



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 03:25 PM UTC

PDB ID : 8F4E / pdb_00008f4e
Title : RT XFEL structure of Photosystem II 250 microseconds after the third illumination at 2.09 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 : 2.09 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

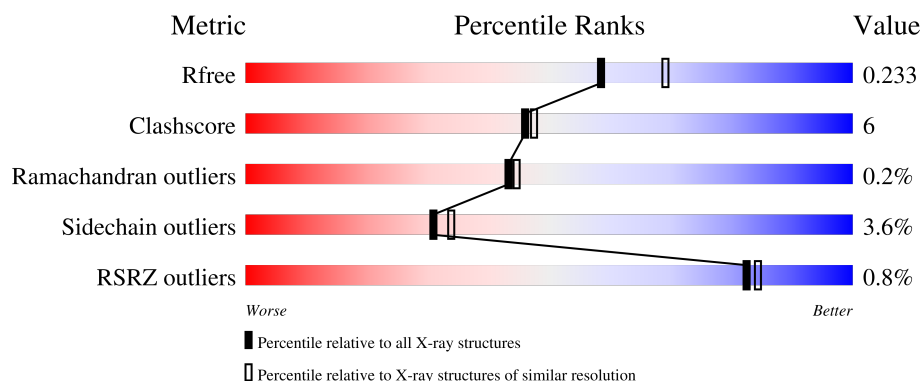
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


The reported resolution of this entry is 2.09 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)






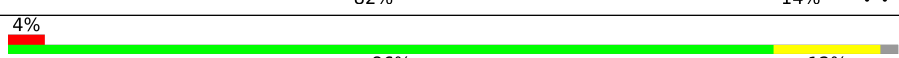


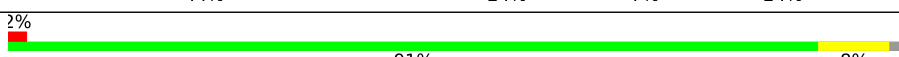


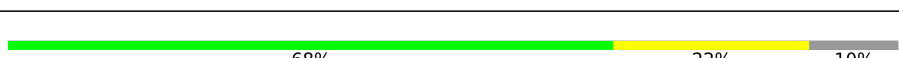


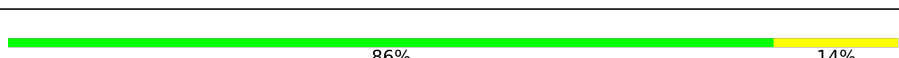
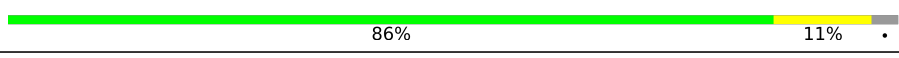
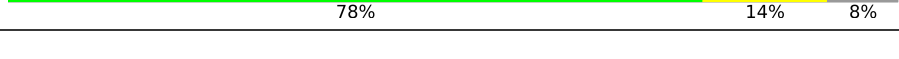
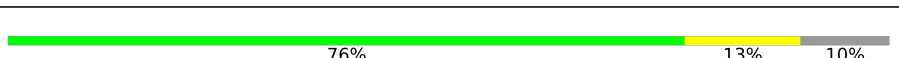
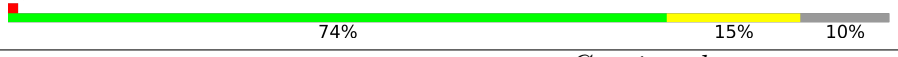



The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	
2	B	510	
2	b	510	
3	C	461	
3	c	461	
4	D	352	
4	d	352	
5	E	84	
5	e	84	
6	F	45	
6	f	45	
7	H	66	
7	h	66	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	46	
10	k	46	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	272	
13	o	272	

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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
25	CLA	A	606	X	-	-	-
25	CLA	A	610	X	-	-	-
25	CLA	A	613	X	-	-	-
25	CLA	B	601	X	-	-	-
25	CLA	B	602	X	-	-	-
25	CLA	B	603	X	-	-	-
25	CLA	B	604	X	-	-	-
25	CLA	B	605	X	-	-	-
25	CLA	B	606	X	-	-	-
25	CLA	B	607	X	-	-	-
25	CLA	B	609	X	-	-	-
25	CLA	B	610	X	-	-	-
25	CLA	B	611	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	B	612	X	-	-	-
25	CLA	B	613	X	-	-	-
25	CLA	B	614	X	-	-	-
25	CLA	B	615	X	-	-	-
25	CLA	C	501	X	-	-	-
25	CLA	C	502	X	-	-	-
25	CLA	C	503	X	-	-	-
25	CLA	C	504	X	-	-	-
25	CLA	C	505	X	-	-	-
25	CLA	C	506	X	-	-	-
25	CLA	C	507	X	-	-	-
25	CLA	C	509	X	-	-	-
25	CLA	C	510	X	-	-	-
25	CLA	C	511	X	-	-	-
25	CLA	C	512	X	-	-	-
25	CLA	C	513	X	-	-	-
25	CLA	D	402	X	-	-	-
25	CLA	H	101	X	-	-	-
25	CLA	a	607	X	-	-	-
25	CLA	a	608	X	-	-	-
25	CLA	a	610	X	-	-	-
25	CLA	a	613	X	-	-	-
25	CLA	b	601	X	-	-	-
25	CLA	b	602	X	-	-	-
25	CLA	b	603	X	-	-	-
25	CLA	b	604	X	-	-	-
25	CLA	b	605	X	-	-	-
25	CLA	b	606	X	-	-	-
25	CLA	b	607	X	-	-	-
25	CLA	b	608	X	-	-	-
25	CLA	b	609	X	-	-	-
25	CLA	b	610	X	-	-	-
25	CLA	b	611	X	-	-	-
25	CLA	b	612	X	-	-	-
25	CLA	b	613	X	-	-	-
25	CLA	b	614	X	-	-	-
25	CLA	b	615	X	-	-	-
25	CLA	c	501	X	-	-	-
25	CLA	c	503	X	-	-	-
25	CLA	c	504	X	-	-	-
25	CLA	c	505	X	-	-	-
25	CLA	c	506	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	c	507	X	-	-	-
25	CLA	c	509	X	-	-	-
25	CLA	c	510	X	-	-	-
25	CLA	c	511	X	-	-	-
25	CLA	c	512	X	-	-	-
25	CLA	c	513	X	-	-	-
25	CLA	d	402	X	-	-	-
25	CLA	d	403	X	-	-	-
25	CLA	h	101	X	-	-	-

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 54466 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				

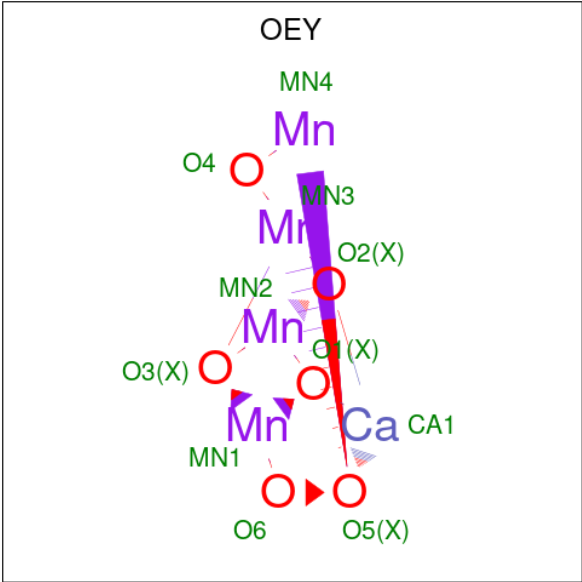
- Molecule 19 is a protein called Photosystem II reaction center protein Z.

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.

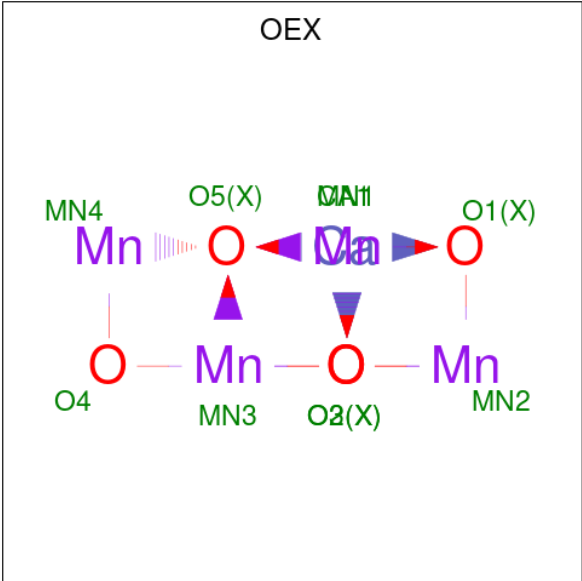
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	R	34	Total	C	N	O		0	0	0
			271	184	47	40				
20	r	31	Total	C	N	O		0	0	0
			246	166	43	37				

- 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
21	A	1	Total	Ca	Mn	O	0	1
			22	2	8	12		
21	a	1	Total	Ca	Mn	O	0	1
			22	2	8	12		

- 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
22	A	1	Total	Ca	Mn	O	0	1
			10	1	4	5		

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

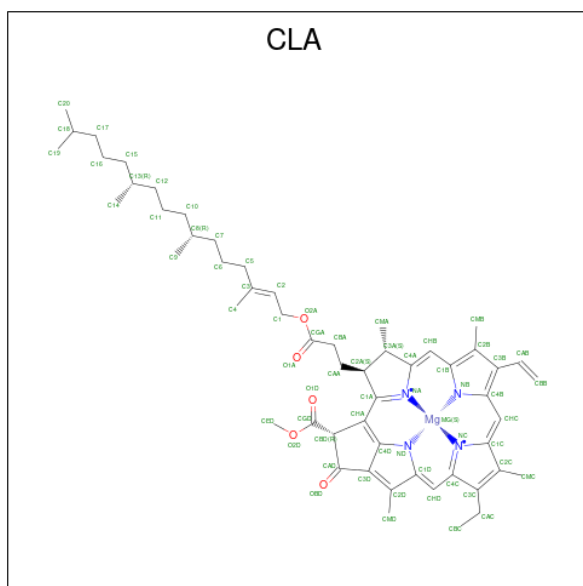
- Molecule 23 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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 CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
25	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
25	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		

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

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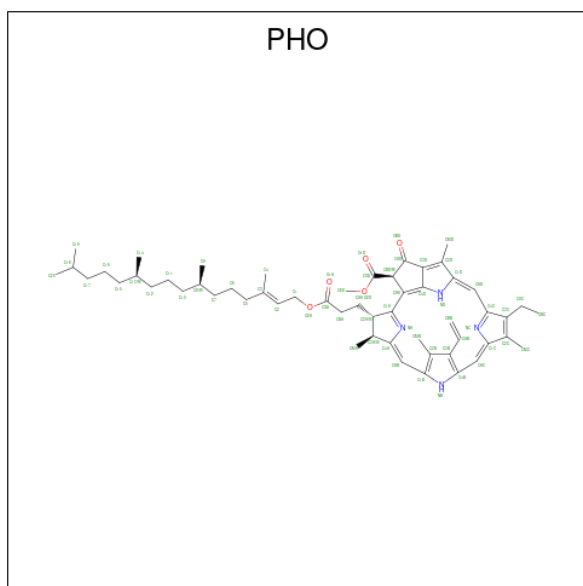
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N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

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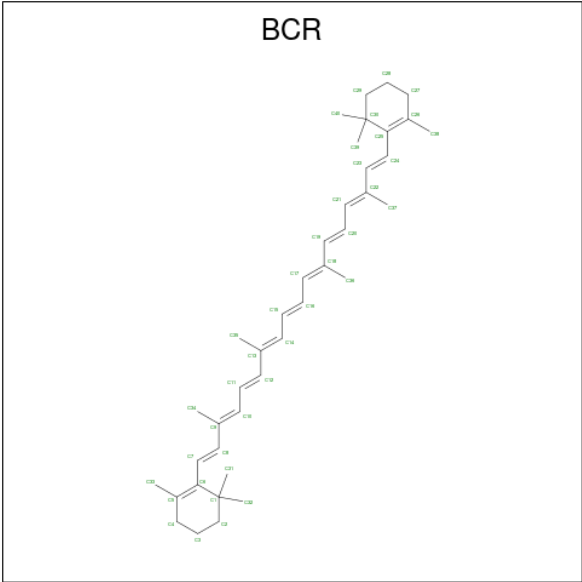
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	h	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 26 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



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

- Molecule 27 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



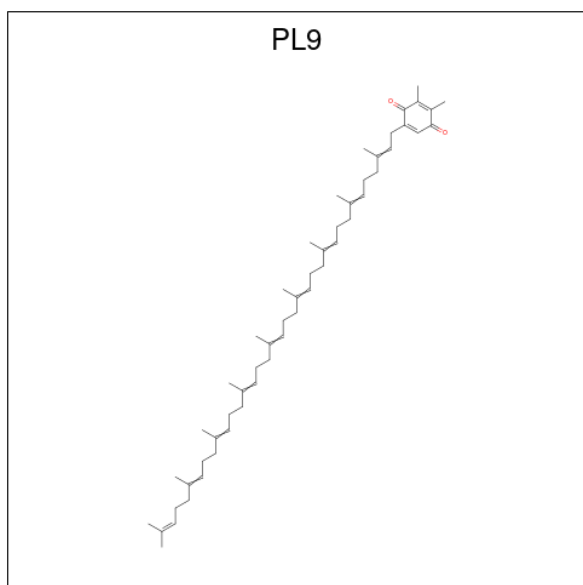
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	C	1	Total C 40 40	0	0
27	D	1	Total C 40 40	0	0
27	H	1	Total C 40 40	0	0
27	K	1	Total C 40 40	0	0
27	K	1	Total C 40 40	0	0
27	K	1	Total C 40 40	0	0
27	T	1	Total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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	b	1	Total C 40 40	0	0
27	c	1	Total C 40 40	0	0
27	c	1	Total C 40 40	0	0
27	c	1	Total C 40 40	0	0
27	d	1	Total C 40 40	0	0
27	k	1	Total C 40 40	0	0
27	t	1	Total C 40 40	0	0
27	x	1	Total C 40 40	0	0

- Molecule 28 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: C₅₃H₈₀O₂).



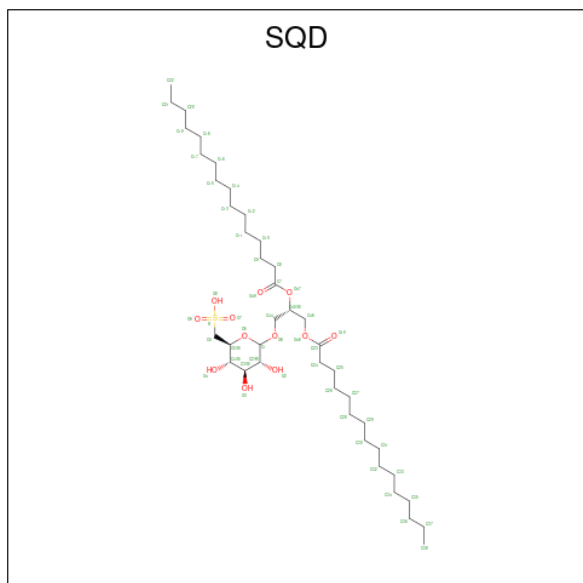
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	A	1	Total C O 55 53 2	0	0
28	D	1	Total C O 55 53 2	0	0

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

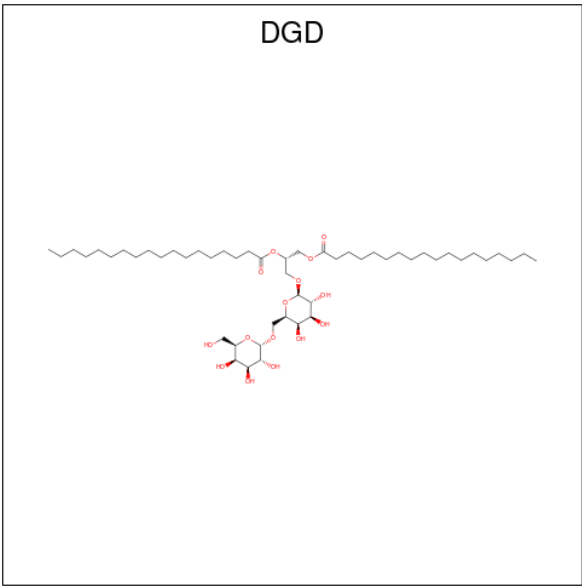
- Molecule 29 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



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

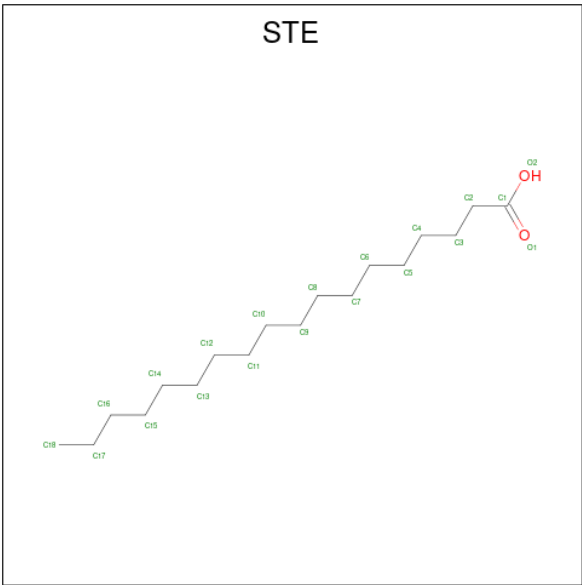
- Molecule 30 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula:

C₅₁H₉₆O₁₅).



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

- Molecule 31 is STEARIC ACID (CCD ID: STE) (formula: C₁₈H₃₆O₂).



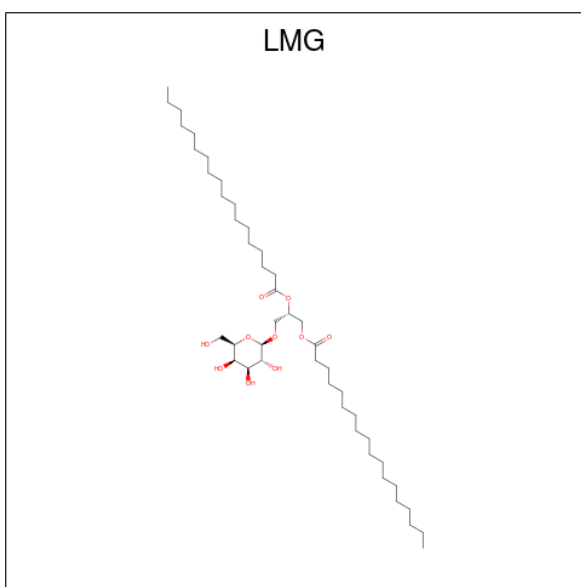
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	B	1	Total	C	O	0	0
			17	15	2		
31	B	1	Total	C	O	0	0
			12	10	2		
31	B	1	Total	C	O	0	0
			18	16	2		
31	B	1	Total	C	O	0	0
			12	10	2		
31	B	1	Total	C		0	0
			16	16			
31	C	1	Total	C	O	0	0
			12	10	2		
31	C	1	Total	C	O	0	0
			12	10	2		
31	C	1	Total	C		0	0
			16	16			
31	D	1	Total	C	O	0	0
			20	18	2		
31	H	1	Total	C		0	0
			18	18			
31	I	1	Total	C		0	0
			15	15			
31	J	1	Total	C	O	0	0
			12	10	2		
31	M	1	Total	C	O	0	0
			15	13	2		
31	M	1	Total	C		0	0
			10	10			

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

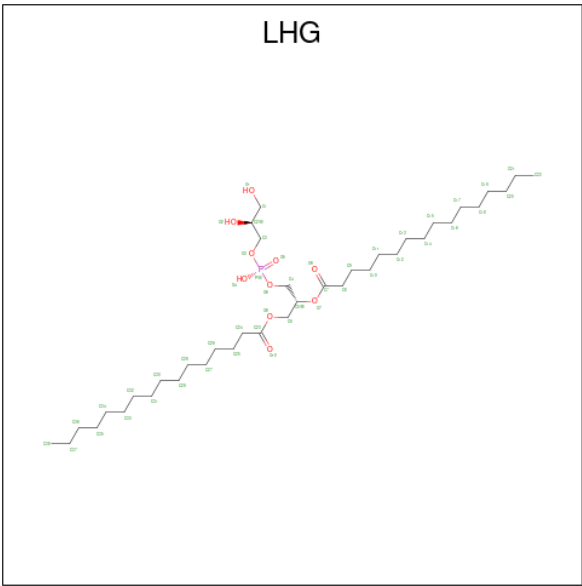
- Molecule 32 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).



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

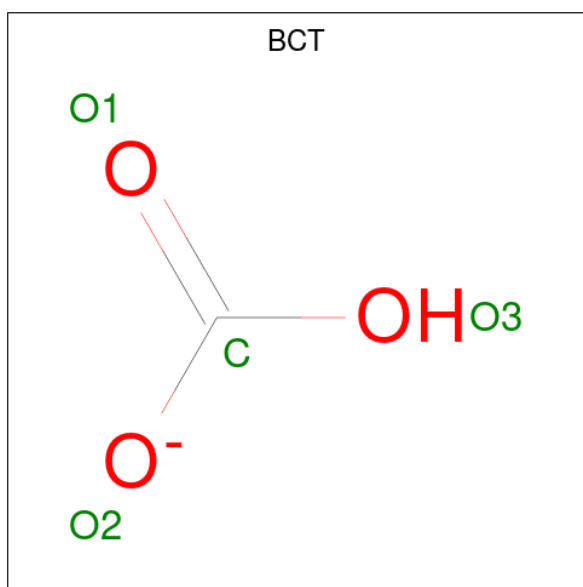
- Molecule 33 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG)

(formula: C₃₈H₇₅O₁₀P).



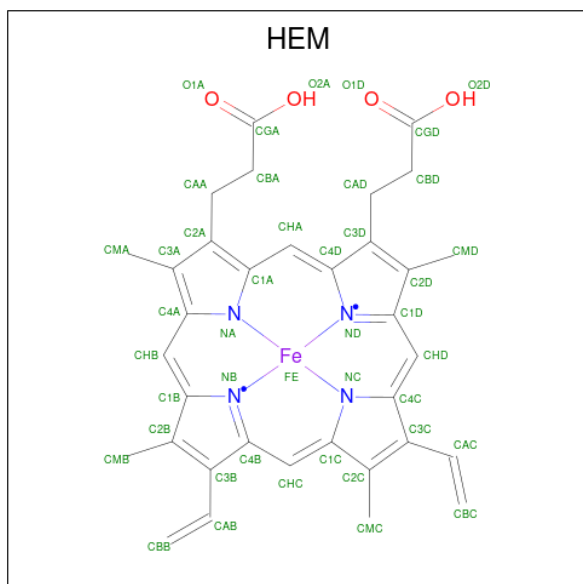
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	B	1	Total	C	O	P	0	0
			49	38	10	1		
33	B	1	Total	C	O	P	0	0
			49	38	10	1		
33	D	1	Total	C	O	P	0	0
			49	38	10	1		
33	D	1	Total	C	O	P	0	0
			47	36	10	1		
33	E	1	Total	C	O	P	0	0
			49	38	10	1		
33	d	1	Total	C	O	P	0	0
			49	38	10	1		
33	d	1	Total	C	O	P	0	0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

- Molecule 34 is BICARBONATE ION (CCD ID: BCT) (formula: CHO₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	D	1	Total	C	O	0	0
			4	1	3		
34	a	1	Total	C	O	0	0
			4	1	3		

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



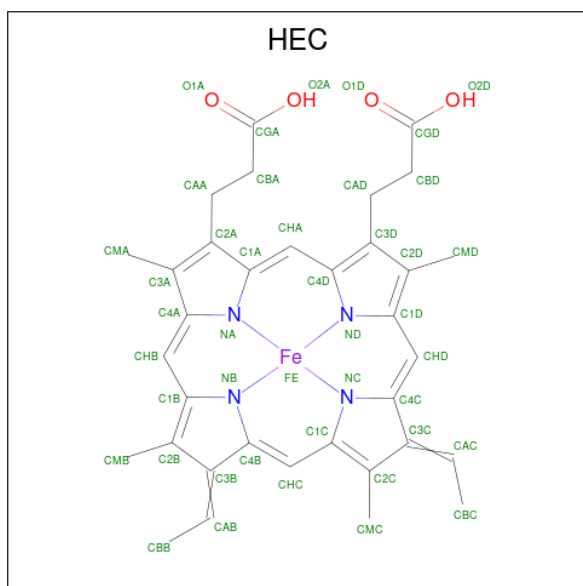
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
35	F	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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

- Molecule 36 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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

- Molecule 37 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	A	130	Total	O	0	4
			138	138		
37	B	191	Total	O	0	0
			191	191		
37	C	159	Total	O	0	0
			159	159		
37	D	119	Total	O	0	0
			119	119		
37	E	28	Total	O	0	0
			28	28		
37	F	9	Total	O	0	0
			9	9		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	H	33	Total 33	O 33	0	0
37	I	21	Total 21	O 21	0	0
37	J	10	Total 10	O 10	0	0
37	K	5	Total 5	O 5	0	0
37	L	7	Total 7	O 7	0	0
37	M	4	Total 4	O 4	0	0
37	O	91	Total 91	O 91	0	0
37	T	13	Total 13	O 13	0	0
37	U	46	Total 46	O 46	0	0
37	V	58	Total 58	O 58	0	0
37	Y	6	Total 6	O 6	0	0
37	X	6	Total 6	O 6	0	0
37	Z	8	Total 8	O 8	0	0
37	R	7	Total 7	O 7	0	0
37	a	117	Total 125	O 125	0	4
37	b	184	Total 184	O 184	0	0
37	c	166	Total 166	O 166	0	0
37	d	105	Total 105	O 105	0	0
37	e	26	Total 26	O 26	0	0
37	f	7	Total 7	O 7	0	0
37	h	23	Total 23	O 23	0	0

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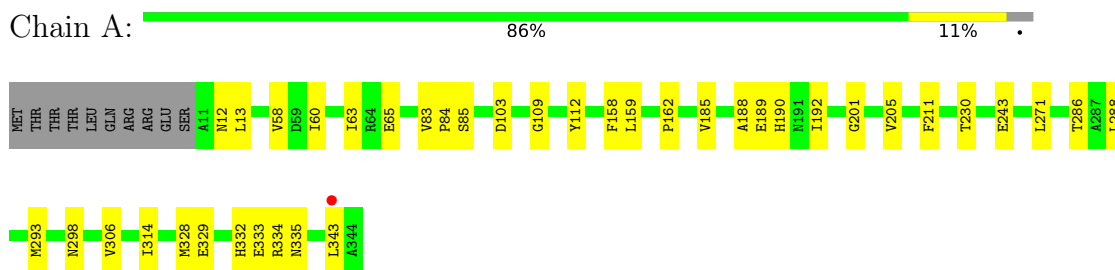
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	i	15	Total 15	O 15	0	0
37	j	5	Total 5	O 5	0	0
37	k	6	Total 6	O 6	0	0
37	l	14	Total 14	O 14	0	0
37	m	9	Total 9	O 9	0	0
37	o	93	Total 93	O 93	0	0
37	t	5	Total 5	O 5	0	0
37	u	52	Total 52	O 52	0	0
37	v	48	Total 48	O 48	0	0
37	y	7	Total 7	O 7	0	0
37	x	8	Total 8	O 8	0	0
37	z	3	Total 3	O 3	0	0
37	r	1	Total 1	O 1	0	0

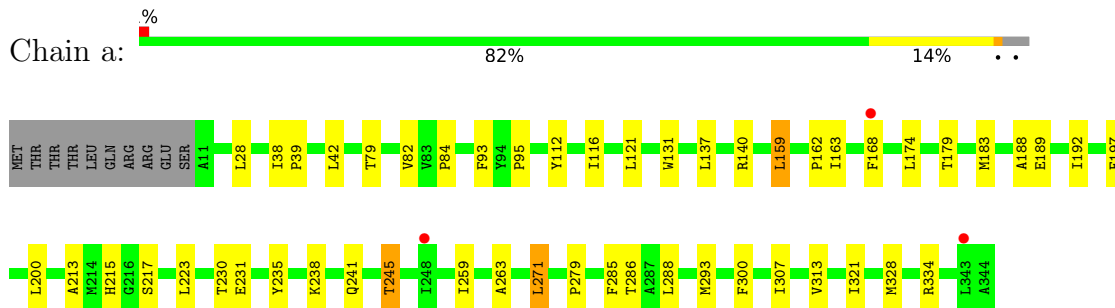
3 Residue-property plots

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.

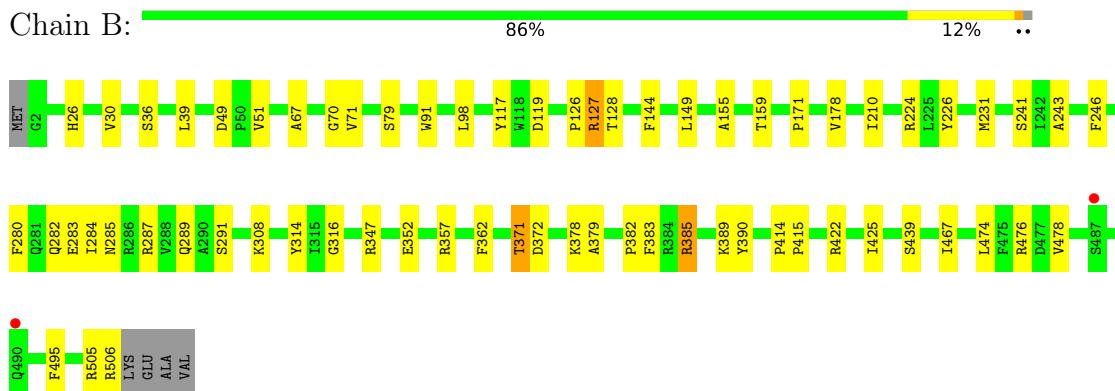
• Molecule 1: Photosystem II protein D1 1



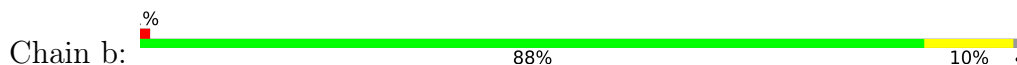
• Molecule 1: Photosystem II protein D1 1

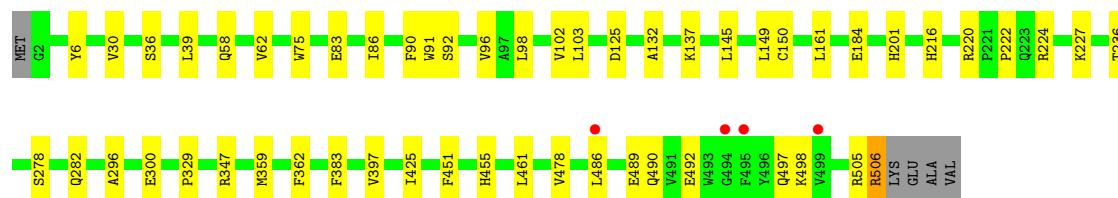


• Molecule 2: Photosystem II CP47 reaction center protein



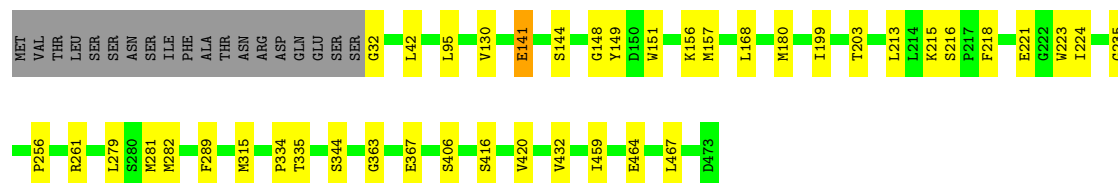
• Molecule 2: Photosystem II CP47 reaction center protein





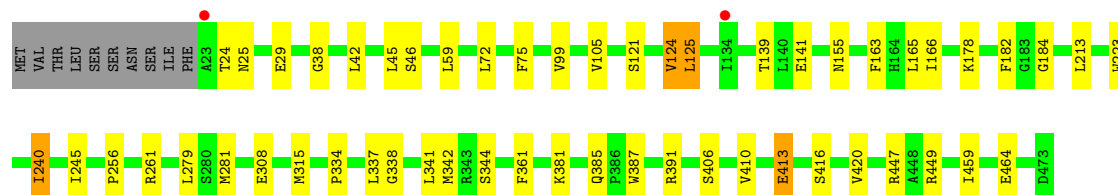
• Molecule 3: Photosystem II CP43 reaction center protein

Chain C: 87% 9% .



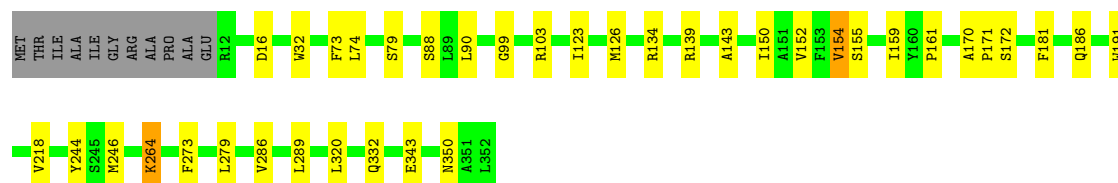
• Molecule 3: Photosystem II CP43 reaction center protein

Chain c: 86% 11% ..



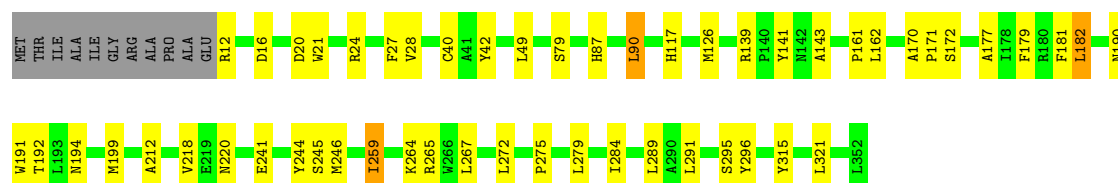
• Molecule 4: Photosystem II D2 protein

Chain D: 86% 10% ..

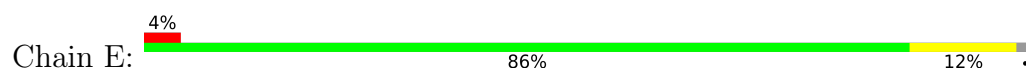


• Molecule 4: Photosystem II D2 protein

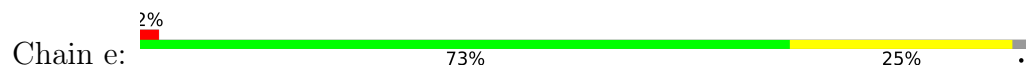
Chain d: 82% 14% ..



• Molecule 5: Cytochrome b559 subunit alpha



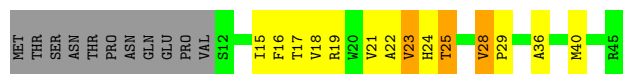
- Molecule 5: Cytochrome b559 subunit alpha



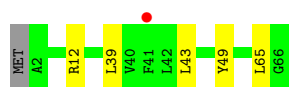
- Molecule 6: Cytochrome b559 subunit beta



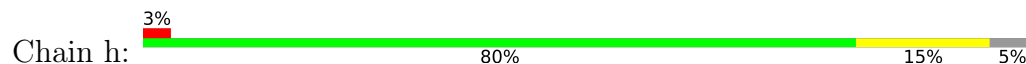
- Molecule 6: Cytochrome b559 subunit beta



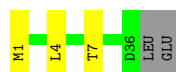
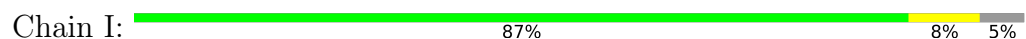
- Molecule 7: Photosystem II reaction center protein H




- Molecule 7: Photosystem II reaction center protein H



- Molecule 8: Photosystem II reaction center protein I



- Molecule 8: Photosystem II reaction center protein I

Chain i:  79% 16% 5%




- Molecule 9: Photosystem II reaction center protein J

Chain J:  68% 22% 10%



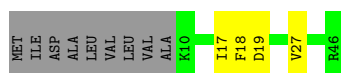
- Molecule 9: Photosystem II reaction center protein J

Chain j:  2% 78% 12% 10%



- Molecule 10: Photosystem II reaction center protein K

Chain K:  72% 9% 20%




- Molecule 10: Photosystem II reaction center protein K

Chain k:  50% 30% 20%




- Molecule 11: Photosystem II reaction center protein L

Chain L:  86% 14%




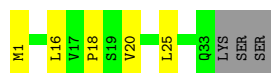
- Molecule 11: Photosystem II reaction center protein L

Chain l:  86% 11% 3%




- Molecule 12: Photosystem II reaction center protein M

Chain M:  78% 14% 8%




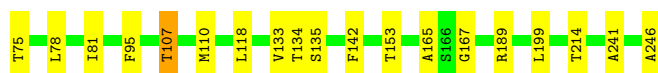
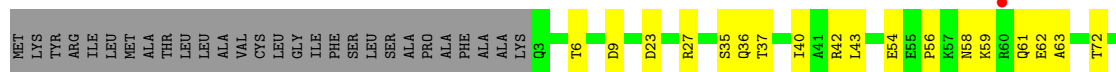
- Molecule 12: Photosystem II reaction center protein M

Chain m:  75% 8% 6% 11%




- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:  76% 13% 10%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:  74% 15% 10%




- Molecule 14: Photosystem II reaction center protein T

Chain T:  3% 72% 22% 6%



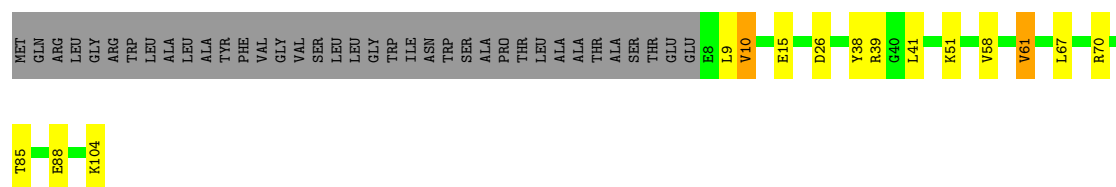
- Molecule 14: Photosystem II reaction center protein T

Chain t:  3% 88% 6%



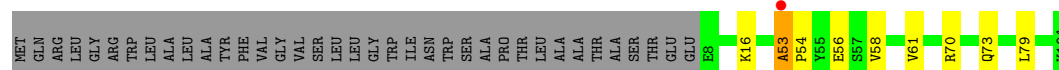
- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:  61% 10% 28%




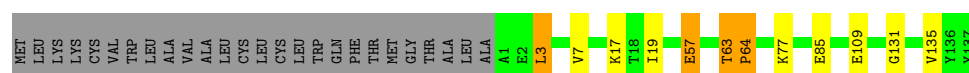
- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u:  66% 6% 28%



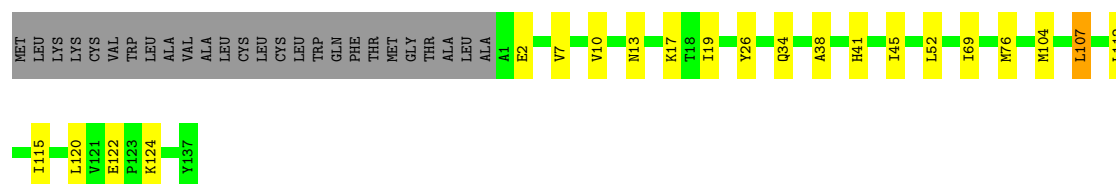
- Molecule 16: Cytochrome c-550

Chain V:  77% 5% 16%

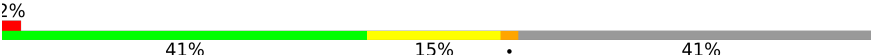


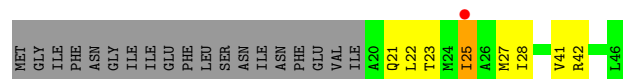
- Molecule 16: Cytochrome c-550

Chain v:  71% 12% 16%



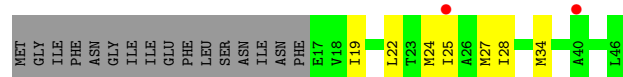
- Molecule 17: Photosystem II reaction center protein Ycf12

Chain Y:  41% 15% 41%

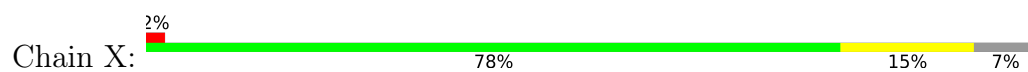


- Molecule 17: Photosystem II reaction center protein Ycf12

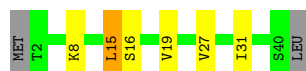
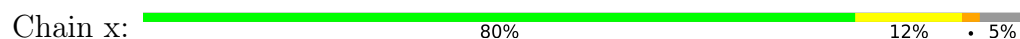
Chain y:  50% 15% 35%



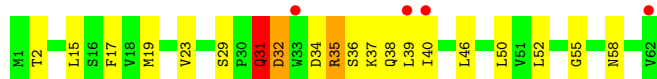
- Molecule 18: Photosystem II reaction center X protein



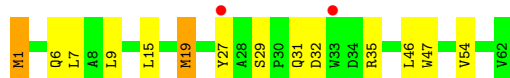
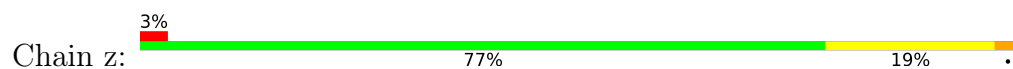
- Molecule 18: Photosystem II reaction center X protein



- 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	117.05Å 221.92Å 308.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.58 – 2.09 33.58 – 2.09	Depositor EDS
% Data completeness (in resolution range)	99.5 (33.58-2.09) 86.0 (33.58-2.09)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.41 (at 2.08Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.182 , 0.233 0.182 , 0.233	Depositor DCC
R_{free} test set	4180 reflections (0.67%)	wwPDB-VP
Wilson B-factor (Å ²)	29.5	Xtriage
Anisotropy	0.201	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 57.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	54466	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.66% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.30	0/3717	0.47	0/5060
1	a	0.28	0/3714	0.46	0/5056
2	B	0.34	0/4155	0.49	0/5661
2	b	0.31	0/4118	0.49	0/5611
3	C	0.32	0/3711	0.47	0/5051
3	c	0.30	0/3791	0.44	0/5158
4	D	0.35	0/2838	0.51	0/3862
4	d	0.35	0/2847	0.51	0/3874
5	E	0.26	0/688	0.42	0/940
5	e	0.24	0/683	0.43	0/932
6	F	0.31	0/284	0.41	0/387
6	f	0.25	0/284	0.49	0/387
7	H	0.33	0/523	0.49	0/713
7	h	0.32	0/511	0.50	0/697
8	I	0.31	0/293	0.46	0/396
8	i	0.33	0/293	0.45	0/396
9	J	0.27	0/263	0.40	0/356
9	j	0.26	0/263	0.44	0/356
10	K	0.27	0/303	0.44	0/416
10	k	0.25	0/303	0.41	0/416
11	L	0.36	0/311	0.46	0/422
11	l	0.32	0/303	0.48	0/412
12	M	0.31	0/249	0.53	0/341
12	m	0.34	0/244	0.48	0/334
13	O	0.32	0/1904	0.51	0/2585
13	o	0.32	0/1905	0.50	0/2583
14	T	0.36	0/257	0.54	0/349
14	t	0.32	0/255	0.48	0/346
15	U	0.30	0/785	0.48	0/1064
15	u	0.32	0/785	0.51	0/1064
16	V	0.32	0/1085	0.50	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.30	0/1085	0.46	0/1473
17	Y	0.23	0/197	0.37	0/264
17	y	0.19	0/219	0.34	0/294
18	X	0.25	0/284	0.36	0/384
18	x	0.21	0/289	0.31	0/391
19	Z	0.21	0/490	0.42	0/669
19	z	0.18	0/488	0.32	0/666
20	R	0.28	0/277	0.46	0/380
20	r	0.24	0/252	0.38	0/347
All	All	0.31	0/45246	0.48	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

There are no bond length outliers.

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

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
1	a	3601	0	3436	41	0
2	B	4005	0	3871	42	0
2	b	3978	0	3836	41	0
3	C	3592	0	3501	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	c	3666	0	3574	36	0
4	D	2745	0	2653	31	0
4	d	2751	0	2659	40	0
5	E	666	0	651	6	0
5	e	664	0	648	16	0
6	F	275	0	282	4	0
6	f	275	0	282	11	0
7	H	510	0	532	5	0
7	h	498	0	518	7	0
8	I	296	0	311	1	0
8	i	296	0	311	3	0
9	J	257	0	268	6	0
9	j	257	0	268	3	0
10	K	293	0	305	2	0
10	k	293	0	305	7	0
11	L	304	0	316	5	0
11	l	296	0	304	1	0
12	M	256	0	269	2	0
12	m	251	0	267	4	0
13	O	1870	0	1830	26	0
13	o	1874	0	1846	22	0
14	T	258	0	261	4	0
14	t	256	0	256	2	0
15	U	774	0	773	10	0
15	u	774	0	773	4	0
16	V	1064	0	1073	9	0
16	v	1064	0	1073	12	0
17	Y	196	0	217	5	0
17	y	218	0	241	3	0
18	X	281	0	312	4	0
18	x	286	0	314	5	0
19	Z	479	0	516	11	0
19	z	477	0	509	6	0
20	R	271	0	298	3	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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	a	2	0	0	0	0
25	A	249	0	264	3	0
25	B	970	0	1067	32	0
25	C	839	0	922	16	0
25	D	130	0	144	7	0
25	H	65	0	72	2	0
25	a	260	0	288	7	0
25	b	970	0	1067	36	0
25	c	839	0	919	22	0
25	d	130	0	144	4	0
25	h	65	0	72	4	0
26	A	128	0	148	3	0
26	a	64	0	74	0	0
26	d	64	0	74	2	0
27	A	40	0	56	0	0
27	B	120	0	168	3	0
27	C	40	0	56	5	0
27	D	40	0	56	1	0
27	H	40	0	56	2	0
27	K	120	0	168	6	0
27	T	40	0	56	1	0
27	a	40	0	56	1	0
27	b	120	0	168	2	0
27	c	120	0	168	11	0
27	d	40	0	56	2	0
27	k	40	0	56	1	0
27	t	40	0	56	1	0
27	x	40	0	56	3	0
28	A	55	0	80	5	0
28	D	55	0	80	1	0
28	a	55	0	80	5	0
28	d	55	0	80	2	0
29	A	91	0	136	2	0
29	F	36	0	46	1	0
29	L	49	0	65	2	0
29	a	90	0	134	2	0
29	f	41	0	49	3	0
29	l	54	0	78	2	0
30	A	66	0	96	8	0
30	C	186	0	246	3	0
30	H	62	0	82	3	0
30	a	44	0	75	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	c	186	0	246	8	0
30	h	62	0	82	1	0
31	B	75	0	117	2	0
31	C	40	0	63	0	0
31	D	20	0	35	3	0
31	H	18	0	35	3	0
31	I	15	0	26	3	0
31	J	12	0	16	0	0
31	M	25	0	38	0	0
31	R	12	0	16	0	0
31	T	31	0	60	0	0
31	a	12	0	16	1	0
31	b	66	0	110	4	0
31	c	32	0	51	2	0
31	d	17	0	26	0	0
31	j	12	0	16	0	0
31	l	18	0	35	0	0
31	m	12	0	16	0	0
31	t	24	0	36	1	0
31	x	20	0	35	2	0
32	B	28	0	40	0	0
32	C	96	0	132	4	0
32	D	84	0	117	5	0
32	M	51	0	72	1	0
32	b	55	0	86	0	0
32	c	134	0	181	6	0
32	d	67	0	92	1	0
32	m	51	0	72	4	0
33	B	98	0	148	4	0
33	D	96	0	141	4	0
33	E	49	0	74	1	0
33	d	137	0	199	11	0
33	e	42	0	57	0	0
33	l	49	0	74	0	0
34	D	4	0	1	0	0
34	a	4	0	1	0	0
35	F	43	0	30	2	0
35	e	43	0	30	2	0
36	V	43	0	30	0	0
36	v	43	0	30	2	0
37	A	138	0	0	3	0
37	B	191	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	C	159	0	0	1	0
37	D	119	0	0	1	0
37	E	28	0	0	0	0
37	F	9	0	0	0	0
37	H	33	0	0	0	0
37	I	21	0	0	0	0
37	J	10	0	0	1	0
37	K	5	0	0	0	0
37	L	7	0	0	0	0
37	M	4	0	0	0	0
37	O	91	0	0	3	0
37	R	7	0	0	0	0
37	T	13	0	0	0	0
37	U	46	0	0	3	0
37	V	58	0	0	3	0
37	X	6	0	0	0	0
37	Y	6	0	0	2	0
37	Z	8	0	0	0	0
37	a	125	0	0	2	0
37	b	184	0	0	1	0
37	c	166	0	0	3	0
37	d	105	0	0	1	0
37	e	26	0	0	1	0
37	f	7	0	0	0	0
37	h	23	0	0	1	0
37	i	15	0	0	0	0
37	j	5	0	0	1	0
37	k	6	0	0	1	0
37	l	14	0	0	0	0
37	m	9	0	0	1	0
37	o	93	0	0	1	0
37	r	1	0	0	0	0
37	t	5	0	0	0	0
37	u	52	0	0	1	0
37	v	48	0	0	2	0
37	x	8	0	0	1	0
37	y	7	0	0	0	0
37	z	3	0	0	0	0
All	All	54466	0	53863	613	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 6.

The worst 5 of 613 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)
37:m:209:HOH:O	14:t:1:FME:SD	2.35	0.84
25:H:101:CLA:H51	31:H:104:STE:H151	1.59	0.84
5:e:57:ALA:H	5:e:60:GLN:HE21	1.29	0.81
21:A:601[C]:OEY:O6	21:A:601[C]:OEY:O5	2.00	0.80
28:A:612:PL9:H361	6:F:25:THR:HG21	1.63	0.80

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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%)	451 (98%)	7 (2%)	0	100	100
1	a	458/344 (133%)	449 (98%)	8 (2%)	1 (0%)	43	44
2	B	507/510 (99%)	500 (99%)	7 (1%)	0	100	100
2	b	503/510 (99%)	496 (99%)	7 (1%)	0	100	100
3	C	461/461 (100%)	451 (98%)	9 (2%)	1 (0%)	43	44
3	c	471/461 (102%)	460 (98%)	10 (2%)	1 (0%)	43	44
4	D	341/352 (97%)	330 (97%)	11 (3%)	0	100	100
4	d	342/352 (97%)	334 (98%)	8 (2%)	0	100	100
5	E	81/84 (96%)	80 (99%)	1 (1%)	0	100	100
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%)	60 (95%)	3 (5%)	0	100	100
7	h	61/66 (92%)	57 (93%)	4 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	I	34/38 (90%)	33 (97%)	1 (3%)	0	100	100
8	i	34/38 (90%)	32 (94%)	2 (6%)	0	100	100
9	J	34/40 (85%)	32 (94%)	2 (6%)	0	100	100
9	j	34/40 (85%)	33 (97%)	1 (3%)	0	100	100
10	K	35/46 (76%)	35 (100%)	0	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%)	31 (100%)	0	0	100	100
12	m	30/36 (83%)	28 (93%)	2 (7%)	0	100	100
13	O	243/272 (89%)	230 (95%)	10 (4%)	3 (1%)	10	7
13	o	242/272 (89%)	234 (97%)	8 (3%)	0	100	100
14	T	28/32 (88%)	28 (100%)	0	0	100	100
14	t	28/32 (88%)	28 (100%)	0	0	100	100
15	U	95/134 (71%)	92 (97%)	3 (3%)	0	100	100
15	u	95/134 (71%)	92 (97%)	2 (2%)	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%)	23 (92%)	2 (8%)	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%)	37 (100%)	0	0	100	100
19	Z	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	7	3
19	z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
20	R	32/41 (78%)	30 (94%)	2 (6%)	0	100	100
20	r	29/41 (71%)	27 (93%)	2 (7%)	0	100	100
All	All	5534/5700 (97%)	5397 (98%)	128 (2%)	9 (0%)	43	44

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
13	O	59	LYS

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Mol	Chain	Res	Type
16	V	64	PRO
19	Z	31	GLN
13	O	62	GLU

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%)	367 (98%)	7 (2%)	50	58
1	a	373/280 (133%)	360 (96%)	13 (4%)	32	35
2	B	407/407 (100%)	396 (97%)	11 (3%)	39	45
2	b	402/407 (99%)	393 (98%)	9 (2%)	45	53
3	C	361/362 (100%)	356 (99%)	5 (1%)	59	67
3	c	370/362 (102%)	357 (96%)	13 (4%)	32	35
4	D	278/283 (98%)	276 (99%)	2 (1%)	76	83
4	d	279/283 (99%)	274 (98%)	5 (2%)	51	60
5	E	72/73 (99%)	70 (97%)	2 (3%)	38	43
5	e	71/73 (97%)	67 (94%)	4 (6%)	19	18
6	F	28/39 (72%)	27 (96%)	1 (4%)	31	34
6	f	28/39 (72%)	24 (86%)	4 (14%)	3	1
7	H	54/55 (98%)	54 (100%)	0	100	100
7	h	53/55 (96%)	51 (96%)	2 (4%)	29	32
8	I	32/34 (94%)	31 (97%)	1 (3%)	35	39
8	i	32/34 (94%)	31 (97%)	1 (3%)	35	39
9	J	24/28 (86%)	23 (96%)	1 (4%)	26	28
9	j	24/28 (86%)	23 (96%)	1 (4%)	26	28
10	K	30/37 (81%)	29 (97%)	1 (3%)	33	37
10	k	30/37 (81%)	25 (83%)	5 (17%)	2	1
11	L	35/35 (100%)	34 (97%)	1 (3%)	37	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	l	34/35 (97%)	31 (91%)	3 (9%)	9	7
12	M	28/32 (88%)	26 (93%)	2 (7%)	13	11
12	m	28/32 (88%)	26 (93%)	2 (7%)	13	11
13	O	206/228 (90%)	201 (98%)	5 (2%)	43	49
13	o	207/228 (91%)	199 (96%)	8 (4%)	28	31
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%)	79 (94%)	5 (6%)	17	15
15	u	84/112 (75%)	82 (98%)	2 (2%)	43	49
16	V	117/138 (85%)	113 (97%)	4 (3%)	32	35
16	v	117/138 (85%)	113 (97%)	4 (3%)	32	35
17	Y	19/37 (51%)	16 (84%)	3 (16%)	2	1
17	y	22/37 (60%)	19 (86%)	3 (14%)	3	2
18	X	31/34 (91%)	29 (94%)	2 (6%)	15	13
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%)	44 (86%)	7 (14%)	3	2
20	R	28/33 (85%)	21 (75%)	7 (25%)	0	0
20	r	25/33 (76%)	20 (80%)	5 (20%)	1	0
All	All	4572/4654 (98%)	4410 (96%)	162 (4%)	31	35

5 of 162 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	f	23	VAL
16	v	19	ILE
7	h	27	THR
12	m	13	LEU
19	z	1	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
5	e	82	GLN

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Mol	Chain	Res	Type
19	z	31	GLN
7	h	59	ASN
13	o	124	ASN
20	r	30	GLN

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	$\# Z > 2$
8	FME	i	1	8	8,9,10	1.06	1 (12%)	8,9,11	1.00	0
14	FME	t	1	14	8,9,10	1.27	1 (12%)	8,9,11	1.01	0
8	FME	I	1	8	8,9,10	1.00	0	8,9,11	1.16	1 (12%)
14	FME	T	1	14	8,9,10	1.03	0	8,9,11	0.94	0
12	FME	m	1	12	8,9,10	1.11	1 (12%)	8,9,11	0.54	0
12	FME	M	1	12	8,9,10	1.04	1 (12%)	8,9,11	1.15	1 (12%)

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
8	FME	i	1	8	-	0/7/9/11	-
14	FME	t	1	14	-	3/7/9/11	-
8	FME	I	1	8	-	0/7/9/11	-
14	FME	T	1	14	-	2/7/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	FME	m	1	12	-	0/7/9/11	-
12	FME	M	1	12	-	0/7/9/11	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	t	1	FME	CA-N	-3.03	1.42	1.46
12	m	1	FME	CA-N	-2.35	1.43	1.46
12	M	1	FME	CA-N	-2.13	1.43	1.46
8	i	1	FME	CA-N	-2.01	1.43	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	I	1	FME	CA-N-CN	-2.33	119.23	122.82
12	M	1	FME	CA-N-CN	-2.02	119.71	122.82

There are no chirality outliers.

All (5) torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	t	1	FME	1	0
14	T	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	PHO	d	401	-	58,69,69	2.11	11 (18%)	55,99,99	1.62	7 (12%)
31	STE	C	520	-	11,11,19	0.67	0	11,11,19	1.38	1 (9%)
25	CLA	C	501	-	69,73,73	1.29	9 (13%)	82,113,113	1.31	8 (9%)
25	CLA	a	613	37	69,73,73	1.30	9 (13%)	82,113,113	1.38	9 (10%)
25	CLA	b	604	-	69,73,73	1.09	6 (8%)	82,113,113	1.33	9 (10%)
27	BCR	c	514	-	41,41,41	1.05	2 (4%)	56,56,56	1.27	7 (12%)
29	SQD	a	615	-	35,35,54	1.77	6 (17%)	37,37,65	1.42	5 (13%)
31	STE	B	626	-	15,15,19	0.38	0	14,14,19	0.78	0
31	STE	c	523	-	11,11,19	0.77	0	11,11,19	1.20	1 (9%)
33	LHG	B	621	-	48,48,48	0.73	1 (2%)	51,54,54	1.20	3 (5%)
31	STE	b	621	-	15,15,19	0.70	0	15,15,19	0.90	0
25	CLA	b	606	37	69,73,73	1.15	6 (8%)	82,113,113	1.31	7 (8%)
32	LMG	d	410	-	44,44,55	0.94	2 (4%)	52,52,63	1.31	6 (11%)
30	DGD	c	518	-	63,63,67	0.94	2 (3%)	77,77,81	1.29	6 (7%)
30	DGD	c	519	-	63,63,67	0.86	3 (4%)	77,77,81	1.44	15 (19%)
25	CLA	a	610	-	69,73,73	1.27	8 (11%)	82,113,113	1.22	7 (8%)
32	LMG	C	515	-	48,48,55	0.92	4 (8%)	56,56,63	1.32	6 (10%)
25	CLA	c	506	-	69,73,73	1.27	9 (13%)	82,113,113	1.31	5 (6%)
32	LMG	M	101	-	51,51,55	0.87	2 (3%)	59,59,63	1.40	6 (10%)
33	LHG	d	407	-	48,48,48	0.64	0	51,54,54	1.19	4 (7%)
25	CLA	C	502	-	69,73,73	1.23	7 (10%)	82,113,113	1.22	7 (8%)
25	CLA	c	502	-	69,73,73	1.18	9 (13%)	82,113,113	1.29	8 (9%)
32	LMG	B	620	-	26,26,55	0.63	0	26,26,63	1.32	1 (3%)
31	STE	B	623	-	11,11,19	0.84	0	11,11,19	1.07	0
26	PHO	a	609	-	58,69,69	2.09	8 (13%)	55,99,99	1.33	10 (18%)
27	BCR	d	404	-	41,41,41	1.11	3 (7%)	56,56,56	1.20	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	b	614	-	69,73,73	1.32	9 (13%)	82,113,113	1.32	7 (8%)
32	LMG	c	522	-	48,48,55	0.99	3 (6%)	56,56,63	1.31	9 (16%)
27	BCR	b	617	-	41,41,41	1.24	3 (7%)	56,56,56	1.20	6 (10%)
31	STE	C	521	-	11,11,19	0.73	0	11,11,19	1.16	0
31	STE	t	103	-	9,9,19	0.44	0	8,8,19	0.63	0
30	DGD	H	103	-	63,63,67	1.12	5 (7%)	77,77,81	1.42	11 (14%)
32	LMG	d	409	-	21,21,55	0.56	0	20,20,63	1.24	3 (15%)
25	CLA	C	505	-	69,73,73	1.33	8 (11%)	82,113,113	1.24	6 (7%)
25	CLA	A	607	37	69,73,73	1.19	6 (8%)	82,113,113	1.43	8 (9%)
25	CLA	c	505	-	69,73,73	1.11	7 (10%)	82,113,113	1.31	9 (10%)
33	LHG	D	408	-	46,46,48	0.91	1 (2%)	49,52,54	1.31	6 (12%)
21	OEY	a	601[C]	3,1,37	0,16,16	-	-	-	-	-
34	BCT	D	401	23	3,3,3	1.09	0	2,3,3	3.15	1 (50%)
27	BCR	B	618	-	41,41,41	1.04	2 (4%)	56,56,56	1.29	4 (7%)
25	CLA	D	402	-	69,73,73	1.30	7 (10%)	82,113,113	1.32	7 (8%)
25	CLA	H	101	37	69,73,73	1.42	9 (13%)	82,113,113	1.34	5 (6%)
25	CLA	a	607	-	69,73,73	1.49	11 (15%)	82,113,113	1.30	7 (8%)
29	SQD	F	102	-	34,36,54	1.55	5 (14%)	42,45,65	1.75	11 (26%)
25	CLA	c	504	37	64,68,73	1.20	7 (10%)	76,107,113	1.33	12 (15%)
25	CLA	C	507	37	69,73,73	1.22	7 (10%)	82,113,113	1.48	8 (9%)
22	OEX	a	602[A]	3,1,37	0,15,15	-	-	-	-	-
28	PL9	A	612	-	55,55,55	0.92	2 (3%)	68,69,69	1.53	13 (19%)
30	DGD	A	616	-	67,67,67	1.08	5 (7%)	81,81,81	1.30	11 (13%)
21	OEY	A	601[C]	3,1,37	0,16,16	-	-	-	-	-
25	CLA	C	512	-	69,73,73	1.40	11 (15%)	82,113,113	1.30	9 (10%)
27	BCR	T	101	-	41,41,41	0.95	1 (2%)	56,56,56	1.24	5 (8%)
27	BCR	A	611	-	41,41,41	0.97	2 (4%)	56,56,56	1.33	8 (14%)
25	CLA	c	503	-	69,73,73	1.30	7 (10%)	82,113,113	1.40	7 (8%)
36	HEC	v	201	16	46,50,50	1.89	4 (8%)	58,82,82	1.73	7 (12%)
25	CLA	C	508	-	69,73,73	1.27	8 (11%)	82,113,113	1.47	10 (12%)
25	CLA	B	610	-	69,73,73	1.32	10 (14%)	82,113,113	1.51	10 (12%)
25	CLA	B	603	-	69,73,73	1.45	8 (11%)	82,113,113	1.58	10 (12%)
32	LMG	b	620	-	55,55,55	0.84	2 (3%)	63,63,63	1.37	9 (14%)
22	OEX	A	602[A]	3,1,37	0,15,15	-	-	-	-	-
29	SQD	l	101	-	52,54,54	1.60	10 (19%)	62,65,65	1.69	11 (17%)
31	STE	B	619	-	16,16,19	0.71	0	16,16,19	1.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	BCR	B	616	-	41,41,41	1.06	3 (7%)	56,56,56	1.23	7 (12%)
25	CLA	c	501	-	69,73,73	1.13	7 (10%)	82,113,113	1.43	8 (9%)
25	CLA	b	608	-	69,73,73	1.19	8 (11%)	82,113,113	1.31	10 (12%)
31	STE	R	101	-	11,11,19	0.74	0	11,11,19	1.14	0
25	CLA	b	605	-	69,73,73	1.43	9 (13%)	82,113,113	1.50	7 (8%)
31	STE	l	103	-	17,17,19	0.29	0	16,16,19	0.93	0
28	PL9	d	405	-	55,55,55	1.08	4 (7%)	68,69,69	1.52	11 (16%)
31	STE	B	624	-	17,17,19	0.64	0	17,17,19	1.10	0
31	STE	D	410	-	19,19,19	0.56	0	19,19,19	1.18	0
31	STE	J	101	-	11,11,19	0.68	0	11,11,19	1.28	2 (18%)
32	LMG	m	101	-	51,51,55	0.98	3 (5%)	59,59,63	1.38	8 (13%)
32	LMG	c	520	-	37,37,55	0.95	1 (2%)	45,45,63	1.33	4 (8%)
32	LMG	D	406	-	51,51,55	0.90	2 (3%)	59,59,63	1.36	5 (8%)
25	CLA	A	606	-	69,73,73	1.29	8 (11%)	82,113,113	1.16	9 (10%)
33	LHG	B	622	-	48,48,48	0.85	2 (4%)	51,54,54	1.35	7 (13%)
25	CLA	B	608	-	69,73,73	1.20	6 (8%)	82,113,113	1.29	5 (6%)
29	SQD	A	615	-	38,38,54	1.77	5 (13%)	40,40,65	1.32	3 (7%)
25	CLA	B	605	-	69,73,73	1.33	8 (11%)	82,113,113	1.38	8 (9%)
31	STE	C	522	-	15,15,19	0.39	0	14,14,19	0.74	0
25	CLA	B	615	-	64,68,73	1.47	6 (9%)	76,107,113	1.48	10 (13%)
25	CLA	C	506	-	69,73,73	1.34	8 (11%)	82,113,113	1.34	10 (12%)
33	LHG	E	101	-	48,48,48	0.74	1 (2%)	51,54,54	1.23	6 (11%)
27	BCR	b	618	-	41,41,41	1.02	2 (4%)	56,56,56	1.28	7 (12%)
31	STE	b	622	-	19,19,19	0.63	0	19,19,19	1.05	1 (5%)
25	CLA	b	603	-	69,73,73	1.29	7 (10%)	82,113,113	1.54	11 (13%)
25	CLA	c	509	-	69,73,73	1.16	6 (8%)	82,113,113	1.46	4 (4%)
35	HEM	e	101	5,6	50,50,50	1.52	9 (18%)	67,82,82	1.27	7 (10%)
27	BCR	H	102	-	41,41,41	0.95	1 (2%)	56,56,56	1.21	6 (10%)
32	LMG	C	519	-	48,48,55	0.91	3 (6%)	56,56,63	1.34	6 (10%)
27	BCR	x	101	-	41,41,41	0.97	1 (2%)	56,56,56	1.21	4 (7%)
25	CLA	C	510	-	69,73,73	1.25	9 (13%)	82,113,113	1.31	8 (9%)
25	CLA	c	510	-	69,73,73	1.22	8 (11%)	82,113,113	1.30	8 (9%)
30	DGD	h	102	-	63,63,67	1.03	4 (6%)	77,77,81	1.45	13 (16%)
25	CLA	D	403	-	69,73,73	1.35	9 (13%)	82,113,113	1.16	4 (4%)
25	CLA	d	403	-	69,73,73	1.26	9 (13%)	82,113,113	1.19	9 (10%)
26	PHO	A	609	-	58,69,69	2.11	10 (17%)	55,99,99	1.59	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	c	513	-	69,73,73	1.15	5 (7%)	82,113,113	1.26	9 (10%)
25	CLA	b	602	-	69,73,73	1.23	6 (8%)	82,113,113	1.31	9 (10%)
25	CLA	b	609	37	69,73,73	1.57	7 (10%)	82,113,113	1.42	9 (10%)
31	STE	H	104	-	17,17,19	0.44	0	16,16,19	0.57	0
27	BCR	C	514	-	41,41,41	1.10	3 (7%)	56,56,56	1.20	6 (10%)
25	CLA	c	507	37	69,73,73	1.22	8 (11%)	82,113,113	1.29	6 (7%)
25	CLA	B	606	37	69,73,73	1.37	5 (7%)	82,113,113	1.43	9 (10%)
30	DGD	a	616	-	43,43,67	0.78	2 (4%)	45,45,81	1.50	8 (17%)
33	LHG	D	407	-	48,48,48	0.77	1 (2%)	51,54,54	1.29	9 (17%)
27	BCR	K	103	-	41,41,41	1.09	2 (4%)	56,56,56	1.11	5 (8%)
33	LHG	e	102	-	41,41,48	0.78	2 (4%)	44,47,54	1.31	5 (11%)
31	STE	M	103	-	9,9,19	0.40	0	8,8,19	0.76	0
29	SQD	A	614	-	50,52,54	1.58	7 (14%)	60,63,65	1.90	15 (25%)
31	STE	t	102	-	13,13,19	0.64	0	13,13,19	1.30	2 (15%)
25	CLA	b	601	-	69,73,73	1.13	4 (5%)	82,113,113	1.38	8 (9%)
25	CLA	B	614	-	69,73,73	1.41	8 (11%)	82,113,113	1.32	5 (6%)
27	BCR	K	101	-	41,41,41	1.05	2 (4%)	56,56,56	1.45	10 (17%)
28	PL9	D	405	-	55,55,55	1.02	3 (5%)	68,69,69	1.58	17 (25%)
30	DGD	C	516	-	63,63,67	1.09	4 (6%)	77,77,81	1.35	9 (11%)
30	DGD	C	518	-	63,63,67	0.98	3 (4%)	77,77,81	1.42	7 (9%)
31	STE	T	103	-	14,14,19	0.30	0	13,13,19	0.96	0
25	CLA	c	511	3	69,73,73	1.36	6 (8%)	82,113,113	1.43	6 (7%)
31	STE	x	102	-	19,19,19	0.66	0	19,19,19	0.92	1 (5%)
25	CLA	B	601	-	69,73,73	1.25	9 (13%)	82,113,113	1.35	8 (9%)
25	CLA	B	613	-	69,73,73	1.40	8 (11%)	82,113,113	1.28	9 (10%)
33	LHG	l	102	-	48,48,48	0.54	0	51,54,54	1.25	7 (13%)
31	STE	b	619	-	19,19,19	0.64	0	19,19,19	0.99	0
31	STE	b	623	-	9,9,19	0.41	0	8,8,19	0.60	0
34	BCT	a	606	23	3,3,3	1.18	0	2,3,3	2.93	1 (50%)
32	LMG	D	409	-	31,31,55	0.67	1 (3%)	33,33,63	1.22	2 (6%)
25	CLA	C	509	-	69,73,73	1.53	11 (15%)	82,113,113	1.41	11 (13%)
31	STE	j	101	-	11,11,19	0.79	0	11,11,19	1.19	1 (9%)
25	CLA	A	610	-	58,62,73	1.23	6 (10%)	68,99,113	1.34	11 (16%)
35	HEM	F	101	5,6	50,50,50	1.42	9 (18%)	67,82,82	1.10	2 (2%)
27	BCR	t	101	-	41,41,41	1.00	2 (4%)	56,56,56	1.46	10 (17%)
31	STE	m	102	-	11,11,19	0.74	0	11,11,19	1.39	2 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	BCR	k	101	-	41,41,41	1.00	3 (7%)	56,56,56	1.11	3 (5%)
27	BCR	K	102	-	41,41,41	1.08	2 (4%)	56,56,56	1.21	5 (8%)
31	STE	M	102	-	14,14,19	0.67	0	14,14,19	1.24	1 (7%)
32	LMG	c	524	-	49,49,55	0.90	4 (8%)	57,57,63	1.25	3 (5%)
25	CLA	d	402	-	69,73,73	1.31	9 (13%)	82,113,113	1.27	8 (9%)
25	CLA	C	503	-	69,73,73	1.28	9 (13%)	82,113,113	1.47	7 (8%)
25	CLA	b	615	-	64,68,73	1.25	7 (10%)	76,107,113	1.39	6 (7%)
25	CLA	B	604	-	69,73,73	1.24	8 (11%)	82,113,113	1.32	8 (9%)
27	BCR	b	616	-	41,41,41	0.99	3 (7%)	56,56,56	1.30	6 (10%)
25	CLA	b	610	-	69,73,73	1.27	5 (7%)	82,113,113	1.35	7 (8%)
31	STE	B	625	-	11,11,19	0.64	0	11,11,19	1.36	2 (18%)
26	PHO	A	608	-	58,69,69	1.95	10 (17%)	55,99,99	1.46	6 (10%)
25	CLA	b	613	-	69,73,73	1.26	8 (11%)	82,113,113	1.26	8 (9%)
27	BCR	D	404	-	41,41,41	1.03	2 (4%)	56,56,56	1.25	7 (12%)
29	SQD	L	101	-	47,49,54	1.66	9 (19%)	57,60,65	1.83	10 (17%)
29	SQD	a	614	-	52,54,54	1.56	6 (11%)	62,65,65	1.92	12 (19%)
25	CLA	c	508	-	68,72,73	1.36	10 (14%)	80,111,113	1.39	12 (15%)
27	BCR	c	515	-	41,41,41	1.07	2 (4%)	56,56,56	1.24	5 (8%)
31	STE	a	617	-	11,11,19	0.77	0	11,11,19	0.99	0
33	LHG	d	408	-	38,38,48	0.77	1 (2%)	41,44,54	1.18	3 (7%)
25	CLA	B	612	-	69,73,73	1.21	8 (11%)	82,113,113	1.41	7 (8%)
21	OEY	A	601[B]	3,1,37	0,16,16	-	-	-	-	-
25	CLA	B	609	37	69,73,73	1.24	10 (14%)	82,113,113	1.43	11 (13%)
33	LHG	d	406	-	48,48,48	0.82	3 (6%)	51,54,54	1.35	7 (13%)
25	CLA	C	513	-	69,73,73	1.23	7 (10%)	82,113,113	1.38	8 (9%)
27	BCR	a	611	-	41,41,41	0.95	2 (4%)	56,56,56	1.17	5 (8%)
31	STE	d	411	-	16,16,19	0.65	0	16,16,19	1.13	1 (6%)
25	CLA	B	607	-	69,73,73	1.44	9 (13%)	82,113,113	1.37	10 (12%)
31	STE	I	101	-	14,14,19	0.41	0	13,13,19	0.72	0
29	SQD	f	101	-	39,41,54	1.70	9 (23%)	49,52,65	1.77	11 (22%)
30	DGD	C	517	-	63,63,67	1.05	6 (9%)	77,77,81	1.45	11 (14%)
25	CLA	C	504	37	63,67,73	1.37	10 (15%)	74,105,113	1.37	13 (17%)
28	PL9	a	612	-	55,55,55	0.72	1 (1%)	68,69,69	1.51	11 (16%)
31	STE	c	521	-	19,19,19	0.65	0	19,19,19	0.94	0
25	CLA	b	607	-	69,73,73	1.49	9 (13%)	82,113,113	1.40	11 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	a	608	37	69,73,73	1.14	6 (8%)	82,113,113	1.23	6 (7%)
25	CLA	B	602	-	69,73,73	1.27	7 (10%)	82,113,113	1.42	11 (13%)
25	CLA	C	511	3	69,73,73	1.28	8 (11%)	82,113,113	1.35	5 (6%)
27	BCR	c	516	-	41,41,41	1.08	2 (4%)	56,56,56	1.15	3 (5%)
25	CLA	b	611	-	69,73,73	1.38	9 (13%)	82,113,113	1.34	9 (10%)
25	CLA	c	512	-	69,73,73	1.23	9 (13%)	82,113,113	1.32	7 (8%)
25	CLA	b	612	-	69,73,73	1.32	9 (13%)	82,113,113	1.42	13 (15%)
25	CLA	h	101	37	69,73,73	1.36	9 (13%)	82,113,113	1.32	9 (10%)
21	OYE	a	601[B]	3,1,37	0,16,16	-	-	-	-	-
31	STE	T	102	-	15,15,19	0.41	0	14,14,19	0.71	0
36	HEC	V	201	16	46,50,50	1.82	5 (10%)	58,82,82	1.94	6 (10%)
30	DGD	c	517	-	63,63,67	0.86	3 (4%)	77,77,81	1.35	9 (11%)
25	CLA	B	611	-	69,73,73	1.21	10 (14%)	82,113,113	1.43	11 (13%)
25	CLA	A	613	37	69,73,73	1.15	6 (8%)	82,113,113	1.25	8 (9%)
27	BCR	B	617	-	41,41,41	1.01	2 (4%)	56,56,56	1.25	6 (10%)

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	PHO	d	401	-	-	7/37/103/103	0/5/6/6
31	STE	C	520	-	-	1/9/9/17	-
25	CLA	C	501	-	1/1/15/20	7/39/115/115	-
25	CLA	a	613	37	1/1/15/20	1/39/115/115	-
25	CLA	b	604	-	1/1/15/20	12/39/115/115	-
27	BCR	c	514	-	-	6/29/63/63	0/2/2/2
29	SQD	a	615	-	-	19/37/37/69	-
31	STE	B	626	-	-	4/13/13/17	-
31	STE	c	523	-	-	4/9/9/17	-
33	LHG	B	621	-	-	21/53/53/53	-
31	STE	b	621	-	-	6/13/13/17	-
25	CLA	b	606	37	1/1/15/20	13/39/115/115	-
32	LMG	d	410	-	-	8/39/59/70	0/1/1/1
30	DGD	c	518	-	-	17/51/91/95	0/2/2/2
30	DGD	c	519	-	-	18/51/91/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	a	610	-	1/1/15/20	10/39/115/115	-
32	LMG	C	515	-	-	22/43/63/70	0/1/1/1
25	CLA	c	506	-	1/1/15/20	15/39/115/115	-
32	LMG	M	101	-	-	25/46/66/70	0/1/1/1
33	LHG	d	407	-	-	19/53/53/53	-
25	CLA	C	502	-	1/1/15/20	8/39/115/115	-
25	CLA	c	502	-	-	5/39/115/115	-
32	LMG	B	620	-	-	14/22/22/70	-
31	STE	B	623	-	-	7/9/9/17	-
26	PHO	a	609	-	-	2/37/103/103	0/5/6/6
27	BCR	d	404	-	-	10/29/63/63	0/2/2/2
25	CLA	b	614	-	1/1/15/20	9/39/115/115	-
32	LMG	c	522	-	-	29/43/63/70	0/1/1/1
27	BCR	b	617	-	-	2/29/63/63	0/2/2/2
31	STE	C	521	-	-	5/9/9/17	-
31	STE	t	103	-	-	4/7/7/17	-
30	DGD	H	103	-	-	16/51/91/95	0/2/2/2
32	LMG	d	409	-	-	8/17/17/70	-
25	CLA	C	505	-	1/1/15/20	13/39/115/115	-
25	CLA	A	607	37	-	11/39/115/115	-
25	CLA	c	505	-	1/1/15/20	12/39/115/115	-
33	LHG	D	408	-	-	23/51/51/53	-
27	BCR	B	618	-	-	5/29/63/63	0/2/2/2
25	CLA	D	402	-	1/1/15/20	6/39/115/115	-
25	CLA	H	101	37	1/1/15/20	18/39/115/115	-
25	CLA	a	607	-	1/1/15/20	4/39/115/115	-
29	SQD	F	102	-	-	10/28/48/69	0/1/1/1
25	CLA	c	504	37	1/1/14/20	8/33/109/115	-
25	CLA	C	507	37	1/1/15/20	9/39/115/115	-
28	PL9	A	612	-	-	27/53/73/73	0/1/1/1
30	DGD	A	616	-	-	28/55/95/95	0/2/2/2
25	CLA	C	512	-	1/1/15/20	14/39/115/115	-
27	BCR	T	101	-	-	6/29/63/63	0/2/2/2
27	BCR	A	611	-	-	4/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	c	503	-	1/1/15/20	7/39/115/115	-
36	HEC	v	201	16	-	6/14/54/54	-
25	CLA	C	508	-	-	8/39/115/115	-
25	CLA	B	610	-	1/1/15/20	7/39/115/115	-
25	CLA	B	603	-	1/1/15/20	12/39/115/115	-
32	LMG	b	620	-	-	31/50/70/70	0/1/1/1
29	SQD	l	101	-	-	28/49/69/69	0/1/1/1
31	STE	B	619	-	-	7/14/14/17	-
27	BCR	B	616	-	-	8/29/63/63	0/2/2/2
25	CLA	c	501	-	1/1/15/20	4/39/115/115	-
25	CLA	b	608	-	1/1/15/20	5/39/115/115	-
31	STE	R	101	-	-	4/9/9/17	-
25	CLA	b	605	-	1/1/15/20	7/39/115/115	-
31	STE	l	103	-	-	8/15/15/17	-
28	PL9	d	405	-	-	13/53/73/73	0/1/1/1
31	STE	B	624	-	-	8/15/15/17	-
31	STE	D	410	-	-	9/17/17/17	-
31	STE	J	101	-	-	4/9/9/17	-
32	LMG	m	101	-	-	24/46/66/70	0/1/1/1
32	LMG	c	520	-	-	14/31/51/70	0/1/1/1
32	LMG	D	406	-	-	18/46/66/70	0/1/1/1
25	CLA	A	606	-	1/1/15/20	3/39/115/115	-
33	LHG	B	622	-	-	15/53/53/53	-
25	CLA	B	608	-	-	4/39/115/115	-
29	SQD	A	615	-	-	17/39/39/69	-
25	CLA	B	605	-	1/1/15/20	14/39/115/115	-
31	STE	C	522	-	-	4/13/13/17	-
25	CLA	B	615	-	1/1/14/20	6/33/109/115	-
25	CLA	C	506	-	1/1/15/20	13/39/115/115	-
33	LHG	E	101	-	-	32/53/53/53	-
27	BCR	b	618	-	-	7/29/63/63	0/2/2/2
31	STE	b	622	-	-	9/17/17/17	-
25	CLA	b	603	-	1/1/15/20	7/39/115/115	-
25	CLA	c	509	-	1/1/15/20	10/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	HEM	e	101	5,6	-	0/14/54/54	-
27	BCR	H	102	-	-	4/29/63/63	0/2/2/2
32	LMG	C	519	-	-	22/43/63/70	0/1/1/1
27	BCR	x	101	-	-	4/29/63/63	0/2/2/2
25	CLA	C	510	-	1/1/15/20	10/39/115/115	-
25	CLA	c	510	-	1/1/15/20	14/39/115/115	-
30	DGD	h	102	-	-	14/51/91/95	0/2/2/2
25	CLA	D	403	-	-	12/39/115/115	-
25	CLA	d	403	-	1/1/15/20	4/39/115/115	-
26	PHO	A	609	-	-	2/37/103/103	0/5/6/6
25	CLA	c	513	-	1/1/15/20	10/39/115/115	-
25	CLA	b	602	-	1/1/15/20	13/39/115/115	-
25	CLA	b	609	37	1/1/15/20	4/39/115/115	-
31	STE	H	104	-	-	9/15/15/17	-
27	BCR	C	514	-	-	6/29/63/63	0/2/2/2
25	CLA	c	507	37	1/1/15/20	12/39/115/115	-
25	CLA	B	606	37	1/1/15/20	10/39/115/115	-
30	DGD	a	616	-	-	26/45/45/95	-
33	LHG	D	407	-	-	23/53/53/53	-
27	BCR	K	103	-	-	7/29/63/63	0/2/2/2
33	LHG	e	102	-	-	25/46/46/53	-
31	STE	M	103	-	-	2/7/7/17	-
29	SQD	A	614	-	-	21/47/67/69	0/1/1/1
31	STE	t	102	-	-	3/11/11/17	-
25	CLA	b	601	-	1/1/15/20	12/39/115/115	-
25	CLA	B	614	-	1/1/15/20	12/39/115/115	-
27	BCR	K	101	-	-	11/29/63/63	0/2/2/2
28	PL9	D	405	-	-	12/53/73/73	0/1/1/1
30	DGD	C	516	-	-	18/51/91/95	0/2/2/2
30	DGD	C	518	-	-	14/51/91/95	0/2/2/2
31	STE	T	103	-	-	11/12/12/17	-
25	CLA	c	511	3	1/1/15/20	4/39/115/115	-
31	STE	x	102	-	-	6/17/17/17	-
25	CLA	B	601	-	1/1/15/20	8/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	B	613	-	1/1/15/20	15/39/115/115	-
33	LHG	l	102	-	-	16/53/53/53	-
31	STE	b	619	-	-	9/17/17/17	-
31	STE	b	623	-	-	2/7/7/17	-
32	LMG	D	409	-	-	18/33/33/70	-
25	CLA	C	509	-	1/1/15/20	13/39/115/115	-
31	STE	j	101	-	-	3/9/9/17	-
25	CLA	A	610	-	1/1/12/20	2/26/102/115	-
35	HEM	F	101	5,6	-	3/14/54/54	-
27	BCR	t	101	-	-	6/29/63/63	0/2/2/2
31	STE	m	102	-	-	4/9/9/17	-
27	BCR	k	101	-	-	5/29/63/63	0/2/2/2
27	BCR	K	102	-	-	6/29/63/63	0/2/2/2
31	STE	M	102	-	-	7/12/12/17	-
32	LMG	c	524	-	-	28/44/64/70	0/1/1/1
25	CLA	d	402	-	1/1/15/20	3/39/115/115	-
25	CLA	C	503	-	1/1/15/20	7/39/115/115	-
25	CLA	b	615	-	1/1/14/20	8/33/109/115	-
25	CLA	B	604	-	1/1/15/20	4/39/115/115	-
27	BCR	b	616	-	-	4/29/63/63	0/2/2/2
25	CLA	b	610	-	1/1/15/20	8/39/115/115	-
31	STE	B	625	-	-	3/9/9/17	-
26	PHO	A	608	-	-	2/37/103/103	0/5/6/6
25	CLA	b	613	-	1/1/15/20	13/39/115/115	-
27	BCR	D	404	-	-	6/29/63/63	0/2/2/2
29	SQD	L	101	-	-	19/44/64/69	0/1/1/1
29	SQD	a	614	-	-	26/49/69/69	0/1/1/1
25	CLA	c	508	-	-	3/38/114/115	-
27	BCR	c	515	-	-	6/29/63/63	0/2/2/2
31	STE	a	617	-	-	4/9/9/17	-
33	LHG	d	408	-	-	12/43/43/53	-
25	CLA	B	612	-	1/1/15/20	16/39/115/115	-
25	CLA	B	609	37	1/1/15/20	6/39/115/115	-
33	LHG	d	406	-	-	22/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	C	513	-	1/1/15/20	12/39/115/115	-
27	BCR	a	611	-	-	1/29/63/63	0/2/2/2
31	STE	d	411	-	-	11/14/14/17	-
25	CLA	B	607	-	1/1/15/20	2/39/115/115	-
31	STE	I	101	-	-	3/12/12/17	-
29	SQD	f	101	-	-	24/36/56/69	0/1/1/1
30	DGD	C	517	-	-	24/51/91/95	0/2/2/2
25	CLA	C	504	37	1/1/13/20	9/32/108/115	-
28	PL9	a	612	-	-	24/53/73/73	0/1/1/1
31	STE	c	521	-	-	11/17/17/17	-
25	CLA	b	607	-	1/1/15/20	3/39/115/115	-
25	CLA	a	608	37	1/1/15/20	12/39/115/115	-
25	CLA	B	602	-	1/1/15/20	10/39/115/115	-
25	CLA	C	511	3	1/1/15/20	8/39/115/115	-
27	BCR	c	516	-	-	4/29/63/63	0/2/2/2
25	CLA	b	611	-	1/1/15/20	8/39/115/115	-
25	CLA	c	512	-	1/1/15/20	22/39/115/115	-
25	CLA	b	612	-	1/1/15/20	4/39/115/115	-
25	CLA	h	101	37	1/1/15/20	18/39/115/115	-
31	STE	T	102	-	-	7/13/13/17	-
36	HEC	V	201	16	-	6/14/54/54	-
30	DGD	c	517	-	-	27/51/91/95	0/2/2/2
25	CLA	B	611	-	1/1/15/20	9/39/115/115	-
25	CLA	A	613	37	1/1/15/20	10/39/115/115	-
27	BCR	B	617	-	-	6/29/63/63	0/2/2/2

The worst 5 of 807 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	a	609	PHO	C1B-C2B	10.05	1.50	1.39
26	A	609	PHO	C1B-C2B	9.34	1.49	1.39
26	d	401	PHO	C1B-C2B	8.96	1.49	1.39
25	b	609	CLA	MG-NB	-8.74	1.88	2.05
26	d	401	PHO	C3B-C4B	8.68	1.50	1.41

The worst 5 of 1138 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	509	CLA	C4A-NA-C1A	8.87	110.73	106.68
36	V	201	HEC	CBB-CAB-C3B	-8.82	109.80	127.43
25	c	511	CLA	C4A-NA-C1A	8.60	110.60	106.68
25	C	507	CLA	C4A-NA-C1A	8.54	110.58	106.68
25	B	603	CLA	C4A-NA-C1A	8.40	110.51	106.68

5 of 64 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
25	A	606	CLA	ND
25	A	610	CLA	ND
25	A	613	CLA	ND
25	B	601	CLA	ND
25	B	602	CLA	ND

5 of 1874 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	B	605	CLA	C4B-C3B-CAB-CBB
25	B	613	CLA	CAD-CBD-CGD-O1D
25	B	613	CLA	CAD-CBD-CGD-O2D
25	B	613	CLA	C14-C13-C15-C16
25	B	614	CLA	C2B-C3B-CAB-CBB

There are no ring outliers.

