



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 09:45 AM UTC

PDB ID : 8F4H / pdb_00008f4h
Title : RT XFEL structure of Photosystem II 1200 microseconds after the third illumination at 2.10 Angstrom resolution
Authors : Bhowmick, A.; Hussein, R.; Bogacz, I.; Simon, P.S.; Ibrahim, M.; Chatterjee, R.; Doyle, M.D.; Cheah, M.H.; Fransson, T.; Chernev, P.; Kim, I.-S.; Makita, H.; Dasgupta, M.; Kaminsky, C.J.; Zhang, M.; Gatcke, J.; Haupt, S.; Nangca, I.I.; Keable, S.M.; Aydin, O.; Tono, K.; Owada, S.; Gee, L.B.; Fuller, F.D.; Batyuk, A.; Alonso-Mori, R.; Holton, J.M.; Paley, D.W.; Moriarty, N.W.; Mamedov, F.; Adams, P.D.; Brewster, A.S.; Dobbek, H.; Sauter, N.K.; Bergmann, U.; Zouni, A.; Messinger, J.; Kern, J.; Yano, J.; Yachandra, V.K.
Deposited on : 2022-11-10
Resolution : 2.10 Å(reported)

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

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

A user guide is available at
<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0

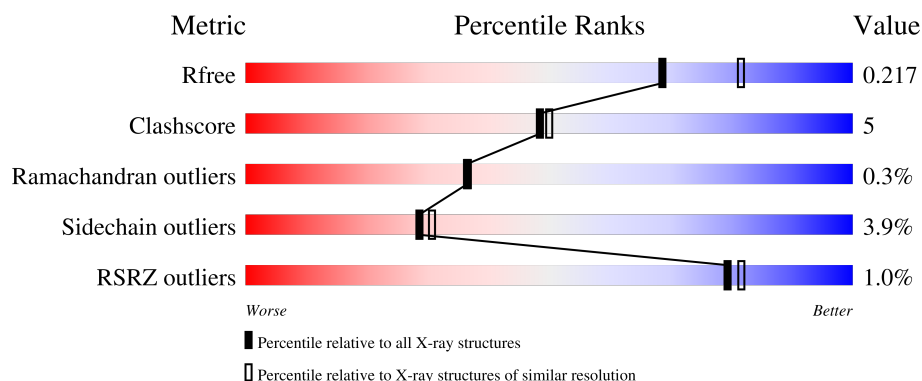
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	344	

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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

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Mol	Chain	Length	Quality of chain
1	a	344	% 83% 12% ..
2	B	510	90% 8% .
2	b	510	88% 10% ..
3	C	461	86% 9% .
3	c	461	88% 10% ..
4	D	352	87% 10% ..
4	d	352	86% 10% ..
5	E	84	% 82% 14% ..
5	e	84	4% 74% 24% .
6	F	45	69% 7% 24%
6	f	45	51% 18% 7% 24%
7	H	66	3% 89% 9% .
7	h	66	3% 74% 20% . 5%
8	I	38	76% 13% 5% 5%
8	i	38	89% 5% 5%
9	J	40	2% 75% 15% 10%
9	j	40	75% 15% 10%
10	K	46	67% 11% . 20%
10	k	46	63% 15% . 20%
11	L	37	3% 81% 16% .
11	l	37	81% 14% . .
12	M	36	78% 14% 8%
12	m	36	86% . 11%
13	O	272	% 78% 11% . 10%
13	o	272	% 76% 12% . 10%

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Mol	Chain	Length	Quality of chain
14	T	32	
14	t	32	
15	U	134	
15	u	134	
16	V	163	
16	v	163	
17	Y	46	
17	y	46	
18	X	41	
18	x	41	
19	Z	62	
19	z	62	
20	R	41	
20	r	41	

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
26	CLA	A	607	X	-	-	-
26	CLA	A	608	X	-	-	-
26	CLA	A	610	X	-	-	-
26	CLA	A	613	X	-	-	-
26	CLA	B	601	X	-	-	-
26	CLA	B	602	X	-	-	-
26	CLA	B	603	X	-	-	-
26	CLA	B	604	X	-	-	-
26	CLA	B	605	X	-	-	-
26	CLA	B	606	X	-	-	-
26	CLA	B	607	X	-	-	-
26	CLA	B	608	X	-	-	-
26	CLA	B	610	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	CLA	B	611	X	-	-	-
26	CLA	B	612	X	-	-	-
26	CLA	B	613	X	-	-	-
26	CLA	B	614	X	-	-	-
26	CLA	B	615	X	-	-	-
26	CLA	B	616	X	-	-	-
26	CLA	C	501	X	-	-	-
26	CLA	C	502	X	-	-	-
26	CLA	C	503	X	-	-	-
26	CLA	C	504	X	-	-	-
26	CLA	C	505	X	-	-	-
26	CLA	C	506	X	-	-	-
26	CLA	C	507	X	-	-	-
26	CLA	C	509	X	-	-	-
26	CLA	C	510	X	-	-	-
26	CLA	C	511	X	-	-	-
26	CLA	C	512	X	-	-	-
26	CLA	C	513	X	-	-	-
26	CLA	D	402	X	-	-	-
26	CLA	a	606	X	-	-	-
26	CLA	a	607	X	-	-	-
26	CLA	a	609	X	-	-	-
26	CLA	a	612	X	-	-	-
26	CLA	b	601	X	-	-	-
26	CLA	b	602	X	-	-	-
26	CLA	b	603	X	-	-	-
26	CLA	b	605	X	-	-	-
26	CLA	b	606	X	-	-	-
26	CLA	b	607	X	-	-	-
26	CLA	b	609	X	-	-	-
26	CLA	b	610	X	-	-	-
26	CLA	b	611	X	-	-	-
26	CLA	b	612	X	-	-	-
26	CLA	b	613	X	-	-	-
26	CLA	b	614	X	-	-	-
26	CLA	b	615	X	-	-	-
26	CLA	c	501	X	-	-	-
26	CLA	c	502	X	-	-	-
26	CLA	c	503	X	-	-	-
26	CLA	c	504	X	-	-	-
26	CLA	c	505	X	-	-	-
26	CLA	c	506	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	CLA	c	507	X	-	-	-
26	CLA	c	509	X	-	-	-
26	CLA	c	510	X	-	-	-
26	CLA	c	511	X	-	-	-
26	CLA	c	512	X	-	-	-
26	CLA	c	513	X	-	-	-
26	CLA	d	403	X	-	-	-
26	CLA	d	404	X	-	-	-
26	CLA	h	101	X	-	-	-

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 54161 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Photosystem II protein D1 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	64	0
			3604	2343	595	643	23			
1	a	334	Total	C	N	O	S	0	64	0
			3601	2340	595	643	23			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	505	Total	C	N	O	S	0	4	0
			4005	2631	666	695	13			
2	b	505	Total	C	N	O	S	0	0	0
			3978	2610	665	690	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	442	Total	C	N	O	S	0	11	0
			3592	2355	601	621	15			
3	c	451	Total	C	N	O	S	0	12	0
			3666	2396	617	638	15			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	341	Total	C	N	O	S	0	2	0
			2745	1818	448	467	12			
4	d	341	Total	C	N	O	S	0	3	0
			2751	1822	448	469	12			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	82	Total	C	N	O	0	1	0
			666	436	107	123			
5	e	82	Total	C	N	O	0	0	0
			664	434	108	122			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	65	Total	C	N	O	S	0	0	0
			510	341	82	85	2			
7	h	63	Total	C	N	O	S	0	0	0
			498	333	80	83	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	36	Total	C	N	O	S	0	0	0
			296	200	46	49	1			
8	i	36	Total	C	N	O	S	0	0	0
			296	200	46	49	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	36	Total	C	N	O	S	0	0	0
			257	174	40	42	1			
9	j	36	Total	C	N	O	S	0	0	0
			257	174	40	42	1			

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

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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
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	36	Total	C	N	O		0	0	0
			296	197	47	52				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	33	Total	C	N	O	S	0	0	0
			256	171	37	47	1			
12	m	32	Total	C	N	O	S	0	0	0
			251	168	36	46	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	244	Total	C	N	O	S	0	1	0
			1870	1168	313	385	4			
13	o	244	Total	C	N	O	S	0	0	0
			1874	1170	317	383	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
			258	181	36	39	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	27	Total	C	N	O	S	0	0	0
			196	128	35	30	3			
17	y	30	Total	C	N	O	S	0	0	0
			218	144	35	36	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	X	38	Total	C	N	O		0	0	0
			281	188	45	48				
18	x	39	Total	C	N	O		0	0	0
			286	191	46	49				

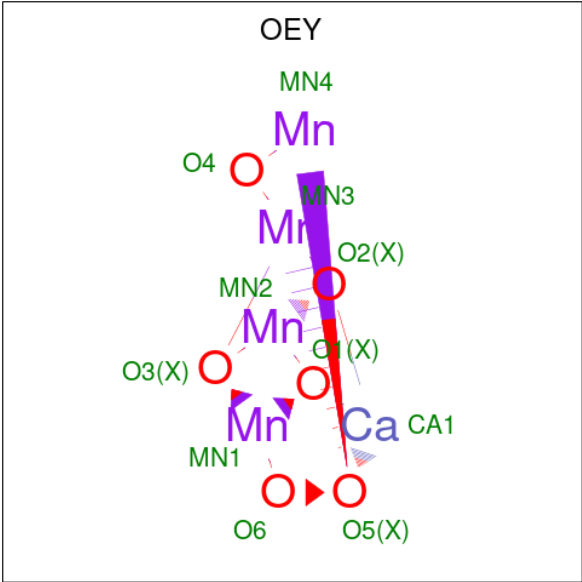
- Molecule 19 is a protein called Photosystem II reaction center protein Z.

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
			477	326	72	77	2			

- Molecule 20 is a protein called Photosystem II protein Y.

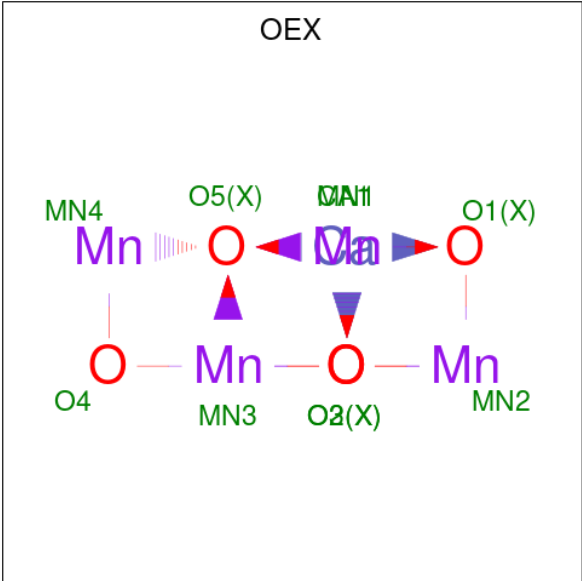
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	R	34	Total	C	N	O		0	0	0
			271	184	47	40				
20	r	31	Total	C	N	O		0	0	0
			246	166	43	37				

- Molecule 21 is CA-MN4-O6 CLUSTER (CCD ID: OEY) (formula: CaMn_4O_6) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	Ca	Mn	O		
21	A	1	22	2	8	12	0	1
21	a	1	22	2	8	12	0	1

- Molecule 22 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5) (labeled as "Ligand of Interest" by depositor).



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

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

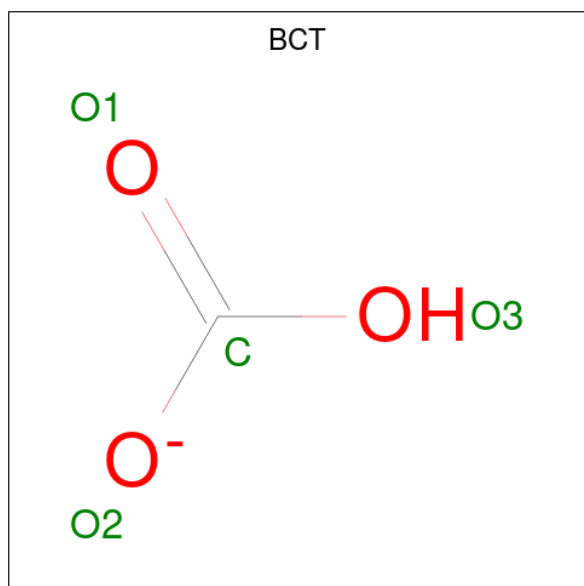
- Molecule 23 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

- Molecule 24 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

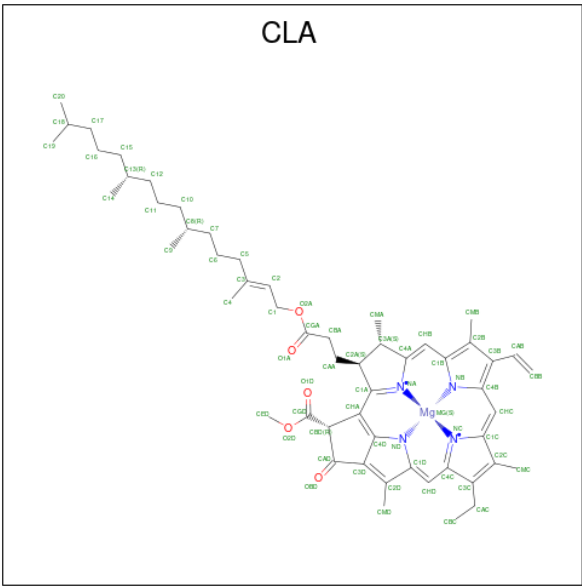
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	A	2	Total	Cl	0	0
			2	2		
24	a	2	Total	Cl	0	0
			2	2		

- Molecule 25 is BICARBONATE ION (CCD ID: BCT) (formula: CHO₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	A	1	Total	C	O	0	0
			4	1	3		
25	d	1	Total	C	O	0	0
			4	1	3		

- Molecule 26 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
26	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
26	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
26	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
26	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
26	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
26	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
26	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
26	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
26	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
26	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
26	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
26	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
26	B	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
26	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
26	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
26	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
26	C	1	Total 59	C 49	Mg 1	N 4	O 5	0	0
26	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
26	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
26	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
26	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
26	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
26	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
26	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
26	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
26	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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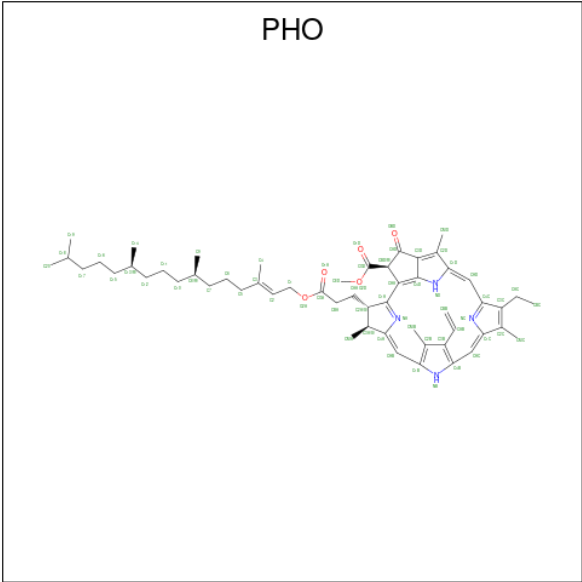
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
26	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
26	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
26	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
26	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
26	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
26	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
26	b	1	Total 65	C 55	Mg 1	N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

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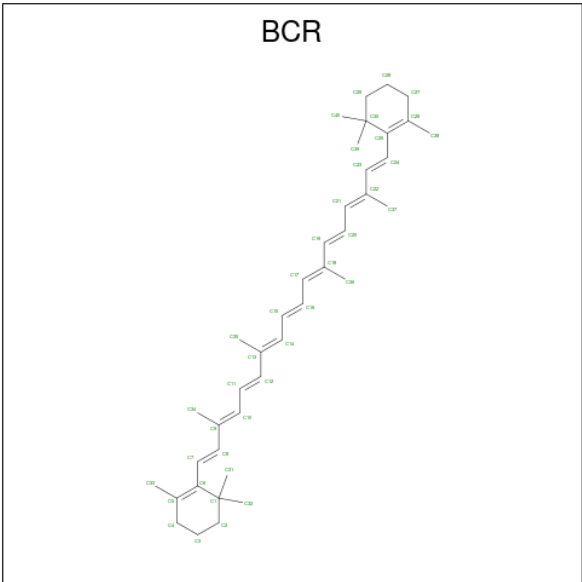
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
26	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
26	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
26	c	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
26	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
26	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
26	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
26	c	1	Total	C	Mg	N	O	0	0
			64	54	1	4	5		
26	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
26	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
26	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
26	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
26	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
26	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
26	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
26	h	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 27 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



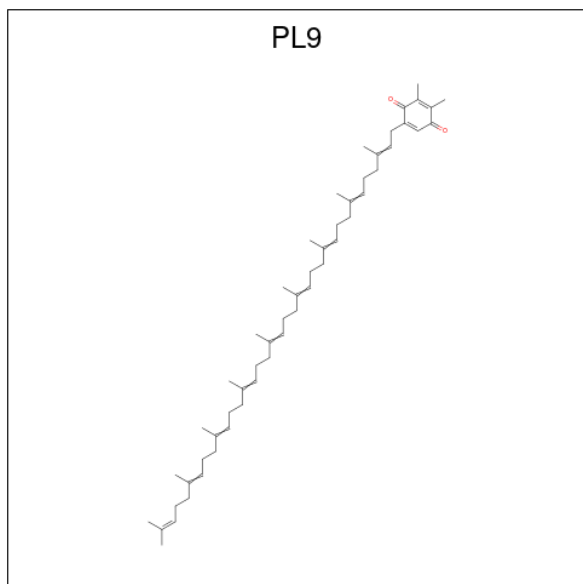
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	A	1	Total	C	N	O	0	0
			64	55	4	5		
27	D	1	Total	C	N	O	0	0
			64	55	4	5		
27	a	1	Total	C	N	O	0	0
			64	55	4	5		
27	d	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 28 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



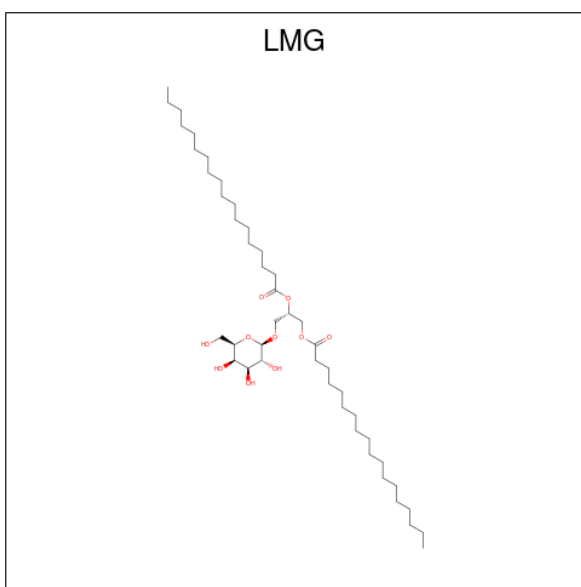
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	A	1	Total C 40 40	0	0
28	B	1	Total C 40 40	0	0
28	B	1	Total C 40 40	0	0
28	B	1	Total C 40 40	0	0
28	C	1	Total C 40 40	0	0
28	D	1	Total C 40 40	0	0
28	K	1	Total C 40 40	0	0
28	K	1	Total C 40 40	0	0
28	T	1	Total C 40 40	0	0
28	X	1	Total C 40 40	0	0
28	Z	1	Total C 40 40	0	0
28	a	1	Total C 40 40	0	0
28	b	1	Total C 40 40	0	0
28	b	1	Total C 40 40	0	0
28	b	1	Total C 40 40	0	0
28	c	1	Total C 40 40	0	0
28	c	1	Total C 40 40	0	0
28	c	1	Total C 40 40	0	0
28	d	1	Total C 40 40	0	0
28	h	1	Total C 40 40	0	0
28	k	1	Total C 40 40	0	0
28	t	1	Total C 40 40	0	0

- Molecule 29 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: $C_{53}H_{80}O_2$).



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

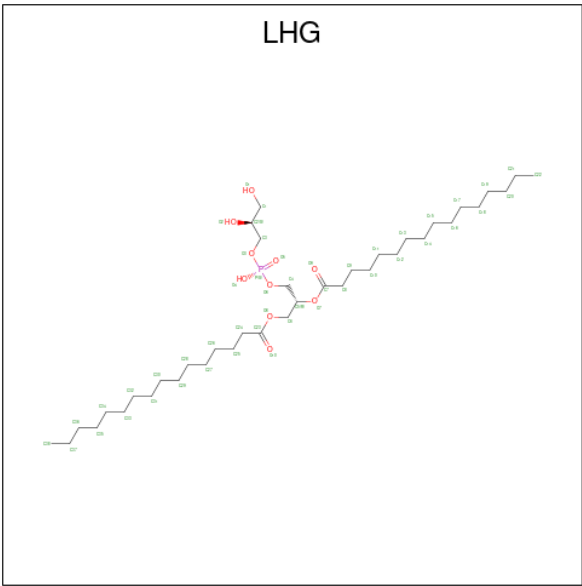
- Molecule 30 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	A	1	Total	C	O	0	0
			48	38	10		
30	B	1	Total	C	O	0	0
			28	24	4		
30	C	1	Total	C	O	0	0
			48	38	10		
30	D	1	Total	C	O	0	0
			51	41	10		
30	D	1	Total	C	O	0	0
			33	27	6		
30	M	1	Total	C	O	0	0
			51	41	10		
30	b	1	Total	C	O	0	0
			55	45	10		
30	c	1	Total	C	O	0	0
			37	27	10		
30	c	1	Total	C	O	0	0
			48	38	10		
30	c	1	Total	C	O	0	0
			49	39	10		
30	d	1	Total	C	O	0	0
			23	21	2		
30	d	1	Total	C	O	0	0
			44	34	10		
30	m	1	Total	C	O	0	0
			51	41	10		

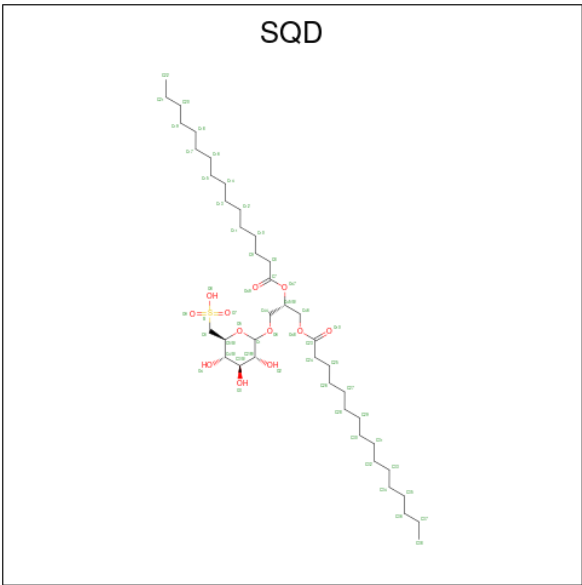
- Molecule 31 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG)

(formula: C₃₈H₇₅O₁₀P).



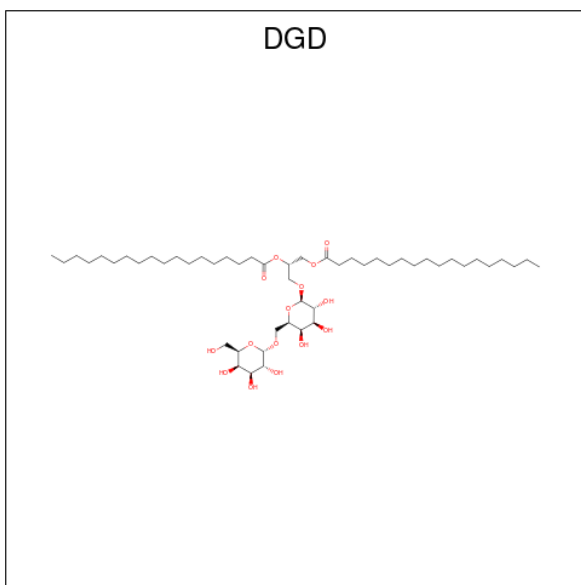
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	A	1	Total	C	O	P	0	0
			47	36	10	1		
31	A	1	Total	C	O	P	0	0
			49	38	10	1		
31	D	1	Total	C	O	P	0	0
			49	38	10	1		
31	D	1	Total	C	O	P	0	0
			49	38	10	1		
31	L	1	Total	C	O	P	0	0
			49	38	10	1		
31	d	1	Total	C	O	P	0	0
			49	38	10	1		
31	d	1	Total	C	O	P	0	0
			49	38	10	1		
31	d	1	Total	C	O	P	0	0
			39	28	10	1		
31	e	1	Total	C	O	P	0	0
			42	31	10	1		
31	l	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 32 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



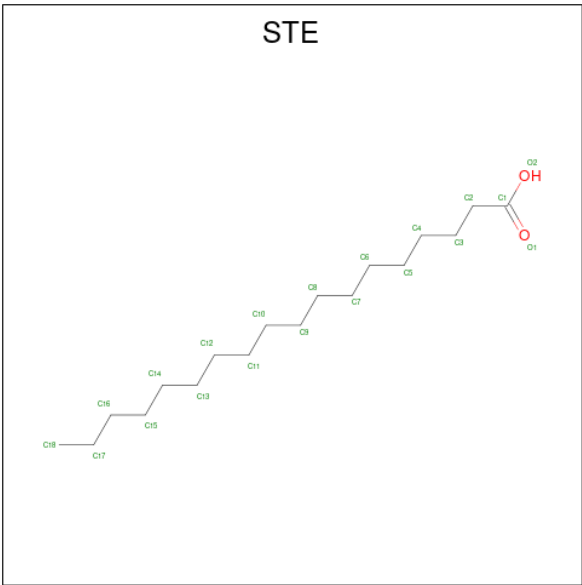
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	A	1	Total	C	O	S	0	0
			52	39	12	1		
32	A	1	Total	C	O		0	0
			39	35	4			
32	B	1	Total	C	O	S	0	0
			54	41	12	1		
32	F	1	Total	C	O	S	0	0
			36	25	10	1		
32	a	1	Total	C	O	S	0	0
			54	41	12	1		
32	b	1	Total	C	O	S	0	0
			49	36	12	1		
32	f	1	Total	C	O	S	0	0
			41	28	12	1		
32	t	1	Total	C	O		0	0
			36	31	5			

- Molecule 33 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: C₅₁H₉₆O₁₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	A	1	Total	C	O	0	0
			66	51	15		
33	C	1	Total	C	O	0	0
			62	47	15		
33	C	1	Total	C	O	0	0
			62	47	15		
33	C	1	Total	C	O	0	0
			62	47	15		
33	H	1	Total	C	O	0	0
			62	47	15		
33	a	1	Total	C	O	0	0
			44	39	5		
33	c	1	Total	C	O	0	0
			62	47	15		
33	c	1	Total	C	O	0	0
			62	47	15		
33	c	1	Total	C	O	0	0
			62	47	15		
33	h	1	Total	C	O	0	0
			62	47	15		

- Molecule 34 is STEARIC ACID (CCD ID: STE) (formula: $C_{18}H_{36}O_2$).



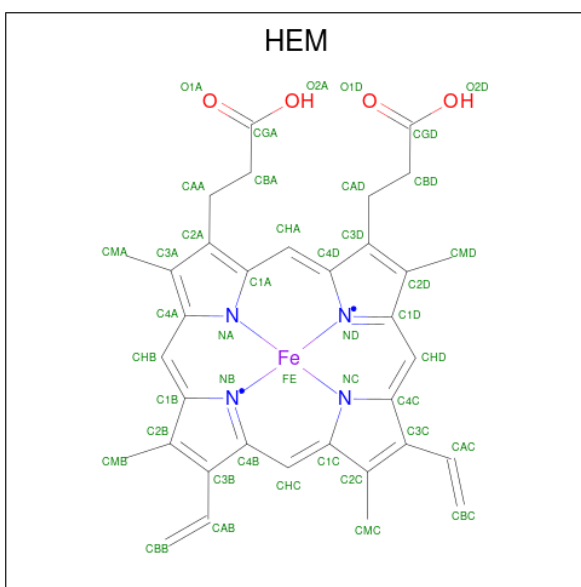
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	B	1	Total	C	O	0	0
			17	15	2		
34	B	1	Total	C	O	0	0
			12	10	2		
34	B	1	Total	C	O	0	0
			12	10	2		
34	B	1	Total	C		0	0
			16	16			
34	C	1	Total	C	O	0	0
			12	10	2		
34	C	1	Total	C	O	0	0
			12	10	2		
34	C	1	Total	C		0	0
			16	16			
34	F	1	Total	C	O	0	0
			12	10	2		
34	H	1	Total	C		0	0
			18	18			
34	I	1	Total	C		0	0
			15	15			
34	J	1	Total	C	O	0	0
			12	10	2		
34	L	1	Total	C	O	0	0
			12	10	2		
34	M	1	Total	C	O	0	0
			15	13	2		
34	M	1	Total	C		0	0
			10	10			

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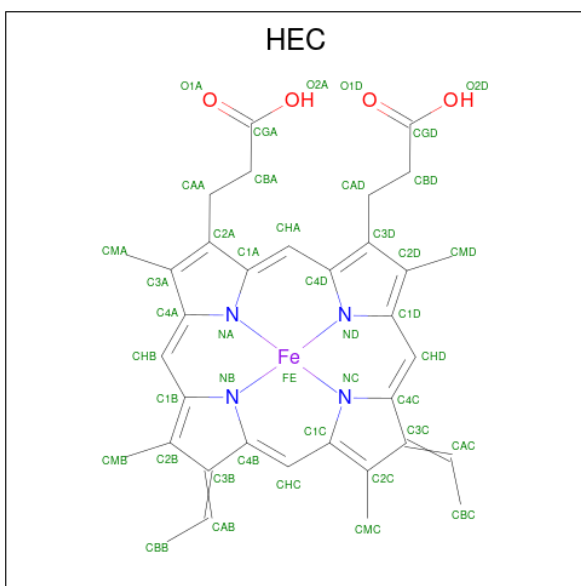
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	T	1	Total C 16 16	0	0
34	T	1	Total C 15 15	0	0
34	X	1	Total C O 20 18 2	0	0
34	a	1	Total C O 12 10 2	0	0
34	b	1	Total C O 20 18 2	0	0
34	b	1	Total C O 20 18 2	0	0
34	b	1	Total C 10 10	0	0
34	c	1	Total C O 20 18 2	0	0
34	d	1	Total C O 16 14 2	0	0
34	d	1	Total C O 17 15 2	0	0
34	d	1	Total C O 20 18 2	0	0
34	j	1	Total C O 12 10 2	0	0
34	k	1	Total C O 12 10 2	0	0
34	l	1	Total C 18 18	0	0
34	t	1	Total C O 14 12 2	0	0
34	t	1	Total C 10 10	0	0
34	t	1	Total C O 18 16 2	0	0

- Molecule 35 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
35	F	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
35	e	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 36 is HEME C (CCD ID: HEC) (formula: $\text{C}_{34}\text{H}_{34}\text{FeN}_4\text{O}_4$).



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

- Molecule 37 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	A	121	Total O 129 129	0	4
37	B	171	Total O 171 171	0	0
37	C	149	Total O 149 149	0	0
37	D	105	Total O 105 105	0	0
37	E	16	Total O 16 16	0	0
37	F	8	Total O 8 8	0	0
37	H	26	Total O 26 26	0	0
37	I	13	Total O 13 13	0	0
37	J	11	Total O 11 11	0	0
37	K	4	Total O 4 4	0	0
37	L	10	Total O 10 10	0	0
37	M	3	Total O 3 3	0	0
37	O	68	Total O 68 68	0	0
37	T	6	Total O 6 6	0	0
37	U	33	Total O 33 33	0	0
37	V	54	Total O 54 54	0	0
37	X	7	Total O 7 7	0	0
37	Z	5	Total O 5 5	0	0
37	a	109	Total O 117 117	0	4
37	b	142	Total O 142 142	0	0
37	c	132	Total O 132 132	0	0

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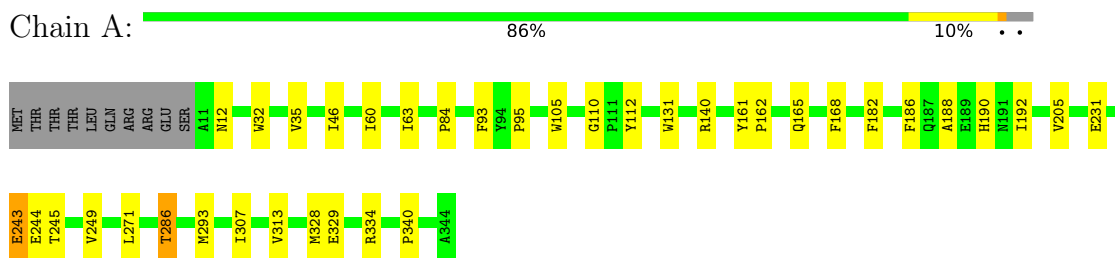
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	d	92	Total 92	O 92	0	0
37	e	13	Total 13	O 13	0	0
37	f	4	Total 4	O 4	0	0
37	h	16	Total 16	O 16	0	0
37	i	12	Total 12	O 12	0	0
37	j	9	Total 9	O 9	0	0
37	k	6	Total 6	O 6	0	0
37	l	8	Total 8	O 8	0	0
37	m	7	Total 7	O 7	0	0
37	o	77	Total 77	O 77	0	0
37	t	10	Total 10	O 10	0	0
37	u	38	Total 38	O 38	0	0
37	v	39	Total 39	O 39	0	0
37	x	4	Total 4	O 4	0	0
37	z	5	Total 5	O 5	0	0
37	r	7	Total 7	O 7	0	0

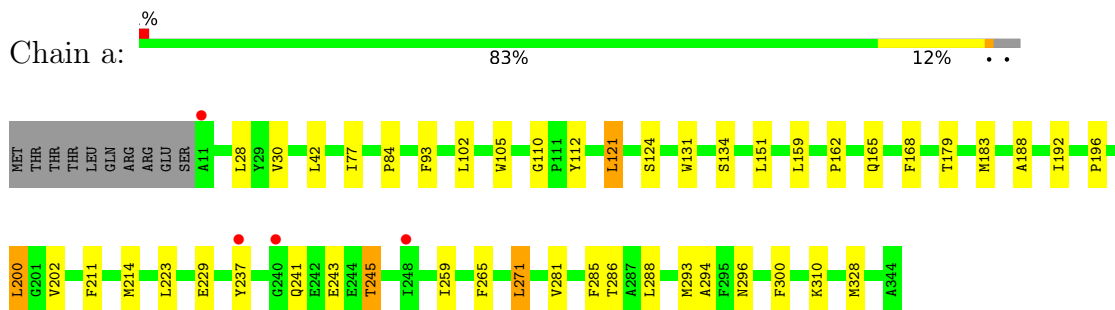
3 Residue-property plots

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

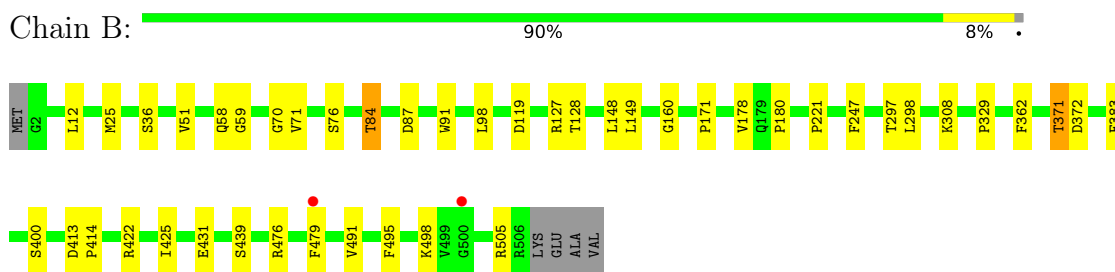
- Molecule 1: Photosystem II protein D1 1



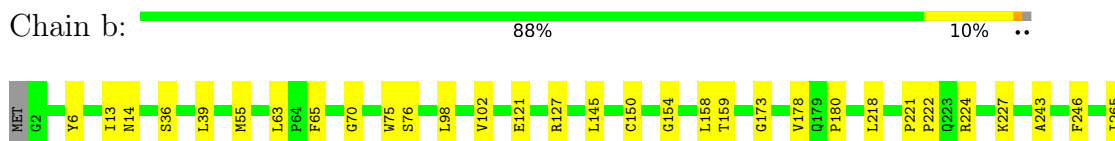
- Molecule 1: Photosystem II protein D1 1



- Molecule 2: Photosystem II CP47 reaction center protein



- Molecule 2: Photosystem II CP47 reaction center protein





• Molecule 3: Photosystem II CP43 reaction center protein

Chain C: 86% 9% .



• Molecule 3: Photosystem II CP43 reaction center protein

Chain c: 88% 10% ..



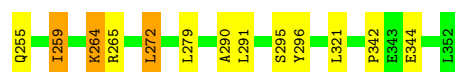
• Molecule 4: Photosystem II D2 protein

Chain D: 87% 10% ..



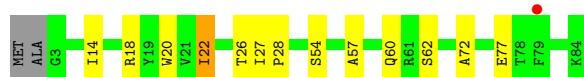
• Molecule 4: Photosystem II D2 protein

Chain d: 86% 10% ..

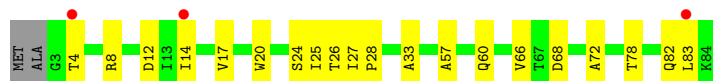
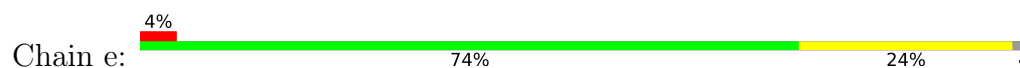


• Molecule 5: Cytochrome b559 subunit alpha

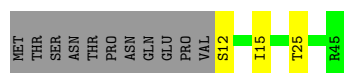
Chain E: 82% 14% ..



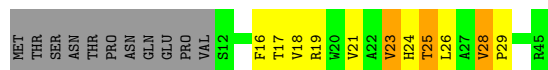
- Molecule 5: Cytochrome b559 subunit alpha



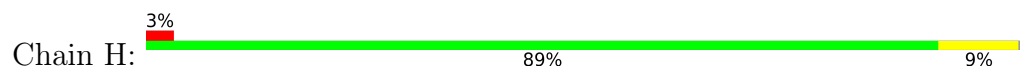
- Molecule 6: Cytochrome b559 subunit beta



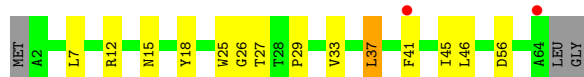
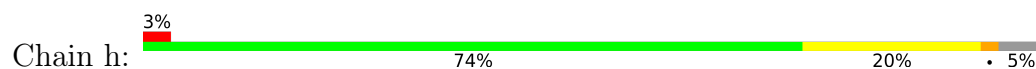
- Molecule 6: Cytochrome b559 subunit beta



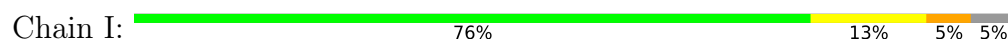
- Molecule 7: Photosystem II reaction center protein H



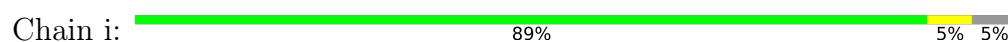
- Molecule 7: Photosystem II reaction center protein H

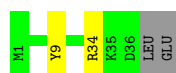


- Molecule 8: Photosystem II reaction center protein I

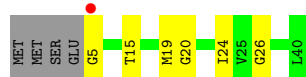
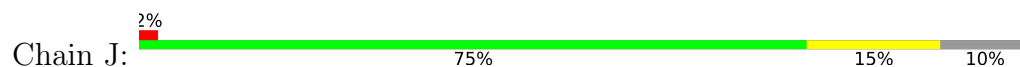


- Molecule 8: Photosystem II reaction center protein I





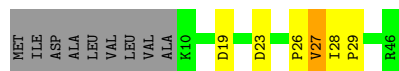
- Molecule 9: Photosystem II reaction center protein J



- Molecule 9: Photosystem II reaction center protein J



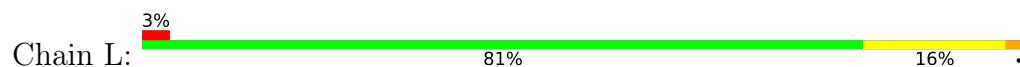
- Molecule 10: Photosystem II reaction center protein K



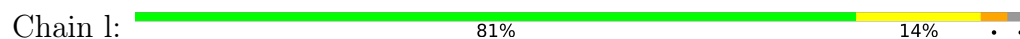
- Molecule 10: Photosystem II reaction center protein K



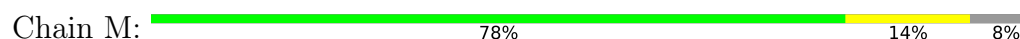
- Molecule 11: Photosystem II reaction center protein L



- Molecule 11: Photosystem II reaction center protein L



- Molecule 12: Photosystem II reaction center protein M





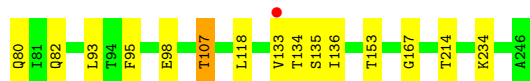
- Molecule 12: Photosystem II reaction center protein M

Chain m: 86% 11%



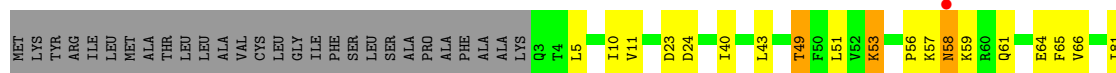
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O: 78% 11% 10%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o: 76% 12% 10%



- Molecule 14: Photosystem II reaction center protein T

Chain T: 81% 12% 6%



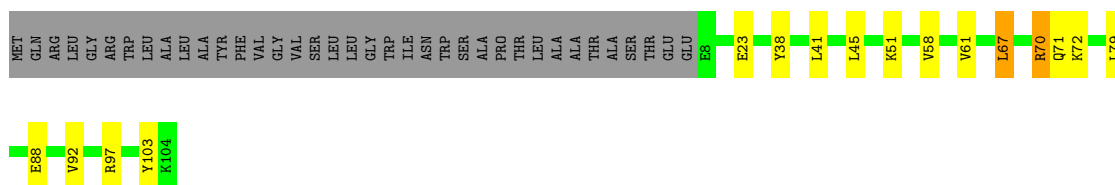
- Molecule 14: Photosystem II reaction center protein T

Chain t: 6% 78% 16% 6%

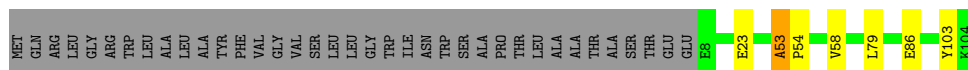


- Molecule 15: Photosystem II 12 kDa extrinsic protein

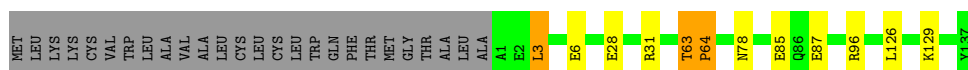
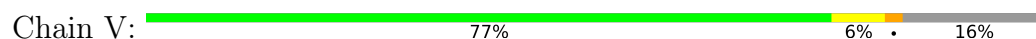
Chain U: 60% 10% 28%



- Molecule 15: Photosystem II 12 kDa extrinsic protein



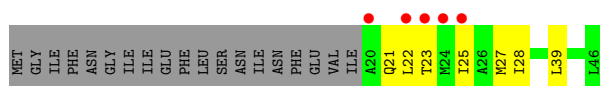
- Molecule 16: Cytochrome c-550



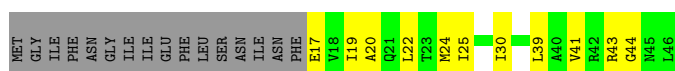
- Molecule 16: Cytochrome c-550



- Molecule 17: Photosystem II reaction center protein Ycf12

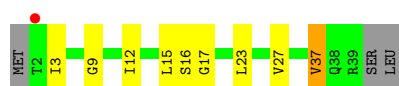


- Molecule 17: Photosystem II reaction center protein Ycf12

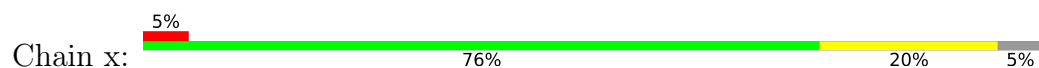


- Molecule 18: Photosystem II reaction center X protein

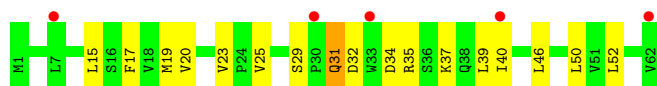




- Molecule 18: Photosystem II reaction center X protein



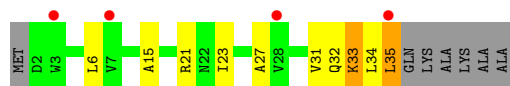
- Molecule 19: Photosystem II reaction center protein Z



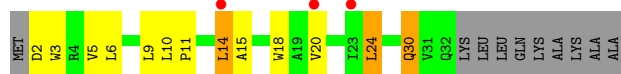
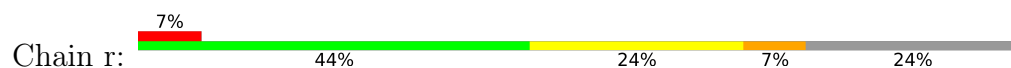
- Molecule 19: Photosystem II reaction center protein Z



- Molecule 20: Photosystem II protein Y



- Molecule 20: Photosystem II protein Y



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	117.56Å 223.17Å 310.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.48 – 2.10 29.48 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.3 (29.48-2.10) 82.6 (29.48-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.34 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.188 , 0.232 (Not available) , 0.217	Depositor DCC
R_{free} test set	4187 reflections (0.67%)	wwPDB-VP
Wilson B-factor (Å ²)	27.6	Xtriage
Anisotropy	0.226	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 59.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	54161	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.29	0/3717	0.44	0/5060
1	a	0.27	0/3714	0.43	0/5056
2	B	0.32	0/4155	0.48	0/5661
2	b	0.32	0/4118	0.48	0/5611
3	C	0.30	0/3711	0.46	0/5051
3	c	0.28	0/3791	0.45	0/5158
4	D	0.34	0/2838	0.50	0/3862
4	d	0.34	0/2847	0.48	0/3874
5	E	0.25	0/688	0.43	0/940
5	e	0.23	0/683	0.41	0/932
6	F	0.28	0/284	0.39	0/387
6	f	0.23	0/284	0.41	0/387
7	H	0.32	0/523	0.48	0/713
7	h	0.28	0/511	0.45	0/697
8	I	0.49	1/293 (0.3%)	0.53	0/396
8	i	0.31	0/293	0.44	0/396
9	J	0.28	0/263	0.38	0/356
9	j	0.25	0/263	0.42	0/356
10	K	0.25	0/303	0.46	0/416
10	k	0.26	0/303	0.49	0/416
11	L	0.35	0/311	0.45	0/422
11	l	0.36	0/303	0.44	0/412
12	M	0.33	0/249	0.49	0/341
12	m	0.34	0/244	0.52	0/334
13	O	0.31	0/1904	0.50	0/2585
13	o	0.32	0/1905	0.50	0/2583
14	T	0.34	0/257	0.57	0/349
14	t	0.31	0/255	0.46	0/346
15	U	0.28	0/785	0.46	0/1064
15	u	0.30	0/785	0.48	0/1064
16	V	0.31	0/1085	0.49	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.26	0/1085	0.43	0/1473
17	Y	0.19	0/197	0.32	0/264
17	y	0.19	0/219	0.38	0/294
18	X	0.25	0/284	0.37	0/384
18	x	0.23	0/289	0.31	0/391
19	Z	0.31	0/490	0.45	0/669
19	z	0.19	0/488	0.29	0/666
20	R	0.24	0/277	0.38	0/380
20	r	0.29	0/252	0.40	0/347
All	All	0.30	1/45246 (0.0%)	0.46	0/61566

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
16	V	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	I	33	LYS	CA-C	5.85	1.55	1.52

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	V	63	THR	Peptide

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	3604	0	3445	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a	3601	0	3436	34	0
2	B	4005	0	3871	31	0
2	b	3978	0	3836	40	0
3	C	3592	0	3501	30	0
3	c	3666	0	3574	31	0
4	D	2745	0	2653	29	0
4	d	2751	0	2659	27	0
5	E	666	0	651	9	0
5	e	664	0	648	13	0
6	F	275	0	282	4	0
6	f	275	0	282	10	0
7	H	510	0	532	4	0
7	h	498	0	518	9	0
8	I	296	0	311	3	0
8	i	296	0	311	2	0
9	J	257	0	268	4	0
9	j	257	0	268	3	0
10	K	293	0	305	4	0
10	k	293	0	305	4	0
11	L	304	0	316	6	0
11	l	296	0	304	4	0
12	M	256	0	269	3	0
12	m	251	0	267	0	0
13	O	1870	0	1830	21	0
13	o	1874	0	1846	20	0
14	T	258	0	261	2	0
14	t	256	0	256	4	0
15	U	774	0	773	9	0
15	u	774	0	773	5	0
16	V	1064	0	1073	8	0
16	v	1064	0	1073	14	0
17	Y	196	0	217	5	0
17	y	218	0	241	5	0
18	X	281	0	312	8	0
18	x	286	0	314	6	0
19	Z	479	0	516	7	0
19	z	477	0	509	13	0
20	R	271	0	298	7	0
20	r	246	0	263	9	0
21	A	22	0	0	2	0
21	a	22	0	0	2	0
22	A	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	a	10	0	0	0	0
23	A	1	0	0	0	0
23	a	1	0	0	0	0
24	A	2	0	0	0	0
24	a	2	0	0	0	0
25	A	4	0	1	0	0
25	d	4	0	1	0	0
26	A	249	0	264	5	0
26	B	1035	0	1139	29	0
26	C	839	0	922	21	0
26	D	130	0	144	7	0
26	a	260	0	288	8	0
26	b	970	0	1067	34	0
26	c	839	0	919	19	0
26	d	130	0	144	1	0
26	h	65	0	72	5	0
27	A	64	0	74	0	0
27	D	64	0	74	2	0
27	a	64	0	74	0	0
27	d	64	0	74	2	0
28	A	40	0	56	2	0
28	B	120	0	168	5	0
28	C	40	0	56	3	0
28	D	40	0	56	1	0
28	K	80	0	112	1	0
28	T	40	0	56	4	0
28	X	40	0	56	1	0
28	Z	40	0	56	3	0
28	a	40	0	56	1	0
28	b	120	0	168	6	0
28	c	120	0	168	9	0
28	d	40	0	56	3	0
28	h	40	0	56	4	0
28	k	40	0	56	1	0
28	t	40	0	56	2	0
29	A	55	0	80	8	0
29	D	55	0	80	1	0
29	a	55	0	80	6	0
29	d	55	0	80	1	0
30	A	48	0	66	2	0
30	B	28	0	40	0	0
30	C	48	0	66	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	D	84	0	117	2	0
30	M	51	0	72	2	0
30	b	55	0	86	0	0
30	c	134	0	181	4	0
30	d	67	0	92	0	0
30	m	51	0	72	2	0
31	A	96	0	141	2	0
31	D	98	0	148	6	0
31	L	49	0	74	3	0
31	d	137	0	199	8	0
31	e	42	0	57	2	0
31	l	49	0	74	3	0
32	A	91	0	136	2	0
32	B	54	0	78	5	0
32	F	36	0	46	2	0
32	a	54	0	78	2	0
32	b	49	0	65	4	0
32	f	41	0	49	4	0
32	t	36	0	56	0	0
33	A	66	0	96	4	0
33	C	186	0	246	3	0
33	H	62	0	82	1	0
33	a	44	0	75	3	0
33	c	186	0	246	3	0
33	h	62	0	82	0	0
34	B	57	0	89	2	0
34	C	40	0	63	2	0
34	F	12	0	16	0	0
34	H	18	0	35	2	0
34	I	15	0	26	1	0
34	J	12	0	16	1	0
34	L	12	0	16	0	0
34	M	25	0	38	0	0
34	T	31	0	60	1	0
34	X	20	0	35	5	0
34	a	12	0	16	0	0
34	b	50	0	86	2	0
34	c	20	0	35	2	0
34	d	53	0	85	6	0
34	j	12	0	16	1	0
34	k	12	0	16	1	0
34	l	18	0	35	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	t	42	0	64	3	0
35	F	43	0	30	1	0
35	e	43	0	30	2	0
36	V	43	0	30	0	0
36	v	43	0	30	2	0
37	A	129	0	0	2	0
37	B	171	0	0	1	0
37	C	149	0	0	1	0
37	D	105	0	0	0	0
37	E	16	0	0	0	0
37	F	8	0	0	1	0
37	H	26	0	0	1	0
37	I	13	0	0	0	0
37	J	11	0	0	1	0
37	K	4	0	0	0	0
37	L	10	0	0	0	0
37	M	3	0	0	0	0
37	O	68	0	0	4	0
37	T	6	0	0	0	0
37	U	33	0	0	1	0
37	V	54	0	0	0	0
37	X	7	0	0	0	0
37	Z	5	0	0	0	0
37	a	117	0	0	0	0
37	b	142	0	0	0	0
37	c	132	0	0	0	0
37	d	92	0	0	0	0
37	e	13	0	0	0	0
37	f	4	0	0	0	0
37	h	16	0	0	0	0
37	i	12	0	0	0	0
37	j	9	0	0	0	0
37	k	6	0	0	0	0
37	l	8	0	0	1	0
37	m	7	0	0	0	0
37	o	77	0	0	1	0
37	r	7	0	0	1	0
37	t	10	0	0	0	0
37	u	38	0	0	1	0
37	v	39	0	0	0	0
37	x	4	0	0	0	0
37	z	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	54161	0	53863	580	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 580 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)
1:A:161[C]:TYR:HH	1:A:190[C]:HIS:HE2	0.96	0.91
21:A:601[C]:OEY:O5	21:A:601[C]:OEY:O6	1.92	0.86
21:a:601[C]:OEY:O5	21:a:601[C]:OEY:O6	1.99	0.79
4:D:103:ARG:HH21	5:E:77:GLU:HG3	1.47	0.78
21:a:601[A]:OEY:O5	21:a:601[A]:OEY:O6	2.04	0.75

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	458/344 (133%)	449 (98%)	9 (2%)	0	100	100
1	a	458/344 (133%)	448 (98%)	8 (2%)	2 (0%)	30	28
2	B	507/510 (99%)	499 (98%)	8 (2%)	0	100	100
2	b	503/510 (99%)	491 (98%)	11 (2%)	1 (0%)	43	44
3	C	461/461 (100%)	451 (98%)	9 (2%)	1 (0%)	43	44
3	c	471/461 (102%)	457 (97%)	13 (3%)	1 (0%)	43	44
4	D	341/352 (97%)	333 (98%)	8 (2%)	0	100	100
4	d	342/352 (97%)	331 (97%)	11 (3%)	0	100	100
5	E	81/84 (96%)	81 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	e	80/84 (95%)	80 (100%)	0	0	100	100
6	F	32/45 (71%)	32 (100%)	0	0	100	100
6	f	32/45 (71%)	32 (100%)	0	0	100	100
7	H	63/66 (96%)	61 (97%)	2 (3%)	0	100	100
7	h	61/66 (92%)	57 (93%)	4 (7%)	0	100	100
8	I	34/38 (90%)	33 (97%)	1 (3%)	0	100	100
8	i	34/38 (90%)	31 (91%)	3 (9%)	0	100	100
9	J	34/40 (85%)	31 (91%)	3 (9%)	0	100	100
9	j	34/40 (85%)	32 (94%)	2 (6%)	0	100	100
10	K	35/46 (76%)	34 (97%)	1 (3%)	0	100	100
10	k	35/46 (76%)	35 (100%)	0	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	34/37 (92%)	34 (100%)	0	0	100	100
12	M	31/36 (86%)	30 (97%)	1 (3%)	0	100	100
12	m	30/36 (83%)	29 (97%)	1 (3%)	0	100	100
13	O	243/272 (89%)	227 (93%)	12 (5%)	4 (2%)	7	4
13	o	242/272 (89%)	236 (98%)	5 (2%)	1 (0%)	30	28
14	T	28/32 (88%)	28 (100%)	0	0	100	100
14	t	28/32 (88%)	27 (96%)	1 (4%)	0	100	100
15	U	95/134 (71%)	93 (98%)	2 (2%)	0	100	100
15	u	95/134 (71%)	90 (95%)	4 (4%)	1 (1%)	11	8
16	V	135/163 (83%)	129 (96%)	5 (4%)	1 (1%)	18	15
16	v	135/163 (83%)	130 (96%)	5 (4%)	0	100	100
17	Y	25/46 (54%)	24 (96%)	1 (4%)	0	100	100
17	y	28/46 (61%)	26 (93%)	2 (7%)	0	100	100
18	X	36/41 (88%)	35 (97%)	1 (3%)	0	100	100
18	x	37/41 (90%)	36 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	57 (95%)	2 (3%)	1 (2%)	7	3
19	z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
20	R	32/41 (78%)	31 (97%)	1 (3%)	0	100	100
20	r	29/41 (71%)	28 (97%)	0	1 (3%)	3	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	5534/5700 (97%)	5381 (97%)	139 (2%)	14 (0%)	36	36

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	O	59	LYS
16	V	64	PRO
13	o	58	ASN
3	C	416	SER
19	Z	31	GLN

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	374/280 (134%)	364 (97%)	10 (3%)	39	45
1	a	373/280 (133%)	358 (96%)	15 (4%)	28	29
2	B	407/407 (100%)	396 (97%)	11 (3%)	39	45
2	b	402/407 (99%)	395 (98%)	7 (2%)	53	62
3	C	361/362 (100%)	350 (97%)	11 (3%)	36	41
3	c	370/362 (102%)	357 (96%)	13 (4%)	32	35
4	D	278/283 (98%)	275 (99%)	3 (1%)	65	74
4	d	279/283 (99%)	273 (98%)	6 (2%)	45	53
5	E	72/73 (99%)	69 (96%)	3 (4%)	26	28
5	e	71/73 (97%)	68 (96%)	3 (4%)	26	28
6	F	28/39 (72%)	28 (100%)	0	100	100
6	f	28/39 (72%)	24 (86%)	4 (14%)	3	1
7	H	54/55 (98%)	52 (96%)	2 (4%)	30	33
7	h	53/55 (96%)	49 (92%)	4 (8%)	12	10
8	I	32/34 (94%)	30 (94%)	2 (6%)	16	14
8	i	32/34 (94%)	31 (97%)	1 (3%)	35	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	J	24/28 (86%)	24 (100%)	0	100	100
9	j	24/28 (86%)	22 (92%)	2 (8%)	10	8
10	K	30/37 (81%)	28 (93%)	2 (7%)	15	12
10	k	30/37 (81%)	26 (87%)	4 (13%)	4	2
11	L	35/35 (100%)	33 (94%)	2 (6%)	18	17
11	l	34/35 (97%)	30 (88%)	4 (12%)	5	3
12	M	28/32 (88%)	26 (93%)	2 (7%)	13	11
12	m	28/32 (88%)	27 (96%)	1 (4%)	31	34
13	O	206/228 (90%)	198 (96%)	8 (4%)	28	31
13	o	207/228 (91%)	197 (95%)	10 (5%)	23	23
14	T	26/28 (93%)	25 (96%)	1 (4%)	29	32
14	t	25/28 (89%)	25 (100%)	0	100	100
15	U	84/112 (75%)	80 (95%)	4 (5%)	23	23
15	u	84/112 (75%)	83 (99%)	1 (1%)	63	72
16	V	117/138 (85%)	116 (99%)	1 (1%)	70	78
16	v	117/138 (85%)	109 (93%)	8 (7%)	14	12
17	Y	19/37 (51%)	19 (100%)	0	100	100
17	y	22/37 (60%)	20 (91%)	2 (9%)	9	6
18	X	31/34 (91%)	28 (90%)	3 (10%)	8	5
18	x	31/34 (91%)	30 (97%)	1 (3%)	34	38
19	Z	52/52 (100%)	43 (83%)	9 (17%)	2	1
19	z	51/52 (98%)	46 (90%)	5 (10%)	7	5
20	R	28/33 (85%)	24 (86%)	4 (14%)	3	1
20	r	25/33 (76%)	19 (76%)	6 (24%)	1	0
All	All	4572/4654 (98%)	4397 (96%)	175 (4%)	28	32

5 of 175 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	d	264	LYS
13	o	53	LYS
5	e	4	THR
8	i	34	ARG
13	o	143	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
5	e	82	GLN
19	z	58	ASN
12	m	5	GLN
16	v	106	ASN
16	V	106	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z > 2$
14	FME	t	1	14	8,9,10	1.23	1 (12%)	8,9,11	0.72	0
8	FME	I	1	8	8,9,10	1.07	1 (12%)	8,9,11	1.45	1 (12%)
14	FME	T	1	14	8,9,10	1.12	1 (12%)	8,9,11	0.96	0
12	FME	m	1	12	8,9,10	0.97	0	8,9,11	0.71	0
8	FME	i	1	8	8,9,10	1.04	0	8,9,11	0.84	0
12	FME	M	1	12	8,9,10	1.12	1 (12%)	8,9,11	1.83	2 (25%)

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
14	FME	t	1	14	-	4/7/9/11	-
8	FME	I	1	8	-	0/7/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	FME	T	1	14	-	1/7/9/11	-
12	FME	m	1	12	-	1/7/9/11	-
8	FME	i	1	8	-	1/7/9/11	-
12	FME	M	1	12	-	1/7/9/11	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	t	1	FME	CA-N	-2.73	1.42	1.46
14	T	1	FME	CA-N	-2.46	1.43	1.46
12	M	1	FME	CA-N	-2.44	1.43	1.46
8	I	1	FME	CA-N	-2.25	1.43	1.46

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	M	1	FME	CA-N-CN	-3.88	116.86	122.82
8	I	1	FME	CA-N-CN	-3.32	117.71	122.82
12	M	1	FME	CB-CA-N	2.36	114.82	110.52

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	M	1	FME	O-C-CA-CB
12	m	1	FME	O-C-CA-CB
14	t	1	FME	N-CA-CB-CG
14	t	1	FME	O-C-CA-CB
14	T	1	FME	CB-CG-SD-CE

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 190 ligands modelled in this entry, 6 are monoatomic - leaving 184 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CLA	b	614	-	69,73,73	1.41	10 (14%)	82,113,113	1.29	6 (7%)
34	STE	F	103	-	11,11,19	0.75	0	11,11,19	1.16	1 (9%)
26	CLA	C	505	-	69,73,73	1.22	6 (8%)	82,113,113	1.32	9 (10%)
30	LMG	m	101	-	51,51,55	0.76	1 (1%)	59,59,63	1.45	8 (13%)
28	BCR	c	515	-	41,41,41	1.13	2 (4%)	56,56,56	1.27	8 (14%)
34	STE	B	623	-	11,11,19	0.73	0	11,11,19	1.37	2 (18%)
26	CLA	c	507	37	69,73,73	1.32	8 (11%)	82,113,113	1.33	9 (10%)
31	LHG	d	407	-	48,48,48	0.75	2 (4%)	51,54,54	1.41	7 (13%)
26	CLA	B	602	-	69,73,73	1.30	6 (8%)	82,113,113	1.39	11 (13%)
26	CLA	C	502	-	69,73,73	1.38	7 (10%)	82,113,113	1.23	7 (8%)
35	HEM	F	101	6,5	50,50,50	1.50	6 (12%)	67,82,82	1.12	3 (4%)
26	CLA	b	615	-	64,68,73	1.19	6 (9%)	76,107,113	1.50	7 (9%)
26	CLA	B	605	-	69,73,73	1.23	6 (8%)	82,113,113	1.27	6 (7%)
28	BCR	B	619	-	41,41,41	0.97	1 (2%)	56,56,56	1.22	5 (8%)
30	LMG	c	522	-	48,48,55	0.91	3 (6%)	56,56,63	1.29	9 (16%)
21	OEY	A	601[A]	1,3,37	0,16,16	-	-	-	-	-
27	PHO	a	608	-	58,69,69	2.08	11 (18%)	55,99,99	1.48	7 (12%)
32	SQD	B	622	-	52,54,54	1.57	8 (15%)	62,65,65	1.80	13 (20%)
33	DGD	A	619	-	67,67,67	1.09	5 (7%)	81,81,81	1.33	11 (13%)
26	CLA	B	615	-	69,73,73	1.42	9 (13%)	82,113,113	1.25	5 (6%)
31	LHG	l	101	-	48,48,48	0.65	0	51,54,54	1.25	8 (15%)
26	CLA	c	510	-	69,73,73	1.48	11 (15%)	82,113,113	1.27	6 (7%)
22	OEX	a	602[B]	1,3,37	0,15,15	-	-	-	-	-
28	BCR	A	611	-	41,41,41	0.99	2 (4%)	56,56,56	1.26	5 (8%)
26	CLA	b	603	-	69,73,73	1.22	8 (11%)	82,113,113	1.56	10 (12%)
28	BCR	h	102	-	41,41,41	0.95	2 (4%)	56,56,56	1.14	3 (5%)
33	DGD	c	517	-	63,63,67	0.94	2 (3%)	77,77,81	1.43	13 (16%)
30	LMG	B	621	-	26,26,55	0.63	0	26,26,63	1.21	1 (3%)
26	CLA	b	605	-	69,73,73	1.36	7 (10%)	82,113,113	1.50	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CLA	c	503	-	69,73,73	1.38	9 (13%)	82,113,113	1.44	6 (7%)
32	SQD	F	102	-	34,36,54	1.53	5 (14%)	42,45,65	1.80	9 (21%)
26	CLA	C	509	-	69,73,73	1.34	8 (11%)	82,113,113	1.43	8 (9%)
26	CLA	b	613	-	69,73,73	1.32	7 (10%)	82,113,113	1.31	9 (10%)
21	OEY	a	601[C]	1,3,37	0,16,16	-	-	-		
32	SQD	f	101	-	39,41,54	1.68	8 (20%)	49,52,65	1.58	10 (20%)
34	STE	M	102	-	14,14,19	0.73	0	14,14,19	1.23	1 (7%)
33	DGD	C	516	-	63,63,67	1.02	5 (7%)	77,77,81	1.41	9 (11%)
34	STE	c	521	-	19,19,19	0.63	0	19,19,19	0.97	0
30	LMG	A	614	-	48,48,55	0.95	5 (10%)	56,56,63	1.26	6 (10%)
34	STE	C	520	-	11,11,19	0.74	0	11,11,19	1.16	1 (9%)
33	DGD	C	515	-	63,63,67	1.04	5 (7%)	77,77,81	1.31	9 (11%)
34	STE	X	102	-	19,19,19	0.61	0	19,19,19	1.14	0
26	CLA	C	513	-	69,73,73	1.34	8 (11%)	82,113,113	1.41	7 (8%)
34	STE	B	620	-	16,16,19	0.66	0	16,16,19	1.04	0
26	CLA	B	611	-	69,73,73	1.32	6 (8%)	82,113,113	1.57	6 (7%)
26	CLA	C	511	3	69,73,73	1.24	7 (10%)	82,113,113	1.40	4 (4%)
25	BCT	A	606	23	3,3,3	1.18	0	2,3,3	2.85	1 (50%)
34	STE	M	103	-	9,9,19	0.35	0	8,8,19	0.79	0
29	PL9	A	612	-	55,55,55	0.88	2 (3%)	68,69,69	1.41	12 (17%)
26	CLA	b	607	-	69,73,73	1.40	8 (11%)	82,113,113	1.34	9 (10%)
36	HEC	v	201	16	46,50,50	1.82	6 (13%)	58,82,82	1.92	8 (13%)
28	BCR	T	101	-	41,41,41	1.09	2 (4%)	56,56,56	1.28	6 (10%)
28	BCR	d	405	-	41,41,41	1.02	2 (4%)	56,56,56	1.23	9 (16%)
34	STE	I	101	-	14,14,19	0.39	0	13,13,19	0.79	0
30	LMG	C	518	-	48,48,55	0.84	2 (4%)	56,56,63	1.34	7 (12%)
26	CLA	c	504	37	64,68,73	1.31	6 (9%)	76,107,113	1.34	9 (11%)
26	CLA	c	509	-	69,73,73	1.21	8 (11%)	82,113,113	1.42	6 (7%)
26	CLA	c	511	3	69,73,73	1.40	8 (11%)	82,113,113	1.56	7 (8%)
32	SQD	b	619	-	47,49,54	1.69	10 (21%)	57,60,65	1.82	13 (22%)
34	STE	k	102	-	11,11,19	0.74	0	11,11,19	1.14	0
34	STE	J	101	-	11,11,19	0.70	0	11,11,19	1.30	2 (18%)
26	CLA	B	612	-	69,73,73	1.21	6 (8%)	82,113,113	1.51	9 (10%)
26	CLA	C	506	-	69,73,73	1.28	7 (10%)	82,113,113	1.30	6 (7%)
31	LHG	d	409	-	38,38,48	0.79	1 (2%)	41,44,54	1.13	3 (7%)
27	PHO	A	609	-	58,69,69	2.05	12 (20%)	55,99,99	1.47	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CLA	c	505	-	69,73,73	1.17	6 (8%)	82,113,113	1.34	7 (8%)
33	DGD	C	517	-	63,63,67	0.98	3 (4%)	77,77,81	1.35	6 (7%)
31	LHG	A	617	-	48,48,48	0.84	3 (6%)	51,54,54	1.20	6 (11%)
26	CLA	A	608	37	69,73,73	1.26	9 (13%)	82,113,113	1.40	10 (12%)
33	DGD	a	614	-	43,43,67	0.89	3 (6%)	45,45,81	1.42	6 (13%)
28	BCR	c	514	-	41,41,41	1.06	2 (4%)	56,56,56	1.18	4 (7%)
32	SQD	A	618	-	38,38,54	1.78	5 (13%)	40,40,65	1.12	2 (5%)
34	STE	t	104	-	9,9,19	0.39	0	8,8,19	0.70	0
31	LHG	D	409	-	48,48,48	0.94	2 (4%)	51,54,54	1.35	7 (13%)
26	CLA	c	502	-	69,73,73	1.30	8 (11%)	82,113,113	1.43	8 (9%)
31	LHG	d	408	-	48,48,48	0.60	0	51,54,54	1.28	6 (11%)
34	STE	B	624	-	11,11,19	0.71	0	11,11,19	1.17	0
26	CLA	a	607	37	69,73,73	1.25	8 (11%)	82,113,113	1.39	8 (9%)
26	CLA	D	402	-	69,73,73	1.29	8 (11%)	82,113,113	1.36	7 (8%)
26	CLA	C	512	-	69,73,73	1.27	9 (13%)	82,113,113	1.45	8 (9%)
30	LMG	M	101	-	51,51,55	0.82	3 (5%)	59,59,63	1.42	7 (11%)
31	LHG	L	101	-	48,48,48	0.74	1 (2%)	51,54,54	1.23	5 (9%)
26	CLA	b	609	37	69,73,73	1.43	7 (10%)	82,113,113	1.33	9 (10%)
26	CLA	A	613	37	69,73,73	1.40	9 (13%)	82,113,113	1.37	7 (8%)
26	CLA	b	601	-	69,73,73	1.24	9 (13%)	82,113,113	1.36	8 (9%)
26	CLA	B	607	37	69,73,73	1.12	7 (10%)	82,113,113	1.24	5 (6%)
34	STE	C	521	-	15,15,19	0.39	0	14,14,19	0.70	0
26	CLA	b	611	-	69,73,73	1.19	6 (8%)	82,113,113	1.28	10 (12%)
34	STE	d	413	-	16,16,19	0.63	0	16,16,19	1.12	1 (6%)
26	CLA	D	403	-	69,73,73	1.29	9 (13%)	82,113,113	1.20	7 (8%)
28	BCR	K	102	-	41,41,41	1.04	2 (4%)	56,56,56	1.11	3 (5%)
26	CLA	b	612	-	69,73,73	1.28	8 (11%)	82,113,113	1.39	9 (10%)
27	PHO	D	401	-	58,69,69	2.17	10 (17%)	55,99,99	1.68	10 (18%)
26	CLA	a	606	-	69,73,73	1.43	11 (15%)	82,113,113	1.29	6 (7%)
34	STE	l	102	-	17,17,19	0.30	0	16,16,19	0.97	0
26	CLA	b	610	-	69,73,73	1.27	6 (8%)	82,113,113	1.40	5 (6%)
33	DGD	c	518	-	63,63,67	0.98	2 (3%)	77,77,81	1.46	12 (15%)
29	PL9	d	406	-	55,55,55	1.03	3 (5%)	68,69,69	1.57	14 (20%)
34	STE	b	620	-	19,19,19	0.59	0	19,19,19	1.15	0
34	STE	d	414	-	19,19,19	0.63	0	19,19,19	1.02	1 (5%)
26	CLA	c	501	-	69,73,73	1.26	6 (8%)	82,113,113	1.47	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	BCR	b	616	-	41,41,41	1.01	2 (4%)	56,56,56	1.35	6 (10%)
30	LMG	b	621	-	55,55,55	0.93	5 (9%)	63,63,63	1.33	7 (11%)
26	CLA	d	403	-	69,73,73	1.29	8 (11%)	82,113,113	1.25	5 (6%)
26	CLA	C	508	-	69,73,73	1.29	7 (10%)	82,113,113	1.40	5 (6%)
33	DGD	H	101	-	63,63,67	1.17	6 (9%)	77,77,81	1.36	10 (12%)
34	STE	C	519	-	11,11,19	0.61	0	11,11,19	1.84	3 (27%)
35	HEM	e	101	6,5	50,50,50	1.59	8 (16%)	67,82,82	1.39	8 (11%)
26	CLA	C	507	37	69,73,73	1.27	6 (8%)	82,113,113	1.42	7 (8%)
33	DGD	h	103	-	63,63,67	0.96	2 (3%)	77,77,81	1.48	12 (15%)
36	HEC	V	201	16	46,50,50	1.83	6 (13%)	58,82,82	1.85	7 (12%)
26	CLA	A	610	-	58,62,73	1.28	6 (10%)	68,99,113	1.37	7 (10%)
28	BCR	Z	101	-	41,41,41	1.09	2 (4%)	56,56,56	1.25	7 (12%)
28	BCR	t	101	-	41,41,41	0.93	1 (2%)	56,56,56	1.29	7 (12%)
26	CLA	B	609	-	69,73,73	1.26	6 (8%)	82,113,113	1.28	6 (7%)
32	SQD	a	613	-	52,54,54	1.57	7 (13%)	62,65,65	1.88	9 (14%)
26	CLA	B	614	-	69,73,73	1.30	6 (8%)	82,113,113	1.37	8 (9%)
34	STE	b	622	-	19,19,19	0.64	0	19,19,19	1.01	1 (5%)
31	LHG	e	102	-	41,41,48	0.79	1 (2%)	44,47,54	1.30	6 (13%)
32	SQD	A	616	-	50,52,54	1.56	8 (16%)	60,63,65	1.85	12 (20%)
28	BCR	c	516	-	41,41,41	1.08	2 (4%)	56,56,56	1.10	2 (3%)
28	BCR	a	610	-	41,41,41	0.98	3 (7%)	56,56,56	1.19	5 (8%)
26	CLA	b	602	-	69,73,73	1.42	9 (13%)	82,113,113	1.36	8 (9%)
28	BCR	b	617	-	41,41,41	1.01	2 (4%)	56,56,56	1.15	4 (7%)
26	CLA	b	608	-	69,73,73	1.38	10 (14%)	82,113,113	1.25	7 (8%)
26	CLA	A	607	-	69,73,73	1.37	8 (11%)	82,113,113	1.29	8 (9%)
34	STE	t	103	-	13,13,19	0.66	0	13,13,19	1.22	1 (7%)
34	STE	j	101	-	11,11,19	0.84	0	11,11,19	1.11	2 (18%)
26	CLA	a	612	37	69,73,73	1.24	7 (10%)	82,113,113	1.31	6 (7%)
27	PHO	d	402	-	58,69,69	2.11	10 (17%)	55,99,99	1.60	8 (14%)
26	CLA	C	504	37	63,67,73	1.40	9 (14%)	74,105,113	1.33	9 (12%)
34	STE	B	625	-	15,15,19	0.39	0	14,14,19	0.75	0
31	LHG	D	407	-	48,48,48	0.73	1 (2%)	51,54,54	1.22	5 (9%)
33	DGD	c	519	-	63,63,67	0.90	3 (4%)	77,77,81	1.39	6 (7%)
29	PL9	a	611	-	55,55,55	0.78	1 (1%)	68,69,69	1.47	11 (16%)
21	OEY	a	601[A]	1,3,37	0,16,16	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	LMG	d	411	-	44,44,55	0.90	2 (4%)	52,52,63	1.31	6 (11%)
28	BCR	B	618	-	41,41,41	1.00	2 (4%)	56,56,56	1.24	6 (10%)
34	STE	a	615	-	11,11,19	0.81	0	11,11,19	1.03	1 (9%)
34	STE	T	103	-	14,14,19	0.31	0	13,13,19	0.97	0
26	CLA	b	606	37	69,73,73	1.07	6 (8%)	82,113,113	1.25	8 (9%)
26	CLA	B	613	-	69,73,73	1.32	8 (11%)	82,113,113	1.44	12 (14%)
34	STE	d	412	-	15,15,19	0.78	0	15,15,19	0.98	1 (6%)
31	LHG	A	615	-	46,46,48	0.81	1 (2%)	49,52,54	1.22	4 (8%)
34	STE	H	102	-	17,17,19	0.42	0	16,16,19	0.69	0
26	CLA	B	606	-	69,73,73	1.49	5 (7%)	82,113,113	1.42	10 (12%)
30	LMG	d	410	-	21,21,55	0.53	0	20,20,63	1.15	2 (10%)
32	SQD	t	102	-	35,35,54	1.78	6 (17%)	37,37,65	1.39	4 (10%)
21	OEY	A	601[C]	1,3,37	0,16,16	-	-	-	-	-
28	BCR	X	101	-	41,41,41	0.95	2 (4%)	56,56,56	1.28	8 (14%)
29	PL9	D	405	-	55,55,55	1.08	1 (1%)	68,69,69	1.55	13 (19%)
26	CLA	d	404	-	69,73,73	1.15	8 (11%)	82,113,113	1.21	6 (7%)
26	CLA	c	513	-	69,73,73	1.36	7 (10%)	82,113,113	1.19	7 (8%)
34	STE	b	623	-	9,9,19	0.40	0	8,8,19	0.64	0
28	BCR	B	617	-	41,41,41	0.95	1 (2%)	56,56,56	1.32	5 (8%)
28	BCR	C	514	-	41,41,41	1.10	3 (7%)	56,56,56	1.08	4 (7%)
34	STE	L	102	-	11,11,19	0.73	0	11,11,19	1.20	1 (9%)
26	CLA	b	604	-	69,73,73	1.40	7 (10%)	82,113,113	1.48	10 (12%)
26	CLA	B	616	-	64,68,73	1.37	10 (15%)	76,107,113	1.48	6 (7%)
26	CLA	C	501	-	69,73,73	1.25	10 (14%)	82,113,113	1.43	8 (9%)
28	BCR	D	404	-	41,41,41	1.06	3 (7%)	56,56,56	1.28	7 (12%)
28	BCR	b	618	-	41,41,41	0.97	2 (4%)	56,56,56	1.09	4 (7%)
26	CLA	C	510	-	69,73,73	1.41	8 (11%)	82,113,113	1.44	9 (10%)
30	LMG	D	406	-	51,51,55	0.78	0	59,59,63	1.34	8 (13%)
26	CLA	c	508	-	68,72,73	1.59	11 (16%)	80,111,113	1.48	10 (12%)
30	LMG	c	520	-	37,37,55	0.97	1 (2%)	45,45,63	1.30	4 (8%)
28	BCR	k	101	-	41,41,41	1.05	3 (7%)	56,56,56	1.10	3 (5%)
25	BCT	d	401	23	3,3,3	1.11	0	2,3,3	2.94	1 (50%)
34	STE	t	105	-	17,17,19	0.61	0	17,17,19	1.09	0
34	STE	T	102	-	15,15,19	0.41	0	14,14,19	0.71	0
26	CLA	C	503	-	69,73,73	1.54	9 (13%)	82,113,113	1.54	10 (12%)
26	CLA	c	506	-	69,73,73	1.35	6 (8%)	82,113,113	1.32	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CLA	h	101	37	69,73,73	1.31	9 (13%)	82,113,113	1.40	7 (8%)
26	CLA	B	610	37	69,73,73	1.29	8 (11%)	82,113,113	1.41	10 (12%)
26	CLA	B	608	-	69,73,73	1.23	7 (10%)	82,113,113	1.34	9 (10%)
26	CLA	B	601	37	69,73,73	1.36	8 (11%)	82,113,113	1.32	7 (8%)
26	CLA	a	609	-	69,73,73	1.17	7 (10%)	82,113,113	1.23	6 (7%)
28	BCR	K	101	-	41,41,41	1.07	3 (7%)	56,56,56	1.12	2 (3%)
30	LMG	c	523	-	49,49,55	1.04	4 (8%)	57,57,63	1.28	4 (7%)
22	OEX	A	602[B]	1,3,37	0,15,15	-	-	-	-	-
26	CLA	B	603	-	69,73,73	1.47	8 (11%)	82,113,113	1.38	9 (10%)
30	LMG	D	408	-	31,31,55	0.74	2 (6%)	33,33,63	1.20	3 (9%)
26	CLA	c	512	-	69,73,73	1.21	9 (13%)	82,113,113	1.37	9 (10%)
26	CLA	B	604	-	69,73,73	1.23	7 (10%)	82,113,113	1.40	8 (9%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	b	614	-	1/1/15/20	9/39/115/115	-
34	STE	F	103	-	-	7/9/9/17	-
26	CLA	C	505	-	1/1/15/20	9/39/115/115	-
30	LMG	m	101	-	-	22/46/66/70	0/1/1/1
28	BCR	c	515	-	-	3/29/63/63	0/2/2/2
34	STE	B	623	-	-	7/9/9/17	-
26	CLA	c	507	37	1/1/15/20	9/39/115/115	-
31	LHG	d	407	-	-	18/53/53/53	-
26	CLA	B	602	-	1/1/15/20	7/39/115/115	-
26	CLA	C	502	-	1/1/15/20	8/39/115/115	-
35	HEM	F	101	6,5	-	2/14/54/54	-
26	CLA	b	615	-	1/1/14/20	8/33/109/115	-
26	CLA	B	605	-	1/1/15/20	11/39/115/115	-
28	BCR	B	619	-	-	2/29/63/63	0/2/2/2
30	LMG	c	522	-	-	22/43/63/70	0/1/1/1
27	PHO	a	608	-	-	2/37/103/103	0/5/6/6
32	SQD	B	622	-	-	25/49/69/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	DGD	A	619	-	-	25/55/95/95	0/2/2/2
26	CLA	B	615	-	1/1/15/20	12/39/115/115	-
31	LHG	l	101	-	-	15/53/53/53	-
26	CLA	c	510	-	1/1/15/20	8/39/115/115	-
28	BCR	A	611	-	-	4/29/63/63	0/2/2/2
26	CLA	b	603	-	1/1/15/20	8/39/115/115	-
28	BCR	h	102	-	-	6/29/63/63	0/2/2/2
33	DGD	c	517	-	-	24/51/91/95	0/2/2/2
30	LMG	B	621	-	-	8/22/22/70	-
26	CLA	b	605	-	1/1/15/20	6/39/115/115	-
26	CLA	c	503	-	1/1/15/20	10/39/115/115	-
32	SQD	F	102	-	-	16/28/48/69	0/1/1/1
26	CLA	C	509	-	1/1/15/20	10/39/115/115	-
26	CLA	b	613	-	1/1/15/20	18/39/115/115	-
32	SQD	f	101	-	-	18/36/56/69	0/1/1/1
34	STE	M	102	-	-	6/12/12/17	-
33	DGD	C	516	-	-	19/51/91/95	0/2/2/2
34	STE	c	521	-	-	8/17/17/17	-
30	LMG	A	614	-	-	19/43/63/70	0/1/1/1
34	STE	C	520	-	-	5/9/9/17	-
33	DGD	C	515	-	-	18/51/91/95	0/2/2/2
34	STE	X	102	-	-	11/17/17/17	-
26	CLA	C	513	-	1/1/15/20	13/39/115/115	-
34	STE	B	620	-	-	7/14/14/17	-
26	CLA	B	611	-	1/1/15/20	5/39/115/115	-
26	CLA	C	511	3	1/1/15/20	5/39/115/115	-
34	STE	M	103	-	-	2/7/7/17	-
29	PL9	A	612	-	-	23/53/73/73	0/1/1/1
26	CLA	b	607	-	1/1/15/20	7/39/115/115	-
36	HEC	v	201	16	-	6/14/54/54	-
28	BCR	T	101	-	-	7/29/63/63	0/2/2/2
28	BCR	d	405	-	-	4/29/63/63	0/2/2/2
34	STE	I	101	-	-	4/12/12/17	-
30	LMG	C	518	-	-	18/43/63/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	c	504	37	1/1/14/20	8/33/109/115	-
26	CLA	c	509	-	1/1/15/20	10/39/115/115	-
26	CLA	c	511	3	1/1/15/20	6/39/115/115	-
32	SQD	b	619	-	-	23/44/64/69	0/1/1/1
34	STE	k	102	-	-	3/9/9/17	-
34	STE	J	101	-	-	6/9/9/17	-
26	CLA	B	612	-	1/1/15/20	5/39/115/115	-
26	CLA	C	506	-	1/1/15/20	9/39/115/115	-
31	LHG	d	409	-	-	9/43/43/53	-
27	PHO	A	609	-	-	4/37/103/103	0/5/6/6
26	CLA	c	505	-	1/1/15/20	11/39/115/115	-
33	DGD	C	517	-	-	15/51/91/95	0/2/2/2
31	LHG	A	617	-	-	24/53/53/53	-
26	CLA	A	608	37	1/1/15/20	8/39/115/115	-
33	DGD	a	614	-	-	18/45/45/95	-
28	BCR	c	514	-	-	0/29/63/63	0/2/2/2
32	SQD	A	618	-	-	16/39/39/69	-
34	STE	t	104	-	-	3/7/7/17	-
31	LHG	D	409	-	-	18/53/53/53	-
26	CLA	c	502	-	1/1/15/20	10/39/115/115	-
31	LHG	d	408	-	-	22/53/53/53	-
34	STE	B	624	-	-	1/9/9/17	-
26	CLA	a	607	37	1/1/15/20	10/39/115/115	-
26	CLA	D	402	-	1/1/15/20	7/39/115/115	-
26	CLA	C	512	-	1/1/15/20	12/39/115/115	-
30	LMG	M	101	-	-	24/46/66/70	0/1/1/1
31	LHG	L	101	-	-	21/53/53/53	-
26	CLA	b	609	37	1/1/15/20	8/39/115/115	-
26	CLA	A	613	37	1/1/15/20	4/39/115/115	-
26	CLA	b	601	-	1/1/15/20	10/39/115/115	-
26	CLA	B	607	37	1/1/15/20	18/39/115/115	-
34	STE	C	521	-	-	10/13/13/17	-
26	CLA	b	611	-	1/1/15/20	14/39/115/115	-
34	STE	d	413	-	-	8/14/14/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	D	403	-	-	8/39/115/115	-
28	BCR	K	102	-	-	4/29/63/63	0/2/2/2
27	PHO	D	401	-	-	4/37/103/103	0/5/6/6
26	CLA	b	612	-	1/1/15/20	8/39/115/115	-
26	CLA	a	606	-	1/1/15/20	6/39/115/115	-
34	STE	l	102	-	-	9/15/15/17	-
26	CLA	b	610	-	1/1/15/20	5/39/115/115	-
33	DGD	c	518	-	-	22/51/91/95	0/2/2/2
29	PL9	d	406	-	-	12/53/73/73	0/1/1/1
34	STE	b	620	-	-	6/17/17/17	-
34	STE	d	414	-	-	7/17/17/17	-
26	CLA	c	501	-	1/1/15/20	6/39/115/115	-
28	BCR	b	616	-	-	6/29/63/63	0/2/2/2
30	LMG	b	621	-	-	27/50/70/70	0/1/1/1
26	CLA	d	403	-	1/1/15/20	5/39/115/115	-
26	CLA	C	508	-	-	6/39/115/115	-
33	DGD	H	101	-	-	18/51/91/95	0/2/2/2
34	STE	C	519	-	-	4/9/9/17	-
35	HEM	e	101	6,5	-	3/14/54/54	-
26	CLA	C	507	37	1/1/15/20	7/39/115/115	-
33	DGD	h	103	-	-	15/51/91/95	0/2/2/2
36	HEC	V	201	16	-	6/14/54/54	-
26	CLA	A	610	-	1/1/12/20	5/26/102/115	-
28	BCR	Z	101	-	-	6/29/63/63	0/2/2/2
28	BCR	t	101	-	-	5/29/63/63	0/2/2/2
26	CLA	B	609	-	-	7/39/115/115	-
32	SQD	a	613	-	-	27/49/69/69	0/1/1/1
26	CLA	B	614	-	1/1/15/20	8/39/115/115	-
34	STE	b	622	-	-	12/17/17/17	-
31	LHG	e	102	-	-	23/46/46/53	-
32	SQD	A	616	-	-	23/47/67/69	0/1/1/1
28	BCR	c	516	-	-	5/29/63/63	0/2/2/2
28	BCR	a	610	-	-	2/29/63/63	0/2/2/2
26	CLA	b	602	-	1/1/15/20	9/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	BCR	b	617	-	-	1/29/63/63	0/2/2/2
26	CLA	b	608	-	-	9/39/115/115	-
26	CLA	A	607	-	1/1/15/20	4/39/115/115	-
34	STE	t	103	-	-	3/11/11/17	-
34	STE	j	101	-	-	5/9/9/17	-
26	CLA	a	612	37	1/1/15/20	5/39/115/115	-
27	PHO	d	402	-	-	4/37/103/103	0/5/6/6
26	CLA	C	504	37	1/1/13/20	7/32/108/115	-
34	STE	B	625	-	-	5/13/13/17	-
31	LHG	D	407	-	-	25/53/53/53	-
33	DGD	c	519	-	-	17/51/91/95	0/2/2/2
29	PL9	a	611	-	-	21/53/73/73	0/1/1/1
30	LMG	d	411	-	-	10/39/59/70	0/1/1/1
34	STE	a	615	-	-	7/9/9/17	-
28	BCR	B	618	-	-	4/29/63/63	0/2/2/2
34	STE	T	103	-	-	9/12/12/17	-
26	CLA	b	606	37	1/1/15/20	12/39/115/115	-
26	CLA	B	613	-	1/1/15/20	8/39/115/115	-
34	STE	d	412	-	-	4/13/13/17	-
31	LHG	A	615	-	-	24/51/51/53	-
34	STE	H	102	-	-	7/15/15/17	-
26	CLA	B	606	-	1/1/15/20	13/39/115/115	-
30	LMG	d	410	-	-	11/17/17/70	-
32	SQD	t	102	-	-	19/37/37/69	-
28	BCR	X	101	-	-	5/29/63/63	0/2/2/2
29	PL9	D	405	-	-	8/53/73/73	0/1/1/1
26	CLA	d	404	-	1/1/15/20	10/39/115/115	-
26	CLA	c	513	-	1/1/15/20	13/39/115/115	-
34	STE	b	623	-	-	6/7/7/17	-
28	BCR	B	617	-	-	5/29/63/63	0/2/2/2
28	BCR	C	514	-	-	7/29/63/63	0/2/2/2
34	STE	L	102	-	-	7/9/9/17	-
26	CLA	b	604	-	-	9/39/115/115	-
26	CLA	B	616	-	1/1/14/20	14/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	C	501	-	1/1/15/20	5/39/115/115	-
28	BCR	D	404	-	-	7/29/63/63	0/2/2/2
28	BCR	b	618	-	-	4/29/63/63	0/2/2/2
26	CLA	C	510	-	1/1/15/20	8/39/115/115	-
30	LMG	D	406	-	-	18/46/66/70	0/1/1/1
26	CLA	c	508	-	-	6/38/114/115	-
30	LMG	c	520	-	-	13/31/51/70	0/1/1/1
28	BCR	k	101	-	-	6/29/63/63	0/2/2/2
34	STE	t	105	-	-	8/15/15/17	-
34	STE	T	102	-	-	7/13/13/17	-
26	CLA	C	503	-	1/1/15/20	4/39/115/115	-
26	CLA	c	506	-	1/1/15/20	13/39/115/115	-
26	CLA	h	101	37	1/1/15/20	16/39/115/115	-
26	CLA	B	610	37	1/1/15/20	7/39/115/115	-
26	CLA	B	608	-	1/1/15/20	5/39/115/115	-
26	CLA	B	601	37	1/1/15/20	13/39/115/115	-
26	CLA	a	609	-	1/1/15/20	11/39/115/115	-
28	BCR	K	101	-	-	7/29/63/63	0/2/2/2
30	LMG	c	523	-	-	22/44/64/70	0/1/1/1
26	CLA	B	603	-	1/1/15/20	13/39/115/115	-
30	LMG	D	408	-	-	18/33/33/70	-
26	CLA	c	512	-	1/1/15/20	16/39/115/115	-
26	CLA	B	604	-	1/1/15/20	14/39/115/115	-

The worst 5 of 793 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	D	401	PHO	C1B-C2B	9.32	1.49	1.39
27	d	402	PHO	C1B-C2B	9.28	1.49	1.39
27	a	608	PHO	C1B-C2B	9.25	1.49	1.39
27	D	401	PHO	C3B-C4B	9.03	1.50	1.41
27	d	402	PHO	C3B-C4B	8.43	1.50	1.41

The worst 5 of 1068 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	c	511	CLA	C4A-NA-C1A	10.05	111.27	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	V	201	HEC	CBB-CAB-C3B	-9.06	109.32	127.43
26	C	511	CLA	C4A-NA-C1A	8.85	110.72	106.68
26	b	603	CLA	C4A-NA-C1A	8.75	110.67	106.68
26	B	611	CLA	C4A-NA-C1A	8.52	110.57	106.68

5 of 64 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
26	A	607	CLA	ND
26	A	608	CLA	ND
26	A	610	CLA	ND
26	A	613	CLA	ND
26	B	601	CLA	ND

5 of 1806 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
26	A	608	CLA	C2B-C3B-CAB-CBB
26	A	608	CLA	C4B-C3B-CAB-CBB
26	B	602	CLA	C6-C7-C8-C9
26	B	614	CLA	CAD-CBD-CGD-O1D
26	B	614	CLA	CAD-CBD-CGD-O2D

There are no ring outliers.

