



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 10:26 AM UTC

PDB ID : 6W1T / pdb_00006w1t
Title : RT XFEL structure of Photosystem II 250 microseconds after the second illumination at 2.01 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 : 2.01 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)

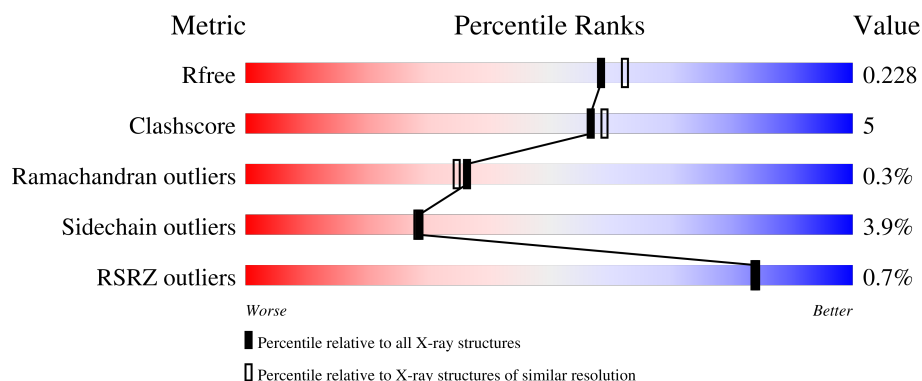
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.01 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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

Mol	Chain	Length	Quality of chain
1	A	344	
1	a	344	

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CCP4 : 9.0.010 (Gargrove)
 Density-Fitness : 1.0.12
 Ideal geometry (proteins) : Engh & Huber (2001)
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Chain	Length	Quality of chain
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
22	CLA	A	402	X	-	-	-
22	CLA	A	403	X	-	-	-
22	CLA	A	406	X	-	-	-
22	CLA	B	601	X	-	-	-
22	CLA	B	602	X	-	-	-
22	CLA	B	603	X	-	-	-
22	CLA	B	604	X	-	-	-
22	CLA	B	605	X	-	-	-
22	CLA	B	606	X	-	-	-
22	CLA	B	607	X	-	-	-
22	CLA	B	610	X	-	-	-
22	CLA	B	611	X	-	-	-
22	CLA	B	612	X	-	-	-
22	CLA	B	613	X	-	-	-
22	CLA	B	614	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	B	615	X	-	-	-
22	CLA	B	616	X	-	-	-
22	CLA	C	501	X	-	-	-
22	CLA	C	503	X	-	-	-
22	CLA	C	504	X	-	-	-
22	CLA	C	505	X	-	-	-
22	CLA	C	506	X	-	-	-
22	CLA	C	507	X	-	-	-
22	CLA	C	509	X	-	-	-
22	CLA	C	510	X	-	-	-
22	CLA	C	511	X	-	-	-
22	CLA	C	512	X	-	-	-
22	CLA	D	402	X	-	-	-
22	CLA	a	402	X	-	-	-
22	CLA	a	404	X	-	-	-
22	CLA	b	601	X	-	-	-
22	CLA	b	603	X	-	-	-
22	CLA	b	604	X	-	-	-
22	CLA	b	605	X	-	-	-
22	CLA	b	606	X	-	-	-
22	CLA	b	607	X	-	-	-
22	CLA	b	609	X	-	-	-
22	CLA	b	610	X	-	-	-
22	CLA	b	611	X	-	-	-
22	CLA	b	612	X	-	-	-
22	CLA	b	613	X	-	-	-
22	CLA	b	614	X	-	-	-
22	CLA	b	615	X	-	-	-
22	CLA	b	616	X	-	-	-
22	CLA	c	501	X	-	-	-
22	CLA	c	503	X	-	-	-
22	CLA	c	504	X	-	-	-
22	CLA	c	505	X	-	-	-
22	CLA	c	506	X	-	-	-
22	CLA	c	507	X	-	-	-
22	CLA	c	509	X	-	-	-
22	CLA	c	510	X	-	-	-
22	CLA	c	511	X	-	-	-
22	CLA	c	512	X	-	-	-
22	CLA	d	403	X	-	-	-
22	CLA	d	404	X	-	-	-
22	CLA	d	405	X	-	-	-

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 105978 atoms, of which 52553 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	60	0
			6031	2014	2942	509	547	19			
1	a	334	Total	C	H	N	O	S	0	60	0
			6019	2011	2933	509	547	19			

- 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	10	0
			6876	2283	3397	580	602	14			
3	c	451	Total	C	H	N	O	S	0	10	0
			7021	2324	3468	596	619	14			

- 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	1	0
			5350	1806	2624	445	463	12			
4	d	341	Total	C	H	N	O	S	0	2	0
			5362	1810	2630	445	465	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			

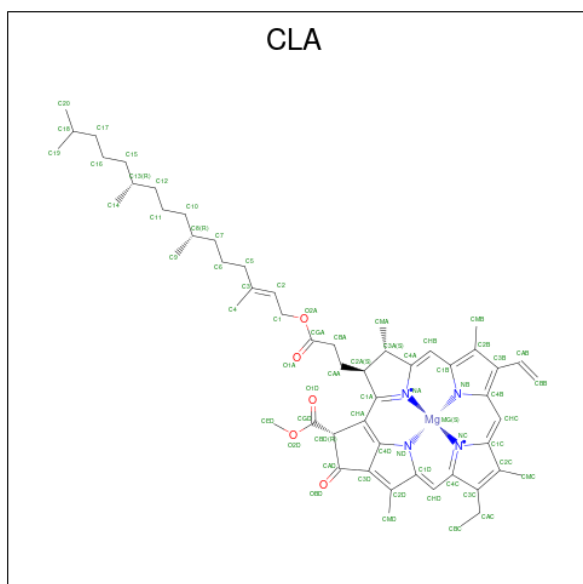
- Molecule 20 is a protein called Photosystem II reaction center protein Z.

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	A	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	A	1	Total 102	C 44	H 48	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
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
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
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
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	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

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
22	C	1	Total	C	H	Mg	N	O	0	0
			117	49	58	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
			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		
22	D	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	a	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	a	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		

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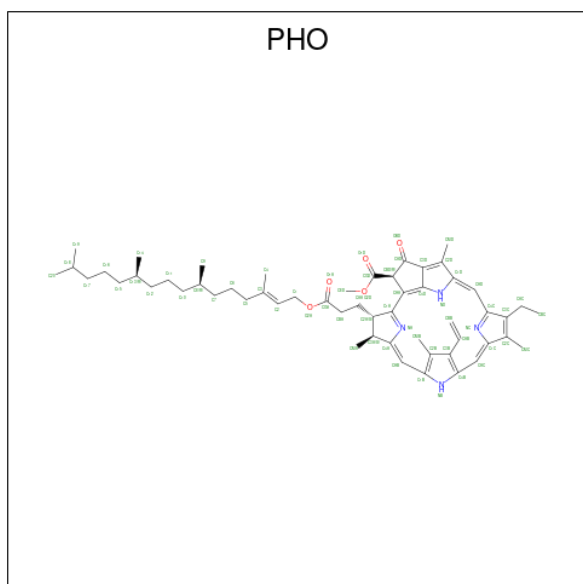
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total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

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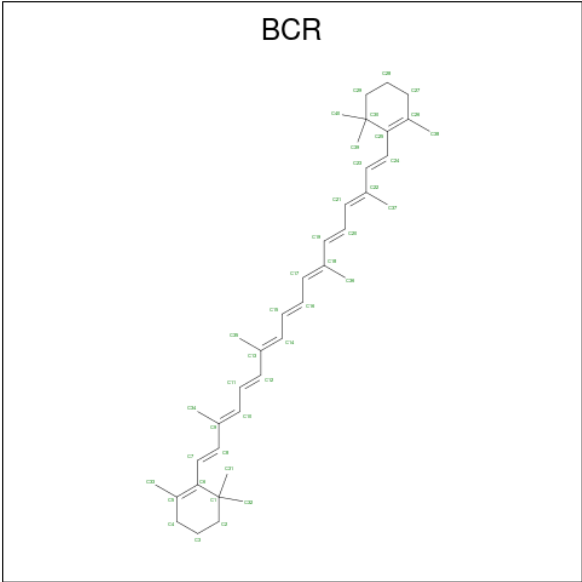
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
22	c	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	c	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	d	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	d	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	d	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	d	1	Total 137	C 55	H 72	Mg 1	N 4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

- 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	A	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	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	T	1	Total	C	H	0	0
			96	40	56		
24	Y	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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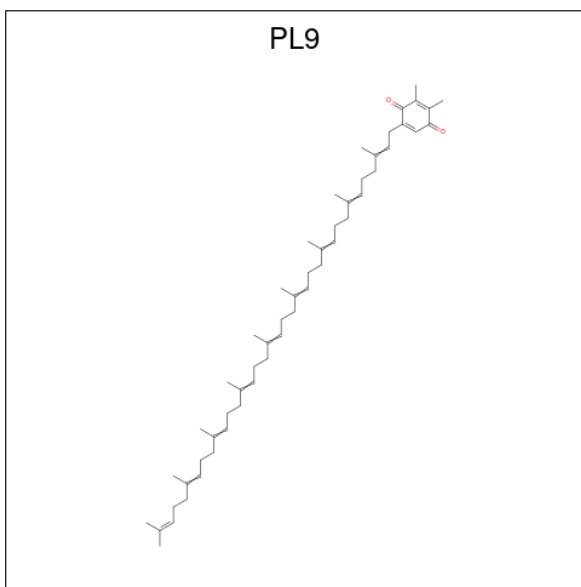
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	b	1	Total	C	H	0	0
			96	40	56		
24	c	1	Total	C	H	0	0
			96	40	56		
24	c	1	Total	C	H	0	0
			96	40	56		
24	c	1	Total	C	H	0	0
			96	40	56		
24	d	1	Total	C	H	0	0
			96	40	56		
24	k	1	Total	C	H	0	0
			96	40	56		
24	t	1	Total	C	H	0	0
			96	40	56		
24	x	1	Total	C	H	0	0
			96	40	56		

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

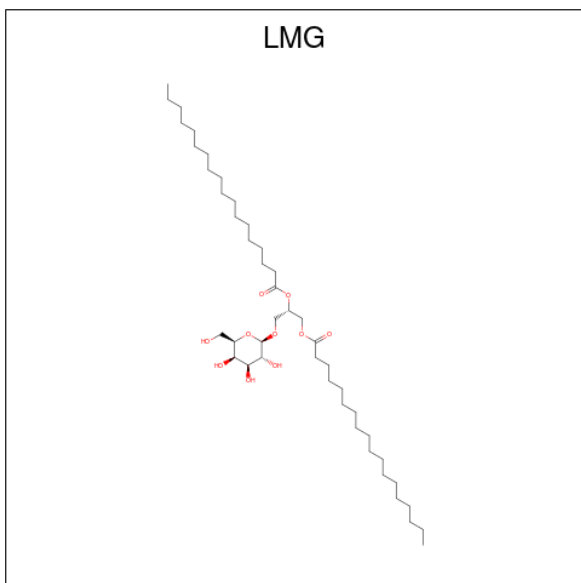
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	A	2	Total	Cl	0	0
			2	2		
25	a	2	Total	Cl	0	0
			2	2		

- 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).



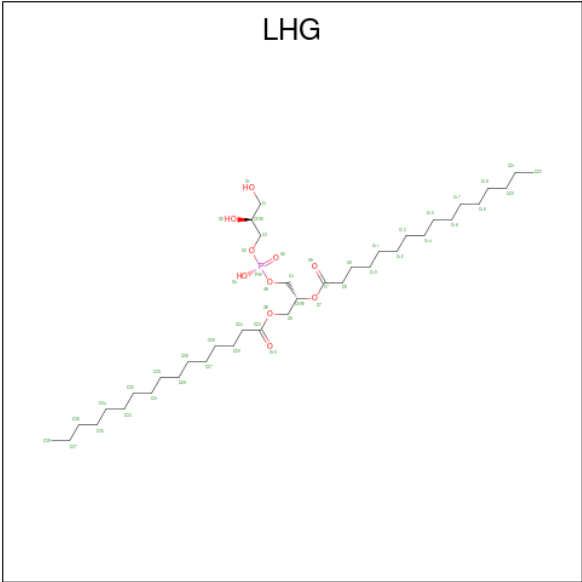
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	A	1	Total	C	H	O	0	0
			135	53	80	2		
26	D	1	Total	C	H	O	0	0
			135	53	80	2		
26	a	1	Total	C	H	O	0	0
			135	53	80	2		
26	d	1	Total	C	H	O	0	0
			135	53	80	2		

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



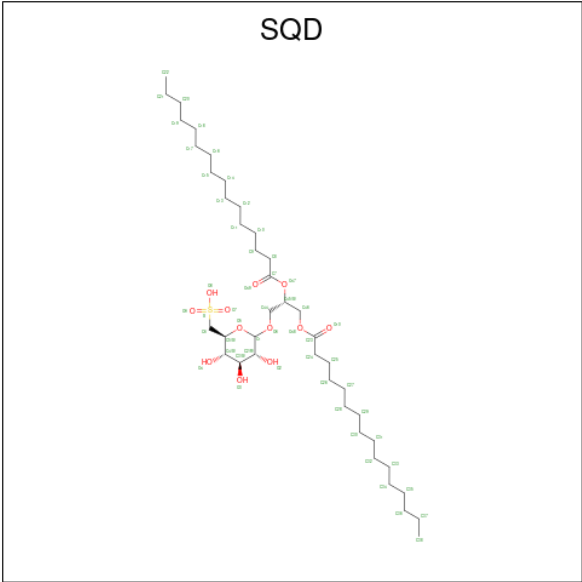
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	A	1	Total	C	H	O	0	0
			113	38	65	10		
27	C	1	Total	C	H	O	0	0
			113	38	65	10		
27	D	1	Total	C	H	O	0	0
			122	41	71	10		
27	D	1	Total	C	H	O	0	0
			78	27	45	6		
27	D	1	Total	C	H	O	0	0
			68	24	40	4		
27	M	1	Total	C	H	O	0	0
			120	41	69	10		
27	a	1	Total	C	H	O	0	0
			138	45	83	10		
27	b	1	Total	C	H	O	0	0
			140	45	85	10		
27	c	1	Total	C	H	O	0	0
			78	27	41	10		
27	c	1	Total	C	H	O	0	0
			116	38	68	10		
27	c	1	Total	C	H	O	0	0
			117	39	68	10		
27	d	1	Total	C	H	O	0	0
			101	34	57	10		
27	m	1	Total	C	H	O	0	0
			120	41	69	10		

- Molecule 28 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



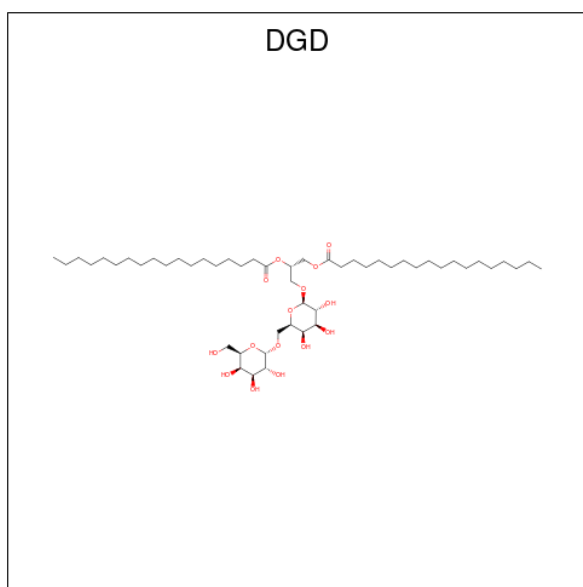
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
28	A	1	Total	C	H	O	P	0	0
			112	36	65	10	1		
28	B	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
28	B	1	Total	C	H	O	P	0	0
			121	38	72	10	1		
28	D	1	Total	C	H	O	P	0	0
			122	38	73	10	1		
28	E	1	Total	C	H	O	P	0	0
			122	38	73	10	1		
28	a	1	Total	C	H	O	P	0	0
			121	38	72	10	1		
28	d	1	Total	C	H	O	P	0	0
			121	38	72	10	1		
28	d	1	Total	C	H	O	P	0	0
			88	28	49	10	1		
28	e	1	Total	C	H	O	P	0	0
			97	31	55	10	1		
28	l	1	Total	C	H	O	P	0	0
			122	38	73	10	1		

- Molecule 29 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



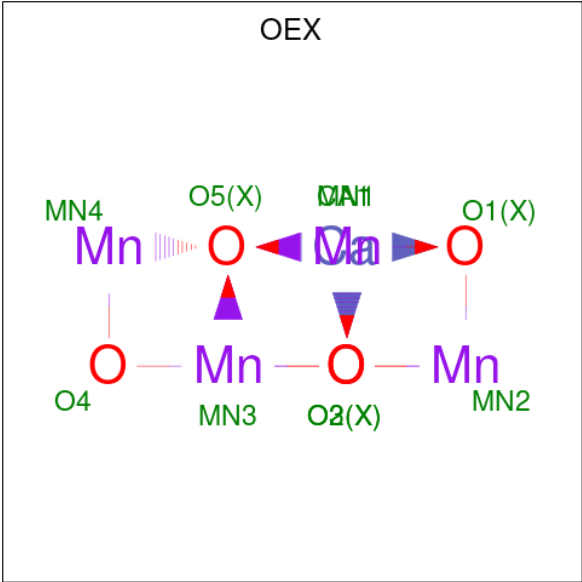
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
29	A	1	Total	C	H	O	S	0	0
			123	39	71	12	1		
29	A	1	Total	C	H	O		0	0
			104	35	65	4			
29	B	1	Total	C	H	O	S	0	0
			131	41	77	12	1		
29	D	1	Total	C	H	O	S	0	0
			81	25	45	10	1		
29	a	1	Total	C	H	O	S	0	0
			131	41	77	12	1		
29	a	1	Total	C	H	O		0	0
			92	31	56	5			
29	b	1	Total	C	H	O	S	0	0
			114	36	65	12	1		
29	f	1	Total	C	H	O	S	0	0
			89	28	48	12	1		

- Molecule 30 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: C₅₁H₉₆O₁₅).



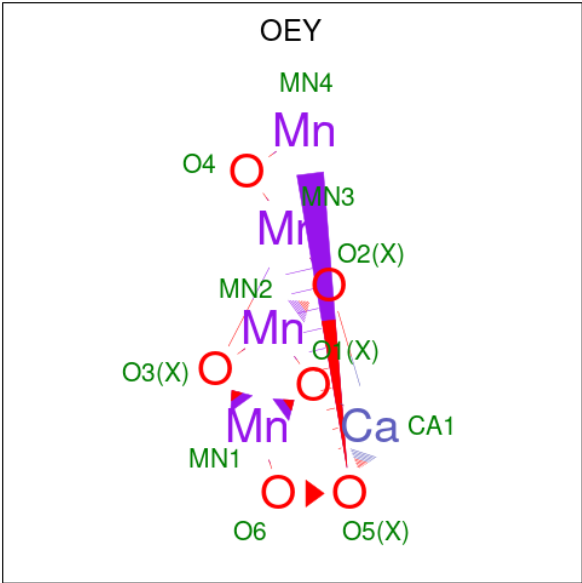
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	A	1	Total	C	H	O	0	0
			160	51	94	15		
30	C	1	Total	C	H	O	0	0
			143	47	81	15		
30	C	1	Total	C	H	O	0	0
			142	47	80	15		
30	C	1	Total	C	H	O	0	0
			142	47	80	15		
30	H	1	Total	C	H	O	0	0
			142	47	80	15		
30	c	1	Total	C	H	O	0	0
			140	47	78	15		
30	c	1	Total	C	H	O	0	0
			138	47	76	15		
30	c	1	Total	C	H	O	0	0
			142	47	80	15		
30	h	1	Total	C	H	O	0	0
			139	47	77	15		

- Molecule 31 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5).



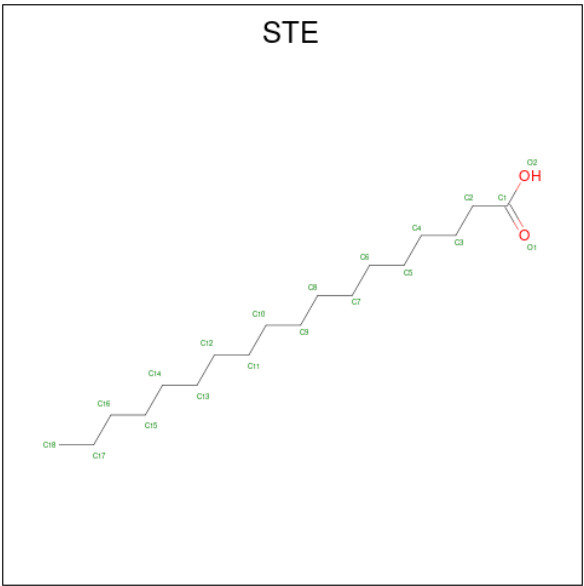
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	A	1	Total	Ca	Mn	O	0	1
			10	1	4	5		
31	a	1	Total	Ca	Mn	O	0	1
			10	1	4	5		

- Molecule 32 is CA-MN4-O6 CLUSTER (CCD ID: OEY) (formula: CaMn_4O_6).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	A	1	Total	Ca	Mn	O	0	1
			11	1	4	6		
32	a	1	Total	Ca	Mn	O	0	1
			11	1	4	6		

- Molecule 33 is STEARIC ACID (CCD ID: STE) (formula: C₁₈H₃₆O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	B	1	Total	C	H	O	0	0
			43	15	26	2		
33	B	1	Total	C	H	O	0	0
			28	10	16	2		
33	B	1	Total	C	H		0	0
			47	16	31			
33	B	1	Total	C	H	O	0	0
			28	10	16	2		
33	C	1	Total	C	H	O	0	0
			28	10	16	2		
33	C	1	Total	C	H		0	0
			47	16	31			
33	C	1	Total	C	H	O	0	0
			28	10	16	2		
33	D	1	Total	C	H	O	0	0
			55	18	35	2		
33	H	1	Total	C	H		0	0
			53	18	35			
33	I	1	Total	C	H		0	0
			41	15	26			
33	J	1	Total	C	H	O	0	0
			28	10	16	2		
33	M	1	Total	C	H	O	0	0
			37	13	22	2		
33	M	1	Total	C	H		0	0
			26	10	16			

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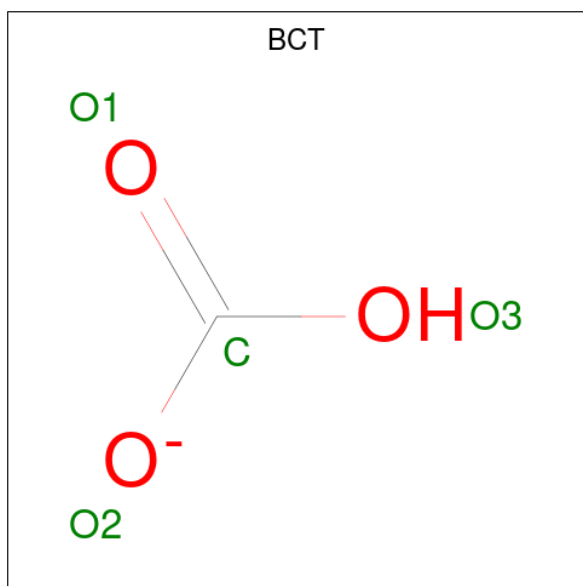
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	R	1	Total C H O 28 10 16 2	0	0
33	T	1	Total C H 44 15 29	0	0
33	Z	1	Total C H 20 8 12	0	0
33	a	1	Total C H 26 10 16	0	0
33	a	1	Total C H O 28 10 16 2	0	0
33	a	1	Total C H 41 15 26	0	0
33	b	1	Total C H 47 16 31	0	0
33	b	1	Total C H O 55 18 35 2	0	0
33	b	1	Total C H O 40 14 24 2	0	0
33	b	1	Total C H O 55 18 35 2	0	0
33	b	1	Total C H 26 10 16	0	0
33	b	1	Total C H 41 14 27	0	0
33	c	1	Total C H O 55 18 35 2	0	0
33	d	1	Total C H O 43 15 26 2	0	0
33	d	1	Total C H O 55 18 35 2	0	0
33	d	1	Total C H O 55 18 35 2	0	0
33	j	1	Total C H O 28 10 16 2	0	0
33	k	1	Total C H O 28 10 16 2	0	0
33	l	1	Total C H 53 18 35	0	0
33	m	1	Total C H O 28 10 16 2	0	0
33	t	1	Total C H O 34 12 20 2	0	0

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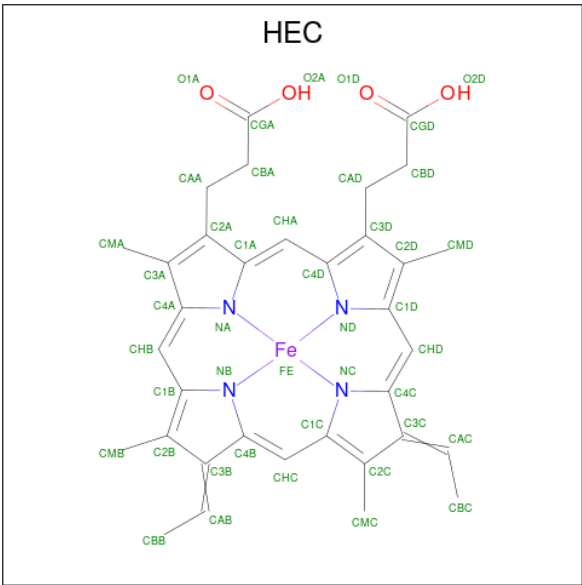
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	t	1	Total	C	H	O	0	0
			46	16	28	2		

- Molecule 34 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3^-).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	D	1	Total	C	H	O	0	0
			5	1	1	3		
34	a	1	Total	C	H	O	0	0
			5	1	1	3		

- Molecule 35 is HEME C (CCD ID: HEC) (formula: $\text{C}_{34}\text{H}_{34}\text{FeN}_4\text{O}_4$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
35	F	1	Total	C	Fe	H	N	O	0	0
			75	34	1	32	4	4		
35	V	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
35	f	1	Total	C	Fe	H	N	O	0	0
			75	34	1	32	4	4		
35	v	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		

- Molecule 36 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	A	146	Total	O	0	8
			146	146		
36	B	211	Total	O	0	0
			211	211		
36	C	185	Total	O	0	0
			185	185		
36	D	129	Total	O	0	0
			129	129		
36	E	34	Total	O	0	0
			34	34		
36	F	13	Total	O	0	0
			13	13		
36	H	33	Total	O	0	0
			33	33		
36	I	11	Total	O	0	0
			11	11		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	J	15	Total 15	O 15	0	0
36	K	9	Total 9	O 9	0	0
36	L	9	Total 9	O 9	0	0
36	M	5	Total 5	O 5	0	0
36	O	104	Total 104	O 104	0	0
36	R	13	Total 13	O 13	0	0
36	T	15	Total 15	O 15	0	0
36	U	51	Total 51	O 51	0	0
36	V	70	Total 70	O 70	0	0
36	X	11	Total 11	O 11	0	0
36	Y	2	Total 2	O 2	0	0
36	Z	5	Total 5	O 5	0	0
36	a	130	Total 130	O 130	0	8
36	b	215	Total 215	O 215	0	0
36	c	190	Total 190	O 190	0	0
36	d	122	Total 122	O 122	0	0
36	e	30	Total 30	O 30	0	0
36	f	9	Total 9	O 9	0	0
36	h	22	Total 22	O 22	0	0
36	i	9	Total 9	O 9	0	0
36	j	10	Total 10	O 10	0	0

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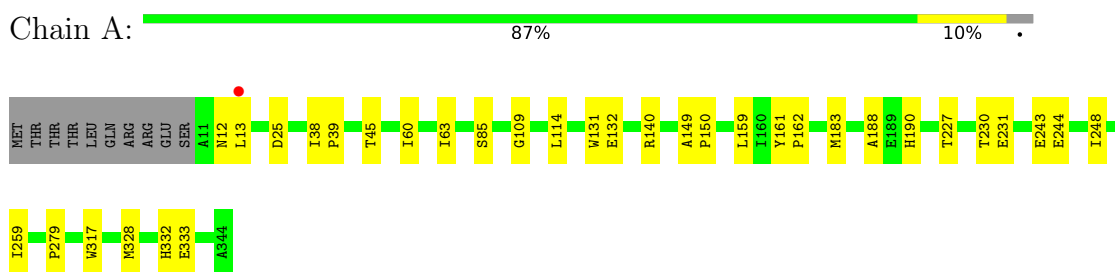
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	k	10	Total 10	O 10	0	0
36	l	9	Total 9	O 9	0	0
36	m	8	Total 8	O 8	0	0
36	o	103	Total 103	O 103	0	0
36	r	2	Total 2	O 2	0	0
36	t	11	Total 11	O 11	0	0
36	u	66	Total 66	O 66	0	0
36	v	58	Total 58	O 58	0	0
36	x	10	Total 10	O 10	0	0
36	y	6	Total 6	O 6	0	0
36	z	6	Total 6	O 6	0	0

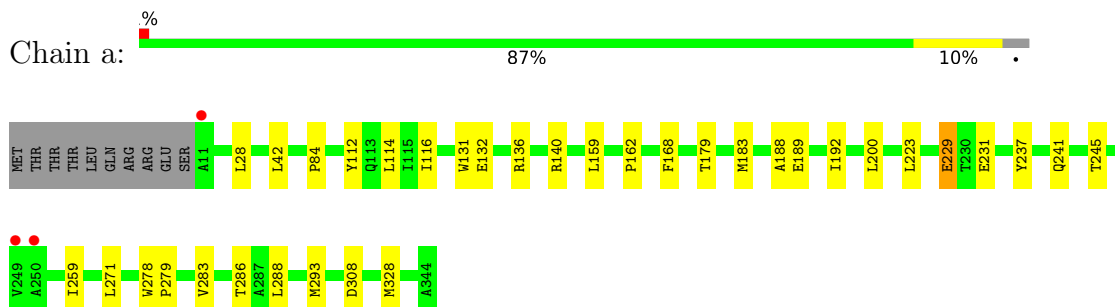
3 Residue-property plots [i](#)

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.

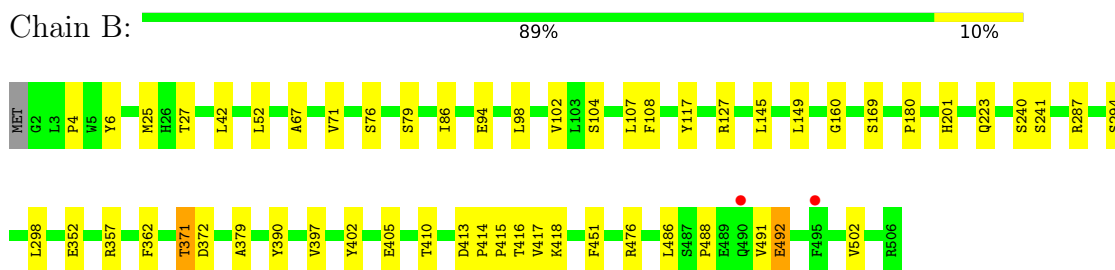
- Molecule 1: Photosystem II protein D1 1



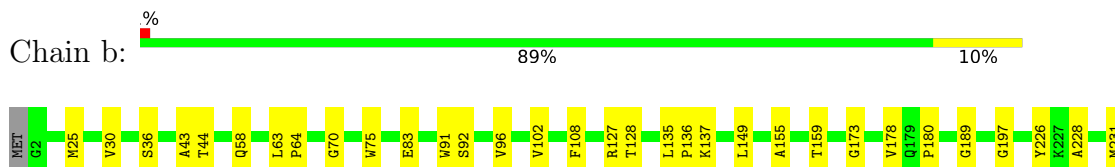
- Molecule 1: Photosystem II protein D1 1

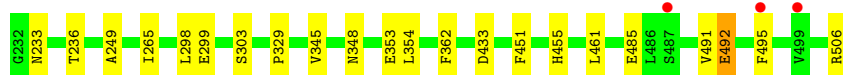


- Molecule 2: Photosystem II CP47 reaction center protein



- Molecule 2: Photosystem II CP47 reaction center protein





- Molecule 3: Photosystem II CP43 reaction center protein

Chain C: 87% 8% .



- Molecule 3: Photosystem II CP43 reaction center protein

Chain c: 89% 9% .



- Molecule 4: Photosystem II D2 protein

Chain D: 88% 8% .



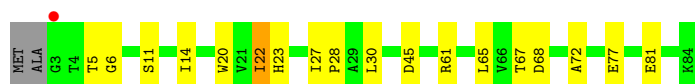
- Molecule 4: Photosystem II D2 protein

Chain d: 85% 11% . .

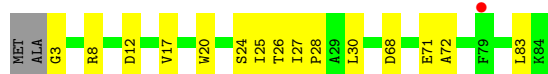
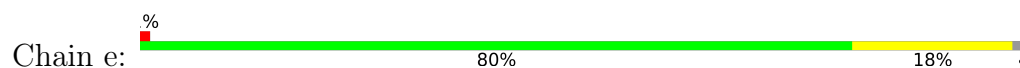


- Molecule 5: Cytochrome b559 subunit alpha

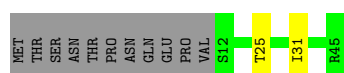
Chain E: 76% 20% . .



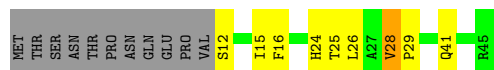
- Molecule 5: Cytochrome b559 subunit alpha



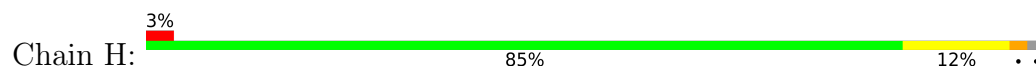
- Molecule 6: Cytochrome b559 subunit beta



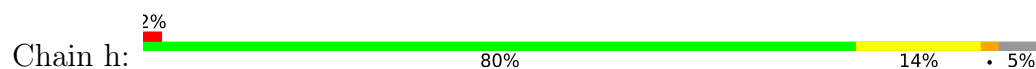
- Molecule 6: Cytochrome b559 subunit beta



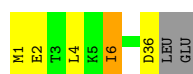
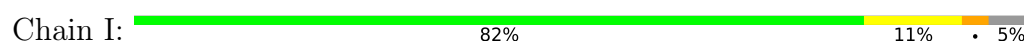
- Molecule 7: Photosystem II reaction center protein H



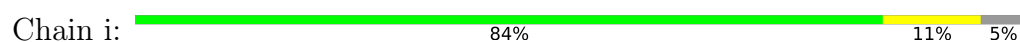
- Molecule 7: Photosystem II reaction center protein H

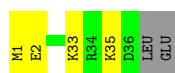


- Molecule 8: Photosystem II reaction center protein I

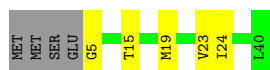
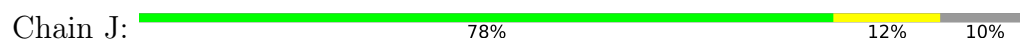


- Molecule 8: Photosystem II reaction center protein I

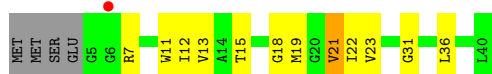




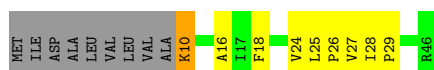
• Molecule 9: Photosystem II reaction center protein J



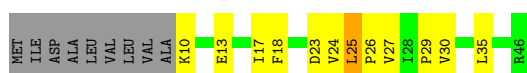
• Molecule 9: Photosystem II reaction center protein J



• Molecule 10: Photosystem II reaction center protein K



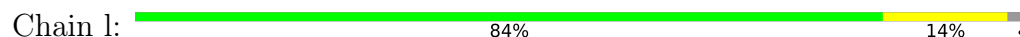
• Molecule 10: Photosystem II reaction center protein K



• Molecule 11: Photosystem II reaction center protein L



• Molecule 11: Photosystem II reaction center protein L



• Molecule 12: Photosystem II reaction center protein M

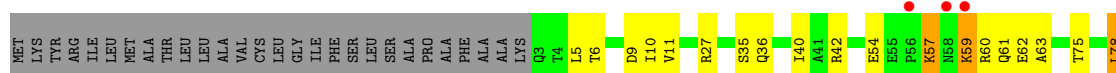
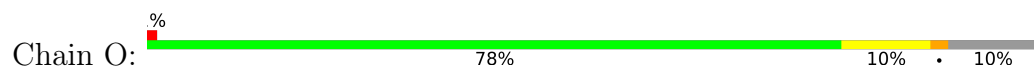




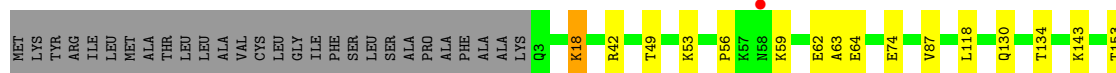
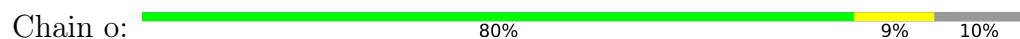
- Molecule 12: Photosystem II reaction center protein M



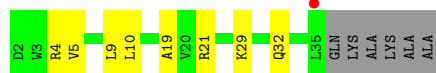
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



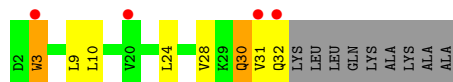
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



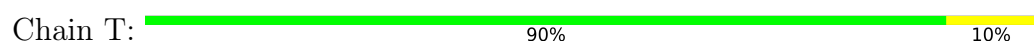
- Molecule 14: Photosystem II protein Y



- Molecule 14: Photosystem II protein Y

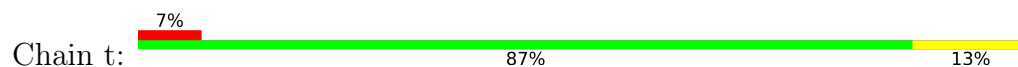


- Molecule 15: Photosystem II reaction center protein T

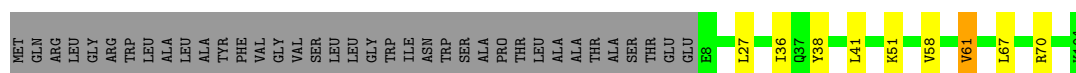




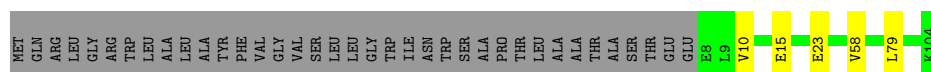
- Molecule 15: Photosystem II reaction center protein T



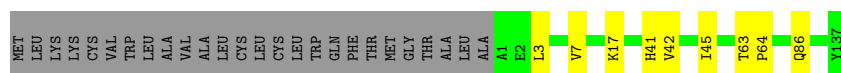
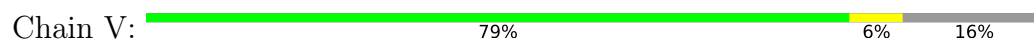
- Molecule 16: Photosystem II 12 kDa extrinsic protein



- Molecule 16: Photosystem II 12 kDa extrinsic protein



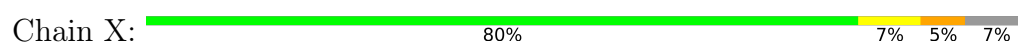
- Molecule 17: Cytochrome c-550



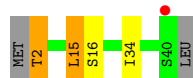
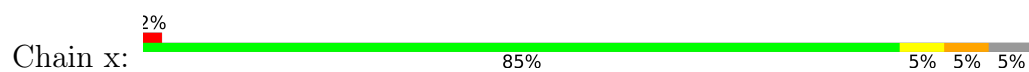
- Molecule 17: Cytochrome c-550



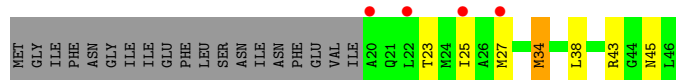
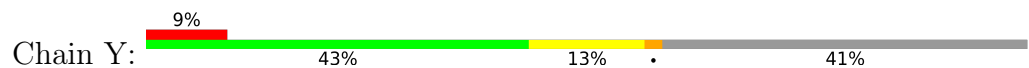
- Molecule 18: Photosystem II reaction center X protein



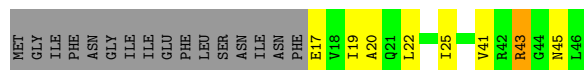
- Molecule 18: Photosystem II reaction center X protein



- Molecule 19: Photosystem II reaction center protein Ycf12



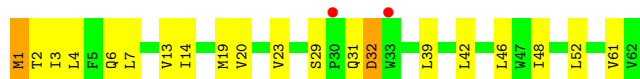
- Molecule 19: Photosystem II reaction center protein Ycf12



- 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	117.04Å 221.92Å 308.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.59 – 2.01 33.59 – 2.01	Depositor EDS
% Data completeness (in resolution range)	99.7 (33.59-2.01) 86.9 (33.59-2.01)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.57 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.175 , 0.228 0.175 , 0.228	Depositor DCC
R_{free} test set	4767 reflections (0.76%)	wwPDB-VP
Wilson B-factor (Å ²)	26.0	Xtriage
Anisotropy	0.205	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 55.6	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	0.96	EDS
Total number of atoms	105978	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.23% 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: FME, HEC, OEX, STE, PL9, DGD, OEY, BCT, FE2, SQD, LHG, CL, BCR, PHO, CLA, LMG

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	0.57	0/3187	0.63	0/4342
1	a	0.53	0/3184	0.63	1/4338 (0.0%)
2	B	0.60	0/4161	0.67	0/5669
2	b	0.56	0/4118	0.65	0/5611
3	C	0.57	0/3621	0.66	2/4930 (0.0%)
3	c	0.53	0/3693	0.64	0/5026
4	D	0.64	0/2820	0.70	0/3840
4	d	0.60	0/2829	0.68	0/3852
5	E	0.50	0/688	0.60	0/940
5	e	0.45	0/683	0.61	0/932
6	F	0.49	0/284	0.62	0/387
6	f	0.48	0/284	0.66	0/387
7	H	0.58	0/523	0.65	0/713
7	h	0.50	0/511	0.62	0/697
8	I	0.56	0/293	0.64	0/396
8	i	0.55	0/293	0.61	0/396
9	J	0.44	0/263	0.64	0/356
9	j	0.43	0/263	0.57	0/356
10	K	0.44	0/303	0.61	0/416
10	k	0.45	0/303	0.55	0/416
11	L	0.61	0/311	0.66	0/422
11	l	0.63	0/303	0.66	0/412
12	M	0.62	0/249	0.70	0/341
12	m	0.56	0/244	0.72	0/334
13	O	0.57	0/1904	0.65	0/2585
13	o	0.58	0/1905	0.65	0/2583
14	R	0.41	0/277	0.54	0/380
14	r	0.32	0/246	0.52	0/339
15	T	0.63	0/257	0.66	0/349
15	t	0.67	0/255	0.63	0/346
16	U	0.50	0/785	0.60	0/1064
16	u	0.52	0/785	0.66	0/1064

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	V	0.56	0/1085	0.68	0/1473
17	v	0.52	0/1085	0.61	0/1473
18	X	0.46	0/284	0.57	0/384
18	x	0.42	0/289	0.51	0/391
19	Y	0.48	0/197	0.57	0/264
19	y	0.40	0/219	0.54	0/294
20	Z	0.39	0/490	0.58	0/669
20	z	0.33	0/488	0.48	0/666
All	All	0.56	0/43962	0.65	3/59833 (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
1	A	0	1
17	V	0	1
All	All	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	88	LEU	CA-C-N	5.36	123.62	120.24
3	C	88	LEU	C-N-CA	5.36	123.62	120.24
1	a	131	TRP	CA-CB-CG	-5.03	104.05	113.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	190[A]	HIS	Mainchain
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	3089	2942	2956	19	0
1	a	3086	2933	2947	19	0
2	B	4005	3859	3867	35	0
2	b	3978	3822	3836	34	0
3	C	3479	3397	3383	23	0
3	c	3553	3468	3466	33	0
4	D	2726	2624	2632	20	0
4	d	2732	2630	2638	32	0
5	E	666	650	651	13	0
5	e	664	647	648	11	0
6	F	275	281	282	2	0
6	f	275	281	282	8	0
7	H	510	532	532	5	0
7	h	498	518	518	7	0
8	I	296	311	311	1	0
8	i	296	311	311	1	0
9	J	257	268	268	4	0
9	j	257	268	268	9	0
10	K	293	305	305	9	0
10	k	293	305	305	6	0
11	L	304	316	316	3	0
11	l	296	304	304	1	0
12	M	256	269	269	6	0
12	m	251	267	267	7	0
13	O	1870	1828	1830	19	0
13	o	1874	1844	1846	11	0
14	R	271	298	298	3	0
14	r	240	253	250	6	0
15	T	258	261	261	0	0
15	t	256	256	256	4	0
16	U	774	772	773	6	0
16	u	774	772	773	1	0
17	V	1064	1068	1073	2	0
17	v	1064	1068	1073	12	0
18	X	281	312	312	4	0
18	x	286	316	314	3	0
19	Y	196	217	217	4	0
19	y	218	241	241	4	0
20	Z	479	516	516	9	0
20	z	477	509	509	10	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	A	184	192	192	1	0
22	B	1035	1139	1139	17	0
22	C	839	922	922	13	0
22	D	195	216	216	5	0
22	a	130	144	144	1	0
22	b	1035	1139	1139	19	0
22	c	839	919	919	15	0
22	d	260	288	288	3	0
23	A	128	148	148	1	0
23	a	64	74	74	1	0
23	d	64	74	74	2	0
24	A	40	56	56	1	0
24	B	120	168	168	9	0
24	C	120	168	168	4	0
24	D	40	56	56	2	0
24	H	40	56	56	4	0
24	T	40	56	56	4	0
24	Y	40	56	56	2	0
24	a	40	56	56	1	0
24	b	120	168	168	5	0
24	c	120	168	168	2	0
24	d	40	56	56	7	0
24	k	40	56	56	0	0
24	t	40	56	56	4	0
24	x	40	56	56	0	0
25	A	2	0	0	0	0
25	a	2	0	0	0	0
26	A	55	80	80	8	0
26	D	55	80	80	0	0
26	a	55	80	80	4	0
26	d	55	80	80	0	0
27	A	48	65	66	0	0
27	C	48	65	66	0	0
27	D	112	156	157	0	0
27	M	51	69	72	0	0
27	a	55	83	86	0	0
27	b	55	85	86	2	0
27	c	134	177	181	3	0
27	d	44	57	58	0	0
27	m	51	69	72	2	0
28	A	47	65	67	0	0
28	B	98	146	148	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	D	49	73	74	0	0
28	E	49	73	74	3	0
28	a	49	72	74	1	0
28	d	88	121	125	0	0
28	e	42	55	57	0	0
28	l	49	73	74	0	0
29	A	91	136	136	1	0
29	B	54	77	77	2	0
29	D	36	45	46	0	0
29	a	90	133	132	3	0
29	b	49	65	65	1	0
29	f	41	48	48	1	0
30	A	66	94	95	1	0
30	C	186	241	246	1	0
30	H	62	80	81	0	0
30	c	186	234	246	1	0
30	h	62	77	79	1	0
31	A	10	0	0	0	0
31	a	10	0	0	0	0
32	A	11	0	0	1	0
32	a	11	0	0	1	0
33	B	57	89	86	3	0
33	C	40	63	60	0	0
33	D	20	35	35	3	0
33	H	18	35	35	0	0
33	I	15	26	26	0	0
33	J	12	16	16	0	0
33	M	25	38	38	1	0
33	R	12	16	16	0	0
33	T	15	29	26	1	0
33	Z	8	12	12	0	0
33	a	37	58	58	0	0
33	b	96	168	165	6	0
33	c	20	35	35	0	0
33	d	57	96	96	4	0
33	j	12	16	16	0	0
33	k	12	16	16	0	0
33	l	18	35	35	0	0
33	m	12	16	16	0	0
33	t	32	48	48	2	0
34	D	4	1	1	0	0
34	a	4	1	1	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	F	43	32	32	5	0
35	V	43	30	30	2	0
35	f	43	32	32	5	0
35	v	43	30	30	3	0
36	A	146	0	0	3	0
36	B	211	0	0	8	0
36	C	185	0	0	1	0
36	D	129	0	0	2	0
36	E	34	0	0	1	0
36	F	13	0	0	1	0
36	H	33	0	0	0	0
36	I	11	0	0	0	0
36	J	15	0	0	2	0
36	K	9	0	0	1	0
36	L	9	0	0	0	0
36	M	5	0	0	2	0
36	O	104	0	0	3	0
36	R	13	0	0	0	0
36	T	15	0	0	0	0
36	U	51	0	0	1	0
36	V	70	0	0	0	0
36	X	11	0	0	0	0
36	Y	2	0	0	0	0
36	Z	5	0	0	1	0
36	a	130	0	0	3	0
36	b	215	0	0	3	0
36	c	190	0	0	9	0
36	d	122	0	0	3	0
36	e	30	0	0	2	0
36	f	9	0	0	1	0
36	h	22	0	0	1	0
36	i	9	0	0	0	0
36	j	10	0	0	1	0
36	k	10	0	0	1	0
36	l	9	0	0	0	0
36	m	8	0	0	2	0
36	o	103	0	0	2	0
36	r	2	0	0	0	0
36	t	11	0	0	1	0
36	u	66	0	0	0	0
36	v	58	0	0	2	0
36	x	10	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	y	6	0	0	2	0
36	z	6	0	0	0	0
All	All	53425	52553	52660	482	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 482 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)
17:v:40:CYS:SG	35:v:201:HEC:CAC	2.04	1.44
3:c:315:MET:SD	36:c:768:HOH:O	2.23	0.94
32:A:417[B]:OEY:O5	32:A:417[B]:OEY:O6	1.92	0.88
5:e:71:GLU:OE1	36:e:201:HOH:O	1.91	0.86
17:v:76:MET:HE2	17:v:112:LEU:HD22	1.58	0.86

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	391/344 (114%)	387 (99%)	3 (1%)	1 (0%)	36	35
1	a	391/344 (114%)	387 (99%)	3 (1%)	1 (0%)	36	35
2	B	508/506 (100%)	497 (98%)	10 (2%)	1 (0%)	43	42
2	b	503/506 (99%)	491 (98%)	12 (2%)	0	100	100
3	C	450/461 (98%)	440 (98%)	9 (2%)	1 (0%)	43	42
3	c	459/461 (100%)	443 (96%)	15 (3%)	1 (0%)	43	42
4	D	339/352 (96%)	329 (97%)	10 (3%)	0	100	100
4	d	340/352 (97%)	331 (97%)	9 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	81/84 (96%)	81 (100%)	0	0	100	100
5	e	80/84 (95%)	79 (99%)	1 (1%)	0	100	100
6	F	32/45 (71%)	32 (100%)	0	0	100	100
6	f	32/45 (71%)	30 (94%)	2 (6%)	0	100	100
7	H	63/66 (96%)	58 (92%)	4 (6%)	1 (2%)	7	3
7	h	61/66 (92%)	57 (93%)	4 (7%)	0	100	100
8	I	34/38 (90%)	33 (97%)	1 (3%)	0	100	100
8	i	34/38 (90%)	31 (91%)	3 (9%)	0	100	100
9	J	34/40 (85%)	32 (94%)	2 (6%)	0	100	100
9	j	34/40 (85%)	34 (100%)	0	0	100	100
10	K	35/46 (76%)	34 (97%)	0	1 (3%)	3	1
10	k	35/46 (76%)	35 (100%)	0	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	34/37 (92%)	34 (100%)	0	0	100	100
12	M	31/36 (86%)	30 (97%)	1 (3%)	0	100	100
12	m	30/36 (83%)	28 (93%)	2 (7%)	0	100	100
13	O	243/272 (89%)	227 (93%)	12 (5%)	4 (2%)	7	3
13	o	242/272 (89%)	233 (96%)	8 (3%)	1 (0%)	30	27
14	R	32/40 (80%)	30 (94%)	2 (6%)	0	100	100
14	r	29/40 (72%)	27 (93%)	2 (7%)	0	100	100
15	T	28/30 (93%)	28 (100%)	0	0	100	100
15	t	28/30 (93%)	28 (100%)	0	0	100	100
16	U	95/134 (71%)	92 (97%)	3 (3%)	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%)	129 (96%)	6 (4%)	0	100	100
18	X	36/41 (88%)	35 (97%)	1 (3%)	0	100	100
18	x	37/41 (90%)	37 (100%)	0	0	100	100
19	Y	25/46 (54%)	23 (92%)	1 (4%)	1 (4%)	2	0
19	y	28/46 (61%)	25 (89%)	2 (7%)	1 (4%)	2	1
20	Z	60/62 (97%)	57 (95%)	3 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	z	60/62 (97%)	55 (92%)	3 (5%)	2 (3%)	3	1
All	All	5374/5686 (94%)	5216 (97%)	141 (3%)	17 (0%)	36	35

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
10	K	16	ALA
13	O	60	ARG
17	V	64	PRO
3	c	416	SER

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	320/280 (114%)	313 (98%)	7 (2%)	45	50
1	a	319/280 (114%)	310 (97%)	9 (3%)	38	41
2	B	408/404 (101%)	396 (97%)	12 (3%)	37	40
2	b	402/404 (100%)	393 (98%)	9 (2%)	45	50
3	C	353/362 (98%)	345 (98%)	8 (2%)	44	49
3	c	361/362 (100%)	351 (97%)	10 (3%)	38	41
4	D	277/283 (98%)	270 (98%)	7 (2%)	42	45
4	d	278/283 (98%)	269 (97%)	9 (3%)	34	35
5	E	72/73 (99%)	66 (92%)	6 (8%)	10	7
5	e	71/73 (97%)	70 (99%)	1 (1%)	59	66
6	F	28/39 (72%)	28 (100%)	0	100	100
6	f	28/39 (72%)	26 (93%)	2 (7%)	13	10
7	H	54/55 (98%)	52 (96%)	2 (4%)	30	30
7	h	53/55 (96%)	51 (96%)	2 (4%)	29	29
8	I	32/34 (94%)	29 (91%)	3 (9%)	8	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	i	32/34 (94%)	31 (97%)	1 (3%)	35	37
9	J	24/28 (86%)	23 (96%)	1 (4%)	26	25
9	j	24/28 (86%)	22 (92%)	2 (8%)	10	7
10	K	30/37 (81%)	29 (97%)	1 (3%)	33	34
10	k	30/37 (81%)	23 (77%)	7 (23%)	1	0
11	L	35/35 (100%)	35 (100%)	0	100	100
11	l	34/35 (97%)	31 (91%)	3 (9%)	9	6
12	M	28/32 (88%)	27 (96%)	1 (4%)	31	31
12	m	28/32 (88%)	26 (93%)	2 (7%)	13	10
13	O	206/228 (90%)	199 (97%)	7 (3%)	32	33
13	o	207/228 (91%)	199 (96%)	8 (4%)	28	28
14	R	28/32 (88%)	24 (86%)	4 (14%)	3	2
14	r	23/32 (72%)	19 (83%)	4 (17%)	2	1
15	T	26/26 (100%)	24 (92%)	2 (8%)	12	8
15	t	25/26 (96%)	25 (100%)	0	100	100
16	U	84/112 (75%)	81 (96%)	3 (4%)	31	31
16	u	84/112 (75%)	81 (96%)	3 (4%)	31	31
17	V	117/138 (85%)	113 (97%)	4 (3%)	32	33
17	v	117/138 (85%)	111 (95%)	6 (5%)	21	19
18	X	31/34 (91%)	29 (94%)	2 (6%)	15	12
18	x	31/34 (91%)	28 (90%)	3 (10%)	8	5
19	Y	19/37 (51%)	17 (90%)	2 (10%)	6	4
19	y	22/37 (60%)	19 (86%)	3 (14%)	3	2
20	Z	52/52 (100%)	46 (88%)	6 (12%)	5	3
20	z	51/52 (98%)	42 (82%)	9 (18%)	2	1
All	All	4444/4642 (96%)	4273 (96%)	171 (4%)	28	29

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

Mol	Chain	Res	Type
5	e	83	LEU
14	r	3	TRP
7	h	12	ARG

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Mol	Chain	Res	Type
11	l	7	ARG
17	v	2	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
13	o	80	GLN
13	o	155	ASN
13	O	155	ASN
13	O	88	ASN
14	r	30	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
12	FME	m	1	12	8,9,10	1.02	1 (12%)	8,9,11	0.97	0
15	FME	t	1	15	8,9,10	1.54	1 (12%)	8,9,11	0.86	1 (12%)
8	FME	I	1	8	8,9,10	0.95	0	8,9,11	1.06	1 (12%)
15	FME	T	1	15	8,9,10	1.04	1 (12%)	8,9,11	1.46	1 (12%)
8	FME	i	1	8	8,9,10	1.16	1 (12%)	8,9,11	1.10	1 (12%)
12	FME	M	1	12	8,9,10	1.10	1 (12%)	8,9,11	0.97	0

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	-	1/7/9/11	-
15	FME	t	1	15	-	1/7/9/11	-
8	FME	I	1	8	-	1/7/9/11	-
15	FME	T	1	15	-	2/7/9/11	-
8	FME	i	1	8	-	0/7/9/11	-
12	FME	M	1	12	-	0/7/9/11	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	t	1	FME	CA-N	-3.67	1.41	1.46
8	i	1	FME	CA-N	-2.58	1.42	1.46
15	T	1	FME	CA-N	-2.38	1.43	1.46
12	M	1	FME	CA-N	-2.22	1.43	1.46
12	m	1	FME	CA-N	-2.20	1.43	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	T	1	FME	O1-CN-N	-2.64	118.51	125.32
8	i	1	FME	CA-N-CN	-2.13	119.54	122.82
15	t	1	FME	CB-CA-N	2.10	114.35	110.52
8	I	1	FME	C-CA-N	2.01	113.37	109.50

There are no chirality outliers.

