



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 09:16 PM UTC

PDB ID : 4PBU / pdb_00004pbu
Title : Serial Time-resolved crystallography of Photosystem II using a femtosecond X-ray laser The S1 state
Authors : Kupitz, C.; Basu, S.; Grotjohann, I.; Fromme, R.; Zatsepin, N.; Rendek, K.N.; Hunter, M.; Shoeman, R.L.; White, T.A.; Wang, D.; James, D.; Yang, J.H.; Cobb, D.E.; Reeder, B.; Sierra, R.G.; Liu, H.; Barty, A.; Aquila, A.; Deponte, D.; Kirian, R.A.; Bari, S.; Bergkamp, J.J.; Beyerlein, K.; Bogan, M.J.; Caleman, C.; Chao, T.-C.; Conrad, C.E.; Davis, K.M.; Fleckenstein, H.; Galli, L.; Hau-Riege, S.P.; Kassemeyer, S.; Laksmono, H.; Liang, M.; Lomb, L.; Marchesini, S.; Martin, A.V.; Messerschmidt, M.; Milathianaki, D.; Nass, K.; Ros, A.; Roy-Chowdhury, S.; Schmidt, K.; Seibert, M.; Steinbrener, J.; Stellato, F.; Yan, L.; Yoon, C.; Moore, T.A.; Moore, A.L.; Pushkar, Y.; Williams, G.J.; Boutet, S.; Doak, R.B.; Weierstall, U.; Frank, M.; Chapman, H.N.; Spence, J.C.H.; Fromme, P.
Deposited on : 2014-04-13
Resolution : 5.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0

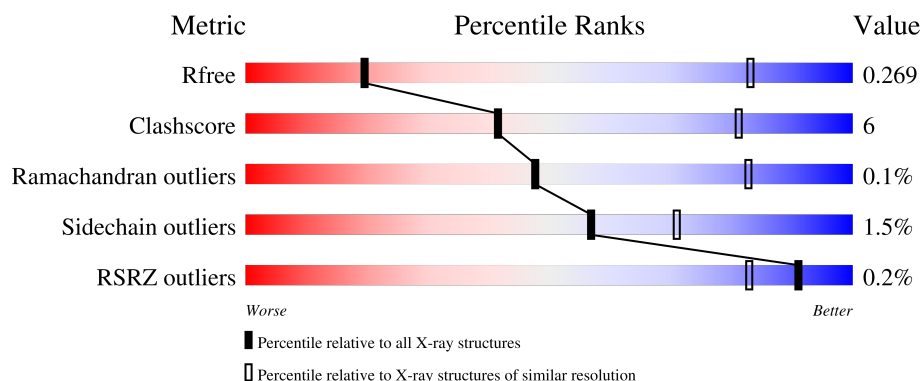
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 5.00 Å.

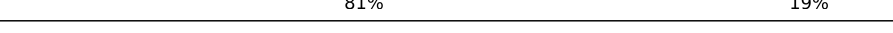
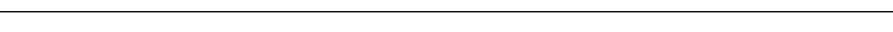
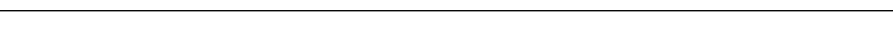
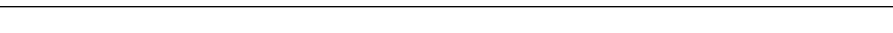
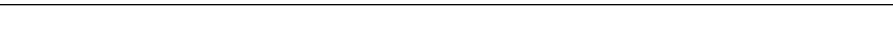
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1009 (6.02-3.98)
Clashscore	190562	1040 (6.00-4.00)
Ramachandran outliers	187476	1015 (6.06-3.92)
Sidechain outliers	187428	1136 (6.10-3.90)
RSRZ outliers	180081	1004 (6.02-3.98)

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.

Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

Mol	Chain	Length	Quality of chain
1	A	334	 90% 10%
1	a	334	 84% 15% .
2	B	504	 91% 9%
2	b	504	 92% 8%
3	C	455	 88% 11% ..
3	c	455	 87% 12%
4	D	342	 90% 10%
4	d	342	 87% 13%
5	E	81	 81% 19%
5	e	81	 84% 16%
6	F	34	 82% 15% .
6	f	34	 3% 71% 24% 6%
7	H	65	 86% 12% .
7	h	65	 89% 11%
8	I	38	 89% 11%
8	i	38	 87% 13%
9	J	40	 82% 12% 5%
9	j	40	 85% 15%
10	K	37	 86% 11% .
10	k	37	 73% 24% .
11	L	37	 78% 19% .
11	l	37	 89% 11%
12	M	34	 3% 82% 18%
12	m	34	 85% 15%
13	O	243	 85% 14% .
13	o	243	 88% 10% .

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Mol	Chain	Length	Quality of chain
14	T	30	
14	t	30	
15	U	97	
15	u	97	
16	V	137	
16	v	137	
17	Y	29	
17	y	29	
18	X	39	
18	x	39	
19	Z	62	
19	z	62	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CL	v	201	-	-	-	X
24	CLA	A	606	X	-	-	-
24	CLA	B	602	X	-	-	-
24	CLA	B	603	X	-	-	-
24	CLA	B	604	X	-	-	-
24	CLA	B	605	X	-	-	-
24	CLA	B	606	X	-	-	-
24	CLA	B	608	X	-	-	-
24	CLA	B	610	X	-	-	-
24	CLA	B	611	X	-	-	-
24	CLA	B	613	X	-	-	-
24	CLA	B	614	X	-	-	-
24	CLA	B	615	X	-	-	-
24	CLA	B	616	X	-	-	-
24	CLA	B	617	X	-	-	-
24	CLA	C	503	X	-	-	-
24	CLA	C	504	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	C	505	X	-	-	-
24	CLA	C	506	X	-	-	-
24	CLA	C	507	X	-	-	-
24	CLA	C	509	X	-	-	-
24	CLA	C	510	X	-	-	-
24	CLA	C	512	X	-	-	-
24	CLA	D	402	X	-	-	-
24	CLA	a	406	X	-	-	-
24	CLA	b	602	X	-	-	-
24	CLA	b	603	X	-	-	-
24	CLA	b	604	X	-	-	-
24	CLA	b	605	X	-	-	-
24	CLA	b	606	X	-	-	-
24	CLA	b	607	X	-	-	-
24	CLA	b	608	X	-	-	-
24	CLA	b	611	X	-	-	-
24	CLA	b	613	X	-	-	-
24	CLA	b	614	X	-	-	-
24	CLA	b	615	X	-	-	-
24	CLA	b	616	X	-	-	-
24	CLA	b	617	X	-	-	-
24	CLA	c	902	X	-	-	-
24	CLA	c	906	X	-	-	-
24	CLA	c	907	X	-	-	-
24	CLA	c	908	X	-	-	-
24	CLA	c	910	X	-	-	-
24	CLA	c	911	X	-	-	-
24	CLA	c	913	X	-	-	-
24	CLA	d	403	X	-	-	-
26	BCR	K	101	-	X	-	-
26	BCR	f	101	-	X	-	-
26	BCR	h	101	-	X	-	-
26	BCR	k	102	-	X	-	-
29	LHG	D	409	-	-	X	-
29	LHG	d	410	-	-	X	-

2 Entry composition [i](#)

There are 33 unique types of molecules in this entry. The entry contains 48924 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 Q(B) protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	0	0
			2620	1716	431	458	15			
1	a	334	Total	C	N	O	S	0	0	0
			2620	1716	431	458	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 core light harvesting protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	504	Total	C	N	O	S	0	0	0
			3969	2605	661	690	13			
2	b	504	Total	C	N	O	S	0	0	0
			3969	2605	661	690	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	451	Total	C	N	O	S	0	0	0
			3486	2281	584	608	13			
3	c	455	Total	C	N	O	S	0	0	0
			3519	2303	589	614	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	341	Total	C	N	O	S	0	0	0
			2717	1800	444	461	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	0	0
			662	432	107	123				
5	e	81	Total	C	N	O		0	0	0
			662	432	107	123				

- 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	32	Total	C	N	O	S	0	0	0
			257	175	43	38	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	0	0
			511	341	82	86	2			
7	h	65	Total	C	N	O	S	0	0	0
			511	341	82	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	0	0
			312	210	48	53	1			
8	i	38	Total	C	N	O	S	0	0	0
			312	210	48	53	1			

- 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	40	Total	C	N	O	S	0	0	0
			288	192	44	49	3			

- 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	0	0
			304	202	48	53	1			
11	l	37	Total	C	N	O	S	0	0	0
			304	202	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	0	0
			267	178	40	48	1			
12	m	34	Total	C	N	O	S	0	0	0
			267	178	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	0	0
			1865	1165	315	381	4			
13	o	243	Total	C	N	O	S	0	0	0
			1865	1165	315	381	4			

- 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	0	0
			256	180	36	38	2			
14	t	30	Total	C	N	O	S	0	0	0
			256	180	36	38	2			

- 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	0	0
			1064	675	177	208	4			
16	v	137	Total	C	N	O	S	0	0	0
			1064	675	177	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			

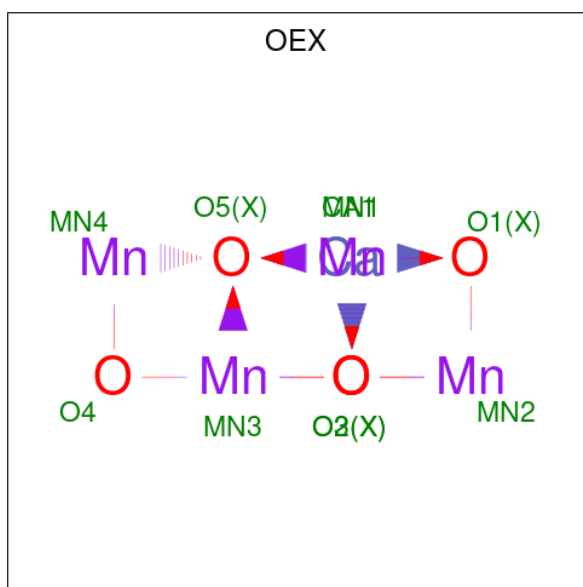
- Molecule 18 is a protein called Photosystem II reaction center X protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	X	39	Total	C	N	O	0	0	0
			287	191	46	50			
18	x	39	Total	C	N	O	0	0	0
			287	191	46	50			

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

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

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



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

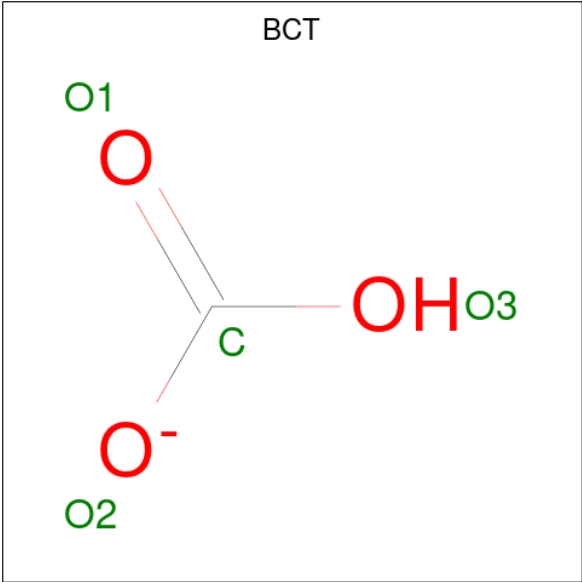
- Molecule 21 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

- Molecule 22 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

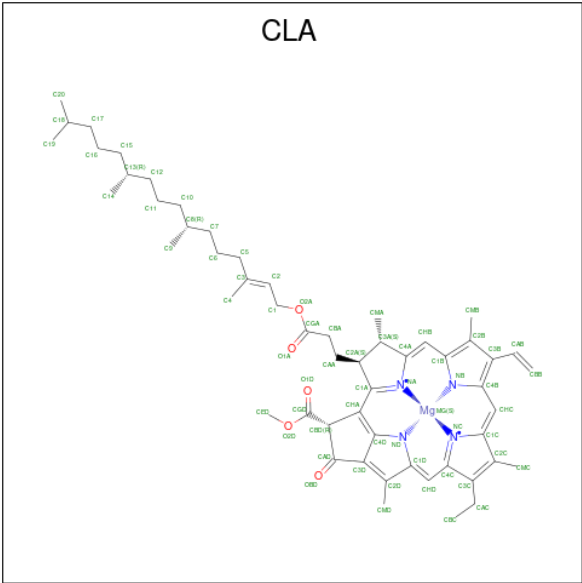
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	2	Total	Cl	0	0
			2	2		
22	V	1	Total	Cl	0	0
			1	1		
22	a	2	Total	Cl	0	0
			2	2		
22	v	1	Total	Cl	0	0
			1	1		

- Molecule 23 is BICARBONATE ION (CCD ID: BCT) (formula: CHO₃).



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

- Molecule 24 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



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

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

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

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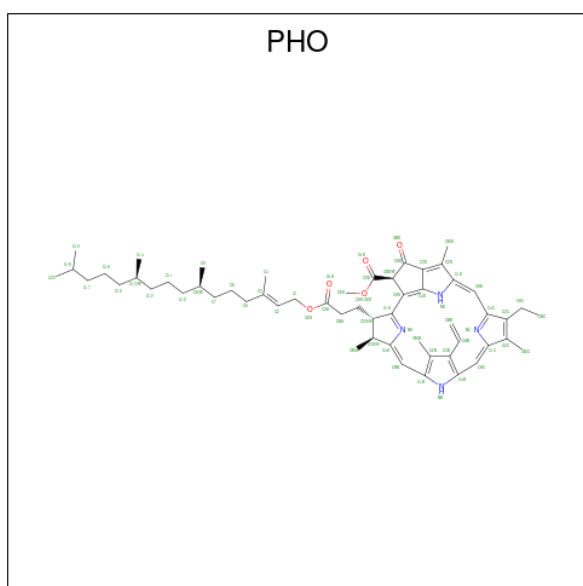
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N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

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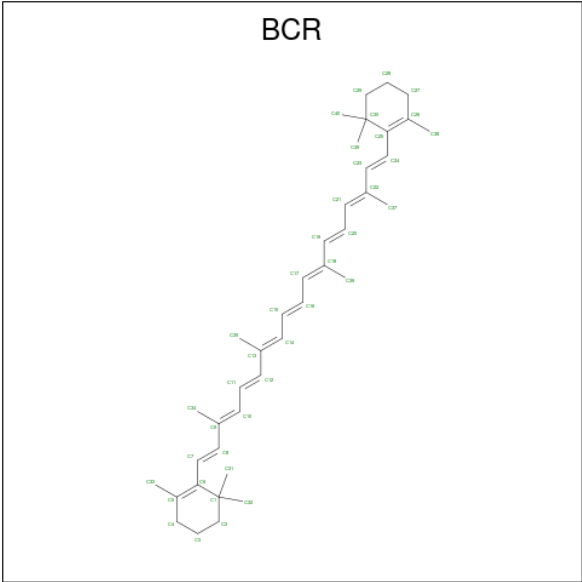
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 25 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



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

- Molecule 26 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



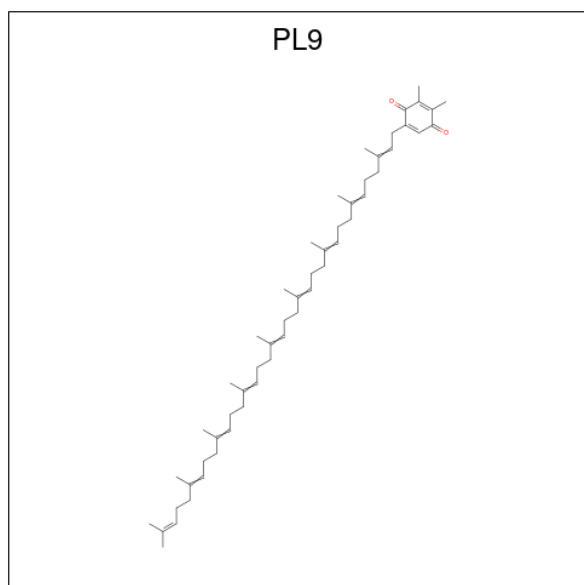
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	D	1	Total C 40 40	0	0
26	H	1	Total C 40 40	0	0
26	K	1	Total C 40 40	0	0
26	T	1	Total C 40 40	0	0
26	T	1	Total C 40 40	0	0
26	Y	1	Total C 40 40	0	0
26	a	1	Total C 40 40	0	0

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

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



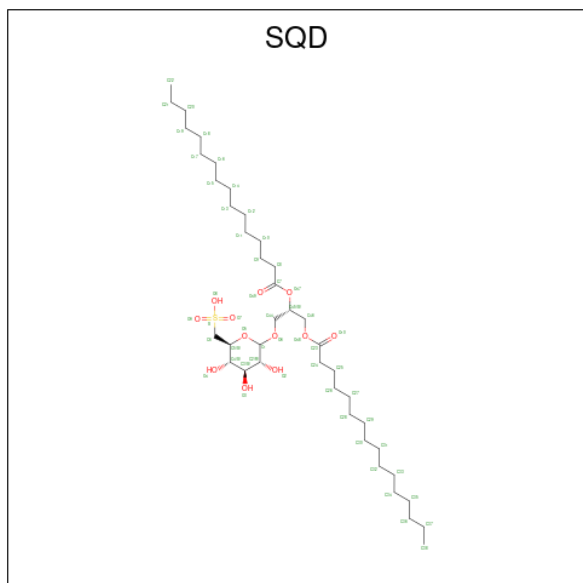
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	1	Total C O 55 53 2	0	0
27	D	1	Total C O 55 53 2	0	0

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

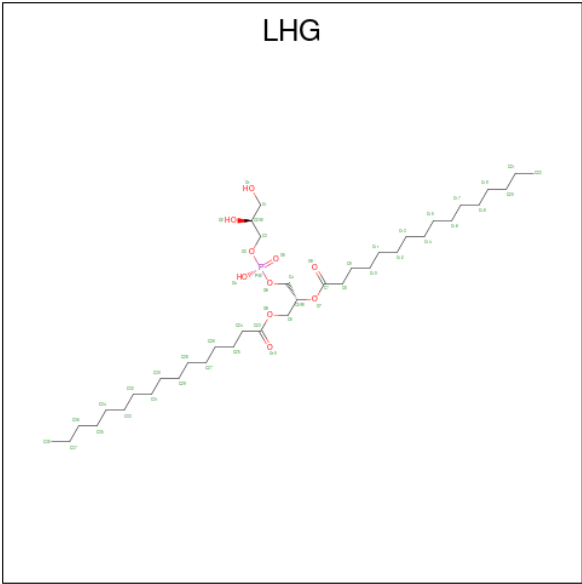
- Molecule 28 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	A	1	Total	C	O	S	0	0
			54	41	12	1		
28	A	1	Total	C	O	S	0	0
			54	41	12	1		
28	F	1	Total	C	O	S	0	0
			43	30	12	1		
28	L	1	Total	C	O	S	0	0
			54	41	12	1		
28	a	1	Total	C	O	S	0	0
			54	41	12	1		
28	a	1	Total	C	O	S	0	0
			54	41	12	1		
28	d	1	Total	C	O	S	0	0
			43	30	12	1		
28	l	1	Total	C	O	S	0	0
			54	41	12	1		

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

(formula: C₃₈H₇₅O₁₀P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	A	1	Total	C	O	P	0	0
			42	31	10	1		
29	B	1	Total	C	O	P	0	0
			49	38	10	1		
29	D	1	Total	C	O	P	0	0
			49	38	10	1		
29	D	1	Total	C	O	P	0	0
			49	38	10	1		
29	D	1	Total	C	O	P	0	0
			49	38	10	1		
29	a	1	Total	C	O	P	0	0
			42	31	10	1		
29	b	1	Total	C	O	P	0	0
			49	38	10	1		
29	d	1	Total	C	O	P	0	0
			49	38	10	1		
29	d	1	Total	C	O	P	0	0
			49	38	10	1		
29	d	1	Total	C	O	P	0	0
			49	38	10	1		

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

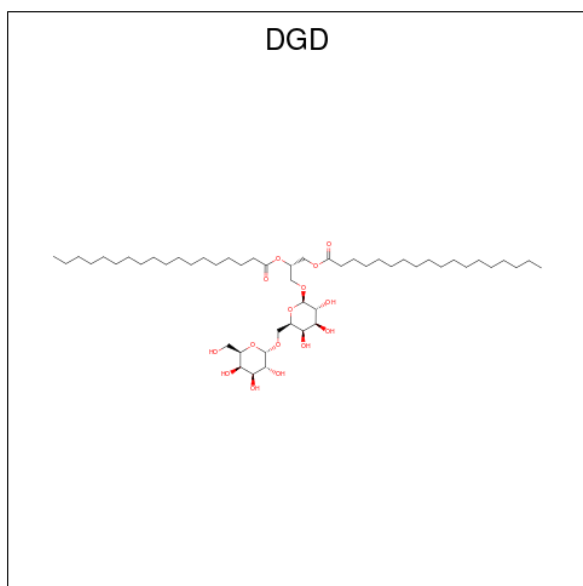
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	B	1	Total	Ca	0	0
			1	1		

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

- Molecule 31 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	C	1	Total 62	C 47	O 15	0	0
31	C	1	Total 62	C 47	O 15	0	0
31	C	1	Total 62	C 47	O 15	0	0
31	D	1	Total 62	C 47	O 15	0	0
31	H	1	Total 62	C 47	O 15	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	c	1	Total C O 62 47 15	0	0
31	c	1	Total C O 62 47 15	0	0
31	d	1	Total C O 62 47 15	0	0
31	h	1	Total C O 62 47 15	0	0
31	j	1	Total C O 62 47 15	0	0

- # HEM

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

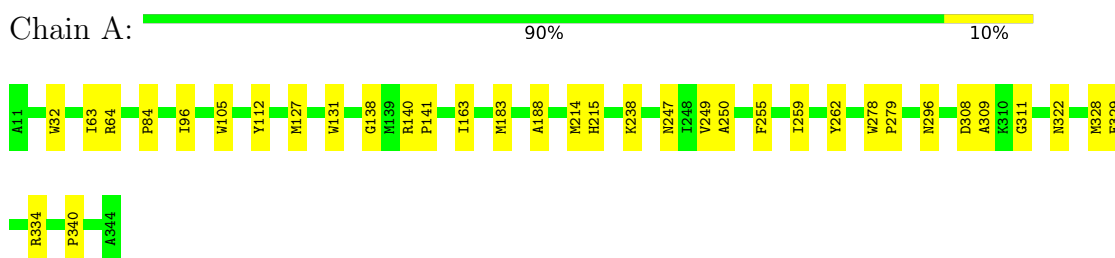
- 

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	j	1	Total	Mg	0	0
			1	1		

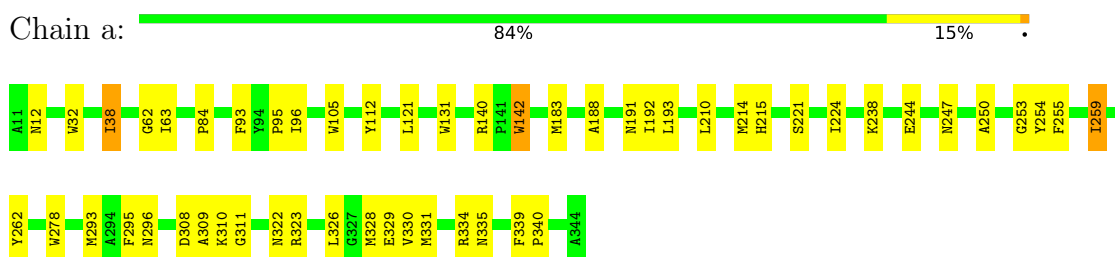
3 Residue-property plots [i](#)

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.

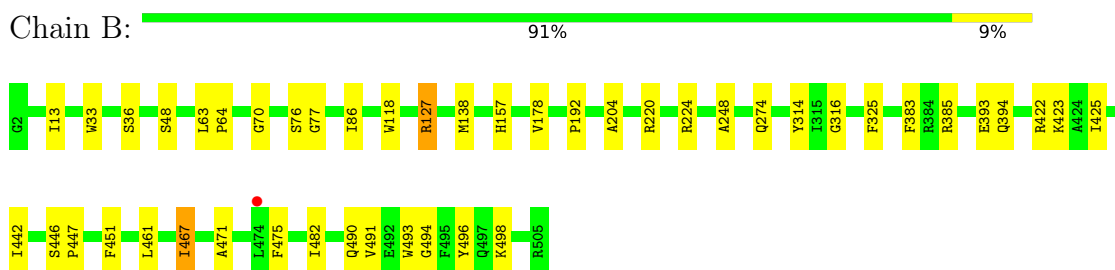
- Molecule 1: Photosystem Q(B) protein 1



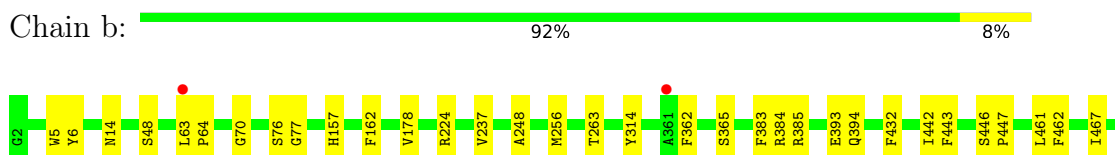
- Molecule 1: Photosystem Q(B) protein 1

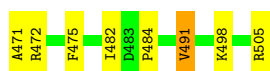


- Molecule 2: Photosystem II core light harvesting protein



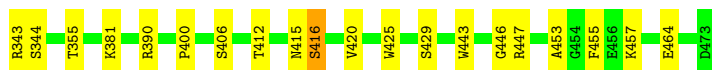
- Molecule 2: Photosystem II core light harvesting protein





• Molecule 3: Photosystem II CP43 protein

Chain C: 88% 11% ..



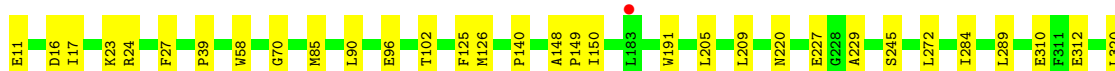
• Molecule 3: Photosystem II CP43 protein

Chain c: 87% 12%



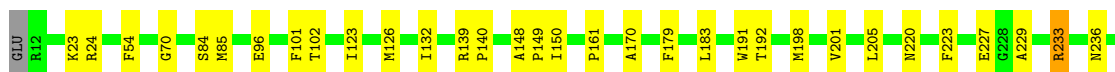
• Molecule 4: Photosystem II D2 protein

Chain D: 90% 10%



• Molecule 4: Photosystem II D2 protein

Chain d: 87% 13%



• Molecule 5: Cytochrome b559 subunit alpha

Chain E: 81% 19%



- Molecule 5: Cytochrome b559 subunit alpha

Chain e: 84% 16%



- Molecule 6: Cytochrome b559 subunit beta

Chain F: 82% 15% .



- Molecule 6: Cytochrome b559 subunit beta

Chain f: 3% 71% 24% 6%



- Molecule 7: Photosystem II reaction center protein H

Chain H: 86% 12% .



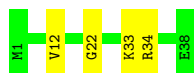
- Molecule 7: Photosystem II reaction center protein H

Chain h: 89% 11%



- Molecule 8: Photosystem II reaction center protein I

Chain I: 89% 11%



- Molecule 8: Photosystem II reaction center protein I

Chain i: 87% 13%



- Molecule 9: Photosystem II reaction center protein J

Chain J: 82% 12% 5%



- Molecule 9: Photosystem II reaction center protein J

Chain j: 85% 15%



- Molecule 10: Photosystem II reaction center protein K

Chain K: 86% 11% .



- Molecule 10: Photosystem II reaction center protein K

Chain k: 73% 24% .



- Molecule 11: Photosystem II reaction center protein L

Chain L: 78% 19% .



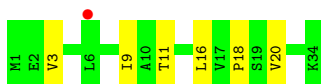
- Molecule 11: Photosystem II reaction center protein L

Chain l: 89% 11%



- Molecule 12: Photosystem II reaction center protein M

Chain M: 3% 82% 18%



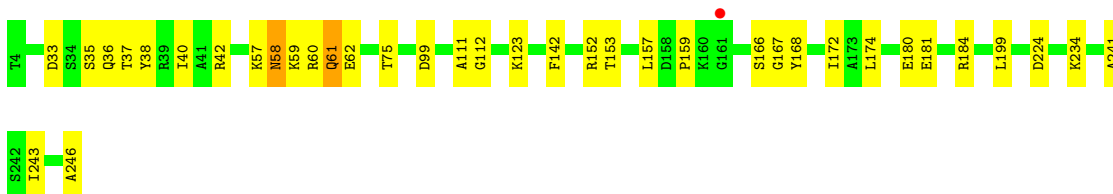
- Molecule 12: Photosystem II reaction center protein M

Chain m: 85% 15%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O: 85% 14%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o: 88% 10%



- Molecule 14: Photosystem II reaction center protein T

Chain T: 90% 10%



- Molecule 14: Photosystem II reaction center protein T

Chain t: 83% 17%



- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U: 85% 15%



- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u:  87% 13%



- Molecule 16: Cytochrome c-550

Chain V:  91% 9%



- Molecule 16: Cytochrome c-550

Chain v:  % 85% 15% .



- Molecule 17: Photosystem II reaction center protein Ycf12

Chain Y:  83% 17%



- Molecule 17: Photosystem II reaction center protein Ycf12

Chain y:  72% 28%



- Molecule 18: Photosystem II reaction center X protein

Chain X:  90% 10%



- Molecule 18: Photosystem II reaction center X protein

Chain x:  85% 15%



- Molecule 19: Photosystem II reaction center protein Z

Chain Z:

97%

.

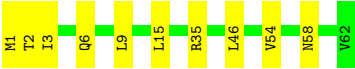


● Molecule 19: Photosystem II reaction center protein Z

Chain z:

84%

16%



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)	100.64 – 5.00 100.64 – 5.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (100.64-5.00) 100.0 (100.64-5.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 5.12Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.261 , 0.262 0.272 , 0.269	Depositor DCC
R_{free} test set	2056 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	285.1	Xtriage
Anisotropy	0.304	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 133.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	48924	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.89% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.62	0/2705	0.80	0/3689
1	a	0.60	1/2705 (0.0%)	0.81	1/3689 (0.0%)
2	B	0.58	0/4109	0.79	0/5600
2	b	0.57	0/4109	0.76	0/5600
3	C	0.55	0/3599	0.78	0/4900
3	c	0.53	0/3633	0.79	0/4946
4	D	0.61	0/2821	0.78	0/3844
4	d	0.56	0/2812	0.77	0/3832
5	E	0.55	0/681	0.81	0/928
5	e	0.54	0/681	0.80	0/928
6	F	0.68	1/284 (0.4%)	0.73	0/387
6	f	0.55	0/265	0.77	0/360
7	H	0.58	0/524	0.77	0/713
7	h	0.54	0/524	0.73	0/713
8	I	0.57	0/319	0.74	0/429
8	i	0.57	0/319	0.77	0/429
9	J	0.59	0/278	0.82	0/376
9	j	0.49	0/294	0.84	0/396
10	K	0.57	0/303	0.81	0/416
10	k	0.63	1/303 (0.3%)	0.87	0/416
11	L	0.57	0/311	0.77	0/422
11	l	0.57	0/311	0.73	0/422
12	M	0.59	0/270	0.86	0/367
12	m	0.60	0/270	0.74	0/367
13	O	0.54	0/1896	0.74	0/2571
13	o	0.52	0/1896	0.75	0/2571
14	T	0.56	0/265	0.76	0/359
14	t	0.60	0/265	0.80	0/359
15	U	0.55	0/785	0.74	0/1064
15	u	0.55	0/785	0.72	0/1064
16	V	0.57	0/1085	0.78	0/1473
16	v	0.53	0/1085	0.82	1/1473 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	Y	0.58	0/216	0.83	0/289
17	y	0.52	0/216	0.97	0/289
18	X	0.53	0/290	0.83	0/392
18	x	0.53	0/290	0.85	0/392
19	Z	0.54	0/490	0.87	0/669
19	z	0.54	0/490	0.91	0/669
All	All	0.57	3/42484 (0.0%)	0.78	2/57803 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	28	VAL	CA-CB	5.69	1.57	1.54
1	a	38	ILE	CA-CB	5.51	1.57	1.54
10	k	28	ILE	CA-CB	5.33	1.56	1.54

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	v	105	ARG	N-CA-C	6.42	119.09	111.33
1	a	142	TRP	N-CA-C	5.90	120.17	112.92

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2620	0	2517	40	0
1	a	2620	0	2517	66	0
2	B	3969	0	3828	57	0
2	b	3969	0	3828	53	0
3	C	3486	0	3407	48	0
3	c	3519	0	3437	53	23
4	D	2726	0	2627	35	0
4	d	2717	0	2621	56	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	662	0	648	12	0
5	e	662	0	648	11	0
6	F	275	0	282	4	0
6	f	257	0	269	5	0
7	H	511	0	532	8	0
7	h	511	0	532	7	0
8	I	312	0	329	4	0
8	i	312	0	329	4	0
9	J	272	0	279	5	0
9	j	288	0	300	6	0
10	K	293	0	305	7	0
10	k	293	0	305	9	0
11	L	304	0	316	8	0
11	l	304	0	316	4	0
12	M	267	0	289	8	0
12	m	267	0	289	8	0
13	O	1865	0	1838	33	23
13	o	1865	0	1838	35	0
14	T	256	0	262	4	0
14	t	256	0	262	4	0
15	U	774	0	773	25	0
15	u	774	0	773	19	0
16	V	1064	0	1073	20	0
16	v	1064	0	1075	30	0
17	Y	215	0	246	3	0
17	y	215	0	246	9	0
18	X	287	0	317	4	0
18	x	287	0	317	10	0
19	Z	479	0	516	0	0
19	z	479	0	516	4	0
20	A	10	0	0	0	0
20	a	10	0	0	0	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	A	2	0	0	0	0
22	V	1	0	0	0	0
22	a	2	0	0	0	0
22	v	1	0	0	0	0
23	A	4	0	0	0	0
23	a	4	0	0	0	0
24	A	260	0	288	8	0
24	B	1040	0	1152	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	C	845	0	936	36	0
24	D	130	0	144	1	0
24	a	195	0	216	7	0
24	b	1040	0	1152	21	0
24	c	845	0	936	45	0
24	d	195	0	216	13	0
25	A	64	0	74	2	0
25	D	64	0	74	4	0
25	a	64	0	74	3	0
25	d	64	0	74	1	0
26	A	40	0	48	0	0
26	B	160	0	188	6	0
26	C	80	0	93	0	0
26	D	40	0	48	2	0
26	H	40	0	46	1	0
26	K	40	0	46	1	0
26	T	80	0	94	2	0
26	Y	40	0	47	1	0
26	a	40	0	48	1	0
26	b	80	0	92	5	0
26	c	80	0	95	3	0
26	f	40	0	46	0	0
26	h	40	0	46	1	0
26	k	80	0	90	5	0
27	A	55	0	80	9	0
27	D	55	0	80	1	0
27	a	55	0	80	8	0
27	d	55	0	80	1	0
28	A	108	0	156	6	0
28	F	43	0	53	0	0
28	L	54	0	78	5	0
28	a	108	0	156	7	0
28	d	43	0	53	1	0
28	l	54	0	78	7	0
29	A	42	0	57	3	0
29	B	49	0	74	3	0
29	D	147	0	222	25	0
29	a	42	0	57	5	0
29	b	49	0	74	6	0
29	d	147	0	222	26	0
30	B	1	0	0	0	0
30	F	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	O	1	0	0	0	0
30	b	1	0	0	0	0
30	c	1	0	0	0	0
30	f	1	0	0	0	0
30	o	1	0	0	0	0
31	C	186	0	246	6	0
31	D	62	0	82	3	0
31	H	62	0	82	2	0
31	c	124	0	164	0	0
31	d	62	0	82	2	0
31	h	62	0	82	1	0
31	j	62	0	82	2	0
32	E	43	0	30	0	0
32	V	43	0	30	9	0
32	e	43	0	30	0	0
32	v	43	0	30	8	0
33	j	1	0	0	0	0
All	All	48924	0	49705	629	23

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 629 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:V:37:CYS:SG	32:V:202:HEM:HAB	1.52	1.49
16:v:40:CYS:SG	32:v:202:HEM:HAC	1.53	1.46
16:V:37:CYS:SG	32:V:202:HEM:CAB	2.03	1.46
16:V:40:CYS:SG	32:V:202:HEM:CAC	2.03	1.44
16:V:40:CYS:SG	32:V:202:HEM:HAC	1.56	1.40

The worst 5 of 23 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:37:THR:O	3:c:19:ASN:CG[2_455]	0.56	1.64
13:O:37:THR:O	3:c:19:ASN:ND2[2_455]	0.91	1.29
13:O:36:GLN:NE2	3:c:19:ASN:CA[2_455]	0.99	1.21
13:O:37:THR:N	3:c:19:ASN:OD1[2_455]	1.04	1.16
13:O:36:GLN:NE2	3:c:19:ASN:C[2_455]	1.05	1.15

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	332/334 (99%)	328 (99%)	3 (1%)	1 (0%)	36	72
1	a	332/334 (99%)	325 (98%)	6 (2%)	1 (0%)	36	72
2	B	502/504 (100%)	496 (99%)	6 (1%)	0	100	100
2	b	502/504 (100%)	492 (98%)	10 (2%)	0	100	100
3	C	449/455 (99%)	440 (98%)	8 (2%)	1 (0%)	43	77
3	c	453/455 (100%)	440 (97%)	12 (3%)	1 (0%)	43	77
4	D	340/342 (99%)	332 (98%)	8 (2%)	0	100	100
4	d	339/342 (99%)	333 (98%)	6 (2%)	0	100	100
5	E	79/81 (98%)	78 (99%)	1 (1%)	0	100	100
5	e	79/81 (98%)	78 (99%)	1 (1%)	0	100	100
6	F	32/34 (94%)	32 (100%)	0	0	100	100
6	f	30/34 (88%)	30 (100%)	0	0	100	100
7	H	63/65 (97%)	58 (92%)	5 (8%)	0	100	100
7	h	63/65 (97%)	56 (89%)	7 (11%)	0	100	100
8	I	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
8	i	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
9	J	36/40 (90%)	36 (100%)	0	0	100	100
9	j	38/40 (95%)	38 (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	35/37 (95%)	35 (100%)	0	0	100	100
11	l	35/37 (95%)	35 (100%)	0	0	100	100
12	M	32/34 (94%)	32 (100%)	0	0	100	100
12	m	32/34 (94%)	32 (100%)	0	0	100	100
13	O	241/243 (99%)	233 (97%)	7 (3%)	1 (0%)	30	67

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	o	241/243 (99%)	231 (96%)	9 (4%)	1 (0%)	30	67
14	T	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
14	t	28/30 (93%)	28 (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	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
16	v	135/137 (98%)	130 (96%)	5 (4%)	0	100	100
17	Y	27/29 (93%)	27 (100%)	0	0	100	100
17	y	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
18	X	37/39 (95%)	36 (97%)	1 (3%)	0	100	100
18	x	37/39 (95%)	35 (95%)	2 (5%)	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	5191/5276 (98%)	5072 (98%)	113 (2%)	6 (0%)	48	83

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	O	58	ASN
13	o	58	ASN
3	C	416	SER
3	c	416	SER
1	A	259	ILE

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	269/269 (100%)	268 (100%)	1 (0%)	84	83
1	a	269/269 (100%)	267 (99%)	2 (1%)	76	80
2	B	402/402 (100%)	399 (99%)	3 (1%)	76	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	b	402/402 (100%)	397 (99%)	5 (1%)	63	74
3	C	352/356 (99%)	345 (98%)	7 (2%)	48	66
3	c	356/356 (100%)	351 (99%)	5 (1%)	59	72
4	D	277/277 (100%)	275 (99%)	2 (1%)	76	80
4	d	276/277 (100%)	274 (99%)	2 (1%)	76	80
5	E	72/72 (100%)	71 (99%)	1 (1%)	59	72
5	e	72/72 (100%)	70 (97%)	2 (3%)	38	59
6	F	28/28 (100%)	27 (96%)	1 (4%)	31	52
6	f	26/28 (93%)	25 (96%)	1 (4%)	29	51
7	H	54/54 (100%)	52 (96%)	2 (4%)	30	51
7	h	54/54 (100%)	54 (100%)	0	100	100
8	I	35/35 (100%)	35 (100%)	0	100	100
8	i	35/35 (100%)	35 (100%)	0	100	100
9	J	26/28 (93%)	26 (100%)	0	100	100
9	j	28/28 (100%)	28 (100%)	0	100	100
10	K	30/30 (100%)	28 (93%)	2 (7%)	15	37
10	k	30/30 (100%)	28 (93%)	2 (7%)	15	37
11	L	35/35 (100%)	33 (94%)	2 (6%)	18	40
11	l	35/35 (100%)	34 (97%)	1 (3%)	37	58
12	M	31/31 (100%)	30 (97%)	1 (3%)	34	55
12	m	31/31 (100%)	31 (100%)	0	100	100
13	O	206/206 (100%)	202 (98%)	4 (2%)	50	66
13	o	206/206 (100%)	201 (98%)	5 (2%)	43	63
14	T	27/27 (100%)	27 (100%)	0	100	100
14	t	27/27 (100%)	25 (93%)	2 (7%)	13	34
15	U	84/84 (100%)	83 (99%)	1 (1%)	63	74
15	u	84/84 (100%)	83 (99%)	1 (1%)	63	74
16	V	117/117 (100%)	116 (99%)	1 (1%)	70	77
16	v	117/117 (100%)	114 (97%)	3 (3%)	40	61
17	Y	22/22 (100%)	21 (96%)	1 (4%)	24	46
17	y	22/22 (100%)	22 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	X	32/32 (100%)	32 (100%)	0	100	100
18	x	32/32 (100%)	31 (97%)	1 (3%)	35	56
19	Z	52/52 (100%)	50 (96%)	2 (4%)	29	51
19	z	52/52 (100%)	49 (94%)	3 (6%)	18	40
All	All	4305/4314 (100%)	4239 (98%)	66 (2%)	57	71

5 of 66 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
14	t	25	GLU
16	v	17	LYS
19	z	35	ARG
13	O	181	GLU
13	O	62	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
3	c	19	ASN
4	d	332	GLN
3	c	28	GLN
4	d	83	ASN
5	e	75	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 152 ligands modelled in this entry, 16 are monoatomic - leaving 136 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
24	CLA	B	605	-	69,73,73	2.37	16 (23%)	82,113,113	2.57	27 (32%)
26	BCR	B	618	-	41,41,41	3.49	14 (34%)	56,56,56	7.56	38 (67%)
26	BCR	D	404	-	41,41,41	3.62	14 (34%)	56,56,56	7.88	40 (71%)
32	HEM	V	202	16	50,50,50	1.86	10 (20%)	67,82,82	1.28	4 (5%)
24	CLA	c	909	-	69,73,73	2.37	19 (27%)	82,113,113	2.50	21 (25%)
24	CLA	b	607	-	69,73,73	2.56	19 (27%)	82,113,113	2.58	25 (30%)
28	SQD	a	402	-	52,54,54	1.01	2 (3%)	62,65,65	1.19	5 (8%)
24	CLA	C	502	-	69,73,73	2.20	17 (24%)	82,113,113	2.42	21 (25%)
24	CLA	c	907	-	69,73,73	2.42	19 (27%)	82,113,113	2.52	22 (26%)
26	BCR	k	102	-	41,41,41	3.62	14 (34%)	56,56,56	8.54	43 (76%)
28	SQD	d	407	-	41,43,54	1.13	2 (4%)	51,54,65	1.40	6 (11%)
24	CLA	c	911	-	69,73,73	2.25	17 (24%)	82,113,113	2.47	24 (29%)
26	BCR	b	619	-	41,41,41	3.62	15 (36%)	56,56,56	8.61	42 (75%)
25	PHO	a	412	-	58,69,69	2.67	11 (18%)	55,99,99	2.85	14 (25%)
26	BCR	k	101	-	41,41,41	3.68	14 (34%)	56,56,56	8.61	42 (75%)
24	CLA	a	406	-	69,73,73	2.11	20 (28%)	82,113,113	2.51	24 (29%)
32	HEM	v	202	16	50,50,50	1.89	10 (20%)	67,82,82	1.43	8 (11%)
24	CLA	B	611	-	69,73,73	2.27	18 (26%)	82,113,113	2.51	24 (29%)
24	CLA	B	609	-	69,73,73	2.09	17 (24%)	82,113,113	2.45	26 (31%)
31	DGD	C	516	-	63,63,67	0.88	3 (4%)	77,77,81	0.98	2 (2%)
26	BCR	f	101	-	41,41,41	3.64	15 (36%)	56,56,56	8.06	46 (82%)
24	CLA	b	605	-	69,73,73	2.39	20 (28%)	82,113,113	2.59	25 (30%)
27	PL9	D	405	-	55,55,55	0.83	2 (3%)	68,69,69	1.32	10 (14%)
31	DGD	C	518	-	63,63,67	0.80	3 (4%)	77,77,81	0.90	3 (3%)
27	PL9	a	410	-	55,55,55	0.71	2 (3%)	68,69,69	1.58	17 (25%)
24	CLA	a	407	-	69,73,73	2.20	17 (24%)	82,113,113	2.42	26 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	BCR	B	619	-	41,41,41	3.49	14 (34%)	56,56,56	7.82	41 (73%)
26	BCR	C	515	-	41,41,41	3.63	14 (34%)	56,56,56	8.33	38 (67%)
28	SQD	L	101	-	52,54,54	1.03	3 (5%)	62,65,65	1.40	9 (14%)
29	LHG	D	407	-	48,48,48	0.87	2 (4%)	51,54,54	1.01	4 (7%)
24	CLA	b	613	-	69,73,73	2.46	15 (21%)	82,113,113	2.50	24 (29%)
24	CLA	c	913	-	69,73,73	2.75	20 (28%)	82,113,113	2.49	26 (31%)
25	PHO	D	401	-	58,69,69	2.68	12 (20%)	55,99,99	2.86	15 (27%)
24	CLA	b	615	-	69,73,73	2.18	16 (23%)	82,113,113	2.68	27 (32%)
24	CLA	b	610	-	69,73,73	2.45	19 (27%)	82,113,113	2.32	21 (25%)
24	CLA	C	508	-	69,73,73	2.50	21 (30%)	82,113,113	2.42	19 (23%)
26	BCR	B	620	-	41,41,41	3.55	14 (34%)	56,56,56	8.51	42 (75%)
24	CLA	B	607	-	69,73,73	2.42	18 (26%)	82,113,113	2.56	26 (31%)
24	CLA	C	505	-	69,73,73	2.35	21 (30%)	82,113,113	2.35	22 (26%)
27	PL9	A	611	-	55,55,55	0.72	2 (3%)	68,69,69	1.55	12 (17%)
24	CLA	b	604	-	69,73,73	2.20	16 (23%)	82,113,113	2.41	24 (29%)
31	DGD	d	406	-	63,63,67	0.97	4 (6%)	77,77,81	0.95	4 (5%)
24	CLA	B	602	-	69,73,73	2.55	21 (30%)	82,113,113	2.60	23 (28%)
24	CLA	B	617	-	69,73,73	2.17	18 (26%)	82,113,113	2.47	26 (31%)
24	CLA	D	402	-	69,73,73	2.09	19 (27%)	82,113,113	2.38	27 (32%)
26	BCR	H	101	-	41,41,41	3.62	14 (34%)	56,56,56	8.34	41 (73%)
24	CLA	C	512	-	69,73,73	2.65	18 (26%)	82,113,113	2.40	26 (31%)
26	BCR	c	915	-	41,41,41	3.61	15 (36%)	56,56,56	8.67	38 (67%)
24	CLA	B	610	-	69,73,73	2.24	19 (27%)	82,113,113	2.43	23 (28%)
26	BCR	A	610	-	41,41,41	3.54	14 (34%)	56,56,56	7.79	37 (66%)
26	BCR	b	618	-	41,41,41	3.52	14 (34%)	56,56,56	8.04	44 (78%)
24	CLA	c	904	-	69,73,73	2.57	18 (26%)	82,113,113	2.48	23 (28%)
29	LHG	A	615	-	41,41,48	1.05	2 (4%)	44,47,54	1.08	3 (6%)
24	CLA	b	614	-	69,73,73	2.15	16 (23%)	82,113,113	2.53	24 (29%)
24	CLA	B	608	-	69,73,73	2.27	18 (26%)	82,113,113	2.41	23 (28%)
24	CLA	C	513	-	69,73,73	2.61	19 (27%)	82,113,113	2.43	24 (29%)
31	DGD	h	102	-	63,63,67	0.91	3 (4%)	77,77,81	0.86	3 (3%)
28	SQD	F	101	-	41,43,54	1.16	3 (7%)	51,54,65	1.42	7 (13%)
24	CLA	A	606	-	69,73,73	2.13	17 (24%)	82,113,113	2.38	24 (29%)
24	CLA	c	908	-	69,73,73	2.45	19 (27%)	82,113,113	2.64	24 (29%)
31	DGD	c	917	-	63,63,67	0.88	2 (3%)	77,77,81	0.80	3 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	A	614	-	69,73,73	1.97	18 (26%)	82,113,113	2.38	24 (29%)
25	PHO	A	608	-	58,69,69	2.53	12 (20%)	55,99,99	2.95	11 (20%)
24	CLA	B	612	-	69,73,73	2.11	16 (23%)	82,113,113	2.51	23 (28%)
24	CLA	c	910	-	69,73,73	2.39	19 (27%)	82,113,113	2.64	25 (30%)
24	CLA	b	609	-	69,73,73	2.34	20 (28%)	82,113,113	2.41	22 (26%)
29	LHG	d	410	-	48,48,48	0.92	2 (4%)	51,54,54	0.97	4 (7%)
24	CLA	C	503	-	69,73,73	2.47	18 (26%)	82,113,113	2.41	21 (25%)
24	CLA	d	404	-	69,73,73	2.39	21 (30%)	82,113,113	2.48	26 (31%)
24	CLA	B	614	-	69,73,73	2.26	18 (26%)	82,113,113	2.47	24 (29%)
24	CLA	b	616	-	69,73,73	2.33	15 (21%)	82,113,113	2.46	24 (29%)
29	LHG	b	620	-	48,48,48	0.89	2 (4%)	51,54,54	0.99	3 (5%)
24	CLA	A	609	-	69,73,73	2.19	16 (23%)	82,113,113	2.55	24 (29%)
32	HEM	e	101	5,6	50,50,50	2.02	11 (22%)	67,82,82	1.27	4 (5%)
24	CLA	c	905	-	69,73,73	2.52	22 (31%)	82,113,113	2.56	23 (28%)
26	BCR	T	101	-	41,41,41	3.62	15 (36%)	56,56,56	7.16	39 (69%)
31	DGD	c	916	-	63,63,67	0.86	3 (4%)	77,77,81	0.90	3 (3%)
28	SQD	A	613	-	52,54,54	0.99	2 (3%)	62,65,65	1.19	6 (9%)
24	CLA	D	403	-	69,73,73	2.37	19 (27%)	82,113,113	2.50	22 (26%)
24	CLA	b	603	-	69,73,73	2.35	20 (28%)	82,113,113	2.33	22 (26%)
24	CLA	a	408	-	69,73,73	2.17	17 (24%)	82,113,113	2.45	26 (31%)
31	DGD	H	102	-	63,63,67	0.92	3 (4%)	77,77,81	0.94	4 (5%)
32	HEM	E	101	5,6	50,50,50	1.98	10 (20%)	67,82,82	1.35	5 (7%)
24	CLA	d	403	-	69,73,73	2.11	17 (24%)	82,113,113	2.41	22 (26%)
24	CLA	B	603	-	69,73,73	2.34	19 (27%)	82,113,113	2.33	21 (25%)
24	CLA	B	606	-	69,73,73	2.31	17 (24%)	82,113,113	2.40	24 (29%)
24	CLA	C	504	-	69,73,73	2.36	19 (27%)	82,113,113	2.49	23 (28%)
24	CLA	d	401	-	69,73,73	2.30	16 (23%)	82,113,113	2.48	23 (28%)
28	SQD	l	101	-	52,54,54	0.99	3 (5%)	62,65,65	1.33	8 (12%)
29	LHG	B	621	-	48,48,48	0.89	2 (4%)	51,54,54	0.99	4 (7%)
23	BCT	a	414	21	3,3,3	1.36	1 (33%)	2,3,3	0.72	0
26	BCR	K	101	-	41,41,41	3.58	14 (34%)	56,56,56	7.86	43 (76%)
29	LHG	a	413	-	41,41,48	1.05	2 (4%)	44,47,54	0.91	2 (4%)
24	CLA	b	606	-	69,73,73	2.30	20 (28%)	82,113,113	2.47	24 (29%)
24	CLA	C	507	-	69,73,73	2.45	20 (28%)	82,113,113	2.59	26 (31%)
24	CLA	B	604	-	69,73,73	2.19	18 (26%)	82,113,113	2.54	26 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	b	617	-	69,73,73	2.29	19 (27%)	82,113,113	2.48	26 (31%)
29	LHG	d	408	-	48,48,48	0.91	2 (4%)	51,54,54	0.96	3 (5%)
26	BCR	C	514	-	41,41,41	3.68	15 (36%)	56,56,56	8.55	36 (64%)
26	BCR	B	622	-	41,41,41	3.60	15 (36%)	56,56,56	7.70	36 (64%)
24	CLA	b	612	-	69,73,73	2.22	15 (21%)	82,113,113	2.46	24 (29%)
20	OEX	A	601	1,3	0,15,15	-	-	-	-	-
24	CLA	c	902	-	69,73,73	2.30	19 (27%)	82,113,113	2.67	25 (30%)
24	CLA	C	511	3	69,73,73	2.46	18 (26%)	82,113,113	2.60	23 (28%)
24	CLA	A	607	-	69,73,73	2.28	18 (26%)	82,113,113	2.56	25 (30%)
26	BCR	T	102	-	41,41,41	3.52	15 (36%)	56,56,56	7.29	38 (67%)
26	BCR	c	918	-	41,41,41	3.44	15 (36%)	56,56,56	7.70	36 (64%)
24	CLA	C	501	-	69,73,73	2.28	18 (26%)	82,113,113	2.53	23 (28%)
31	DGD	D	406	-	63,63,67	1.00	4 (6%)	77,77,81	1.03	6 (7%)
24	CLA	c	906	-	69,73,73	2.27	19 (27%)	82,113,113	2.45	22 (26%)
29	LHG	D	408	-	48,48,48	0.90	3 (6%)	51,54,54	0.85	2 (3%)
26	BCR	h	101	-	41,41,41	3.61	14 (34%)	56,56,56	8.48	42 (75%)
24	CLA	C	509	-	69,73,73	2.44	19 (27%)	82,113,113	2.60	27 (32%)
24	CLA	b	602	-	69,73,73	2.54	20 (28%)	82,113,113	2.49	26 (31%)
25	PHO	d	402	-	58,69,69	2.51	13 (22%)	55,99,99	2.81	13 (23%)
23	BCT	A	605	21	3,3,3	1.46	1 (33%)	2,3,3	0.26	0
24	CLA	b	611	-	69,73,73	2.35	18 (26%)	82,113,113	2.49	22 (26%)
24	CLA	b	608	-	69,73,73	2.38	17 (24%)	82,113,113	2.35	24 (29%)
31	DGD	j	101	-	63,63,67	0.88	3 (4%)	77,77,81	0.87	3 (3%)
24	CLA	B	613	-	69,73,73	2.35	19 (27%)	82,113,113	2.44	21 (25%)
24	CLA	C	510	-	69,73,73	2.31	20 (28%)	82,113,113	2.53	26 (31%)
27	PL9	d	405	-	55,55,55	0.82	2 (3%)	68,69,69	1.30	8 (11%)
24	CLA	C	506	-	69,73,73	2.33	20 (28%)	82,113,113	2.48	24 (29%)
31	DGD	C	517	-	63,63,67	0.89	2 (3%)	77,77,81	0.86	4 (5%)
28	SQD	a	411	-	52,54,54	0.93	2 (3%)	62,65,65	1.53	10 (16%)
26	BCR	a	409	-	41,41,41	3.48	14 (34%)	56,56,56	7.87	34 (60%)
24	CLA	B	616	-	69,73,73	2.44	20 (28%)	82,113,113	2.50	21 (25%)
20	OEX	a	401	1,3	0,15,15	-	-	-	-	-
29	LHG	d	409	-	48,48,48	0.85	2 (4%)	51,54,54	0.92	3 (5%)
24	CLA	c	912	3	69,73,73	2.57	20 (28%)	82,113,113	2.52	23 (28%)
24	CLA	c	914	-	69,73,73	2.75	21 (30%)	82,113,113	2.37	25 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	LHG	D	409	-	48,48,48	0.95	2 (4%)	51,54,54	0.91	3 (5%)
28	SQD	A	612	-	52,54,54	0.92	2 (3%)	62,65,65	1.49	11 (17%)
24	CLA	c	903	-	69,73,73	2.29	17 (24%)	82,113,113	2.59	22 (26%)
26	BCR	Y	101	-	41,41,41	3.65	14 (34%)	56,56,56	8.11	36 (64%)
24	CLA	B	615	-	69,73,73	2.23	19 (27%)	82,113,113	2.51	27 (32%)

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
24	CLA	B	605	-	1/1/15/20	4/39/115/115	-
26	BCR	B	618	-	-	5/29/63/63	0/2/2/2
26	BCR	D	404	-	-	6/29/63/63	0/2/2/2
32	HEM	V	202	16	-	6/14/54/54	-
24	CLA	c	909	-	-	4/39/115/115	-
24	CLA	b	607	-	1/1/15/20	10/39/115/115	-
28	SQD	a	402	-	-	21/49/69/69	0/1/1/1
24	CLA	C	502	-	-	7/39/115/115	-
24	CLA	c	907	-	1/1/15/20	11/39/115/115	-
26	BCR	k	102	-	-	10/29/63/63	0/2/2/2
28	SQD	d	407	-	-	21/38/58/69	0/1/1/1
24	CLA	c	911	-	1/1/15/20	6/39/115/115	-
26	BCR	b	619	-	-	2/29/63/63	0/2/2/2
25	PHO	a	412	-	-	2/37/103/103	0/5/6/6
26	BCR	k	101	-	-	8/29/63/63	0/2/2/2
24	CLA	a	406	-	1/1/15/20	2/39/115/115	-
32	HEM	v	202	16	-	6/14/54/54	-
24	CLA	B	611	-	1/1/15/20	7/39/115/115	-
24	CLA	B	609	-	-	1/39/115/115	-
31	DGD	C	516	-	-	24/51/91/95	0/2/2/2
26	BCR	f	101	-	-	7/29/63/63	0/2/2/2
24	CLA	b	605	-	1/1/15/20	5/39/115/115	-
27	PL9	D	405	-	-	1/53/73/73	0/1/1/1
31	DGD	C	518	-	-	16/51/91/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	PL9	a	410	-	-	10/53/73/73	0/1/1/1
24	CLA	a	407	-	-	11/39/115/115	-
26	BCR	B	619	-	-	4/29/63/63	0/2/2/2
26	BCR	C	515	-	-	4/29/63/63	0/2/2/2
28	SQD	L	101	-	-	29/49/69/69	0/1/1/1
29	LHG	D	407	-	-	13/53/53/53	-
24	CLA	b	613	-	1/1/15/20	5/39/115/115	-
24	CLA	c	913	-	1/1/15/20	13/39/115/115	-
25	PHO	D	401	-	-	4/37/103/103	0/5/6/6
24	CLA	b	615	-	1/1/15/20	17/39/115/115	-
24	CLA	b	610	-	-	2/39/115/115	-
24	CLA	C	508	-	-	5/39/115/115	-
26	BCR	B	620	-	-	1/29/63/63	0/2/2/2
24	CLA	C	505	-	1/1/15/20	2/39/115/115	-
24	CLA	B	607	-	-	7/39/115/115	-
27	PL9	A	611	-	-	9/53/73/73	0/1/1/1
24	CLA	b	604	-	1/1/15/20	6/39/115/115	-
31	DGD	d	406	-	-	33/51/91/95	0/2/2/2
24	CLA	B	602	-	1/1/15/20	18/39/115/115	-
24	CLA	B	617	-	1/1/15/20	15/39/115/115	-
24	CLA	D	402	-	1/1/15/20	5/39/115/115	-
26	BCR	H	101	-	-	8/29/63/63	0/2/2/2
24	CLA	C	512	-	1/1/15/20	9/39/115/115	-
26	BCR	c	915	-	-	8/29/63/63	0/2/2/2
24	CLA	B	610	-	1/1/15/20	0/39/115/115	-
26	BCR	A	610	-	-	4/29/63/63	0/2/2/2
26	BCR	b	618	-	-	3/29/63/63	0/2/2/2
24	CLA	c	904	-	-	3/39/115/115	-
29	LHG	A	615	-	-	24/46/46/53	-
24	CLA	b	614	-	1/1/15/20	6/39/115/115	-
24	CLA	B	608	-	1/1/15/20	2/39/115/115	-
24	CLA	C	513	-	-	9/39/115/115	-
31	DGD	h	102	-	-	13/51/91/95	0/2/2/2
28	SQD	F	101	-	-	17/38/58/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	A	606	-	1/1/15/20	3/39/115/115	-
24	CLA	c	908	-	1/1/15/20	10/39/115/115	-
31	DGD	c	917	-	-	18/51/91/95	0/2/2/2
24	CLA	A	614	-	-	2/39/115/115	-
25	PHO	A	608	-	-	2/37/103/103	0/5/6/6
24	CLA	B	612	-	-	3/39/115/115	-
24	CLA	c	910	-	1/1/15/20	9/39/115/115	-
24	CLA	b	609	-	-	1/39/115/115	-
29	LHG	d	410	-	-	17/53/53/53	-
24	CLA	C	503	-	1/1/15/20	1/39/115/115	-
24	CLA	d	404	-	-	7/39/115/115	-
24	CLA	B	614	-	1/1/15/20	3/39/115/115	-
24	CLA	b	616	-	1/1/15/20	11/39/115/115	-
29	LHG	b	620	-	-	17/53/53/53	-
24	CLA	A	609	-	-	13/39/115/115	-
32	HEM	e	101	5,6	-	4/14/54/54	-
24	CLA	c	905	-	-	9/39/115/115	-
26	BCR	T	101	-	-	1/29/63/63	0/2/2/2
31	DGD	c	916	-	-	20/51/91/95	0/2/2/2
28	SQD	A	613	-	-	23/49/69/69	0/1/1/1
24	CLA	b	603	-	1/1/15/20	2/39/115/115	-
24	CLA	D	403	-	-	14/39/115/115	-
24	CLA	a	408	-	-	11/39/115/115	-
31	DGD	H	102	-	-	15/51/91/95	0/2/2/2
32	HEM	E	101	5,6	-	4/14/54/54	-
24	CLA	d	403	-	1/1/15/20	5/39/115/115	-
24	CLA	B	603	-	1/1/15/20	0/39/115/115	-
24	CLA	B	606	-	1/1/15/20	5/39/115/115	-
24	CLA	C	504	-	1/1/15/20	9/39/115/115	-
24	CLA	d	401	-	-	2/39/115/115	-
28	SQD	l	101	-	-	28/49/69/69	0/1/1/1
29	LHG	B	621	-	-	17/53/53/53	-
29	LHG	a	413	-	-	25/46/46/53	-
26	BCR	K	101	-	-	11/29/63/63	0/2/2/2
24	CLA	b	606	-	1/1/15/20	4/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	C	507	-	1/1/15/20	11/39/115/115	-
24	CLA	B	604	-	1/1/15/20	5/39/115/115	-
24	CLA	b	617	-	1/1/15/20	12/39/115/115	-
29	LHG	d	408	-	-	11/53/53/53	-
26	BCR	C	514	-	-	5/29/63/63	0/2/2/2
26	BCR	B	622	-	-	4/29/63/63	0/2/2/2
24	CLA	b	612	-	-	4/39/115/115	-
24	CLA	c	902	-	1/1/15/20	3/39/115/115	-
24	CLA	C	511	3	-	0/39/115/115	-
24	CLA	A	607	-	-	7/39/115/115	-
26	BCR	T	102	-	-	3/29/63/63	0/2/2/2
26	BCR	c	918	-	-	13/29/63/63	0/2/2/2
24	CLA	C	501	-	-	9/39/115/115	-
31	DGD	D	406	-	-	33/51/91/95	0/2/2/2
24	CLA	c	906	-	1/1/15/20	4/39/115/115	-
29	LHG	D	408	-	-	13/53/53/53	-
26	BCR	h	101	-	-	9/29/63/63	0/2/2/2
24	CLA	C	509	-	1/1/15/20	8/39/115/115	-
24	CLA	b	602	-	1/1/15/20	18/39/115/115	-
25	PHO	d	402	-	-	1/37/103/103	0/5/6/6
24	CLA	b	611	-	1/1/15/20	4/39/115/115	-
24	CLA	b	608	-	1/1/15/20	1/39/115/115	-
31	DGD	j	101	-	-	18/51/91/95	0/2/2/2
24	CLA	B	613	-	1/1/15/20	3/39/115/115	-
24	CLA	C	510	-	1/1/15/20	6/39/115/115	-
27	PL9	d	405	-	-	3/53/73/73	0/1/1/1
24	CLA	C	506	-	1/1/15/20	14/39/115/115	-
31	DGD	C	517	-	-	24/51/91/95	0/2/2/2
28	SQD	a	411	-	-	23/49/69/69	0/1/1/1
26	BCR	a	409	-	-	2/29/63/63	0/2/2/2
24	CLA	B	616	-	1/1/15/20	11/39/115/115	-
29	LHG	d	409	-	-	10/53/53/53	-
24	CLA	c	912	3	-	7/39/115/115	-
24	CLA	c	914	-	-	15/39/115/115	-
29	LHG	D	409	-	-	12/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	SQD	A	612	-	-	17/49/69/69	0/1/1/1
24	CLA	c	903	-	-	4/39/115/115	-
26	BCR	Y	101	-	-	2/29/63/63	0/2/2/2
24	CLA	B	615	-	1/1/15/20	10/39/115/115	-

The worst 5 of 1773 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	512	CLA	MG-NA	14.06	2.39	2.06
24	c	914	CLA	MG-NC	12.56	2.36	2.06
24	b	613	CLA	MG-NA	12.54	2.36	2.06
24	c	913	CLA	MG-NA	12.23	2.35	2.06
24	B	605	CLA	MG-NA	12.05	2.34	2.06

The worst 5 of 2793 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b	619	BCR	C20-C21-C22	30.76	170.41	127.28
26	H	101	BCR	C20-C21-C22	27.39	165.69	127.28
26	c	915	BCR	C20-C21-C22	27.33	165.60	127.28
26	k	101	BCR	C16-C17-C18	27.12	165.32	127.28
26	h	101	BCR	C20-C21-C22	27.12	165.32	127.28

5 of 45 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	A	606	CLA	ND
24	B	602	CLA	ND
24	B	603	CLA	ND
24	B	604	CLA	ND
24	B	605	CLA	ND

5 of 1196 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	B	602	CLA	CAD-CBD-CGD-O2D
24	B	615	CLA	CAD-CBD-CGD-O1D
24	B	615	CLA	CAD-CBD-CGD-O2D
24	B	617	CLA	CHA-CBD-CGD-O1D
24	C	502	CLA	CAD-CBD-CGD-O1D

There are no ring outliers.