144 monomers are involved in 267 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	b	614	CLA	4	0
26	C	505	CLA	2	0
30	m	101	LMG	2	0
28	c	515	BCR	3	0
26	c	507	CLA	2	0
31	d	407	LHG	5	0
26	B	602	CLA	1	0
26	C	502	CLA	2	0
35	F	101	HEM	1	0
26	b	615	CLA	4	0
26	B	605	CLA	5	0
28	B	619	BCR	2	0
30	c	522	LMG	2	0
21	A	601[A]	OEY	1	0
32	B	622	SQD	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	A	619	DGD	4	0
26	B	615	CLA	1	0
31	l	101	LHG	3	0
26	c	510	CLA	1	0
28	A	611	BCR	2	0
26	b	603	CLA	3	0
28	h	102	BCR	4	0
33	c	517	DGD	1	0
26	b	605	CLA	2	0
26	c	503	CLA	2	0
32	F	102	SQD	2	0
26	C	509	CLA	1	0
26	b	613	CLA	5	0
21	a	601[C]	OEY	1	0
32	f	101	SQD	4	0
33	C	516	DGD	2	0
34	c	521	STE	2	0
30	A	614	LMG	2	0
34	X	102	STE	5	0
26	C	513	CLA	3	0
34	B	620	STE	2	0
26	C	511	CLA	3	0
29	A	612	PL9	8	0
26	b	607	CLA	1	0
36	v	201	HEC	2	0
28	T	101	BCR	4	0
28	d	405	BCR	3	0
34	I	101	STE	1	0
30	C	518	LMG	3	0
26	c	504	CLA	2	0
26	c	511	CLA	4	0
32	b	619	SQD	4	0
34	k	102	STE	1	0
34	J	101	STE	1	0
26	B	612	CLA	3	0
26	C	506	CLA	2	0
31	d	409	LHG	1	0
26	c	505	CLA	3	0
33	C	517	DGD	1	0
31	A	617	LHG	1	0
26	A	608	CLA	1	0
33	a	614	DGD	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	c	514	BCR	4	0
32	A	618	SQD	1	0
31	D	409	LHG	3	0
31	d	408	LHG	2	0
26	a	607	CLA	2	0
26	D	402	CLA	4	0
26	C	512	CLA	3	0
30	M	101	LMG	2	0
31	L	101	LHG	3	0
26	b	609	CLA	2	0
26	A	613	CLA	3	0
26	b	601	CLA	1	0
26	B	607	CLA	1	0
34	C	521	STE	2	0
26	b	611	CLA	3	0
34	d	413	STE	1	0
26	D	403	CLA	3	0
28	K	102	BCR	1	0
26	b	612	CLA	5	0
27	D	401	PHO	2	0
26	a	606	CLA	2	0
34	l	102	STE	1	0
29	d	406	PL9	1	0
34	d	414	STE	5	0
26	c	501	CLA	3	0
28	b	616	BCR	2	0
26	C	508	CLA	2	0
33	H	101	DGD	1	0
35	e	101	HEM	2	0
26	C	507	CLA	1	0
28	Z	101	BCR	3	0
28	t	101	BCR	2	0
26	B	609	CLA	1	0
32	a	613	SQD	2	0
26	B	614	CLA	4	0
34	b	622	STE	1	0
31	e	102	LHG	2	0
32	A	616	SQD	1	0
28	c	516	BCR	2	0
28	a	610	BCR	1	0
26	b	602	CLA	3	0
28	b	617	BCR	3	0

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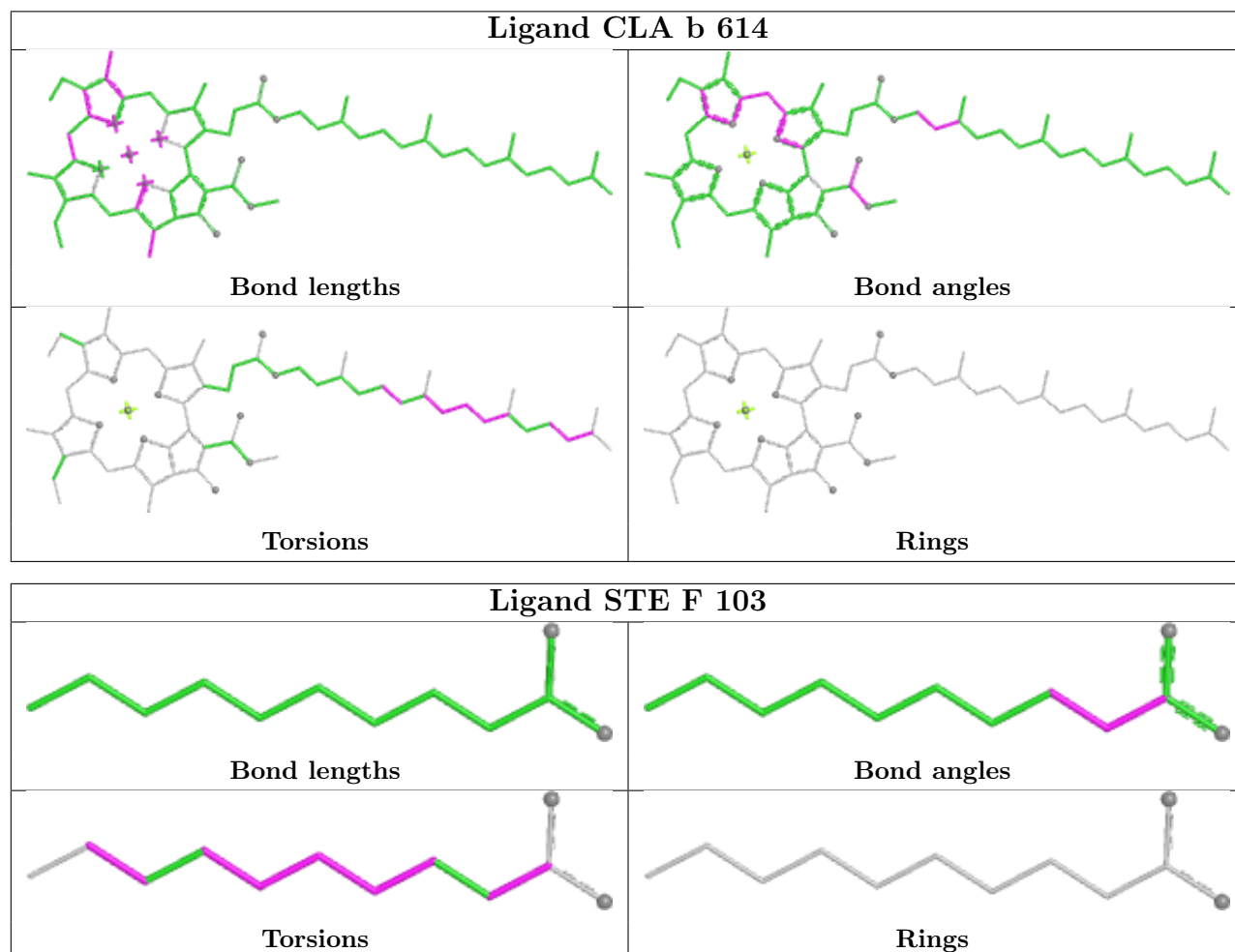
Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	b	608	CLA	2	0
26	A	607	CLA	2	0
34	j	101	STE	1	0
26	a	612	CLA	2	0
27	d	402	PHO	2	0
26	C	504	CLA	2	0
31	D	407	LHG	3	0
33	c	519	DGD	2	0
29	a	611	PL9	6	0
21	a	601[A]	OEY	1	0
28	B	618	BCR	2	0
26	b	606	CLA	3	0
26	B	613	CLA	1	0
31	A	615	LHG	1	0
34	H	102	STE	2	0
26	B	606	CLA	3	0
21	A	601[C]	OEY	1	0
28	X	101	BCR	1	0
29	D	405	PL9	1	0
26	d	404	CLA	1	0
26	c	513	CLA	4	0
34	b	623	STE	1	0
28	B	617	BCR	1	0
28	C	514	BCR	3	0
26	b	604	CLA	2	0
26	B	616	CLA	1	0
26	C	501	CLA	1	0
28	D	404	BCR	1	0
28	b	618	BCR	1	0
30	D	406	LMG	1	0
26	c	508	CLA	1	0
28	k	101	BCR	1	0
34	t	105	STE	3	0
34	T	102	STE	1	0
26	C	503	CLA	3	0
26	h	101	CLA	5	0
26	B	610	CLA	1	0
26	B	608	CLA	1	0
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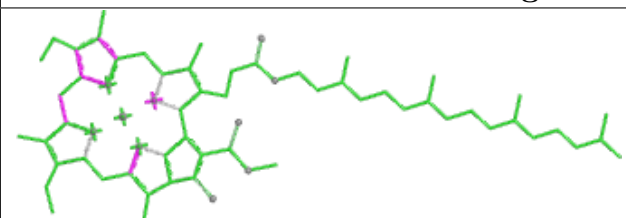
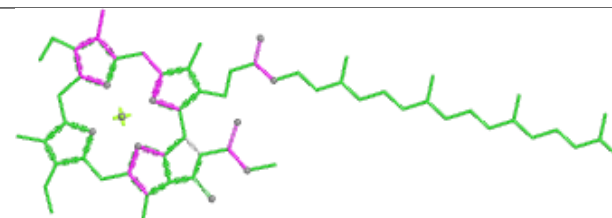
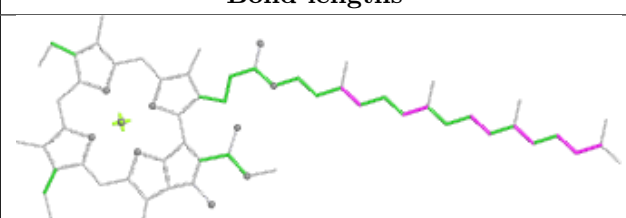
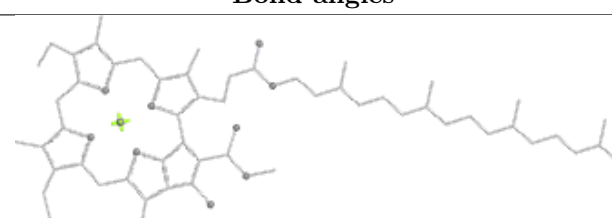
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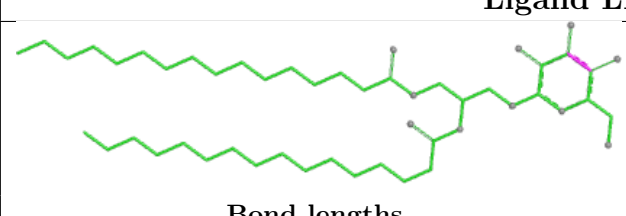
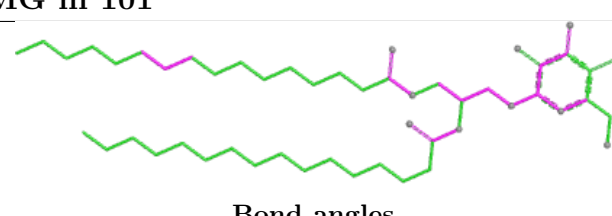
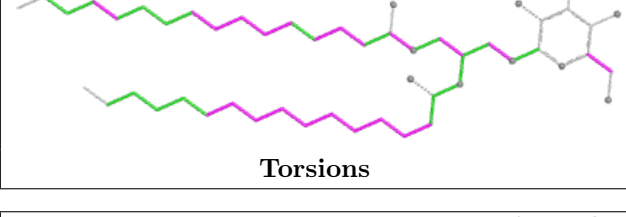
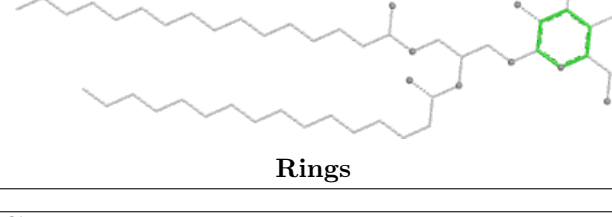
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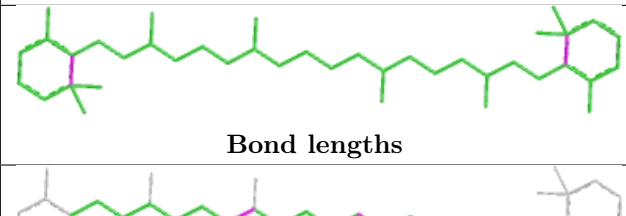
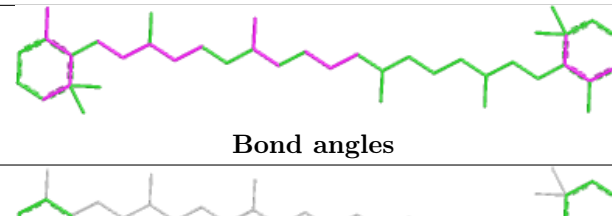
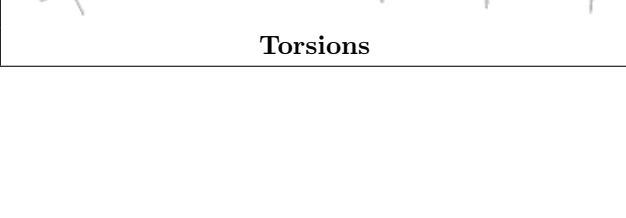
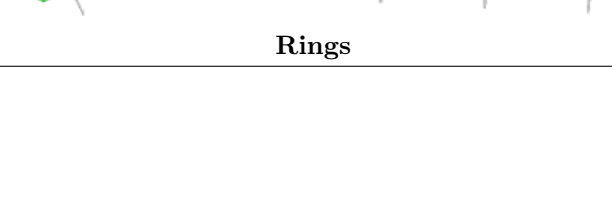
Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	D	408	LMG	1	0
26	c	512	CLA	3	0
26	B	604	CLA	4	0

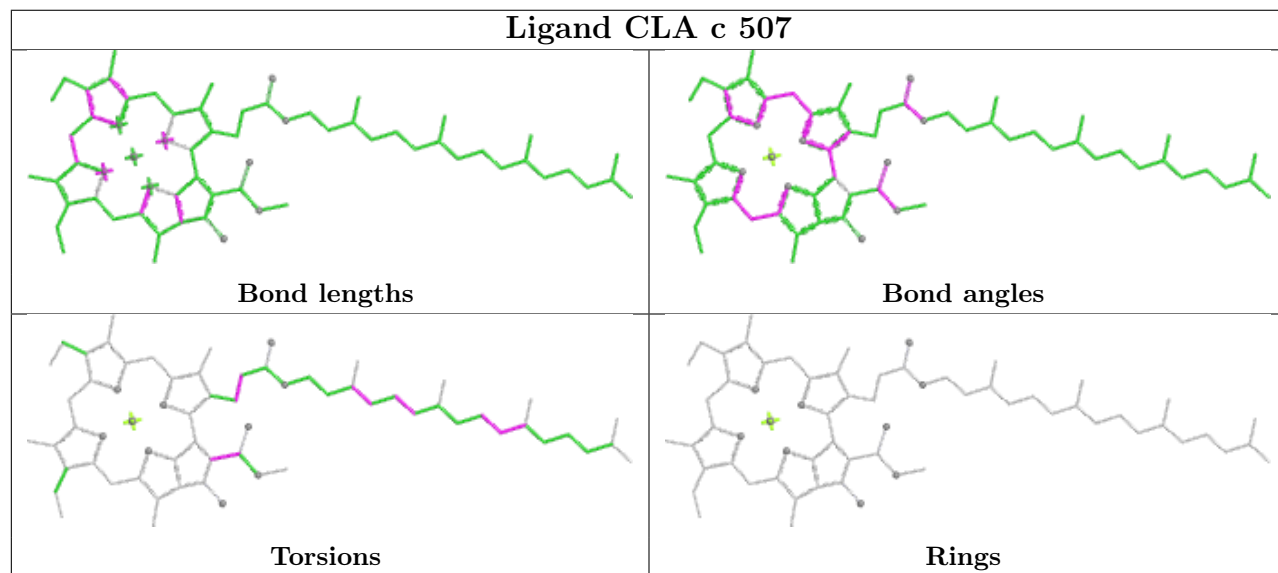
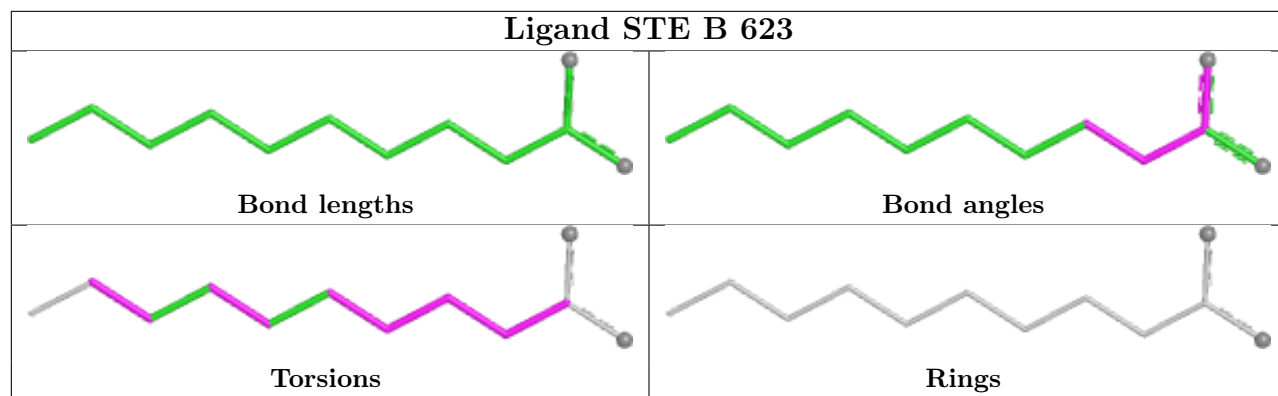
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



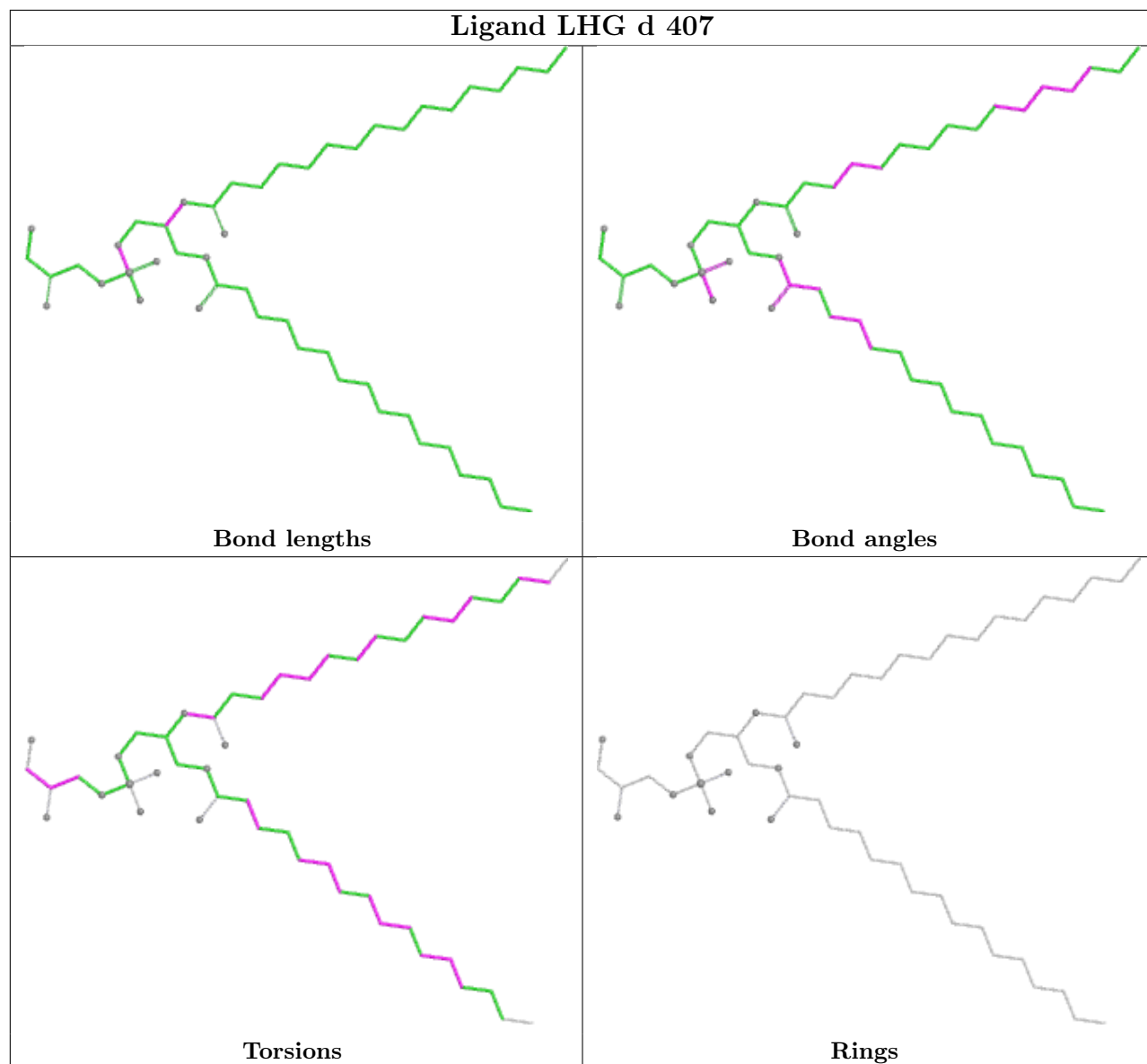
Ligand CLA C 505	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LMG m 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

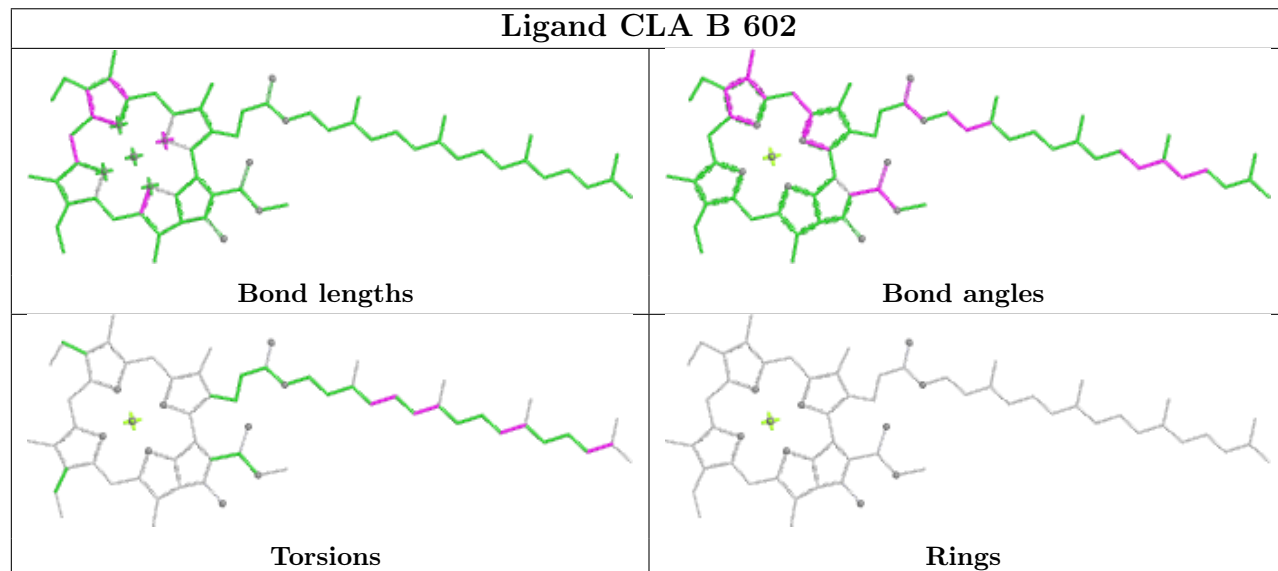
Ligand BCR c 515	
	
Bond lengths	Bond angles
	
Torsions	Rings



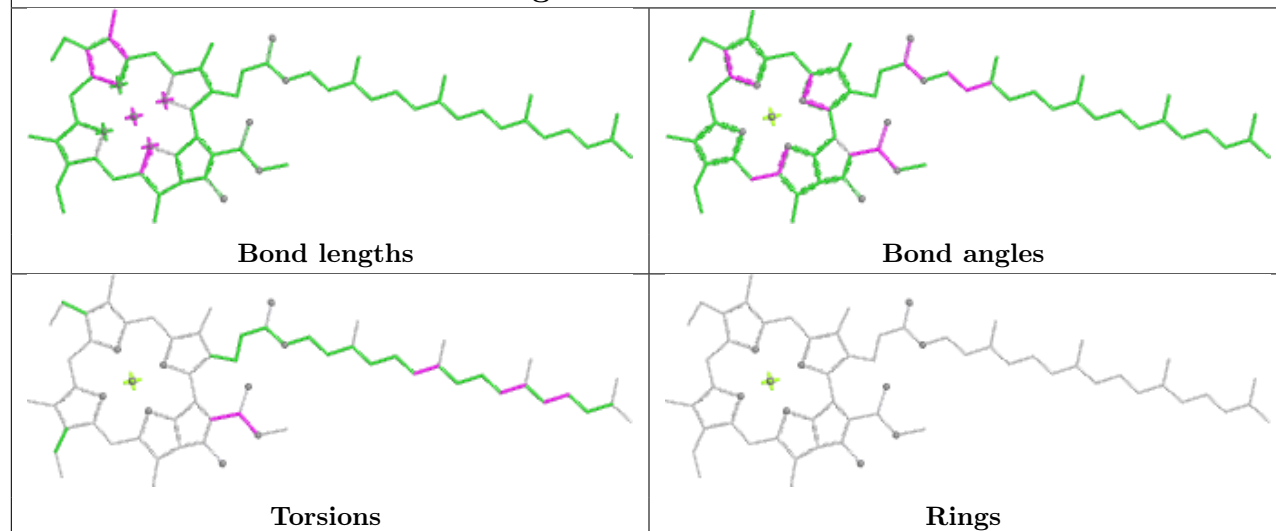
Ligand LHG d 407



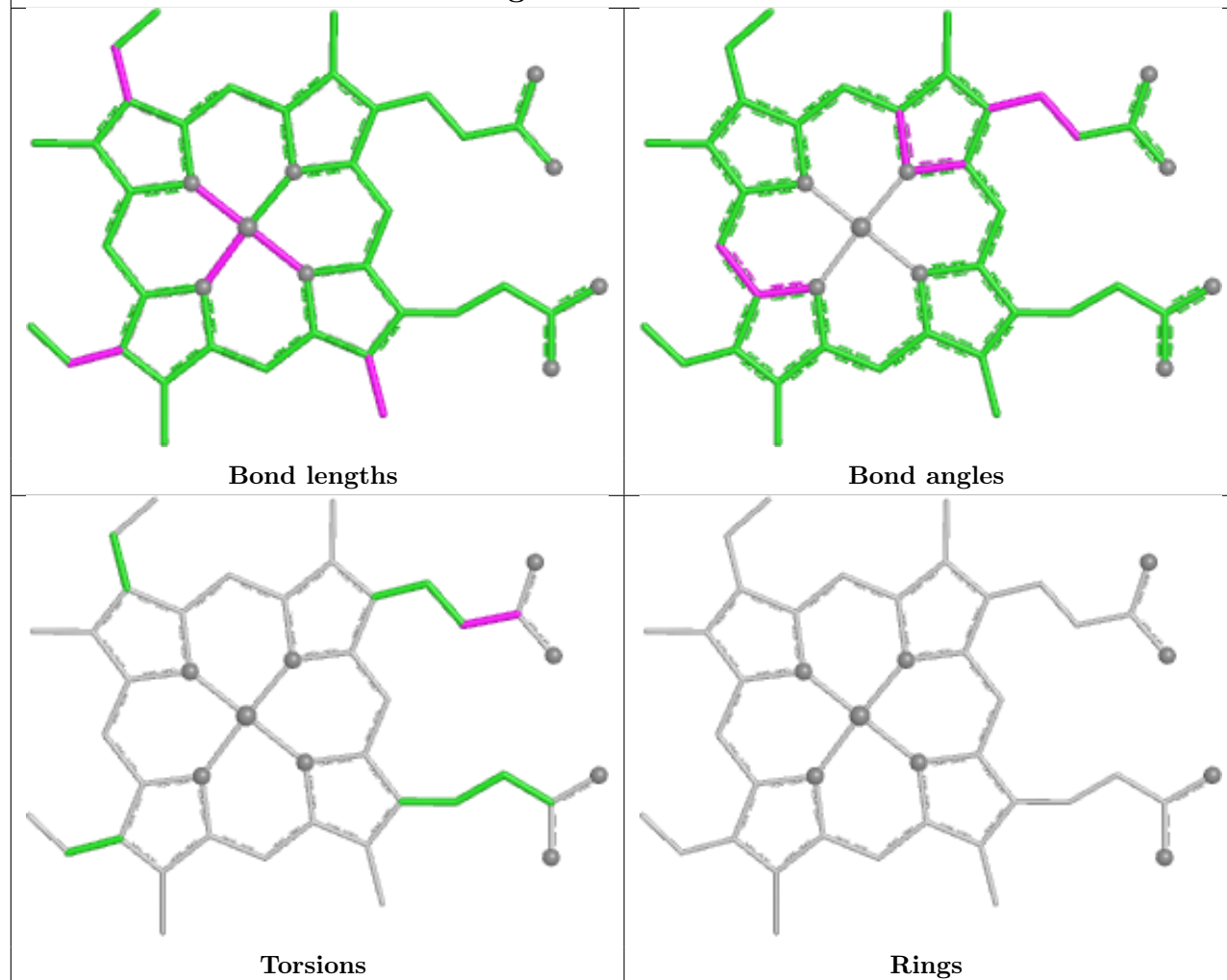
Ligand CLA B 602

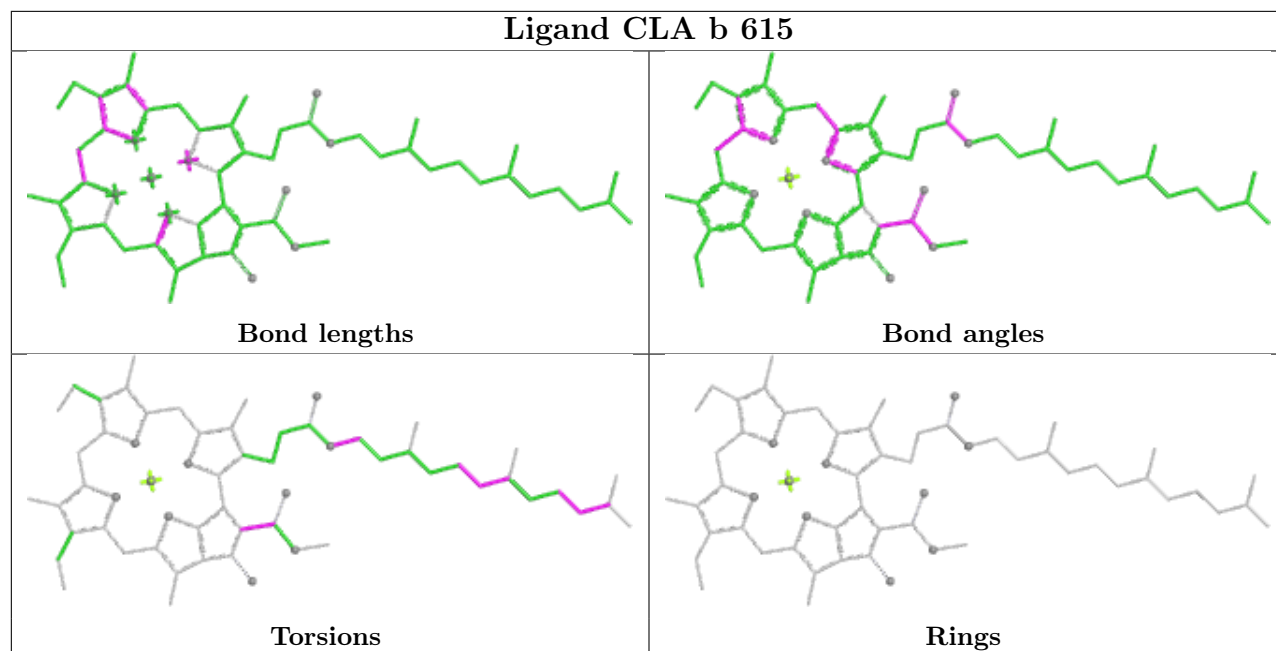
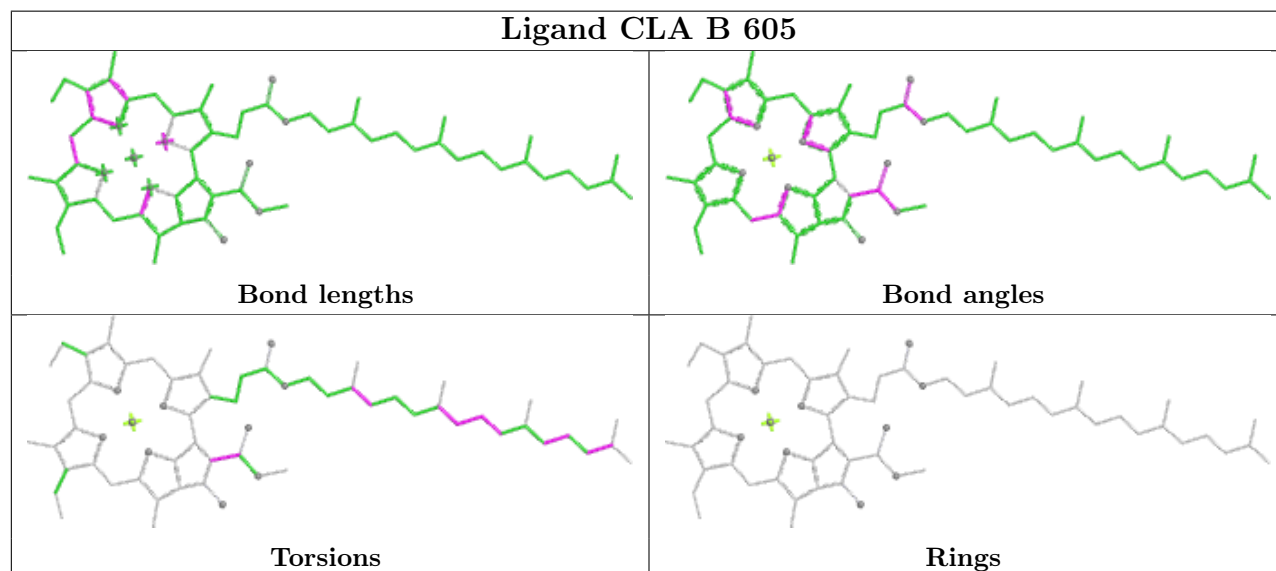
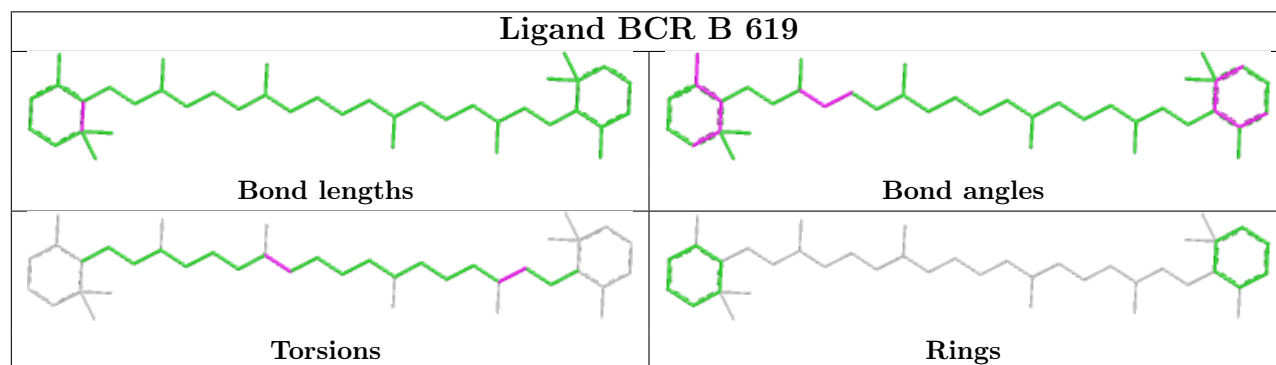


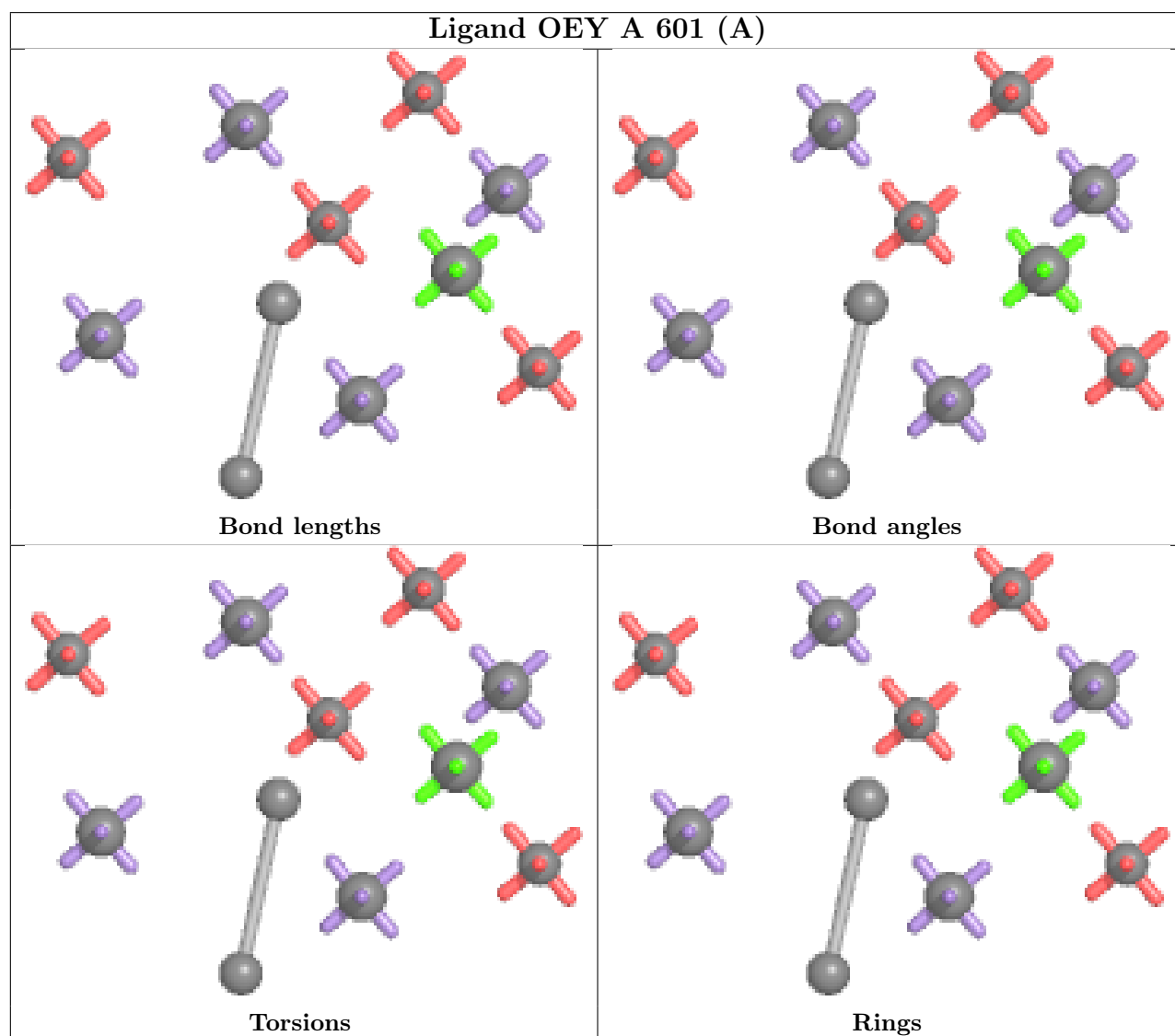
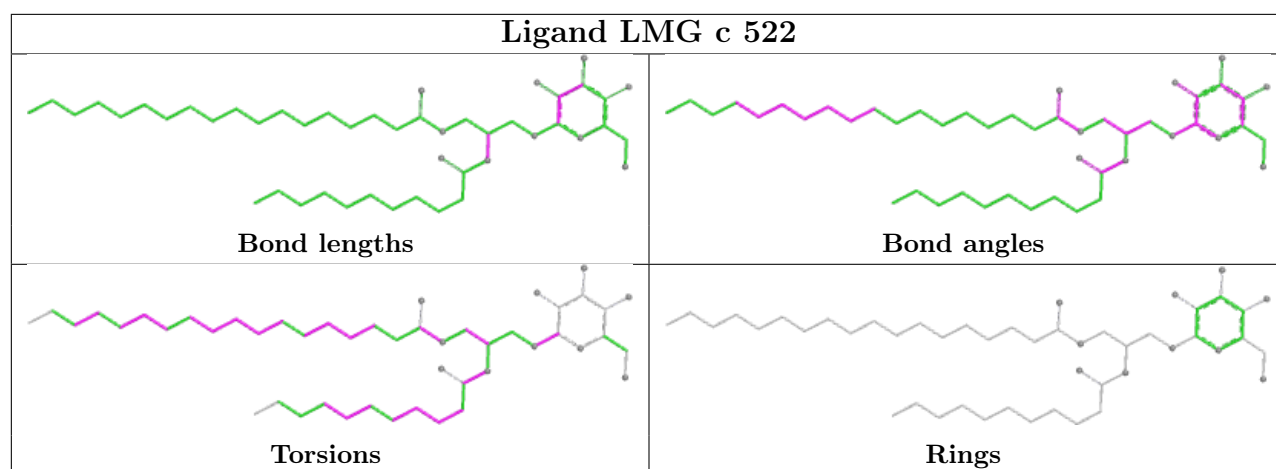
Ligand CLA C 502

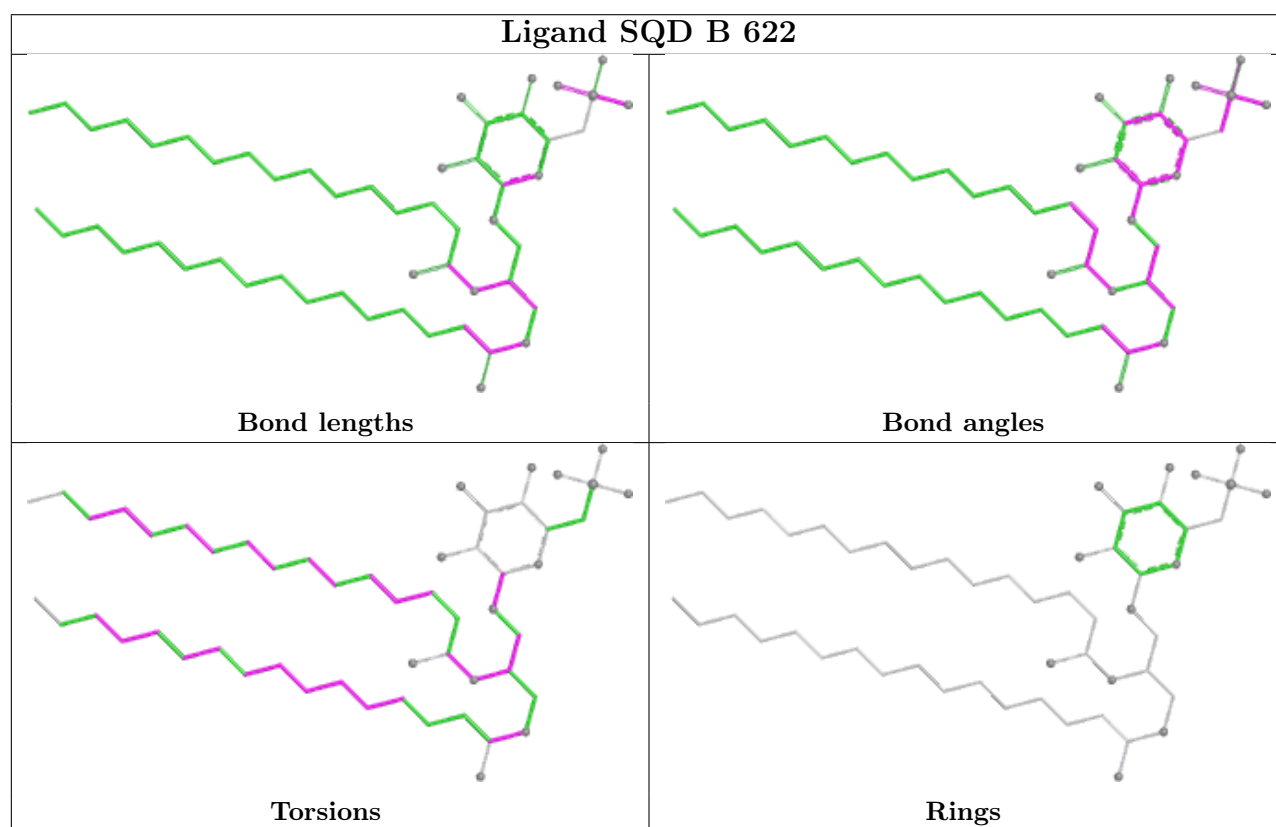
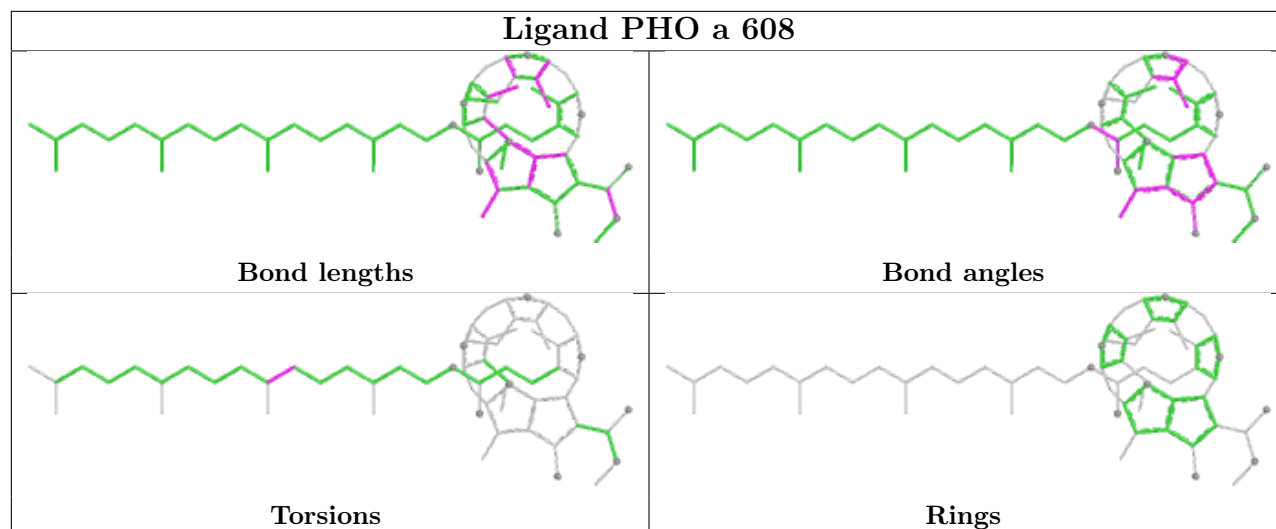


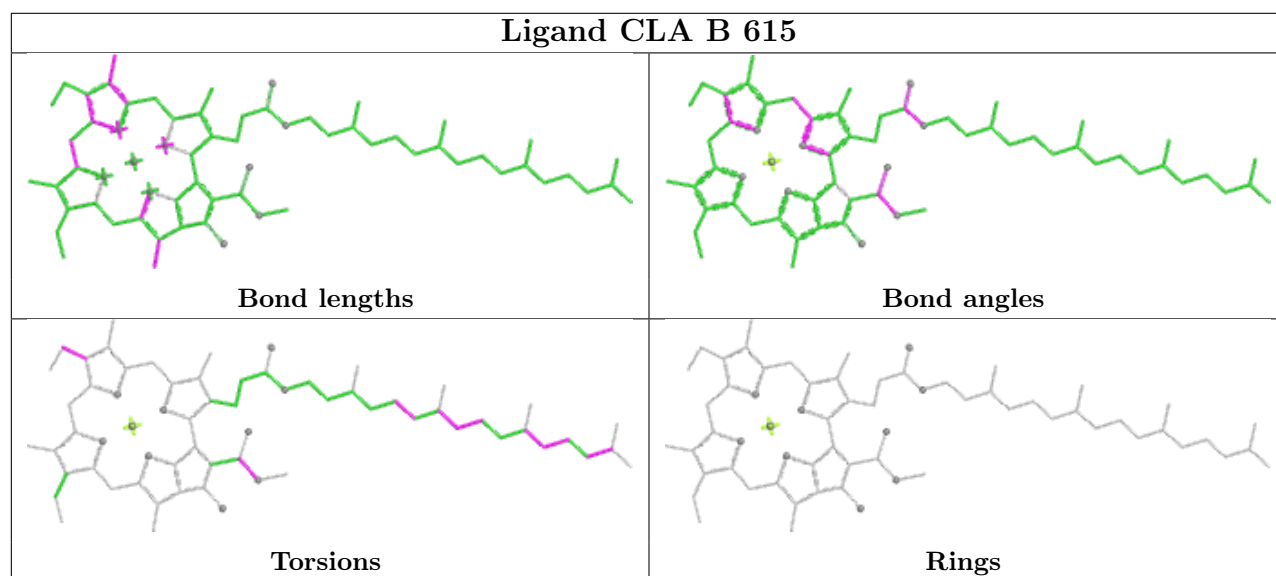
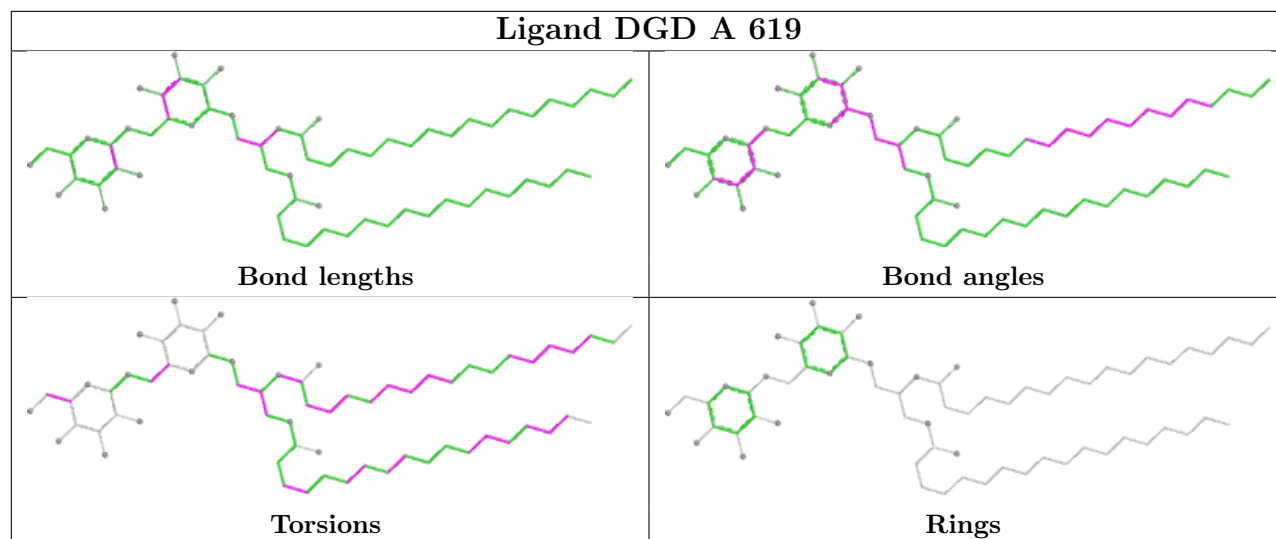
Ligand HEM F 101

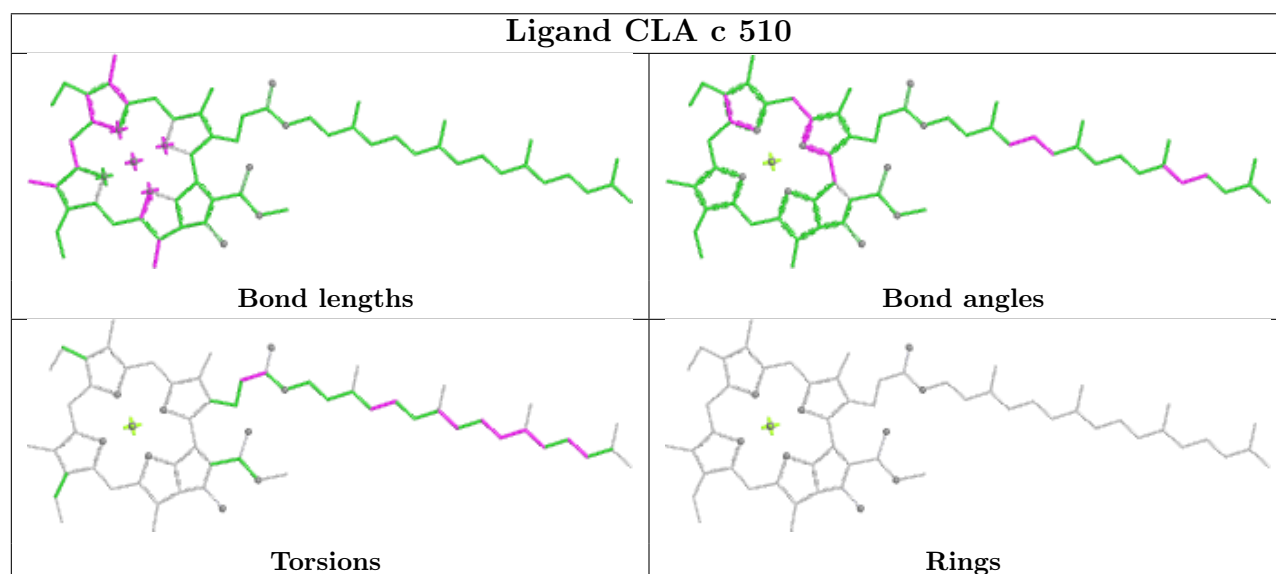
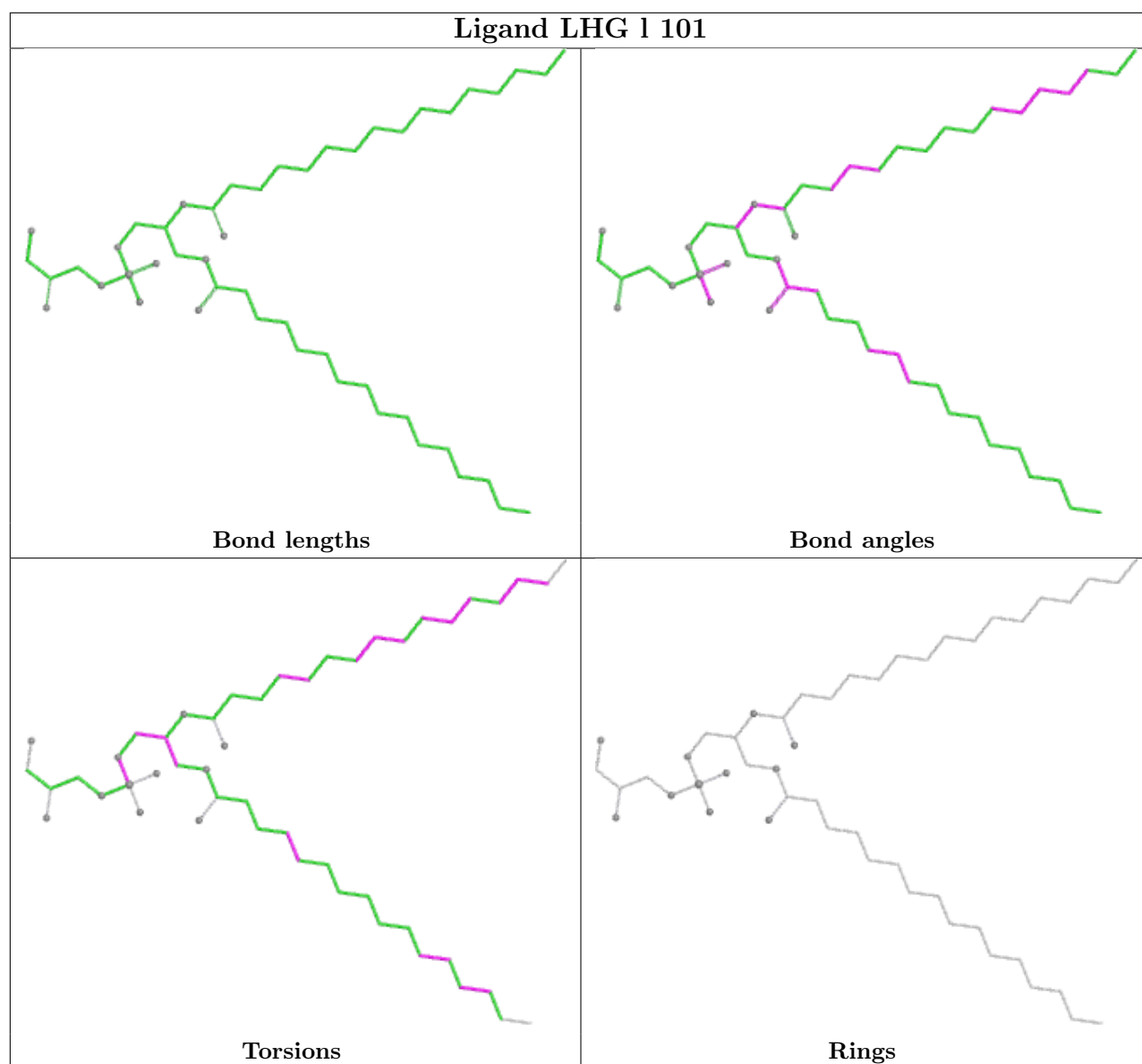


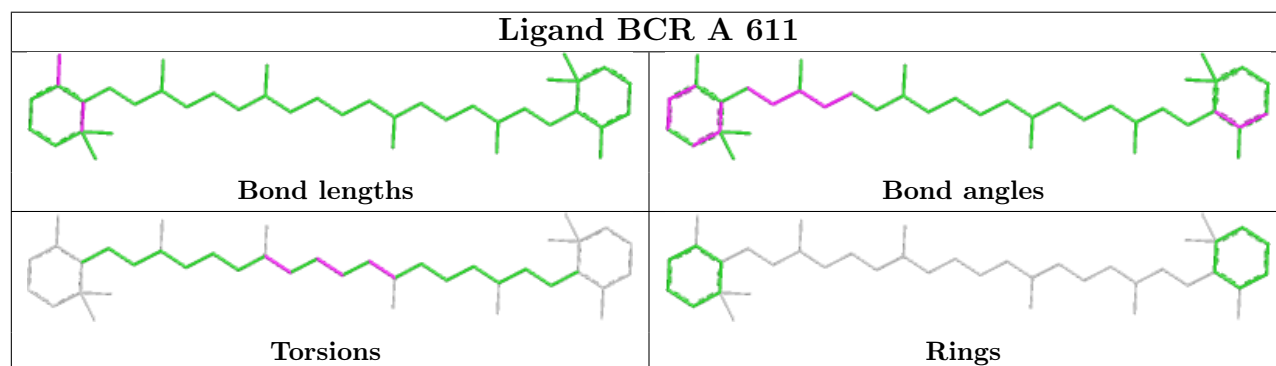
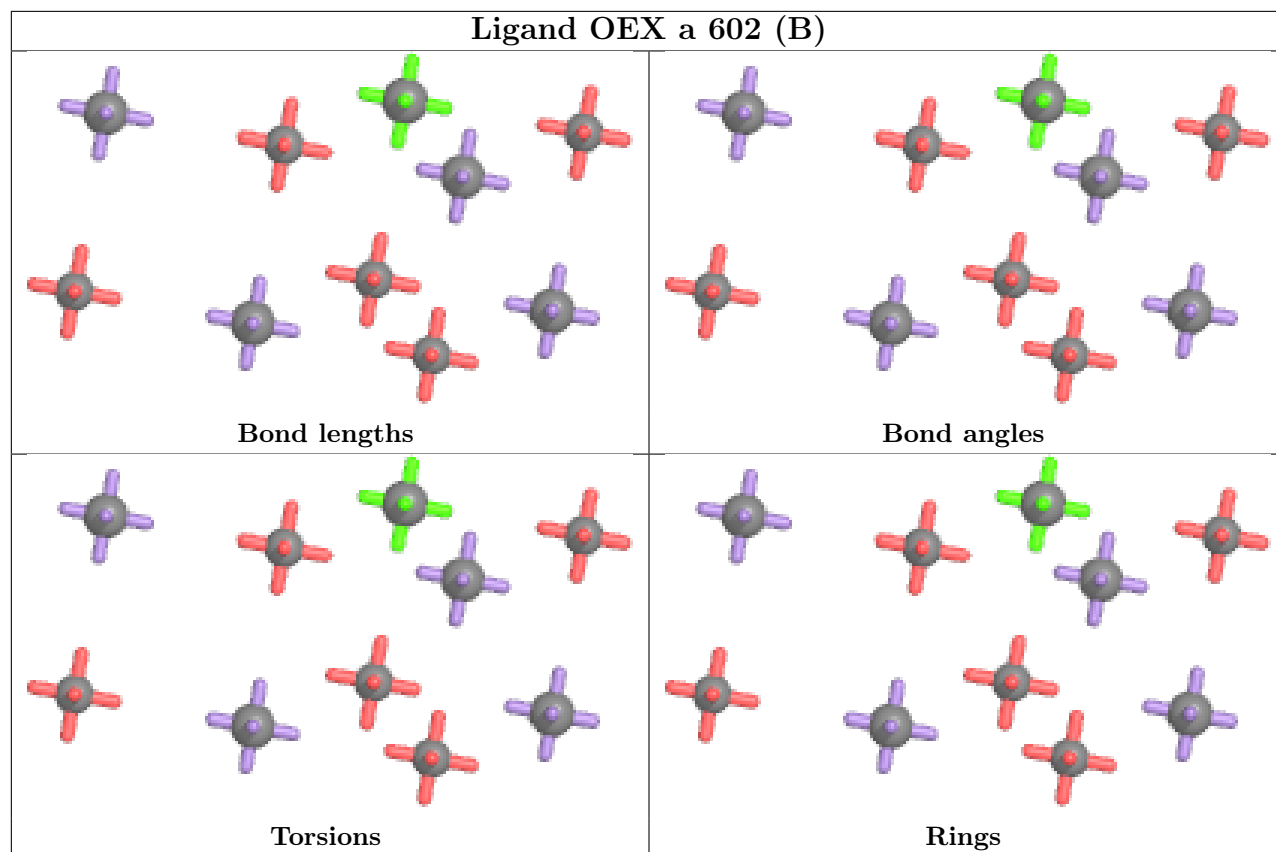
Ligand CLA b 615**Ligand CLA B 605****Ligand BCR B 619**

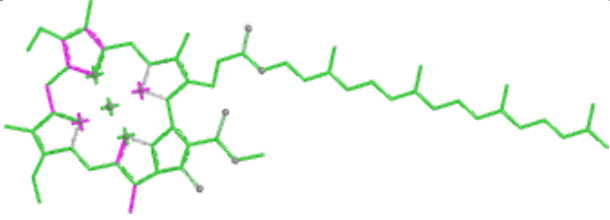
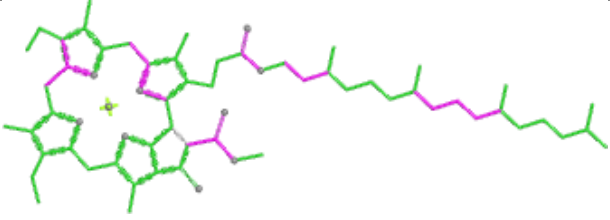
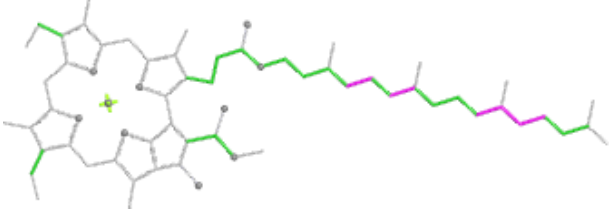
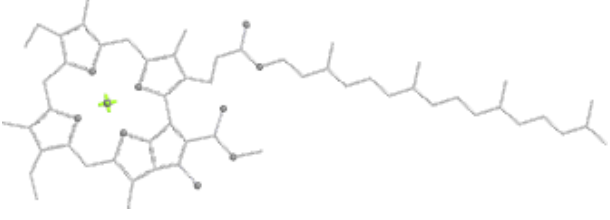
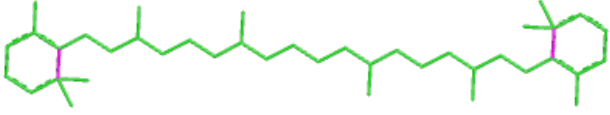
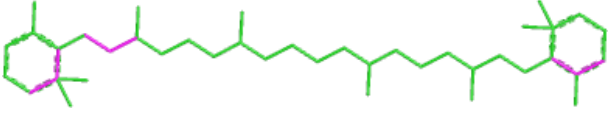
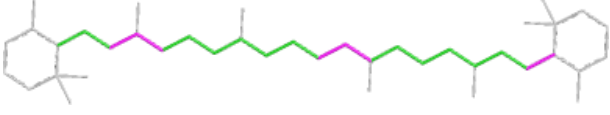
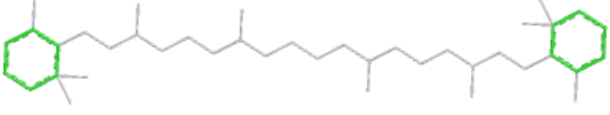
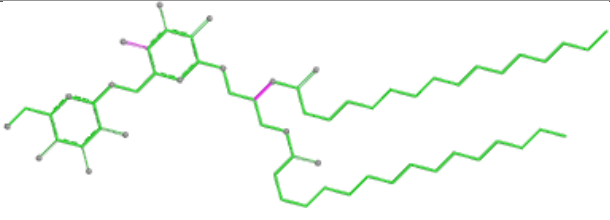
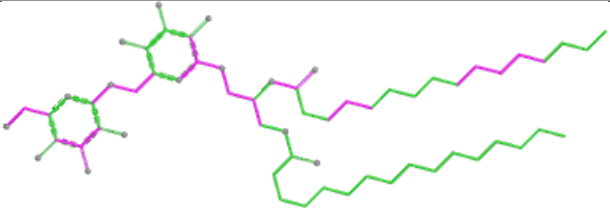
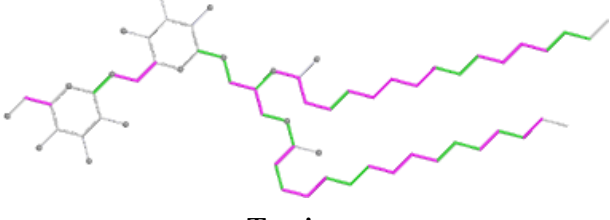
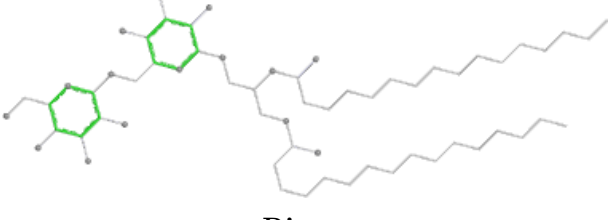


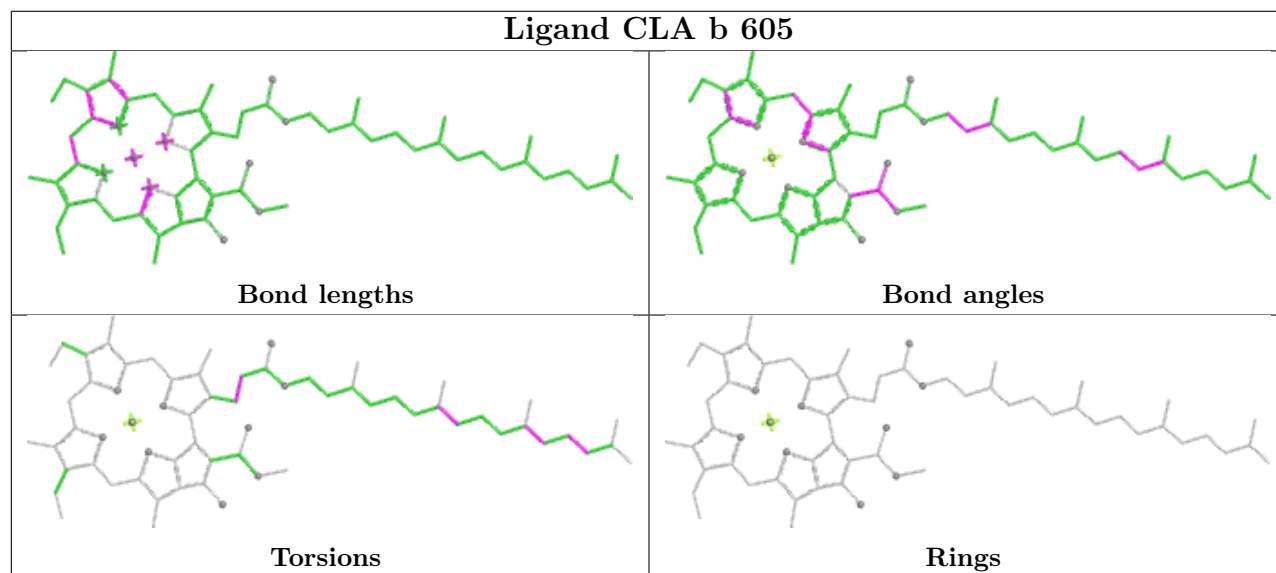
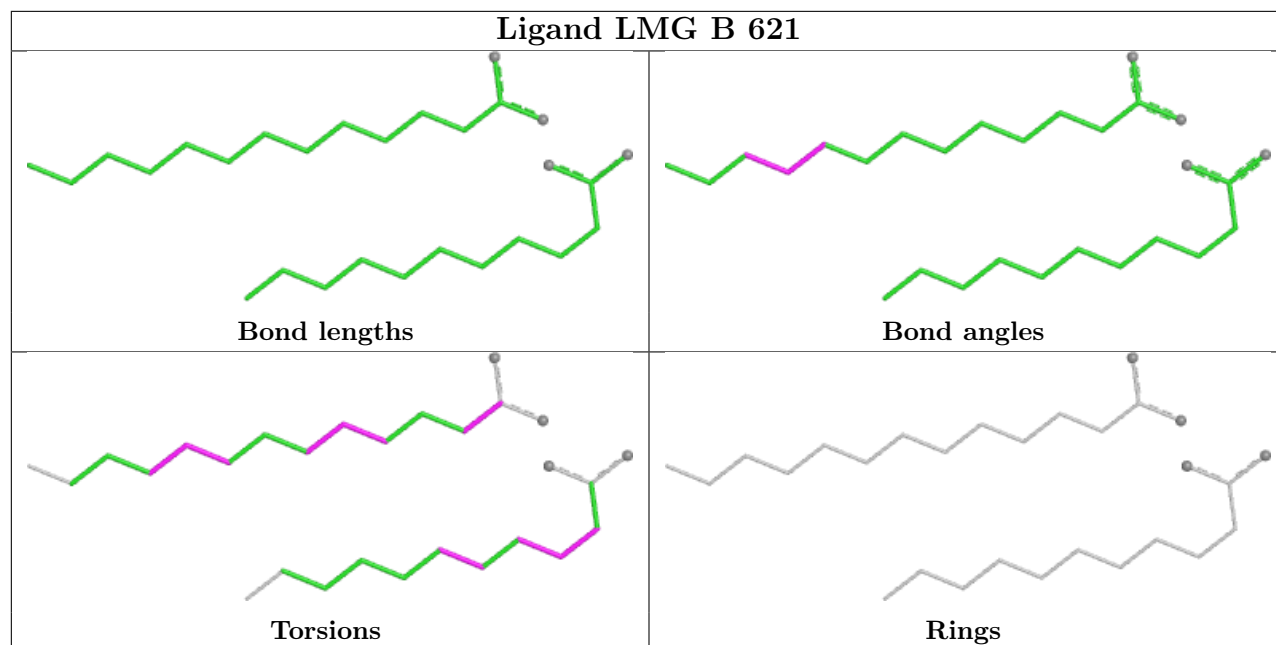


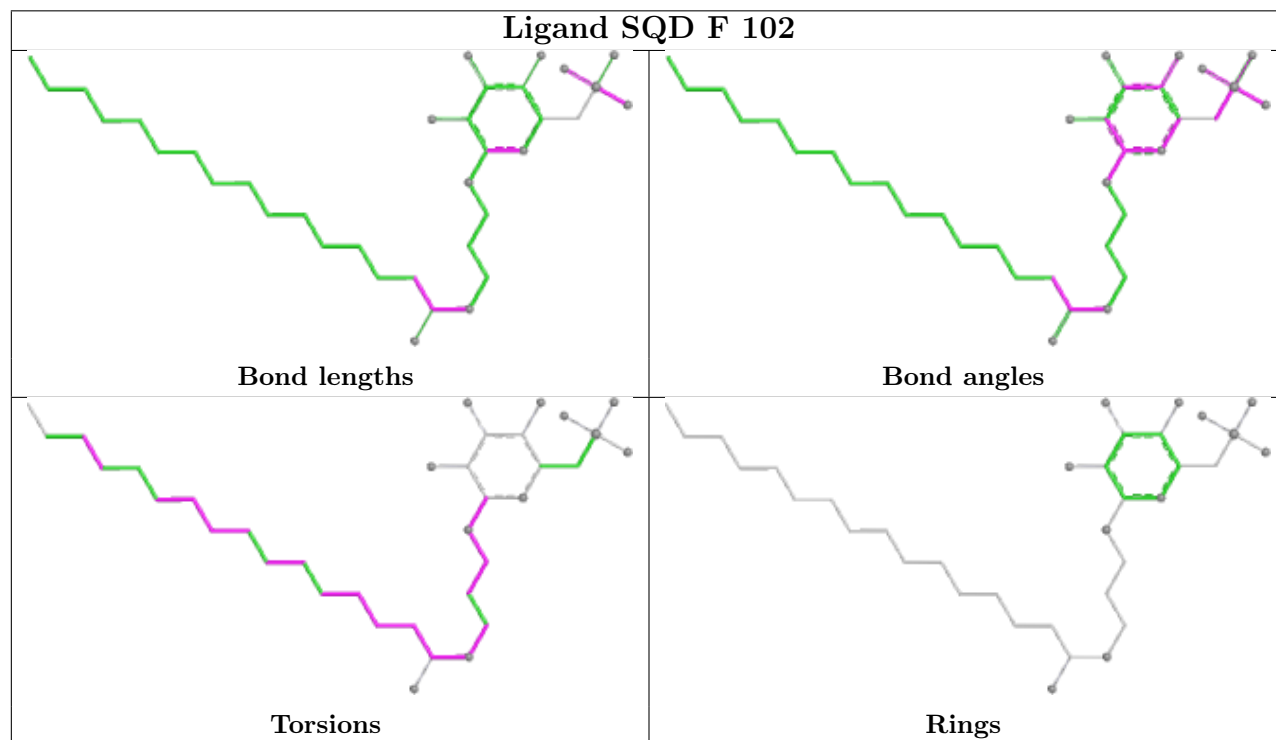
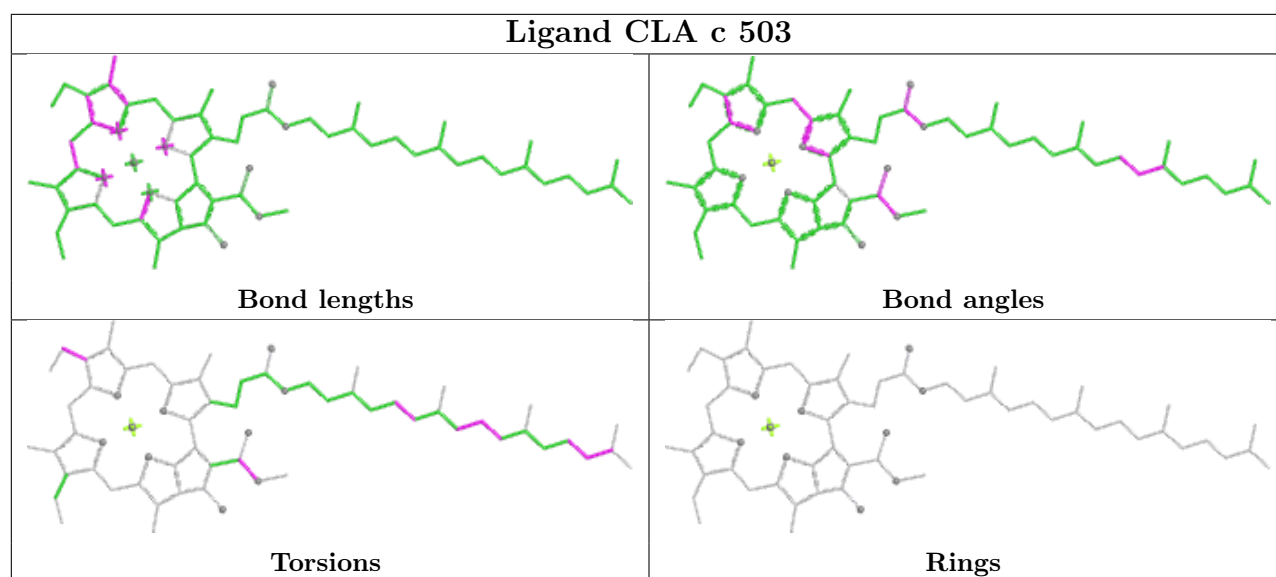


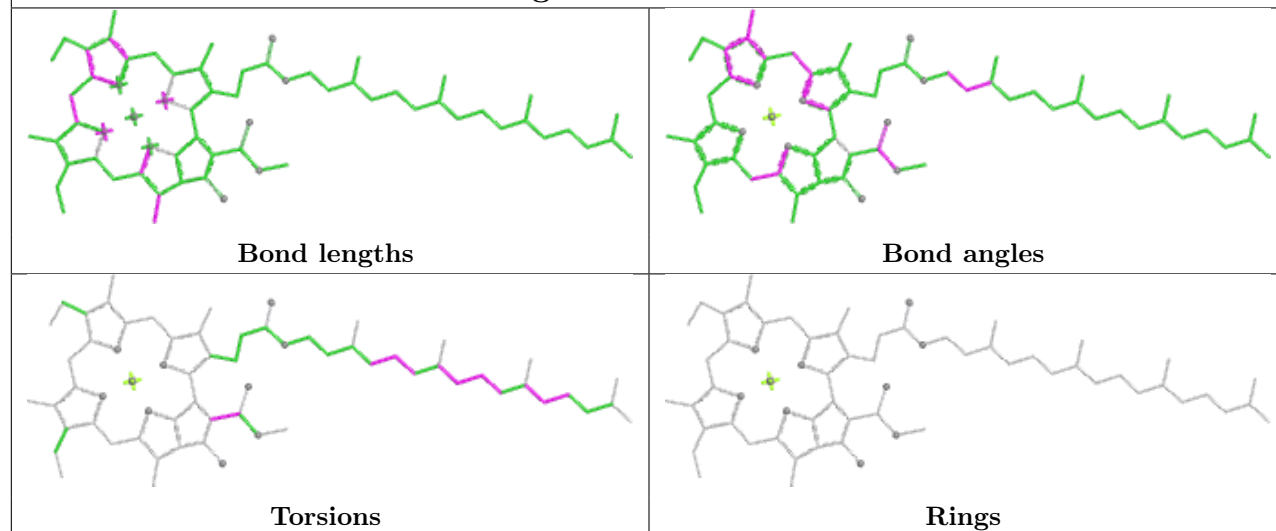
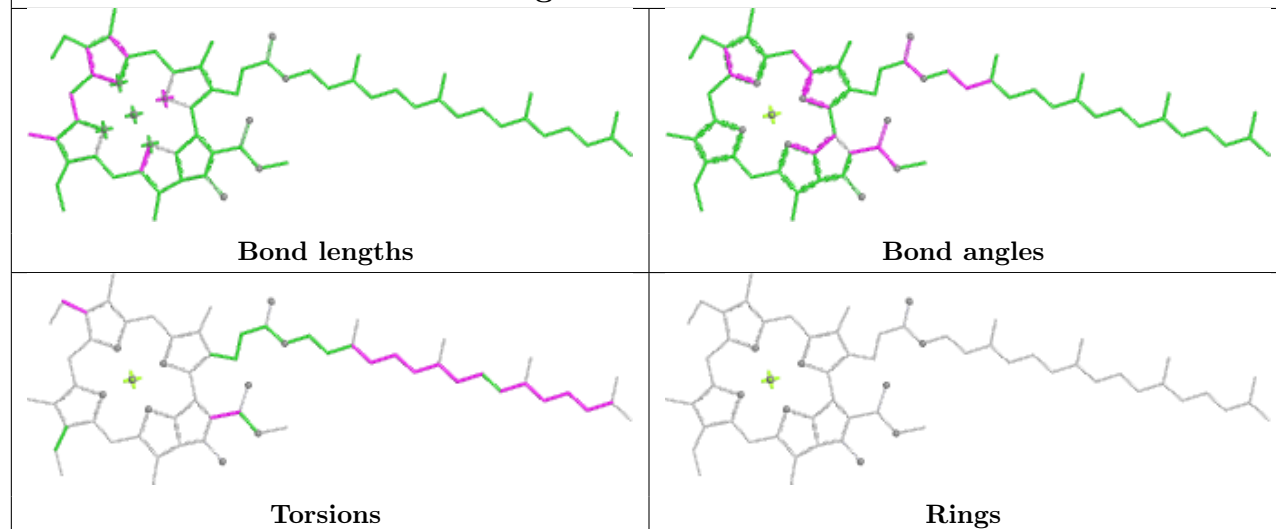


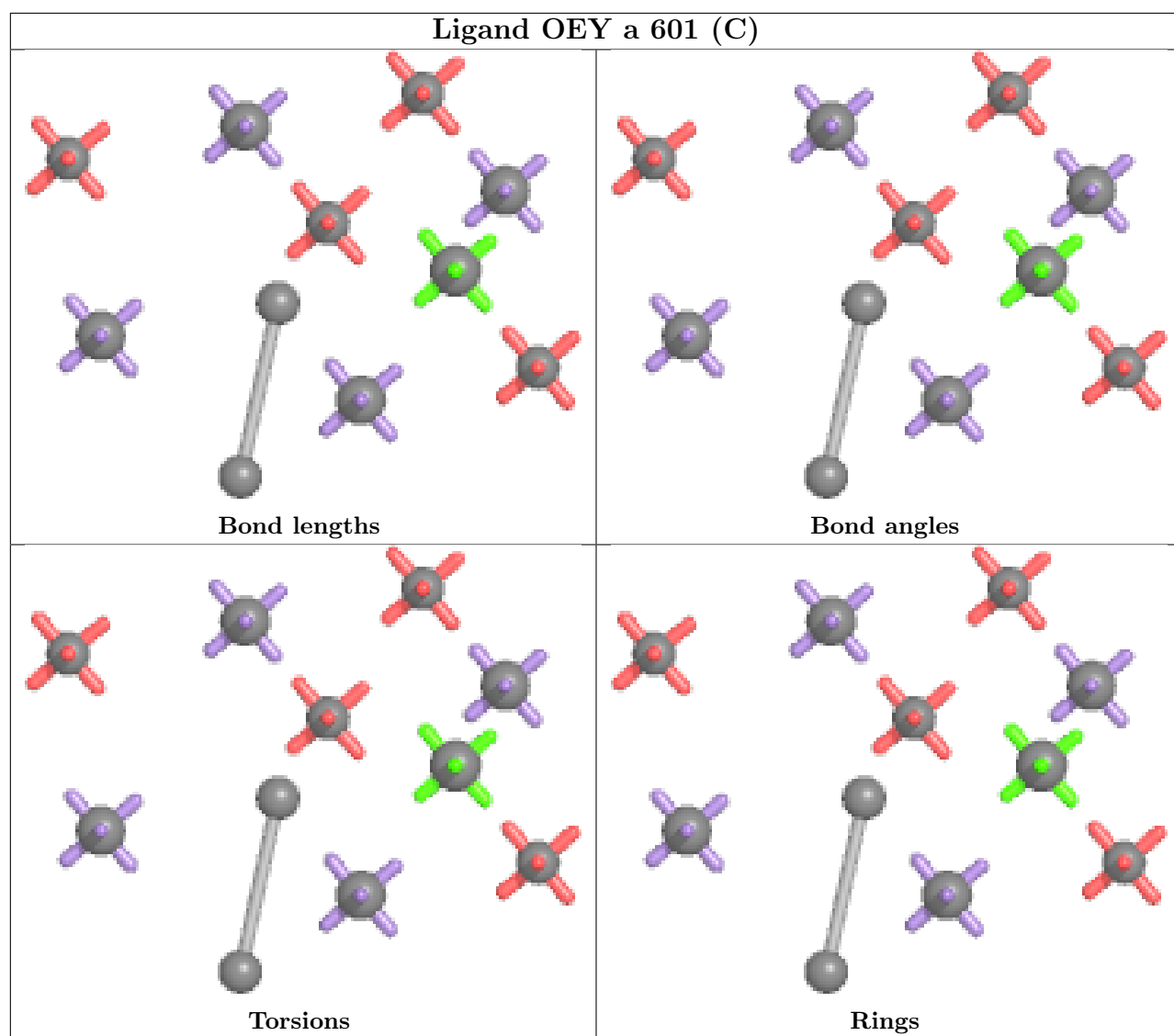


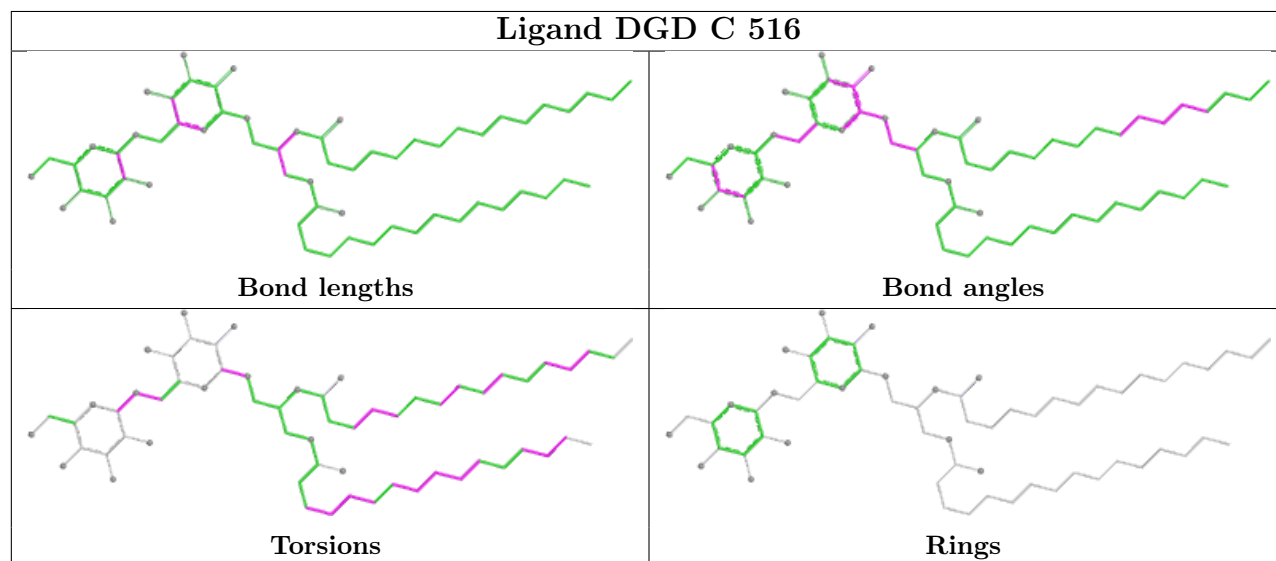
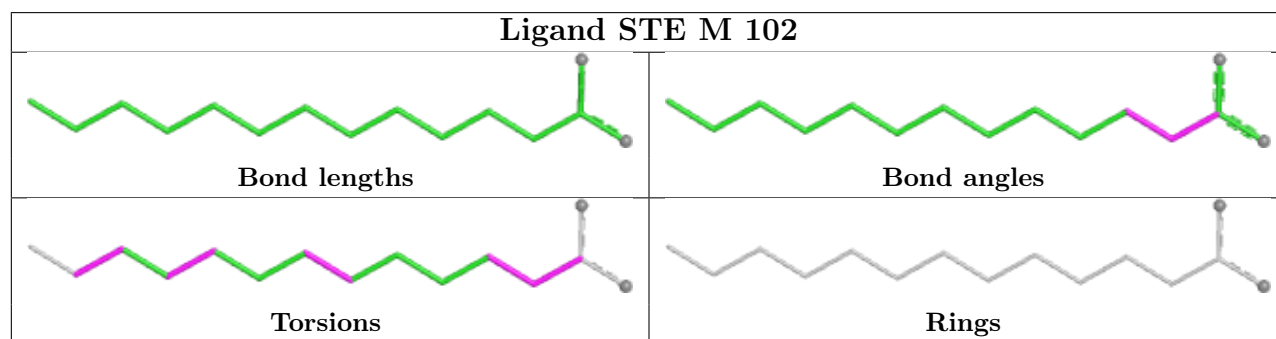
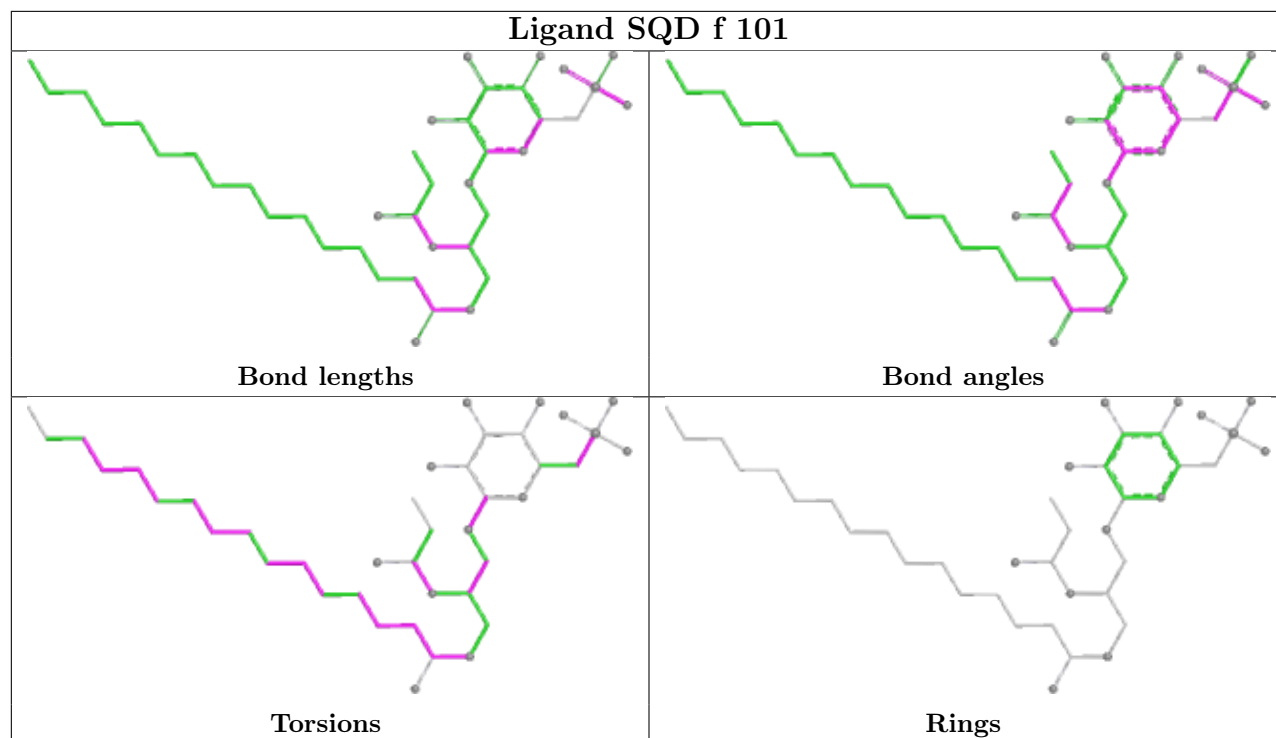
Ligand CLA b 603	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR h 102	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand DGD c 517	
 Bond lengths	 Bond angles
 Torsions	 Rings