All (5) 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	CB-CA-N-CN

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 191 ligands modelled in this entry, 6 are monoatomic - leaving 185 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$
22	CLA	A	402	-	69,73,73	1.27	7 (10%)	82,113,113	1.24	10 (12%)
33	STE	R	101	-	11,11,19	0.98	0	11,11,19	0.93	0
22	CLA	d	403	-	69,73,73	1.29	8 (11%)	82,113,113	1.36	9 (10%)
22	CLA	B	616	-	64,68,73	1.39	7 (10%)	76,107,113	1.48	8 (10%)
22	CLA	B	608	-	69,73,73	1.07	5 (7%)	82,113,113	1.29	10 (12%)
22	CLA	c	512	-	69,73,73	1.12	8 (11%)	82,113,113	1.34	7 (8%)
33	STE	d	412	-	19,19,19	0.81	1 (5%)	19,19,19	1.15	2 (10%)
24	BCR	c	514	-	41,41,41	1.18	3 (7%)	56,56,56	1.34	7 (12%)
24	BCR	a	405	-	41,41,41	1.01	3 (7%)	56,56,56	1.28	5 (8%)
22	CLA	b	614	-	69,73,73	1.26	8 (11%)	82,113,113	1.45	10 (12%)
33	STE	j	101	-	11,11,19	0.98	1 (9%)	11,11,19	1.11	2 (18%)
30	DGD	c	519	-	63,63,67	1.13	3 (4%)	77,77,81	1.38	8 (10%)
27	LMG	M	101	-	51,51,55	1.03	4 (7%)	59,59,63	1.55	9 (15%)
33	STE	M	102	-	14,14,19	0.61	0	14,14,19	1.16	0
22	CLA	B	612	-	69,73,73	1.30	8 (11%)	82,113,113	1.53	12 (14%)
28	LHG	D	409	-	48,48,48	1.14	3 (6%)	51,54,54	1.26	6 (11%)
33	STE	b	622	-	19,19,19	0.62	0	19,19,19	1.01	0
29	SQD	b	620	-	47,49,54	0.98	2 (4%)	57,60,65	1.92	14 (24%)
33	STE	C	521	-	11,11,19	0.80	0	11,11,19	1.22	1 (9%)
30	DGD	H	102	-	63,63,67	1.41	12 (19%)	77,77,81	1.42	9 (11%)
29	SQD	A	414	-	38,38,54	1.03	4 (10%)	40,40,65	1.56	4 (10%)
22	CLA	B	601	36	69,73,73	1.30	8 (11%)	82,113,113	1.47	7 (8%)
34	BCT	a	408	21	3,3,3	1.33	0	2,3,3	3.58	2 (100%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	b	607	36	69,73,73	1.20	8 (11%)	82,113,113	1.18	8 (9%)
22	CLA	c	508	-	68,72,73	1.37	7 (10%)	80,111,113	1.38	10 (12%)
33	STE	b	624	-	15,15,19	0.82	0	15,15,19	1.00	1 (6%)
33	STE	D	412	-	19,19,19	0.55	0	19,19,19	1.34	2 (10%)
22	CLA	B	602	-	69,73,73	1.36	8 (11%)	82,113,113	1.25	10 (12%)
22	CLA	b	606	-	69,73,73	1.72	9 (13%)	82,113,113	1.55	8 (9%)
24	BCR	B	617	-	41,41,41	1.15	4 (9%)	56,56,56	1.30	11 (19%)
22	CLA	d	401	36	69,73,73	1.45	12 (17%)	82,113,113	1.42	11 (13%)
23	PHO	A	405	-	58,69,69	1.95	12 (20%)	55,99,99	1.45	9 (16%)
22	CLA	b	603	-	69,73,73	1.35	7 (10%)	82,113,113	1.37	13 (15%)
33	STE	C	522	-	15,15,19	0.49	0	14,14,19	0.65	0
33	STE	m	102	-	11,11,19	0.79	0	11,11,19	1.24	1 (9%)
22	CLA	A	406	-	58,62,73	1.34	7 (12%)	68,99,113	1.37	9 (13%)
24	BCR	k	101	-	41,41,41	1.10	4 (9%)	56,56,56	1.11	4 (7%)
28	LHG	l	101	-	48,48,48	0.88	1 (2%)	51,54,54	1.31	7 (13%)
22	CLA	b	610	36	69,73,73	1.44	9 (13%)	82,113,113	1.51	12 (14%)
28	LHG	A	412	-	46,46,48	1.18	5 (10%)	49,52,54	1.40	7 (14%)
22	CLA	D	403	36	69,73,73	1.20	8 (11%)	82,113,113	1.29	6 (7%)
24	BCR	B	619	-	41,41,41	1.18	3 (7%)	56,56,56	1.36	5 (8%)
31	OEX	a	417[A]	1,3,36	0,15,15	-	-	-	-	-
33	STE	Z	101	-	7,7,19	0.48	0	6,6,19	0.55	0
22	CLA	b	611	-	69,73,73	1.25	7 (10%)	82,113,113	1.34	10 (12%)
22	CLA	c	501	-	69,73,73	1.15	7 (10%)	82,113,113	1.41	9 (10%)
28	LHG	d	408	-	48,48,48	0.98	1 (2%)	51,54,54	1.21	4 (7%)
22	CLA	b	601	36	69,73,73	1.26	9 (13%)	82,113,113	1.29	5 (6%)
24	BCR	C	516	-	41,41,41	1.20	3 (7%)	56,56,56	1.20	4 (7%)
24	BCR	d	406	-	41,41,41	1.11	2 (4%)	56,56,56	1.31	6 (10%)
33	STE	b	627	-	13,13,19	0.54	0	12,12,19	0.46	0
29	SQD	A	413	-	50,52,54	1.10	7 (14%)	60,63,65	1.98	9 (15%)
22	CLA	a	404	-	69,73,73	1.58	8 (11%)	82,113,113	1.33	11 (13%)
22	CLA	D	402	-	69,73,73	1.15	7 (10%)	82,113,113	1.36	8 (9%)
22	CLA	C	502	-	69,73,73	1.29	9 (13%)	82,113,113	1.35	11 (13%)
22	CLA	B	610	36	69,73,73	1.46	11 (15%)	82,113,113	1.39	9 (10%)
22	CLA	C	511	3	69,73,73	1.48	11 (15%)	82,113,113	1.37	7 (8%)
33	STE	C	523	-	11,11,19	0.63	0	11,11,19	1.42	2 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	DGD	C	518	-	63,63,67	1.22	8 (12%)	77,77,81	1.33	9 (11%)
33	STE	T	102	-	14,14,19	0.49	0	13,13,19	0.65	0
29	SQD	a	411	-	52,54,54	1.02	4 (7%)	62,65,65	1.84	11 (17%)
33	STE	t	103	-	17,17,19	0.63	0	17,17,19	1.12	1 (5%)
27	LMG	c	523	-	49,49,55	0.85	1 (2%)	57,57,63	1.29	6 (10%)
33	STE	M	103	-	9,9,19	0.44	0	8,8,19	0.82	0
29	SQD	B	623	-	52,54,54	0.97	3 (5%)	62,65,65	1.84	14 (22%)
27	LMG	c	522	-	48,48,55	1.06	5 (10%)	56,56,63	1.28	4 (7%)
22	CLA	b	608	-	69,73,73	1.23	7 (10%)	82,113,113	1.26	11 (13%)
24	BCR	A	407	-	41,41,41	1.15	4 (9%)	56,56,56	1.47	11 (19%)
22	CLA	A	403	36	69,73,73	1.33	8 (11%)	82,113,113	1.27	7 (8%)
23	PHO	a	403	-	58,69,69	1.93	10 (17%)	55,99,99	1.59	10 (18%)
27	LMG	D	411	-	26,26,55	0.67	0	26,26,63	1.25	1 (3%)
33	STE	c	521	-	19,19,19	0.66	0	19,19,19	0.94	0
33	STE	d	413	-	19,19,19	0.54	0	19,19,19	1.01	0
22	CLA	b	613	-	69,73,73	1.15	7 (10%)	82,113,113	1.25	5 (6%)
28	LHG	e	101	-	41,41,48	0.95	3 (7%)	44,47,54	1.32	5 (11%)
33	STE	a	414	-	11,11,19	0.89	0	11,11,19	1.07	1 (9%)
22	CLA	B	611	-	69,73,73	1.33	7 (10%)	82,113,113	1.63	9 (10%)
33	STE	b	626	-	9,9,19	0.51	0	8,8,19	0.55	0
22	CLA	C	504	36	63,67,73	1.18	6 (9%)	74,105,113	1.33	10 (13%)
24	BCR	c	516	-	41,41,41	1.14	3 (7%)	56,56,56	1.17	3 (5%)
24	BCR	b	619	-	41,41,41	1.06	2 (4%)	56,56,56	1.30	6 (10%)
27	LMG	C	520	-	48,48,55	0.86	3 (6%)	56,56,63	1.36	8 (14%)
30	DGD	c	517	-	63,63,67	1.21	9 (14%)	77,77,81	1.42	15 (19%)
24	BCR	x	101	-	41,41,41	1.08	2 (4%)	56,56,56	1.27	8 (14%)
33	STE	a	413	-	9,9,19	0.56	0	8,8,19	0.53	0
22	CLA	B	604	-	69,73,73	1.26	6 (8%)	82,113,113	1.56	6 (7%)
28	LHG	B	621	-	48,48,48	0.92	2 (4%)	51,54,54	1.14	2 (3%)
35	HEC	f	101	6,5	46,50,50	1.85	6 (13%)	58,82,82	2.14	7 (12%)
22	CLA	c	505	-	69,73,73	1.28	11 (15%)	82,113,113	1.30	8 (9%)
22	CLA	B	609	-	69,73,73	1.51	9 (13%)	82,113,113	1.43	11 (13%)
22	CLA	c	502	-	69,73,73	1.19	7 (10%)	82,113,113	1.30	8 (9%)
28	LHG	B	622	-	48,48,48	0.92	3 (6%)	51,54,54	1.29	5 (9%)
29	SQD	D	408	-	34,36,54	1.00	3 (8%)	42,45,65	2.17	10 (23%)
22	CLA	C	505	-	69,73,73	1.27	8 (11%)	82,113,113	1.30	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	STE	k	102	-	11,11,19	0.82	0	11,11,19	1.12	1 (9%)
33	STE	t	102	-	13,13,19	0.73	0	13,13,19	1.34	2 (15%)
27	LMG	b	623	-	55,55,55	1.00	2 (3%)	63,63,63	1.50	8 (12%)
33	STE	b	621	-	15,15,19	0.42	0	14,14,19	0.80	0
26	PL9	a	409	-	55,55,55	1.13	5 (9%)	68,69,69	1.63	13 (19%)
24	BCR	C	515	-	41,41,41	1.20	4 (9%)	56,56,56	1.32	9 (16%)
33	STE	B	625	-	15,15,19	0.48	0	14,14,19	0.62	0
33	STE	B	626	-	11,11,19	0.98	0	11,11,19	0.85	0
22	CLA	C	513	-	69,73,73	1.15	5 (7%)	82,113,113	1.41	6 (7%)
27	LMG	D	410	-	31,31,55	1.14	3 (9%)	33,33,63	1.12	2 (6%)
22	CLA	d	404	36	69,73,73	1.82	11 (15%)	82,113,113	1.46	11 (13%)
22	CLA	b	616	-	64,68,73	1.16	7 (10%)	76,107,113	1.39	8 (10%)
33	STE	I	101	-	14,14,19	0.58	0	13,13,19	0.53	0
22	CLA	C	509	-	69,73,73	1.25	8 (11%)	82,113,113	1.46	9 (10%)
31	OEX	A	416[A]	1,3,36	0,15,15	-	-	-	-	-
30	DGD	A	415	-	67,67,67	1.39	11 (16%)	81,81,81	1.34	9 (11%)
30	DGD	c	518	-	63,63,67	1.24	10 (15%)	77,77,81	1.38	9 (11%)
22	CLA	c	511	3	69,73,73	1.47	10 (14%)	82,113,113	1.29	7 (8%)
22	CLA	C	506	-	69,73,73	1.56	9 (13%)	82,113,113	1.18	6 (7%)
22	CLA	B	613	-	69,73,73	1.32	9 (13%)	82,113,113	1.07	6 (7%)
35	HEC	V	201	17	46,50,50	1.83	5 (10%)	58,82,82	2.01	5 (8%)
26	PL9	D	406	-	55,55,55	1.61	8 (14%)	68,69,69	1.72	16 (23%)
28	LHG	d	409	-	38,38,48	1.04	2 (5%)	41,44,54	1.18	4 (9%)
22	CLA	C	507	36	69,73,73	1.21	8 (11%)	82,113,113	1.57	10 (12%)
22	CLA	B	605	-	69,73,73	1.24	7 (10%)	82,113,113	1.39	10 (12%)
27	LMG	A	411	-	48,48,55	1.10	5 (10%)	56,56,63	1.34	7 (12%)
33	STE	B	620	-	16,16,19	0.77	0	16,16,19	1.00	0
34	BCT	D	401	21	3,3,3	0.95	0	2,3,3	3.63	2 (100%)
27	LMG	D	407	-	51,51,55	0.99	5 (9%)	59,59,63	1.25	4 (6%)
32	OXY	A	417[B]	1,3,36	0,16,16	-	-	-	-	-
24	BCR	c	515	-	41,41,41	1.27	4 (9%)	56,56,56	1.44	9 (16%)
30	DGD	C	517	-	63,63,67	1.30	10 (15%)	77,77,81	1.41	11 (14%)
30	DGD	C	519	-	63,63,67	1.23	6 (9%)	77,77,81	1.33	8 (10%)
22	CLA	b	615	-	69,73,73	1.65	10 (14%)	82,113,113	1.58	11 (13%)
22	CLA	C	503	-	69,73,73	1.30	7 (10%)	82,113,113	1.76	11 (13%)
24	BCR	b	618	-	41,41,41	1.21	3 (7%)	56,56,56	1.27	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	BCR	b	617	-	41,41,41	1.12	3 (7%)	56,56,56	1.50	9 (16%)
22	CLA	c	509	-	69,73,73	1.27	7 (10%)	82,113,113	1.47	7 (8%)
22	CLA	d	405	-	69,73,73	1.37	10 (14%)	82,113,113	1.21	9 (10%)
22	CLA	b	604	-	69,73,73	1.19	6 (8%)	82,113,113	1.56	16 (19%)
33	STE	B	624	-	11,11,19	0.83	0	11,11,19	1.31	1 (9%)
22	CLA	B	606	-	69,73,73	1.36	11 (15%)	82,113,113	1.46	13 (15%)
24	BCR	Y	101	-	41,41,41	1.13	2 (4%)	56,56,56	1.39	8 (14%)
30	DGD	h	101	-	63,63,67	1.18	7 (11%)	77,77,81	1.37	9 (11%)
24	BCR	B	618	-	41,41,41	1.16	2 (4%)	56,56,56	1.33	9 (16%)
22	CLA	C	501	-	69,73,73	1.38	9 (13%)	82,113,113	1.40	6 (7%)
22	CLA	C	510	-	69,73,73	1.16	10 (14%)	82,113,113	1.39	7 (8%)
32	OEY	a	418[B]	1,3,36	0,16,16	-	-	-	-	-
33	STE	H	103	-	17,17,19	0.51	0	16,16,19	0.69	0
22	CLA	b	612	-	69,73,73	1.62	10 (14%)	82,113,113	1.32	9 (10%)
28	LHG	E	101	-	48,48,48	0.92	2 (4%)	51,54,54	1.27	5 (9%)
22	CLA	D	404	-	69,73,73	1.69	11 (15%)	82,113,113	1.16	4 (4%)
22	CLA	b	609	-	69,73,73	1.34	8 (11%)	82,113,113	1.51	11 (13%)
22	CLA	c	504	36	64,68,73	1.22	7 (10%)	76,107,113	1.29	10 (13%)
24	BCR	t	101	-	41,41,41	1.11	4 (9%)	56,56,56	1.44	12 (21%)
24	BCR	D	405	-	41,41,41	1.22	3 (7%)	56,56,56	1.39	10 (17%)
22	CLA	c	506	-	69,73,73	1.55	9 (13%)	82,113,113	1.33	9 (10%)
22	CLA	B	607	36	69,73,73	1.13	7 (10%)	82,113,113	1.29	8 (9%)
22	CLA	c	510	-	69,73,73	1.41	8 (11%)	82,113,113	1.35	9 (10%)
22	CLA	B	614	-	69,73,73	1.06	5 (7%)	82,113,113	1.31	9 (10%)
27	LMG	d	410	-	44,44,55	1.12	3 (6%)	52,52,63	1.30	7 (13%)
23	PHO	d	402	-	58,69,69	2.11	9 (15%)	55,99,99	1.73	10 (18%)
33	STE	J	101	-	11,11,19	0.66	0	11,11,19	1.36	2 (18%)
26	PL9	d	407	-	55,55,55	1.60	10 (18%)	68,69,69	1.85	15 (22%)
33	STE	l	102	-	17,17,19	0.38	0	16,16,19	0.91	0
35	HEC	F	101	6,5	46,50,50	1.87	6 (13%)	58,82,82	2.01	10 (17%)
23	PHO	A	404	-	58,69,69	1.82	12 (20%)	55,99,99	1.74	12 (21%)
22	CLA	C	512	-	69,73,73	1.20	6 (8%)	82,113,113	1.32	11 (13%)
22	CLA	C	508	-	69,73,73	1.50	10 (14%)	82,113,113	1.51	11 (13%)
22	CLA	c	503	-	69,73,73	1.23	9 (13%)	82,113,113	1.27	6 (7%)
29	SQD	f	102	-	39,41,54	1.08	3 (7%)	49,52,65	2.00	11 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	b	602	-	69,73,73	1.10	7 (10%)	82,113,113	1.45	12 (14%)
24	BCR	C	514	-	41,41,41	1.19	3 (7%)	56,56,56	1.41	10 (17%)
27	LMG	a	416	-	55,55,55	1.06	2 (3%)	63,63,63	1.36	7 (11%)
22	CLA	b	605	-	69,73,73	1.20	8 (11%)	82,113,113	1.51	15 (18%)
33	STE	b	625	-	19,19,19	0.73	0	19,19,19	0.82	0
22	CLA	B	603	-	69,73,73	1.28	10 (14%)	82,113,113	1.60	11 (13%)
24	BCR	H	101	-	41,41,41	1.06	1 (2%)	56,56,56	1.35	8 (14%)
28	LHG	a	410	-	48,48,48	0.91	2 (4%)	51,54,54	1.50	8 (15%)
27	LMG	c	520	-	37,37,55	1.22	5 (13%)	45,45,63	1.36	8 (17%)
26	PL9	A	410	-	55,55,55	1.24	6 (10%)	68,69,69	1.42	12 (17%)
33	STE	a	415	-	14,14,19	0.40	0	13,13,19	0.73	0
22	CLA	c	513	-	69,73,73	1.27	10 (14%)	82,113,113	1.18	5 (6%)
27	LMG	m	101	-	51,51,55	0.95	2 (3%)	59,59,63	1.48	8 (13%)
22	CLA	c	507	36	69,73,73	1.16	6 (8%)	82,113,113	1.40	12 (14%)
29	SQD	a	412	-	35,35,54	1.11	2 (5%)	37,37,65	1.63	5 (13%)
24	BCR	T	101	-	41,41,41	1.09	3 (7%)	56,56,56	1.41	7 (12%)
22	CLA	a	402	-	69,73,73	1.37	10 (14%)	82,113,113	1.40	9 (10%)
35	HEC	v	201	17	46,50,50	1.92	4 (8%)	58,82,82	1.98	7 (12%)
33	STE	d	411	-	16,16,19	0.63	0	16,16,19	1.43	3 (18%)
22	CLA	B	615	-	69,73,73	1.26	9 (13%)	82,113,113	1.28	9 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	A	402	-	1/1/20/20	5/39/115/115	-
33	STE	R	101	-	-	4/9/9/17	-
22	CLA	d	403	-	1/1/20/20	6/39/115/115	-
22	CLA	B	616	-	1/1/19/20	7/33/109/115	-
22	CLA	B	608	-	-	1/39/115/115	-
22	CLA	c	512	-	1/1/20/20	20/39/115/115	-
33	STE	d	412	-	-	8/17/17/17	-
24	BCR	c	514	-	-	15/29/63/63	0/2/2/2
24	BCR	a	405	-	-	1/29/63/63	0/2/2/2
22	CLA	b	614	-	1/1/20/20	11/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	STE	j	101	-	-	3/9/9/17	-
30	DGD	c	519	-	-	13/51/91/95	0/2/2/2
27	LMG	M	101	-	-	23/46/66/70	0/1/1/1
33	STE	M	102	-	-	5/12/12/17	-
22	CLA	B	612	-	1/1/20/20	6/39/115/115	-
28	LHG	D	409	-	-	20/53/53/53	-
33	STE	b	622	-	-	8/17/17/17	-
29	SQD	b	620	-	-	21/44/64/69	0/1/1/1
33	STE	C	521	-	-	7/9/9/17	-
30	DGD	H	102	-	-	16/51/91/95	0/2/2/2
29	SQD	A	414	-	-	21/39/39/69	-
22	CLA	B	601	36	1/1/20/20	13/39/115/115	-
22	CLA	b	607	36	1/1/20/20	13/39/115/115	-
22	CLA	c	508	-	-	9/38/114/115	-
33	STE	b	624	-	-	7/13/13/17	-
33	STE	D	412	-	-	9/17/17/17	-
22	CLA	B	602	-	1/1/20/20	5/39/115/115	-
22	CLA	b	606	-	1/1/20/20	5/39/115/115	-
24	BCR	B	617	-	-	8/29/63/63	0/2/2/2
22	CLA	d	401	36	-	12/39/115/115	-
23	PHO	A	405	-	-	2/37/103/103	0/5/6/6
22	CLA	b	603	-	1/1/20/20	5/39/115/115	-
33	STE	C	522	-	-	5/13/13/17	-
33	STE	m	102	-	-	4/9/9/17	-
22	CLA	A	406	-	1/1/17/20	3/26/102/115	-
24	BCR	k	101	-	-	10/29/63/63	0/2/2/2
28	LHG	l	101	-	-	15/53/53/53	-
22	CLA	b	610	36	1/1/20/20	5/39/115/115	-
28	LHG	A	412	-	-	18/51/51/53	-
22	CLA	D	403	36	-	5/39/115/115	-
24	BCR	B	619	-	-	4/29/63/63	0/2/2/2
33	STE	Z	101	-	-	2/5/5/17	-
22	CLA	b	611	-	1/1/20/20	6/39/115/115	-
22	CLA	c	501	-	1/1/20/20	2/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	LHG	d	408	-	-	18/53/53/53	-
22	CLA	b	601	36	1/1/20/20	14/39/115/115	-
24	BCR	C	516	-	-	9/29/63/63	0/2/2/2
24	BCR	d	406	-	-	8/29/63/63	0/2/2/2
33	STE	b	627	-	-	5/11/11/17	-
29	SQD	A	413	-	-	14/47/67/69	0/1/1/1
22	CLA	a	404	-	1/1/20/20	8/39/115/115	-
22	CLA	D	402	-	1/1/20/20	6/39/115/115	-
22	CLA	C	511	3	1/1/20/20	4/39/115/115	-
22	CLA	B	610	36	1/1/20/20	5/39/115/115	-
22	CLA	C	502	-	-	5/39/115/115	-
33	STE	C	523	-	-	3/9/9/17	-
30	DGD	C	518	-	-	22/51/91/95	0/2/2/2
33	STE	T	102	-	-	11/12/12/17	-
29	SQD	a	411	-	-	23/49/69/69	0/1/1/1
33	STE	t	103	-	-	8/15/15/17	-
27	LMG	c	523	-	-	20/44/64/70	0/1/1/1
33	STE	M	103	-	-	2/7/7/17	-
29	SQD	B	623	-	-	24/49/69/69	0/1/1/1
27	LMG	c	522	-	-	24/43/63/70	0/1/1/1
22	CLA	b	608	-	-	1/39/115/115	-
24	BCR	A	407	-	-	8/29/63/63	0/2/2/2
22	CLA	A	403	36	1/1/20/20	9/39/115/115	-
23	PHO	a	403	-	-	1/37/103/103	0/5/6/6
27	LMG	D	411	-	-	7/22/22/70	-
33	STE	c	521	-	-	7/17/17/17	-
33	STE	d	413	-	-	8/17/17/17	-
22	CLA	b	613	-	1/1/20/20	9/39/115/115	-
28	LHG	e	101	-	-	29/46/46/53	-
33	STE	a	414	-	-	3/9/9/17	-
22	CLA	B	611	-	1/1/20/20	9/39/115/115	-
33	STE	b	626	-	-	4/7/7/17	-
22	CLA	C	504	36	1/1/18/20	6/32/108/115	-
24	BCR	c	516	-	-	3/29/63/63	0/2/2/2
24	BCR	b	619	-	-	0/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	LMG	C	520	-	-	12/43/63/70	0/1/1/1
30	DGD	c	517	-	-	28/51/91/95	0/2/2/2
24	BCR	x	101	-	-	5/29/63/63	0/2/2/2
33	STE	a	413	-	-	3/7/7/17	-
22	CLA	B	604	-	1/1/20/20	7/39/115/115	-
28	LHG	B	621	-	-	25/53/53/53	-
35	HEC	f	101	6,5	-	5/14/54/54	-
22	CLA	c	505	-	1/1/20/20	10/39/115/115	-
22	CLA	B	609	-	-	5/39/115/115	-
22	CLA	c	502	-	-	4/39/115/115	-
28	LHG	B	622	-	-	18/53/53/53	-
29	SQD	D	408	-	-	12/28/48/69	0/1/1/1
22	CLA	C	505	-	1/1/20/20	11/39/115/115	-
33	STE	k	102	-	-	6/9/9/17	-
33	STE	t	102	-	-	3/11/11/17	-
27	LMG	b	623	-	-	21/50/70/70	0/1/1/1
33	STE	b	621	-	-	8/13/13/17	-
26	PL9	a	409	-	-	27/53/73/73	0/1/1/1
24	BCR	C	515	-	-	5/29/63/63	0/2/2/2
33	STE	B	625	-	-	9/13/13/17	-
33	STE	B	626	-	-	5/9/9/17	-
22	CLA	C	513	-	-	8/39/115/115	-
27	LMG	D	410	-	-	15/33/33/70	-
22	CLA	d	404	36	1/1/20/20	2/39/115/115	-
22	CLA	b	616	-	1/1/19/20	7/33/109/115	-
33	STE	I	101	-	-	3/12/12/17	-
22	CLA	C	509	-	1/1/20/20	11/39/115/115	-
30	DGD	A	415	-	-	20/55/95/95	0/2/2/2
30	DGD	c	518	-	-	18/51/91/95	0/2/2/2
22	CLA	c	511	3	1/1/20/20	11/39/115/115	-
22	CLA	C	506	-	1/1/20/20	8/39/115/115	-
22	CLA	B	613	-	1/1/20/20	10/39/115/115	-
35	HEC	V	201	17	-	6/14/54/54	-
26	PL9	D	406	-	-	9/53/73/73	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	LHG	d	409	-	-	13/43/43/53	-
22	CLA	C	507	36	1/1/20/20	10/39/115/115	-
22	CLA	B	605	-	1/1/20/20	9/39/115/115	-
27	LMG	A	411	-	-	21/43/63/70	0/1/1/1
33	STE	B	620	-	-	5/14/14/17	-
27	LMG	D	407	-	-	15/46/66/70	0/1/1/1
24	BCR	c	515	-	-	5/29/63/63	0/2/2/2
30	DGD	C	517	-	-	24/51/91/95	0/2/2/2
30	DGD	C	519	-	-	11/51/91/95	0/2/2/2
22	CLA	b	615	-	1/1/20/20	7/39/115/115	-
22	CLA	C	503	-	1/1/20/20	3/39/115/115	-
24	BCR	b	618	-	-	6/29/63/63	0/2/2/2
24	BCR	b	617	-	-	7/29/63/63	0/2/2/2
22	CLA	c	509	-	1/1/20/20	9/39/115/115	-
22	CLA	d	405	-	1/1/20/20	11/39/115/115	-
22	CLA	b	604	-	1/1/20/20	7/39/115/115	-
33	STE	B	624	-	-	3/9/9/17	-
22	CLA	B	606	-	1/1/20/20	9/39/115/115	-
24	BCR	Y	101	-	-	6/29/63/63	0/2/2/2
30	DGD	h	101	-	-	19/51/91/95	0/2/2/2
24	BCR	B	618	-	-	2/29/63/63	0/2/2/2
22	CLA	C	501	-	1/1/20/20	3/39/115/115	-
22	CLA	C	510	-	1/1/20/20	8/39/115/115	-
33	STE	H	103	-	-	10/15/15/17	-
22	CLA	b	612	-	1/1/20/20	3/39/115/115	-
28	LHG	E	101	-	-	23/53/53/53	-
22	CLA	D	404	-	-	9/39/115/115	-
22	CLA	b	609	-	1/1/20/20	8/39/115/115	-
22	CLA	c	504	36	1/1/19/20	7/33/109/115	-
24	BCR	t	101	-	-	6/29/63/63	0/2/2/2
24	BCR	D	405	-	-	6/29/63/63	0/2/2/2
22	CLA	c	506	-	1/1/20/20	16/39/115/115	-
22	CLA	B	607	36	1/1/20/20	4/39/115/115	-
22	CLA	c	510	-	1/1/20/20	10/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	B	614	-	1/1/20/20	15/39/115/115	-
27	LMG	d	410	-	-	10/39/59/70	0/1/1/1
23	PHO	d	402	-	-	0/37/103/103	0/5/6/6
33	STE	J	101	-	-	6/9/9/17	-
26	PL9	d	407	-	-	12/53/73/73	0/1/1/1
33	STE	l	102	-	-	9/15/15/17	-
35	HEC	F	101	6,5	-	6/14/54/54	-
23	PHO	A	404	-	-	0/37/103/103	0/5/6/6
22	CLA	C	512	-	1/1/20/20	13/39/115/115	-
22	CLA	C	508	-	-	8/39/115/115	-
22	CLA	c	503	-	1/1/20/20	6/39/115/115	-
29	SQD	f	102	-	-	11/36/56/69	0/1/1/1
22	CLA	b	602	-	-	3/39/115/115	-
24	BCR	C	514	-	-	10/29/63/63	0/2/2/2
27	LMG	a	416	-	-	30/50/70/70	0/1/1/1
22	CLA	b	605	-	1/1/20/20	5/39/115/115	-
33	STE	b	625	-	-	9/17/17/17	-
22	CLA	B	603	-	1/1/20/20	5/39/115/115	-
24	BCR	H	101	-	-	6/29/63/63	0/2/2/2
28	LHG	a	410	-	-	23/53/53/53	-
27	LMG	c	520	-	-	11/31/51/70	0/1/1/1
26	PL9	A	410	-	-	25/53/73/73	0/1/1/1
33	STE	a	415	-	-	6/12/12/17	-
22	CLA	c	513	-	-	6/39/115/115	-
27	LMG	m	101	-	-	24/46/66/70	0/1/1/1
22	CLA	c	507	36	1/1/20/20	6/39/115/115	-
29	SQD	a	412	-	-	17/37/37/69	-
24	BCR	T	101	-	-	7/29/63/63	0/2/2/2
22	CLA	a	402	-	1/1/20/20	6/39/115/115	-
35	HEC	v	201	17	-	6/14/54/54	-
33	STE	d	411	-	-	5/14/14/17	-
22	CLA	B	615	-	1/1/20/20	9/39/115/115	-

The worst 5 of 901 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	402	PHO	C1B-C2B	9.62	1.50	1.39
22	D	404	CLA	MG-NB	-9.28	1.87	2.05
22	b	606	CLA	MG-NA	9.01	2.27	2.06
23	a	403	PHO	C1B-C2B	8.94	1.49	1.39
23	d	402	PHO	C3B-C4B	8.35	1.49	1.41

The worst 5 of 1254 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	503	CLA	C4A-NA-C1A	10.48	111.46	106.68
35	V	201	HEC	CBB-CAB-C3B	-10.07	107.30	127.43
35	f	101	HEC	CBC-CAC-C3C	-9.90	107.64	127.43
35	F	101	HEC	CBC-CAC-C3C	-9.59	108.27	127.43
22	B	604	CLA	C4A-NA-C1A	9.39	110.97	106.68

5 of 57 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	A	402	CLA	ND
22	A	403	CLA	ND
22	A	406	CLA	ND
22	B	601	CLA	ND
22	B	602	CLA	ND

5 of 1712 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	B	601	CLA	C1A-C2A-CAA-CBA
22	B	606	CLA	C2B-C3B-CAB-CBB
22	B	606	CLA	C4B-C3B-CAB-CBB
22	B	614	CLA	CAD-CBD-CGD-O1D
22	B	614	CLA	CAD-CBD-CGD-O2D

There are no ring outliers.

99 monomers are involved in 179 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A	402	CLA	1	0
22	d	403	CLA	2	0
22	B	616	CLA	1	0
22	c	512	CLA	2	0
33	d	412	STE	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	c	514	BCR	1	0
24	a	405	BCR	1	0
22	b	614	CLA	1	0
33	M	102	STE	1	0
22	B	612	CLA	1	0
33	b	622	STE	2	0
29	b	620	SQD	1	0
29	A	414	SQD	1	0
22	B	601	CLA	1	0
22	c	508	CLA	3	0
33	D	412	STE	3	0
22	B	602	CLA	1	0
22	b	606	CLA	4	0
23	A	405	PHO	1	0
22	b	610	CLA	1	0
22	D	403	CLA	3	0
24	B	619	BCR	4	0
22	b	611	CLA	1	0
22	c	501	CLA	2	0
24	d	406	BCR	7	0
33	b	627	STE	2	0
22	a	404	CLA	1	0
22	B	610	CLA	3	0
30	C	518	DGD	1	0
33	T	102	STE	1	0
33	t	103	STE	1	0
27	c	523	LMG	1	0
29	B	623	SQD	2	0
27	c	522	LMG	2	0
22	b	608	CLA	1	0
24	A	407	BCR	1	0
23	a	403	PHO	1	0
33	d	413	STE	2	0
24	c	516	BCR	1	0
24	b	619	BCR	1	0
30	c	517	DGD	1	0
22	B	604	CLA	5	0
35	f	101	HEC	5	0
28	B	622	LHG	1	0
22	C	505	CLA	2	0
33	t	102	STE	1	0
27	b	623	LMG	2	0

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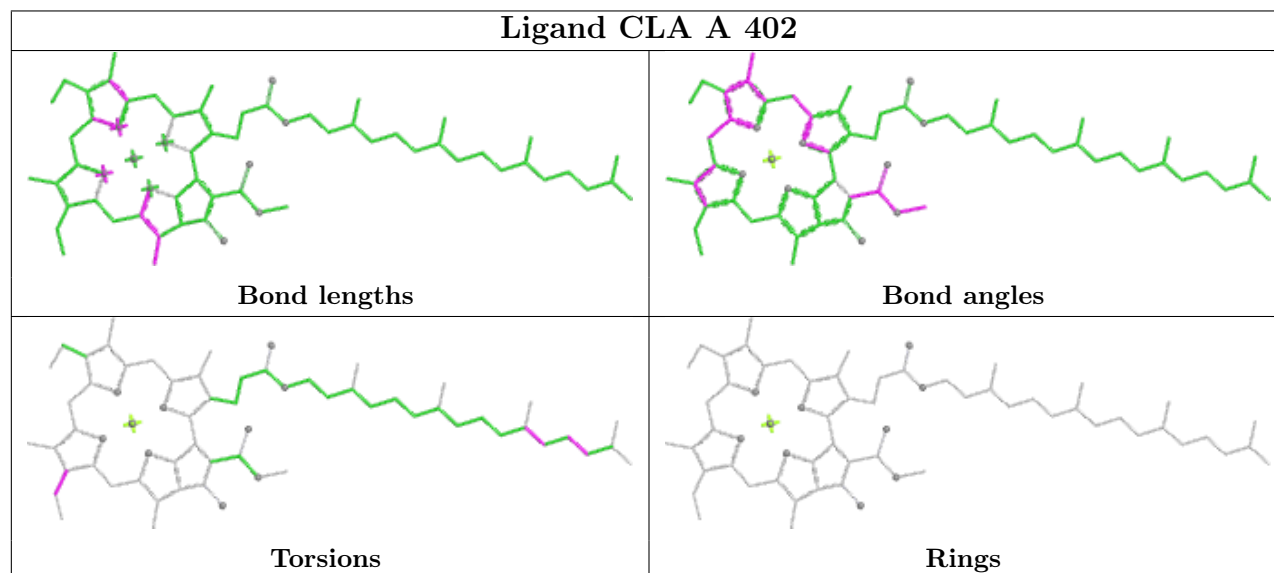
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26	a	409	PL9	4	0
24	C	515	BCR	2	0
22	C	513	CLA	4	0
22	d	404	CLA	1	0
22	b	616	CLA	1	0
22	C	509	CLA	5	0
30	A	415	DGD	1	0
22	c	511	CLA	2	0
22	C	506	CLA	1	0
22	B	613	CLA	1	0
35	V	201	HEC	2	0
22	B	605	CLA	3	0
33	B	620	STE	1	0
32	A	417[B]	OEY	1	0
22	b	615	CLA	3	0
22	C	503	CLA	1	0
24	b	618	BCR	4	0
22	c	509	CLA	1	0
22	b	604	CLA	4	0
33	B	624	STE	2	0
22	B	606	CLA	2	0
24	Y	101	BCR	2	0
30	h	101	DGD	1	0
24	B	618	BCR	5	0
22	C	501	CLA	1	0
32	a	418[B]	OEY	1	0
22	b	612	CLA	1	0
28	E	101	LHG	3	0
22	D	404	CLA	2	0
22	b	609	CLA	2	0
22	c	504	CLA	4	0
24	t	101	BCR	4	0
24	D	405	BCR	2	0
22	c	506	CLA	1	0
22	B	607	CLA	2	0
23	d	402	PHO	2	0
35	F	101	HEC	5	0
29	f	102	SQD	1	0
22	b	602	CLA	1	0
24	C	514	BCR	2	0
22	b	605	CLA	2	0

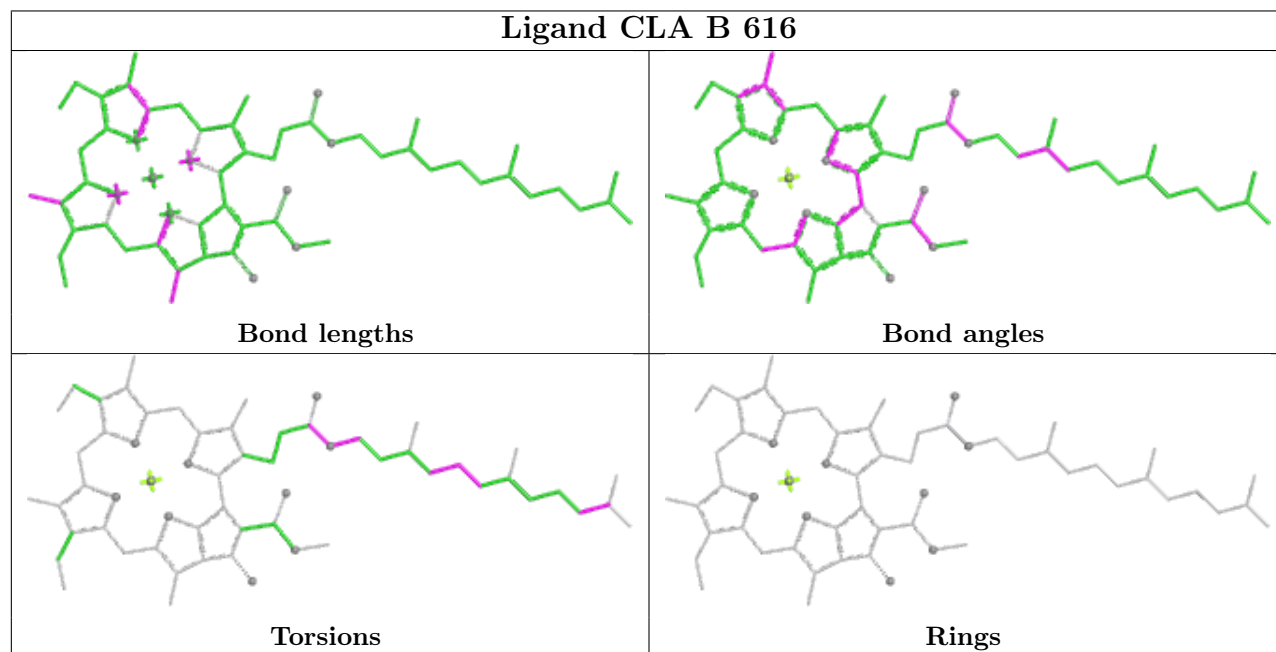
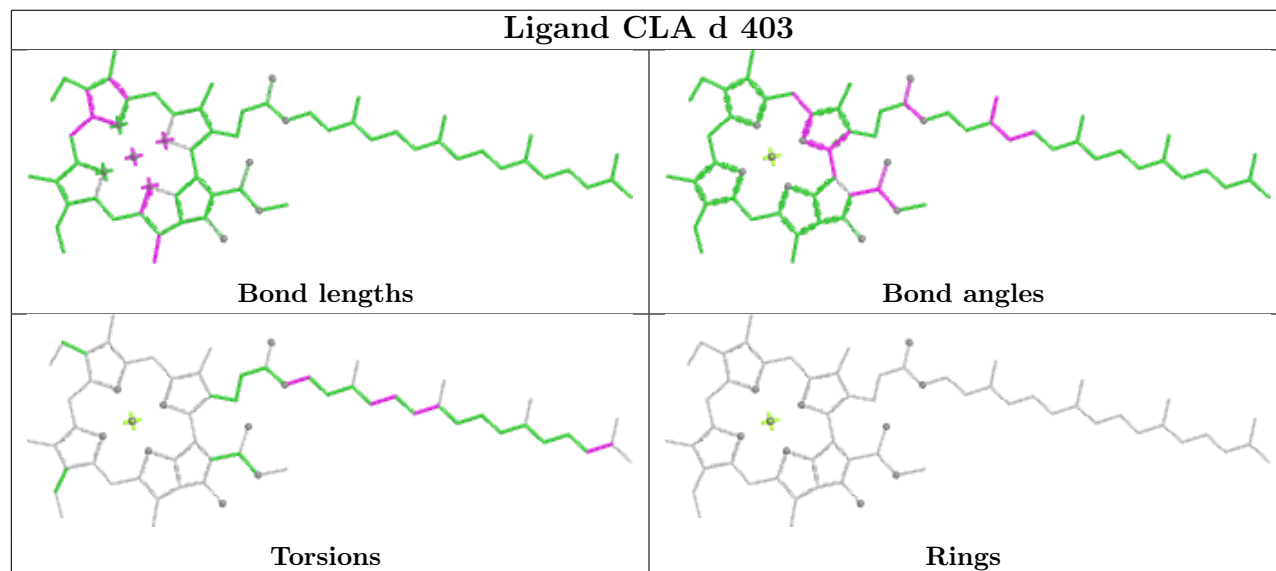
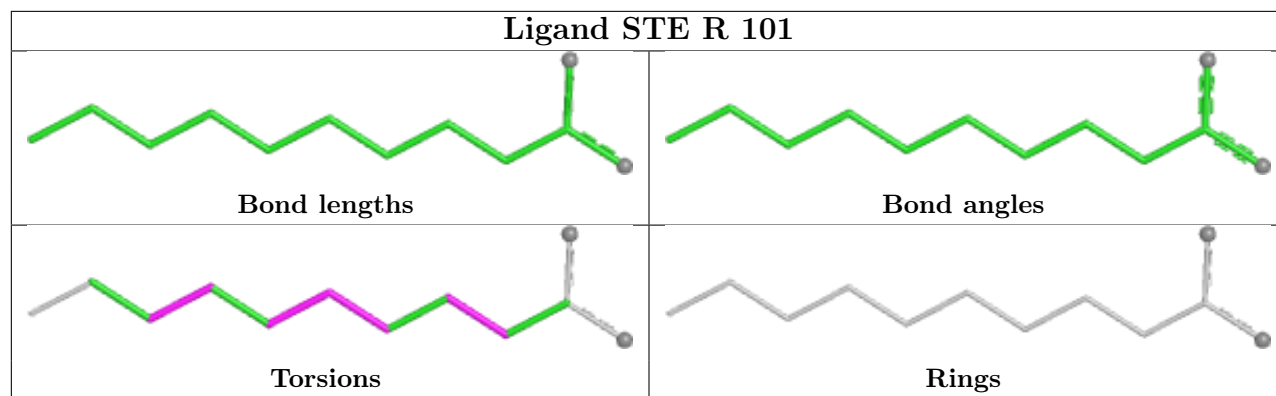
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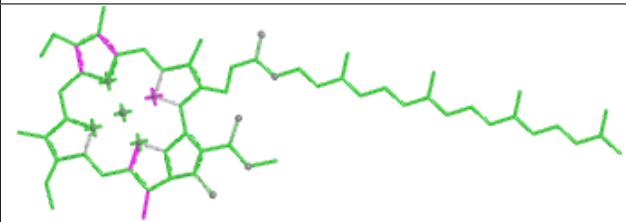
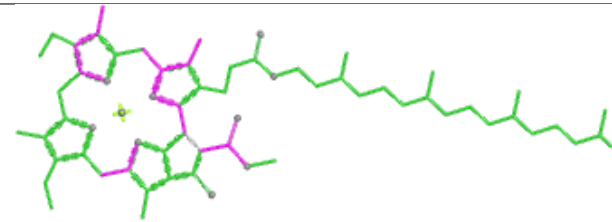
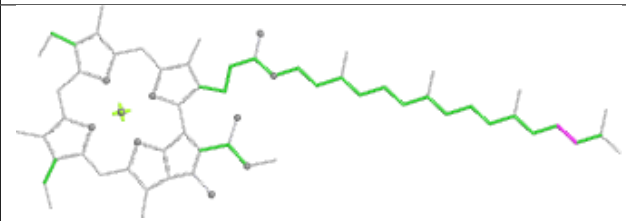
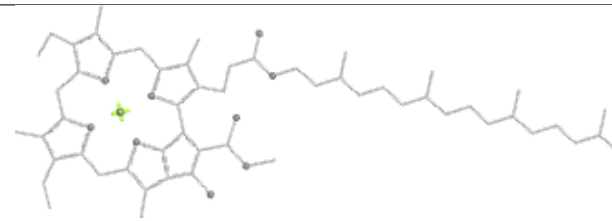
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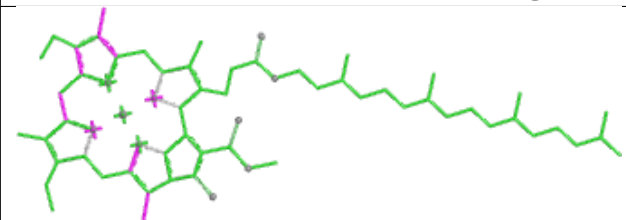
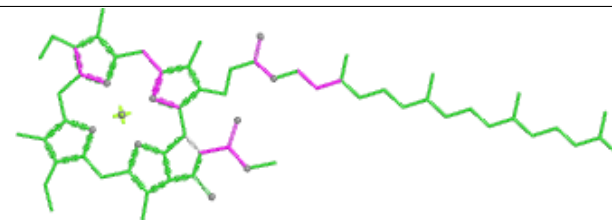
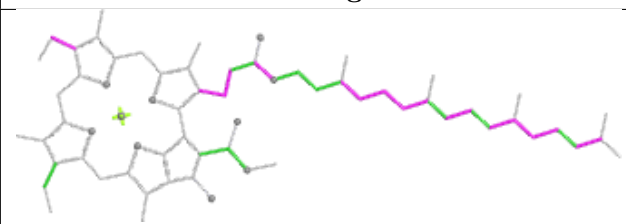
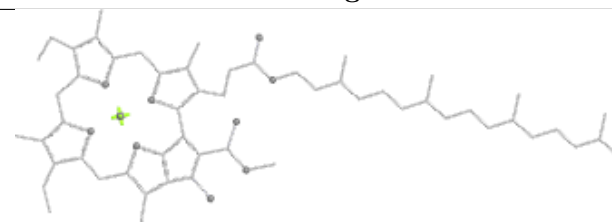
Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	H	101	BCR	4	0
28	a	410	LHG	1	0
26	A	410	PL9	8	0
22	c	513	CLA	2	0
27	m	101	LMG	2	0
22	c	507	CLA	2	0
29	a	412	SQD	3	0
24	T	101	BCR	4	0
35	v	201	HEC	3	0
33	d	411	STE	1	0

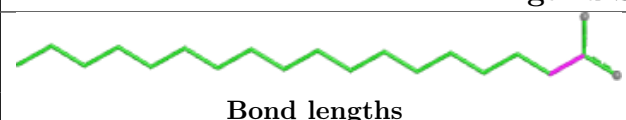
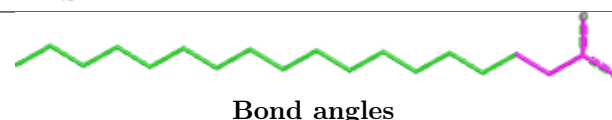
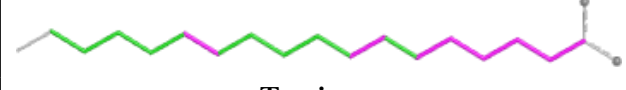
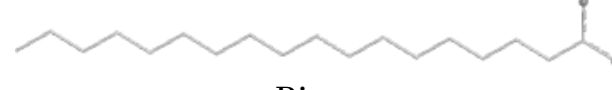
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

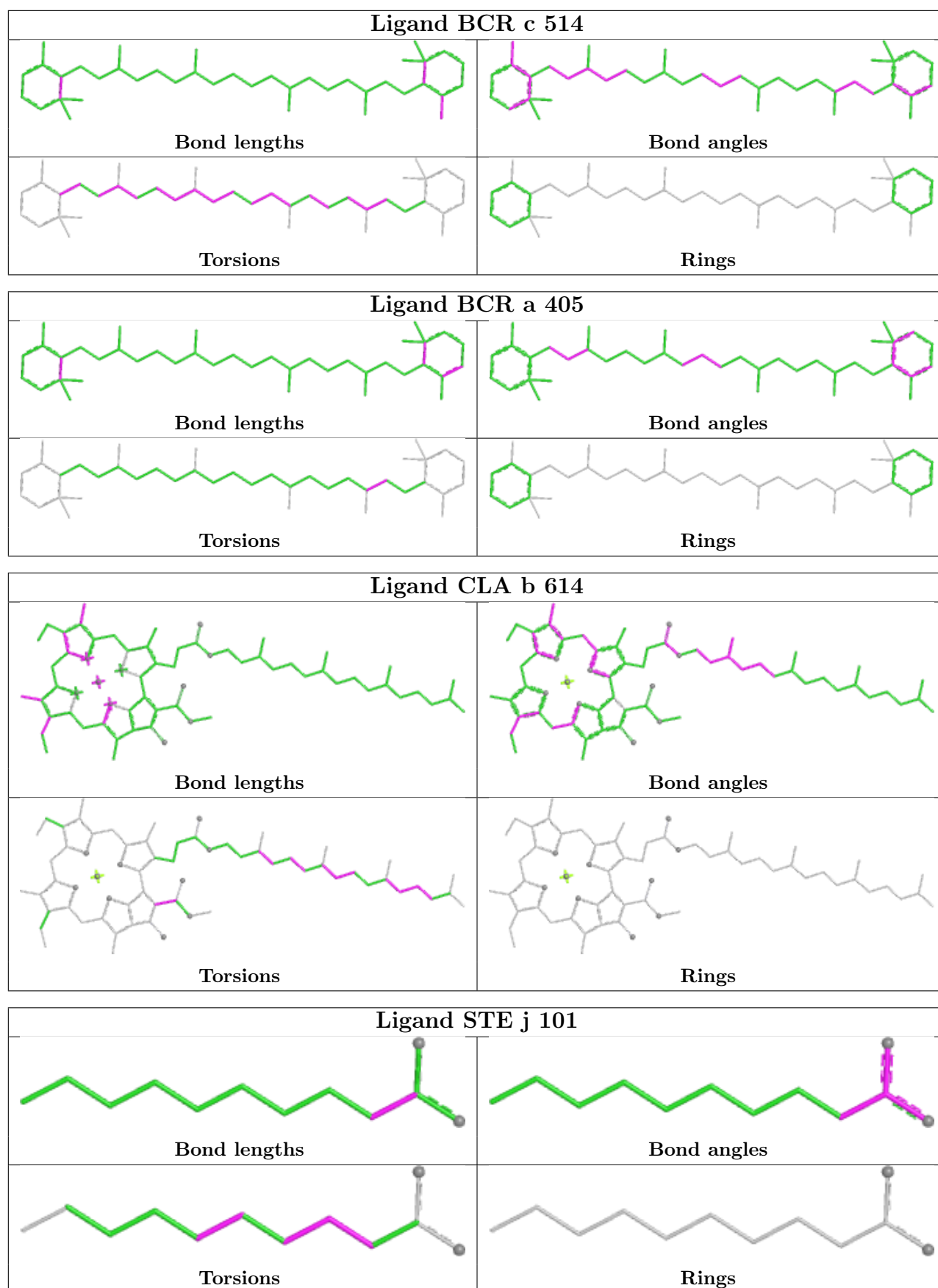


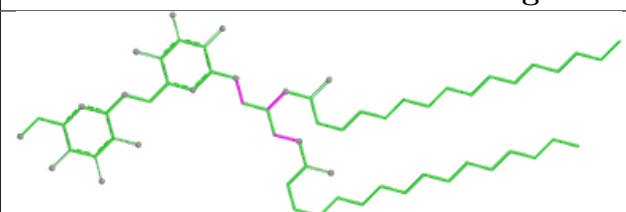
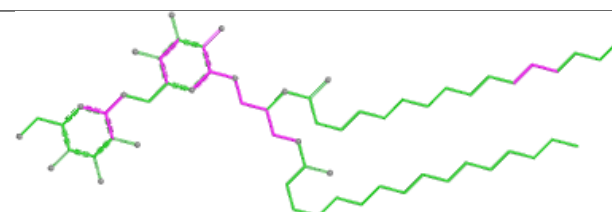
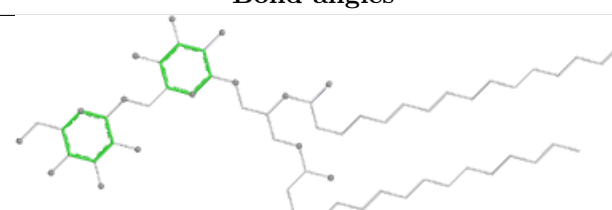


