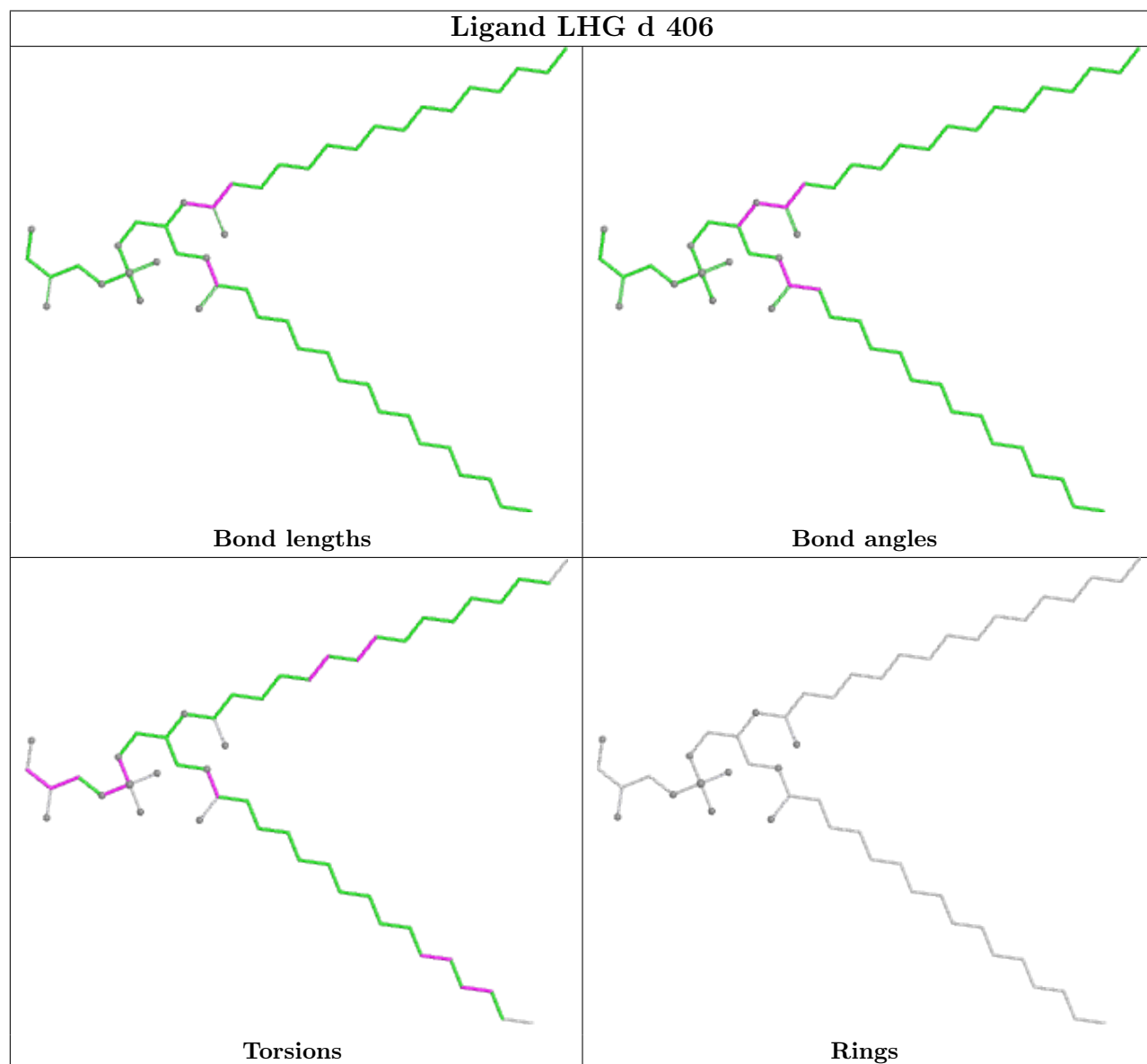
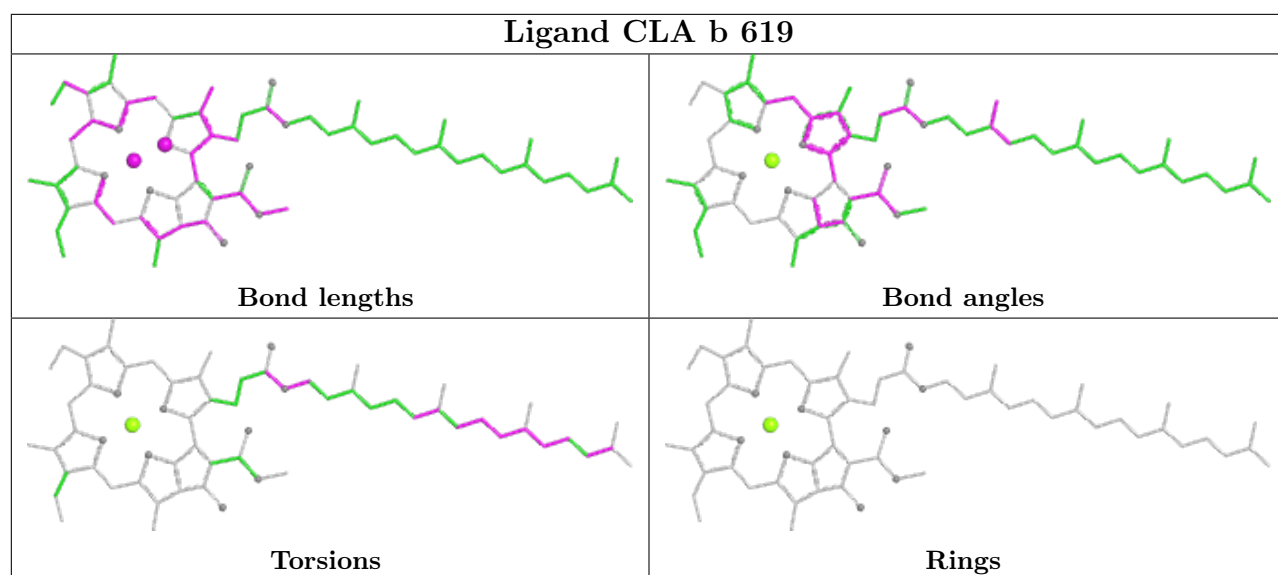


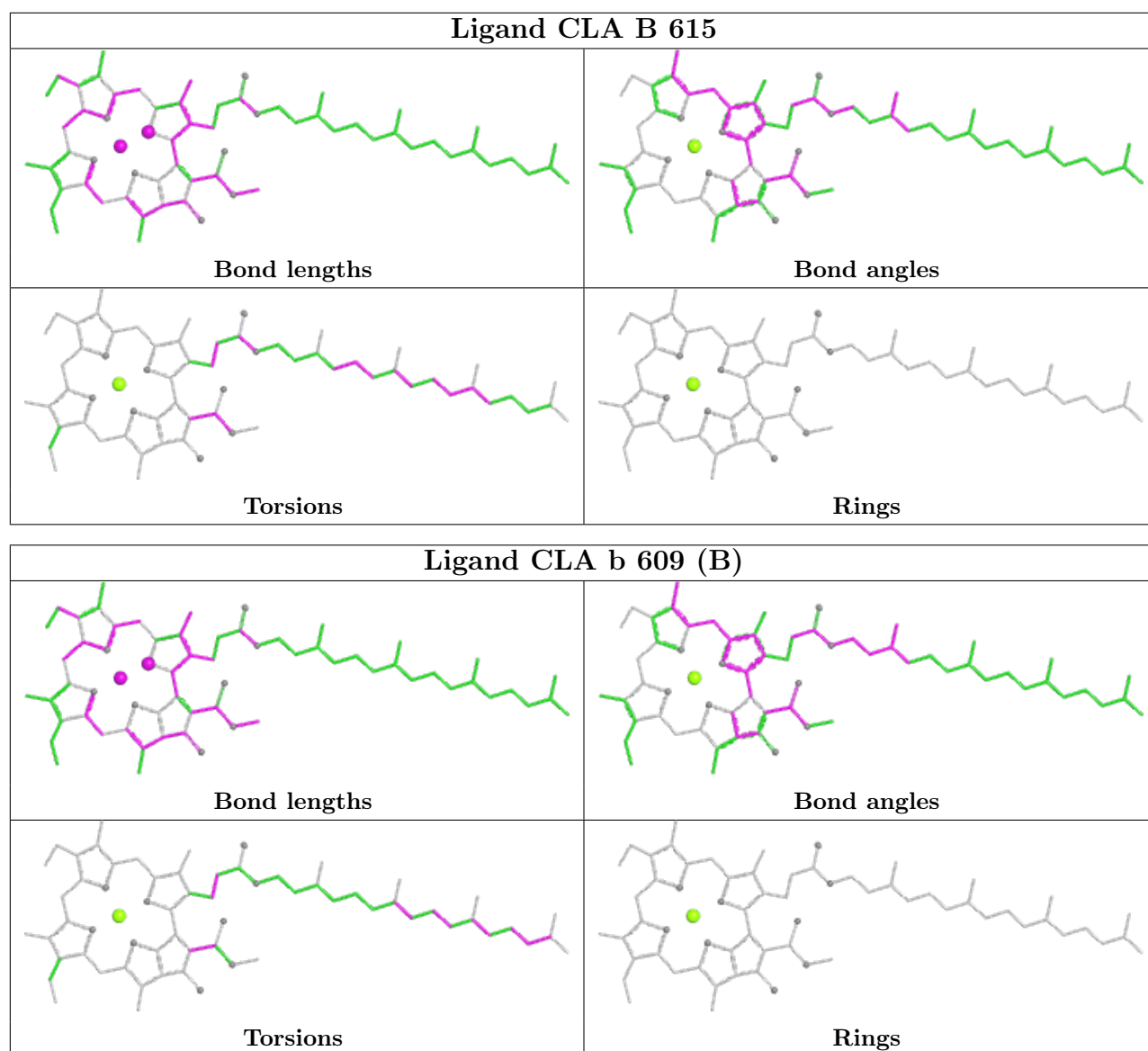


Ligand CLA D 403	
	
Bond lengths	Bond angles
	
Torsions	Rings

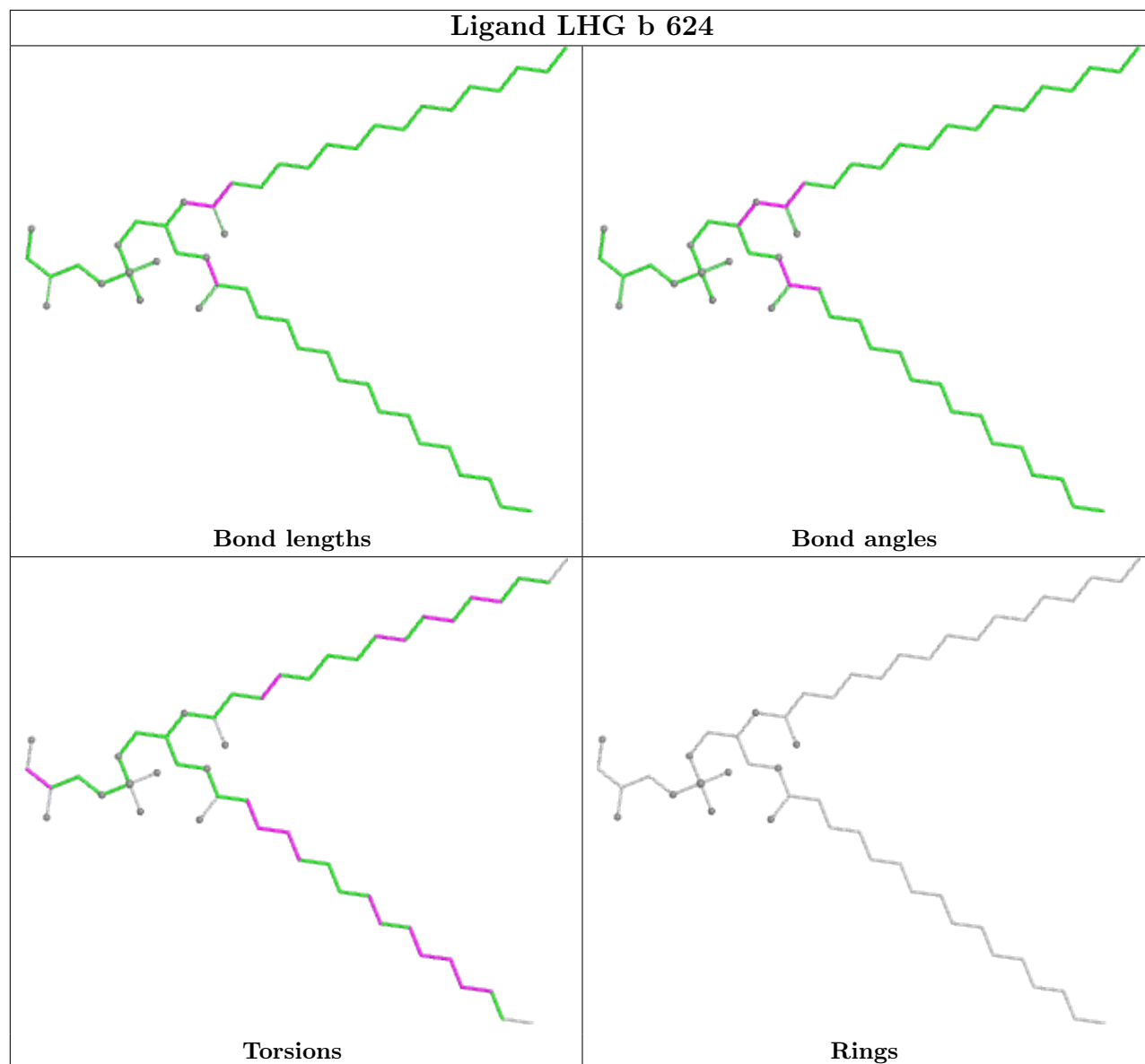
Ligand CLA b 611	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LMG j 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

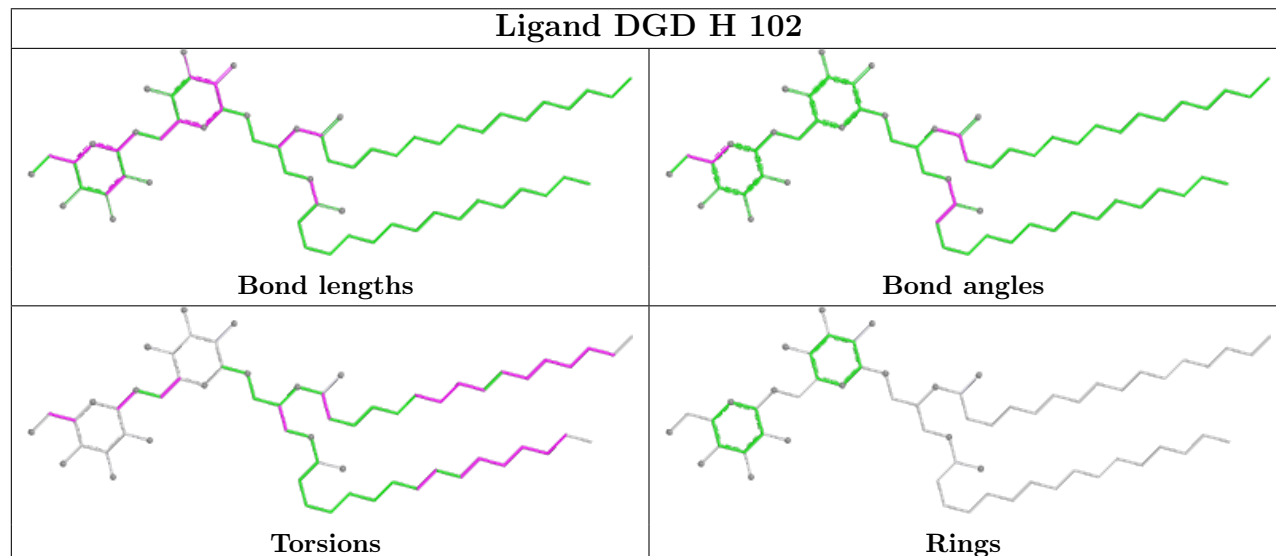


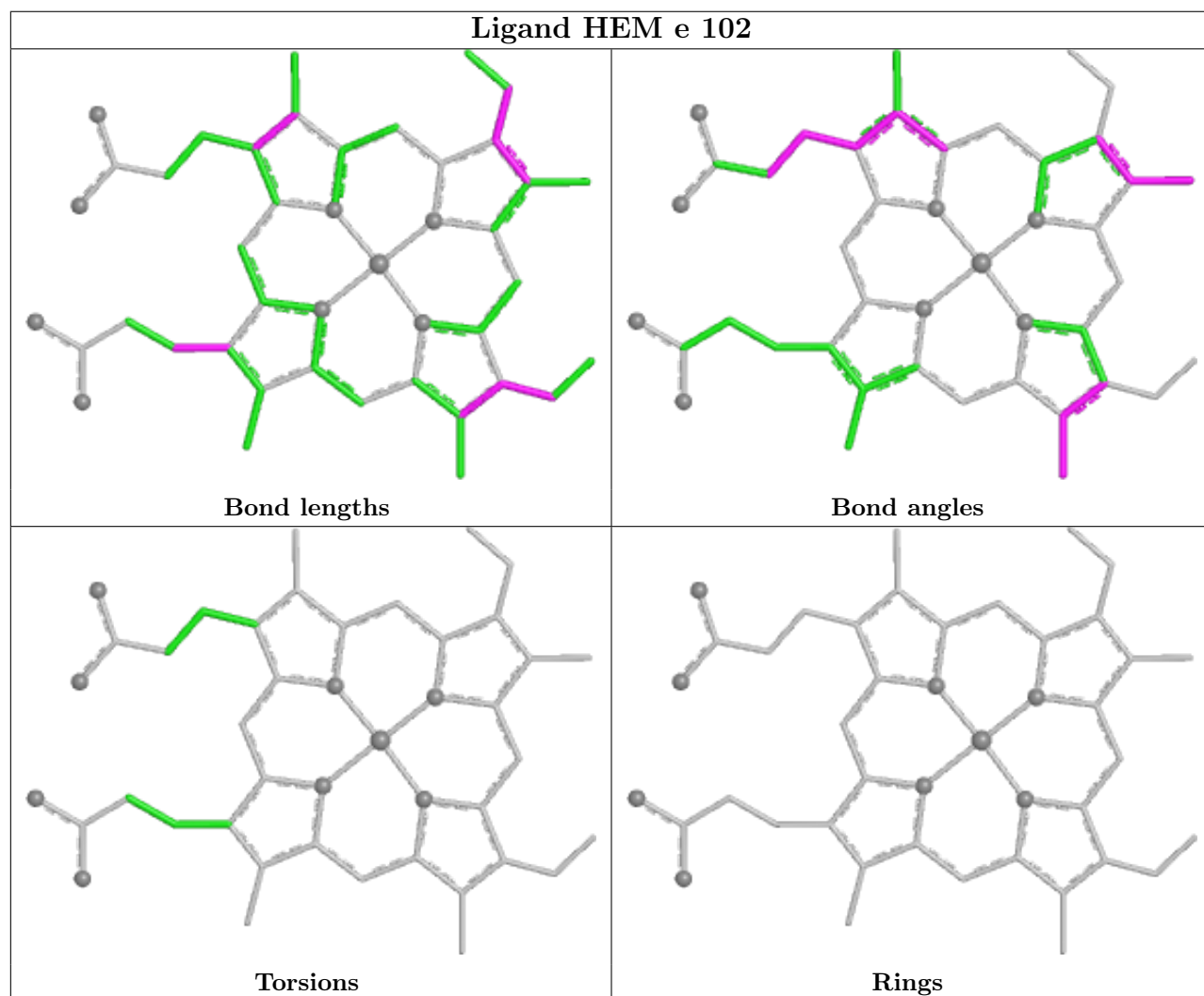
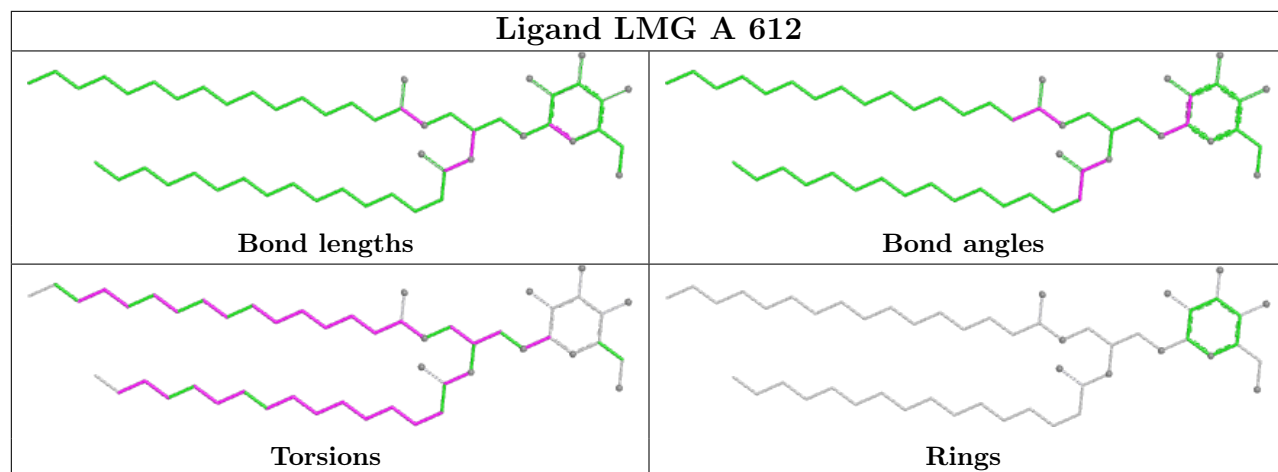


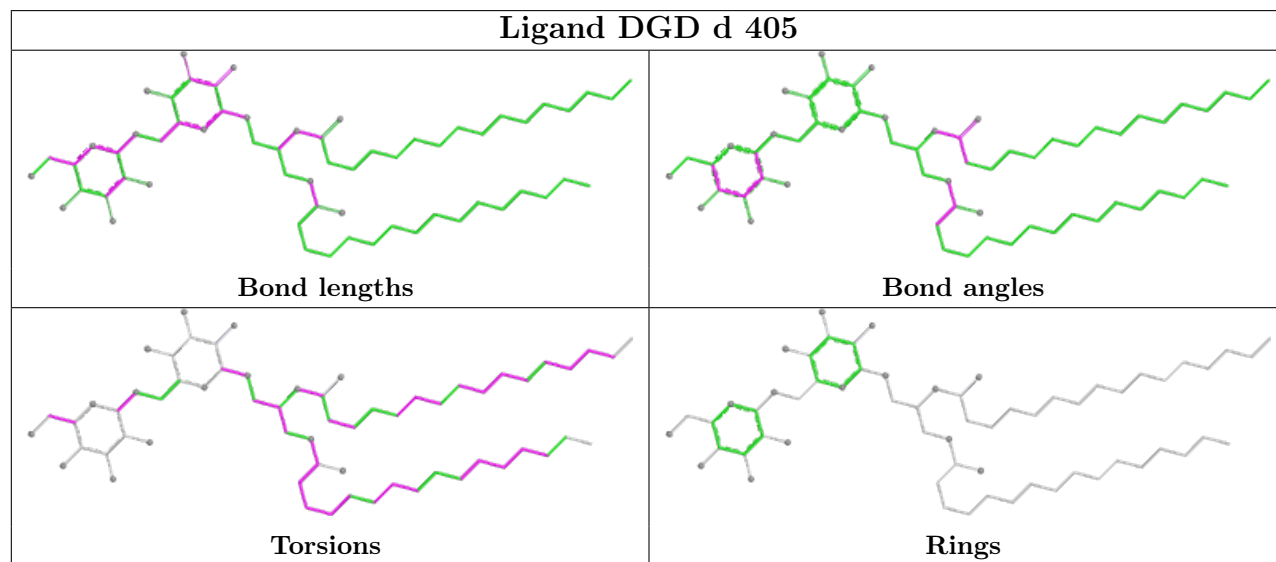
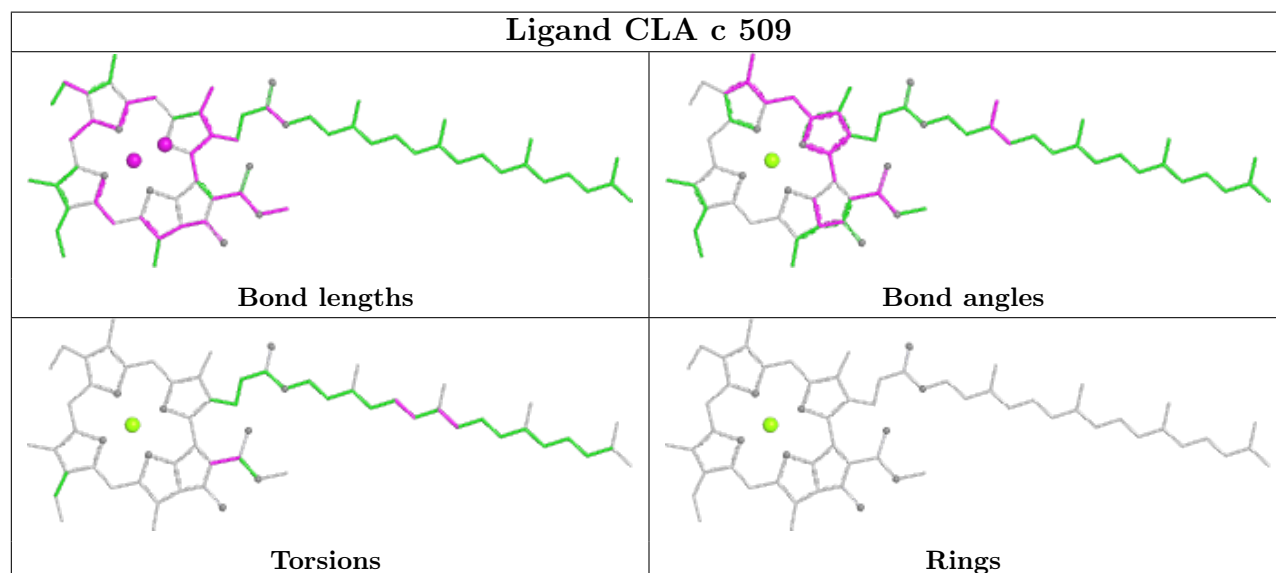
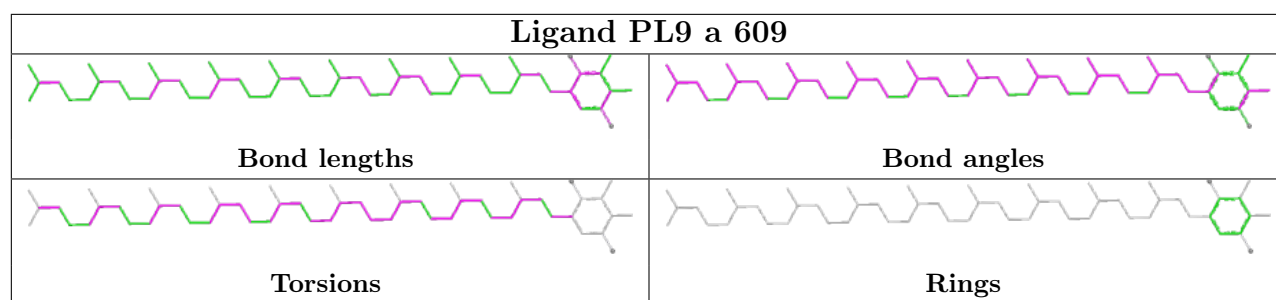
Ligand LHG b 624

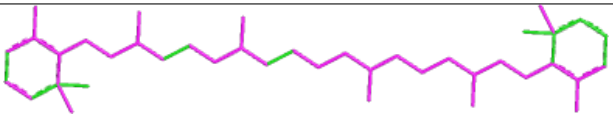
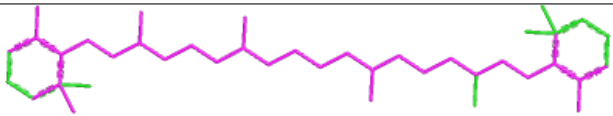
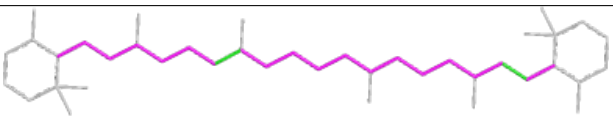
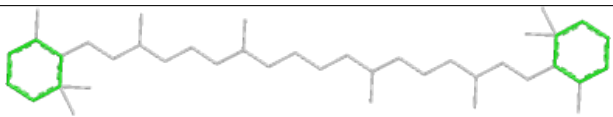


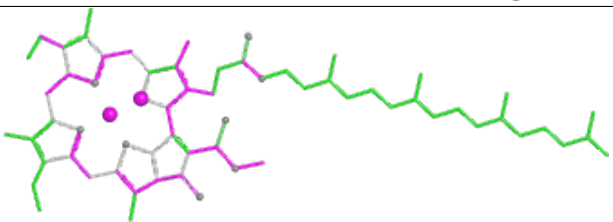
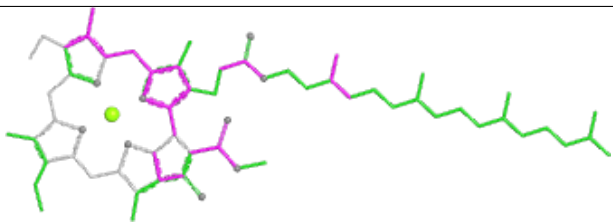
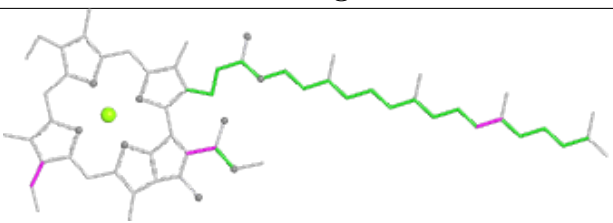
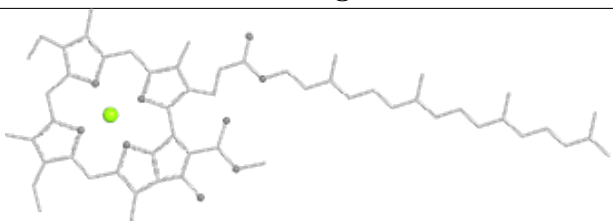
Ligand DGD H 102

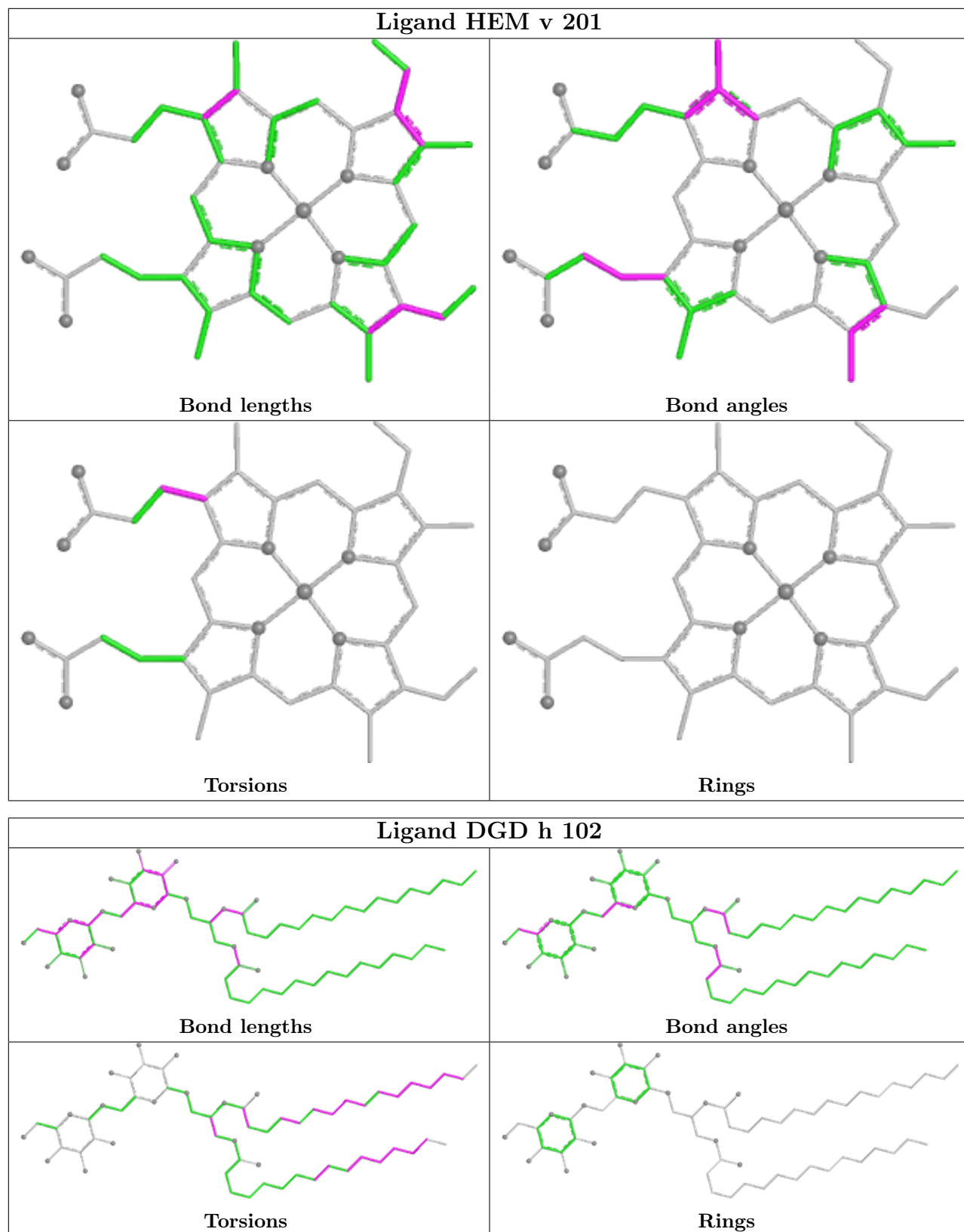


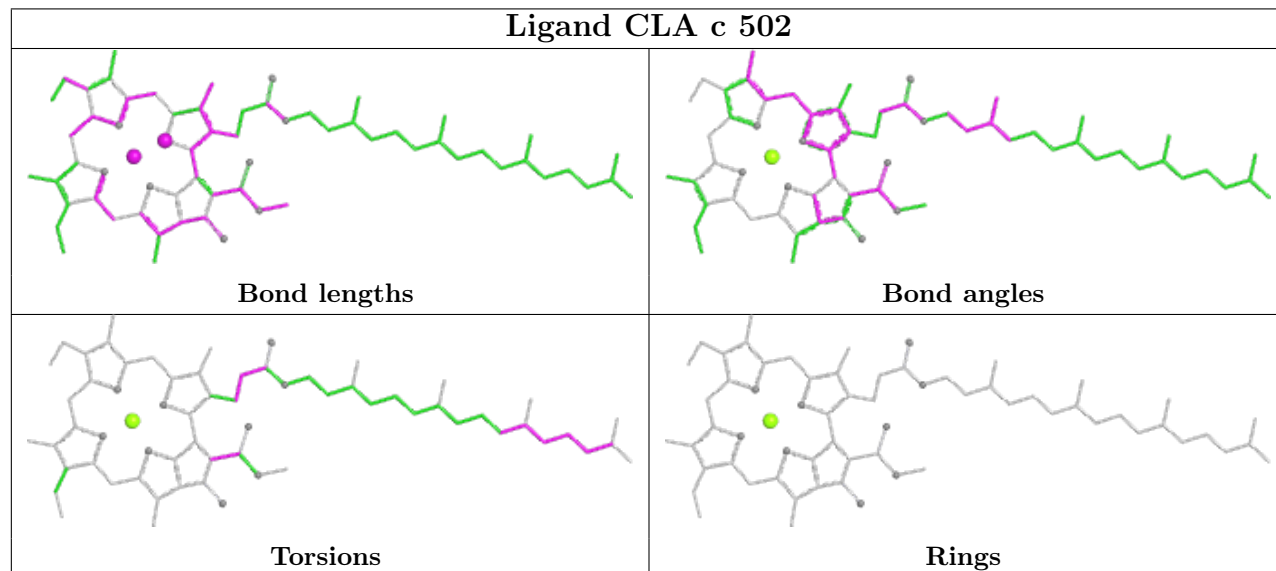
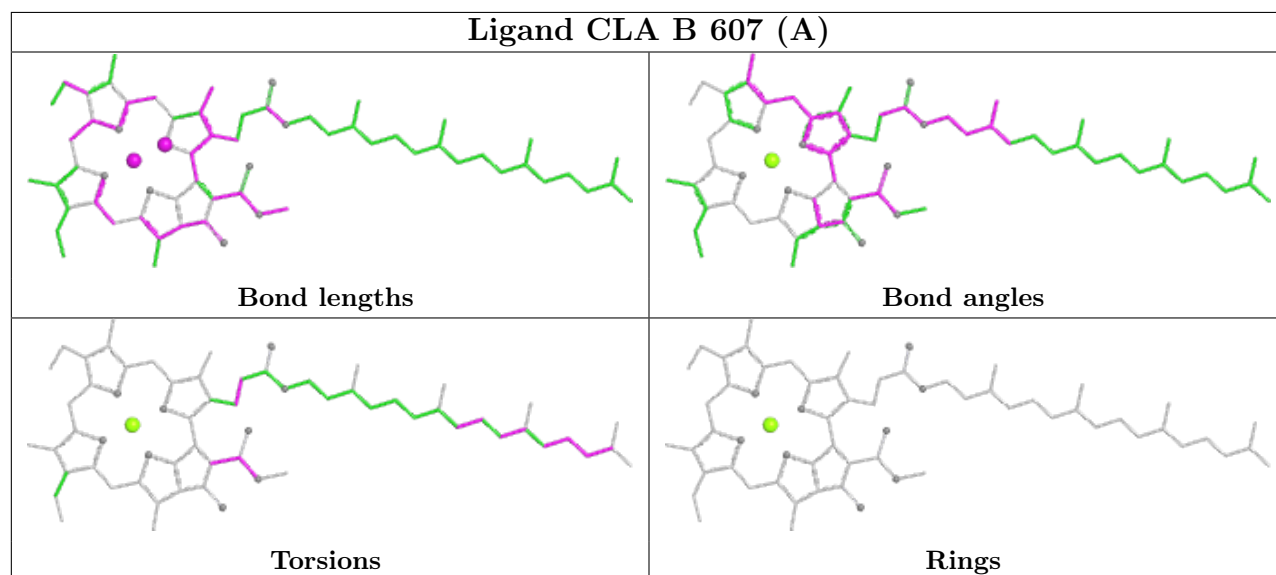
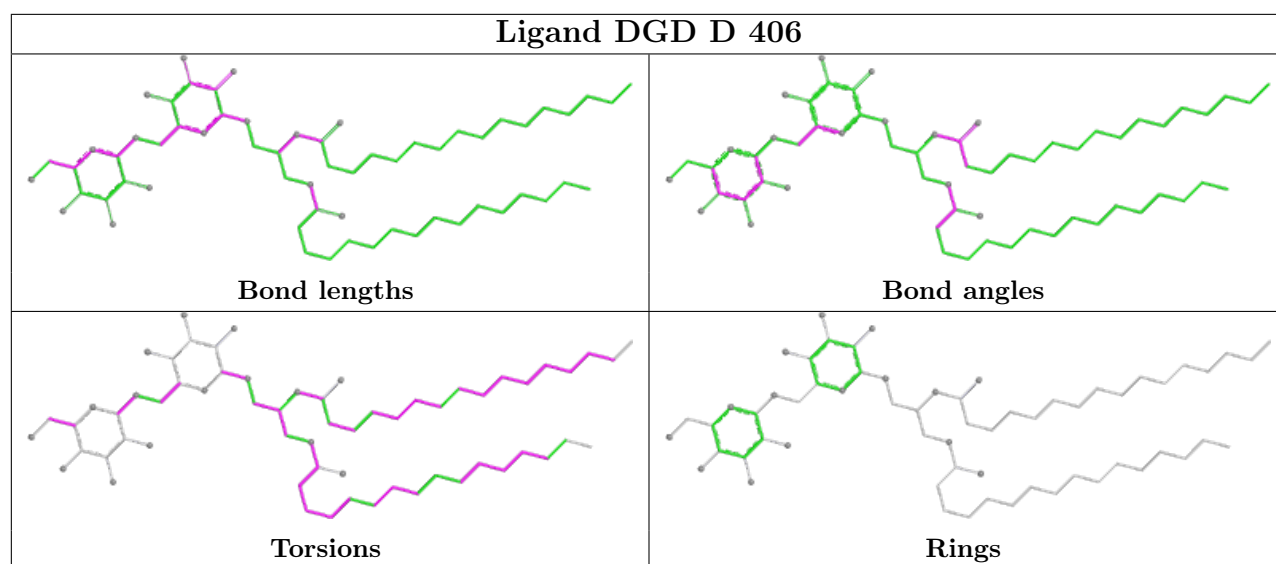


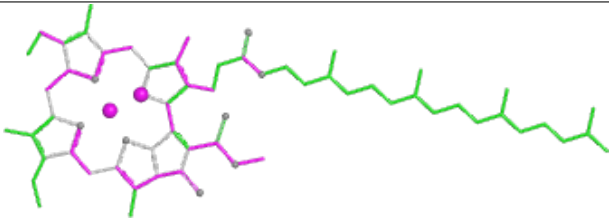
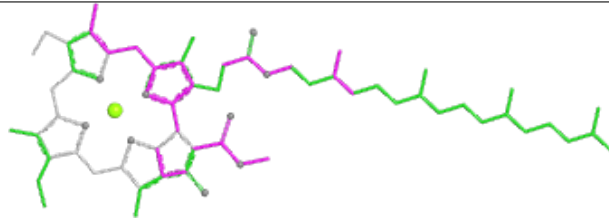
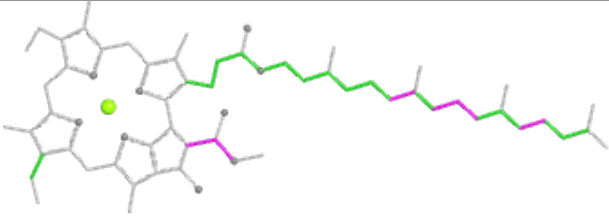
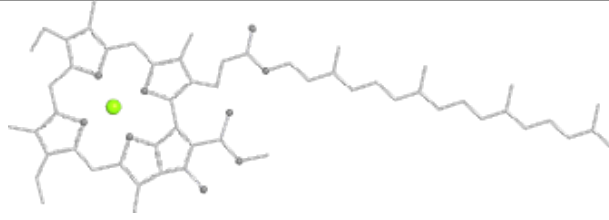


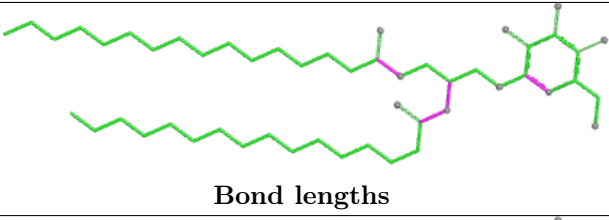
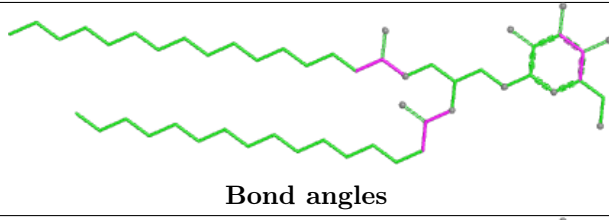
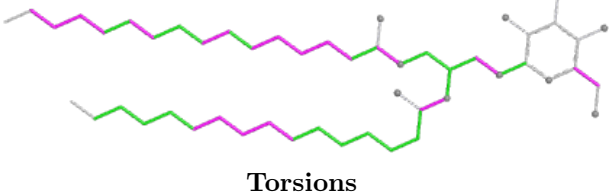
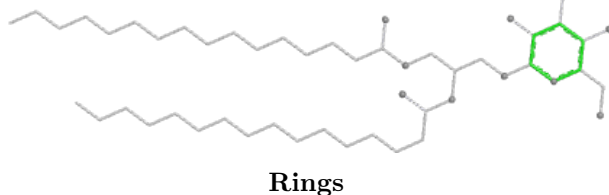
Ligand BCR b 622	
	
