



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 6, 2026 – 01:25 AM EDT

PDB ID : 6W1O / pdb_00006w1o
Title : RT XFEL structure of the dark-stable state of Photosystem II (0F, S1-rich) at 2.08 Angstrom resolution
Authors : Ibrahim, M.; Fransson, T.; Chatterjee, R.; Cheah, M.H.; Hussein, R.; Lassalle, L.; Sutherlin, K.D.; Young, I.D.; Fuller, F.D.; Gul, S.; Kim, I.-S.; Simon, P.S.; de Lichtenberg, C.; Chernev, P.; Bogacz, I.; Pham, C.; Orville, A.M.; Saichek, N.; Northen, T.R.; Batyuk, A.; Carbajo, S.; Alonso-Mori, R.; Tono, K.; Owada, S.; Bhowmick, A.; Bolotovskii, R.; Mendez, D.; Moriarty, N.W.; Holton, J.M.; Dobbek, H.; Brewster, A.S.; Adams, P.D.; Sauter, N.K.; Bergmann, U.; Zouni, A.; Messinger, J.; Kern, J.; Yachandra, V.K.; Yano, J.
Deposited on : 2020-03-04
Resolution : 2.08 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

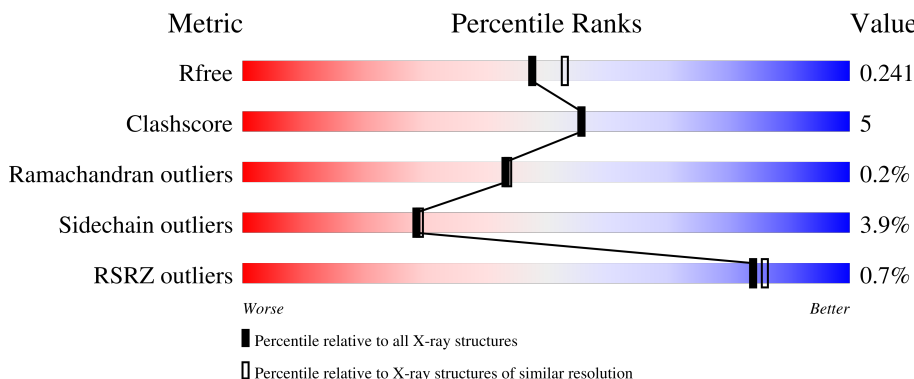
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.08 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	8172 (2.10-2.06)
Clashscore	190562	8714 (2.10-2.06)
Ramachandran outliers	187476	8641 (2.10-2.06)
Sidechain outliers	187428	8642 (2.10-2.06)
RSRZ outliers	180081	8177 (2.10-2.06)

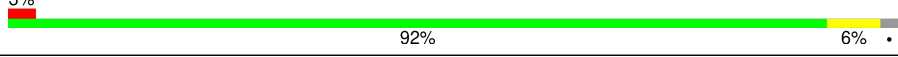
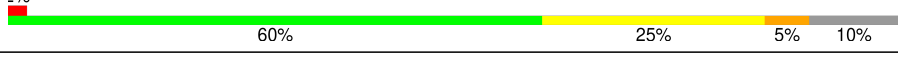
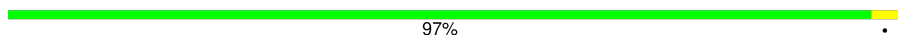
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively.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

Mol	Chain	Length	Quality of chain
1	A	334	 88% 12%
1	a	334	 89% 11%

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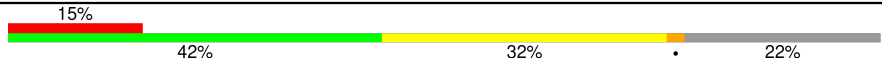
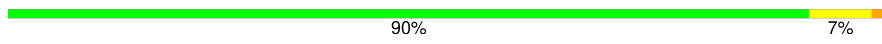
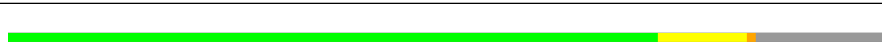
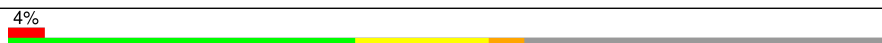
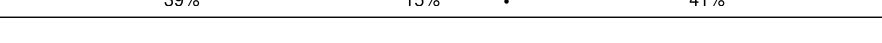
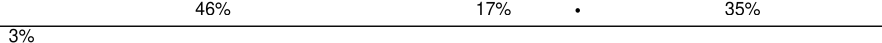
CCP4 : 9.0.015 (Gargrove)
 Density-Fitness : 1.0.12
 Ideal geometry (proteins) : Engh & Huber (2001)
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.50

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Mol	Chain	Length	Quality of chain
2	B	506	
2	b	506	
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	
14	R	40	

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Mol	Chain	Length	Quality of chain
14	r	40	
15	T	30	
15	t	30	
16	U	134	
16	u	134	
17	V	163	
17	v	163	
18	X	41	
18	x	41	
19	Y	46	
19	y	46	
20	Z	62	
20	z	62	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
34	HEC	F	102	X	-	-	-
34	HEC	V	201	X	-	-	-
34	HEC	f	101	X	-	-	-
34	HEC	v	201	X	-	-	-

2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 103895 atoms, of which 51610 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	H	N	O	S	0	0	0
			5130	1717	2508	431	459	15			
1	a	334	Total	C	H	N	O	S	0	0	0
			5118	1714	2499	431	459	15			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	505	Total	C	H	N	O	S	0	5	0
			7864	2631	3859	666	695	13			
2	b	505	Total	C	H	N	O	S	0	0	0
			7800	2610	3822	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	H	N	O	S	0	2	0
			6768	2249	3342	571	593	13			
3	c	451	Total	C	H	N	O	S	0	2	0
			6913	2290	3413	587	610	13			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	D	341	Total	C	H	N	O	S	0	0	0
			5330	1800	2613	444	461	12			
4	d	341	Total	C	H	N	O	S	0	1	0
			5342	1804	2619	444	463	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	82	Total	C	H	N	O	0	1	0
			1316	436	650	107	123			
5	e	82	Total	C	H	N	O	0	0	0
			1311	434	647	108	122			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	34	Total	C	H	N	O	0	0	0
			556	187	281	45	42			
6	f	34	Total	C	H	N	O	0	0	0
			556	187	281	45	42			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	65	Total	C	H	N	O	0	0	0
			1042	341	532	82	85			
7	h	63	Total	C	H	N	O	0	0	0
			1016	333	518	80	83			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	36	Total	C	H	N	O	0	0	0
			607	200	311	46	49			
8	i	36	Total	C	H	N	O	0	0	0
			607	200	311	46	49			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	1	FME	-	initiating methionine	UNP Q8DJZ6
i	1	FME	-	initiating methionine	UNP Q8DJZ6

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	36	Total	C	H	N	O	0	0	0
			525	174	268	40	42			
9	j	36	Total	C	H	N	O	0	0	0
			525	174	268	40	42			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	K	37	Total	C	H	N	O	0	0	0
			598	204	305	43	46			
10	k	37	Total	C	H	N	O	0	0	0
			598	204	305	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	H	N	O	0	0	0
			620	202	316	48	53			
11	l	36	Total	C	H	N	O	0	0	0
			600	197	304	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	H	N	O	0	0	0
			525	171	269	37	47			
12	m	32	Total	C	H	N	O	0	0	0
			518	168	267	36	46			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	1	FME	-	initiating methionine	UNP Q8DHA7
m	1	FME	-	initiating methionine	UNP Q8DHA7

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	244	Total	C	H	N	O	0	1	0
			3698	1168	1828	313	385			
13	o	244	Total	C	H	N	O	0	0	0
			3718	1170	1844	317	383			

- Molecule 14 is a protein called Photosystem II protein Y.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	R	34	Total	C	H	N	O	0	0	0
			569	184	298	47	40			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	r	31	Total	C	H	N	O	0	0	0
			493	162	253	42	36			

- Molecule 15 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	T	30	Total	C	H	N	O	S	0	0
			519	181	261	36	39	2		
15	t	30	Total	C	H	N	O	S	0	0
			512	180	256	36	38	2		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	1	FME	-	initiating methionine	UNP Q8DIQ0
t	1	FME	-	initiating methionine	UNP Q8DIQ0

- Molecule 16 is a protein called Photosystem II 12 kDa extrinsic protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	U	97	Total	C	H	N	O	0	0	0
			1546	491	772	129	154			
16	u	97	Total	C	H	N	O	0	0	0
			1546	491	772	129	154			

- Molecule 17 is a protein called Cytochrome c-550.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	V	137	Total	C	H	N	O	S	0	0
			2132	675	1068	177	208	4		
17	v	137	Total	C	H	N	O	S	0	0
			2132	675	1068	177	208	4		

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	X	38	Total	C	H	N	O	0	0	0
			593	188	312	45	48			
18	x	39	Total	C	H	N	O	0	0	0
			602	191	316	46	49			

- Molecule 19 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
19	Y	27	Total	C	H	N	O	S	0	0	0
			413	128	217	35	30	3			
19	y	30	Total	C	H	N	O	S	0	0	0
			459	144	241	35	36	3			

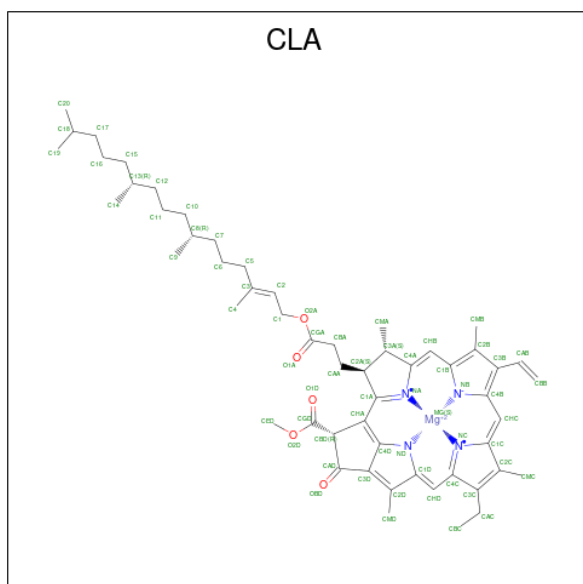
- Molecule 20 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
20	Z	62	Total 995	C 328	H 516	N 72	O 77	S 2	0	0	0
20	z	62	Total 986	C 326	H 509	N 72	O 77	S 2	0	0	0

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

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

- Molecule 22 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
22	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	D	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	D	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	D	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	H	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	a	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	a	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	a	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	a	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0

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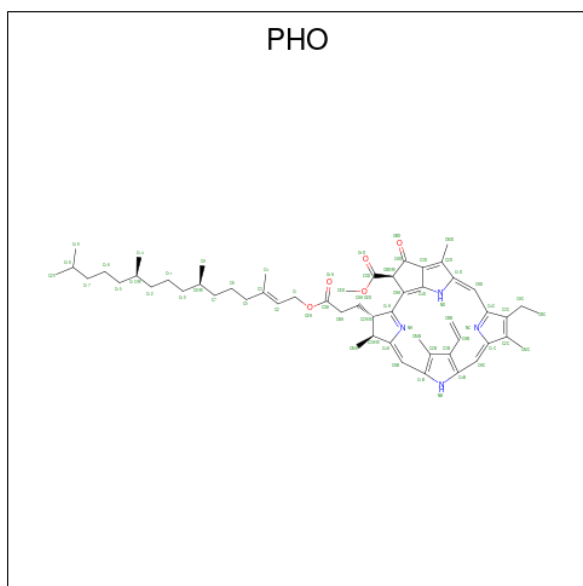
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			119	50	59	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			132	54	68	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

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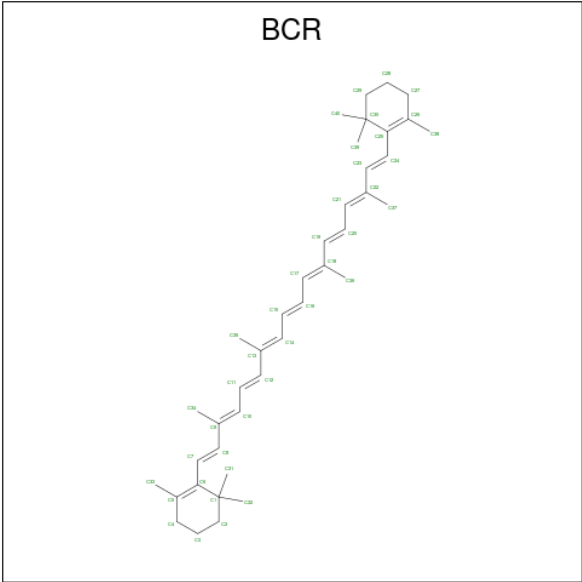
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

- Molecule 23 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
23	A	1	Total	C	H	N	O		0	0
			138	55	74	4	5			
23	D	1	Total	C	H	N	O		0	0
			138	55	74	4	5			
23	a	1	Total	C	H	N	O		0	0
			138	55	74	4	5			
23	d	1	Total	C	H	N	O		0	0
			138	55	74	4	5			

- Molecule 24 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	A	1	Total	C	H	0	0
			96	40	56		
24	B	1	Total	C	H	0	0
			96	40	56		
24	B	1	Total	C	H	0	0
			96	40	56		
24	B	1	Total	C	H	0	0
			96	40	56		
24	C	1	Total	C	H	0	0
			96	40	56		
24	F	1	Total	C	H	0	0
			96	40	56		
24	H	1	Total	C	H	0	0
			96	40	56		
24	K	1	Total	C	H	0	0
			96	40	56		
24	K	1	Total	C	H	0	0
			96	40	56		
24	K	1	Total	C	H	0	0
			96	40	56		
24	T	1	Total	C	H	0	0
			96	40	56		
24	a	1	Total	C	H	0	0
			96	40	56		
24	b	1	Total	C	H	0	0
			96	40	56		
24	b	1	Total	C	H	0	0
			96	40	56		

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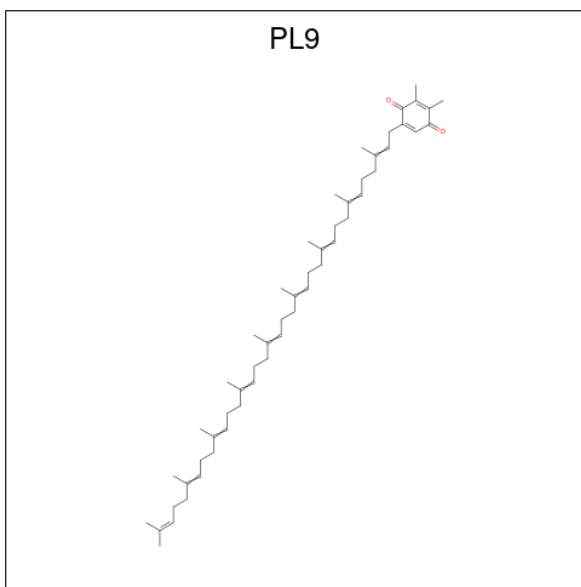
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	b	1	Total	C	H	0	0
			96	40	56		
24	c	1	Total	C	H	0	0
			96	40	56		
24	c	1	Total	C	H	0	0
			96	40	56		
24	d	1	Total	C	H	0	0
			96	40	56		
24	h	1	Total	C	H	0	0
			96	40	56		
24	k	1	Total	C	H	0	0
			96	40	56		
24	k	1	Total	C	H	0	0
			96	40	56		
24	t	1	Total	C	H	0	0
			96	40	56		

- Molecule 25 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

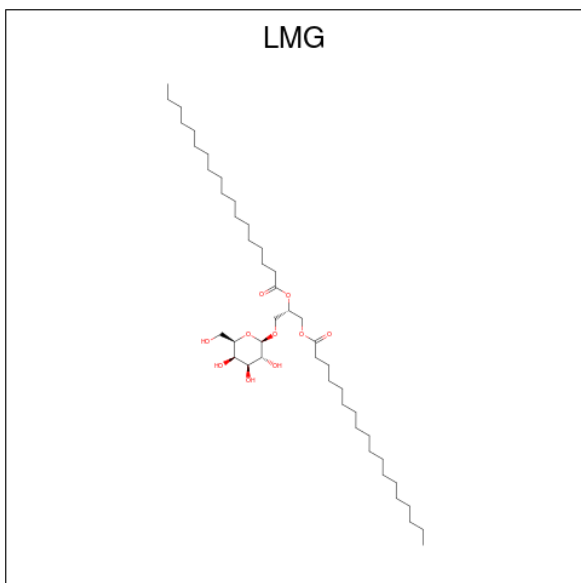
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	A	2	Total	Cl	0	0
			2	2		
25	a	2	Total	Cl	0	0
			2	2		

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



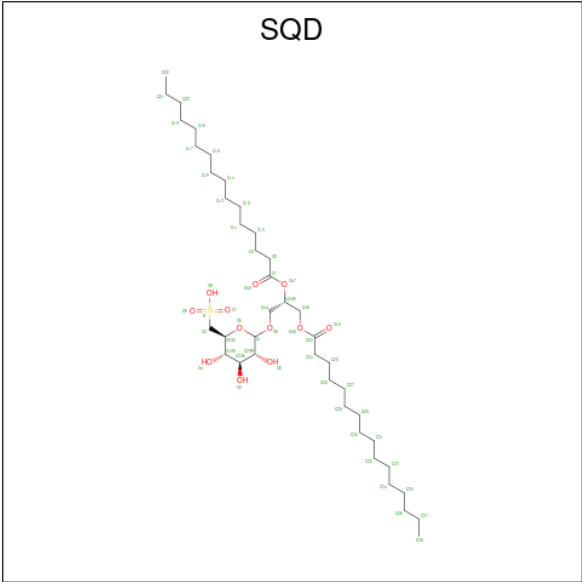
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	A	1	Total	C	H	O	0	0
			135	53	80	2		
26	D	1	Total	C	H	O	0	0
			135	53	80	2		
26	a	1	Total	C	H	O	0	0
			135	53	80	2		
26	d	1	Total	C	H	O	0	0
			135	53	80	2		

- Molecule 27 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



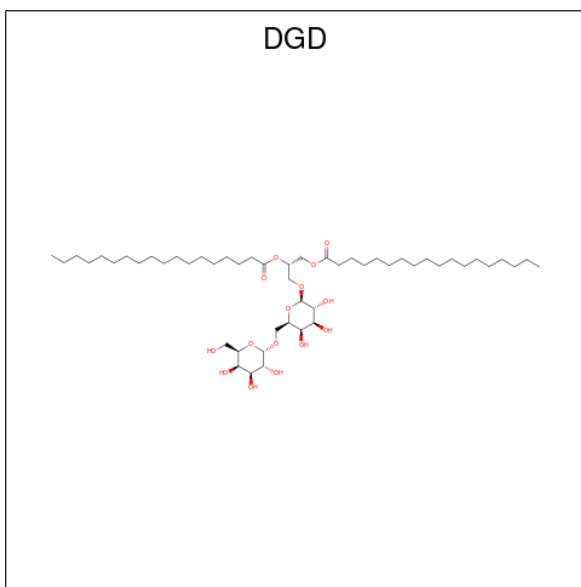
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	A	1	Total	C	H	O	0	0
			114	38	66	10		
27	B	1	Total	C	H	O	0	0
			68	24	40	4		
27	D	1	Total	C	H	O	0	0
			123	41	72	10		
27	D	1	Total	C	H	O	0	0
			78	27	45	6		
27	M	1	Total	C	H	O	0	0
			123	41	72	10		
27	Y	1	Total	C	H	O	0	0
			114	38	66	10		
27	a	1	Total	C	H	O	0	0
			141	45	86	10		
27	b	1	Total	C	H	O	0	0
			123	41	72	10		
27	b	1	Total	C	H	O	0	0
			141	45	86	10		
27	c	1	Total	C	H	O	0	0
			81	27	44	10		
27	c	1	Total	C	H	O	0	0
			117	38	69	10		
27	c	1	Total	C	H	O	0	0
			117	39	68	10		
27	d	1	Total	C	H	O	0	0
			102	34	58	10		

- Molecule 28 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



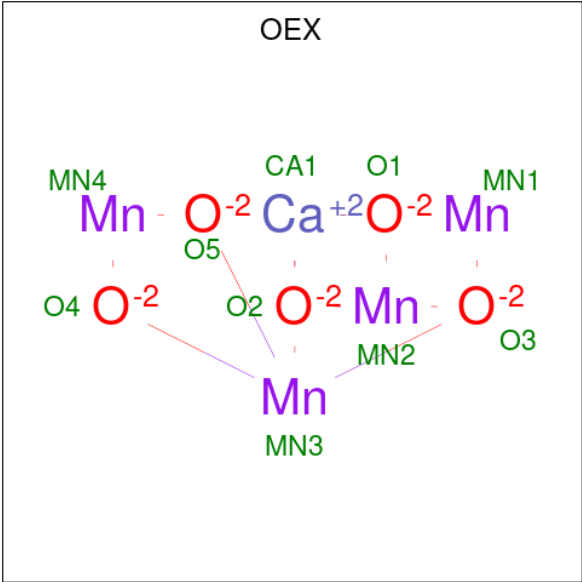
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
28	A	1	Total	C	H	O	S	0	0
			123	39	71	12	1		
28	A	1	Total	C	H	O		0	0
			104	35	65	4			
28	B	1	Total	C	H	O	S	0	0
			132	41	78	12	1		
28	D	1	Total	C	H	O	S	0	0
			82	25	46	10	1		
28	L	1	Total	C	H	O	S	0	0
			114	36	65	12	1		
28	a	1	Total	C	H	O	S	0	0
			132	41	78	12	1		
28	a	1	Total	C	H	O		0	0
			92	31	56	5			
28	f	1	Total	C	H	O	S	0	0
			89	28	48	12	1		

- Molecule 29 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: C₅₁H₉₆O₁₅).



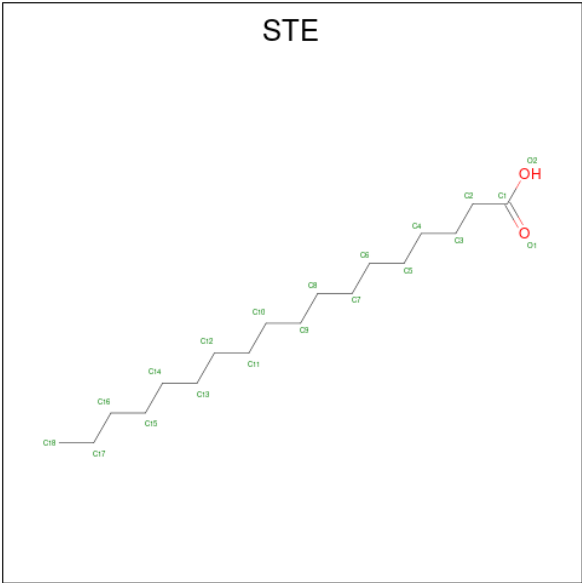
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	A	1	Total	C	H	O	0	0
			162	51	96	15		
29	C	1	Total	C	H	O	0	0
			144	47	82	15		
29	C	1	Total	C	H	O	0	0
			144	47	82	15		
29	C	1	Total	C	H	O	0	0
			144	47	82	15		
29	H	1	Total	C	H	O	0	0
			144	47	82	15		
29	c	1	Total	C	H	O	0	0
			143	47	81	15		
29	c	1	Total	C	H	O	0	0
			144	47	82	15		
29	c	1	Total	C	H	O	0	0
			144	47	82	15		
29	h	1	Total	C	H	O	0	0
			144	47	82	15		

- Molecule 30 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5).



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

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	B	1	Total	C	H	O	0	0
			28	10	16	2		
31	B	1	Total	C	H	O	0	0
			43	15	26	2		

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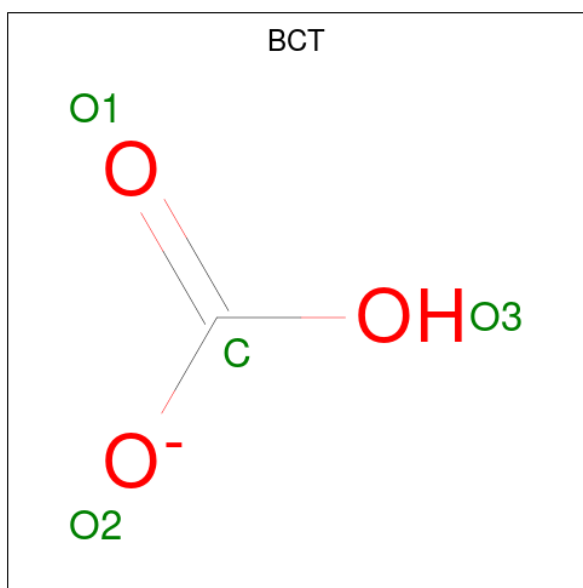
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	B	1	Total	C	H	O	0	0
			34	12	20	2		
31	B	1	Total	C	H	O	0	0
			28	10	16	2		
31	B	1	Total	C	H	O	0	0
			46	16	28	2		
31	B	1	Total	C	H		0	0
			47	16	31			
31	B	1	Total	C	H		0	0
			41	15	26			
31	C	1	Total	C	H	O	0	0
			28	10	16	2		
31	C	1	Total	C	H		0	0
			47	16	31			
31	C	1	Total	C	H	O	0	0
			28	10	16	2		
31	D	1	Total	C	H	O	0	0
			55	18	35	2		
31	E	1	Total	C	H	O	0	0
			28	10	16	2		
31	H	1	Total	C	H		0	0
			53	18	35			
31	I	1	Total	C	H		0	0
			41	15	26			
31	J	1	Total	C	H	O	0	0
			28	10	16	2		
31	M	1	Total	C	H	O	0	0
			37	13	22	2		
31	M	1	Total	C	H		0	0
			26	10	16			
31	T	1	Total	C	H		0	0
			44	15	29			
31	Z	1	Total	C	H		0	0
			20	8	12			
31	a	1	Total	C	H		0	0
			26	10	16			
31	a	1	Total	C	H	O	0	0
			28	10	16	2		
31	b	1	Total	C	H		0	0
			47	16	31			
31	b	1	Total	C	H	O	0	0
			55	18	35	2		

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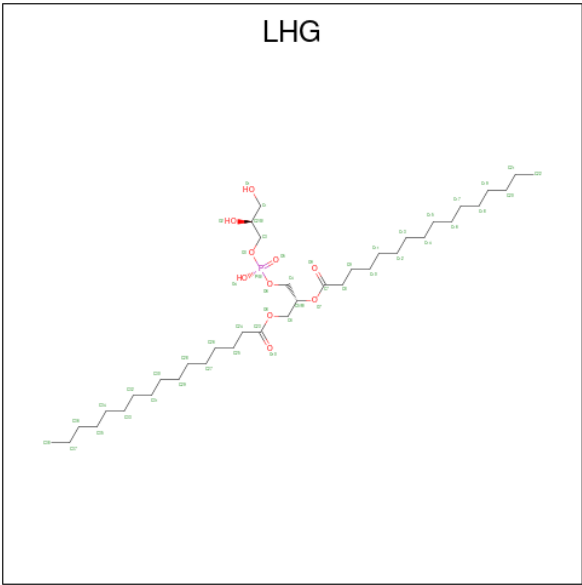
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	b	1	Total C H O 55 18 35 2	0	0
31	b	1	Total C H 26 10 16	0	0
31	b	1	Total C H 41 14 27	0	0
31	b	1	Total C H O 55 18 35 2	0	0
31	c	1	Total C H O 28 10 16 2	0	0
31	c	1	Total C H O 55 18 35 2	0	0
31	d	1	Total C H O 40 14 24 2	0	0
31	d	1	Total C H O 43 15 26 2	0	0
31	d	1	Total C H O 55 18 35 2	0	0
31	j	1	Total C H O 28 10 16 2	0	0
31	m	1	Total C H 53 18 35	0	0
31	m	1	Total C H O 28 10 16 2	0	0

- Molecule 32 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	D	1	Total	C	H	O	0	0
			5	1	1	3		
32	d	1	Total	C	H	O	0	0
			5	1	1	3		

- Molecule 33 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



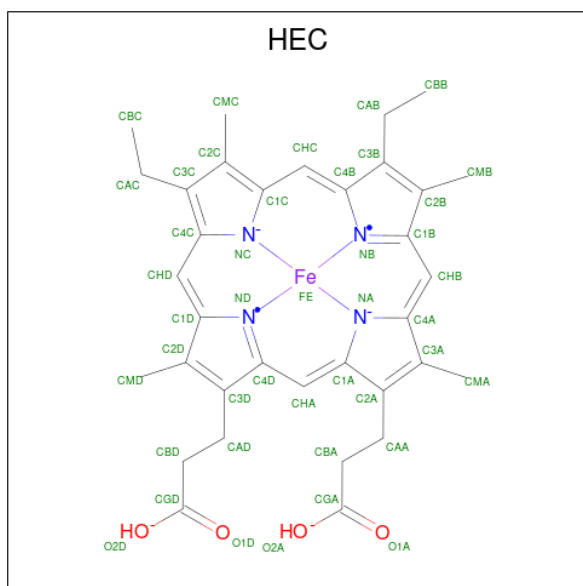
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
33	D	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
33	D	1	Total	C	H	O	P	0	0
			114	36	67	10	1		
33	D	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
33	E	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
33	L	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
33	d	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
33	d	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
33	d	1	Total	C	H	O	P	0	0
			90	28	51	10	1		
33	e	1	Total	C	H	O	P	0	0
			99	31	57	10	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
33	1	1	Total	C	H	O	P	0	0
			123	38	74	10	1		

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



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
34	F	1	Total 73	C 34	Fe 1	H 30	N 4	O 4	0	0
34	V	1	Total 73	C 34	Fe 1	H 30	N 4	O 4	0	0
34	f	1	Total 73	C 34	Fe 1	H 30	N 4	O 4	0	0
34	v	1	Total 73	C 34	Fe 1	H 30	N 4	O 4	0	0

- Molecule 35 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	A	142	Total O 142 142	0	0
35	B	212	Total O 212 212	0	0
35	C	184	Total O 184 184	0	0
35	D	138	Total O 138 138	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	E	36	Total O 36 36	0	0
35	F	8	Total O 8 8	0	0
35	H	40	Total O 40 40	0	0
35	I	24	Total O 24 24	0	0
35	J	15	Total O 15 15	0	0
35	K	7	Total O 7 7	0	0
35	L	9	Total O 9 9	0	0
35	M	11	Total O 11 11	0	0
35	O	104	Total O 104 104	0	0
35	R	4	Total O 4 4	0	0
35	T	10	Total O 10 10	0	0
35	U	52	Total O 52 52	0	0
35	V	59	Total O 59 59	0	0
35	X	15	Total O 15 15	0	0
35	Y	5	Total O 5 5	0	0
35	Z	6	Total O 6 6	0	0
35	a	116	Total O 116 116	0	0
35	b	201	Total O 201 201	0	0
35	c	187	Total O 187 187	0	0
35	d	115	Total O 115 115	0	0
35	e	21	Total O 21 21	0	0

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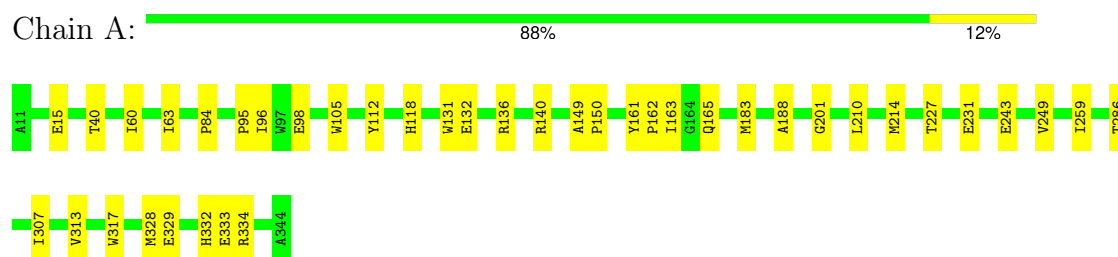
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	f	6	Total 6	O 6	0	0
35	h	31	Total 31	O 31	0	0
35	i	12	Total 12	O 12	0	0
35	j	6	Total 6	O 6	0	0
35	k	7	Total 7	O 7	0	0
35	l	5	Total 5	O 5	0	0
35	m	10	Total 10	O 10	0	0
35	o	86	Total 86	O 86	0	0
35	r	6	Total 6	O 6	0	0
35	t	9	Total 9	O 9	0	0
35	u	53	Total 53	O 53	0	0
35	v	62	Total 62	O 62	0	0
35	x	8	Total 8	O 8	0	0
35	y	4	Total 4	O 4	0	0
35	z	11	Total 11	O 11	0	0

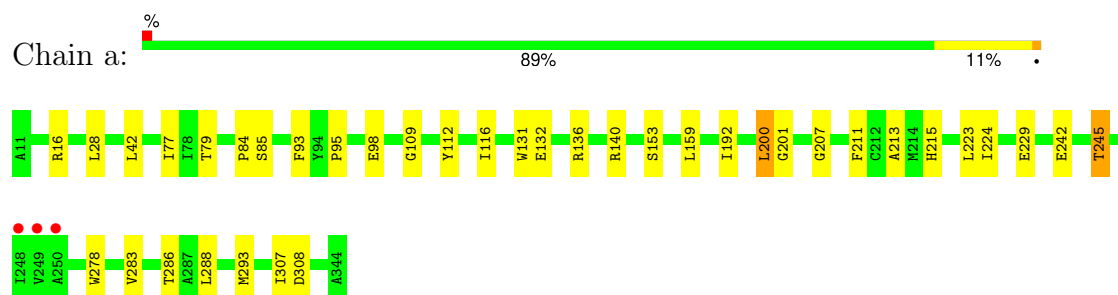
3 Residue-property plots [i](#)

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

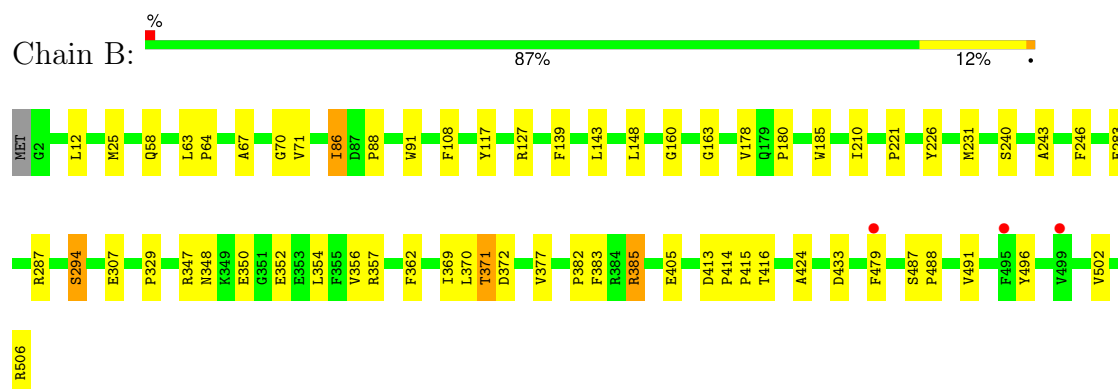
- Molecule 1: Photosystem II protein D1 1



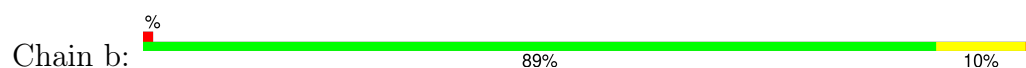
- Molecule 1: Photosystem II protein D1 1

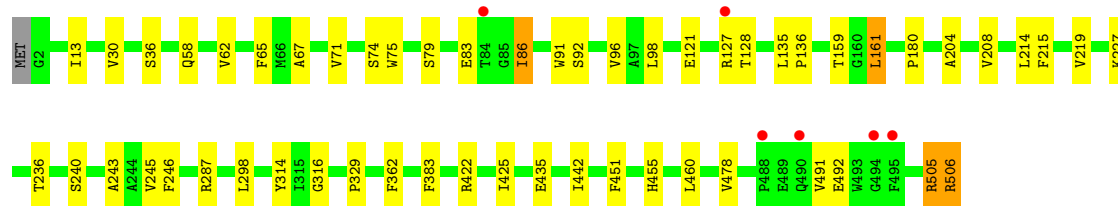


- Molecule 2: Photosystem II CP47 reaction center protein



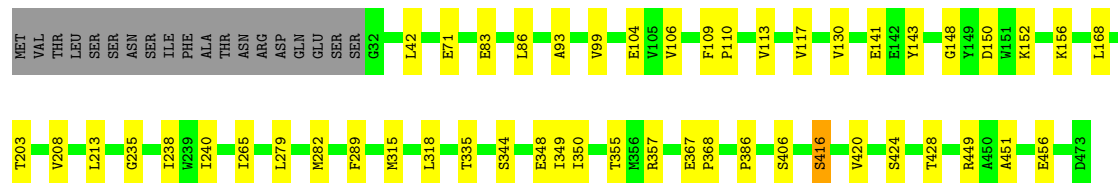
- Molecule 2: Photosystem II CP47 reaction center protein





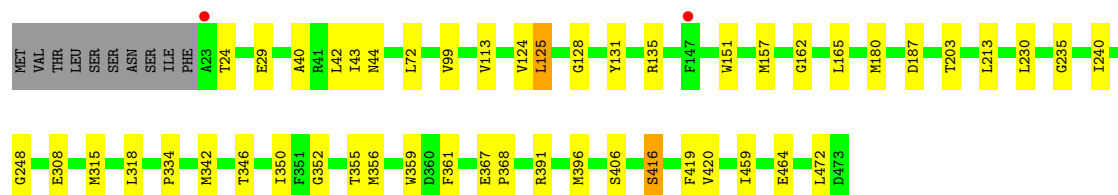
• Molecule 3: Photosystem II CP43 reaction center protein

Chain C: 85% 11% •



• Molecule 3: Photosystem II CP43 reaction center protein

Chain c: 87% 10% •



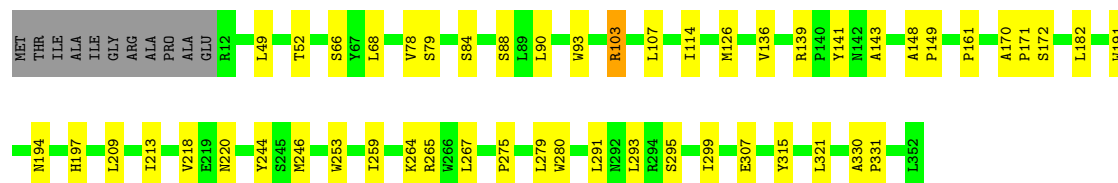
• Molecule 4: Photosystem II D2 protein

Chain D: 87% 9% • •

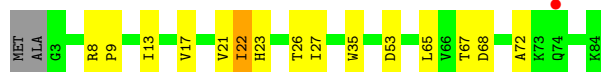
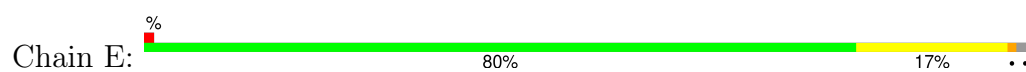


• Molecule 4: Photosystem II D2 protein

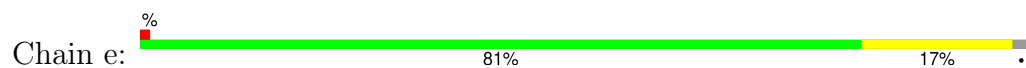
Chain d: 82% 14% •



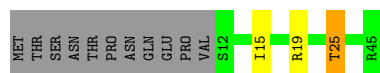
• Molecule 5: Cytochrome b559 subunit alpha



- Molecule 5: Cytochrome b559 subunit alpha



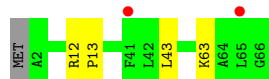
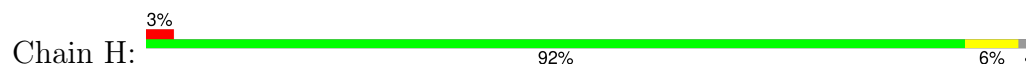
- Molecule 6: Cytochrome b559 subunit beta



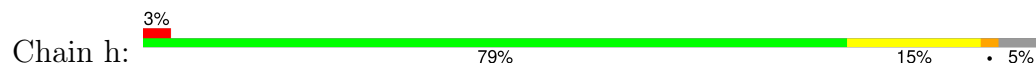
- Molecule 6: Cytochrome b559 subunit beta



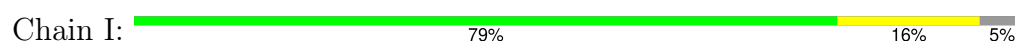
- Molecule 7: Photosystem II reaction center protein H



- Molecule 7: Photosystem II reaction center protein H

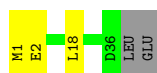


- Molecule 8: Photosystem II reaction center protein I



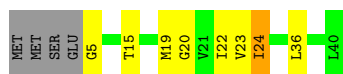
- Molecule 8: Photosystem II reaction center protein I

Chain i:  87% 8% 5%



• Molecule 9: Photosystem II reaction center protein J

Chain J:  70% 18% 10%



• Molecule 9: Photosystem II reaction center protein J

Chain j:  2% 60% 25% 5% 10%



• Molecule 10: Photosystem II reaction center protein K

Chain K:  65% 15% 20%

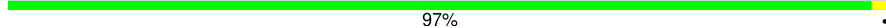


• Molecule 10: Photosystem II reaction center protein K

Chain k:  61% 20% 20%



• Molecule 11: Photosystem II reaction center protein L

Chain L:  97% 1% 2%



• Molecule 11: Photosystem II reaction center protein L

Chain l:  86% 11% 3%



• Molecule 12: Photosystem II reaction center protein M

Chain M:  75% 17% 8%



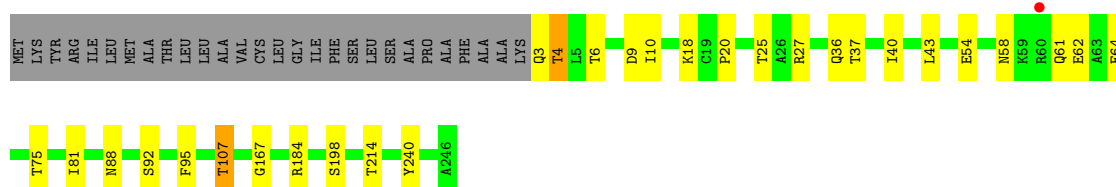
- Molecule 12: Photosystem II reaction center protein M

Chain m:  75% 14% 11%



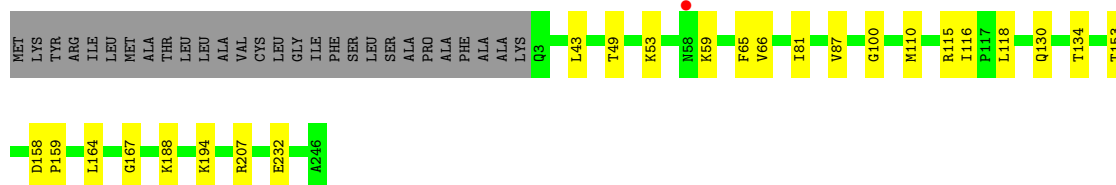
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:  79% 10% 10%



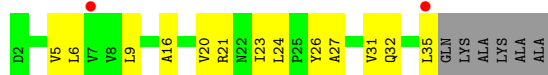
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:  81% 9% 10%



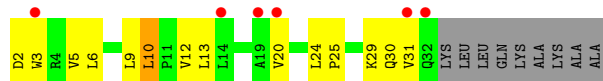
- Molecule 14: Photosystem II protein Y

Chain R:  5% 52% 32% 15%



- Molecule 14: Photosystem II protein Y

Chain r:  15% 42% 32% 22%



- Molecule 15: Photosystem II reaction center protein T

Chain T:  90% 7% •



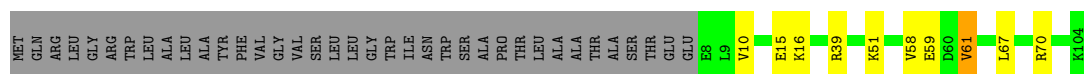
- Molecule 15: Photosystem II reaction center protein T

Chain t:  7% 90% 10%



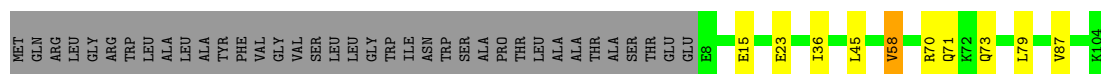
- Molecule 16: Photosystem II 12 kDa extrinsic protein

Chain U:  65% 7% • 28%



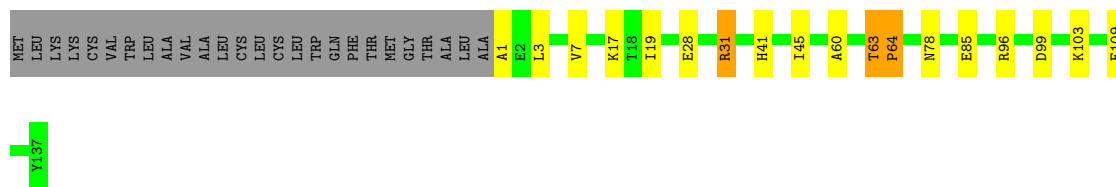
- Molecule 16: Photosystem II 12 kDa extrinsic protein

Chain u:  65% 7% • 28%



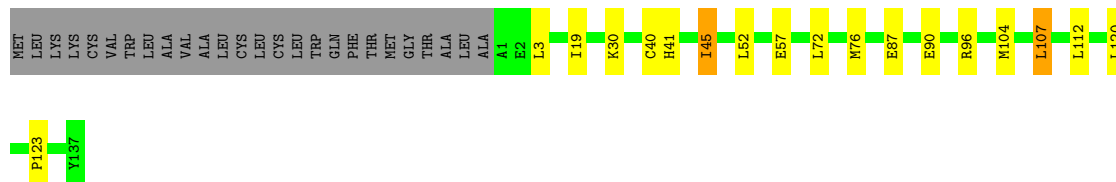
- Molecule 17: Cytochrome c-550

Chain V:  73% 9% • 16%



- Molecule 17: Cytochrome c-550

Chain v:  73% 10% • 16%

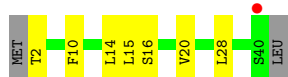
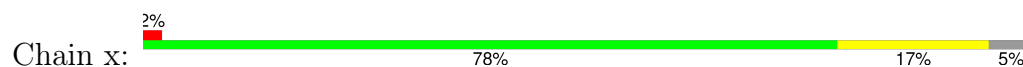


- Molecule 18: Photosystem II reaction center X protein

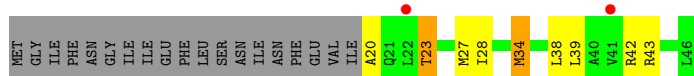
Chain X:  83% 7% • 7%



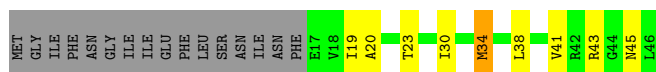
- Molecule 18: Photosystem II reaction center X protein



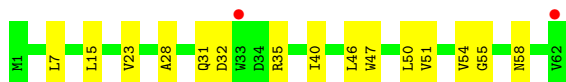
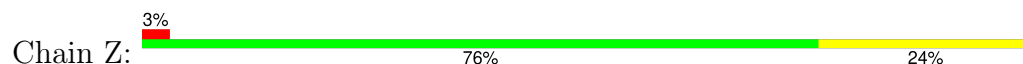
- Molecule 19: Photosystem II reaction center protein Ycf12



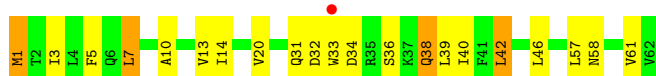
- Molecule 19: Photosystem II reaction center protein Ycf12



- Molecule 20: Photosystem II reaction center protein Z



- Molecule 20: Photosystem II reaction center protein Z



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	116.92Å 221.63Å 307.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.64 – 2.08 33.64 – 2.08	Depositor EDS
% Data completeness (in resolution range)	99.6 (33.64-2.08) 85.0 (33.64-2.08)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.55 (at 2.08Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.181 , 0.240 0.182 , 0.241	Depositor DCC
R_{free} test set	4226 reflections (0.67%)	wwPDB-VP
Wilson B-factor (Å ²)	26.3	Xtriage
Anisotropy	0.197	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 53.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	103895	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.55% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.64	0/2707	0.72	0/3692
1	a	0.61	0/2704	0.71	1/3688 (0.0%)
2	B	0.59	0/4161	0.66	0/5669
2	b	0.59	0/4118	0.67	0/5611
3	C	0.59	0/3547	0.68	0/4830
3	c	0.55	0/3619	0.63	0/4926
4	D	0.62	0/2812	0.70	0/3832
4	d	0.59	0/2821	0.69	0/3844
5	E	0.48	0/688	0.60	0/940
5	e	0.43	0/683	0.61	0/932
6	F	0.50	0/284	0.60	0/387
6	f	0.45	0/284	0.69	0/387
7	H	0.61	0/523	0.67	0/713
7	h	0.51	0/511	0.62	0/697
8	I	0.55	0/293	0.70	0/396
8	i	0.60	0/293	0.67	0/396
9	J	0.46	0/263	0.67	0/356
9	j	0.44	0/263	0.57	0/356
10	K	0.45	0/303	0.60	0/416
10	k	0.45	0/303	0.55	0/416
11	L	0.68	0/311	0.68	0/422
11	l	0.67	0/303	0.63	0/412
12	M	0.66	0/249	0.80	0/341
12	m	0.63	0/244	0.74	0/334
13	O	0.58	0/1904	0.67	0/2585
13	o	0.58	0/1905	0.67	0/2583
14	R	0.42	0/277	0.55	0/380
14	r	0.38	0/246	0.46	0/339
15	T	0.62	0/257	0.72	0/349
15	t	0.56	0/255	0.65	0/346
16	U	0.49	0/785	0.62	0/1064
16	u	0.58	0/785	0.67	0/1064

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	V	0.59	0/1085	0.66	0/1473
17	v	0.51	0/1085	0.62	0/1473
18	X	0.44	0/284	0.61	0/384
18	x	0.35	0/289	0.48	0/391
19	Y	0.42	0/197	0.64	0/264
19	y	0.37	0/219	0.54	0/294
20	Z	0.37	0/490	0.53	0/669
20	z	0.35	0/488	0.49	0/666
All	All	0.57	0/42838	0.66	1/58317 (0.0%)

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
17	V	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	131	TRP	CA-CB-CG	-5.11	103.89	113.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
17	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	2622	2508	2519	26	0
1	a	2619	2499	2510	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	4005	3859	3867	43	0
2	b	3978	3822	3836	30	0
3	C	3426	3342	3343	23	0
3	c	3500	3413	3426	28	0
4	D	2717	2613	2621	27	0
4	d	2723	2619	2627	34	0
5	E	666	650	651	12	0
5	e	664	647	648	11	0
6	F	275	281	282	3	0
6	f	275	281	282	10	0
7	H	510	532	532	3	0
7	h	498	518	518	5	0
8	I	296	311	311	3	0
8	i	296	311	311	1	0
9	J	257	268	268	6	0
9	j	257	268	268	10	0
10	K	293	305	305	3	0
10	k	293	305	305	5	0
11	L	304	316	316	1	0
11	l	296	304	304	0	0
12	M	256	269	269	4	0
12	m	251	267	267	2	0
13	O	1870	1828	1830	21	0
13	o	1874	1844	1846	13	0
14	R	271	298	298	5	0
14	r	240	253	250	8	0
15	T	258	261	261	3	0
15	t	256	256	256	2	0
16	U	774	772	773	5	0
16	u	774	772	773	5	0
17	V	1064	1068	1073	11	0
17	v	1064	1068	1073	11	0
18	X	281	312	312	2	0
18	x	286	316	314	3	0
19	Y	196	217	217	6	0
19	y	218	241	241	4	0
20	Z	479	516	516	7	0
20	z	477	509	509	12	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	A	184	192	192	3	0
22	B	970	1067	1067	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	C	839	922	922	8	0
22	D	195	216	216	6	0
22	H	65	72	72	2	0
22	a	260	288	288	4	0
22	b	1035	1139	1139	16	0
22	c	839	919	919	12	0
22	d	130	144	144	1	0
23	A	64	74	74	1	0
23	D	64	74	74	1	0
23	a	64	74	74	1	0
23	d	64	74	74	1	0
24	A	40	56	56	1	0
24	B	120	168	168	7	0
24	C	40	56	56	0	0
24	F	40	56	56	5	0
24	H	40	56	56	3	0
24	K	120	168	168	4	0
24	T	40	56	56	4	0
24	a	40	56	56	2	0
24	b	120	168	168	2	0
24	c	80	112	112	6	0
24	d	40	56	56	3	0
24	h	40	56	56	1	0
24	k	80	112	112	2	0
24	t	40	56	56	3	0
25	A	2	0	0	0	0
25	a	2	0	0	0	0
26	A	55	80	80	2	0
26	D	55	80	80	0	0
26	a	55	80	80	3	0
26	d	55	80	80	1	0
27	A	48	66	66	0	0
27	B	28	40	40	0	0
27	D	84	117	117	4	0
27	M	51	72	72	1	0
27	Y	48	66	66	0	0
27	a	55	86	86	2	0
27	b	106	158	158	1	0
27	c	134	181	181	1	0
27	d	44	58	58	0	0
28	A	91	136	134	3	0
28	B	54	78	78	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	D	36	46	45	0	0
28	L	49	65	65	0	0
28	a	90	134	133	1	0
28	f	41	48	48	1	0
29	A	66	96	96	1	0
29	C	186	246	246	1	0
29	H	62	82	82	1	0
29	c	186	245	241	3	0
29	h	62	82	81	0	0
30	A	10	0	0	0	0
30	a	10	0	0	0	0
31	B	104	163	163	2	0
31	C	40	63	63	0	0
31	D	20	35	35	0	0
31	E	12	16	16	0	0
31	H	18	35	35	0	0
31	I	15	26	26	0	0
31	J	12	16	16	0	0
31	M	25	38	38	0	0
31	T	15	29	29	0	0
31	Z	8	12	12	1	0
31	a	22	32	32	1	0
31	b	100	179	179	2	0
31	c	32	51	51	2	0
31	d	53	85	85	1	0
31	j	12	16	16	0	0
31	m	30	51	51	1	0
32	D	4	1	1	0	0
32	d	4	1	1	0	0
33	D	145	215	215	6	0
33	E	49	74	74	1	0
33	L	49	74	74	1	0
33	d	137	199	199	3	0
33	e	42	57	57	1	0
33	l	49	74	74	0	0
34	F	43	30	32	3	0
34	V	43	30	30	2	0
34	f	43	30	32	5	0
34	v	43	30	30	1	0
35	A	142	0	0	3	0
35	B	212	0	0	4	0
35	C	184	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	D	138	0	0	4	0
35	E	36	0	0	0	0
35	F	8	0	0	0	0
35	H	40	0	0	1	0
35	I	24	0	0	1	0
35	J	15	0	0	2	0
35	K	7	0	0	0	0
35	L	9	0	0	0	0
35	M	11	0	0	1	0
35	O	104	0	0	3	0
35	R	4	0	0	0	0
35	T	10	0	0	1	0
35	U	52	0	0	1	0
35	V	59	0	0	1	0
35	X	15	0	0	0	0
35	Y	5	0	0	0	0
35	Z	6	0	0	0	0
35	a	116	0	0	0	0
35	b	201	0	0	2	0
35	c	187	0	0	2	0
35	d	115	0	0	1	0
35	e	21	0	0	0	0
35	f	6	0	0	0	0
35	h	31	0	0	0	0
35	i	12	0	0	0	0
35	j	6	0	0	2	0
35	k	7	0	0	1	0
35	l	5	0	0	0	0
35	m	10	0	0	1	0
35	o	86	0	0	2	0
35	r	6	0	0	1	0
35	t	9	0	0	0	0
35	u	53	0	0	1	0
35	v	62	0	0	3	0
35	x	8	0	0	0	0
35	y	4	0	0	0	0
35	z	11	0	0	0	0
All	All	52285	51610	51694	478	0

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

The worst 5 of 478 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)
13:O:27:ARG:NH1	35:O:301:HOH:O	2.09	0.85
3:c:391[B]:ARG:NE	35:c:602:HOH:O	2.15	0.80
5:e:30:LEU:HD11	34:f:101:HEC:HBB3	1.64	0.78
17:v:76:MET:HE2	17:v:112:LEU:HD22	1.66	0.78
9:j:36:LEU:O	35:j:201:HOH:O	2.00	0.76

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	332/334 (99%)	325 (98%)	6 (2%)	1 (0%)	36	36
1	a	332/334 (99%)	326 (98%)	6 (2%)	0	100	100
2	B	508/506 (100%)	499 (98%)	9 (2%)	0	100	100
2	b	503/506 (99%)	490 (97%)	13 (3%)	0	100	100
3	C	442/461 (96%)	433 (98%)	8 (2%)	1 (0%)	43	44
3	c	451/461 (98%)	435 (96%)	15 (3%)	1 (0%)	43	44
4	D	339/352 (96%)	329 (97%)	10 (3%)	0	100	100
4	d	340/352 (97%)	333 (98%)	7 (2%)	0	100	100
5	E	81/84 (96%)	79 (98%)	2 (2%)	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%)	59 (94%)	4 (6%)	0	100	100
7	h	61/66 (92%)	56 (92%)	4 (7%)	1 (2%)	7	4
8	I	34/38 (90%)	32 (94%)	2 (6%)	0	100	100
8	i	34/38 (90%)	32 (94%)	2 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	J	34/40 (85%)	30 (88%)	4 (12%)	0	100	100
9	j	34/40 (85%)	33 (97%)	1 (3%)	0	100	100
10	K	35/46 (76%)	34 (97%)	1 (3%)	0	100	100
10	k	35/46 (76%)	35 (100%)	0	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	34/37 (92%)	34 (100%)	0	0	100	100
12	M	31/36 (86%)	31 (100%)	0	0	100	100
12	m	30/36 (83%)	28 (93%)	2 (7%)	0	100	100
13	O	243/272 (89%)	224 (92%)	18 (7%)	1 (0%)	30	28
13	o	242/272 (89%)	230 (95%)	12 (5%)	0	100	100
14	R	32/40 (80%)	30 (94%)	2 (6%)	0	100	100
14	r	29/40 (72%)	26 (90%)	2 (7%)	1 (3%)	3	1
15	T	28/30 (93%)	28 (100%)	0	0	100	100
15	t	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
16	U	95/134 (71%)	91 (96%)	4 (4%)	0	100	100
16	u	95/134 (71%)	93 (98%)	2 (2%)	0	100	100
17	V	135/163 (83%)	129 (96%)	5 (4%)	1 (1%)	18	14
17	v	135/163 (83%)	131 (97%)	4 (3%)	0	100	100
18	X	36/41 (88%)	35 (97%)	1 (3%)	0	100	100
18	x	37/41 (90%)	36 (97%)	1 (3%)	0	100	100
19	Y	25/46 (54%)	23 (92%)	1 (4%)	1 (4%)	2	0
19	y	28/46 (61%)	25 (89%)	3 (11%)	0	100	100
20	Z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
20	z	60/62 (97%)	54 (90%)	5 (8%)	1 (2%)	7	3
All	All	5240/5666 (92%)	5072 (97%)	159 (3%)	9 (0%)	43	44

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
17	V	64	PRO
3	c	416	SER
13	O	62	GLU
19	Y	43	ARG

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	270/270 (100%)	268 (99%)	2 (1%)	76	82
1	a	269/270 (100%)	257 (96%)	12 (4%)	24	24
2	B	408/404 (101%)	399 (98%)	9 (2%)	45	51
2	b	402/404 (100%)	386 (96%)	16 (4%)	28	28
3	C	346/362 (96%)	334 (96%)	12 (4%)	32	33
3	c	354/362 (98%)	342 (97%)	12 (3%)	32	34
4	D	276/283 (98%)	272 (99%)	4 (1%)	59	66
4	d	277/283 (98%)	269 (97%)	8 (3%)	37	40
5	E	72/73 (99%)	70 (97%)	2 (3%)	38	42
5	e	71/73 (97%)	69 (97%)	2 (3%)	38	42
6	F	28/39 (72%)	27 (96%)	1 (4%)	31	32
6	f	28/39 (72%)	25 (89%)	3 (11%)	6	3
7	H	54/55 (98%)	54 (100%)	0	100	100
7	h	53/55 (96%)	49 (92%)	4 (8%)	12	9
8	I	32/34 (94%)	30 (94%)	2 (6%)	16	13
8	i	32/34 (94%)	31 (97%)	1 (3%)	35	38
9	J	24/28 (86%)	23 (96%)	1 (4%)	26	26
9	j	24/28 (86%)	22 (92%)	2 (8%)	10	7
10	K	30/37 (81%)	27 (90%)	3 (10%)	7	4
10	k	30/37 (81%)	27 (90%)	3 (10%)	7	4
11	L	35/35 (100%)	35 (100%)	0	100	100
11	l	34/35 (97%)	30 (88%)	4 (12%)	5	3
12	M	28/32 (88%)	27 (96%)	1 (4%)	31	32
12	m	28/32 (88%)	26 (93%)	2 (7%)	13	10
13	O	206/228 (90%)	199 (97%)	7 (3%)	32	34
13	o	207/228 (91%)	200 (97%)	7 (3%)	32	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	R	28/32 (88%)	23 (82%)	5 (18%)	2	1
14	r	23/32 (72%)	19 (83%)	4 (17%)	2	1
15	T	26/26 (100%)	25 (96%)	1 (4%)	29	30
15	t	25/26 (96%)	25 (100%)	0	100	100
16	U	84/112 (75%)	80 (95%)	4 (5%)	23	22
16	u	84/112 (75%)	81 (96%)	3 (4%)	31	32
17	V	117/138 (85%)	112 (96%)	5 (4%)	26	26
17	v	117/138 (85%)	112 (96%)	5 (4%)	26	26
18	X	31/34 (91%)	28 (90%)	3 (10%)	8	5
18	x	31/34 (91%)	29 (94%)	2 (6%)	15	12
19	Y	19/37 (51%)	17 (90%)	2 (10%)	6	4
19	y	22/37 (60%)	18 (82%)	4 (18%)	2	1
20	Z	52/52 (100%)	47 (90%)	5 (10%)	8	5
20	z	51/52 (98%)	43 (84%)	8 (16%)	2	1
All	All	4328/4622 (94%)	4157 (96%)	171 (4%)	28	28

5 of 171 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	d	307	GLU
13	o	134	THR
6	f	15	ILE
10	k	30	VAL
16	u	23	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 44 such sidechains are listed below:

Mol	Chain	Res	Type
3	c	373	ASN
13	o	124	ASN
3	c	378	ASN
4	d	350	ASN
13	o	155	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	FME	M	1	12	8,9,10	1.10	1 (12%)	8,9,11	0.80	0
15	FME	T	1	15	8,9,10	1.18	0	8,9,11	0.92	0
8	FME	I	1	8	8,9,10	1.03	0	8,9,11	1.08	0
8	FME	i	1	8	8,9,10	1.23	1 (12%)	8,9,11	1.44	2 (25%)
12	FME	m	1	12	8,9,10	1.15	1 (12%)	8,9,11	0.73	0
15	FME	t	1	15	8,9,10	1.04	0	8,9,11	1.25	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
12	FME	M	1	12	-	2/7/9/11	-
15	FME	T	1	15	-	2/7/9/11	-
8	FME	I	1	8	-	1/7/9/11	-
8	FME	i	1	8	-	0/7/9/11	-
12	FME	m	1	12	-	0/7/9/11	-
15	FME	t	1	15	-	1/7/9/11	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	i	1	FME	CA-N	-2.86	1.42	1.46
12	m	1	FME	CA-N	-2.42	1.43	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	M	1	FME	CA-N	-2.16	1.43	1.46

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	i	1	FME	CB-CA-N	2.52	115.11	110.52
8	i	1	FME	CA-N-CN	-2.41	119.12	122.82
15	t	1	FME	C-CA-N	2.37	114.06	109.50

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	M	1	FME	O-C-CA-CB
15	T	1	FME	O-C-CA-CB
15	t	1	FME	CB-CG-SD-CE
15	T	1	FME	CB-CG-SD-CE
8	I	1	FME	C-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 189 ligands modelled in this entry, 6 are monoatomic - leaving 183 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	$\# Z > 2$
31	STE	M	102	-	14,14,19	1.03	1 (7%)	14,14,19	0.69	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	SQD	L	101	-	47,49,54	0.93	2 (4%)	57,60,65	2.35	14 (24%)
33	LHG	D	412	-	48,48,48	0.79	1 (2%)	51,54,54	1.34	5 (9%)
22	CLA	c	509	3	68,72,73	1.48	10 (14%)	80,111,113	1.38	9 (11%)
33	LHG	D	410	-	46,46,48	1.06	3 (6%)	49,52,54	1.24	4 (8%)
24	BCR	F	101	-	41,41,41	1.13	3 (7%)	56,56,56	1.30	6 (10%)
22	CLA	b	608	2	69,73,73	1.36	8 (11%)	82,113,113	1.36	8 (9%)
31	STE	a	413	-	9,9,19	0.57	0	8,8,19	0.57	0
22	CLA	H	101	35	69,73,73	1.47	10 (14%)	82,113,113	1.48	7 (8%)
27	LMG	b	623	-	55,55,55	0.88	2 (3%)	63,63,63	1.61	11 (17%)
22	CLA	C	510	3	69,73,73	1.13	7 (10%)	82,113,113	1.24	8 (9%)
23	PHO	D	401	-	58,69,69	1.94	9 (15%)	55,99,99	1.39	6 (10%)
24	BCR	k	101	-	41,41,41	1.08	4 (9%)	56,56,56	1.12	3 (5%)
26	PL9	D	406	-	55,55,55	1.33	7 (12%)	68,69,69	1.60	14 (20%)
24	BCR	C	514	-	41,41,41	1.23	3 (7%)	56,56,56	1.25	9 (16%)
31	STE	H	104	-	17,17,19	0.42	0	16,16,19	0.89	0
22	CLA	C	503	3	69,73,73	1.38	8 (11%)	82,113,113	1.48	13 (15%)
28	SQD	a	411	-	52,54,54	1.01	4 (7%)	62,65,65	2.15	15 (24%)
22	CLA	A	403	35	69,73,73	1.28	10 (14%)	82,113,113	1.31	12 (14%)
27	LMG	A	410	-	48,48,55	1.01	2 (4%)	56,56,63	1.44	7 (12%)
27	LMG	D	407	-	51,51,55	0.92	2 (3%)	59,59,63	1.38	8 (13%)
31	STE	d	412	-	16,16,19	0.63	0	16,16,19	1.07	1 (6%)
22	CLA	C	506	3	69,73,73	1.84	10 (14%)	82,113,113	1.25	8 (9%)
31	STE	B	626	-	15,15,19	0.48	0	14,14,19	0.71	0
29	DGD	c	519	-	63,63,67	1.21	8 (12%)	77,77,81	1.40	8 (10%)
22	CLA	d	403	4	69,73,73	1.21	8 (11%)	82,113,113	1.18	7 (8%)
22	CLA	a	405	1	69,73,73	1.22	8 (11%)	82,113,113	1.32	8 (9%)
22	CLA	C	504	35	63,67,73	1.33	10 (15%)	74,105,113	1.37	11 (14%)
31	STE	m	102	-	11,11,19	0.76	0	11,11,19	1.32	2 (18%)
33	LHG	D	409	-	48,48,48	0.96	2 (4%)	51,54,54	1.29	6 (11%)
27	LMG	a	415	-	55,55,55	1.44	6 (10%)	63,63,63	1.46	7 (11%)
22	CLA	C	508	3	69,73,73	1.41	8 (11%)	82,113,113	1.40	5 (6%)
33	LHG	e	101	-	41,41,48	0.93	1 (2%)	44,47,54	1.24	4 (9%)
24	BCR	K	101	-	41,41,41	1.11	2 (4%)	56,56,56	1.46	8 (14%)
31	STE	B	624	-	11,11,19	0.96	2 (18%)	11,11,19	1.06	0
28	SQD	a	412	-	35,35,54	1.22	2 (5%)	37,37,65	1.48	4 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	STE	C	518	-	11,11,19	0.79	0	11,11,19	0.96	0
28	SQD	A	412	-	38,38,54	1.04	3 (7%)	40,40,65	1.30	4 (10%)
33	LHG	d	409	-	38,38,48	1.02	2 (5%)	41,44,54	1.08	2 (4%)
22	CLA	c	512	3	69,73,73	1.50	8 (11%)	82,113,113	1.43	6 (7%)
22	CLA	D	403	4	69,73,73	1.14	7 (10%)	82,113,113	1.37	12 (14%)
23	PHO	a	404	-	58,69,69	1.94	7 (12%)	55,99,99	1.57	9 (16%)
31	STE	b	620	-	15,15,19	0.46	0	14,14,19	0.82	0
33	LHG	l	101	-	48,48,48	0.62	0	51,54,54	1.16	4 (7%)
22	CLA	b	612	2	69,73,73	1.15	7 (10%)	82,113,113	1.35	13 (15%)
22	CLA	D	404	35	69,73,73	1.37	7 (10%)	82,113,113	1.31	5 (6%)
27	LMG	c	522	-	48,48,55	1.13	5 (10%)	56,56,63	1.19	3 (5%)
31	STE	B	601	-	11,11,19	0.62	0	11,11,19	1.30	1 (9%)
27	LMG	d	410	-	44,44,55	1.16	4 (9%)	52,52,63	1.32	5 (9%)
24	BCR	K	102	-	41,41,41	1.03	3 (7%)	56,56,56	1.27	5 (8%)
22	CLA	a	402	1	69,73,73	1.41	8 (11%)	82,113,113	1.45	13 (15%)
26	PL9	A	409	-	55,55,55	0.97	1 (1%)	68,69,69	1.55	13 (19%)
22	CLA	A	402	1	69,73,73	1.42	9 (13%)	82,113,113	1.34	6 (7%)
34	HEC	f	101	6,5	50,50,50	1.55	9 (18%)	68,82,82	1.66	13 (19%)
22	CLA	C	502	3	69,73,73	1.27	8 (11%)	82,113,113	1.23	8 (9%)
29	DGD	h	102	-	63,63,67	1.16	11 (17%)	77,77,81	1.37	10 (12%)
22	CLA	c	506	3	69,73,73	1.14	8 (11%)	82,113,113	1.35	8 (9%)
22	CLA	c	504	3	69,73,73	1.22	11 (15%)	82,113,113	1.53	10 (12%)
29	DGD	C	516	-	63,63,67	1.20	10 (15%)	77,77,81	1.38	10 (12%)
31	STE	m	101	-	17,17,19	0.44	0	16,16,19	0.80	0
22	CLA	C	511	3	69,73,73	1.22	9 (13%)	82,113,113	1.20	4 (4%)
24	BCR	d	405	-	41,41,41	1.22	3 (7%)	56,56,56	1.29	6 (10%)
28	SQD	D	408	-	34,36,54	0.94	2 (5%)	42,45,65	1.75	9 (21%)
22	CLA	B	611	2	69,73,73	1.26	7 (10%)	82,113,113	1.50	14 (17%)
33	LHG	L	102	-	48,48,48	0.82	2 (4%)	51,54,54	1.20	2 (3%)
31	STE	b	627	-	19,19,19	0.61	0	19,19,19	1.23	2 (10%)
22	CLA	C	509	3	69,73,73	1.30	13 (18%)	82,113,113	1.26	10 (12%)
24	BCR	B	618	-	41,41,41	1.00	1 (2%)	56,56,56	1.42	9 (16%)
31	STE	c	501	-	11,11,19	0.86	0	11,11,19	1.06	0
24	BCR	t	101	-	41,41,41	0.98	2 (4%)	56,56,56	1.48	14 (25%)
24	BCR	b	618	-	41,41,41	1.17	2 (4%)	56,56,56	1.30	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	B	616	2	64,68,73	1.70	10 (15%)	76,107,113	1.56	10 (13%)
22	CLA	D	405	4	69,73,73	1.38	9 (13%)	82,113,113	1.10	5 (6%)
22	CLA	b	607	35	69,73,73	1.45	9 (13%)	82,113,113	1.32	10 (12%)
22	CLA	B	614	2	69,73,73	1.27	9 (13%)	82,113,113	1.27	10 (12%)
24	BCR	T	101	-	41,41,41	1.24	4 (9%)	56,56,56	1.21	4 (7%)
30	OEX	a	416	1,3,35	0,14,14	-	-	-	-	-
24	BCR	b	617	-	41,41,41	1.14	4 (9%)	56,56,56	1.38	10 (17%)
24	BCR	a	406	-	41,41,41	1.26	3 (7%)	56,56,56	1.24	6 (10%)
23	PHO	d	401	-	58,69,69	2.06	10 (17%)	55,99,99	1.74	10 (18%)
22	CLA	C	505	3	69,73,73	1.31	8 (11%)	82,113,113	1.38	9 (10%)
31	STE	E	102	-	11,11,19	0.98	1 (9%)	11,11,19	0.99	1 (9%)
31	STE	T	102	-	14,14,19	0.44	0	13,13,19	0.86	0
31	STE	Z	101	-	7,7,19	0.44	0	6,6,19	0.57	0
31	STE	C	520	-	11,11,19	0.80	0	11,11,19	1.44	1 (9%)
31	STE	B	625	-	17,17,19	0.66	0	17,17,19	1.27	1 (5%)
22	CLA	c	503	3	69,73,73	1.15	8 (11%)	82,113,113	1.35	7 (8%)
26	PL9	a	409	-	55,55,55	1.03	4 (7%)	68,69,69	1.59	10 (14%)
22	CLA	c	513	3	69,73,73	1.26	11 (15%)	82,113,113	1.31	6 (7%)
22	CLA	C	512	3	69,73,73	1.55	9 (13%)	82,113,113	1.28	10 (12%)
22	CLA	B	606	2	69,73,73	1.60	9 (13%)	82,113,113	1.44	7 (8%)
22	CLA	C	513	3	69,73,73	1.21	10 (14%)	82,113,113	1.46	11 (13%)
22	CLA	c	508	35	69,73,73	1.28	6 (8%)	82,113,113	1.26	8 (9%)
22	CLA	B	608	2	69,73,73	1.62	9 (13%)	82,113,113	1.40	10 (12%)
23	PHO	A	404	-	58,69,69	1.92	12 (20%)	55,99,99	1.46	9 (16%)
22	CLA	B	605	2	69,73,73	1.32	9 (13%)	82,113,113	1.58	13 (15%)
22	CLA	b	609	2	69,73,73	1.49	8 (11%)	82,113,113	1.31	11 (13%)
22	CLA	B	613	2	69,73,73	1.52	11 (15%)	82,113,113	1.40	9 (10%)
32	BCT	d	402	21	3,3,3	1.13	0	2,3,3	3.61	2 (100%)
22	CLA	B	612	2	69,73,73	1.11	5 (7%)	82,113,113	1.38	12 (14%)
27	LMG	M	101	-	51,51,55	1.17	3 (5%)	59,59,63	1.49	10 (16%)
33	LHG	d	407	-	48,48,48	1.03	2 (4%)	51,54,54	1.46	5 (9%)
24	BCR	B	617	-	41,41,41	1.11	2 (4%)	56,56,56	1.29	5 (8%)
24	BCR	B	619	-	41,41,41	1.13	2 (4%)	56,56,56	1.47	9 (16%)
24	BCR	k	102	-	41,41,41	0.98	2 (4%)	56,56,56	1.22	4 (7%)
33	LHG	E	101	-	48,48,48	0.88	3 (6%)	51,54,54	1.22	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	B	602	2	69,73,73	1.33	6 (8%)	82,113,113	1.36	10 (12%)
22	CLA	b	611	2	69,73,73	1.41	8 (11%)	82,113,113	1.72	11 (13%)
22	CLA	C	507	35	69,73,73	1.39	7 (10%)	82,113,113	1.64	13 (15%)
22	CLA	a	403	35	69,73,73	1.25	9 (13%)	82,113,113	1.44	11 (13%)
31	STE	c	521	-	19,19,19	0.74	1 (5%)	19,19,19	0.92	1 (5%)
24	BCR	c	516	-	41,41,41	1.26	5 (12%)	56,56,56	1.31	6 (10%)
27	LMG	Y	101	-	48,48,55	0.97	2 (4%)	56,56,63	1.35	6 (10%)
22	CLA	b	610	35	69,73,73	1.30	8 (11%)	82,113,113	1.48	17 (20%)
22	CLA	b	615	2	69,73,73	1.82	11 (15%)	82,113,113	1.44	10 (12%)
31	STE	B	620	-	16,16,19	0.99	2 (12%)	16,16,19	0.90	0
22	CLA	d	404	4	69,73,73	1.15	8 (11%)	82,113,113	1.19	10 (12%)
32	BCT	D	402	21	3,3,3	1.14	0	2,3,3	2.97	2 (100%)
22	CLA	b	613	2	69,73,73	1.15	9 (13%)	82,113,113	1.37	11 (13%)
31	STE	b	626	-	13,13,19	0.41	0	12,12,19	0.77	0
31	STE	d	411	-	15,15,19	0.90	1 (6%)	15,15,19	0.95	2 (13%)
22	CLA	b	603	2	69,73,73	1.33	8 (11%)	82,113,113	1.51	13 (15%)
22	CLA	b	606	2	69,73,73	1.48	9 (13%)	82,113,113	1.45	6 (7%)
27	LMG	B	621	-	26,26,55	0.67	0	26,26,63	1.27	2 (7%)
28	SQD	A	411	-	50,52,54	1.11	5 (10%)	60,63,65	1.69	12 (20%)
31	STE	M	103	-	9,9,19	0.50	0	8,8,19	0.73	0
31	STE	b	624	-	19,19,19	0.69	0	19,19,19	1.33	3 (15%)
22	CLA	B	609	2	69,73,73	1.38	7 (10%)	82,113,113	1.31	6 (7%)
34	HEC	F	102	6,5	50,50,50	1.54	5 (10%)	68,82,82	1.33	8 (11%)
22	CLA	c	505	35	64,68,73	1.25	8 (12%)	76,107,113	1.38	11 (14%)
29	DGD	c	518	-	63,63,67	1.14	6 (9%)	77,77,81	1.41	11 (14%)
31	STE	b	622	-	19,19,19	0.72	0	19,19,19	0.90	0
22	CLA	B	615	2	69,73,73	1.47	10 (14%)	82,113,113	1.43	9 (10%)
24	BCR	A	406	-	41,41,41	1.17	3 (7%)	56,56,56	1.43	7 (12%)
31	STE	j	101	-	11,11,19	1.06	1 (9%)	11,11,19	1.41	2 (18%)
24	BCR	h	101	-	41,41,41	1.03	2 (4%)	56,56,56	1.37	8 (14%)
31	STE	C	519	-	15,15,19	0.60	0	14,14,19	0.50	0
27	LMG	D	411	-	31,31,55	1.12	3 (9%)	33,33,63	1.17	2 (6%)
28	SQD	B	622	-	52,54,54	1.01	3 (5%)	62,65,65	1.83	12 (19%)
31	STE	J	101	-	11,11,19	0.70	0	11,11,19	1.50	2 (18%)
29	DGD	c	517	-	63,63,67	1.37	7 (11%)	77,77,81	1.34	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	b	605	2	69,73,73	1.11	7 (10%)	82,113,113	1.51	16 (19%)
29	DGD	C	517	-	63,63,67	1.17	6 (9%)	77,77,81	1.47	12 (15%)
31	STE	d	413	-	19,19,19	0.70	0	19,19,19	0.94	1 (5%)
27	LMG	c	520	-	37,37,55	1.17	4 (10%)	45,45,63	1.28	6 (13%)
29	DGD	H	103	-	63,63,67	1.31	9 (14%)	77,77,81	1.53	14 (18%)
30	OEX	A	414	1,3,35	0,14,14	-	-	-	-	-
31	STE	B	627	-	14,14,19	0.55	0	13,13,19	0.64	0
22	CLA	b	604	2	69,73,73	1.49	9 (13%)	82,113,113	1.62	10 (12%)
22	CLA	c	502	3	69,73,73	1.27	7 (10%)	82,113,113	1.50	6 (7%)
33	LHG	d	408	-	48,48,48	1.01	2 (4%)	51,54,54	1.17	3 (5%)
22	CLA	b	616	2	64,68,73	1.15	5 (7%)	76,107,113	1.64	12 (15%)
29	DGD	A	413	-	67,67,67	1.33	10 (14%)	81,81,81	1.53	13 (16%)
34	HEC	V	201	17	50,50,50	1.41	4 (8%)	68,82,82	1.38	15 (22%)
22	CLA	c	511	3	69,73,73	1.20	8 (11%)	82,113,113	1.45	7 (8%)
24	BCR	H	102	-	41,41,41	0.98	1 (2%)	56,56,56	1.36	7 (12%)
31	STE	D	413	-	19,19,19	0.70	0	19,19,19	0.99	0
24	BCR	c	515	-	41,41,41	1.11	2 (4%)	56,56,56	1.18	4 (7%)
22	CLA	B	604	2	69,73,73	1.19	6 (8%)	82,113,113	1.65	14 (17%)
22	CLA	B	607	35	69,73,73	1.16	8 (11%)	82,113,113	1.40	9 (10%)
22	CLA	b	602	2	69,73,73	1.48	9 (13%)	82,113,113	1.33	11 (13%)
34	HEC	v	201	17	50,50,50	1.40	6 (12%)	68,82,82	1.35	7 (10%)
22	CLA	c	514	3	69,73,73	1.52	10 (14%)	82,113,113	1.16	10 (12%)
31	STE	B	623	-	13,13,19	0.64	0	13,13,19	1.31	2 (15%)
22	CLA	b	601	35	69,73,73	1.42	8 (11%)	82,113,113	1.34	9 (10%)
27	LMG	c	523	-	49,49,55	1.06	5 (10%)	57,57,63	1.30	5 (8%)
28	SQD	f	102	-	39,41,54	1.11	4 (10%)	49,52,65	1.79	10 (20%)
22	CLA	B	610	35	69,73,73	1.38	11 (15%)	82,113,113	1.37	14 (17%)
22	CLA	c	507	3	69,73,73	1.32	10 (14%)	82,113,113	1.25	11 (13%)
22	CLA	a	410	35	69,73,73	1.43	7 (10%)	82,113,113	1.40	9 (10%)
22	CLA	c	510	3	69,73,73	1.19	6 (8%)	82,113,113	1.64	9 (10%)
22	CLA	C	501	3	69,73,73	1.52	12 (17%)	82,113,113	1.45	11 (13%)
24	BCR	b	619	-	41,41,41	1.12	2 (4%)	56,56,56	1.30	9 (16%)
29	DGD	C	515	-	63,63,67	1.46	10 (15%)	77,77,81	1.45	12 (15%)
22	CLA	B	603	2	69,73,73	1.27	6 (8%)	82,113,113	1.43	13 (15%)
31	STE	b	625	-	9,9,19	0.53	0	8,8,19	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	STE	a	414	-	11,11,19	0.84	1 (9%)	11,11,19	1.24	1 (9%)
22	CLA	A	405	1	58,62,73	1.46	10 (17%)	68,99,113	1.42	8 (11%)
27	LMG	b	621	-	51,51,55	1.02	4 (7%)	59,59,63	1.43	10 (16%)
22	CLA	b	614	2	69,73,73	1.17	9 (13%)	82,113,113	1.15	6 (7%)
24	BCR	K	103	-	41,41,41	1.10	2 (4%)	56,56,56	1.33	7 (12%)
31	STE	I	101	-	14,14,19	0.56	0	13,13,19	0.45	0
26	PL9	d	406	-	55,55,55	1.58	10 (18%)	68,69,69	1.80	15 (22%)

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
31	STE	M	102	-	-	6/12/12/17	-
28	SQD	L	101	-	-	24/44/64/69	0/1/1/1
33	LHG	D	412	-	-	20/53/53/53	-
22	CLA	c	509	3	-	5/38/114/115	-
33	LHG	D	410	-	-	21/51/51/53	-
24	BCR	F	101	-	-	6/29/63/63	0/2/2/2
22	CLA	b	608	2	-	5/39/115/115	-
31	STE	a	413	-	-	5/7/7/17	-
22	CLA	H	101	35	-	19/39/115/115	-
27	LMG	b	623	-	-	27/50/70/70	0/1/1/1
22	CLA	C	510	3	-	6/39/115/115	-
23	PHO	D	401	-	-	1/37/103/103	0/5/6/6
24	BCR	k	101	-	-	10/29/63/63	0/2/2/2
26	PL9	D	406	-	-	12/53/73/73	0/1/1/1
24	BCR	C	514	-	-	6/29/63/63	0/2/2/2
31	STE	H	104	-	-	9/15/15/17	-
22	CLA	C	503	3	-	7/39/115/115	-
28	SQD	a	411	-	-	22/49/69/69	0/1/1/1
22	CLA	A	403	35	-	15/39/115/115	-
27	LMG	A	410	-	-	18/43/63/70	0/1/1/1
27	LMG	D	407	-	-	16/46/66/70	0/1/1/1
31	STE	d	412	-	-	7/14/14/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	C	506	3	-	7/39/115/115	-
31	STE	B	626	-	-	8/13/13/17	-
29	DGD	c	519	-	-	17/51/91/95	0/2/2/2
22	CLA	d	403	4	-	12/39/115/115	-
22	CLA	a	405	1	-	5/39/115/115	-
22	CLA	C	504	35	-	6/32/108/115	-
31	STE	m	102	-	-	5/9/9/17	-
33	LHG	D	409	-	-	26/53/53/53	-
27	LMG	a	415	-	-	31/50/70/70	0/1/1/1
22	CLA	C	508	3	-	6/39/115/115	-
33	LHG	e	101	-	-	22/46/46/53	-
24	BCR	K	101	-	-	9/29/63/63	0/2/2/2
31	STE	B	624	-	-	5/9/9/17	-
28	SQD	a	412	-	-	15/37/37/69	-
31	STE	C	518	-	-	6/9/9/17	-
28	SQD	A	412	-	-	17/39/39/69	-
33	LHG	d	409	-	-	12/43/43/53	-
22	CLA	c	512	3	-	8/39/115/115	-
22	CLA	D	403	4	-	5/39/115/115	-
23	PHO	a	404	-	-	6/37/103/103	0/5/6/6
31	STE	b	620	-	-	7/13/13/17	-
33	LHG	l	101	-	-	17/53/53/53	-
22	CLA	b	612	2	-	5/39/115/115	-
22	CLA	D	404	35	-	8/39/115/115	-
27	LMG	c	522	-	-	25/43/63/70	0/1/1/1
31	STE	B	601	-	-	4/9/9/17	-
27	LMG	d	410	-	-	11/39/59/70	0/1/1/1
24	BCR	K	102	-	-	6/29/63/63	0/2/2/2
22	CLA	a	402	1	-	6/39/115/115	-
34	HEC	f	101	6,5	1/1/7/7	9/14/54/54	-
22	CLA	A	402	1	-	3/39/115/115	-
26	PL9	A	409	-	-	22/53/73/73	0/1/1/1
22	CLA	C	502	3	-	9/39/115/115	-
29	DGD	h	102	-	-	18/51/91/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	c	506	3	-	8/39/115/115	-
22	CLA	c	504	3	-	10/39/115/115	-
29	DGD	C	516	-	-	22/51/91/95	0/2/2/2
31	STE	m	101	-	-	7/15/15/17	-
22	CLA	C	511	3	-	7/39/115/115	-
24	BCR	d	405	-	-	6/29/63/63	0/2/2/2
28	SQD	D	408	-	-	12/28/48/69	0/1/1/1
22	CLA	B	611	2	-	2/39/115/115	-
33	LHG	L	102	-	-	18/53/53/53	-
31	STE	b	627	-	-	9/17/17/17	-
22	CLA	C	509	3	-	10/39/115/115	-
24	BCR	B	618	-	-	8/29/63/63	0/2/2/2
31	STE	c	501	-	-	3/9/9/17	-
24	BCR	t	101	-	-	4/29/63/63	0/2/2/2
24	BCR	b	618	-	-	5/29/63/63	0/2/2/2
22	CLA	B	616	2	-	12/33/109/115	-
22	CLA	D	405	4	-	6/39/115/115	-
22	CLA	b	607	35	-	13/39/115/115	-
22	CLA	B	614	2	-	8/39/115/115	-
24	BCR	T	101	-	-	14/29/63/63	0/2/2/2
24	BCR	b	617	-	-	8/29/63/63	0/2/2/2
24	BCR	a	406	-	-	3/29/63/63	0/2/2/2
23	PHO	d	401	-	-	5/37/103/103	0/5/6/6
22	CLA	C	505	3	-	10/39/115/115	-
31	STE	E	102	-	-	4/9/9/17	-
31	STE	T	102	-	-	7/12/12/17	-
31	STE	Z	101	-	-	2/5/5/17	-
31	STE	C	520	-	-	2/9/9/17	-
31	STE	B	625	-	-	15/15/15/17	-
22	CLA	c	503	3	-	7/39/115/115	-
26	PL9	a	409	-	-	21/53/73/73	0/1/1/1
22	CLA	c	513	3	-	19/39/115/115	-
22	CLA	C	512	3	-	14/39/115/115	-
22	CLA	B	606	2	-	11/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	C	513	3	-	16/39/115/115	-
22	CLA	c	508	35	-	10/39/115/115	-
22	CLA	B	608	2	-	4/39/115/115	-
23	PHO	A	404	-	-	3/37/103/103	0/5/6/6
22	CLA	B	605	2	-	9/39/115/115	-
22	CLA	b	609	2	-	10/39/115/115	-
22	CLA	B	613	2	-	12/39/115/115	-
22	CLA	B	612	2	-	11/39/115/115	-
27	LMG	M	101	-	-	27/46/66/70	0/1/1/1
33	LHG	d	407	-	-	14/53/53/53	-
24	BCR	B	617	-	-	7/29/63/63	0/2/2/2
24	BCR	B	619	-	-	6/29/63/63	0/2/2/2
24	BCR	k	102	-	-	3/29/63/63	0/2/2/2
33	LHG	E	101	-	-	29/53/53/53	-
22	CLA	B	602	2	-	7/39/115/115	-
22	CLA	b	611	2	-	8/39/115/115	-
22	CLA	C	507	35	-	5/39/115/115	-
22	CLA	a	403	35	-	10/39/115/115	-
31	STE	c	521	-	-	11/17/17/17	-
24	BCR	c	516	-	-	5/29/63/63	0/2/2/2
27	LMG	Y	101	-	-	24/43/63/70	0/1/1/1
22	CLA	b	610	35	-	2/39/115/115	-
22	CLA	b	615	2	-	8/39/115/115	-
31	STE	B	620	-	-	9/14/14/17	-
22	CLA	d	404	4	-	3/39/115/115	-
22	CLA	b	613	2	-	7/39/115/115	-
31	STE	b	626	-	-	5/11/11/17	-
31	STE	d	411	-	-	6/13/13/17	-
22	CLA	b	603	2	-	6/39/115/115	-
22	CLA	b	606	2	-	5/39/115/115	-
27	LMG	B	621	-	-	10/22/22/70	-
28	SQD	A	411	-	-	9/47/67/69	0/1/1/1
31	STE	M	103	-	-	3/7/7/17	-
31	STE	b	624	-	-	10/17/17/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	B	609	2	-	7/39/115/115	-
34	HEC	F	102	6,5	1/1/7/7	6/14/54/54	-
22	CLA	c	505	35	-	4/33/109/115	-
29	DGD	c	518	-	-	21/51/91/95	0/2/2/2
31	STE	b	622	-	-	8/17/17/17	-
22	CLA	B	615	2	-	10/39/115/115	-
24	BCR	A	406	-	-	9/29/63/63	0/2/2/2
31	STE	j	101	-	-	4/9/9/17	-
24	BCR	h	101	-	-	4/29/63/63	0/2/2/2
31	STE	C	519	-	-	5/13/13/17	-
27	LMG	D	411	-	-	15/33/33/70	-
28	SQD	B	622	-	-	19/49/69/69	0/1/1/1
31	STE	J	101	-	-	5/9/9/17	-
29	DGD	c	517	-	-	23/51/91/95	0/2/2/2
22	CLA	b	605	2	-	6/39/115/115	-
29	DGD	C	517	-	-	14/51/91/95	0/2/2/2
31	STE	d	413	-	-	11/17/17/17	-
27	LMG	c	520	-	-	10/31/51/70	0/1/1/1
29	DGD	H	103	-	-	17/51/91/95	0/2/2/2
31	STE	B	627	-	-	5/12/12/17	-
22	CLA	b	604	2	-	6/39/115/115	-
22	CLA	c	502	3	-	1/39/115/115	-
33	LHG	d	408	-	-	19/53/53/53	-
22	CLA	b	616	2	-	9/33/109/115	-
29	DGD	A	413	-	-	28/55/95/95	0/2/2/2
34	HEC	V	201	17	1/1/7/7	4/14/54/54	-
22	CLA	c	511	3	-	6/39/115/115	-
24	BCR	H	102	-	-	5/29/63/63	0/2/2/2
31	STE	D	413	-	-	9/17/17/17	-
24	BCR	c	515	-	-	10/29/63/63	0/2/2/2
22	CLA	B	604	2	-	10/39/115/115	-
22	CLA	B	607	35	-	5/39/115/115	-
34	HEC	v	201	17	1/1/7/7	5/14/54/54	-
22	CLA	b	602	2	-	5/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	c	514	3	-	8/39/115/115	-
31	STE	B	623	-	-	3/11/11/17	-
22	CLA	b	601	35	-	16/39/115/115	-
27	LMG	c	523	-	-	23/44/64/70	0/1/1/1
28	SQD	f	102	-	-	15/36/56/69	0/1/1/1
22	CLA	B	610	35	-	5/39/115/115	-
22	CLA	c	507	3	-	13/39/115/115	-
22	CLA	a	410	35	-	4/39/115/115	-
22	CLA	c	510	3	-	15/39/115/115	-
22	CLA	C	501	3	-	3/39/115/115	-
24	BCR	b	619	-	-	8/29/63/63	0/2/2/2
29	DGD	C	515	-	-	22/51/91/95	0/2/2/2
22	CLA	B	603	2	-	12/39/115/115	-
31	STE	b	625	-	-	6/7/7/17	-
31	STE	a	414	-	-	2/9/9/17	-
22	CLA	A	405	1	-	3/26/102/115	-
27	LMG	b	621	-	-	15/46/66/70	0/1/1/1
22	CLA	b	614	2	-	15/39/115/115	-
24	BCR	K	103	-	-	6/29/63/63	0/2/2/2
31	STE	I	101	-	-	7/12/12/17	-
26	PL9	d	406	-	-	15/53/73/73	0/1/1/1

The worst 5 of 908 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	506	CLA	MG-ND	-9.62	1.86	2.05
23	d	401	PHO	C1B-C2B	9.55	1.50	1.39
23	a	404	PHO	C1B-C2B	8.80	1.49	1.39
22	b	615	CLA	MG-NA	8.66	2.26	2.06
23	D	401	PHO	C1B-C2B	8.33	1.48	1.39

The worst 5 of 1286 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	L	101	SQD	O6-C1-C2	10.63	124.41	108.27
28	a	411	SQD	O6-C1-C2	10.10	123.61	108.27
22	b	604	CLA	C4A-NA-C1A	9.40	110.97	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	611	CLA	C4A-NA-C1A	9.36	110.95	106.68
22	c	510	CLA	C4A-NA-C1A	9.18	110.87	106.68

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
34	F	102	HEC	NA
34	V	201	HEC	NA
34	f	101	HEC	NA
34	v	201	HEC	NA

5 of 1812 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	A	405	CLA	C2-C3-C5-C6
22	A	405	CLA	C4-C3-C5-C6
22	B	614	CLA	CAD-CBD-CGD-O1D
22	B	614	CLA	CAD-CBD-CGD-O2D
22	C	502	CLA	CAD-CBD-CGD-O2D

There are no ring outliers.