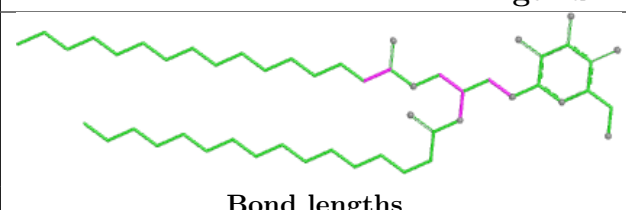
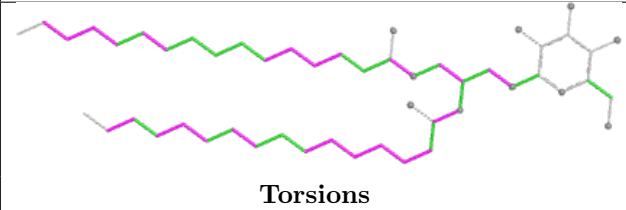
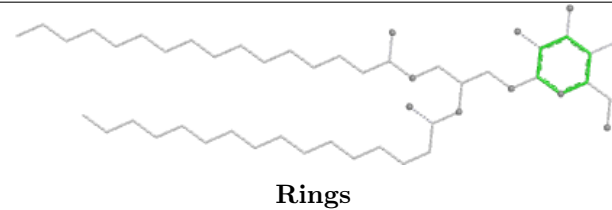
Ligand CLA B 608	
	
Bond lengths	Bond angles
	
Torsions	Rings

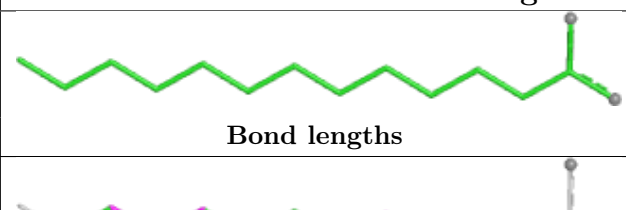
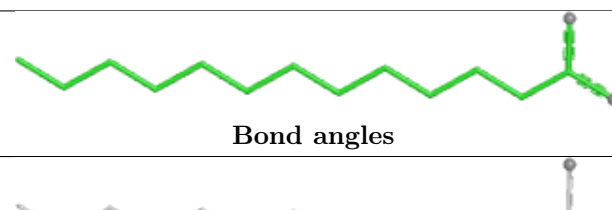
Ligand CLA c 512	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand STE d 412	
	
Bond lengths	Bond angles
	
Torsions	Rings

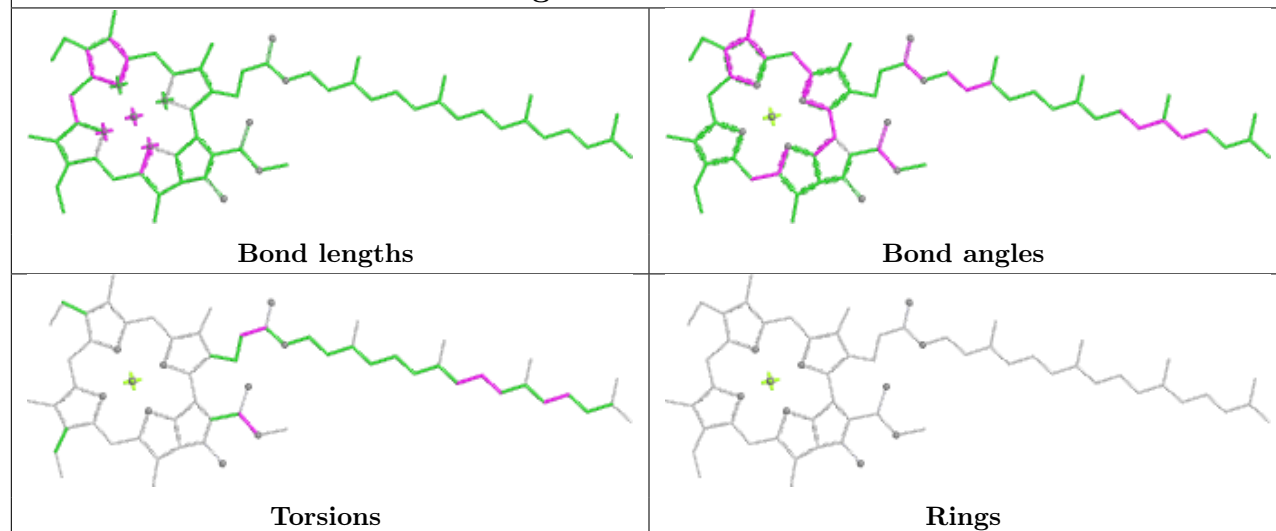


Ligand DGD c 519	
	
Bond lengths	Bond angles
	
Torsions	Rings

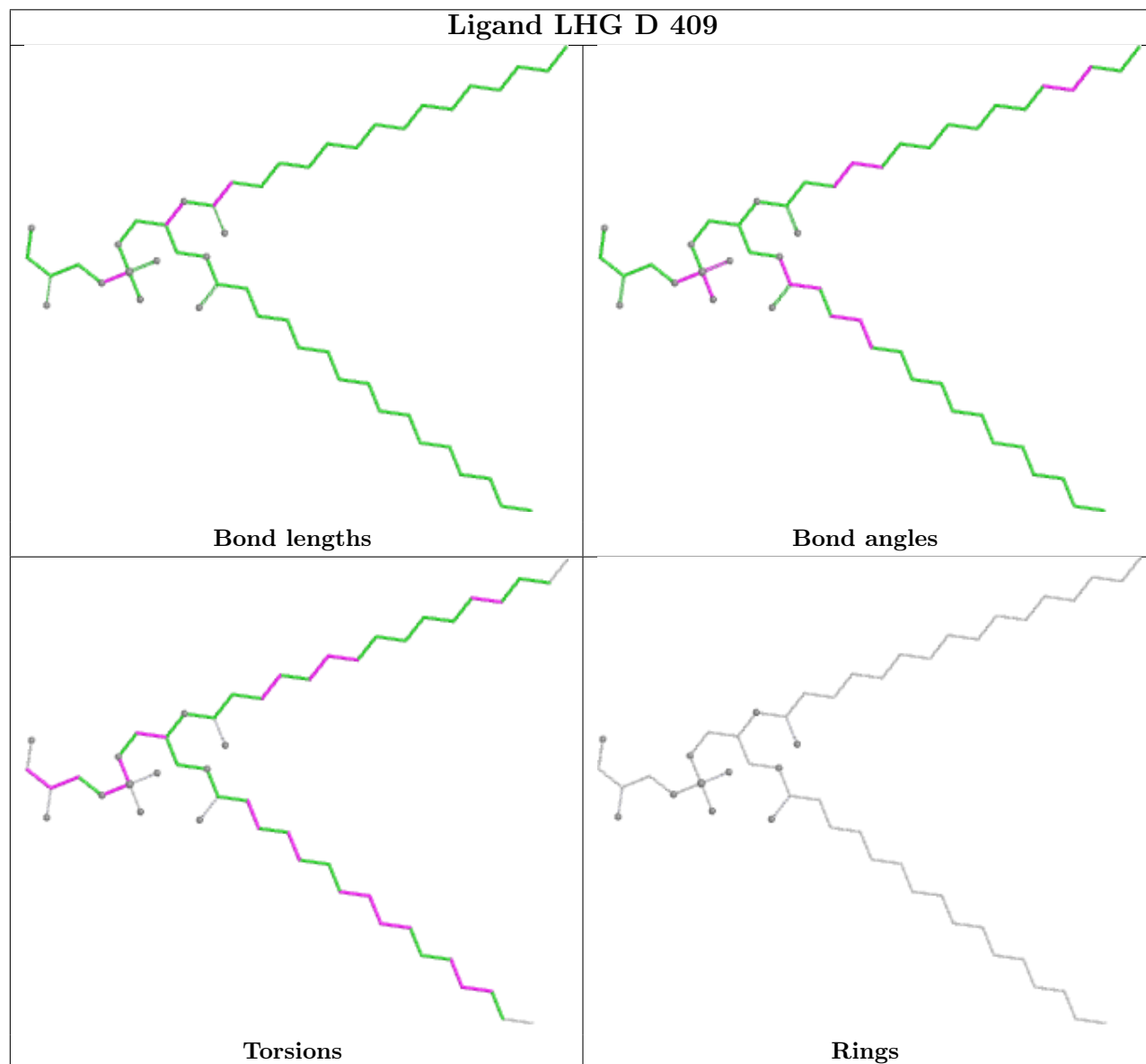
Ligand LMG M 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

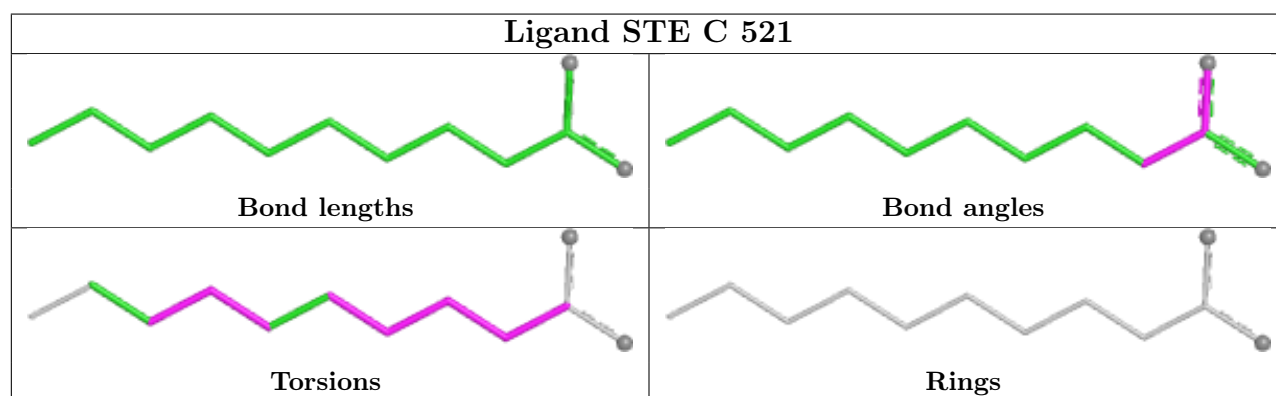
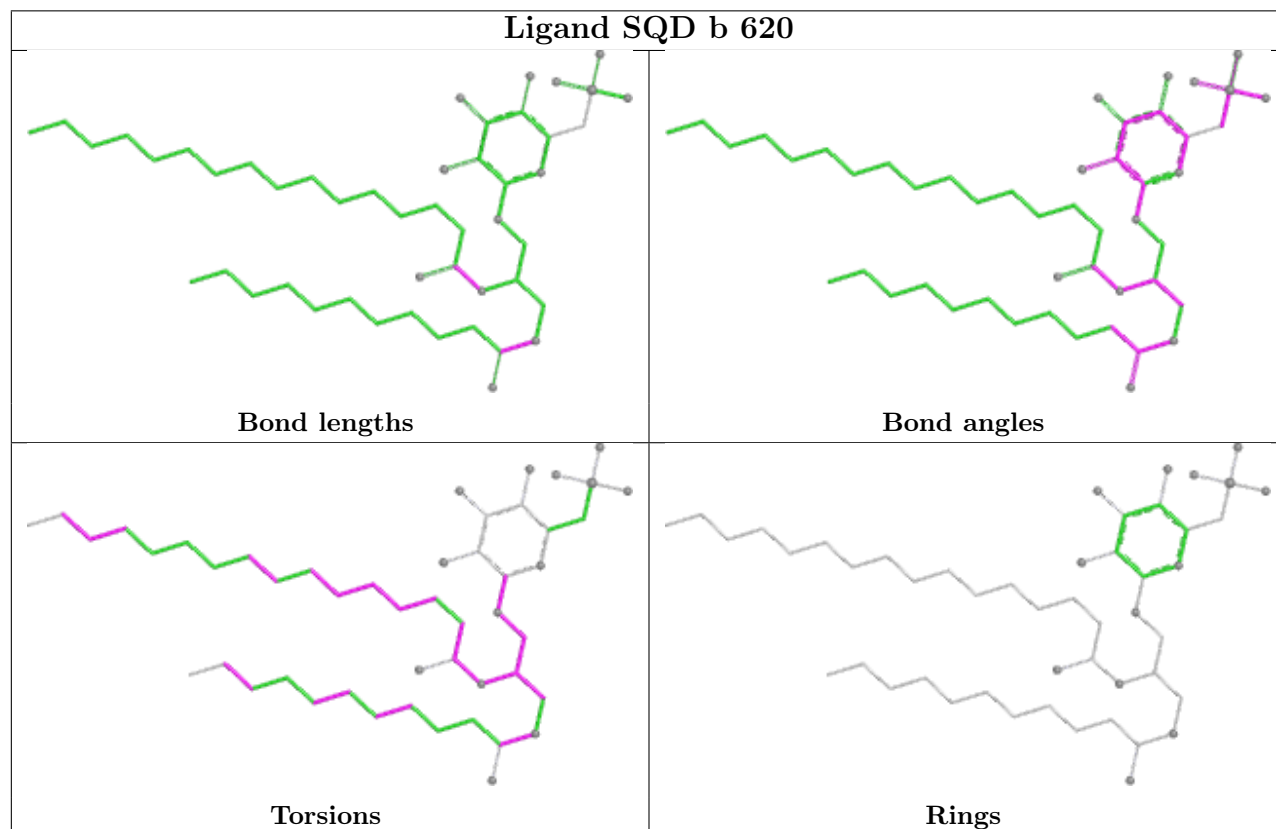
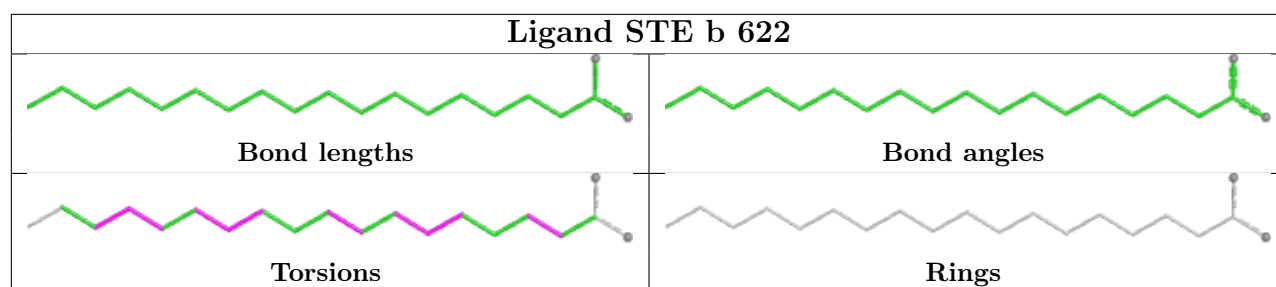
Ligand STE M 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

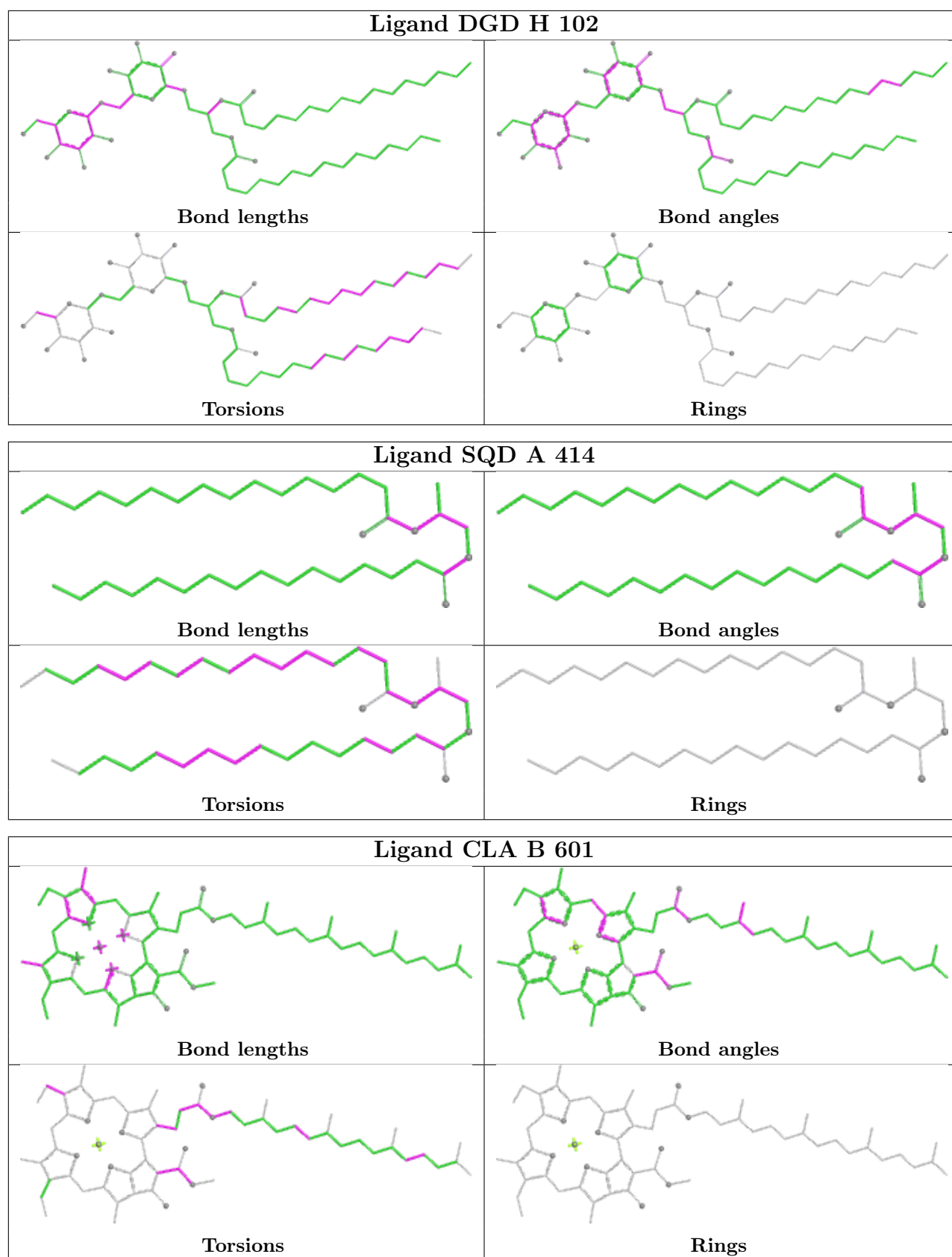
Ligand CLA B 612

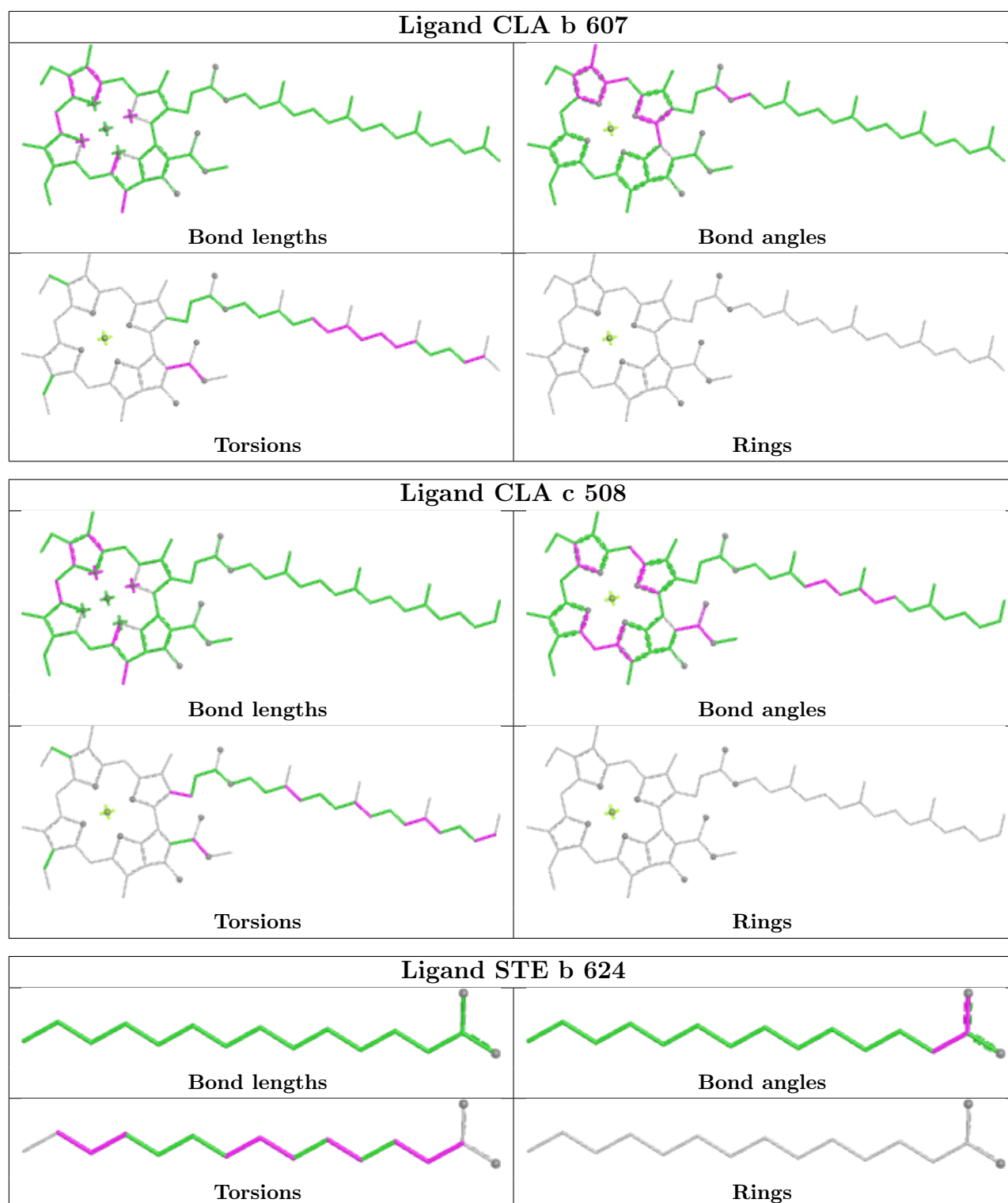


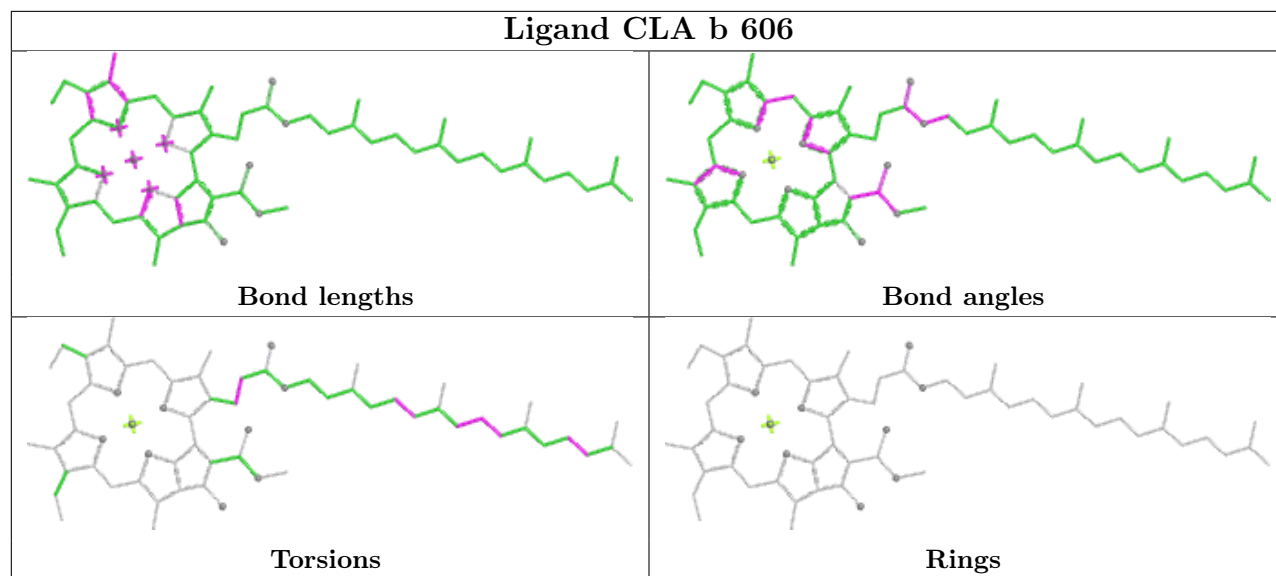
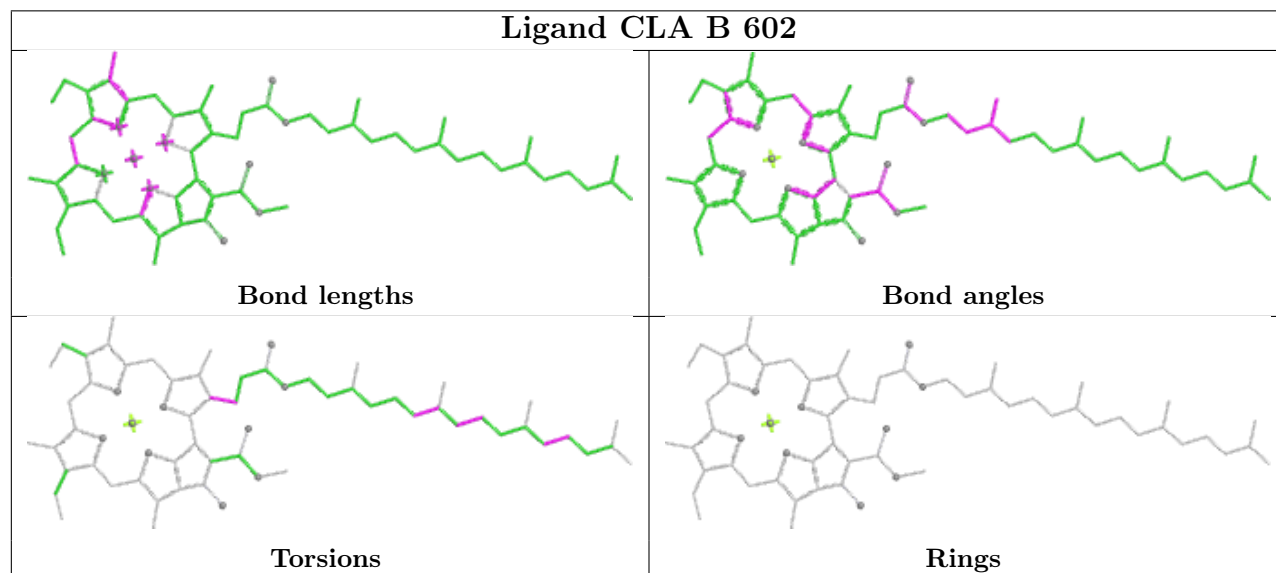
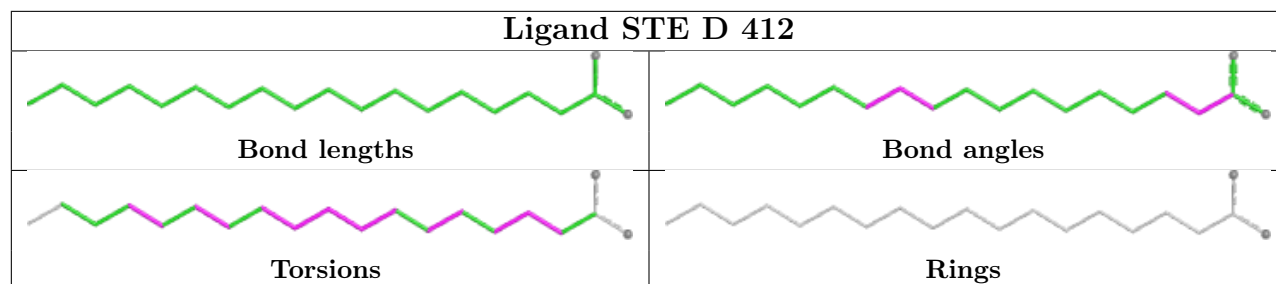
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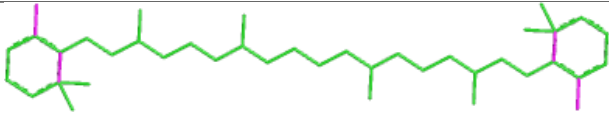
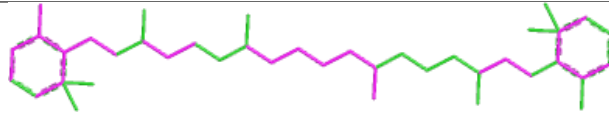
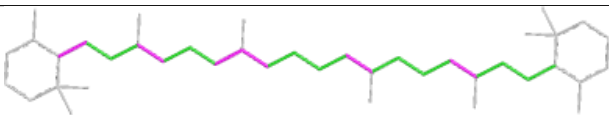
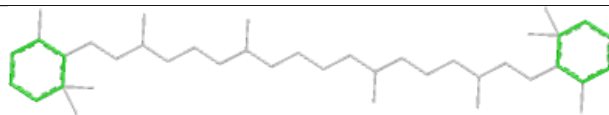


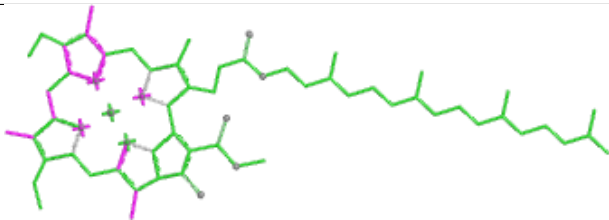
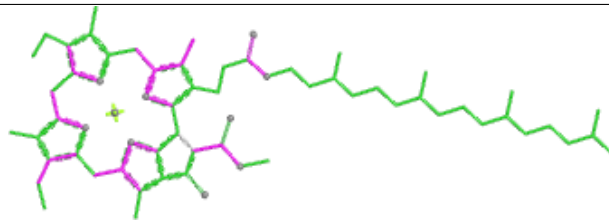
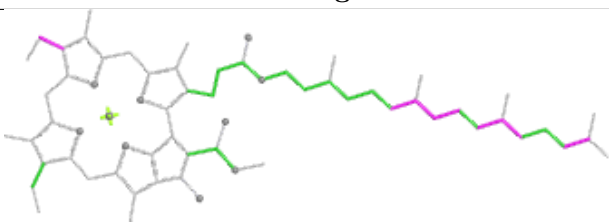
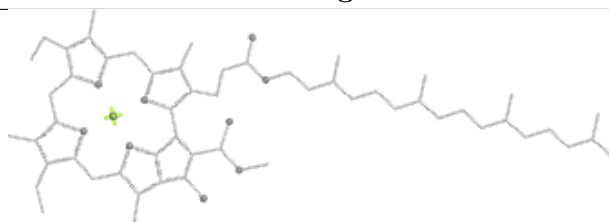


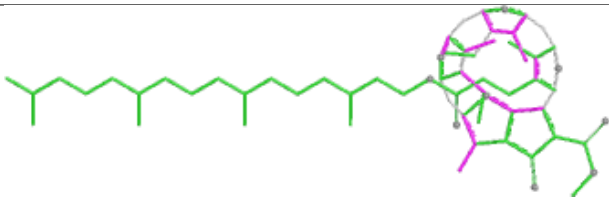
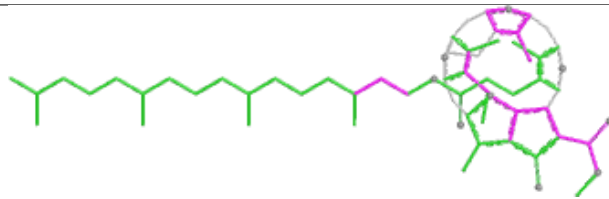
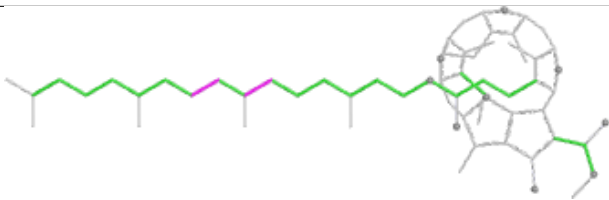
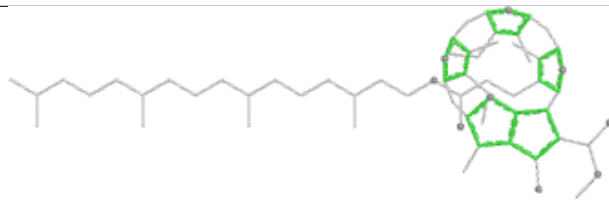


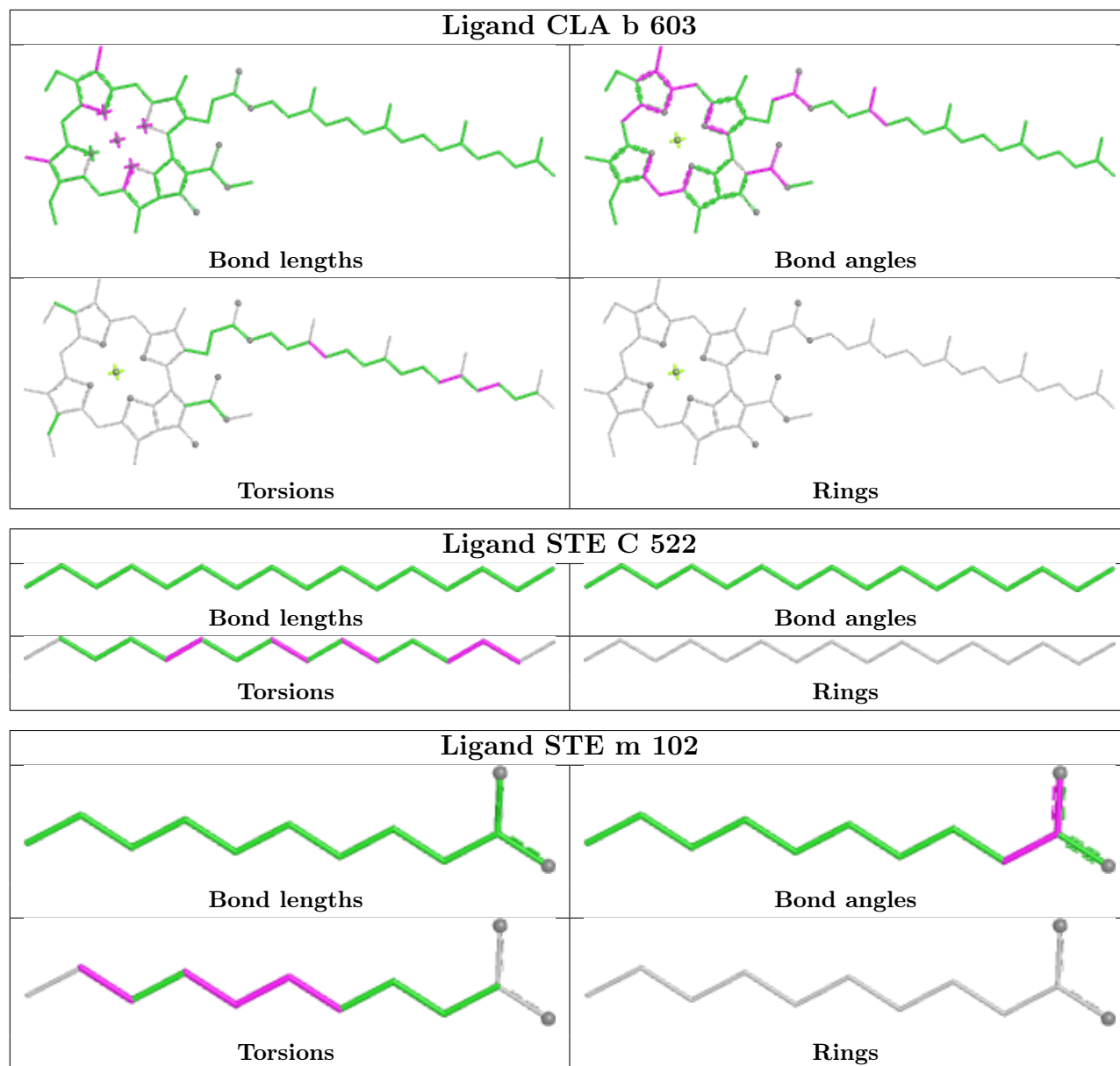


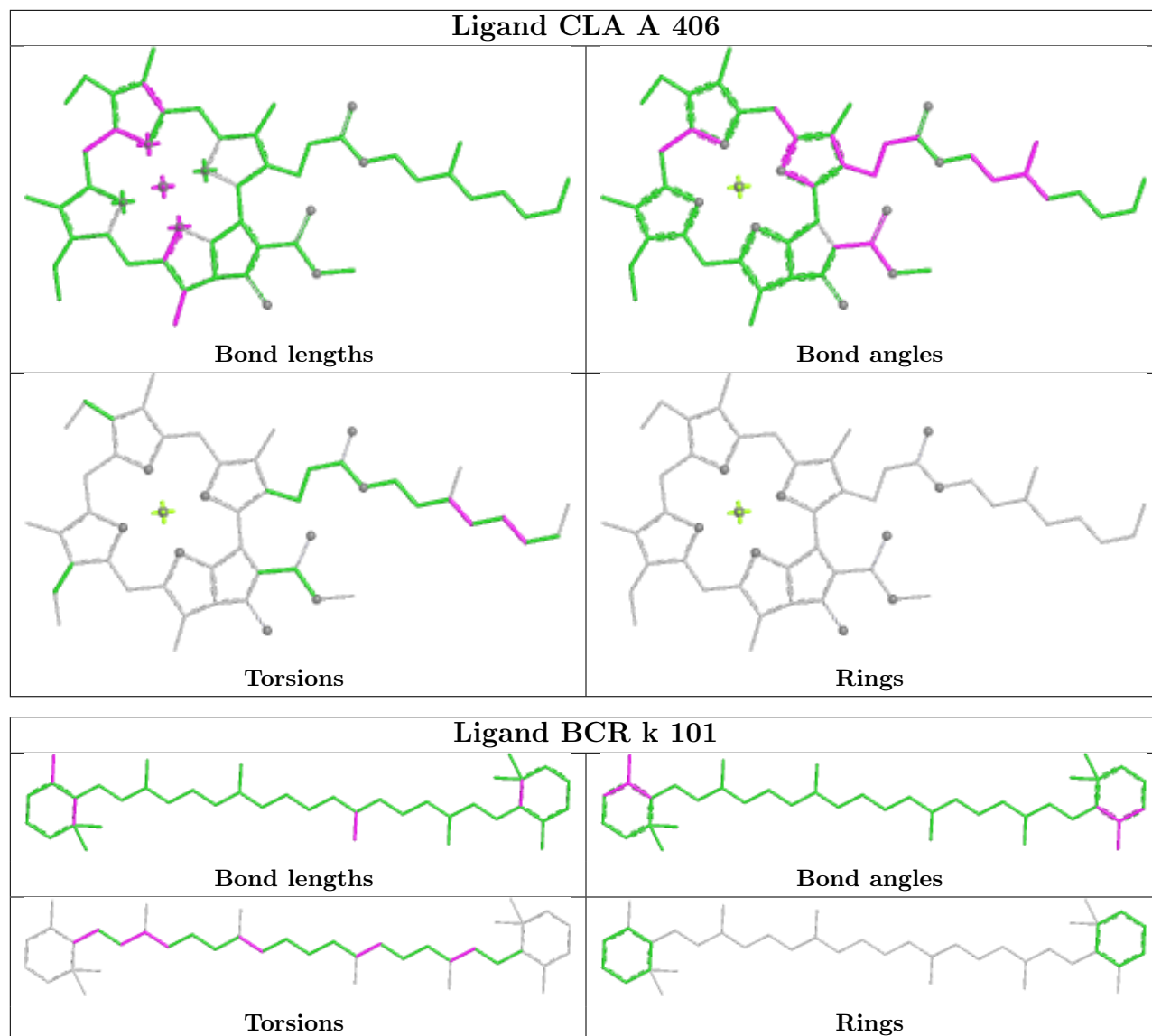


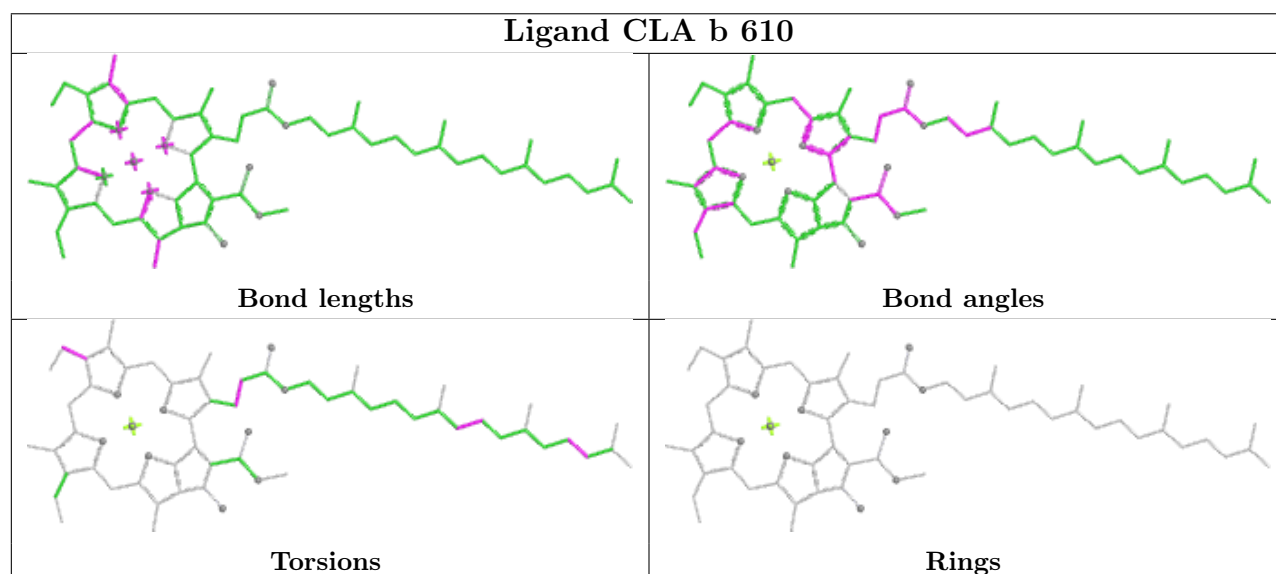
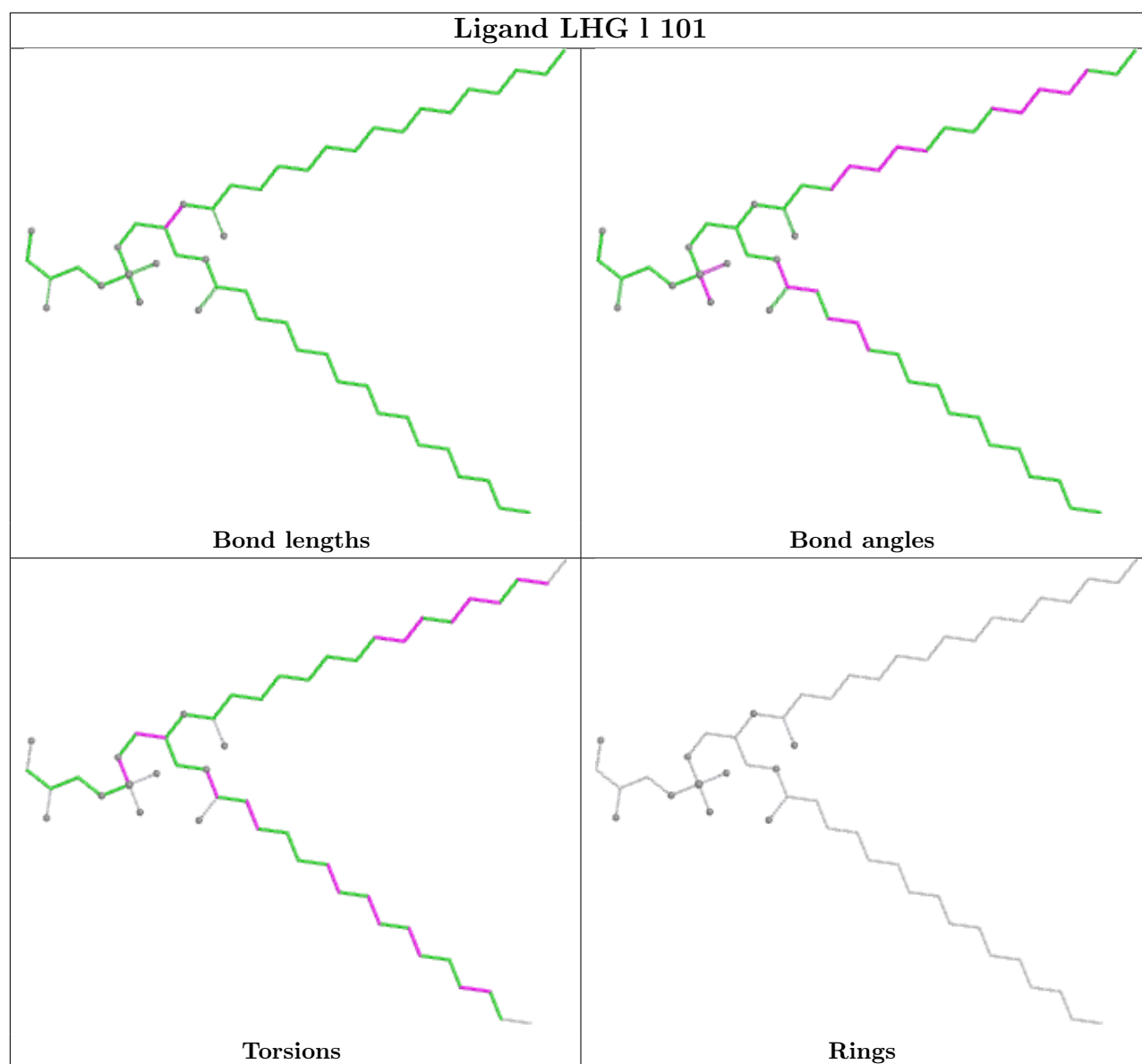
Ligand BCR B 617	
	
Bond lengths	Bond angles
	
Torsions	Rings

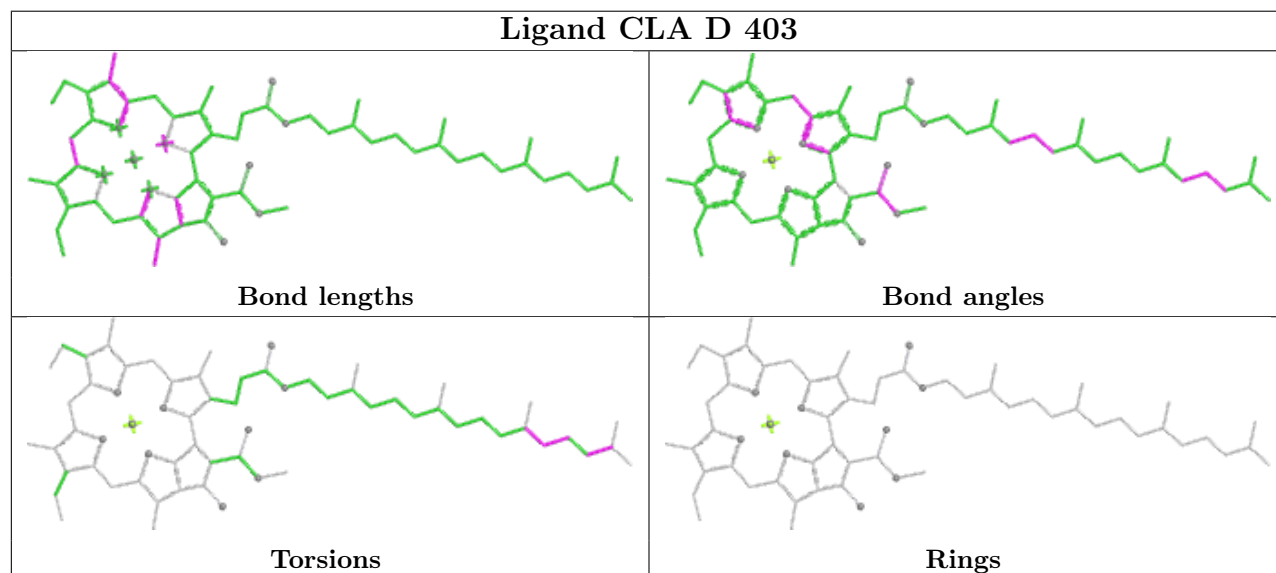
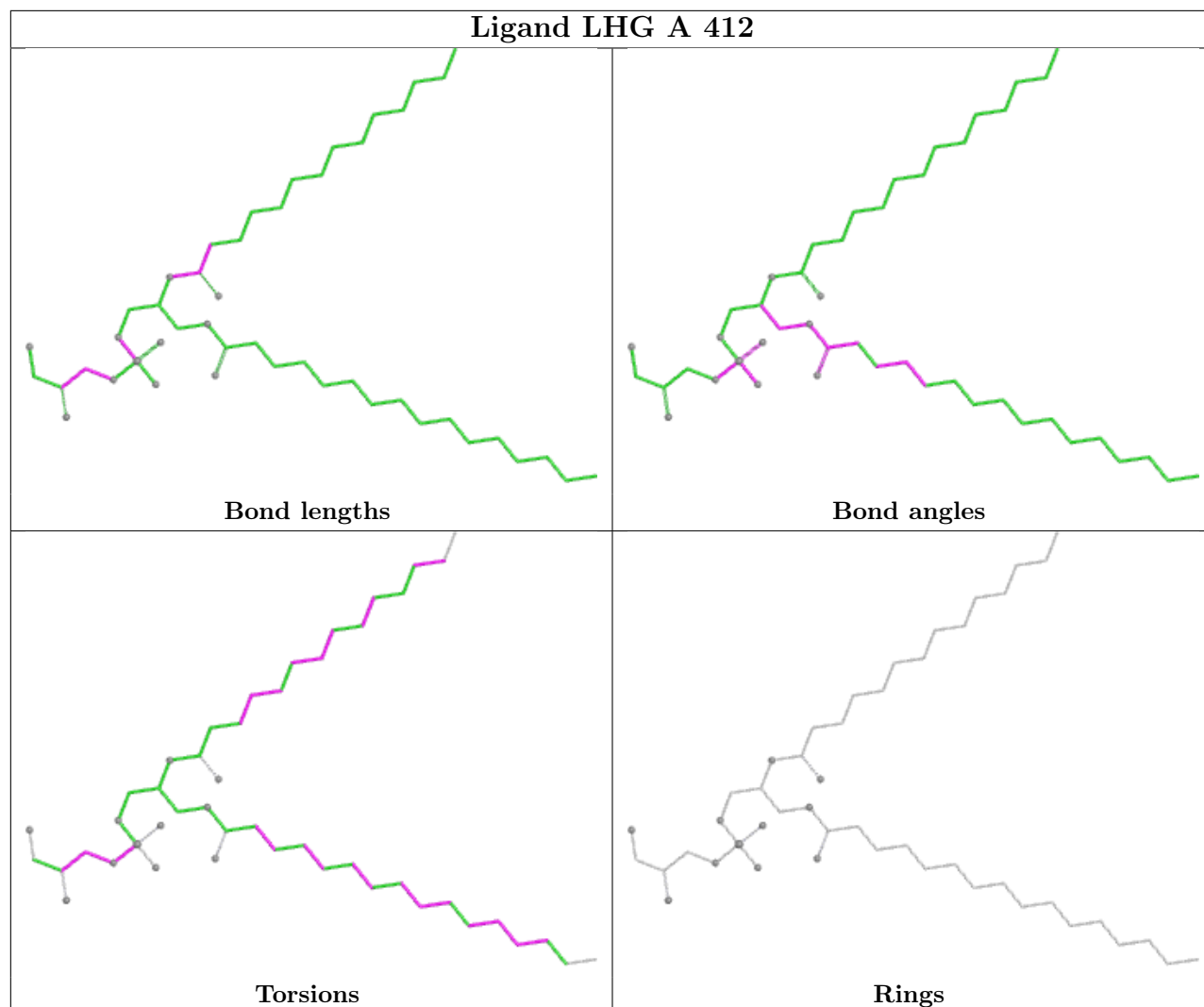
Ligand CLA d 401	
	
Bond lengths	Bond angles
	
Torsions	Rings

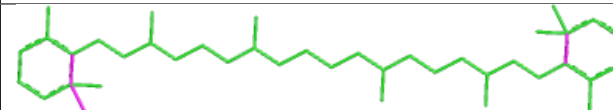
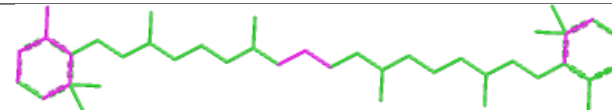
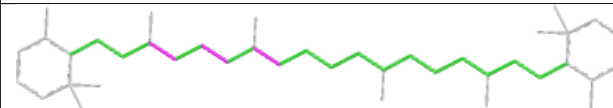
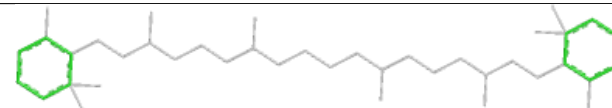
Ligand PHO A 405	
	