140 monomers are involved in 269 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	d	401	PHO	2	0
25	C	501	CLA	1	0
25	a	613	CLA	1	0
25	b	604	CLA	4	0
27	c	514	BCR	2	0
29	a	615	SQD	1	0
31	B	626	STE	1	0
33	B	621	LHG	3	0
31	b	621	STE	1	0
25	b	606	CLA	2	0
30	c	518	DGD	2	0
30	c	519	DGD	4	0
25	a	610	CLA	3	0
32	C	515	LMG	3	0
25	c	506	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	M	101	LMG	1	0
33	d	407	LHG	3	0
25	C	502	CLA	3	0
27	d	404	BCR	2	0
25	b	614	CLA	5	0
32	c	522	LMG	2	0
27	b	617	BCR	2	0
31	t	103	STE	1	0
30	H	103	DGD	3	0
32	d	409	LMG	1	0
25	C	505	CLA	2	0
25	c	505	CLA	3	0
33	D	408	LHG	2	0
21	a	601[C]	OEY	1	0
25	D	402	CLA	4	0
25	H	101	CLA	2	0
25	a	607	CLA	4	0
29	F	102	SQD	1	0
25	c	504	CLA	2	0
25	C	507	CLA	2	0
28	A	612	PL9	5	0
30	A	616	DGD	8	0
21	A	601[C]	OEY	1	0
25	C	512	CLA	1	0
27	T	101	BCR	1	0
25	c	503	CLA	2	0
36	v	201	HEC	2	0
25	C	508	CLA	1	0
25	B	610	CLA	2	0
25	B	603	CLA	2	0
29	l	101	SQD	2	0
31	B	619	STE	1	0
27	B	616	BCR	2	0
25	c	501	CLA	2	0
25	b	608	CLA	4	0
25	b	605	CLA	3	0
28	d	405	PL9	2	0
31	D	410	STE	3	0
32	m	101	LMG	4	0
32	c	520	LMG	1	0
32	D	406	LMG	4	0
25	A	606	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	B	622	LHG	1	0
25	B	608	CLA	3	0
25	B	605	CLA	2	0
25	B	615	CLA	2	0
25	C	506	CLA	2	0
33	E	101	LHG	1	0
31	b	622	STE	1	0
25	b	603	CLA	2	0
25	c	509	CLA	2	0
35	e	101	HEM	2	0
27	H	102	BCR	2	0
32	C	519	LMG	1	0
27	x	101	BCR	3	0
25	C	510	CLA	2	0
25	c	510	CLA	1	0
30	h	102	DGD	1	0
25	D	403	CLA	3	0
25	d	403	CLA	3	0
26	A	609	PHO	3	0
25	c	513	CLA	2	0
25	b	602	CLA	4	0
25	b	609	CLA	3	0
31	H	104	STE	3	0
27	C	514	BCR	5	0
25	c	507	CLA	3	0
25	B	606	CLA	4	0
30	a	616	DGD	1	0
33	D	407	LHG	2	0
27	K	103	BCR	1	0
29	A	614	SQD	2	0
25	b	601	CLA	5	0
25	B	614	CLA	2	0
27	K	101	BCR	2	0
28	D	405	PL9	1	0
30	C	518	DGD	1	0
25	c	511	CLA	3	0
31	x	102	STE	2	0
25	B	601	CLA	2	0
25	B	613	CLA	4	0
31	b	619	STE	2	0
32	D	409	LMG	1	0
25	C	509	CLA	3	0

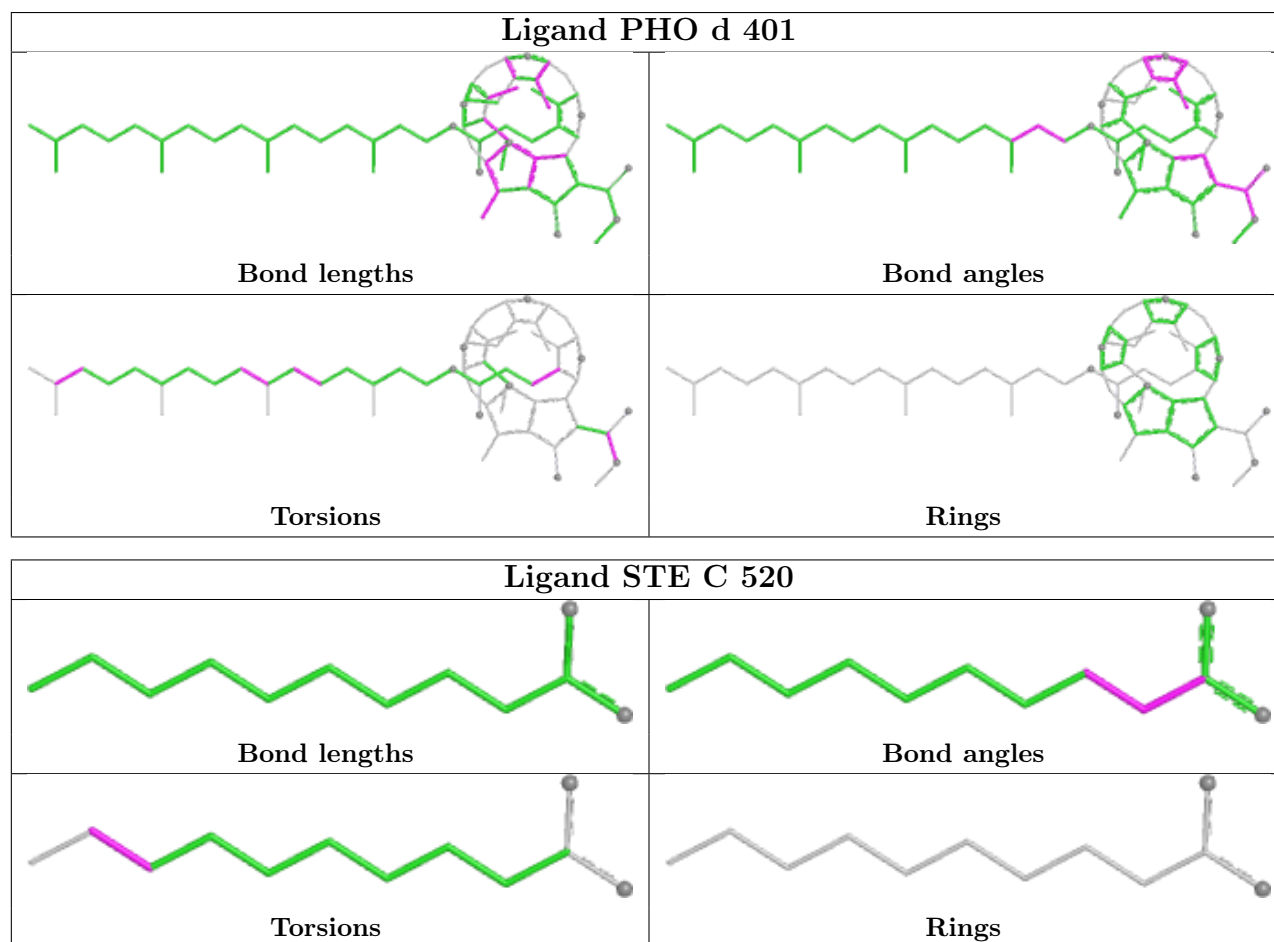
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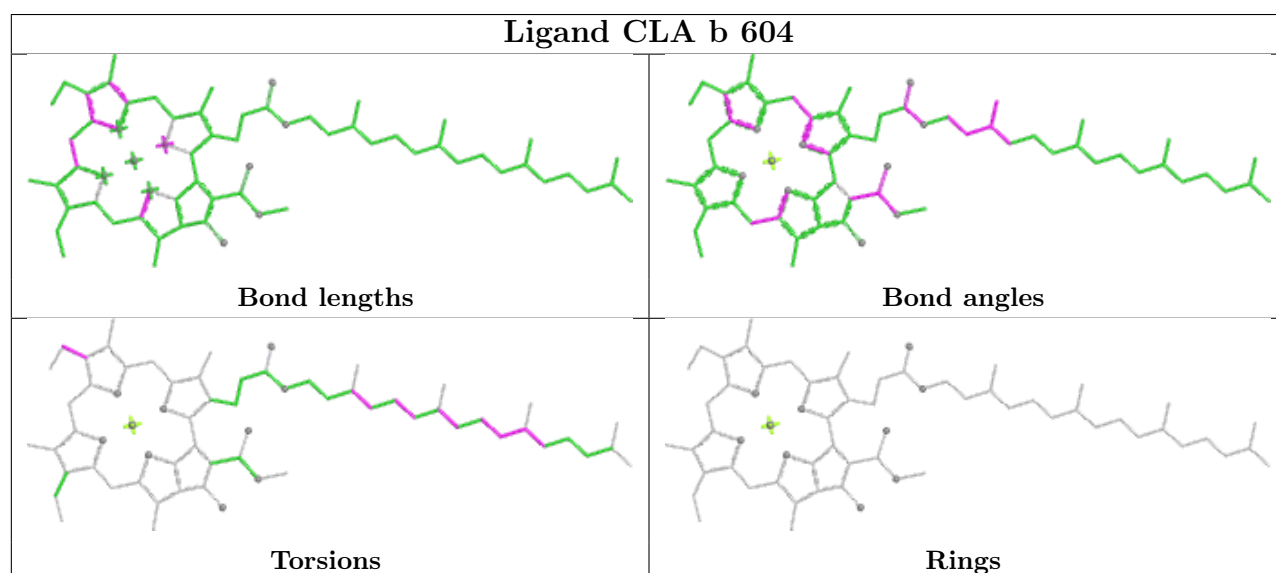
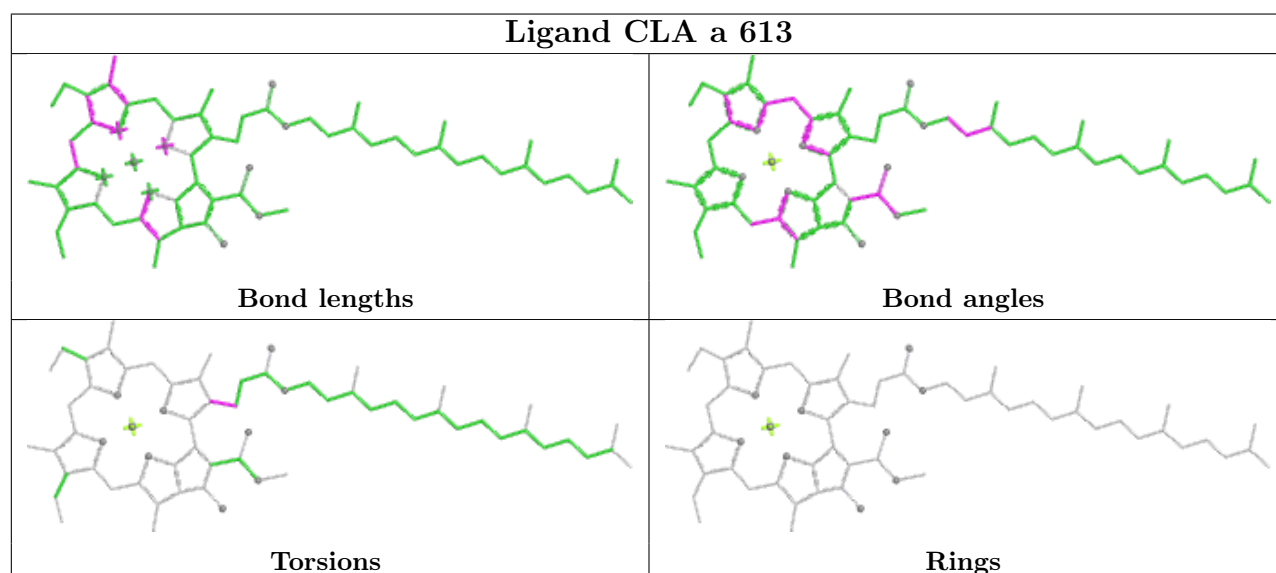
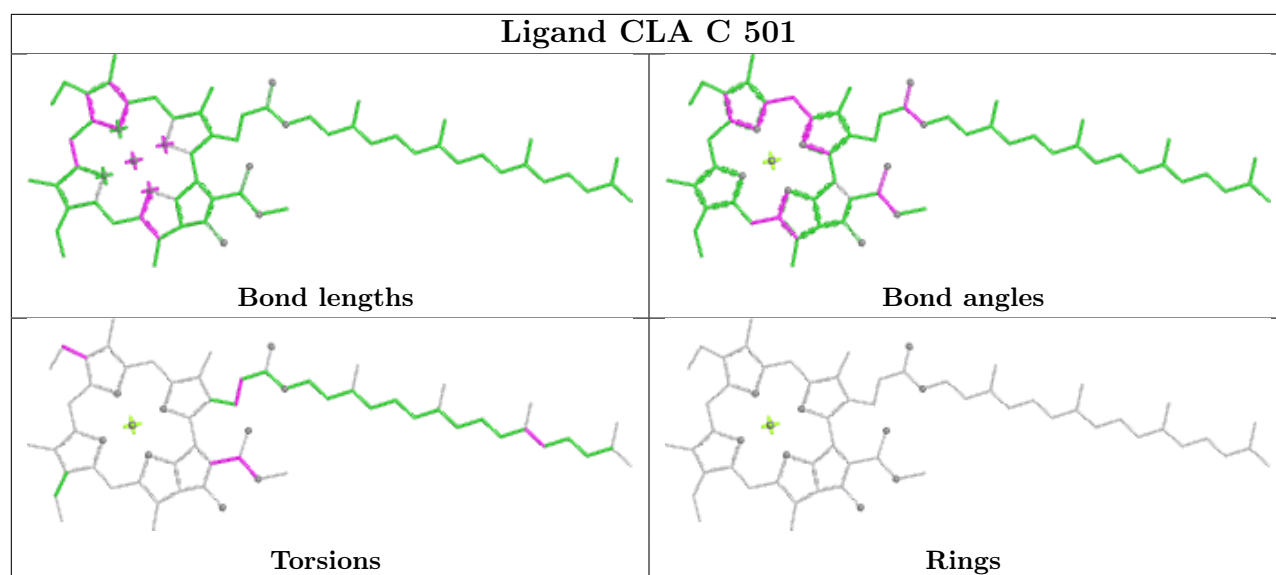
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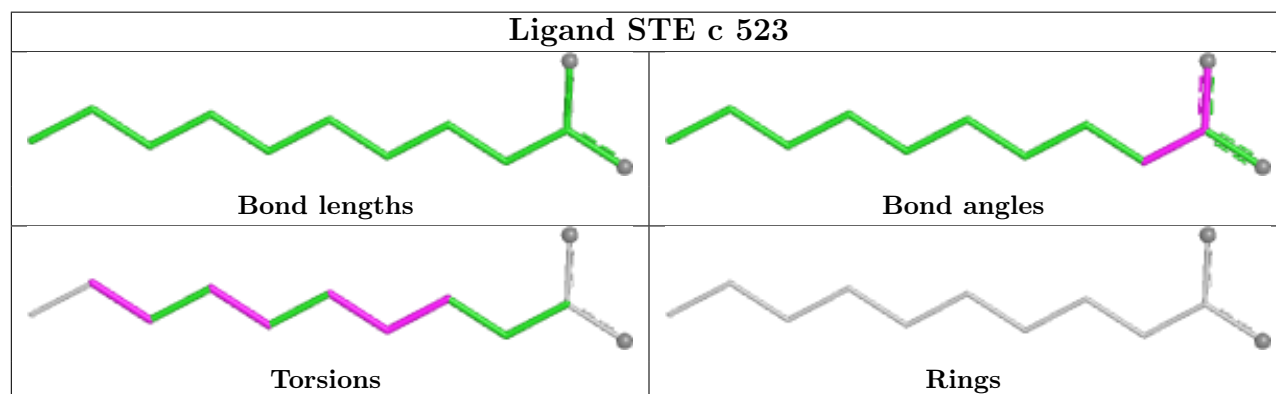
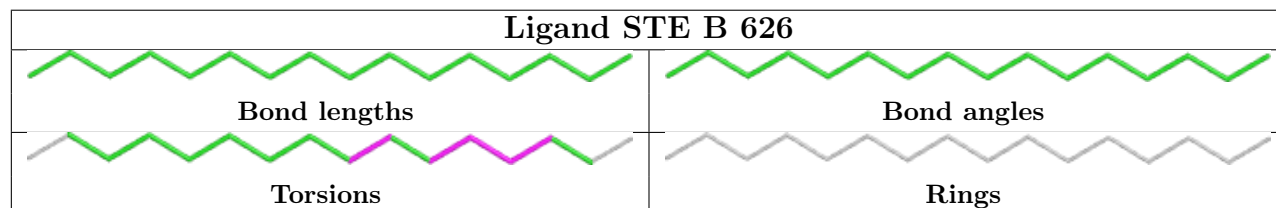
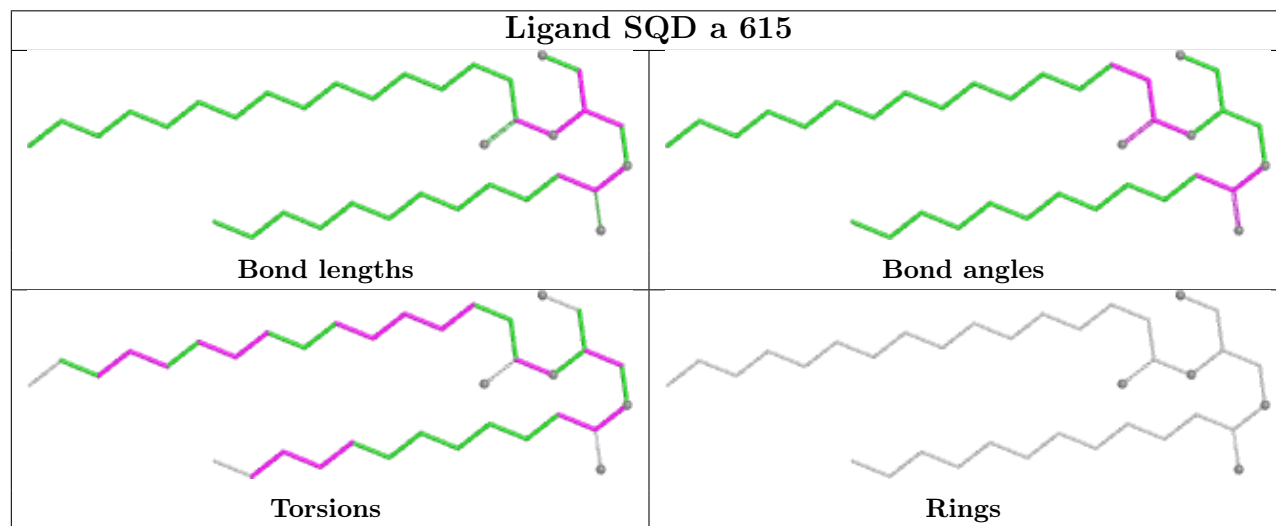
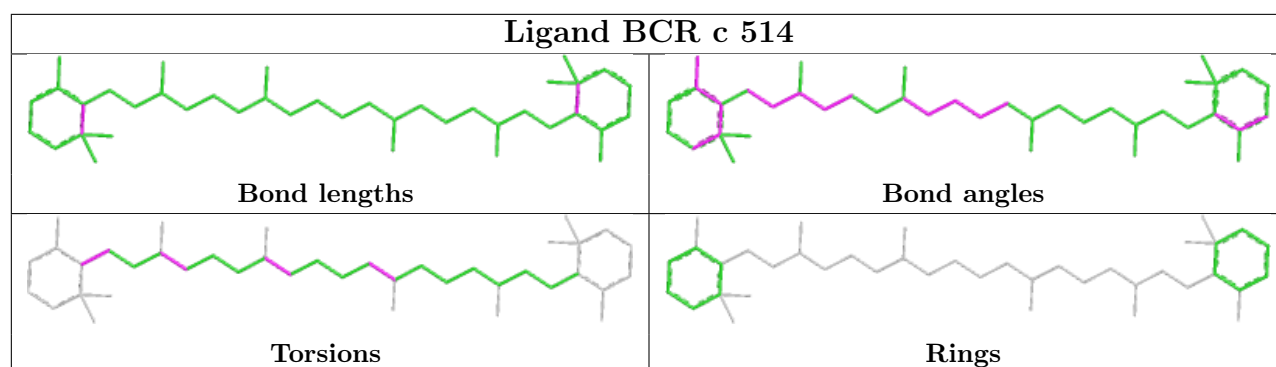
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	A	610	CLA	1	0
35	F	101	HEM	2	0
27	t	101	BCR	1	0
27	k	101	BCR	1	0
27	K	102	BCR	3	0
32	c	524	LMG	3	0
25	d	402	CLA	1	0
25	C	503	CLA	1	0
25	b	615	CLA	3	0
25	B	604	CLA	5	0
25	b	610	CLA	1	0
25	b	613	CLA	2	0
27	D	404	BCR	1	0
29	L	101	SQD	2	0
29	a	614	SQD	1	0
25	c	508	CLA	1	0
27	c	515	BCR	6	0
31	a	617	STE	1	0
33	d	408	LHG	1	0
25	B	612	CLA	3	0
21	A	601[B]	OEY	1	0
25	B	609	CLA	2	0
33	d	406	LHG	7	0
27	a	611	BCR	1	0
31	I	101	STE	3	0
29	f	101	SQD	3	0
30	C	517	DGD	2	0
25	C	504	CLA	1	0
28	a	612	PL9	5	0
31	c	521	STE	2	0
25	B	602	CLA	4	0
25	C	511	CLA	1	0
27	c	516	BCR	3	0
25	b	611	CLA	3	0
25	c	512	CLA	3	0
25	b	612	CLA	3	0
25	h	101	CLA	4	0
21	a	601[B]	OEY	1	0
30	c	517	DGD	3	0
25	B	611	CLA	4	0
27	B	617	BCR	1	0

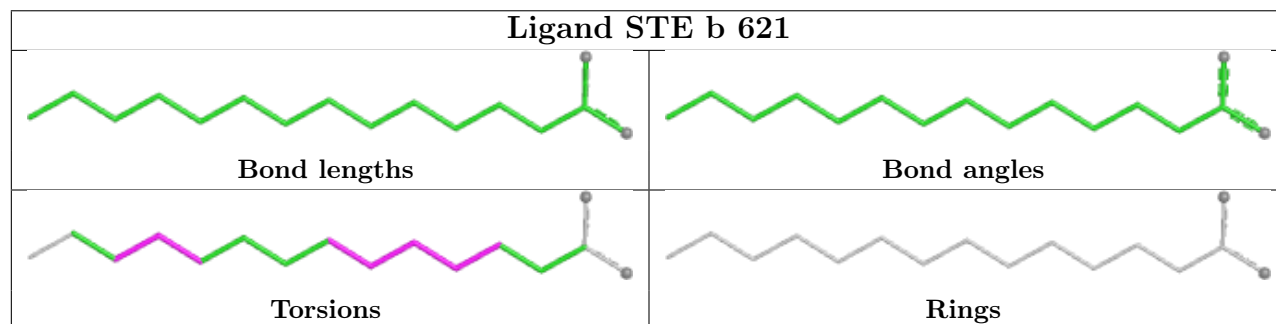
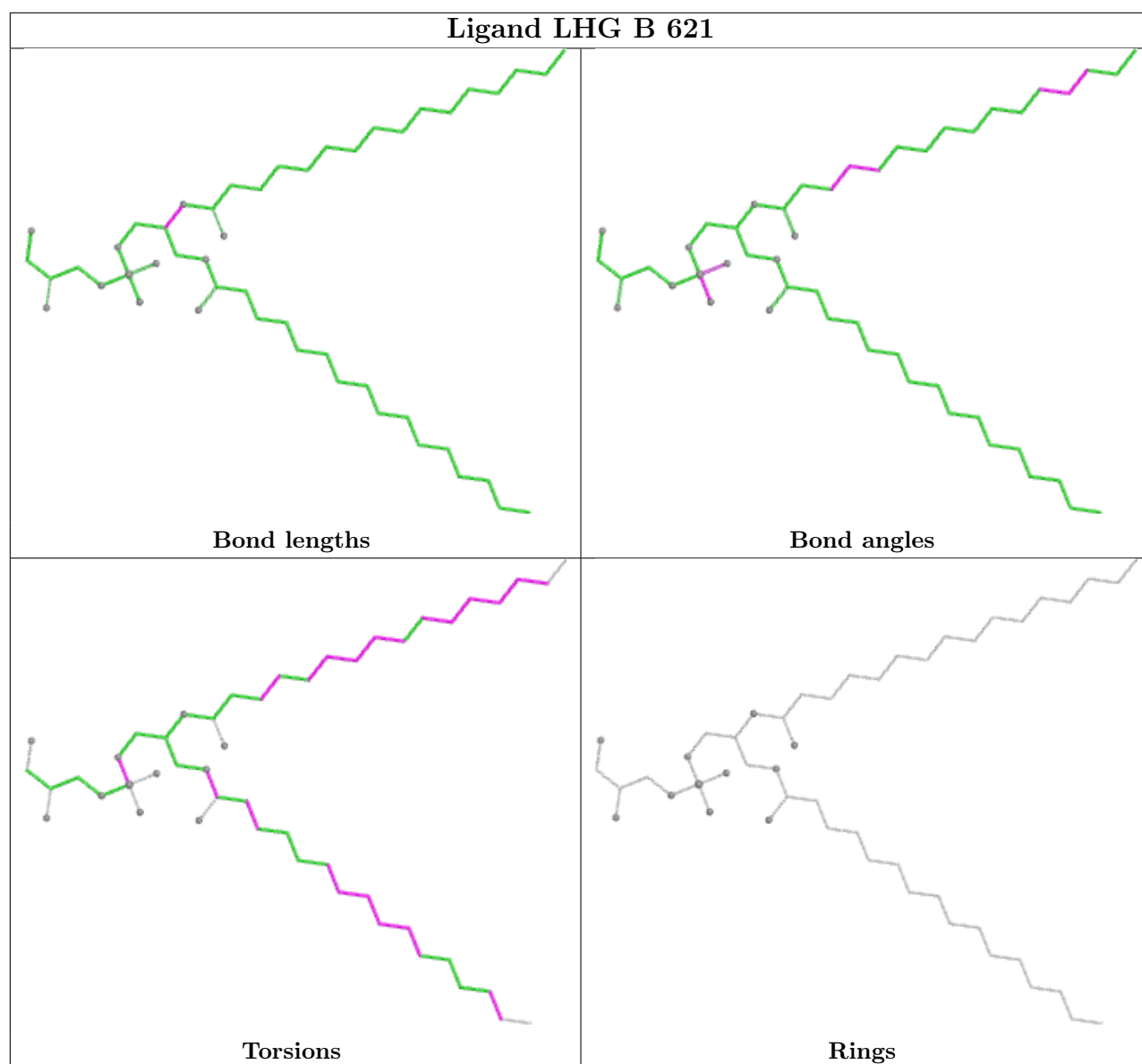
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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

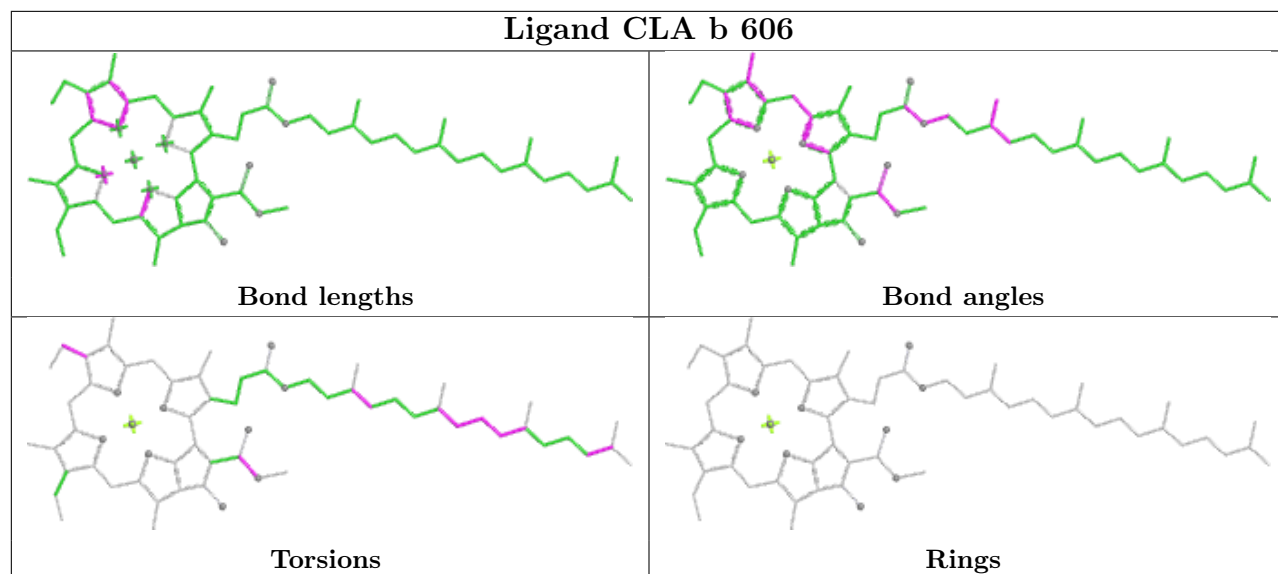




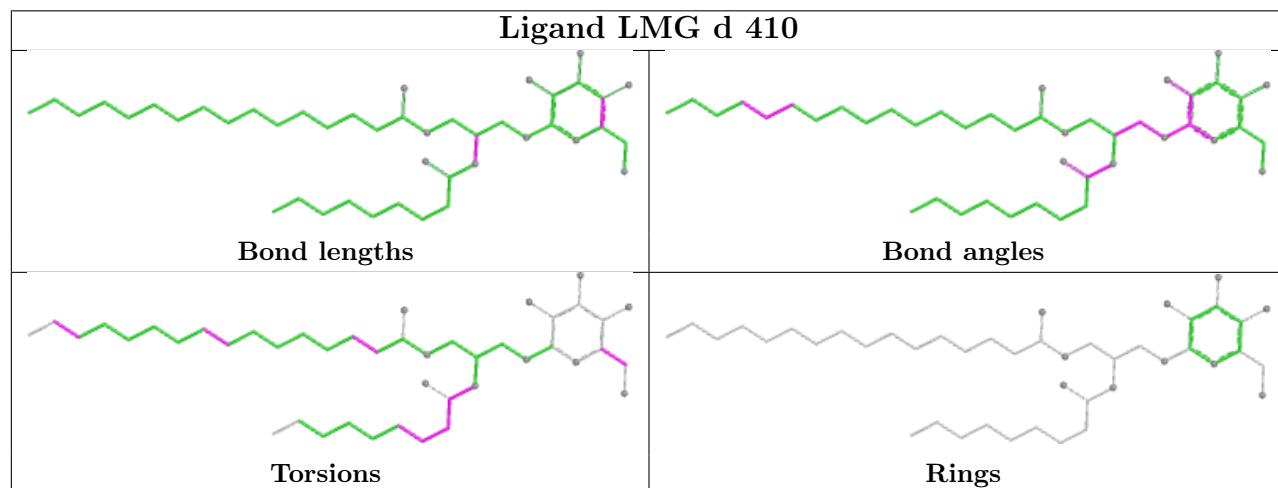




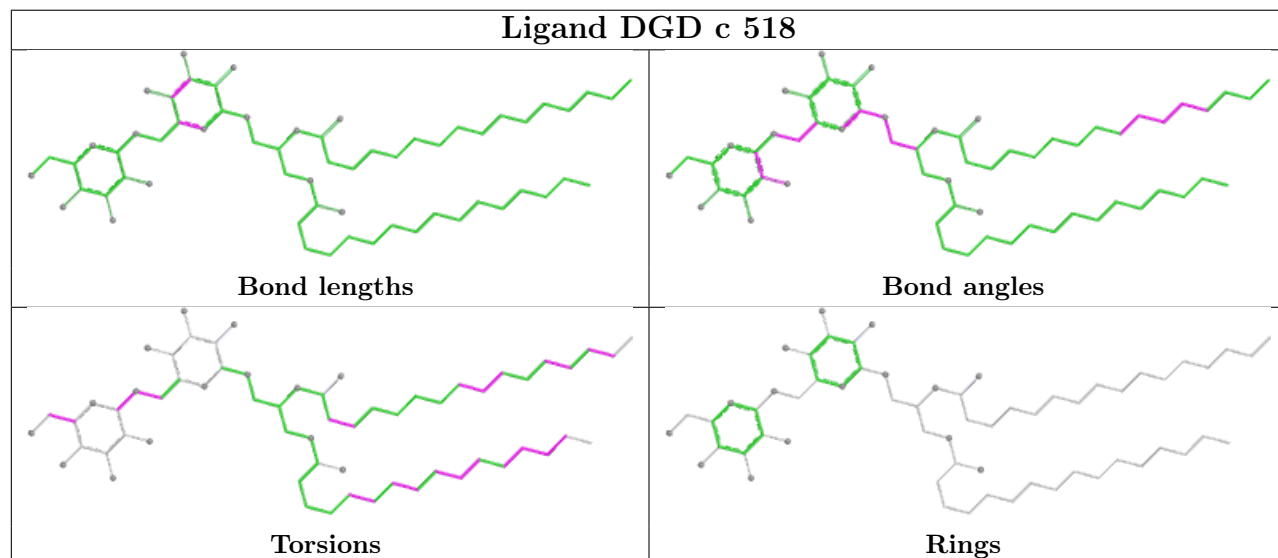
Ligand CLA b 606

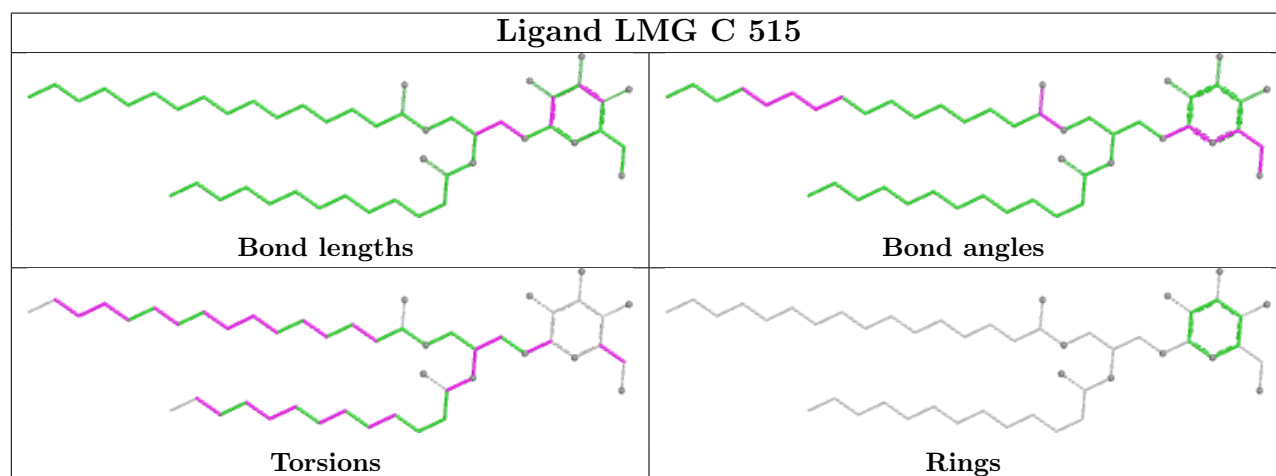
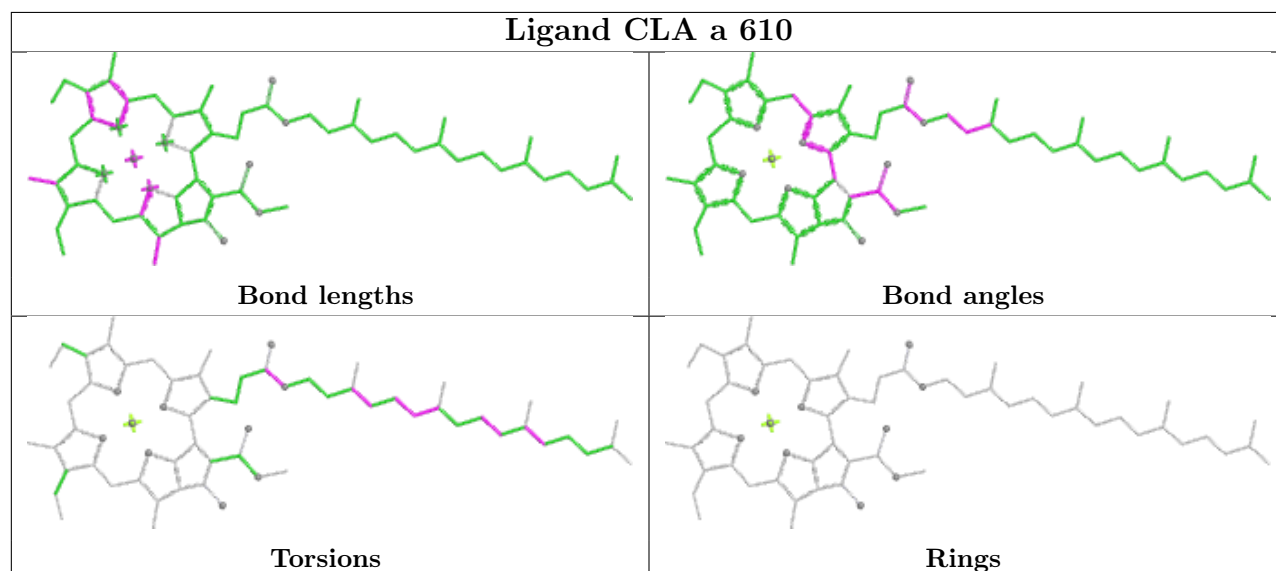
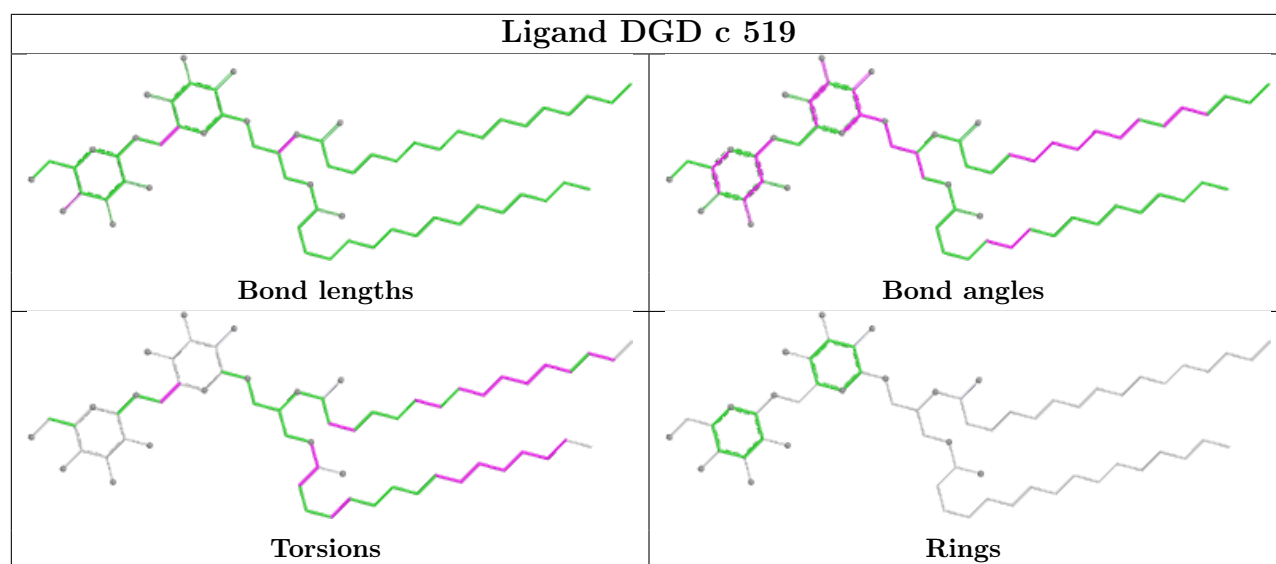


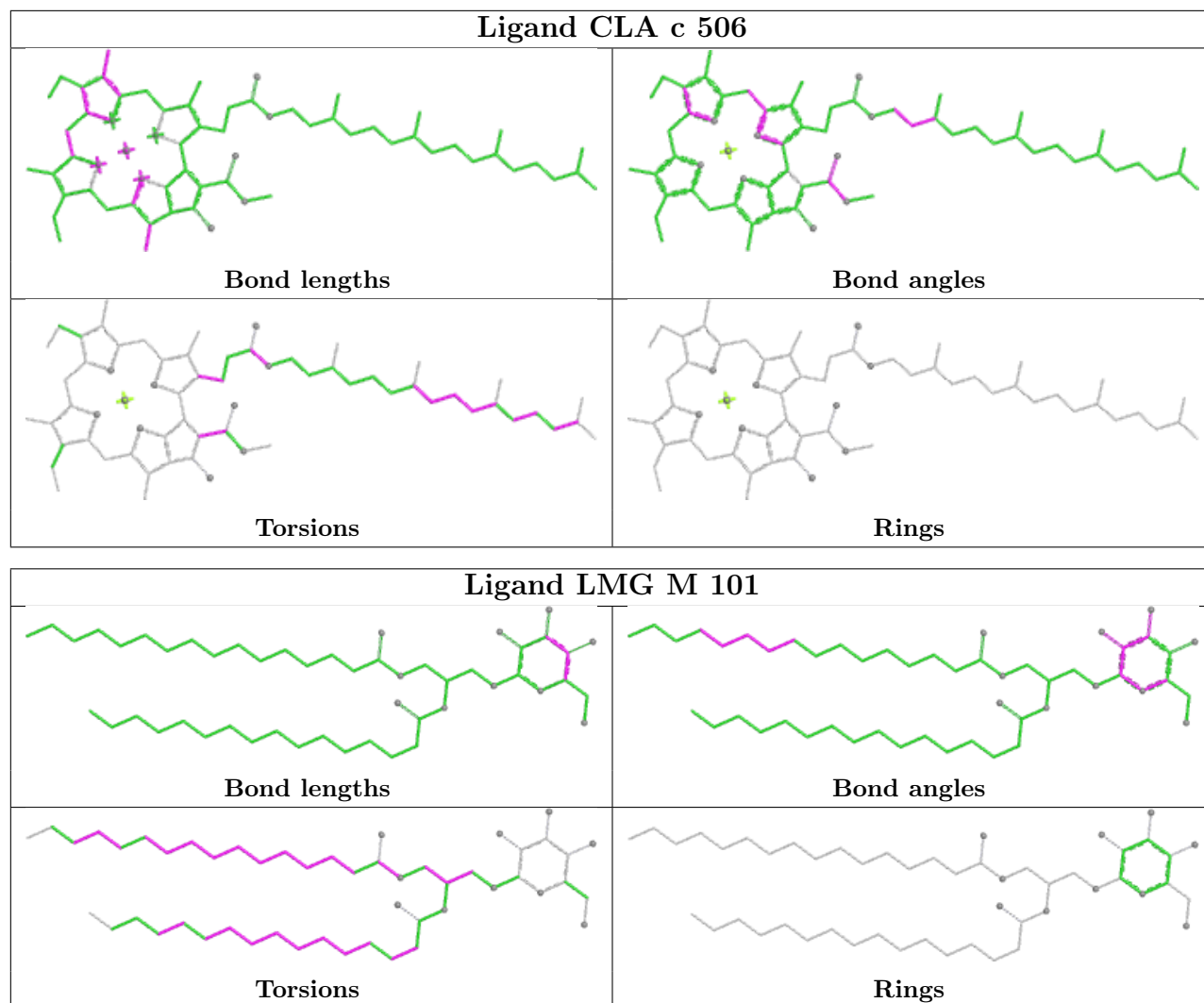
Ligand LMG d 410

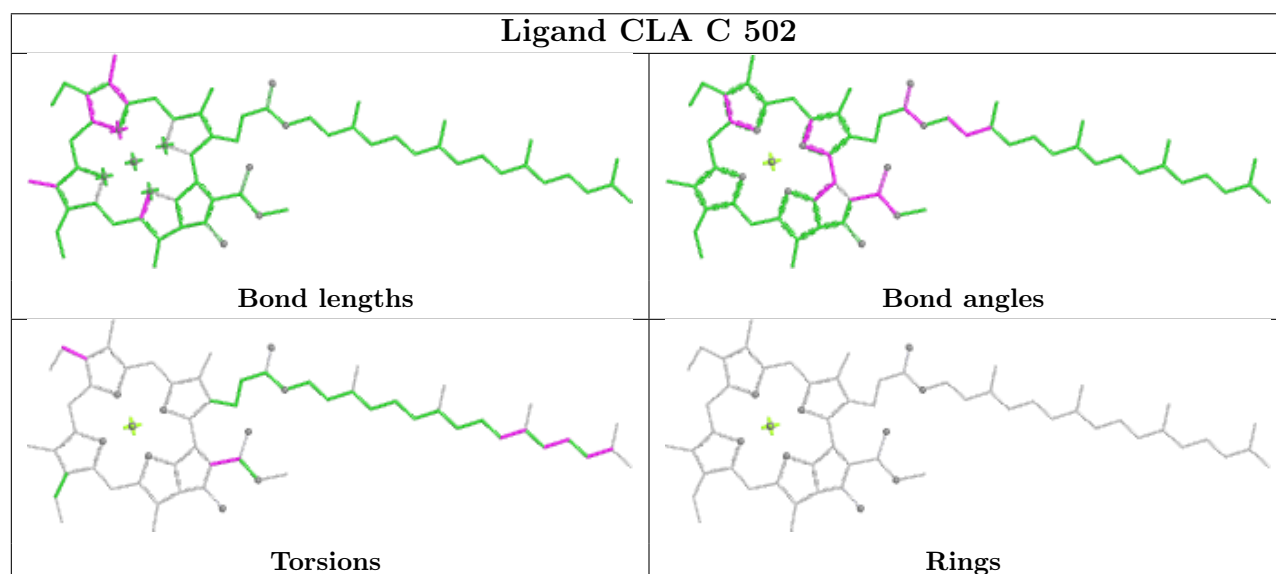
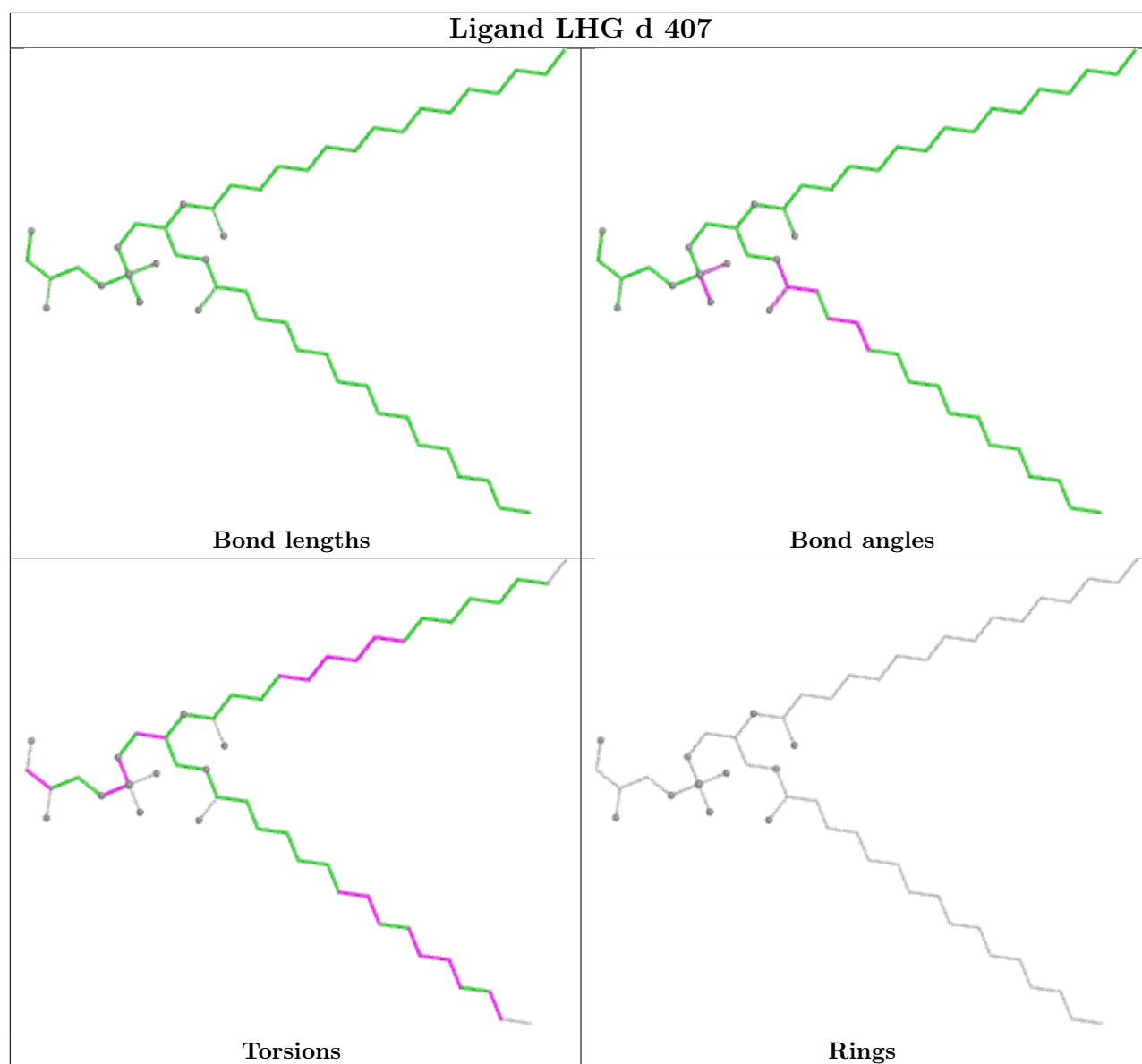


Ligand DGD c 518

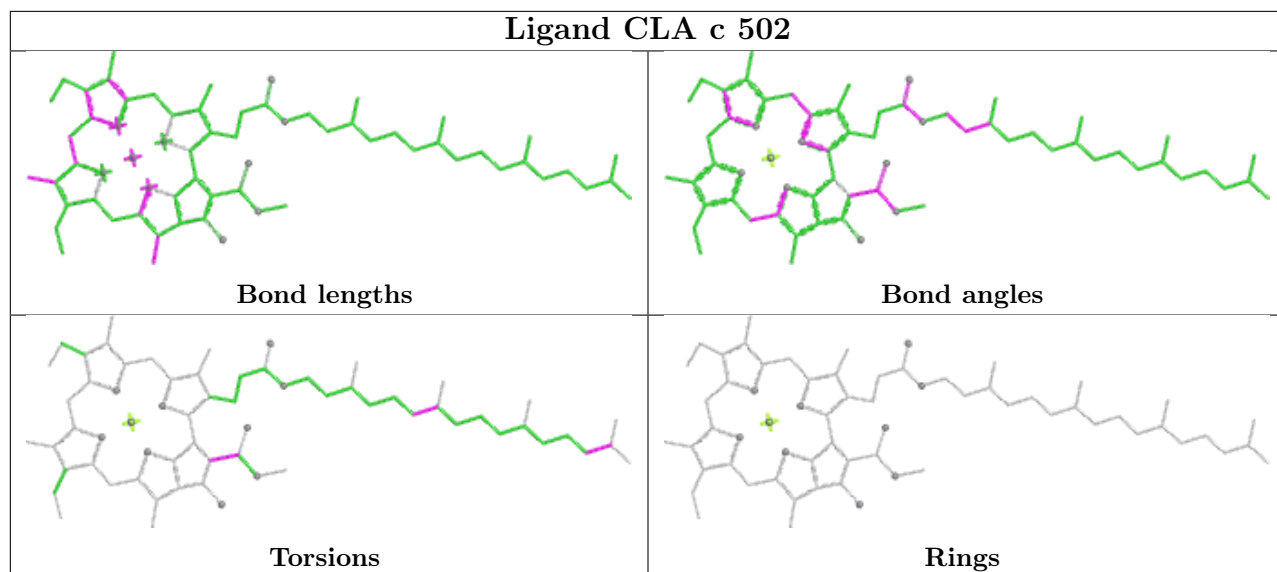




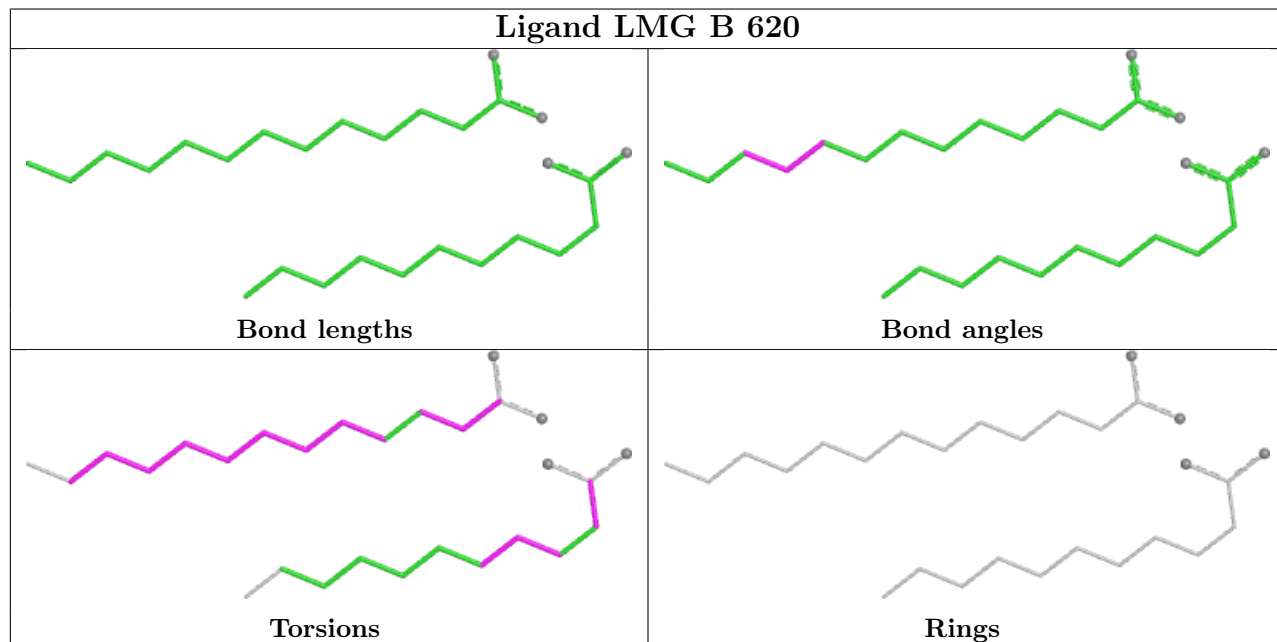




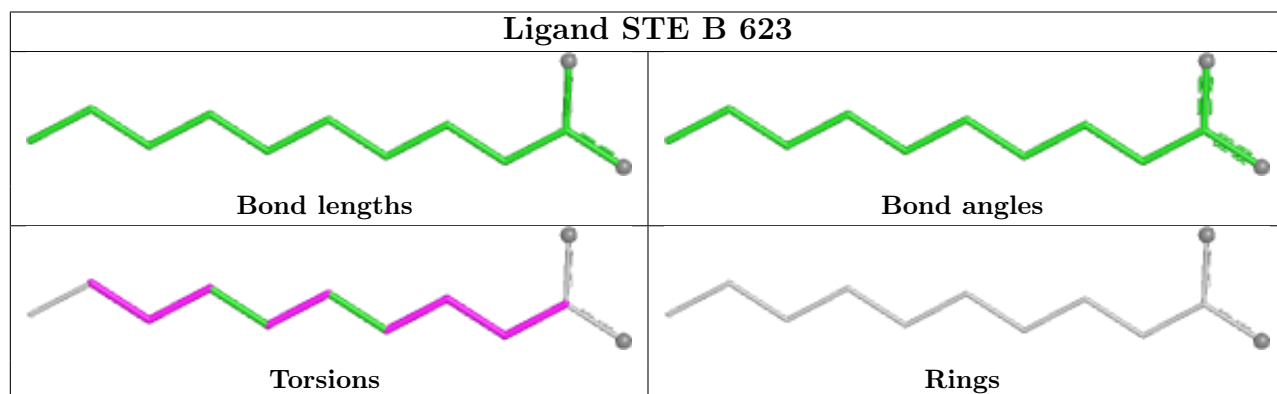
Ligand CLA c 502



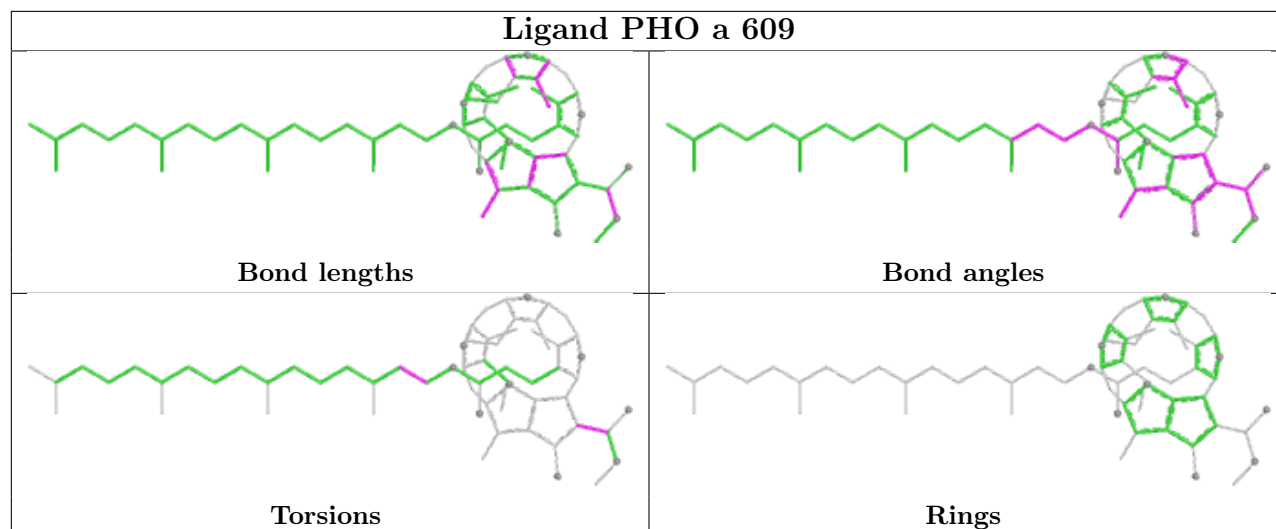
Ligand LMG B 620



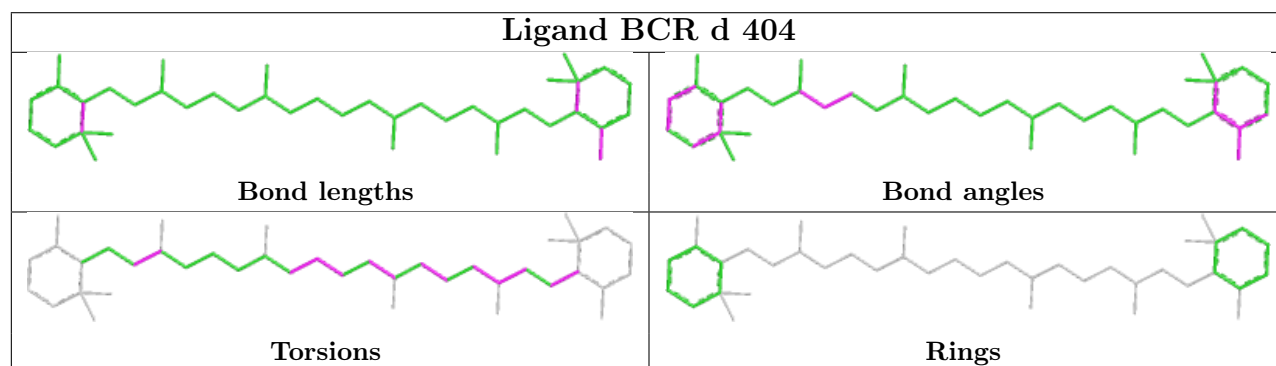
Ligand STE B 623



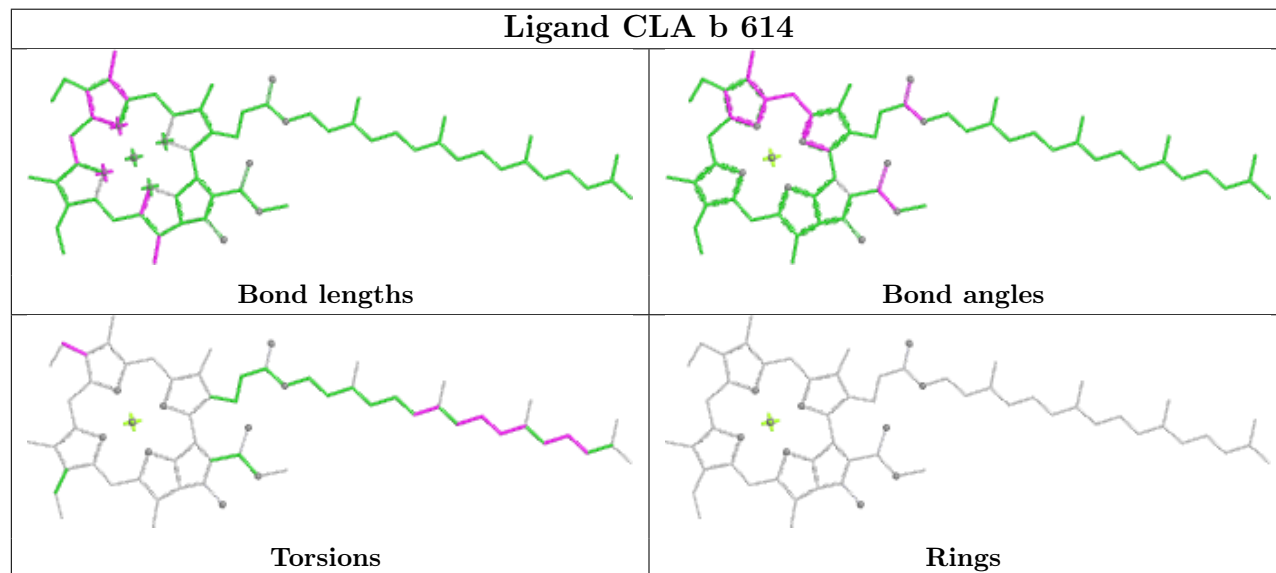
Ligand PHO a 609

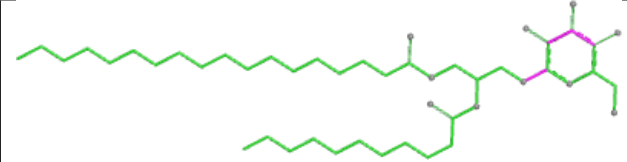
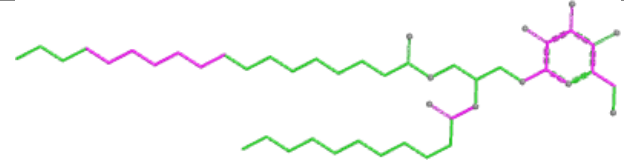
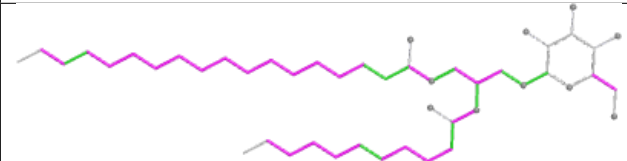
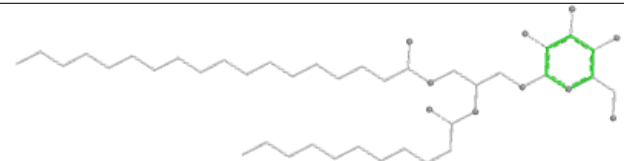
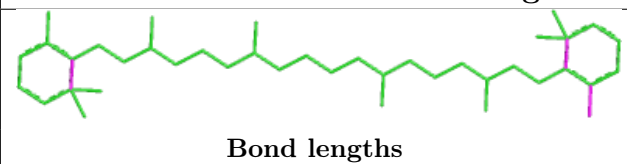
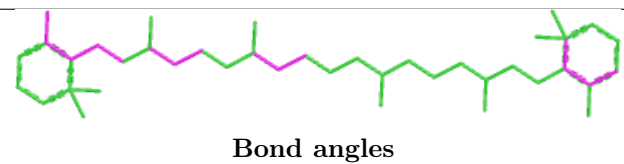
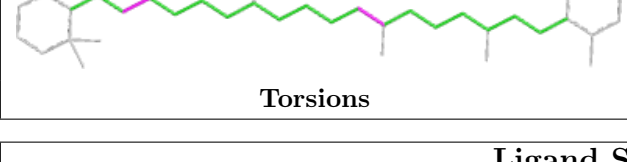
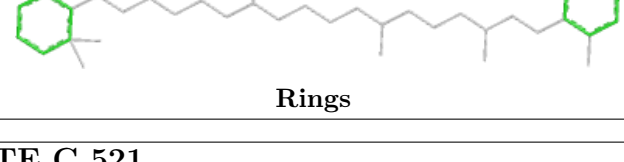
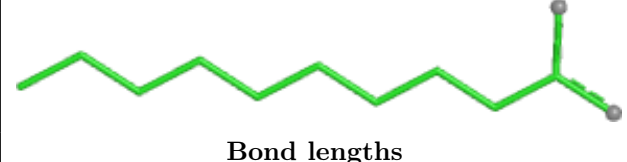
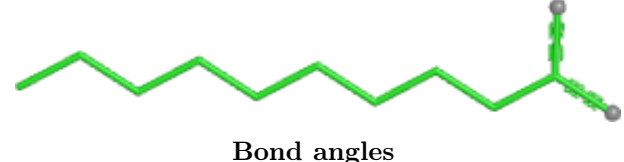
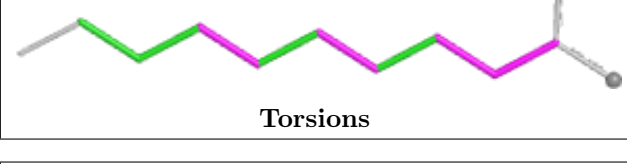
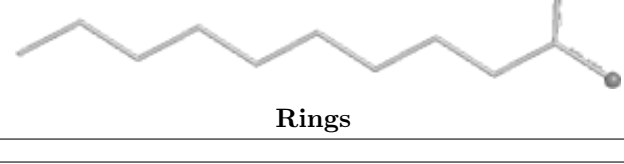
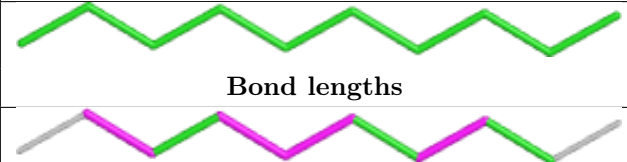
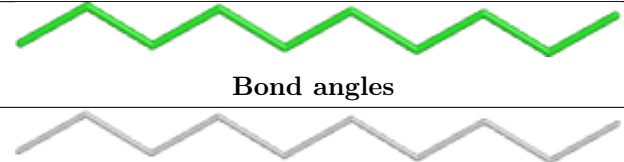
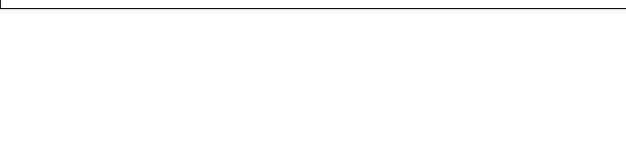
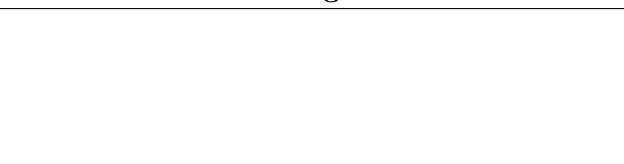


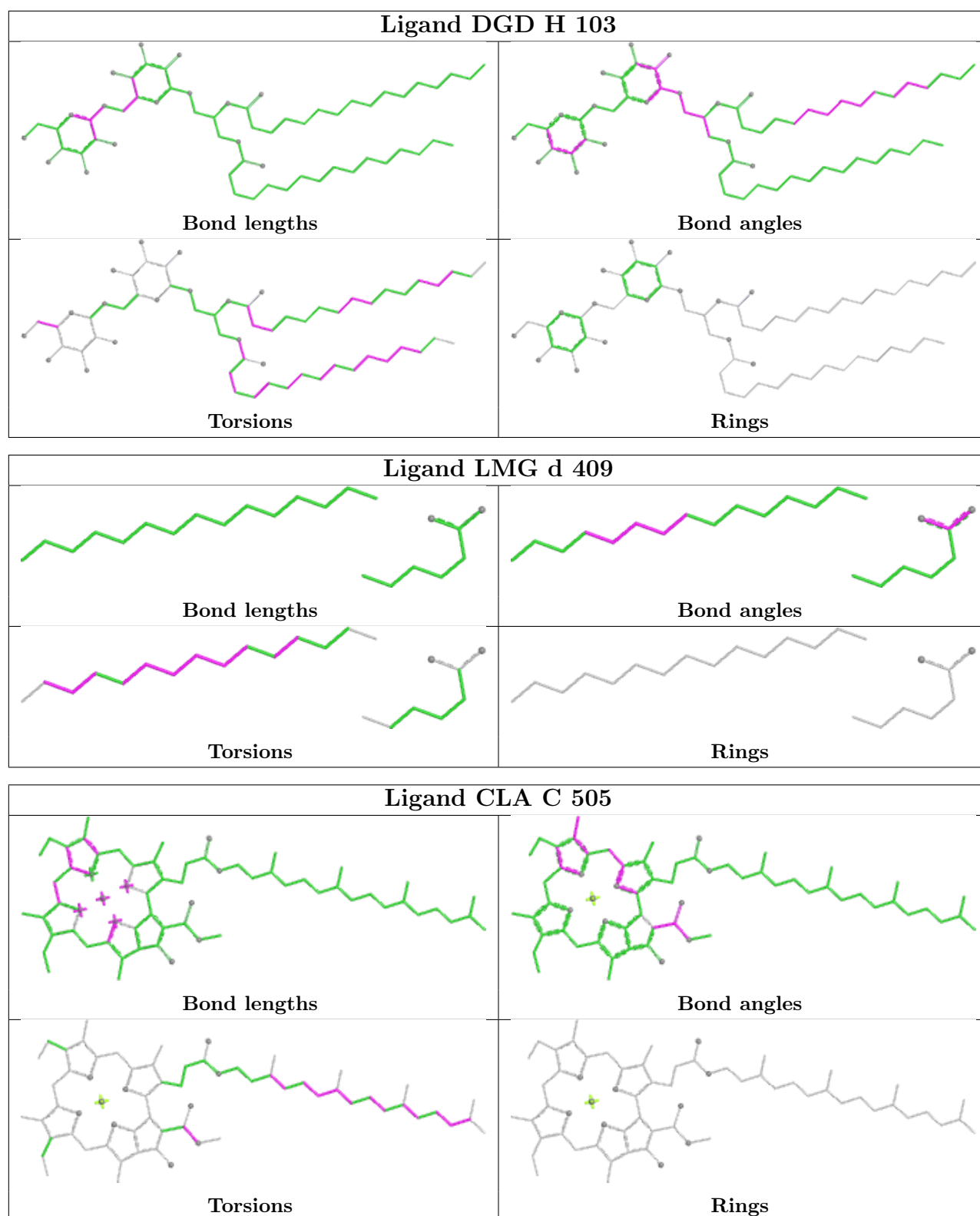
Ligand BCR d 404

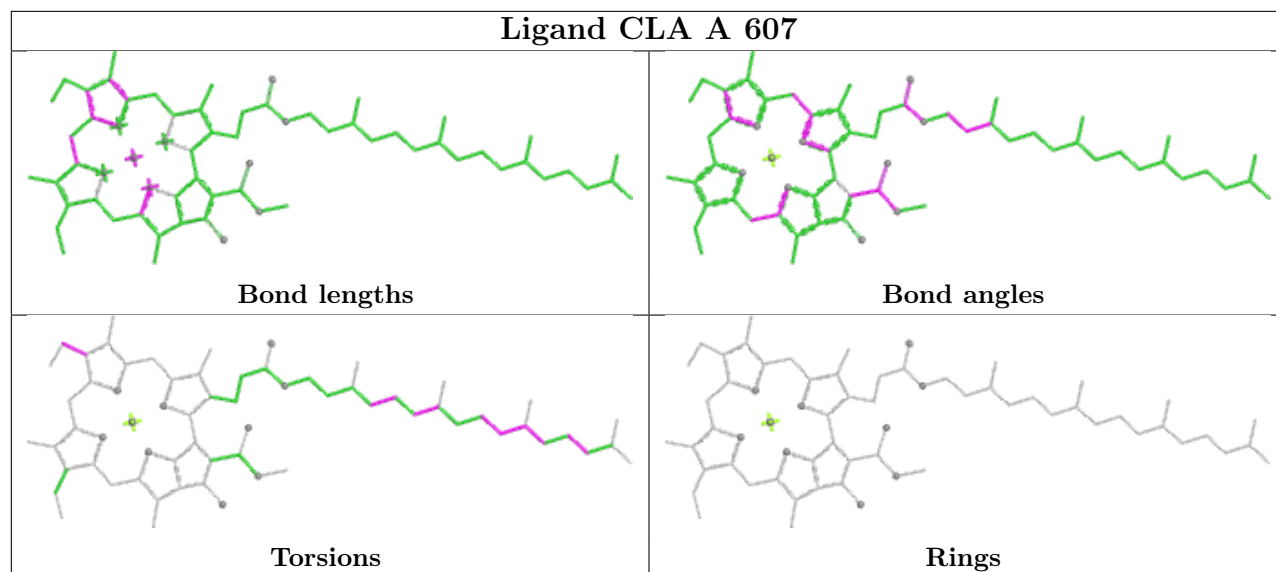
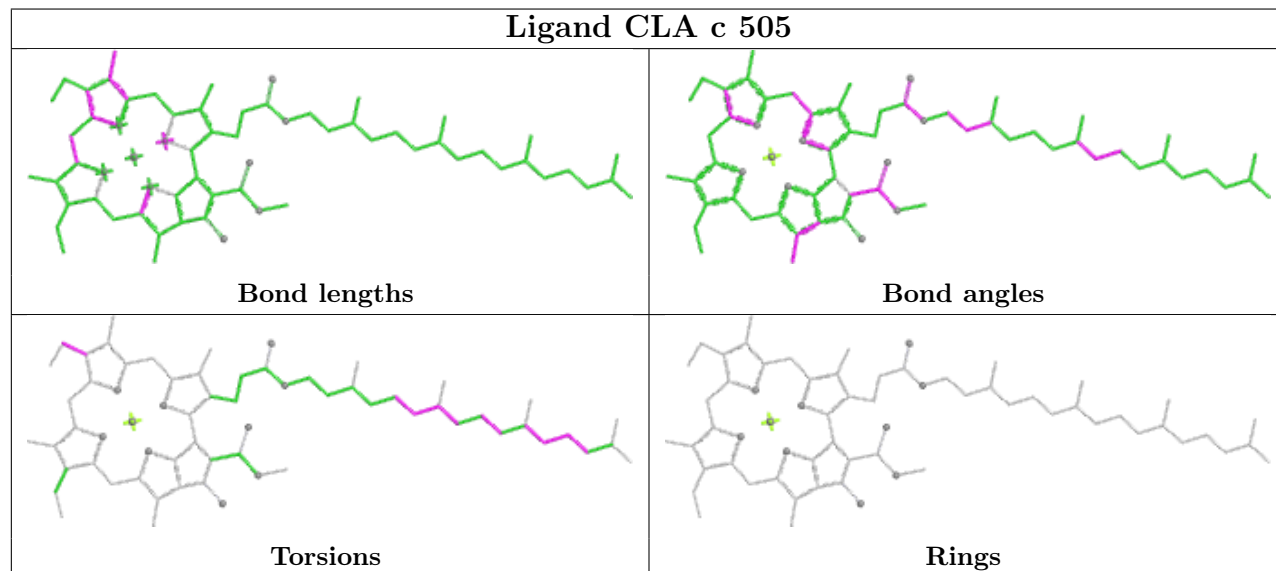


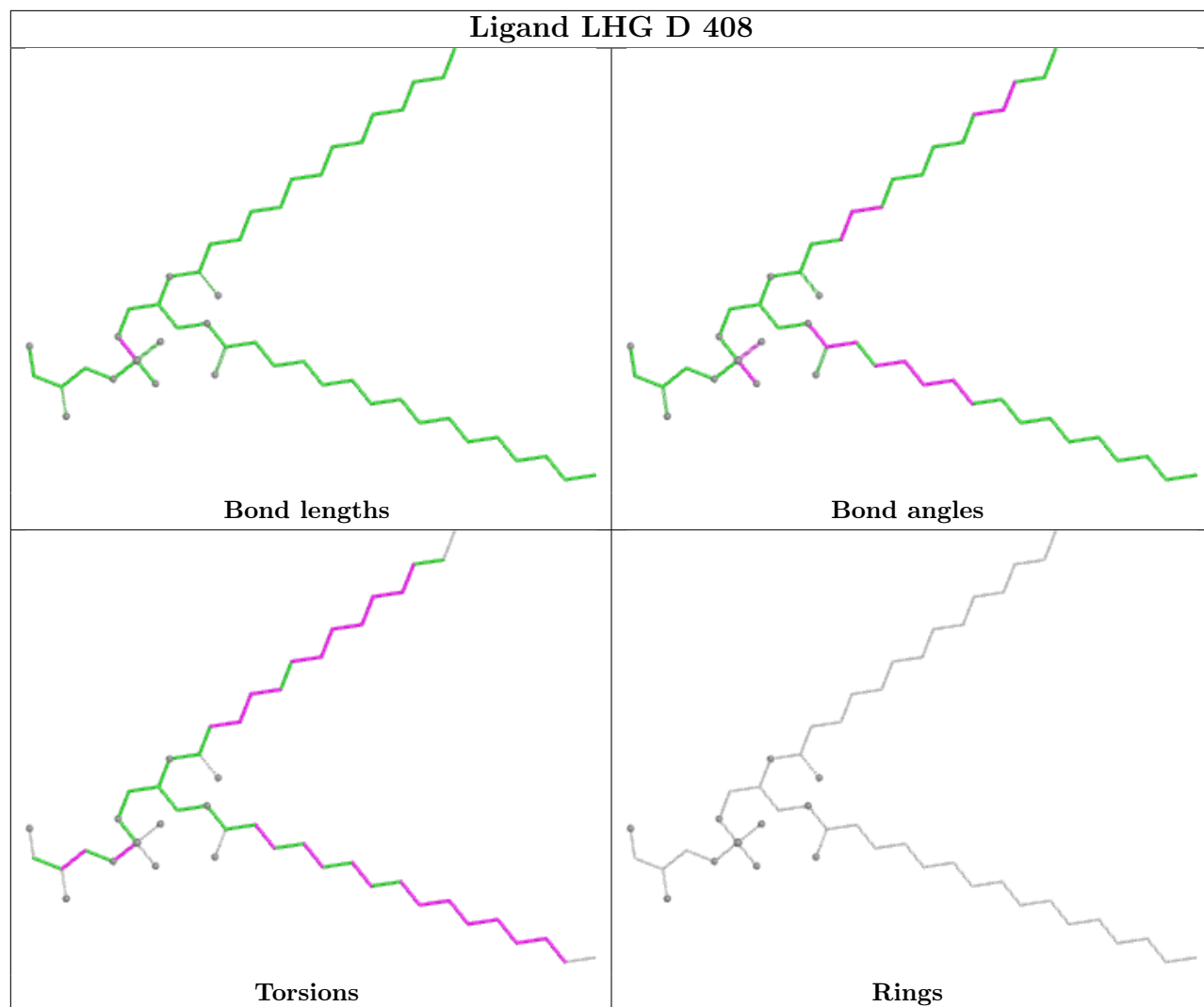
Ligand CLA b 614

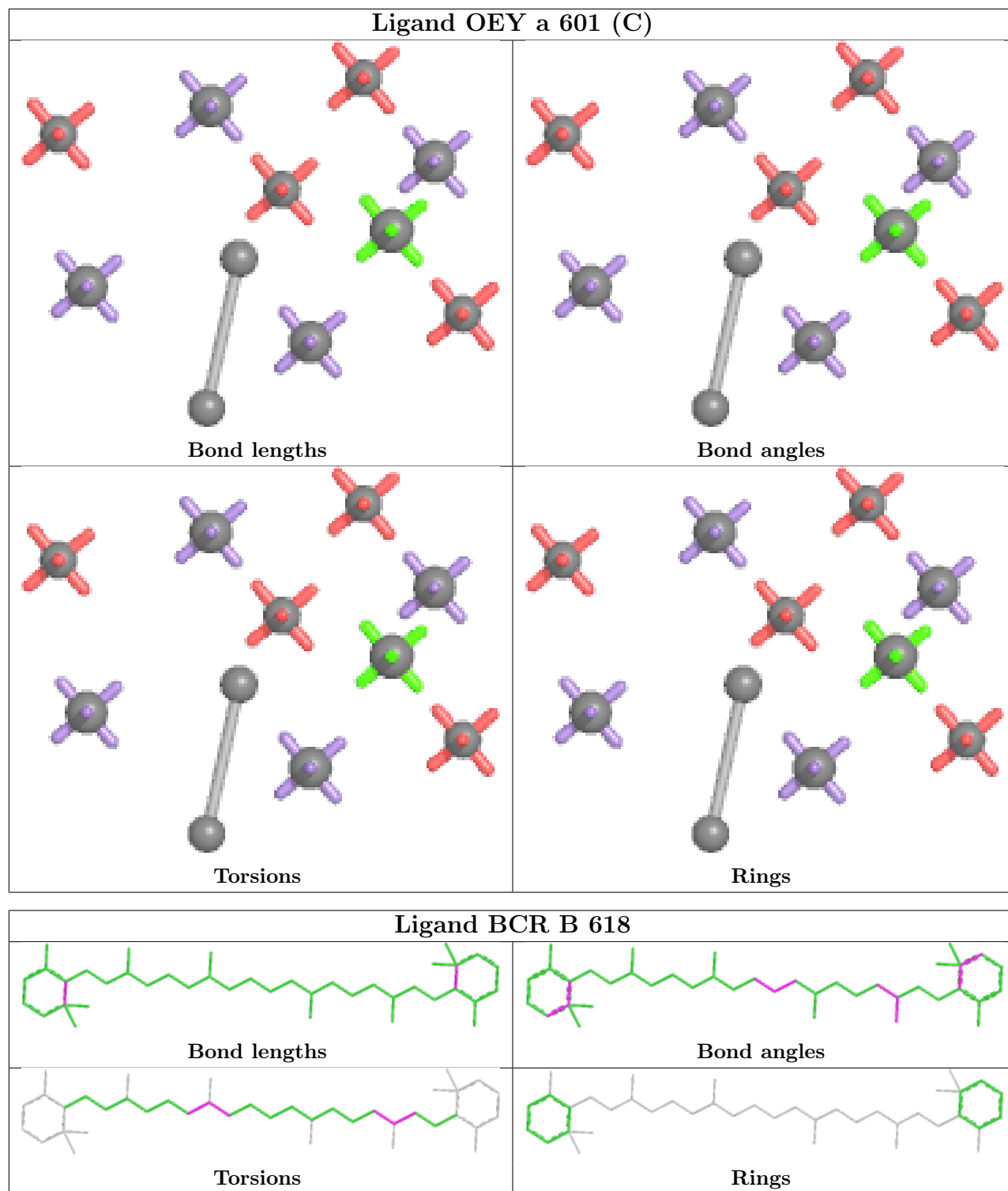


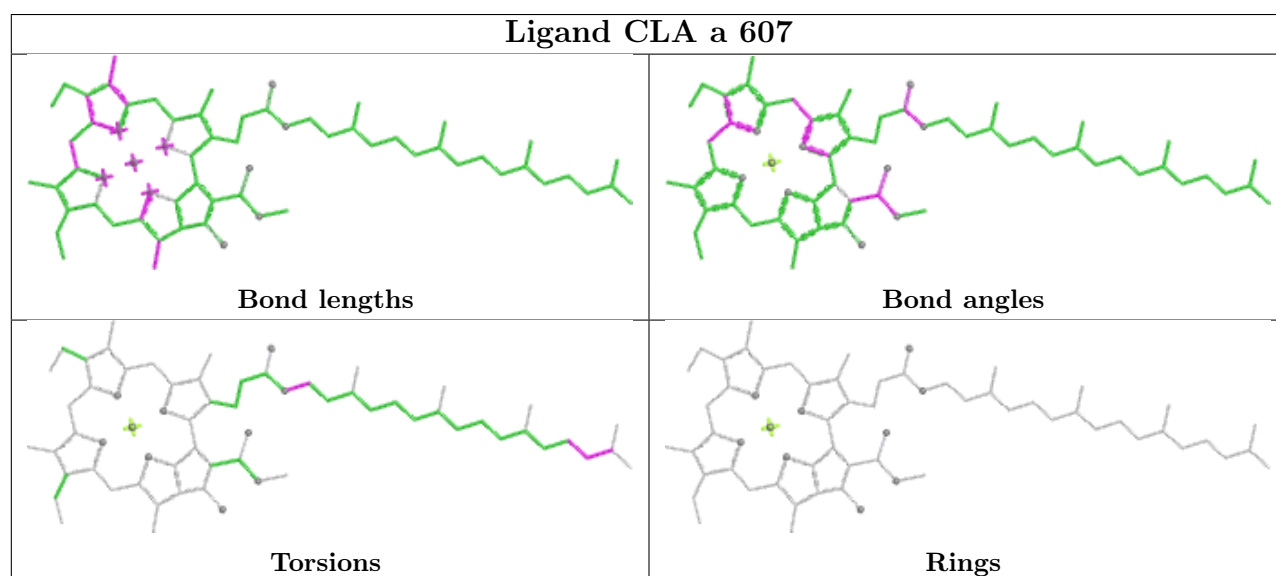
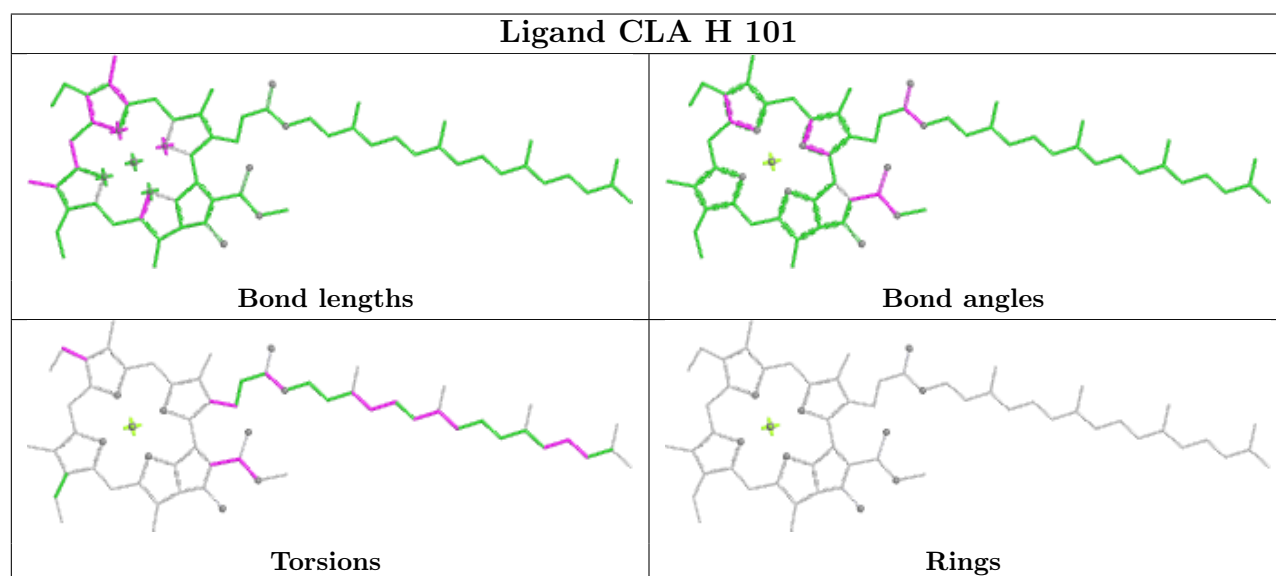
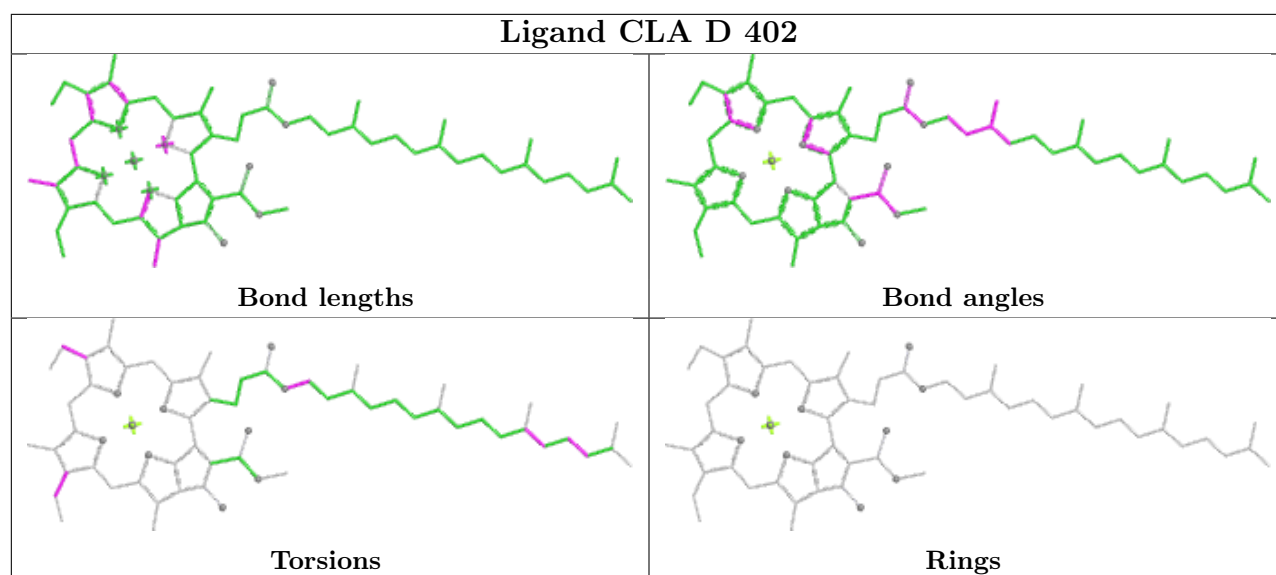
Ligand LMG c 522	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR b 617	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand STE C 521	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand STE t 103	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

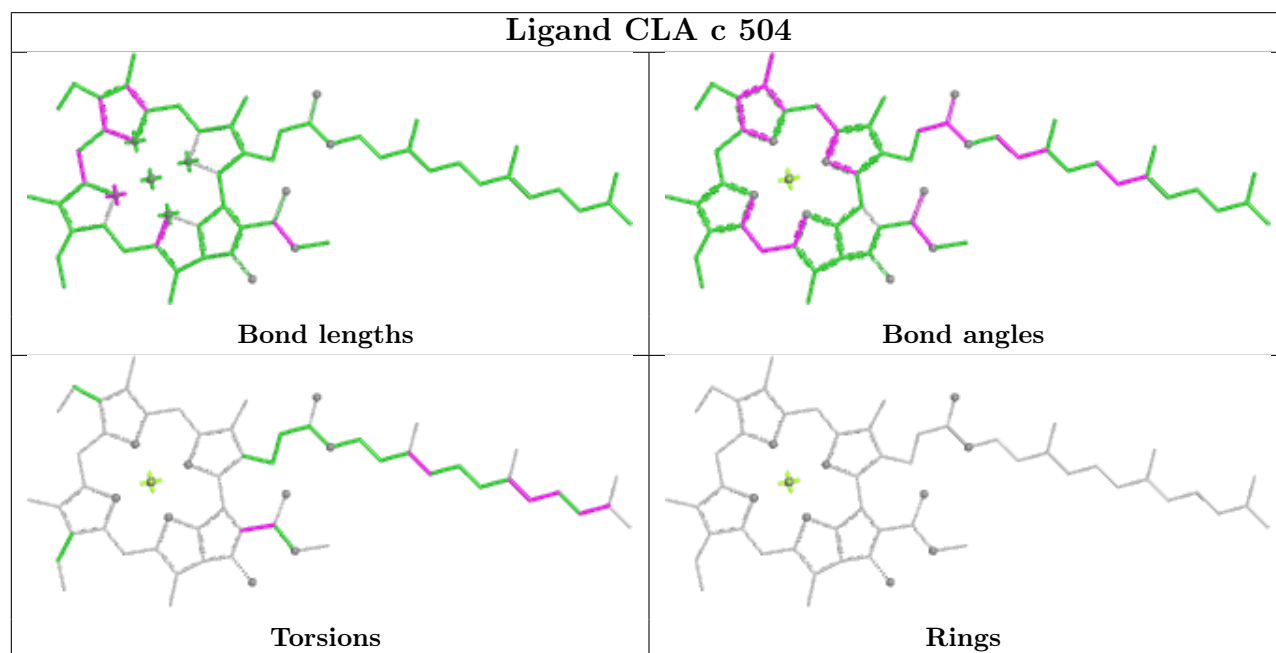
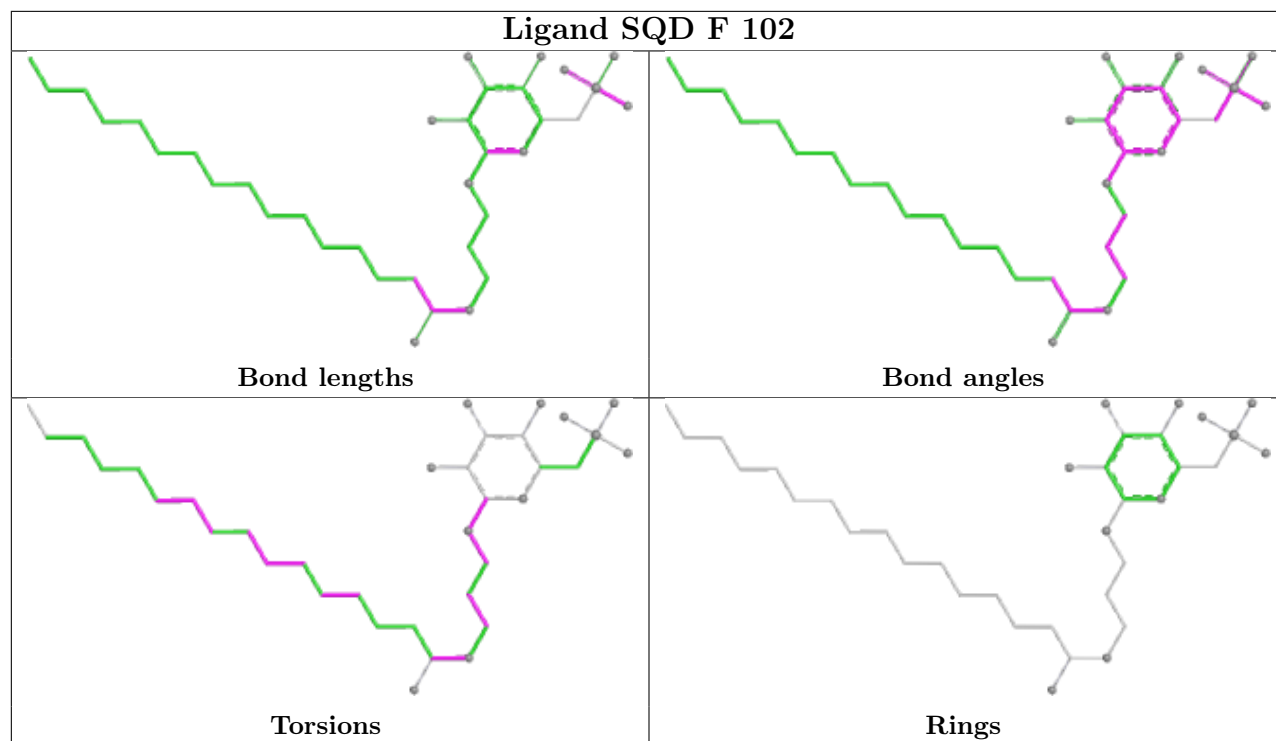