110 monomers are involved in 277 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	B	605	CLA	2	0
26	B	618	BCR	1	0
26	D	404	BCR	2	0
32	V	202	HEM	9	0
24	c	909	CLA	8	0
24	b	607	CLA	4	0
28	a	402	SQD	3	0
24	C	502	CLA	3	0
24	c	907	CLA	3	0
26	k	102	BCR	2	0
28	d	407	SQD	1	0
24	c	911	CLA	9	0
26	b	619	BCR	3	0
25	a	412	PHO	3	0
26	k	101	BCR	3	0
24	a	406	CLA	2	0
32	v	202	HEM	8	0
24	B	611	CLA	4	0
24	B	609	CLA	2	0
31	C	516	DGD	2	0
24	b	605	CLA	1	0
27	D	405	PL9	1	0
31	C	518	DGD	3	0
27	a	410	PL9	8	0
24	a	407	CLA	3	0
26	B	619	BCR	2	0
28	L	101	SQD	5	0
29	D	407	LHG	3	0
24	b	613	CLA	1	0
24	c	913	CLA	5	0
25	D	401	PHO	4	0
24	b	615	CLA	1	0
24	C	508	CLA	9	0
26	B	620	BCR	1	0
24	B	607	CLA	1	0
24	C	505	CLA	3	0
27	A	611	PL9	9	0
24	b	604	CLA	2	0
31	d	406	DGD	2	0
24	B	617	CLA	4	0

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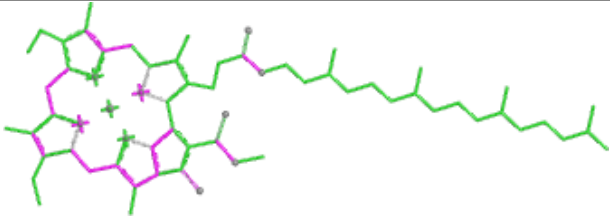
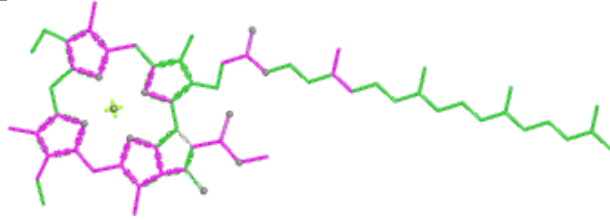
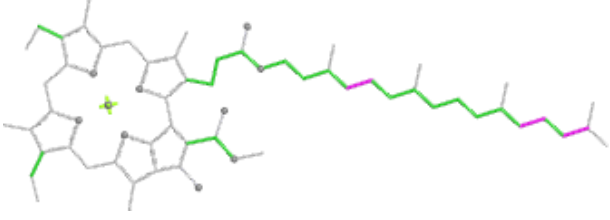
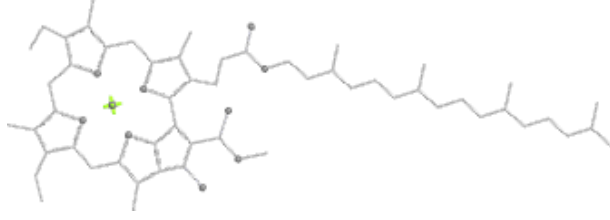
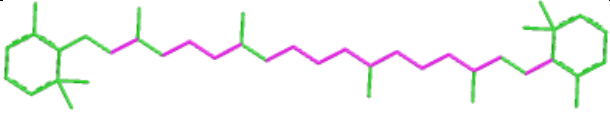
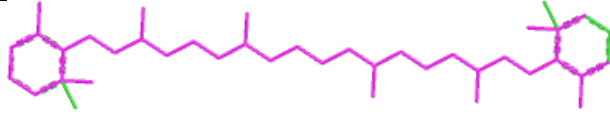
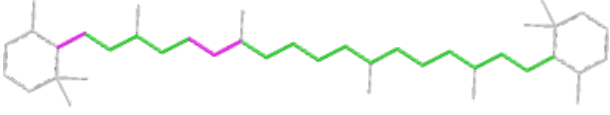
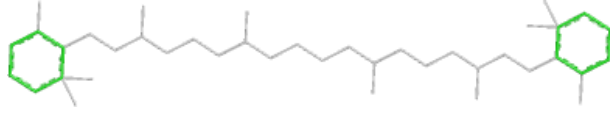
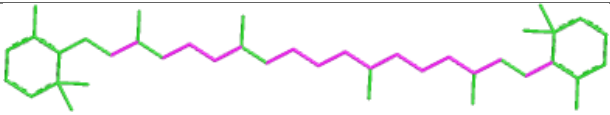
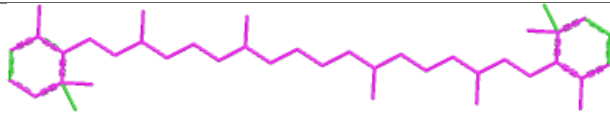
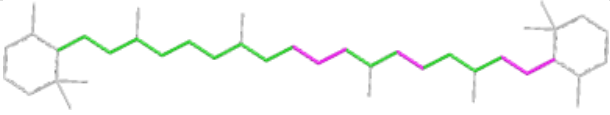
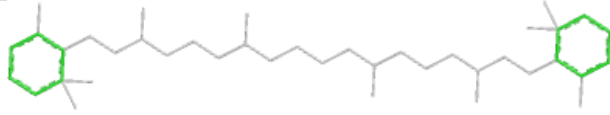
Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	H	101	BCR	1	0
24	C	512	CLA	2	0
26	c	915	BCR	2	0
24	B	610	CLA	1	0
26	b	618	BCR	2	0
24	c	904	CLA	2	0
29	A	615	LHG	3	0
24	b	614	CLA	3	0
31	h	102	DGD	1	0
24	A	606	CLA	4	0
24	c	908	CLA	1	0
24	A	614	CLA	3	0
25	A	608	PHO	2	0
24	B	612	CLA	3	0
24	c	910	CLA	2	0
29	d	410	LHG	23	0
24	C	503	CLA	2	0
24	d	404	CLA	5	0
24	B	614	CLA	2	0
24	b	616	CLA	3	0
29	b	620	LHG	6	0
24	A	609	CLA	3	0
24	c	905	CLA	5	0
26	T	101	BCR	2	0
28	A	613	SQD	1	0
24	D	403	CLA	1	0
24	a	408	CLA	2	0
31	H	102	DGD	2	0
24	d	403	CLA	4	0
24	B	603	CLA	2	0
24	B	606	CLA	4	0
24	C	504	CLA	6	0
24	d	401	CLA	4	0
28	l	101	SQD	7	0
29	B	621	LHG	3	0
26	K	101	BCR	1	0
29	a	413	LHG	5	0
24	b	606	CLA	3	0
24	C	507	CLA	2	0
24	B	604	CLA	2	0
24	b	617	CLA	3	0
29	d	408	LHG	2	0

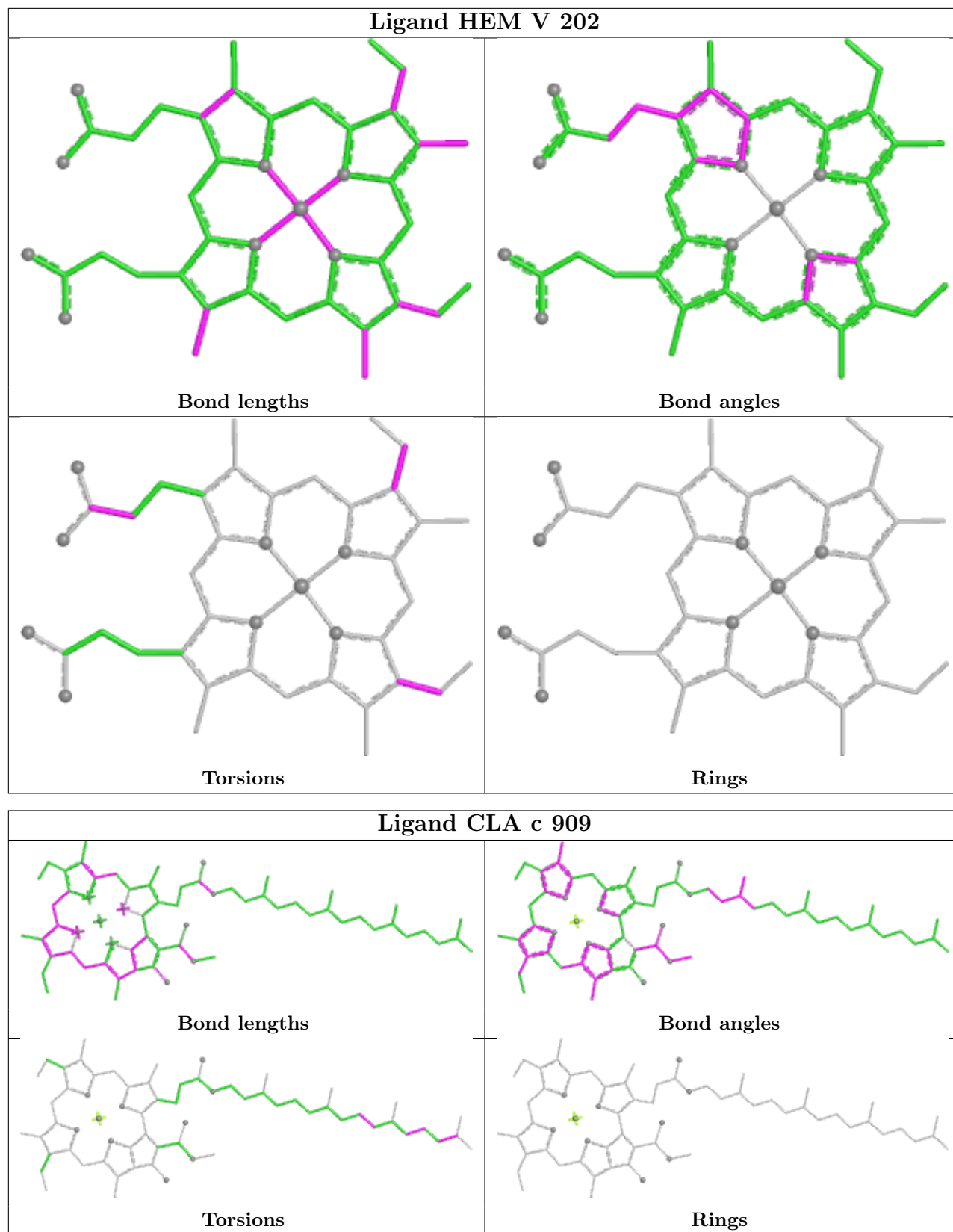
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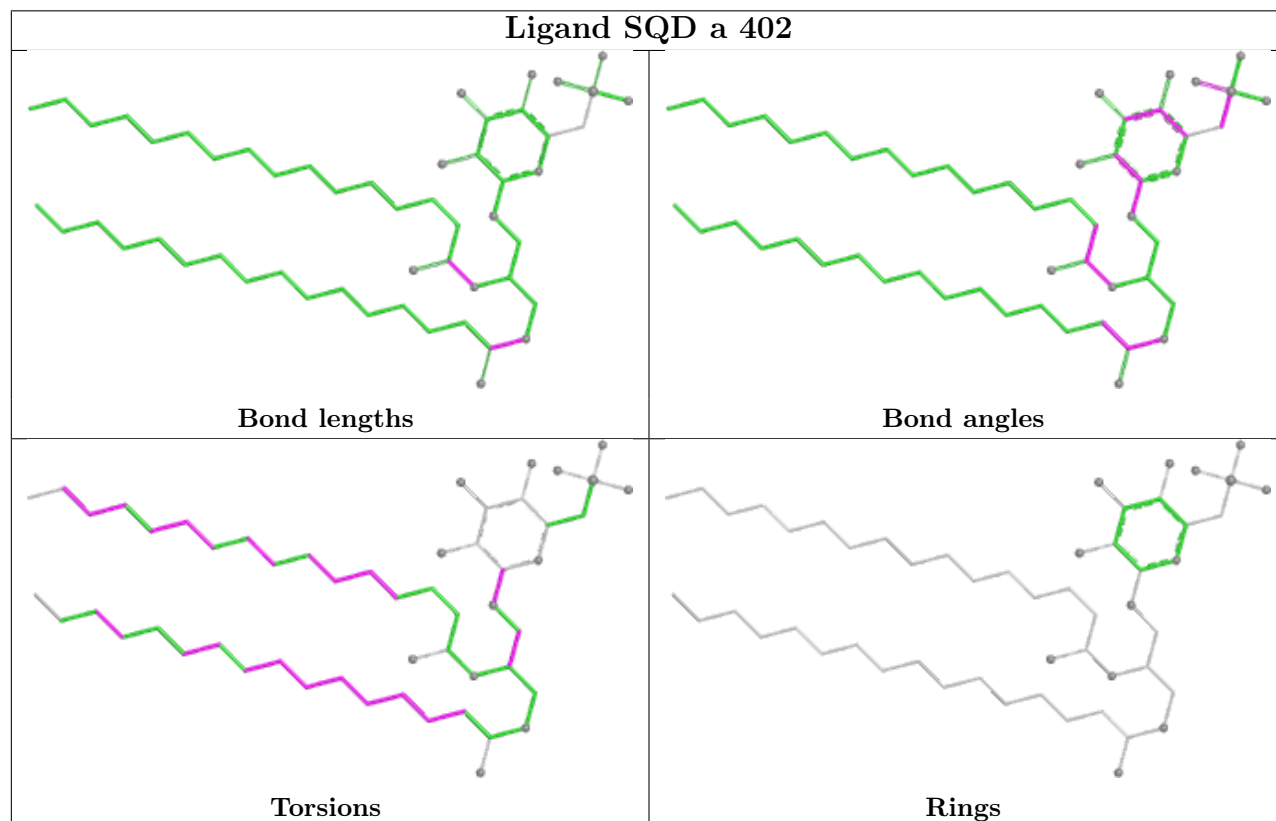
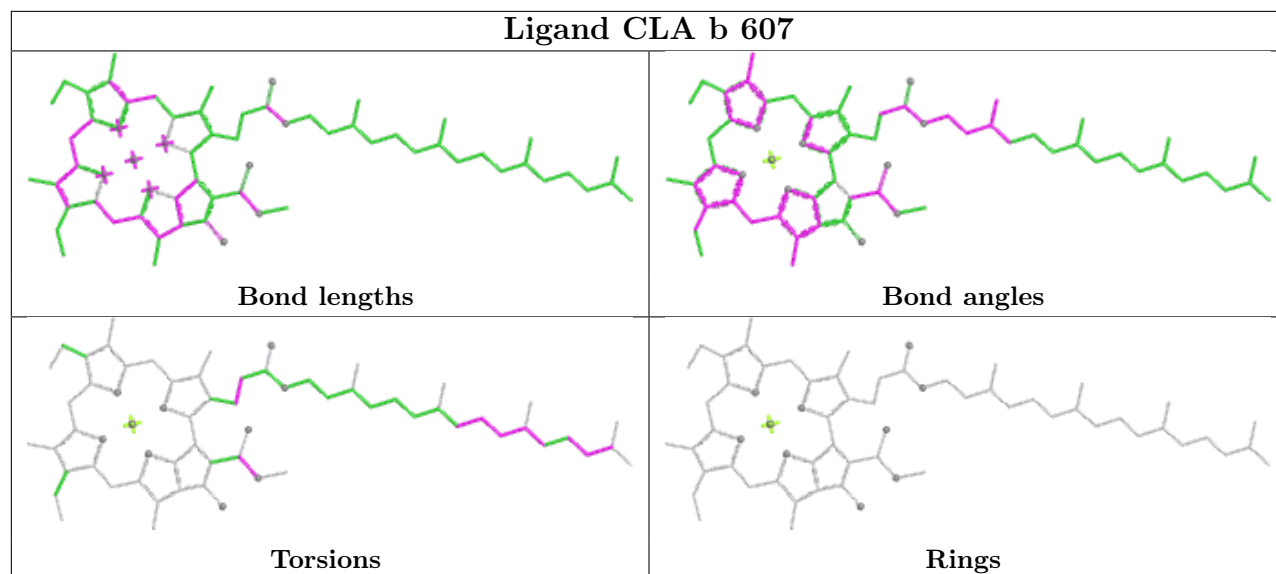
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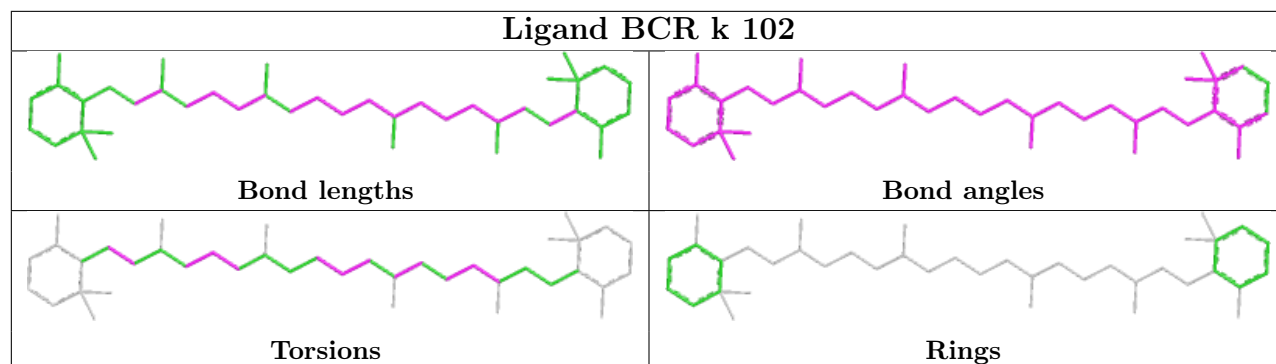
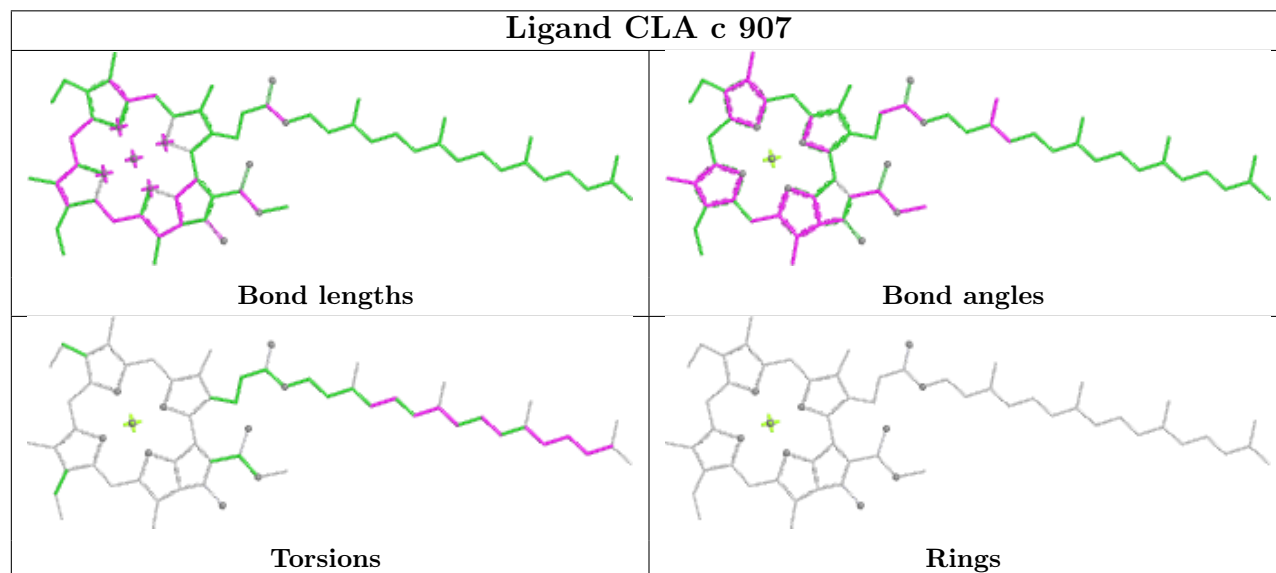
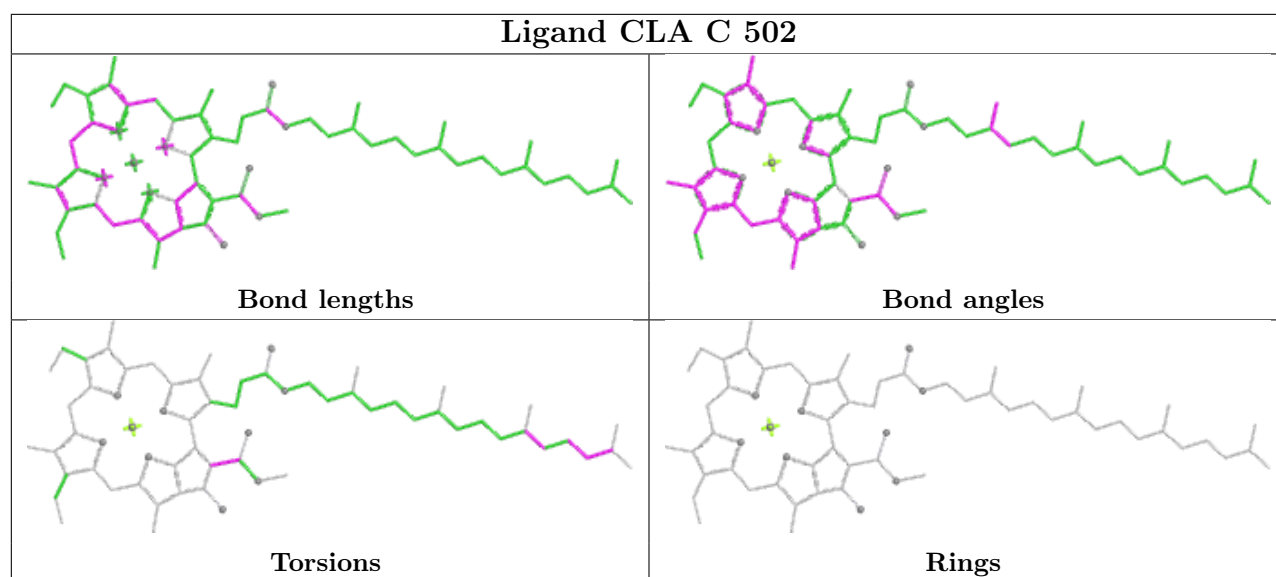
Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	B	622	BCR	3	0
24	b	612	CLA	3	0
24	c	902	CLA	2	0
24	C	511	CLA	1	0
26	c	918	BCR	1	0
24	C	501	CLA	2	0
31	D	406	DGD	3	0
24	c	906	CLA	7	0
26	h	101	BCR	1	0
24	C	509	CLA	3	0
25	d	402	PHO	1	0
24	b	611	CLA	2	0
31	j	101	DGD	2	0
24	B	613	CLA	1	0
24	C	510	CLA	4	0
27	d	405	PL9	1	0
24	C	506	CLA	3	0
31	C	517	DGD	1	0
28	a	411	SQD	4	0
26	a	409	BCR	1	0
24	B	616	CLA	3	0
29	d	409	LHG	1	0
24	c	912	CLA	2	0
24	c	914	CLA	2	0
29	D	409	LHG	22	0
28	A	612	SQD	5	0
24	c	903	CLA	3	0
26	Y	101	BCR	1	0

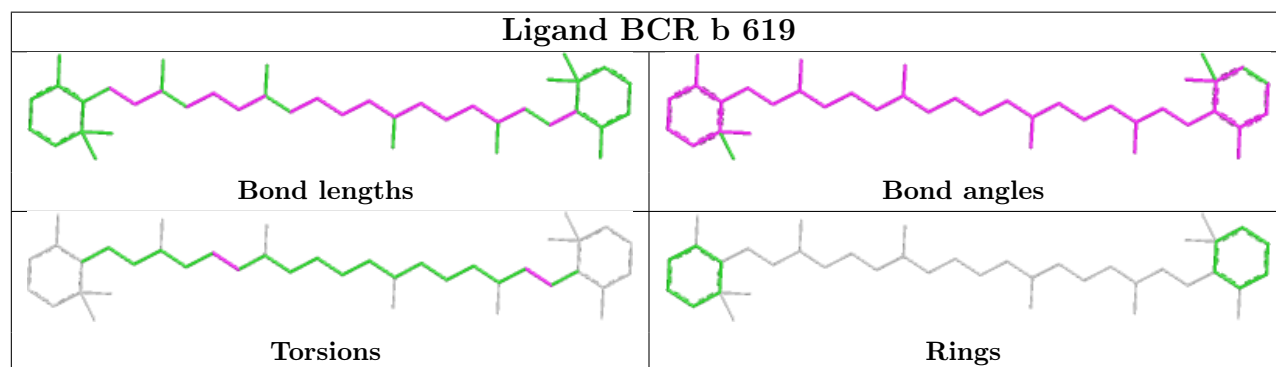
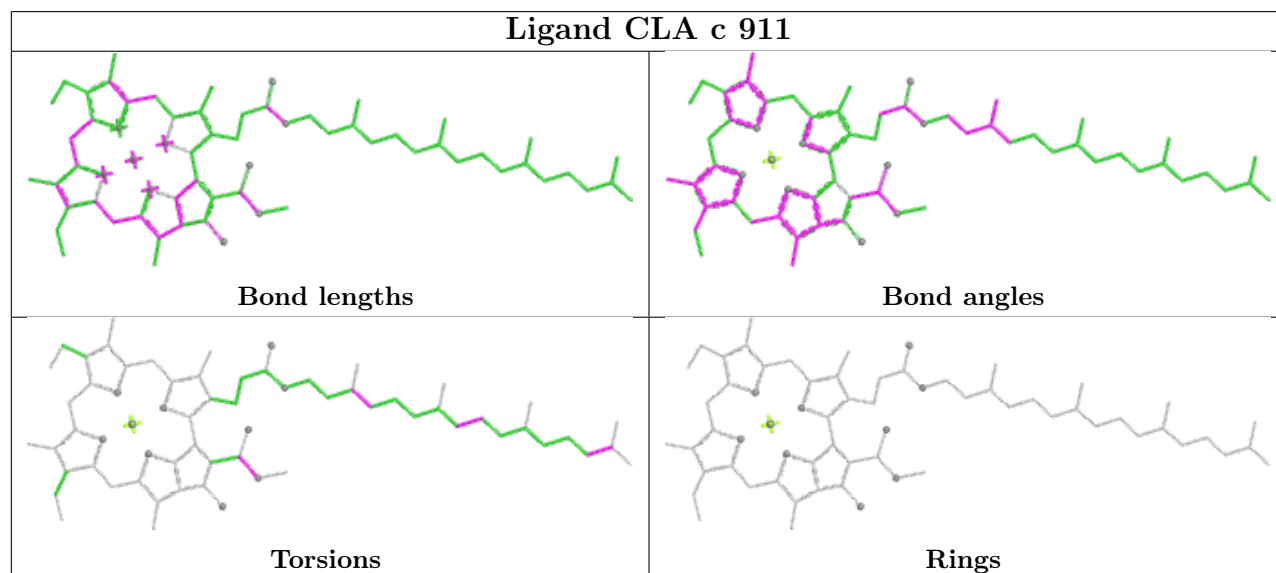
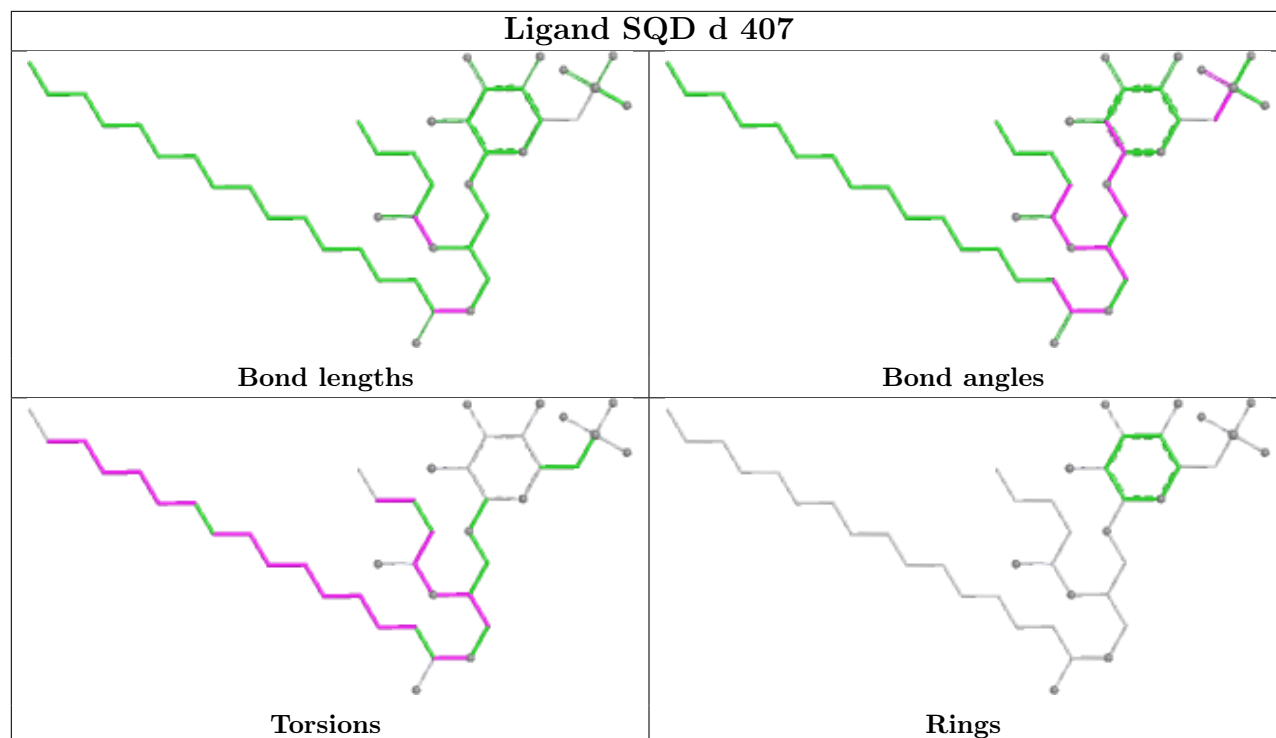
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

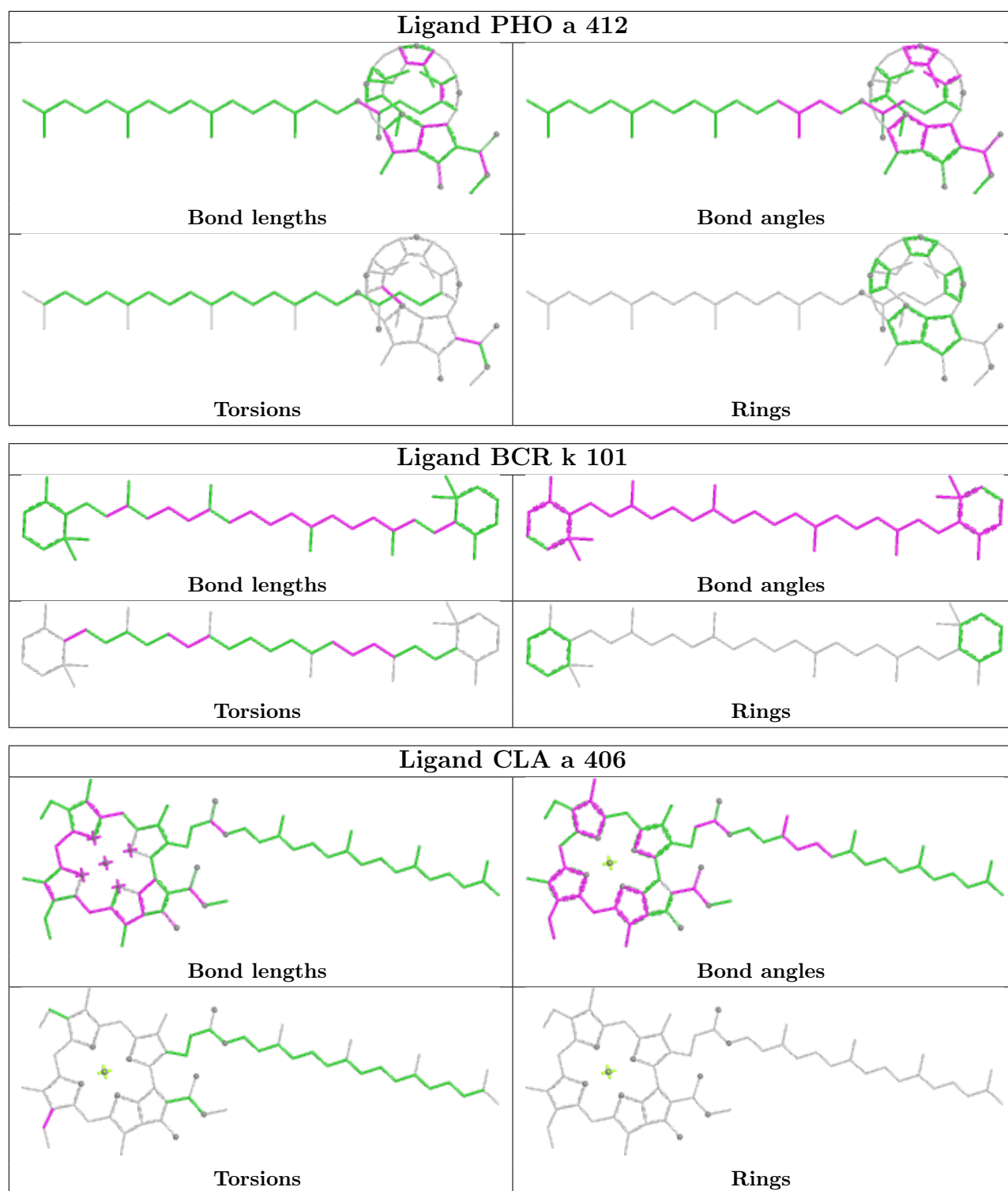
Ligand CLA B 605	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR B 618	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR D 404	
 Bond lengths	 Bond angles
 Torsions	 Rings



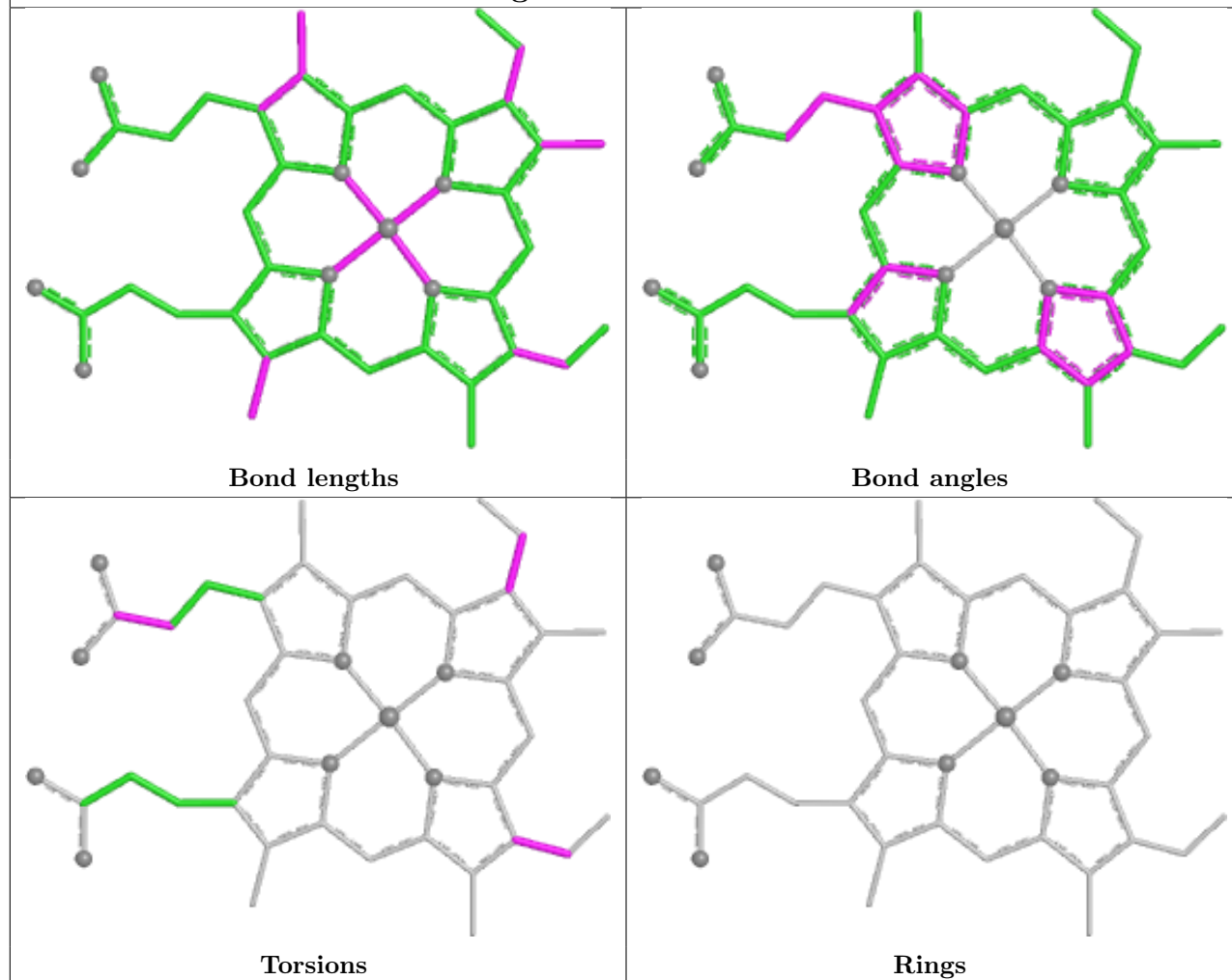




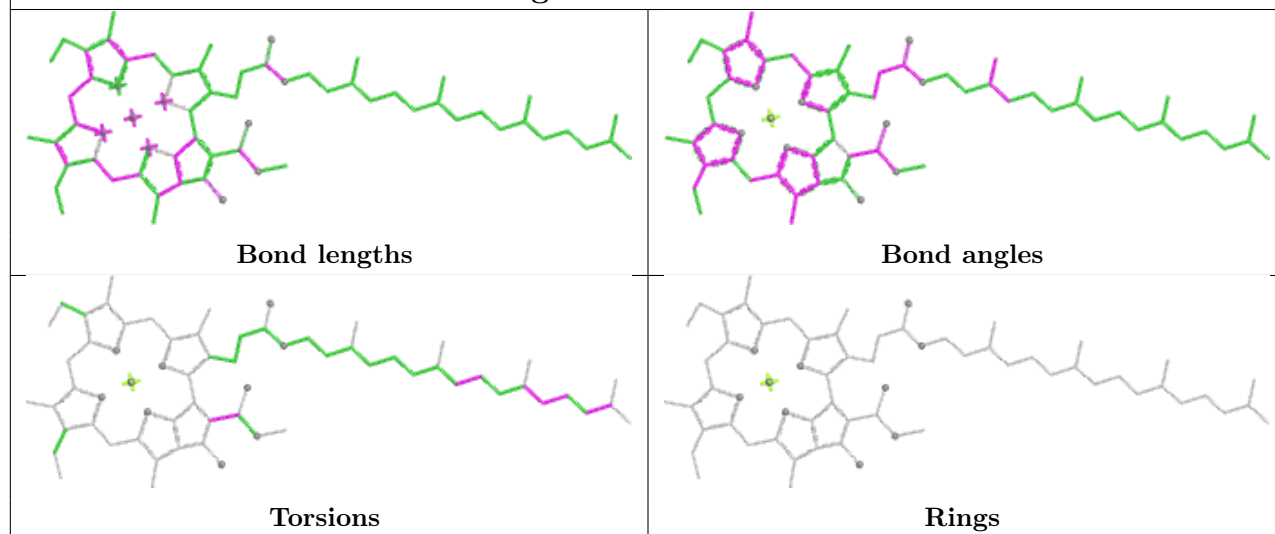


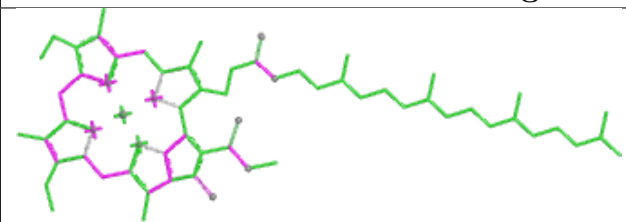
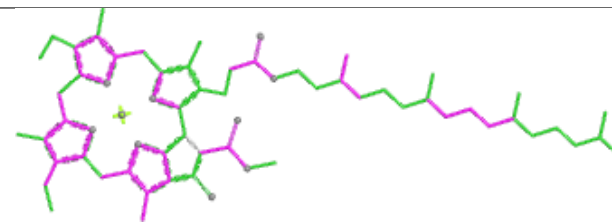
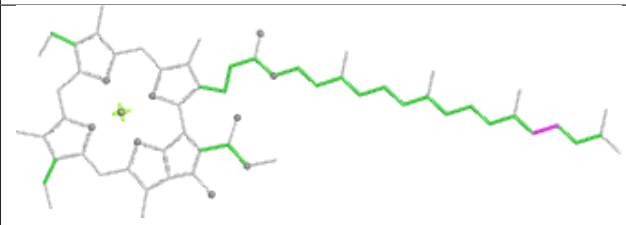
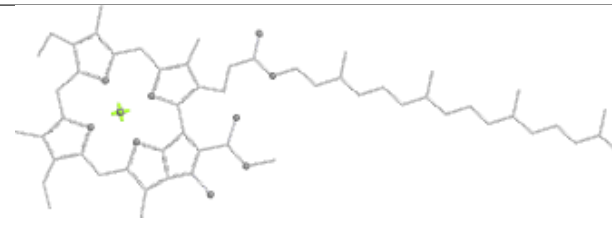


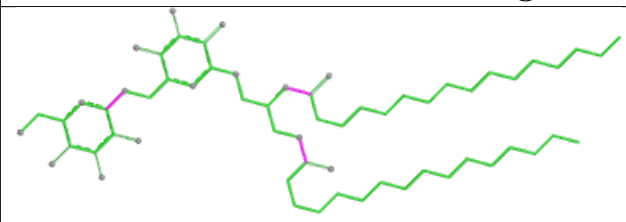
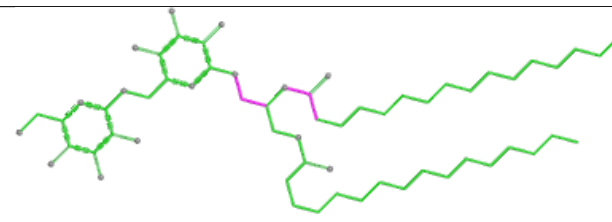
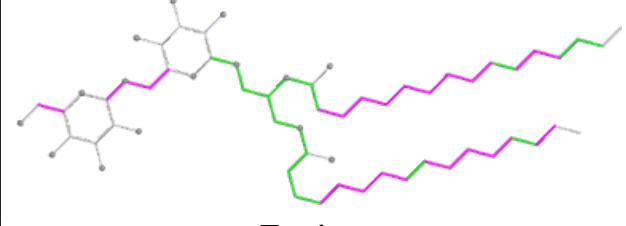
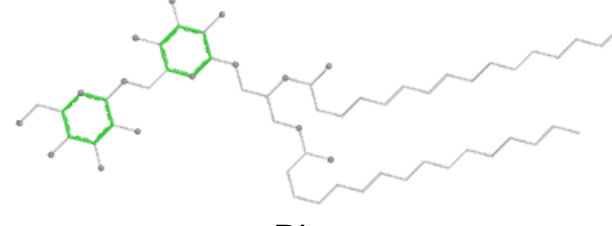
Ligand HEM v 202

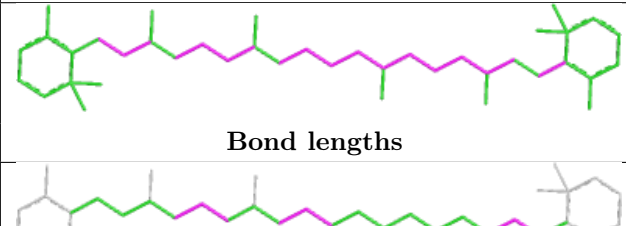
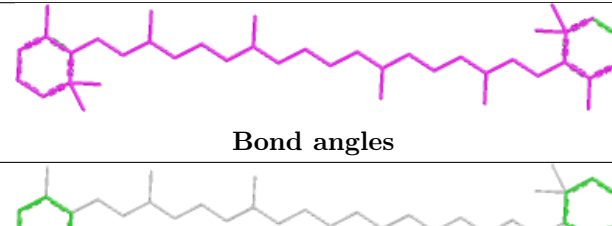
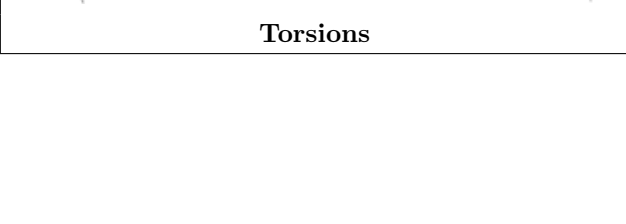
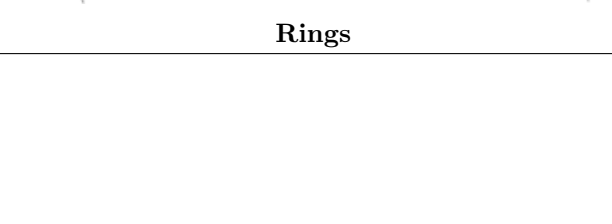


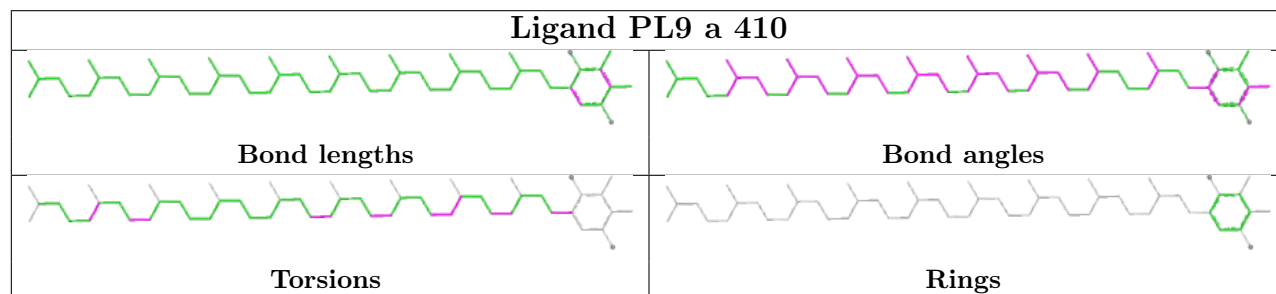
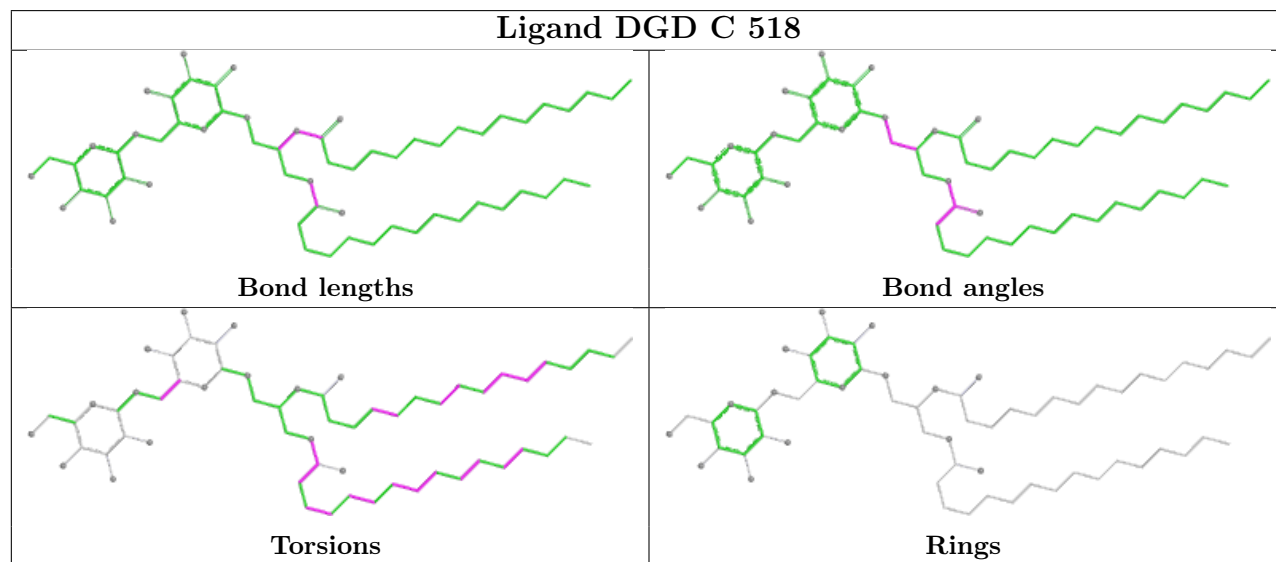
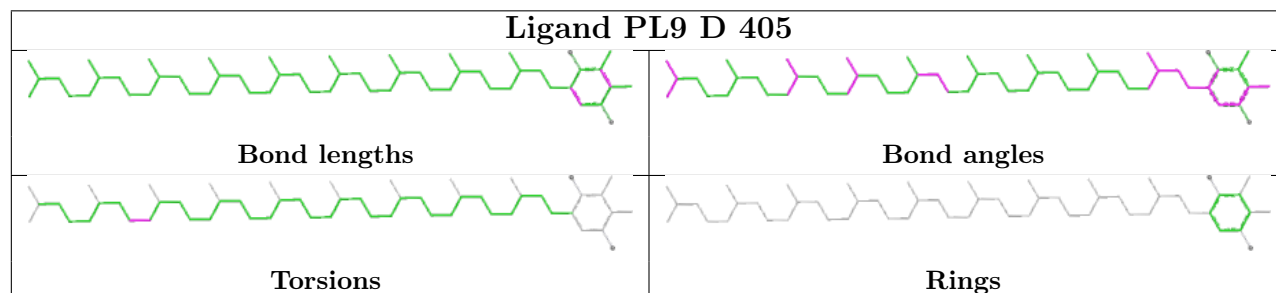
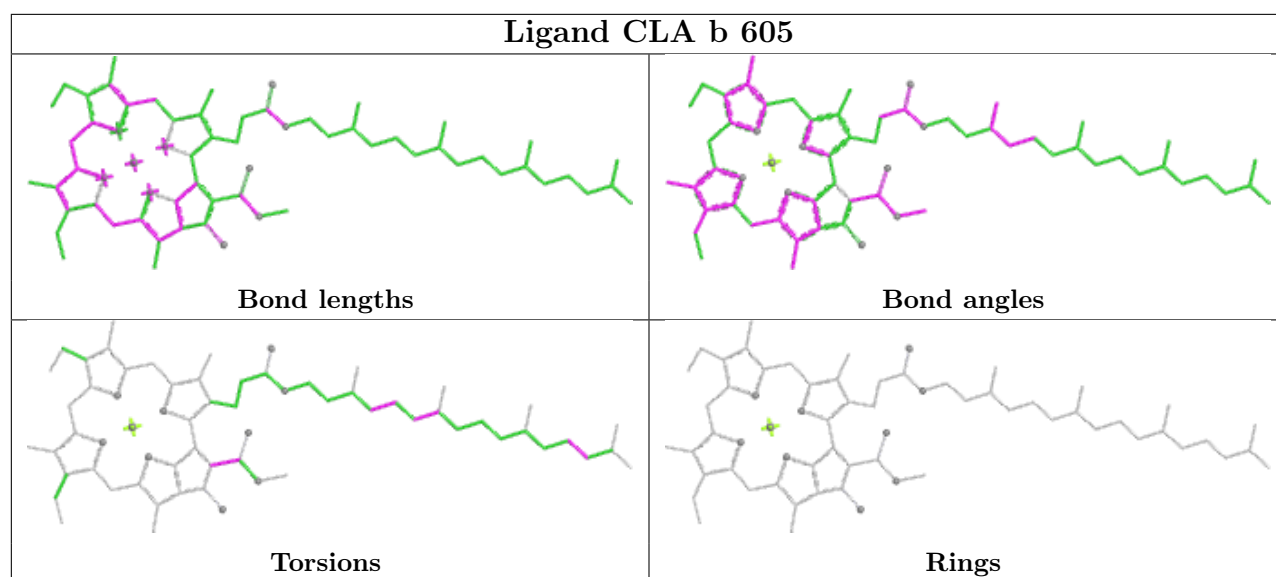
Ligand CLA B 611

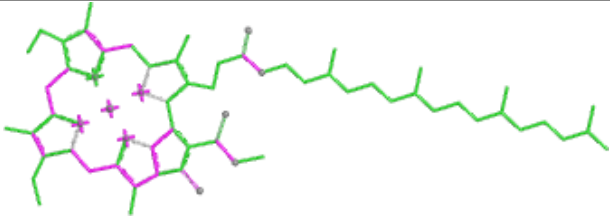
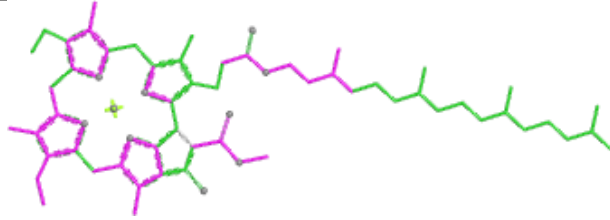
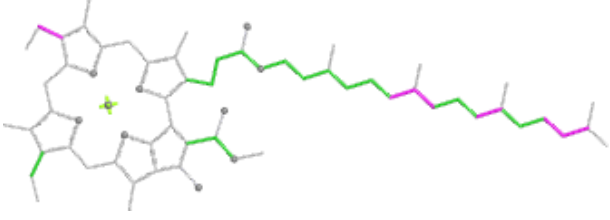
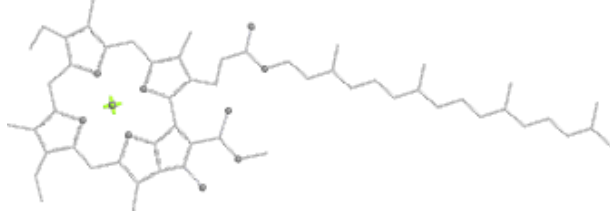
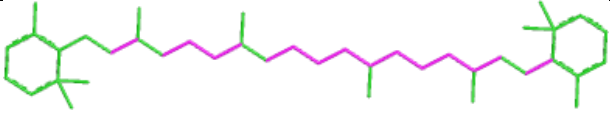
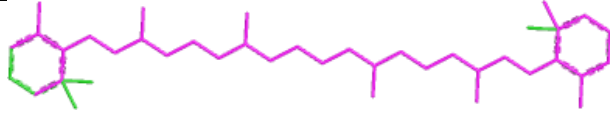
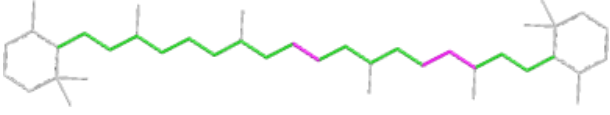
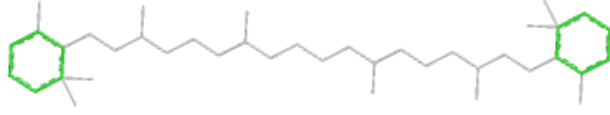
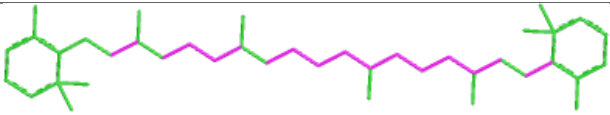
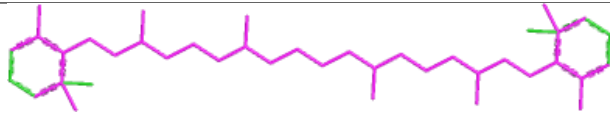
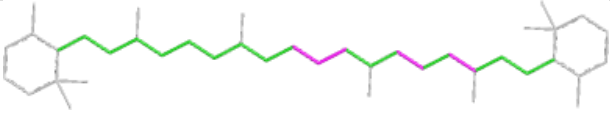
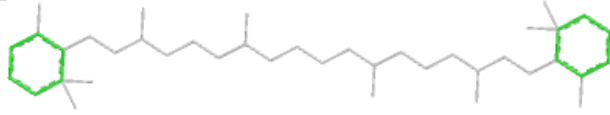


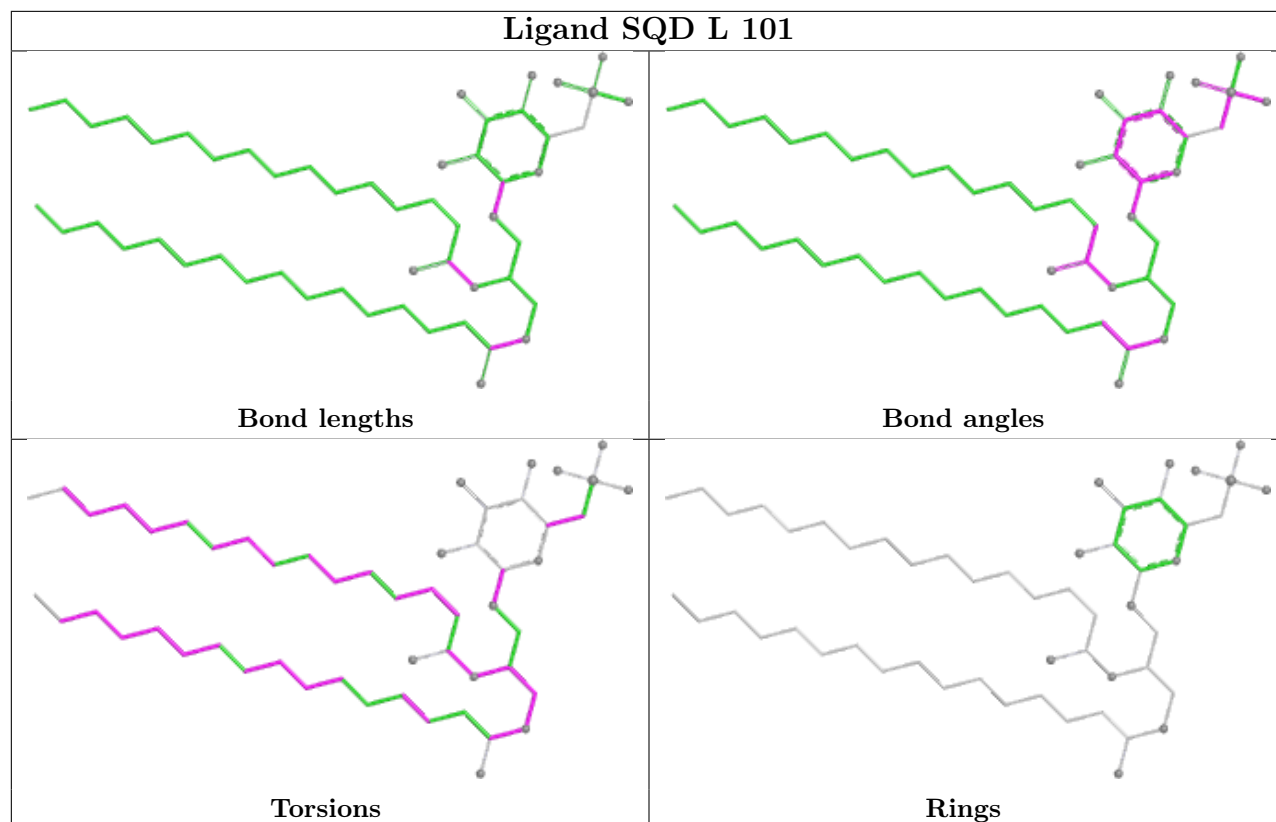
Ligand CLA B 609	
	
Bond lengths	Bond angles
	
Torsions	Rings

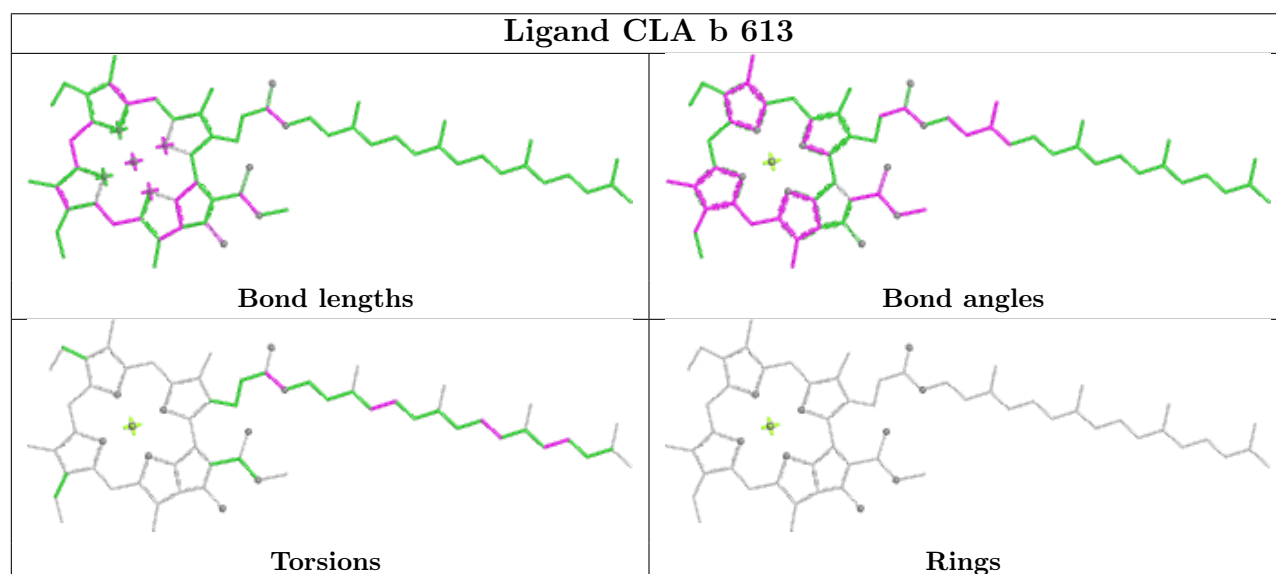
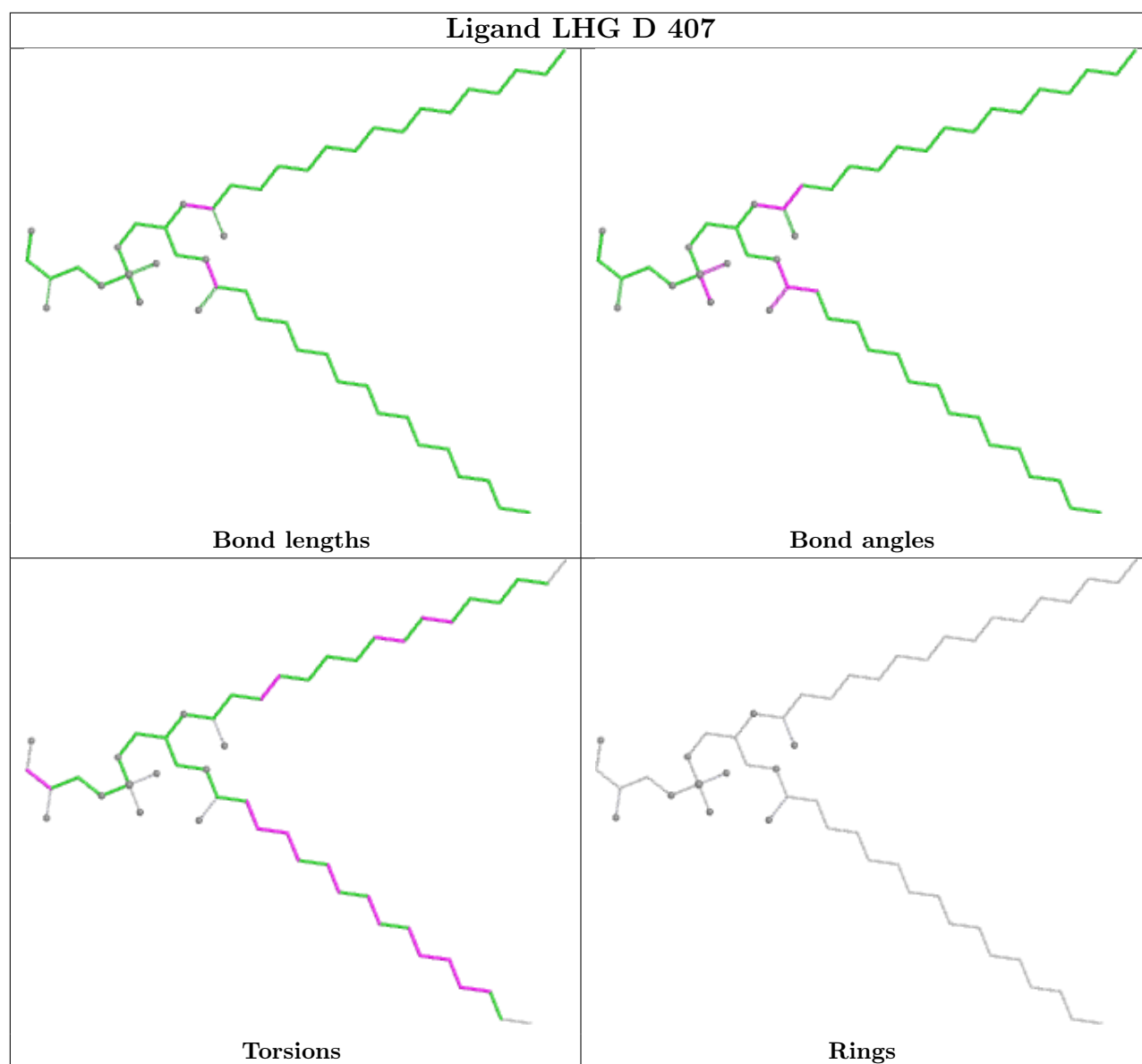
Ligand DGD C 516	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR f 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

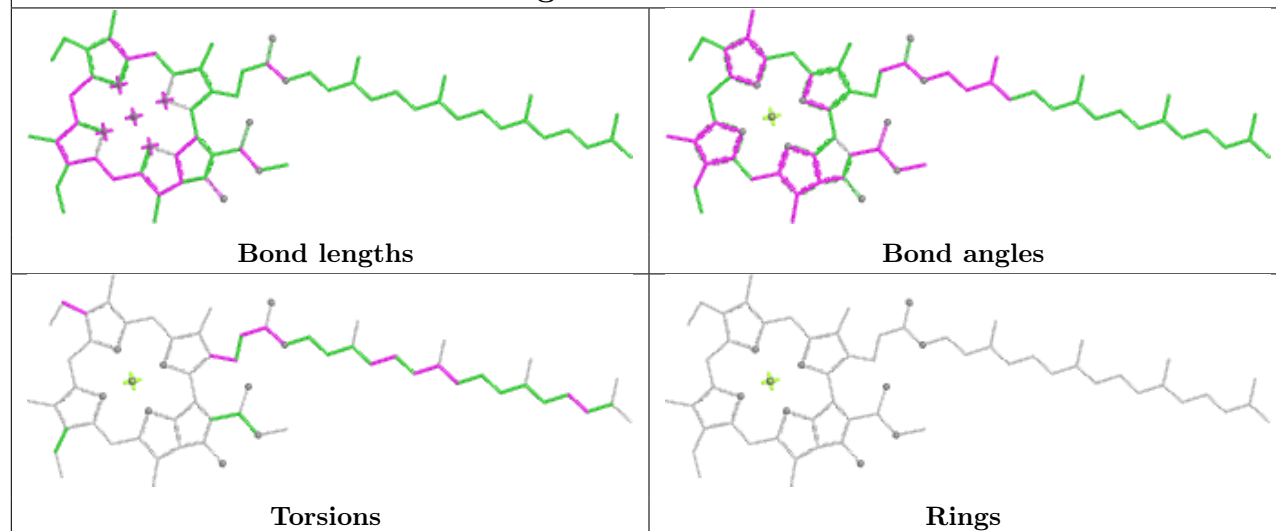


Ligand CLA a 407	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR B 619	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR C 515	
 Bond lengths	 Bond angles
 Torsions	 Rings