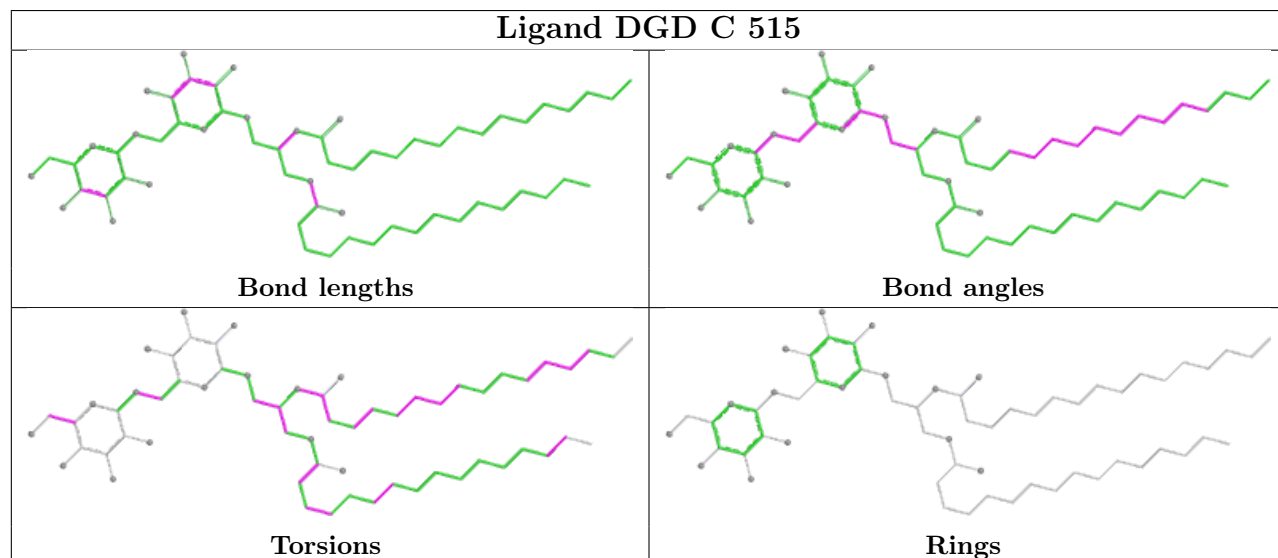
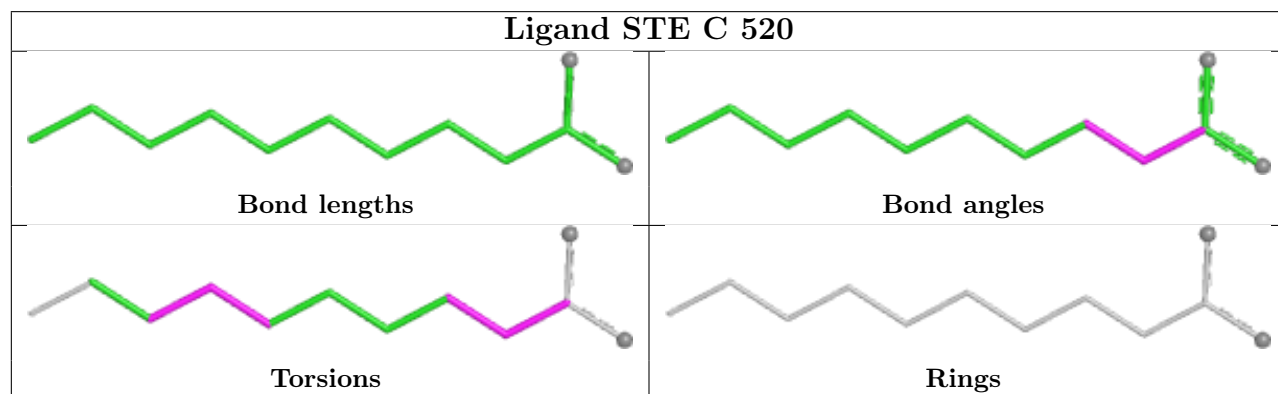
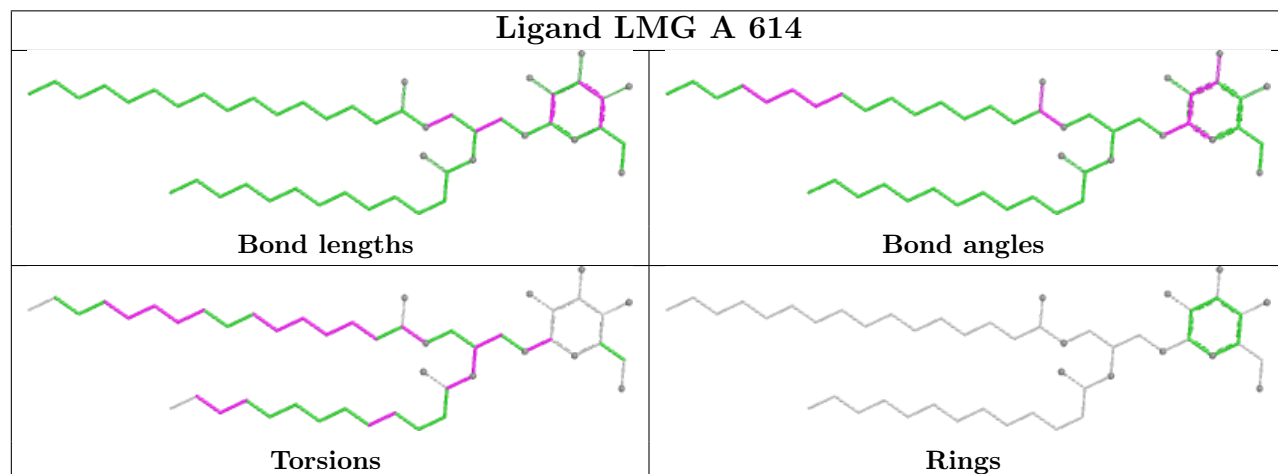
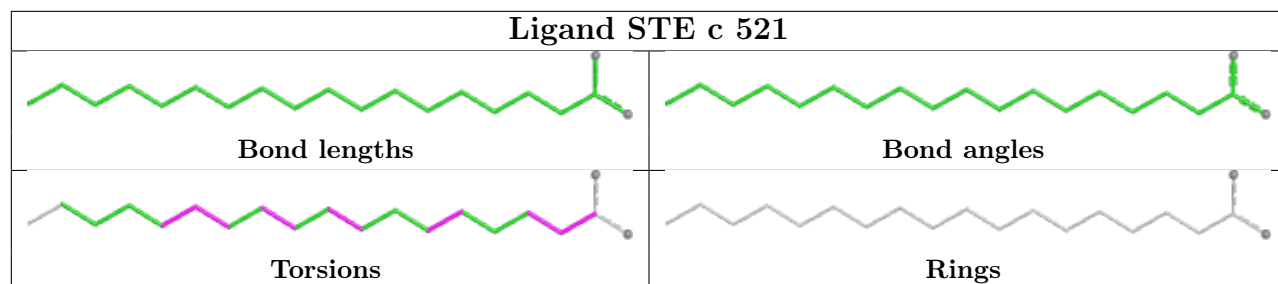


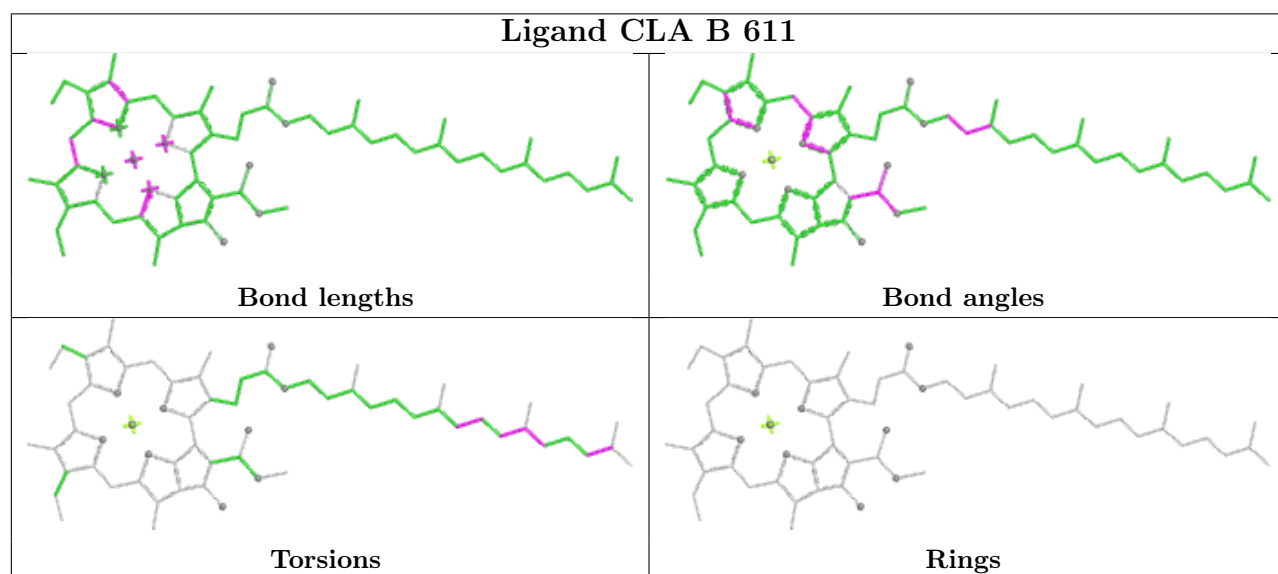
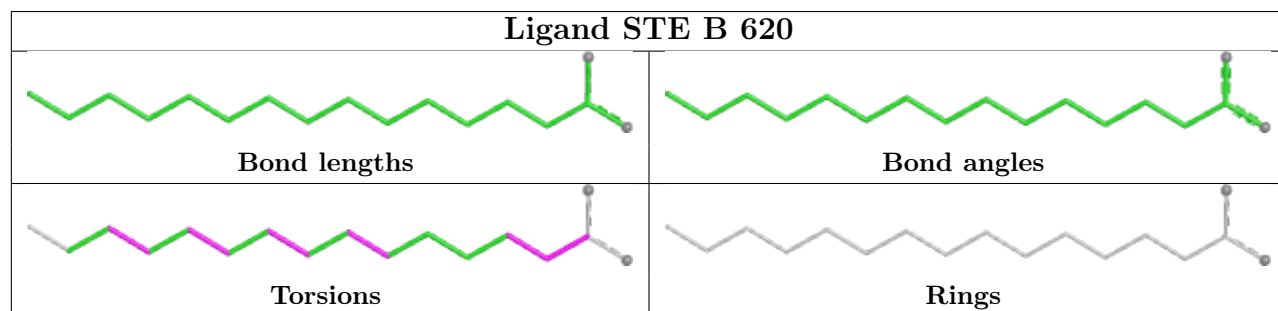
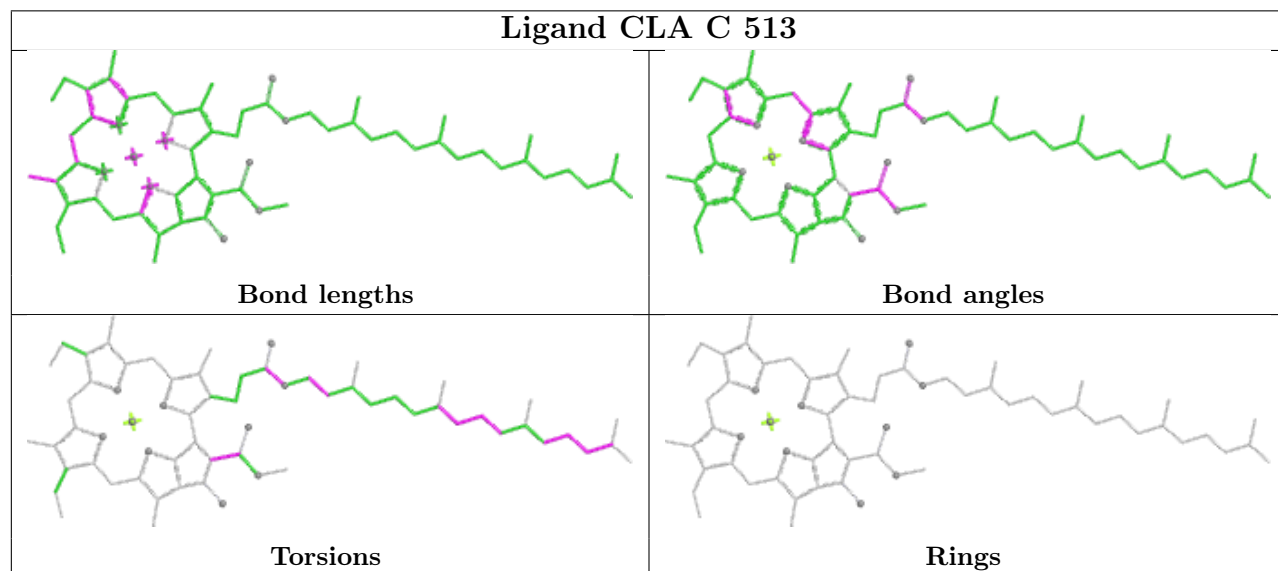
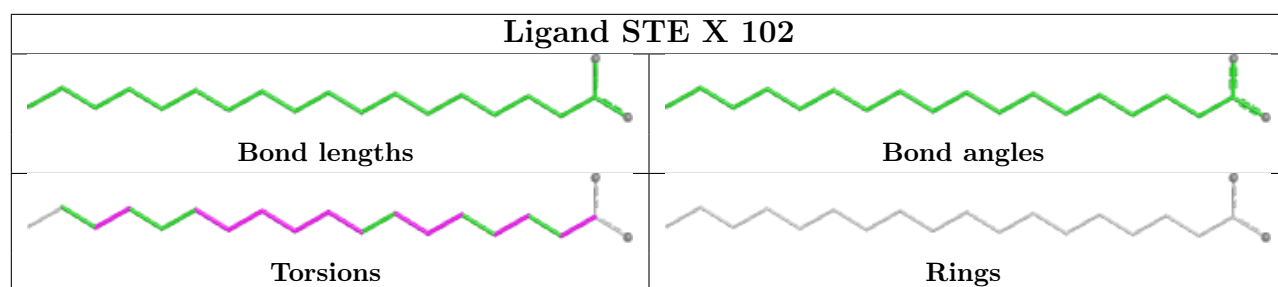


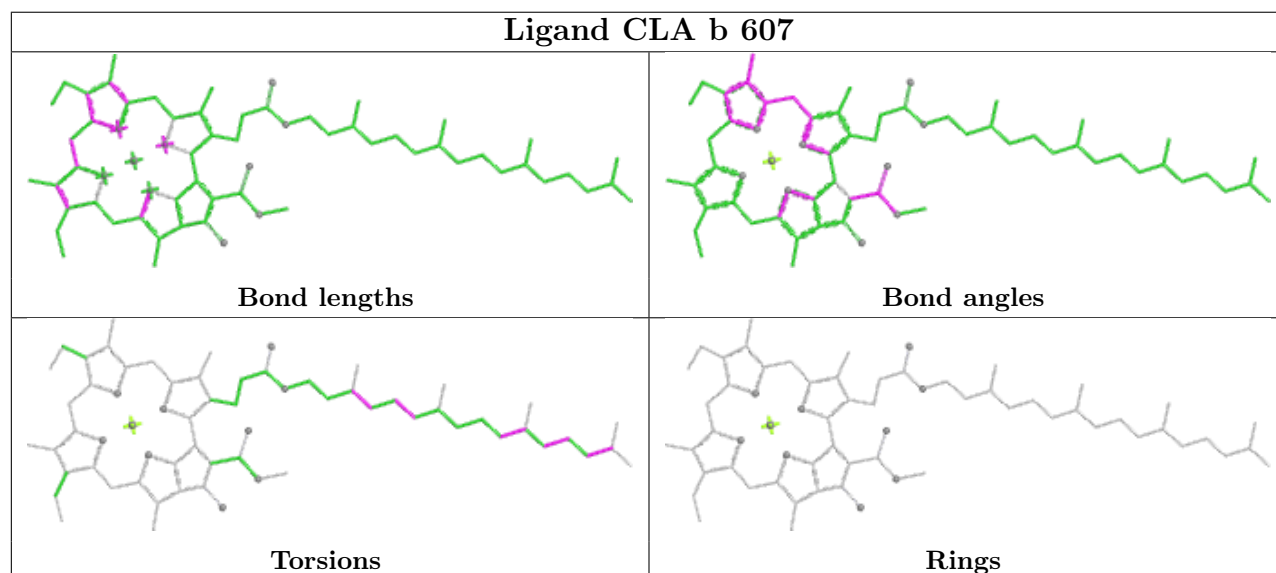
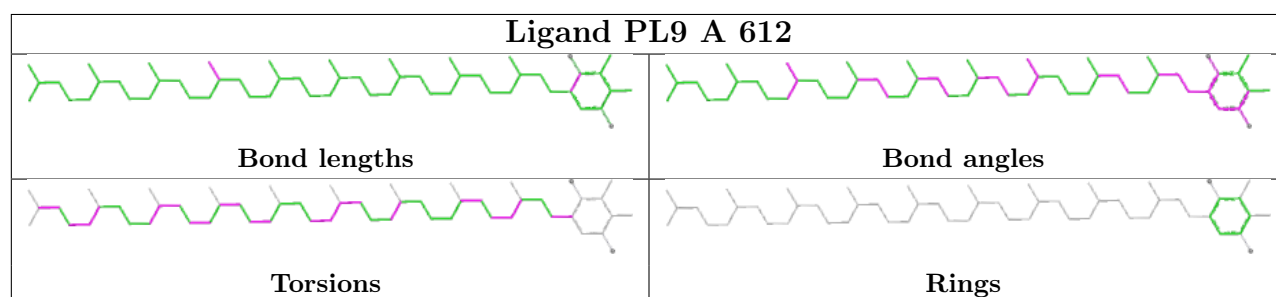
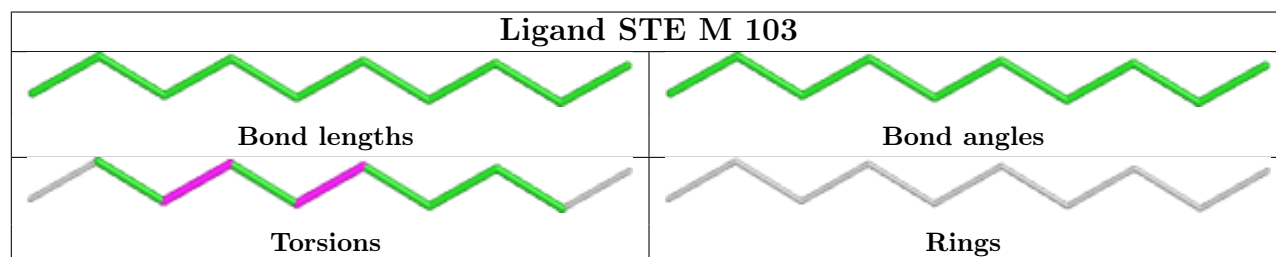
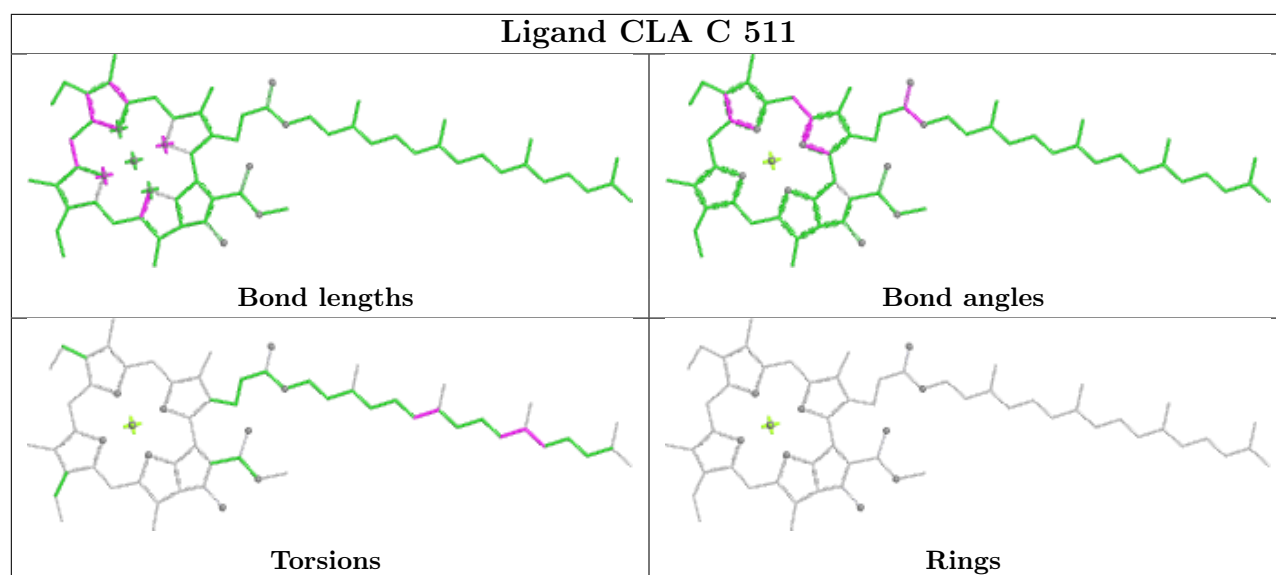
Ligand CLA C 509**Ligand CLA b 613**



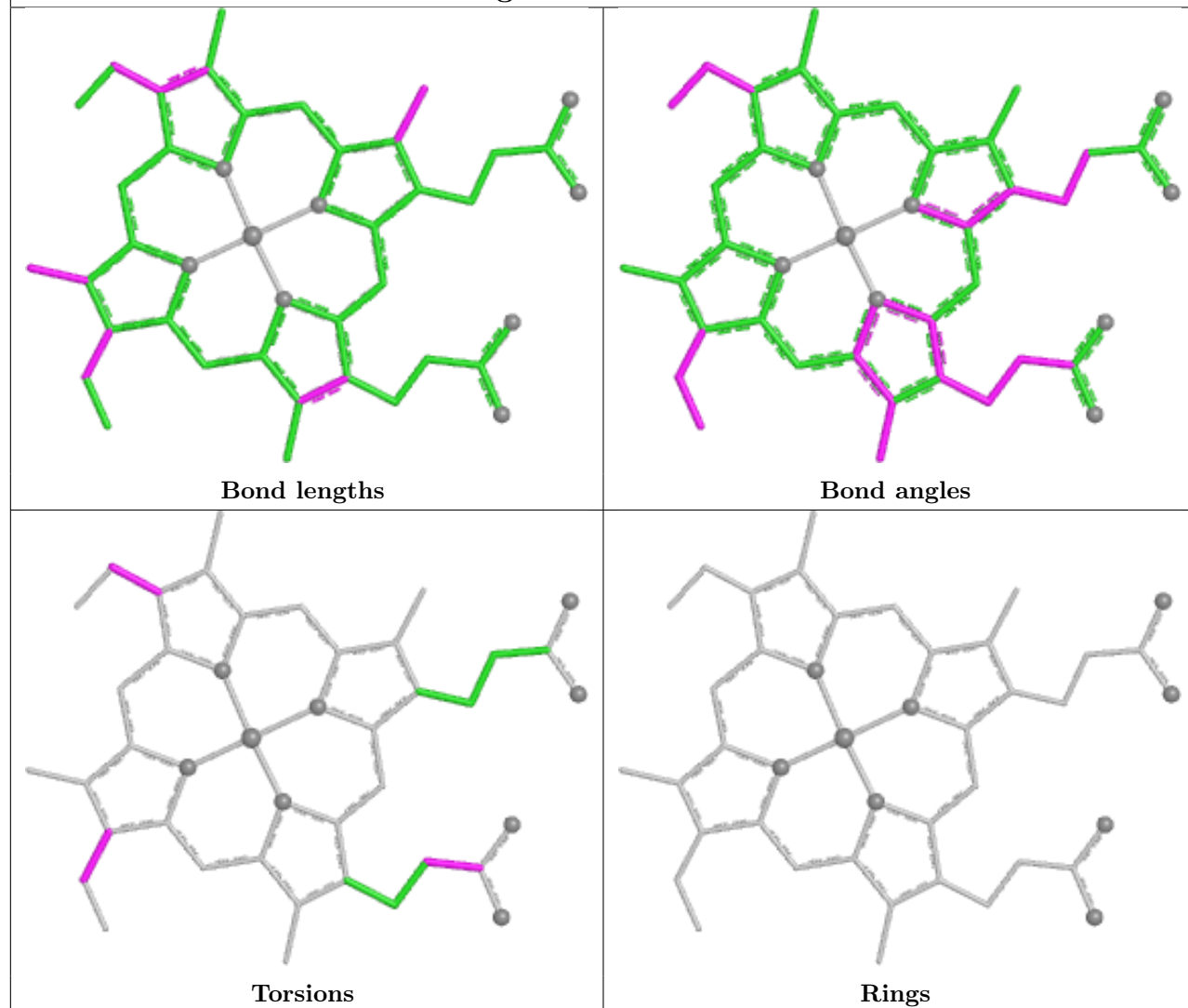




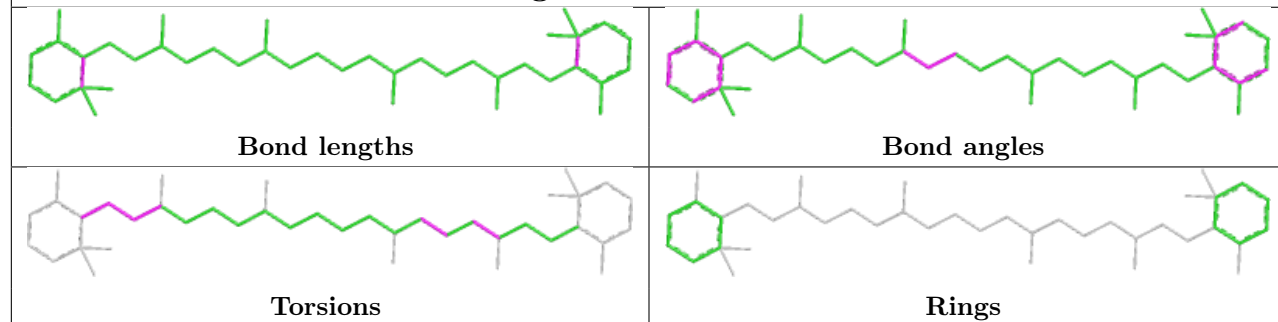


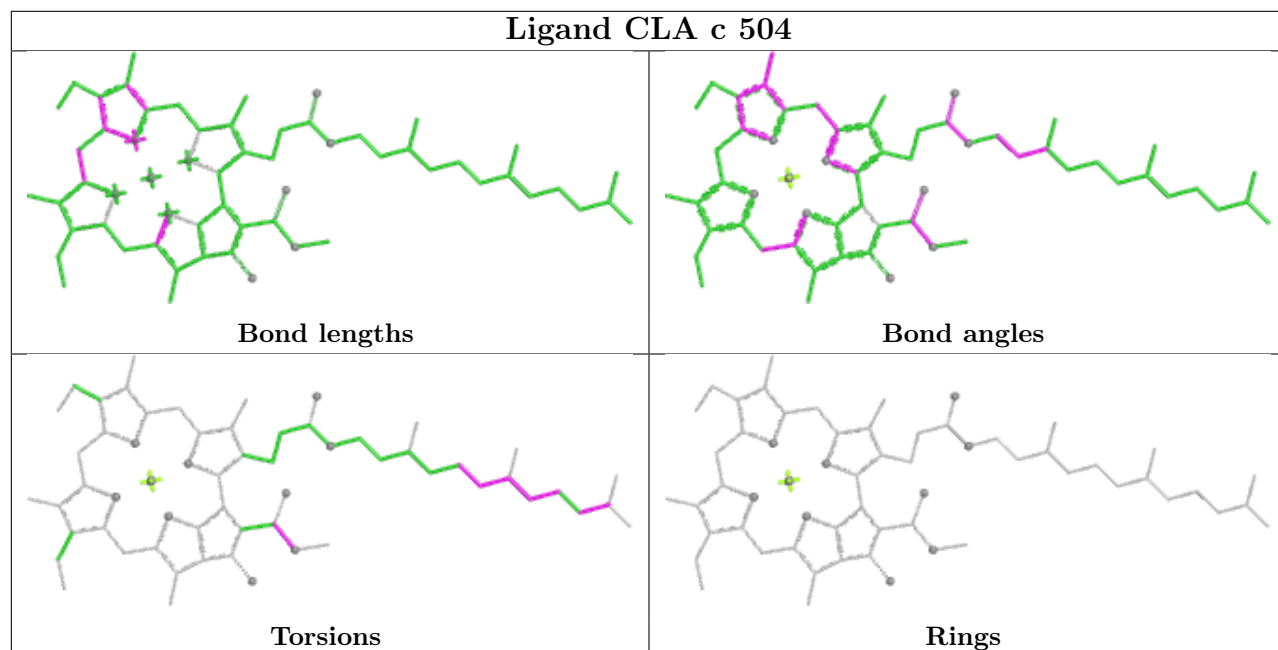
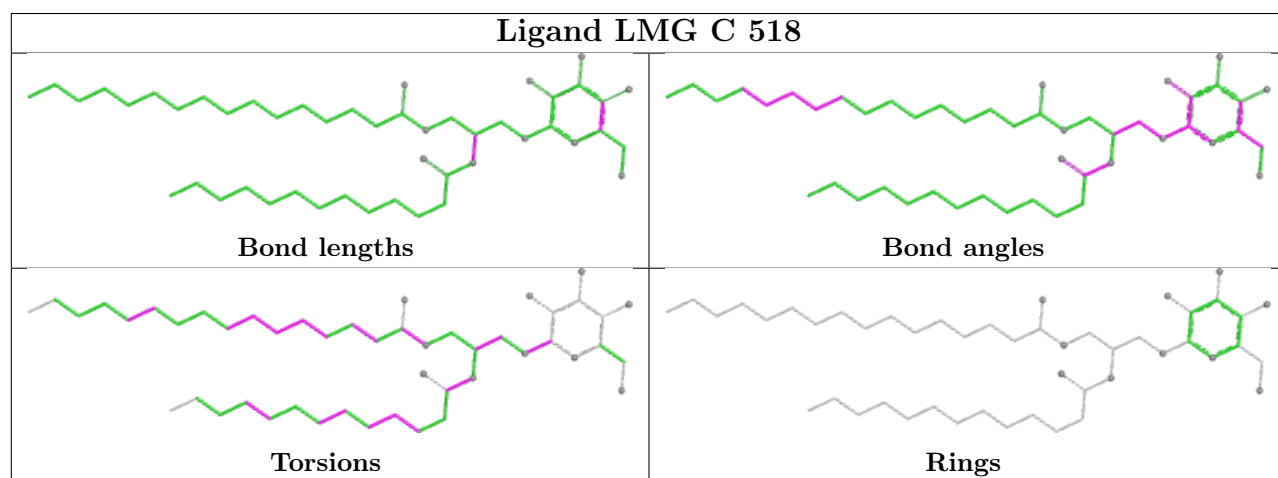
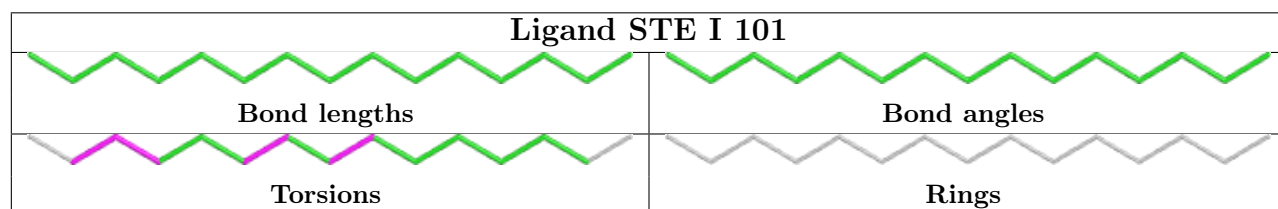
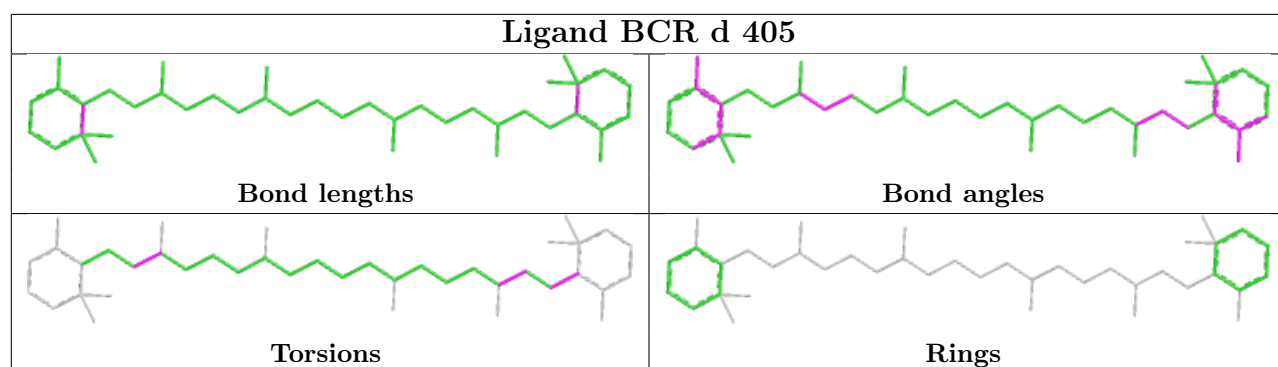


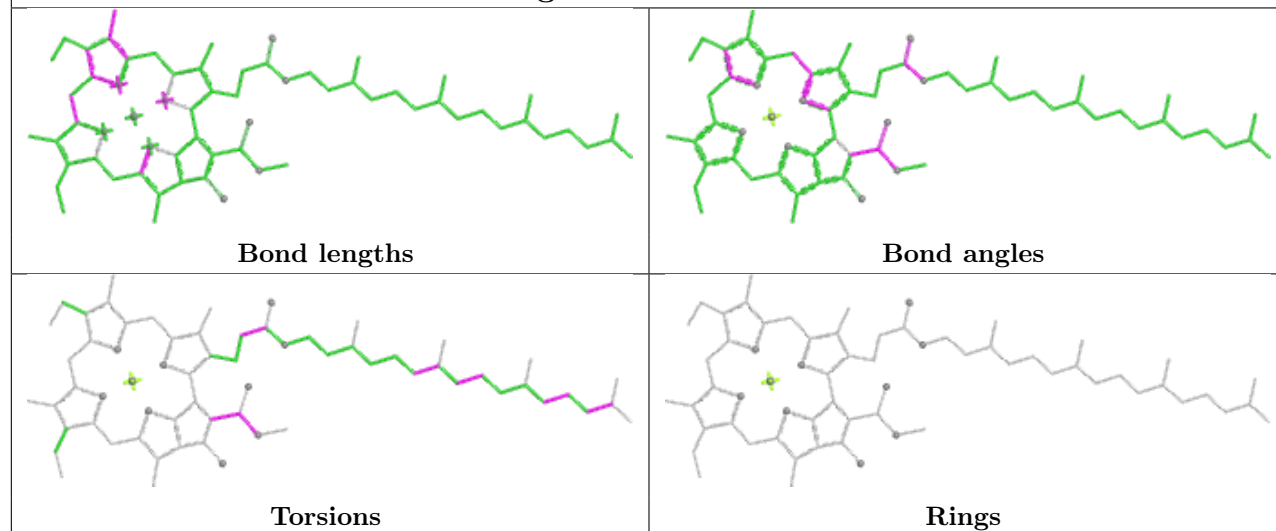
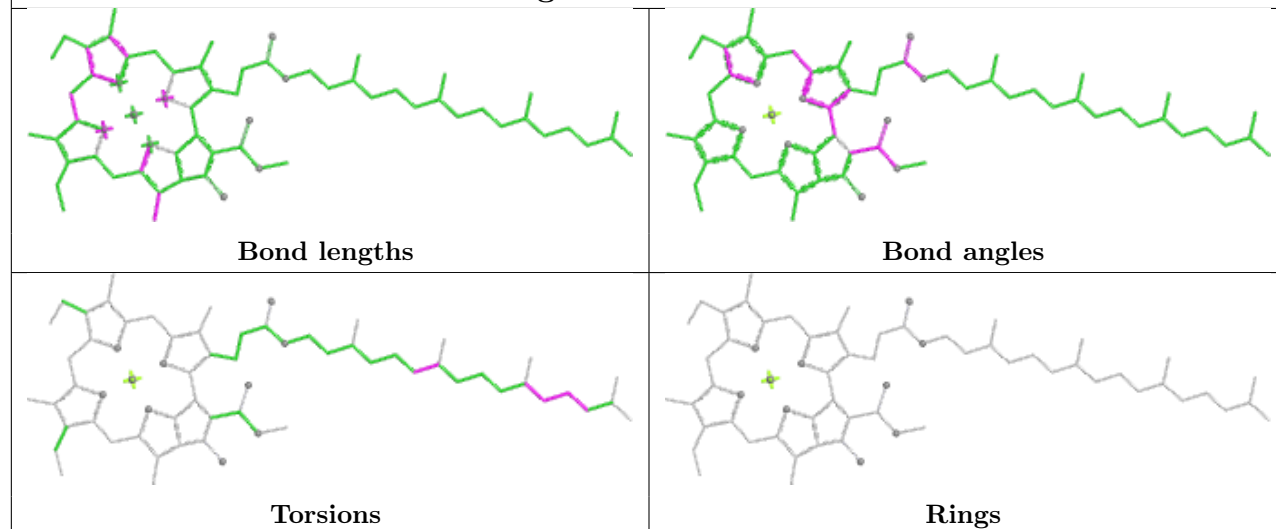
Ligand HEC v 201

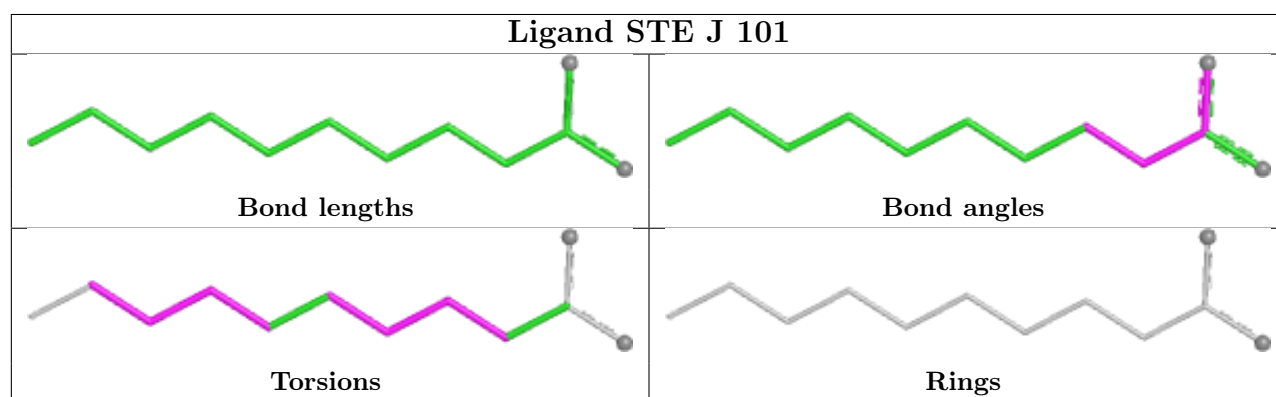
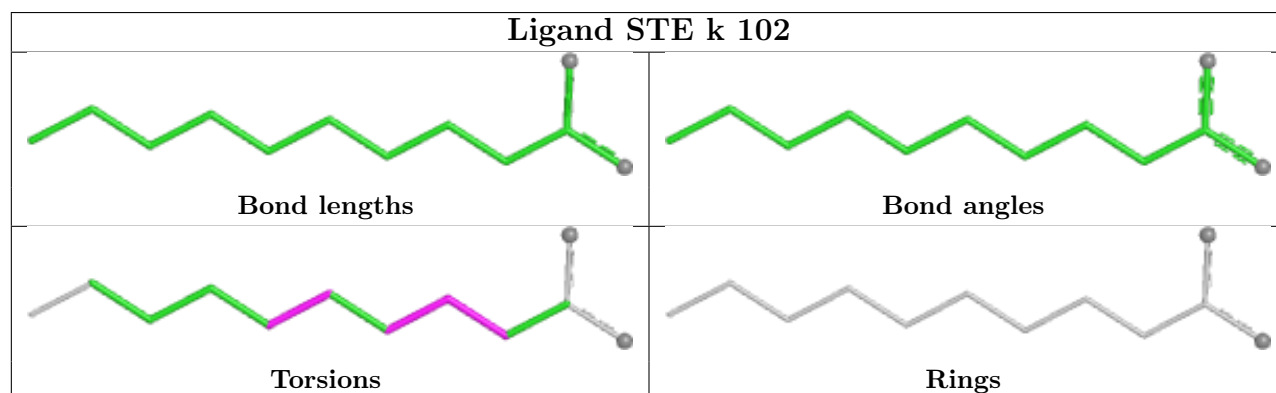
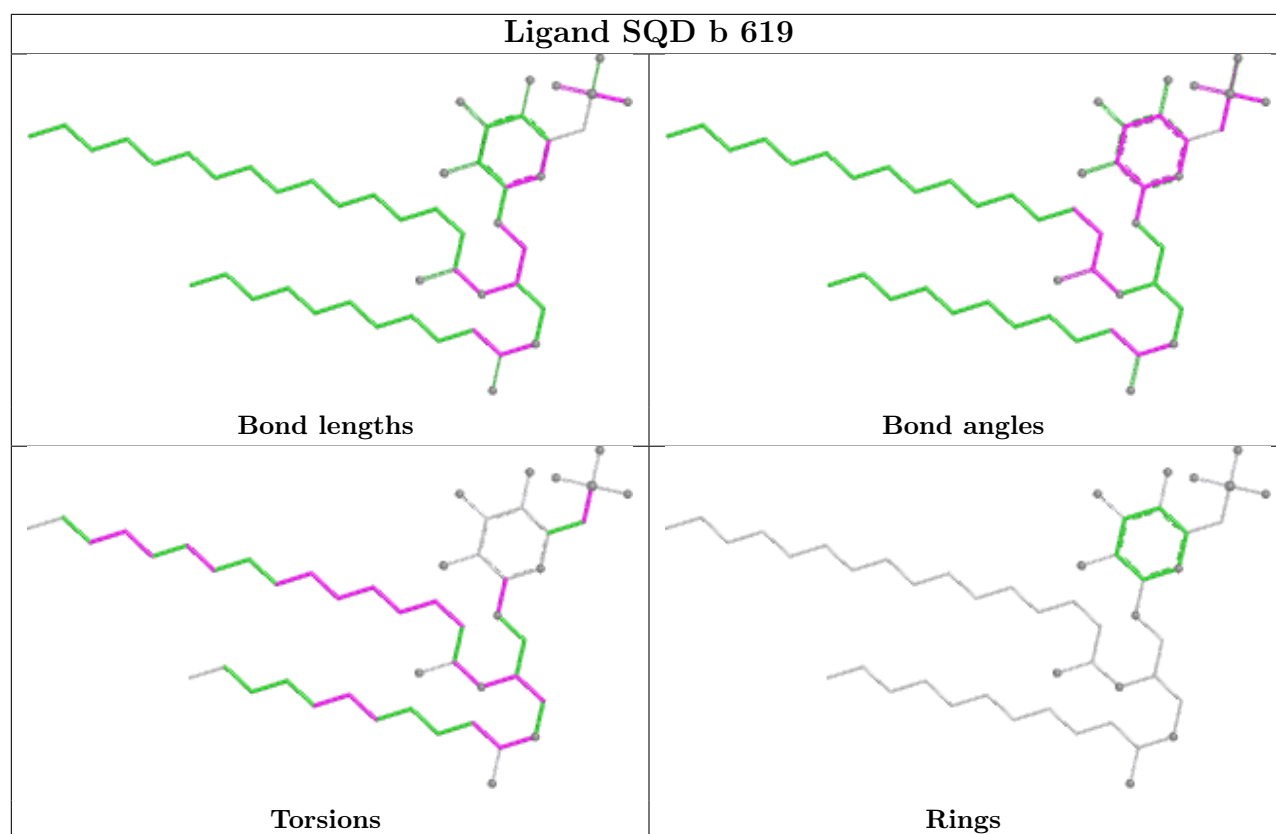


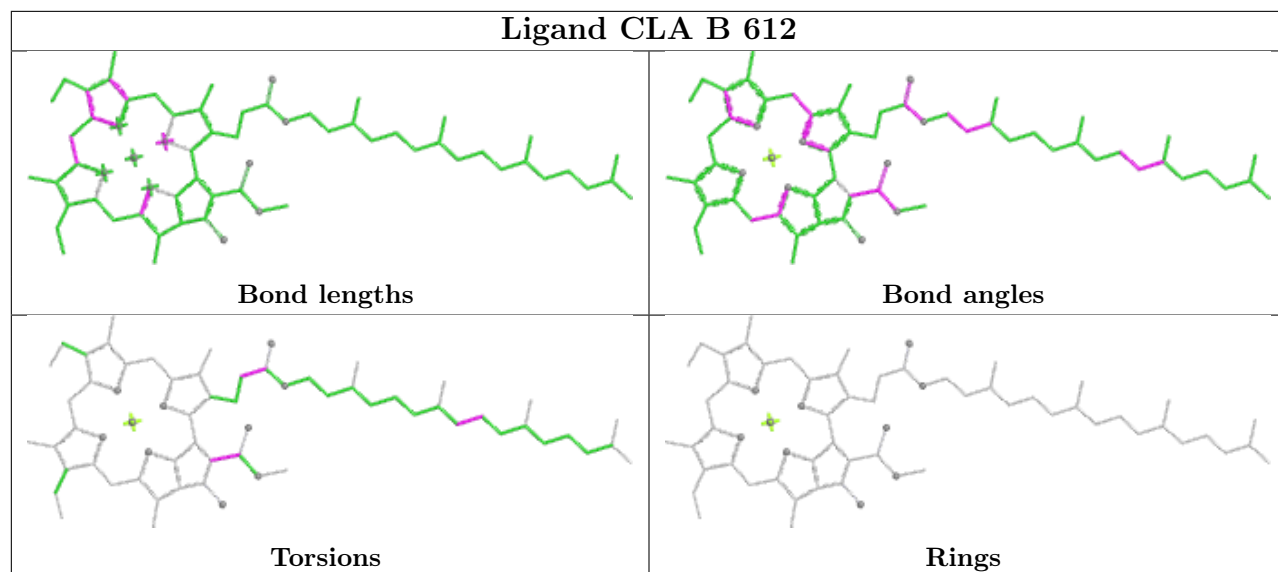
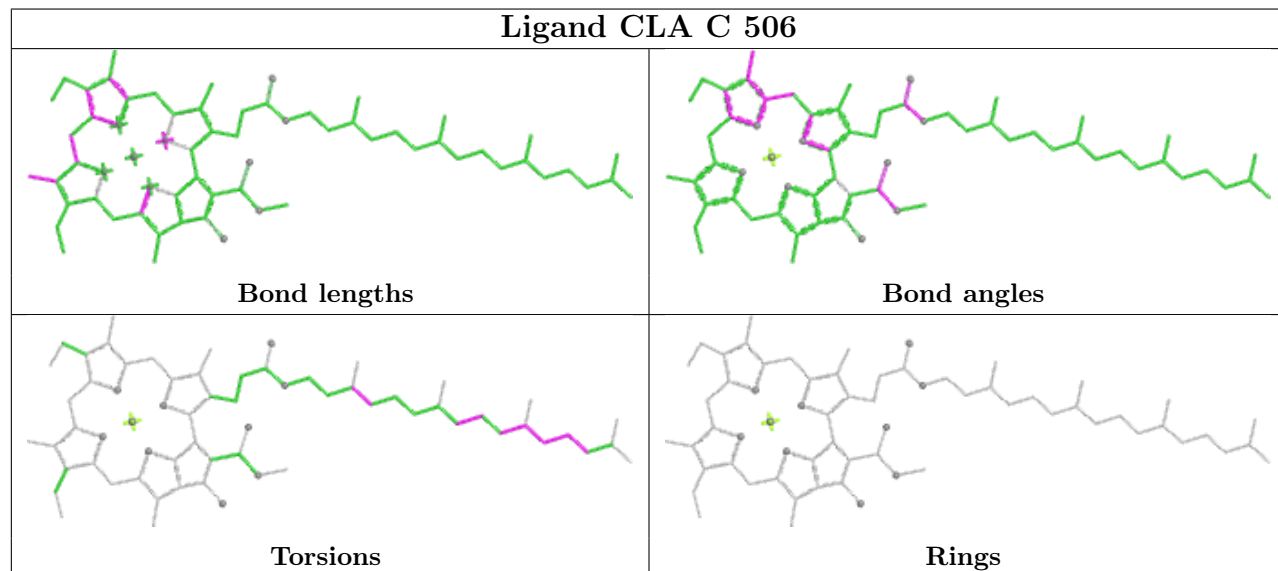
Ligand BCR T 101

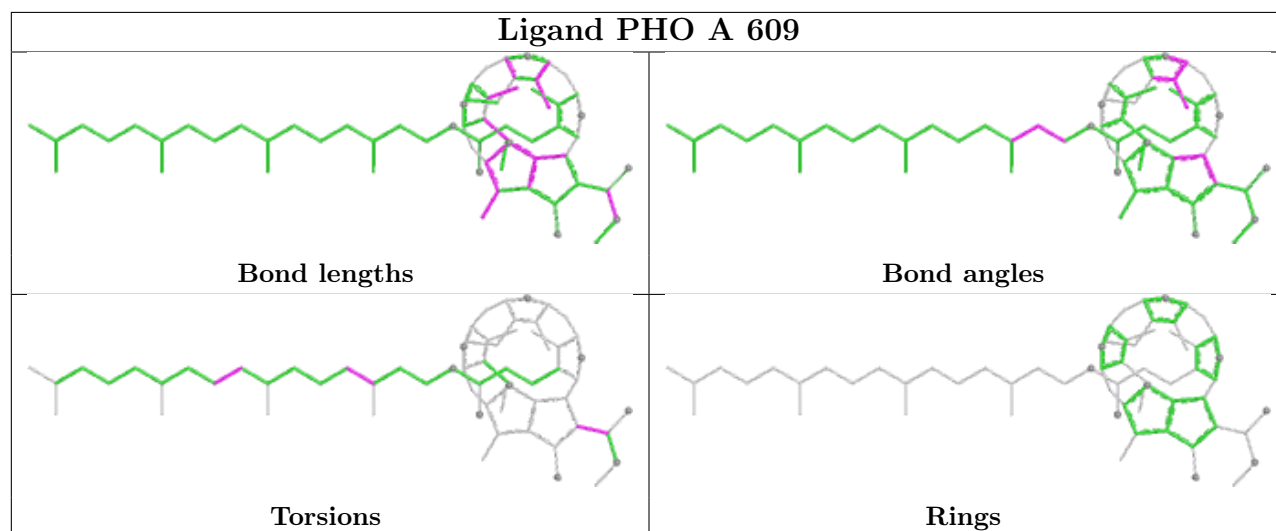
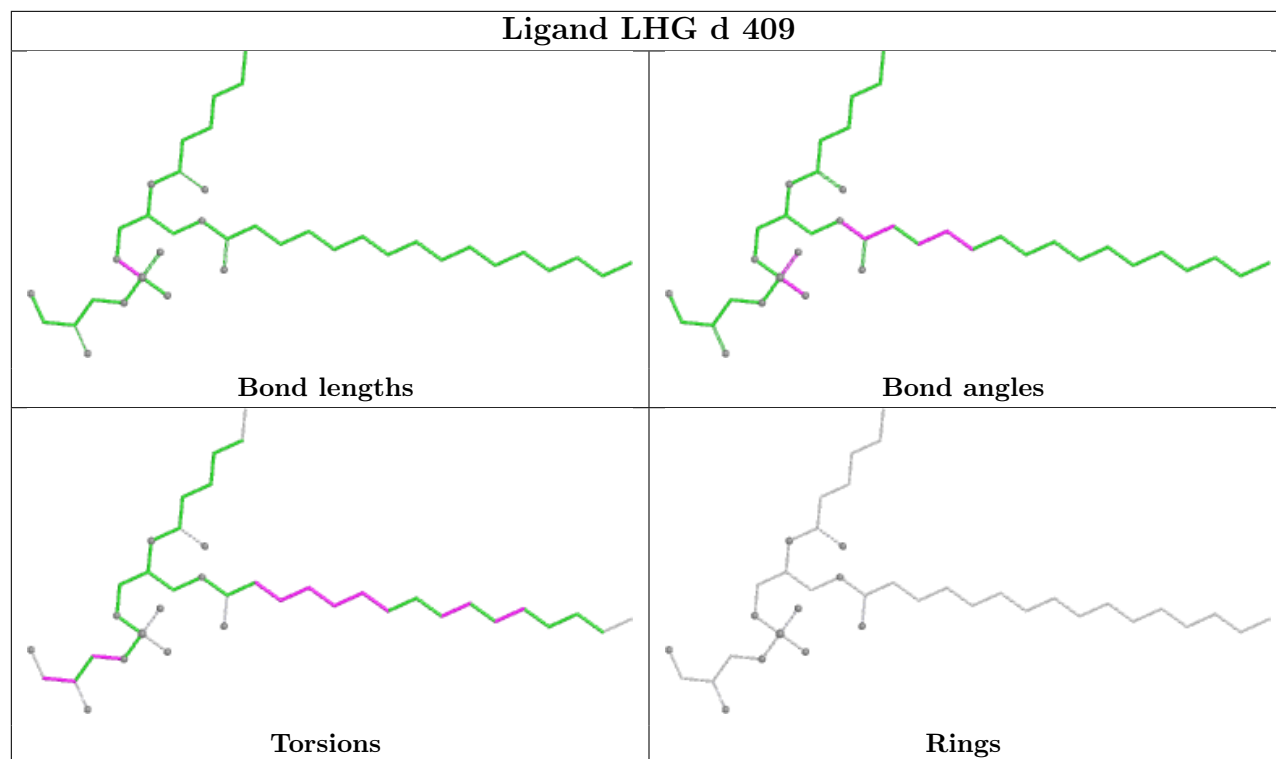




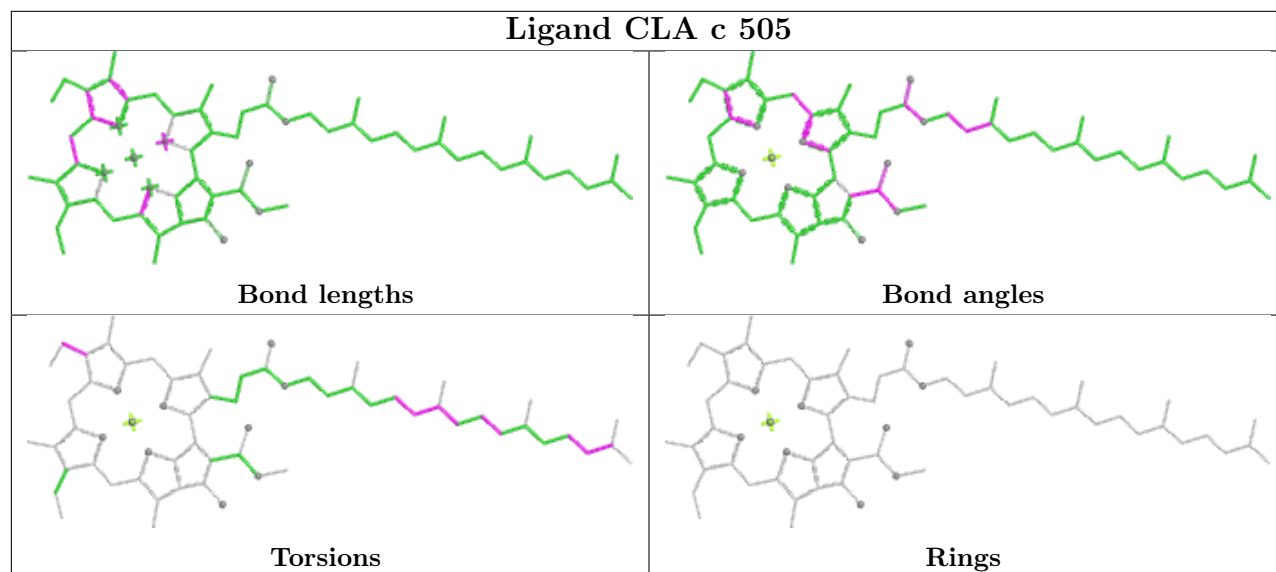
Ligand CLA c 509**Ligand CLA c 511**



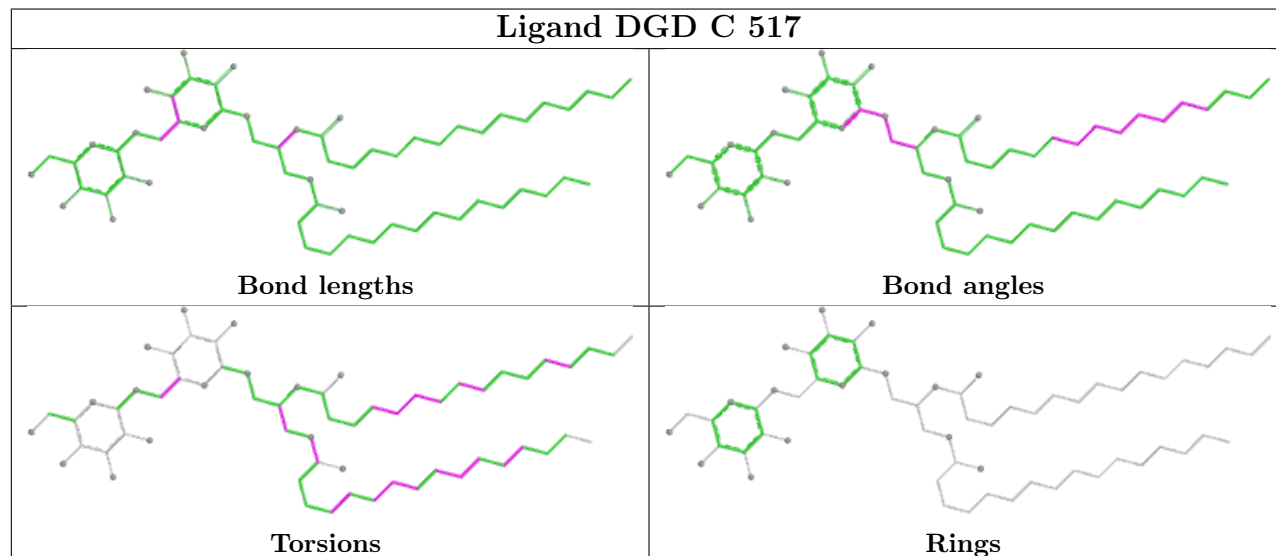
Ligand CLA B 612**Ligand CLA C 506**

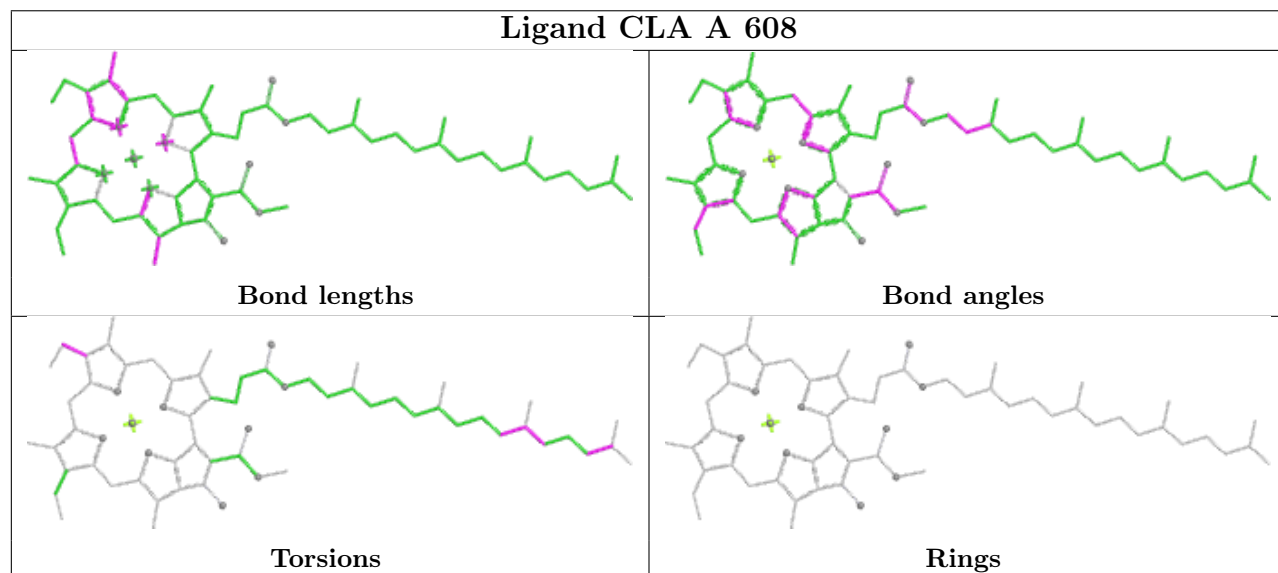
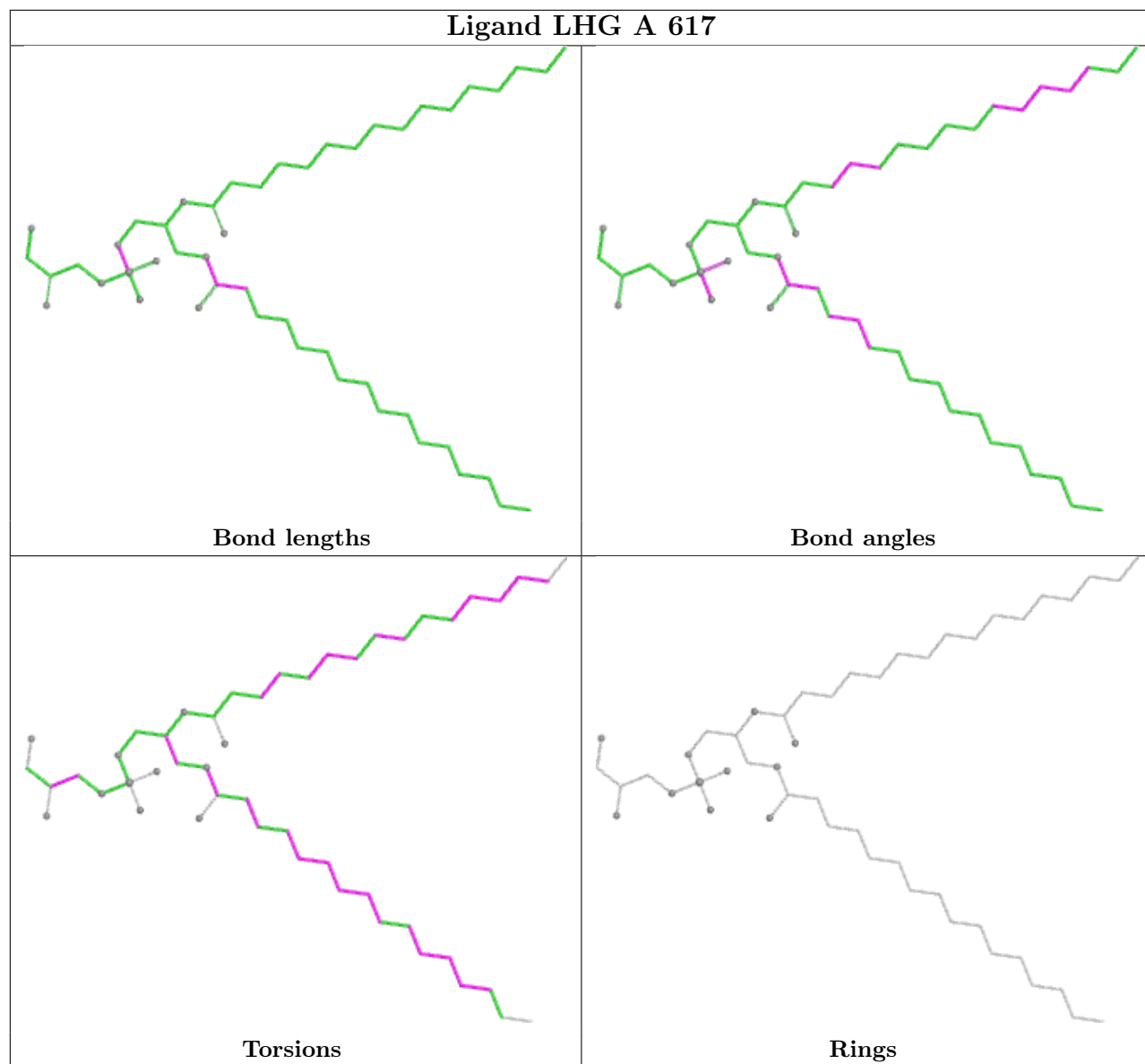


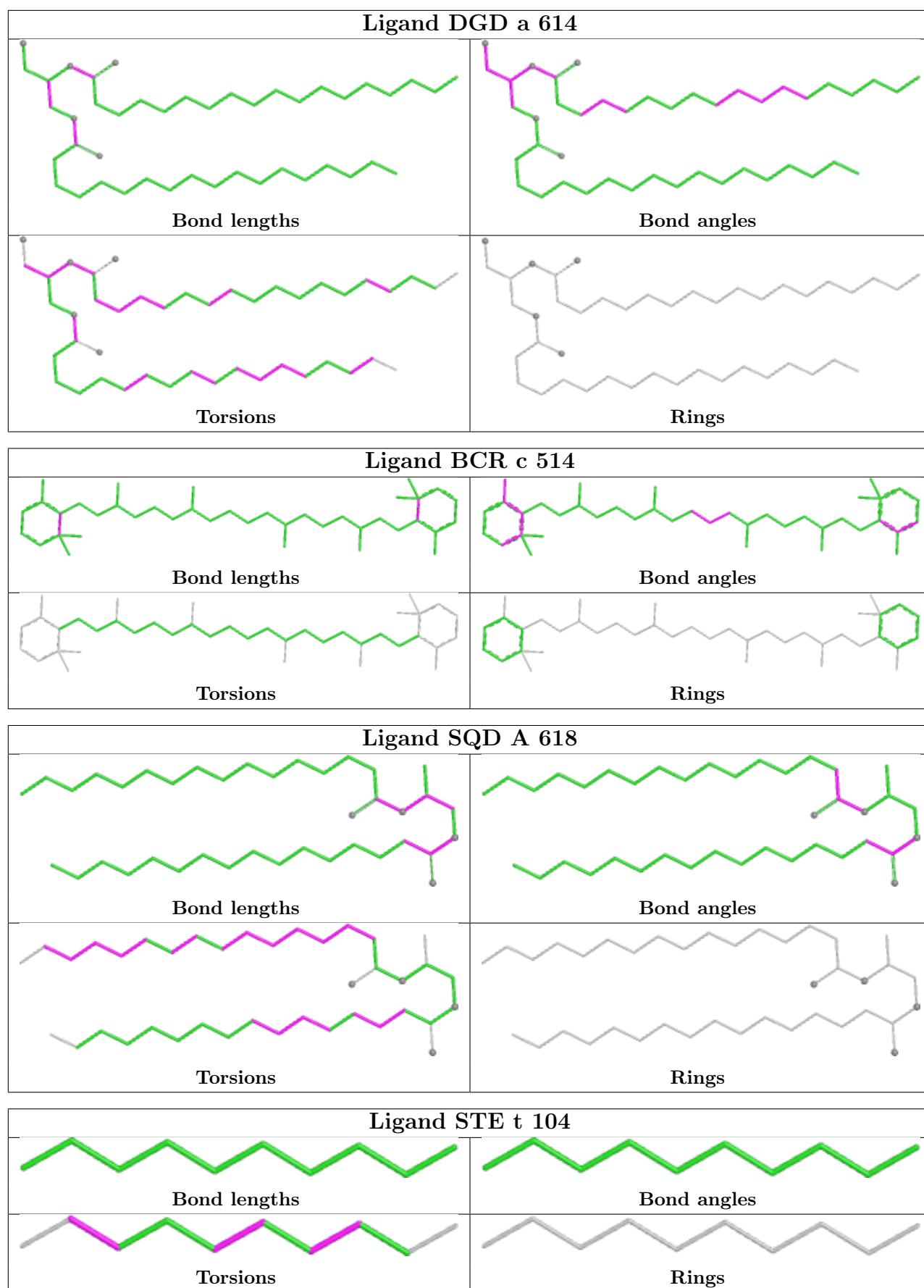
Ligand CLA c 505

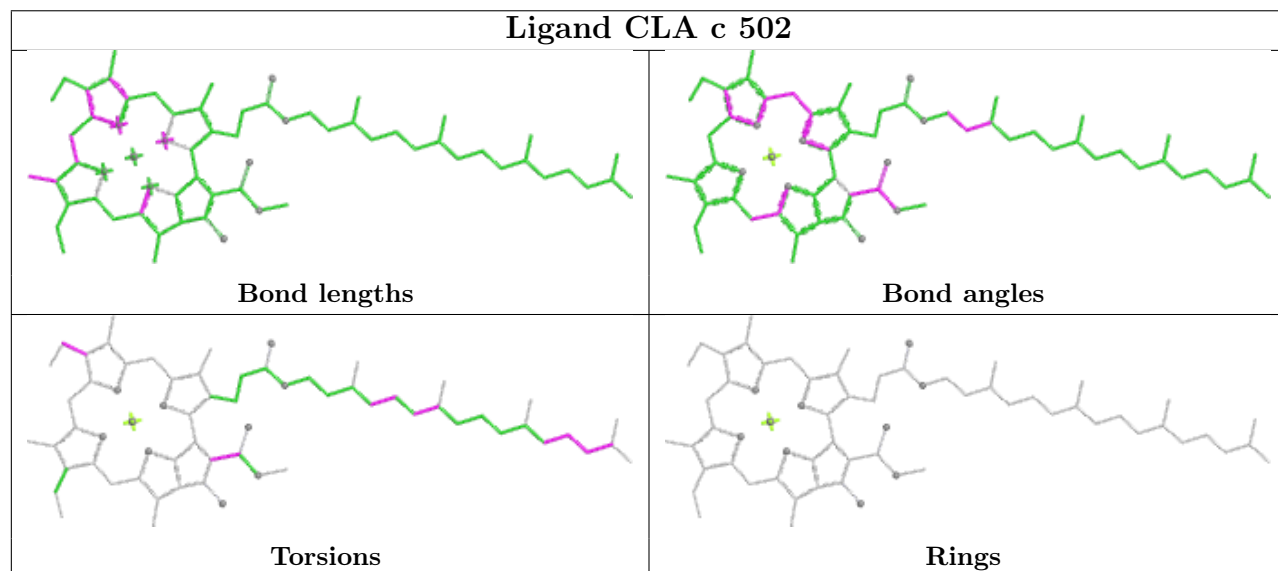
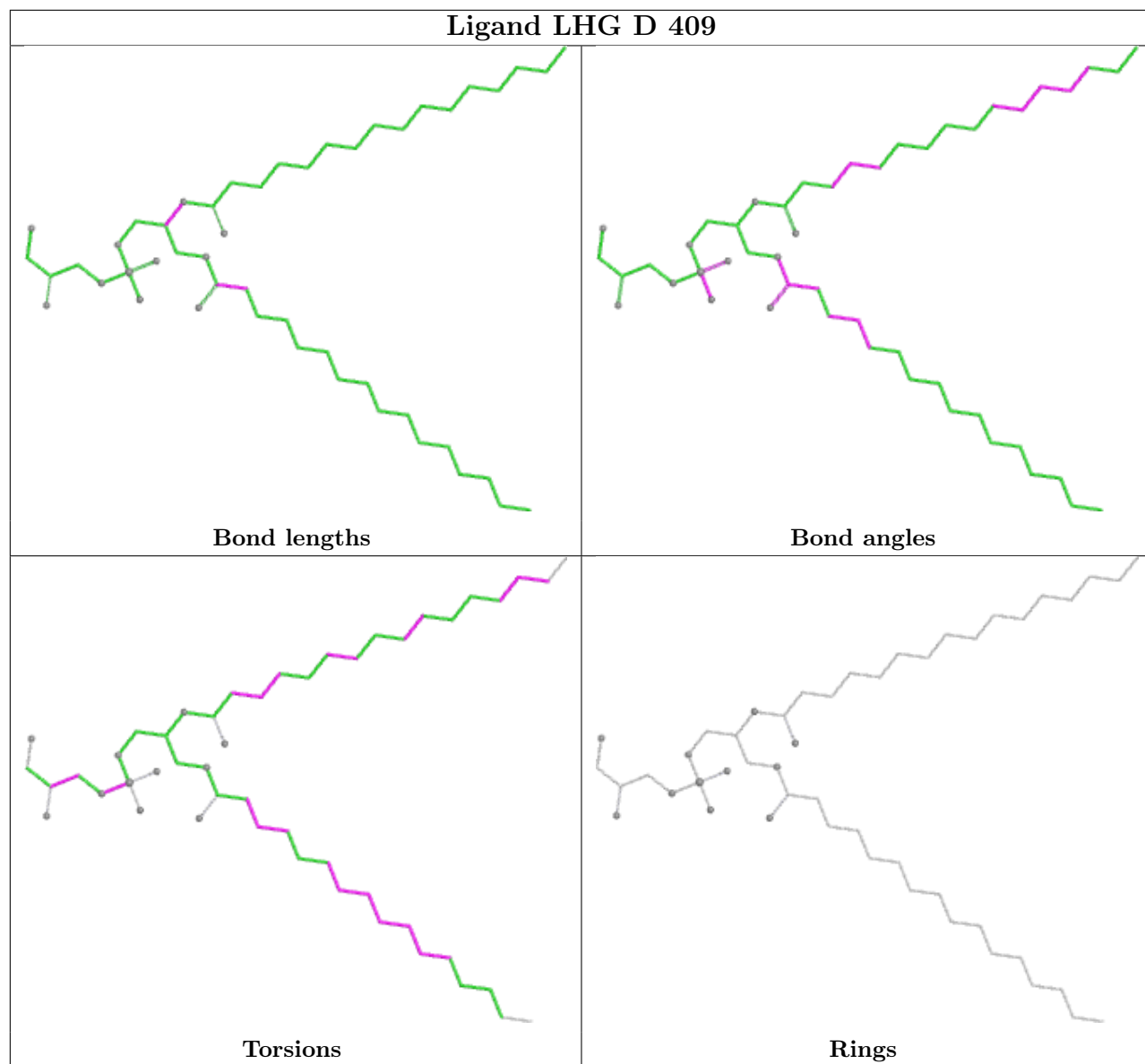


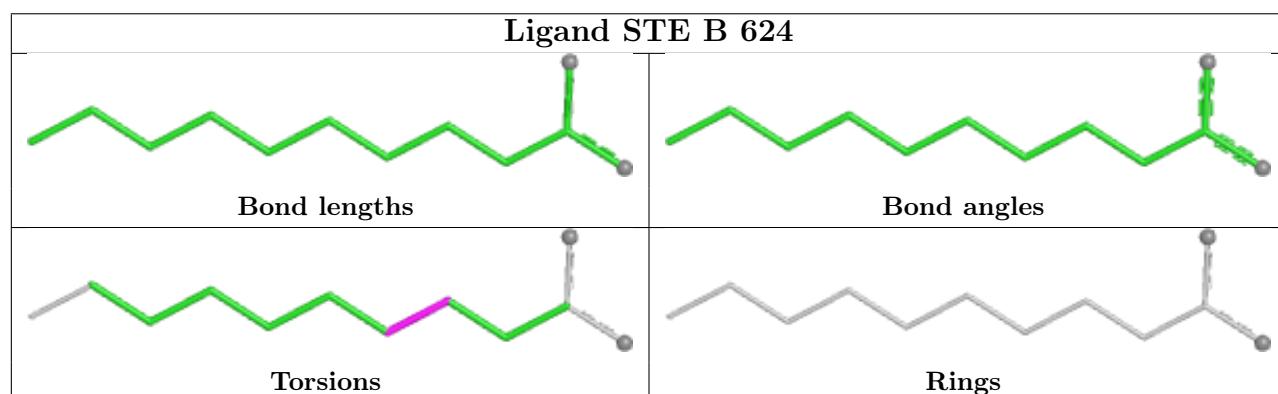
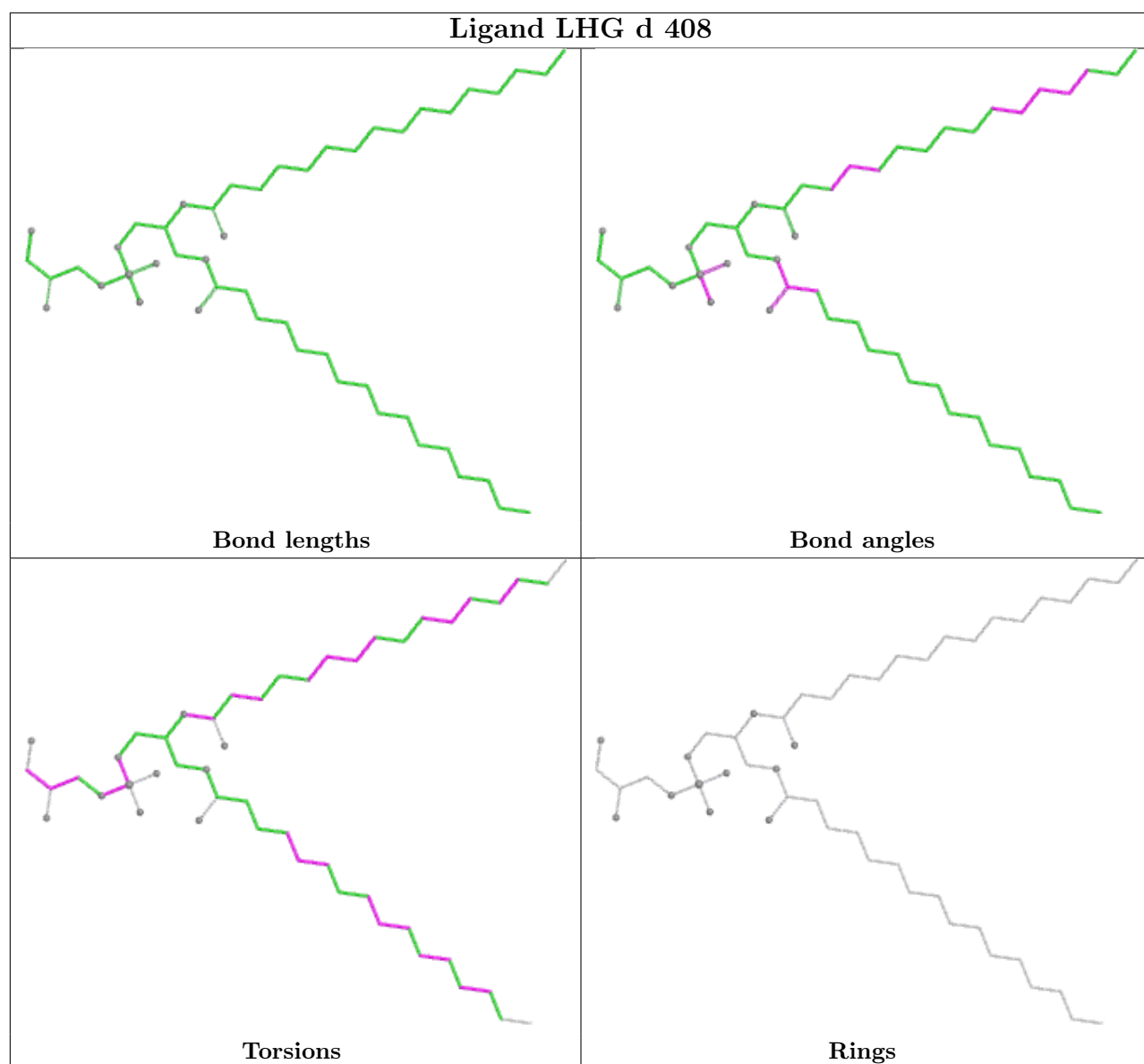
Ligand DGD C 517



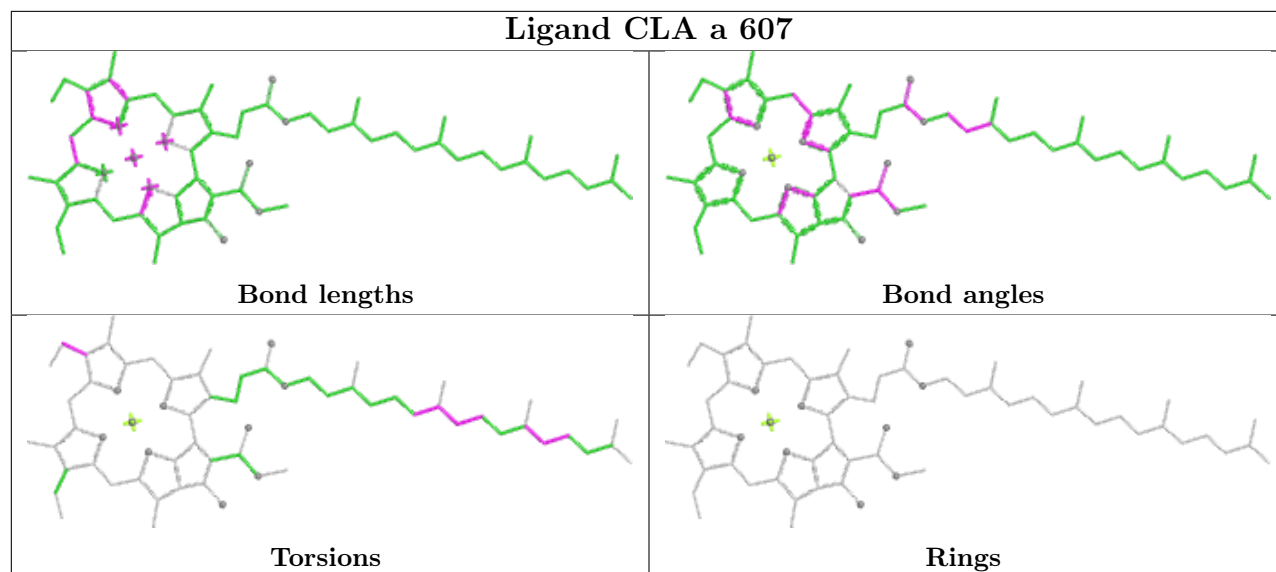




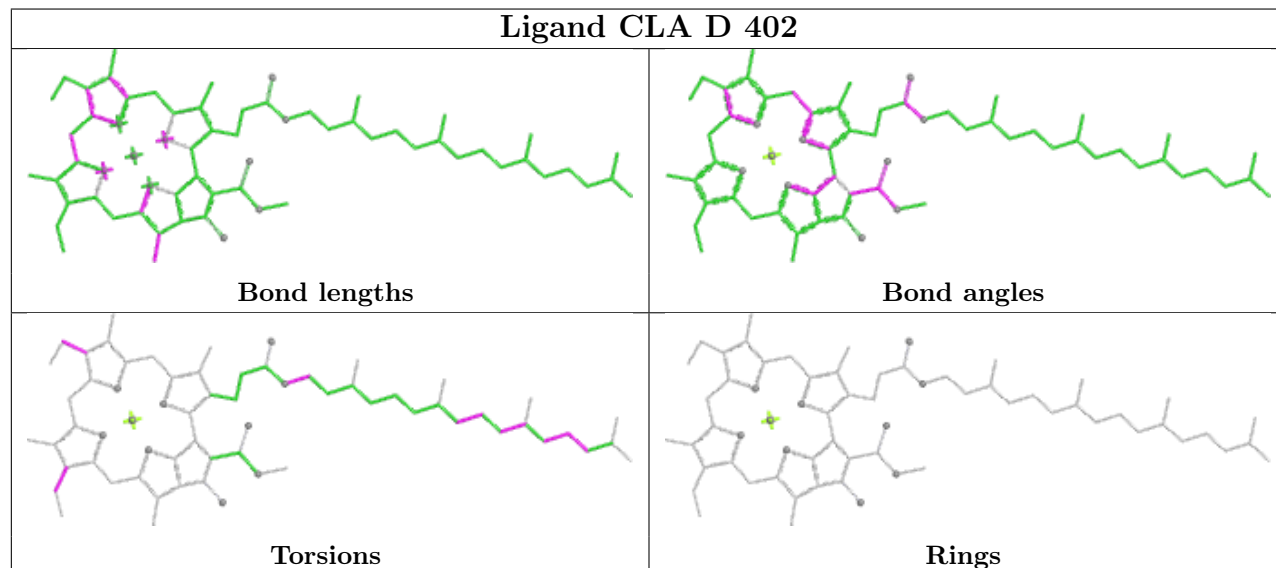




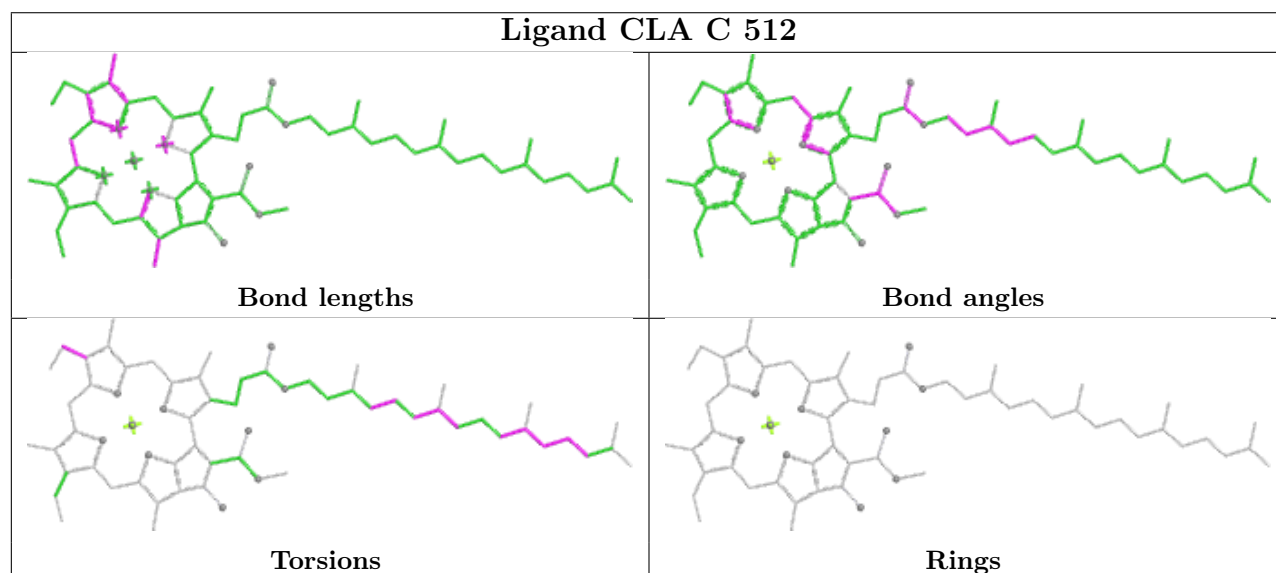
Ligand CLA a 607

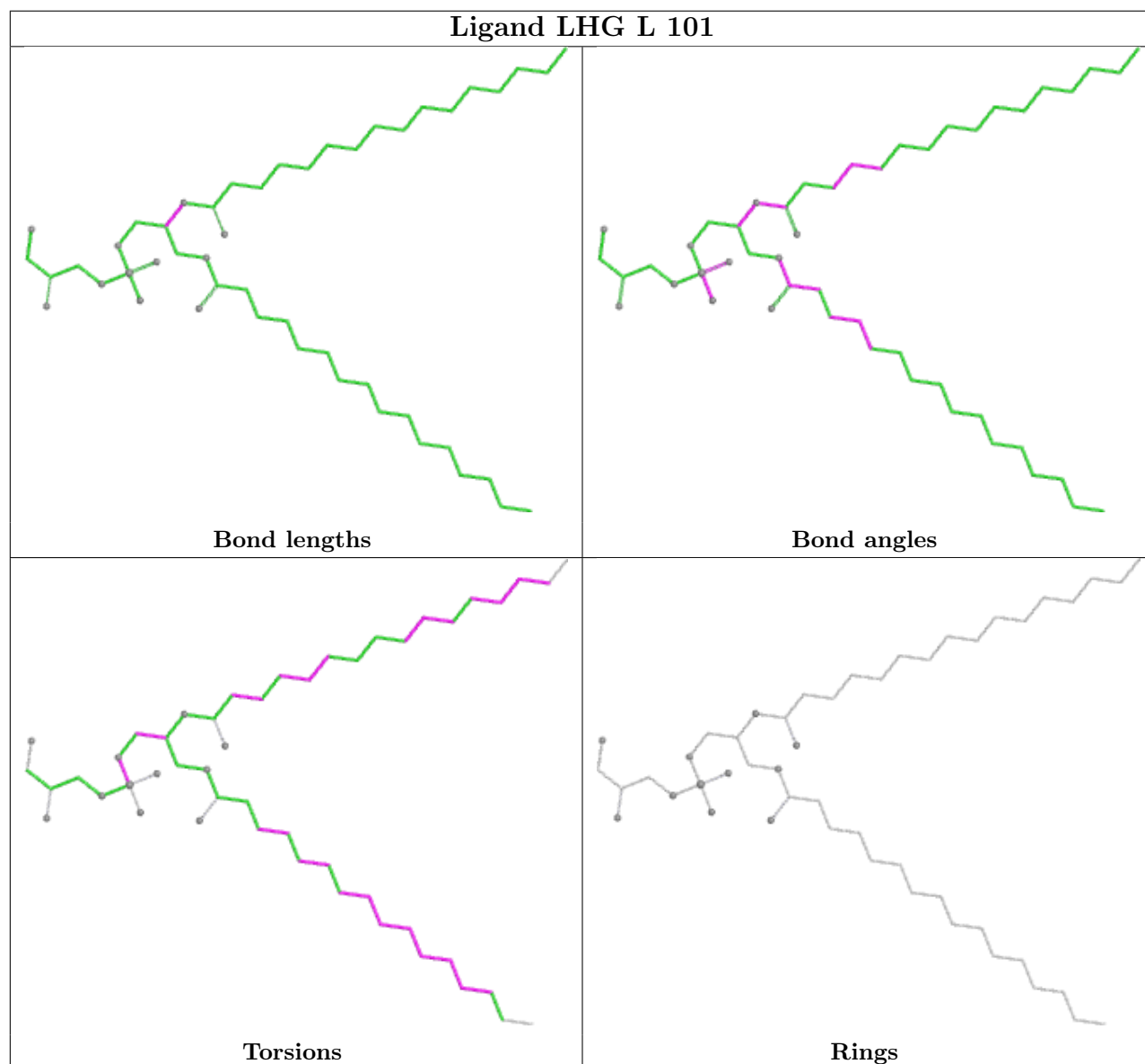
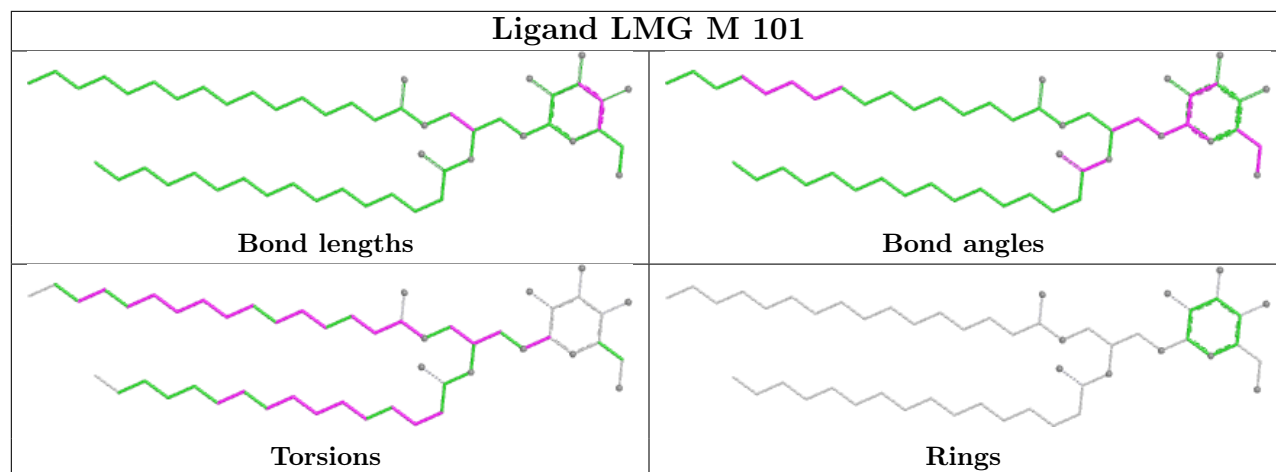


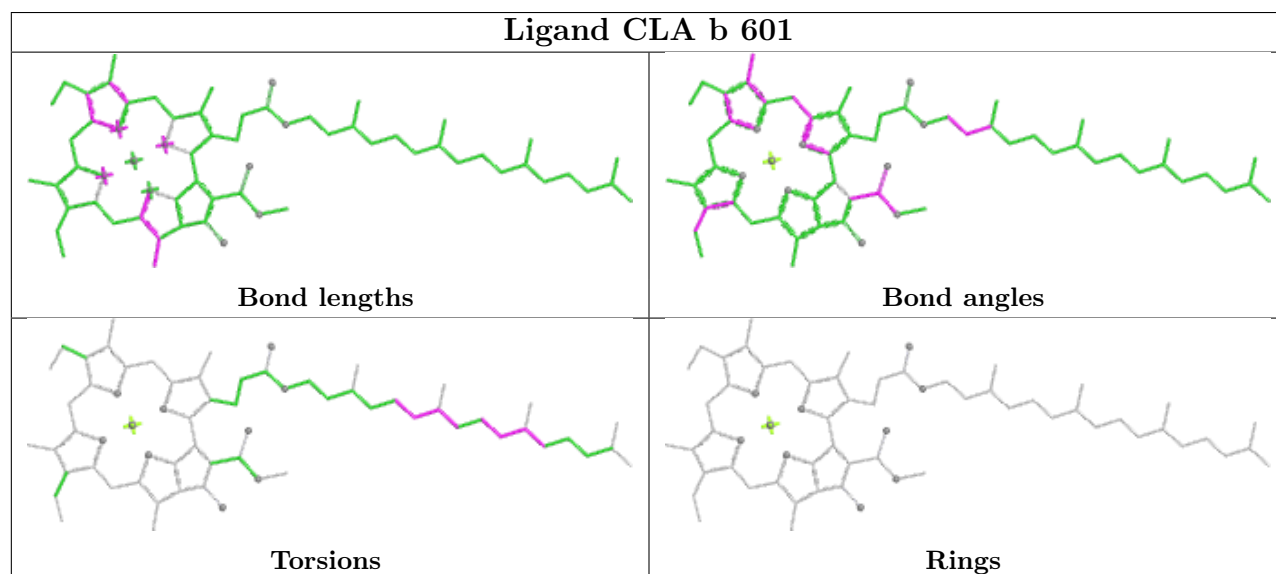
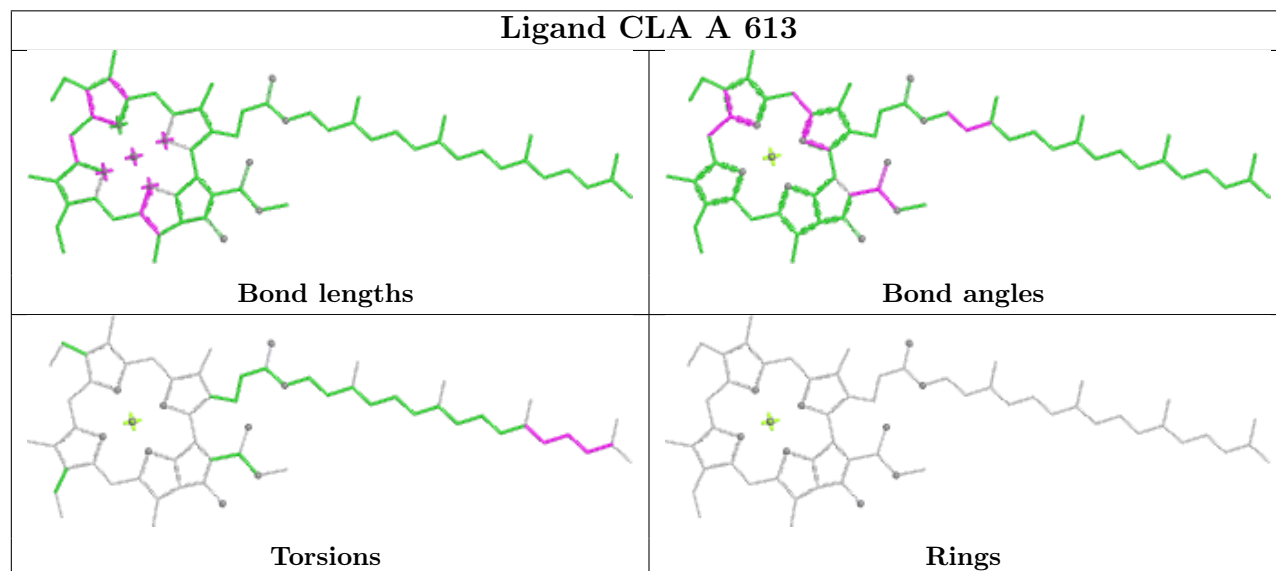
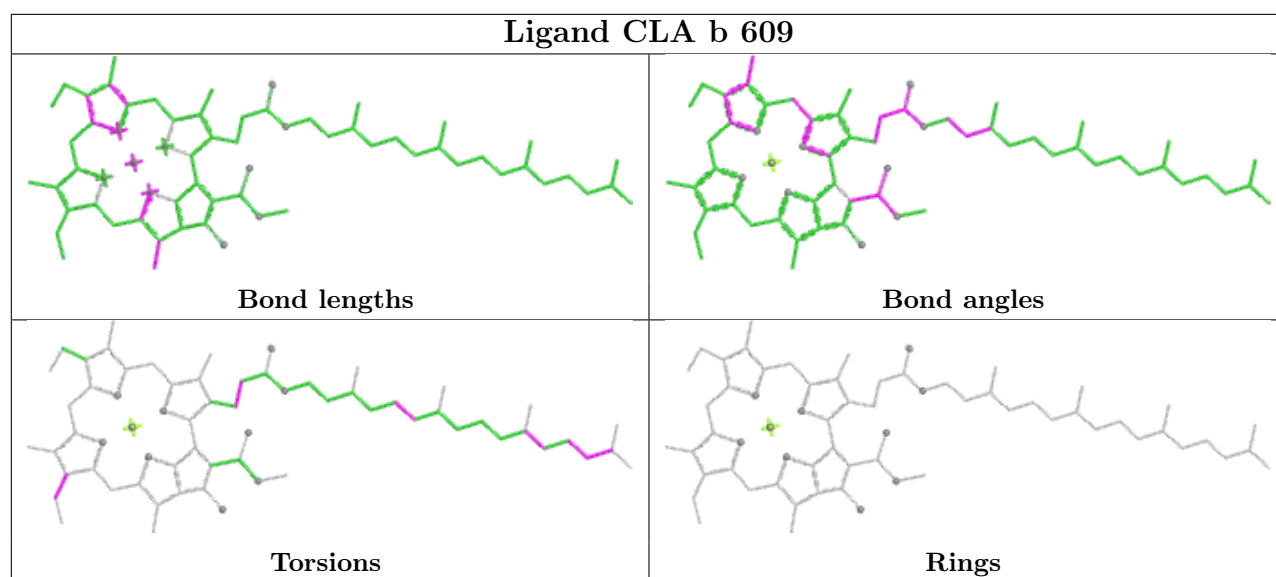
Ligand CLA D 402