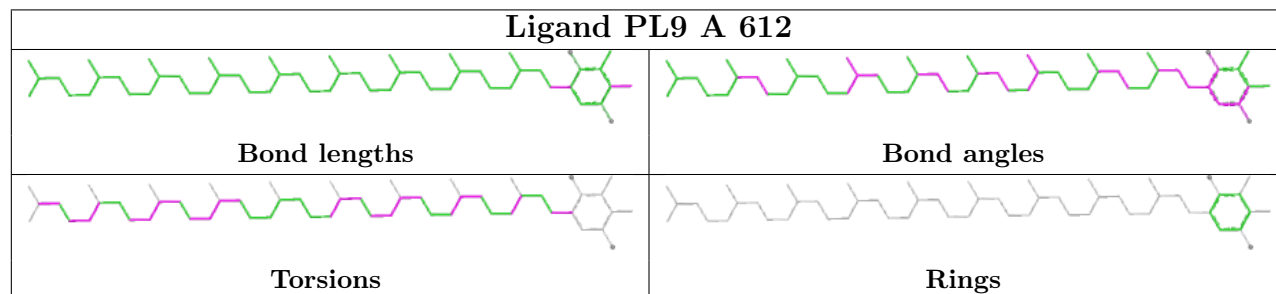
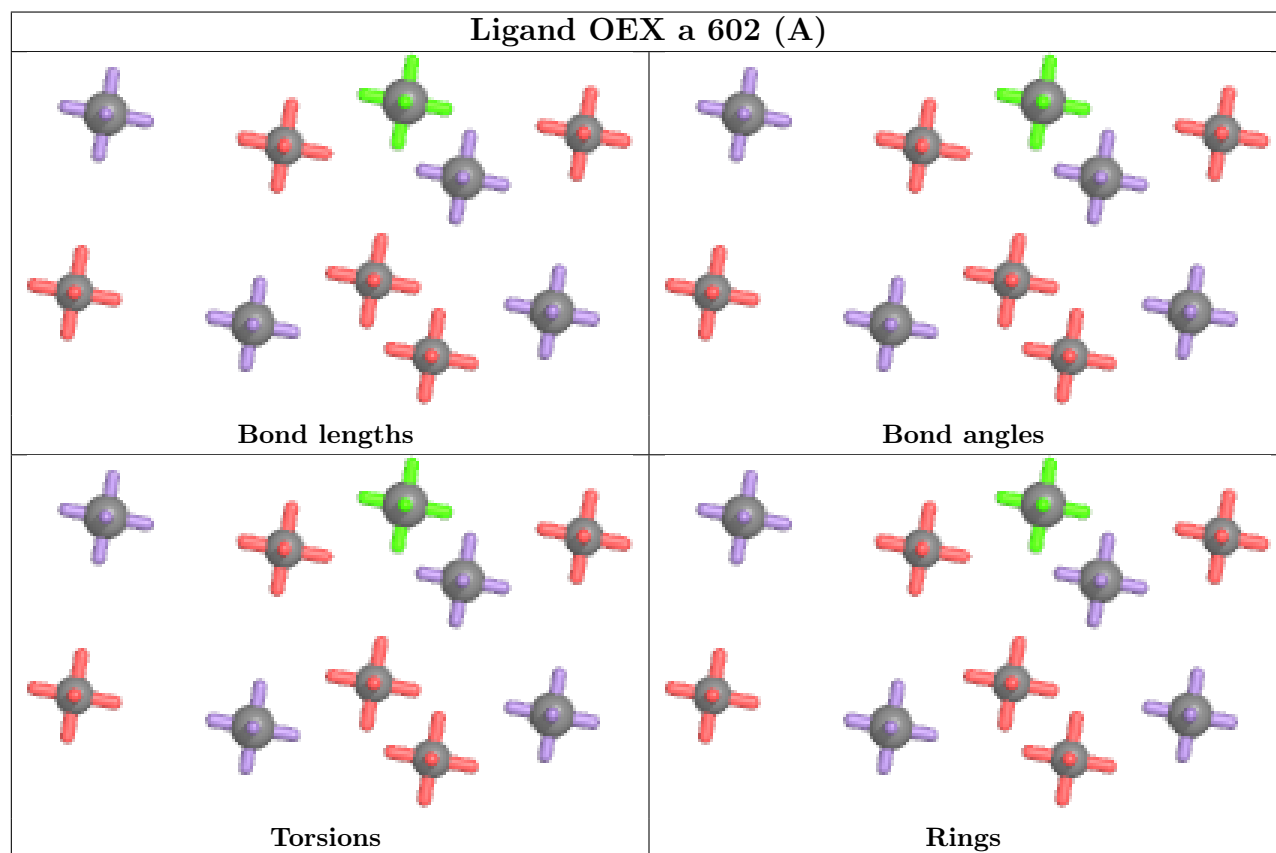
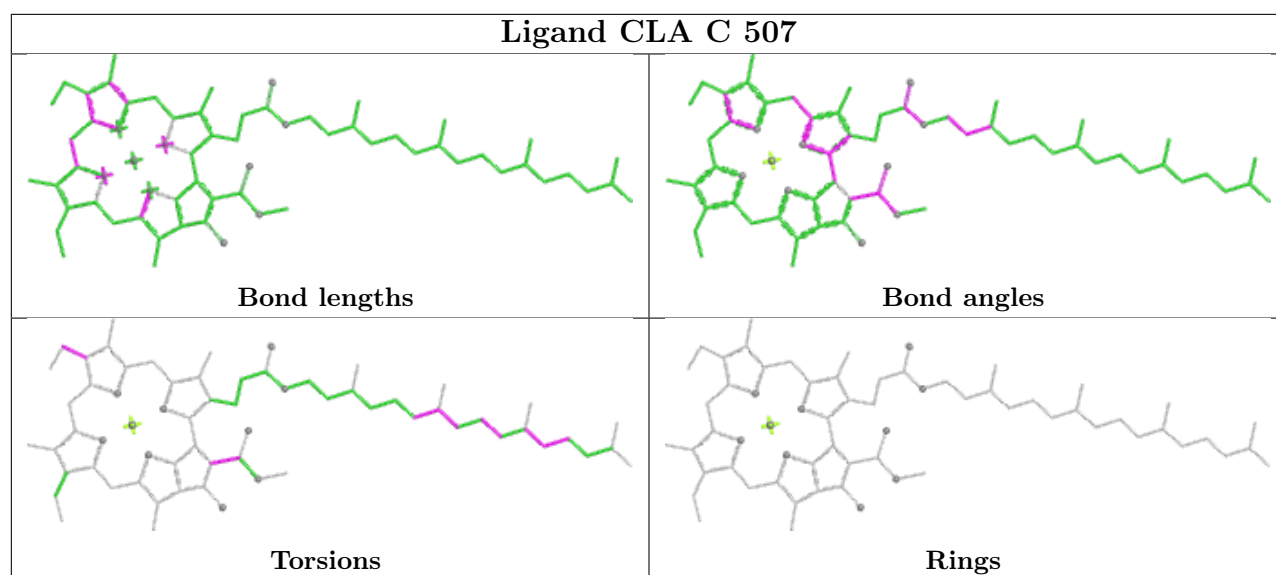
Ligand CLA A 607**Ligand CLA c 505**

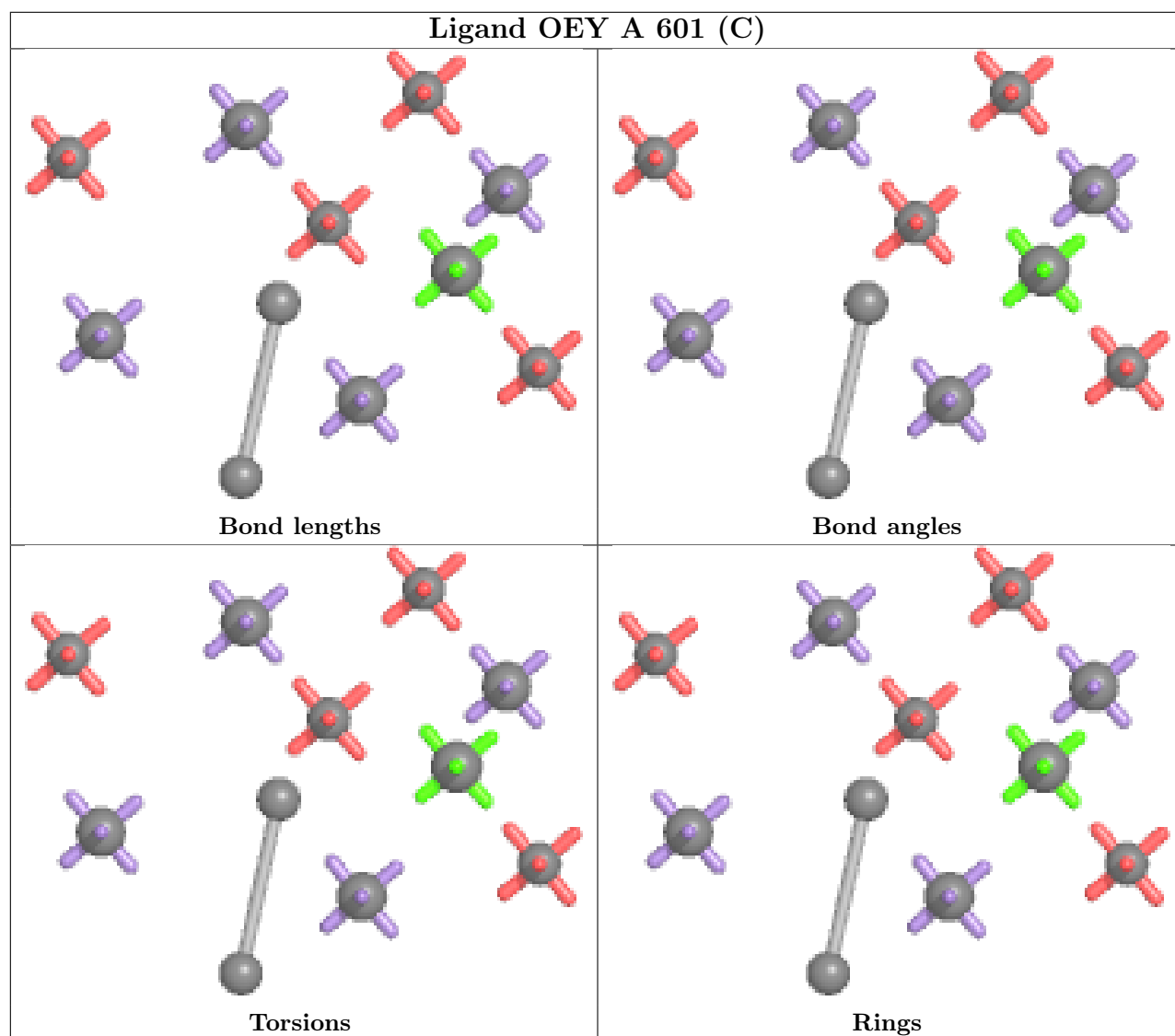
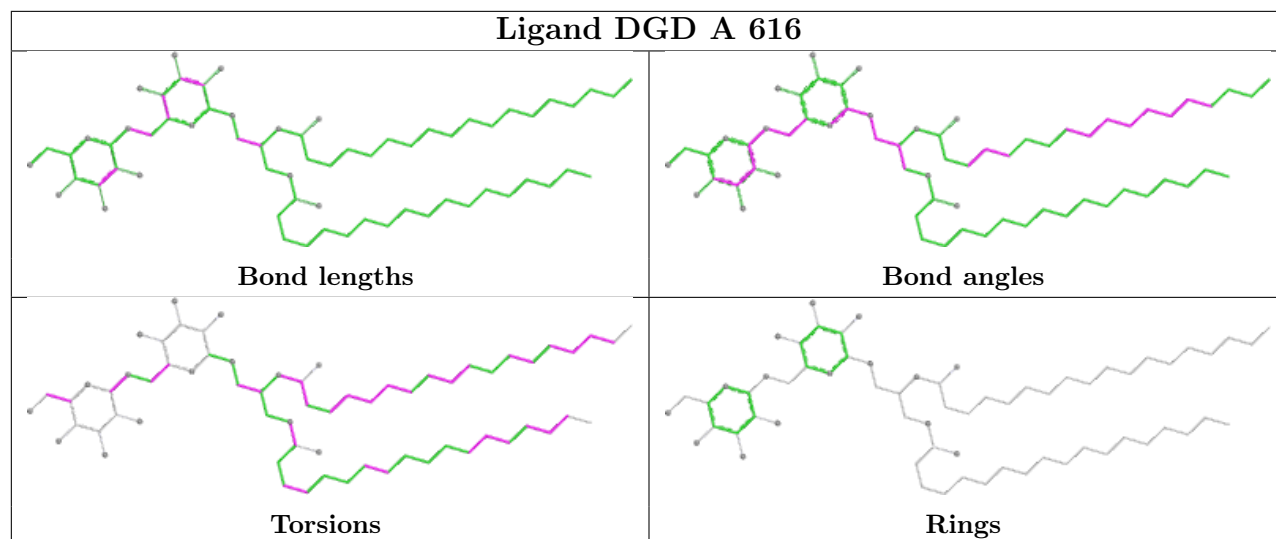


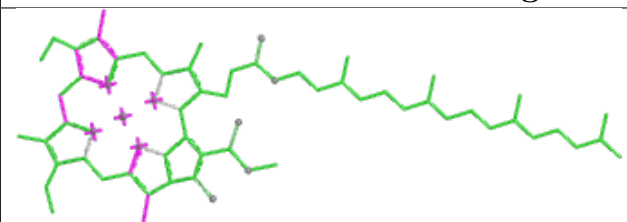
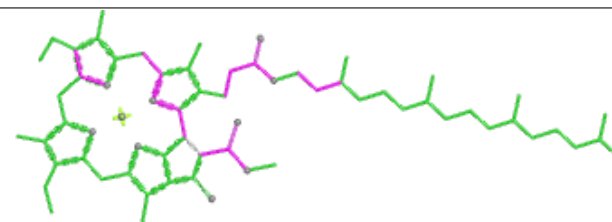
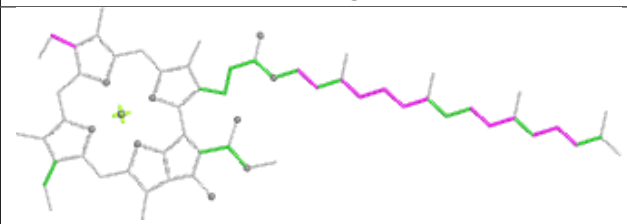
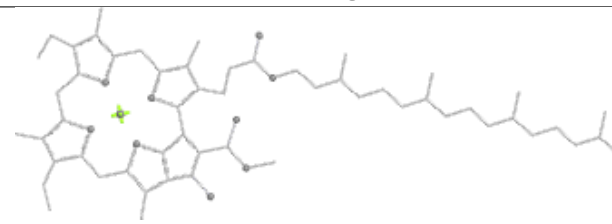



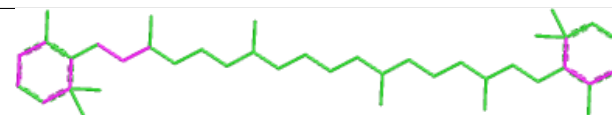
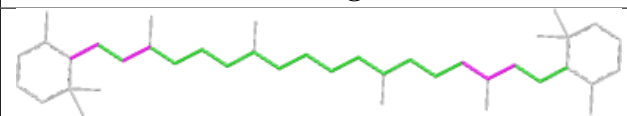
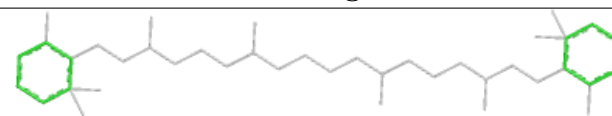



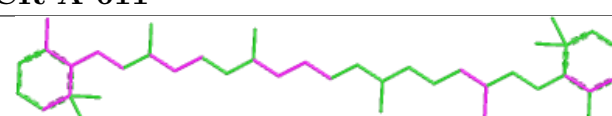

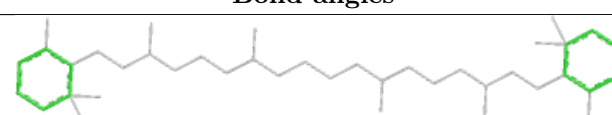




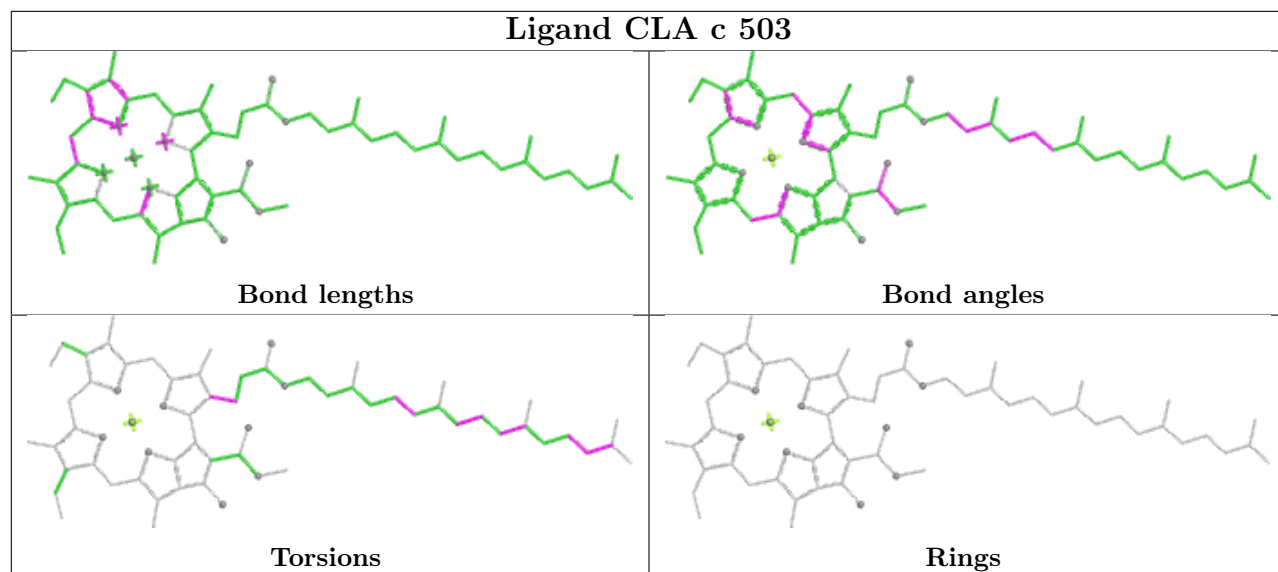


Ligand CLA C 512	
	
Bond lengths	Bond angles
	
Torsions	Rings

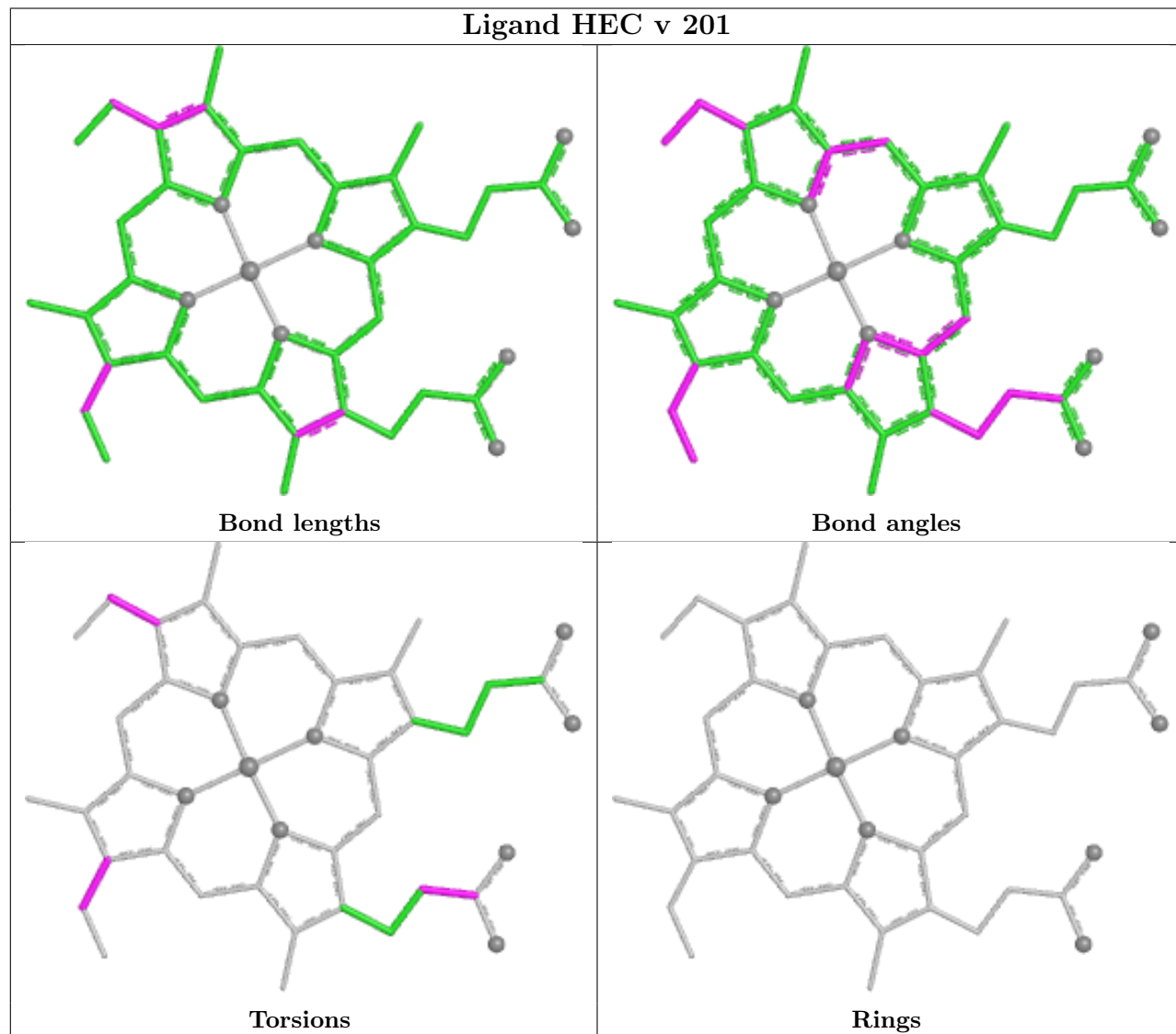
Ligand BCR T 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

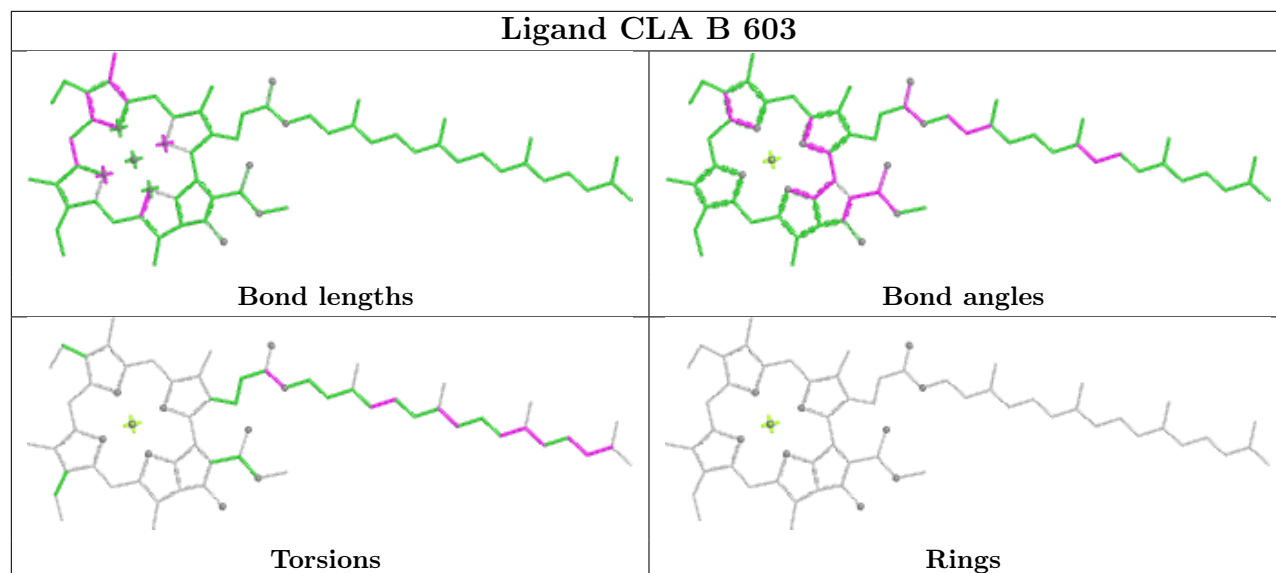
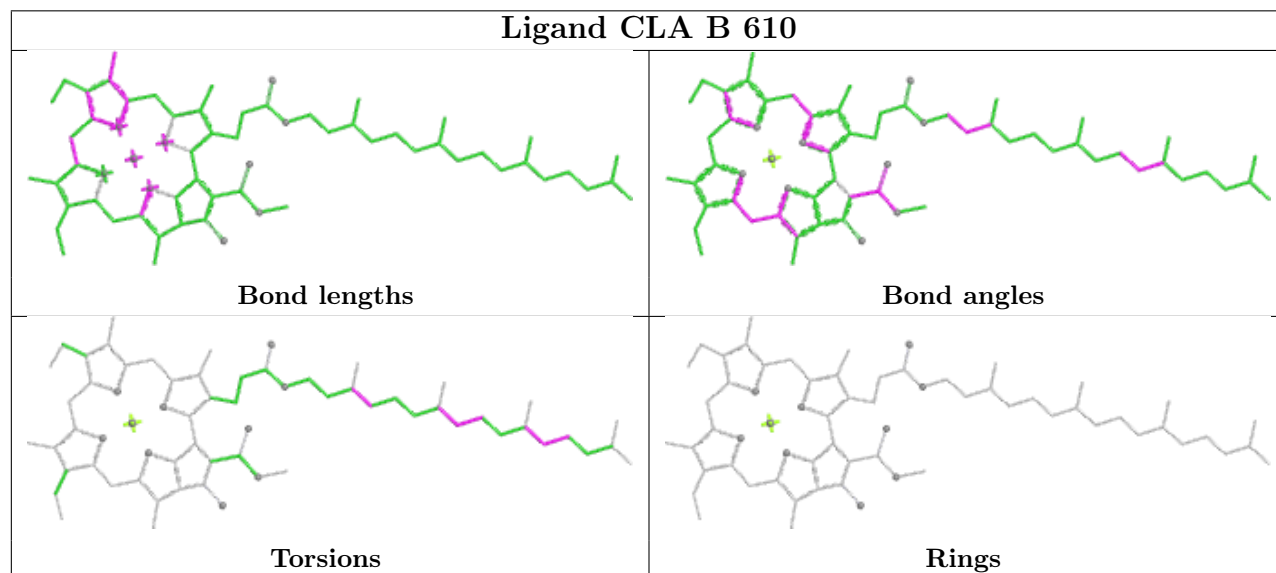
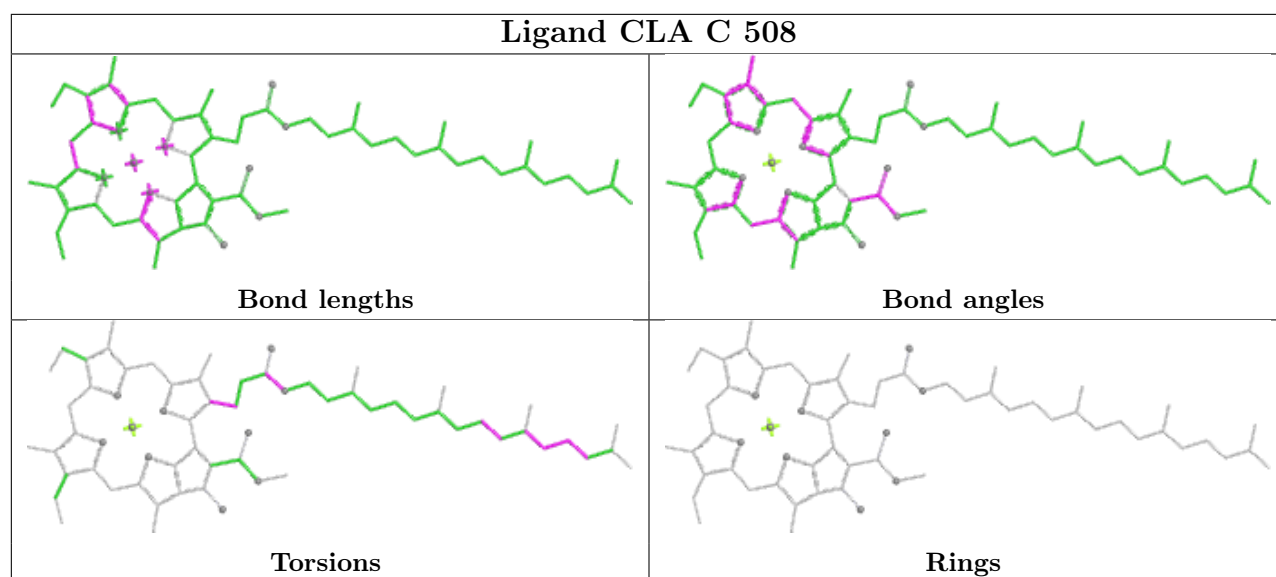
Ligand BCR A 611	
	
Bond lengths	Bond angles
	
Torsions	Rings

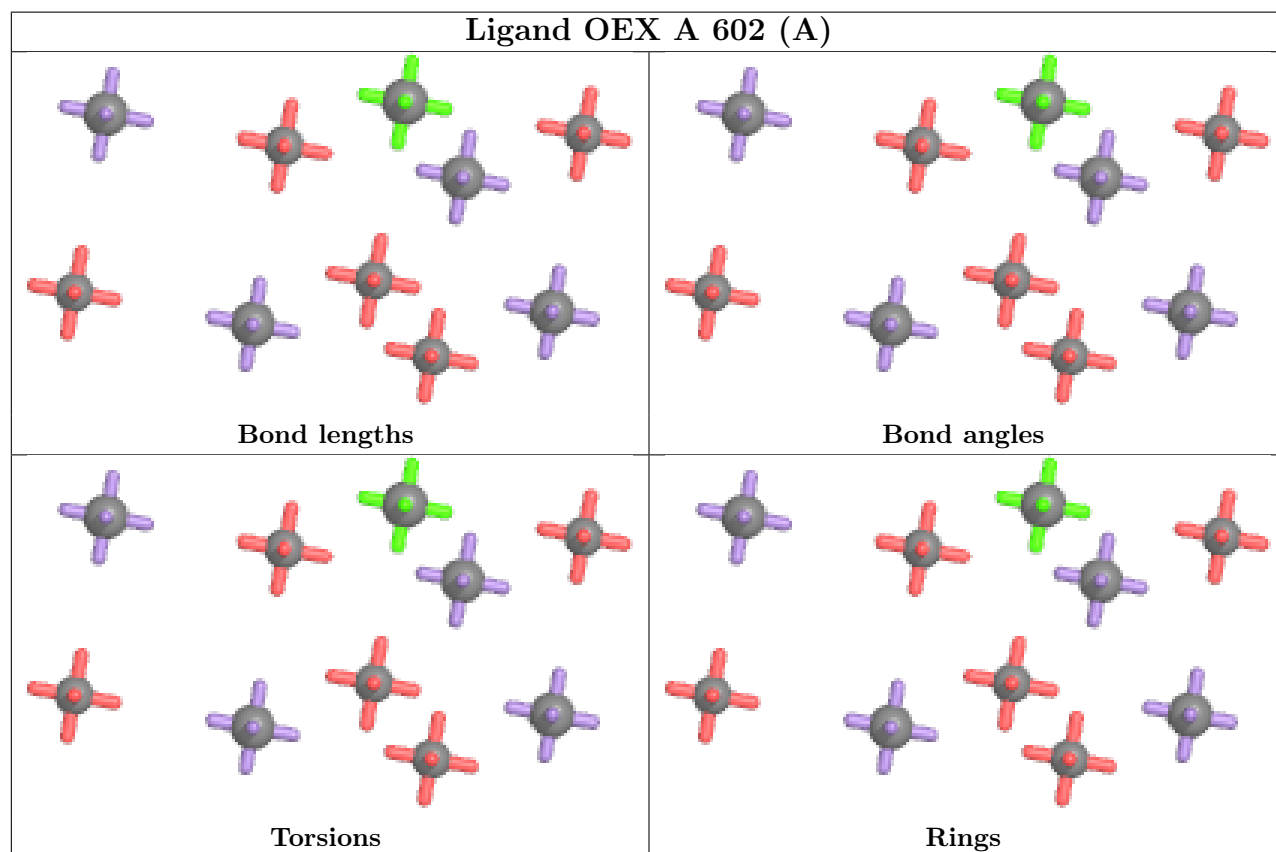
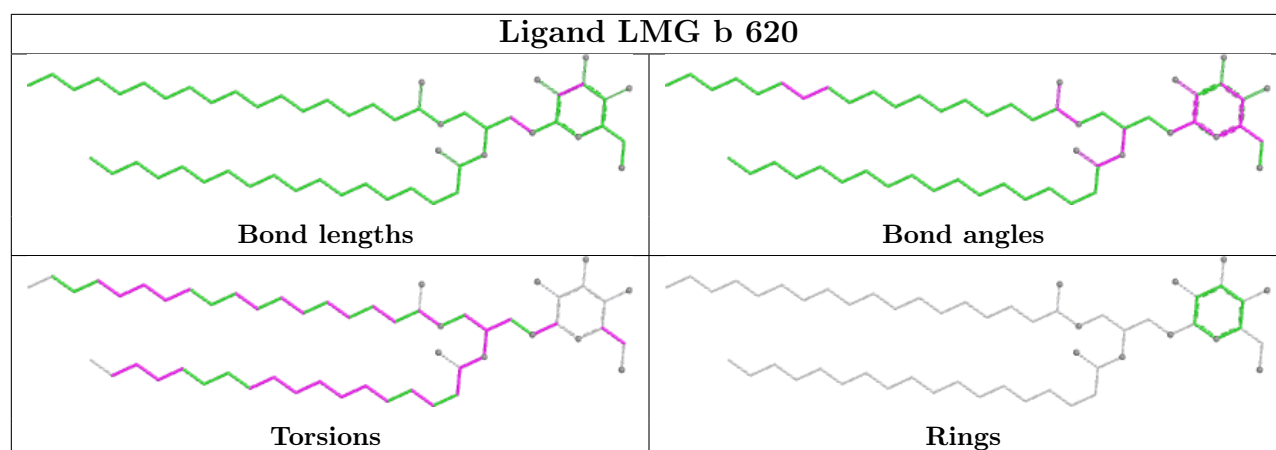
Ligand CLA c 503

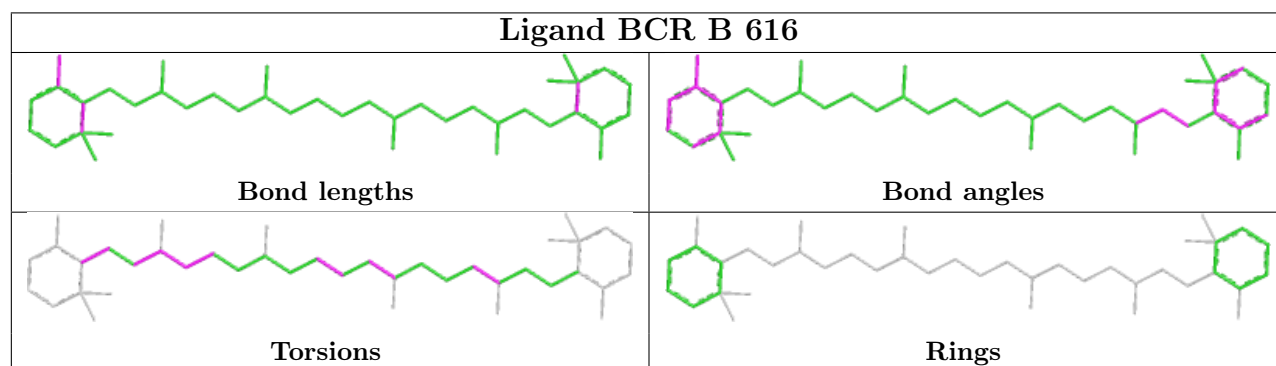
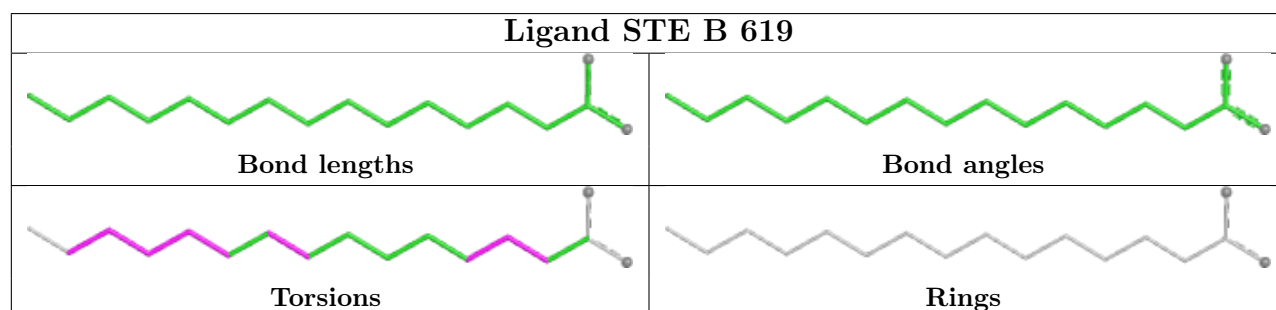
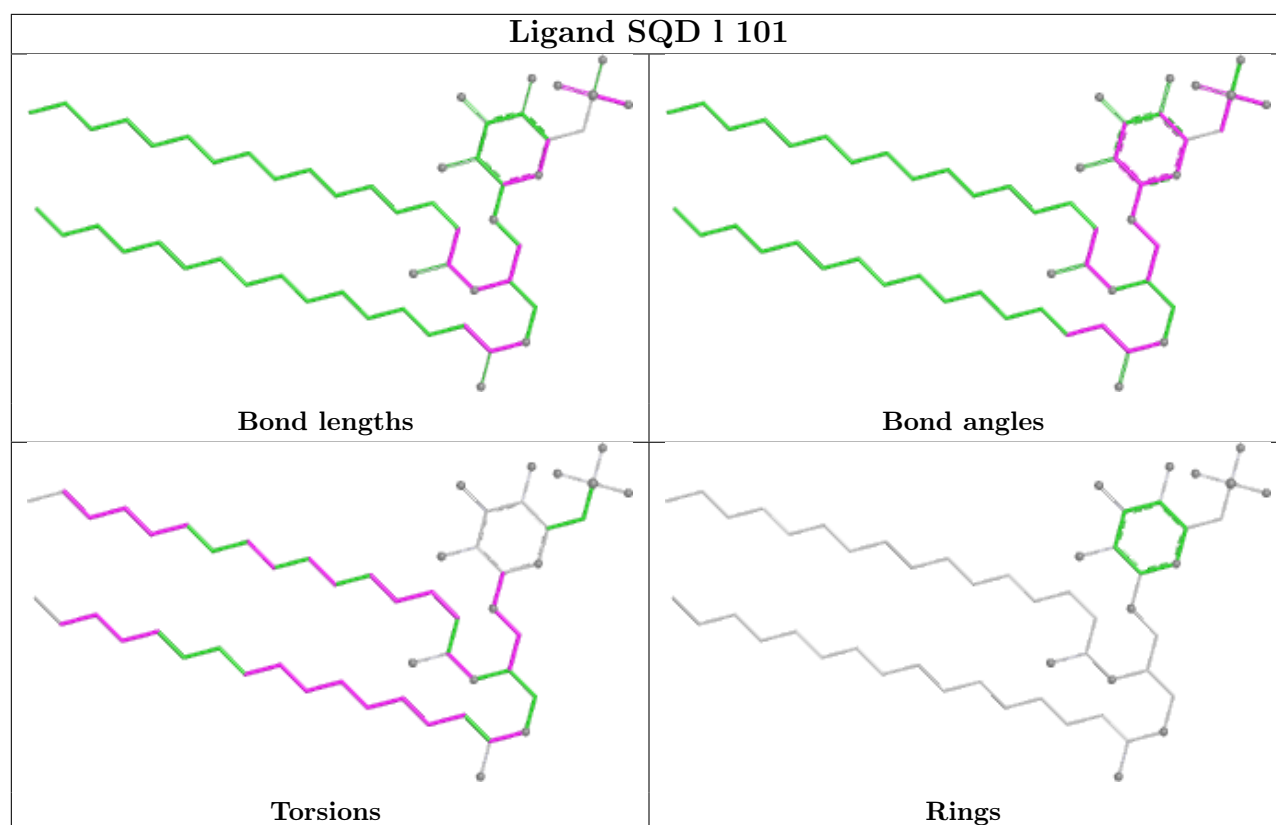


Ligand HEC v 201

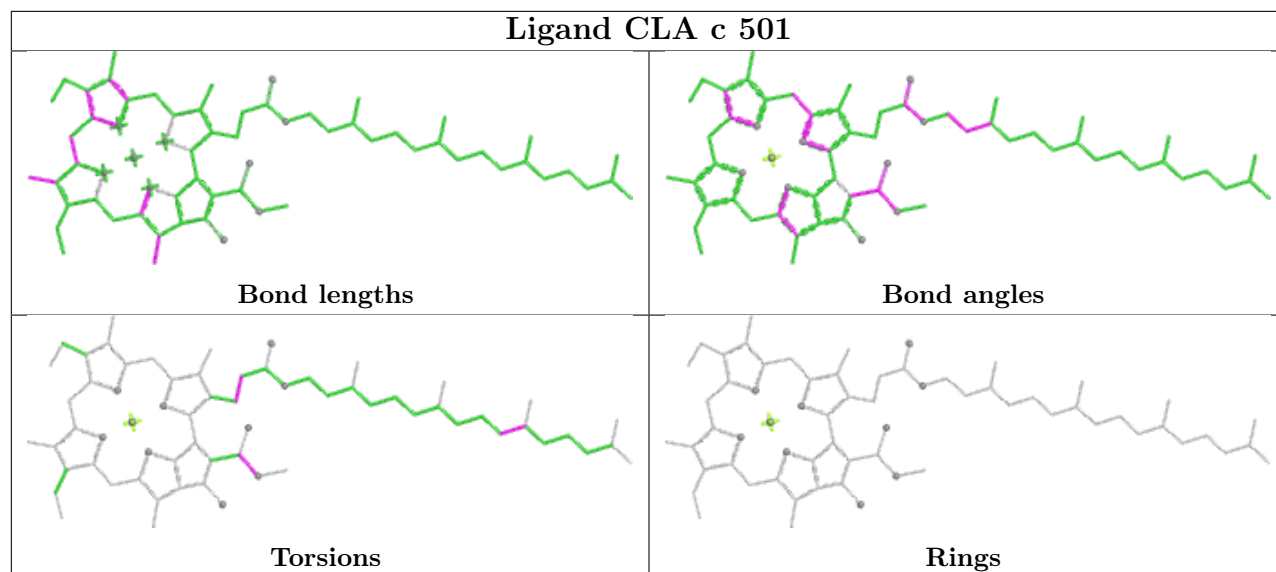




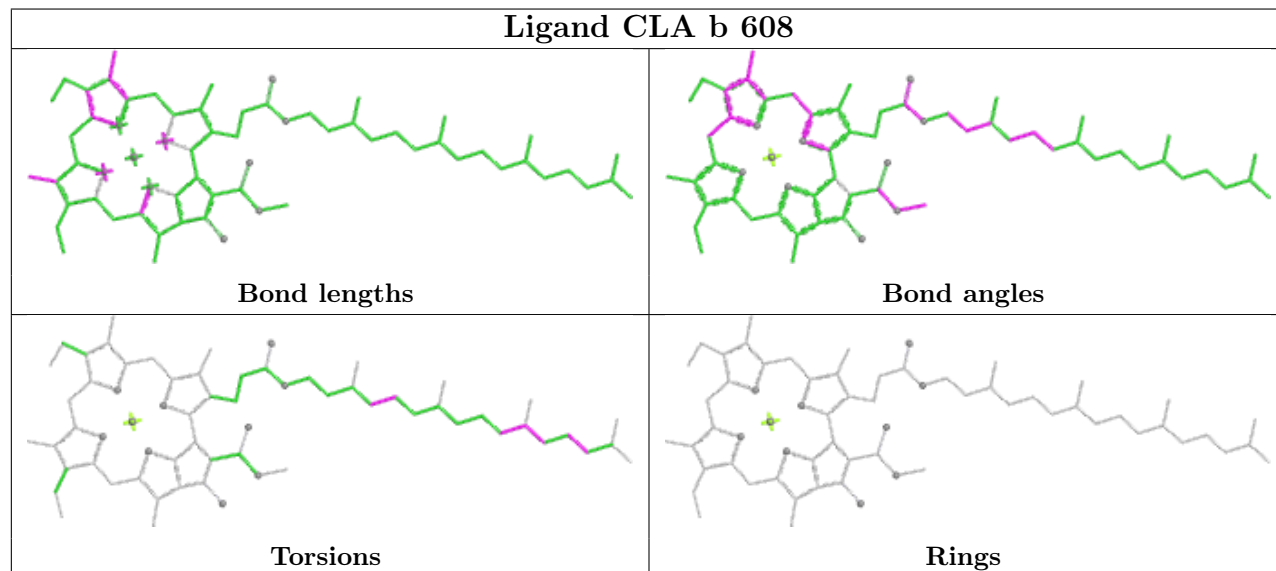




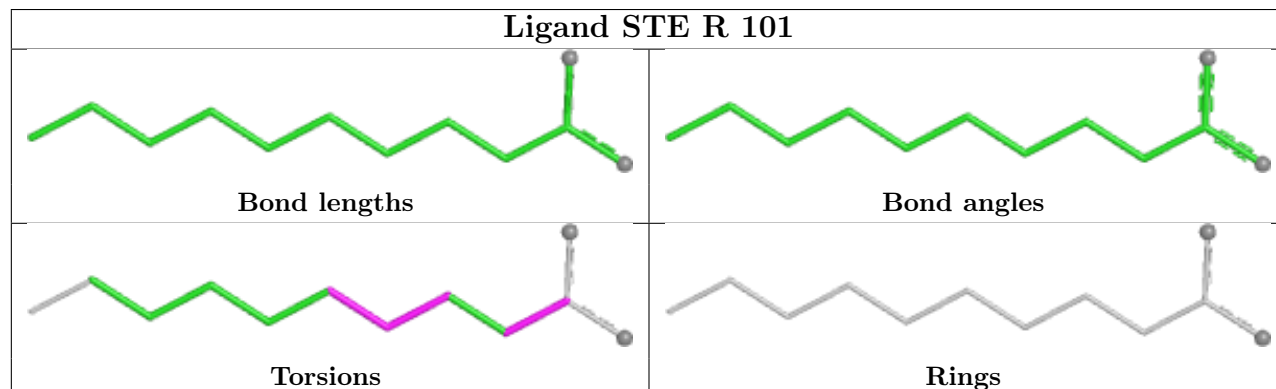
Ligand CLA c 501

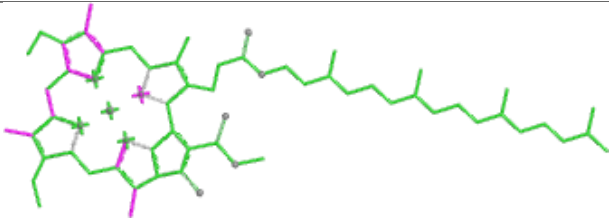
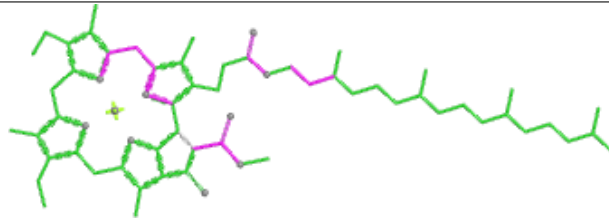
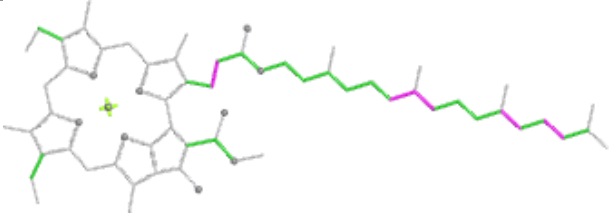
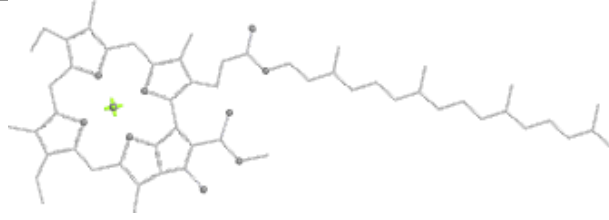






Ligand CLA b 608


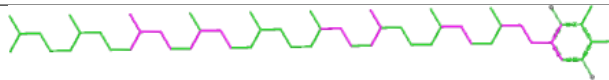
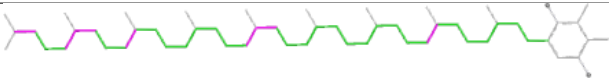



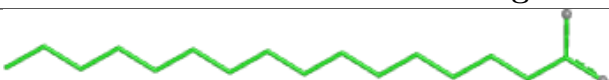
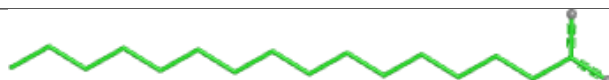
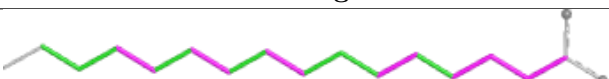
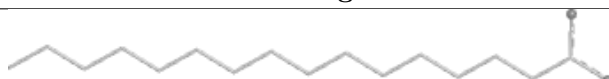
Ligand STE R 101

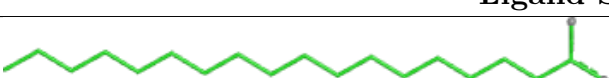
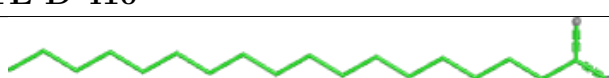
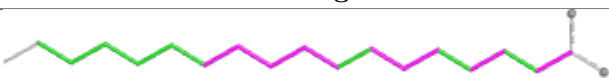
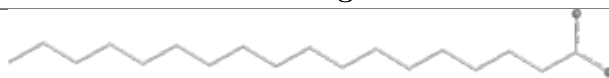


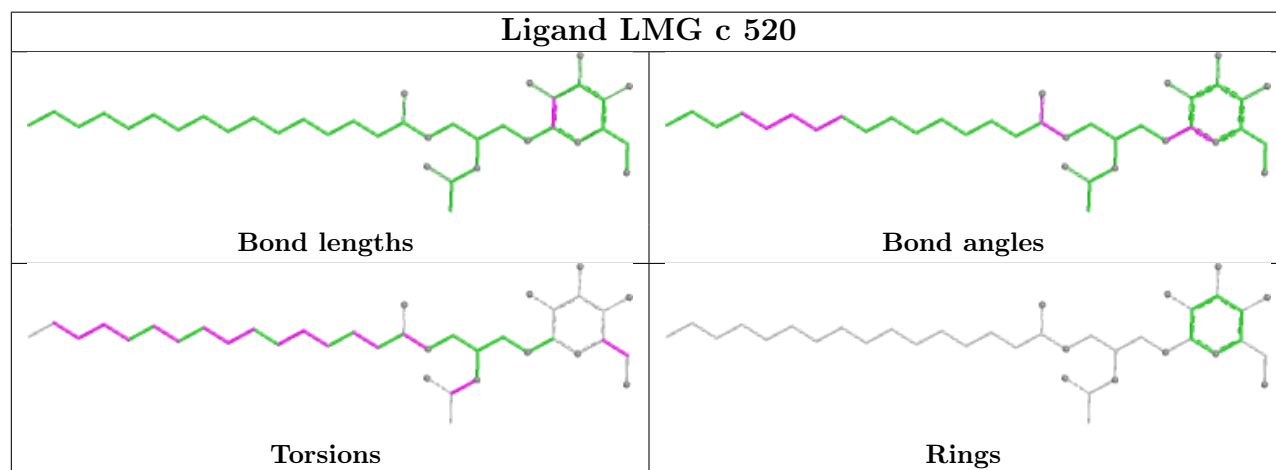
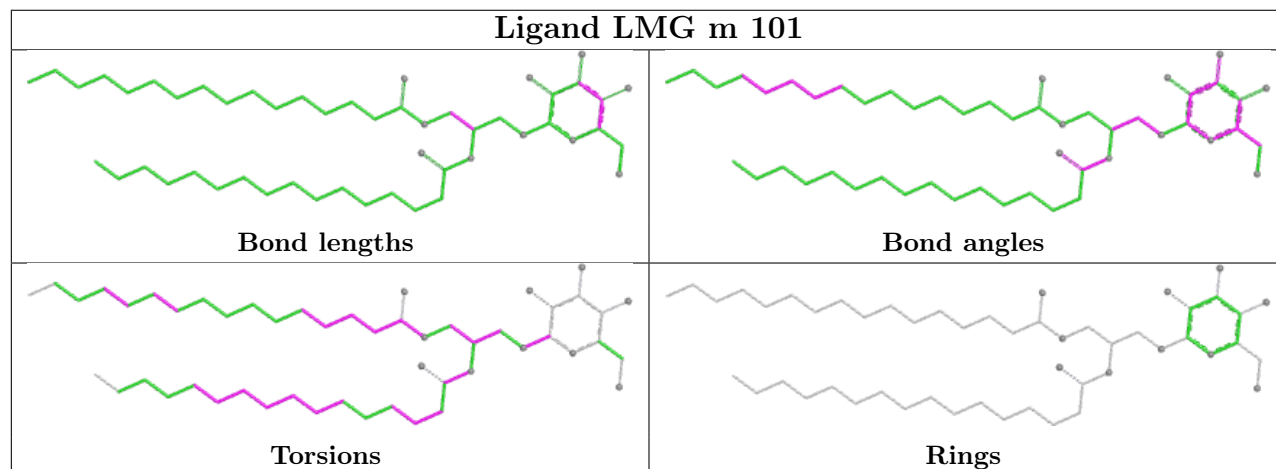
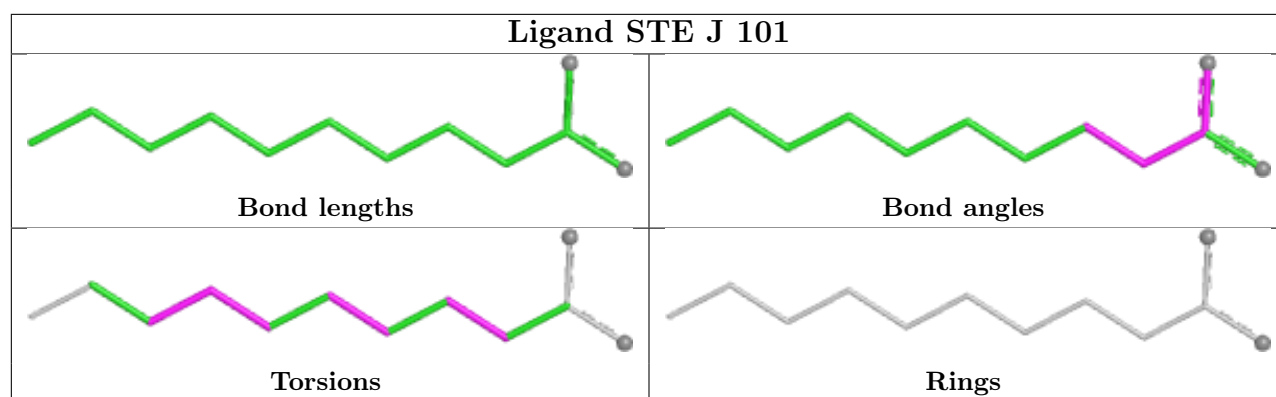
Ligand CLA b 605			
			
Bond lengths		Bond angles	
			
Torsions		Rings	

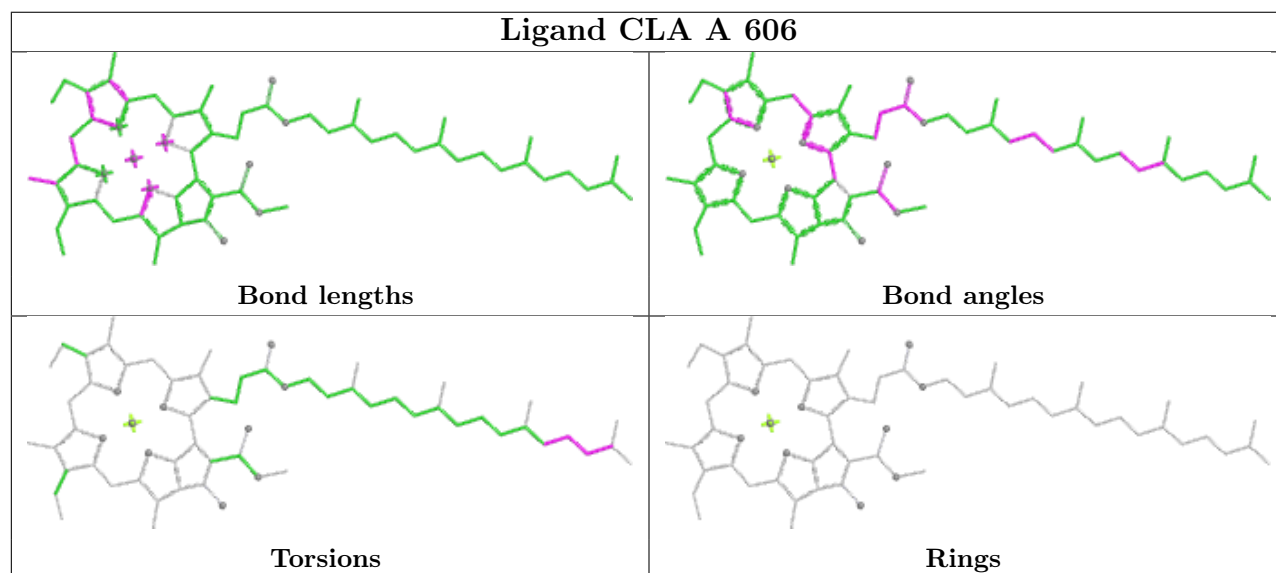
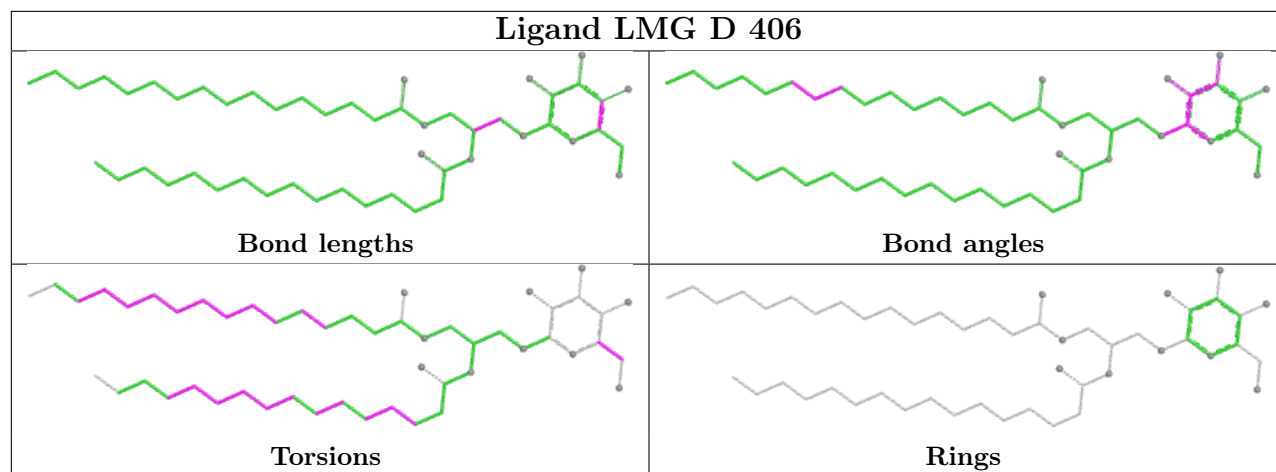
Ligand STE l 103			
			
Bond lengths		Bond angles	
			
Torsions		Rings	

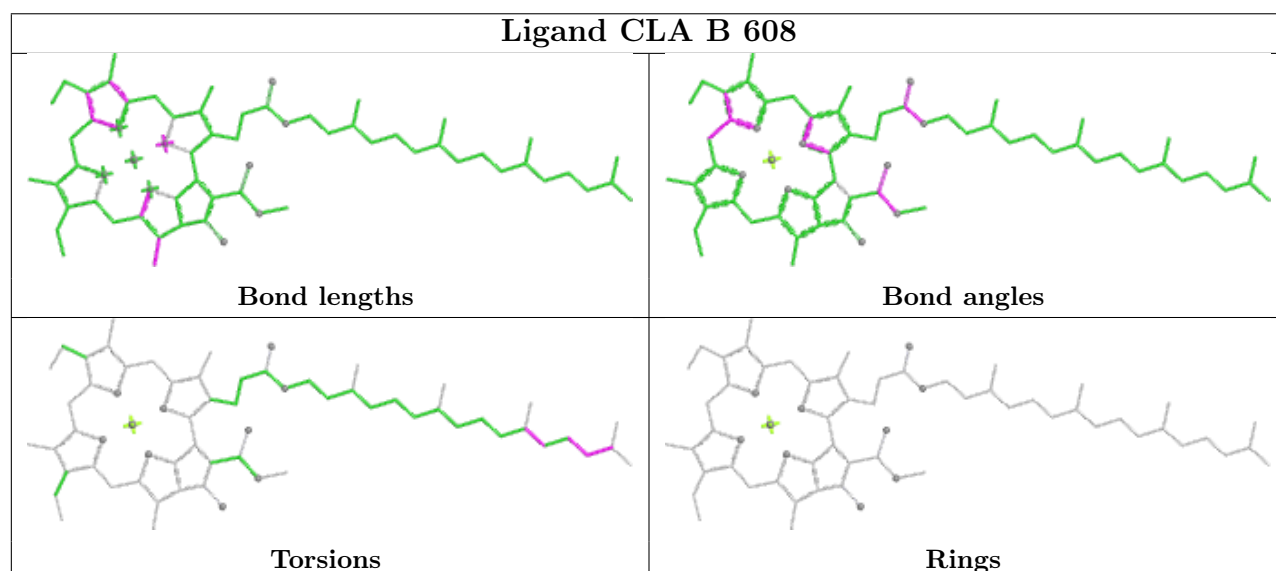
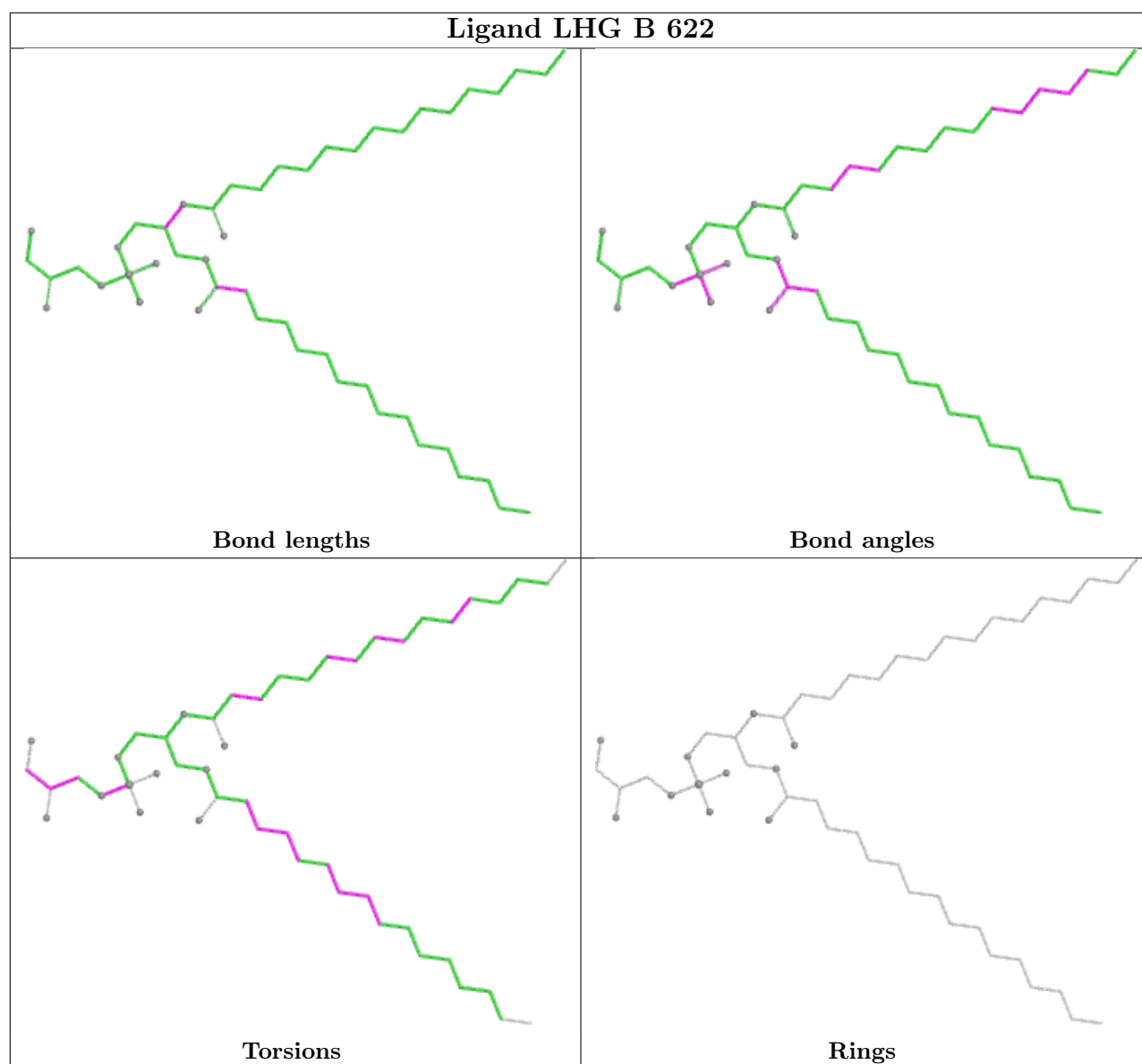
Ligand PL9 d 405			
			
Bond lengths		Bond angles	
			
Torsions		Rings	

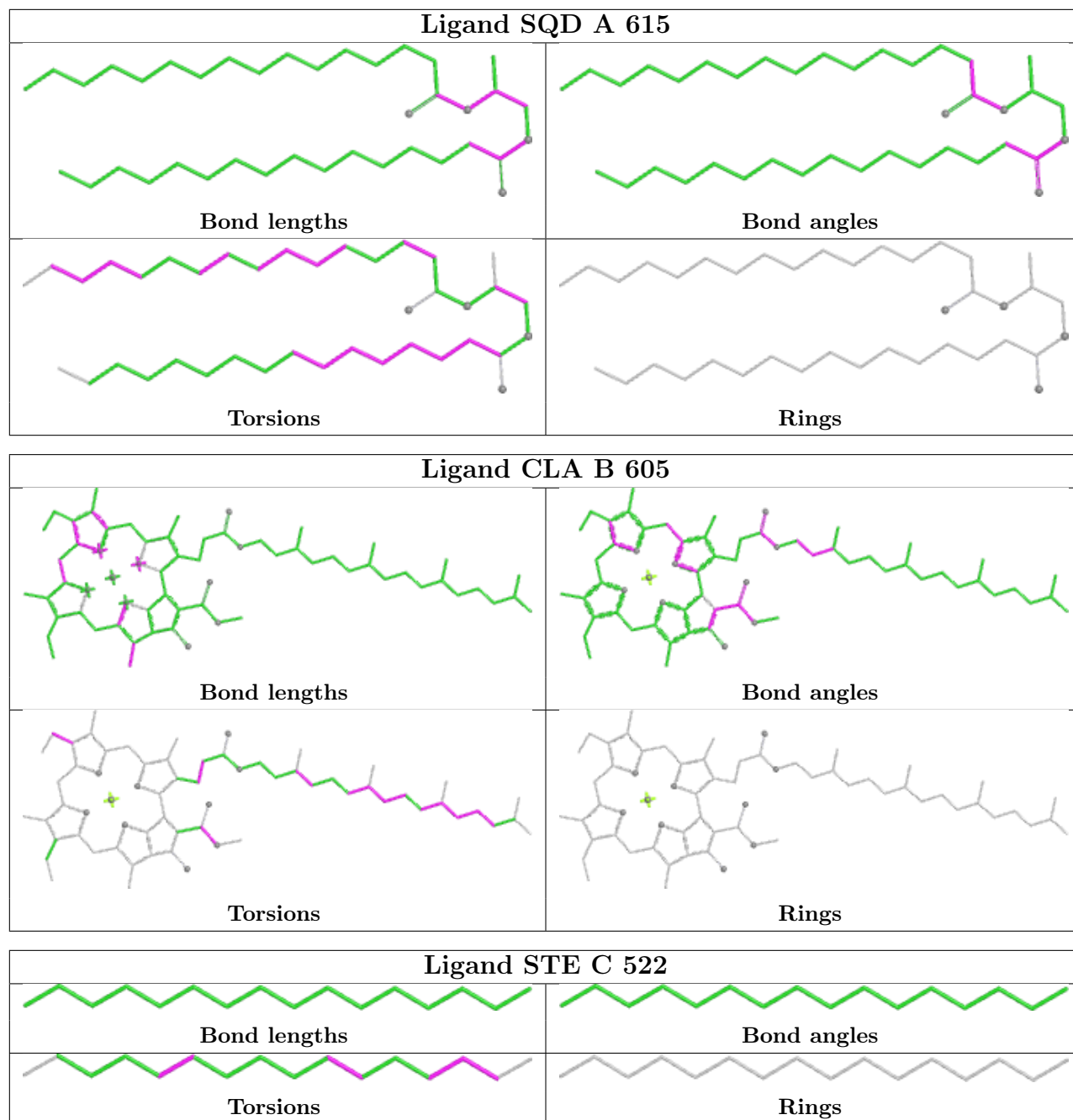
Ligand STE B 624			
			
Bond lengths		Bond angles	
			
Torsions		Rings	

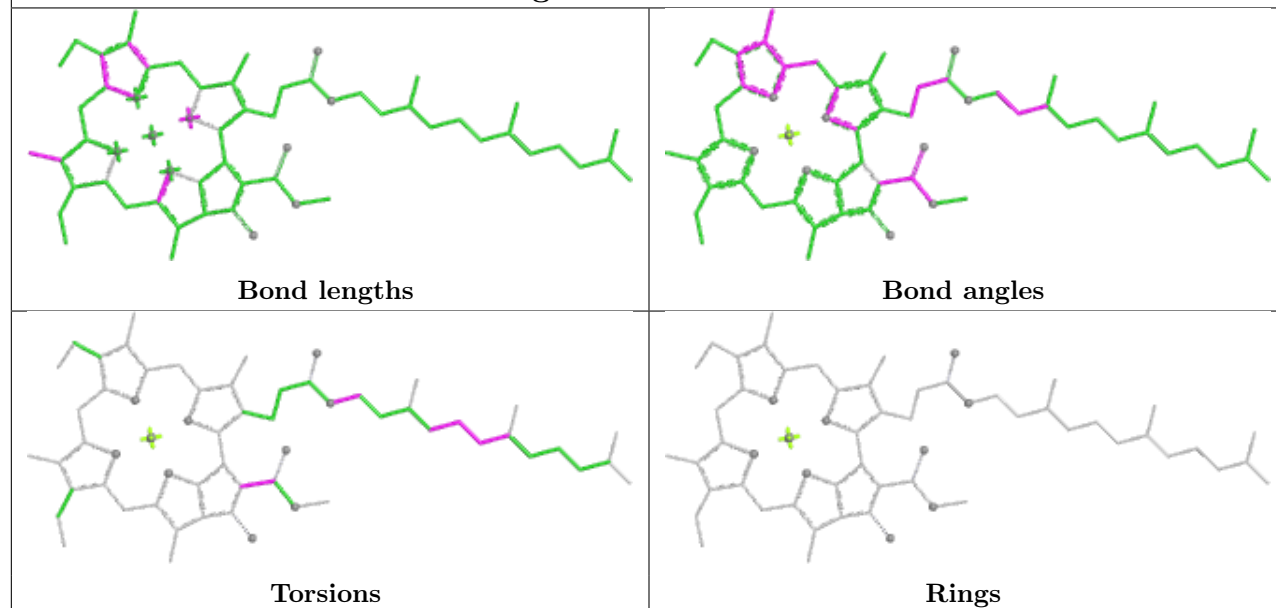
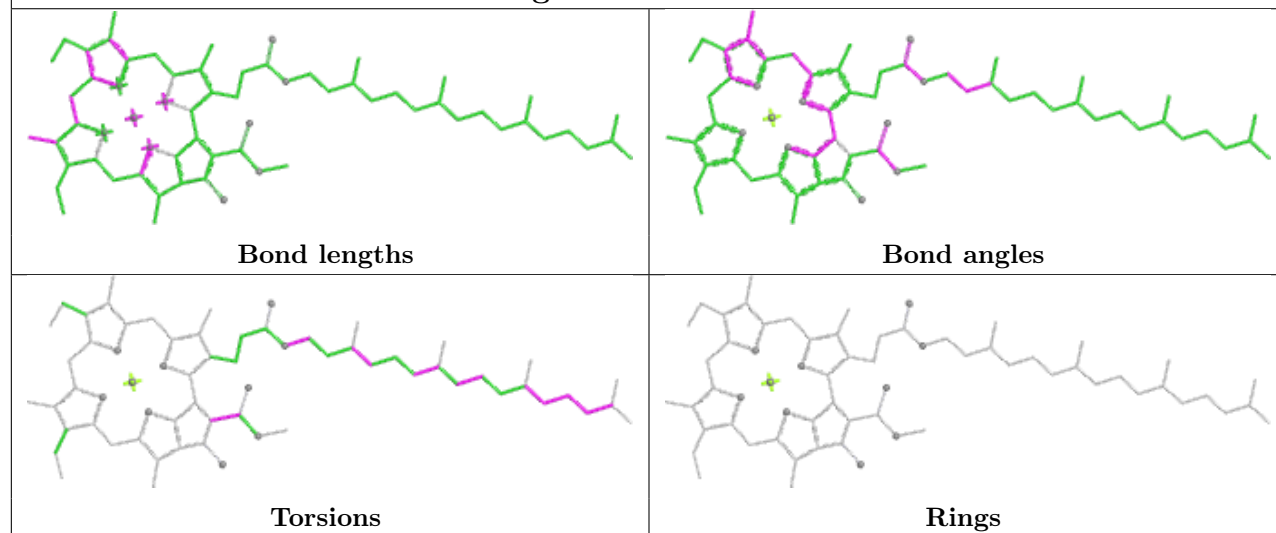
Ligand STE D 410			
			
Bond lengths		Bond angles	
			
Torsions		Rings	

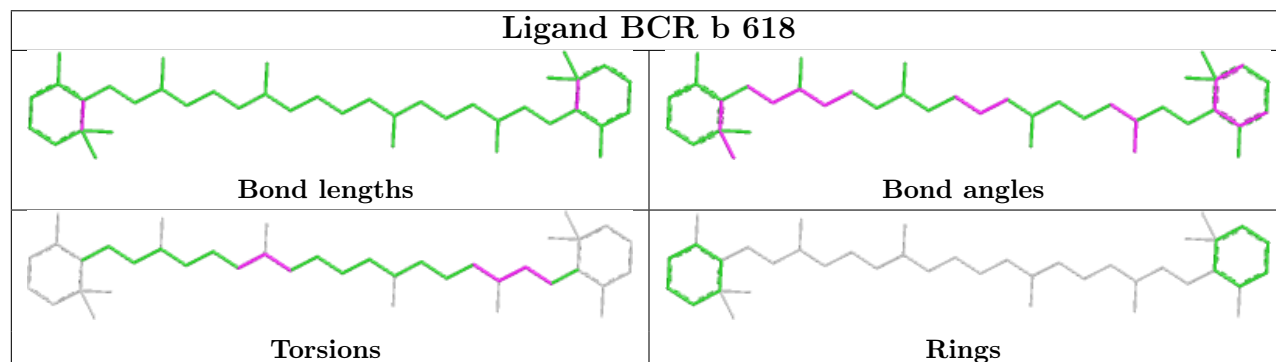
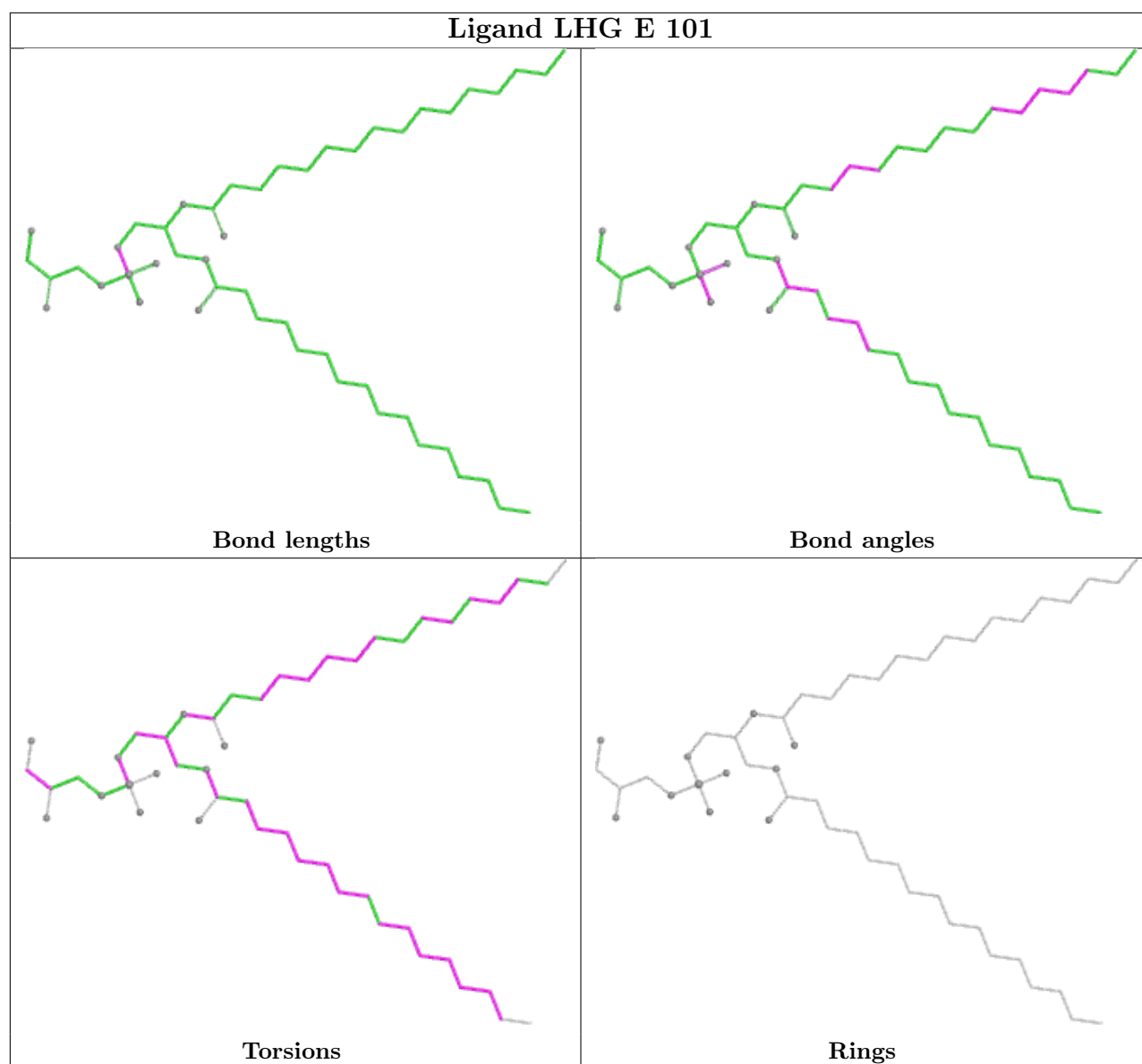


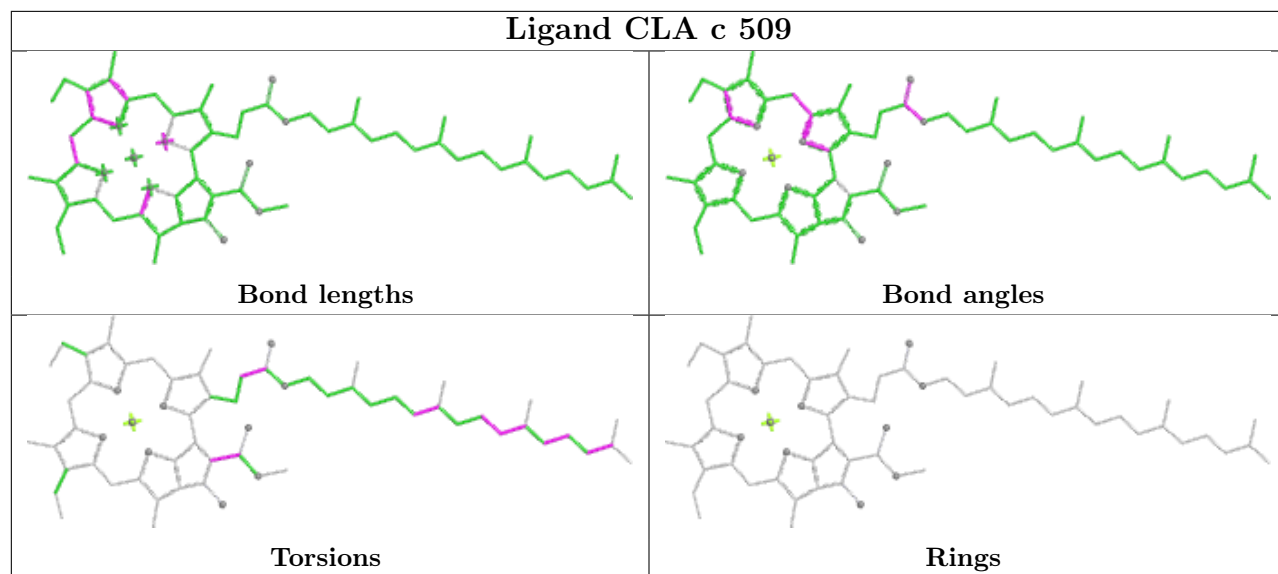
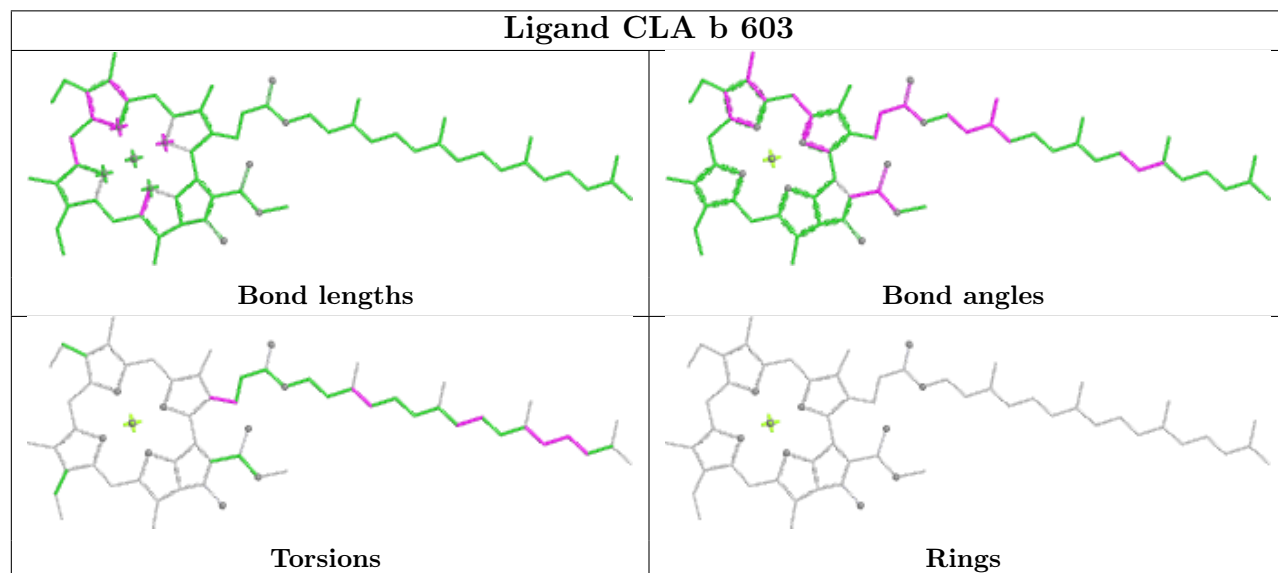
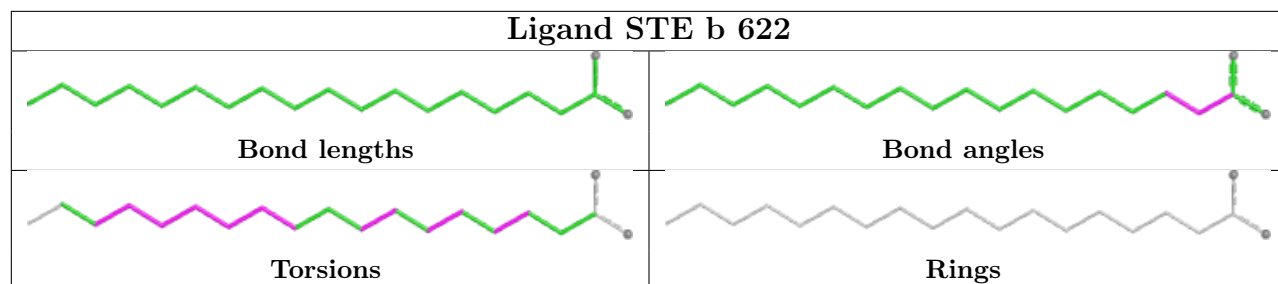




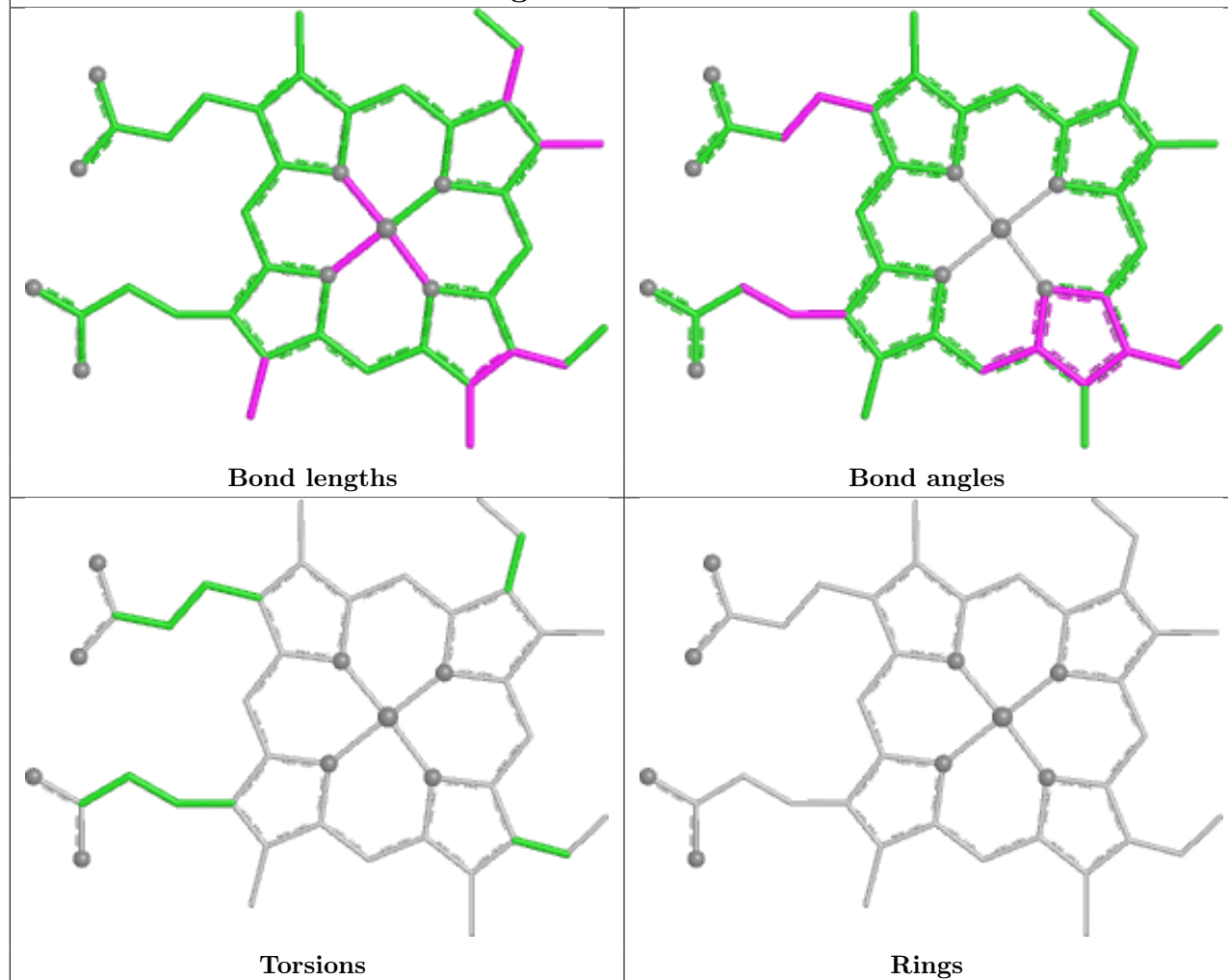


Ligand CLA B 615**Ligand CLA C 506**

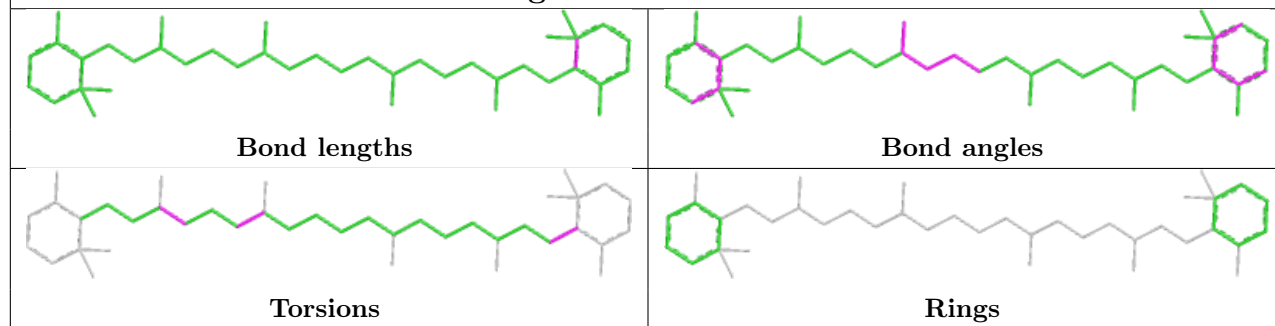


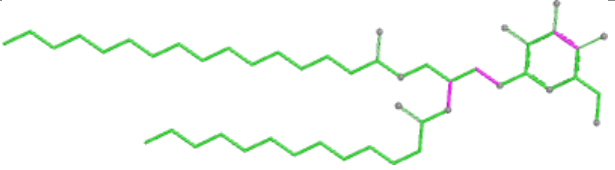
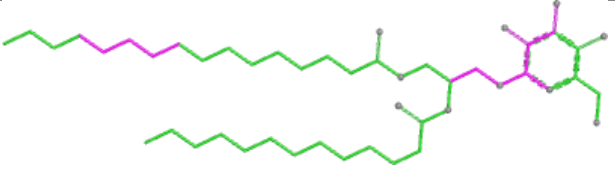
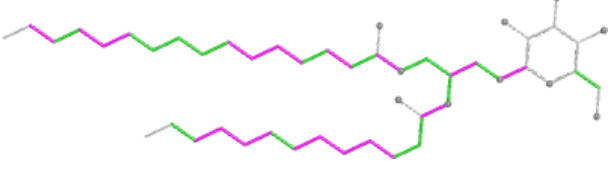
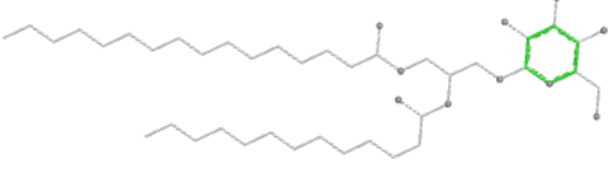
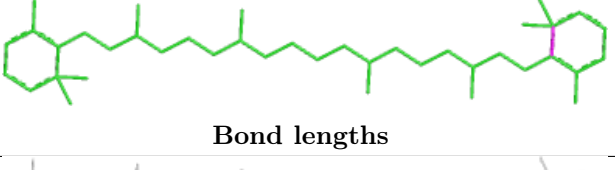
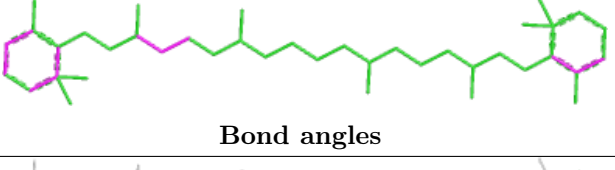
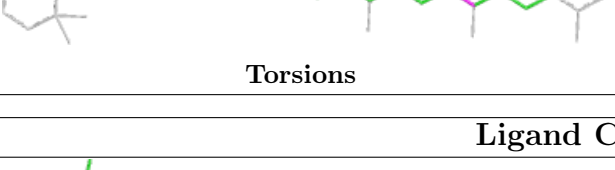