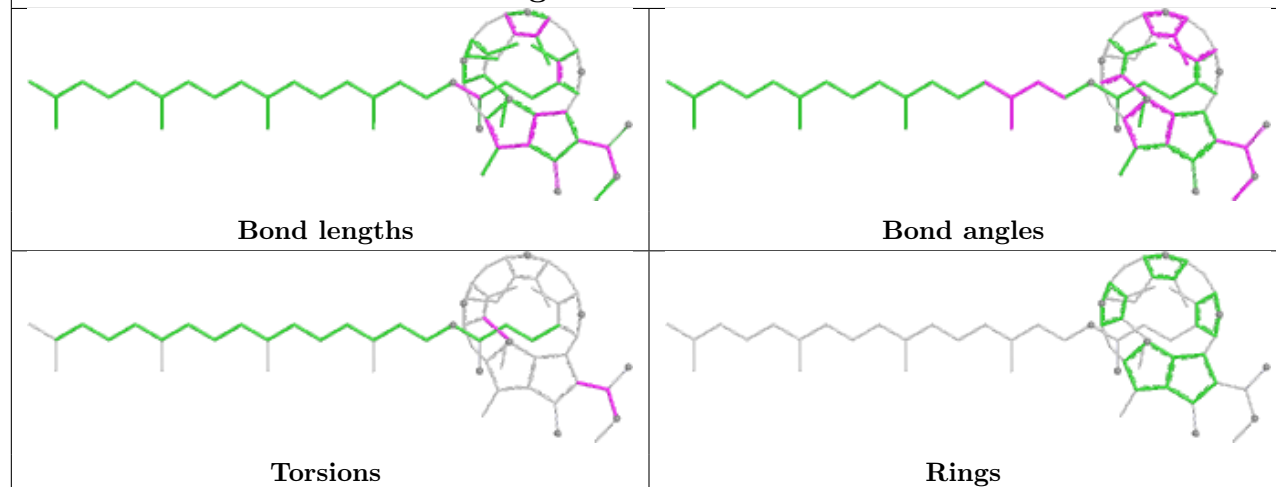




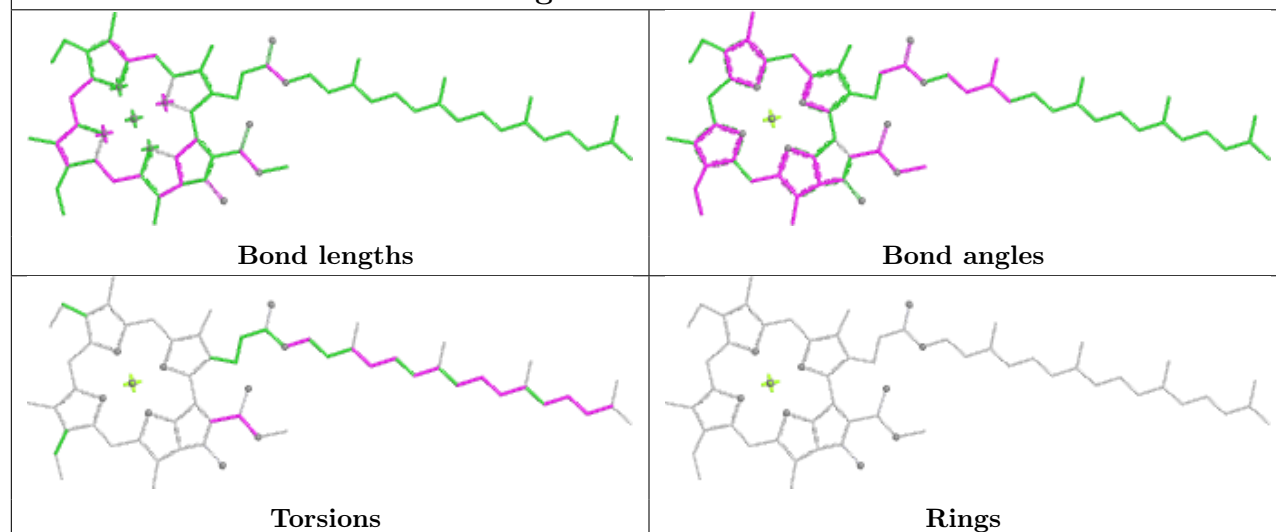
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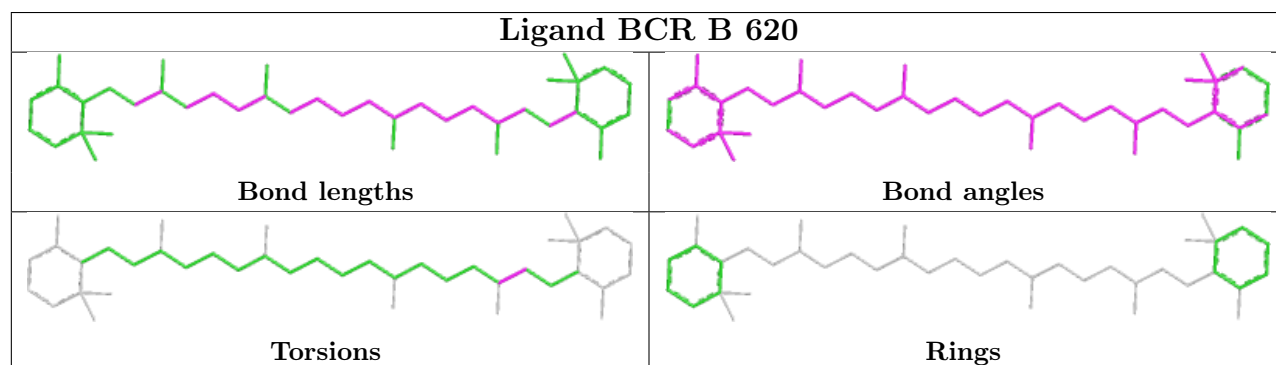
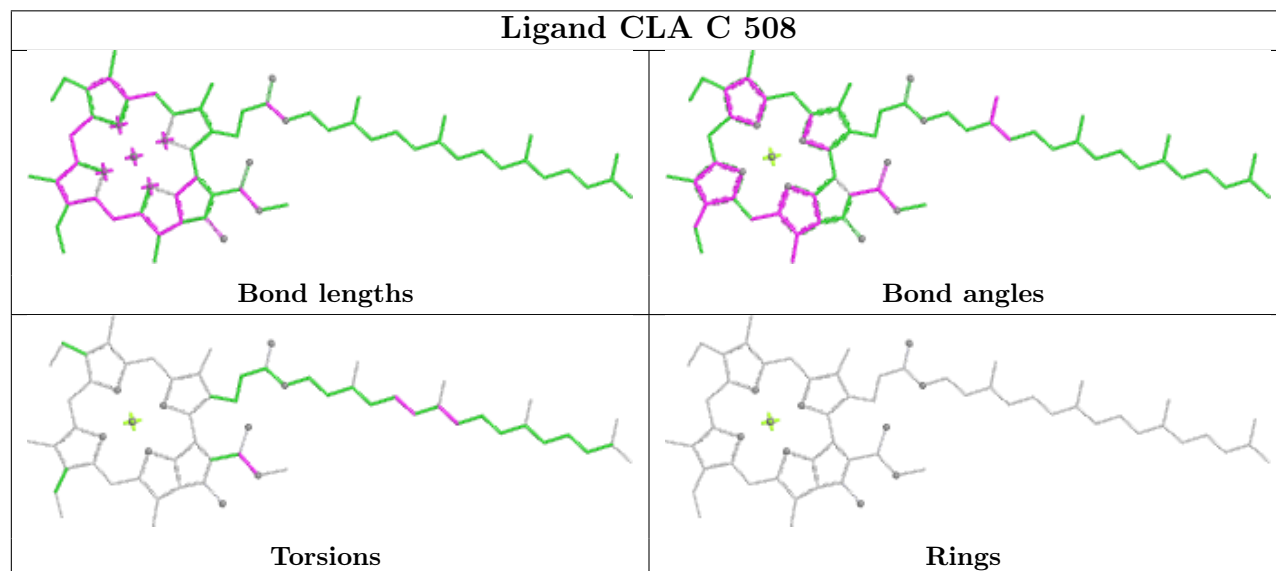
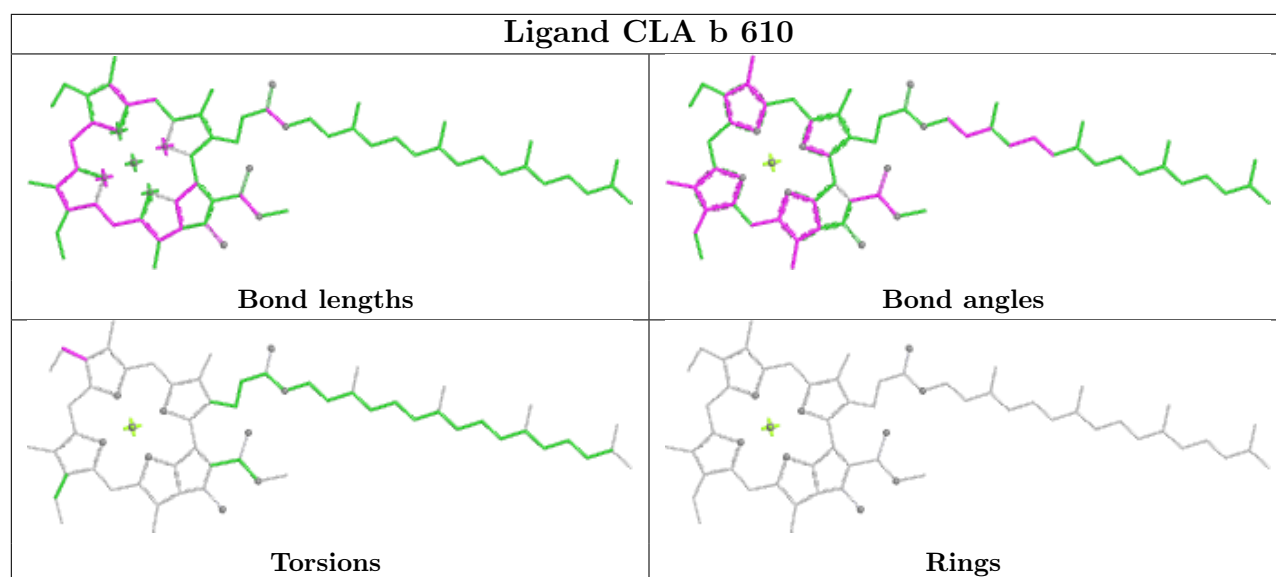


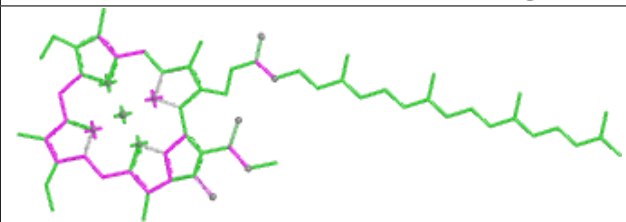
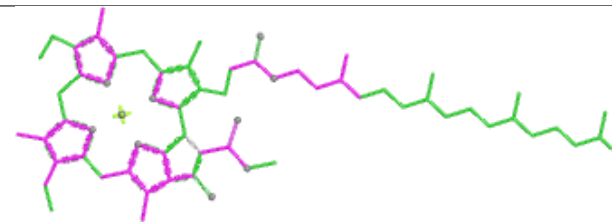
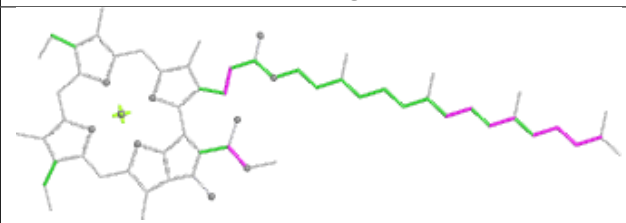
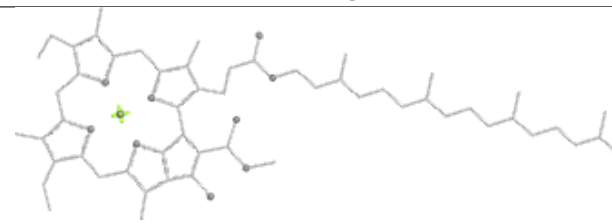
Ligand PHO D 401

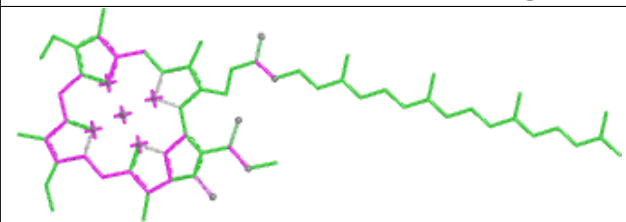
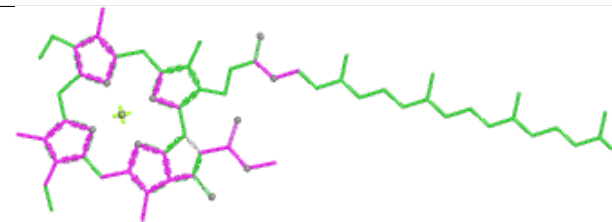
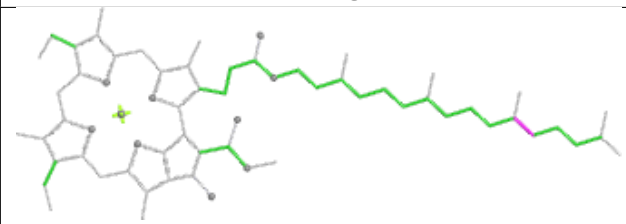
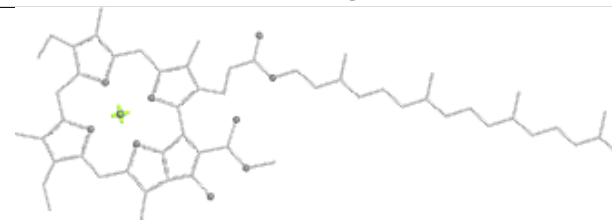


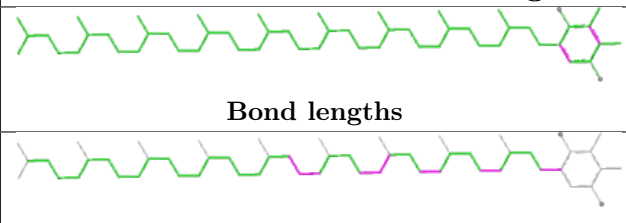
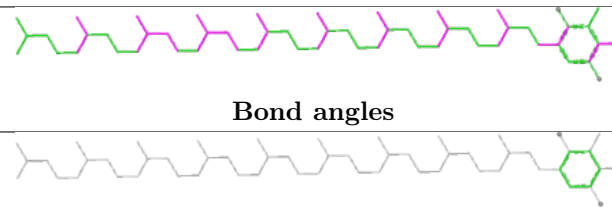
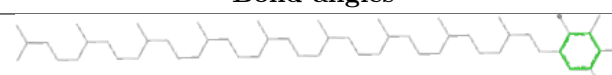
Ligand CLA b 615

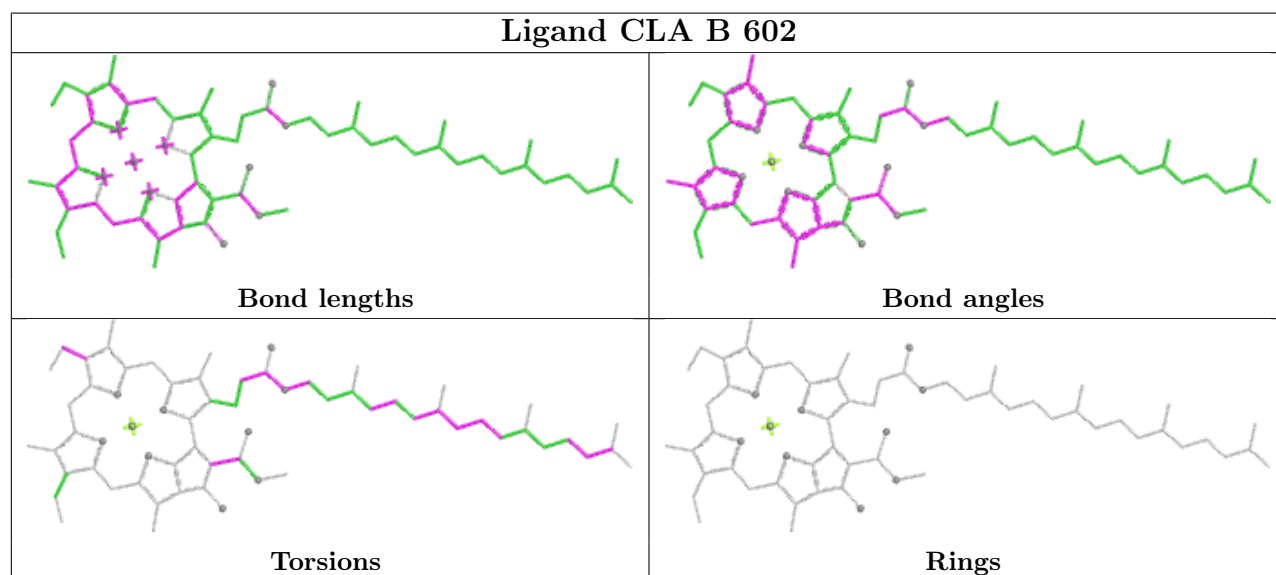
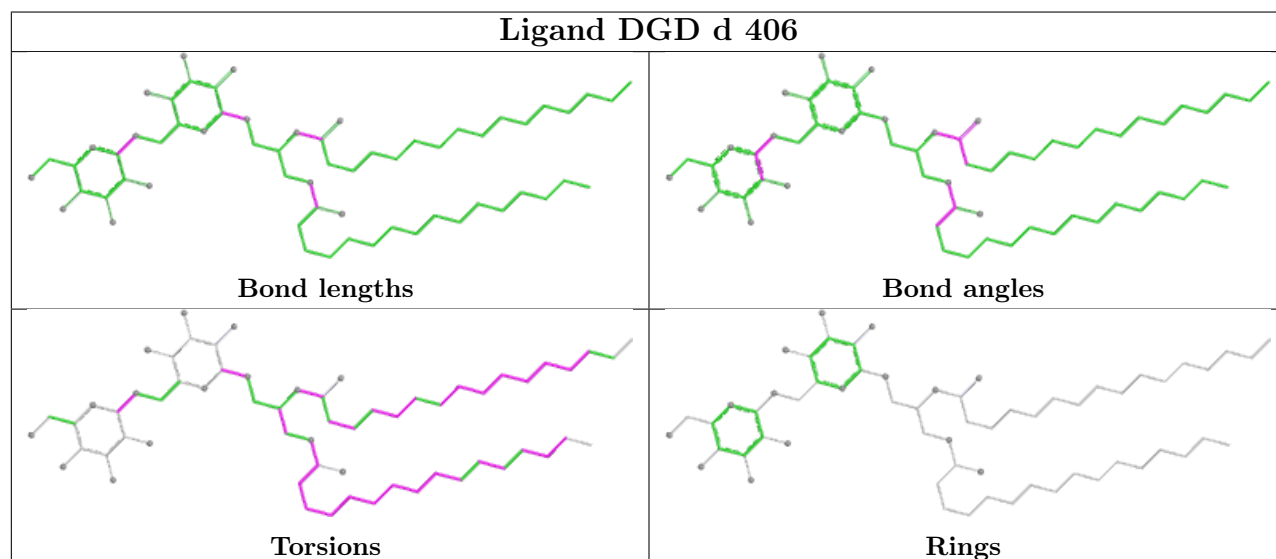
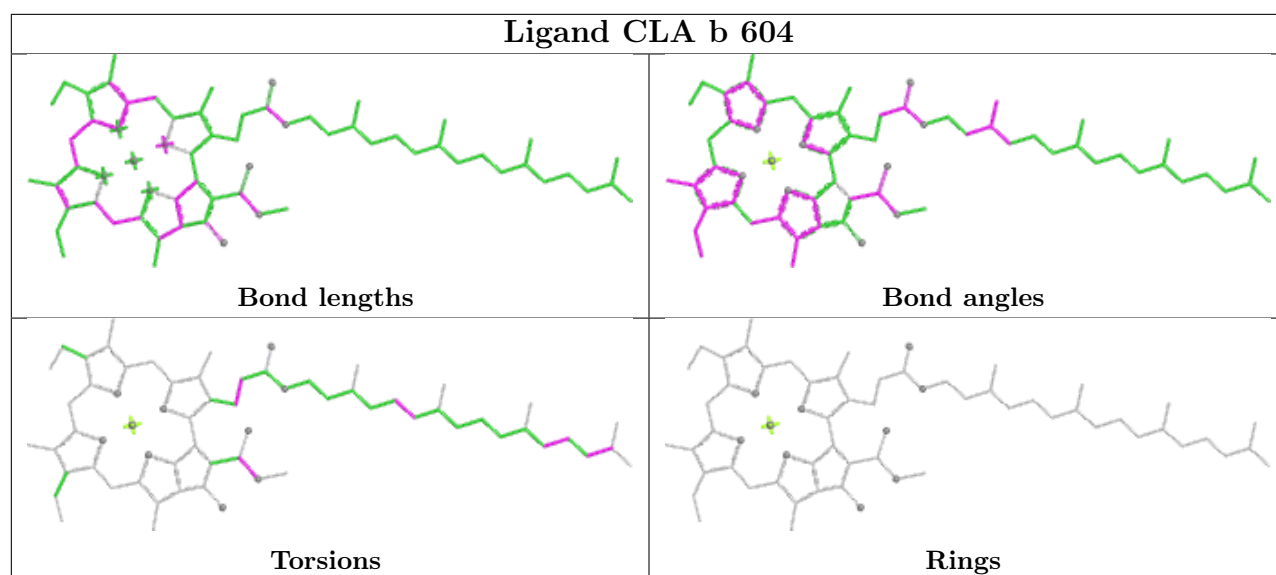


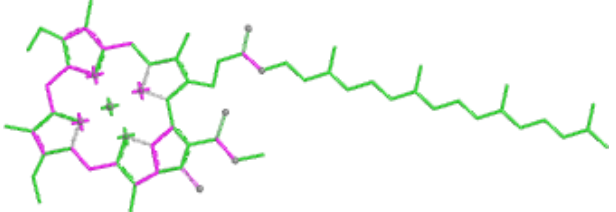
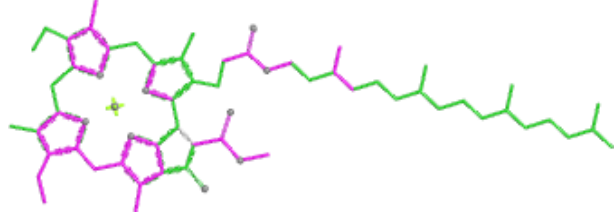
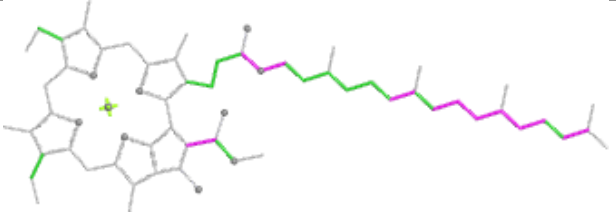
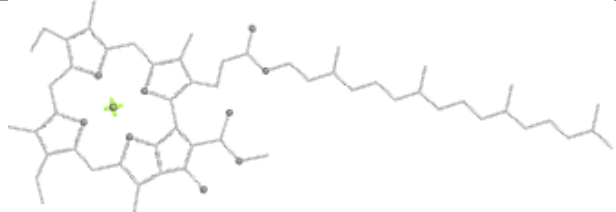
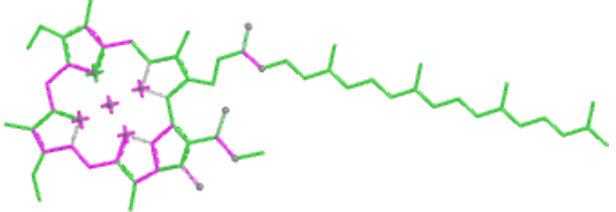
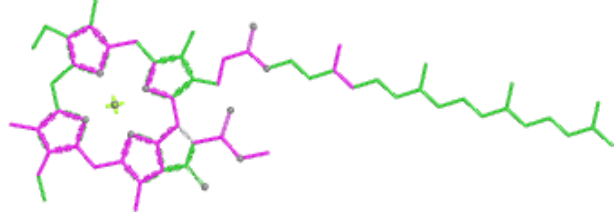
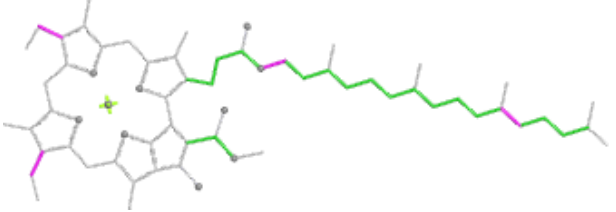
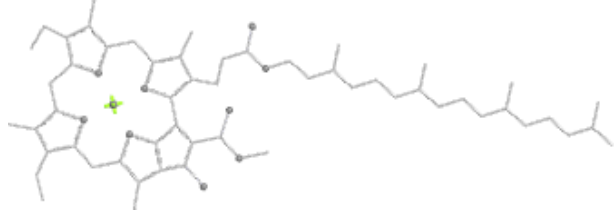
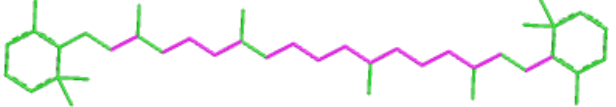
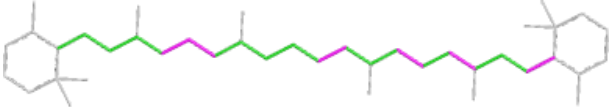
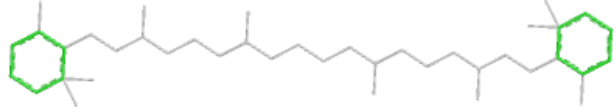


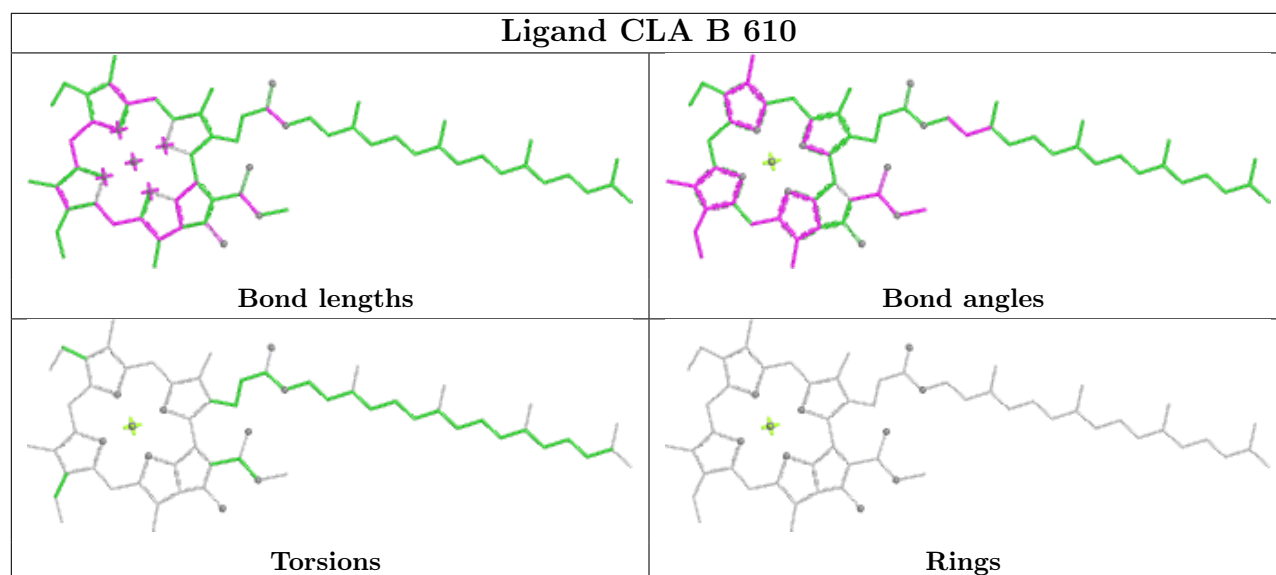
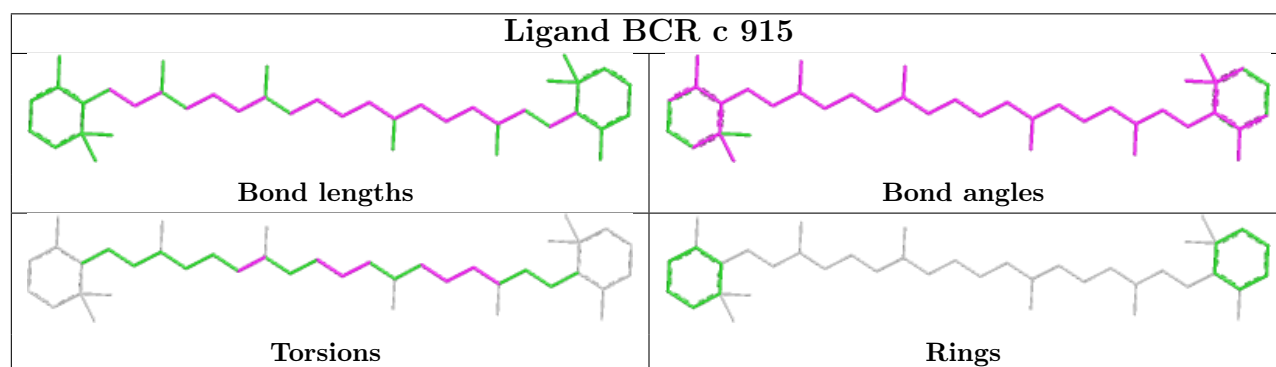
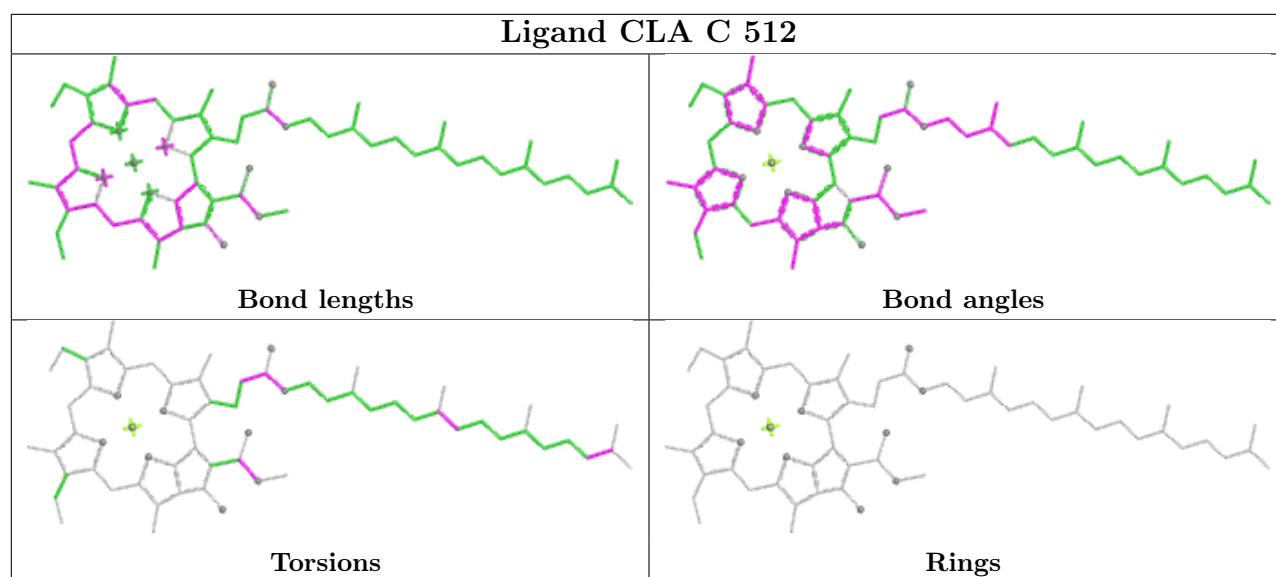
Ligand CLA B 607	
	
Bond lengths	Bond angles
	
Torsions	Rings

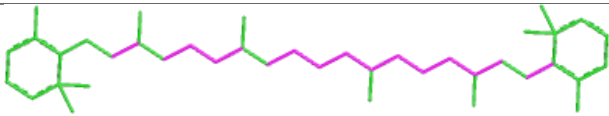
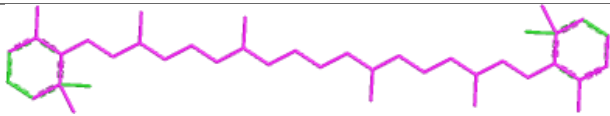
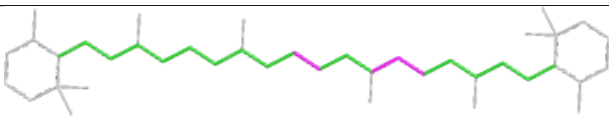
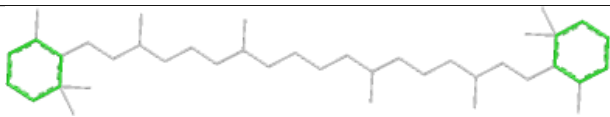
Ligand CLA C 505	
	
Bond lengths	Bond angles
	
Torsions	Rings

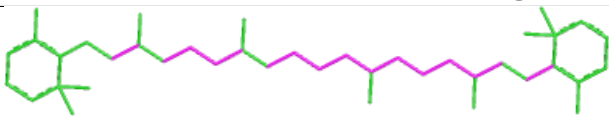
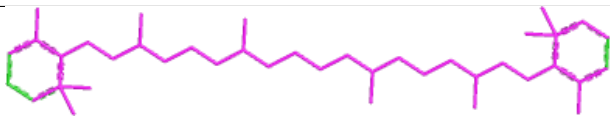
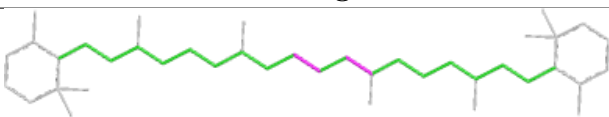
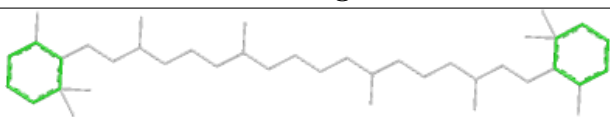
Ligand PL9 A 611	
	
Bond lengths	Bond angles
	
Torsions	Rings

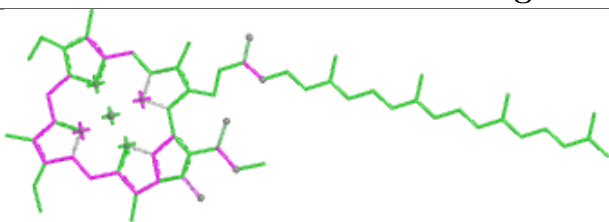
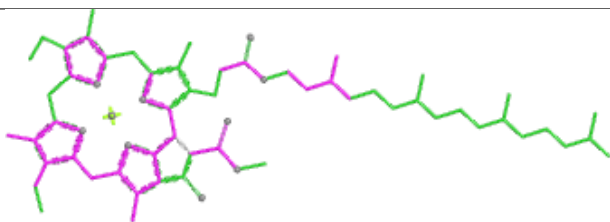
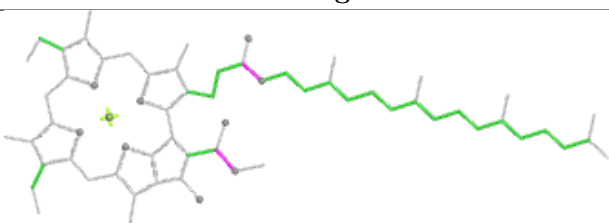
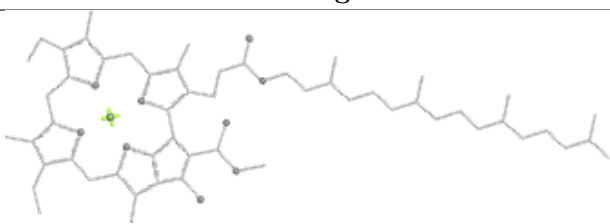


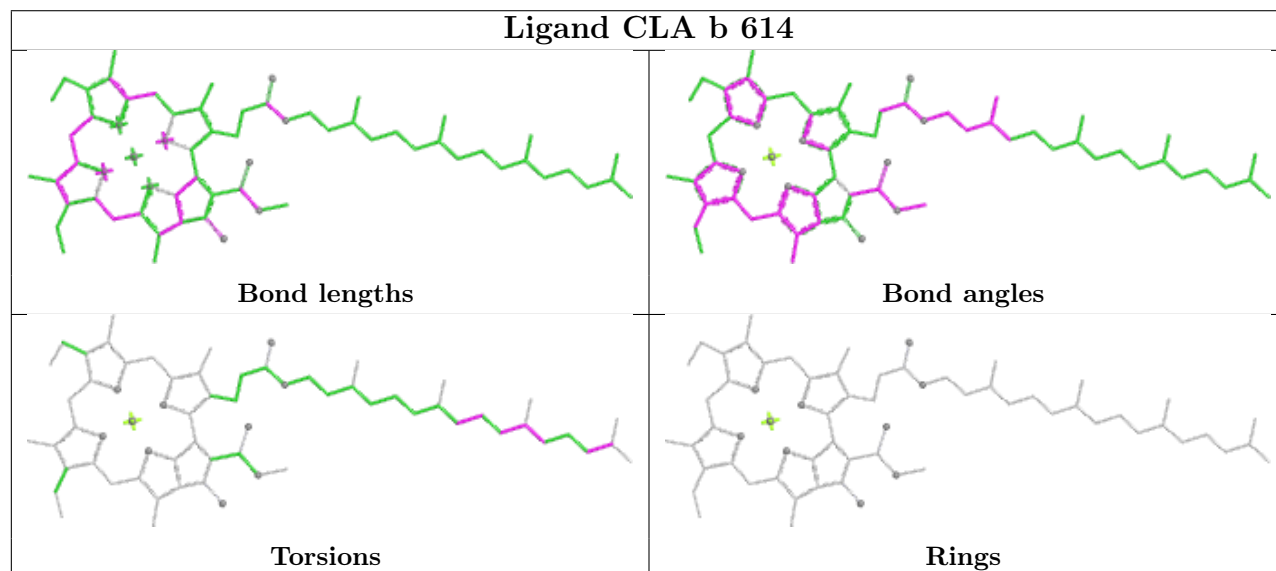
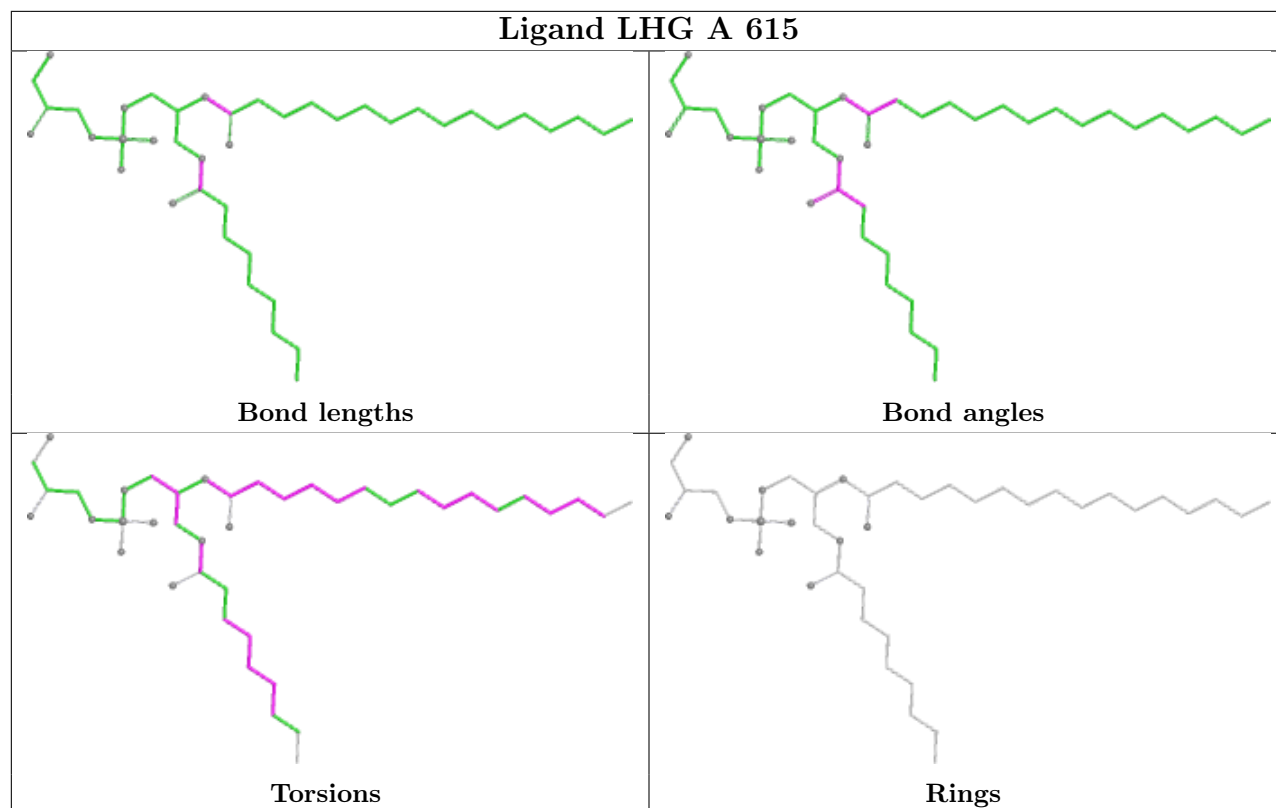
Ligand CLA B 617	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA D 402	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR H 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

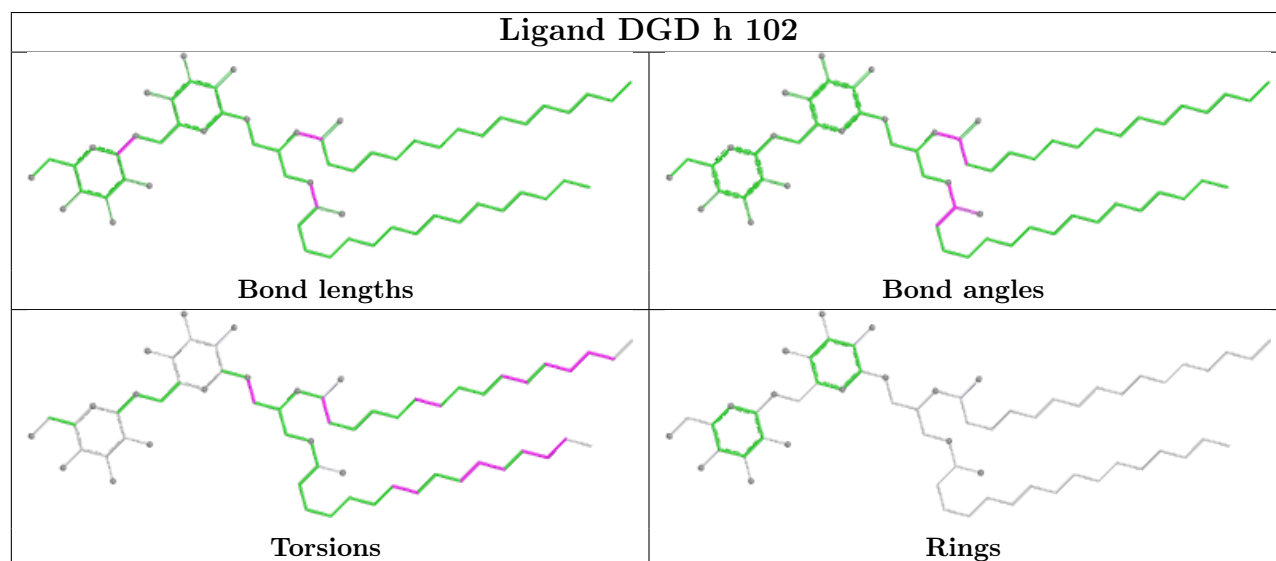
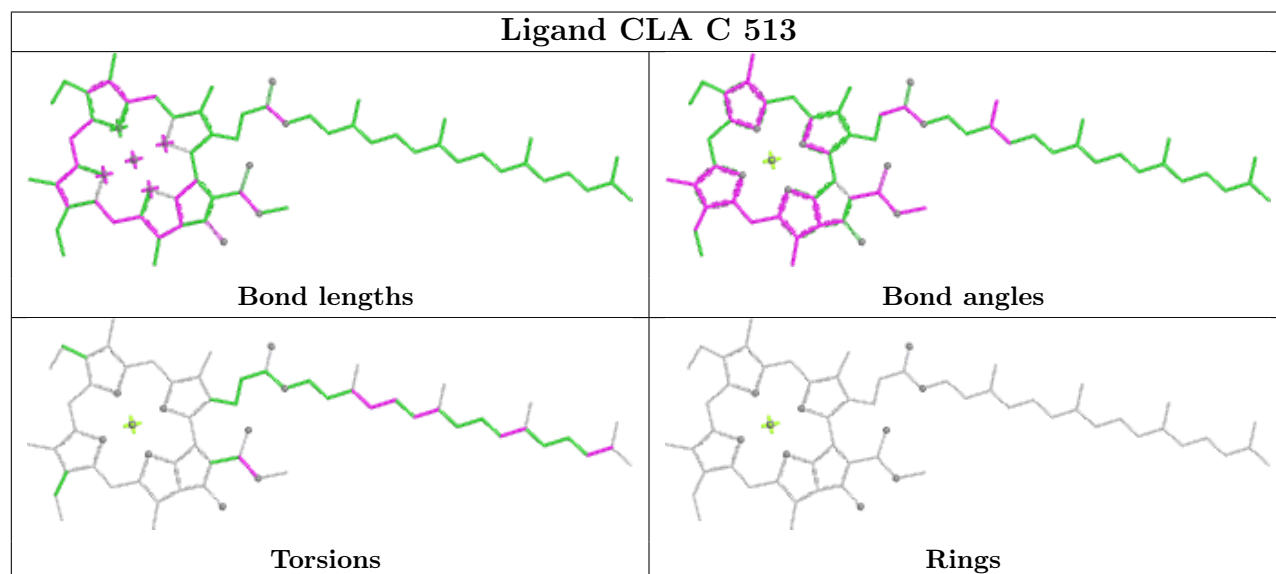
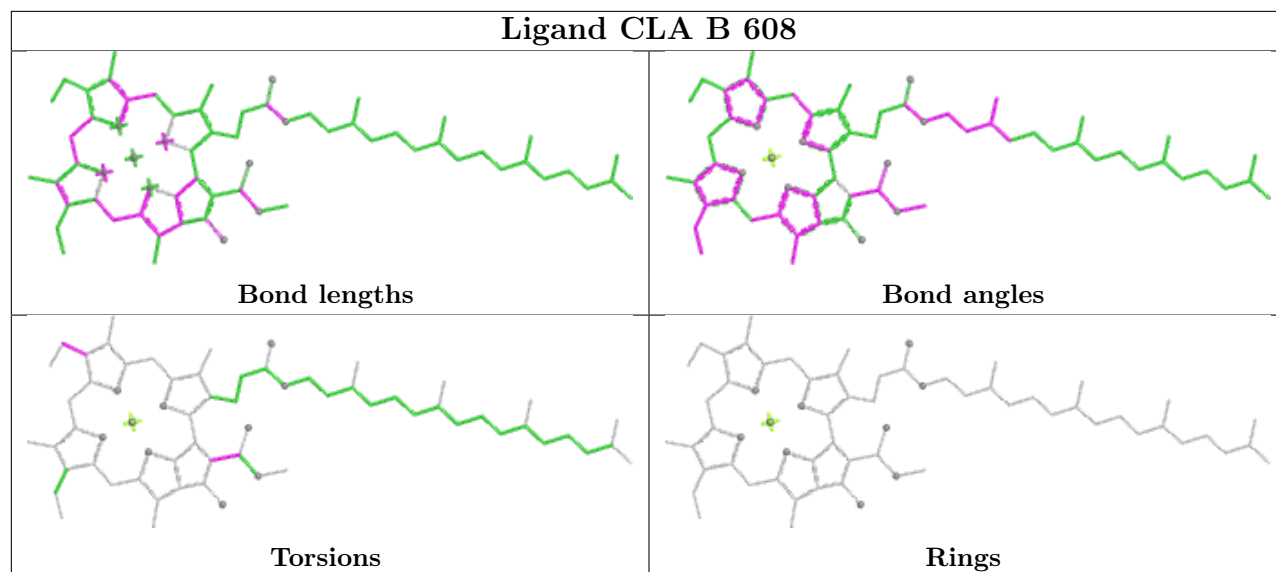


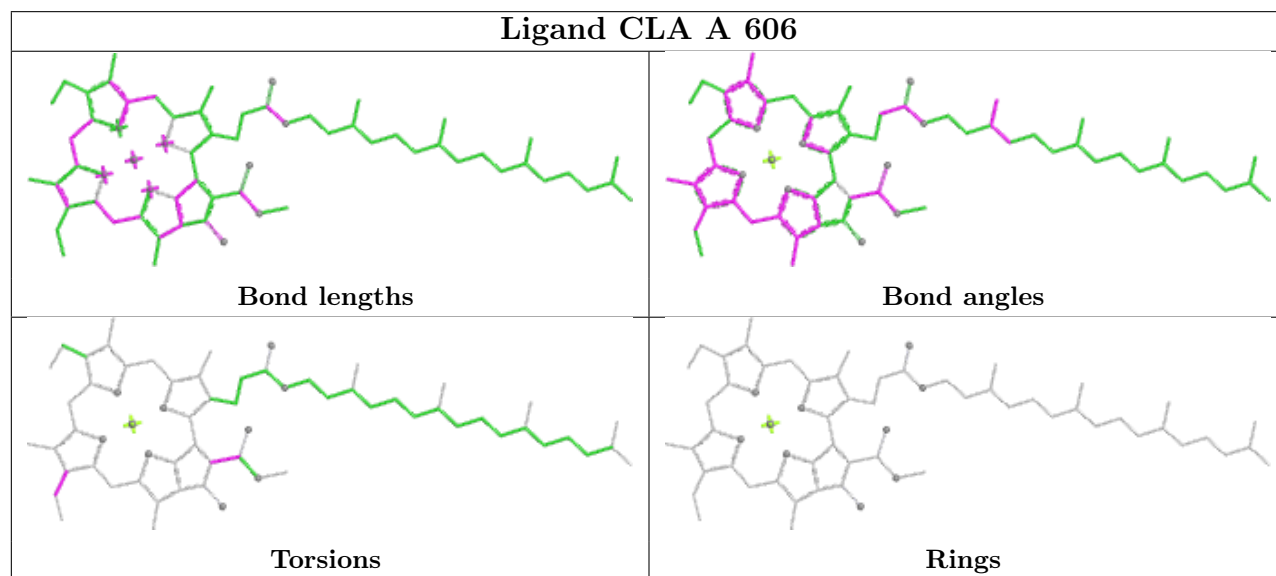
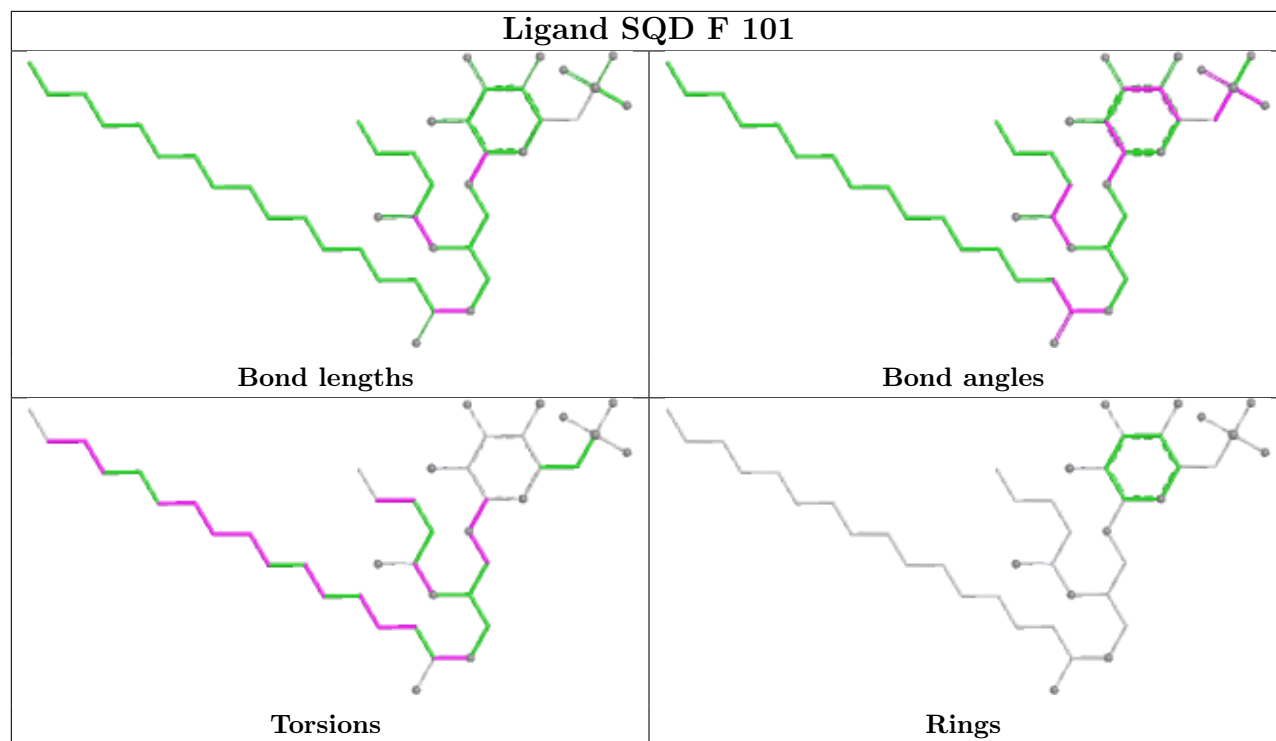
Ligand BCR A 610	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR b 618	
	
Bond lengths	Bond angles
	
Torsions	Rings

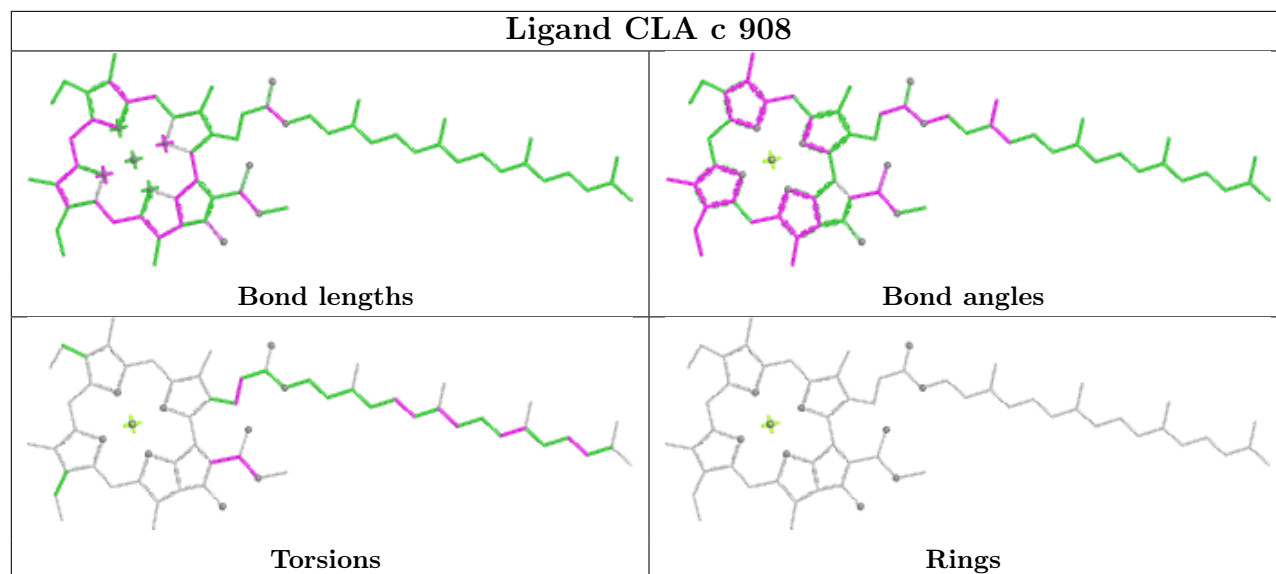
Ligand CLA c 904	
	
Bond lengths	Bond angles
	
Torsions	Rings



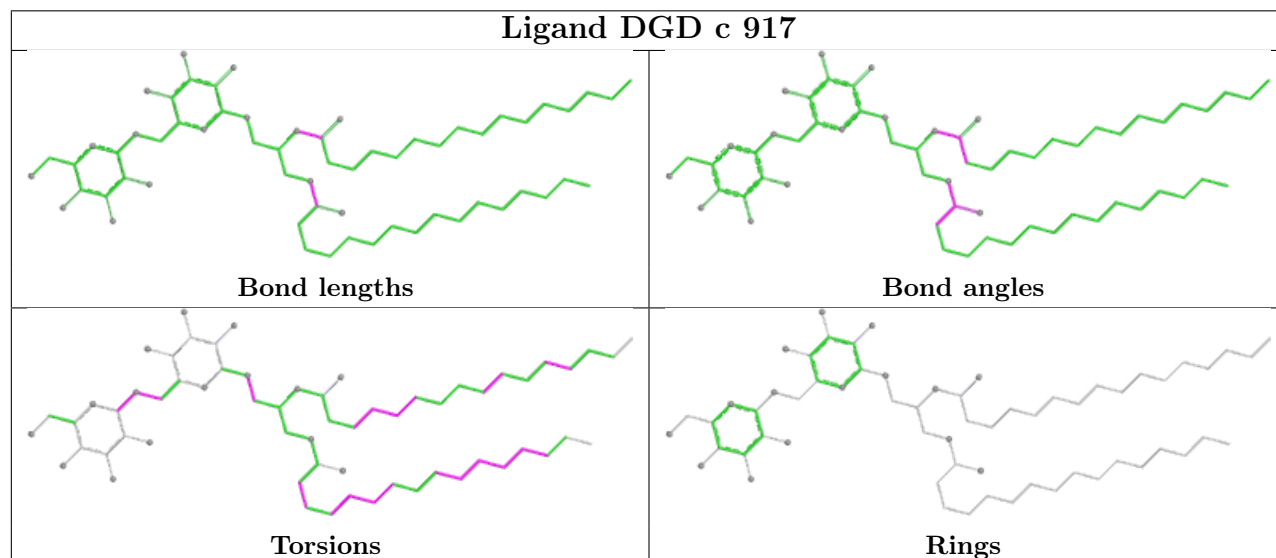




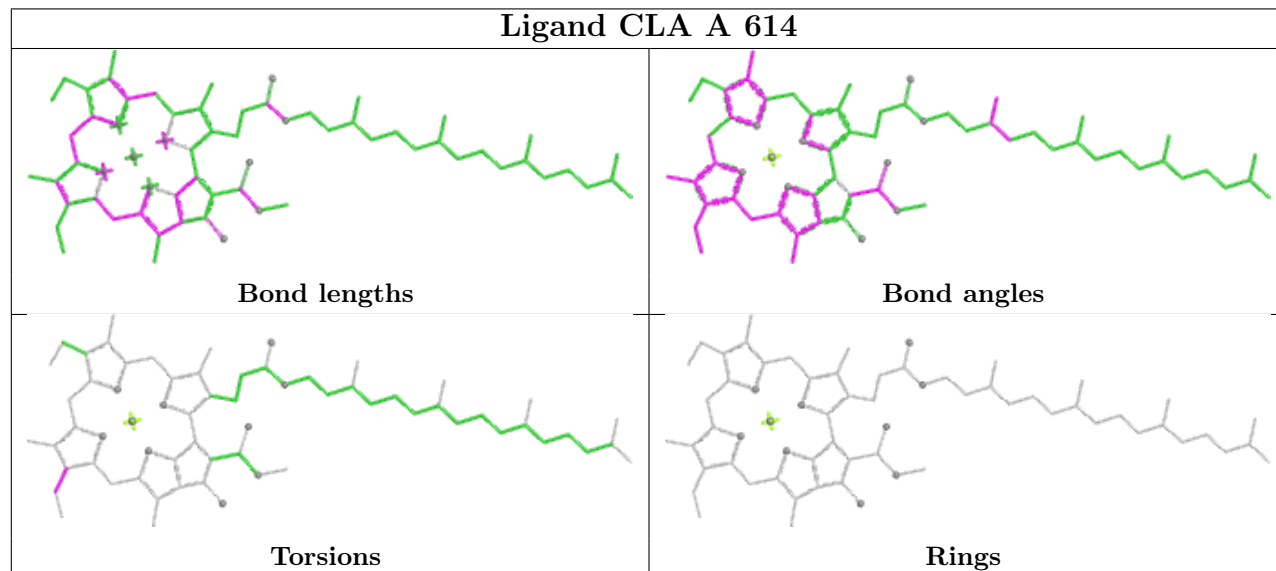
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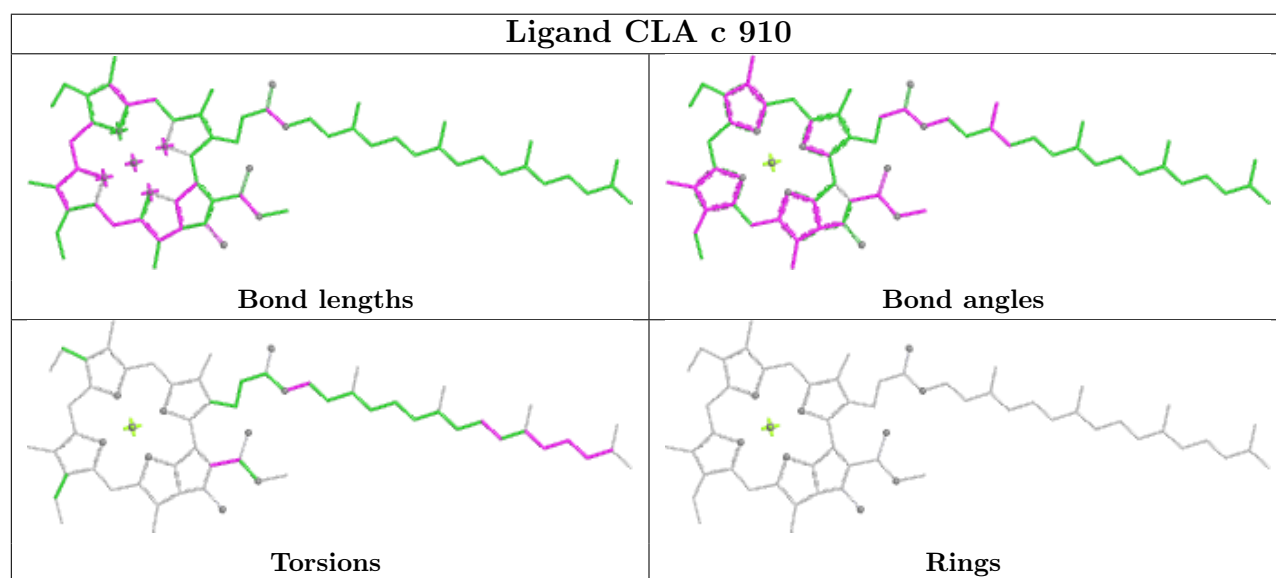
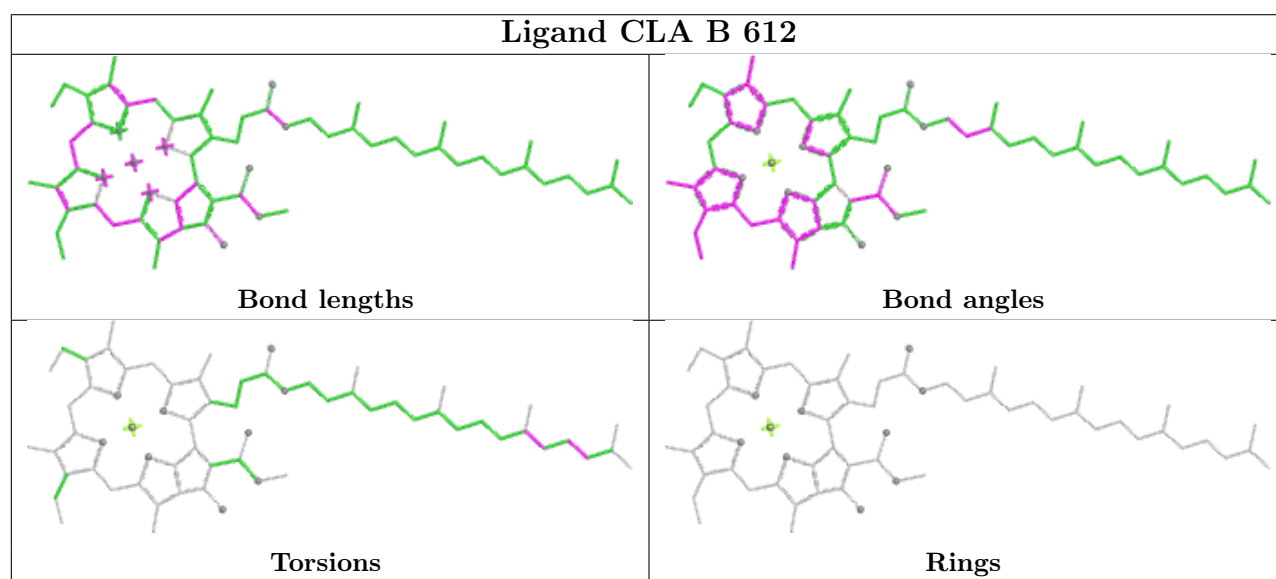
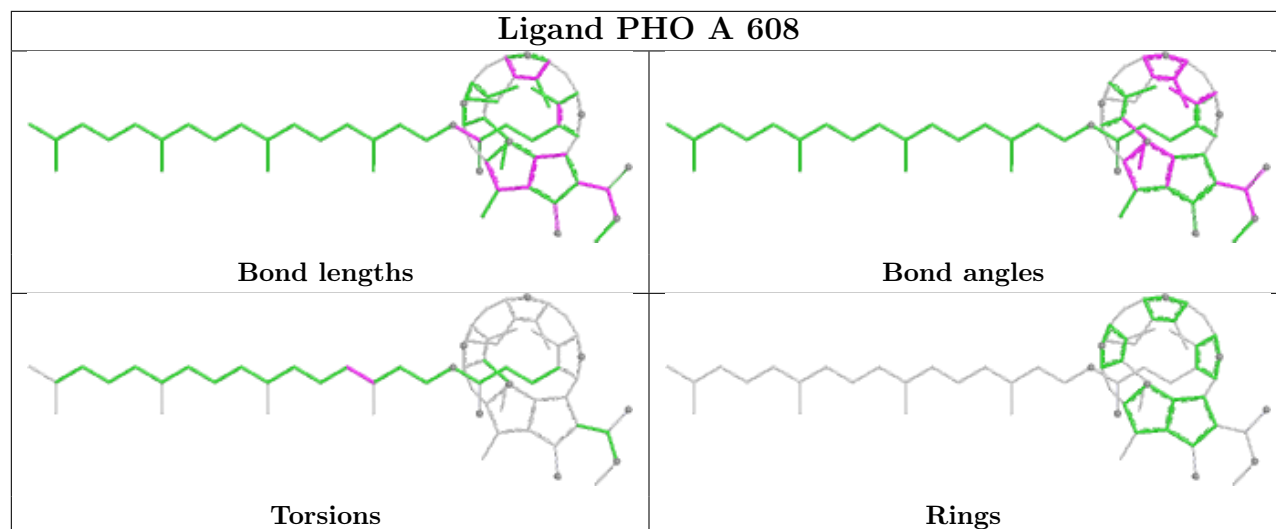