101 monomers are involved in 153 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	D	412	LHG	5	0
24	F	101	BCR	5	0
22	b	608	CLA	1	0
31	a	413	STE	1	0
22	H	101	CLA	2	0
23	D	401	PHO	1	0
28	a	411	SQD	1	0
27	D	407	LMG	1	0
29	c	519	DGD	2	0
22	d	403	CLA	1	0
31	m	102	STE	1	0
33	D	409	LHG	1	0
27	a	415	LMG	2	0
33	e	101	LHG	1	0
24	K	101	BCR	2	0
28	A	412	SQD	2	0
22	c	512	CLA	1	0
22	D	403	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	a	404	PHO	1	0
22	D	404	CLA	2	0
27	c	522	LMG	1	0
24	K	102	BCR	2	0
22	a	402	CLA	3	0
26	A	409	PL9	2	0
22	A	402	CLA	2	0
34	f	101	HEC	5	0
22	C	502	CLA	1	0
22	c	506	CLA	1	0
22	c	504	CLA	3	0
22	C	511	CLA	1	0
24	d	405	BCR	3	0
33	L	102	LHG	1	0
22	C	509	CLA	1	0
24	B	618	BCR	2	0
24	t	101	BCR	3	0
24	b	618	BCR	2	0
22	B	616	CLA	1	0
22	D	405	CLA	3	0
22	B	614	CLA	1	0
24	T	101	BCR	4	0
24	a	406	BCR	2	0
23	d	401	PHO	1	0
31	Z	101	STE	1	0
26	a	409	PL9	3	0
22	C	512	CLA	2	0
22	B	606	CLA	2	0
22	C	513	CLA	2	0
22	c	508	CLA	1	0
22	B	608	CLA	1	0
23	A	404	PHO	1	0
22	B	605	CLA	2	0
22	B	613	CLA	2	0
22	B	612	CLA	1	0
27	M	101	LMG	1	0
33	d	407	LHG	2	0
24	B	617	BCR	2	0
24	B	619	BCR	3	0
24	k	102	BCR	2	0
33	E	101	LHG	1	0
31	c	521	STE	2	0

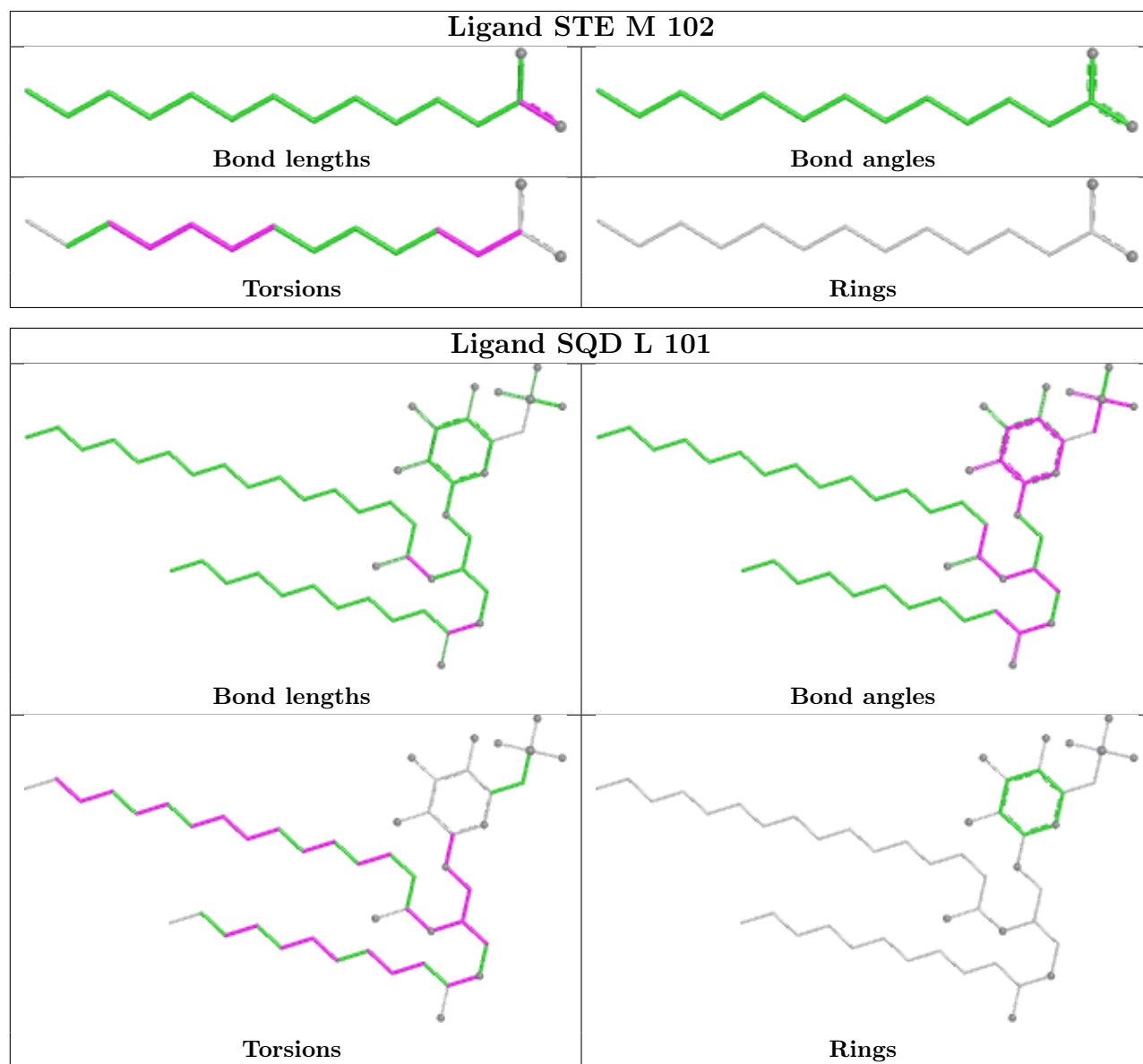
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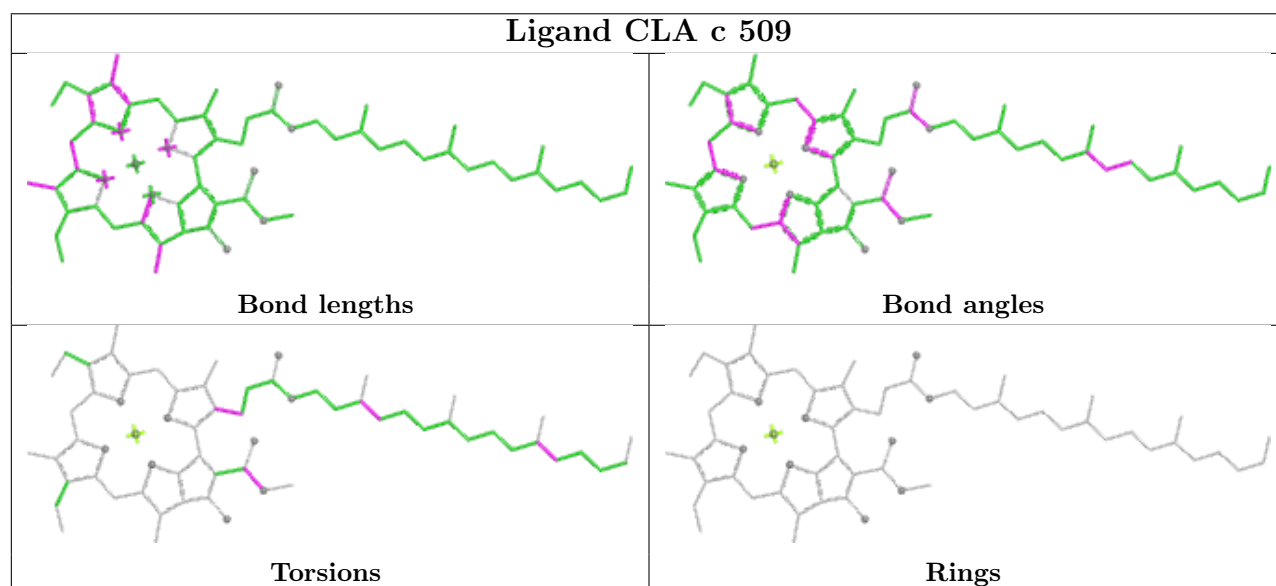
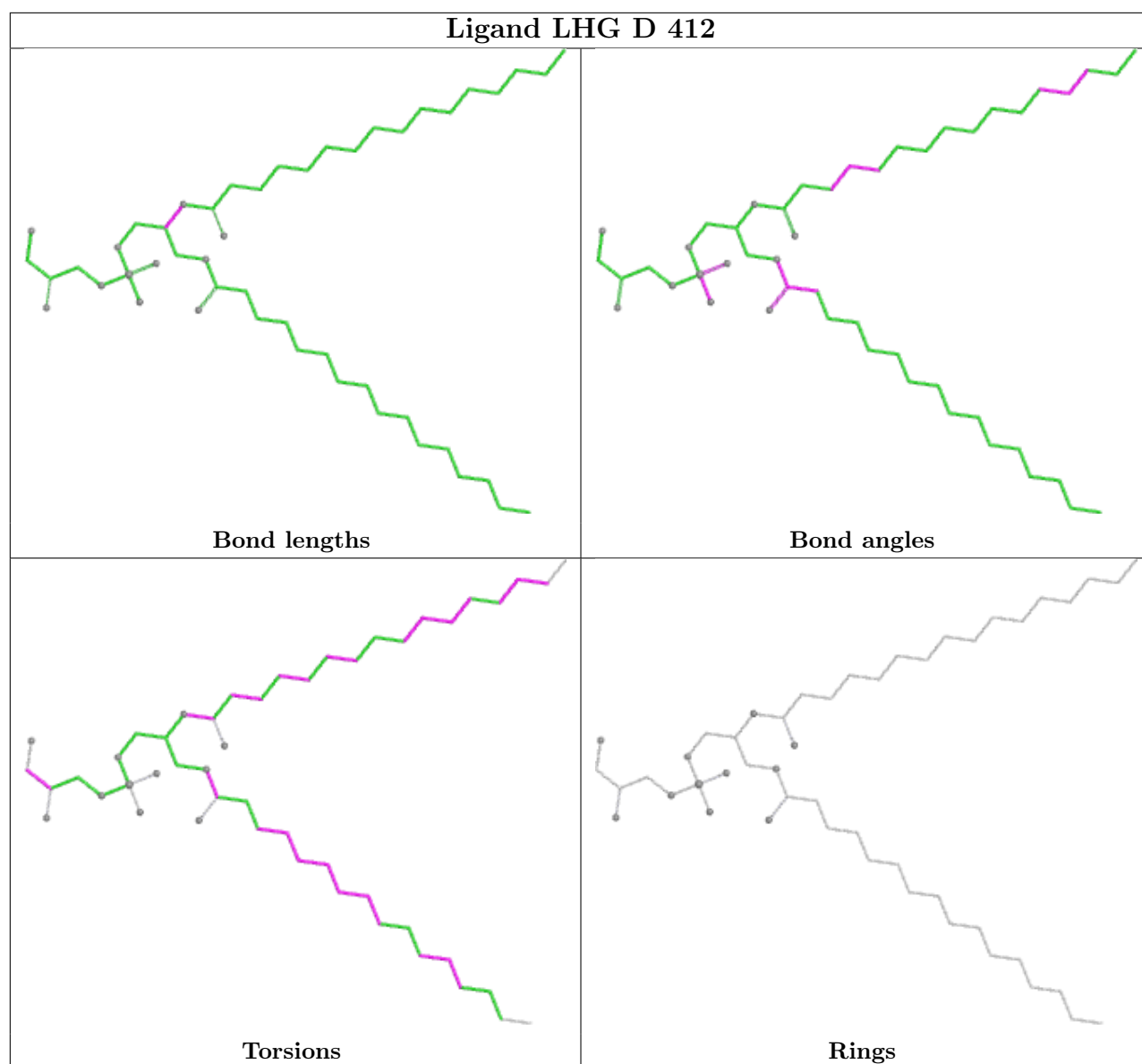
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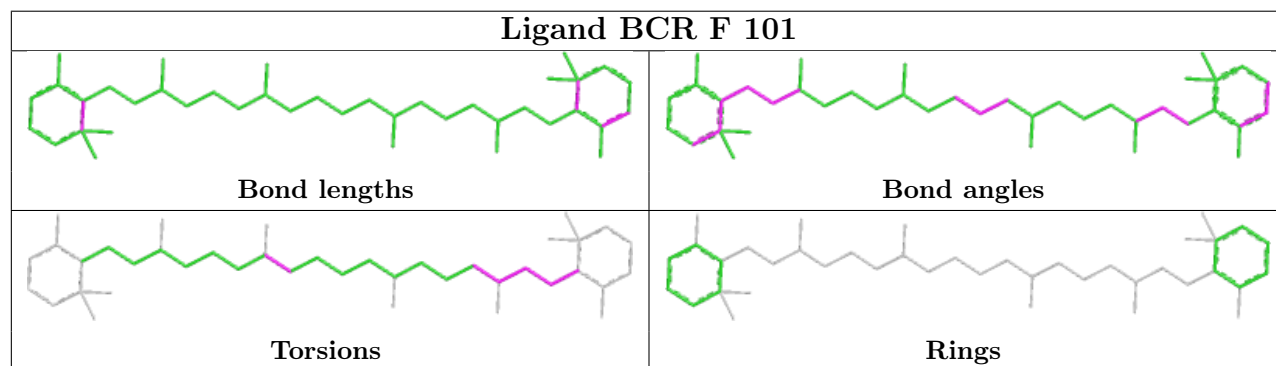
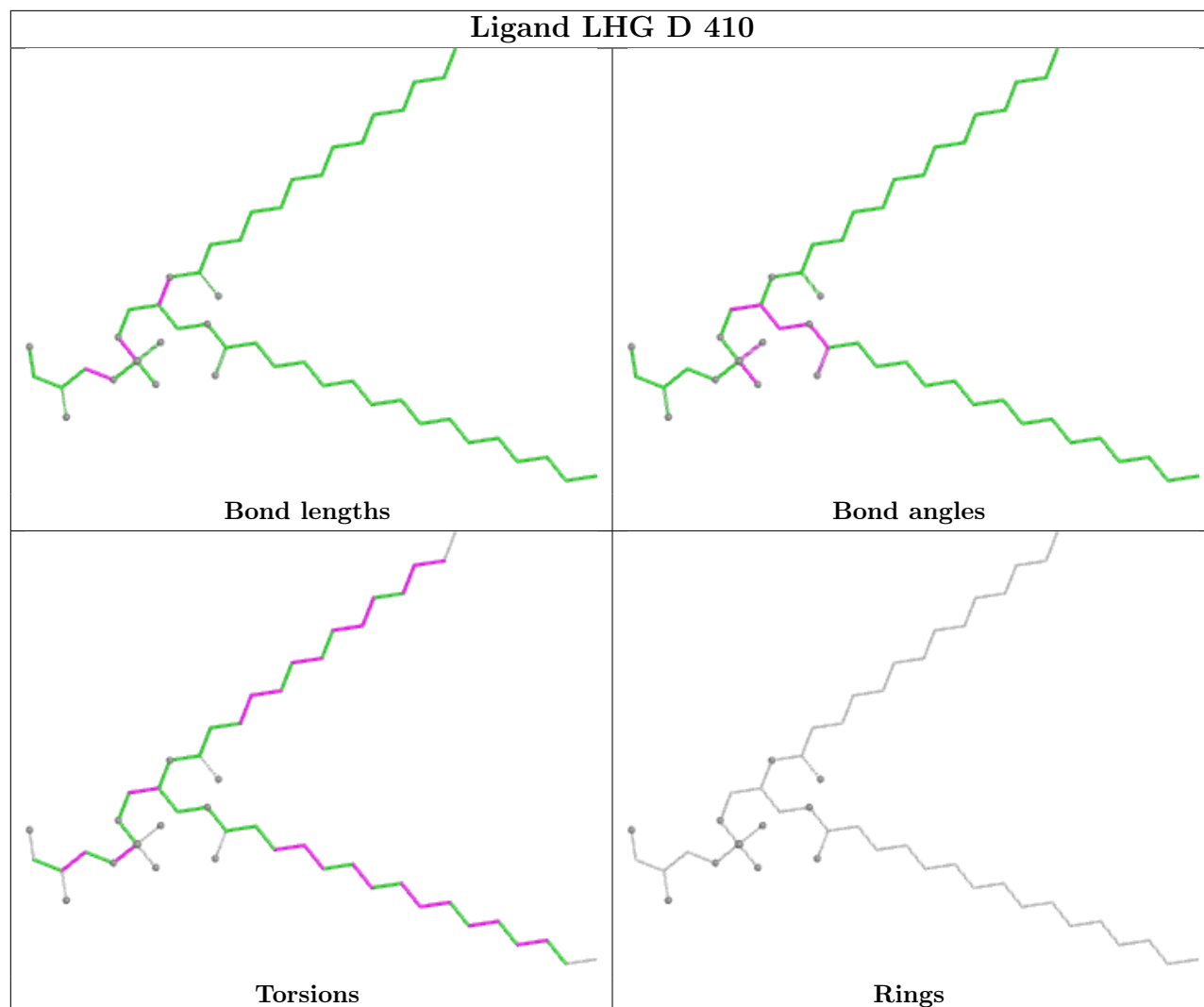
Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	c	516	BCR	3	0
22	b	615	CLA	4	0
31	B	620	STE	1	0
22	b	613	CLA	1	0
22	b	606	CLA	3	0
28	A	411	SQD	1	0
22	B	609	CLA	2	0
34	F	102	HEC	3	0
22	c	505	CLA	1	0
29	c	518	DGD	1	0
31	b	622	STE	2	0
24	A	406	BCR	1	0
24	h	101	BCR	1	0
27	D	411	LMG	3	0
28	B	622	SQD	1	0
22	b	605	CLA	3	0
31	d	413	STE	1	0
29	H	103	DGD	1	0
31	B	627	STE	1	0
22	b	604	CLA	2	0
22	c	502	CLA	2	0
33	d	408	LHG	1	0
22	b	616	CLA	1	0
29	A	413	DGD	1	0
34	V	201	HEC	2	0
22	c	511	CLA	1	0
24	H	102	BCR	3	0
24	c	515	BCR	3	0
22	B	604	CLA	1	0
22	b	602	CLA	1	0
34	v	201	HEC	1	0
22	c	514	CLA	5	0
22	b	601	CLA	1	0
28	f	102	SQD	1	0
22	a	410	CLA	1	0
22	C	501	CLA	2	0
29	C	515	DGD	1	0
22	A	405	CLA	1	0
27	b	621	LMG	1	0
22	b	614	CLA	1	0
26	d	406	PL9	1	0

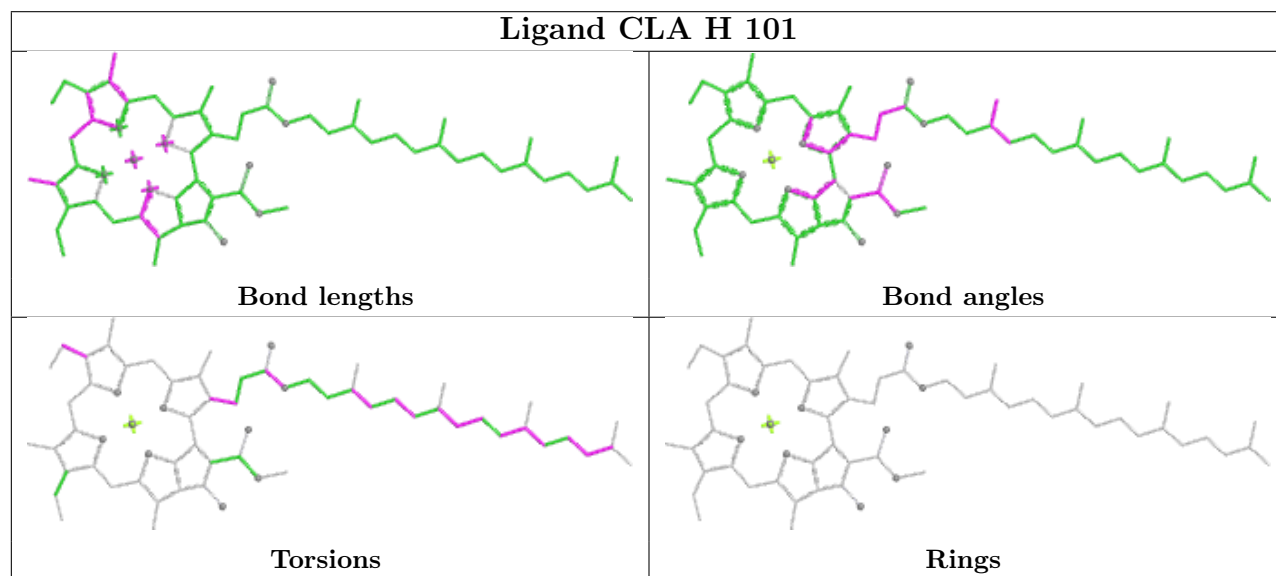
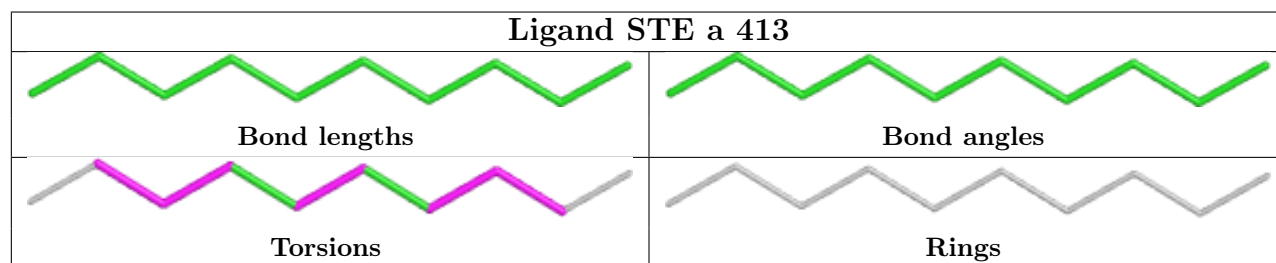
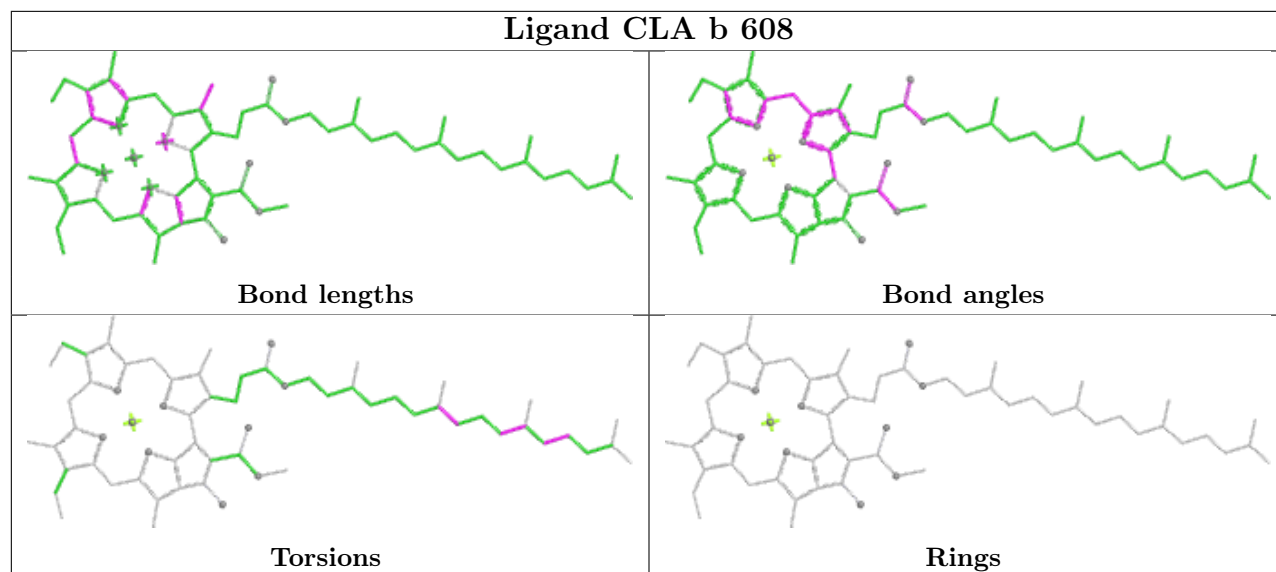
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

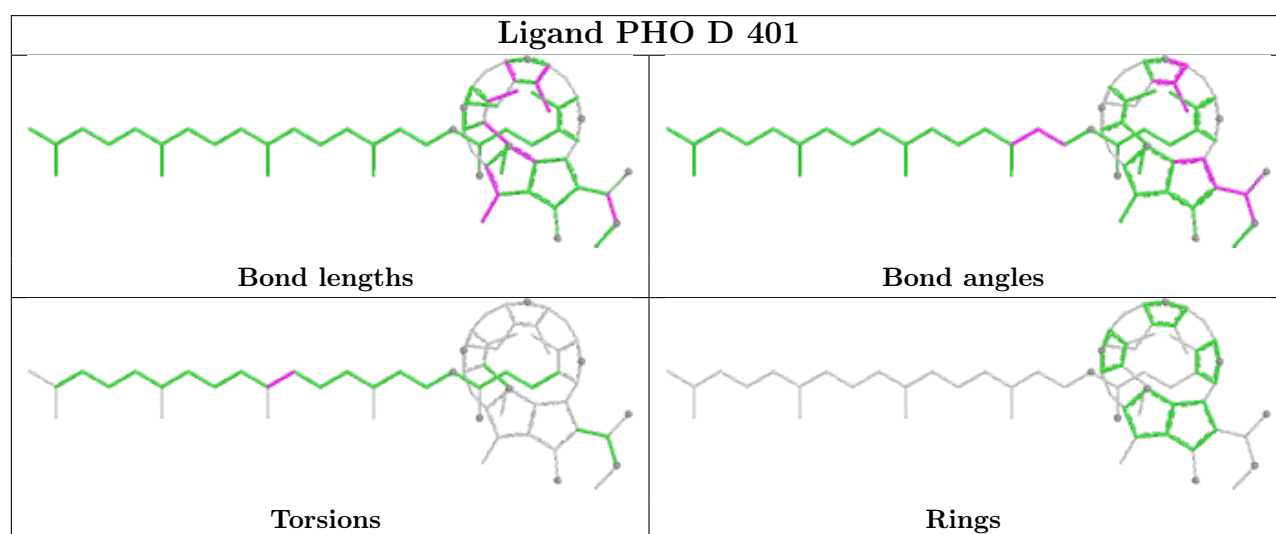
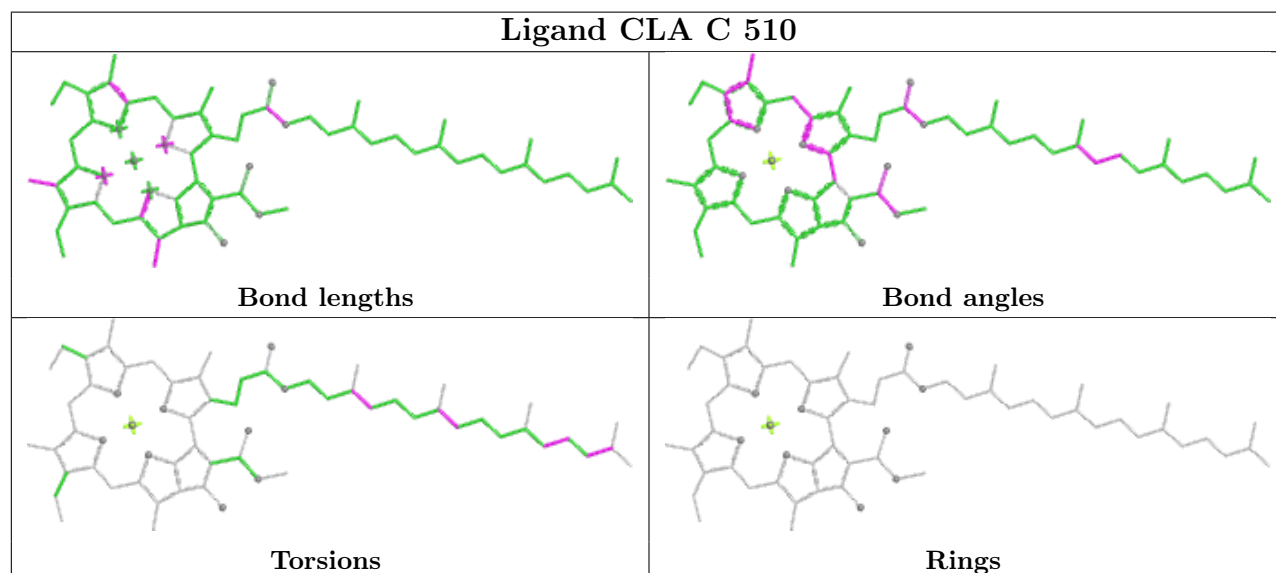
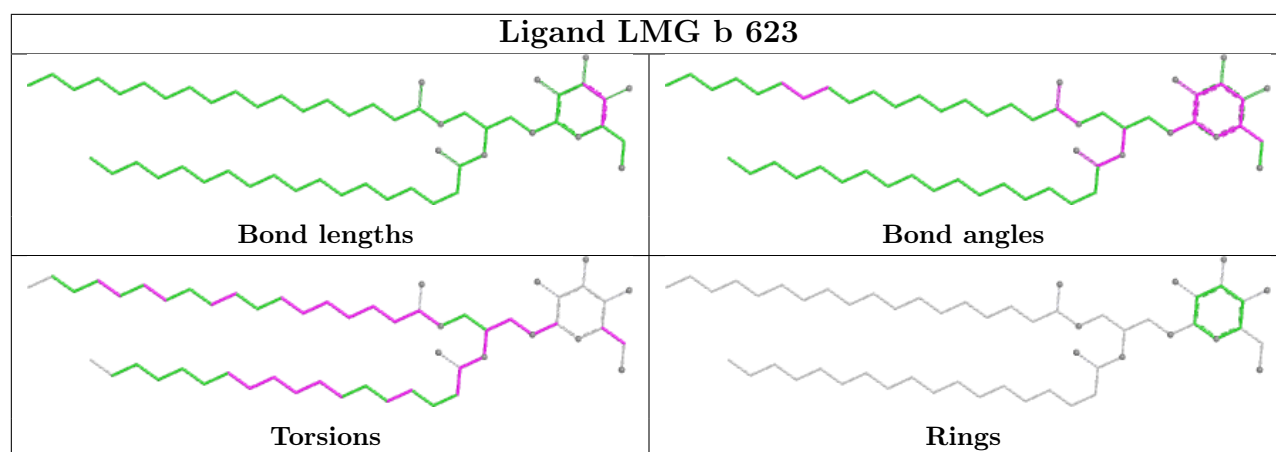
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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.

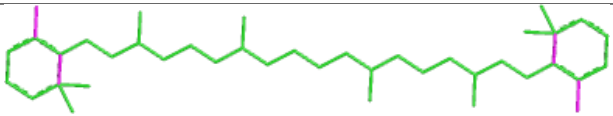
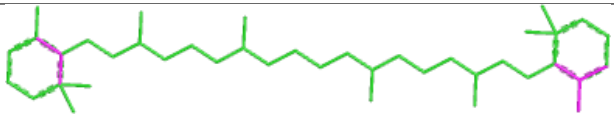
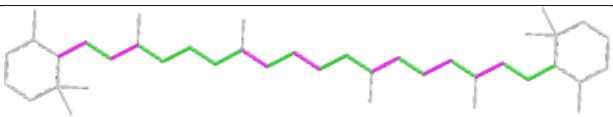
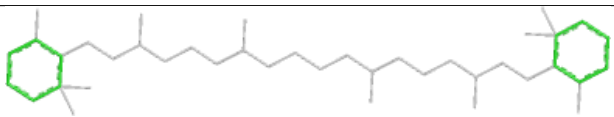




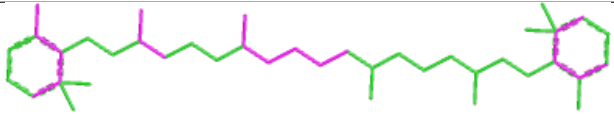
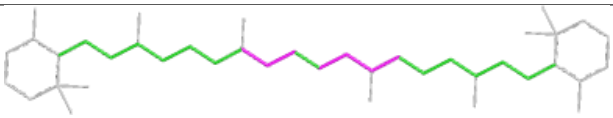
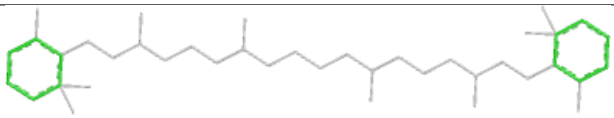




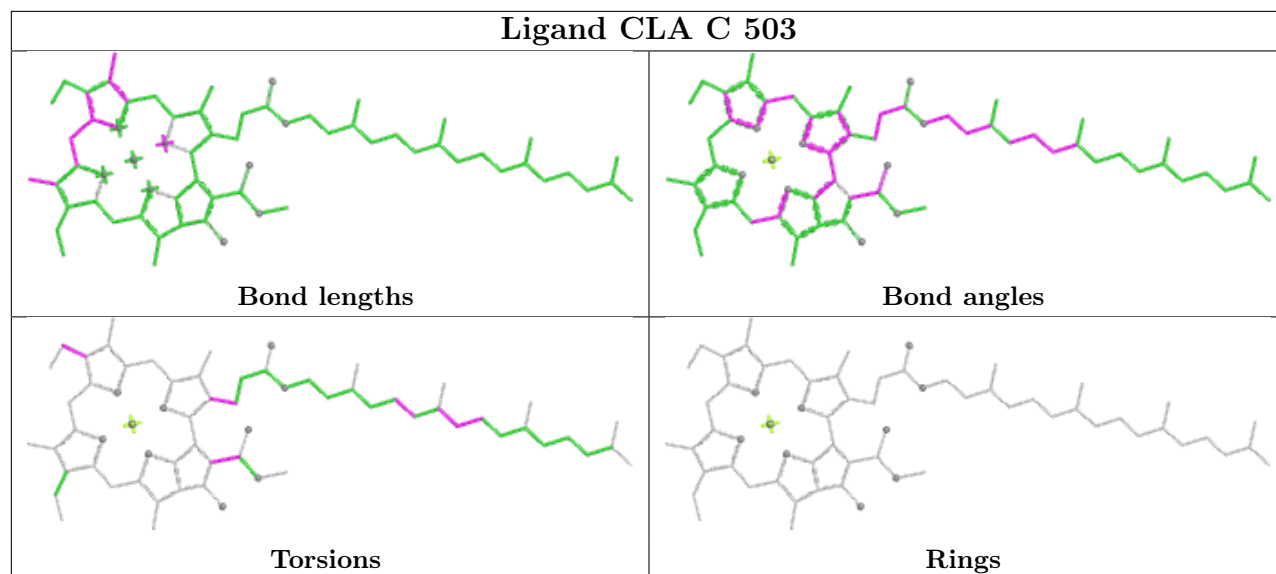
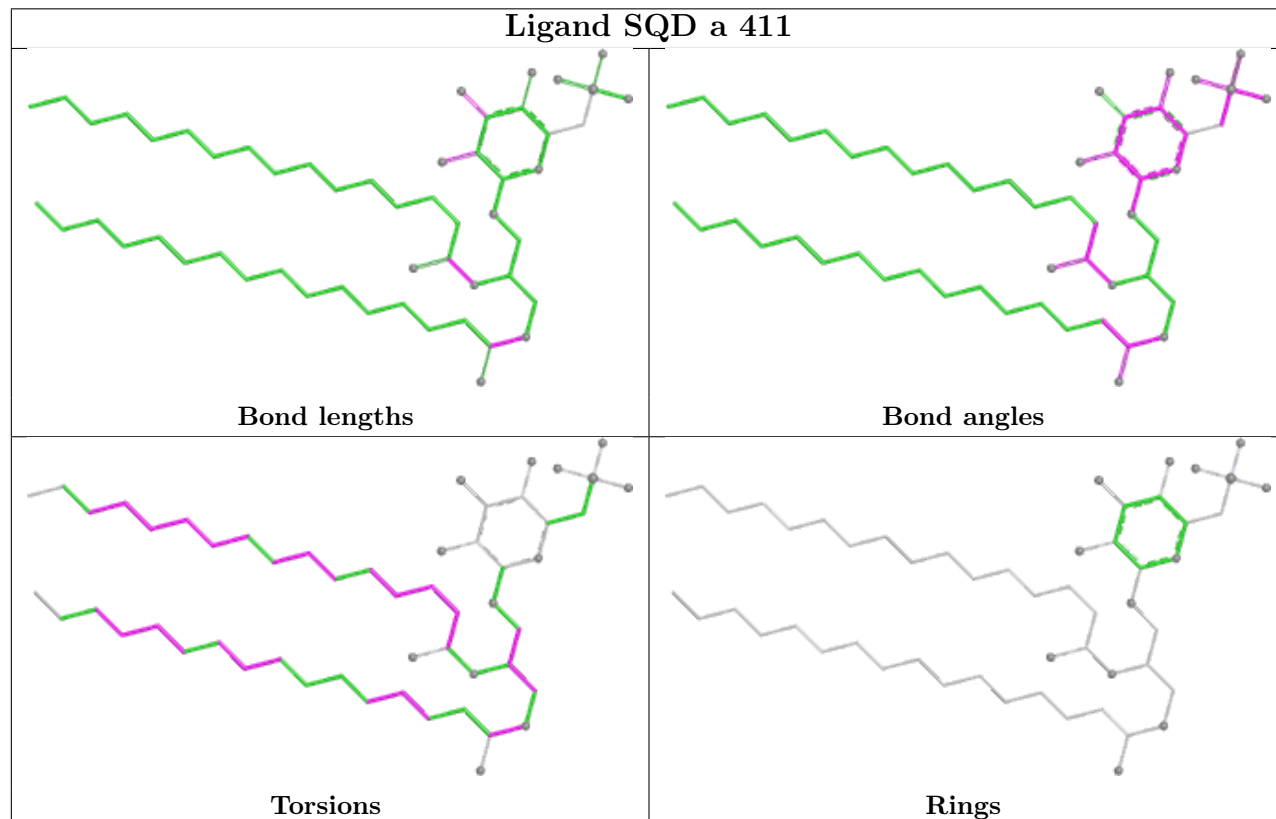


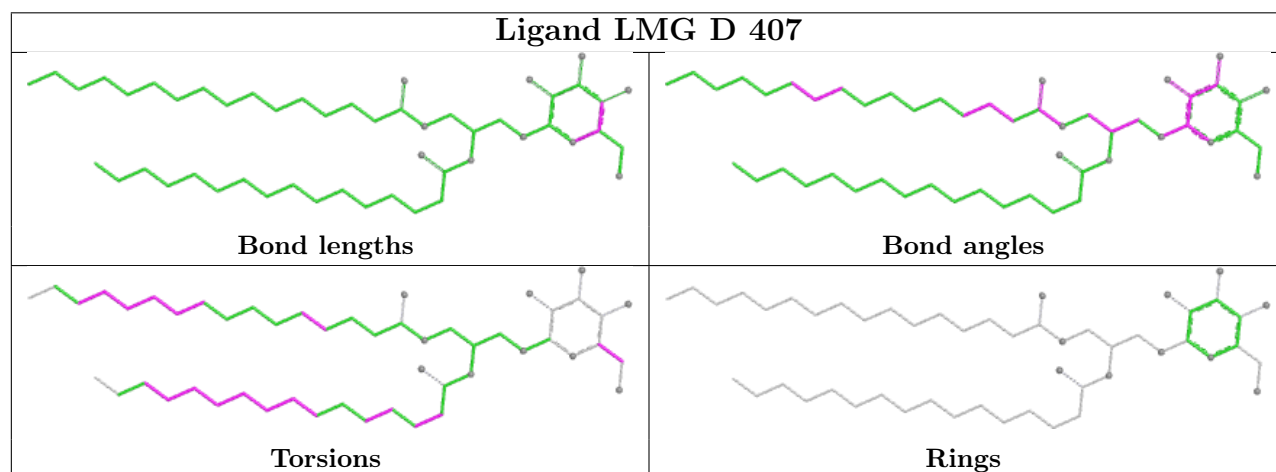
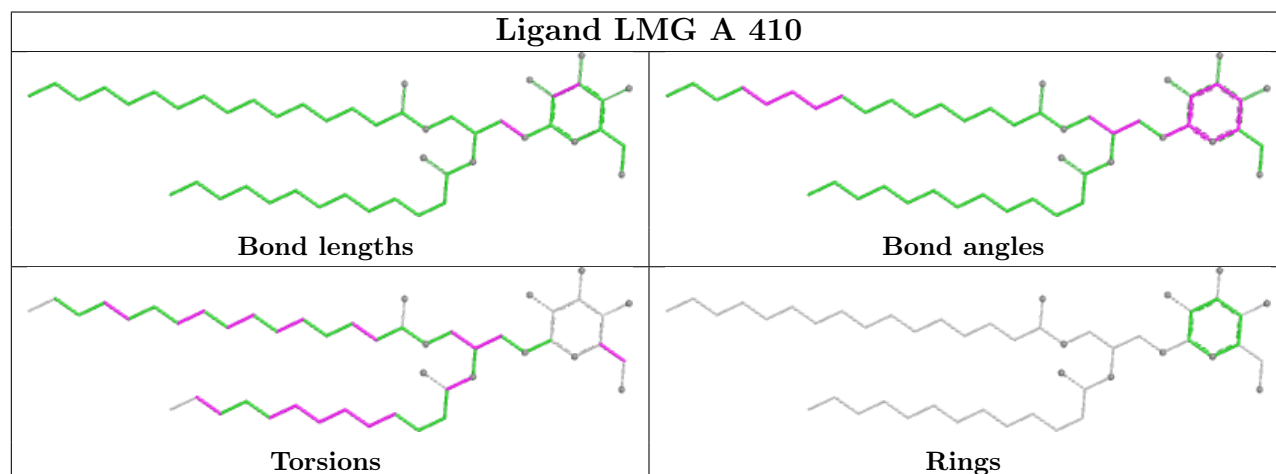
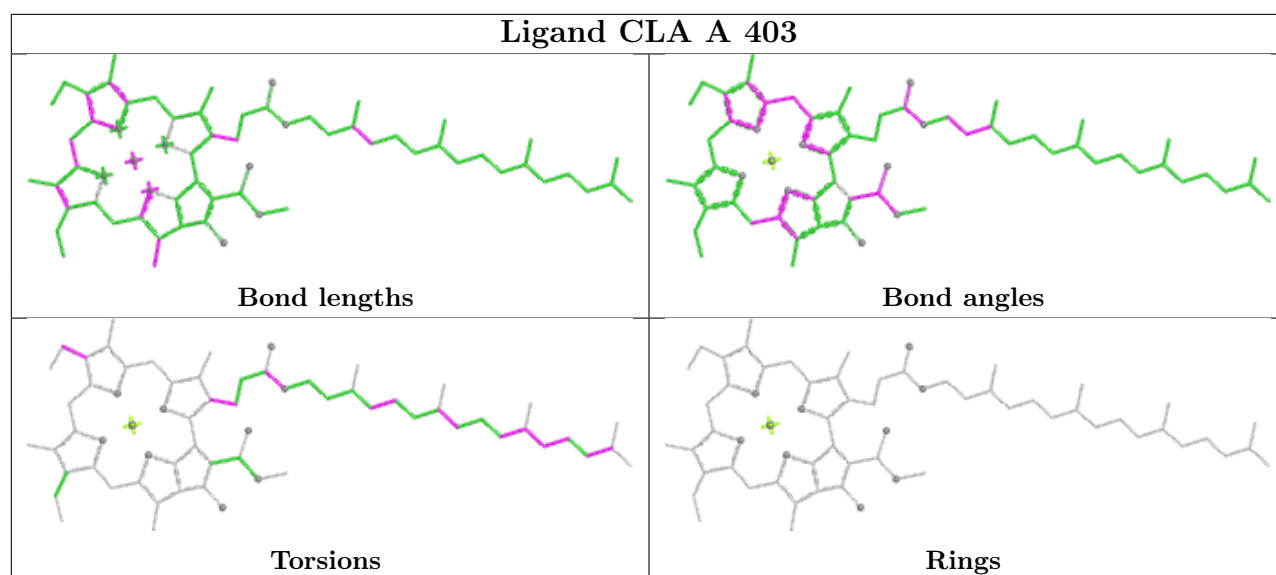
Ligand BCR k 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

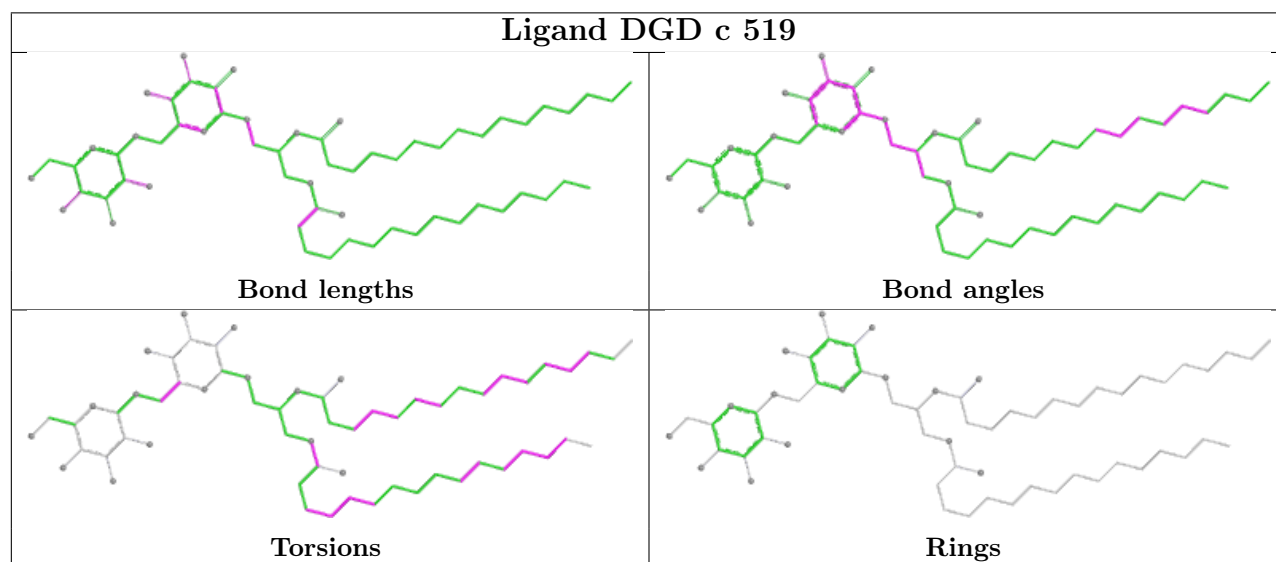
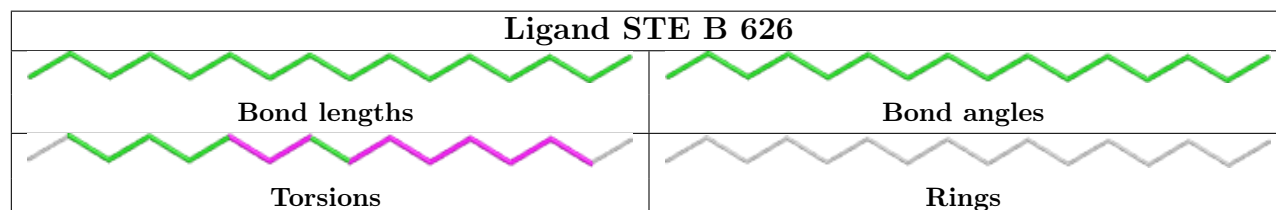
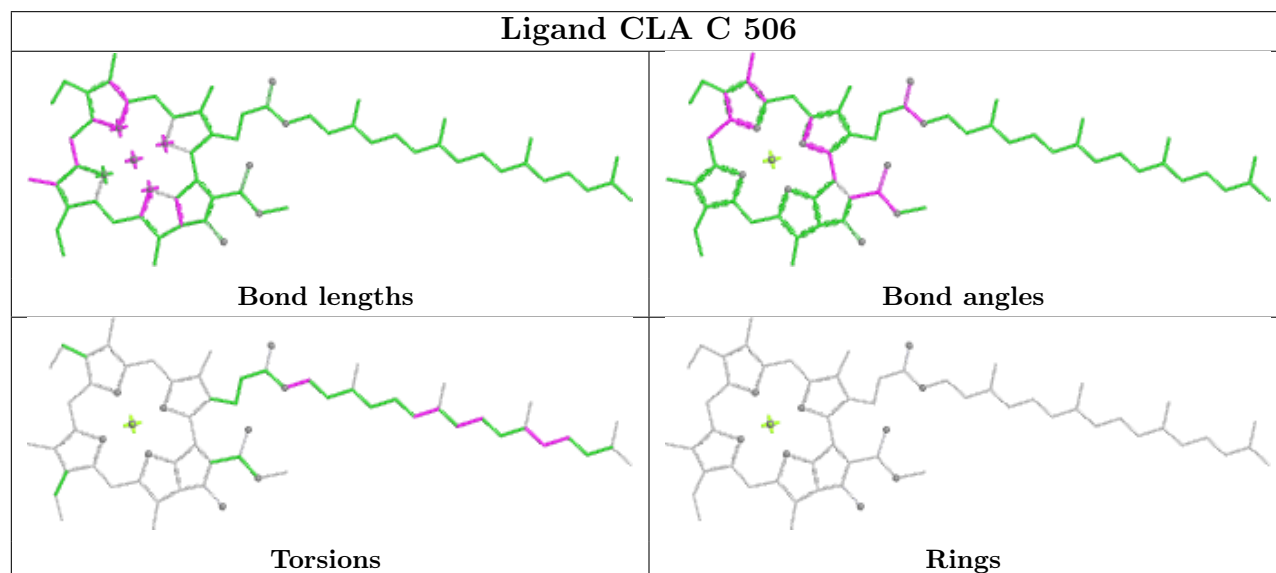
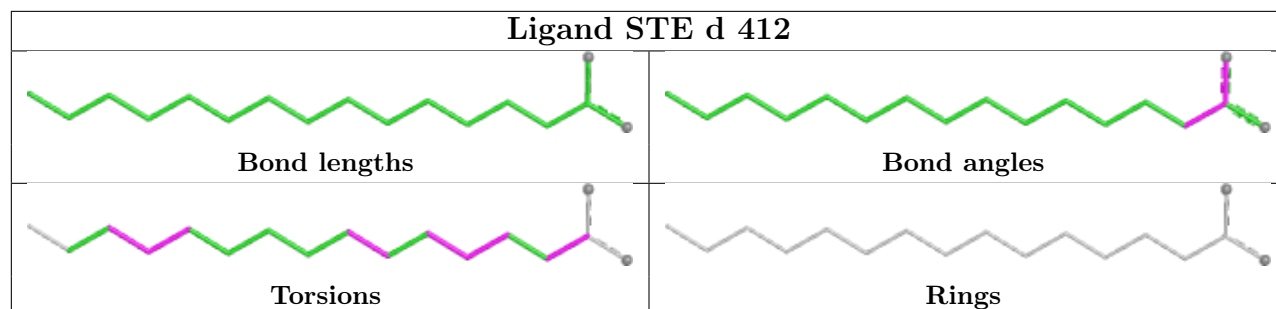
Ligand PL9 D 406	
 Bond lengths	 Bond angles
 Torsions	 Rings

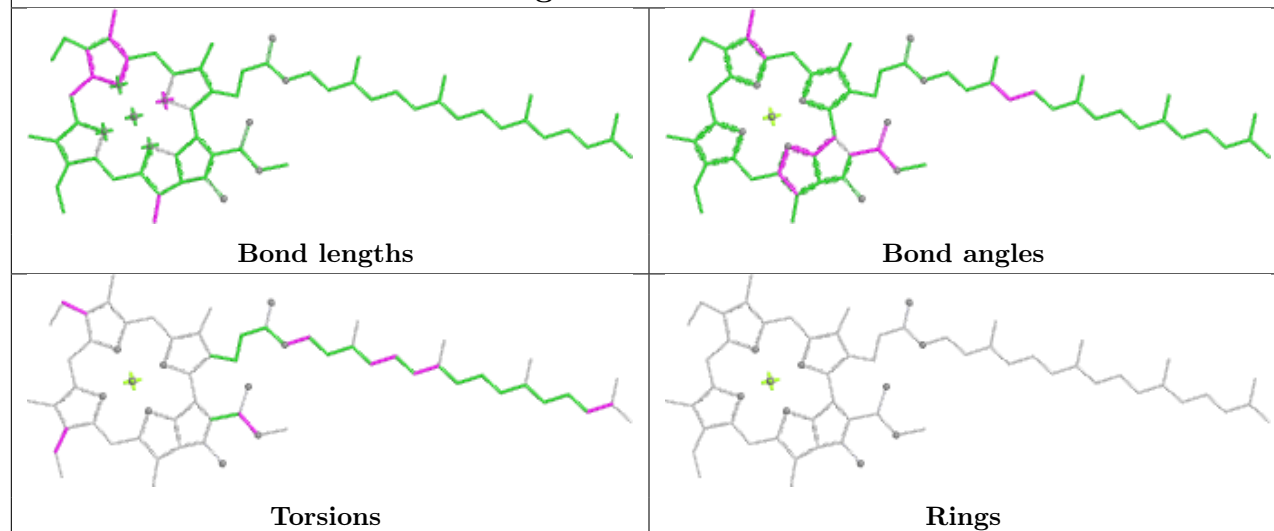
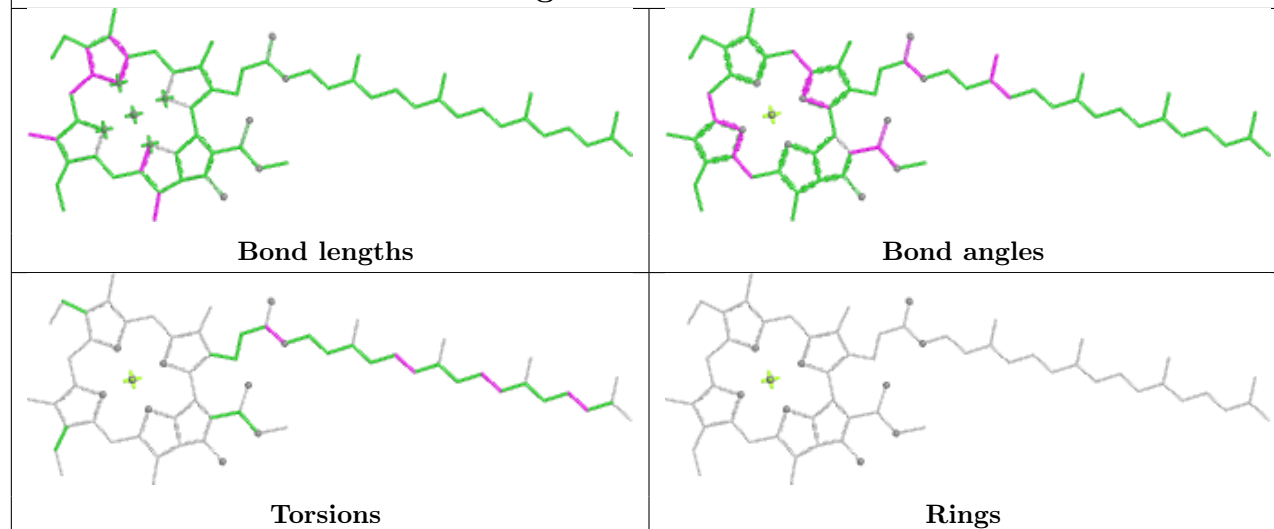
Ligand BCR C 514	
 Bond lengths	 Bond angles
 Torsions	 Rings

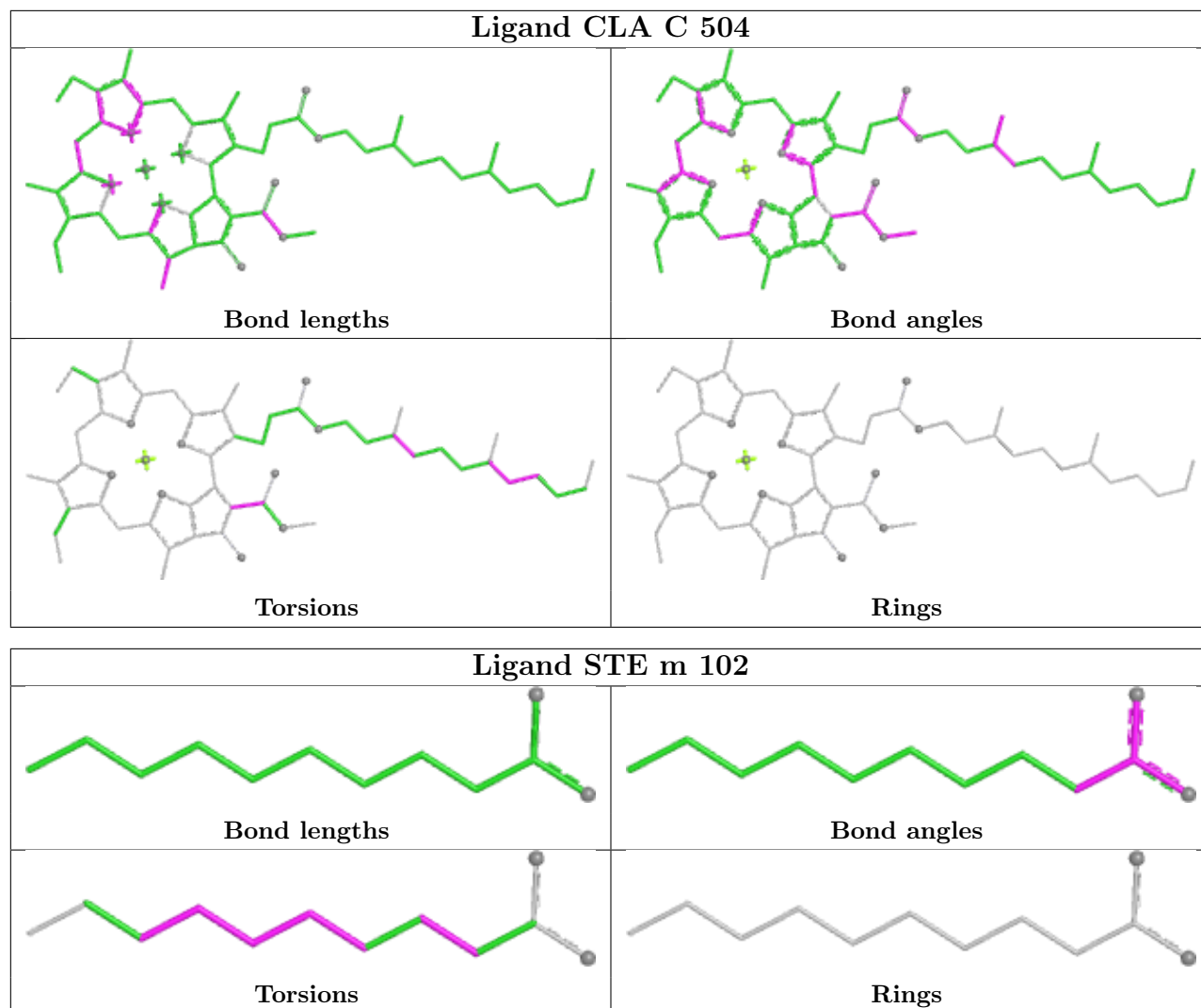
Ligand STE H 104	
 Bond lengths	 Bond angles
 Torsions	 Rings

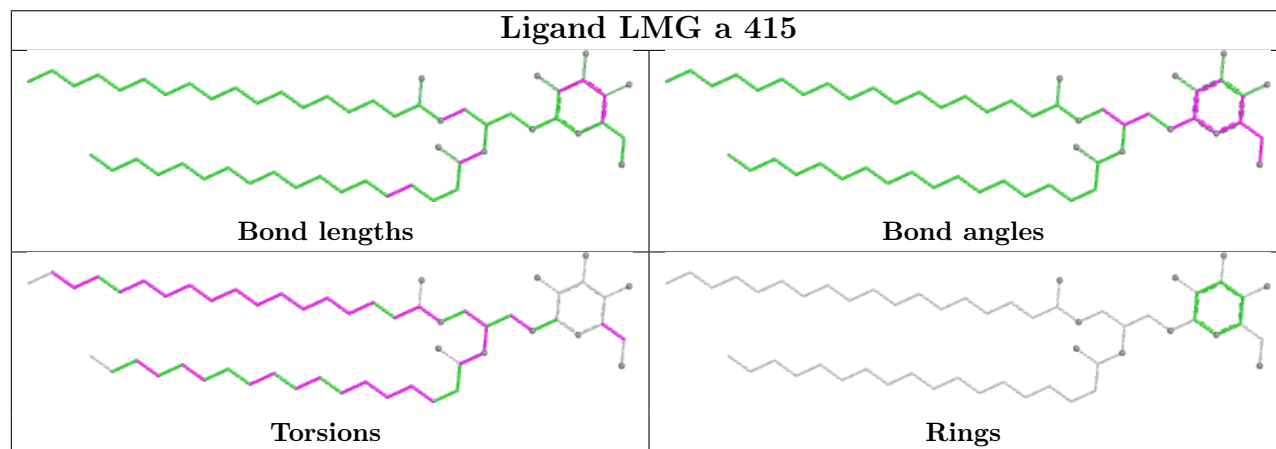
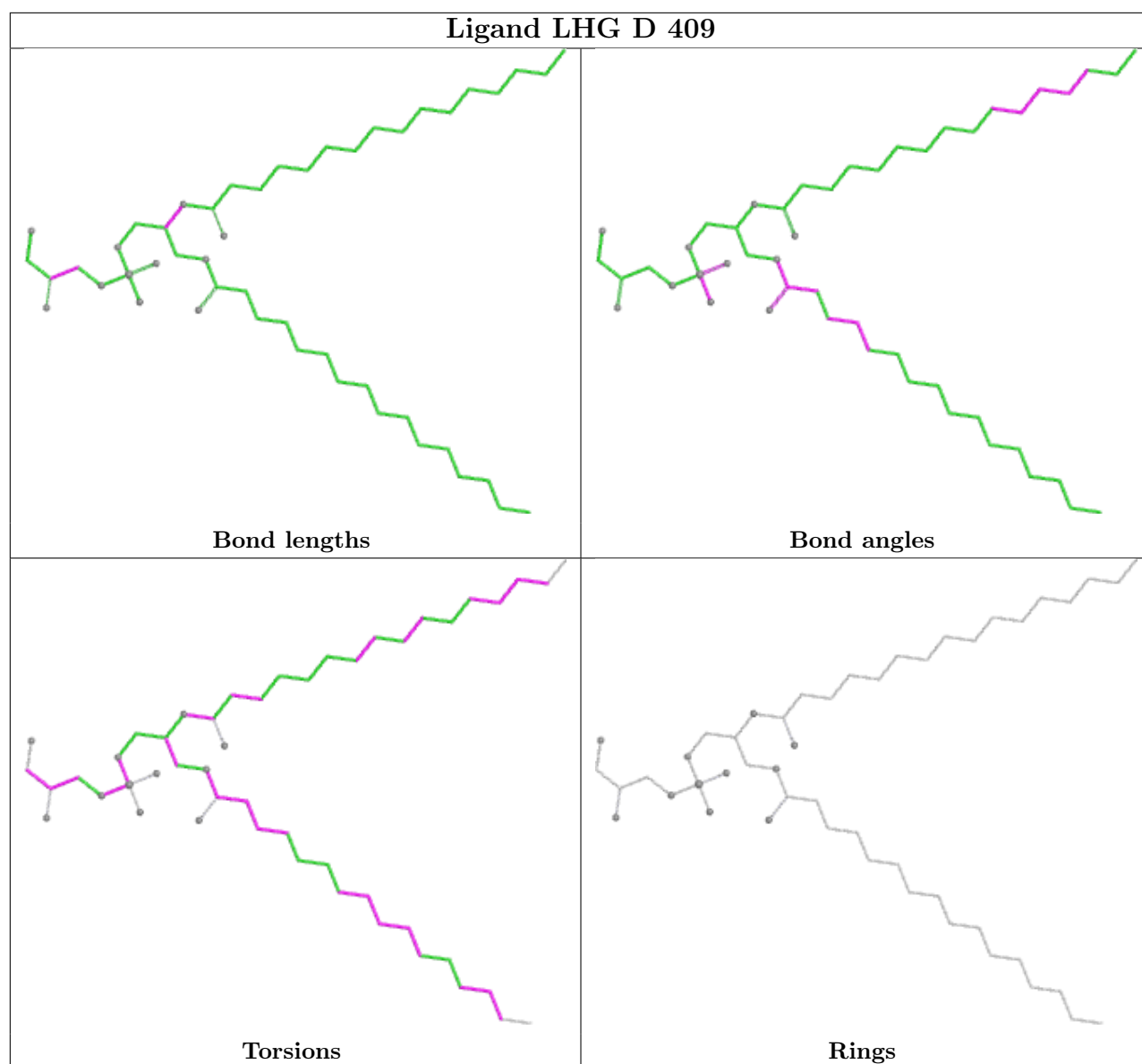
Ligand CLA C 503**Ligand SQD a 411**

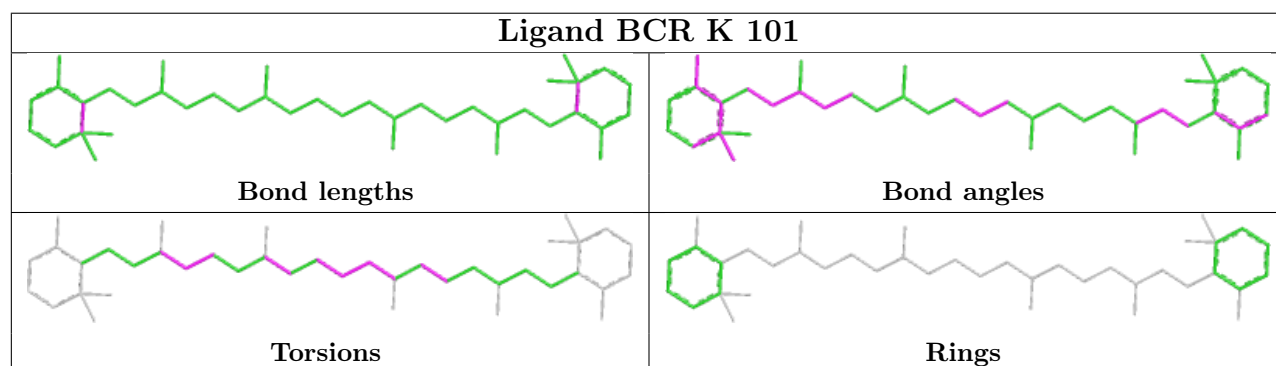
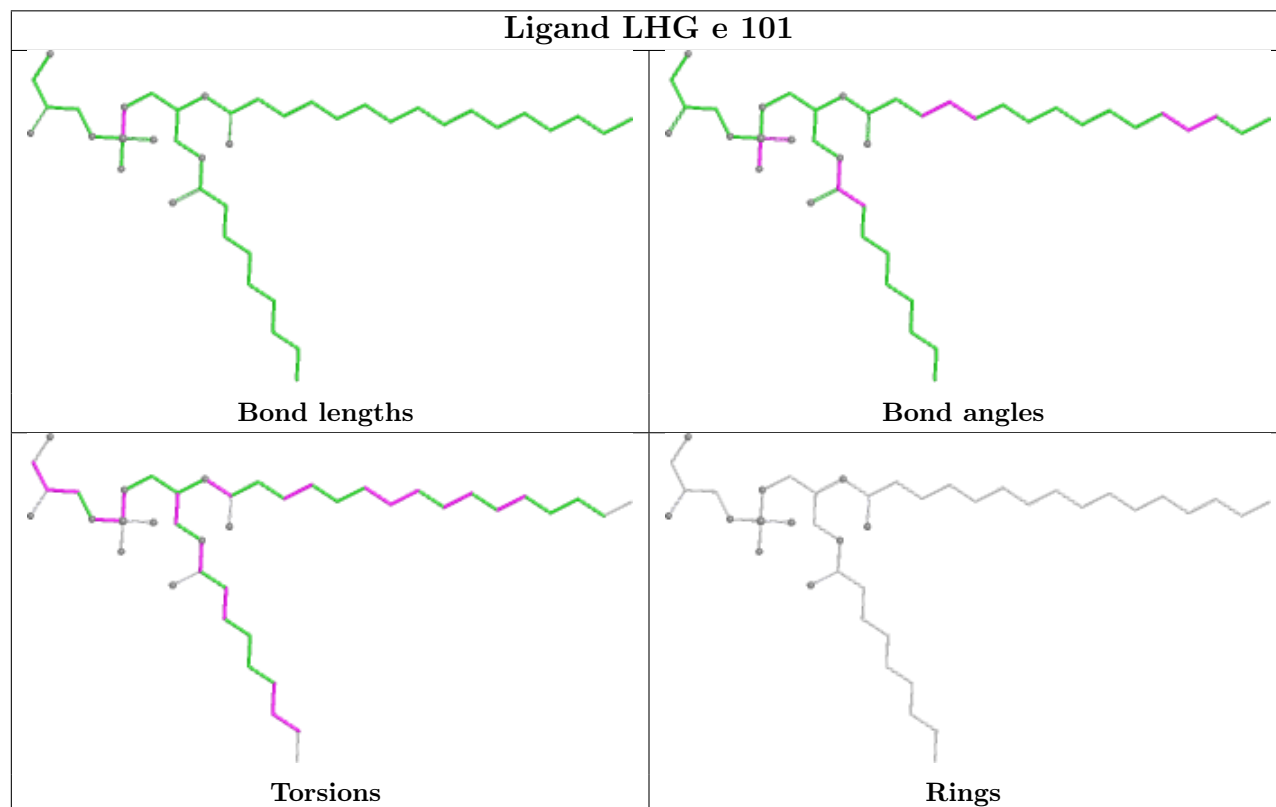
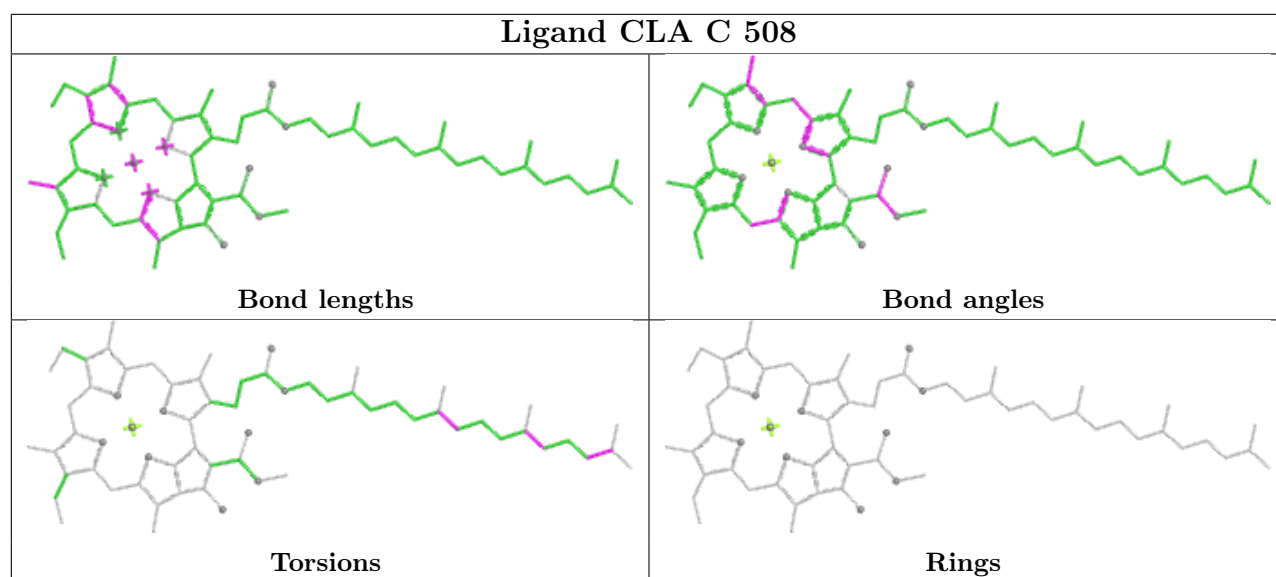


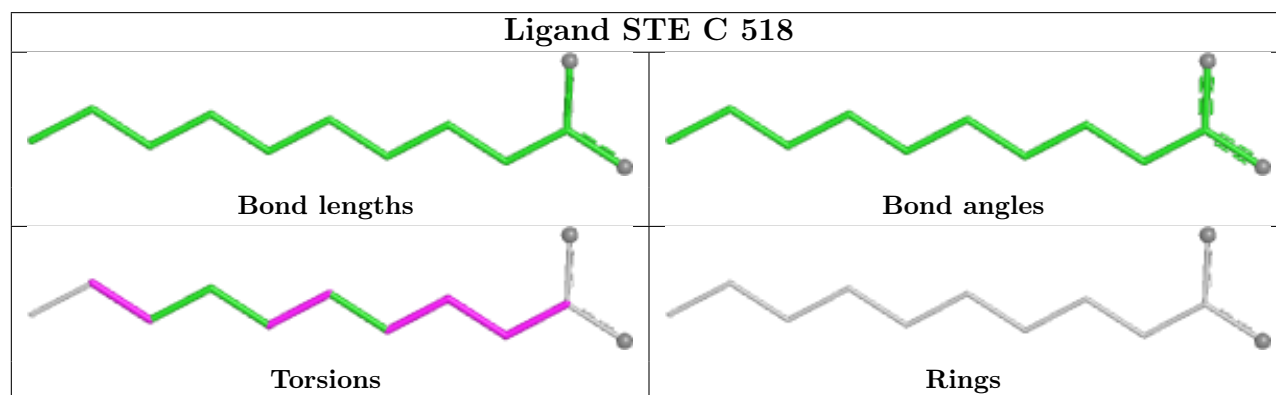
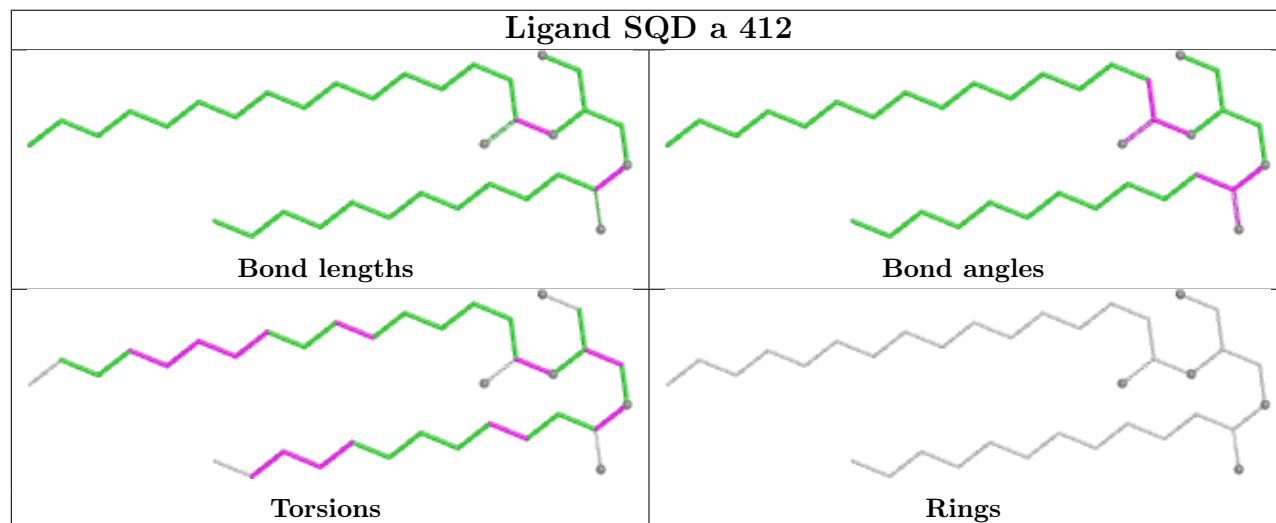
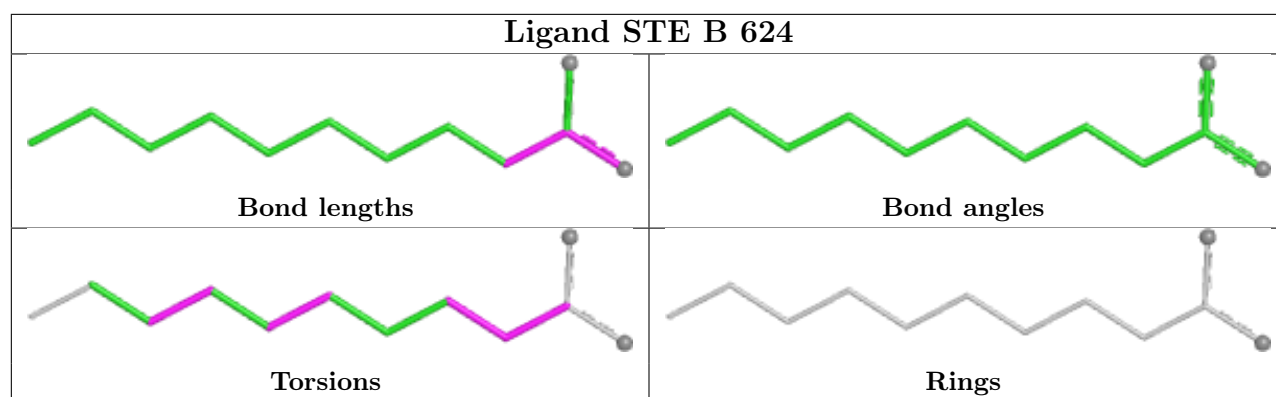


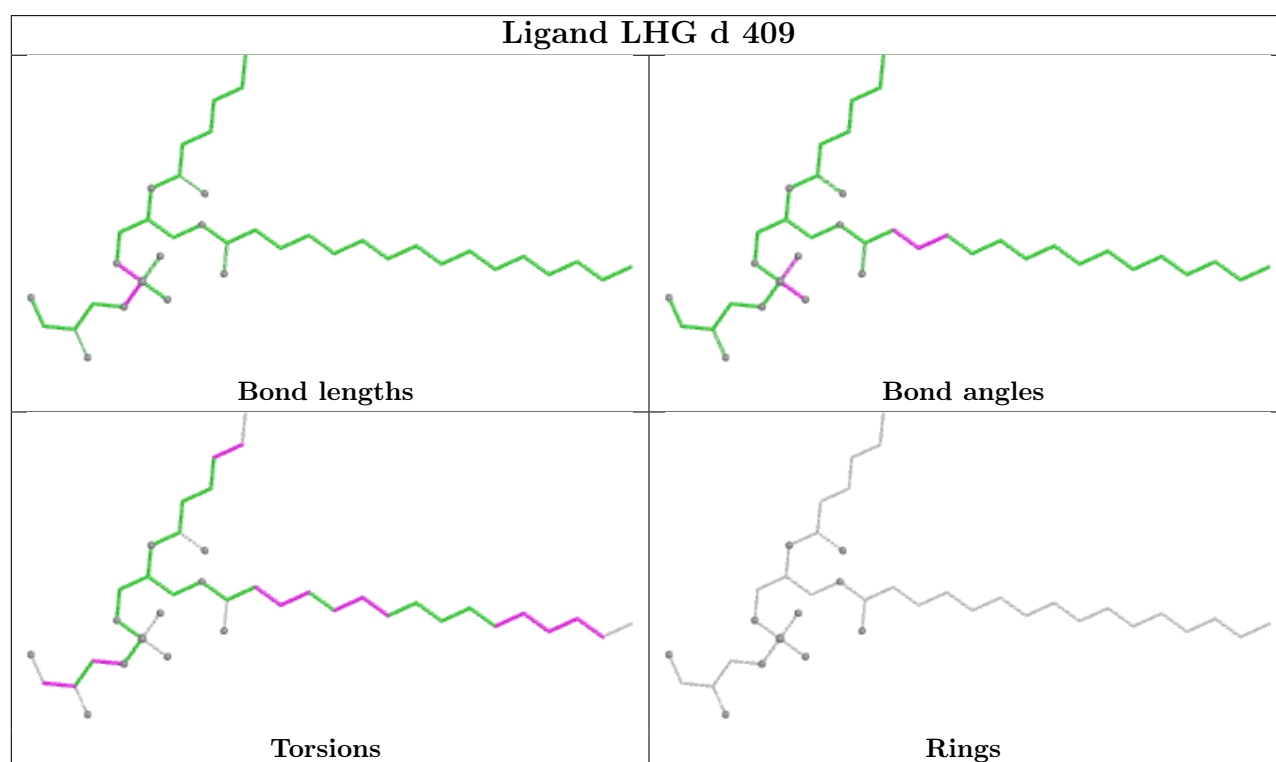
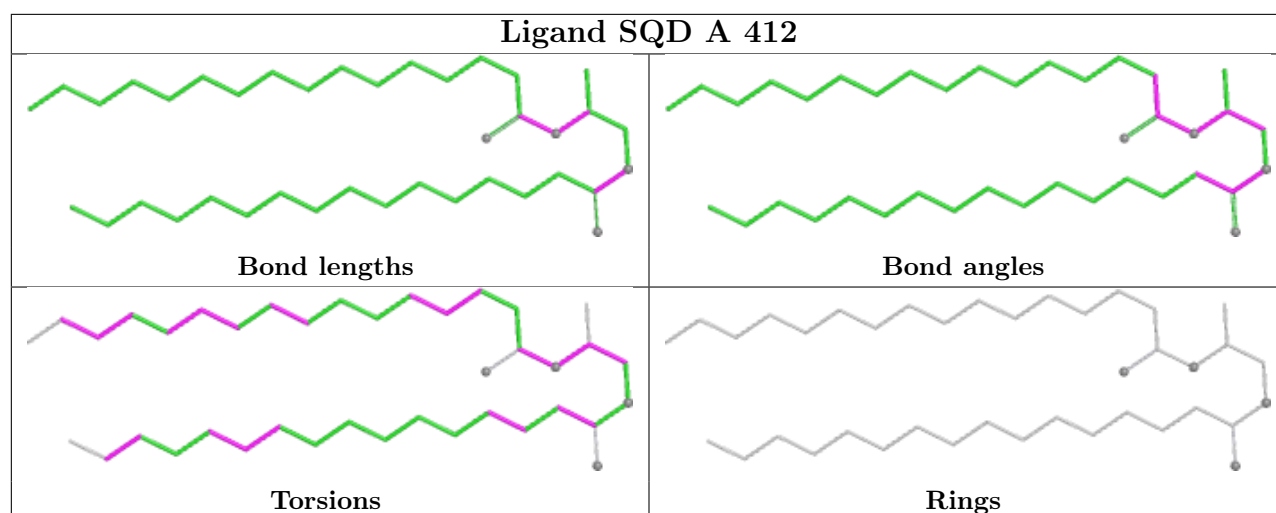
Ligand CLA d 403**Ligand CLA a 405**