Bond lengths	Bond angles
	
Torsions	Rings

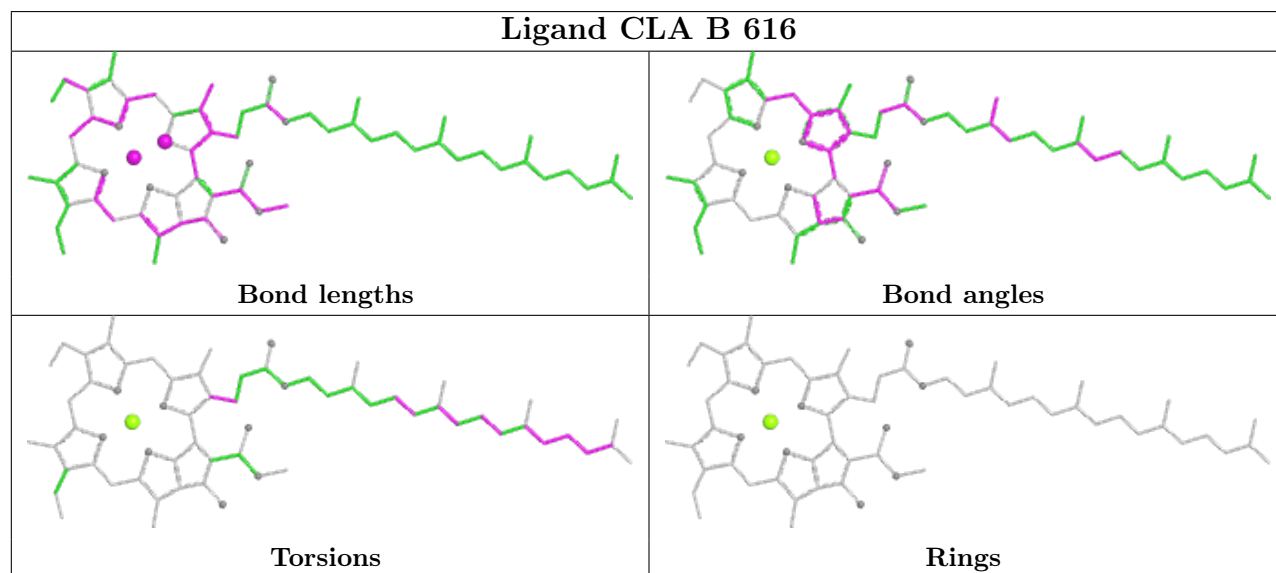
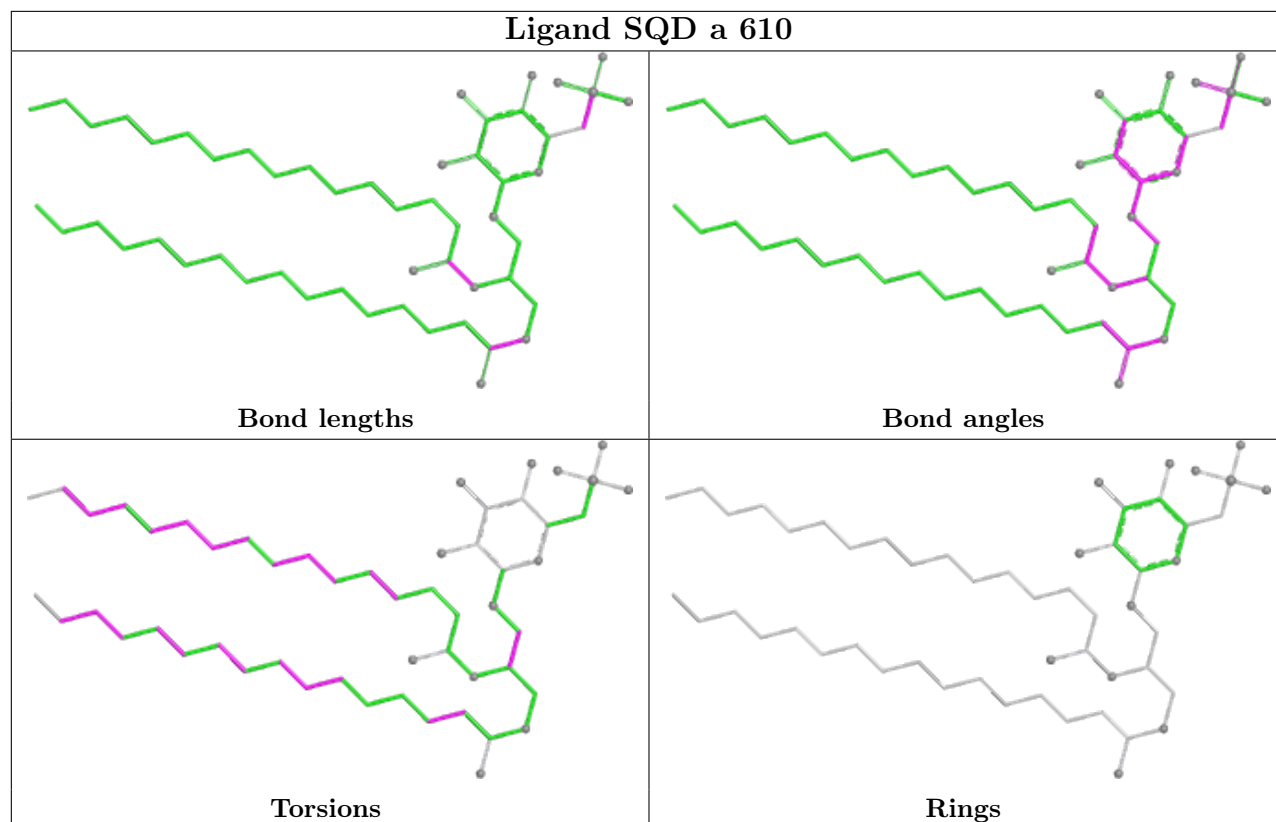
Ligand CLA D 402	
	
Bond lengths	Bond angles
	
Torsions	Rings

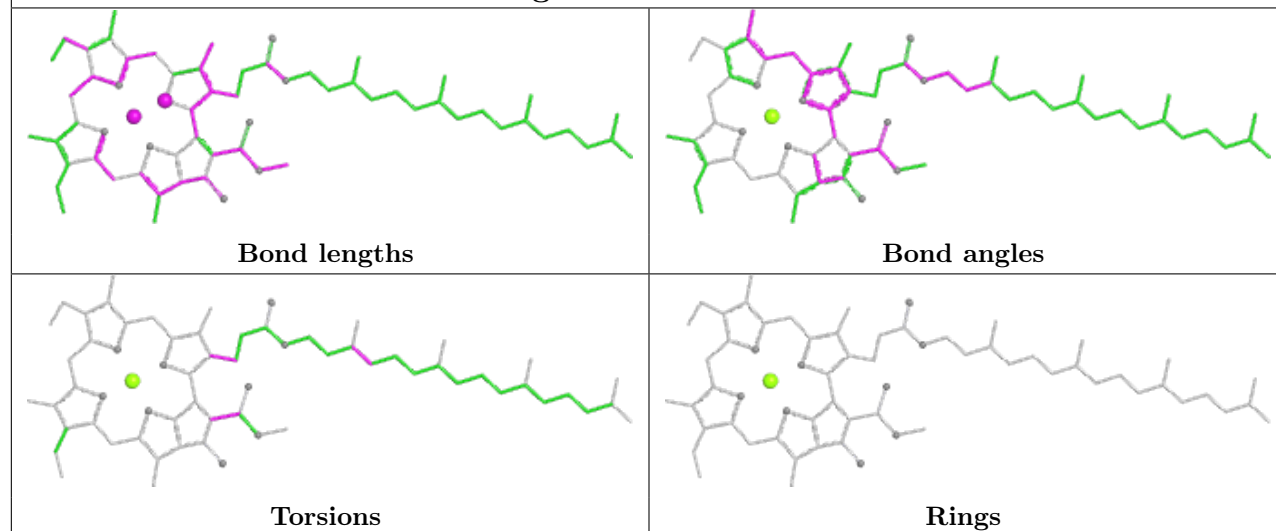
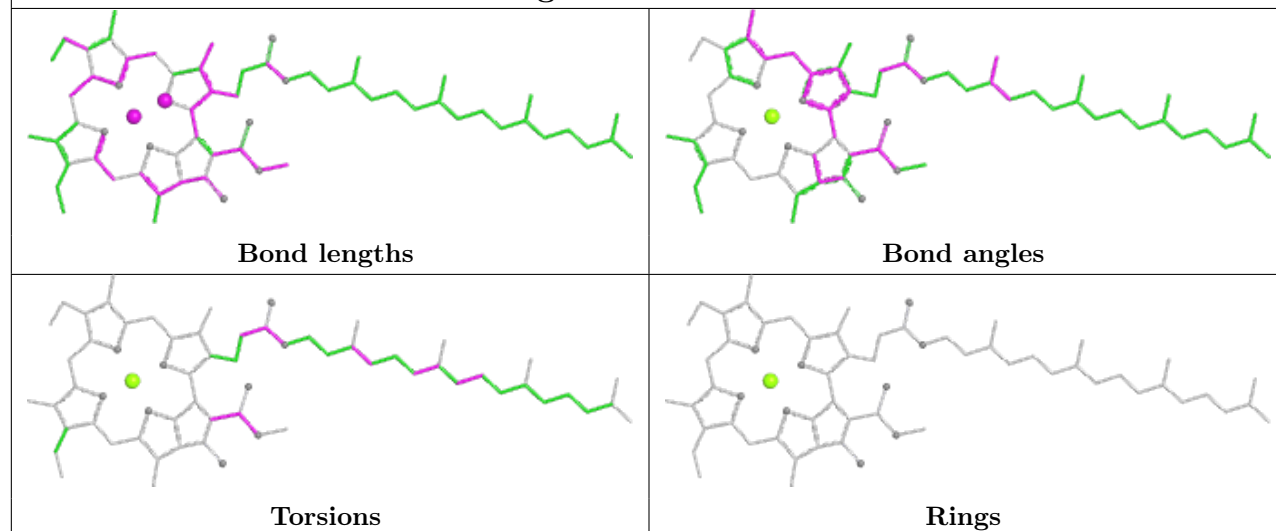


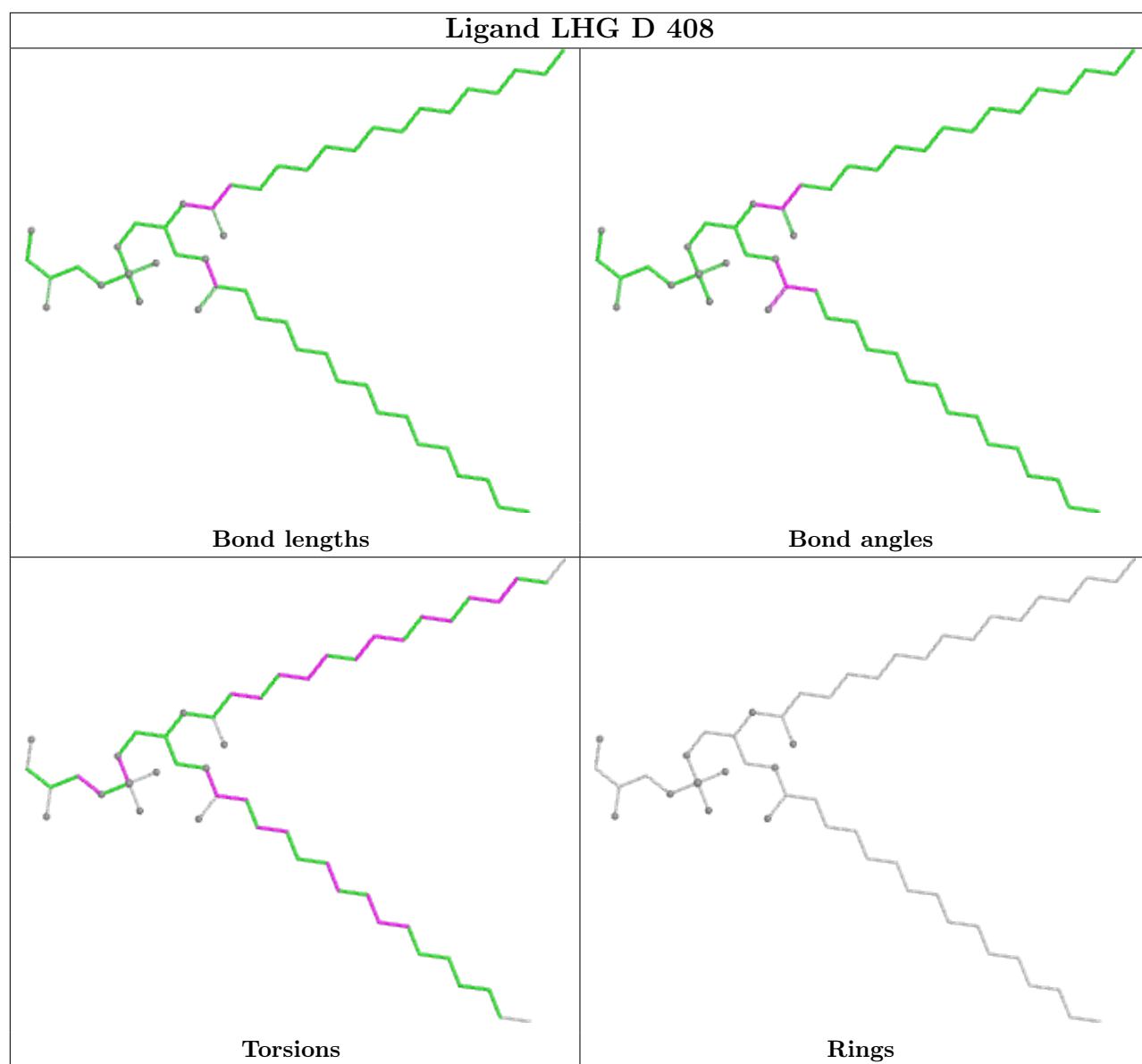


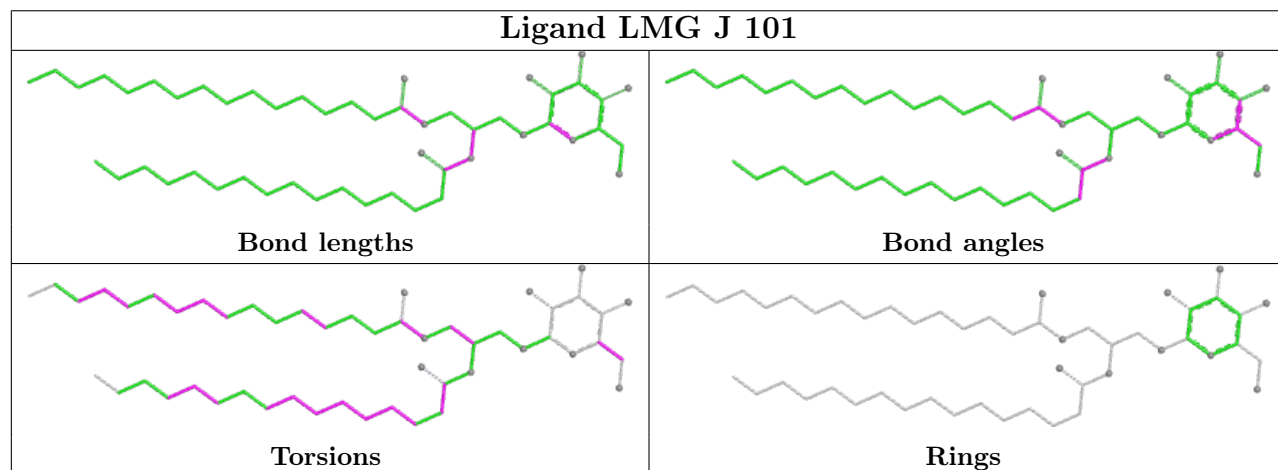
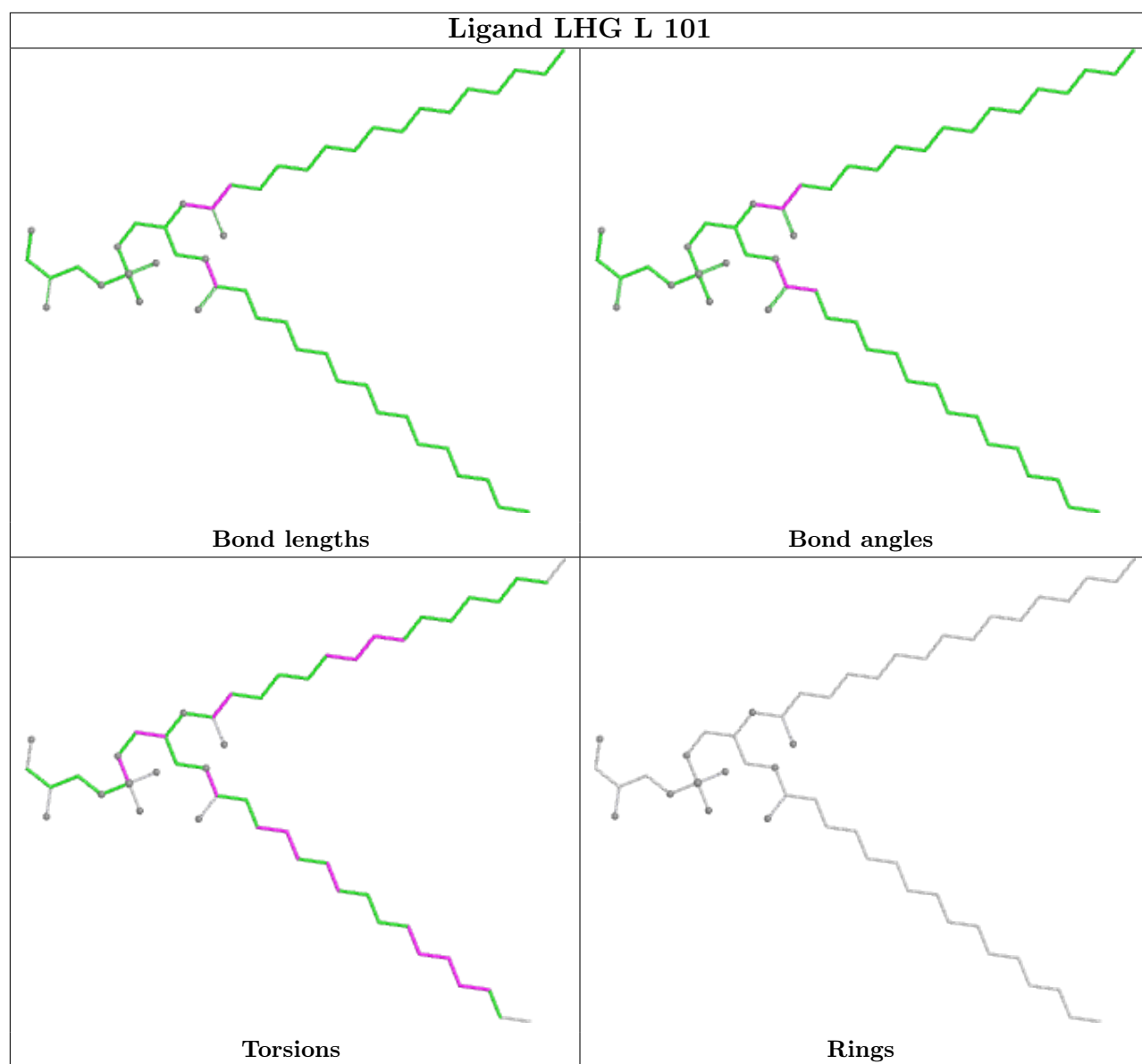
Ligand CLA C 509	
	
Bond lengths	Bond angles
	
Torsions	Rings

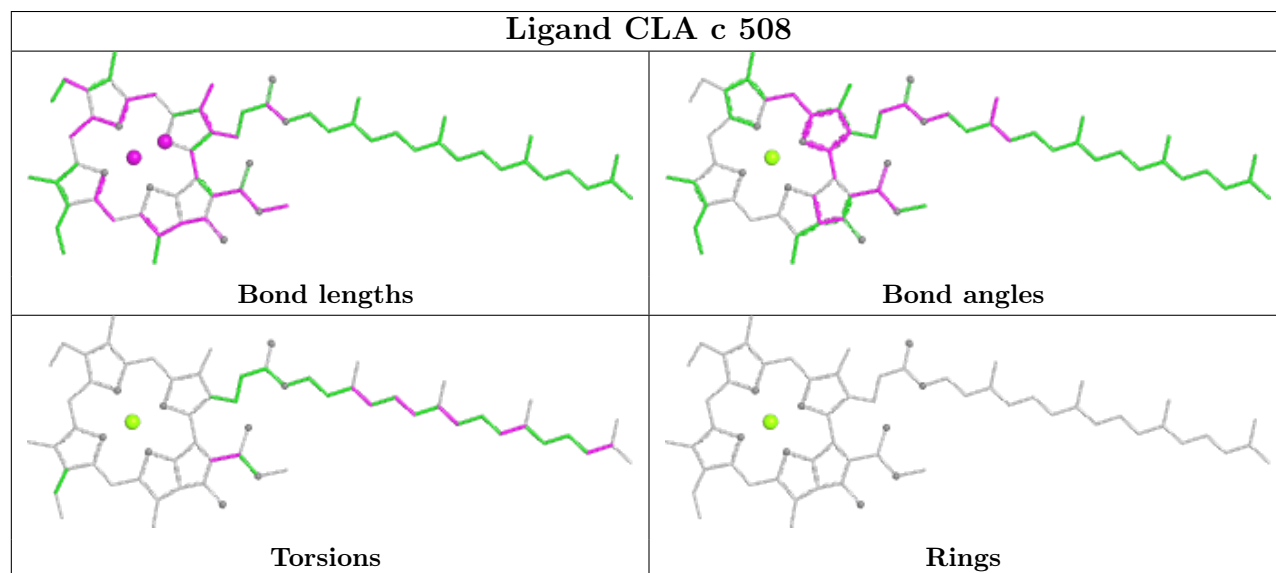
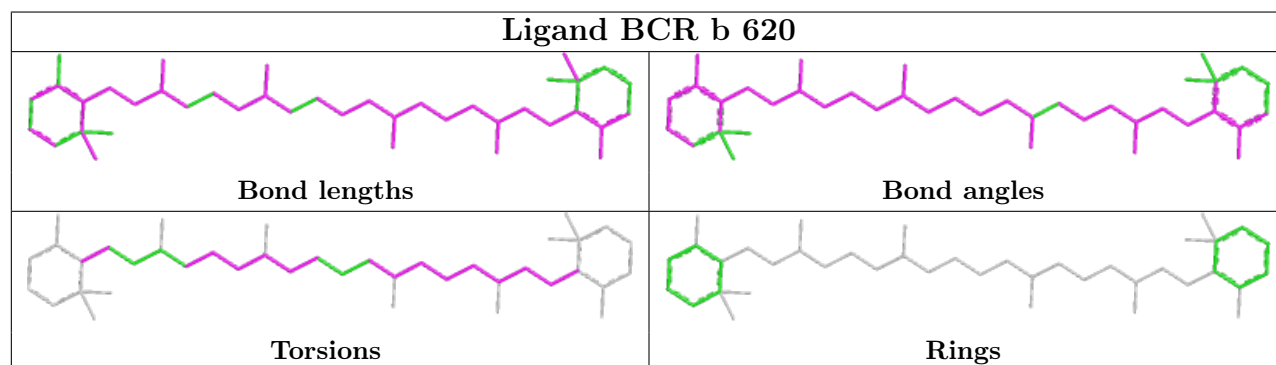
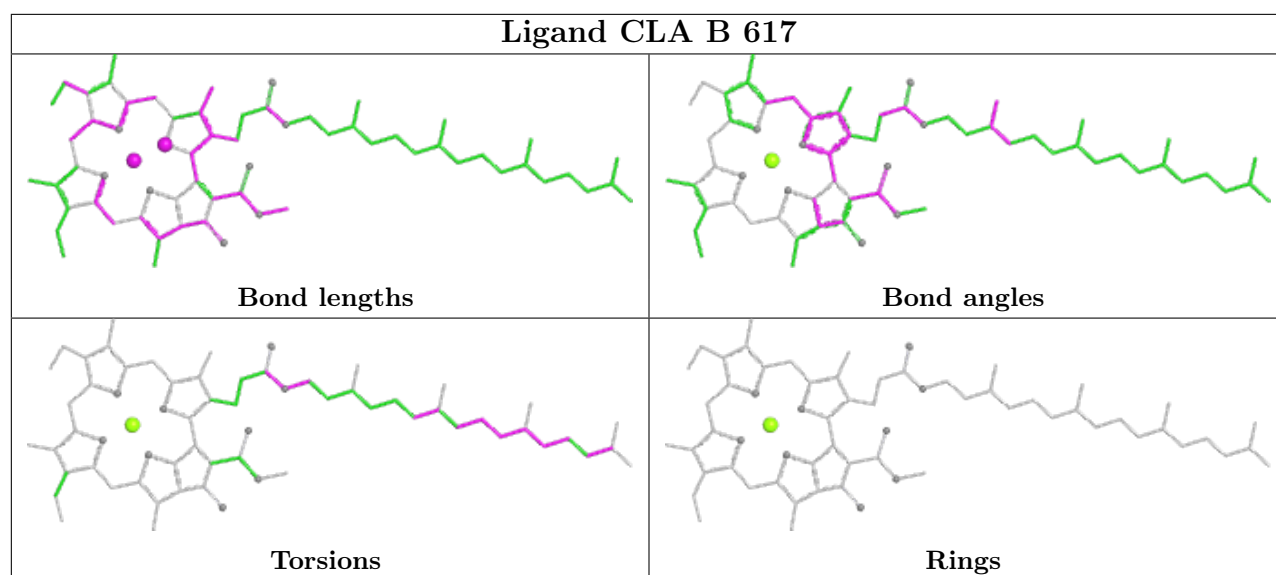
Ligand LMG c 521	
	
Bond lengths	Bond angles
	
Torsions	Rings

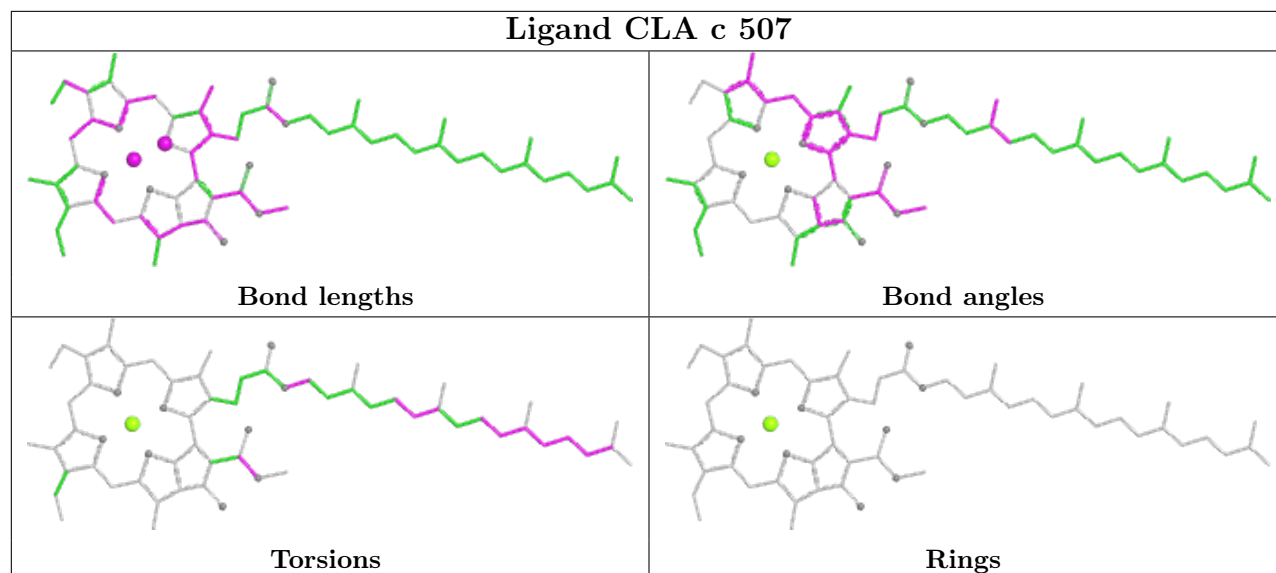
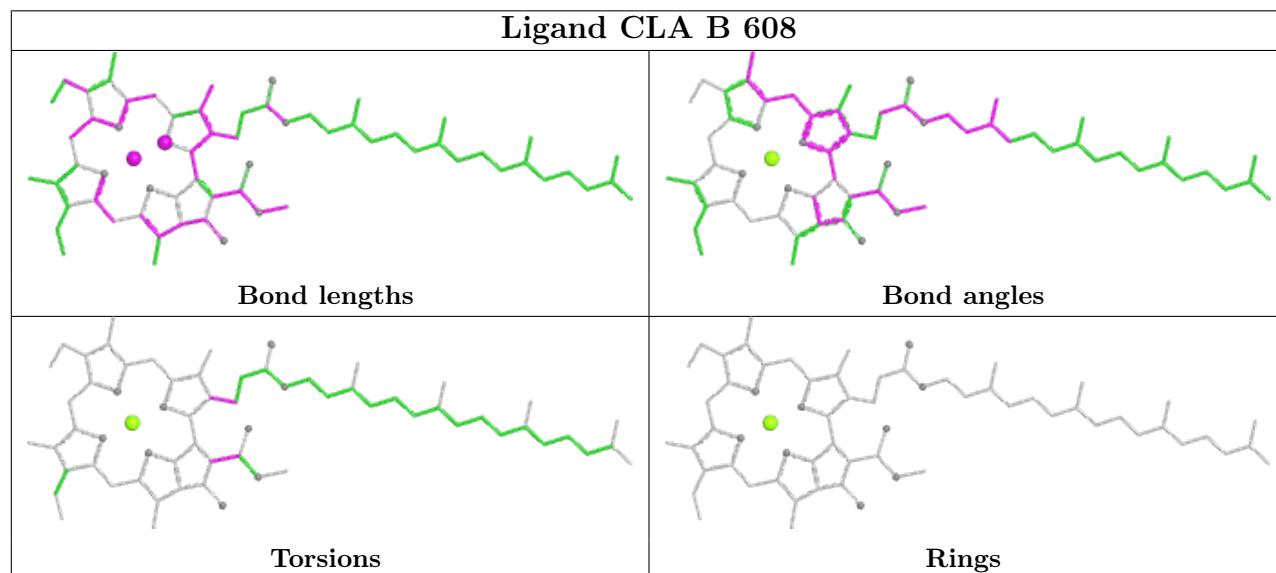
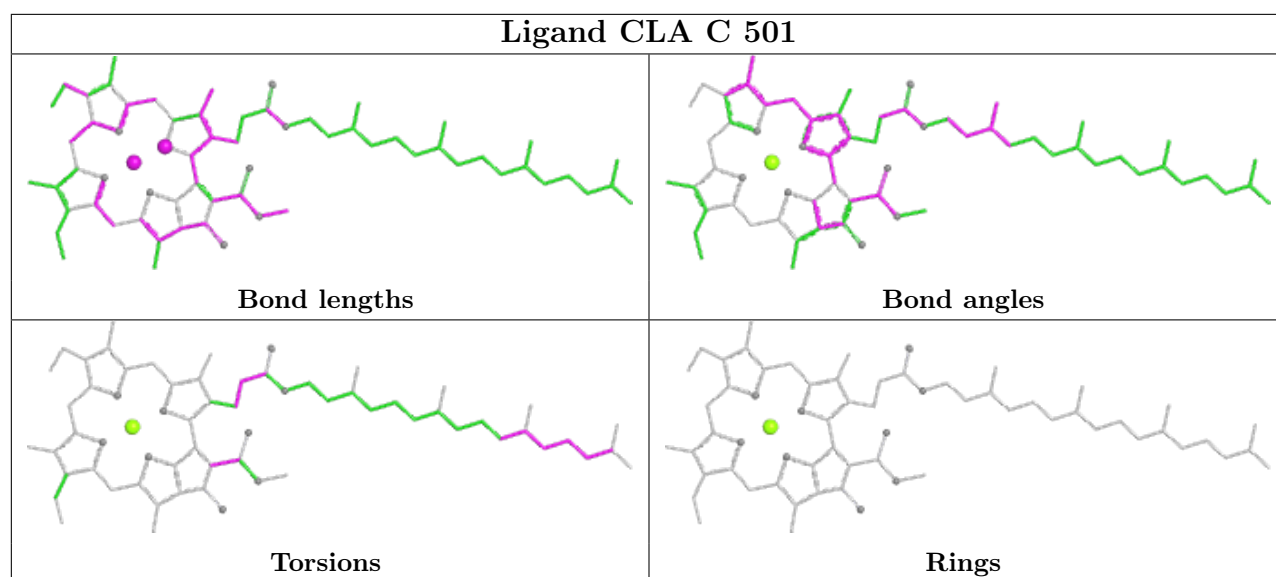


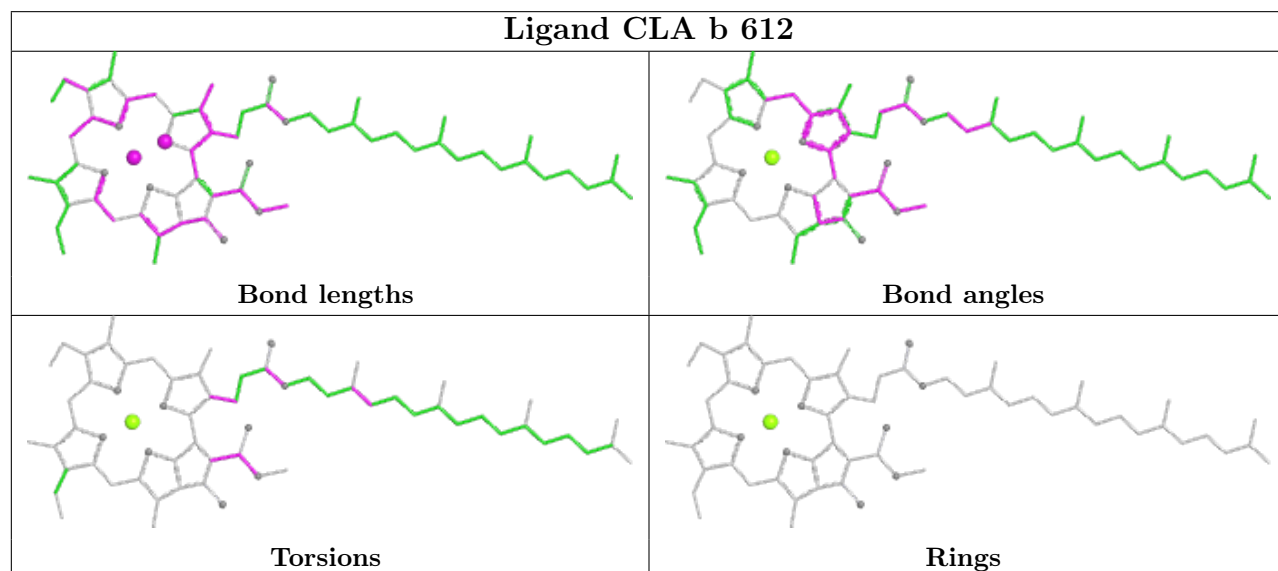
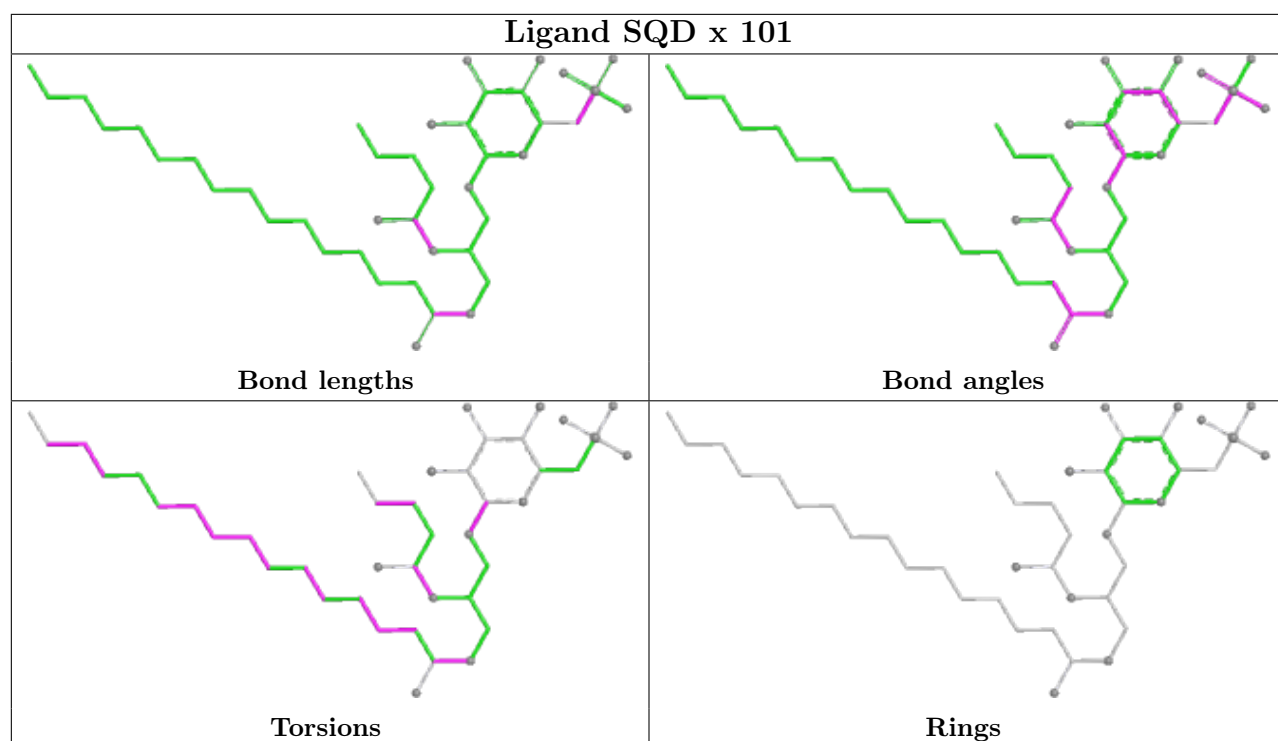
Ligand CLA B 610**Ligand CLA c 511**

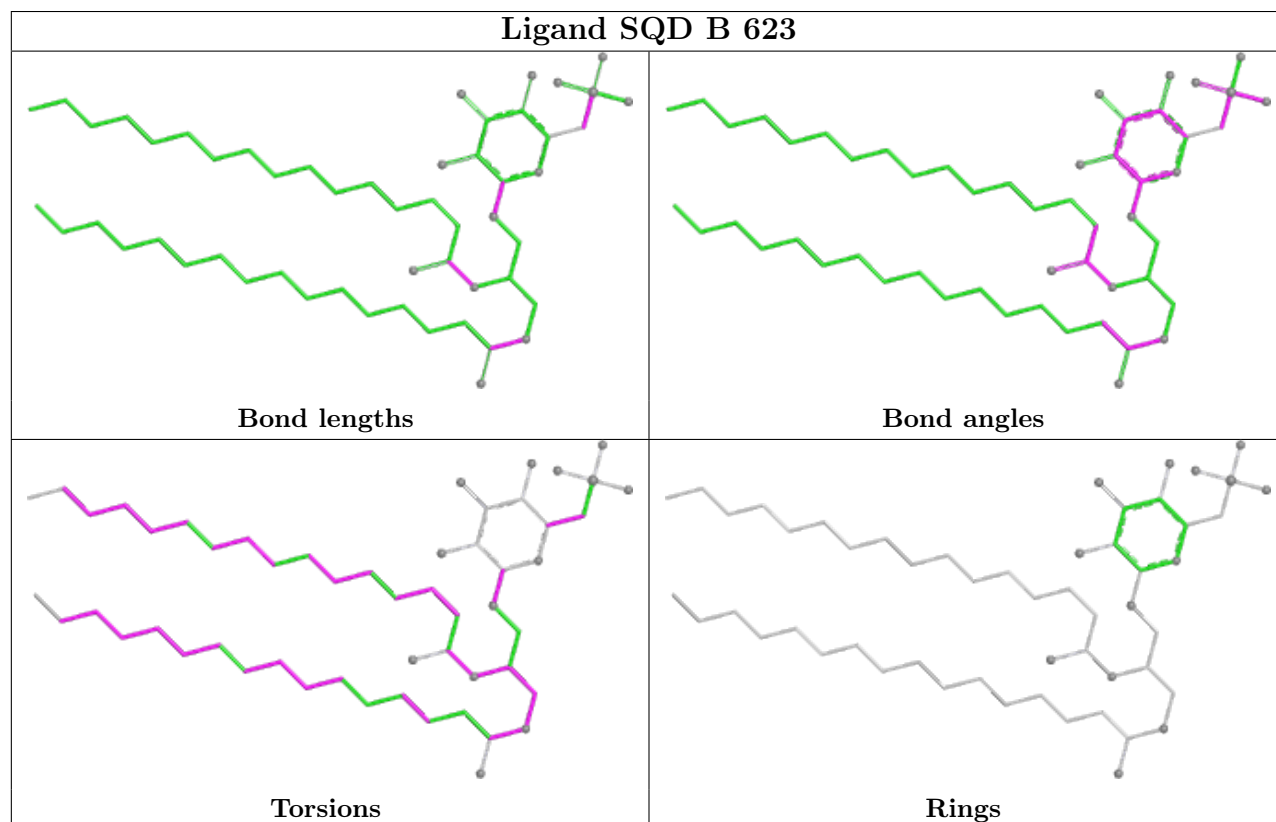
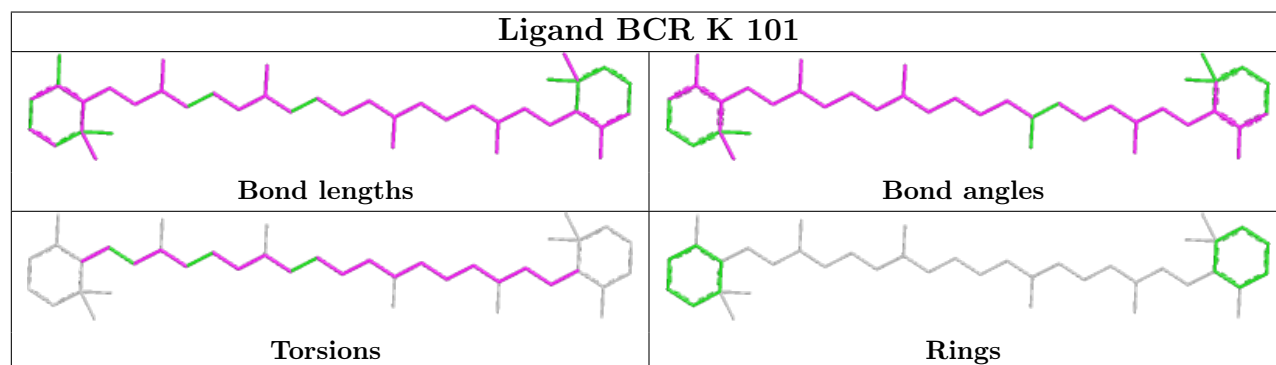
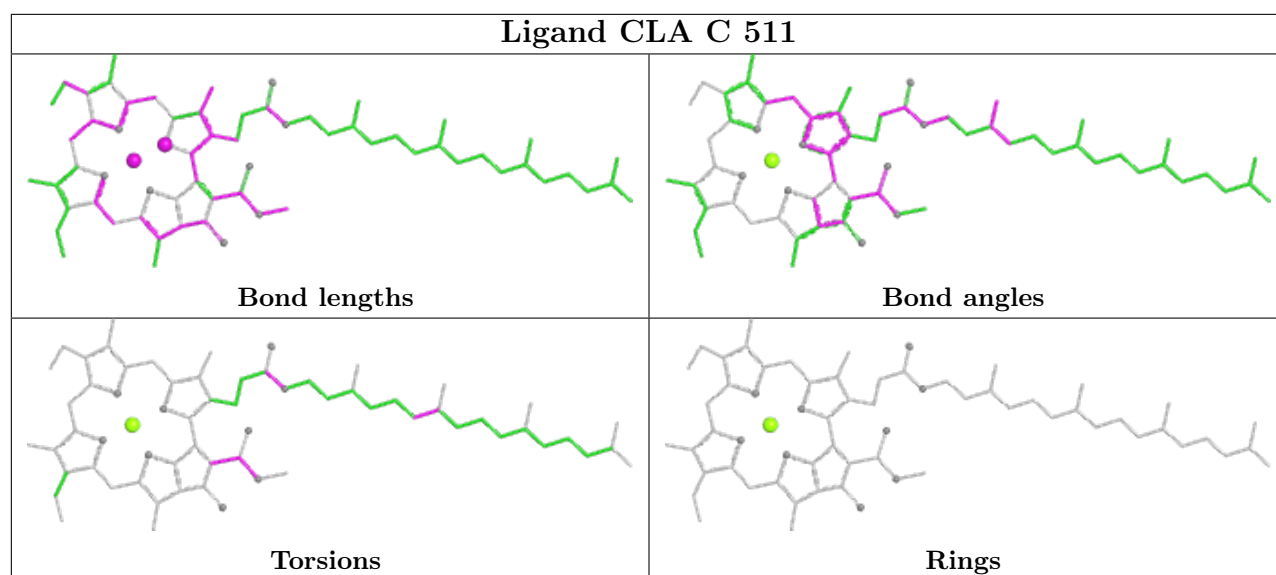