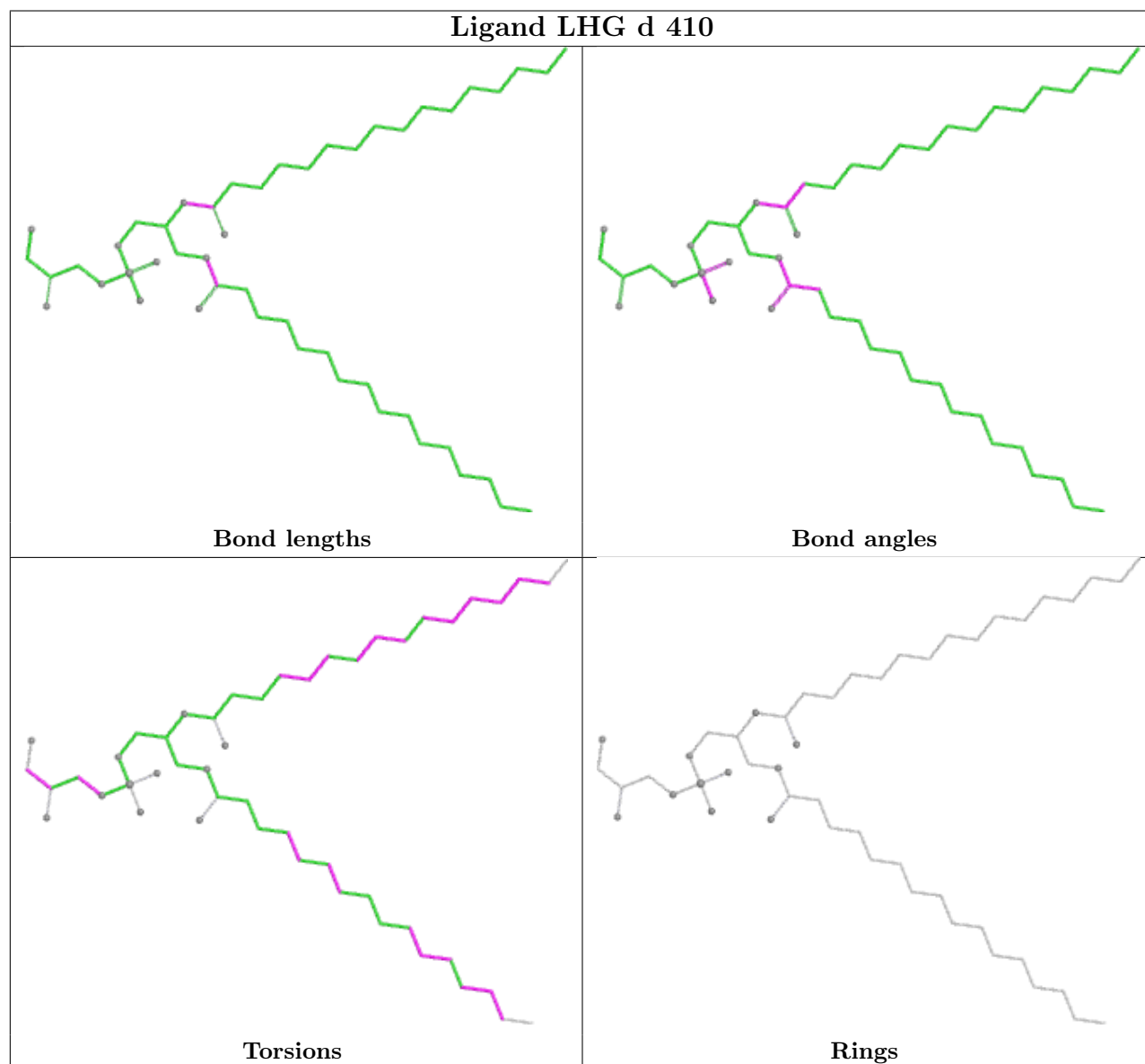
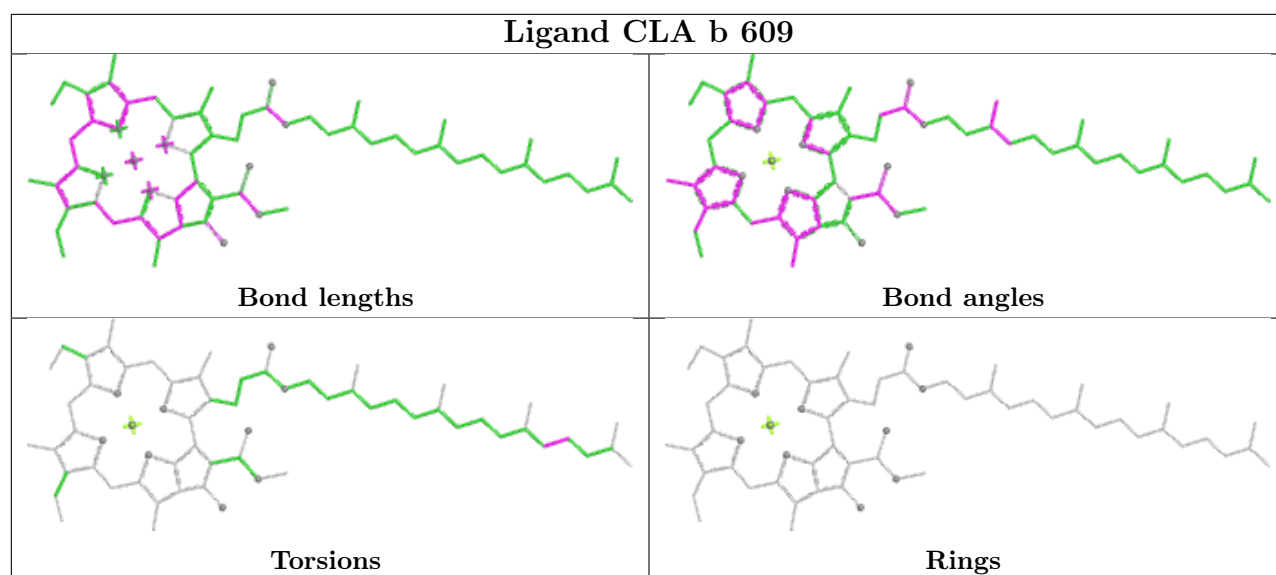
Ligand DGD c 917

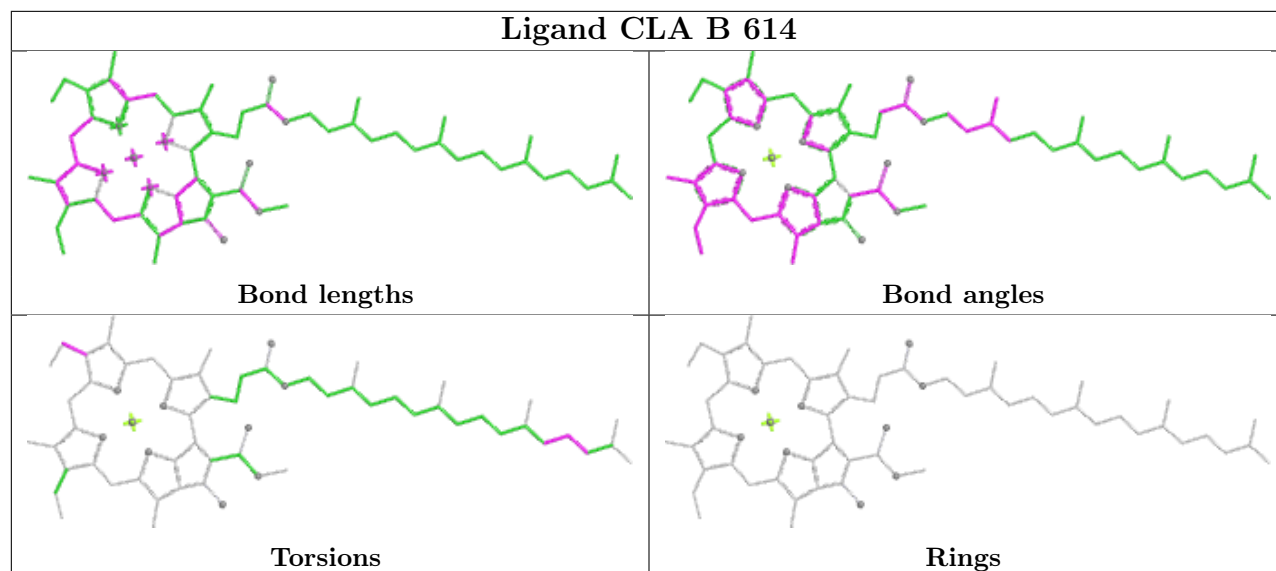
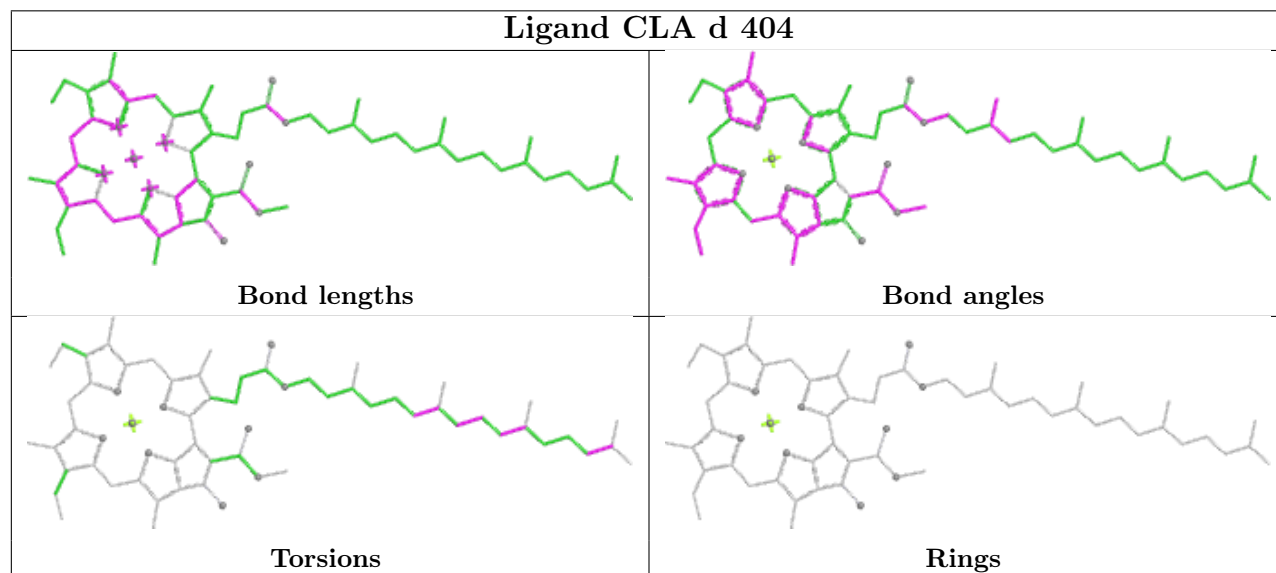
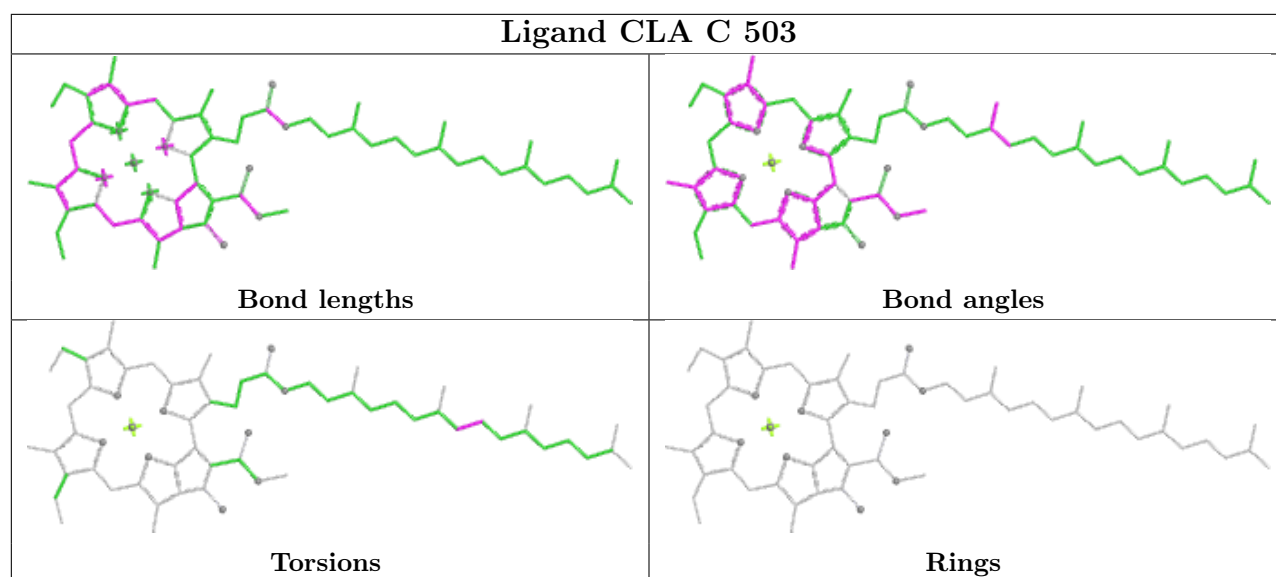


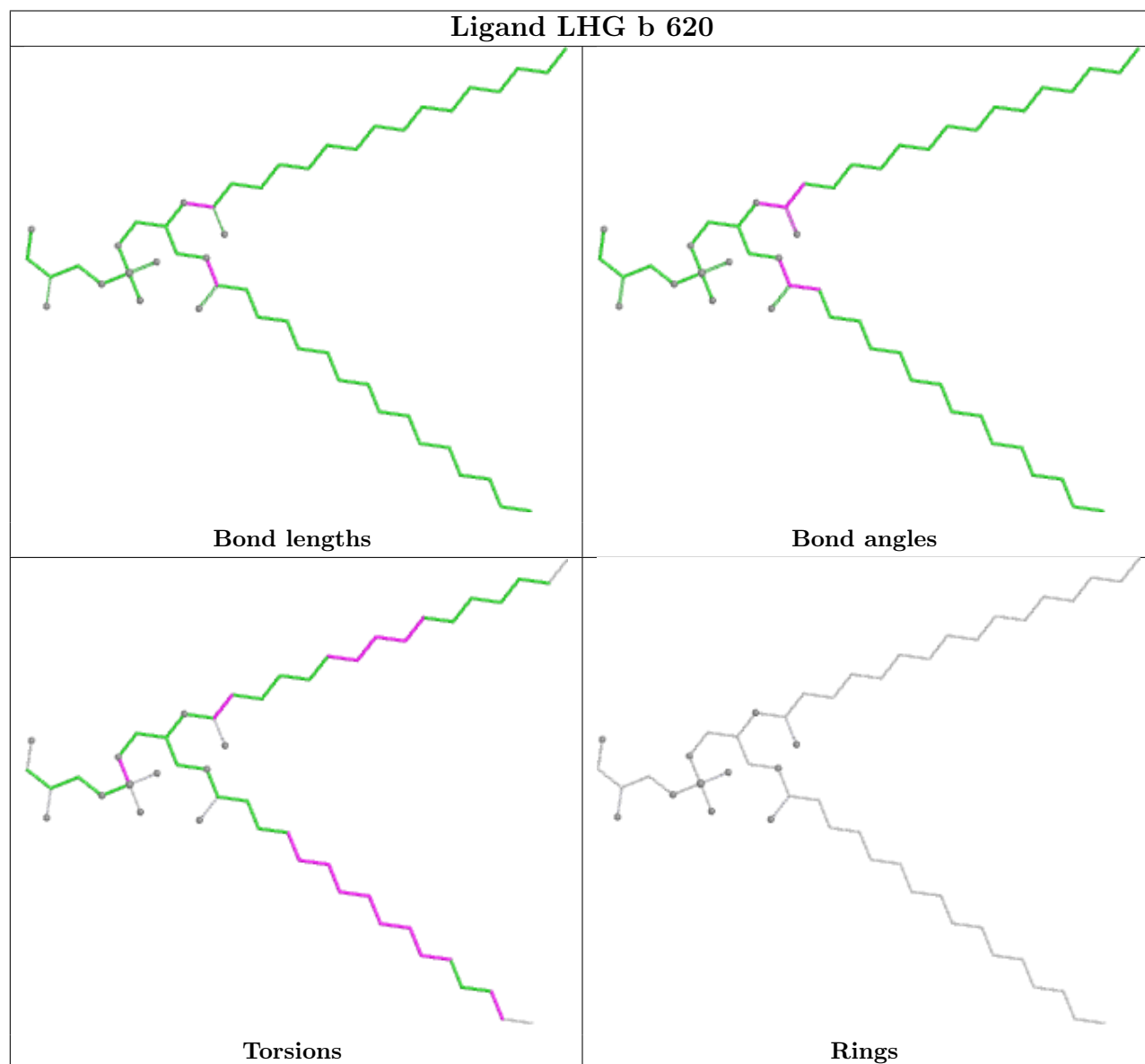
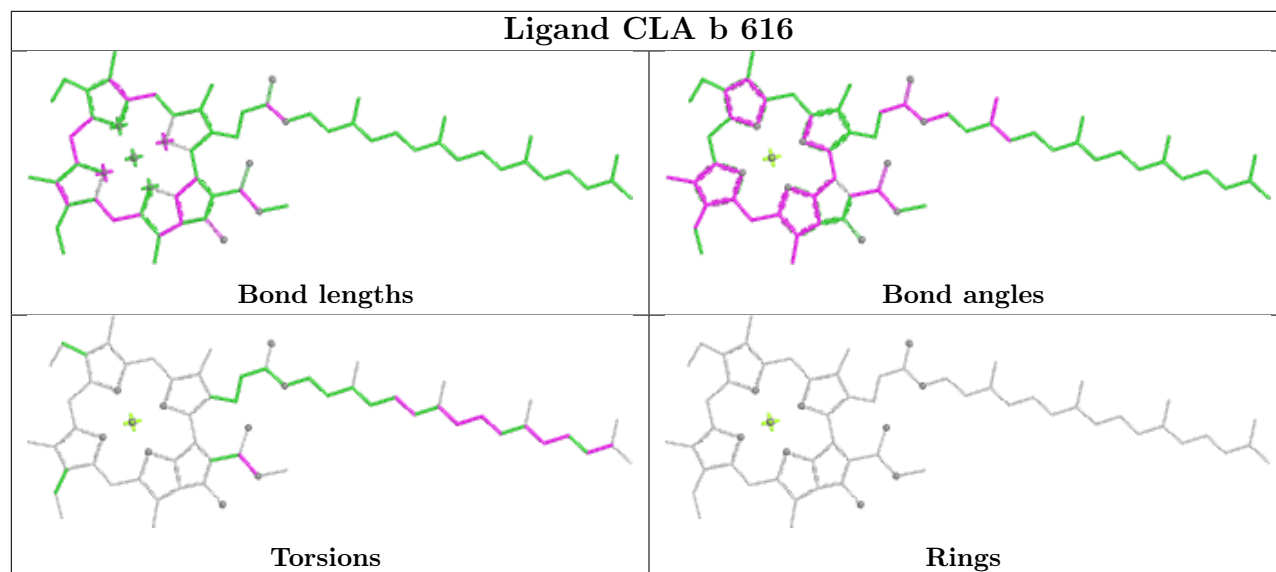
Ligand CLA A 614



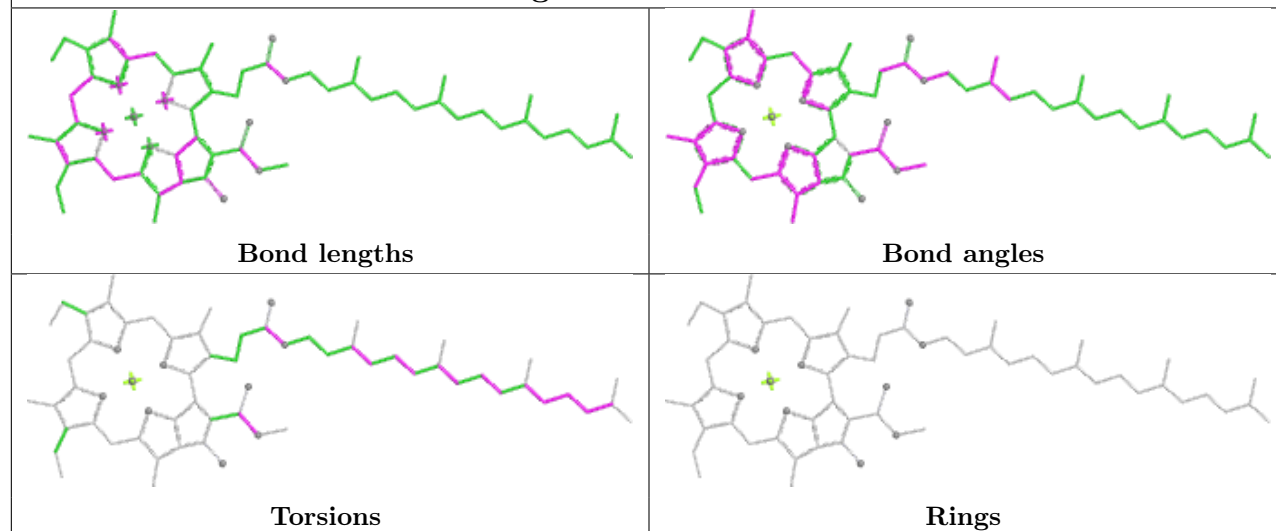




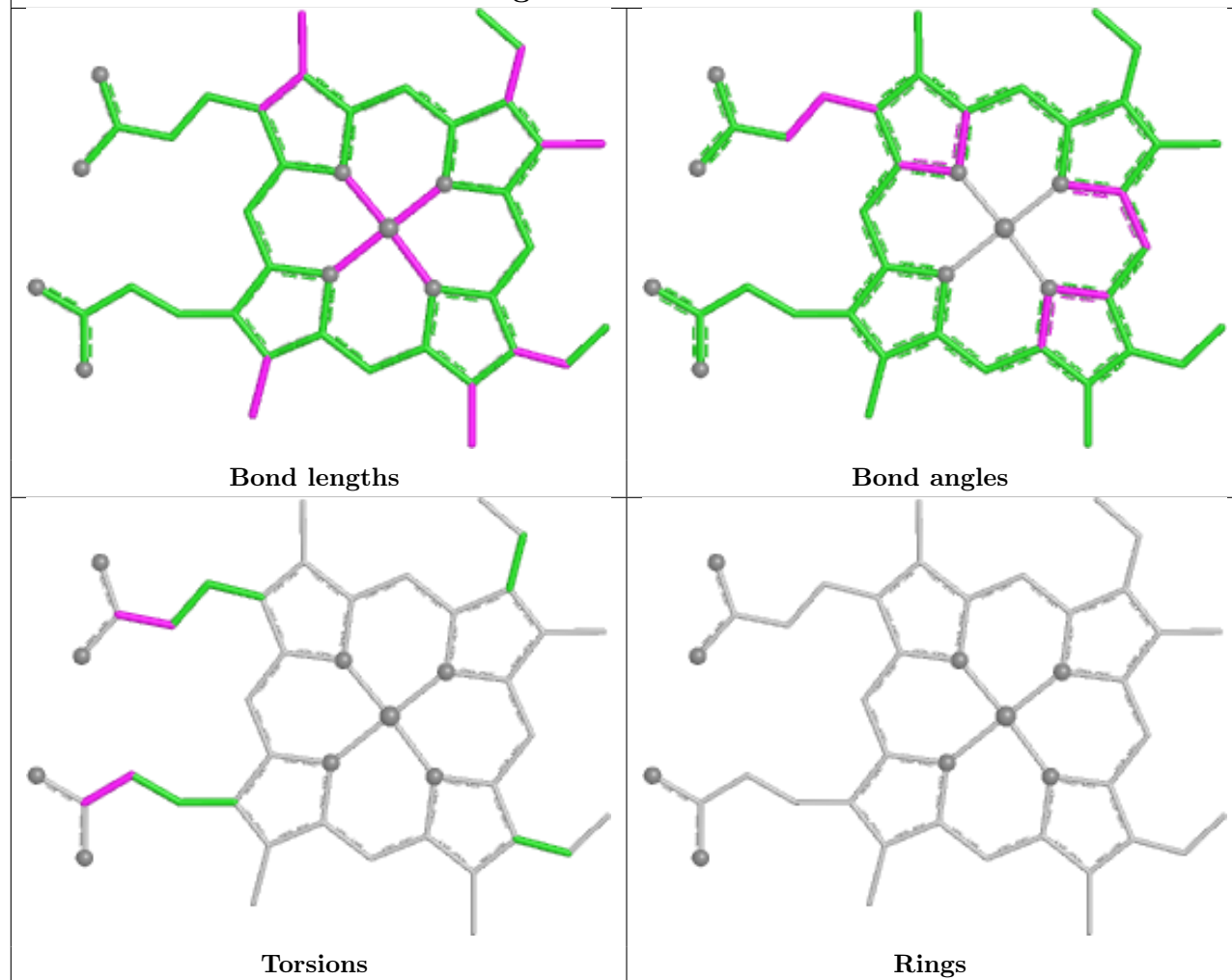


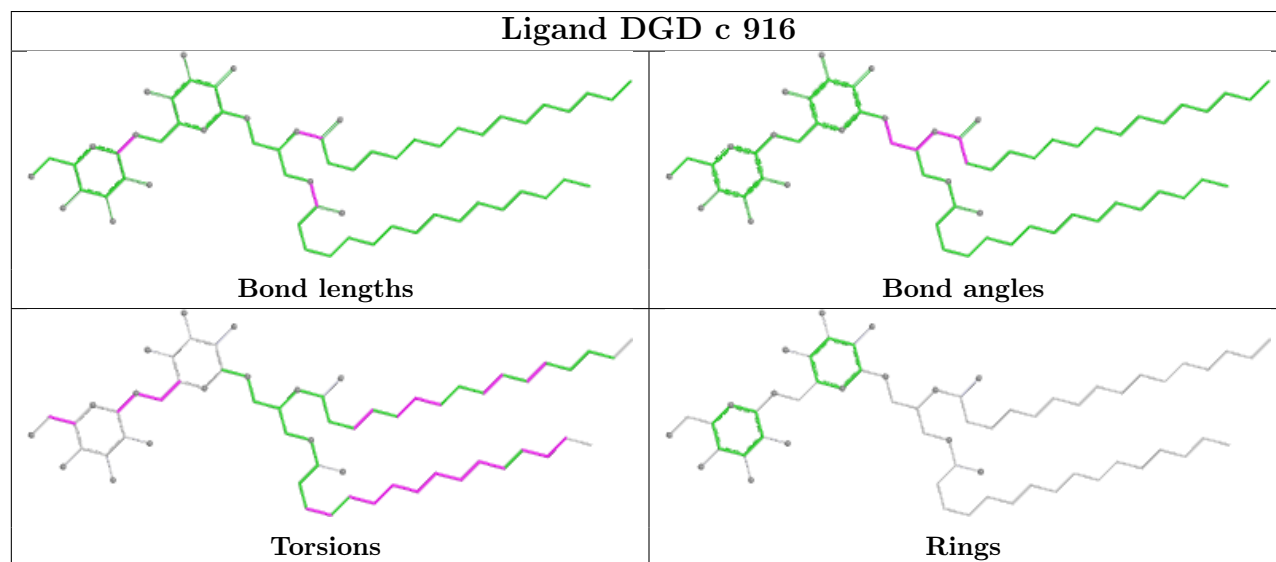
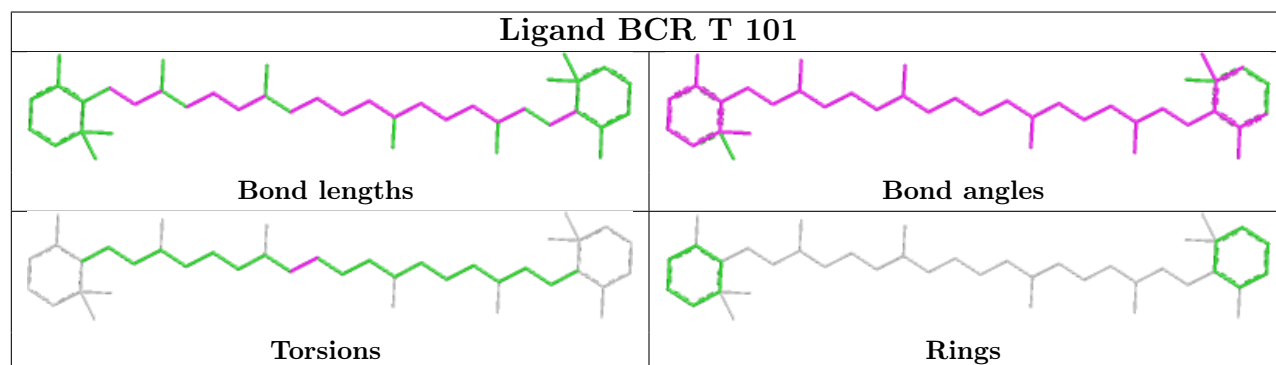
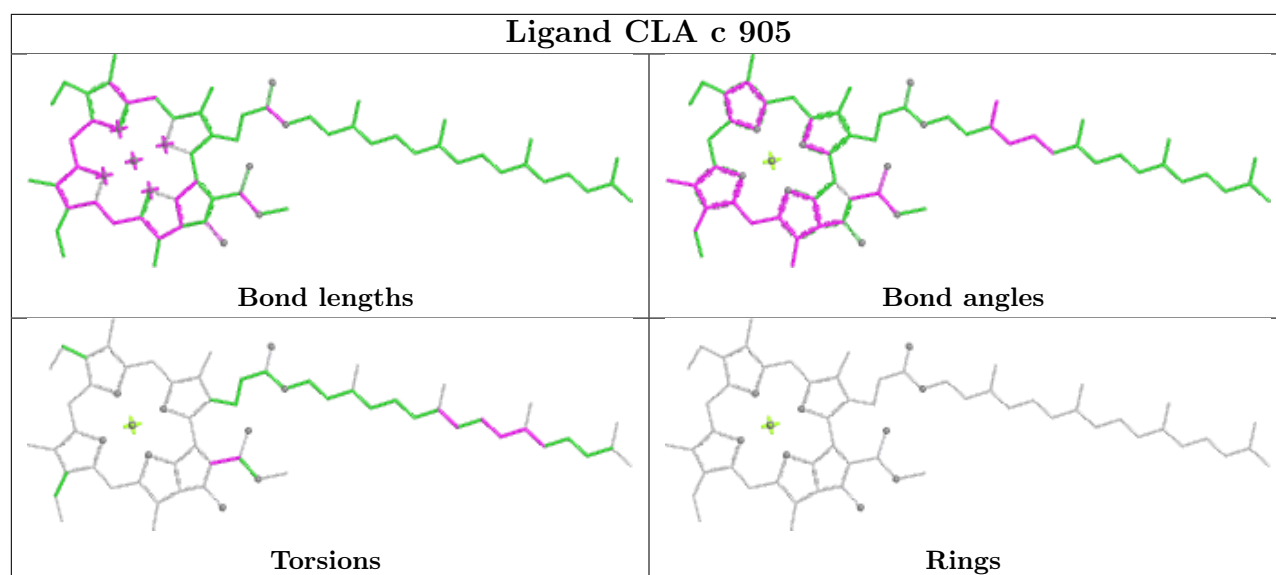


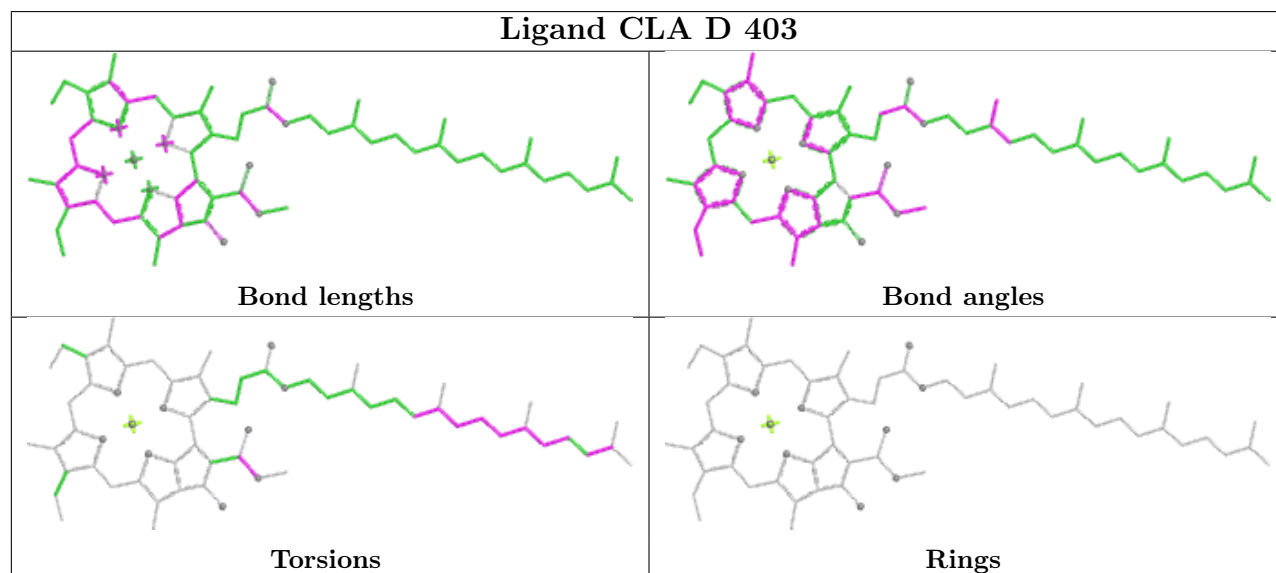
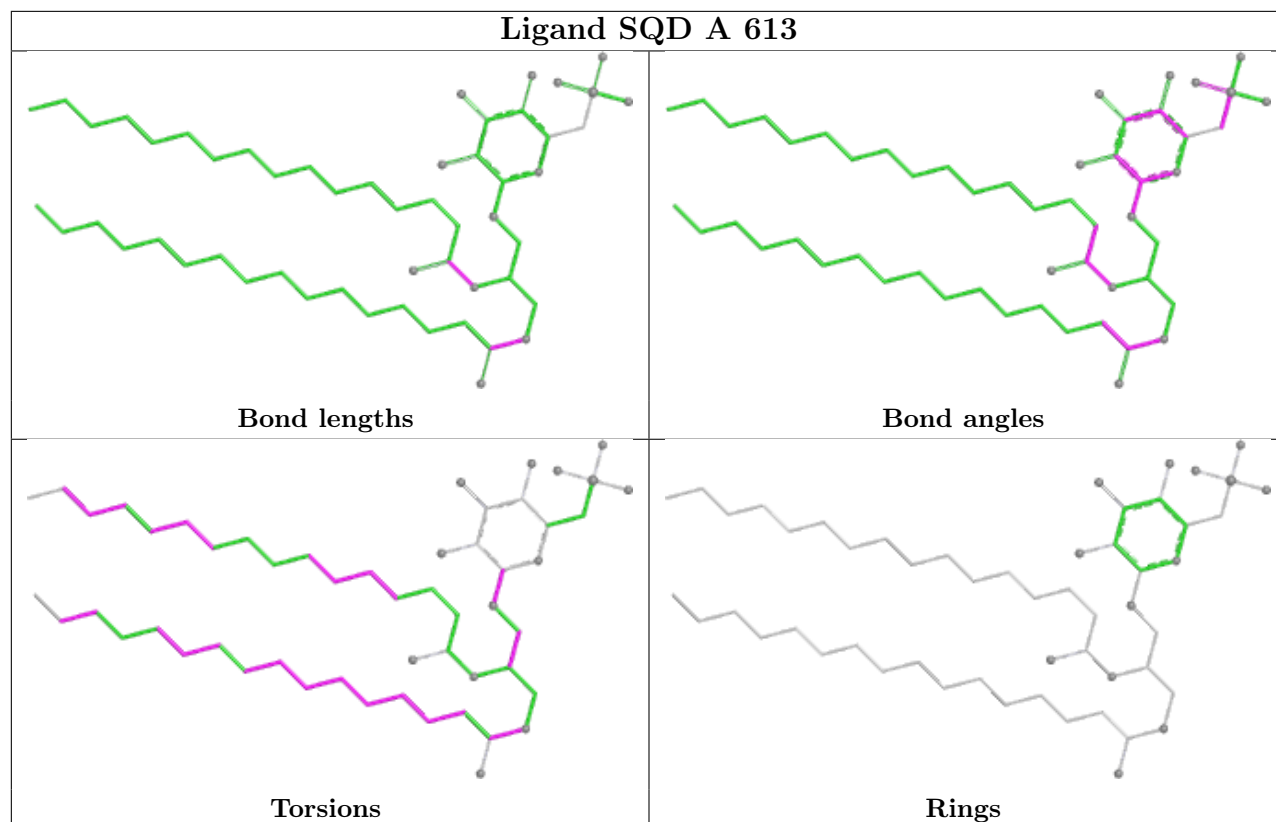
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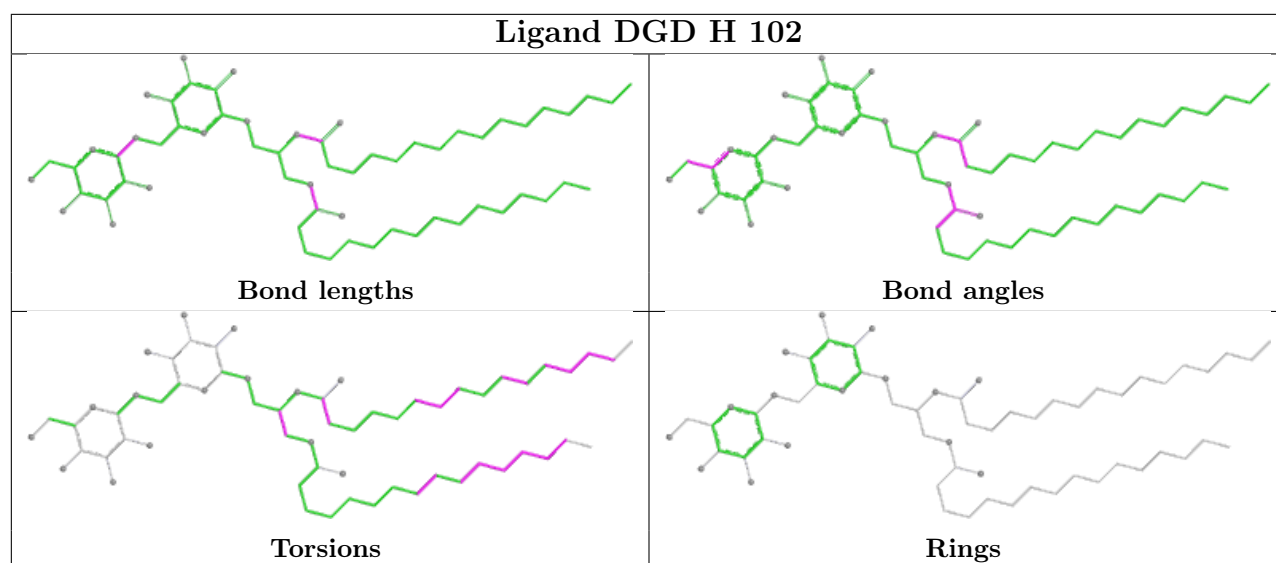
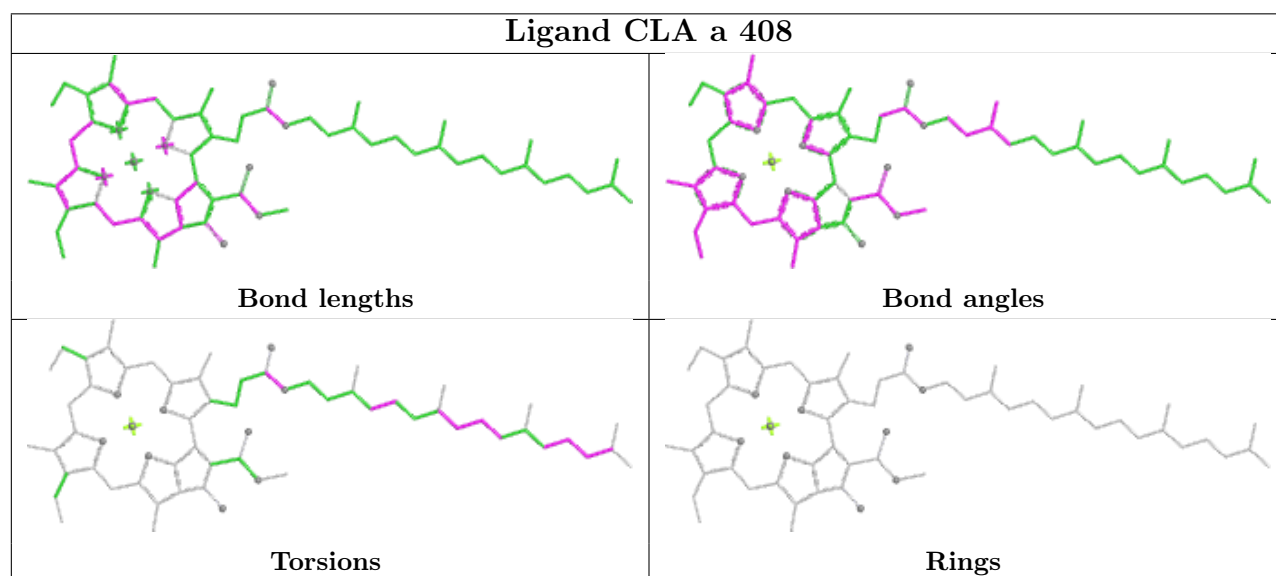
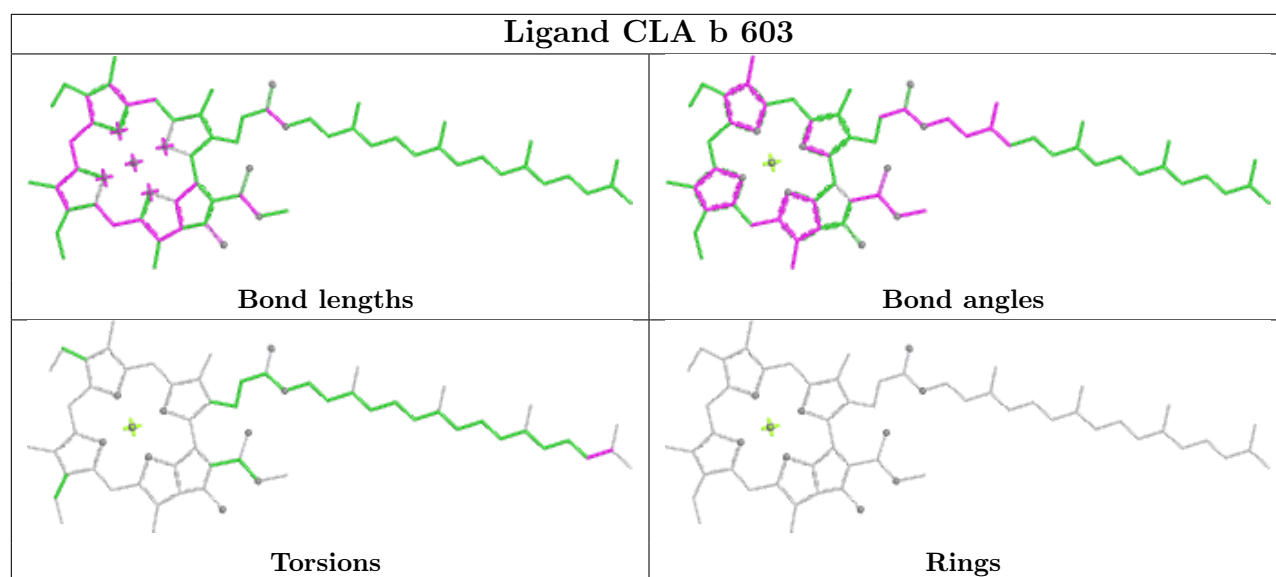


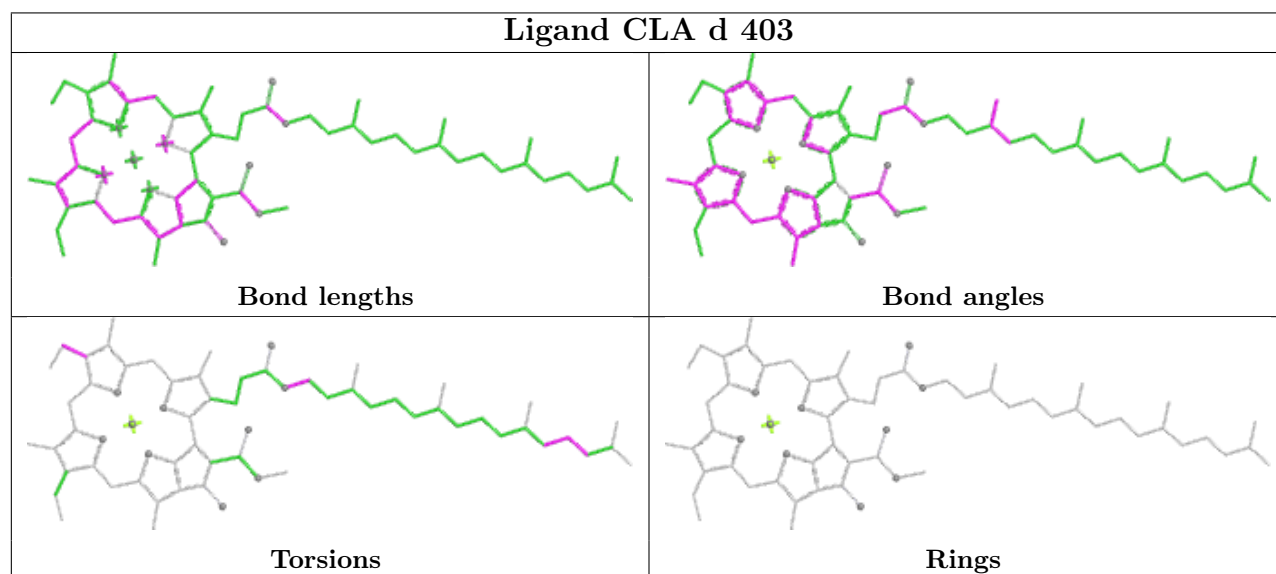
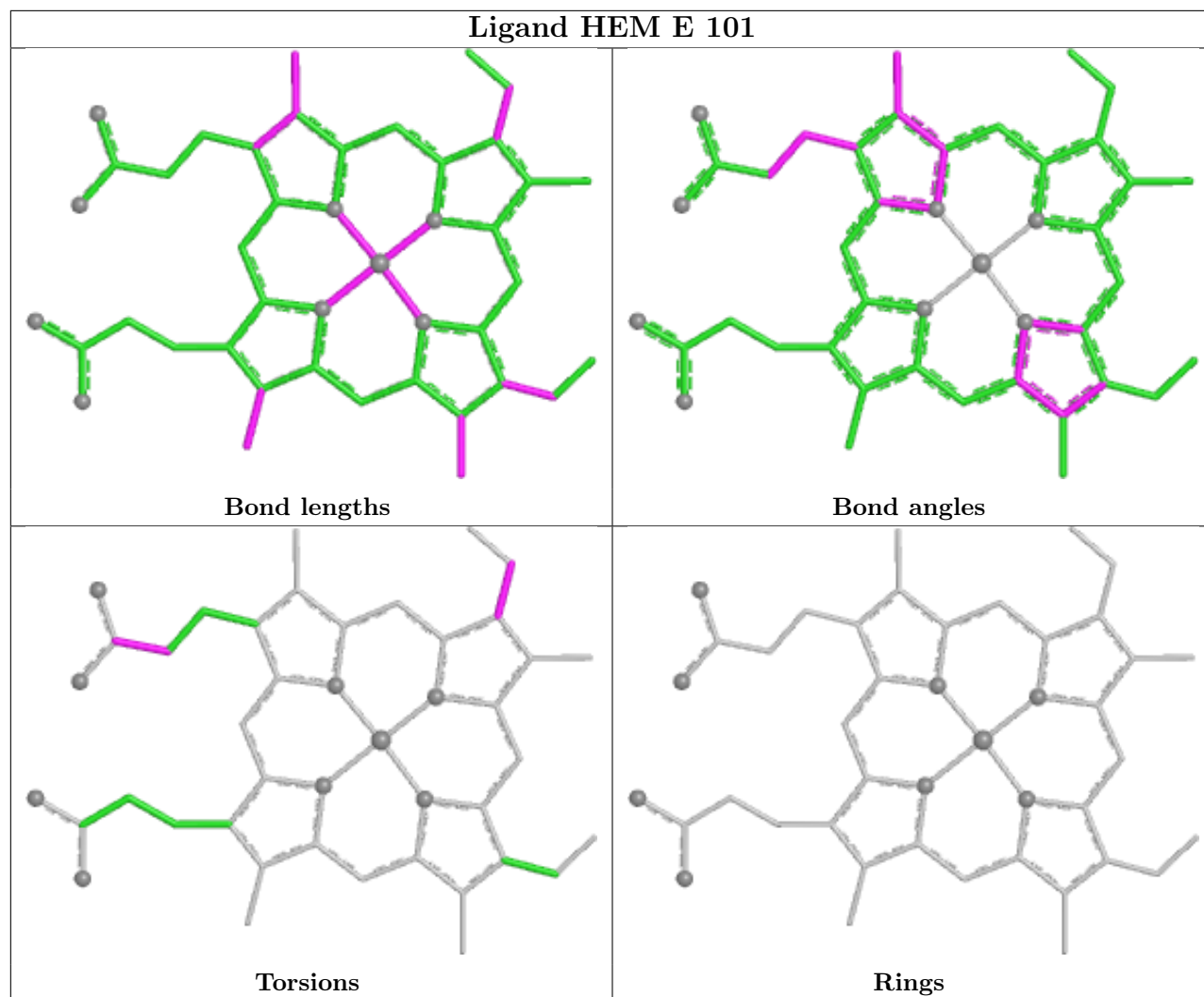
Ligand HEM e 101

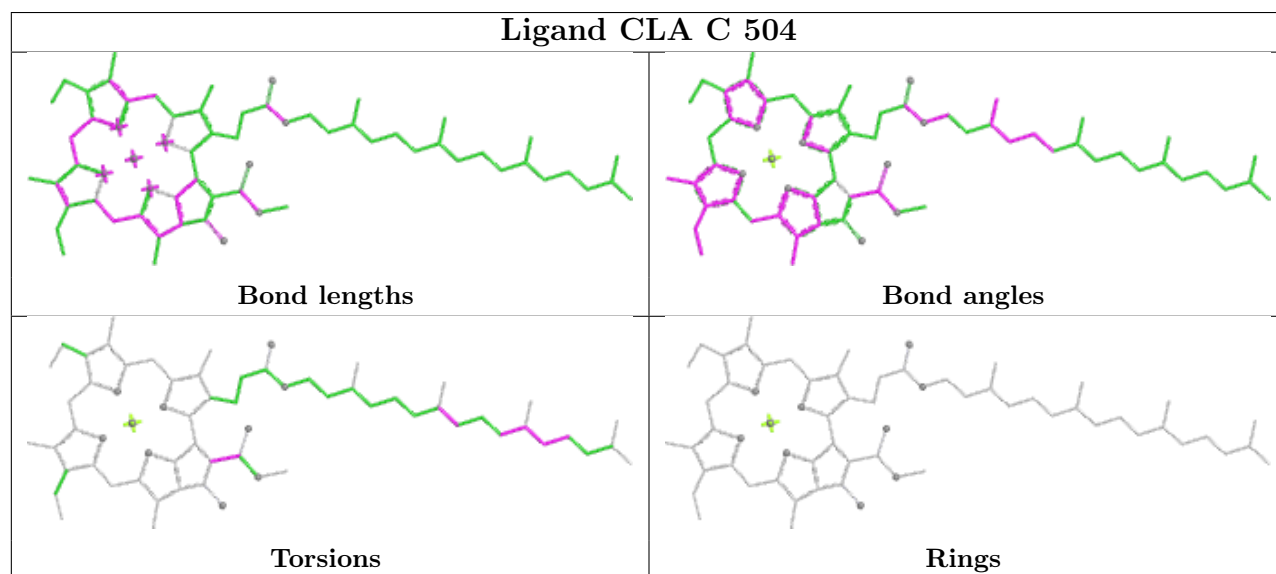
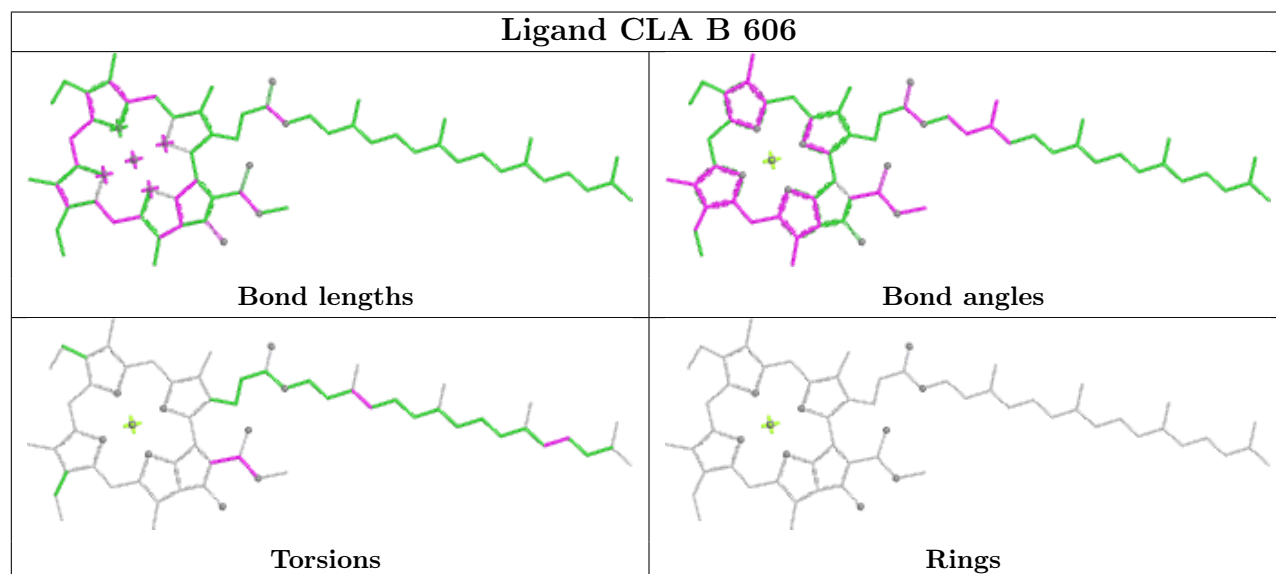
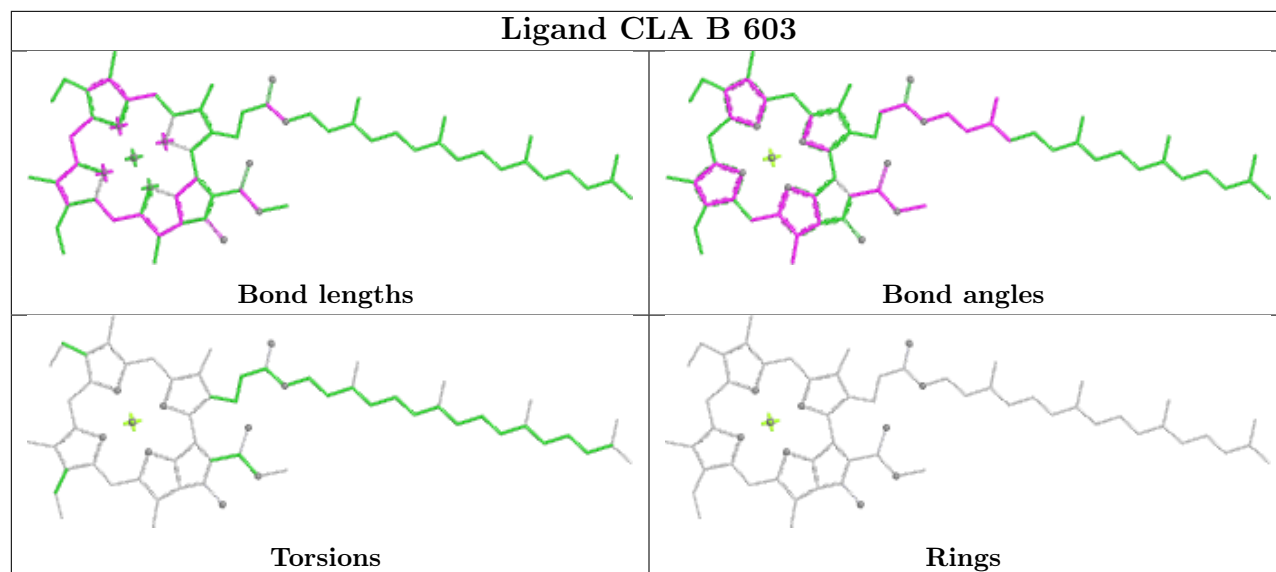




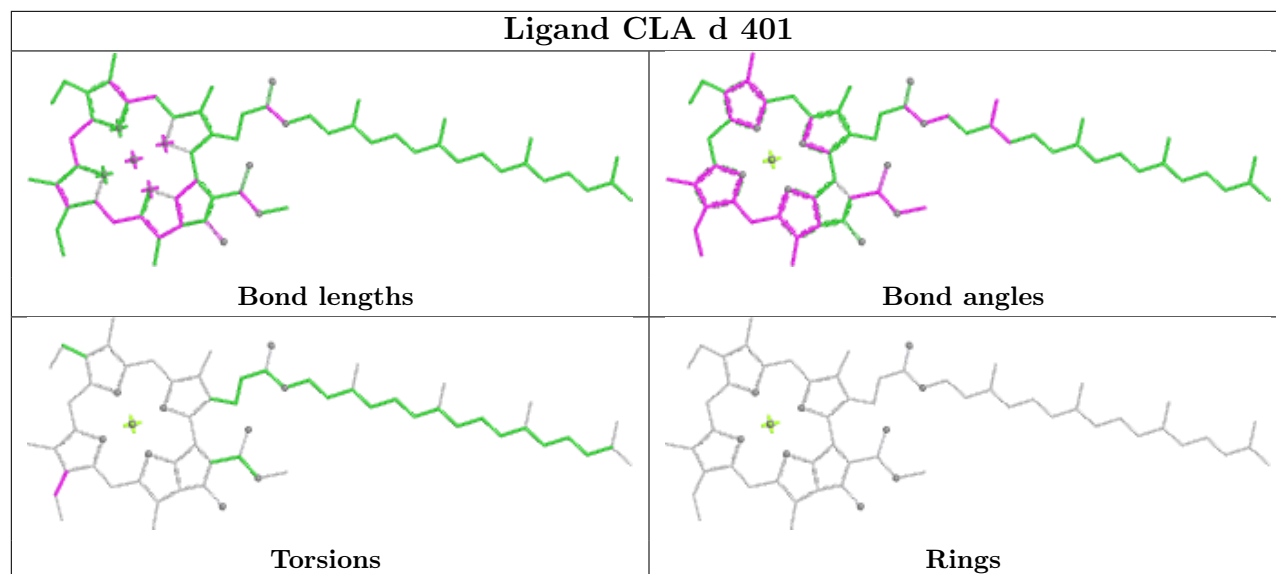




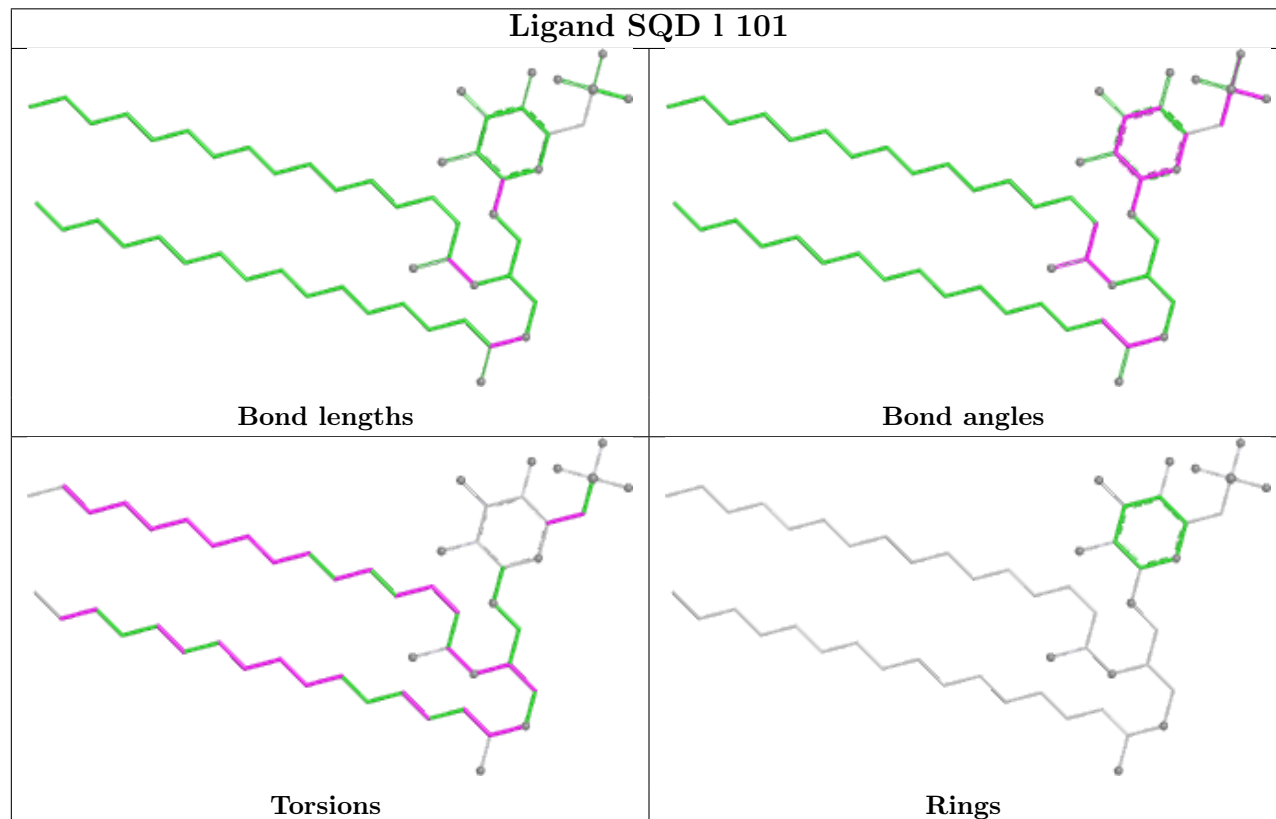


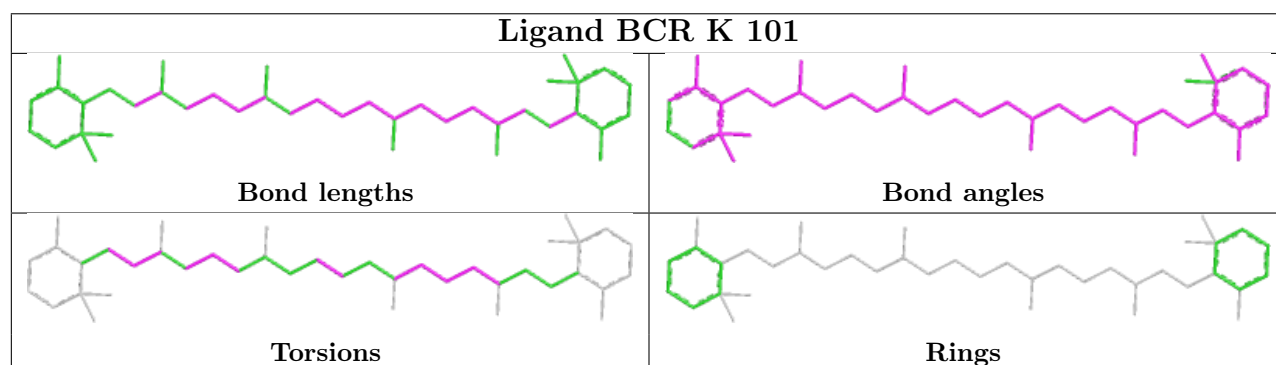
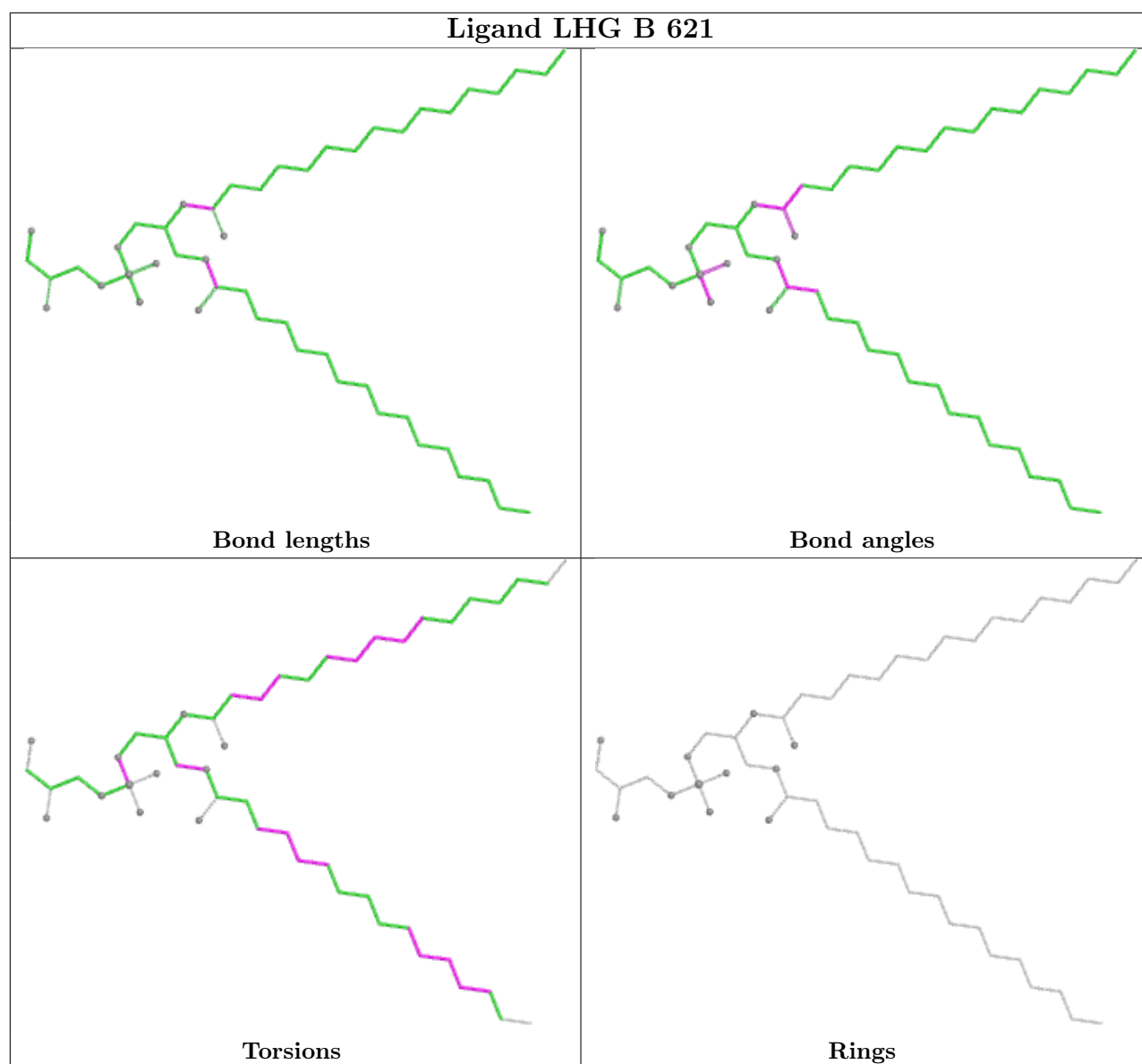