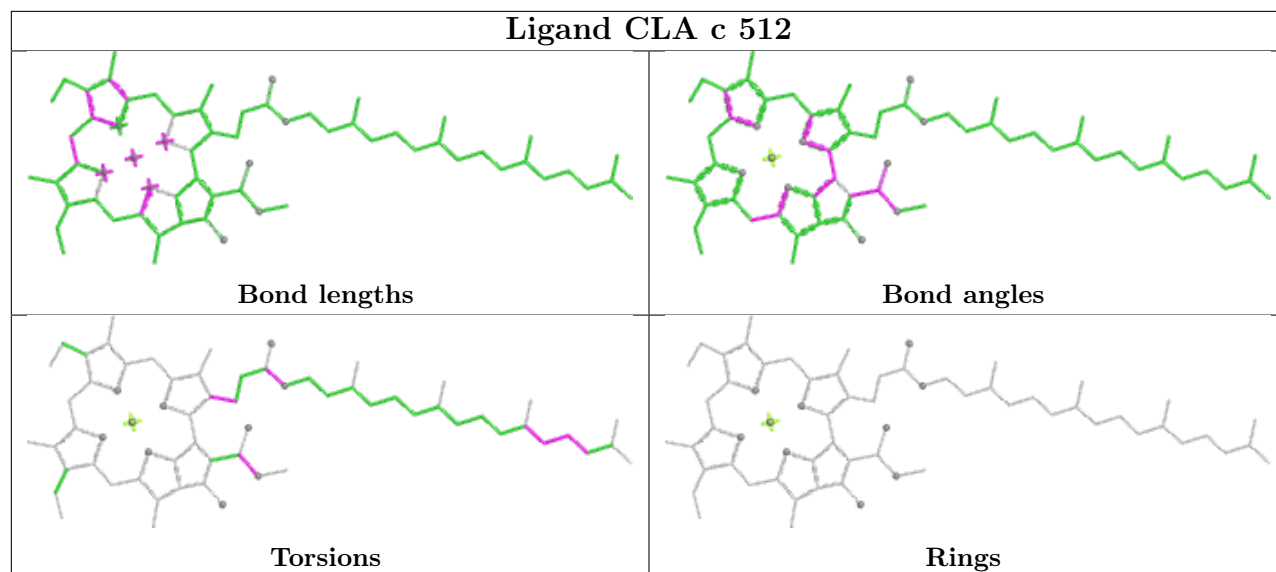




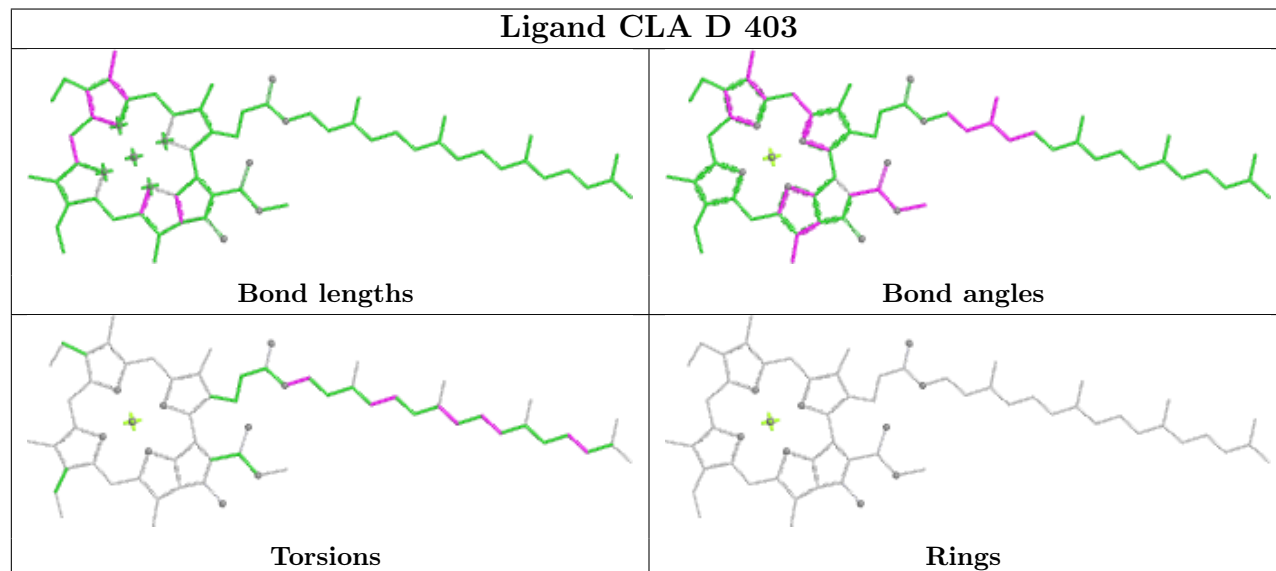




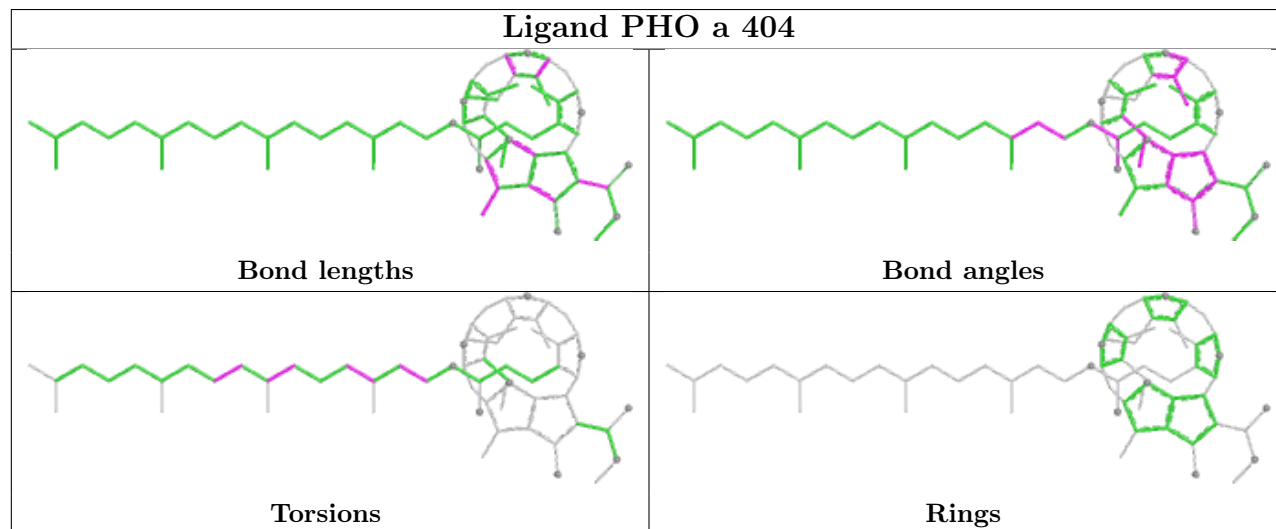
Ligand CLA c 512

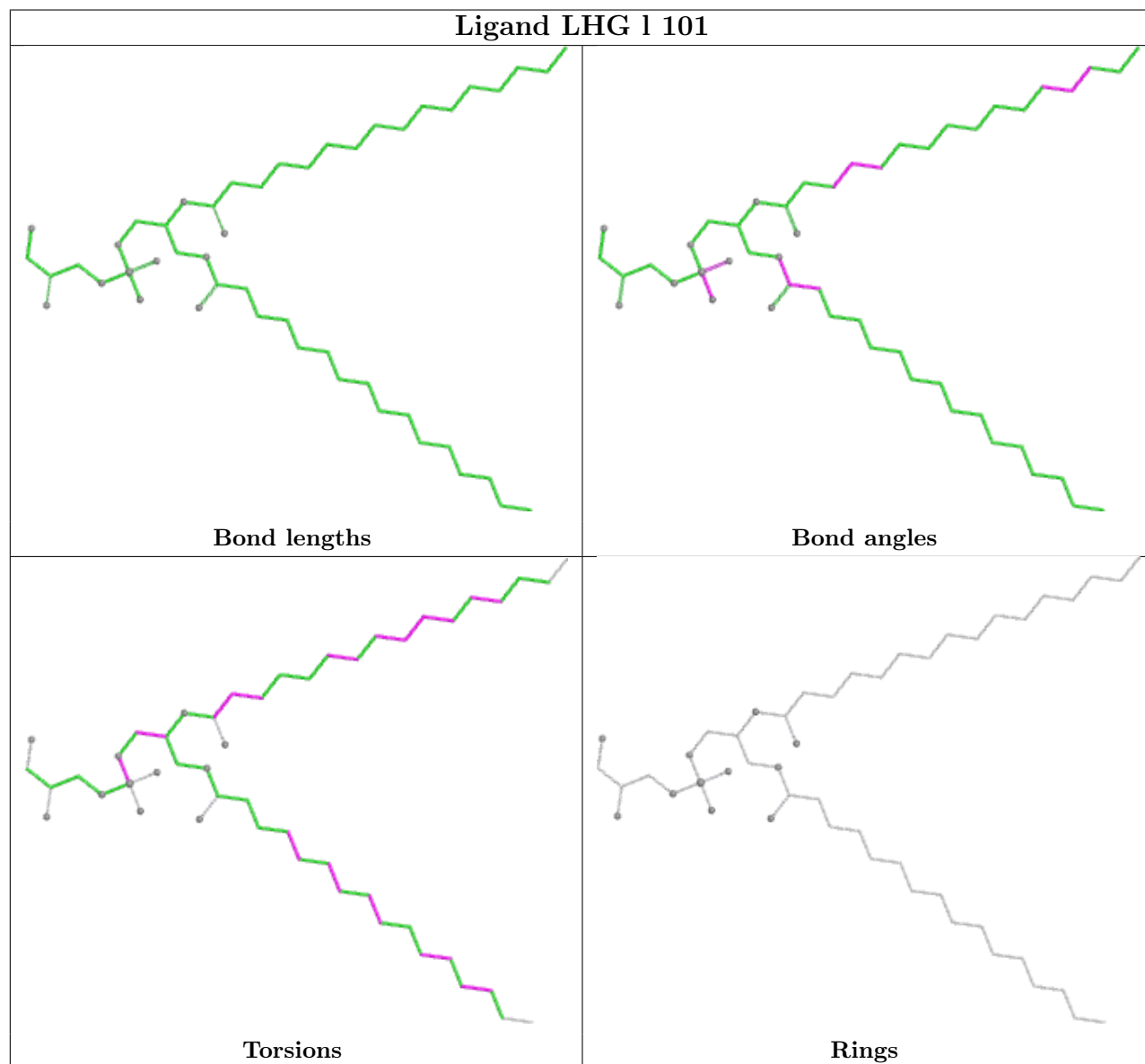
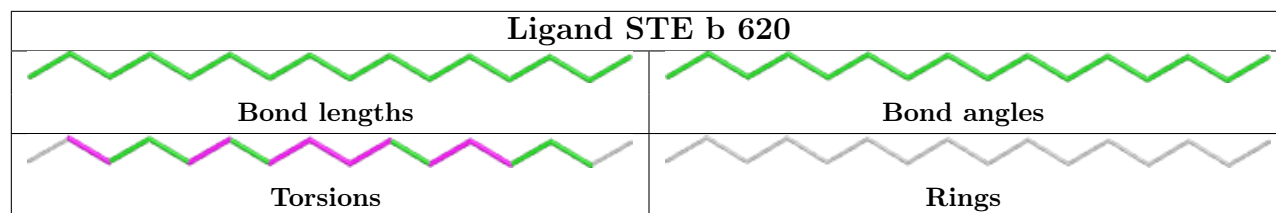


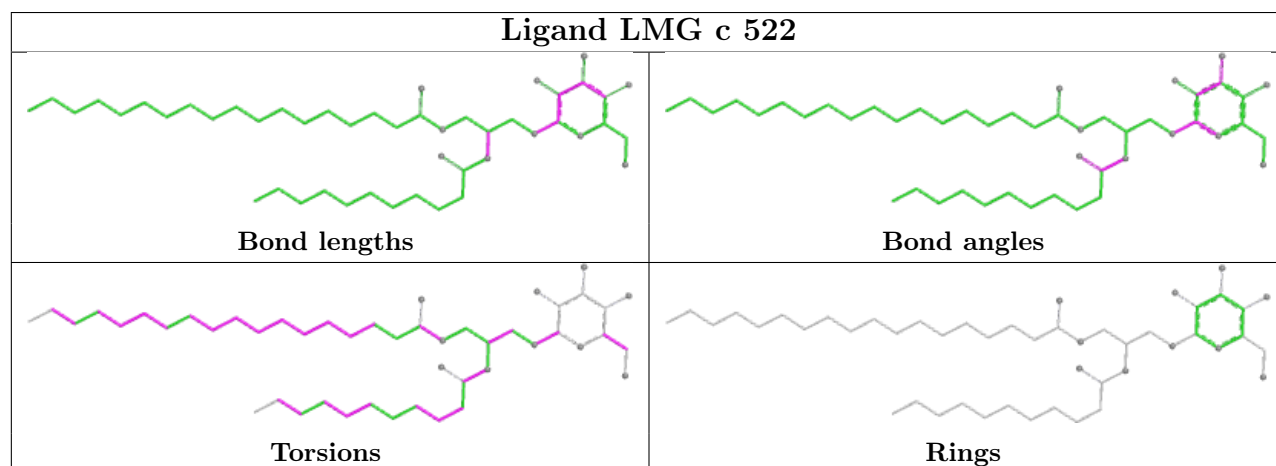
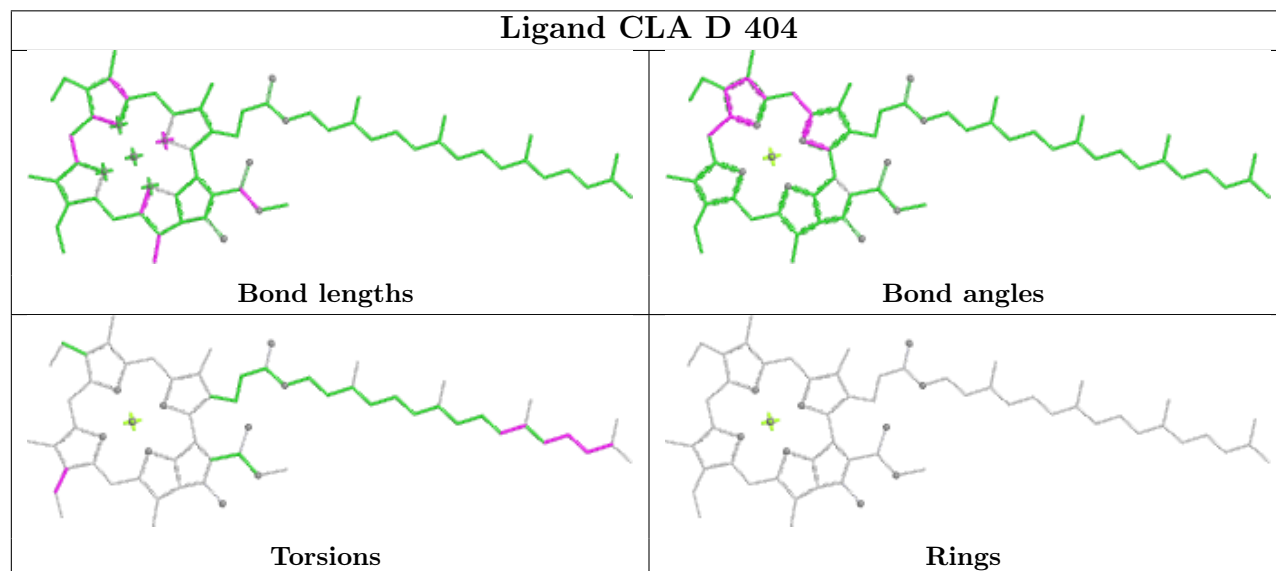
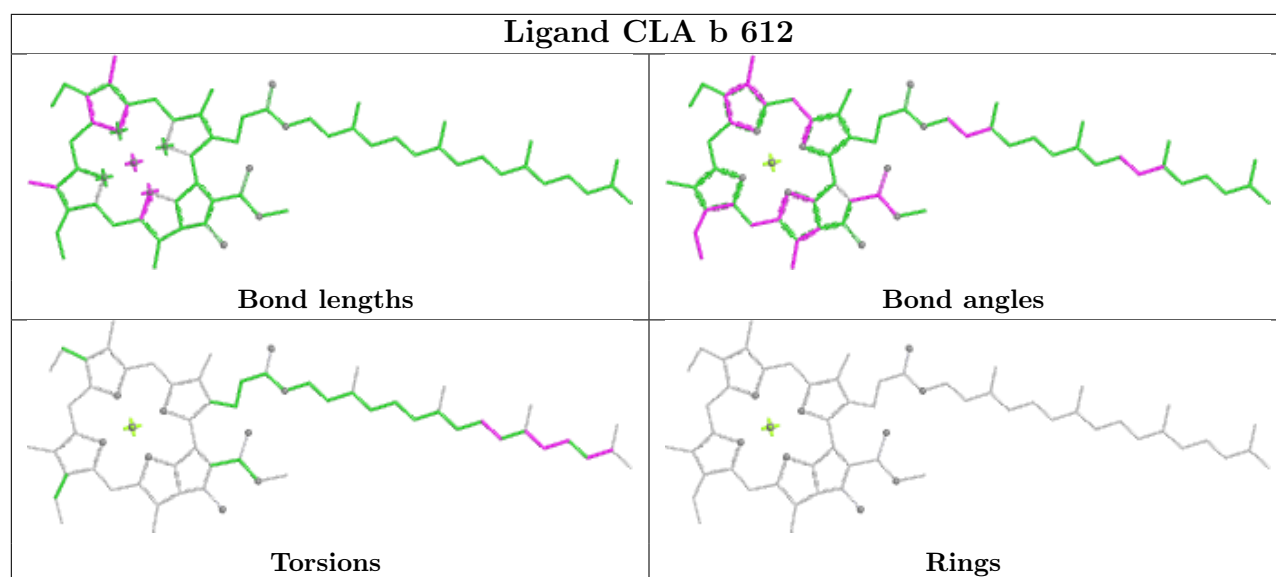
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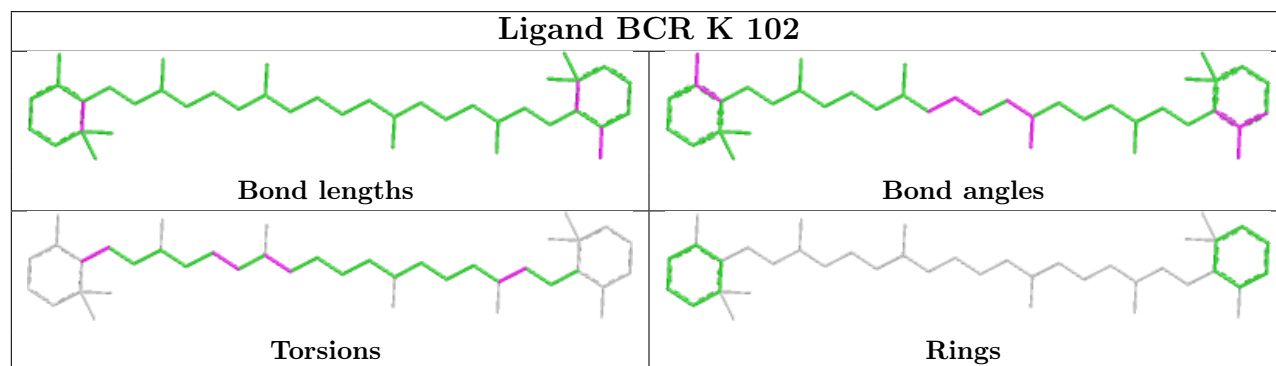
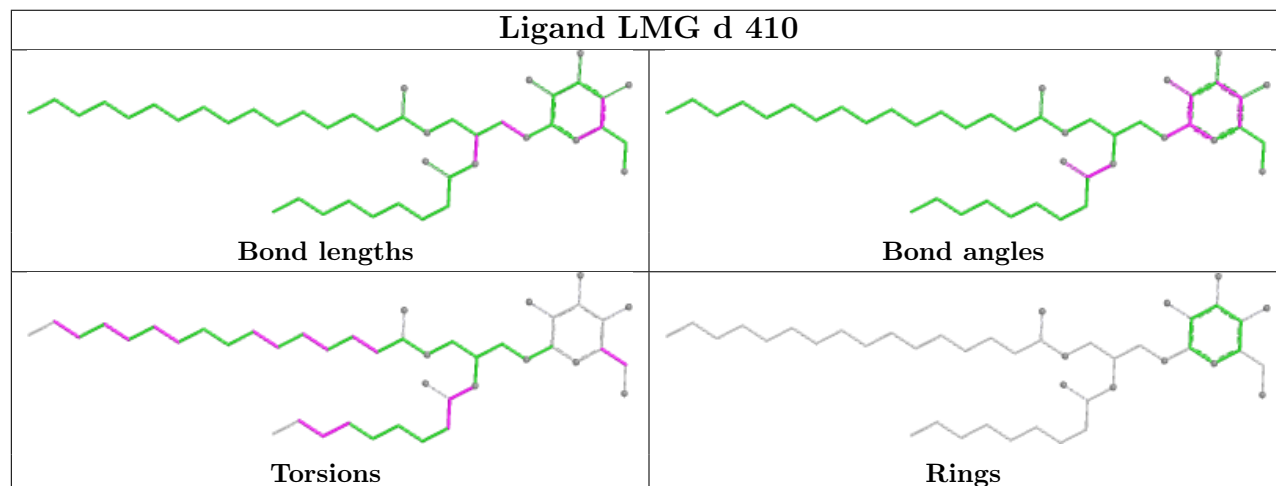
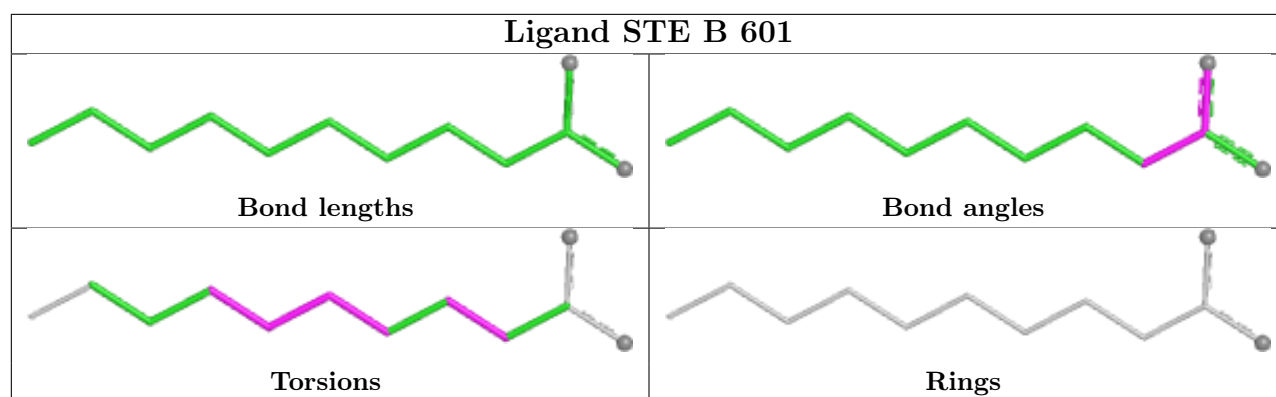


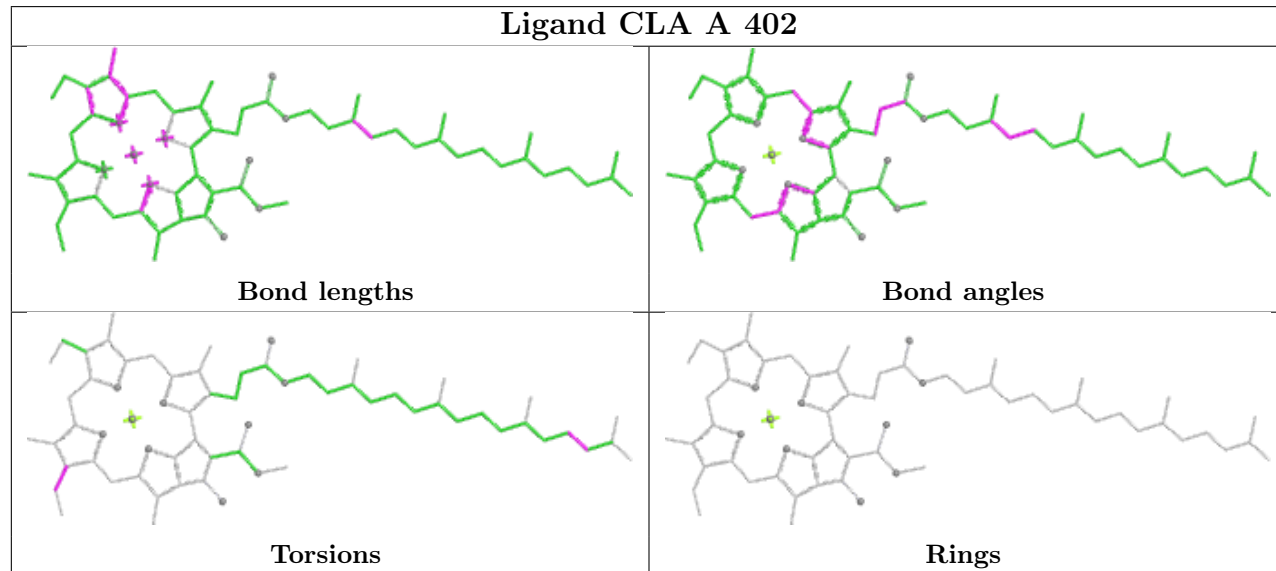
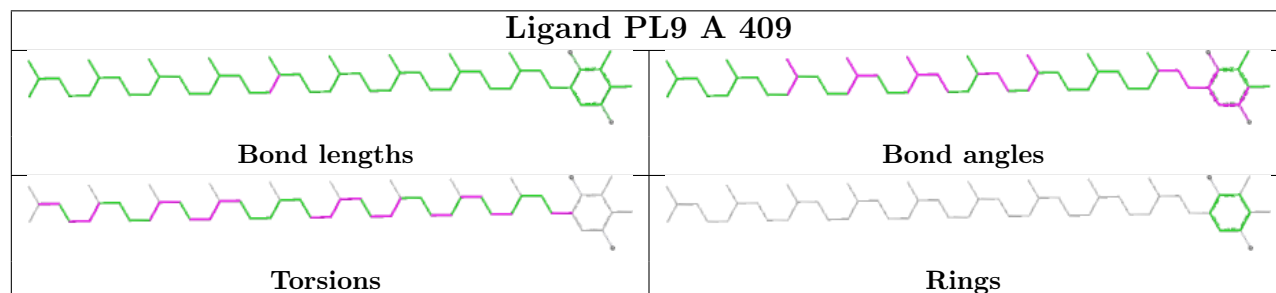
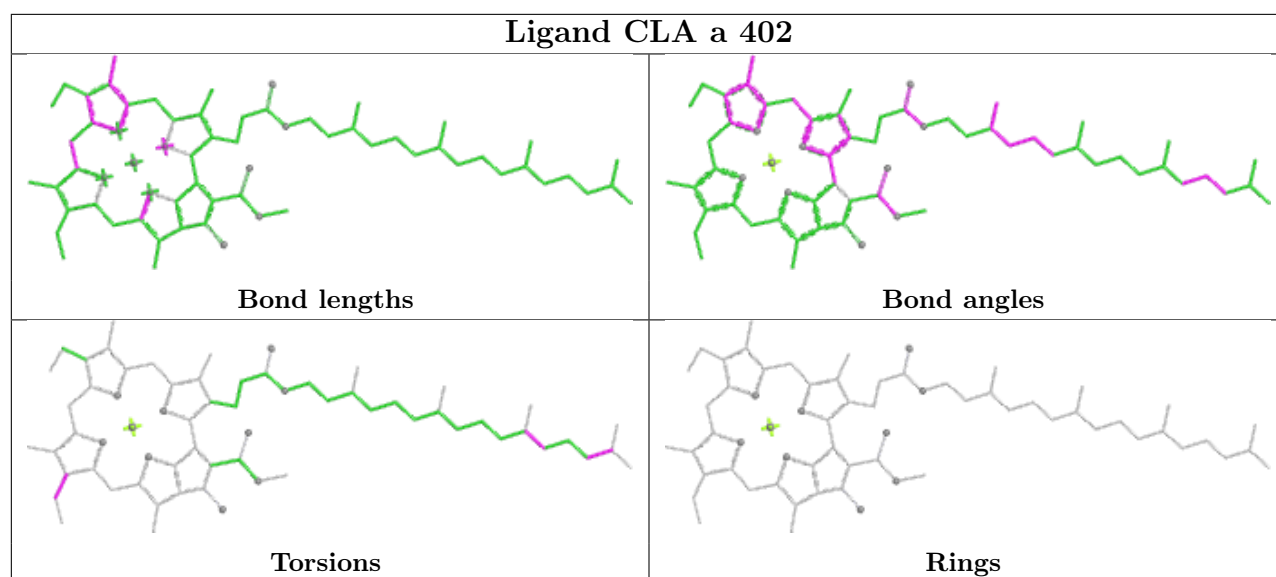
Ligand PHO a 404



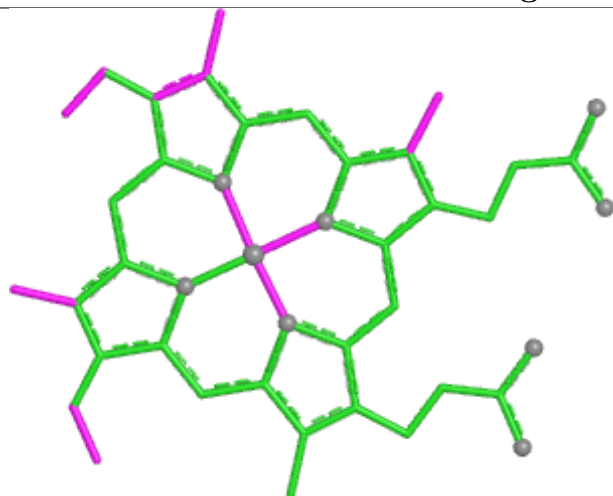




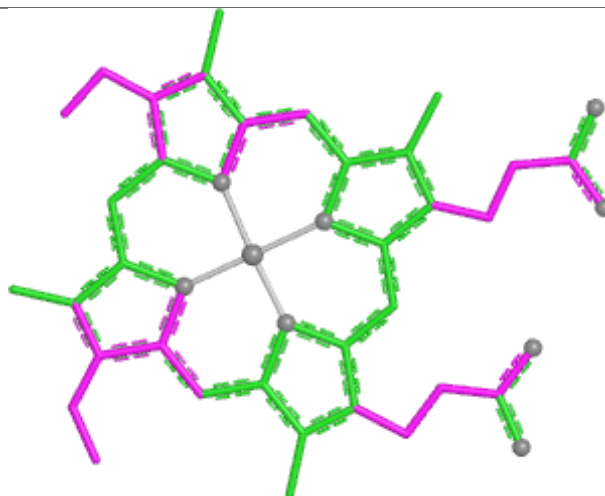




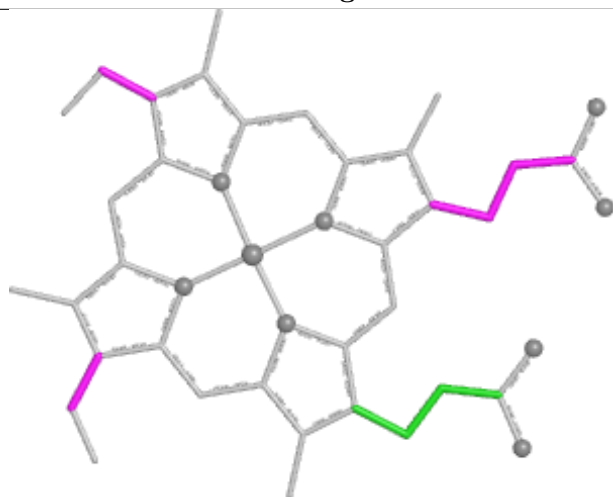
Ligand HEC f 101



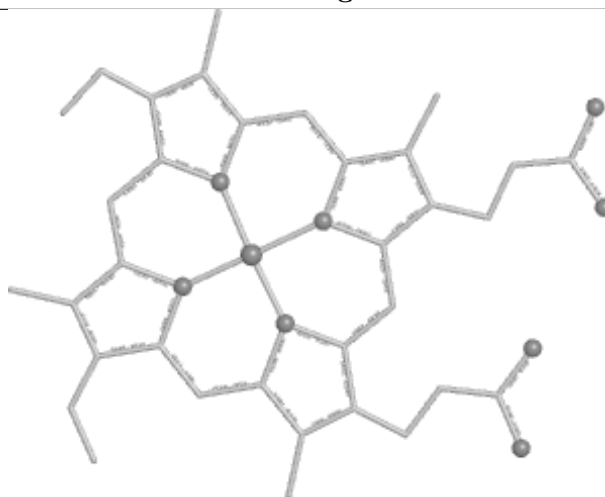
Bond lengths



Bond angles

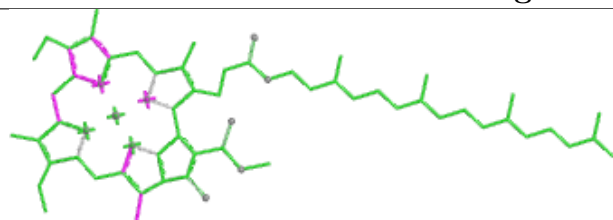


Torsions

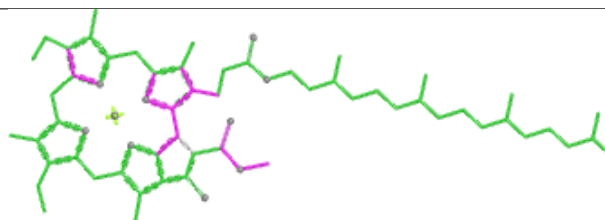


Rings

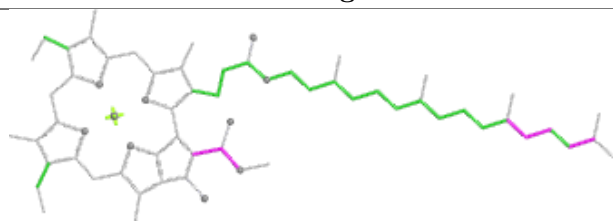
Ligand CLA C 502



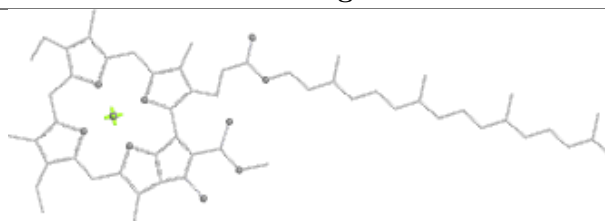
Bond lengths



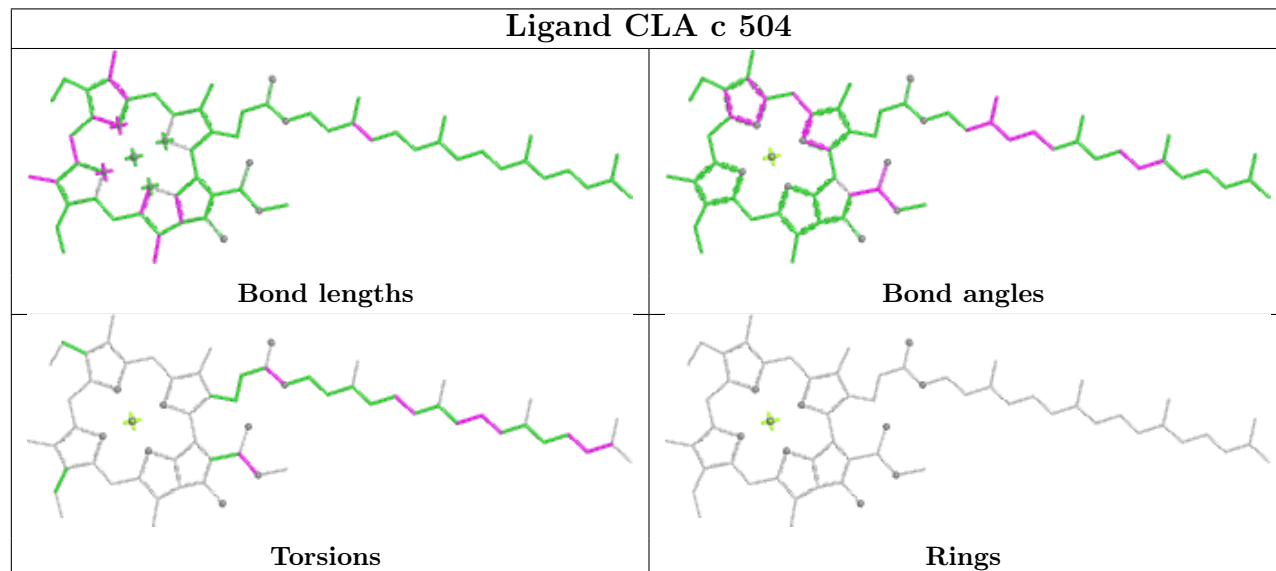
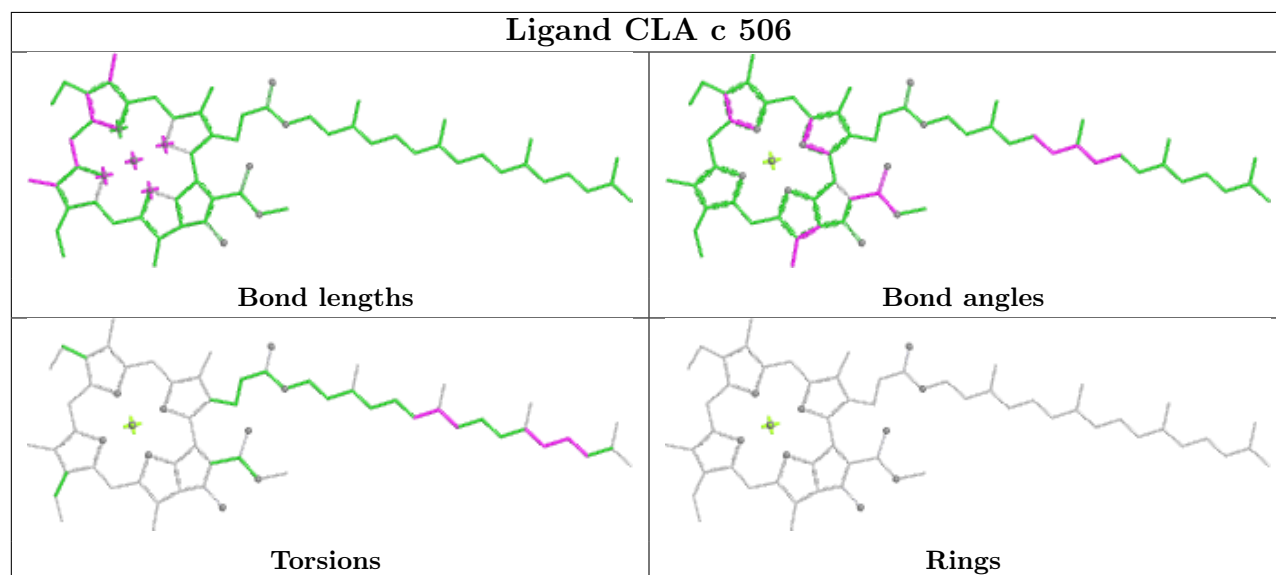
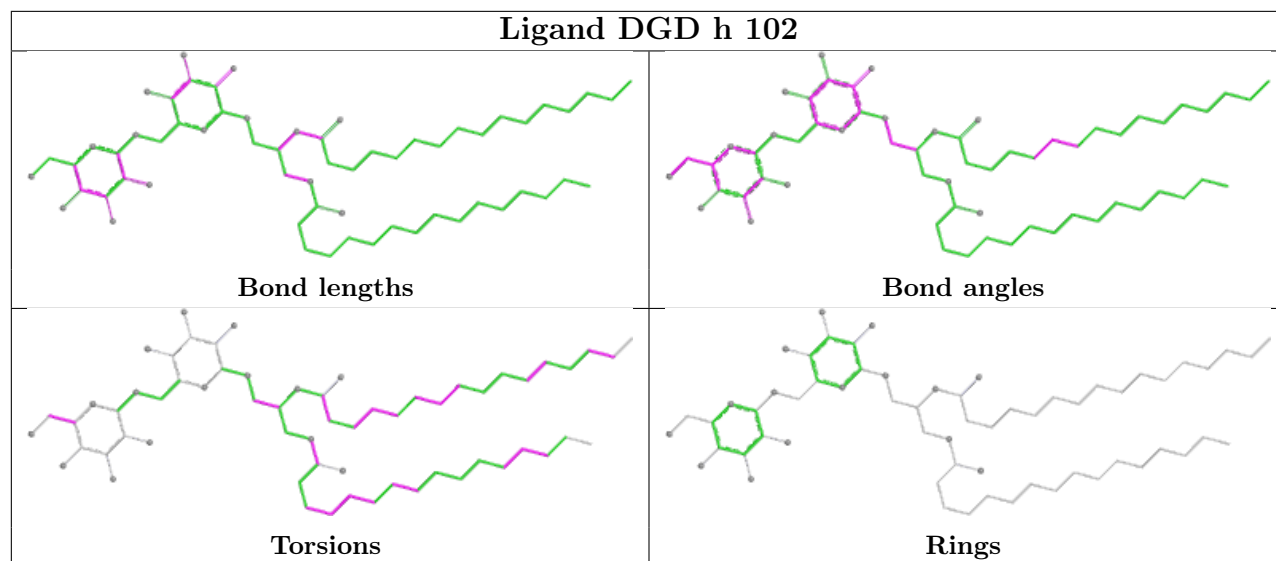
Bond angles

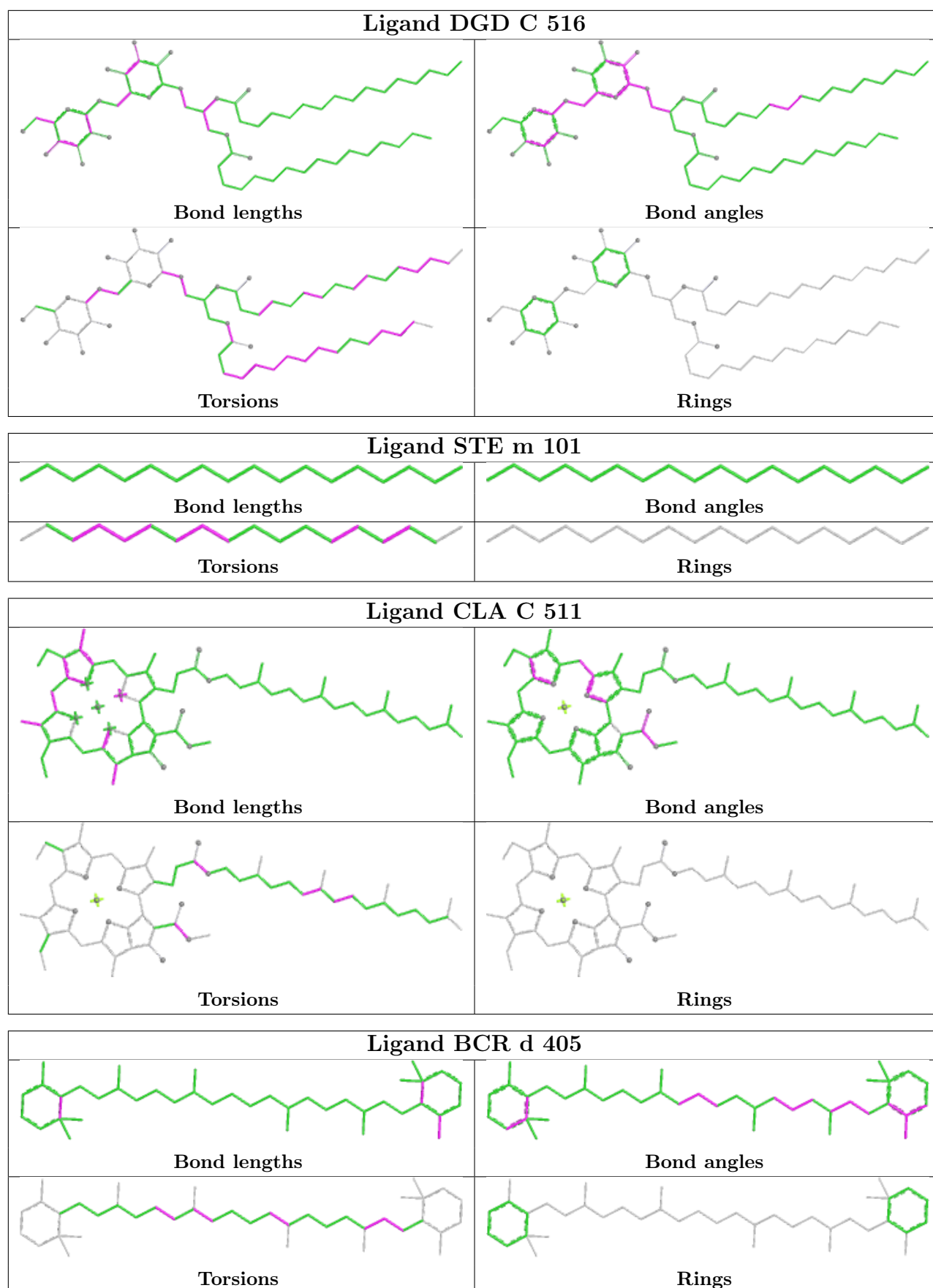


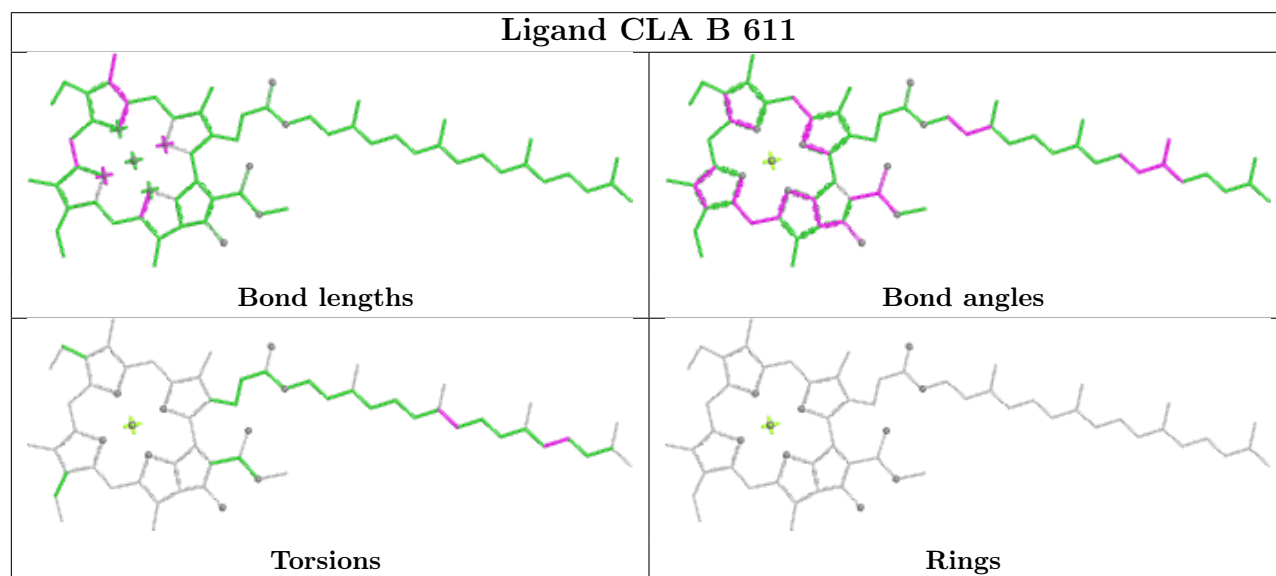
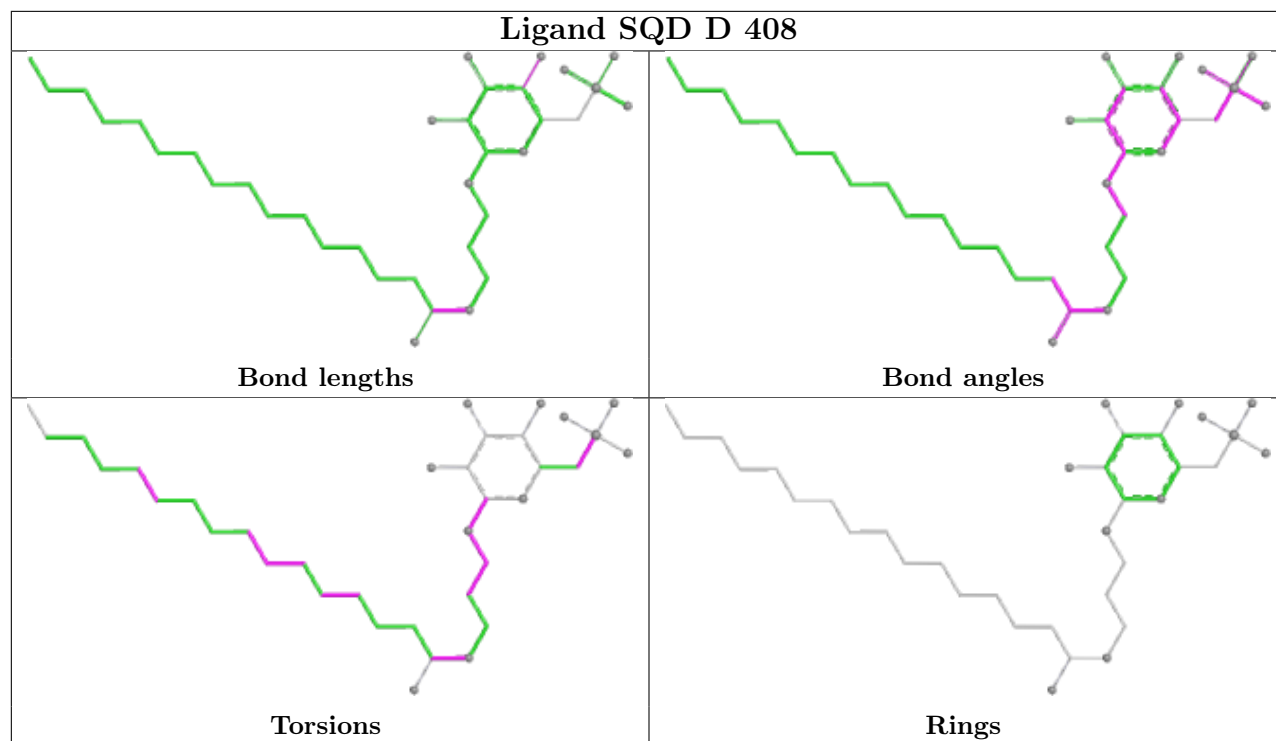
Torsions

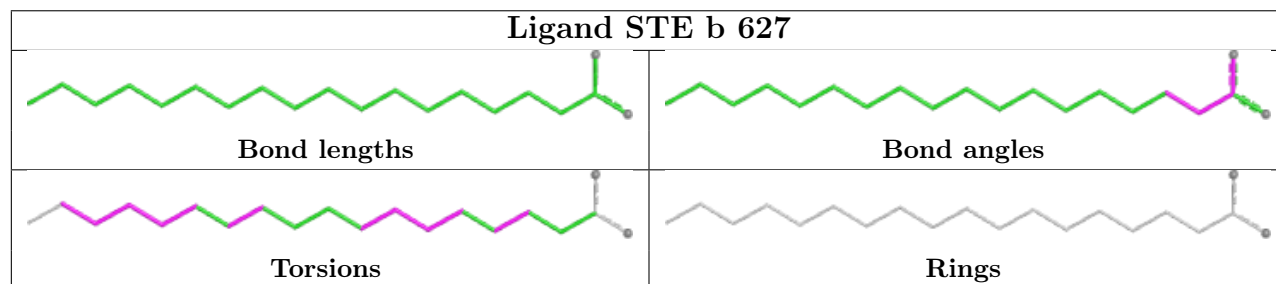
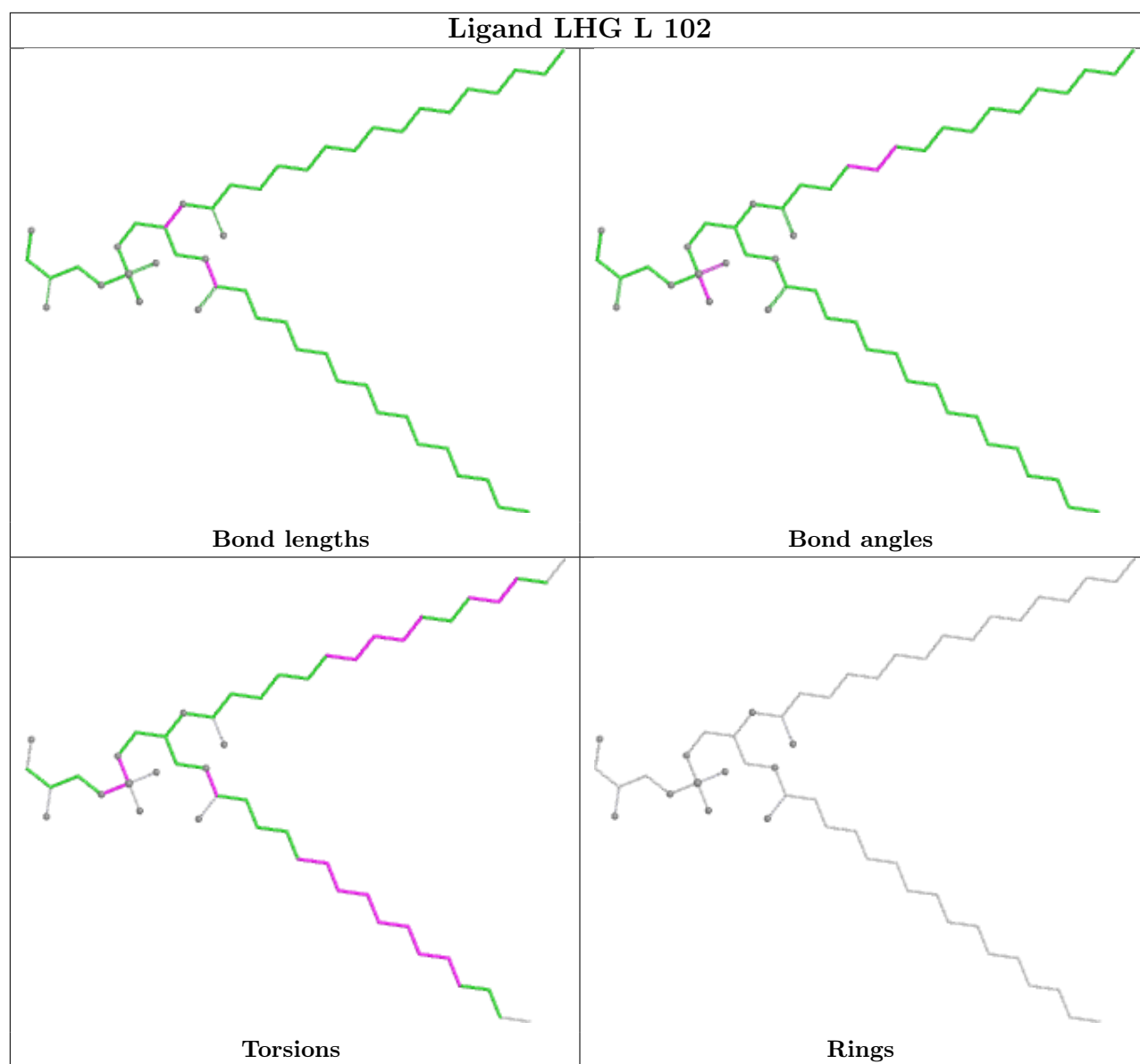


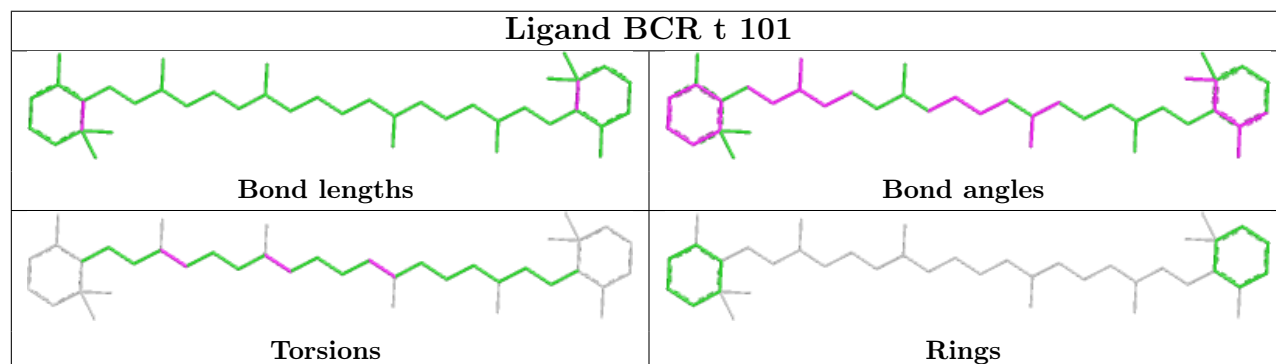
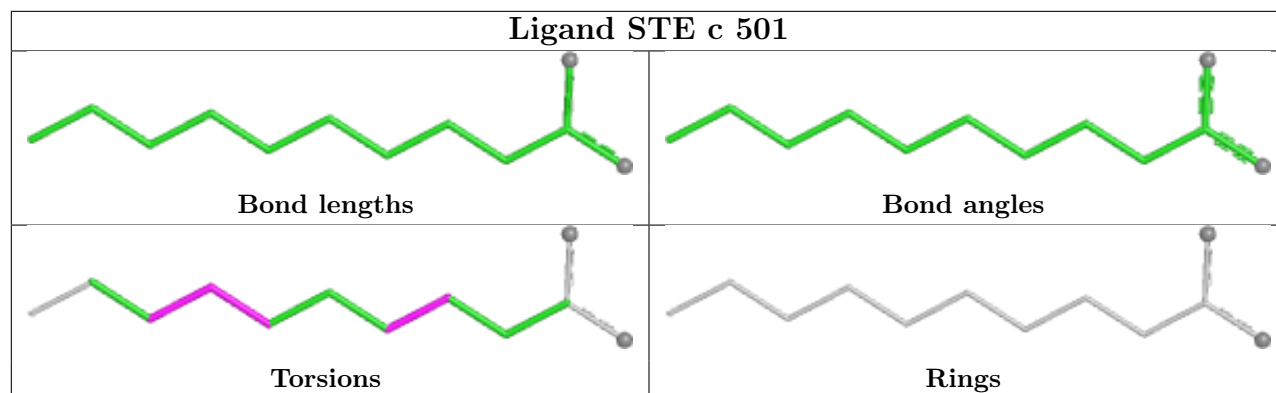
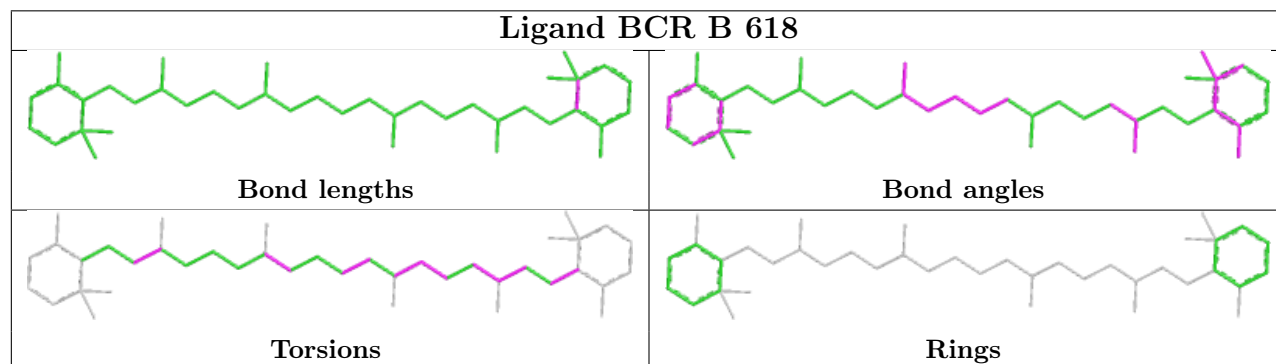
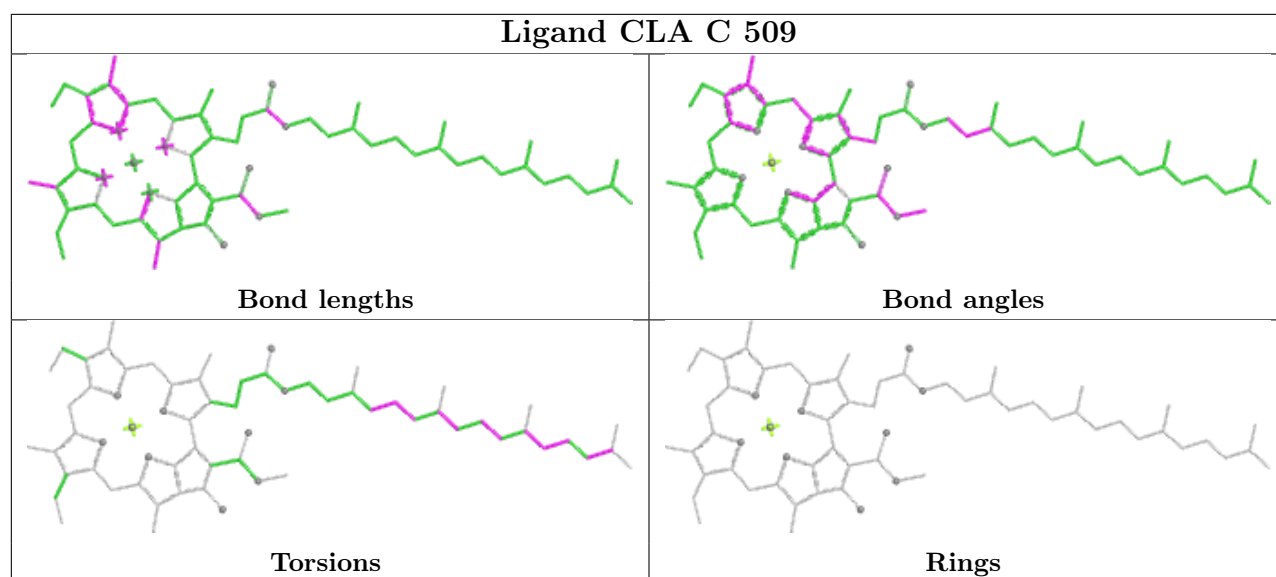
Rings

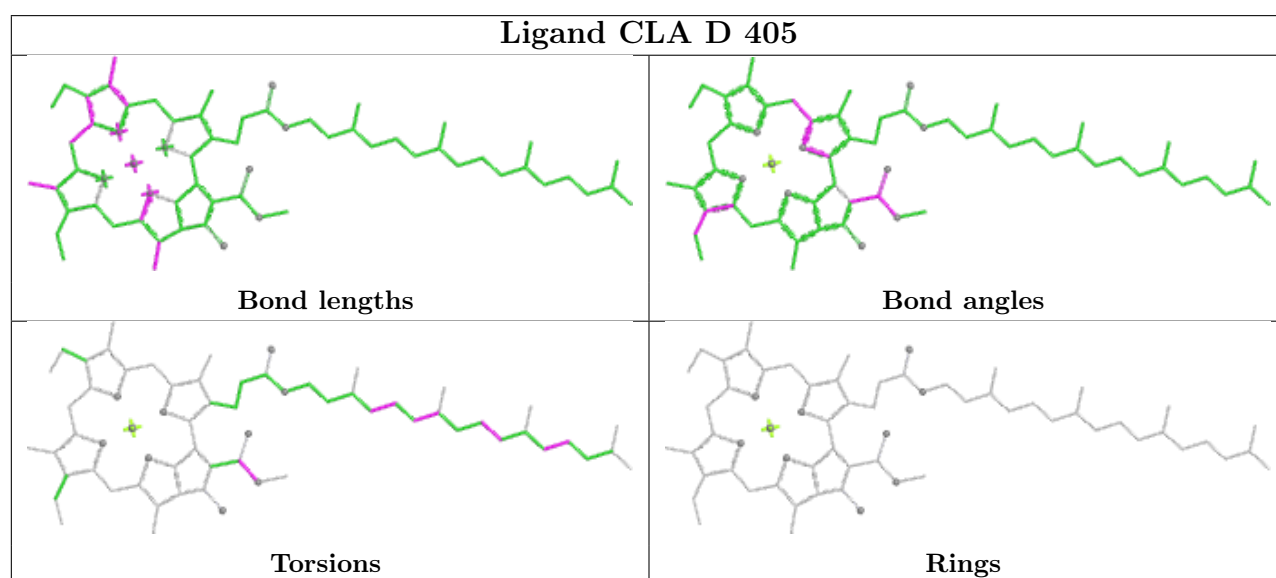
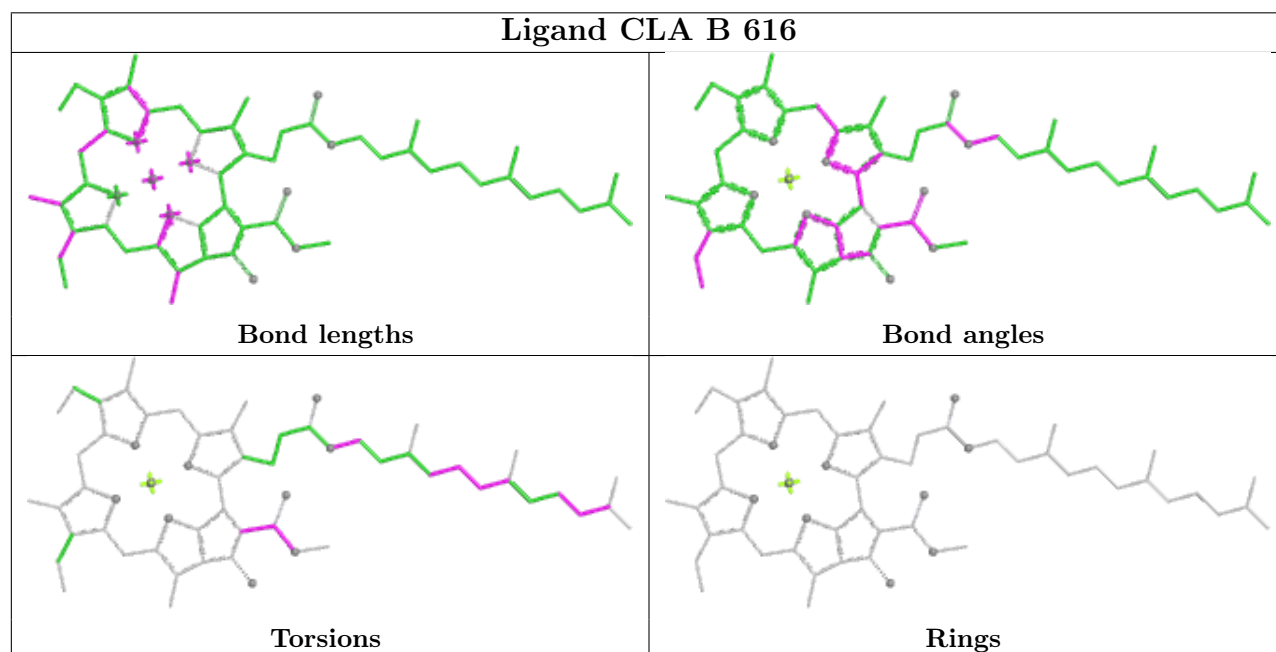
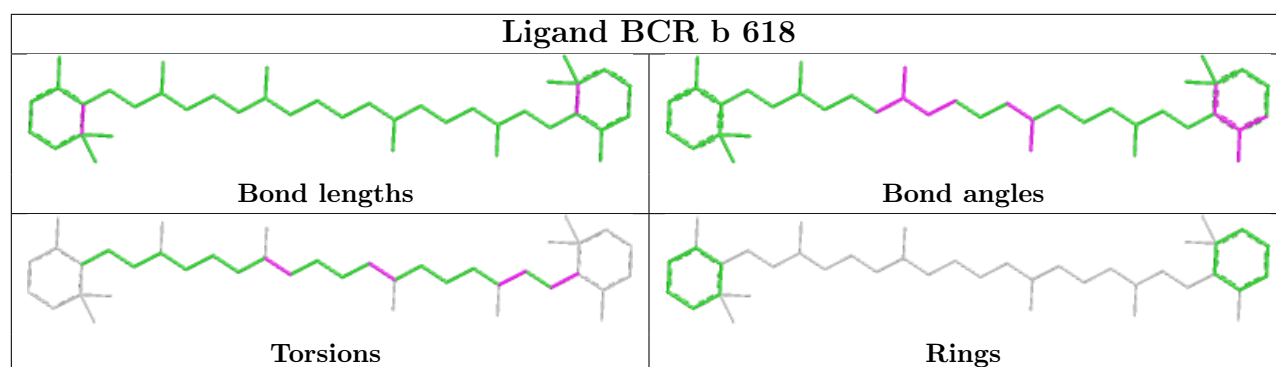


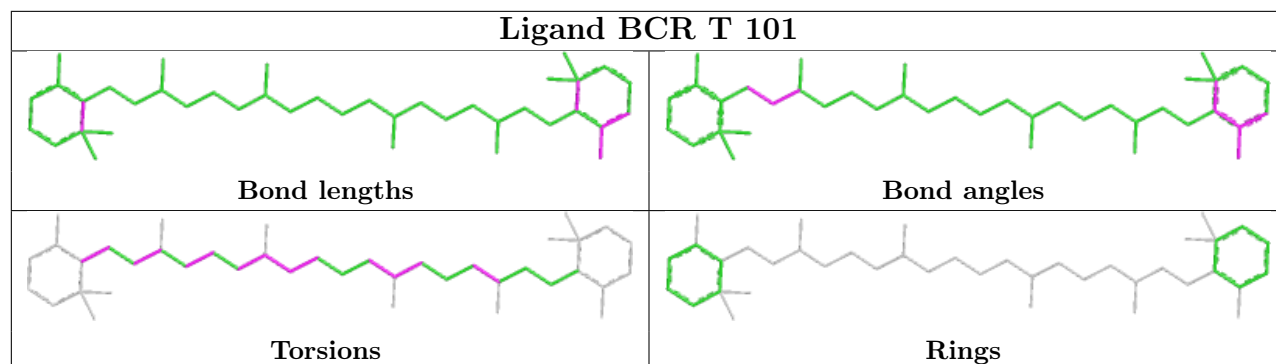
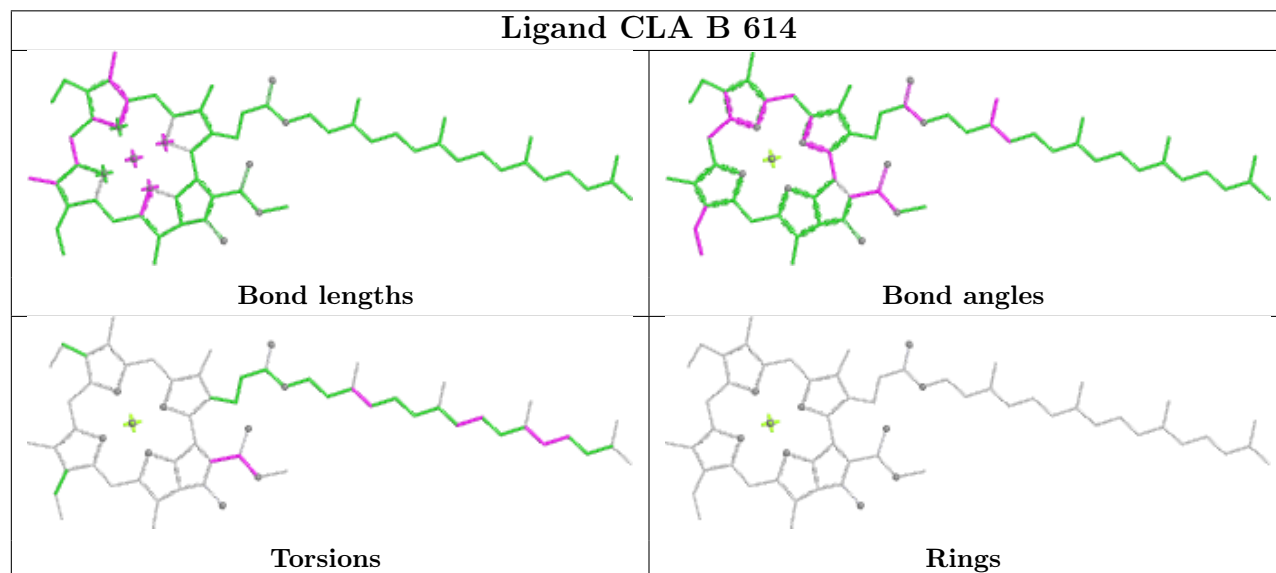
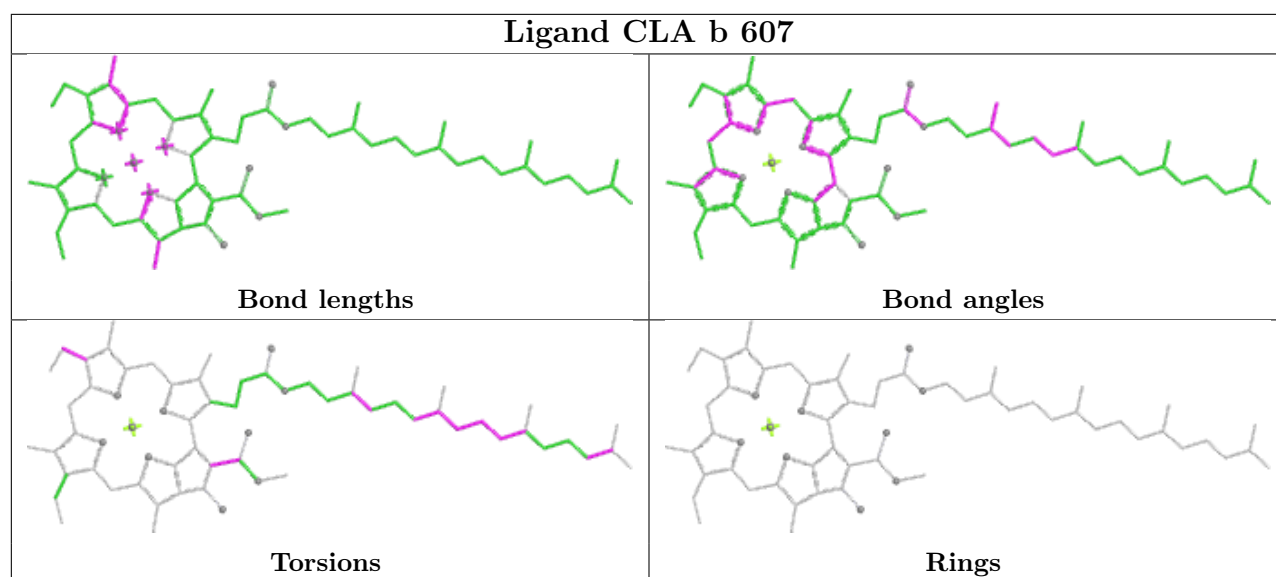


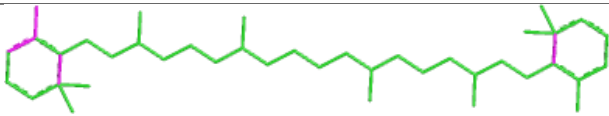
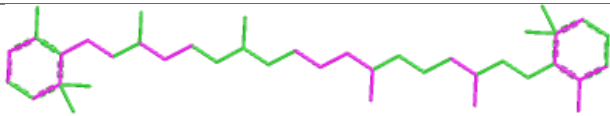
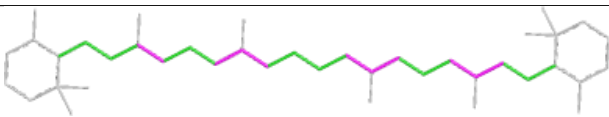
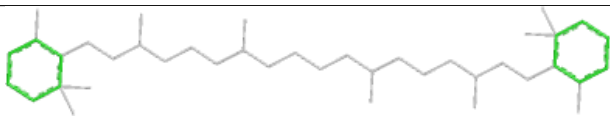


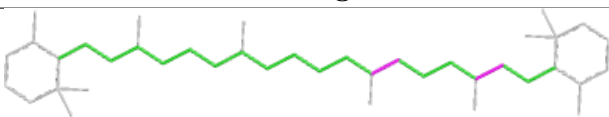
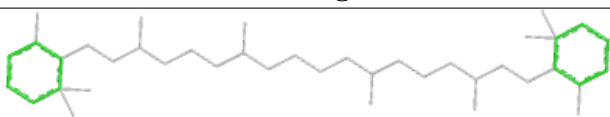


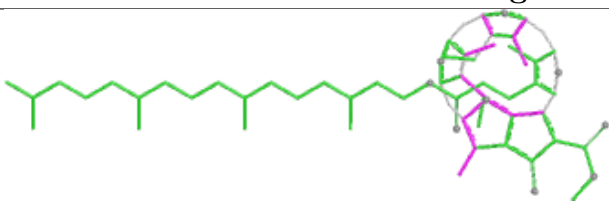
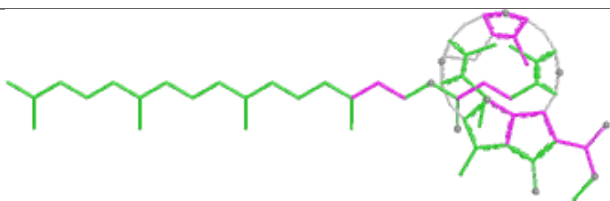
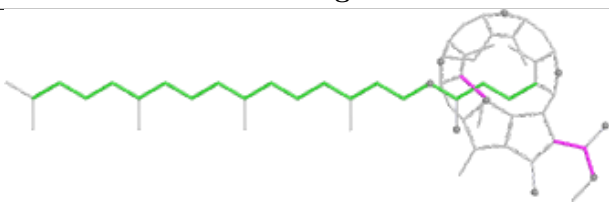
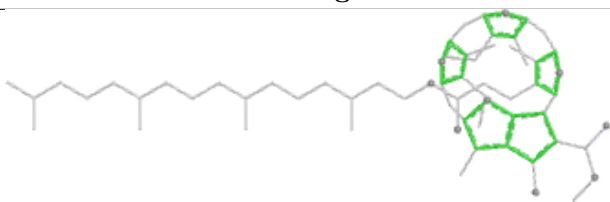


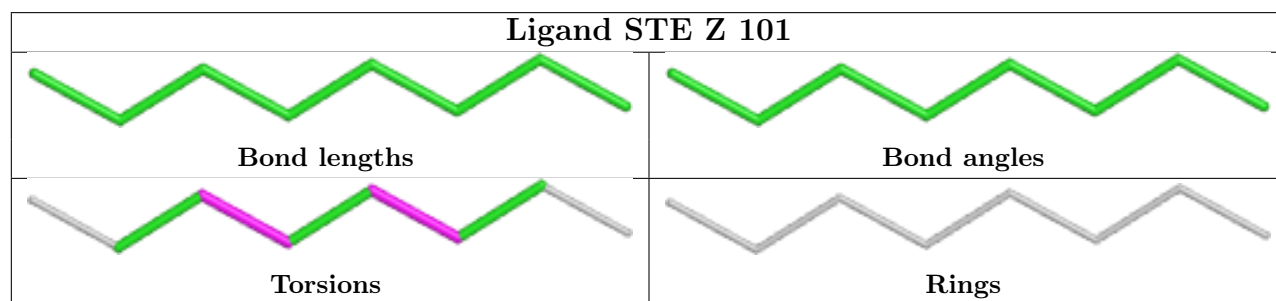
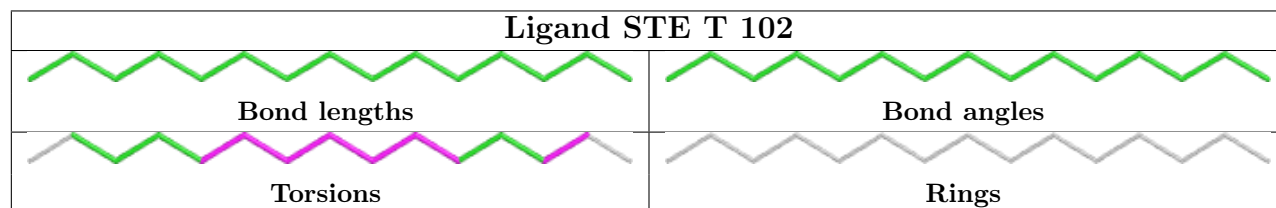
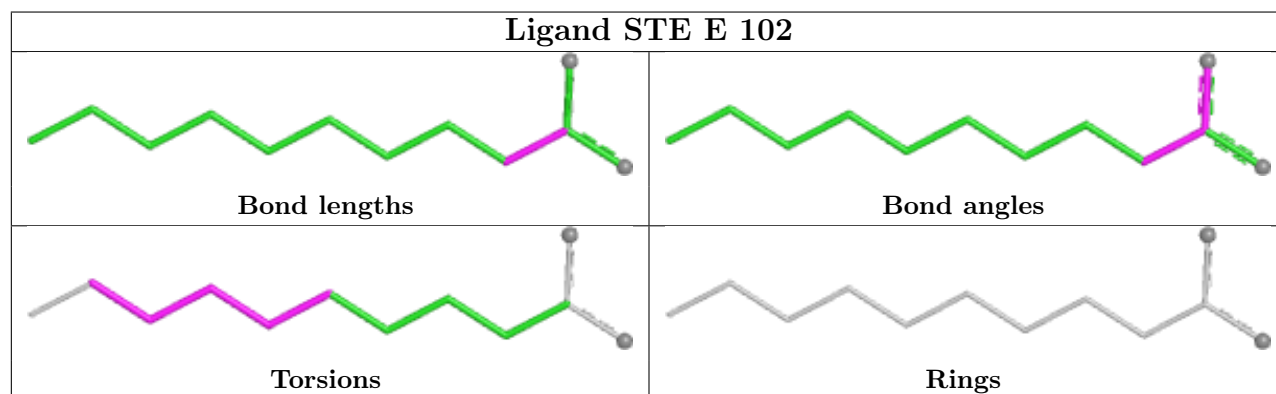
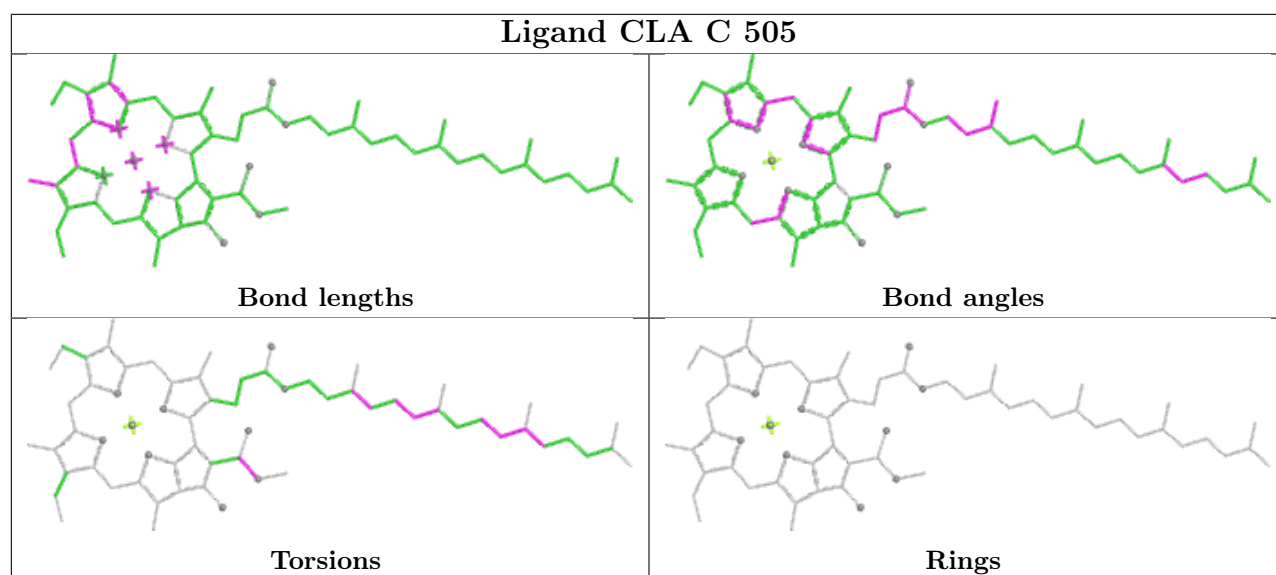


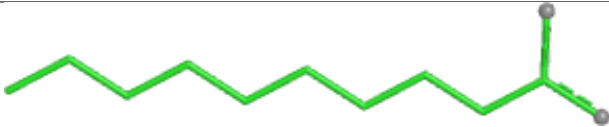
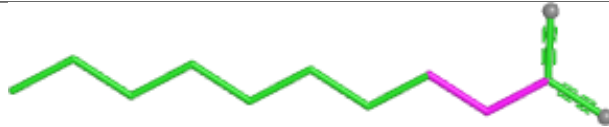
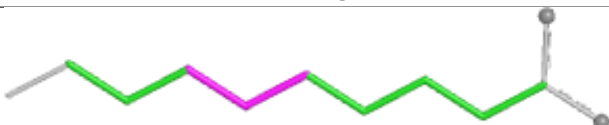
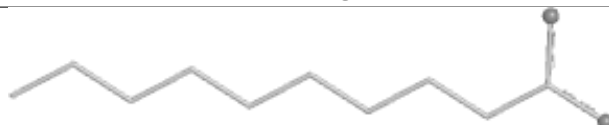


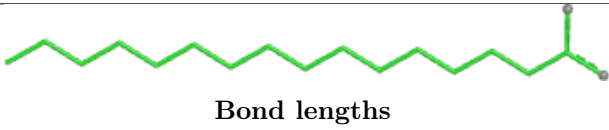
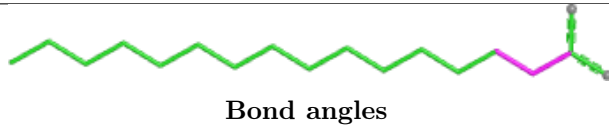
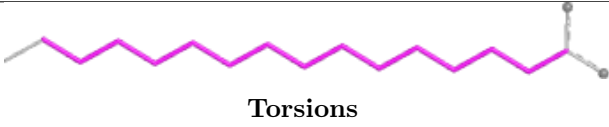
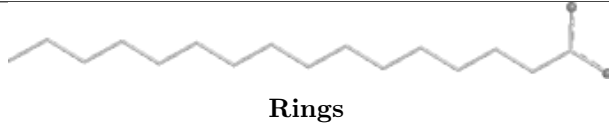
Ligand BCR b 617	
	
Bond lengths	Bond angles
	
Torsions	Rings

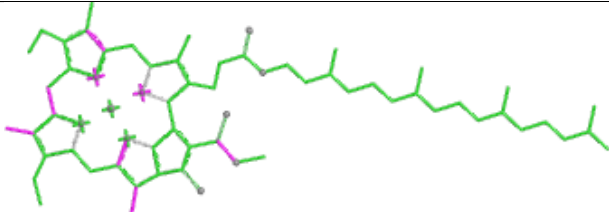
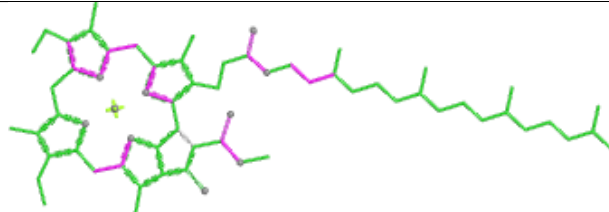
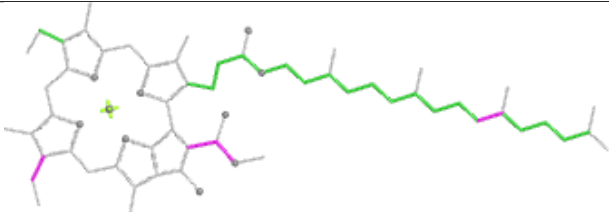
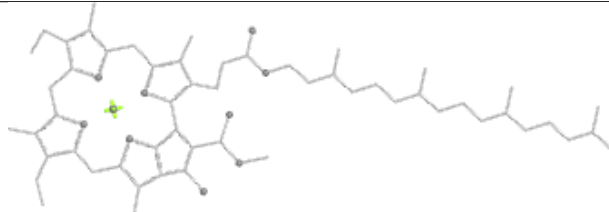
Ligand BCR a 406	
	
Bond lengths	Bond angles
	
Torsions	Rings

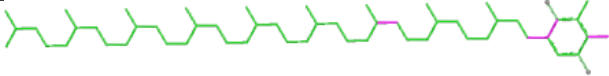
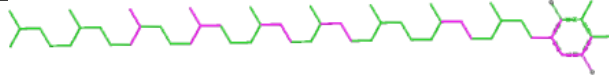
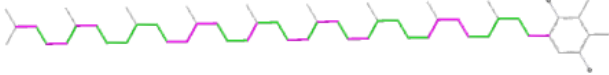
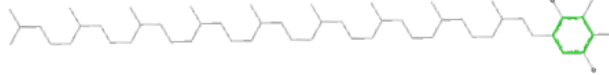
Ligand PHO d 401	
	