Bond lengths	Bond angles
	
Torsions	Rings



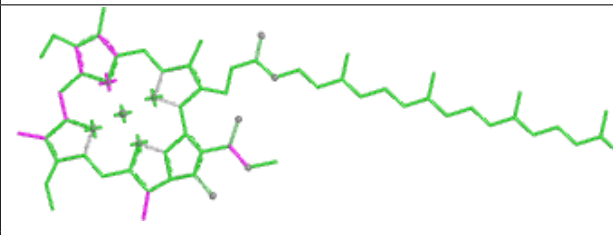
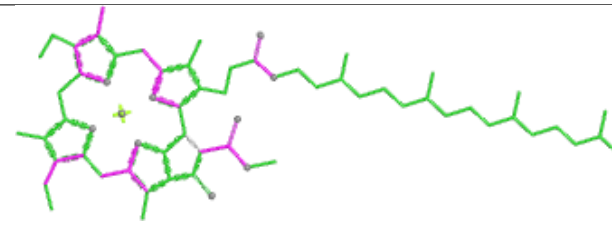
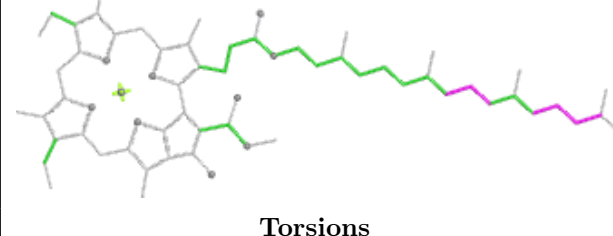
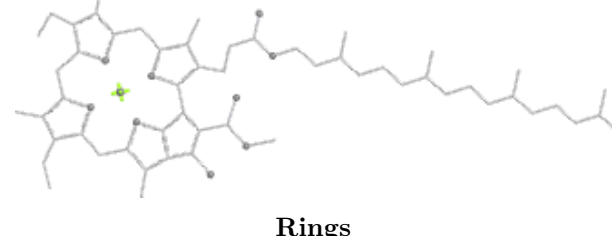




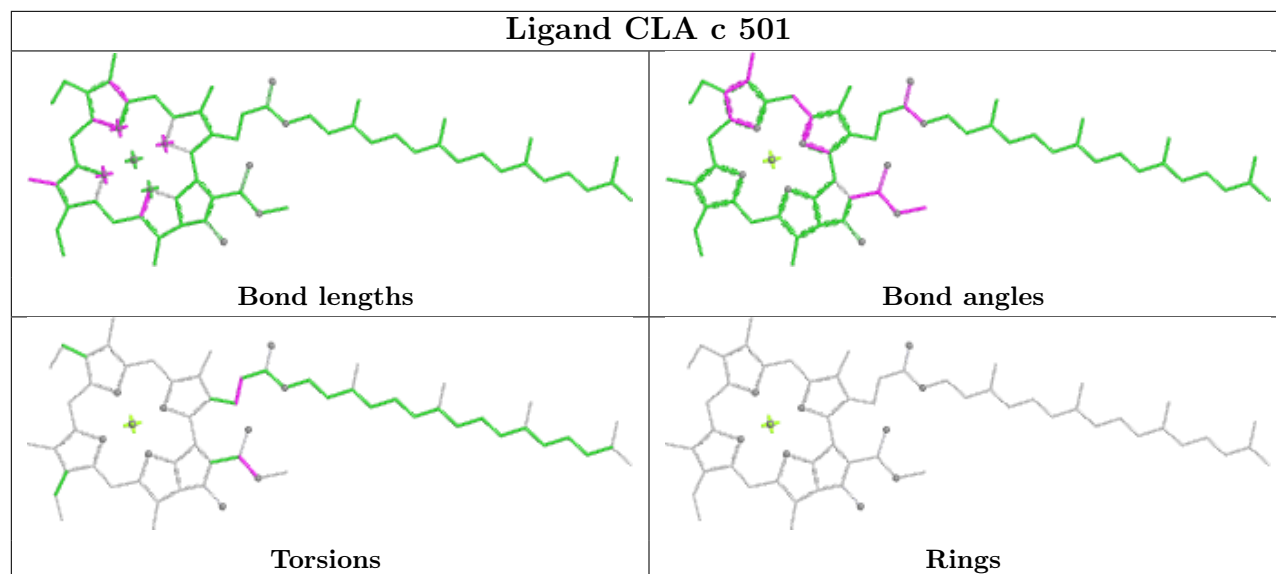


Ligand BCR B 619	
	
Bond lengths	Bond angles
	
Torsions	Rings

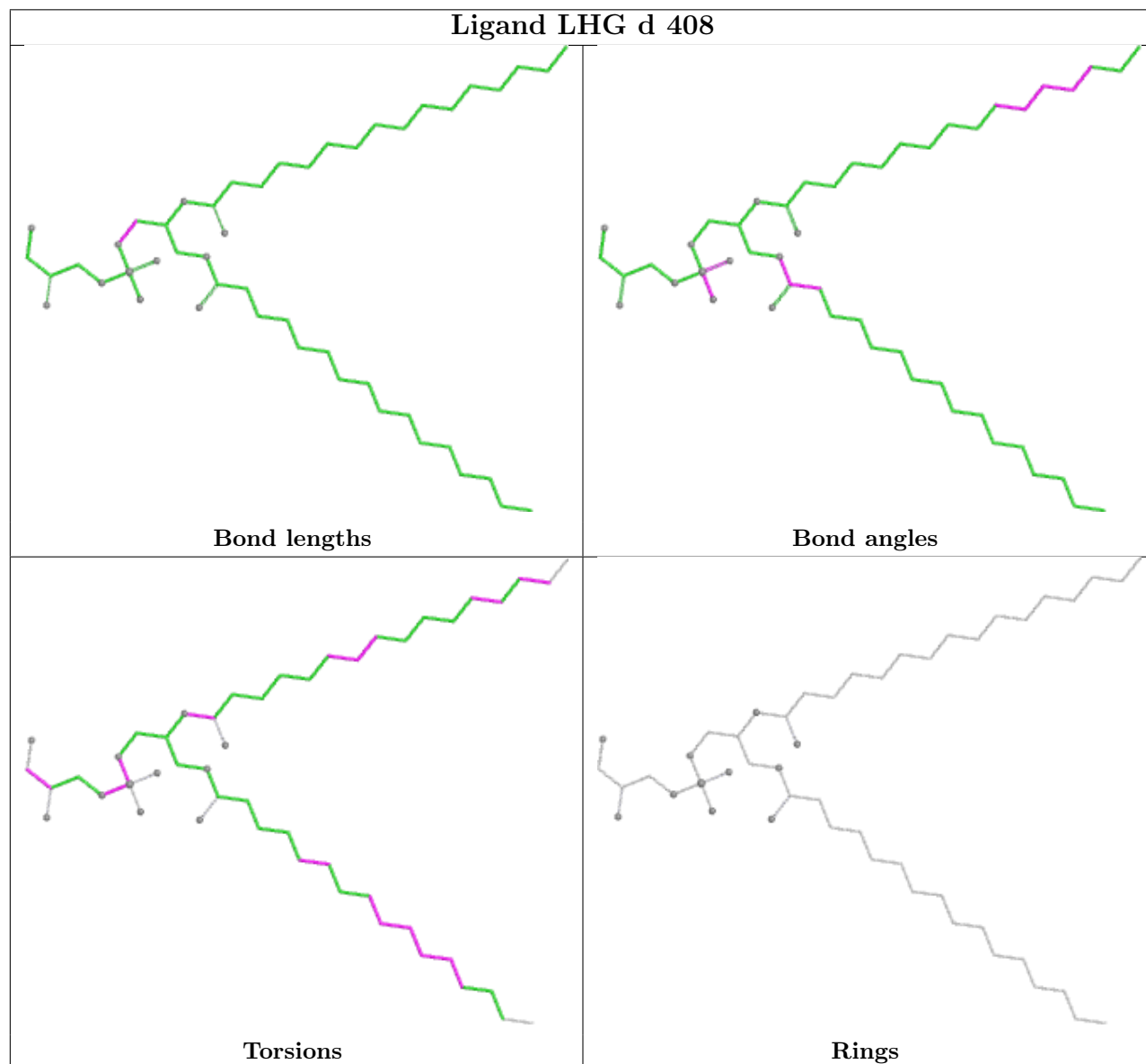
Ligand STE Z 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

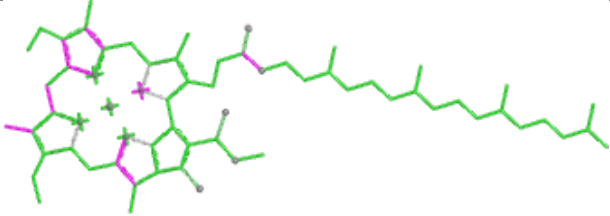
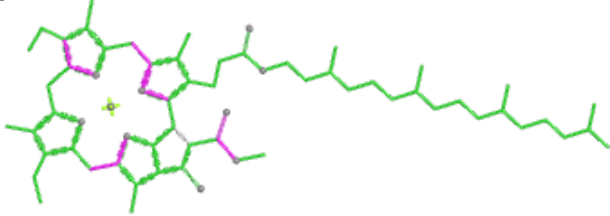
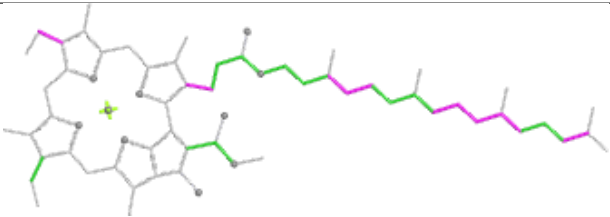
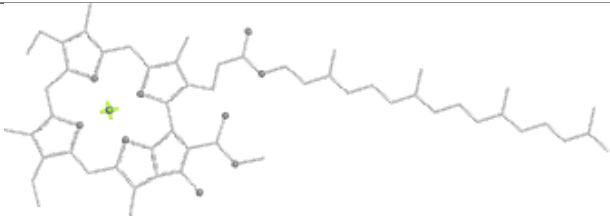
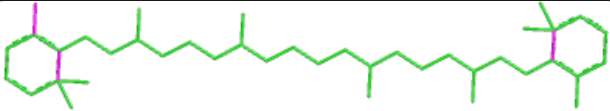
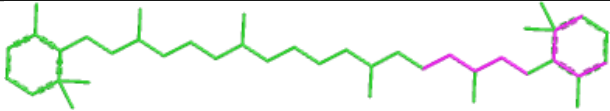
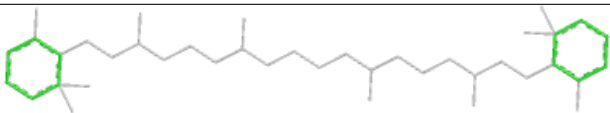
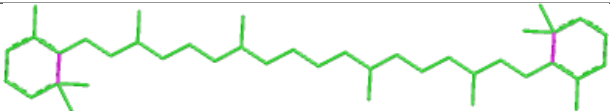
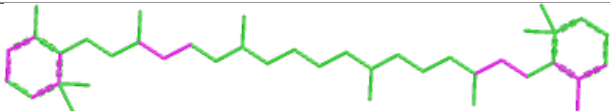
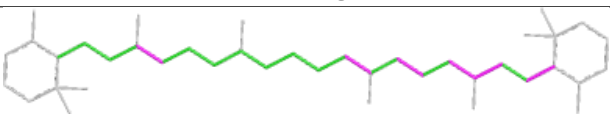
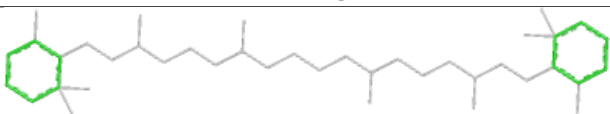
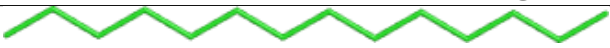
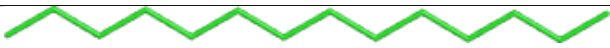
Ligand CLA b 611	
	
Bond lengths	Bond angles
	
Torsions	Rings

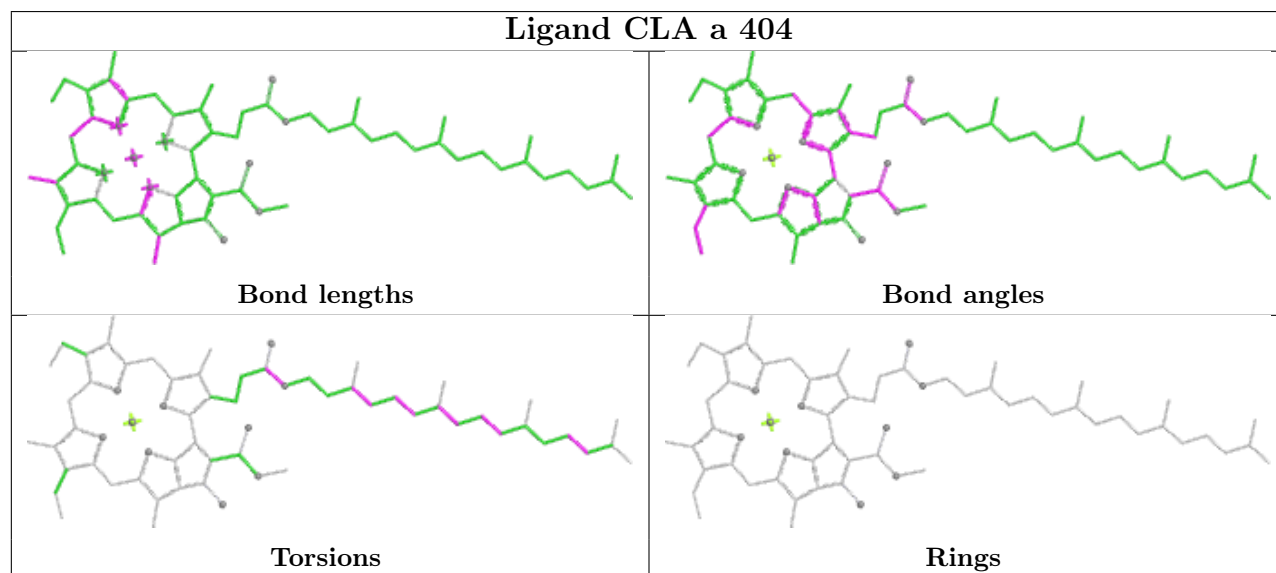
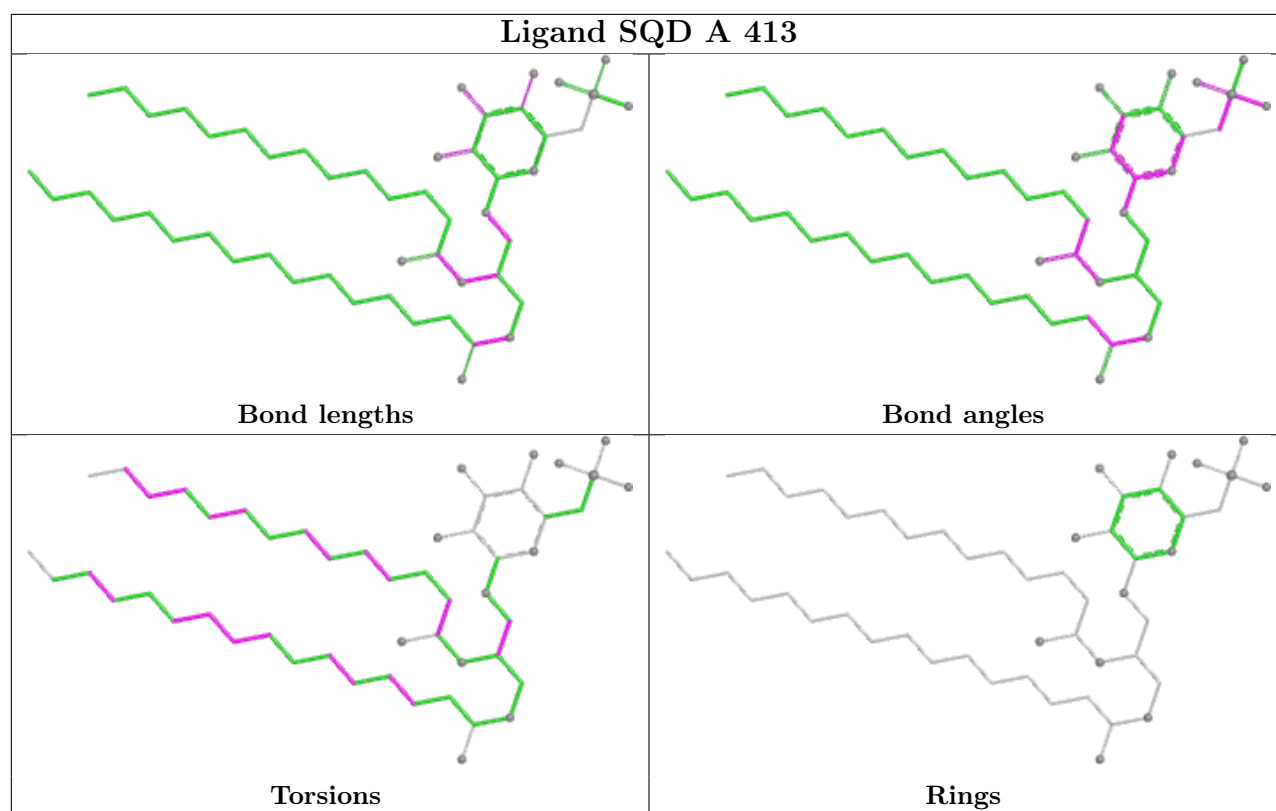
Ligand CLA c 501

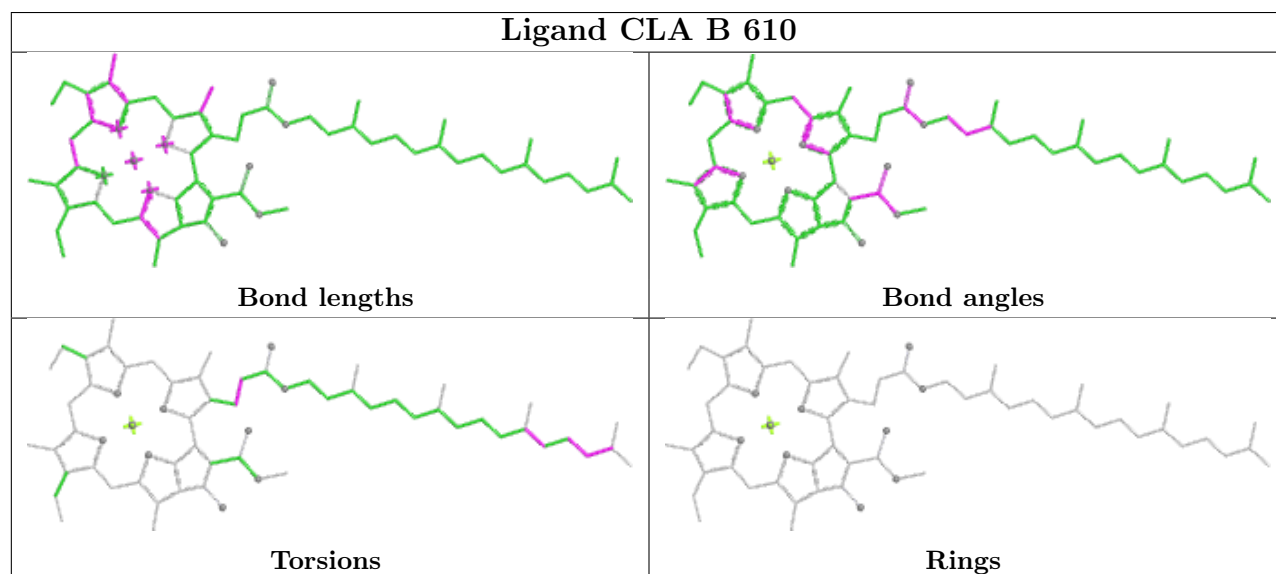
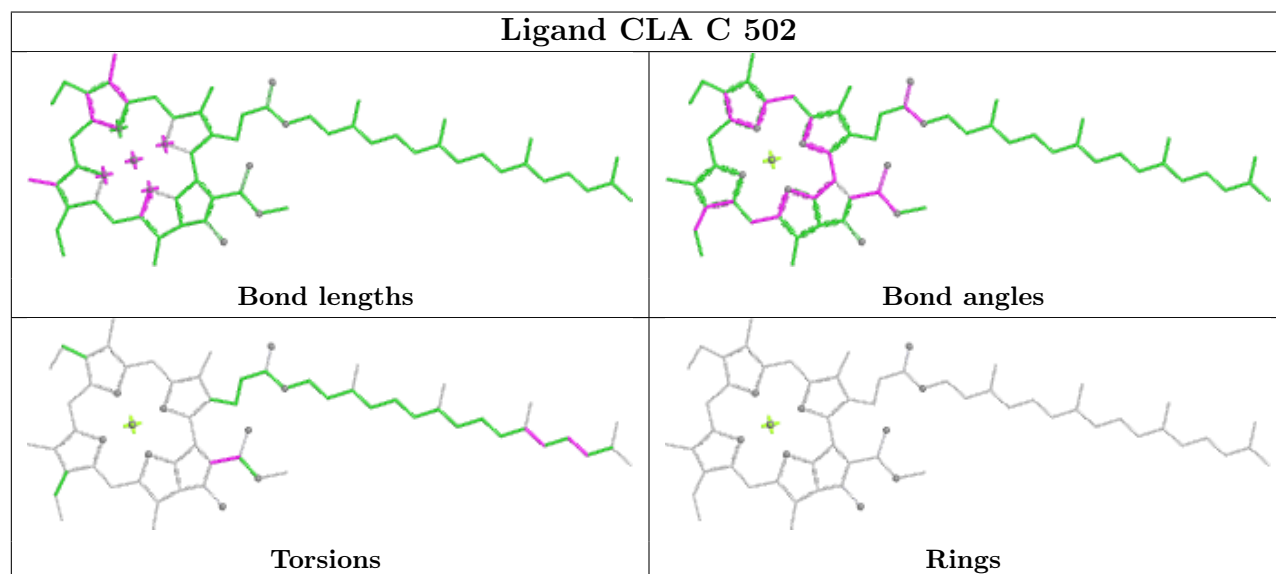
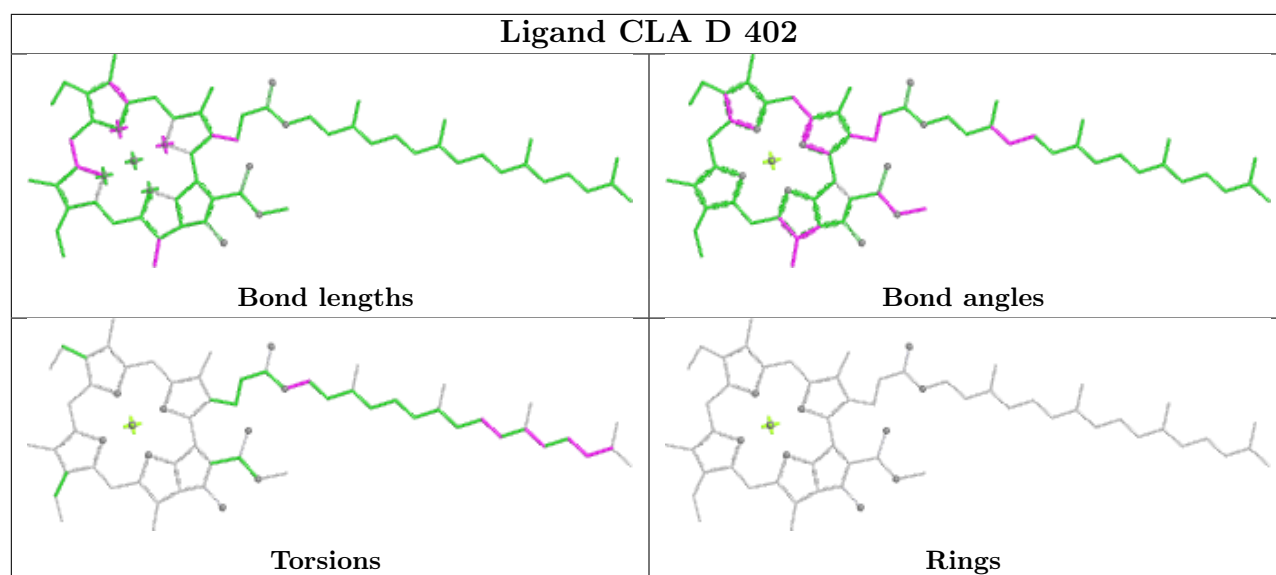


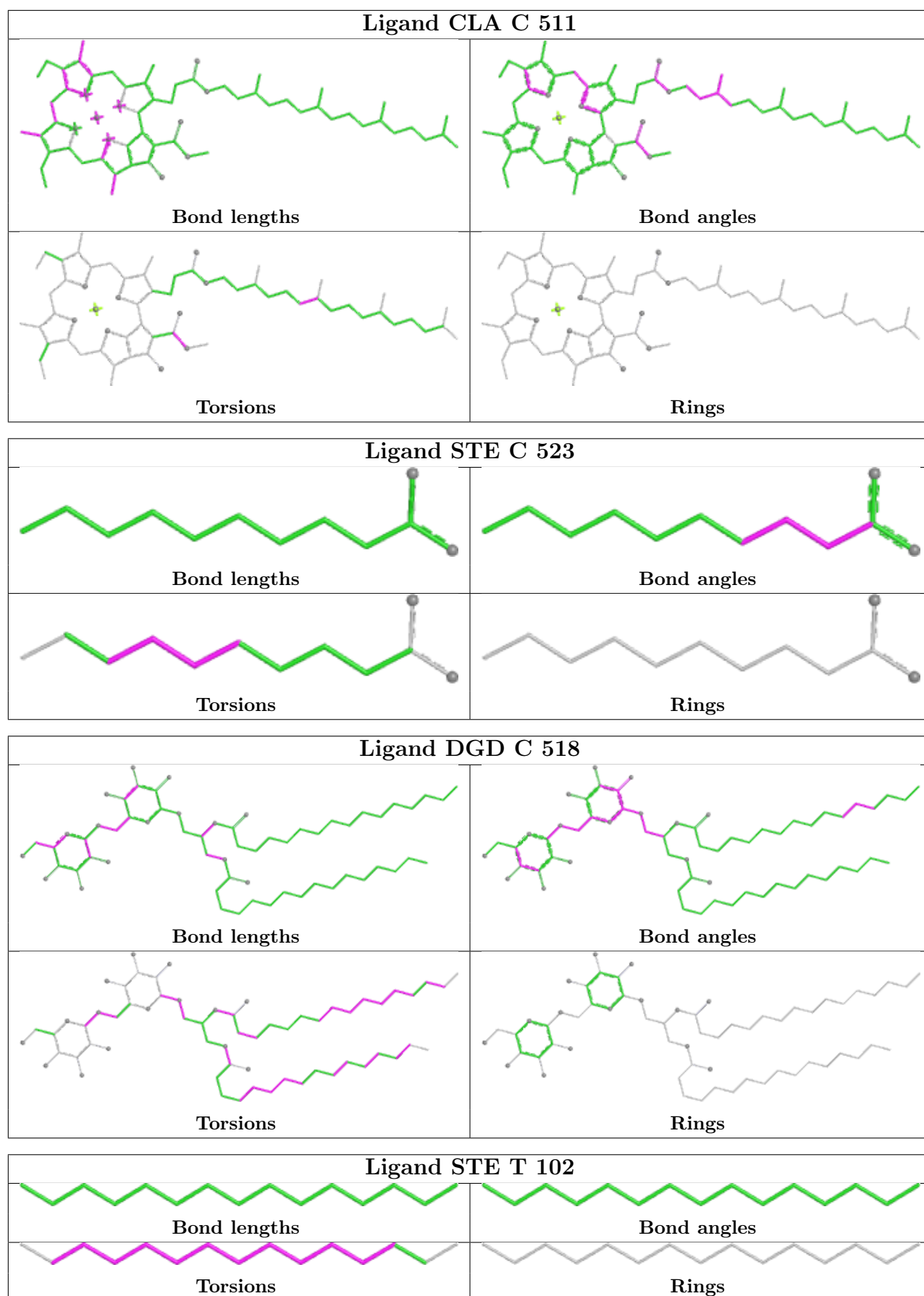
Ligand LHG d 408

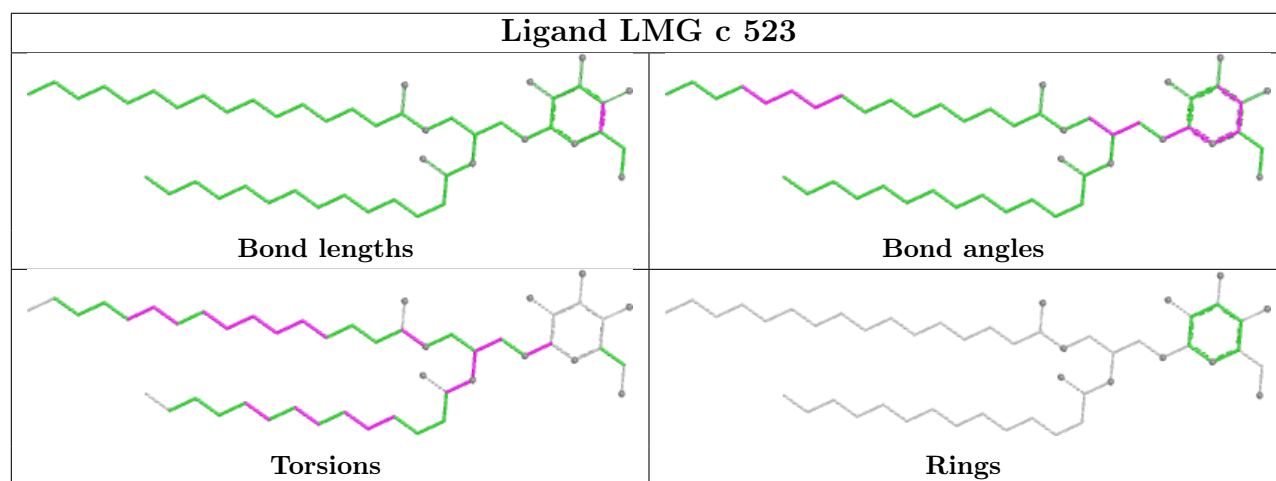
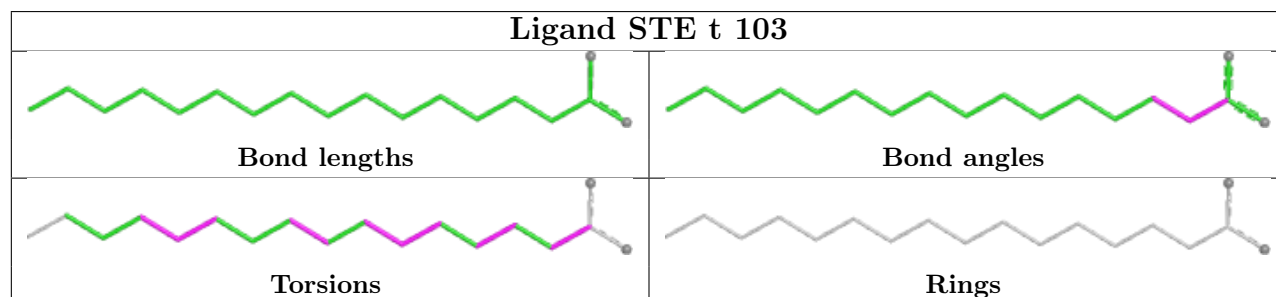
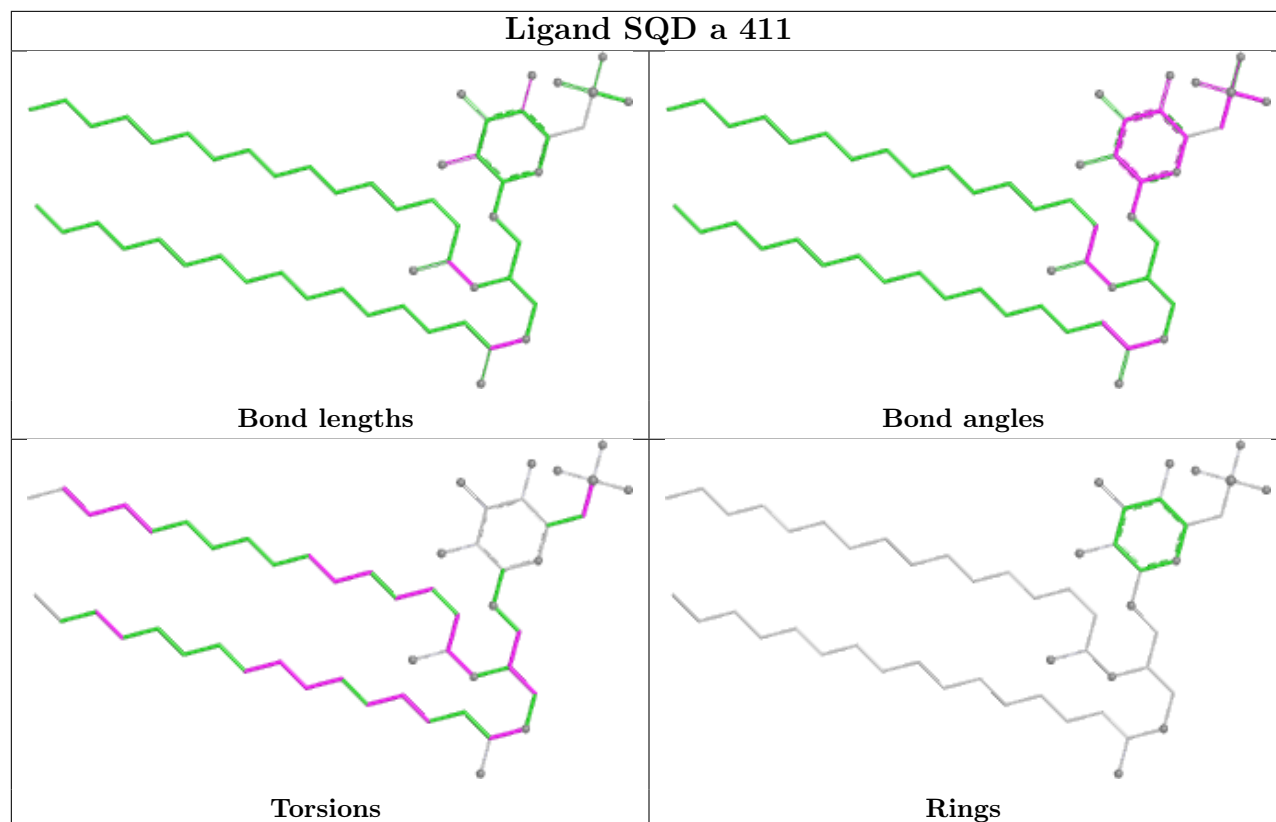


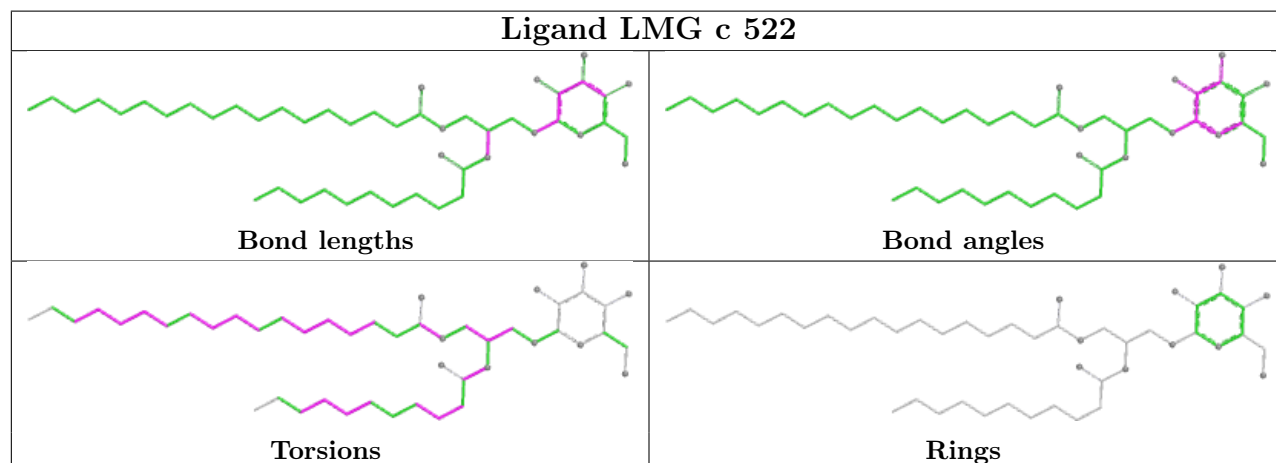
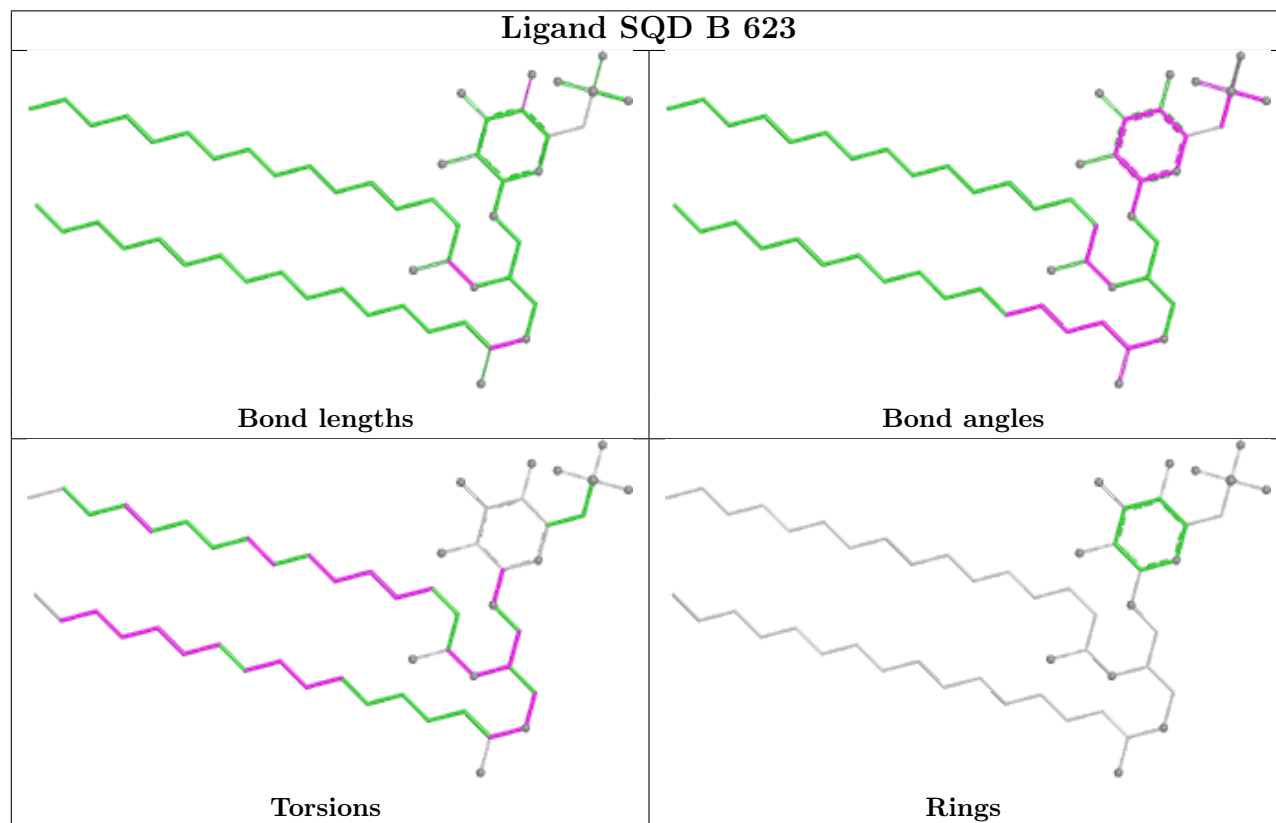
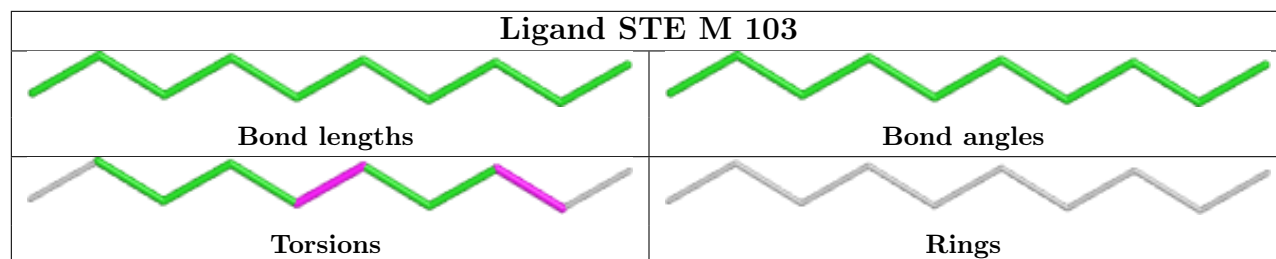
Ligand CLA b 601			
			
Bond lengths			
		Bond angles	
			
Torsions			
		Rings	
Ligand BCR C 516			
			
Bond lengths			
		Bond angles	
			
Torsions			
		Rings	
Ligand BCR d 406			
			
Bond lengths			
		Bond angles	
			
Torsions			
		Rings	
Ligand STE b 627			
			
Bond lengths			
		Bond angles	
			
Torsions			
		Rings	

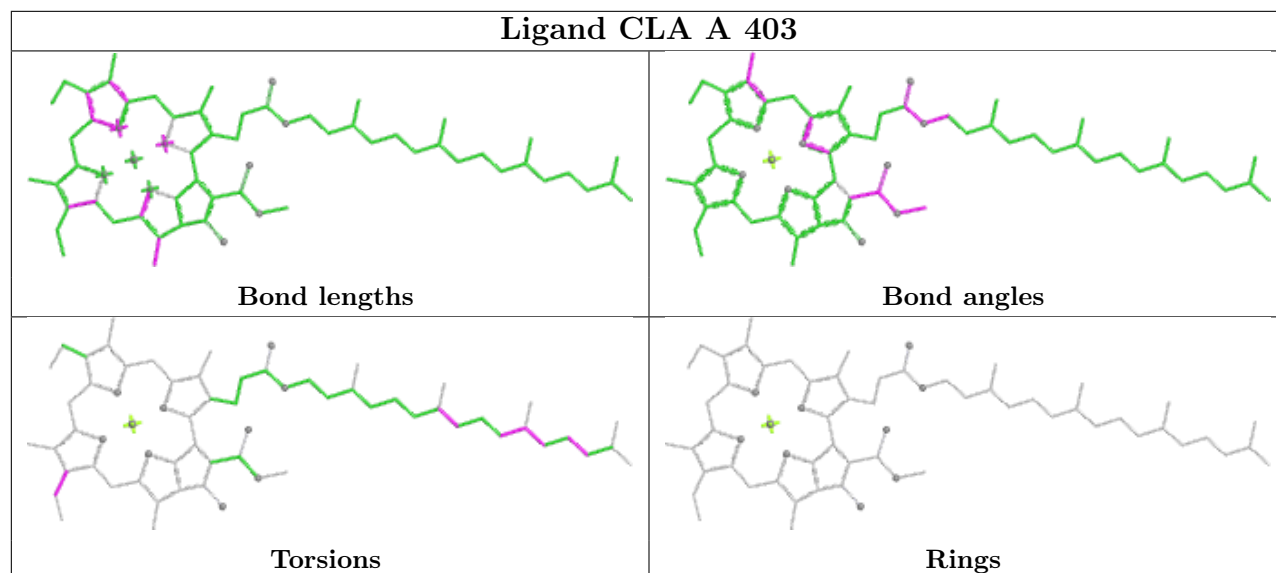
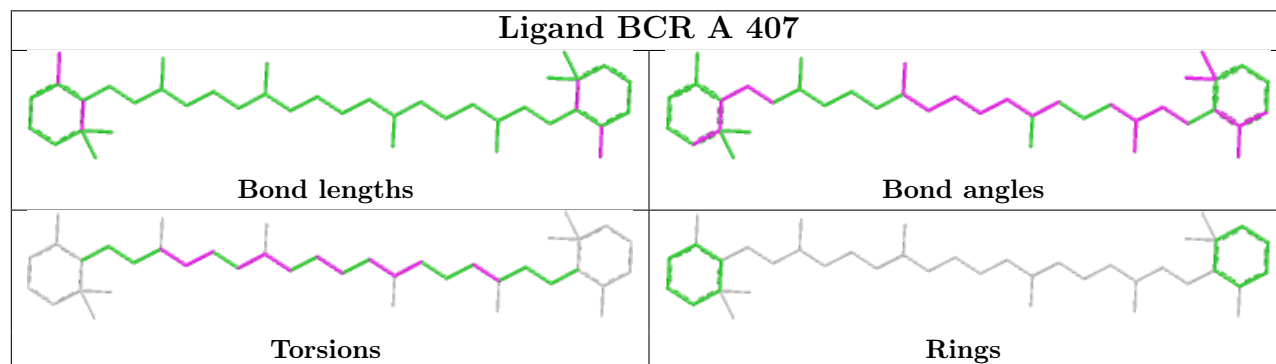
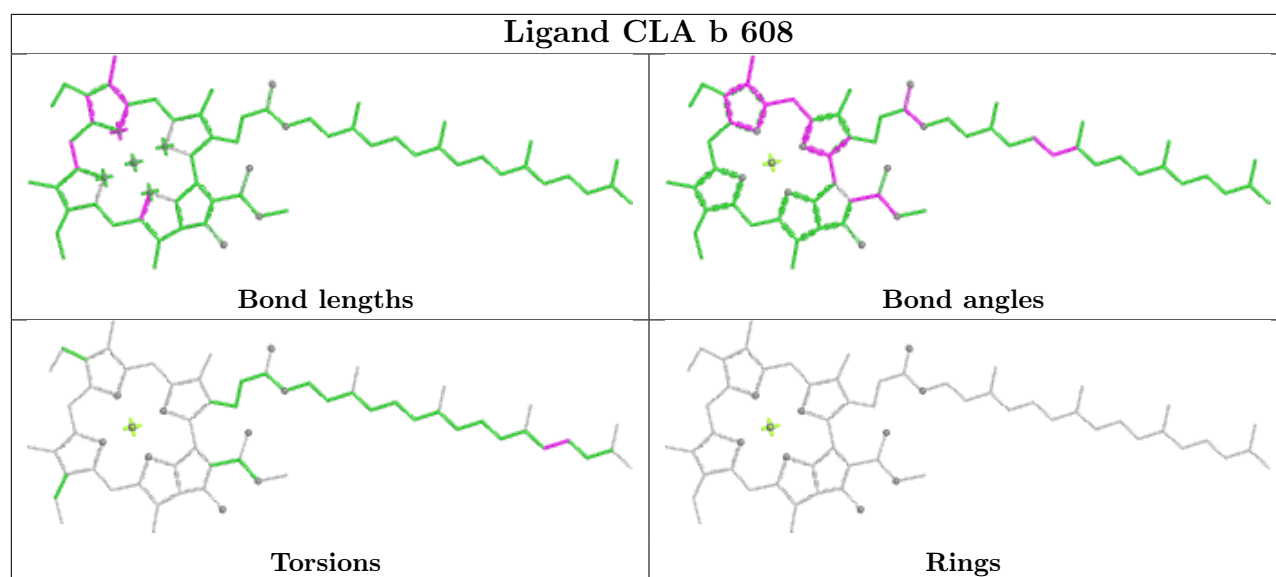


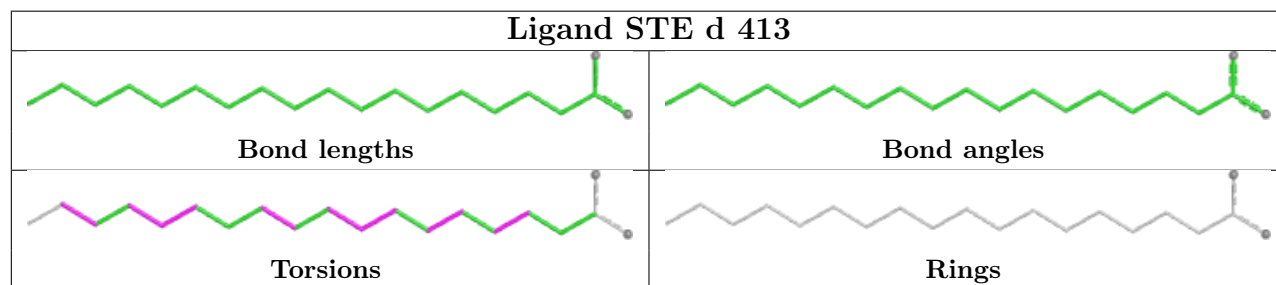
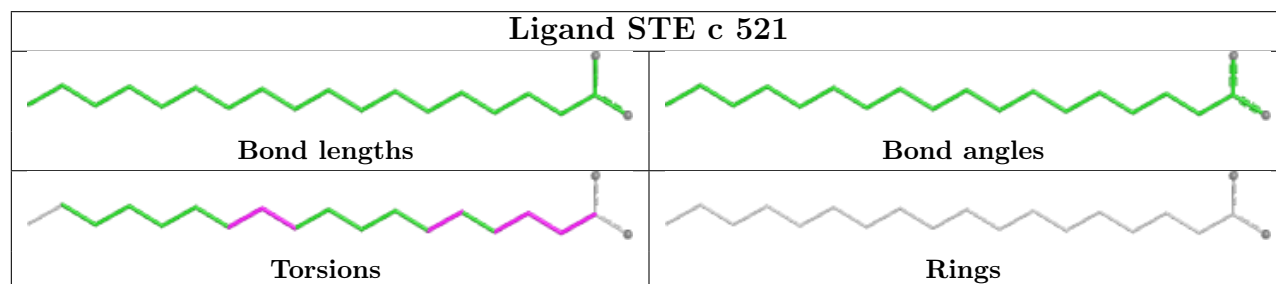
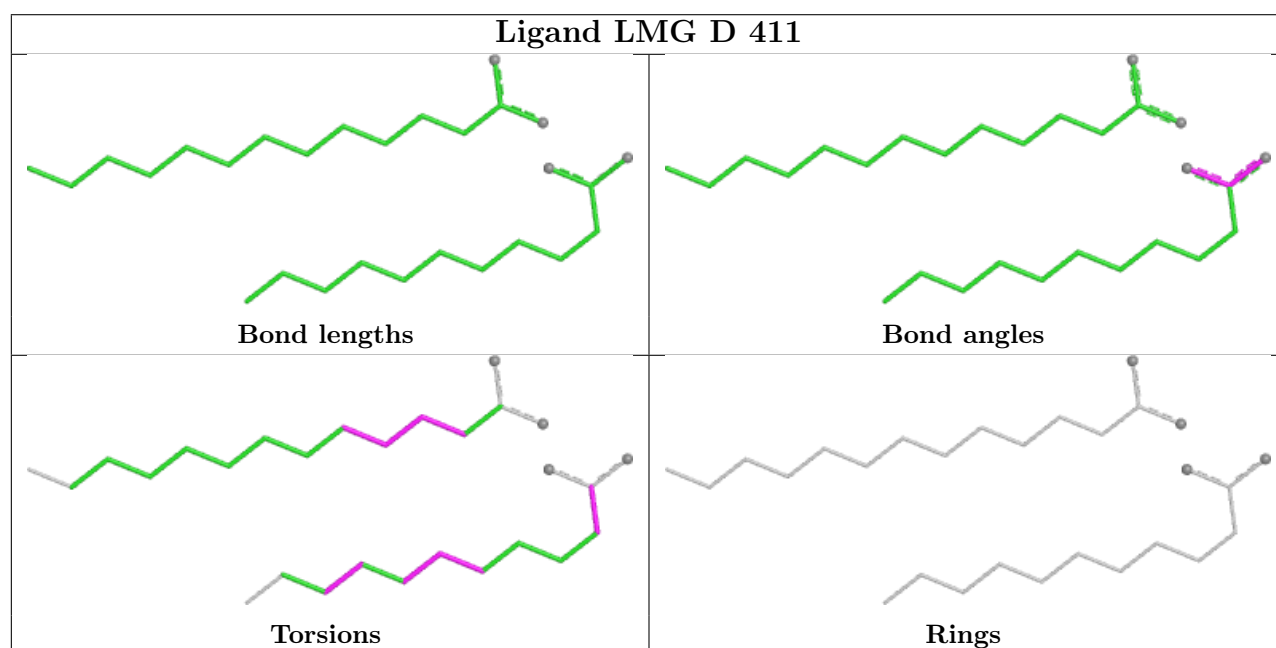
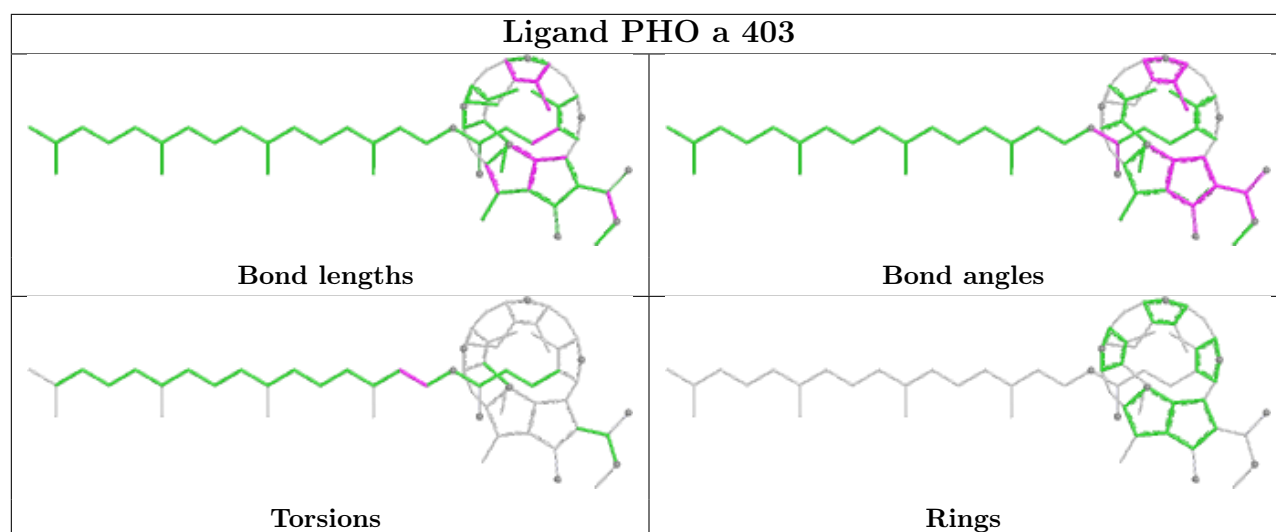