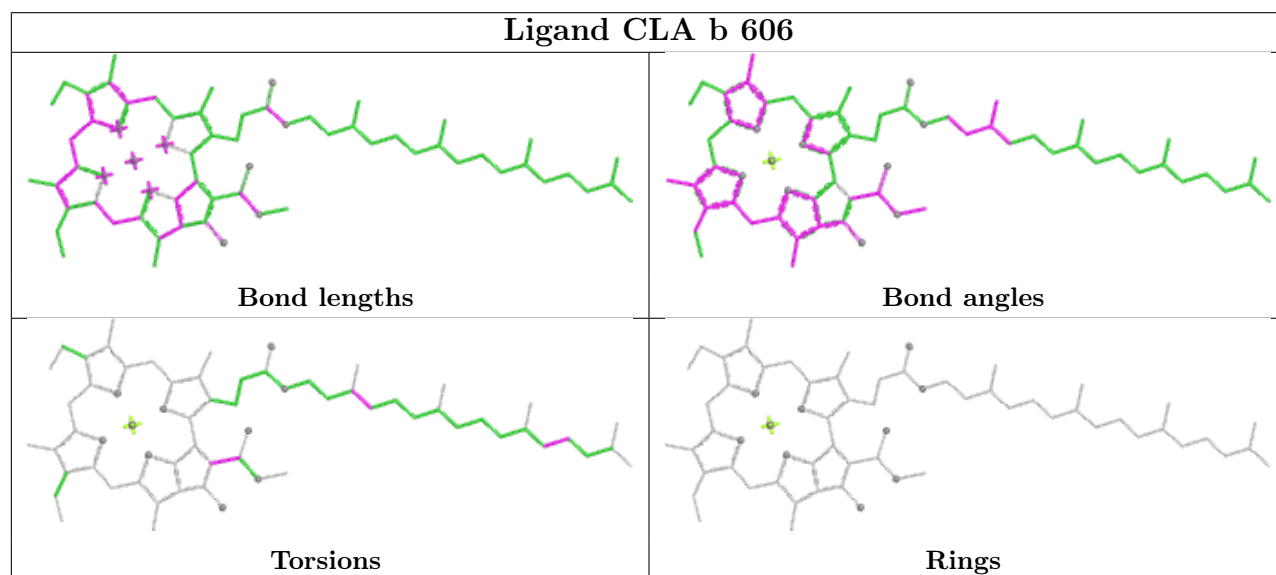
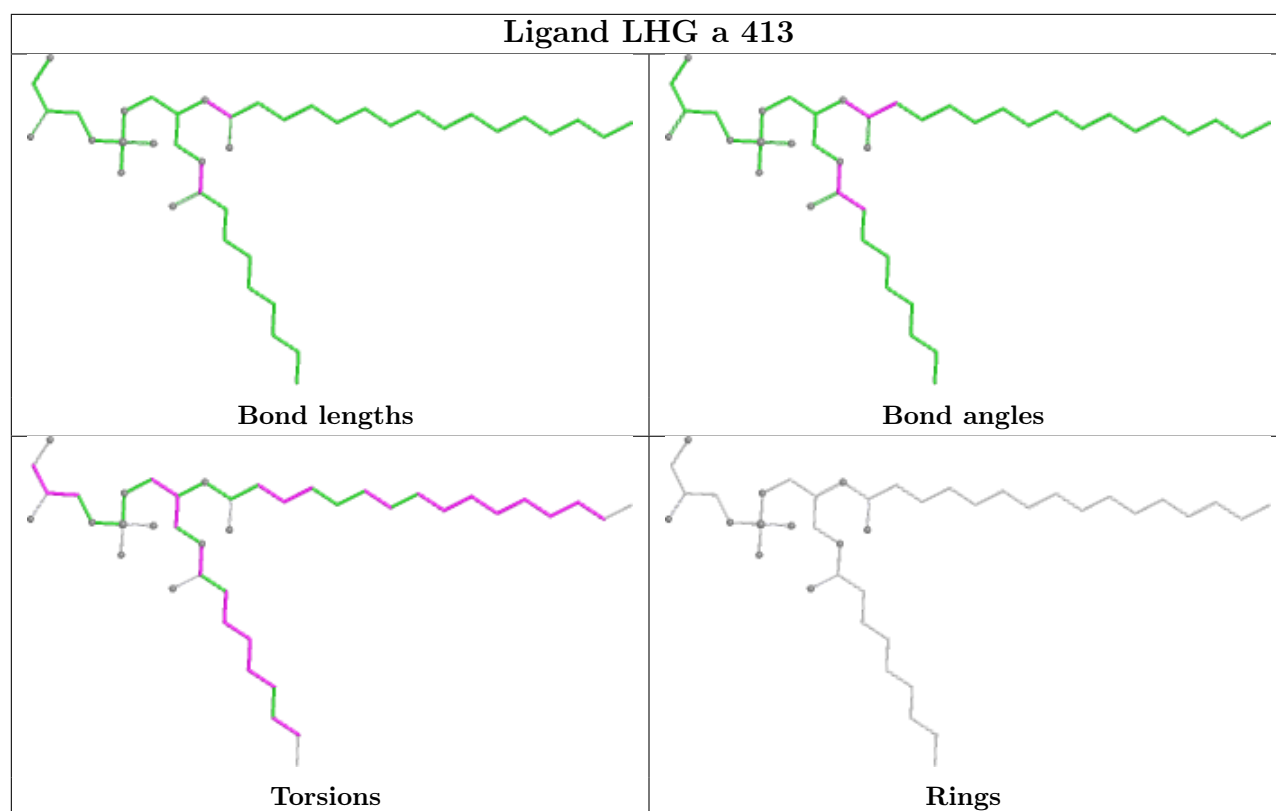
Ligand CLA d 401

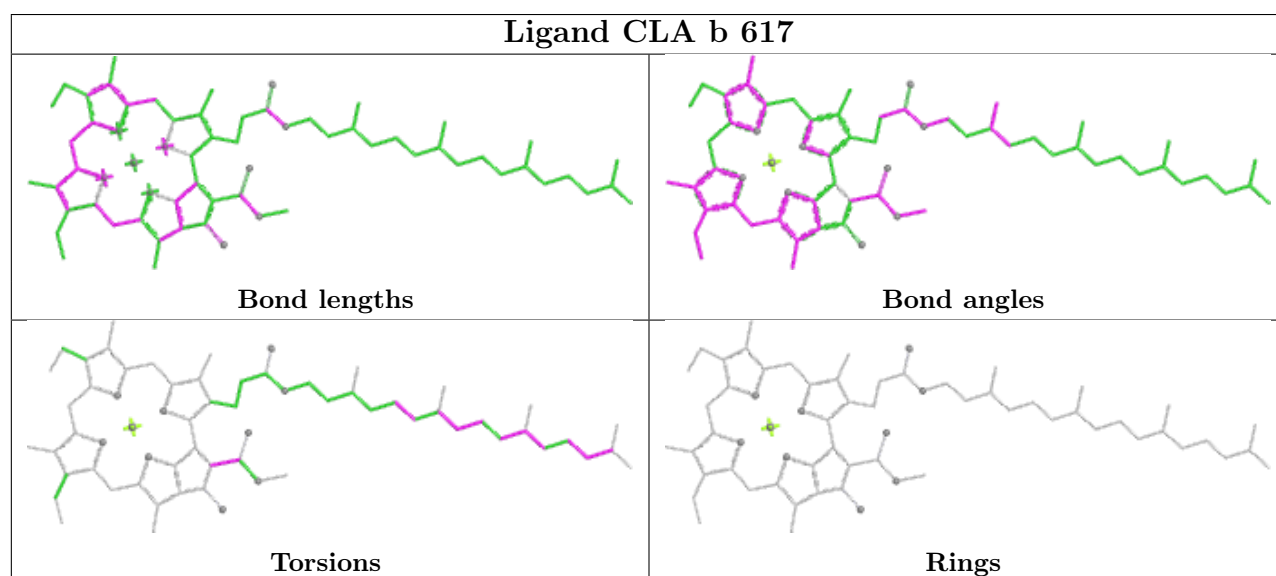
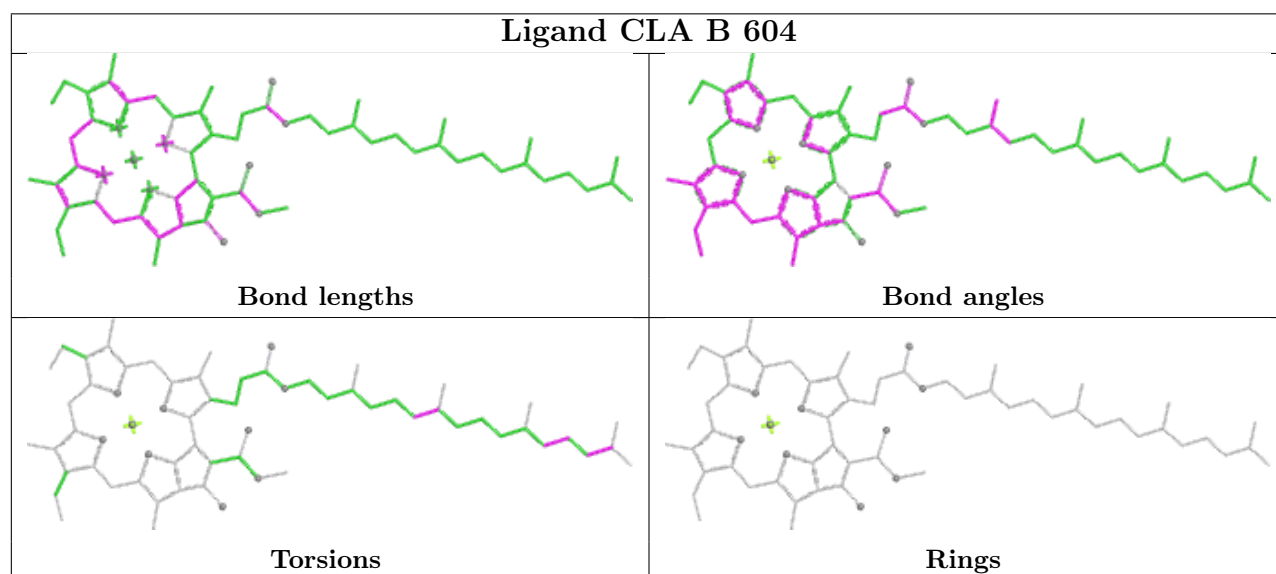
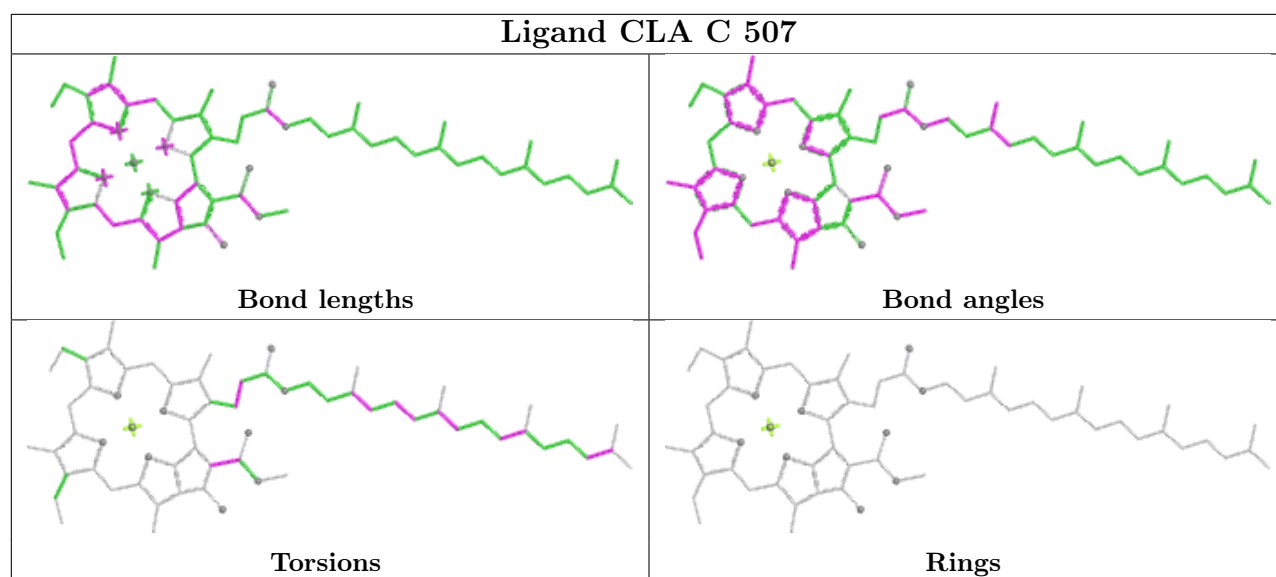


Ligand SQD l 101

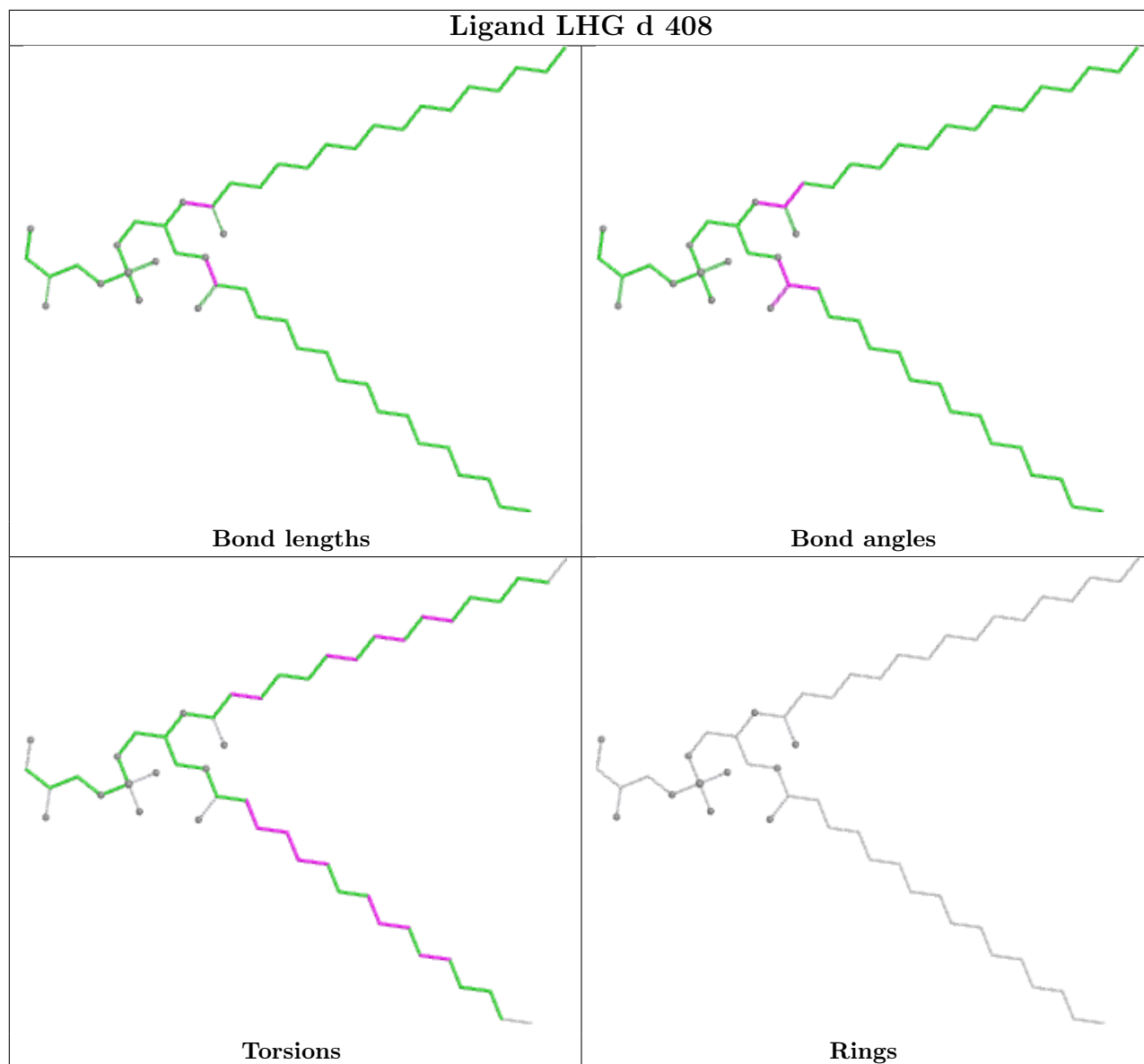




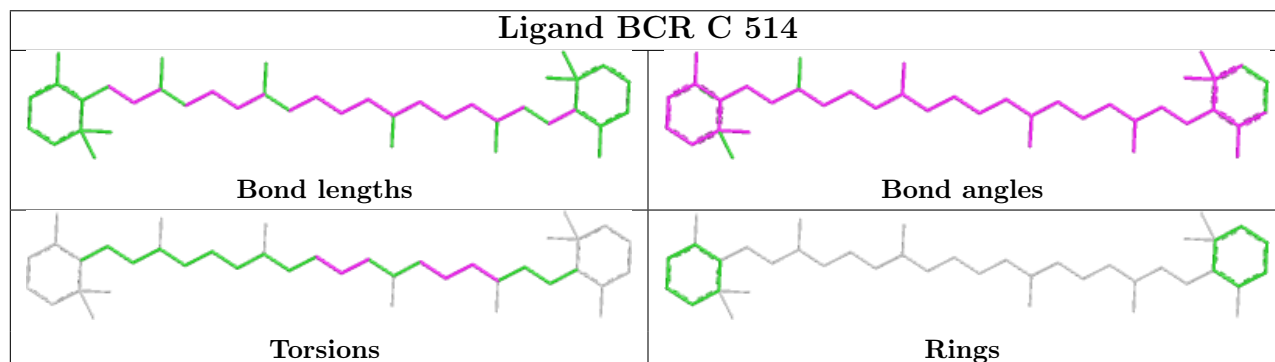


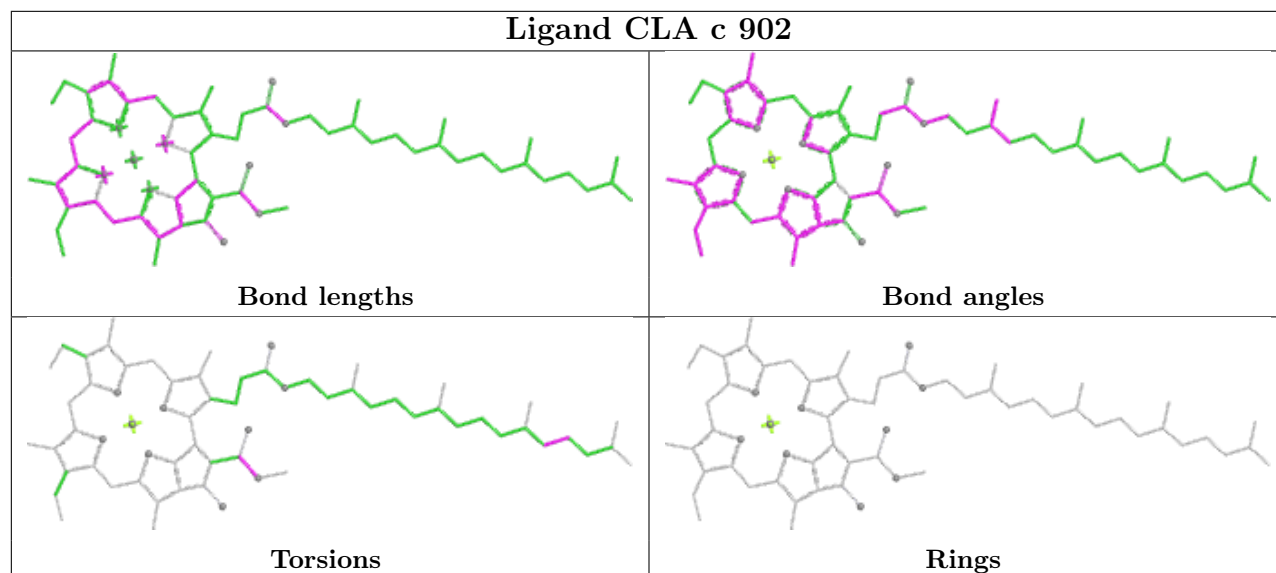
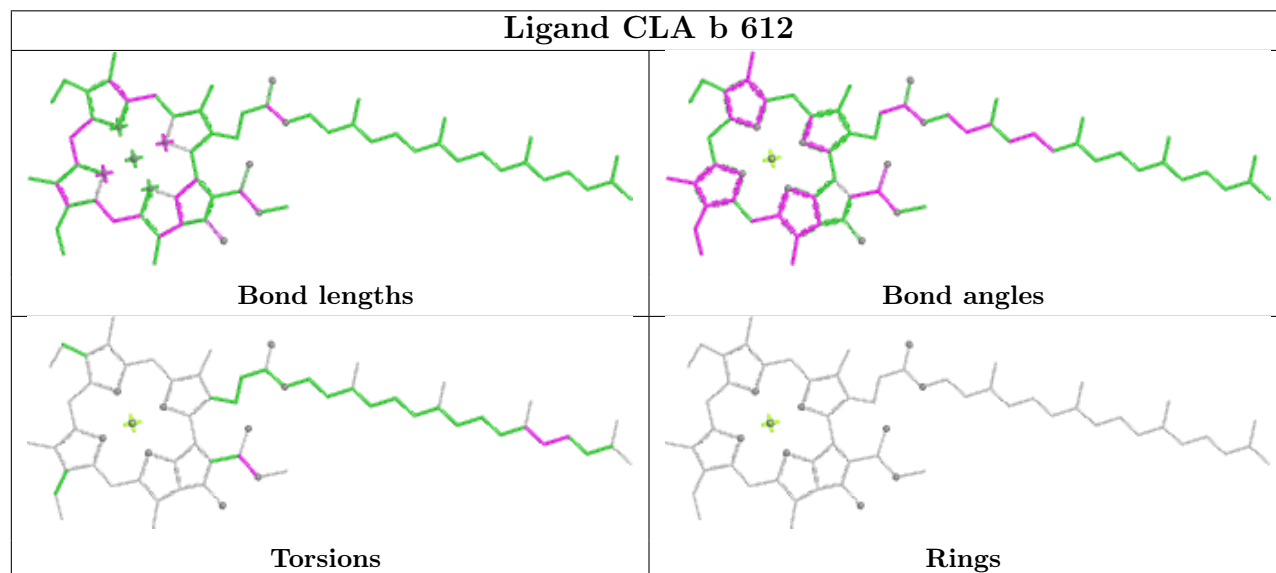
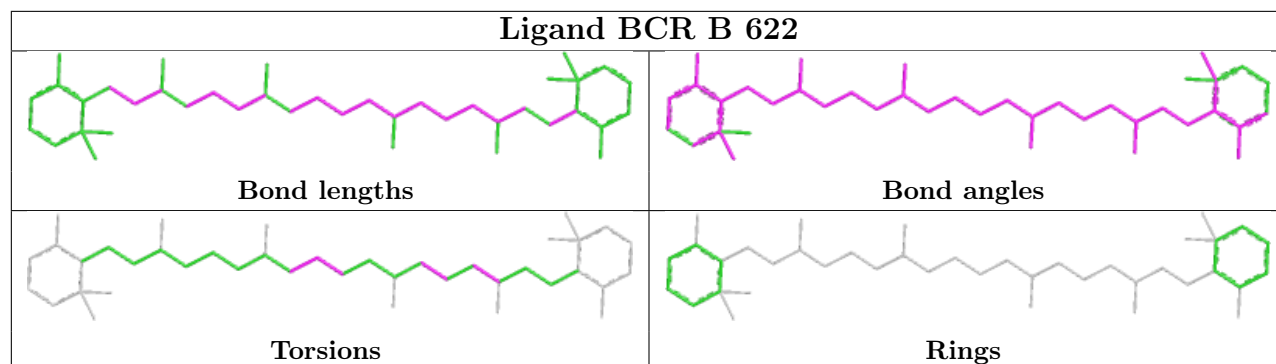


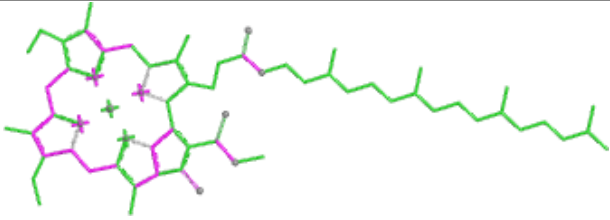
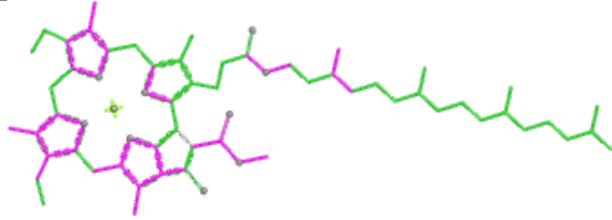
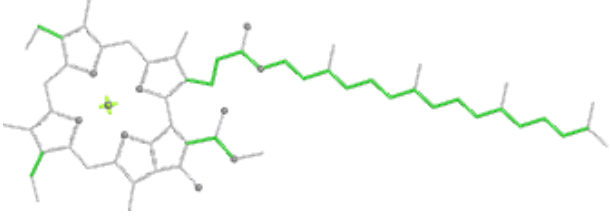
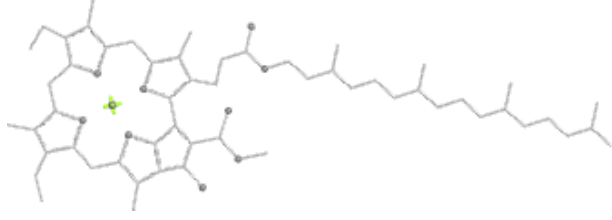
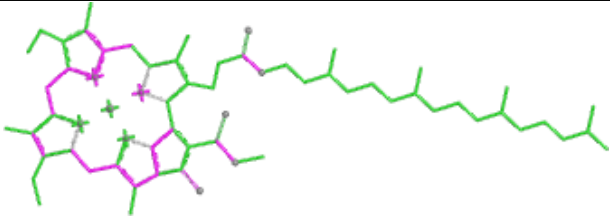
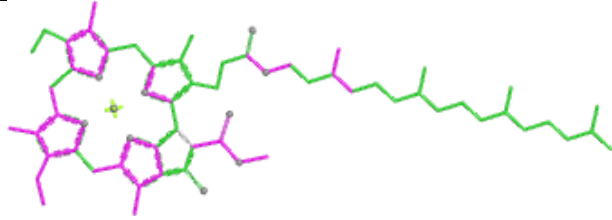
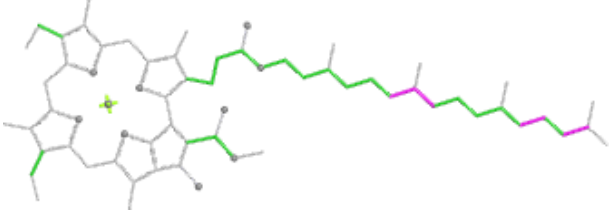
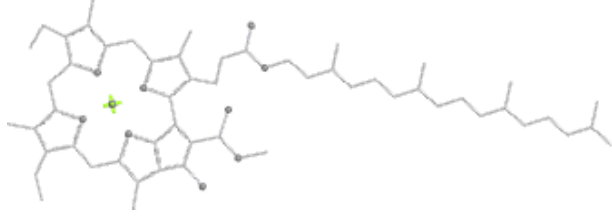
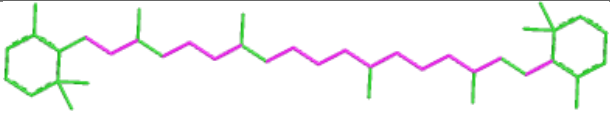
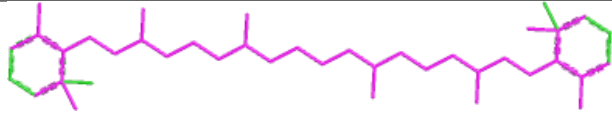
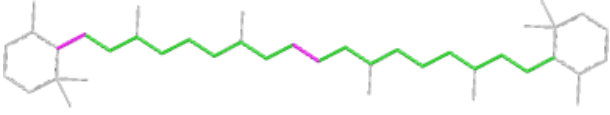
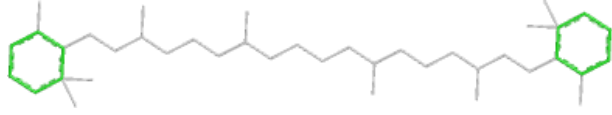
Ligand LHG d 408

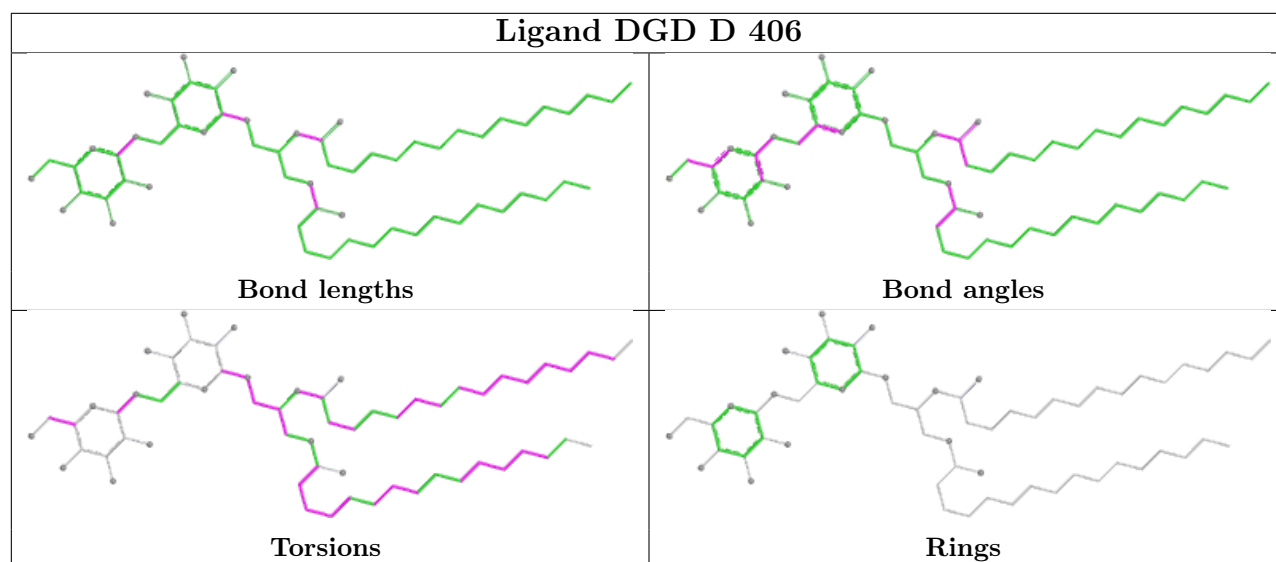
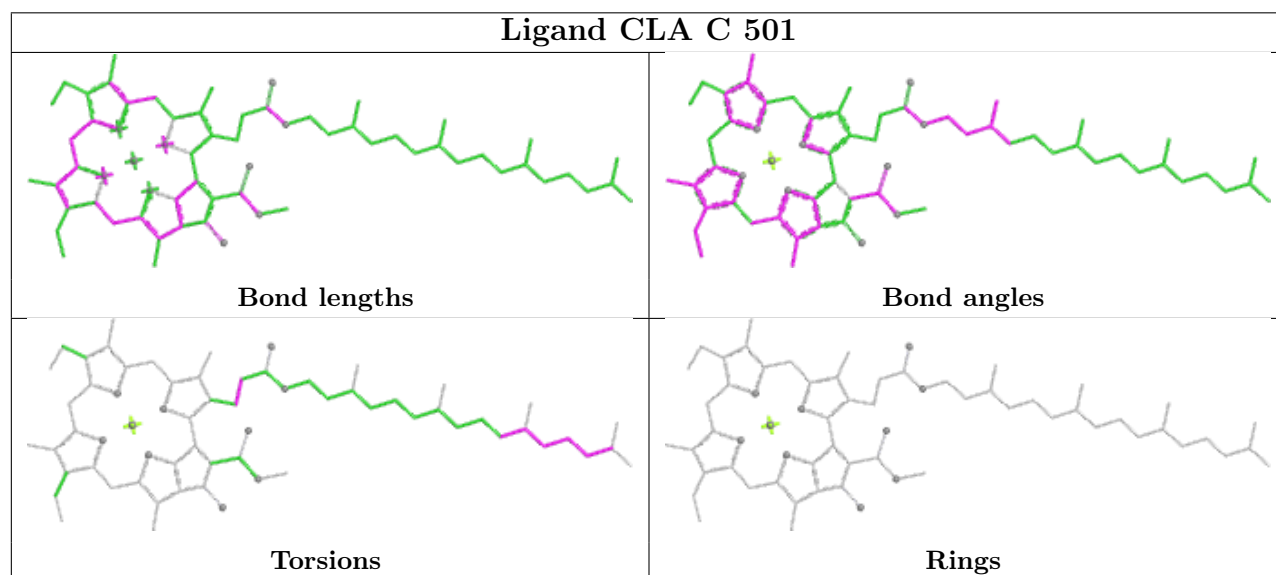
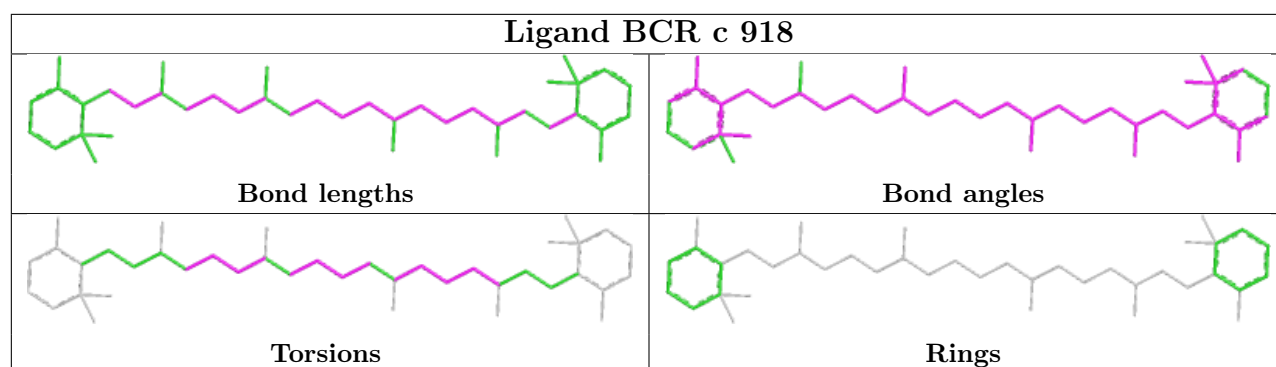


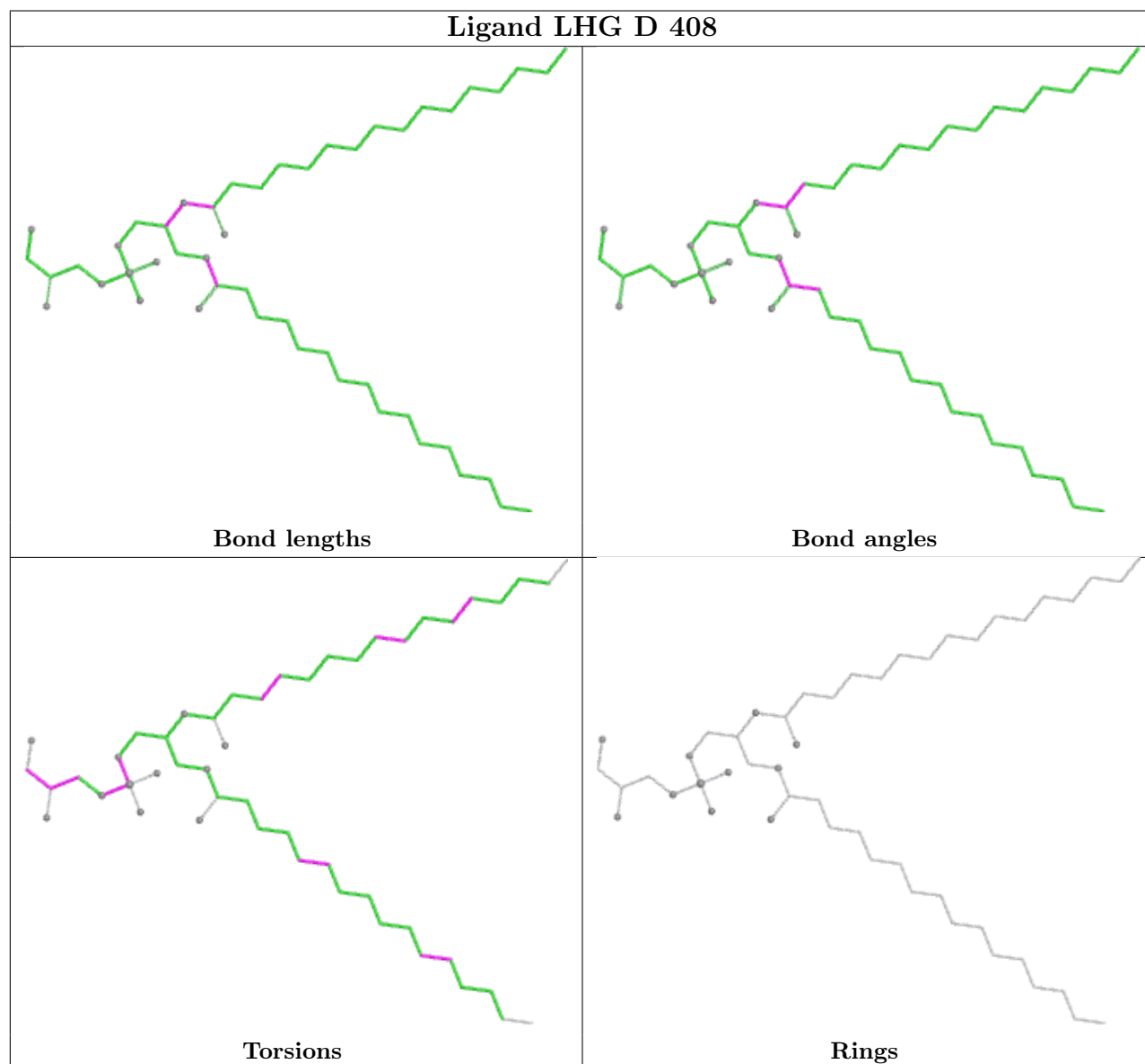
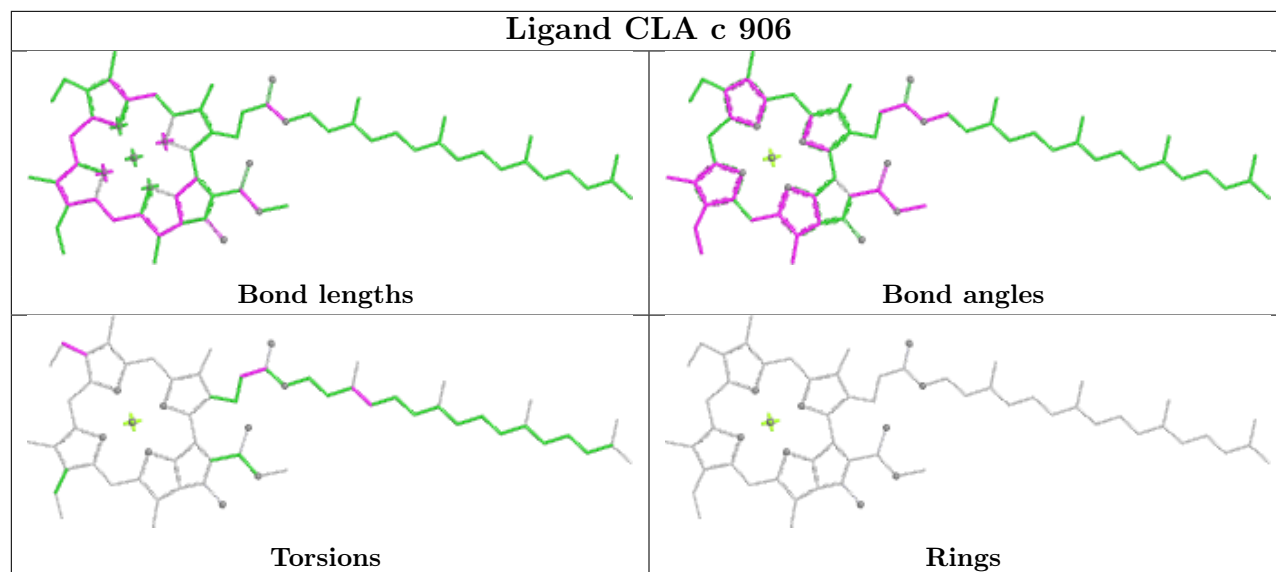
Ligand BCR C 514

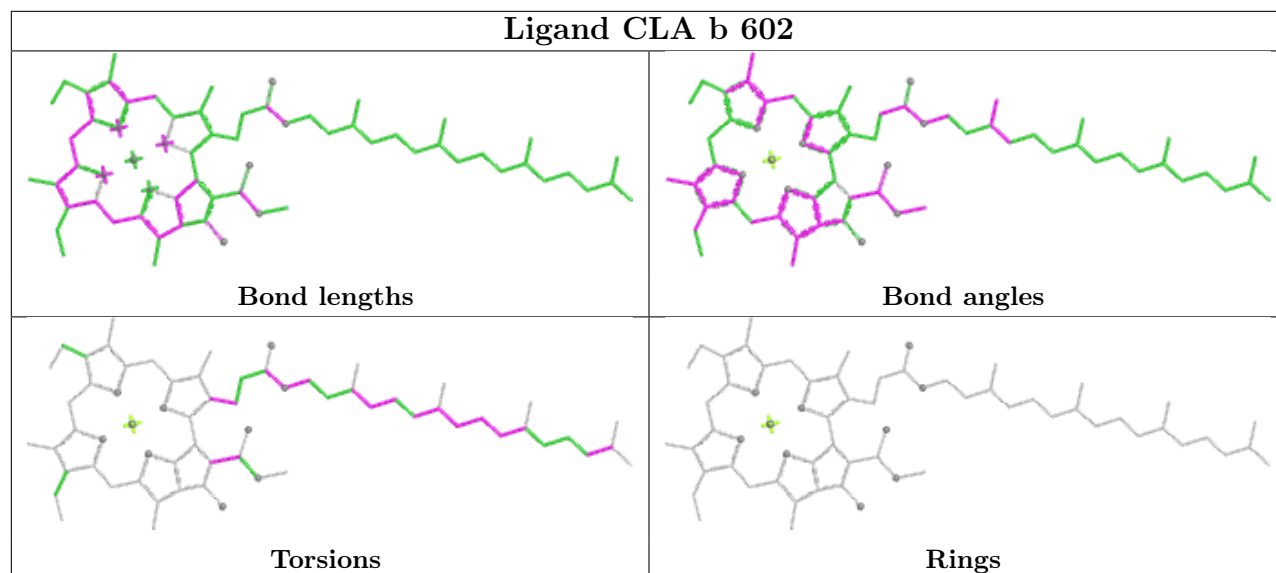
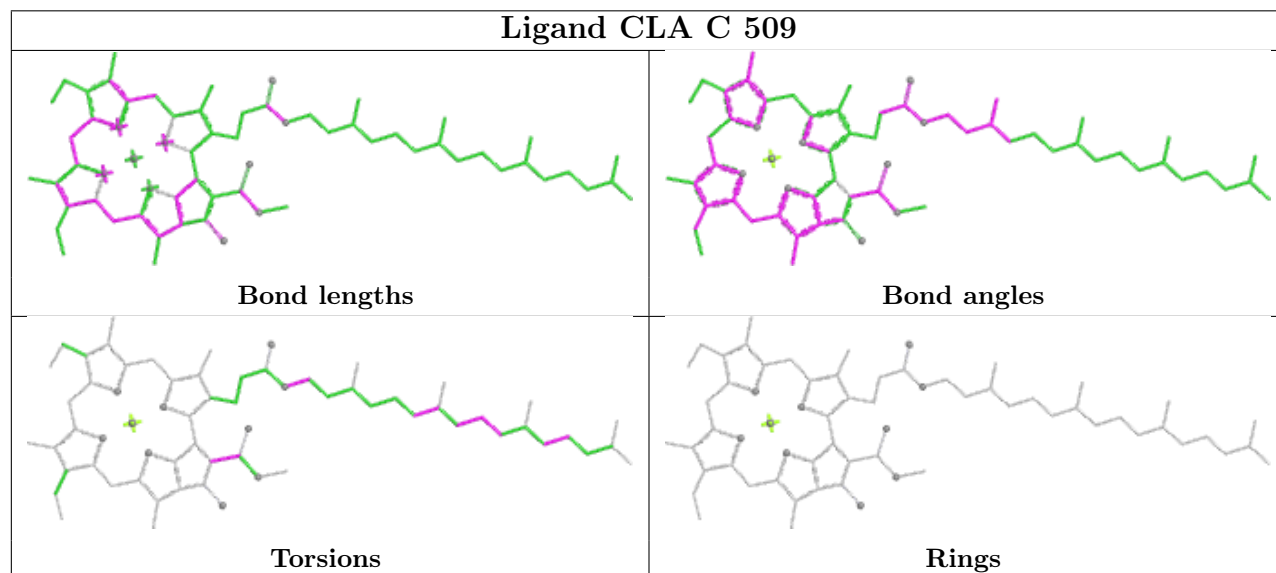
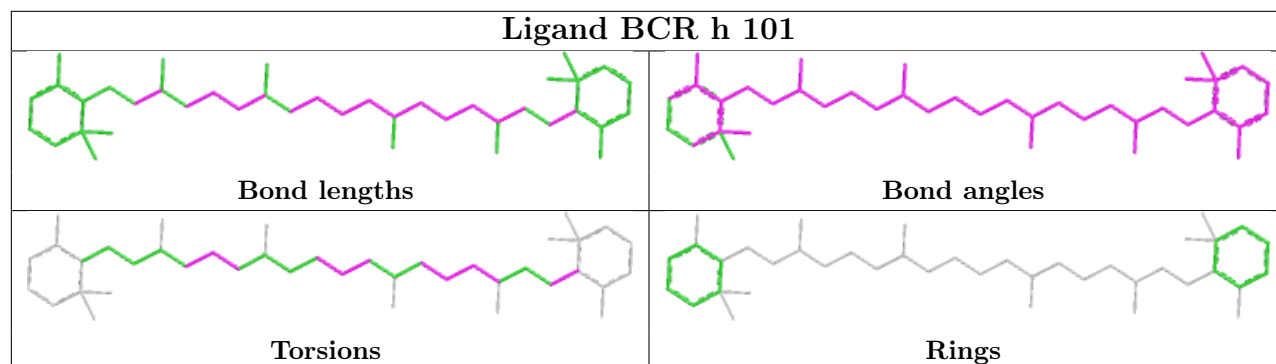


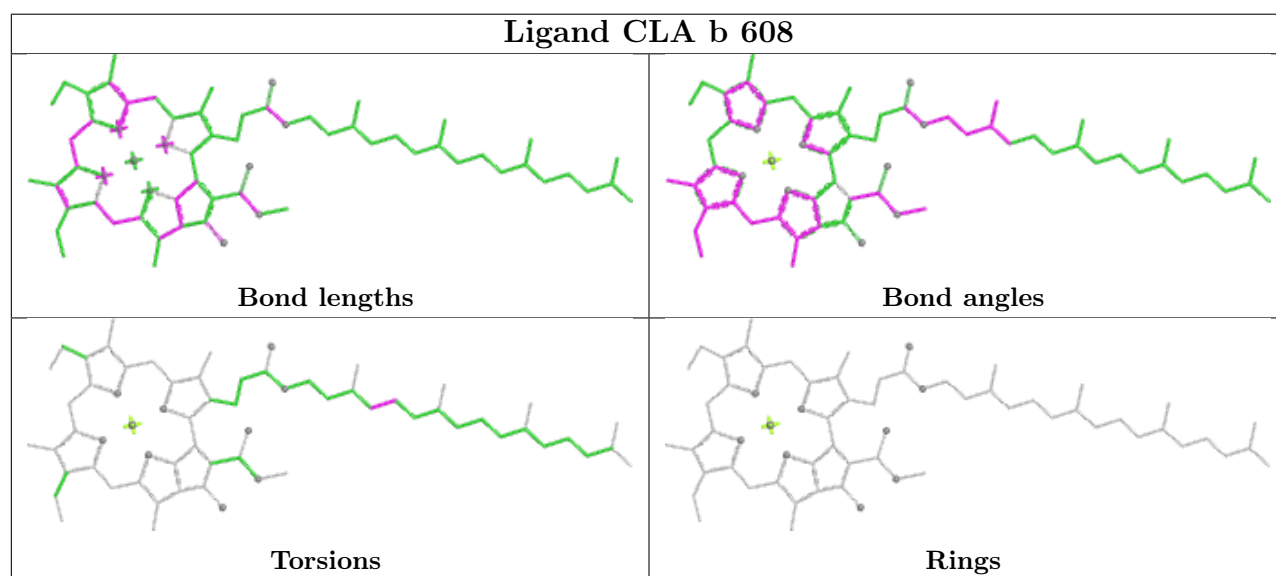
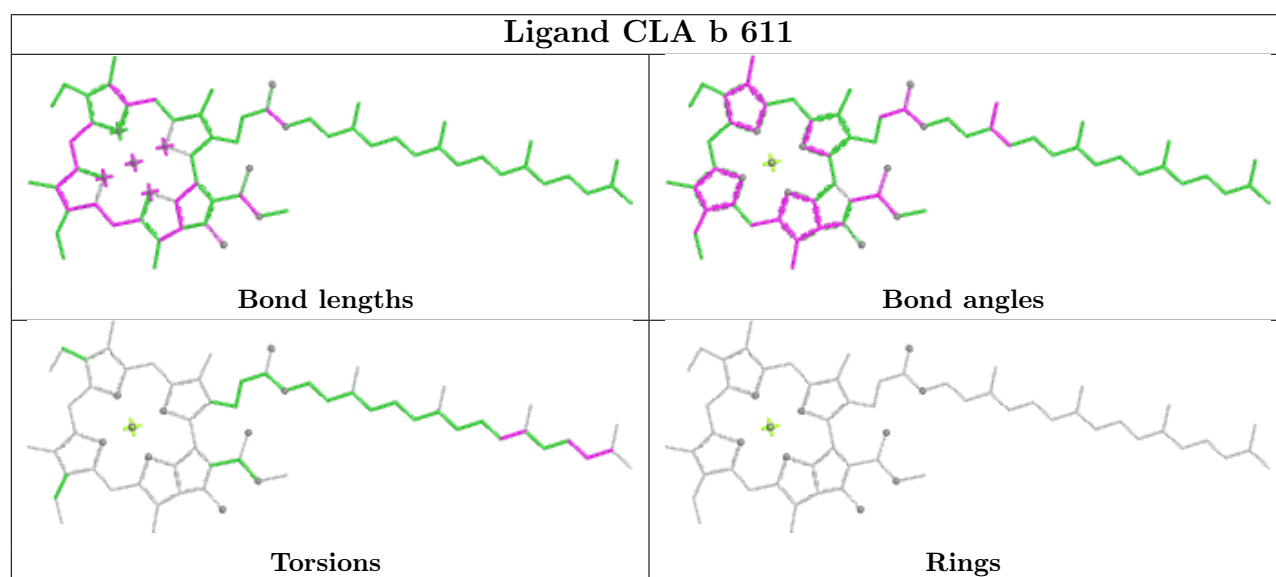
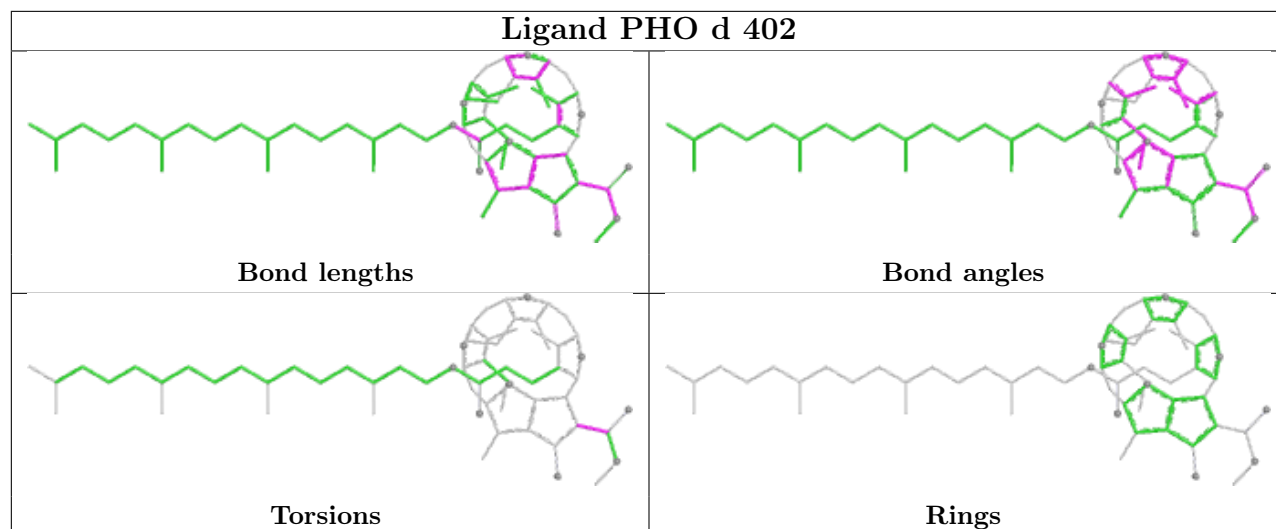


Ligand CLA C 511	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA A 607	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR T 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

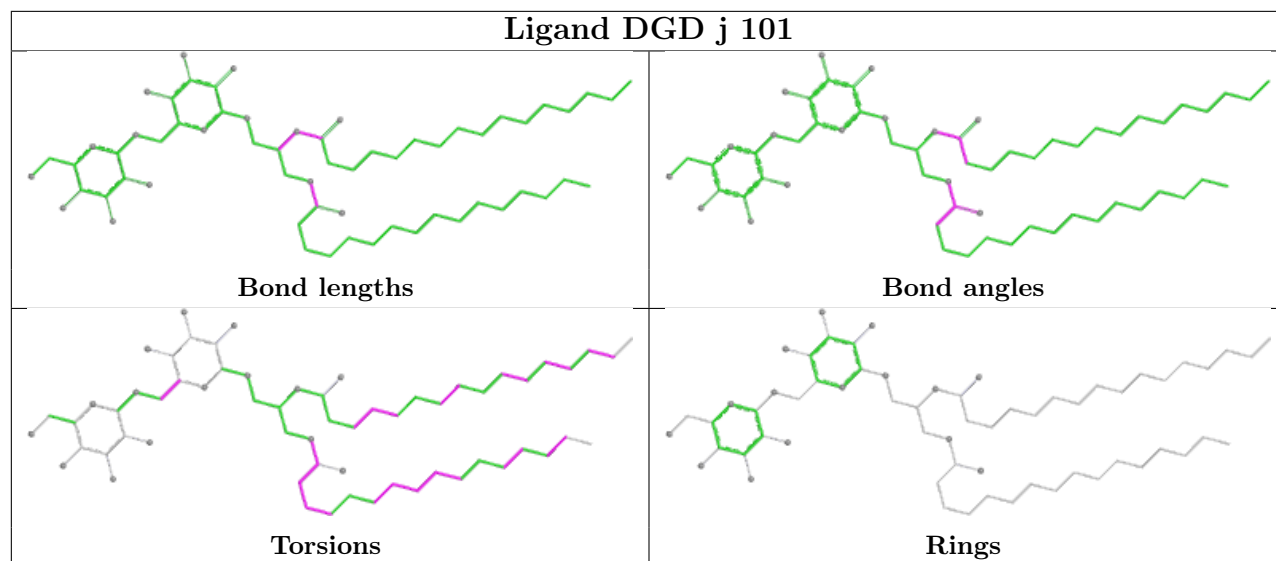




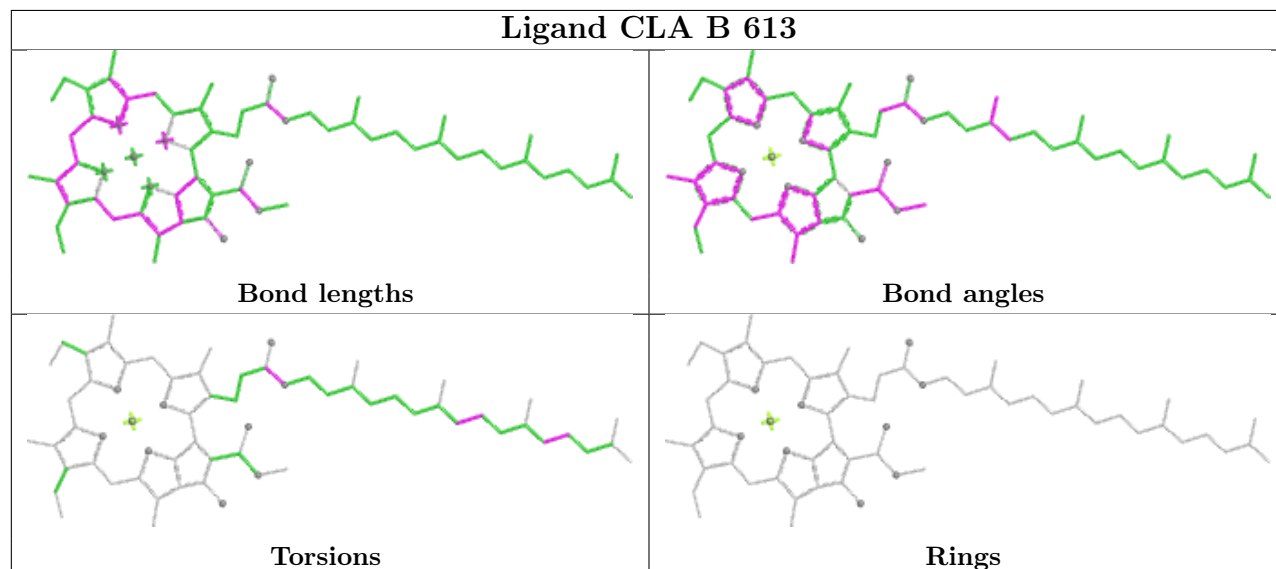




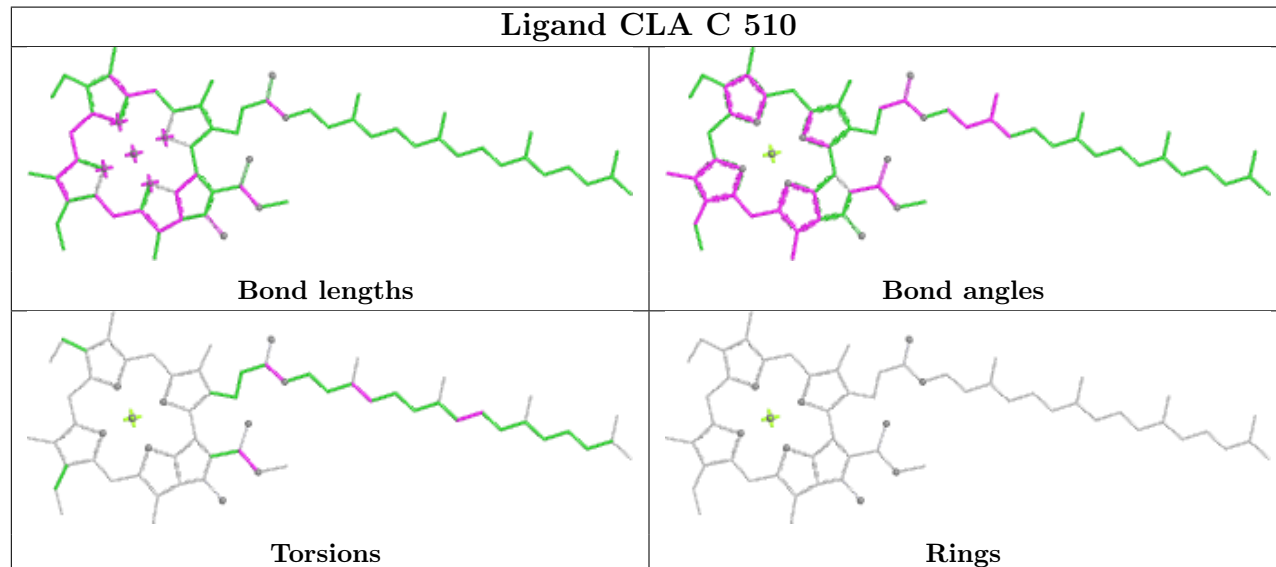
Ligand DGD j 101

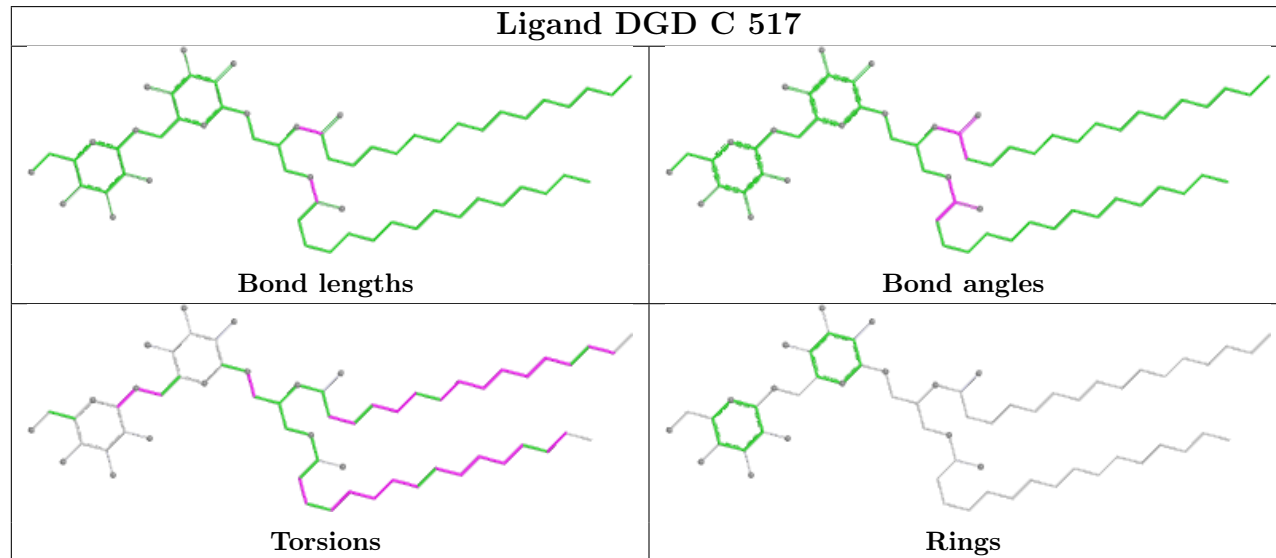
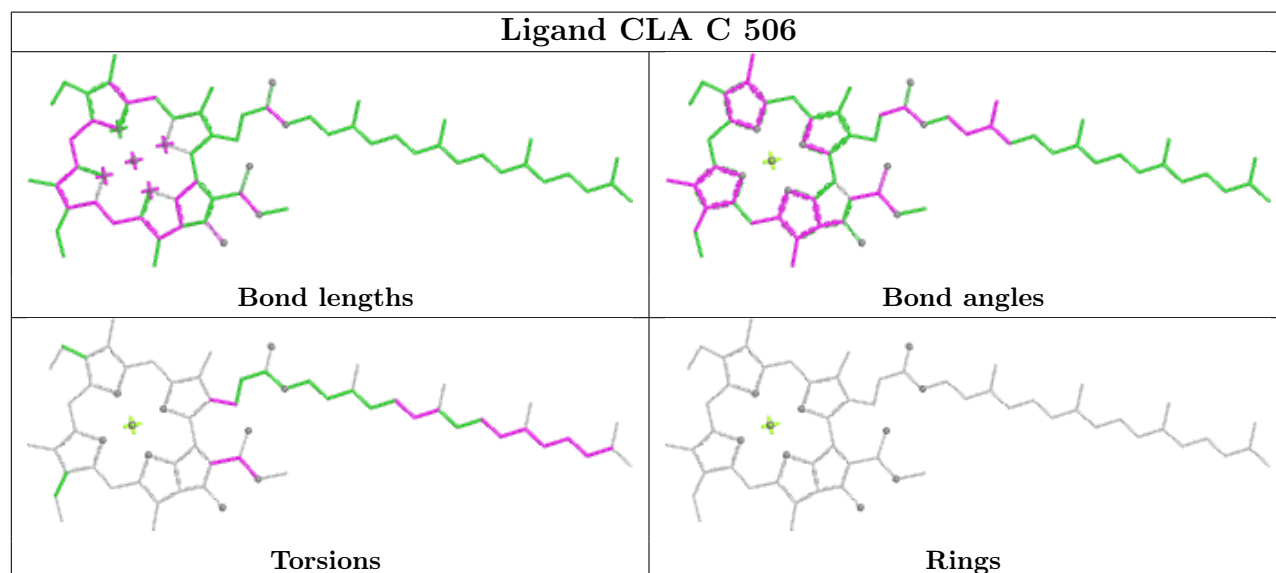
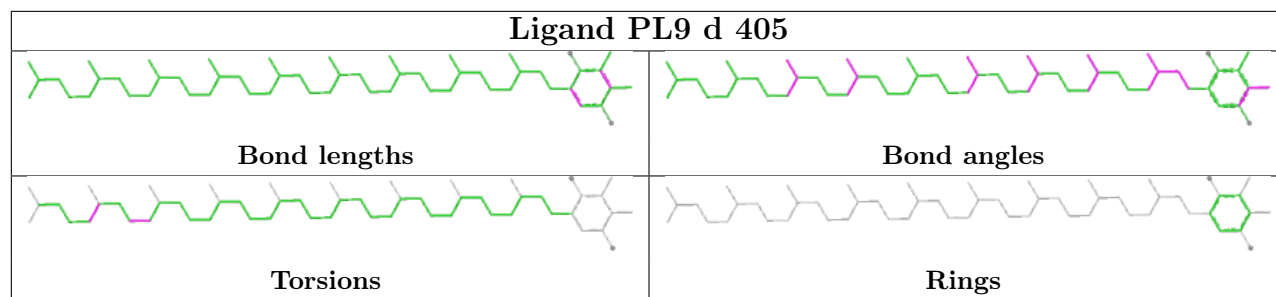