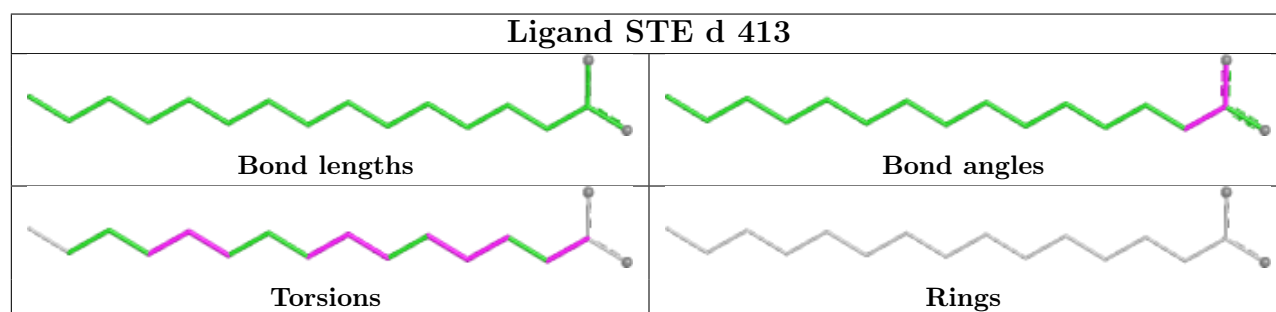
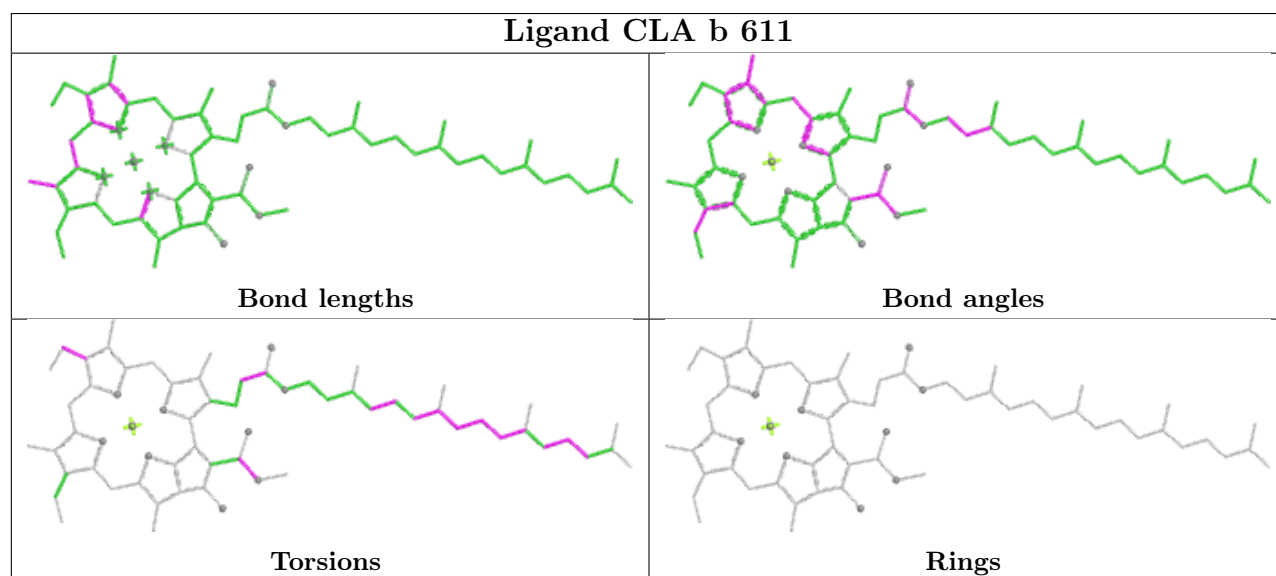
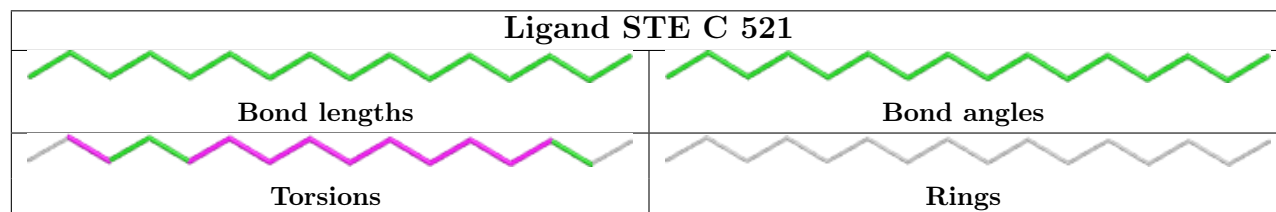
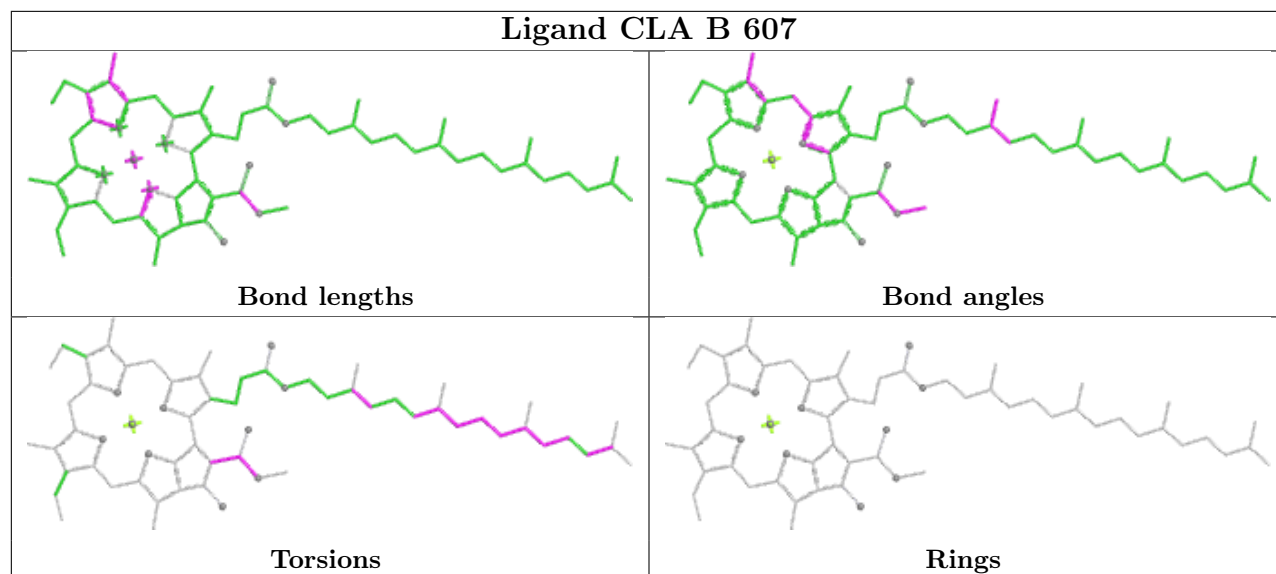


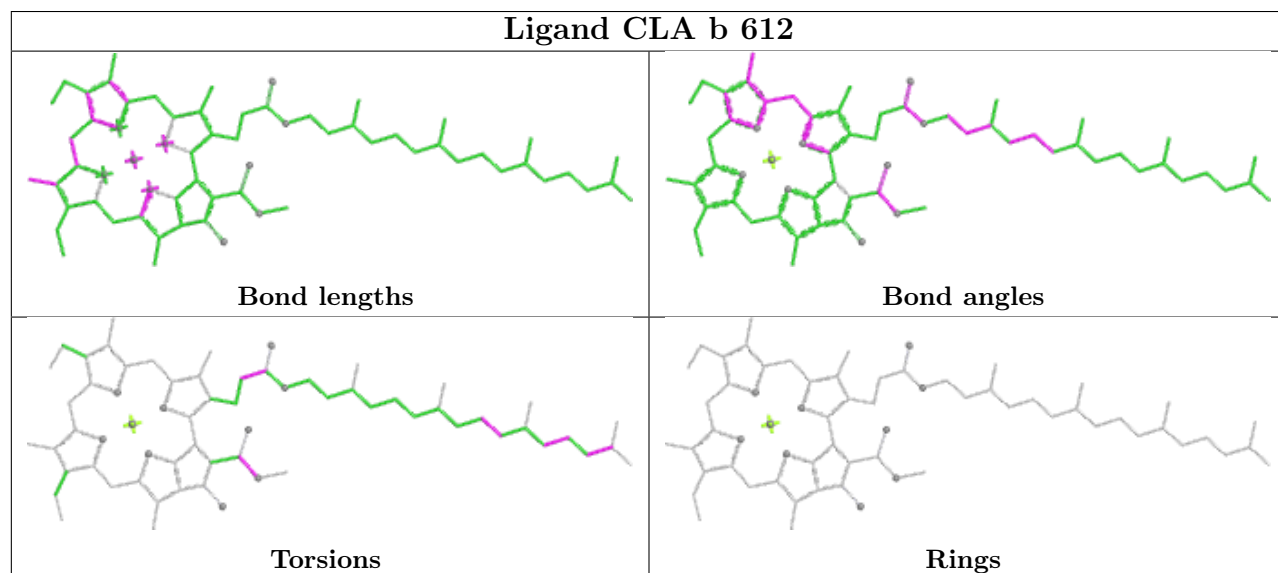
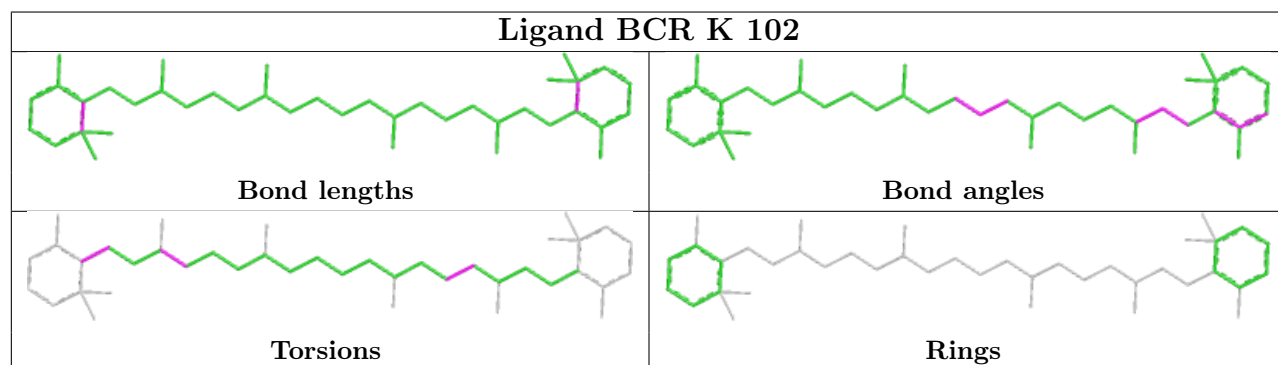
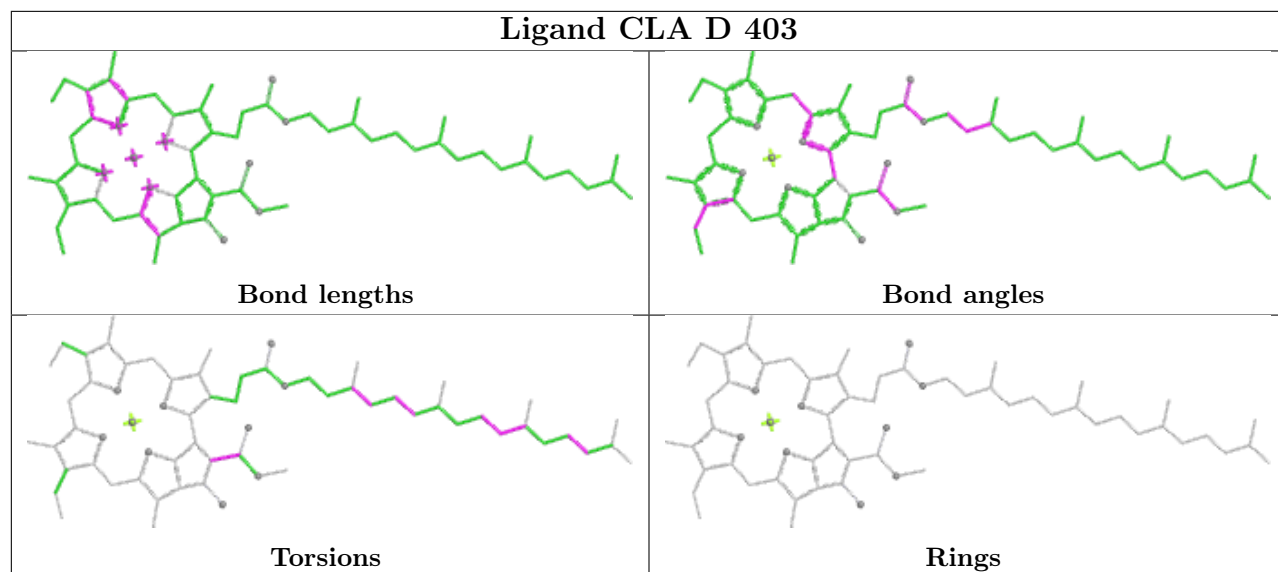
Ligand CLA C 512

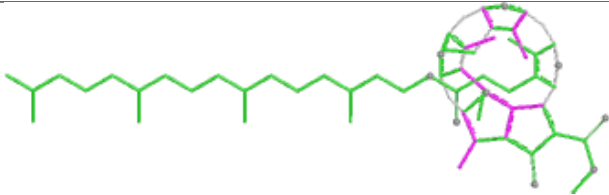
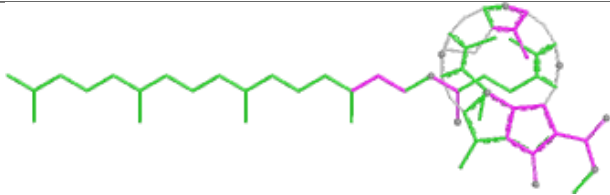
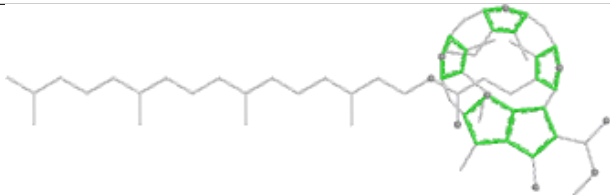
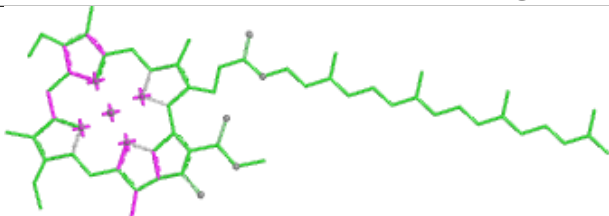
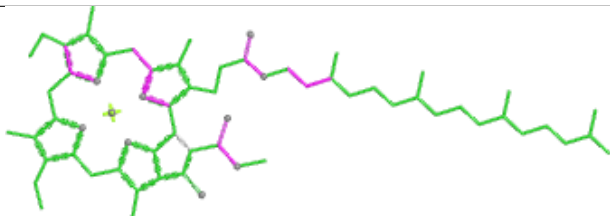
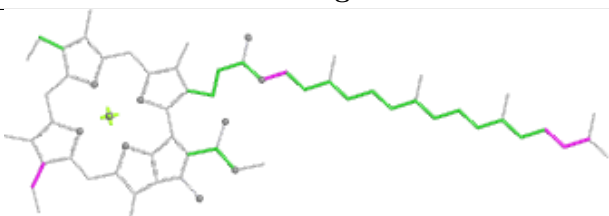
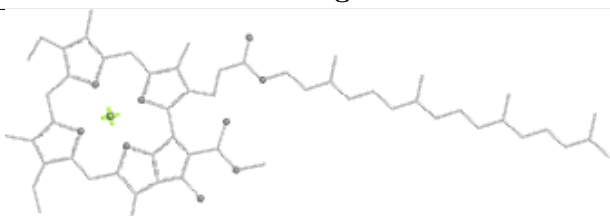
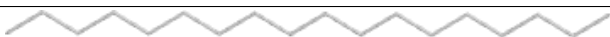




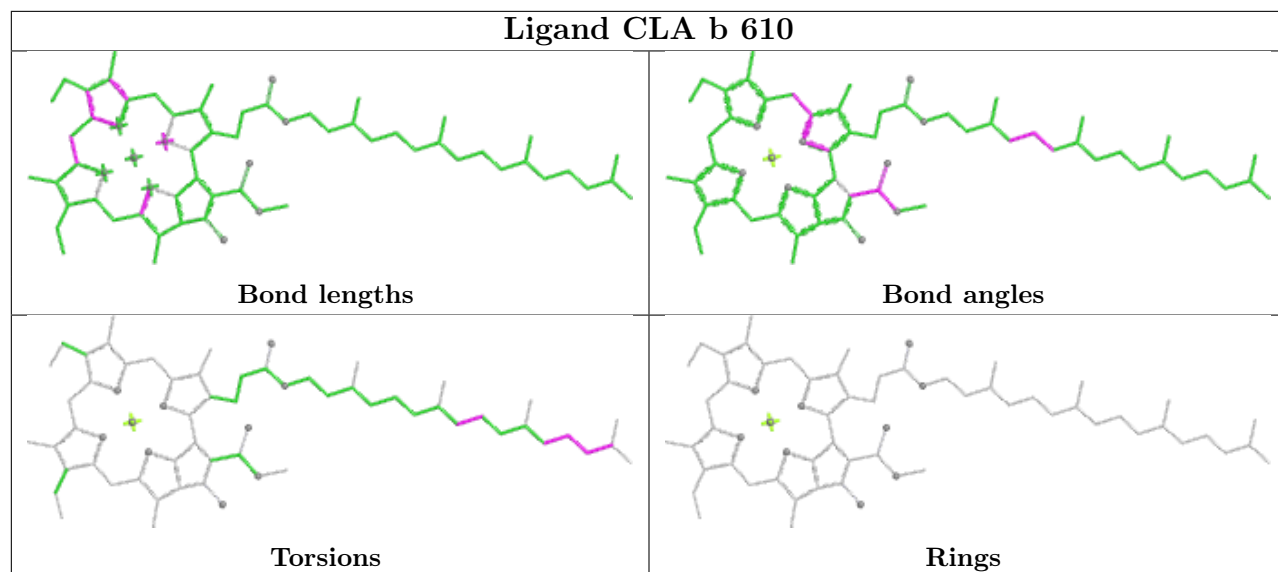




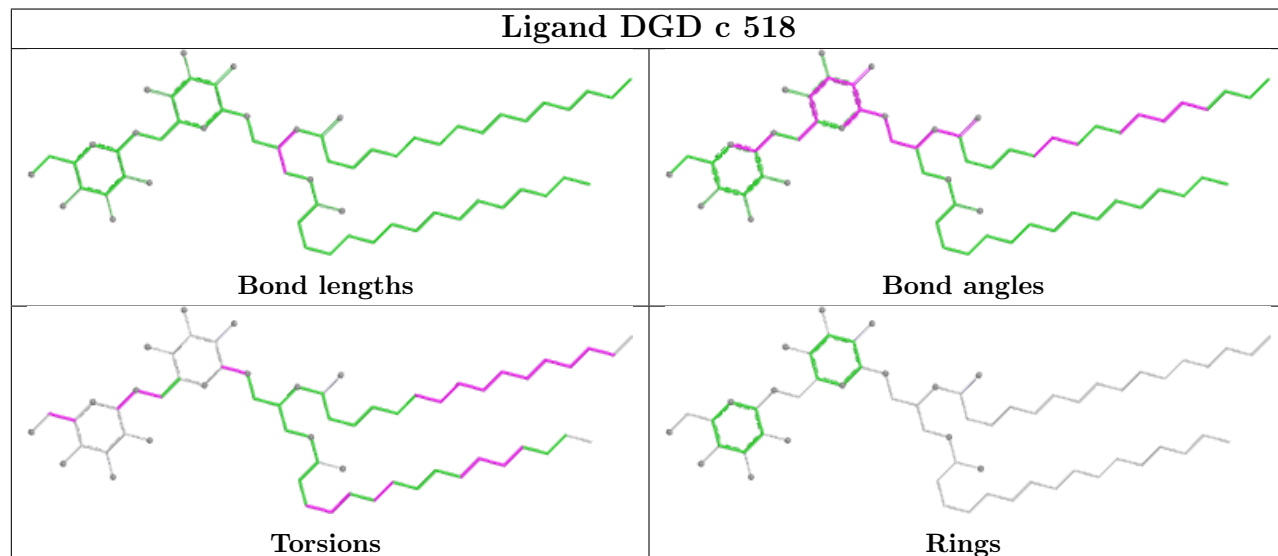


Ligand PHO D 401	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA a 606	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand STE l 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

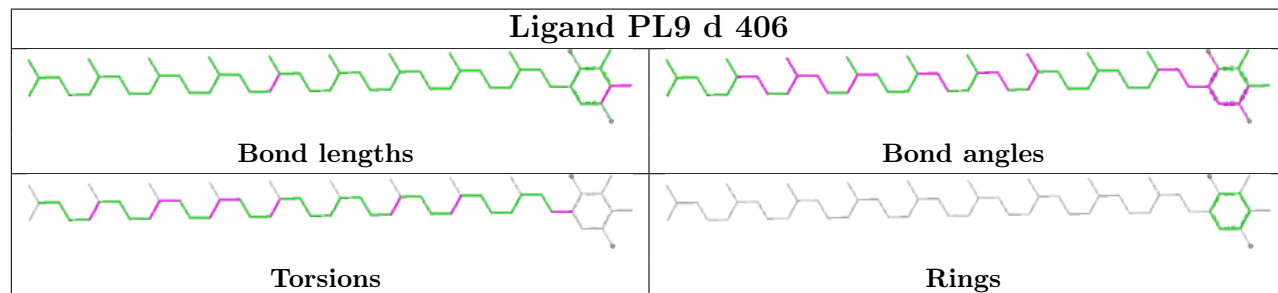
Ligand CLA b 610



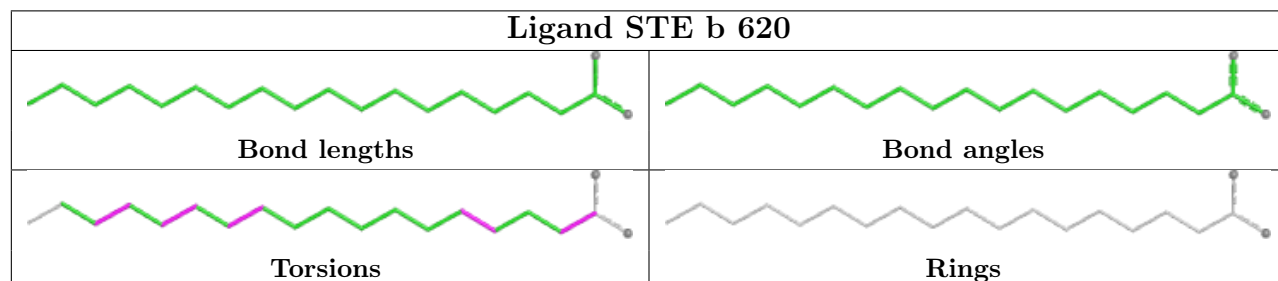
Ligand DGD c 518

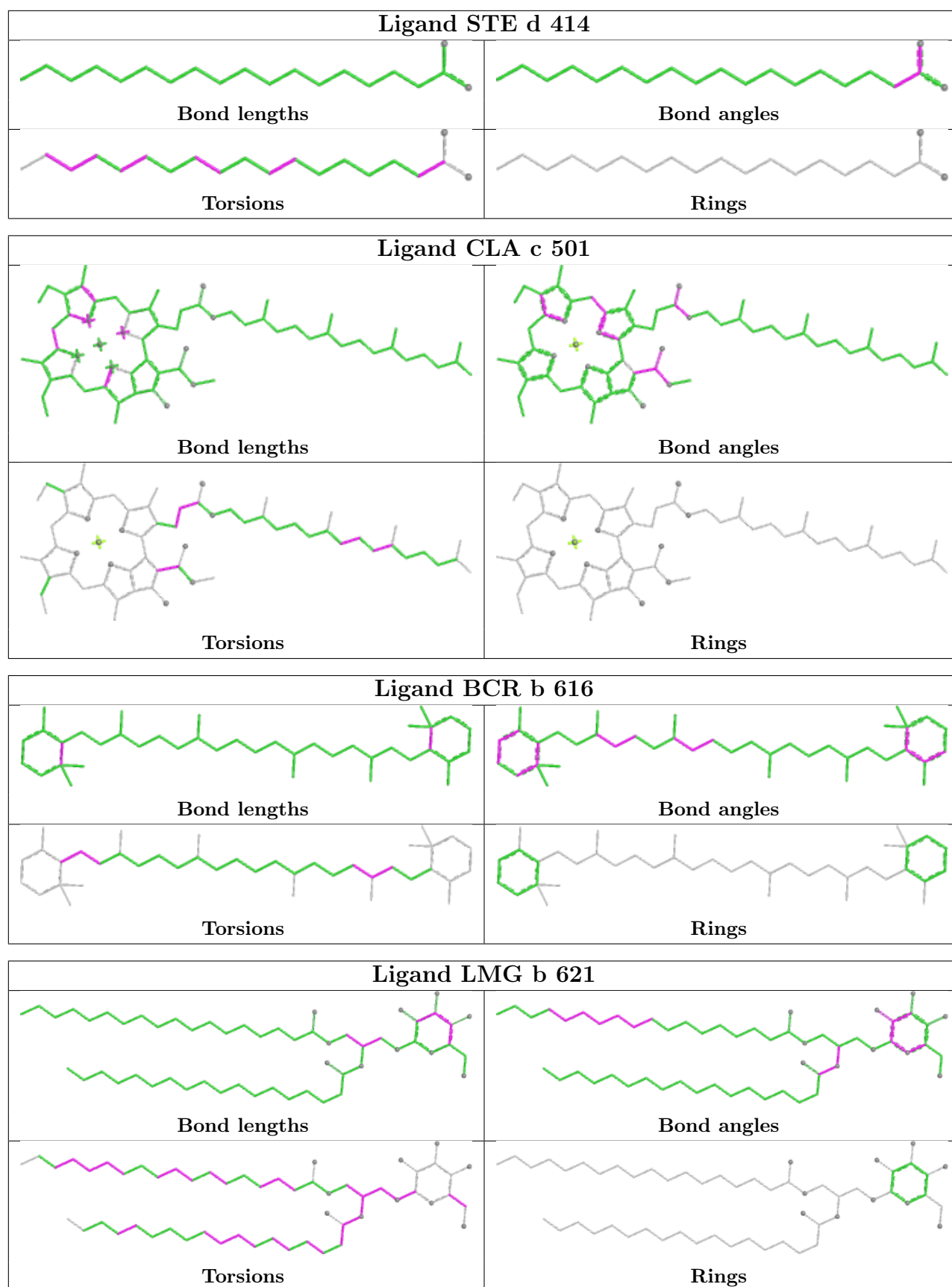


Ligand PL9 d 406

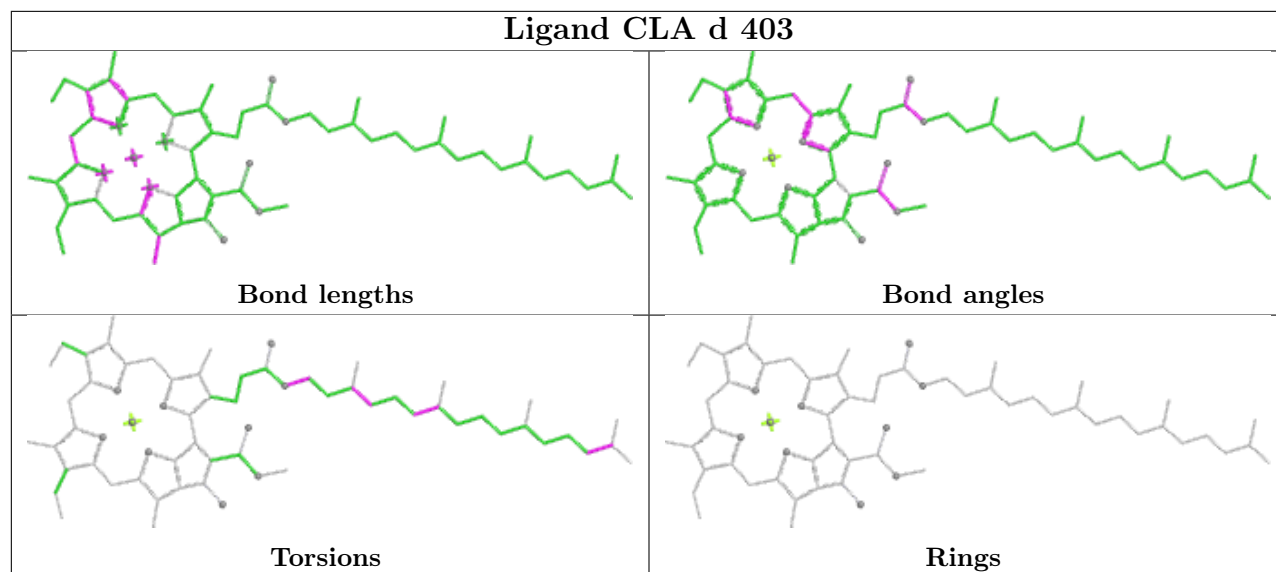


Ligand STE b 620

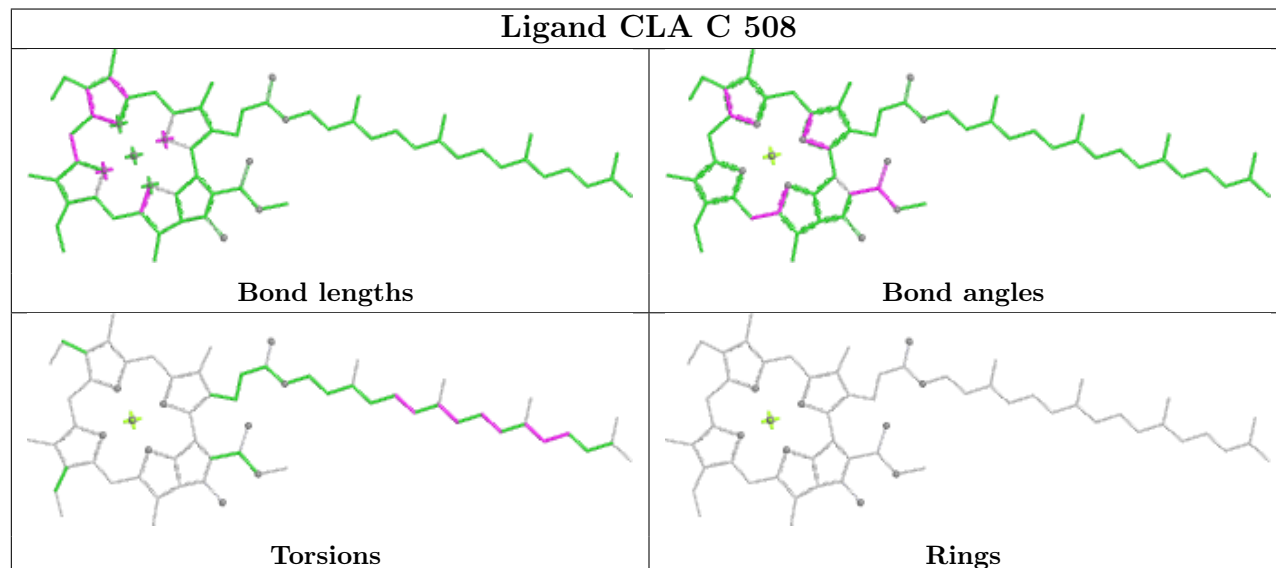




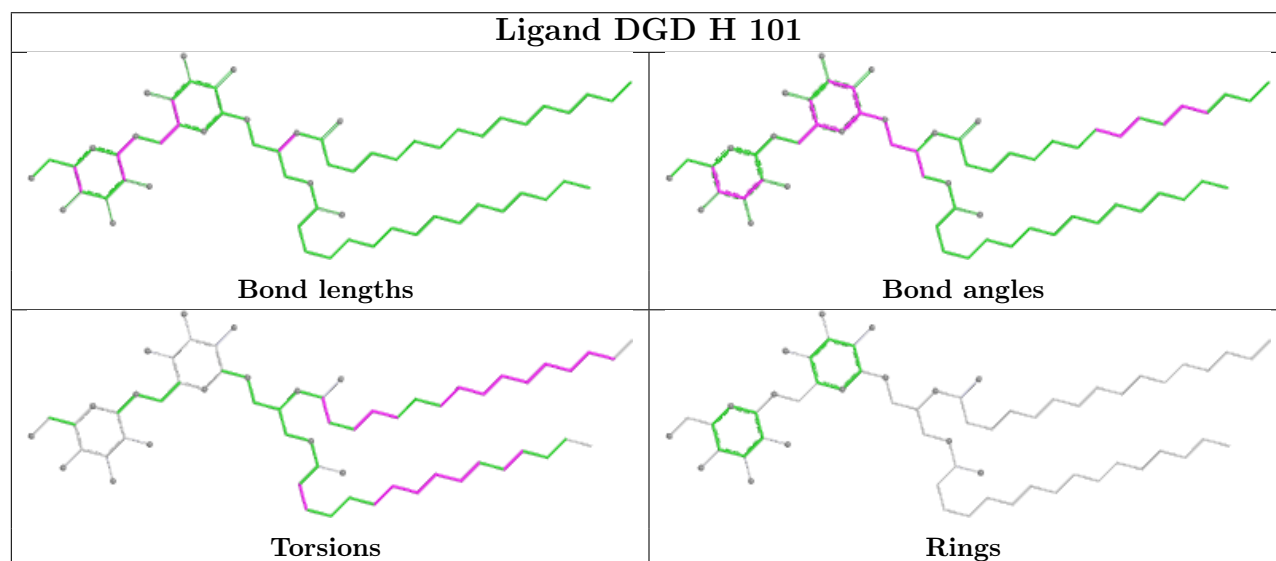
Ligand CLA d 403

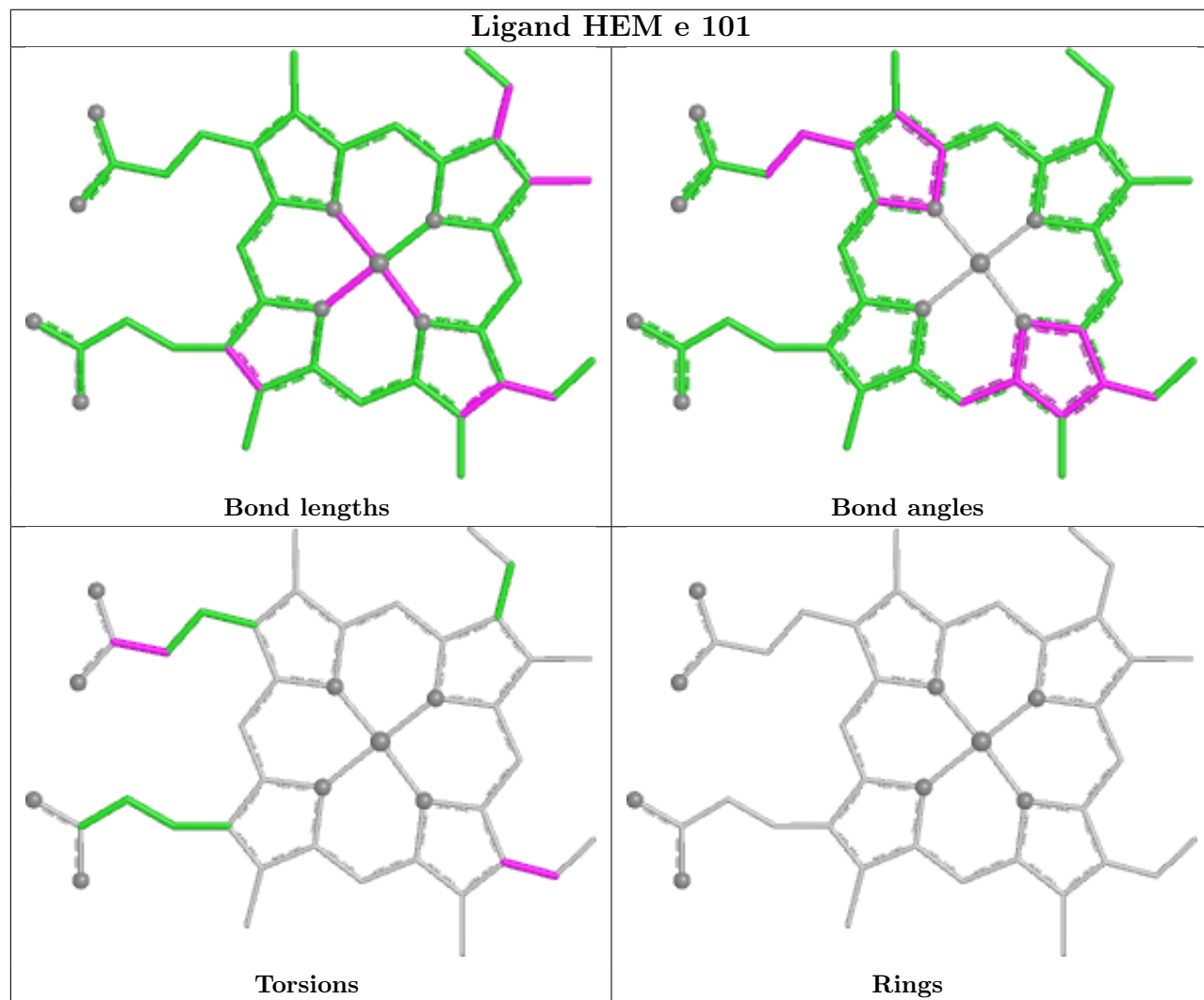
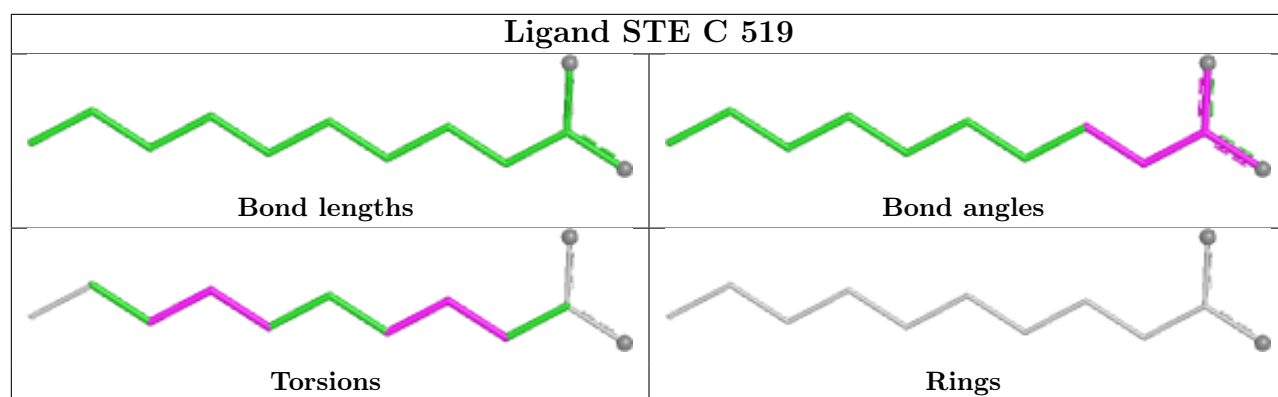


Ligand CLA C 508

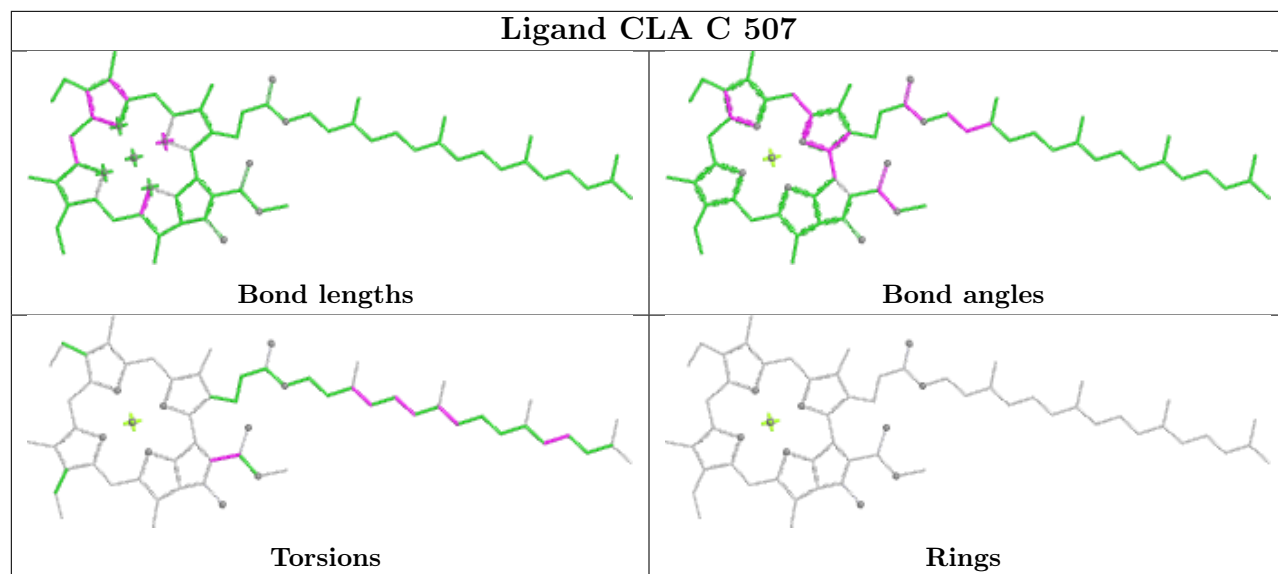


Ligand DGD H 101

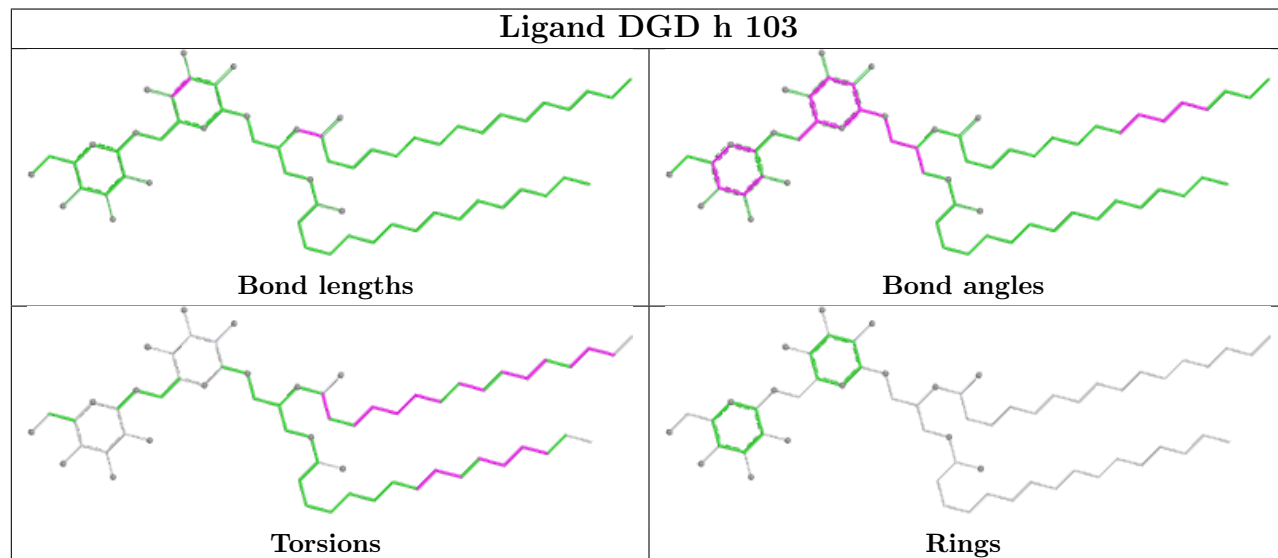




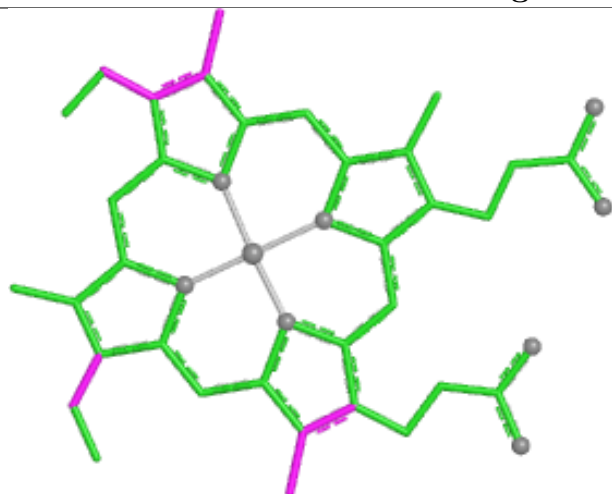
Ligand CLA C 507



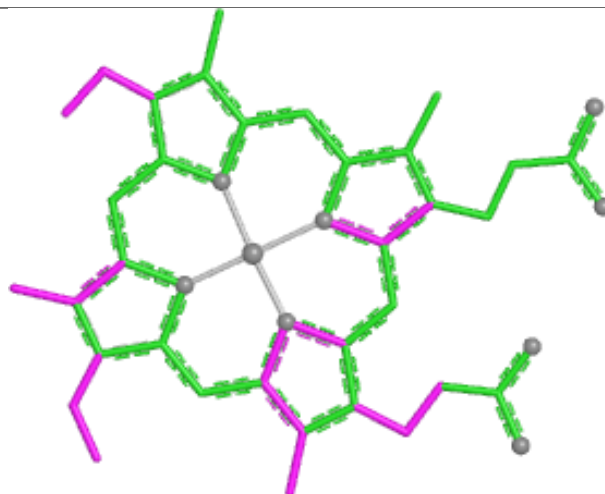
Ligand DGD h 103



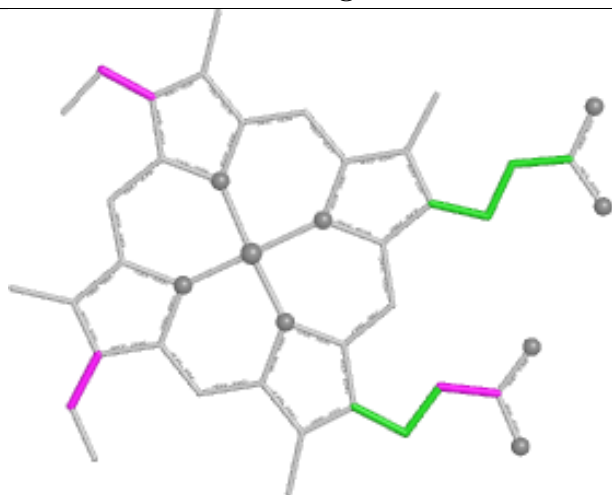
Ligand HEC V 201



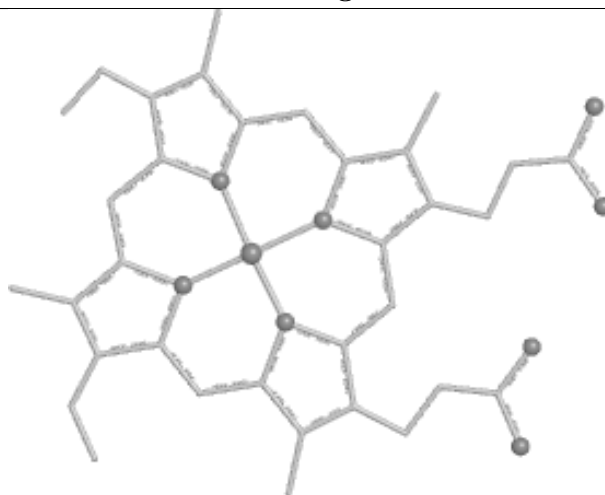
Bond lengths



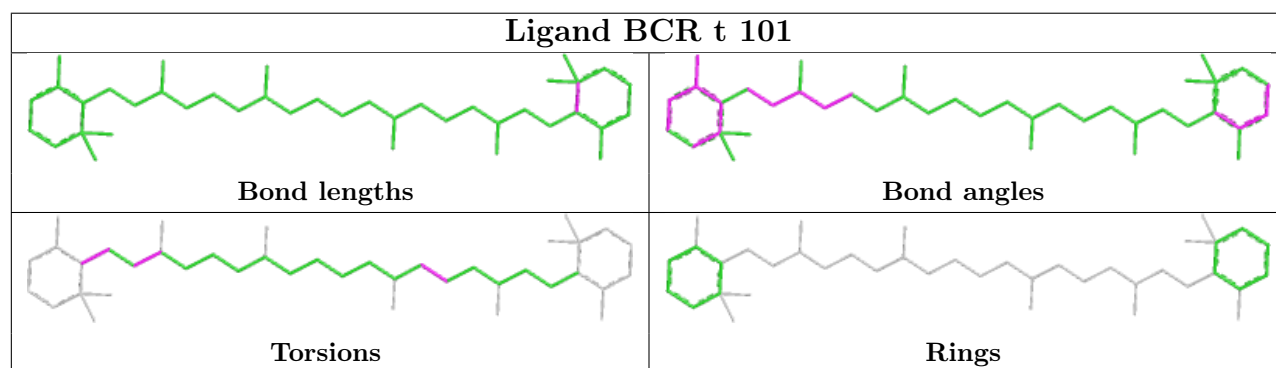
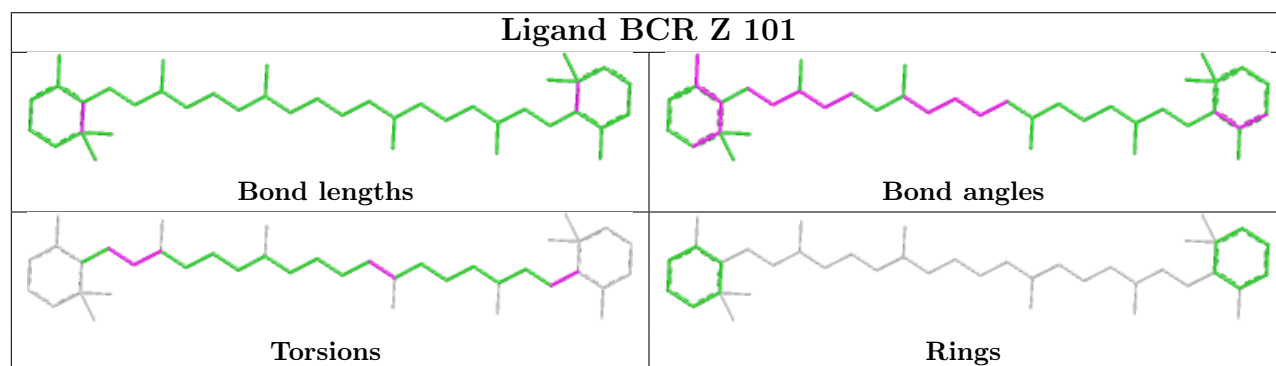
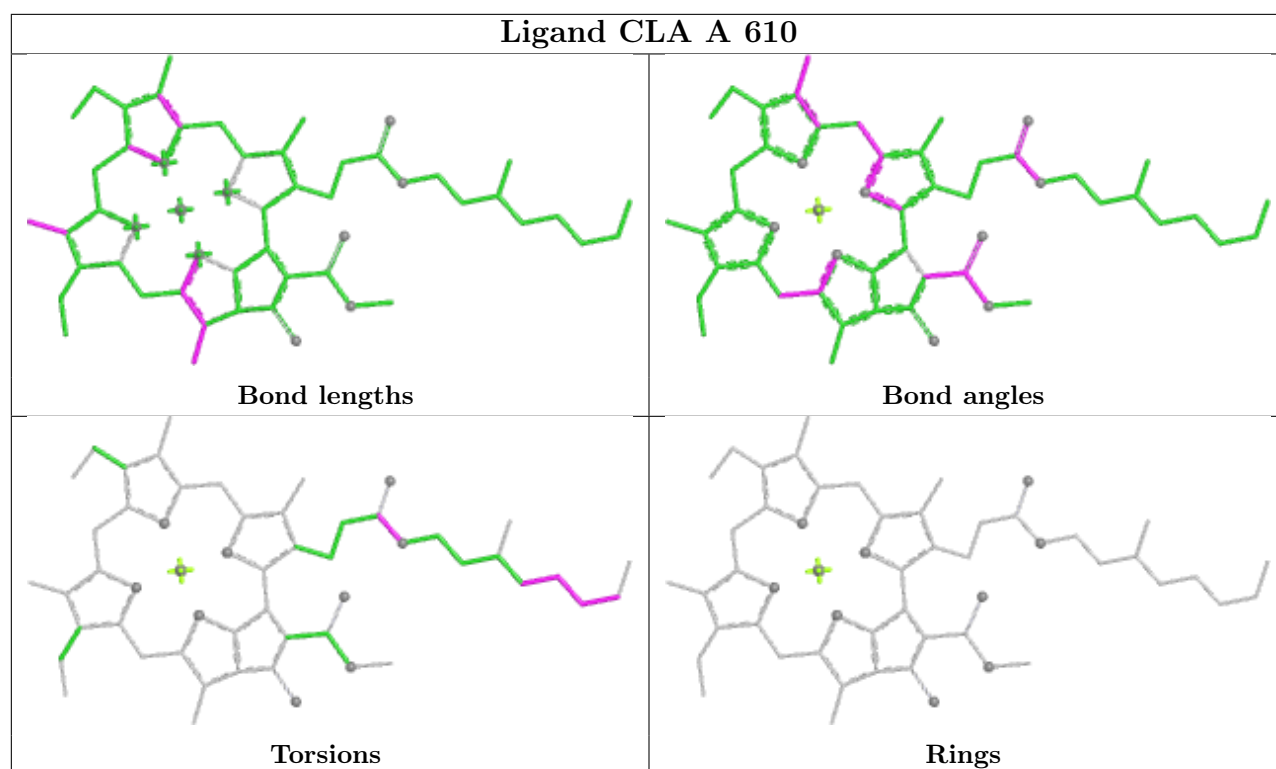
Bond angles

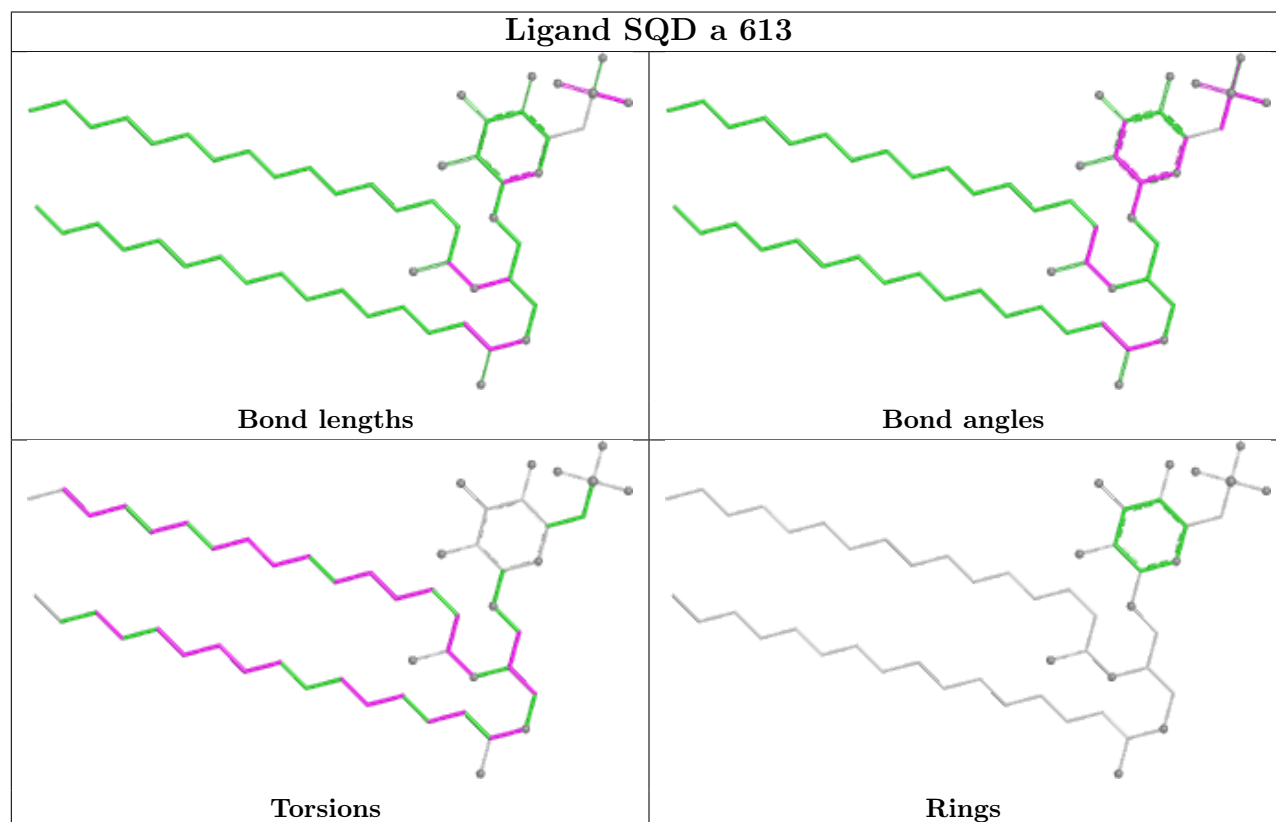
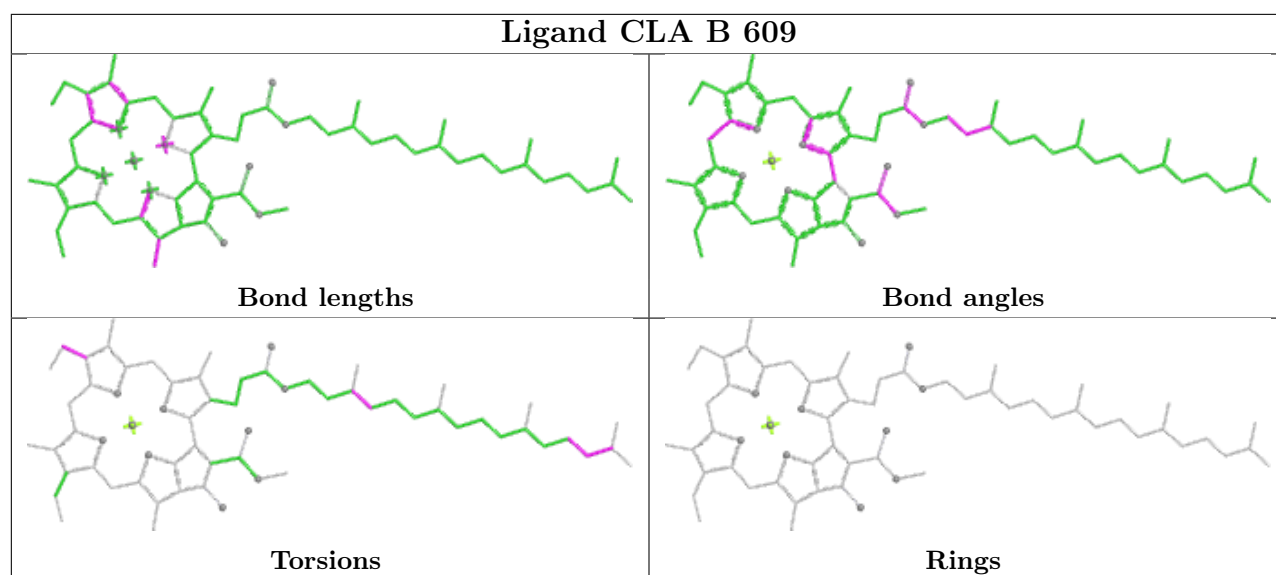


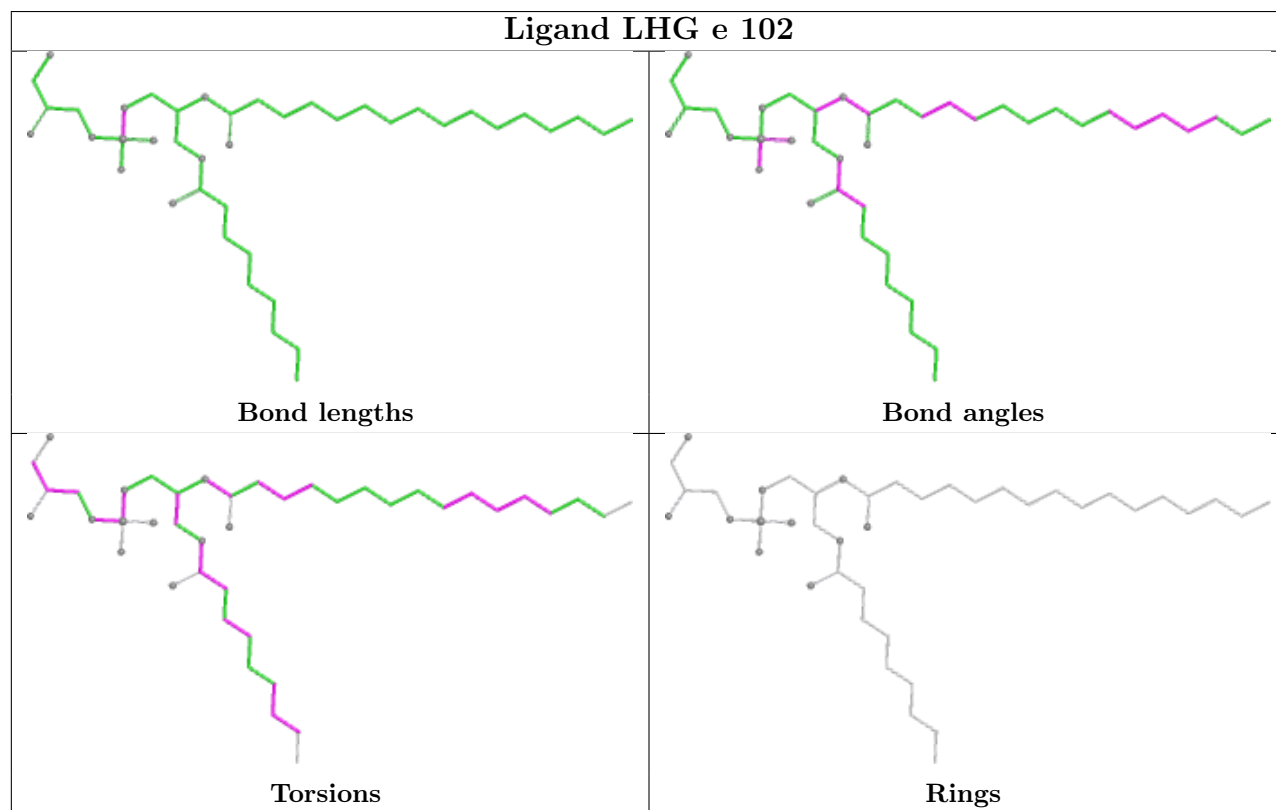
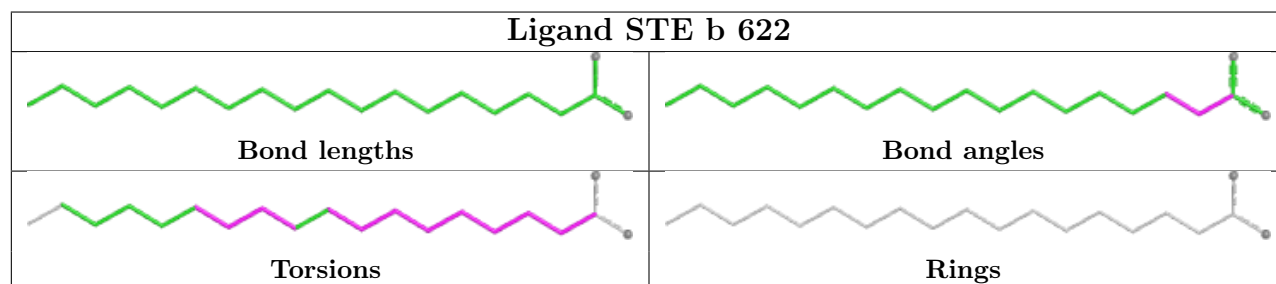
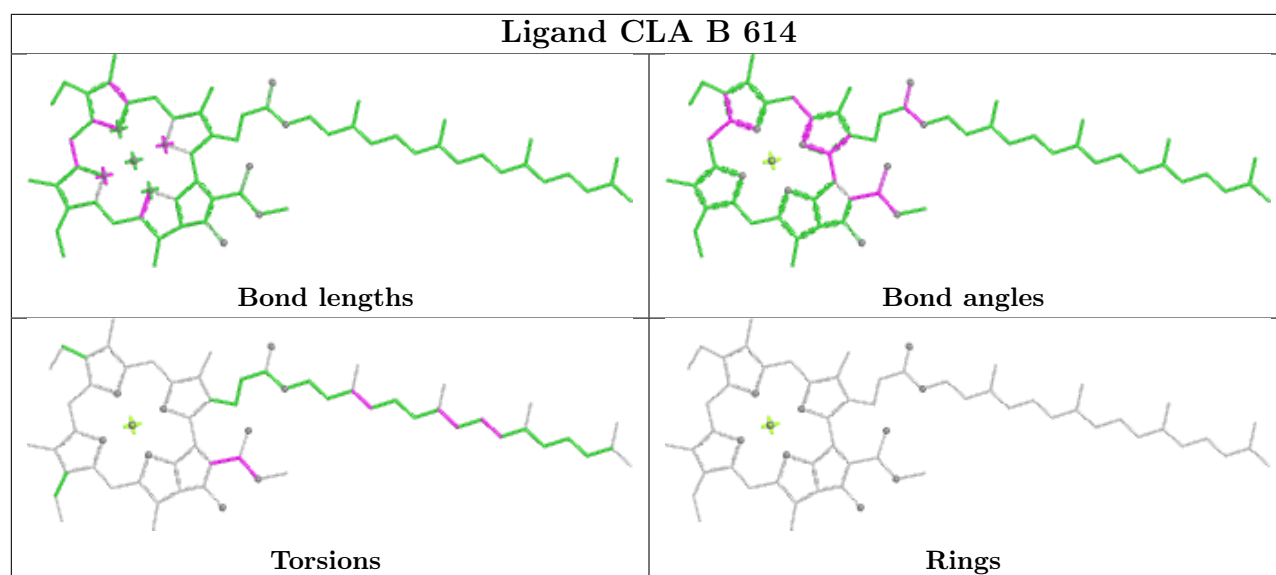
Torsions

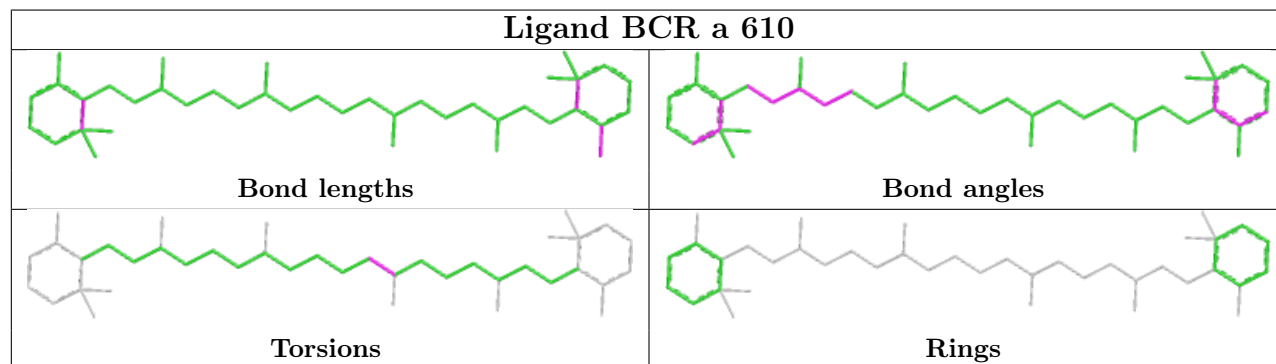
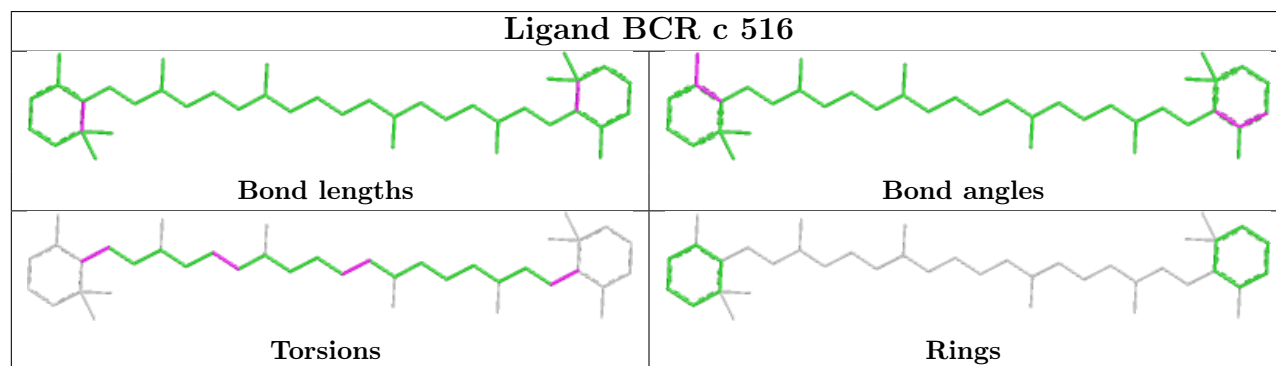
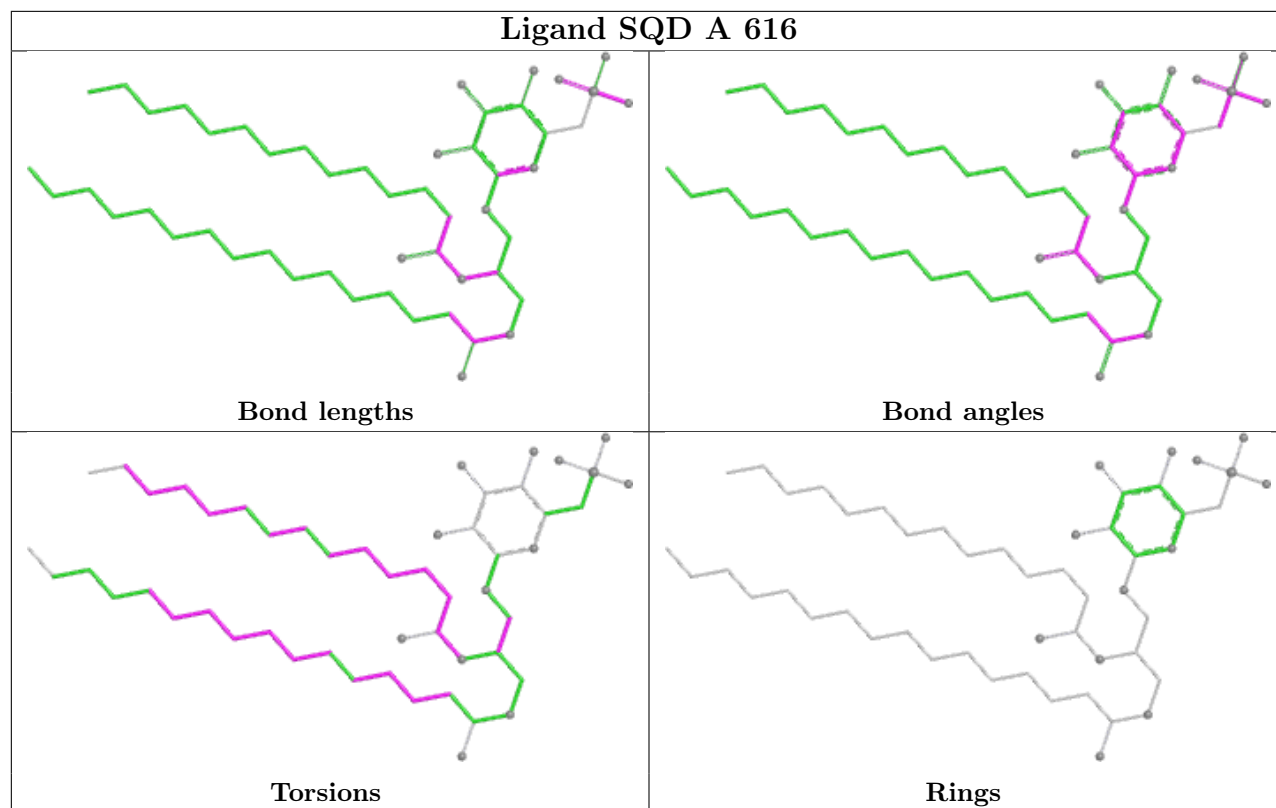


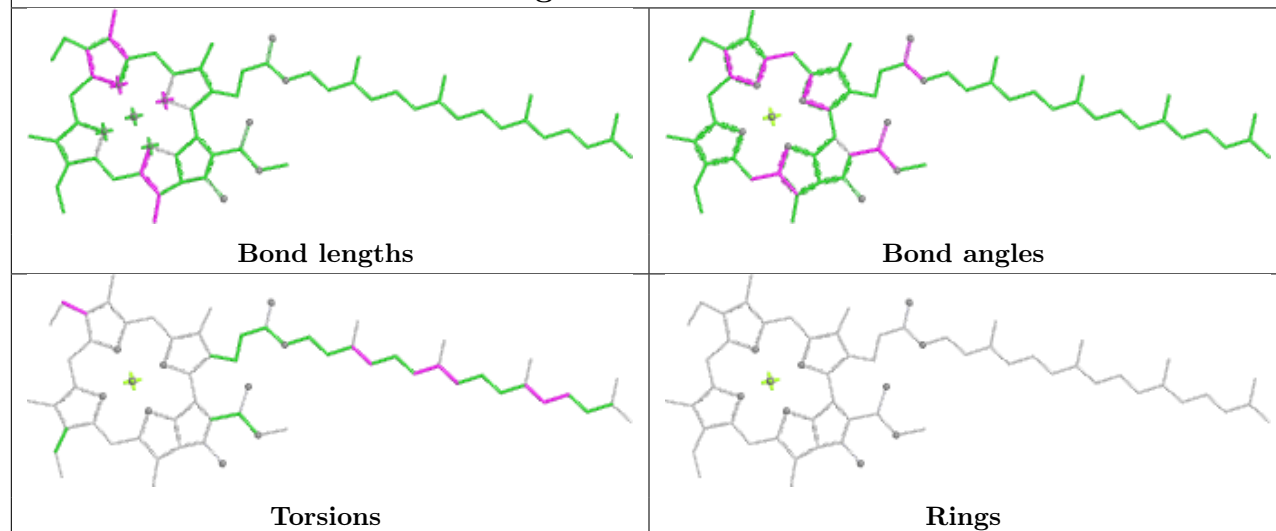
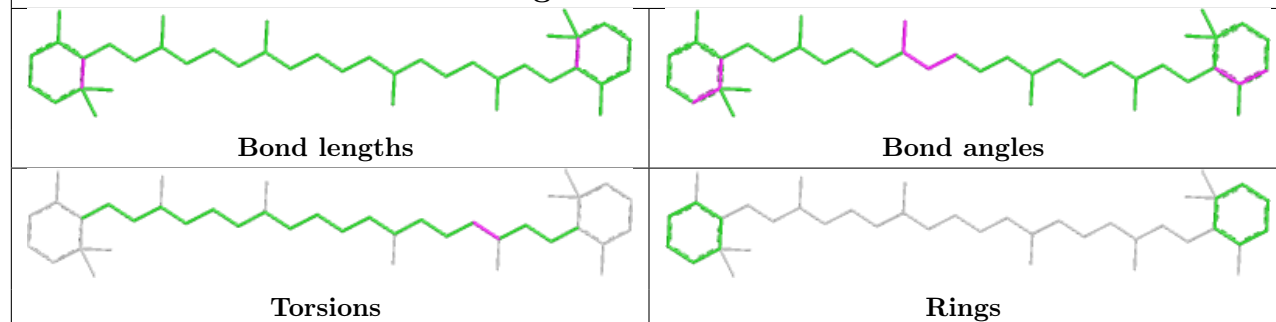
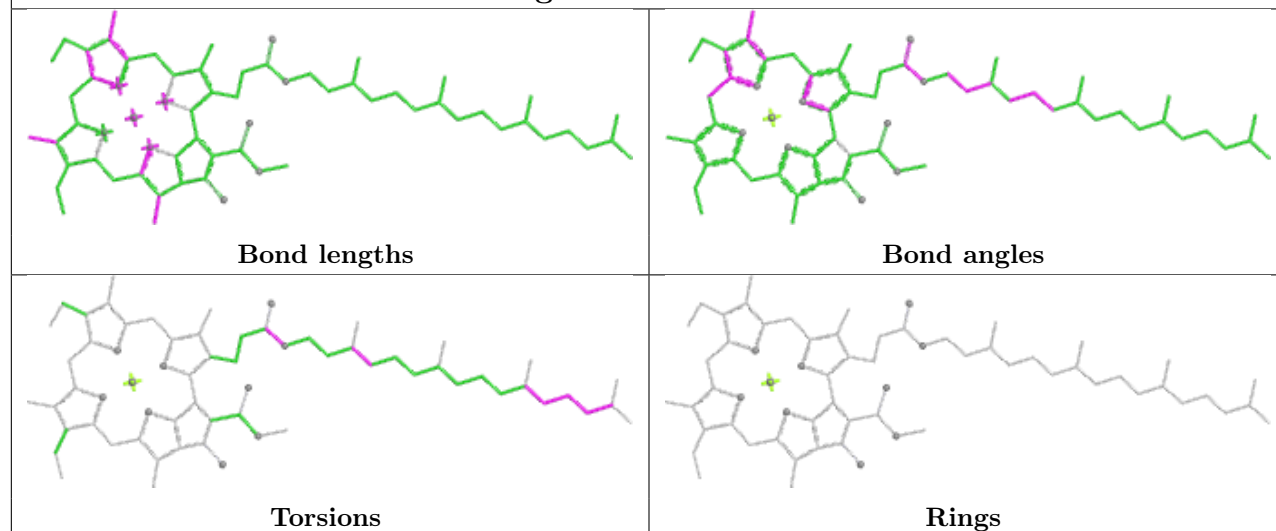
Rings

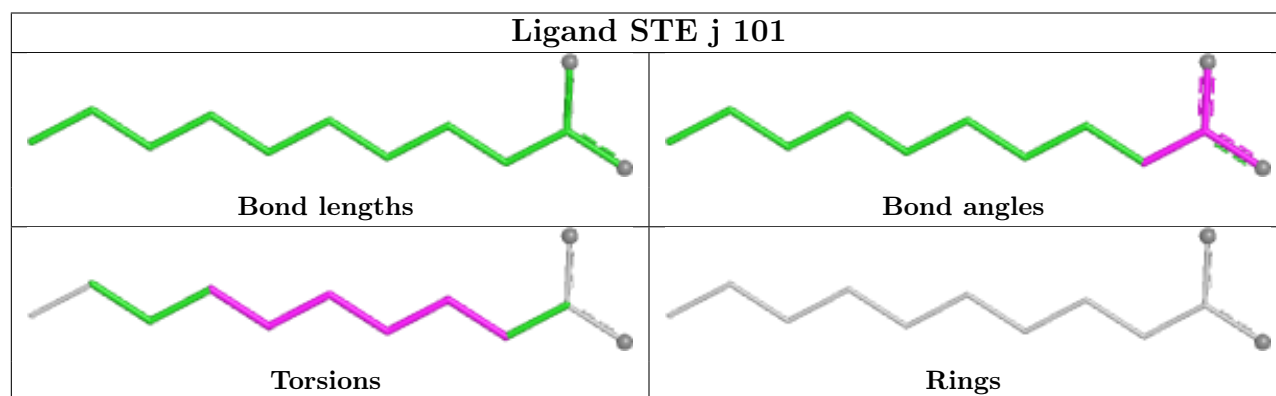
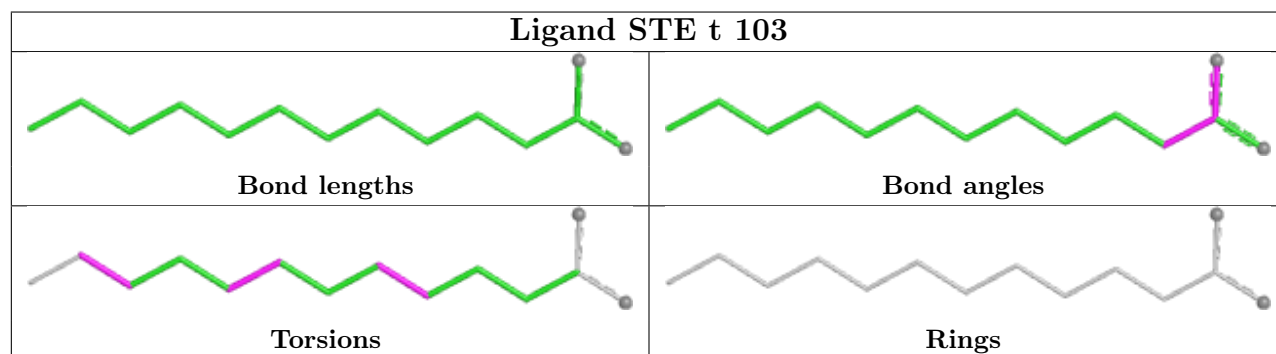
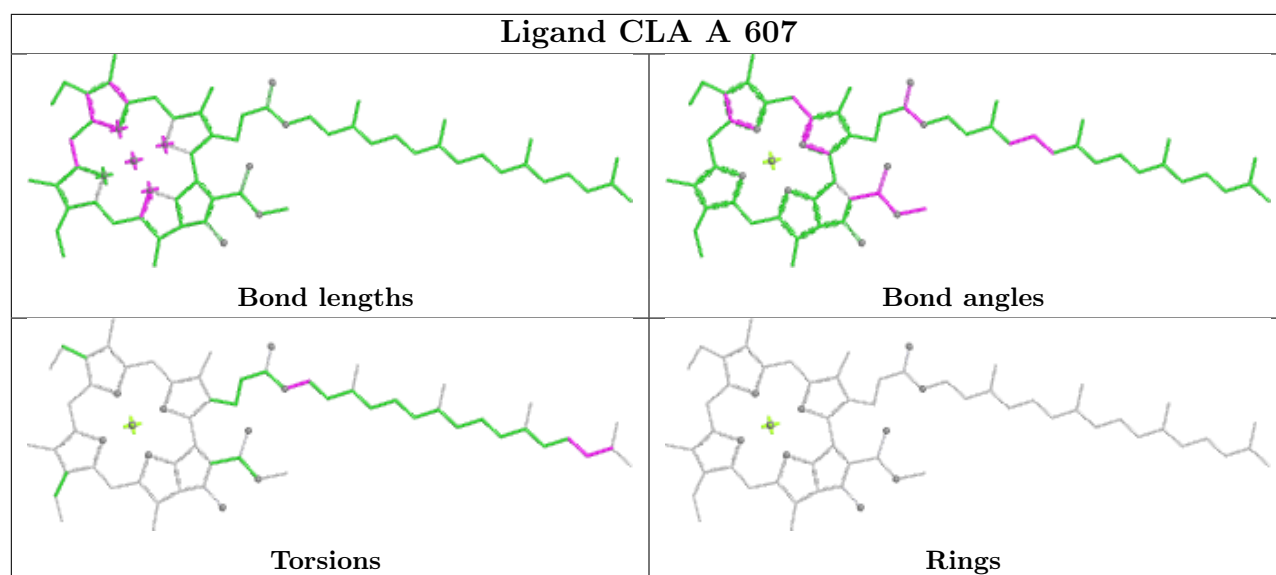




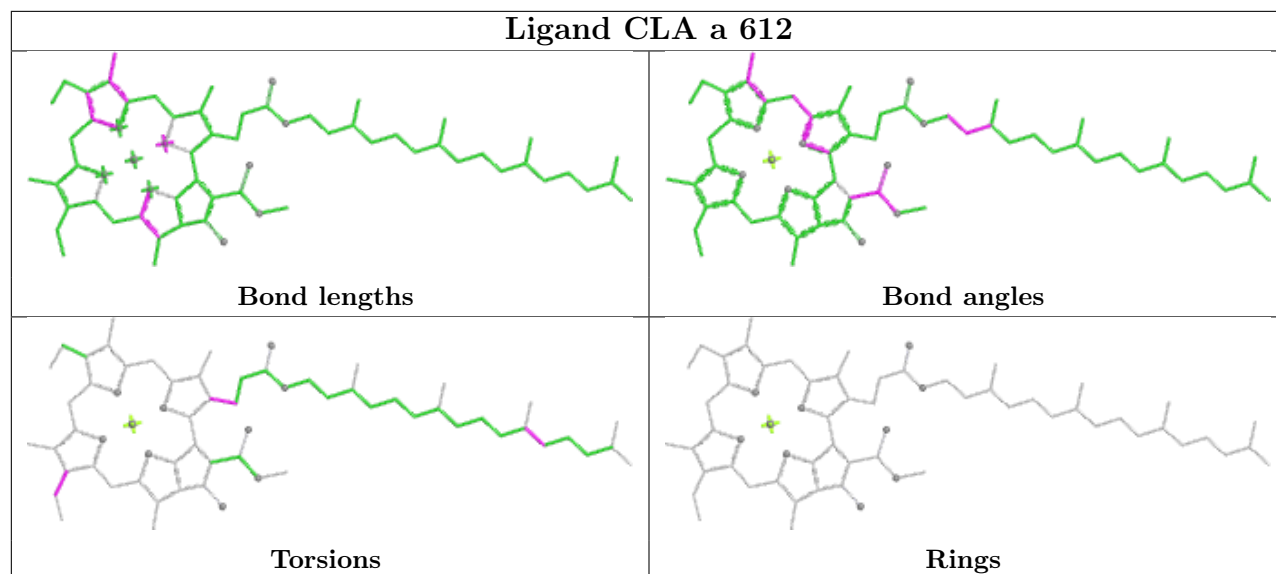




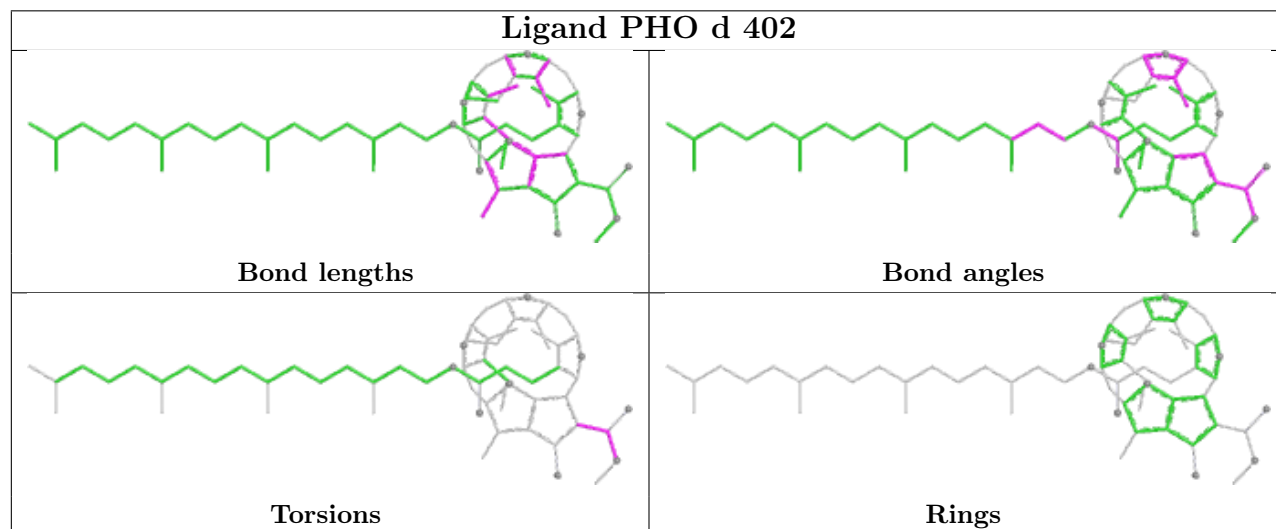
Ligand CLA b 602**Ligand BCR b 617****Ligand CLA b 608**