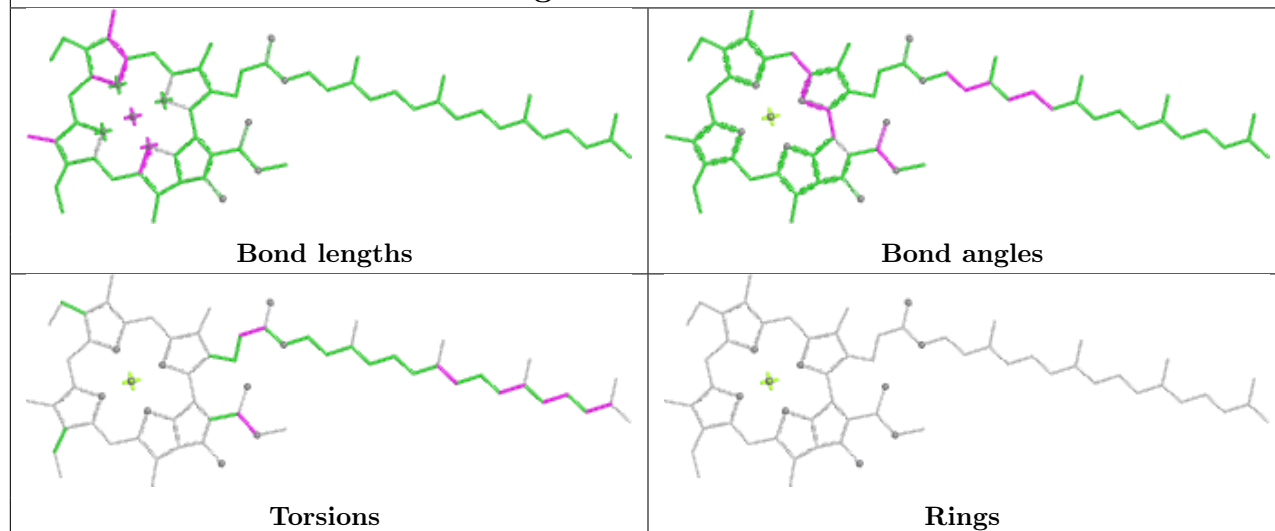




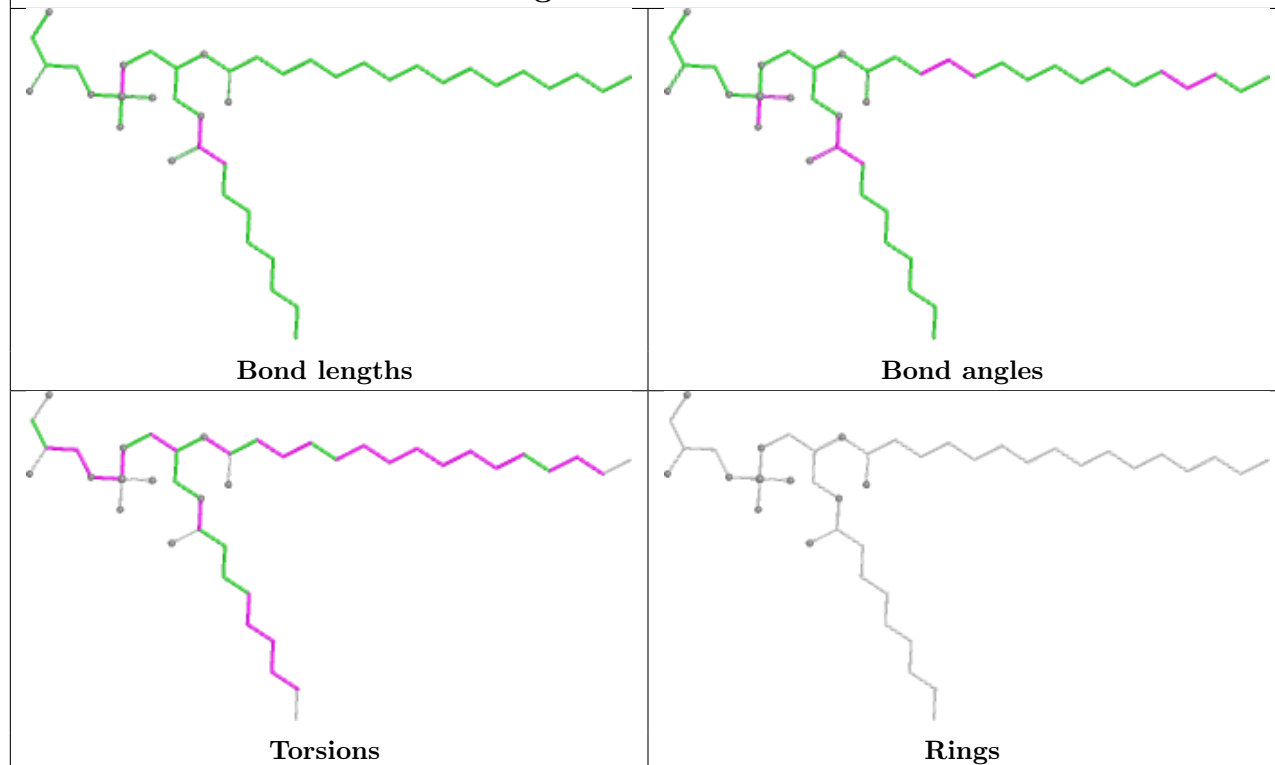




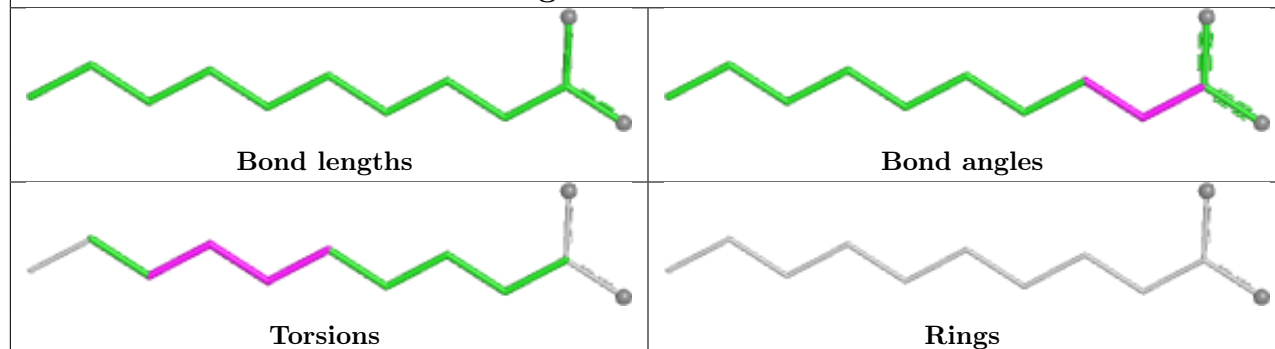
Ligand CLA b 613

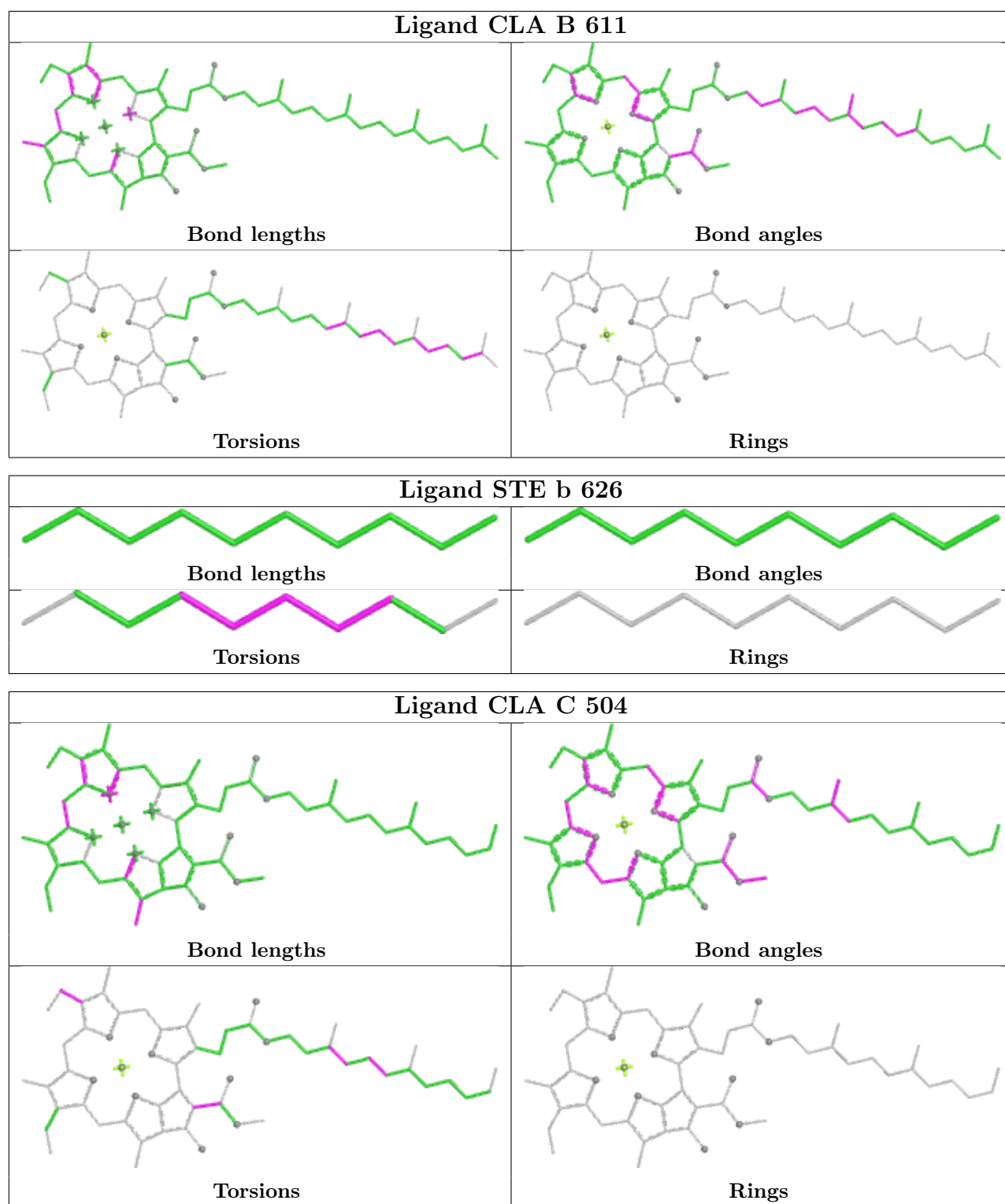


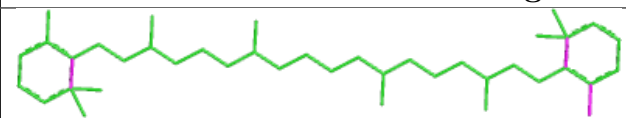
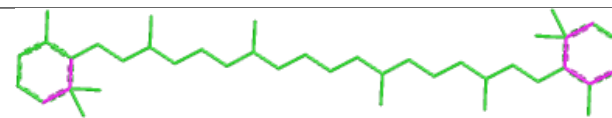
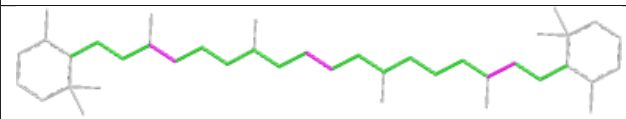
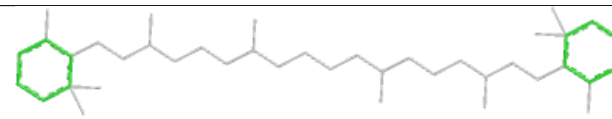
Ligand LHG e 101

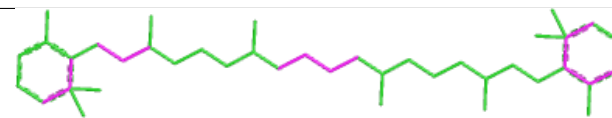
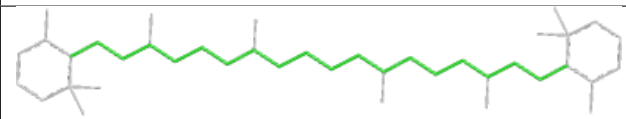
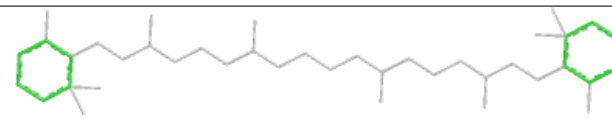


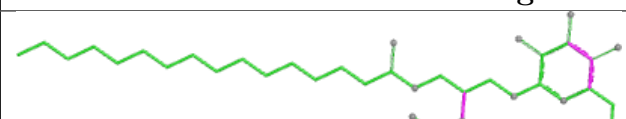
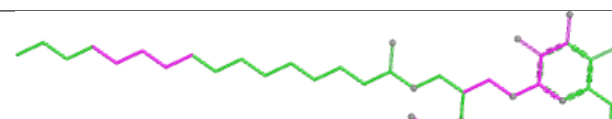
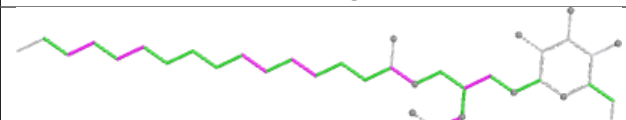
Ligand STE a 414

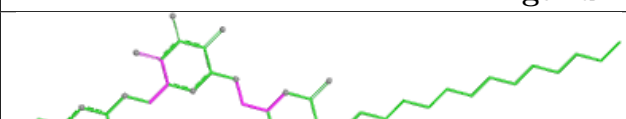
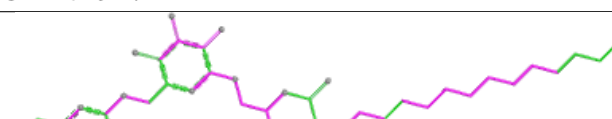
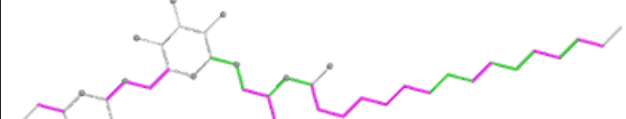
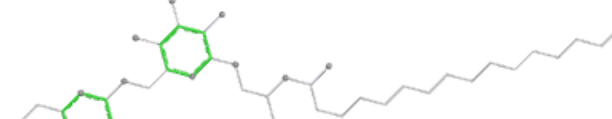


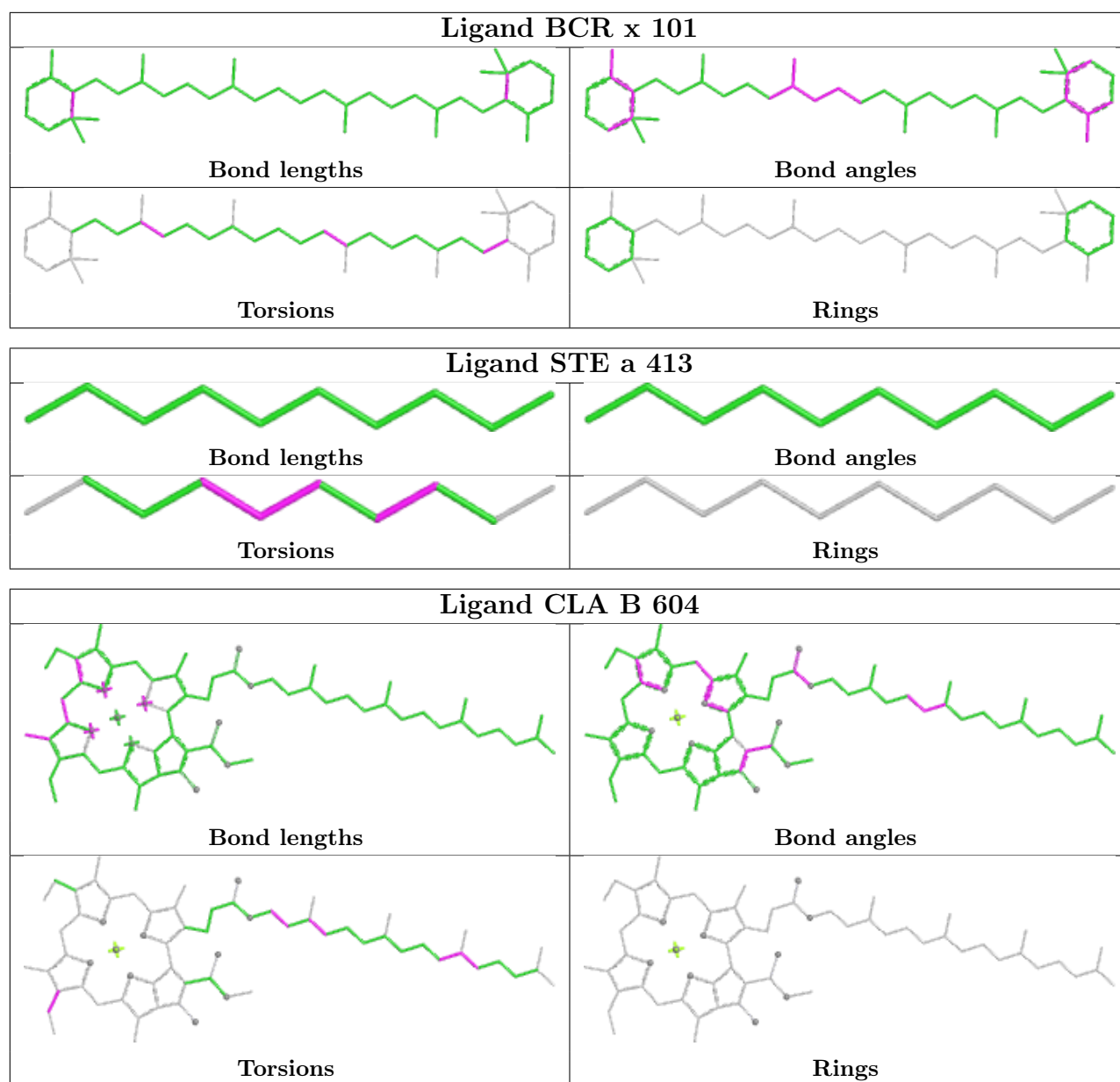


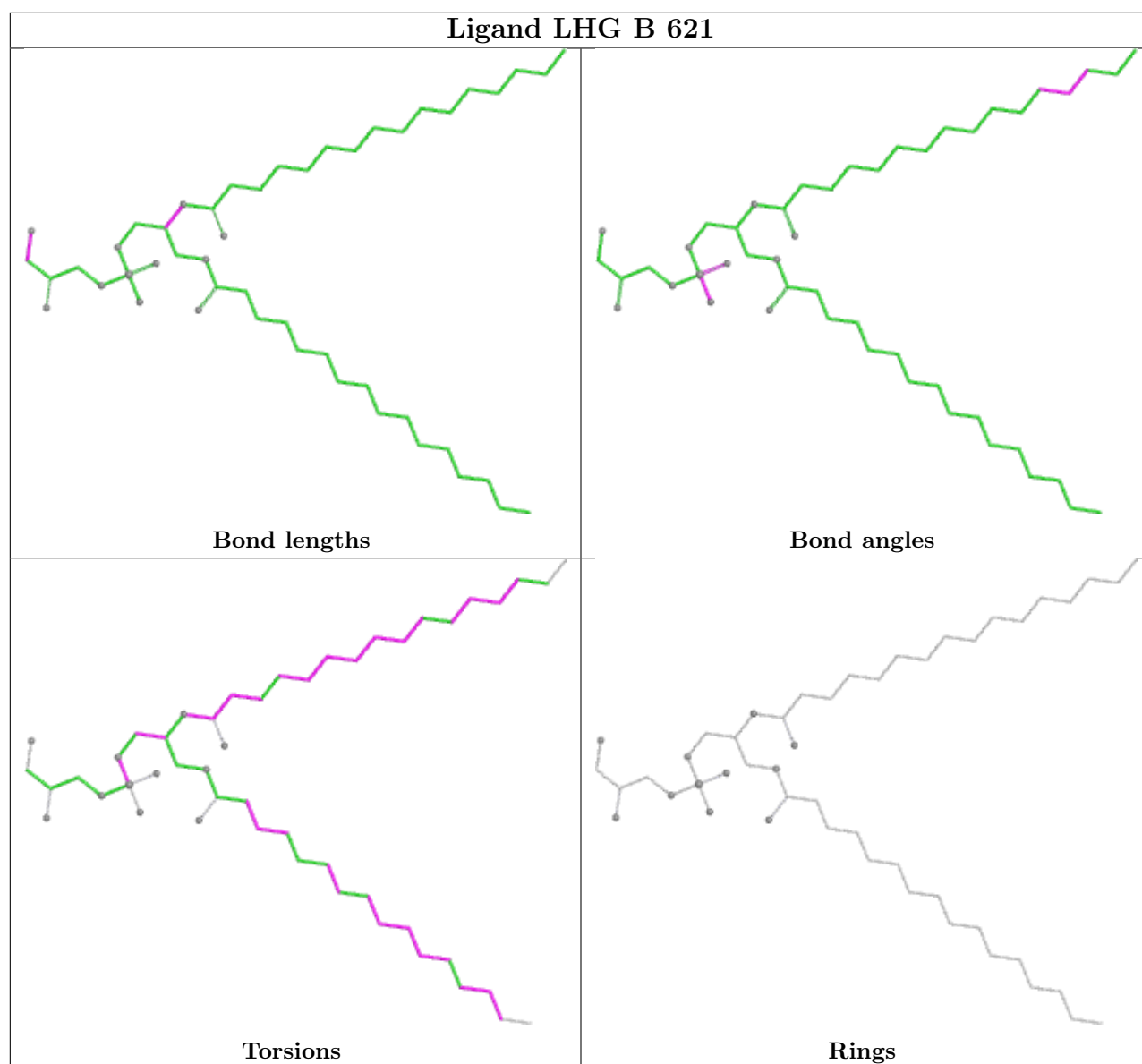
Ligand BCR c 516	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR b 619	
	
Bond lengths	Bond angles
	
Torsions	Rings

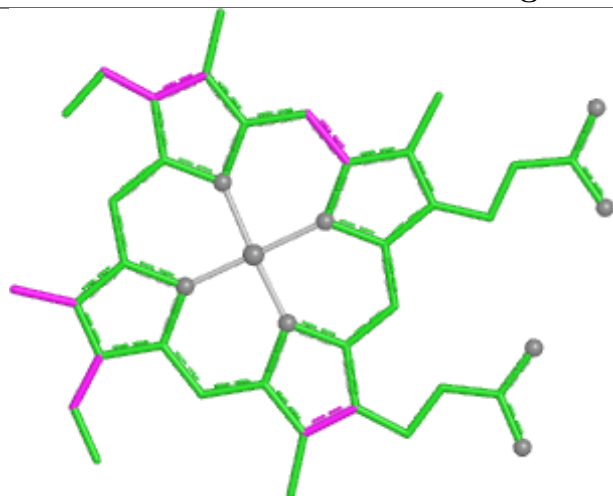
Ligand LMG C 520	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand DGD c 517	
	
Bond lengths	Bond angles
	
Torsions	Rings

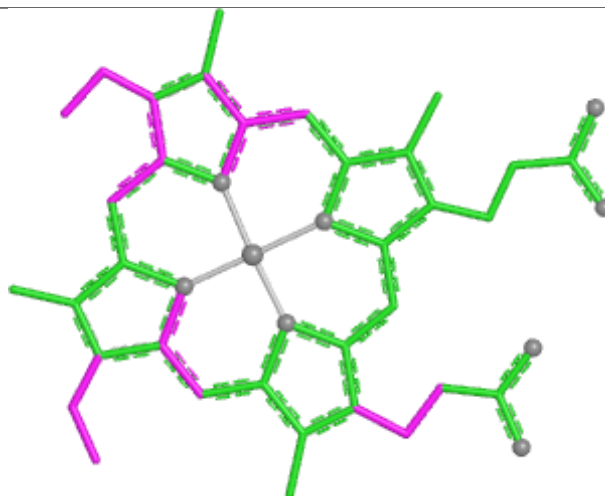




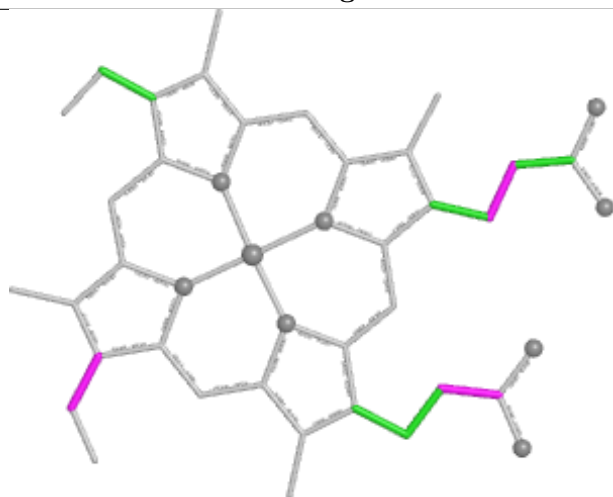
Ligand HEC f 101



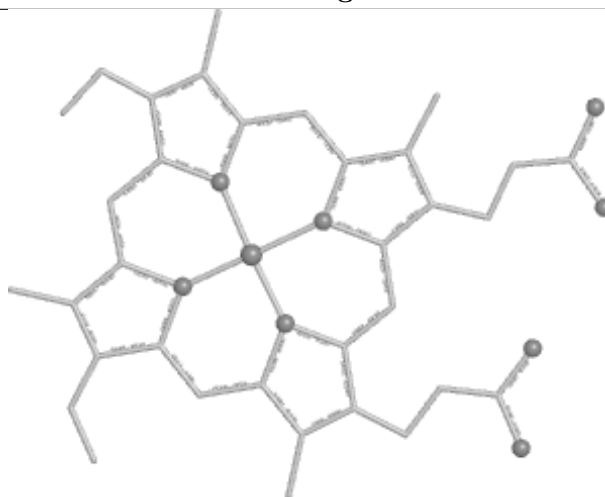
Bond lengths



Bond angles

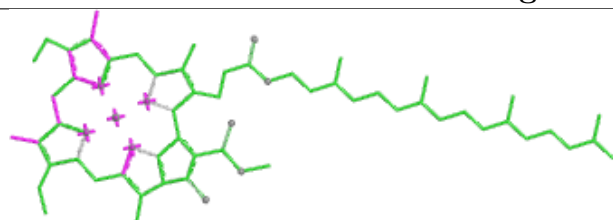


Torsions

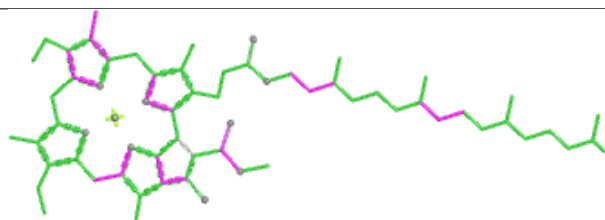


Rings

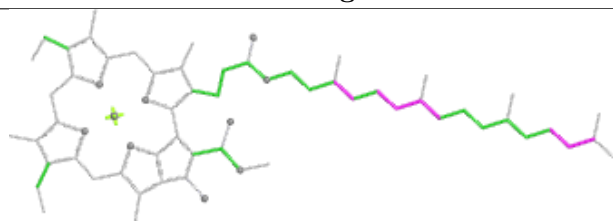
Ligand CLA c 505



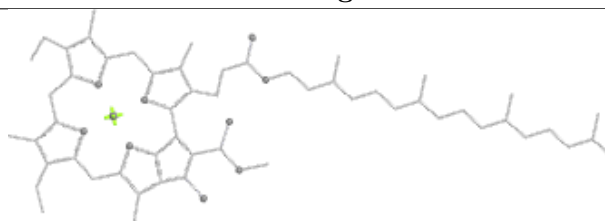
Bond lengths



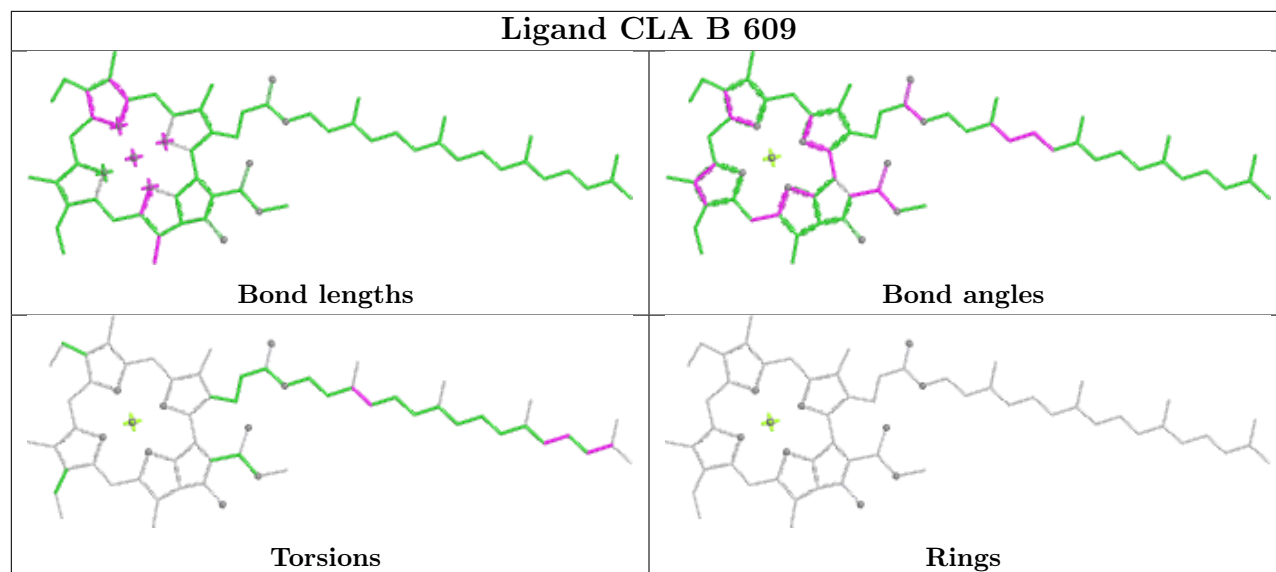
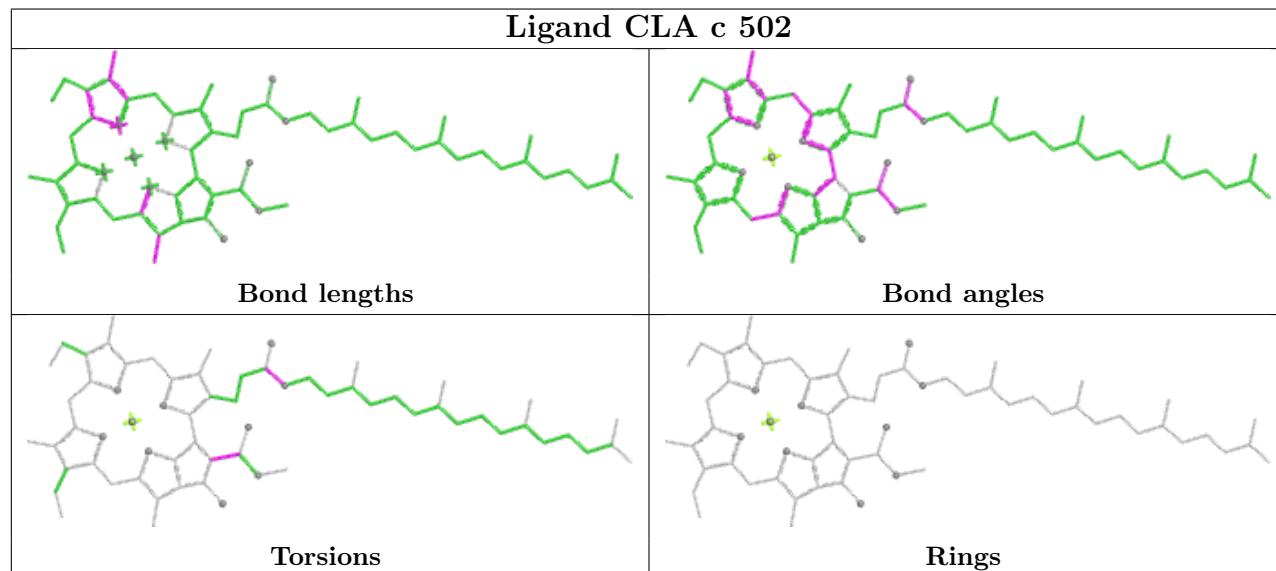
Bond angles

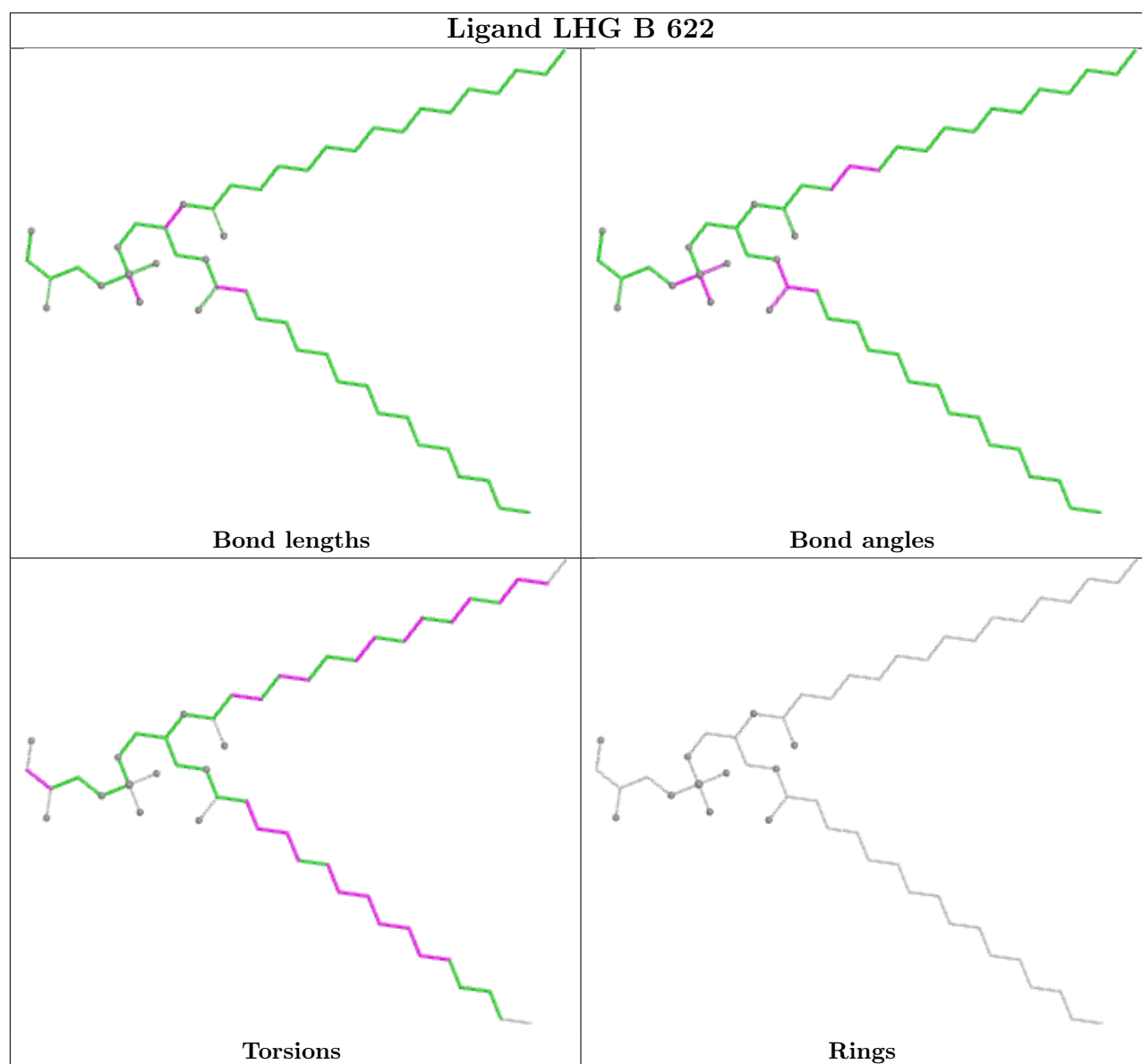


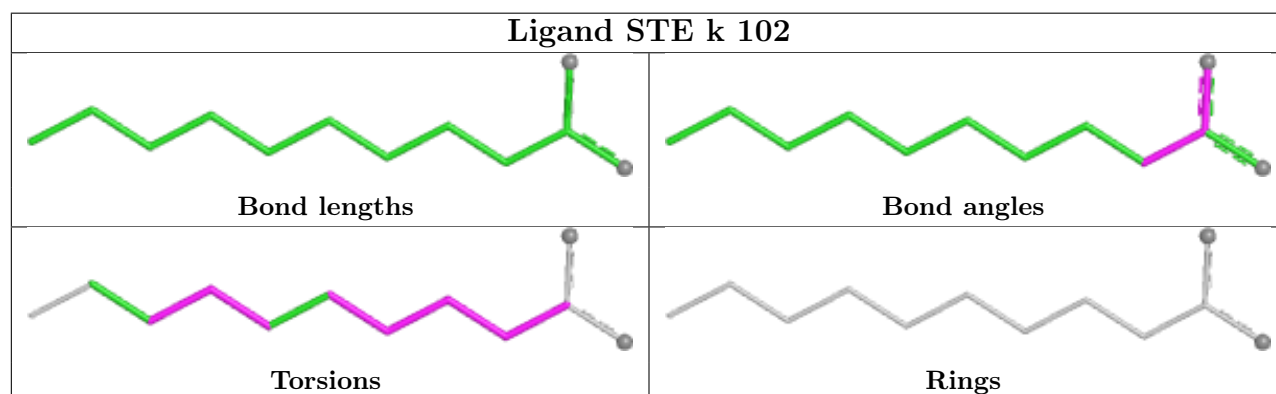
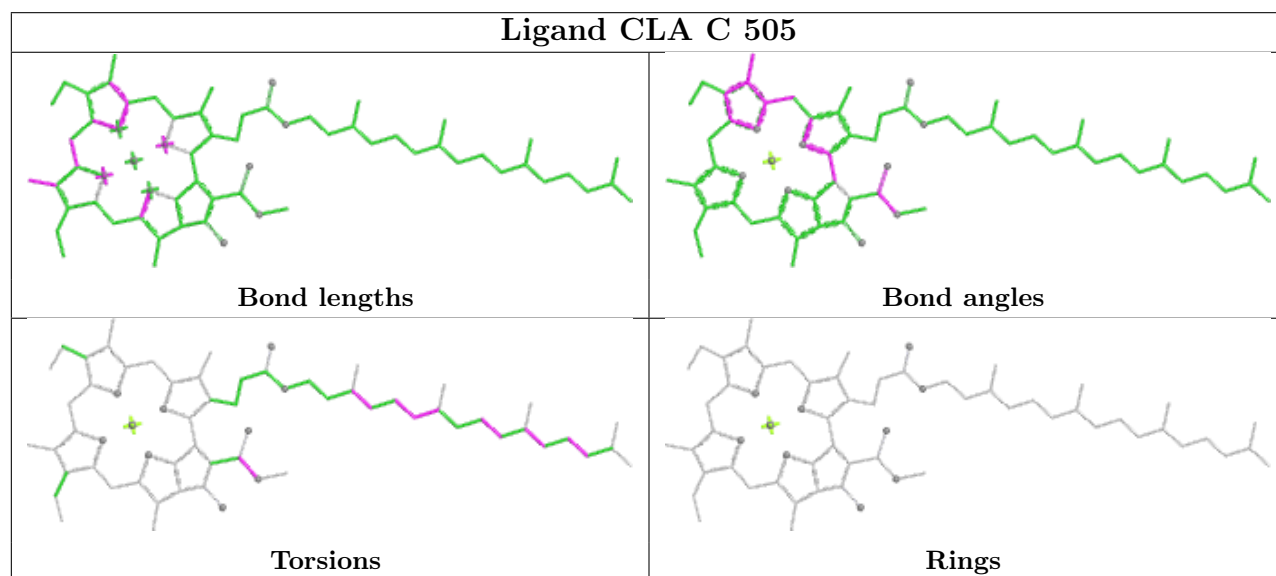
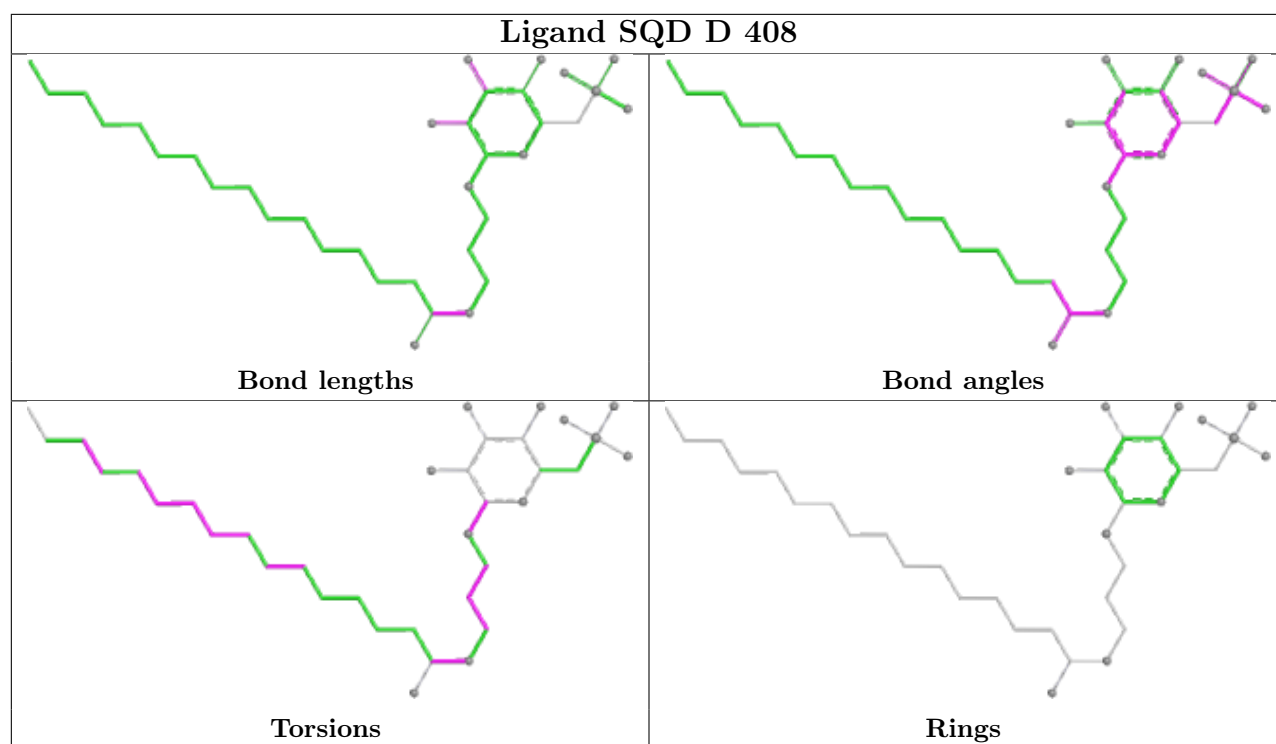
Torsions

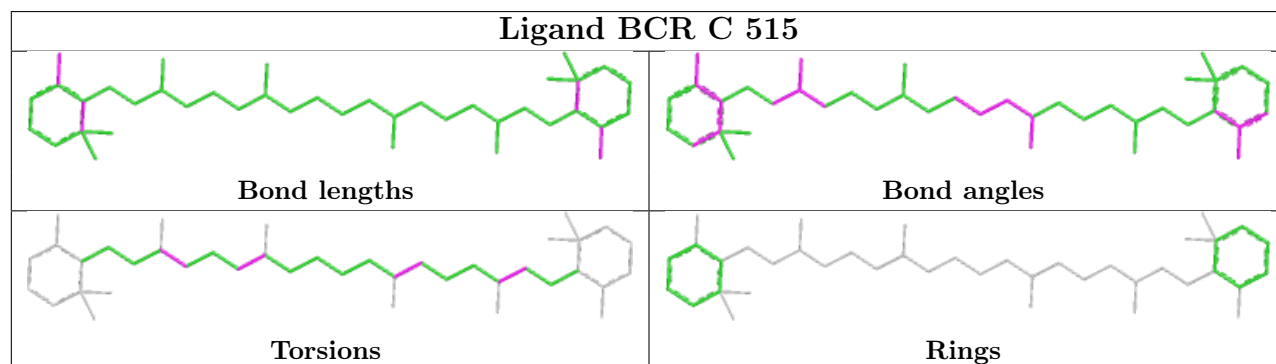
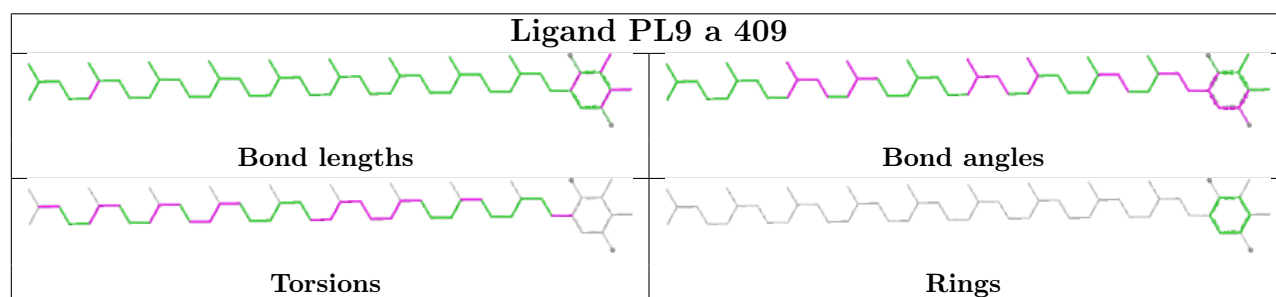
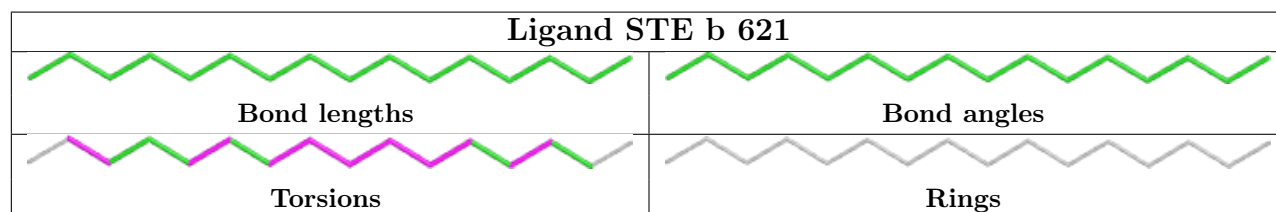
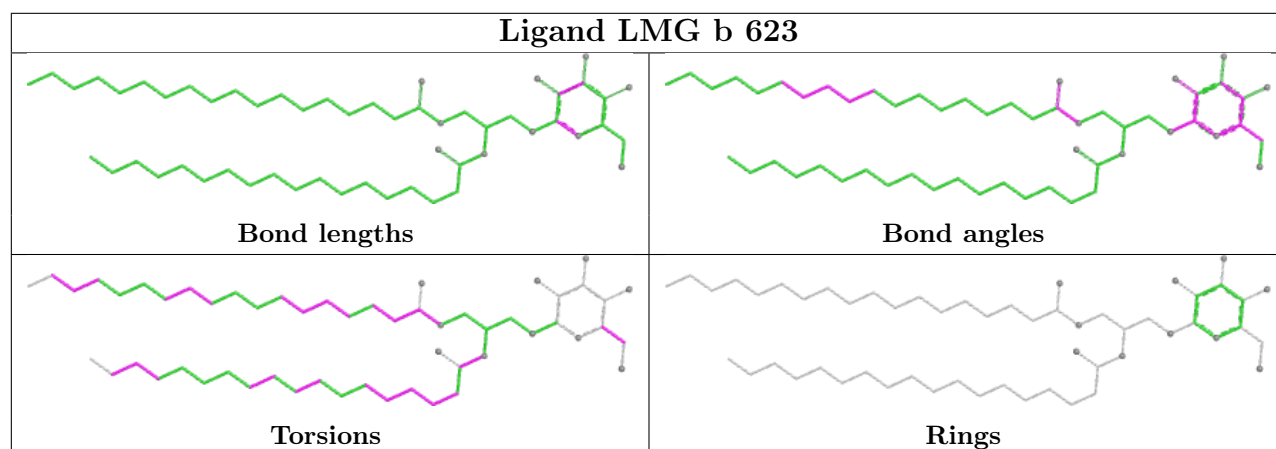
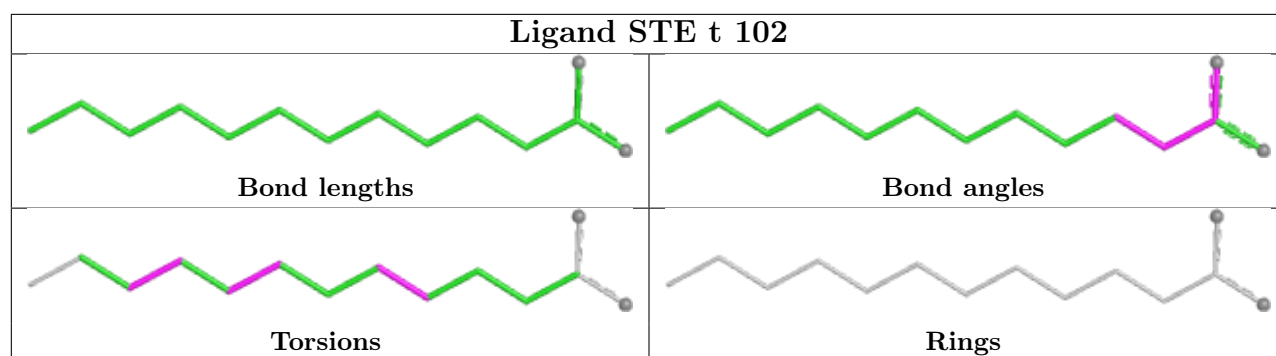


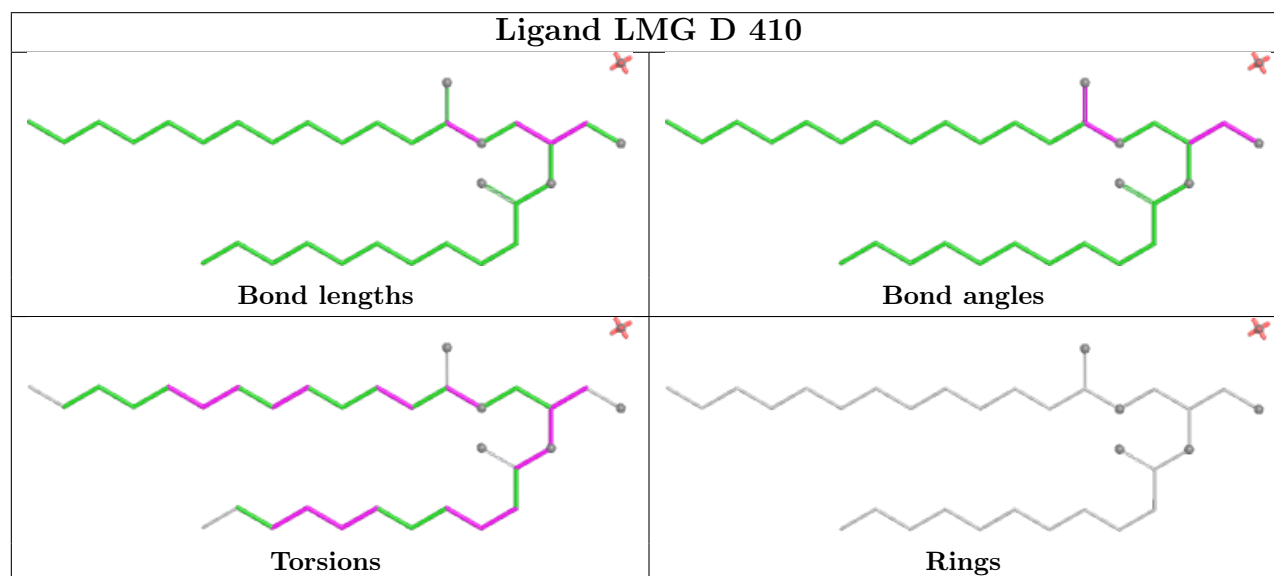
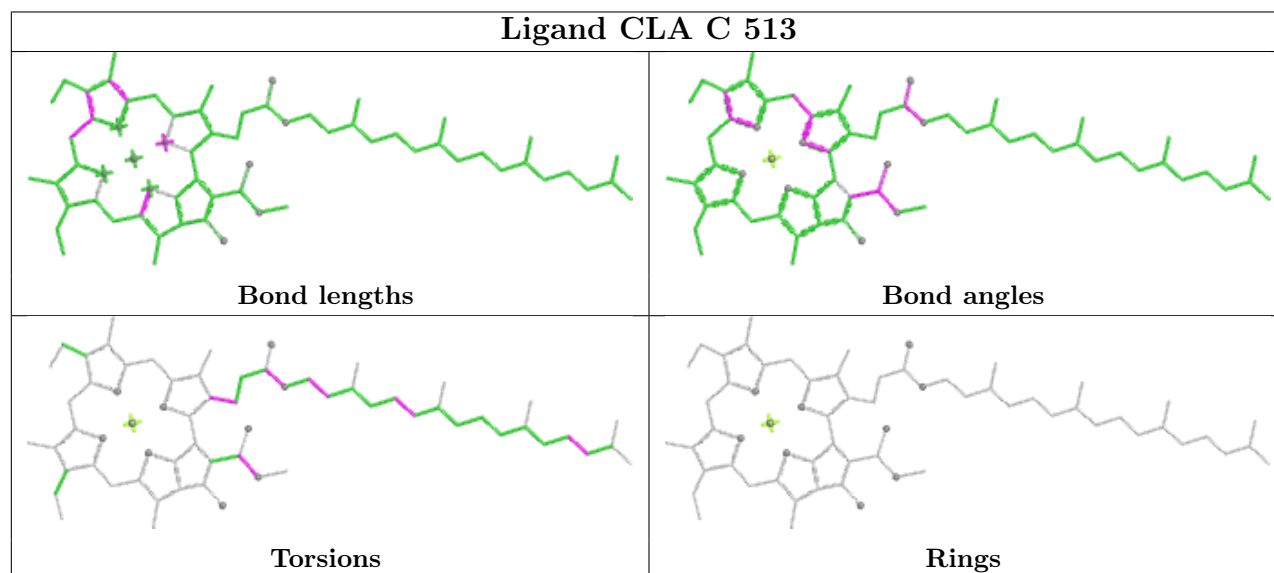
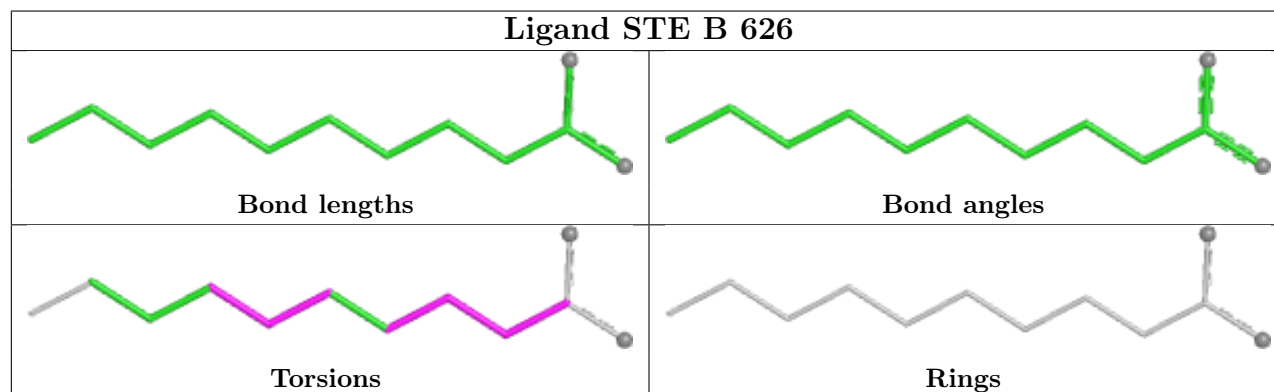
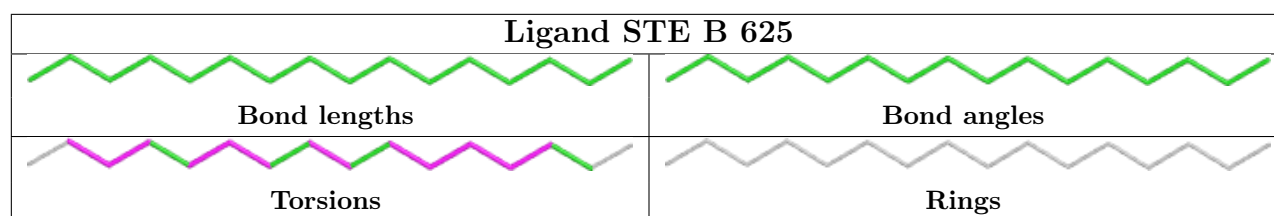
Rings