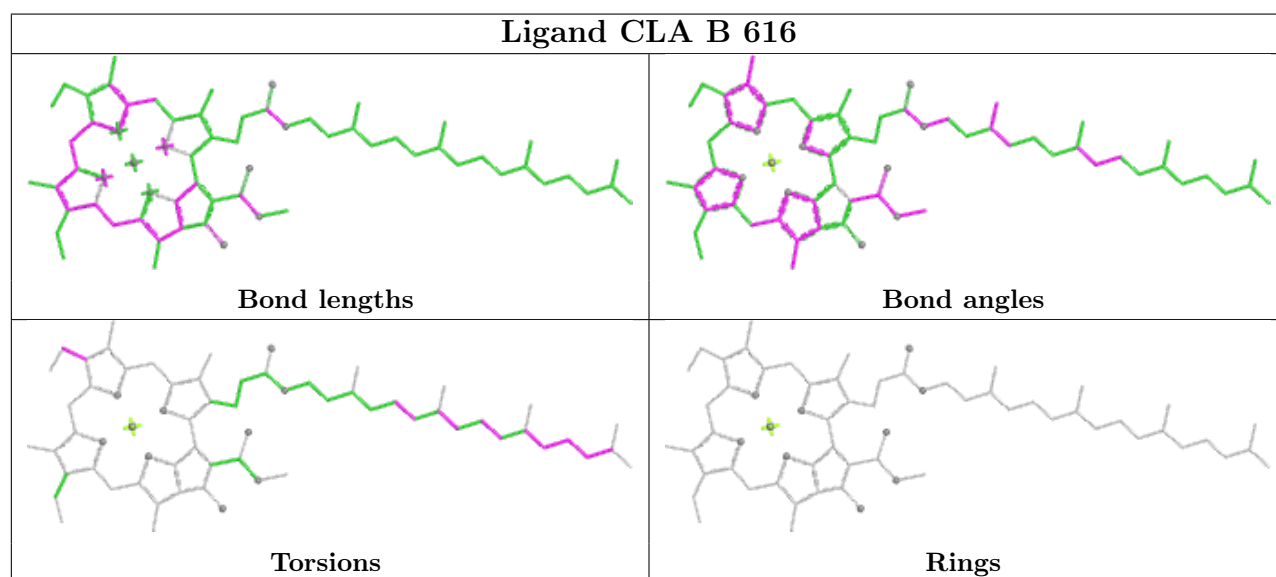
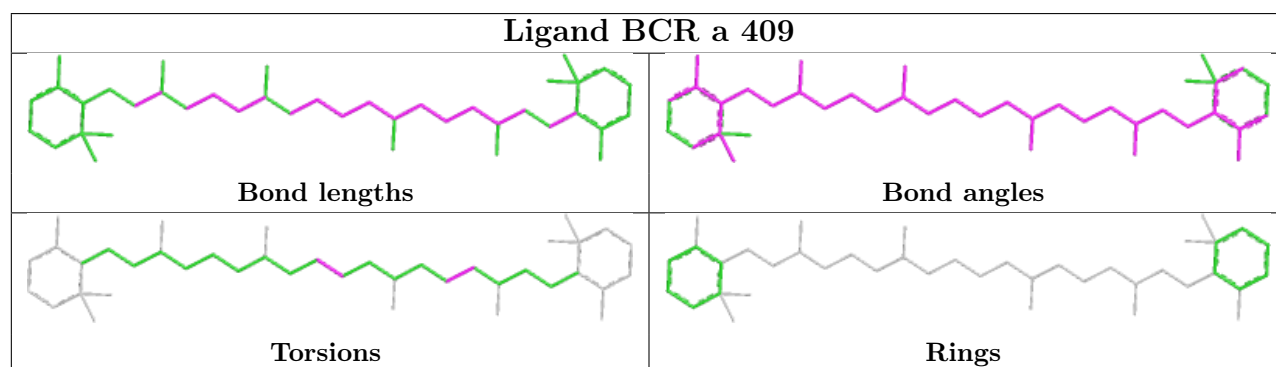
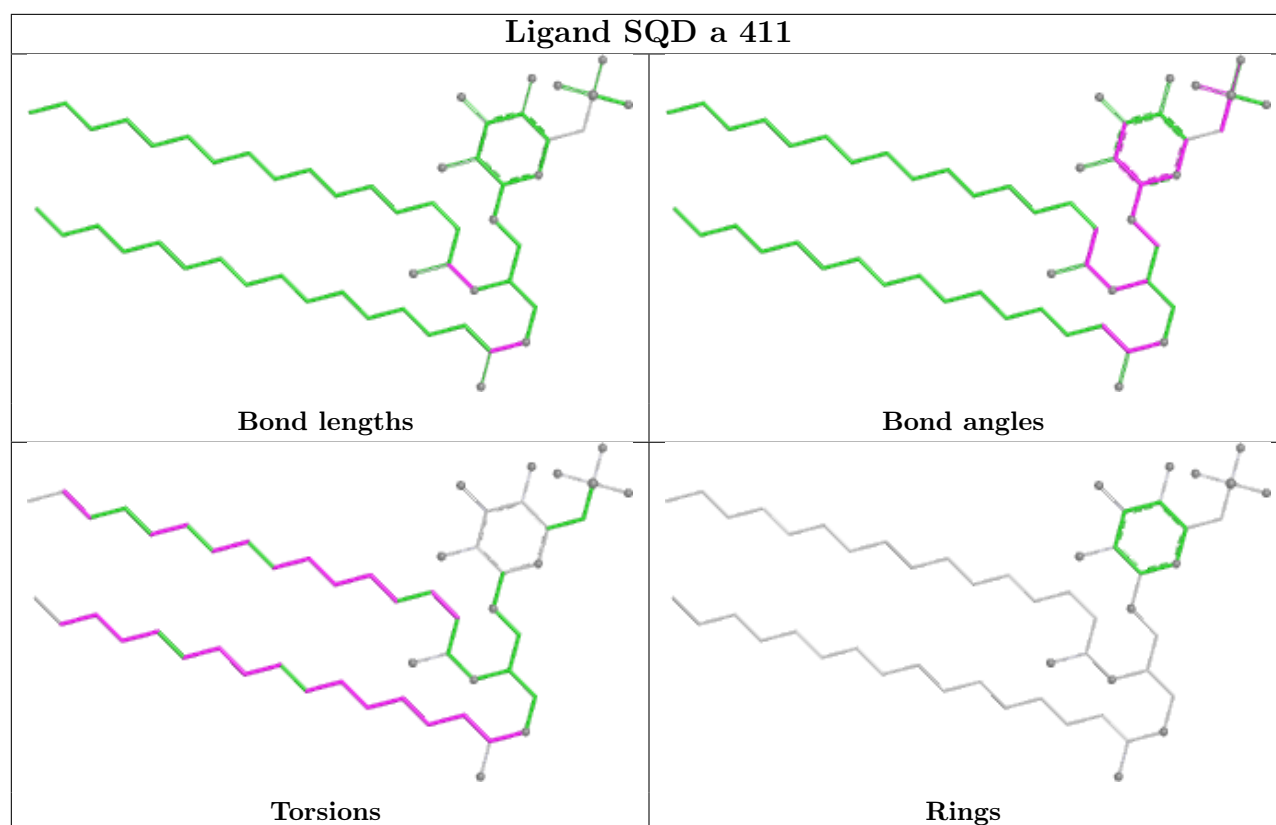
Ligand CLA B 613

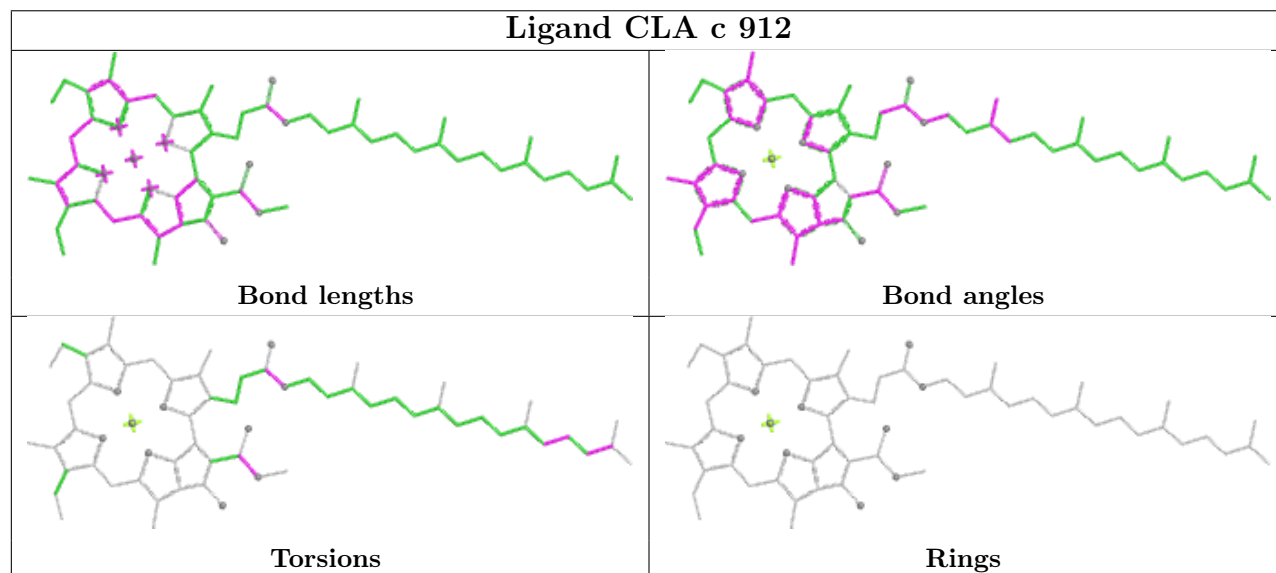
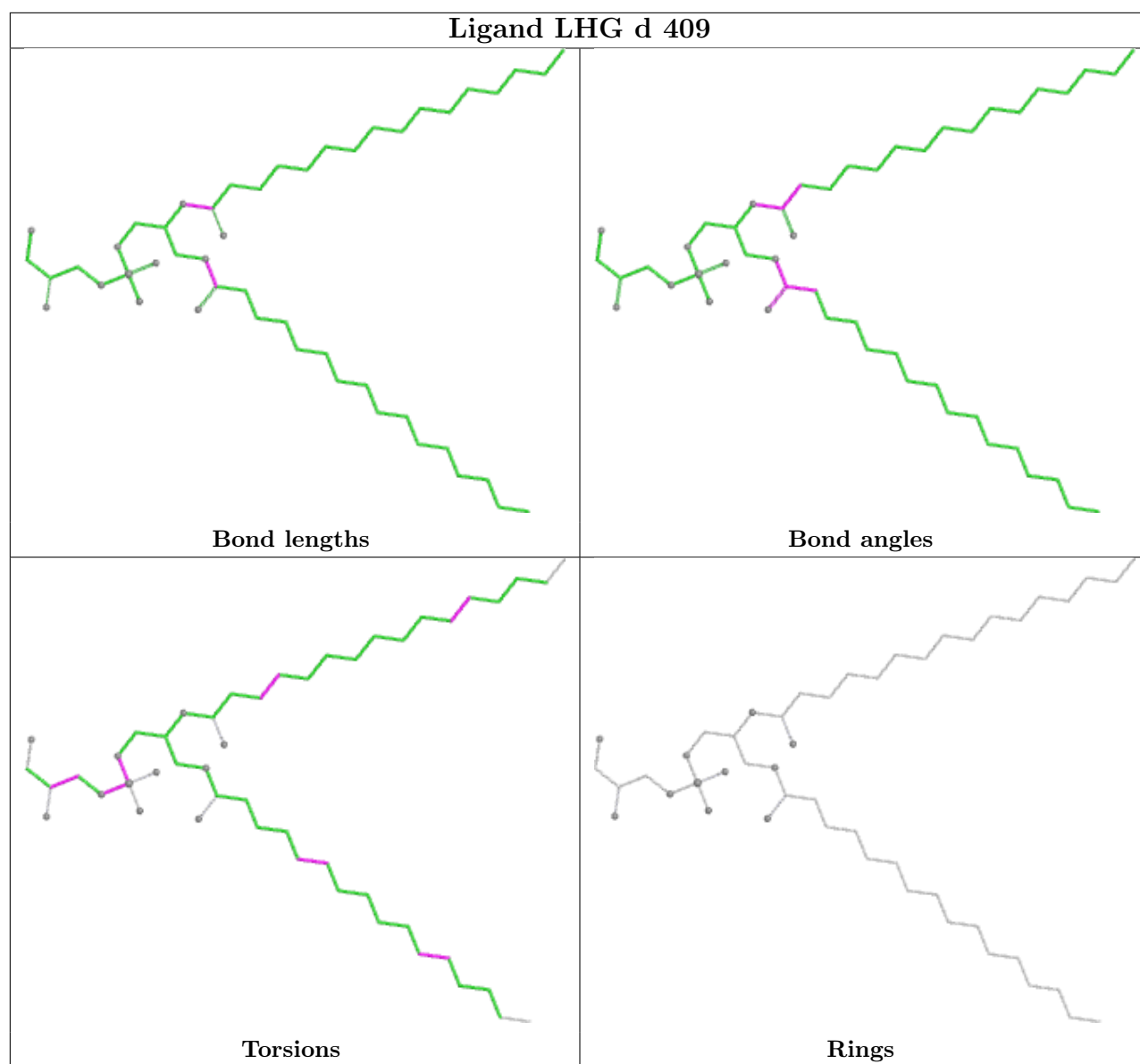


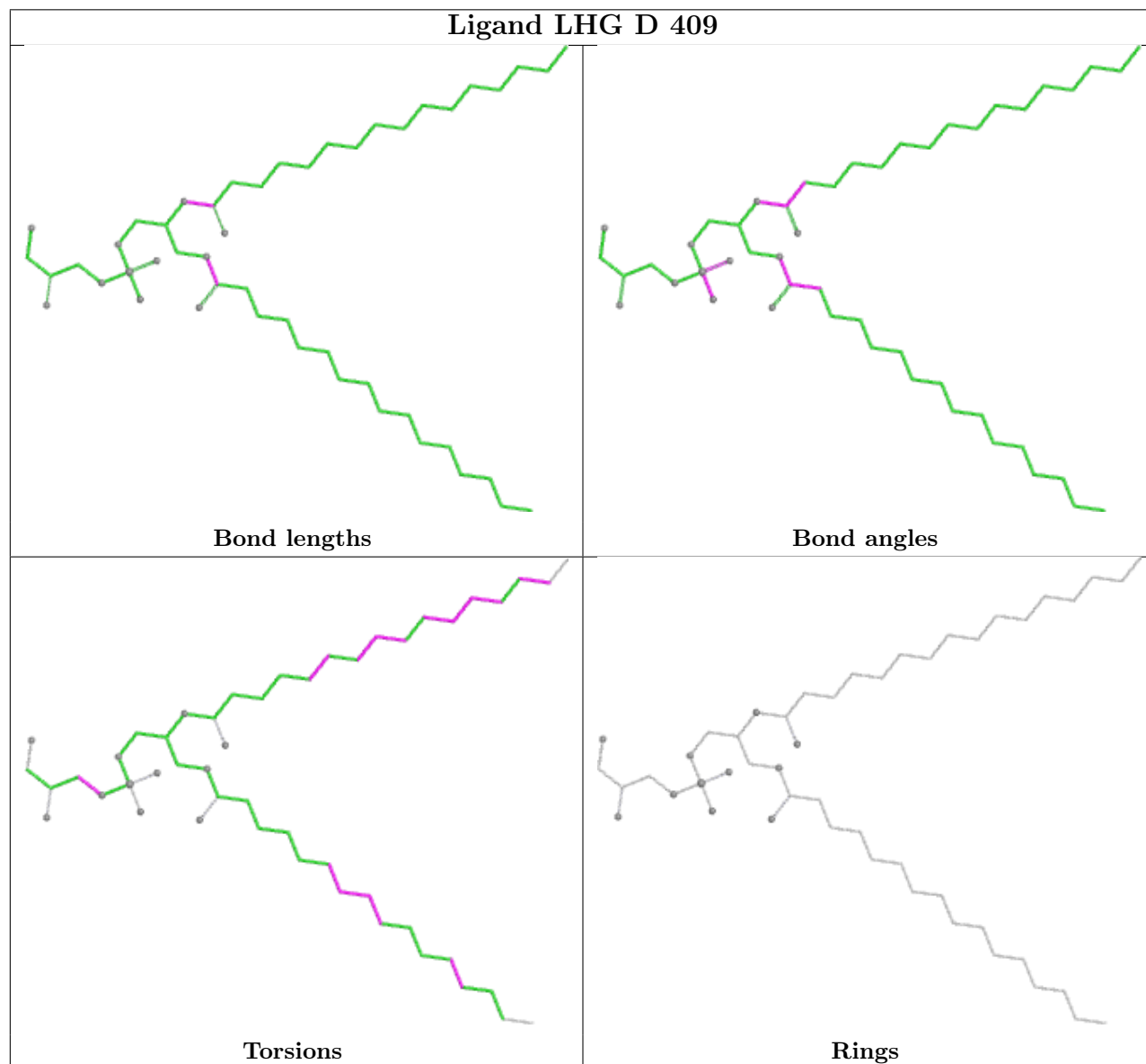
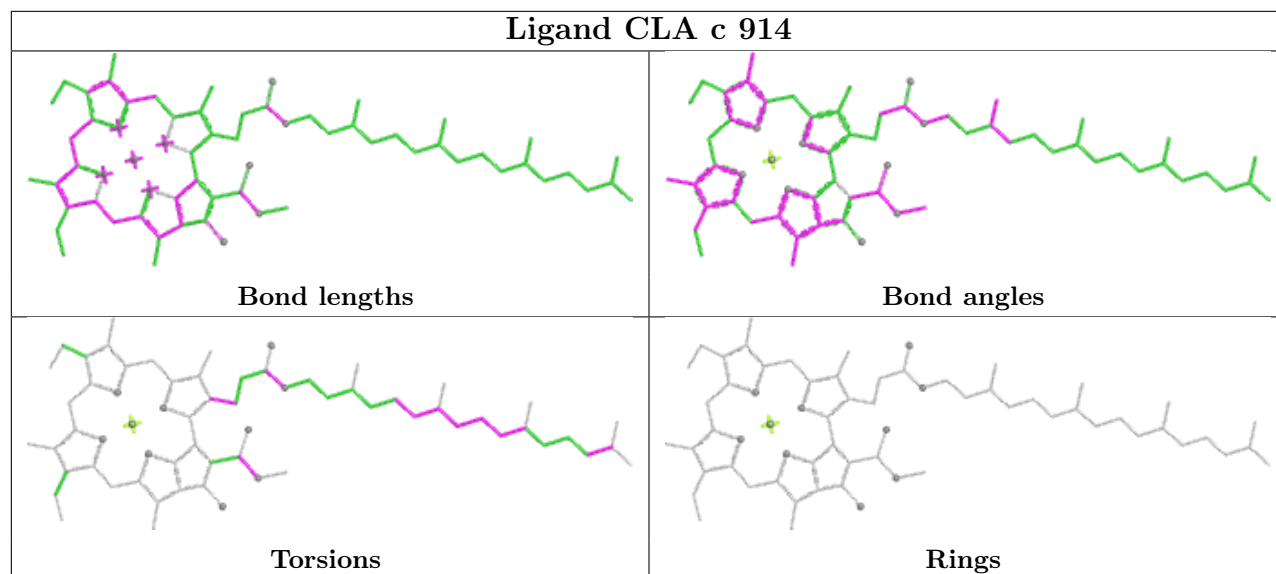
Ligand CLA C 510

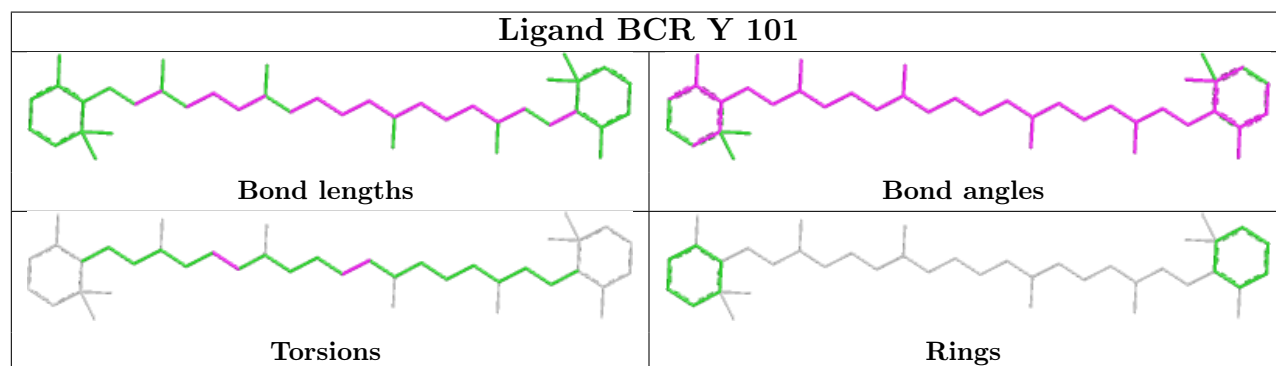
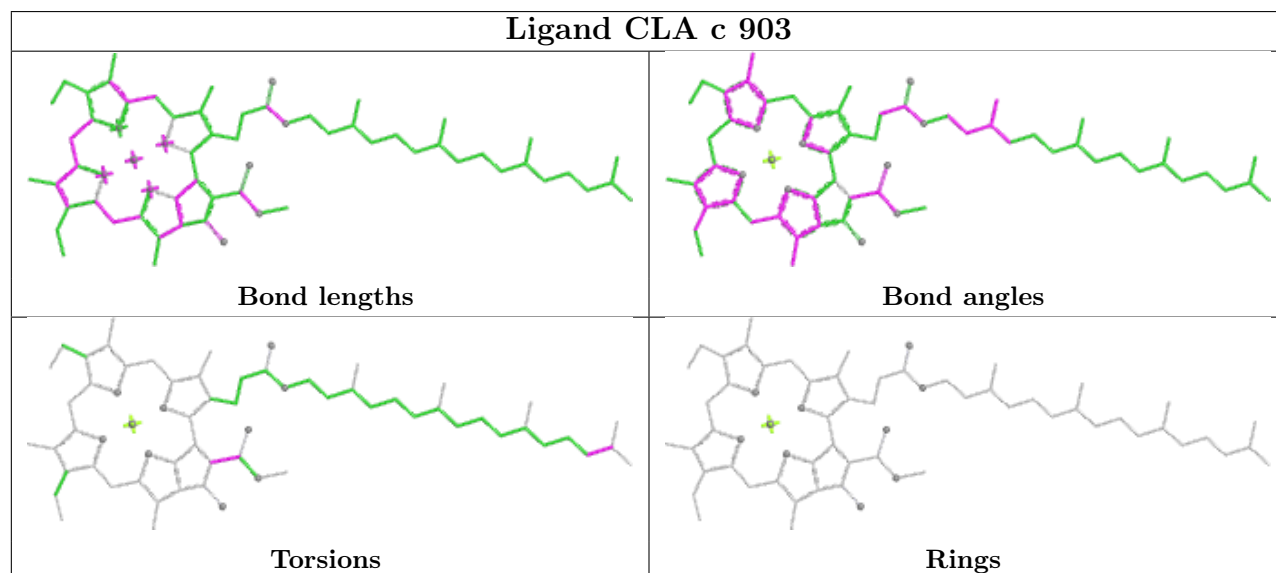
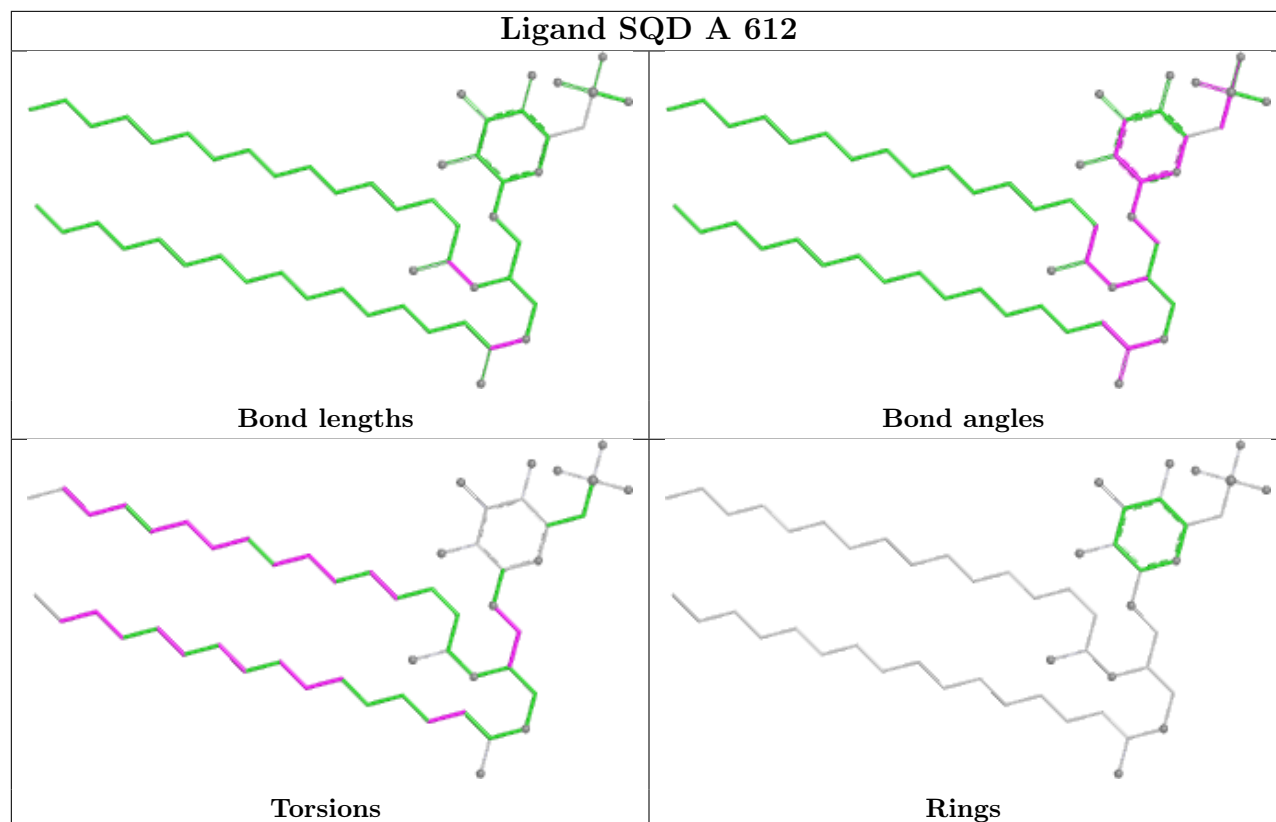


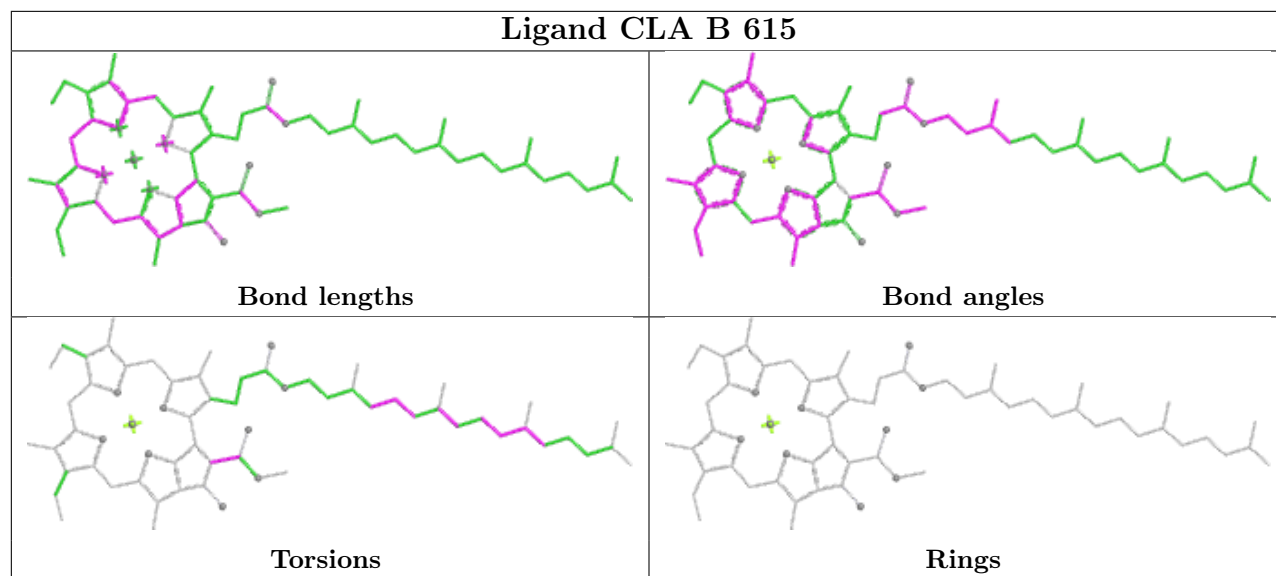












5.7 Other polymers [i](#)

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%)	-0.66	0 100 100	16, 22, 43, 53	0
1	a	334/334 (100%)	-0.70	0 100 100	19, 24, 45, 62	0
2	B	504/504 (100%)	-0.64	1 (0%) 91 83	18, 27, 49, 70	0
2	b	504/504 (100%)	-0.67	2 (0%) 88 77	20, 29, 52, 93	0
3	C	451/455 (99%)	-0.67	0 100 100	21, 31, 44, 56	0
3	c	455/455 (100%)	-0.74	1 (0%) 91 83	24, 34, 45, 59	0
4	D	342/342 (100%)	-0.63	1 (0%) 90 80	17, 23, 39, 61	0
4	d	341/342 (99%)	-0.64	1 (0%) 90 80	19, 26, 42, 59	0
5	E	81/81 (100%)	-0.66	0 100 100	27, 40, 57, 63	0
5	e	81/81 (100%)	-0.74	0 100 100	34, 45, 67, 76	0
6	F	34/34 (100%)	-0.65	0 100 100	28, 33, 58, 61	0
6	f	32/34 (94%)	-0.59	1 (3%) 51 42	30, 36, 60, 62	0
7	H	65/65 (100%)	-0.69	0 100 100	23, 34, 40, 58	0
7	h	65/65 (100%)	-0.67	0 100 100	28, 37, 48, 58	0
8	I	38/38 (100%)	-0.64	0 100 100	26, 33, 65, 68	0
8	i	38/38 (100%)	-0.91	0 100 100	29, 34, 62, 65	0
9	J	38/40 (95%)	-0.77	0 100 100	26, 37, 68, 72	0
9	j	40/40 (100%)	-0.71	0 100 100	31, 42, 76, 80	0
10	K	37/37 (100%)	-0.88	0 100 100	33, 38, 45, 47	0
10	k	37/37 (100%)	-0.59	0 100 100	38, 43, 55, 58	0
11	L	37/37 (100%)	-0.72	0 100 100	17, 22, 50, 59	0
11	l	37/37 (100%)	-0.81	0 100 100	19, 22, 55, 62	0
12	M	34/34 (100%)	-0.32	1 (2%) 53 44	21, 23, 36, 52	0
12	m	34/34 (100%)	-0.53	0 100 100	21, 25, 37, 53	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/243 (100%)	-0.67	1 (0%) 88 77	18, 32, 55, 71	0
13	o	243/243 (100%)	-0.63	0 100 100	21, 35, 61, 72	0
14	T	30/30 (100%)	-0.46	0 100 100	19, 23, 44, 52	0
14	t	30/30 (100%)	-0.54	0 100 100	20, 24, 44, 50	0
15	U	97/97 (100%)	-0.60	0 100 100	23, 30, 48, 50	0
15	u	97/97 (100%)	-0.71	0 100 100	25, 31, 37, 47	0
16	V	137/137 (100%)	-0.71	0 100 100	23, 28, 39, 48	0
16	v	137/137 (100%)	-0.76	1 (0%) 84 71	27, 37, 51, 57	0
17	Y	29/29 (100%)	-0.76	0 100 100	42, 48, 75, 77	0
17	y	29/29 (100%)	-0.57	0 100 100	50, 56, 75, 76	0
18	X	39/39 (100%)	-0.82	0 100 100	33, 40, 66, 68	0
18	x	39/39 (100%)	-0.75	0 100 100	37, 43, 75, 77	0
19	Z	62/62 (100%)	-0.77	0 100 100	39, 48, 68, 72	0
19	z	62/62 (100%)	-0.55	0 100 100	53, 61, 82, 87	0
All	All	5267/5276 (99%)	-0.67	10 (0%) 91 83	16, 30, 56, 93	0

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	f	14	PRO	3.1
4	D	183	LEU	2.6
13	O	161	GLY	2.3
4	d	292	ASN	2.2
2	b	361	ALA	2.2

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
22	CL	V	201	1/1	-0.02	0.10	50,50,50,50	0
30	CA	F	102	1/1	0.32	0.10	56,56,56,56	0
33	MG	j	102	1/1	0.34	0.13	34,34,34,34	0
22	CL	v	201	1/1	0.37	0.49	60,60,60,60	0
30	CA	B	601	1/1	0.47	0.09	76,76,76,76	0
30	CA	f	102	1/1	0.56	0.14	58,58,58,58	0
30	CA	b	601	1/1	0.78	0.07	77,77,77,77	0
23	BCT	a	414	4/4	0.79	0.20	34,34,35,37	0
22	CL	A	603	1/1	0.80	0.09	24,24,24,24	0
26	BCR	B	620	40/40	0.81	0.11	27,33,39,39	0
24	CLA	a	407	65/65	0.82	0.13	19,23,63,65	0
24	CLA	b	602	65/65	0.82	0.10	38,46,68,68	0
24	CLA	b	617	65/65	0.83	0.10	27,33,74,75	0
26	BCR	b	619	40/40	0.84	0.11	30,34,41,42	0
24	CLA	B	602	65/65	0.84	0.10	32,41,66,66	0
26	BCR	C	514	40/40	0.84	0.12	37,43,47,47	0
27	PL9	A	611	55/55	0.85	0.13	52,69,78,78	0
26	BCR	T	102	40/40	0.85	0.14	25,29,31,31	0
31	DGD	d	406	62/66	0.85	0.12	80,91,105,105	0
24	CLA	b	607	65/65	0.85	0.10	26,30,41,42	0
25	PHO	D	401	64/64	0.86	0.09	19,22,28,32	0
31	DGD	D	406	62/66	0.86	0.12	77,89,103,103	0
27	PL9	a	410	55/55	0.86	0.14	63,80,85,85	0
28	SQD	d	407	43/54	0.86	0.10	84,90,93,94	0
29	LHG	A	615	42/49	0.87	0.11	69,83,86,86	0
27	PL9	D	405	55/55	0.87	0.13	19,23,29,32	0
26	BCR	k	101	40/40	0.87	0.09	37,41,45,45	0
24	CLA	b	608	65/65	0.87	0.13	19,23,30,32	0
24	CLA	B	616	65/65	0.88	0.12	25,27,45,46	0
29	LHG	D	408	49/49	0.88	0.16	24,28,37,40	0
26	BCR	c	915	40/40	0.88	0.09	30,37,41,42	0
26	BCR	c	918	40/40	0.88	0.09	50,52,58,58	0
26	BCR	C	515	40/40	0.88	0.09	30,37,40,41	0
26	BCR	H	101	40/40	0.88	0.12	26,33,42,42	0
22	CL	A	604	1/1	0.88	0.08	21,21,21,21	0
26	BCR	a	409	40/40	0.88	0.12	21,26,29,29	0
26	BCR	b	618	40/40	0.88	0.13	24,28,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	CLA	C	513	65/65	0.89	0.10	39,45,64,64	0
24	CLA	a	406	65/65	0.89	0.10	18,20,28,33	0
29	LHG	a	413	42/49	0.89	0.12	95,107,110,111	0
29	LHG	d	410	49/49	0.89	0.10	28,34,66,67	0
24	CLA	B	608	65/65	0.89	0.10	17,20,32,34	0
24	CLA	C	504	65/65	0.89	0.11	25,28,54,54	0
27	PL9	d	405	55/55	0.89	0.12	19,25,29,31	0
28	SQD	A	612	54/54	0.89	0.10	49,57,66,67	0
31	DGD	C	517	62/66	0.89	0.11	23,35,62,63	0
28	SQD	A	613	54/54	0.89	0.14	50,63,68,68	0
26	BCR	A	610	40/40	0.89	0.11	22,27,32,32	0
28	SQD	l	101	54/54	0.89	0.15	57,69,84,85	0
24	CLA	B	617	65/65	0.90	0.10	22,29,77,78	0
26	BCR	T	101	40/40	0.90	0.10	25,37,44,45	0
29	LHG	b	620	49/49	0.90	0.11	24,31,46,50	0
24	CLA	D	403	65/65	0.90	0.12	24,27,65,67	0
26	BCR	B	618	40/40	0.90	0.11	23,27,28,29	0
26	BCR	B	619	40/40	0.90	0.11	21,28,40,40	0
24	CLA	B	607	65/65	0.90	0.08	24,28,40,41	0
24	CLA	C	509	65/65	0.90	0.09	29,32,46,47	0
28	SQD	a	402	54/54	0.90	0.13	51,67,75,76	0
24	CLA	c	914	65/65	0.90	0.09	46,51,73,74	0
26	BCR	f	101	40/40	0.90	0.09	30,34,48,49	0
26	BCR	h	101	40/40	0.90	0.10	29,37,45,45	0
24	CLA	D	402	65/65	0.91	0.10	13,18,34,35	0
24	CLA	b	612	65/65	0.91	0.10	20,23,37,41	0
24	CLA	b	616	65/65	0.91	0.09	27,30,45,46	0
24	CLA	B	613	65/65	0.91	0.11	20,24,30,31	0
26	BCR	k	102	40/40	0.91	0.09	33,44,47,48	0
26	BCR	D	404	40/40	0.91	0.12	25,30,48,49	0
24	CLA	c	902	65/65	0.91	0.09	30,33,41,45	0
24	CLA	C	508	65/65	0.91	0.08	25,29,54,58	0
24	CLA	d	404	65/65	0.91	0.10	26,31,67,68	0
24	CLA	A	606	65/65	0.91	0.12	15,19,25,34	0
25	PHO	a	412	64/64	0.91	0.09	20,25,30,33	0
31	DGD	C	518	62/66	0.91	0.09	22,31,52,56	0
24	CLA	C	512	65/65	0.91	0.10	37,41,62,63	0
28	SQD	a	411	54/54	0.91	0.10	50,60,75,76	0
31	DGD	j	101	62/66	0.91	0.09	25,34,52,55	0
22	CL	a	405	1/1	0.91	0.08	26,26,26,26	0
24	CLA	c	912	65/65	0.92	0.09	32,37,43,44	0
29	LHG	D	409	49/49	0.92	0.09	26,33,62,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	CLA	c	913	65/65	0.92	0.09	38,42,62,63	0
24	CLA	a	408	65/65	0.92	0.10	20,24,75,75	0
24	CLA	b	613	65/65	0.92	0.11	21,26,33,35	0
26	BCR	K	101	40/40	0.92	0.08	29,33,37,37	0
25	PHO	A	608	64/64	0.92	0.07	16,21,25,26	0
24	CLA	A	607	65/65	0.92	0.14	19,21,63,65	0
26	BCR	Y	101	40/40	0.92	0.08	34,38,39,39	0
22	CL	a	404	1/1	0.92	0.08	28,28,28,28	0
24	CLA	C	511	65/65	0.92	0.07	29,34,37,38	0
24	CLA	c	904	65/65	0.92	0.08	26,37,39,40	0
31	DGD	c	916	62/66	0.92	0.12	24,35,60,61	0
31	DGD	c	917	62/66	0.92	0.10	28,36,64,65	0
24	CLA	c	905	65/65	0.92	0.08	28,30,55,56	0
24	CLA	c	907	65/65	0.92	0.09	30,35,64,64	0
26	BCR	B	622	40/40	0.92	0.10	23,34,41,41	0
24	CLA	c	910	65/65	0.93	0.07	27,30,46,46	0
24	CLA	b	614	65/65	0.93	0.10	21,24,44,45	0
29	LHG	d	409	49/49	0.93	0.10	23,27,38,40	0
24	CLA	c	903	65/65	0.93	0.10	25,28,42,45	0
24	CLA	b	615	65/65	0.93	0.09	22,26,65,66	0
24	CLA	C	507	65/65	0.93	0.07	29,33,52,53	0
24	CLA	A	614	65/65	0.93	0.09	14,18,29,35	0
32	HEM	e	101	43/43	0.93	0.09	43,46,52,55	0
28	SQD	L	101	54/54	0.93	0.11	58,66,80,80	0
24	CLA	b	603	65/65	0.94	0.09	26,29,36,37	0
24	CLA	B	609	65/65	0.94	0.09	20,24,31,31	0
30	CA	c	901	1/1	0.94	0.22	46,46,46,46	0
24	CLA	B	606	65/65	0.94	0.08	19,23,34,35	0
29	LHG	D	407	49/49	0.94	0.09	29,34,41,41	0
24	CLA	C	501	65/65	0.94	0.08	29,32,44,46	0
24	CLA	d	401	65/65	0.94	0.10	17,20,27,31	0
24	CLA	C	503	65/65	0.94	0.09	27,31,35,36	0
24	CLA	B	615	65/65	0.94	0.11	20,24,60,61	0
29	LHG	d	408	49/49	0.94	0.09	29,37,41,42	0
24	CLA	C	505	65/65	0.94	0.10	28,30,44,45	0
24	CLA	c	908	65/65	0.94	0.08	28,32,50,51	0
24	CLA	c	909	65/65	0.94	0.08	27,29,57,60	0
30	CA	O	301	1/1	0.95	0.04	49,49,49,49	0
25	PHO	d	402	64/64	0.95	0.10	18,22,24,25	0
24	CLA	b	605	65/65	0.95	0.08	20,25,53,55	0
24	CLA	c	911	65/65	0.95	0.07	26,30,39,40	0
30	CA	o	301	1/1	0.95	0.05	51,51,51,51	0

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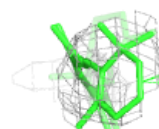
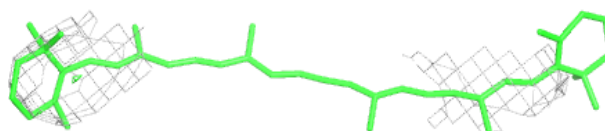
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	DGD	C	516	62/66	0.95	0.08	23,33,61,62	0
24	CLA	B	605	65/65	0.95	0.07	19,22,50,51	0
24	CLA	B	611	65/65	0.95	0.09	21,25,32,37	0
23	BCT	A	605	4/4	0.95	0.06	39,39,40,42	0
24	CLA	C	510	65/65	0.95	0.06	24,28,35,37	0
28	SQD	F	101	43/54	0.95	0.07	67,74,78,79	0
24	CLA	c	906	65/65	0.95	0.07	28,31,44,44	0
31	DGD	h	102	62/66	0.95	0.13	29,36,43,44	0
24	CLA	A	609	65/65	0.95	0.08	21,24,71,72	0
24	CLA	B	603	65/65	0.95	0.07	23,26,32,32	0
24	CLA	C	506	65/65	0.95	0.07	31,38,74,75	0
31	DGD	H	102	62/66	0.96	0.08	26,32,38,40	0
24	CLA	b	610	65/65	0.96	0.07	28,31,33,36	0
29	LHG	B	621	49/49	0.96	0.09	23,31,43,44	0
24	CLA	b	611	65/65	0.96	0.08	25,28,34,37	0
24	CLA	d	403	65/65	0.96	0.09	18,21,38,39	0
24	CLA	B	610	65/65	0.96	0.07	23,28,31,32	0
32	HEM	E	101	43/43	0.96	0.07	39,42,45,47	0
24	CLA	b	606	65/65	0.96	0.06	21,24,32,33	0
32	HEM	v	202	43/43	0.96	0.08	28,31,34,36	0
24	CLA	b	609	65/65	0.96	0.07	22,27,38,39	0
24	CLA	B	614	65/65	0.97	0.06	19,22,45,47	0
24	CLA	b	604	65/65	0.97	0.06	23,26,35,38	0
32	HEM	V	202	43/43	0.97	0.07	23,24,27,29	0
24	CLA	B	612	65/65	0.97	0.07	19,21,32,34	0
24	CLA	C	502	65/65	0.97	0.07	24,26,39,42	0
24	CLA	B	604	65/65	0.97	0.10	18,22,31,35	0
20	OEX	A	601	10/10	0.99	0.07	22,23,26,26	0
20	OEX	a	401	10/10	0.99	0.09	25,27,28,28	0
21	FE2	A	602	1/1	1.00	0.03	26,26,26,26	0
21	FE2	a	403	1/1	1.00	0.15	27,27,27,27	0

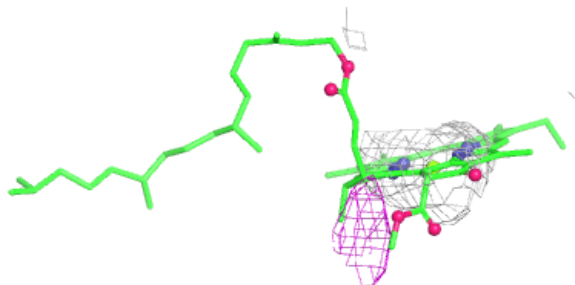
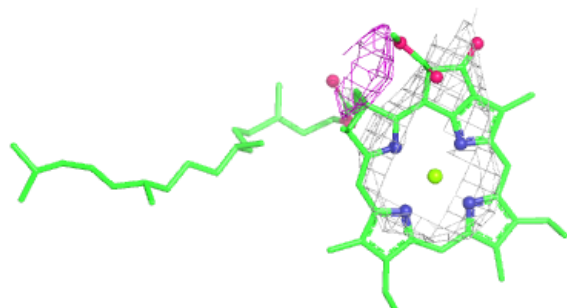
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around BCR 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)

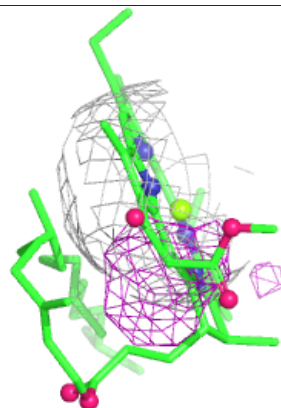
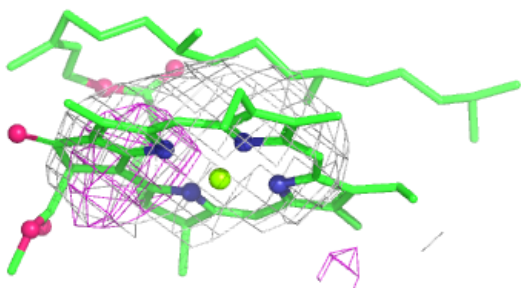
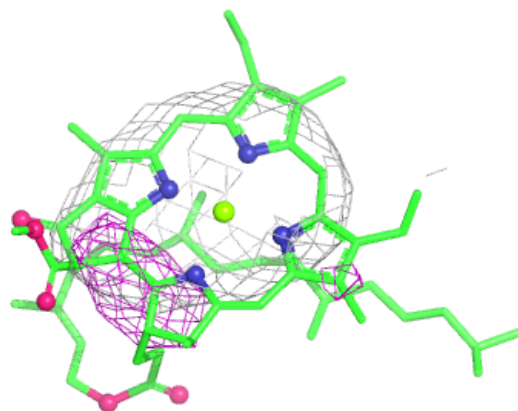
**Electron density around CLA a 407:**

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



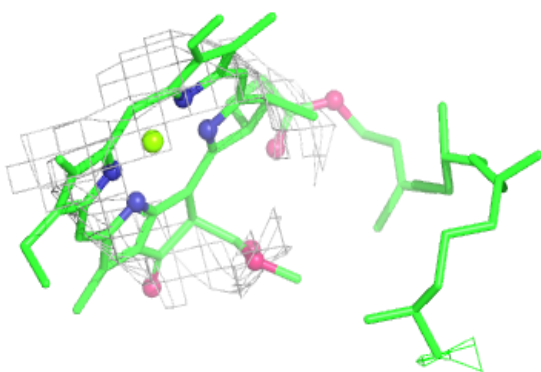
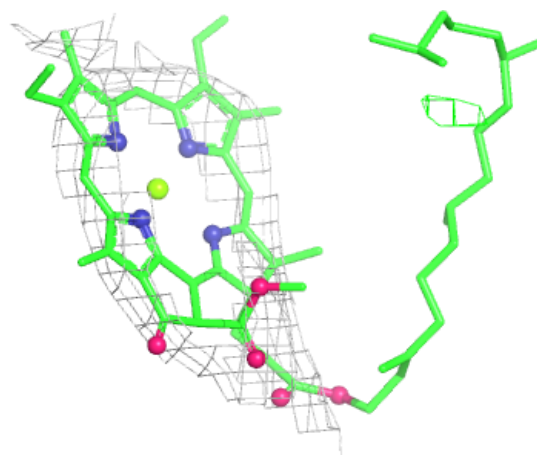
Electron density around CLA b 602:

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



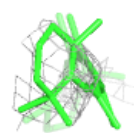
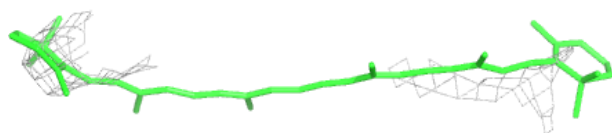
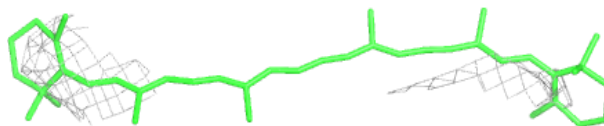
Electron density around CLA b 617:

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

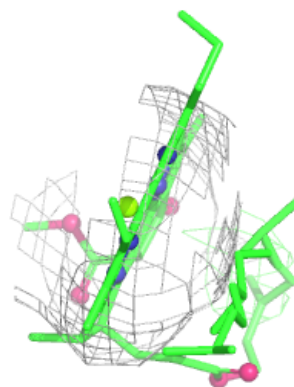
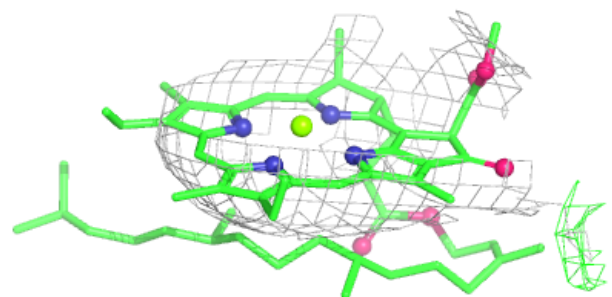
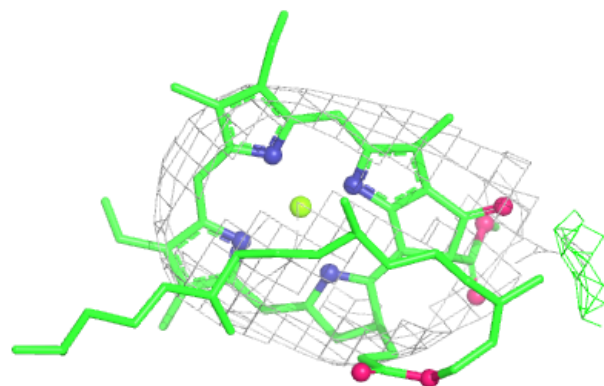


Electron density around BCR b 619:

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

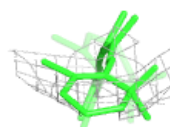
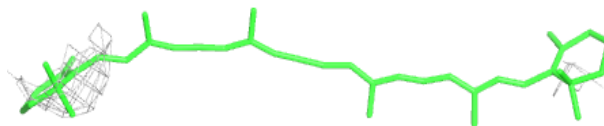
**Electron density around CLA B 602:**

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

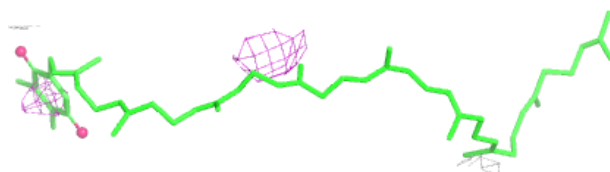
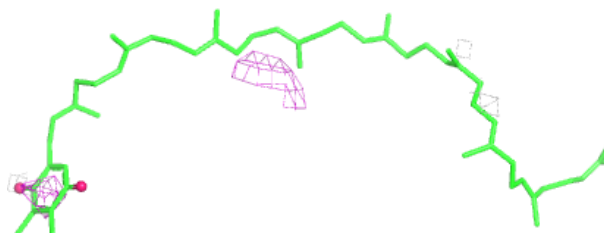


Electron density around BCR C 514:

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

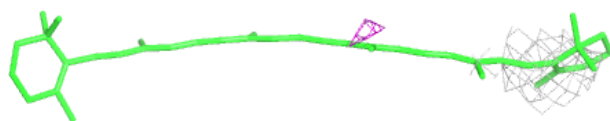
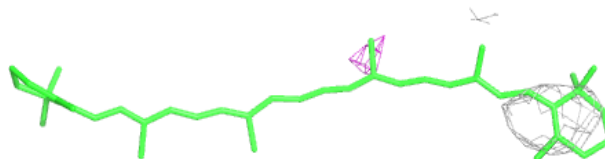
**Electron density around PL9 A 611:**

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

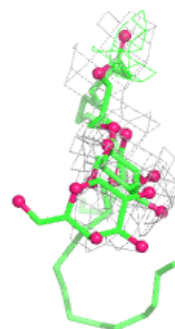
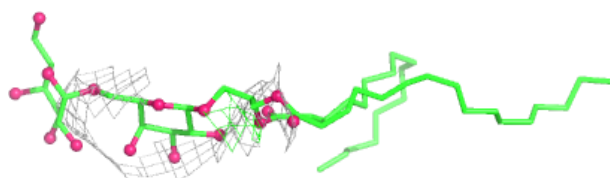


Electron density around BCR T 102:

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

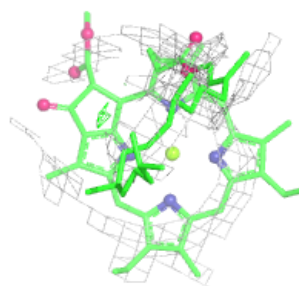
**Electron density around DGD d 406:**

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



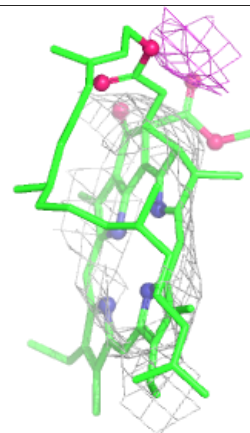
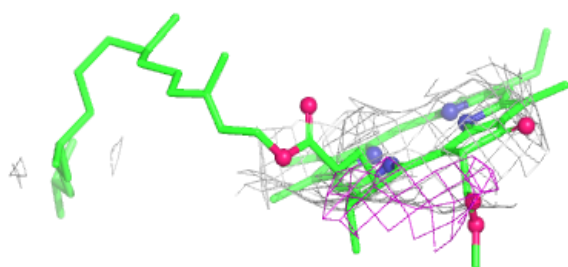
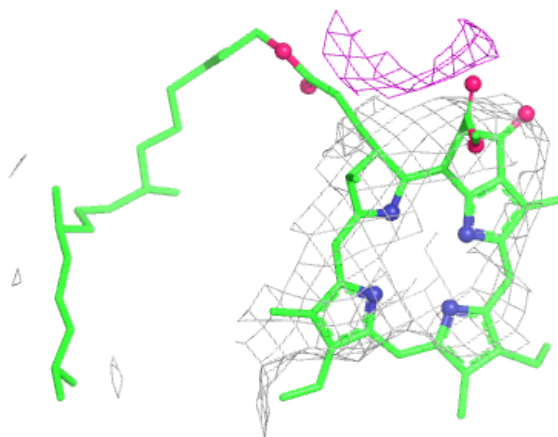
Electron density around CLA b 607:

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

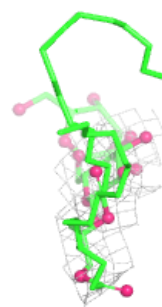
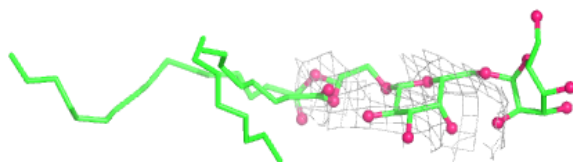
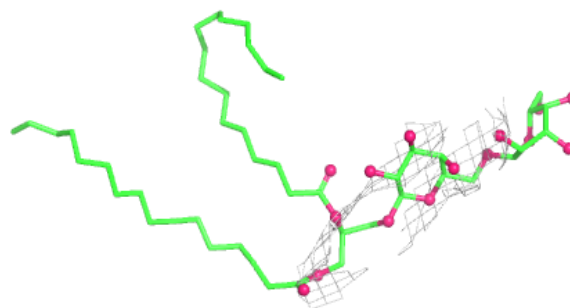


Electron density around PHO D 401:

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

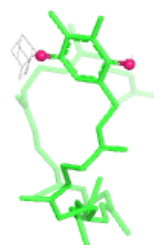
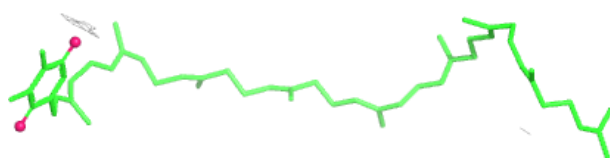
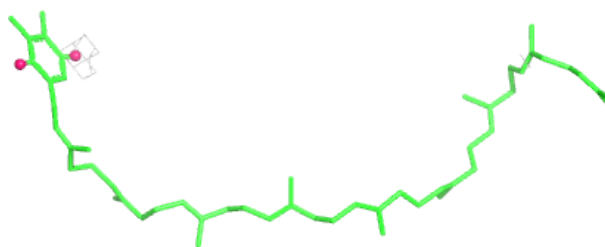
**Electron density around DGD D 406:**

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

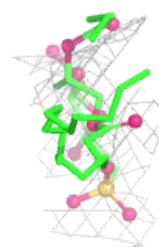
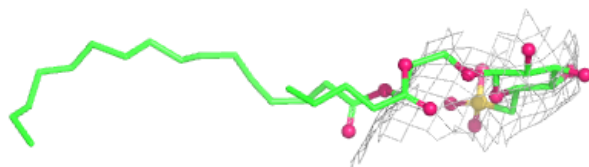
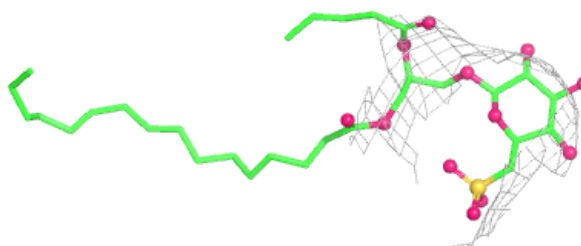


Electron density around PL9 a 410:

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

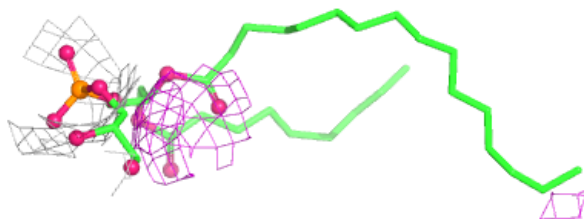
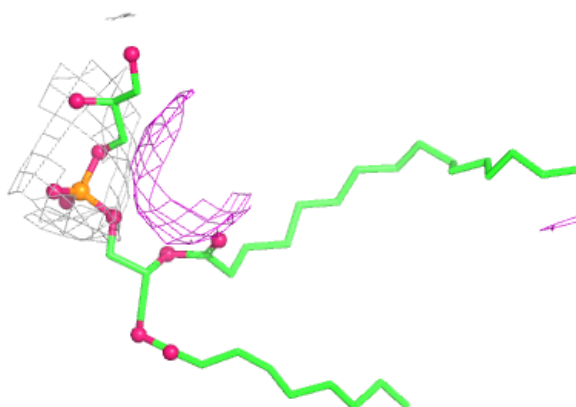
**Electron density around SQD d 407:**

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

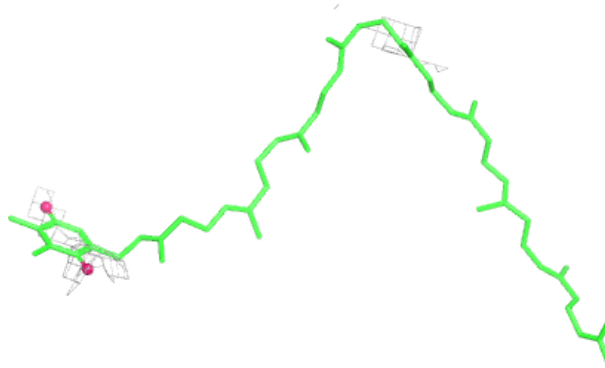


Electron density around LHG A 615:

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

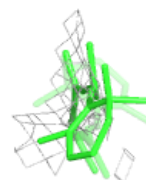
**Electron density around PL9 D 405:**

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

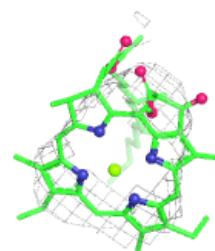
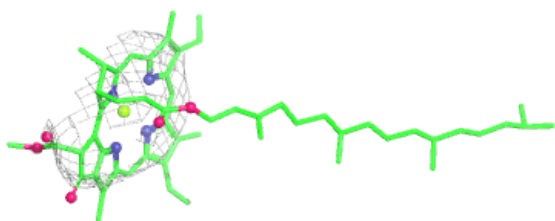
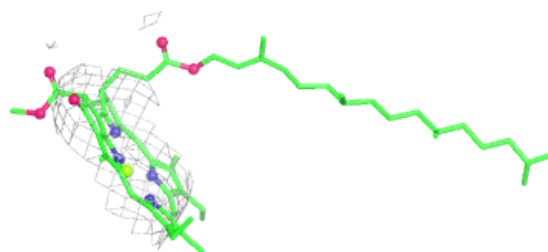


Electron density around BCR k 101:

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

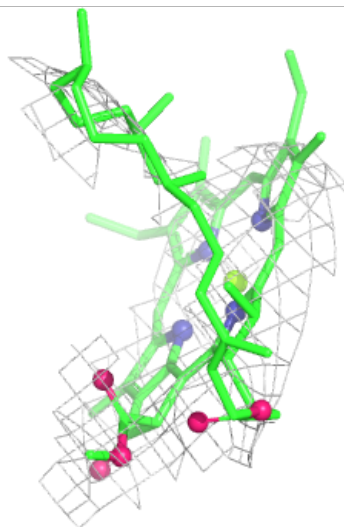
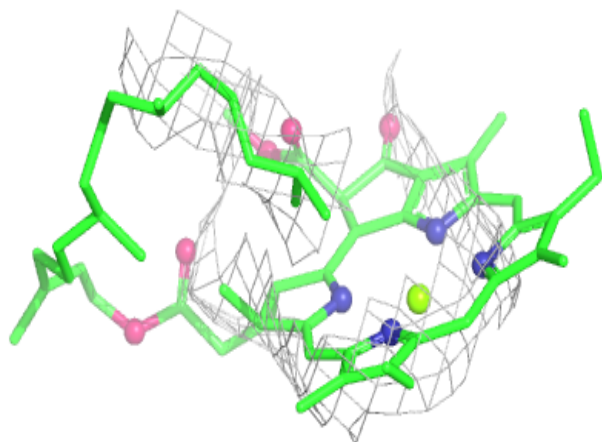
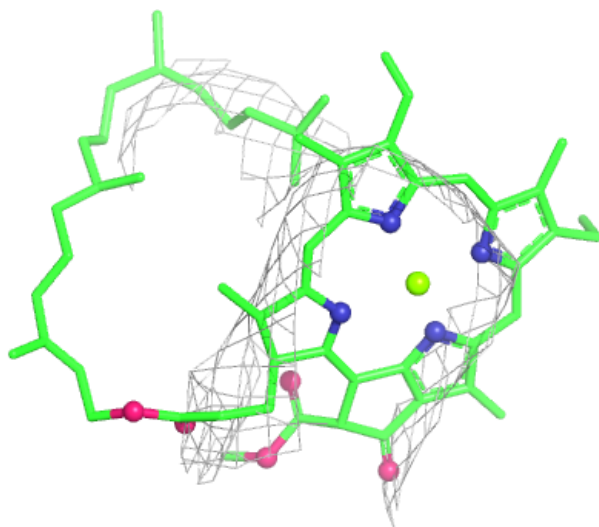
**Electron density around CLA b 608:**

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



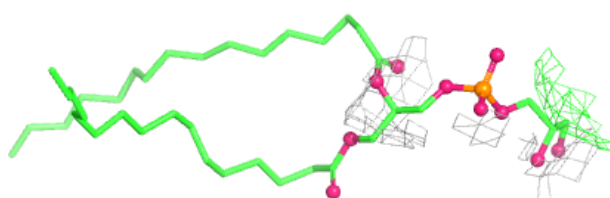
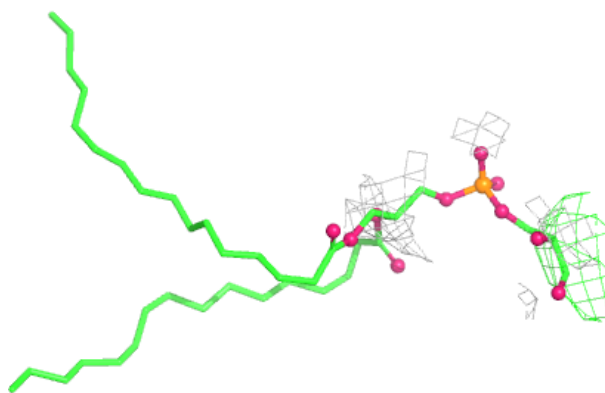
Electron density around CLA B 616:

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

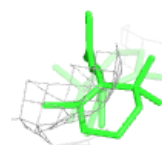
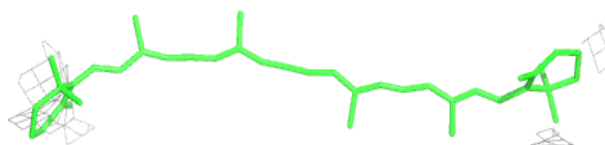


Electron density around LHG D 408:

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

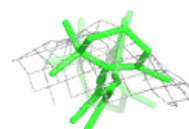
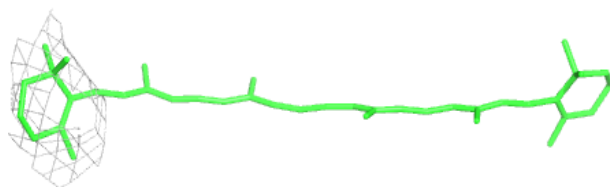
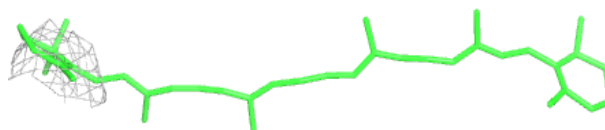
**Electron density around BCR c 915:**