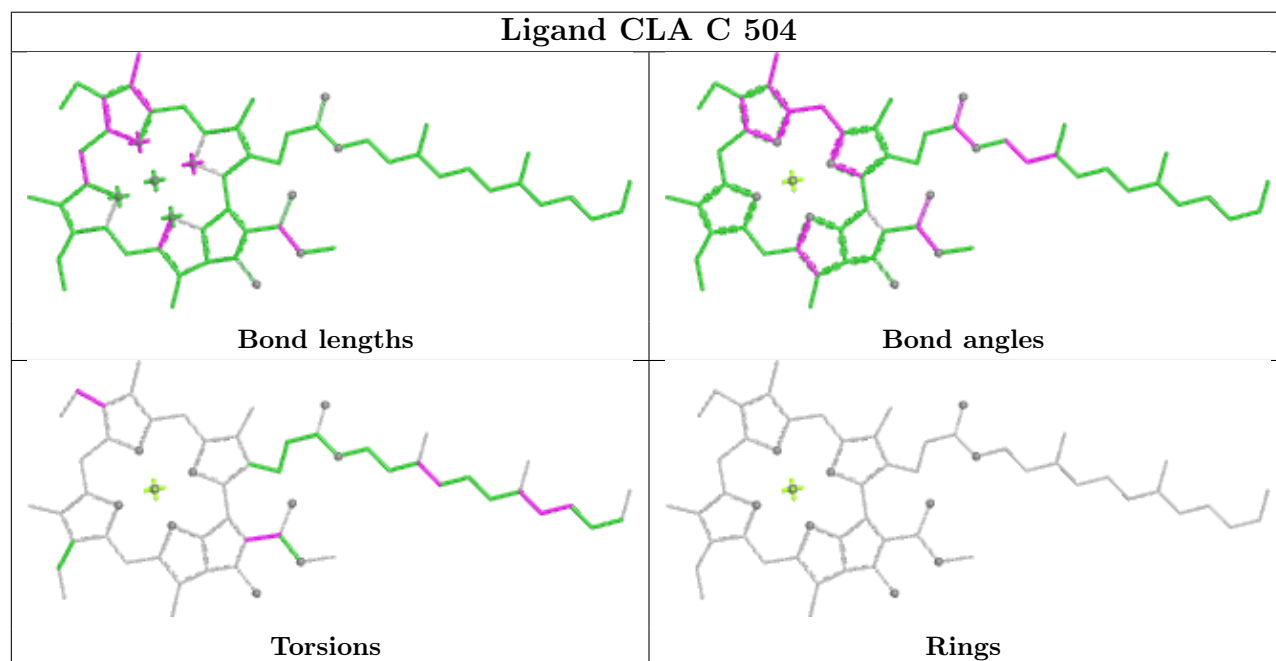
Ligand CLA a 612

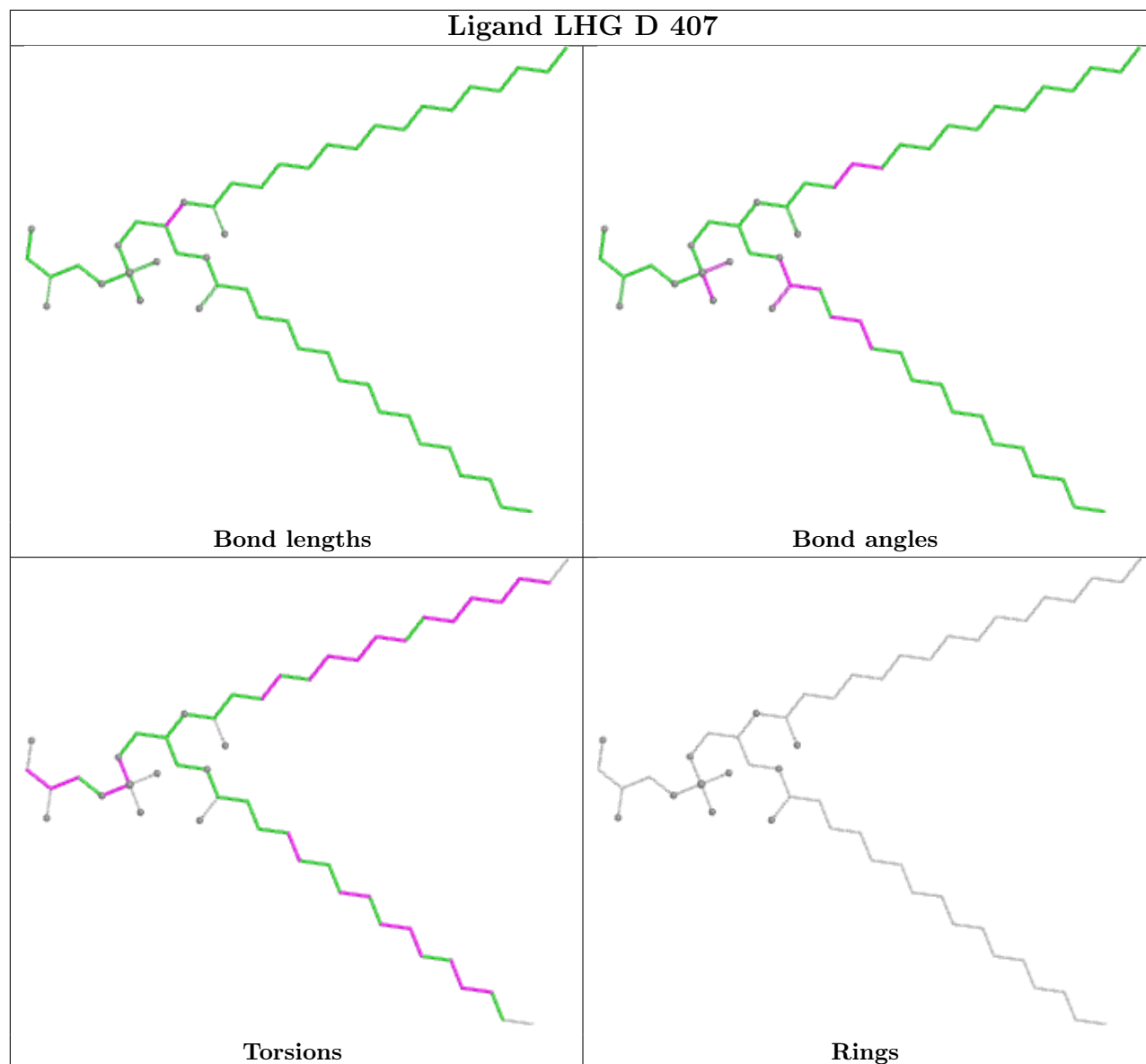
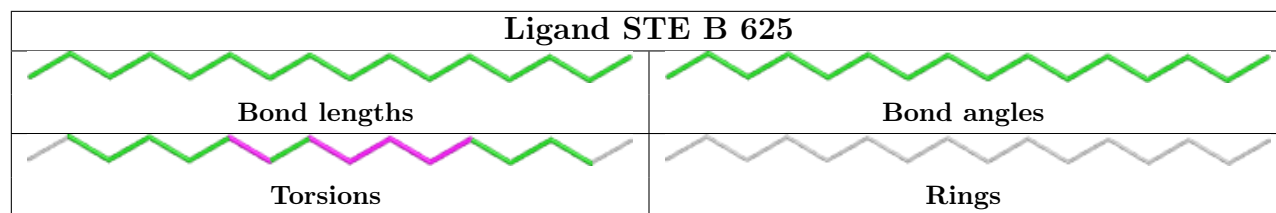


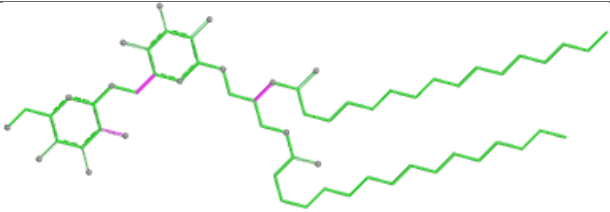
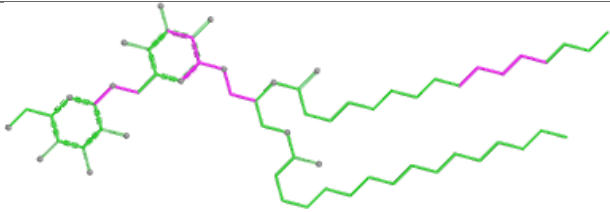
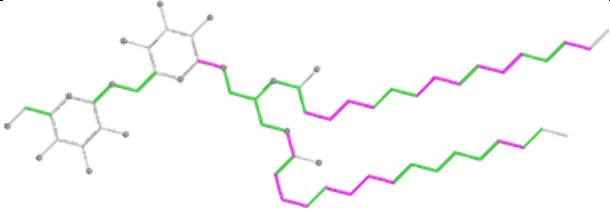
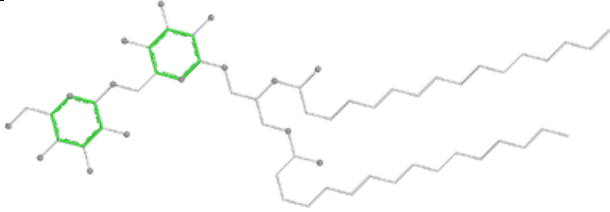
Ligand PHO d 402

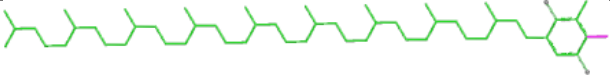
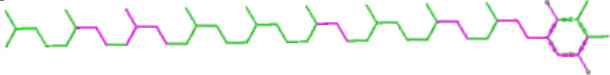
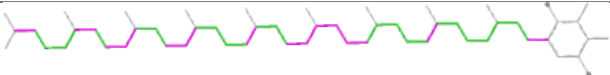
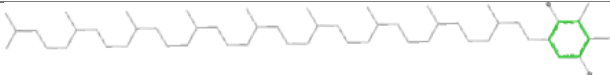


Ligand CLA C 504

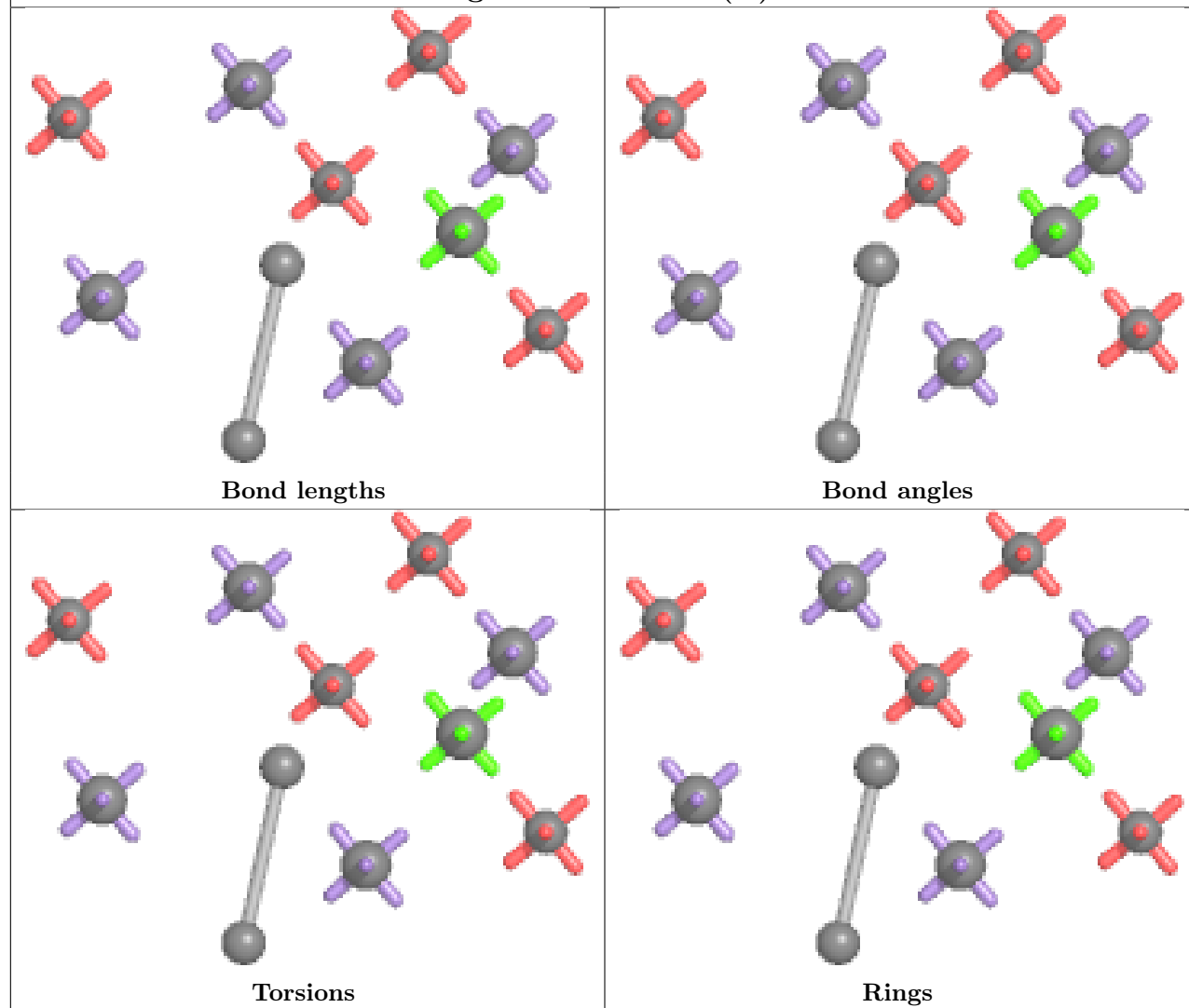




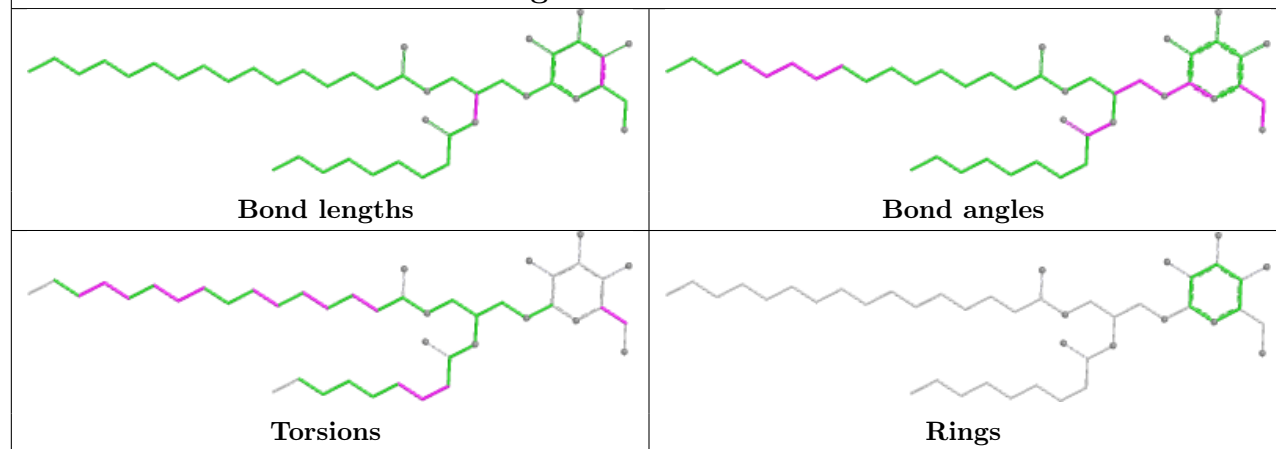
Ligand DGD c 519			
			
Bond lengths	Bond angles		
			
Torsions	Rings		

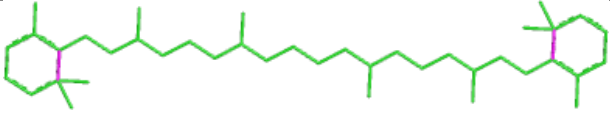
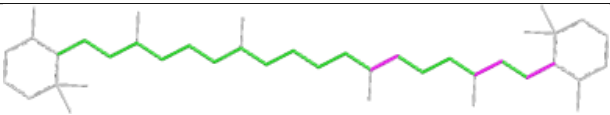
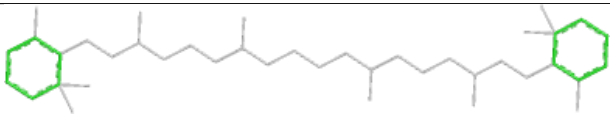
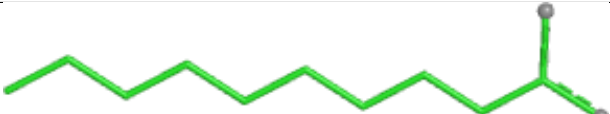
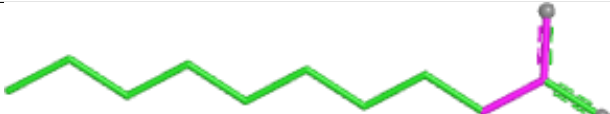
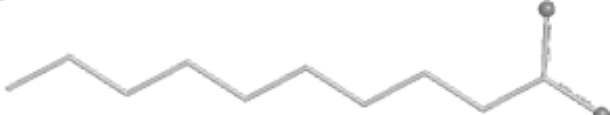
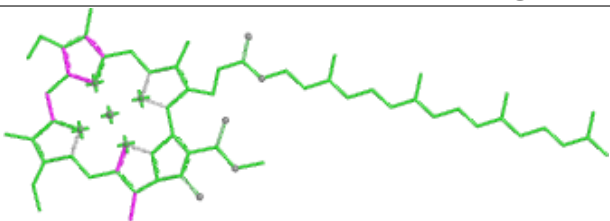
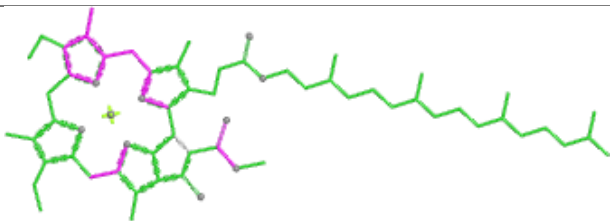
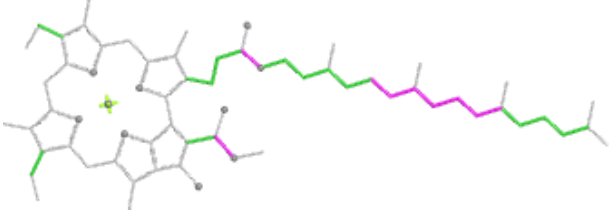
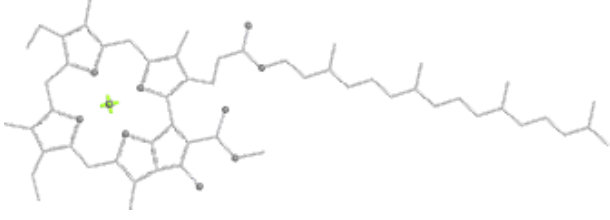
Ligand PL9 a 611			
			
Bond lengths	Bond angles		
			
Torsions	Rings		

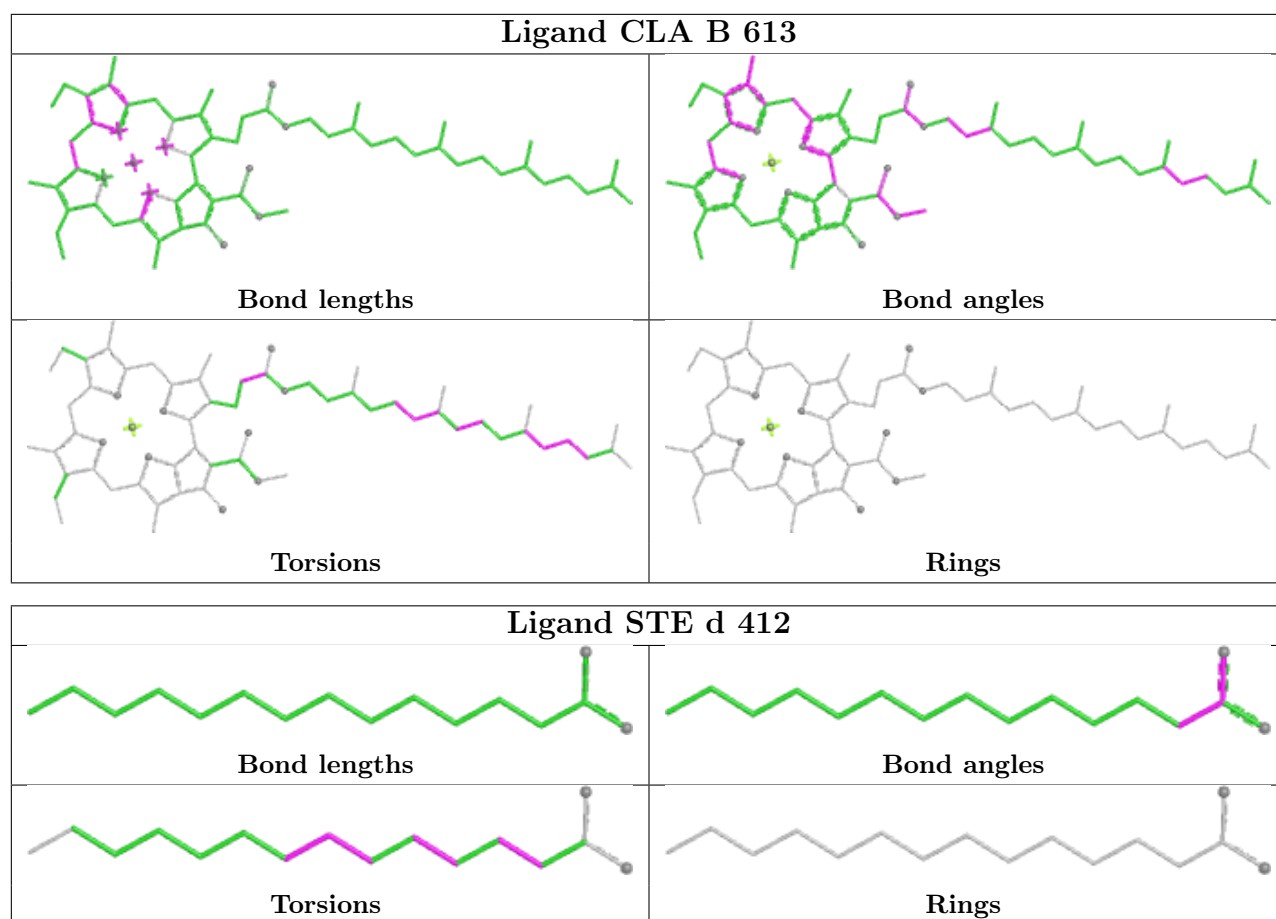
Ligand OEY a 601 (A)

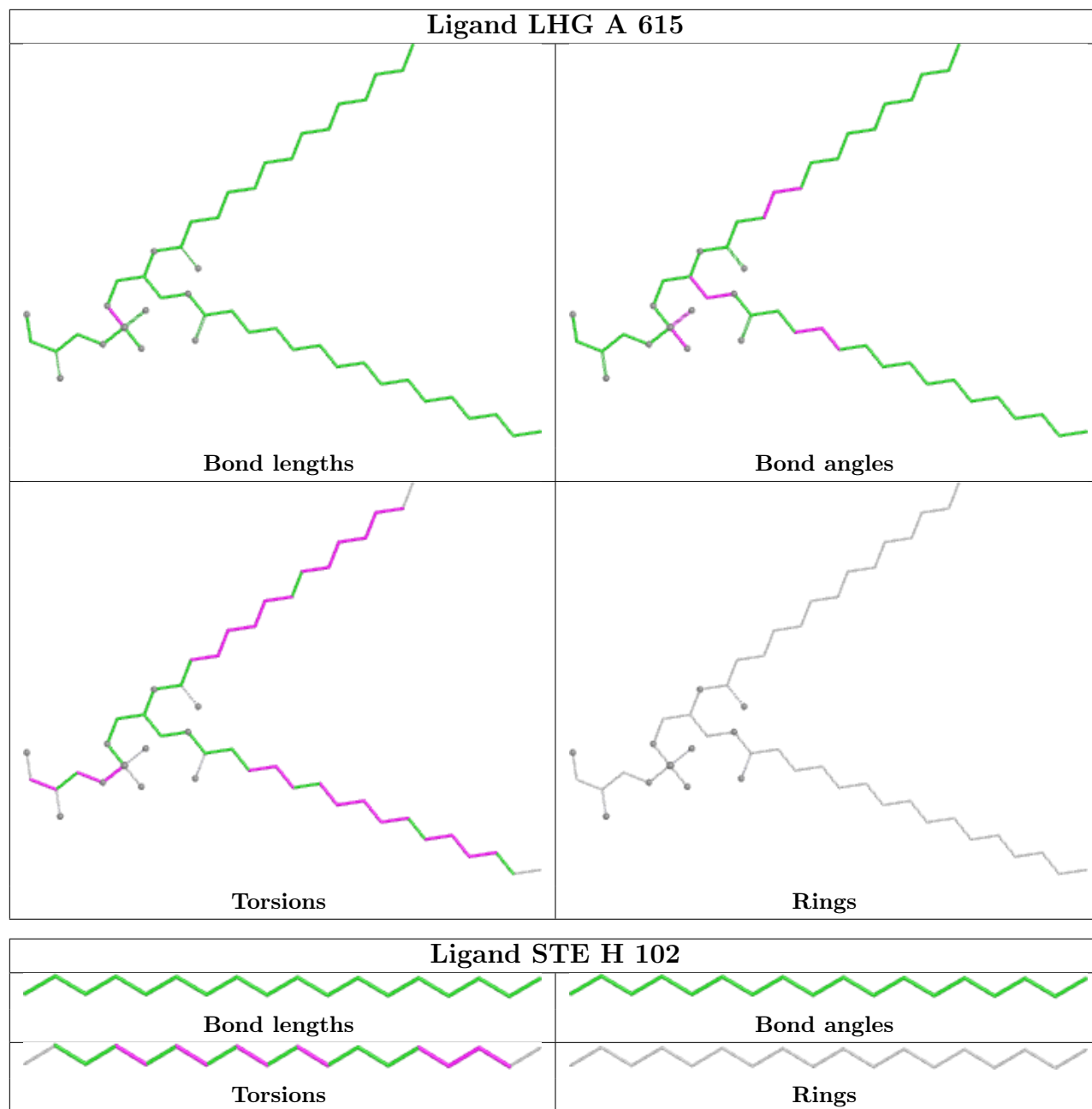


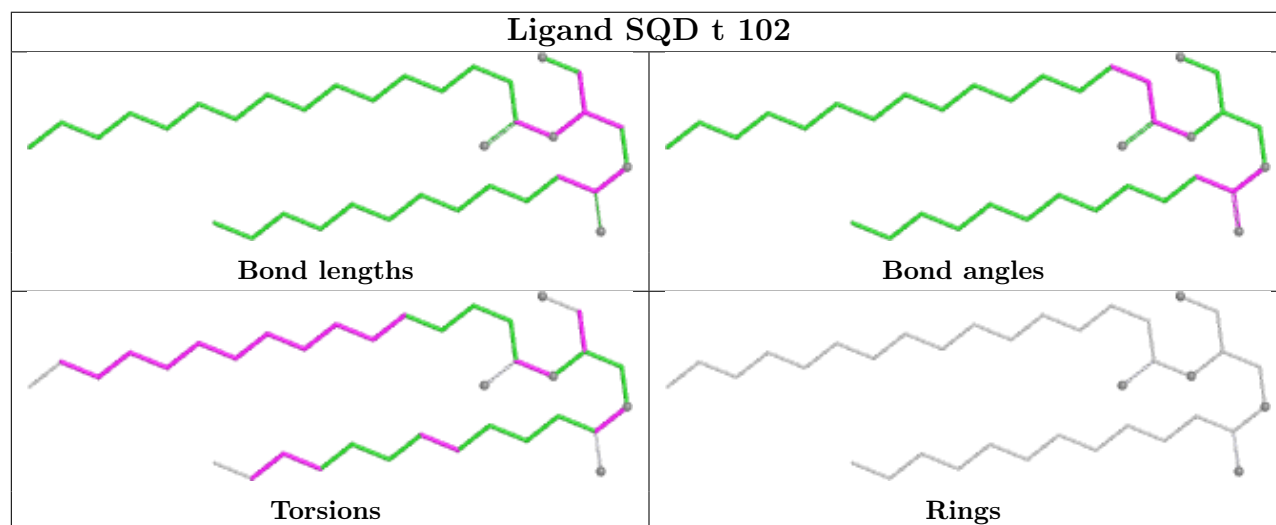
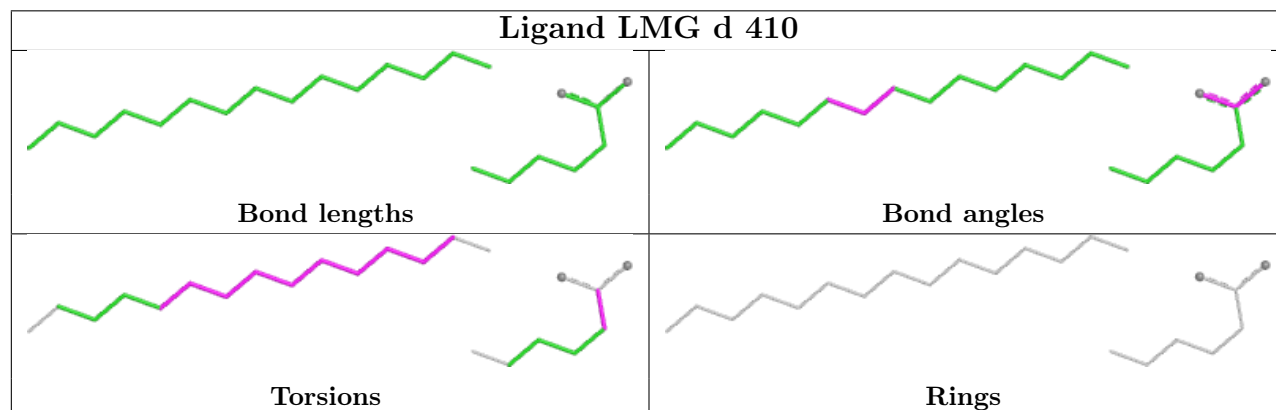
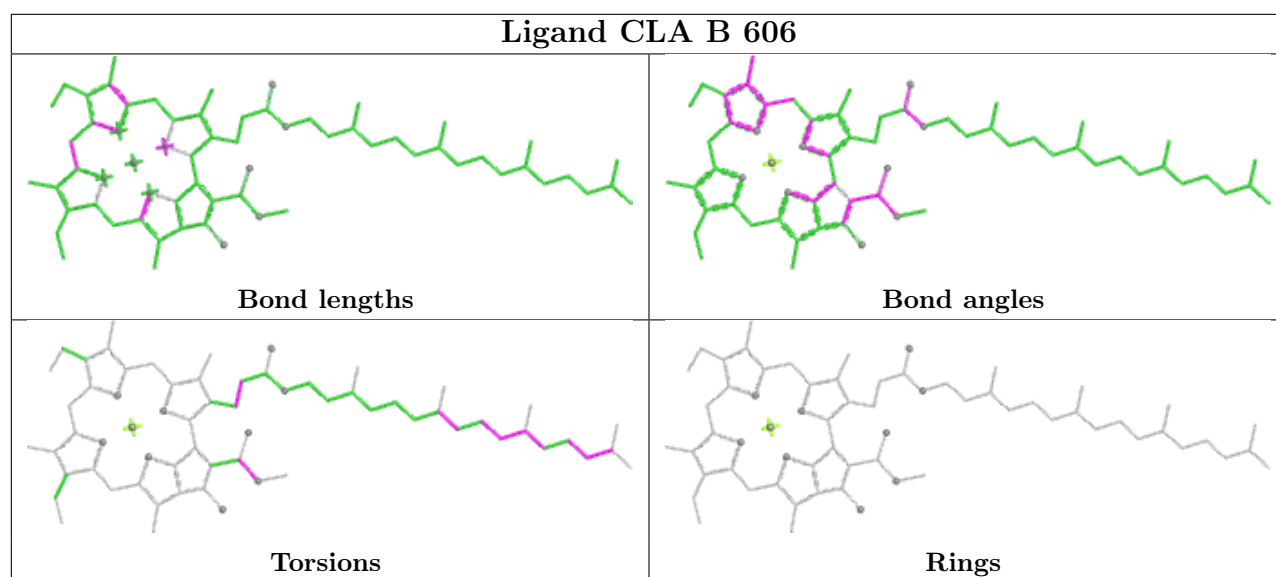
Ligand LMG d 411

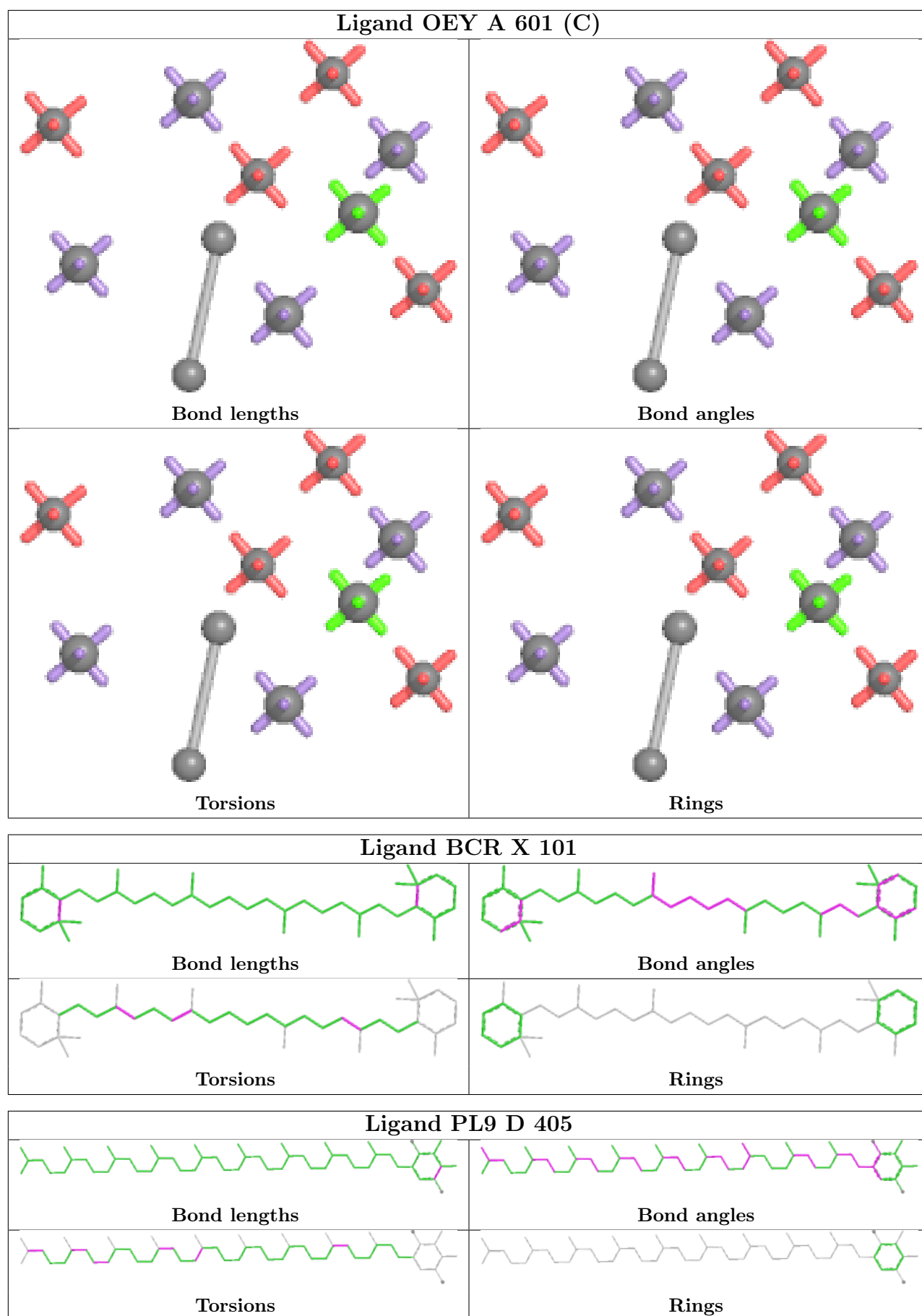


Ligand BCR B 618	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand STE a 615	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand STE T 103	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA b 606	
 Bond lengths	 Bond angles
 Torsions	 Rings

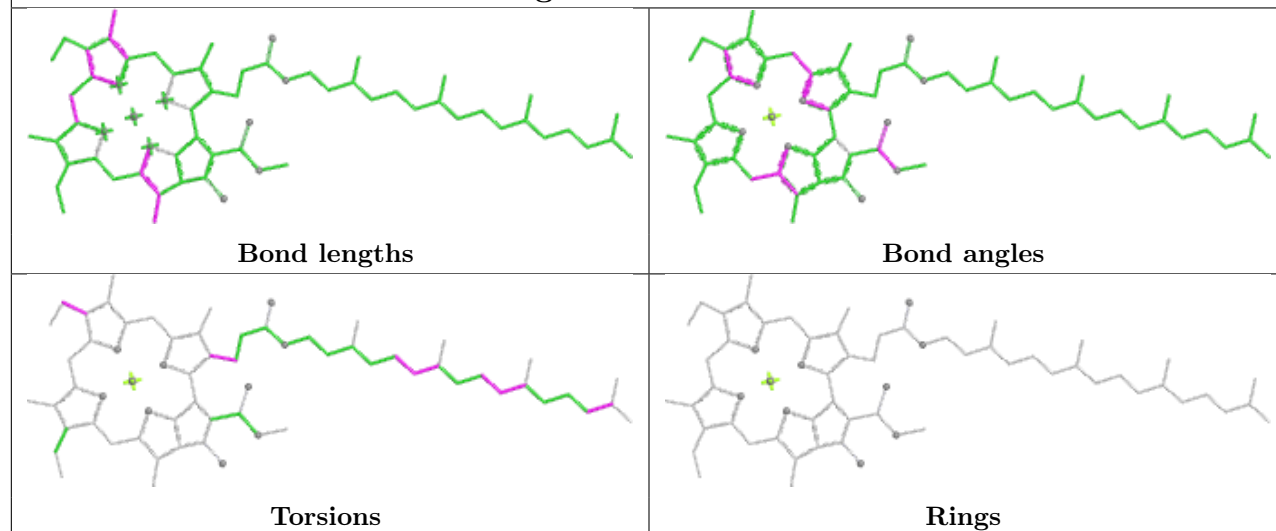




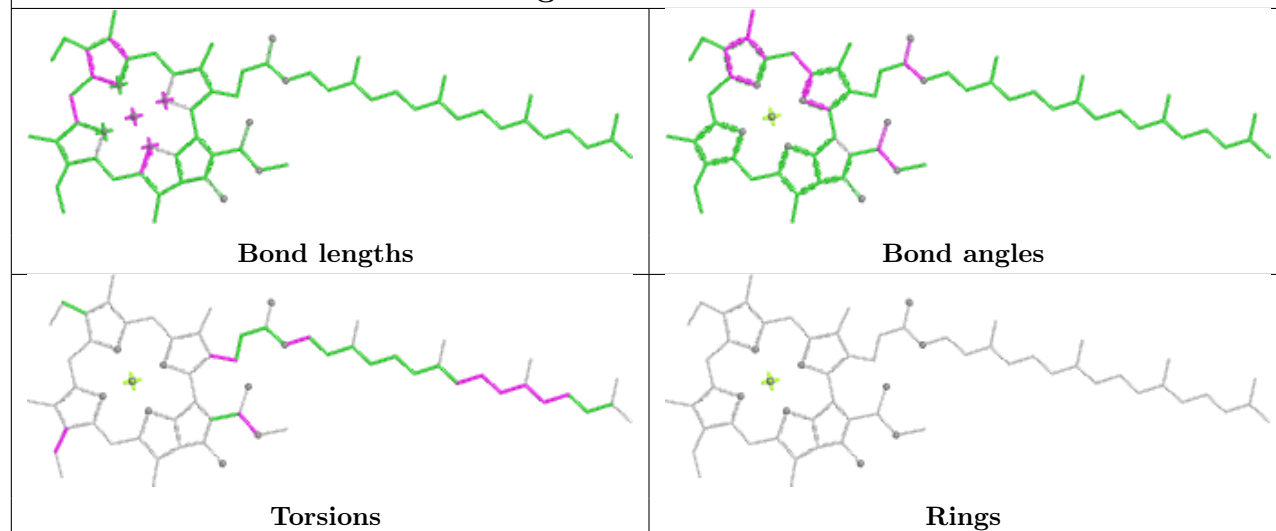




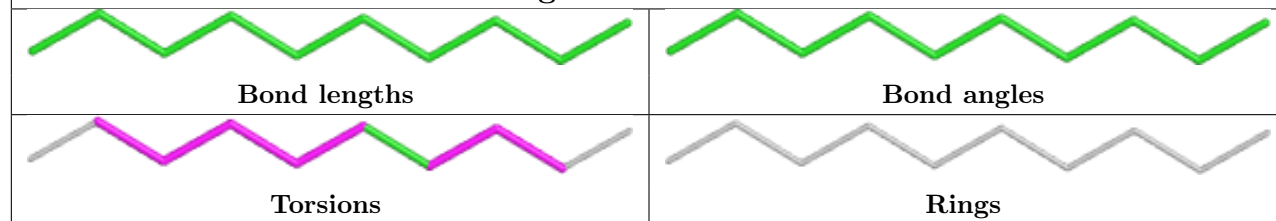
Ligand CLA d 404

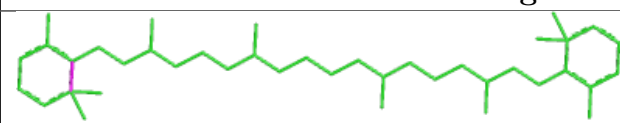
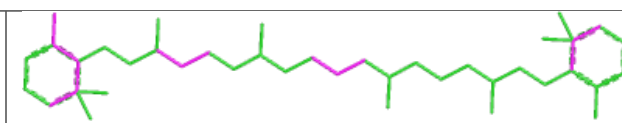
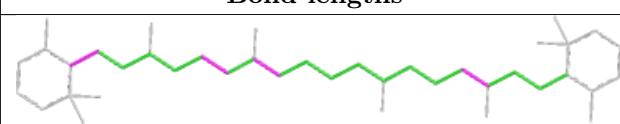
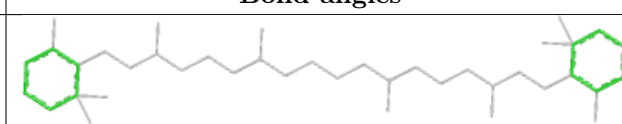


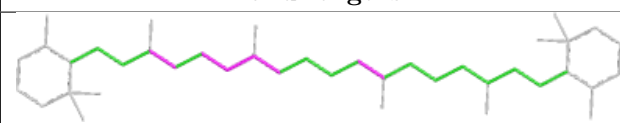
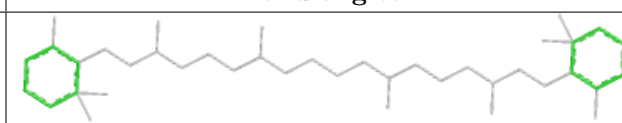
Ligand CLA c 513

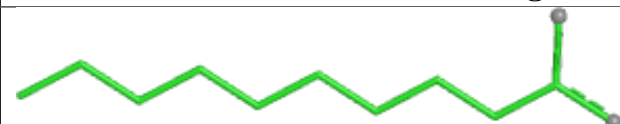
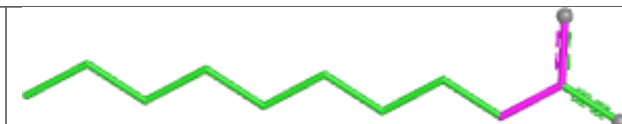
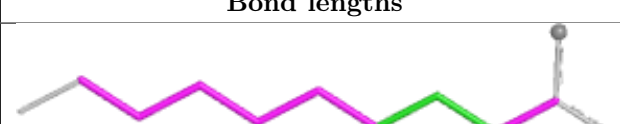
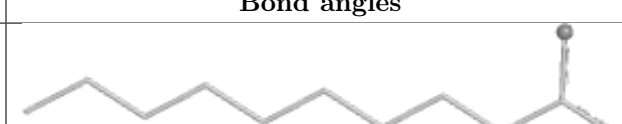


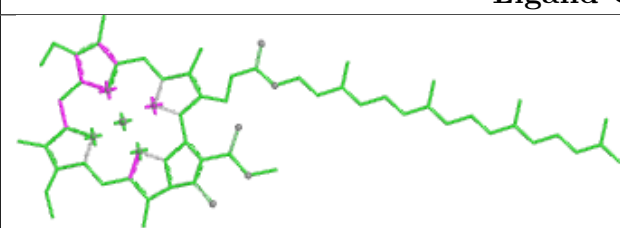
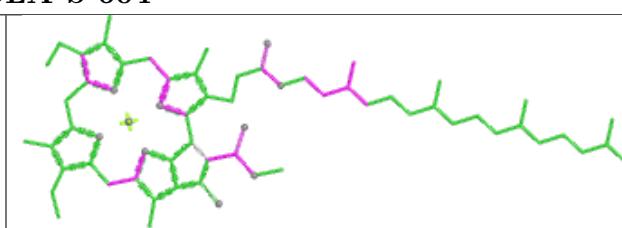
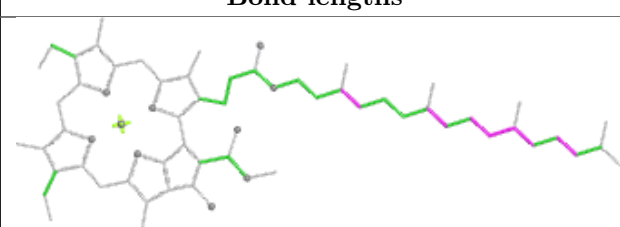
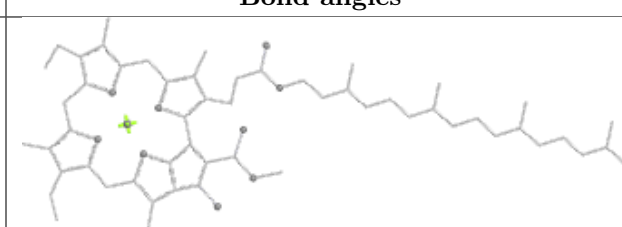
Ligand STE b 623

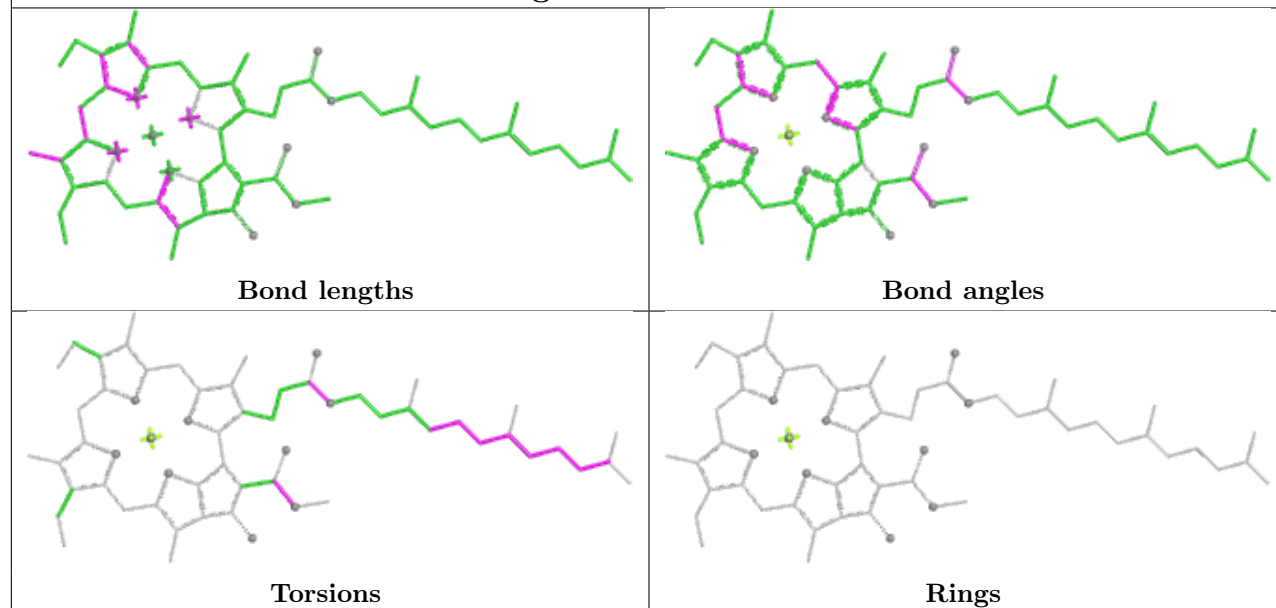
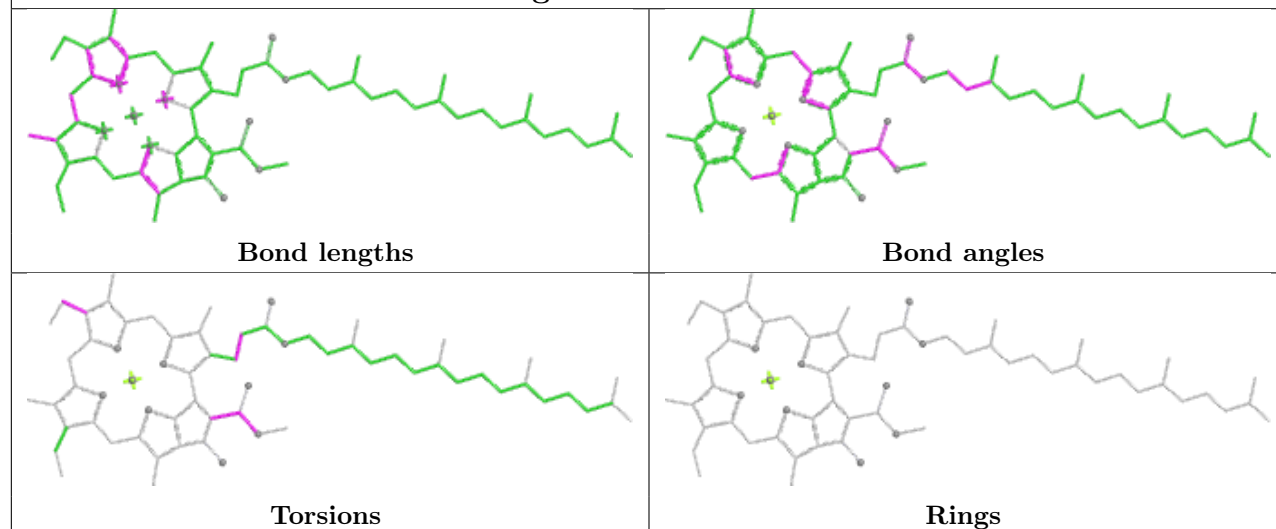
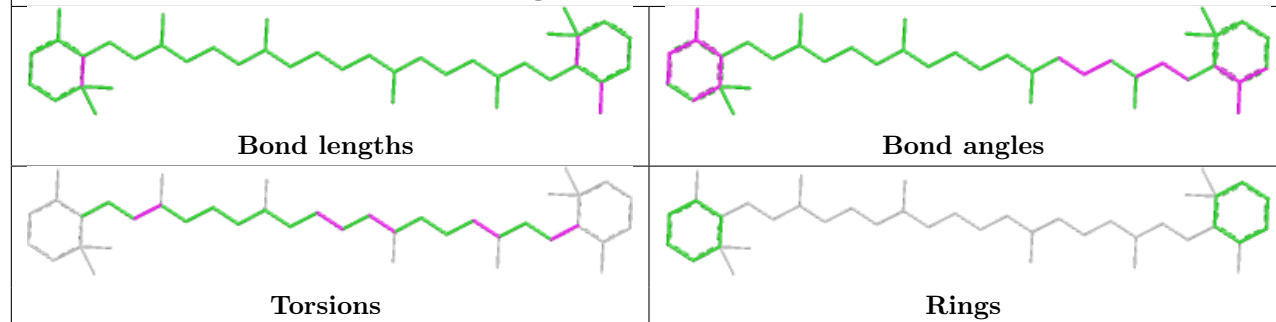


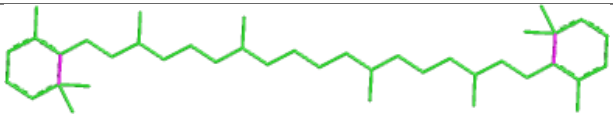
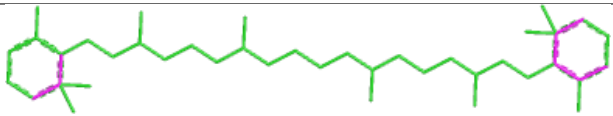
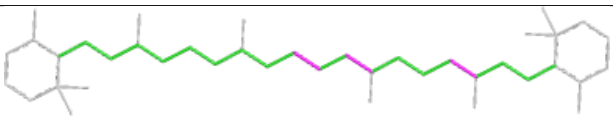
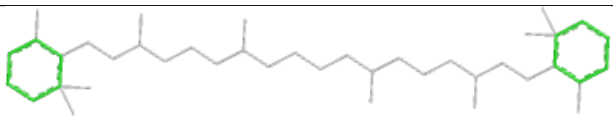
Ligand BCR B 617	
	
Bond lengths	Bond angles
	
Torsions	Rings

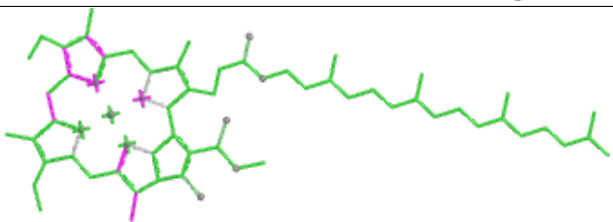
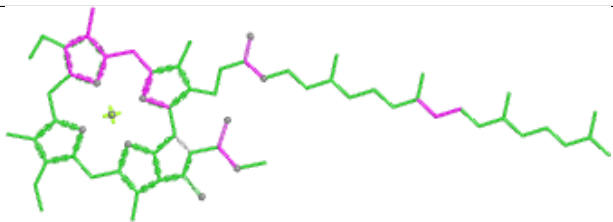
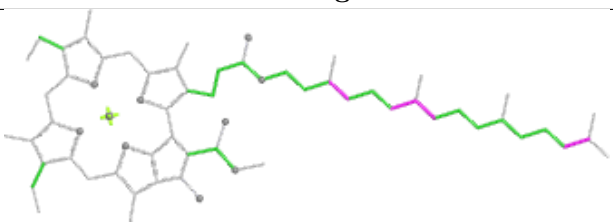
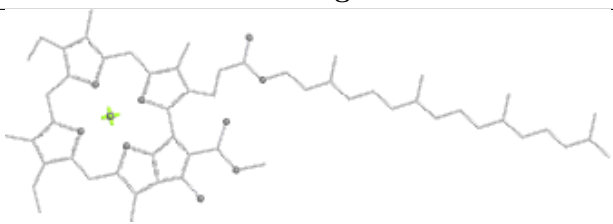
Ligand BCR C 514	
	
Bond lengths	Bond angles
	
Torsions	Rings

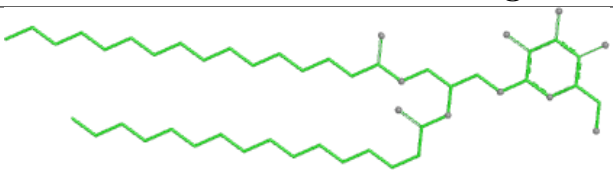
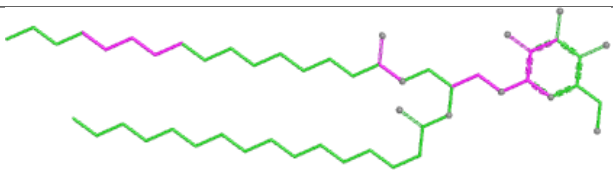
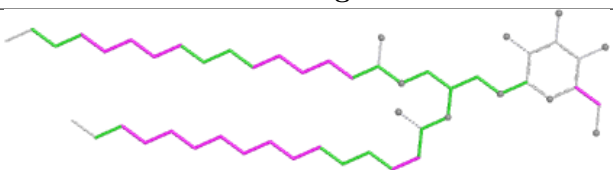
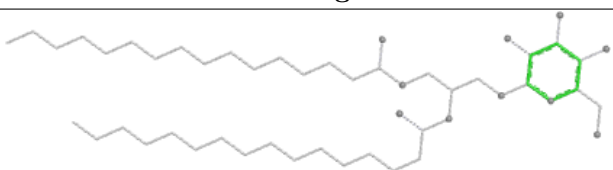
Ligand STE L 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

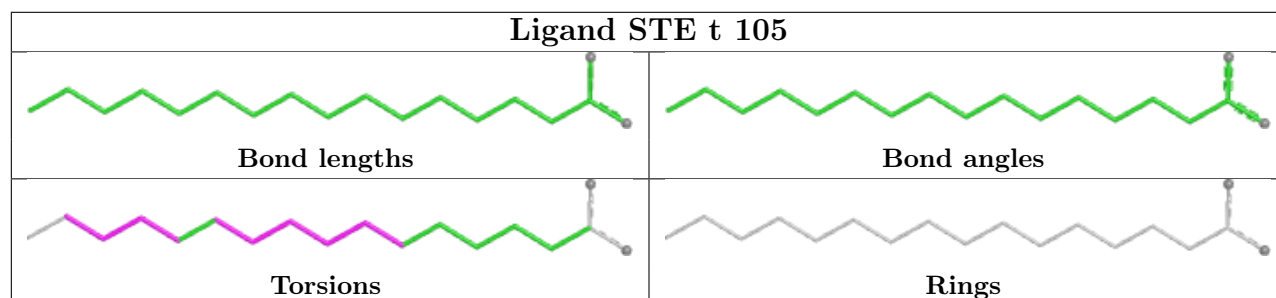
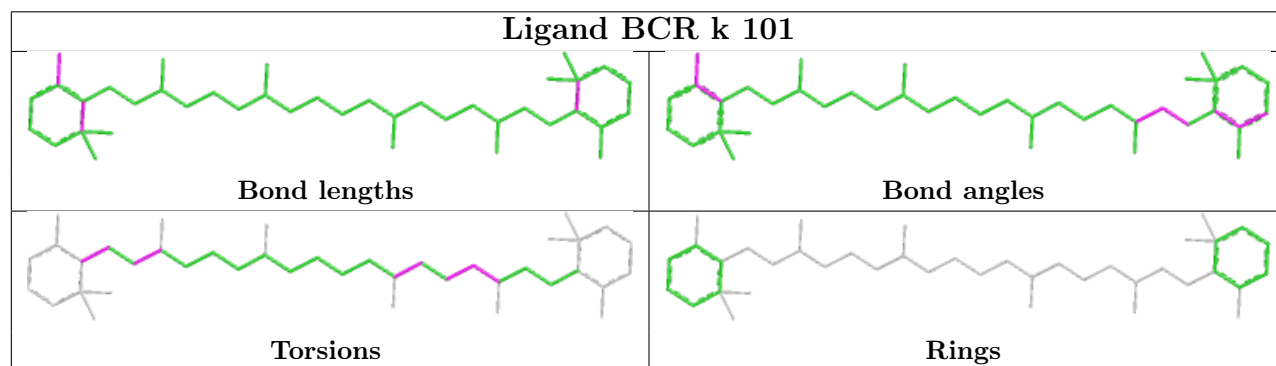
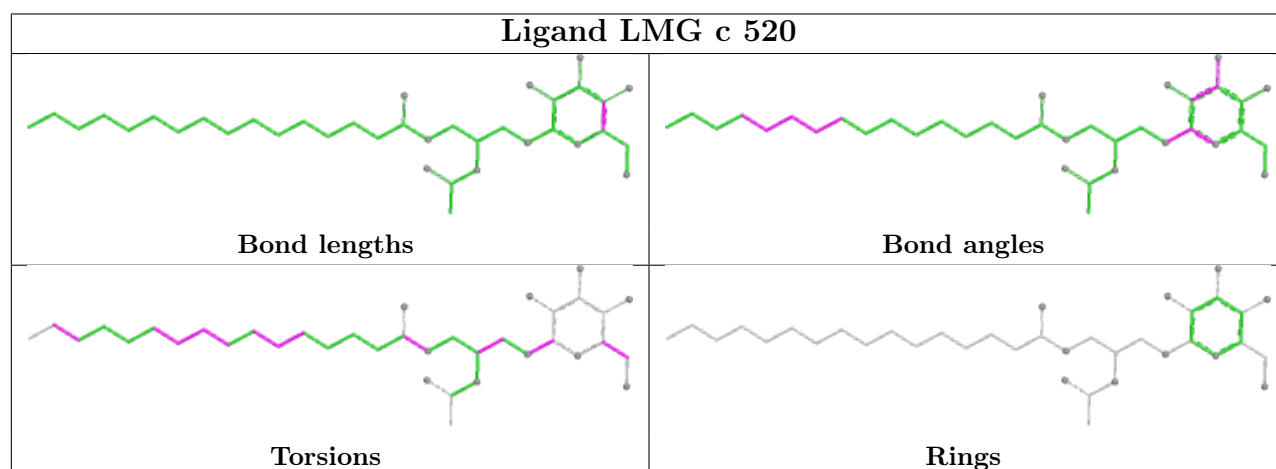
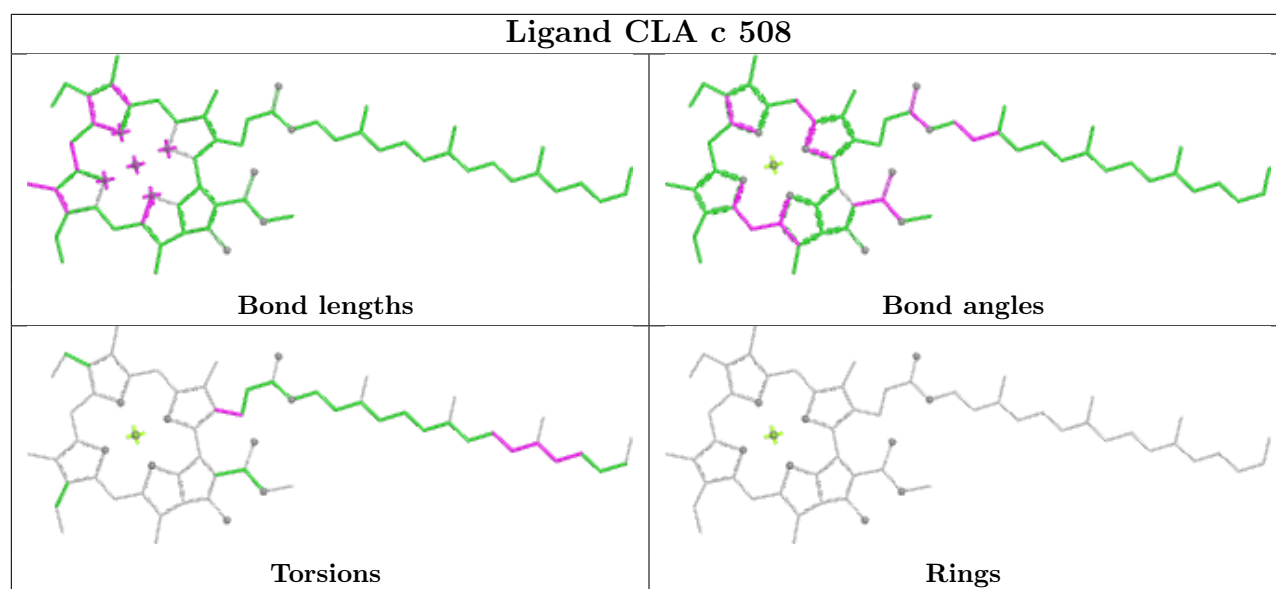
Ligand CLA b 604	
	
Bond lengths	Bond angles
	
Torsions	Rings

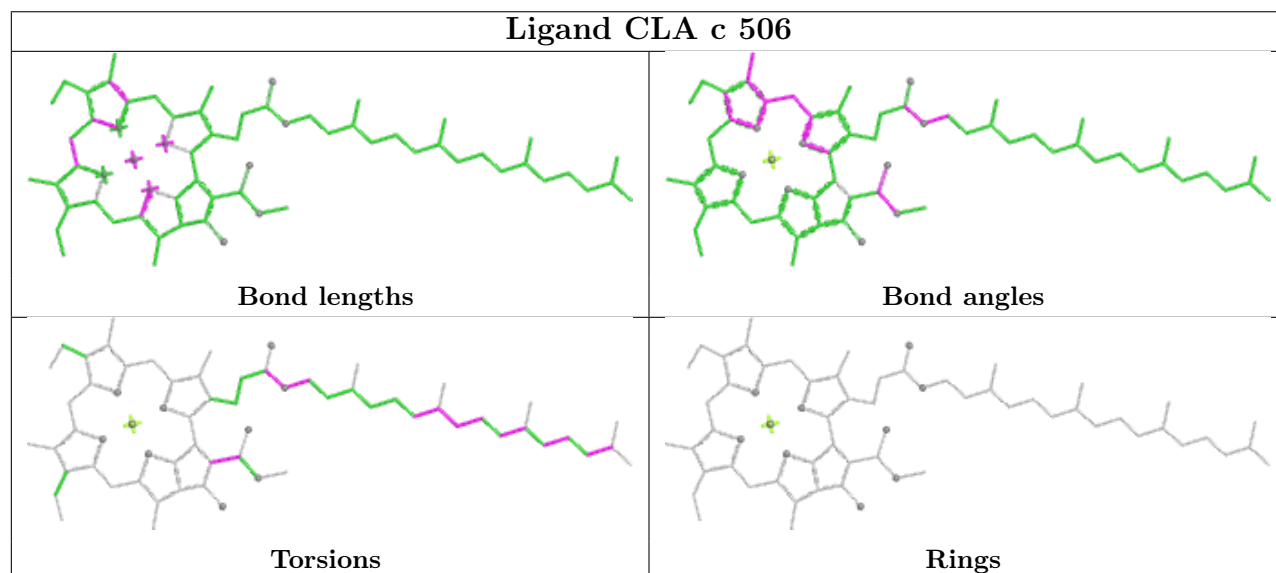
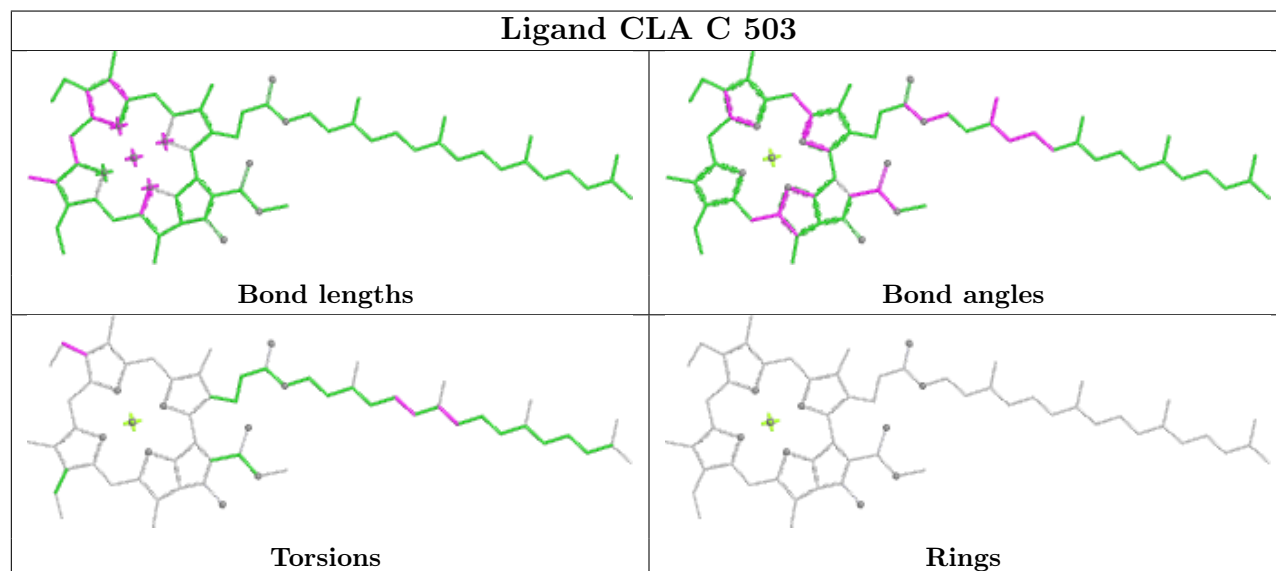
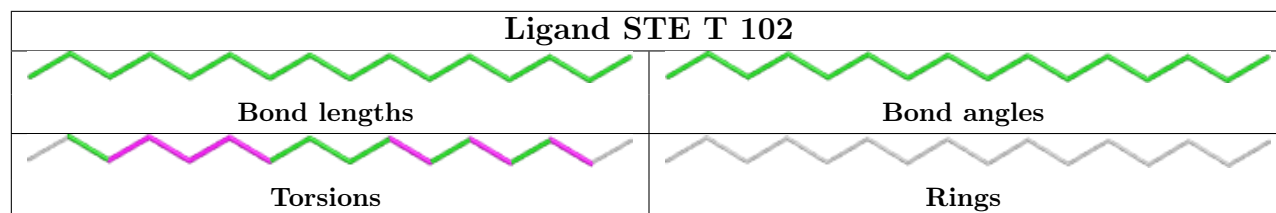
Ligand CLA B 616**Ligand CLA C 501****Ligand BCR D 404**

Ligand BCR b 618	
	
Bond lengths	Bond angles
	
Torsions	Rings

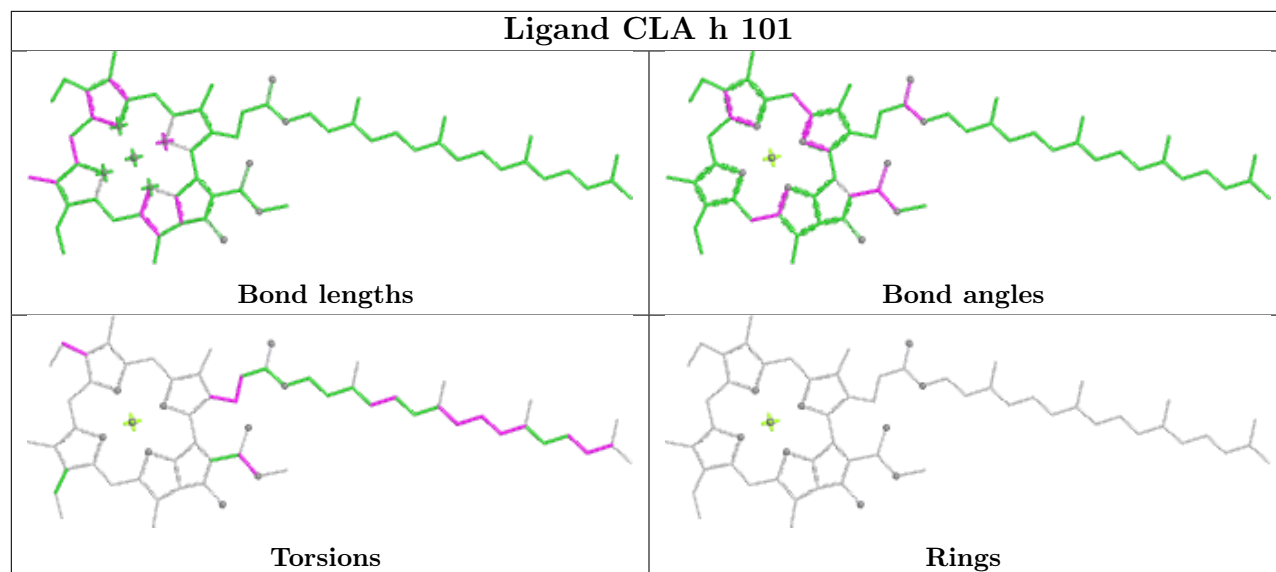
Ligand CLA C 510	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LMG D 406	
	
Bond lengths	Bond angles
	
Torsions	Rings

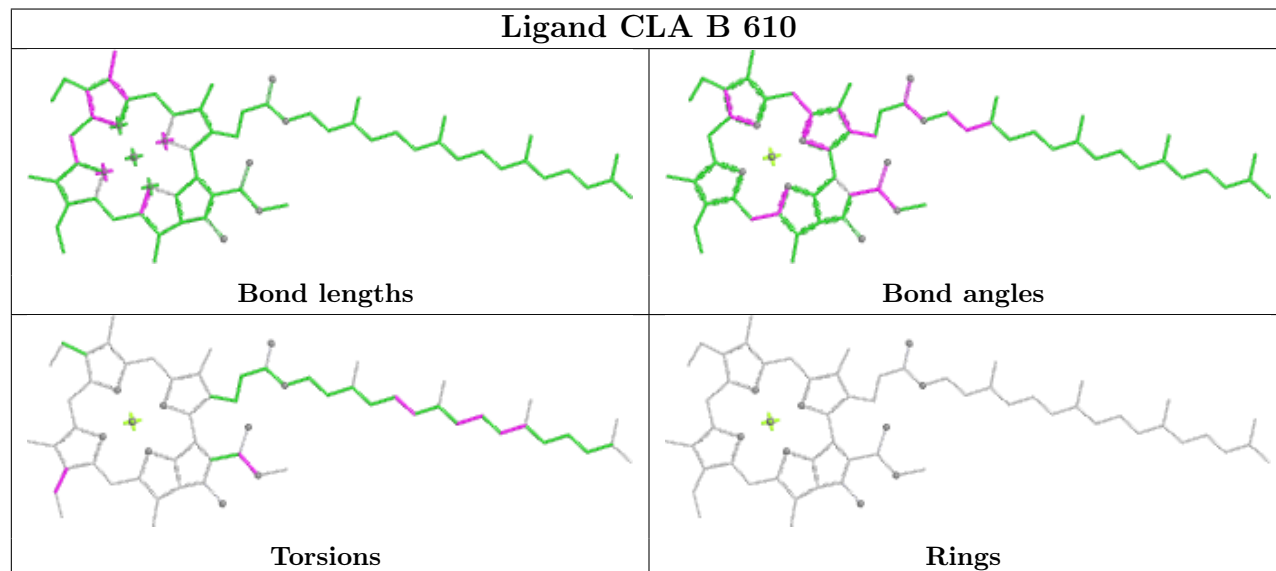




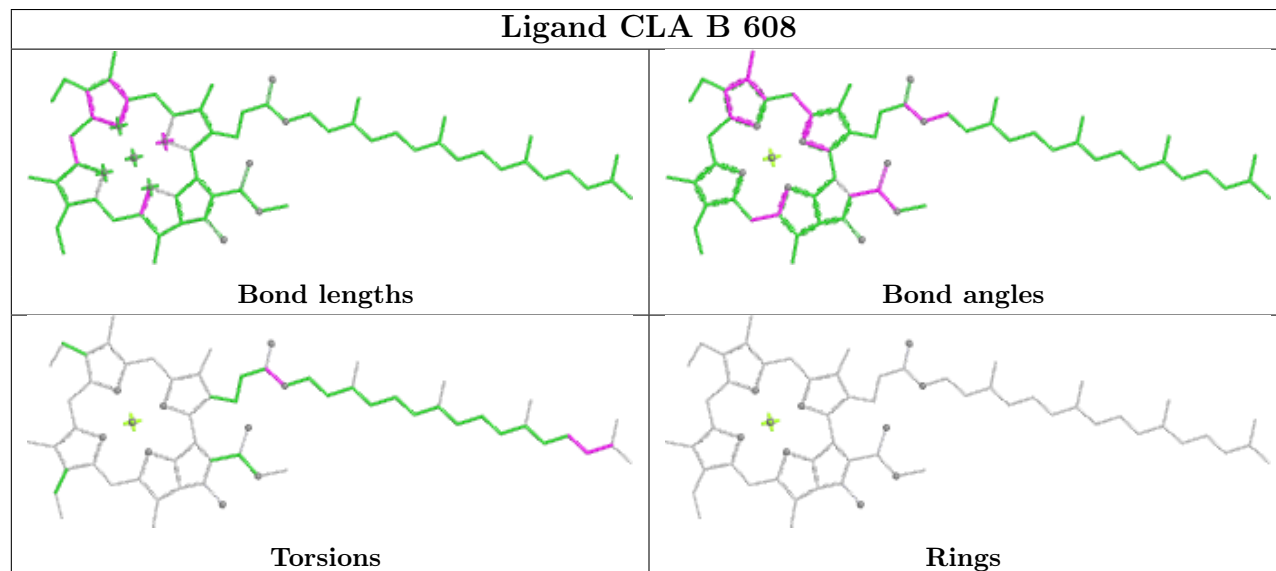
Ligand CLA h 101

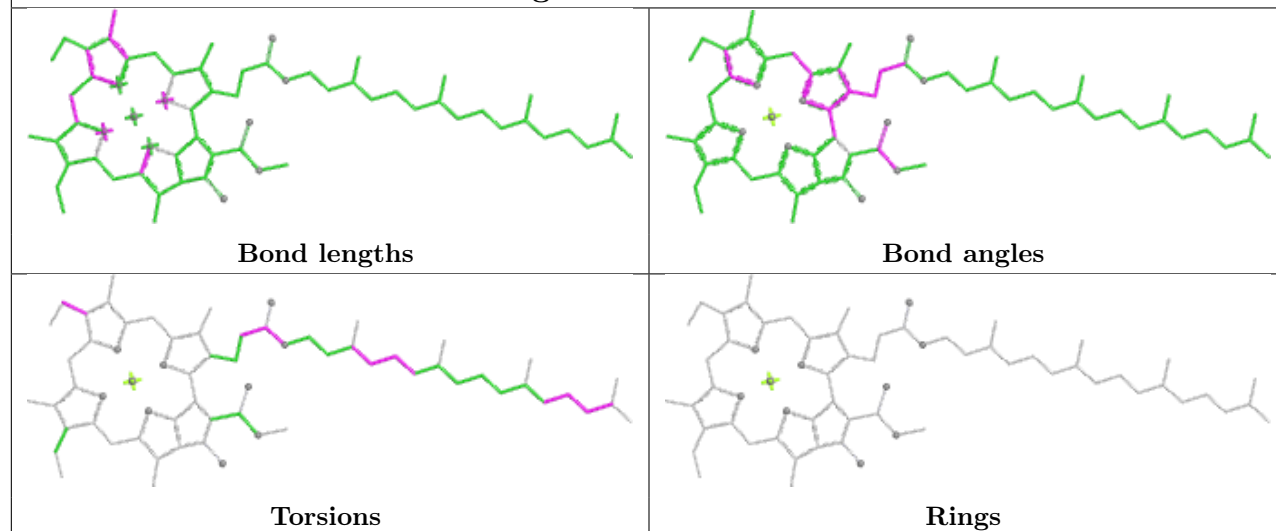
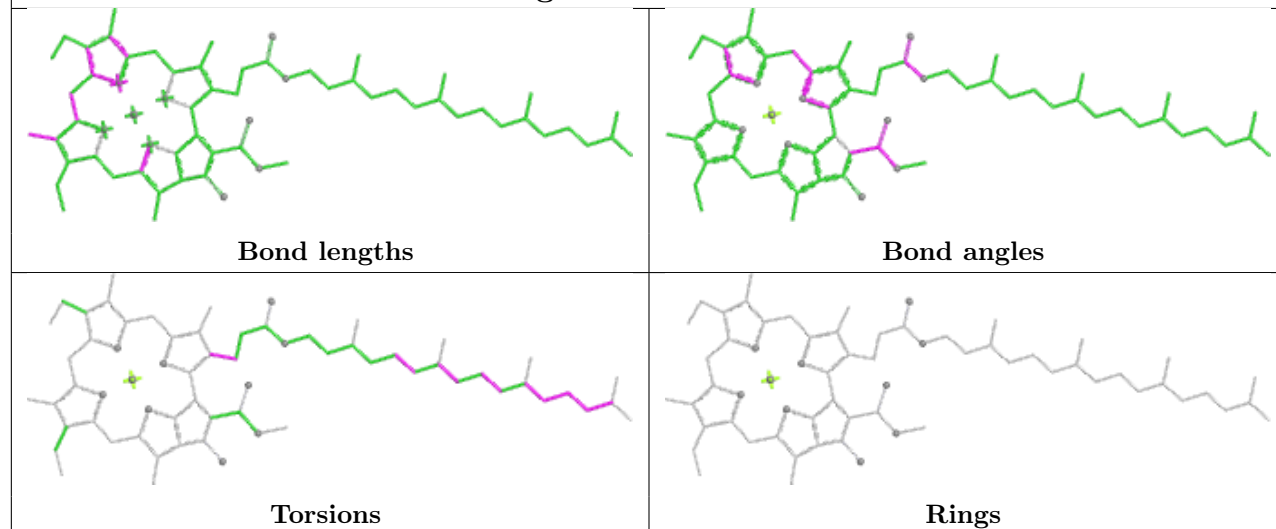
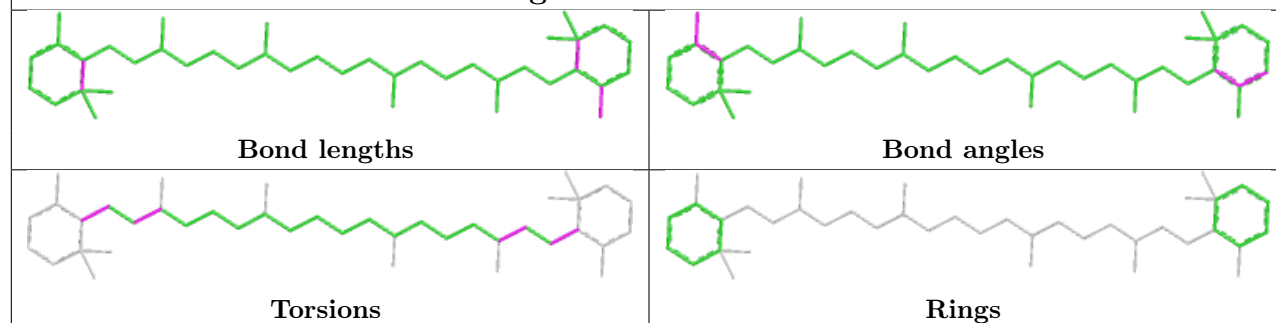


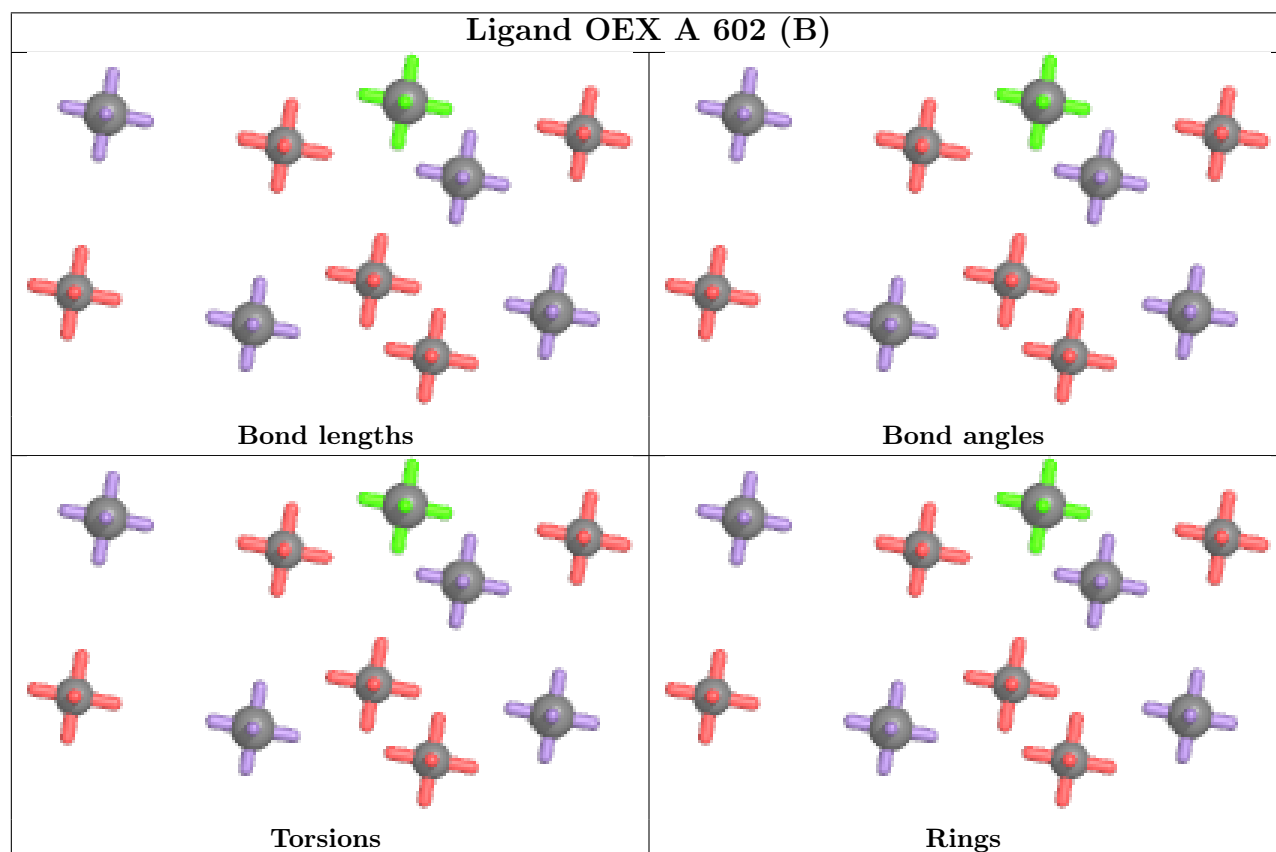
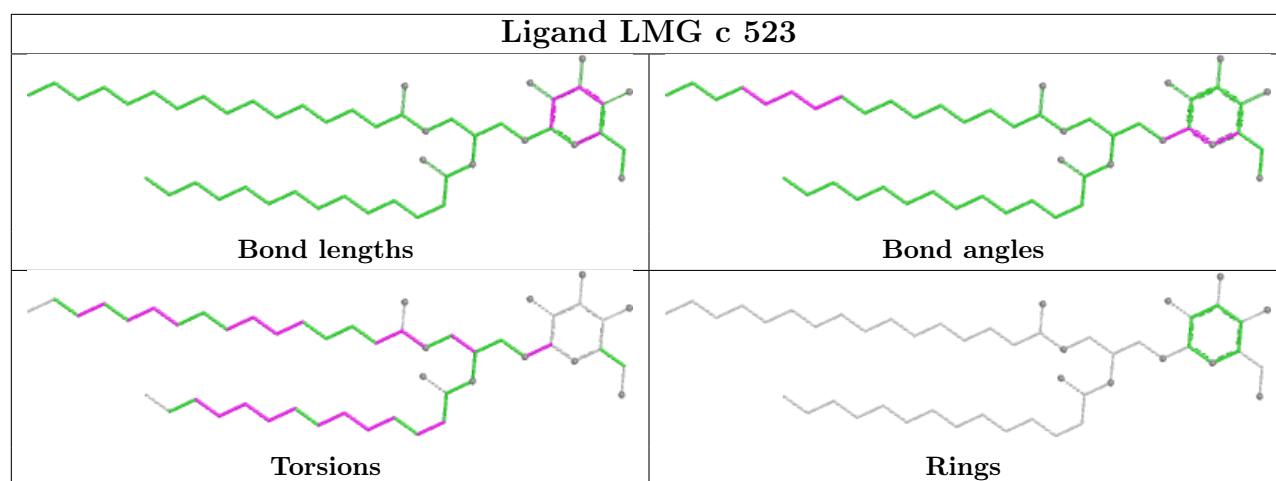
Ligand CLA B 610



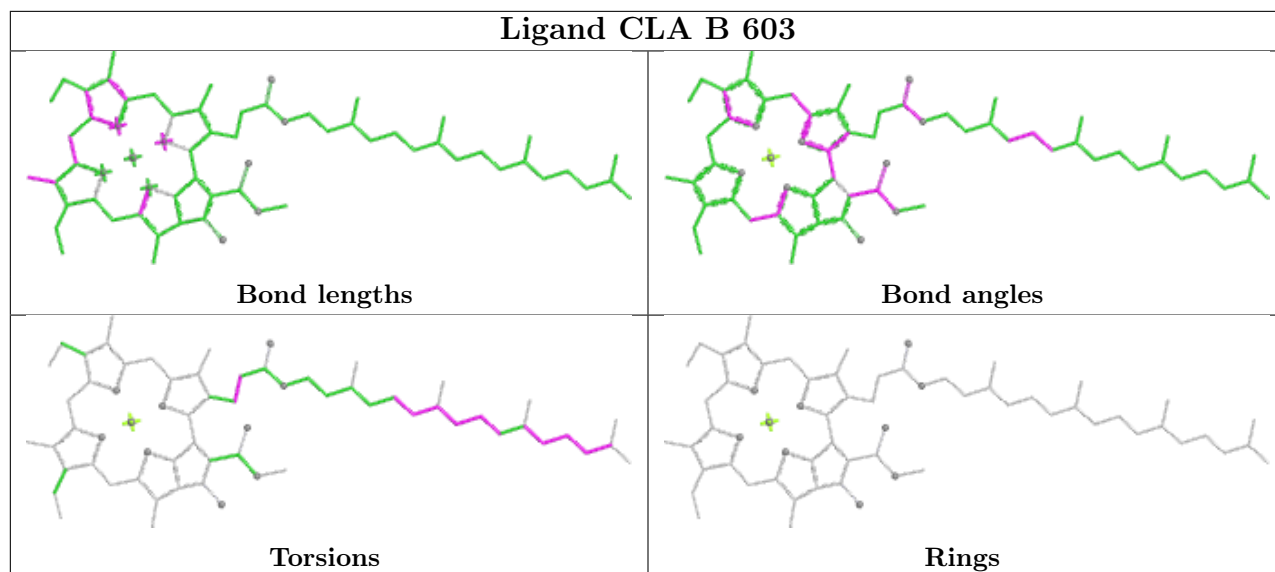
Ligand CLA B 608



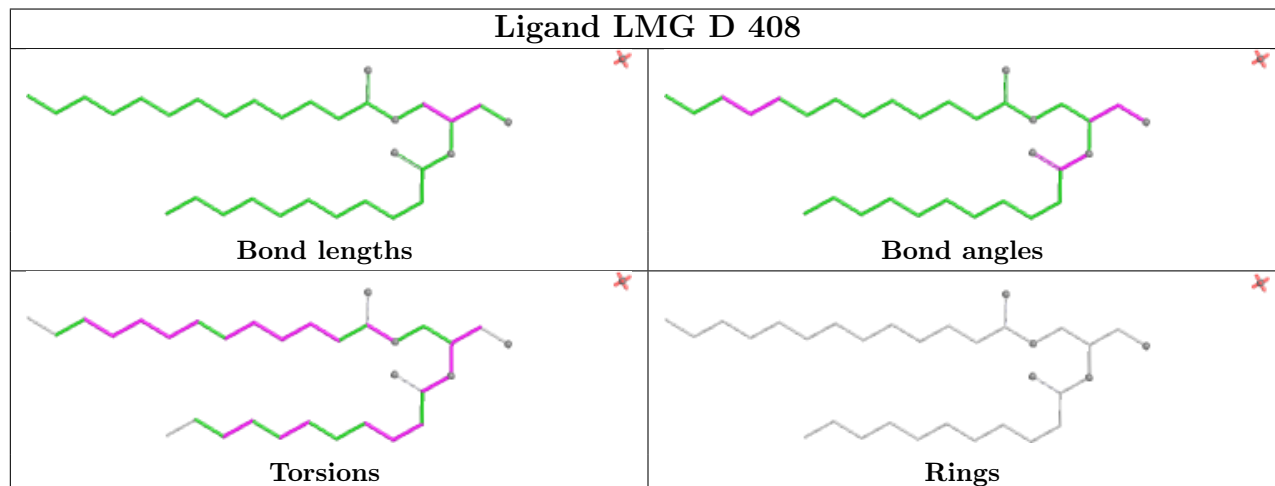
Ligand CLA B 601**Ligand CLA a 609****Ligand BCR K 101**



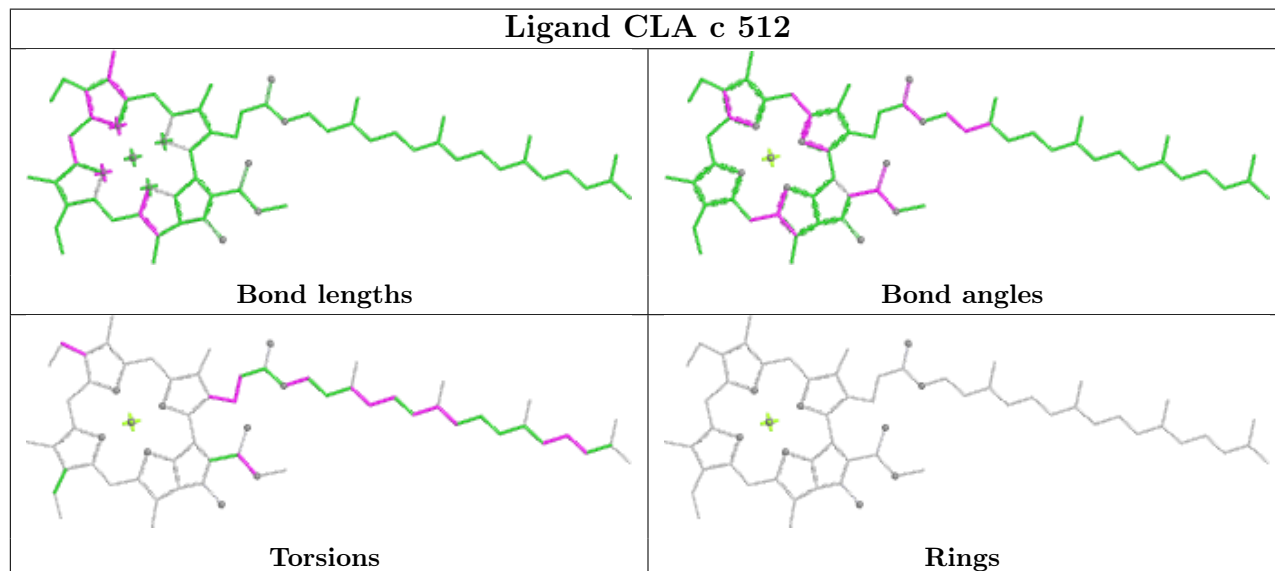
Ligand CLA B 603

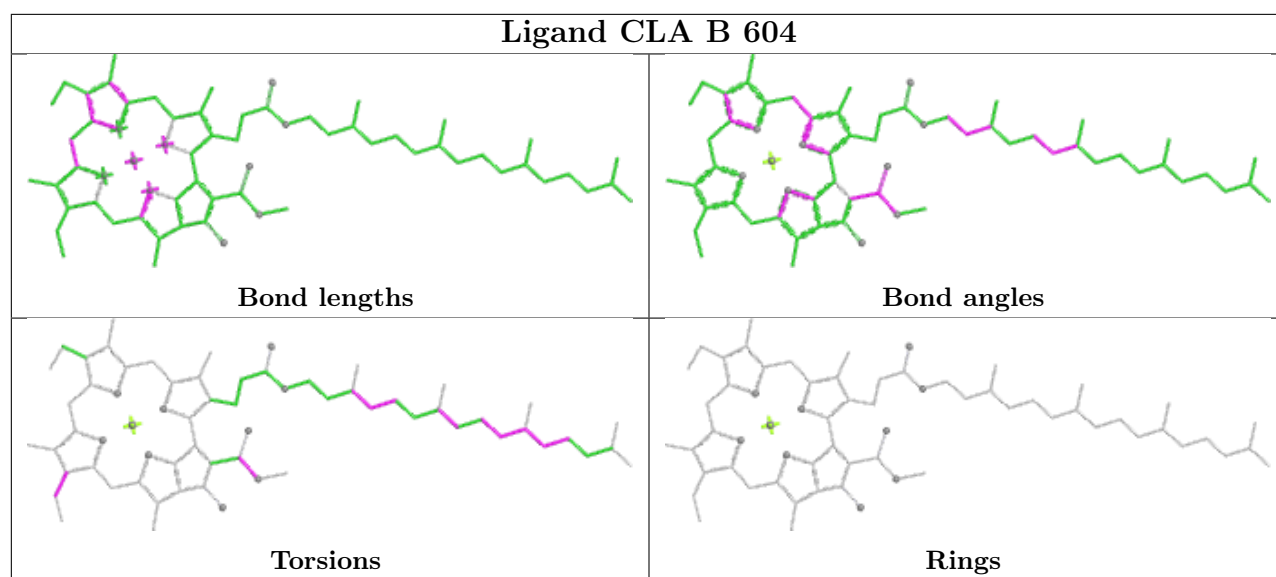


Ligand LMG D 408



Ligand CLA c 512





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	334/344 (97%)	-0.40	0 100 100	9, 31, 53, 81	64 (19%)
1	a	334/344 (97%)	-0.32	4 (1%) 76 78	9, 33, 64, 83	64 (19%)
2	B	505/510 (99%)	-0.33	2 (0%) 88 90	20, 35, 65, 96	4 (0%)
2	b	505/510 (99%)	-0.21	1 (0%) 91 92	27, 38, 78, 109	0
3	C	442/461 (95%)	-0.28	0 100 100	10, 39, 55, 78	11 (2%)
3	c	451/461 (97%)	-0.15	2 (0%) 88 90	10, 43, 63, 98	12 (2%)
4	D	341/352 (96%)	-0.45	0 100 100	11, 33, 52, 76	2 (0%)
4	d	341/352 (96%)	-0.33	1 (0%) 90 91	11, 37, 63, 86	3 (0%)
5	E	82/84 (97%)	0.35	1 (1%) 76 78	38, 57, 76, 87	1 (1%)
5	e	82/84 (97%)	0.58	3 (3%) 45 47	41, 65, 86, 97	0
6	F	34/45 (75%)	0.14	0 100 100	41, 49, 67, 88	0
6	f	34/45 (75%)	0.28	0 100 100	46, 55, 89, 108	0
7	H	65/66 (98%)	0.08	2 (3%) 51 54	37, 45, 62, 78	0
7	h	63/66 (95%)	0.38	2 (3%) 50 53	48, 56, 66, 72	0
8	I	35/38 (92%)	-0.16	0 100 100	32, 41, 65, 81	0
8	i	35/38 (92%)	-0.07	0 100 100	34, 43, 70, 86	0
9	J	36/40 (90%)	0.32	1 (2%) 55 57	40, 54, 84, 95	0
9	j	36/40 (90%)	0.43	0 100 100	41, 61, 97, 109	0
10	K	37/46 (80%)	0.16	0 100 100	48, 56, 70, 81	0
10	k	37/46 (80%)	0.33	0 100 100	53, 60, 77, 83	0
11	L	37/37 (100%)	-0.45	1 (2%) 56 59	27, 32, 63, 71	0
11	l	36/37 (97%)	-0.47	0 100 100	27, 33, 64, 79	0
12	M	32/36 (88%)	-0.36	0 100 100	29, 35, 61, 76	0
12	m	31/36 (86%)	-0.31	0 100 100	31, 36, 55, 66	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/272 (89%)	-0.06	4 (1%) 70 73	28, 44, 79, 137	1 (0%)
13	o	244/272 (89%)	-0.09	2 (0%) 82 84	28, 42, 78, 122	0
14	T	29/32 (90%)	-0.48	0 100 100	28, 33, 58, 77	0
14	t	29/32 (90%)	-0.26	2 (6%) 23 24	29, 35, 75, 90	0
15	U	97/134 (72%)	-0.12	0 100 100	35, 45, 68, 90	0
15	u	97/134 (72%)	-0.16	0 100 100	33, 43, 59, 85	0
16	V	137/163 (84%)	-0.22	0 100 100	33, 42, 58, 70	0
16	v	137/163 (84%)	0.00	0 100 100	38, 50, 69, 86	0
17	Y	27/46 (58%)	1.07	5 (18%) 3 3	58, 76, 110, 114	0
17	y	30/46 (65%)	0.94	0 100 100	68, 80, 98, 101	0
18	X	38/41 (92%)	0.23	1 (2%) 57 60	47, 59, 77, 83	0
18	x	39/41 (95%)	0.61	2 (5%) 33 35	59, 69, 92, 104	0
19	Z	62/62 (100%)	0.96	5 (8%) 18 19	59, 75, 112, 129	0
19	z	62/62 (100%)	0.90	4 (6%) 25 26	65, 76, 116, 122	0
20	R	34/41 (82%)	1.07	4 (11%) 9 9	68, 74, 87, 93	0
20	r	31/41 (75%)	1.29	3 (9%) 13 14	77, 89, 107, 110	0
All	All	5302/5700 (93%)	-0.13	52 (0%) 79 81	9, 41, 77, 137	162 (3%)