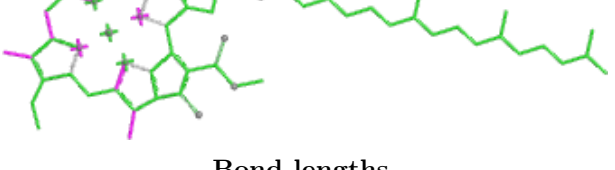
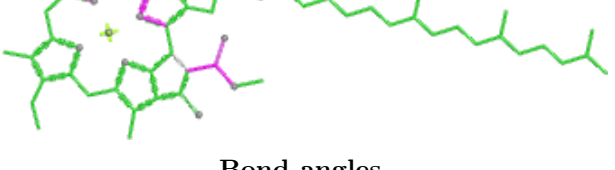
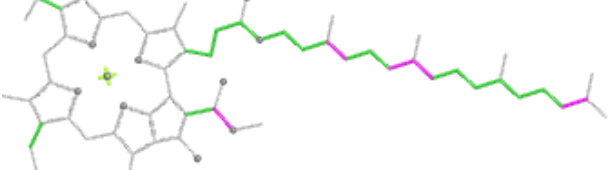
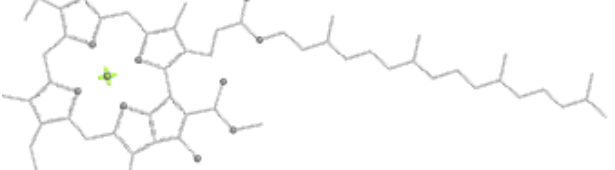


Ligand HEM e 101

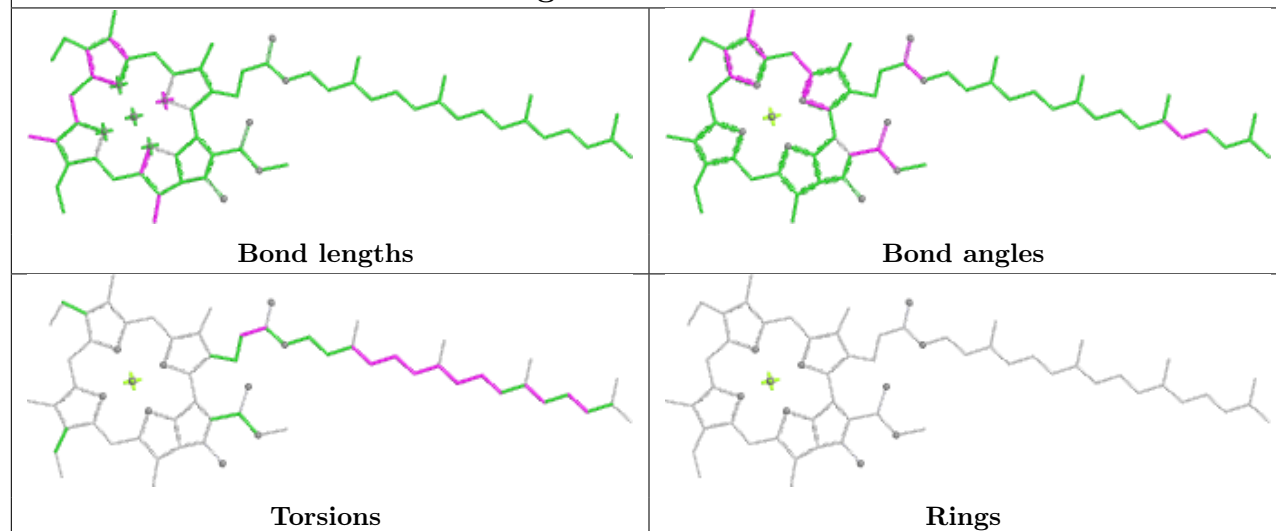


Ligand BCR H 102

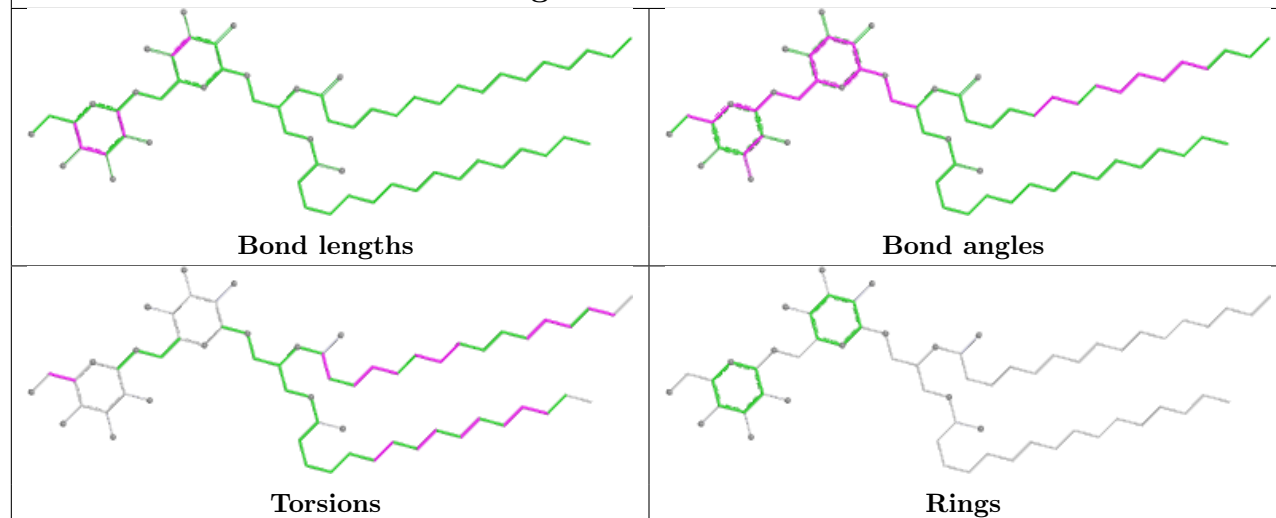


Ligand LMG C 519	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR x 101	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand CLA C 510	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

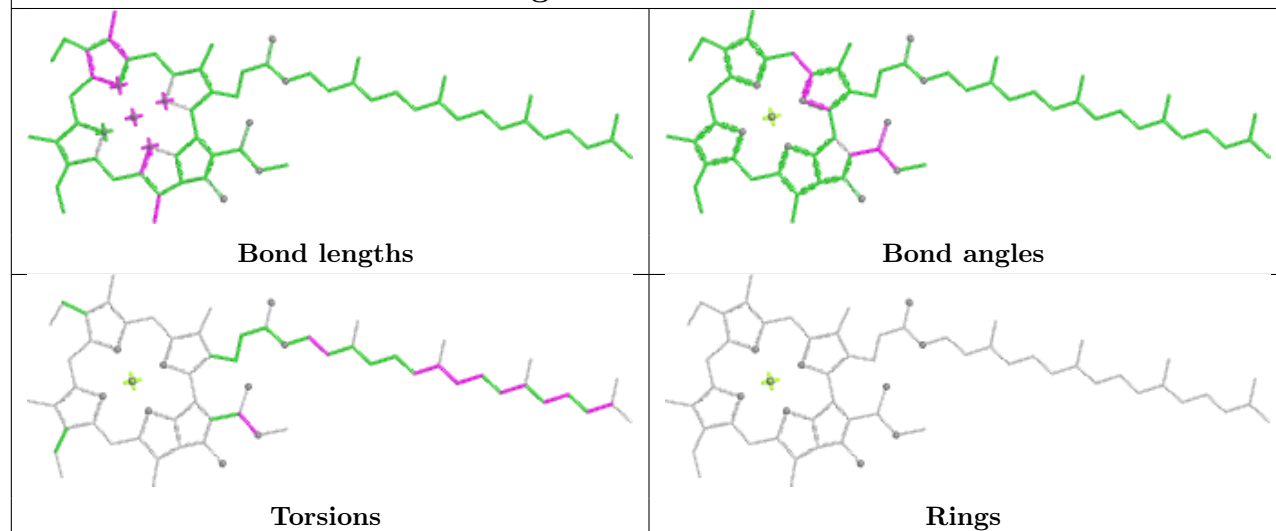
Ligand CLA c 510



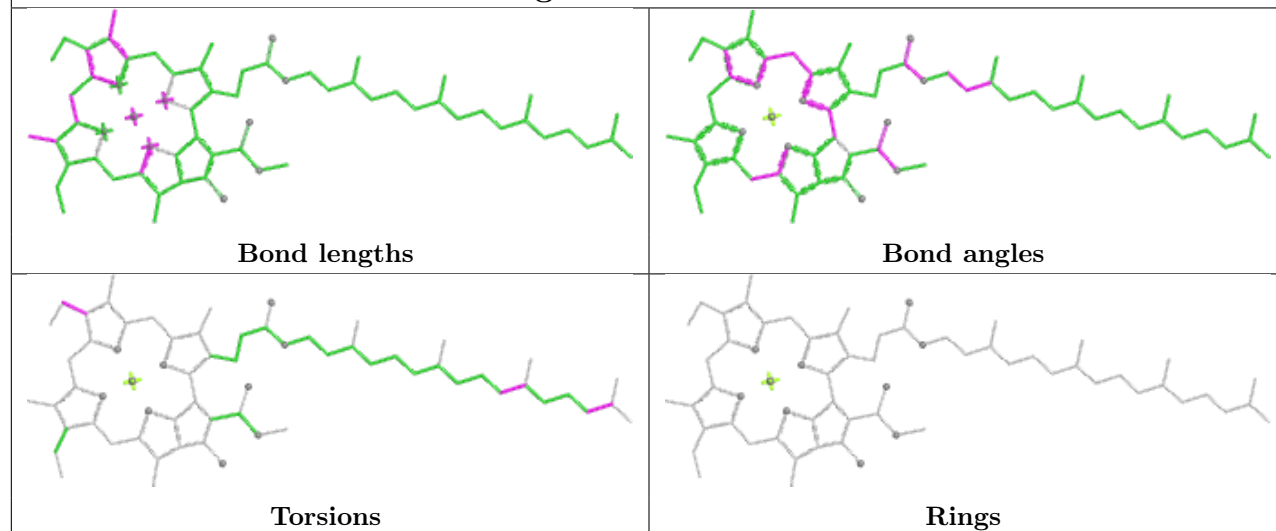
Ligand DGD h 102



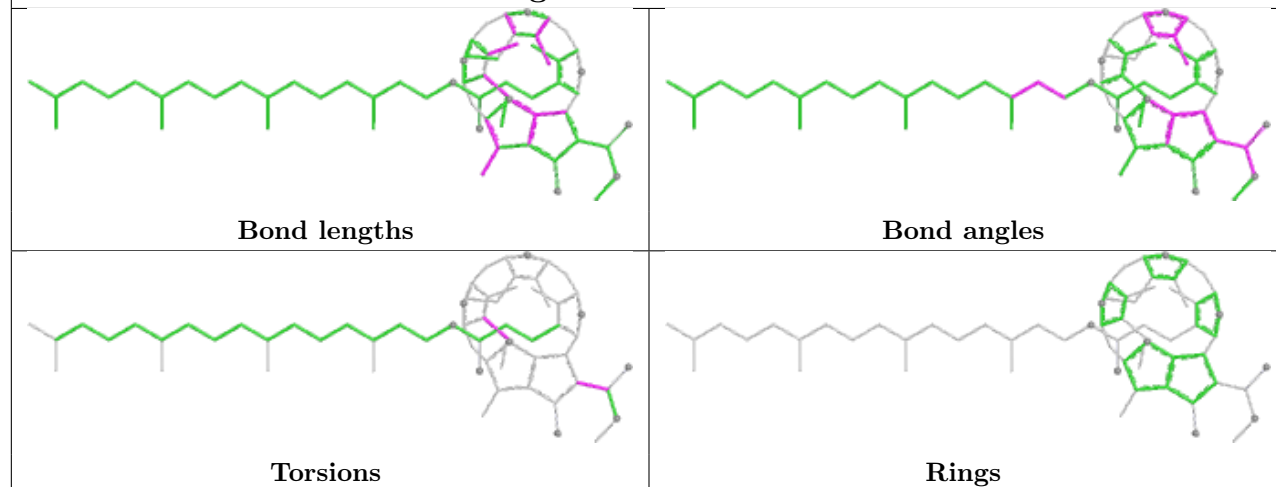
Ligand CLA D 403



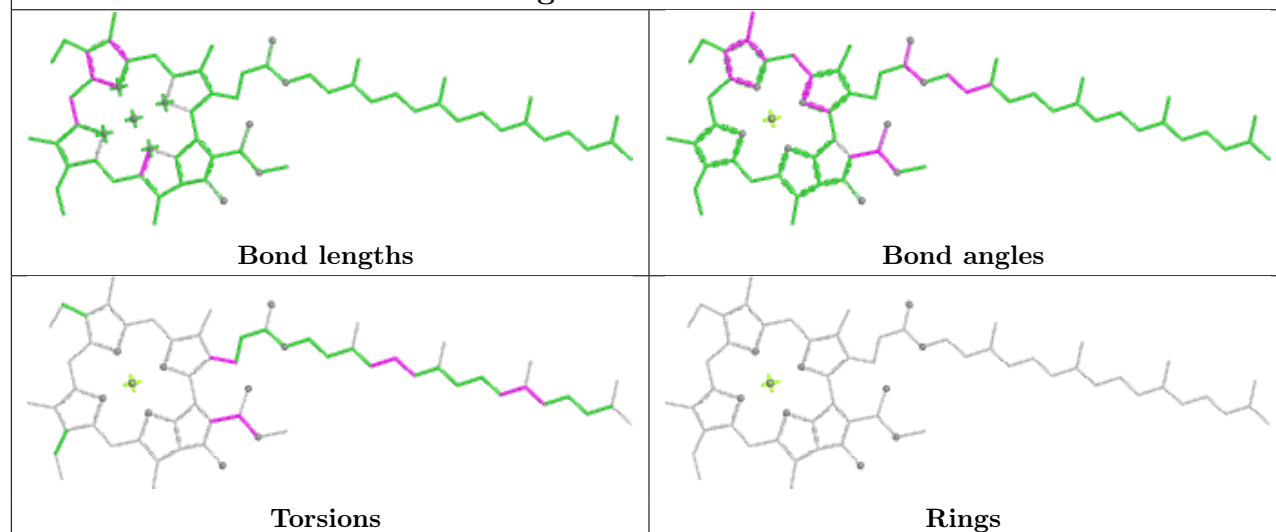
Ligand CLA d 403

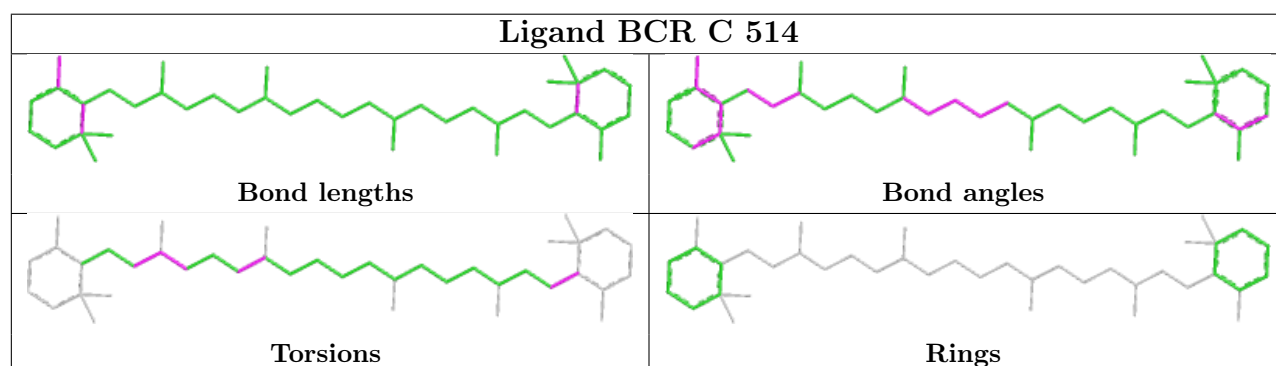
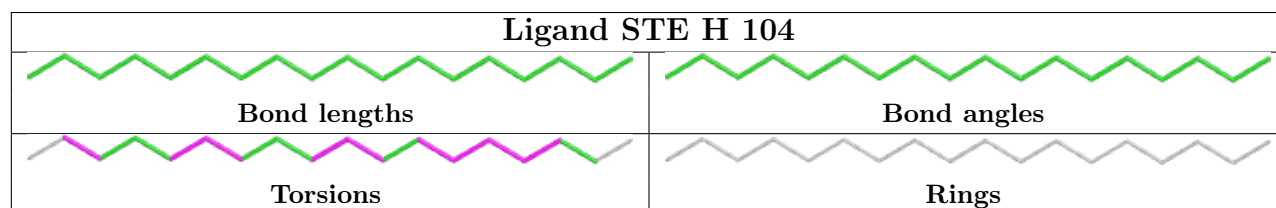
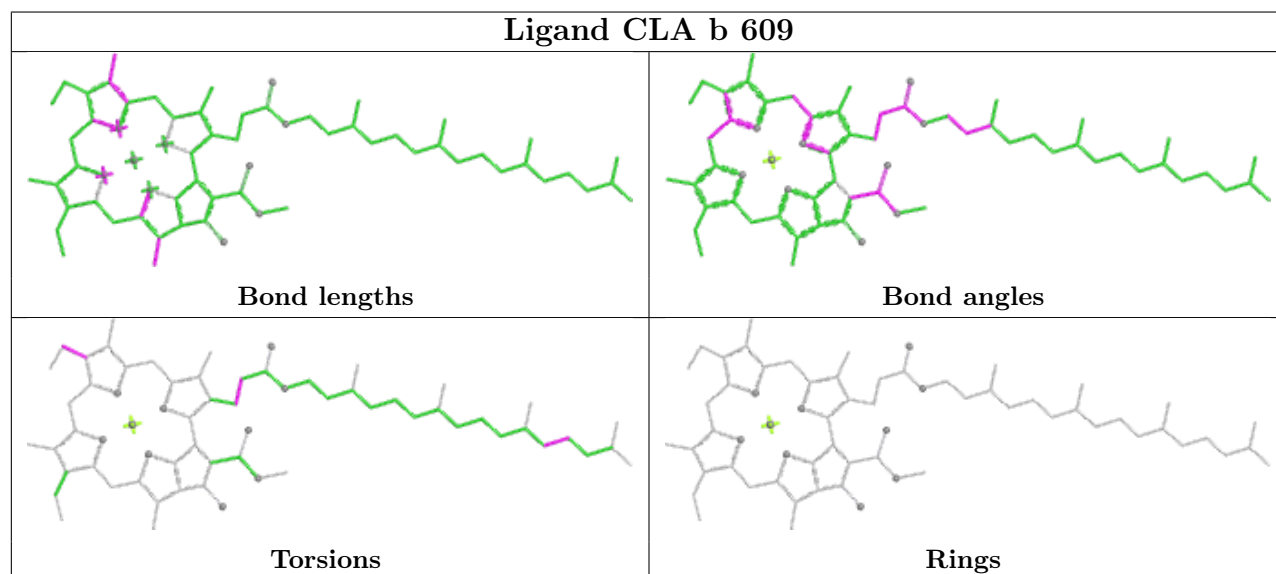
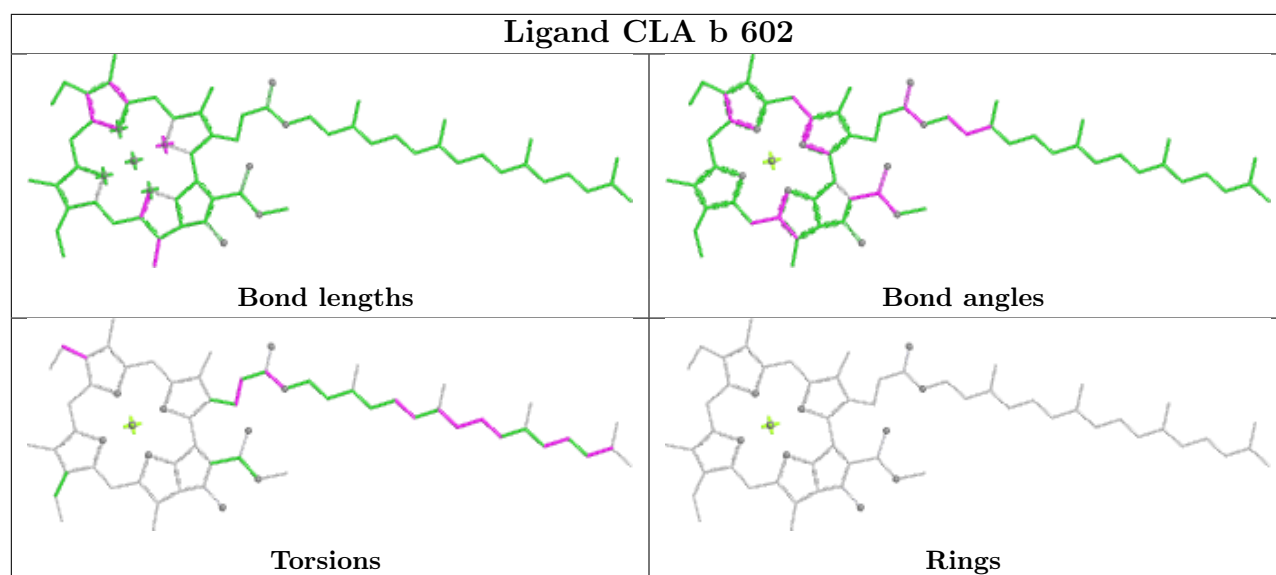


Ligand PHO A 609

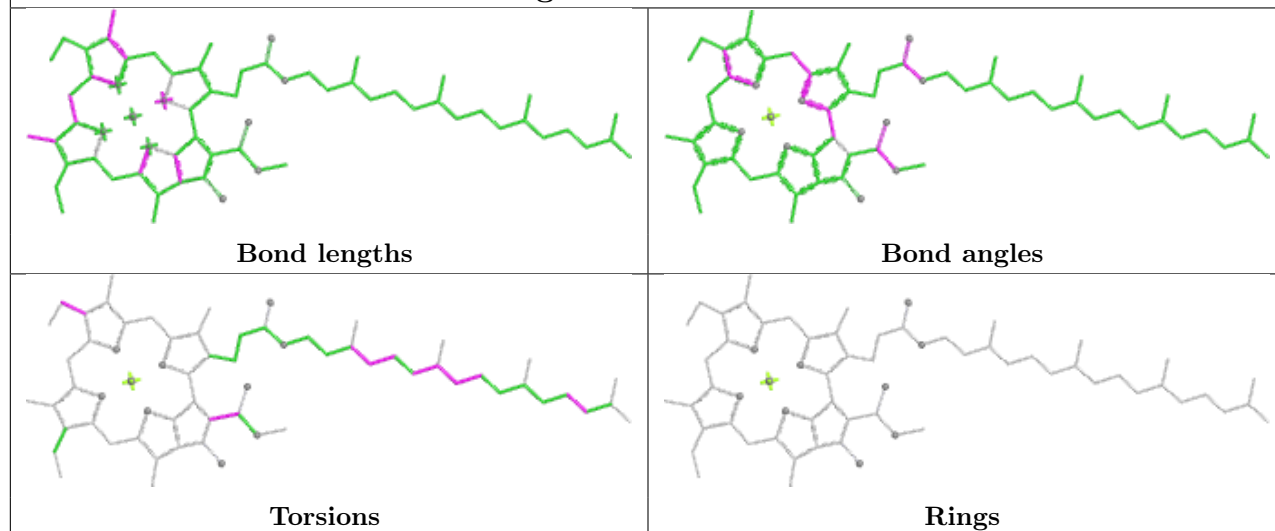


Ligand CLA c 513

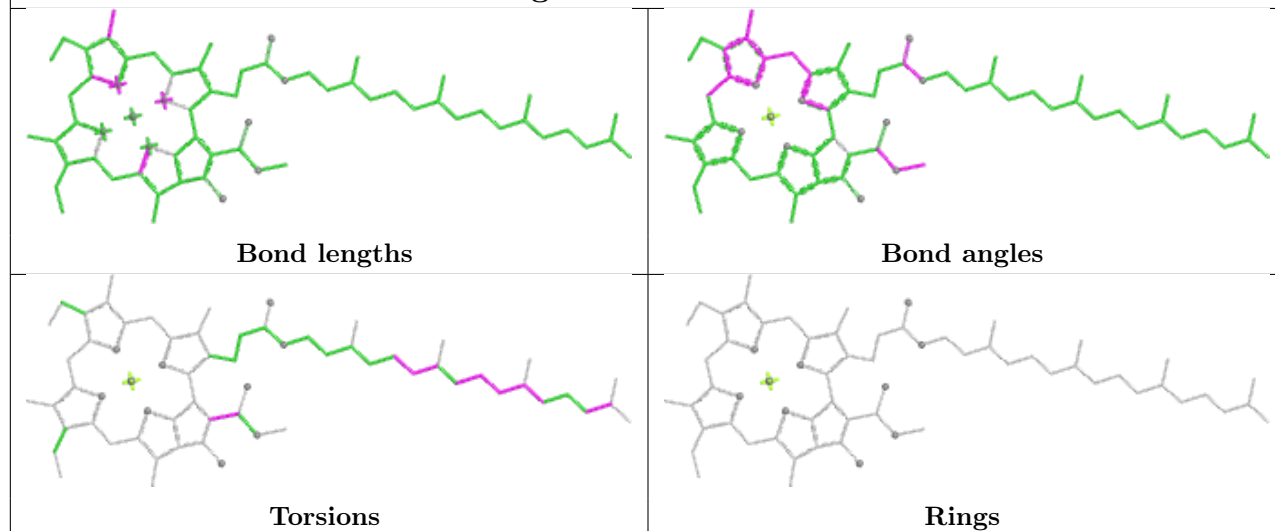




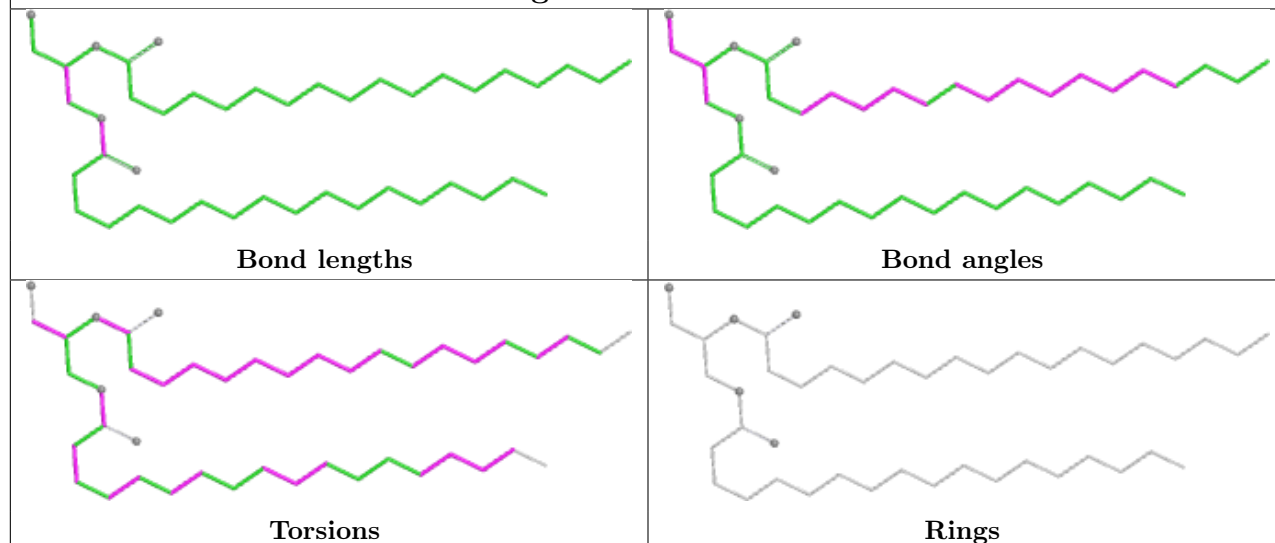
Ligand CLA c 507

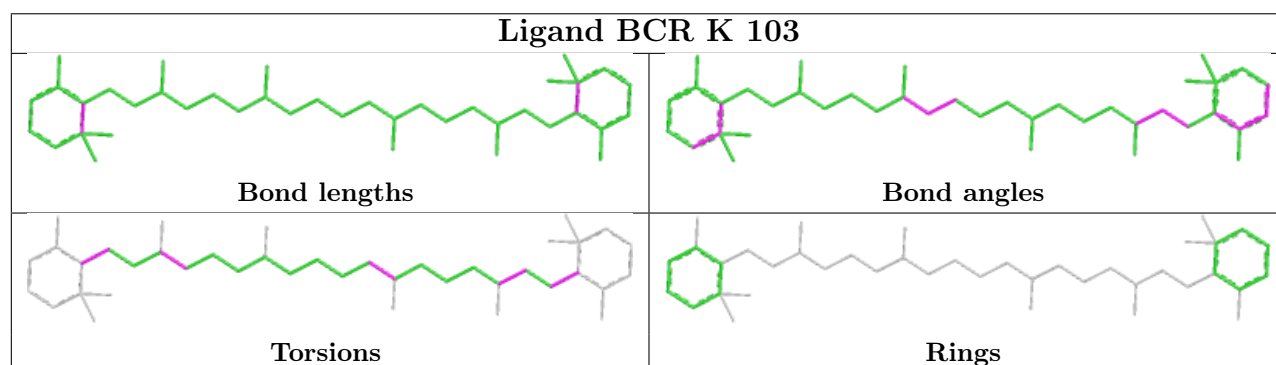
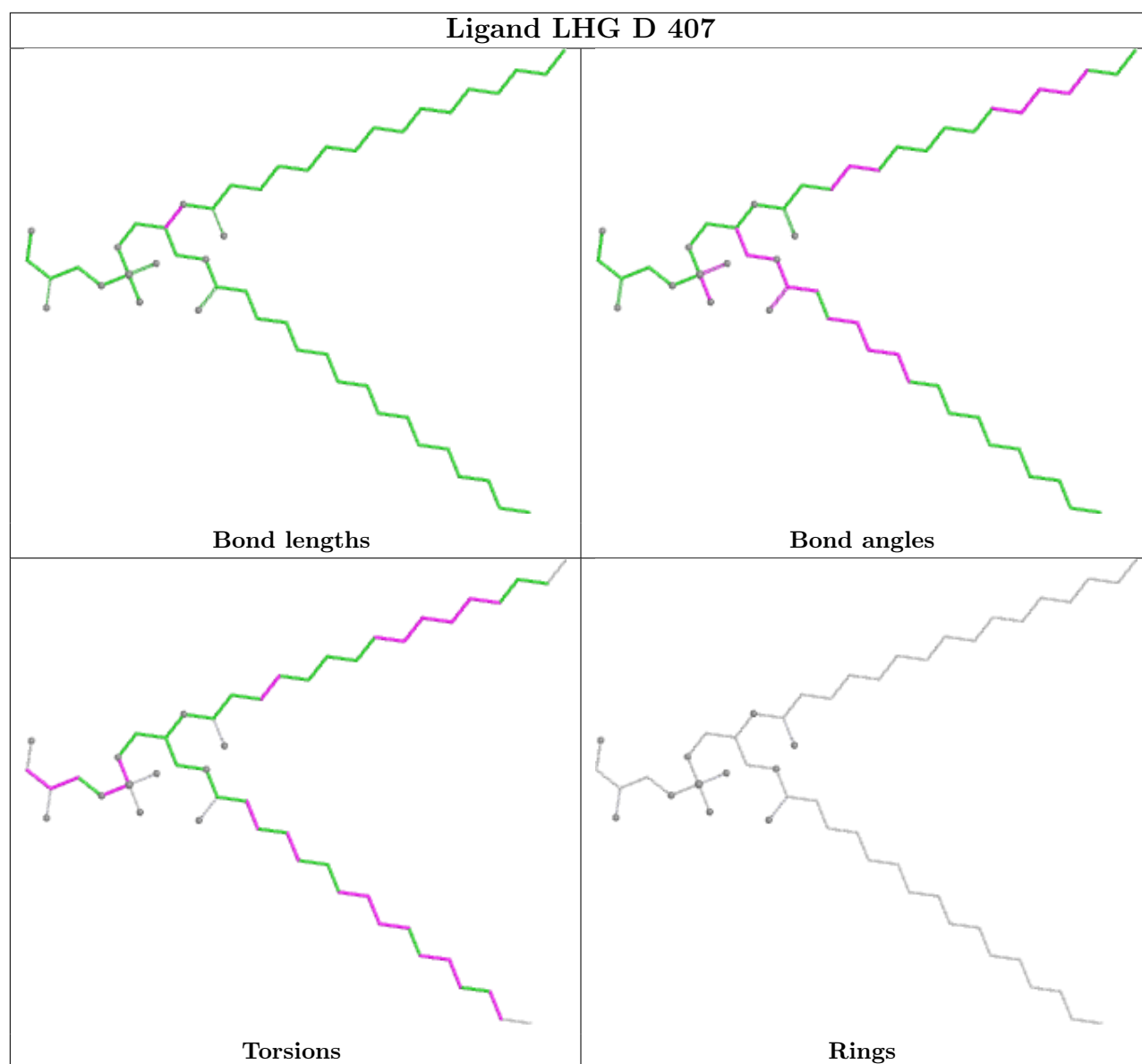


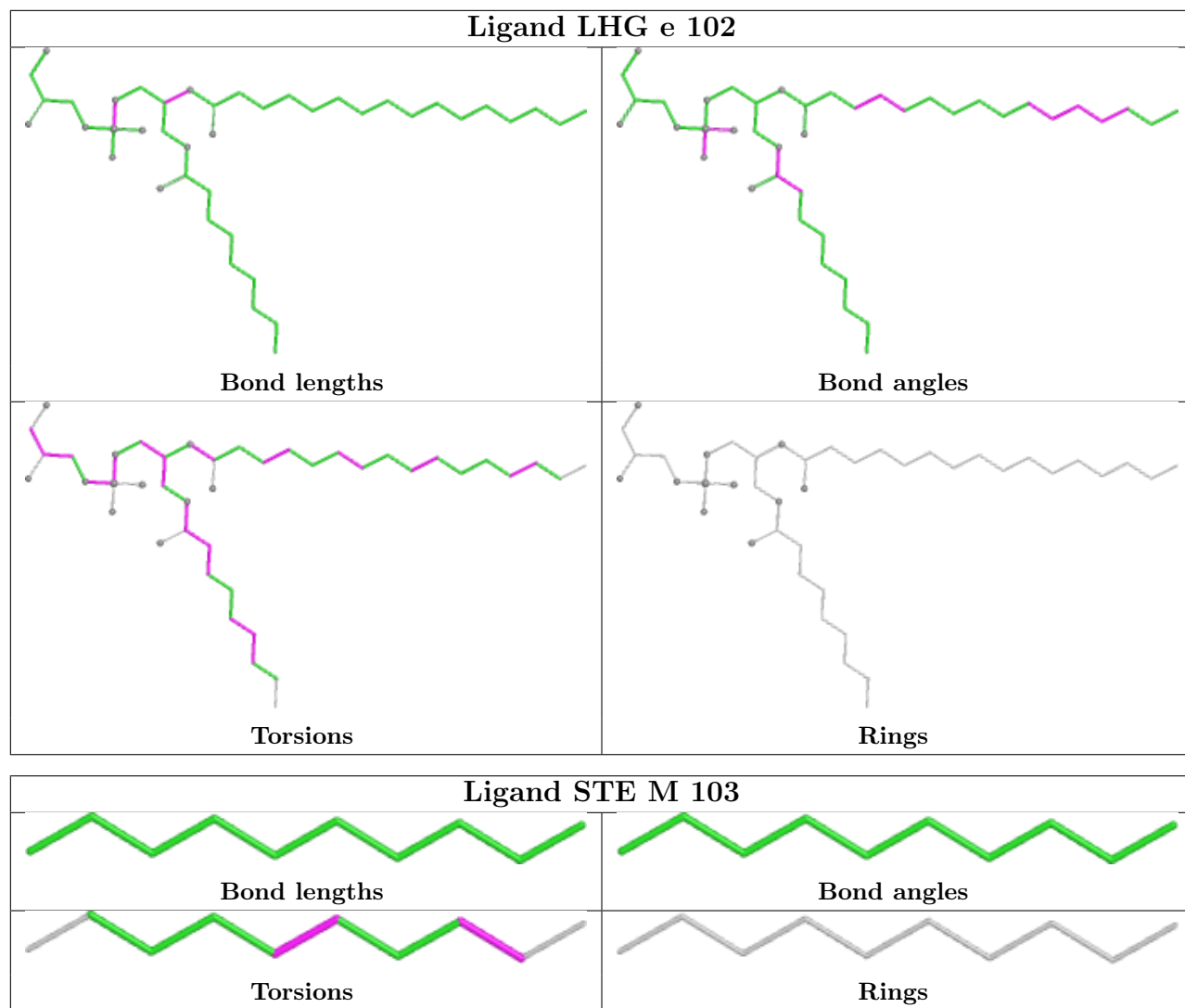
Ligand CLA B 606

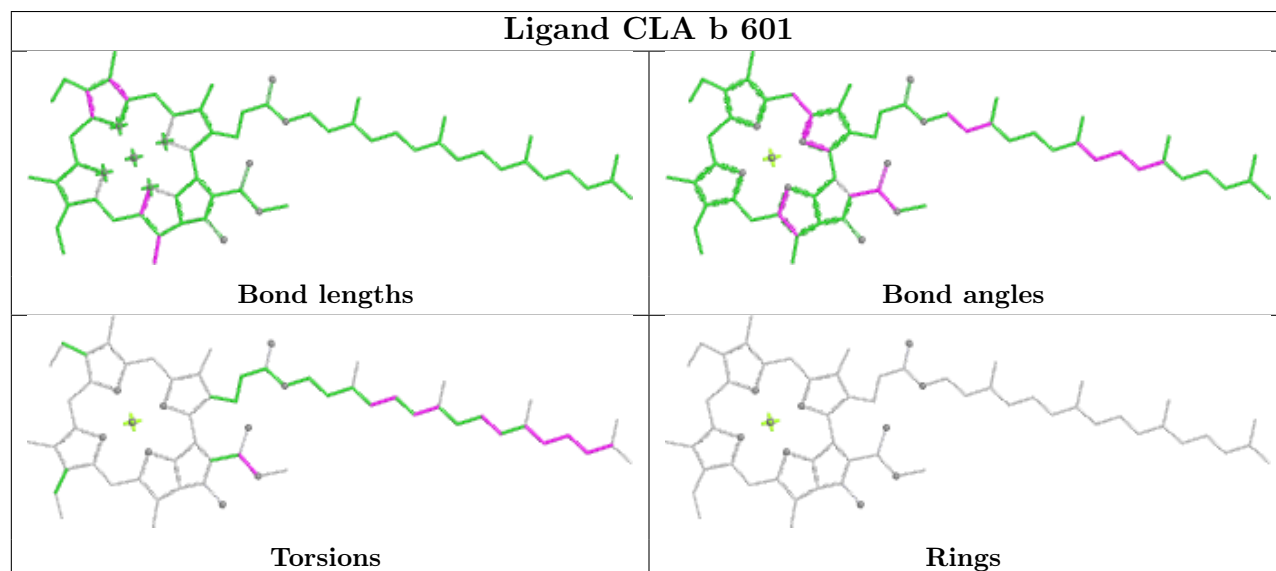
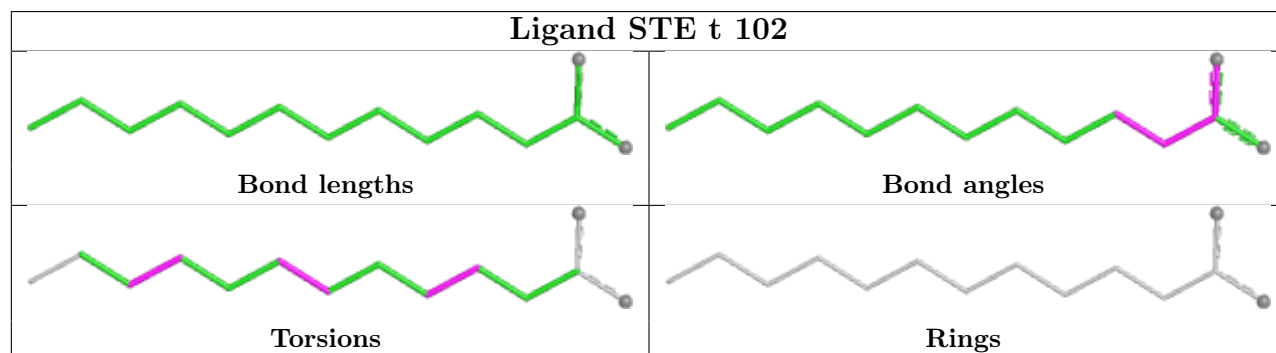
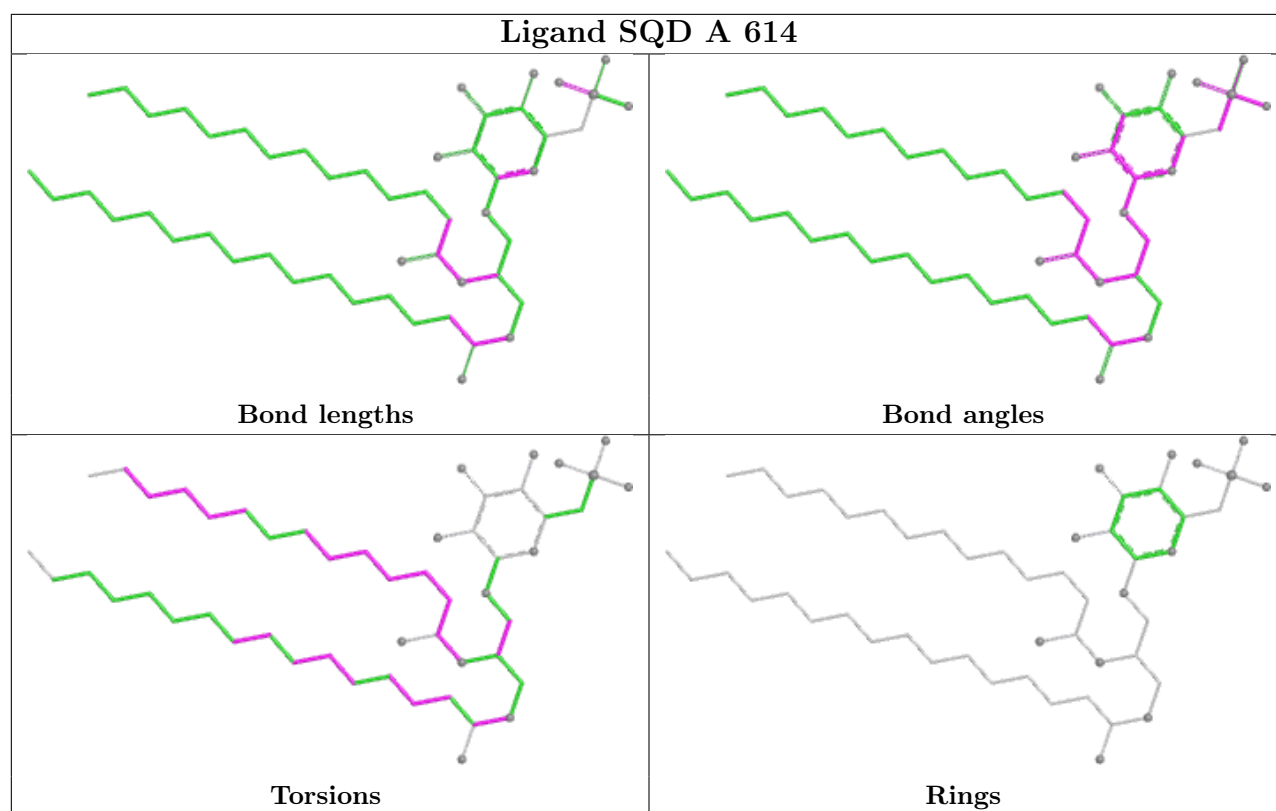


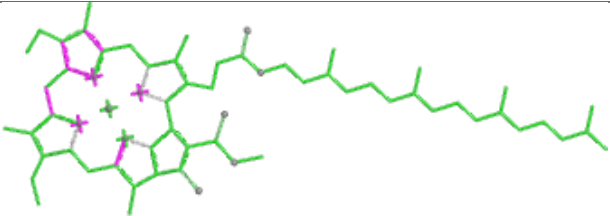
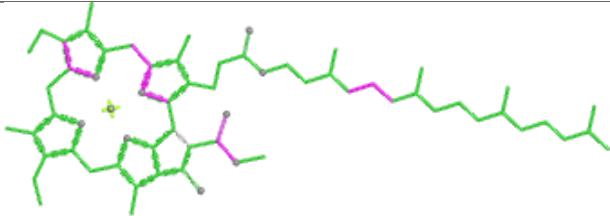
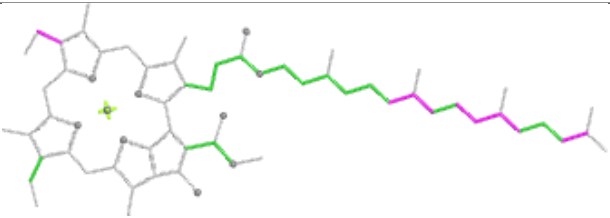
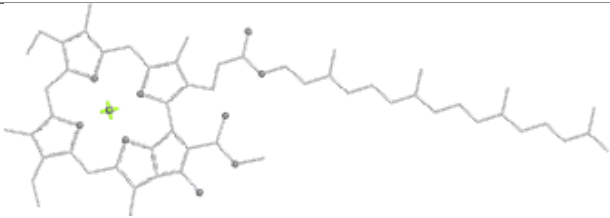
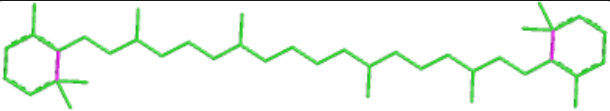
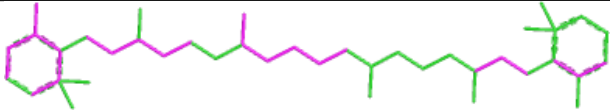
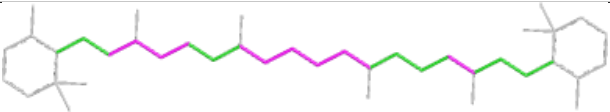
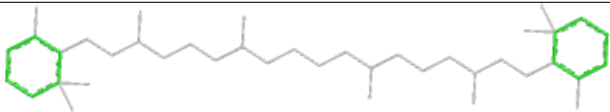
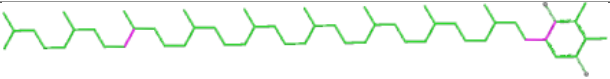
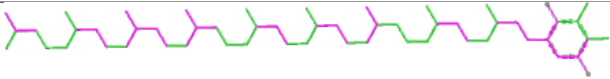
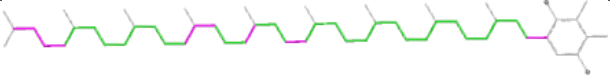
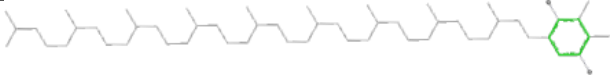
Ligand DGD a 616

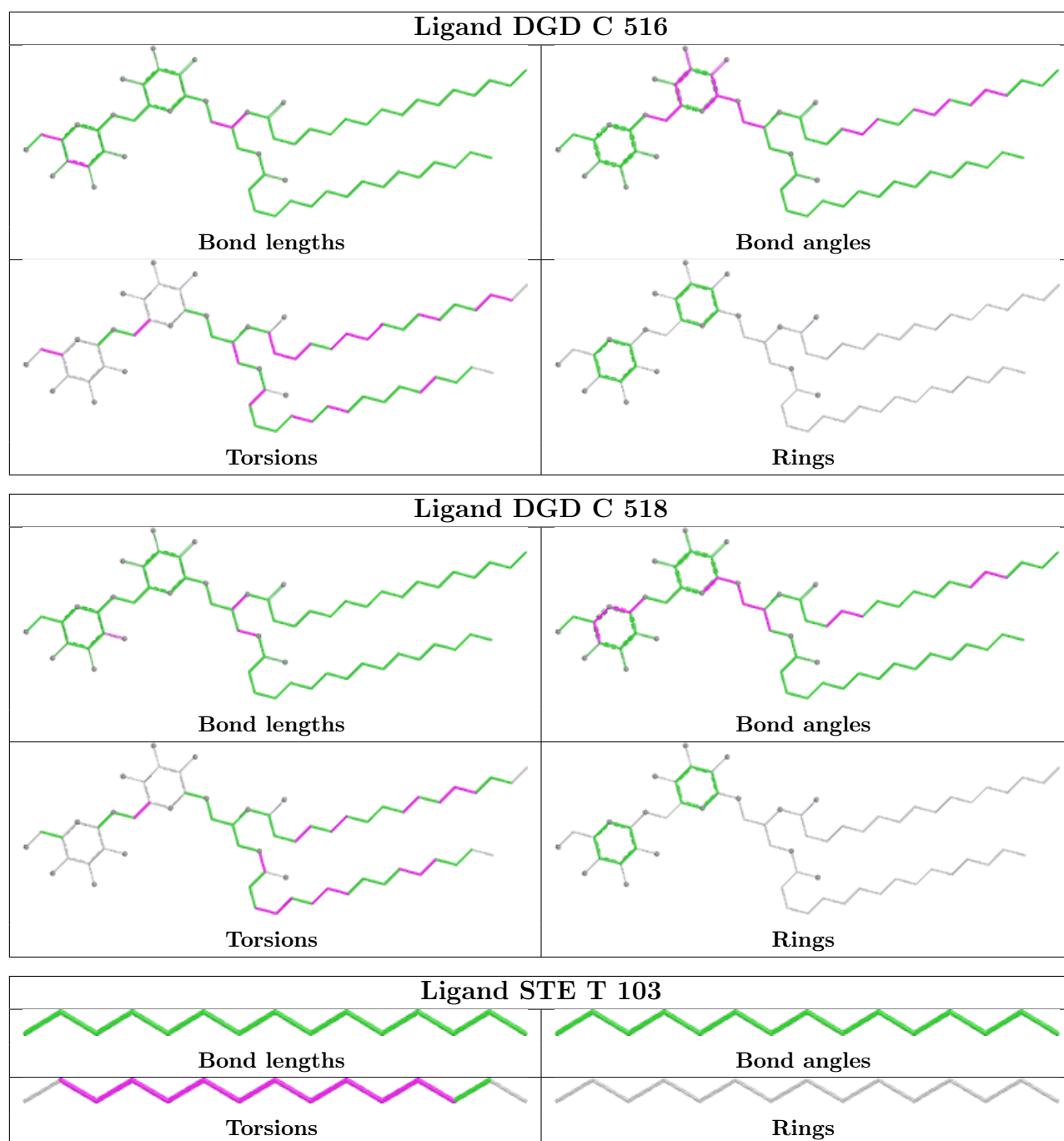


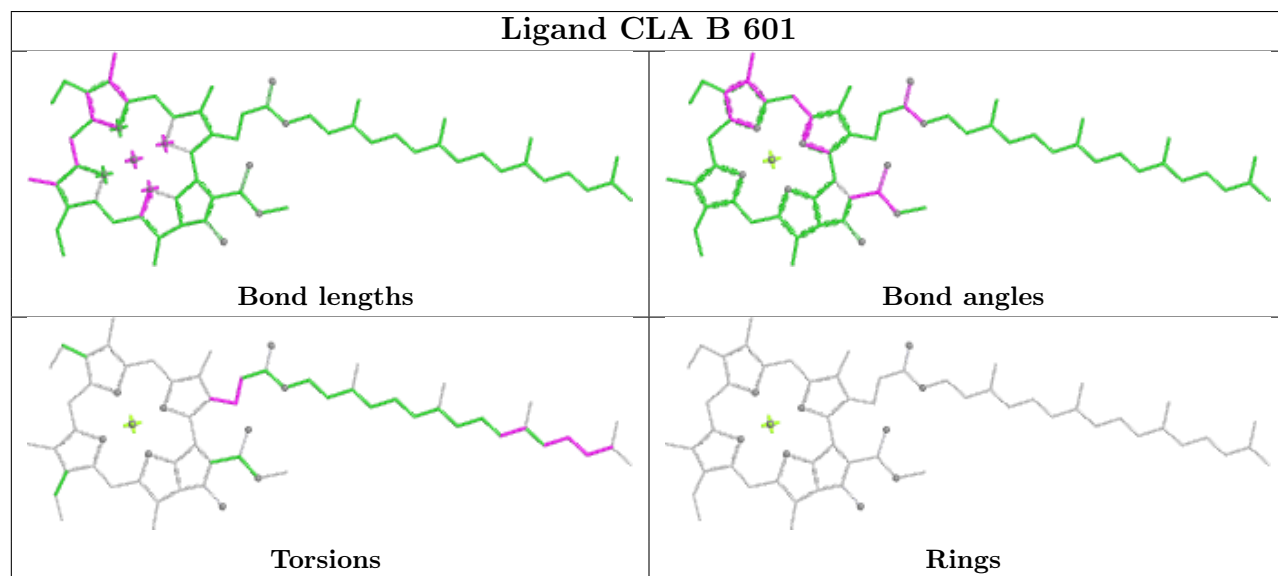
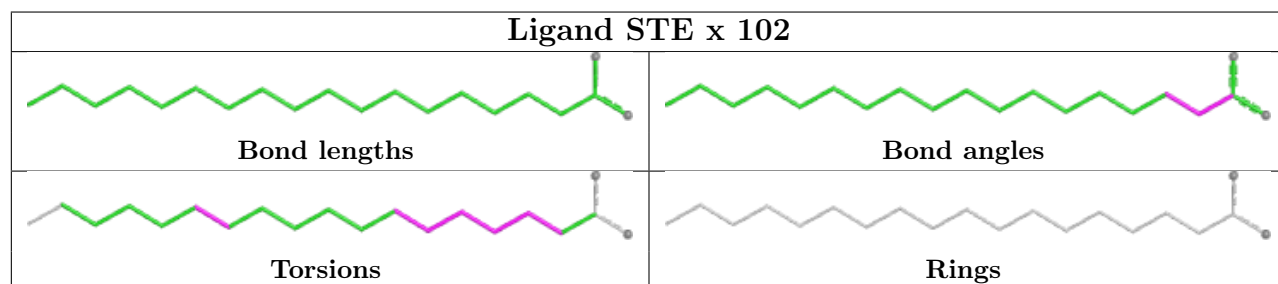
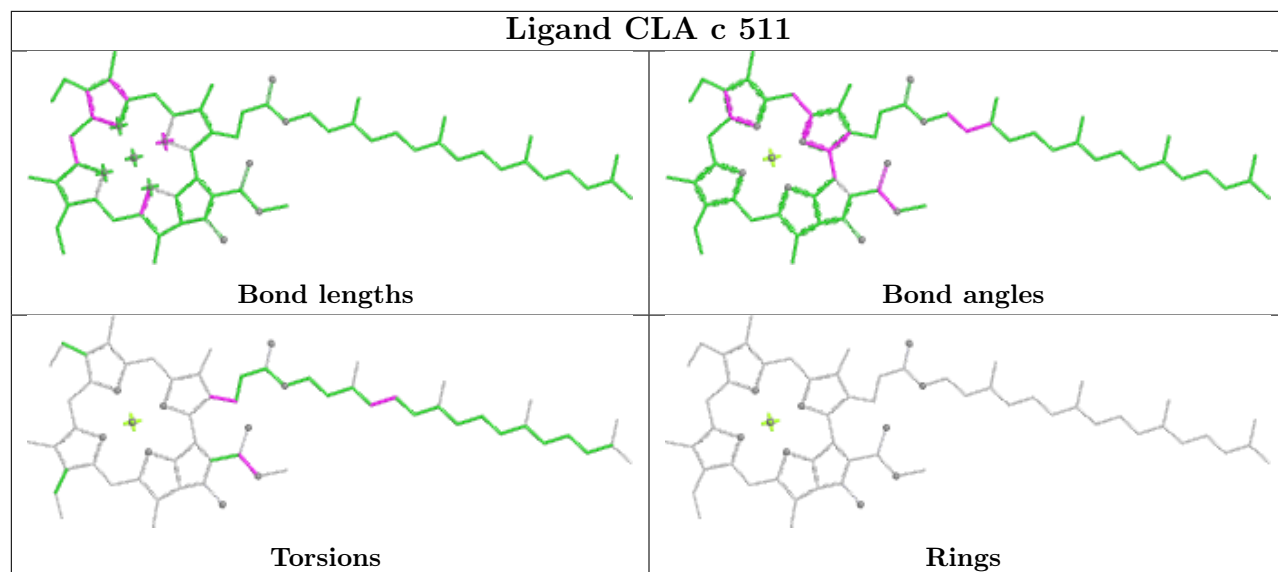


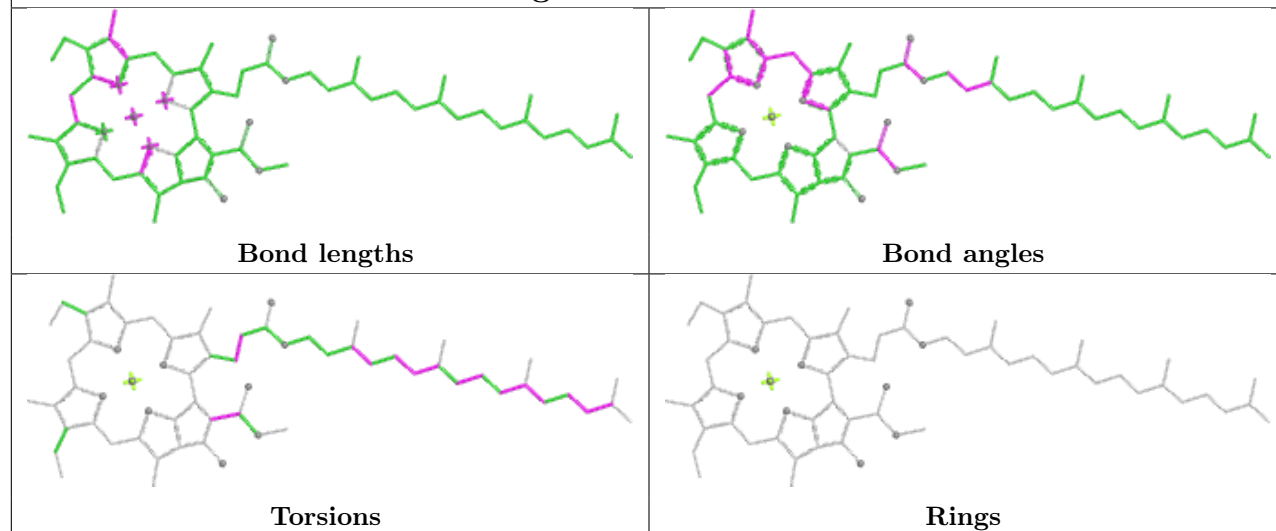
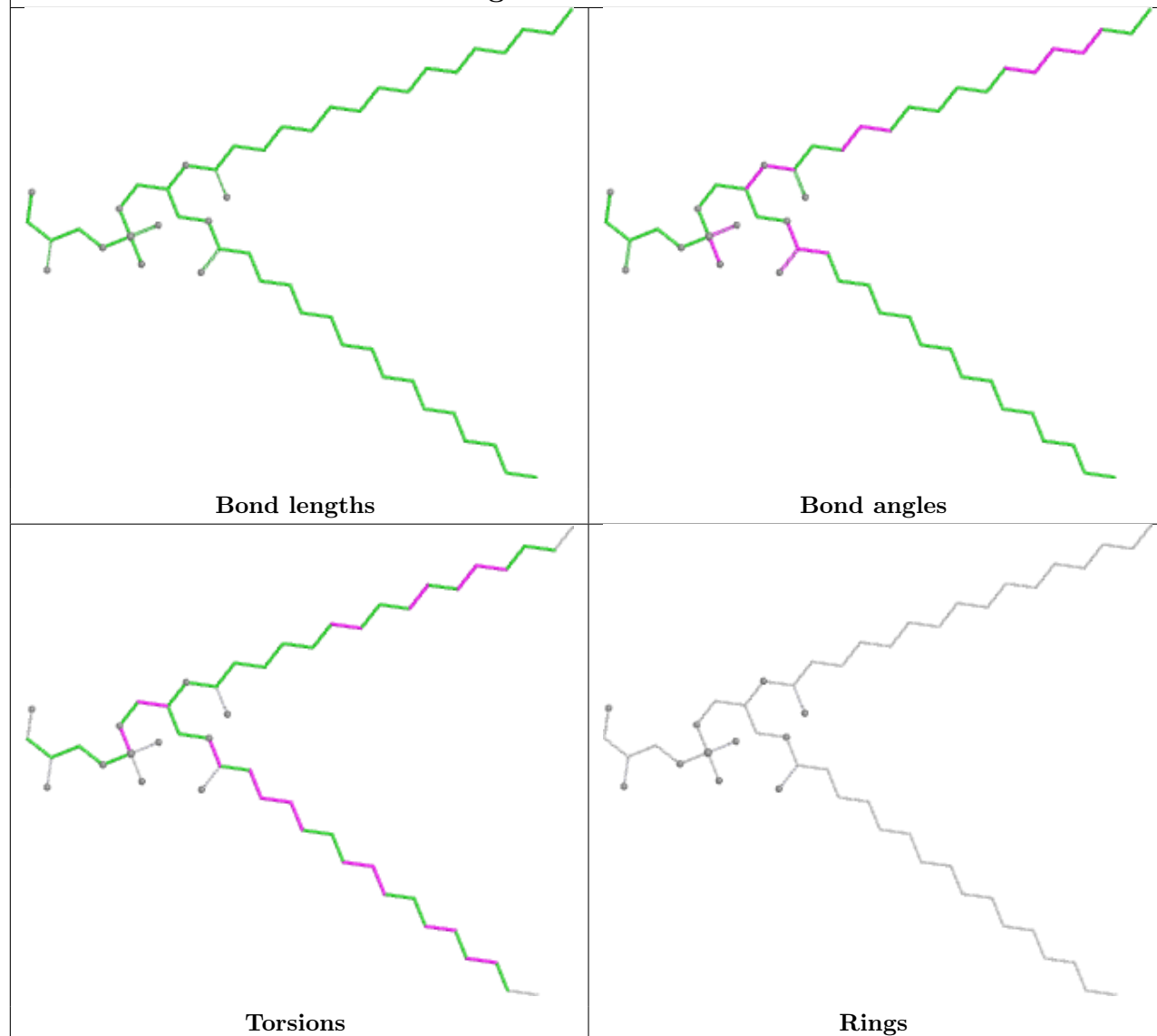


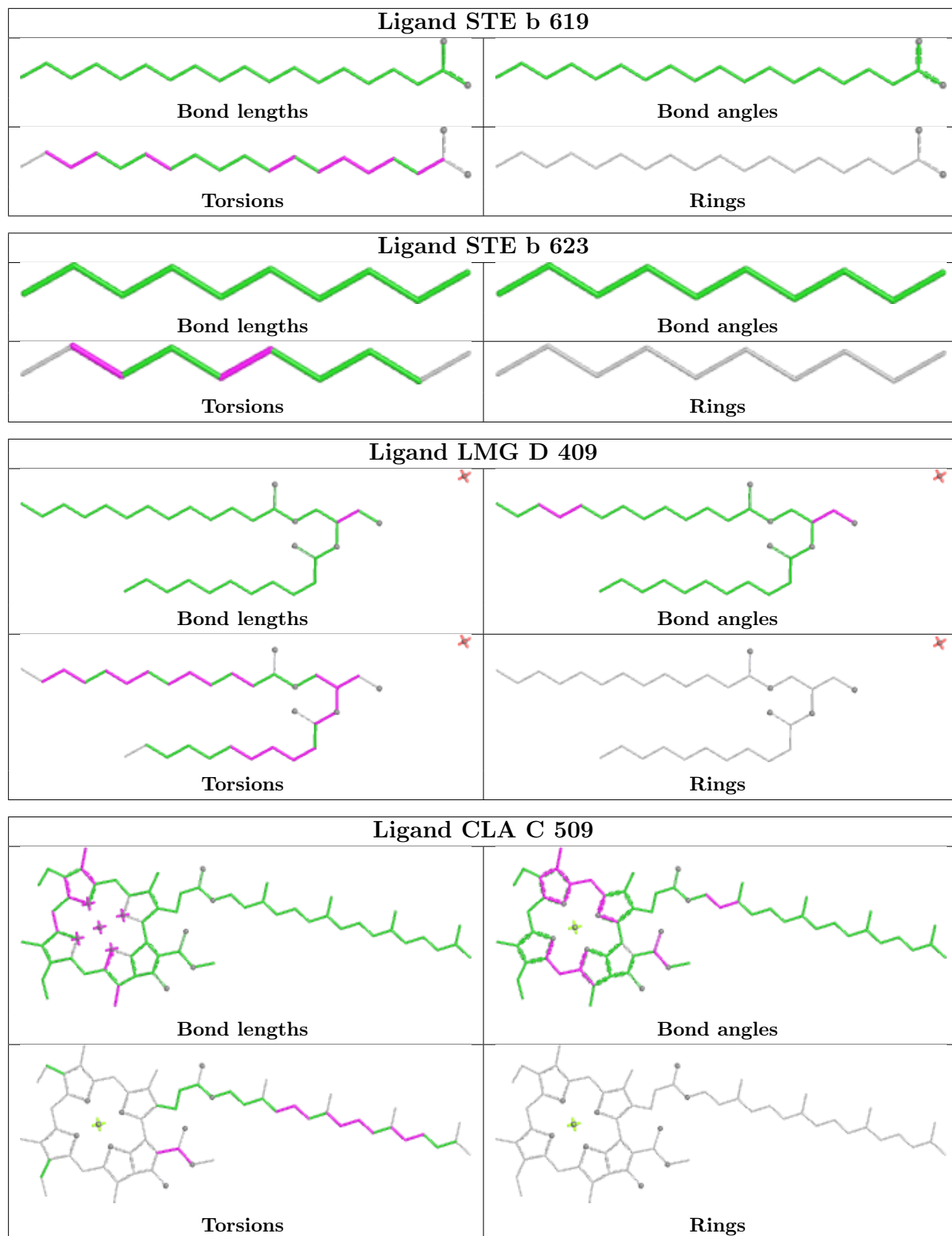


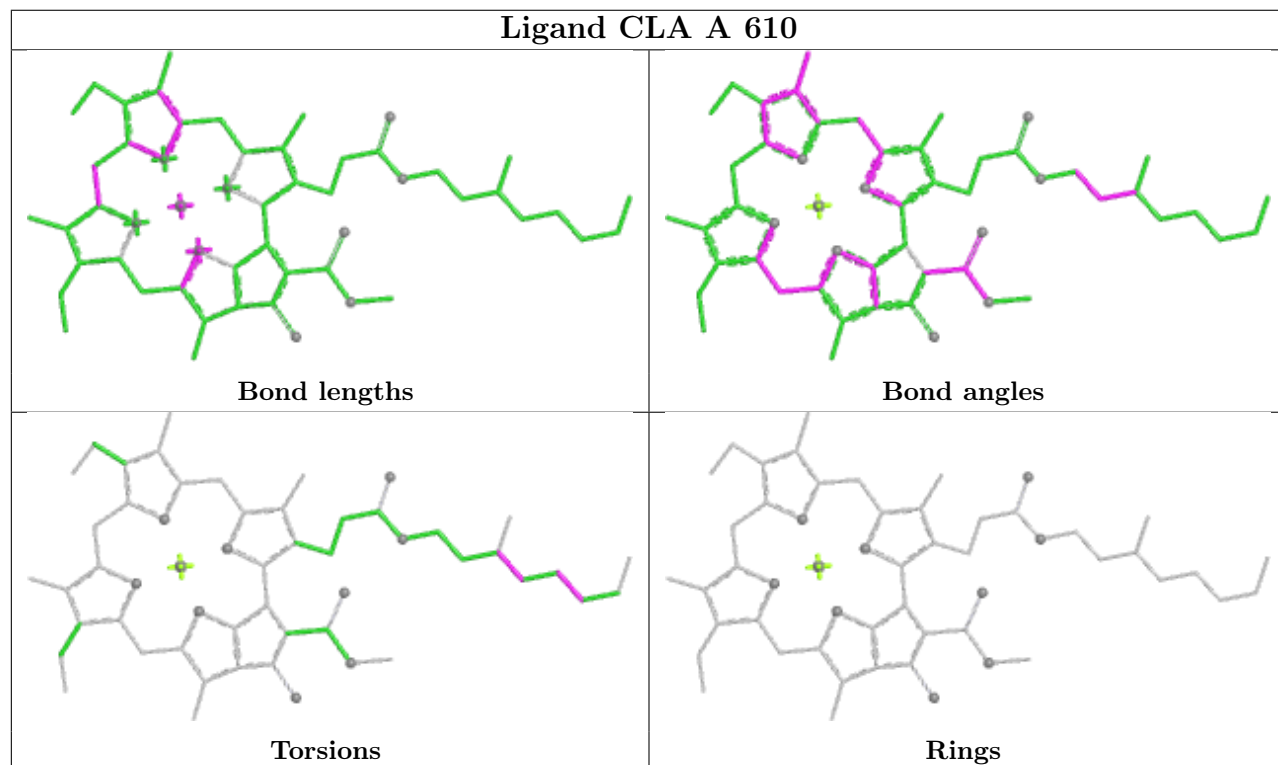
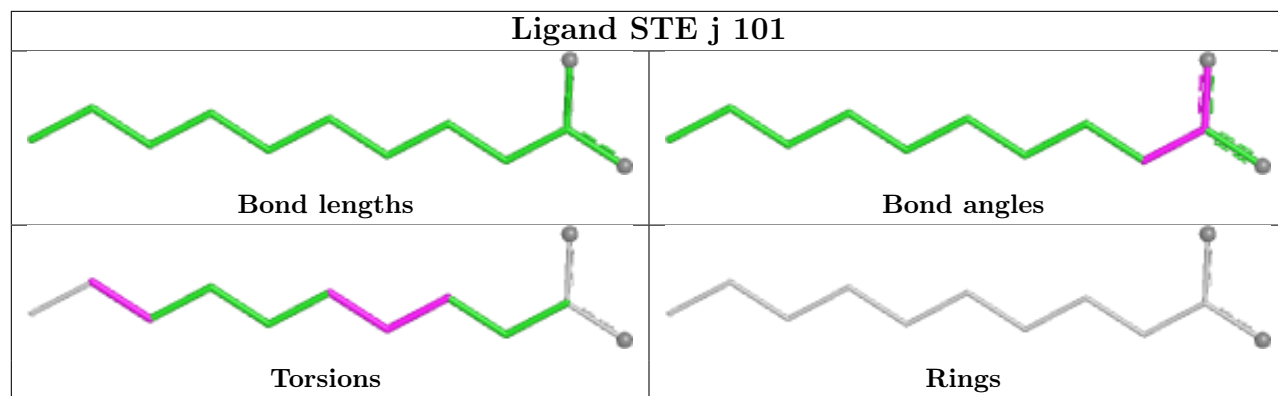
Ligand CLA B 614	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR K 101	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand PL9 D 405	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

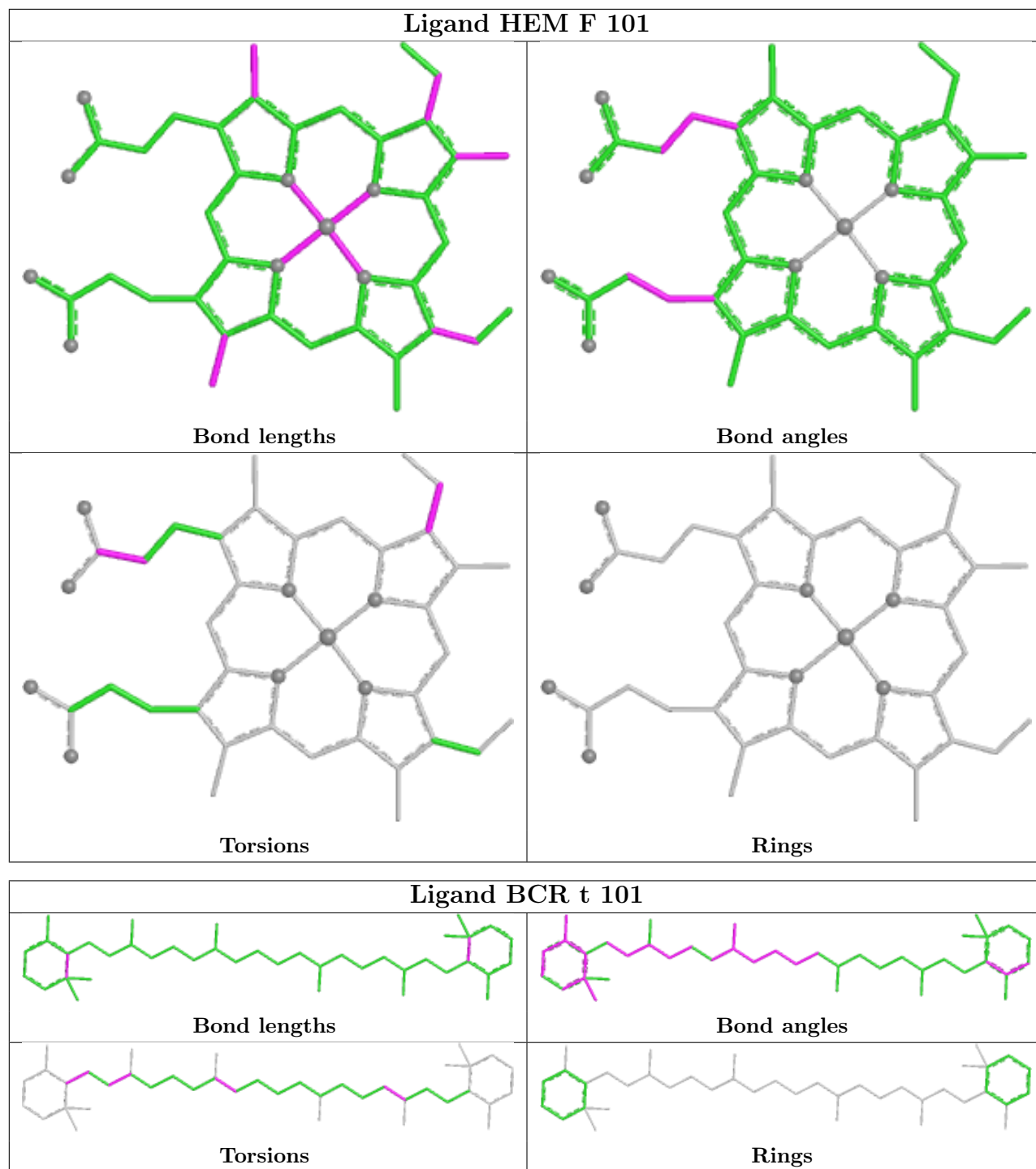


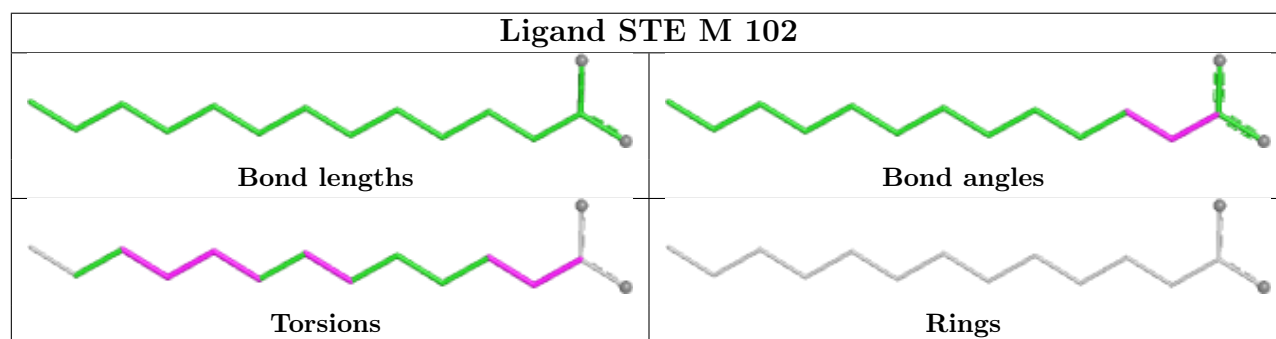
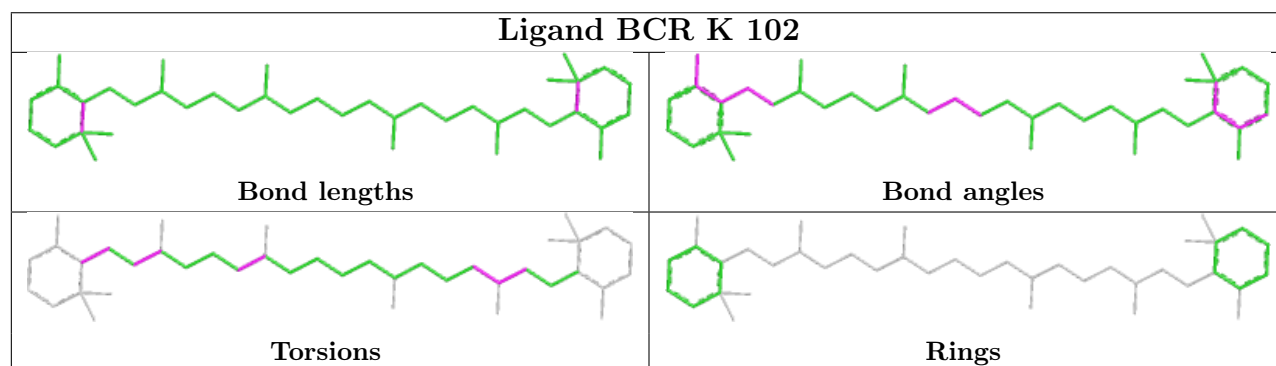
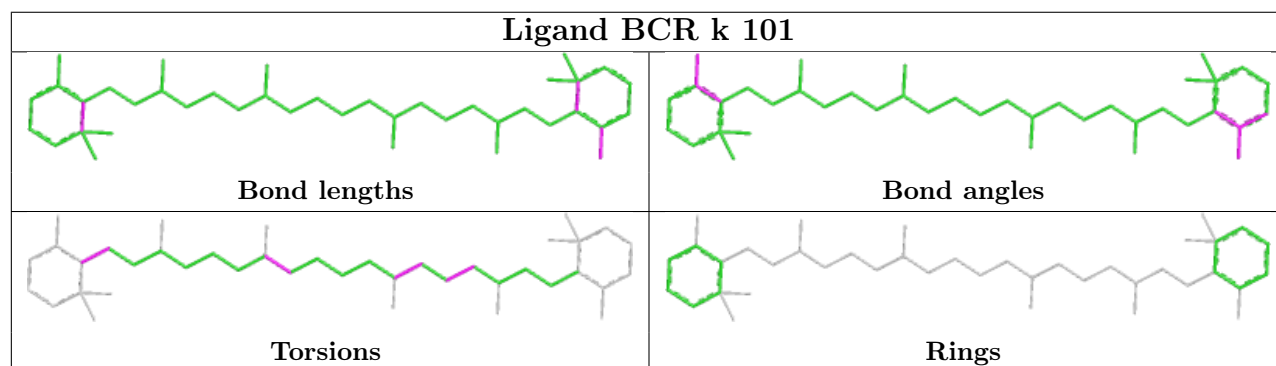
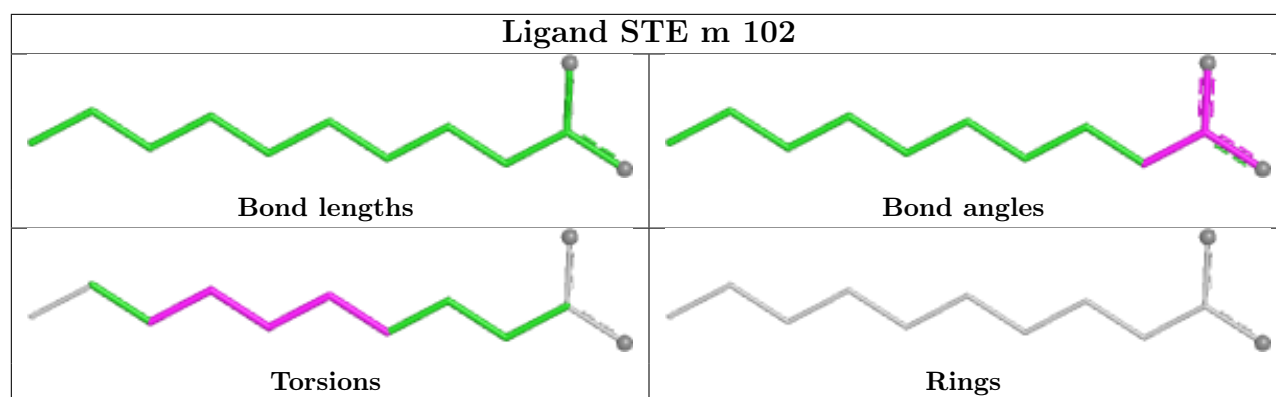


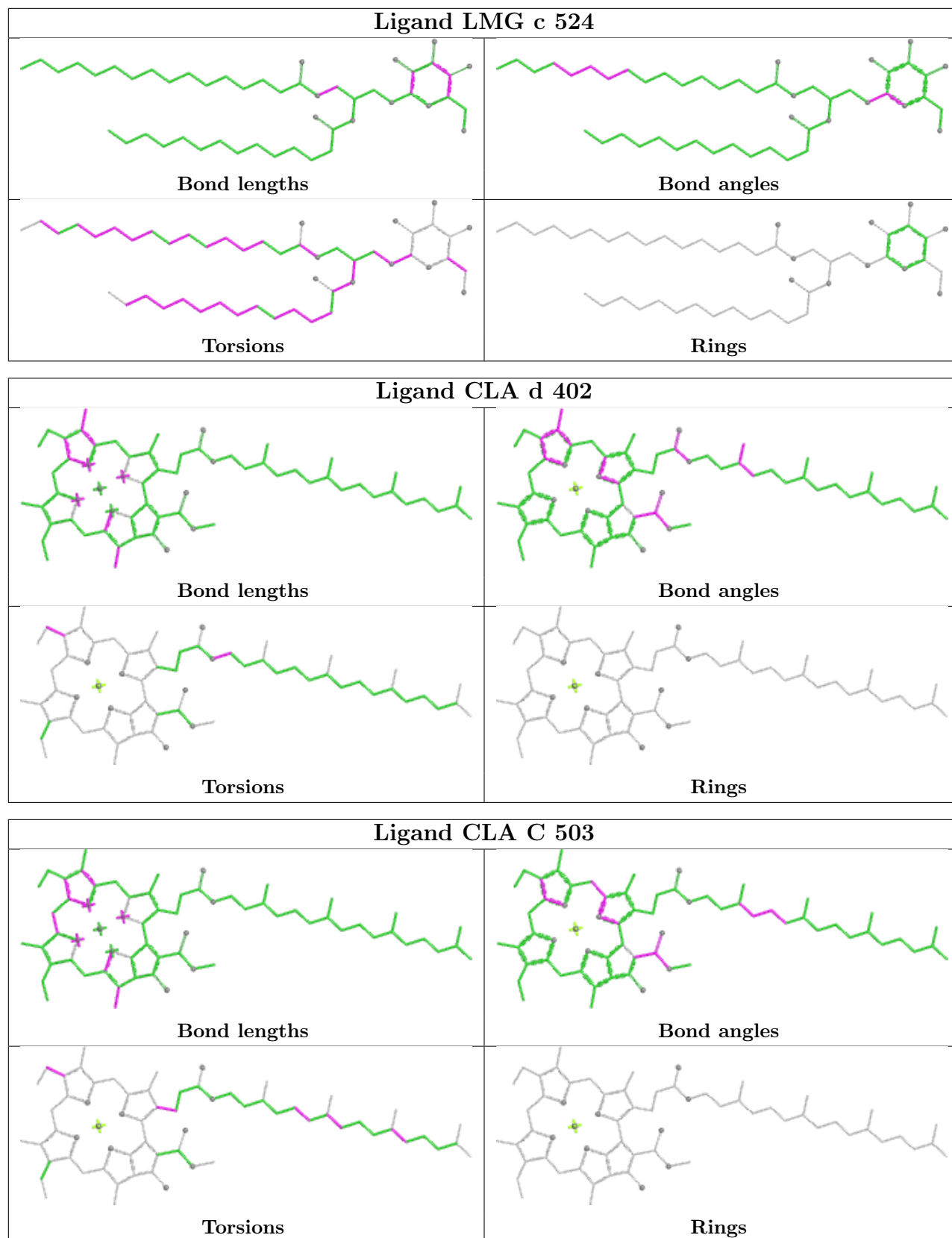
Ligand CLA B 613**Ligand LHG 1 102**

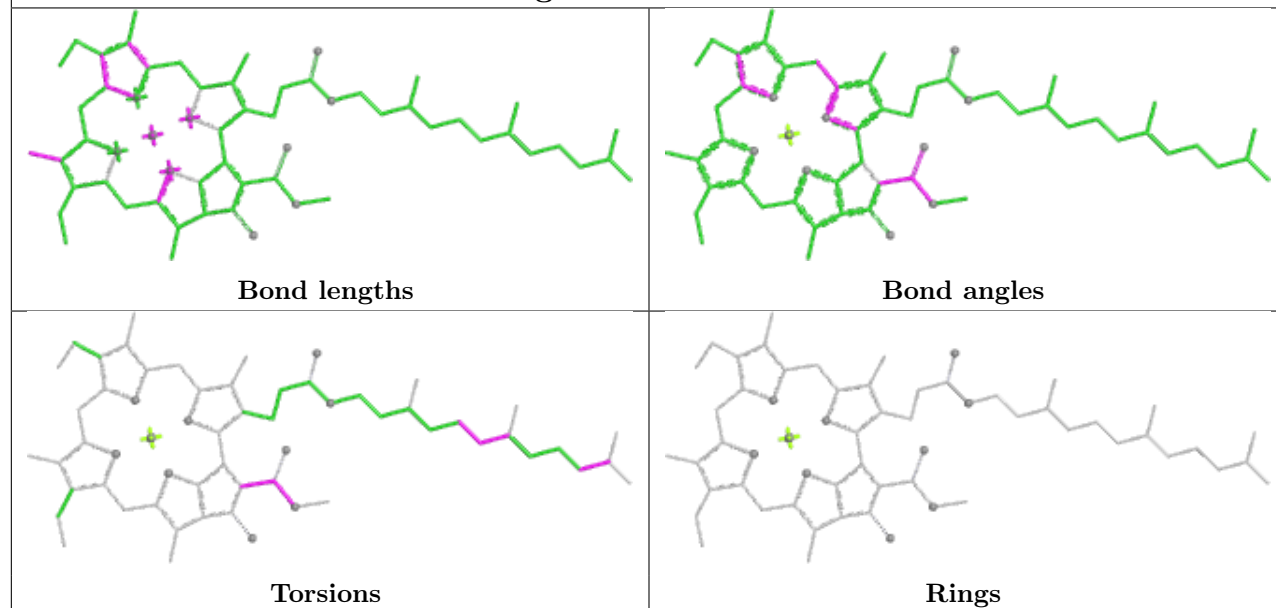
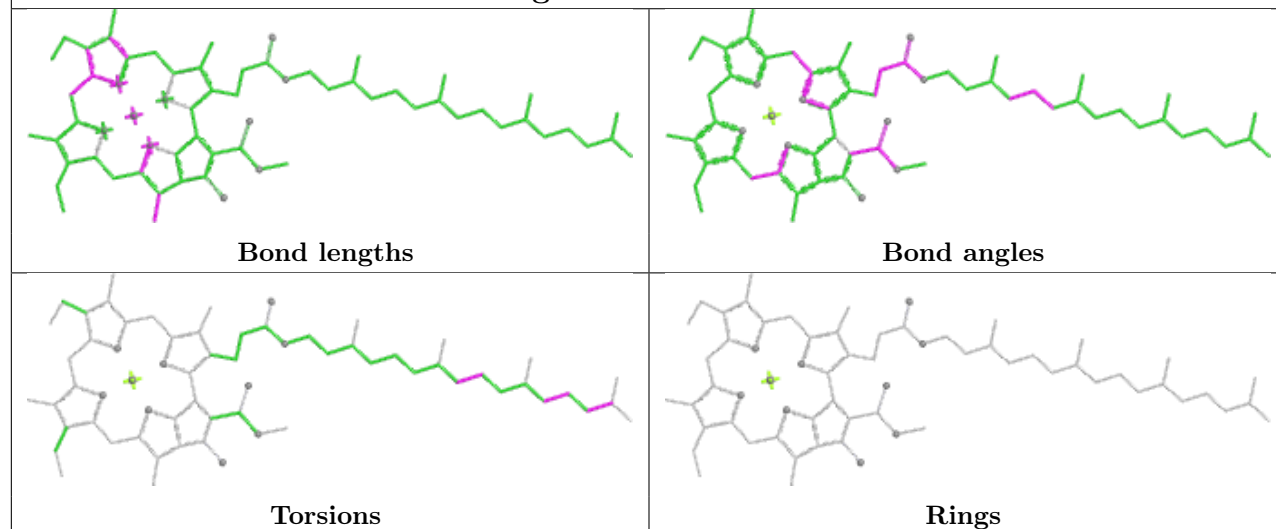
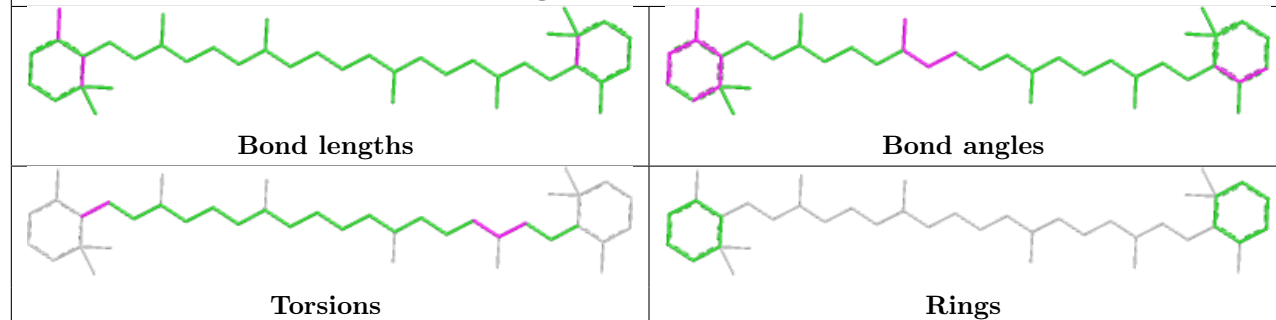