5.7 Other polymers [i](#)

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%)	-0.32	3 (0%) 84 77	57, 63, 84, 93	0
1	a	334/334 (100%)	-0.22	2 (0%) 89 84	78, 84, 104, 114	0
2	B	504/504 (100%)	-0.20	4 (0%) 86 79	59, 68, 89, 111	0
2	b	504/504 (100%)	-0.12	6 (1%) 79 70	80, 88, 110, 131	0
3	C	451/451 (100%)	-0.06	8 (1%) 68 59	61, 72, 85, 97	0
3	c	451/451 (100%)	-0.19	6 (1%) 77 68	82, 93, 105, 118	0
4	D	342/342 (100%)	-0.29	3 (0%) 84 77	57, 64, 80, 102	0
4	d	342/342 (100%)	-0.22	4 (1%) 79 70	78, 85, 101, 123	0
5	E	81/81 (100%)	-0.12	0 100 100	68, 81, 98, 104	0
5	e	81/81 (100%)	0.09	1 (1%) 79 70	89, 102, 119, 125	0
6	F	34/34 (100%)	-0.29	1 (2%) 51 41	68, 74, 99, 102	0
6	f	34/34 (100%)	-0.22	1 (2%) 51 41	89, 95, 120, 122	0
7	H	65/65 (100%)	0.25	6 (9%) 9 8	64, 74, 81, 99	0
7	h	65/65 (100%)	0.37	4 (6%) 20 17	85, 95, 102, 120	0
8	I	38/38 (100%)	-0.24	0 100 100	70, 74, 105, 109	0
8	i	38/38 (100%)	-0.10	1 (2%) 56 46	90, 95, 126, 130	0
9	J	38/38 (100%)	-0.17	1 (2%) 56 46	66, 78, 109, 112	0
9	j	38/38 (100%)	-0.18	1 (2%) 56 46	87, 99, 129, 133	0
10	K	37/37 (100%)	-0.55	0 100 100	74, 79, 86, 88	0
10	k	37/37 (100%)	-0.02	1 (2%) 54 45	94, 100, 107, 108	0
11	L	37/37 (100%)	0.01	4 (10%) 5 6	58, 62, 90, 99	0
11	l	37/37 (100%)	-0.04	2 (5%) 25 22	79, 83, 111, 120	0
12	M	34/34 (100%)	-0.63	0 100 100	62, 64, 77, 93	0
12	m	34/34 (100%)	-0.46	0 100 100	83, 84, 98, 114	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/243 (100%)	-0.25	0 100 100	59, 73, 95, 111	0
13	o	243/243 (100%)	0.03	5 (2%) 63 54	79, 94, 116, 132	0
14	T	30/30 (100%)	-0.12	3 (10%) 7 7	60, 64, 85, 93	0
14	t	30/30 (100%)	-0.43	0 100 100	80, 85, 105, 114	0
15	U	97/97 (100%)	-0.10	1 (1%) 82 74	64, 71, 89, 90	0
15	u	97/97 (100%)	-0.20	1 (1%) 82 74	84, 92, 110, 111	0
16	V	137/137 (100%)	-0.30	1 (0%) 87 82	64, 69, 80, 88	0
16	v	137/137 (100%)	-0.24	3 (2%) 62 52	84, 89, 101, 109	0
17	Y	29/29 (100%)	-0.15	1 (3%) 45 36	82, 89, 115, 118	0
17	y	29/29 (100%)	-0.31	0 100 100	103, 110, 136, 138	0
18	X	39/39 (100%)	0.06	7 (17%) 1 2	74, 80, 107, 108	0
18	x	39/39 (100%)	-0.11	3 (7%) 13 12	95, 101, 127, 129	0
19	Z	62/62 (100%)	-0.31	1 (1%) 72 62	80, 89, 109, 112	0
19	z	62/62 (100%)	-0.14	2 (3%) 47 38	101, 110, 129, 133	0
All	All	5264/5264 (100%)	-0.17	87 (1%) 70 61	57, 83, 107, 138	0

The worst 5 of 87 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
11	L	2	GLU	4.5
7	H	2	ALA	4.2
11	L	3	PRO	4.2
7	h	2	ALA	4.1
18	X	2	THR	4.0

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 monosaccharides 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	u	201	1/1	0.09	0.16	112,112,112,112	0
21	CL	V	201	1/1	0.20	0.34	91,91,91,91	0
30	CA	B	601	1/1	0.21	1.14	117,117,117,117	0
30	CA	b	603	1/1	0.22	0.57	137,137,137,137	0
26	PL9	A	610	55/55	0.48	0.36	93,109,118,119	0
25	BCR	h	101	40/40	0.51	0.62	87,94,103,104	0
25	BCR	c	522	40/40	0.58	0.39	91,95,98,99	0
32	DGD	d	405	62/66	0.58	0.48	138,151,164,165	0
26	PL9	a	609	55/55	0.59	0.45	113,130,139,140	0
25	BCR	H	101	40/40	0.62	0.56	67,74,83,83	0
25	BCR	a	608	40/40	0.63	0.64	83,89,93,94	0
21	CL	a	602	1/1	0.63	0.17	86,86,86,86	0
28	LMG	C	520	51/55	0.64	0.54	83,117,122,123	0
26	PL9	d	404	55/55	0.67	0.31	80,84,91,93	0
25	BCR	C	521	40/40	0.69	0.30	70,74,78,78	0
32	DGD	D	406	62/66	0.69	0.45	118,130,143,144	0
27	SQD	a	610	54/54	0.69	0.51	110,119,128,128	0
25	BCR	T	101	40/40	0.70	0.40	65,78,85,86	0
25	BCR	b	622	40/40	0.71	0.54	89,94,100,101	0
31	LHG	E	101	42/49	0.72	0.39	110,124,127,127	0
27	SQD	x	101	43/54	0.72	0.50	128,136,140,140	0
23	CLA	C	513	65/65	0.72	0.47	80,85,105,105	0
28	LMG	c	521	51/55	0.73	0.51	104,137,142,143	0
31	LHG	e	101	42/49	0.74	0.40	131,145,147,148	0
27	SQD	A	611	54/54	0.75	0.41	90,98,107,108	0
23	CLA	C	512	65/65	0.75	0.41	78,82,103,104	0
27	SQD	b	602	54/54	0.75	0.42	99,107,121,121	0
23	CLA	B	617	65/65	0.75	0.44	63,69,118,119	0
25	BCR	C	515	40/40	0.75	0.34	71,78,81,82	0
25	BCR	f	101	40/40	0.75	0.35	87,91,109,110	0
25	BCR	F	101	40/40	0.76	0.33	66,71,88,90	0
23	CLA	b	609[B]	65/65	0.76	0.45	83,87,93,95	65
25	BCR	C	514	40/40	0.76	0.39	78,84,87,88	0
23	CLA	C	507	65/65	0.76	0.41	70,74,92,94	0
25	BCR	b	621	40/40	0.76	0.39	83,89,101,101	0
23	CLA	b	609[A]	65/65	0.76	0.45	85,90,102,103	65

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
25	BCR	b	620	40/40	0.77	0.61	84,88,90,90	0
25	BCR	A	609	40/40	0.77	0.56	63,68,73,73	0
23	CLA	b	604	65/65	0.77	0.72	94,102,127,128	0
23	CLA	c	502	65/65	0.77	0.35	90,93,106,108	0
23	CLA	c	513	65/65	0.77	0.41	99,102,124,124	0
28	LMG	z	101	37/55	0.77	0.52	117,145,149,150	0
25	BCR	t	101	40/40	0.78	0.36	86,99,106,106	0
27	SQD	B	623	54/54	0.78	0.30	119,127,141,142	0
23	CLA	b	618	65/65	0.78	0.39	86,89,107,108	0
28	LMG	c	520	51/55	0.78	0.38	92,118,134,135	0
21	CL	A	602	1/1	0.79	0.23	65,65,65,65	0
28	LMG	b	623	51/55	0.80	0.39	91,100,112,116	0
23	CLA	B	607[A]	65/65	0.80	0.40	65,69,81,82	65
27	SQD	X	101	43/54	0.80	0.39	108,115,119,119	0
25	BCR	c	515	40/40	0.80	0.44	99,105,108,108	0
23	CLA	c	504	65/65	0.80	0.29	89,93,96,97	0
30	CA	F	102	1/1	0.80	0.59	97,97,97,97	0
23	CLA	B	607[B]	65/65	0.80	0.40	63,67,72,75	65
30	CA	f	102	1/1	0.80	0.37	118,118,118,118	0
28	LMG	C	519	51/55	0.80	0.41	72,98,113,114	0
25	BCR	K	101	40/40	0.80	0.37	75,78,79,80	0
28	LMG	J	101	51/55	0.80	0.34	66,76,106,108	0
28	LMG	Z	101	37/55	0.80	0.41	96,124,129,129	0
27	SQD	b	601	54/54	0.81	0.33	91,103,109,109	0
23	CLA	c	503	65/65	0.81	0.36	85,87,101,103	0
25	BCR	B	620	40/40	0.81	0.39	68,74,80,80	0
23	CLA	C	511	65/65	0.81	0.33	70,75,78,79	0
23	CLA	c	508	65/65	0.81	0.32	91,94,113,115	0
29	FE2	a	615	1/1	0.81	0.16	88,88,88,88	0
23	CLA	B	602	65/65	0.81	0.40	73,82,107,107	0
25	BCR	c	516	40/40	0.82	0.27	92,98,102,102	0
23	CLA	b	619	65/65	0.82	0.43	83,90,139,139	0
31	LHG	l	101	49/49	0.82	0.29	84,92,104,106	0
25	BCR	B	618	40/40	0.82	0.37	63,68,69,70	0
32	DGD	c	519	62/66	0.82	0.47	83,93,113,117	0
23	CLA	b	617	65/65	0.82	0.37	82,86,121,122	0
23	CLA	B	616	65/65	0.83	0.35	65,68,86,87	0
23	CLA	C	506	65/65	0.83	0.30	72,79,115,115	0
23	CLA	a	605	65/65	0.83	0.33	80,83,124,126	0
23	CLA	d	403	65/65	0.84	0.33	86,89,126,128	0
23	CLA	a	607	65/65	0.84	0.42	83,85,133,133	0
28	LMG	A	612	51/55	0.85	0.30	94,100,105,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
28	LMG	B	621	51/55	0.85	0.34	70,80,92,95	0
23	CLA	B	608	65/65	0.85	0.35	58,61,73,74	0
27	SQD	a	612	54/54	0.85	0.31	111,124,129,130	0
24	PHO	D	401	64/64	0.85	0.31	59,63,69,73	0
23	CLA	a	604	65/65	0.85	0.30	77,80,87,95	0
23	CLA	C	505	65/65	0.85	0.30	69,71,85,85	0
31	LHG	D	408	49/49	0.86	0.36	67,74,103,104	0
26	PL9	D	405	55/55	0.86	0.21	60,64,70,72	0
31	LHG	a	614	49/49	0.86	0.35	87,94,124,125	0
23	CLA	c	514	65/65	0.86	0.30	101,106,125,126	0
28	LMG	a	611	51/55	0.86	0.26	114,121,126,126	0
32	DGD	C	518	62/66	0.86	0.35	62,72,93,97	0
25	BCR	k	101	40/40	0.86	0.32	95,99,100,100	0
32	DGD	c	517	62/66	0.86	0.26	84,94,122,124	0
23	CLA	b	613	65/65	0.86	0.43	82,86,94,98	0
23	CLA	c	507	65/65	0.86	0.30	93,100,136,136	0
34	MG	j	102	1/1	0.86	0.18	89,89,89,89	0
23	CLA	b	615	65/65	0.87	0.35	81,85,91,92	0
24	PHO	d	401	64/64	0.87	0.28	80,84,90,94	0
23	CLA	c	510	65/65	0.87	0.26	91,93,108,108	0
23	CLA	D	404	65/65	0.87	0.34	65,68,106,107	0
29	FE2	A	613	1/1	0.87	0.28	67,67,67,67	0
23	CLA	b	612	65/65	0.87	0.27	85,90,92,93	0
23	CLA	C	508	65/65	0.87	0.30	66,70,95,99	0
23	CLA	C	501	65/65	0.88	0.35	69,73,85,87	0
31	LHG	b	624	49/49	0.88	0.25	91,96,102,102	0
31	LHG	d	406	49/49	0.88	0.35	85,89,98,102	0
23	CLA	b	606	65/65	0.88	0.28	79,84,92,96	0
24	PHO	a	606	64/64	0.88	0.32	78,83,86,87	0
32	DGD	C	517	62/66	0.88	0.31	63,75,103,104	0
23	CLA	C	509	65/65	0.88	0.24	70,72,87,88	0
23	CLA	c	512	65/65	0.88	0.25	90,95,99,99	0
23	CLA	b	616	65/65	0.88	0.32	80,84,106,108	0
32	DGD	c	518	62/66	0.88	0.30	84,96,124,124	0
25	BCR	B	619	40/40	0.88	0.30	62,69,81,81	0
23	CLA	B	615	65/65	0.88	0.27	61,65,101,102	0
28	LMG	j	101	51/55	0.88	0.24	87,96,126,129	0
23	CLA	A	608	65/65	0.89	0.35	62,65,112,113	0
32	DGD	C	516	62/66	0.89	0.22	64,73,102,103	0
22	BCT	a	603	4/4	0.89	0.48	100,101,101,103	0
31	LHG	B	622	49/49	0.89	0.25	70,75,81,82	0
23	CLA	B	610	65/65	0.89	0.30	64,69,72,73	0

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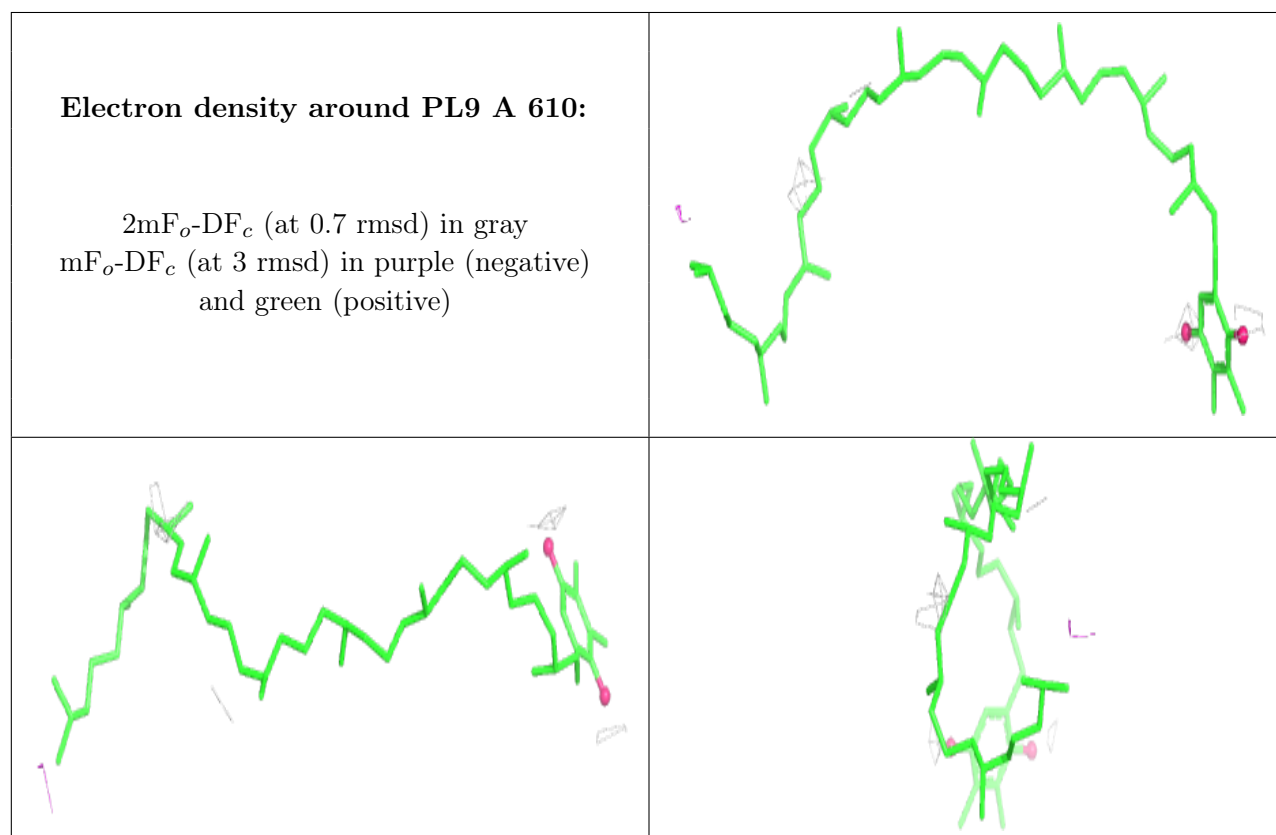
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	DGD	H	102	62/66	0.89	0.23	66,72,79,81	0
23	CLA	C	504	65/65	0.89	0.29	66,68,95,95	0
23	CLA	B	611	65/65	0.89	0.27	62,65,73,77	0
23	CLA	b	605	65/65	0.89	0.24	85,88,93,94	0
23	CLA	A	606	65/65	0.89	0.31	60,62,104,106	0
32	DGD	h	102	62/66	0.89	0.25	87,93,99,101	0
33	HEM	e	102	43/43	0.89	0.45	101,103,107,108	0
23	CLA	b	608	65/65	0.89	0.27	80,84,95,97	0
23	CLA	B	606	65/65	0.90	0.23	59,64,75,76	0
23	CLA	c	506	65/65	0.90	0.22	89,92,106,106	0
33	HEM	E	102	43/43	0.90	0.28	80,82,86,87	0
23	CLA	b	610	65/65	0.90	0.31	79,82,94,95	0
23	CLA	b	611	65/65	0.90	0.26	82,86,92,93	0
23	CLA	C	502	65/65	0.91	0.33	65,67,80,83	0
23	CLA	c	509	65/65	0.91	0.27	87,90,115,119	0
23	CLA	C	503	65/65	0.91	0.33	68,72,76,77	0
23	CLA	B	604	65/65	0.91	0.25	58,63,72,76	0
23	CLA	a	613	65/65	0.91	0.34	75,79,91,96	0
23	CLA	B	605	65/65	0.91	0.25	60,63,91,91	0
23	CLA	B	613	65/65	0.91	0.29	61,64,71,72	0
23	CLA	D	403	65/65	0.91	0.28	54,59,75,76	0
23	CLA	B	614	65/65	0.91	0.26	60,63,85,87	0
33	HEM	v	201	43/43	0.91	0.30	84,86,88,90	0
34	MG	J	102	1/1	0.91	0.48	68,68,68,68	0
31	LHG	D	407	49/49	0.91	0.21	64,69,78,81	0
23	CLA	B	609	65/65	0.92	0.24	61,65,71,72	0
23	CLA	A	605	65/65	0.92	0.26	56,59,66,75	0
23	CLA	B	603	65/65	0.92	0.23	64,67,72,73	0
23	CLA	b	614	65/65	0.92	0.29	80,83,94,96	0
31	LHG	L	101	49/49	0.92	0.23	63,72,83,85	0
23	CLA	D	402	65/65	0.93	0.28	54,59,70,76	0
23	CLA	c	505	65/65	0.93	0.26	86,89,115,116	0
21	CL	A	603	1/1	0.93	0.20	62,62,62,62	0
24	PHO	A	607	64/64	0.93	0.26	57,62,65,67	0
23	CLA	c	511	65/65	0.93	0.24	86,90,96,99	0
23	CLA	b	607	65/65	0.93	0.24	81,84,111,112	0
20	OEX	A	601	10/10	0.94	0.31	63,64,67,67	0
23	CLA	B	612	65/65	0.94	0.24	60,62,73,75	0
23	CLA	d	402	65/65	0.94	0.25	75,80,95,96	0
33	HEM	V	202	43/43	0.94	0.26	63,65,68,69	0
21	CL	c	501	1/1	0.95	0.18	83,83,83,83	0
23	CLA	C	510	65/65	0.95	0.23	65,69,76,78	0

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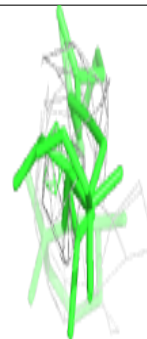
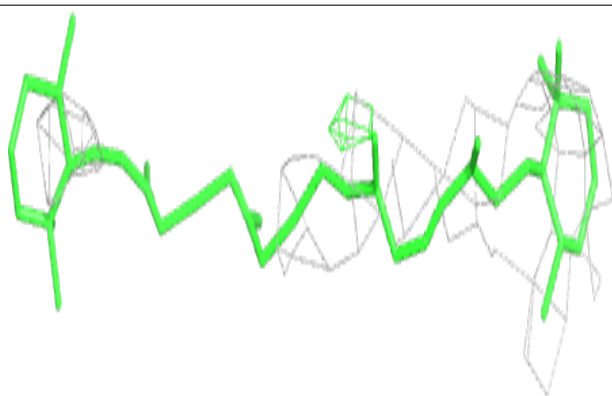
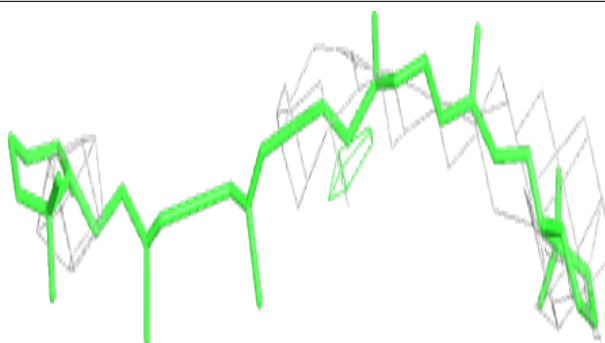
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
20	OEX	a	601	10/10	0.96	0.32	83,84,87,88	0
30	CA	o	301	1/1	0.96	0.24	110,110,110,110	0
30	CA	O	301	1/1	0.97	0.17	90,90,90,90	0
22	BCT	A	604	4/4	0.97	0.21	79,80,81,82	0

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.

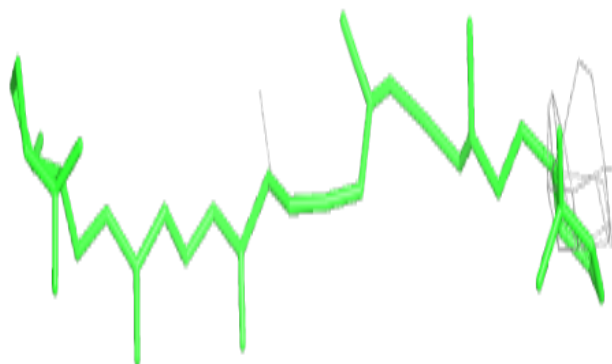
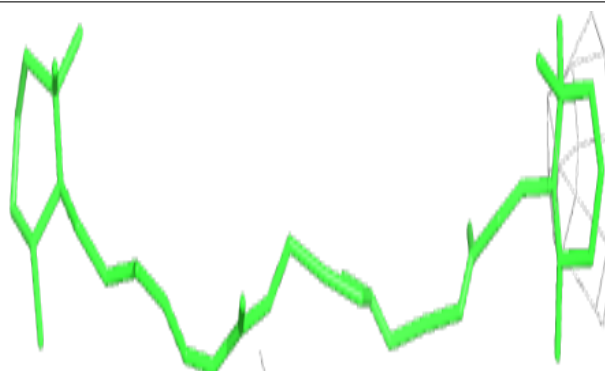


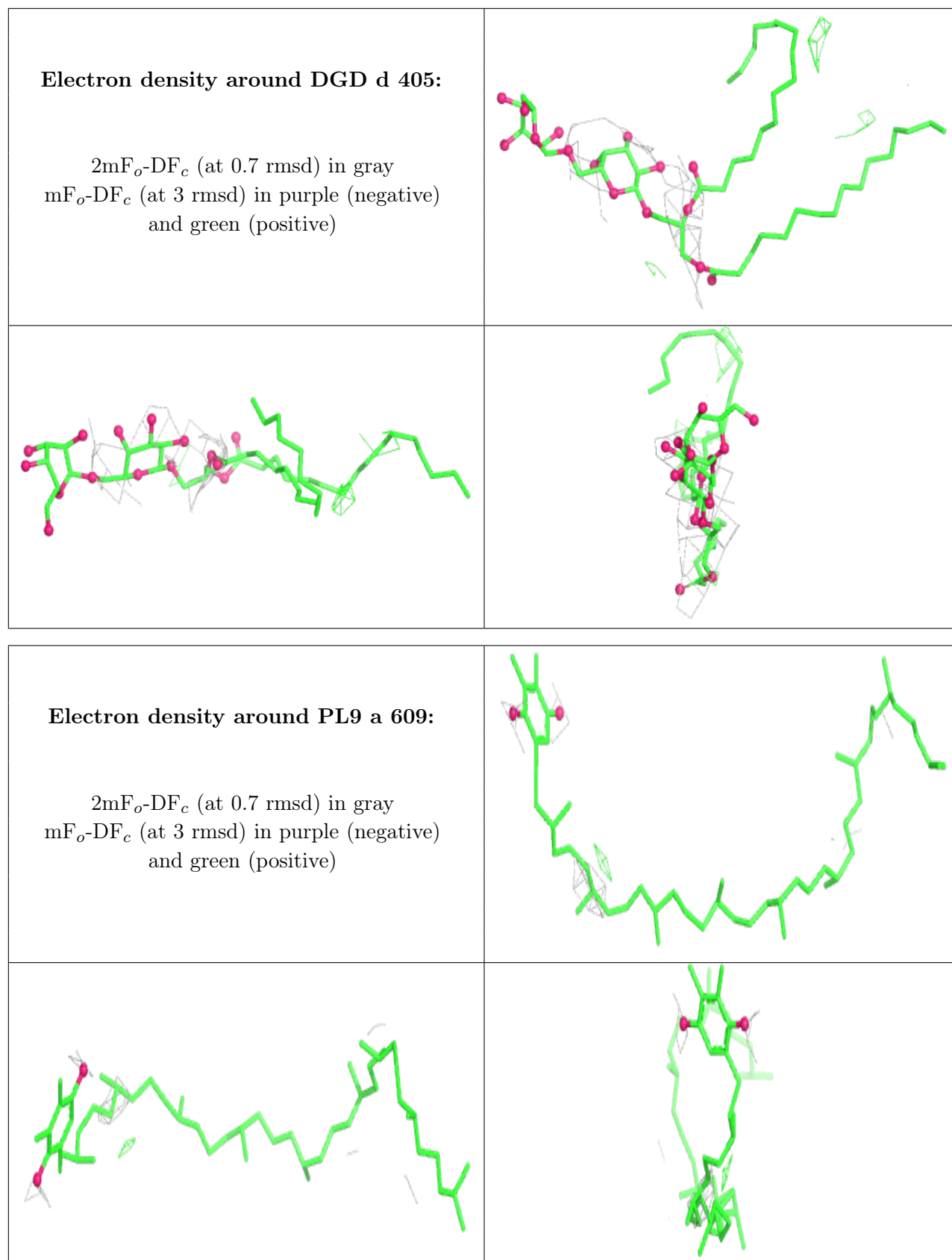
Electron density around BCR h 101:

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

**Electron density around BCR c 522:**

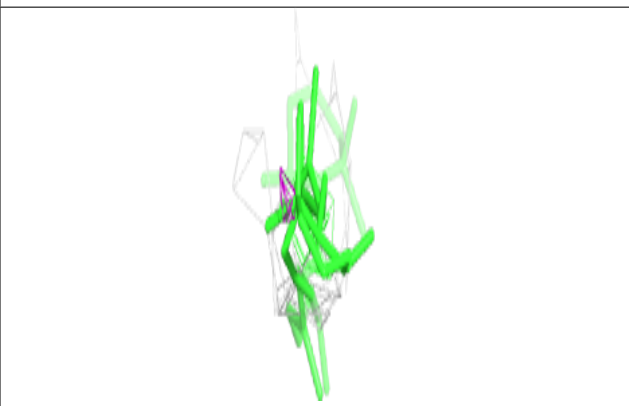
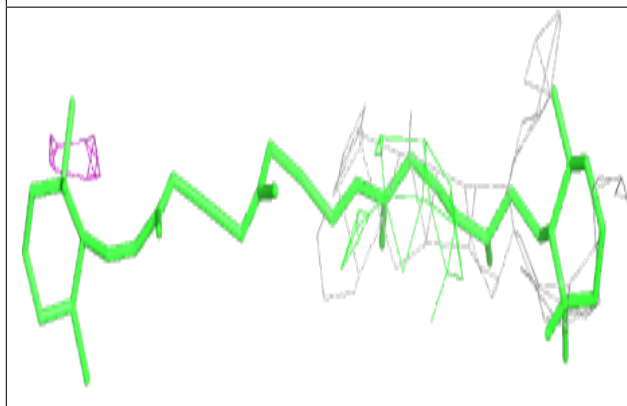
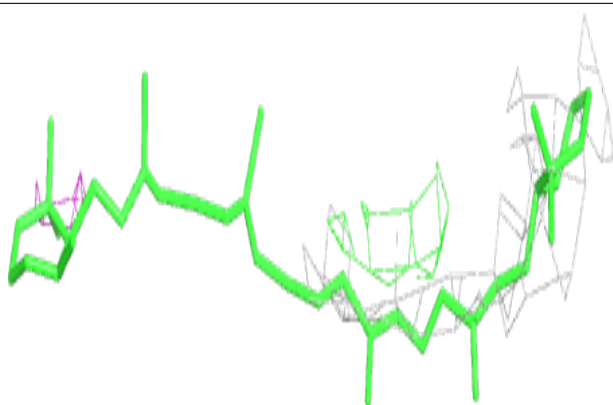
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



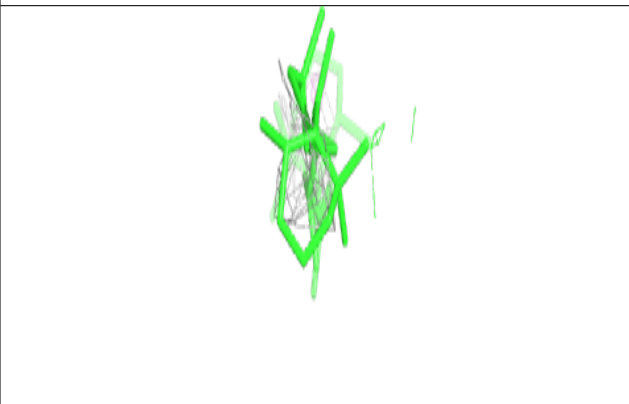
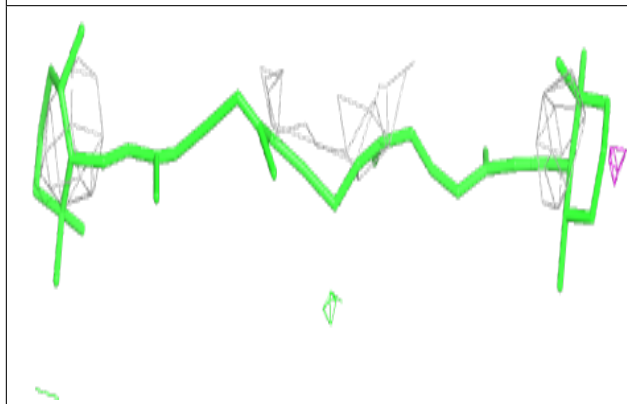
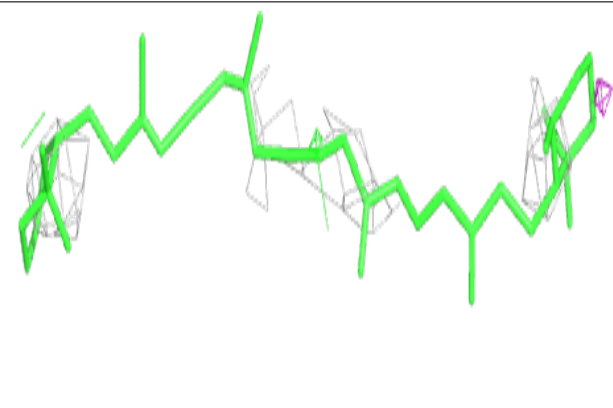


Electron density around BCR H 101:

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

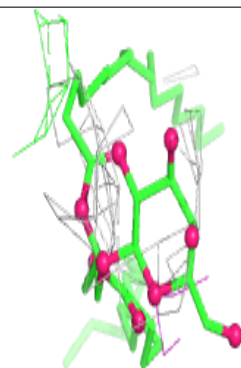
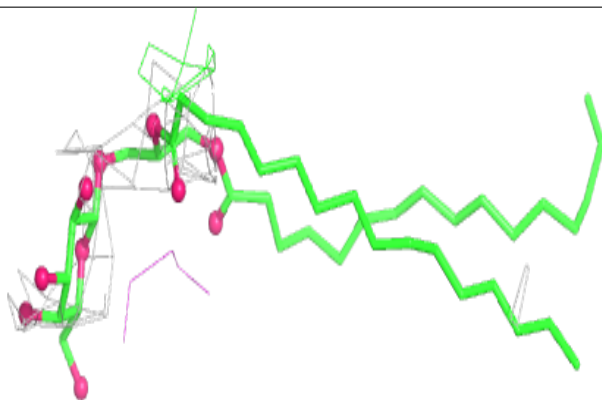
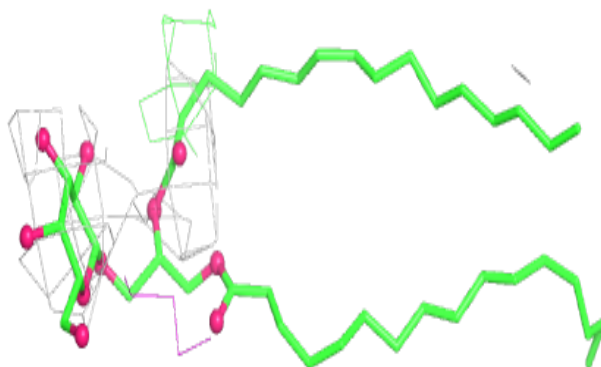
**Electron density around BCR a 608:**

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

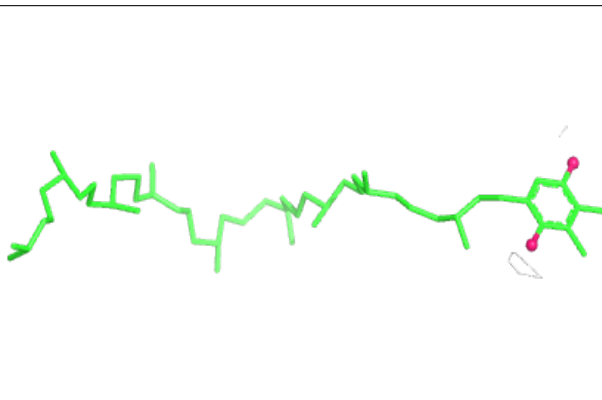
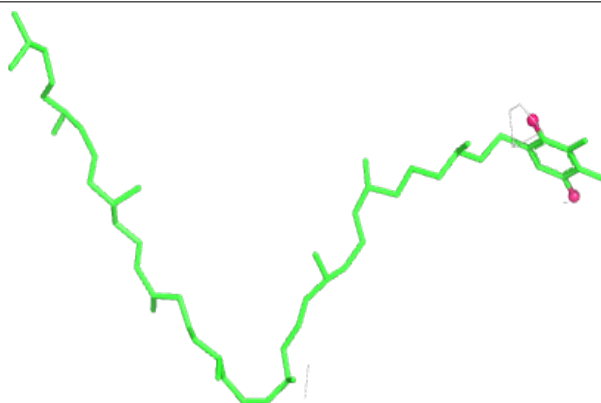


Electron density around LMG C 520:

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

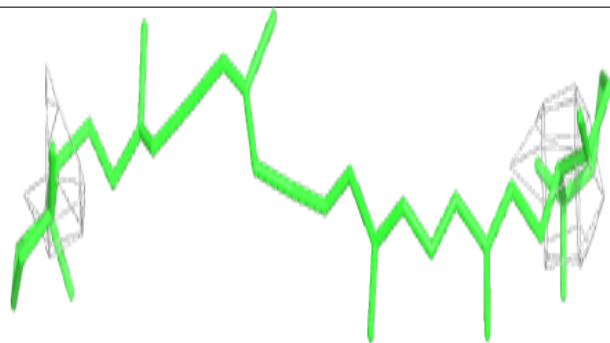
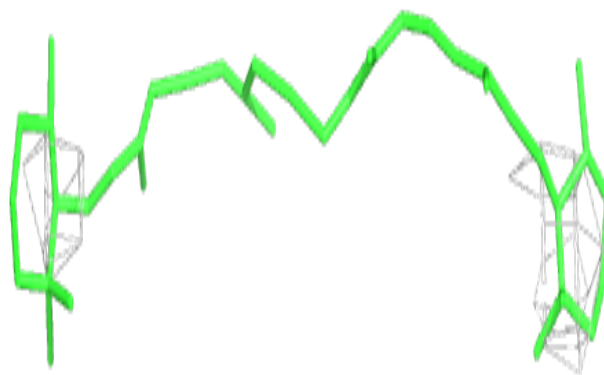
**Electron density around PL9 d 404:**

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

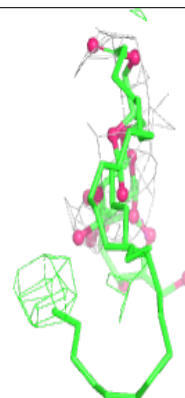
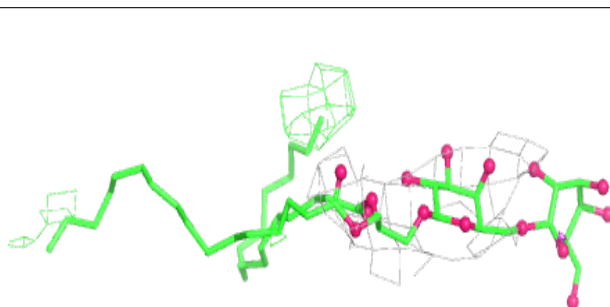


Electron density around BCR C 521:

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

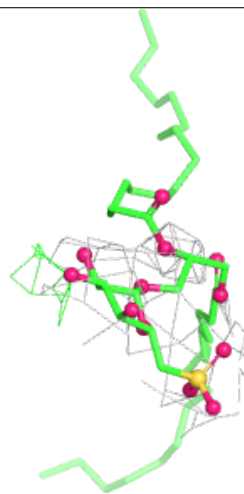
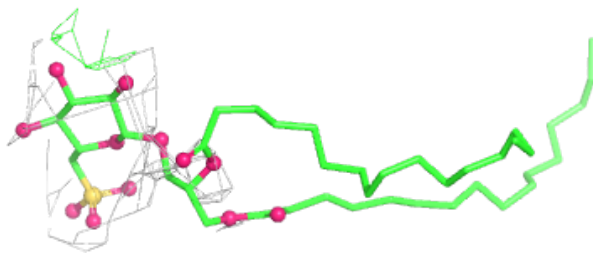
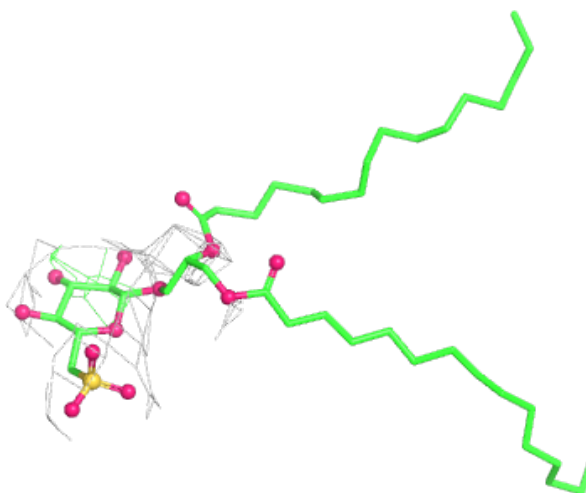
**Electron density around DGD D 406:**

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



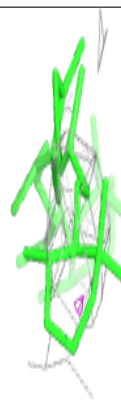
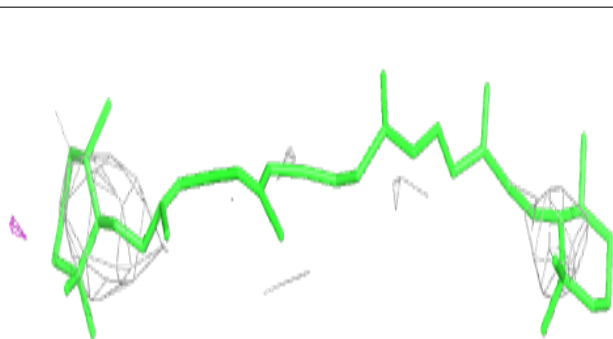
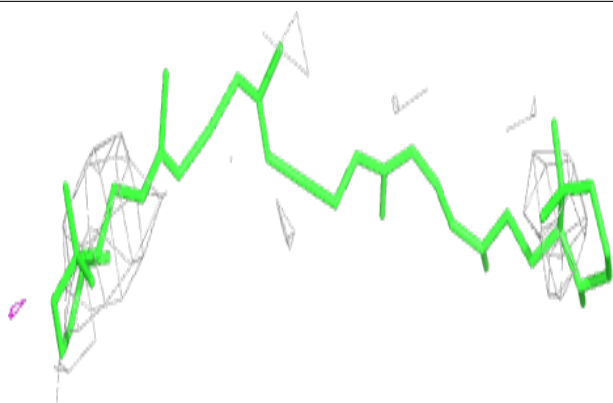
Electron density around SQD a 610:

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

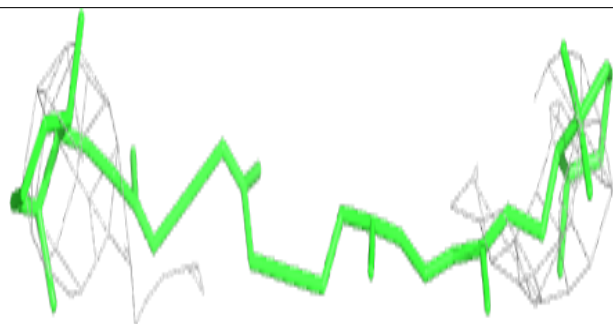
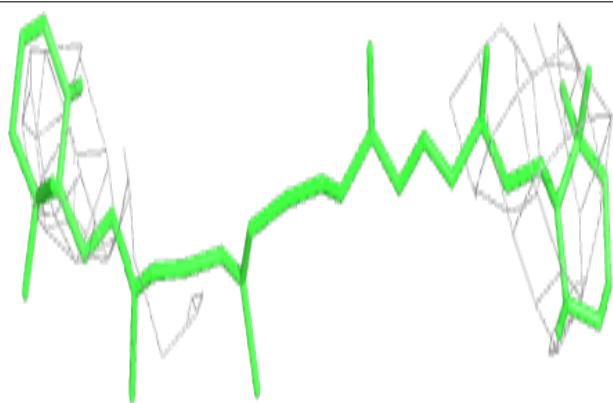


Electron density around BCR T 101:

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

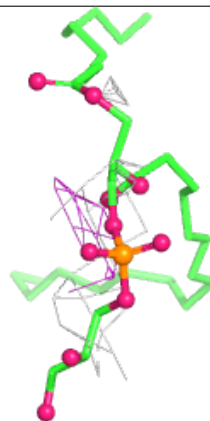
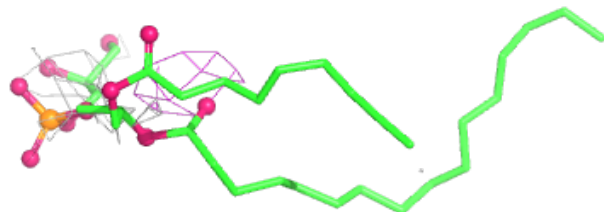
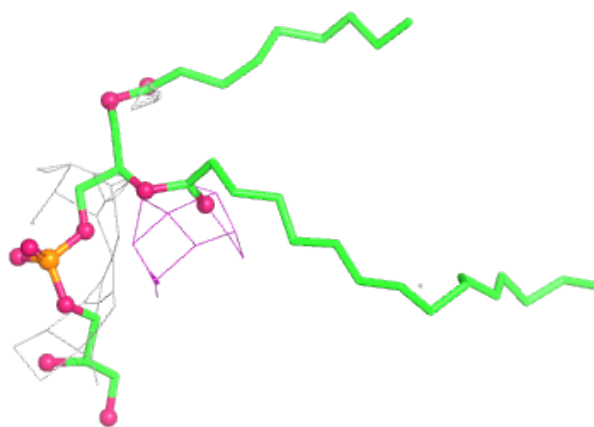
**Electron density around BCR b 622:**

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



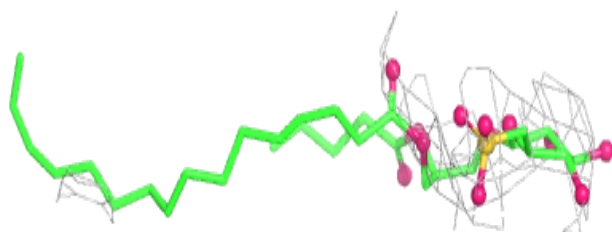
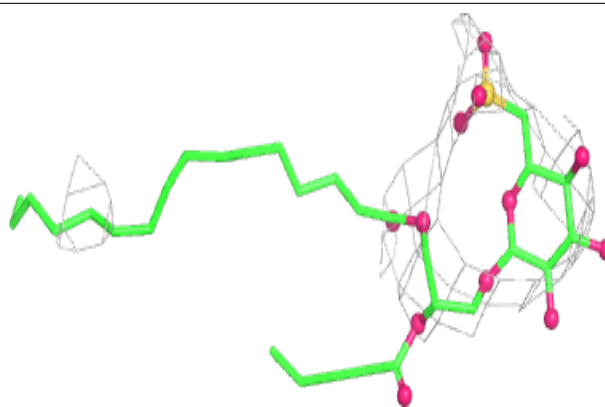
Electron density around LHG E 101:

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

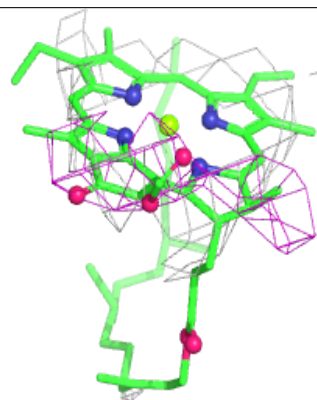
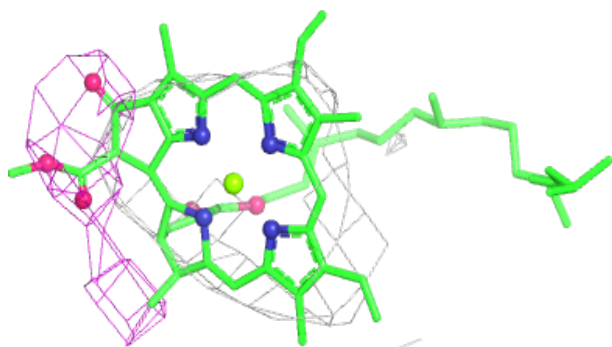
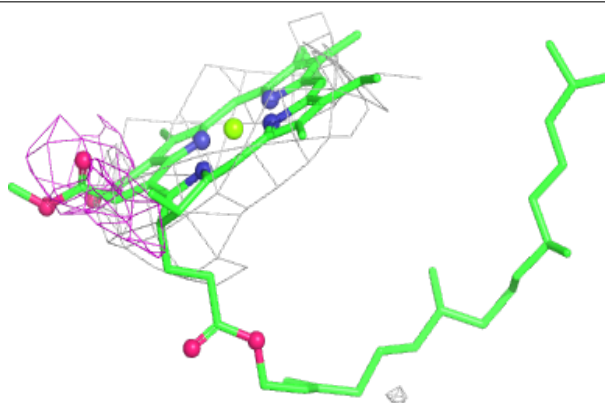


Electron density around SQD x 101:

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

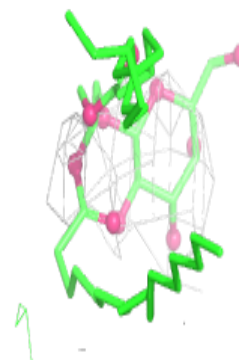
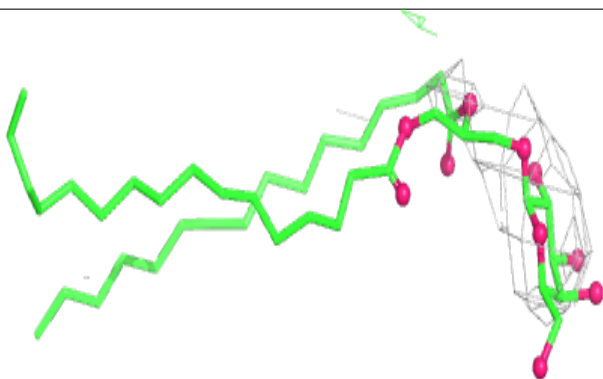
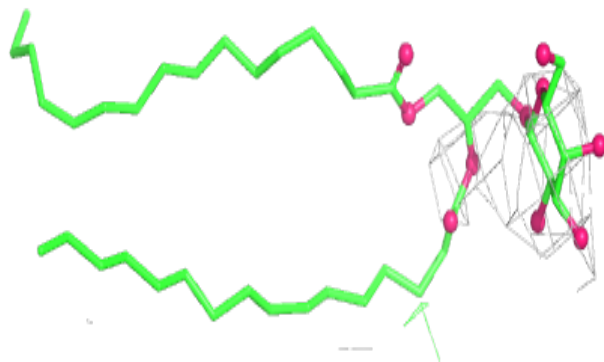
**Electron density around CLA C 513:**

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

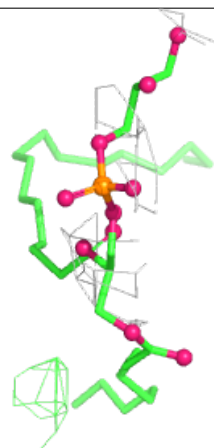
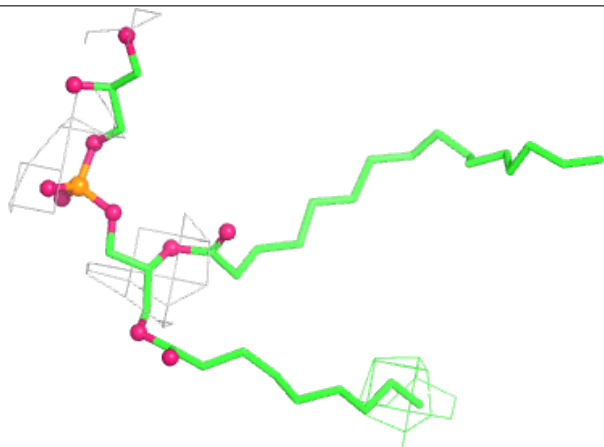


Electron density around LMG c 521:

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

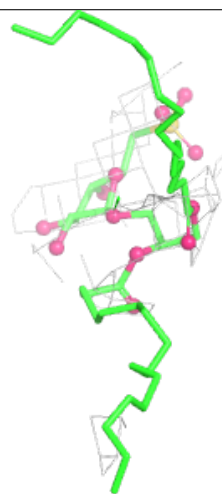
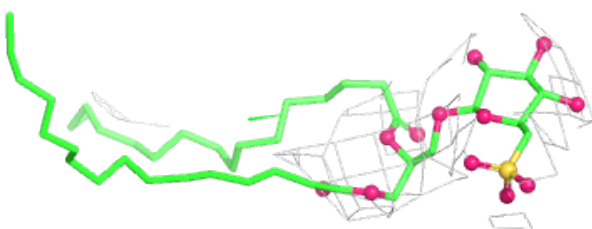
**Electron density around LHG e 101:**

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



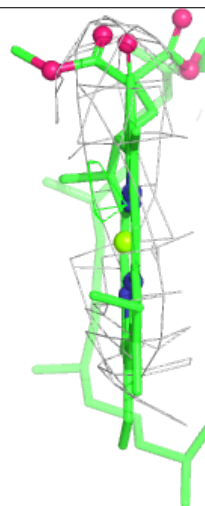
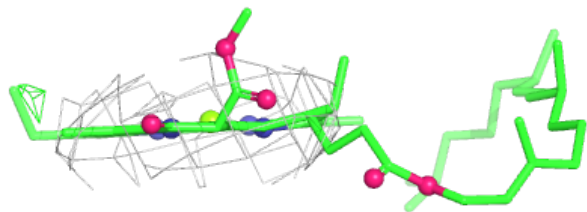
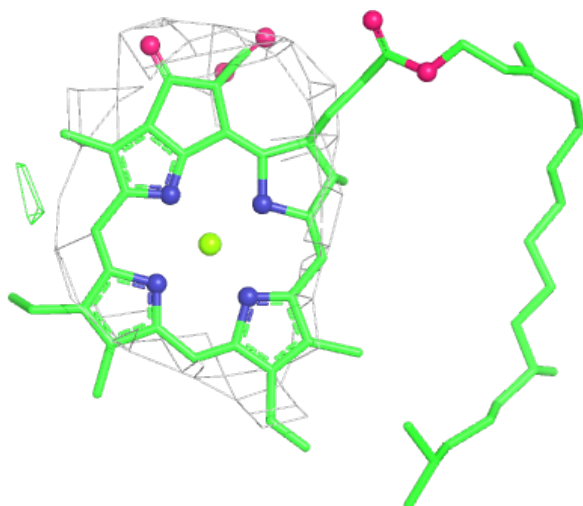
Electron density around SQD A 611:

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



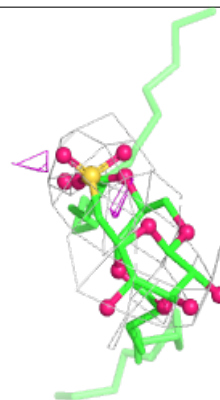
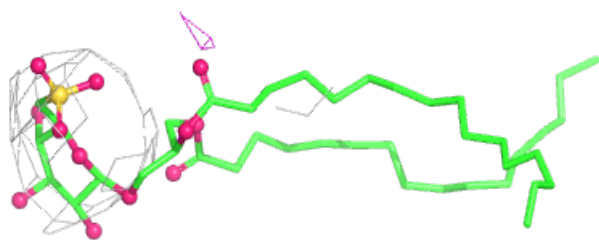
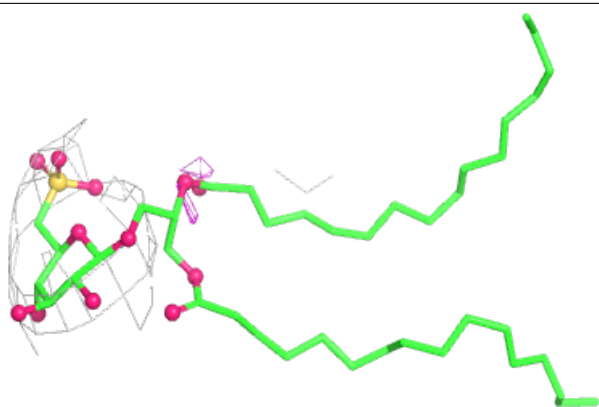
Electron density around CLA C 512:

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



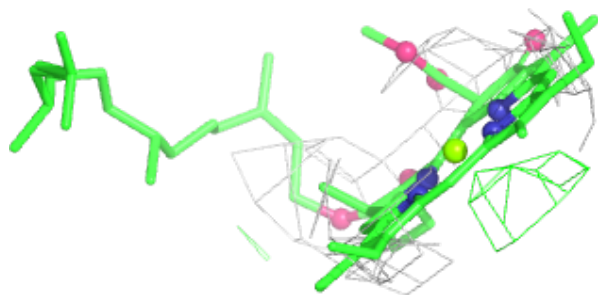
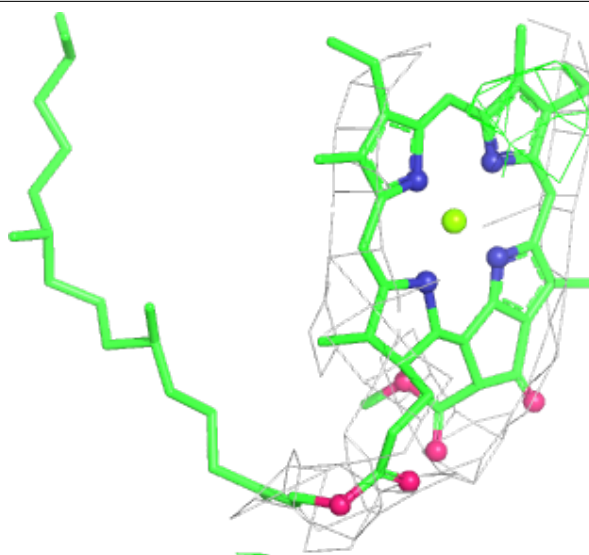
Electron density around SQD b 602:

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



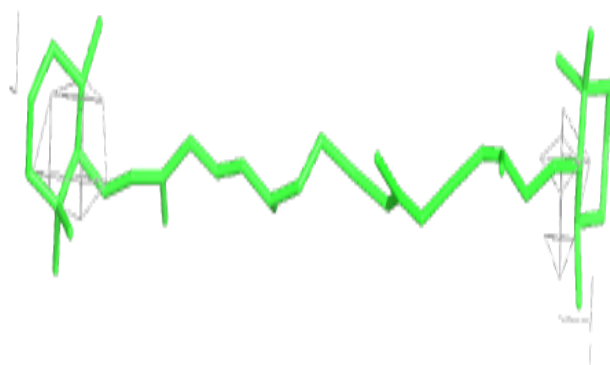
Electron density around CLA B 617:

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

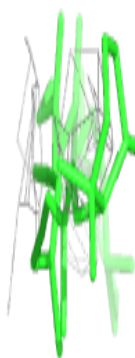
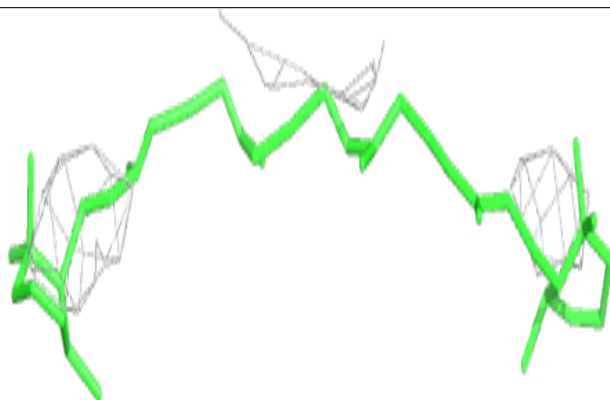
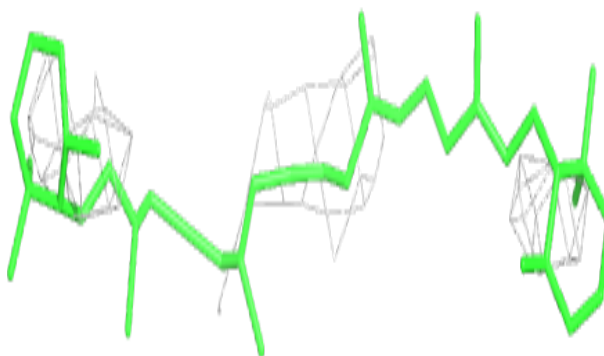


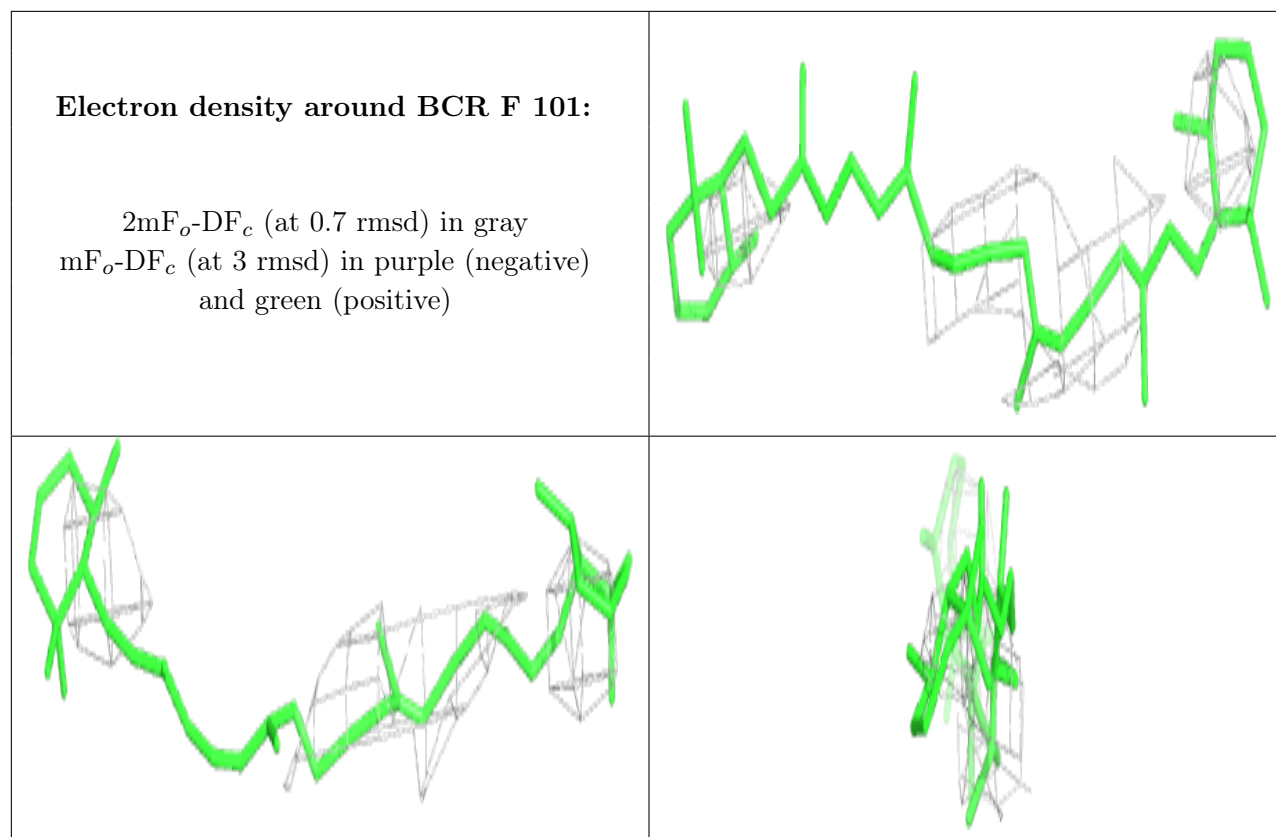
Electron density around BCR C 515:

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

**Electron density around BCR f 101:**

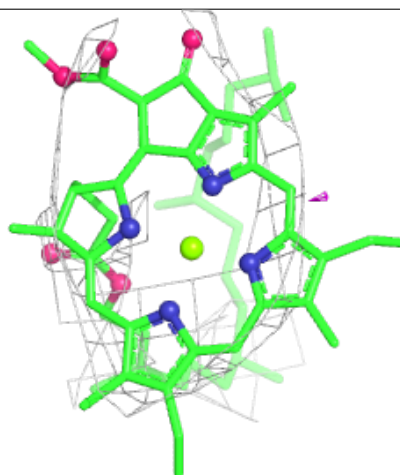
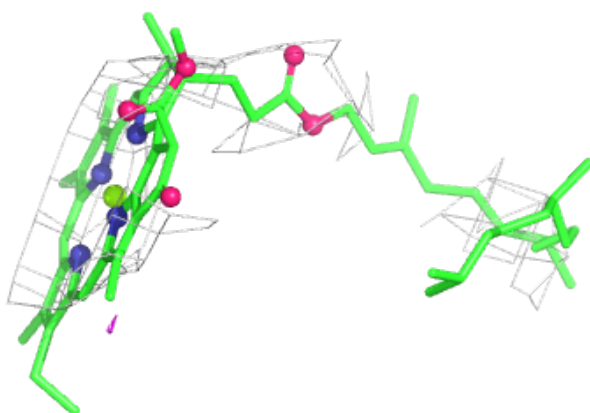
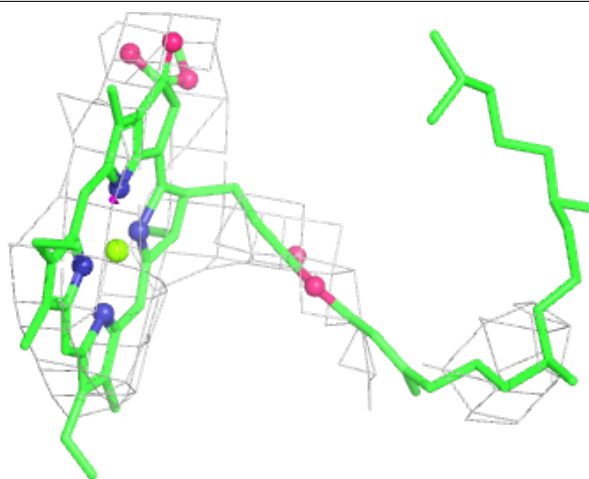
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





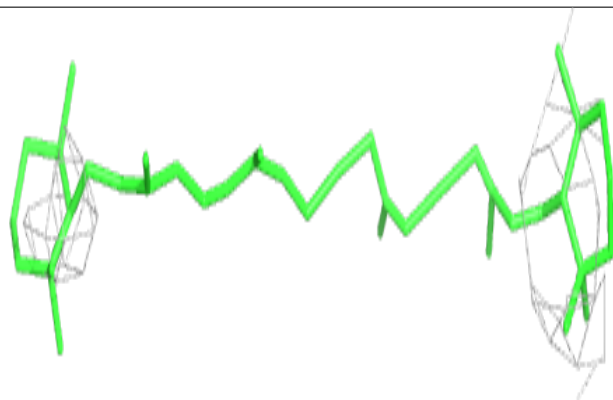
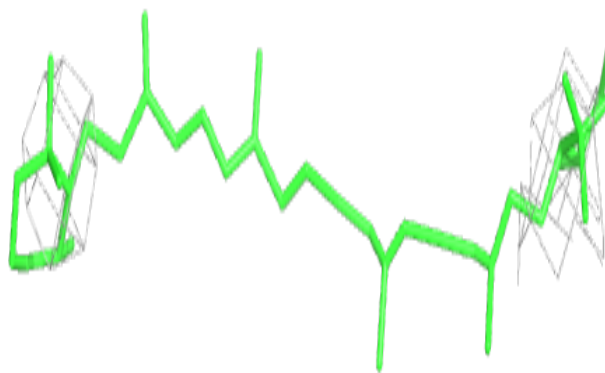
Electron density around CLA b 609 (B):

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



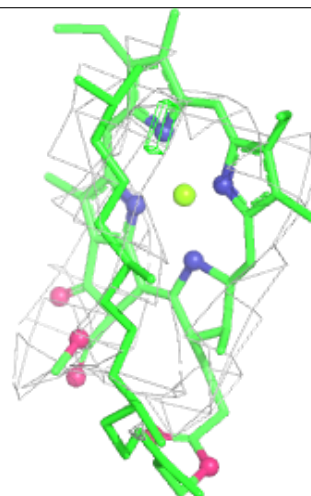
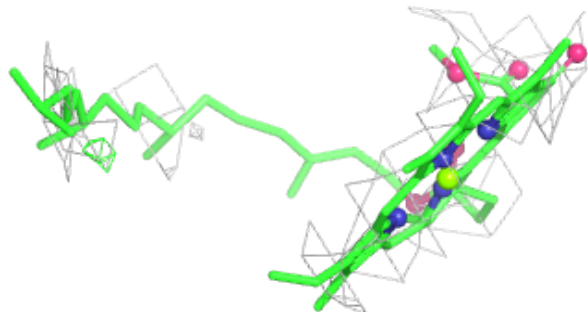
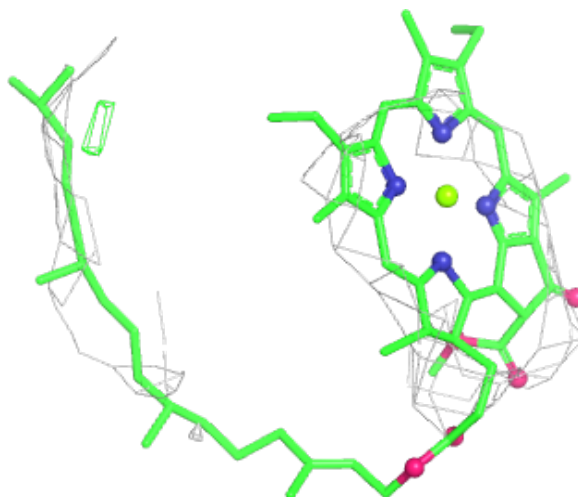
Electron density around BCR C 514:

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



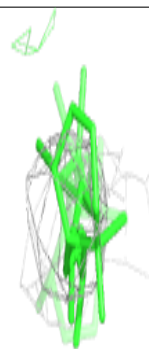
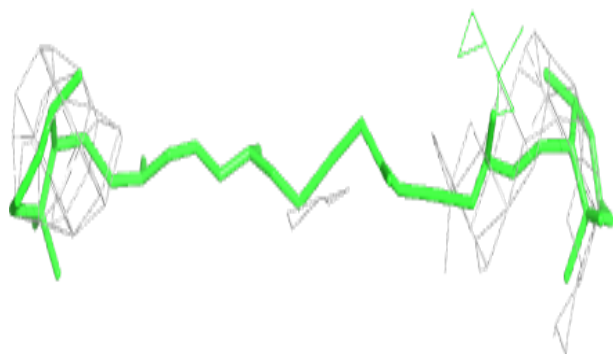
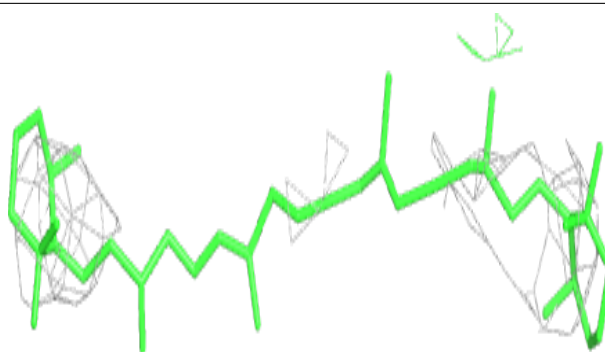
Electron density around CLA C 507:

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

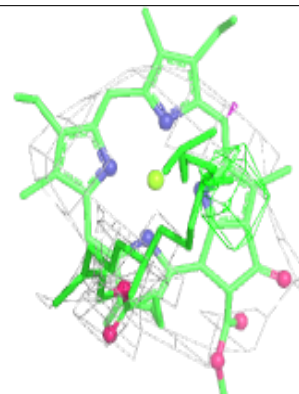
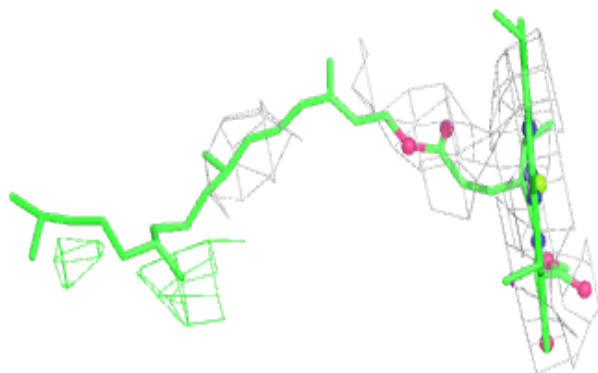
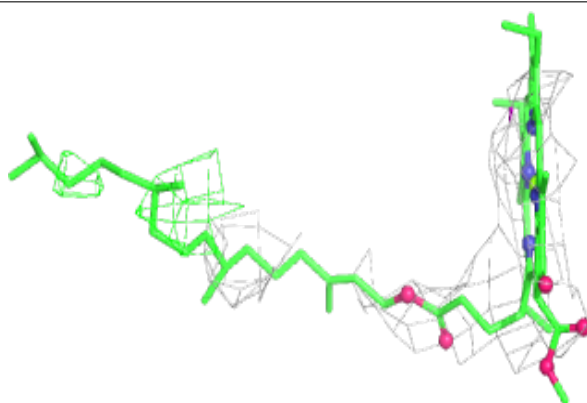


Electron density around BCR b 621:

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

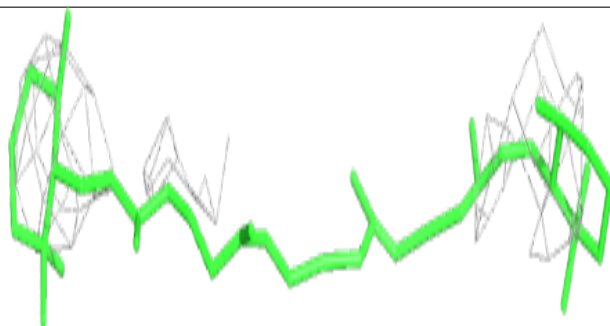
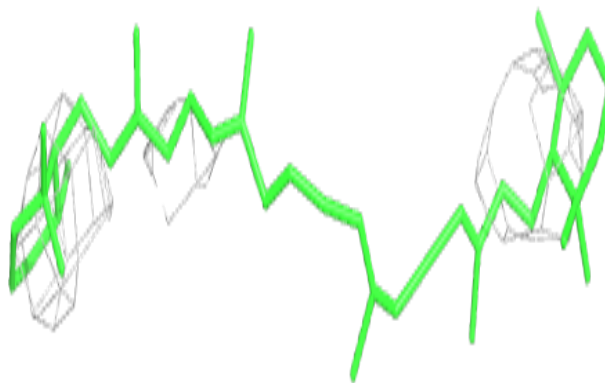
**Electron density around CLA b 609 (A):**

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

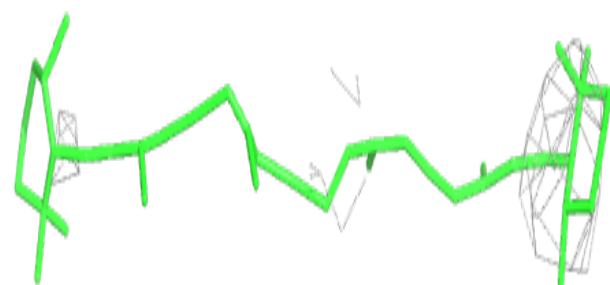


Electron density around BCR b 620:

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

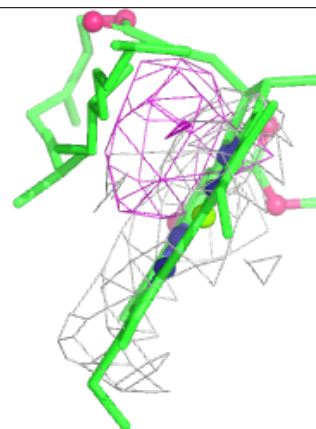
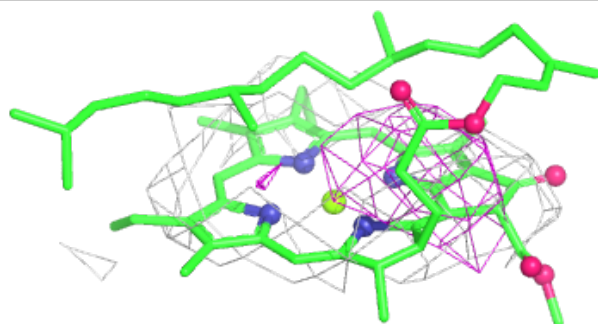
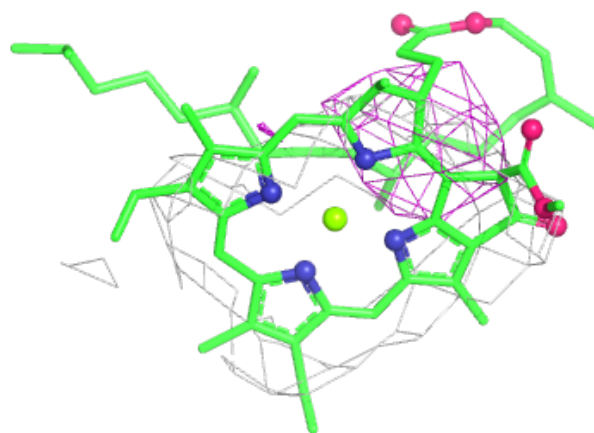
**Electron density around BCR A 609:**

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

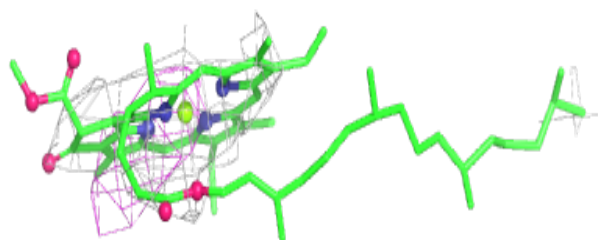
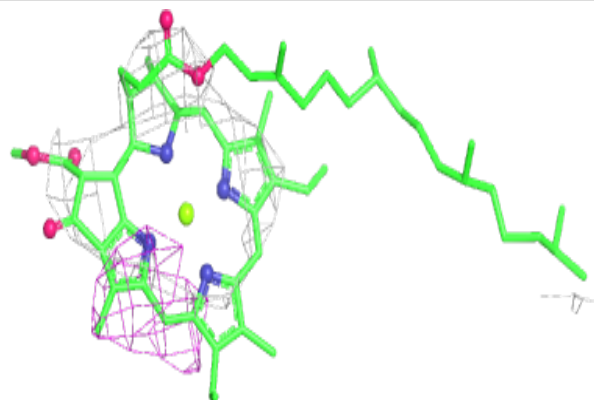


Electron density around CLA b 604:

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

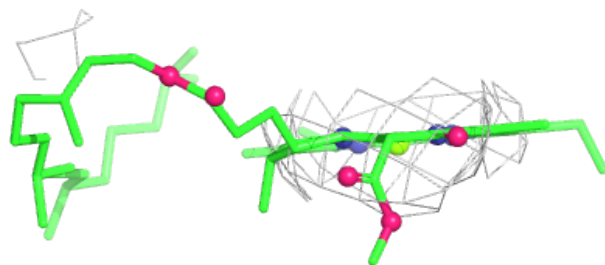
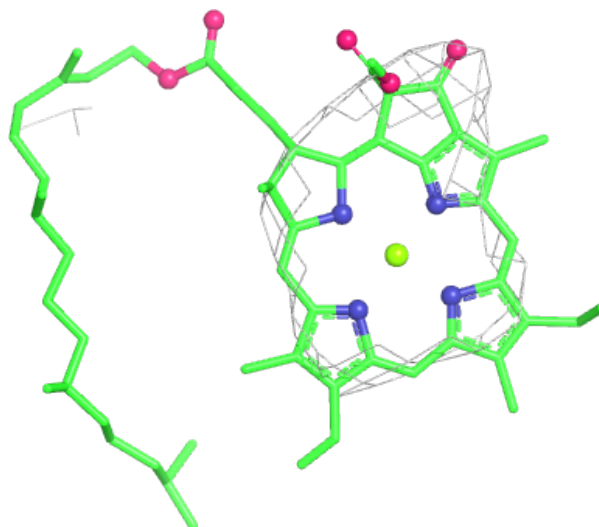
**Electron density around CLA c 502:**

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



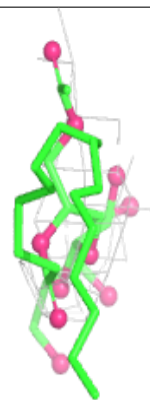
Electron density around CLA c 513:

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

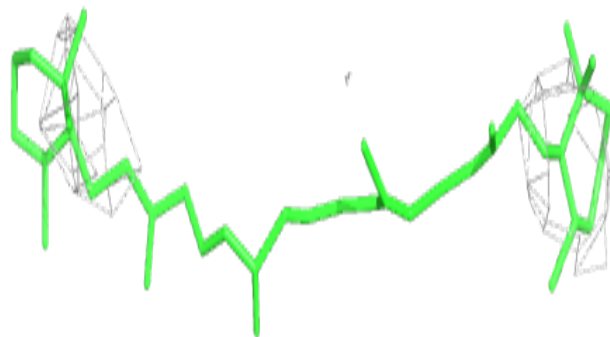
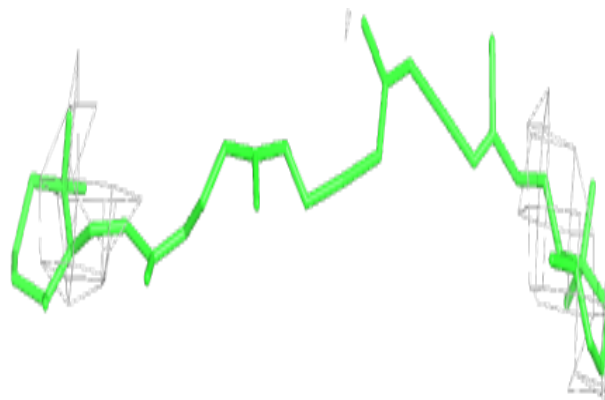


Electron density around LMG z 101:

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

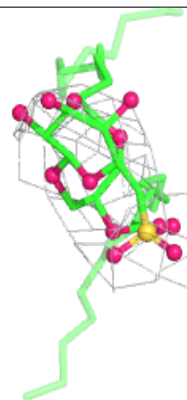
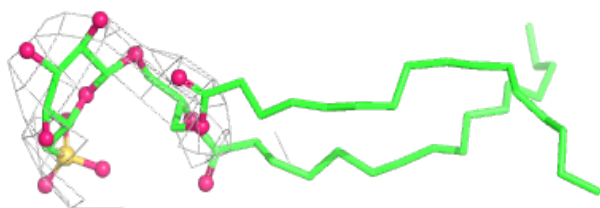
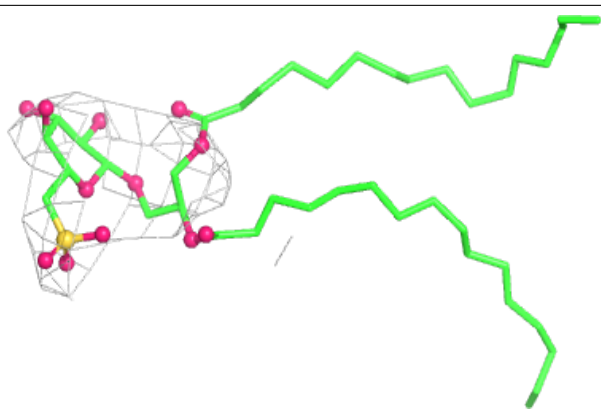
**Electron density around BCR t 101:**

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



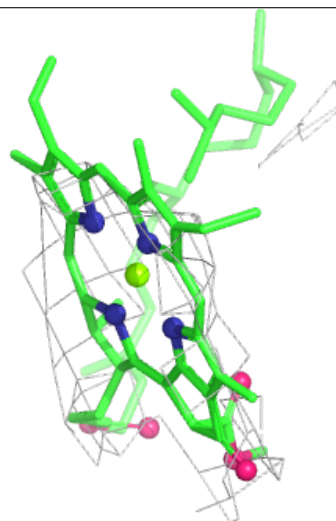
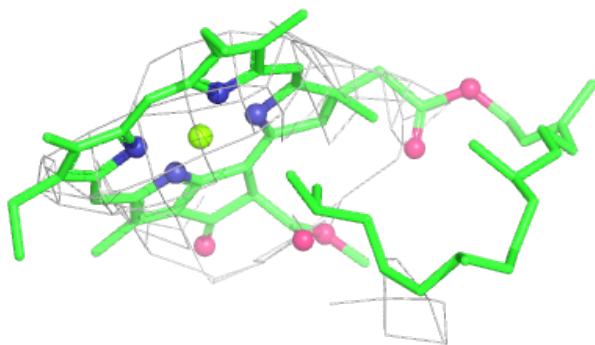
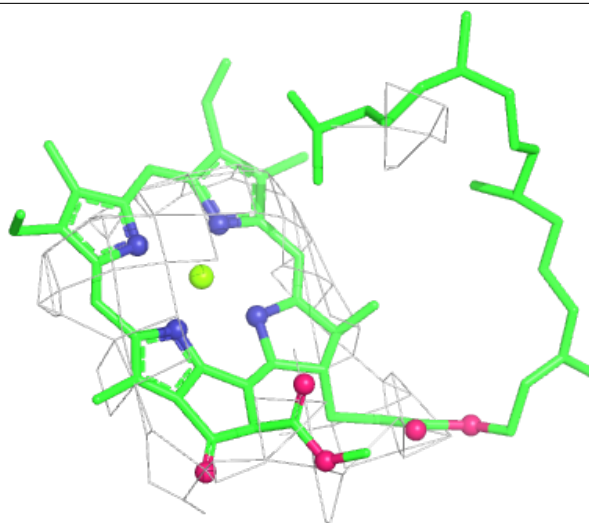
Electron density around SQD B 623:

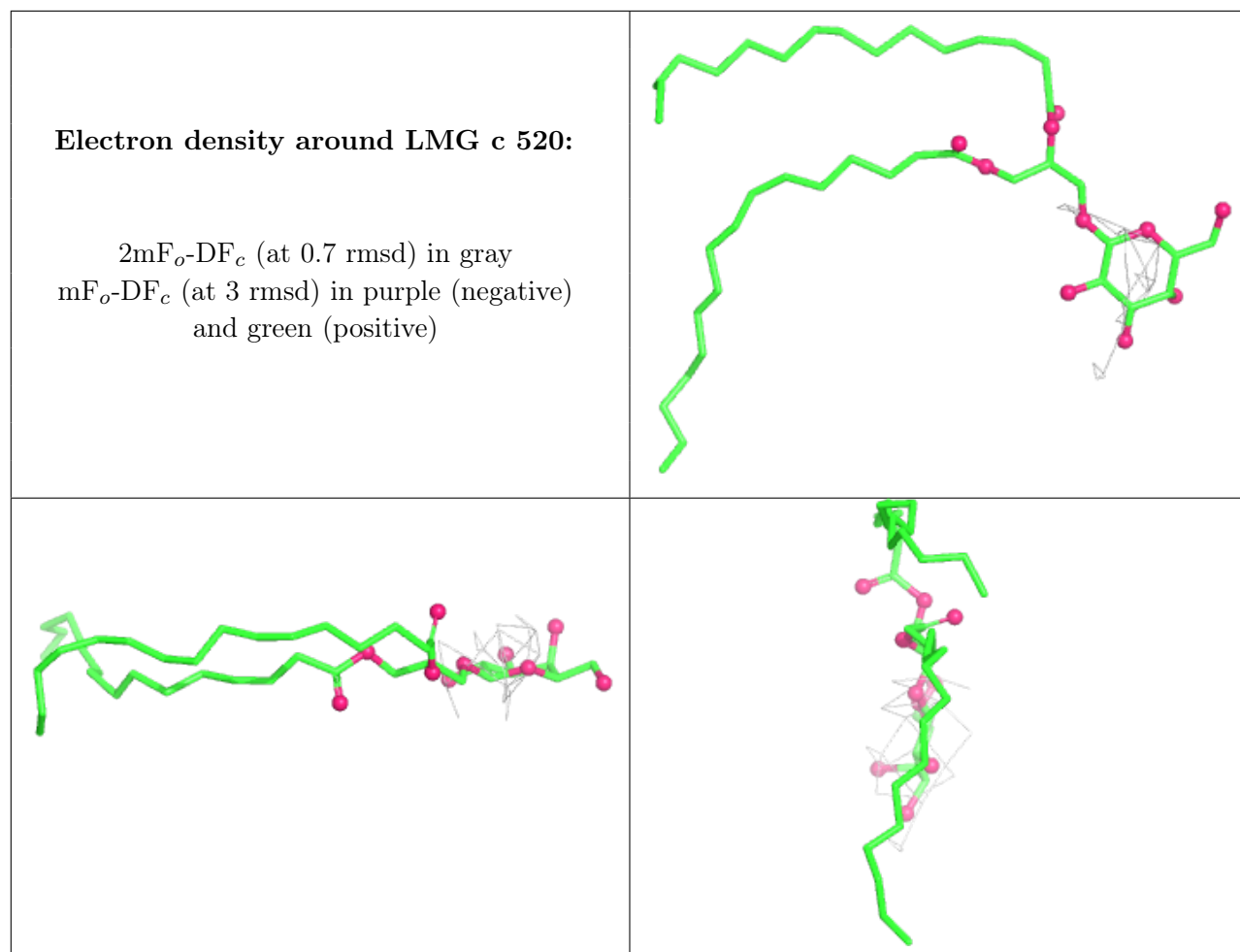
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA b 618:

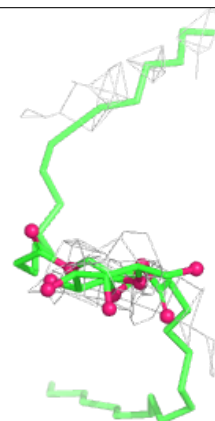
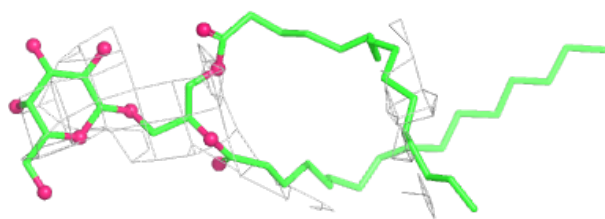
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



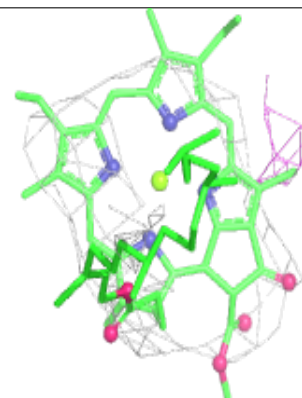
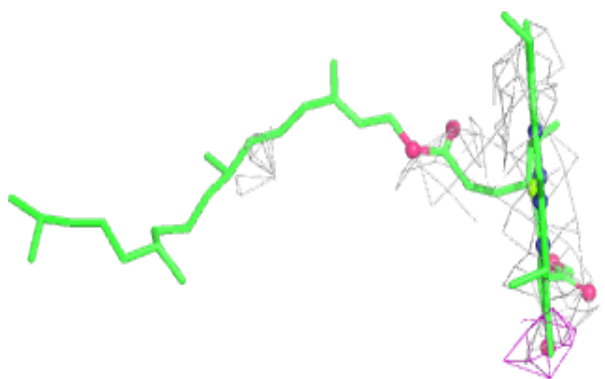
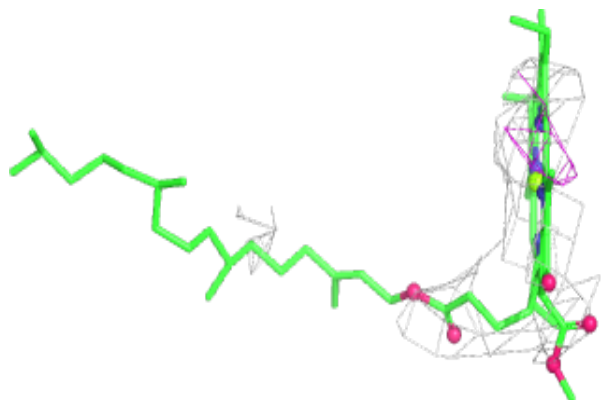