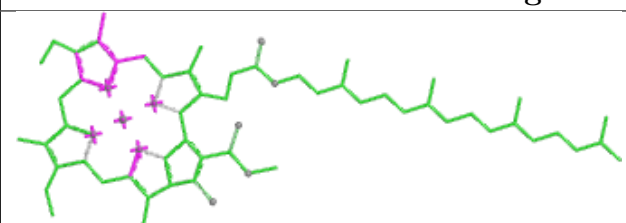
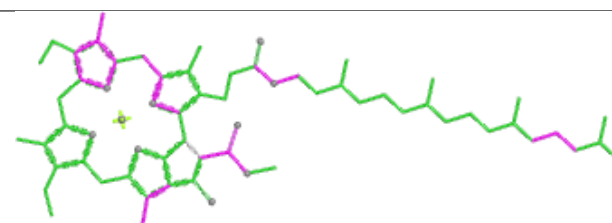
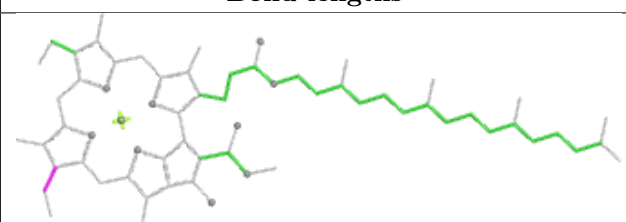
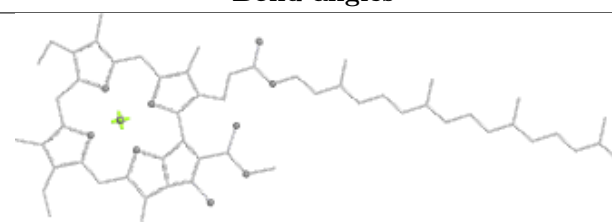
Ligand CLA B 609**Ligand CLA c 502**

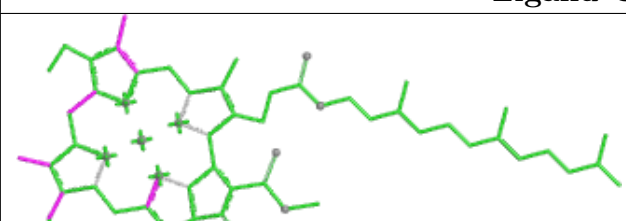
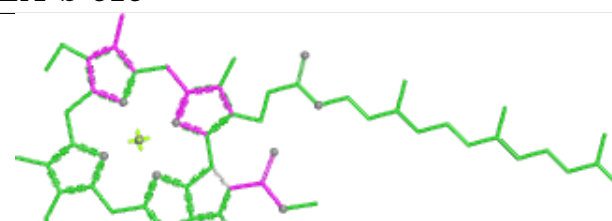
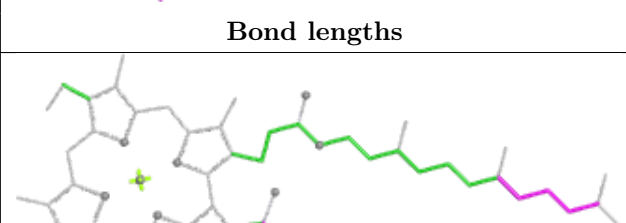
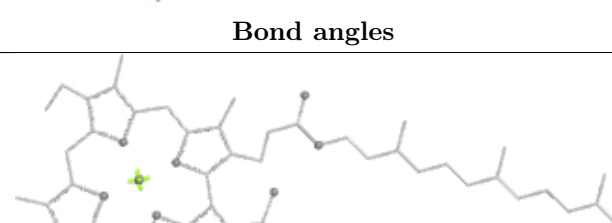


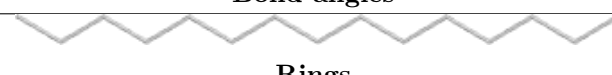


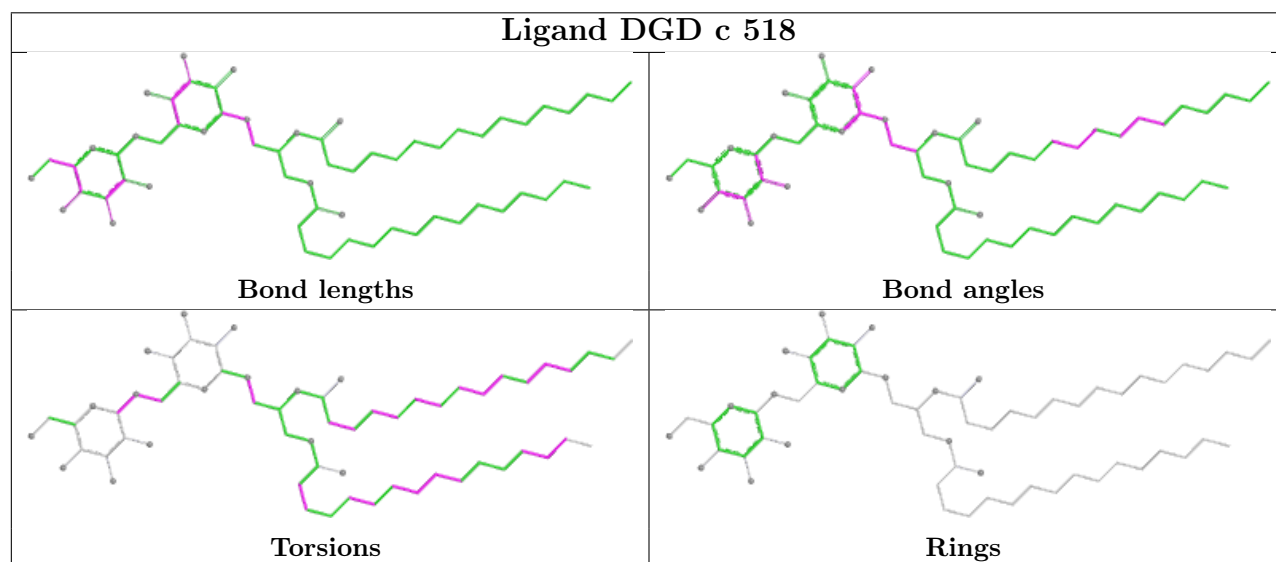
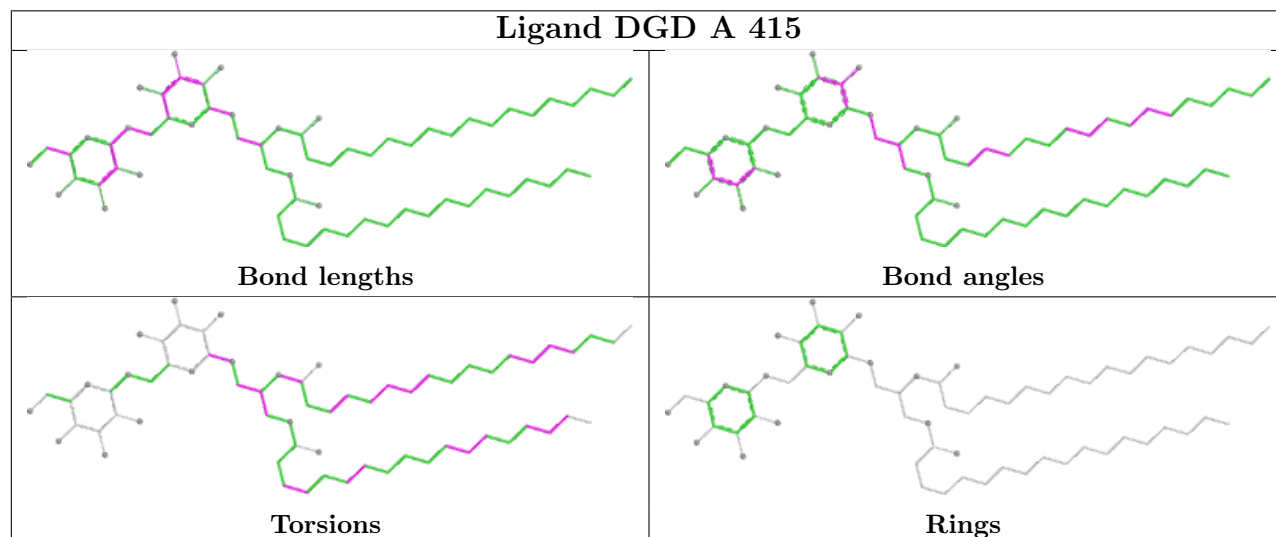
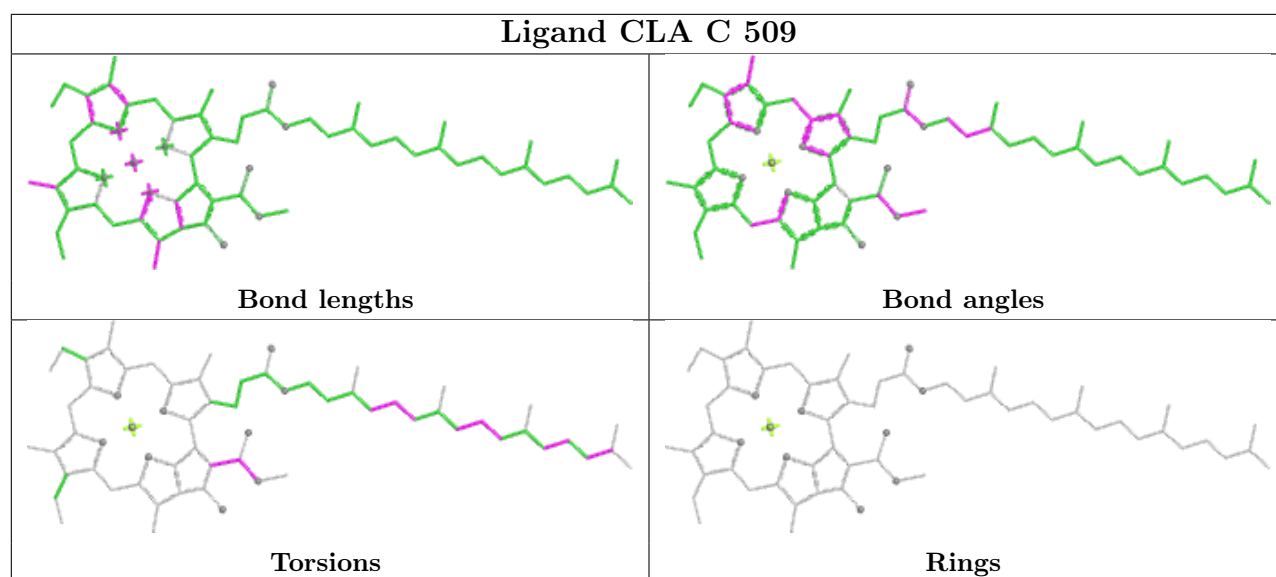




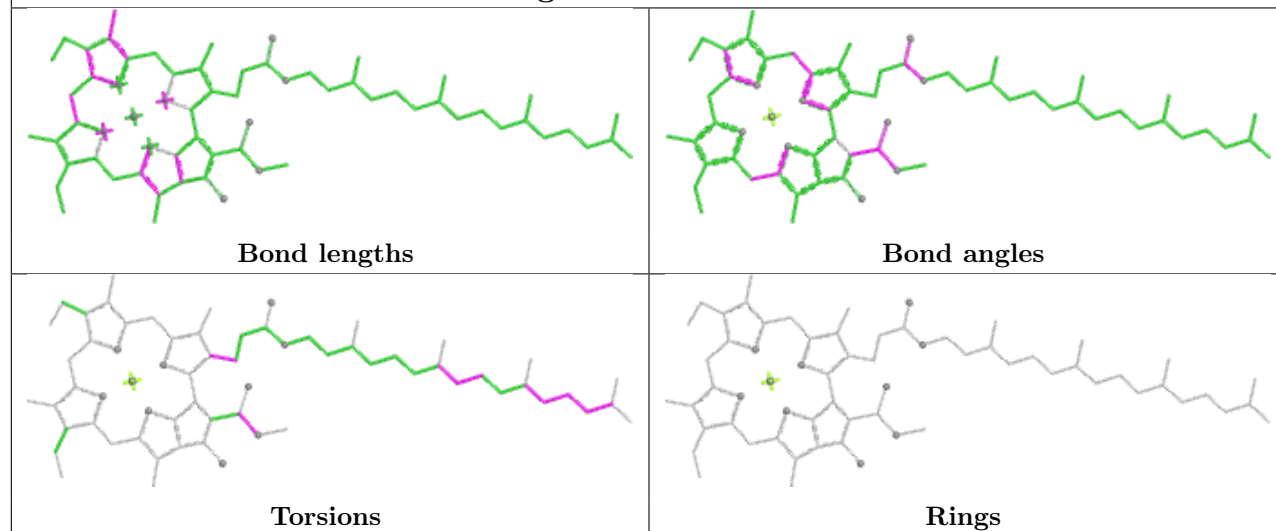
Ligand CLA d 404	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 616	
	
Bond lengths	Bond angles
	
Torsions	Rings

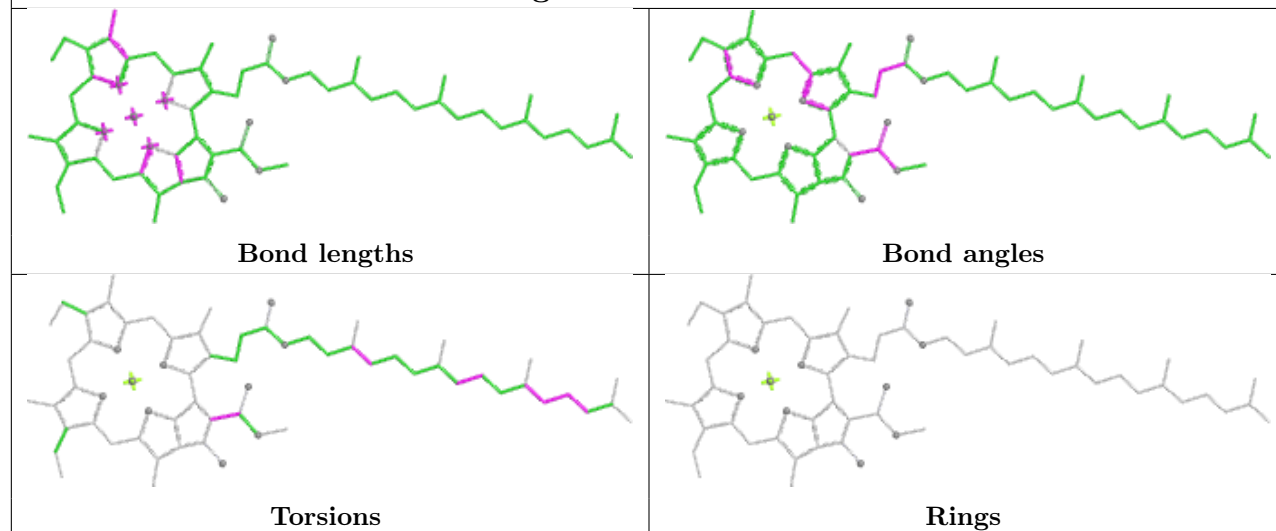
Ligand STE I 101	
	
Bond lengths	Bond angles
	
Torsions	Rings



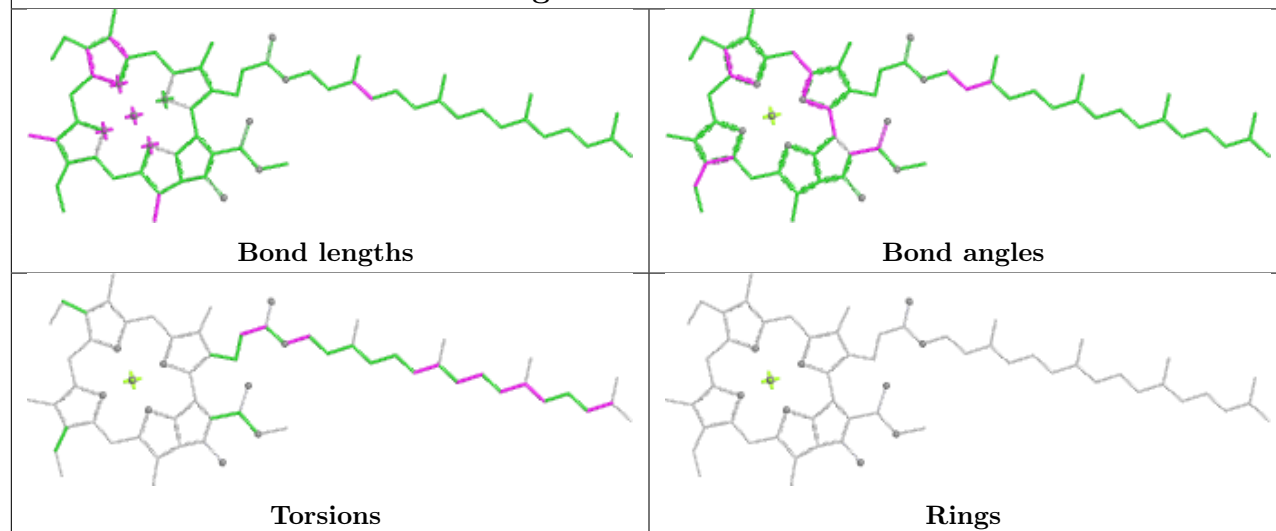
Ligand CLA c 511



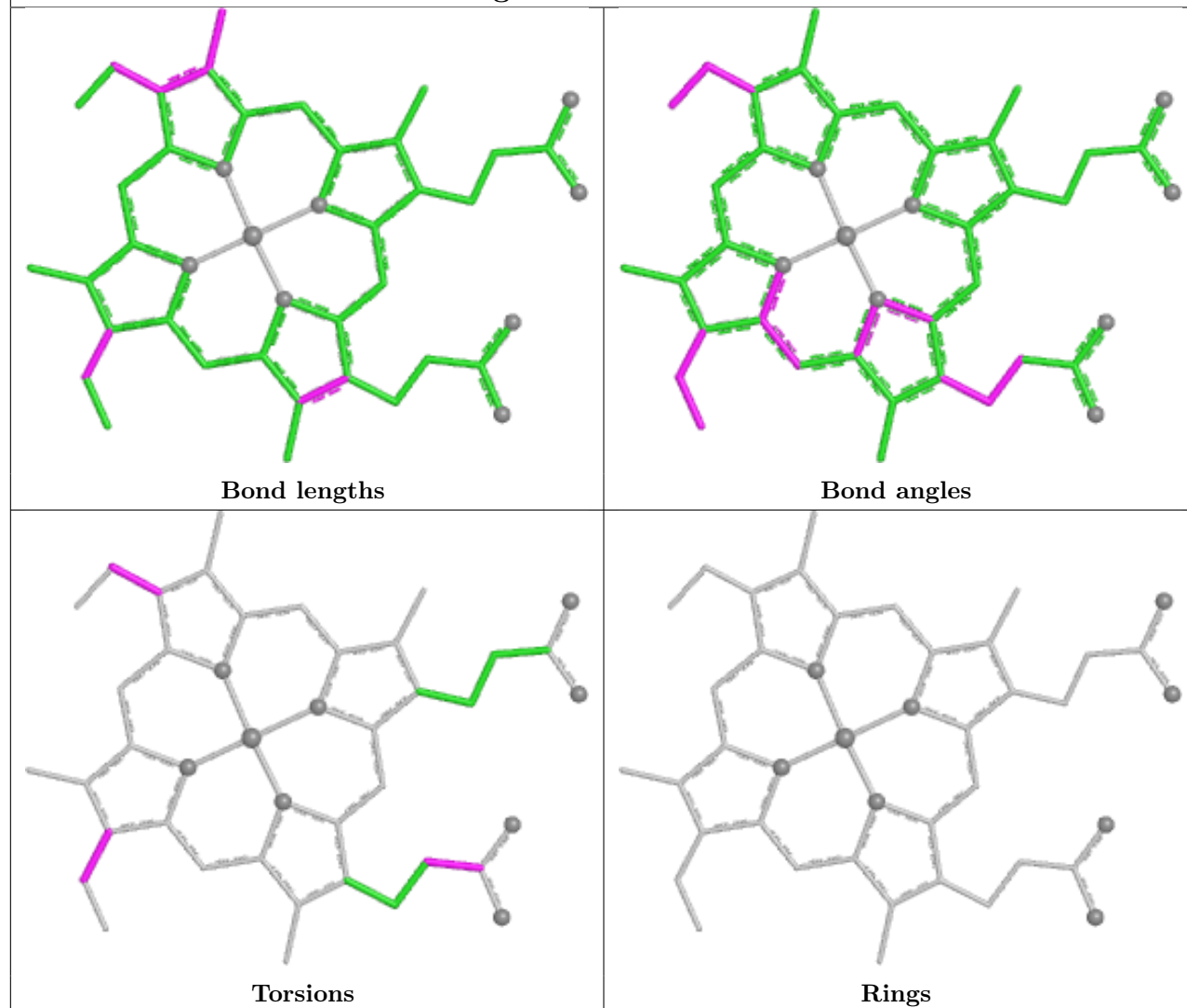
Ligand CLA C 506



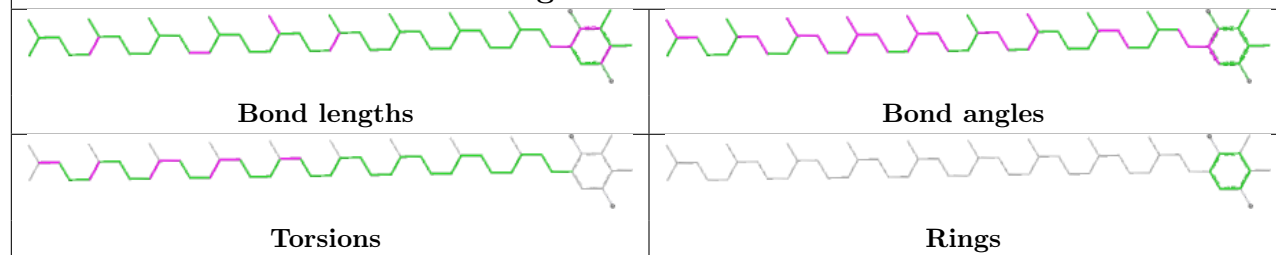
Ligand CLA B 613

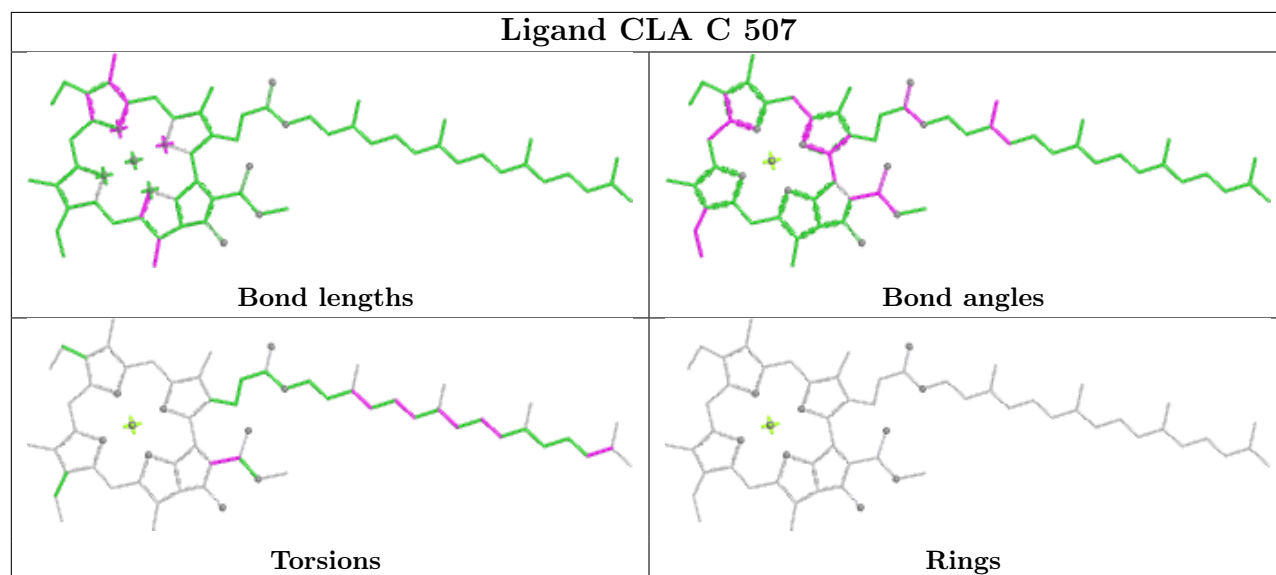
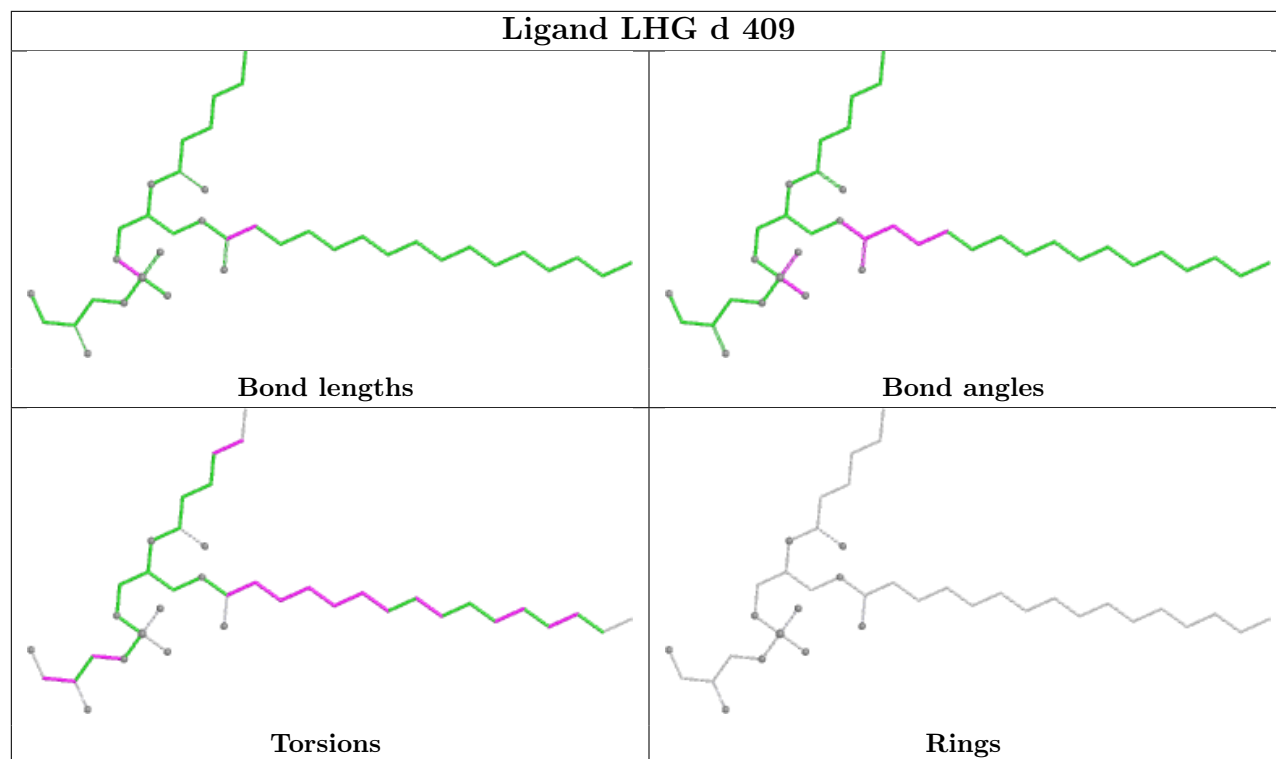


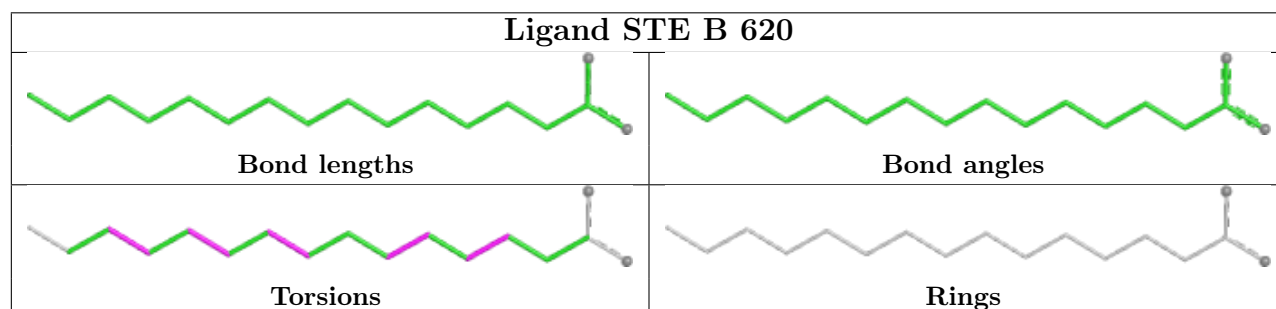
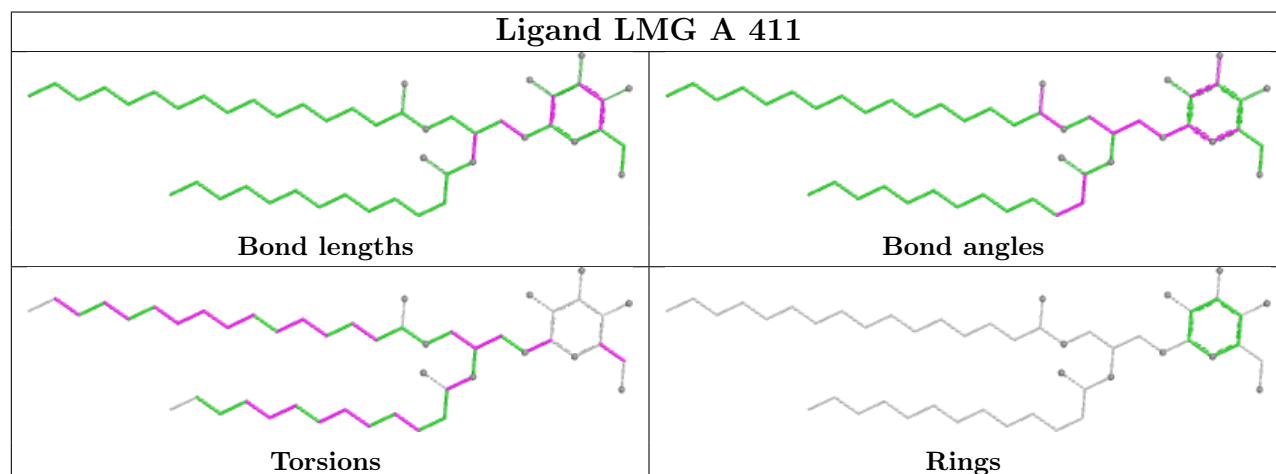
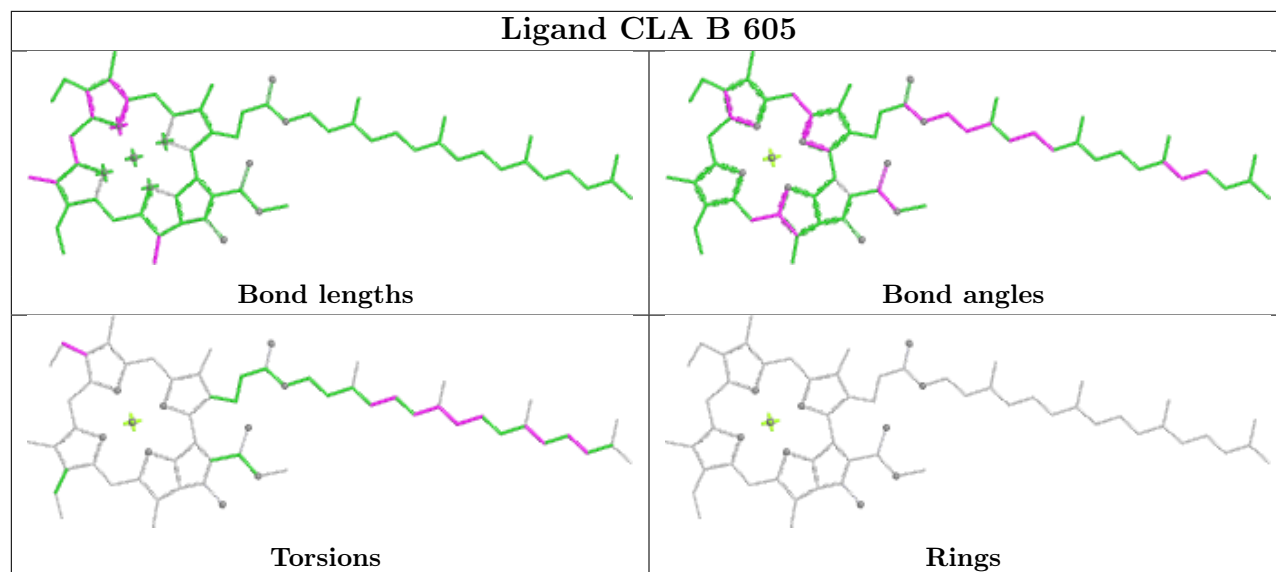
Ligand HEC V 201

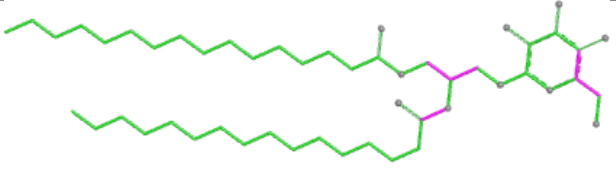
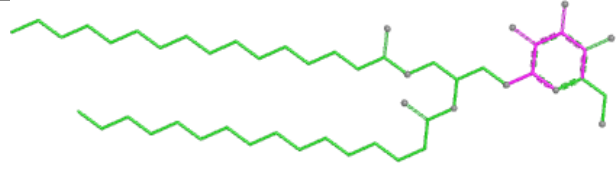
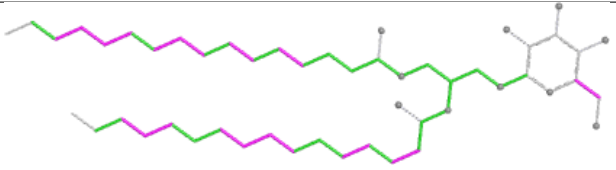
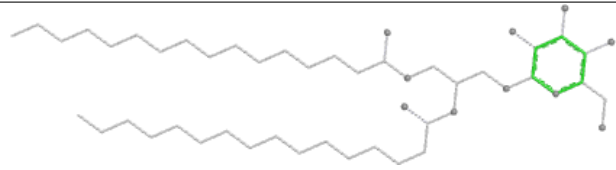


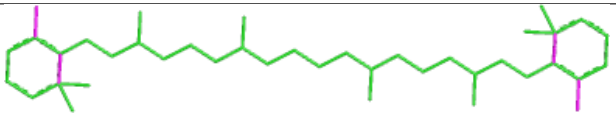
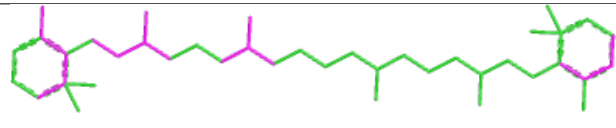
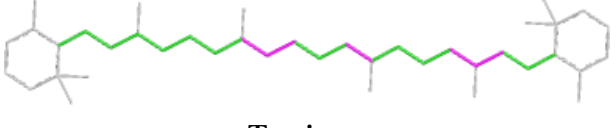
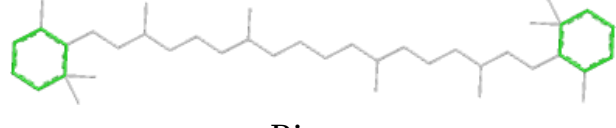
Ligand PL9 D 406

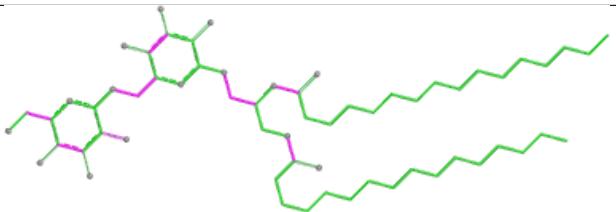
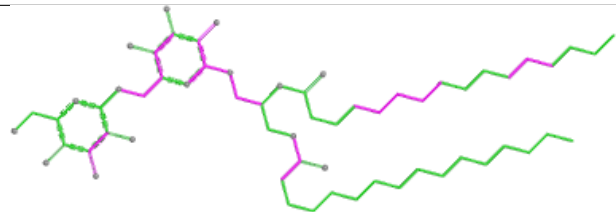
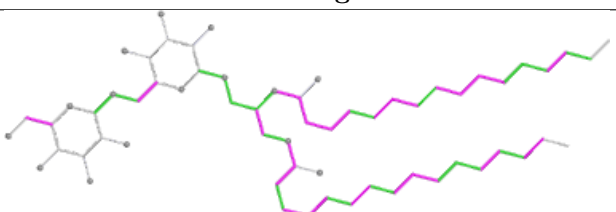
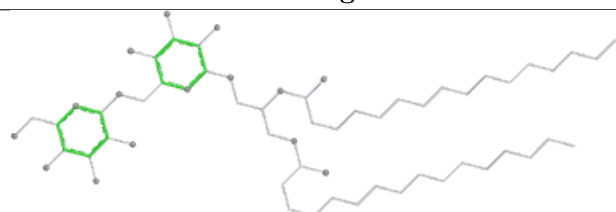


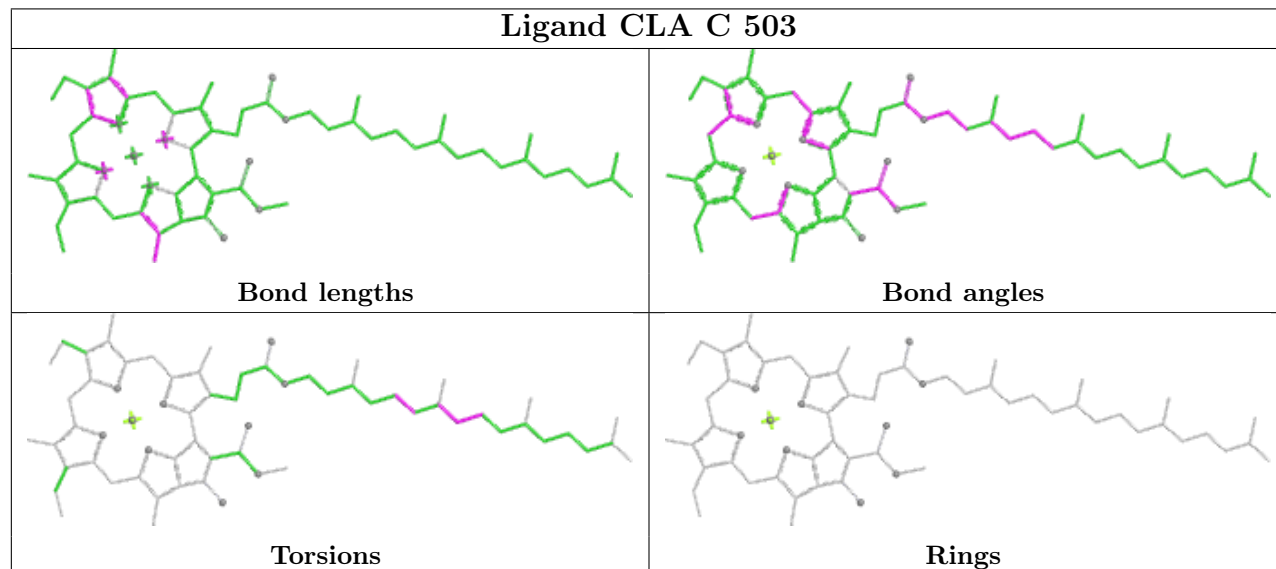
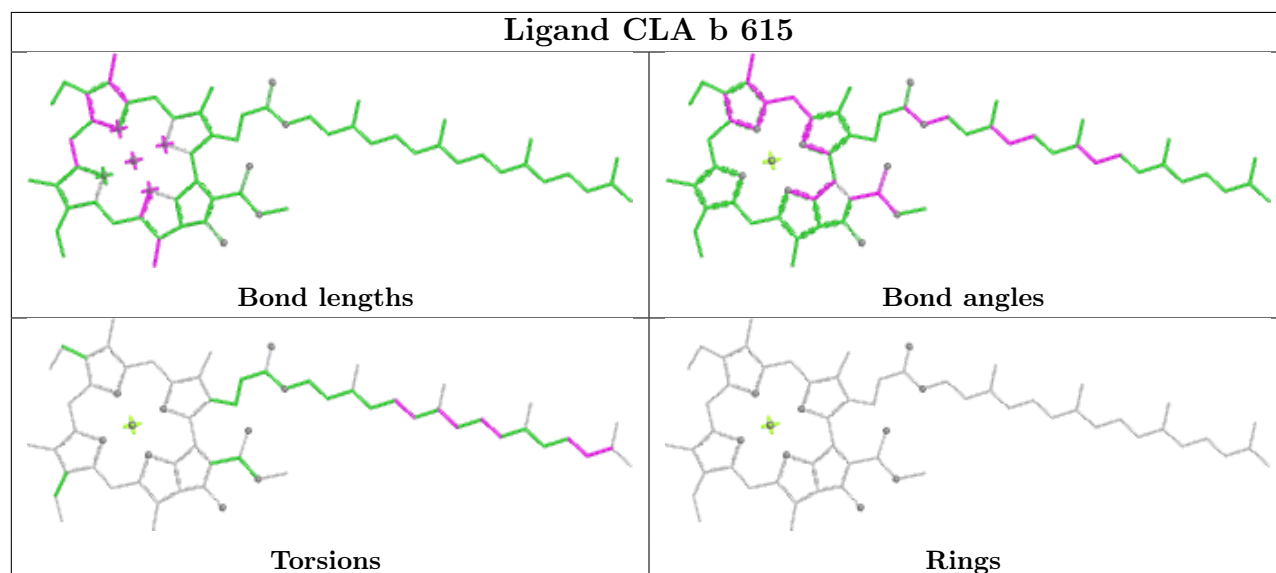
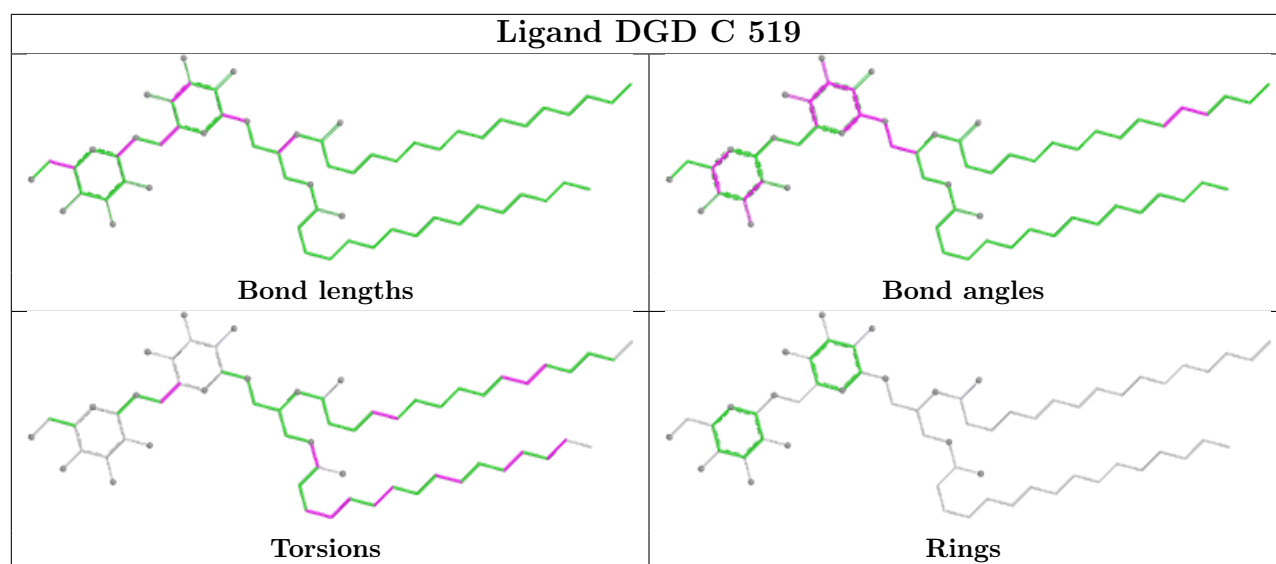


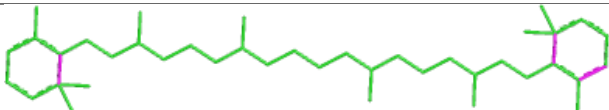
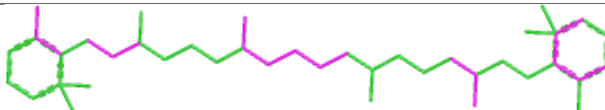
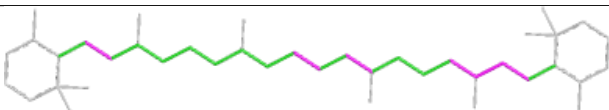
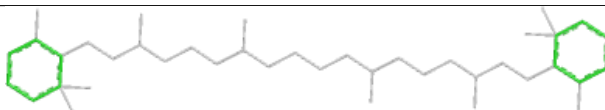


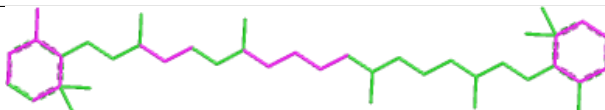
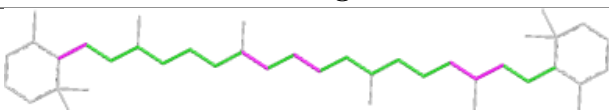
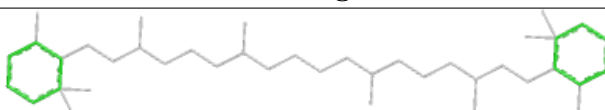
Ligand LMG D 407	
	
Bond lengths	Bond angles
	
Torsions	Rings

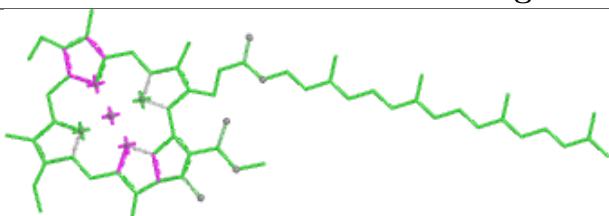
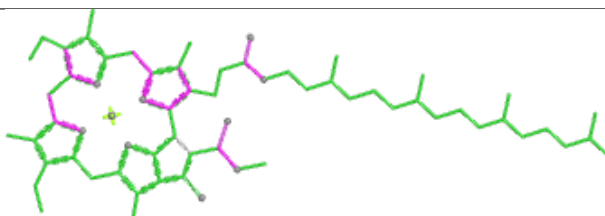
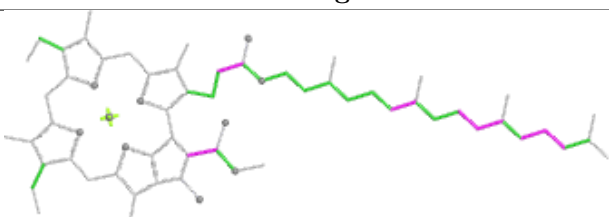
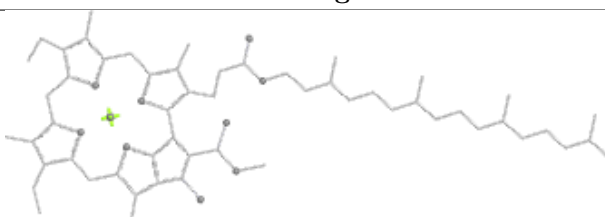
Ligand BCR c 515	
	
Bond lengths	Bond angles
	
Torsions	Rings

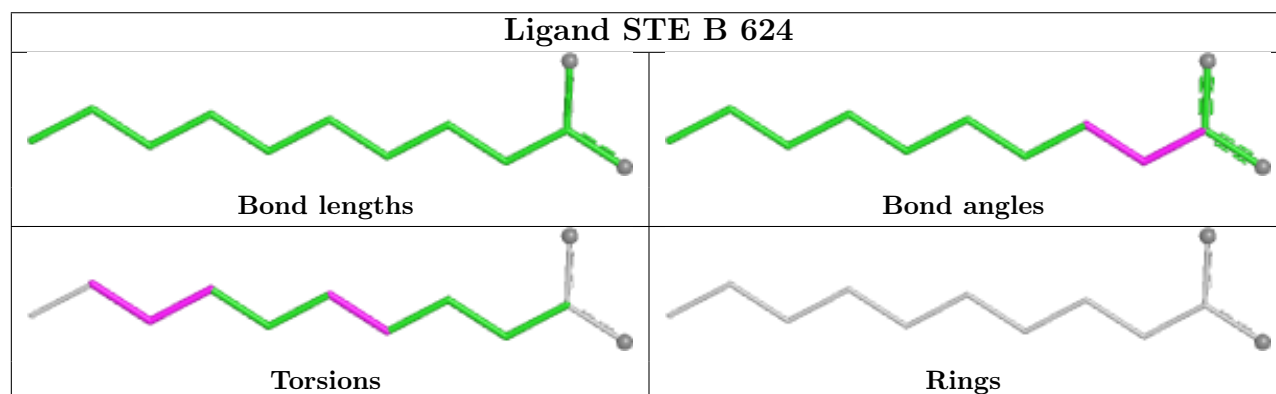
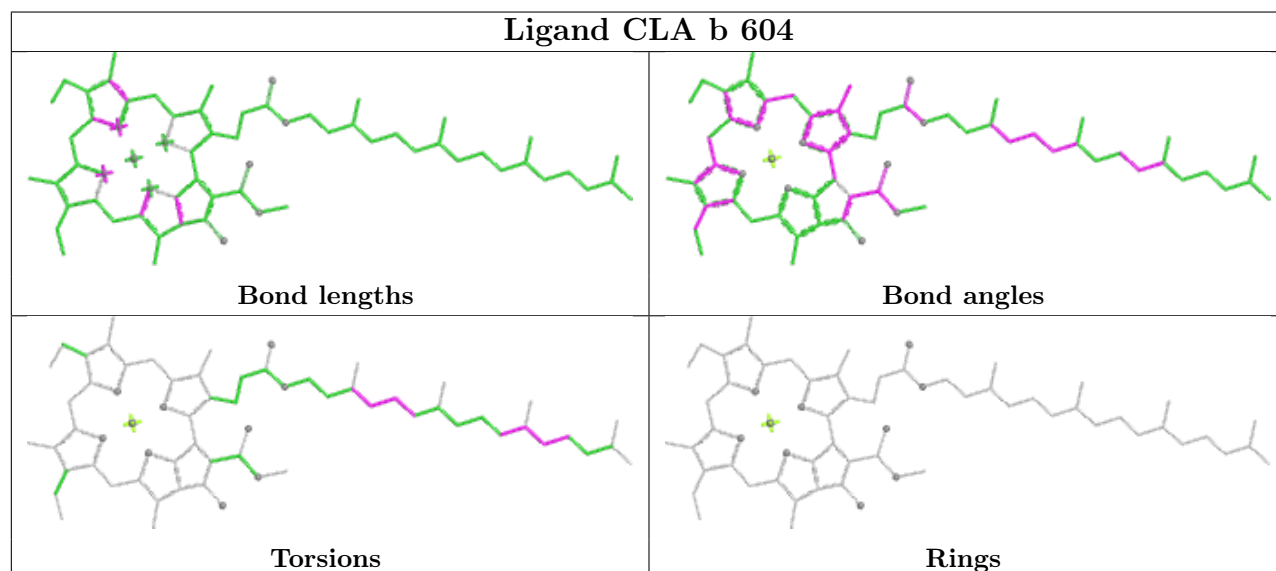
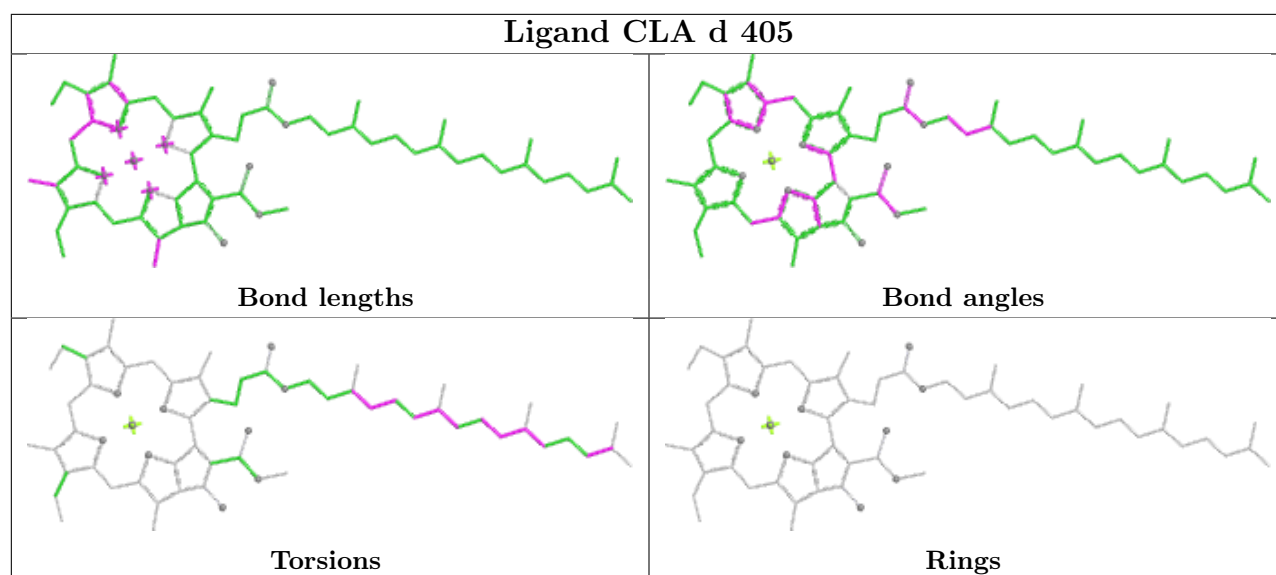
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Bond lengths	Bond angles
	