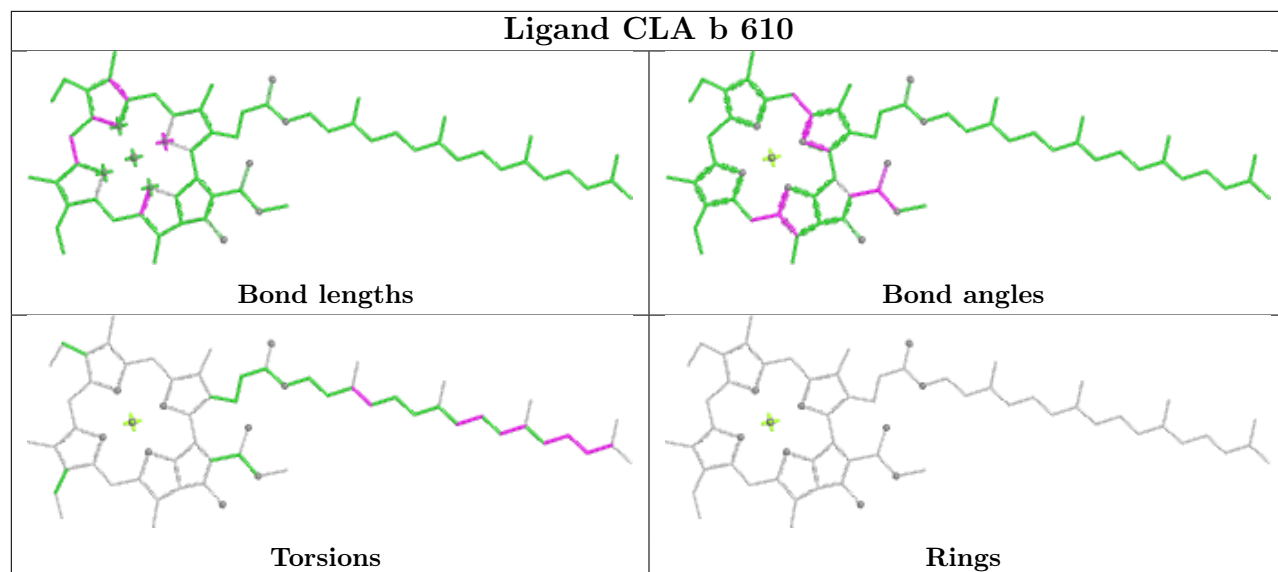
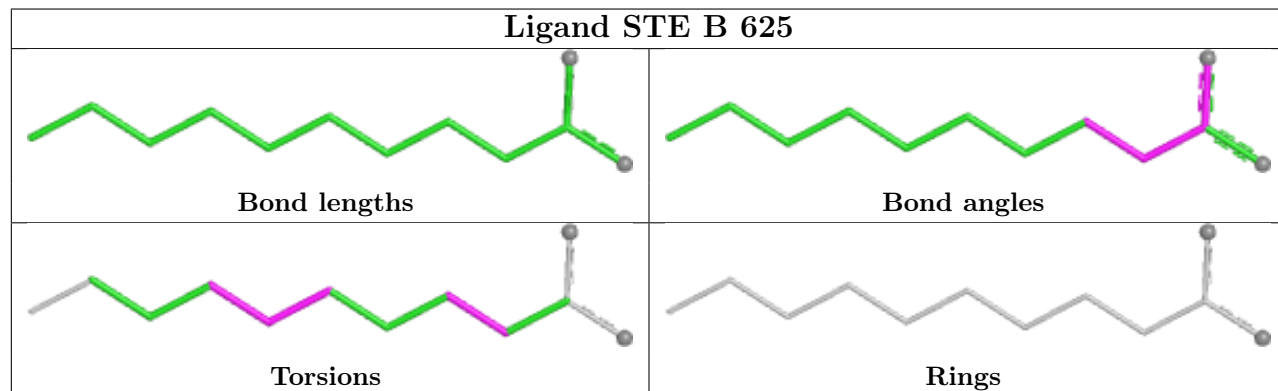
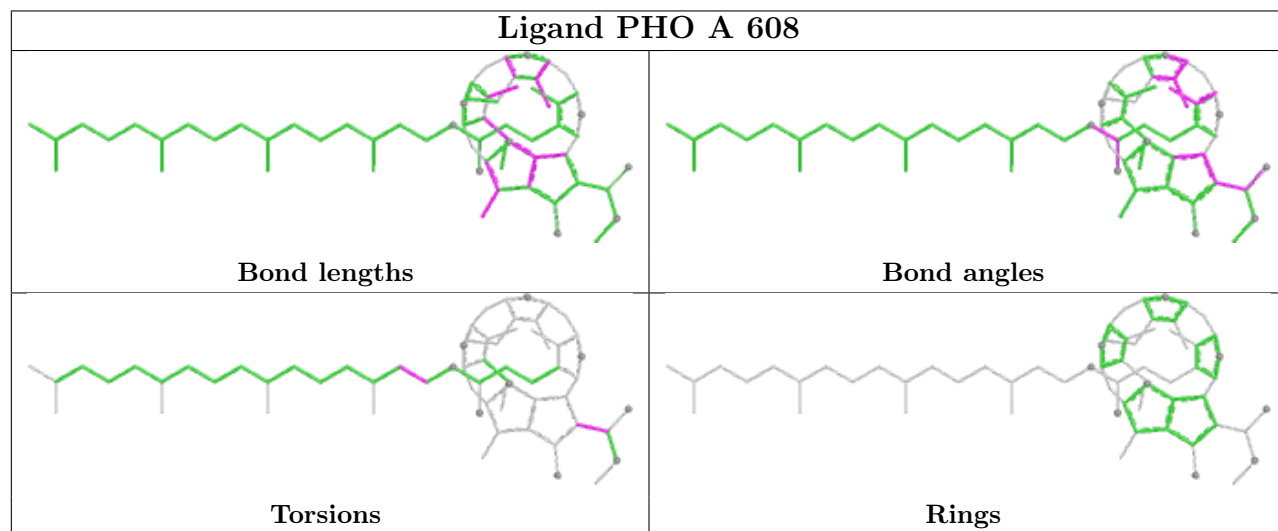




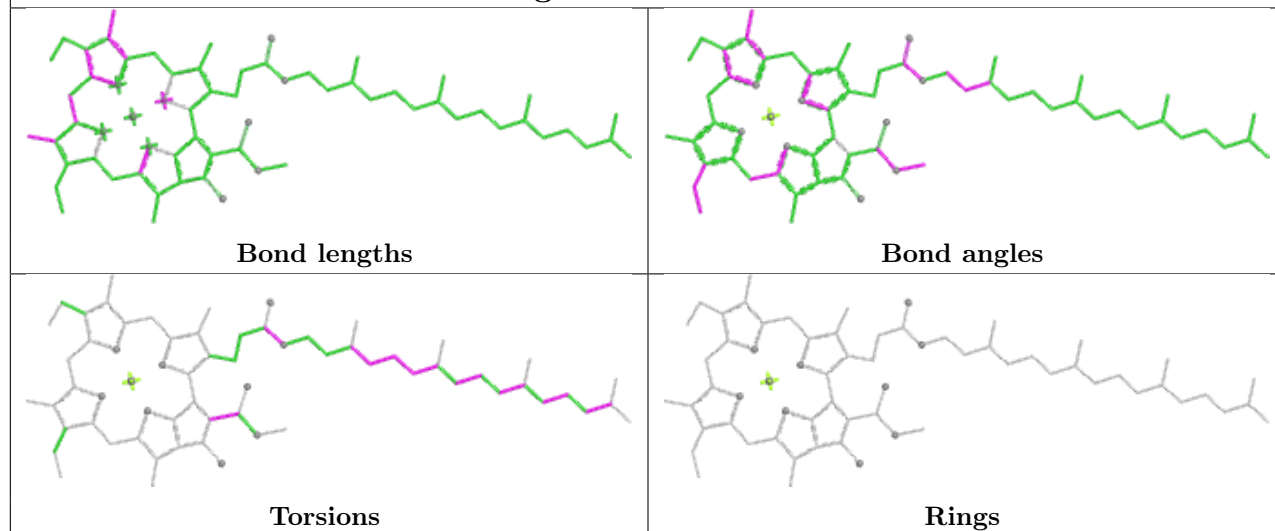




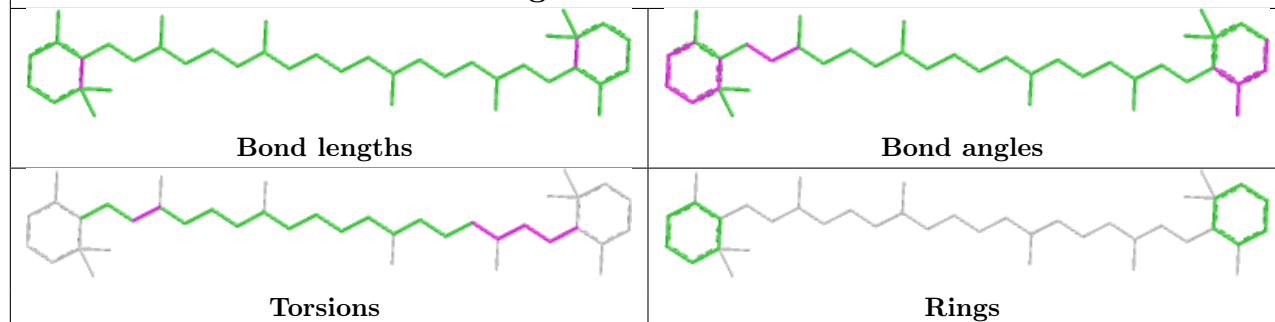
Ligand CLA b 615**Ligand CLA B 604****Ligand BCR b 616**

Ligand CLA b 610**Ligand STE B 625****Ligand PHO A 608**

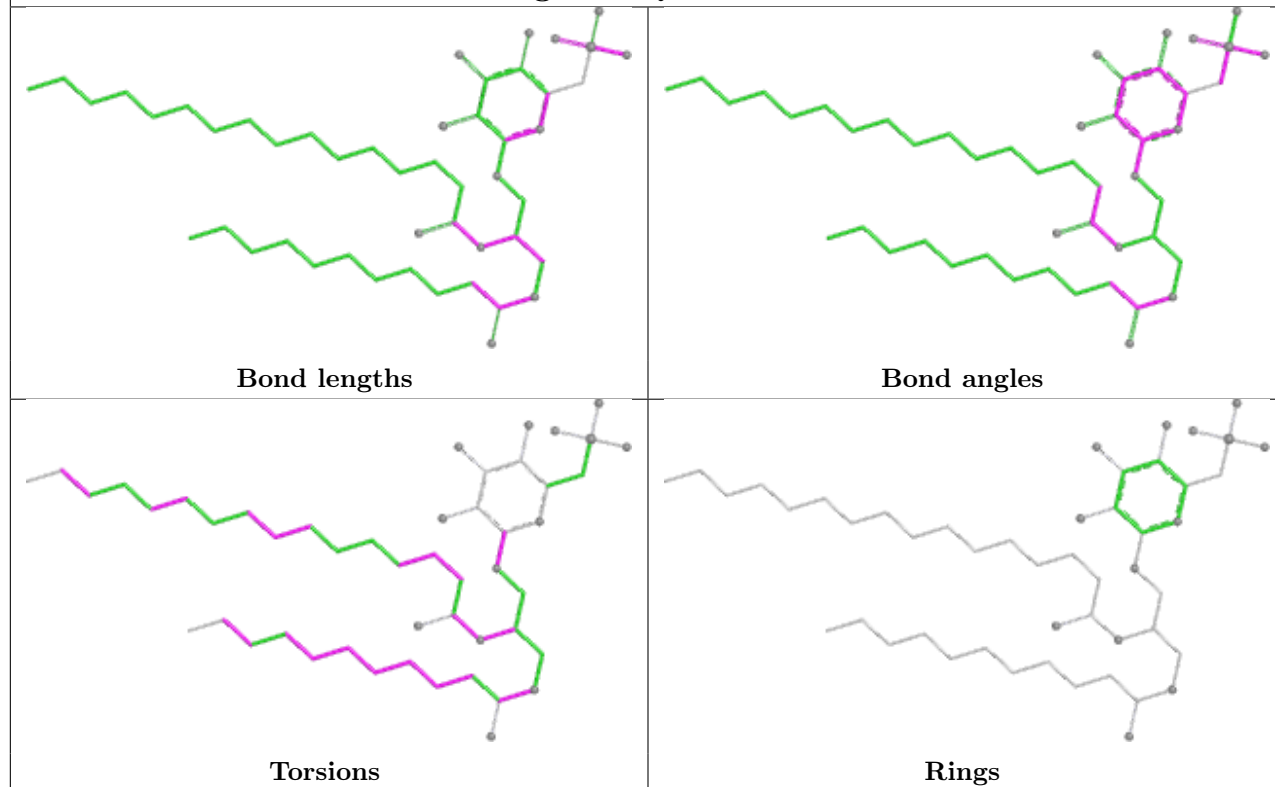
Ligand CLA b 613

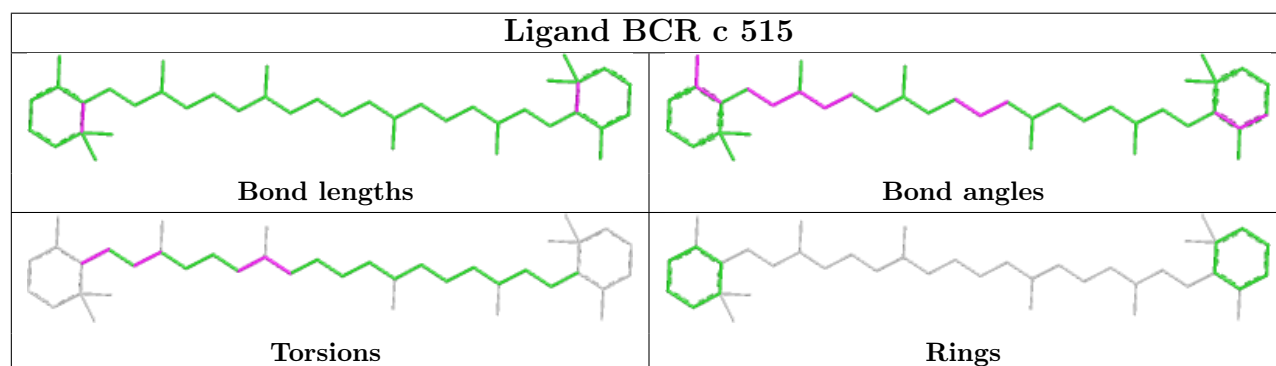
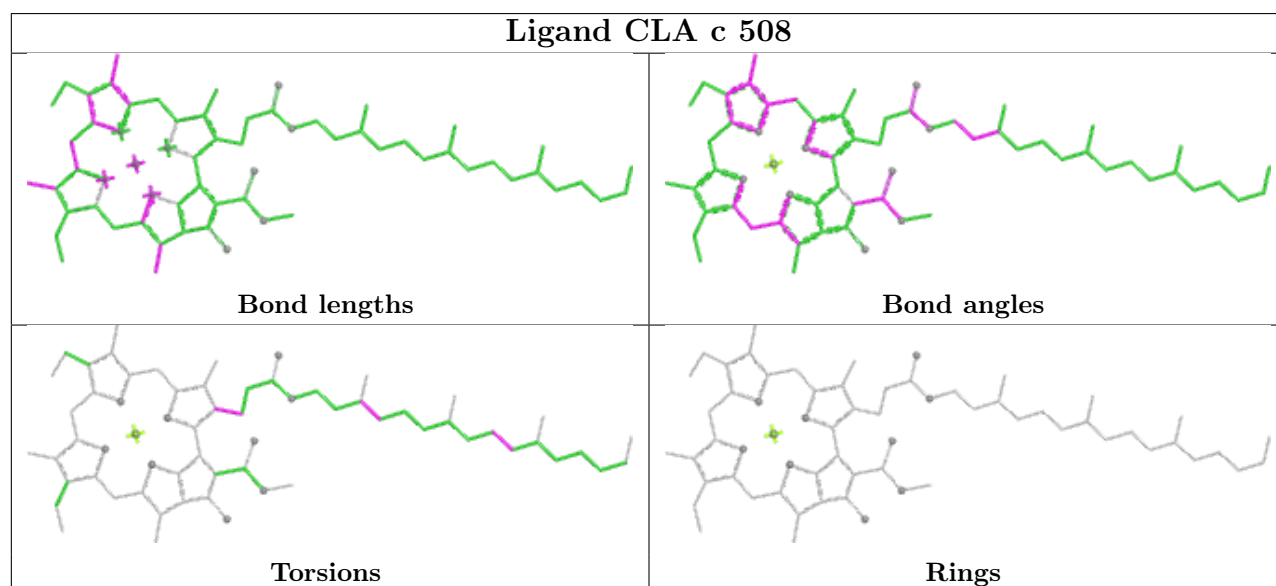
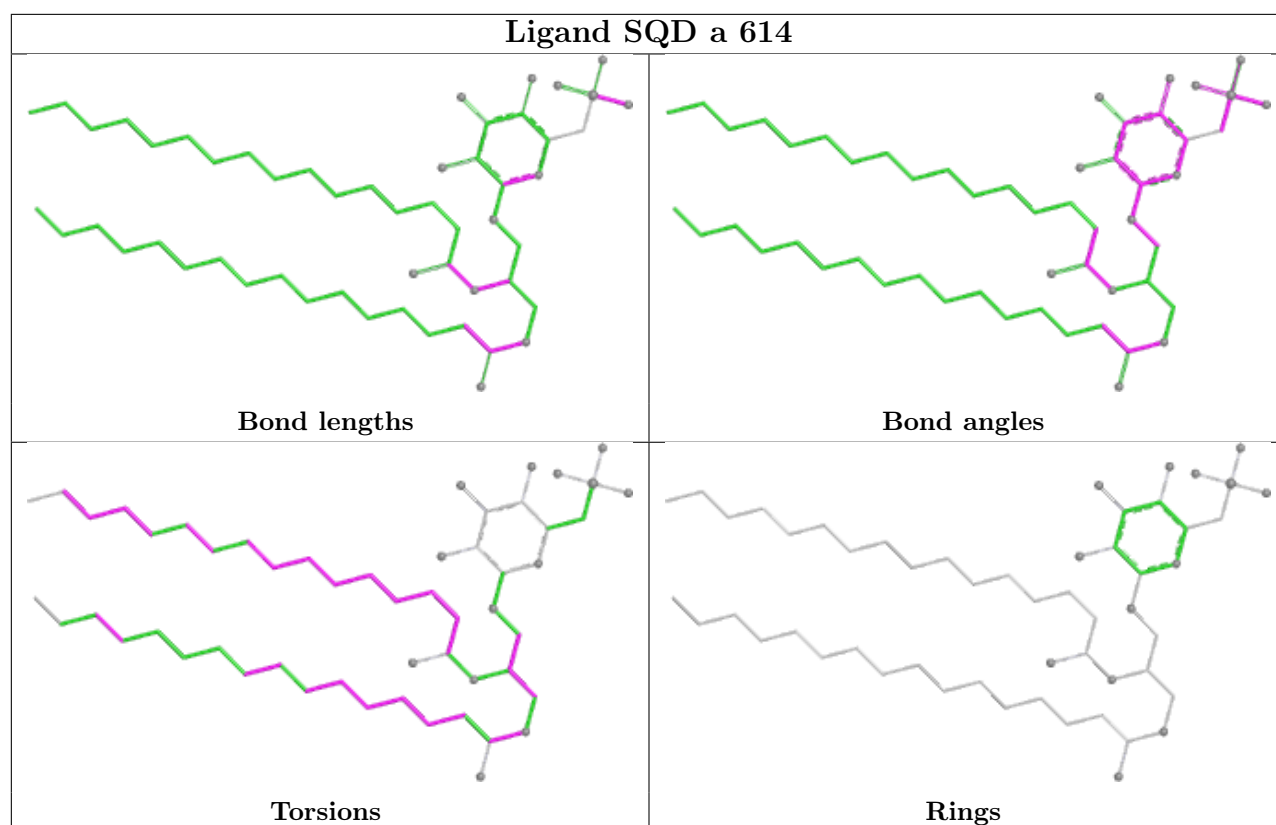


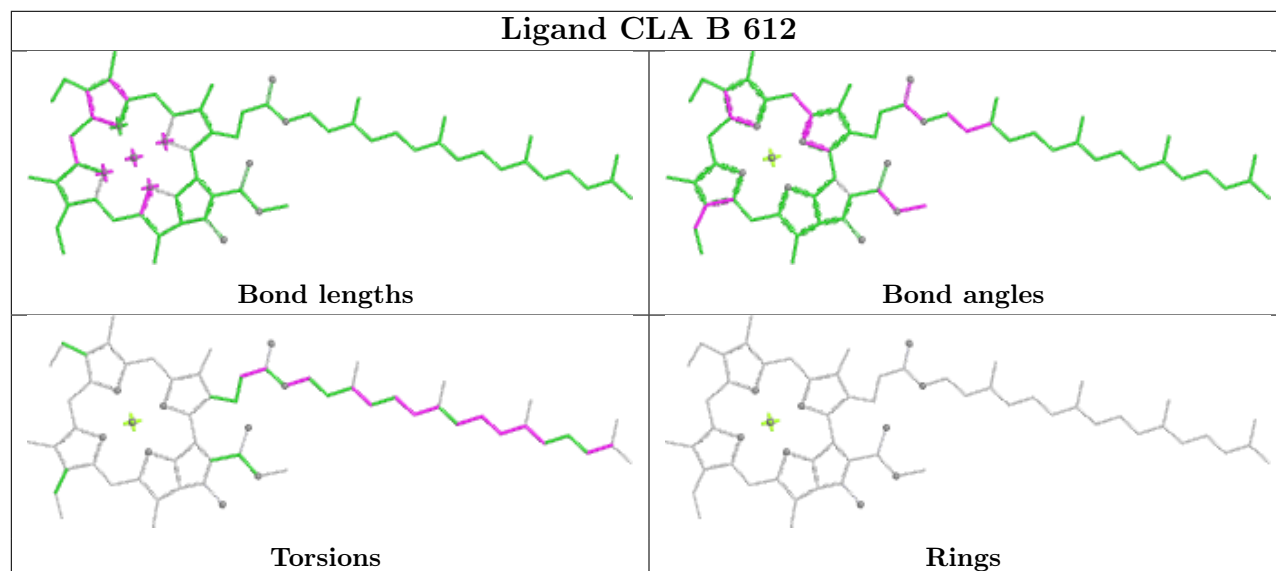
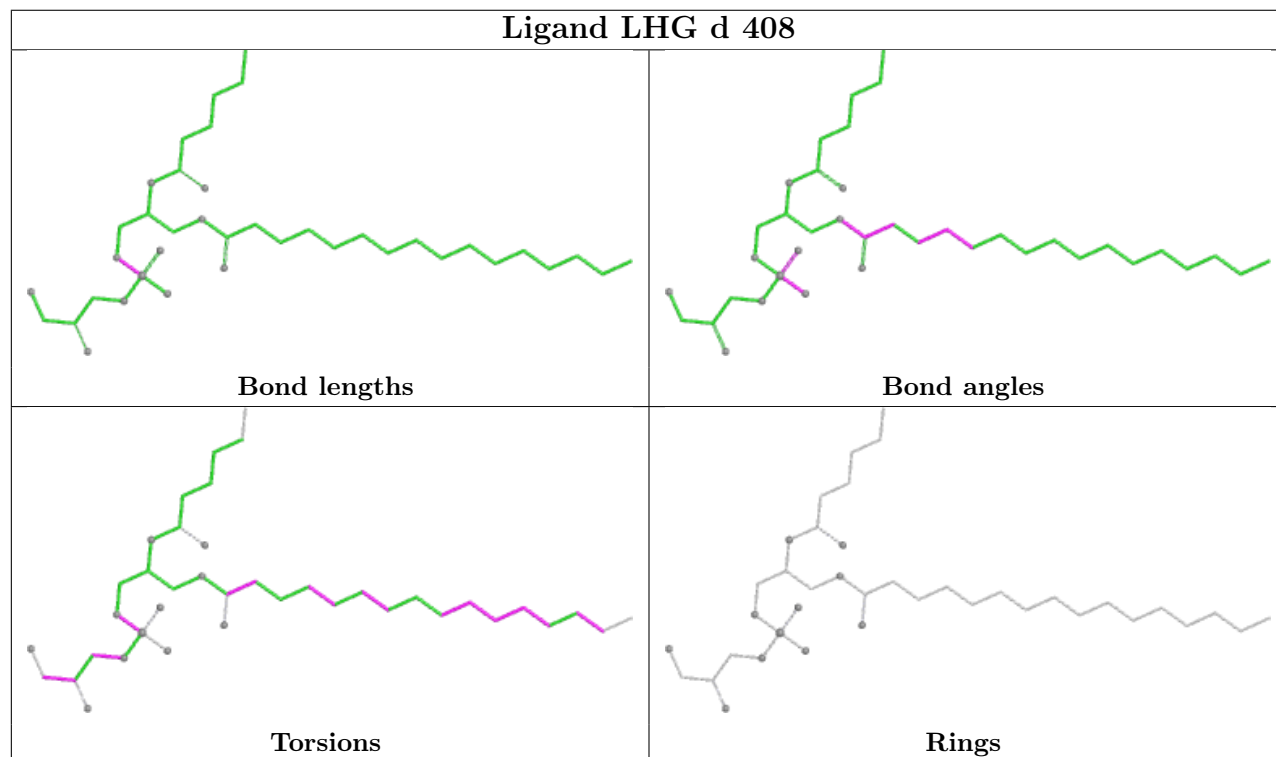
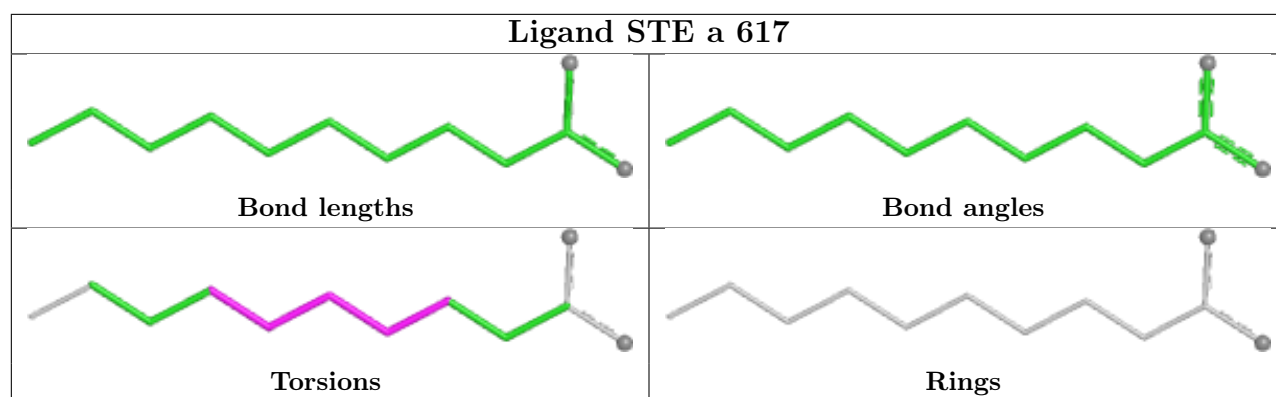
Ligand BCR D 404



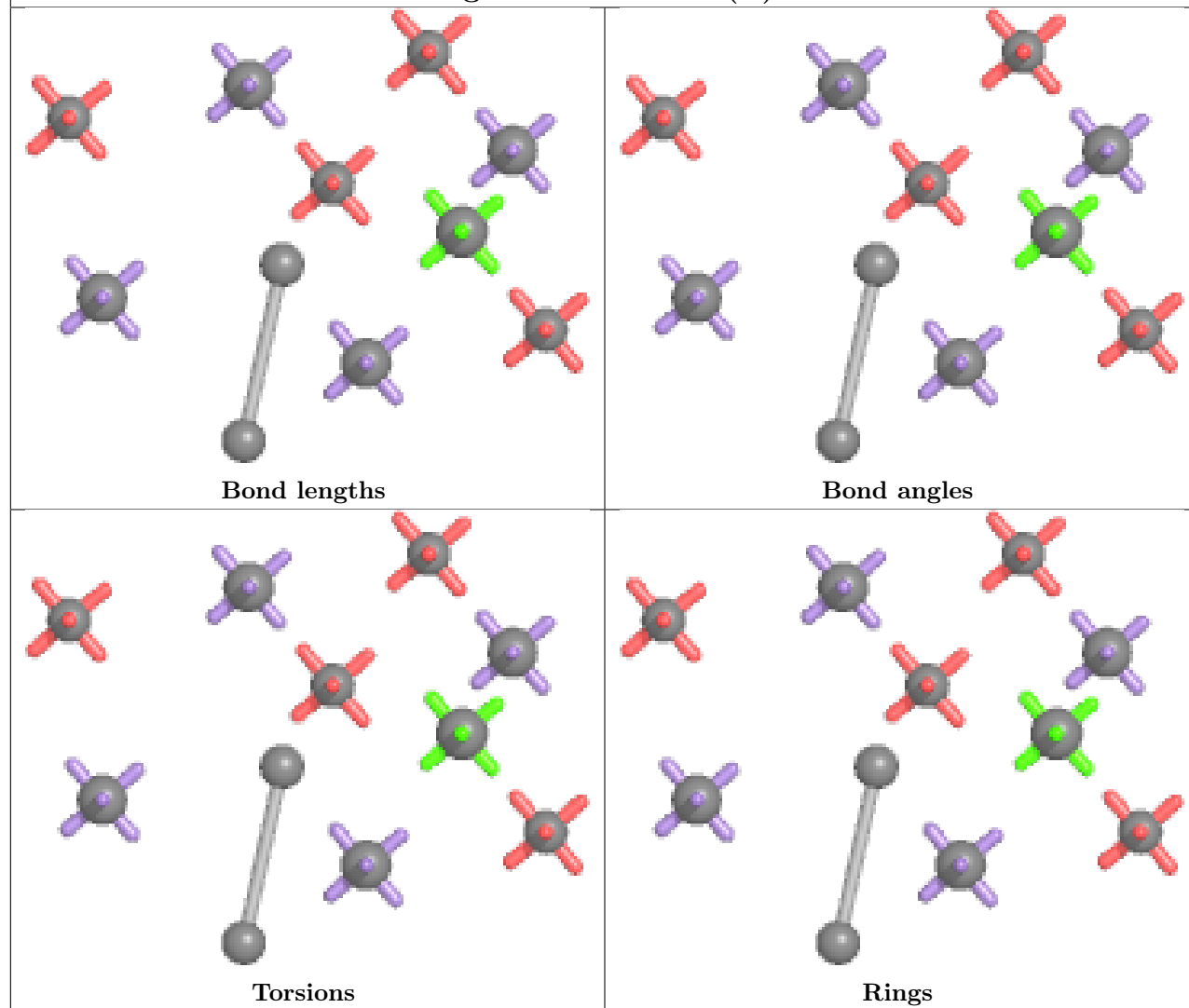
Ligand SQD L 101



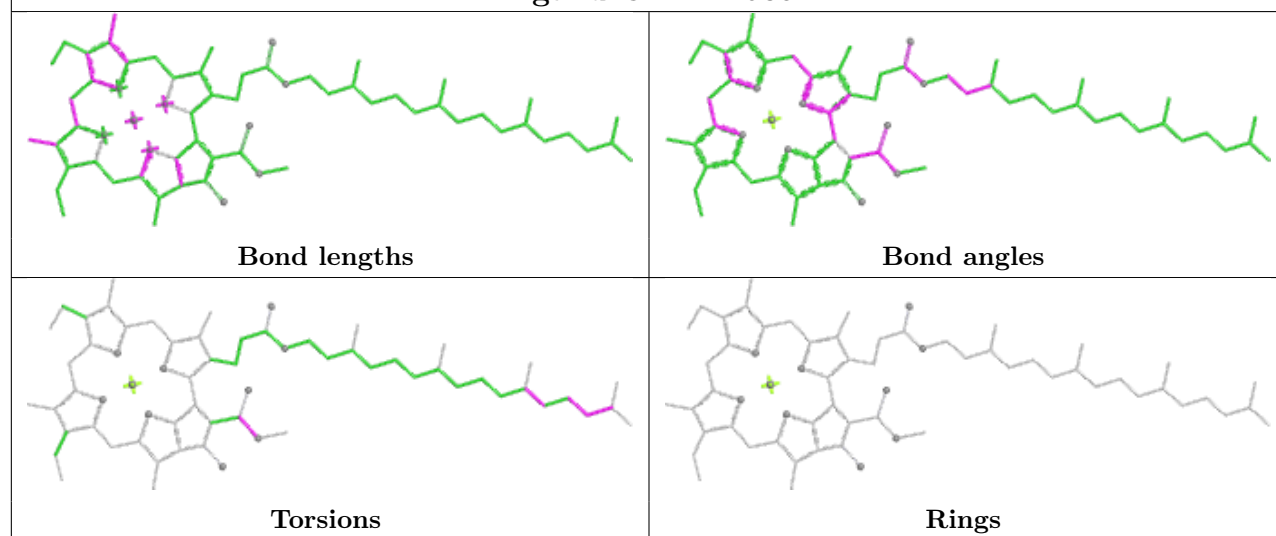


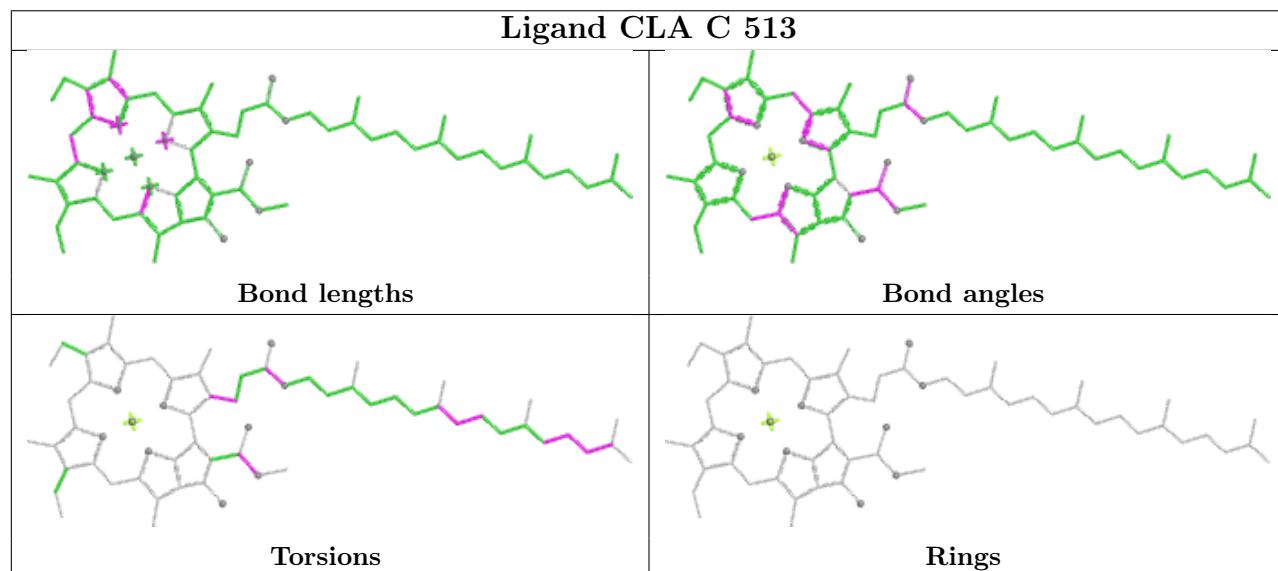
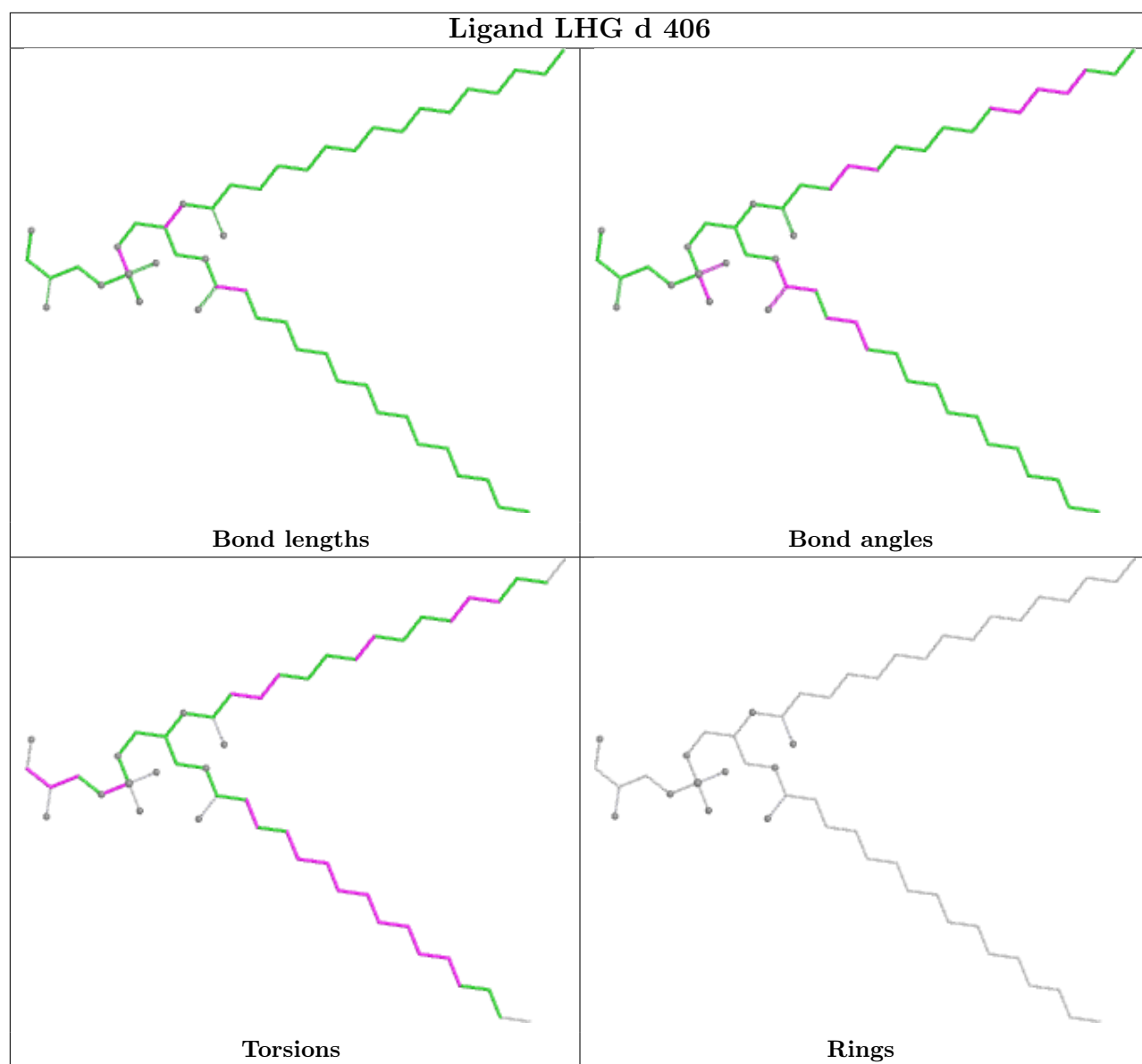


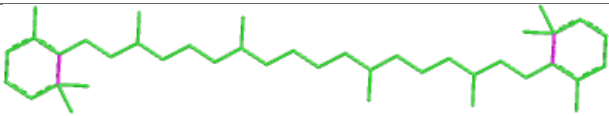
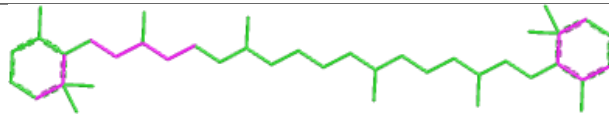
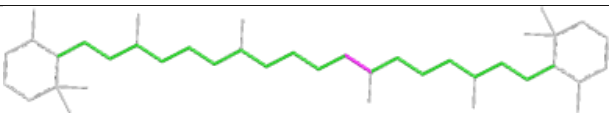
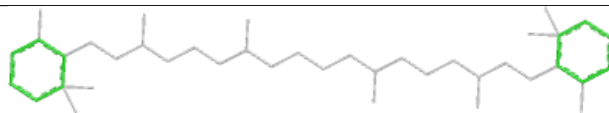
Ligand OEY A 601 (B)



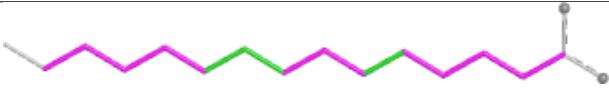
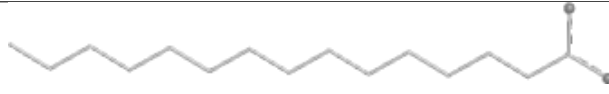


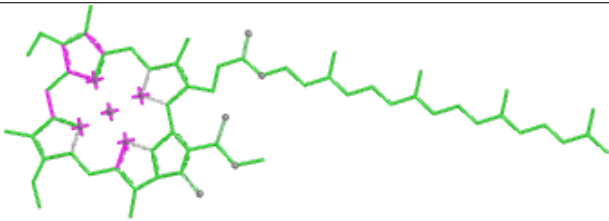
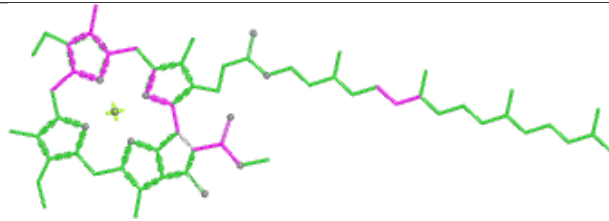
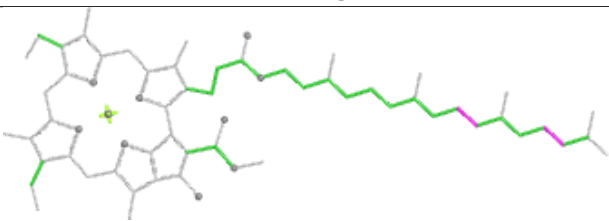
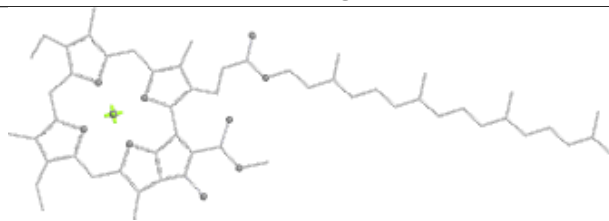
Ligand CLA B 609







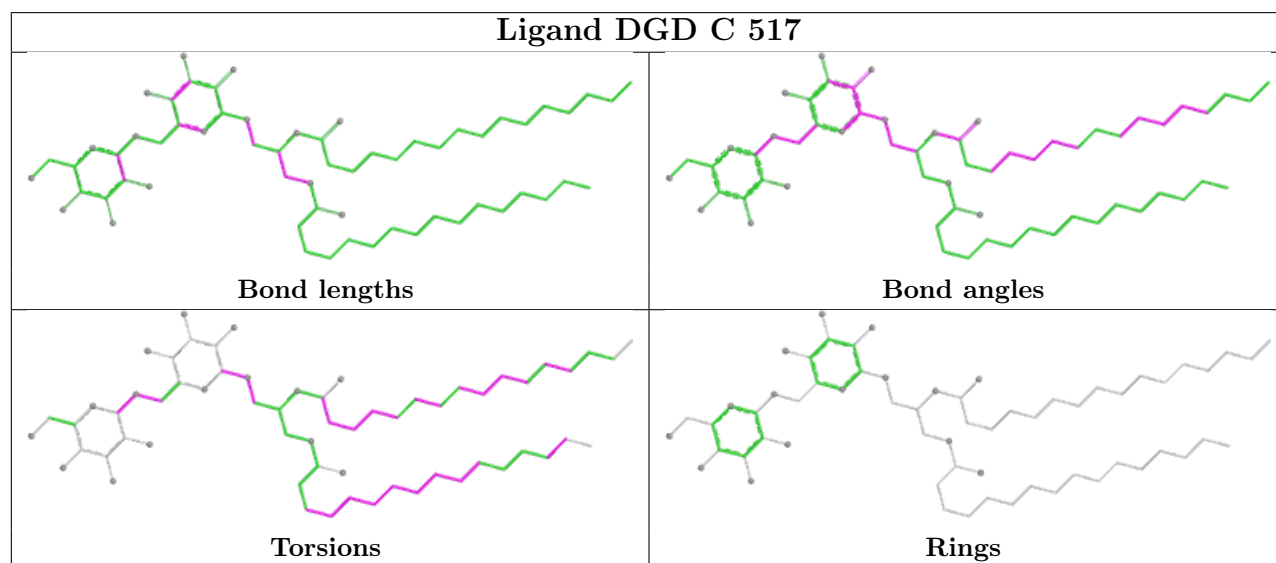
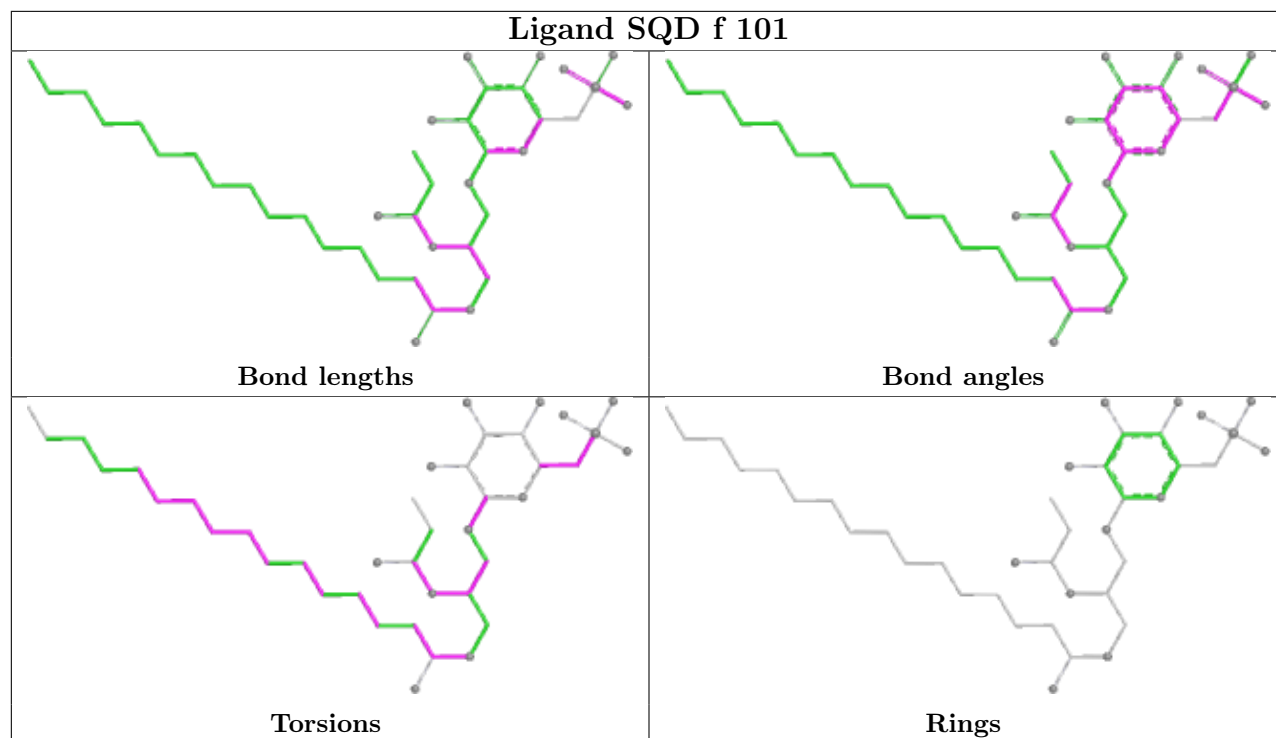


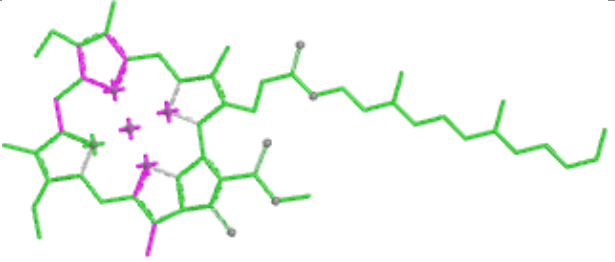
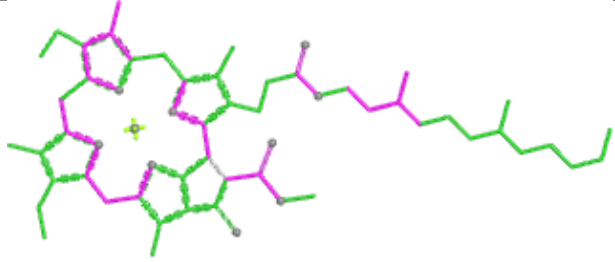
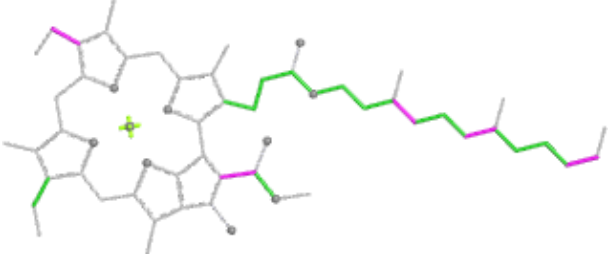
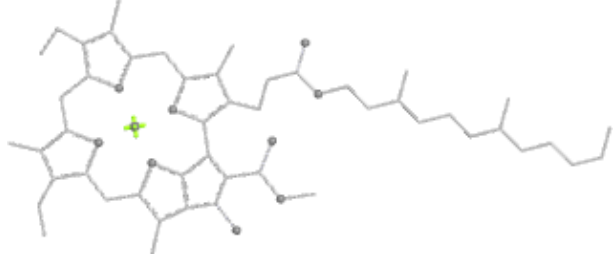
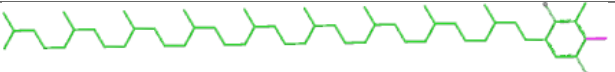
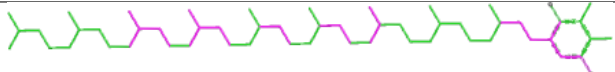
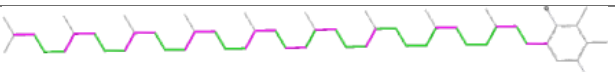
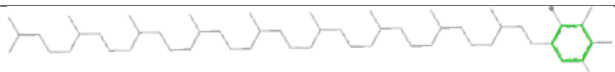
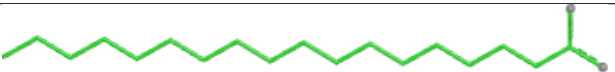
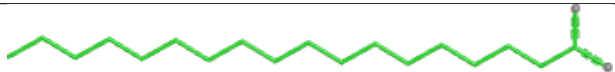
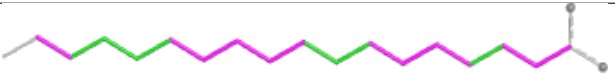

Ligand BCR a 611	
	
Bond lengths	Bond angles
	
Torsions	Rings

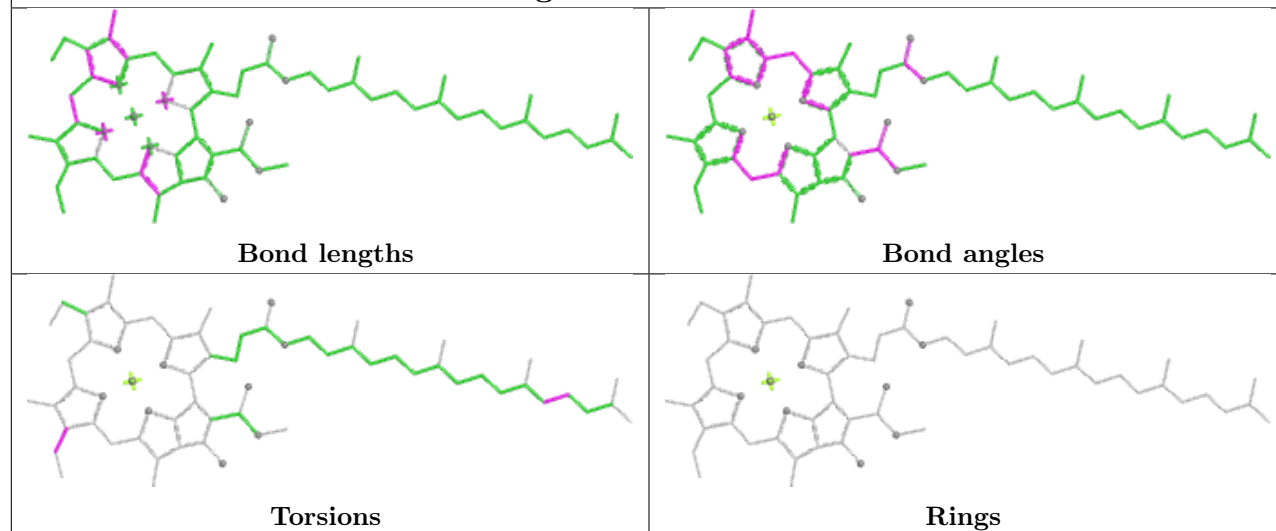
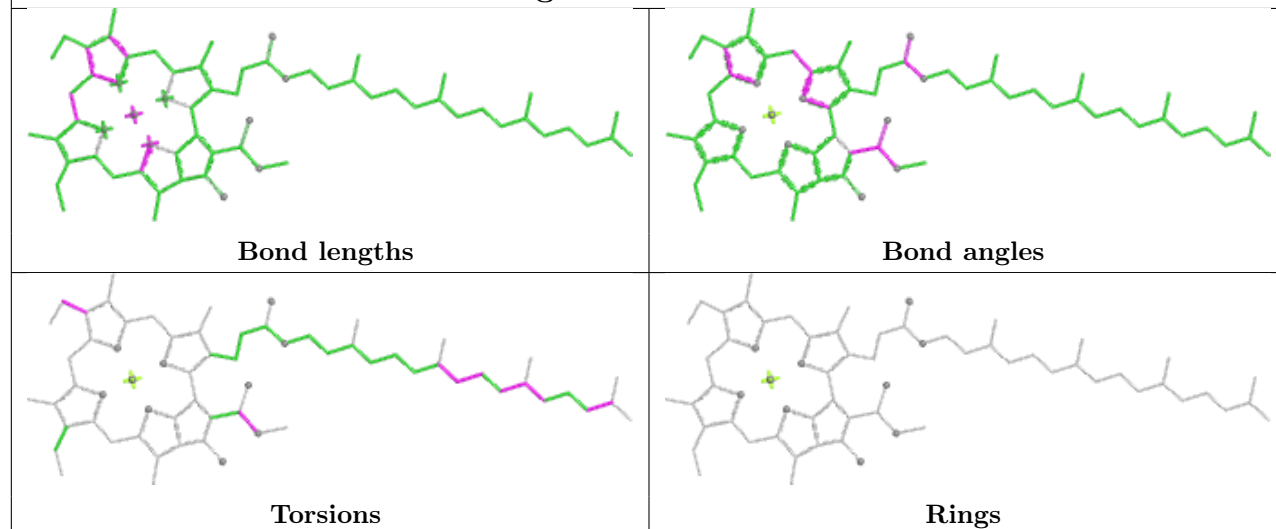
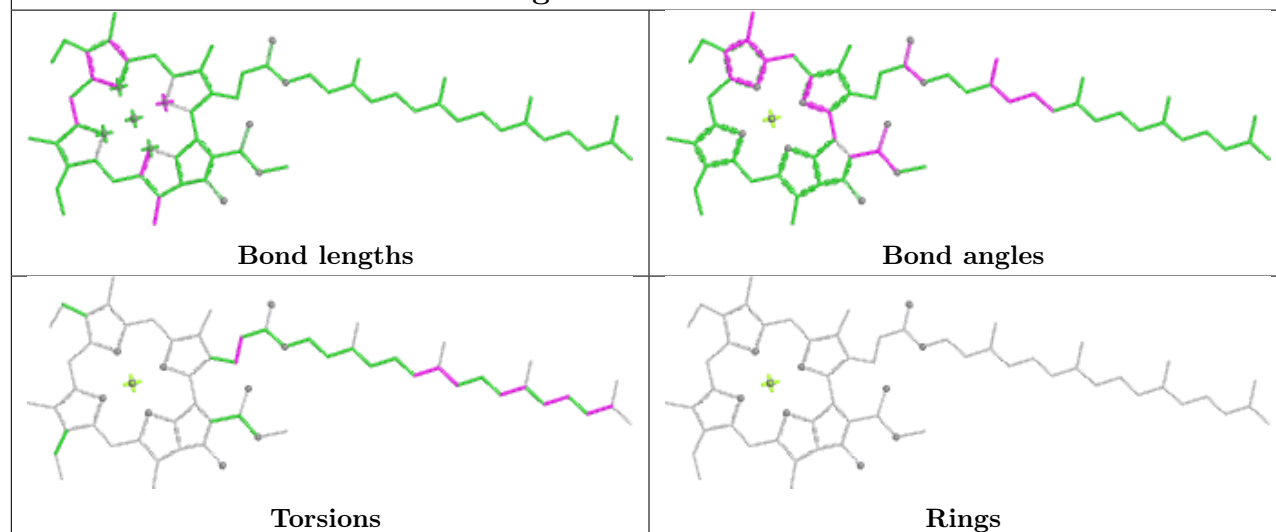
Ligand STE d 411	
	
Bond lengths	Bond angles
	
Torsions	Rings

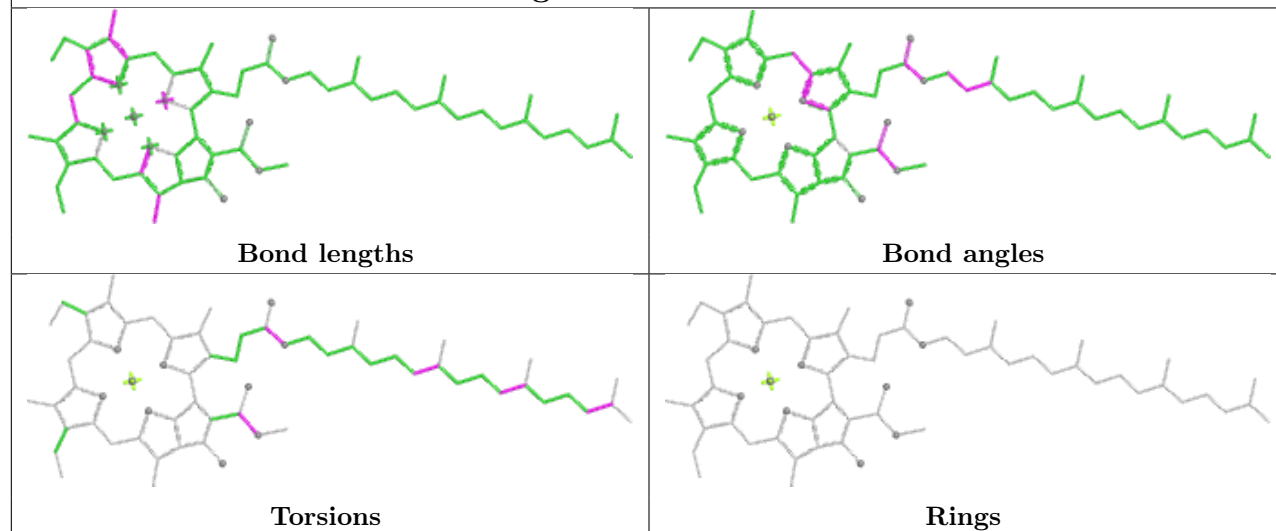
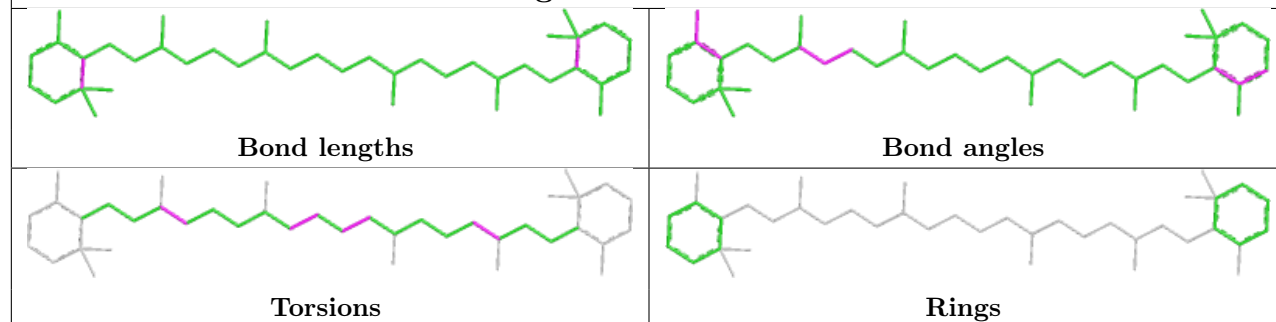
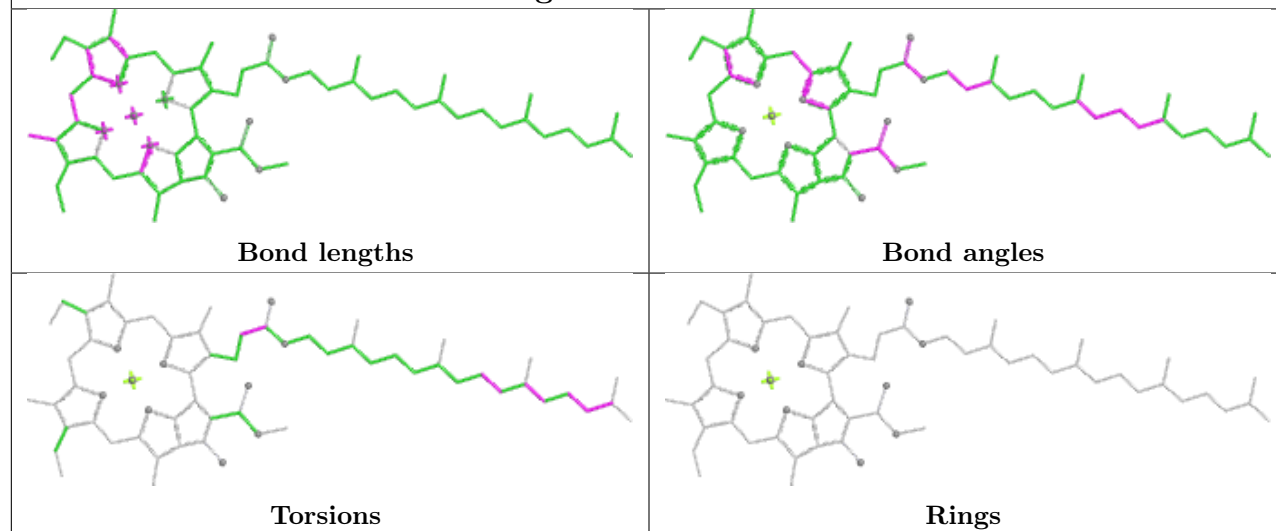
Ligand CLA B 607	
	
Bond lengths	Bond angles
	
Torsions	Rings

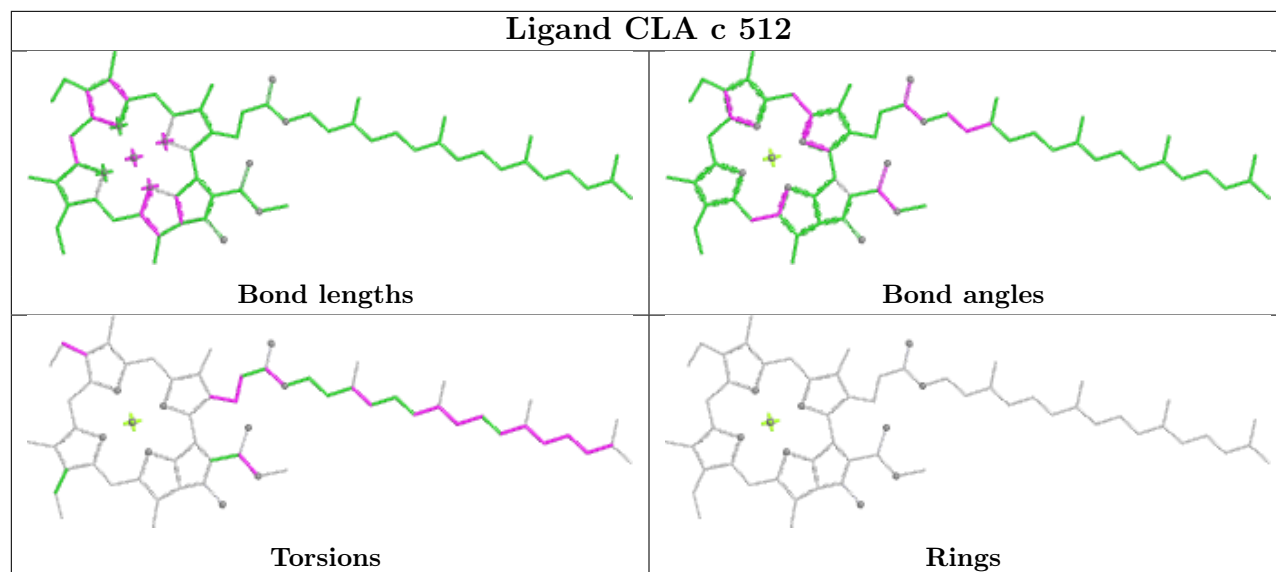
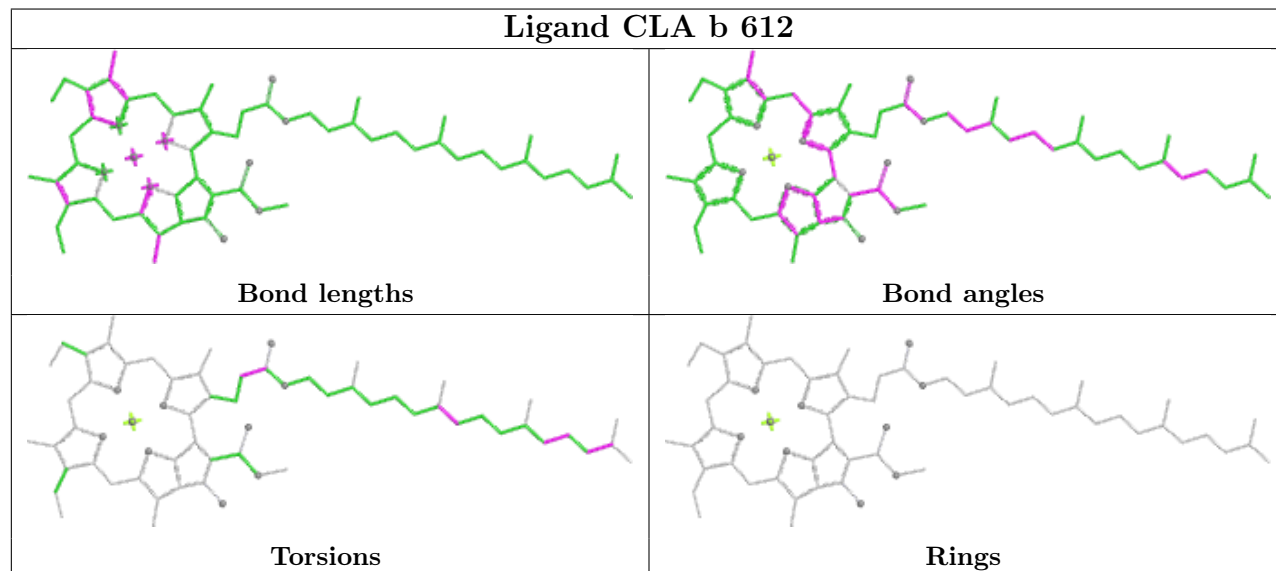
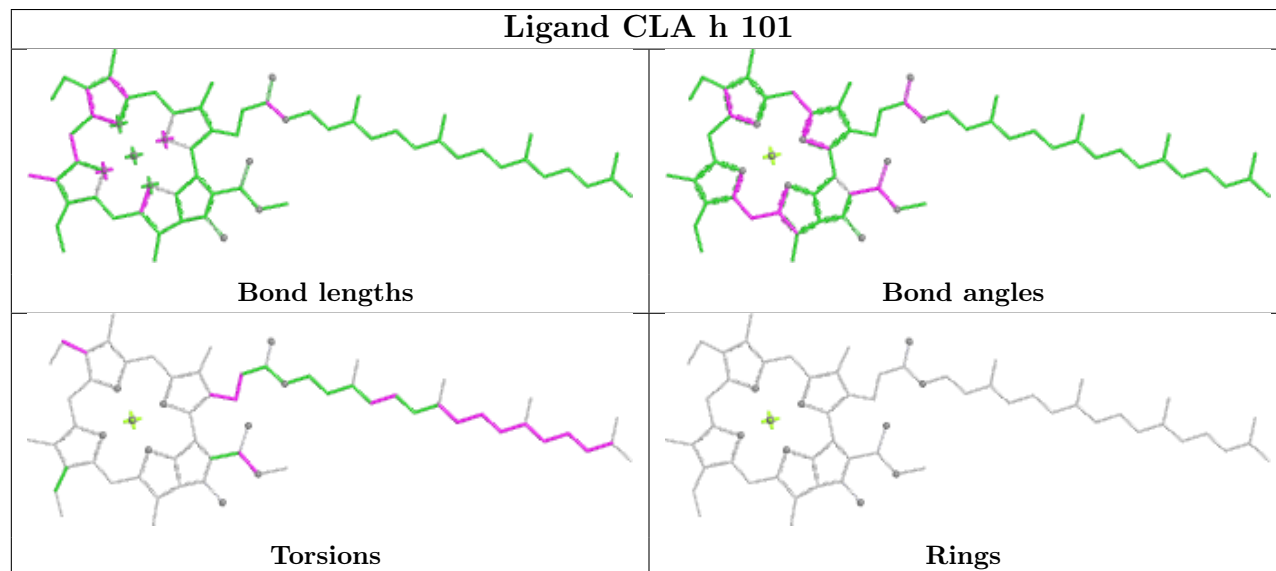
Ligand STE I 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

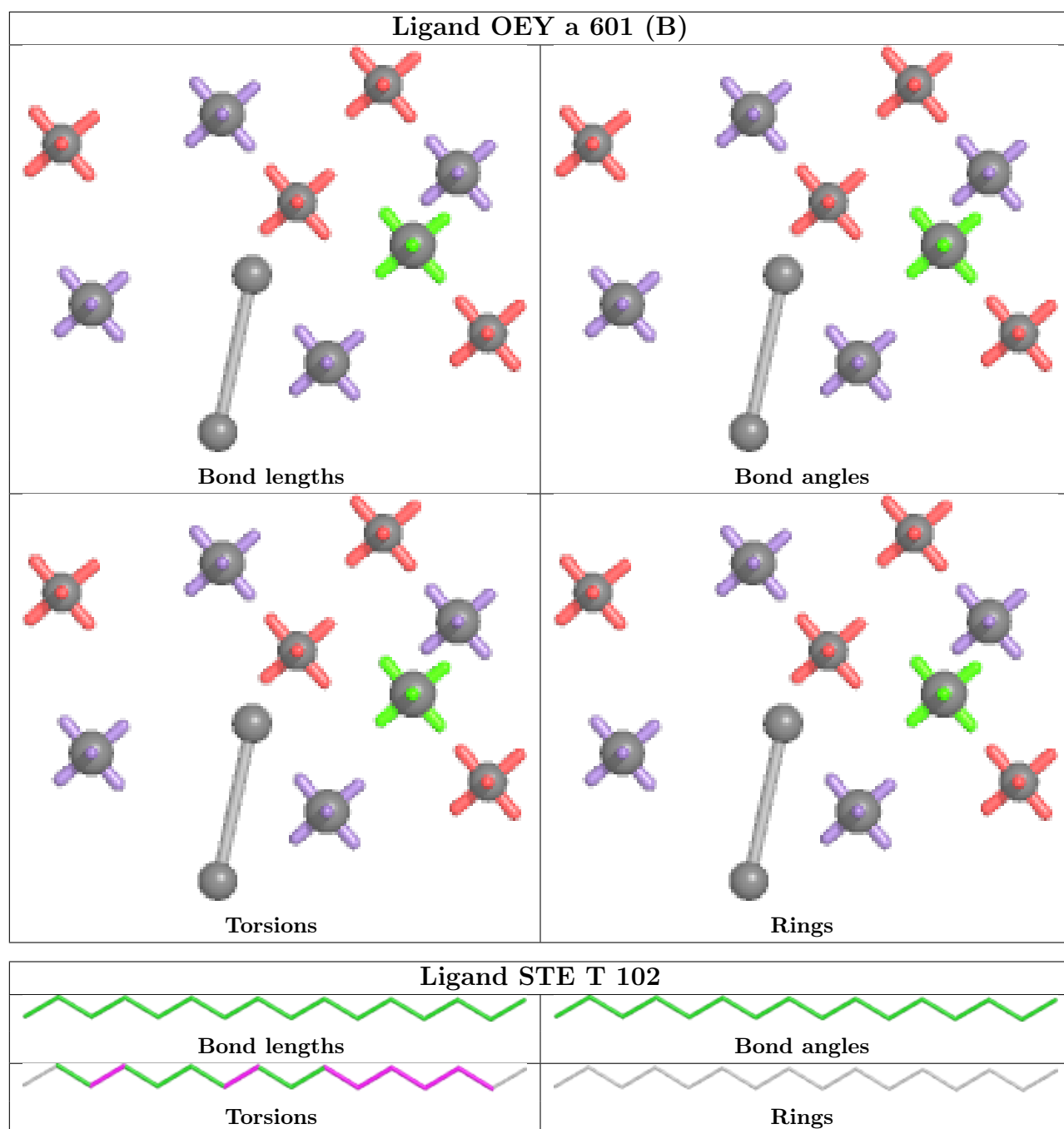


Ligand CLA C 504	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand PL9 a 612	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand STE c 521	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

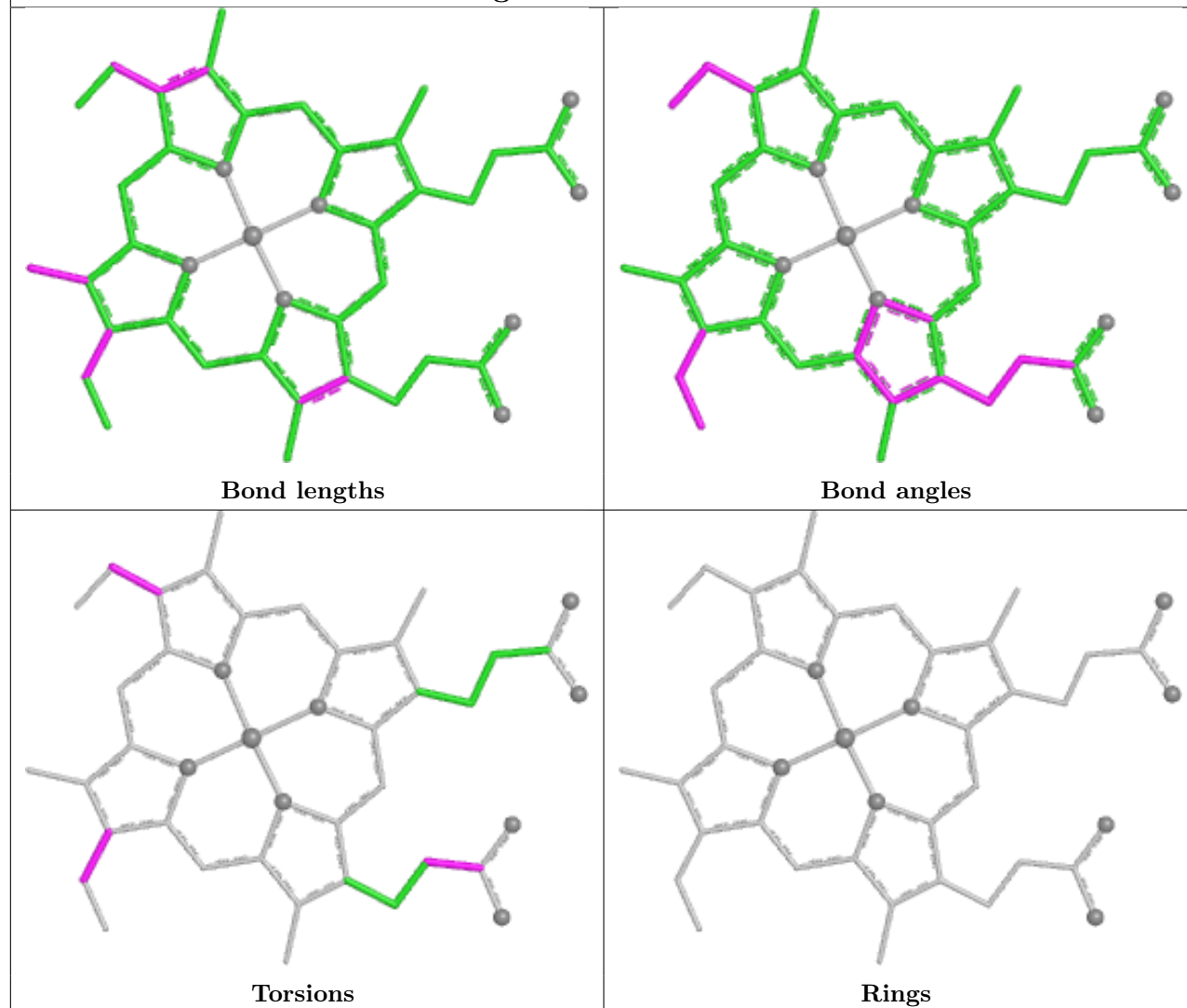
Ligand CLA b 607**Ligand CLA a 608****Ligand CLA B 602**

Ligand CLA C 511**Ligand BCR c 516****Ligand CLA b 611**

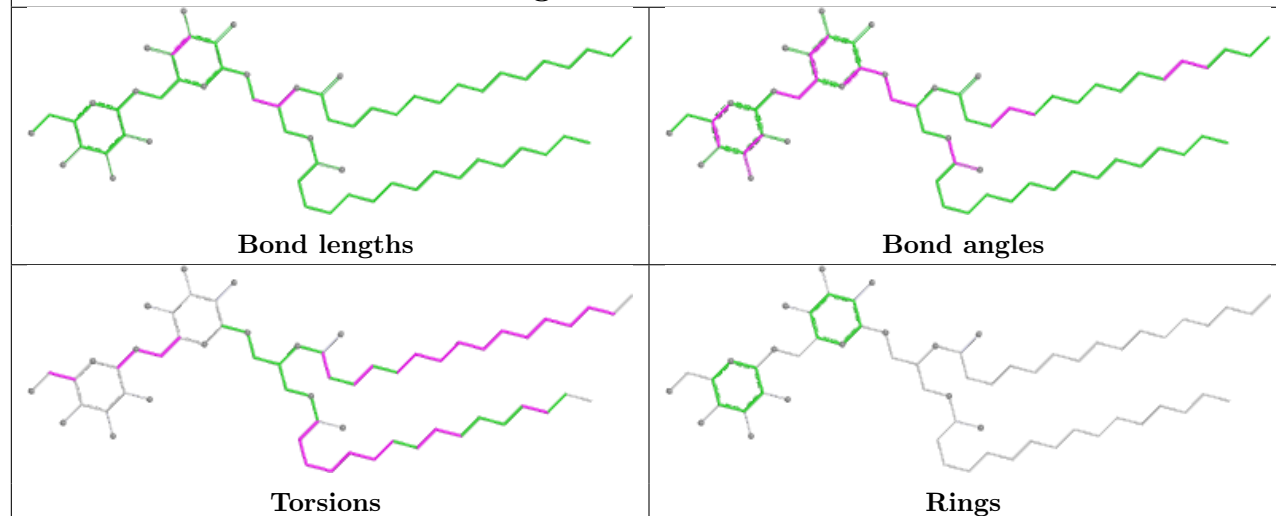
Ligand CLA c 512**Ligand CLA b 612****Ligand CLA h 101**

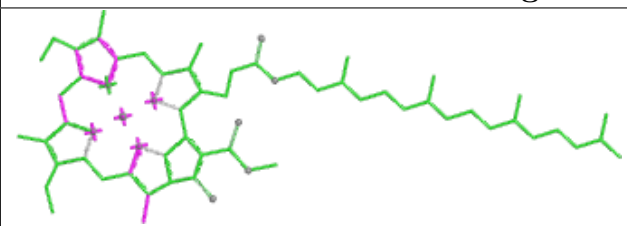
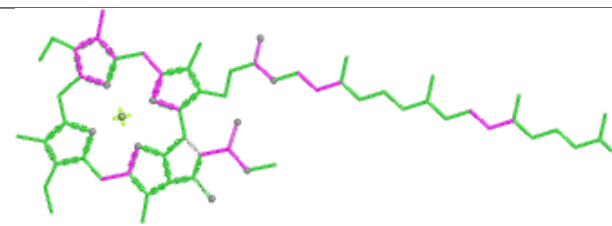
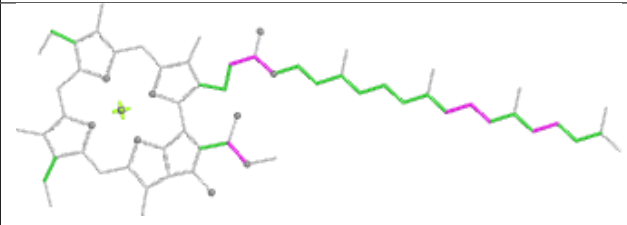
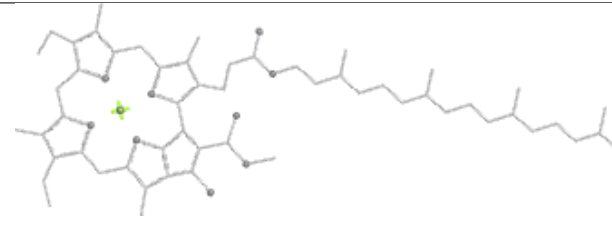


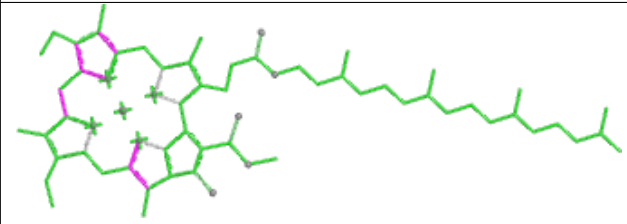
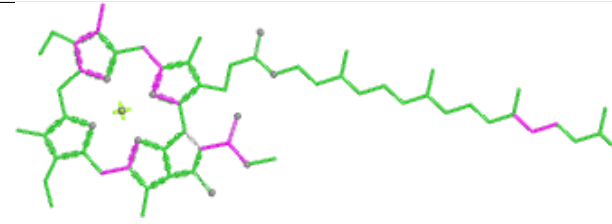
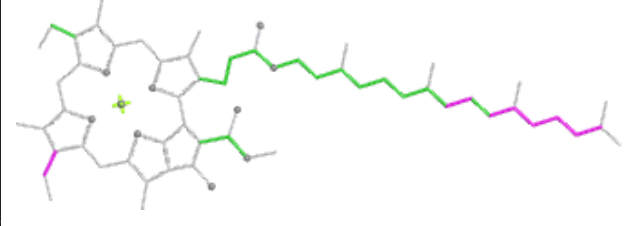
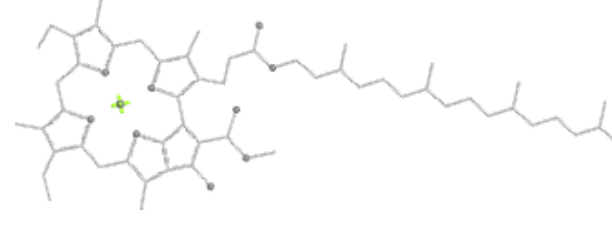
Ligand HEC V 201

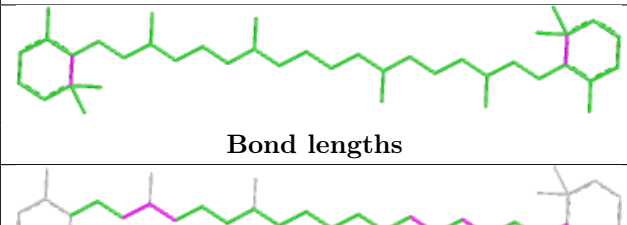
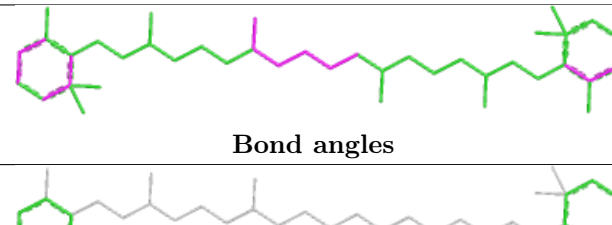
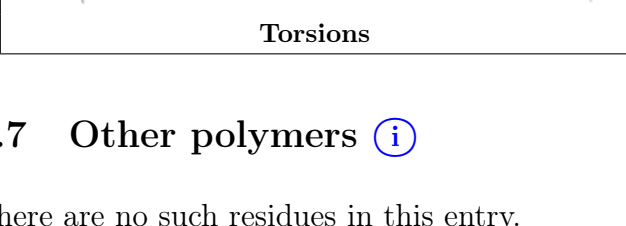
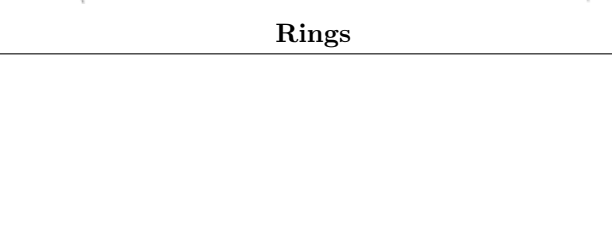


Ligand DGD c 517



Ligand CLA B 611	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 613	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR B 617	
	
Bond lengths	Bond angles
	
Torsions	Rings

5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.25	1 (0%) 90 91	9, 30, 50, 82	64 (19%)
1	a	334/344 (97%)	-0.16	3 (0%) 81 83	9, 32, 58, 81	64 (19%)
2	B	505/510 (99%)	-0.34	2 (0%) 88 90	19, 35, 62, 88	4 (0%)
2	b	505/510 (99%)	-0.19	4 (0%) 82 84	27, 39, 71, 112	0
3	C	442/461 (95%)	-0.24	0 100 100	9, 38, 54, 75	11 (2%)
3	c	451/461 (97%)	-0.14	2 (0%) 88 90	10, 42, 62, 99	12 (2%)
4	D	341/352 (96%)	-0.44	0 100 100	10, 32, 49, 73	2 (0%)
4	d	341/352 (96%)	-0.30	0 100 100	11, 36, 60, 80	3 (0%)
5	E	82/84 (97%)	0.37	3 (3%) 45 47	34, 53, 70, 85	1 (1%)
5	e	82/84 (97%)	0.45	2 (2%) 59 62	42, 60, 78, 86	0
6	F	34/45 (75%)	0.06	0 100 100	40, 45, 59, 87	0
6	f	34/45 (75%)	0.26	0 100 100	44, 52, 79, 92	0
7	H	65/66 (98%)	-0.04	1 (1%) 72 74	35, 42, 58, 72	0
7	h	63/66 (95%)	0.21	2 (3%) 50 53	42, 51, 62, 66	0
8	I	35/38 (92%)	-0.25	0 100 100	35, 41, 68, 77	0
8	i	35/38 (92%)	-0.06	0 100 100	34, 43, 77, 88	0
9	J	36/40 (90%)	0.09	0 100 100	38, 51, 78, 86	0
9	j	36/40 (90%)	0.41	1 (2%) 55 57	41, 54, 87, 92	0
10	K	37/46 (80%)	0.13	0 100 100	46, 52, 69, 77	0
10	k	37/46 (80%)	0.19	0 100 100	51, 57, 72, 78	0
11	L	37/37 (100%)	-0.41	0 100 100	27, 31, 61, 68	0
11	l	36/37 (97%)	-0.46	0 100 100	30, 33, 68, 88	0
12	M	32/36 (88%)	-0.37	0 100 100	30, 35, 58, 71	0
12	m	31/36 (86%)	-0.33	0 100 100	31, 36, 54, 65	0

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Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/272 (89%)	-0.09	1 (0%) 88 90	27, 44, 80, 133	1 (0%)
13	o	244/272 (89%)	-0.08	2 (0%) 82 84	29, 42, 79, 123	0
14	T	29/32 (90%)	-0.44	1 (3%) 48 50	28, 33, 57, 71	0
14	t	29/32 (90%)	-0.37	1 (3%) 48 50	30, 34, 71, 87	0
15	U	97/134 (72%)	-0.08	0 100 100	34, 45, 71, 88	0
15	u	97/134 (72%)	-0.15	1 (1%) 79 81	33, 42, 58, 84	0
16	V	137/163 (84%)	-0.20	0 100 100	33, 42, 58, 77	0
16	v	137/163 (84%)	-0.02	0 100 100	36, 48, 66, 86	0
17	Y	27/46 (58%)	0.96	1 (3%) 45 47	55, 75, 93, 95	0
17	y	30/46 (65%)	0.84	2 (6%) 24 25	64, 76, 89, 104	0
18	X	38/41 (92%)	0.12	1 (2%) 57 60	41, 53, 67, 74	0
18	x	39/41 (95%)	0.24	0 100 100	50, 60, 87, 102	0
19	Z	62/62 (100%)	0.85	4 (6%) 25 26	57, 69, 111, 126	0
19	z	62/62 (100%)	0.74	2 (3%) 50 53	61, 72, 115, 119	0
20	R	34/41 (82%)	0.83	1 (2%) 53 56	61, 69, 81, 84	0
20	r	31/41 (75%)	1.23	3 (9%) 13 14	73, 88, 108, 116	0
All	All	5302/5700 (93%)	-0.12	41 (0%) 82 84	9, 40, 73, 133	162 (3%)