The worst 5 of 52 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
19	Z	62	VAL	5.3
7	h	64	ALA	3.6
18	x	37	VAL	3.4
20	R	35	LEU	3.4
3	c	23	ALA	3.1

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

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
14	FME	t	1	10/11	0.91	0.10	33,37,56,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
12	FME	M	1	10/11	0.93	0.10	37,53,63,64	0
12	FME	m	1	10/11	0.95	0.09	30,49,65,66	0
14	FME	T	1	10/11	0.95	0.11	33,37,51,70	0
8	FME	I	1	10/11	0.97	0.07	37,48,53,55	0
8	FME	i	1	10/11	0.97	0.07	41,49,53,55	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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($\text{\AA}^2$)	Q<0.9
34	STE	H	102	18/20	0.71	0.18	58,70,75,81	0
31	LHG	A	617	49/49	0.73	0.17	55,79,98,109	0
34	STE	a	615	12/20	0.73	0.14	54,63,79,81	0
30	LMG	b	621	55/55	0.74	0.19	57,69,86,89	0
30	LMG	c	522	48/55	0.76	0.15	60,73,85,89	0
33	DGD	a	614	44/66	0.78	0.15	38,54,67,71	0
30	LMG	d	410	23/55	0.78	0.19	52,65,73,74	0
26	CLA	h	101	65/65	0.78	0.14	55,72,92,97	0
31	LHG	e	102	42/49	0.79	0.14	60,86,104,113	0
29	PL9	A	612	55/55	0.79	0.16	44,63,82,88	0
34	STE	b	622	20/20	0.79	0.14	51,60,67,70	0
34	STE	d	414	20/20	0.79	0.16	46,52,62,65	0
34	STE	L	102	12/20	0.80	0.19	48,60,76,76	0
34	STE	k	102	12/20	0.80	0.12	60,70,74,75	0
29	PL9	a	611	55/55	0.82	0.15	50,66,78,86	0
32	SQD	t	102	36/54	0.82	0.14	40,59,75,76	0
30	LMG	D	408	33/55	0.82	0.14	44,59,81,83	0
34	STE	d	412	16/20	0.83	0.16	54,63,78,81	0
34	STE	J	101	12/20	0.83	0.15	57,62,72,72	0
33	DGD	A	619	66/66	0.83	0.12	47,59,67,76	0
34	STE	B	625	16/20	0.84	0.14	51,55,66,69	0
30	LMG	A	614	48/55	0.84	0.11	37,58,68,72	0
34	STE	b	623	10/20	0.84	0.15	46,56,62,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	LMG	c	520	37/55	0.84	0.12	52,68,80,83	0
26	CLA	B	601	65/65	0.84	0.12	41,63,87,94	0
34	STE	T	103	15/20	0.84	0.16	46,51,67,68	0
34	STE	F	103	12/20	0.85	0.13	58,75,86,89	0
34	STE	T	102	16/20	0.85	0.16	38,48,58,60	0
32	SQD	A	618	39/54	0.85	0.13	42,55,78,80	0
34	STE	C	520	12/20	0.85	0.13	48,55,59,63	0
34	STE	j	101	12/20	0.85	0.12	52,56,64,65	0
34	STE	b	620	20/20	0.85	0.13	42,56,76,78	0
34	STE	t	104	10/20	0.85	0.12	46,53,59,60	0
34	STE	B	624	12/20	0.86	0.12	50,52,71,73	0
32	SQD	f	101	41/54	0.86	0.14	62,81,91,95	0
30	LMG	C	518	48/55	0.86	0.13	48,68,82,86	0
30	LMG	c	523	49/55	0.86	0.10	41,56,78,83	0
30	LMG	B	621	28/55	0.86	0.13	40,50,64,67	0
34	STE	B	620	17/20	0.86	0.13	40,51,67,68	0
34	STE	C	519	12/20	0.87	0.14	39,47,51,53	0
34	STE	B	623	12/20	0.87	0.13	47,58,66,68	0
34	STE	C	521	16/20	0.87	0.11	39,49,64,64	0
34	STE	X	102	20/20	0.87	0.12	37,49,70,73	0
34	STE	c	521	20/20	0.87	0.13	50,56,82,82	0
34	STE	I	101	15/20	0.88	0.13	44,52,59,62	0
32	SQD	F	102	36/54	0.88	0.14	55,72,80,82	0
28	BCR	K	101	40/40	0.88	0.10	46,55,61,68	0
34	STE	t	103	14/20	0.88	0.11	38,49,60,60	0
34	STE	d	413	17/20	0.88	0.13	43,52,67,69	0
34	STE	t	105	18/20	0.88	0.12	44,57,86,87	0
28	BCR	d	405	40/40	0.89	0.10	42,50,79,84	0
28	BCR	h	102	40/40	0.89	0.11	42,58,68,68	0
33	DGD	C	516	62/66	0.89	0.11	36,49,88,96	0
32	SQD	B	622	54/54	0.89	0.11	39,60,80,86	0
30	LMG	m	101	51/55	0.89	0.10	33,48,64,66	0
32	SQD	a	613	54/54	0.89	0.11	45,60,75,81	0
32	SQD	b	619	49/54	0.89	0.10	37,56,72,77	0
30	LMG	M	101	51/55	0.89	0.10	31,48,67,68	0
33	DGD	H	101	62/66	0.90	0.10	38,47,56,61	0
26	CLA	C	513	65/65	0.90	0.10	50,57,77,85	0
33	DGD	h	103	62/66	0.90	0.10	38,50,59,62	0
34	STE	M	103	10/20	0.90	0.13	44,48,59,61	0
28	BCR	D	404	40/40	0.91	0.09	37,45,79,85	0
33	DGD	c	518	62/66	0.91	0.10	39,52,76,81	0
26	CLA	c	512	65/65	0.91	0.10	46,58,77,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
28	BCR	k	101	40/40	0.91	0.11	49,61,68,73	0
28	BCR	X	101	40/40	0.91	0.10	39,50,56,63	0
34	STE	l	102	18/20	0.91	0.12	36,41,68,73	0
28	BCR	Z	101	40/40	0.91	0.11	50,56,62,64	0
28	BCR	b	618	40/40	0.91	0.09	33,45,59,61	0
28	BCR	c	514	40/40	0.91	0.11	52,61,65,68	0
32	SQD	A	616	52/54	0.92	0.10	35,56,80,84	0
26	CLA	c	513	65/65	0.92	0.10	53,66,83,88	0
34	STE	M	102	15/20	0.92	0.10	37,44,53,64	0
26	CLA	C	503	65/65	0.92	0.09	36,42,49,54	0
28	BCR	B	618	40/40	0.92	0.07	26,37,46,48	0
28	BCR	c	516	40/40	0.92	0.12	52,59,63,68	0
30	LMG	D	406	51/55	0.92	0.09	36,52,71,74	0
28	BCR	t	101	40/40	0.93	0.07	29,38,48,51	0
28	BCR	b	616	40/40	0.93	0.08	30,40,48,48	0
28	BCR	b	617	40/40	0.93	0.07	27,36,46,47	0
26	CLA	C	512	65/65	0.93	0.10	40,51,75,81	0
26	CLA	c	508	64/65	0.93	0.09	36,43,81,96	0
28	BCR	K	102	40/40	0.93	0.10	38,51,62,64	0
31	LHG	A	615	47/49	0.93	0.11	30,45,70,80	0
28	BCR	T	101	40/40	0.93	0.07	33,39,47,52	0
31	LHG	d	409	39/49	0.93	0.09	37,43,51,54	0
28	BCR	B	619	40/40	0.93	0.08	33,41,54,60	0
28	BCR	C	514	40/40	0.93	0.09	31,41,51,54	0
26	CLA	c	511	65/65	0.94	0.10	44,56,70,72	0
31	LHG	D	409	49/49	0.94	0.09	29,40,53,59	0
31	LHG	d	407	49/49	0.94	0.09	32,45,61,66	0
25	BCT	d	401	4/4	0.94	0.08	32,36,43,48	0
26	CLA	C	506	65/65	0.94	0.09	32,42,74,77	0
26	CLA	C	508	65/65	0.94	0.09	34,41,87,91	0
28	BCR	A	611	40/40	0.94	0.07	25,33,38,41	0
28	BCR	B	617	40/40	0.94	0.08	30,38,48,53	0
26	CLA	C	510	65/65	0.94	0.08	30,43,57,73	0
26	CLA	C	511	65/65	0.94	0.10	33,48,60,63	0
26	CLA	B	606	65/65	0.94	0.08	27,35,61,69	0
26	CLA	B	616	60/65	0.94	0.08	26,36,76,89	0
26	CLA	a	607	65/65	0.94	0.09	29,37,86,95	0
26	CLA	b	605	65/65	0.94	0.08	31,39,60,71	0
33	DGD	C	515	62/66	0.94	0.09	25,36,63,70	0
26	CLA	b	613	65/65	0.94	0.09	28,37,66,71	0
33	DGD	C	517	62/66	0.94	0.08	30,44,69,75	0
26	CLA	c	503	65/65	0.94	0.08	37,45,51,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
26	CLA	c	504	60/65	0.94	0.08	31,45,69,74	0
33	DGD	c	517	62/66	0.94	0.08	30,38,60,67	0
26	CLA	c	506	65/65	0.94	0.09	39,46,72,76	0
33	DGD	c	519	62/66	0.94	0.09	33,48,71,80	0
26	CLA	c	507	65/65	0.94	0.08	33,41,50,53	0
26	CLA	C	502	65/65	0.94	0.08	30,39,51,56	0
30	LMG	d	411	44/55	0.94	0.09	41,52,72,76	0
26	CLA	c	510	65/65	0.94	0.08	34,44,56,63	0
28	BCR	c	515	40/40	0.94	0.09	33,47,53,56	0
26	CLA	c	502	65/65	0.95	0.07	34,41,53,58	0
26	CLA	C	501	65/65	0.95	0.07	25,35,49,53	0
25	BCT	A	606	4/4	0.95	0.09	35,35,39,40	0
26	CLA	c	505	65/65	0.95	0.07	33,41,56,64	0
26	CLA	a	606	65/65	0.95	0.07	23,31,37,47	0
29	PL9	D	405	55/55	0.95	0.07	24,31,38,39	0
26	CLA	C	509	65/65	0.95	0.09	34,42,57,59	0
29	PL9	d	406	55/55	0.95	0.07	25,33,38,41	0
26	CLA	a	609	65/65	0.95	0.09	24,30,68,76	0
26	CLA	c	509	65/65	0.95	0.09	38,45,57,61	0
26	CLA	b	601	65/65	0.95	0.08	34,42,54,60	0
26	CLA	B	602	65/65	0.95	0.07	28,37,55,57	0
28	BCR	a	610	40/40	0.95	0.06	20,34,43,45	0
26	CLA	b	607	65/65	0.95	0.07	33,41,59,66	0
26	CLA	C	504	59/65	0.95	0.08	35,43,75,82	0
26	CLA	d	404	65/65	0.95	0.08	34,43,83,86	0
26	CLA	b	614	65/65	0.95	0.07	31,40,53,58	0
27	PHO	d	402	64/64	0.95	0.06	30,39,45,49	0
26	CLA	b	615	60/65	0.95	0.08	31,41,84,91	0
26	CLA	b	611	65/65	0.96	0.07	26,32,40,42	0
26	CLA	b	612	65/65	0.96	0.07	25,32,62,72	0
26	CLA	C	507	65/65	0.96	0.07	31,38,51,52	0
26	CLA	B	610	65/65	0.96	0.07	24,31,40,42	0
26	CLA	B	611	65/65	0.96	0.06	20,30,38,46	0
26	CLA	c	501	65/65	0.96	0.07	28,38,47,53	0
26	CLA	B	612	65/65	0.96	0.06	22,28,35,42	0
26	CLA	B	614	65/65	0.96	0.08	23,35,64,75	0
26	CLA	B	615	65/65	0.96	0.07	25,37,51,61	0
31	LHG	L	101	49/49	0.96	0.07	31,38,51,54	0
26	CLA	A	613	65/65	0.96	0.06	24,29,38,46	0
31	LHG	d	408	49/49	0.96	0.07	27,39,48,55	0
26	CLA	D	403	65/65	0.96	0.08	30,36,90,103	0
26	CLA	B	603	65/65	0.96	0.07	26,31,54,59	0

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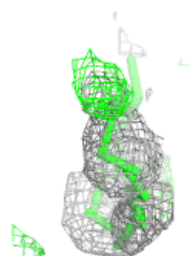
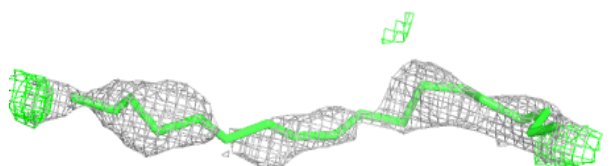
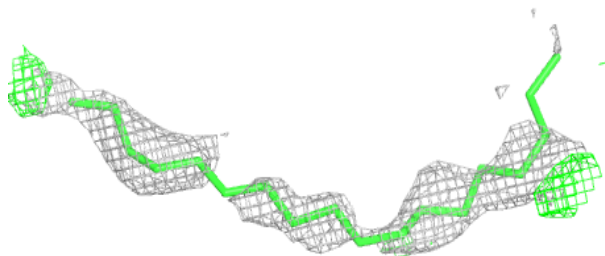
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	LHG	l	101	49/49	0.96	0.07	31,41,48,56	0
26	CLA	B	604	65/65	0.96	0.07	22,30,65,68	0
26	CLA	A	608	65/65	0.96	0.08	24,33,83,90	0
26	CLA	a	612	65/65	0.96	0.06	22,30,39,44	0
26	CLA	B	607	65/65	0.96	0.06	20,29,54,58	0
26	CLA	b	602	65/65	0.96	0.07	25,34,59,70	0
26	CLA	b	603	65/65	0.96	0.07	26,33,66,79	0
26	CLA	d	403	65/65	0.96	0.07	24,32,52,56	0
26	CLA	b	604	65/65	0.96	0.06	24,35,44,49	0
26	CLA	C	505	65/65	0.96	0.08	24,37,56,59	0
27	PHO	A	609	64/64	0.96	0.06	23,27,35,38	0
27	PHO	D	401	64/64	0.96	0.06	25,33,38,43	0
27	PHO	a	608	64/64	0.96	0.06	24,29,35,40	0
26	CLA	b	606	65/65	0.96	0.07	23,30,54,62	0
26	CLA	B	609	65/65	0.96	0.07	27,40,51,62	0
26	CLA	b	608	65/65	0.96	0.07	32,43,63,70	0
26	CLA	b	609	65/65	0.96	0.07	30,37,45,49	0
26	CLA	b	610	65/65	0.96	0.06	25,32,45,53	0
35	HEM	e	101	43/43	0.96	0.10	54,63,79,83	0
26	CLA	D	402	65/65	0.97	0.06	22,27,47,58	0
26	CLA	B	605	65/65	0.97	0.06	23,31,41,45	0
31	LHG	D	407	49/49	0.97	0.06	26,37,44,54	0
26	CLA	B	608	65/65	0.97	0.06	25,34,53,56	0
26	CLA	A	607	65/65	0.97	0.05	21,29,37,41	0
35	HEM	F	101	43/43	0.97	0.08	45,52,63,72	0
26	CLA	B	613	65/65	0.97	0.06	22,29,60,68	0
26	CLA	A	610	54/65	0.98	0.05	22,28,58,60	0
24	CL	A	604	1/1	0.98	0.04	34,34,34,34	0
36	HEC	V	201	43/43	0.98	0.05	26,33,40,47	0
36	HEC	v	201	43/43	0.98	0.07	32,38,46,50	0
24	CL	a	604	1/1	0.99	0.05	32,32,32,32	0
24	CL	a	605	1/1	0.99	0.12	30,30,30,30	0
21	OEY	A	601[C]	11/11	0.99	0.04	28,30,33,36	11
21	OEY	a	601[A]	11/11	0.99	0.03	31,35,39,39	11
21	OEY	a	601[C]	11/11	0.99	0.03	26,28,35,37	11
22	OEX	A	602[B]	10/10	0.99	0.03	27,31,34,34	10
22	OEX	a	602[B]	10/10	0.99	0.03	26,31,33,33	10
21	OEY	A	601[A]	11/11	0.99	0.04	31,34,38,38	11
24	CL	A	605	1/1	0.99	0.04	35,35,35,35	0
23	FE2	A	603	1/1	1.00	0.02	29,29,29,29	0
23	FE2	a	603	1/1	1.00	0.03	36,36,36,36	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.

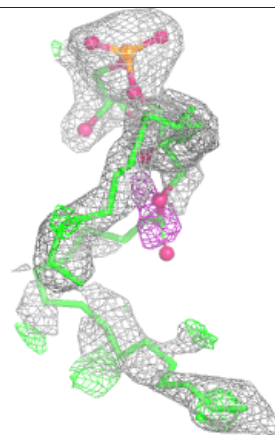
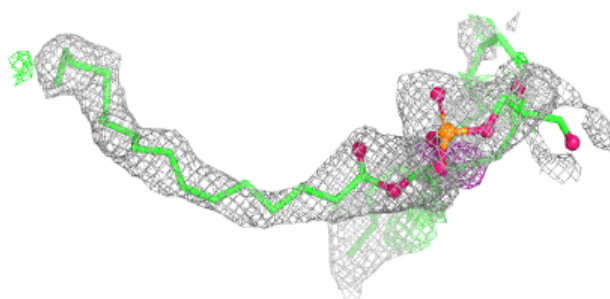
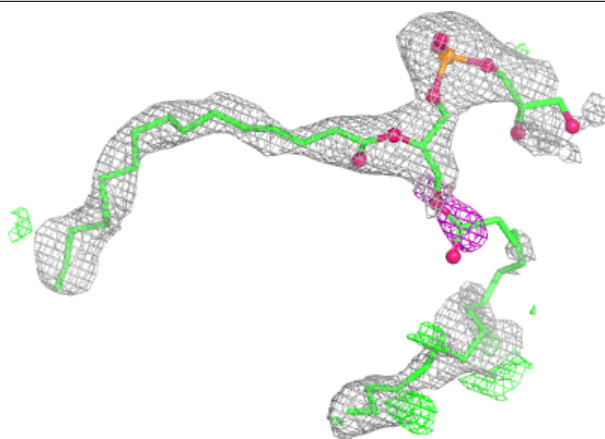
Electron density around STE H 102:

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

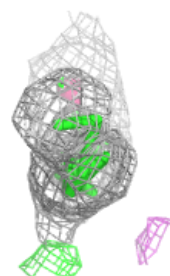
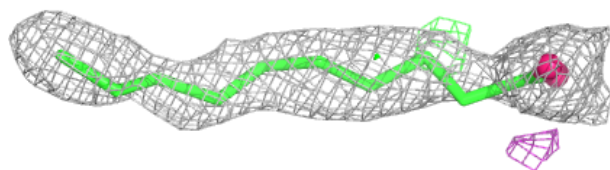
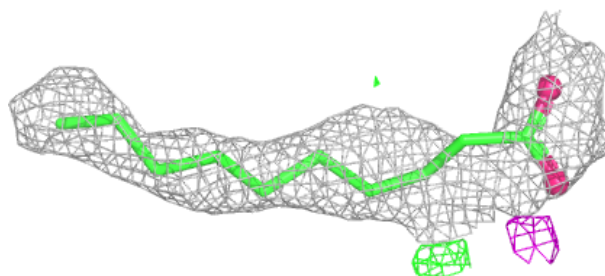


Electron density around LHG A 617:

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

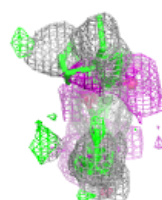
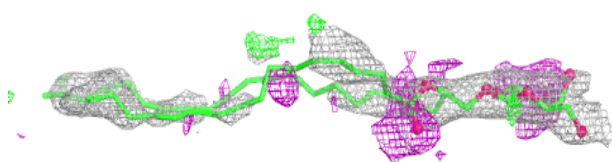
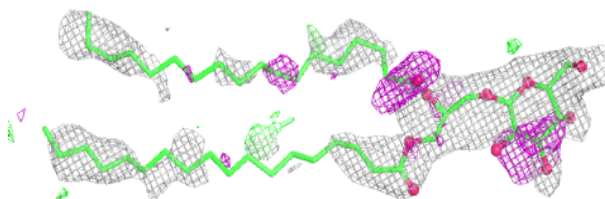
**Electron density around STE a 615:**

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

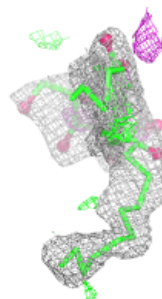
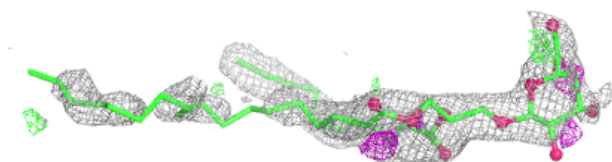
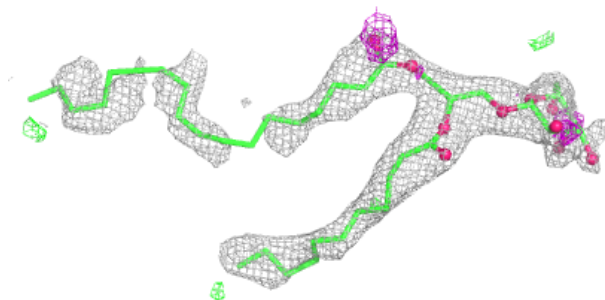


Electron density around LMG b 621:

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

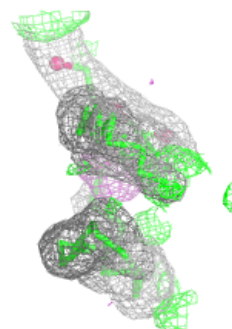
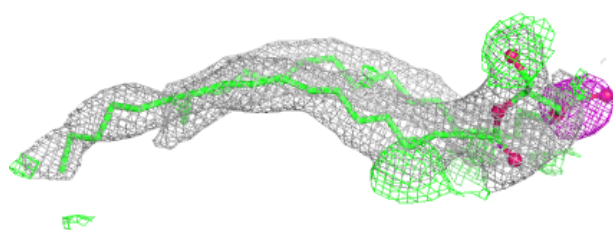
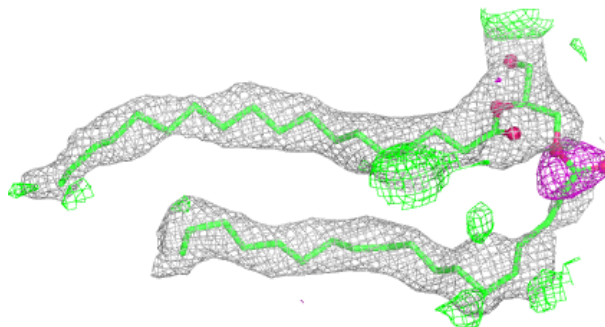
**Electron density around LMG c 522:**

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

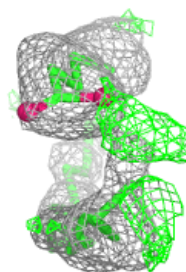
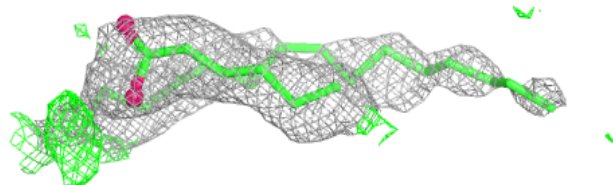
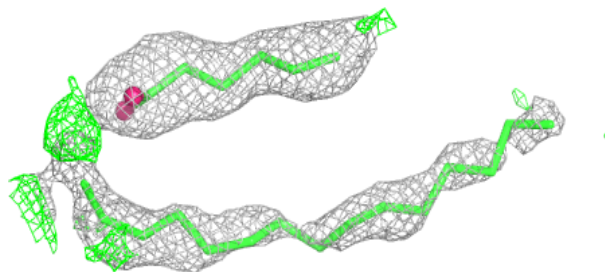


Electron density around DGD a 614:

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

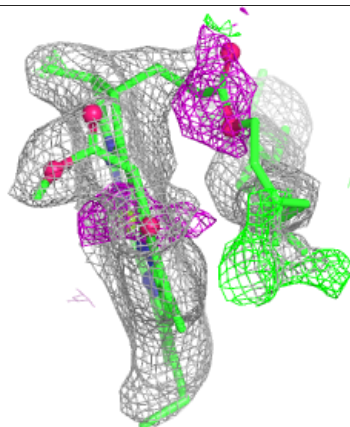
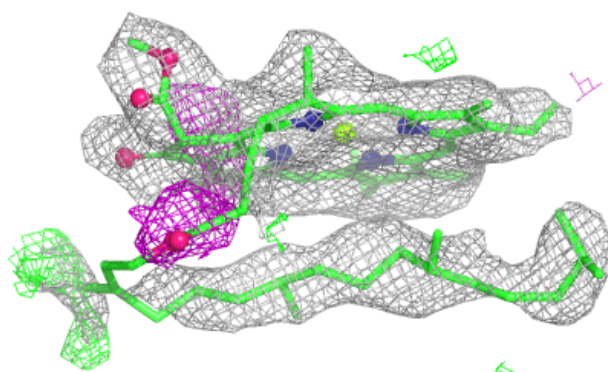
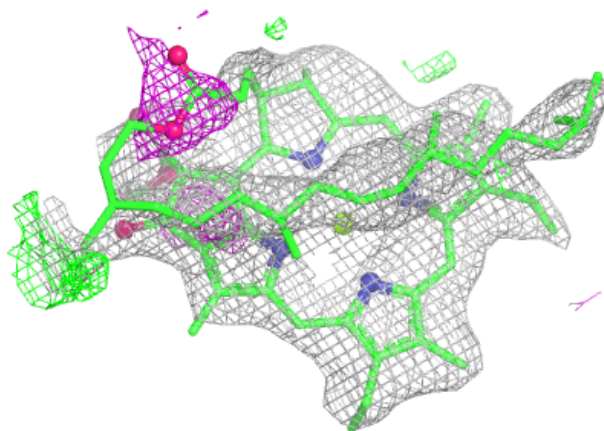
**Electron density around LMG d 410:**

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

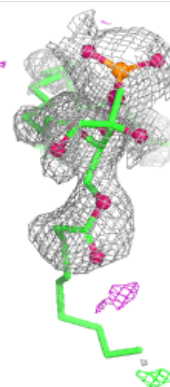
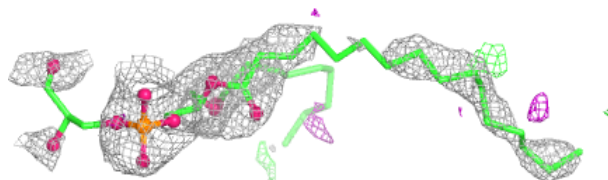
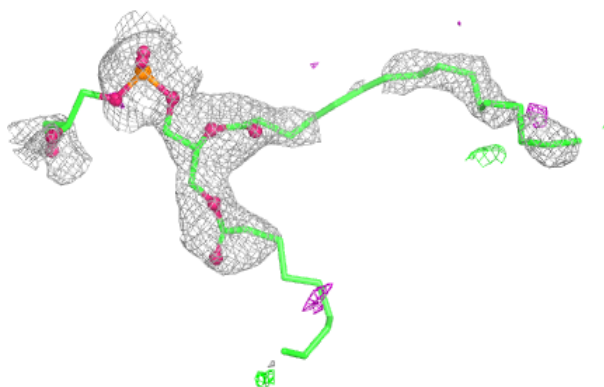


Electron density around CLA h 101:

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

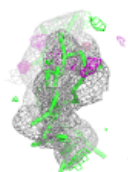
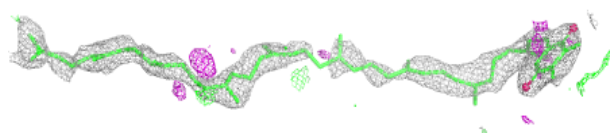
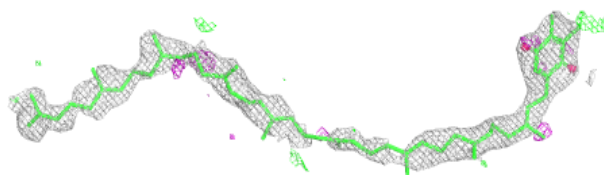
**Electron density around LHG e 102:**

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

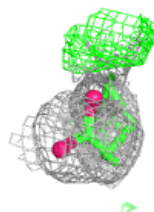
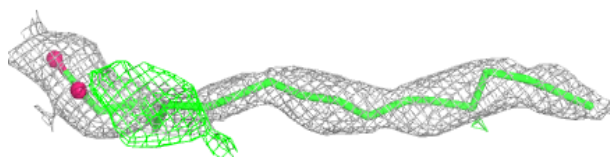
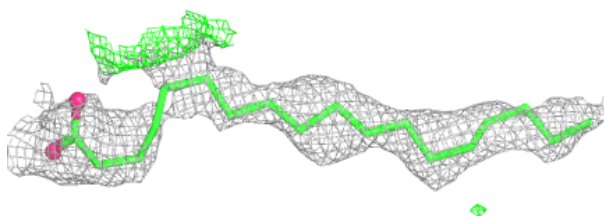


Electron density around PL9 A 612:

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

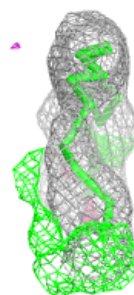
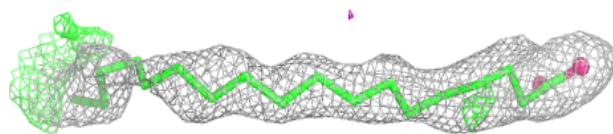
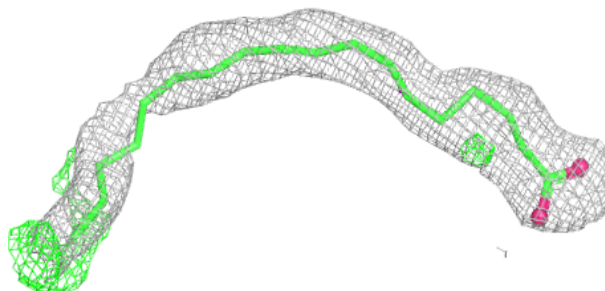
**Electron density around STE b 622:**

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

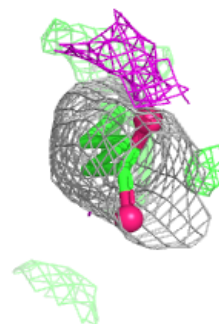
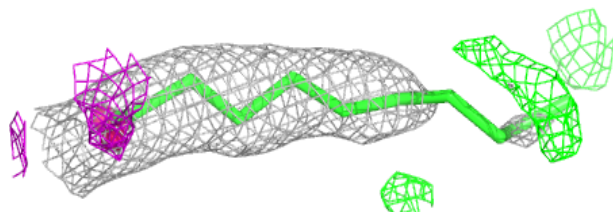
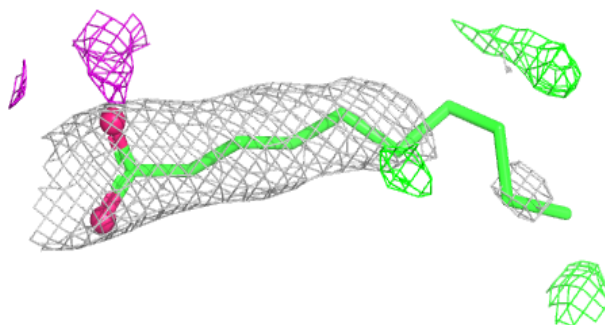


Electron density around STE d 414:

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

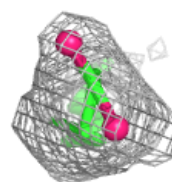
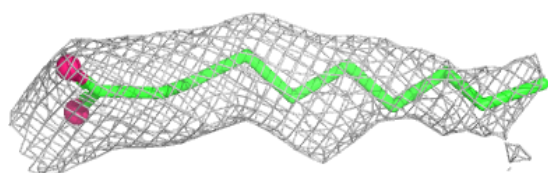
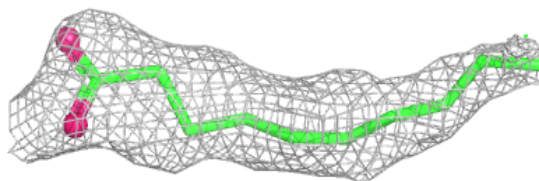
**Electron density around STE L 102:**

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

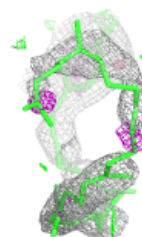
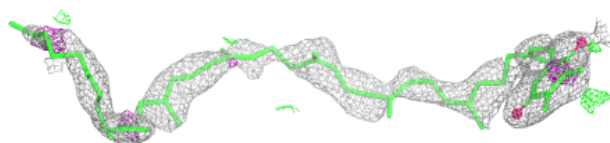
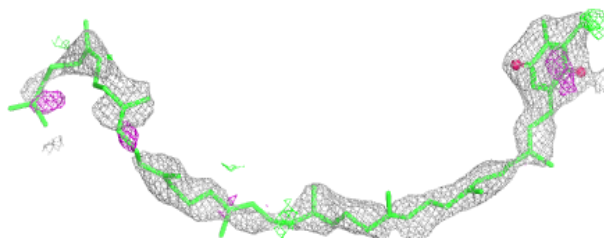


Electron density around STE k 102:

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

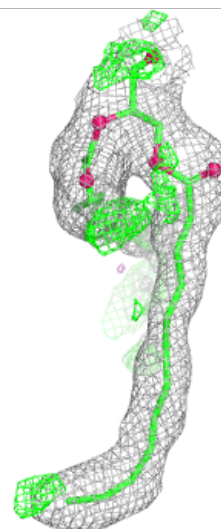
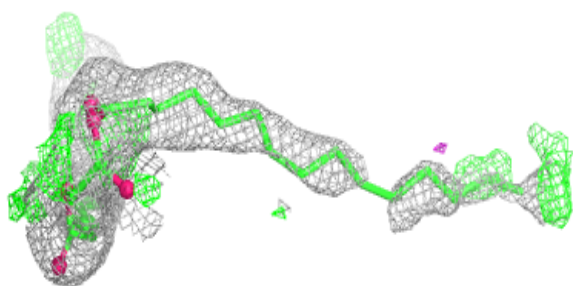
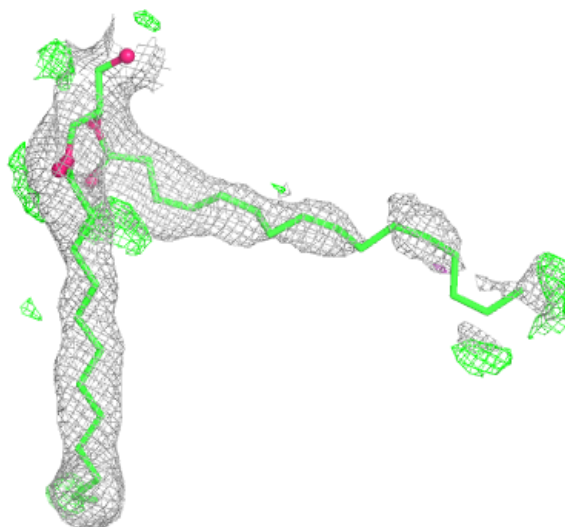
**Electron density around PL9 a 611:**

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



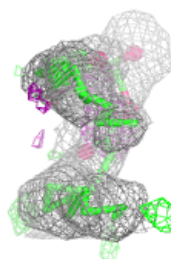
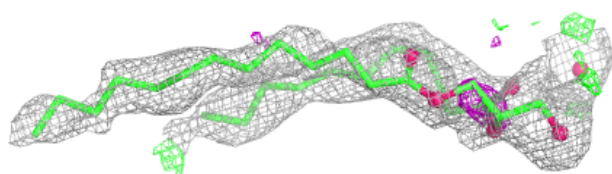
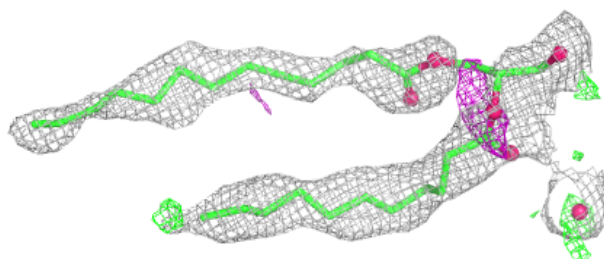
Electron density around SQD t 102:

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

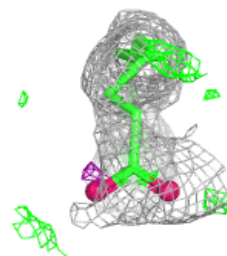
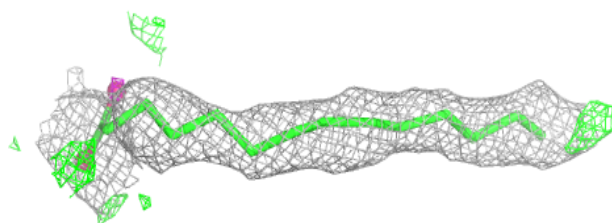
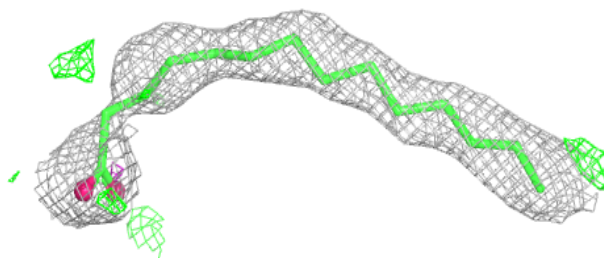


Electron density around LMG D 408:

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

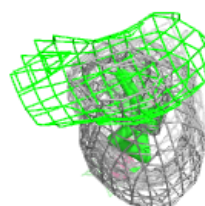
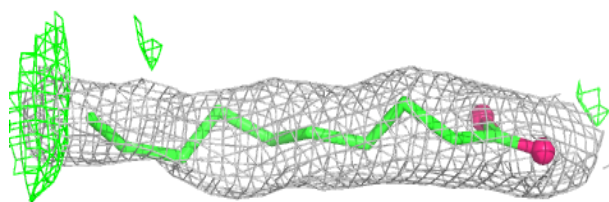
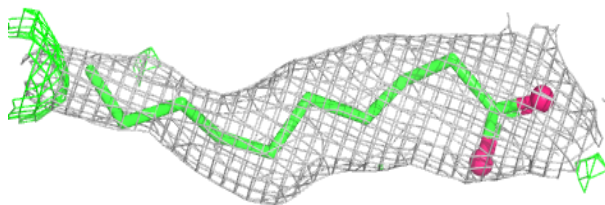
**Electron density around STE d 412:**

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

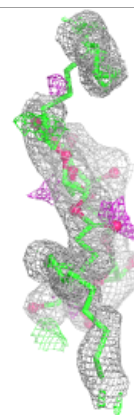
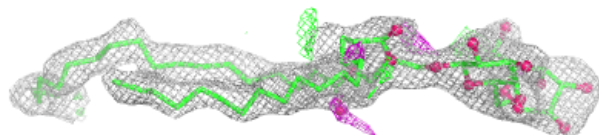
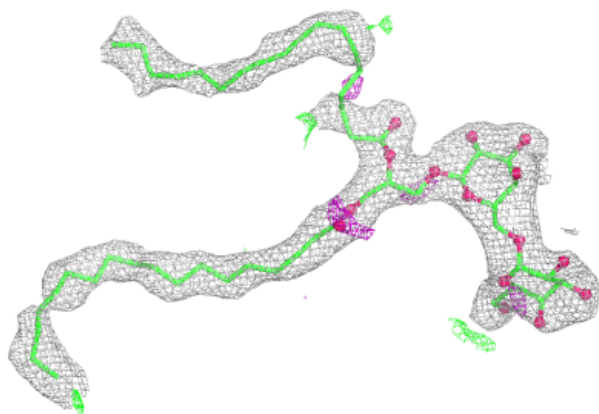


Electron density around STE J 101:

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

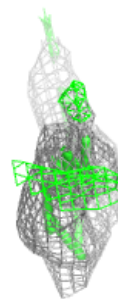
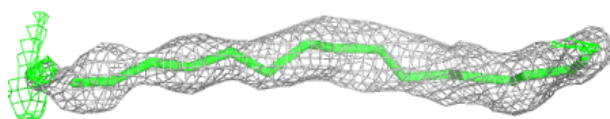
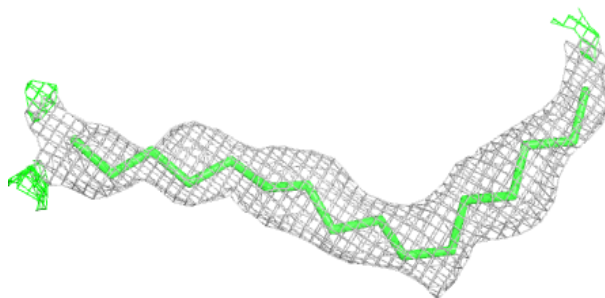
**Electron density around DGD A 619:**

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

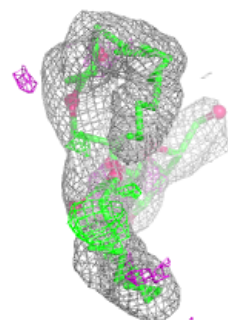
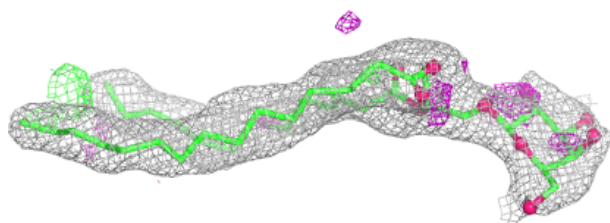
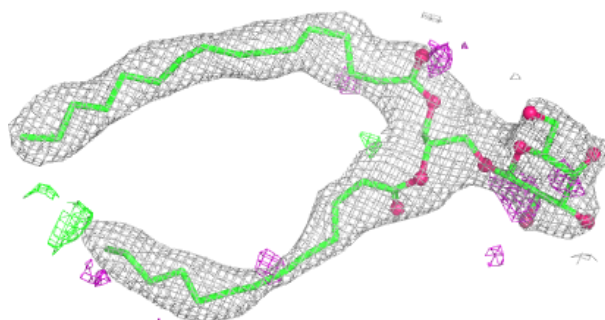


Electron density around STE B 625:

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

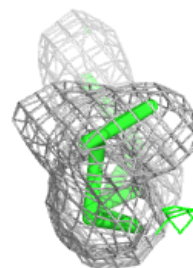
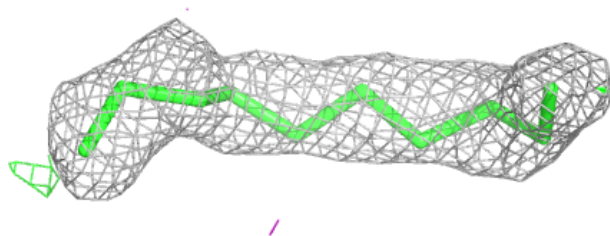
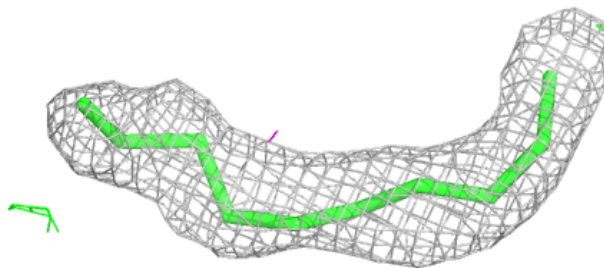
**Electron density around LMG A 614:**

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

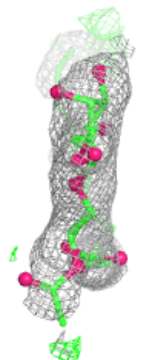
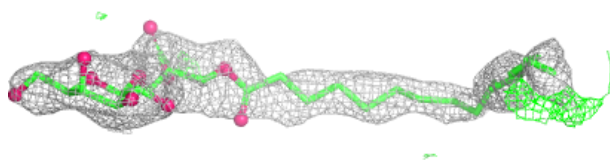
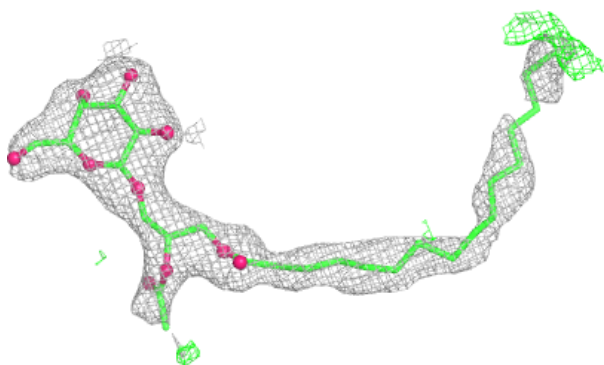


Electron density around STE b 623:

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

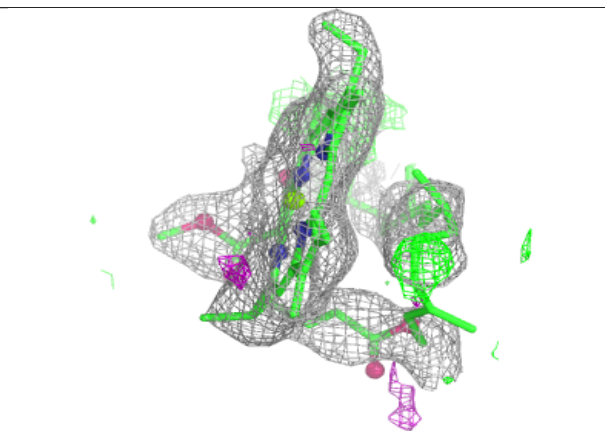
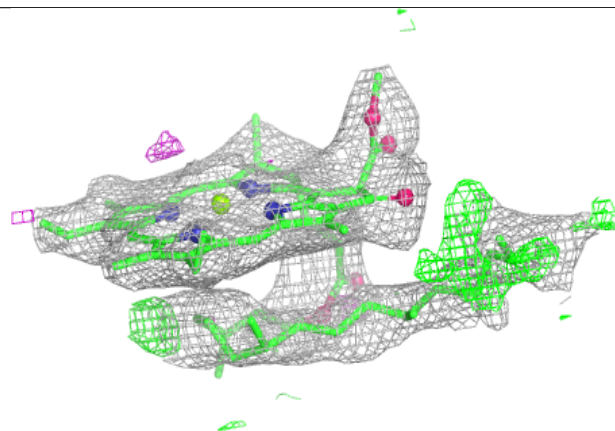
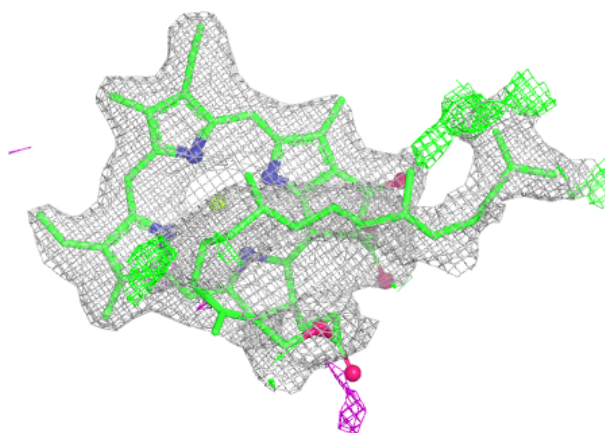
**Electron density around LMG c 520:**

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

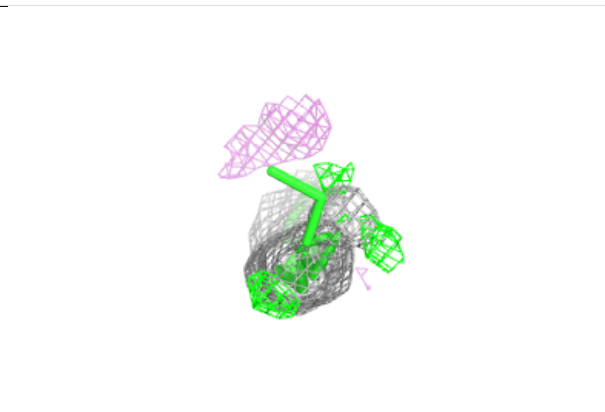
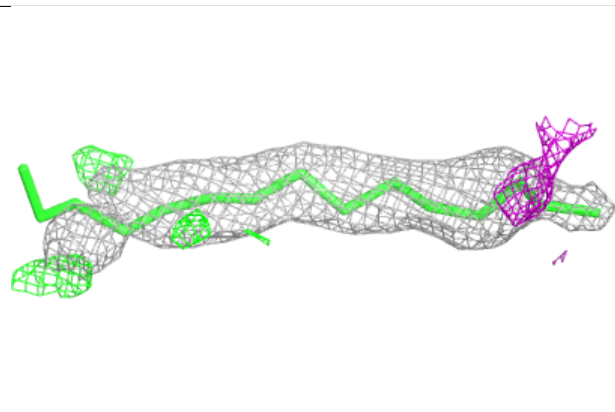
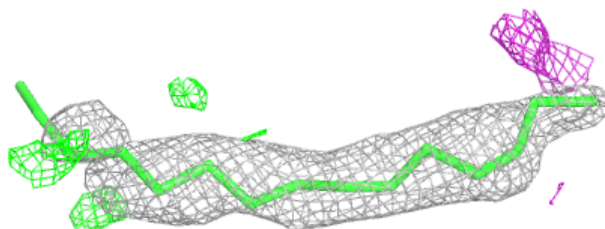


Electron density around CLA B 601:

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

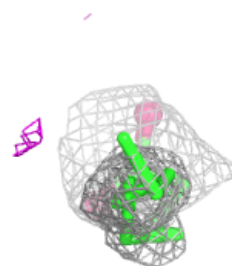
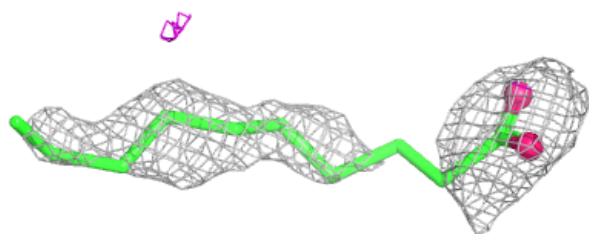
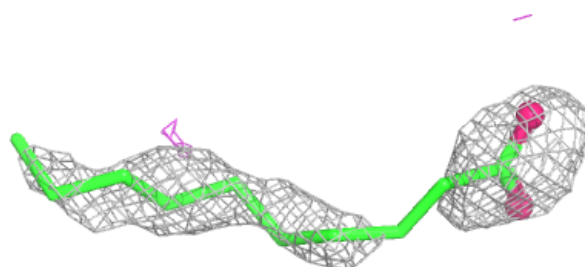
**Electron density around STE T 103:**

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

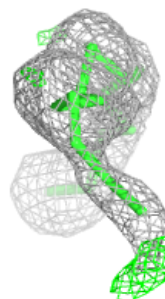
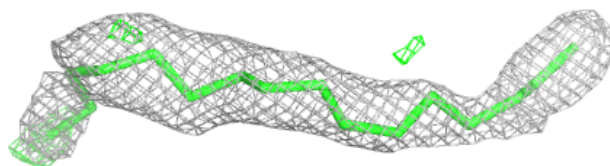
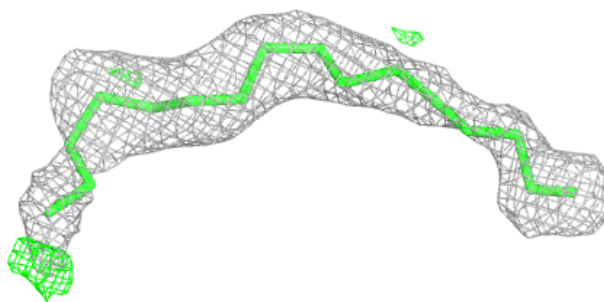


Electron density around STE F 103:

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

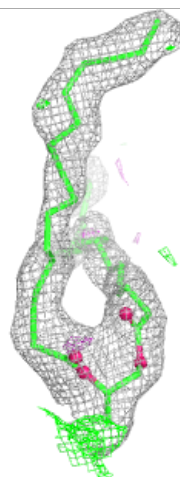
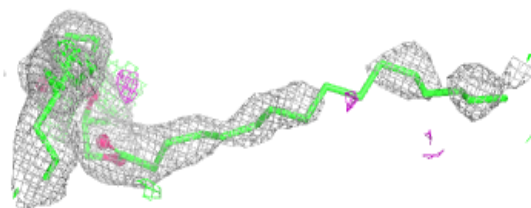
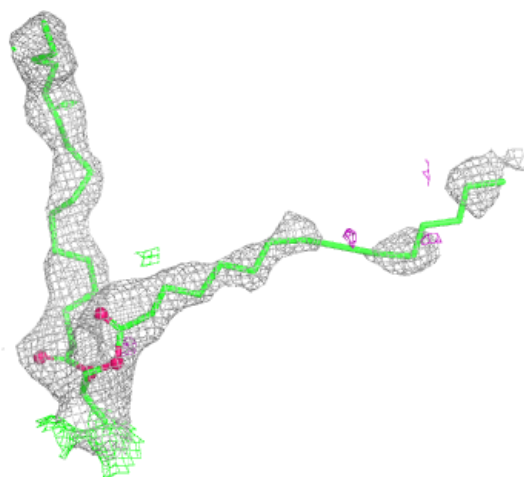
**Electron density around STE T 102:**

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



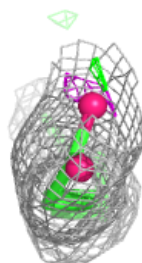
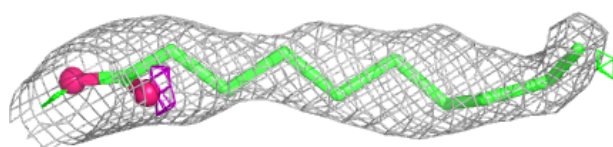
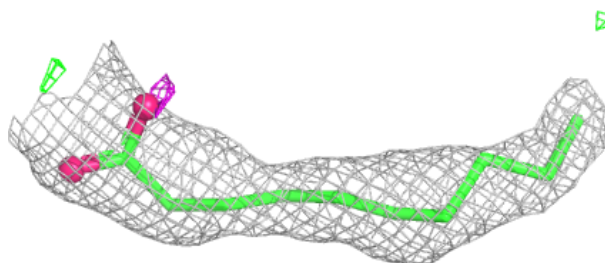
Electron density around SQD A 618:

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

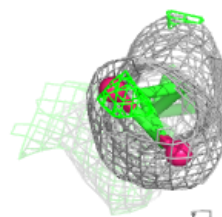
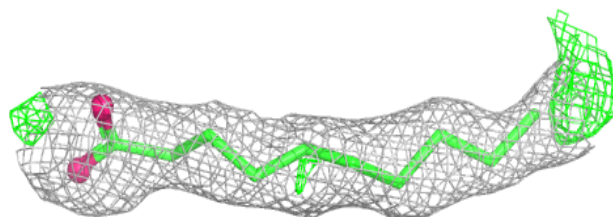
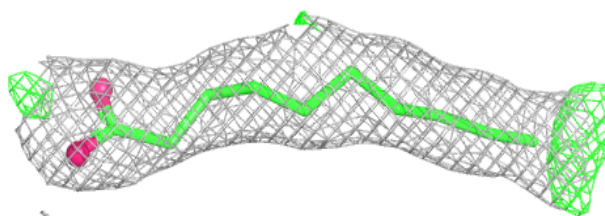


Electron density around STE C 520:

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

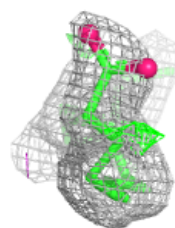
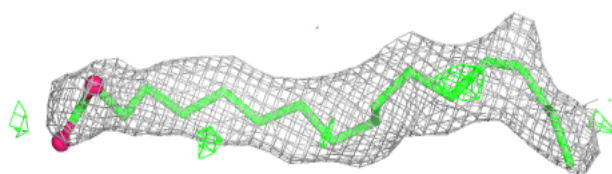
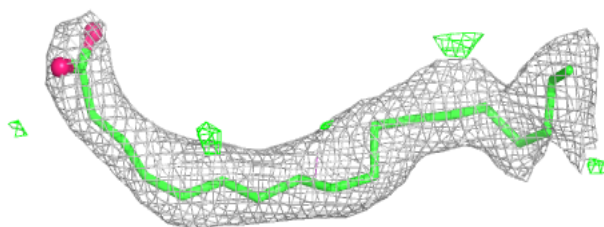
**Electron density around STE j 101:**

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

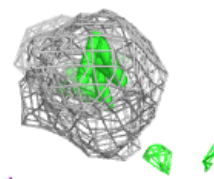
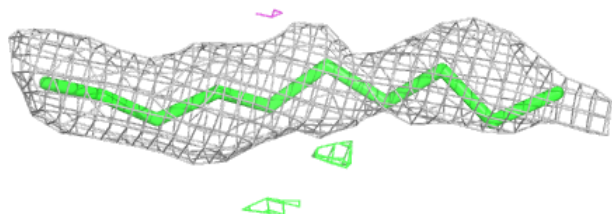
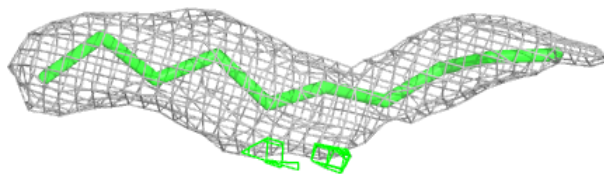


Electron density around STE b 620:

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

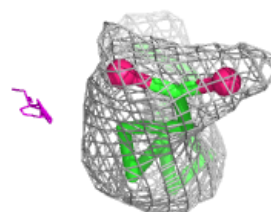
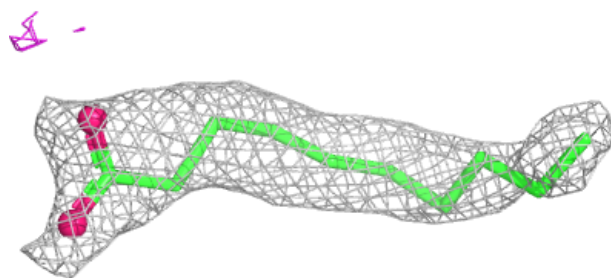
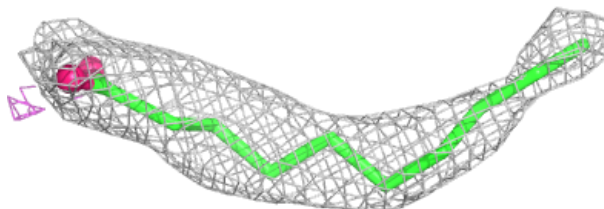
**Electron density around STE t 104:**

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

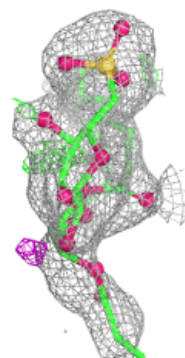
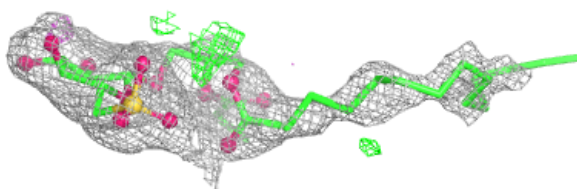
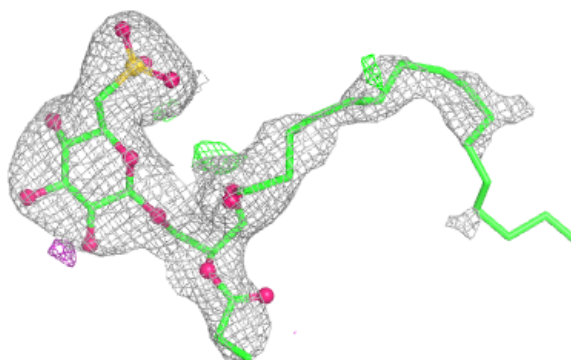


Electron density around STE B 624:

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

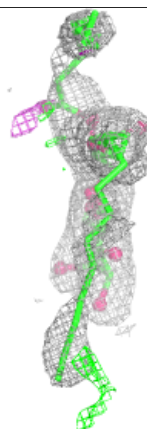
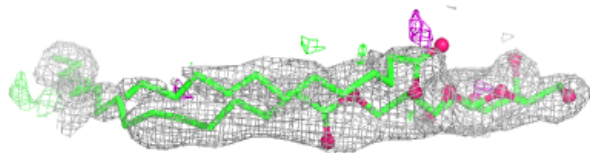
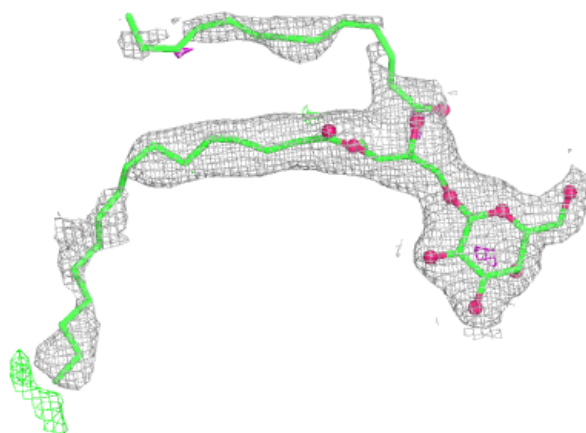
**Electron density around SQD f 101:**

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

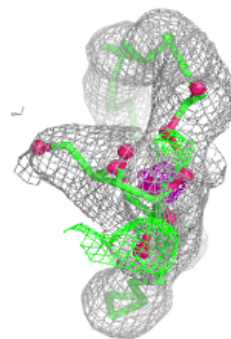
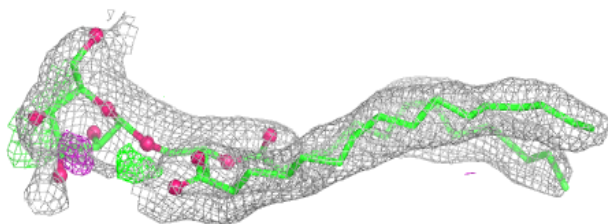
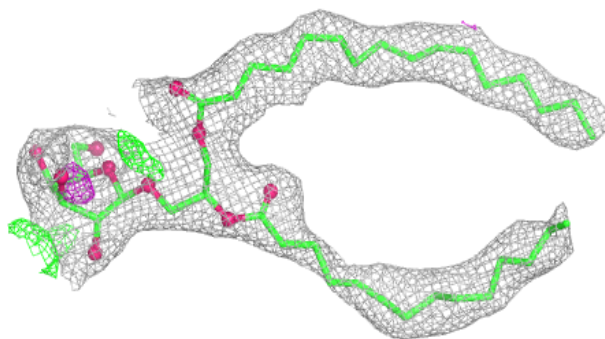


Electron density around LMG C 518:

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

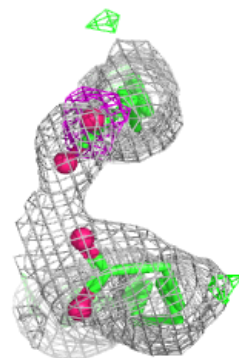
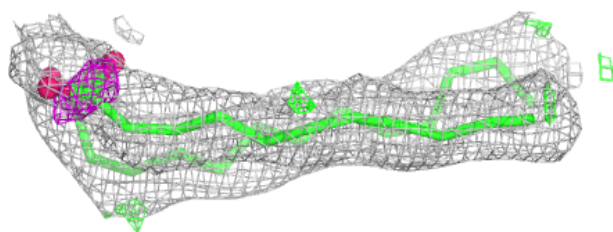
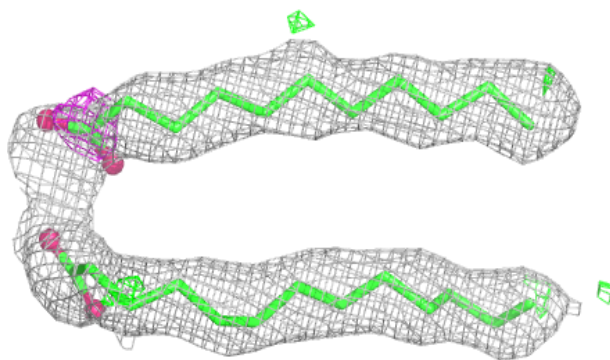
**Electron density around LMG c 523:**

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

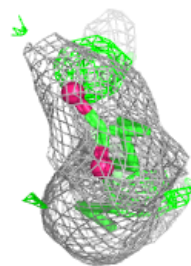
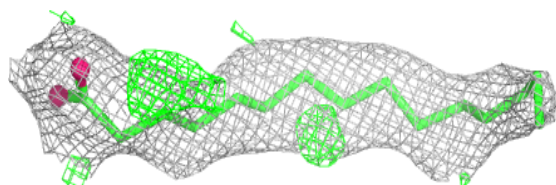
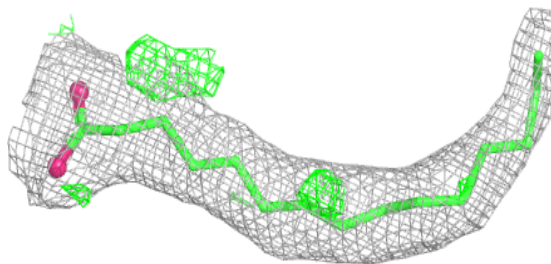


Electron density around LMG B 621:

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

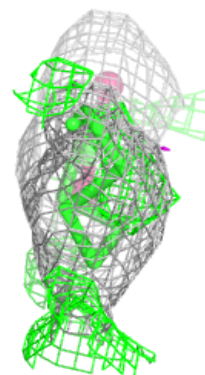
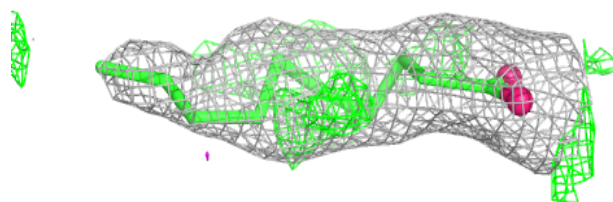
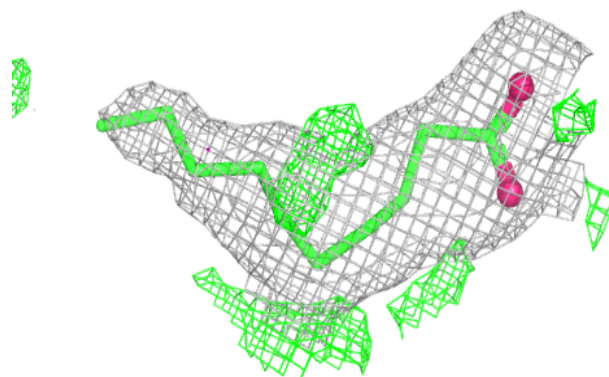
**Electron density around STE B 620:**

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

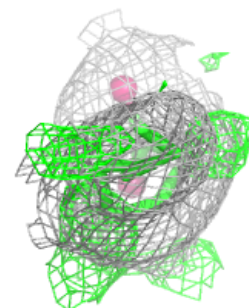
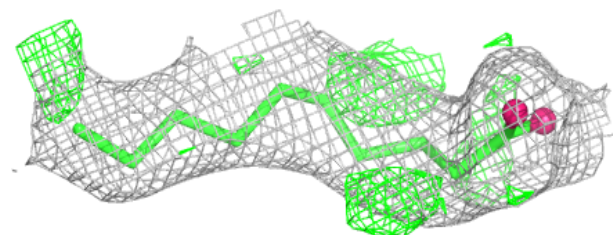
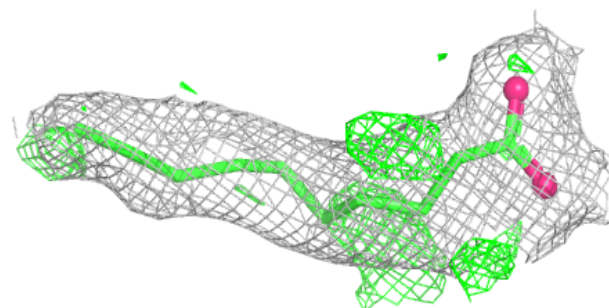


Electron density around STE C 519:

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

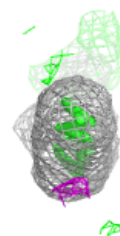
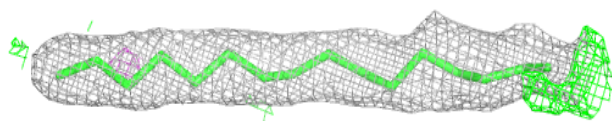
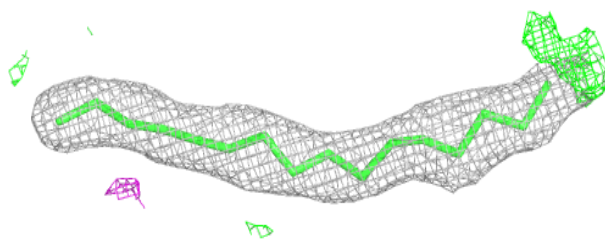
**Electron density around STE B 623:**

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

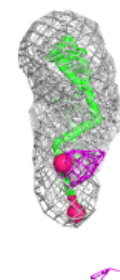
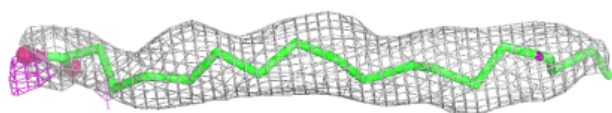
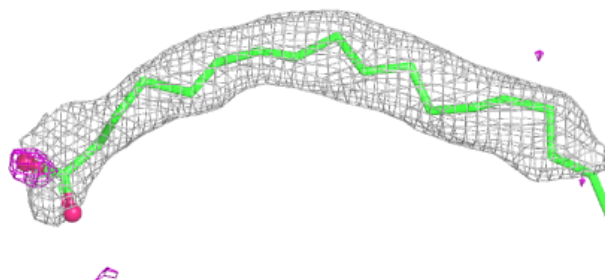


Electron density around STE C 521:

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

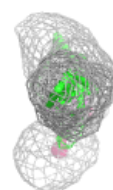
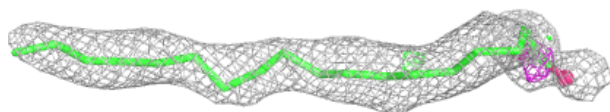
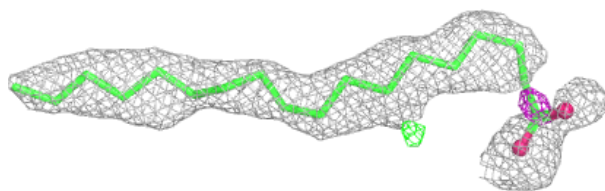
**Electron density around STE X 102:**

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

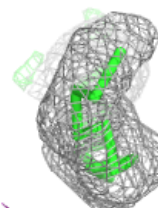
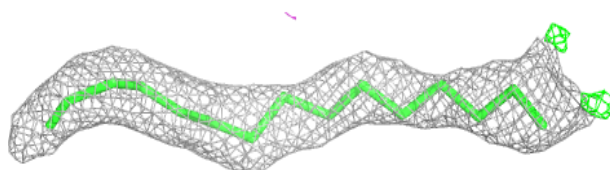
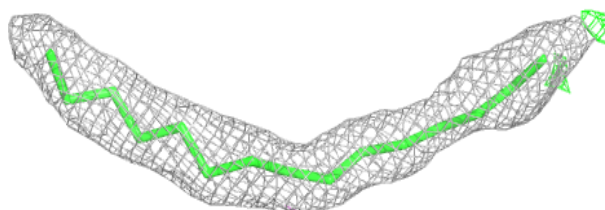


Electron density around STE c 521:

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

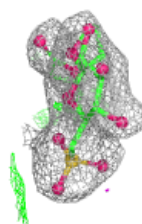
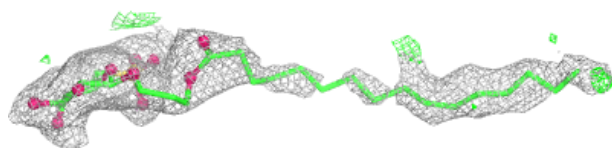
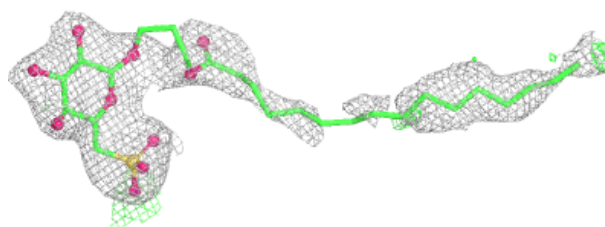
**Electron density around STE I 101:**

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

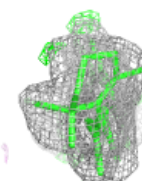
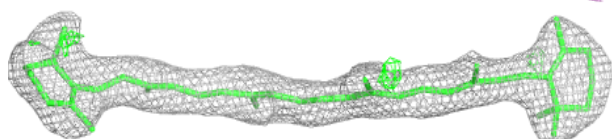
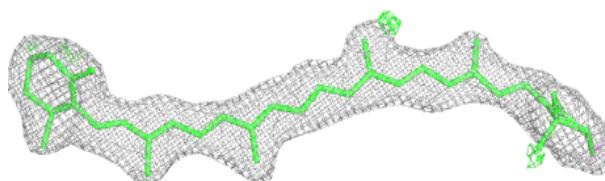


Electron density around SQD F 102:

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

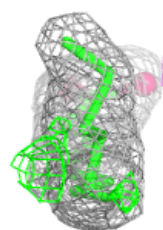
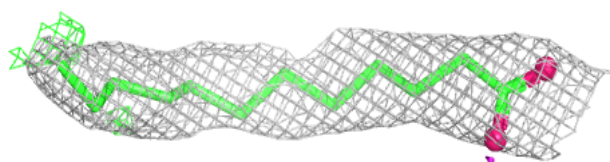
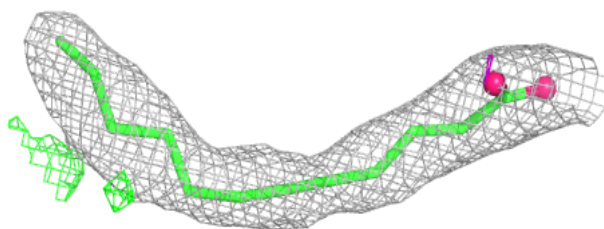
**Electron density around BCR K 101:**

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

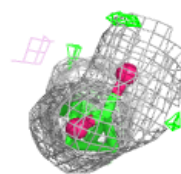
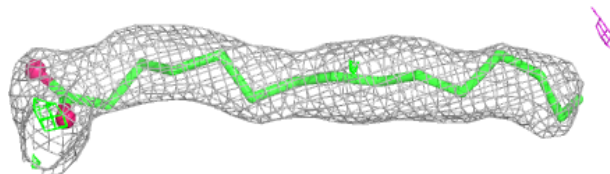
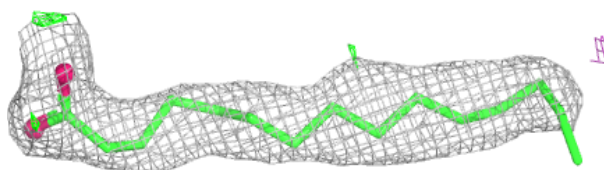


Electron density around STE t 103:

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

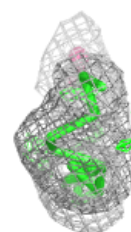
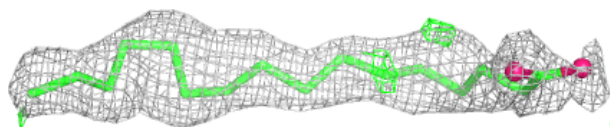
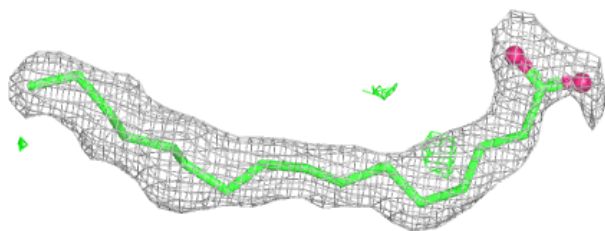
**Electron density around STE d 413:**

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

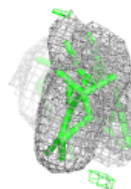
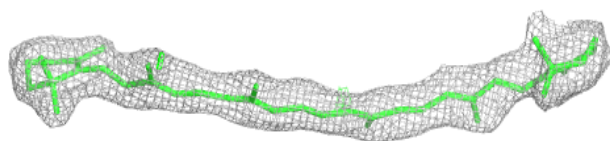
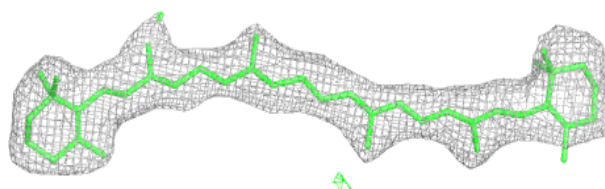


Electron density around STE t 105:

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

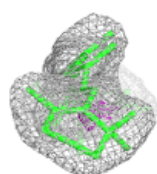
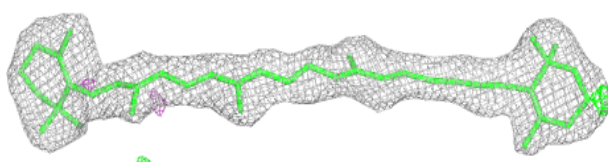
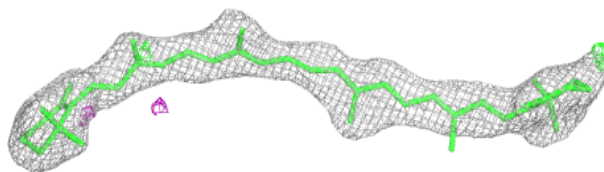
**Electron density around BCR d 405:**

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

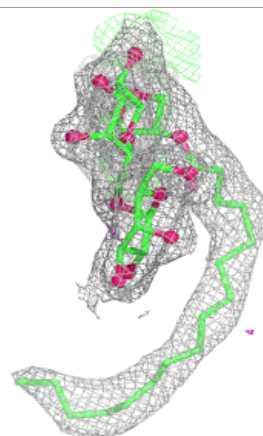
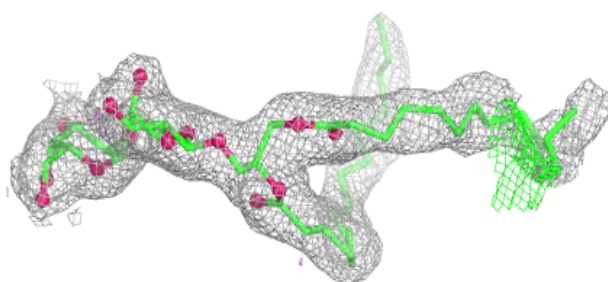
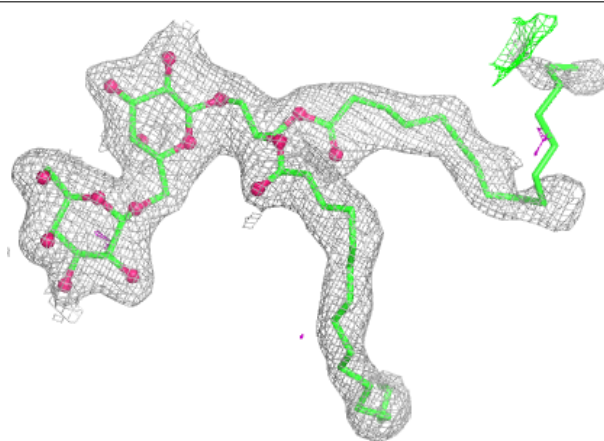


Electron density around BCR h 102:

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

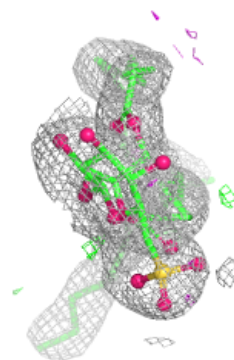
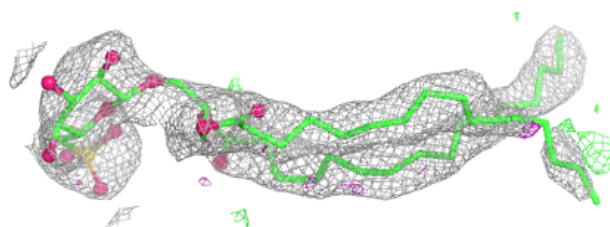
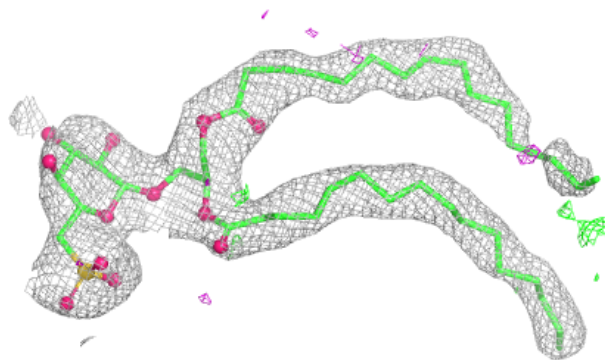
**Electron density around DGD C 516:**

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

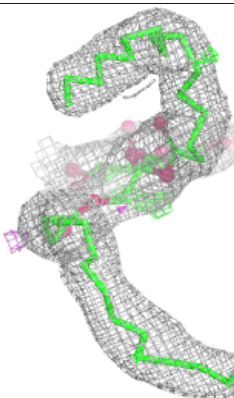
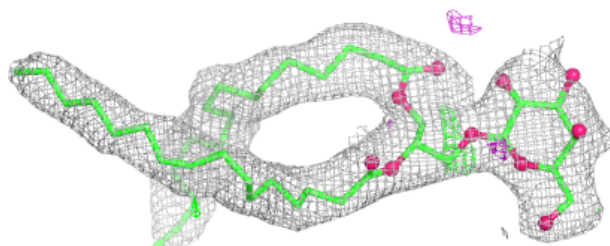
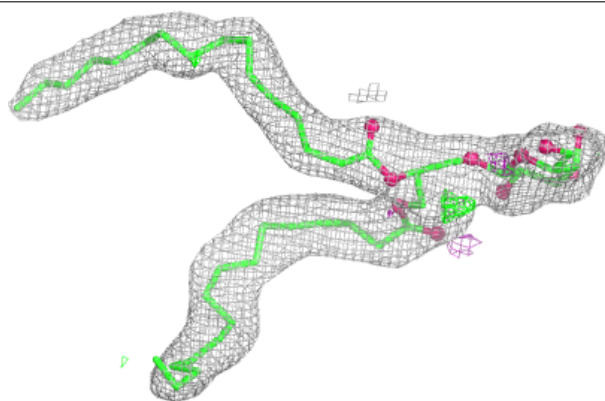


Electron density around SQD B 622:

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

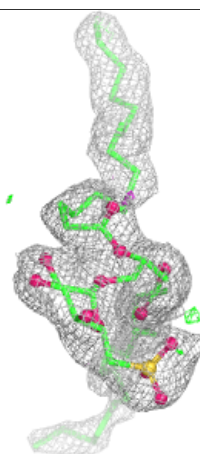
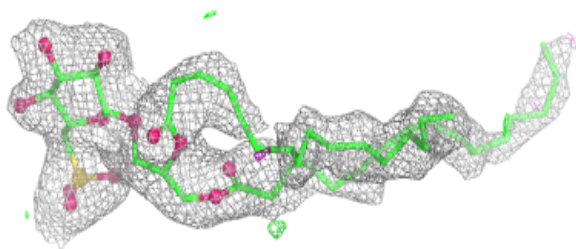
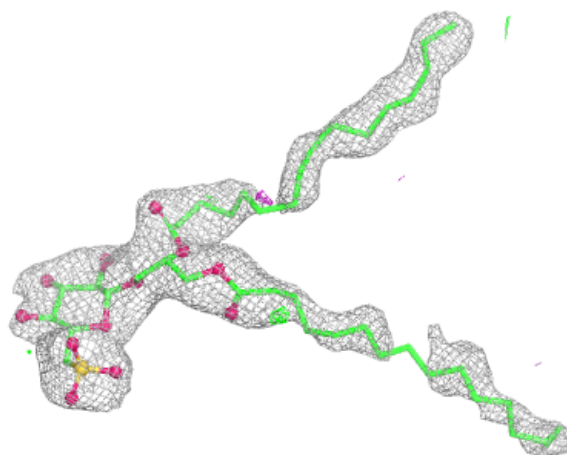
**Electron density around LMG m 101:**

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



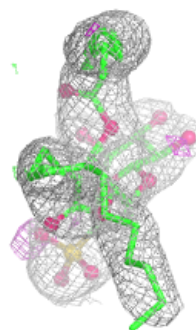
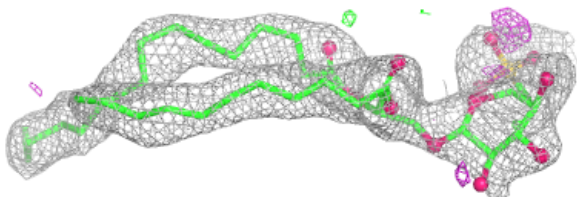
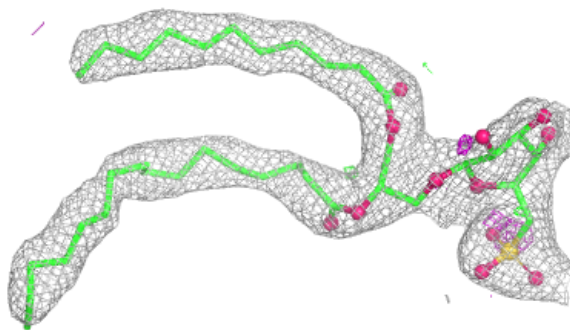
Electron density around SQD a 613:

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

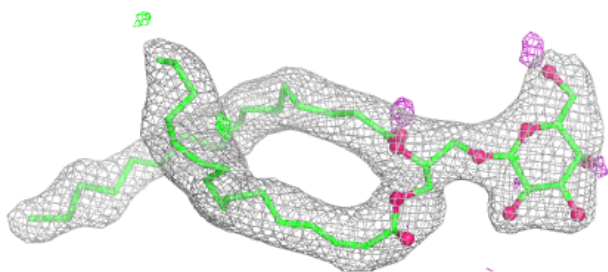
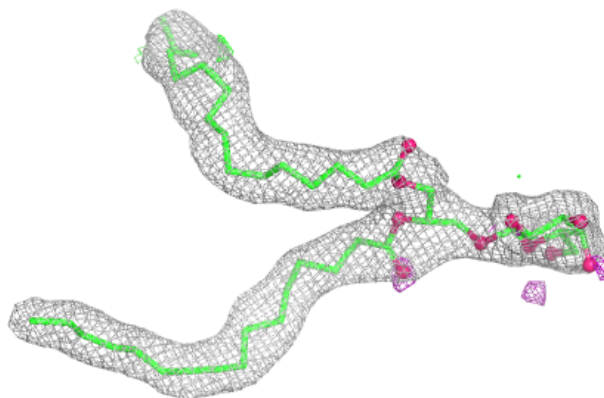


Electron density around SQD b 619:

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

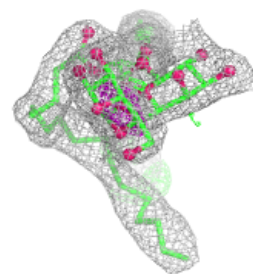
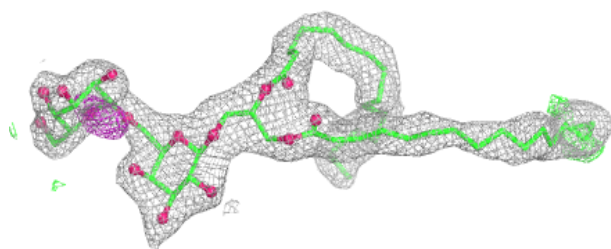
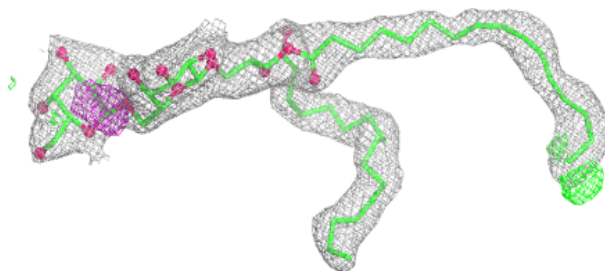
**Electron density around LMG M 101:**

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

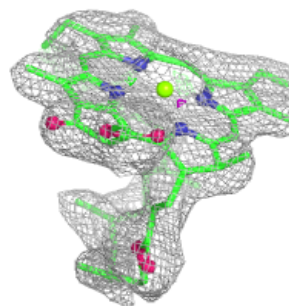
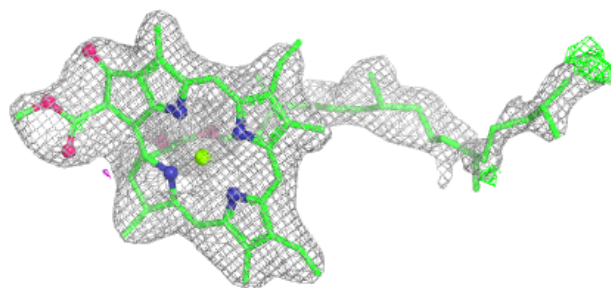
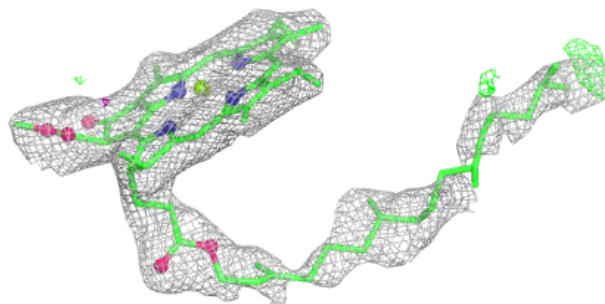


Electron density around DGD H 101:

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

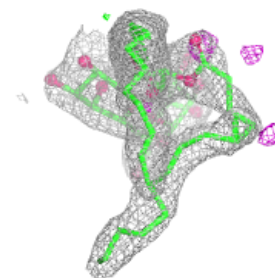
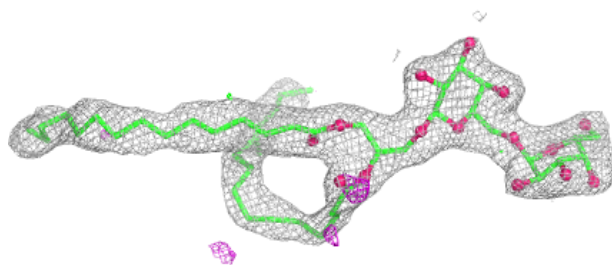
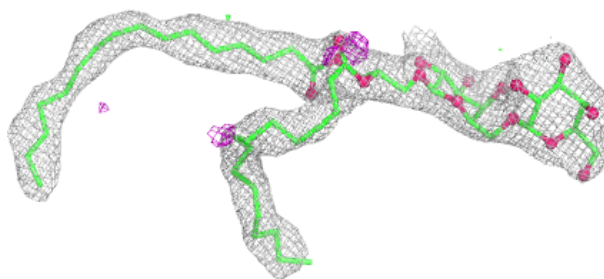
**Electron density around CLA C 513:**

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

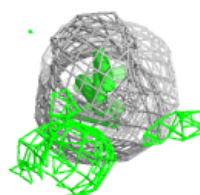
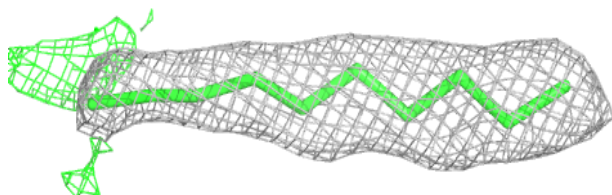
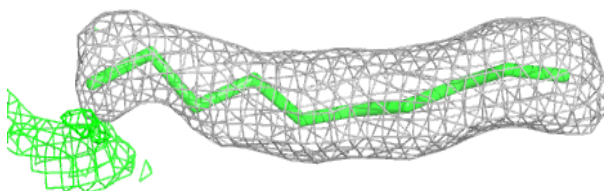