Electron density around LMG b 623:

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

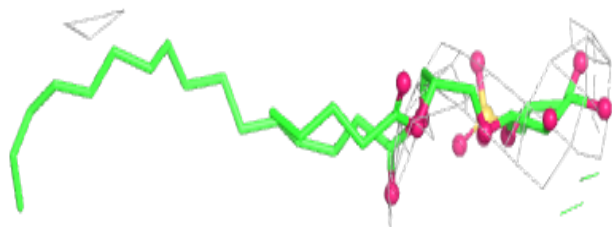
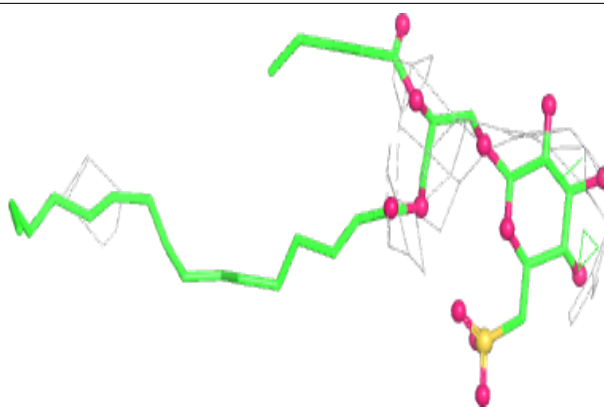
**Electron density around CLA B 607 (A):**

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

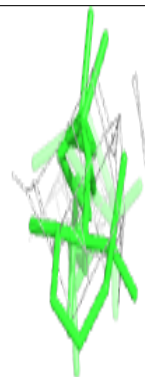
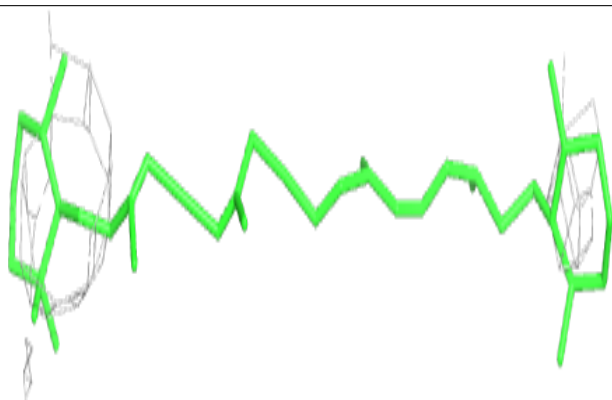
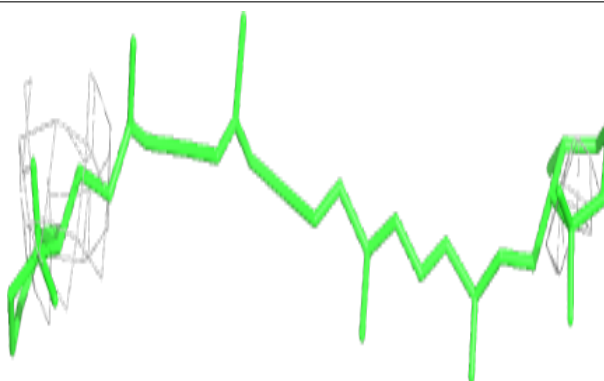


Electron density around SQD X 101:

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

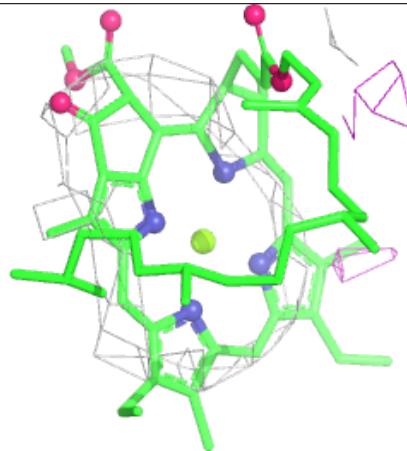
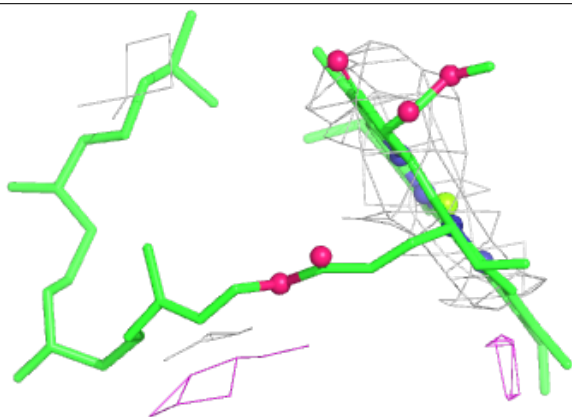
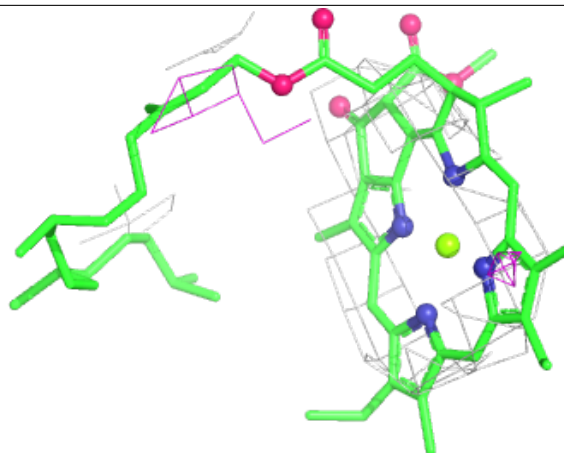
**Electron density around BCR c 515:**

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



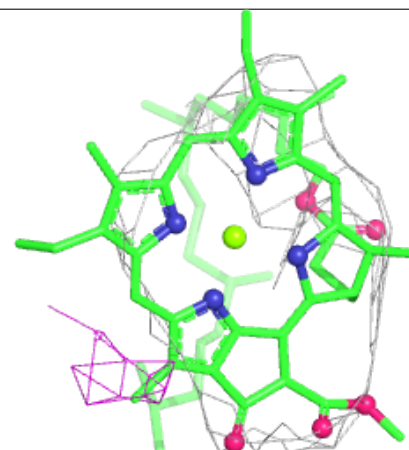
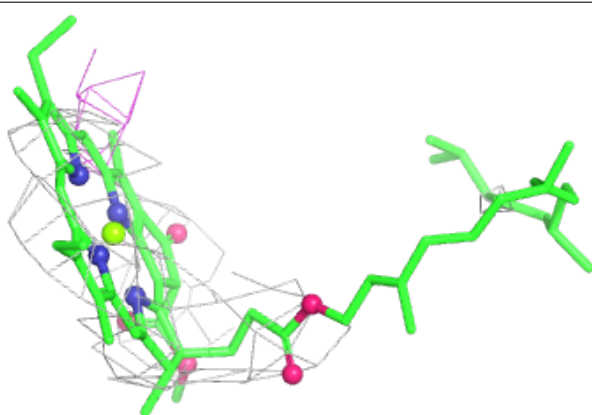
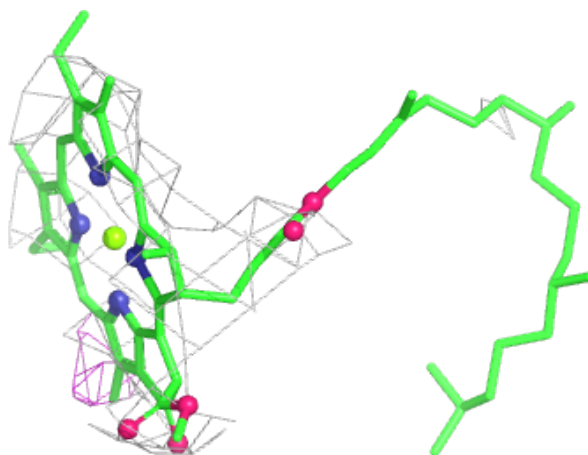
Electron density around CLA c 504:

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



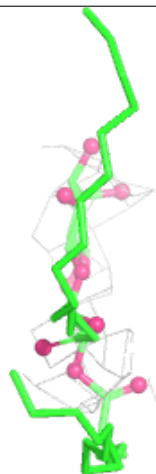
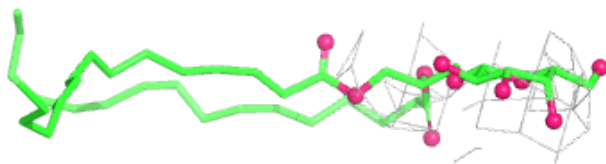
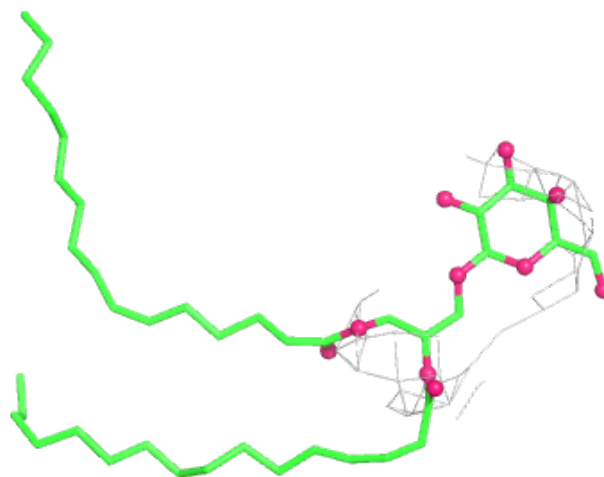
Electron density around CLA B 607 (B):

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



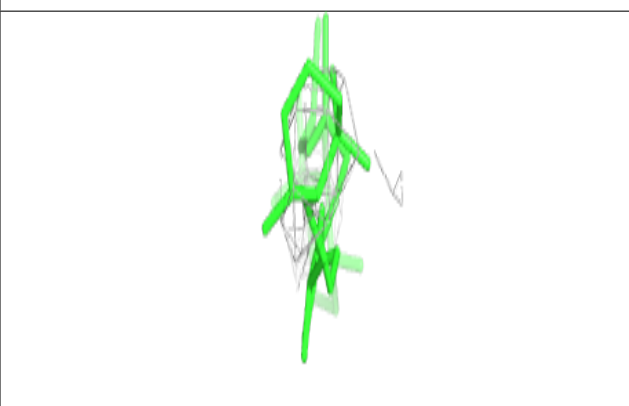
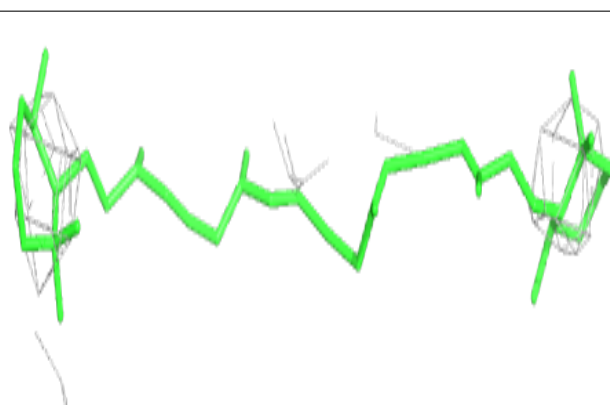
Electron density around LMG C 519:

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

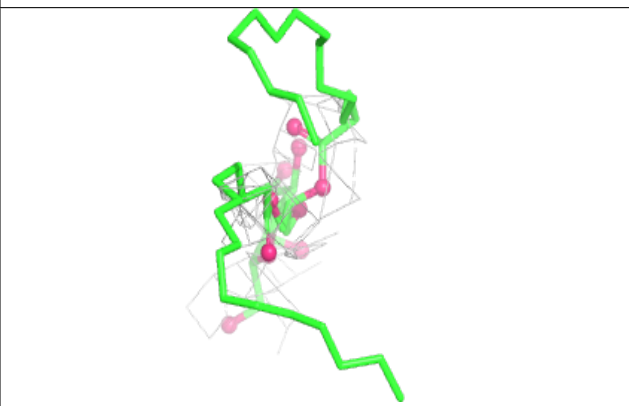
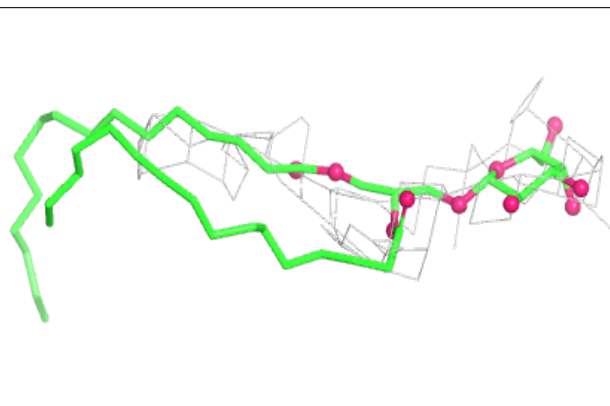
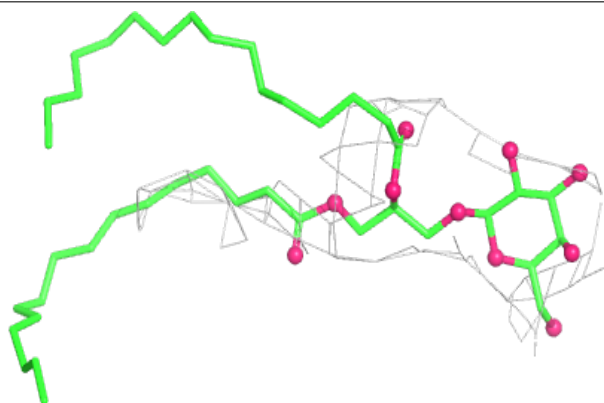


Electron density around BCR K 101:

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

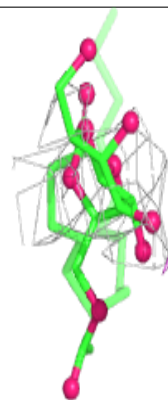
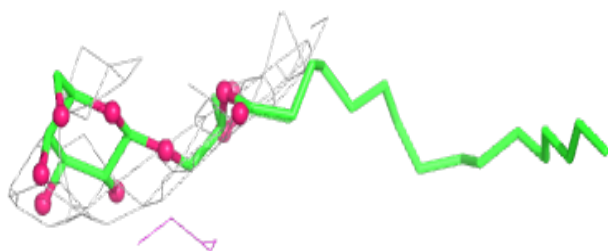
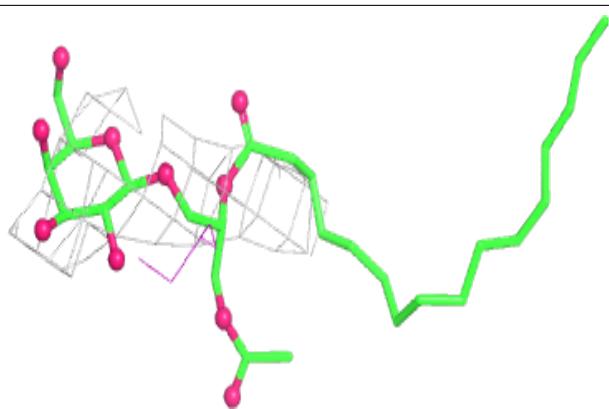
**Electron density around LMG J 101:**

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

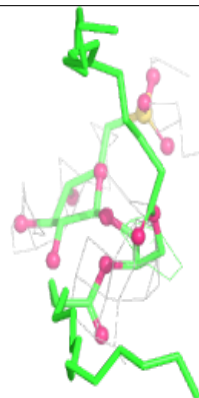
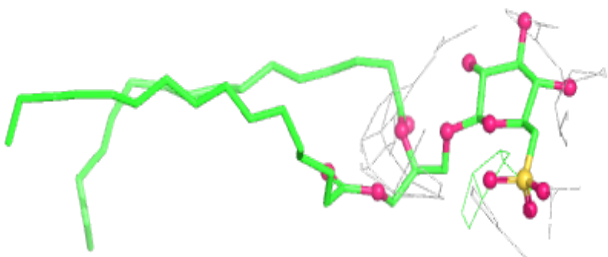
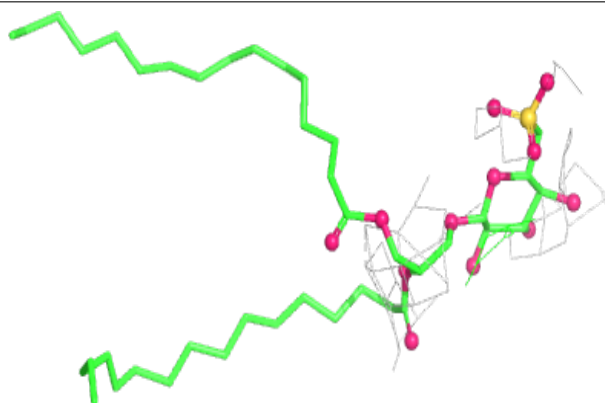


Electron density around LMG Z 101:

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

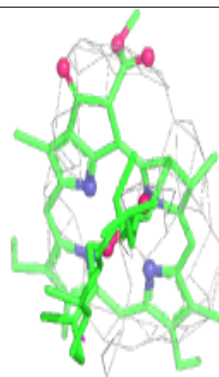
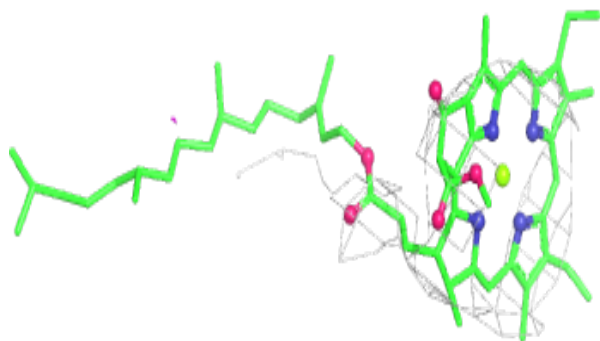
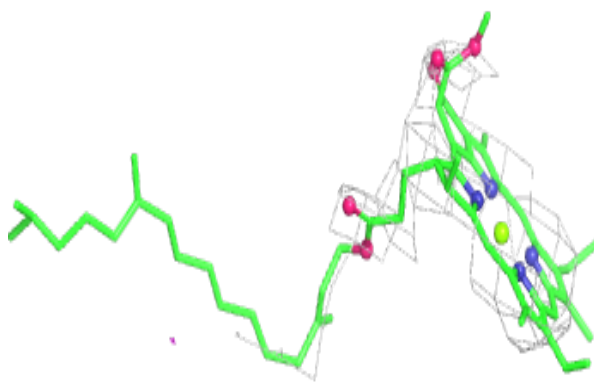
**Electron density around SQD b 601:**

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

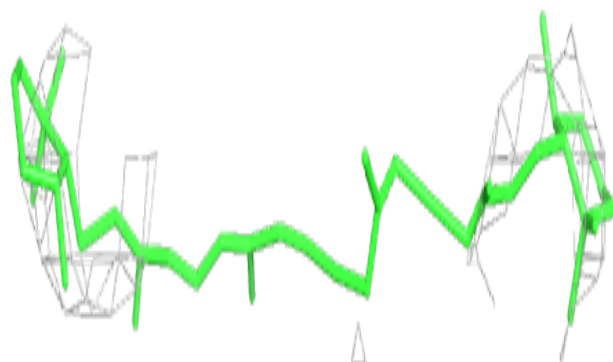
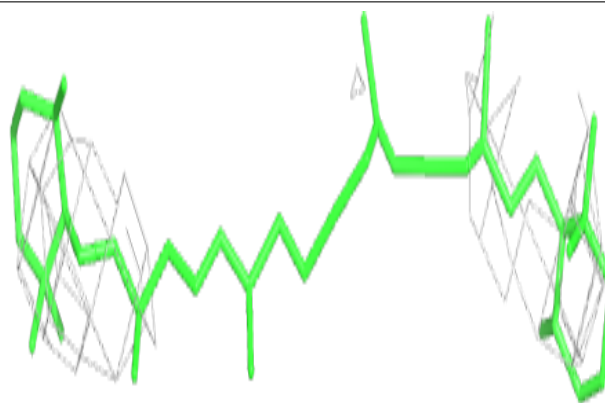


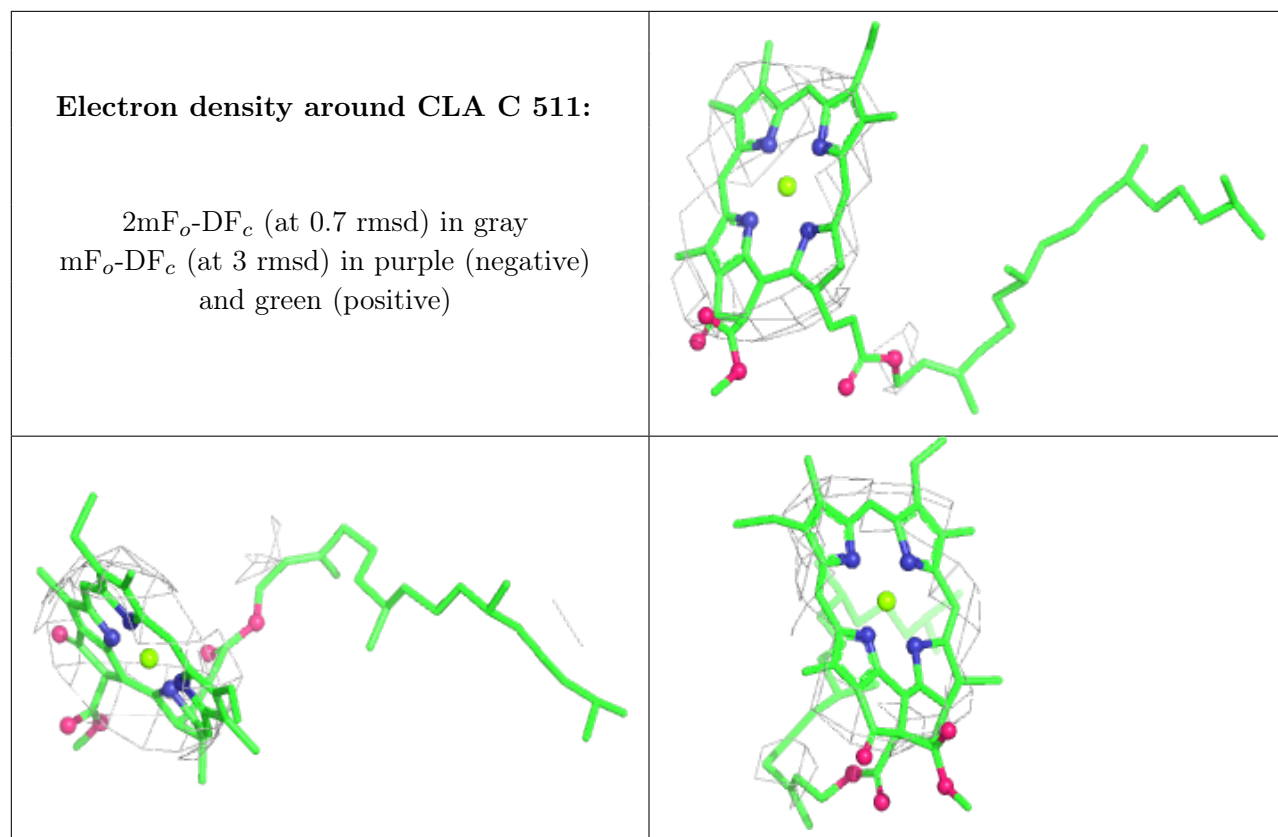
Electron density around CLA c 503:

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

**Electron density around BCR B 620:**

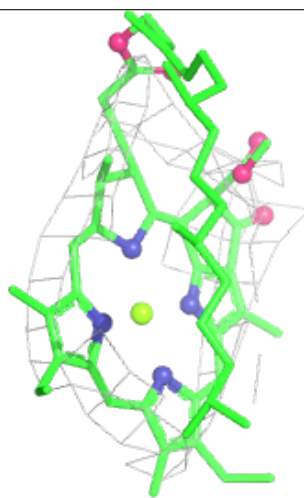
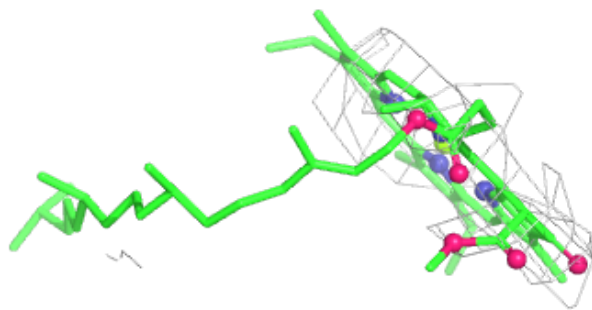
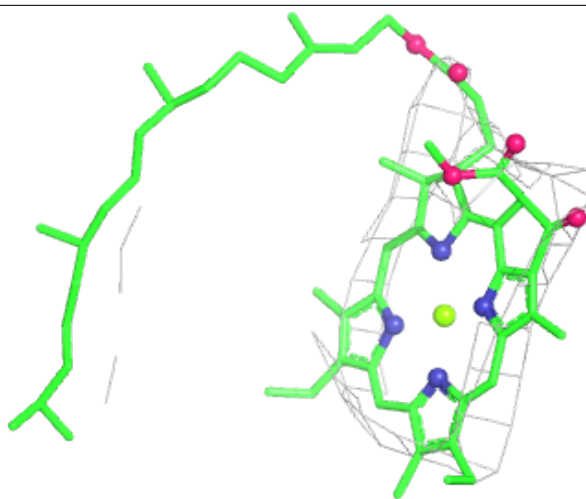
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





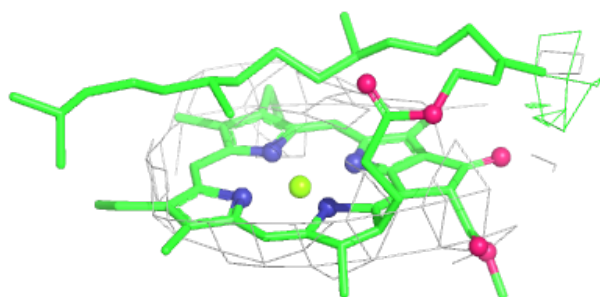
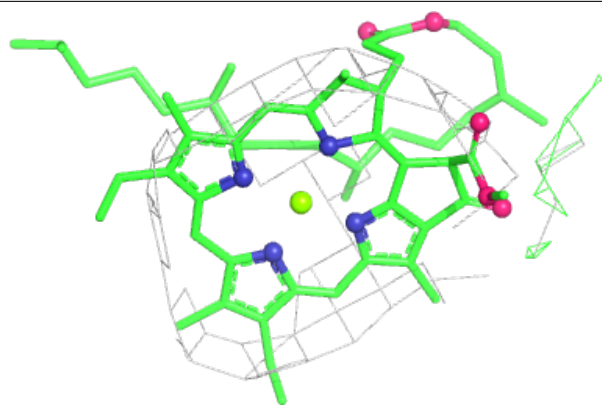
Electron density around CLA c 508:

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

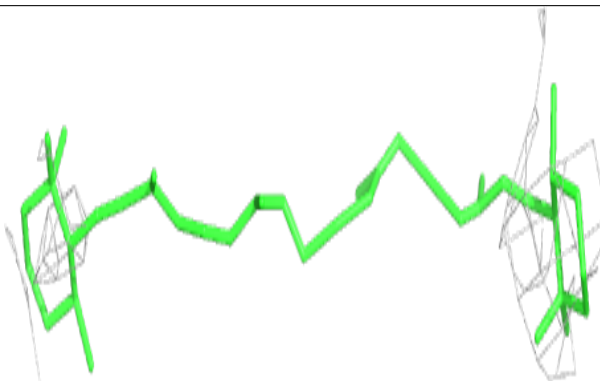


Electron density around CLA B 602:

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

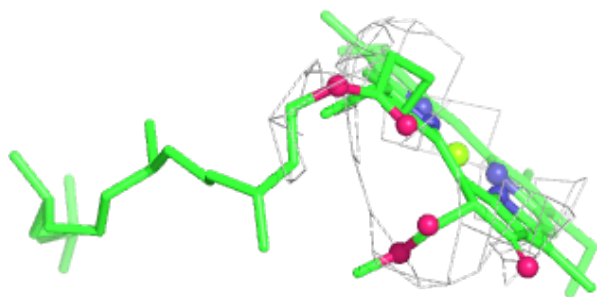
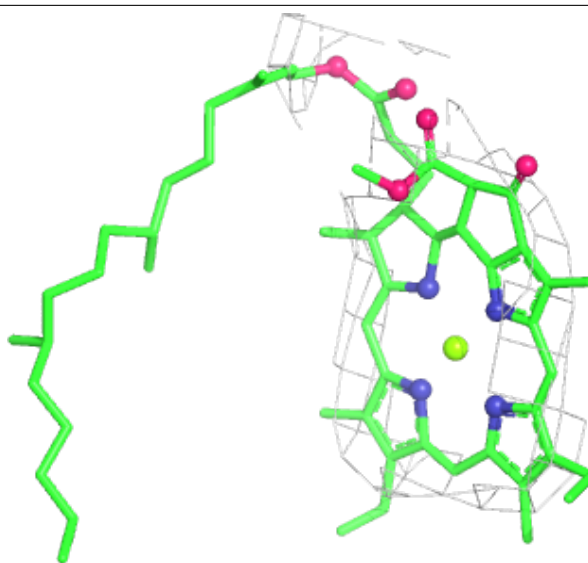
**Electron density around BCR c 516:**

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



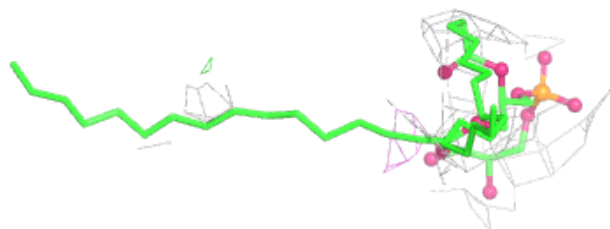
Electron density around CLA b 619:

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



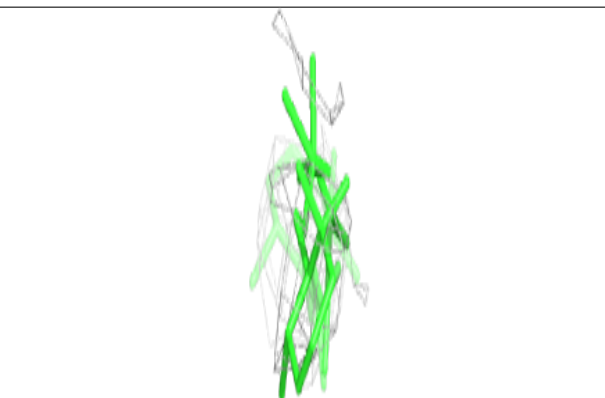
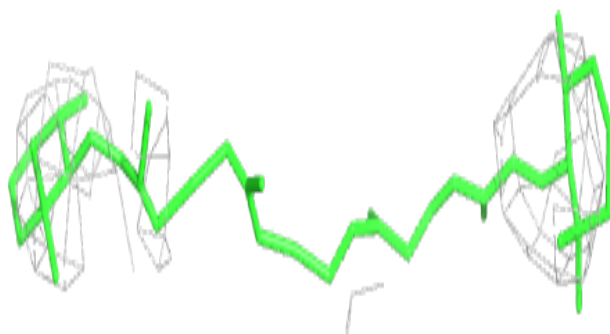
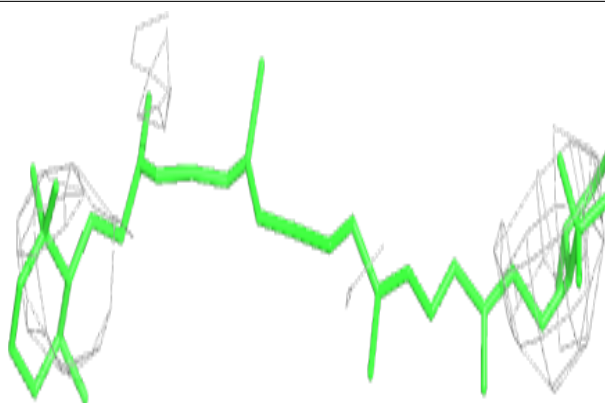
Electron density around LHG 1 101:

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

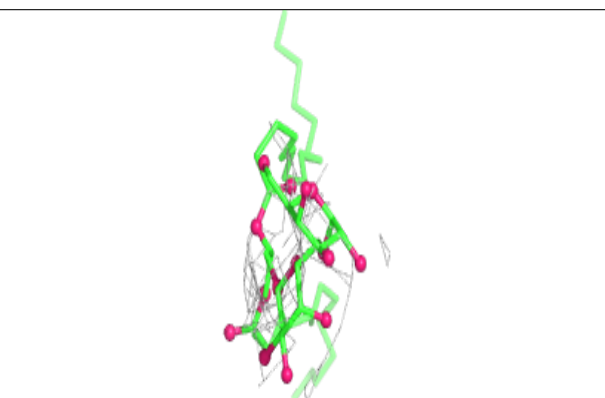
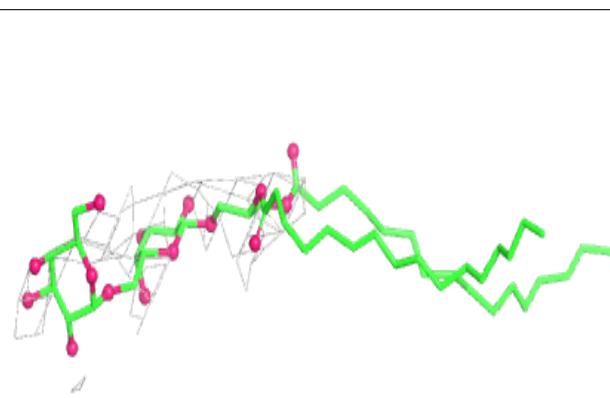
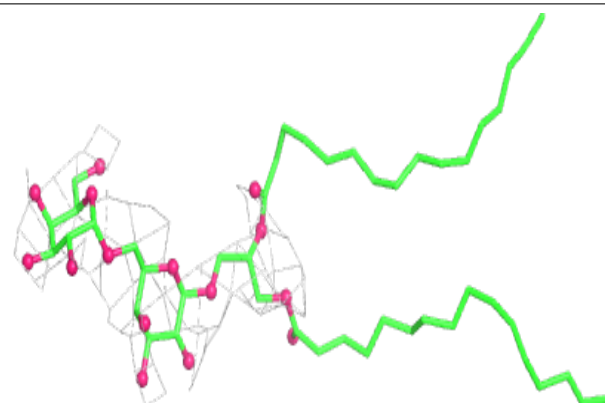


Electron density around BCR B 618:

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

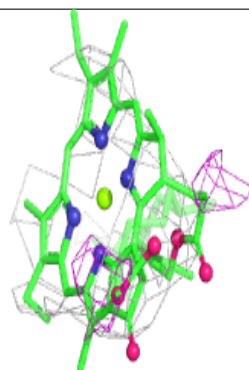
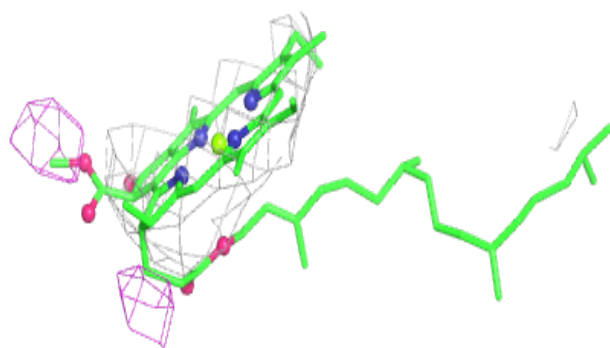
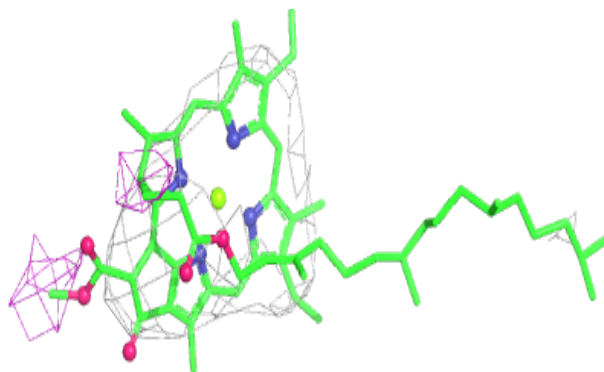
**Electron density around DGD c 519:**

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



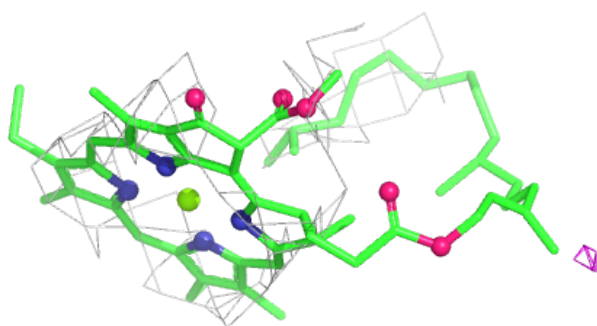
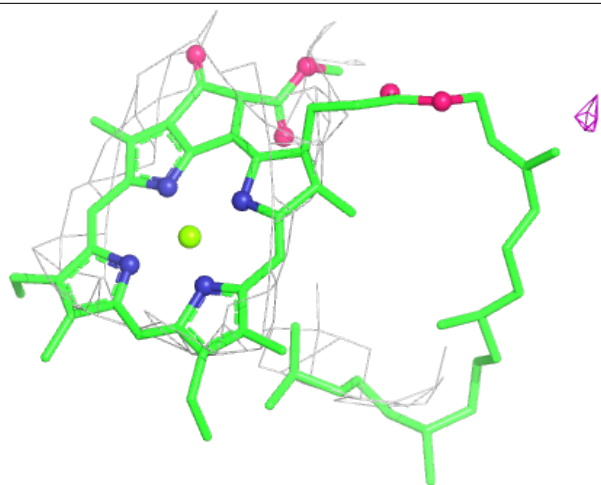
Electron density around CLA b 617:

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



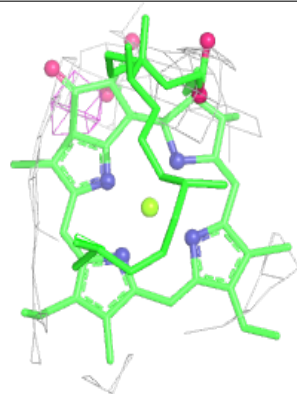
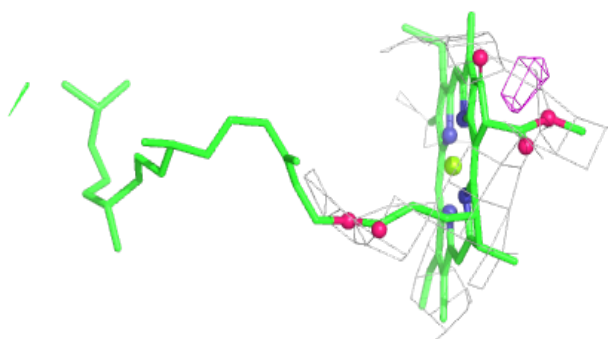
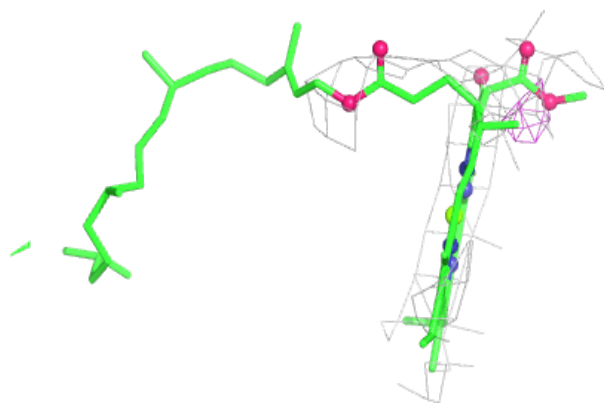
Electron density around CLA B 616:

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

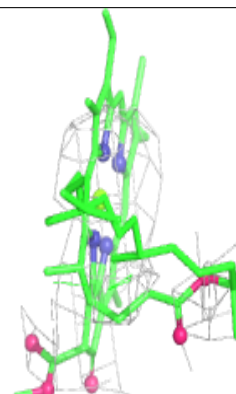
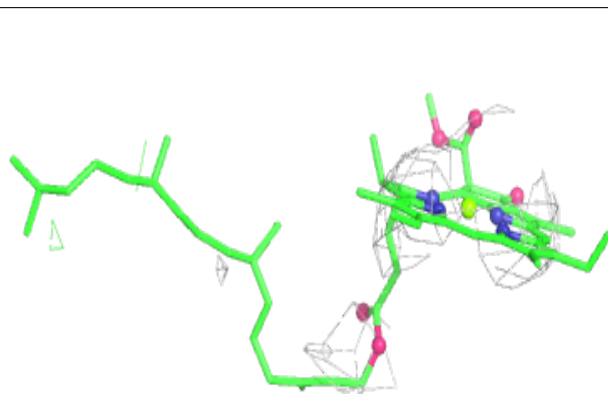
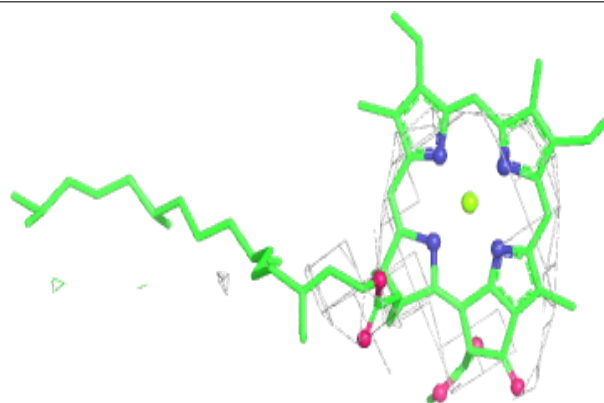


Electron density around CLA C 506:

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

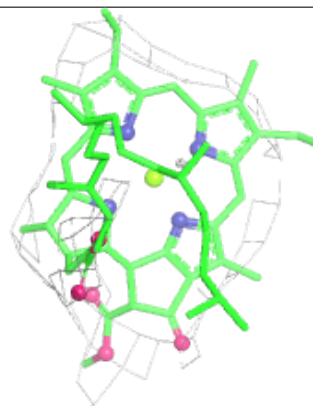
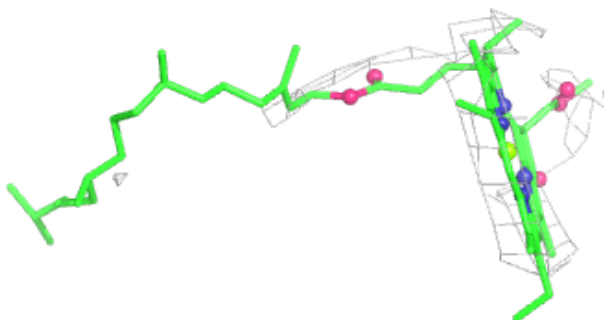
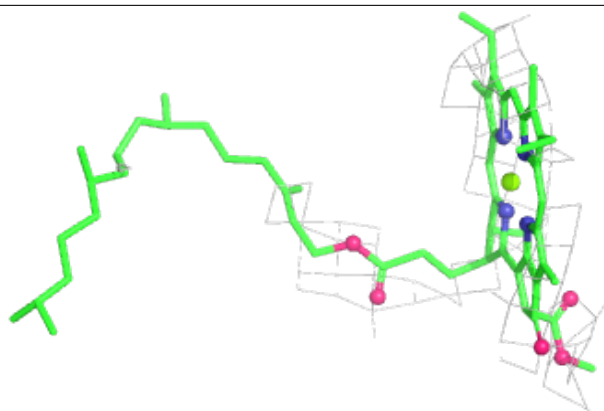
**Electron density around CLA a 605:**

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

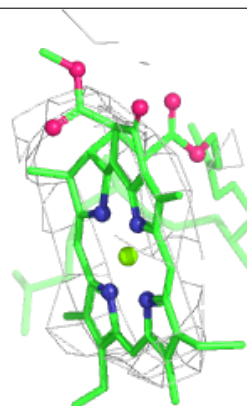
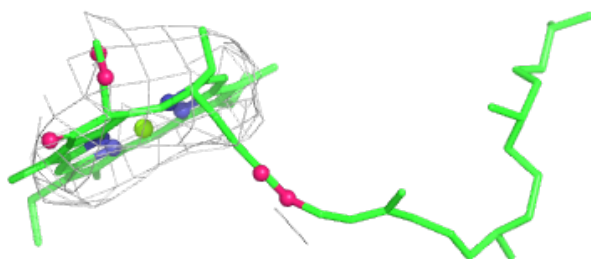
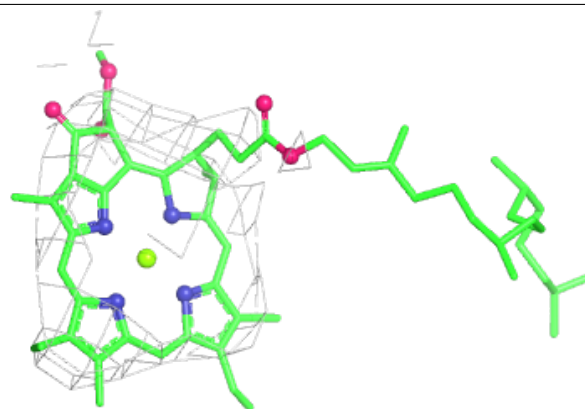