The worst 5 of 41 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	o	58	ASN	3.8
20	R	35	LEU	3.7
1	a	248	ILE	3.4
9	j	6	GLY	3.0
5	e	79	PHE	3.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
12	FME	M	1	10/11	0.92	0.11	44,51,67,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
14	FME	t	1	10/11	0.93	0.09	33,38,54,78	0
12	FME	m	1	10/11	0.95	0.09	33,45,62,66	0
14	FME	T	1	10/11	0.95	0.07	33,41,57,63	0
8	FME	I	1	10/11	0.96	0.07	39,49,57,57	0
8	FME	i	1	10/11	0.96	0.09	37,50,52,53	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(\AA^2)	Q<0.9
31	STE	H	104	18/20	0.73	0.20	52,68,74,75	0
31	STE	b	622	20/20	0.75	0.15	47,57,75,76	0
32	LMG	b	620	55/55	0.78	0.17	50,66,81,84	0
33	LHG	E	101	49/49	0.78	0.15	52,74,93,101	0
32	LMG	d	409	23/55	0.79	0.18	49,63,69,72	0
31	STE	x	102	20/20	0.80	0.16	43,54,63,69	0
32	LMG	c	522	48/55	0.80	0.15	51,71,81,87	0
31	STE	b	623	10/20	0.81	0.14	44,50,52,55	0
31	STE	a	617	12/20	0.81	0.12	50,56,71,72	0
25	CLA	h	101	65/65	0.82	0.13	52,66,86,94	0
28	PL9	A	612	55/55	0.82	0.16	39,62,73,75	0
28	PL9	a	612	55/55	0.82	0.17	46,67,79,83	0
31	STE	B	626	16/20	0.82	0.15	48,58,64,69	0
31	STE	t	103	10/20	0.82	0.14	43,53,58,60	0
33	LHG	e	102	42/49	0.82	0.14	58,80,99,107	0
31	STE	m	102	12/20	0.83	0.15	48,52,66,67	0
31	STE	B	624	18/20	0.83	0.13	41,50,72,75	0
30	DGD	a	616	44/66	0.83	0.14	36,52,82,85	0
31	STE	c	523	12/20	0.83	0.12	57,67,75,76	0
29	SQD	a	615	36/54	0.84	0.13	30,52,69,74	0
31	STE	B	625	12/20	0.84	0.13	49,56,65,65	0
32	LMG	D	409	33/55	0.84	0.14	37,52,69,72	0
31	STE	B	619	17/20	0.84	0.13	37,49,69,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
31	STE	b	621	16/20	0.85	0.14	53,59,78,79	0
31	STE	J	101	12/20	0.85	0.13	49,54,61,65	0
30	DGD	A	616	66/66	0.85	0.12	47,57,66,70	0
32	LMG	C	515	48/55	0.85	0.12	40,54,65,71	0
31	STE	b	619	20/20	0.85	0.13	40,52,66,68	0
31	STE	c	521	20/20	0.86	0.12	44,55,77,78	0
29	SQD	A	615	39/54	0.86	0.13	40,51,77,78	0
31	STE	I	101	15/20	0.86	0.15	43,51,64,65	0
31	STE	C	521	12/20	0.86	0.12	43,50,56,61	0
31	STE	T	102	16/20	0.86	0.15	36,45,56,61	0
31	STE	R	101	12/20	0.86	0.14	63,68,83,84	0
32	LMG	c	520	37/55	0.87	0.11	49,59,71,73	0
32	LMG	B	620	28/55	0.87	0.13	37,48,61,67	0
29	SQD	f	101	41/54	0.87	0.14	65,78,88,91	0
31	STE	C	522	16/20	0.87	0.14	37,52,58,59	0
31	STE	d	411	17/20	0.87	0.13	49,52,64,66	0
31	STE	C	520	12/20	0.88	0.11	34,44,52,56	0
31	STE	j	101	12/20	0.88	0.11	51,57,60,61	0
29	SQD	l	101	54/54	0.88	0.11	38,60,76,82	0
25	CLA	H	101	65/65	0.88	0.11	39,53,77,84	0
32	LMG	c	524	49/55	0.88	0.10	39,54,70,76	0
31	STE	T	103	15/20	0.88	0.14	45,53,69,73	0
32	LMG	m	101	51/55	0.88	0.10	34,49,63,71	0
31	STE	D	410	20/20	0.88	0.12	35,45,64,73	0
31	STE	B	623	12/20	0.88	0.11	39,47,59,59	0
31	STE	l	103	18/20	0.89	0.12	37,44,63,64	0
29	SQD	L	101	49/54	0.89	0.10	42,58,80,82	0
32	LMG	C	519	48/55	0.89	0.12	43,65,81,85	0
27	BCR	K	102	40/40	0.90	0.10	43,51,61,62	0
29	SQD	a	614	54/54	0.90	0.10	38,59,75,81	0
27	BCR	d	404	40/40	0.90	0.11	38,47,79,85	0
31	STE	t	102	14/20	0.90	0.09	38,43,50,54	0
27	BCR	k	101	40/40	0.90	0.11	50,57,65,70	0
29	SQD	F	102	36/54	0.90	0.12	48,64,72,75	0
27	BCR	c	514	40/40	0.91	0.10	46,56,63,65	0
31	STE	M	102	15/20	0.91	0.10	36,43,60,62	0
27	BCR	x	101	40/40	0.91	0.10	38,53,61,64	0
32	LMG	M	101	51/55	0.91	0.09	33,46,61,62	0
27	BCR	H	102	40/40	0.91	0.09	34,45,55,57	0
30	DGD	C	517	62/66	0.91	0.10	36,45,83,98	0
27	BCR	B	617	40/40	0.92	0.07	27,36,46,48	0
27	BCR	D	404	40/40	0.92	0.10	33,43,70,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
30	DGD	H	103	62/66	0.92	0.09	34,42,50,52	0
25	CLA	c	512	65/65	0.92	0.10	47,55,78,83	0
30	DGD	h	102	62/66	0.92	0.09	34,45,52,54	0
25	CLA	C	513	65/65	0.92	0.09	45,55,79,83	0
27	BCR	K	103	40/40	0.92	0.11	42,48,58,59	0
27	BCR	b	618	40/40	0.92	0.09	33,43,53,55	0
29	SQD	A	614	52/54	0.92	0.10	33,52,68,74	0
31	STE	M	103	10/20	0.92	0.10	35,46,53,54	0
27	BCR	c	516	40/40	0.93	0.11	47,52,61,64	0
32	LMG	D	406	51/55	0.93	0.10	32,47,64,68	0
25	CLA	C	512	65/65	0.93	0.10	39,48,69,79	0
25	CLA	c	513	65/65	0.93	0.10	48,60,86,92	0
27	BCR	t	101	40/40	0.93	0.07	27,39,48,48	0
27	BCR	K	101	40/40	0.93	0.10	41,53,58,60	0
25	CLA	B	605	65/65	0.93	0.09	26,34,63,72	0
25	CLA	C	510	65/65	0.93	0.08	31,43,51,53	0
27	BCR	b	616	40/40	0.93	0.08	28,42,48,51	0
27	BCR	B	618	40/40	0.93	0.08	31,42,50,52	0
30	DGD	c	518	62/66	0.93	0.09	39,47,75,81	0
27	BCR	C	514	40/40	0.93	0.09	31,41,49,50	0
25	CLA	C	511	65/65	0.94	0.09	36,48,57,62	0
27	BCR	A	611	40/40	0.94	0.07	26,34,38,39	0
27	BCR	T	101	40/40	0.94	0.07	29,38,47,48	0
30	DGD	C	516	62/66	0.94	0.10	30,35,70,79	0
28	PL9	D	405	55/55	0.94	0.07	24,31,40,42	0
30	DGD	C	518	62/66	0.94	0.08	31,43,61,66	0
25	CLA	c	503	65/65	0.94	0.08	36,44,50,55	0
27	BCR	b	617	40/40	0.94	0.07	29,39,45,49	0
25	CLA	c	508	64/65	0.94	0.09	36,42,77,93	0
30	DGD	c	519	62/66	0.94	0.08	33,46,66,68	0
25	CLA	c	509	65/65	0.94	0.10	38,46,56,58	0
32	LMG	d	410	44/55	0.94	0.09	38,48,71,76	0
25	CLA	c	511	65/65	0.94	0.10	44,53,59,63	0
33	LHG	B	622	49/49	0.94	0.09	32,41,53,61	0
33	LHG	D	408	47/49	0.94	0.10	31,40,69,74	0
25	CLA	C	502	65/65	0.94	0.08	33,39,49,58	0
33	LHG	d	406	49/49	0.94	0.10	32,45,59,65	0
25	CLA	C	501	65/65	0.94	0.07	26,35,45,45	0
34	BCT	a	606	4/4	0.94	0.08	33,36,41,45	0
28	PL9	d	405	55/55	0.95	0.07	25,34,39,41	0
25	CLA	B	614	65/65	0.95	0.07	25,35,51,62	0
25	CLA	B	615	60/65	0.95	0.09	28,35,74,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
25	CLA	d	402	65/65	0.95	0.07	21,32,51,55	0
25	CLA	d	403	65/65	0.95	0.08	34,42,70,74	0
25	CLA	A	607	65/65	0.95	0.09	23,32,80,84	0
26	PHO	A	609	64/64	0.95	0.06	27,32,38,42	0
26	PHO	a	609	64/64	0.95	0.06	26,31,36,39	0
26	PHO	d	401	64/64	0.95	0.07	28,38,44,46	0
25	CLA	B	609	65/65	0.95	0.07	25,32,37,42	0
27	BCR	B	616	40/40	0.95	0.07	31,36,46,55	0
25	CLA	C	503	65/65	0.95	0.07	35,41,45,52	0
25	CLA	a	607	65/65	0.95	0.07	24,29,37,47	0
25	CLA	a	608	65/65	0.95	0.08	28,37,85,93	0
25	CLA	b	601	65/65	0.95	0.08	31,39,52,55	0
25	CLA	b	603	65/65	0.95	0.08	25,33,62,71	0
25	CLA	b	605	65/65	0.95	0.07	30,37,62,65	0
25	CLA	b	607	65/65	0.95	0.07	32,40,53,56	0
25	CLA	b	608	65/65	0.95	0.07	32,43,54,64	0
25	CLA	b	609	65/65	0.95	0.08	30,37,43,49	0
27	BCR	a	611	40/40	0.95	0.07	23,32,42,45	0
25	CLA	b	614	65/65	0.95	0.07	29,39,51,56	0
25	CLA	b	615	60/65	0.95	0.08	33,40,77,79	0
25	CLA	c	502	65/65	0.95	0.07	33,41,53,59	0
25	CLA	C	506	65/65	0.95	0.09	30,41,74,79	0
27	BCR	c	515	40/40	0.95	0.08	32,44,50,53	0
25	CLA	c	504	60/65	0.95	0.08	30,42,68,72	0
25	CLA	c	505	65/65	0.95	0.08	31,39,58,60	0
25	CLA	c	506	65/65	0.95	0.08	37,43,71,77	0
25	CLA	c	507	65/65	0.95	0.07	32,40,49,55	0
25	CLA	C	507	65/65	0.95	0.07	29,38,49,51	0
25	CLA	C	508	65/65	0.95	0.08	33,39,83,94	0
33	LHG	d	408	39/49	0.95	0.09	34,44,55,60	0
25	CLA	c	510	65/65	0.95	0.07	33,45,52,54	0
33	LHG	l	102	49/49	0.95	0.07	32,41,46,49	0
25	CLA	C	509	65/65	0.95	0.08	32,40,53,55	0
25	CLA	a	613	65/65	0.96	0.06	25,30,40,42	0
25	CLA	B	604	65/65	0.96	0.07	26,31,39,42	0
25	CLA	b	602	65/65	0.96	0.07	27,33,56,68	0
25	CLA	A	606	65/65	0.96	0.06	21,27,37,41	0
25	CLA	b	604	65/65	0.96	0.07	25,34,42,45	0
25	CLA	C	504	59/65	0.96	0.07	35,41,66,72	0
25	CLA	b	606	65/65	0.96	0.07	25,33,54,60	0
26	PHO	A	608	64/64	0.96	0.05	21,27,33,37	0
25	CLA	C	505	65/65	0.96	0.08	28,36,58,65	0

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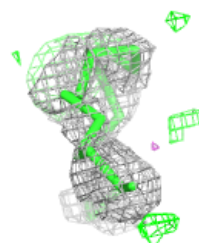
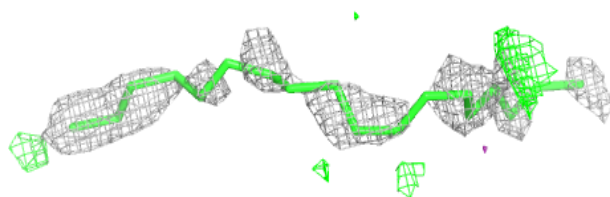
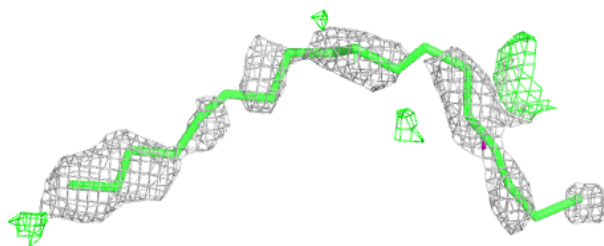
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
25	CLA	B	606	65/65	0.96	0.07	21,30,54,57	0
25	CLA	B	607	65/65	0.96	0.06	25,33,47,50	0
25	CLA	b	610	65/65	0.96	0.06	25,33,45,50	0
25	CLA	b	611	65/65	0.96	0.07	25,33,39,45	0
25	CLA	b	612	65/65	0.96	0.07	26,31,64,67	0
25	CLA	b	613	65/65	0.96	0.07	27,37,63,73	0
25	CLA	B	608	65/65	0.96	0.07	28,37,49,52	0
25	CLA	A	610	54/65	0.96	0.07	22,30,58,60	0
25	CLA	c	501	65/65	0.96	0.07	29,38,46,48	0
25	CLA	B	610	65/65	0.96	0.06	23,30,40,43	0
33	LHG	B	621	49/49	0.96	0.07	30,36,45,53	0
25	CLA	B	611	65/65	0.96	0.07	24,31,40,47	0
33	LHG	D	407	49/49	0.96	0.07	25,35,45,46	0
25	CLA	B	612	65/65	0.96	0.06	22,30,56,65	0
25	CLA	B	613	65/65	0.96	0.08	26,36,57,67	0
25	CLA	B	601	65/65	0.96	0.07	28,36,49,54	0
33	LHG	d	407	49/49	0.96	0.07	30,40,47,52	0
25	CLA	B	602	65/65	0.96	0.07	25,31,52,54	0
25	CLA	B	603	65/65	0.96	0.07	25,30,63,65	0
30	DGD	c	517	62/66	0.96	0.08	27,38,58,67	0
25	CLA	a	610	65/65	0.96	0.08	24,31,66,74	0
35	HEM	e	101	43/43	0.96	0.09	54,58,72,85	0
25	CLA	D	403	65/65	0.97	0.07	28,34,77,92	0
25	CLA	A	613	65/65	0.97	0.06	21,28,41,45	0
35	HEM	F	101	43/43	0.97	0.08	42,48,58,63	0
25	CLA	D	402	65/65	0.97	0.06	22,28,47,52	0
34	BCT	D	401	4/4	0.98	0.07	35,37,38,38	0
22	OEX	a	602[A]	10/10	0.98	0.03	35,37,42,42	10
24	CL	A	604	1/1	0.98	0.04	34,34,34,34	0
22	OEX	A	602[A]	10/10	0.98	0.03	36,38,41,43	10
36	HEC	V	201	43/43	0.98	0.07	29,36,44,52	0
36	HEC	v	201	43/43	0.98	0.06	29,38,41,44	0
21	OEY	A	601[C]	11/11	0.99	0.03	29,31,35,37	11
23	FE2	a	603	1/1	0.99	0.02	36,36,36,36	0
21	OEY	a	601[B]	11/11	0.99	0.03	20,25,29,30	11
24	CL	A	605	1/1	0.99	0.08	31,31,31,31	0
24	CL	a	604	1/1	0.99	0.04	32,32,32,32	0
24	CL	a	605	1/1	0.99	0.09	34,34,34,34	0
21	OEY	a	601[C]	11/11	0.99	0.03	30,32,34,36	11
21	OEY	A	601[B]	11/11	0.99	0.03	20,24,27,30	11
23	FE2	A	603	1/1	1.00	0.01	28,28,28,28	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.

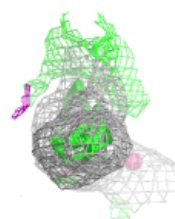
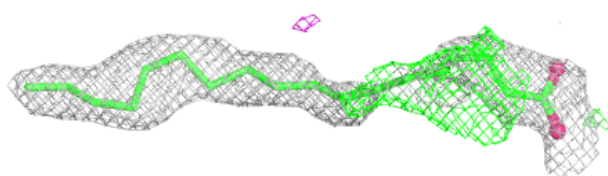
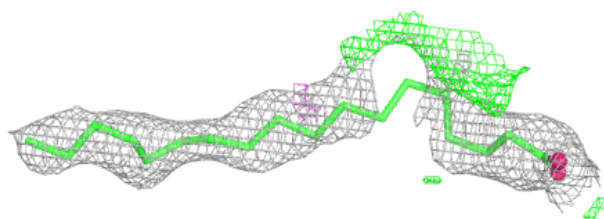
Electron density around STE H 104:

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

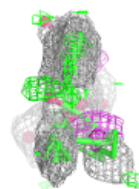
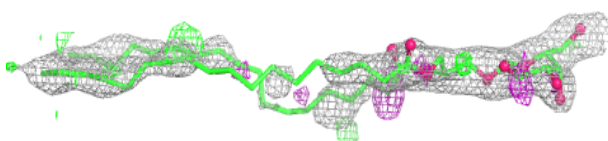
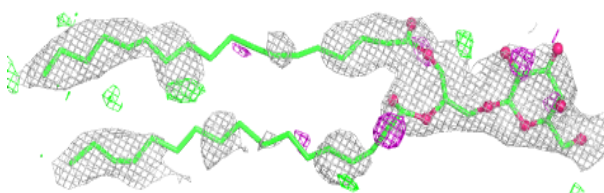


Electron density around STE b 622:

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

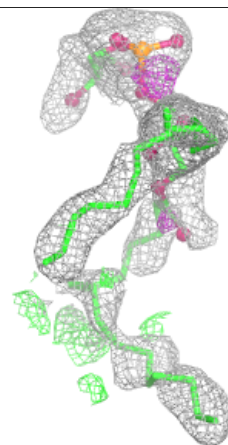
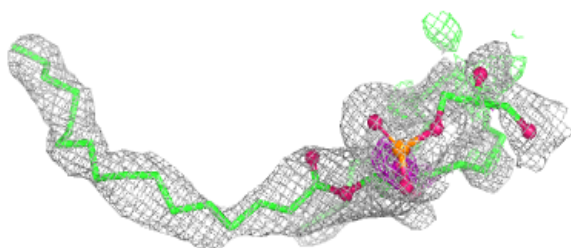
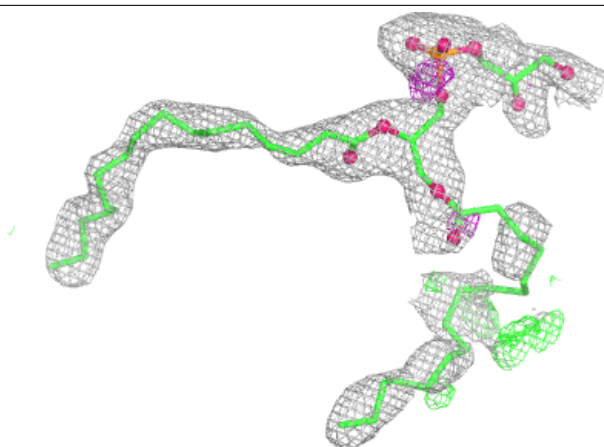
**Electron density around LMG b 620:**

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

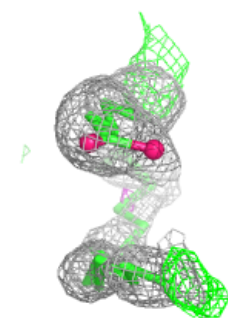
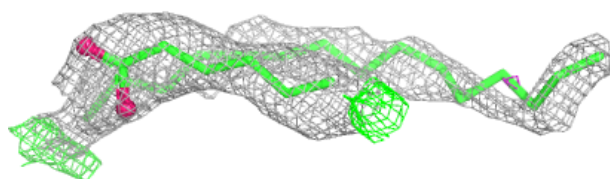
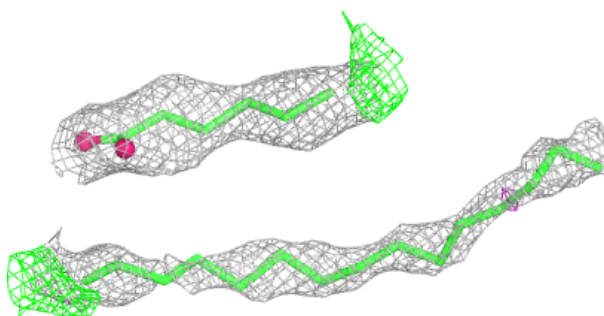


Electron density around LHG E 101:

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

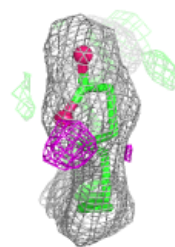
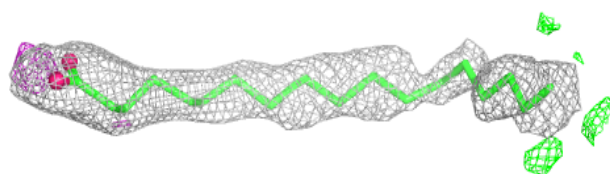
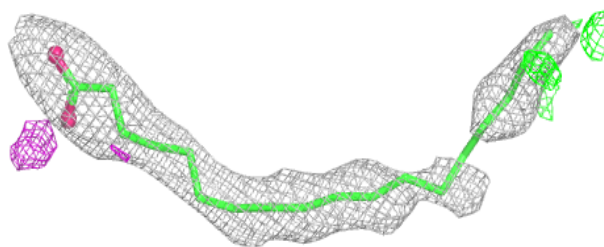
**Electron density around LMG d 409:**

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

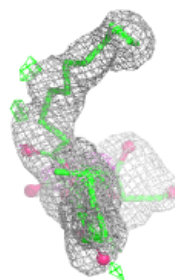
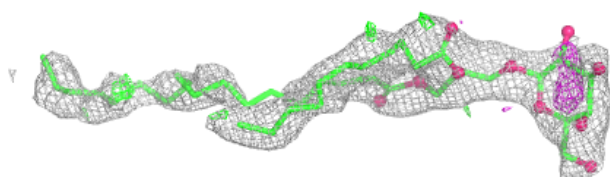
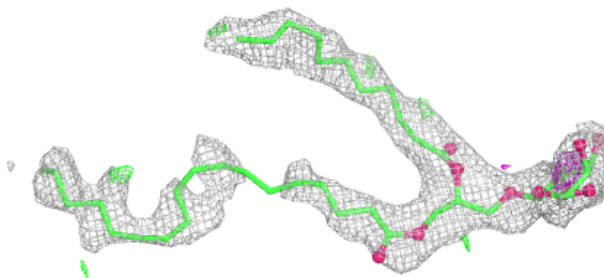


Electron density around STE x 102:

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

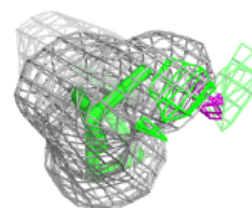
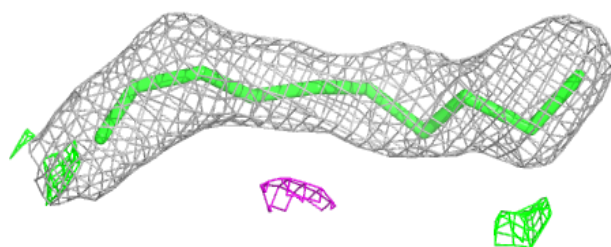
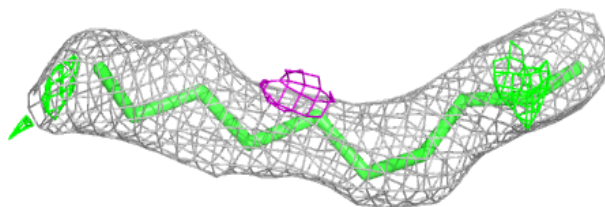
**Electron density around LMG c 522:**

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

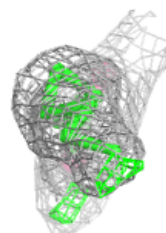
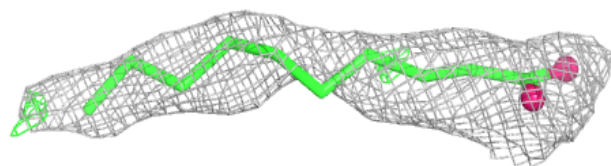
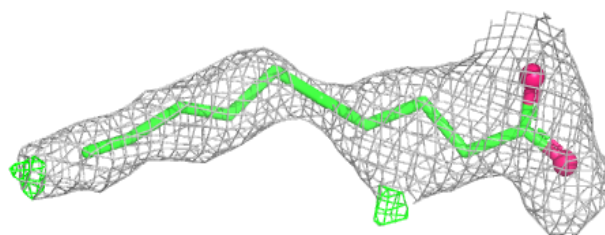


Electron density around STE b 623:

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

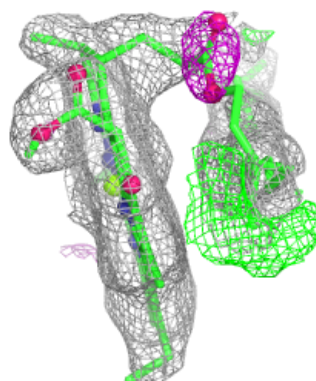
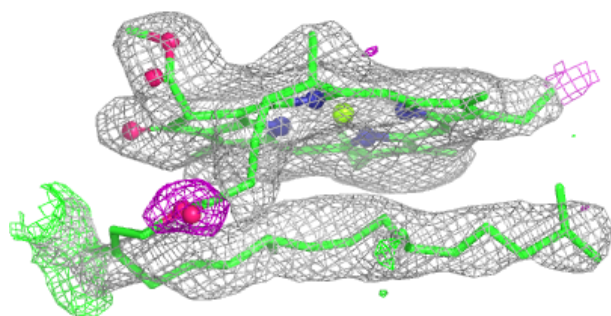
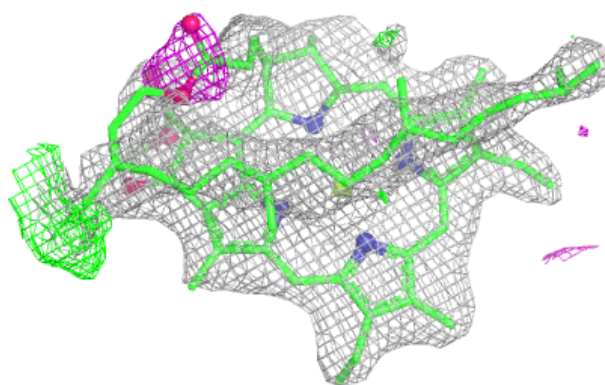
**Electron density around STE a 617:**

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

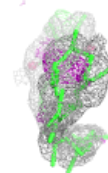
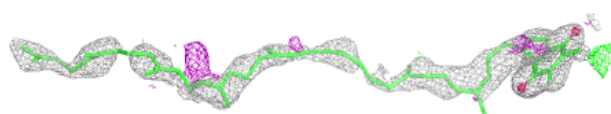
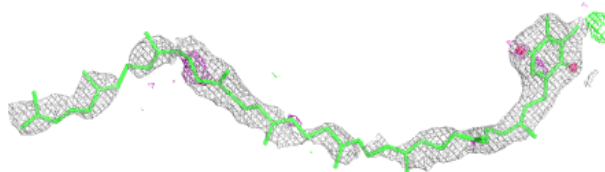


Electron density around CLA h 101:

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

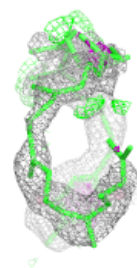
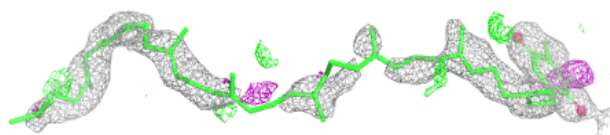
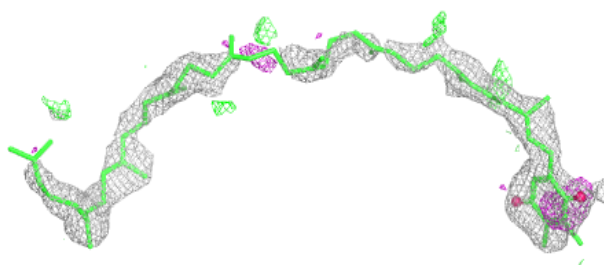
**Electron density around PL9 A 612:**

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

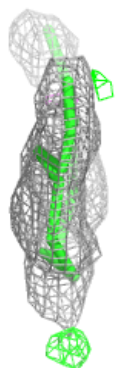
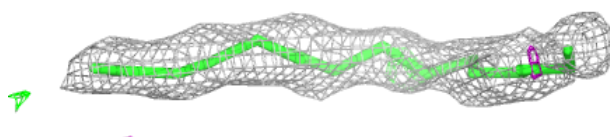
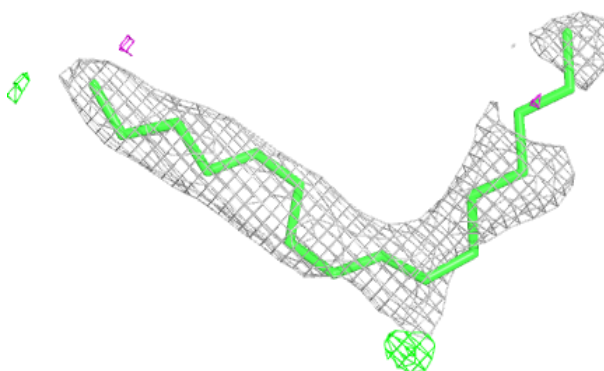


Electron density around PL9 a 612:

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

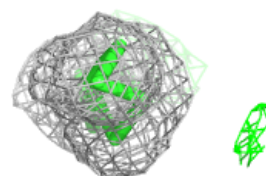
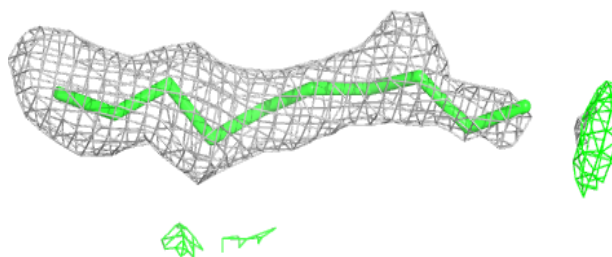
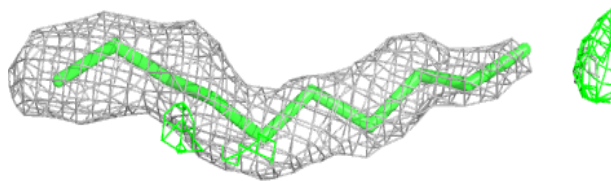
**Electron density around STE B 626:**

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

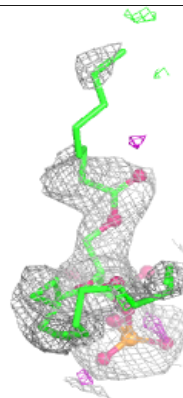
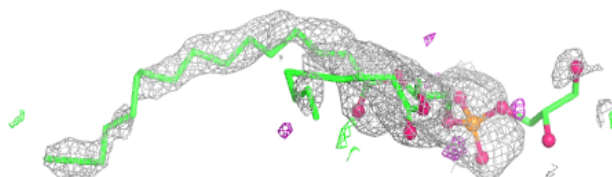
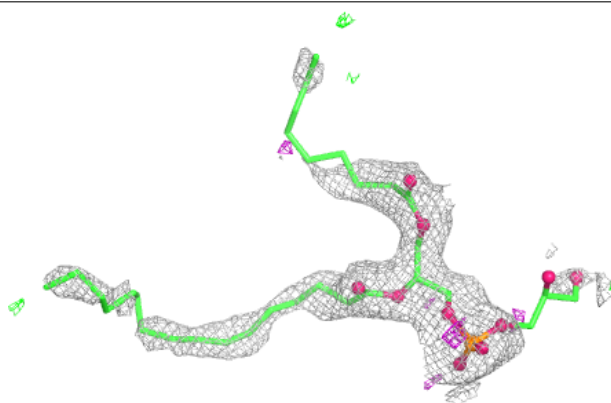


Electron density around STE t 103:

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

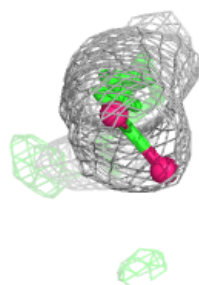
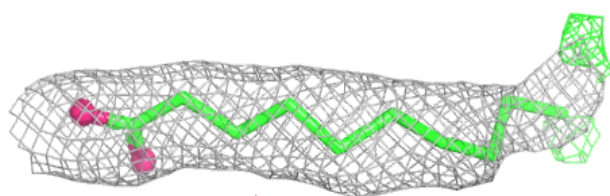
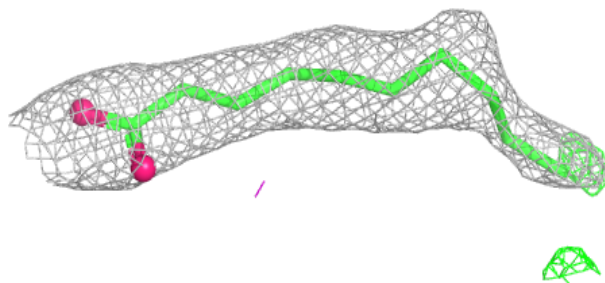
**Electron density around LHG e 102:**

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

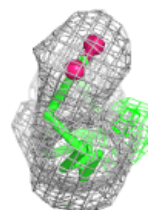
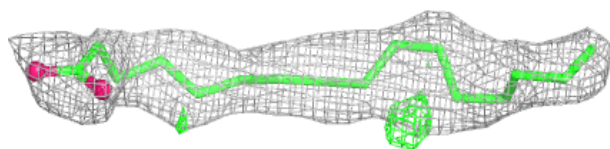
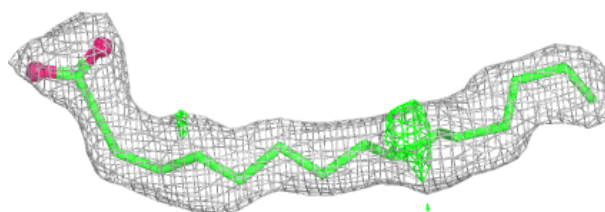


Electron density around STE m 102:

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

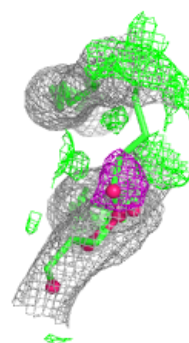
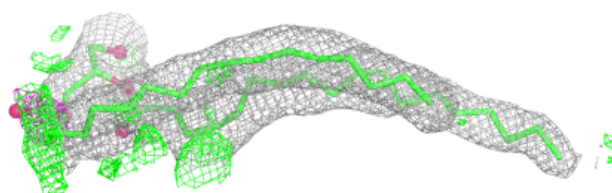
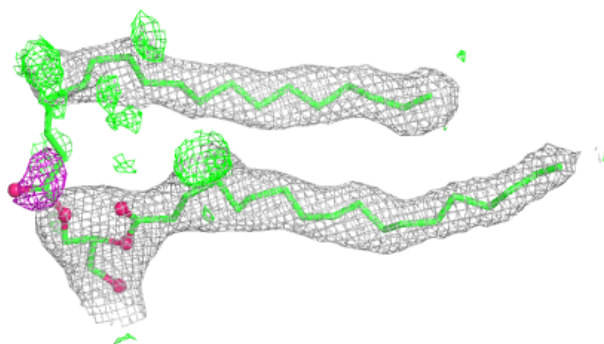
**Electron density around STE B 624:**

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

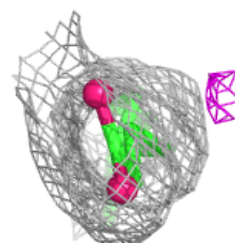
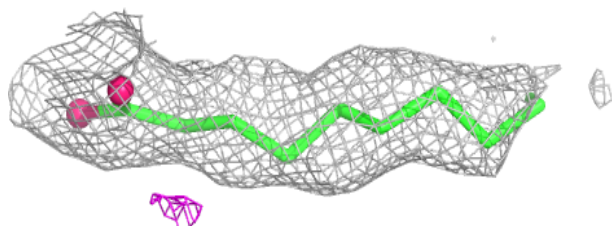
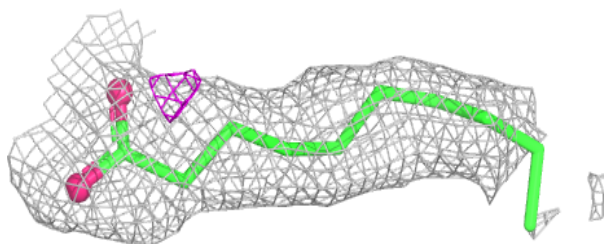


Electron density around DGD a 616:

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

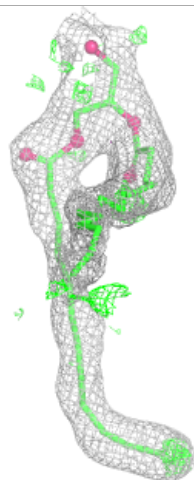
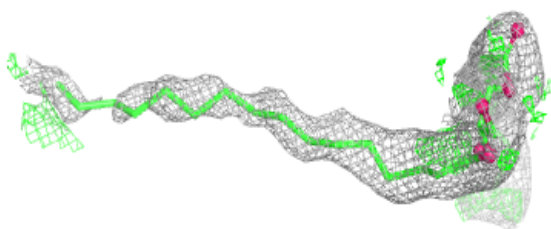
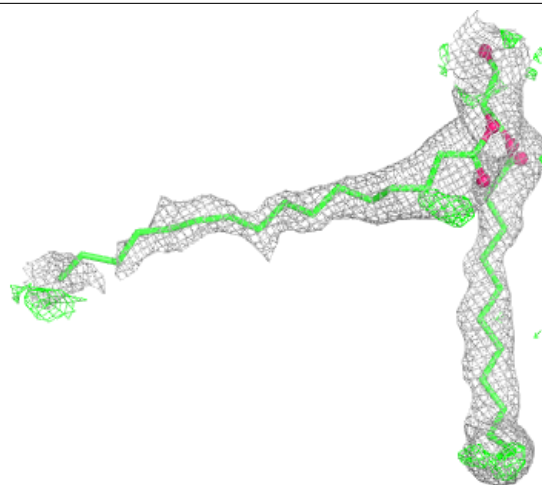
**Electron density around STE c 523:**

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



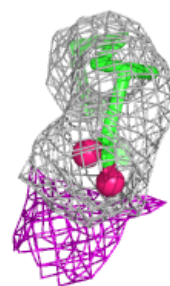
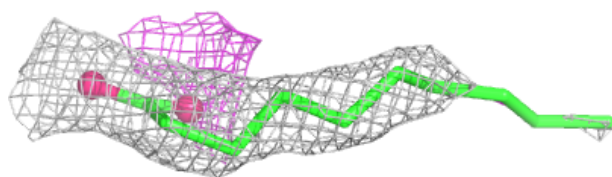
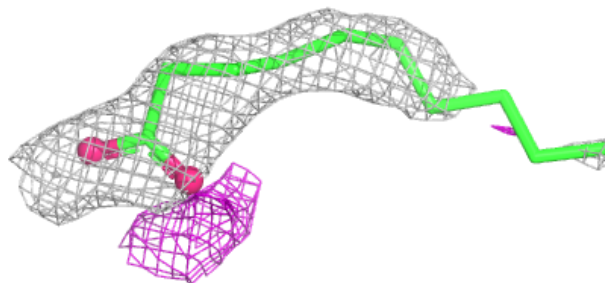
Electron density around SQD a 615:

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

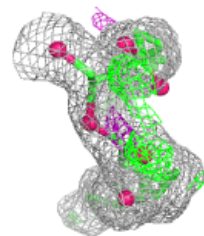
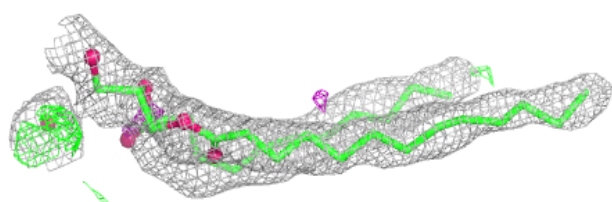
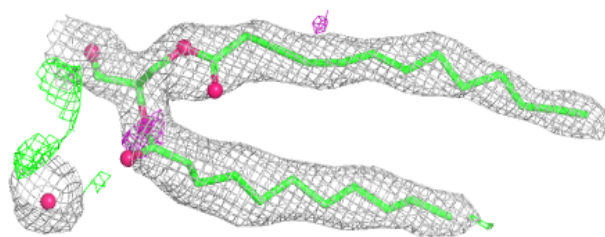


Electron density around STE B 625:

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

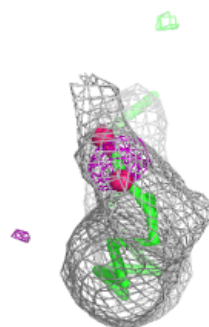
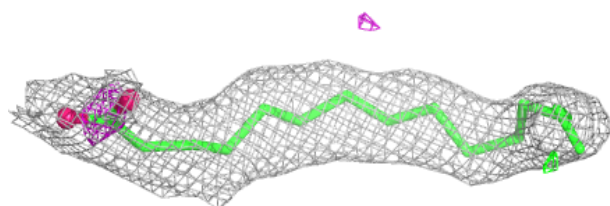
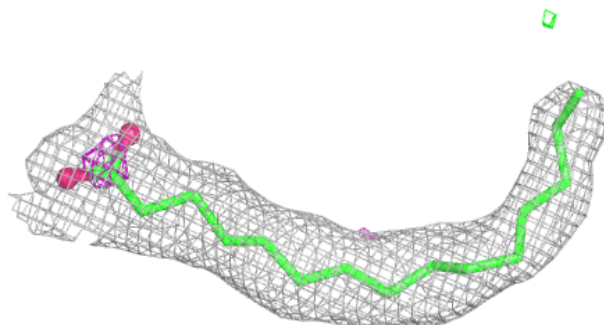
**Electron density around LMG D 409:**

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

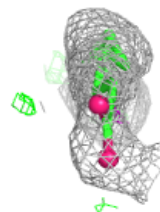
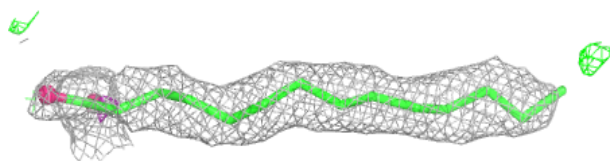
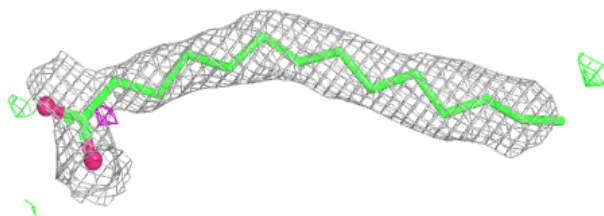


Electron density around STE B 619:

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

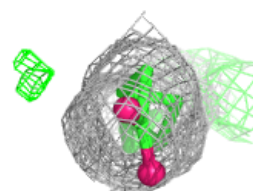
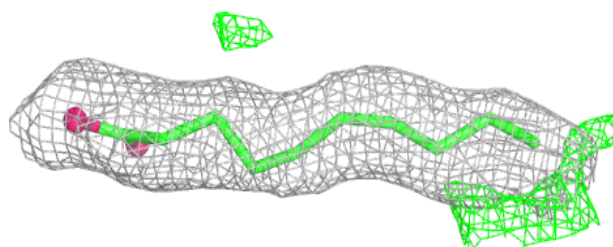
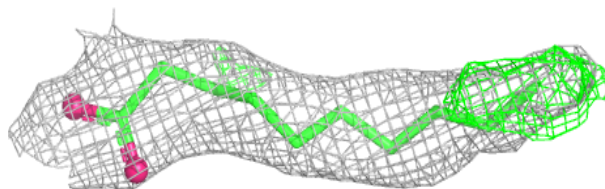
**Electron density around STE b 621:**

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

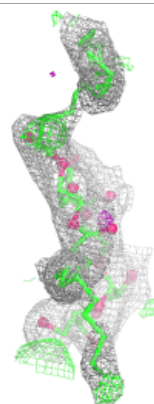
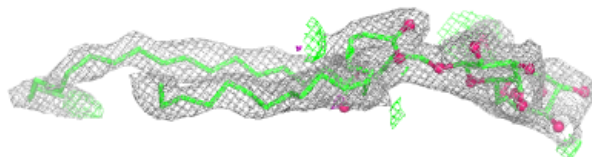
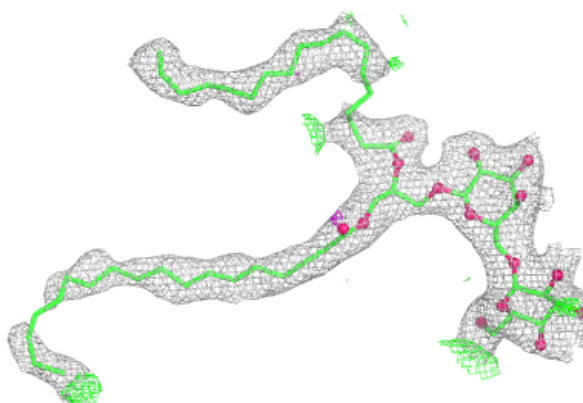


Electron density around STE J 101:

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

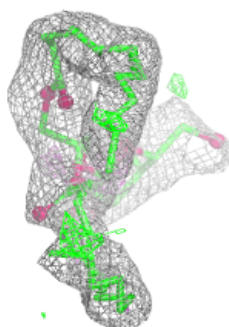
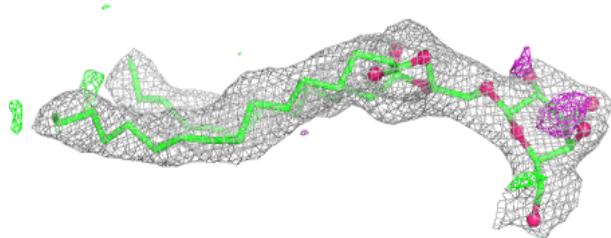
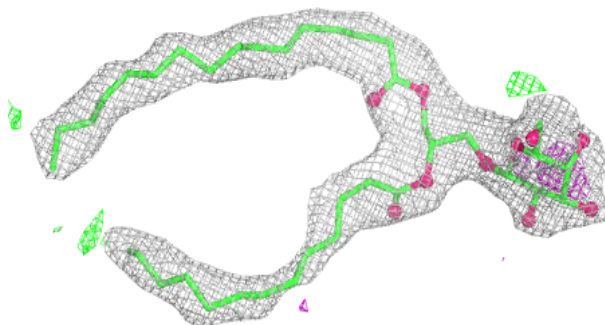
**Electron density around DGD A 616:**

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

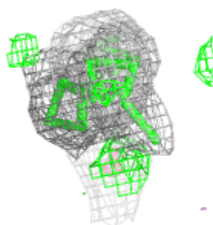
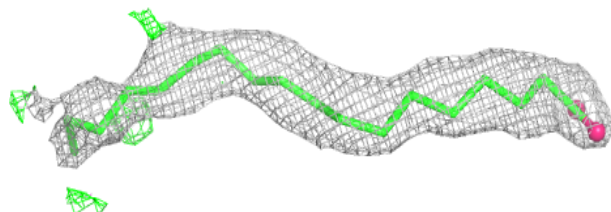
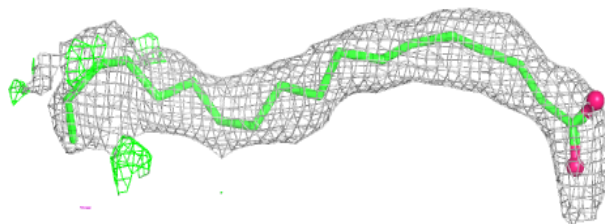


Electron density around LMG C 515:

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

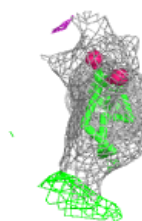
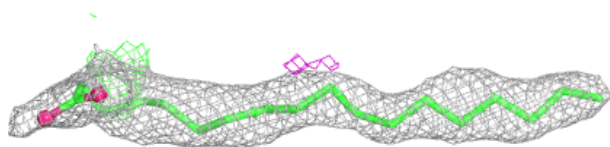
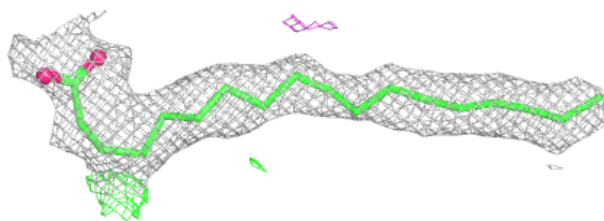
**Electron density around STE b 619:**

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



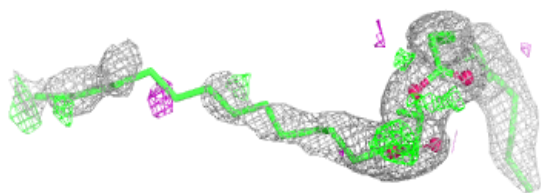
Electron density around STE c 521:

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



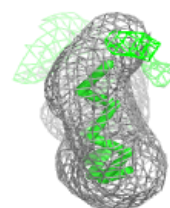
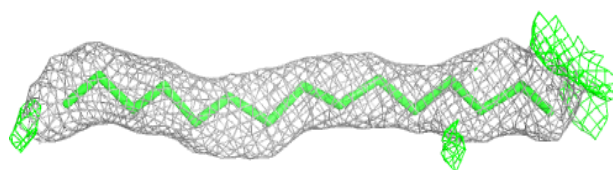
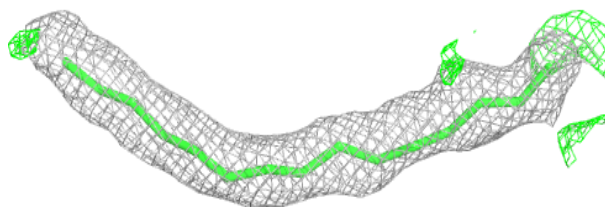
Electron density around SQD A 615:

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

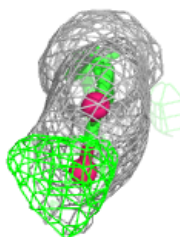
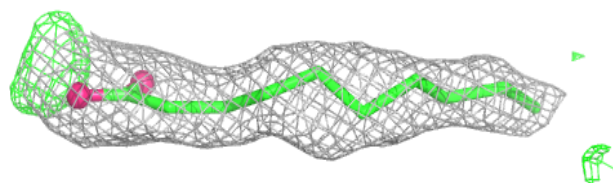
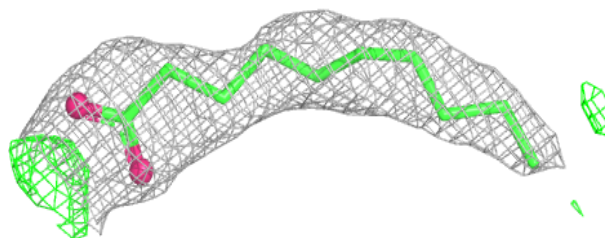


Electron density around STE I 101:

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

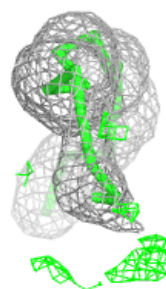
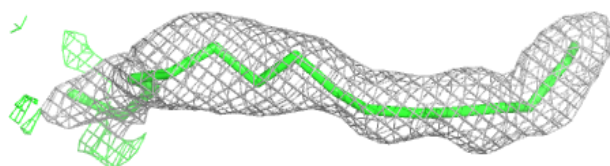
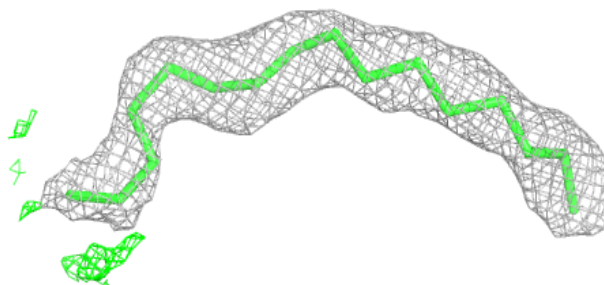
**Electron density around STE C 521:**

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

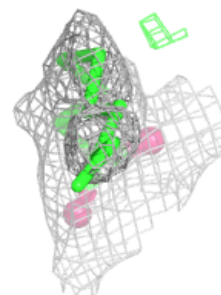
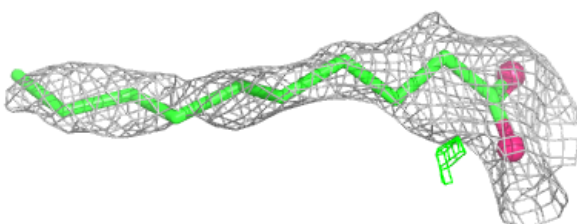
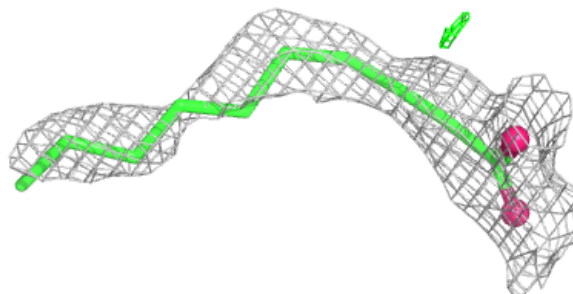


Electron density around STE T 102:

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

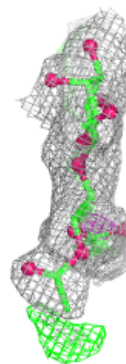
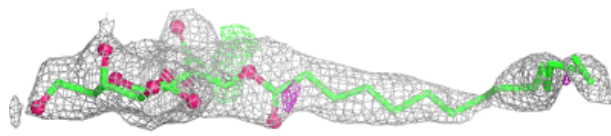
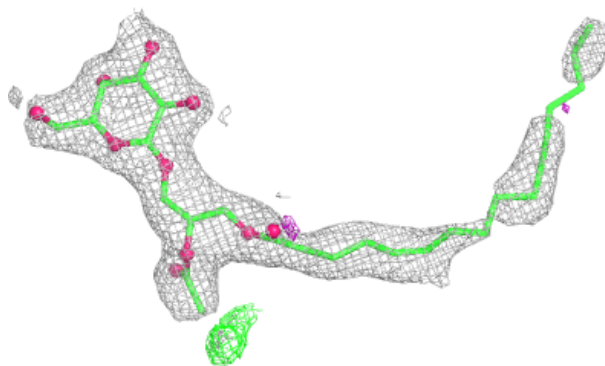
**Electron density around STE R 101:**

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

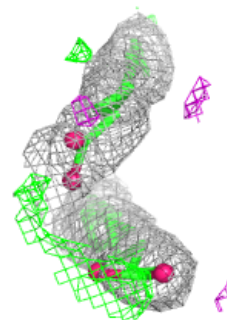
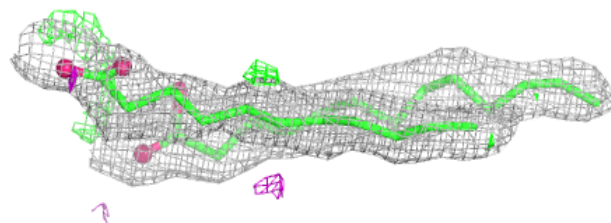
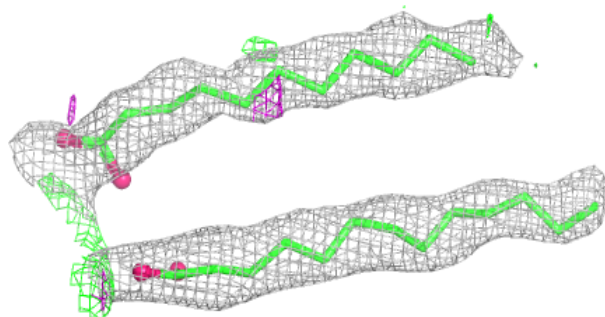


Electron density around LMG c 520:

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

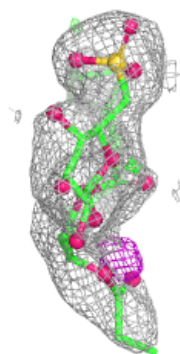
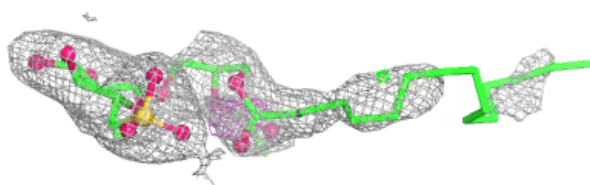
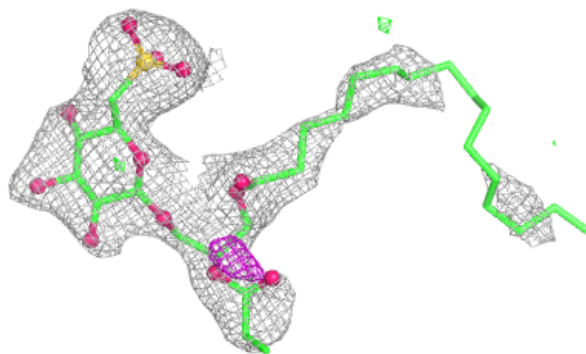
**Electron density around LMG B 620:**

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

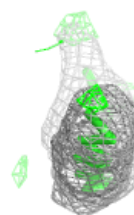
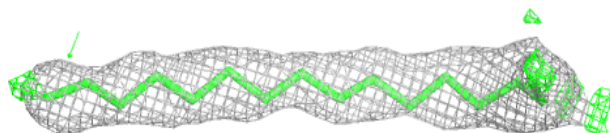
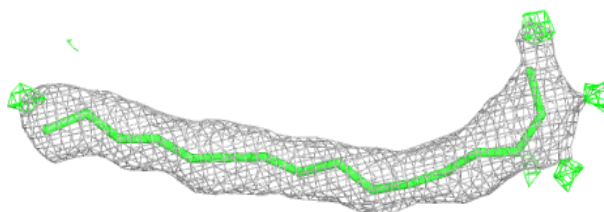


Electron density around SQD f 101:

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

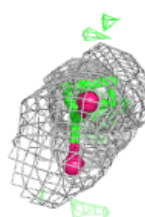
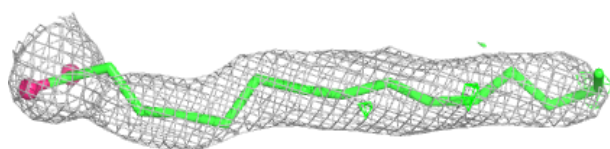
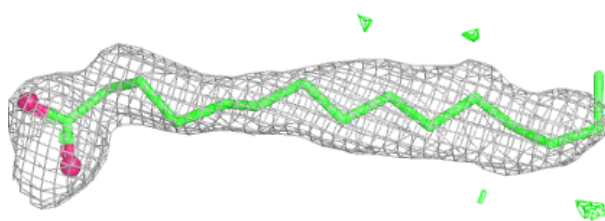
**Electron density around STE C 522:**

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

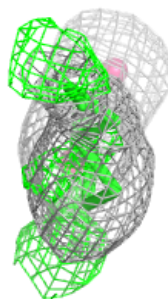
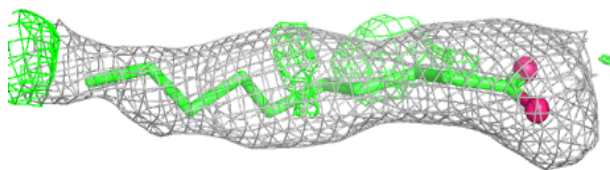
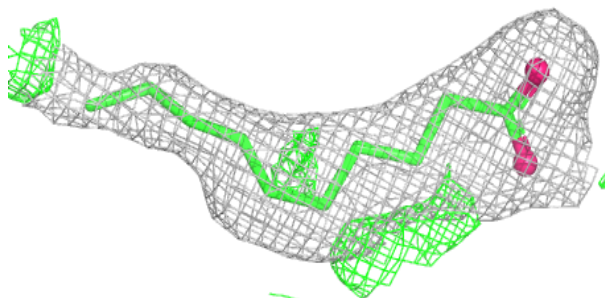


Electron density around STE d 411:

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

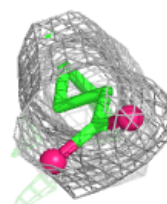
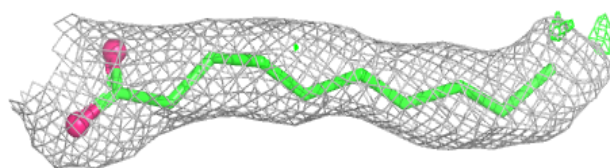
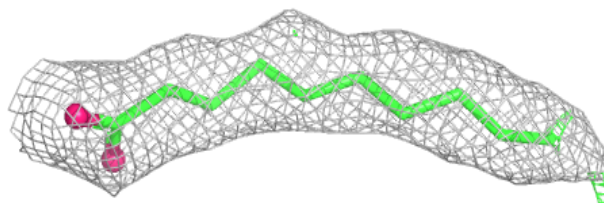
**Electron density around STE C 520:**

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

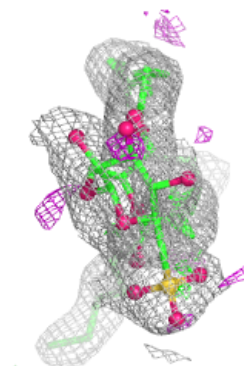
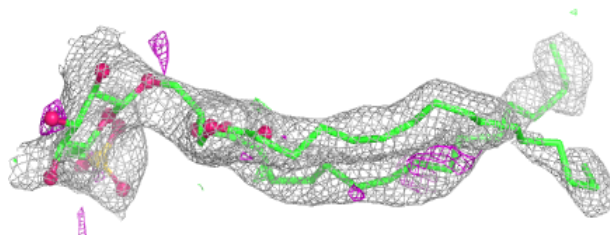
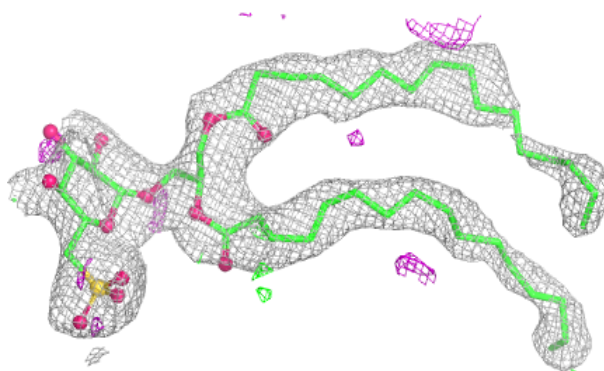


Electron density around STE j 101:

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

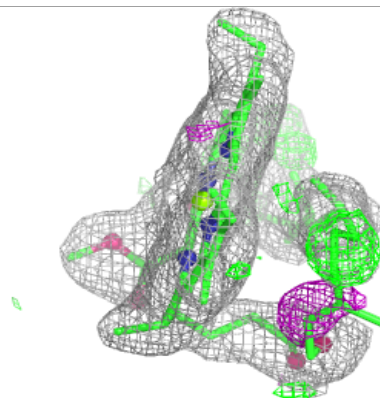
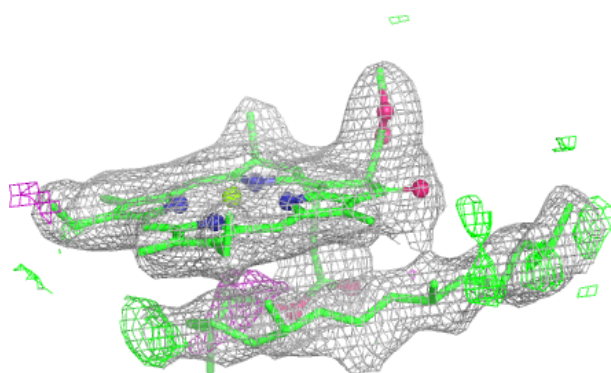
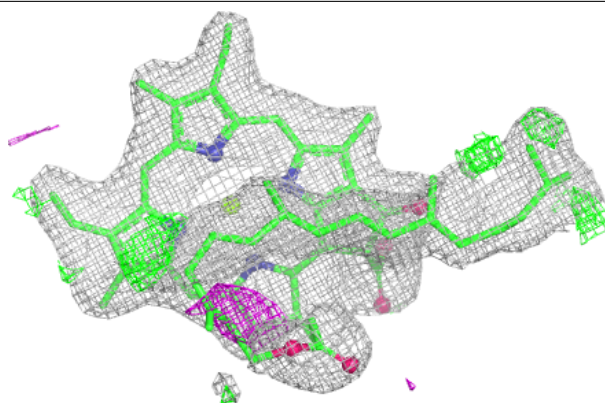
**Electron density around SQD l 101:**

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

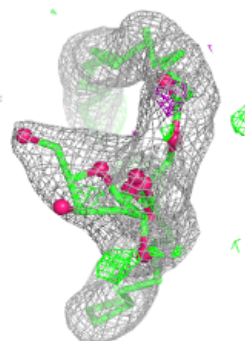
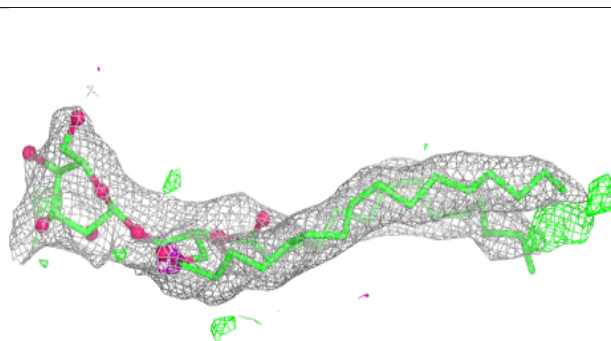
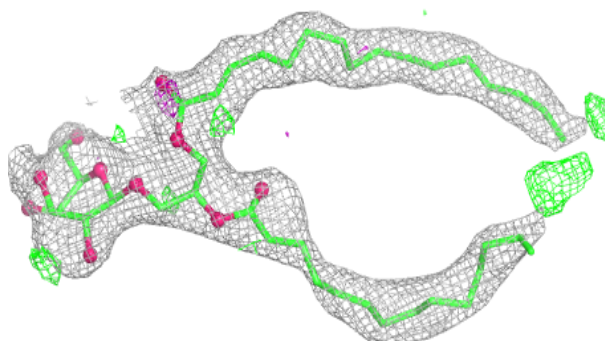


Electron density around CLA H 101:

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

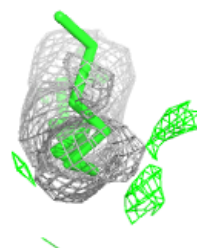
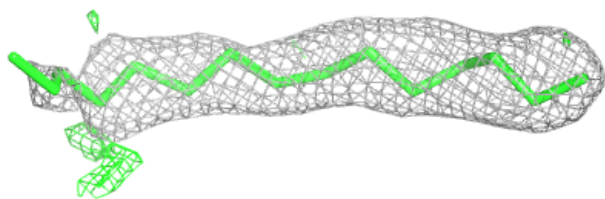
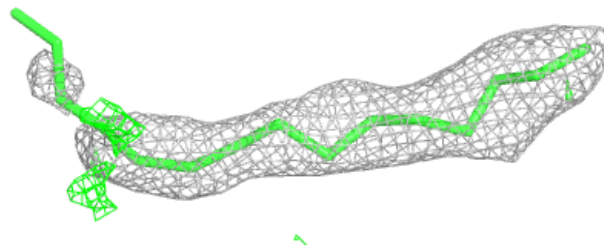
**Electron density around LMG c 524:**

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

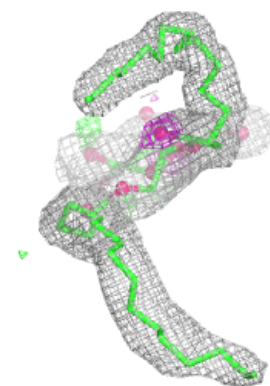
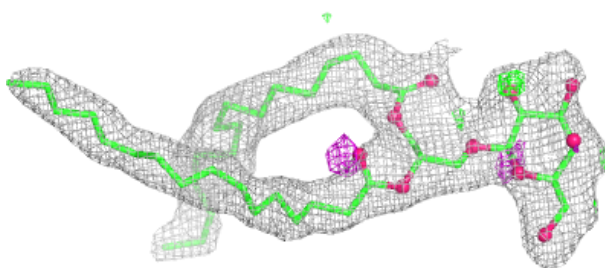
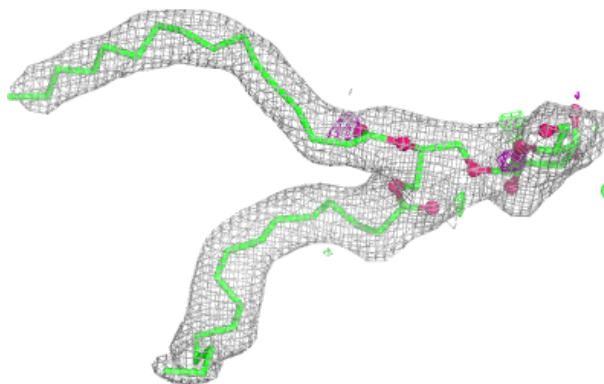


Electron density around STE T 103:

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

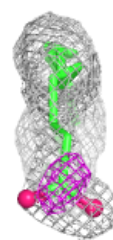
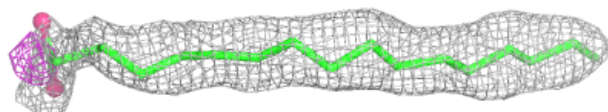
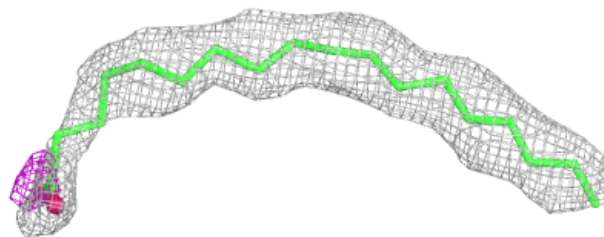
**Electron density around LMG m 101:**

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

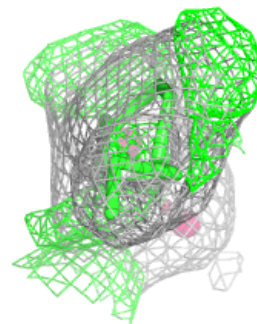
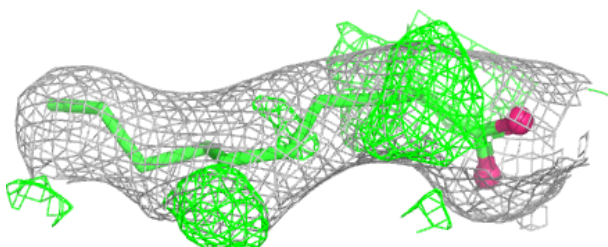
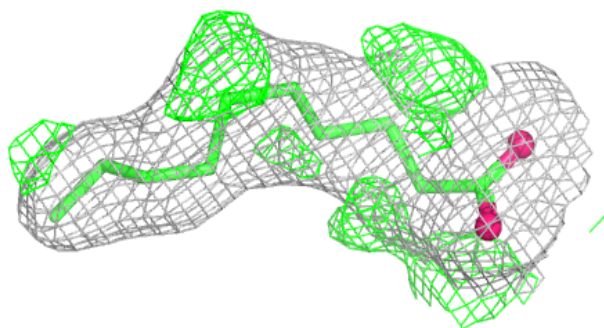


Electron density around STE D 410:

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

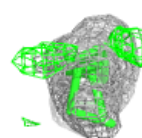
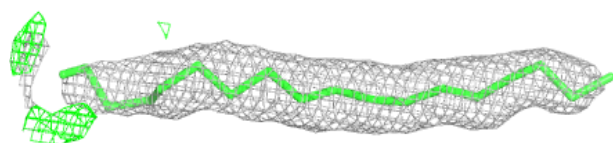
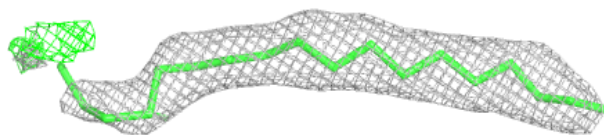
**Electron density around STE B 623:**

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

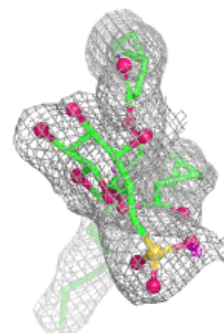
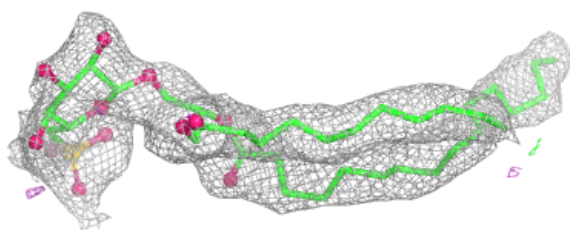
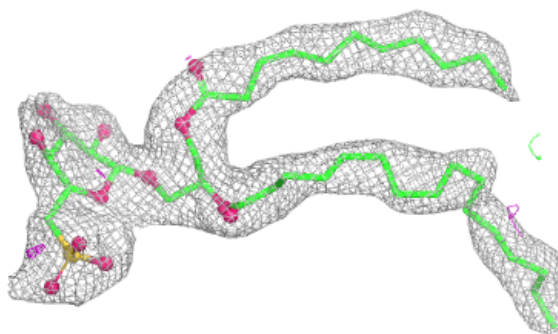


Electron density around STE I 103:

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

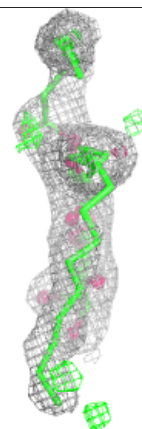
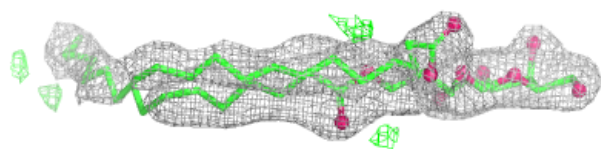
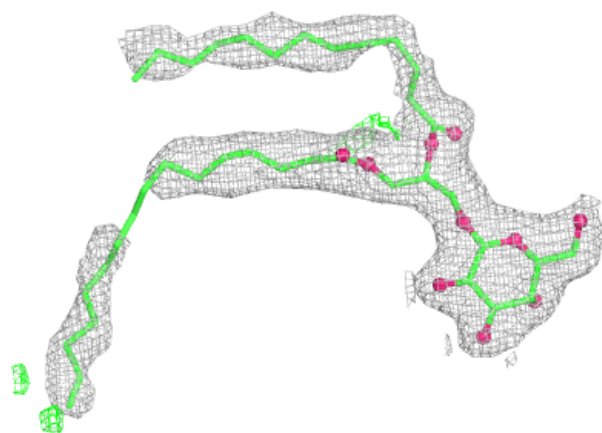
**Electron density around SQD L 101:**

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

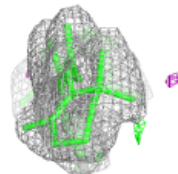
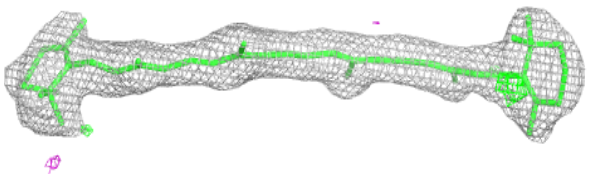
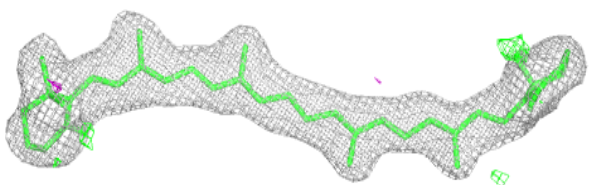


Electron density around LMG C 519:

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

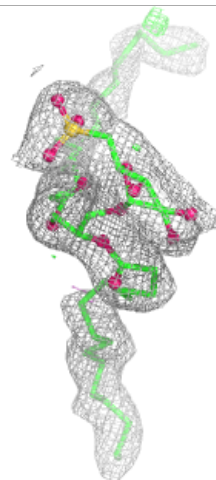
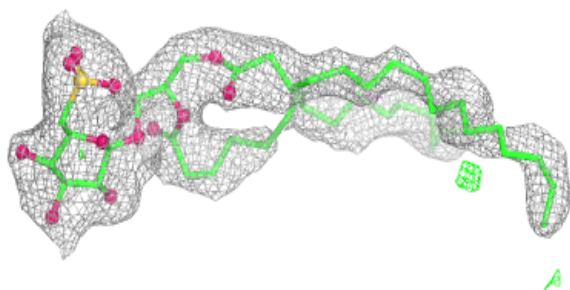
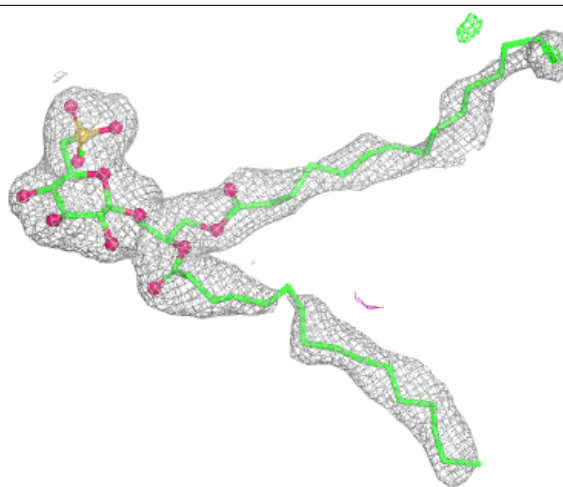
**Electron density around BCR K 102:**

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



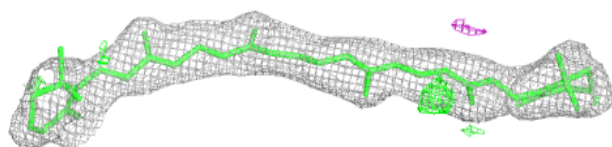
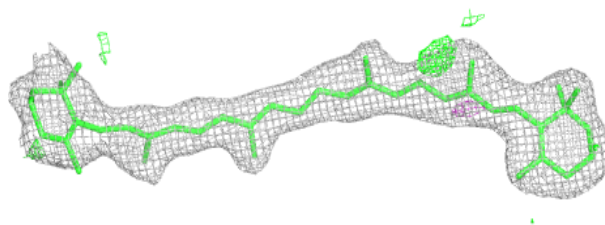
Electron density around SQD a 614:

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

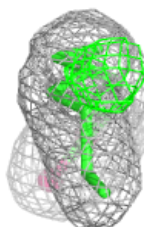
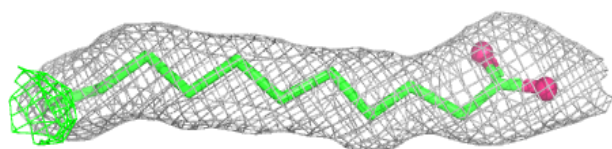
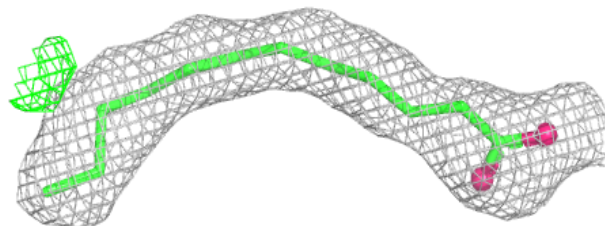


Electron density around BCR d 404:

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

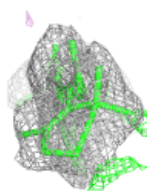
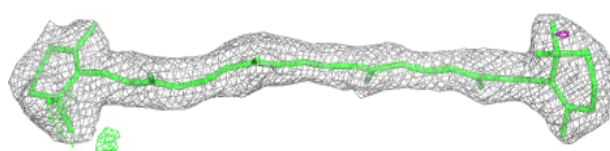
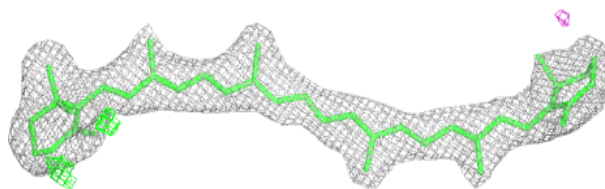
**Electron density around STE t 102:**

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

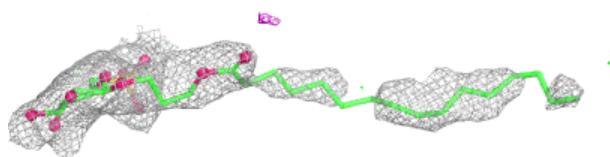
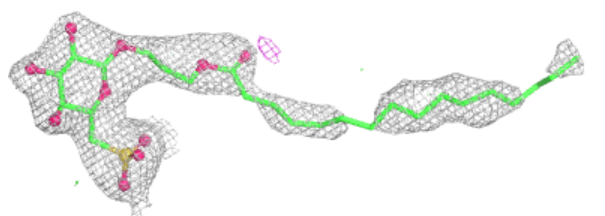


Electron density around BCR k 101:

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

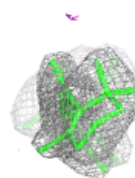
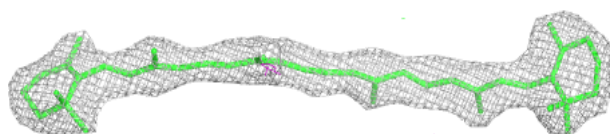
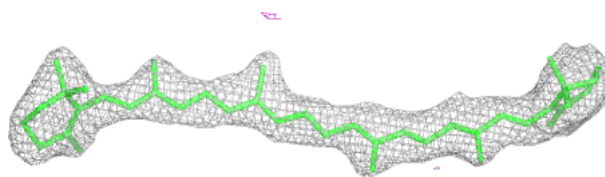
**Electron density around SQD F 102:**

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

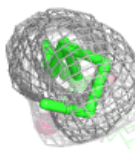
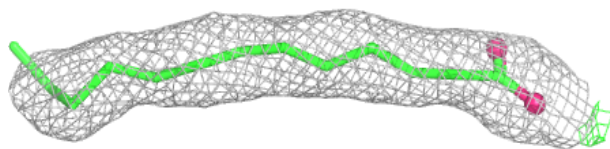
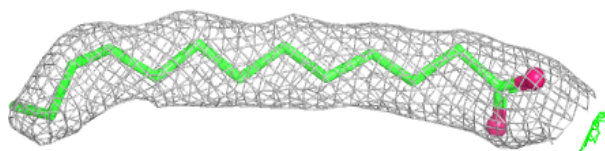


Electron density around BCR c 514:

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

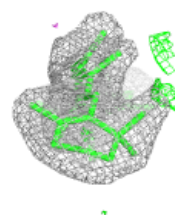
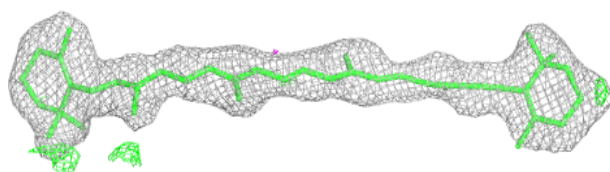
**Electron density around STE M 102:**

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

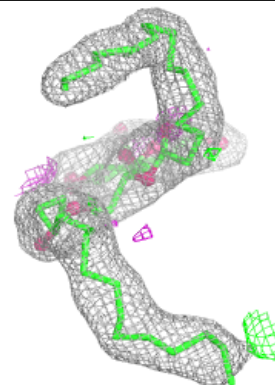
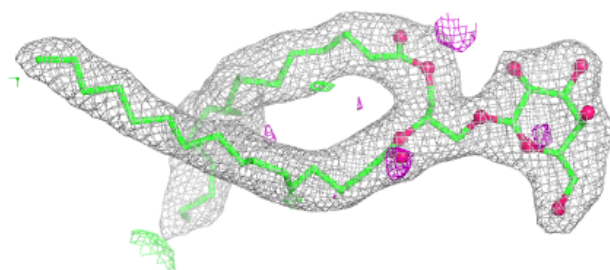
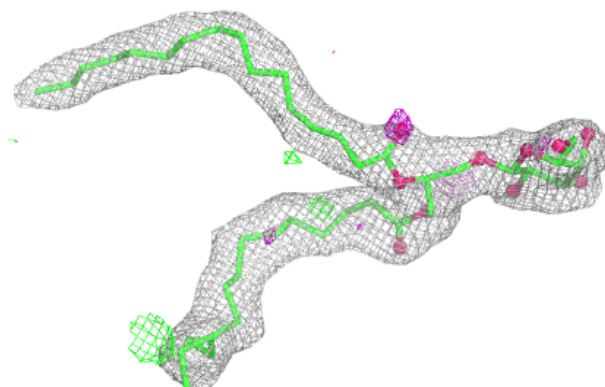


Electron density around BCR x 101:

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

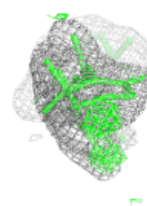
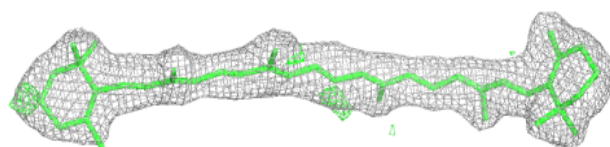
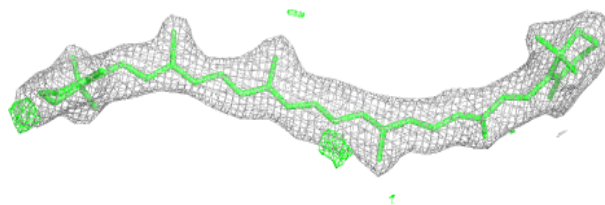
**Electron density around LMG M 101:**

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

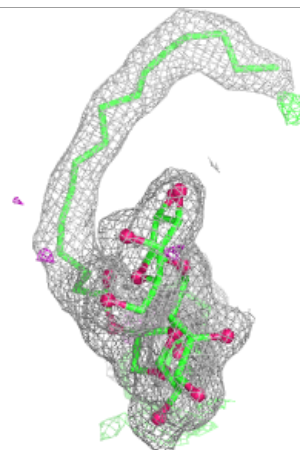
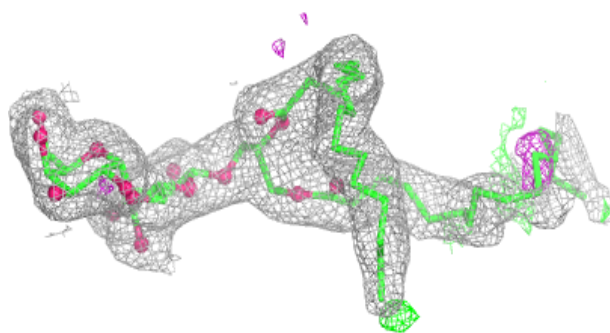
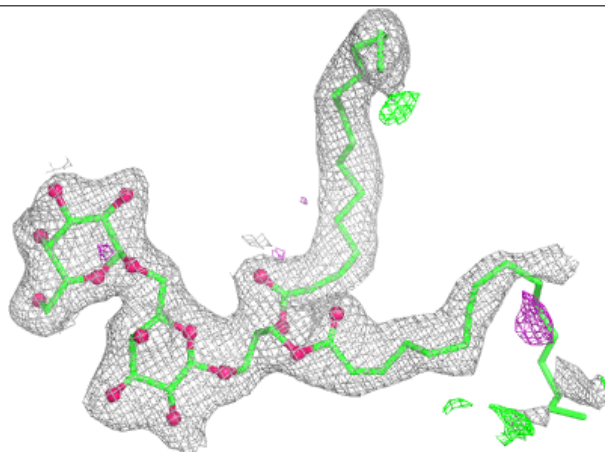


Electron density around BCR H 102:

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

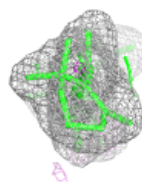
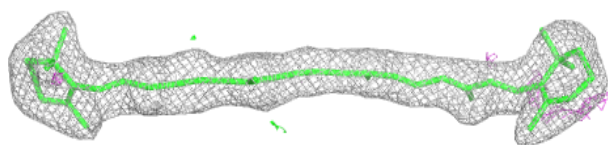
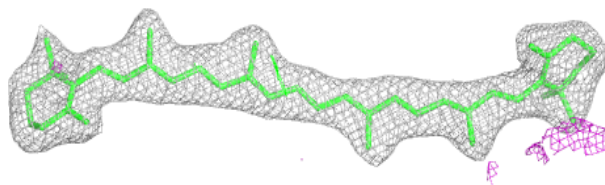
**Electron density around DGD C 517:**

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

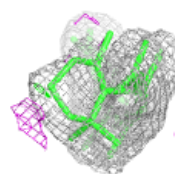
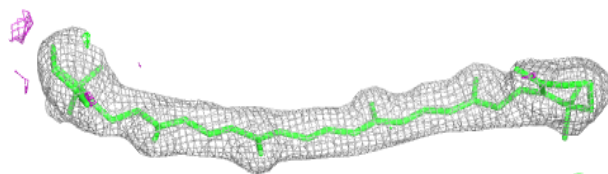
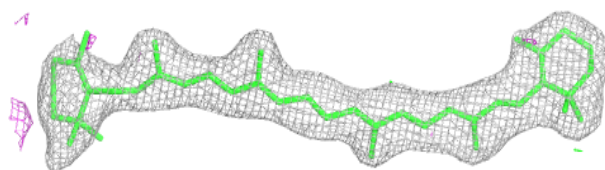


Electron density around BCR B 617:

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

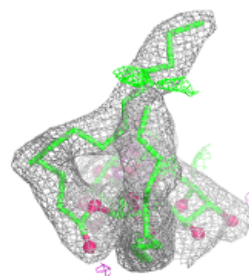
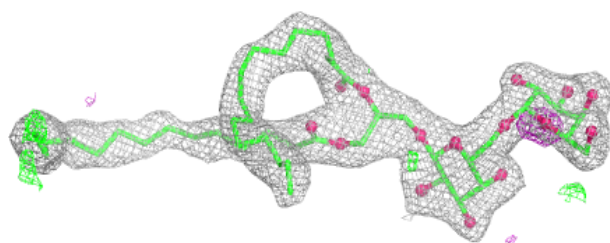
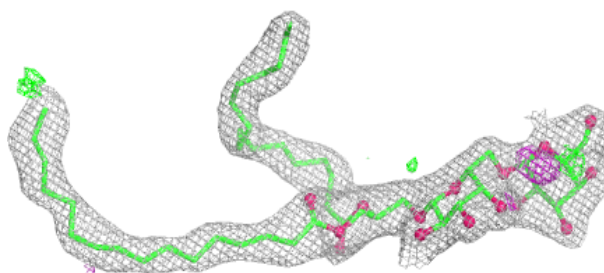
**Electron density around BCR D 404:**

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



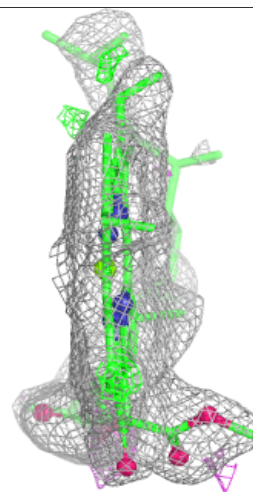
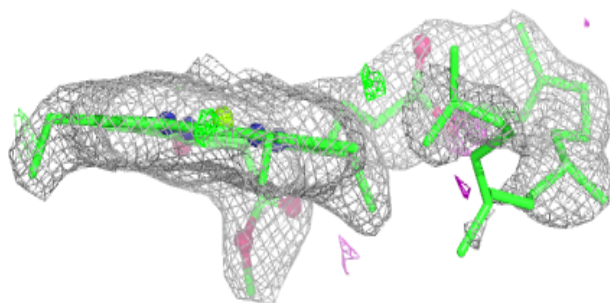
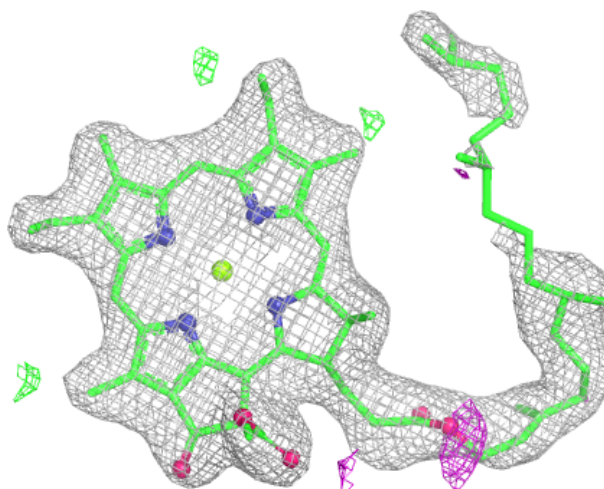
Electron density around DGD H 103:

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



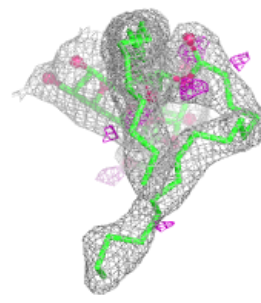
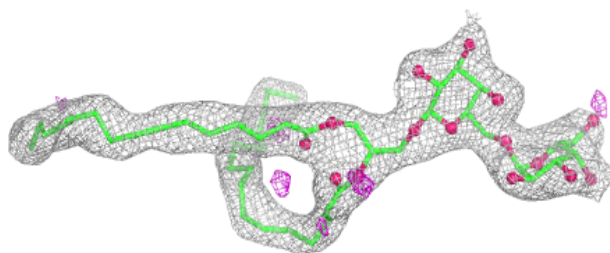
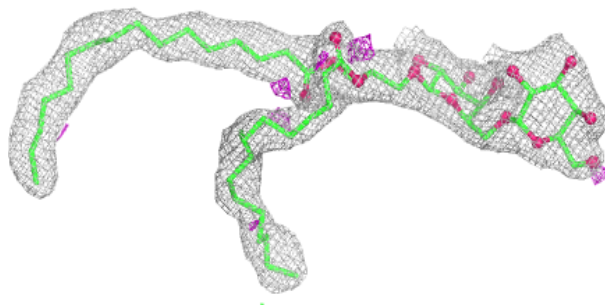
Electron density around CLA c 512:

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

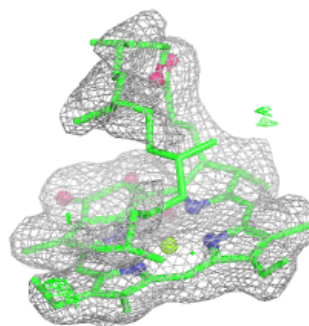
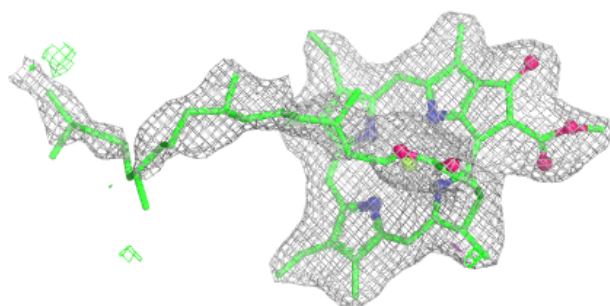
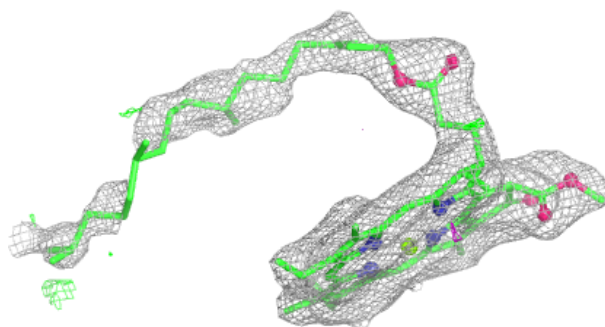


Electron density around DGD h 102:

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

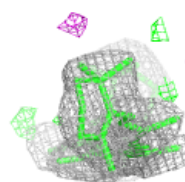
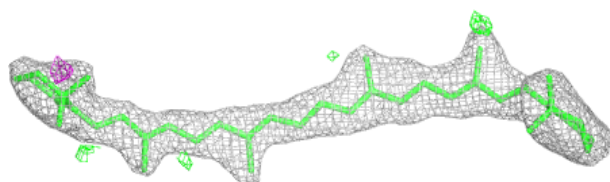
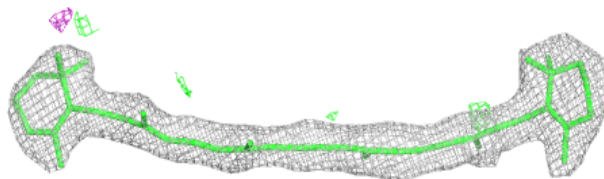
**Electron density around CLA C 513:**

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

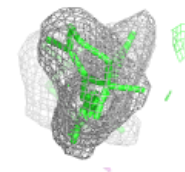
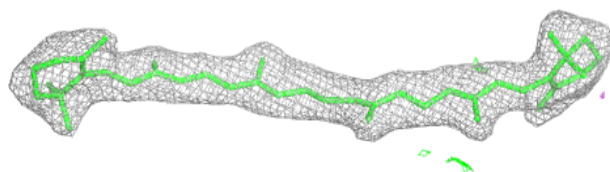
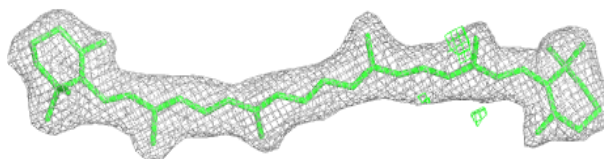


Electron density around BCR K 103:

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

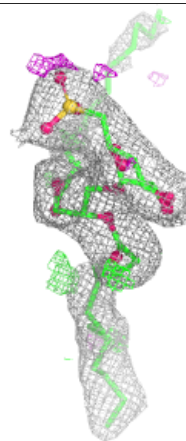
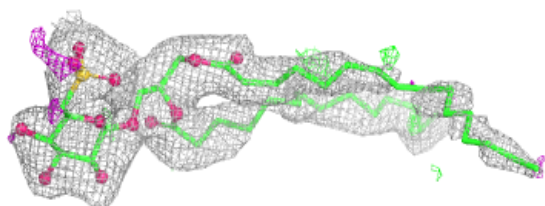
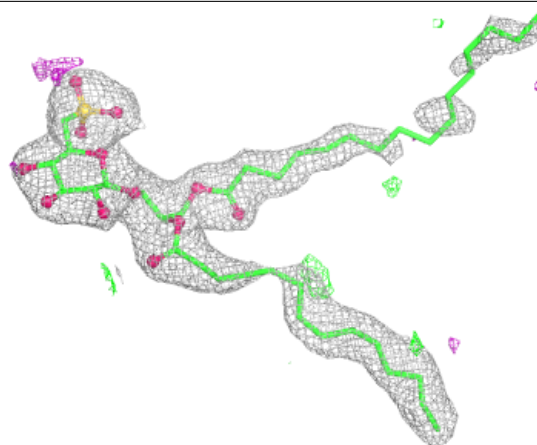
**Electron density around BCR b 618:**

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

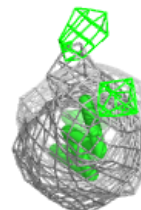
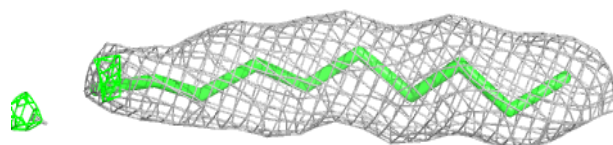
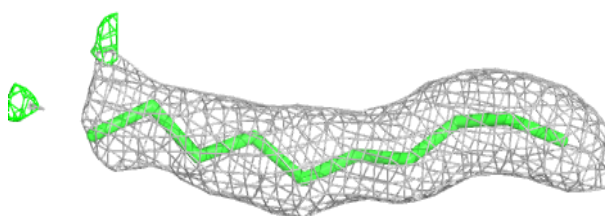


Electron density around SQD A 614:

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

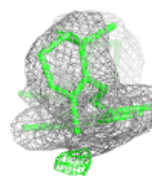
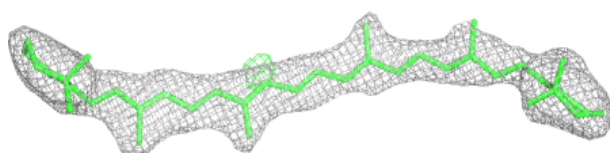
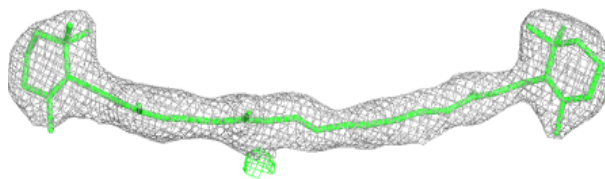
**Electron density around STE M 103:**

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

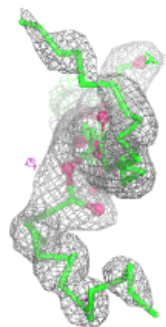
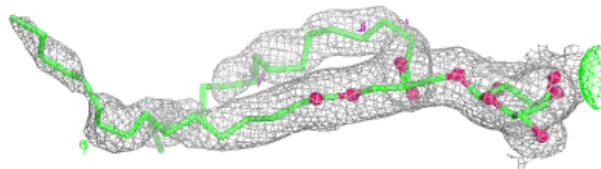
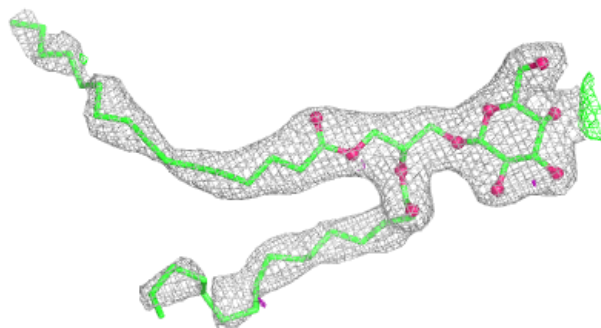


Electron density around BCR c 516:

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

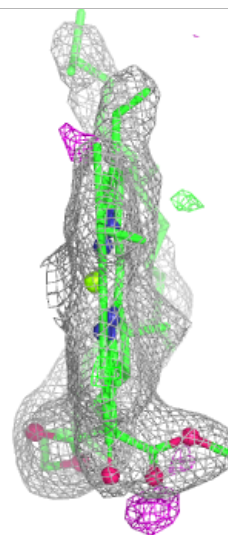
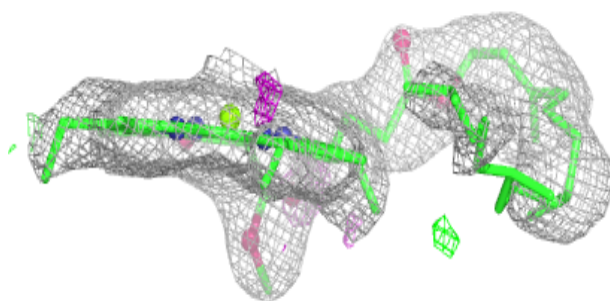
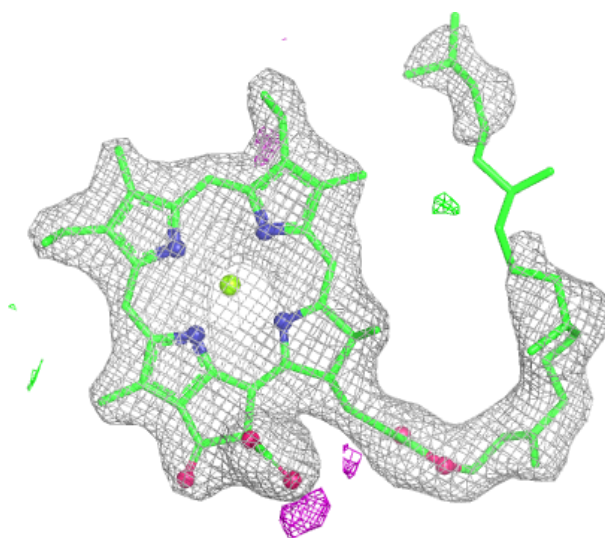
**Electron density around LMG D 406:**

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



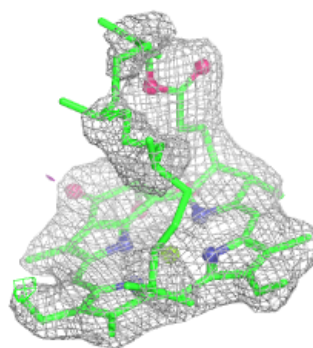
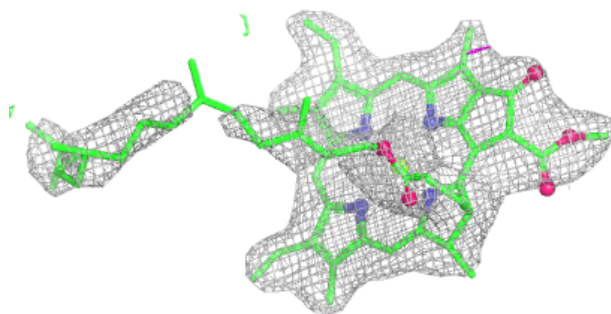
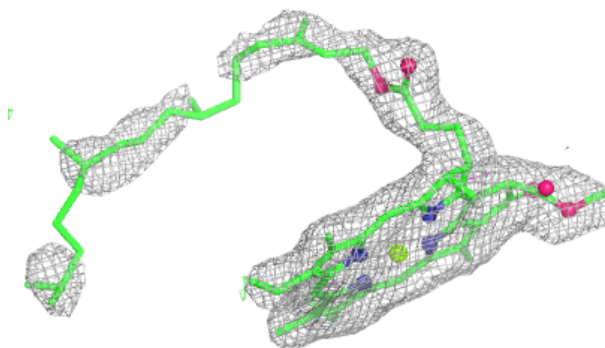
Electron density around CLA C 512:

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

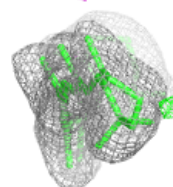
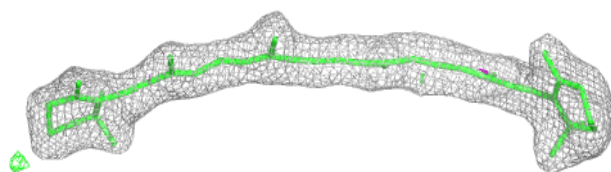
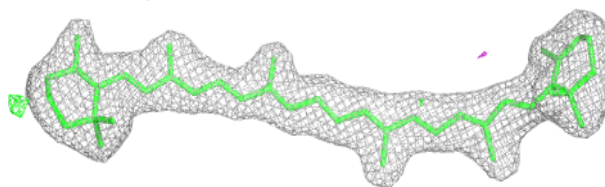


Electron density around CLA c 513:

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

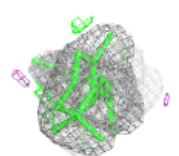
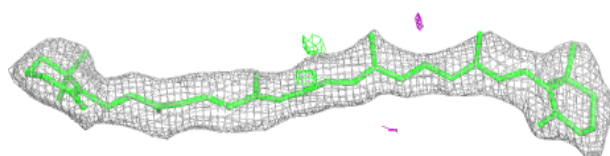
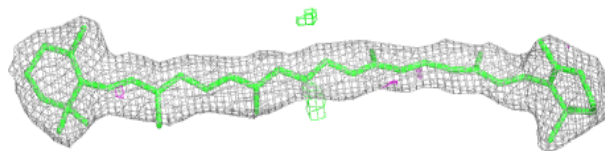
**Electron density around BCR t 101:**

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

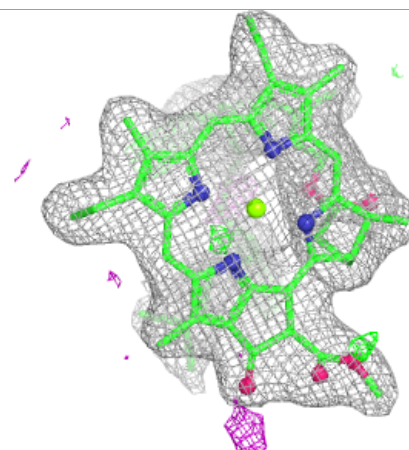
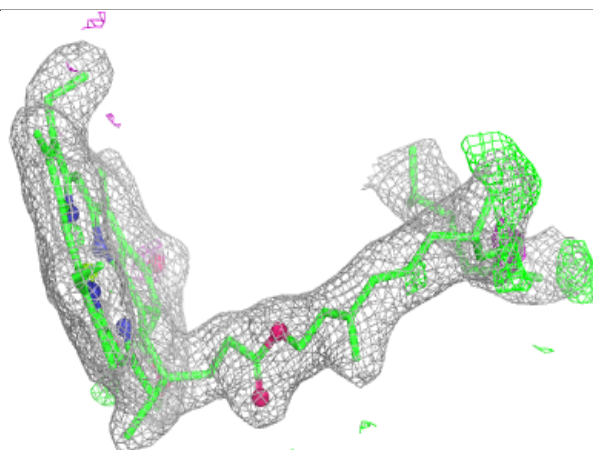
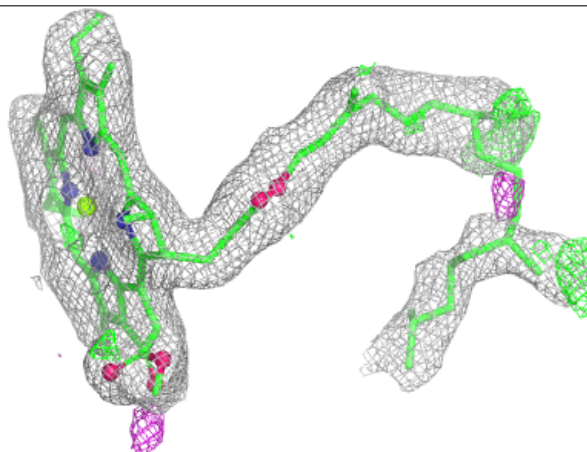


Electron density around BCR K 101:

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

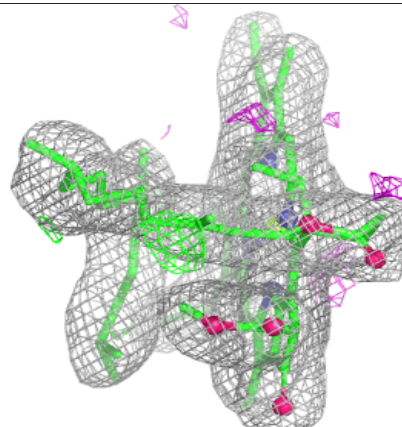
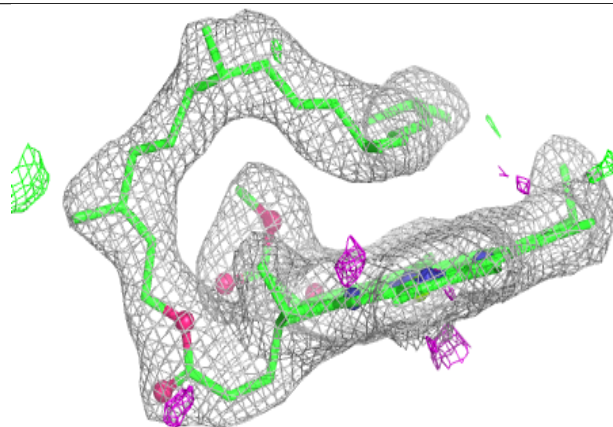
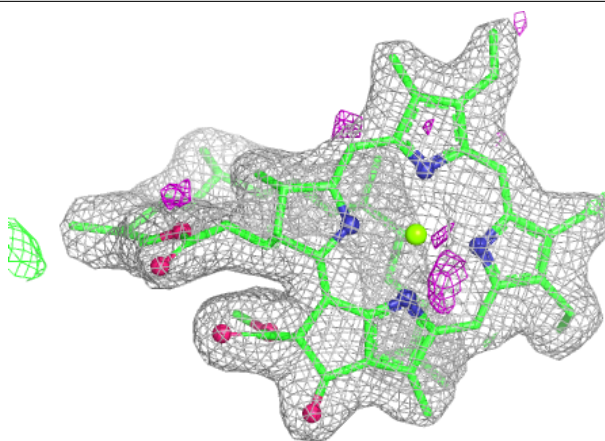
**Electron density around CLA B 605:**

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

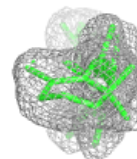
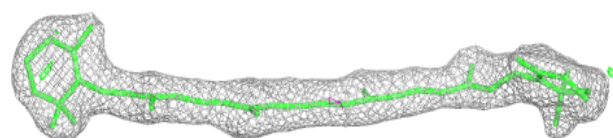
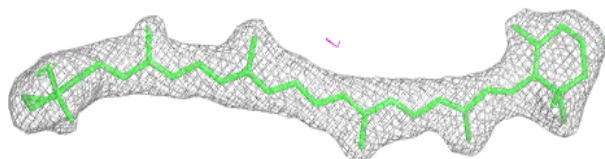


Electron density around CLA C 510:

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

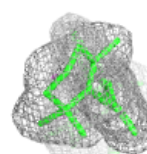
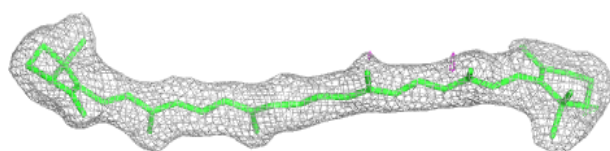
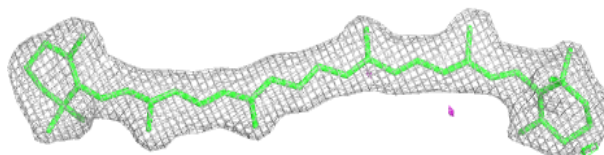
**Electron density around BCR b 616:**

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

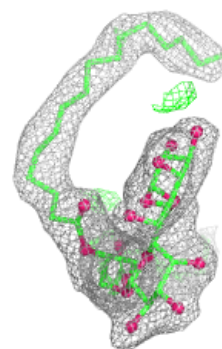
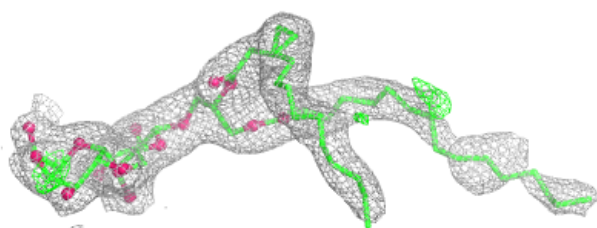
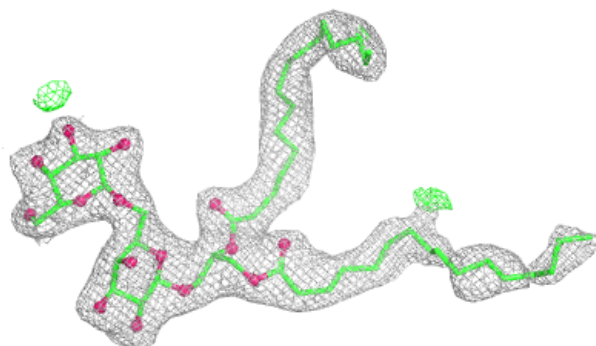


Electron density around BCR B 618:

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

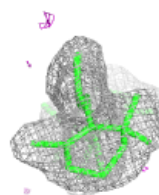
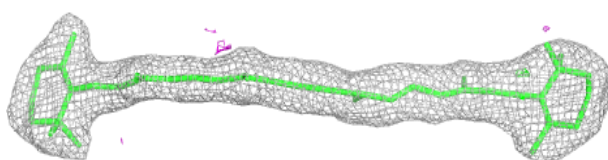
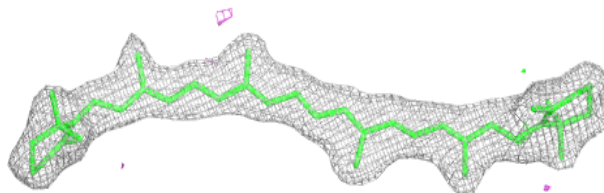
**Electron density around DGD c 518:**

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

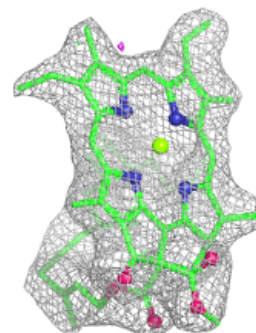
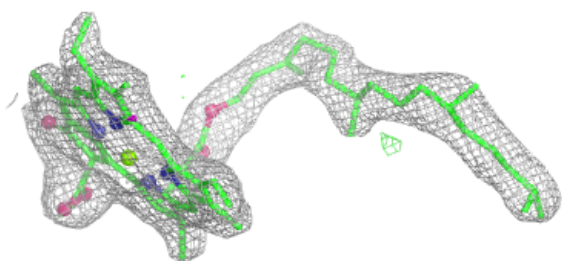
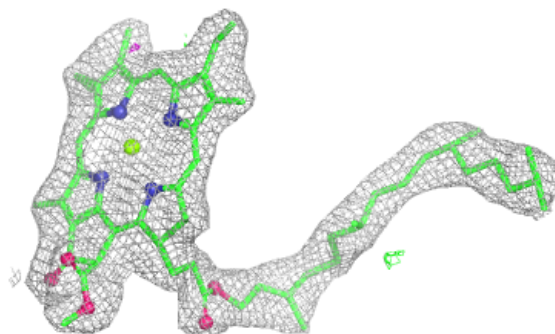


Electron density around BCR C 514:

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

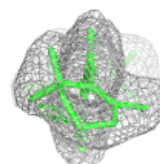
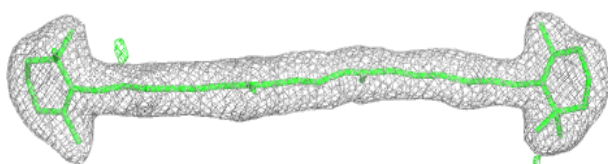
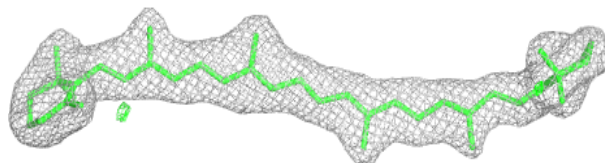
**Electron density around CLA C 511:**

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

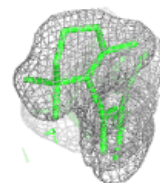
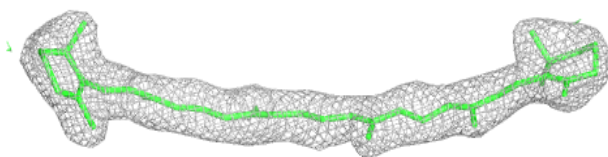
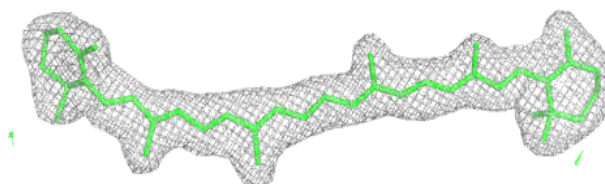


Electron density around BCR A 611:

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

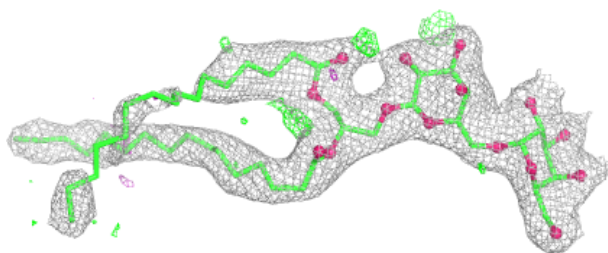
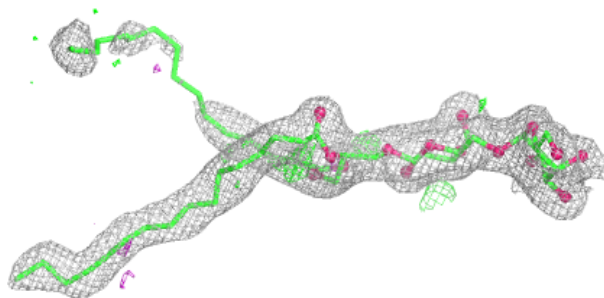
**Electron density around BCR T 101:**

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

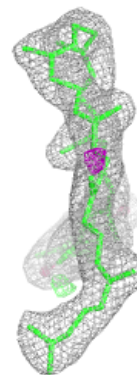
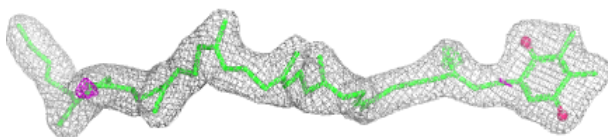
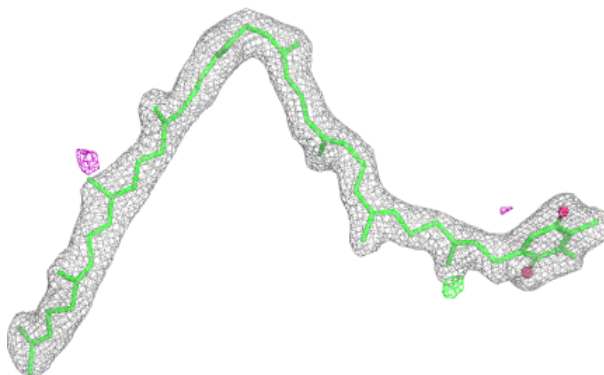


Electron density around DGD C 516:

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

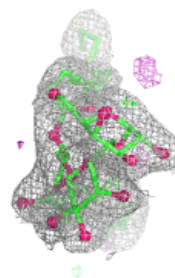
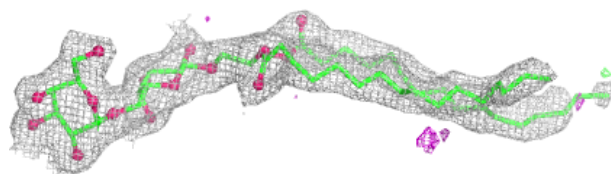
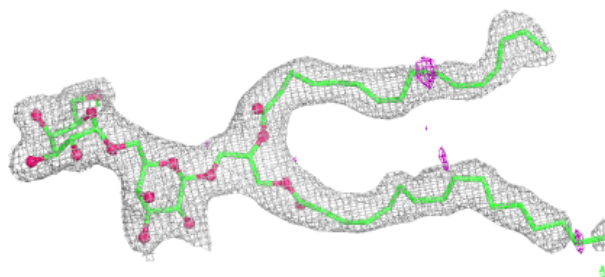
**Electron density around PL9 D 405:**

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



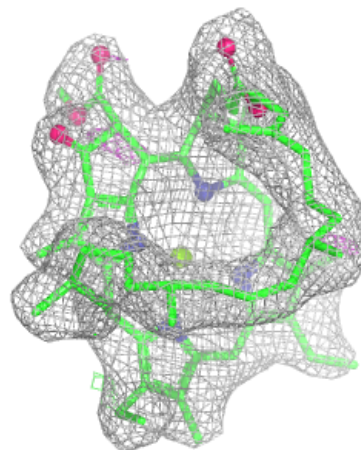
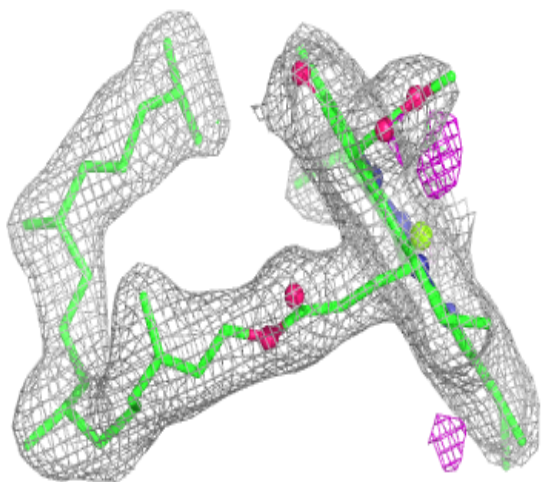
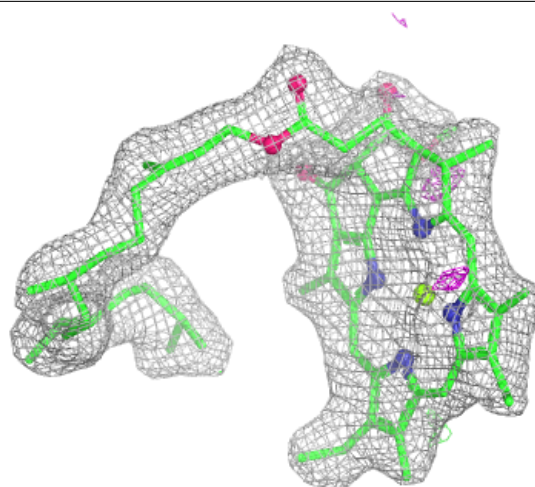
Electron density around DGD C 518:

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



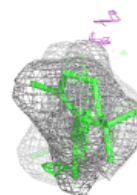
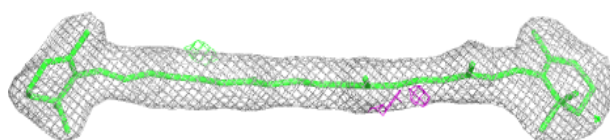
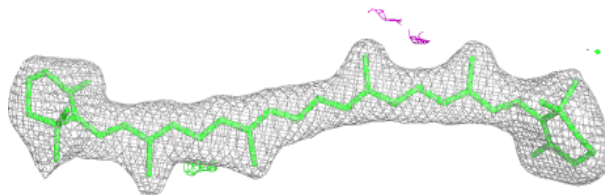
Electron density around CLA c 503:

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

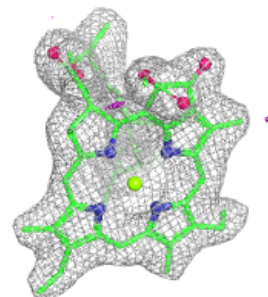
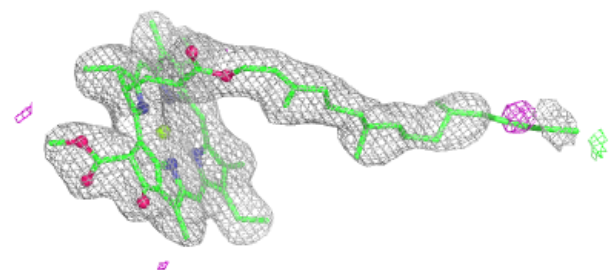
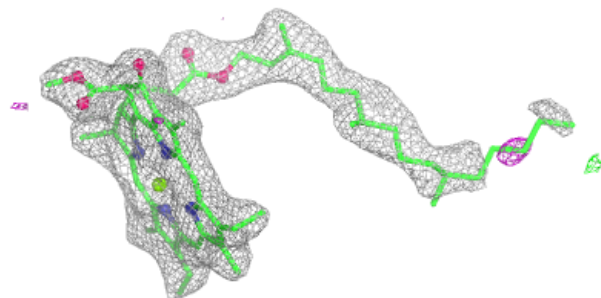


Electron density around BCR b 617:

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

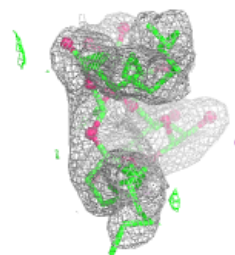
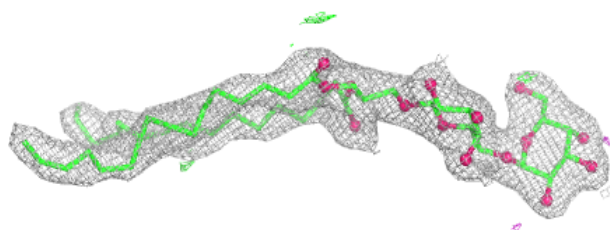
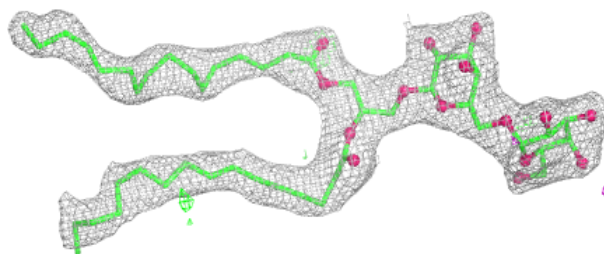
**Electron density around CLA c 508:**

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



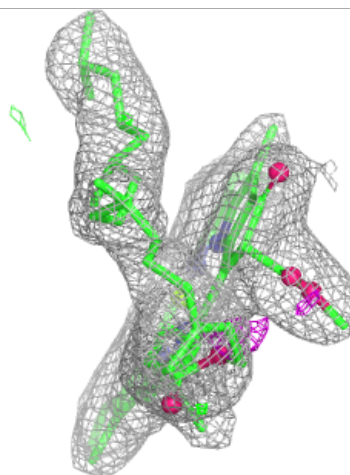
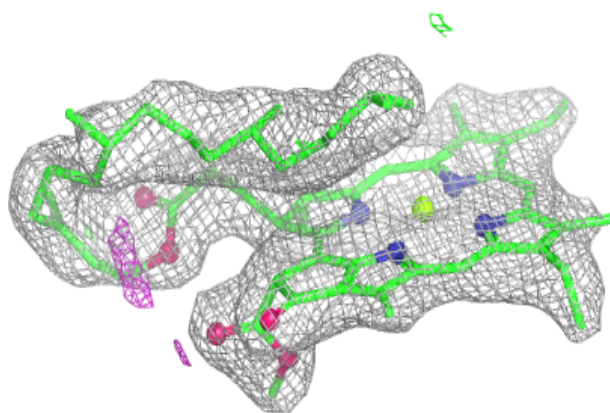
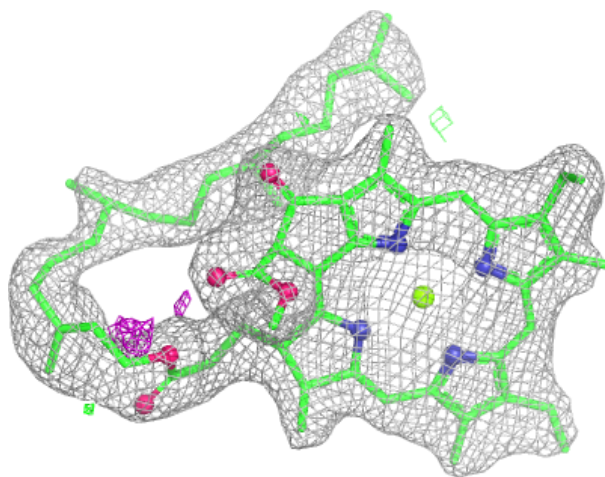
Electron density around DGD c 519:

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



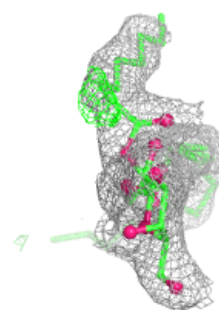
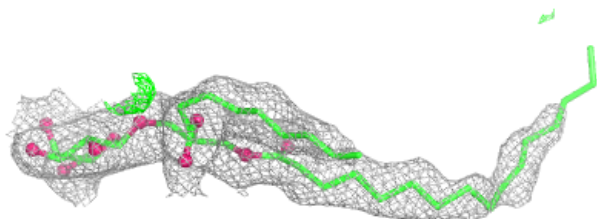
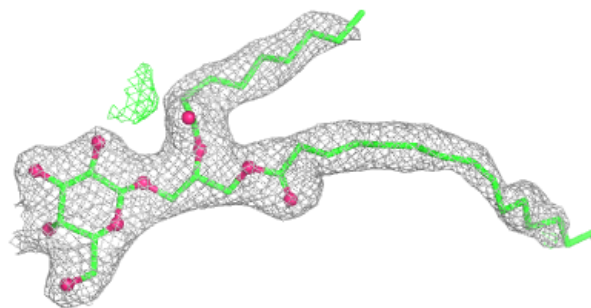
Electron density around CLA c 509:

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

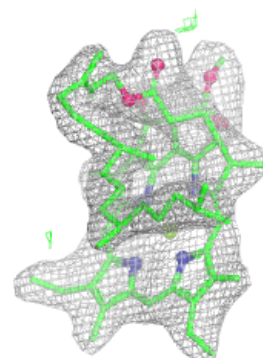
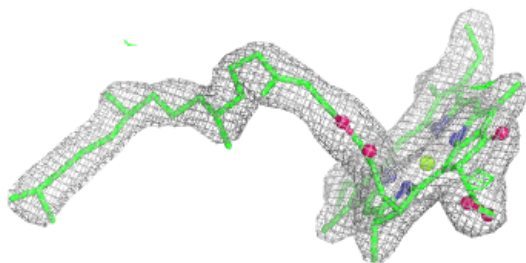
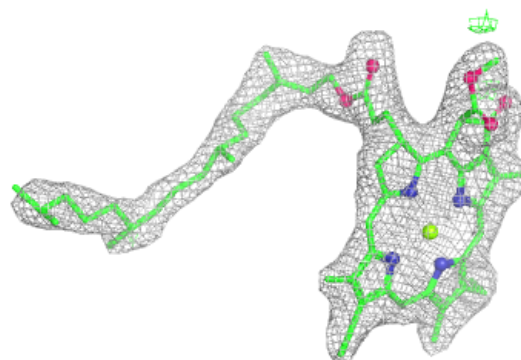


Electron density around LMG d 410:

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

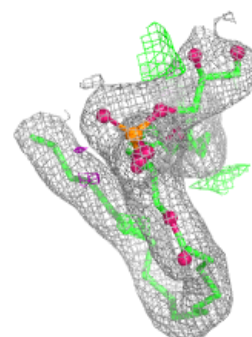
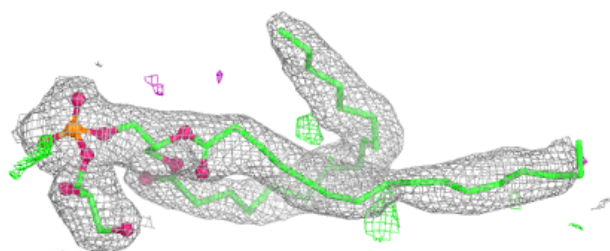
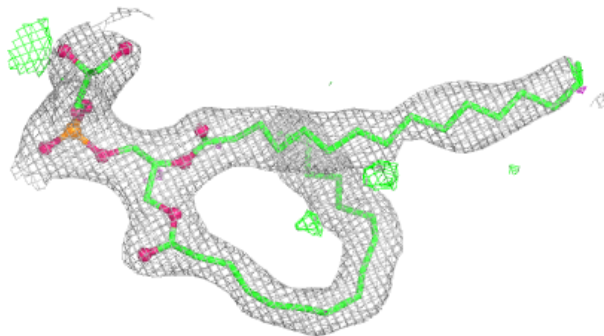
**Electron density around CLA c 511:**

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

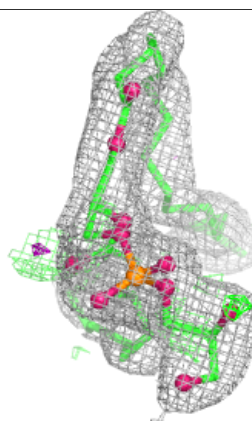
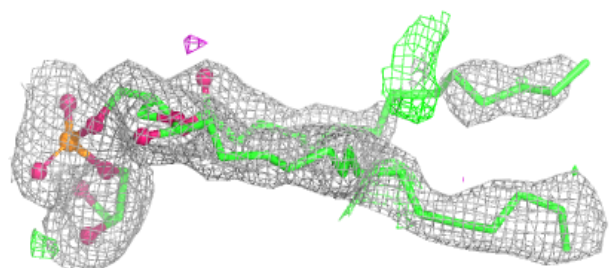
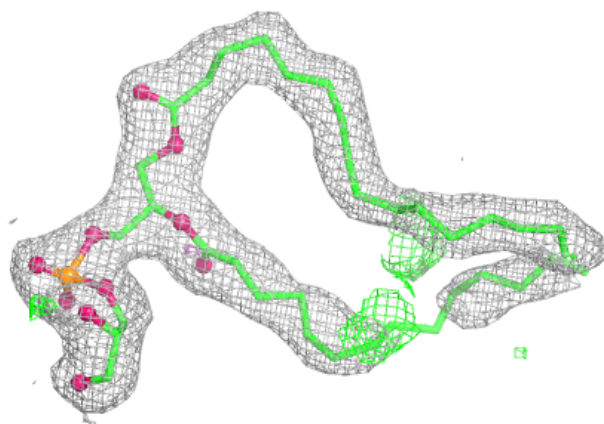


Electron density around LHG B 622:

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

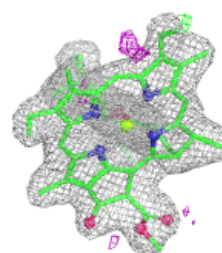
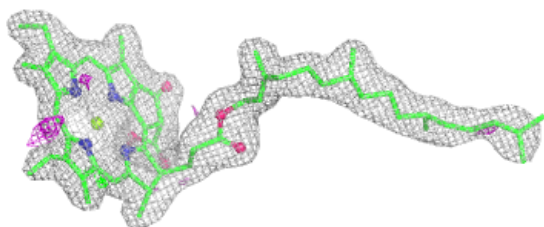
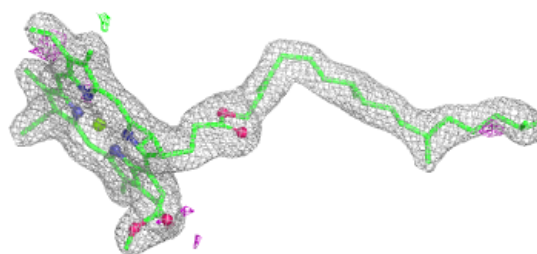
**Electron density around LHG D 408:**

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

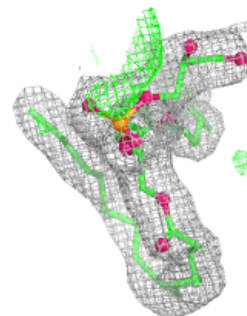
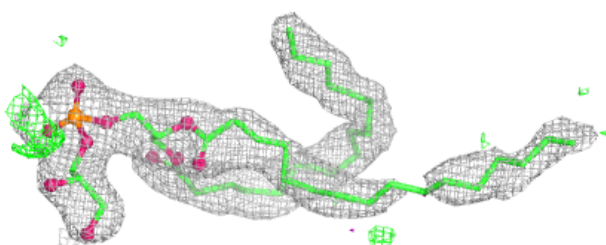
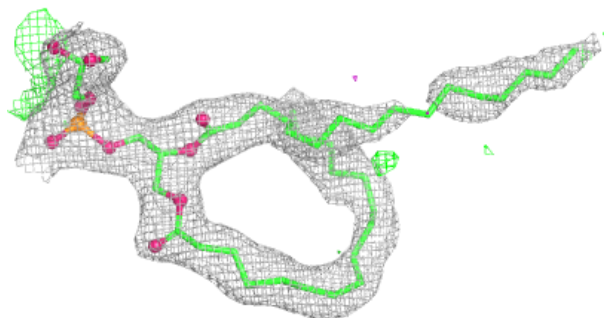


Electron density around CLA C 502:

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

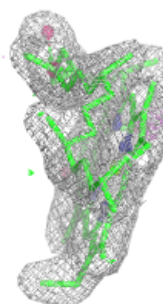
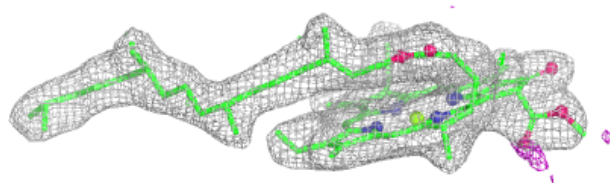
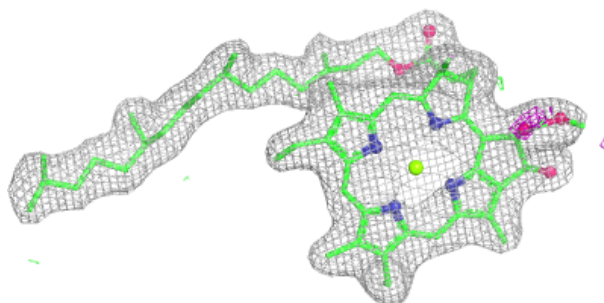
**Electron density around LHG d 406:**

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

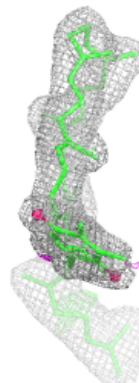
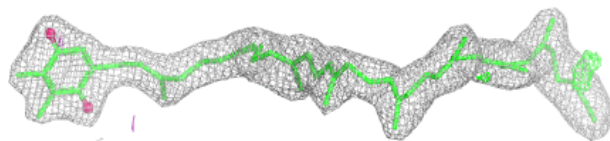
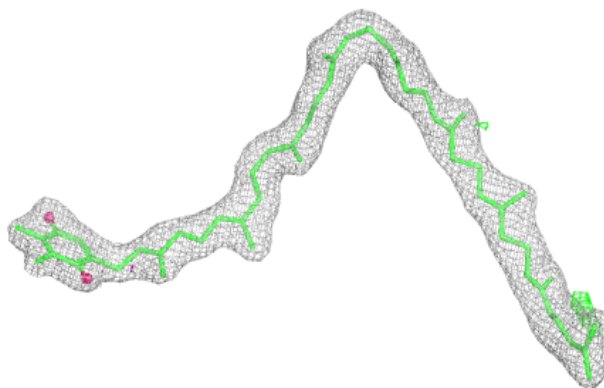


Electron density around CLA C 501:

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

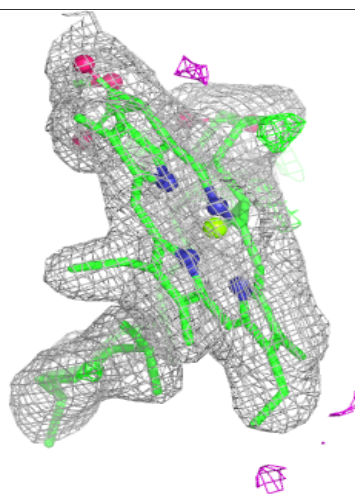
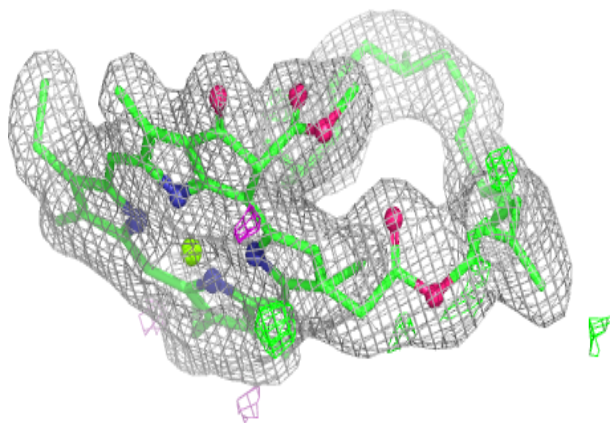
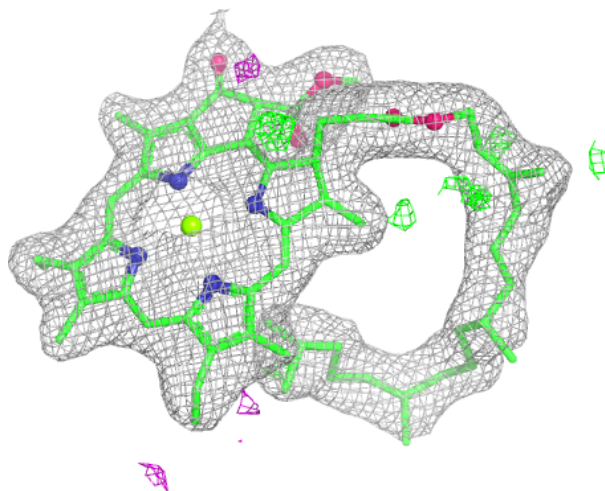
**Electron density around PL9 d 405:**

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



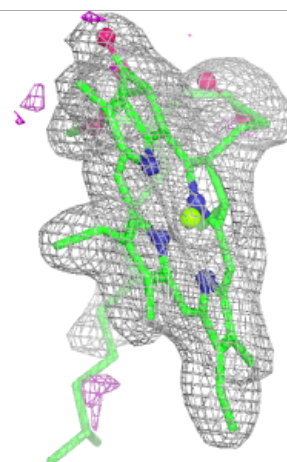
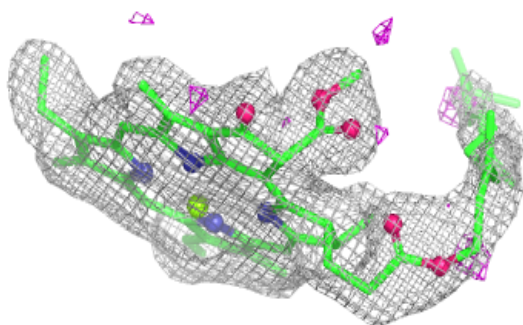
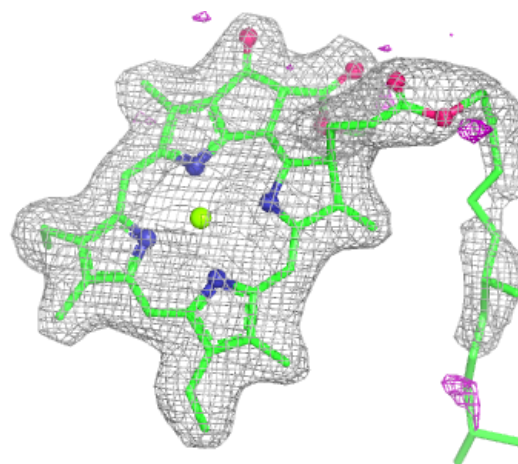
Electron density around CLA B 614:

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



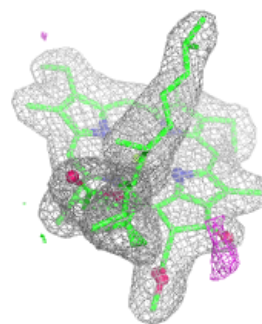
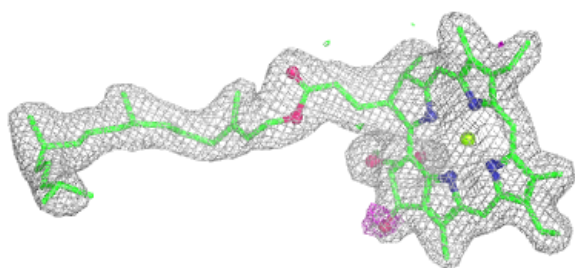
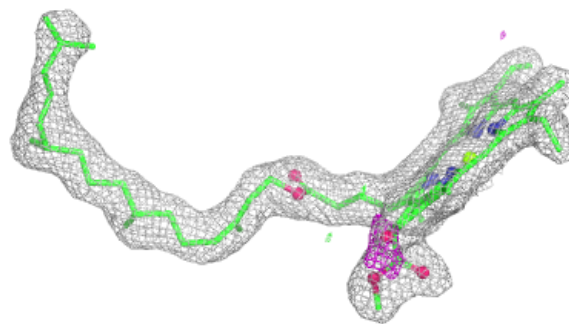
Electron density around CLA B 615:

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

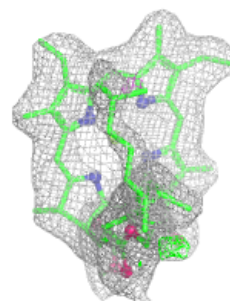
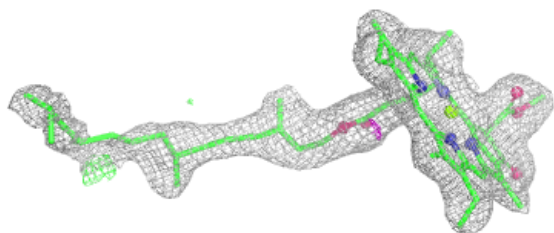
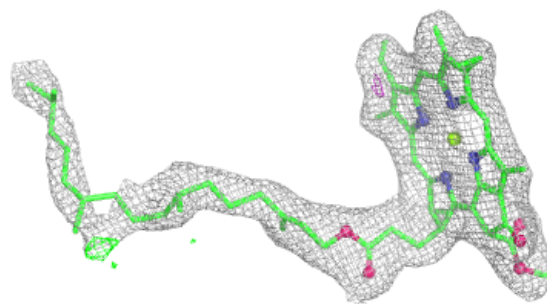


Electron density around CLA d 402:

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

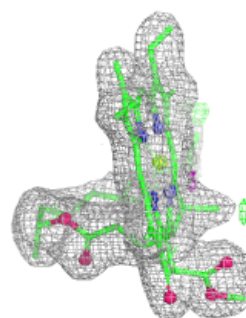
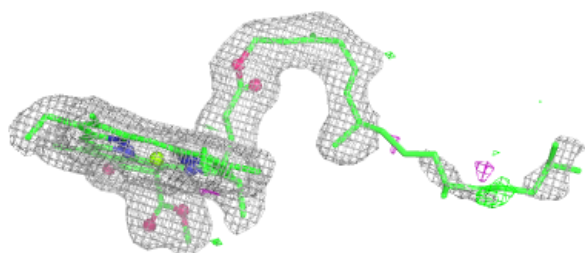
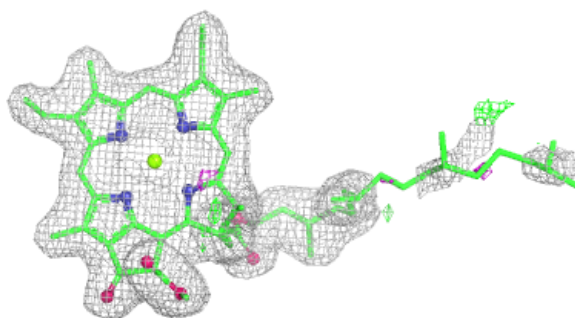
**Electron density around CLA d 403:**

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



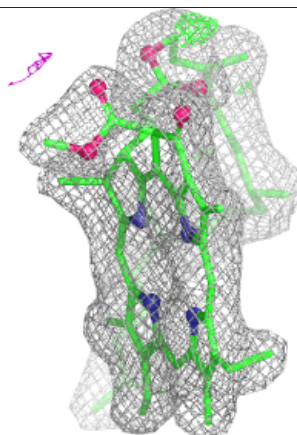
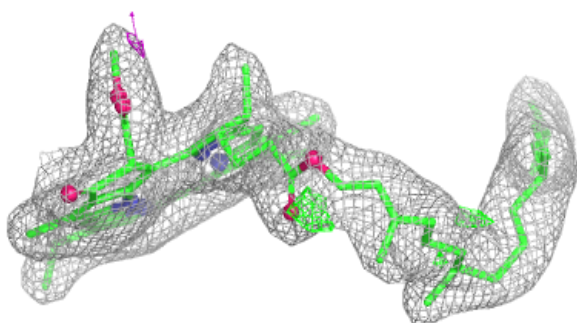
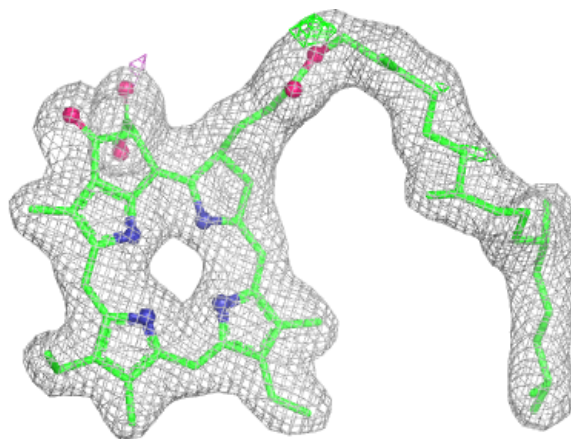
Electron density around CLA A 607:

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



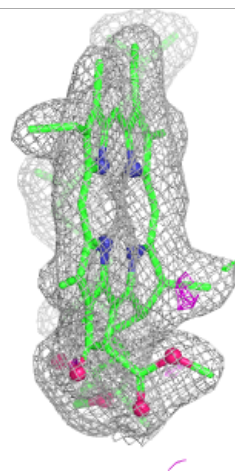
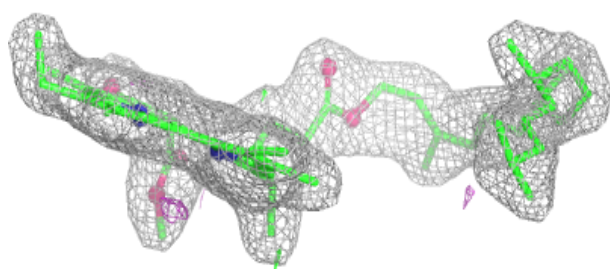
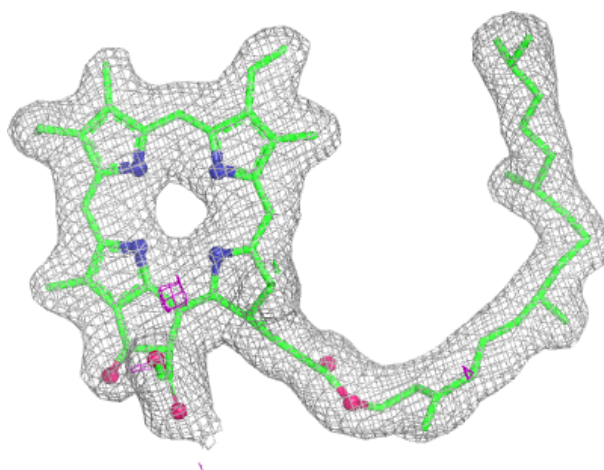
Electron density around PHO A 609:

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



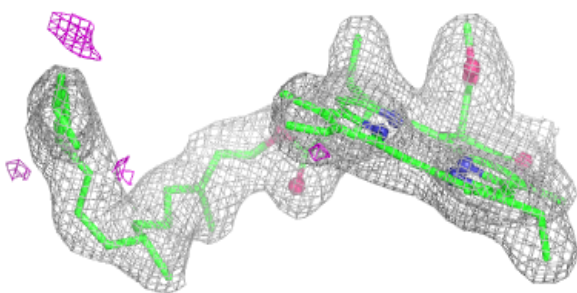
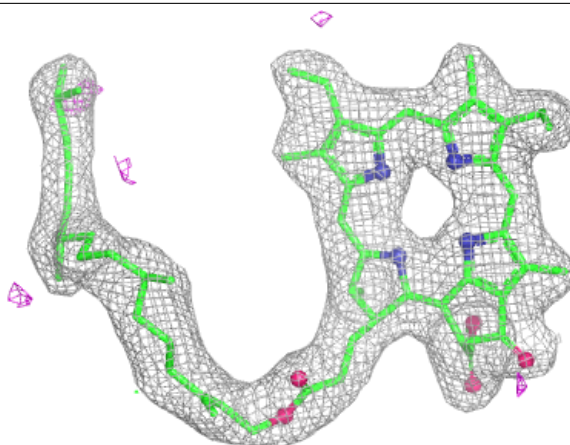
Electron density around PHO a 609:

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



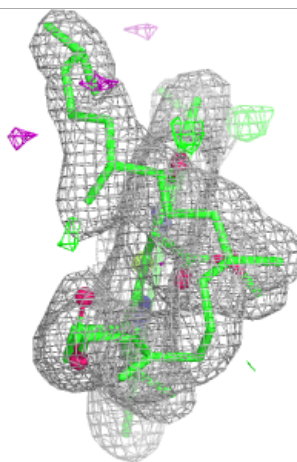
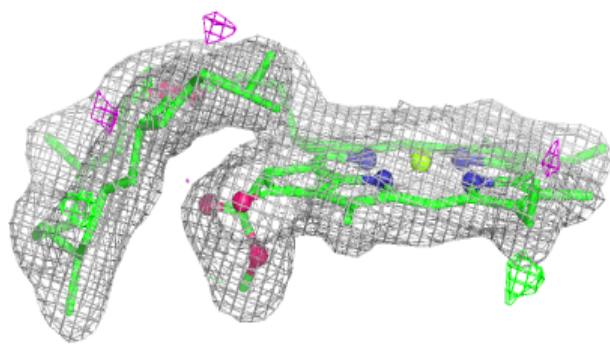
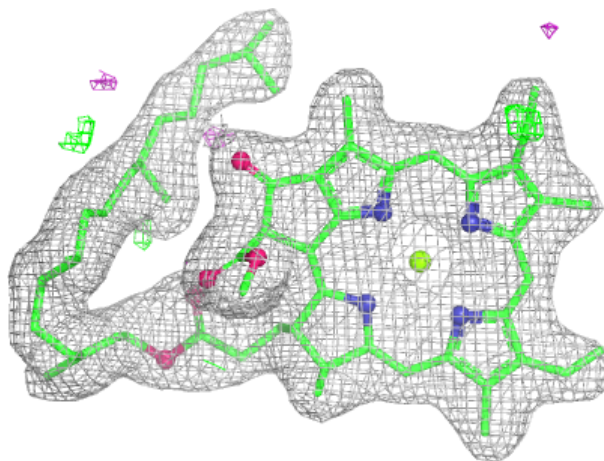
Electron density around PHO d 401:

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



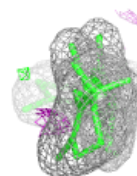
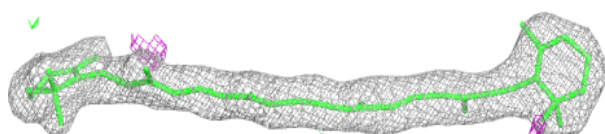
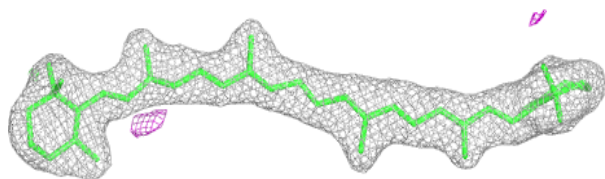
Electron density around CLA B 609:

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

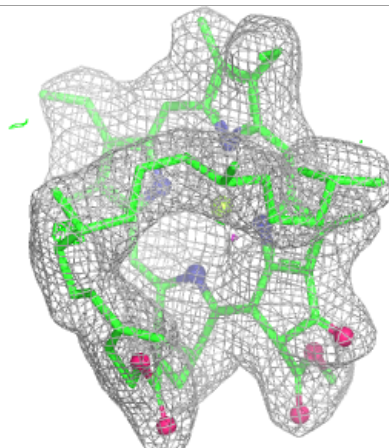
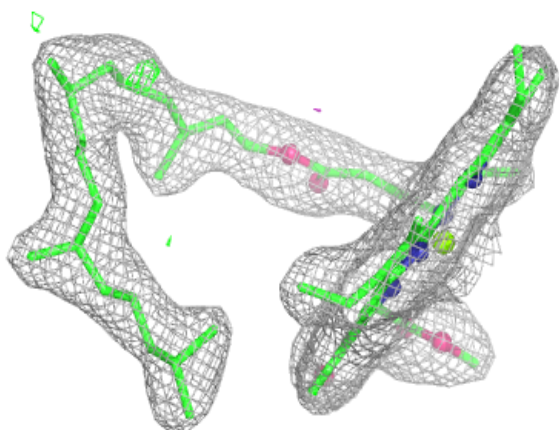
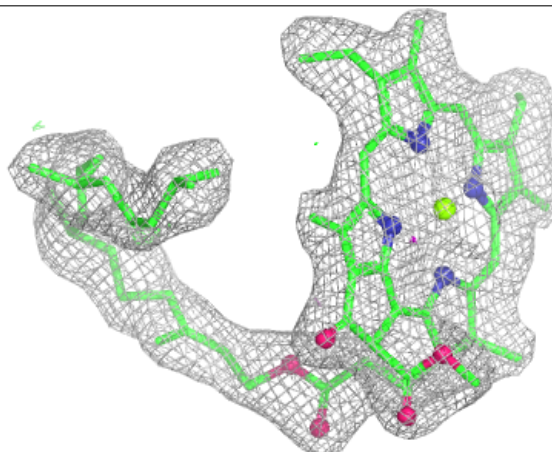


Electron density around BCR B 616:

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

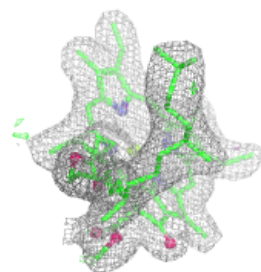
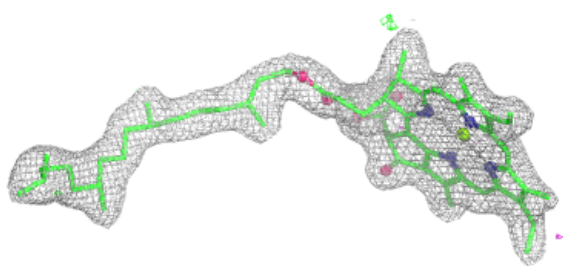
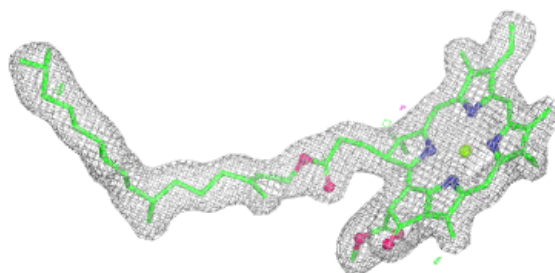
**Electron density around CLA C 503:**

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

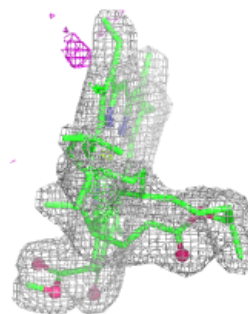
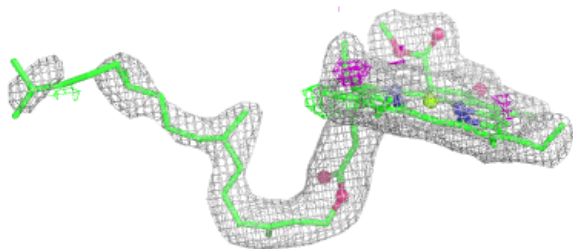
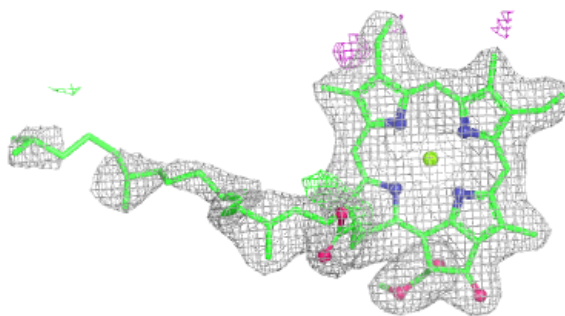


Electron density around CLA a 607:

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

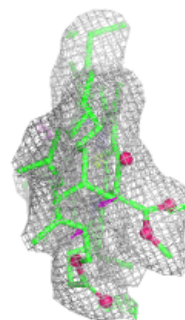
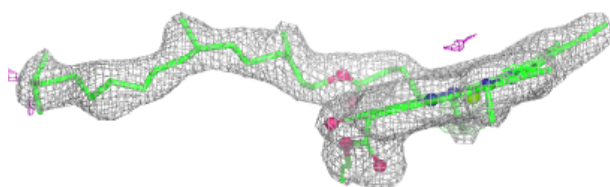
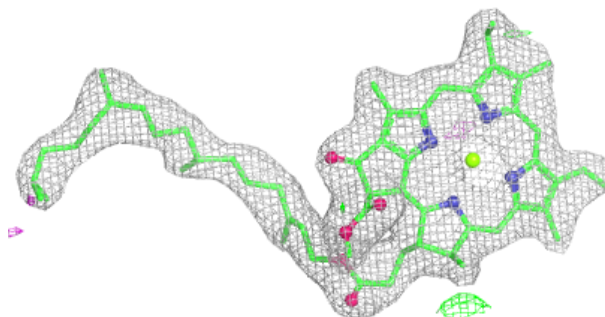
**Electron density around CLA a 608:**

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

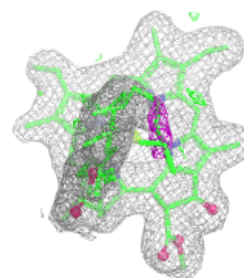
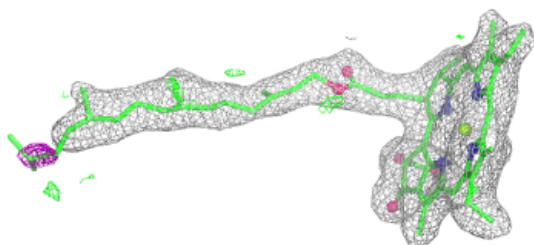
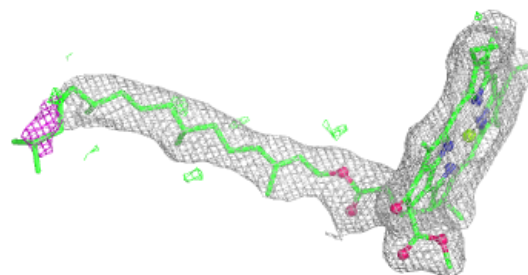


Electron density around CLA b 601:

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

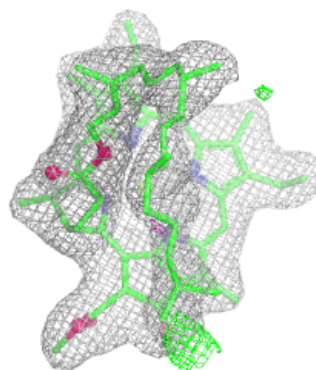
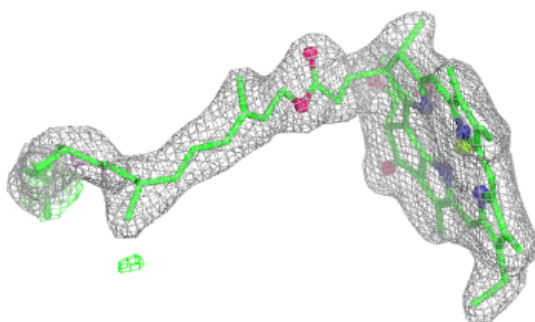
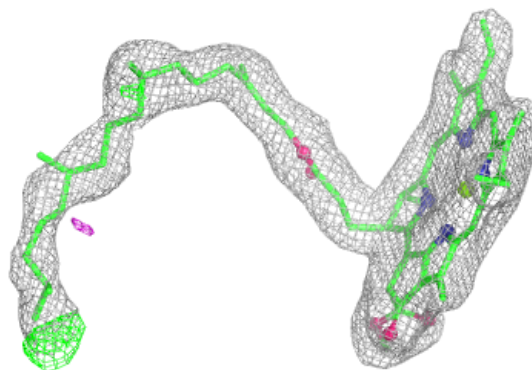
**Electron density around CLA b 603:**

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

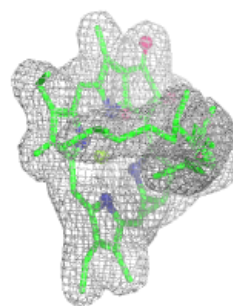
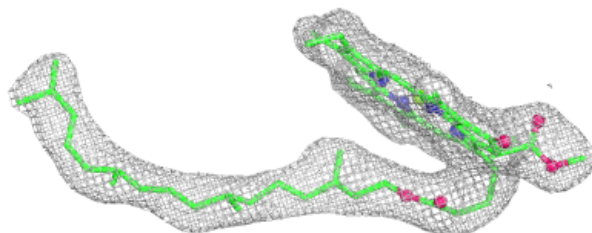
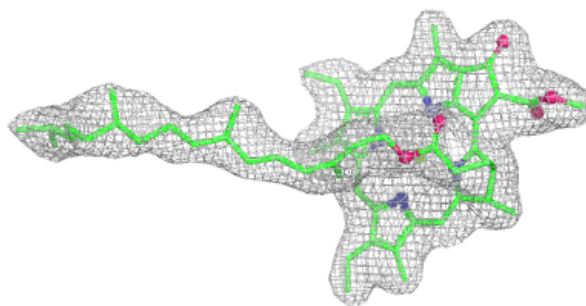


Electron density around CLA b 605:

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

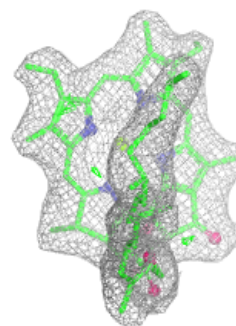
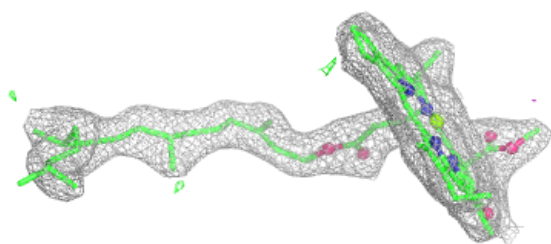
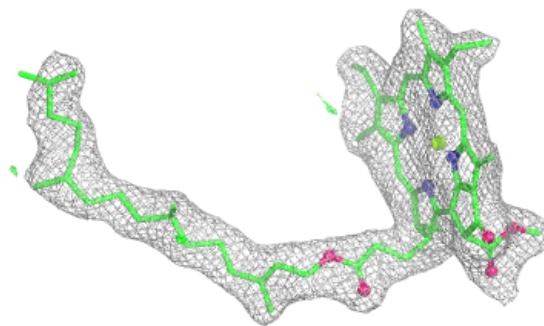
**Electron density around CLA b 607:**

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



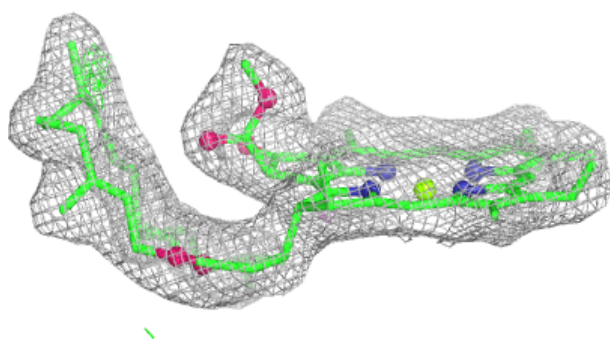
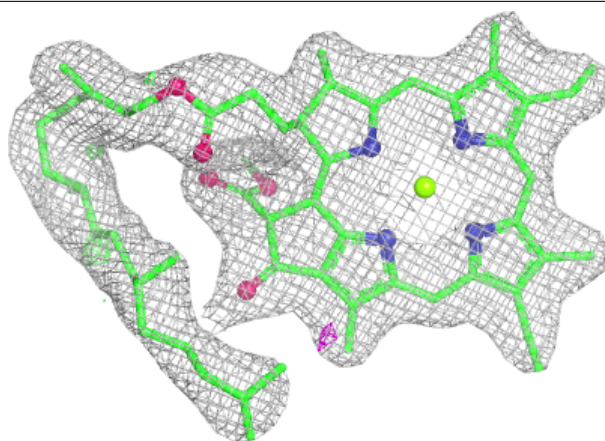
Electron density around CLA b 608:

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

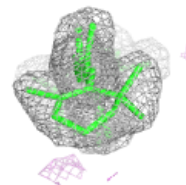
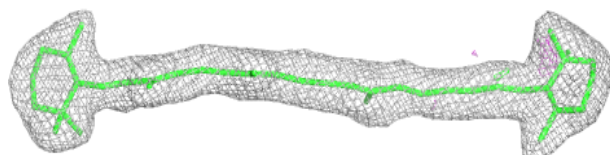
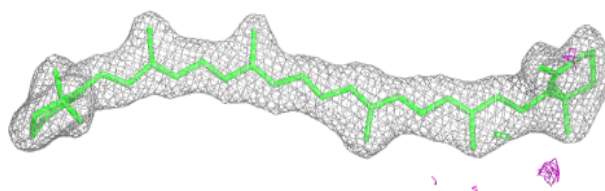


Electron density around CLA b 609:

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

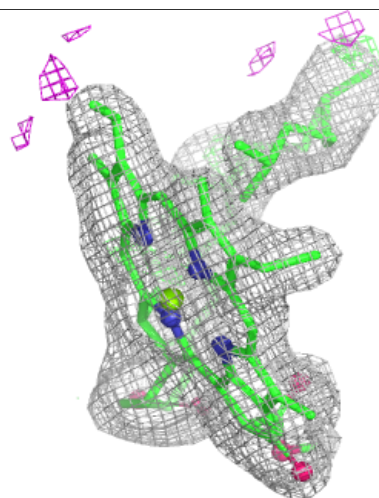
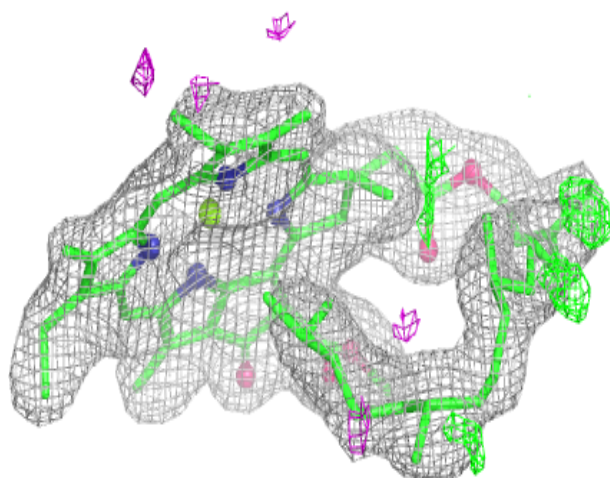
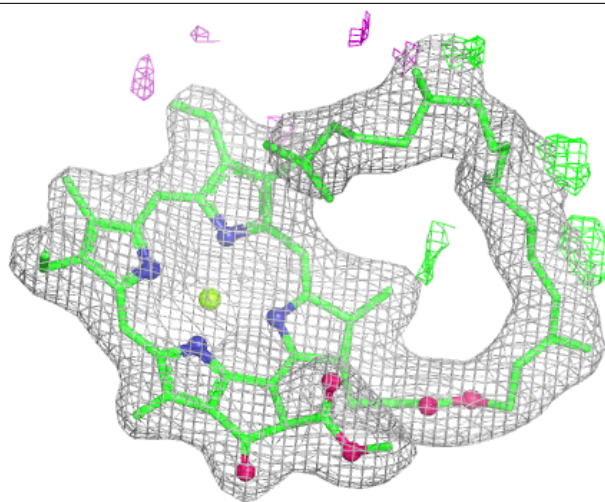
**Electron density around BCR a 611:**

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



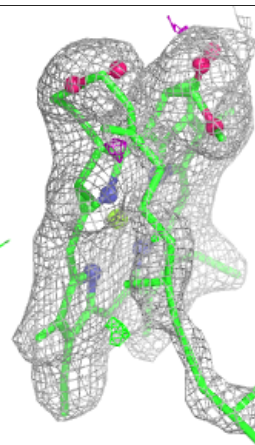
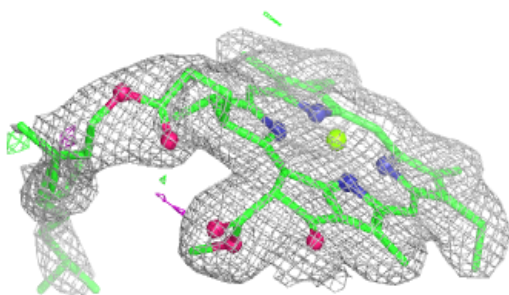
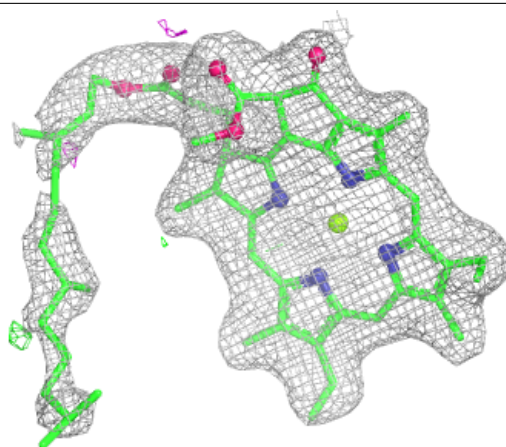
Electron density around CLA b 614:

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



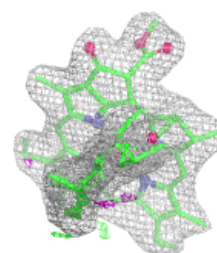
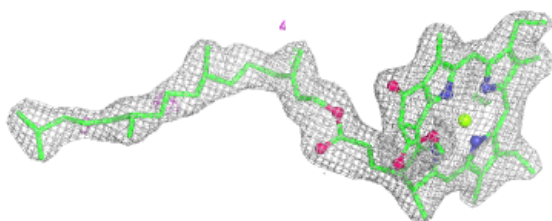
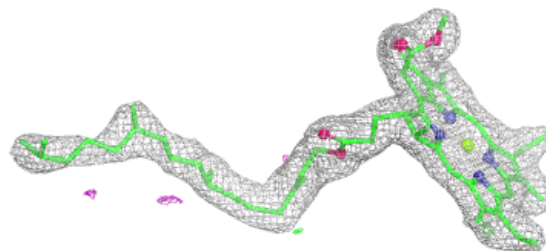
Electron density around CLA b 615:

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

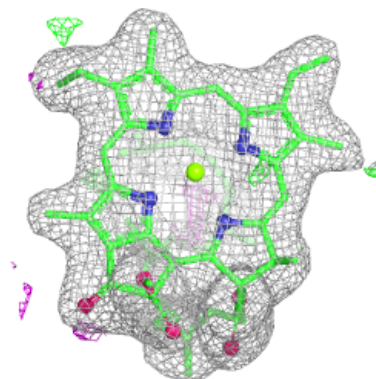
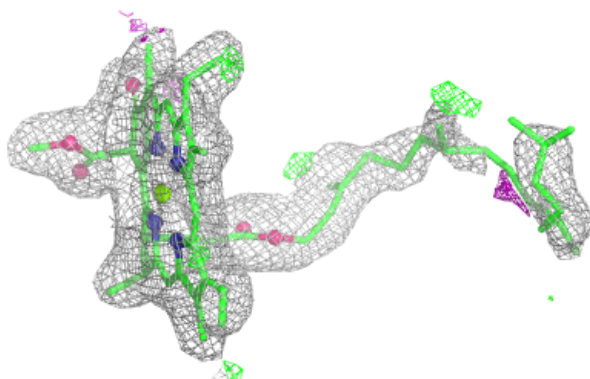
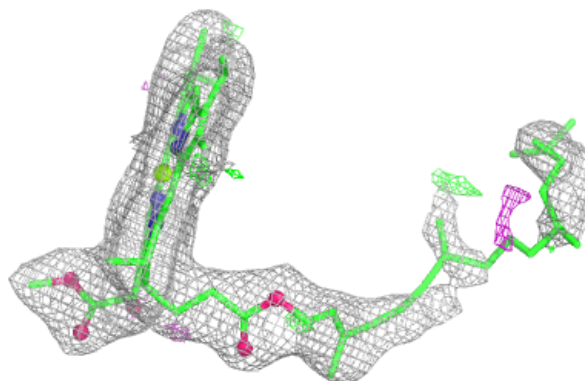


Electron density around CLA c 502:

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

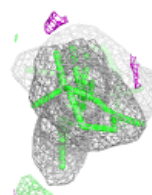
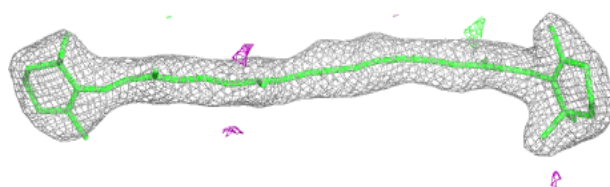
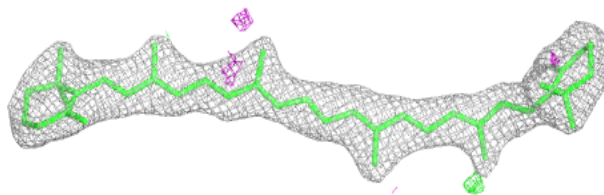
**Electron density around CLA C 506:**

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

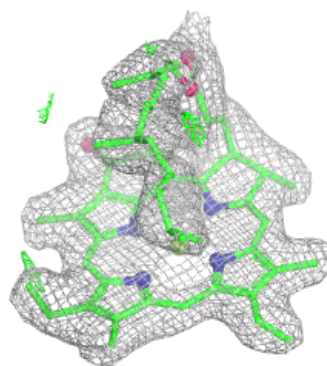
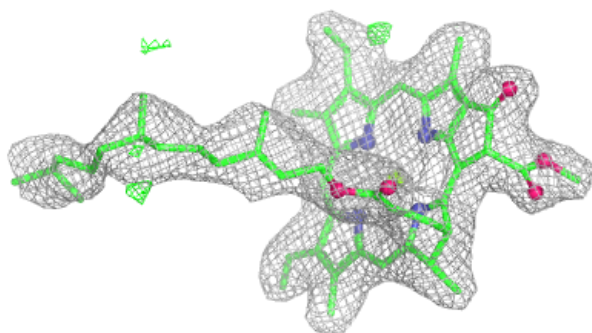
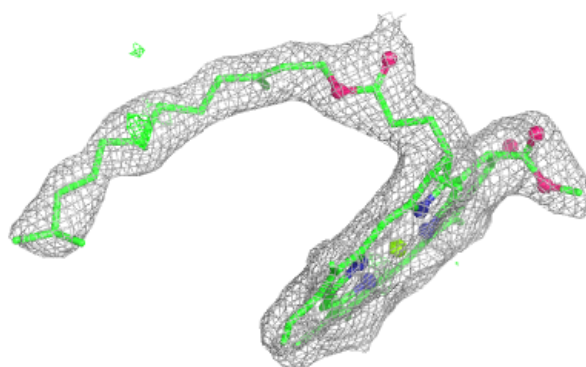


Electron density around BCR c 515:

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

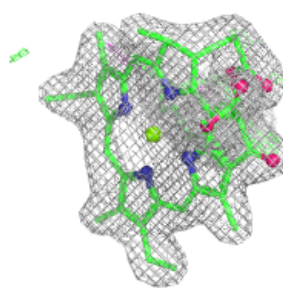
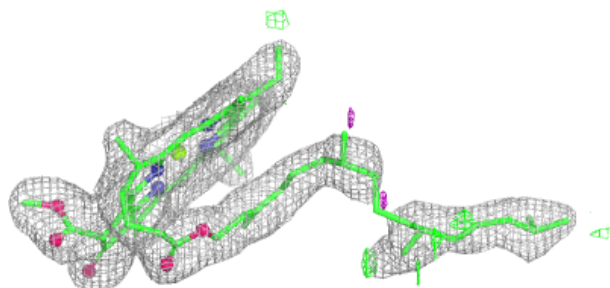
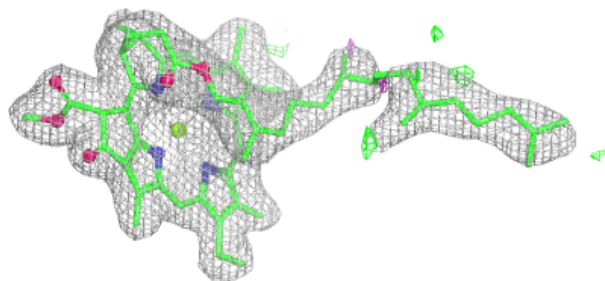
**Electron density around CLA c 504:**