Bond lengths	Bond angles
	
Torsions	Rings

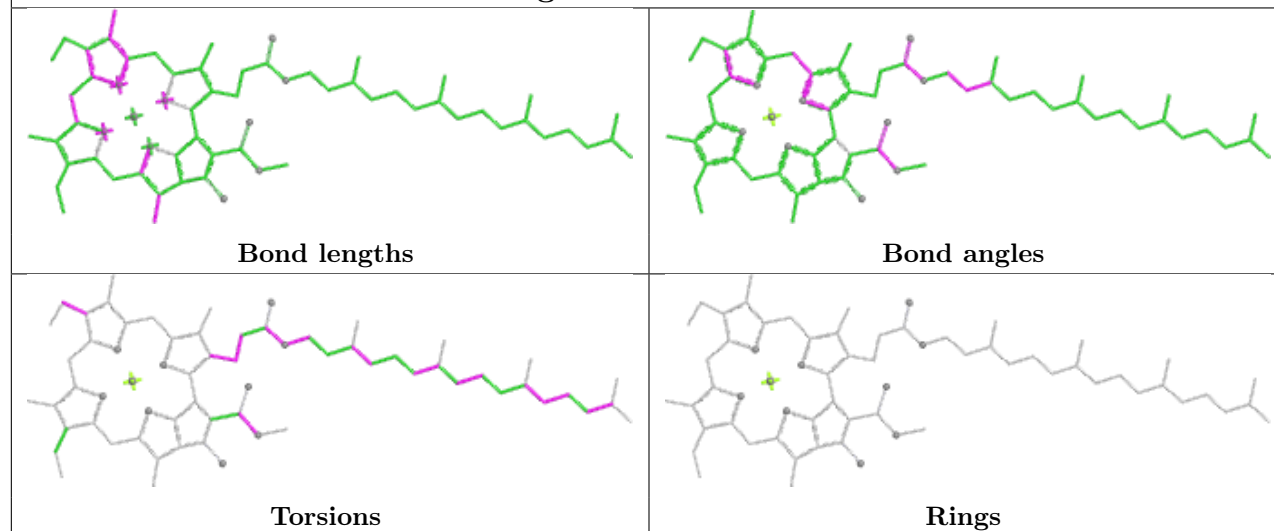
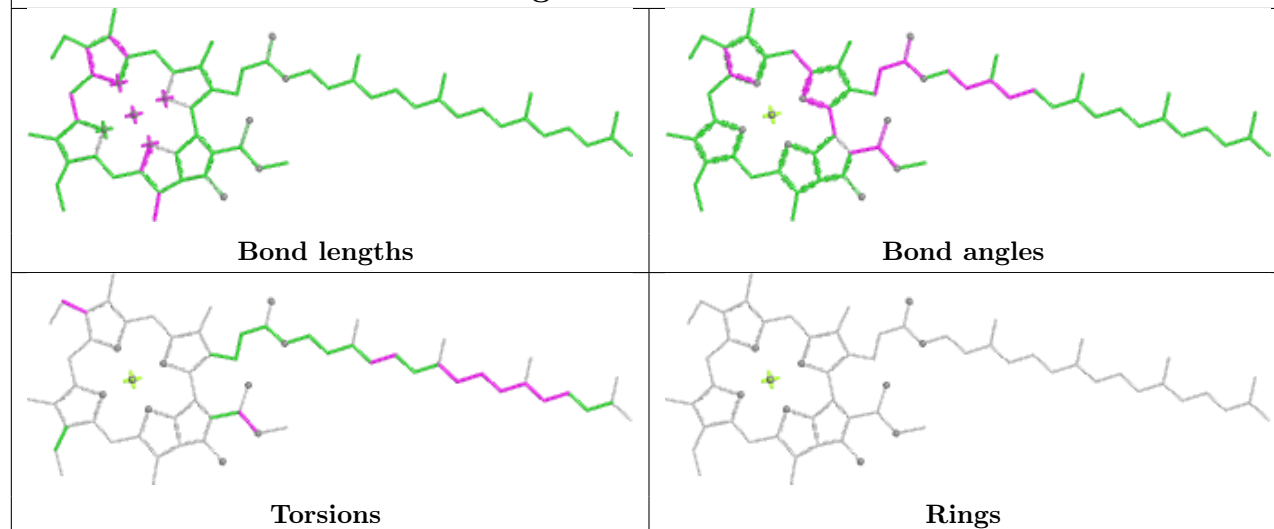
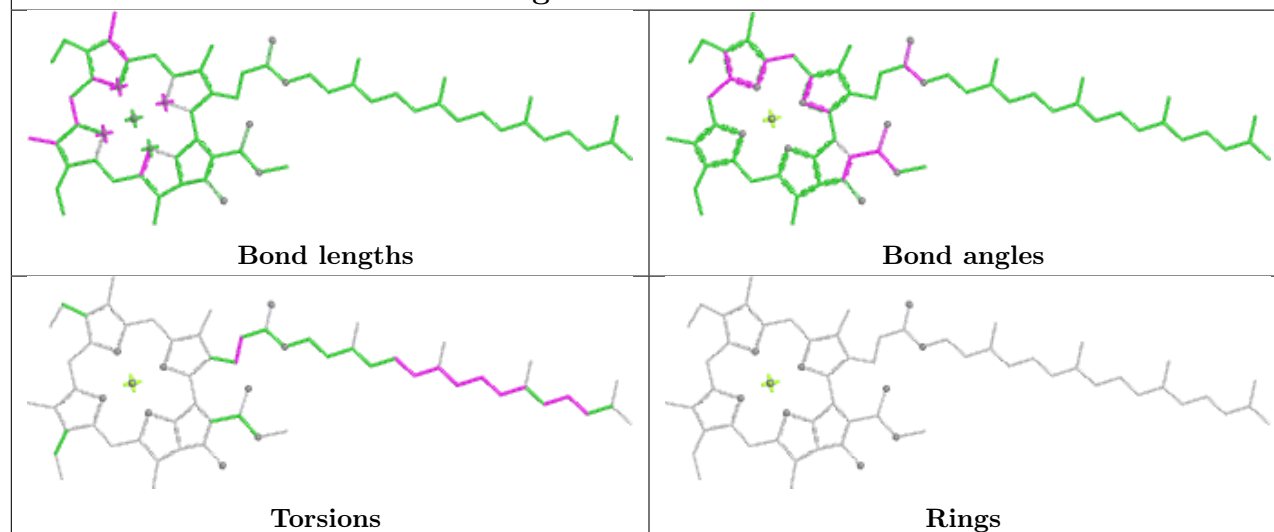


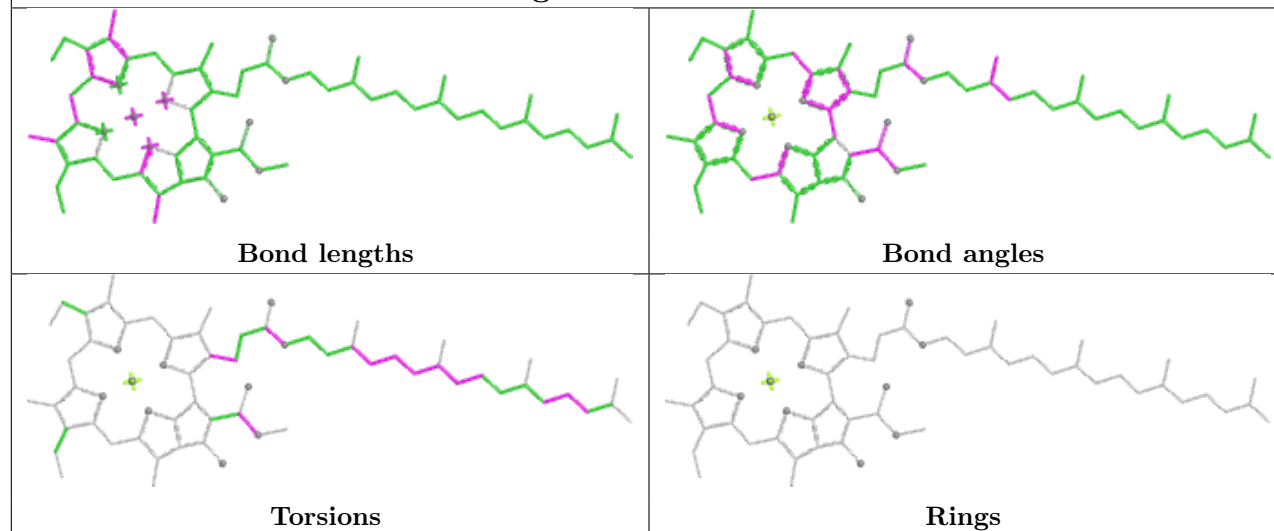
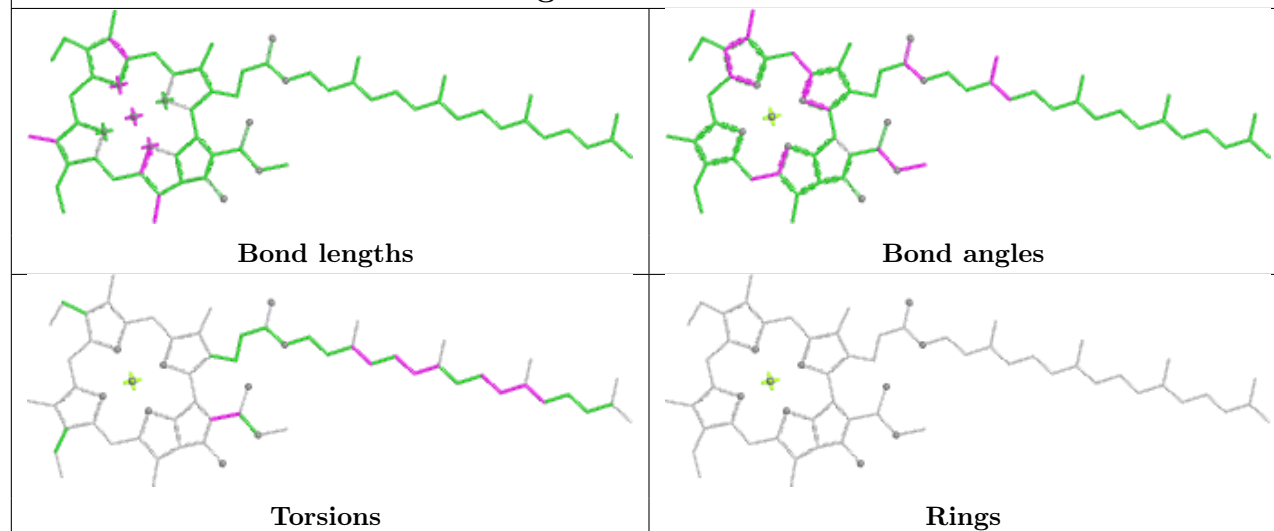
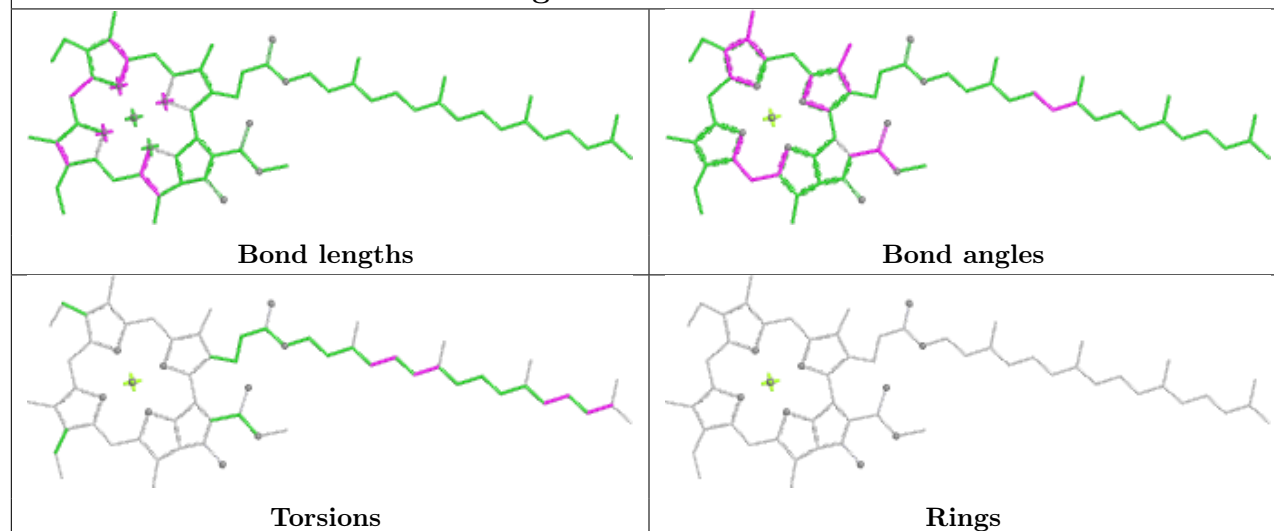
Ligand STE C 520	
	
Bond lengths	Bond angles
	
Torsions	Rings

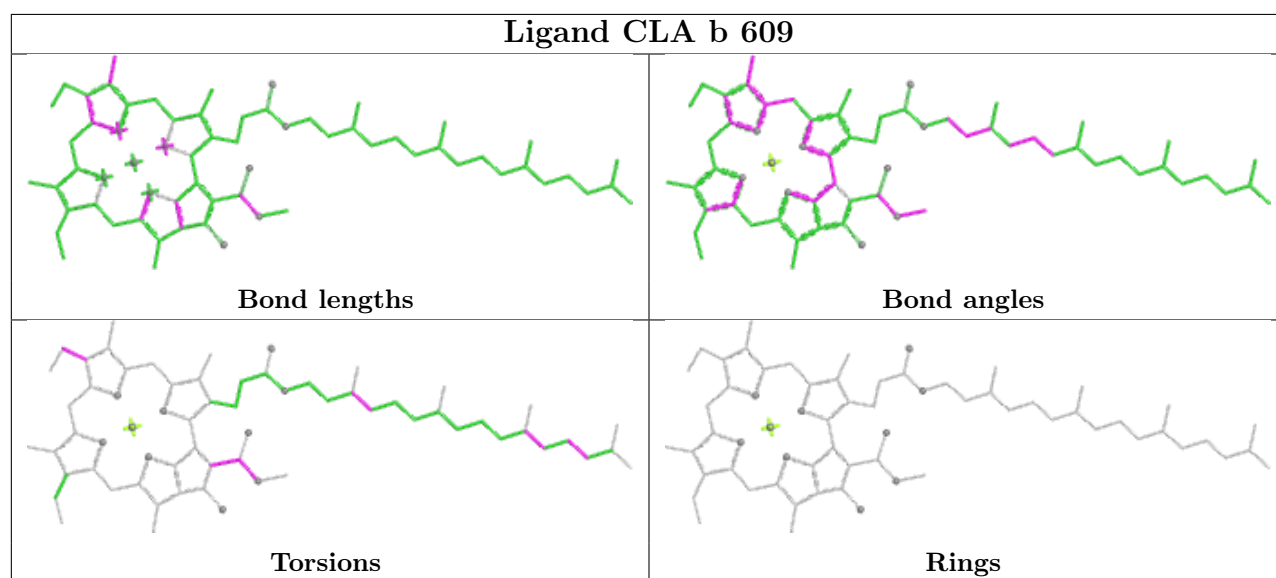
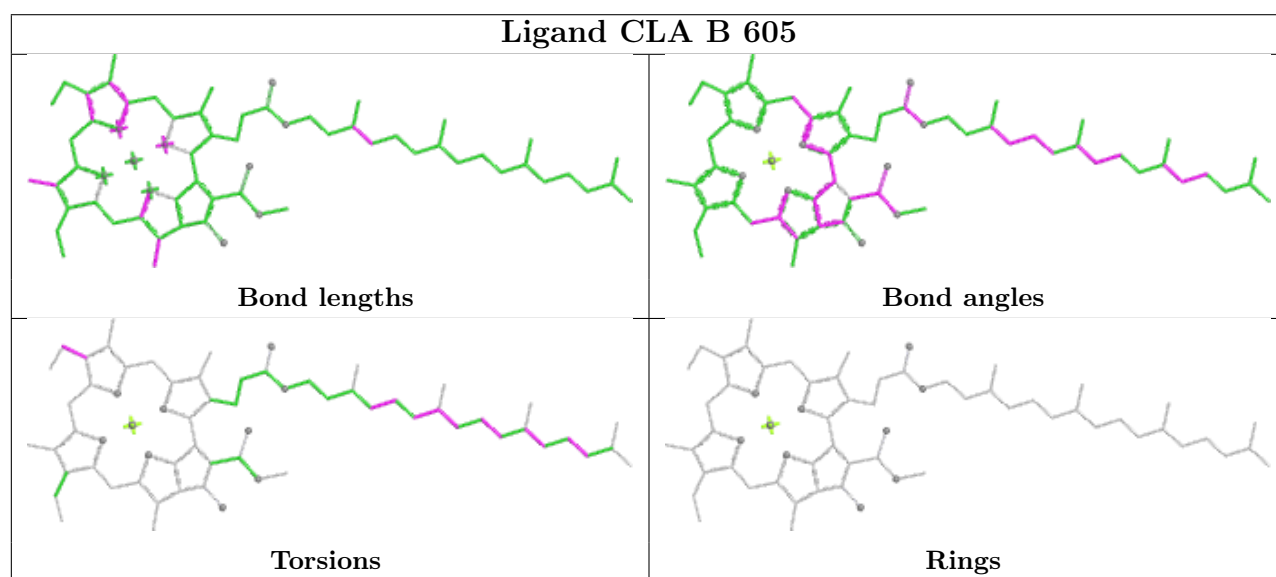
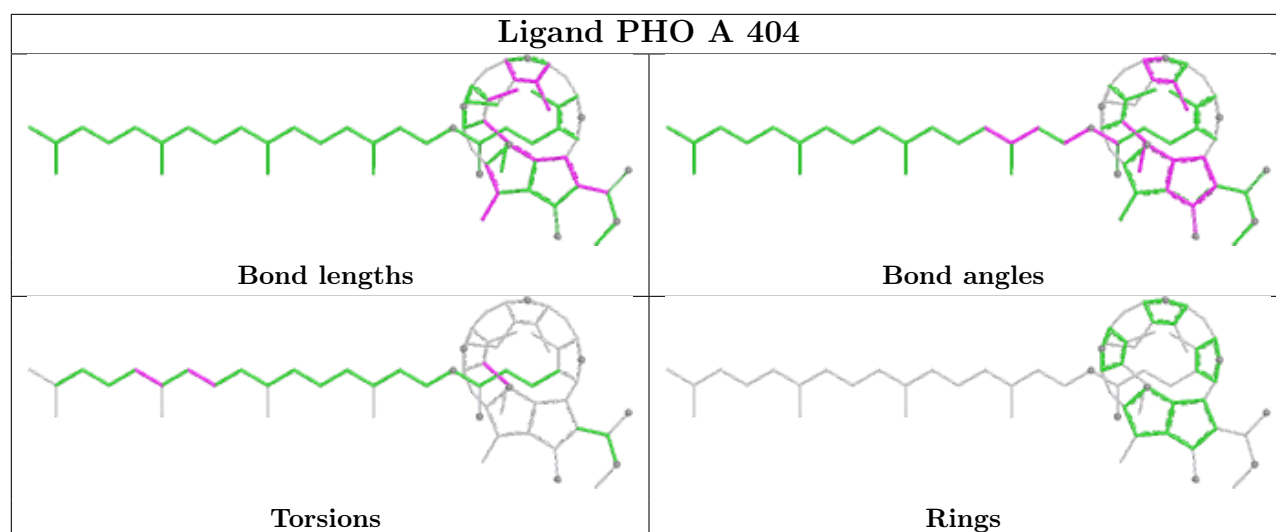
Ligand STE B 625	
	
Bond lengths	Bond angles
	
Torsions	Rings

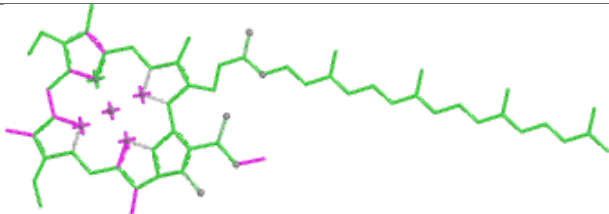
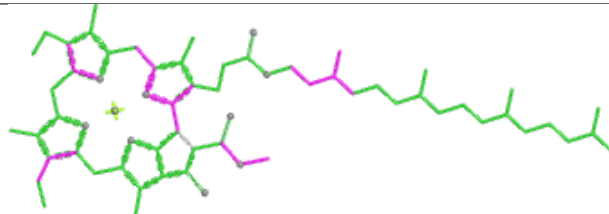
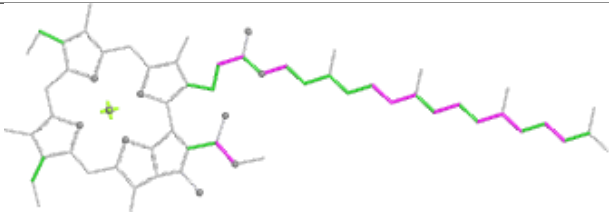
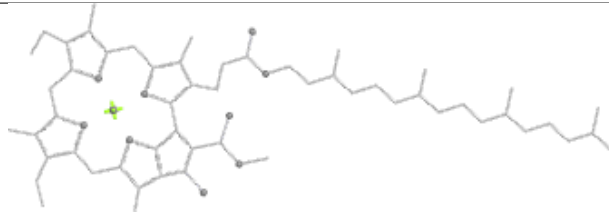
Ligand CLA c 503	
	
Bond lengths	Bond angles
	
Torsions	Rings

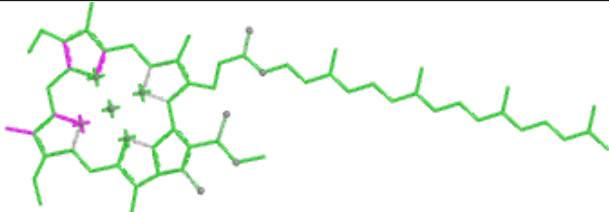
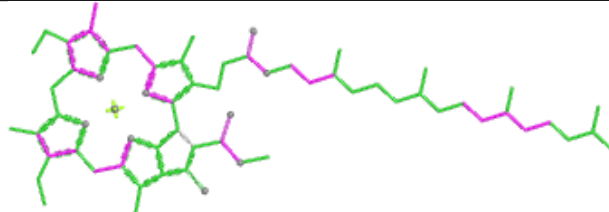
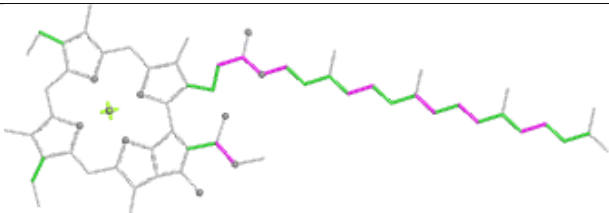
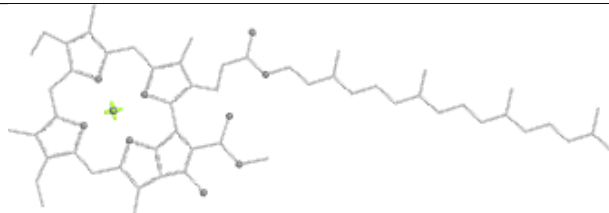
Ligand PL9 a 409	
	
Bond lengths	Bond angles
	
Torsions	Rings

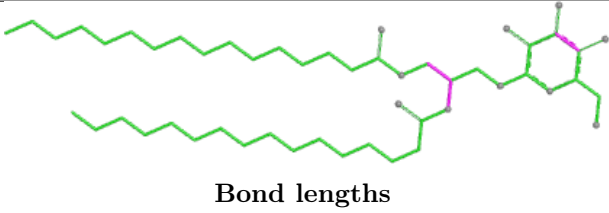
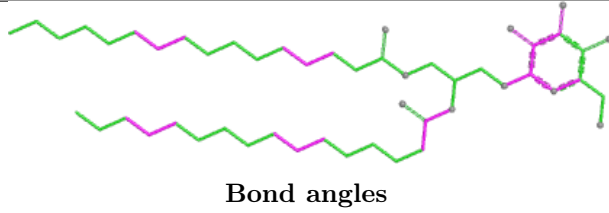
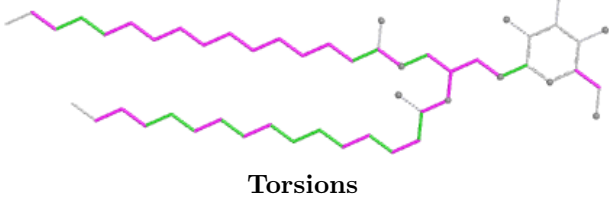
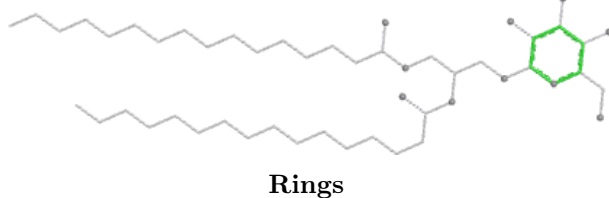
Ligand CLA c 513**Ligand CLA C 512****Ligand CLA B 606**

Ligand CLA C 513**Ligand CLA c 508****Ligand CLA B 608**

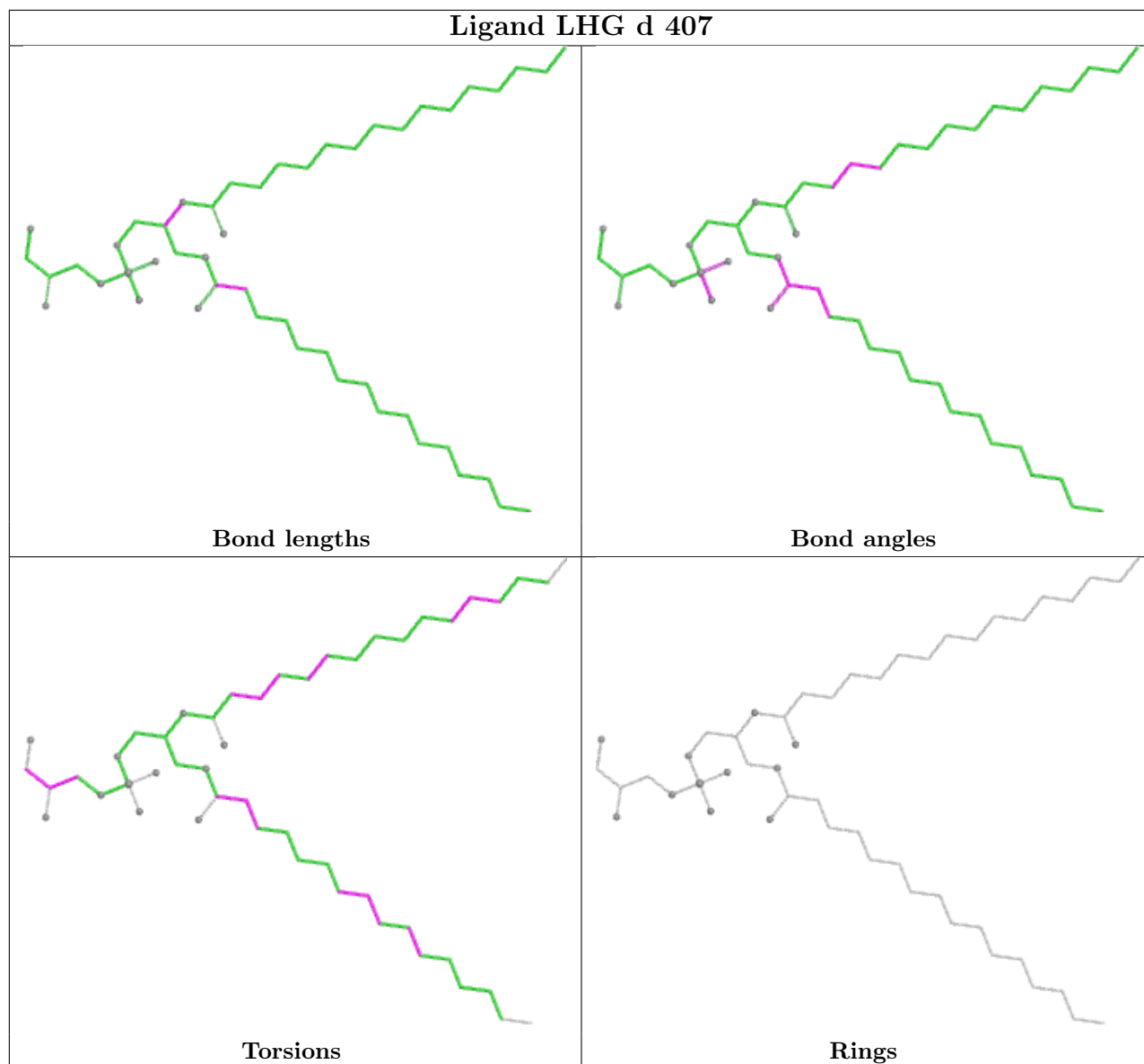


Ligand CLA B 613	
	
Bond lengths	Bond angles
	
Torsions	Rings

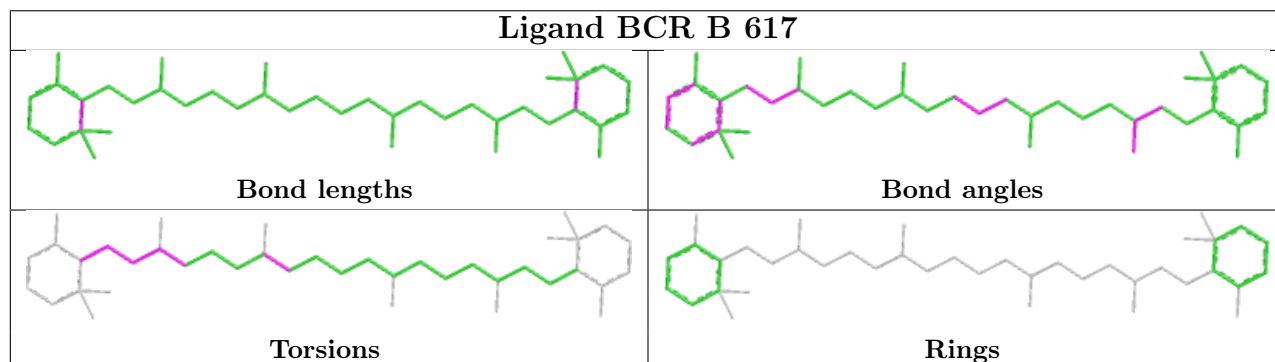
Ligand CLA B 612	
	
Bond lengths	Bond angles
	
Torsions	Rings

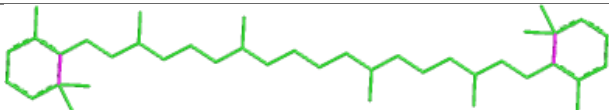
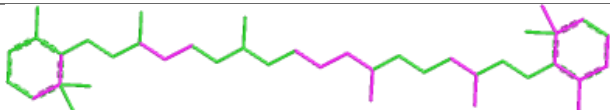
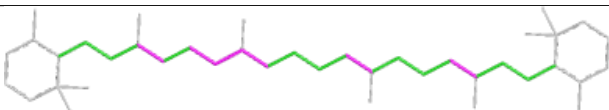
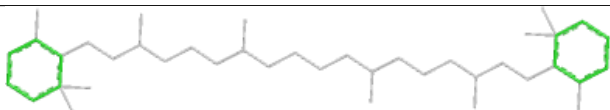
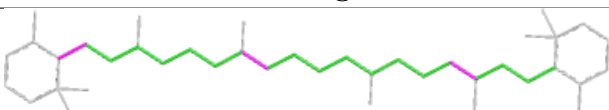
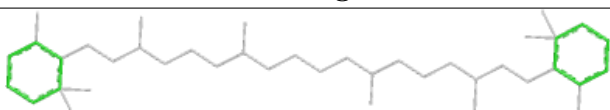
Ligand LMG M 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

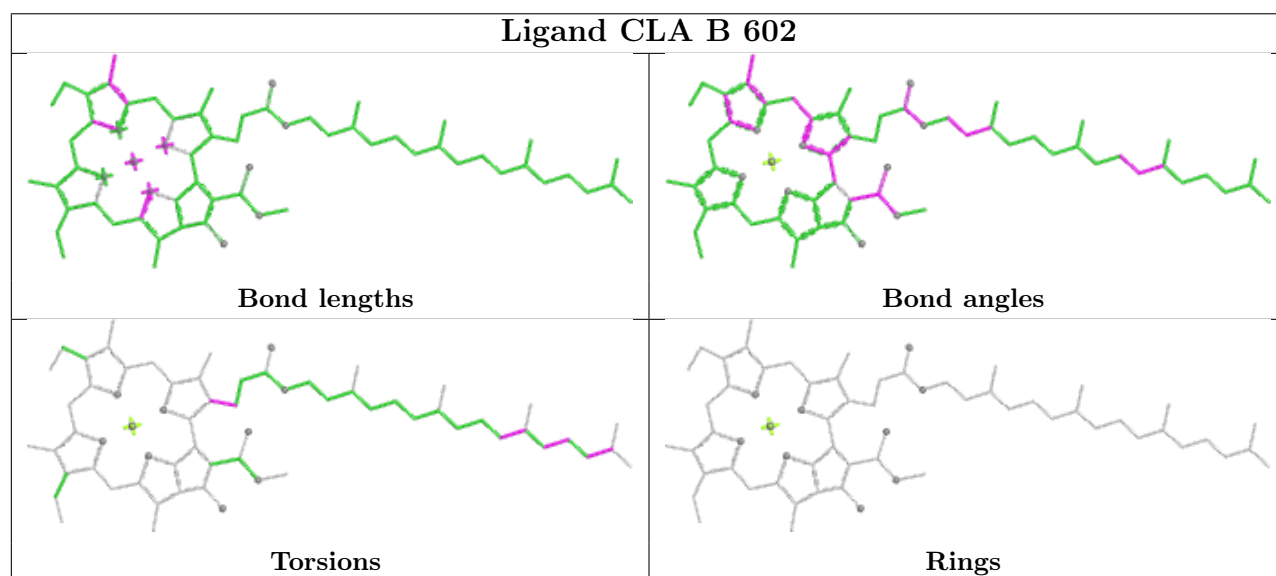
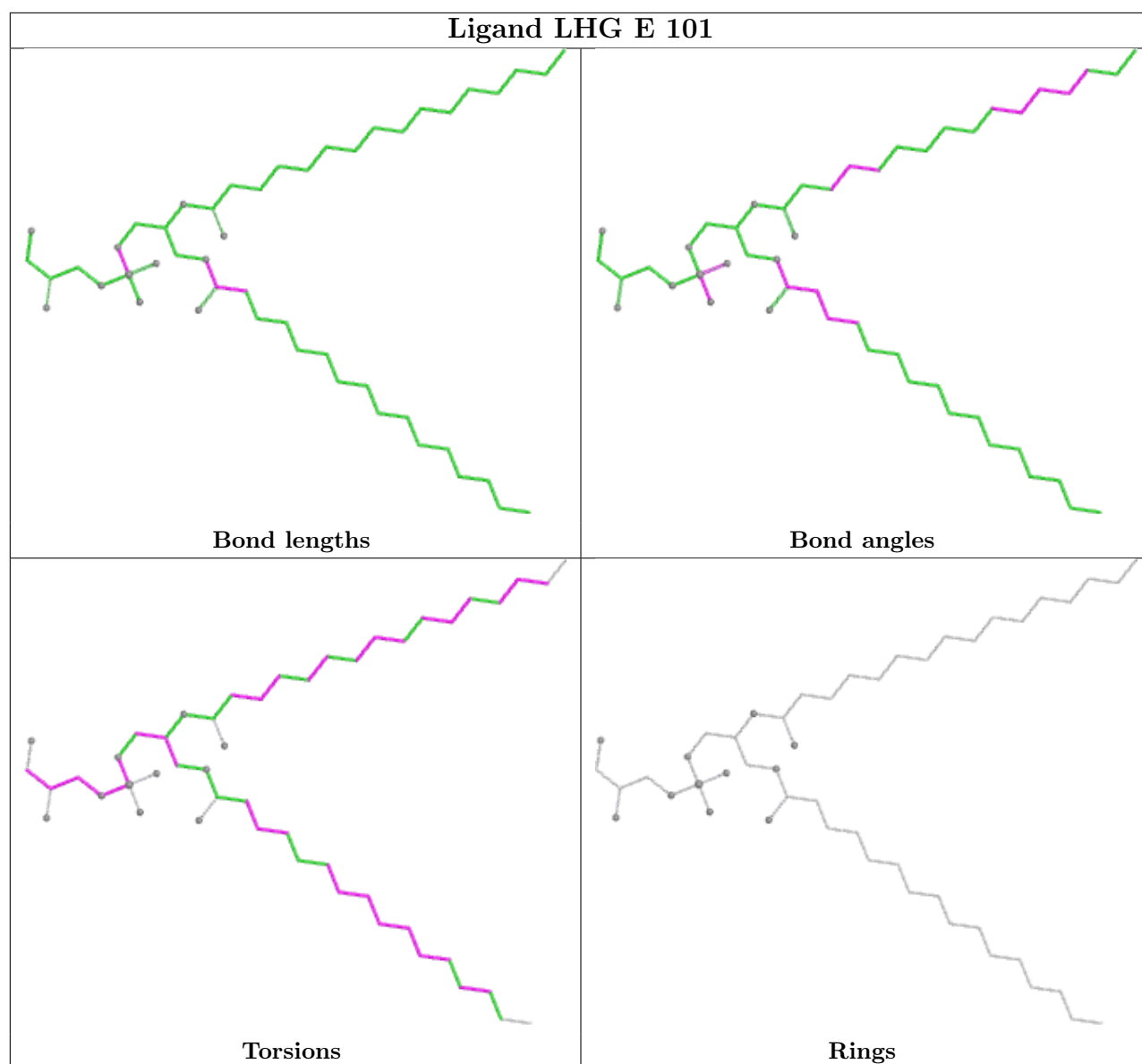
Ligand LHG d 407

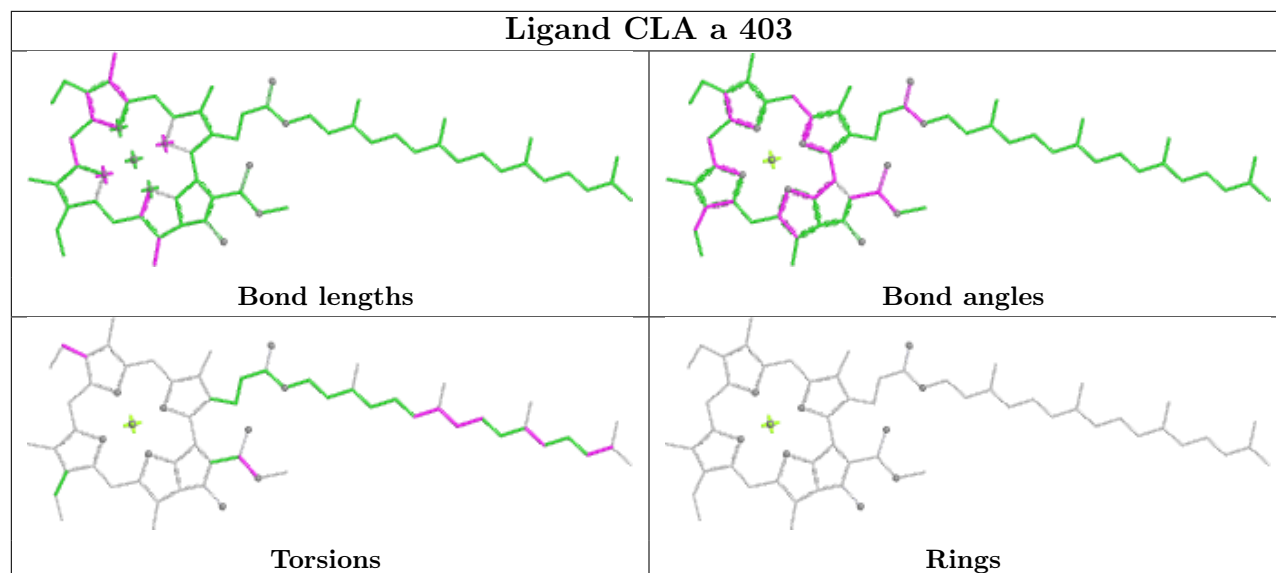
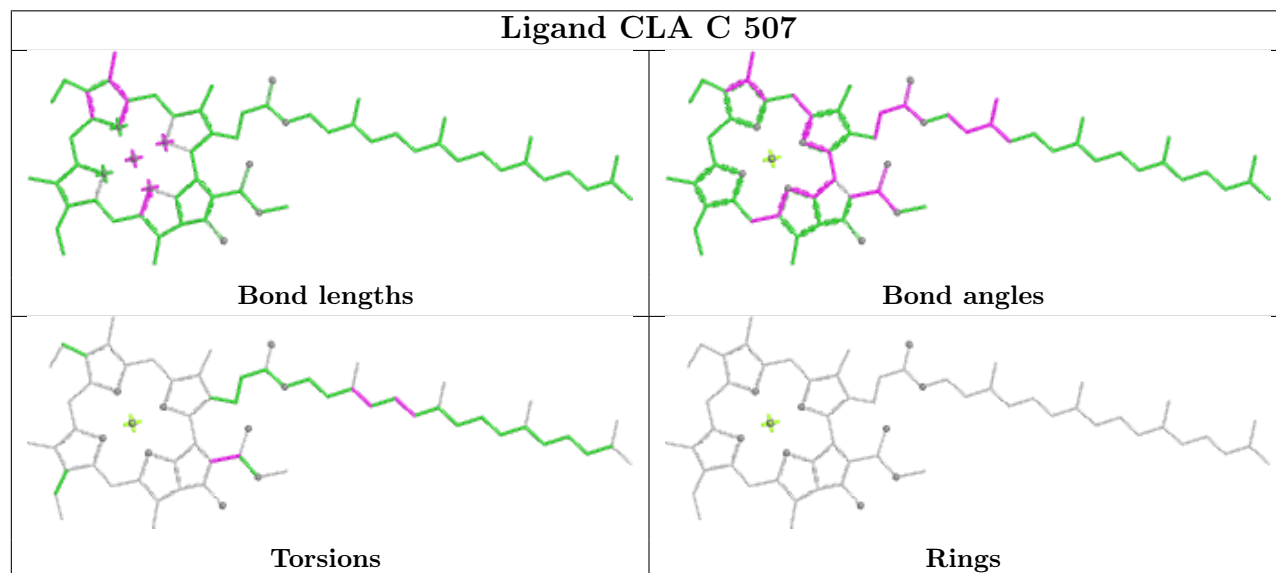
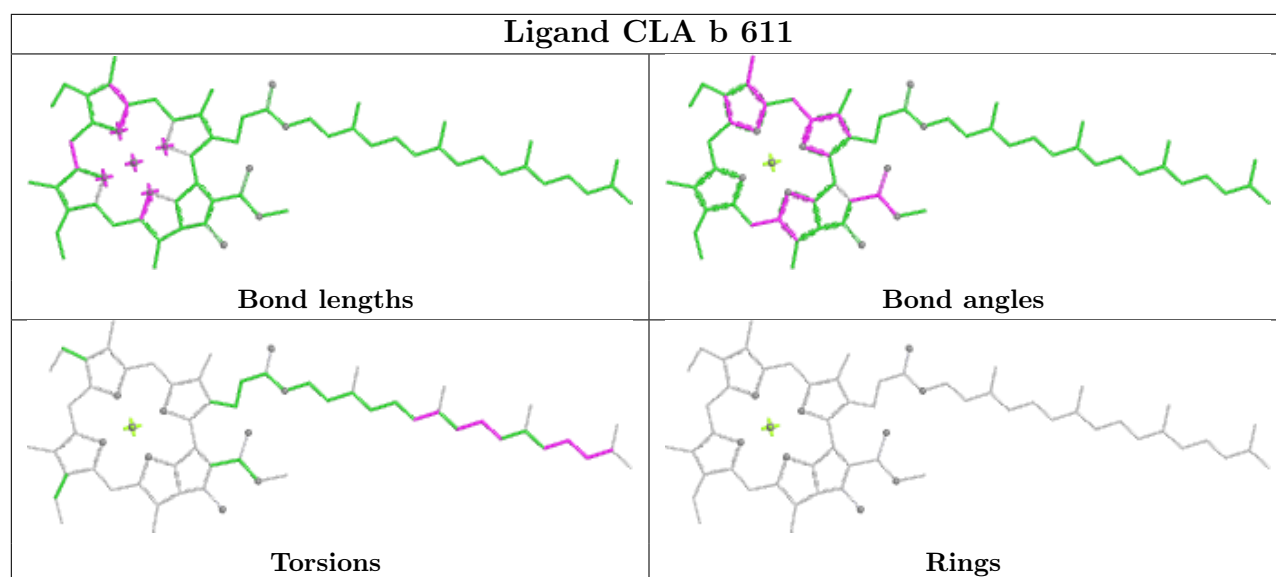


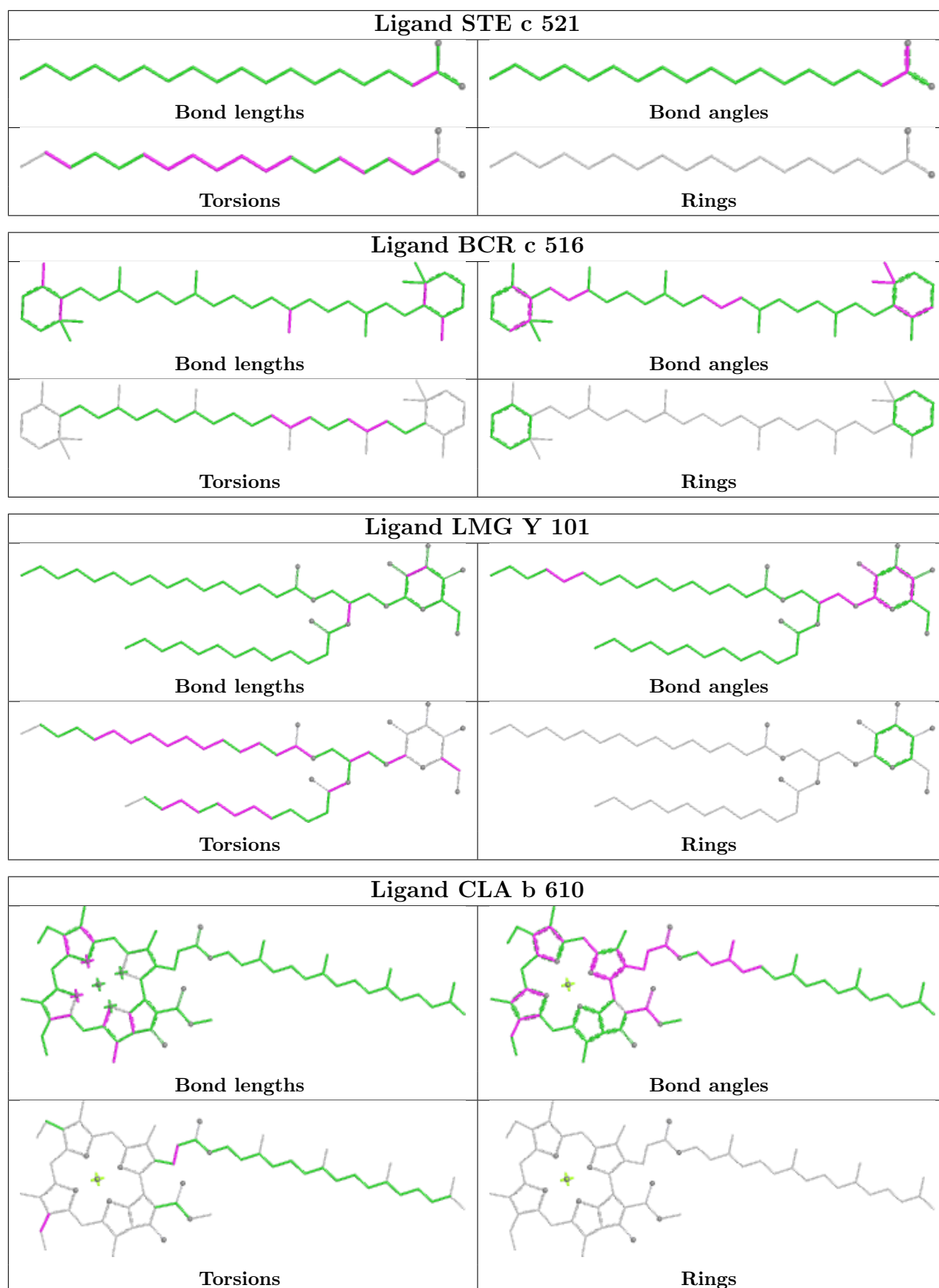
Ligand BCR B 617



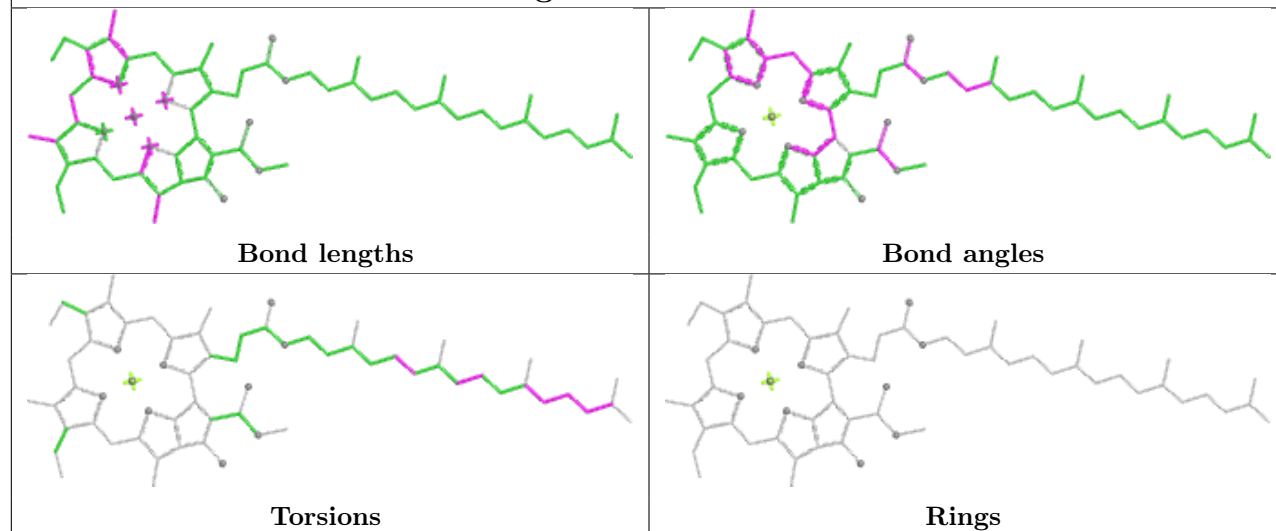
Ligand BCR B 619	
	Bond lengths
	Bond angles
	Torsions
	Rings
Ligand BCR k 102	
	Bond lengths
	Bond angles
	Torsions
	Rings



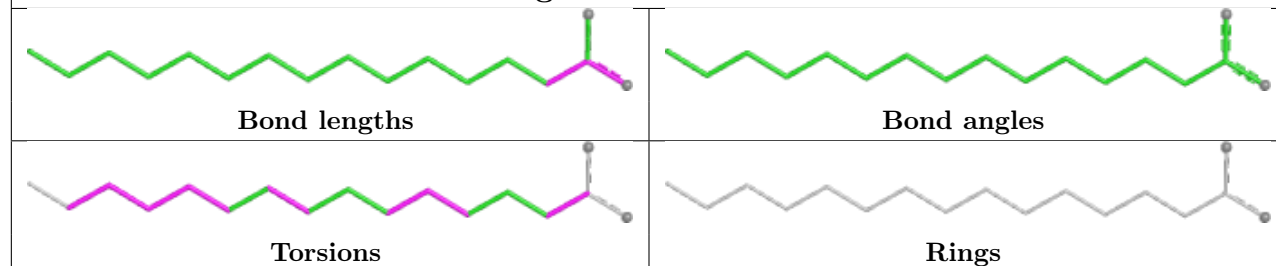




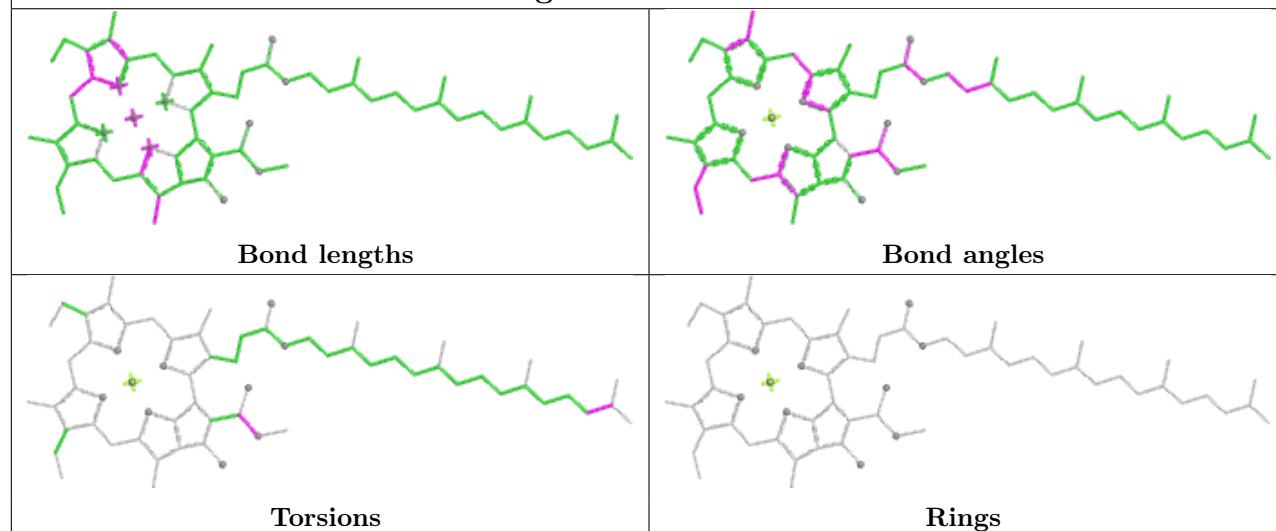
Ligand CLA b 615

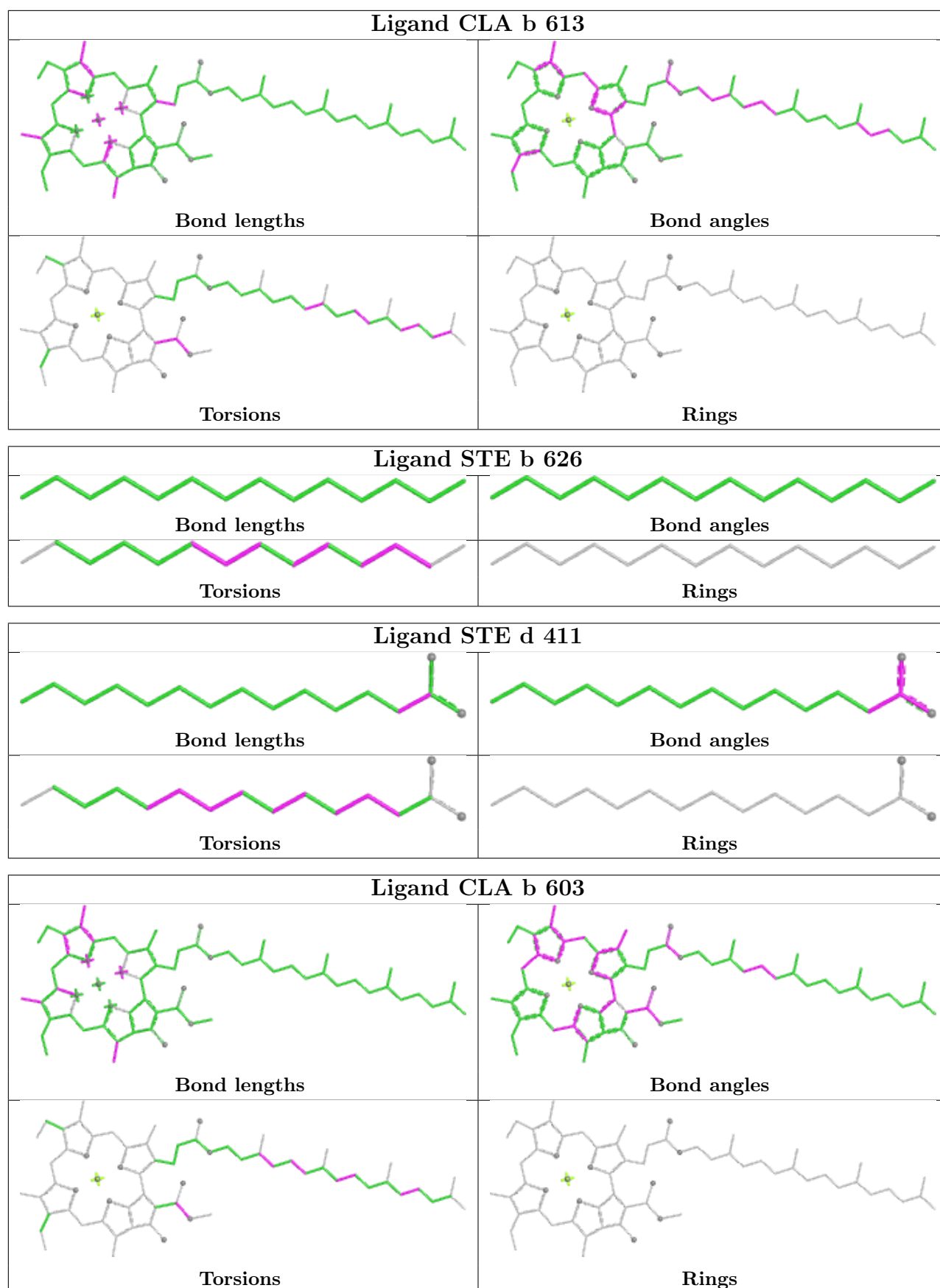


Ligand STE B 620

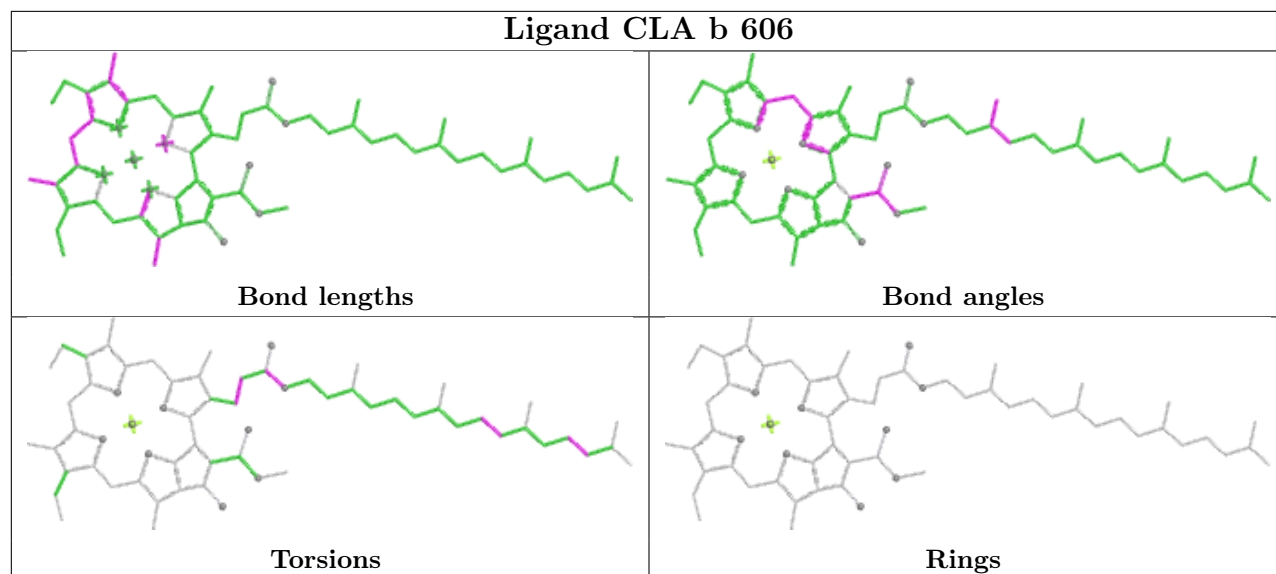


Ligand CLA d 404

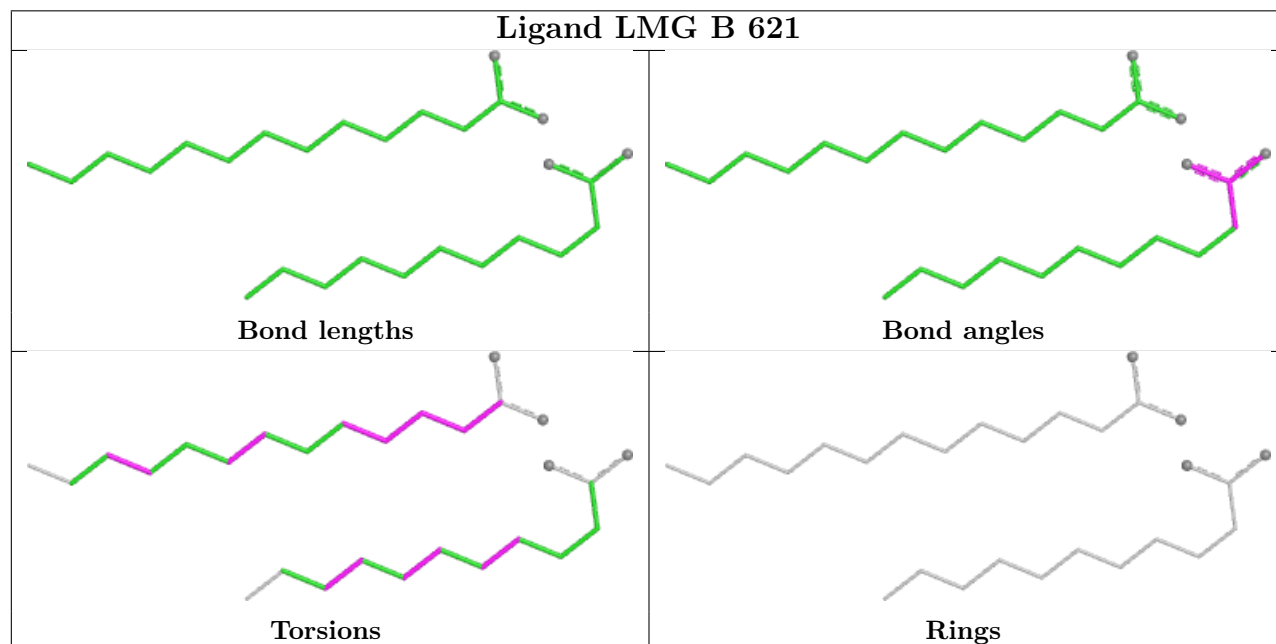


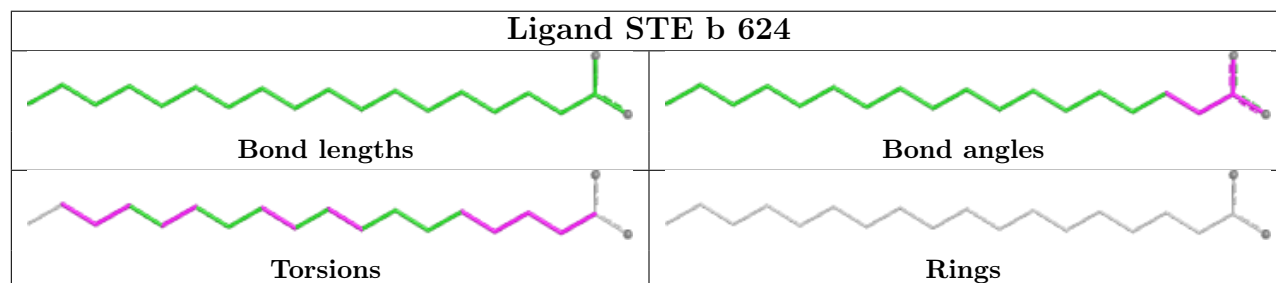
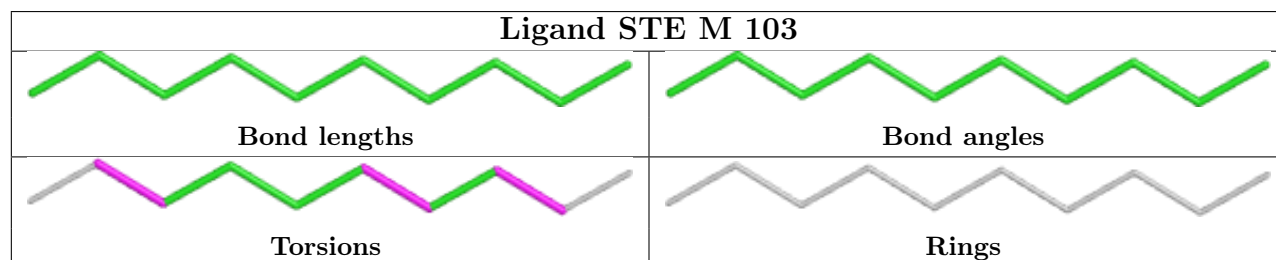
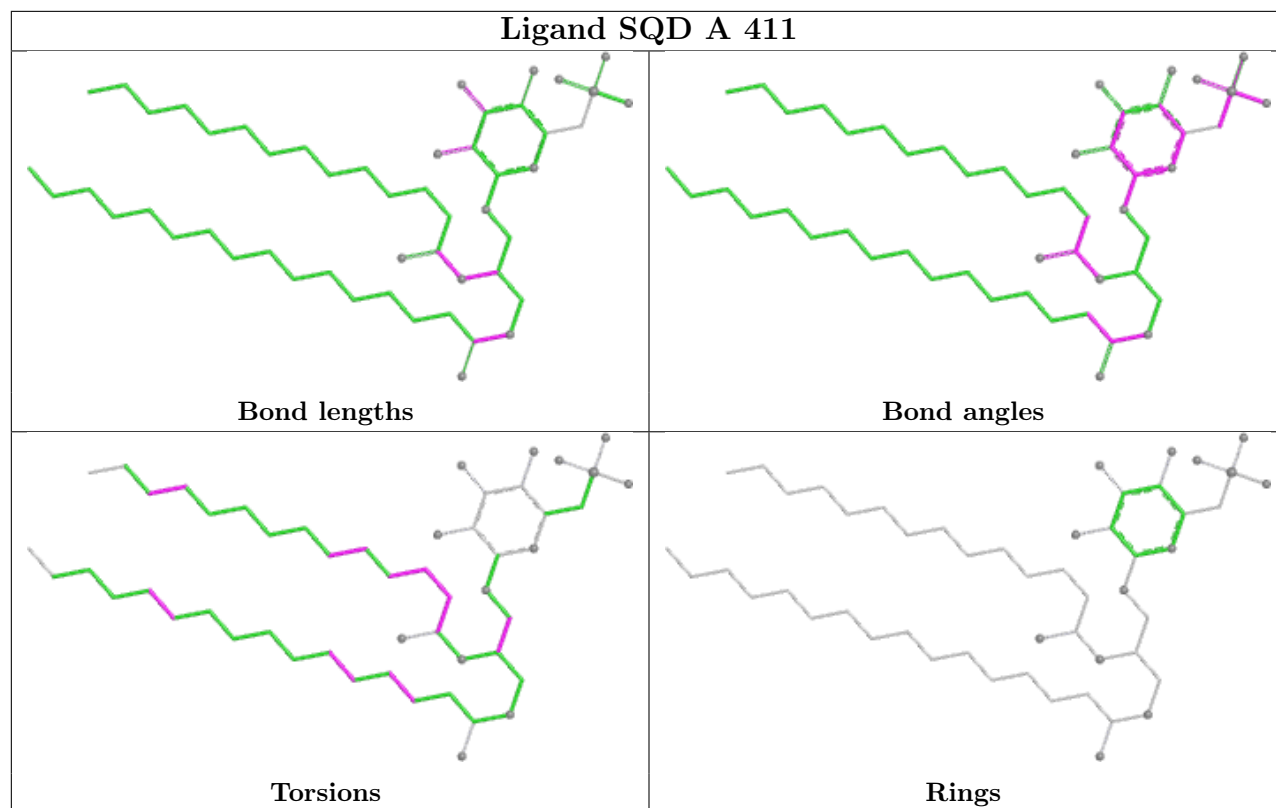


Ligand CLA b 606

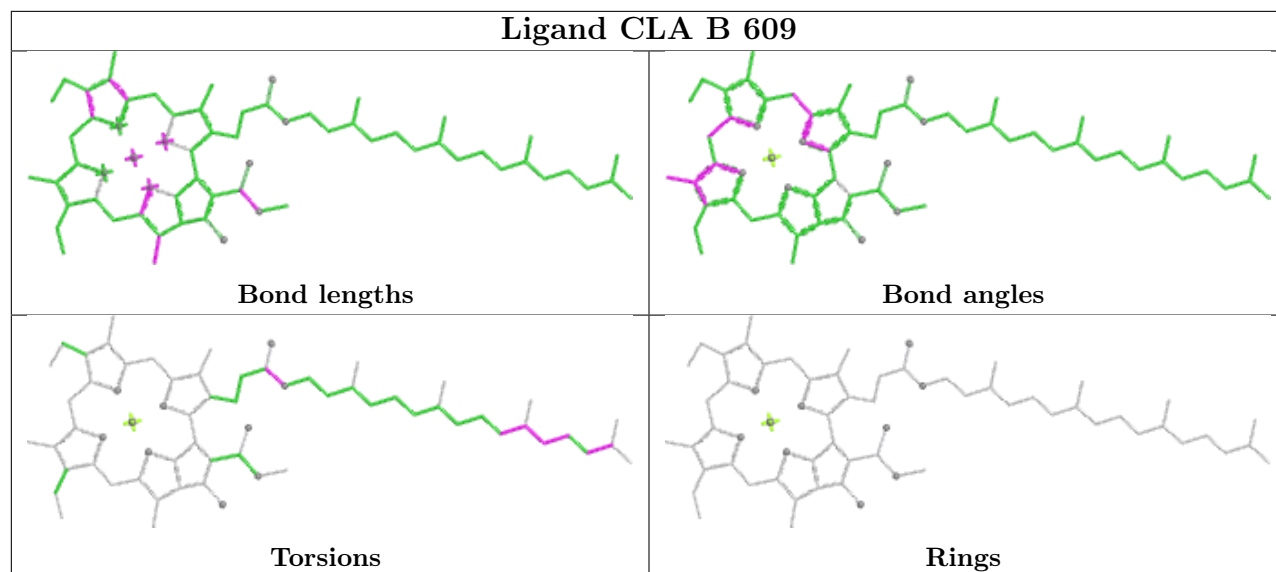


Ligand LMG B 621

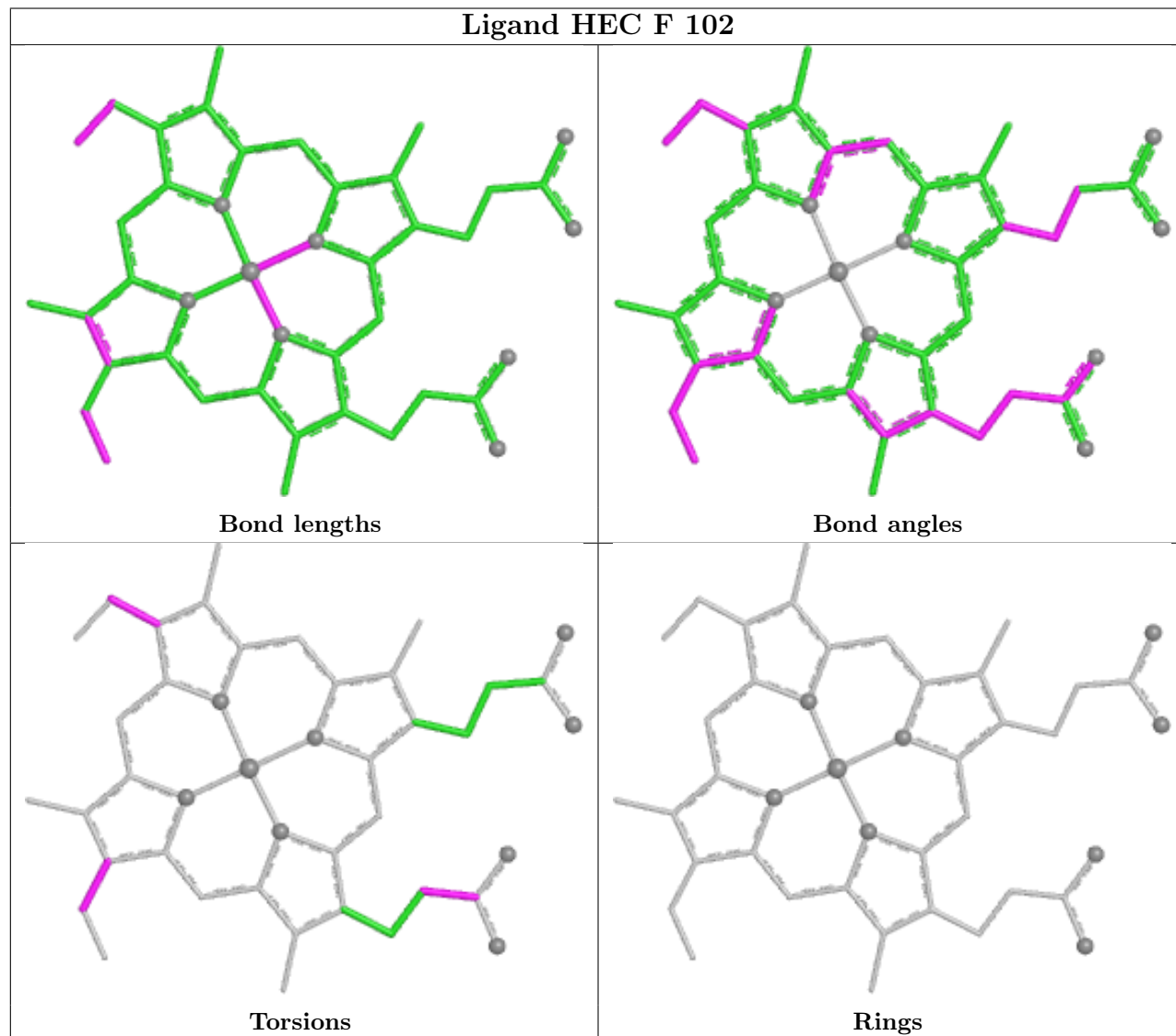


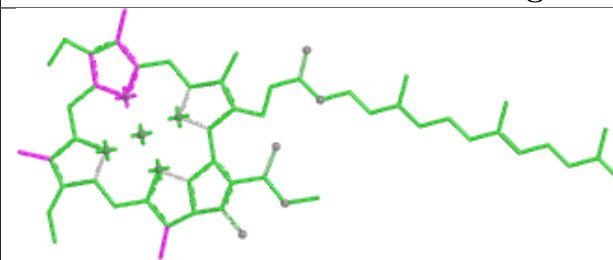
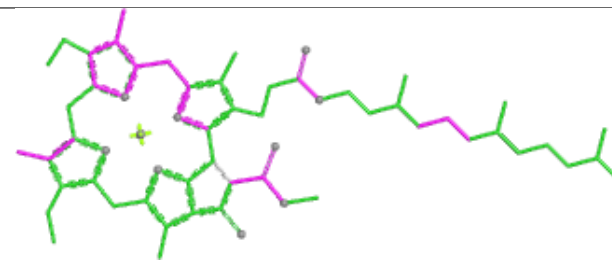
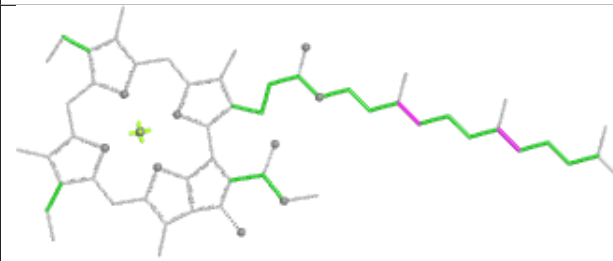
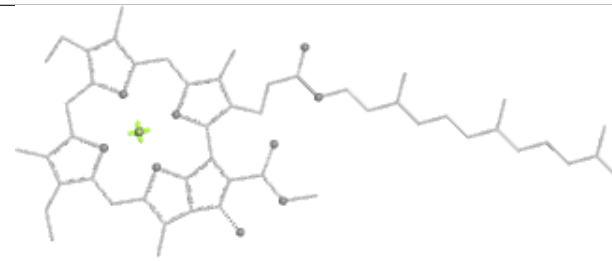


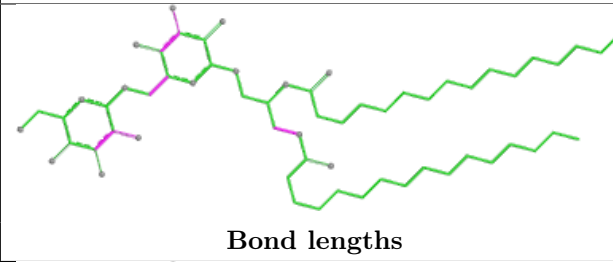
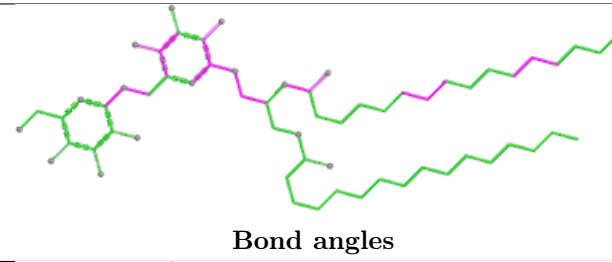
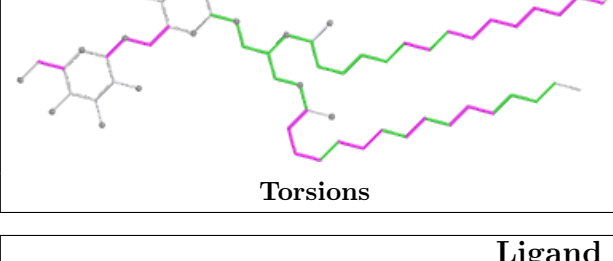
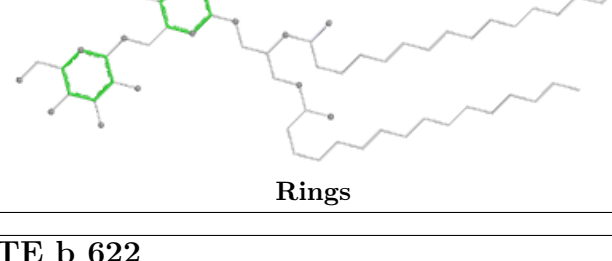
Ligand CLA B 609

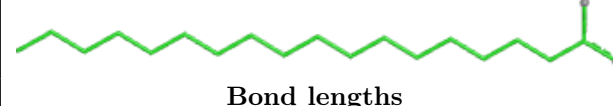
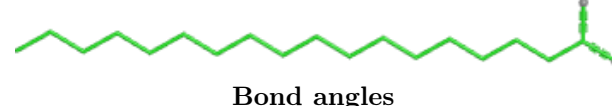
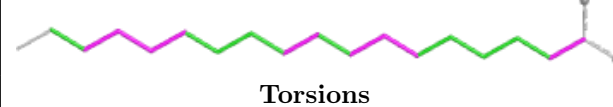


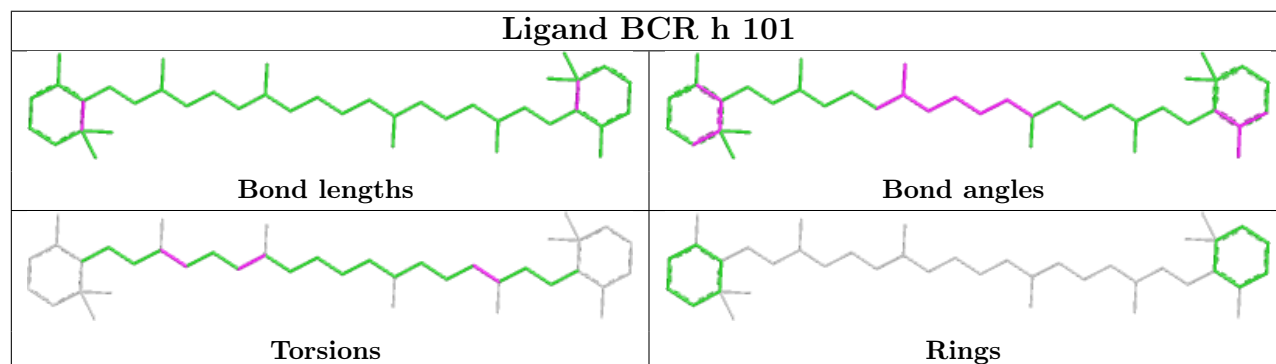
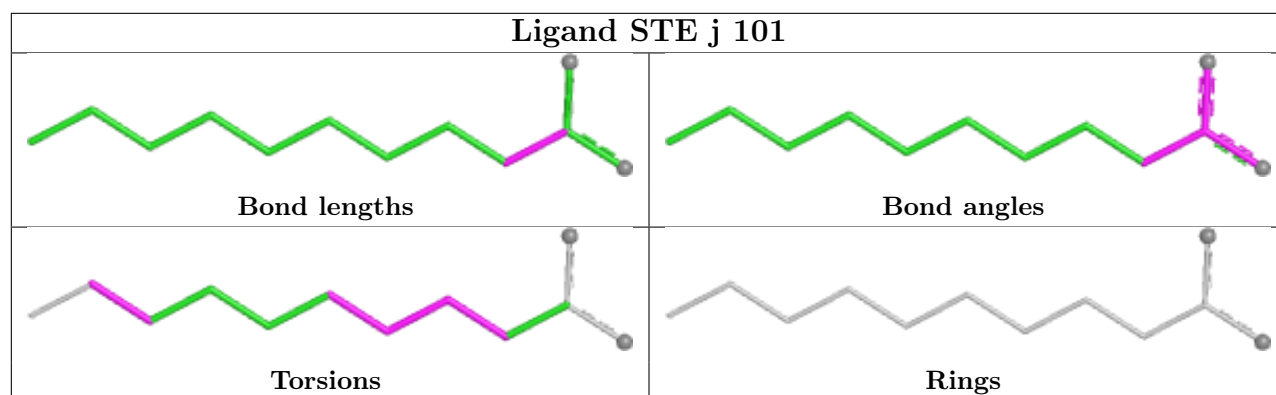
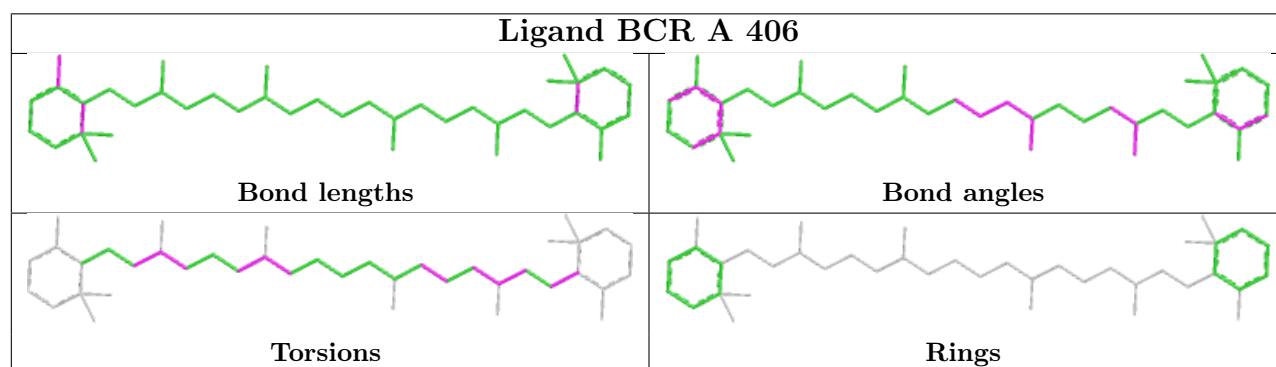
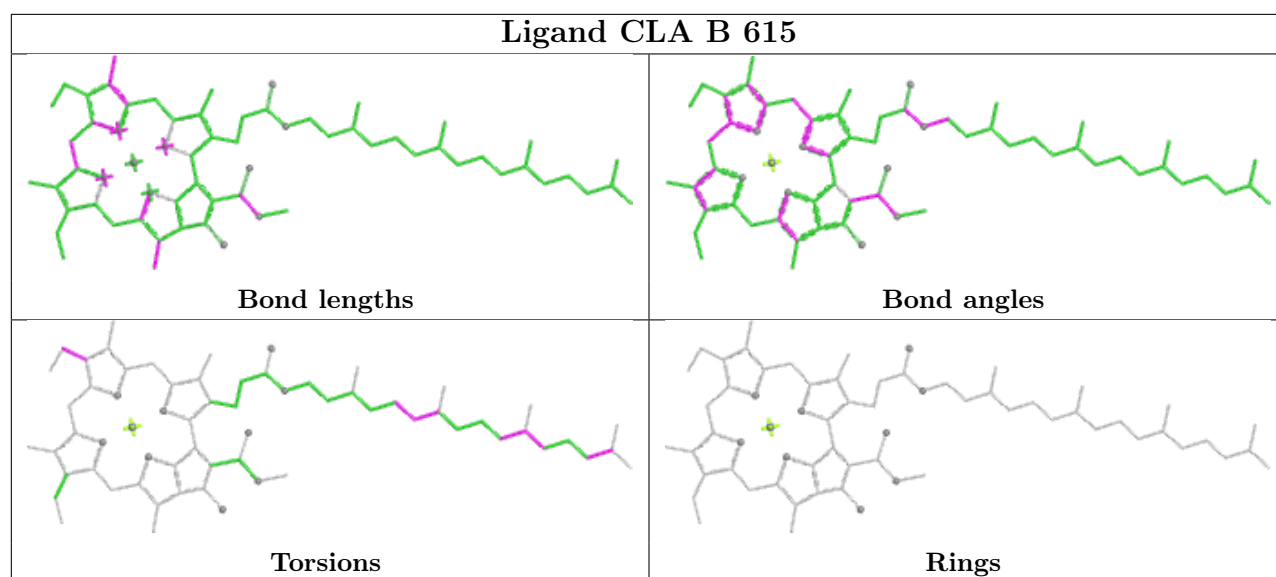
Ligand HEC F 102

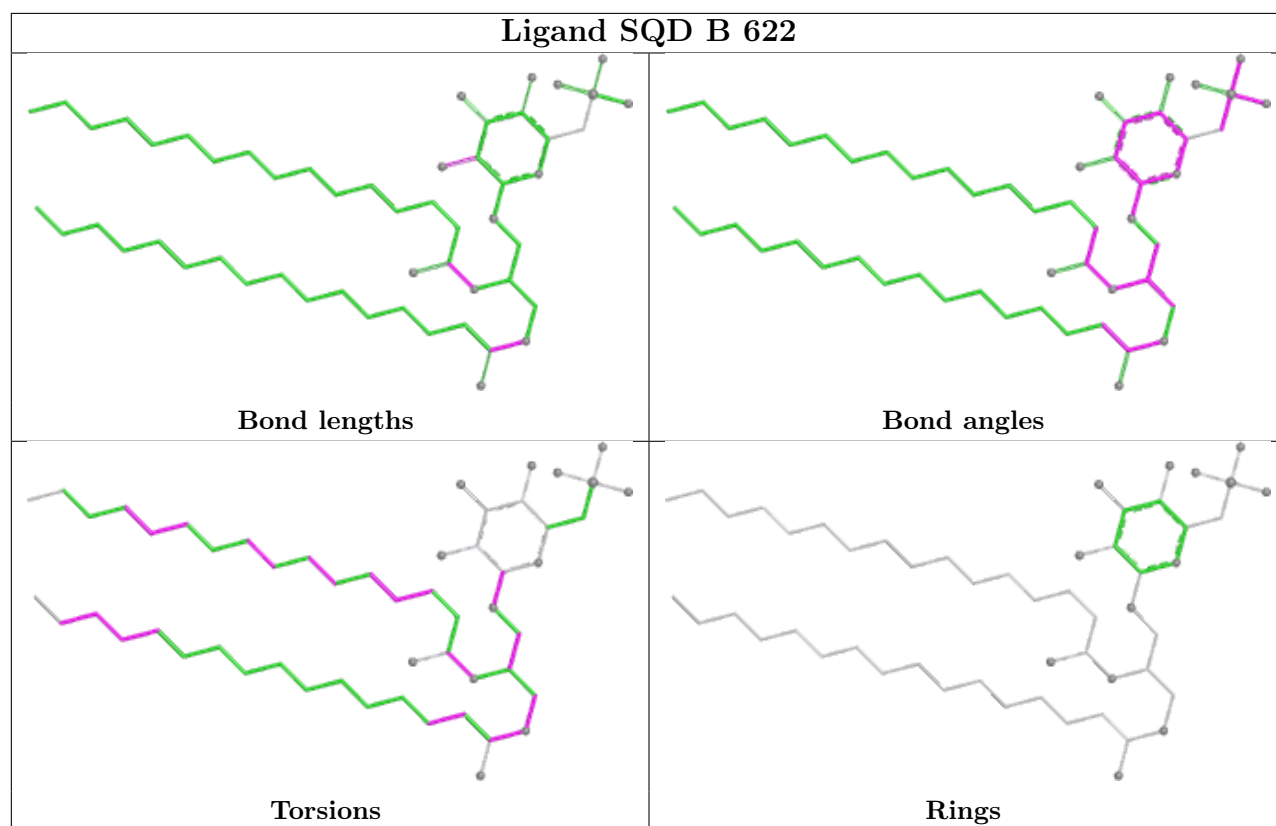
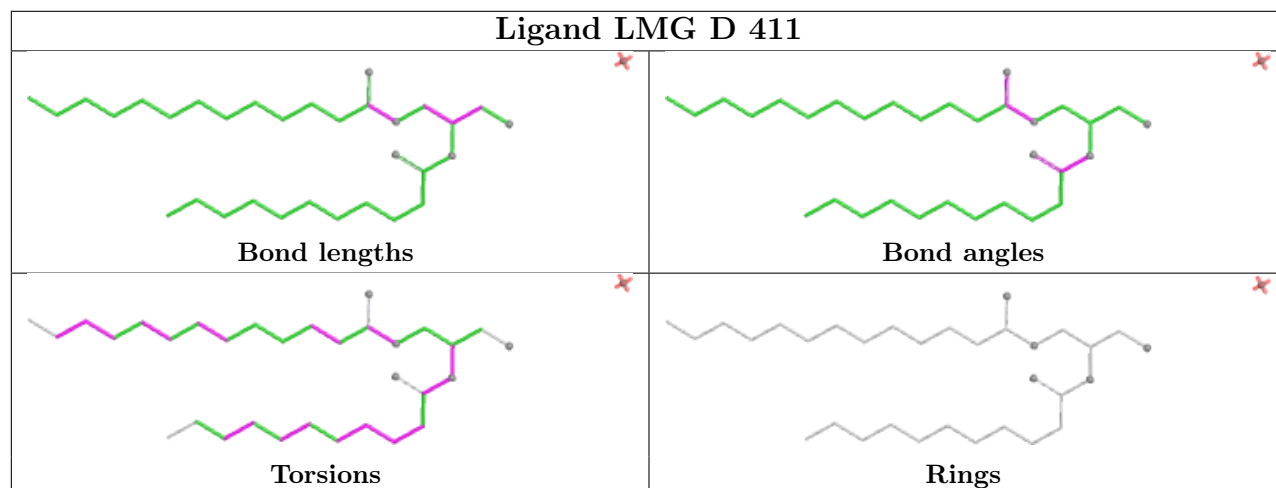
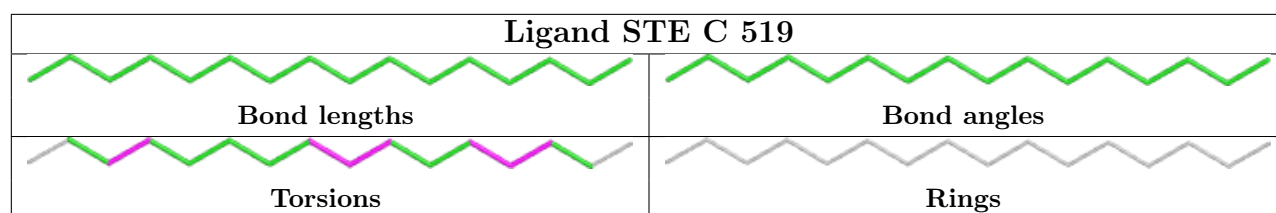