Electron density around DGD h 103:

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

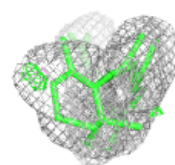
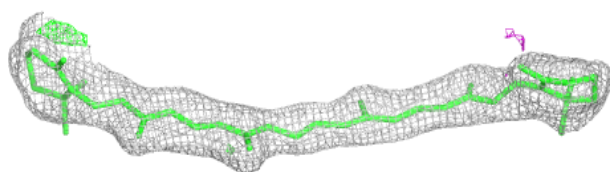
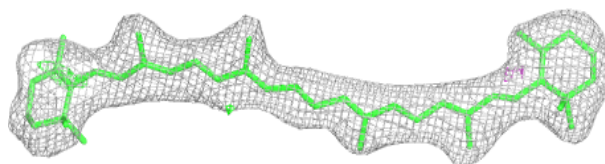
**Electron density around STE M 103:**

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

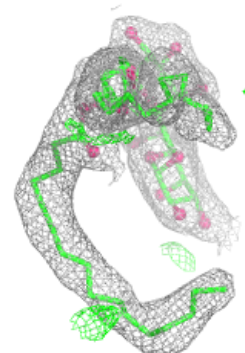
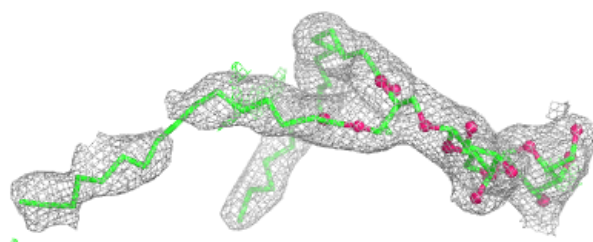
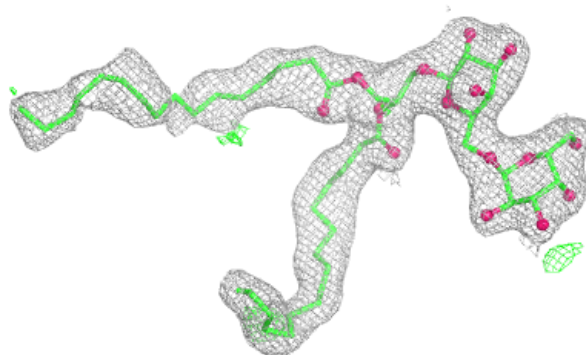


Electron density around BCR D 404:

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

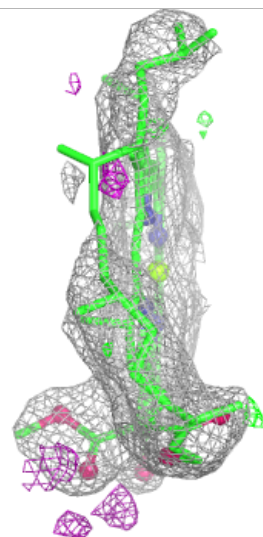
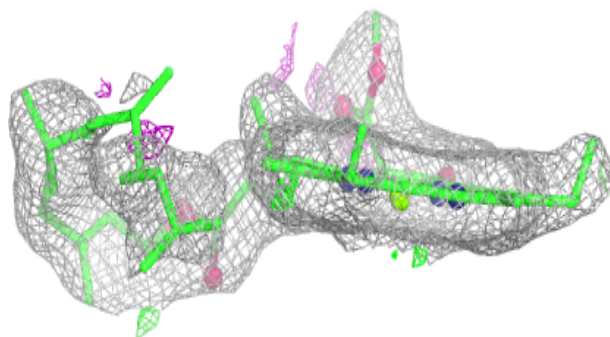
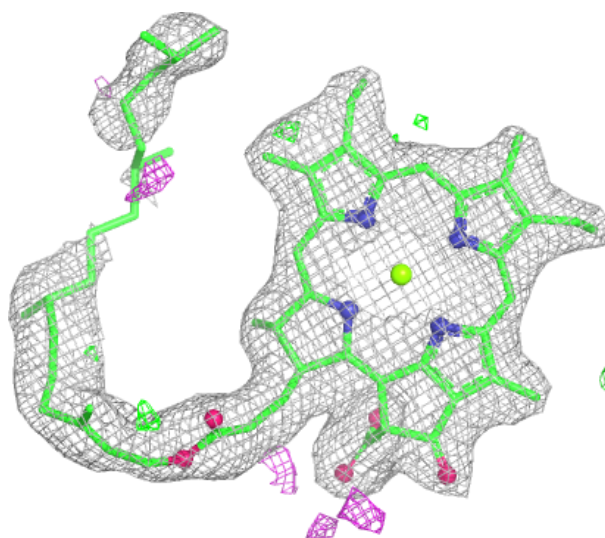
**Electron density around DGD c 518:**

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



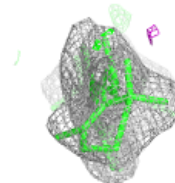
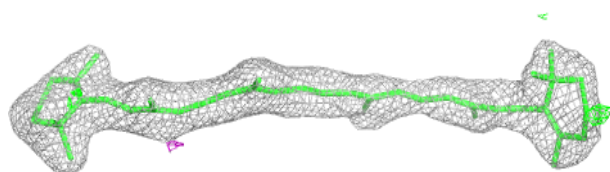
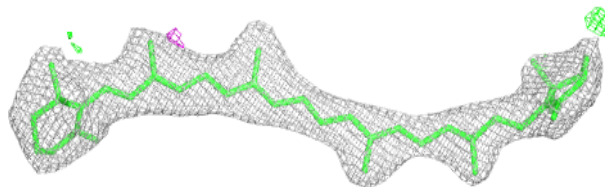
Electron density around CLA c 512:

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

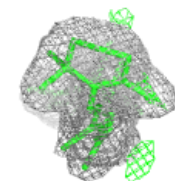
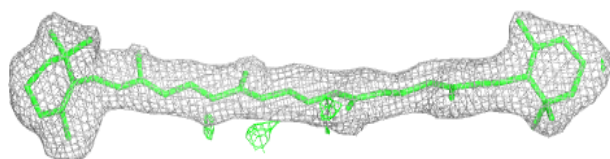
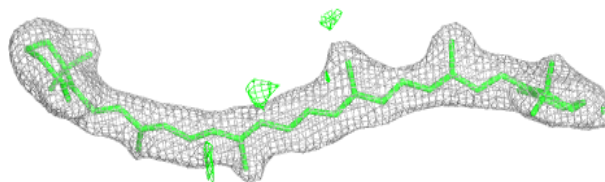


Electron density around BCR k 101:

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

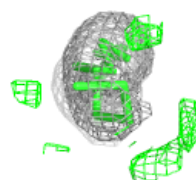
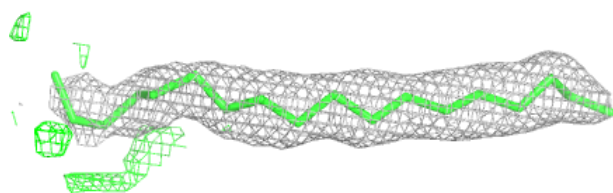
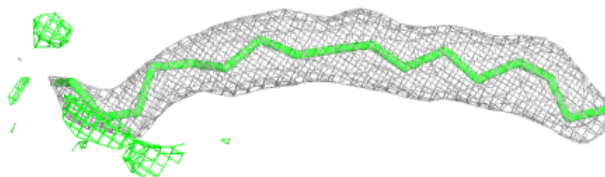
**Electron density around BCR X 101:**

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

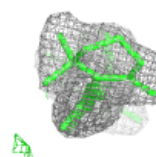
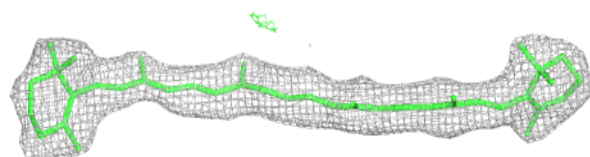
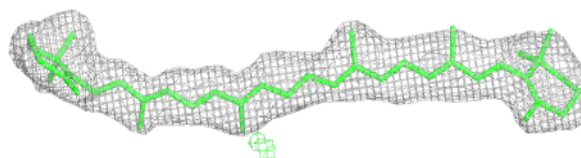


Electron density around STE I 102:

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

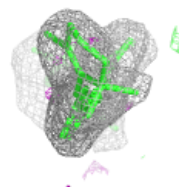
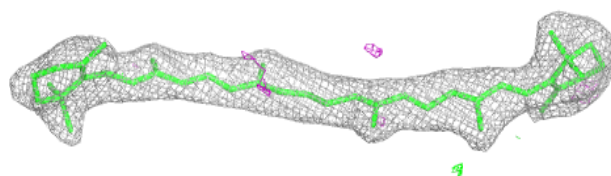
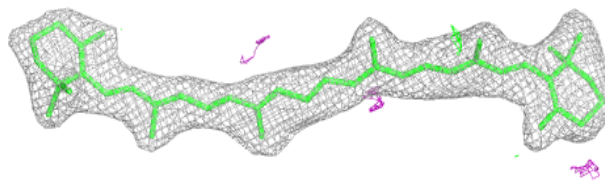
**Electron density around BCR Z 101:**

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

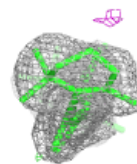
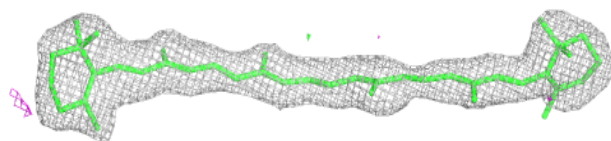
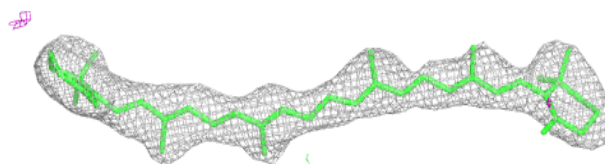


Electron density around BCR b 618:

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

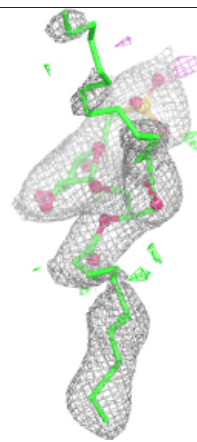
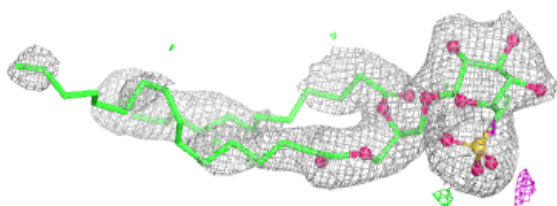
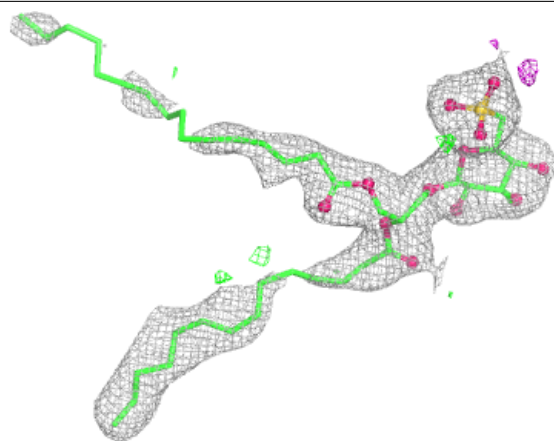
**Electron density around BCR c 514:**

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

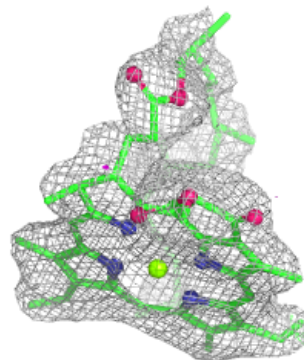
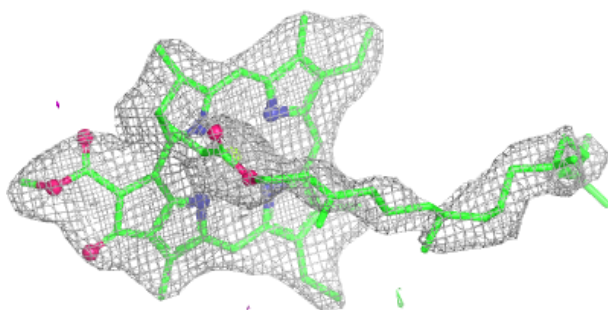
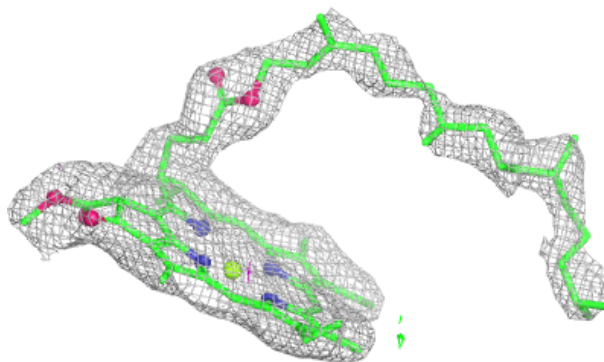


Electron density around SQD A 616:

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

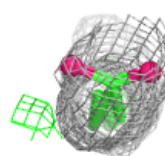
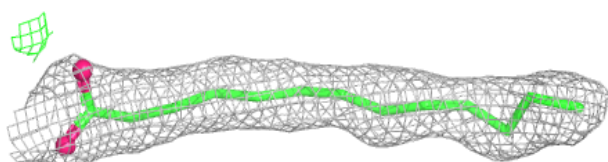
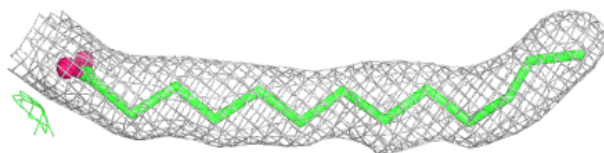
**Electron density around CLA c 513:**

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

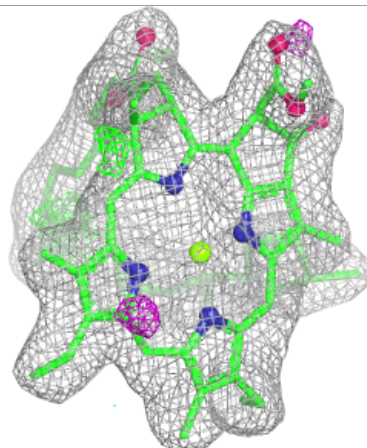
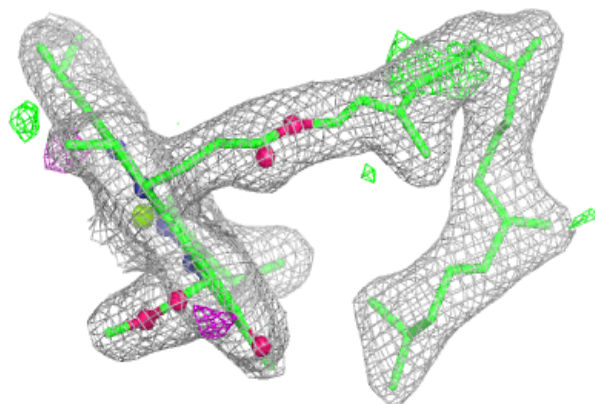
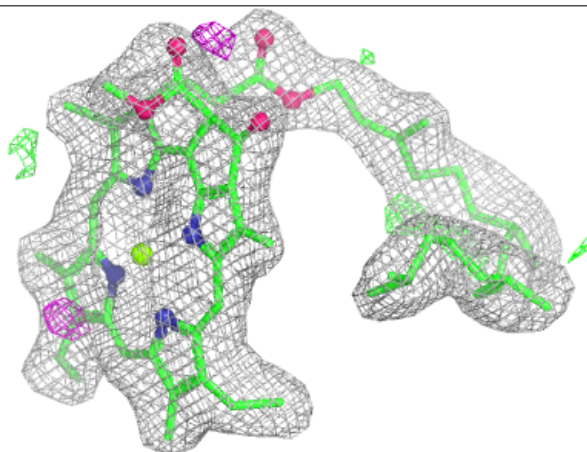


Electron density around STE M 102:

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

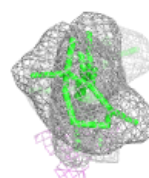
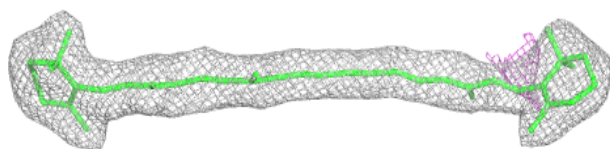
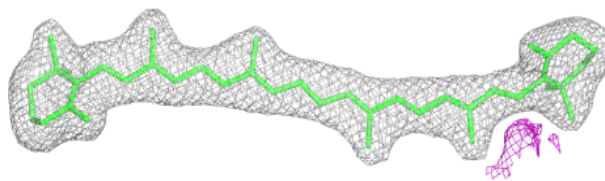
**Electron density around CLA C 503:**

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

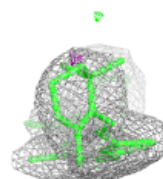
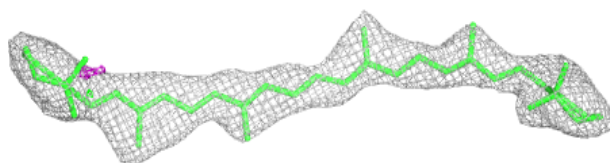
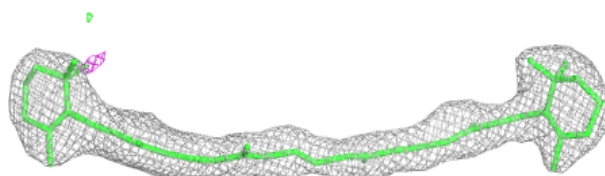


Electron density around BCR B 618:

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

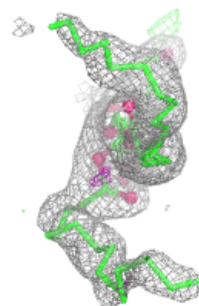
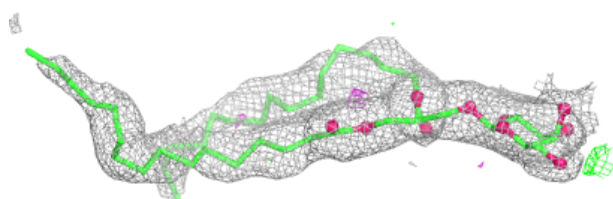
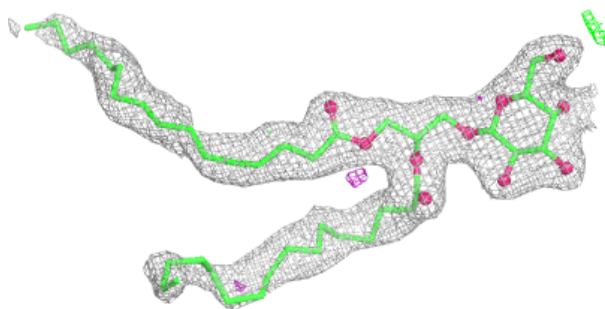
**Electron density around BCR c 516:**

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

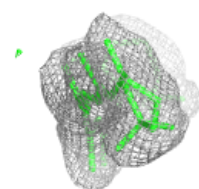
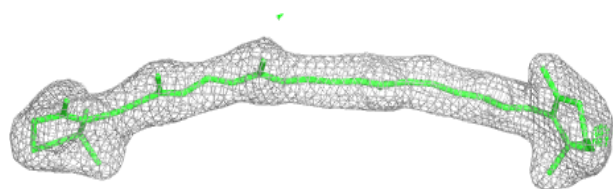
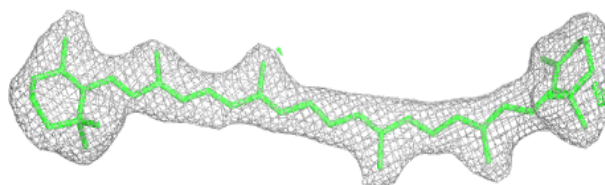


Electron density around LMG D 406:

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

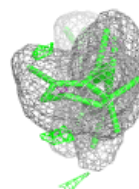
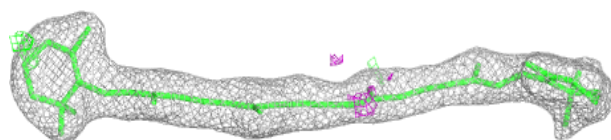
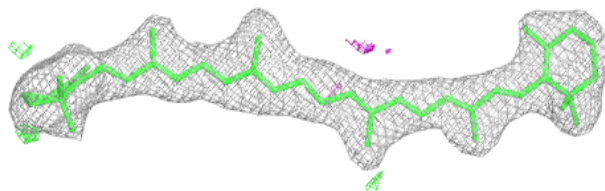
**Electron density around BCR t 101:**

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

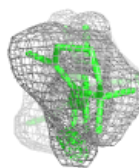
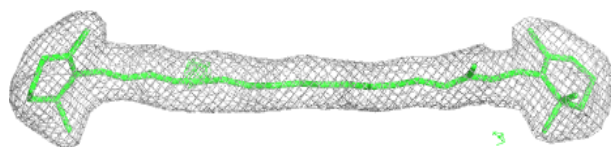
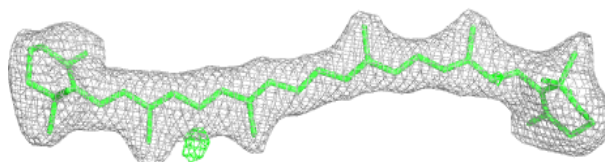


Electron density around BCR b 616:

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

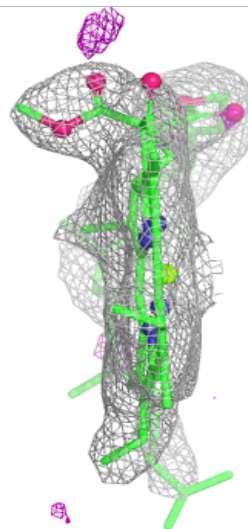
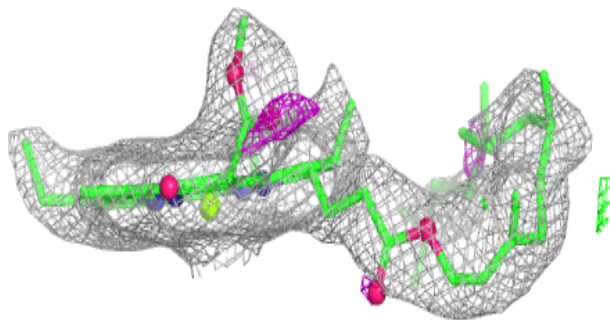
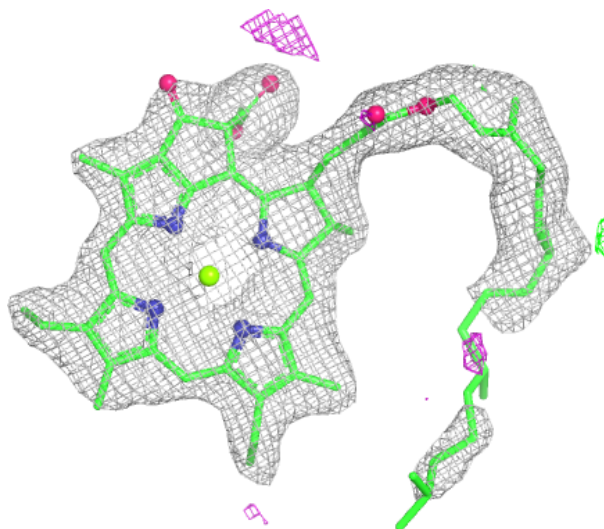
**Electron density around BCR b 617:**

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



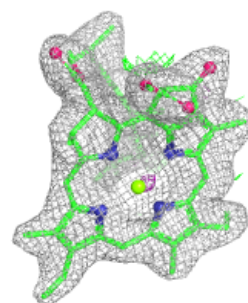
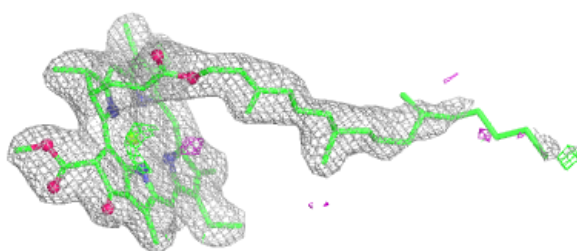
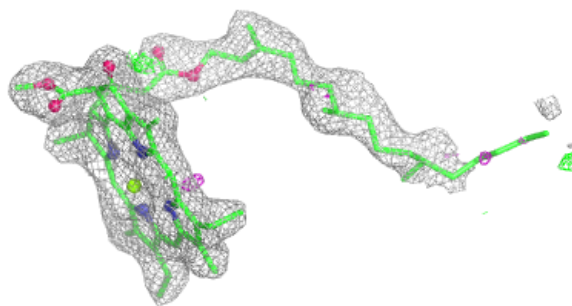
Electron density around CLA C 512:

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

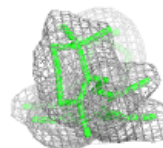
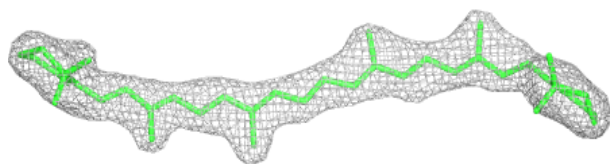
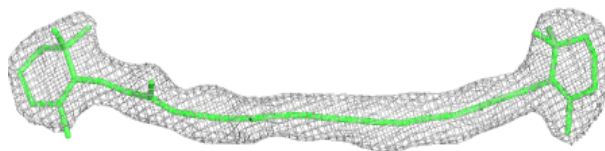


Electron density around CLA c 508:

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

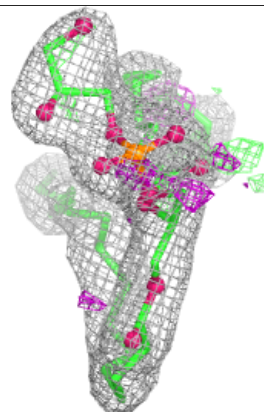
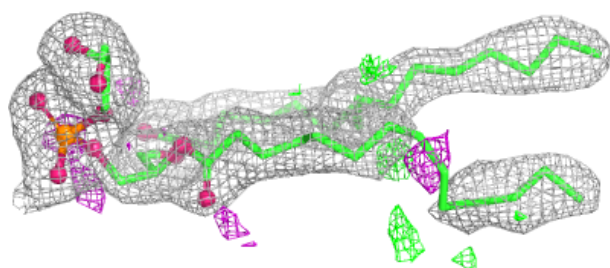
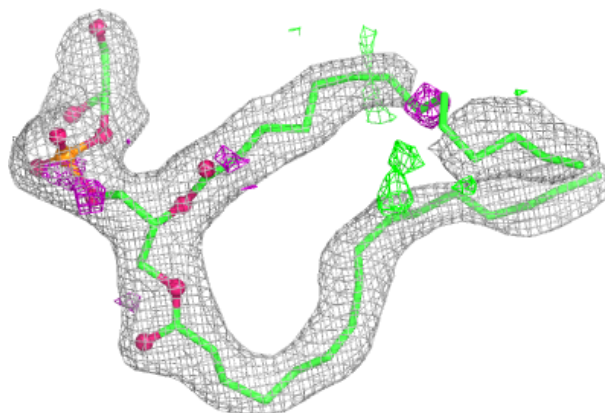
**Electron density around BCR K 102:**

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

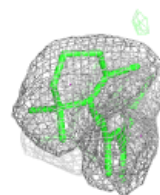
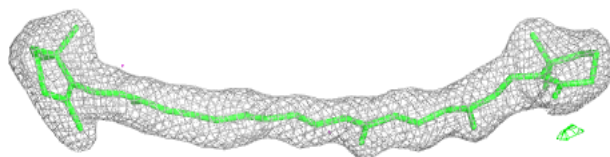
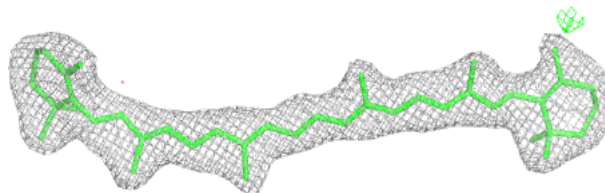


Electron density around LHG A 615:

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

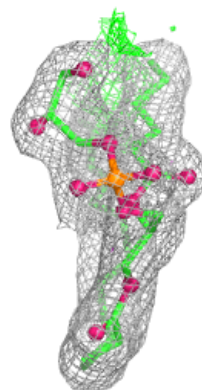
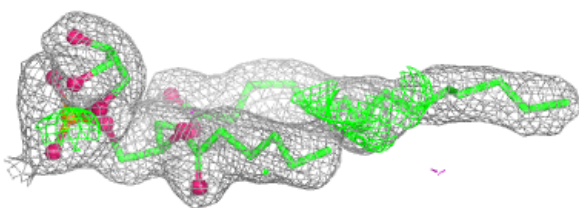
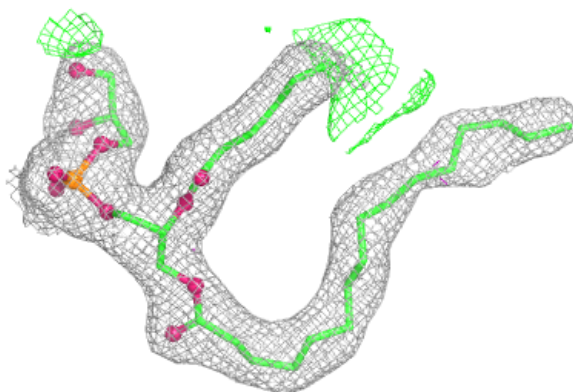
**Electron density around BCR T 101:**

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

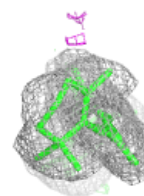
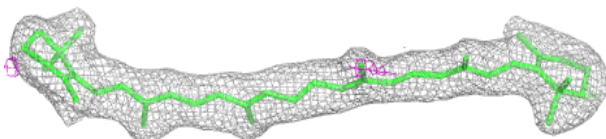
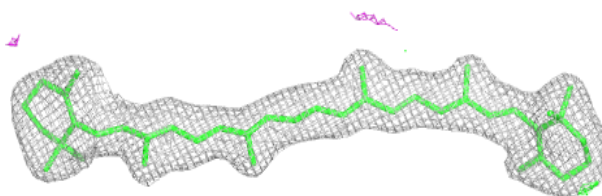


Electron density around LHG d 409:

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

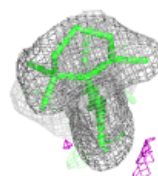
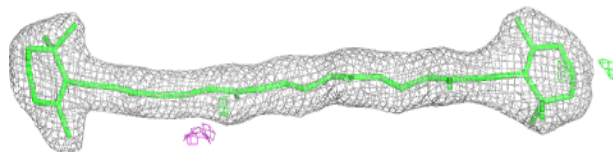
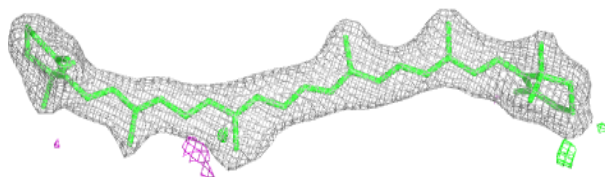
**Electron density around BCR B 619:**

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

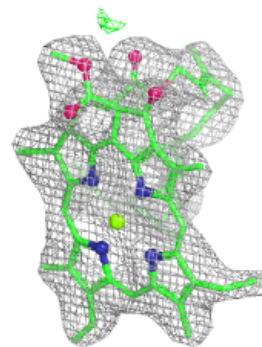
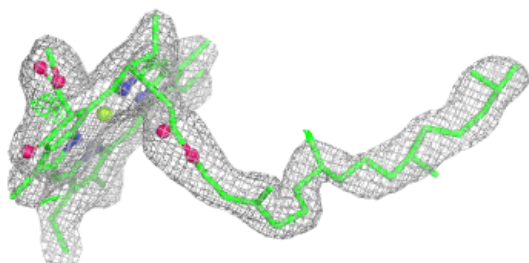
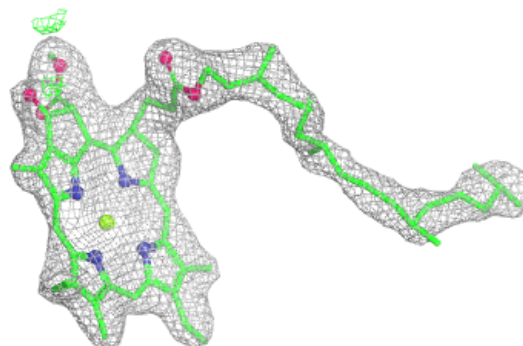


Electron density around BCR C 514:

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

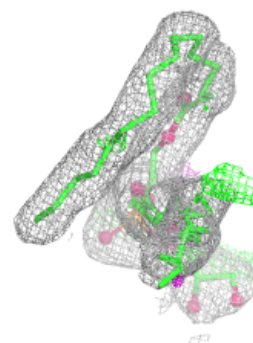
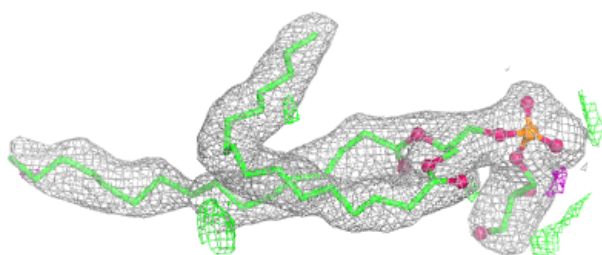
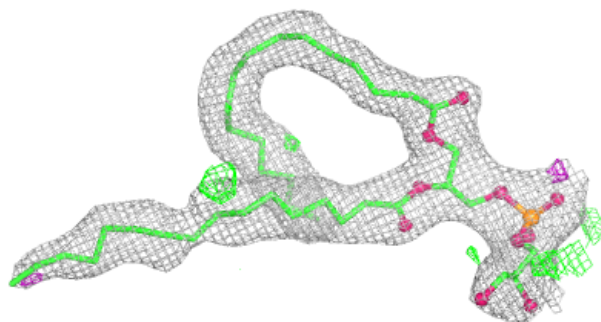
**Electron density around CLA c 511:**

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

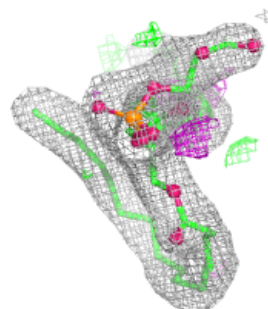
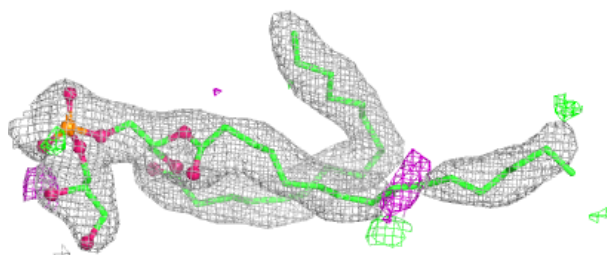
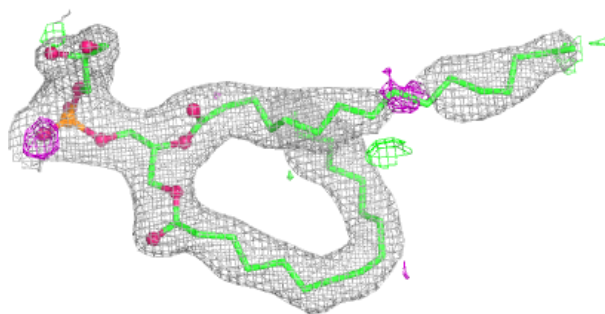


Electron density around LHG D 409:

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

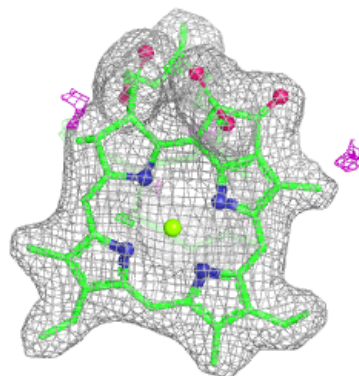
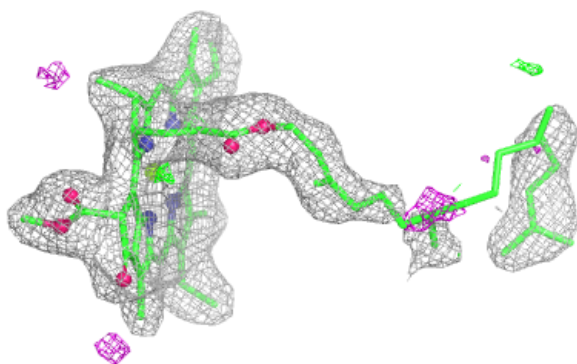
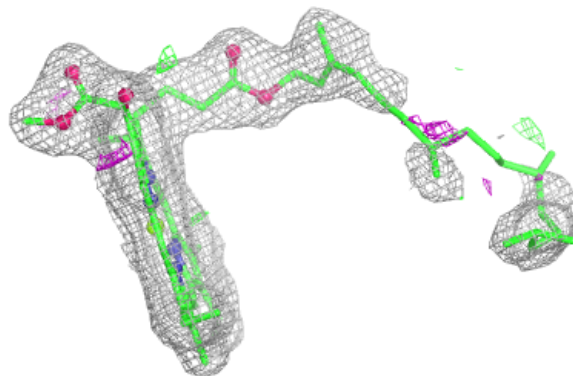
**Electron density around LHG d 407:**

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

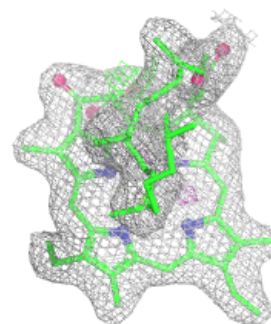
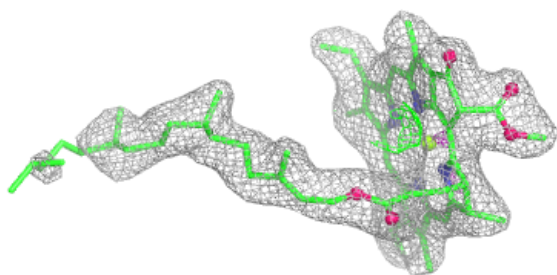
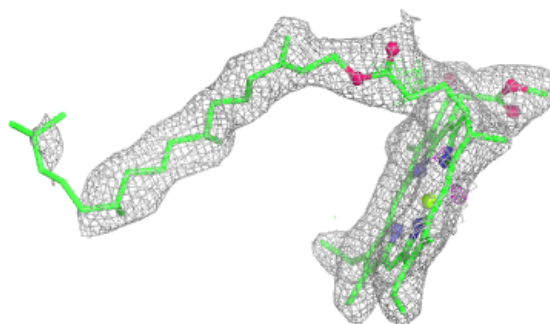


Electron density around CLA C 506:

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

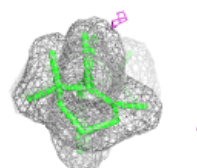
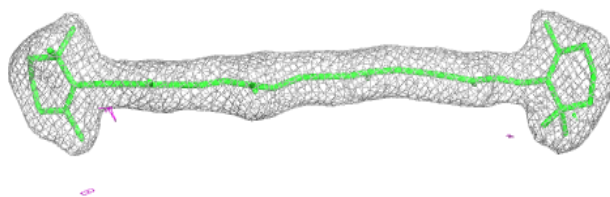
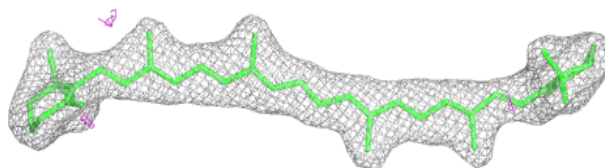
**Electron density around CLA C 508:**

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

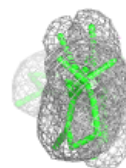
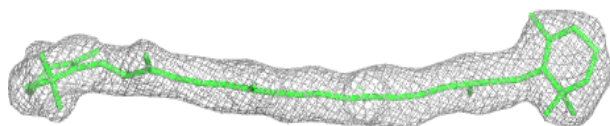
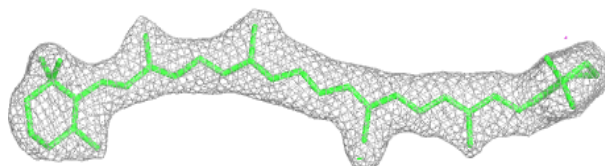


Electron density around BCR A 611:

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

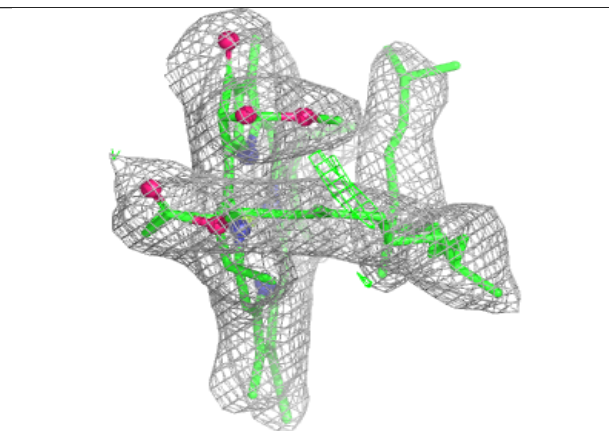
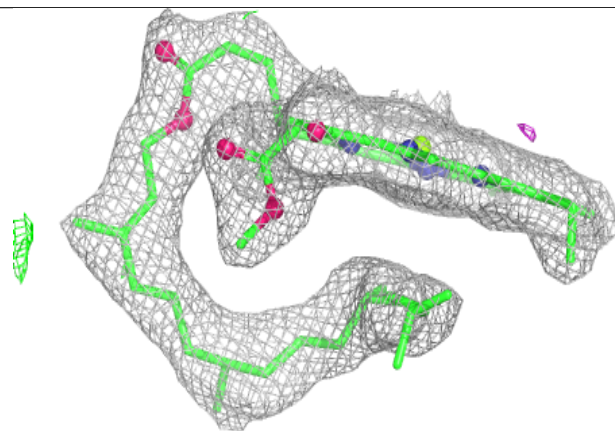
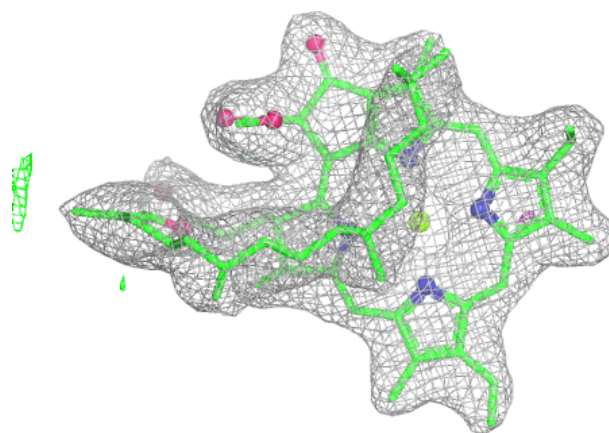
**Electron density around BCR B 617:**

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

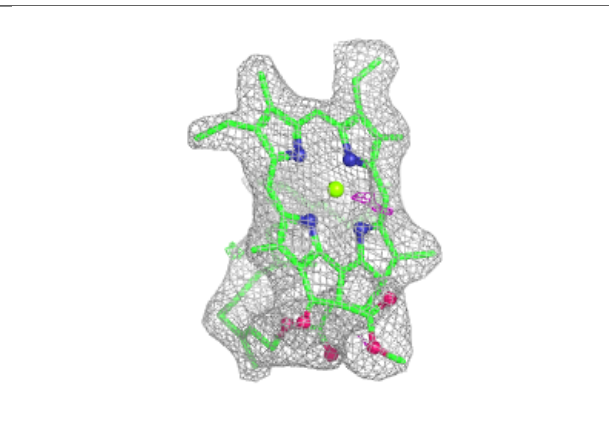
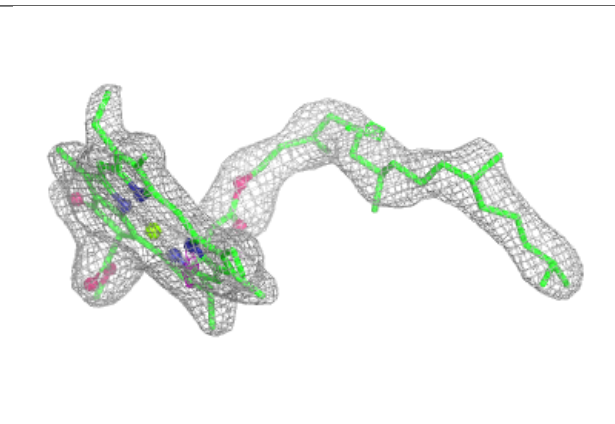
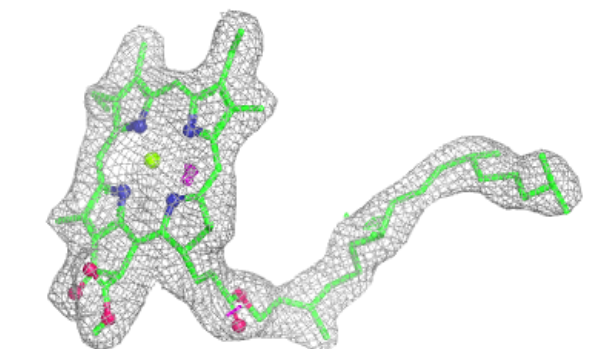


Electron density around CLA C 510:

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

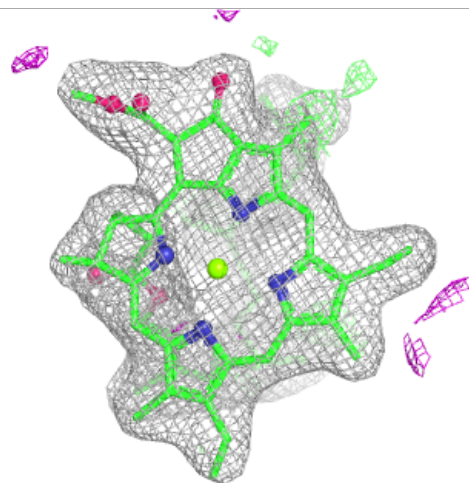
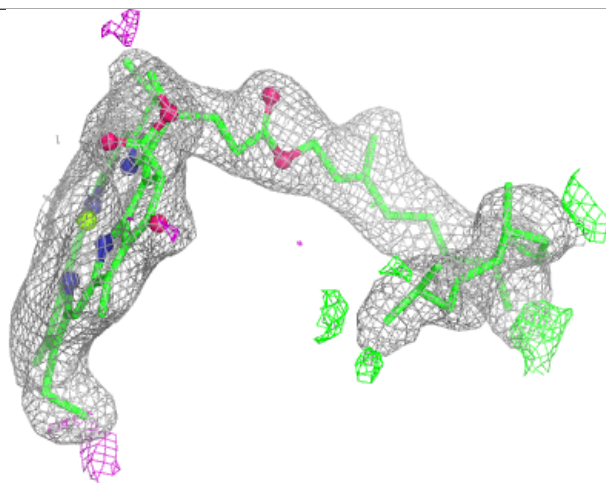
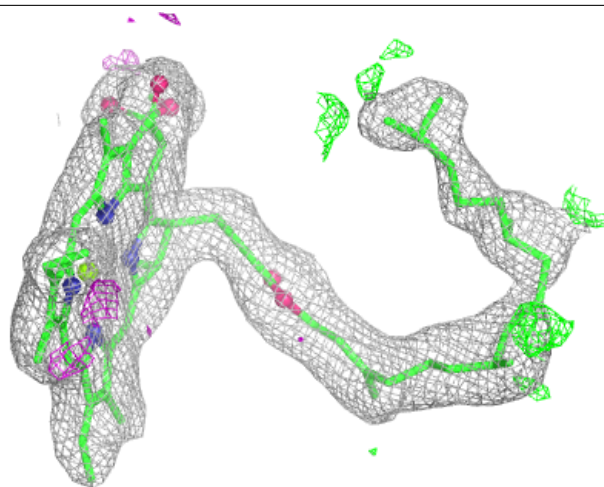
**Electron density around CLA C 511:**

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



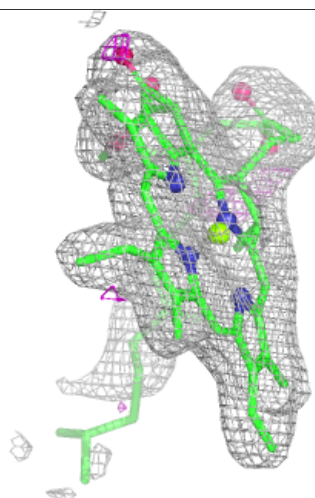
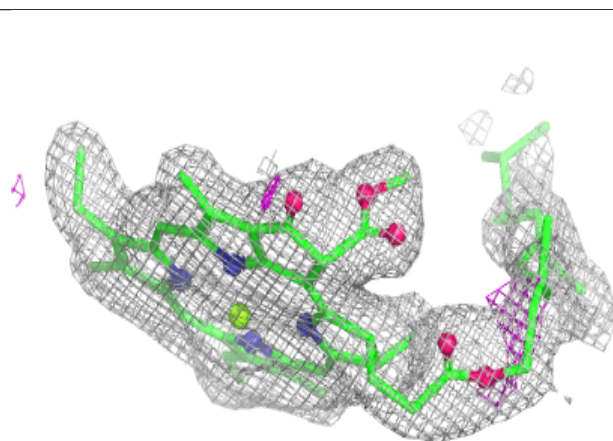
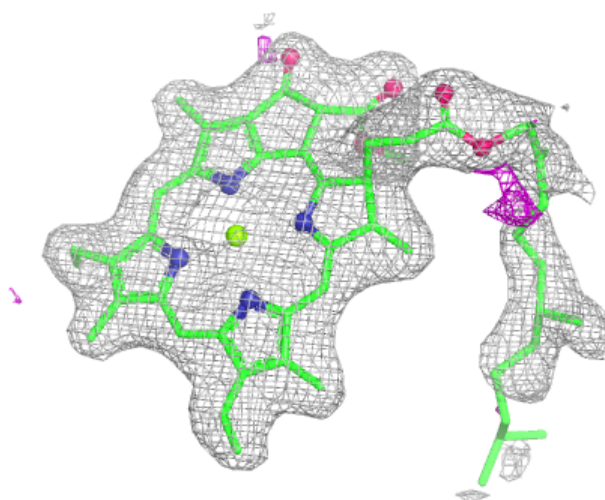
Electron density around CLA B 606:

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



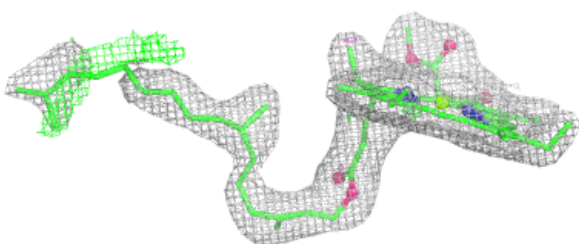
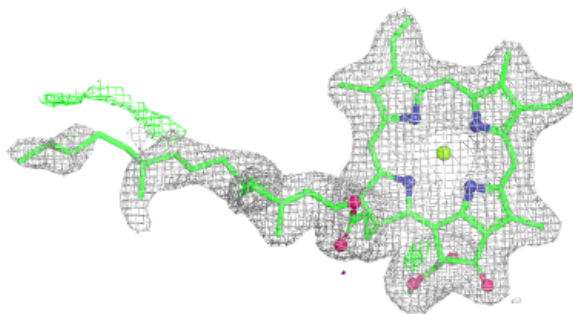
Electron density around CLA B 616:

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

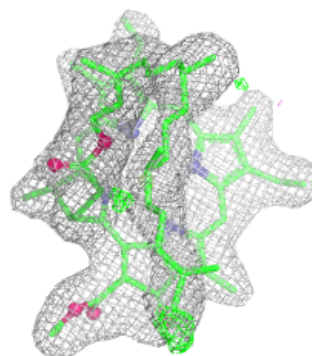
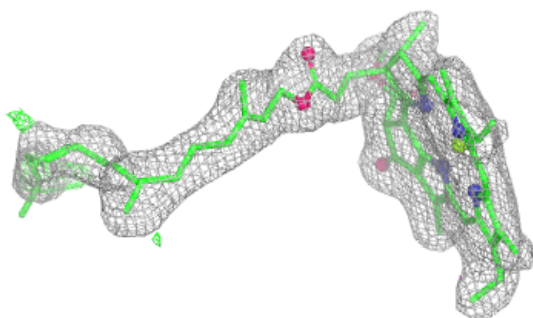
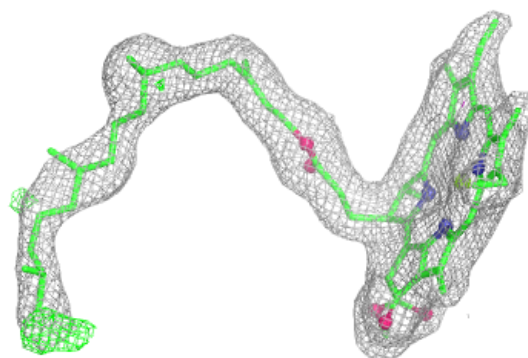


Electron density around CLA a 607:

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

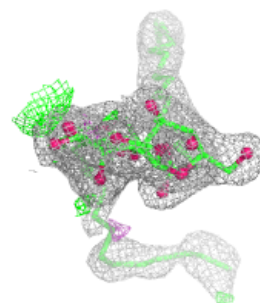
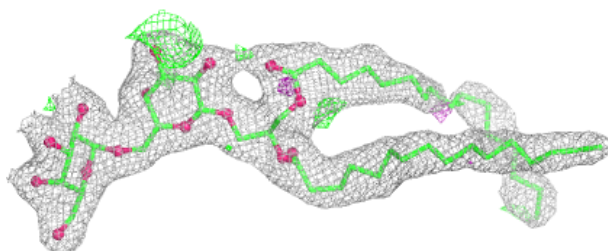
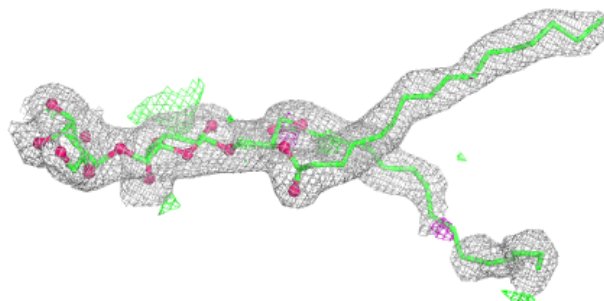
**Electron density around CLA b 605:**

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

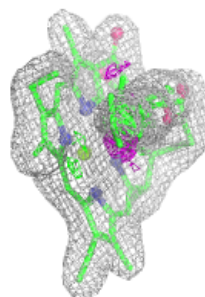
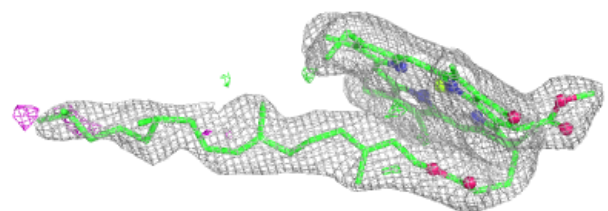
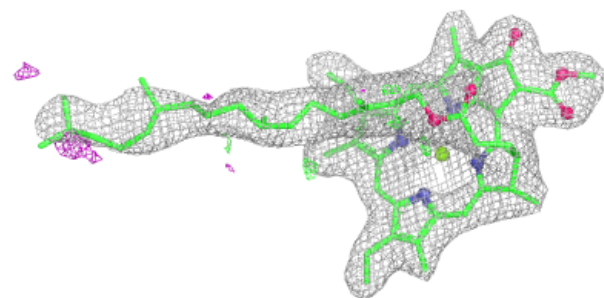


Electron density around DGD C 515:

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

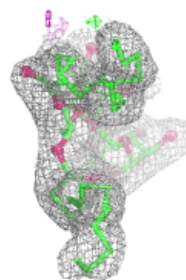
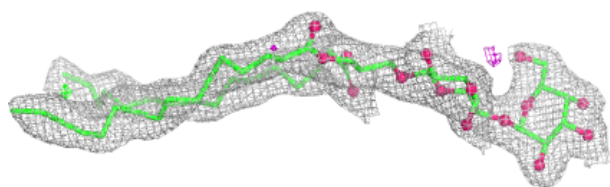
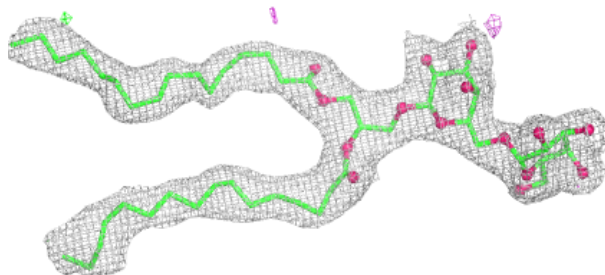
**Electron density around CLA b 613:**

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



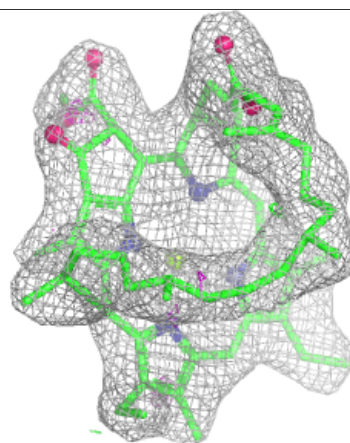
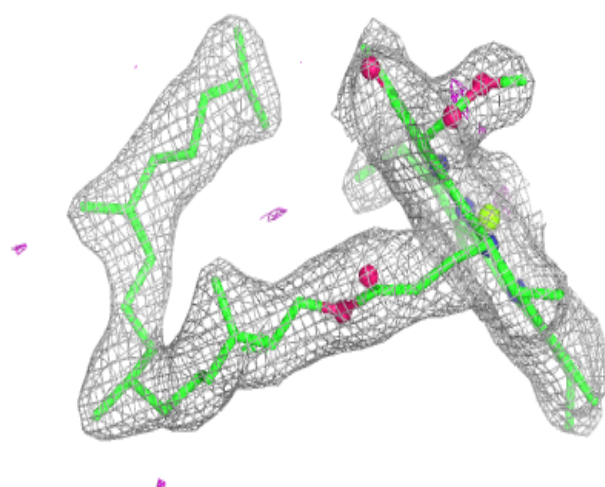
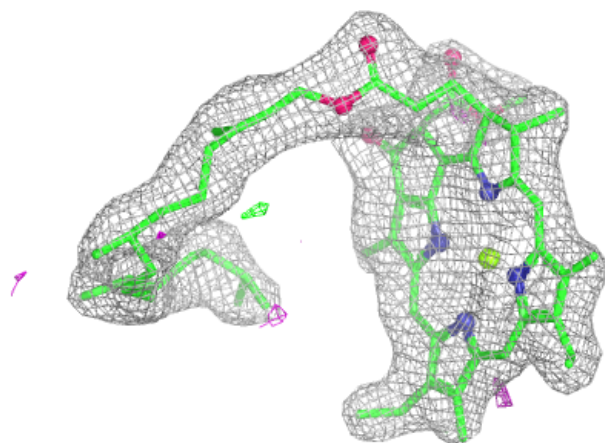
Electron density around DGD C 517:

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



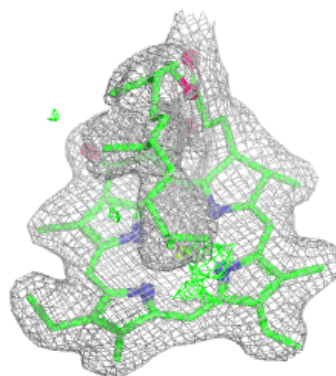
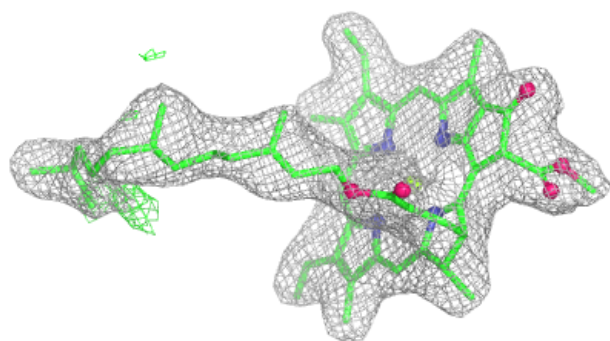
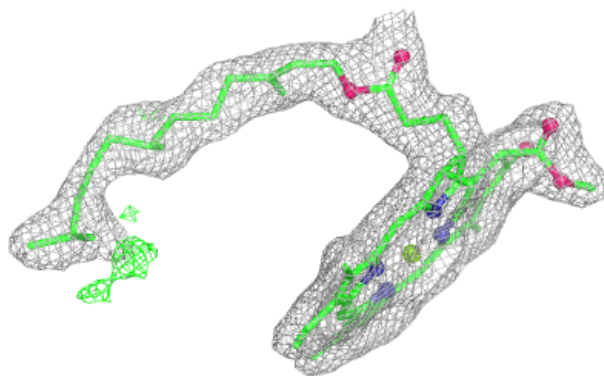
Electron density around CLA c 503:

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

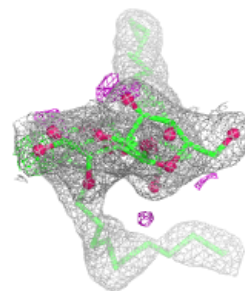
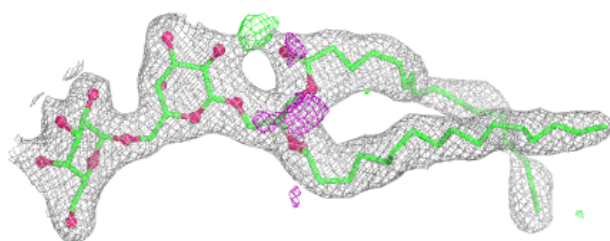
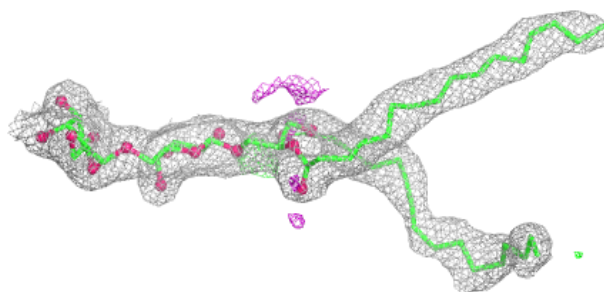


Electron density around CLA c 504:

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

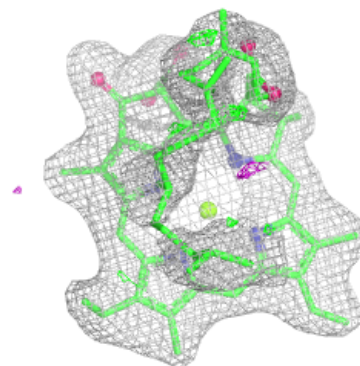
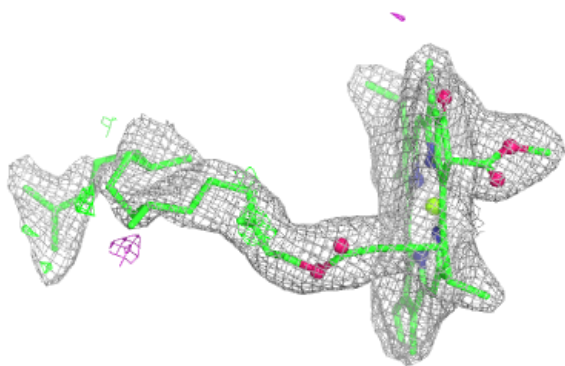
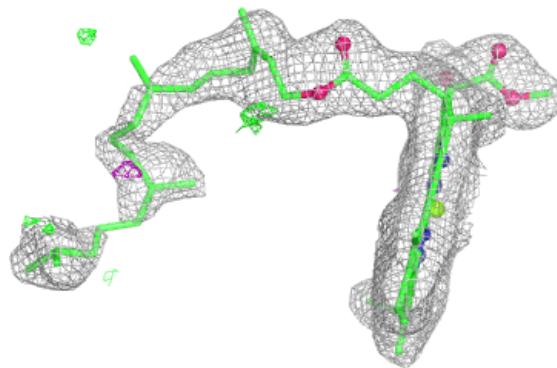
**Electron density around DGD c 517:**

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

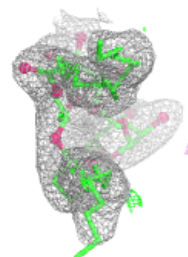
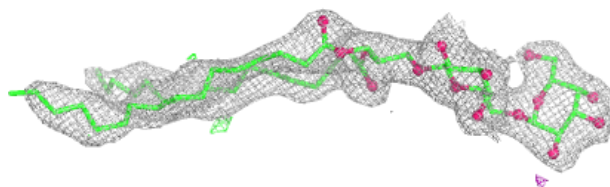
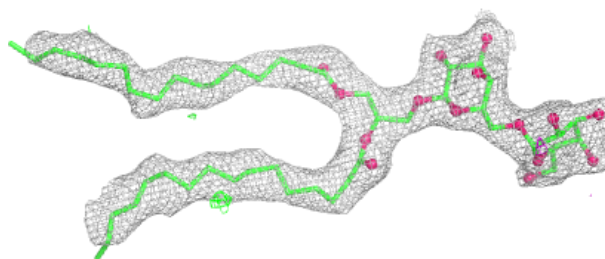


Electron density around CLA c 506:

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

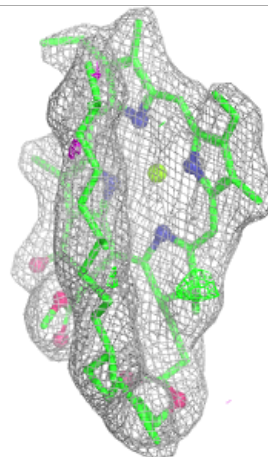
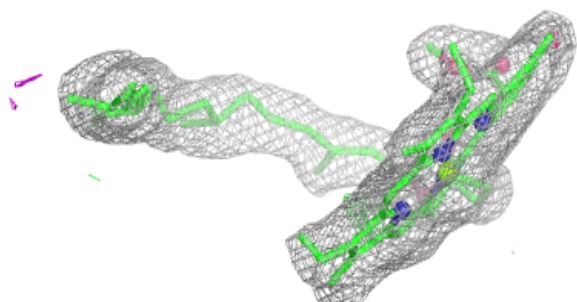
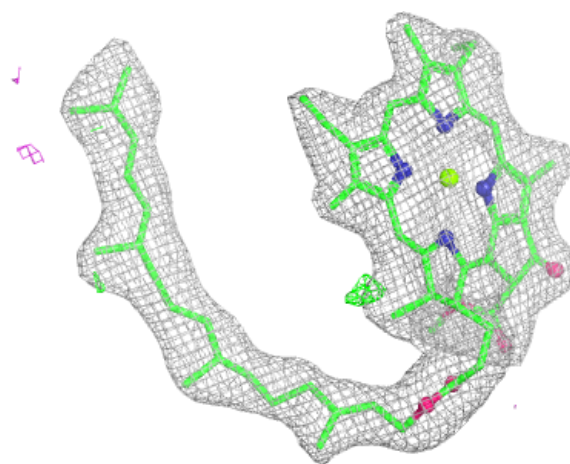
**Electron density around DGD c 519:**

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



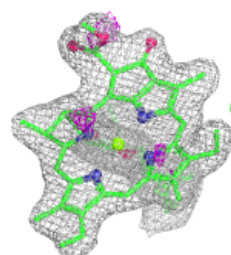
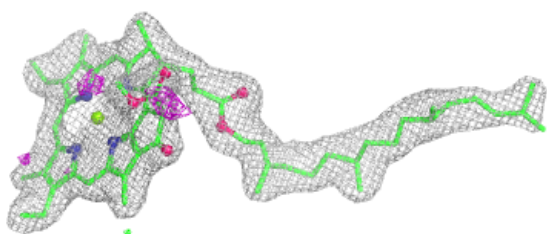
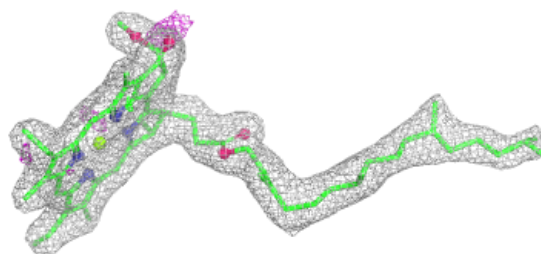
Electron density around CLA c 507:

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

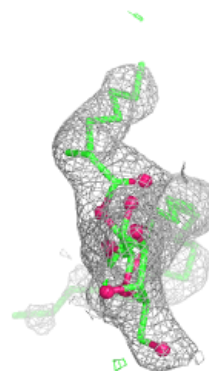
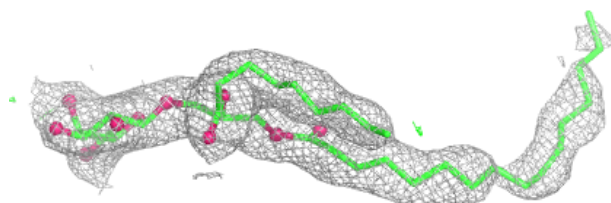
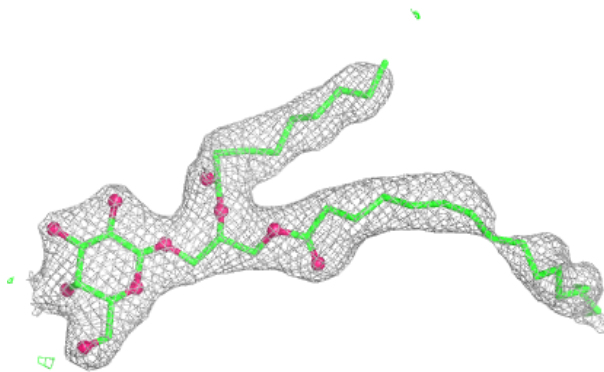


Electron density around CLA C 502:

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

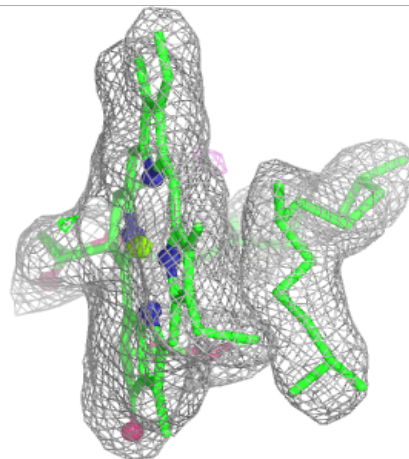
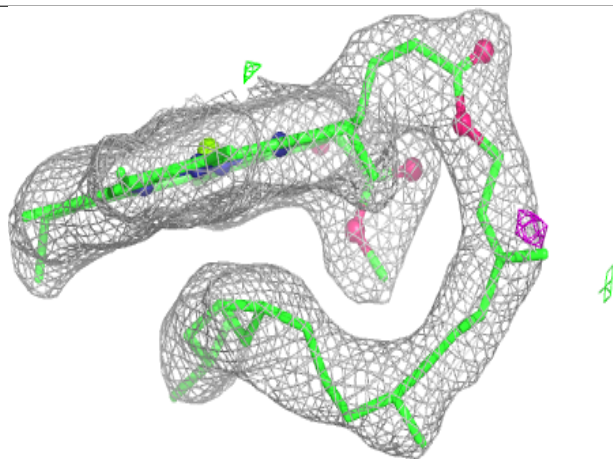
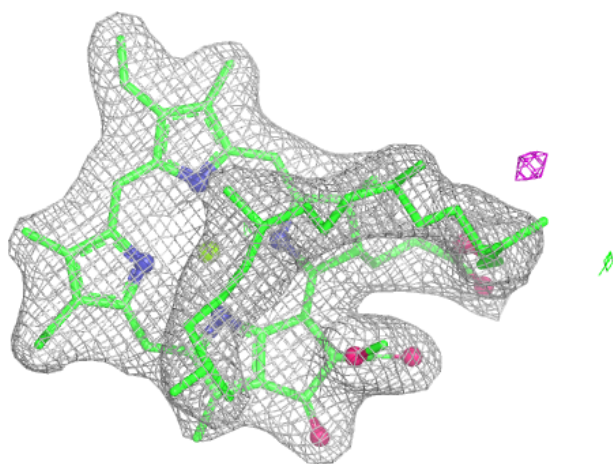
**Electron density around LMG d 411:**

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



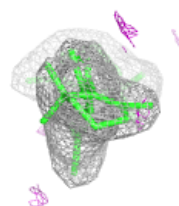
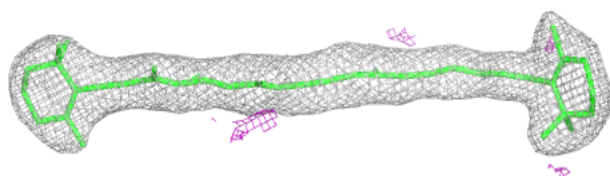
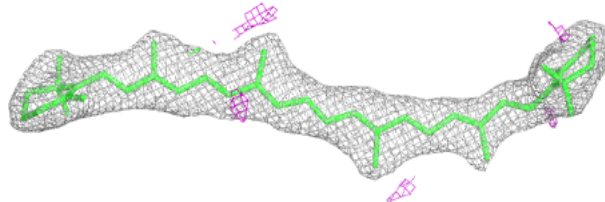
Electron density around CLA c 510:

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

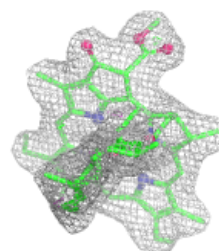
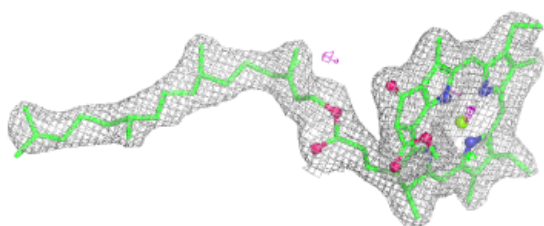
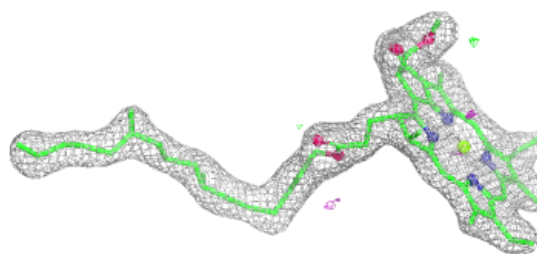


Electron density around BCR c 515:

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

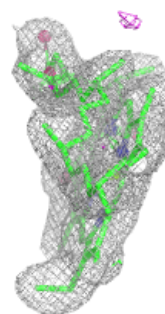
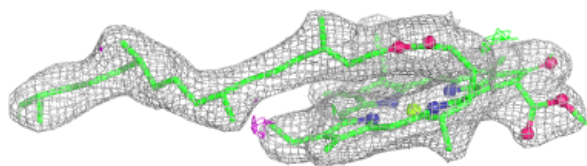
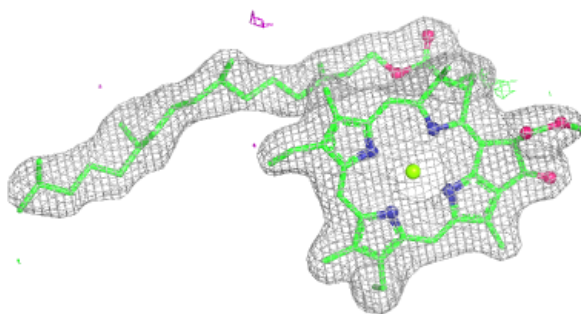
**Electron density around CLA c 502:**

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

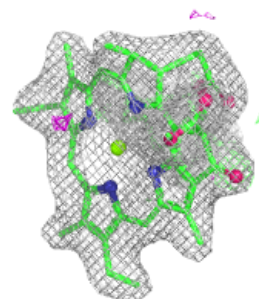
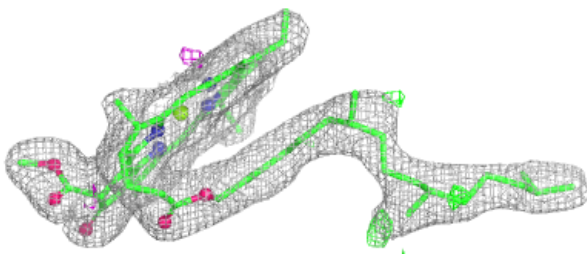
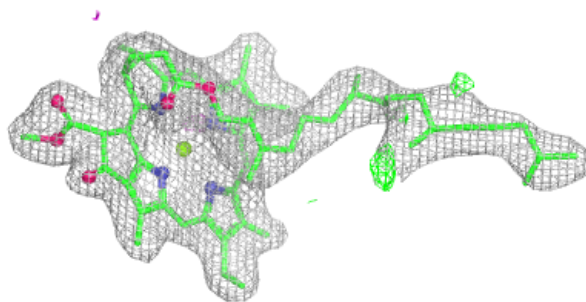


Electron density around CLA C 501:

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

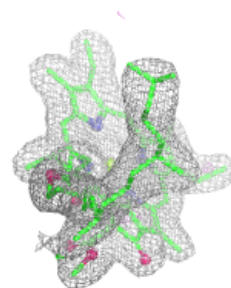
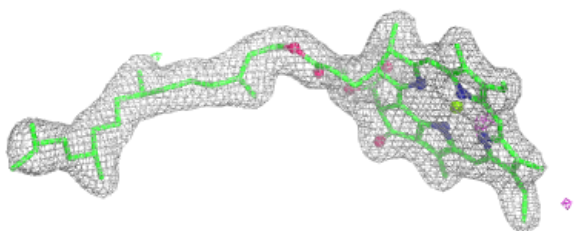
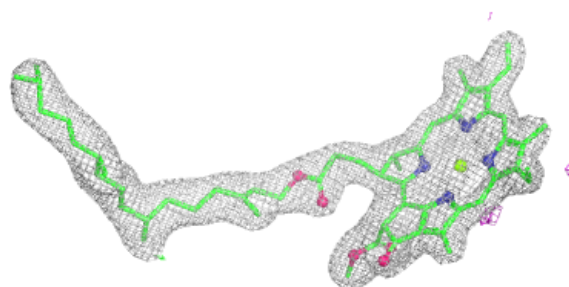
**Electron density around CLA c 505:**

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

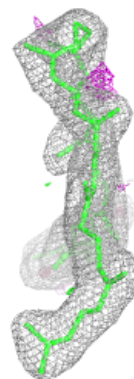
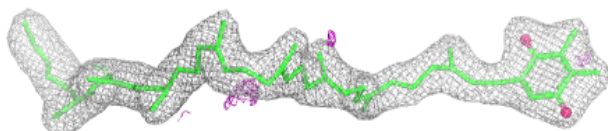
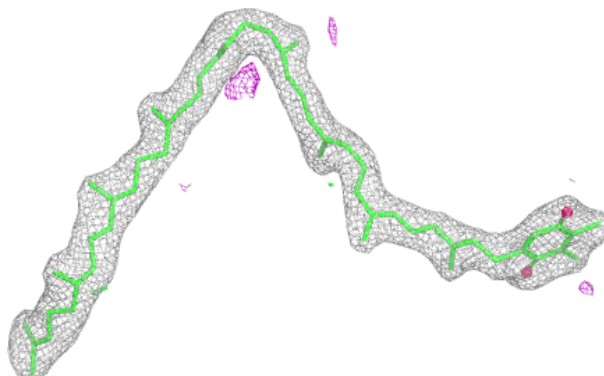


Electron density around CLA a 606:

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

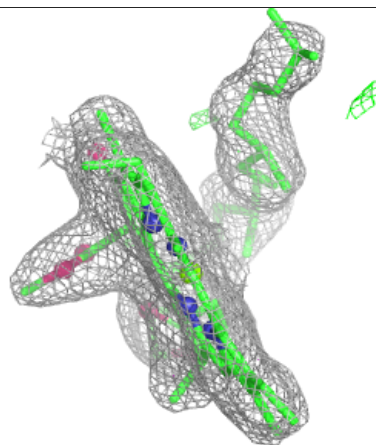
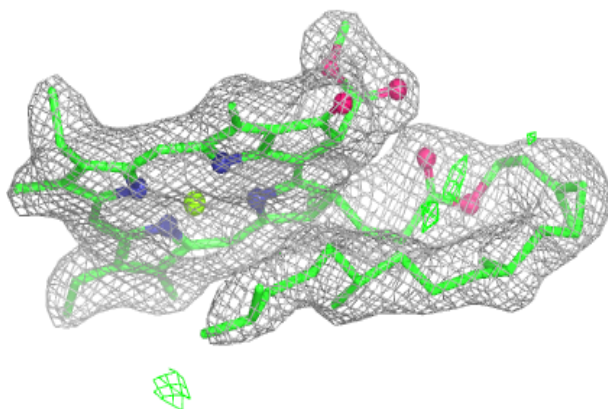
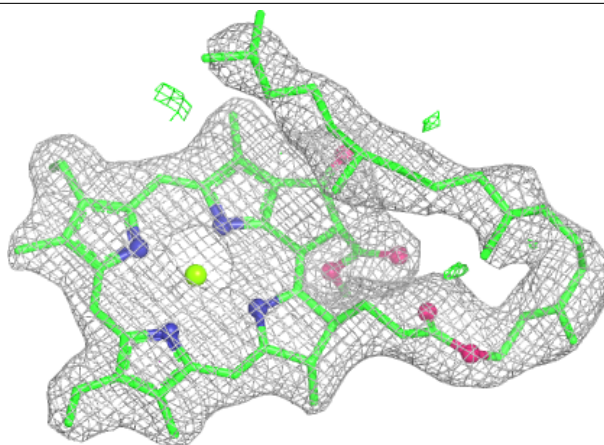
**Electron density around PL9 D 405:**

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

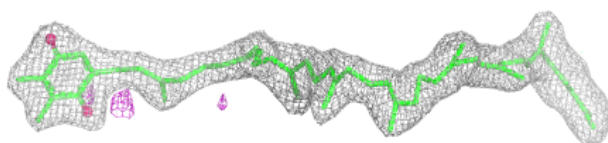
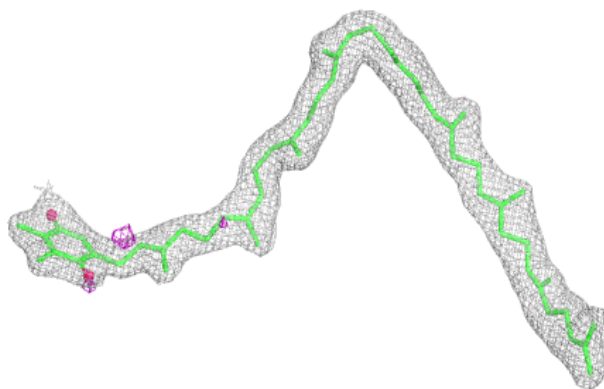


Electron density around CLA C 509:

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

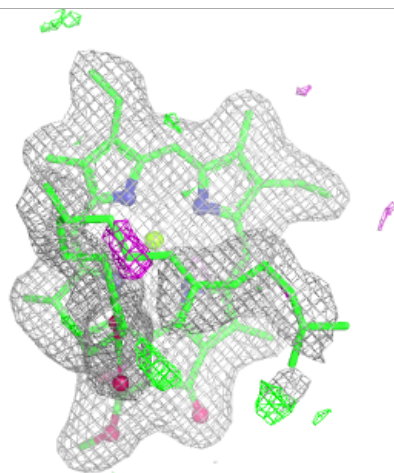
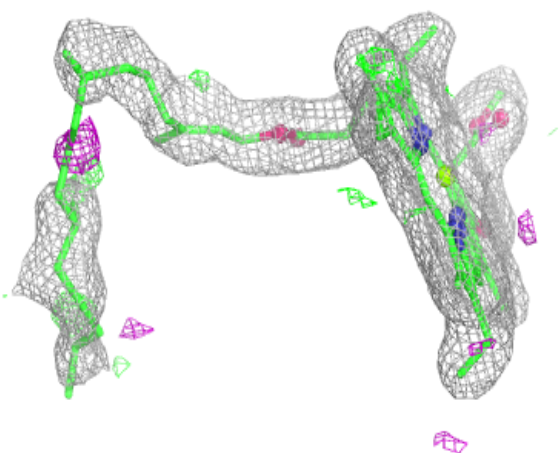
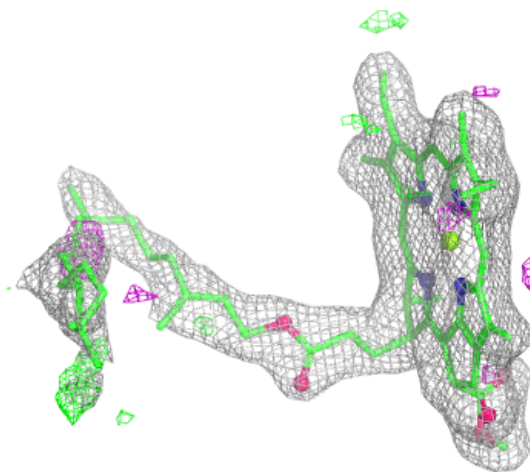
**Electron density around PL9 d 406:**

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



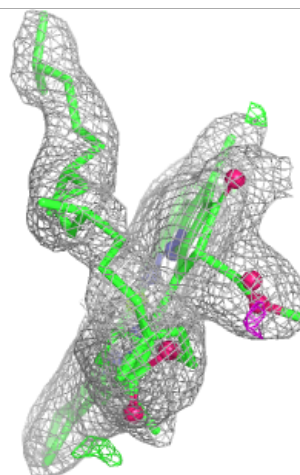
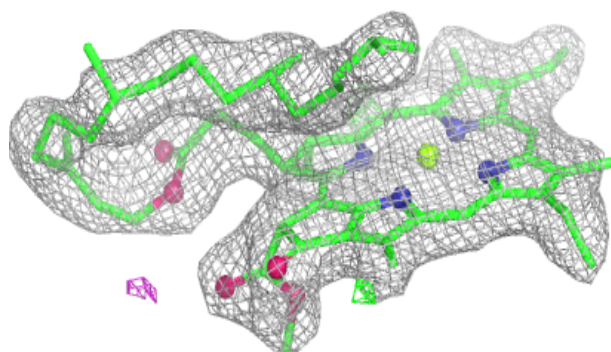
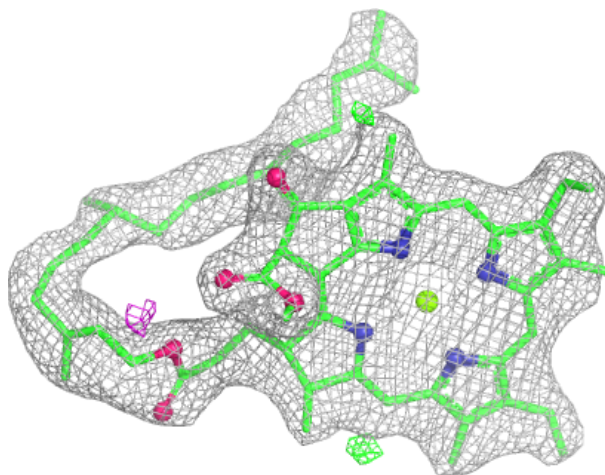
Electron density around CLA a 609:

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



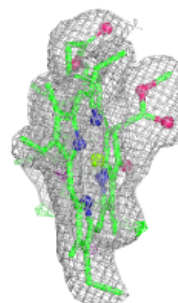
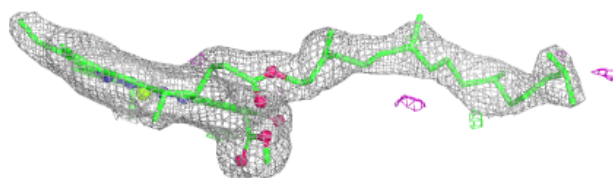
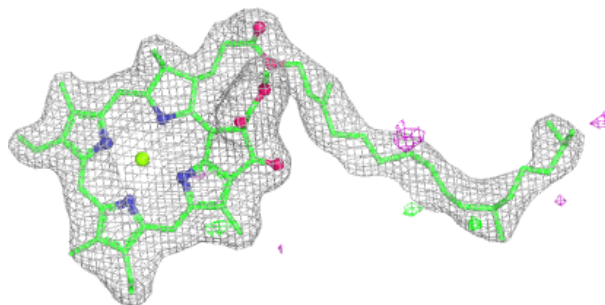
Electron density around CLA c 509:

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

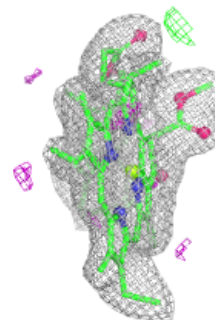
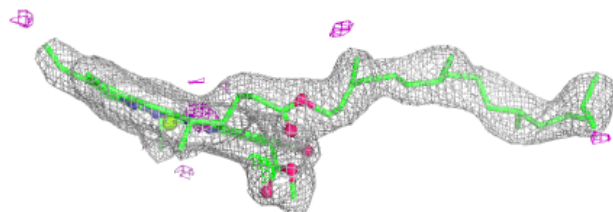
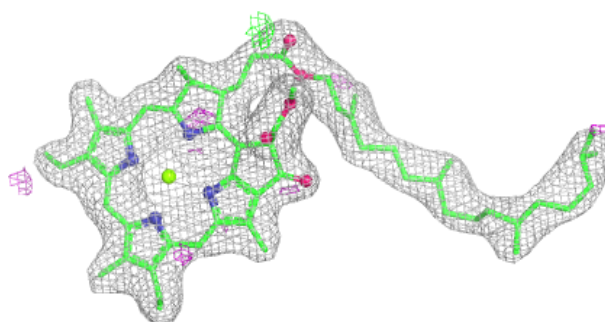


Electron density around CLA b 601:

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

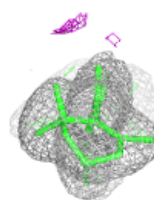
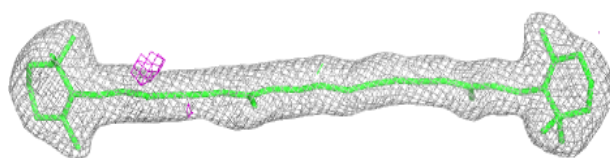
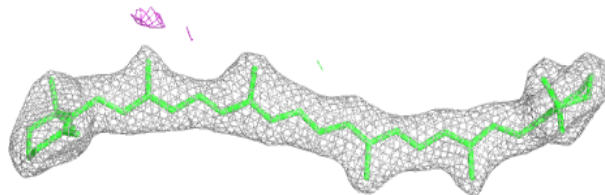
**Electron density around CLA B 602:**

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

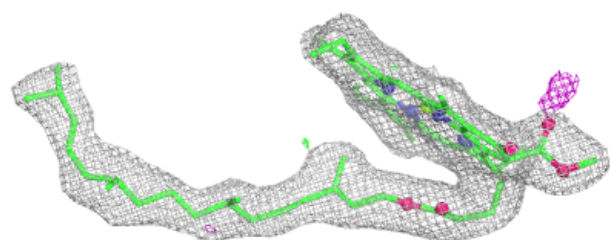
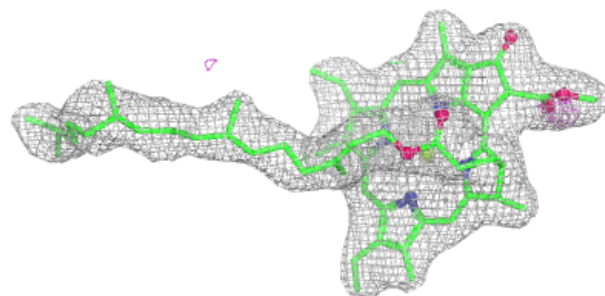


Electron density around BCR a 610:

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

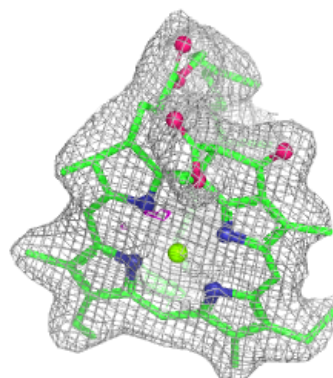
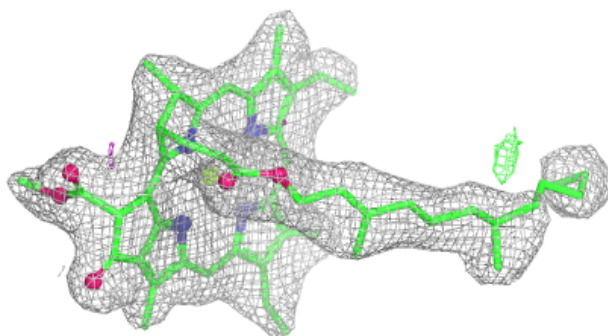
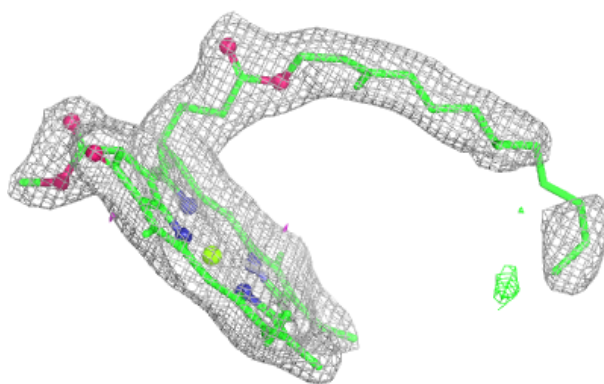
**Electron density around CLA b 607:**

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

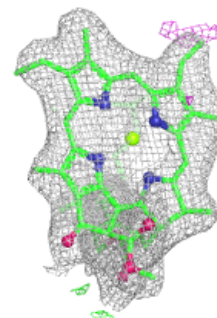
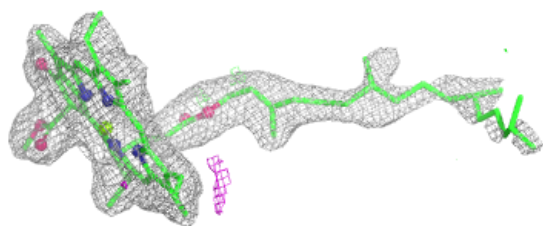
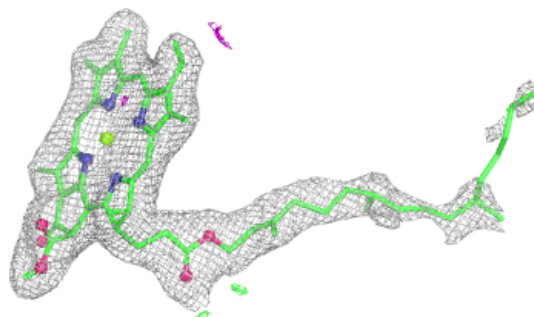