Torsions	Rings

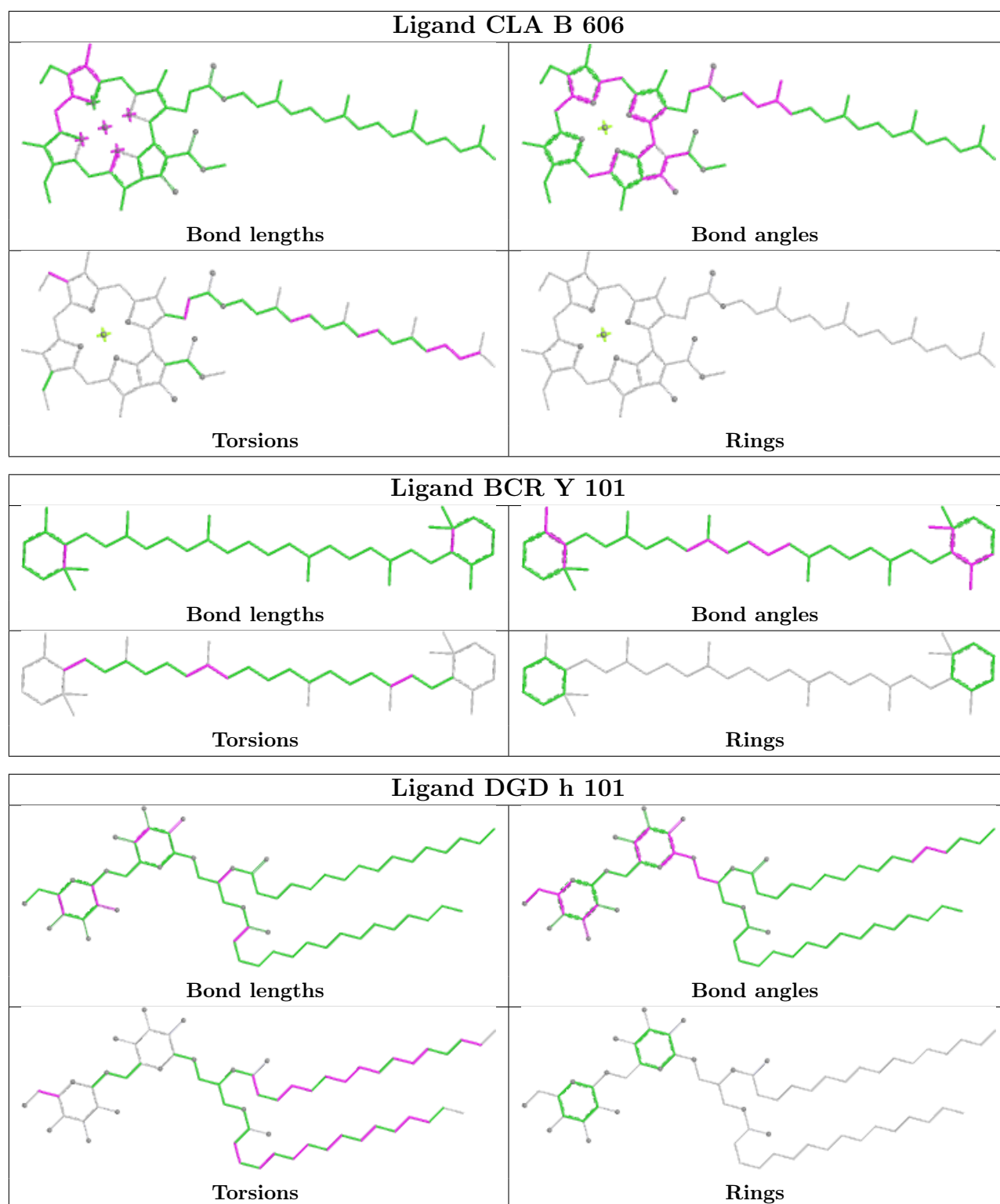


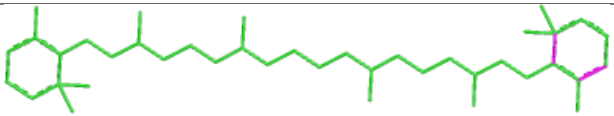
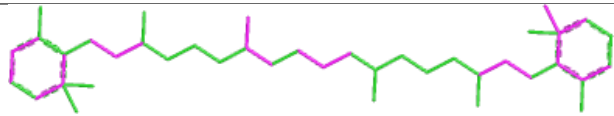
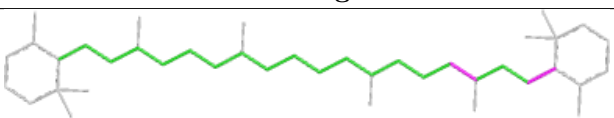
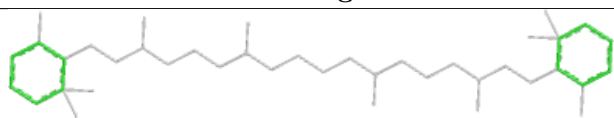
Ligand BCR b 618	
	
Bond lengths	Bond angles
	
Torsions	Rings

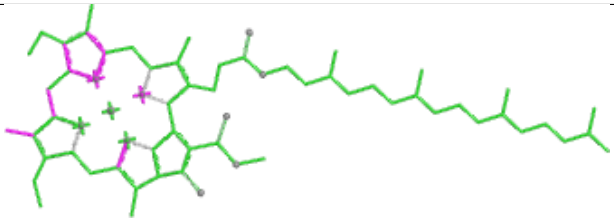
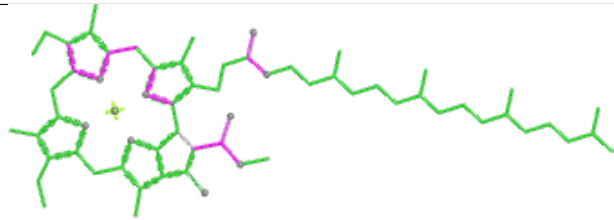
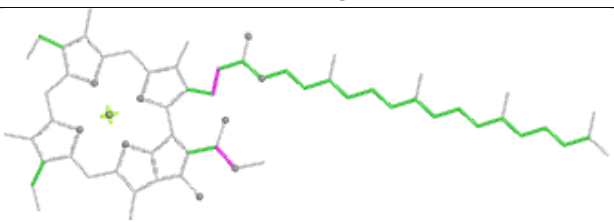
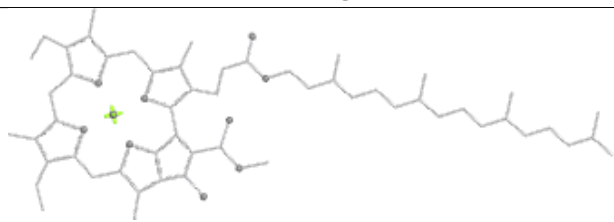
Ligand BCR b 617	
	
Bond lengths	Bond angles
	
Torsions	Rings

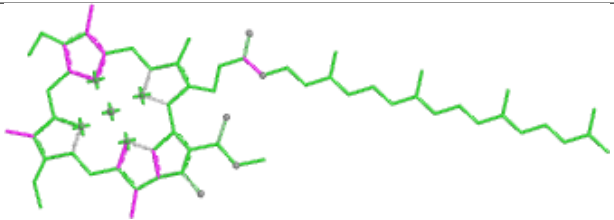
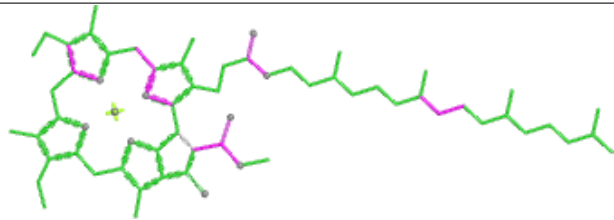
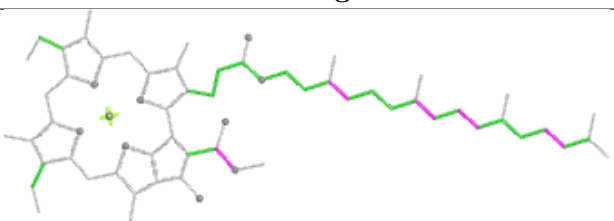
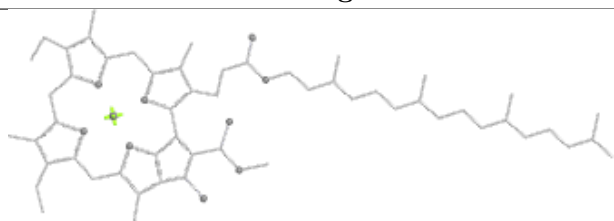
Ligand CLA c 509	
	
Bond lengths	Bond angles
	
Torsions	Rings





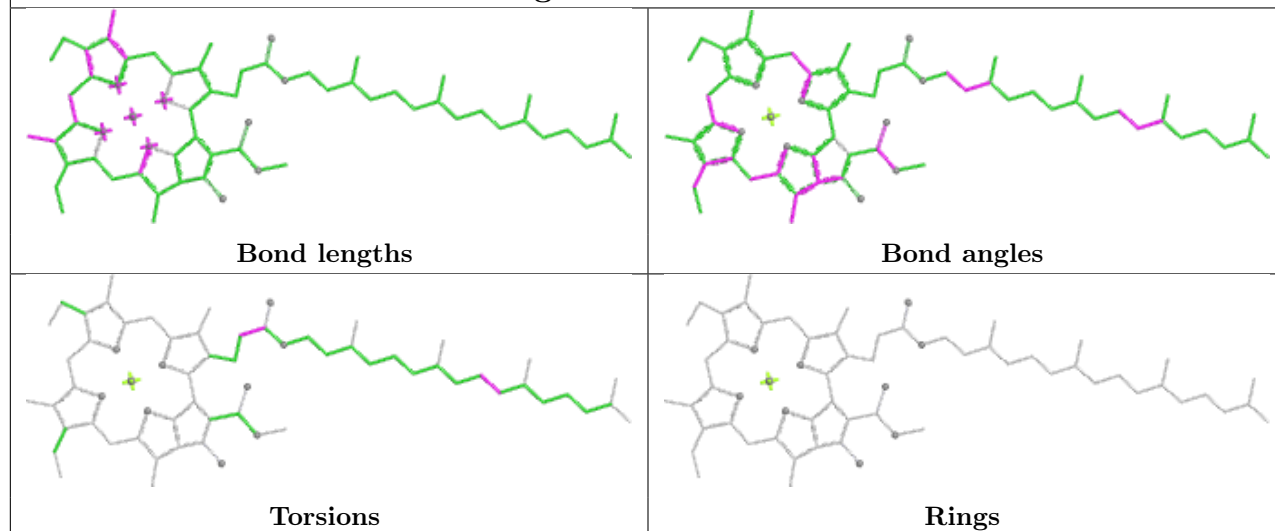
Ligand BCR B 618	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA C 501	
	
Bond lengths	Bond angles
	
Torsions	Rings

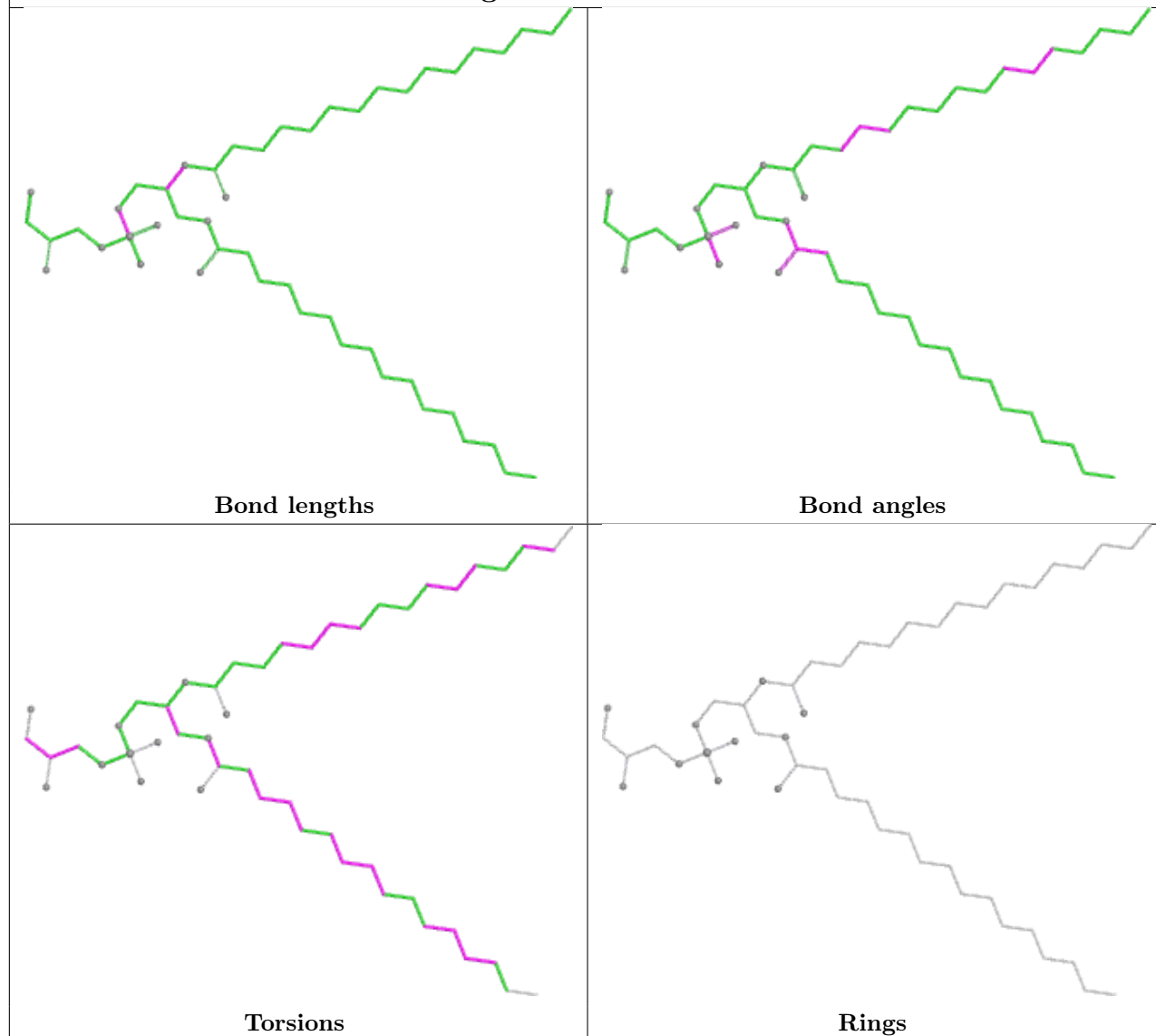
Ligand CLA C 510	
	
Bond lengths	Bond angles
	
Torsions	Rings

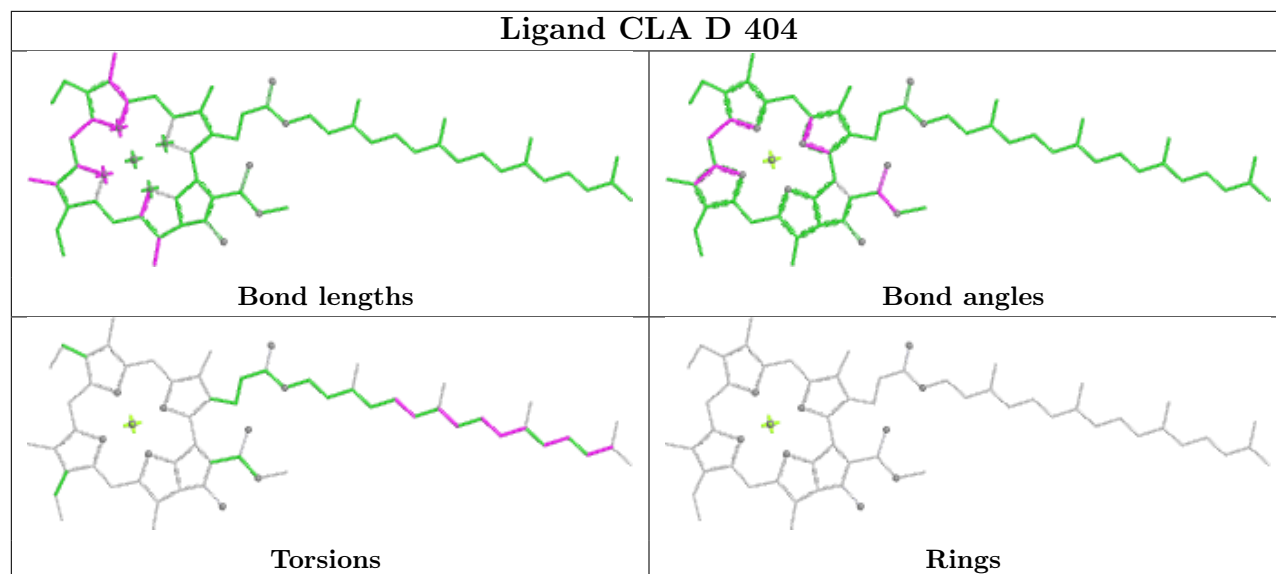
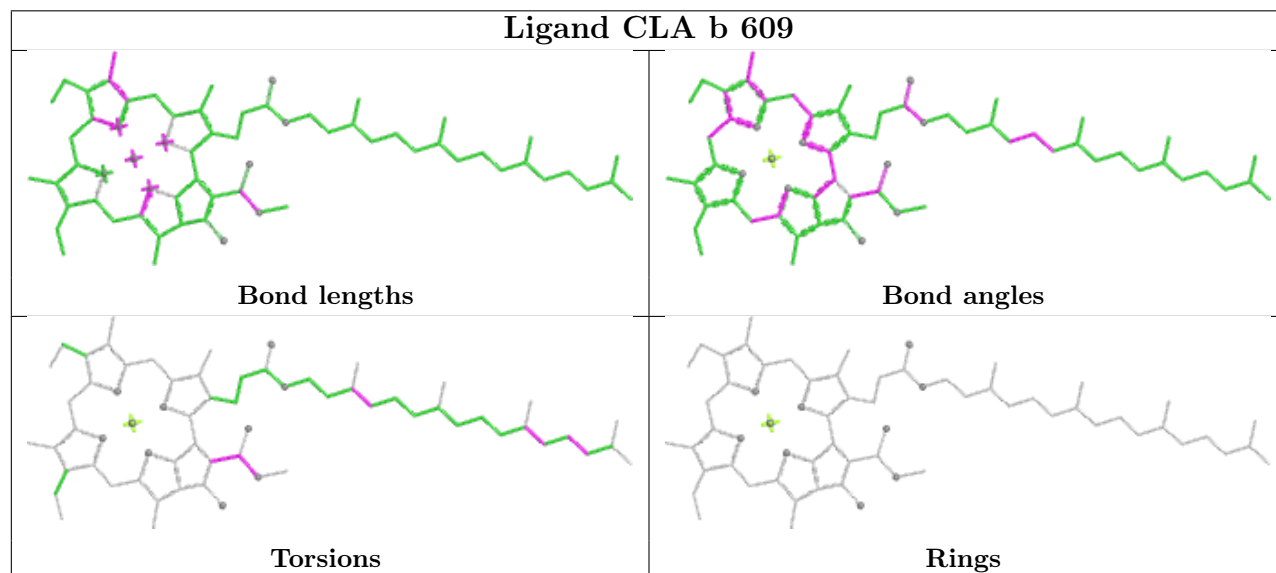
Ligand STE H 103	
	
Bond lengths	Bond angles
	
Torsions	Rings

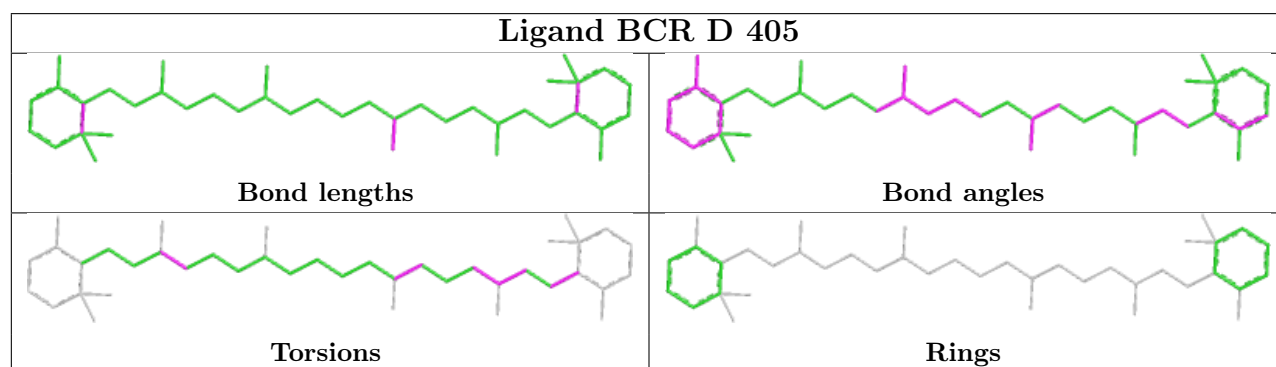
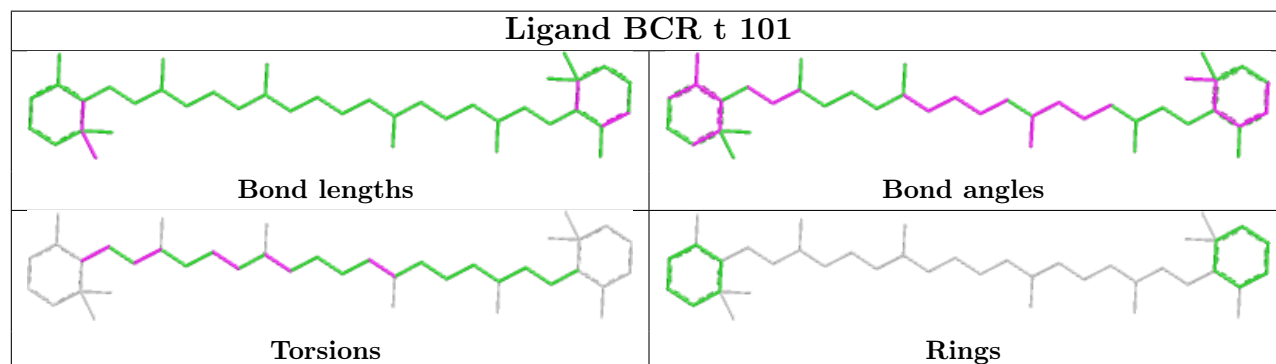
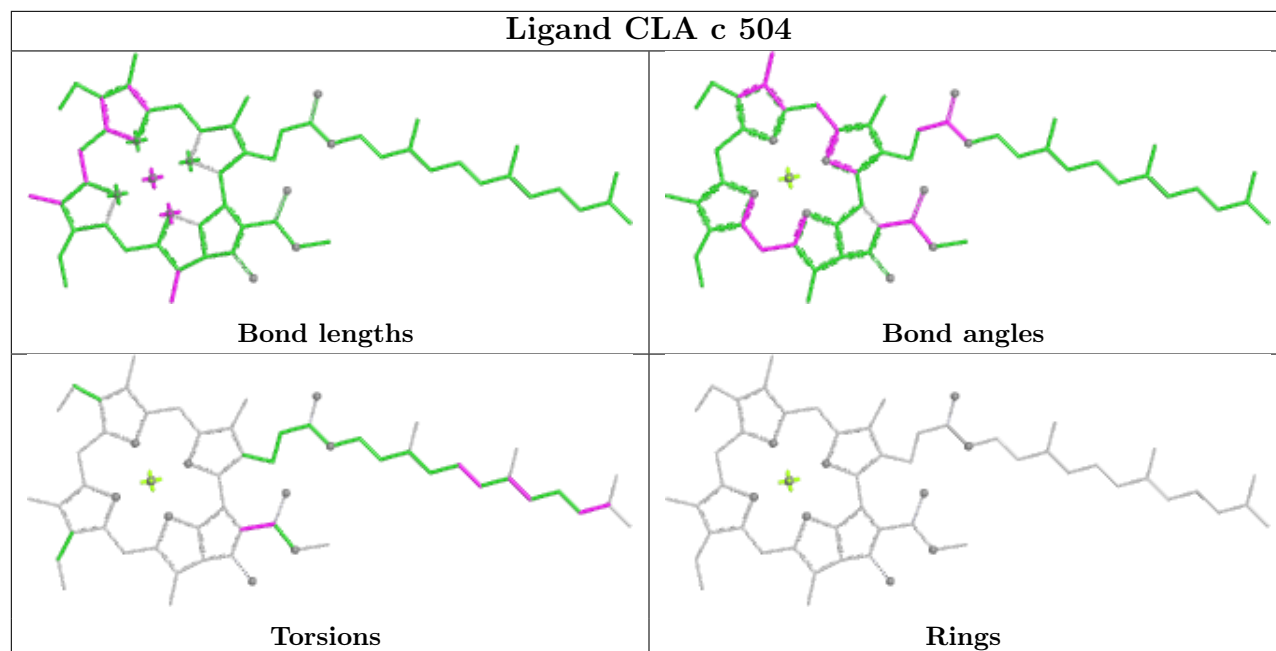
Ligand CLA b 612

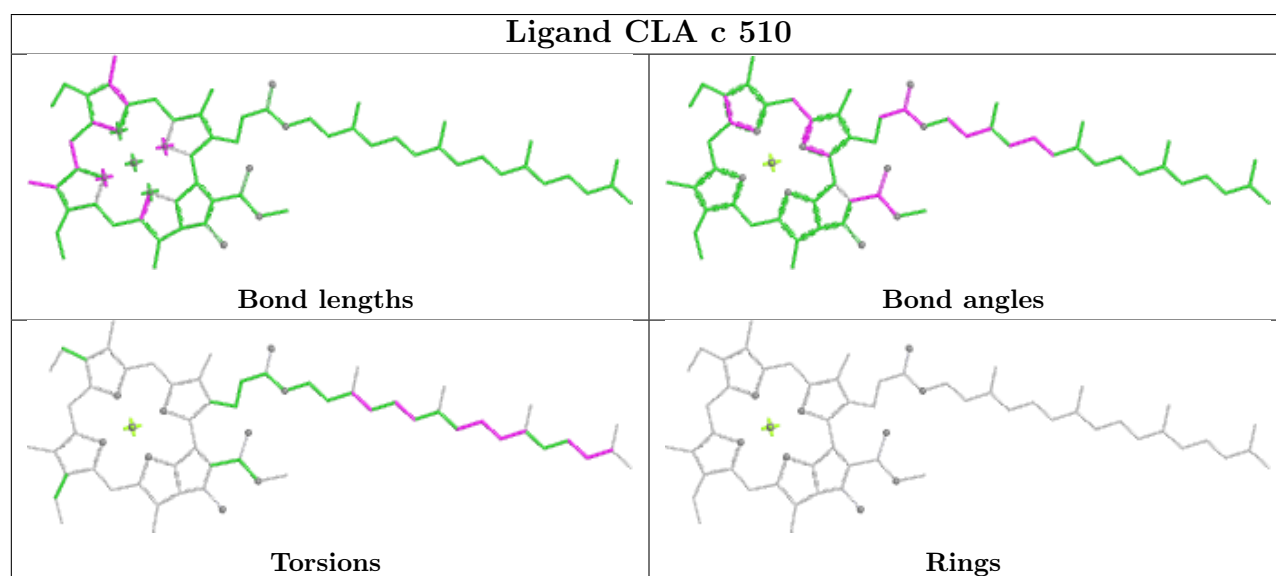
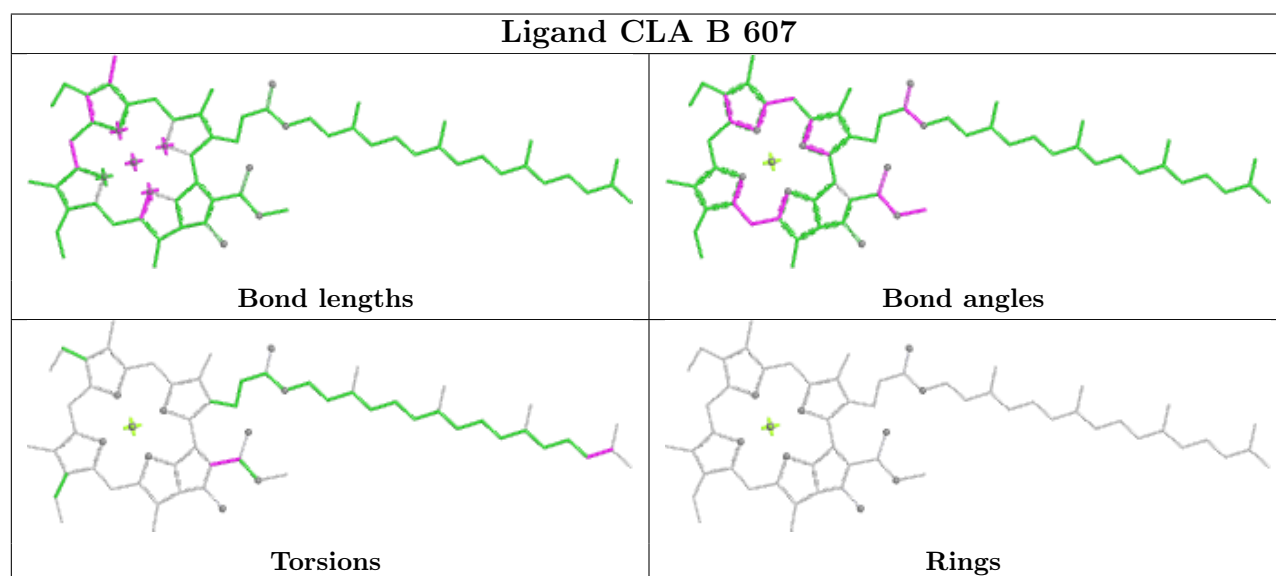
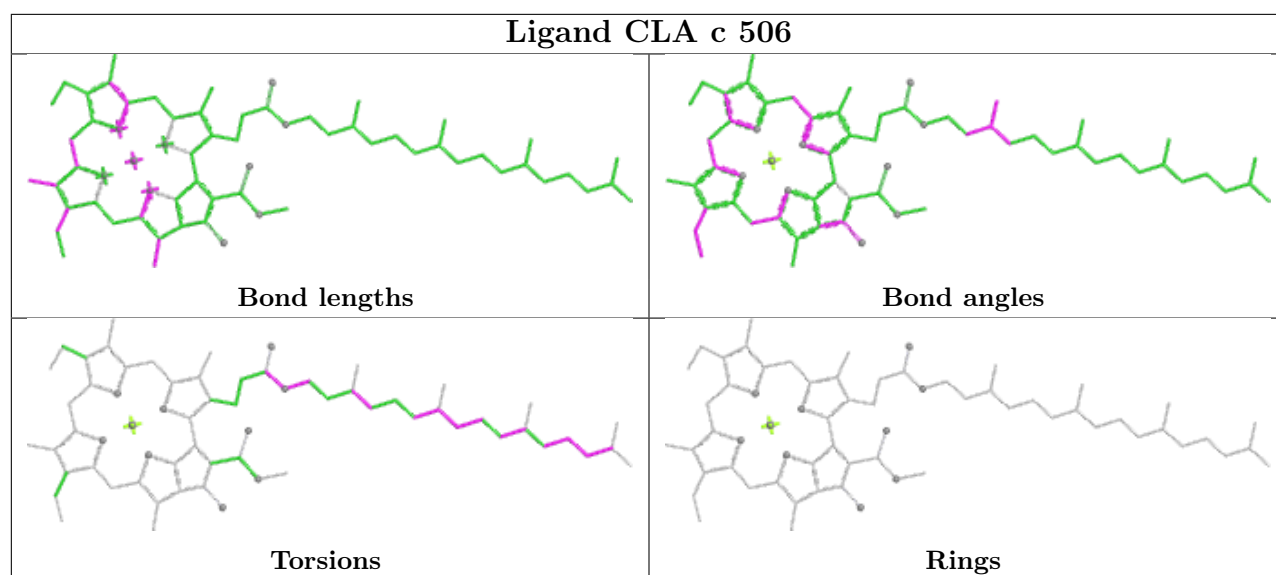


Ligand LHG E 101

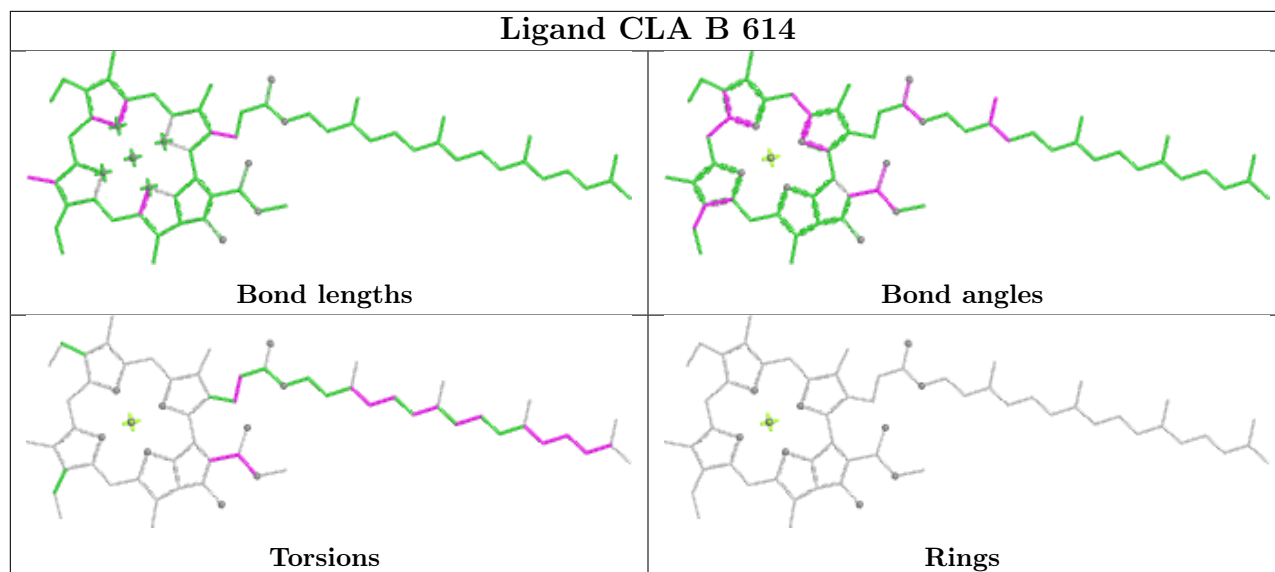


Ligand CLA D 404**Ligand CLA b 609**

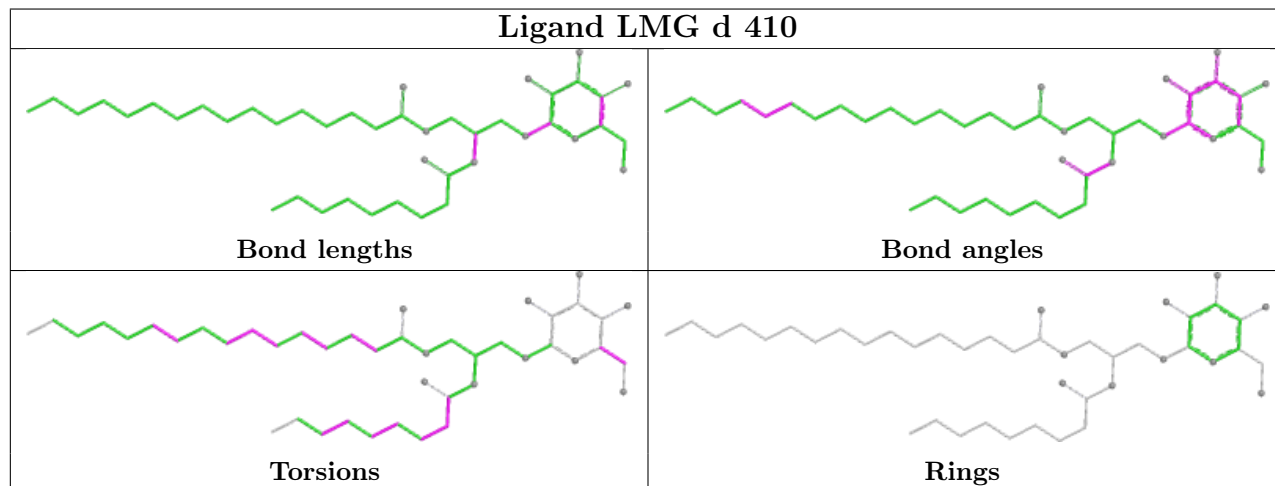




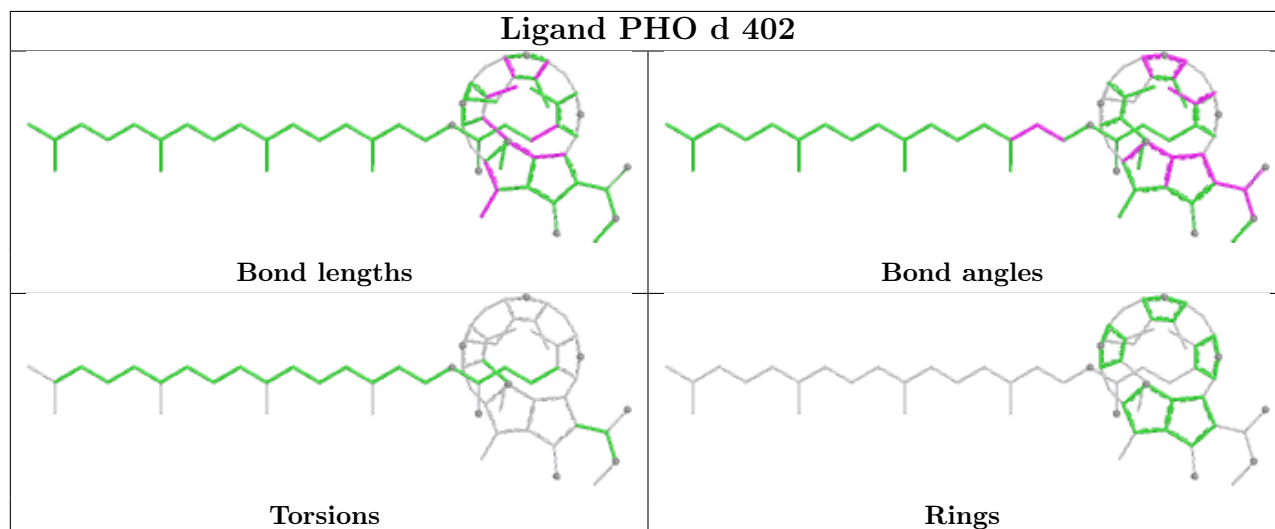
Ligand CLA B 614

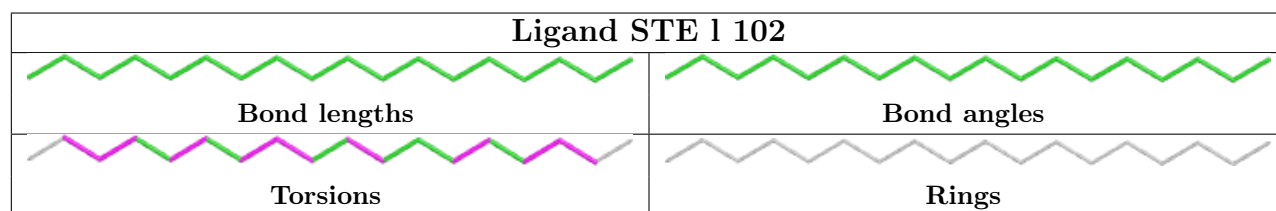
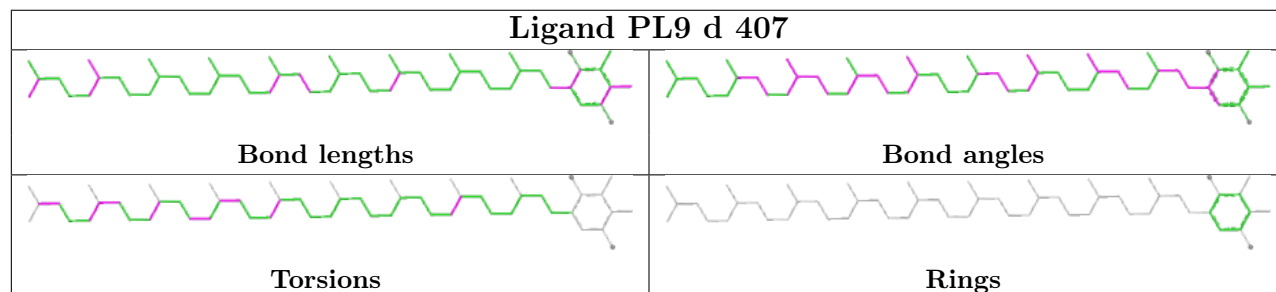
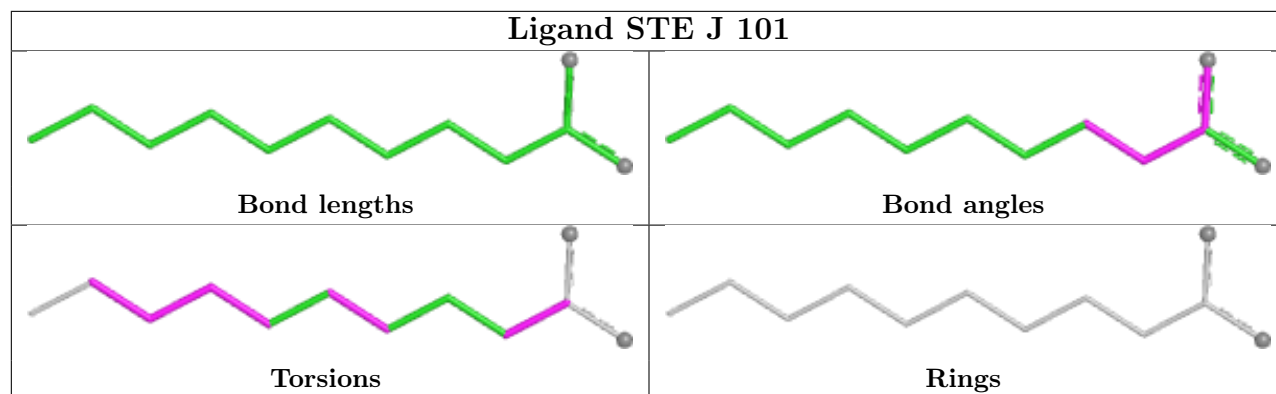


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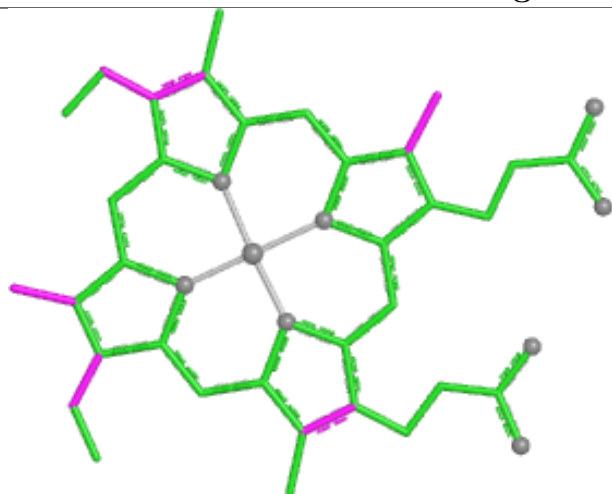


Ligand PHO d 402

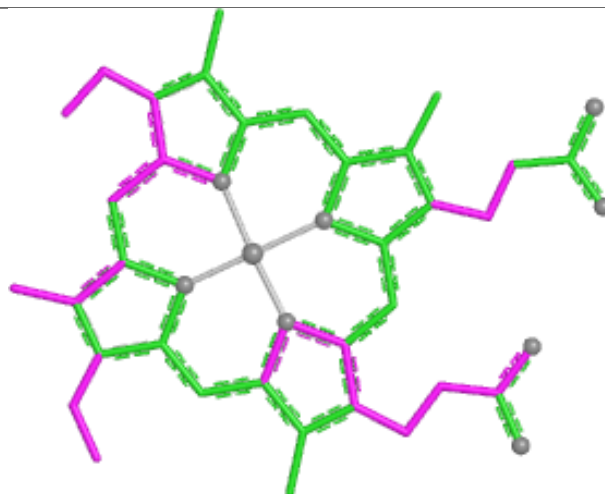




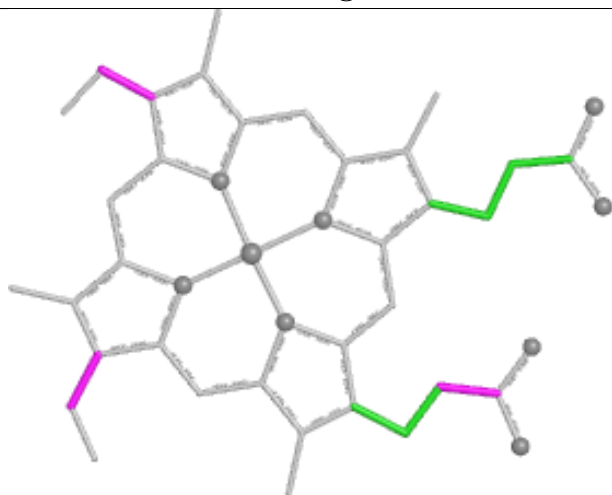
Ligand HEC F 101



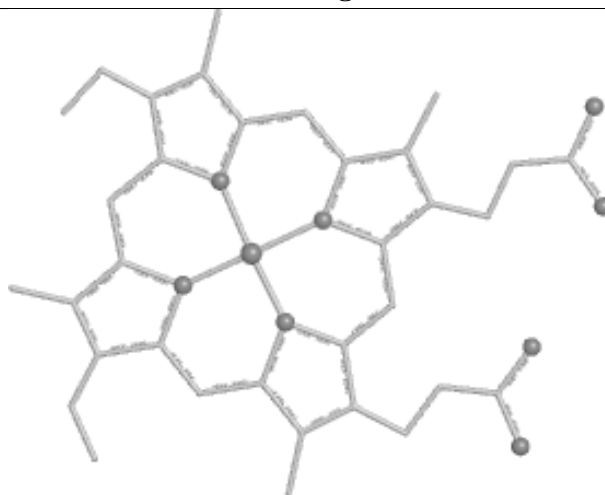
Bond lengths



Bond angles

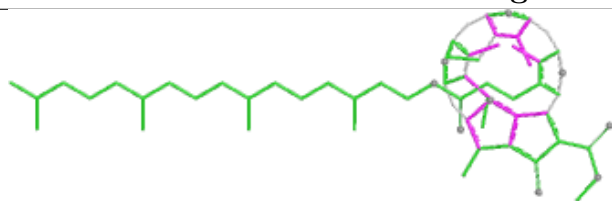


Torsions

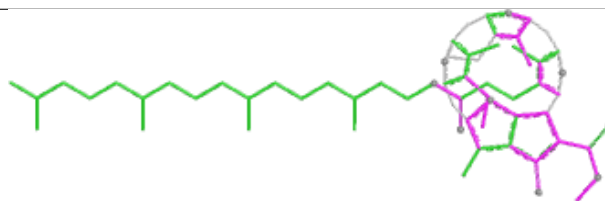


Rings

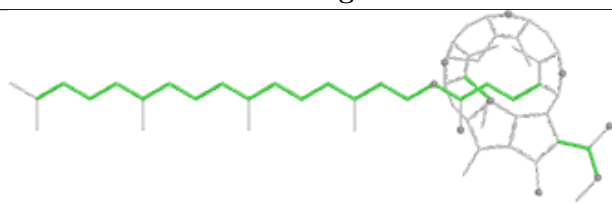
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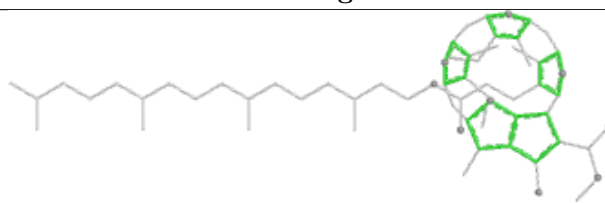
Bond lengths



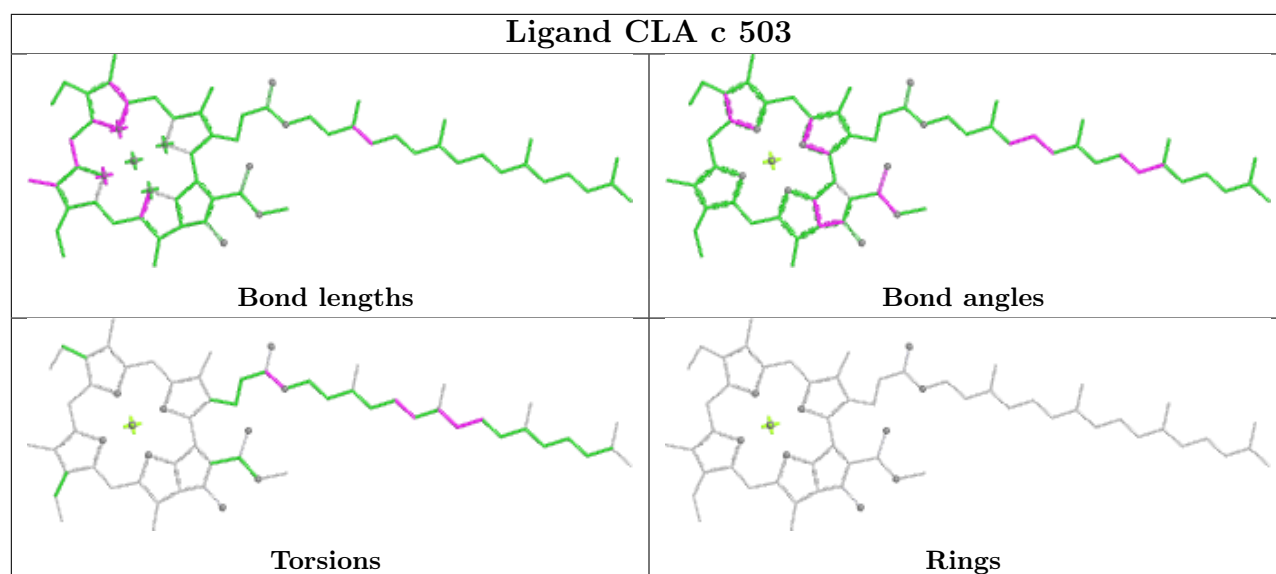
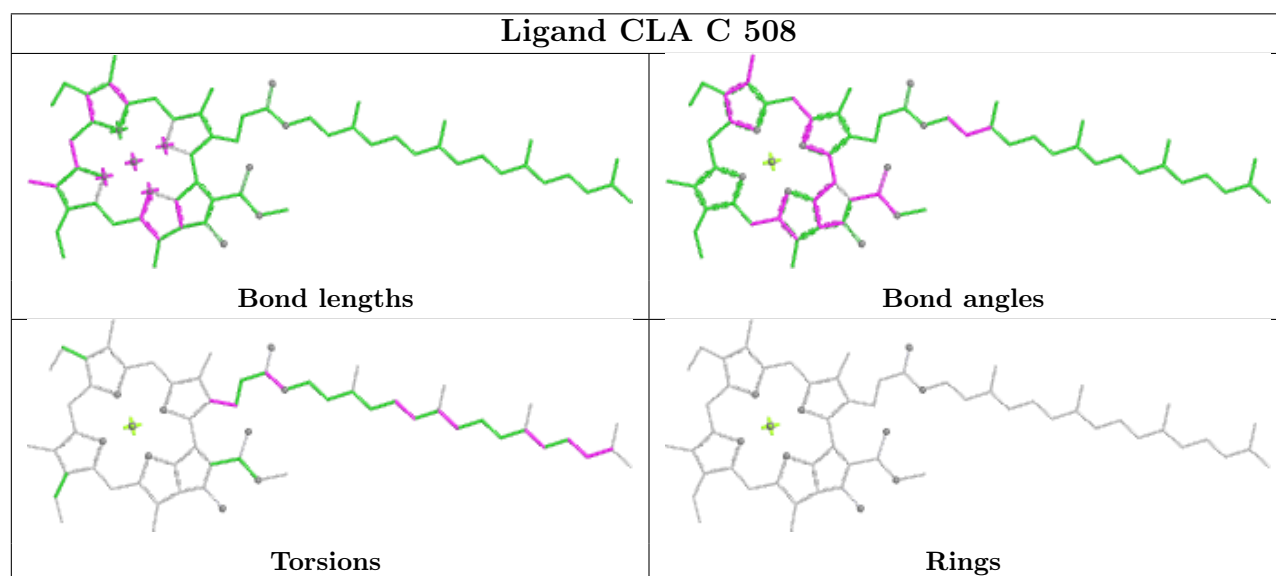
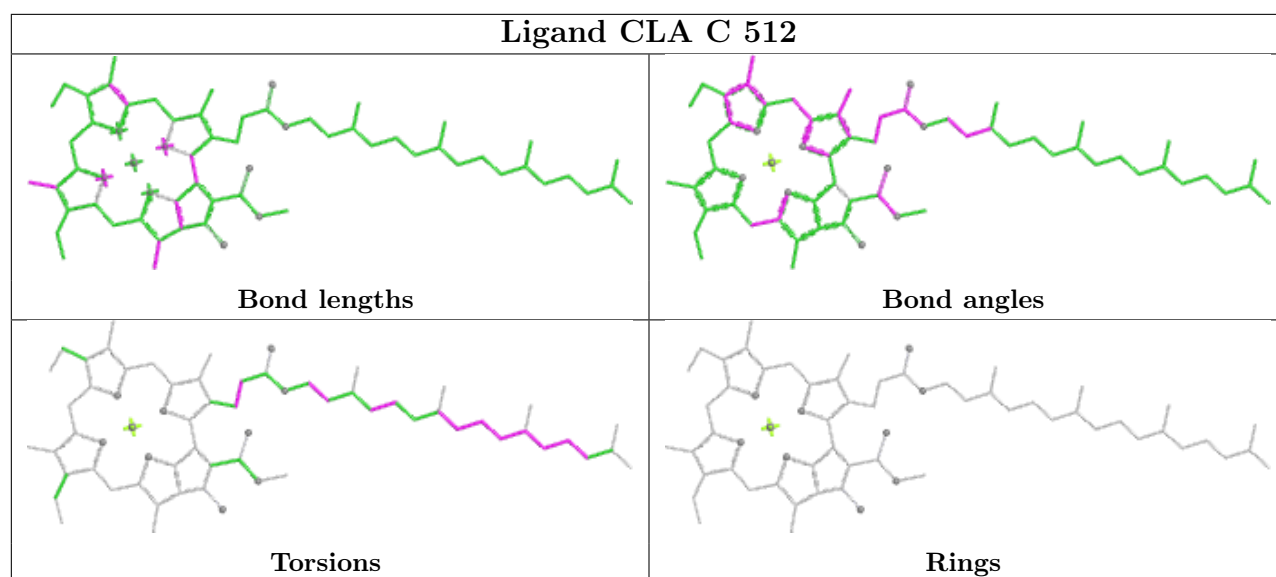
Bond angles