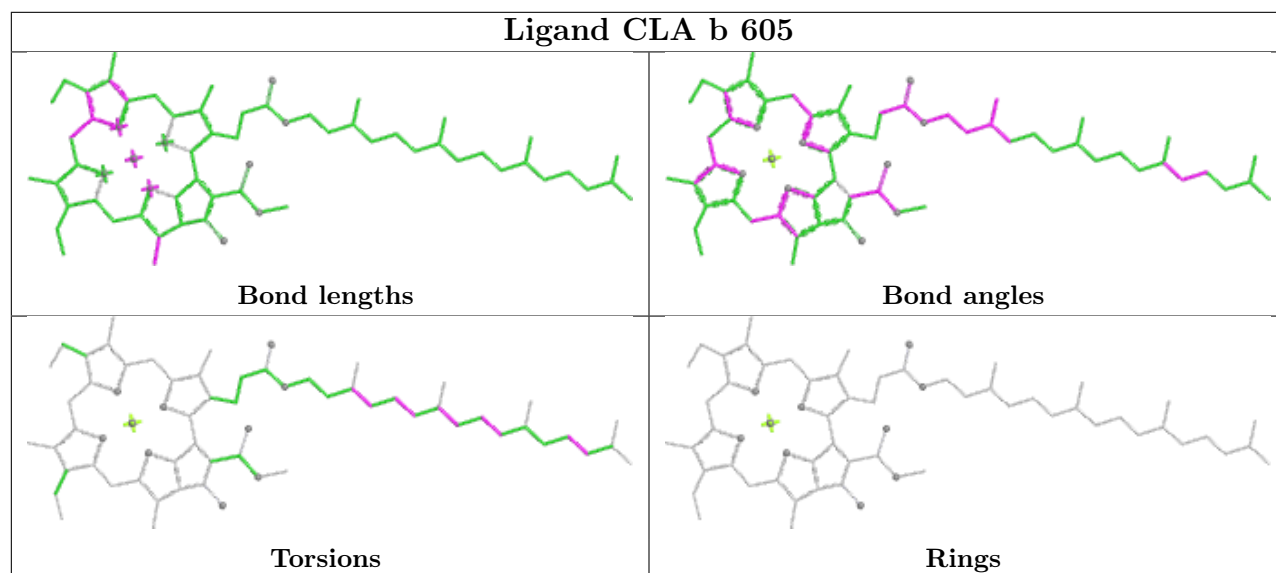
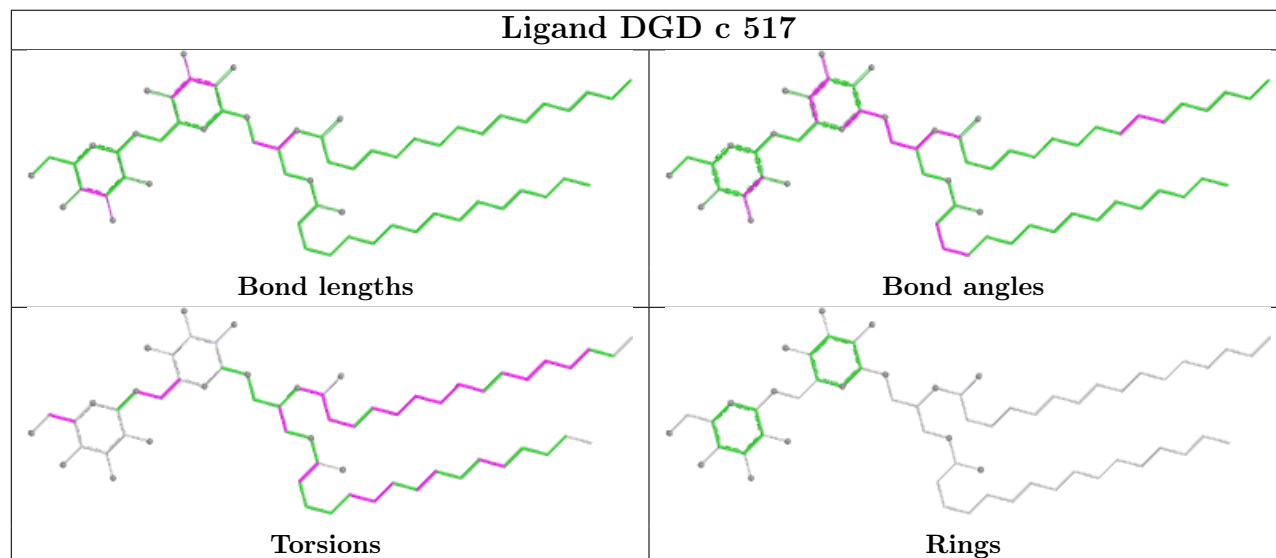
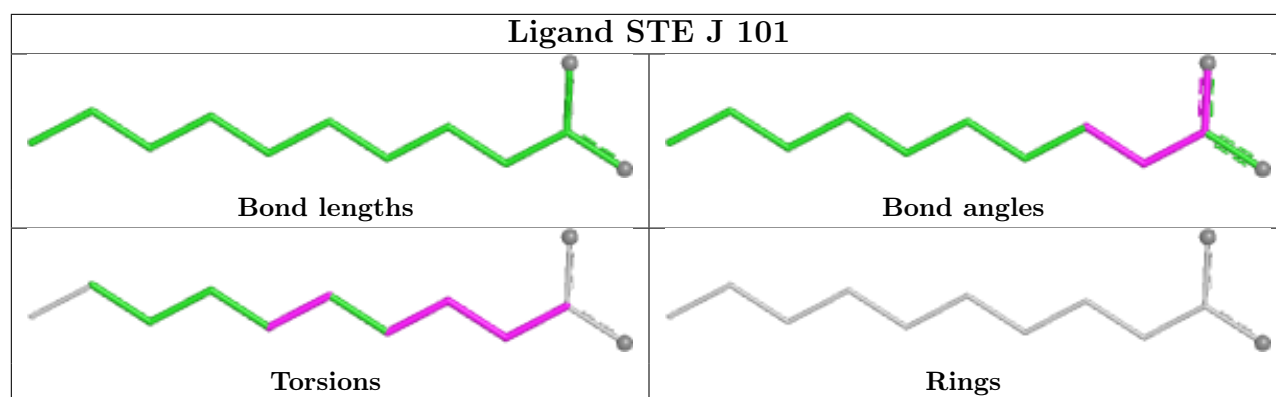
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Bond lengths	Bond angles
	
Torsions	Rings

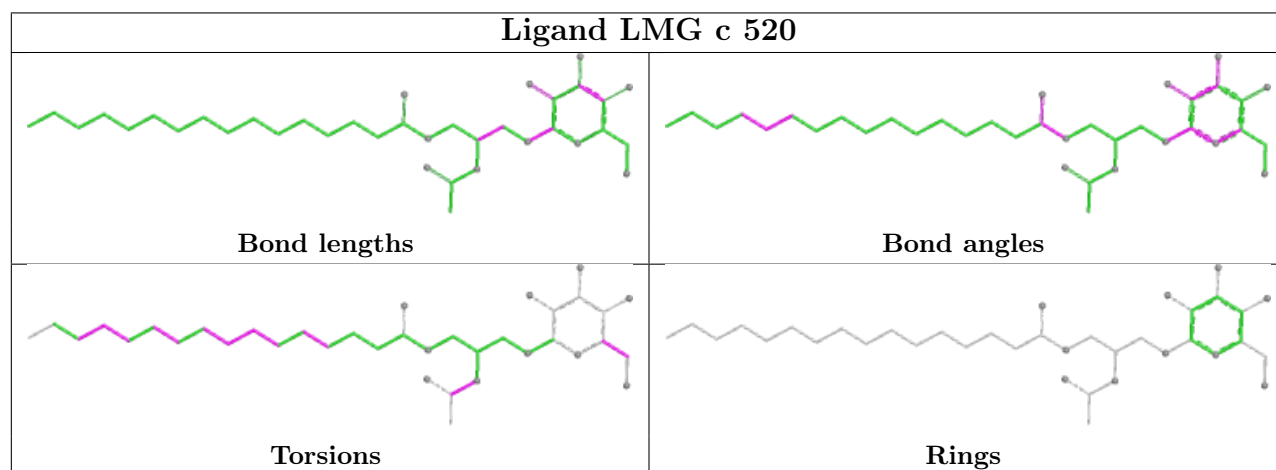
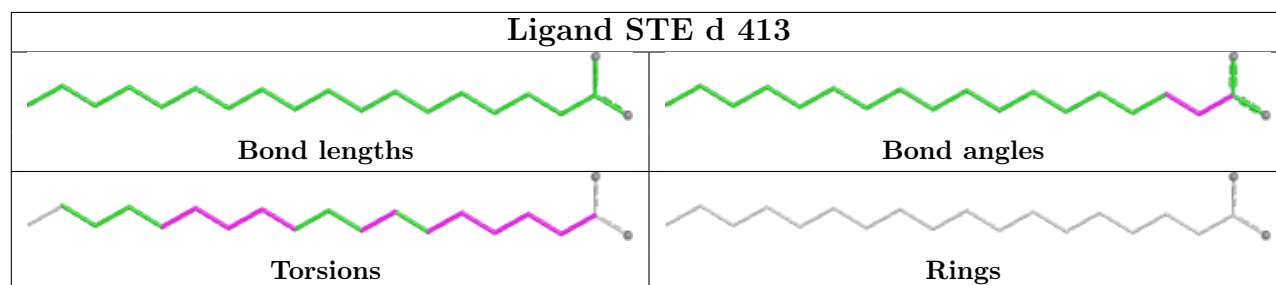
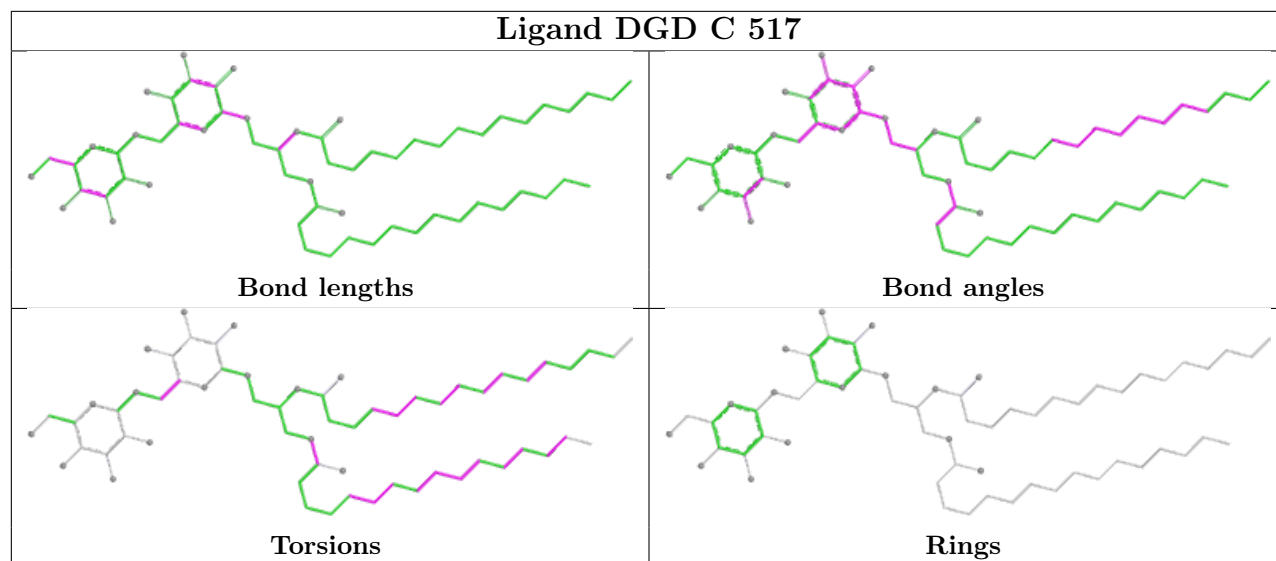
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Bond lengths	Bond angles
	
Torsions	Rings

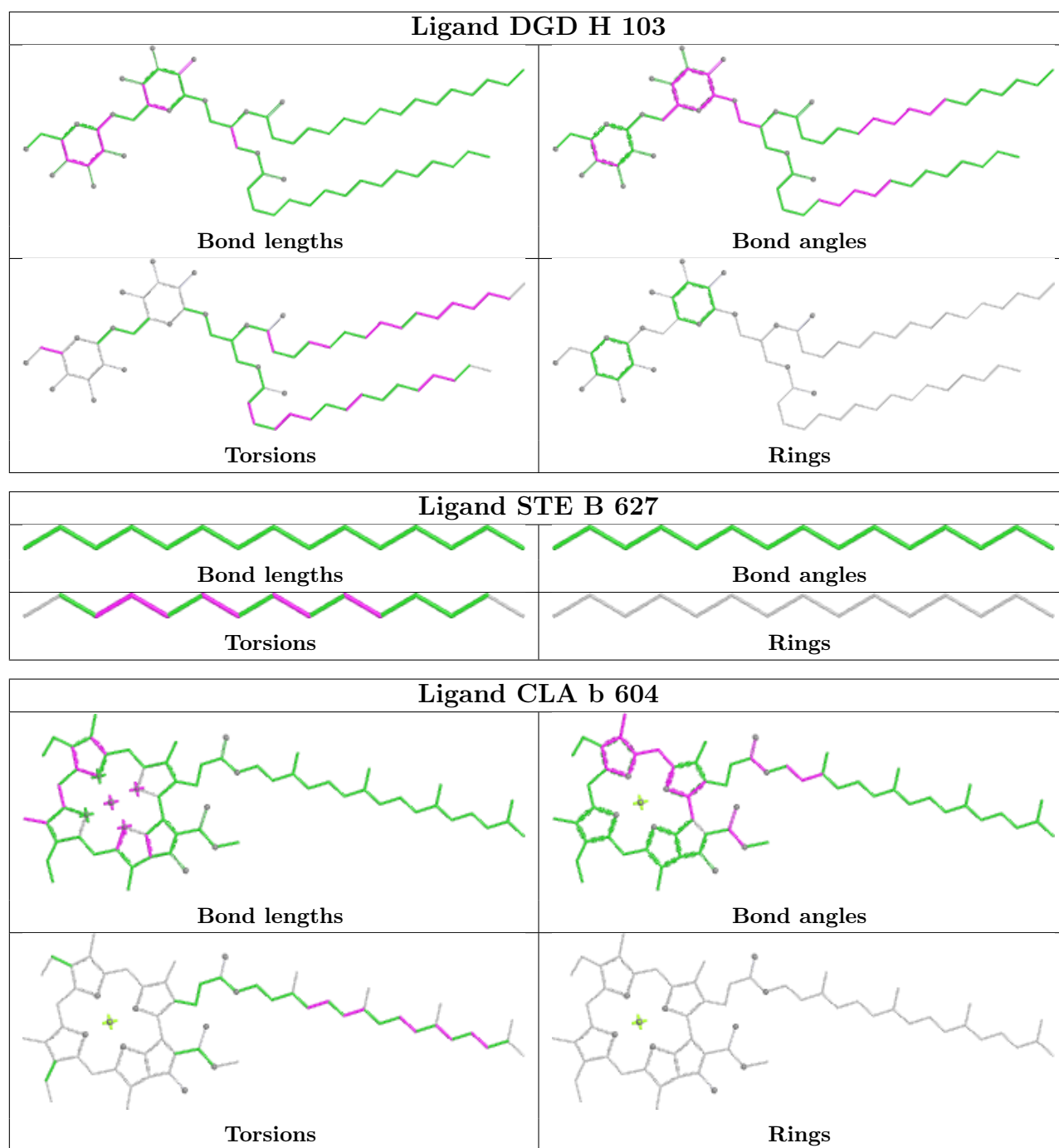
Ligand STE b 622	
	
Bond lengths	Bond angles
	
Torsions	Rings



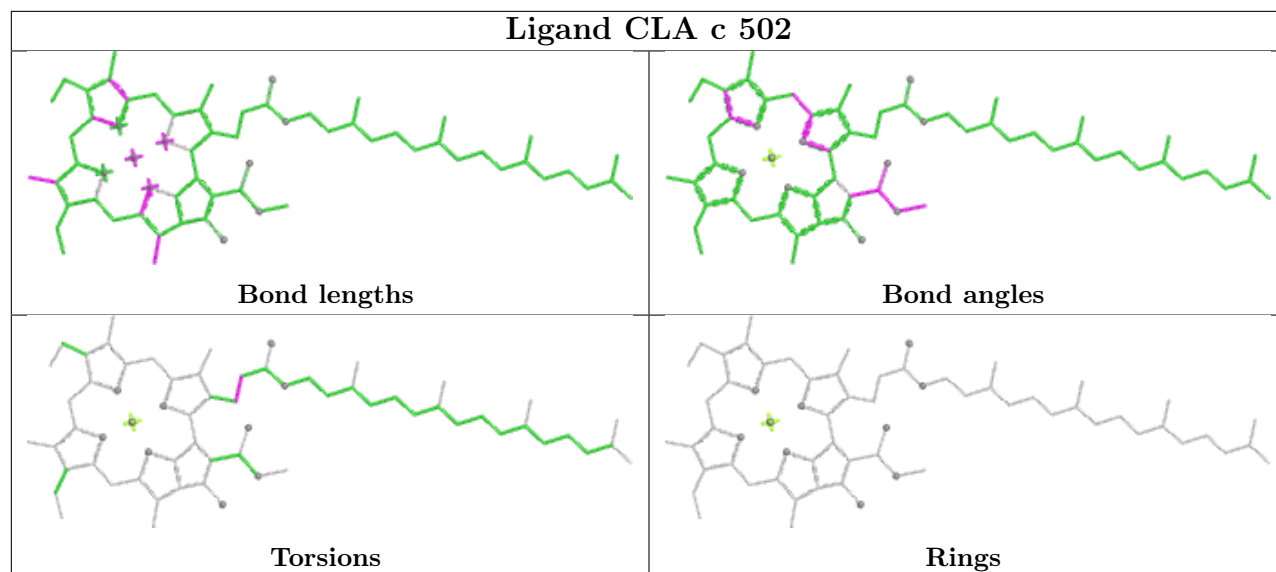




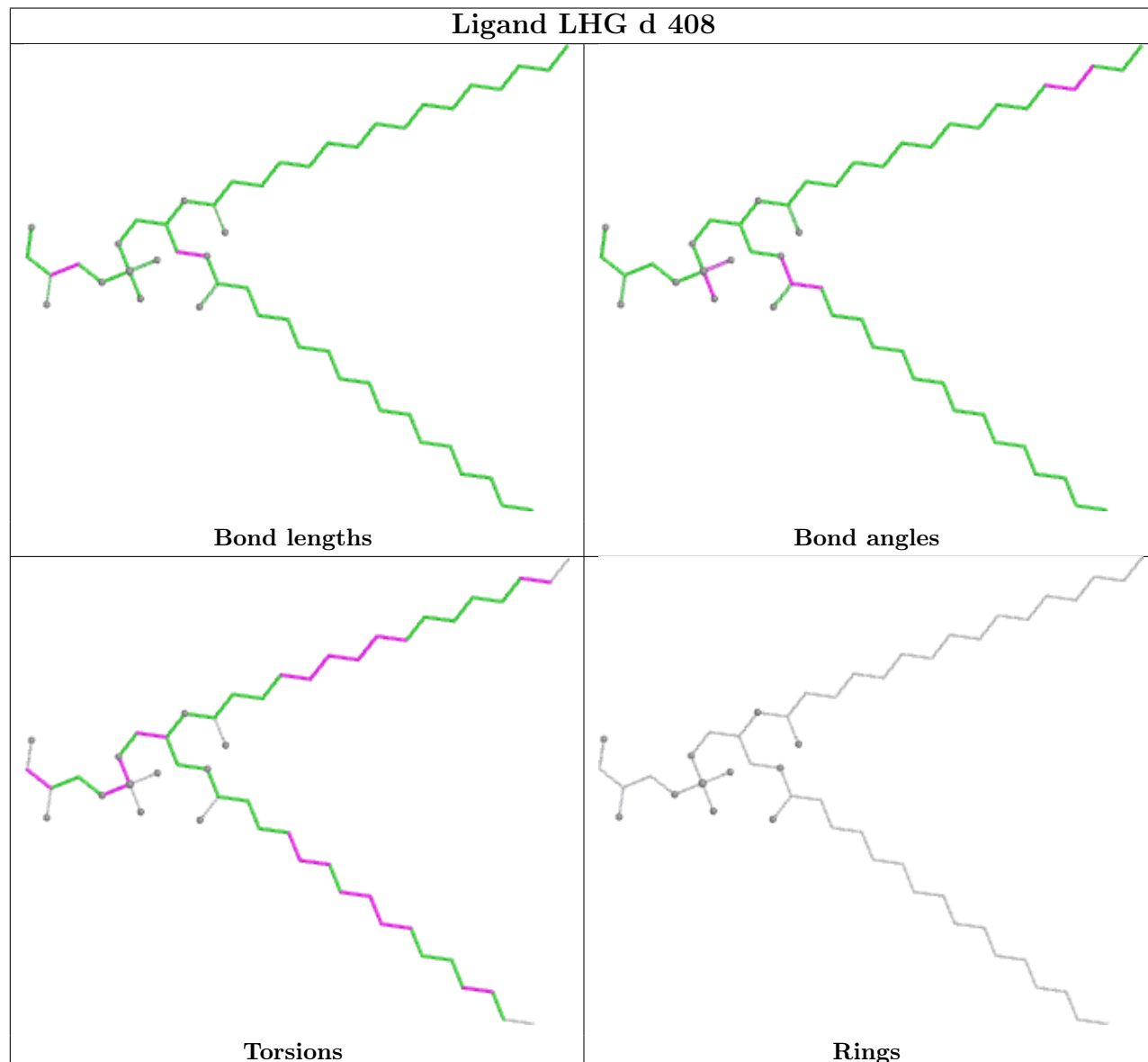


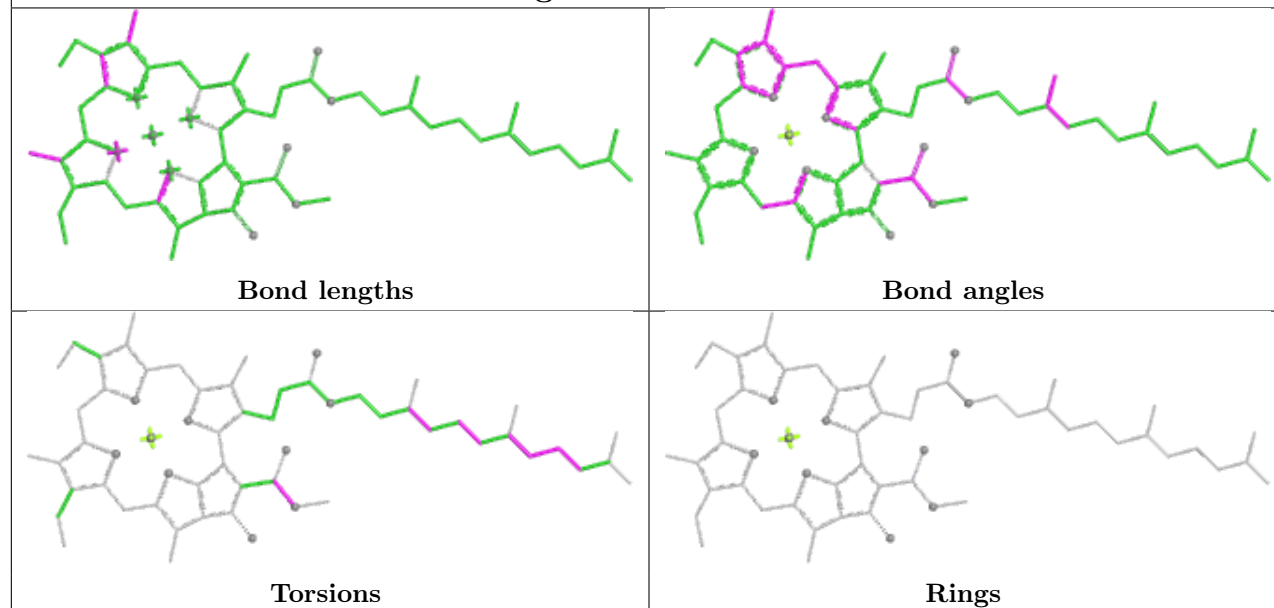
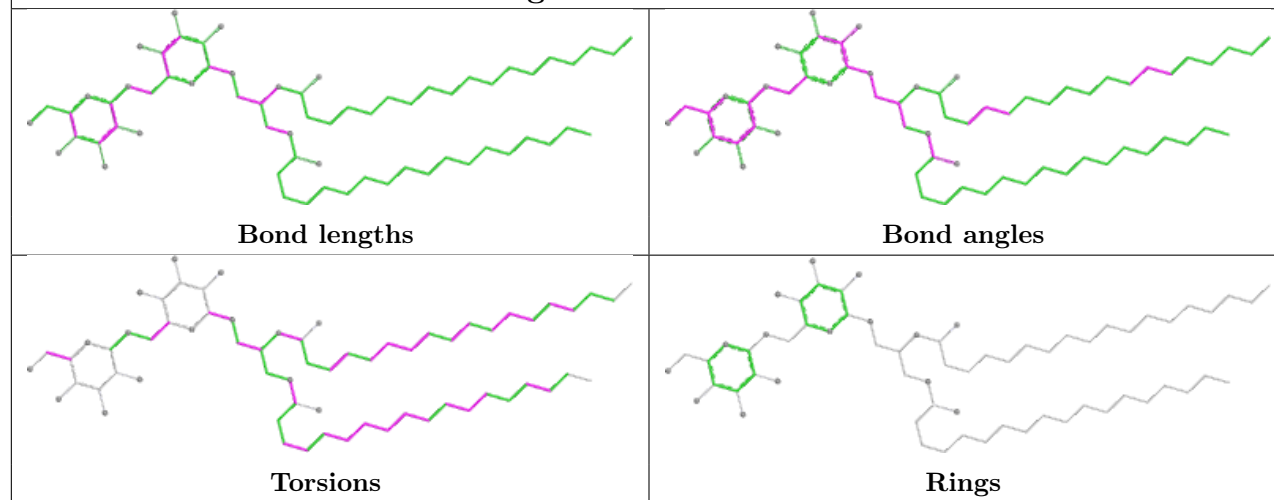


Ligand CLA c 502

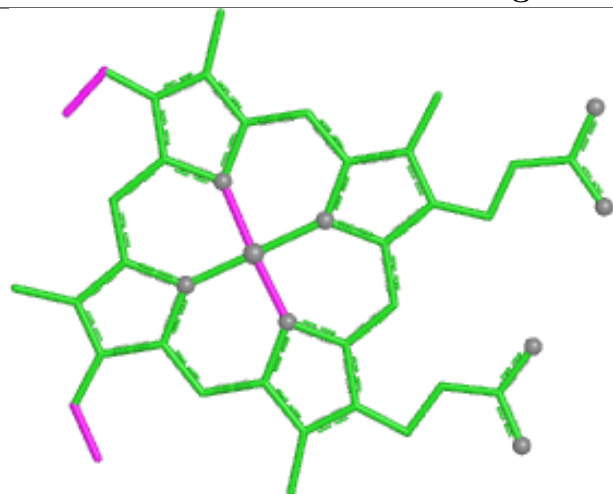


Ligand LHG d 408

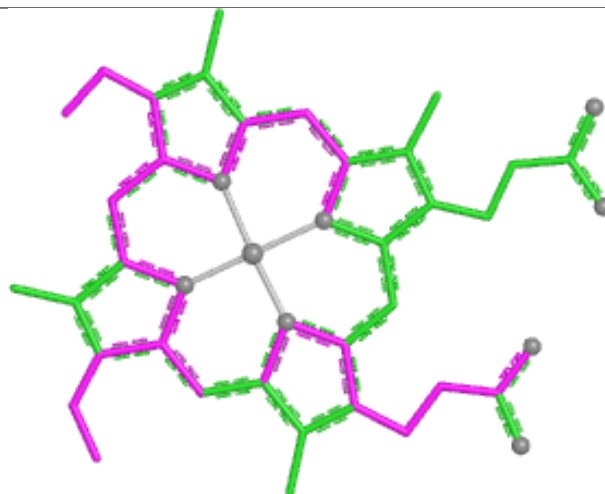


Ligand CLA b 616**Ligand DGD A 413**

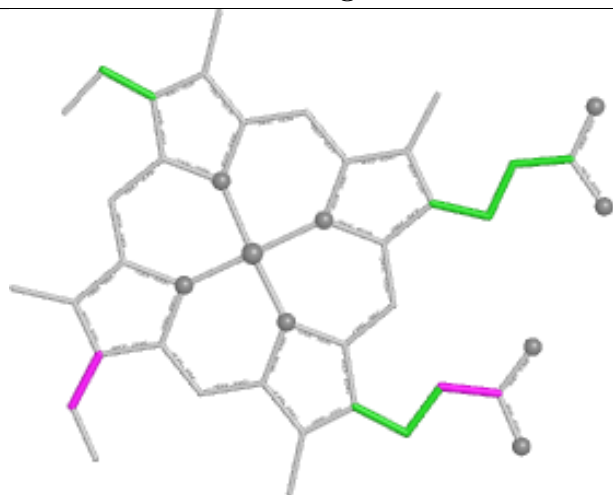
Ligand HEC V 201



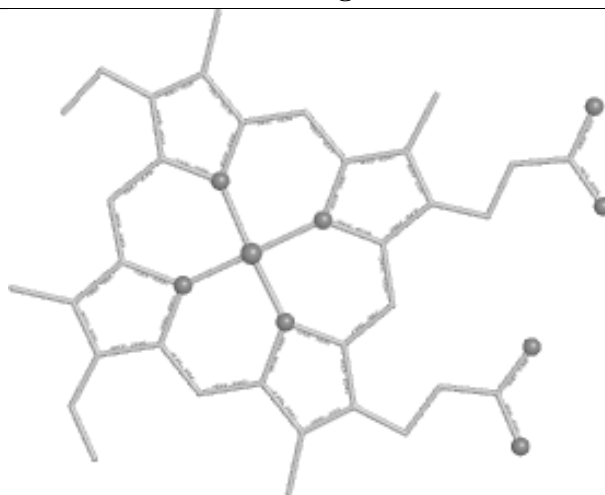
Bond lengths



Bond angles

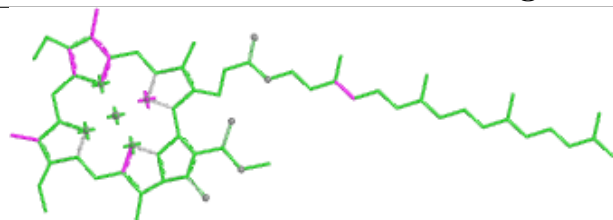


Torsions

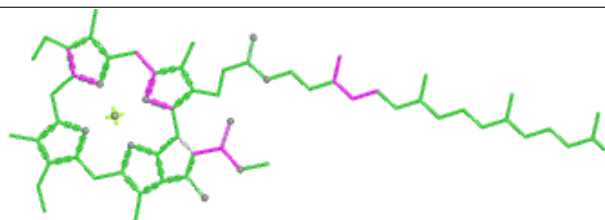


Rings

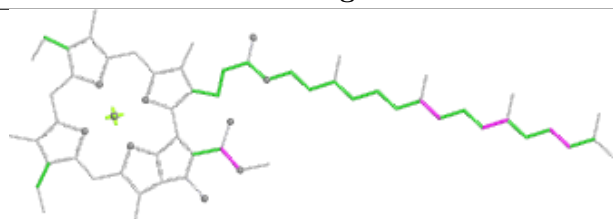
Ligand CLA c 511



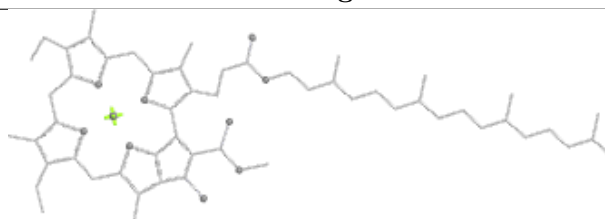
Bond lengths



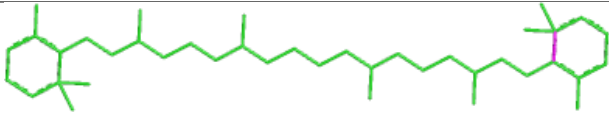
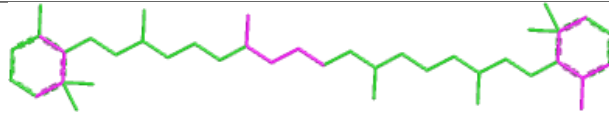
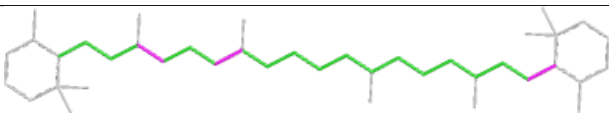
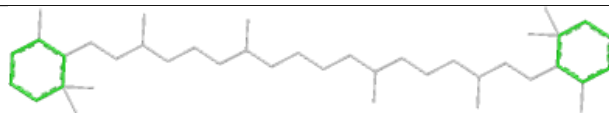
Bond angles

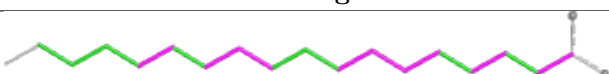
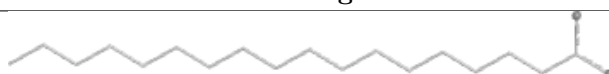


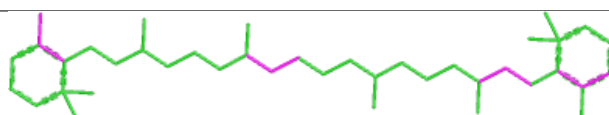
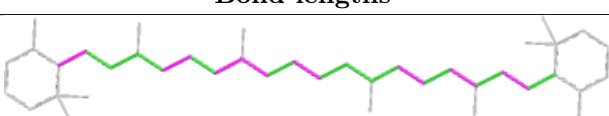
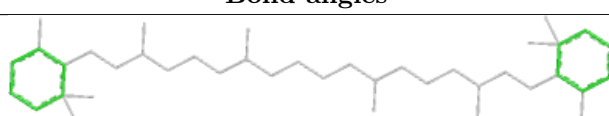
Torsions

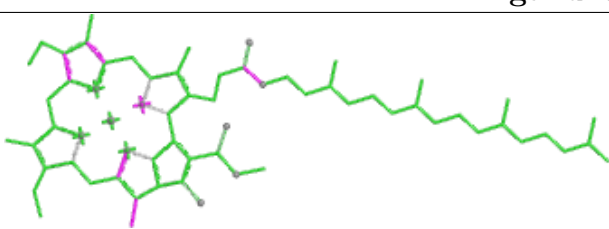
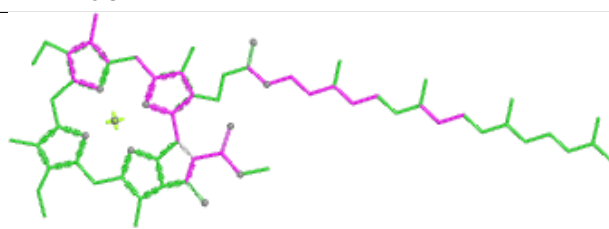
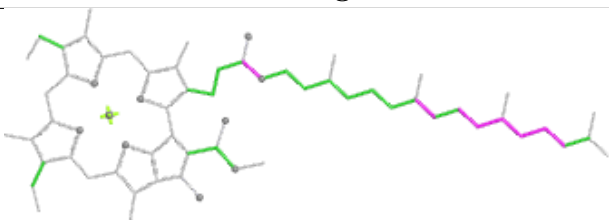
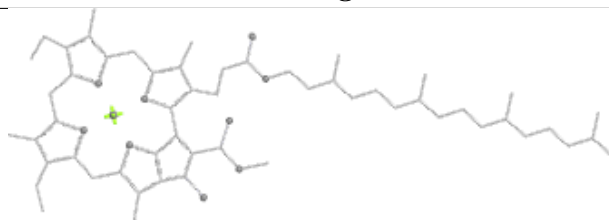


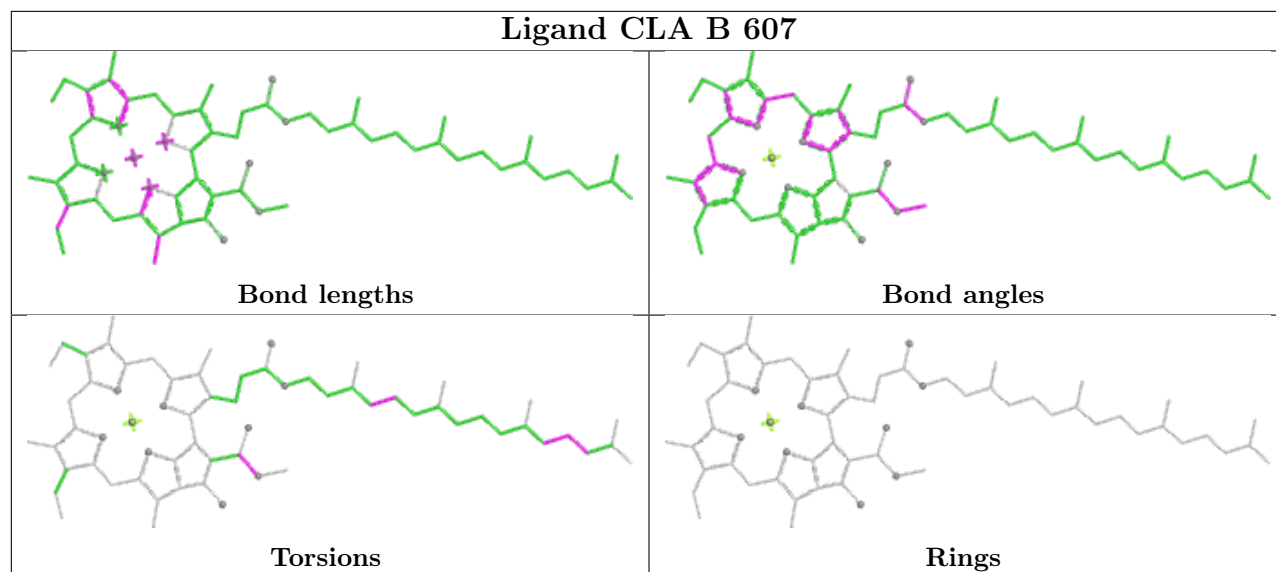
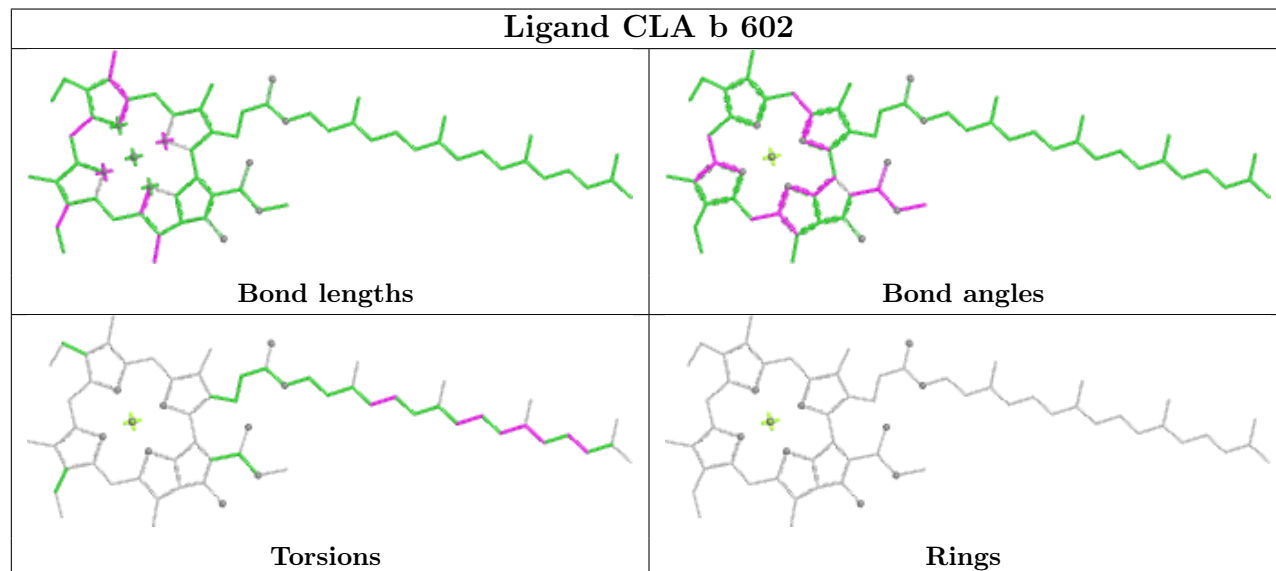
Rings

Ligand BCR H 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

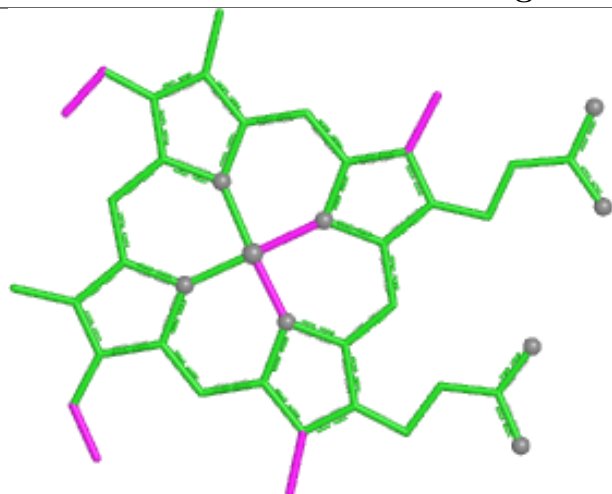
Ligand STE D 413	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR c 515	
	
Bond lengths	Bond angles
	
Torsions	Rings

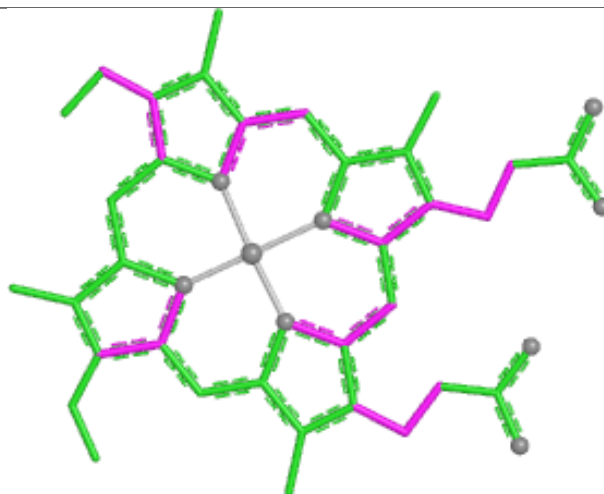
Ligand CLA B 604	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 607**Ligand CLA b 602**

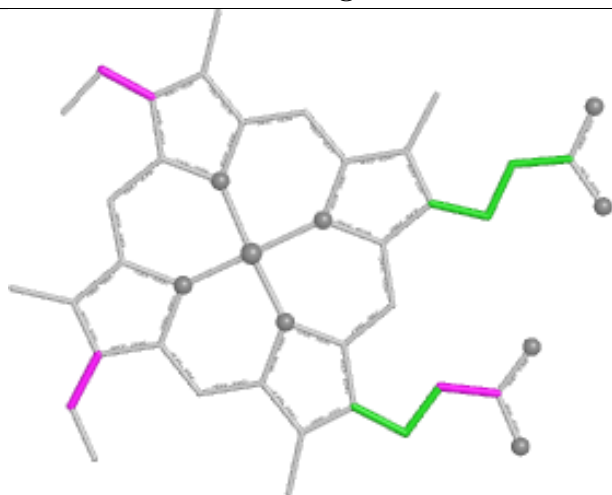
Ligand HEC v 201



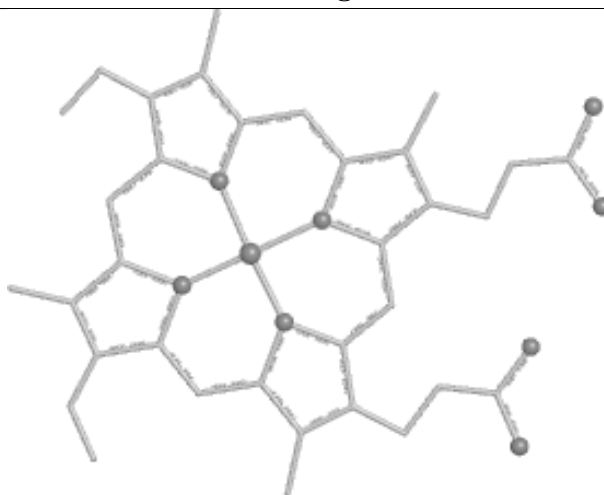
Bond lengths



Bond angles

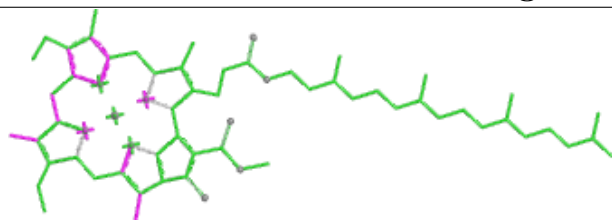


Torsions

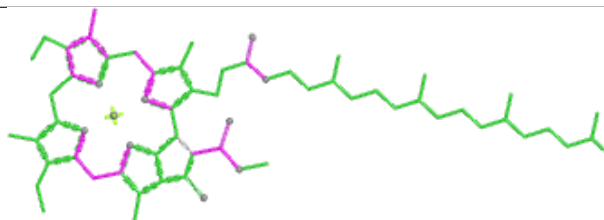


Rings

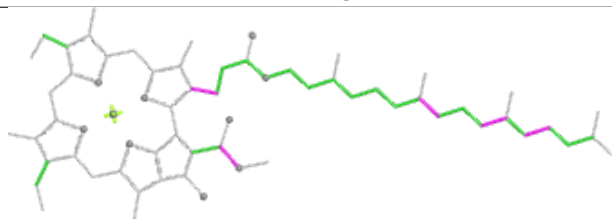
Ligand CLA c 514



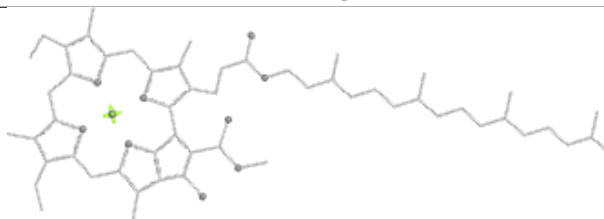
Bond lengths



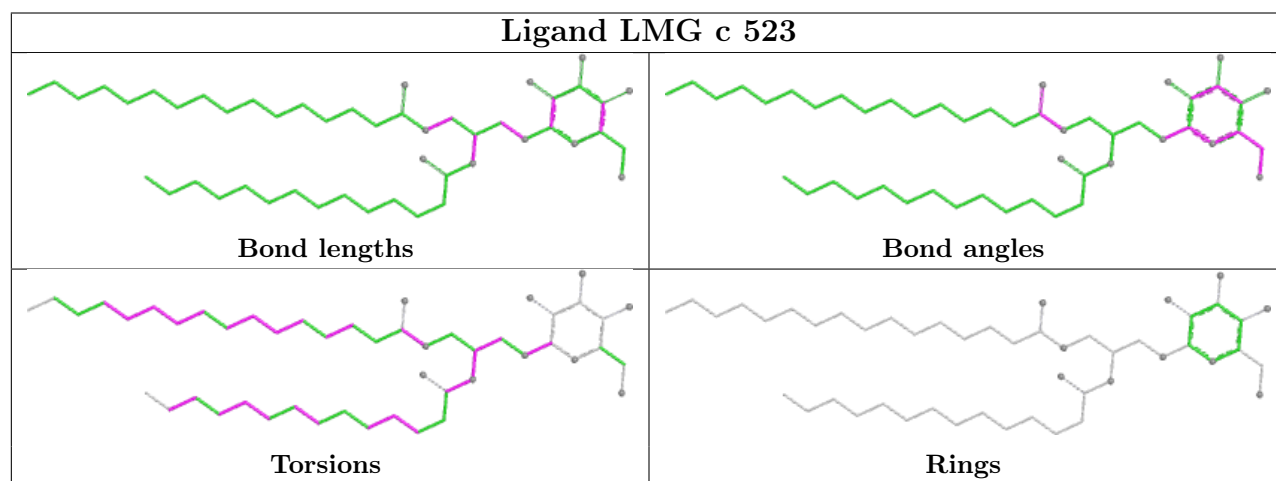
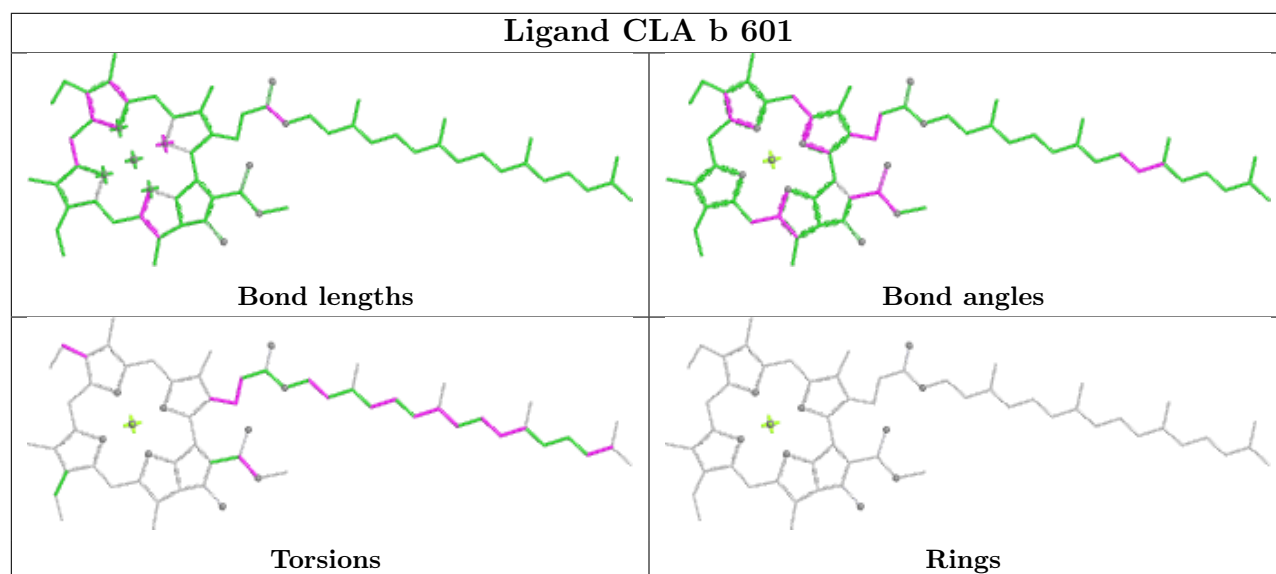
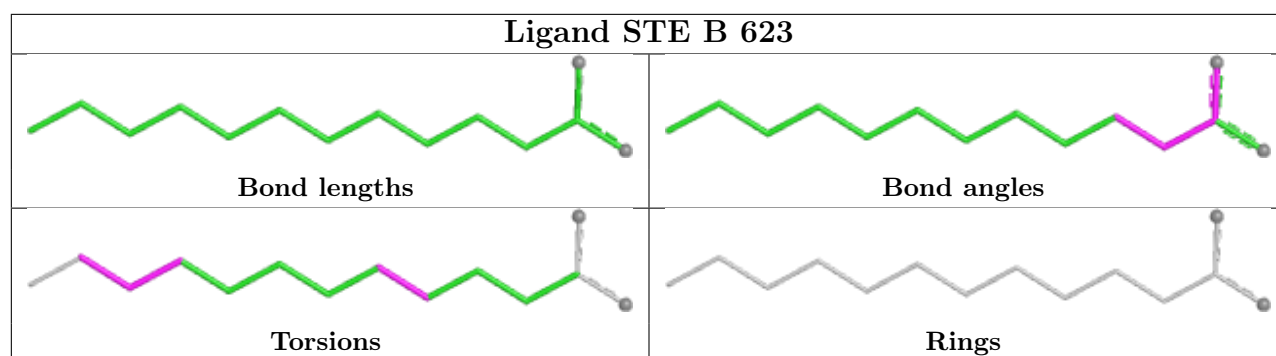
Bond angles

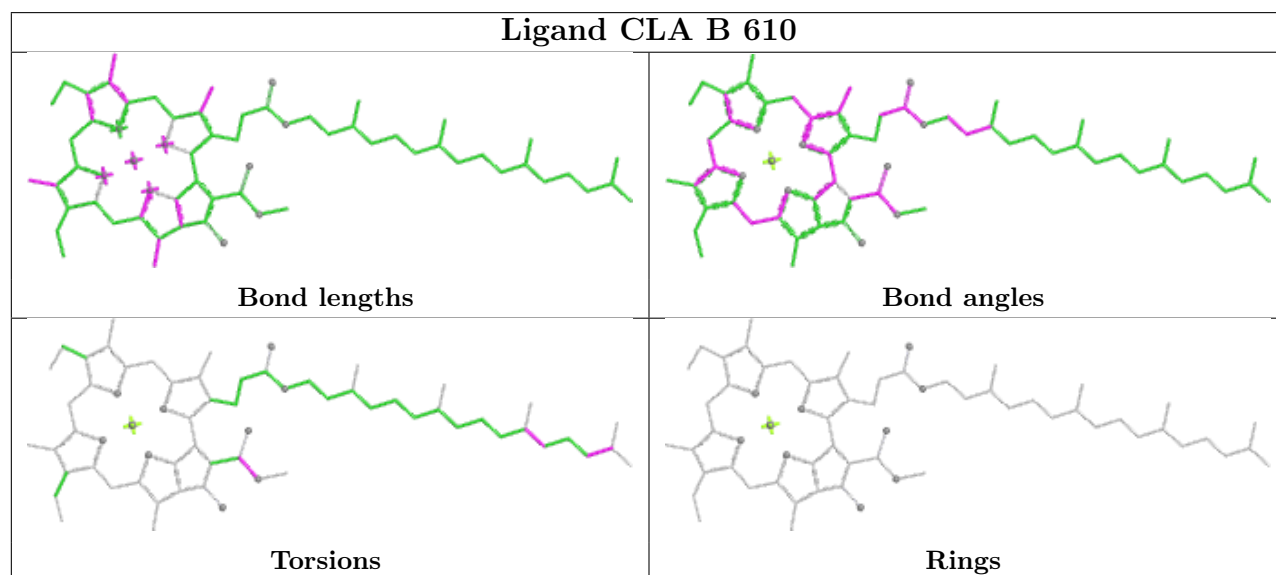
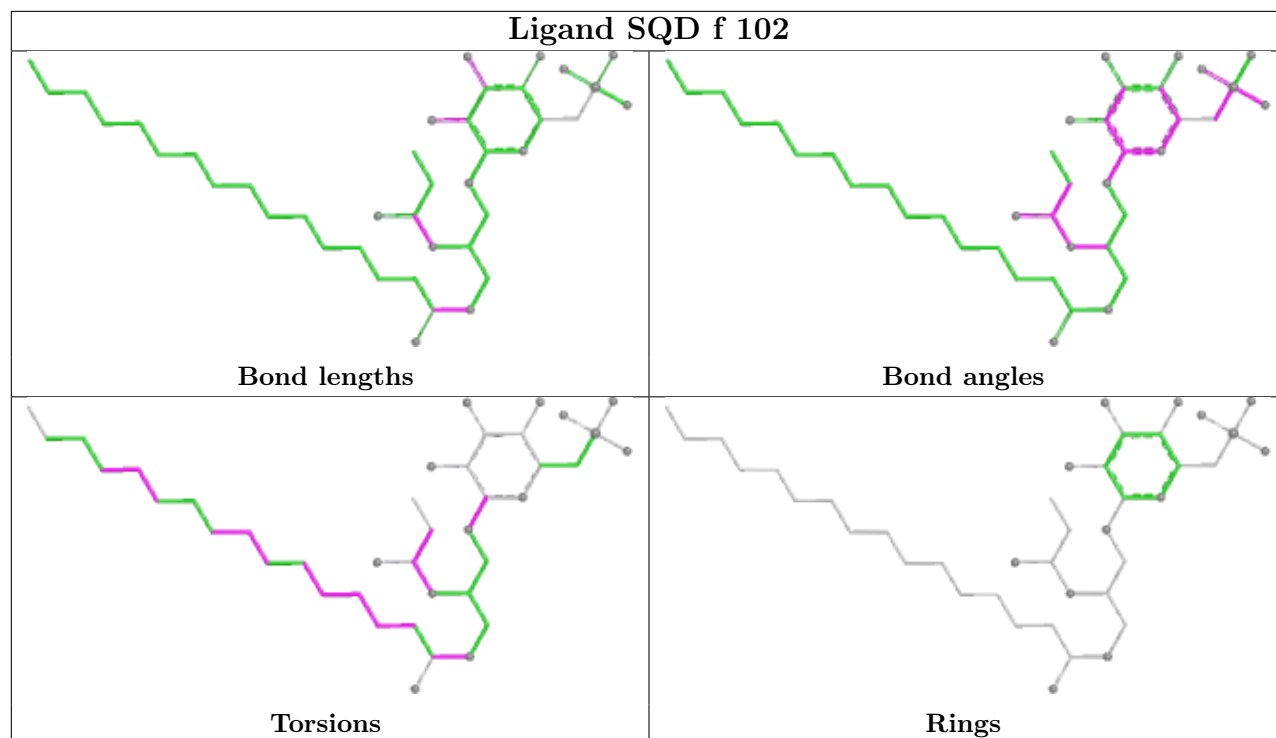


Torsions

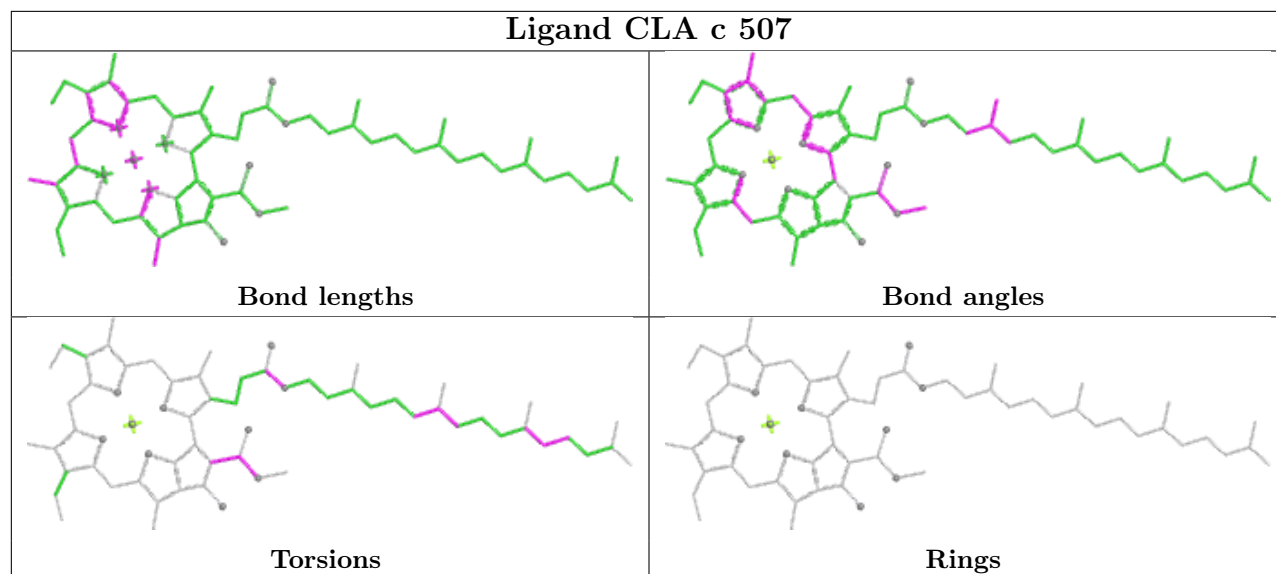


Rings

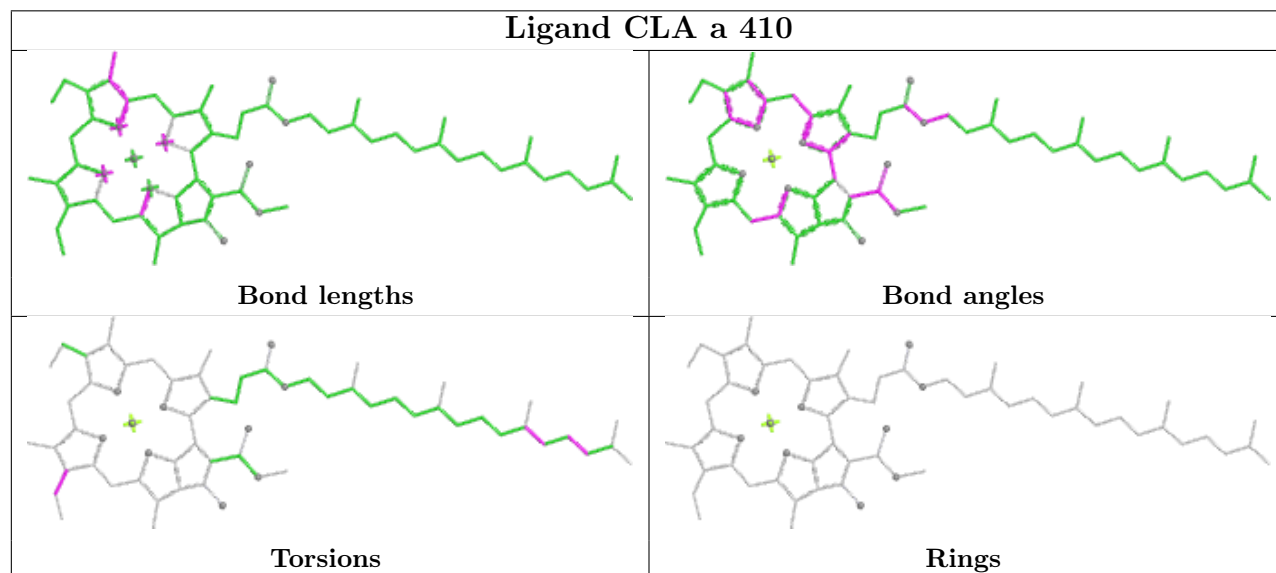




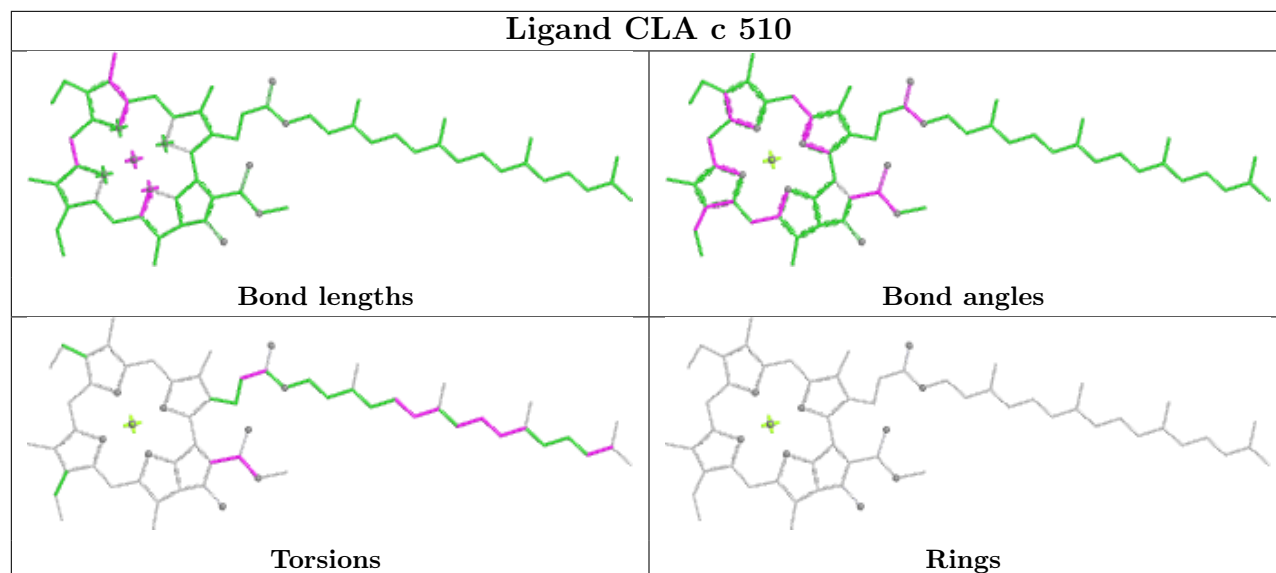
Ligand CLA c 507

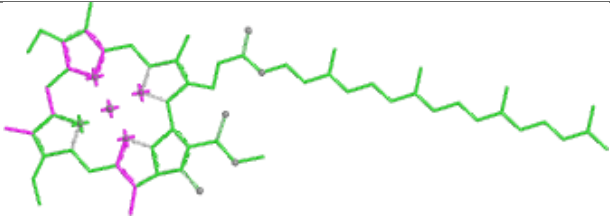
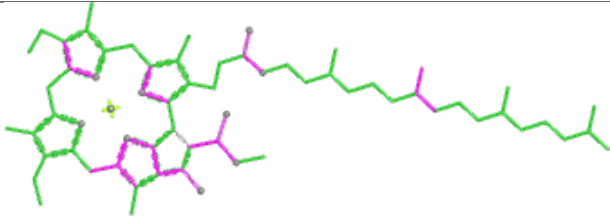
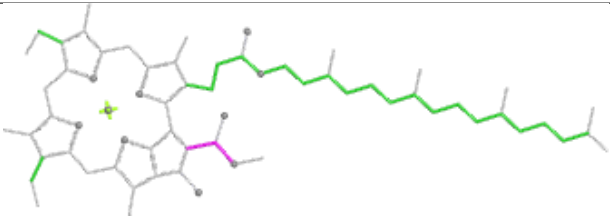
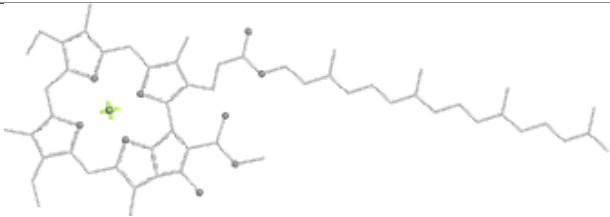
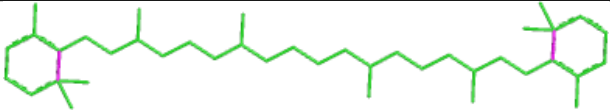
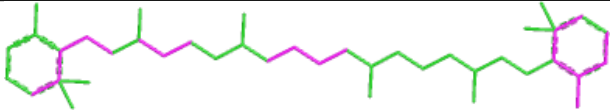
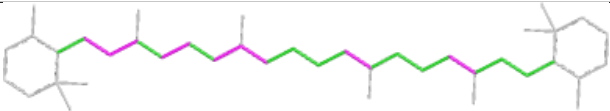
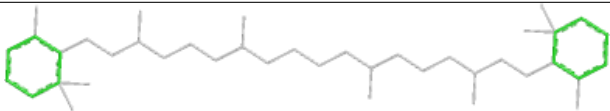
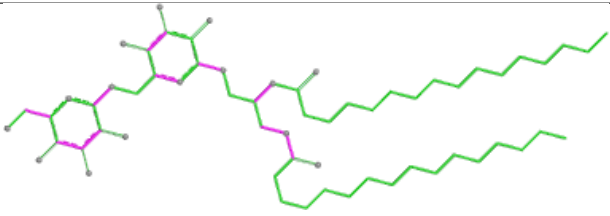
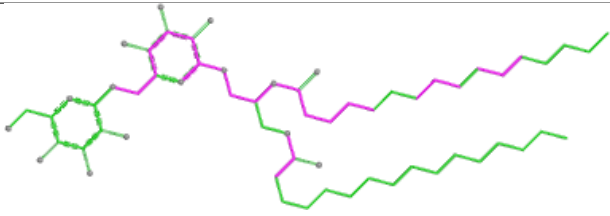
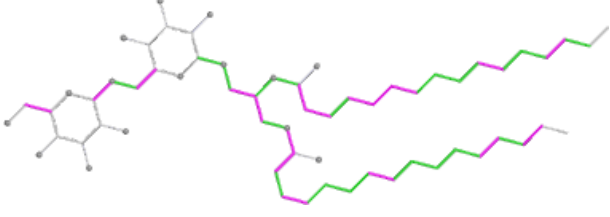
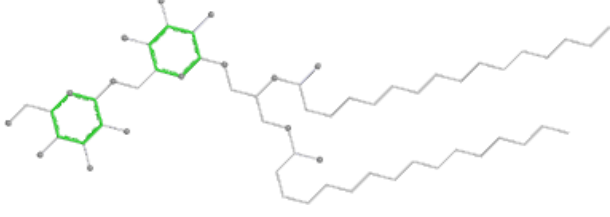


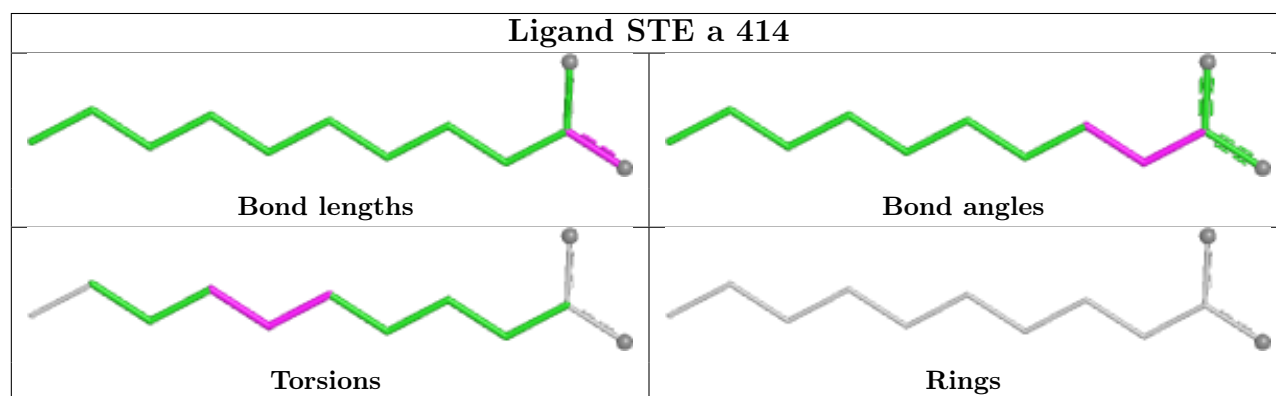
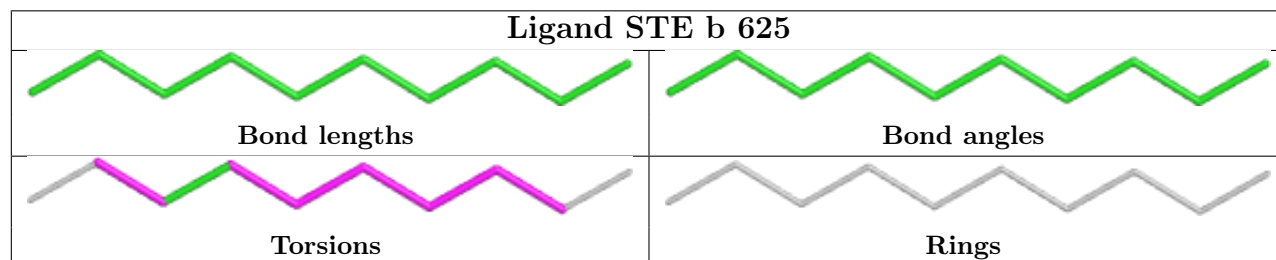
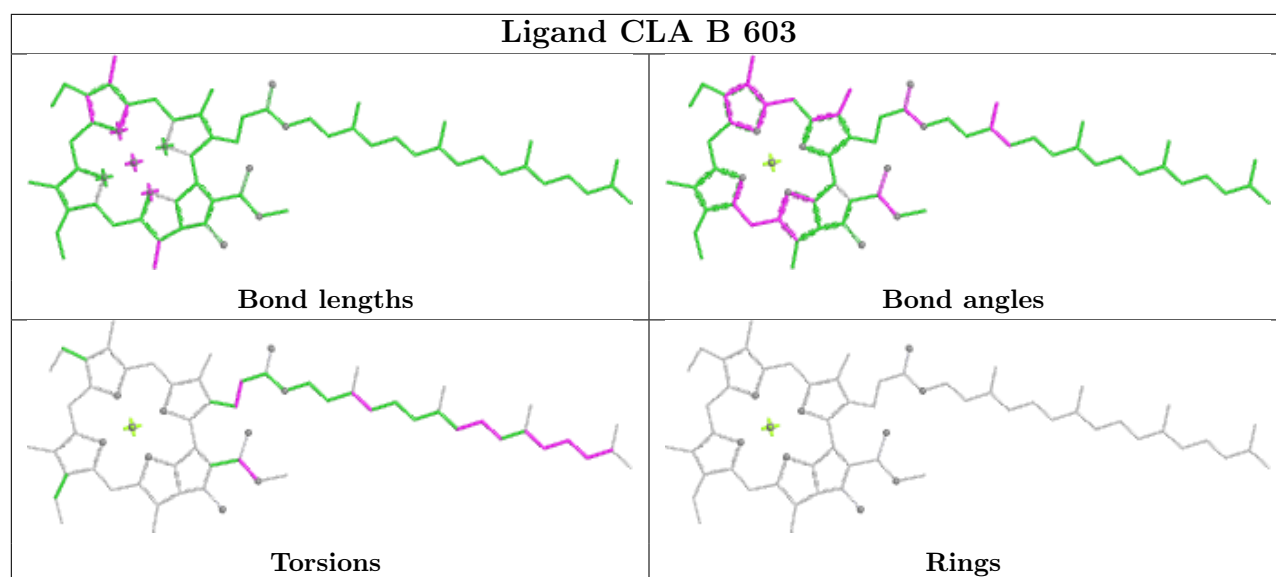
Ligand CLA a 410

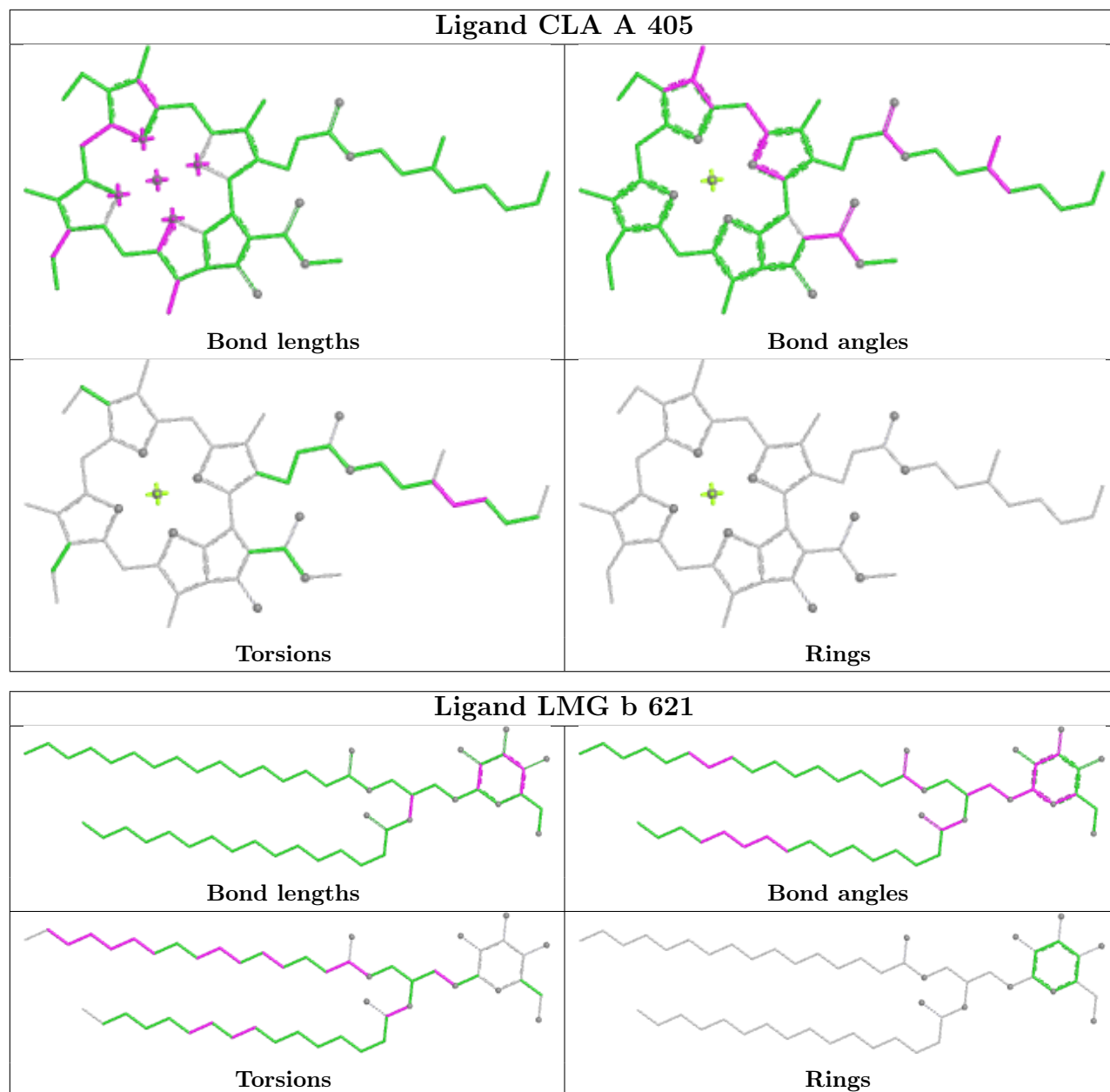


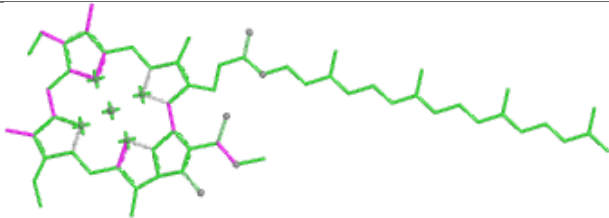
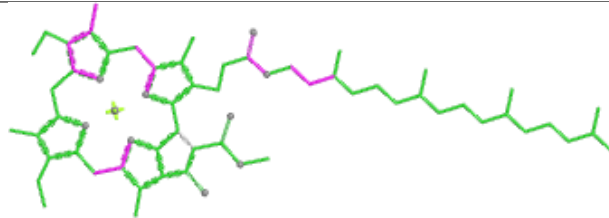
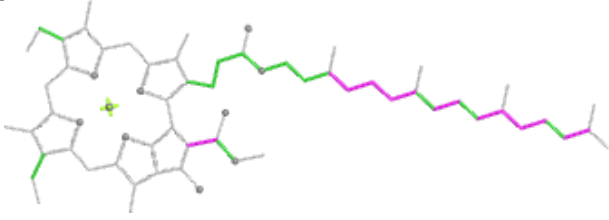
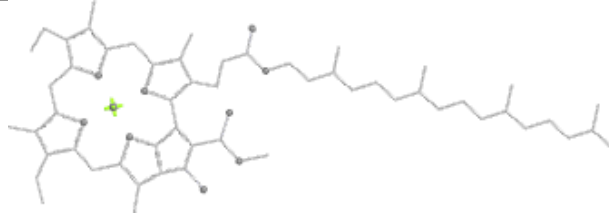
Ligand CLA c 510

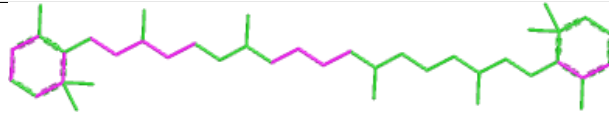
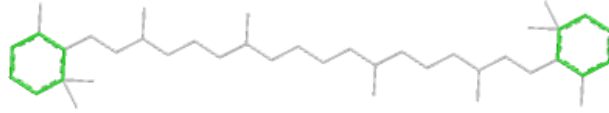


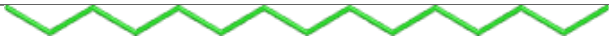
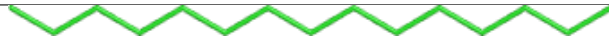
Ligand CLA C 501	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR b 619	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand DGD C 515	
 Bond lengths	 Bond angles
 Torsions	 Rings

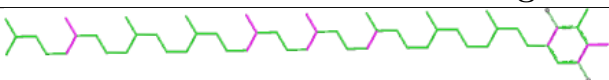
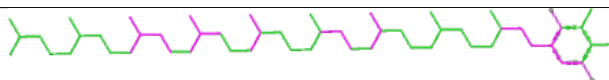
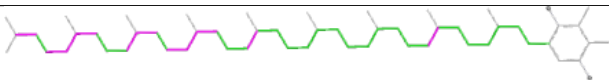
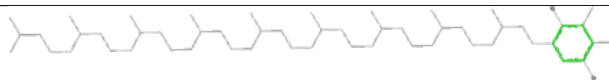




Ligand CLA b 614	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR K 103	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand STE I 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PL9 d 406	
	
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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	334/334 (100%)	-0.61	0 100 100	22, 30, 53, 81	0
1	a	334/334 (100%)	-0.51	3 (0%) 81 83	23, 33, 62, 80	0
2	B	505/506 (99%)	-0.46	3 (0%) 85 87	18, 35, 66, 99	4 (0%)
2	b	505/506 (99%)	-0.32	6 (1%) 76 78	23, 39, 75, 113	0
3	C	442/461 (95%)	-0.42	0 100 100	16, 38, 57, 84	1 (0%)
3	c	451/461 (97%)	-0.29	2 (0%) 88 90	20, 42, 66, 95	2 (0%)
4	D	341/352 (96%)	-0.60	0 100 100	21, 32, 52, 89	0
4	d	341/352 (96%)	-0.45	0 100 100	23, 36, 59, 85	1 (0%)
5	E	82/84 (97%)	0.17	1 (1%) 76 78	31, 54, 74, 82	1 (1%)
5	e	82/84 (97%)	0.22	1 (1%) 76 78	42, 63, 81, 91	0
6	F	34/45 (75%)	-0.11	0 100 100	38, 46, 70, 95	0
6	f	34/45 (75%)	0.13	0 100 100	45, 52, 83, 93	0
7	H	65/66 (98%)	-0.21	2 (3%) 51 53	33, 44, 63, 74	0
7	h	63/66 (95%)	0.04	2 (3%) 50 52	43, 54, 64, 82	0
8	I	35/38 (92%)	-0.36	0 100 100	31, 41, 72, 87	0
8	i	35/38 (92%)	-0.22	0 100 100	33, 43, 81, 85	0
9	J	36/40 (90%)	-0.06	0 100 100	37, 52, 80, 96	0
9	j	36/40 (90%)	0.08	1 (2%) 55 57	41, 56, 84, 101	0
10	K	37/46 (80%)	-0.05	0 100 100	45, 56, 75, 81	0
10	k	37/46 (80%)	0.16	0 100 100	51, 60, 72, 79	0
11	L	37/37 (100%)	-0.64	0 100 100	26, 33, 66, 71	0
11	l	36/37 (97%)	-0.57	0 100 100	26, 33, 76, 87	0
12	M	32/36 (88%)	-0.51	0 100 100	28, 36, 57, 72	0
12	m	31/36 (86%)	-0.50	0 100 100	29, 37, 53, 72	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/272 (89%)	-0.29	1 (0%) 88 90	26, 43, 85, 134	1 (0%)
13	o	244/272 (89%)	-0.26	1 (0%) 88 90	25, 42, 80, 113	0
14	R	34/40 (85%)	0.84	2 (5%) 28 29	66, 80, 102, 111	0
14	r	31/40 (77%)	1.46	6 (19%) 3 3	73, 100, 118, 130	0
15	T	29/30 (96%)	-0.64	0 100 100	27, 33, 65, 80	0
15	t	29/30 (96%)	-0.39	2 (6%) 23 24	26, 34, 80, 96	0
16	U	97/134 (72%)	-0.25	0 100 100	32, 46, 70, 92	0
16	u	97/134 (72%)	-0.36	0 100 100	31, 42, 57, 82	0
17	V	137/163 (84%)	-0.38	0 100 100	31, 43, 60, 79	0
17	v	137/163 (84%)	-0.12	0 100 100	33, 49, 71, 88	0
18	X	38/41 (92%)	-0.14	0 100 100	42, 55, 78, 84	0
18	x	39/41 (95%)	0.19	1 (2%) 57 60	50, 65, 94, 109	0
19	Y	27/46 (58%)	0.81	2 (7%) 20 22	54, 78, 93, 103	0
19	y	30/46 (65%)	0.61	0 100 100	63, 77, 92, 99	0
20	Z	62/62 (100%)	0.61	2 (3%) 50 52	57, 74, 120, 131	0
20	z	62/62 (100%)	0.58	1 (1%) 70 73	59, 75, 112, 130	0
All	All	5302/5666 (93%)	-0.30	39 (0%) 84 86	16, 40, 78, 134	10 (0%)