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

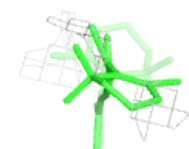
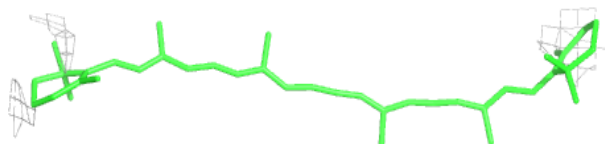


Electron density around BCR c 918:

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

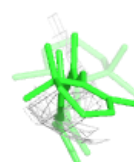
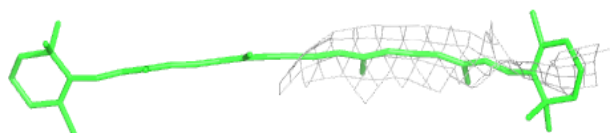
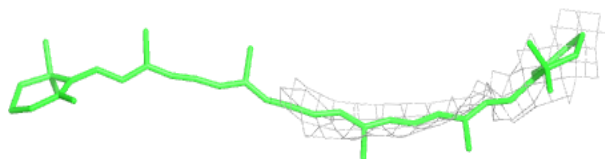
**Electron density around BCR C 515:**

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

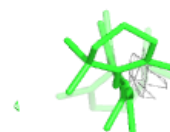
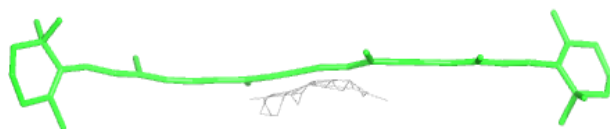
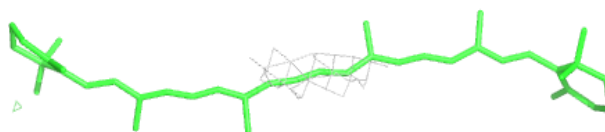


Electron density around BCR H 101:

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

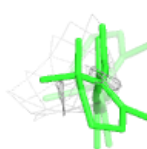
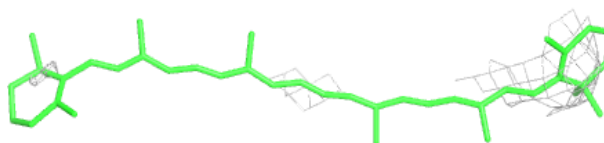
**Electron density around BCR a 409:**

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

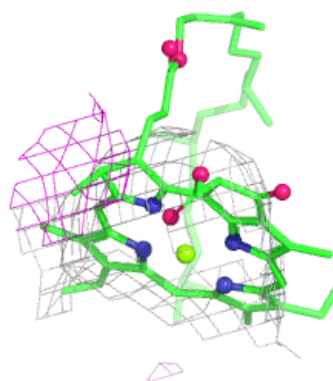
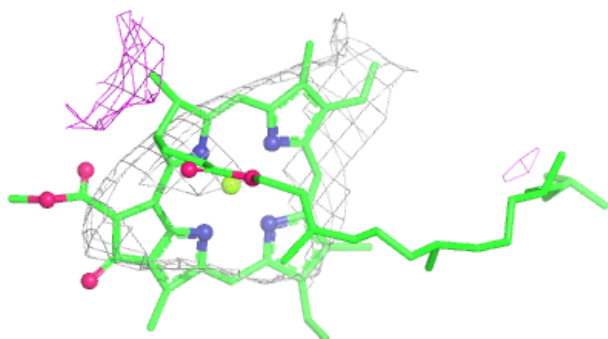
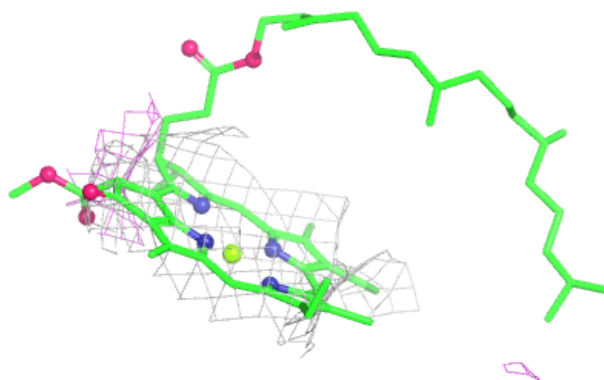


Electron density around BCR b 618:

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

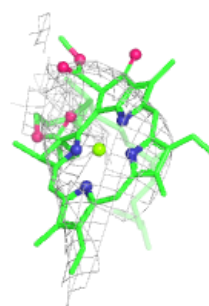
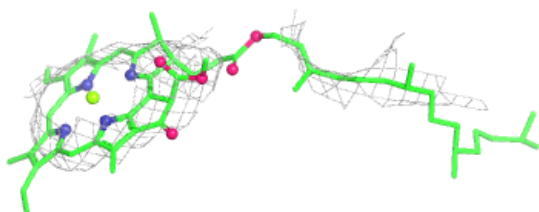
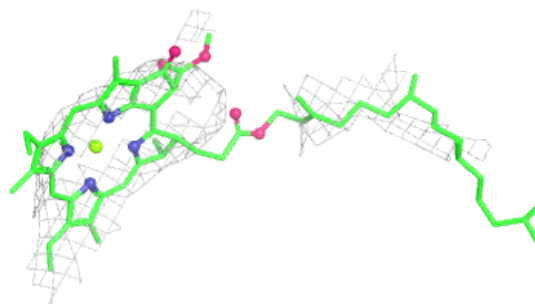
**Electron density around CLA C 513:**

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

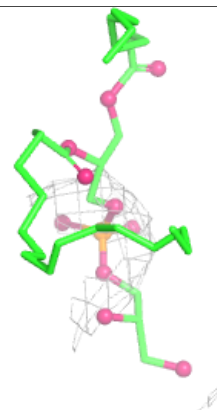
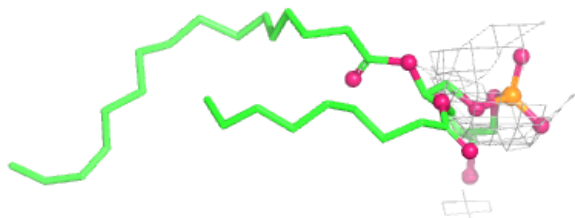
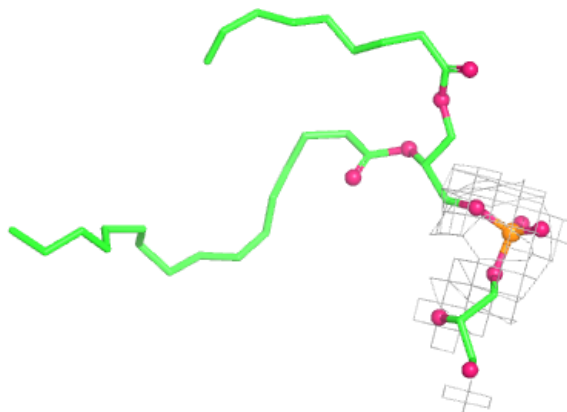


Electron density around CLA a 406:

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

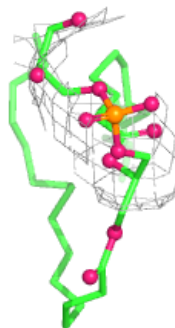
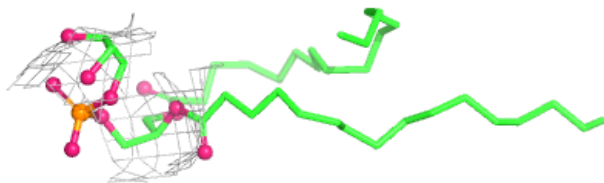
**Electron density around LHG a 413:**

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

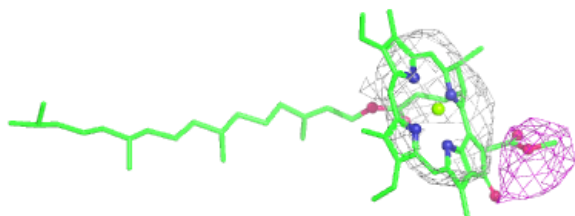
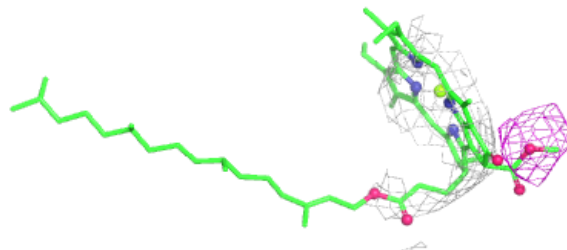


Electron density around LHG d 410:

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

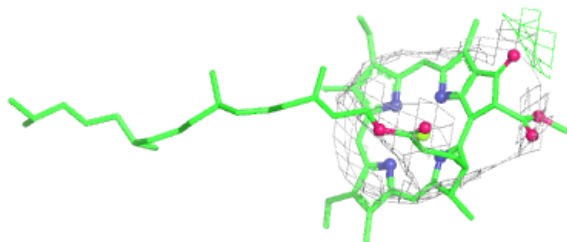
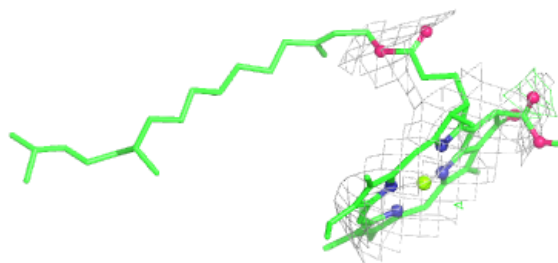
**Electron density around CLA B 608:**

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

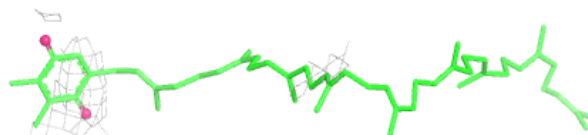
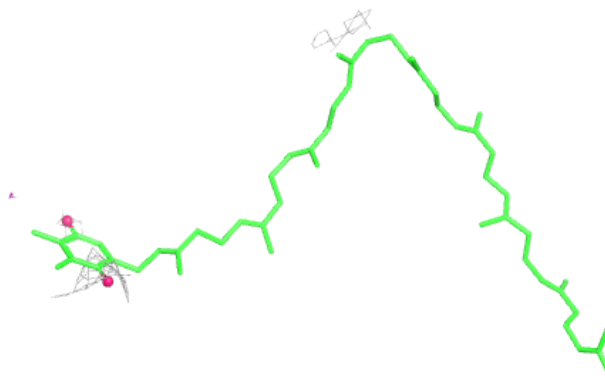


Electron density around CLA C 504:

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

**Electron density around 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)



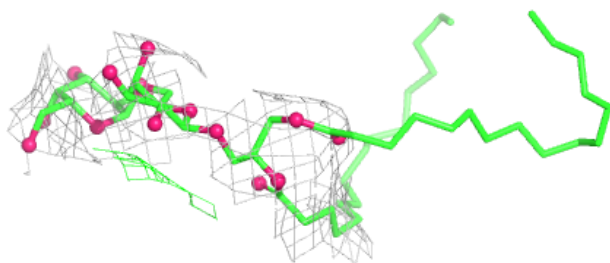
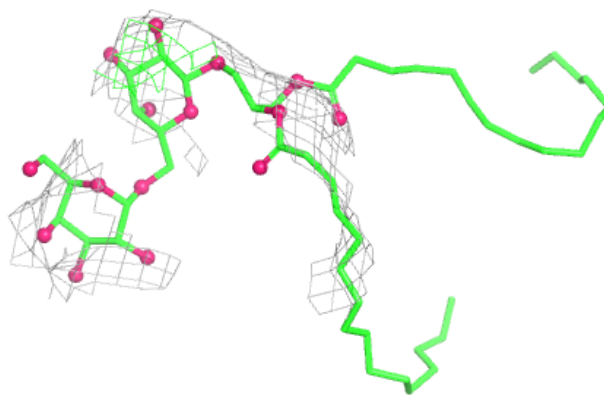
Electron density around SQD A 612:

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

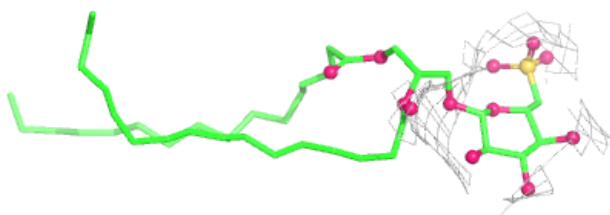
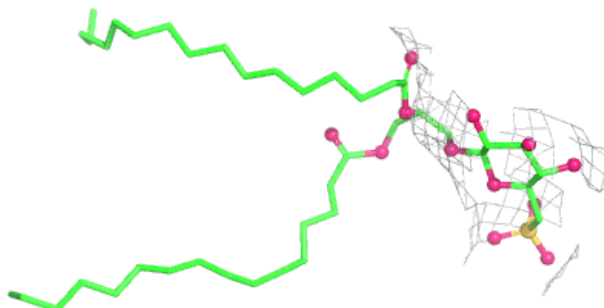


Electron density around DGD C 517:

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

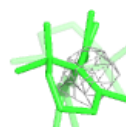
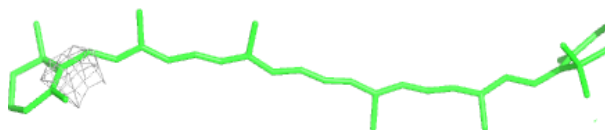
**Electron density around SQD A 613:**

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

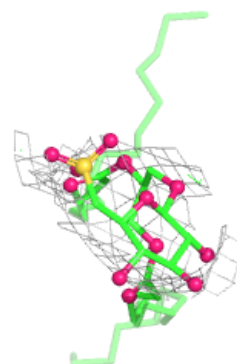
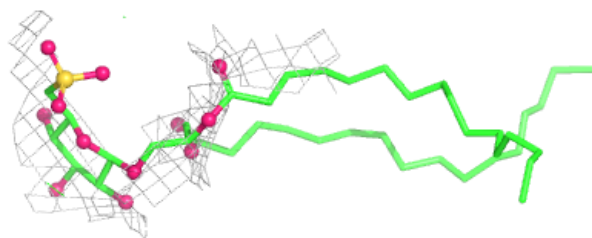
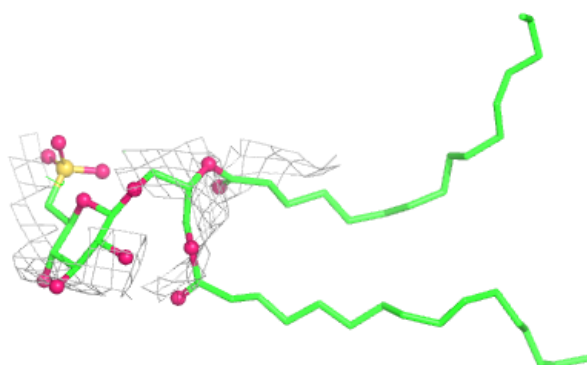


Electron density around BCR A 610:

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

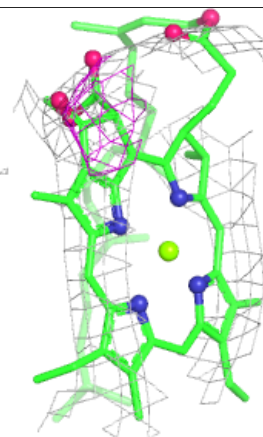
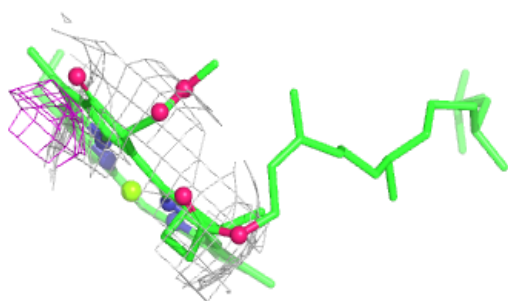
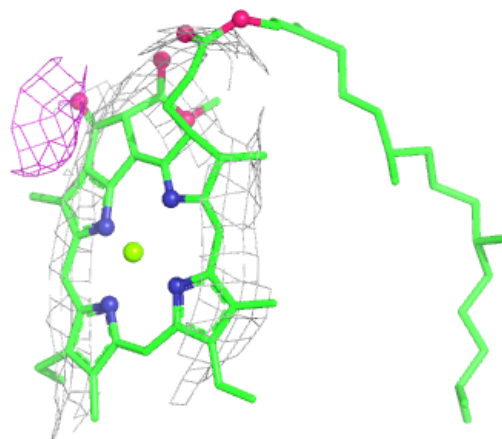
**Electron density around SQD 1 101:**

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

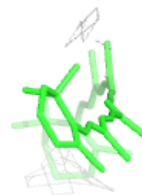
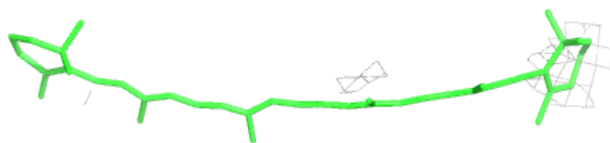
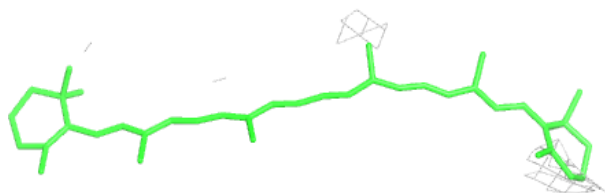


Electron density around CLA B 617:

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

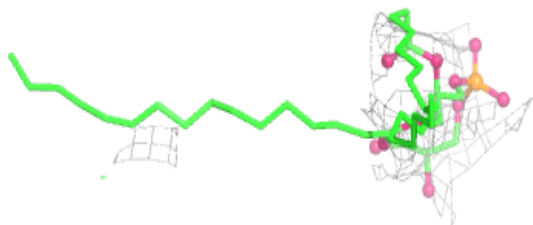
**Electron density around BCR T 101:**

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



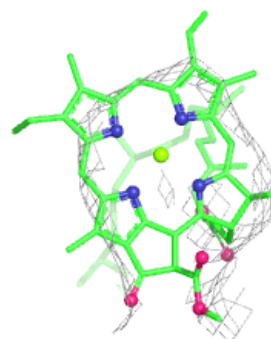
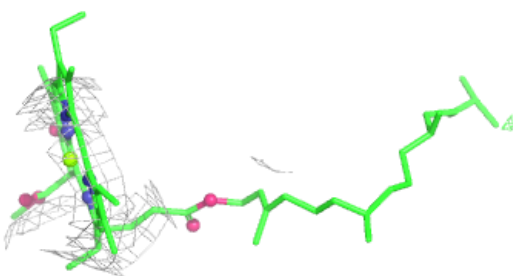
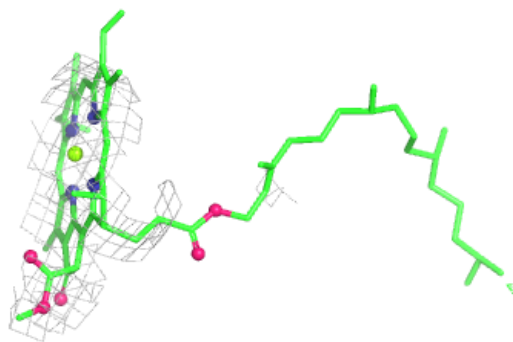
Electron density around LHG b 620:

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

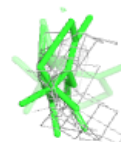
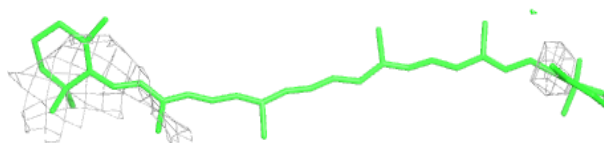


Electron density around CLA D 403:

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

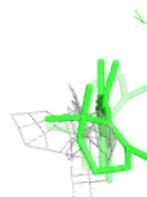
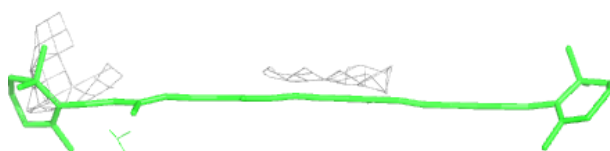
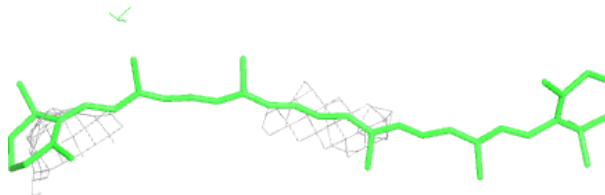
**Electron density around BCR B 618:**

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

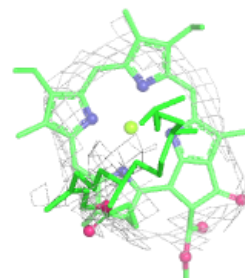
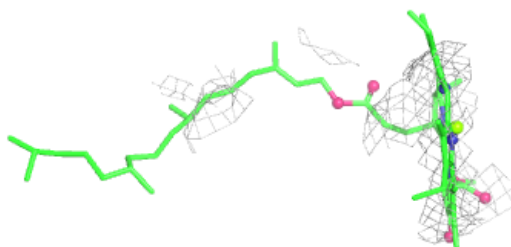
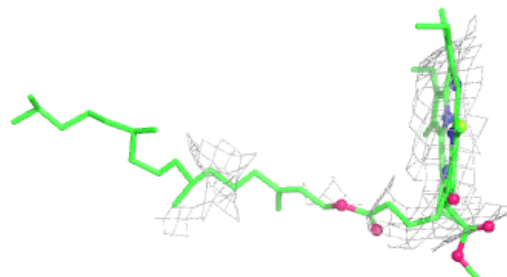


Electron density around BCR B 619:

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

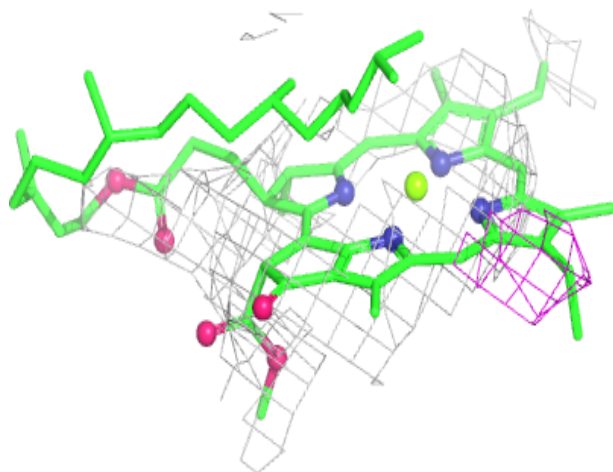
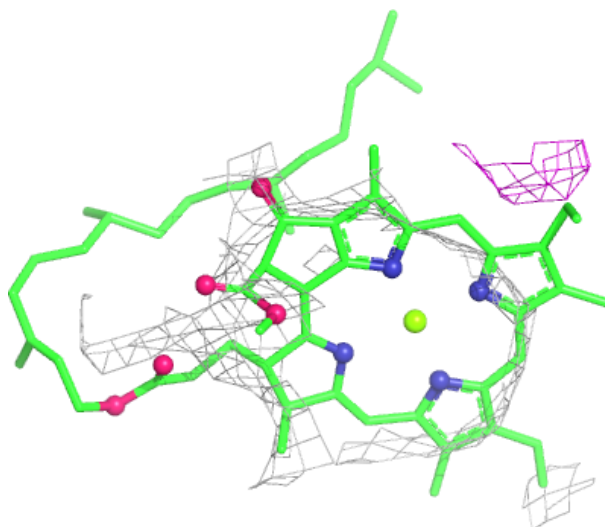
**Electron density around CLA B 607:**

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



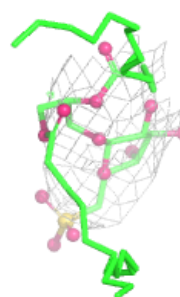
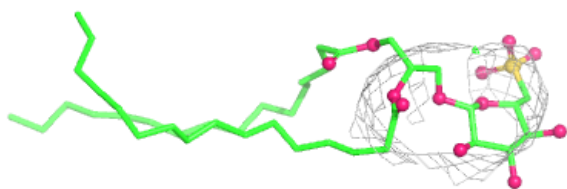
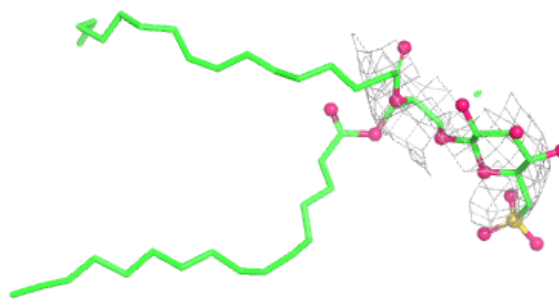
Electron density around CLA C 509:

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

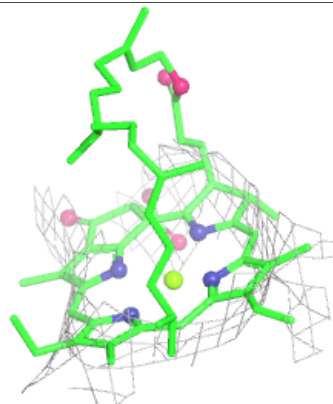
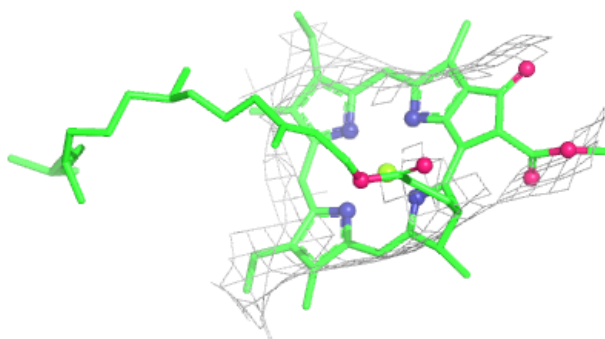
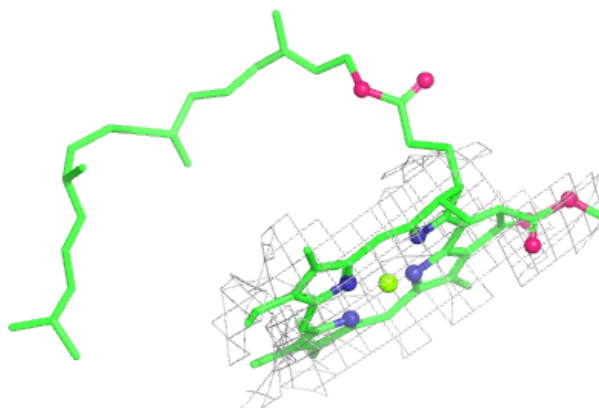


Electron density around SQD a 402:

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

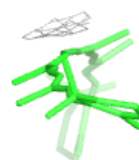
**Electron density around CLA c 914:**

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

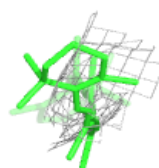
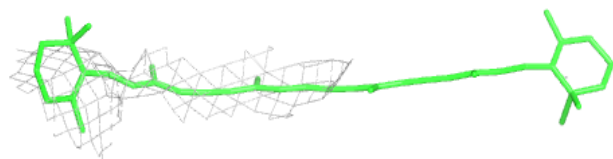
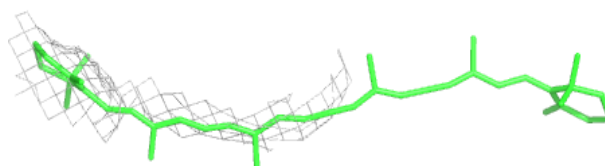


Electron density around BCR f 101:

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

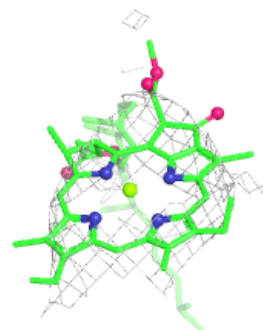
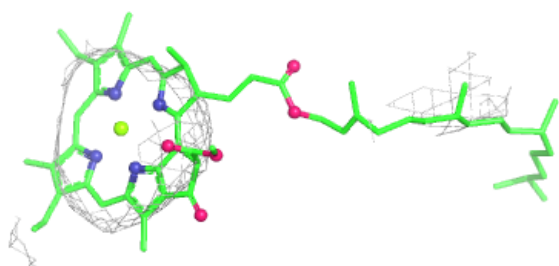
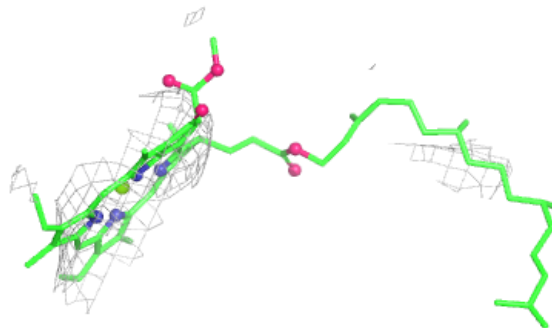
**Electron density around BCR h 101:**

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



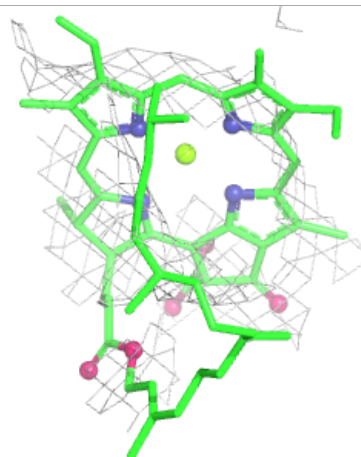
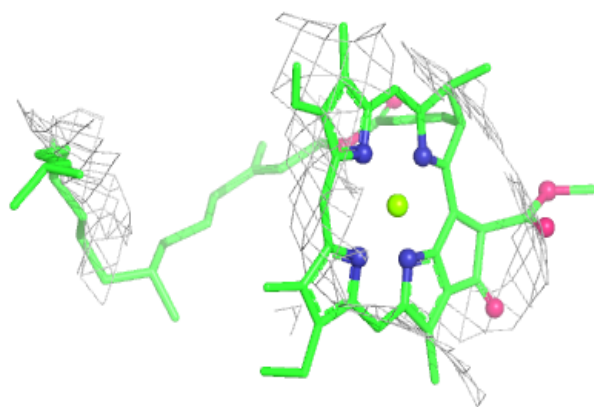
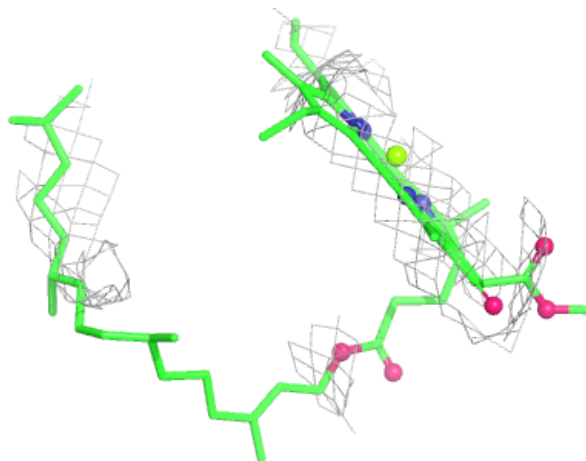
Electron density around CLA D 402:

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



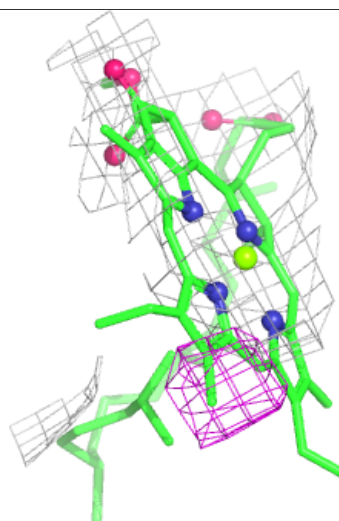
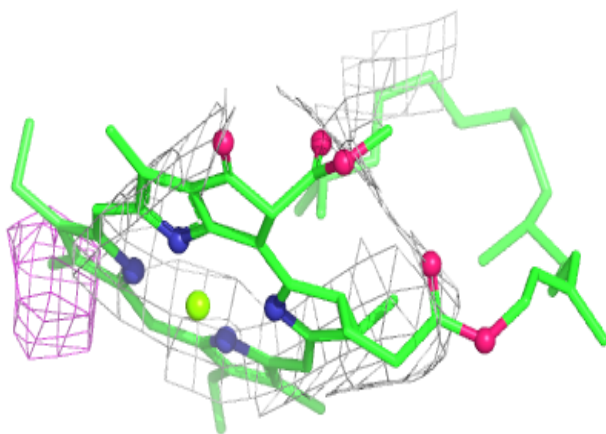
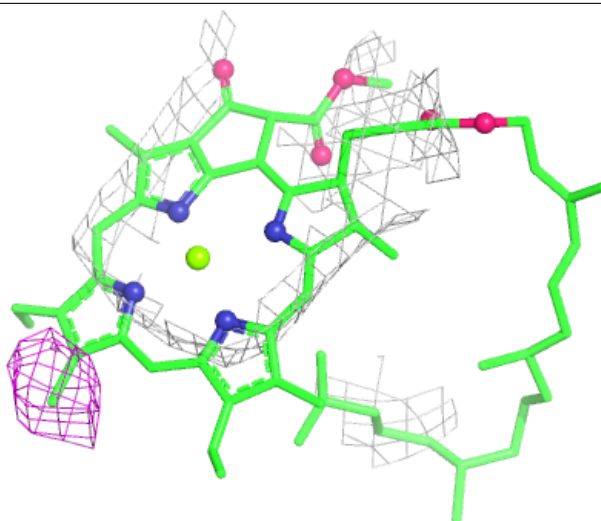
Electron density around CLA b 612:

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



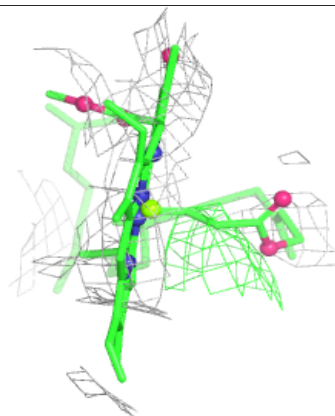
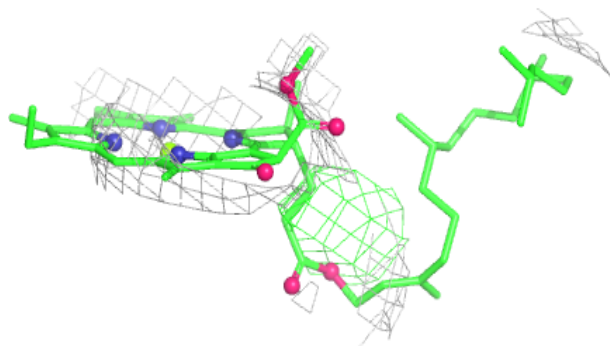
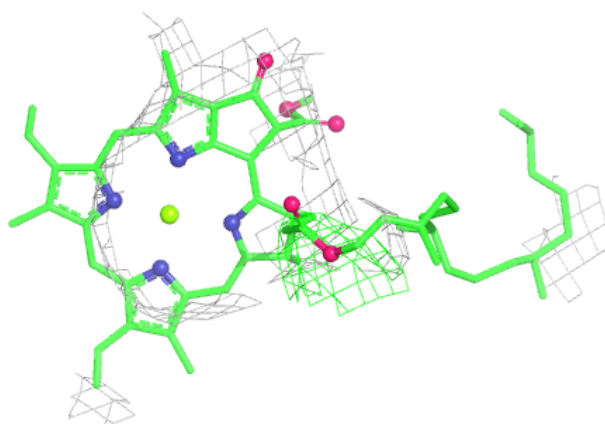
Electron density around CLA b 616:

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

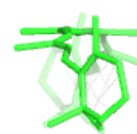
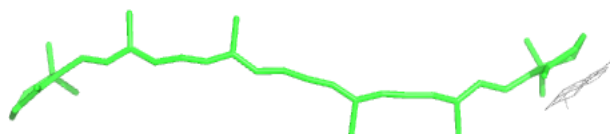
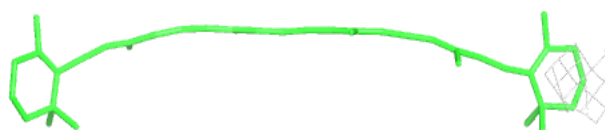


Electron density around CLA B 613:

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

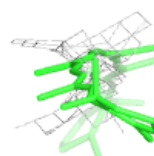
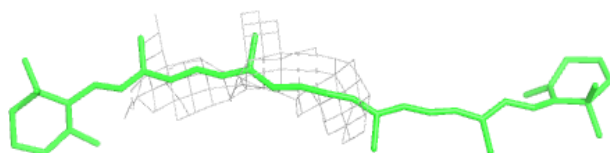
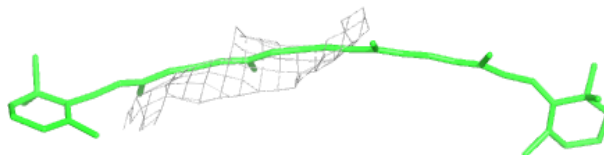
**Electron density around BCR k 102:**

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

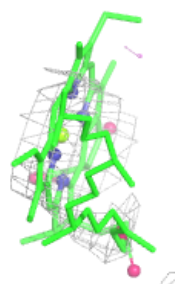
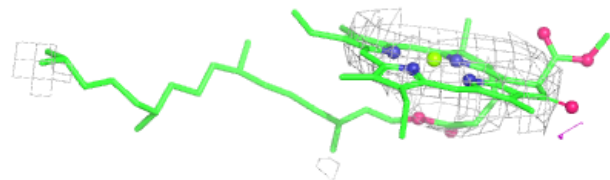
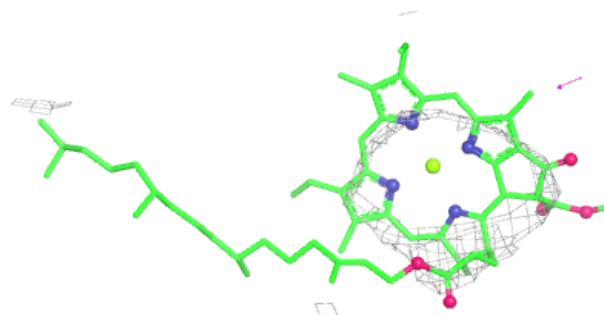


Electron density around BCR D 404:

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

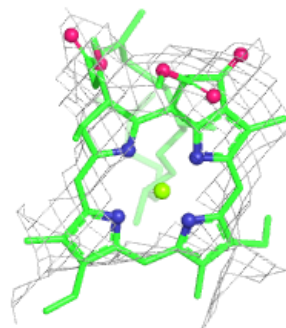
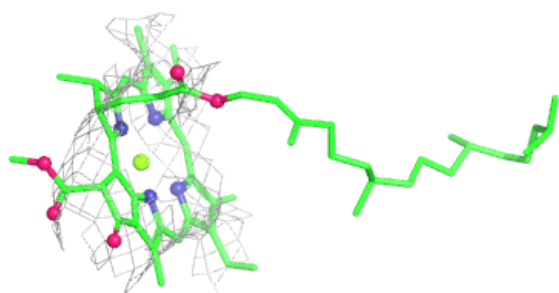
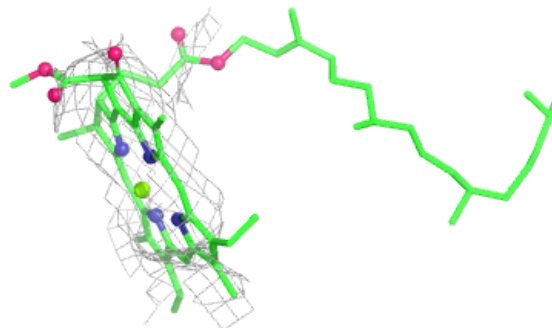
**Electron density around CLA c 902:**

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

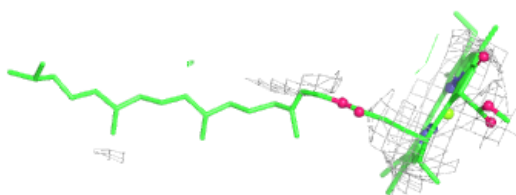
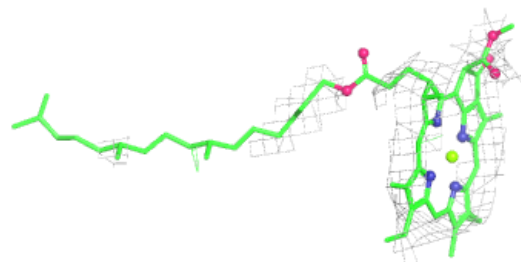


Electron density around CLA C 508:

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

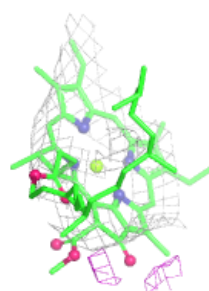
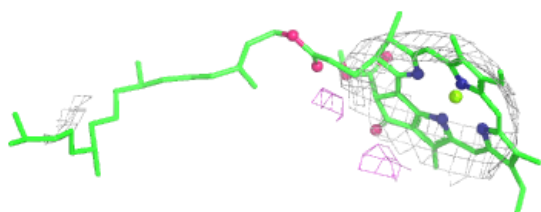
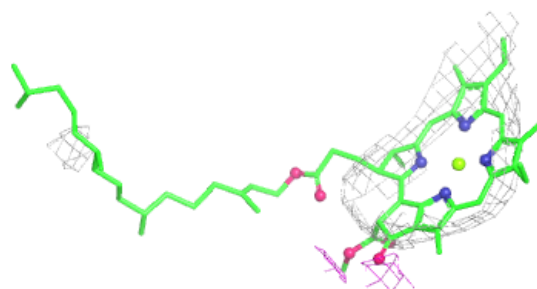
**Electron density around CLA d 404:**

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

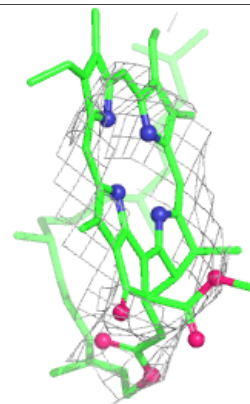
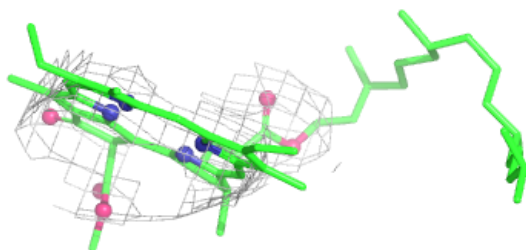
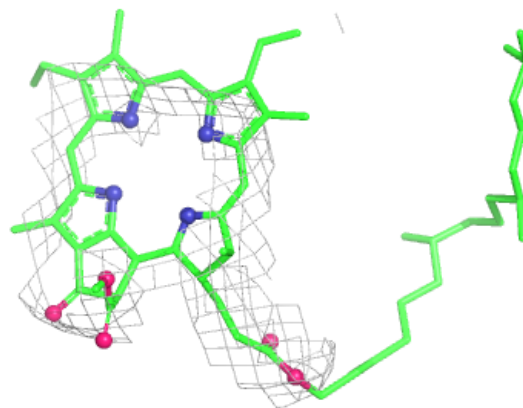


Electron density around CLA A 606:

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

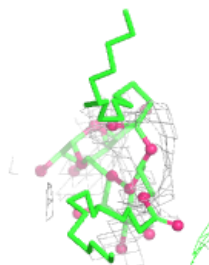
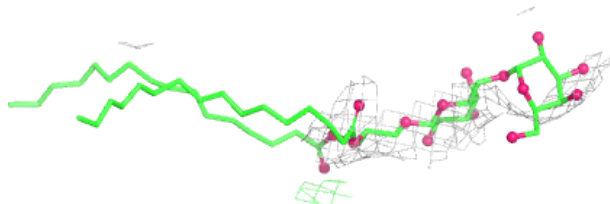
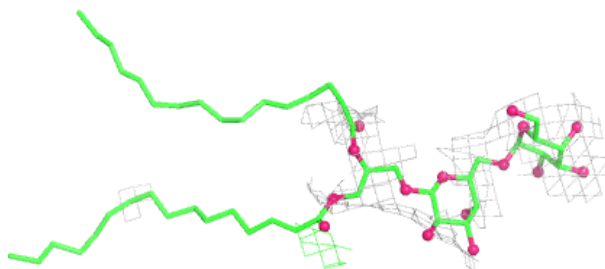
**Electron density around PHO a 412:**

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



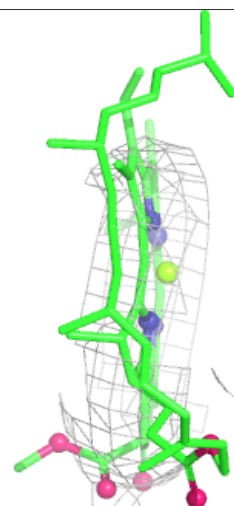
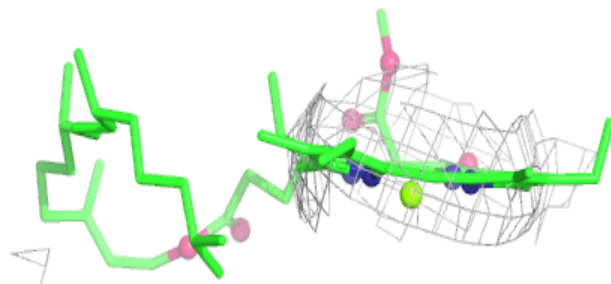
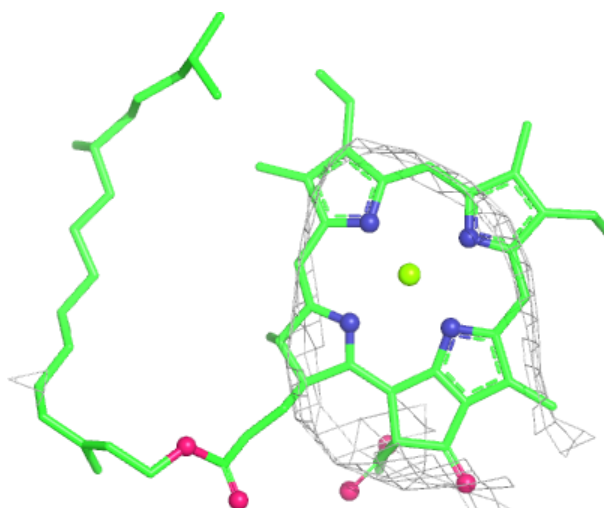
Electron density around DGD C 518:

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



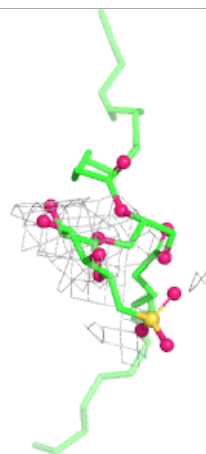
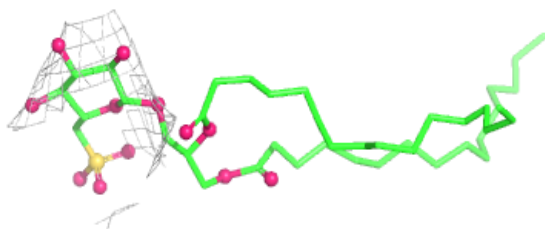
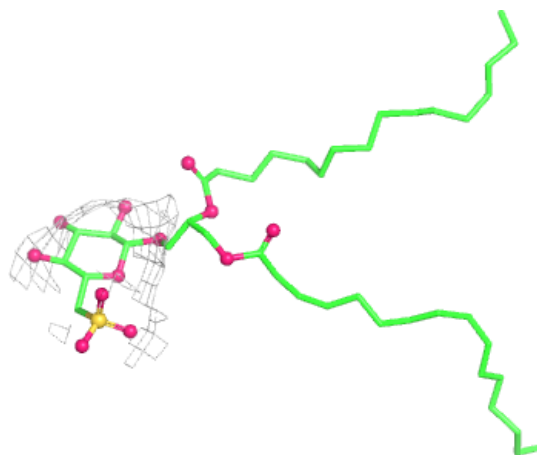
Electron density around CLA C 512:

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



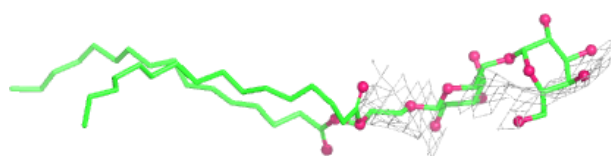
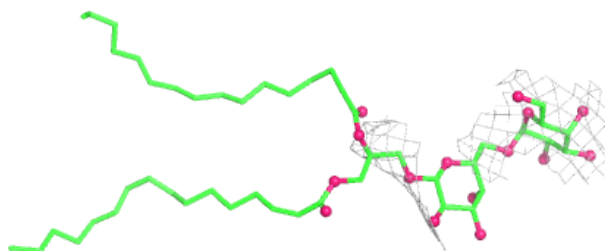
Electron density around SQD a 411:

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

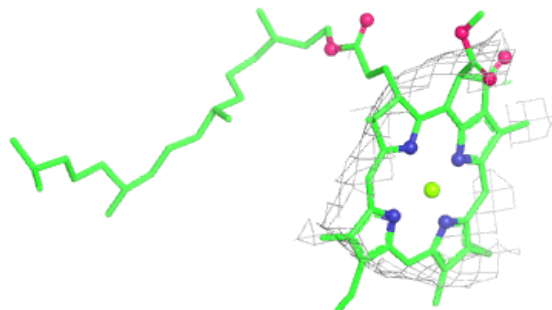


Electron density around DGD j 101:

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

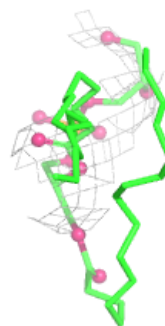
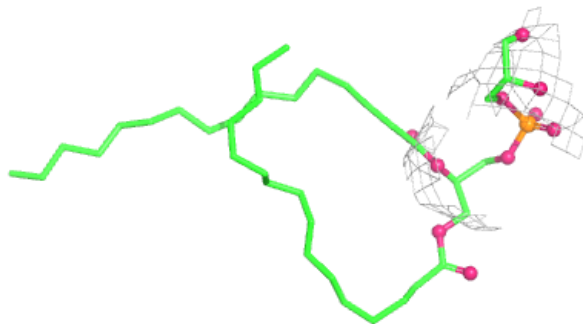
**Electron density around CLA c 912:**

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



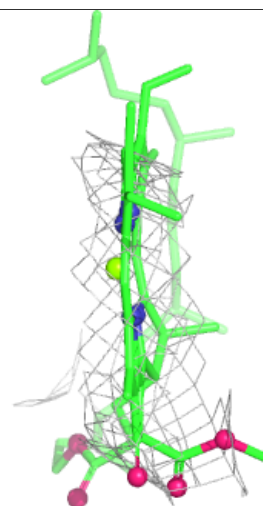
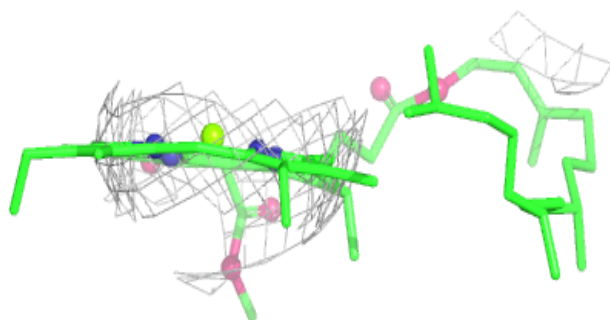
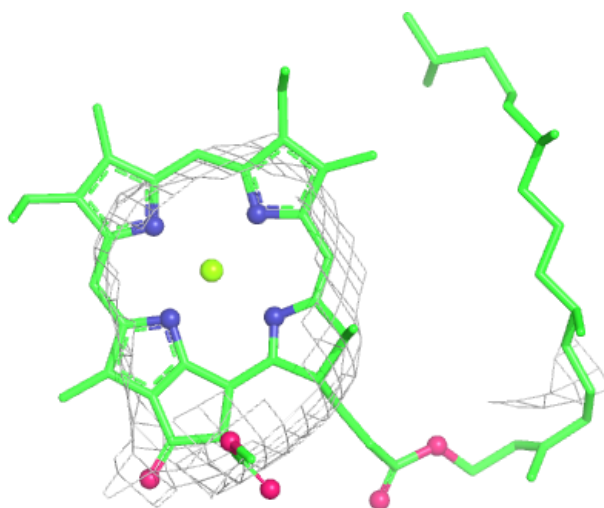
Electron density around LHG D 409:

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



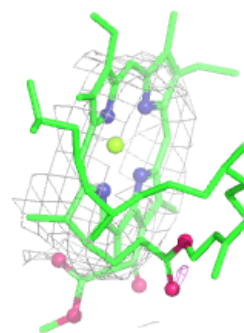
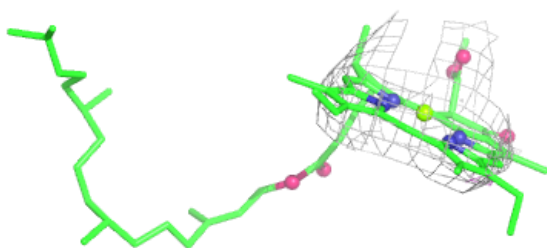
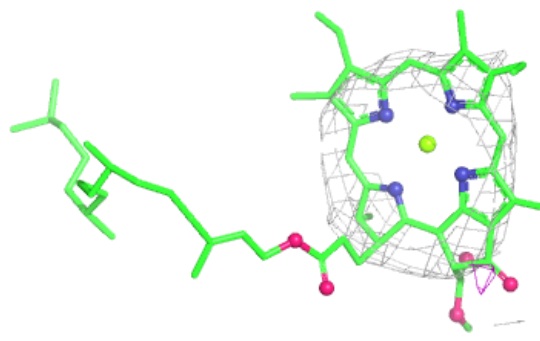
Electron density around CLA c 913:

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

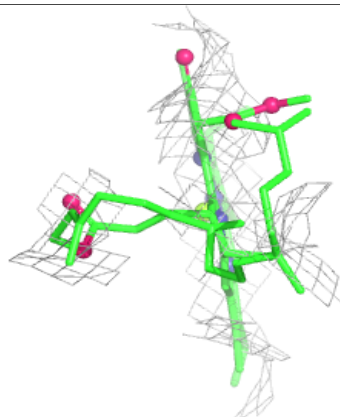
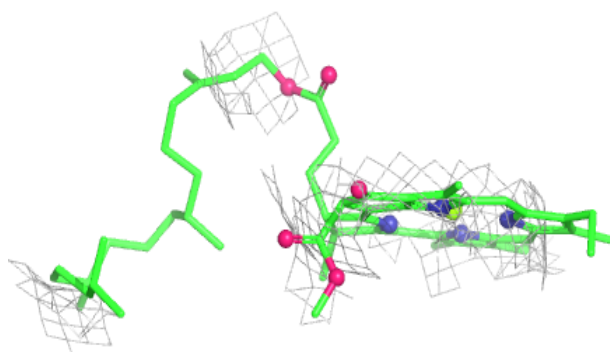
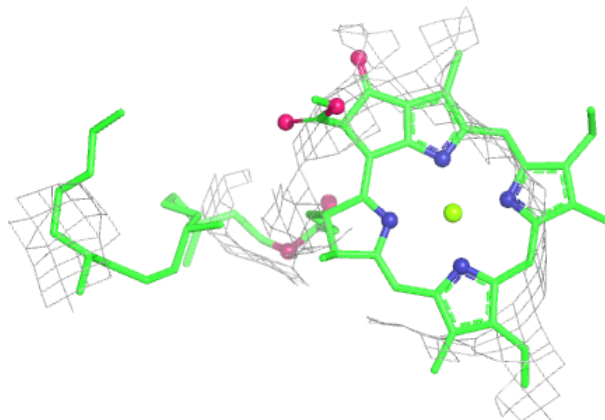


Electron density around CLA a 408:

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

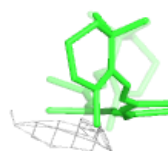
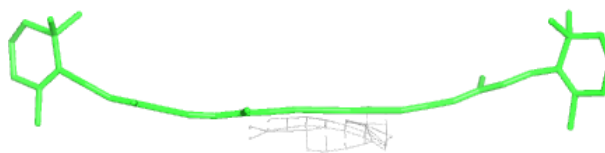
**Electron density around CLA b 613:**

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

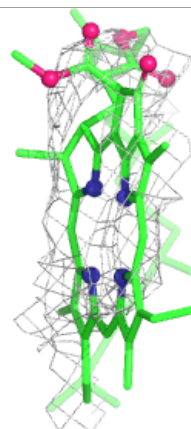
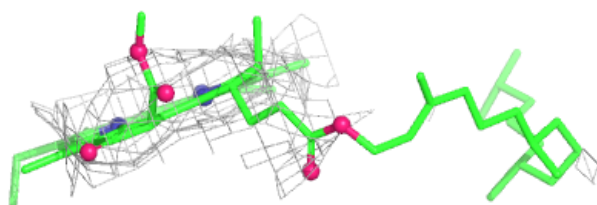
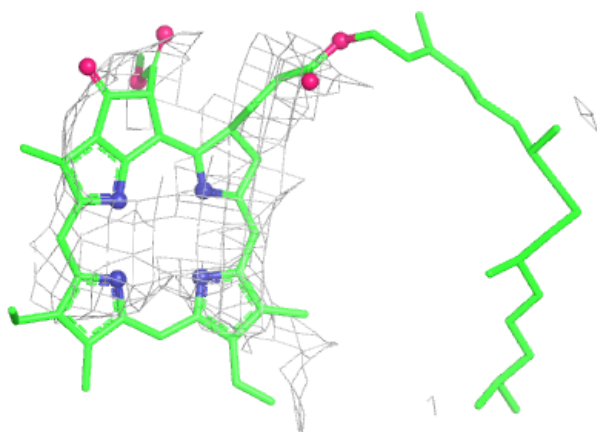


Electron density around BCR K 101:

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

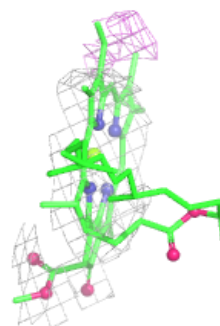
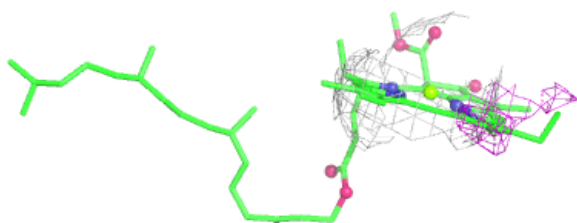
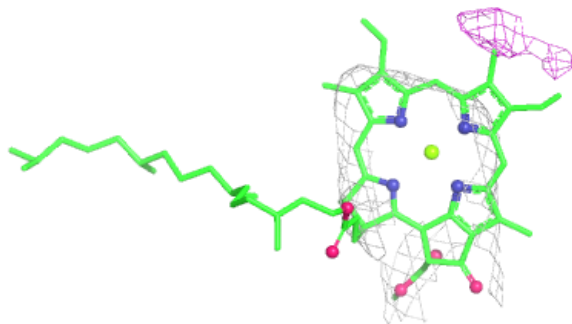
**Electron density around PHO A 608:**

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

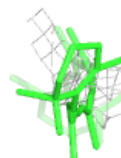
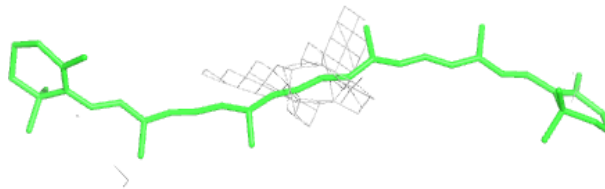


Electron density around CLA A 607:

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

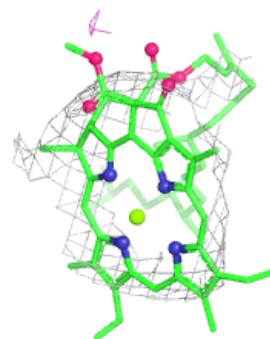
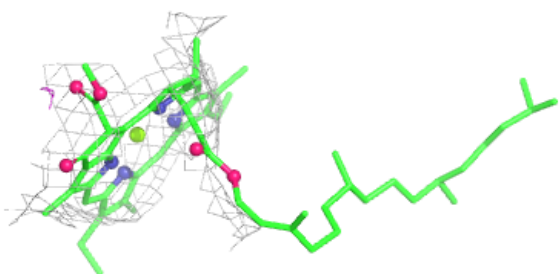
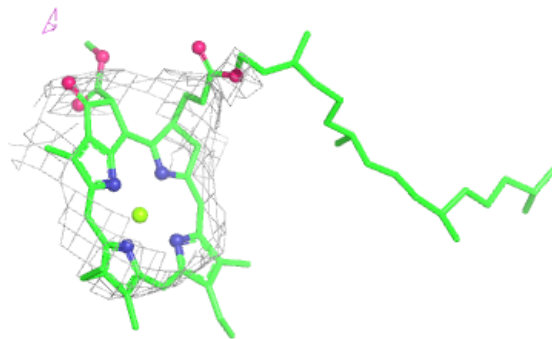
**Electron density around BCR Y 101:**

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



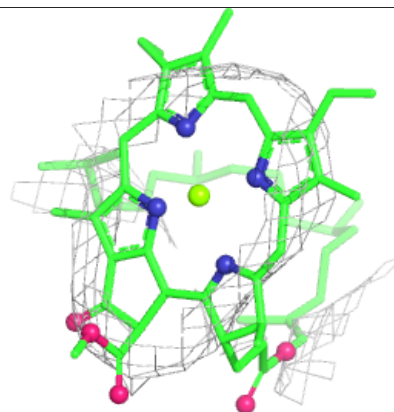
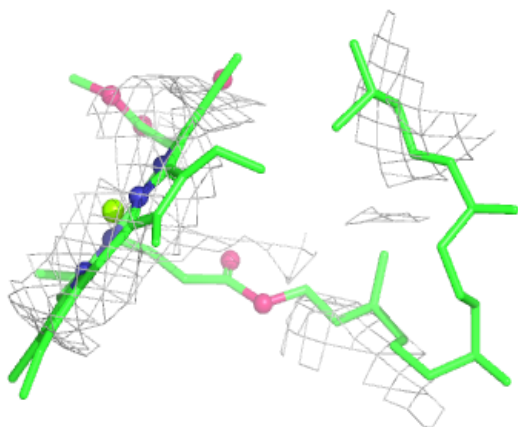
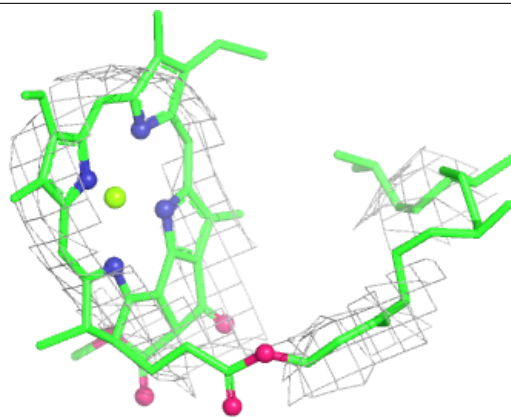
Electron density around CLA C 511:

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

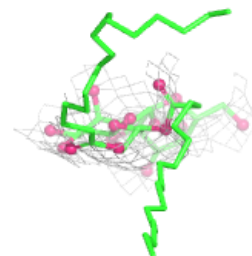
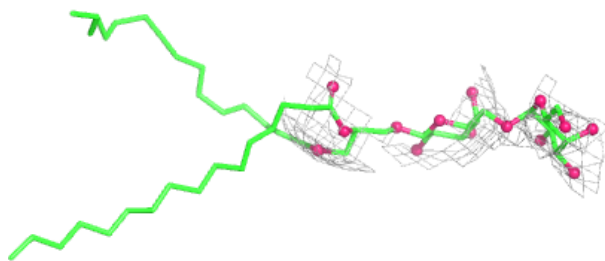


Electron density around CLA c 904:

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

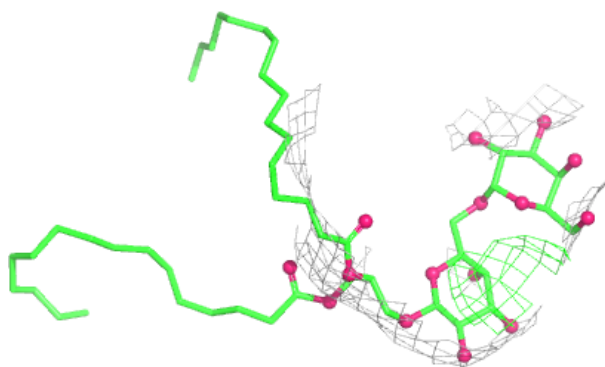
**Electron density around DGD c 916:**

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

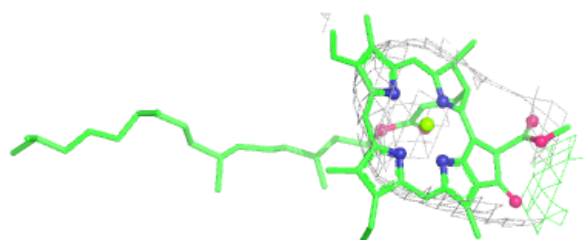
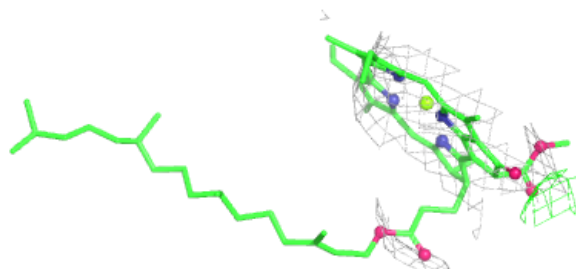


Electron density around DGD c 917:

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

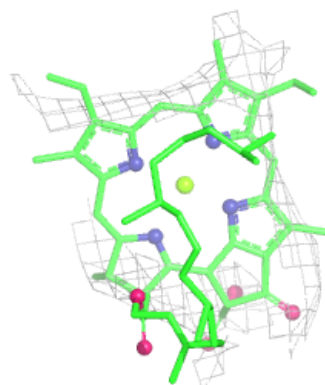
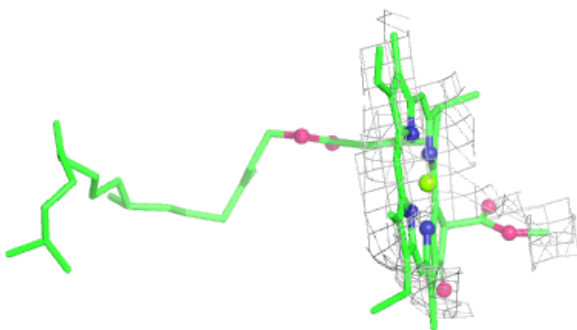
**Electron density around CLA c 905:**

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

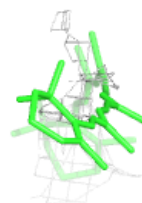
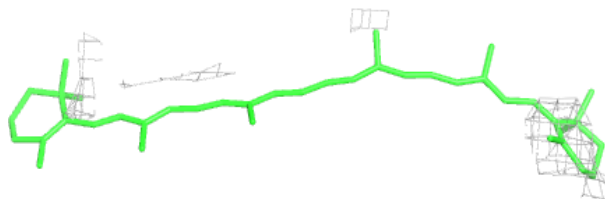


Electron density around CLA c 907:

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

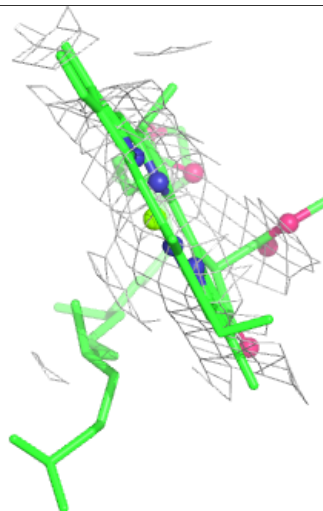
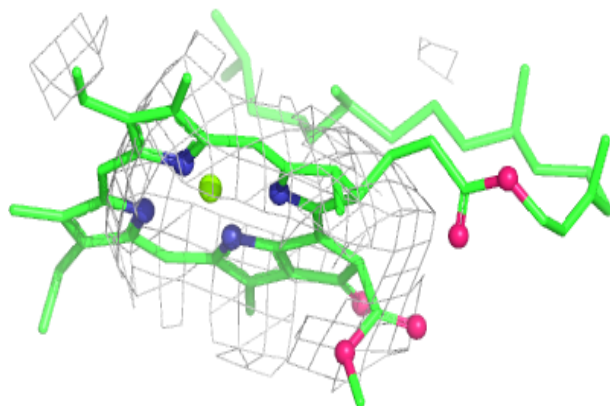
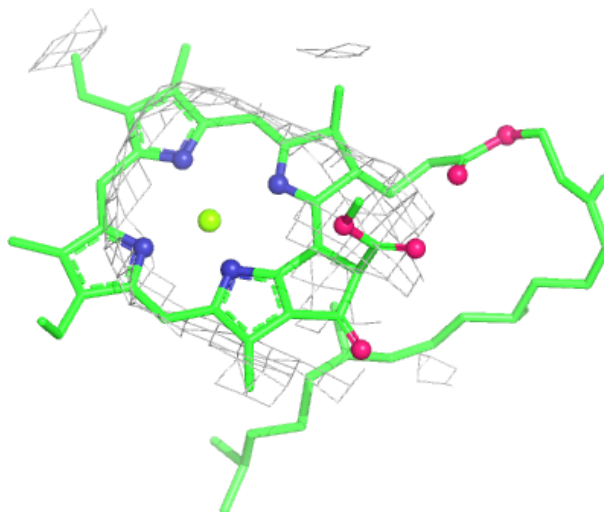
**Electron density around BCR B 622:**

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



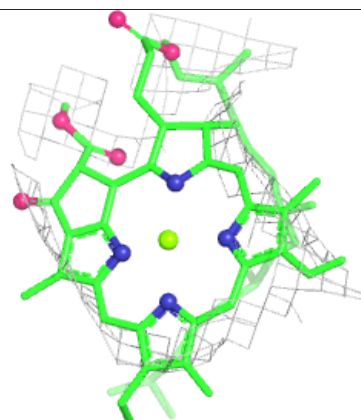
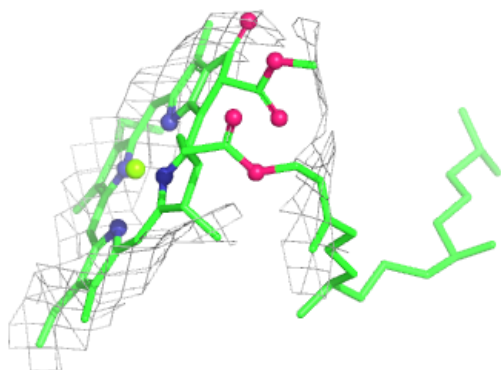
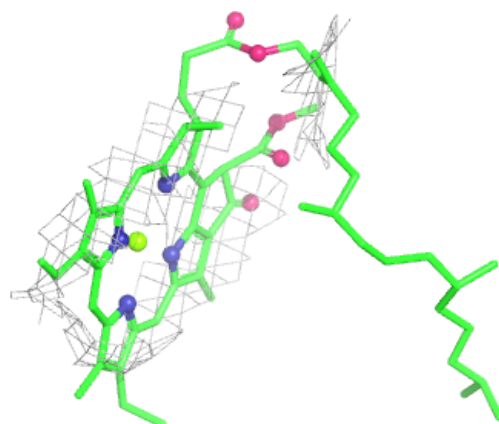
Electron density around CLA c 910:

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

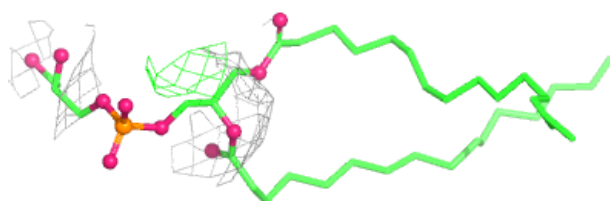
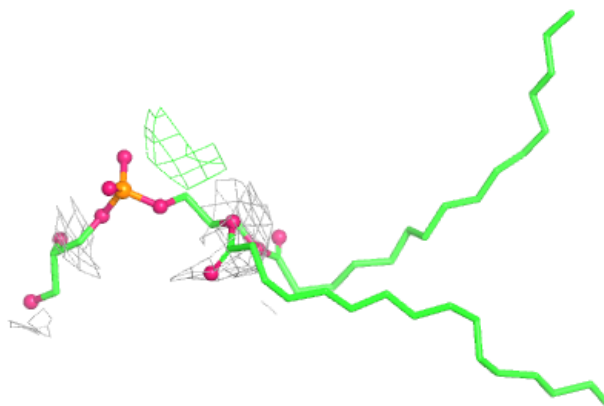


Electron density around CLA b 614:

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

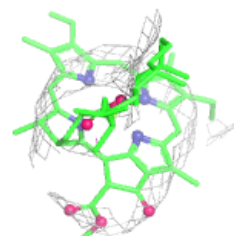
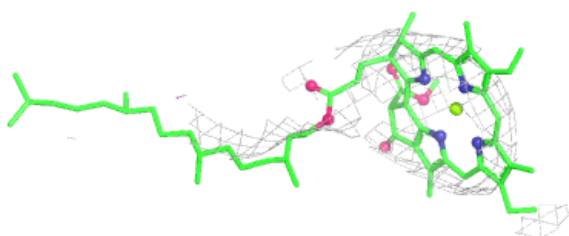
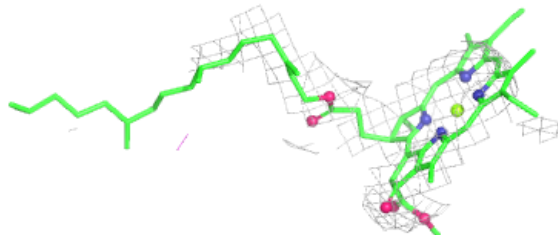
**Electron density around LHG d 409:**

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

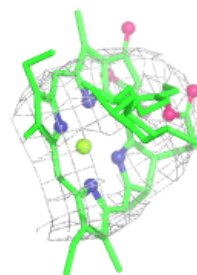
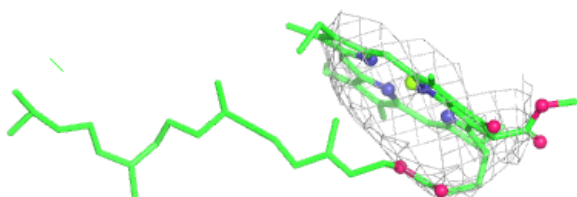
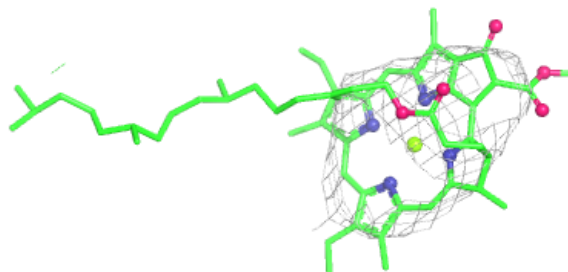


Electron density around CLA c 903:

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

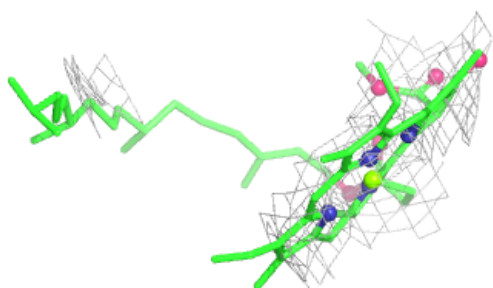
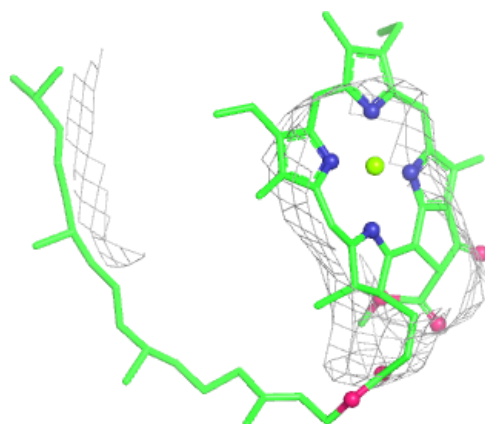
**Electron density around CLA b 615:**

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

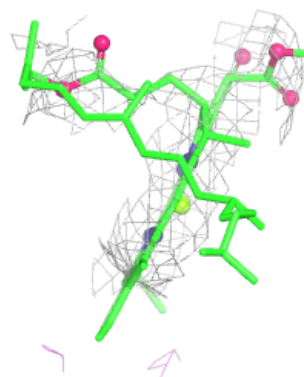
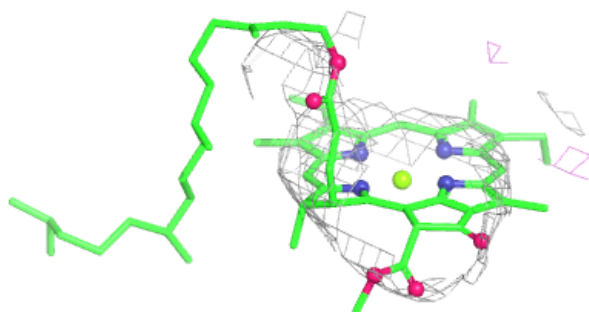
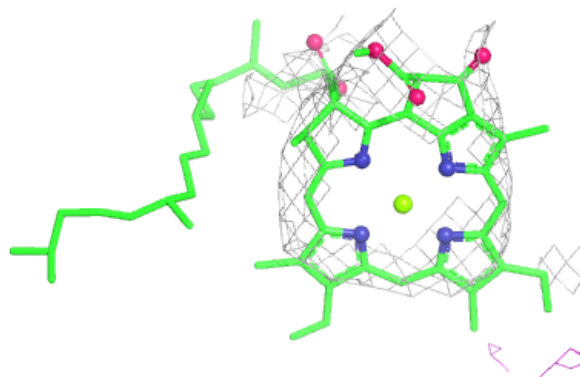


Electron density around CLA C 507:

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

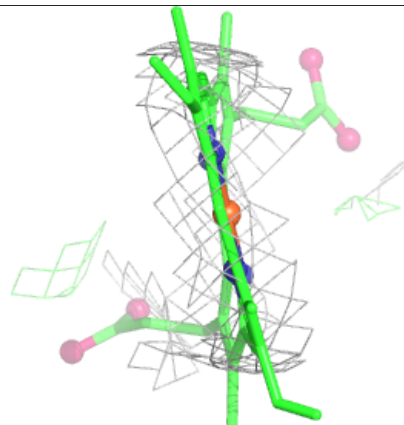
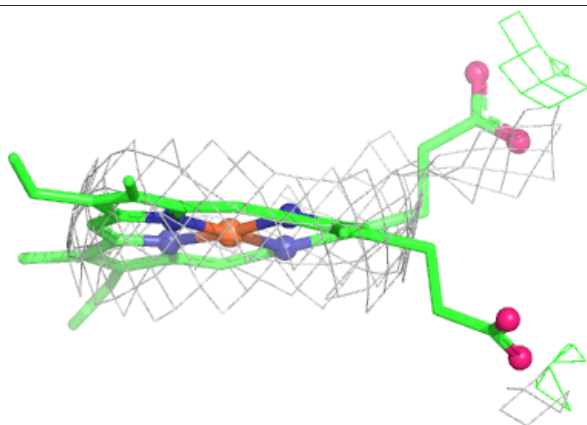
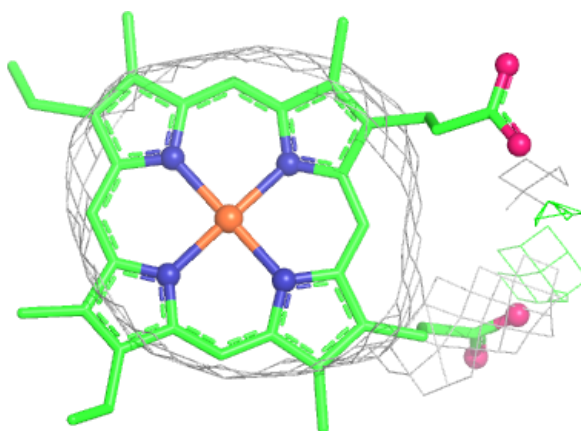
**Electron density around CLA A 614:**

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

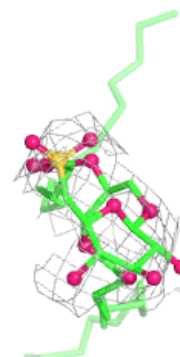
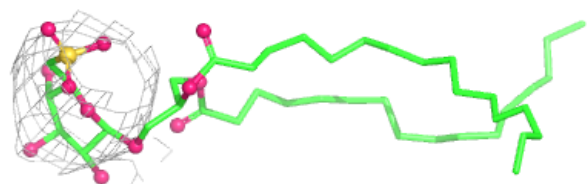
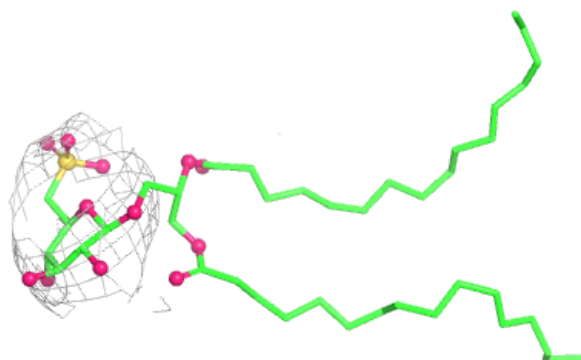


Electron density around HEM e 101:

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

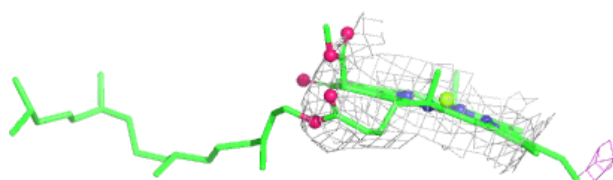
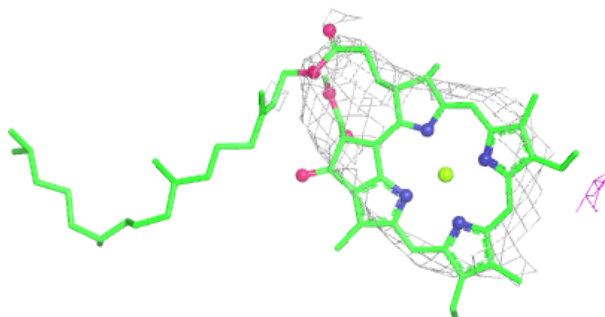
**Electron density around SQD L 101:**

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

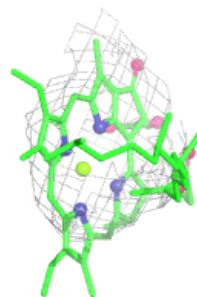
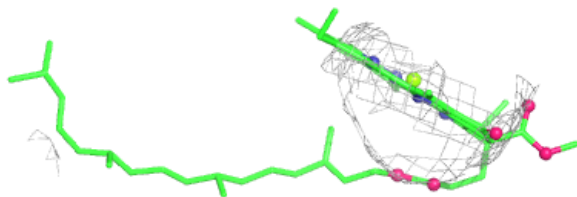


Electron density around CLA b 603:

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

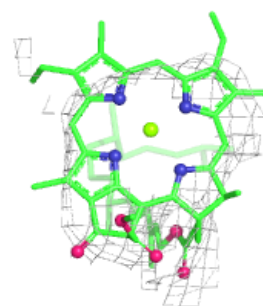
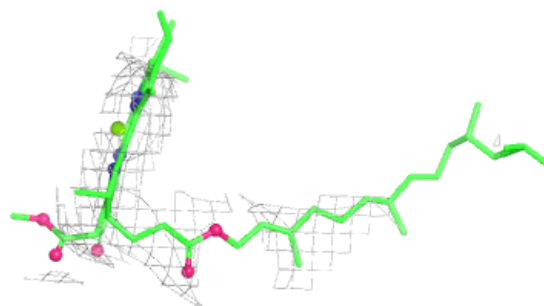
**Electron density around CLA B 609:**

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

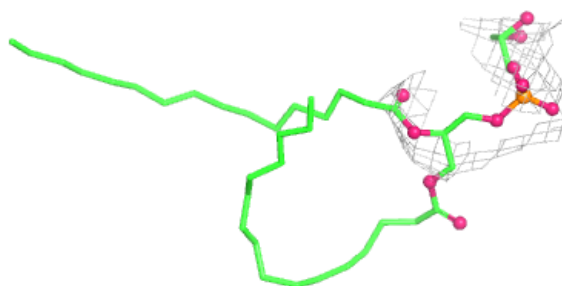


Electron density around CLA B 606:

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

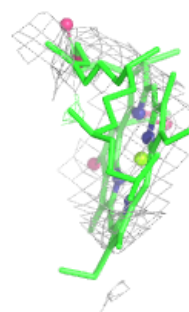
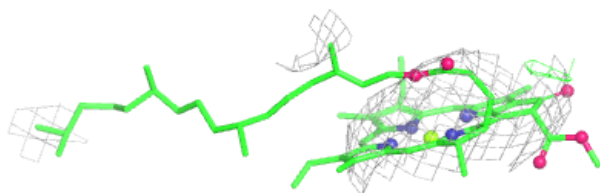
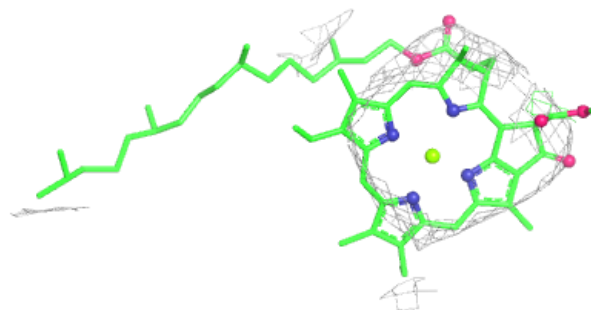
**Electron density around LHG D 407:**

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

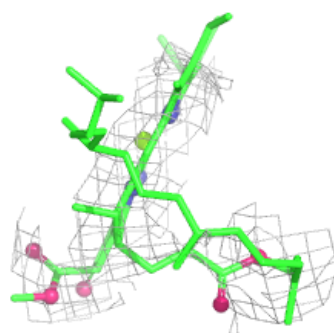
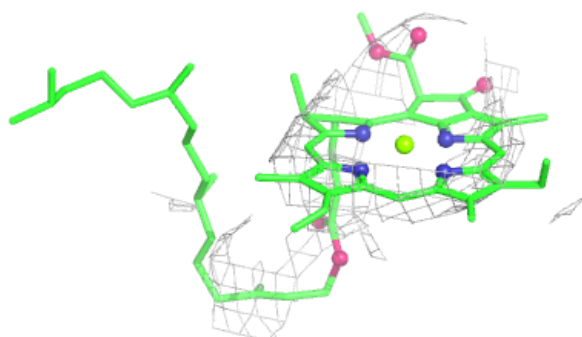
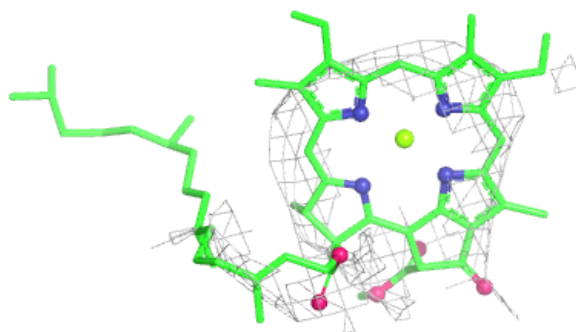


Electron density around CLA C 501:

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

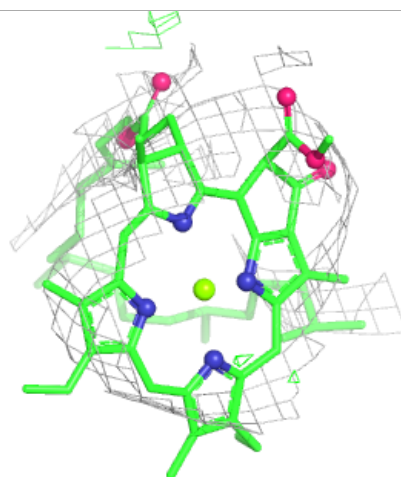
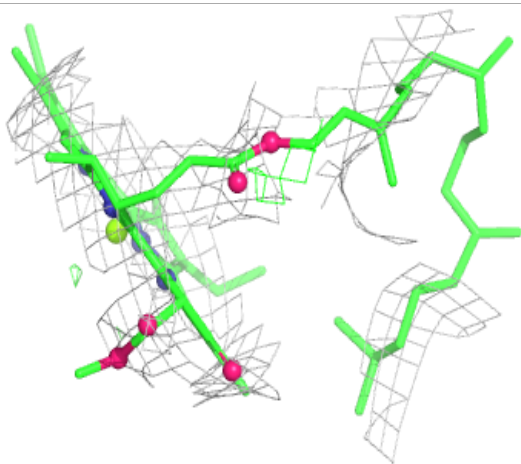
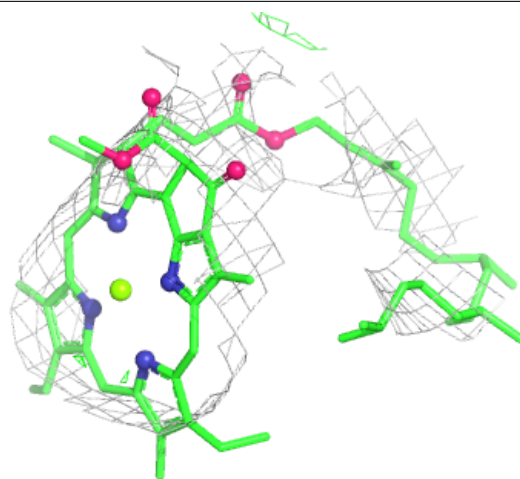
**Electron density around CLA d 401:**

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



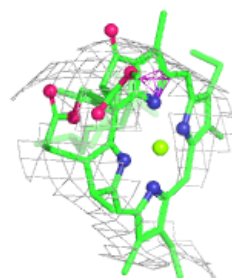
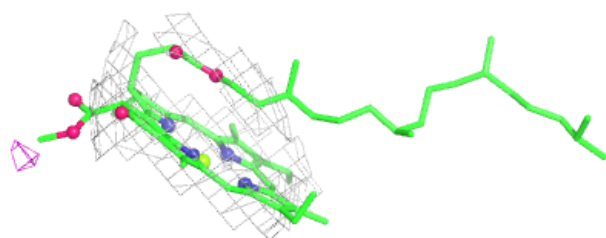
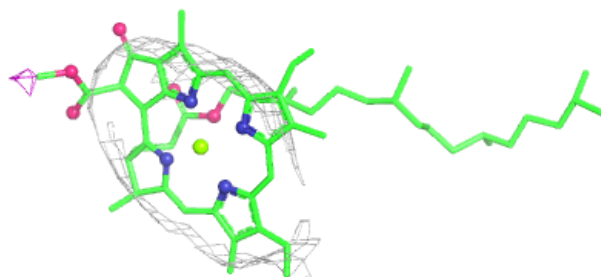
Electron density around CLA C 503:

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

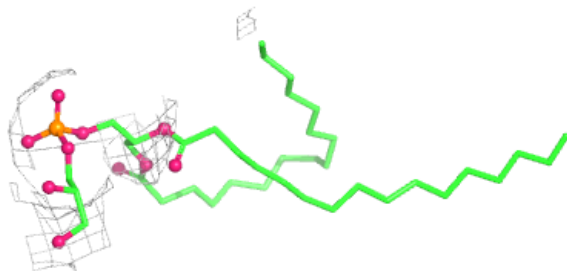


Electron density around CLA B 615:

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

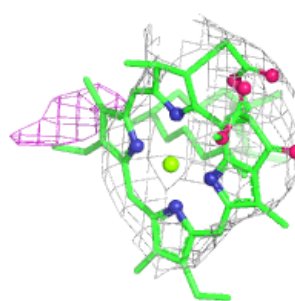
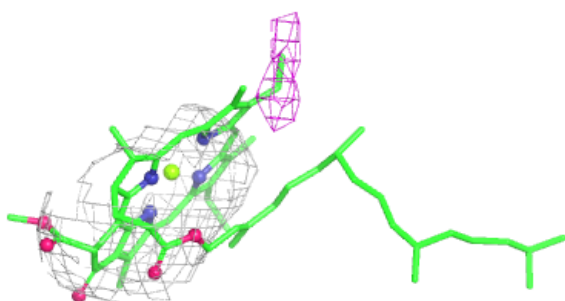
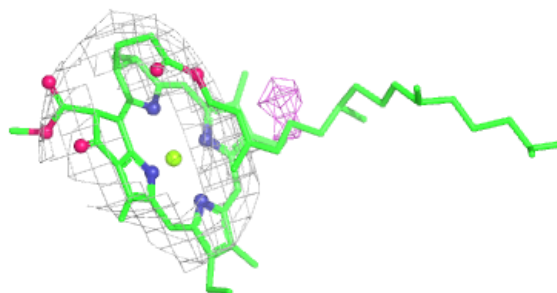
**Electron density around LHG d 408:**

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

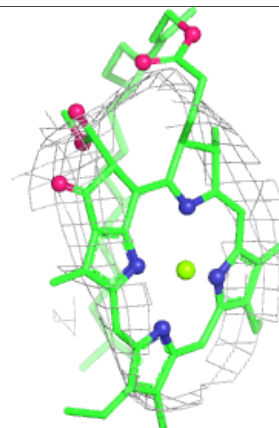
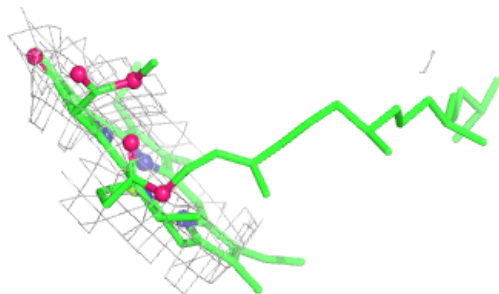
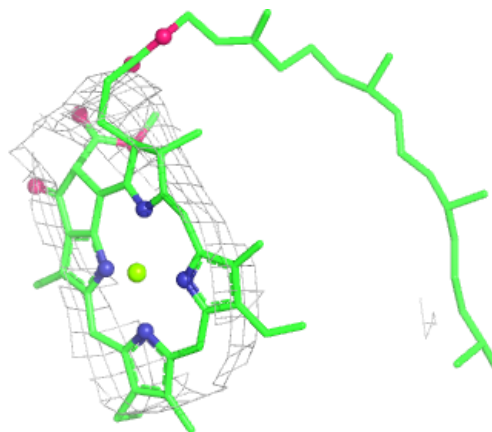


Electron density around CLA C 505:

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

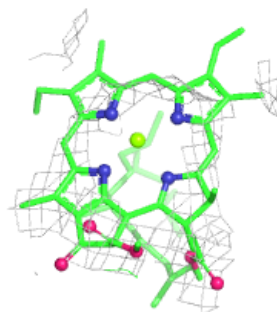
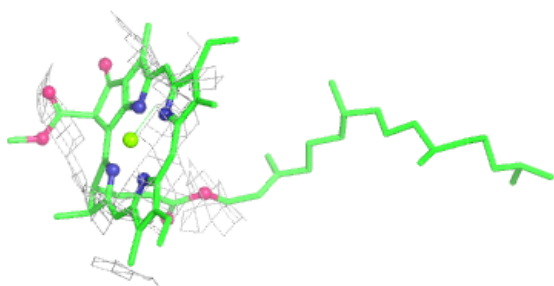
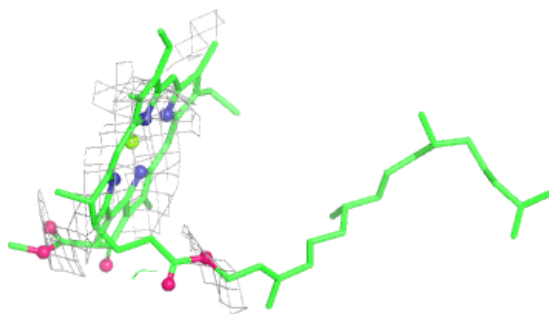
**Electron density around CLA c 908:**

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



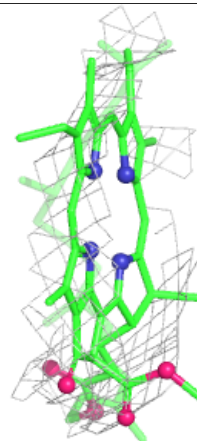
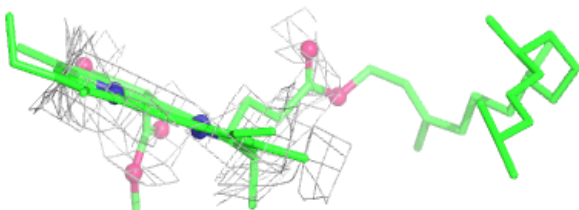
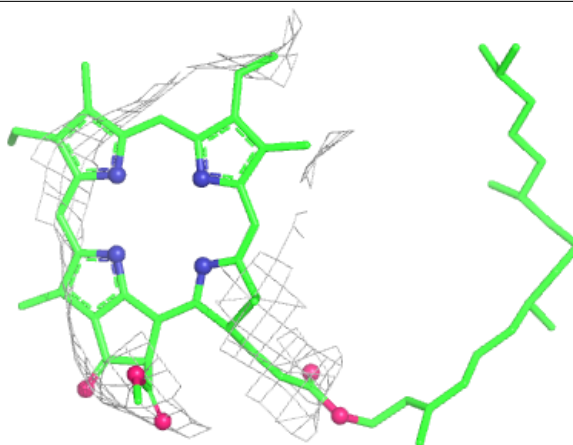
Electron density around CLA c 909:

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



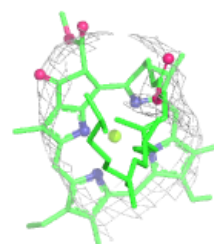
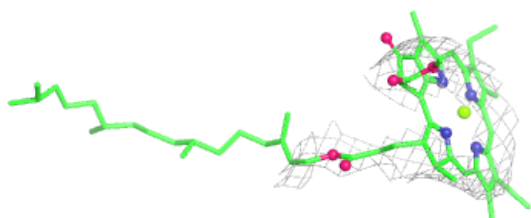
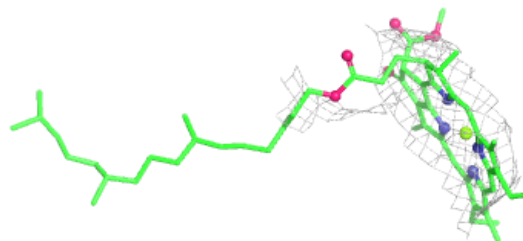
Electron density around PHO d 402:

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



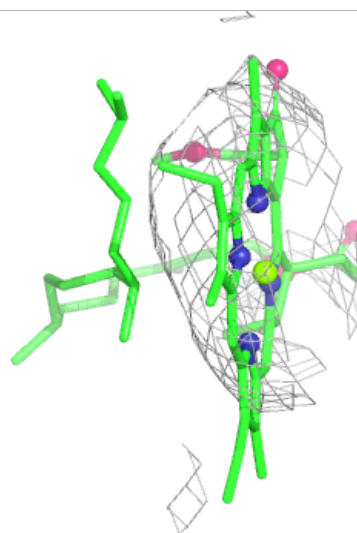
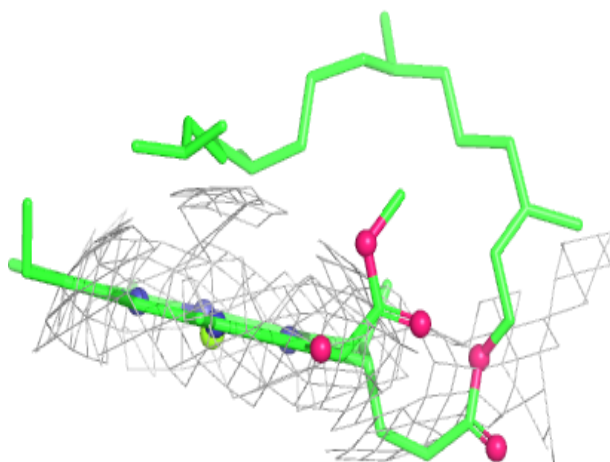
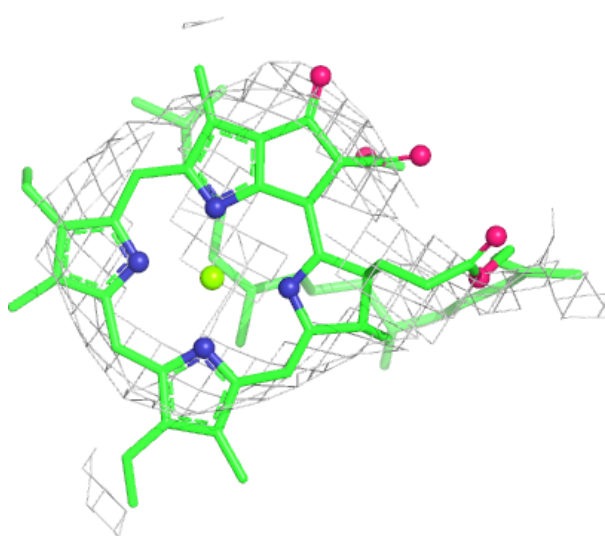
Electron density around CLA b 605:

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



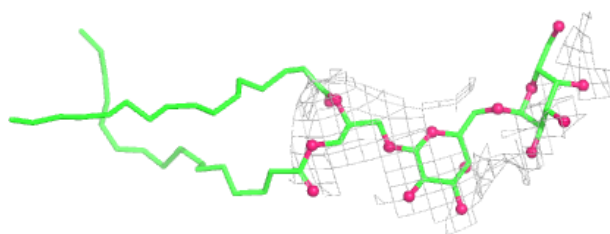
Electron density around CLA c 911:

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

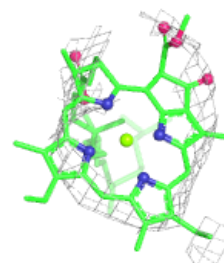
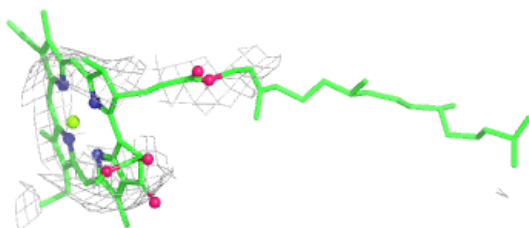
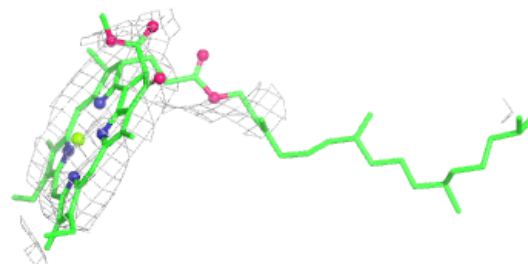


Electron density around DGD C 516:

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

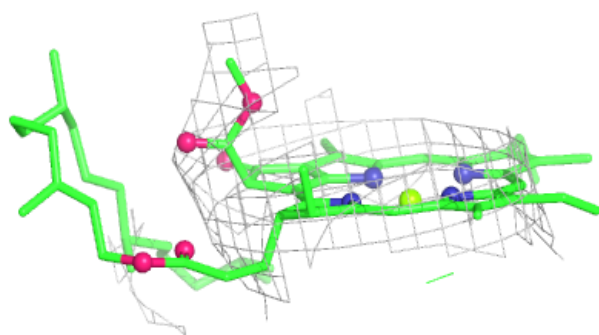
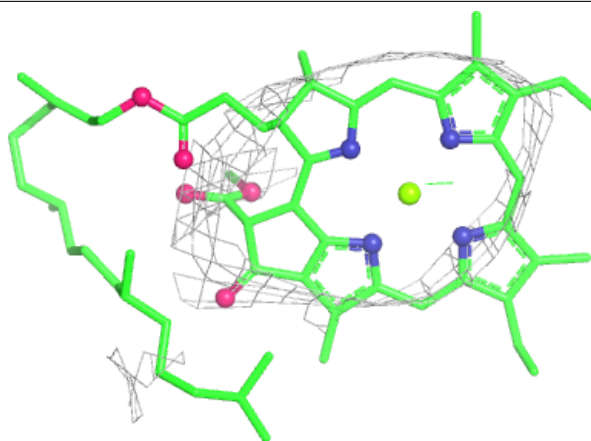
**Electron density around CLA B 605:**

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



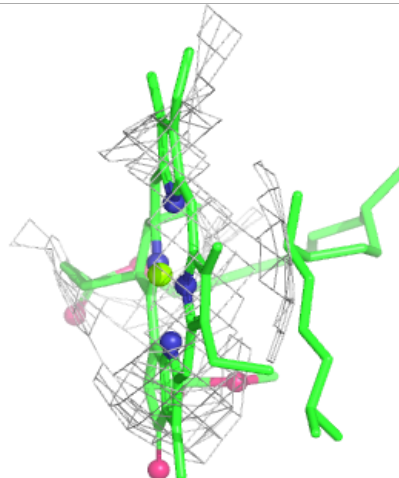
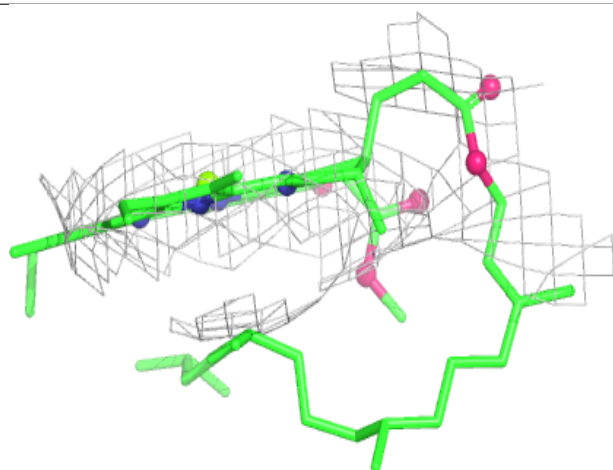
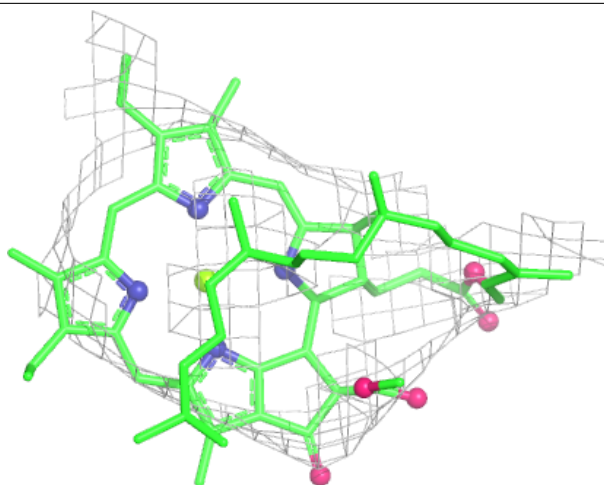
Electron density around CLA B 611:

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



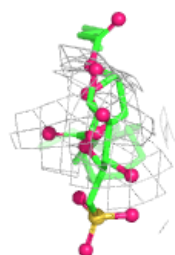
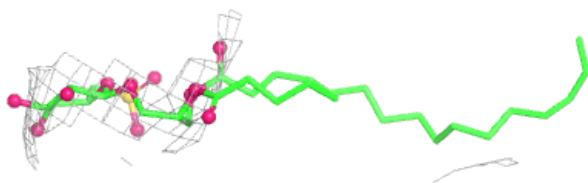
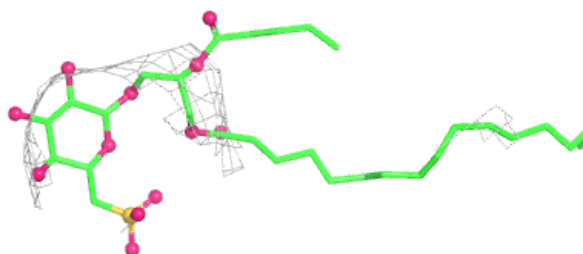
Electron density around CLA C 510:

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

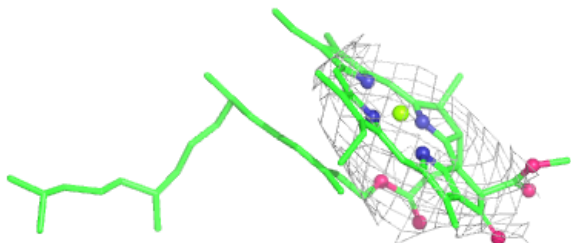
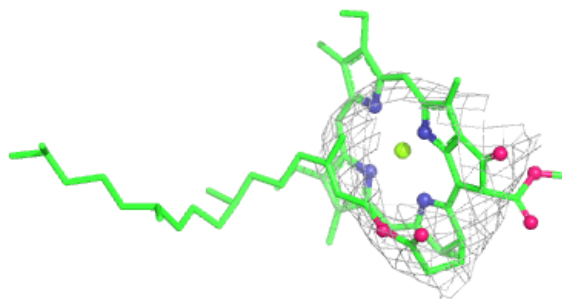


Electron density around SQD F 101:

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

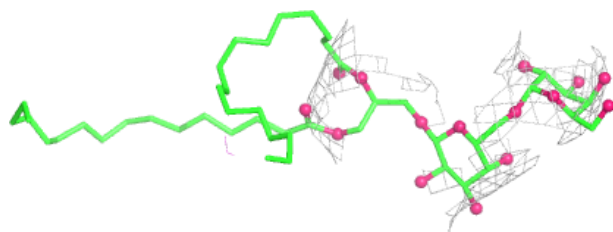
**Electron density around CLA c 906:**

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

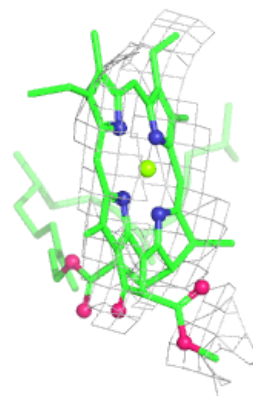
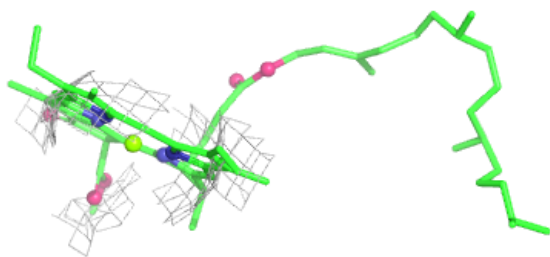
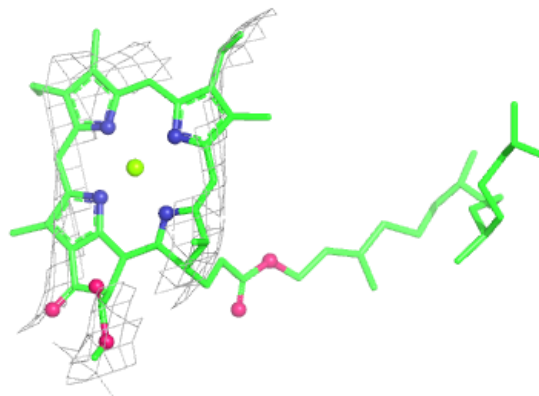


Electron density around DGD h 102:

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

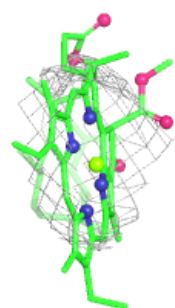
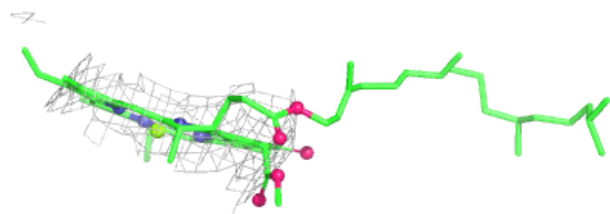
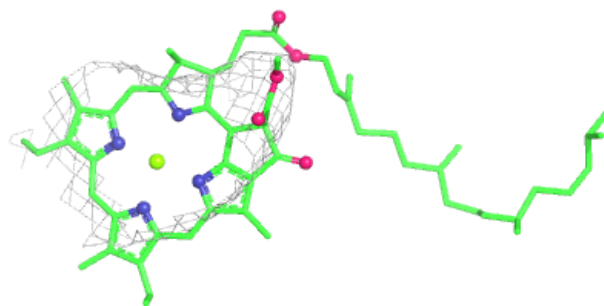
**Electron density around CLA A 609:**

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

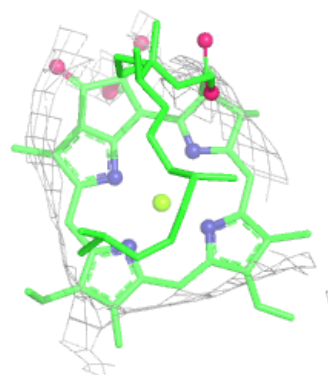
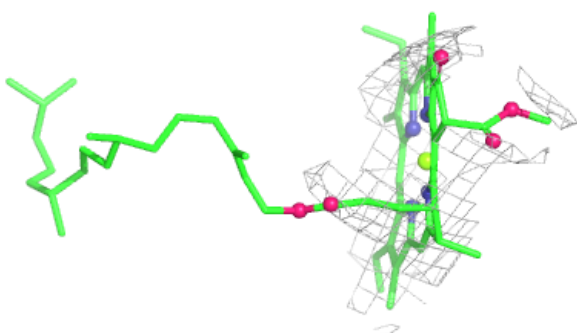
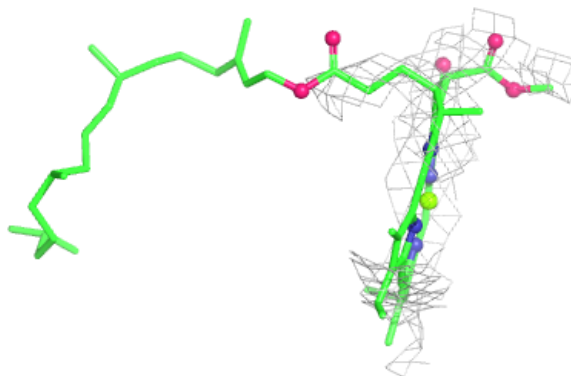


Electron density around CLA B 603:

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

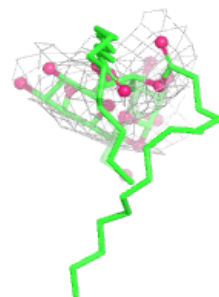
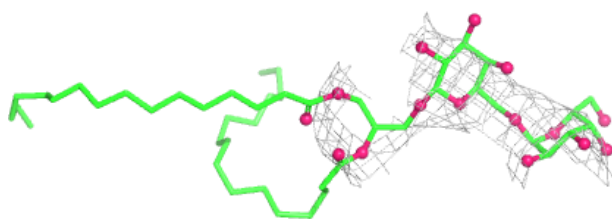
**Electron density around CLA C 506:**

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

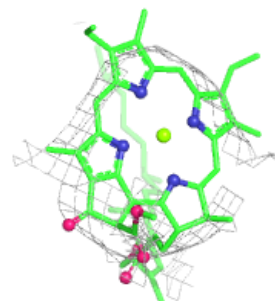
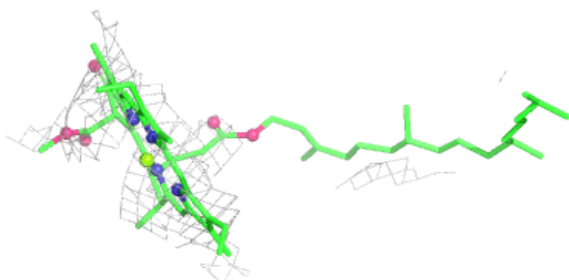
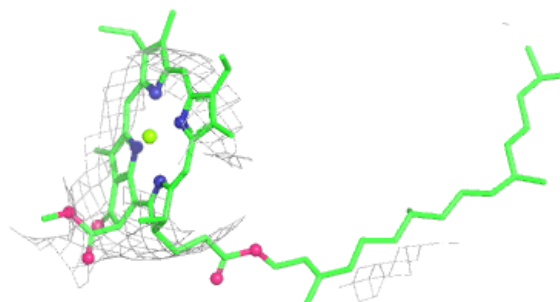


Electron density around DGD H 102:

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

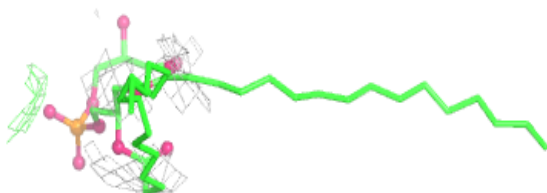
**Electron density around CLA b 610:**

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



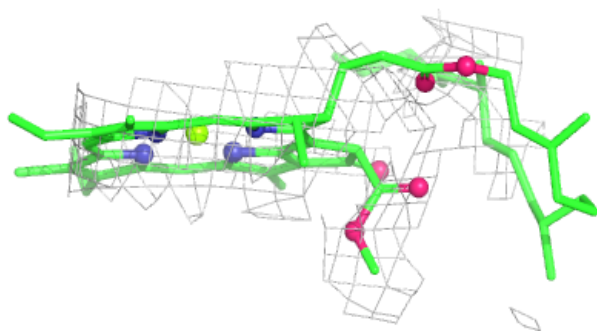
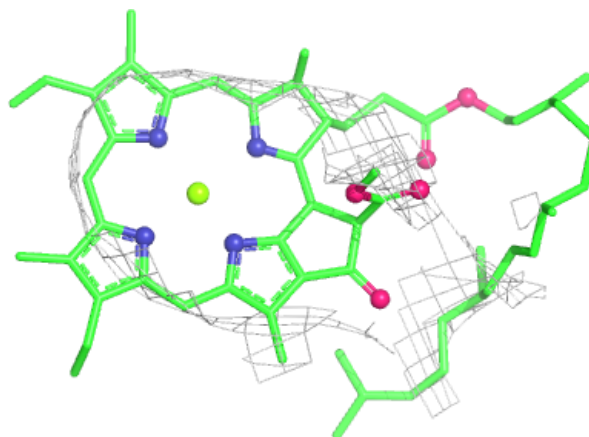
Electron density around LHG B 621:

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



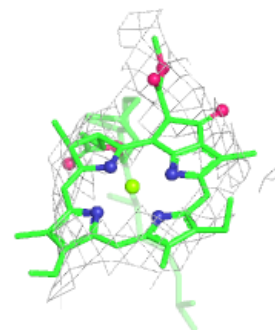
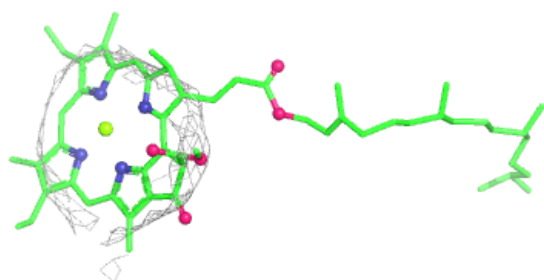
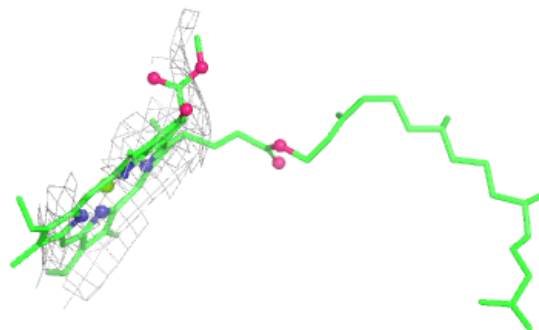
Electron density around CLA b 611:

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

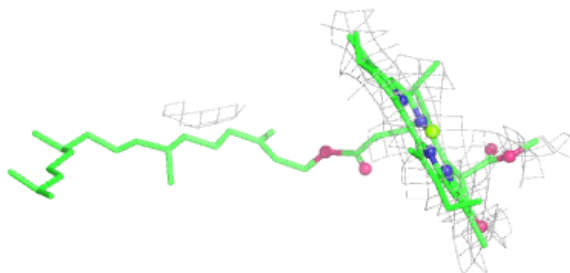
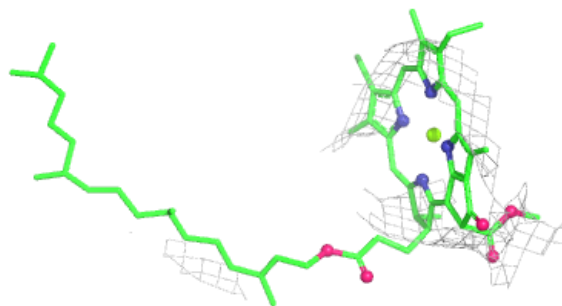


Electron density around CLA d 403:

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

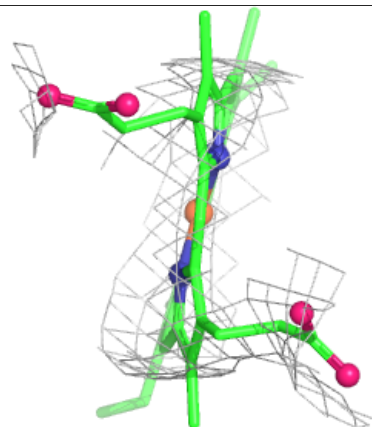
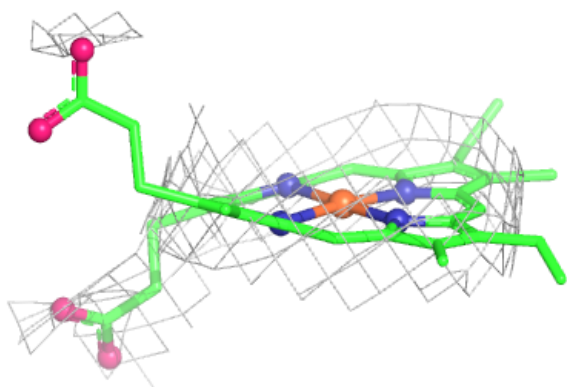
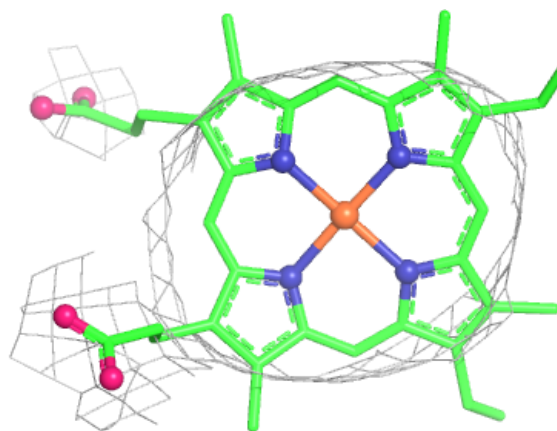
**Electron density around CLA B 610:**

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

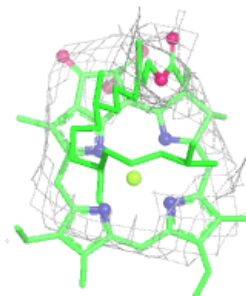
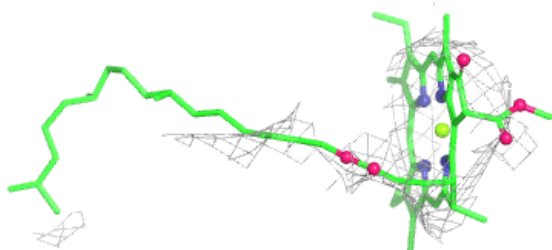
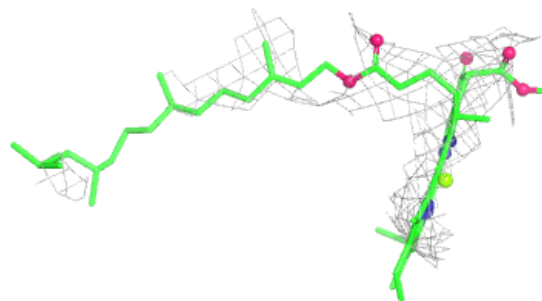


Electron density around HEM E 101:

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

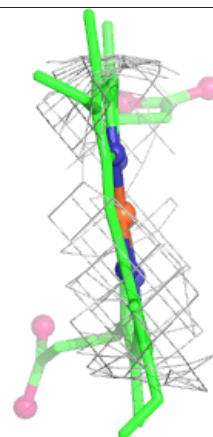
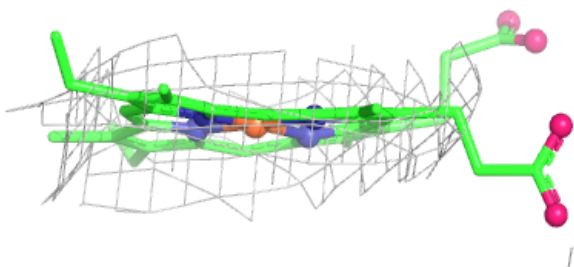
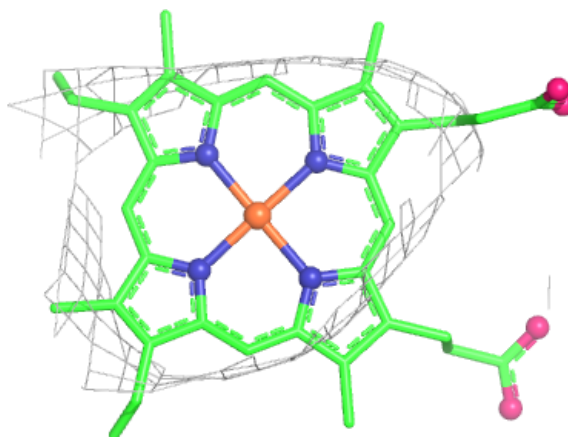
**Electron density around CLA b 606:**

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



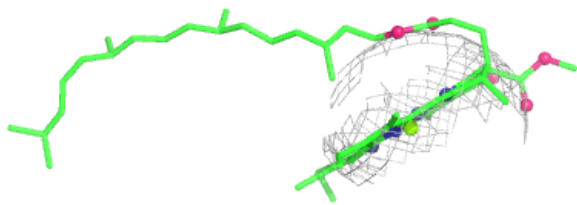
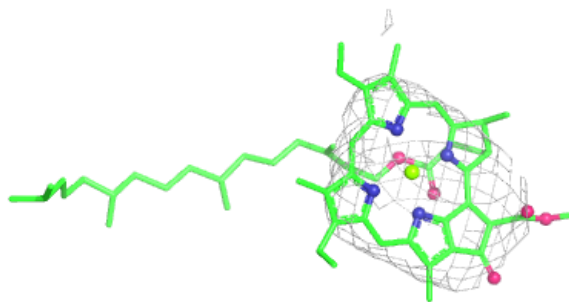
Electron density around HEM v 202:

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



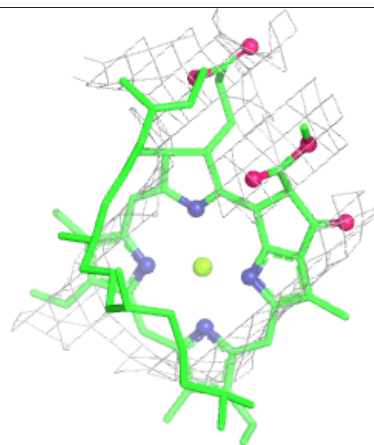
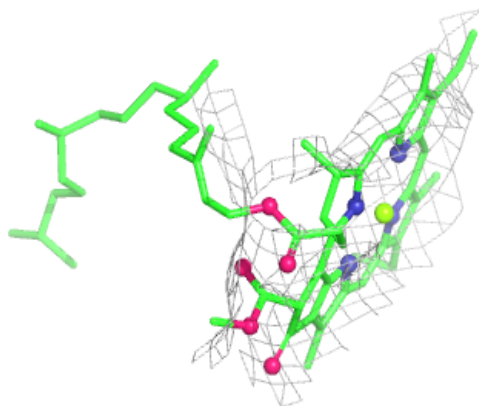
Electron density around CLA b 609:

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



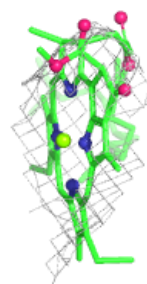
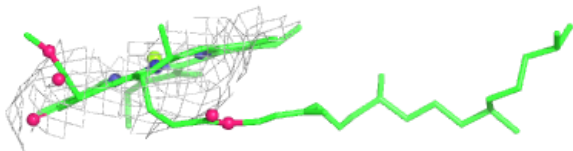
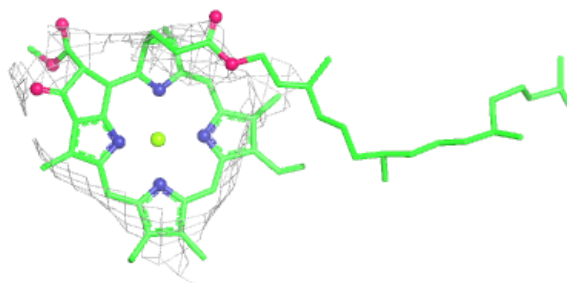
Electron density around CLA B 614:

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

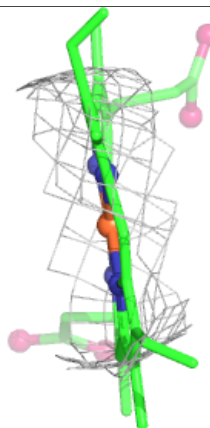
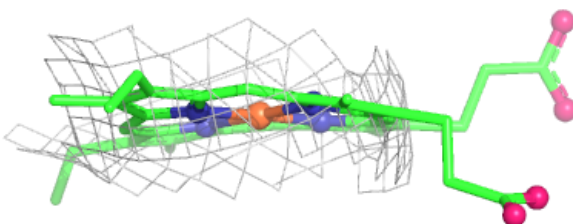
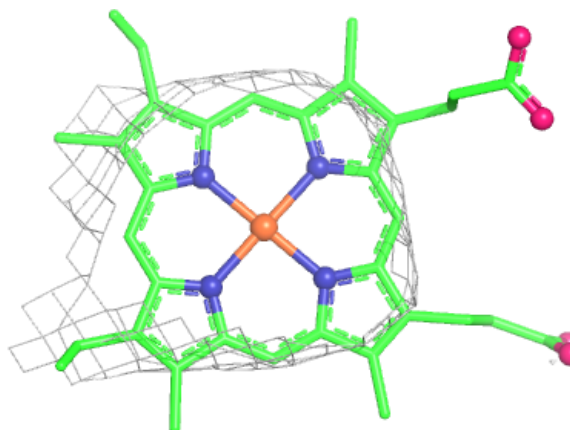


Electron density around CLA b 604:

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

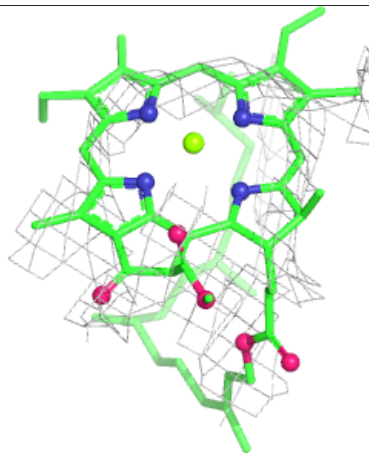
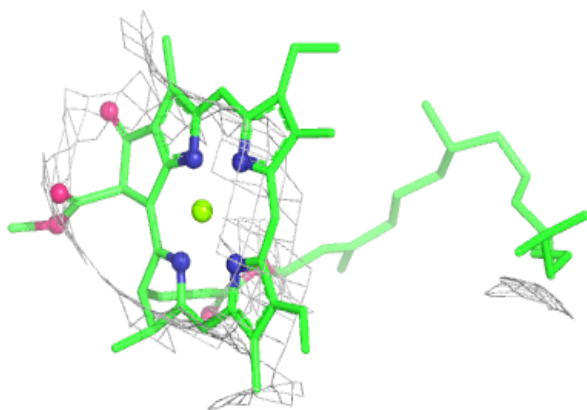
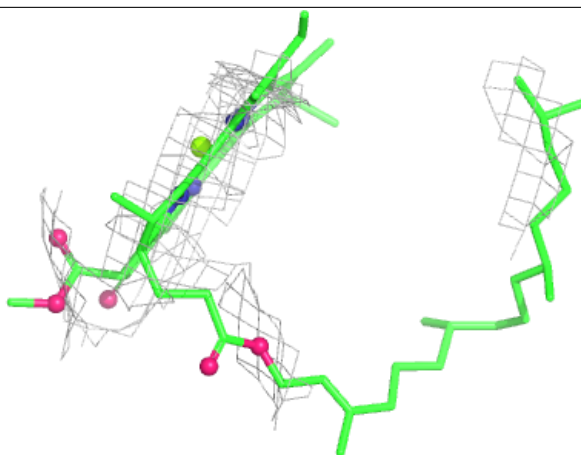
**Electron density around HEM V 202:**

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



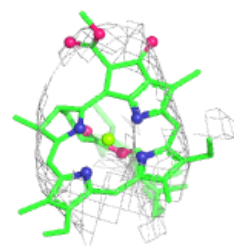
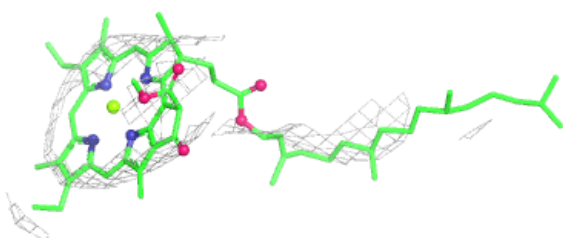
Electron density around CLA B 612:

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

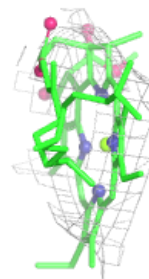
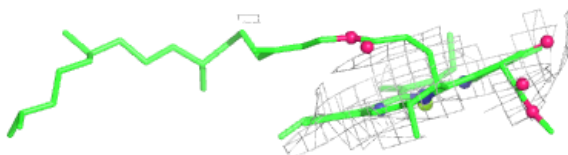
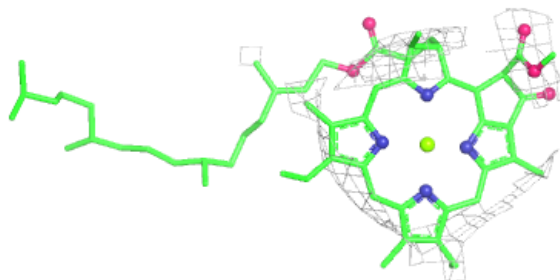


Electron density around CLA C 502:

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

**Electron density around CLA 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.