Electron density around CLA d 403:

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

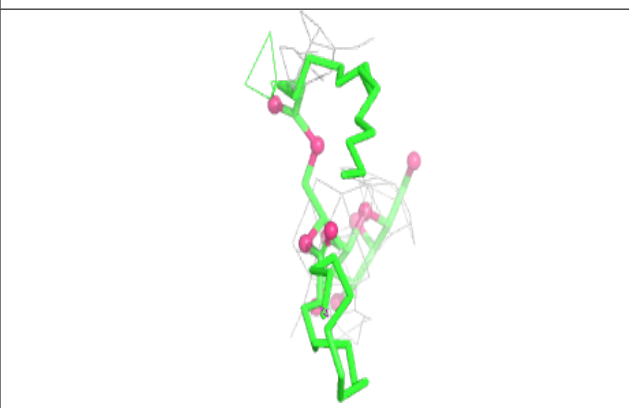
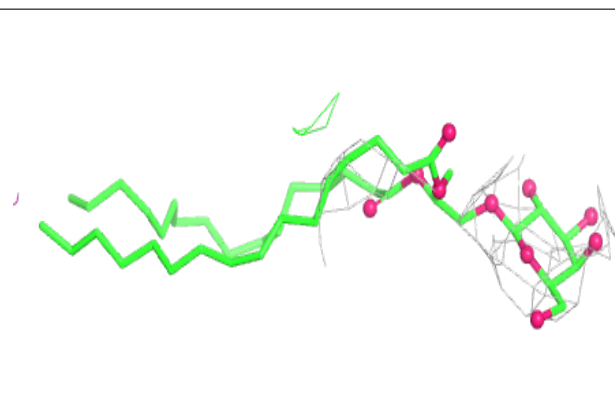
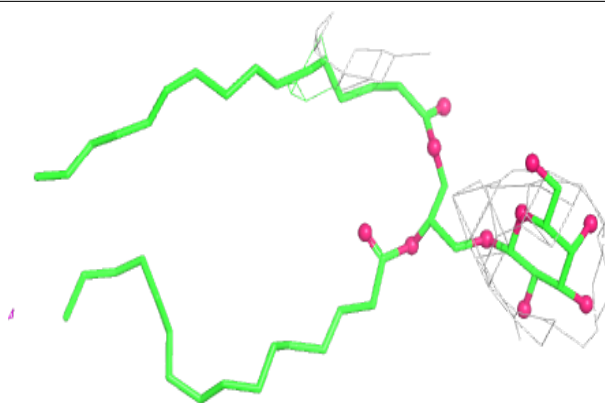
**Electron density around CLA a 607:**

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

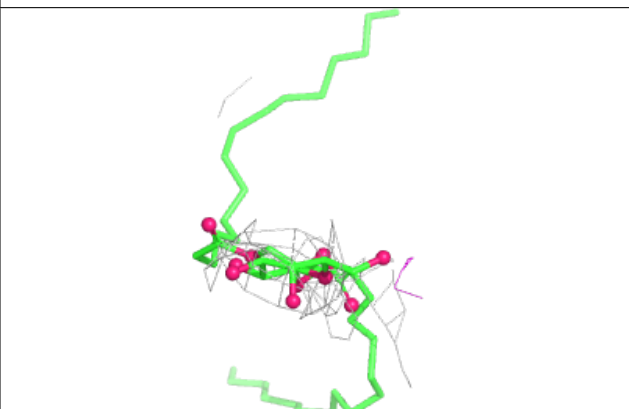
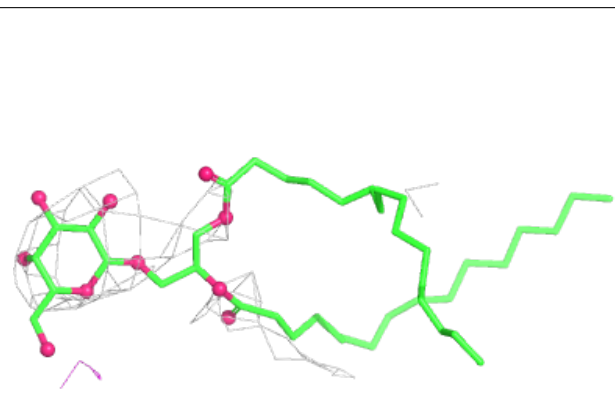
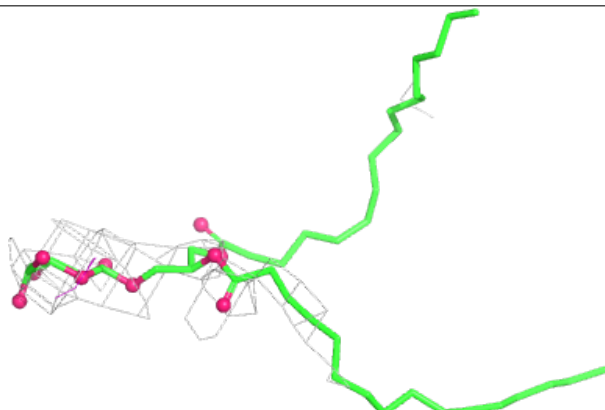


Electron density around LMG A 612:

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

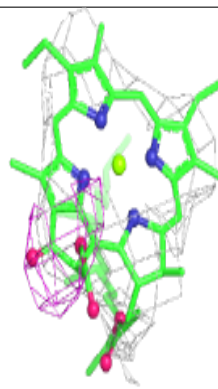
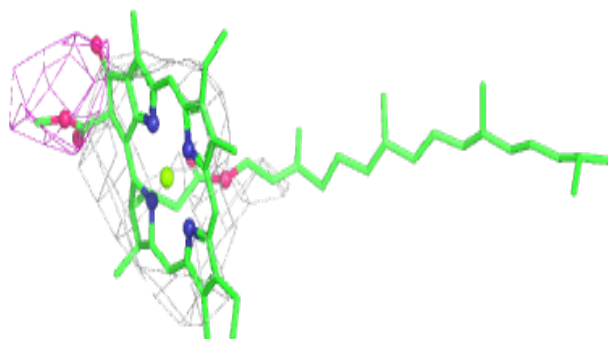
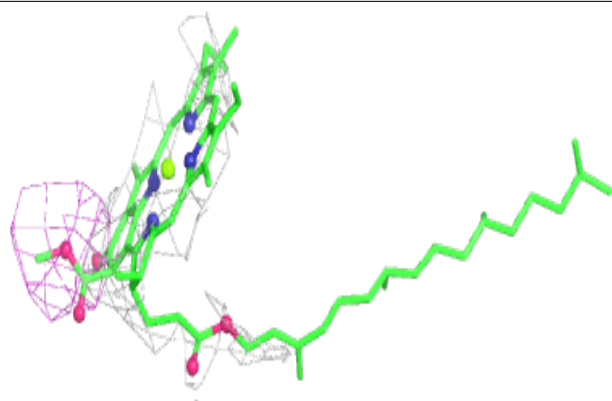
**Electron density around LMG B 621:**

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

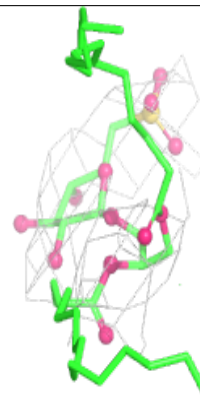
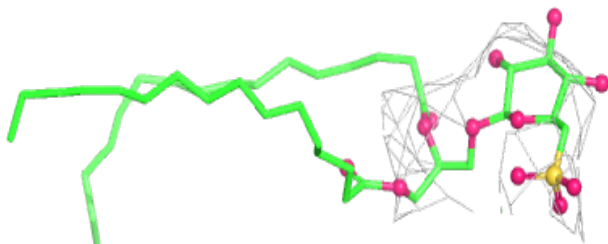
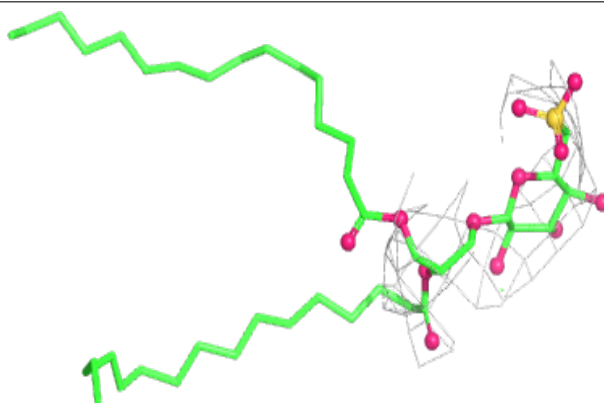


Electron density around CLA B 608:

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

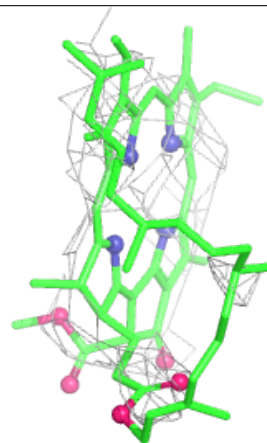
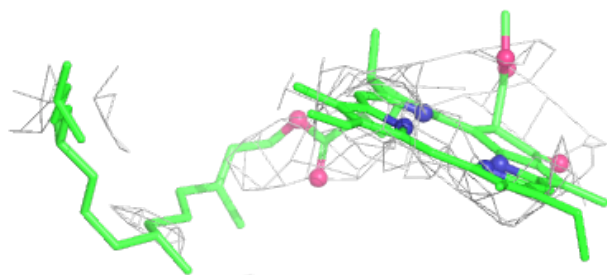
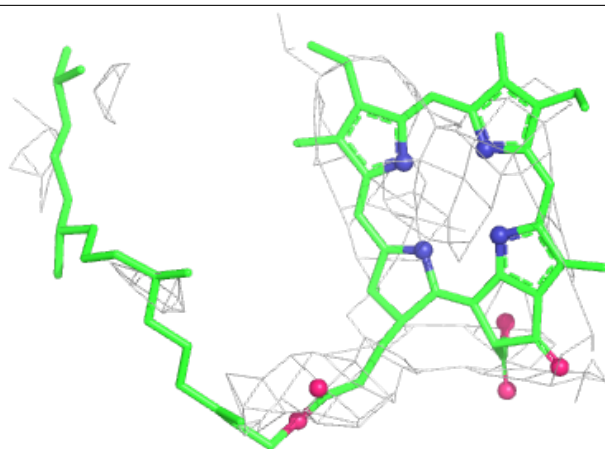
**Electron density around SQD a 612:**

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

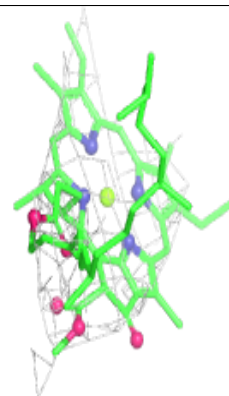
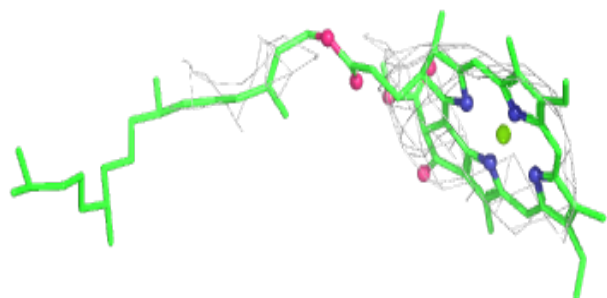
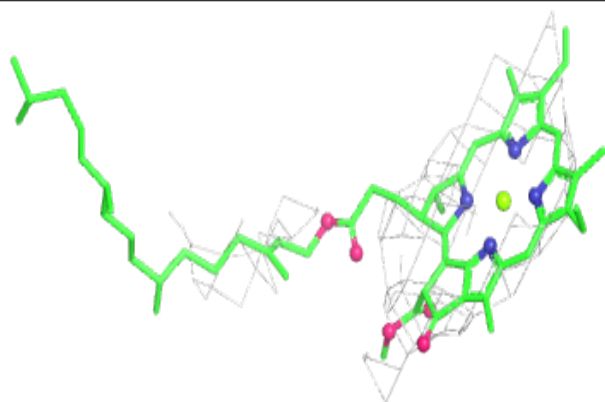


Electron density around PHO D 401:

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

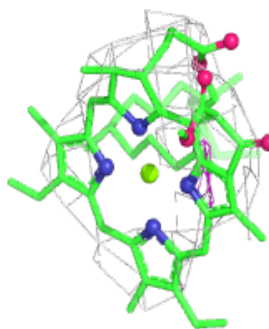
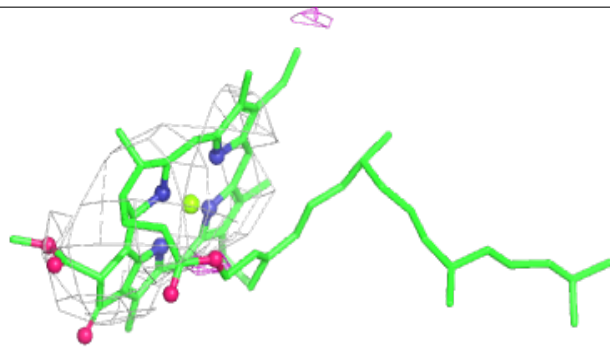
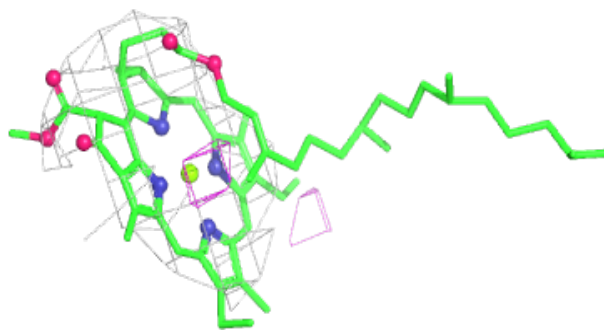
**Electron density around CLA a 604:**

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

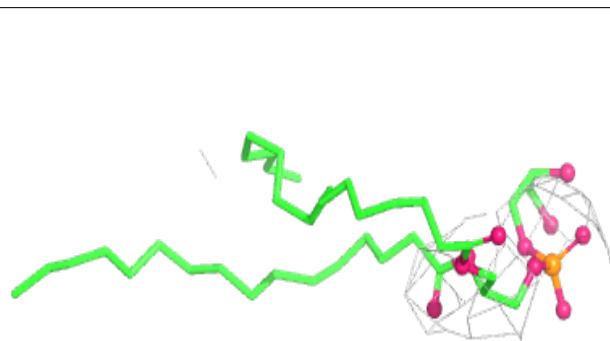
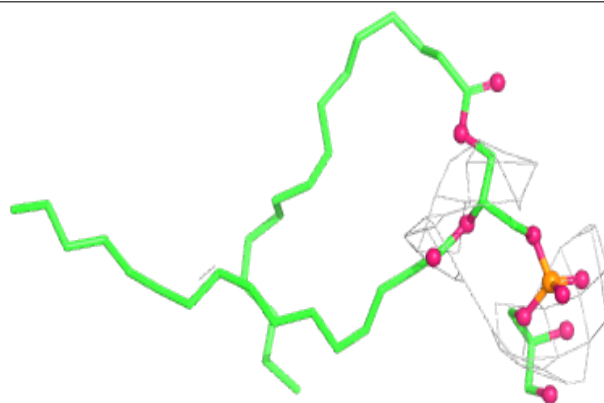


Electron density around CLA C 505:

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

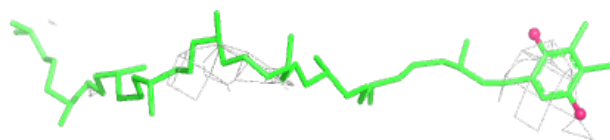
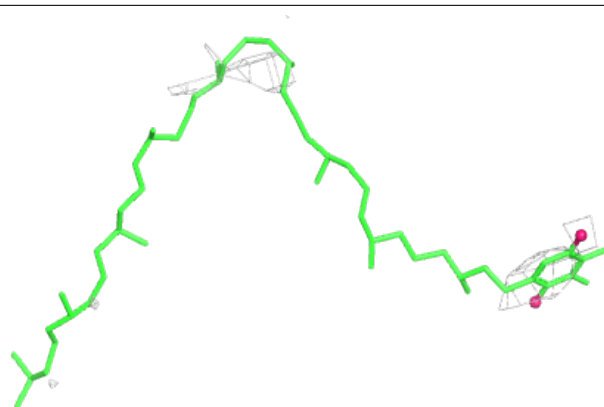
**Electron density around LHG D 408:**

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

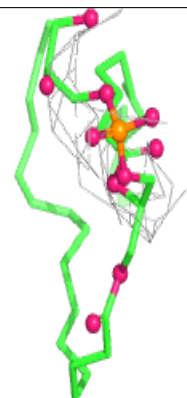


Electron density around PL9 D 405:

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

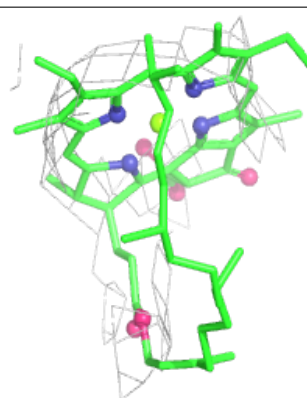
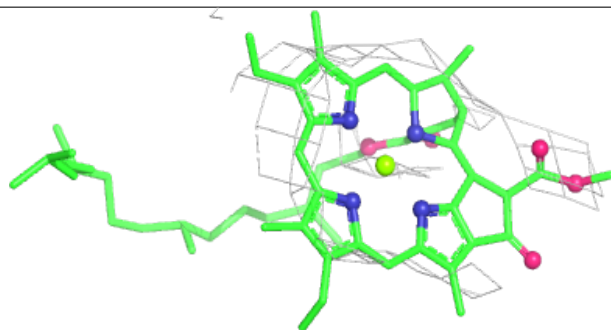
**Electron density around LHG a 614:**

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

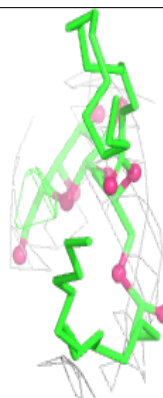
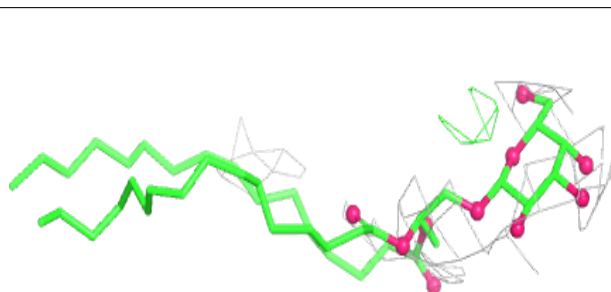
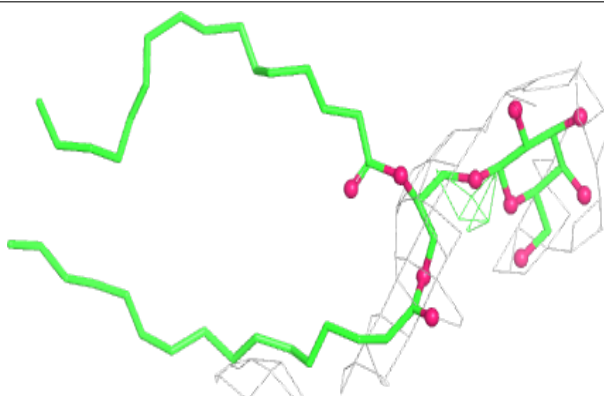


Electron density around CLA c 514:

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

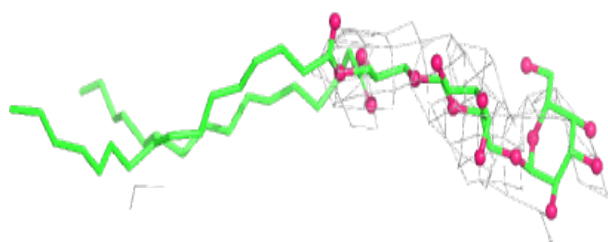
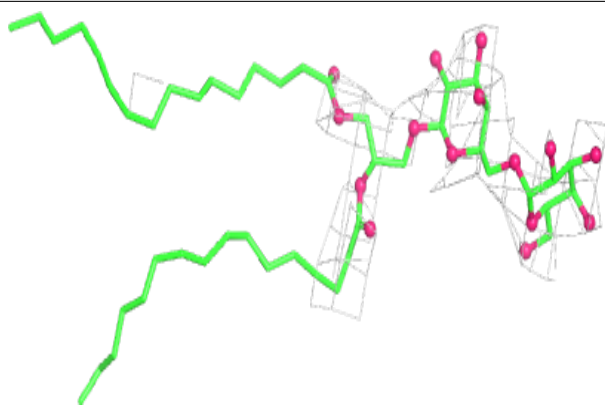
**Electron density around LMG a 611:**

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

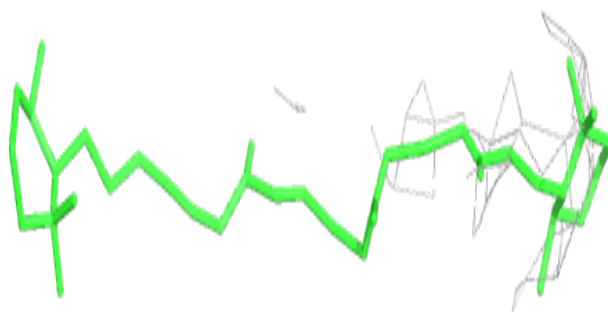
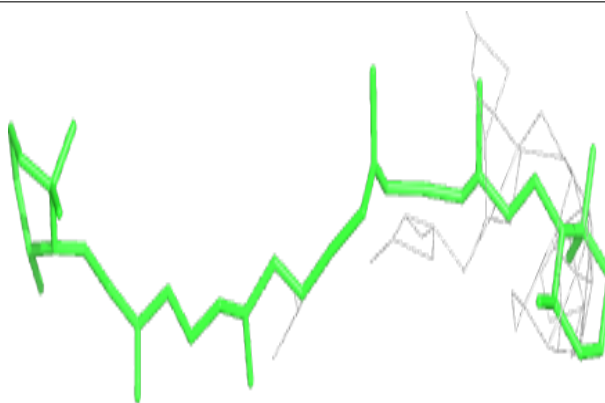


Electron density around DGD C 518:

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

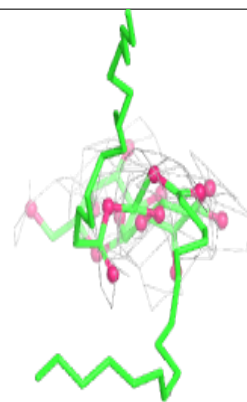
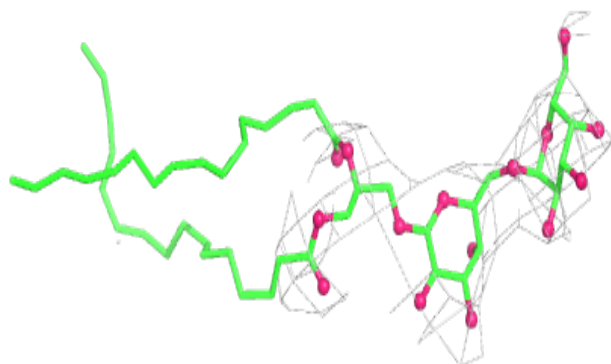
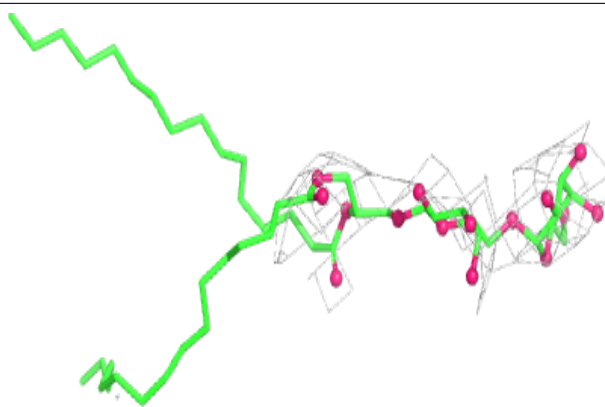
**Electron density around BCR k 101:**

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

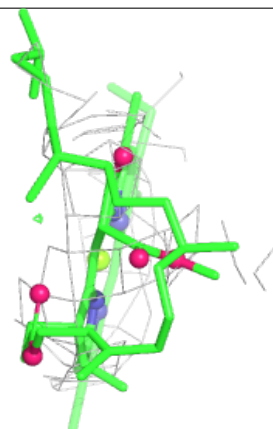
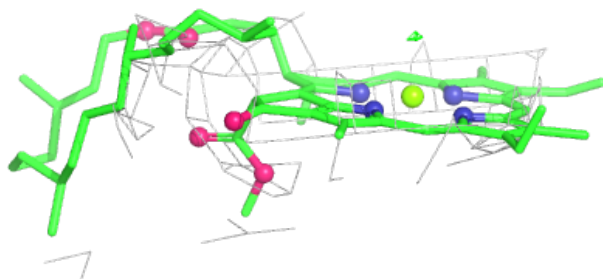
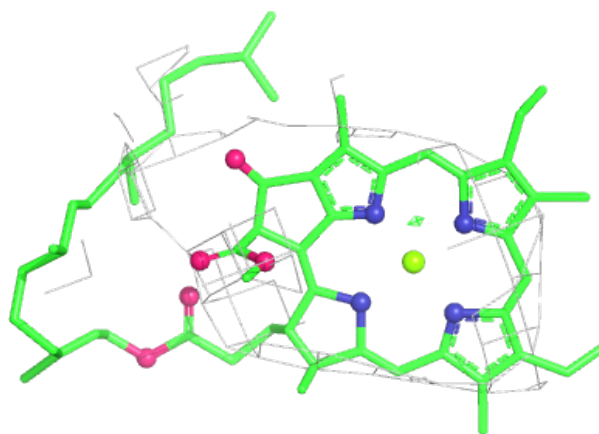


Electron density around DGD c 517:

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

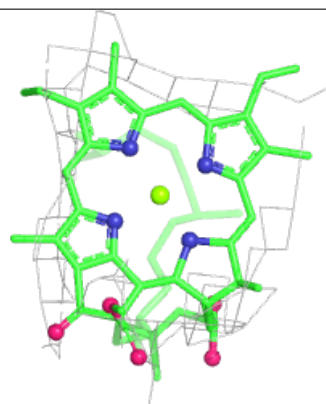
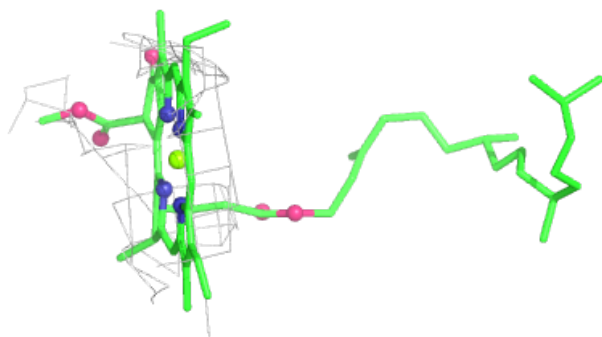
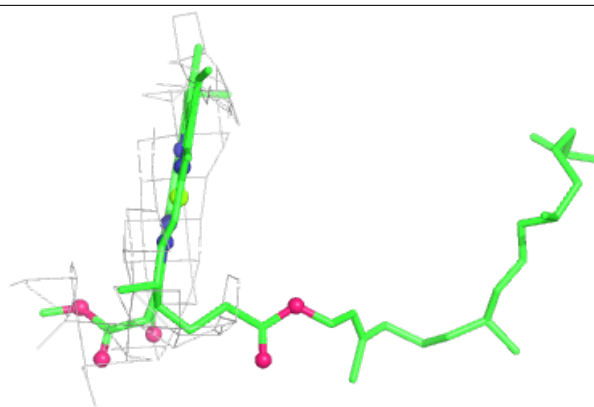
**Electron density around CLA b 613:**

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

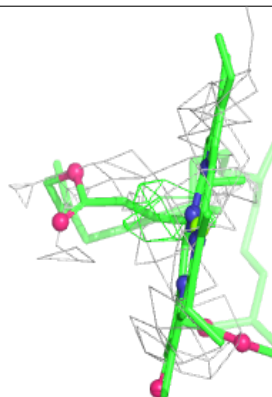
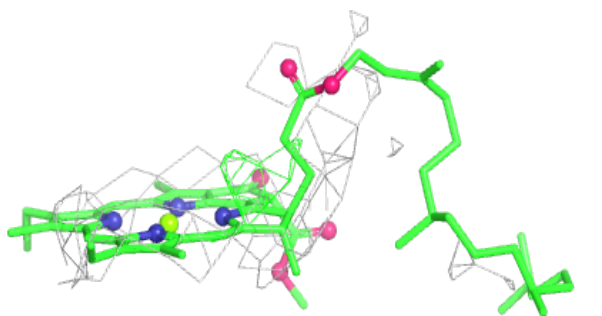
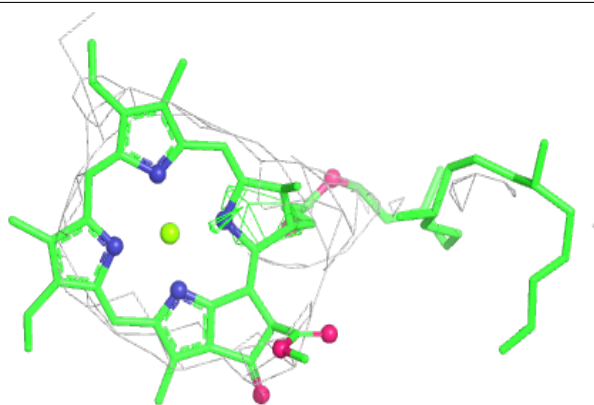


Electron density around CLA c 507:

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

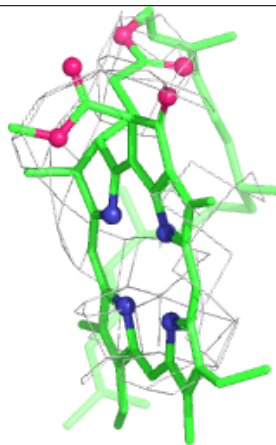
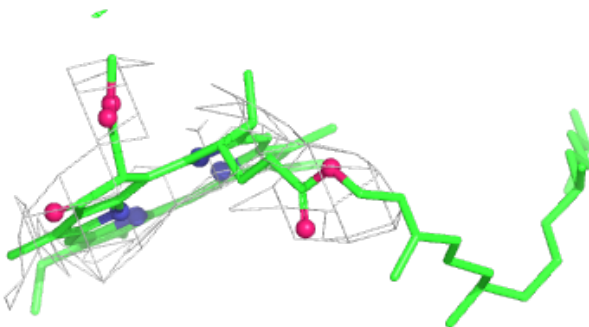
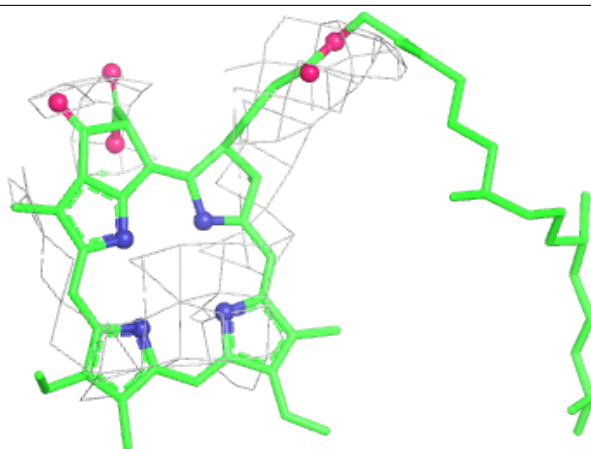
**Electron density around CLA b 615:**

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



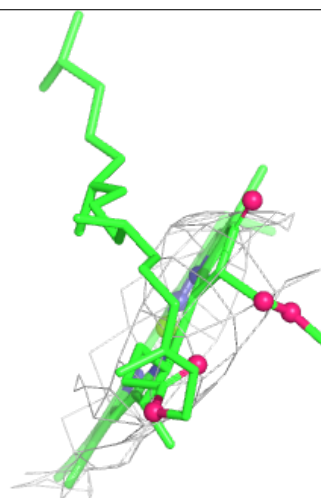
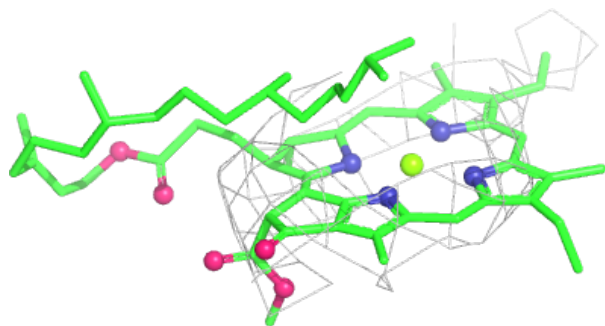
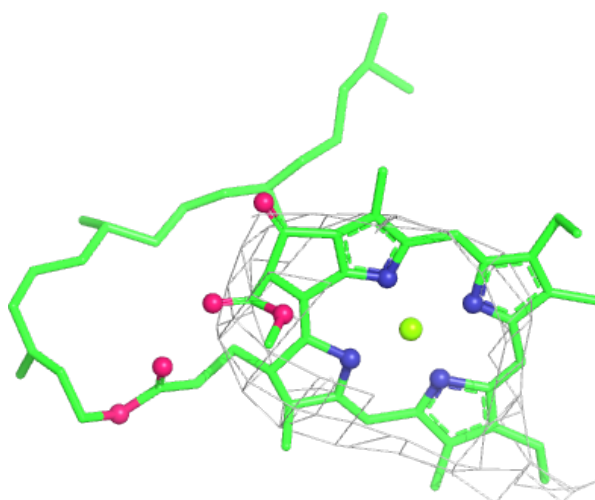
Electron density around PHO d 401:

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



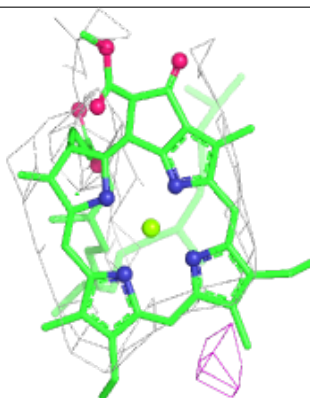
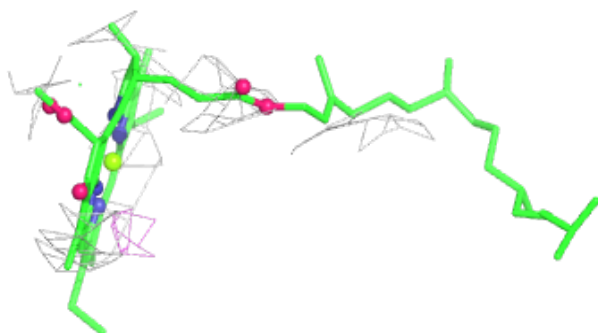
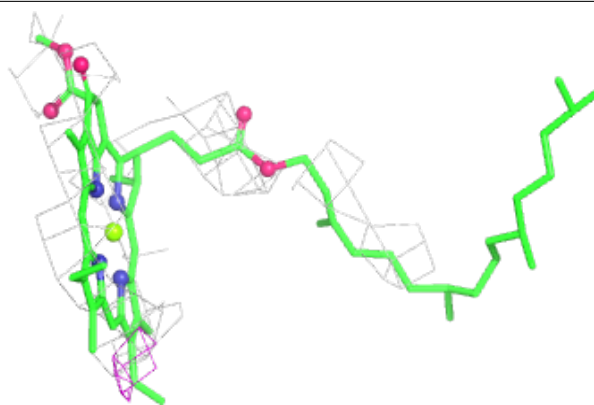
Electron density around CLA c 510:

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

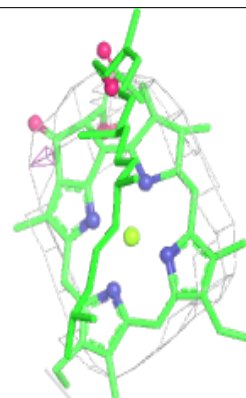
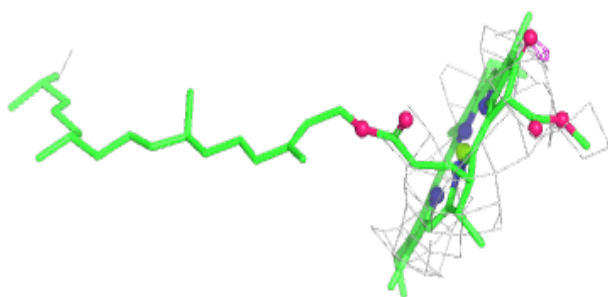
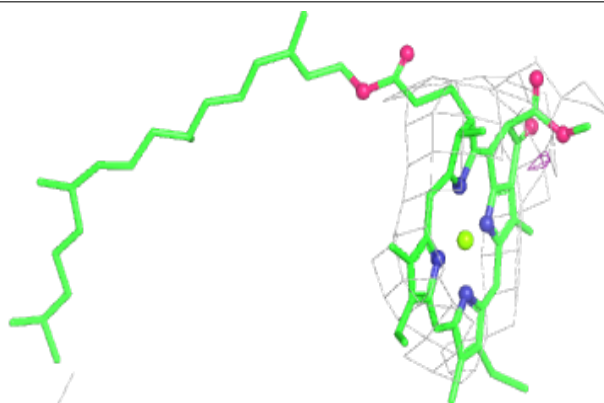


Electron density around CLA D 404:

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

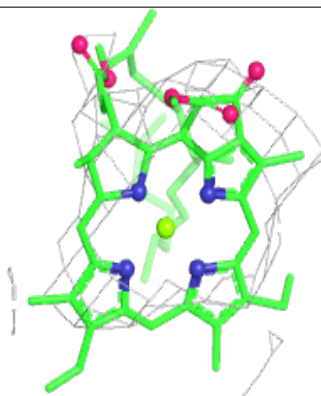
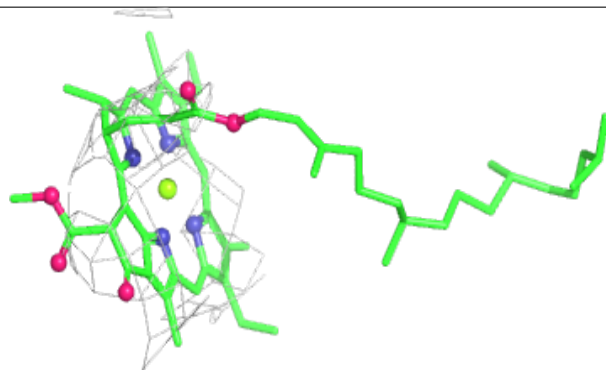
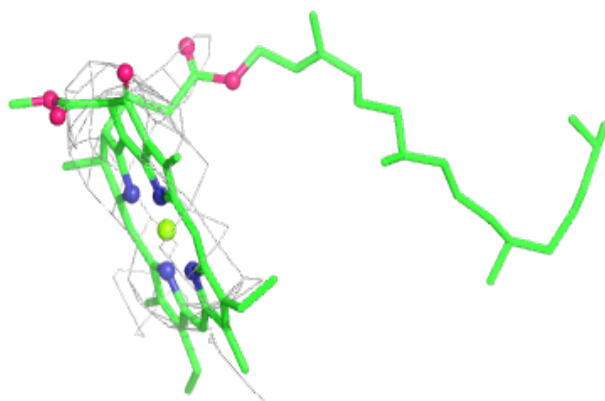
**Electron density around CLA b 612:**

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

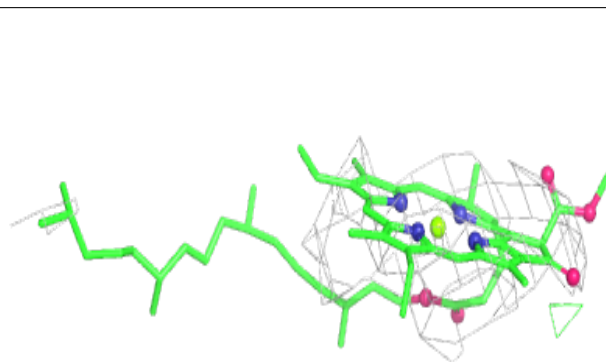
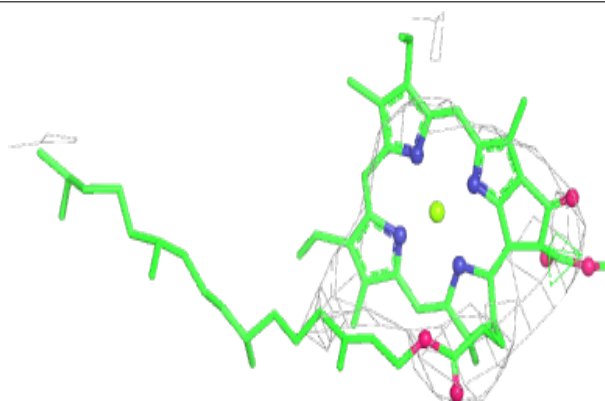


Electron density around CLA C 508:

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

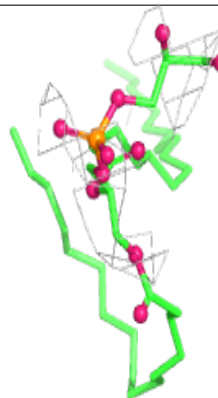
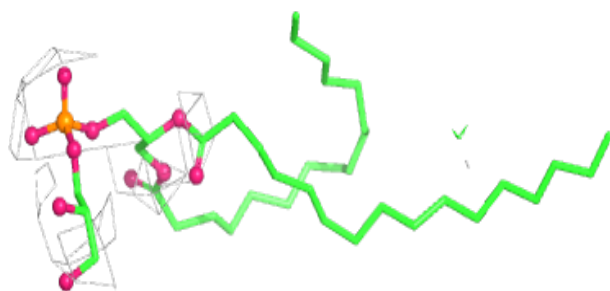
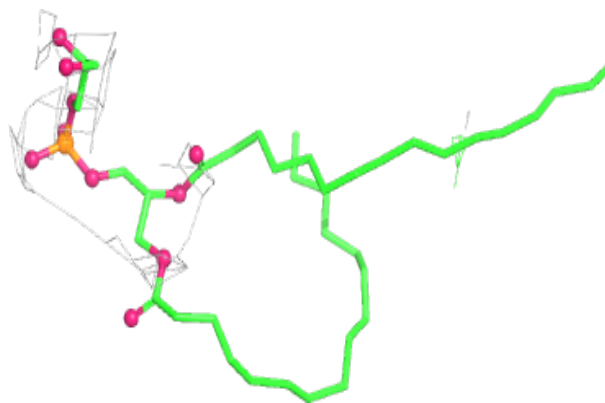
**Electron density around CLA C 501:**

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

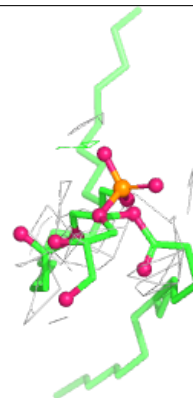
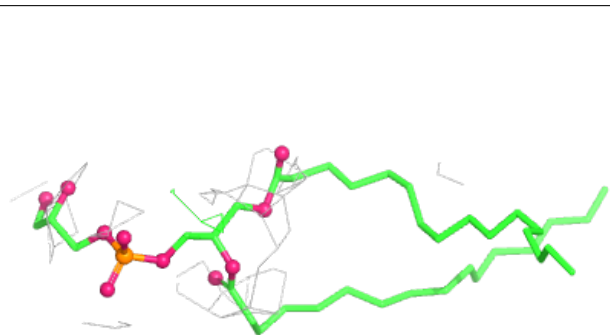
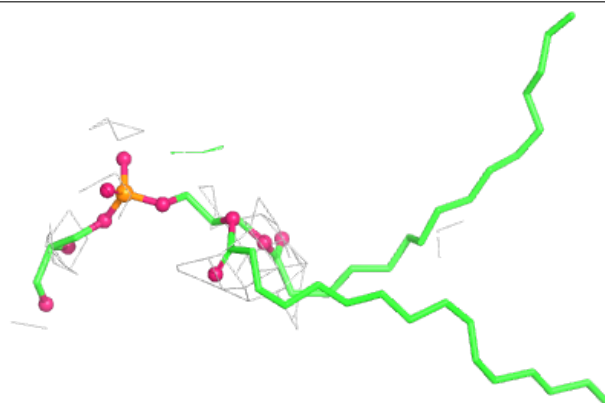


Electron density around LHG b 624:

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

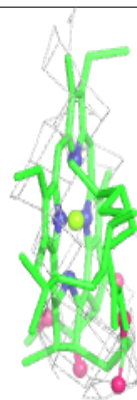
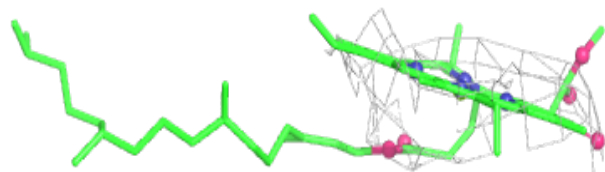
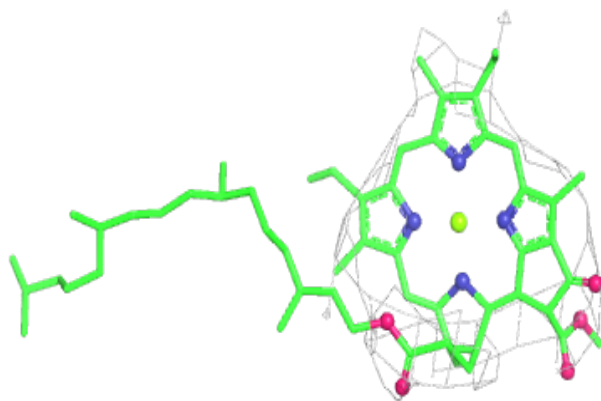
**Electron density around LHG d 406:**

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

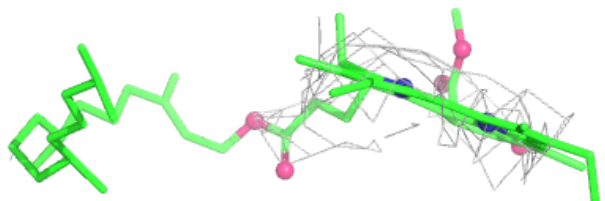
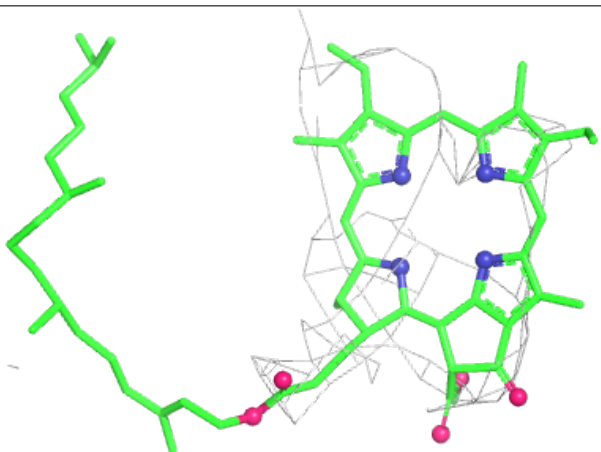


Electron density around CLA b 606:

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

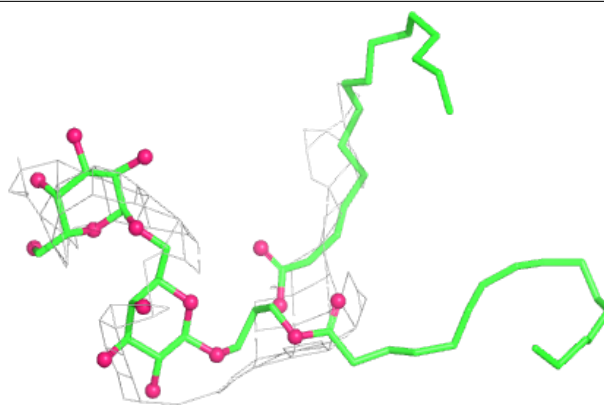
**Electron density around PHO a 606:**

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



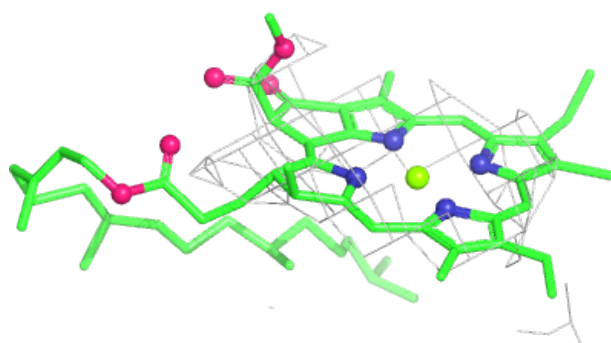
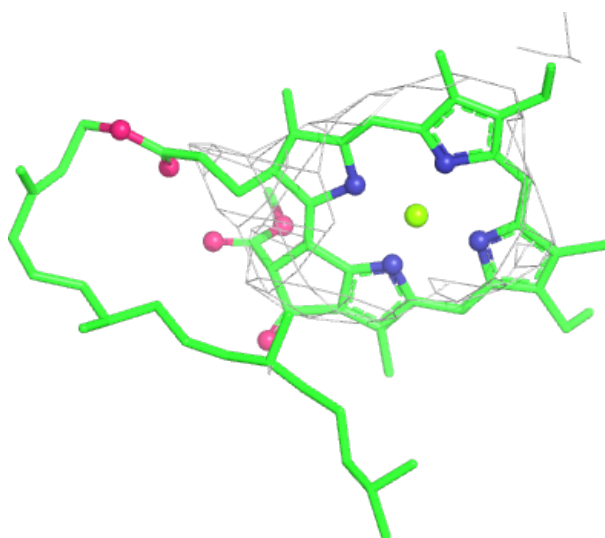
Electron density around DGD C 517:

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



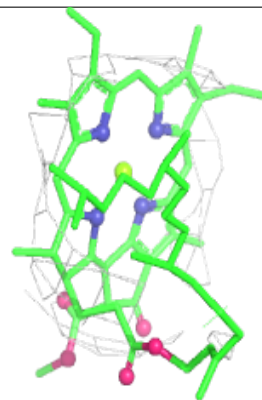
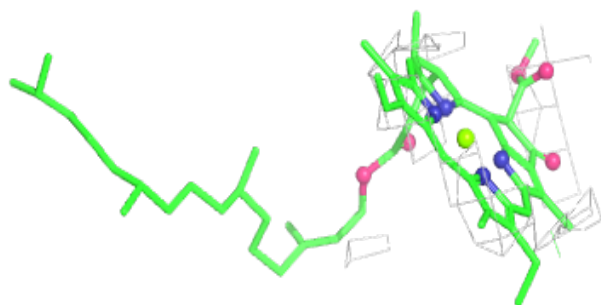
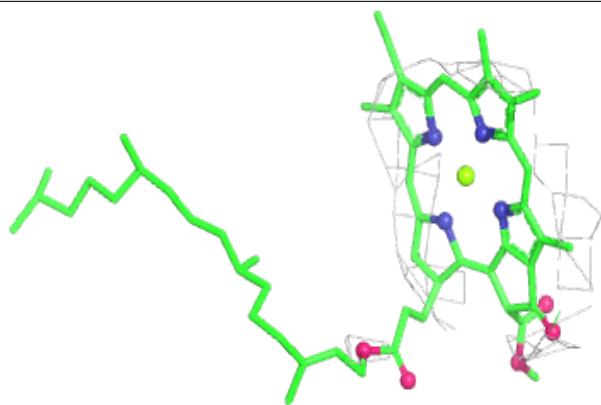
Electron density around CLA C 509:

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



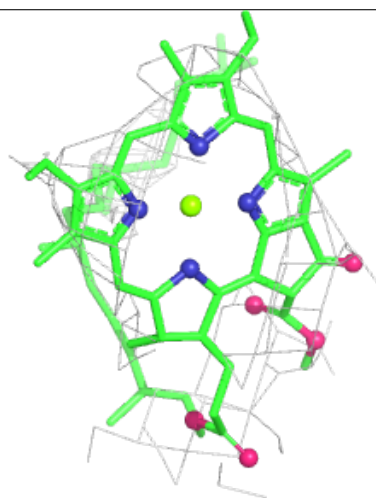
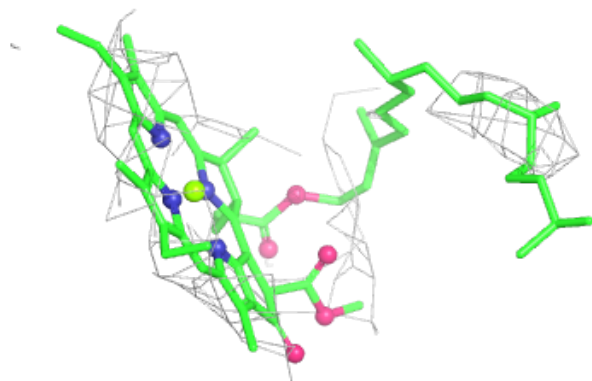
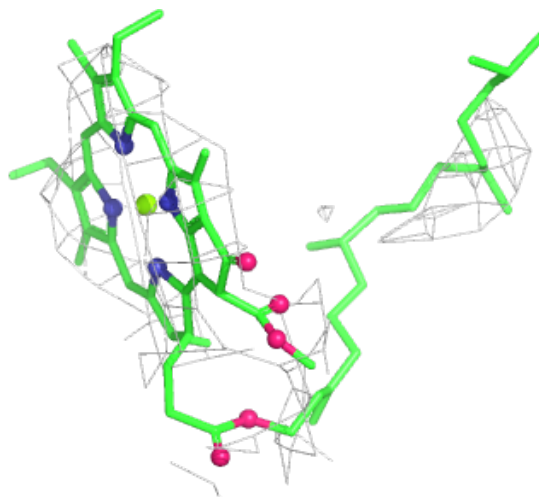
Electron density around CLA c 512:

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



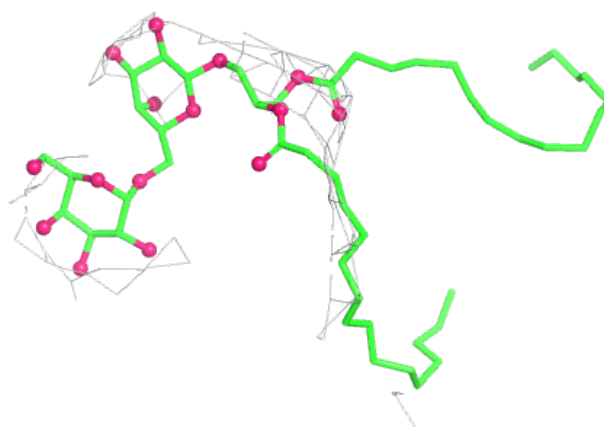
Electron density around CLA b 616:

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

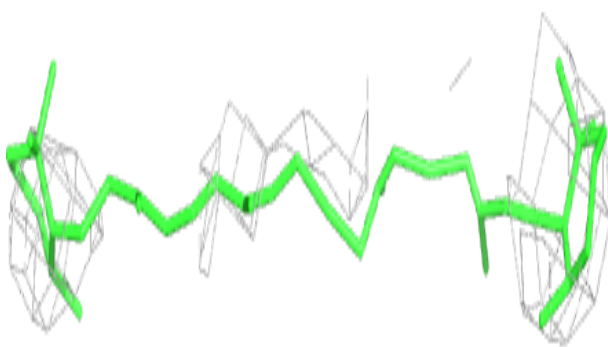
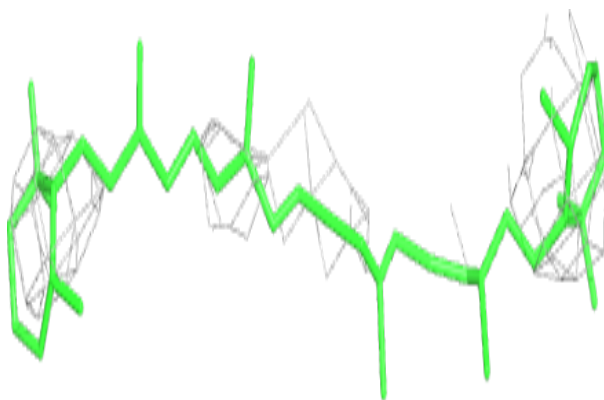


Electron density around DGD c 518:

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

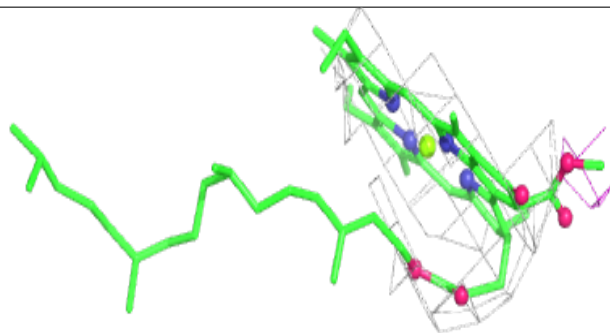
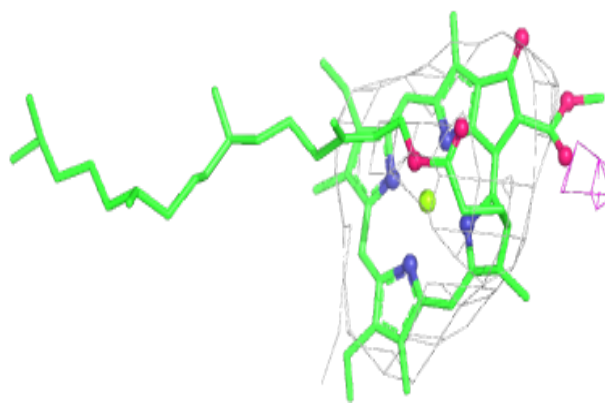
**Electron density around BCR B 619:**

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

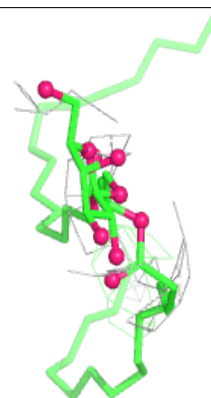
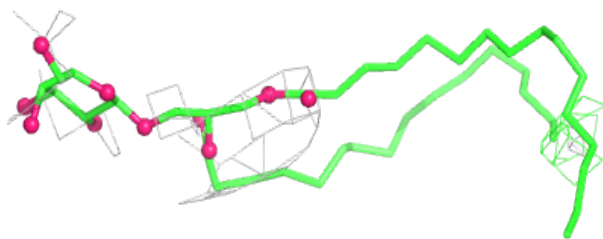
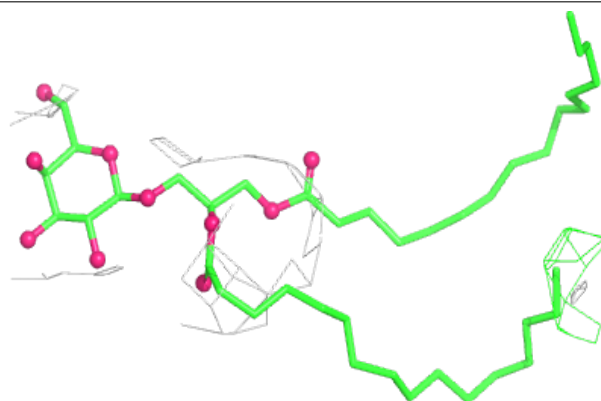


Electron density around CLA B 615:

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

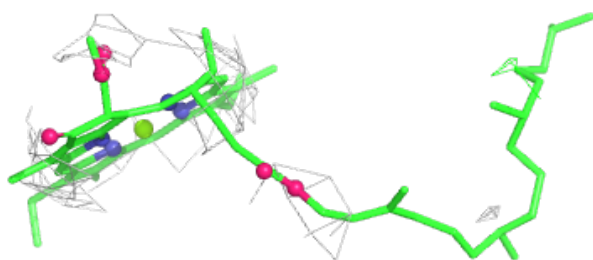
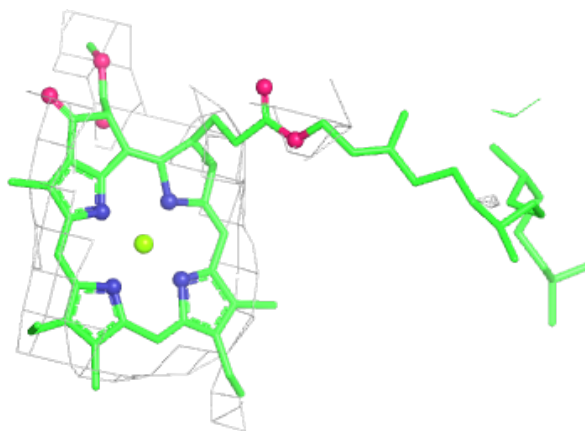
**Electron density around LMG j 101:**

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

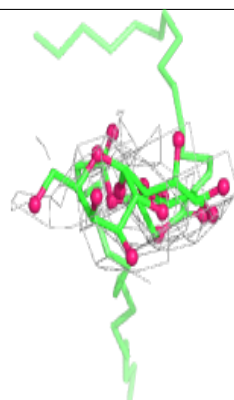
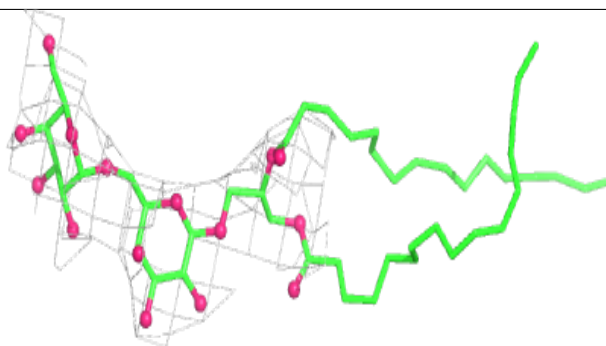
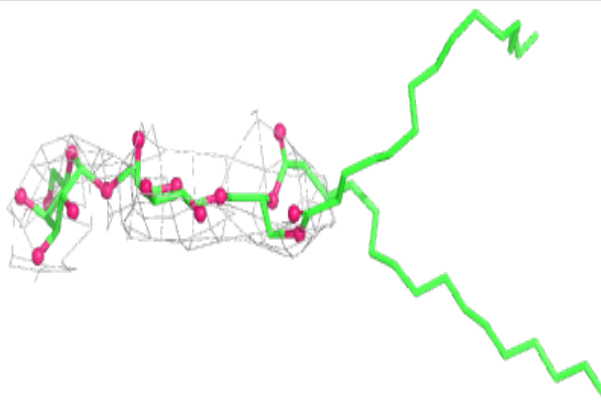


Electron density around CLA A 608:

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

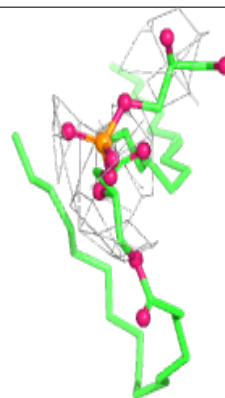
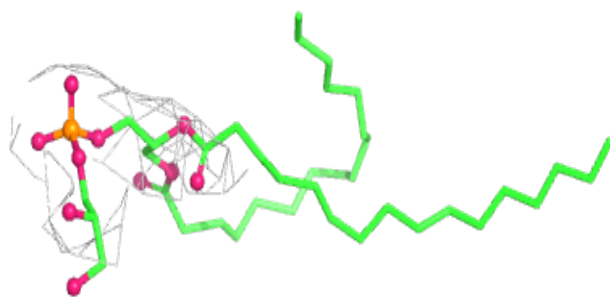
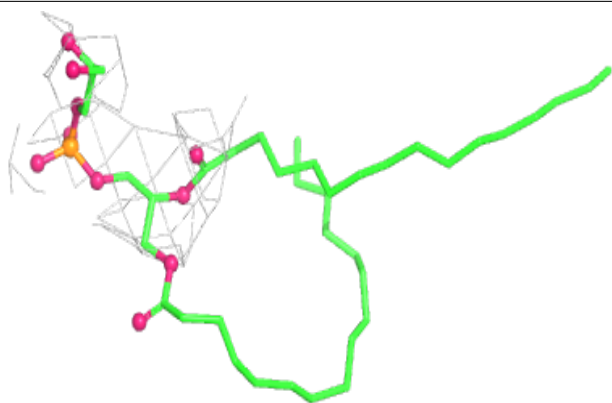
**Electron density around DGD C 516:**

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

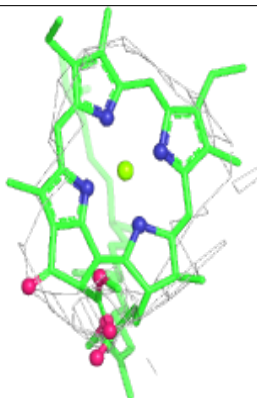
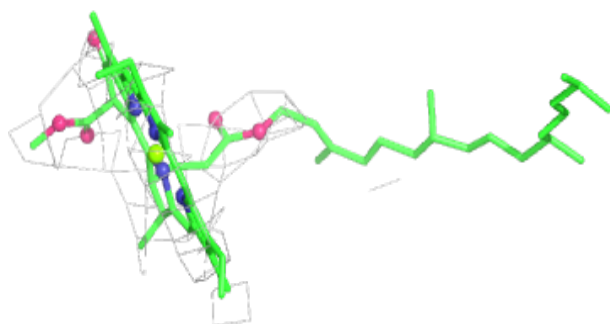
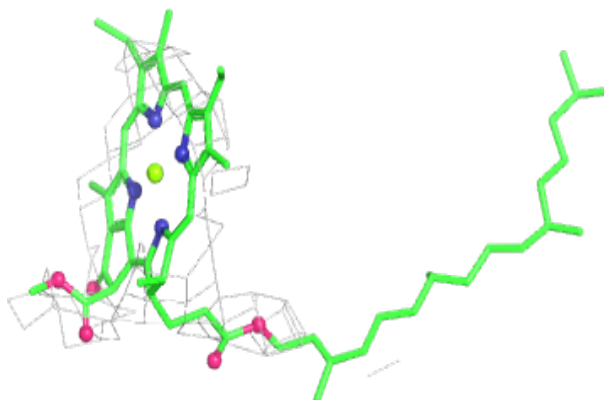


Electron density around LHG B 622:

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

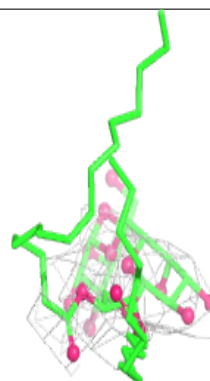
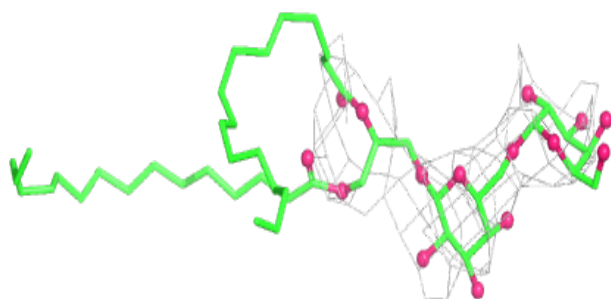
**Electron density around CLA B 610:**

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

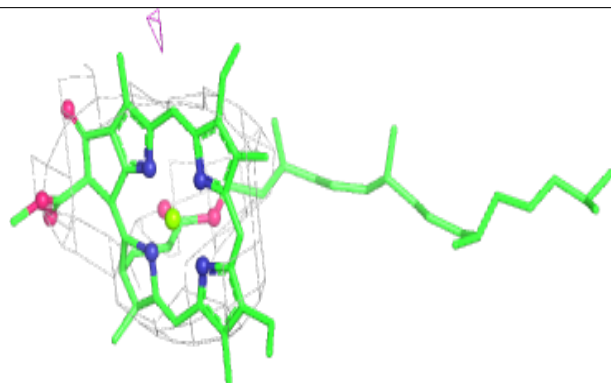
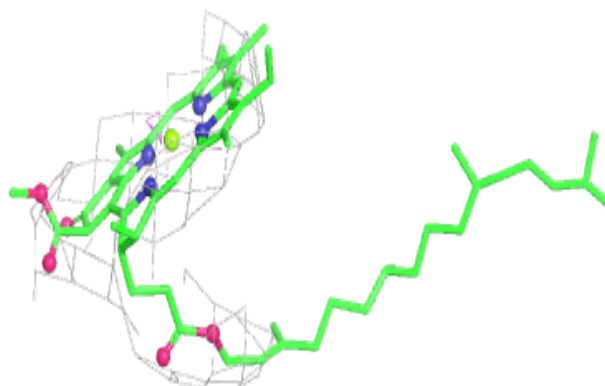


Electron density around DGD H 102:

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

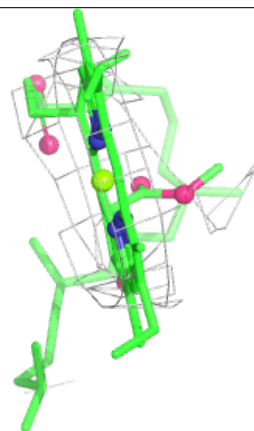
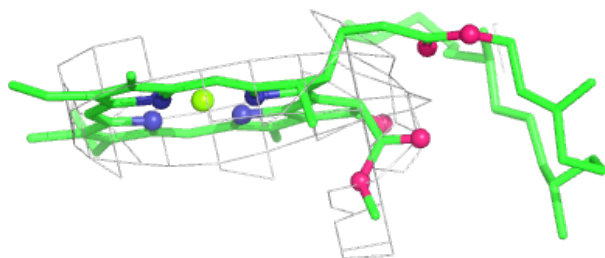
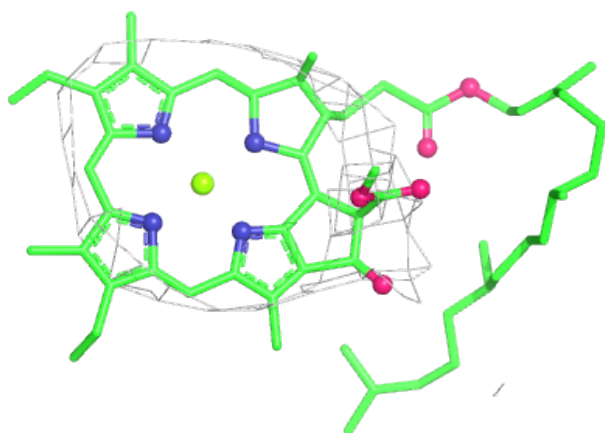
**Electron density around CLA C 504:**

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

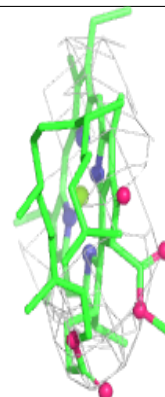
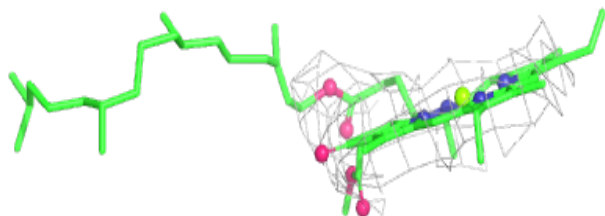
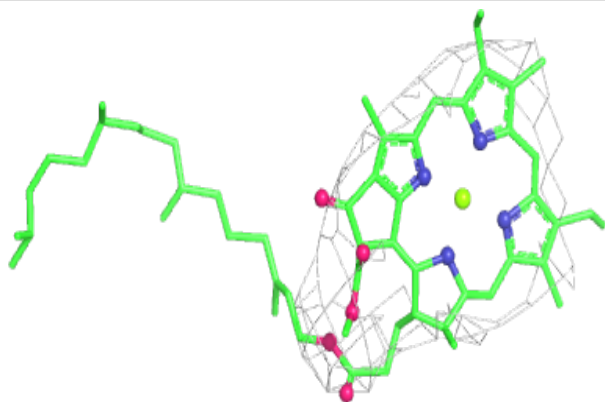


Electron density around CLA B 611:

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

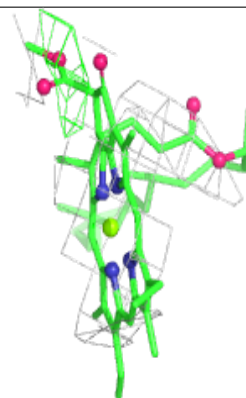
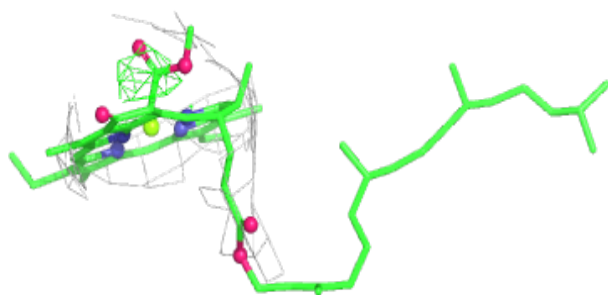
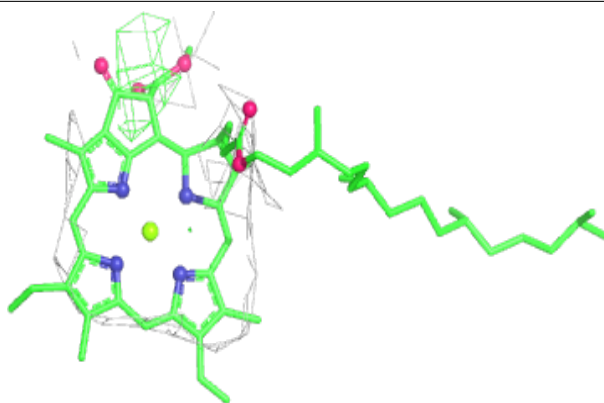
**Electron density around CLA b 605:**

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

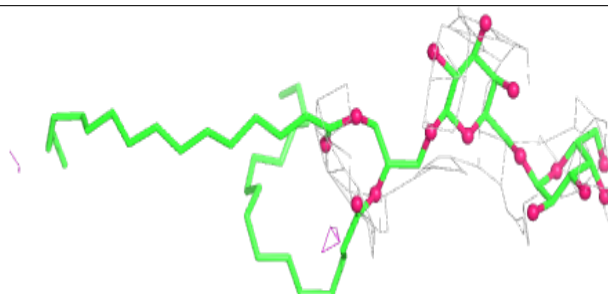


Electron density around CLA A 606:

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

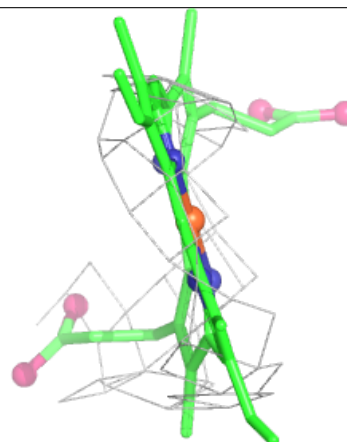
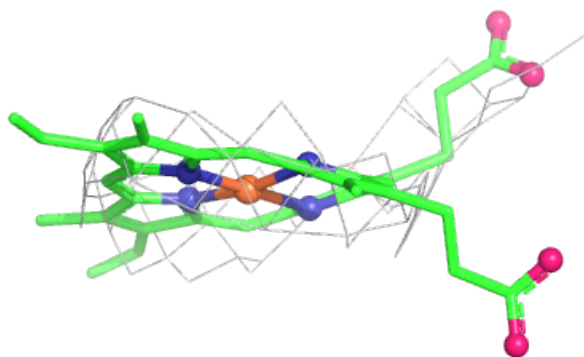
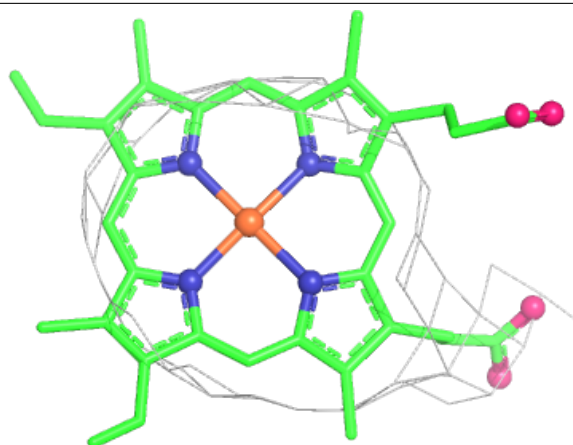
**Electron density around DGD h 102:**

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

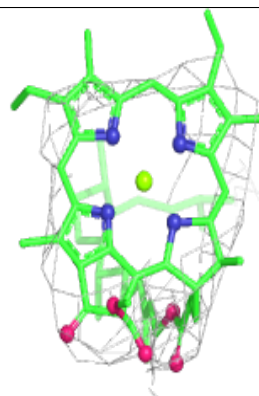
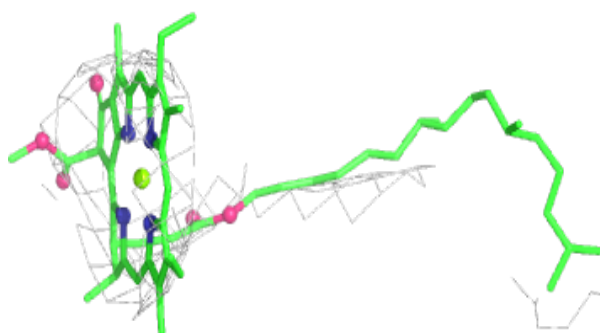
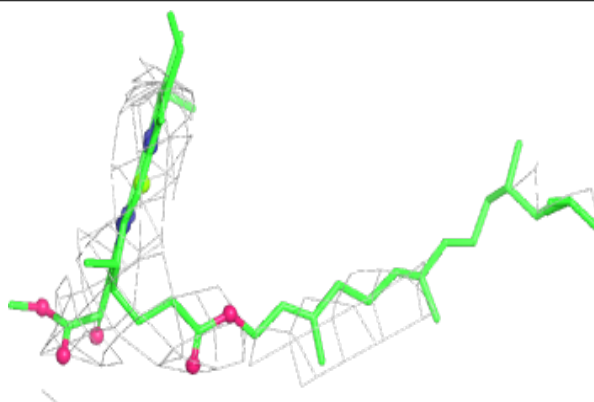


Electron density around HEM e 102:

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

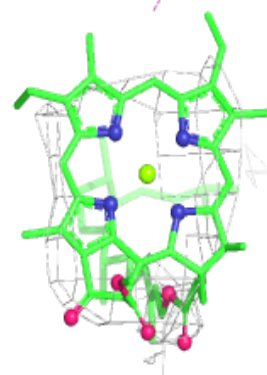
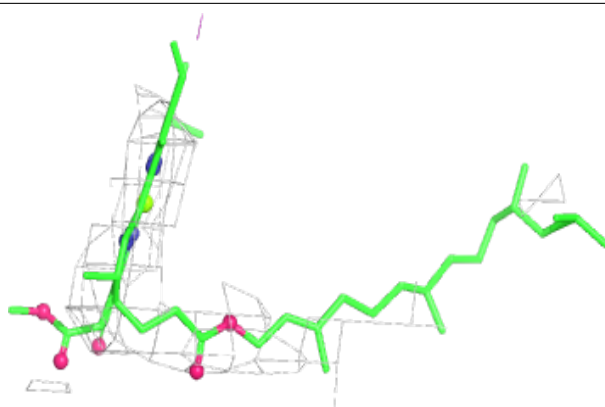
**Electron density around CLA b 608:**

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

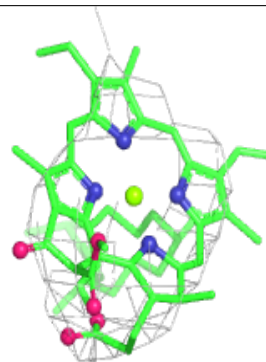
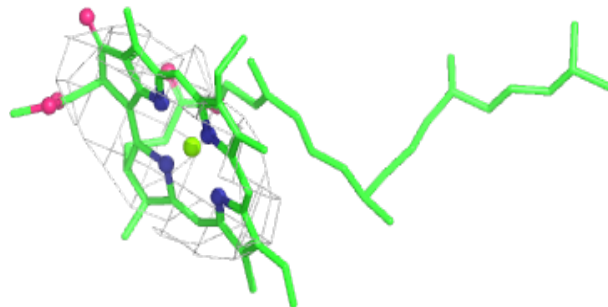
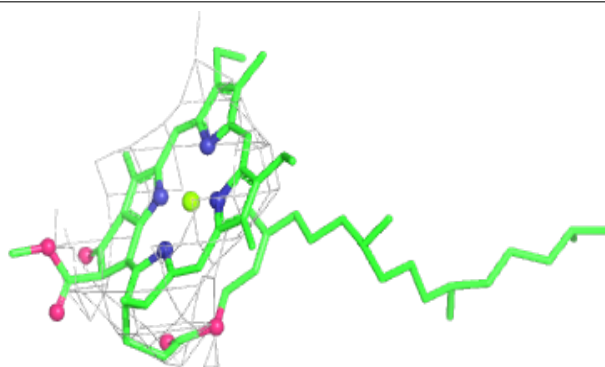


Electron density around CLA B 606:

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

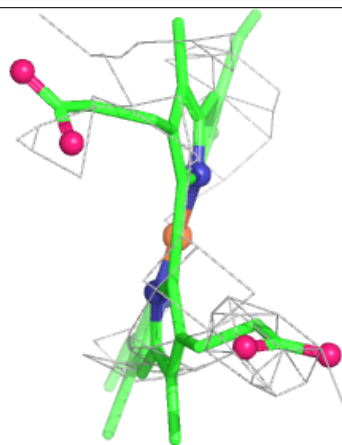
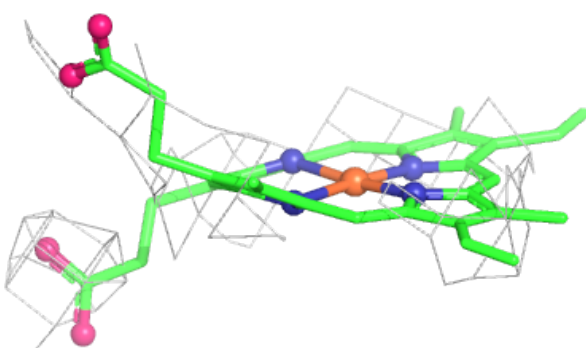
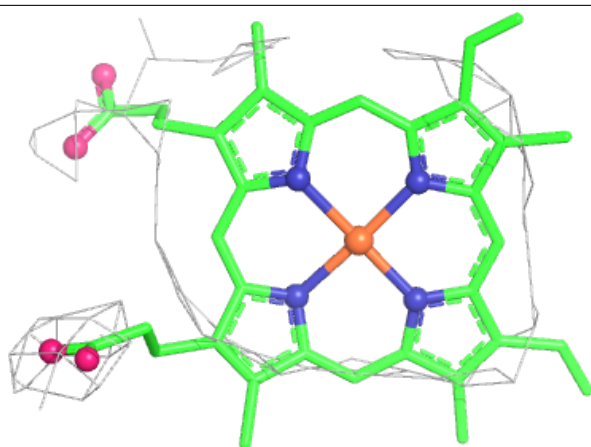
**Electron density around CLA c 506:**

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

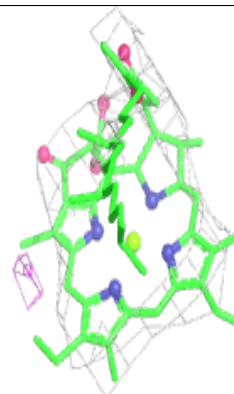
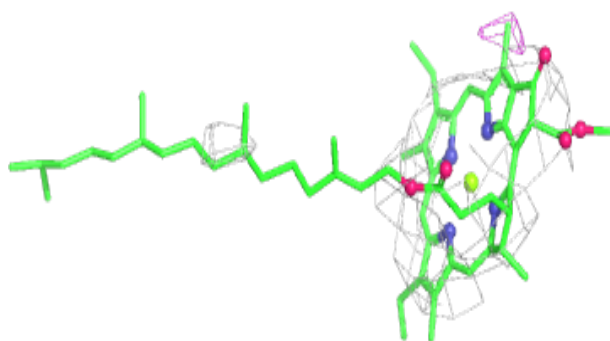
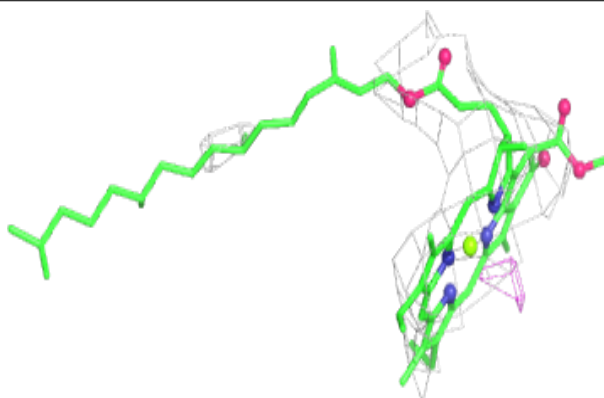


Electron density around HEM E 102:

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

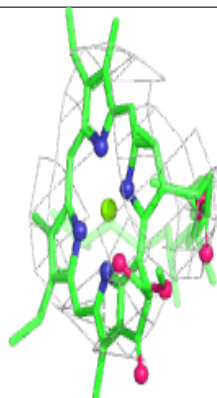
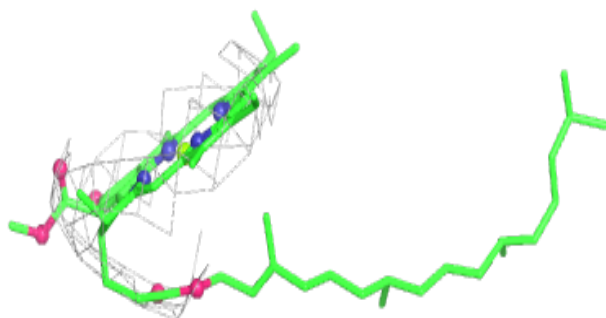
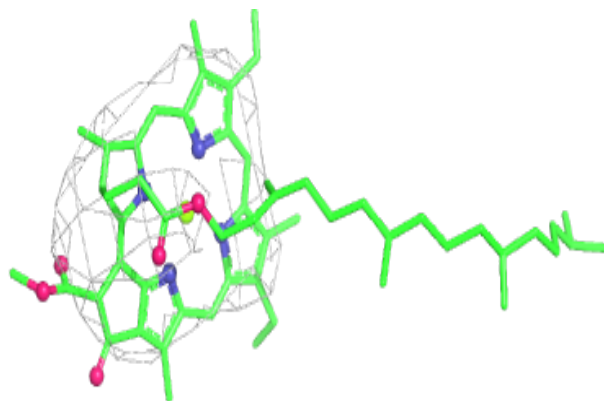
**Electron density around CLA b 610:**

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

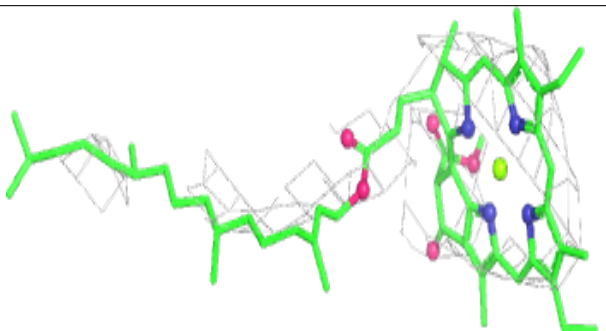
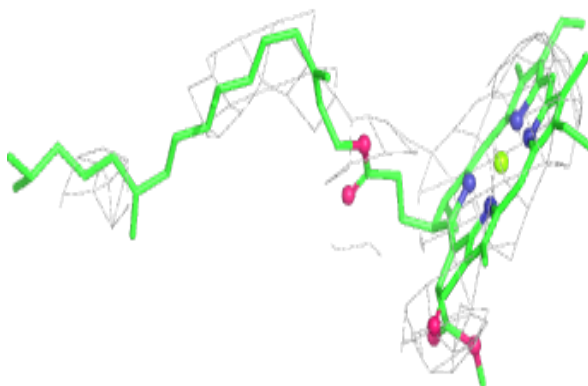


Electron density around CLA b 611:

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

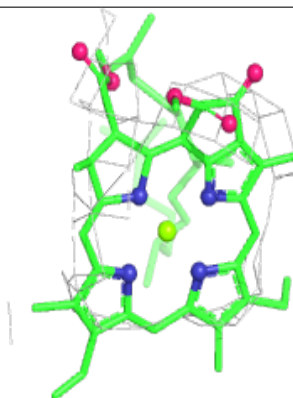
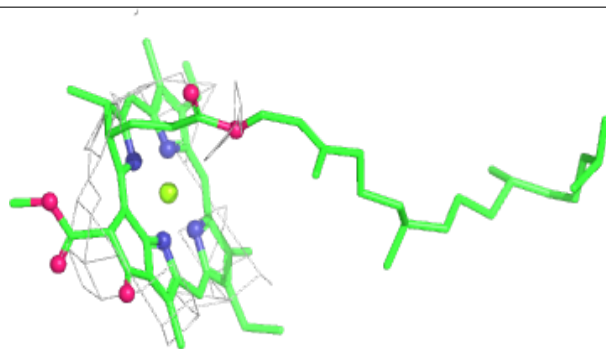
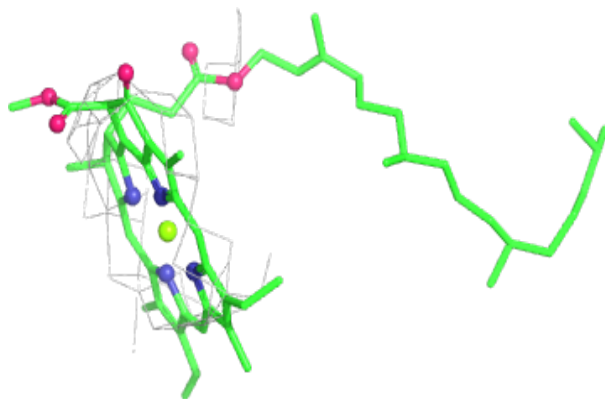
**Electron density around CLA C 502:**