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

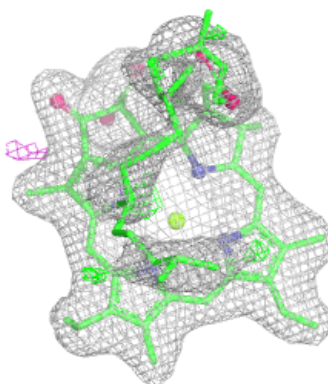
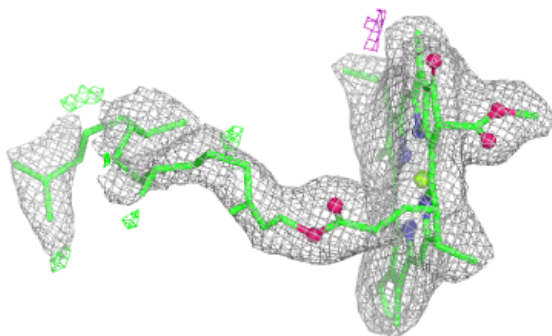
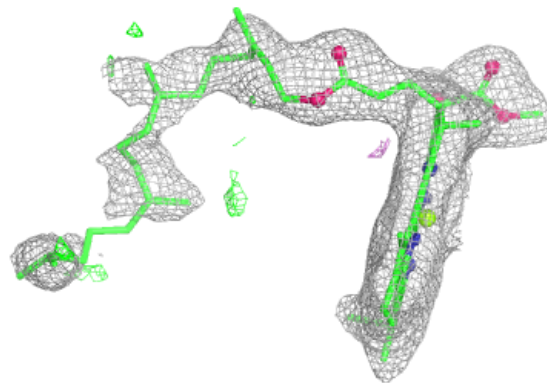


Electron density around CLA c 505:

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

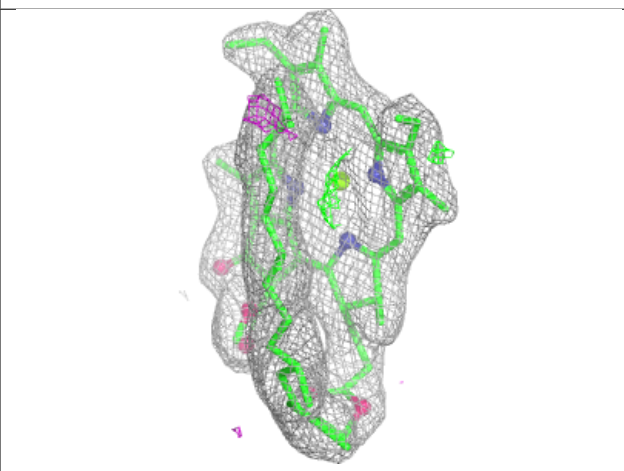
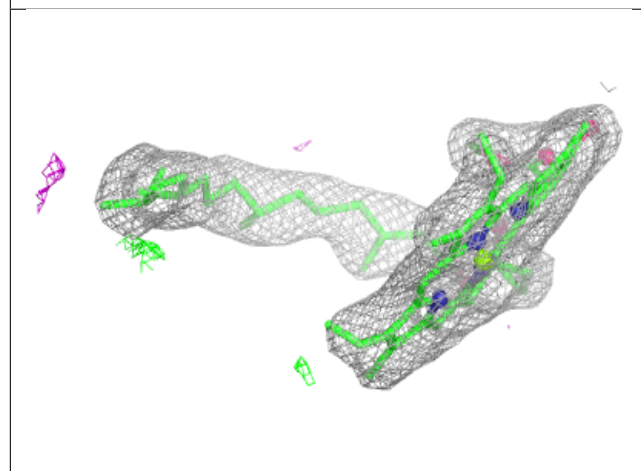
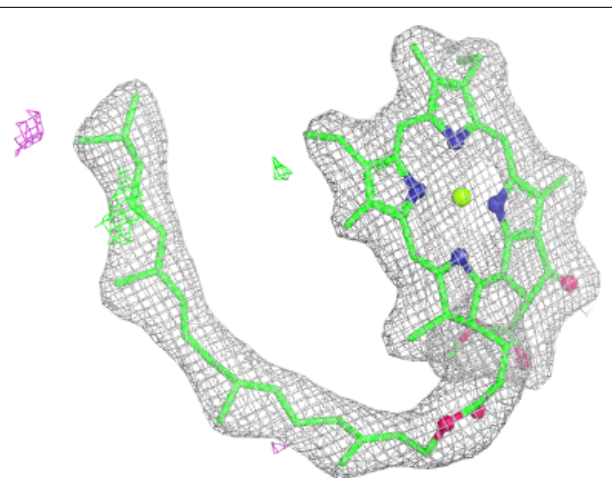
**Electron density around CLA c 506:**

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



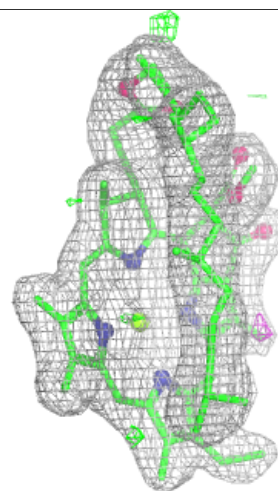
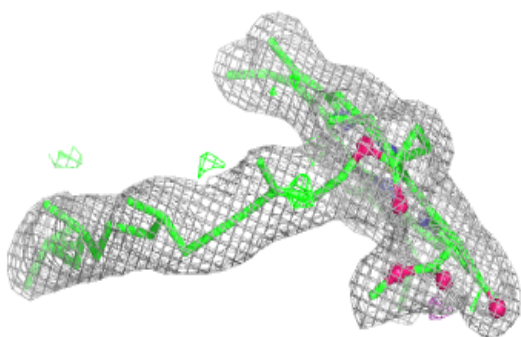
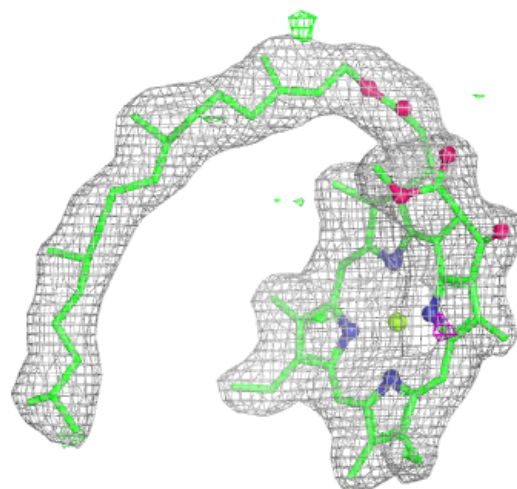
Electron density around CLA c 507:

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



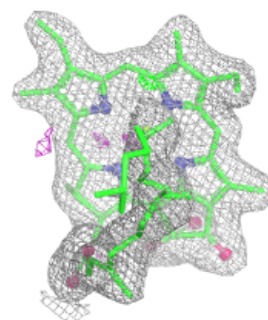
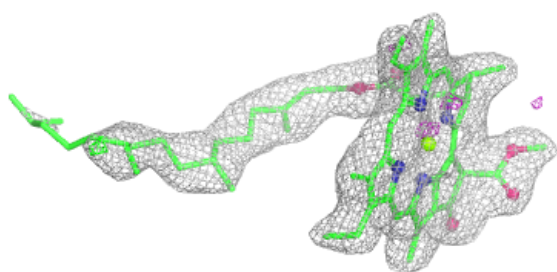
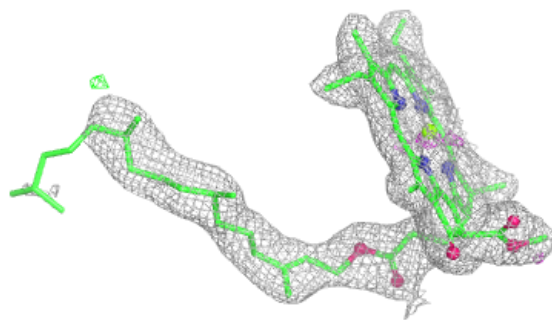
Electron density around CLA C 507:

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

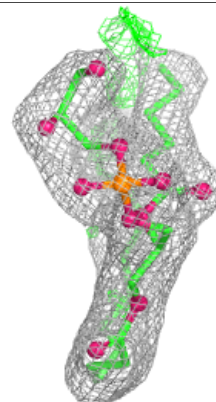
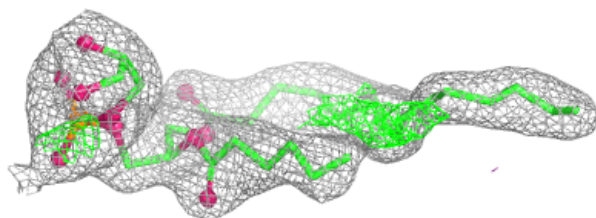
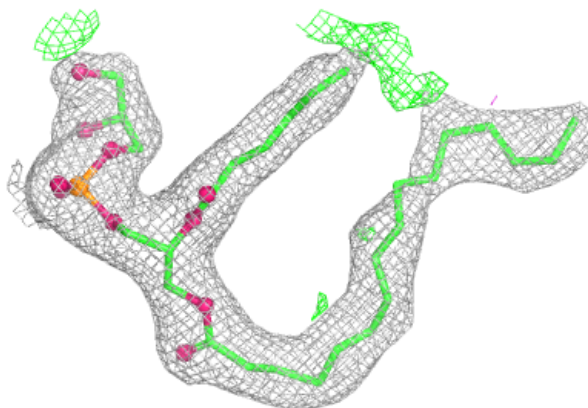


Electron density around CLA C 508:

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

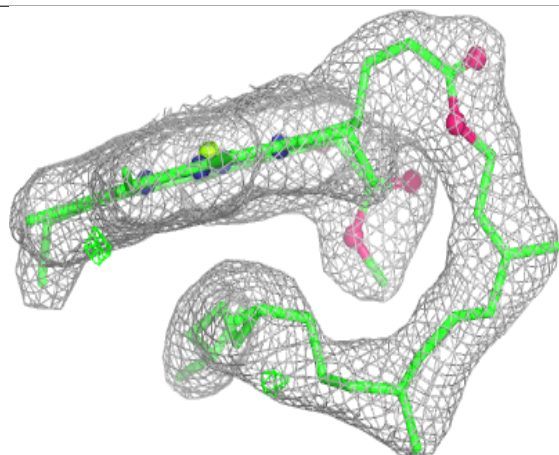
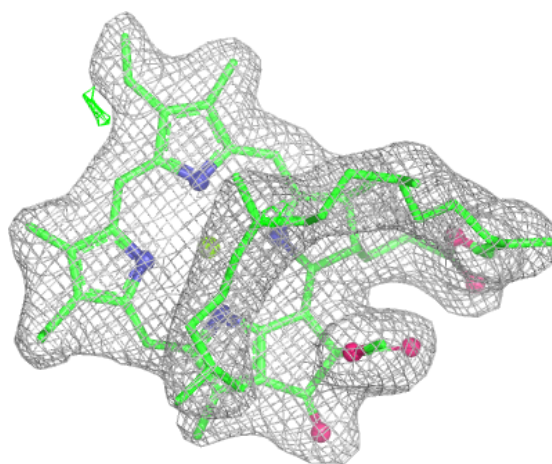
**Electron density around LHG d 408:**

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



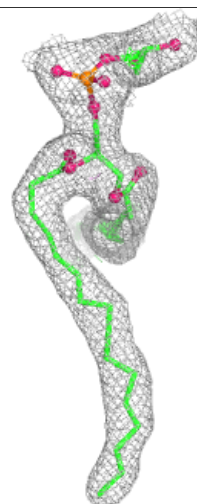
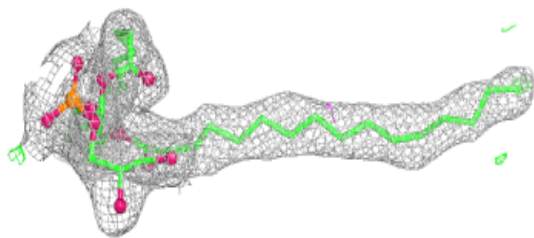
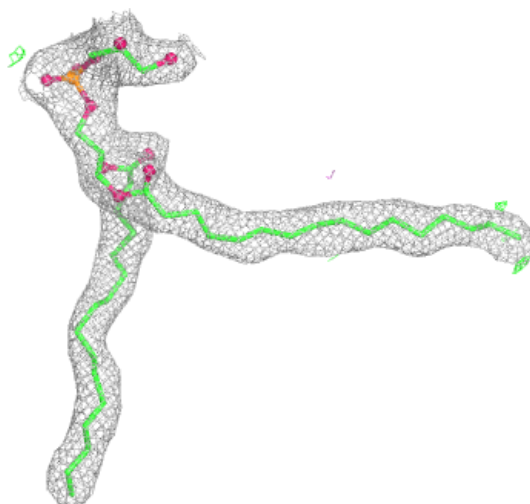
Electron density around CLA c 510:

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



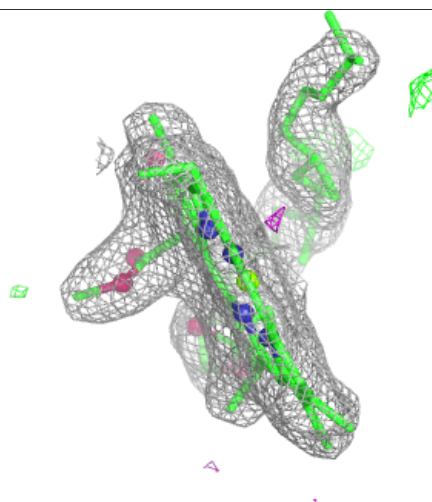
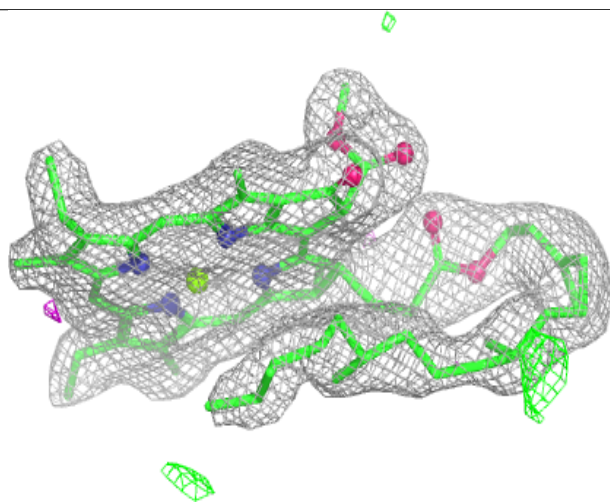
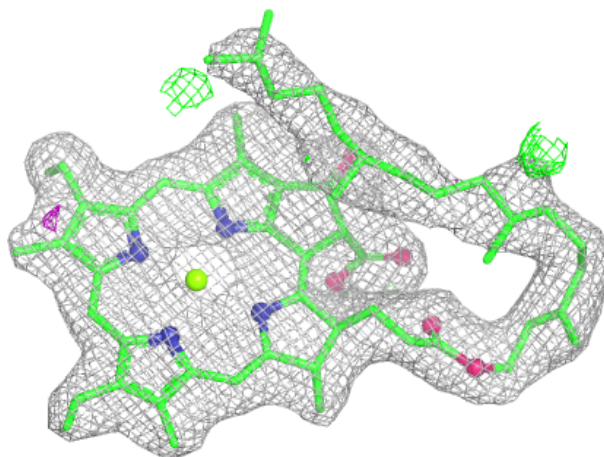
Electron density around LHG 1 102:

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



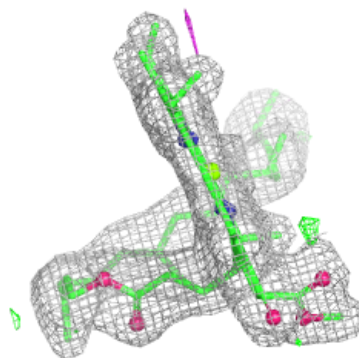
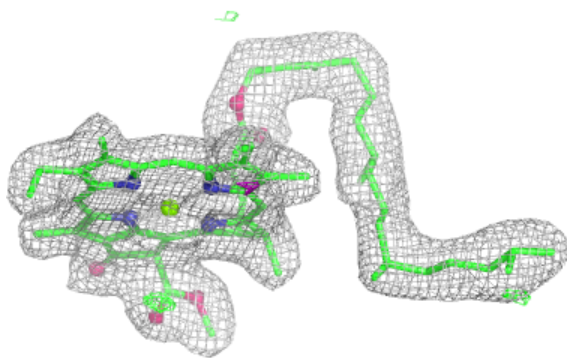
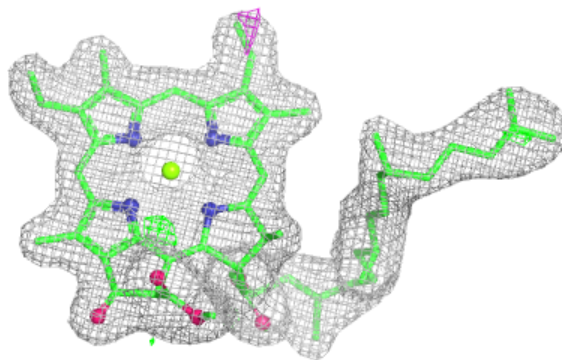
Electron density around CLA C 509:

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

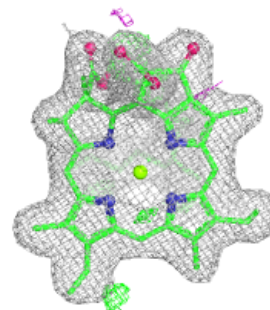
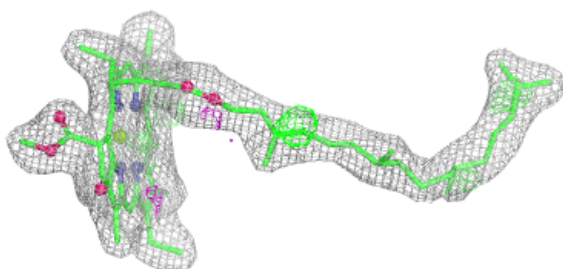
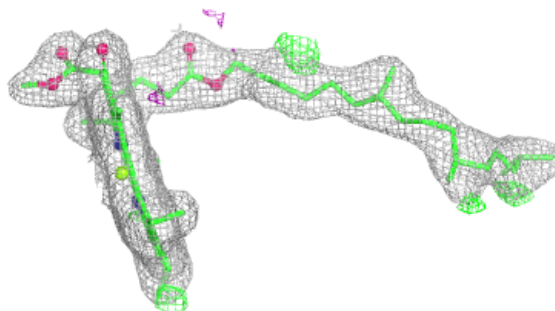


Electron density around CLA a 613:

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

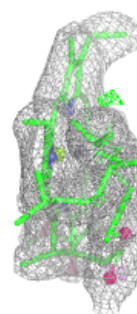
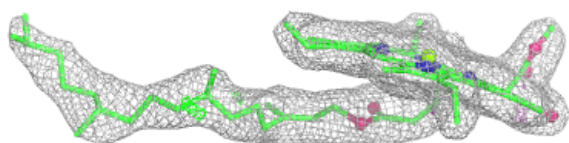
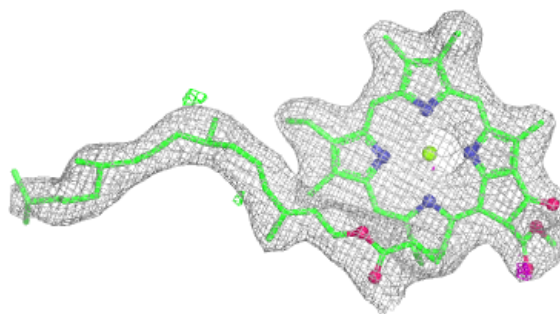
**Electron density around CLA B 604:**

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

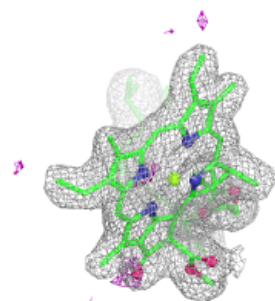
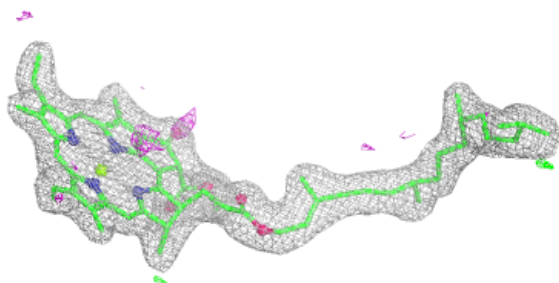
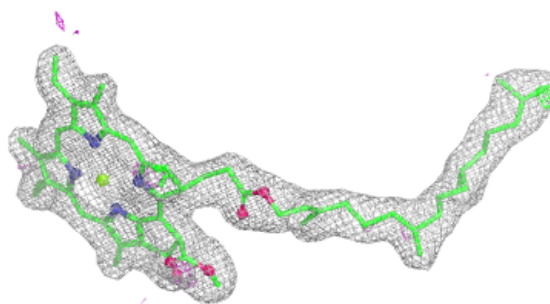


Electron density around CLA b 602:

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

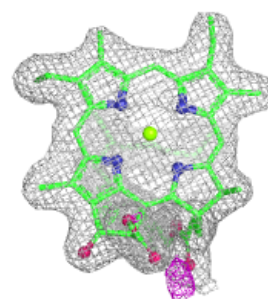
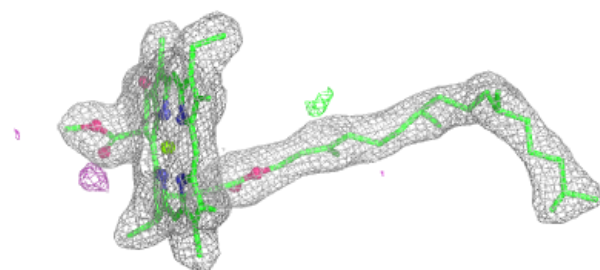
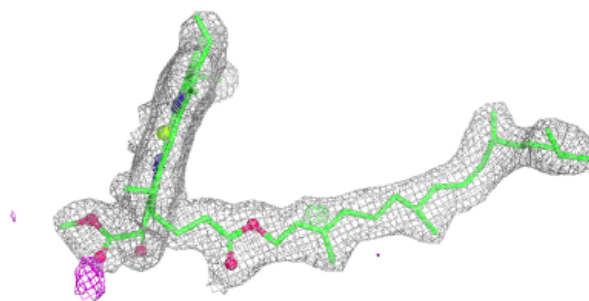
**Electron density around CLA A 606:**

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

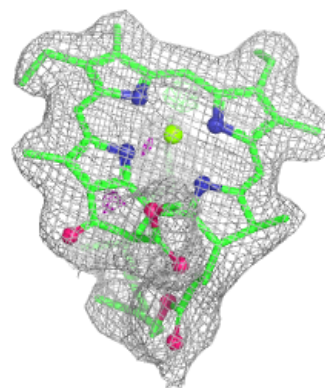
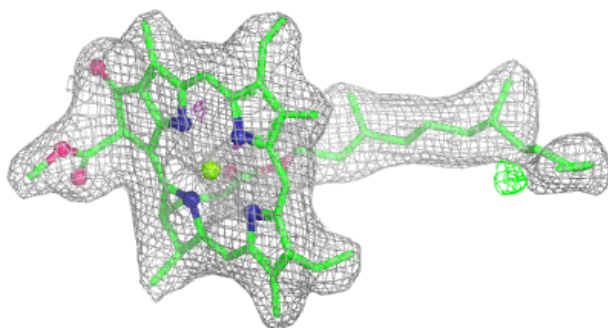
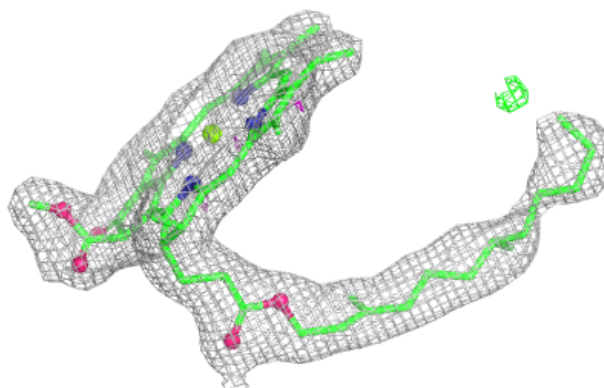


Electron density around CLA b 604:

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

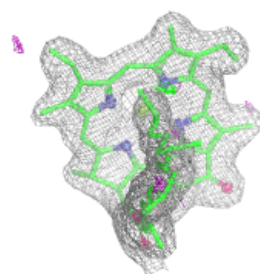
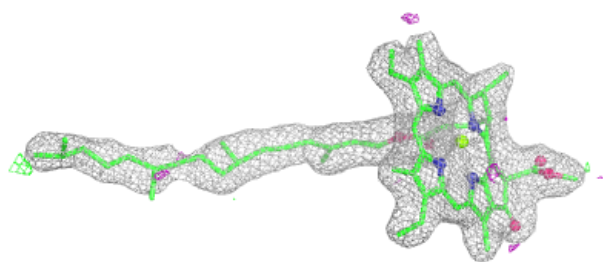
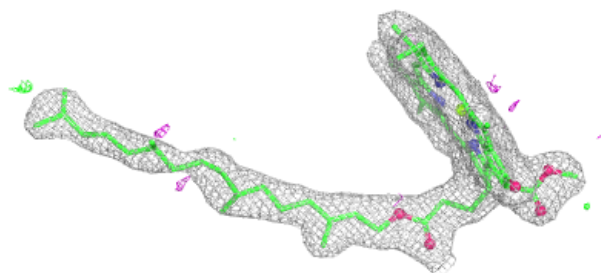
**Electron density around CLA C 504:**

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

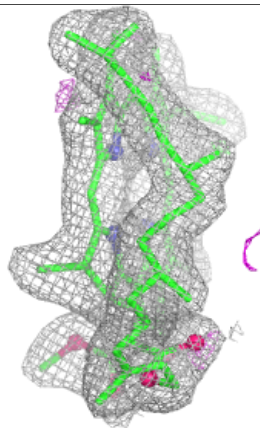
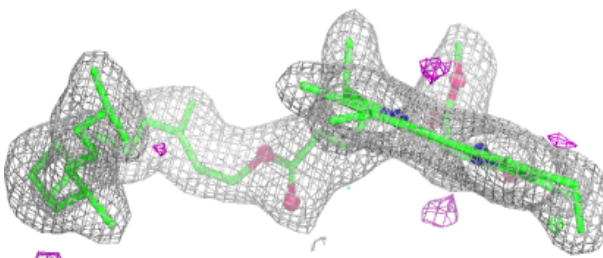
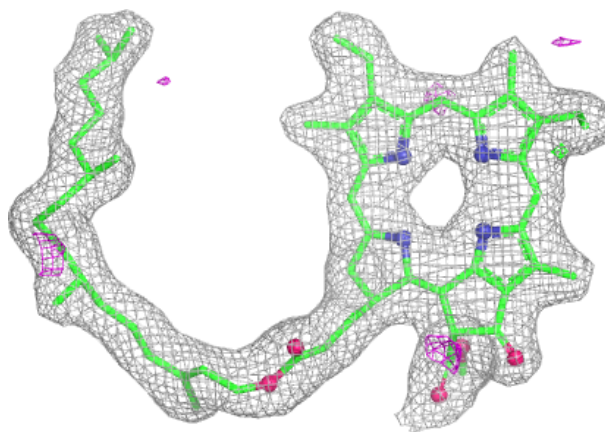


Electron density around CLA b 606:

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

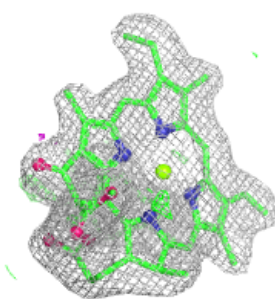
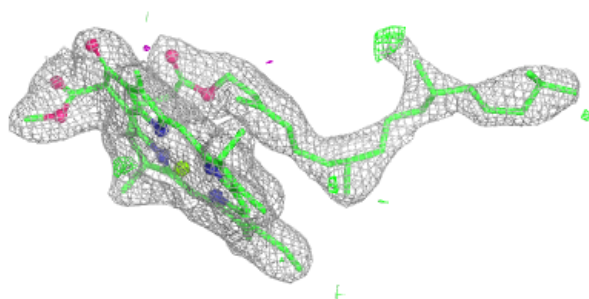
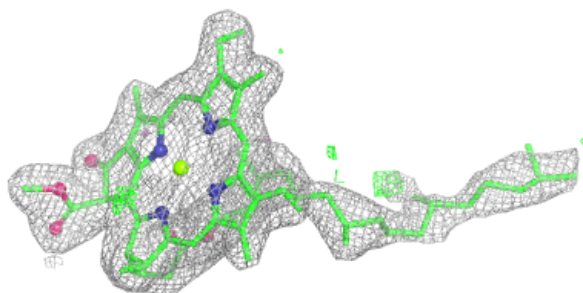
**Electron density around PHO A 608:**

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

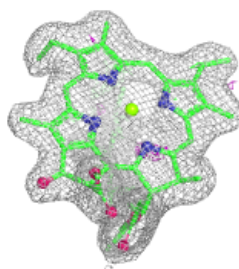
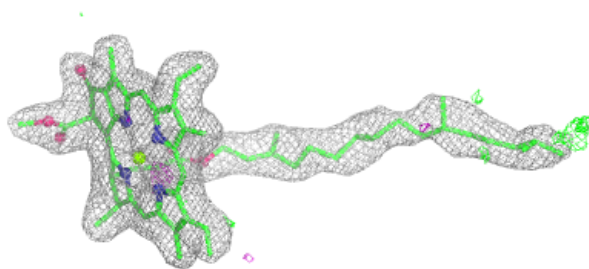
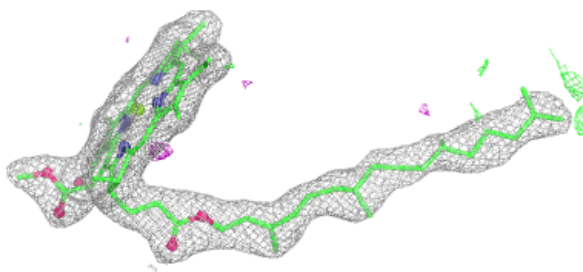


Electron density around CLA C 505:

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

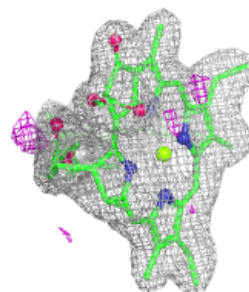
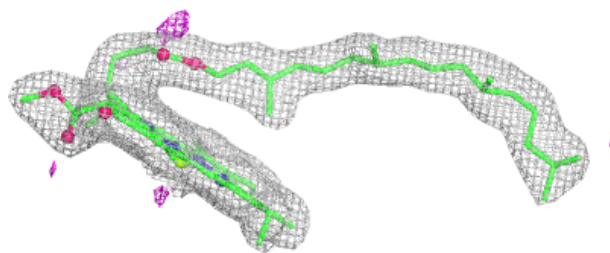
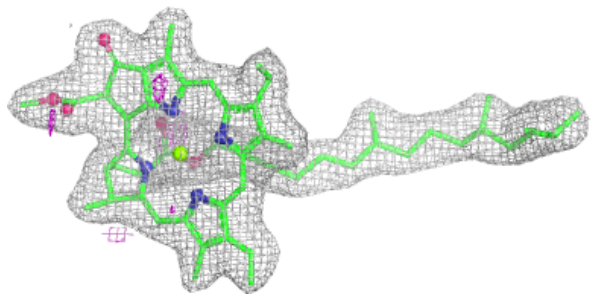
**Electron density around CLA B 606:**

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



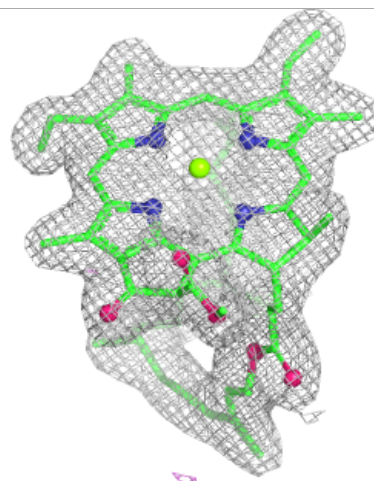
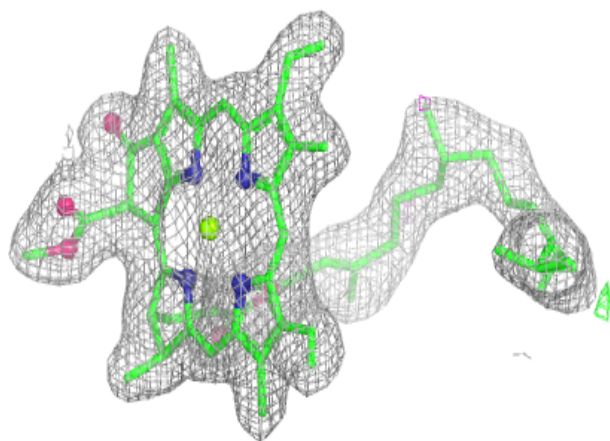
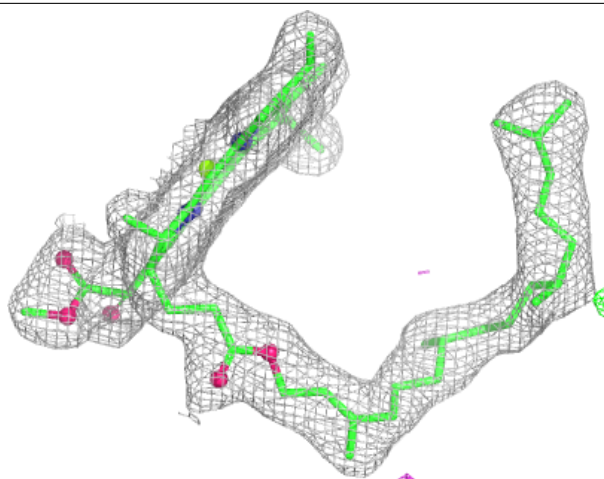
Electron density around CLA B 607:

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



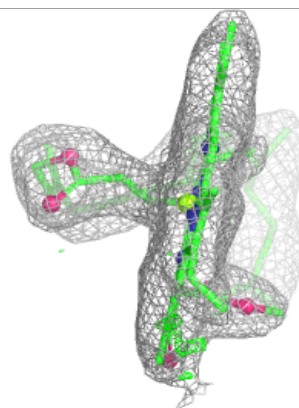
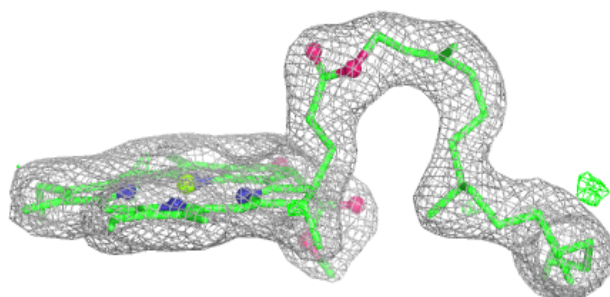
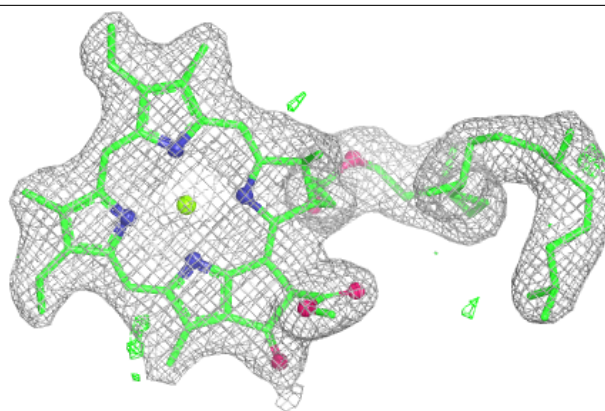
Electron density around CLA b 610:

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

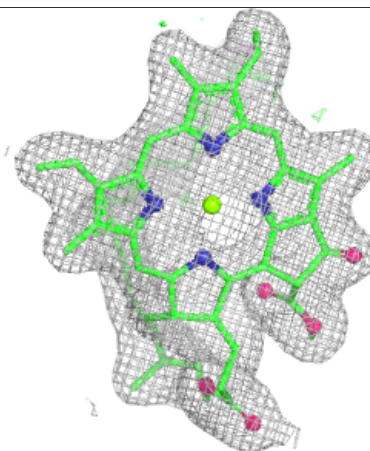
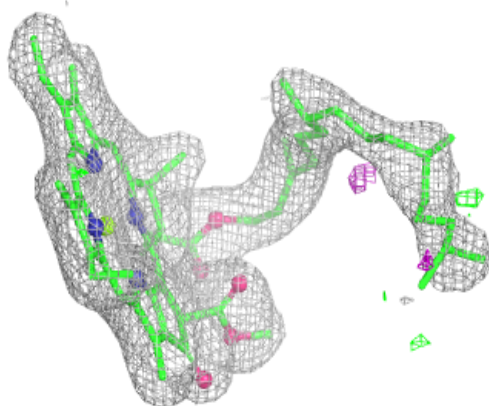
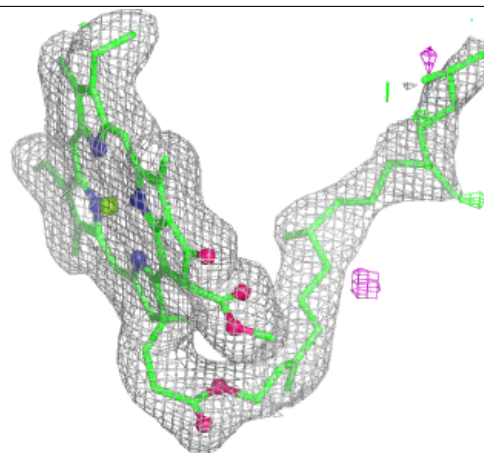


Electron density around CLA b 611:

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

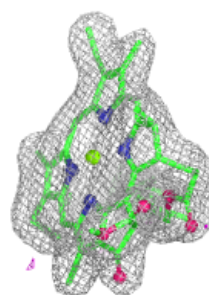
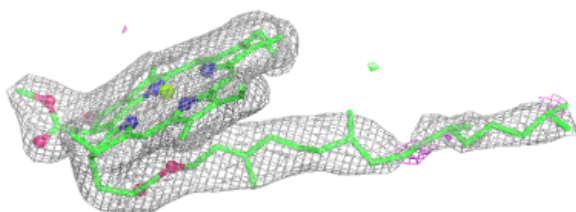
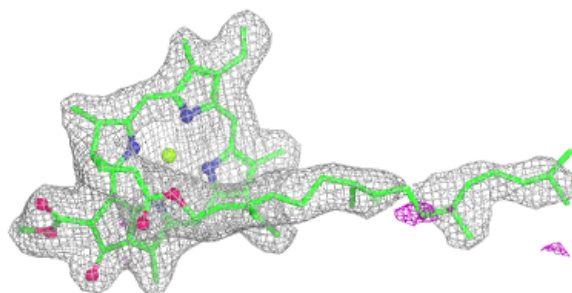
**Electron density around CLA b 612:**

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

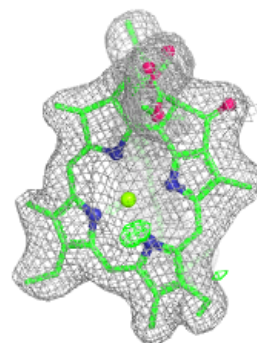
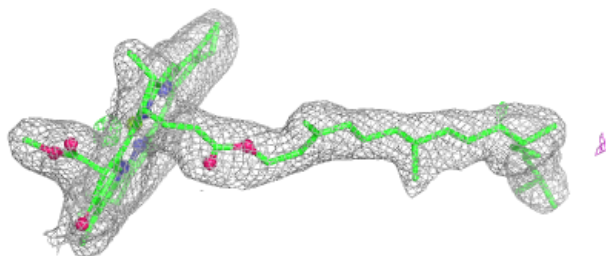
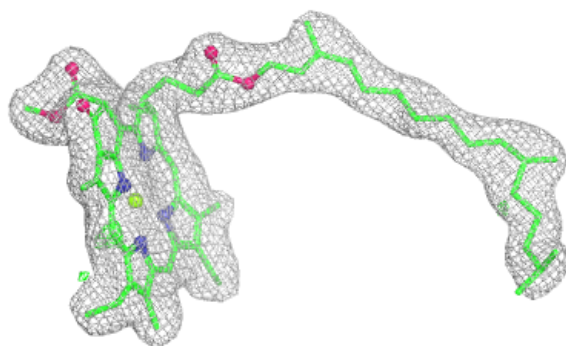


Electron density around CLA b 613:

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

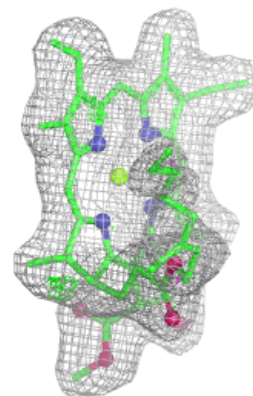
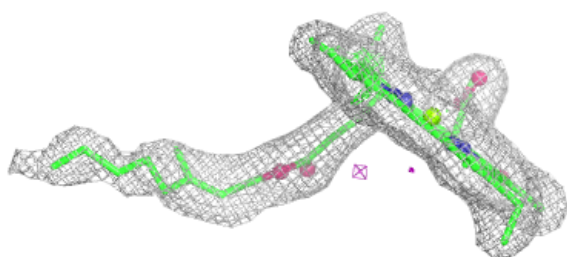
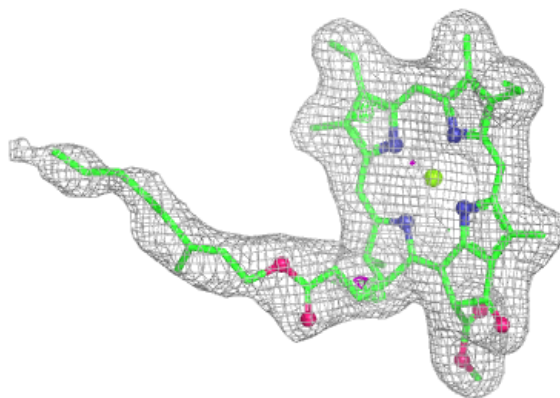
**Electron density around CLA B 608:**

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

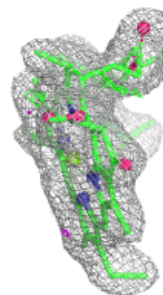
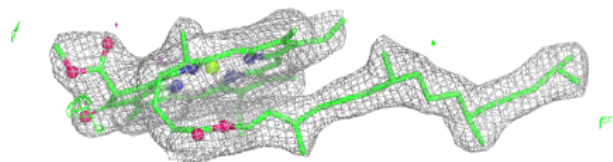
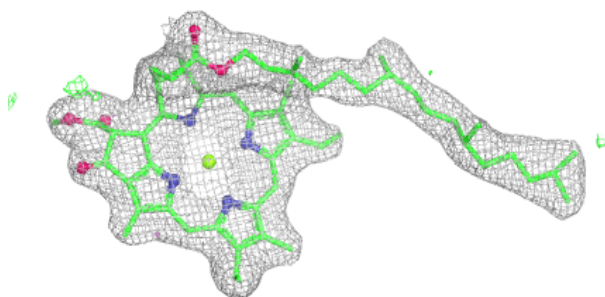


Electron density around CLA A 610:

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

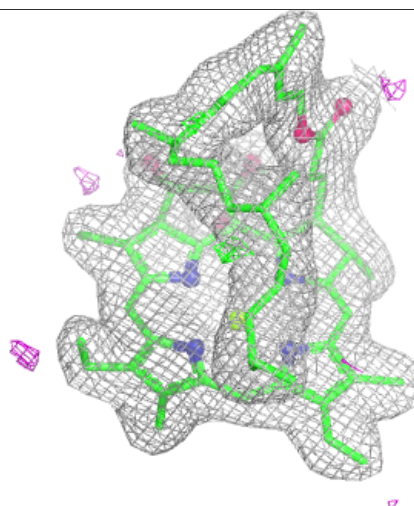
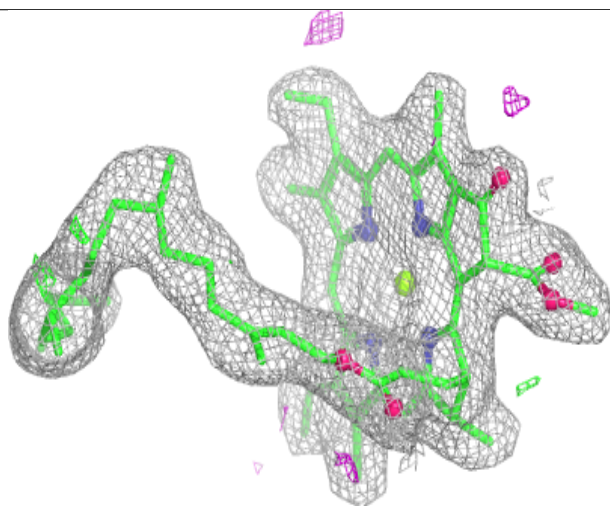
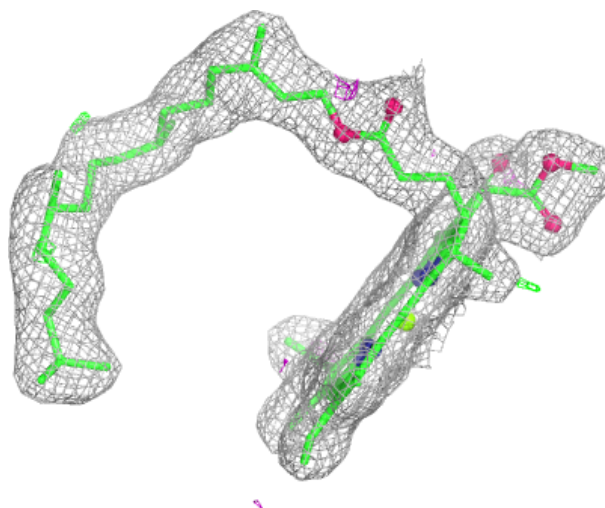
**Electron density around CLA c 501:**

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



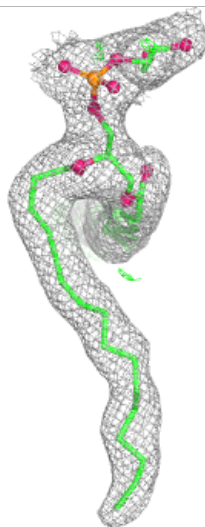
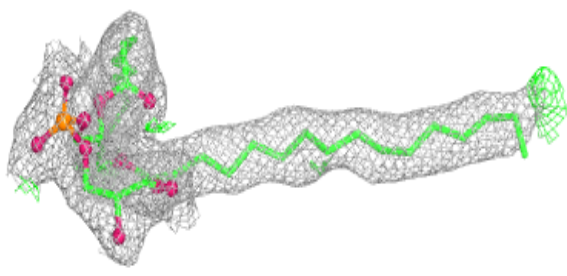
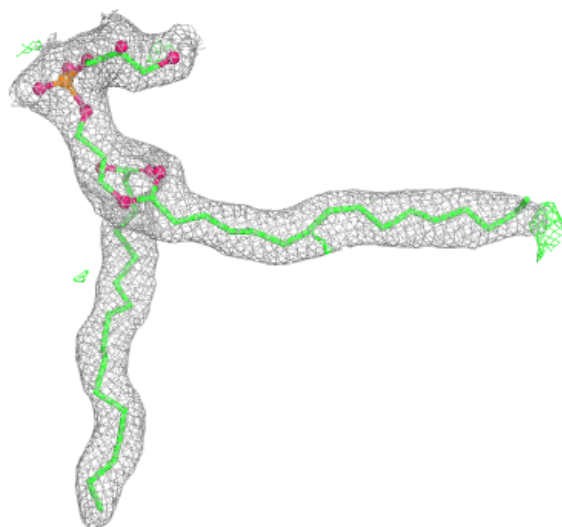
Electron density around CLA B 610:

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



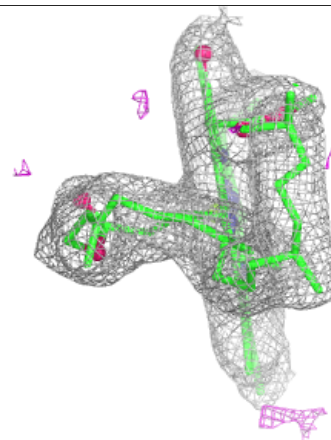
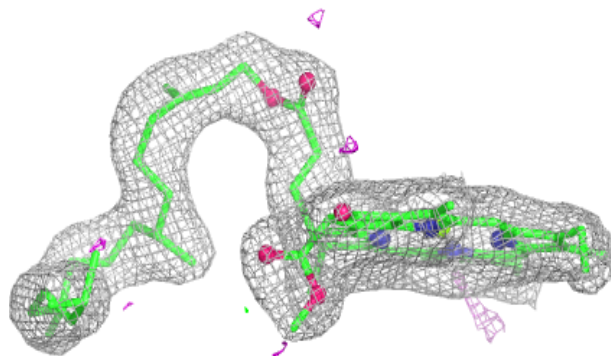
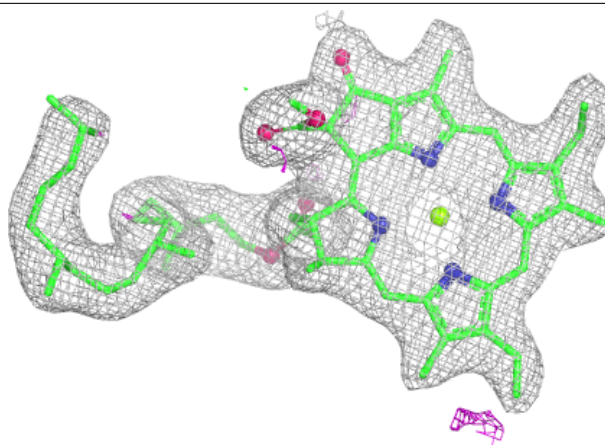
Electron density around LHG B 621:

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

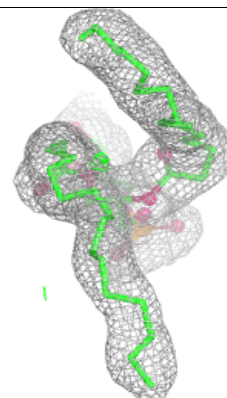
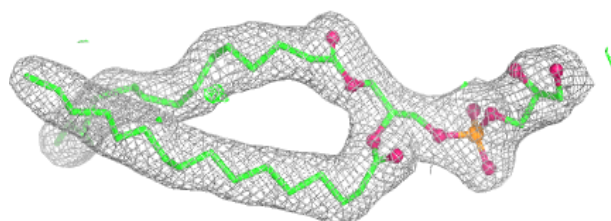
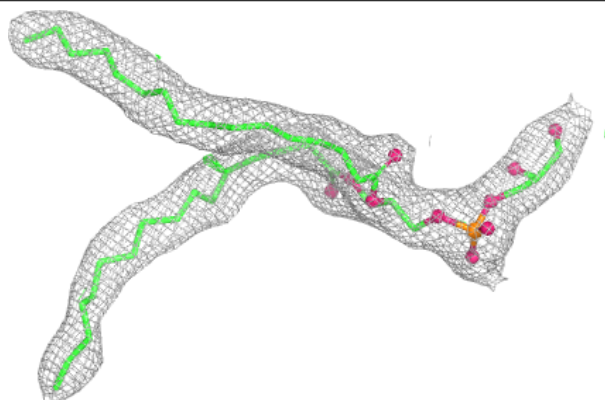


Electron density around CLA B 611:

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

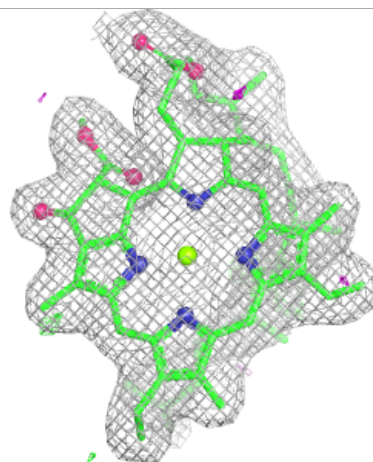
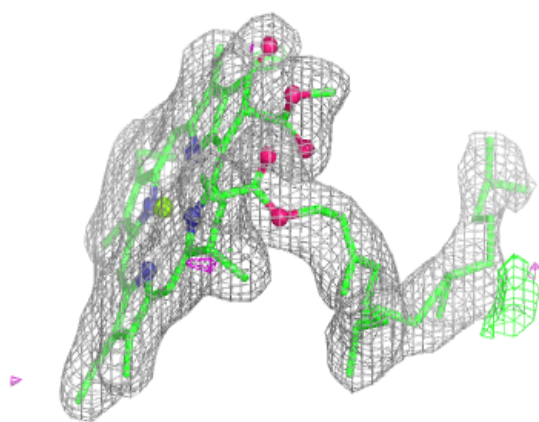
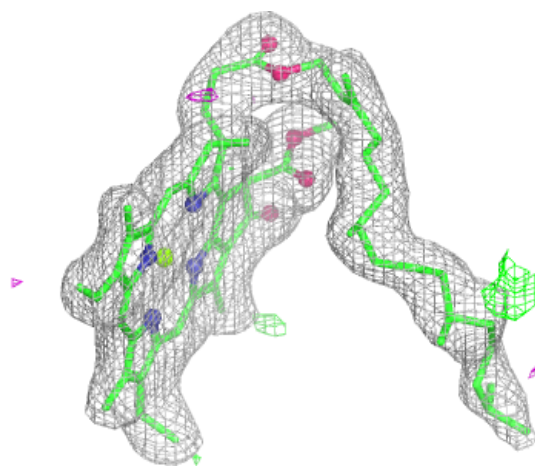
**Electron density around LHG D 407:**

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



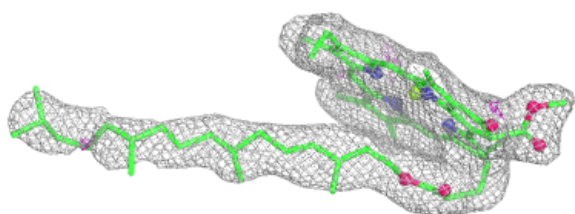
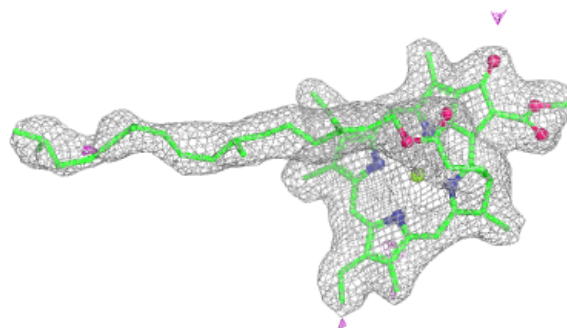
Electron density around CLA B 612:

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

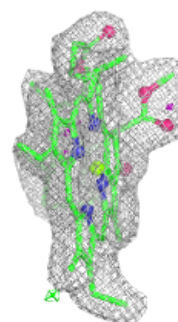
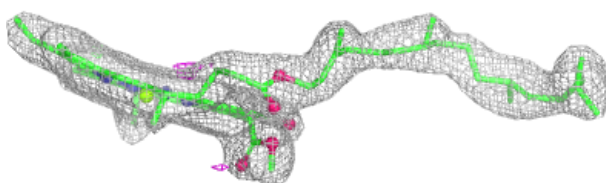
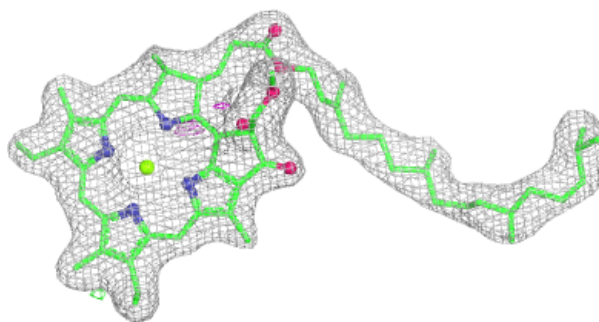


Electron density around CLA B 613:

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

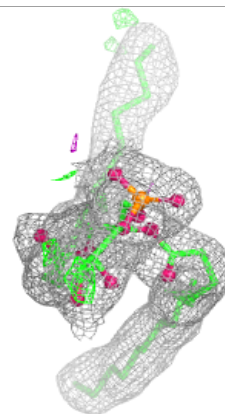
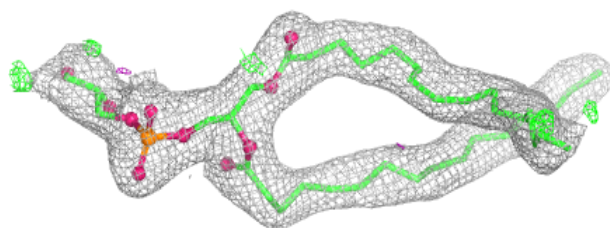
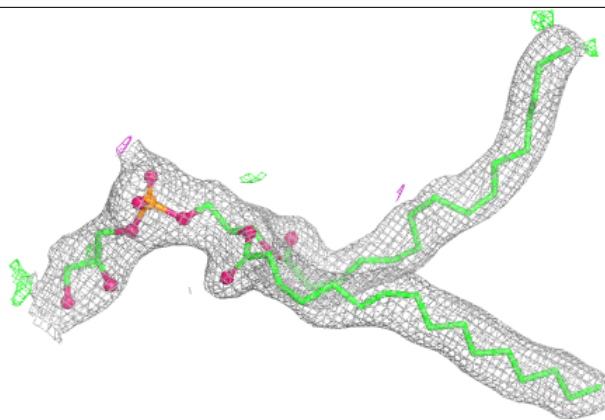
**Electron density around CLA B 601:**

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

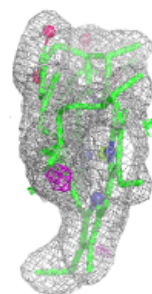
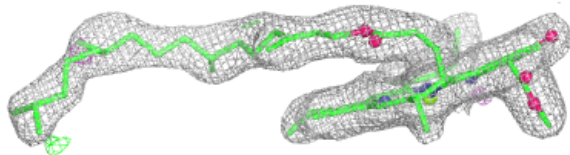
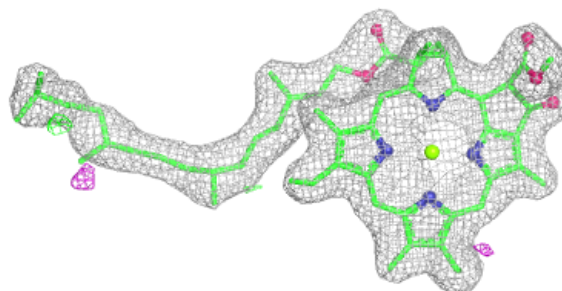


Electron density around LHG d 407:

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

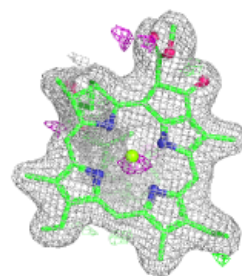
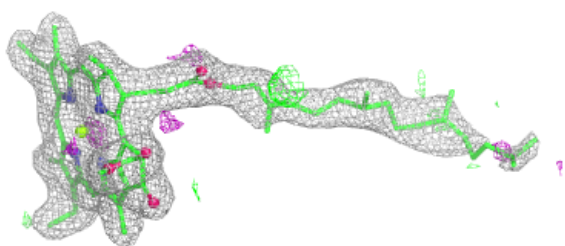
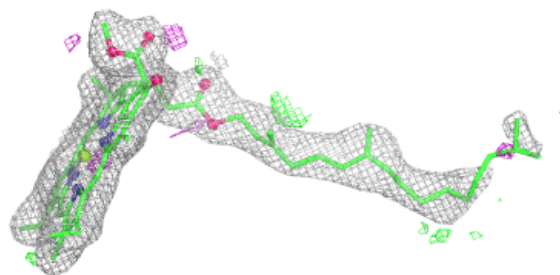
**Electron density around CLA B 602:**

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

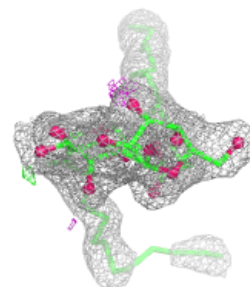
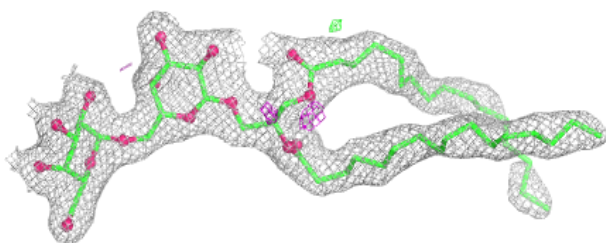
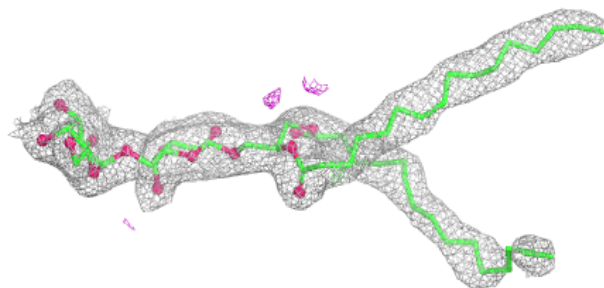


Electron density around CLA B 603:

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

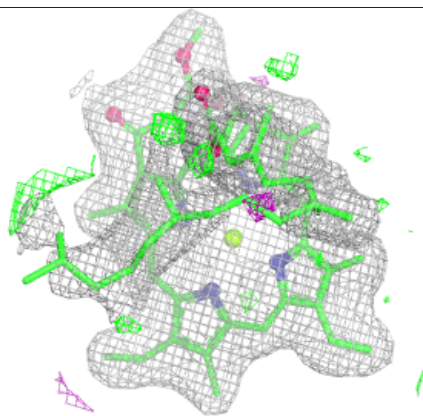
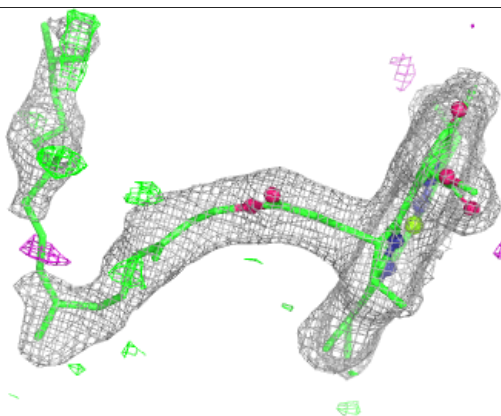
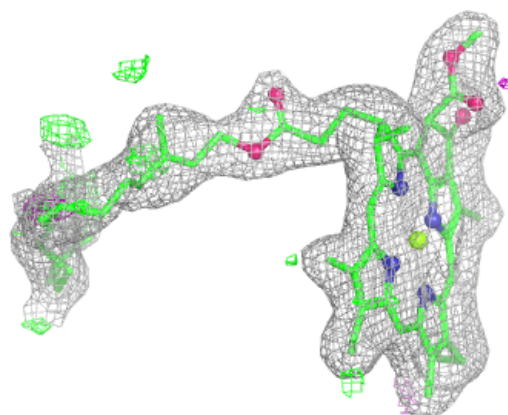
**Electron density around DGD c 517:**

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



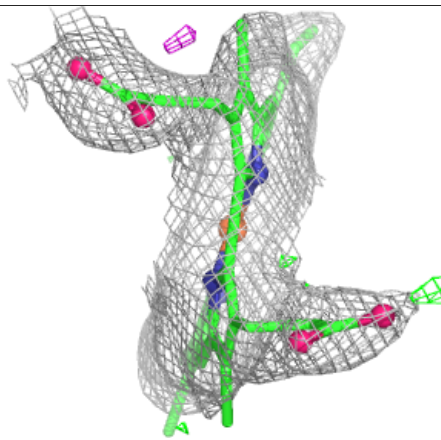
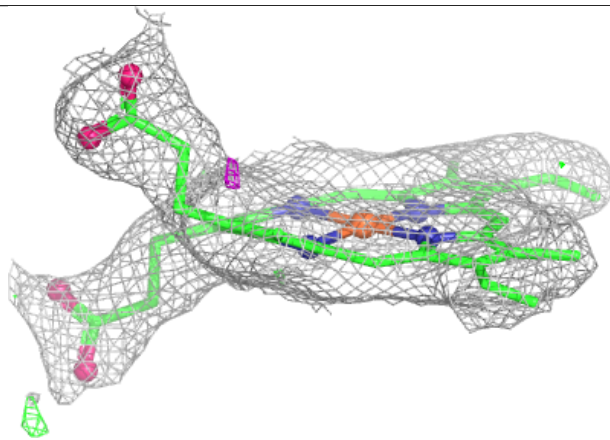
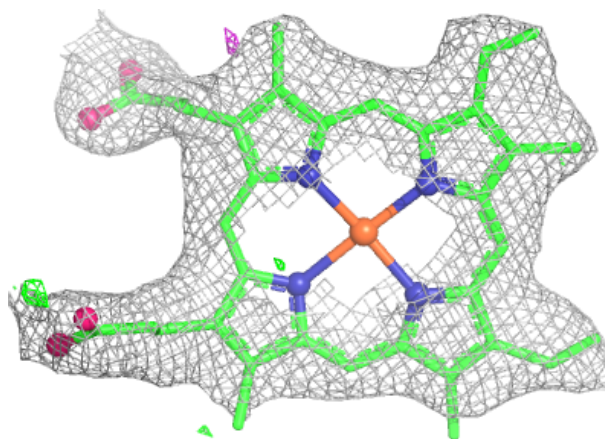
Electron density around CLA a 610:

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



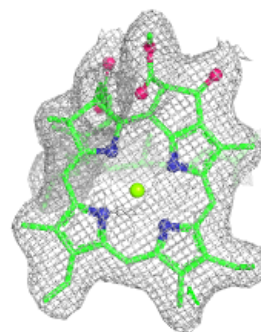
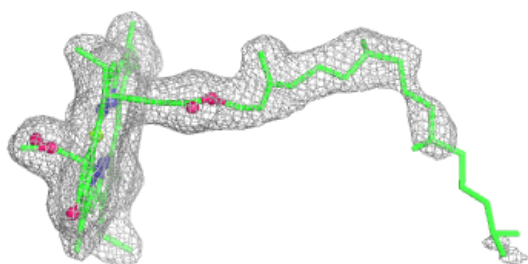
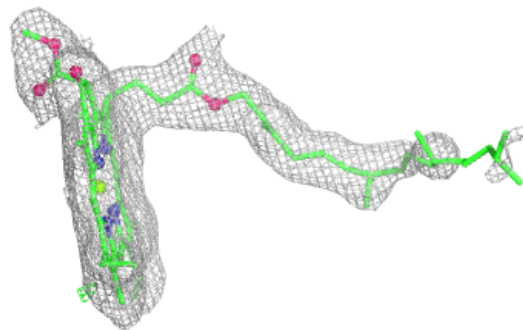
Electron density around HEM e 101:

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

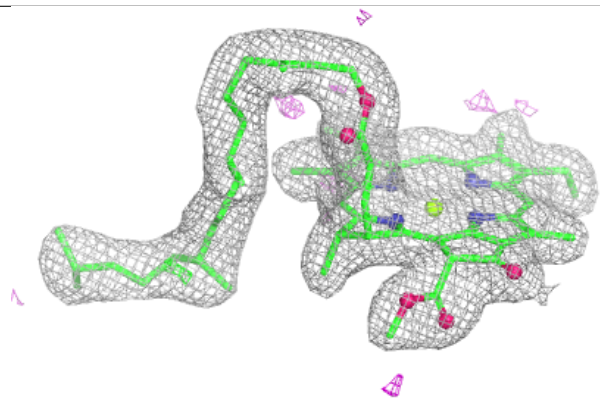
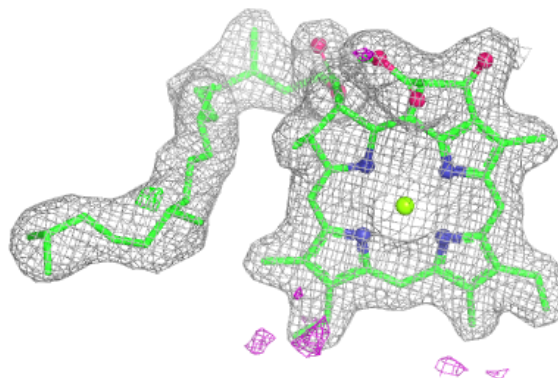


Electron density around CLA D 403:

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

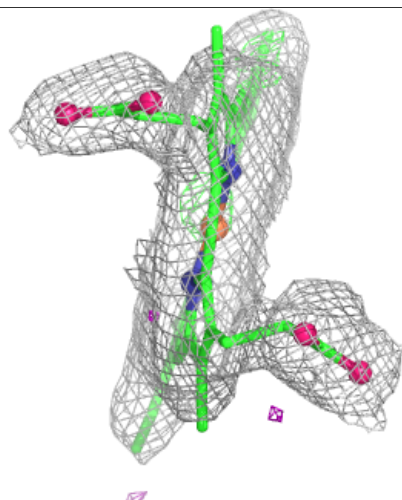
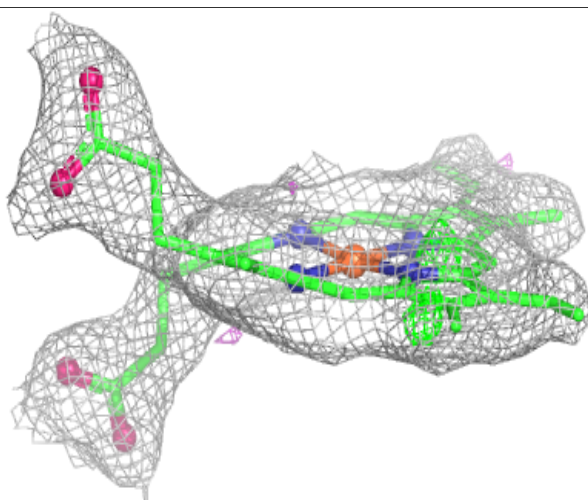
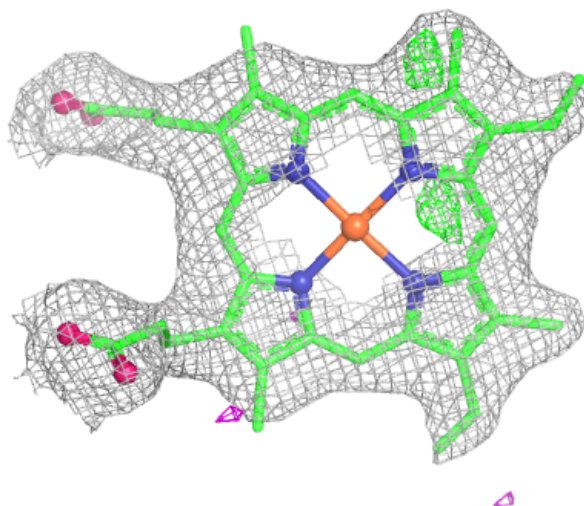
**Electron density around CLA A 613:**

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



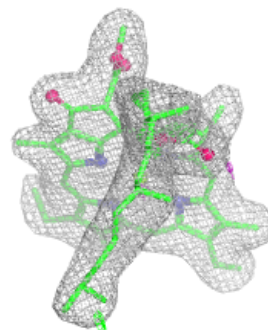
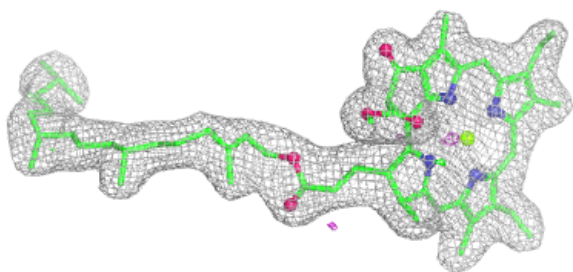
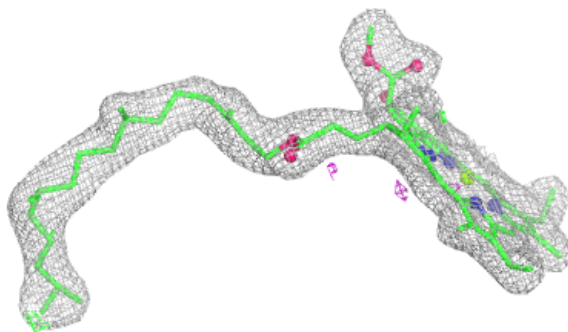
Electron density around HEM F 101:

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



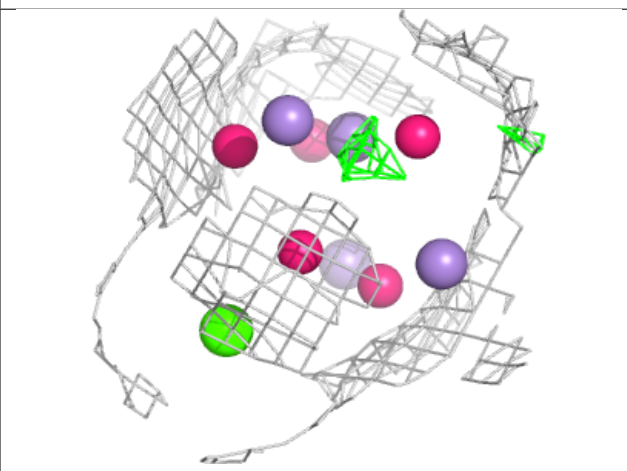
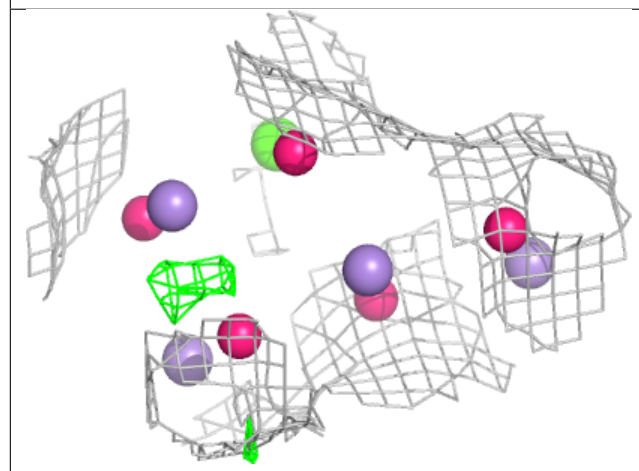
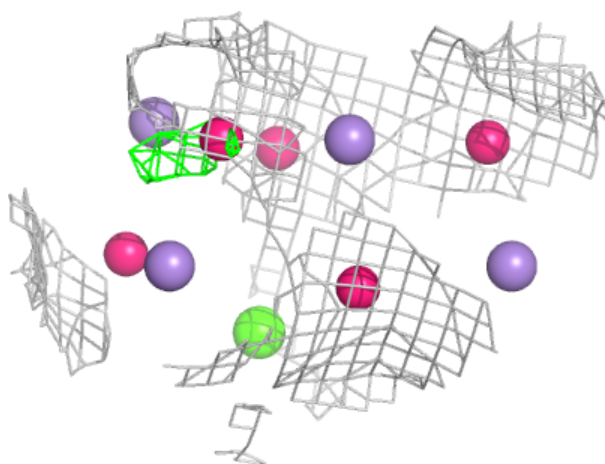
Electron density around CLA D 402:

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



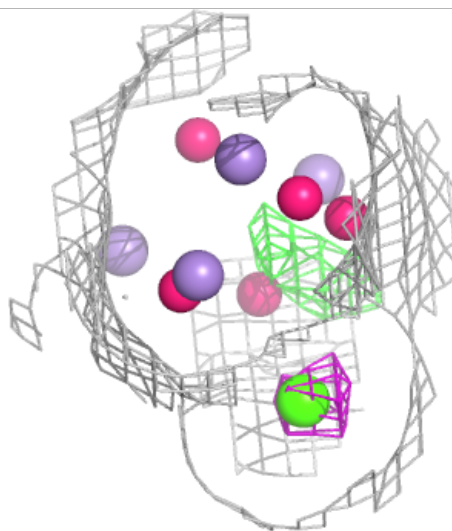
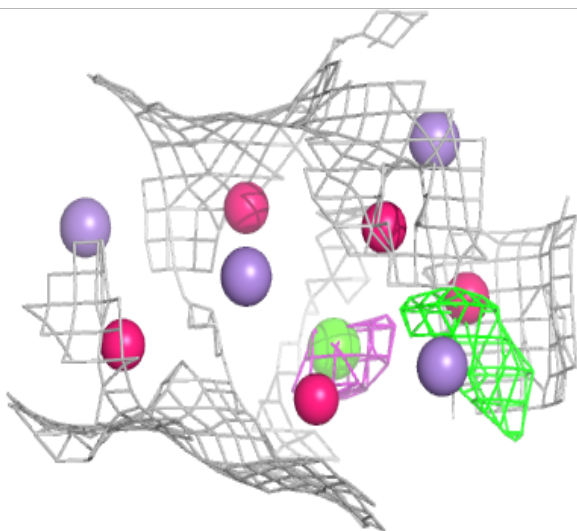
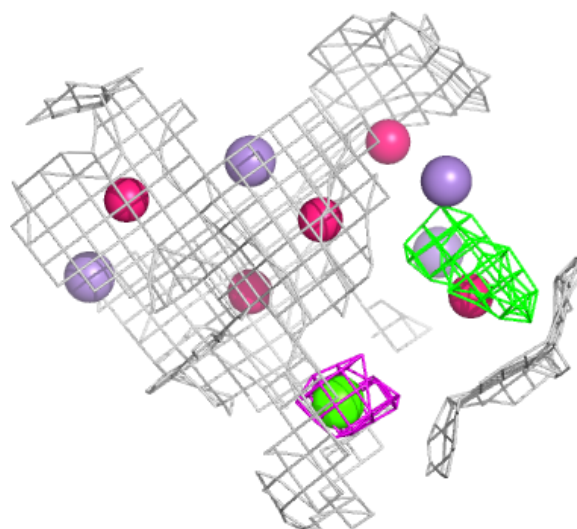
Electron density around OEX a 602 (Å):

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



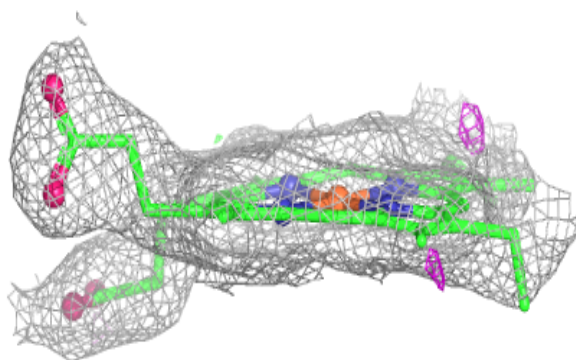
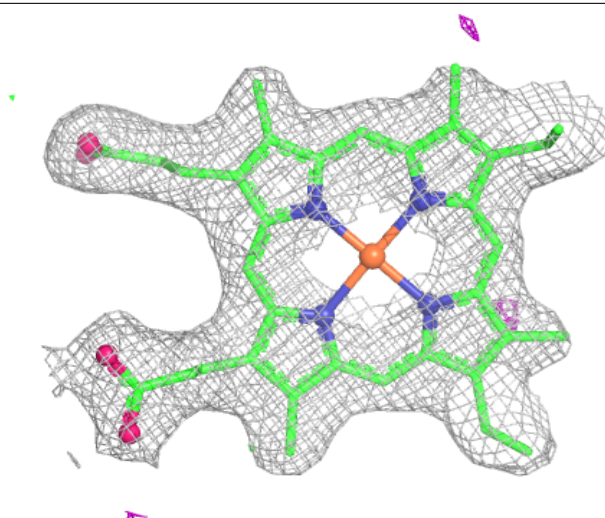
Electron density around OEX A 602 (A):

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



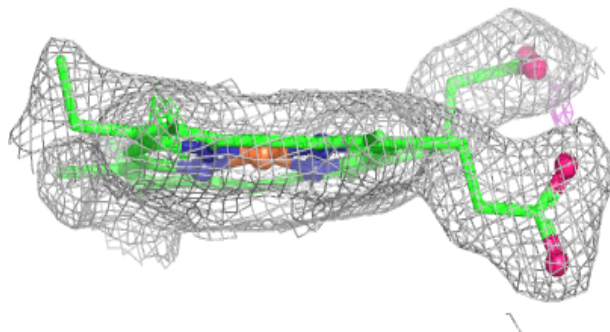
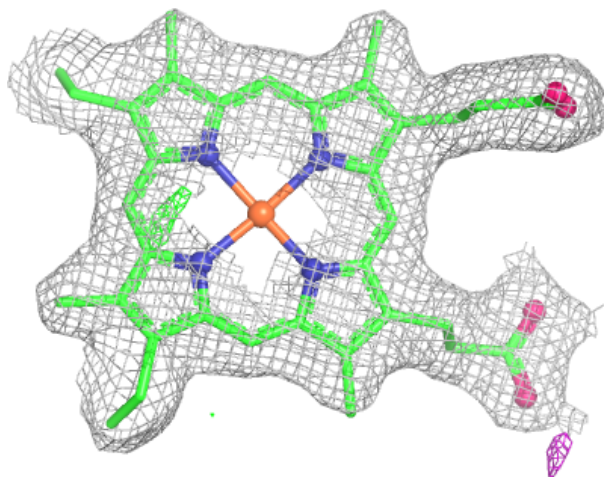
Electron density around HEC V 201:

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



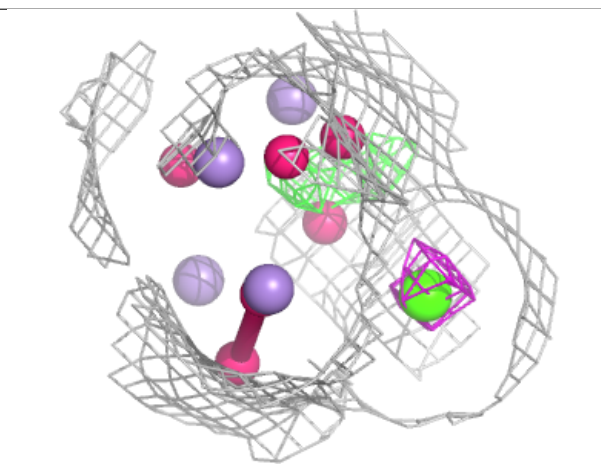
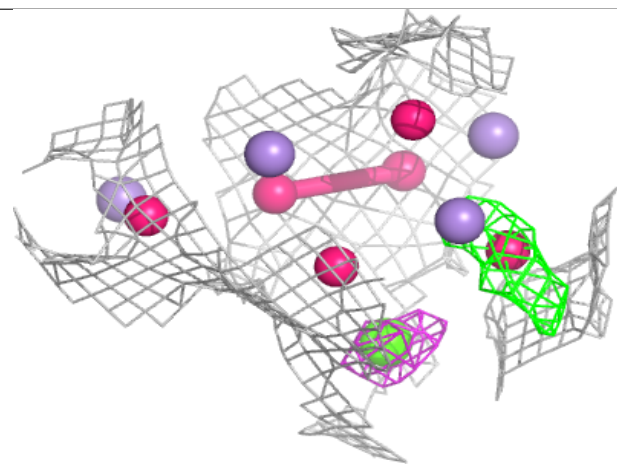
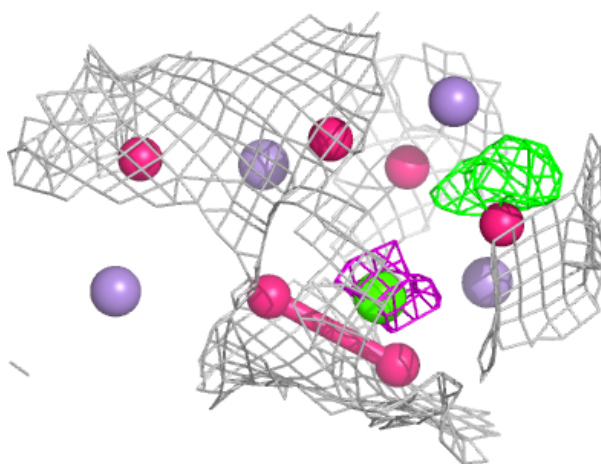
Electron density around HEC v 201:

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



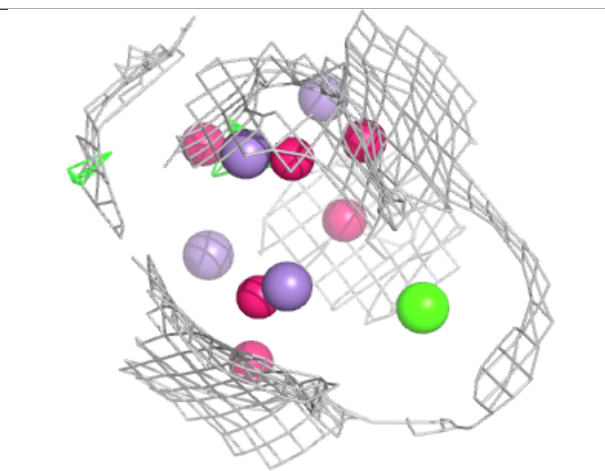
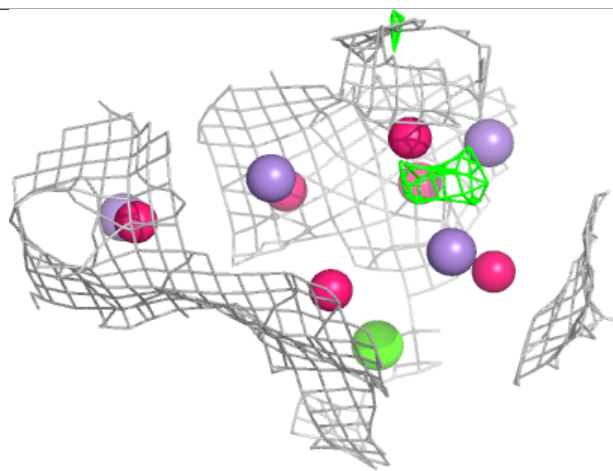
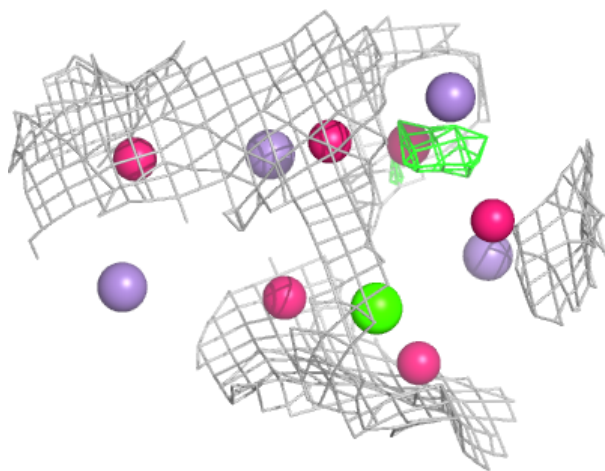
Electron density around OEY A 601 (C):

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



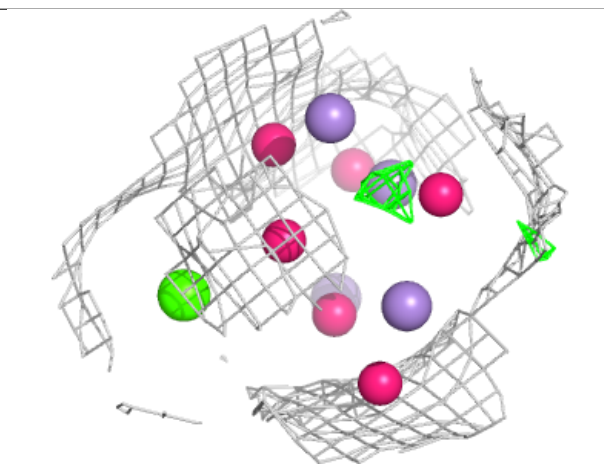
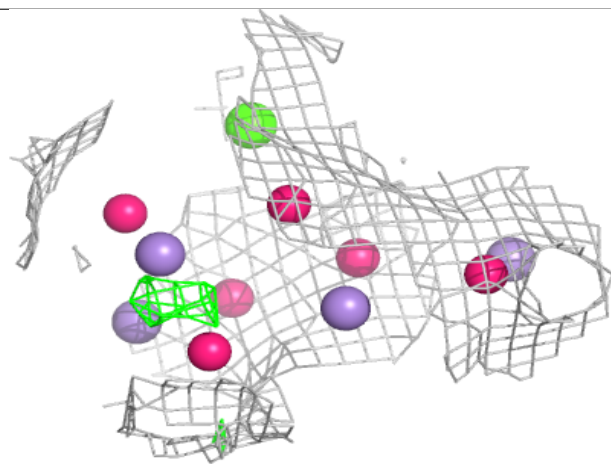
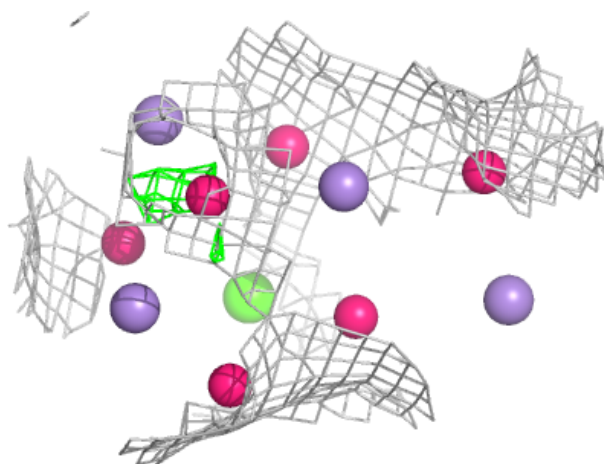
Electron density around OEY a 601 (B):

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



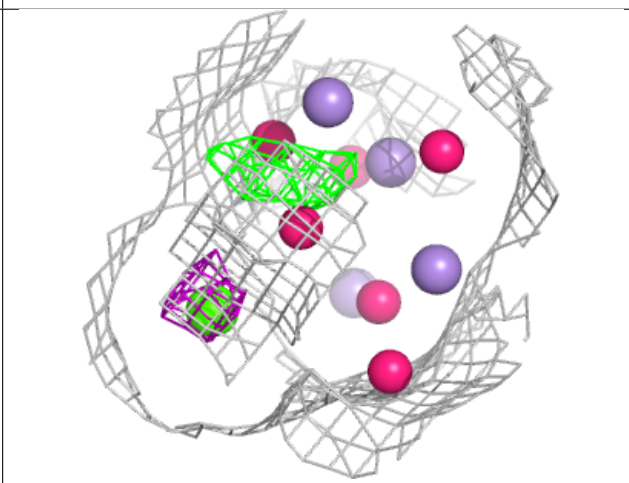
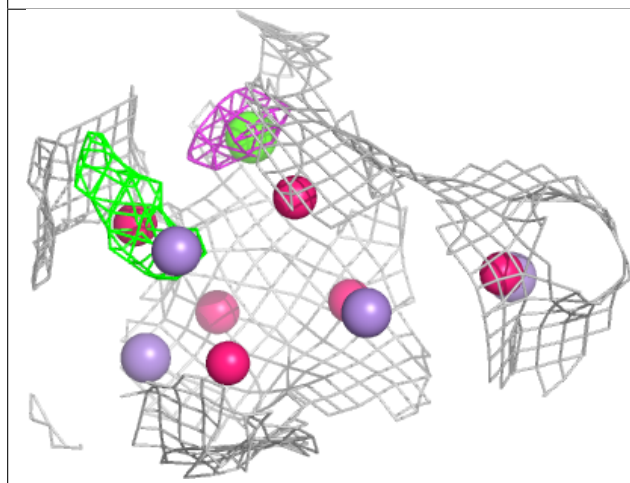
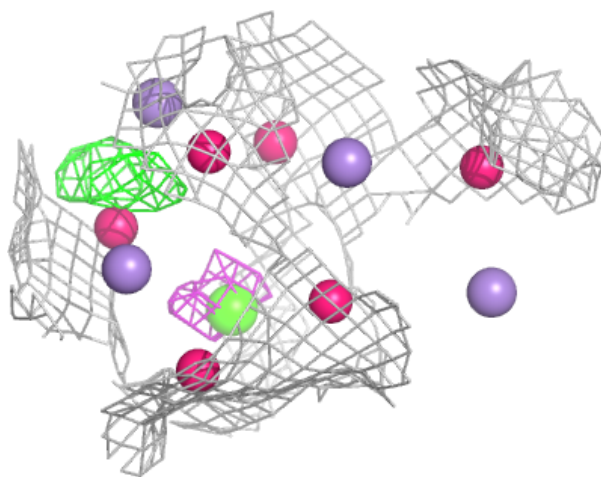
Electron density around OEY a 601 (C):

$2mF_o-DF_c$ (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 (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.