The worst 5 of 39 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	o	58	ASN	4.3
14	R	35	LEU	4.2
15	t	30	THR	3.9
14	r	32	GLN	3.7
20	Z	62	VAL	3.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
12	FME	M	1	10/11	0.94	0.09	40,53,69,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	FME	I	1	10/11	0.95	0.07	40,48,64,66	0
15	FME	T	1	10/11	0.95	0.08	29,44,67,67	0
12	FME	m	1	10/11	0.96	0.07	33,47,65,76	0
8	FME	i	1	10/11	0.96	0.09	40,50,65,66	0
15	FME	t	1	10/11	0.96	0.07	28,43,73,73	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	STE	E	102	12/20	0.74	0.17	46,78,92,94	0
31	STE	b	625	10/20	0.74	0.17	44,53,61,73	0
31	STE	I	101	15/20	0.77	0.17	37,55,73,76	0
33	LHG	E	101	49/49	0.77	0.14	50,83,110,126	0
31	STE	b	624	20/20	0.79	0.15	41,60,75,89	0
31	STE	b	627	20/20	0.80	0.14	38,64,84,90	0
33	LHG	e	101	42/49	0.80	0.14	65,87,116,127	0
31	STE	H	104	18/20	0.81	0.16	44,73,89,94	0
31	STE	B	627	15/20	0.81	0.19	36,61,74,77	0
31	STE	j	101	12/20	0.81	0.13	42,56,74,75	0
31	STE	a	414	12/20	0.81	0.13	40,65,71,75	0
26	PL9	a	409	55/55	0.81	0.17	47,74,93,96	0
31	STE	m	102	12/20	0.82	0.17	46,61,76,76	0
27	LMG	b	623	55/55	0.82	0.15	42,70,95,101	0
26	PL9	A	409	55/55	0.82	0.16	47,68,94,97	0
27	LMG	c	522	48/55	0.83	0.14	46,80,104,108	0
27	LMG	a	415	55/55	0.83	0.13	34,58,80,92	0
31	STE	C	519	16/20	0.83	0.13	42,58,73,77	0
31	STE	a	413	10/20	0.83	0.13	38,61,67,68	0
31	STE	B	626	16/20	0.84	0.13	35,58,78,79	0
31	STE	c	501	12/20	0.84	0.12	54,68,87,89	0
29	DGD	A	413	66/66	0.85	0.11	44,62,78,99	0
31	STE	T	102	15/20	0.85	0.14	44,59,83,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
27	LMG	D	411	33/55	0.85	0.13	34,56,84,89	0
28	SQD	a	412	36/54	0.85	0.13	29,63,90,97	0
31	STE	d	411	16/20	0.86	0.14	45,62,78,83	0
22	CLA	b	601	65/65	0.86	0.12	43,68,89,92	0
31	STE	m	101	18/20	0.86	0.12	34,51,78,79	0
31	STE	b	626	14/20	0.86	0.14	51,65,84,88	0
31	STE	B	620	17/20	0.86	0.11	32,50,63,71	0
27	LMG	Y	101	48/55	0.86	0.12	34,68,86,99	0
31	STE	b	622	20/20	0.87	0.10	36,54,79,85	0
28	SQD	f	102	41/54	0.87	0.13	55,91,113,119	0
31	STE	b	620	16/20	0.87	0.12	35,46,64,71	0
31	STE	C	518	12/20	0.88	0.10	41,55,62,66	0
27	LMG	c	520	37/55	0.88	0.11	40,67,80,83	0
31	STE	B	625	18/20	0.88	0.11	40,58,76,83	0
27	LMG	A	410	48/55	0.88	0.10	38,57,72,87	0
28	SQD	A	412	39/54	0.88	0.11	42,61,90,93	0
31	STE	c	521	20/20	0.88	0.11	37,55,93,103	0
24	BCR	K	101	40/40	0.89	0.12	40,58,75,82	0
31	STE	B	601	12/20	0.89	0.13	51,67,78,86	0
28	SQD	B	622	54/54	0.89	0.10	37,61,91,101	0
31	STE	d	413	20/20	0.89	0.10	42,57,76,84	0
28	SQD	L	101	49/54	0.89	0.09	38,60,89,107	0
22	CLA	H	101	65/65	0.89	0.11	33,63,91,110	0
31	STE	J	101	12/20	0.89	0.12	45,59,69,77	0
27	LMG	c	523	49/55	0.89	0.10	30,56,82,98	0
31	STE	Z	101	8/20	0.89	0.16	50,61,70,70	0
31	STE	M	102	15/20	0.90	0.11	32,48,69,74	0
31	STE	M	103	10/20	0.90	0.11	34,47,64,70	0
27	LMG	b	621	51/55	0.90	0.10	32,53,76,97	0
31	STE	B	623	14/20	0.90	0.10	36,47,56,62	0
31	STE	B	624	12/20	0.90	0.10	32,48,63,76	0
31	STE	d	412	17/20	0.90	0.11	41,56,67,74	0
31	STE	C	520	12/20	0.91	0.09	34,46,57,58	0
31	STE	D	413	20/20	0.91	0.10	34,54,71,79	0
24	BCR	h	101	40/40	0.91	0.09	35,54,73,79	0
27	LMG	B	621	28/55	0.91	0.11	35,51,65,73	0
24	BCR	k	101	40/40	0.91	0.10	42,60,81,85	0
24	BCR	K	102	40/40	0.91	0.09	33,53,68,74	0
24	BCR	c	515	40/40	0.91	0.10	41,62,76,77	0
22	CLA	c	513	65/65	0.92	0.10	38,56,91,106	0
27	LMG	M	101	51/55	0.92	0.08	31,48,72,90	0
22	CLA	C	513	65/65	0.92	0.10	38,64,97,109	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
29	DGD	C	516	62/66	0.92	0.09	34,51,97,119	0
29	DGD	h	102	62/66	0.92	0.09	29,48,65,68	0
28	SQD	D	408	36/54	0.92	0.11	46,75,89,100	0
24	BCR	d	405	40/40	0.92	0.10	28,54,85,95	0
24	BCR	C	514	40/40	0.93	0.08	23,38,55,63	0
28	SQD	a	411	54/54	0.93	0.10	39,62,94,96	0
24	BCR	F	101	40/40	0.93	0.09	21,44,82,90	0
24	BCR	H	102	40/40	0.93	0.08	30,50,66,75	0
22	CLA	c	514	65/65	0.93	0.10	39,67,109,116	0
24	BCR	k	102	40/40	0.93	0.10	40,55,67,68	0
29	DGD	H	103	62/66	0.93	0.08	29,46,61,73	0
24	BCR	B	618	40/40	0.93	0.07	23,39,50,52	0
24	BCR	T	101	40/40	0.93	0.07	23,39,52,52	0
29	DGD	c	518	62/66	0.94	0.08	33,50,90,96	0
27	LMG	d	410	44/55	0.94	0.09	31,51,89,104	0
28	SQD	A	411	52/54	0.94	0.09	34,59,84,88	0
27	LMG	D	407	51/55	0.94	0.09	27,56,86,93	0
24	BCR	c	516	40/40	0.94	0.09	22,44,60,72	0
24	BCR	B	619	40/40	0.94	0.07	25,42,61,72	0
22	CLA	c	512	65/65	0.94	0.09	39,52,65,74	0
24	BCR	K	103	40/40	0.94	0.10	36,54,67,69	0
24	BCR	A	406	40/40	0.94	0.07	23,35,43,47	0
24	BCR	b	617	40/40	0.94	0.07	25,41,54,59	0
24	BCR	b	618	40/40	0.94	0.07	22,38,51,52	0
33	LHG	D	410	47/49	0.94	0.09	24,46,82,99	0
24	BCR	b	619	40/40	0.94	0.08	31,47,63,67	0
33	LHG	d	407	49/49	0.94	0.10	33,49,76,80	0
33	LHG	d	409	39/49	0.94	0.09	29,45,72,80	0
22	CLA	C	512	65/65	0.94	0.09	35,55,82,95	0
22	CLA	C	510	65/65	0.95	0.07	27,46,62,66	0
22	CLA	d	404	65/65	0.95	0.09	32,49,89,106	0
24	BCR	t	101	40/40	0.95	0.06	23,38,51,52	0
23	PHO	d	401	64/64	0.95	0.07	20,37,47,61	0
26	PL9	D	406	55/55	0.95	0.06	21,34,49,54	0
29	DGD	C	515	62/66	0.95	0.09	21,40,73,87	0
22	CLA	C	511	65/65	0.95	0.07	27,49,66,77	0
29	DGD	C	517	62/66	0.95	0.08	26,46,77,87	0
24	BCR	B	617	40/40	0.95	0.06	24,38,59,60	0
22	CLA	B	615	65/65	0.95	0.07	21,38,60,69	0
29	DGD	c	519	62/66	0.95	0.08	28,54,83,91	0
22	CLA	C	503	65/65	0.95	0.07	32,42,51,61	0
22	CLA	C	504	59/65	0.95	0.07	27,41,81,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	CLA	C	505	65/65	0.95	0.08	19,39,71,77	0
22	CLA	b	606	65/65	0.95	0.07	22,37,73,77	0
22	CLA	b	609	65/65	0.95	0.07	27,43,64,74	0
22	CLA	b	610	65/65	0.95	0.08	23,36,50,56	0
22	CLA	b	616	60/65	0.95	0.08	24,42,86,88	0
22	CLA	c	503	65/65	0.95	0.07	29,41,62,66	0
22	CLA	c	504	65/65	0.95	0.07	28,41,54,58	0
22	CLA	c	506	65/65	0.95	0.08	24,40,64,70	0
22	CLA	c	507	65/65	0.95	0.09	29,48,102,109	0
22	CLA	c	509	64/65	0.95	0.08	27,46,86,103	0
22	CLA	c	510	65/65	0.95	0.08	33,47,70,77	0
22	CLA	C	506	65/65	0.95	0.09	28,45,83,99	0
22	CLA	C	508	65/65	0.95	0.07	25,42,97,107	0
22	CLA	C	501	65/65	0.96	0.06	19,36,51,56	0
22	CLA	a	402	65/65	0.96	0.06	19,29,46,56	0
22	CLA	d	403	65/65	0.96	0.06	19,34,54,65	0
22	CLA	a	403	65/65	0.96	0.08	25,40,97,106	0
23	PHO	A	404	64/64	0.96	0.06	18,28,40,48	0
23	PHO	D	401	64/64	0.96	0.06	21,32,44,48	0
23	PHO	a	404	64/64	0.96	0.06	19,29,40,44	0
22	CLA	a	405	65/65	0.96	0.08	18,35,82,91	0
22	CLA	a	410	65/65	0.96	0.06	17,29,48,54	0
22	CLA	C	502	65/65	0.96	0.06	26,42,52,53	0
22	CLA	b	602	65/65	0.96	0.08	26,44,65,72	0
22	CLA	b	603	65/65	0.96	0.06	18,36,65,76	0
22	CLA	B	605	65/65	0.96	0.07	19,31,47,52	0
22	CLA	b	608	65/65	0.96	0.07	25,42,60,69	0
22	CLA	B	606	65/65	0.96	0.07	23,36,69,86	0
22	CLA	B	608	65/65	0.96	0.06	20,34,56,61	0
22	CLA	b	611	65/65	0.96	0.06	19,34,53,61	0
22	CLA	b	612	65/65	0.96	0.07	15,33,48,57	0
22	CLA	b	614	65/65	0.96	0.07	21,38,78,86	0
24	BCR	a	406	40/40	0.96	0.06	19,32,50,55	0
22	CLA	b	615	65/65	0.96	0.07	24,39,59,63	0
22	CLA	B	609	65/65	0.96	0.07	24,39,57,69	0
22	CLA	c	502	65/65	0.96	0.06	26,41,53,57	0
22	CLA	C	507	65/65	0.96	0.06	20,40,56,66	0
22	CLA	B	610	65/65	0.96	0.07	18,33,46,50	0
22	CLA	c	505	60/65	0.96	0.07	32,45,76,89	0
29	DGD	c	517	62/66	0.96	0.08	24,42,84,94	0
22	CLA	C	509	65/65	0.96	0.08	25,46,62,69	0
22	CLA	B	611	65/65	0.96	0.06	19,30,46,50	0

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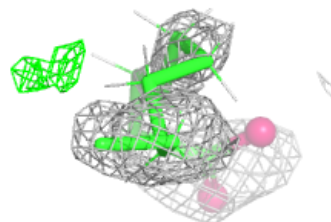
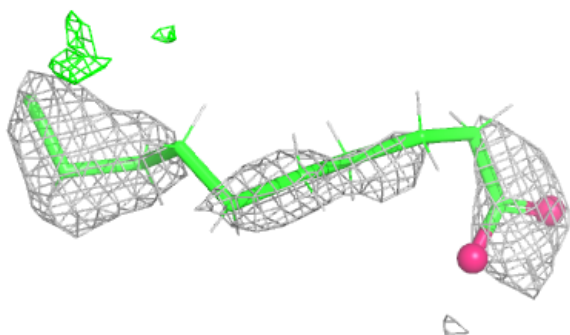
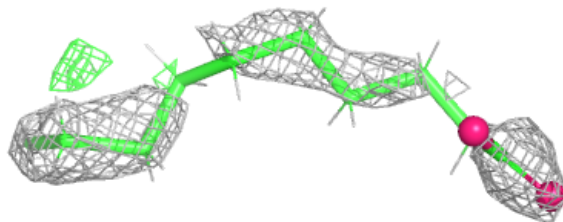
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	CLA	c	508	65/65	0.96	0.07	28,44,59,63	0
32	BCT	d	402	4/4	0.96	0.08	31,35,44,53	0
22	CLA	B	612	65/65	0.96	0.07	19,31,47,56	0
33	LHG	D	412	49/49	0.96	0.07	30,44,65,76	0
22	CLA	B	604	65/65	0.96	0.07	19,32,79,84	0
33	LHG	L	102	49/49	0.96	0.07	26,41,53,60	0
22	CLA	c	511	65/65	0.96	0.07	29,47,64,68	0
22	CLA	B	616	60/65	0.96	0.09	25,39,94,110	0
26	PL9	d	406	55/55	0.96	0.06	22,33,42,53	0
33	LHG	l	101	49/49	0.96	0.06	26,45,55,64	0
22	CLA	A	403	65/65	0.97	0.08	21,34,97,110	0
22	CLA	B	602	65/65	0.97	0.06	20,36,55,66	0
22	CLA	B	607	65/65	0.97	0.06	14,34,62,66	0
22	CLA	b	613	65/65	0.97	0.07	17,34,73,87	0
22	CLA	B	613	65/65	0.97	0.06	17,31,71,73	0
22	CLA	B	614	65/65	0.97	0.07	20,36,75,87	0
33	LHG	D	409	49/49	0.97	0.06	26,41,53,56	0
22	CLA	B	603	65/65	0.97	0.07	15,32,63,67	0
22	CLA	D	403	65/65	0.97	0.06	15,29,52,61	0
22	CLA	b	604	65/65	0.97	0.07	20,33,81,91	0
22	CLA	b	605	65/65	0.97	0.06	21,34,49,53	0
22	CLA	D	404	65/65	0.97	0.06	19,28,52,62	0
33	LHG	d	408	49/49	0.97	0.06	23,42,57,68	0
22	CLA	b	607	65/65	0.97	0.07	18,35,69,78	0
22	CLA	D	405	65/65	0.97	0.07	22,42,107,119	0
22	CLA	A	402	65/65	0.97	0.06	16,26,46,49	0
34	HEC	F	102	43/43	0.97	0.08	37,48,64,66	0
34	HEC	f	101	43/43	0.97	0.08	42,58,81,84	0
32	BCT	D	402	4/4	0.98	0.07	22,26,32,36	0
34	HEC	V	201	43/43	0.98	0.06	19,35,43,44	0
22	CLA	A	405	54/65	0.98	0.06	18,31,66,72	0
34	HEC	v	201	43/43	0.98	0.06	27,37,50,51	0
21	FE2	a	401	1/1	0.99	0.02	34,34,34,34	0
25	CL	A	407	1/1	0.99	0.03	29,29,29,29	0
25	CL	a	407	1/1	0.99	0.03	28,28,28,28	0
30	OEX	A	414	10/10	0.99	0.02	22,26,28,29	0
30	OEX	a	416	10/10	0.99	0.03	23,26,30,31	0
25	CL	a	408	1/1	0.99	0.07	28,28,28,28	0
21	FE2	A	401	1/1	0.99	0.02	26,26,26,26	0
25	CL	A	408	1/1	1.00	0.02	30,30,30,30	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.

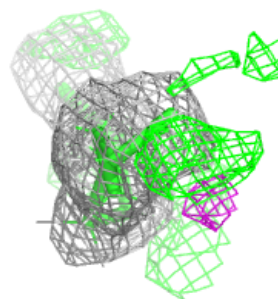
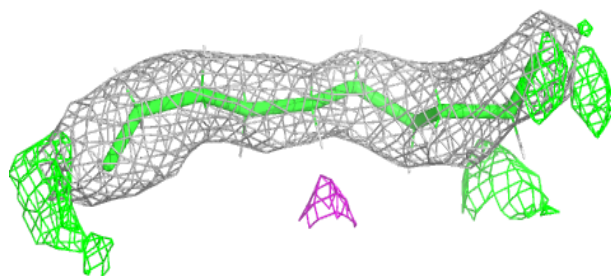
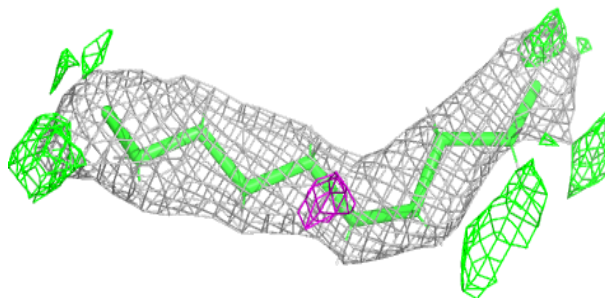
Electron density around STE E 102:

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

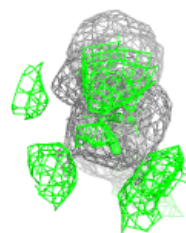
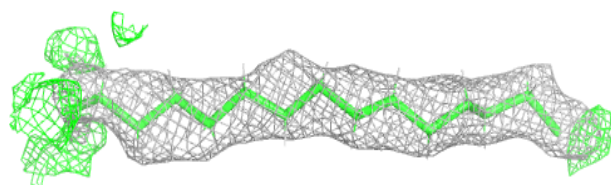
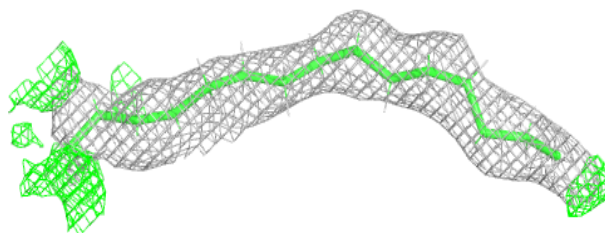


Electron density around STE b 625:

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

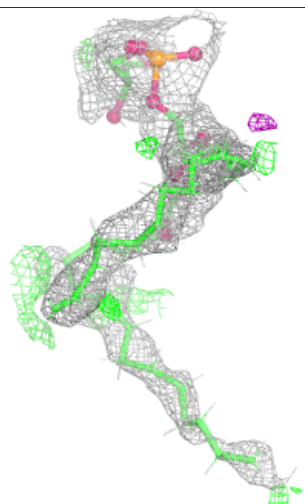
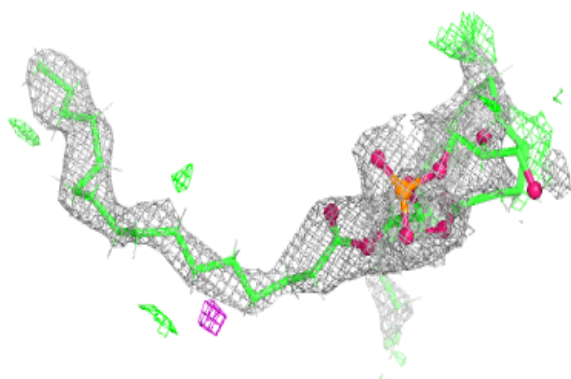
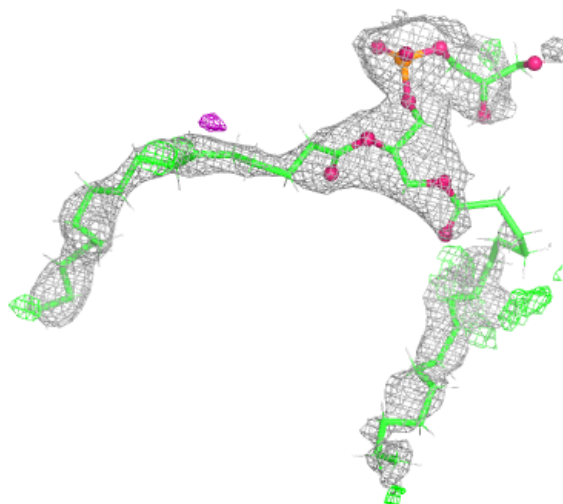
**Electron density around STE I 101:**

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



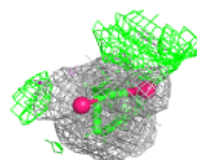
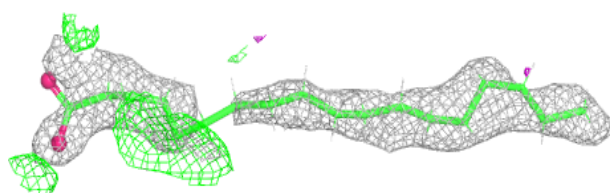
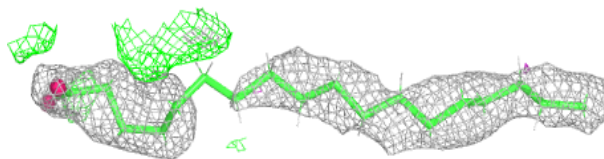
Electron density around LHG E 101:

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

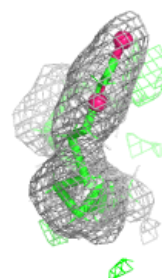
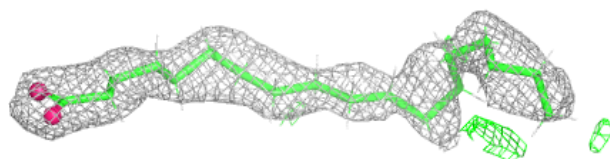
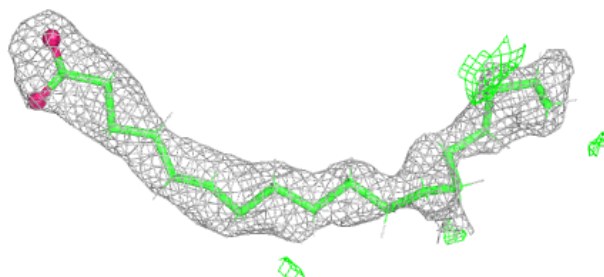


Electron density around STE b 624:

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

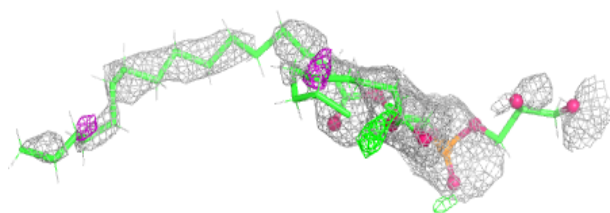
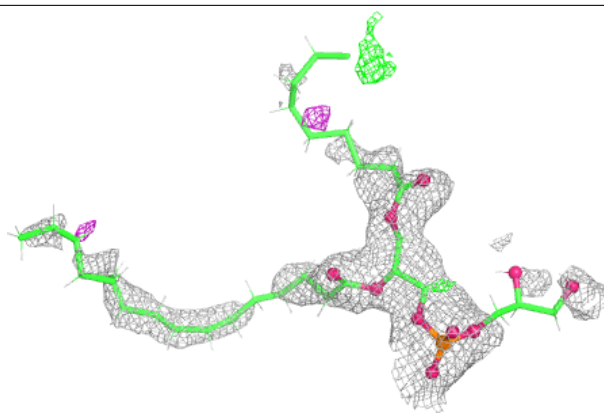
**Electron density around STE b 627:**

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

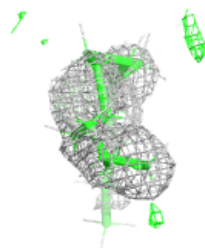
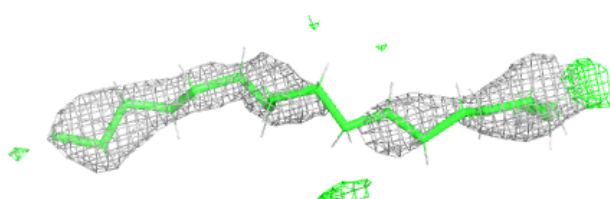
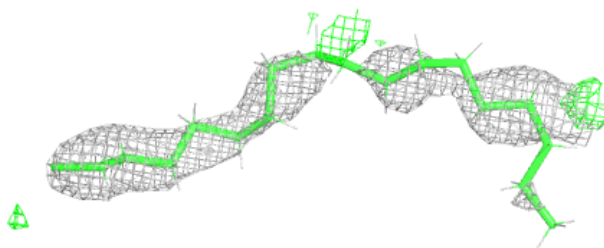


Electron density around LHG e 101:

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

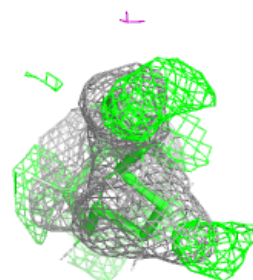
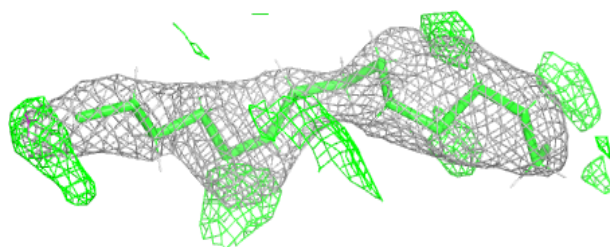
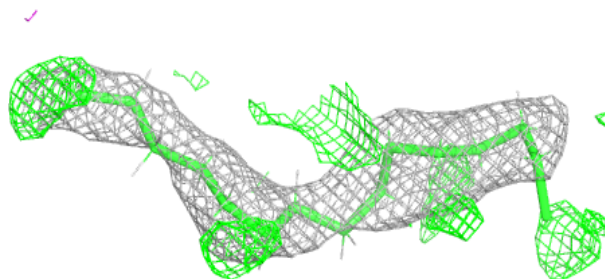
**Electron density around STE H 104:**

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

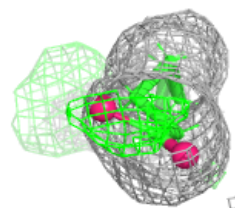
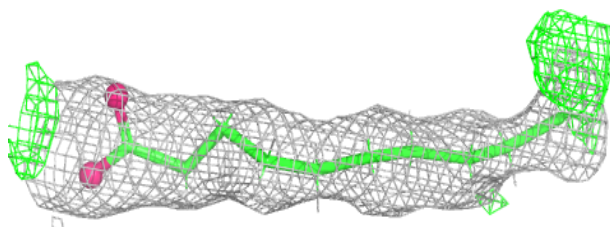
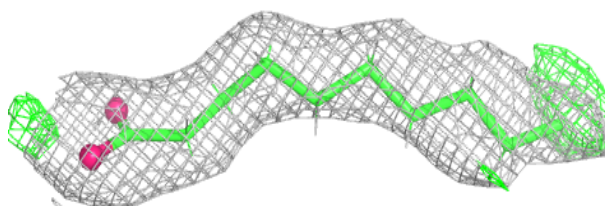


Electron density around STE B 627:

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

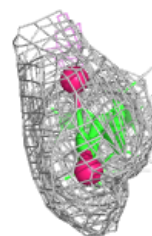
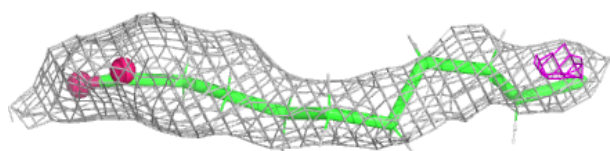
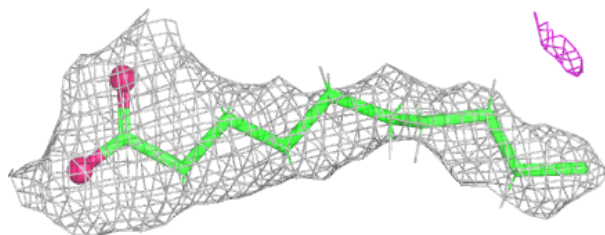
**Electron density around STE j 101:**

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

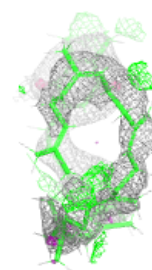
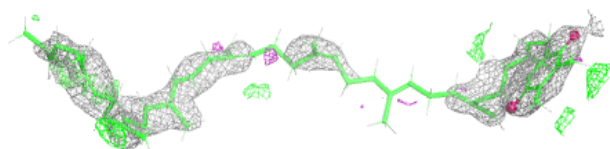
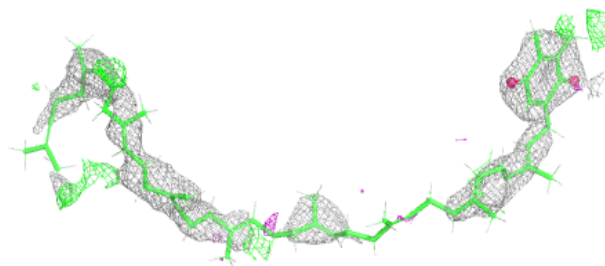


Electron density around STE a 414:

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

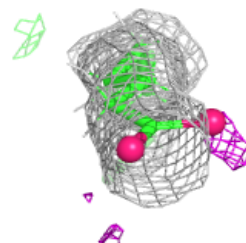
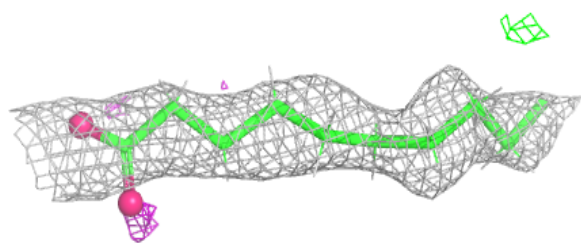
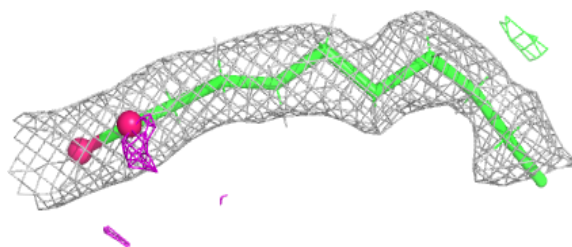
**Electron density around PL9 a 409:**

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

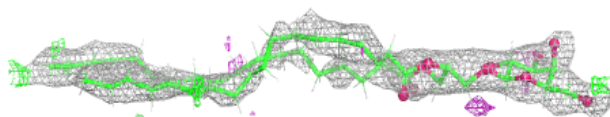
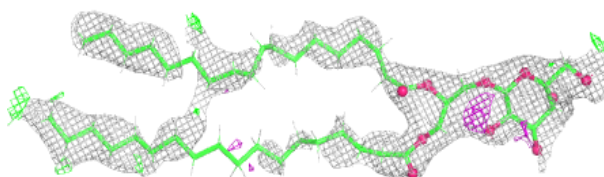


Electron density around STE m 102:

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

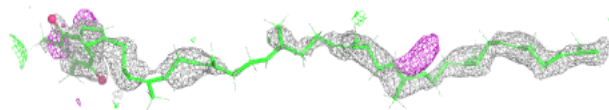
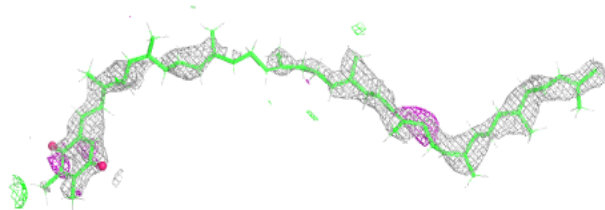
**Electron density around LMG b 623:**

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

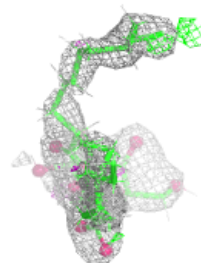
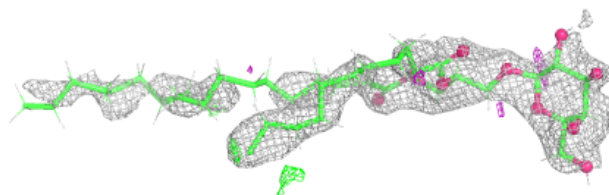
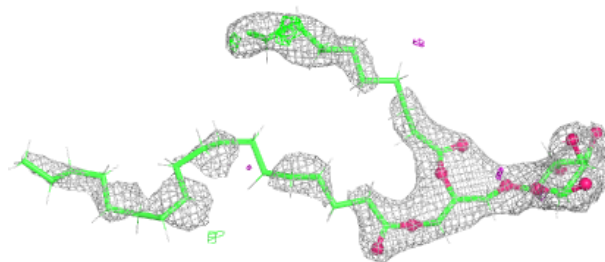


Electron density around PL9 A 409:

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

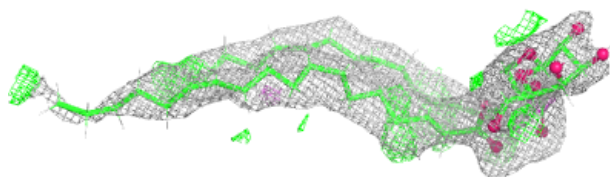
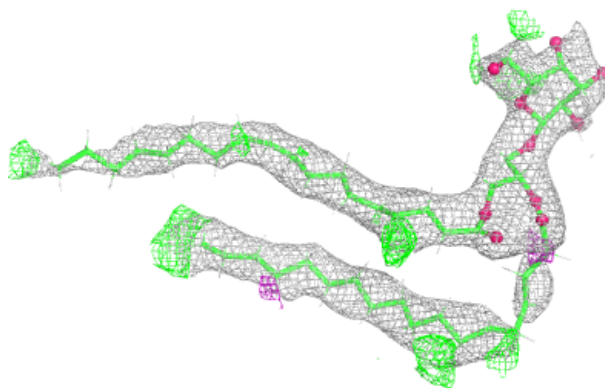
**Electron density around LMG c 522:**

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

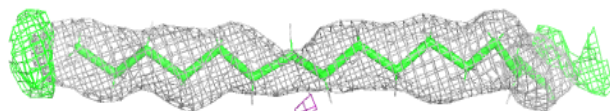
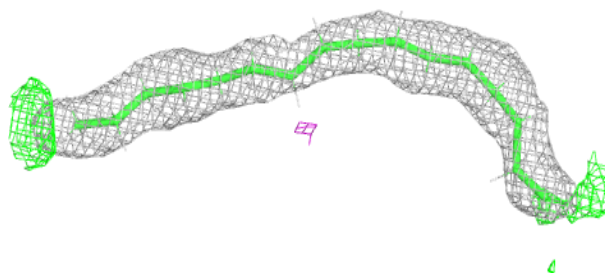


Electron density around LMG a 415:

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

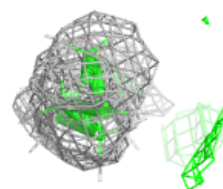
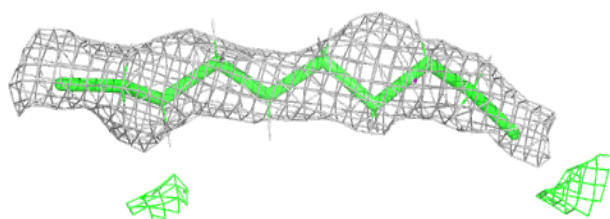
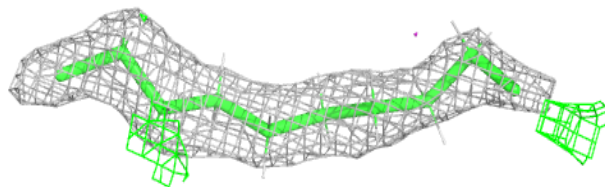
**Electron density around STE C 519:**

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

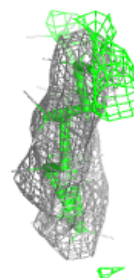
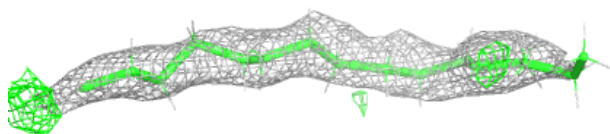
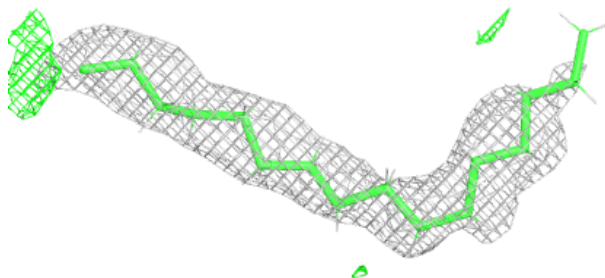


Electron density around STE a 413:

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

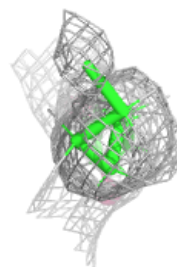
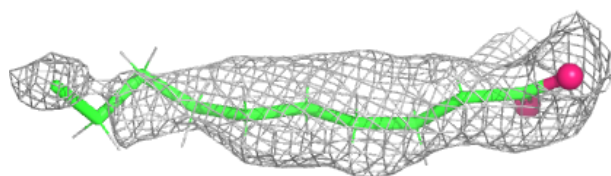
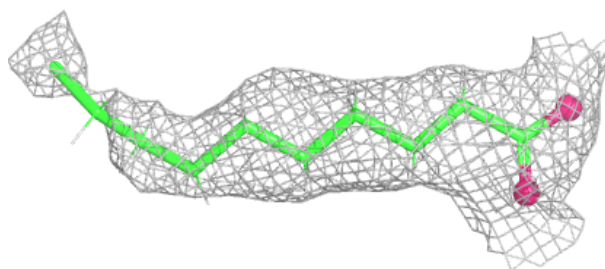
**Electron density around STE B 626:**

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

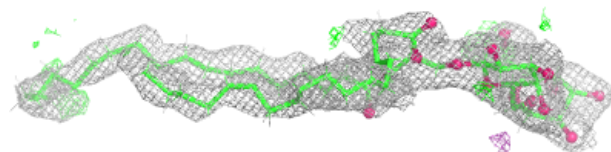
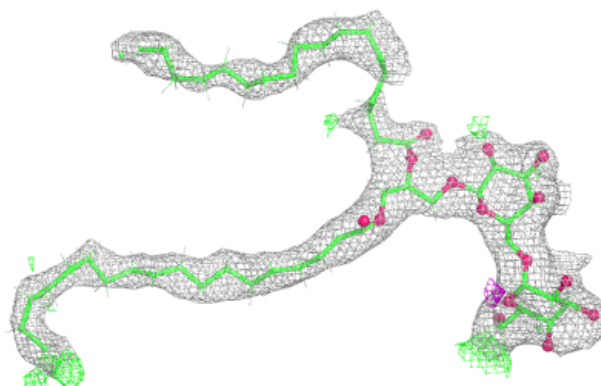


Electron density around STE c 501:

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

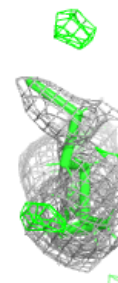
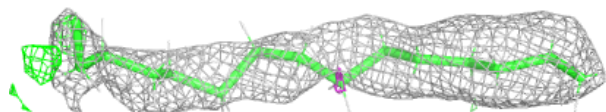
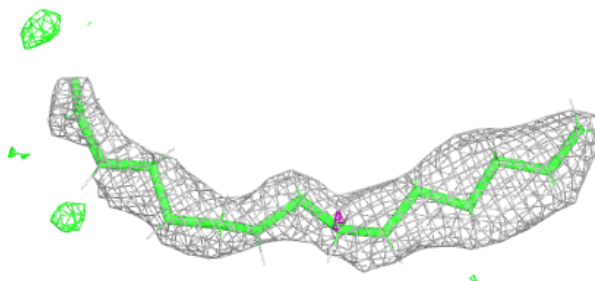
**Electron density around DGD A 413:**

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

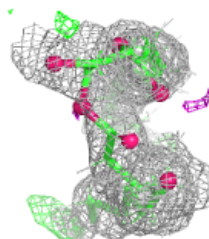
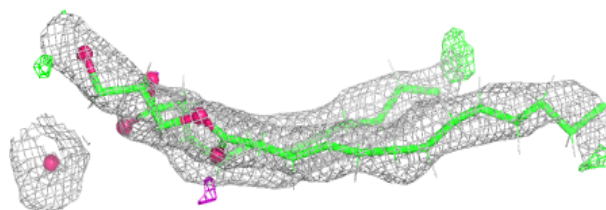
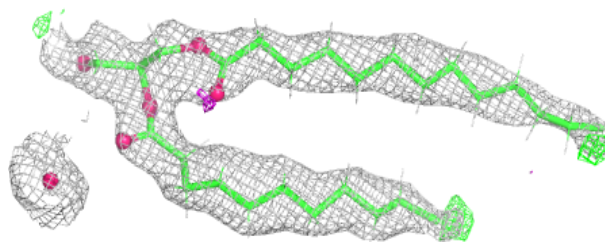


Electron density around STE T 102:

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

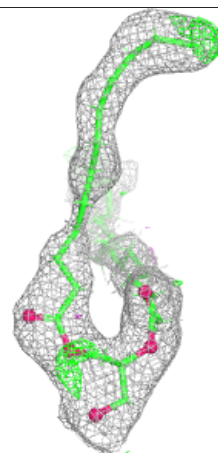
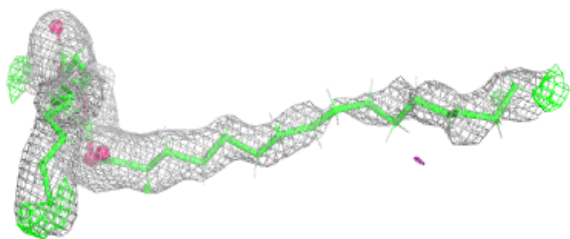
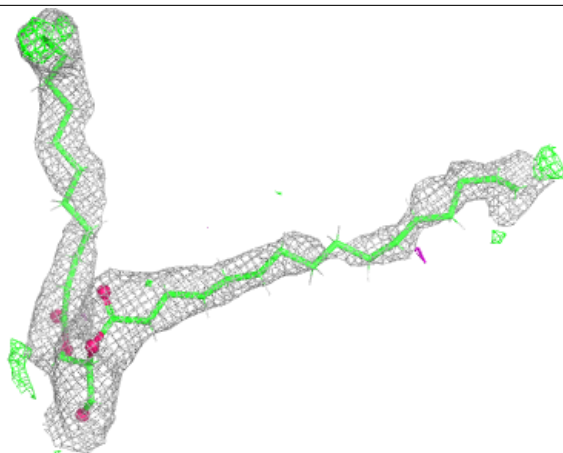
**Electron density around LMG D 411:**

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

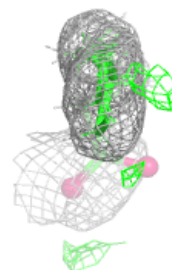
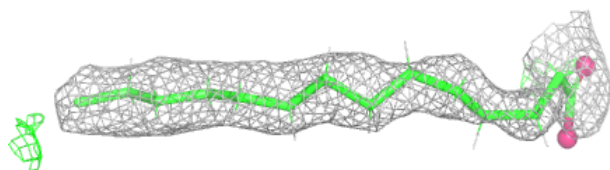
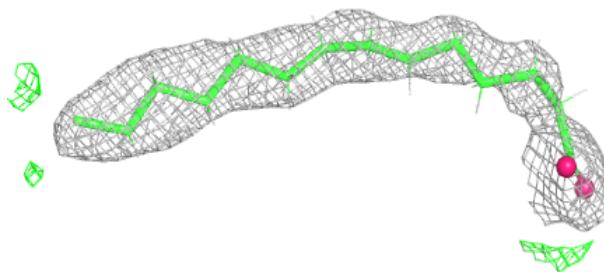


Electron density around SQD a 412:

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

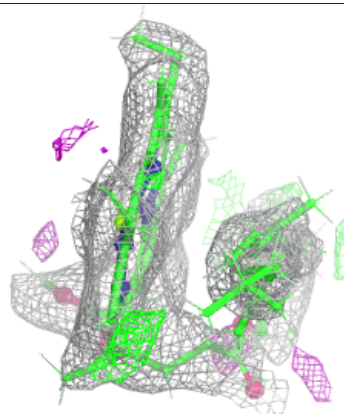
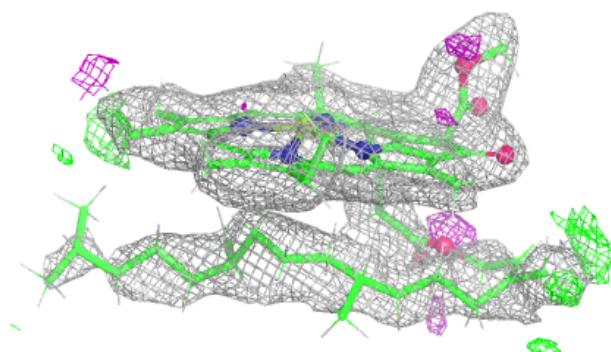
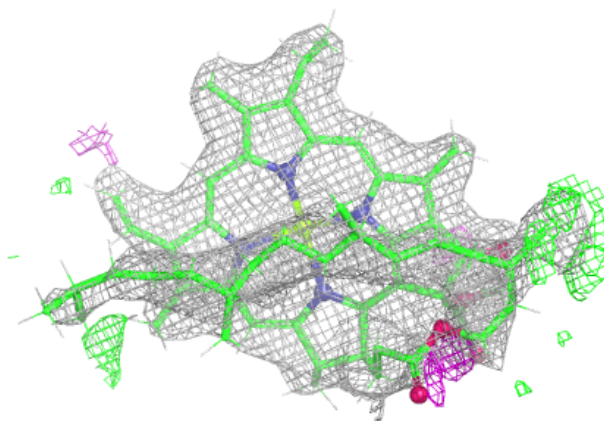
**Electron density around STE d 411:**

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

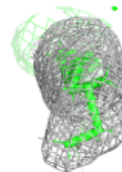
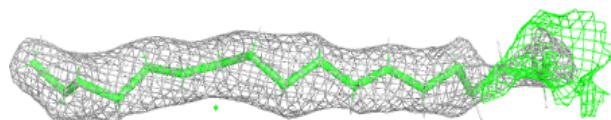
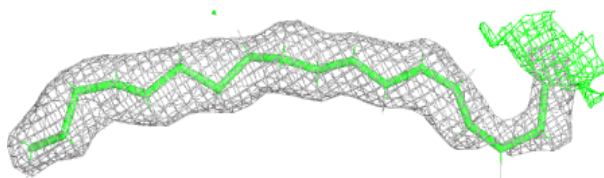


Electron density around CLA b 601:

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

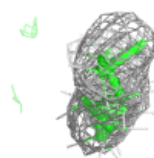
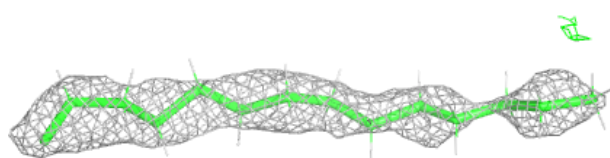
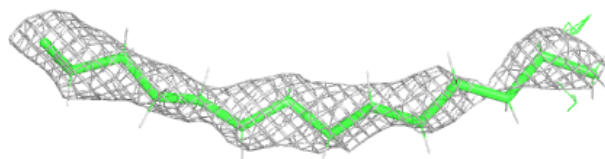
**Electron density around STE m 101:**

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

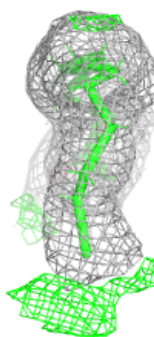
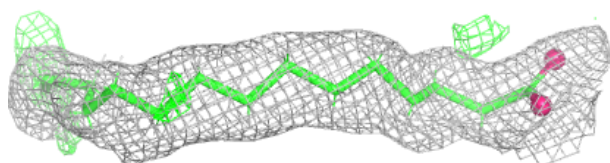
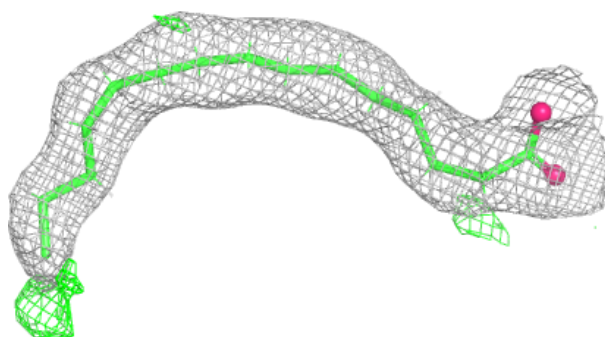


Electron density around STE b 626:

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

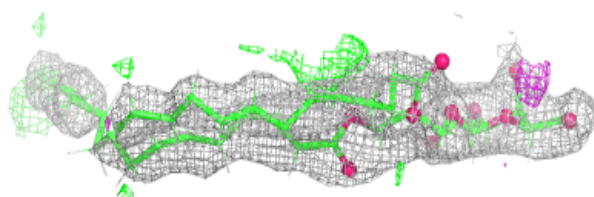
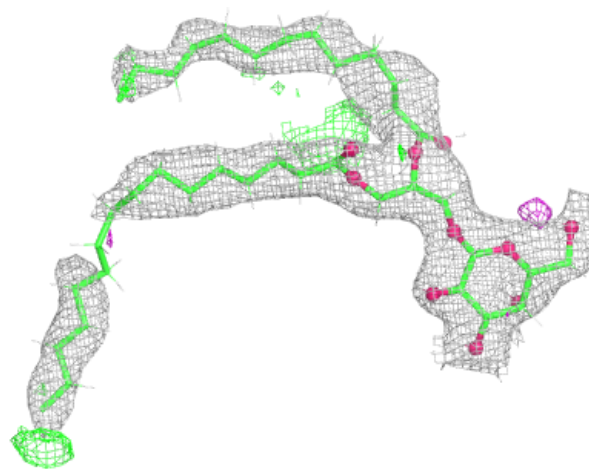
**Electron density around STE B 620:**

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



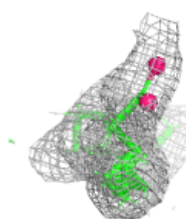
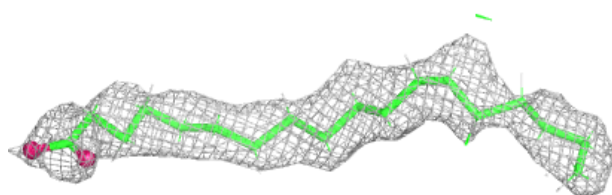
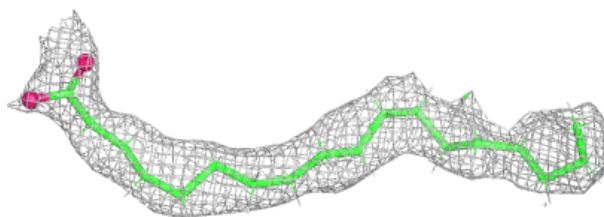
Electron density around LMG Y 101:

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

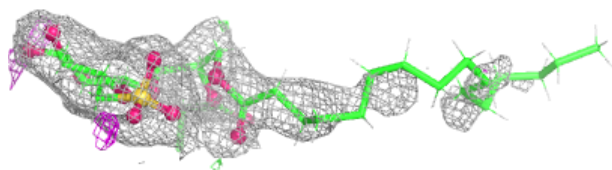
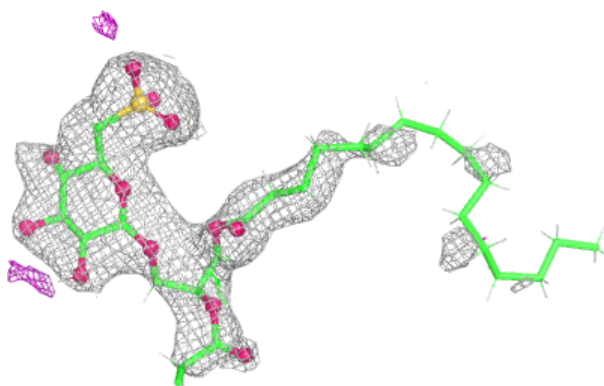


Electron density around STE b 622:

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

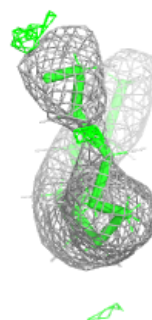
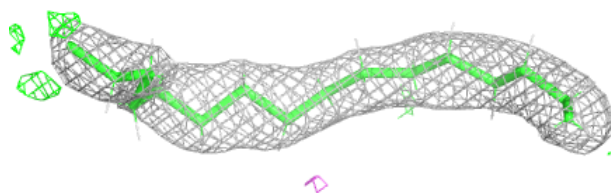
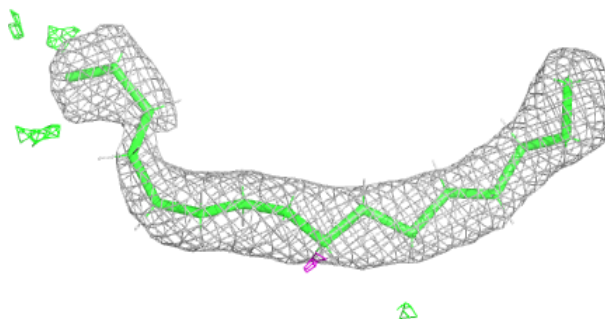
**Electron density around SQD f 102:**

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

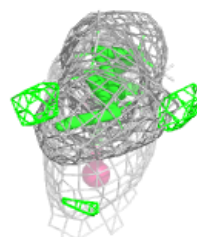
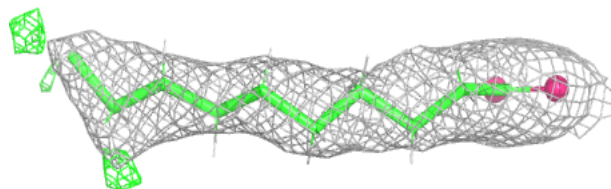
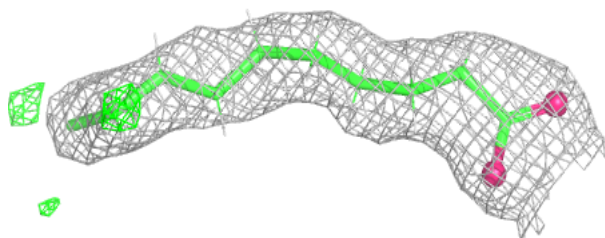


Electron density around STE b 620:

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

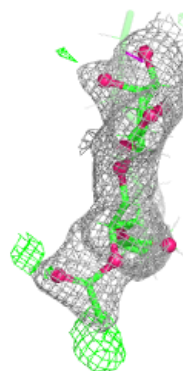
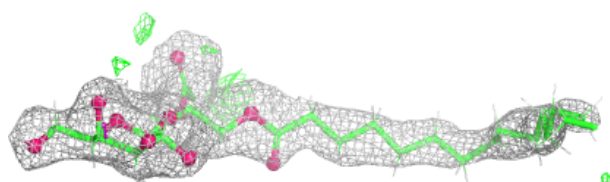
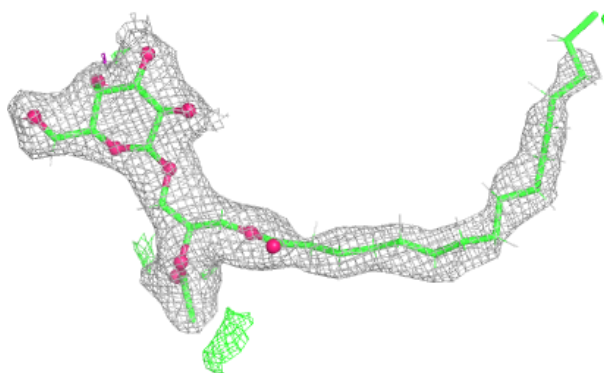
**Electron density around STE C 518:**

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

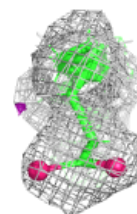
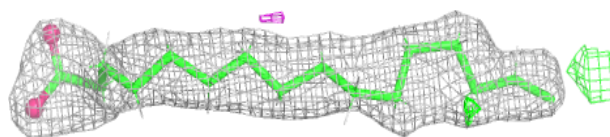
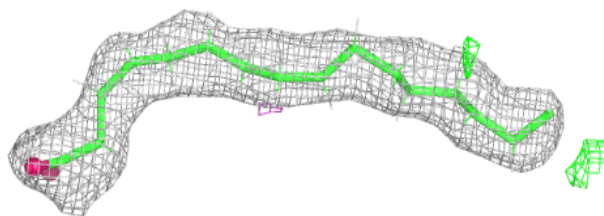


Electron density around LMG c 520:

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

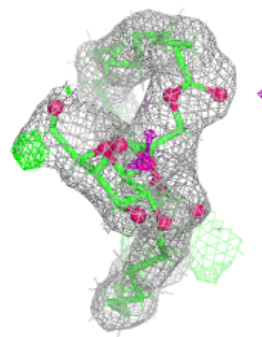
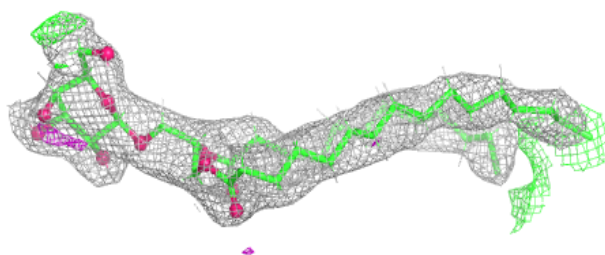
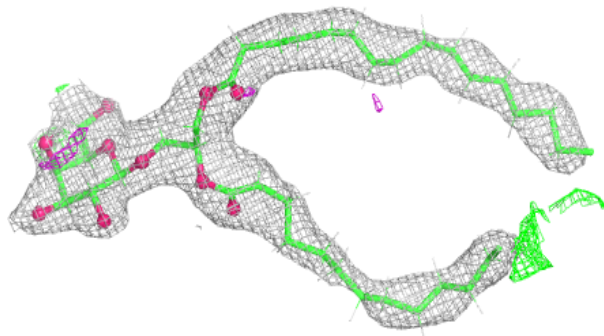
**Electron density around STE B 625:**

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



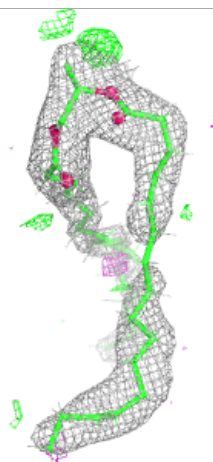
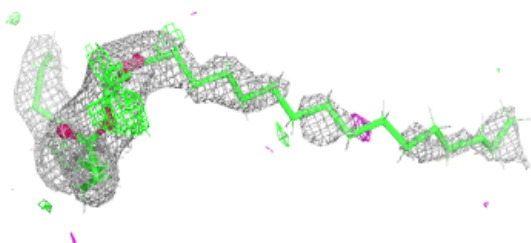
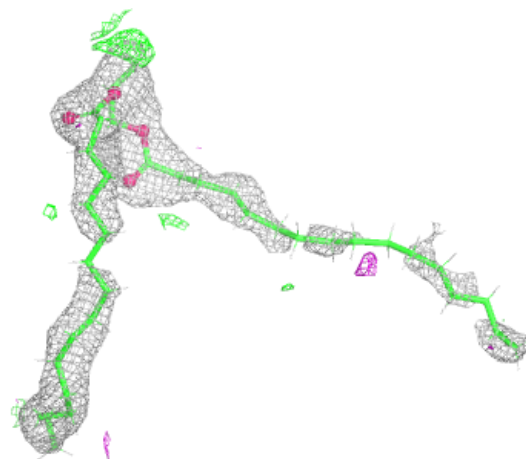
Electron density around LMG A 410:

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



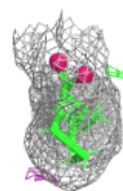
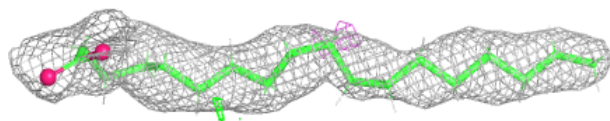
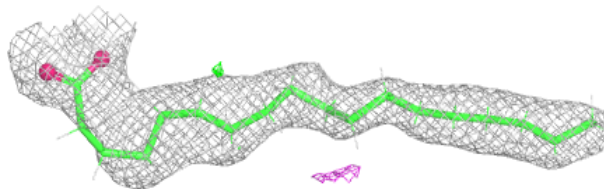
Electron density around SQD A 412:

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

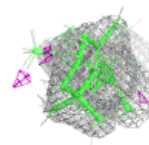
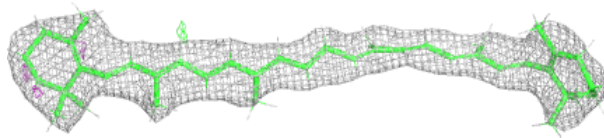


Electron density around STE c 521:

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

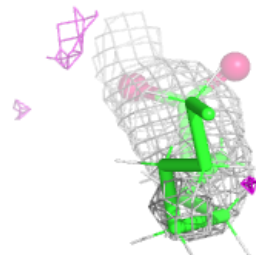
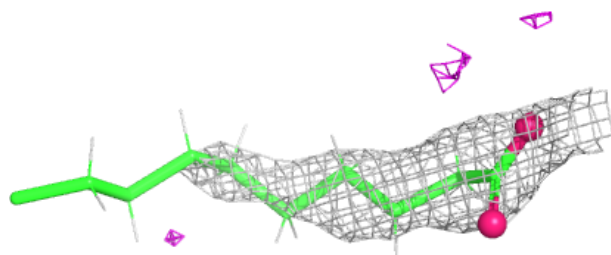
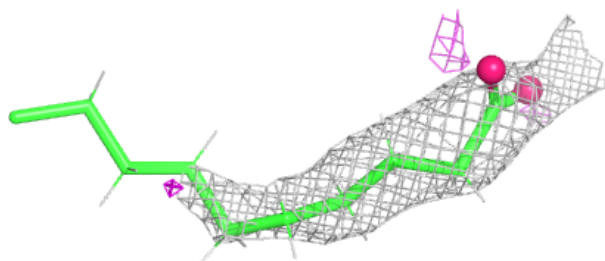
**Electron density around BCR K 101:**

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

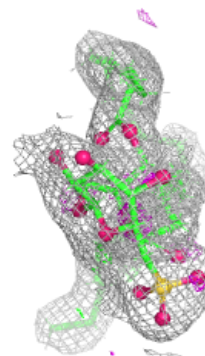
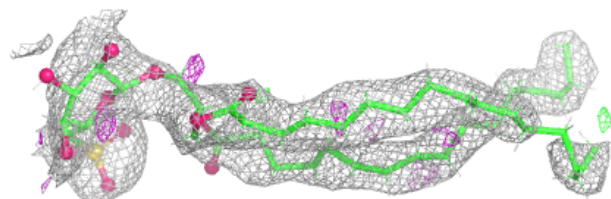
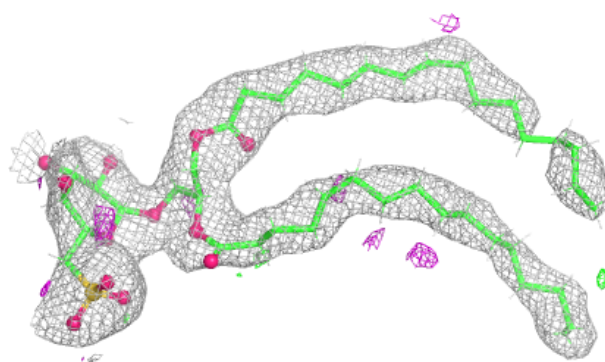


Electron density around STE B 601:

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

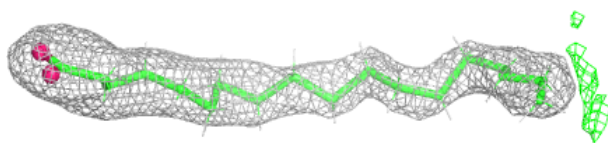
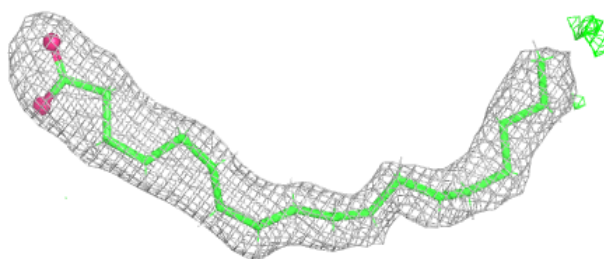
**Electron density around SQD B 622:**

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

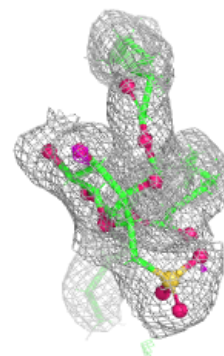
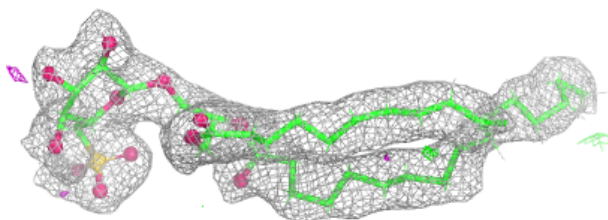
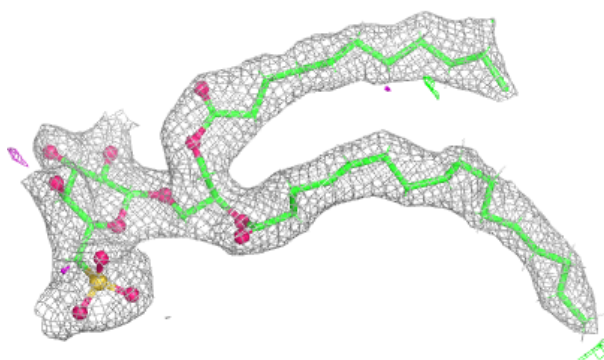


Electron density around STE d 413:

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

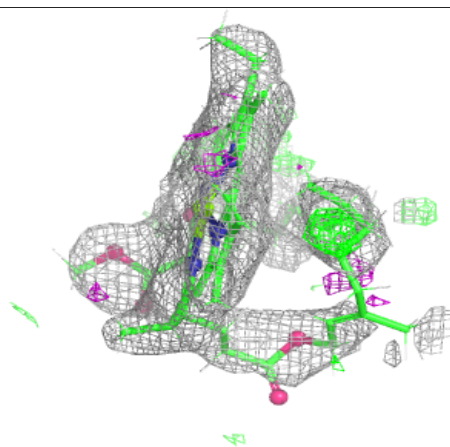
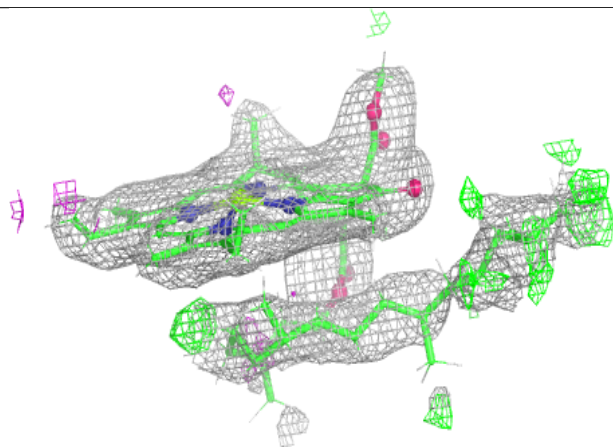
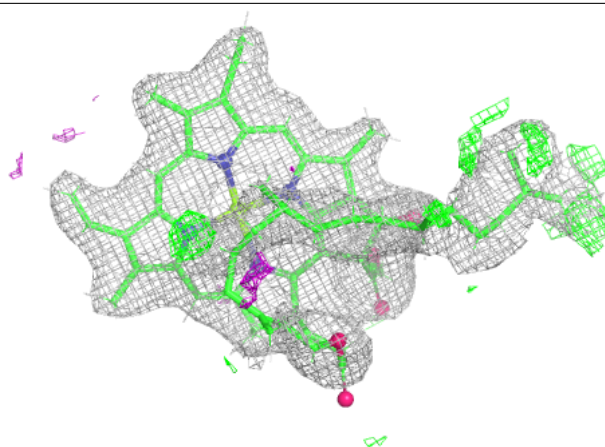
**Electron density around SQD L 101:**

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

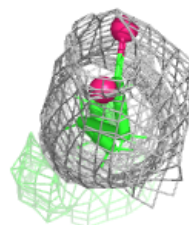
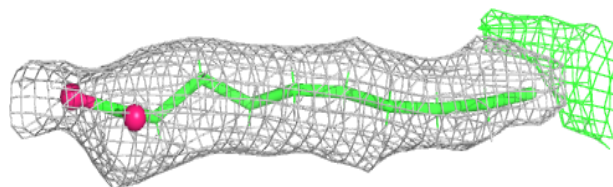
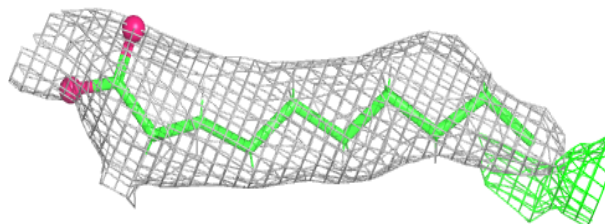


Electron density around CLA H 101:

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

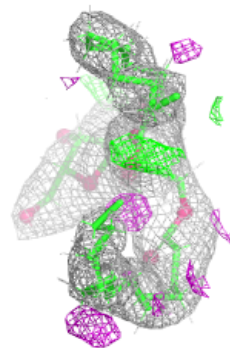
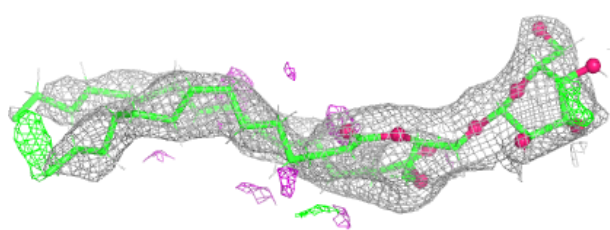
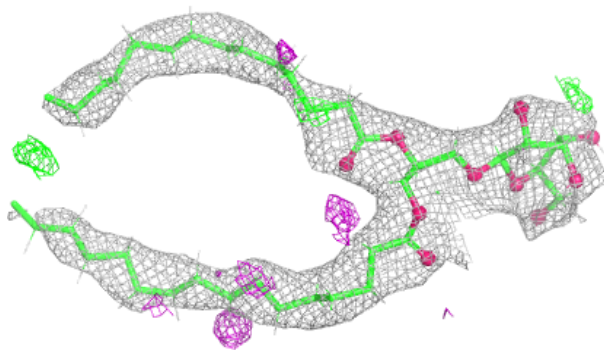
**Electron density around STE J 101:**

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

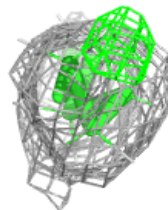
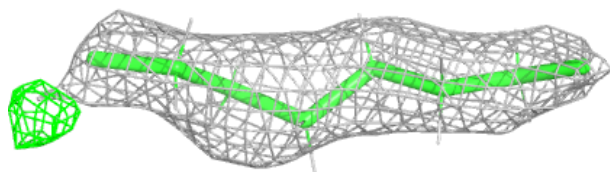
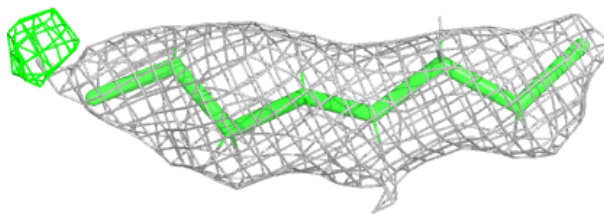


Electron density around LMG c 523:

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

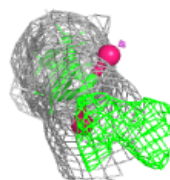
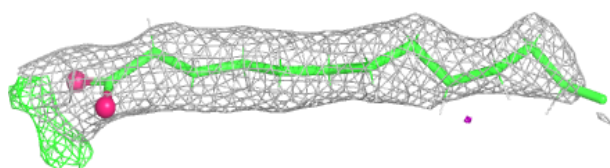
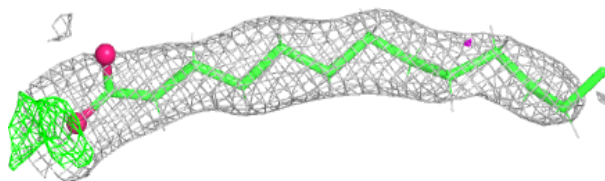
**Electron density around STE Z 101:**

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

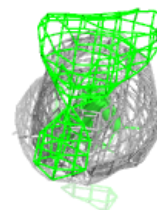
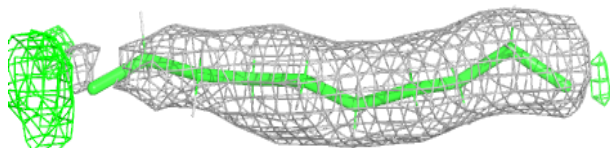
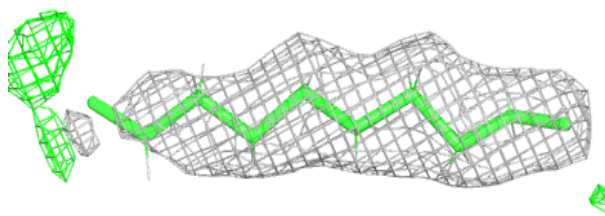


Electron density around STE M 102:

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

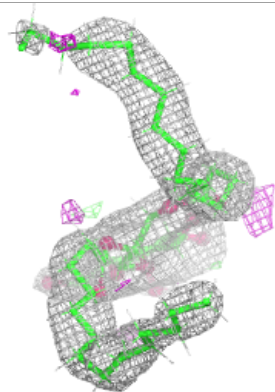
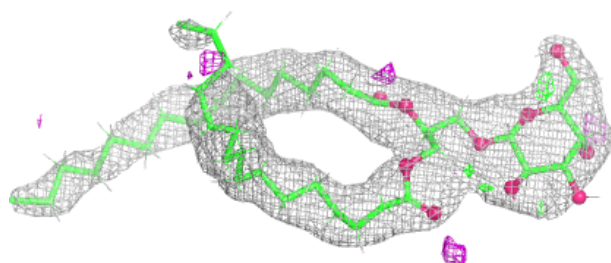
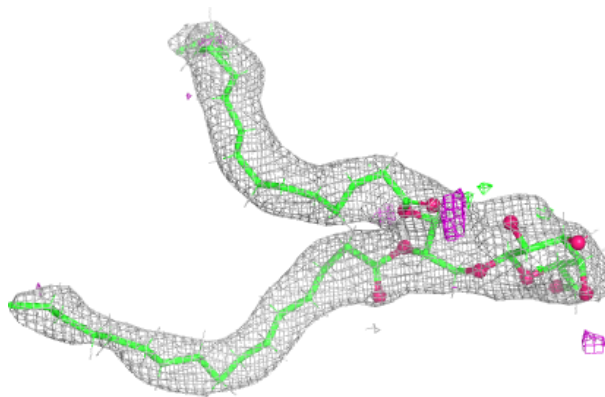
**Electron density around STE M 103:**

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

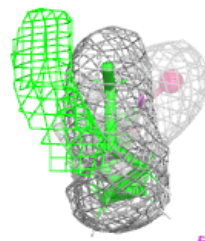
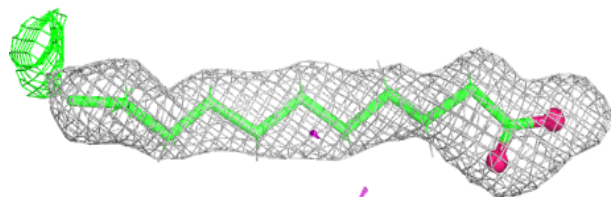
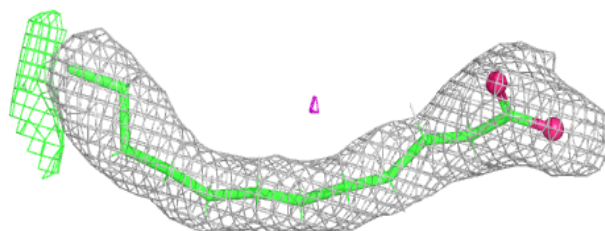


Electron density around LMG b 621:

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

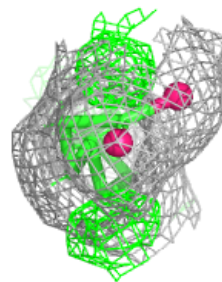
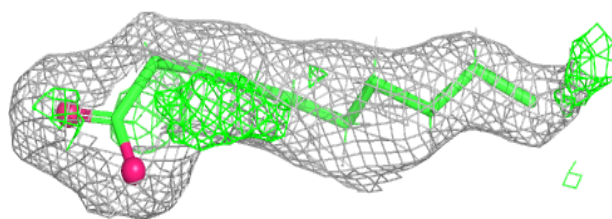
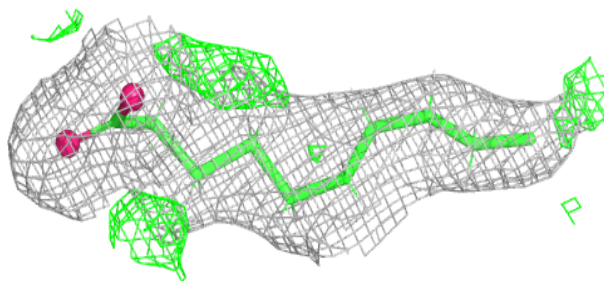
**Electron density around STE B 623:**

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

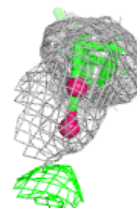
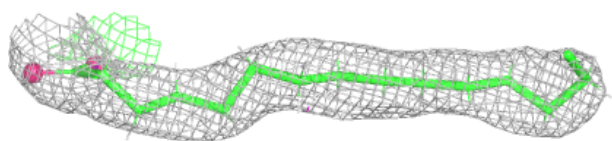
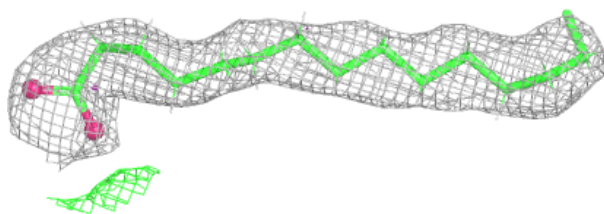


Electron density around STE B 624:

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

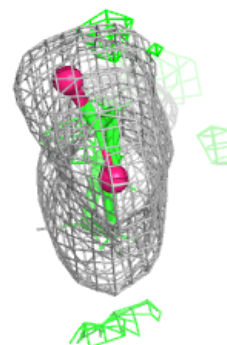
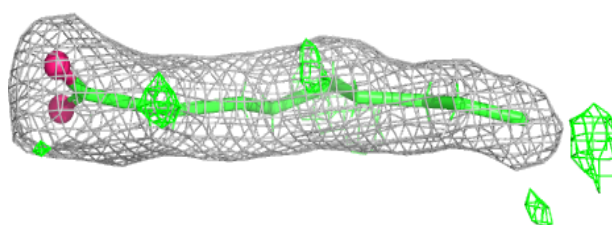
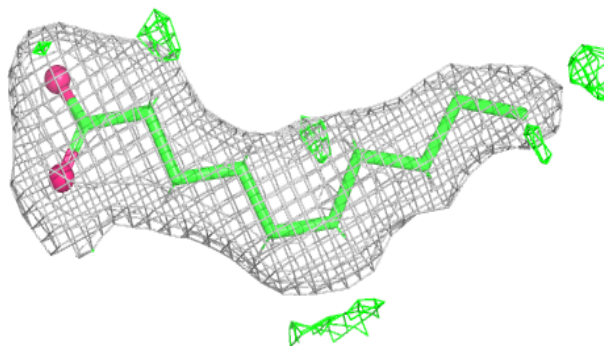
**Electron density around STE d 412:**

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

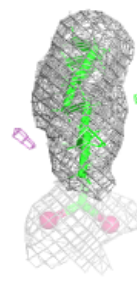
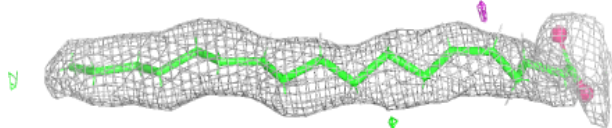
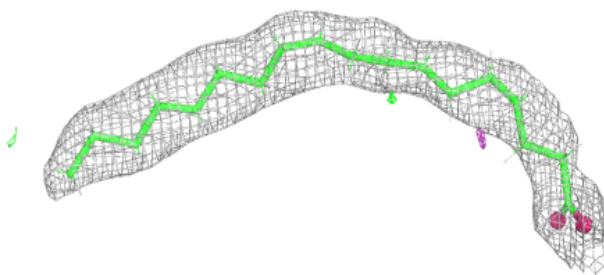


Electron density around STE C 520:

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

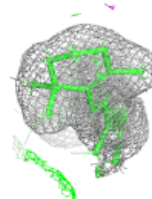
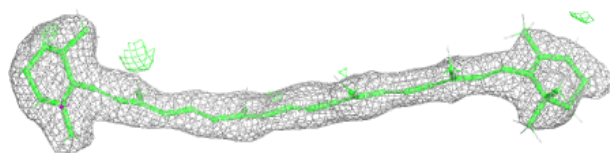
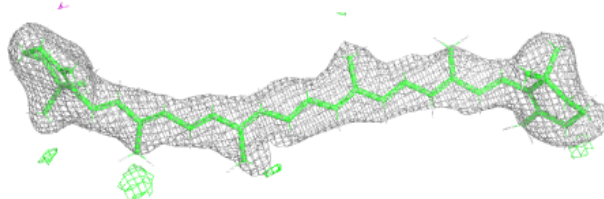
**Electron density around STE D 413:**

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

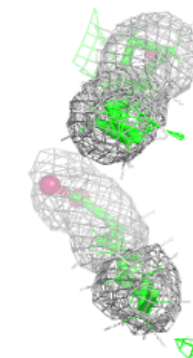
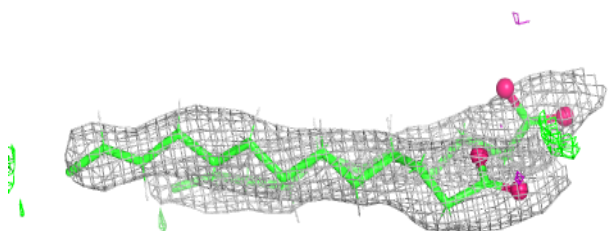
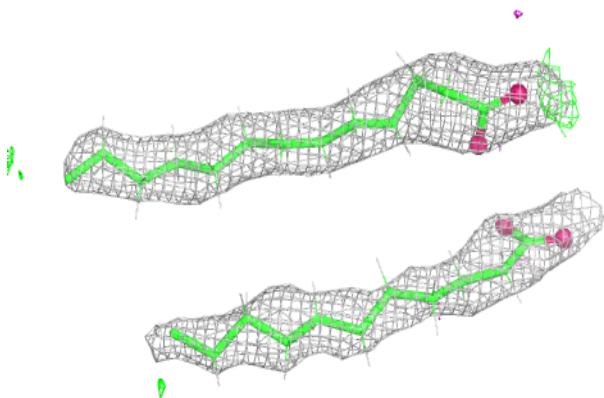


Electron density around BCR h 101:

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

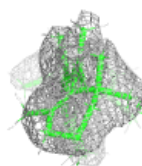
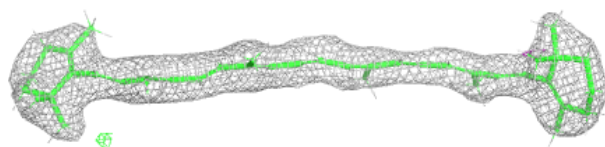
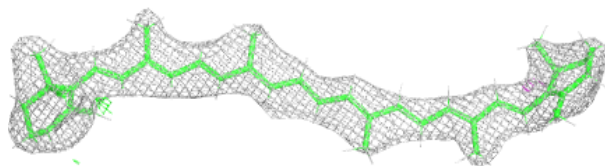
**Electron density around LMG B 621:**

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

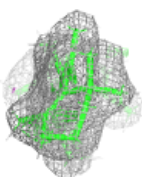
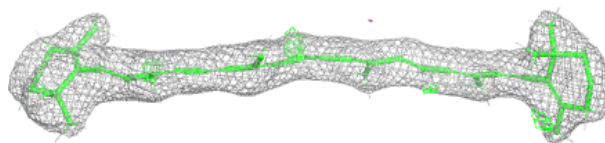


Electron density around BCR k 101:

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

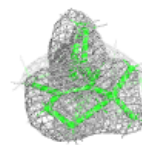
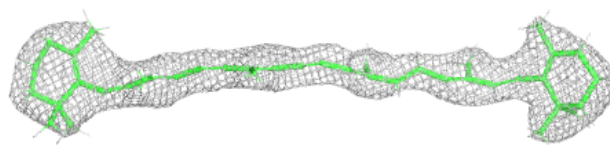
**Electron density around BCR K 102:**

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



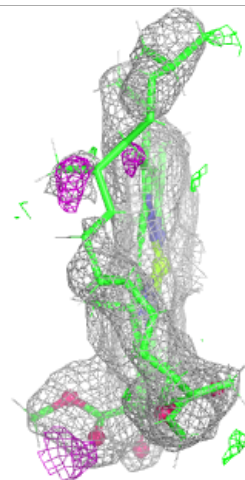
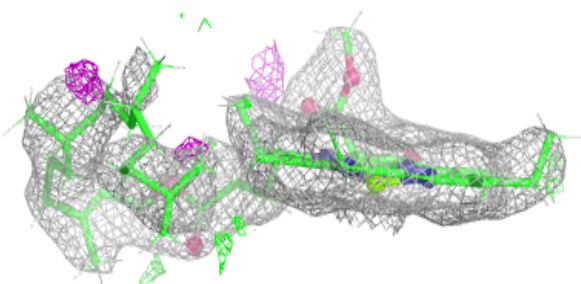
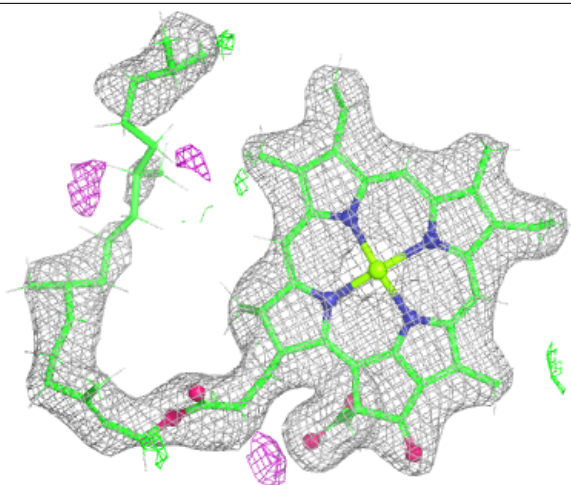
Electron density around BCR c 515:

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



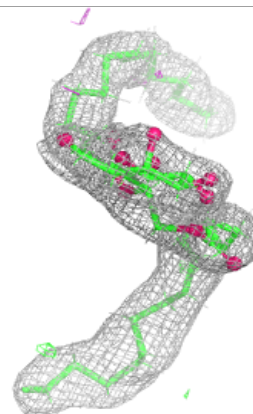
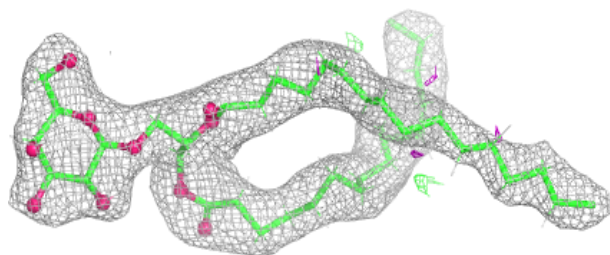
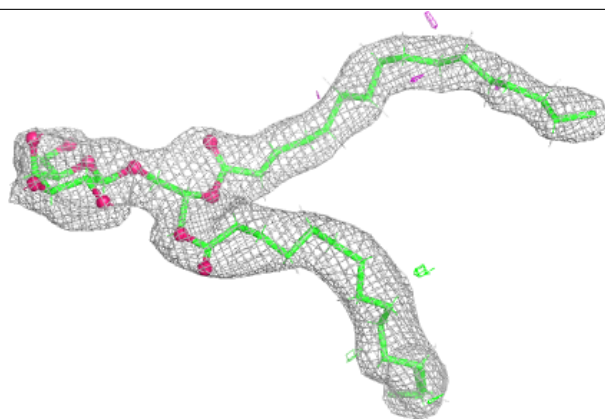
Electron density around CLA c 513:

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

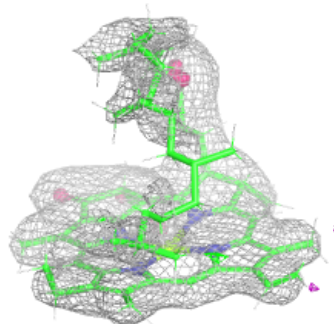
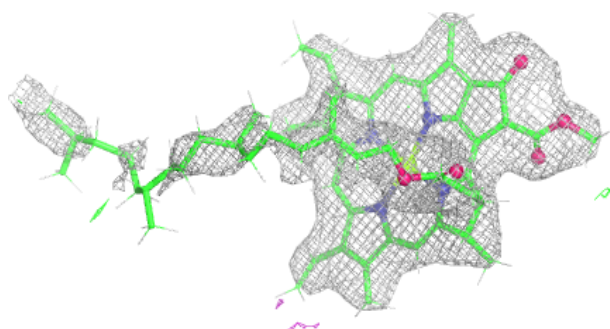
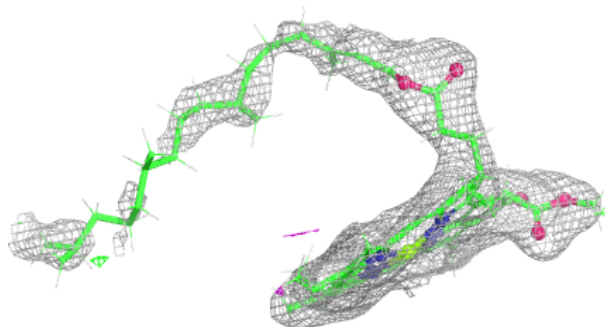