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



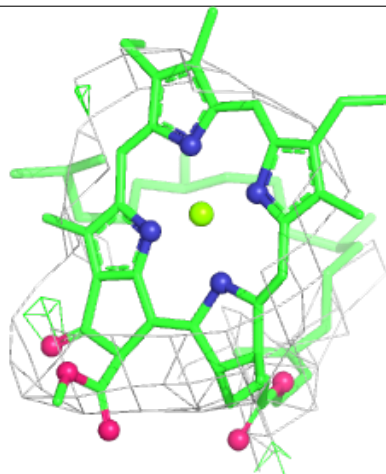
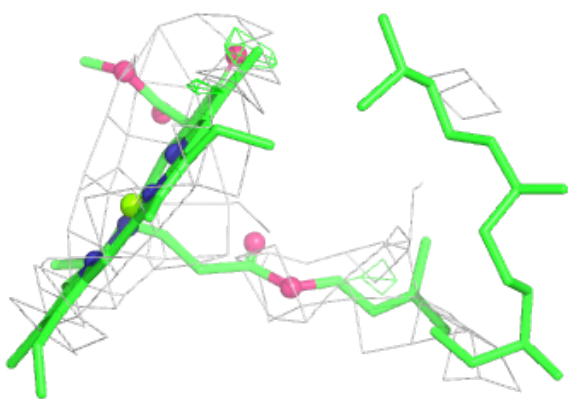
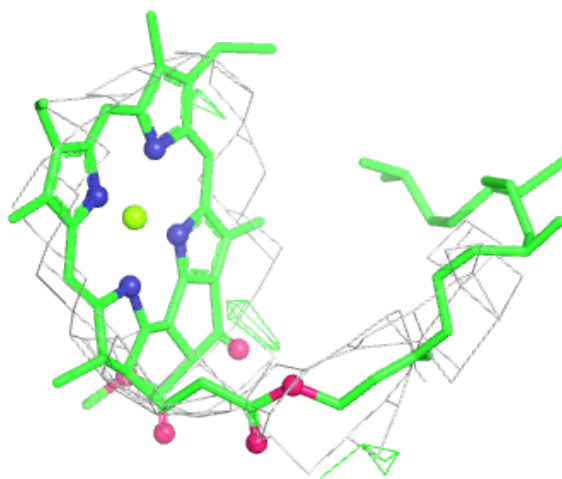
Electron density around CLA c 509:

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



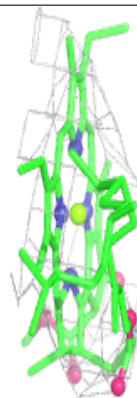
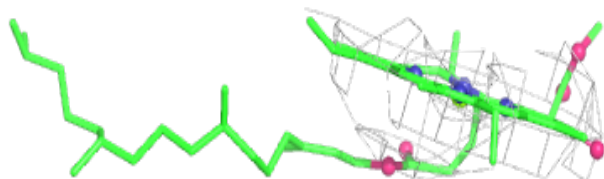
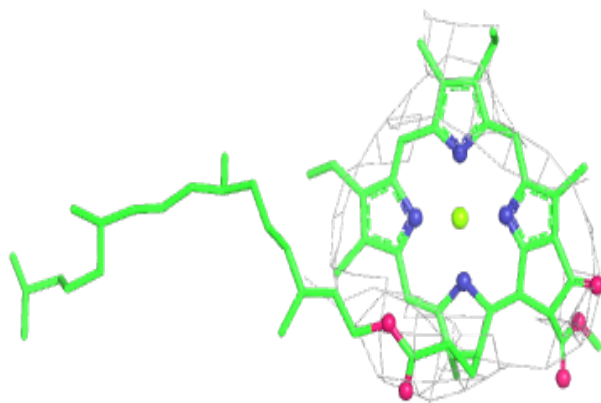
Electron density around CLA C 503:

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

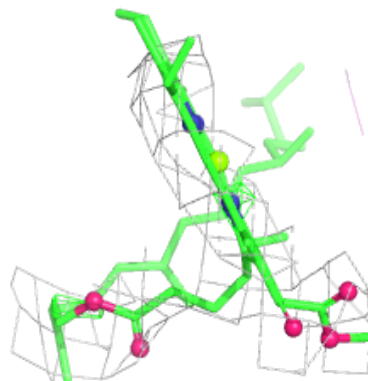
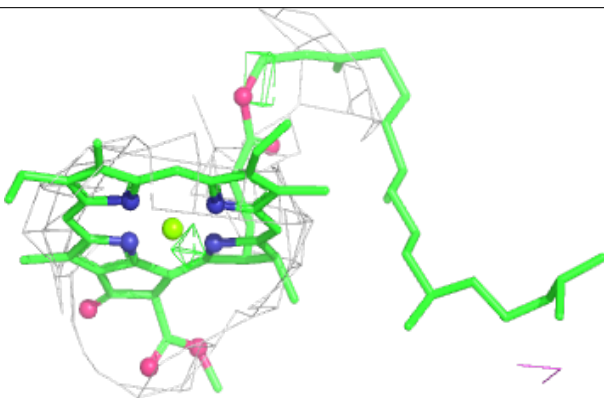
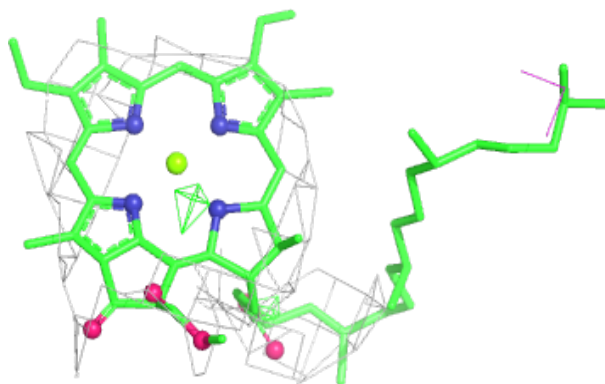


Electron density around CLA B 604:

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

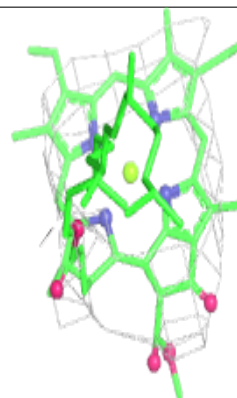
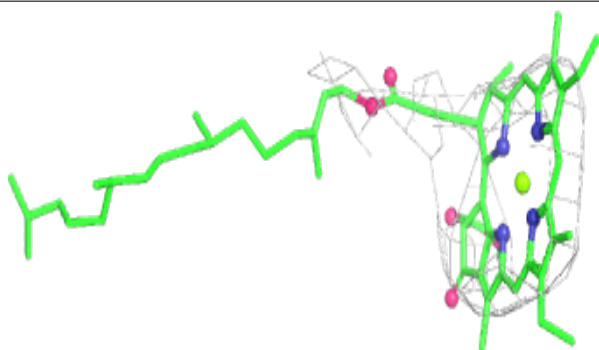
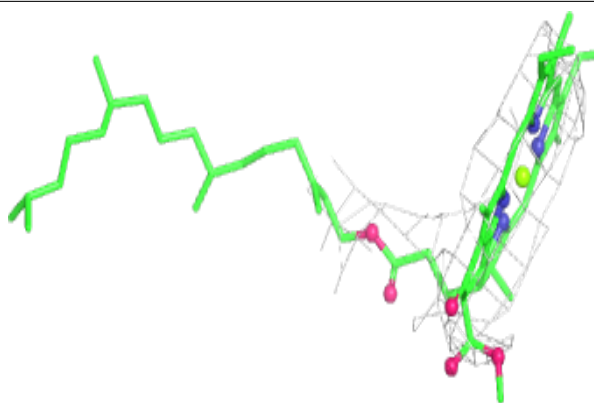
**Electron density around CLA a 613:**

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

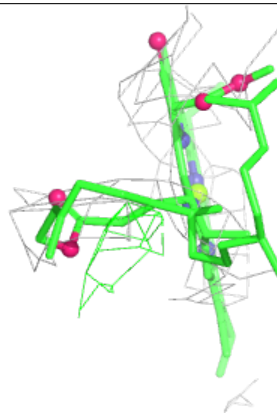
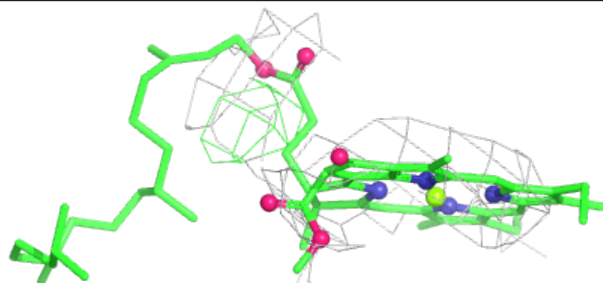
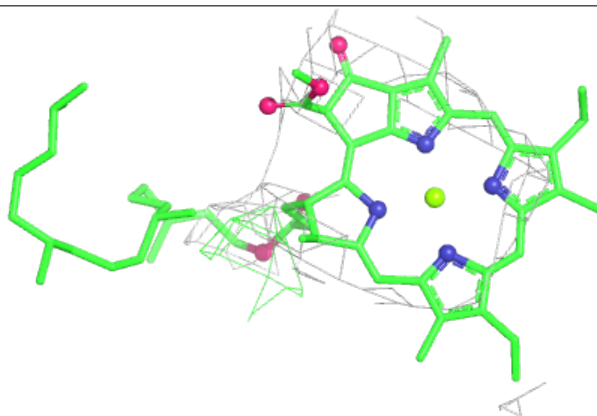


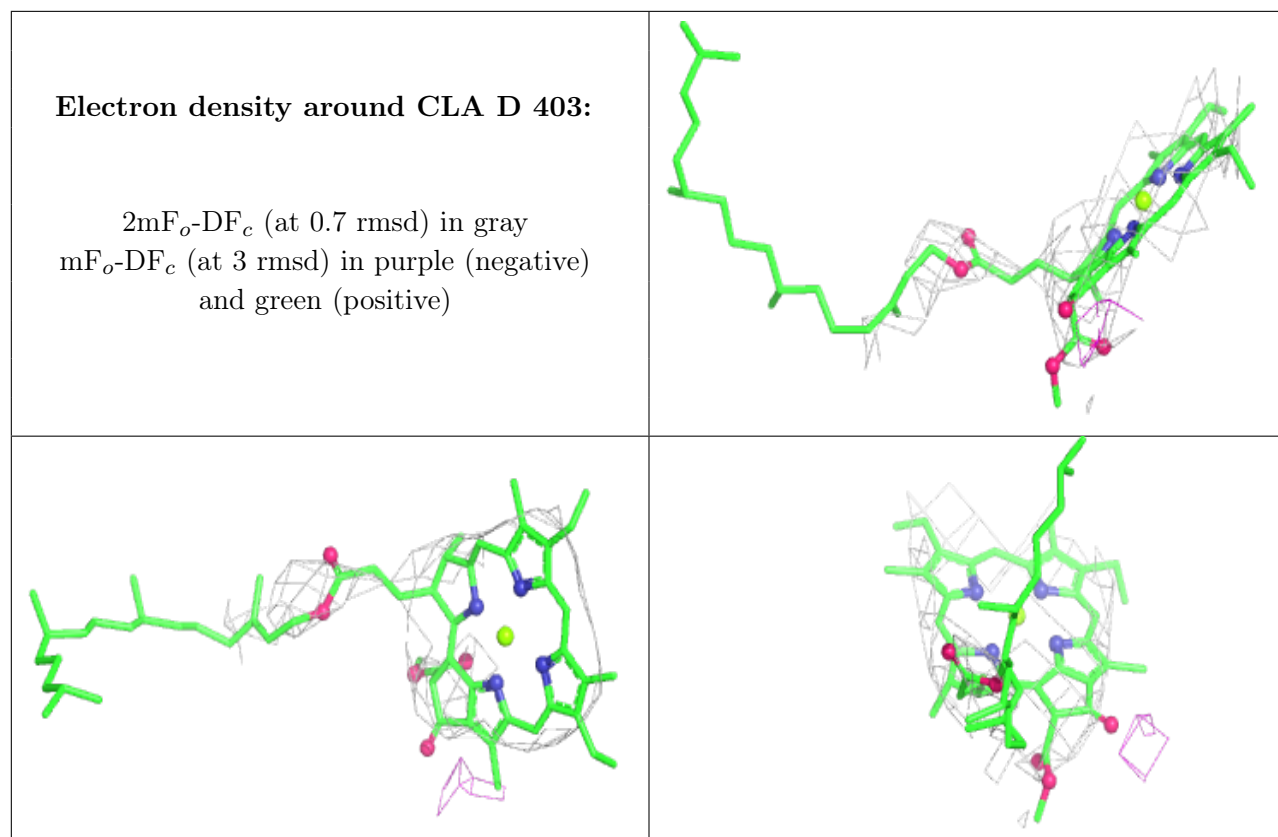
Electron density around CLA B 605:

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

**Electron density around CLA B 613:**

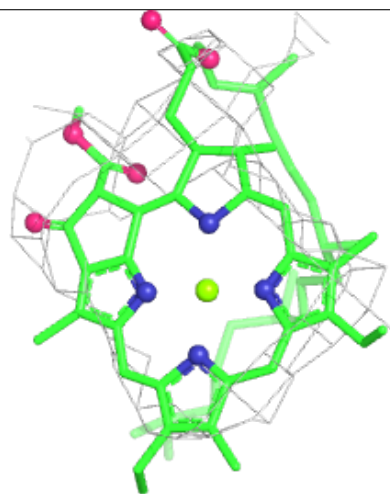
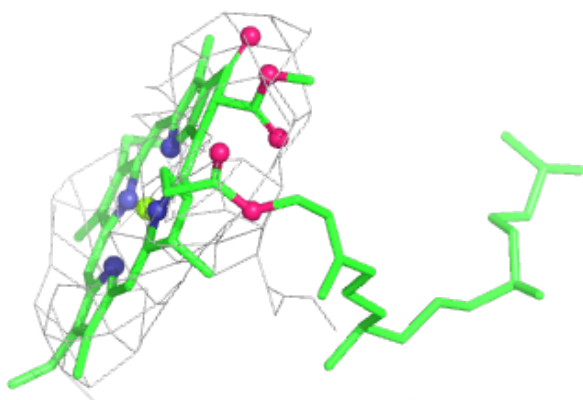
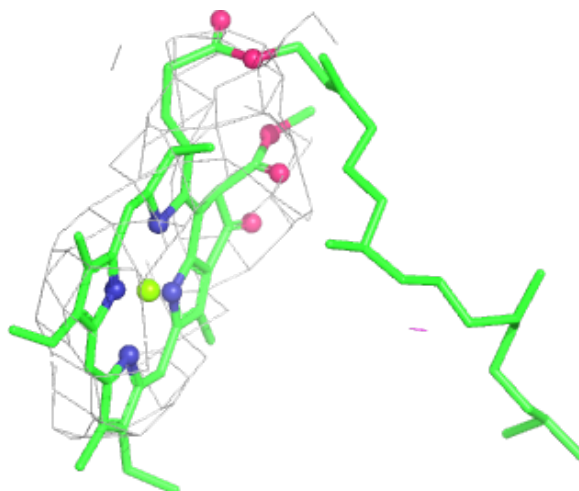
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





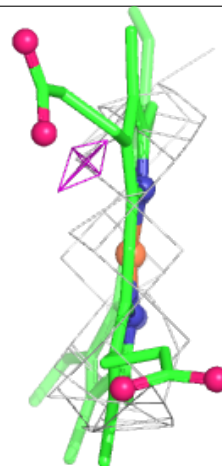
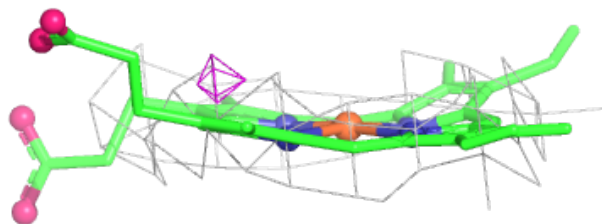
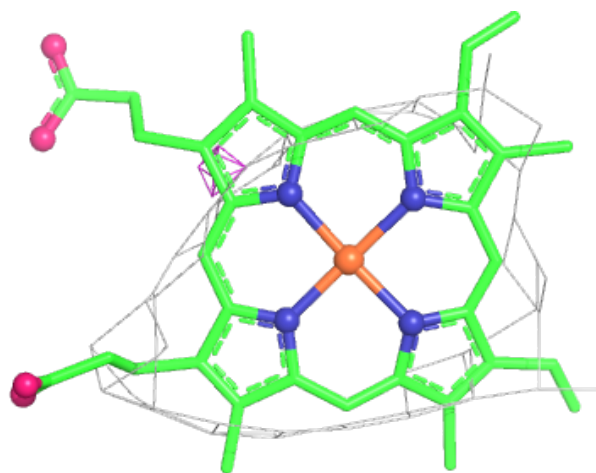
Electron density around CLA B 614:

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



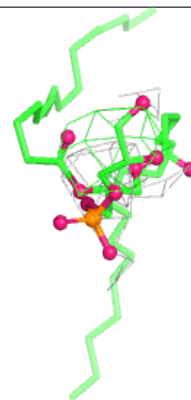
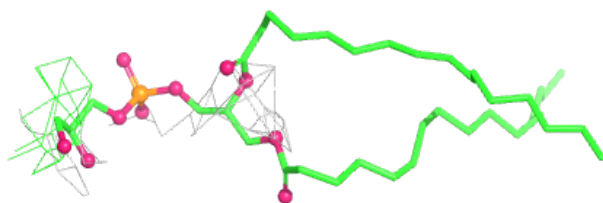
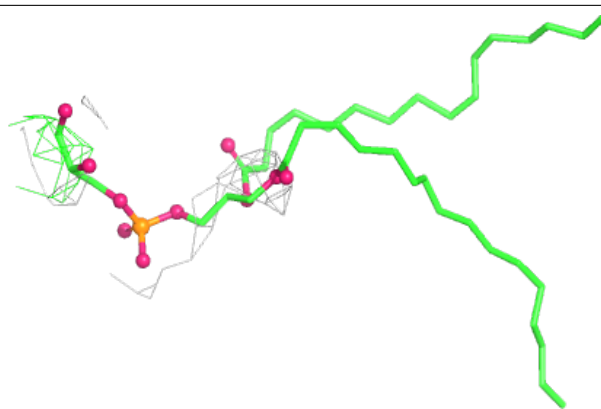
Electron density around HEM v 201:

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

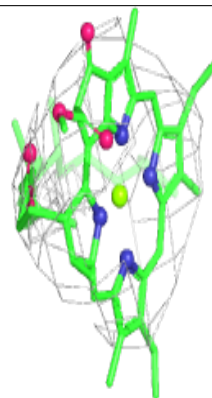
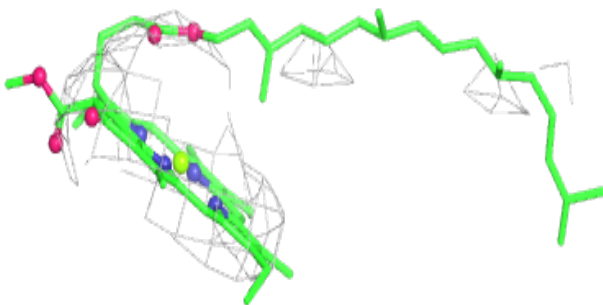
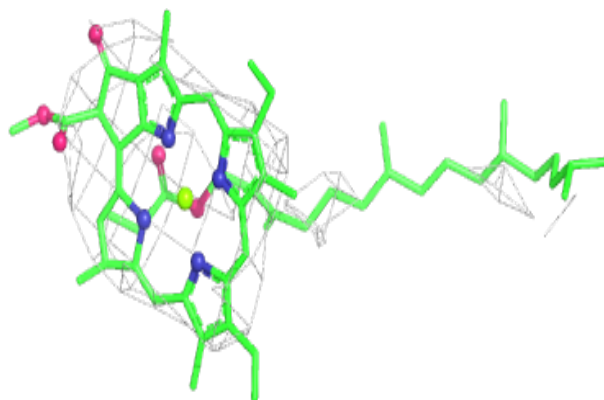


Electron density around LHG D 407:

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

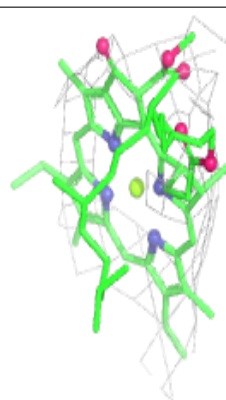
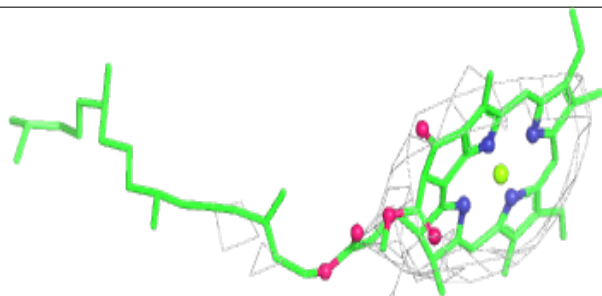
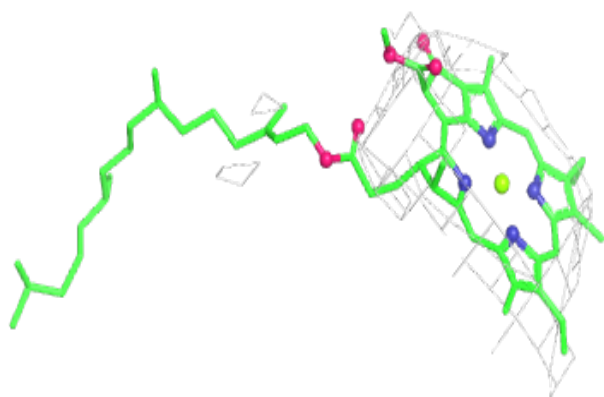
**Electron density around CLA B 609:**

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

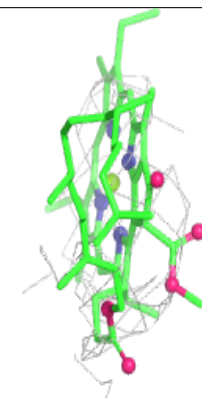
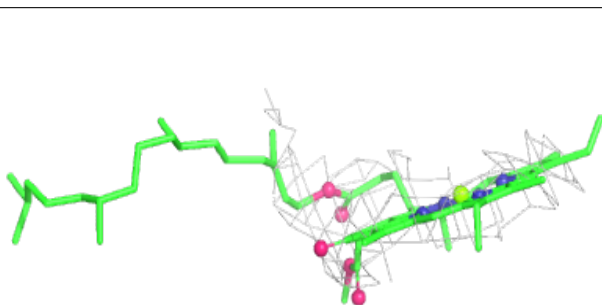
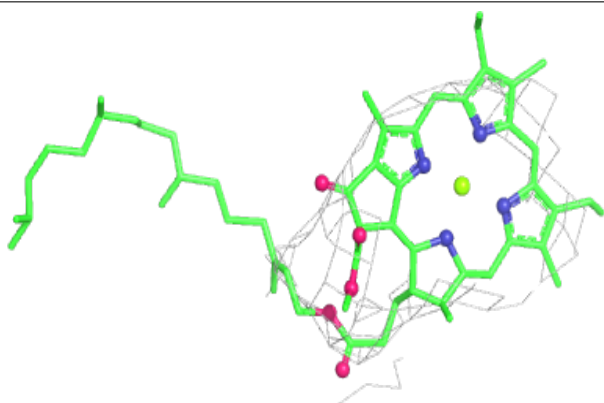


Electron density around CLA A 605:

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

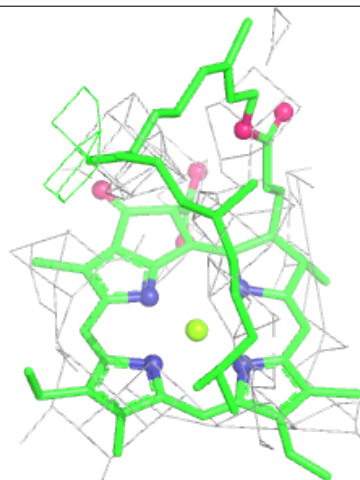
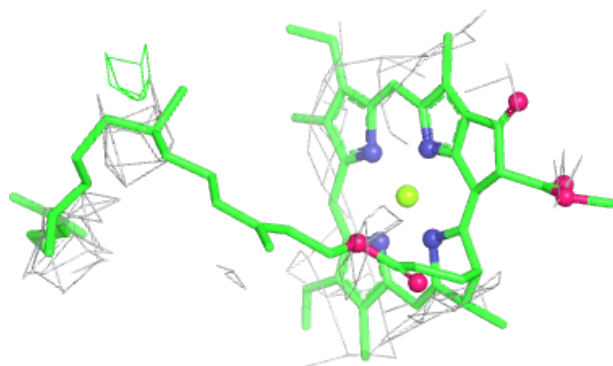
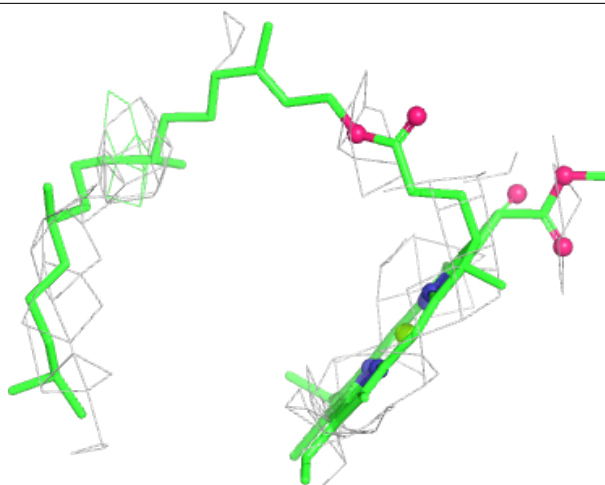
**Electron density around CLA B 603:**

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



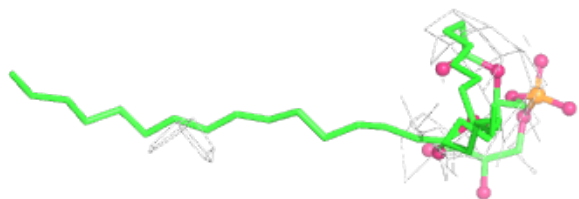
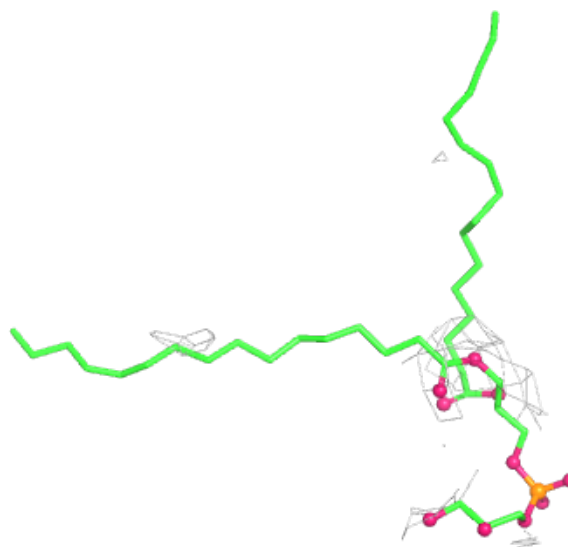
Electron density around CLA b 614:

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



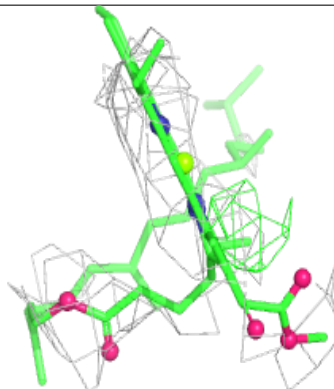
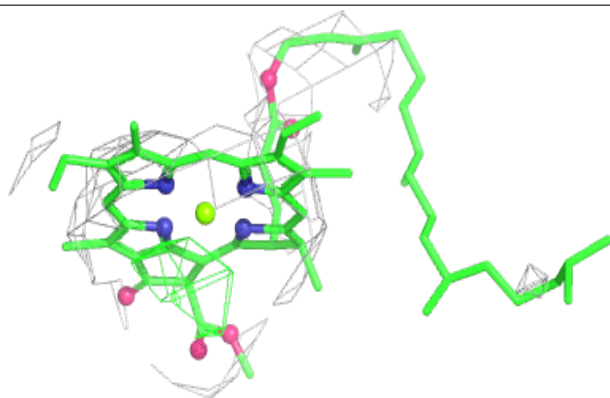
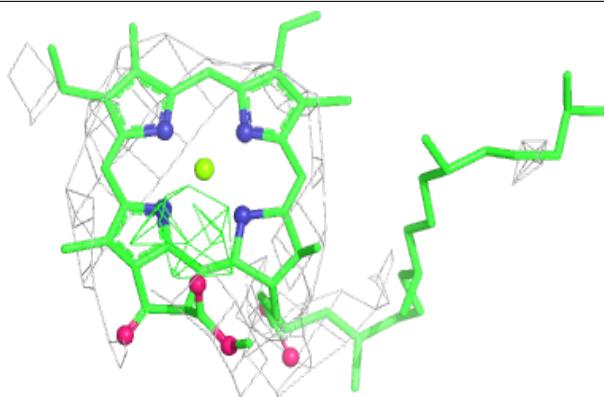
Electron density around LHG L 101:

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

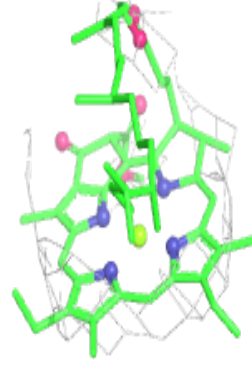
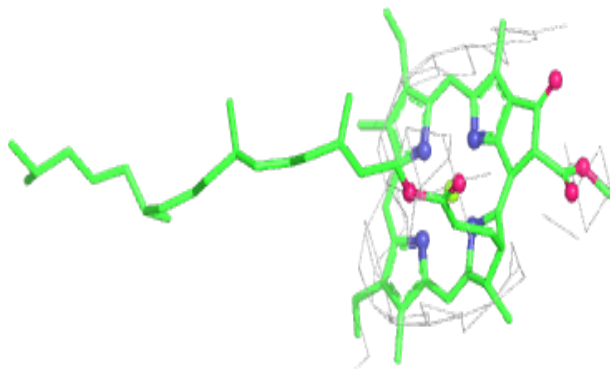
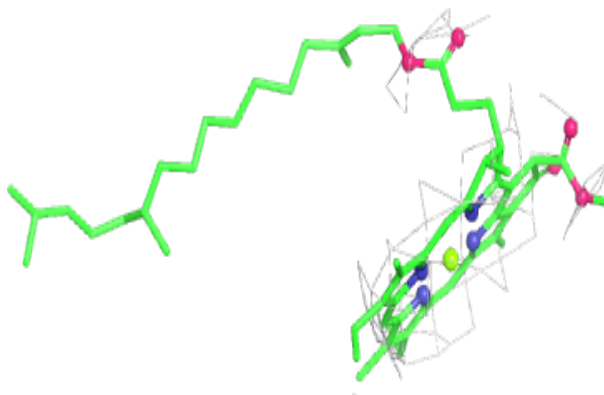


Electron density around CLA D 402:

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

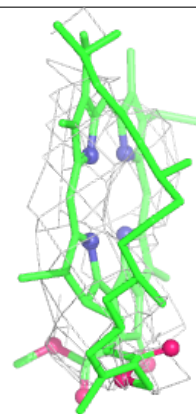
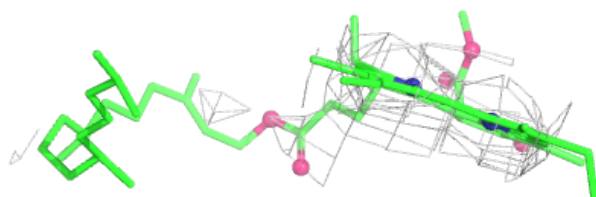
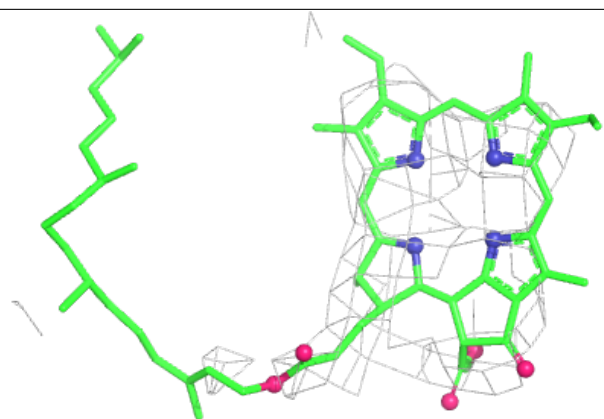
**Electron density around CLA c 505:**

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



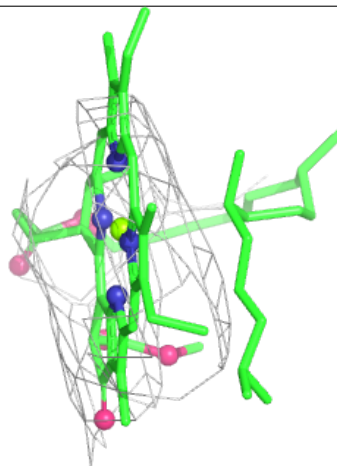
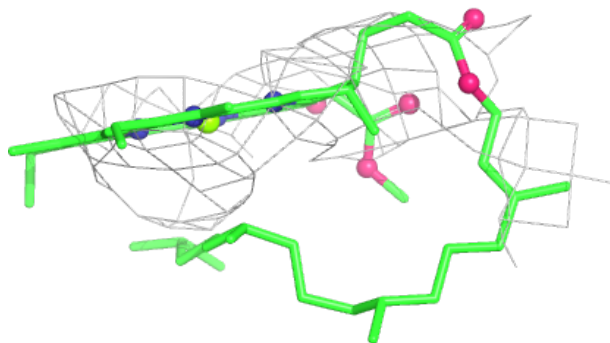
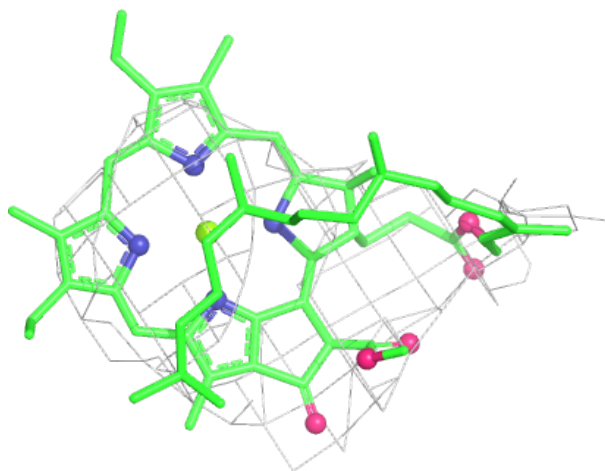
Electron density around PHO A 607:

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



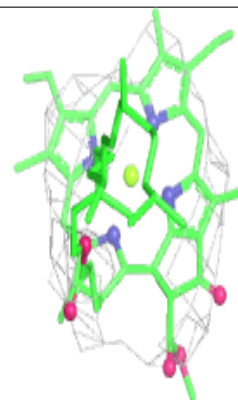
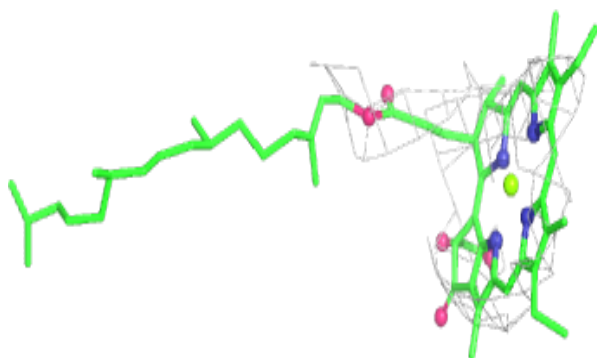
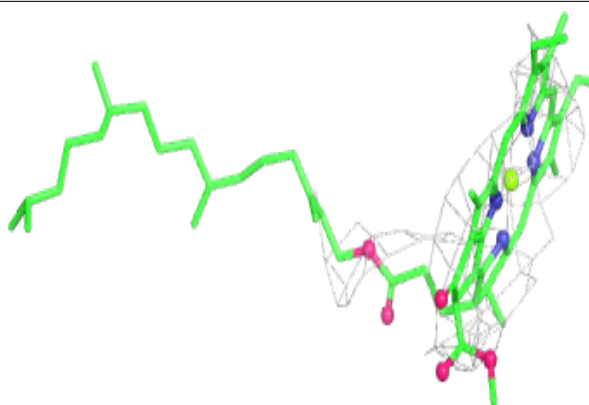
Electron density around CLA c 511:

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



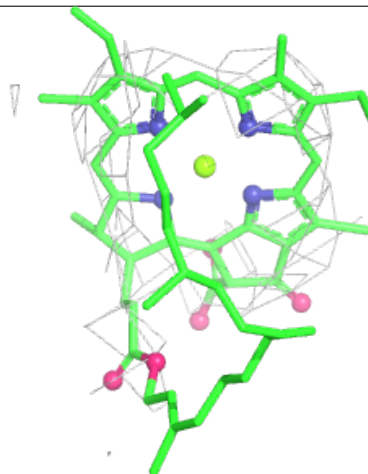
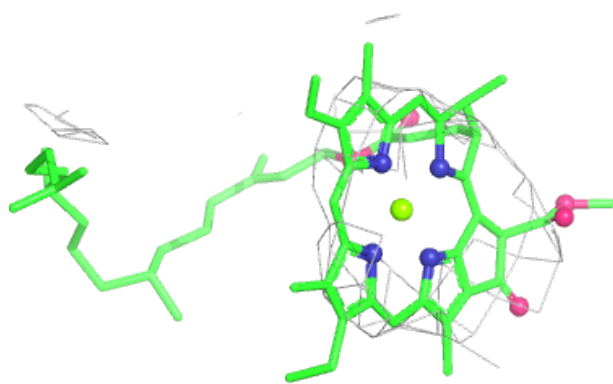
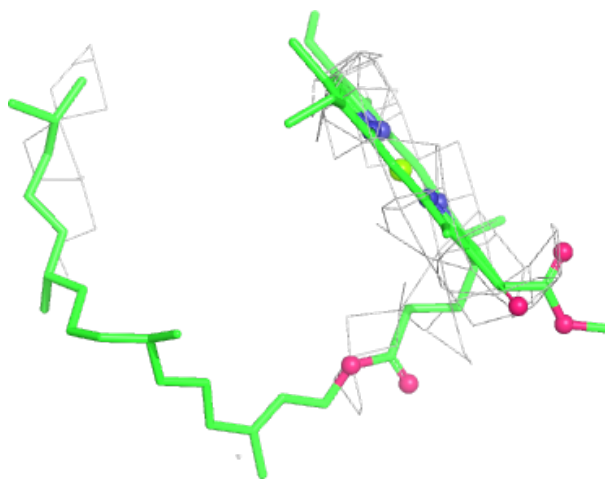
Electron density around CLA b 607:

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



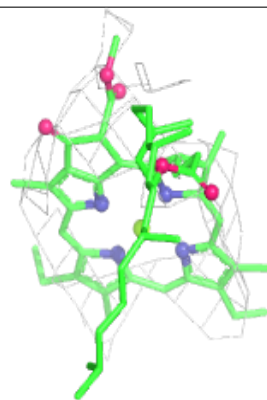
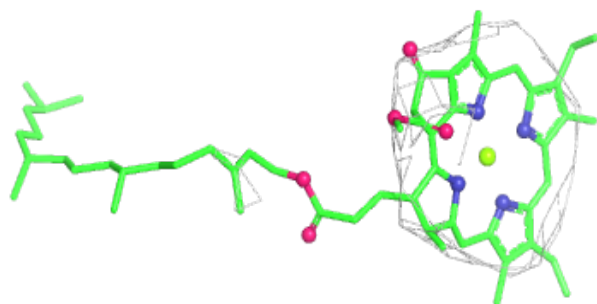
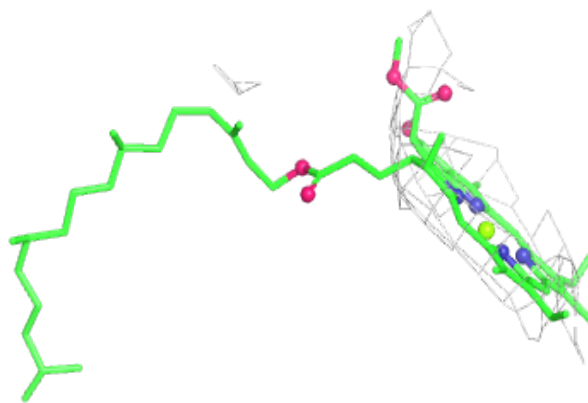
Electron density around CLA B 612:

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



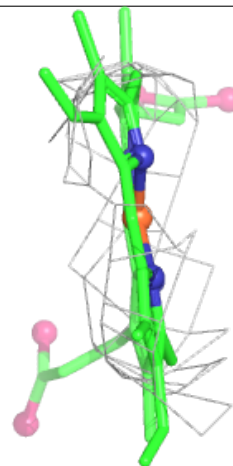
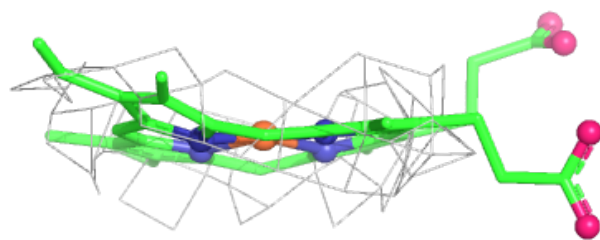
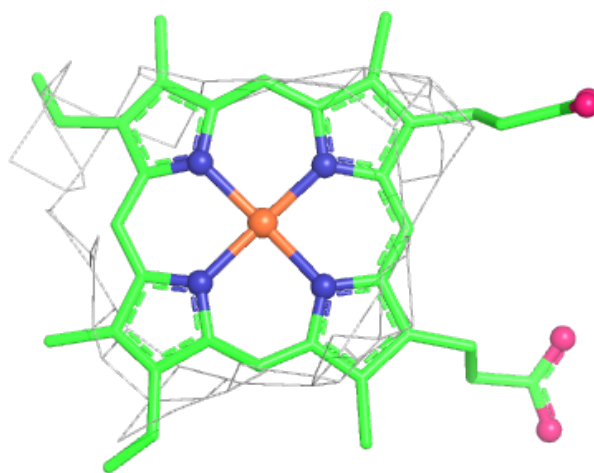
Electron density around CLA d 402:

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



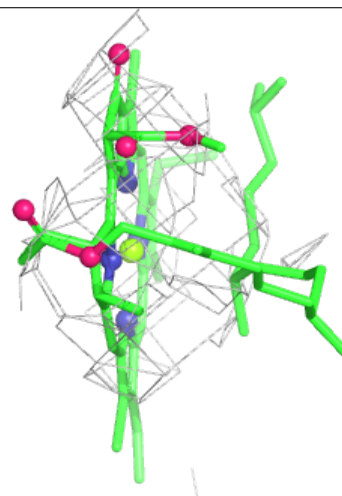
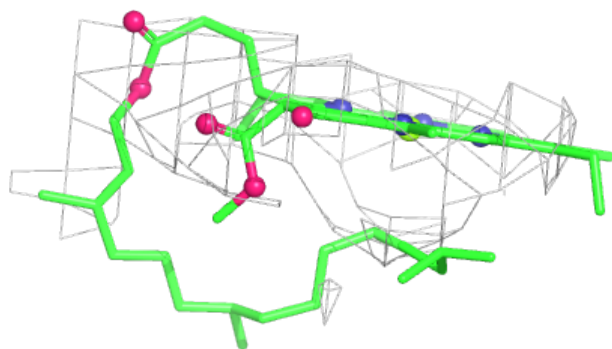
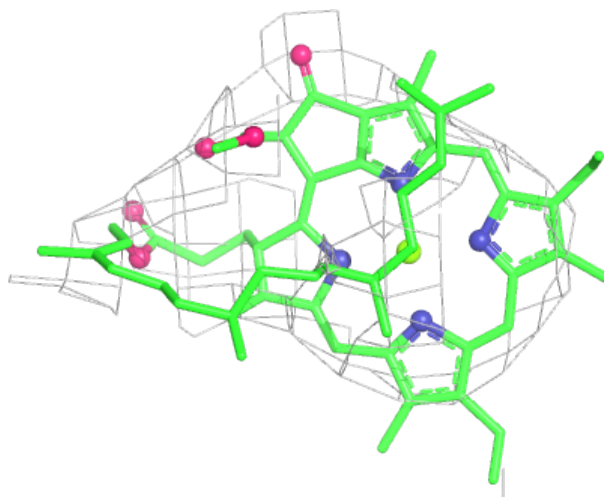
Electron density around HEM V 202:

$2mF_o-DF_c$ (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)



6.5 Other polymers [i](#)

There are no such residues in this entry.