Electron density around CLA C 504:

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

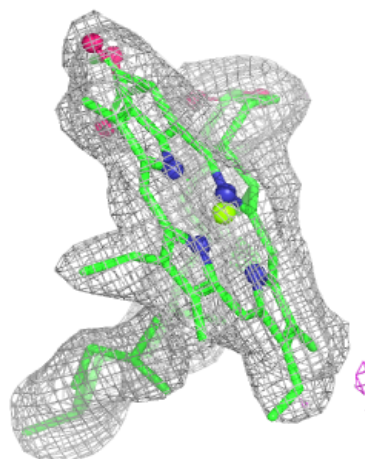
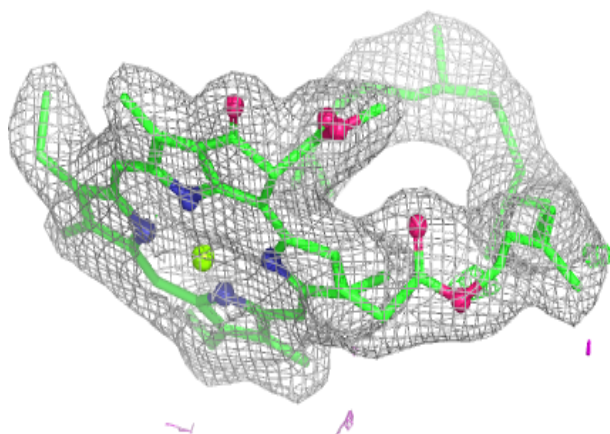
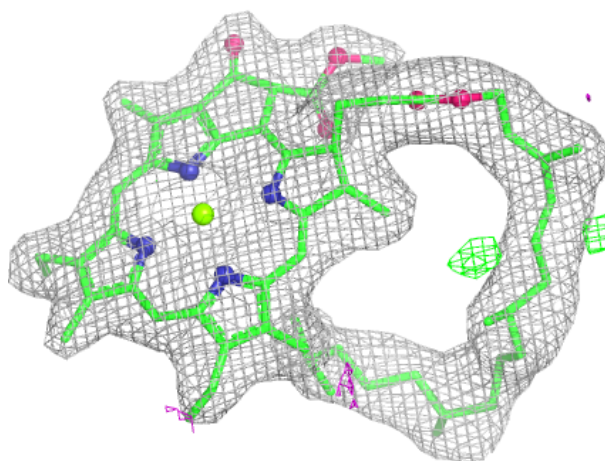
**Electron density around CLA d 404:**

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



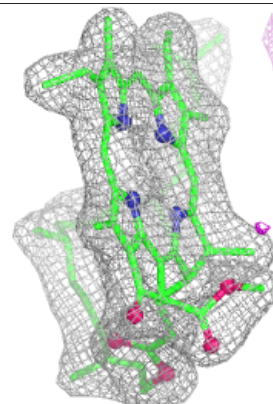
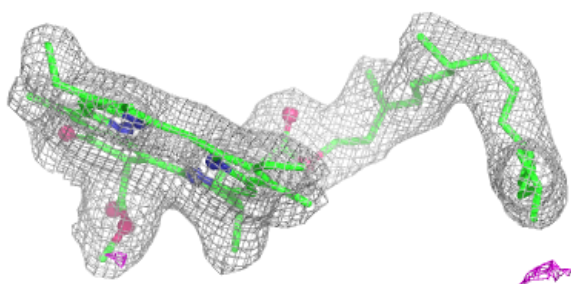
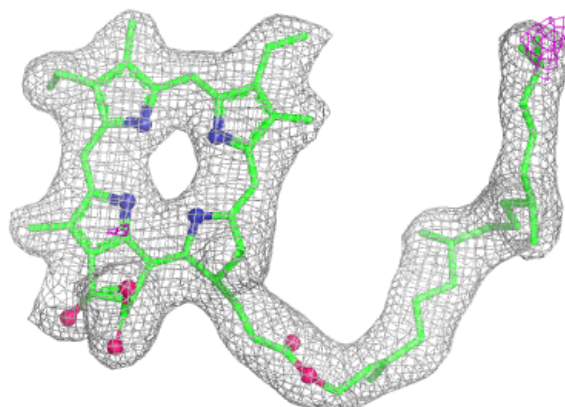
Electron density around CLA b 614:

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

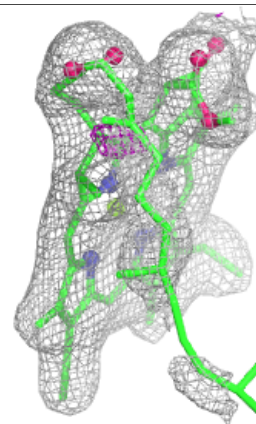
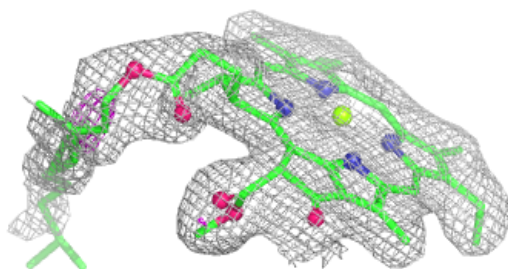
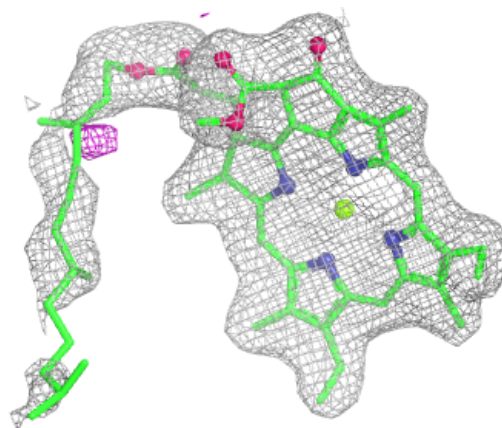


Electron density around PHO d 402:

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

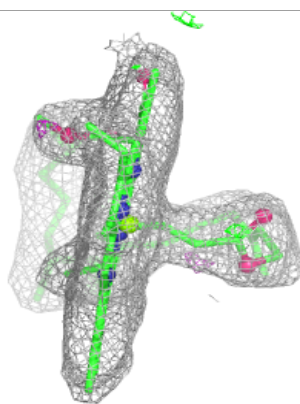
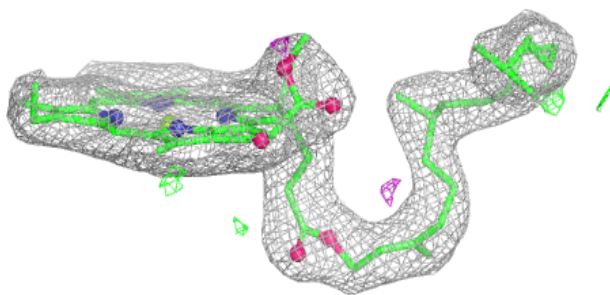
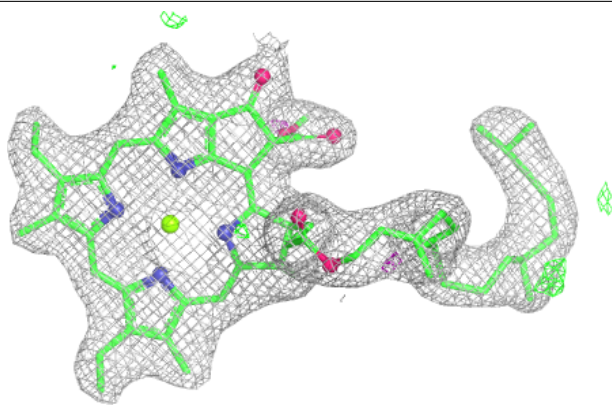
**Electron density around CLA b 615:**

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



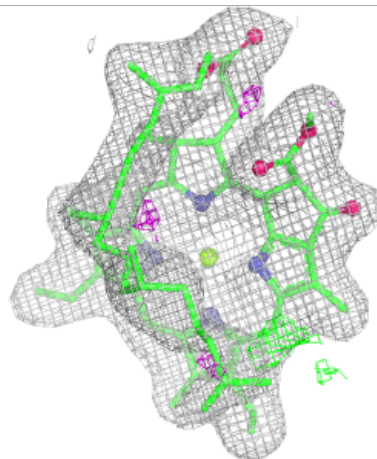
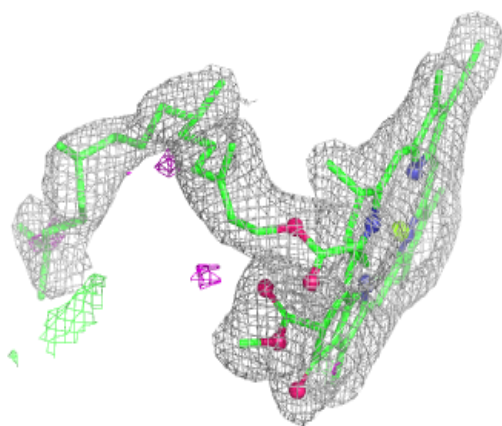
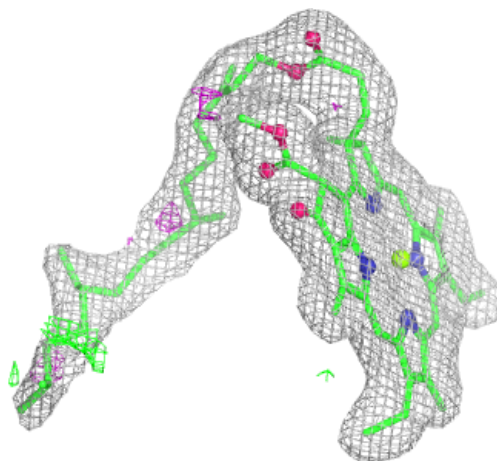
Electron density around CLA b 611:

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



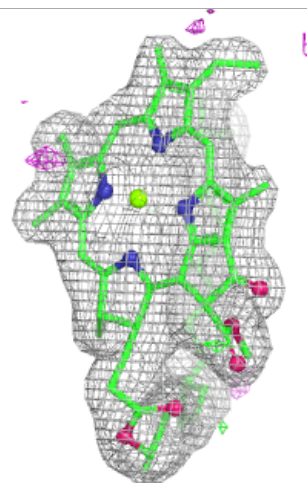
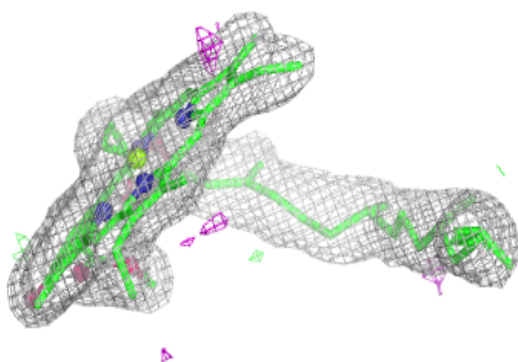
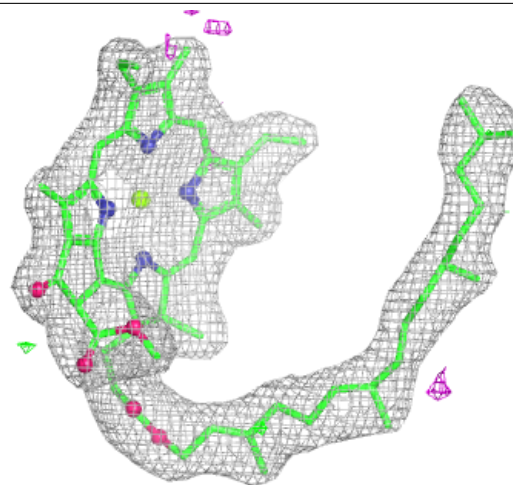
Electron density around CLA b 612:

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



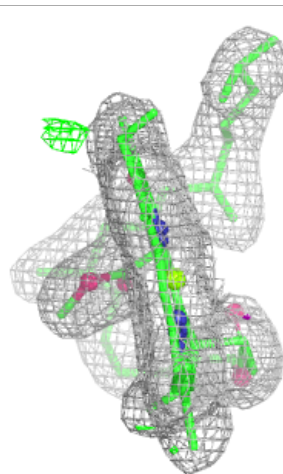
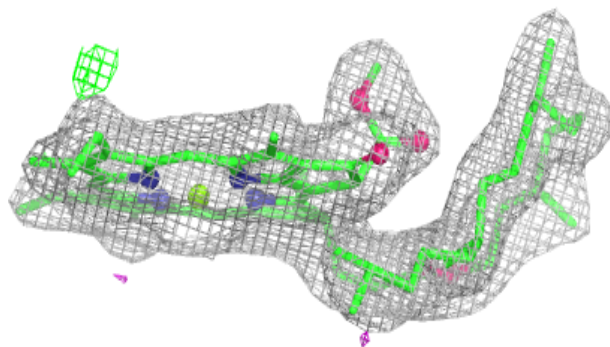
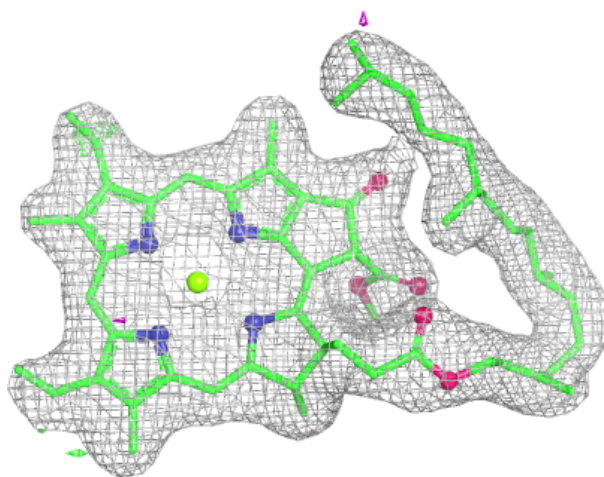
Electron density around CLA C 507:

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



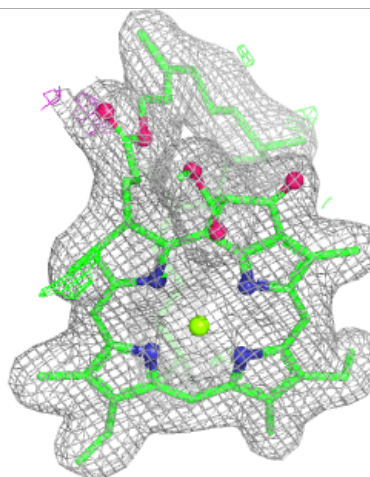
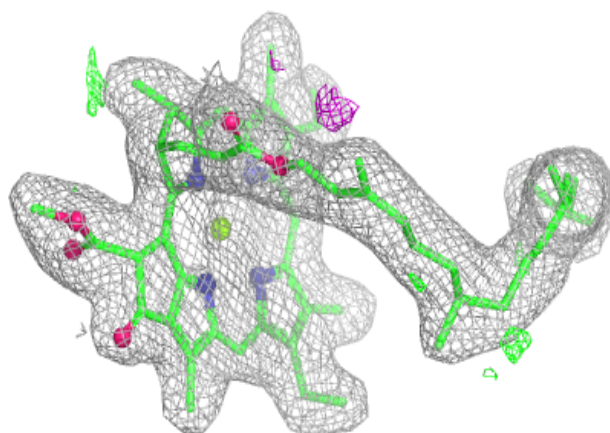
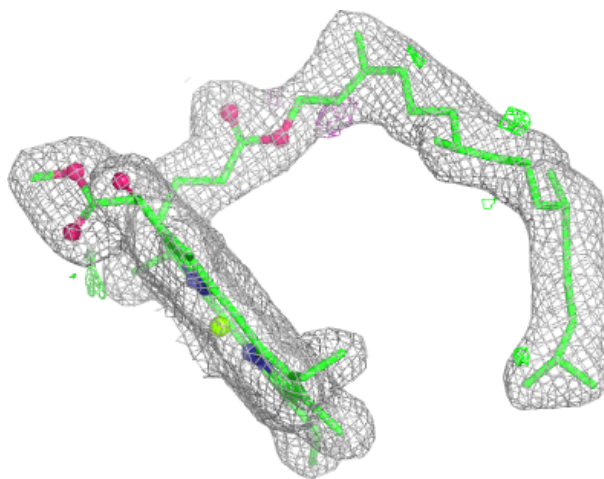
Electron density around CLA B 610:

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



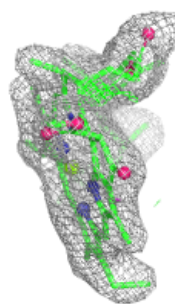
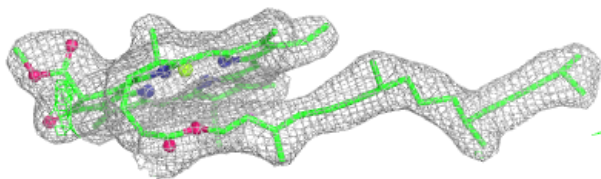
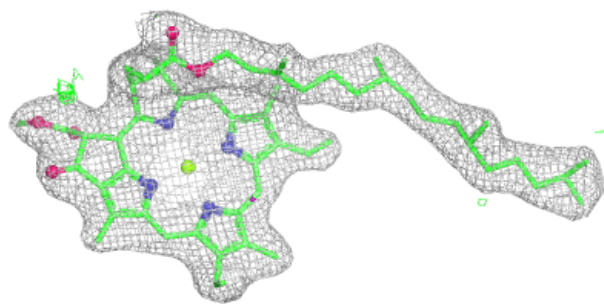
Electron density around CLA B 611:

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

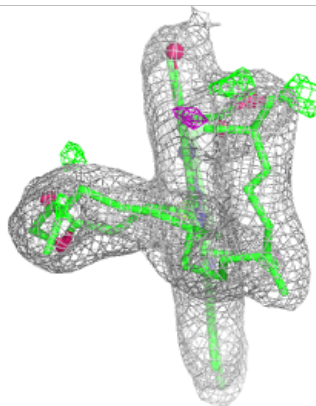
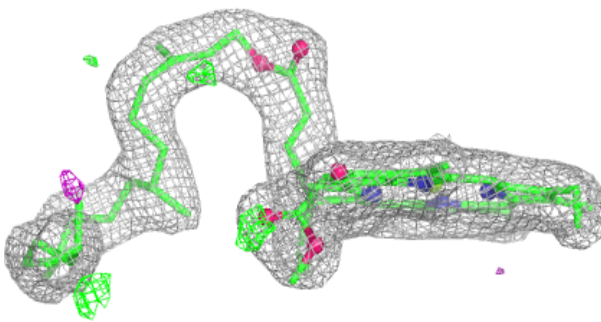
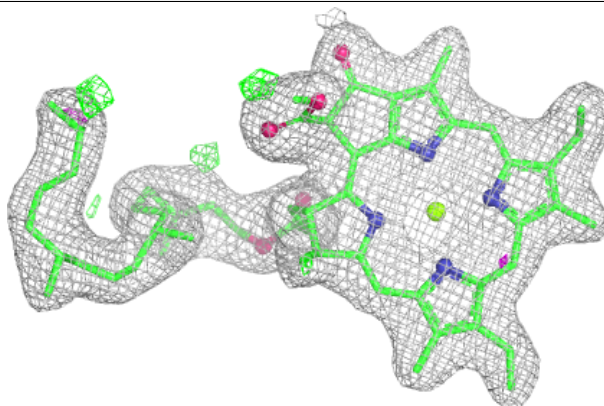


Electron density around CLA c 501:

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

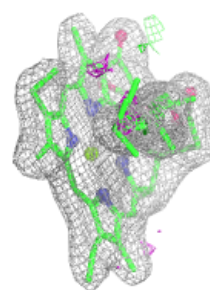
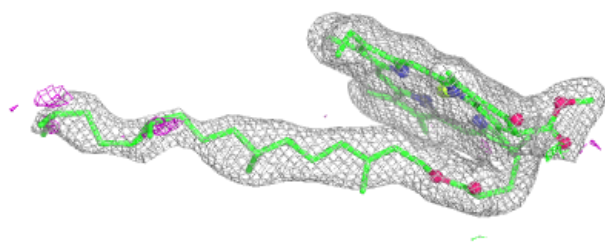
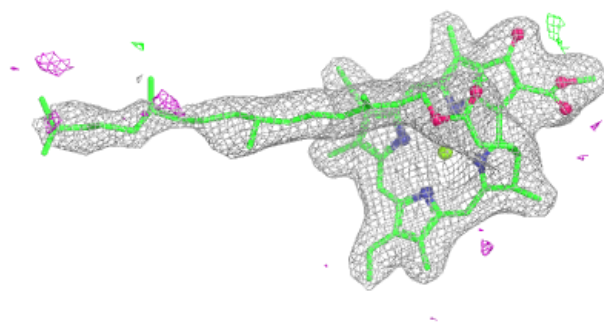
**Electron density around CLA B 612:**

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



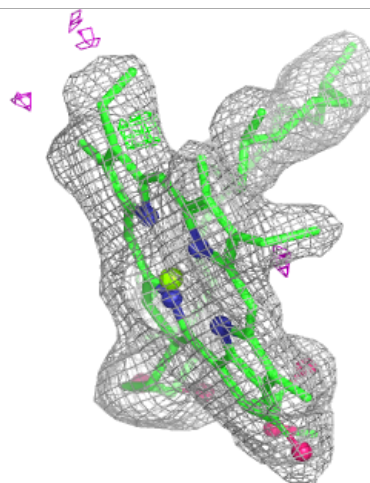
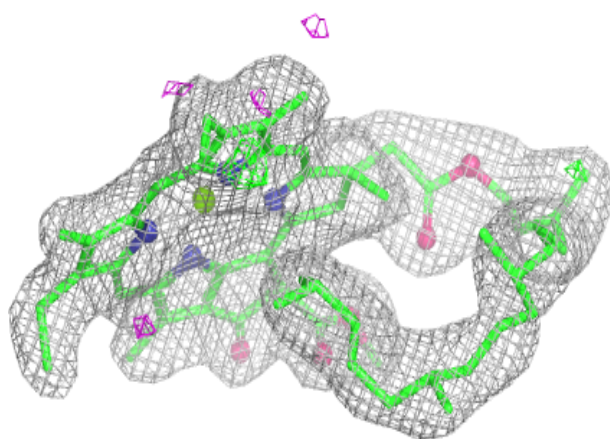
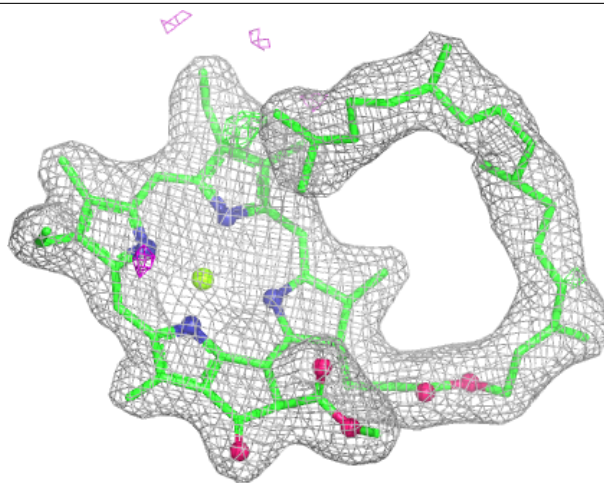
Electron density around CLA B 614:

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



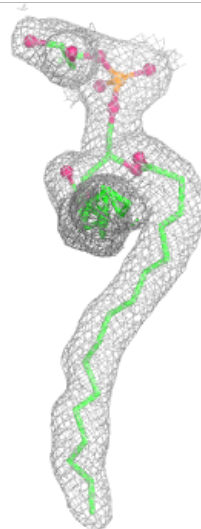
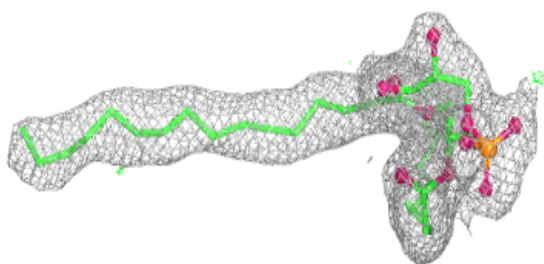
Electron density around CLA B 615:

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



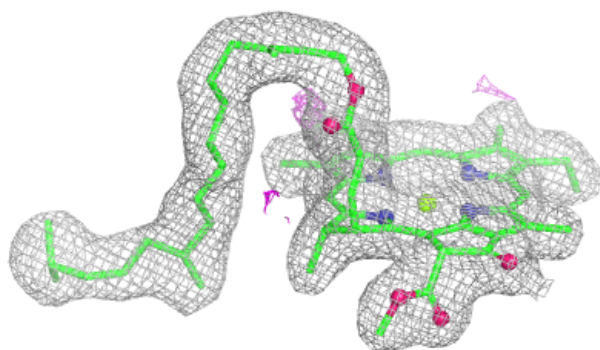
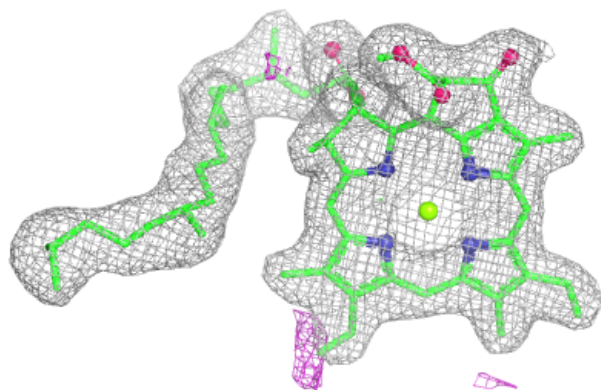
Electron density around LHG L 101:

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

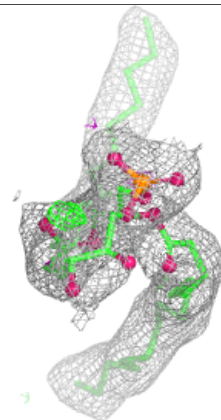
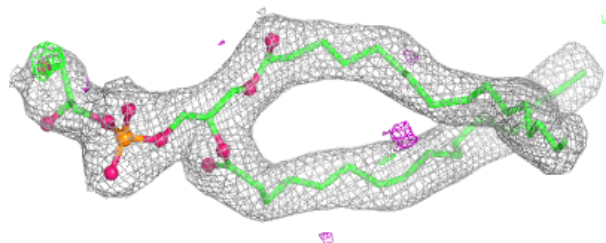
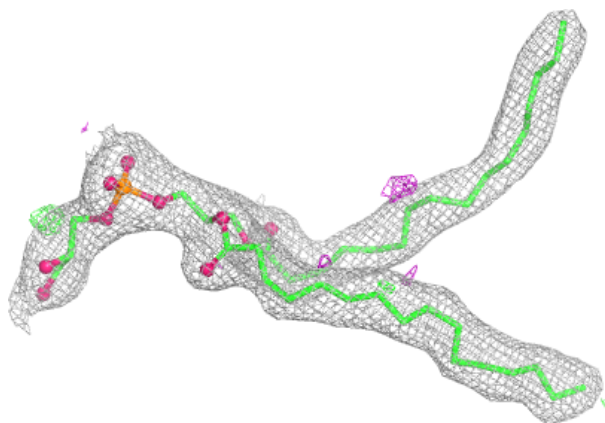


Electron density around CLA A 613:

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

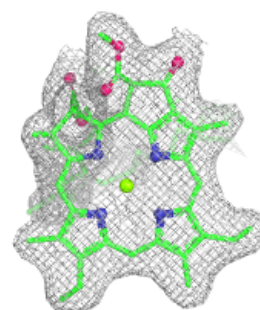
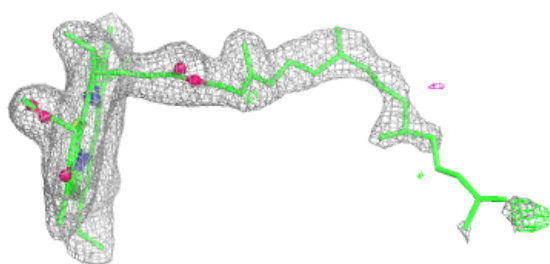
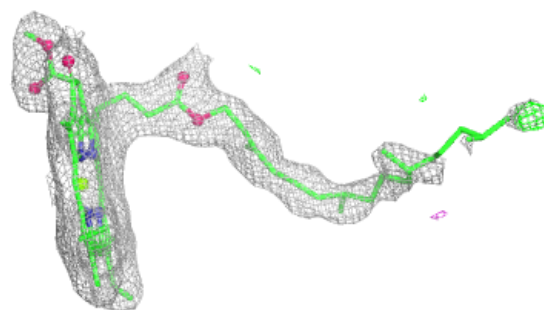
**Electron density around LHG d 408:**

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

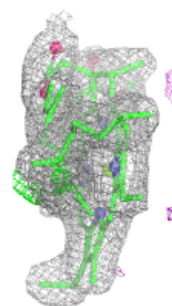
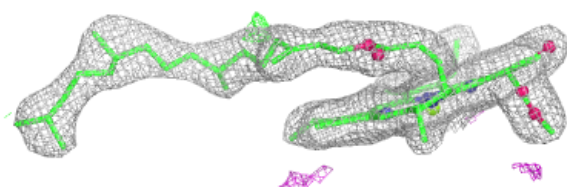
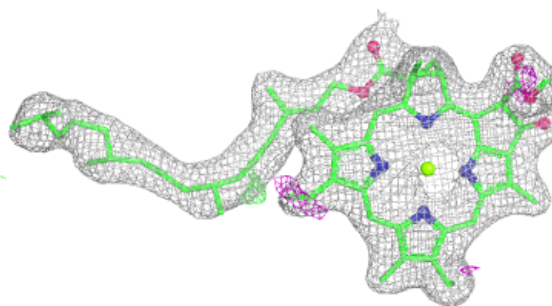


Electron density around CLA D 403:

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

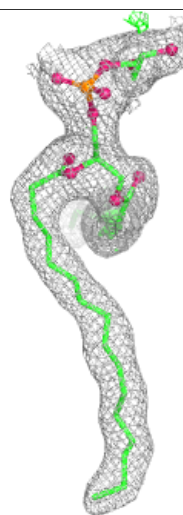
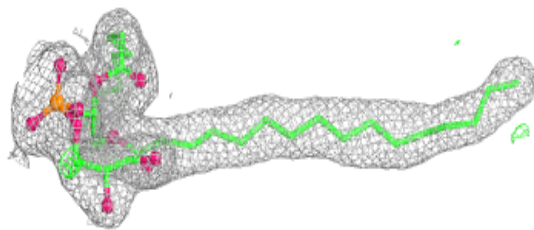
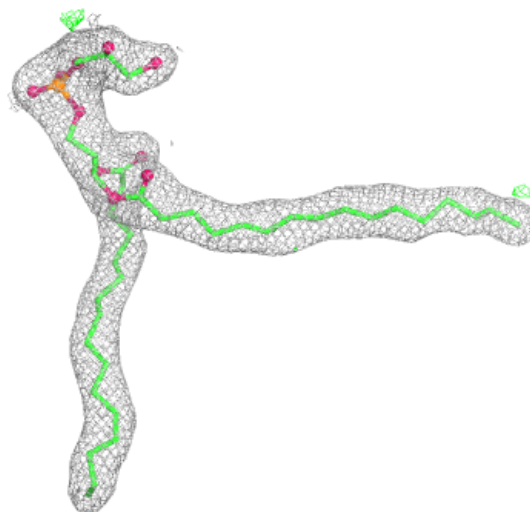
**Electron density around CLA B 603:**

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



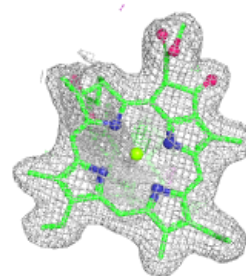
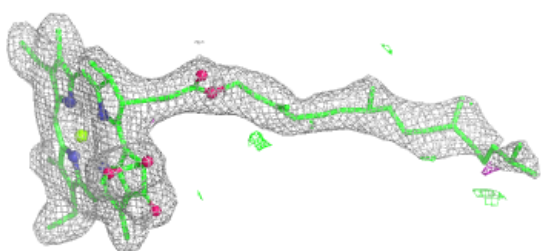
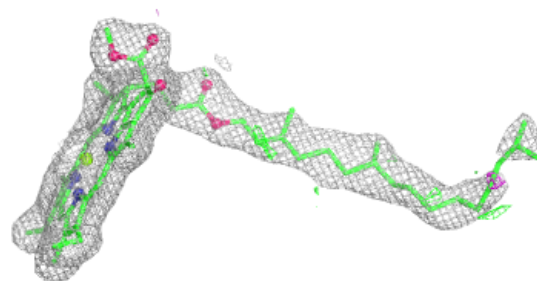
Electron density around LHG 1 101:

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

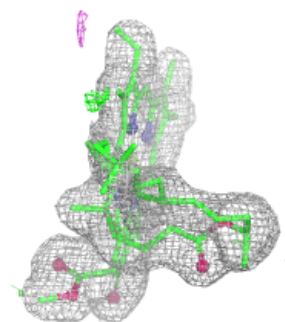
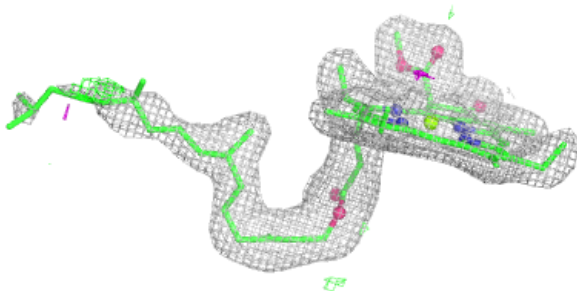
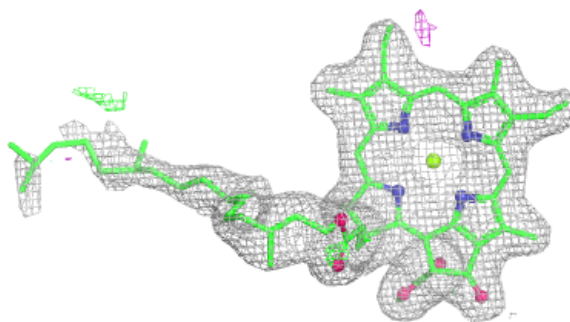


Electron density around CLA B 604:

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

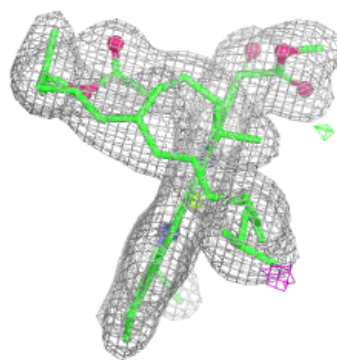
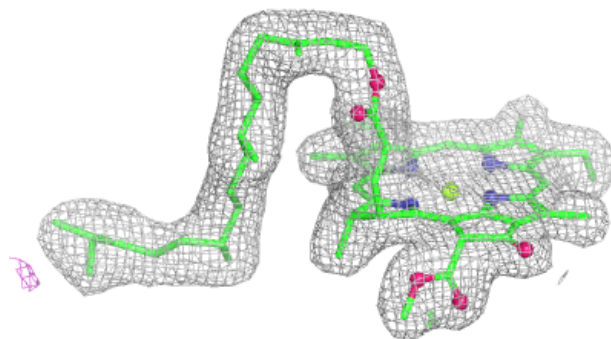
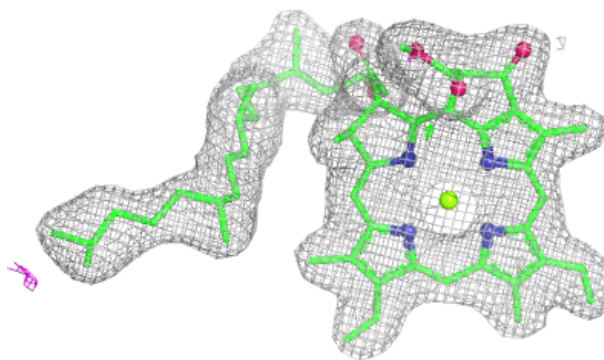
**Electron density around CLA A 608:**

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

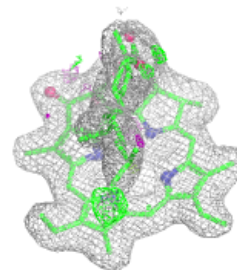
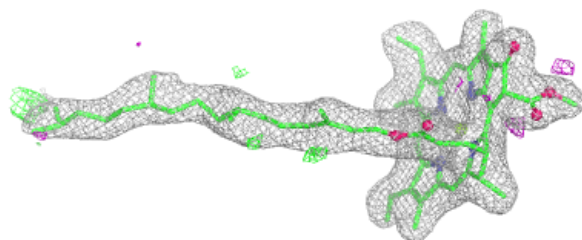
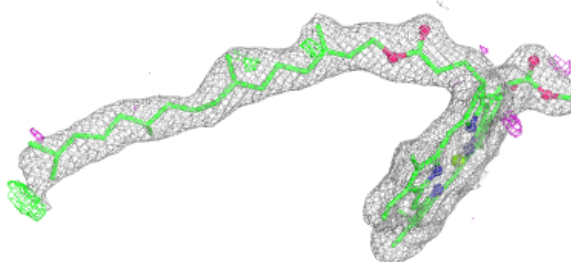


Electron density around CLA a 612:

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

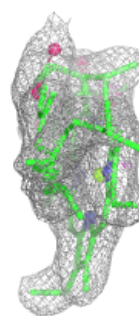
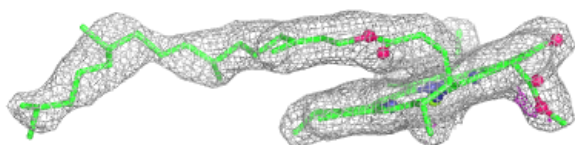
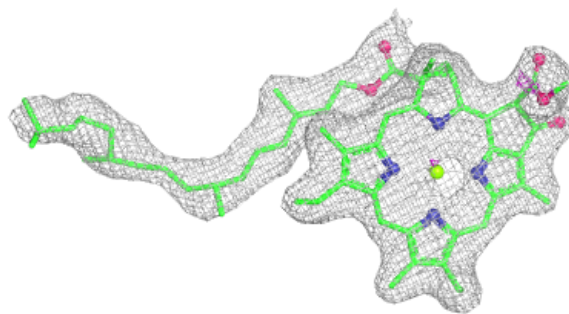
**Electron density around CLA B 607:**

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

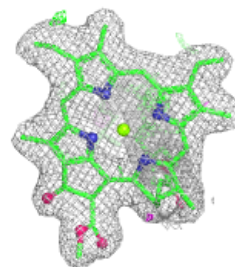
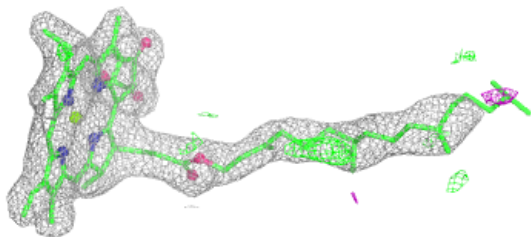
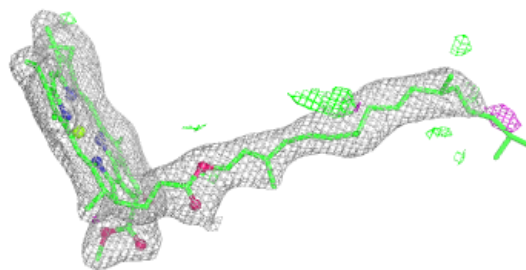


Electron density around CLA b 602:

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

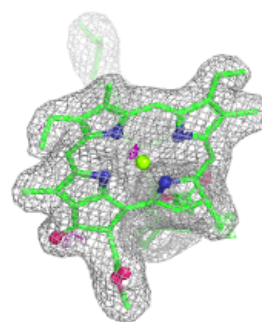
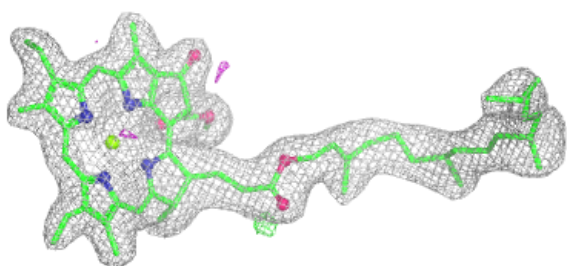
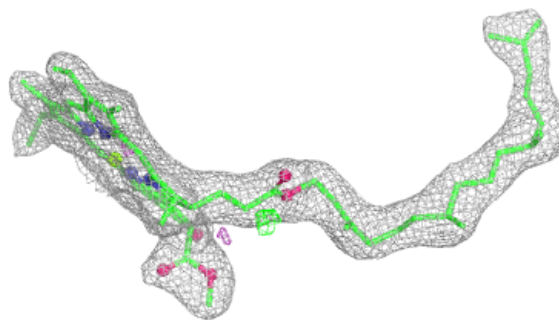
**Electron density around CLA b 603:**

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

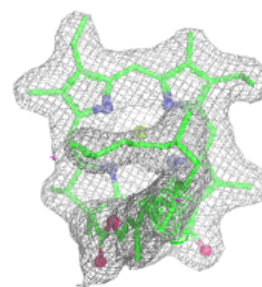
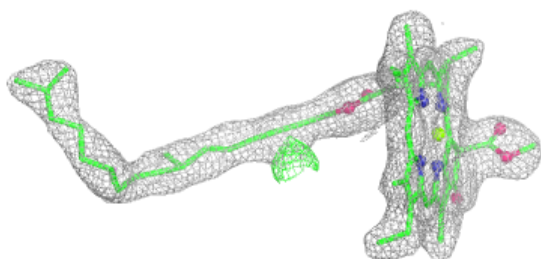
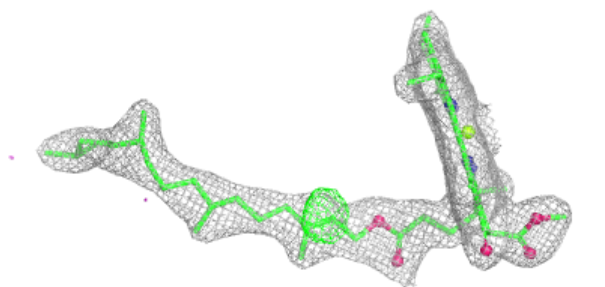


Electron density around CLA d 403:

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

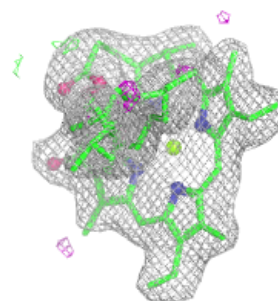
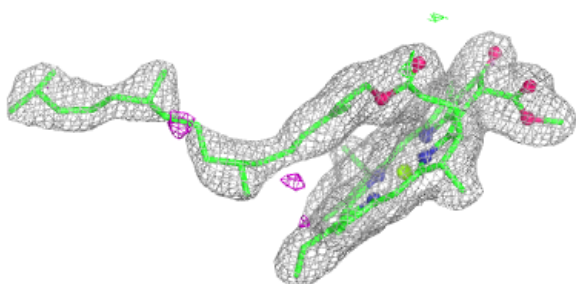
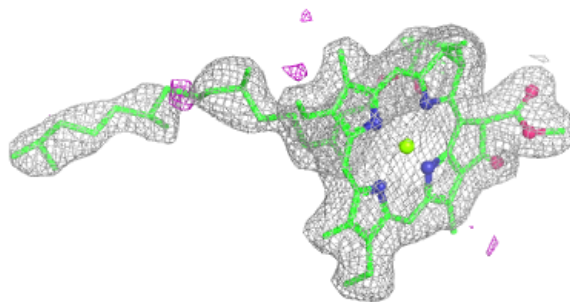
**Electron density around CLA b 604:**

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

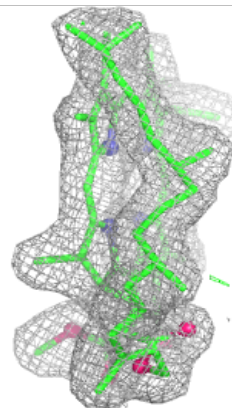
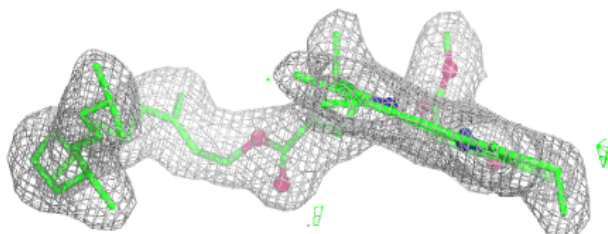
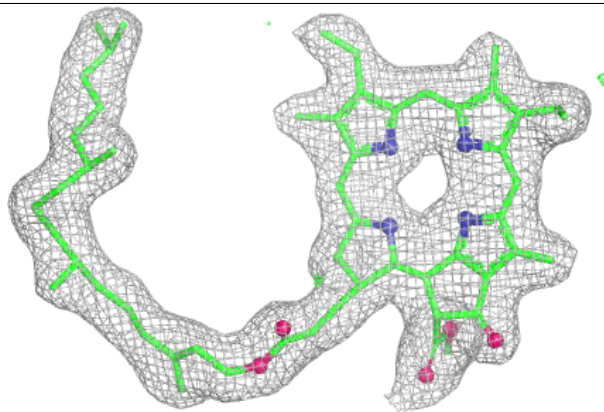


Electron density around CLA C 505:

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

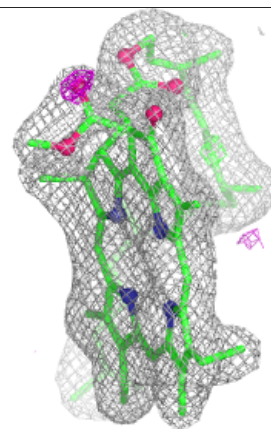
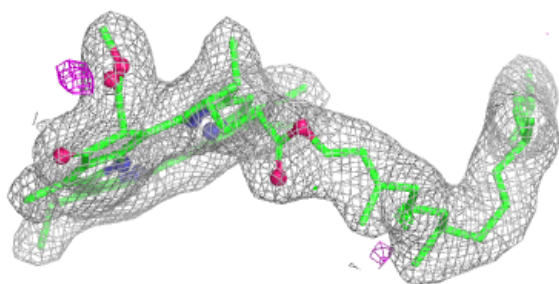
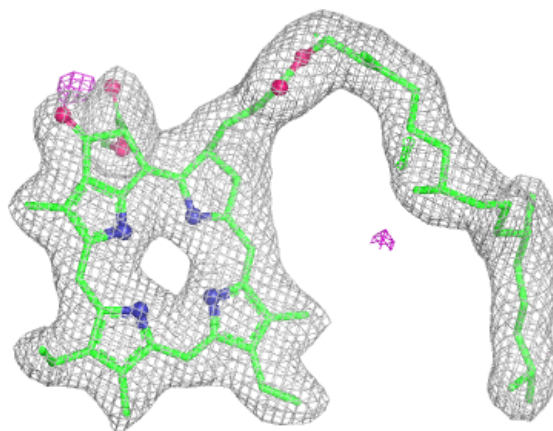
**Electron density around PHO A 609:**

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



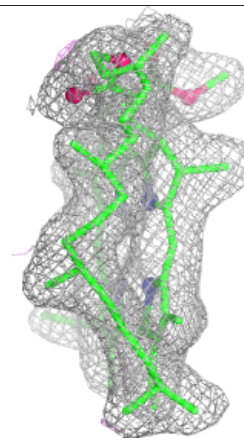
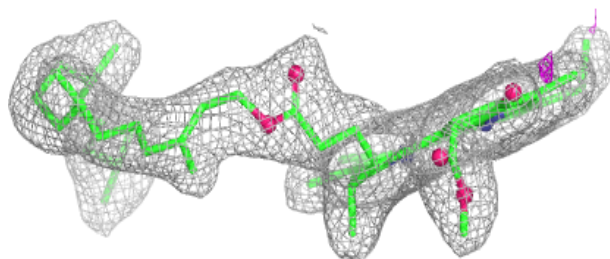
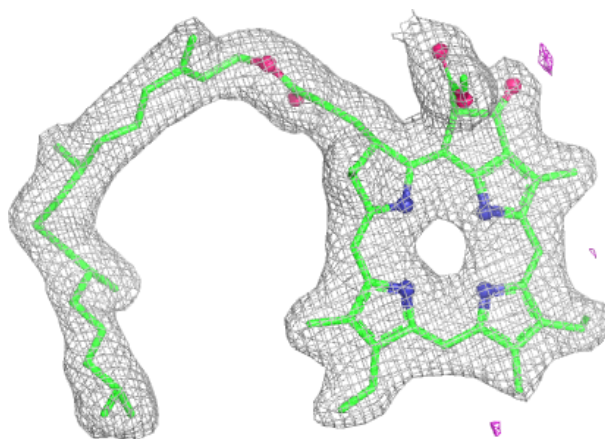
Electron density around PHO D 401:

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



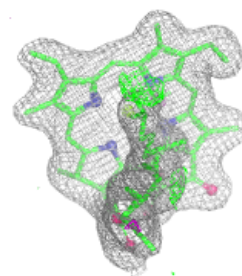
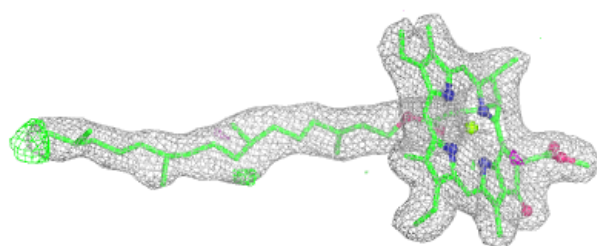
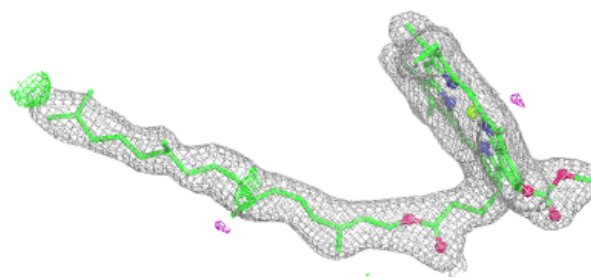
Electron density around PHO a 608:

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

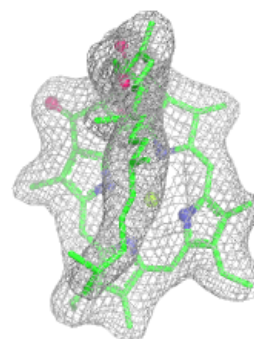
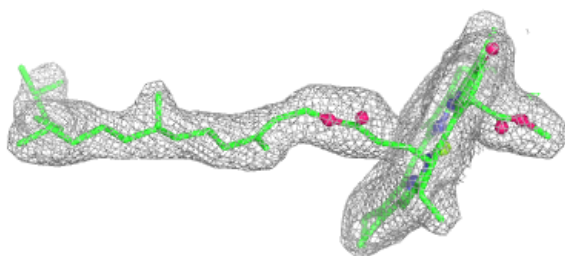
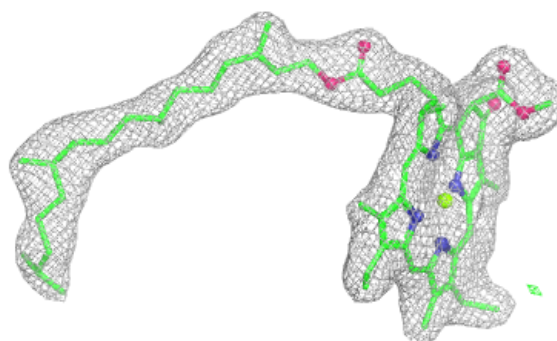


Electron density around CLA b 606:

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

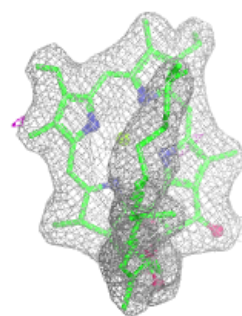
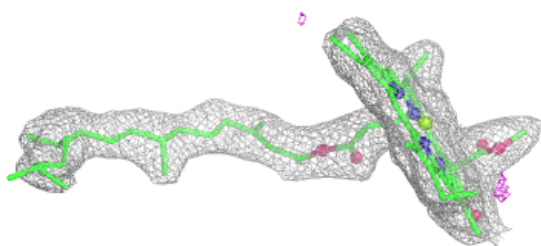
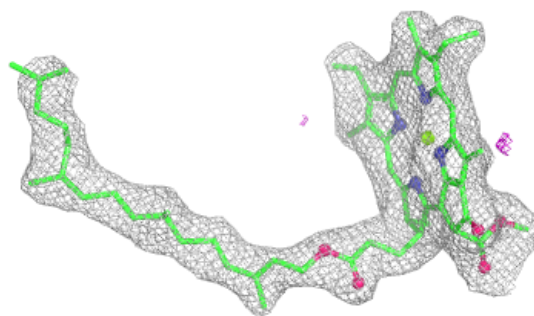
**Electron density around CLA B 609:**

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



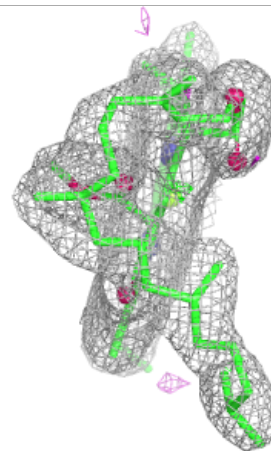
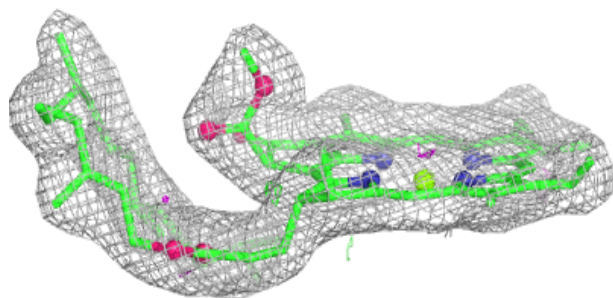
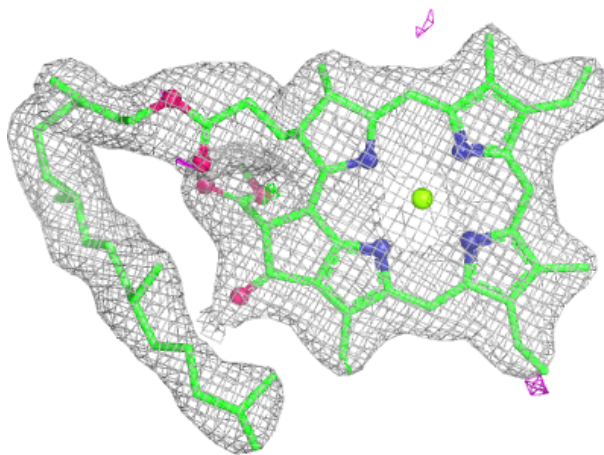
Electron density around CLA b 608:

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



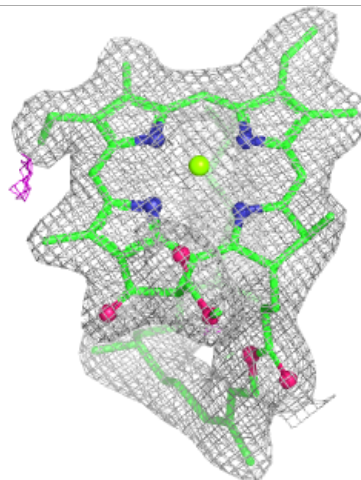
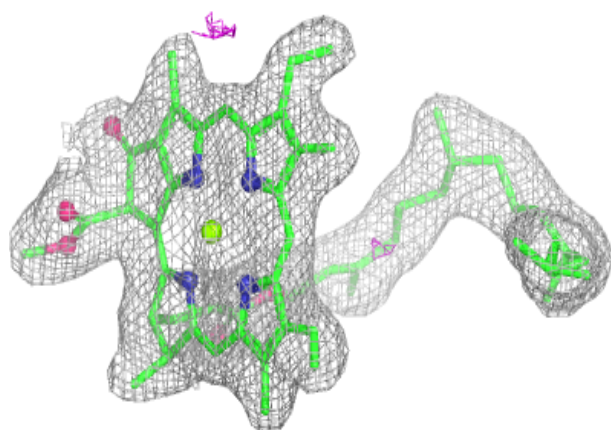
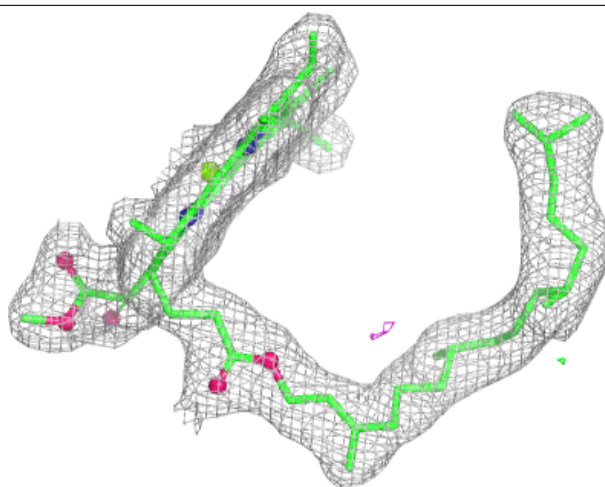
Electron density around CLA b 609:

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



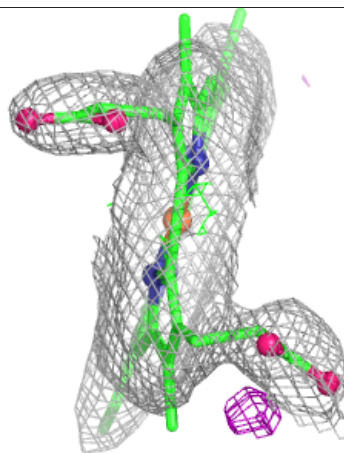
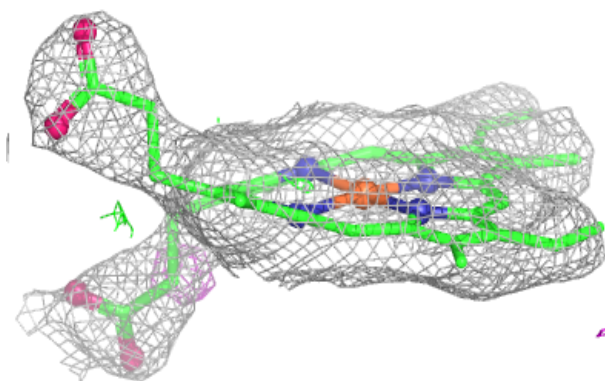
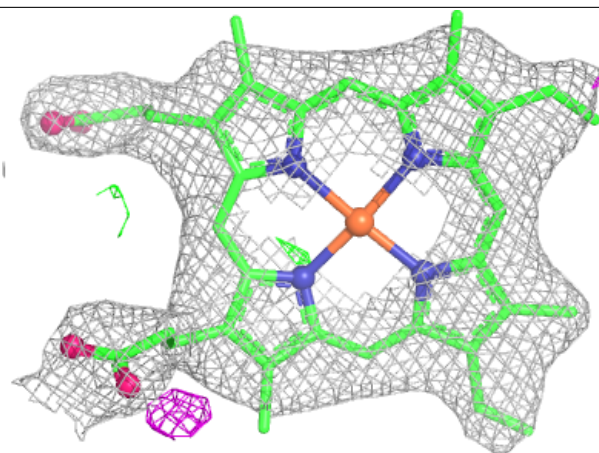
Electron density around CLA b 610:

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



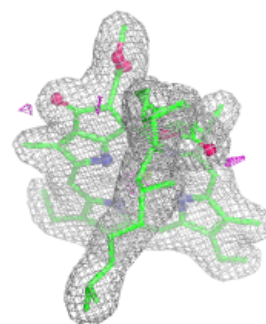
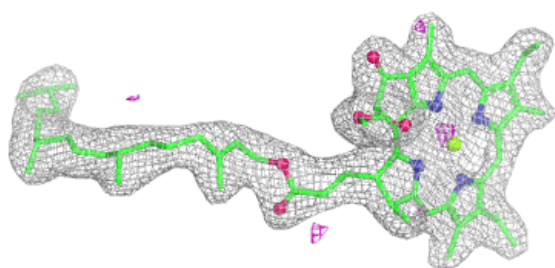
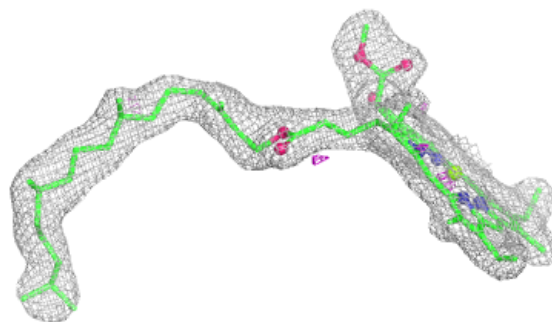
Electron density around HEM e 101:

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

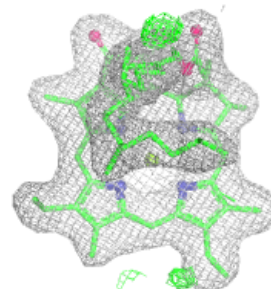
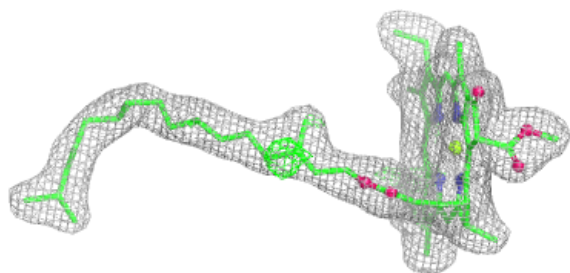
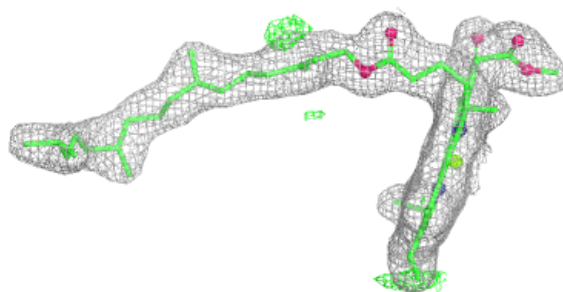


Electron density around CLA D 402:

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

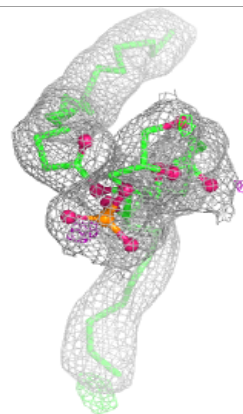
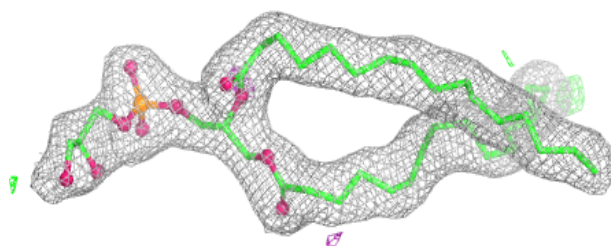
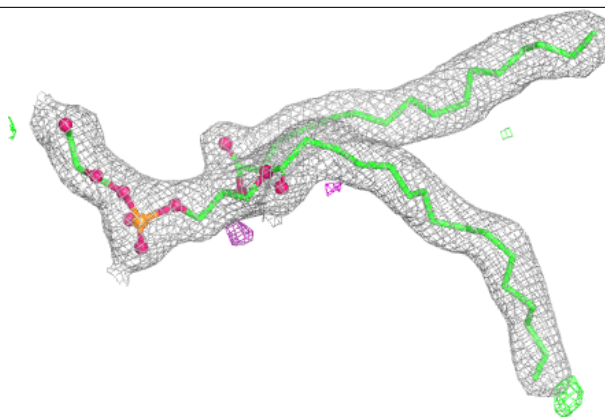
**Electron density around CLA B 605:**

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

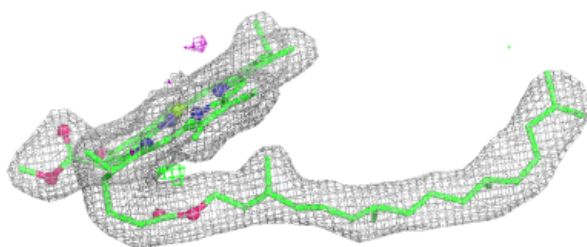
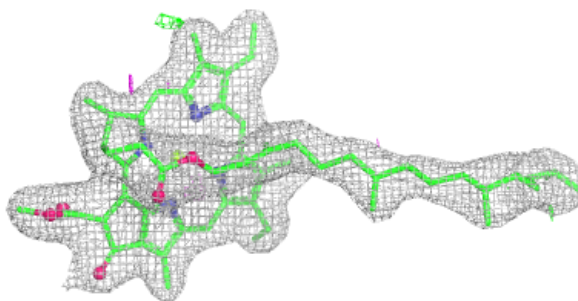


Electron density around LHG D 407:

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

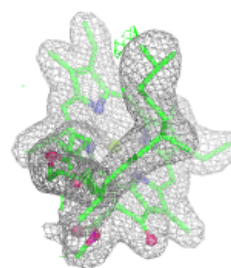
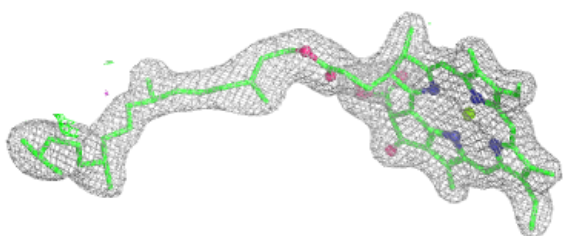
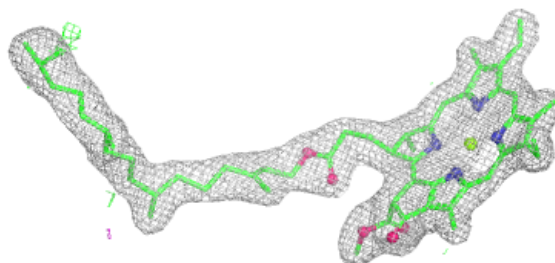
**Electron density around CLA B 608:**

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



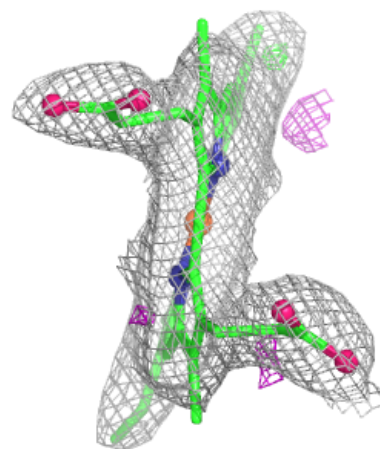
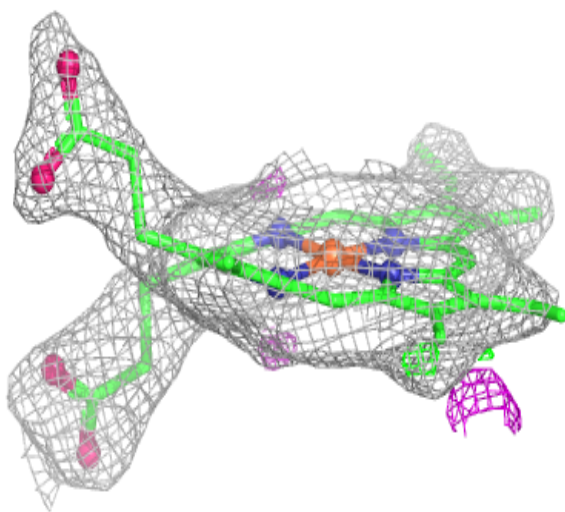
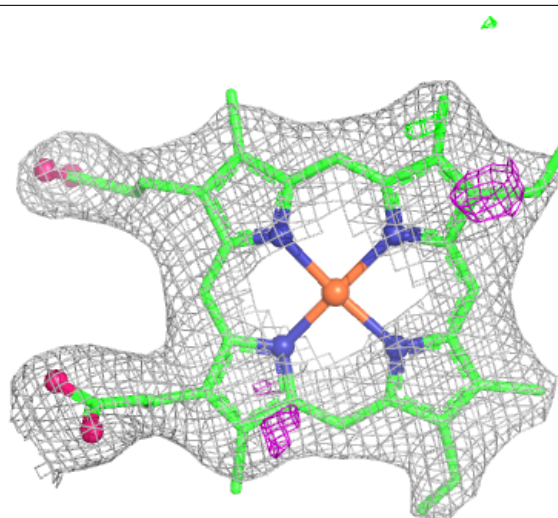
Electron density around CLA A 607:

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



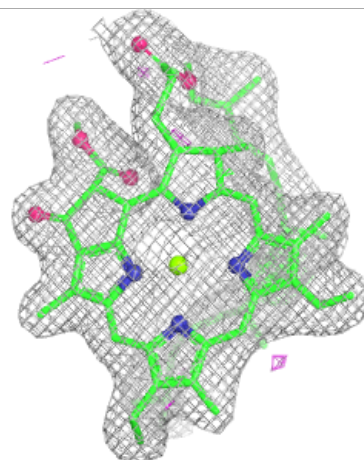
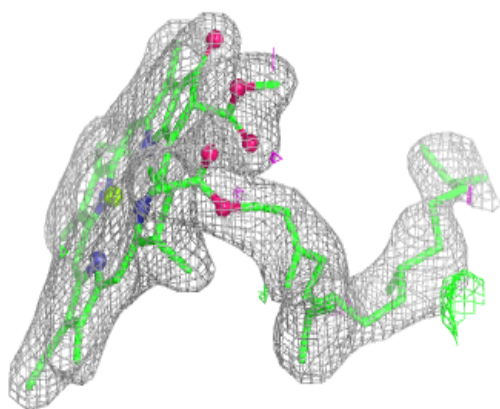
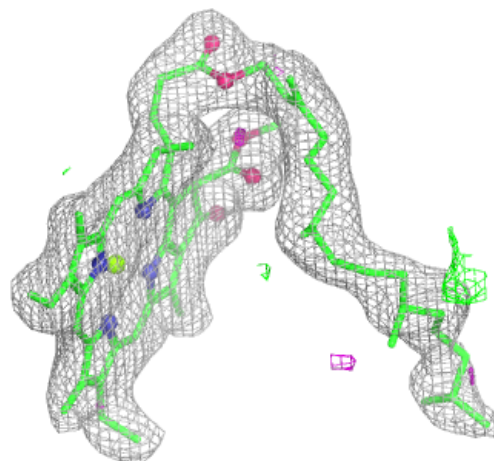
Electron density around HEM F 101:

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



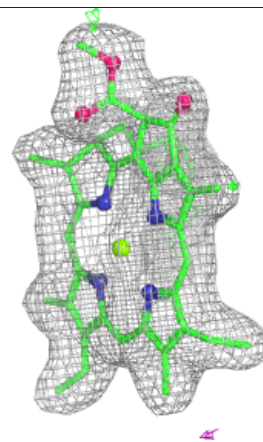
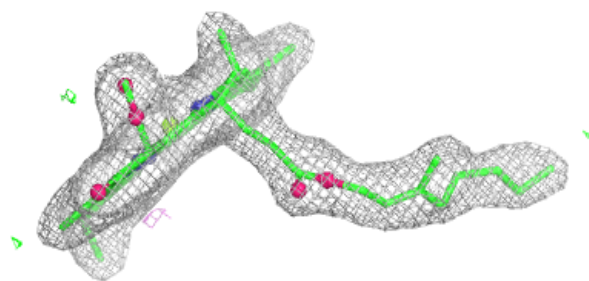
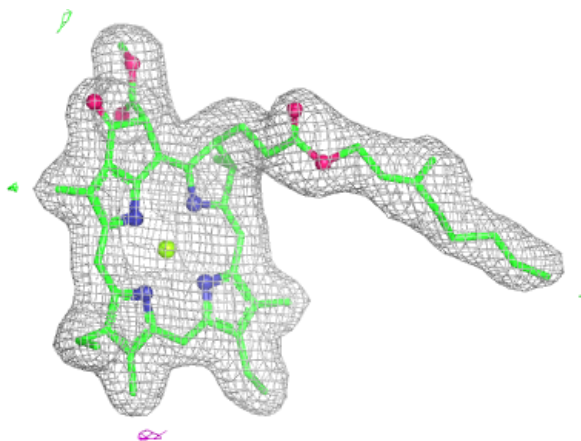
Electron density around CLA B 613:

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



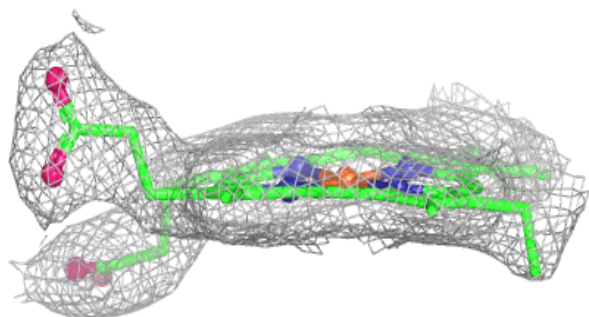
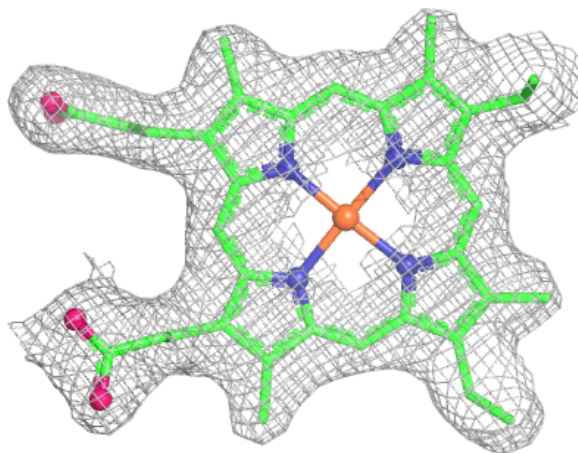
Electron density around CLA A 610:

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



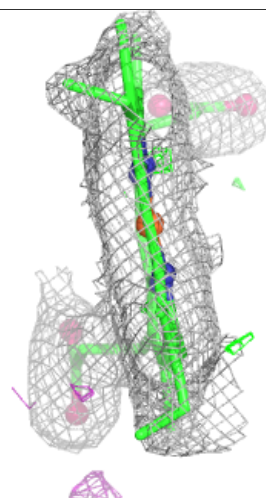
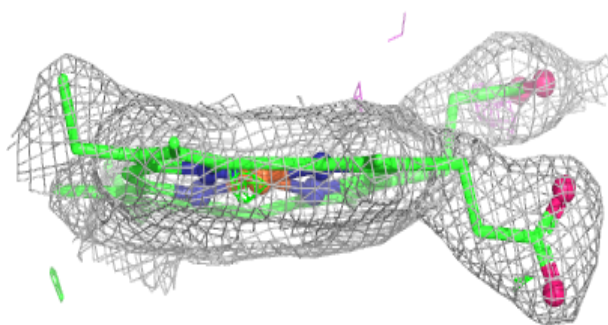
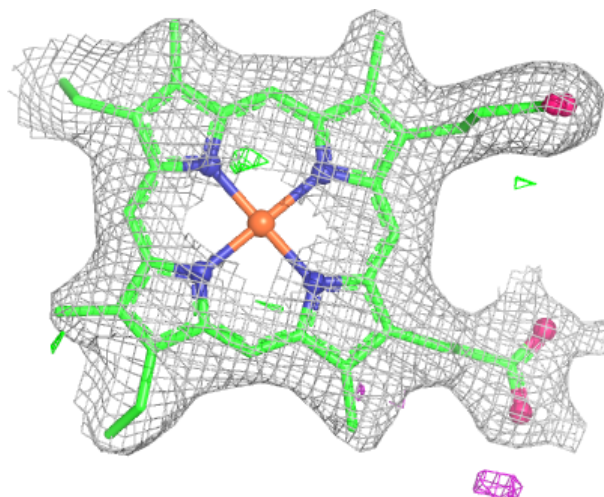
Electron density around HEC V 201:

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



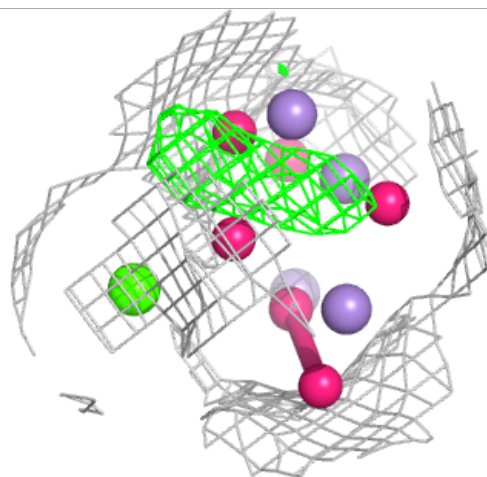
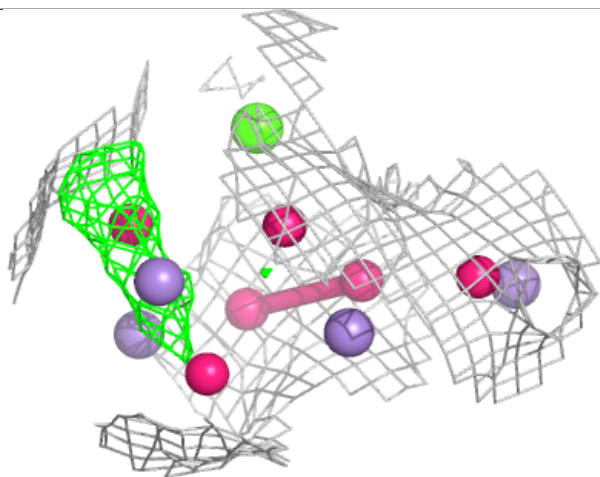
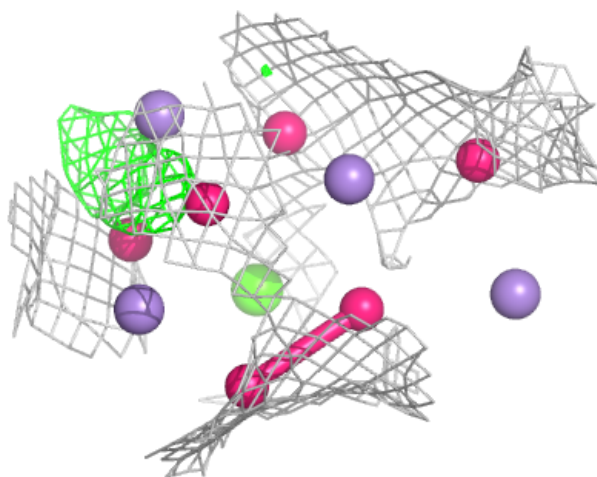
Electron density around HEC v 201:

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



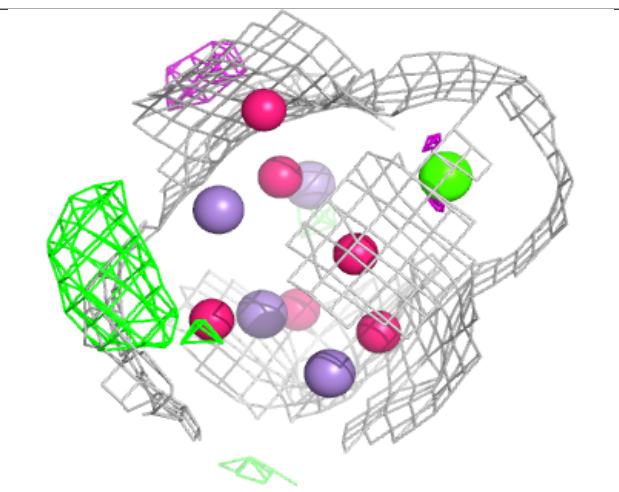
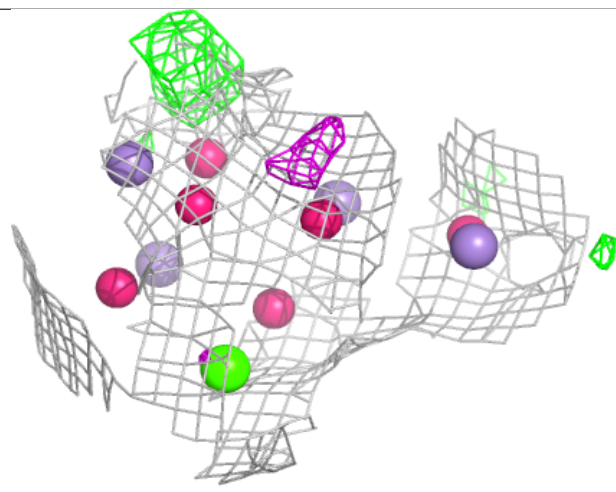
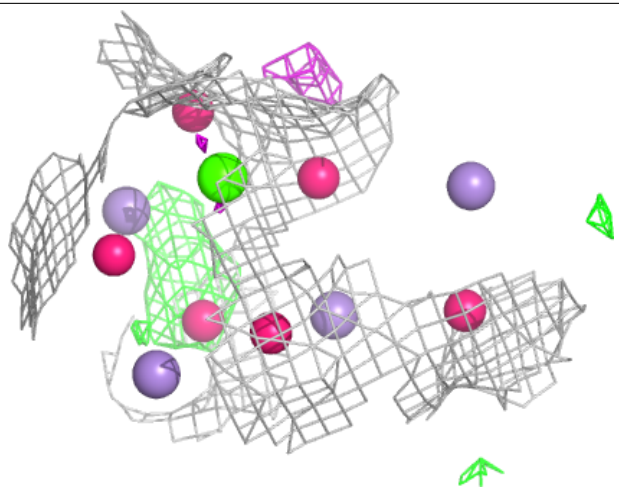
Electron density around OEY A 601 (C):

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



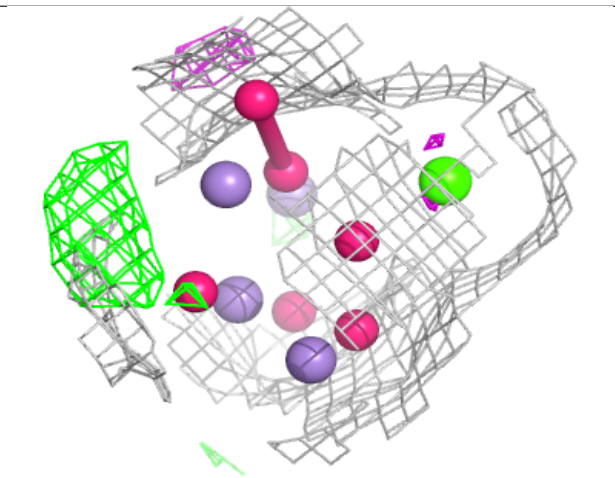
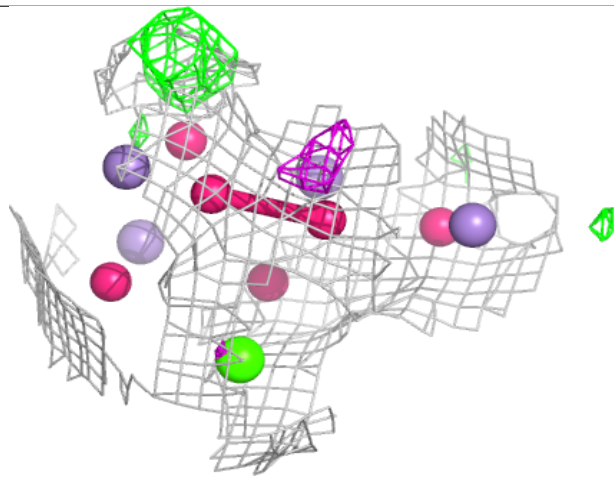
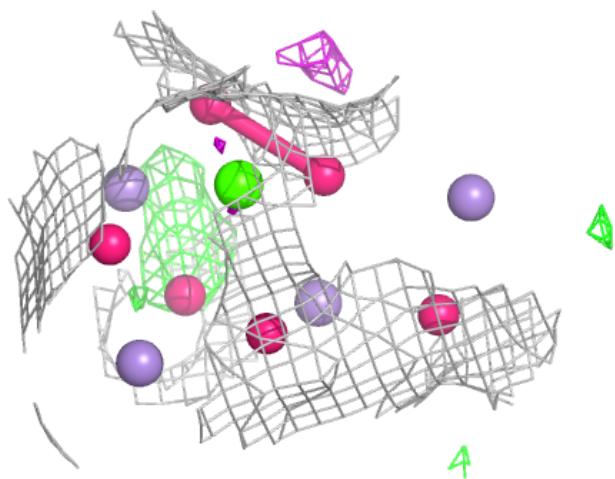
Electron density around OEY a 601 (A):

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



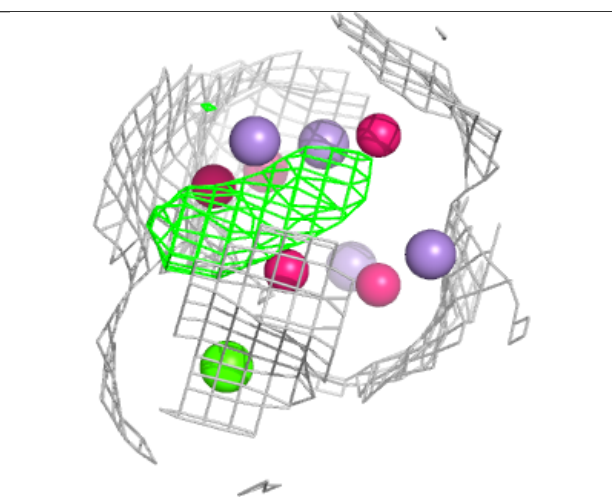
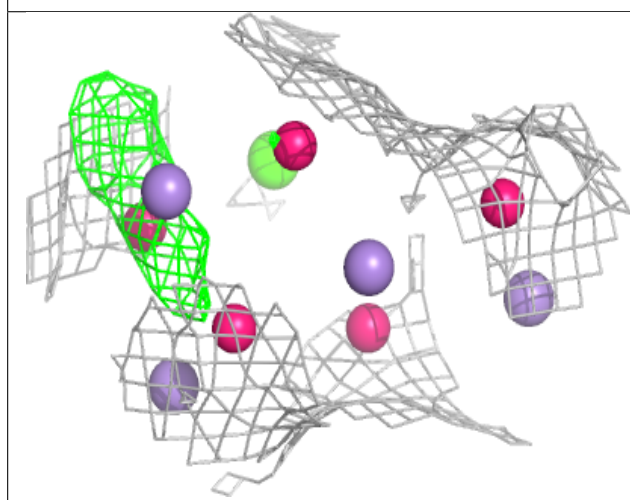
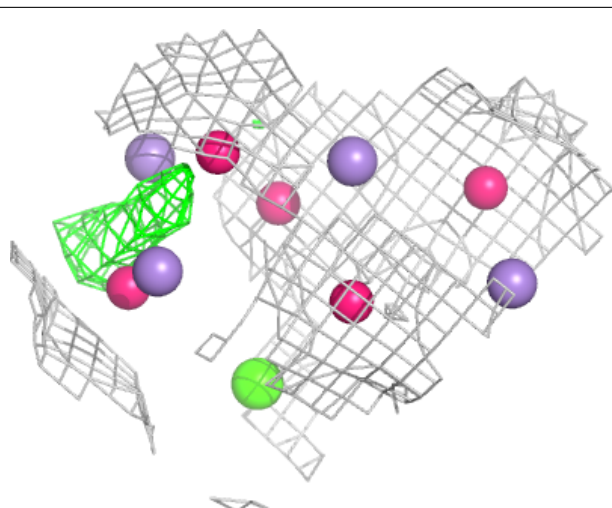
Electron density around OEY a 601 (C):

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



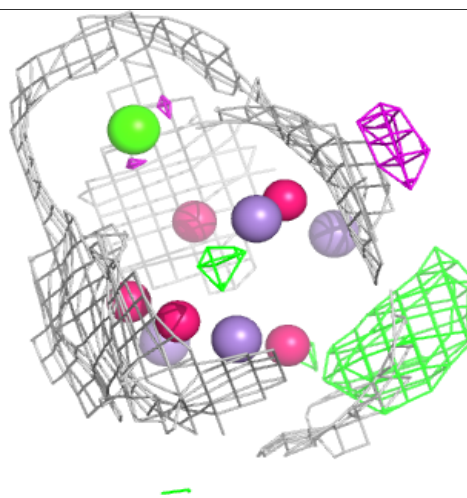
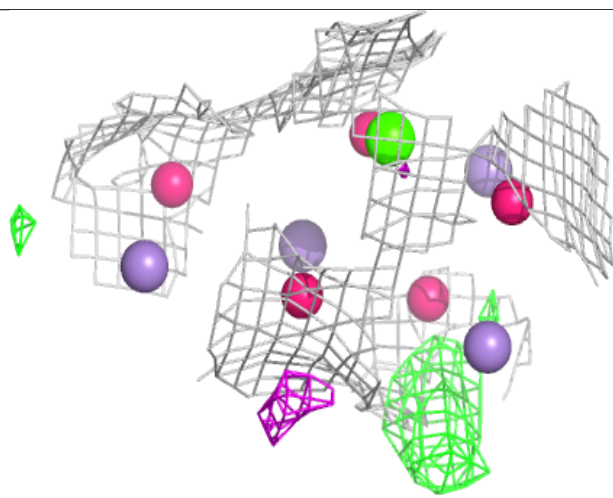
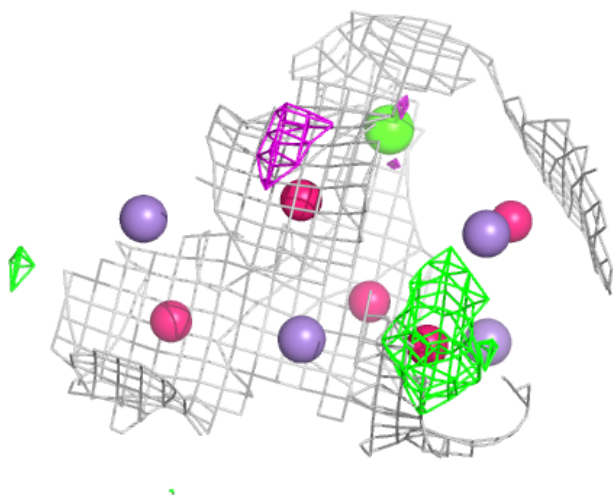
Electron density around OEX A 602 (B):

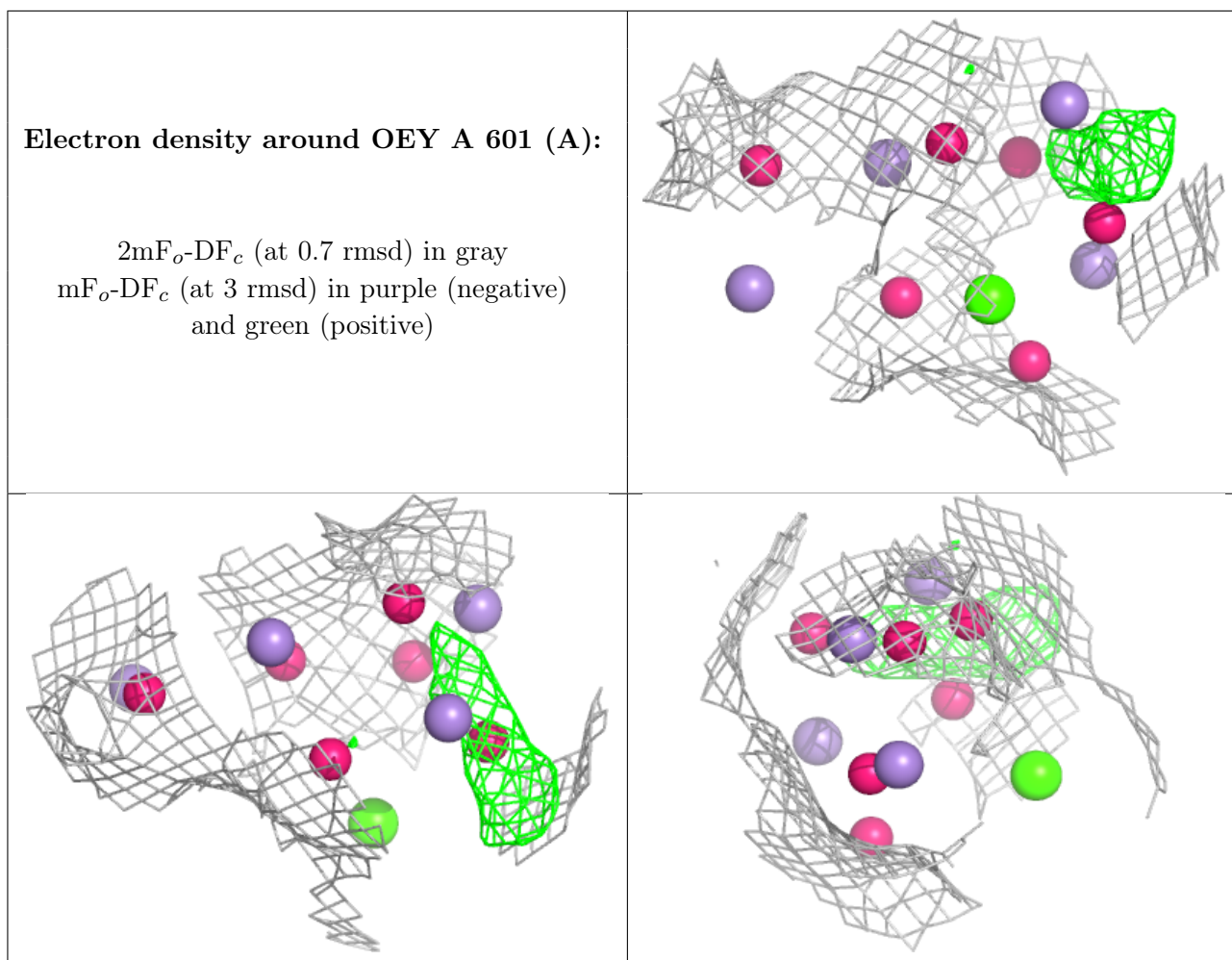
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around OEX a 602 (B):

$2mF_o-DF_c$ (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.