Electron density around LMG M 101:

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

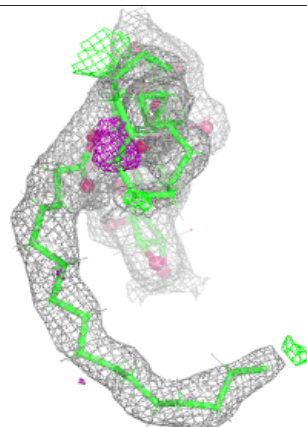
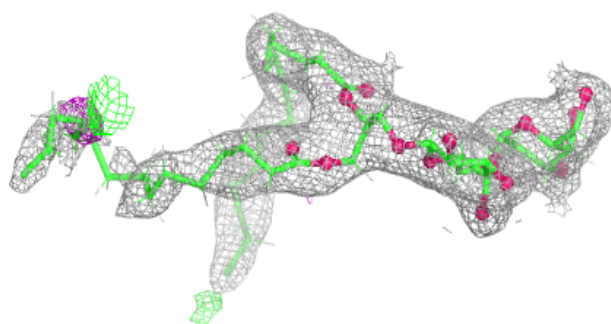
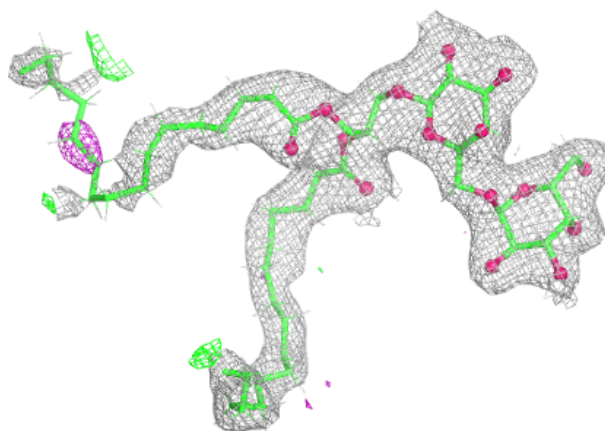
**Electron density around CLA C 513:**

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

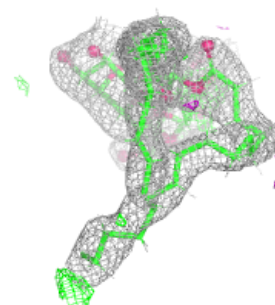
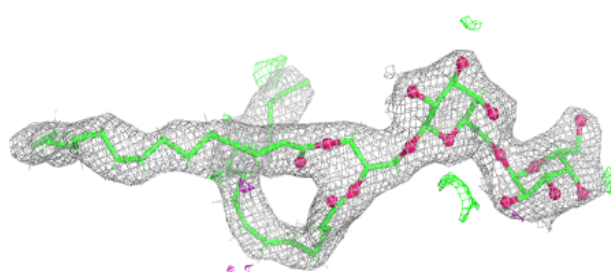
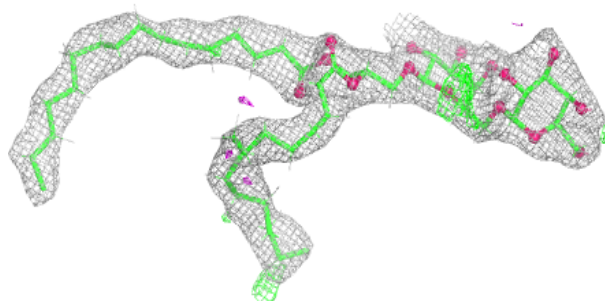


Electron density around DGD C 516:

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

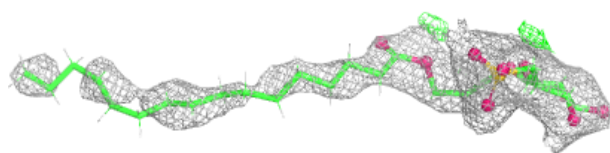
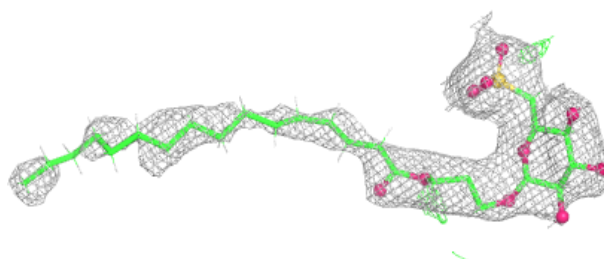
**Electron density around DGD h 102:**

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

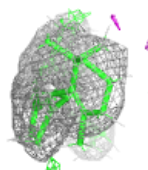
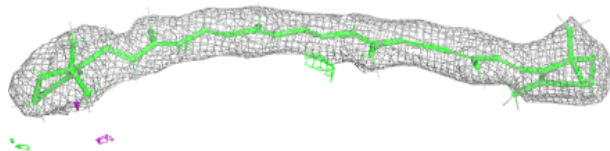


Electron density around SQD D 408:

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

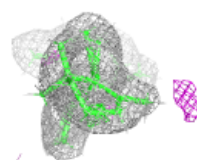
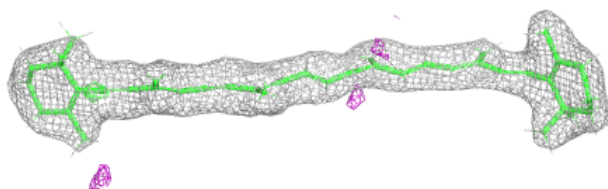
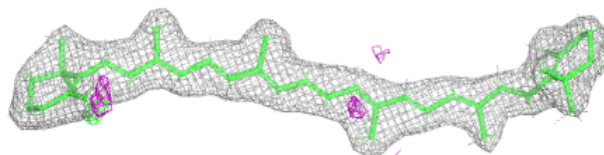
**Electron density around BCR d 405:**

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



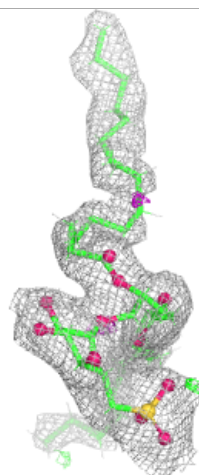
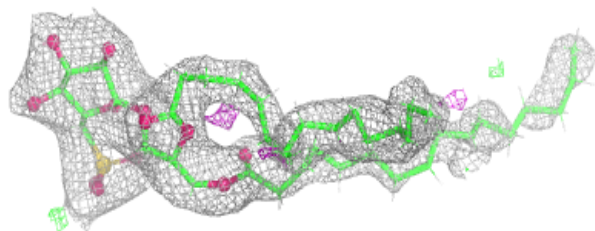
Electron density around BCR C 514:

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



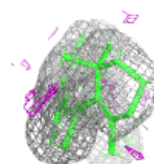
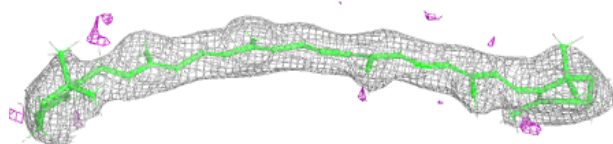
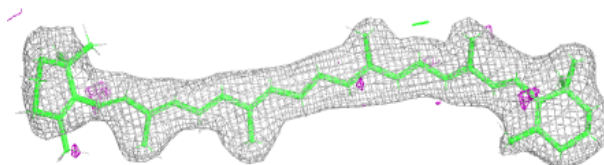
Electron density around SQD a 411:

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

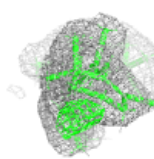
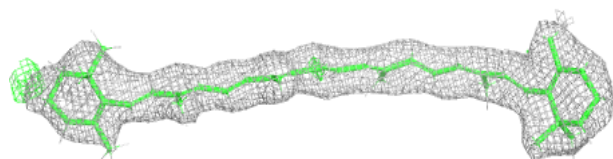
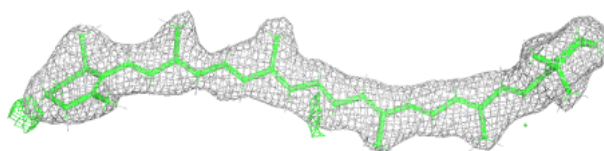


Electron density around BCR F 101:

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

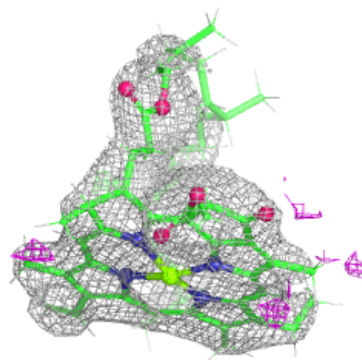
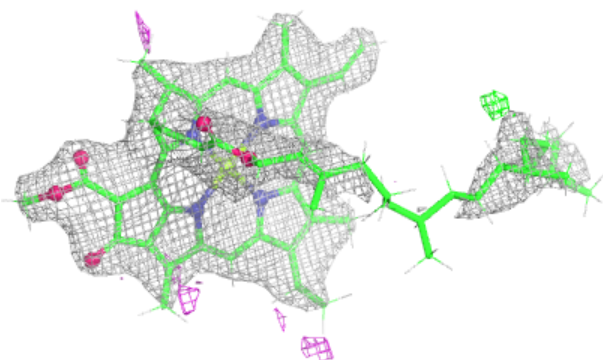
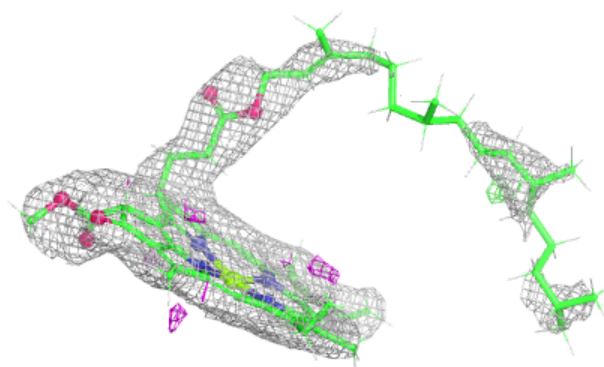
**Electron density around BCR H 102:**

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

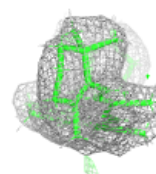
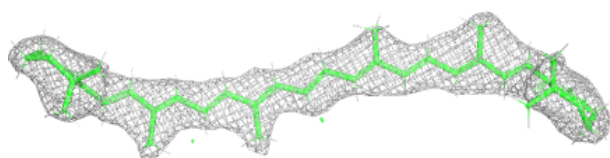
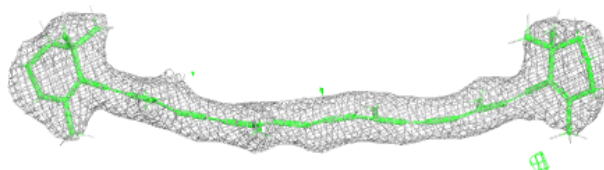


Electron density around CLA c 514:

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

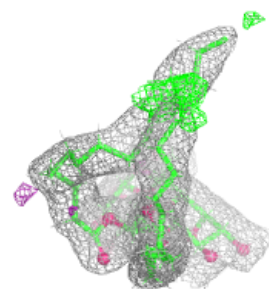
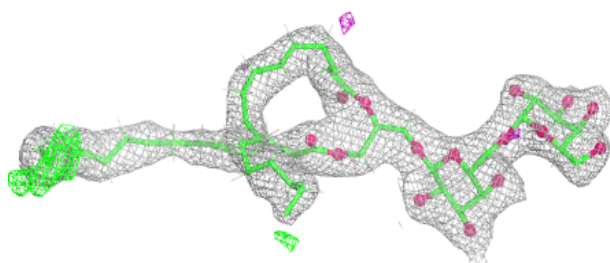
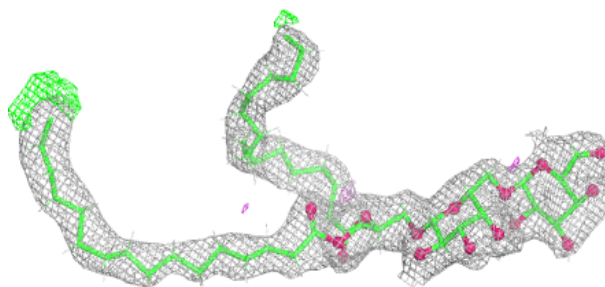
**Electron density around BCR k 102:**

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

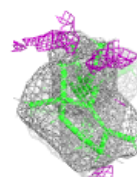
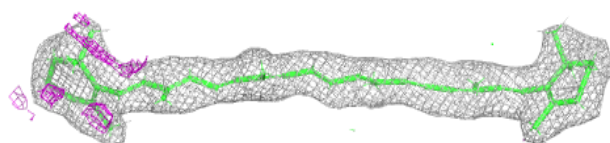
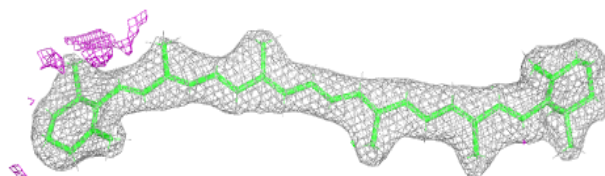


Electron density around DGD H 103:

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

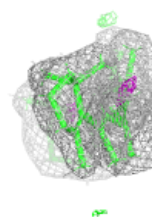
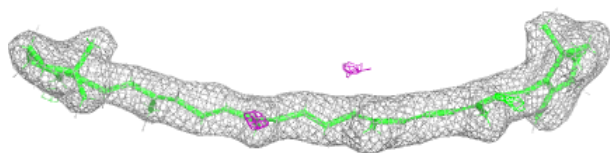
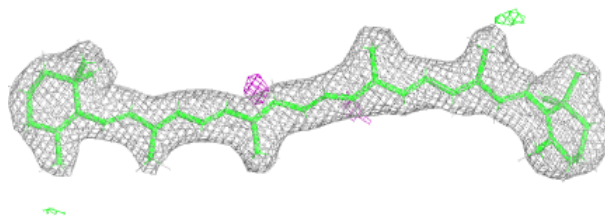
**Electron density around BCR B 618:**

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

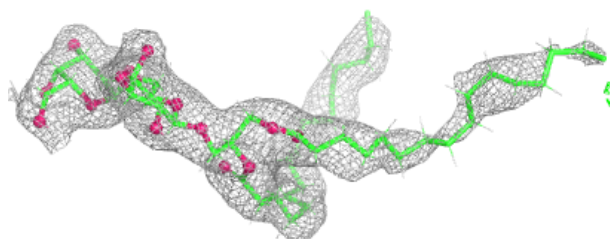
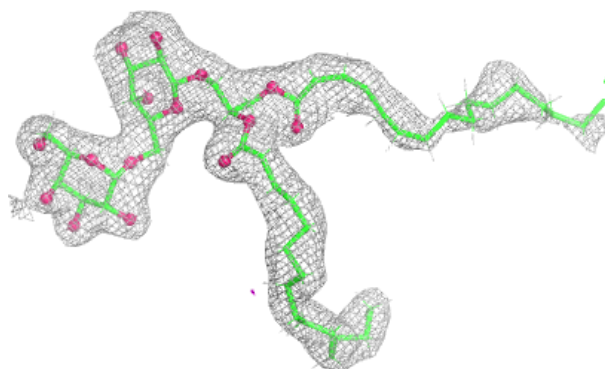


Electron density around BCR T 101:

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

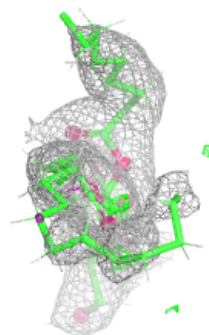
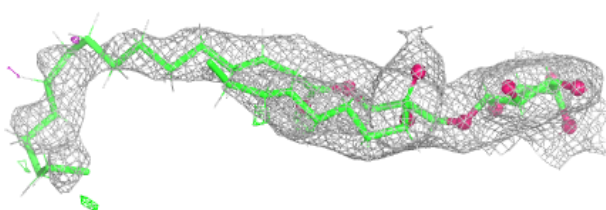
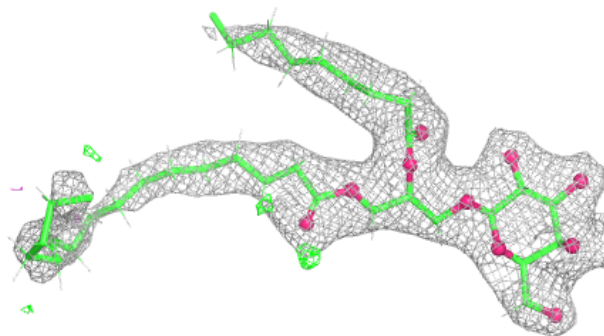
**Electron density around DGD c 518:**

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

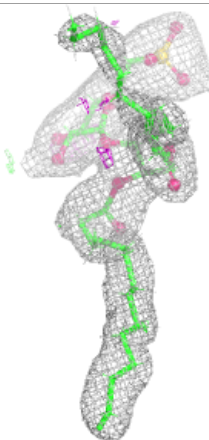
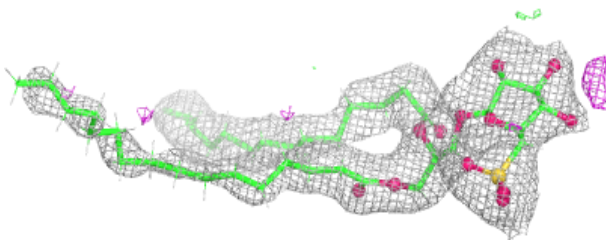
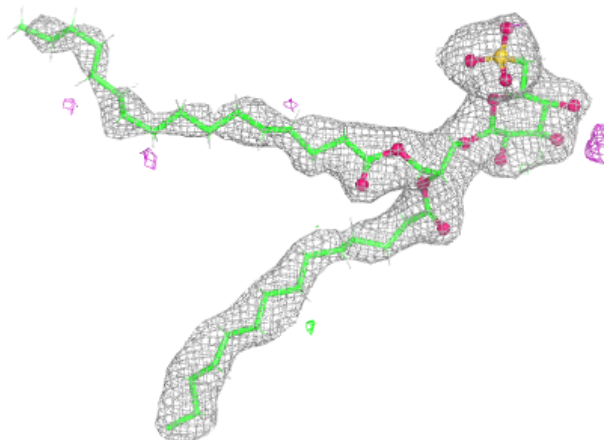


Electron density around LMG d 410:

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

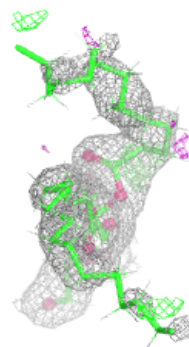
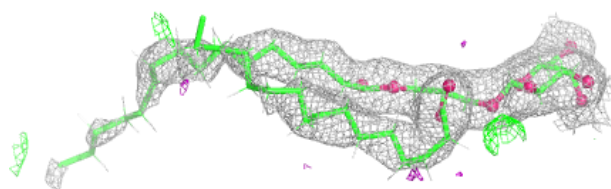
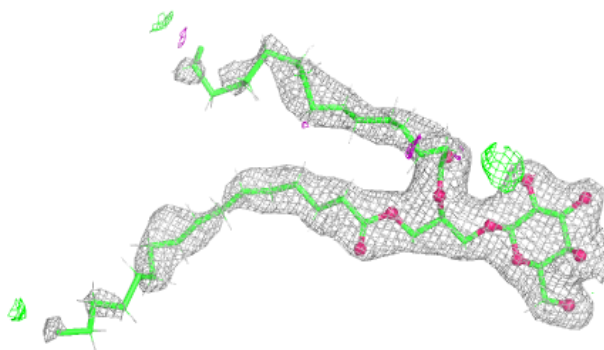
**Electron density around SQD A 411:**

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

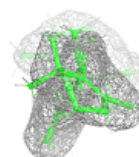
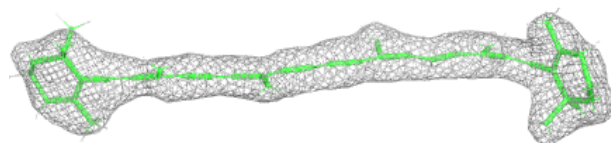
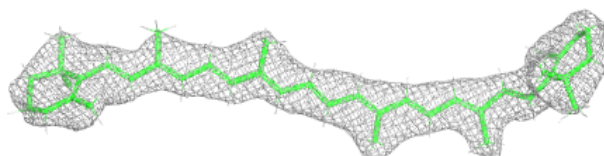


Electron density around LMG D 407:

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

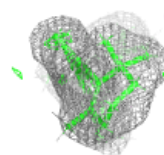
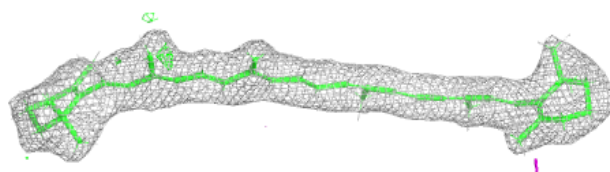
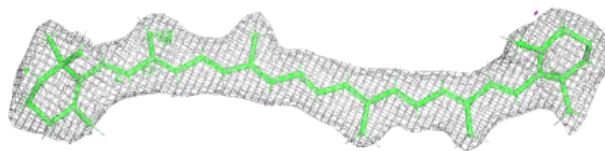
**Electron density around BCR c 516:**

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

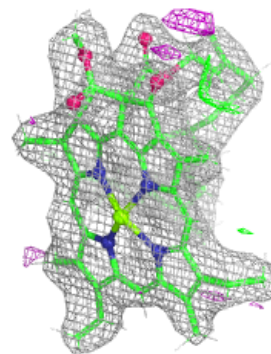
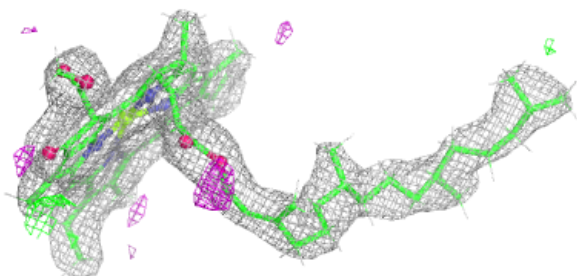
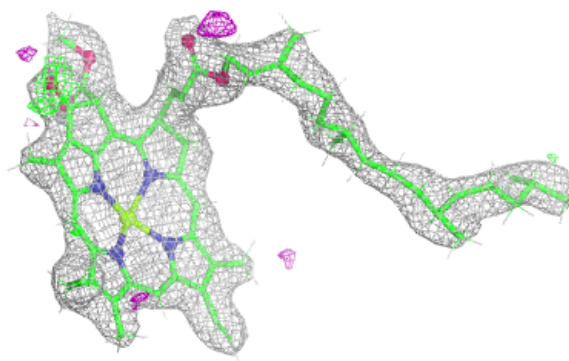


Electron density around BCR B 619:

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

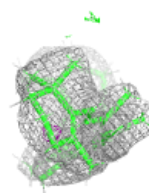
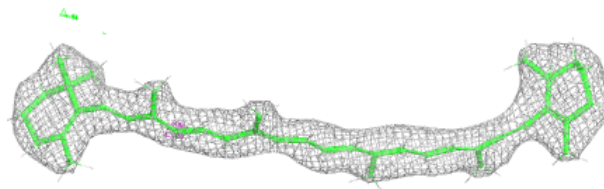
**Electron density around CLA c 512:**

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

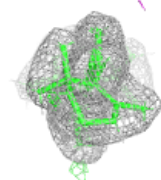
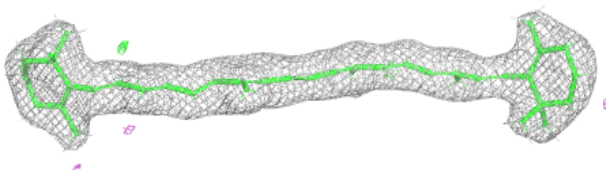
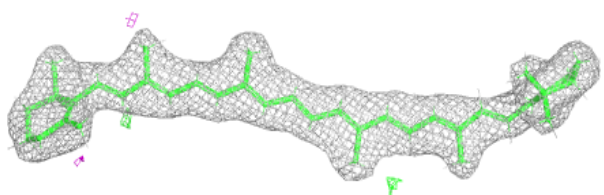


Electron density around BCR K 103:

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

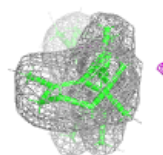
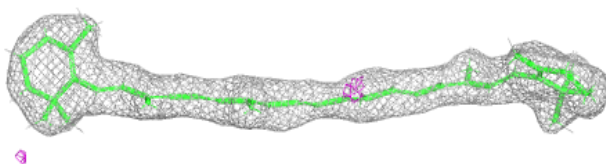
**Electron density around BCR A 406:**

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

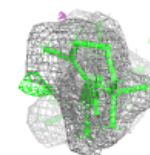
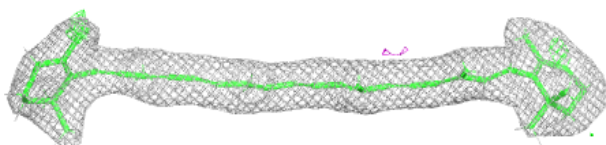
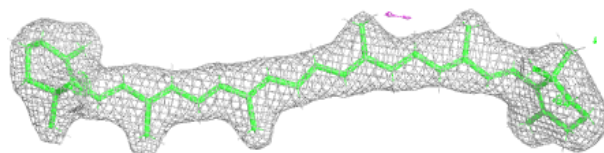


Electron density around BCR b 617:

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

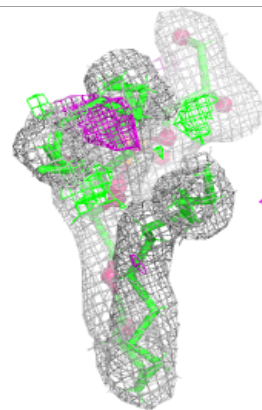
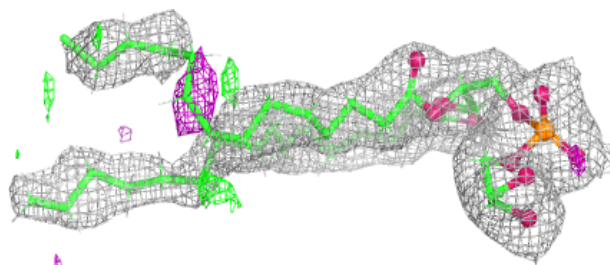
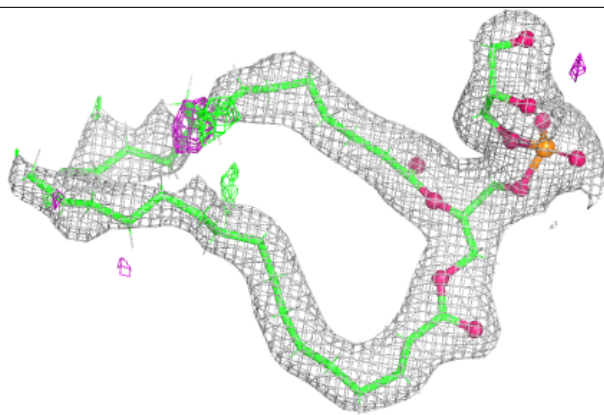
**Electron density around BCR b 618:**

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

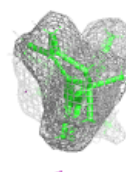
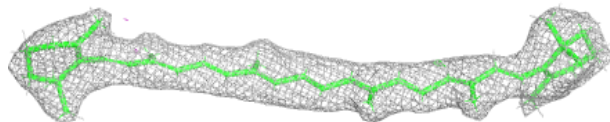
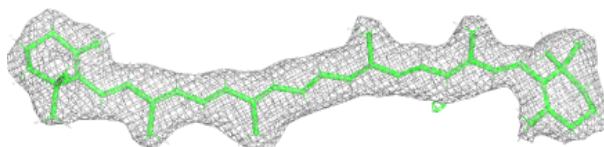


Electron density around LHG D 410:

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

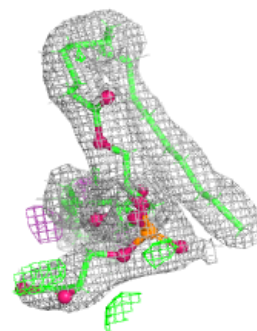
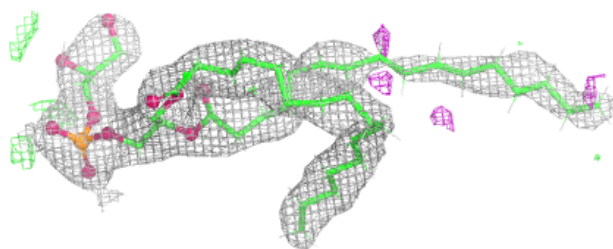
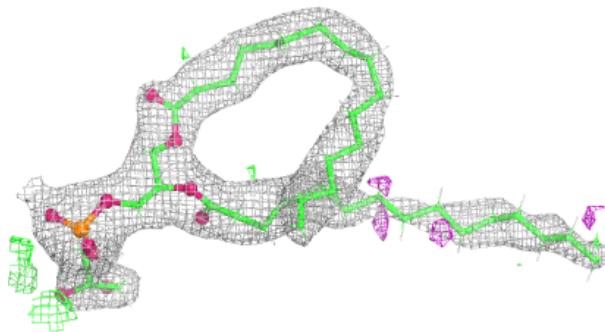
**Electron density around BCR b 619:**

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

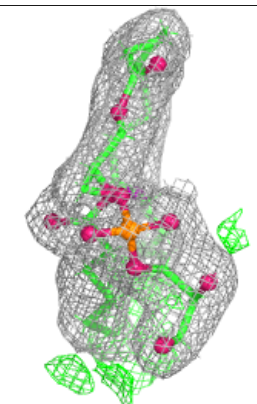
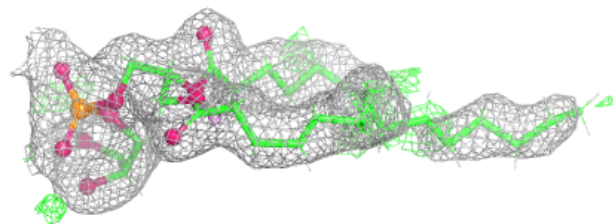
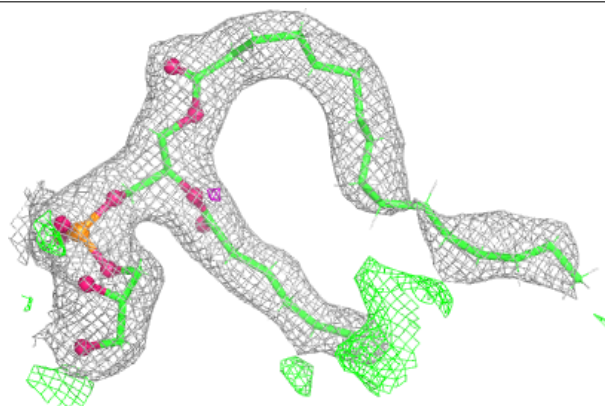


Electron density around LHG d 407:

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

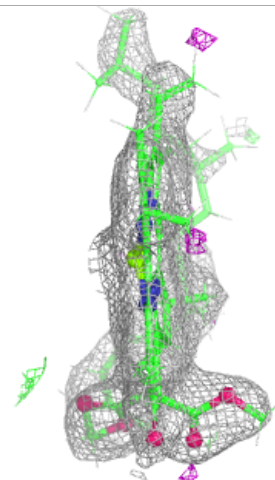
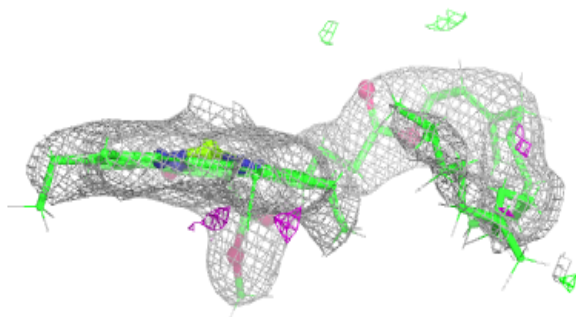
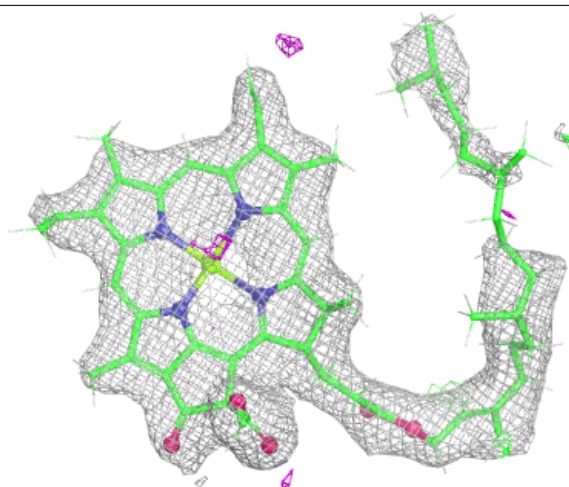
**Electron density around LHG d 409:**

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



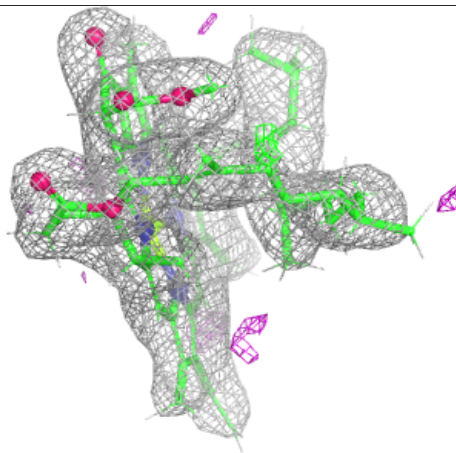
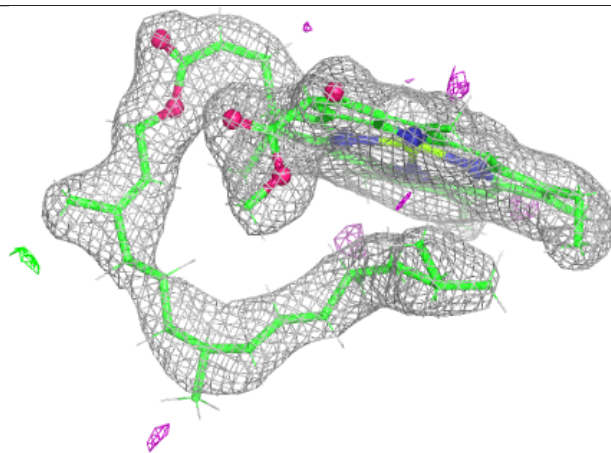
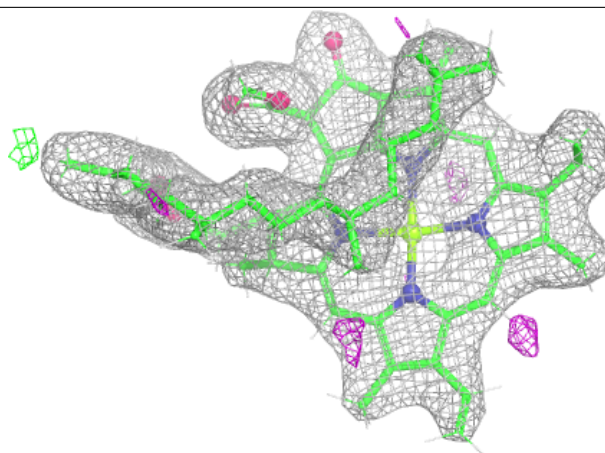
Electron density around CLA C 512:

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



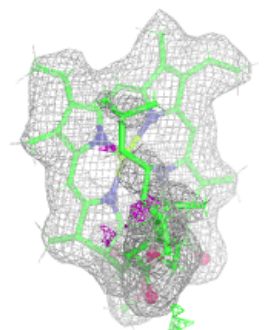
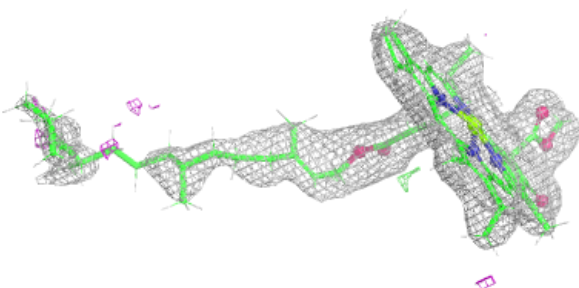
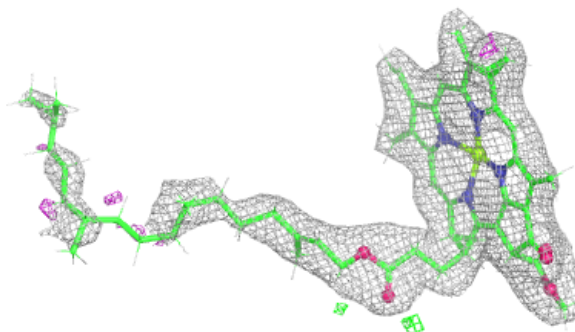
Electron density around CLA C 510:

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

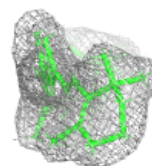
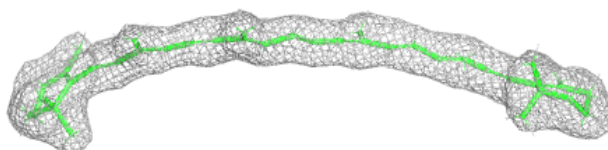
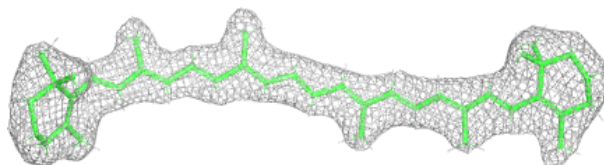


Electron density around CLA d 404:

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

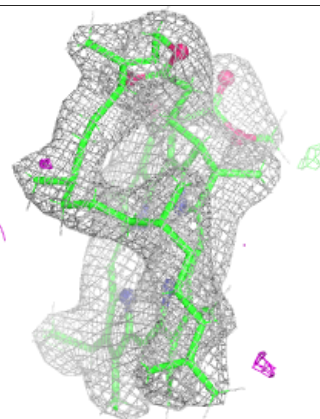
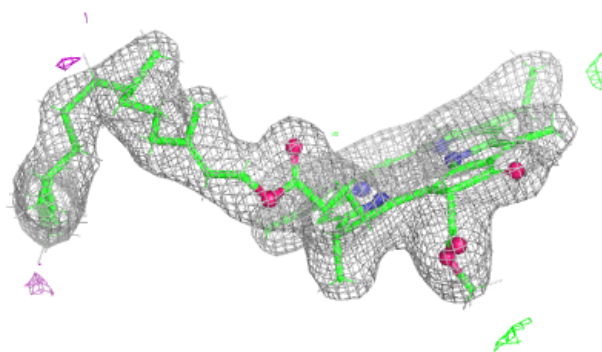
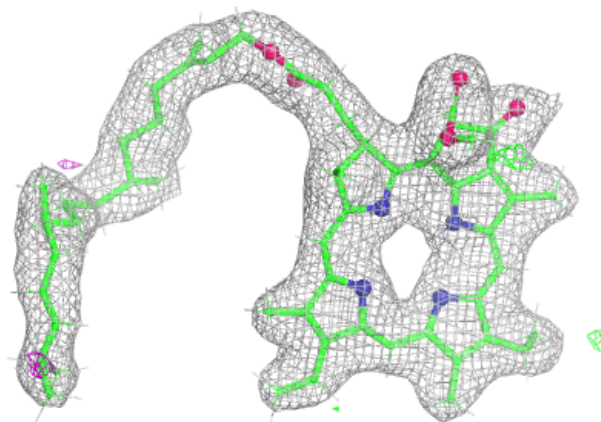
**Electron density around BCR t 101:**

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

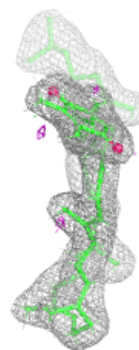
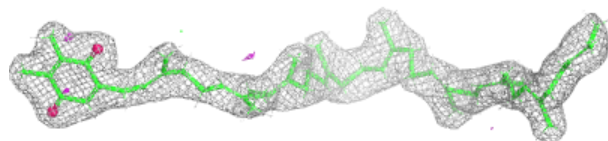
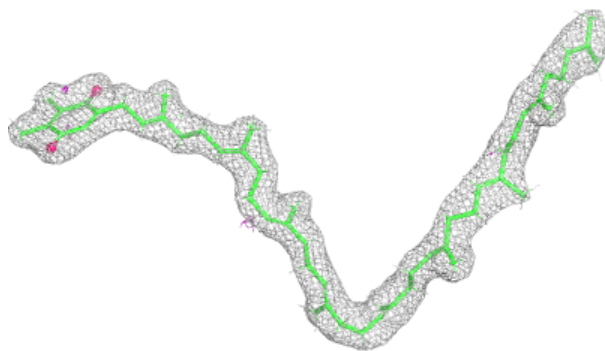


Electron density around PHO d 401:

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

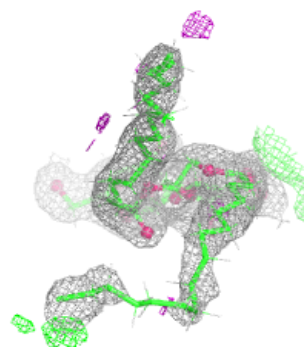
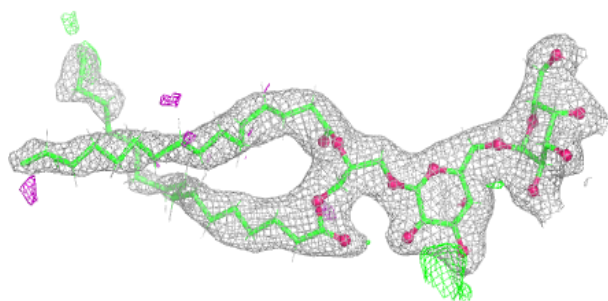
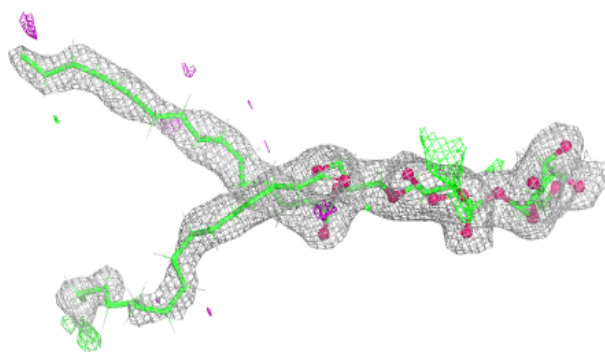
**Electron density around PL9 D 406:**

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

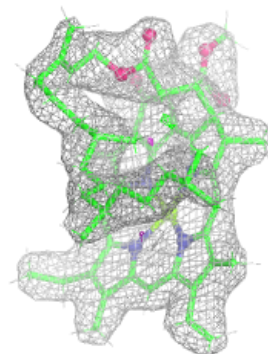
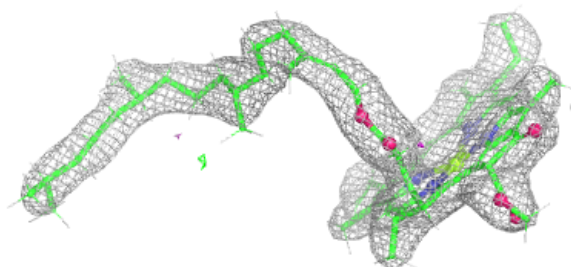
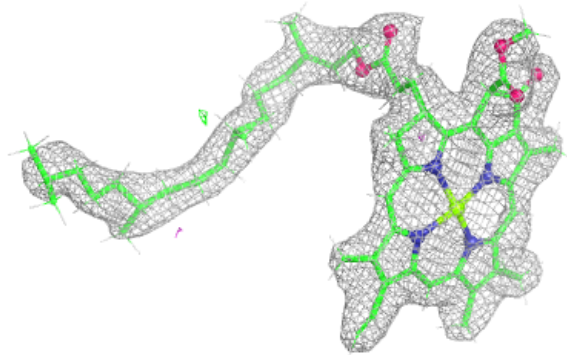


Electron density around DGD C 515:

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

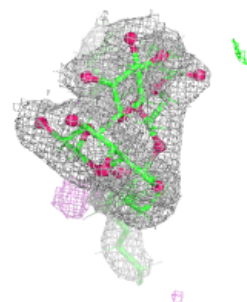
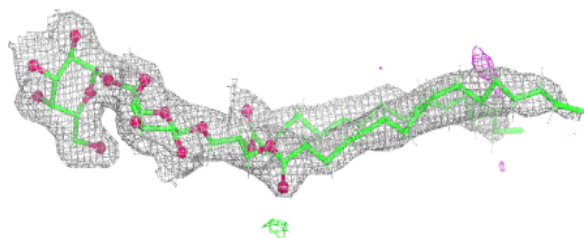
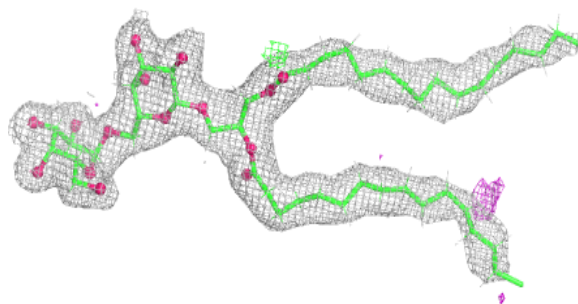
**Electron density around CLA C 511:**

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

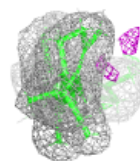
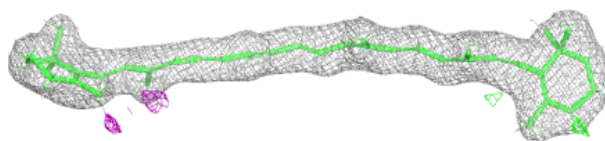
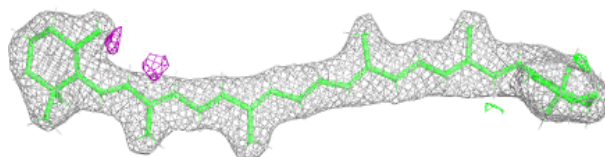


Electron density around DGD C 517:

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

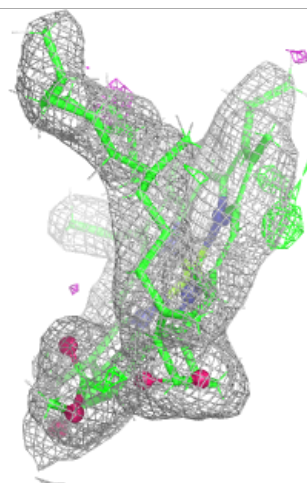
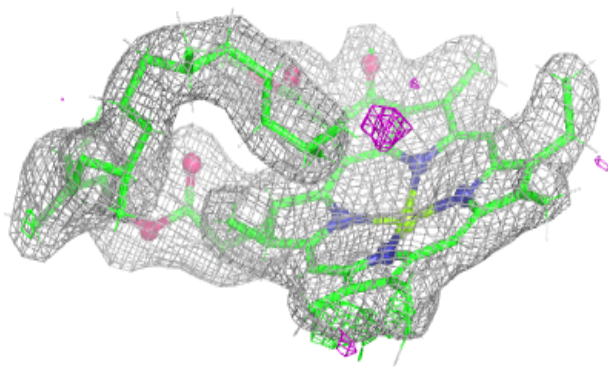
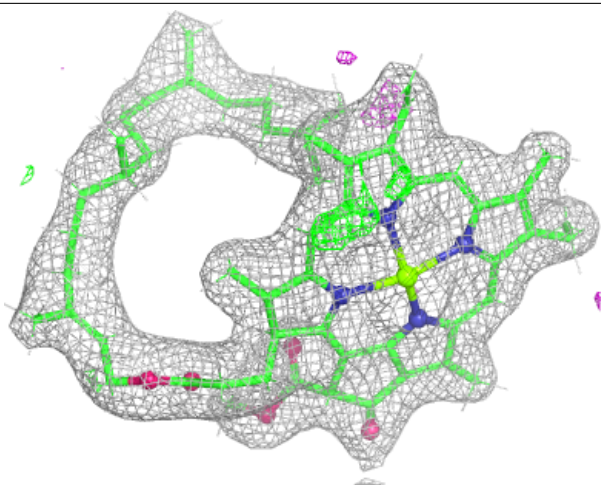
**Electron density around BCR B 617:**

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



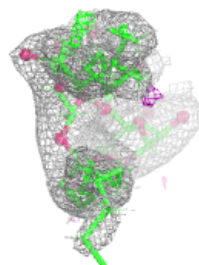
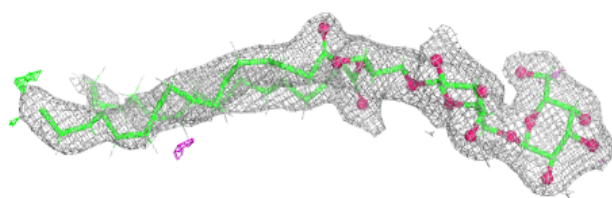
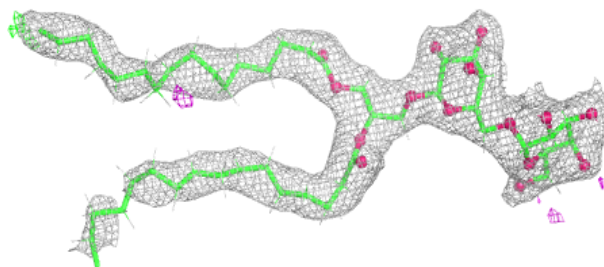
Electron density around CLA B 615:

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

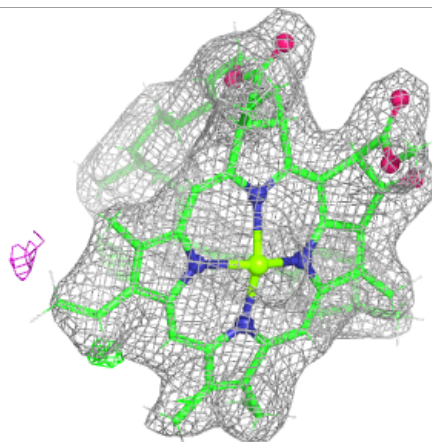
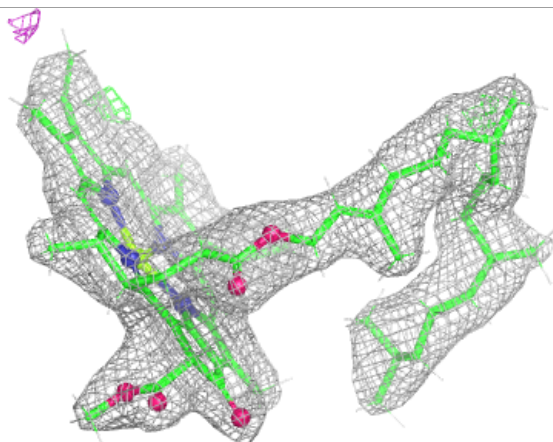
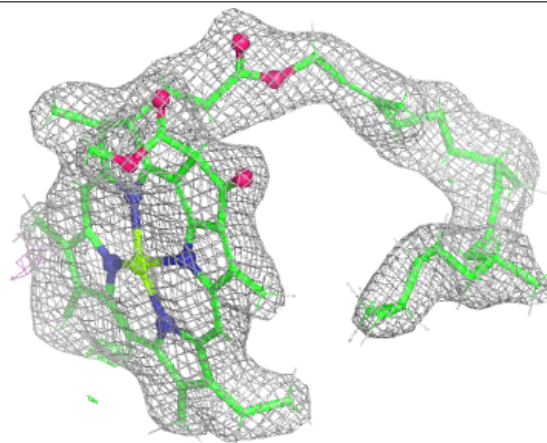


Electron density around DGD c 519:

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

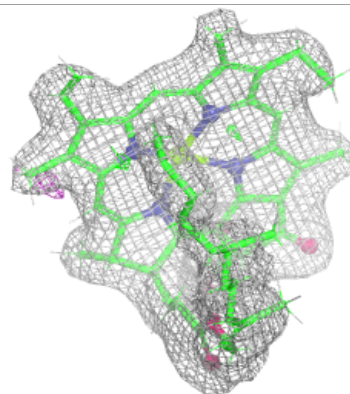
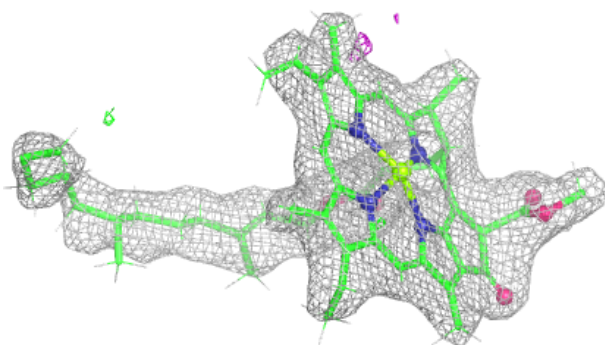
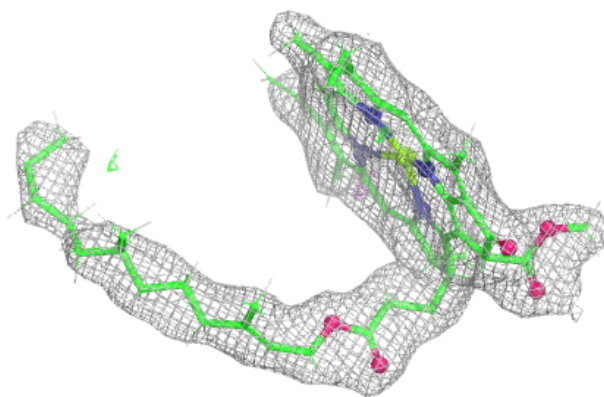
**Electron density around CLA C 503:**

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

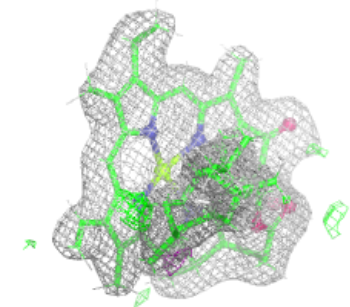
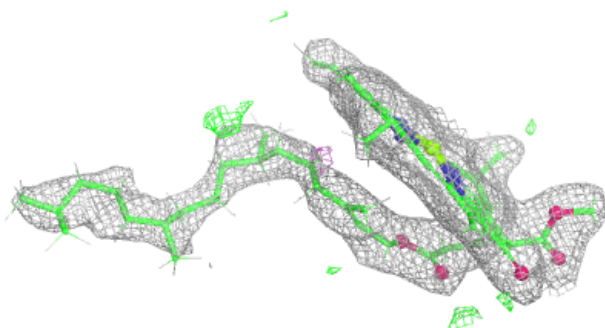
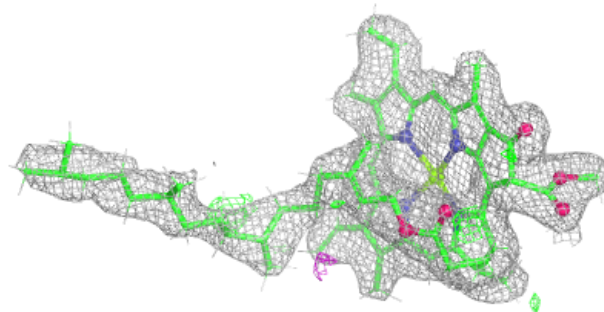


Electron density around CLA C 504:

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

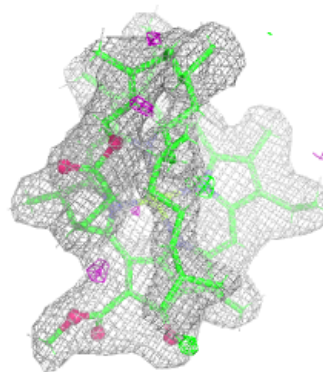
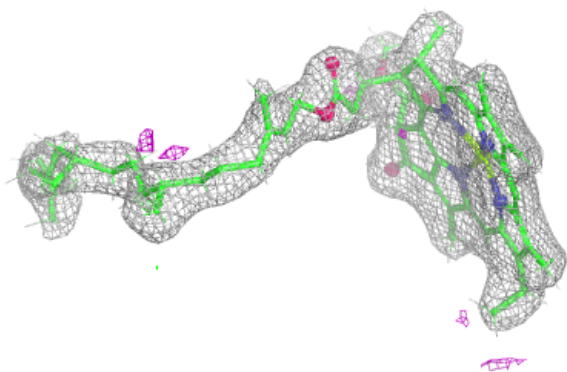
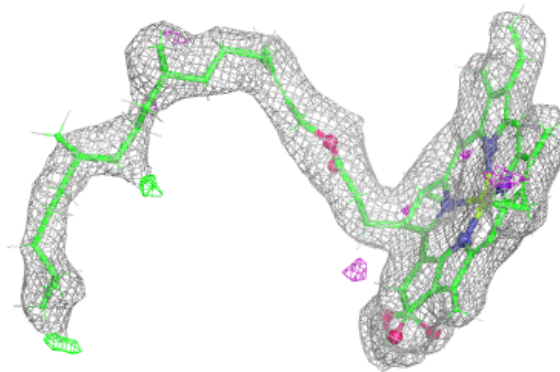
**Electron density around CLA C 505:**

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

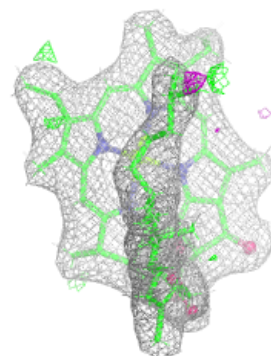
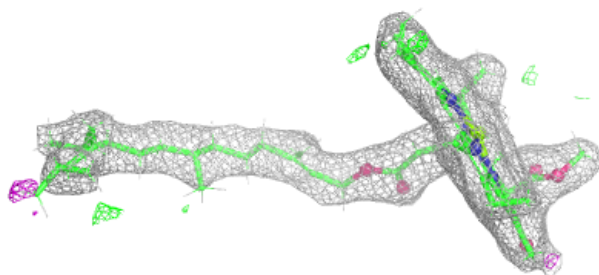
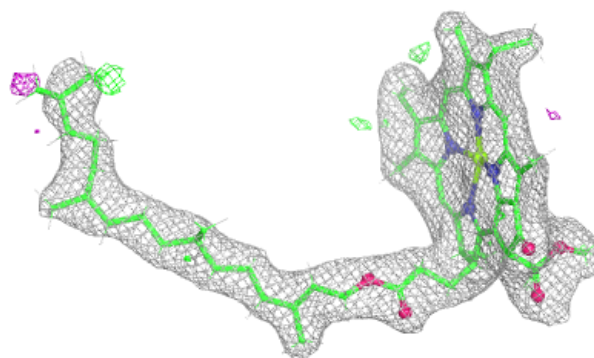


Electron density around CLA b 606:

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

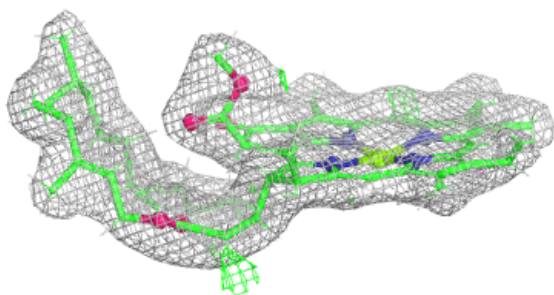
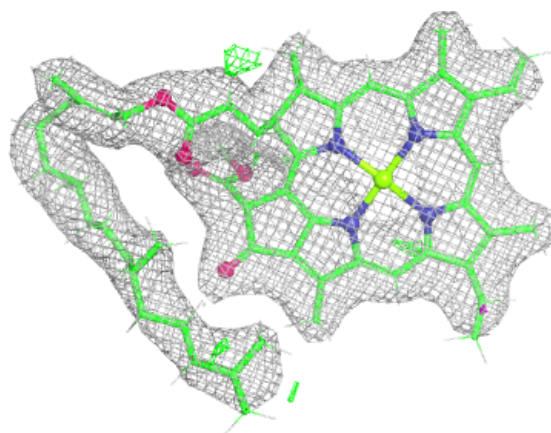
**Electron density around CLA b 609:**

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



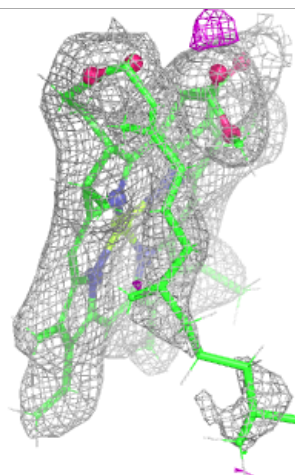
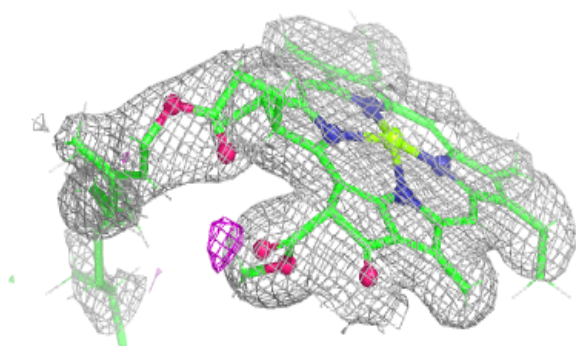
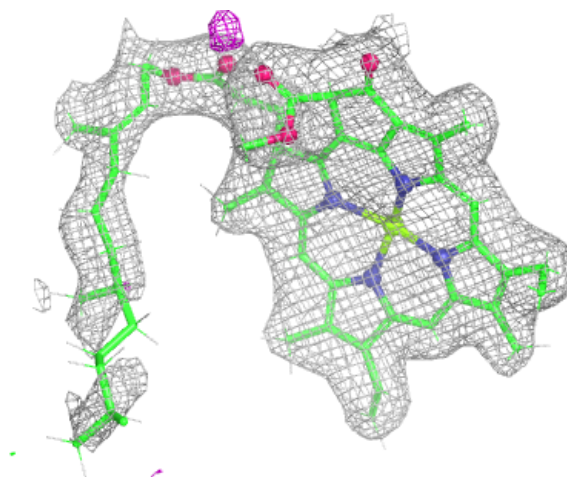
Electron density around CLA b 610:

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



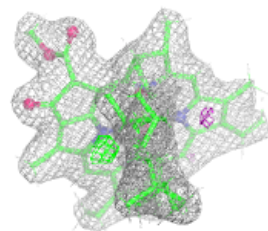
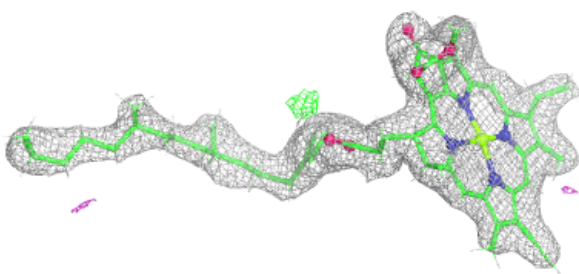
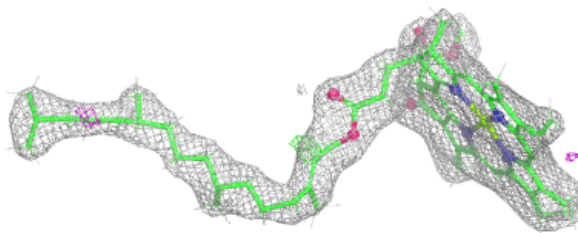
Electron density around CLA b 616:

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



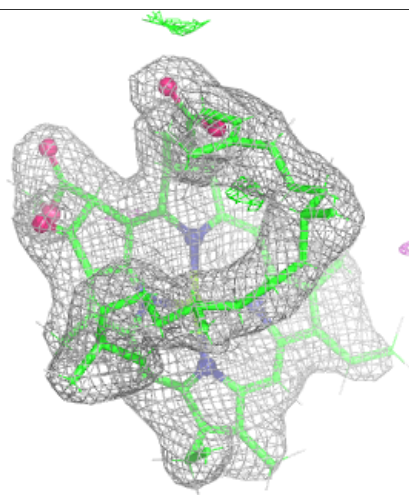
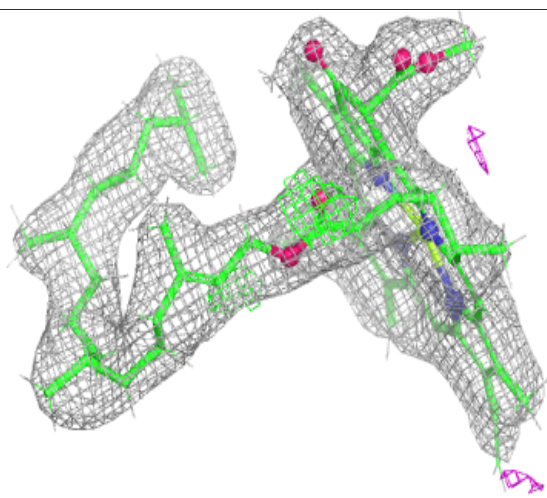
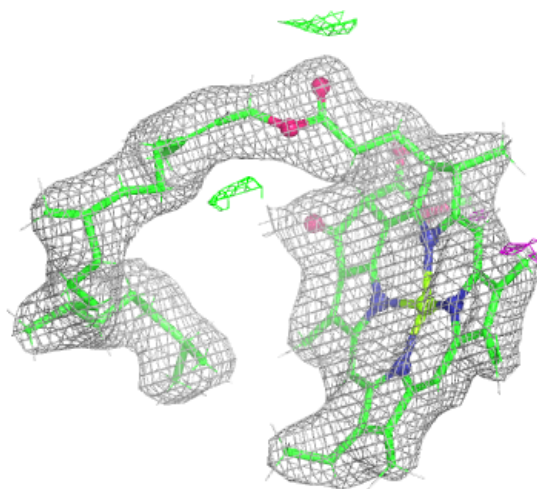
Electron density around CLA c 503:

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



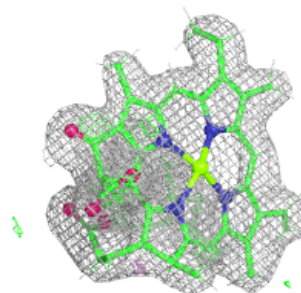
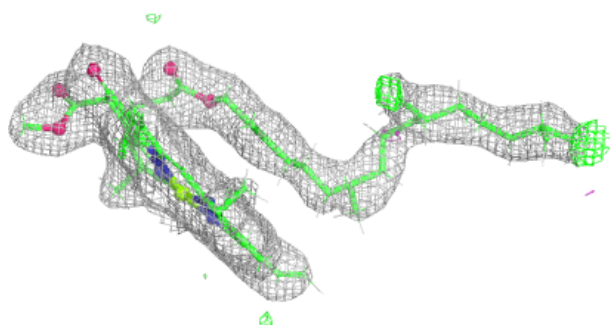
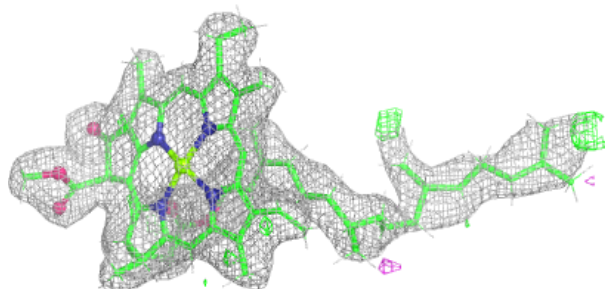
Electron density around CLA c 504:

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

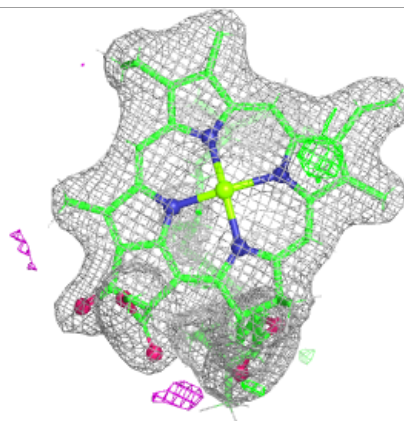
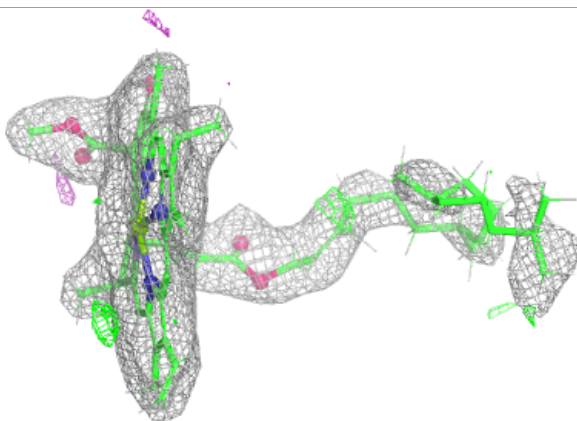
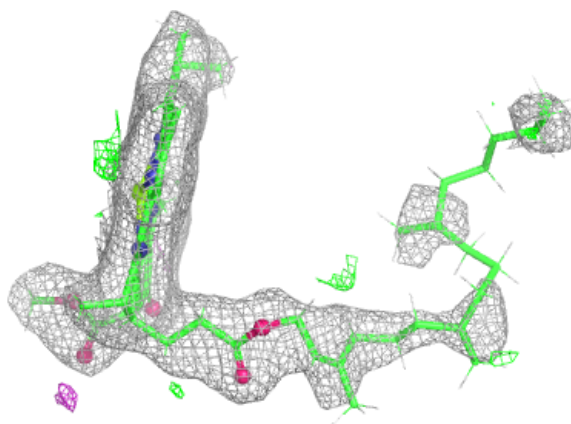


Electron density around CLA c 506:

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

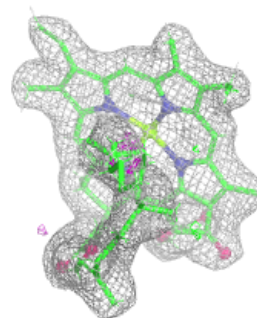
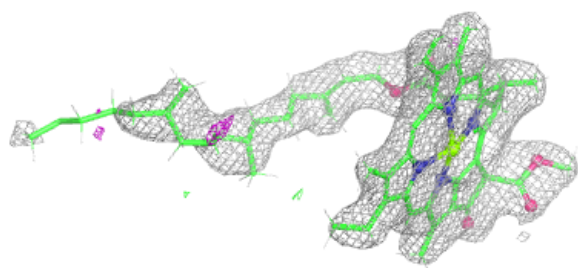
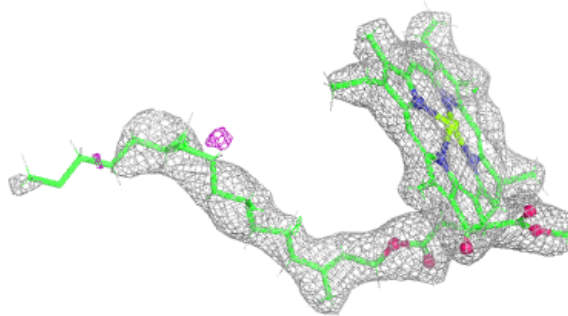
**Electron density around CLA c 507:**

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



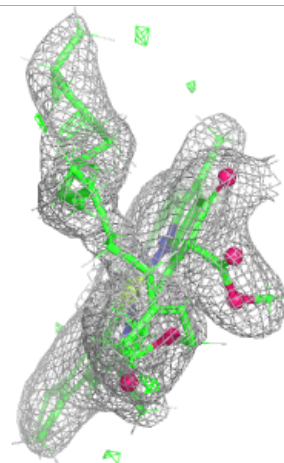
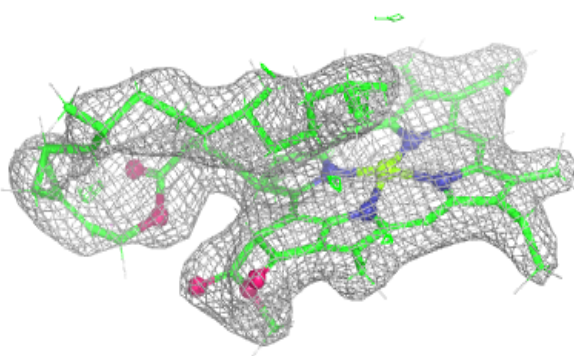
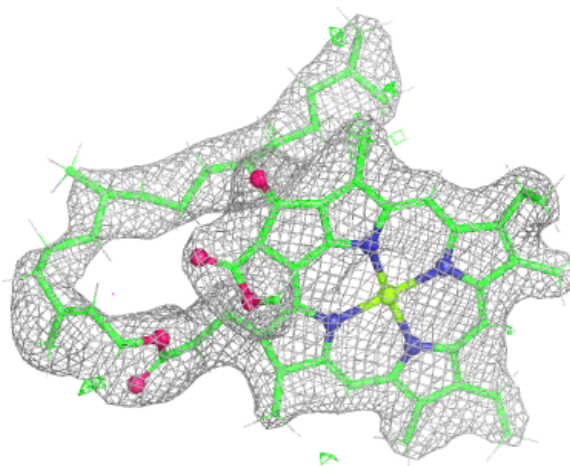
Electron density around CLA c 509:

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



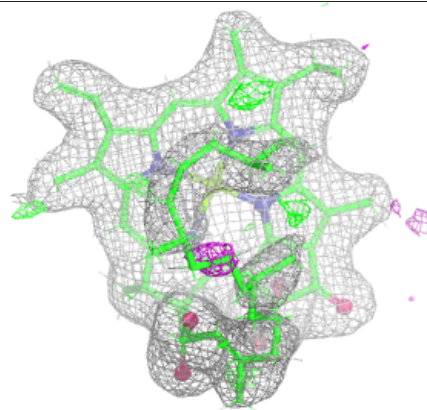
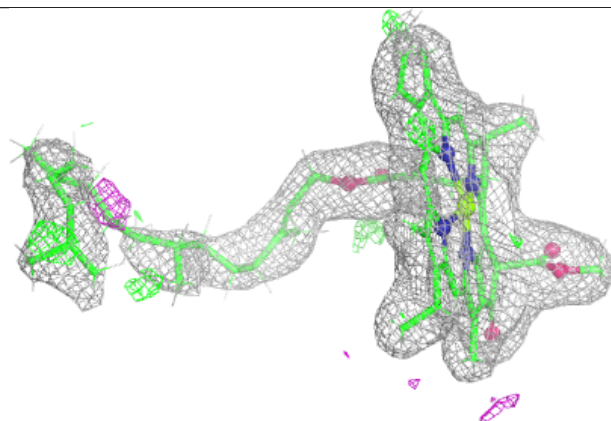
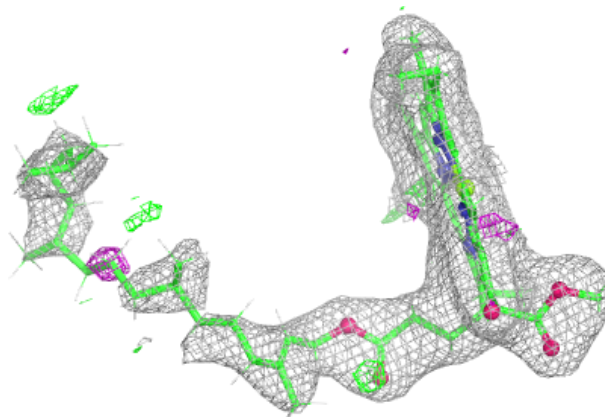
Electron density around CLA c 510:

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

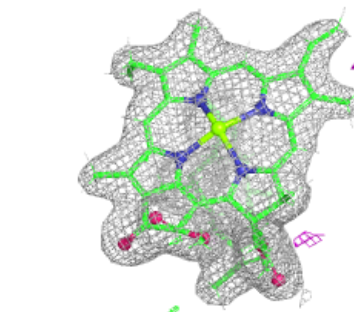
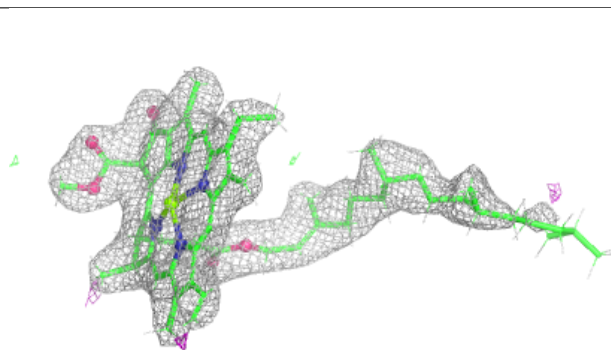
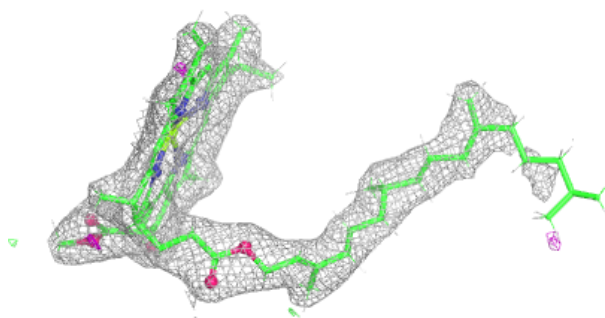


Electron density around CLA C 506:

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

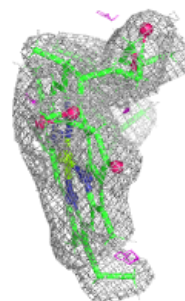
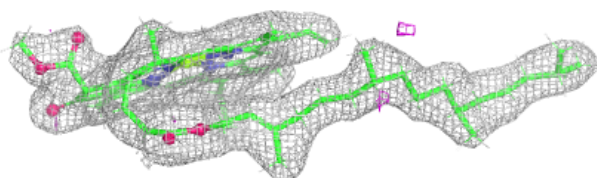
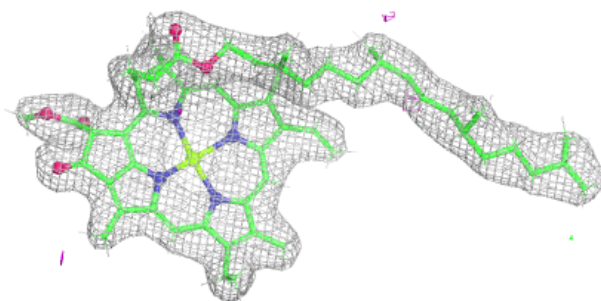
**Electron density around CLA C 508:**

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

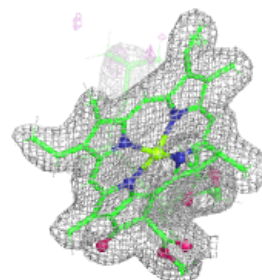
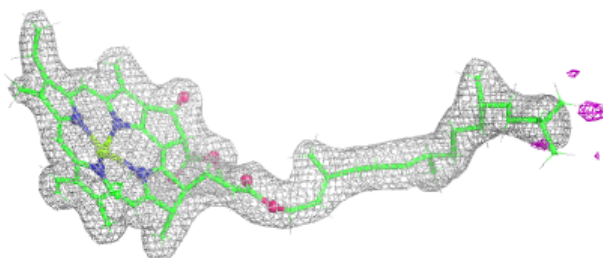
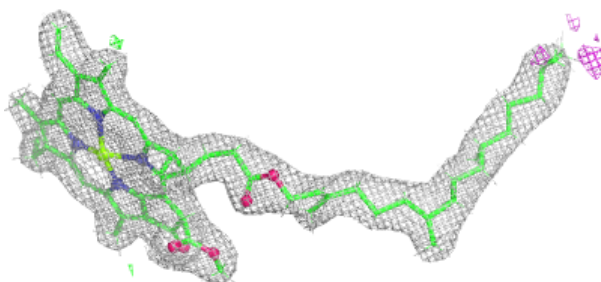


Electron density around CLA C 501:

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

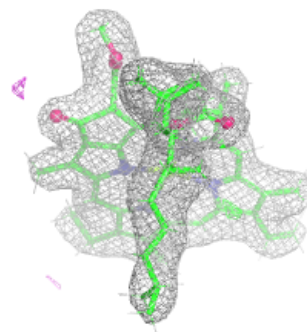
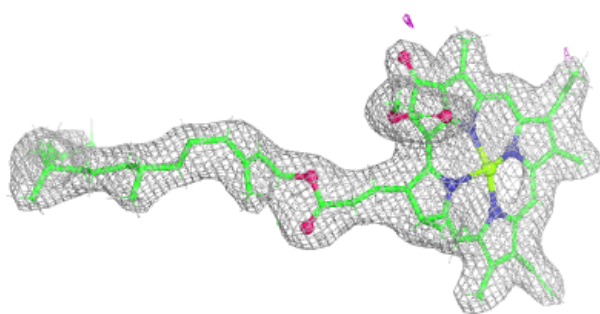
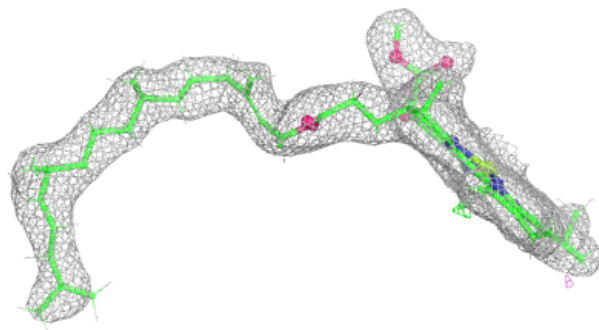
**Electron density around CLA a 402:**

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

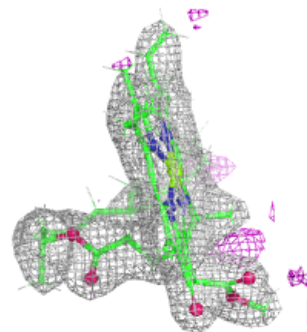
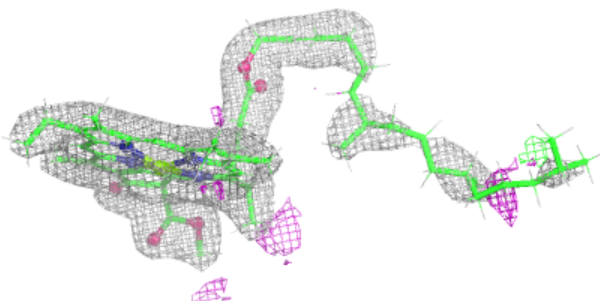
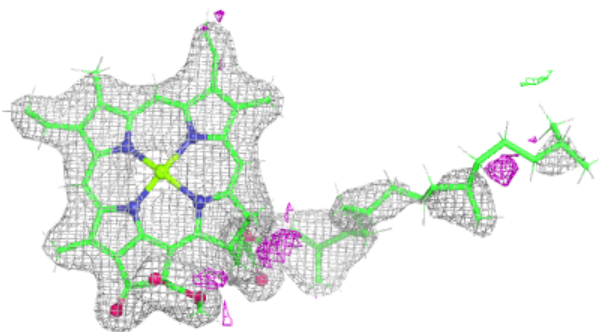


Electron density around CLA d 403:

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

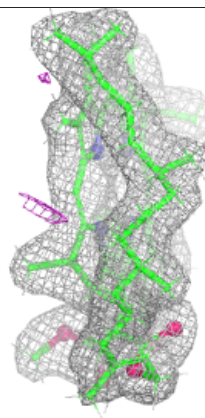
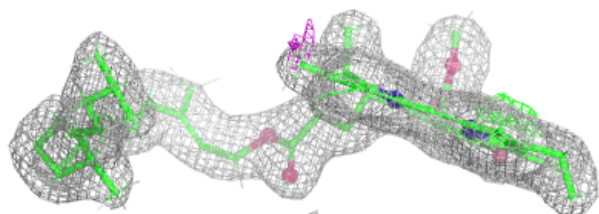
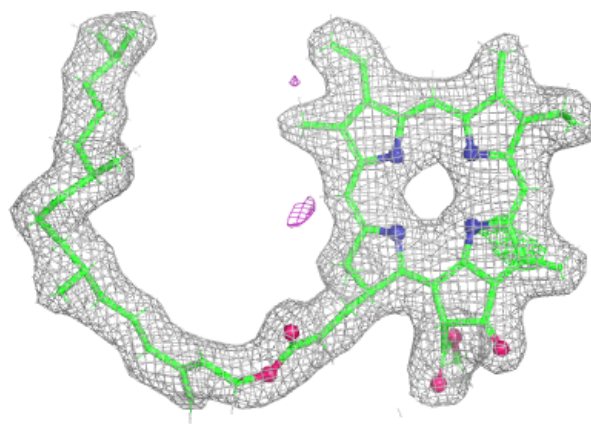
**Electron density around CLA a 403:**

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



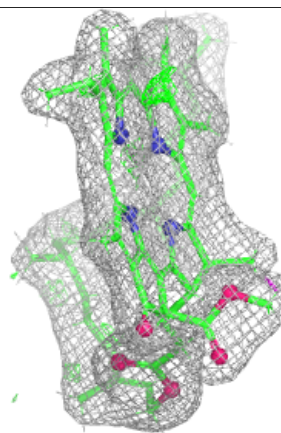
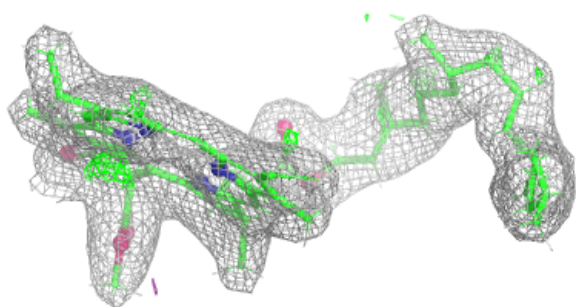
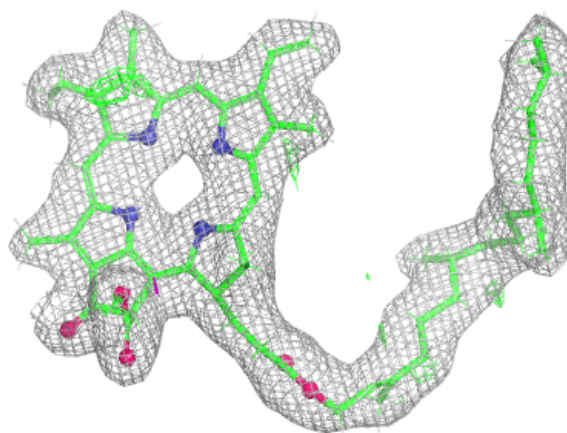
Electron density around PHO A 404:

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



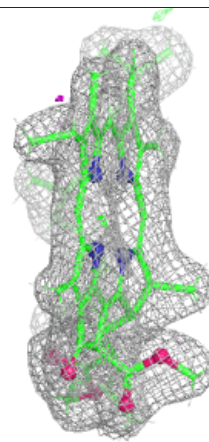
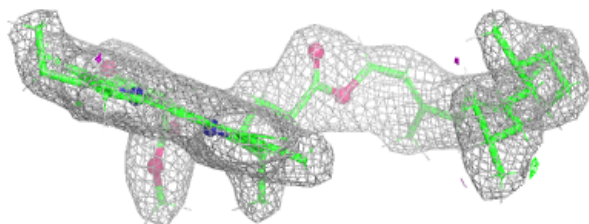
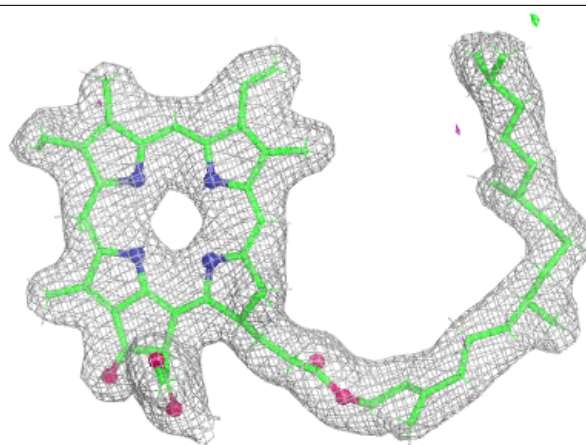
Electron density around PHO D 401:

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



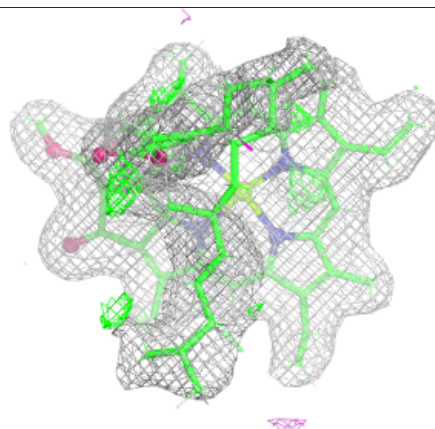
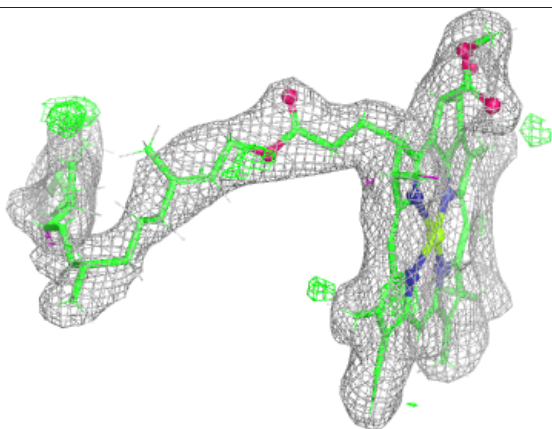
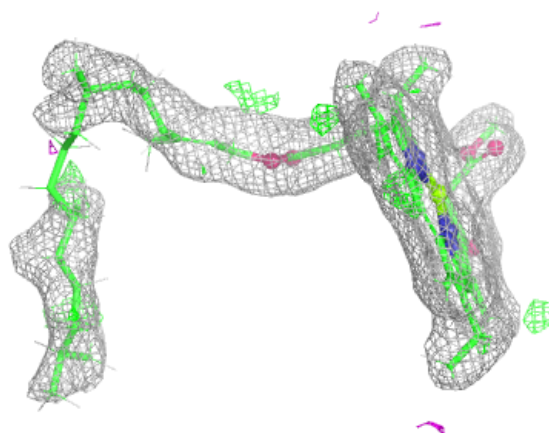
Electron density around PHO a 404:

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

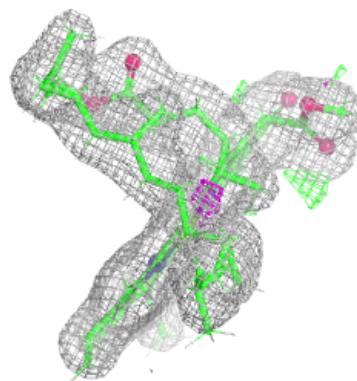
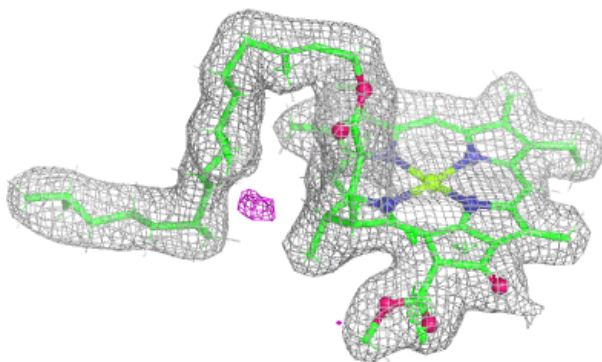
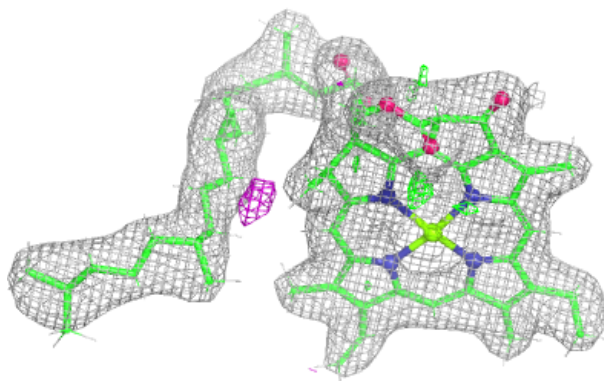


Electron density around CLA a 405:

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

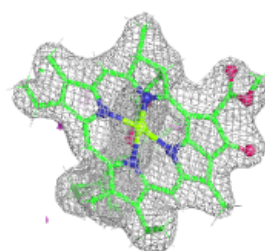
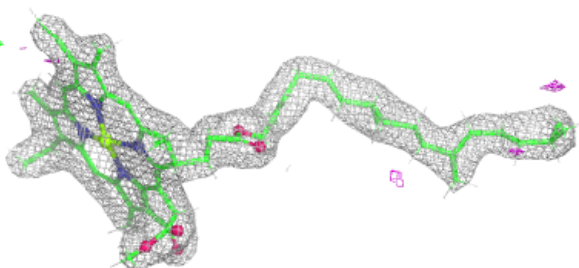
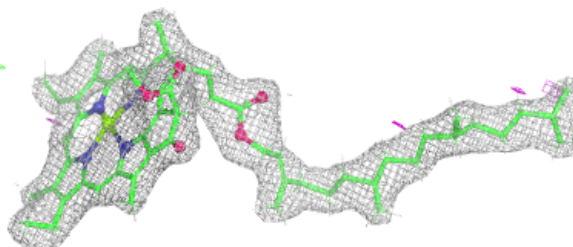
**Electron density around CLA a 410:**

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

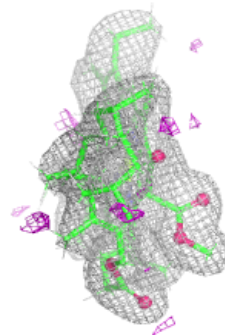
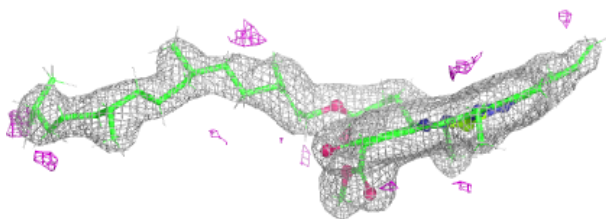
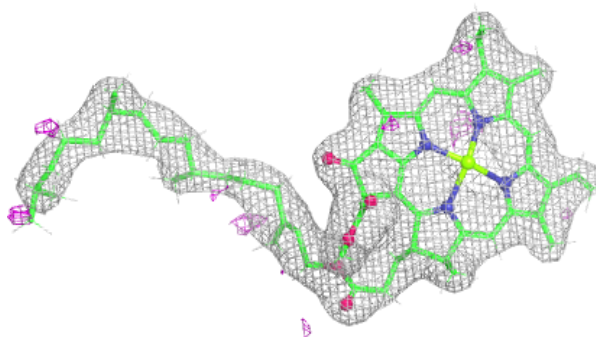


Electron density around CLA C 502:

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

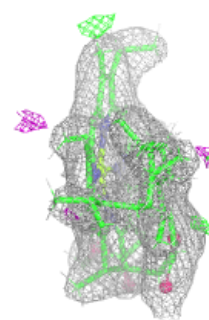
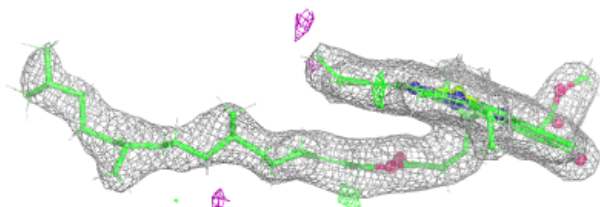
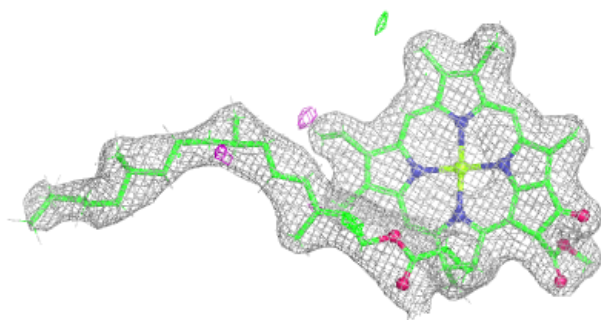
**Electron density around CLA b 602:**

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

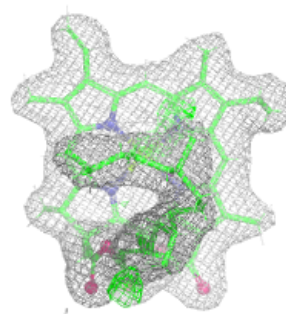
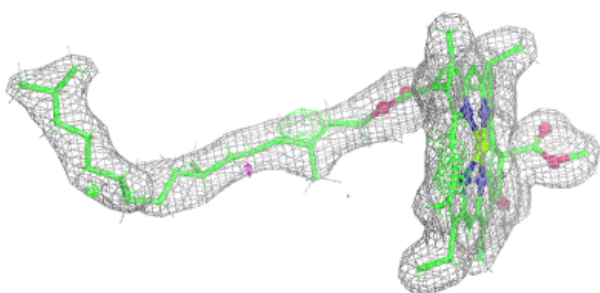
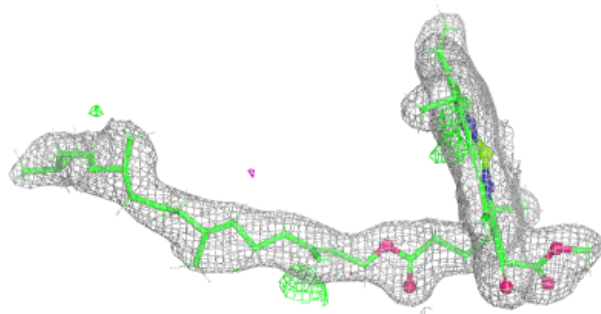


Electron density around CLA b 603:

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

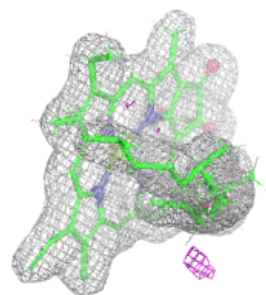
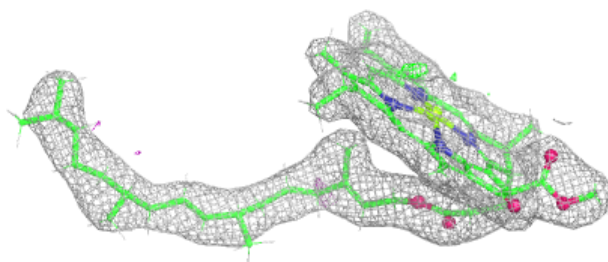
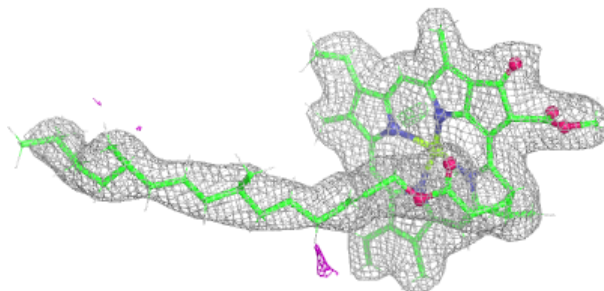
**Electron density around CLA B 605:**

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



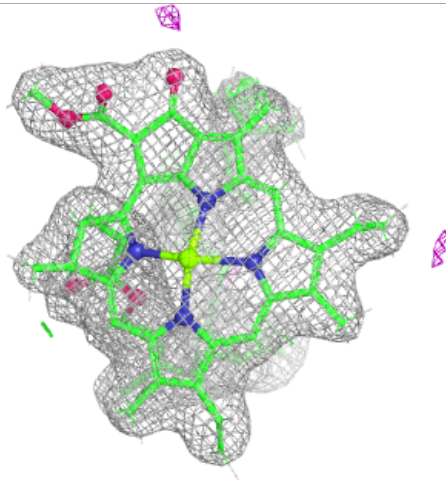
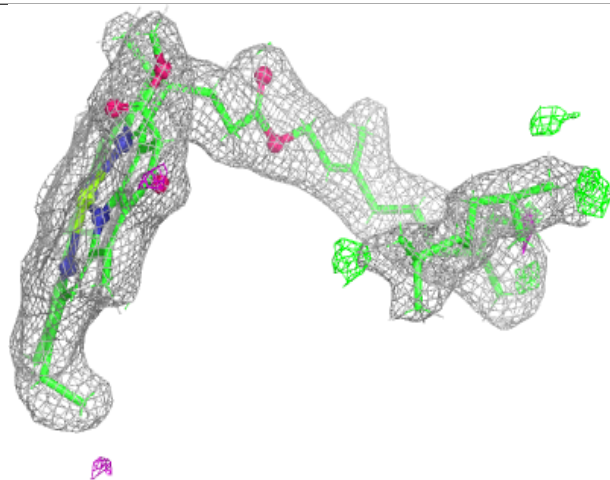
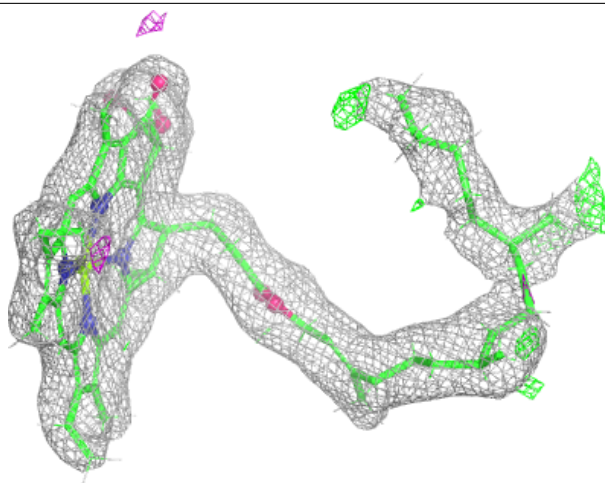
Electron density around CLA b 608:

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



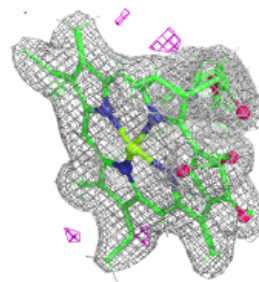
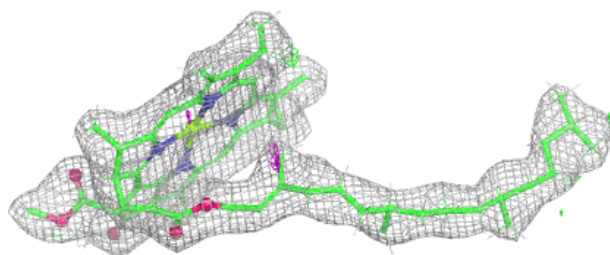
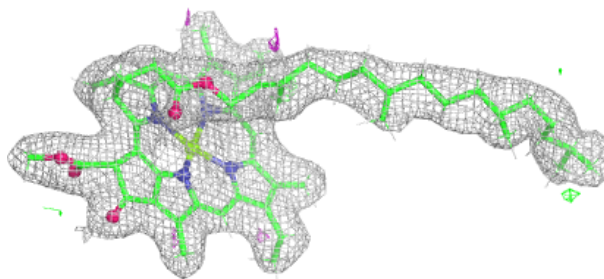
Electron density around CLA B 606:

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



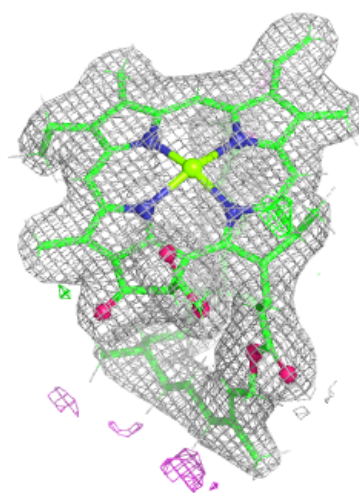
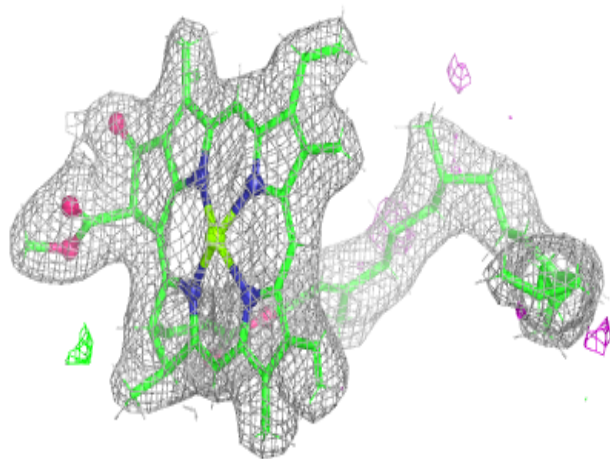
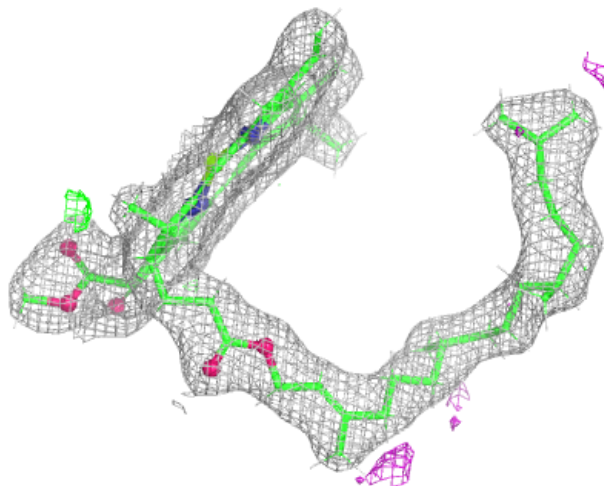
Electron density around CLA B 608:

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



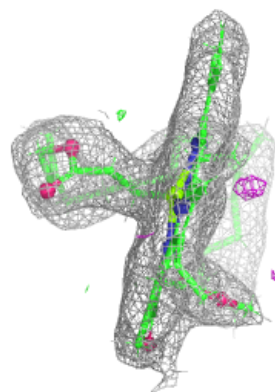
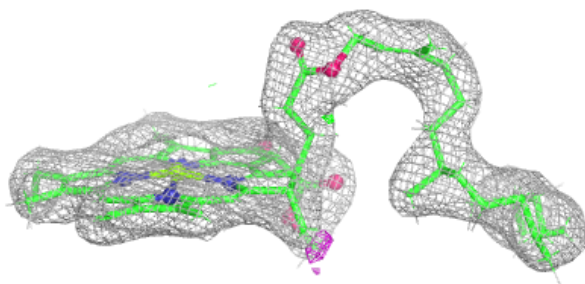
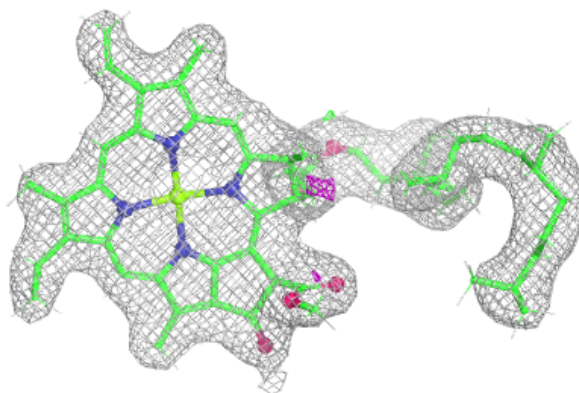
Electron density around CLA b 611:

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

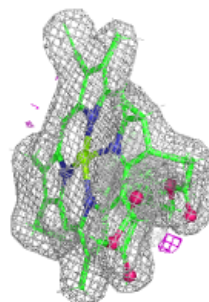
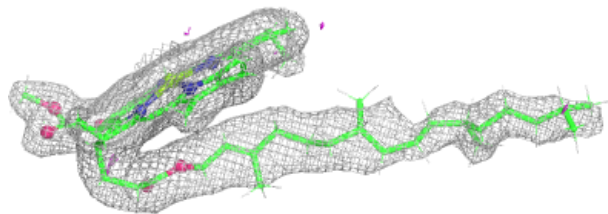
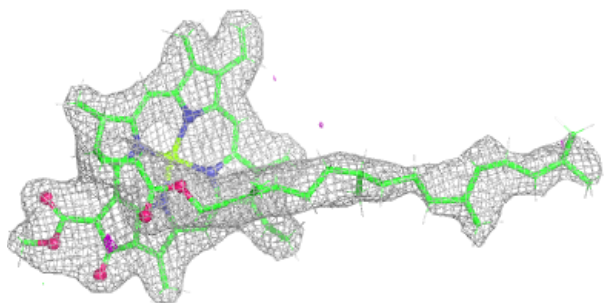


Electron density around CLA b 612:

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

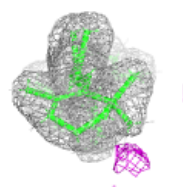
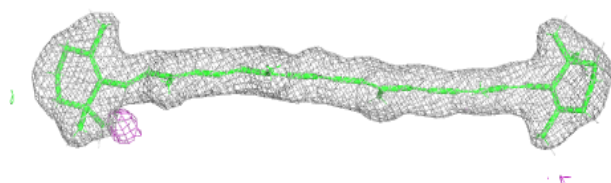
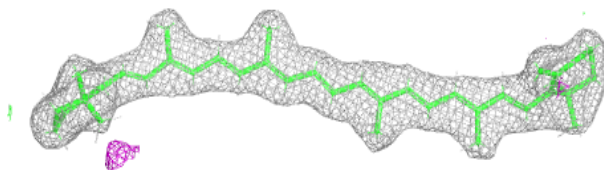
**Electron density around CLA b 614:**

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



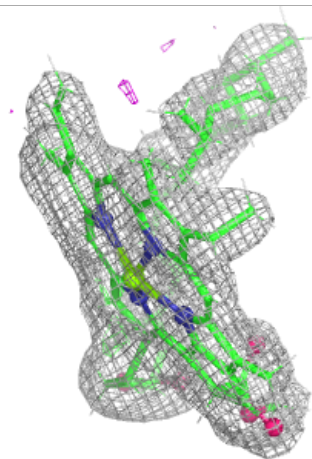
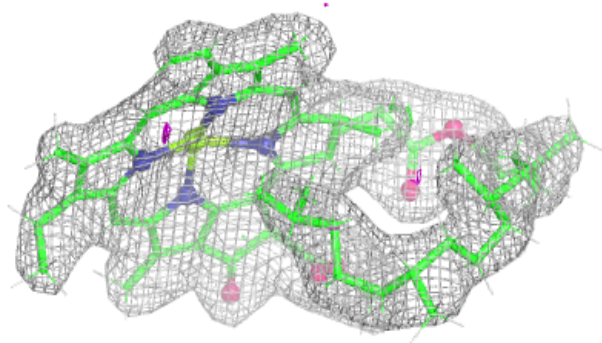
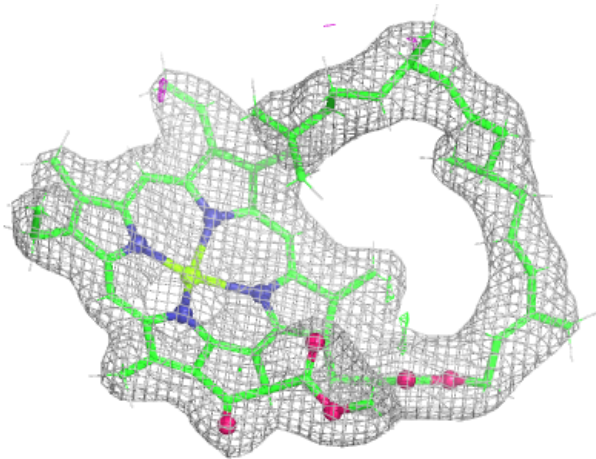
Electron density around BCR a 406:

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



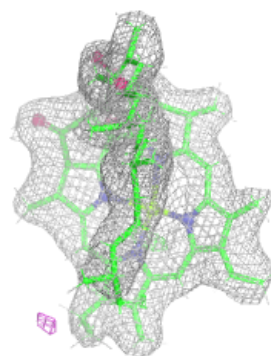
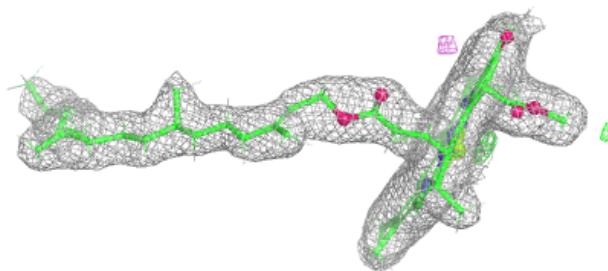
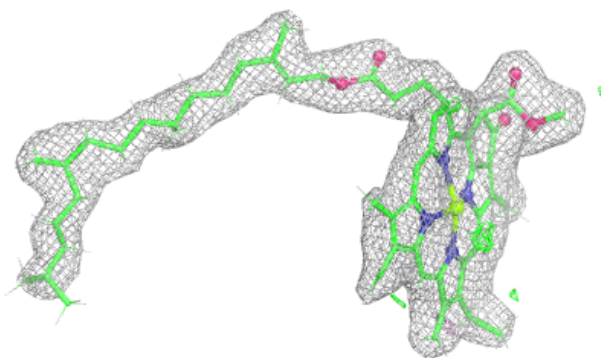
Electron density around CLA b 615:

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

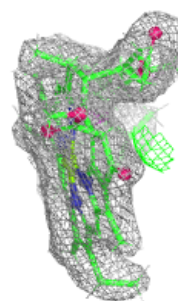
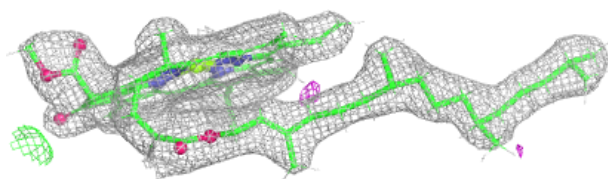
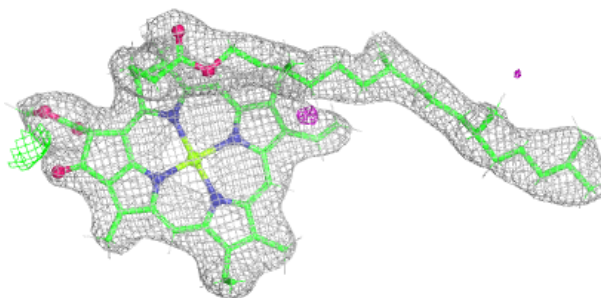


Electron density around CLA B 609:

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

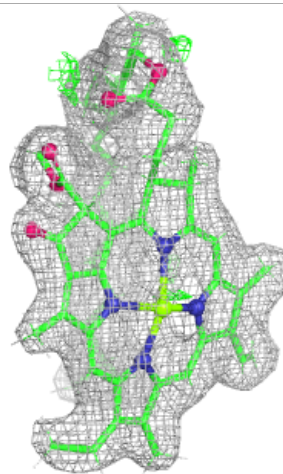
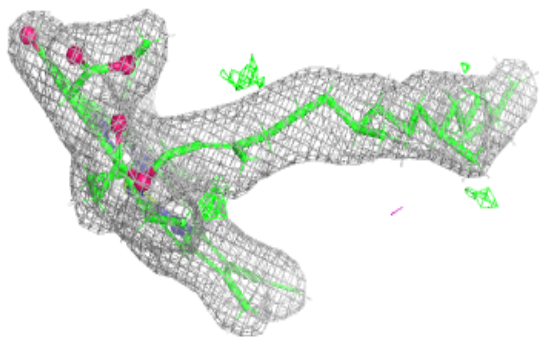
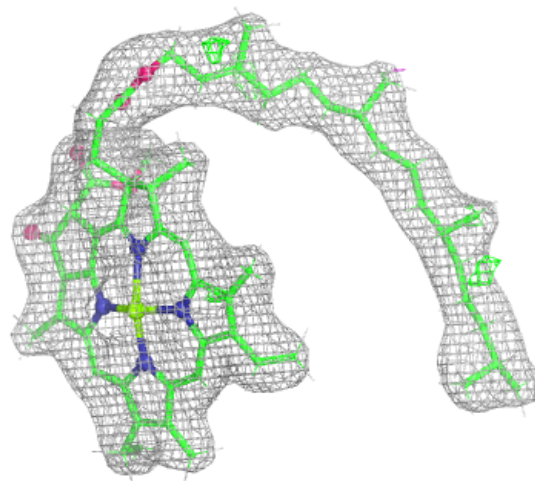
**Electron density around CLA c 502:**

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



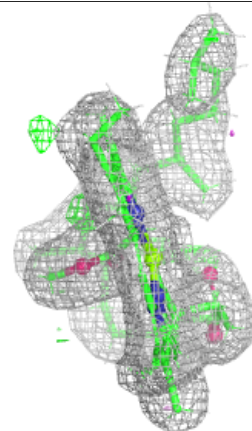
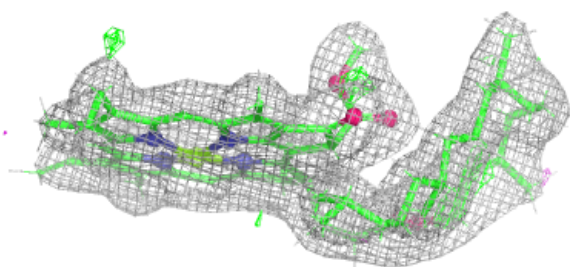
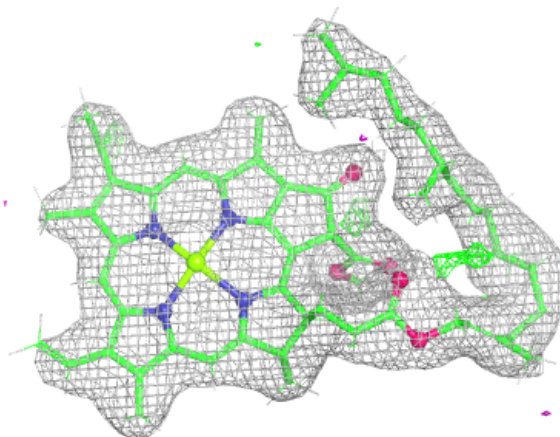
Electron density around CLA C 507:

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

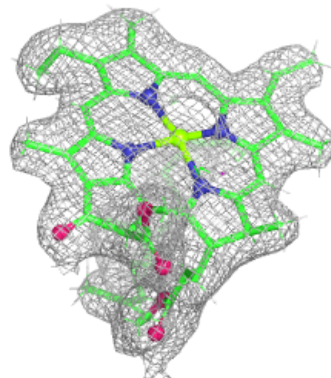
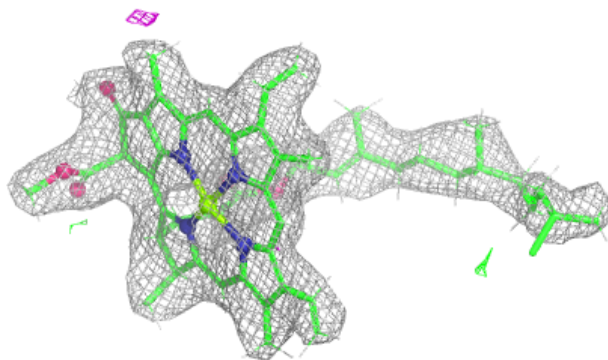
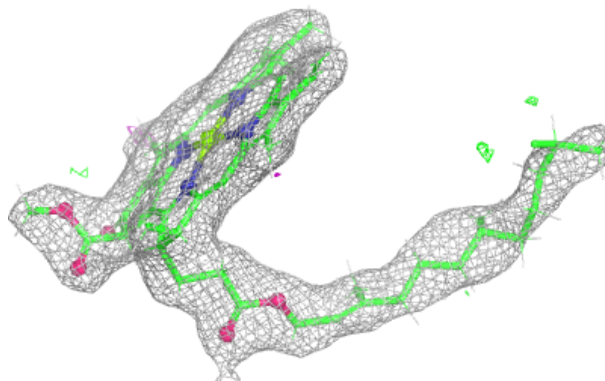


Electron density around CLA B 610:

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

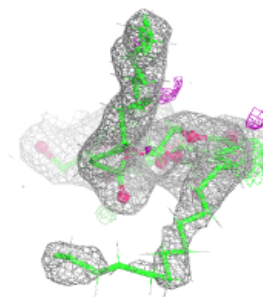
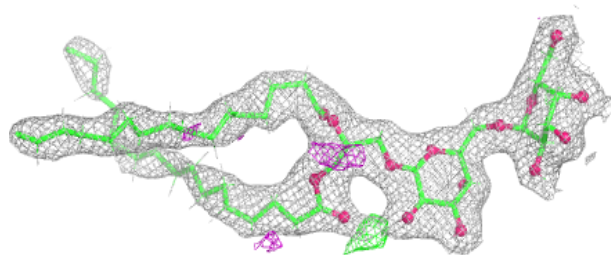
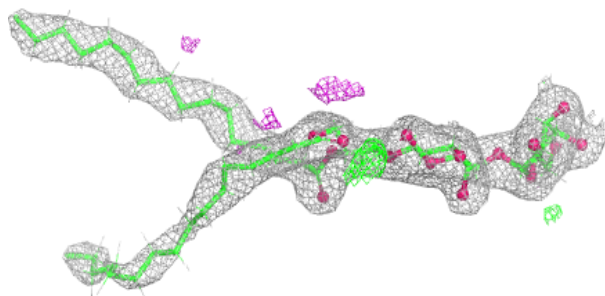
**Electron density around CLA c 505:**

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



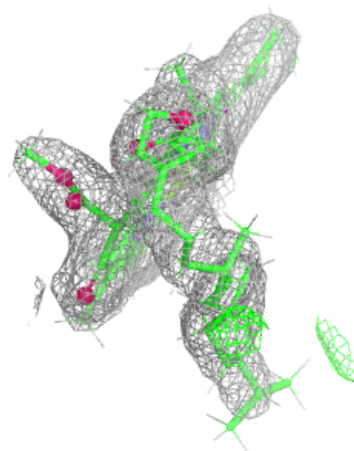
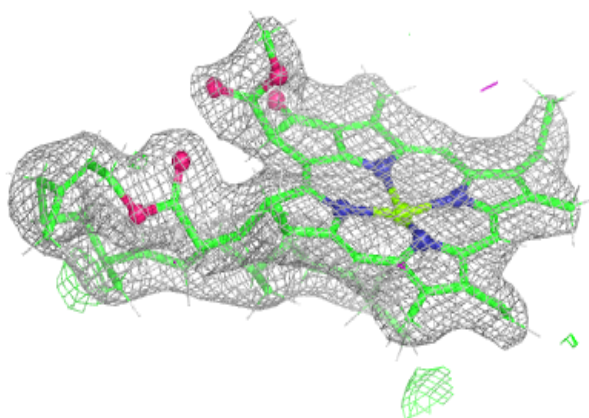
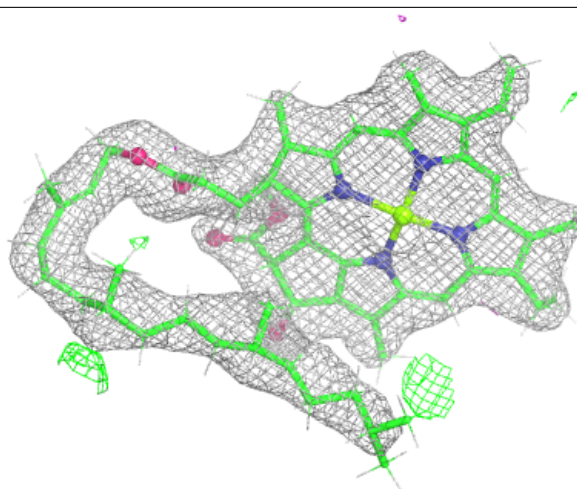
Electron density around DGD c 517:

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



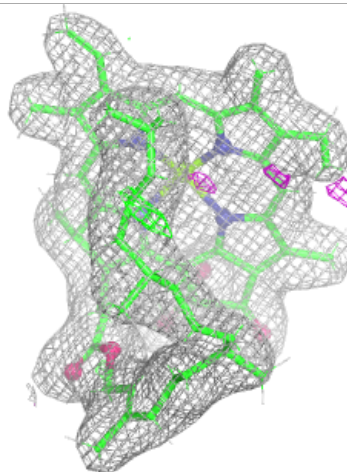
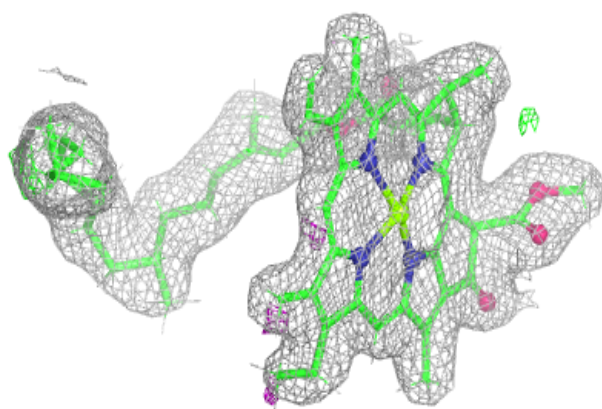
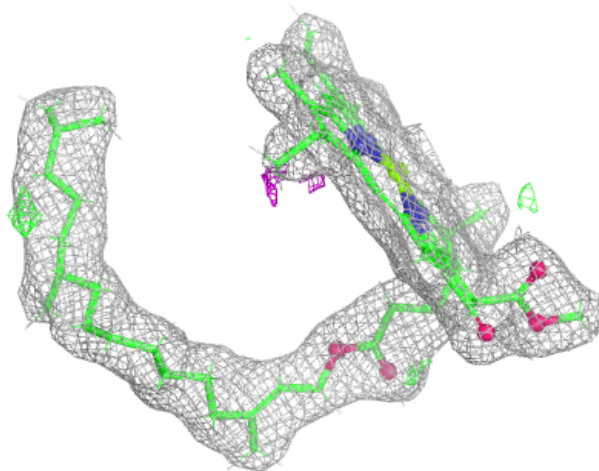
Electron density around CLA C 509:

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



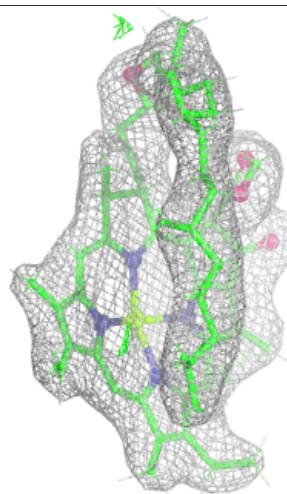
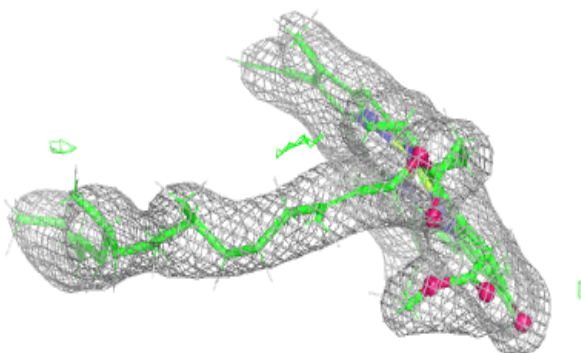
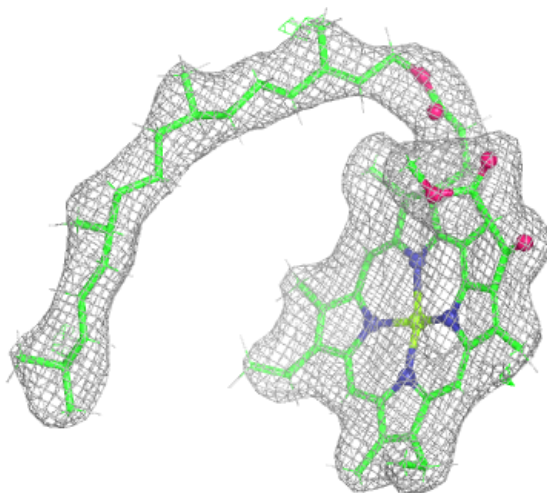
Electron density around CLA B 611:

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



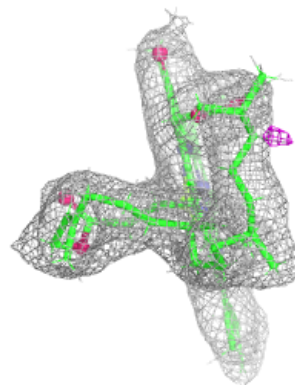
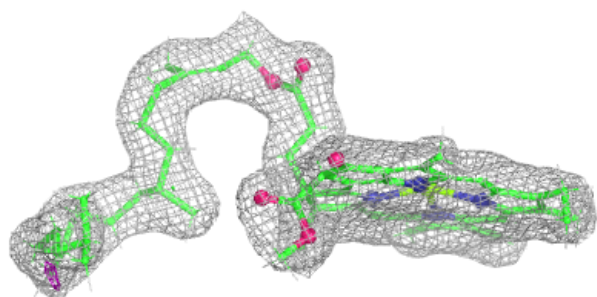
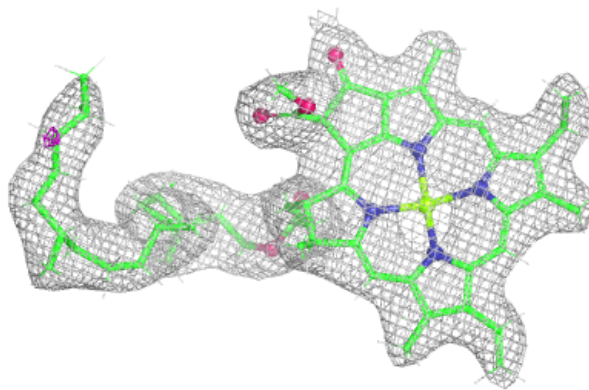
Electron density around CLA c 508:

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

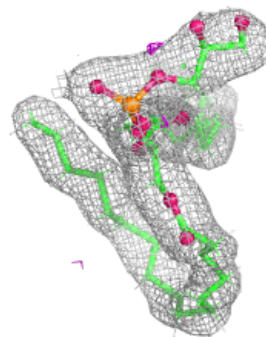
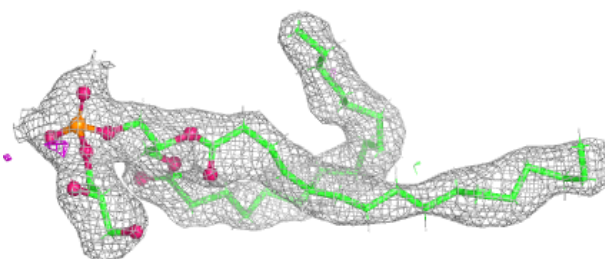
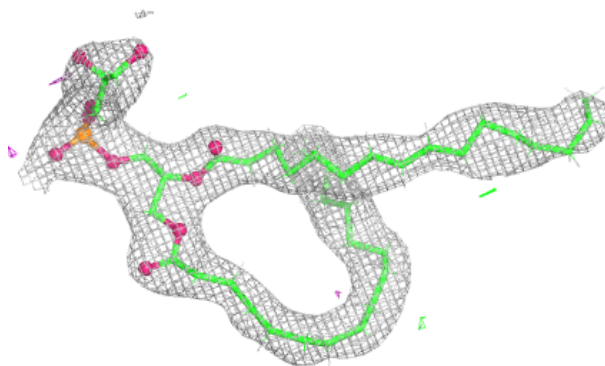


Electron density around CLA B 612:

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

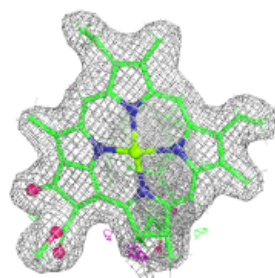
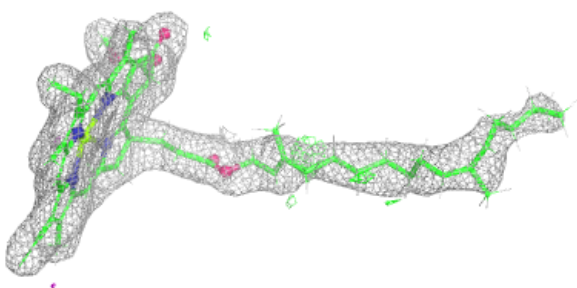
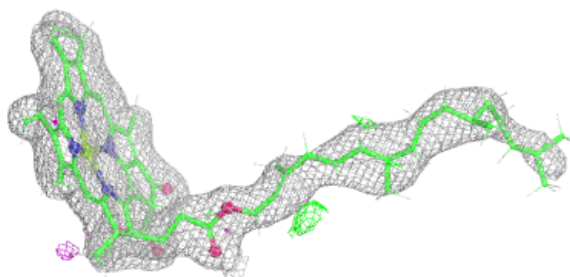
**Electron density around LHG D 412:**

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



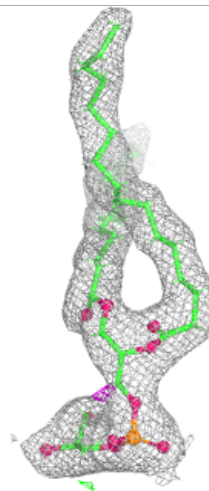
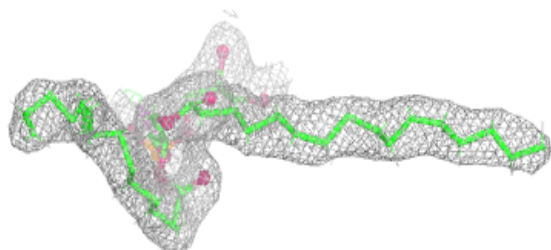
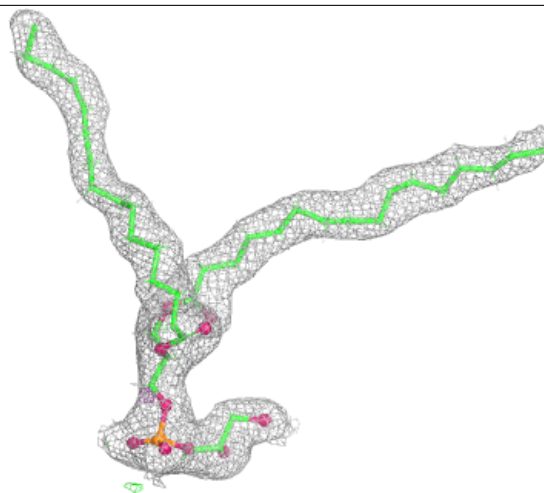
Electron density around CLA B 604:

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



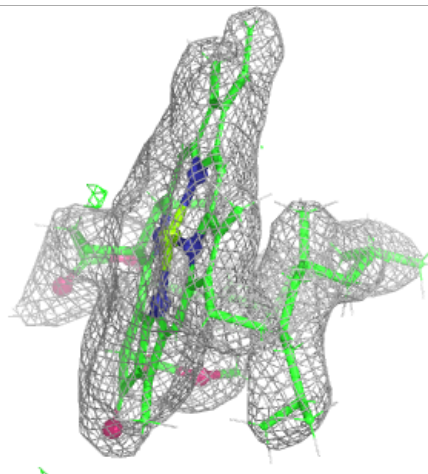
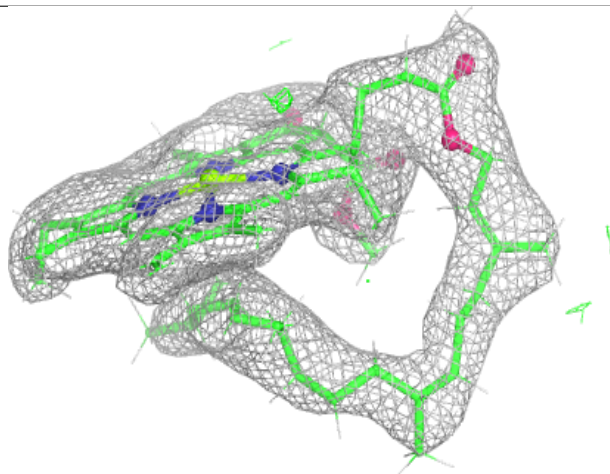
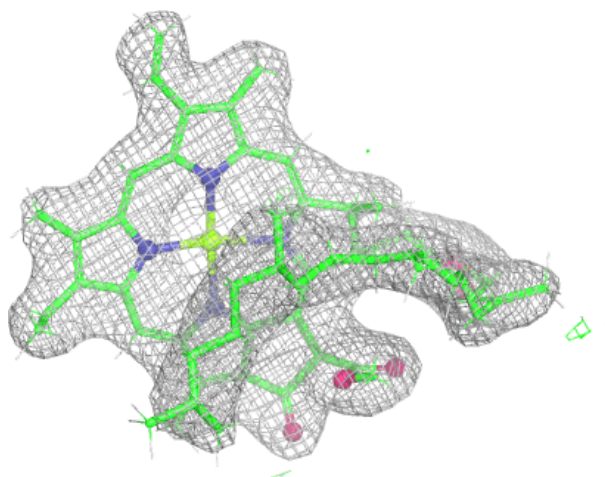
Electron density around LHG L 102:

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



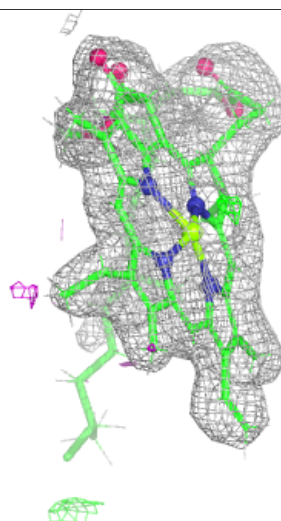
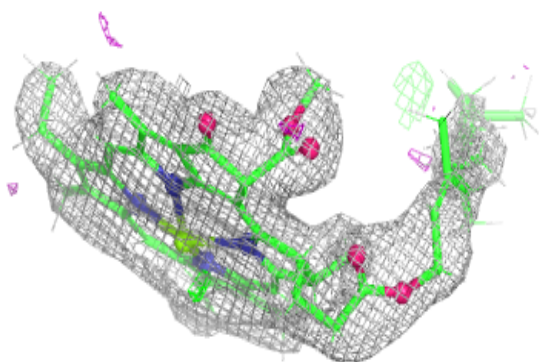
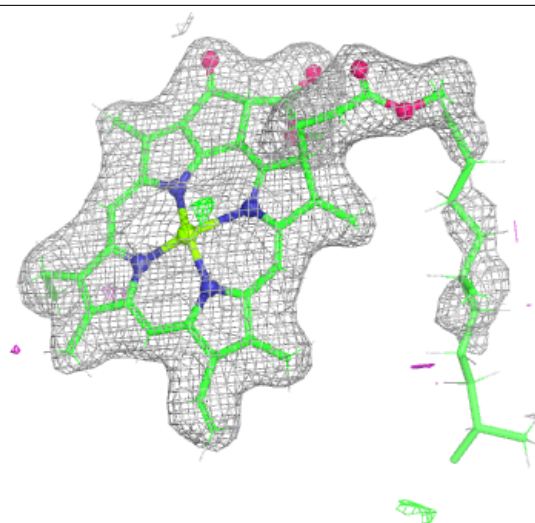
Electron density around CLA c 511:

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



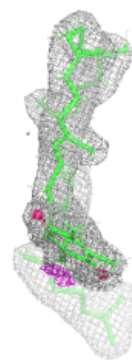
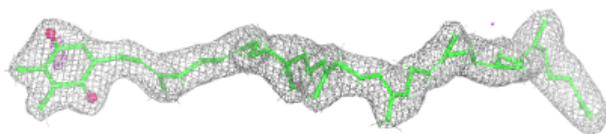
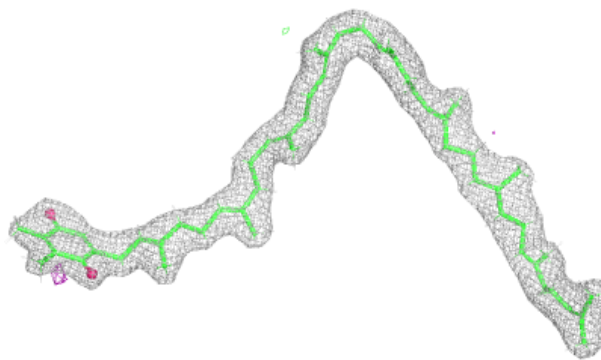
Electron density around CLA B 616:

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



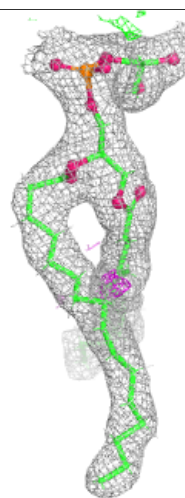
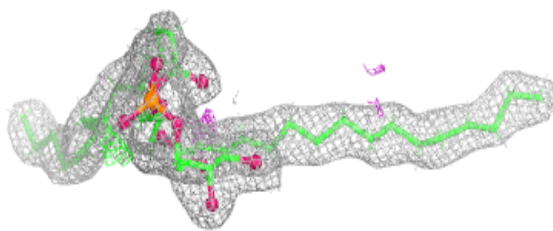
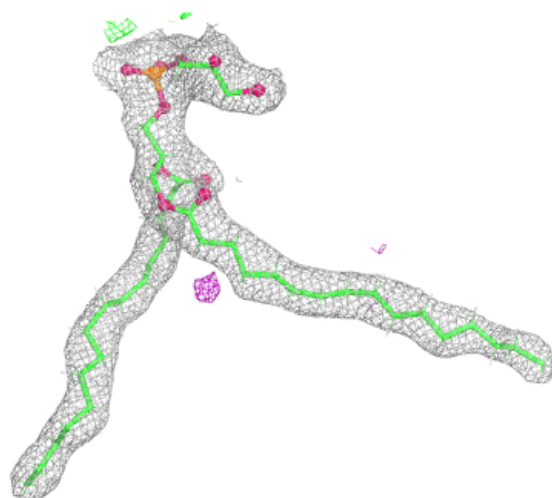
Electron density around PL9 d 406:

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



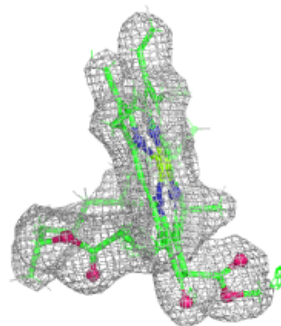
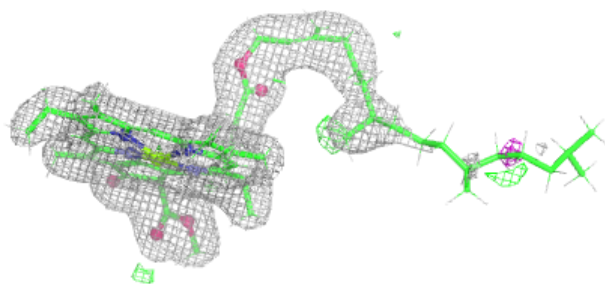
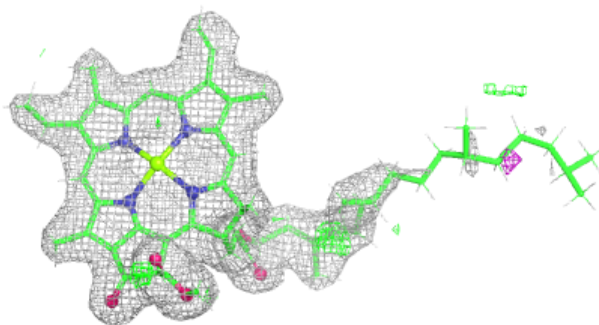
Electron density around LHG 1 101:

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

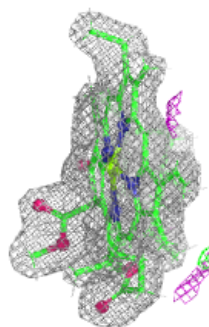
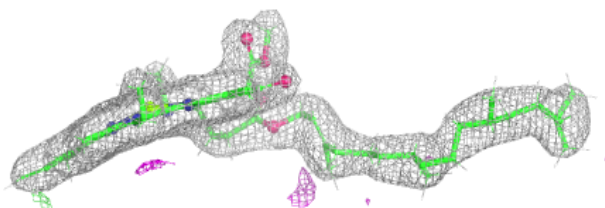
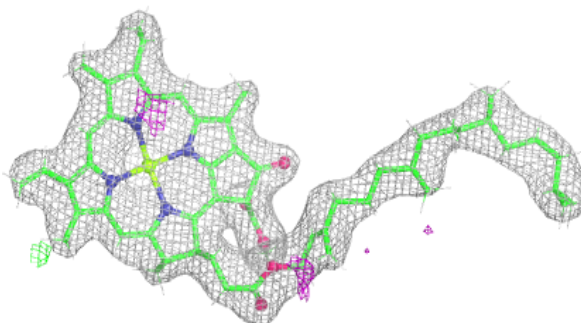


Electron density around CLA A 403:

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

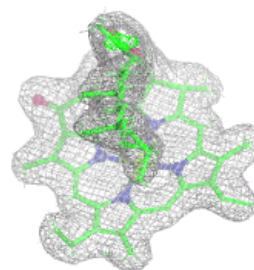
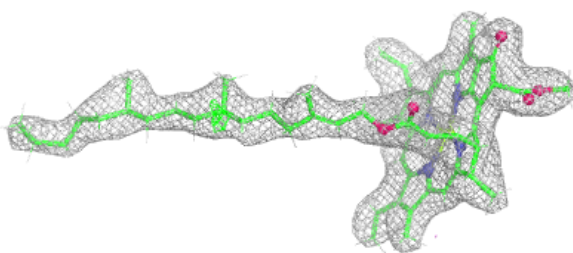
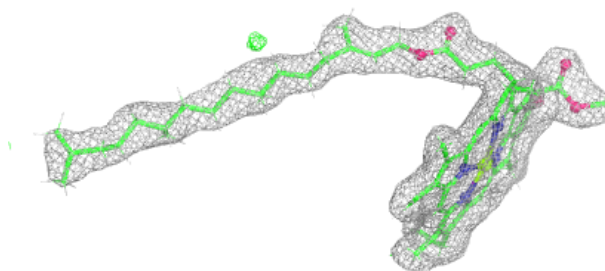
**Electron density around CLA B 602:**

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



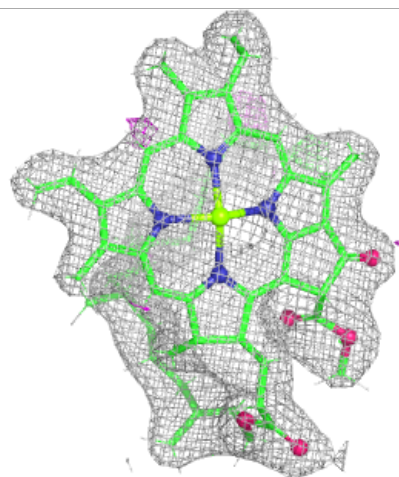
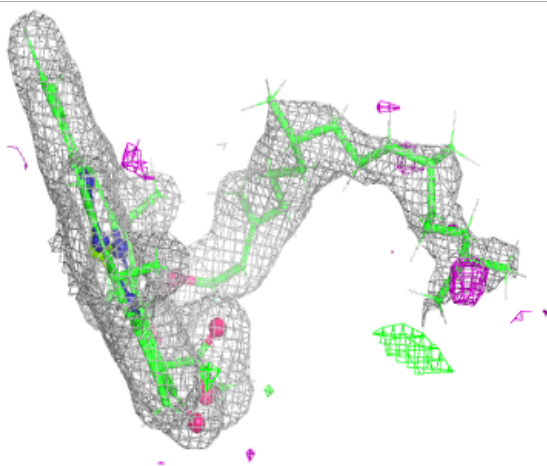
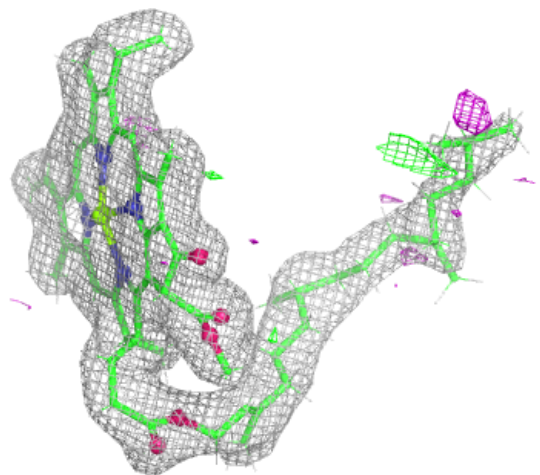
Electron density around CLA B 607:

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



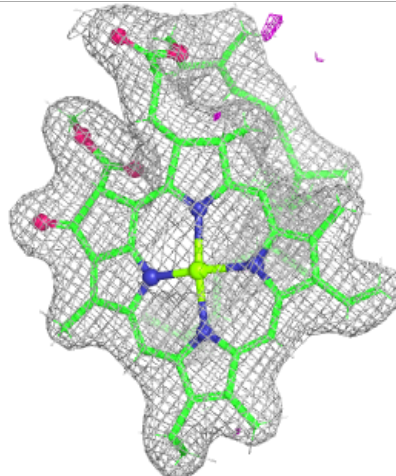
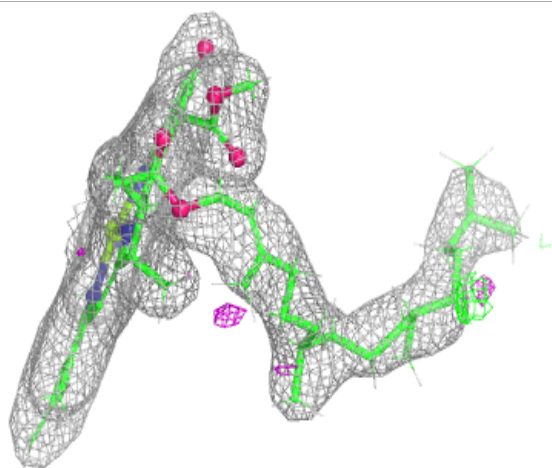
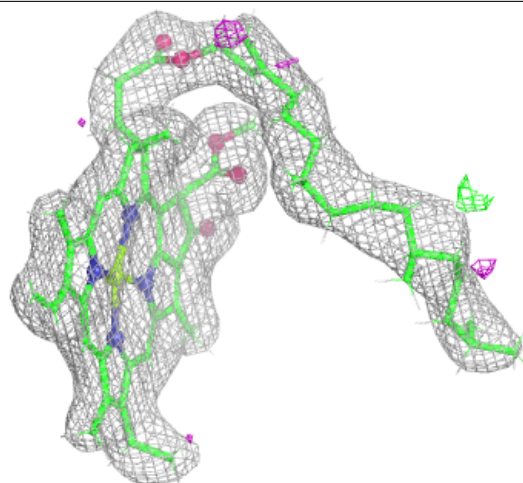
Electron density around CLA b 613:

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



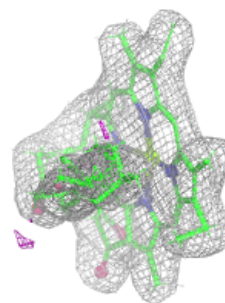
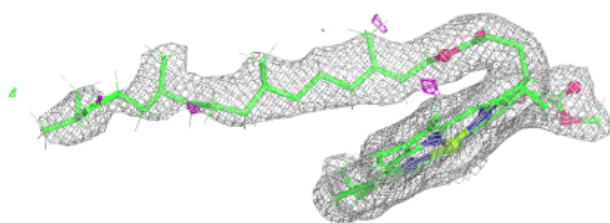
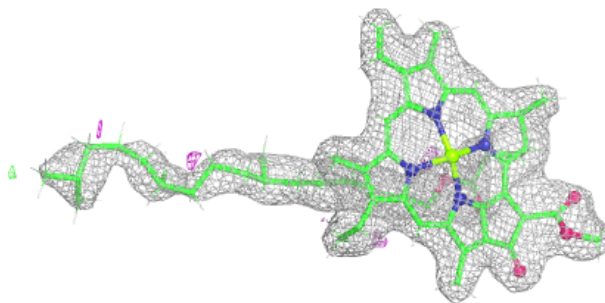
Electron density around CLA B 613:

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



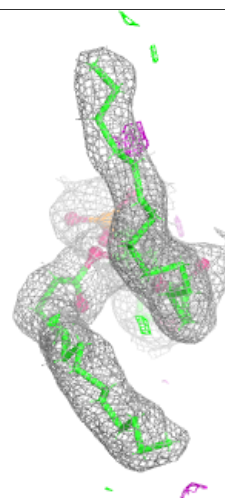
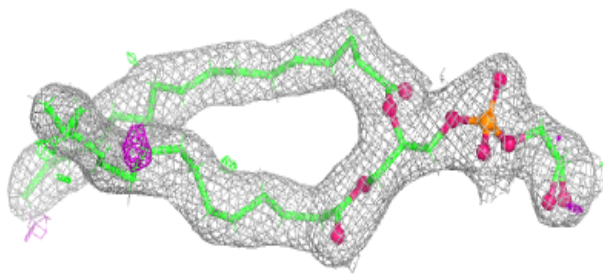
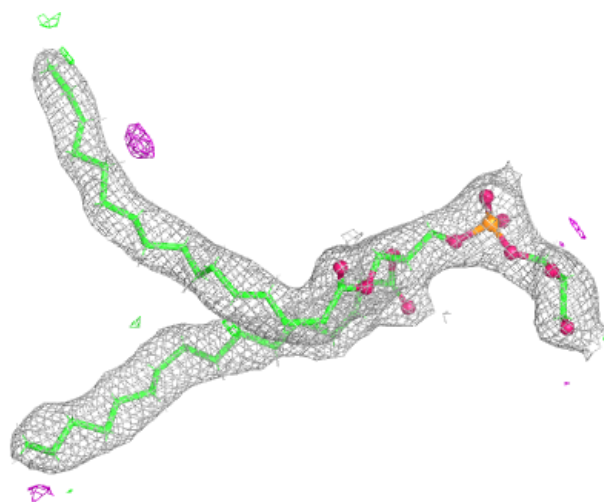
Electron density around CLA B 614:

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



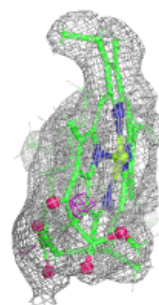
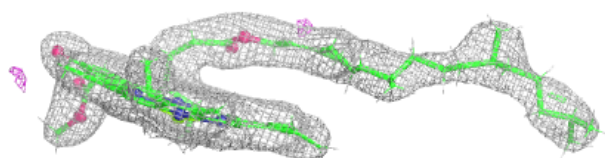
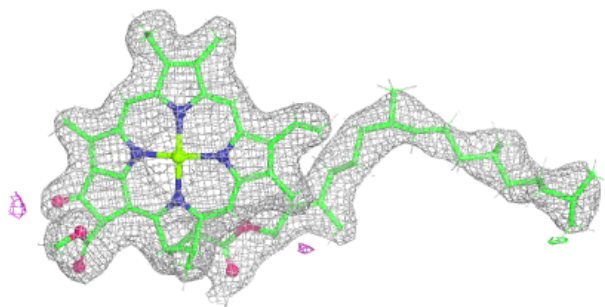
Electron density around LHG D 409:

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

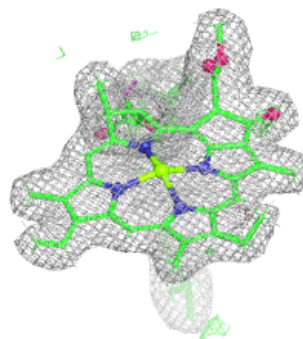
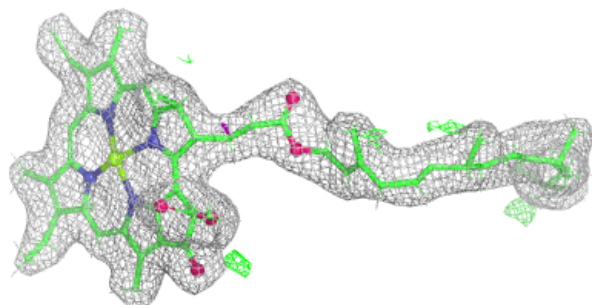
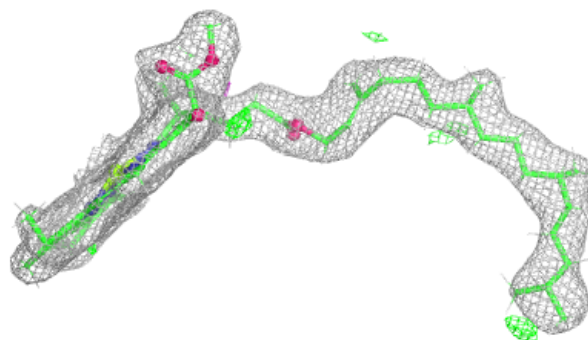


Electron density around CLA B 603:

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

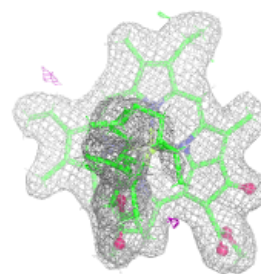
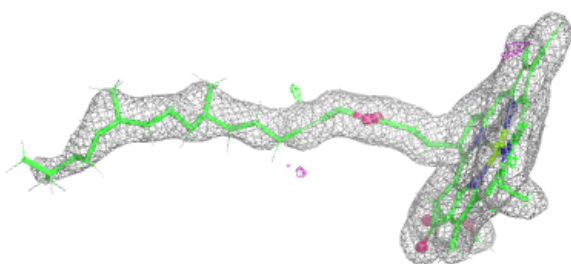
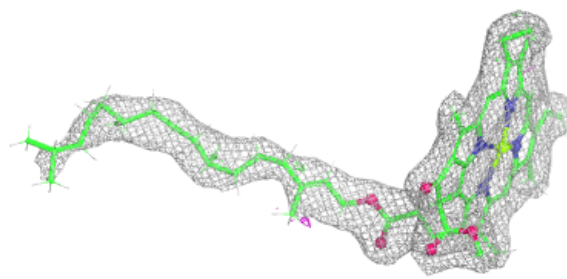
**Electron density around CLA D 403:**

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

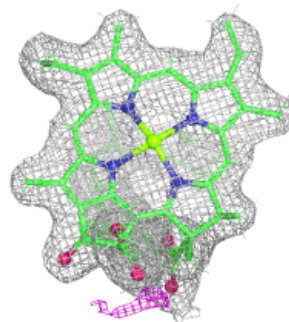
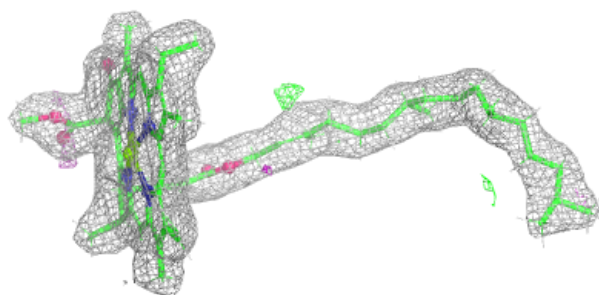
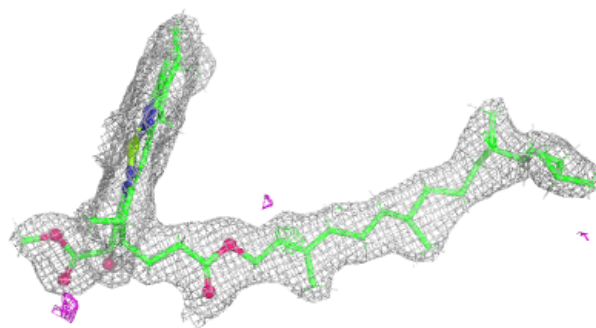


Electron density around CLA b 604:

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

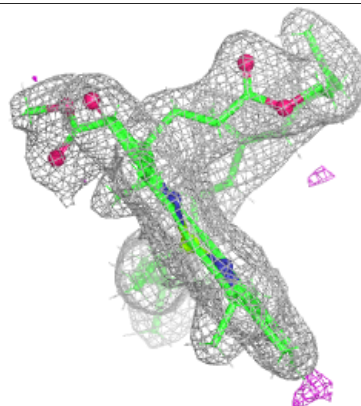
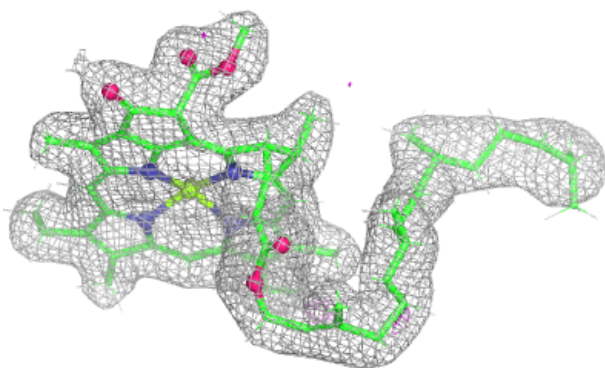
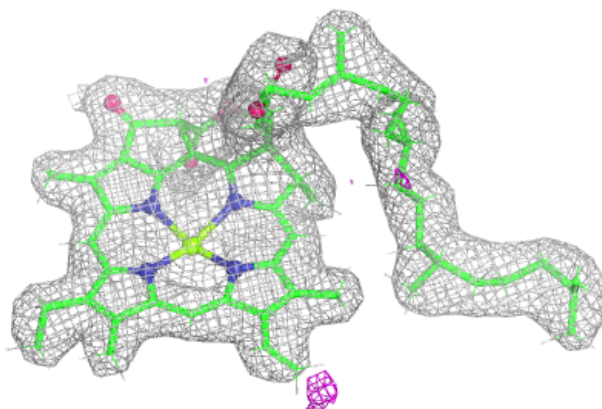
**Electron density around CLA b 605:**

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

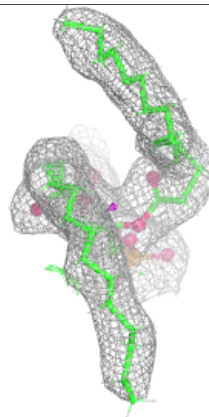
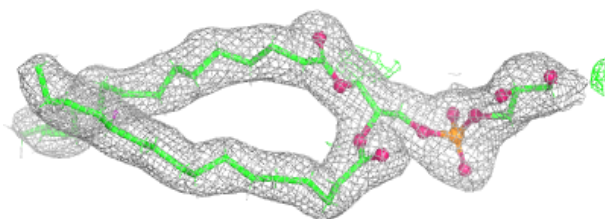
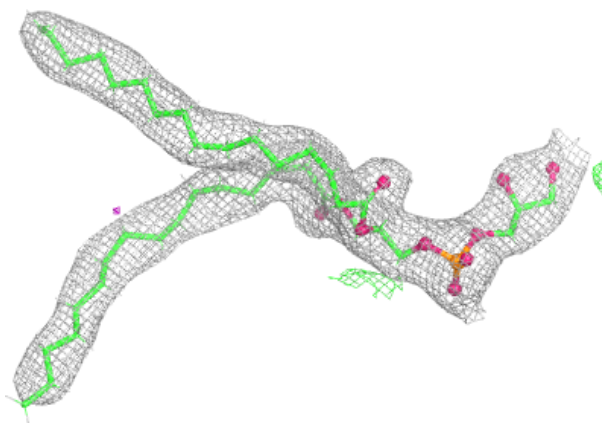


Electron density around CLA D 404:

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

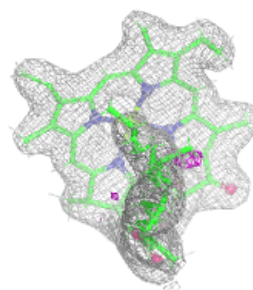
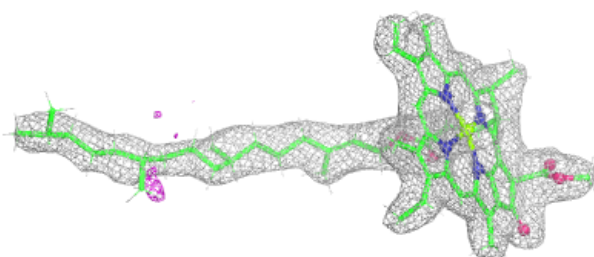
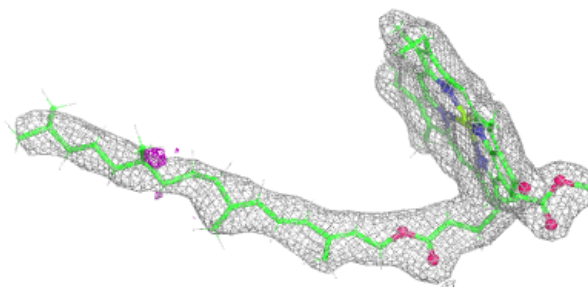
**Electron density around LHG d 408:**

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

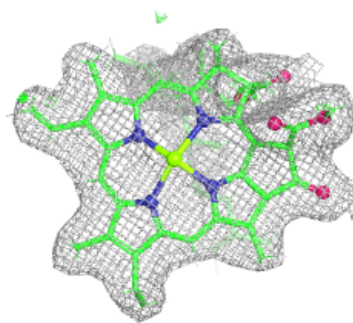
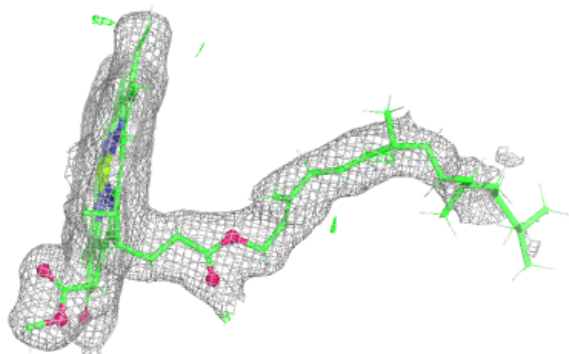
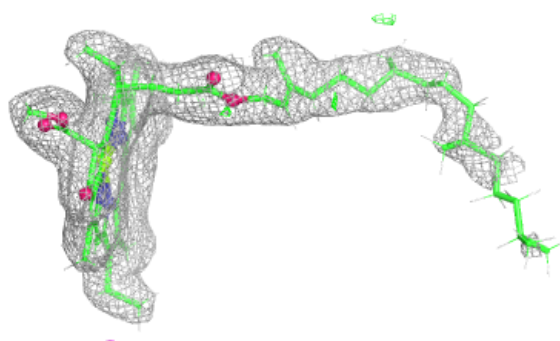


Electron density around CLA b 607:

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

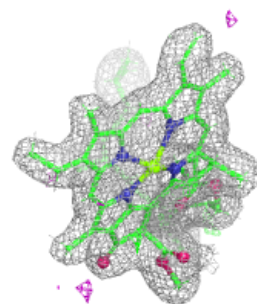
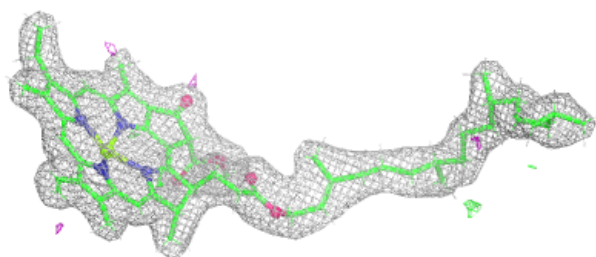
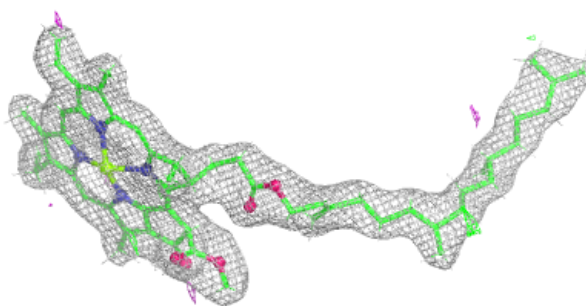
**Electron density around CLA D 405:**

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



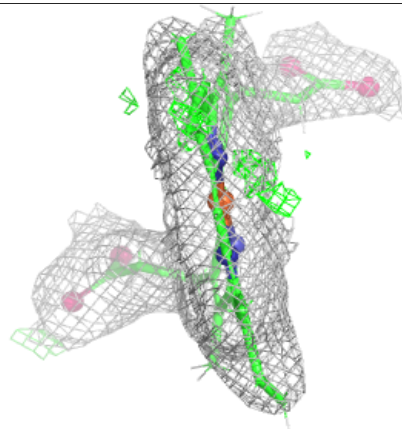
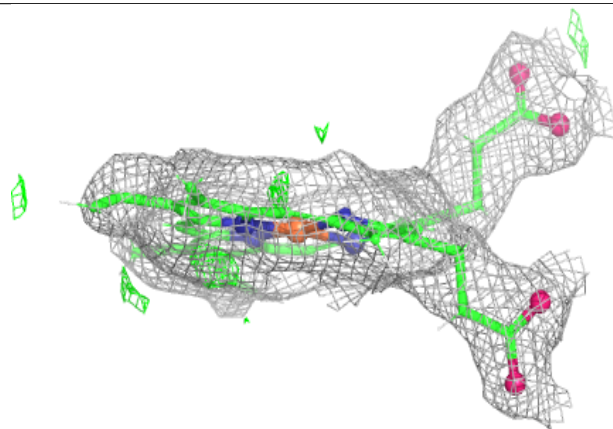
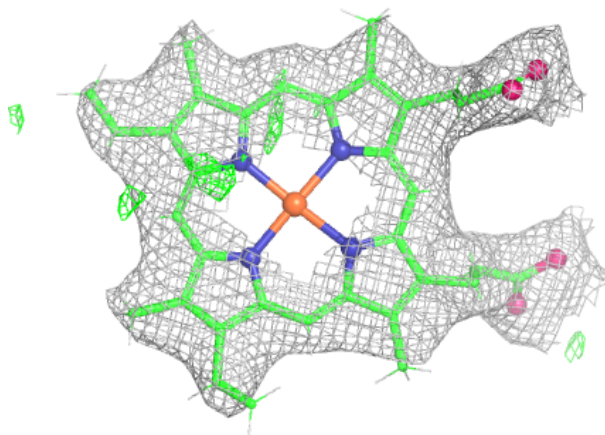
Electron density around CLA A 402:

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



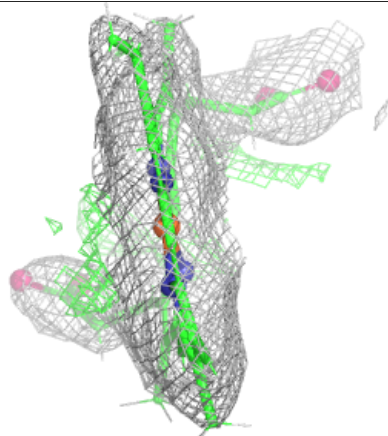
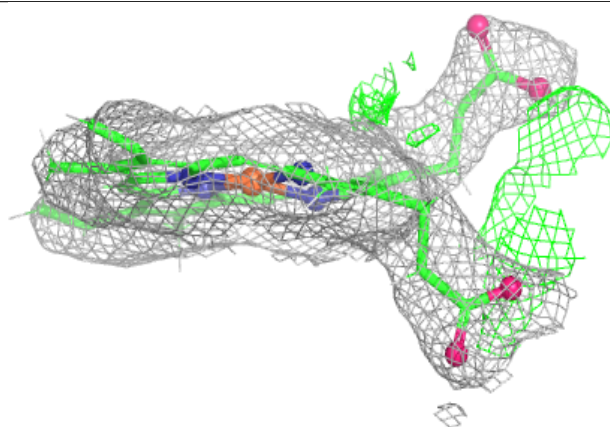
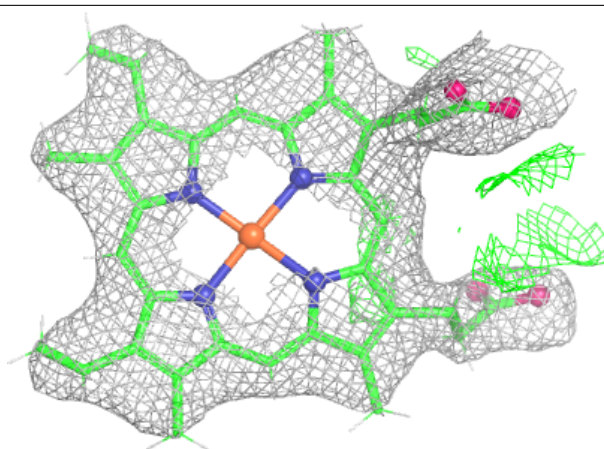
Electron density around HEC F 102:

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



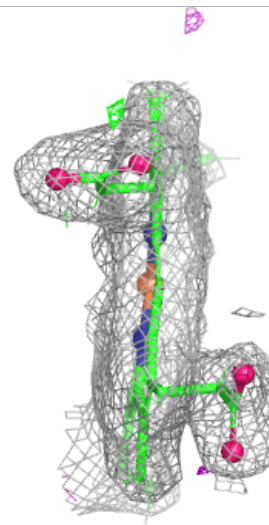
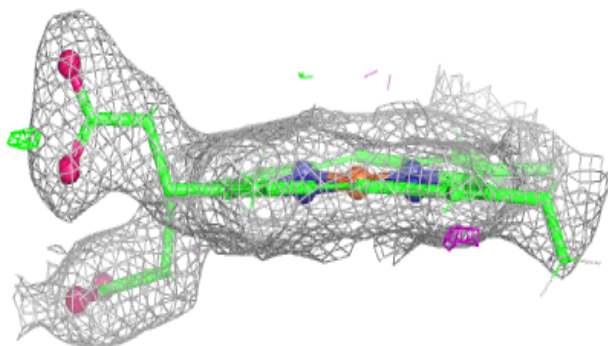
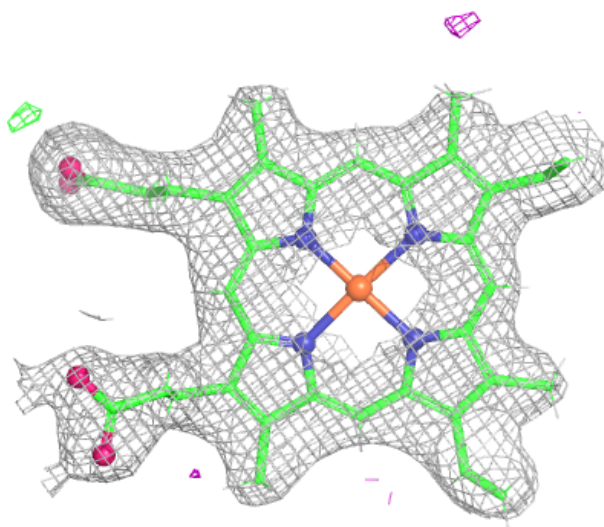
Electron density around HEC f 101:

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



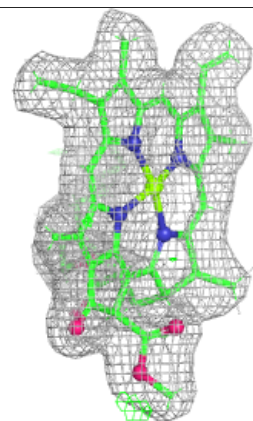
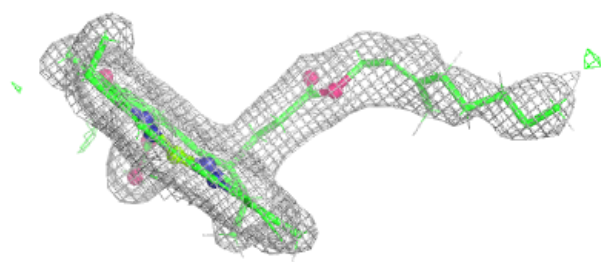
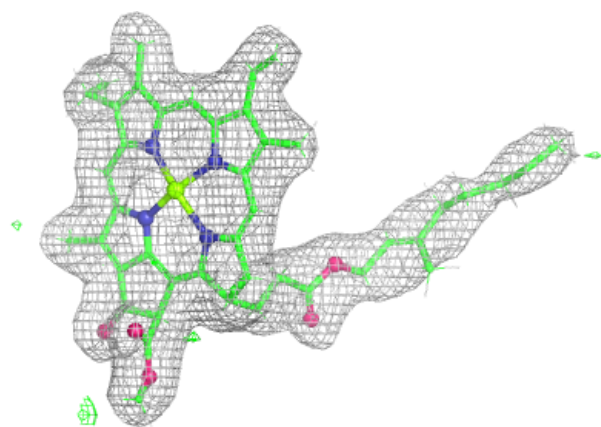
Electron density around HEC V 201:

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



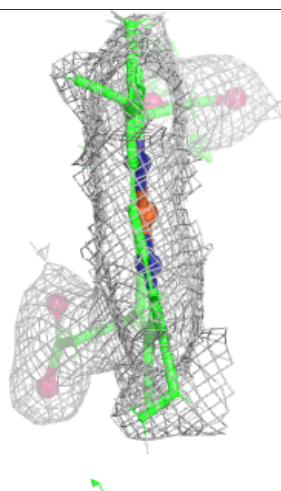
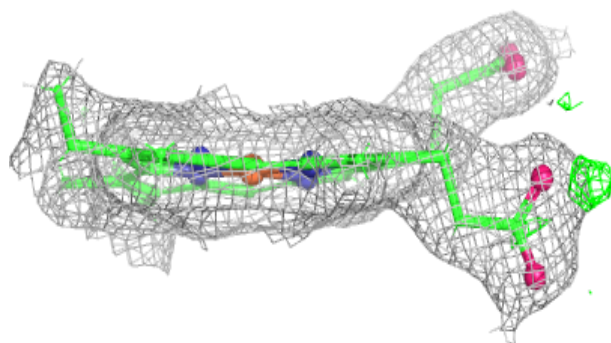
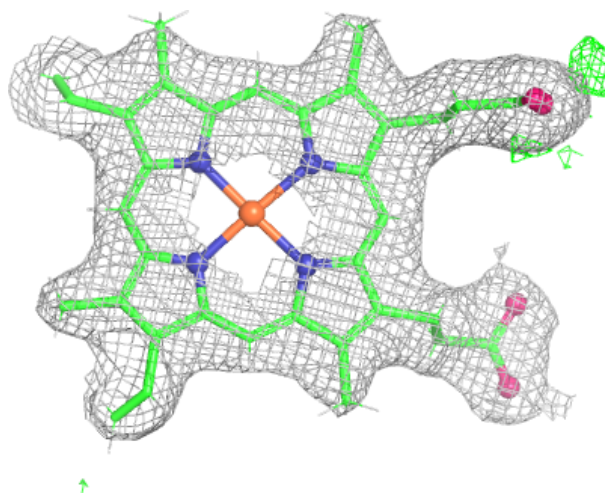
Electron density around CLA A 405:

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



Electron density around 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.