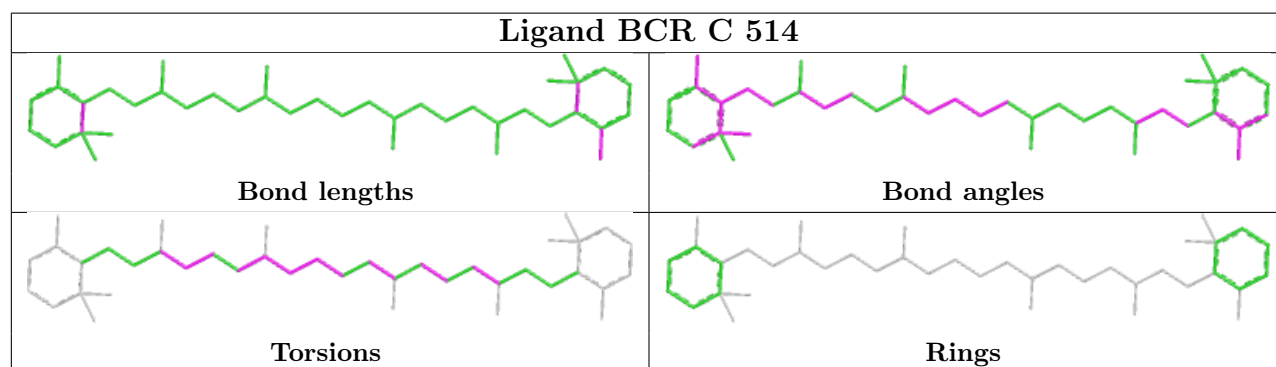
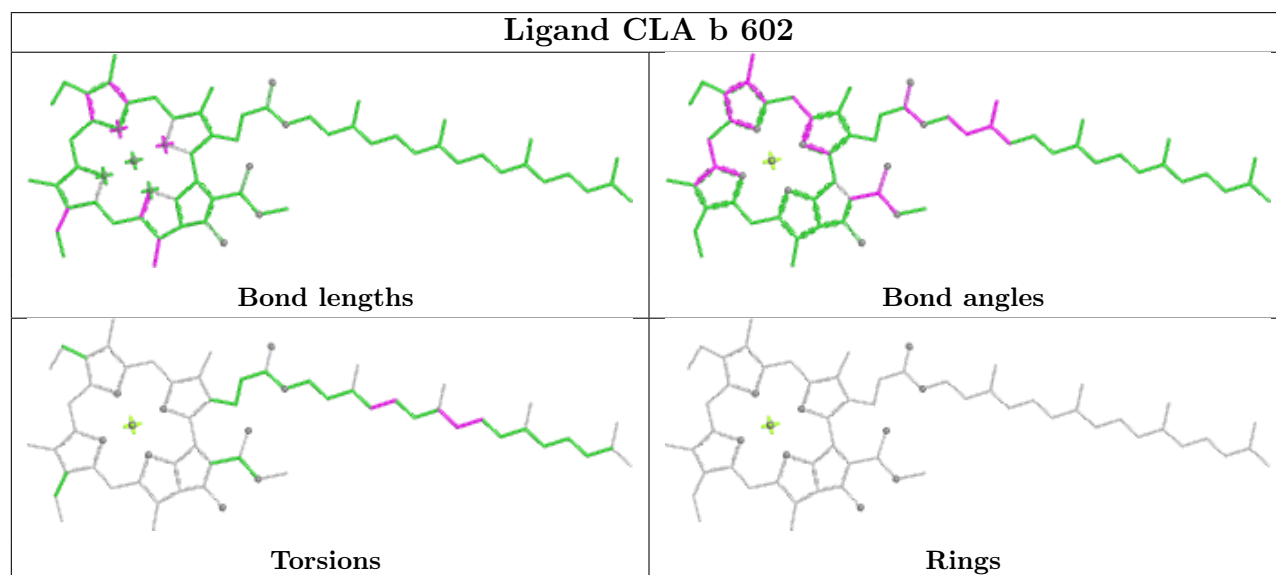
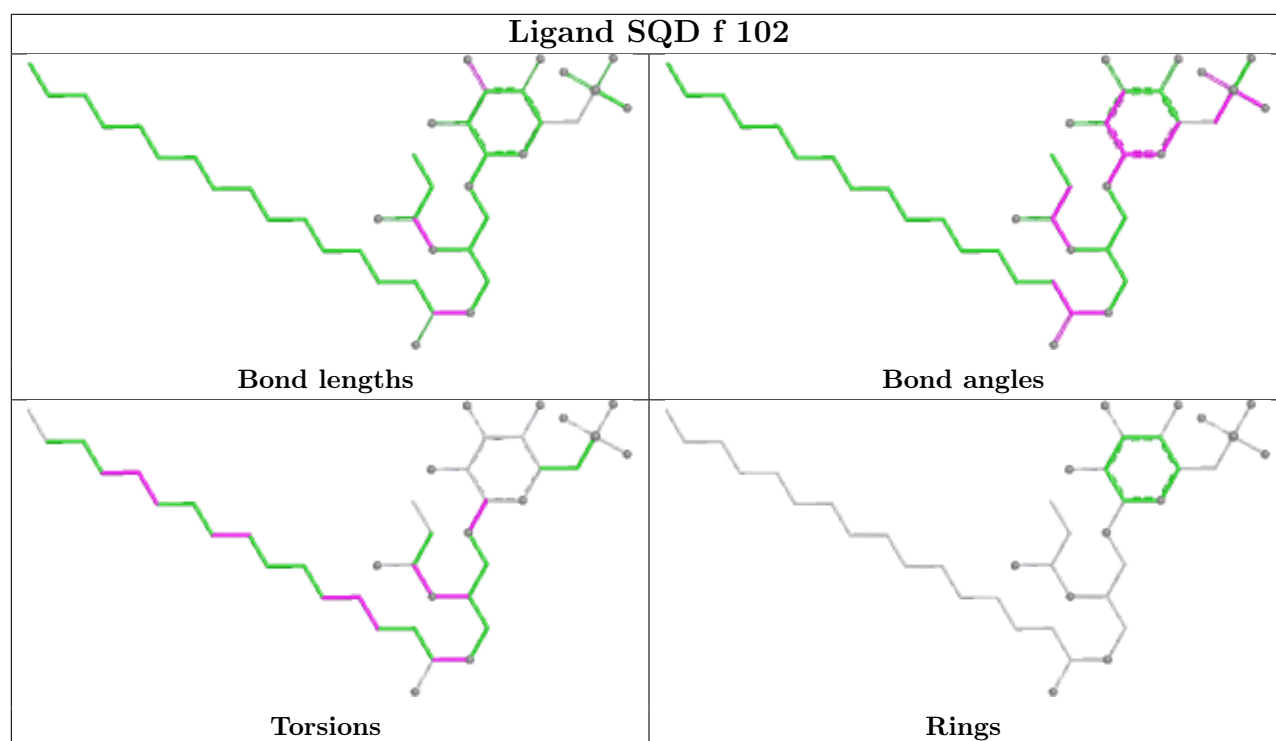


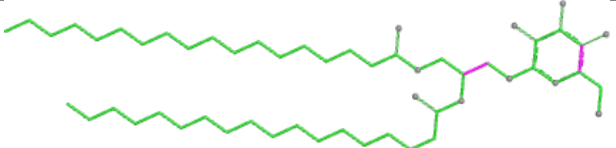
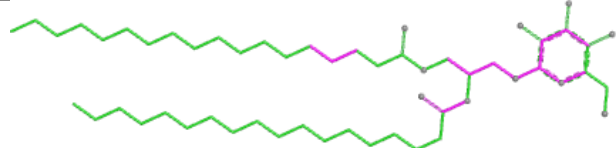
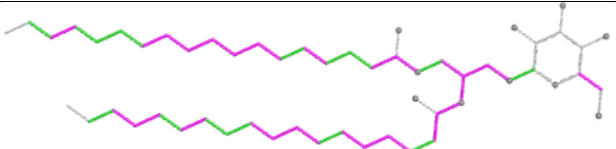
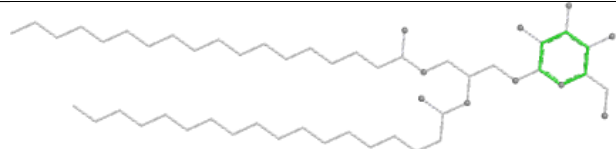
Torsions

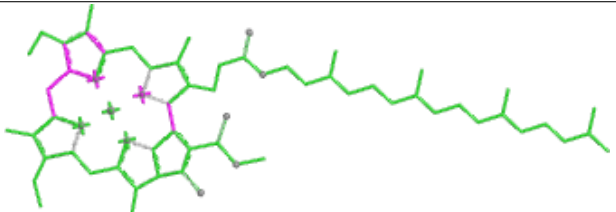
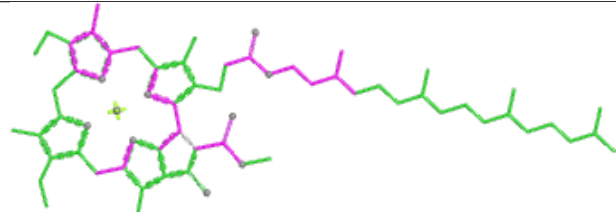
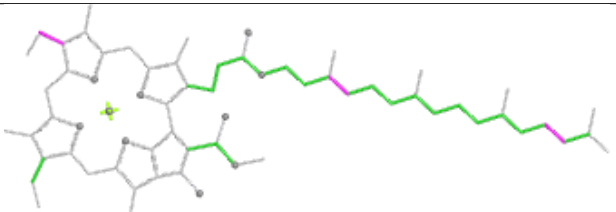
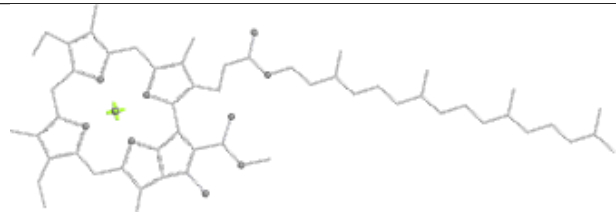


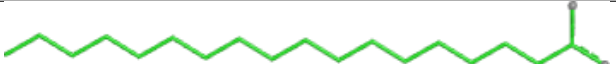
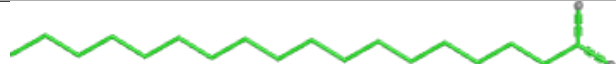
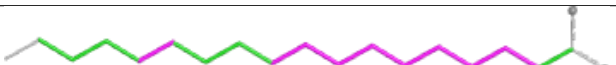
Rings

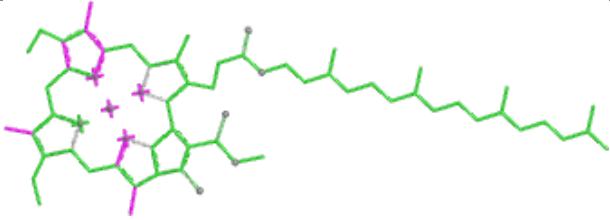
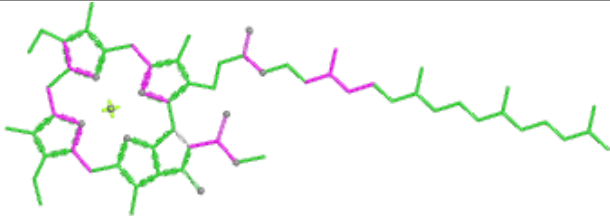
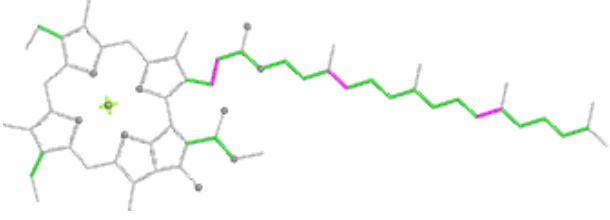
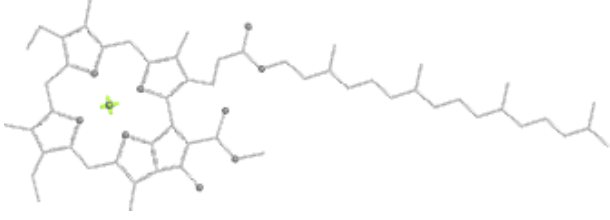


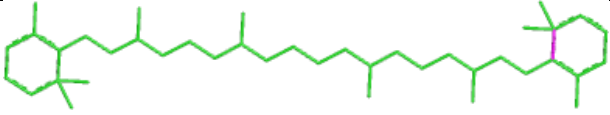
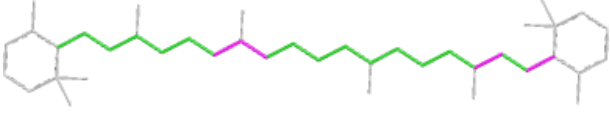
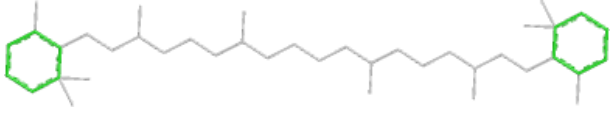


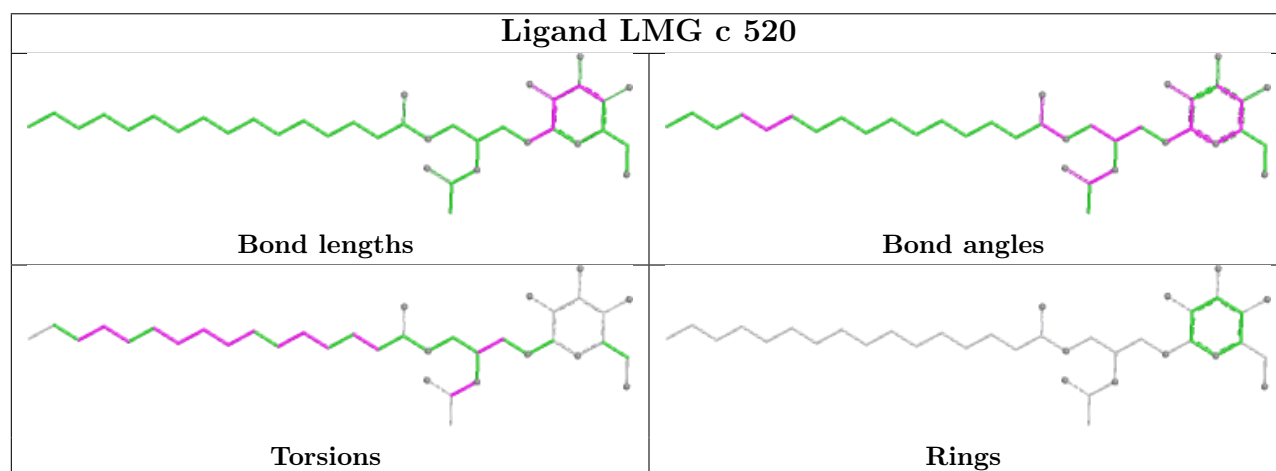
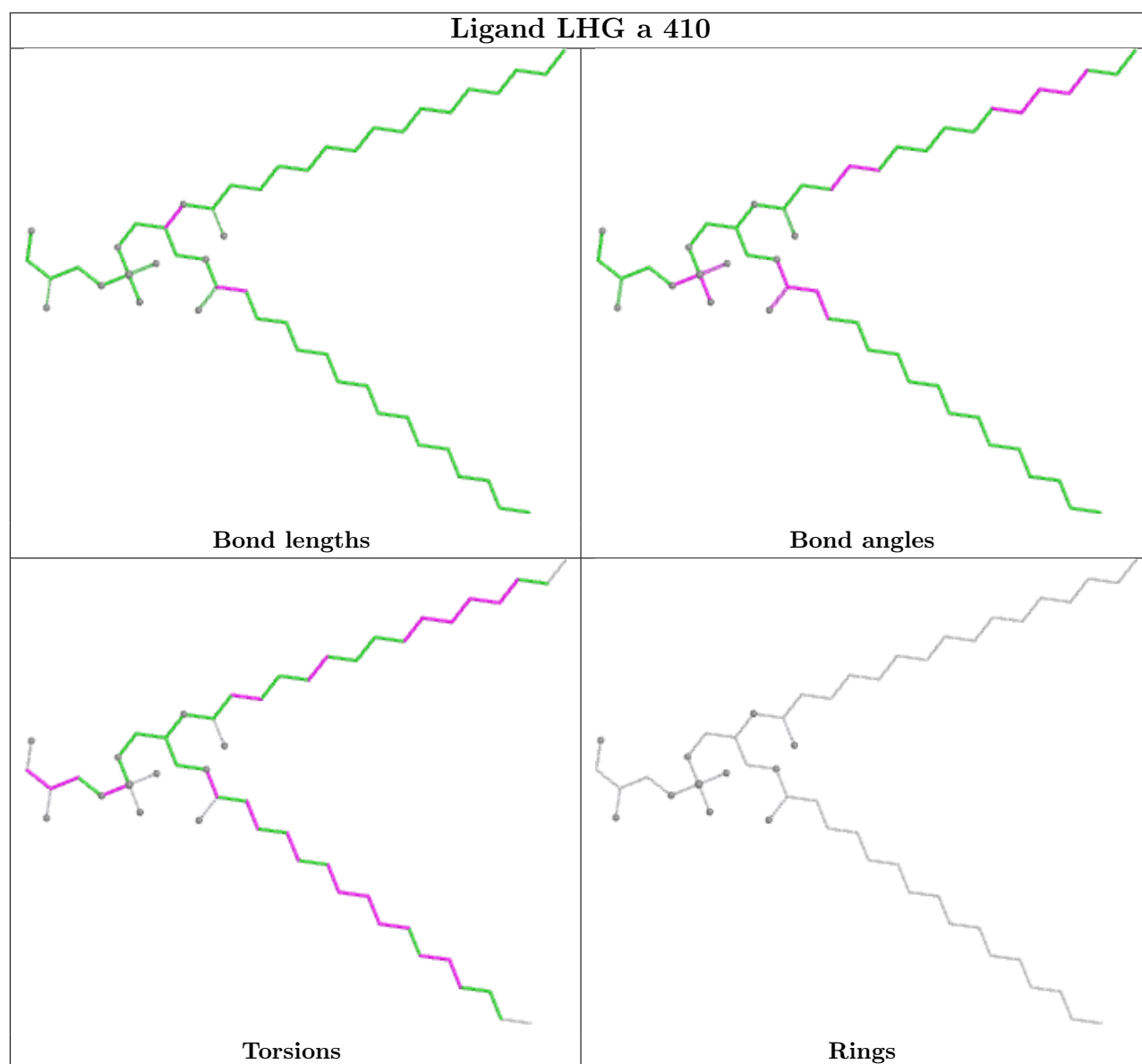
Ligand LMG a 416	
	
Bond lengths	Bond angles
	
Torsions	Rings

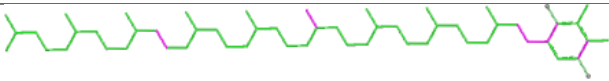
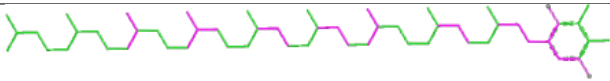
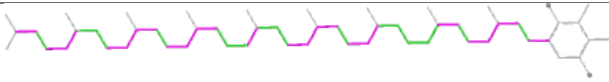
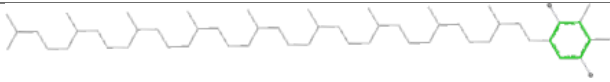
Ligand CLA b 605	
	
Bond lengths	Bond angles
	
Torsions	Rings

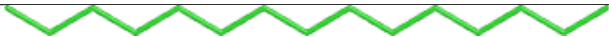
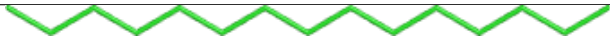
Ligand STE b 625	
	
Bond lengths	Bond angles
	
Torsions	Rings

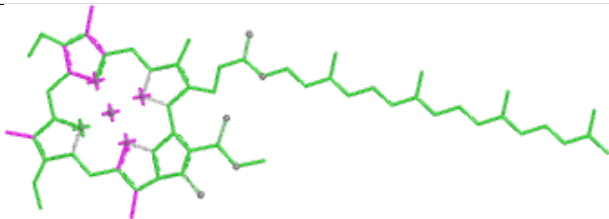
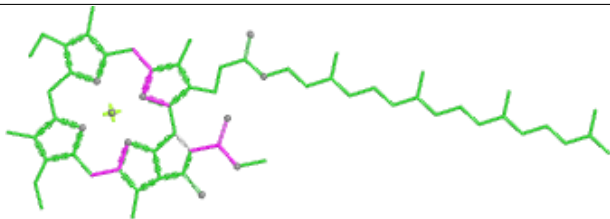
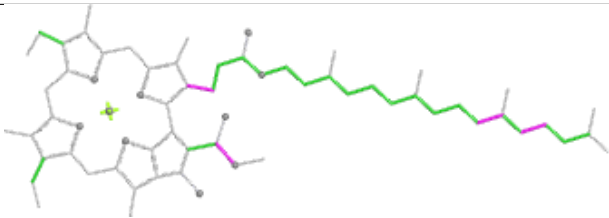
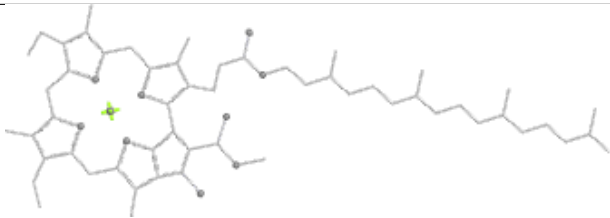
Ligand CLA B 603			
			
Bond lengths	Bond angles		
			
Torsions	Rings		

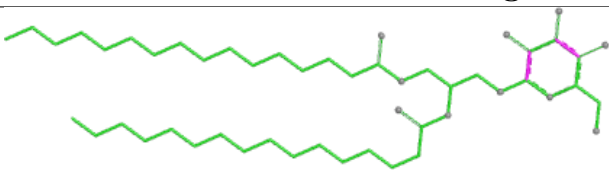
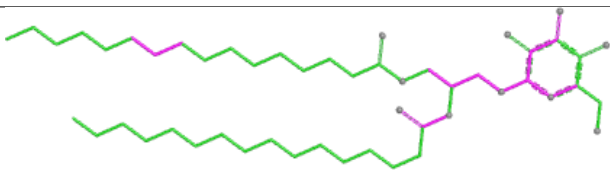
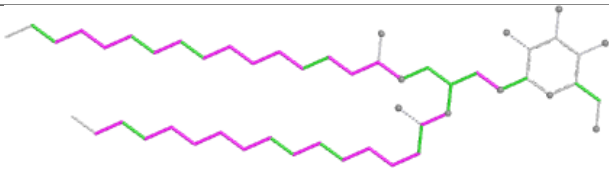
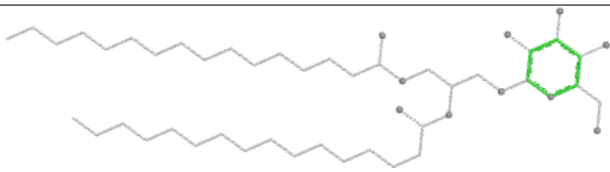
Ligand BCR H 101			
			
Bond lengths	Bond angles		
			
Torsions	Rings		

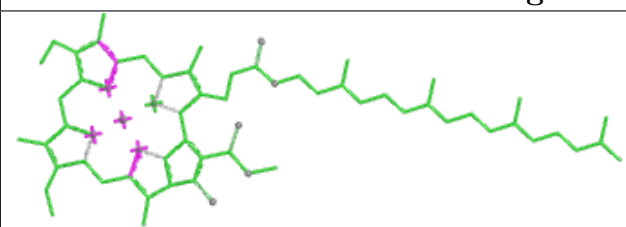
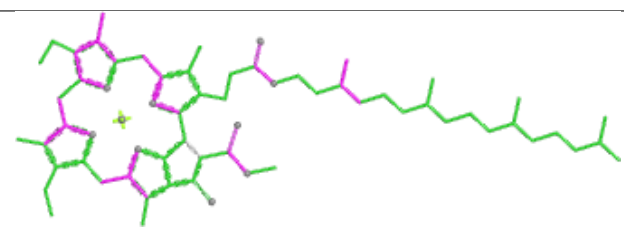
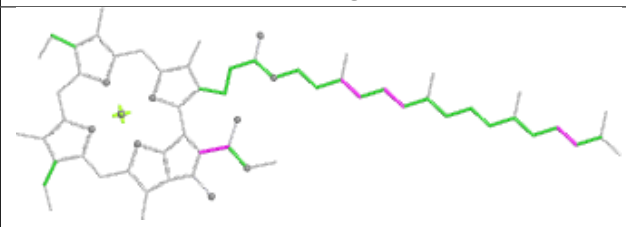
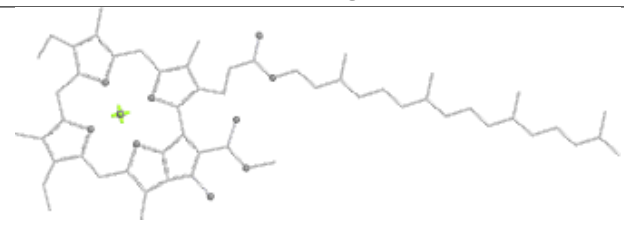


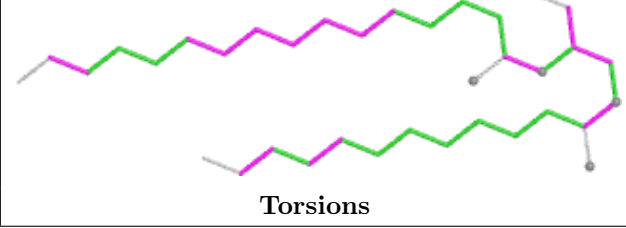
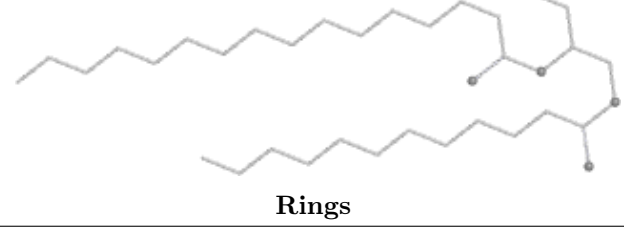
Ligand PL9 A 410	
 Bond lengths	 Bond angles
 Torsions	 Rings

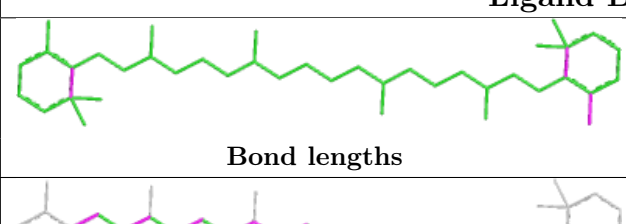
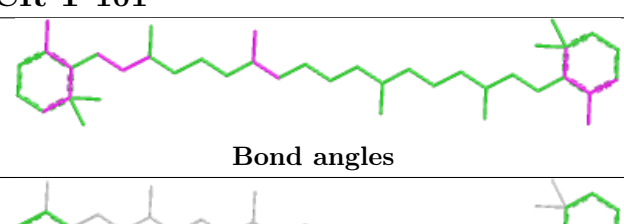
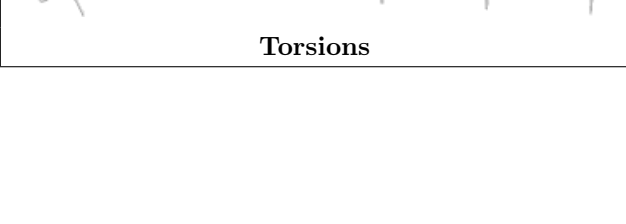
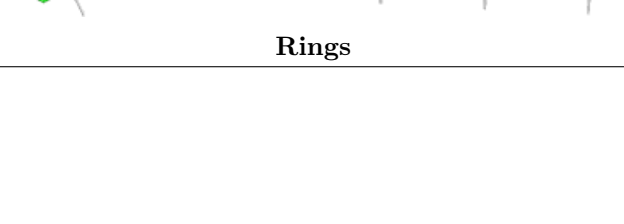
Ligand STE a 415	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA c 513	
 Bond lengths	 Bond angles
 Torsions	 Rings

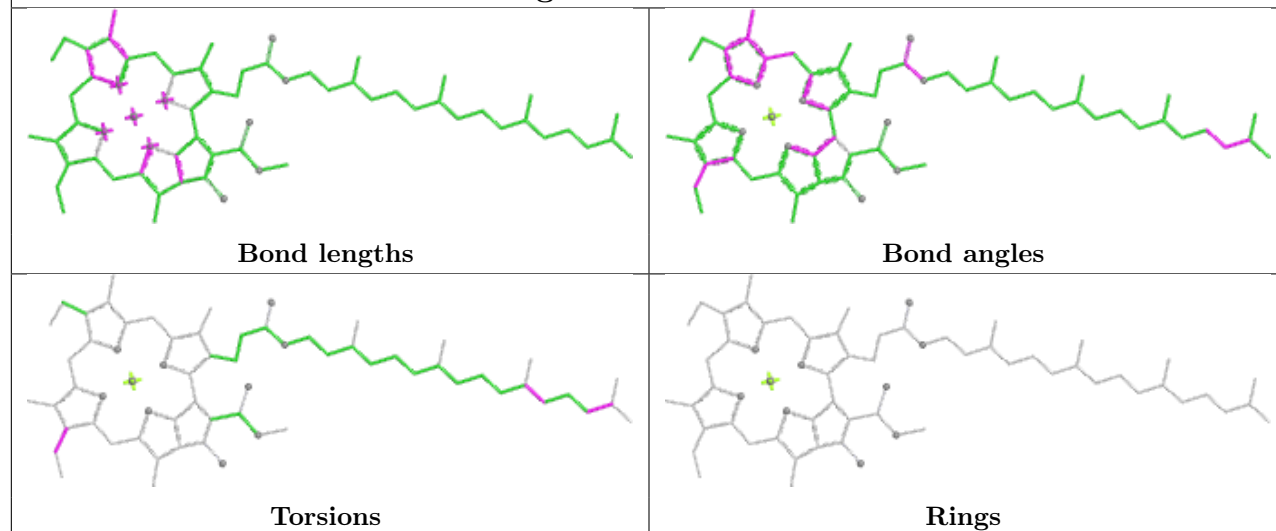
Ligand LMG m 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA c 507	
	
Bond lengths	Bond angles
	
Torsions	Rings

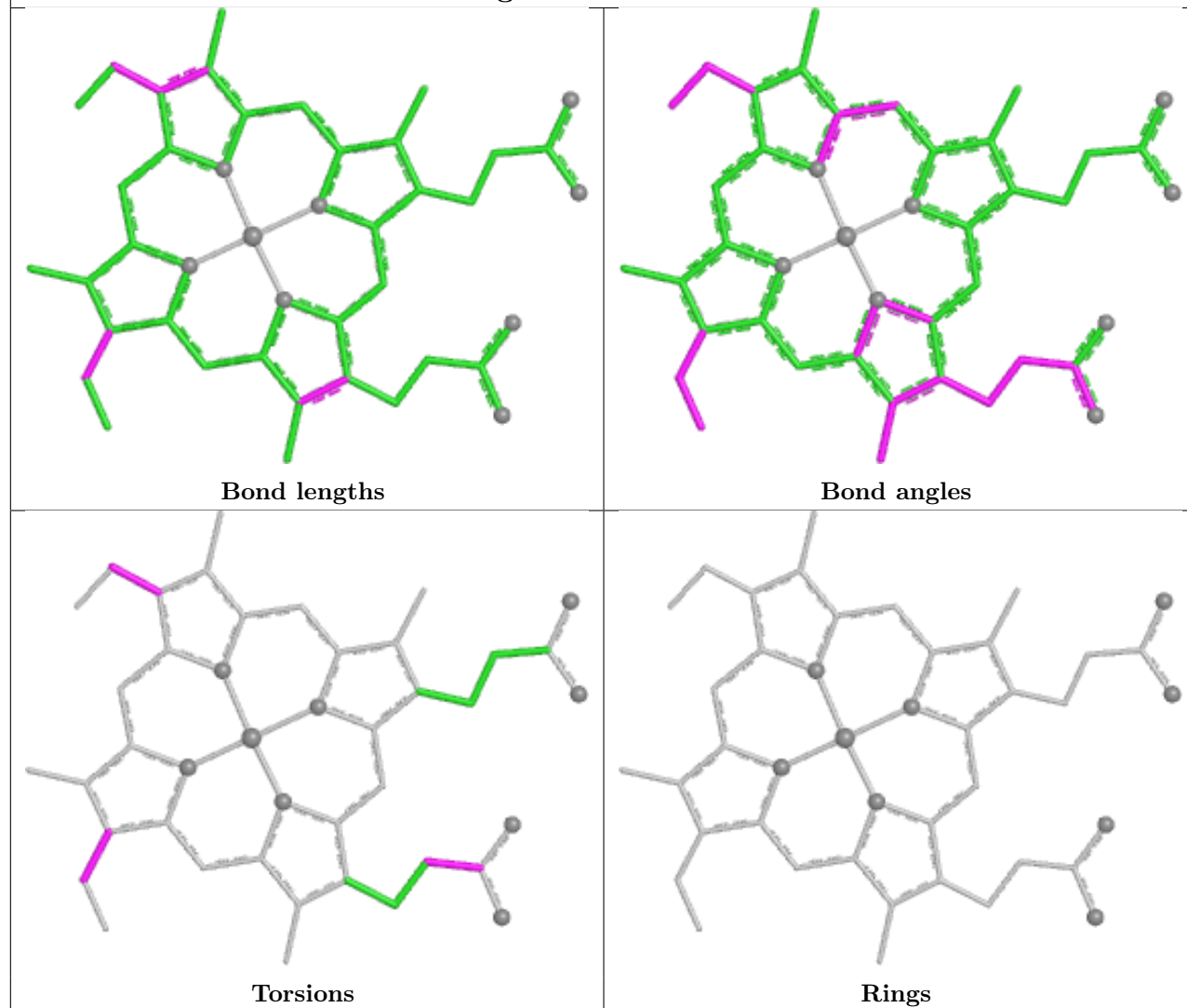
Ligand SQD a 412	
	
Bond lengths	Bond angles
	
Torsions	Rings

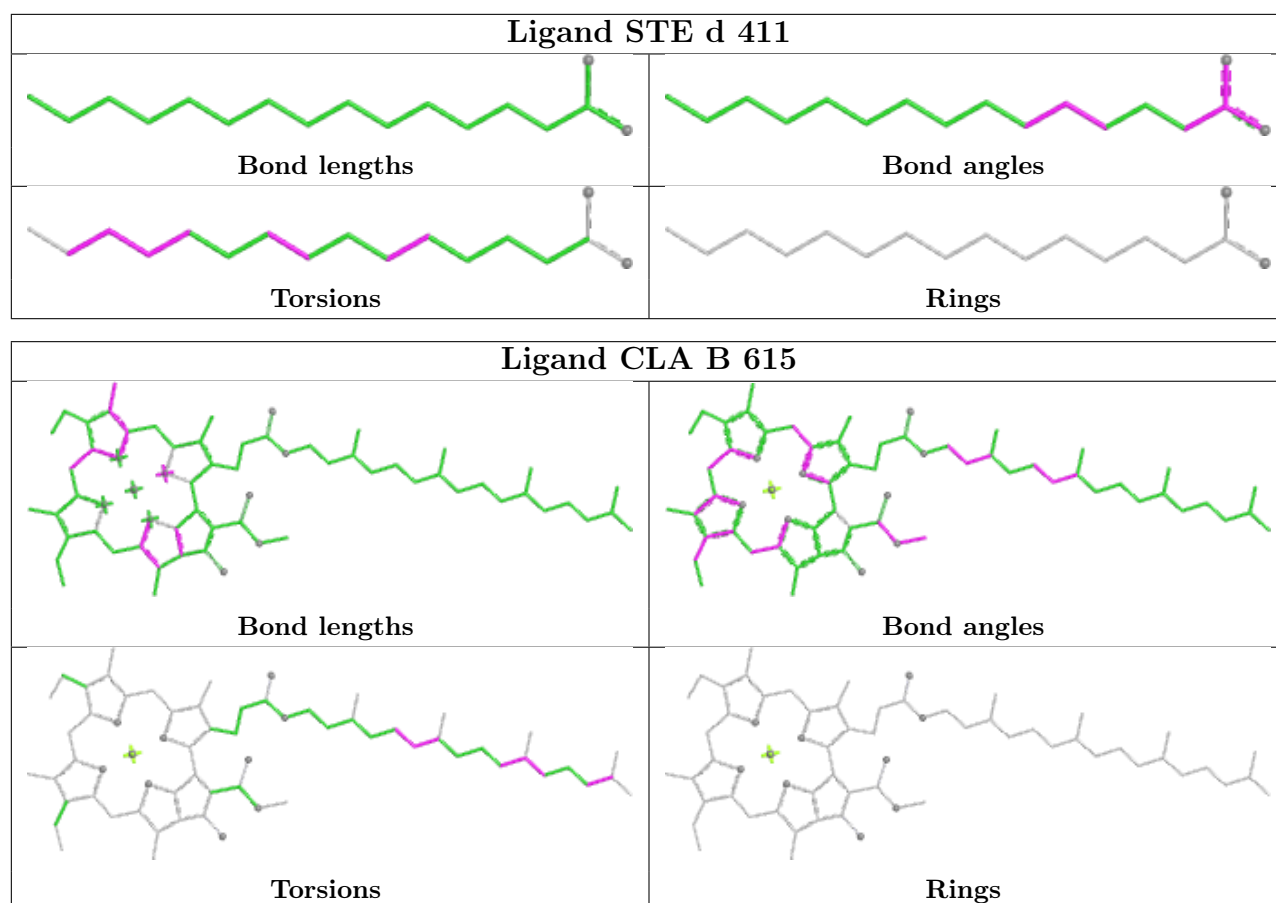
Ligand BCR T 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA a 402



Ligand HEC v 201





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	334/344 (97%)	-0.63	1 (0%) 90 89	13, 29, 48, 84	60 (17%)
1	a	334/344 (97%)	-0.50	3 (0%) 81 80	12, 31, 57, 89	60 (17%)
2	B	505/506 (99%)	-0.50	2 (0%) 88 88	17, 34, 63, 91	4 (0%)
2	b	505/506 (99%)	-0.35	3 (0%) 85 85	24, 38, 72, 105	0
3	C	442/461 (95%)	-0.49	0 100 100	14, 37, 54, 80	7 (1%)
3	c	451/461 (97%)	-0.35	2 (0%) 88 88	14, 41, 65, 109	8 (1%)
4	D	341/352 (96%)	-0.69	0 100 100	15, 31, 48, 87	1 (0%)
4	d	341/352 (96%)	-0.50	0 100 100	16, 35, 57, 84	2 (0%)
5	E	82/84 (97%)	0.14	1 (1%) 76 76	28, 51, 74, 86	1 (1%)
5	e	82/84 (97%)	0.26	1 (1%) 76 76	39, 60, 79, 92	0
6	F	34/45 (75%)	-0.20	0 100 100	36, 43, 64, 85	0
6	f	34/45 (75%)	-0.03	0 100 100	40, 48, 78, 92	0
7	H	65/66 (98%)	-0.33	2 (3%) 51 50	32, 42, 62, 74	0
7	h	63/66 (95%)	0.00	1 (1%) 70 70	40, 52, 67, 76	0
8	I	35/38 (92%)	-0.46	0 100 100	33, 40, 75, 90	0
8	i	35/38 (92%)	-0.25	0 100 100	31, 42, 77, 93	0
9	J	36/40 (90%)	-0.18	0 100 100	34, 51, 71, 98	0
9	j	36/40 (90%)	0.01	1 (2%) 55 54	38, 53, 93, 112	0
10	K	37/46 (80%)	-0.11	0 100 100	42, 52, 74, 80	0
10	k	37/46 (80%)	0.06	0 100 100	46, 55, 72, 80	0
11	L	37/37 (100%)	-0.60	0 100 100	25, 31, 66, 71	0
11	l	36/37 (97%)	-0.52	0 100 100	25, 32, 80, 89	0
12	M	32/36 (88%)	-0.52	1 (3%) 51 50	25, 36, 61, 77	0
12	m	31/36 (86%)	-0.51	0 100 100	26, 36, 51, 75	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/272 (89%)	-0.20	3 (1%) 76 76	26, 43, 83, 137	1 (0%)
13	o	244/272 (89%)	-0.24	1 (0%) 88 88	26, 42, 82, 138	0
14	R	34/40 (85%)	0.71	1 (2%) 53 52	58, 72, 93, 105	0
14	r	31/40 (77%)	1.07	4 (12%) 7 6	69, 92, 108, 120	0
15	T	29/30 (96%)	-0.57	0 100 100	27, 33, 66, 79	0
15	t	29/30 (96%)	-0.45	2 (6%) 23 21	28, 33, 85, 86	0
16	U	97/134 (72%)	-0.25	0 100 100	33, 46, 70, 91	0
16	u	97/134 (72%)	-0.33	0 100 100	32, 41, 58, 87	0
17	V	137/163 (84%)	-0.41	0 100 100	30, 41, 59, 83	0
17	v	137/163 (84%)	-0.18	0 100 100	33, 48, 70, 86	0
18	X	38/41 (92%)	-0.09	0 100 100	38, 51, 73, 82	0
18	x	39/41 (95%)	0.18	1 (2%) 57 56	48, 58, 84, 102	0
19	Y	27/46 (58%)	0.94	4 (14%) 5 5	51, 72, 96, 97	0
19	y	30/46 (65%)	0.68	0 100 100	60, 70, 92, 103	0
20	Z	62/62 (100%)	0.64	1 (1%) 70 70	51, 66, 117, 129	0
20	z	62/62 (100%)	0.65	2 (3%) 50 49	57, 72, 111, 122	0
All	All	5302/5686 (93%)	-0.33	37 (0%) 84 84	12, 39, 76, 138	144 (2%)

The worst 5 of 37 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	o	58	ASN	4.2
13	O	59	LYS	4.1
14	R	35	LEU	3.8
7	H	41	PHE	3.8
5	e	79	PHE	3.4

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	40,51,73,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
15	FME	t	1	10/11	0.94	0.08	32,45,72,72	0
8	FME	I	1	10/11	0.95	0.08	33,44,65,71	0
12	FME	m	1	10/11	0.96	0.09	34,45,71,80	0
15	FME	T	1	10/11	0.96	0.06	27,46,65,65	0
8	FME	i	1	10/11	0.96	0.08	36,50,62,65	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
33	STE	H	103	18/20	0.75	0.18	51,74,87,90	0
33	STE	a	414	12/20	0.78	0.14	35,62,69,75	0
33	STE	d	413	20/20	0.78	0.16	38,68,92,97	0
33	STE	b	625	20/20	0.79	0.17	49,66,82,85	0
33	STE	a	413	10/20	0.80	0.15	40,62,75,75	0
33	STE	b	627	14/20	0.81	0.16	52,65,84,93	0
33	STE	b	626	10/20	0.81	0.16	39,53,59,69	0
27	LMG	b	623	55/55	0.82	0.15	49,71,96,103	0
27	LMG	a	416	55/55	0.82	0.16	37,63,101,136	0
33	STE	R	101	12/20	0.82	0.16	55,77,85,87	0
33	STE	I	101	15/20	0.83	0.14	38,55,77,81	0
28	LHG	E	101	49/49	0.83	0.14	43,76,103,113	0
28	LHG	e	101	42/49	0.83	0.14	51,78,103,123	0
27	LMG	c	522	48/55	0.83	0.14	43,75,106,112	0
33	STE	m	102	12/20	0.83	0.17	49,62,82,84	0
33	STE	T	102	15/20	0.84	0.14	42,58,79,80	0
33	STE	k	102	12/20	0.84	0.11	43,65,78,83	0
33	STE	C	521	12/20	0.84	0.13	41,58,69,70	0
33	STE	a	415	15/20	0.85	0.18	39,68,86,93	0
33	STE	b	621	16/20	0.85	0.13	29,47,69,70	0
33	STE	B	626	12/20	0.85	0.15	49,62,79,84	0
33	STE	B	625	16/20	0.85	0.14	43,62,82,84	0
27	LMG	D	410	33/55	0.86	0.13	35,55,80,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	CLA	b	601	65/65	0.86	0.11	46,65,86,102	0
33	STE	d	412	20/20	0.86	0.11	36,54,71,77	0
29	SQD	a	412	36/54	0.86	0.12	31,63,87,91	0
33	STE	b	622	20/20	0.86	0.12	34,60,72,74	0
33	STE	B	620	17/20	0.86	0.12	33,52,69,70	0
33	STE	t	103	18/20	0.86	0.12	44,57,78,85	0
27	LMG	c	520	37/55	0.87	0.13	43,67,84,90	0
33	STE	c	521	20/20	0.87	0.10	37,59,72,75	0
27	LMG	A	411	48/55	0.87	0.11	35,56,78,89	0
30	DGD	A	415	66/66	0.87	0.11	42,64,85,88	0
33	STE	j	101	12/20	0.87	0.12	45,57,71,73	0
33	STE	b	624	16/20	0.87	0.12	42,62,79,80	0
33	STE	C	523	12/20	0.87	0.11	36,48,55,59	0
33	STE	t	102	14/20	0.87	0.11	34,50,66,67	0
26	PL9	A	410	55/55	0.87	0.13	32,65,86,92	0
26	PL9	a	409	55/55	0.88	0.13	34,68,87,99	0
27	LMG	c	523	49/55	0.88	0.11	36,57,92,106	0
33	STE	Z	101	8/20	0.88	0.14	37,55,66,66	0
29	SQD	A	414	39/54	0.88	0.13	40,64,96,106	0
33	STE	J	101	12/20	0.88	0.12	46,57,67,69	0
29	SQD	B	623	54/54	0.89	0.10	37,61,86,98	0
33	STE	C	522	16/20	0.89	0.12	34,51,75,83	0
27	LMG	C	520	48/55	0.89	0.11	41,67,88,95	0
33	STE	M	103	10/20	0.89	0.13	32,43,56,63	0
29	SQD	b	620	49/54	0.90	0.09	40,58,92,111	0
33	STE	D	412	20/20	0.90	0.10	34,52,73,77	0
29	SQD	f	102	41/54	0.90	0.13	52,83,112,115	0
33	STE	l	102	18/20	0.90	0.11	36,48,82,86	0
27	LMG	m	101	51/55	0.90	0.10	34,50,80,88	0
33	STE	d	411	17/20	0.90	0.12	39,56,68,71	0
24	BCR	C	514	40/40	0.90	0.10	39,54,67,68	0
33	STE	B	624	12/20	0.91	0.10	31,47,59,67	0
27	LMG	D	411	28/55	0.91	0.11	34,48,64,74	0
22	CLA	B	601	65/65	0.91	0.10	27,57,88,102	0
29	SQD	D	408	36/54	0.92	0.11	42,67,91,95	0
29	SQD	a	411	54/54	0.92	0.10	39,62,89,99	0
22	CLA	C	513	65/65	0.92	0.09	38,62,94,108	0
27	LMG	M	101	51/55	0.92	0.08	30,46,67,80	0
24	BCR	D	405	40/40	0.92	0.09	26,42,77,91	0
24	BCR	Y	101	40/40	0.92	0.09	32,48,64,68	0
24	BCR	d	406	40/40	0.92	0.10	35,52,96,100	0
24	BCR	x	101	40/40	0.92	0.09	34,49,67,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	DGD	h	101	62/66	0.93	0.09	32,46,57,68	0
24	BCR	c	514	40/40	0.93	0.09	44,57,70,72	0
24	BCR	H	101	40/40	0.93	0.08	28,44,58,65	0
24	BCR	k	101	40/40	0.93	0.09	34,57,72,73	0
30	DGD	H	102	62/66	0.93	0.08	26,43,57,60	0
24	BCR	c	516	40/40	0.94	0.09	35,48,63,67	0
24	BCR	C	515	40/40	0.94	0.08	26,39,52,64	0
22	CLA	c	512	65/65	0.94	0.09	37,54,91,108	0
22	CLA	c	513	65/65	0.94	0.10	41,66,110,114	0
24	BCR	B	618	40/40	0.94	0.07	24,36,49,50	0
24	BCR	b	617	40/40	0.94	0.07	28,40,50,53	0
24	BCR	b	618	40/40	0.94	0.06	27,38,52,52	0
27	LMG	d	410	44/55	0.94	0.09	30,49,84,89	0
33	STE	M	102	15/20	0.94	0.08	35,45,62,62	0
30	DGD	C	518	62/66	0.94	0.09	27,49,99,122	0
24	BCR	b	619	40/40	0.94	0.08	27,47,63,72	0
30	DGD	c	518	62/66	0.94	0.08	29,51,95,99	0
27	LMG	D	407	51/55	0.94	0.10	26,54,85,89	0
28	LHG	a	410	49/49	0.94	0.10	28,48,77,84	0
22	CLA	C	512	65/65	0.94	0.09	32,52,84,94	0
29	SQD	A	413	52/54	0.94	0.10	34,58,103,107	0
28	LHG	A	412	47/49	0.95	0.10	26,49,84,100	0
24	BCR	C	516	40/40	0.95	0.08	33,48,64,65	0
22	CLA	c	511	65/65	0.95	0.09	30,50,70,75	0
28	LHG	d	409	39/49	0.95	0.09	30,45,75,83	0
22	CLA	C	511	65/65	0.95	0.08	27,48,66,69	0
24	BCR	T	101	40/40	0.95	0.06	23,36,52,54	0
22	CLA	C	506	65/65	0.95	0.09	26,41,85,102	0
24	BCR	a	405	40/40	0.95	0.06	23,33,43,46	0
22	CLA	d	405	65/65	0.95	0.08	26,48,89,100	0
23	PHO	d	402	64/64	0.95	0.06	25,35,45,52	0
24	BCR	A	407	40/40	0.95	0.06	19,33,41,42	0
24	BCR	B	617	40/40	0.95	0.07	25,38,57,65	0
24	BCR	c	515	40/40	0.95	0.07	28,41,58,63	0
22	CLA	b	606	65/65	0.95	0.08	26,39,76,82	0
30	DGD	C	517	62/66	0.95	0.09	22,42,80,92	0
24	BCR	B	619	40/40	0.95	0.06	24,41,59,71	0
22	CLA	b	609	65/65	0.95	0.07	28,42,65,68	0
22	CLA	c	509	65/65	0.95	0.08	32,45,61,69	0
22	CLA	B	616	60/65	0.96	0.08	23,36,91,109	0
22	CLA	b	610	65/65	0.96	0.07	22,35,51,53	0
22	CLA	b	612	65/65	0.96	0.07	20,33,47,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	DGD	C	519	62/66	0.96	0.08	24,47,77,91	0
22	CLA	b	614	65/65	0.96	0.07	23,37,75,82	0
30	DGD	c	517	62/66	0.96	0.07	20,42,74,76	0
22	CLA	b	615	65/65	0.96	0.07	26,38,61,66	0
30	DGD	c	519	62/66	0.96	0.09	26,52,87,92	0
22	CLA	b	616	60/65	0.96	0.07	26,40,82,91	0
22	CLA	c	501	65/65	0.96	0.07	28,38,50,55	0
22	CLA	c	502	65/65	0.96	0.06	28,39,58,65	0
24	BCR	t	101	40/40	0.96	0.06	24,36,51,57	0
22	CLA	c	503	65/65	0.96	0.06	27,42,53,57	0
22	CLA	c	504	60/65	0.96	0.08	29,44,81,89	0
26	PL9	D	406	55/55	0.96	0.06	18,33,46,50	0
22	CLA	c	505	65/65	0.96	0.07	23,40,71,74	0
26	PL9	d	407	55/55	0.96	0.06	18,34,43,47	0
22	CLA	c	506	65/65	0.96	0.08	29,45,94,103	0
22	CLA	c	507	65/65	0.96	0.07	26,42,60,70	0
22	CLA	c	508	64/65	0.96	0.08	28,42,82,101	0
22	CLA	C	501	65/65	0.96	0.06	21,35,47,53	0
22	CLA	c	510	65/65	0.96	0.07	26,45,59,77	0
22	CLA	C	502	65/65	0.96	0.06	25,39,52,58	0
22	CLA	C	503	65/65	0.96	0.06	26,39,47,50	0
22	CLA	C	504	59/65	0.96	0.07	27,40,82,87	0
22	CLA	d	401	65/65	0.96	0.08	24,37,86,97	0
22	CLA	d	404	65/65	0.96	0.06	19,28,45,54	0
22	CLA	C	505	65/65	0.96	0.08	23,38,71,87	0
23	PHO	A	405	64/64	0.96	0.05	21,30,38,40	0
23	PHO	a	403	64/64	0.96	0.05	19,29,37,48	0
22	CLA	B	605	65/65	0.96	0.06	20,31,46,48	0
28	LHG	B	622	49/49	0.96	0.07	29,43,69,78	0
22	CLA	C	507	65/65	0.96	0.07	24,39,57,59	0
22	CLA	C	508	65/65	0.96	0.07	24,38,99,119	0
22	CLA	C	509	65/65	0.96	0.07	25,42,62,65	0
22	CLA	C	510	65/65	0.96	0.07	26,42,63,69	0
22	CLA	B	606	65/65	0.96	0.07	20,34,67,72	0
22	CLA	B	609	65/65	0.96	0.07	24,36,56,65	0
22	CLA	B	610	65/65	0.96	0.07	20,32,40,47	0
22	CLA	a	404	65/65	0.96	0.08	19,35,84,101	0
22	CLA	B	614	65/65	0.96	0.08	19,37,81,90	0
22	CLA	b	605	65/65	0.96	0.06	20,34,50,55	0
22	CLA	B	615	65/65	0.96	0.07	24,35,63,75	0
22	CLA	b	608	65/65	0.96	0.07	23,41,63,71	0
34	BCT	a	408	4/4	0.96	0.09	27,33,39,46	0

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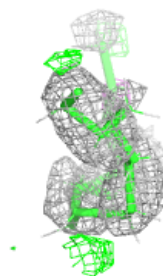
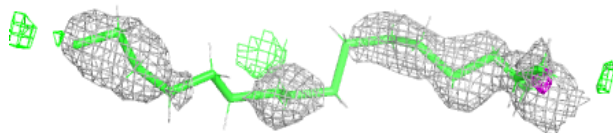
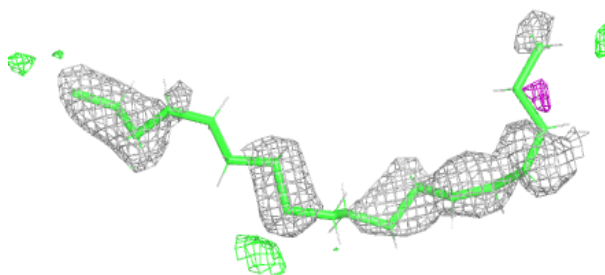
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	CLA	D	404	65/65	0.97	0.07	22,43,109,119	0
22	CLA	a	402	65/65	0.97	0.05	17,28,49,59	0
22	CLA	B	603	65/65	0.97	0.06	18,31,65,69	0
22	CLA	B	611	65/65	0.97	0.05	19,30,46,51	0
22	CLA	b	602	65/65	0.97	0.07	25,40,64,71	0
22	CLA	b	603	65/65	0.97	0.06	21,35,71,79	0
22	CLA	b	604	65/65	0.97	0.07	17,37,86,98	0
22	CLA	B	612	65/65	0.97	0.06	17,31,49,54	0
22	CLA	B	613	65/65	0.97	0.06	17,31,70,80	0
22	CLA	b	607	65/65	0.97	0.07	19,35,69,74	0
22	CLA	B	604	65/65	0.97	0.07	20,32,74,85	0
22	CLA	A	403	65/65	0.97	0.07	22,33,88,98	0
22	CLA	A	402	65/65	0.97	0.06	16,26,45,55	0
22	CLA	d	403	65/65	0.97	0.06	18,31,53,65	0
22	CLA	b	611	65/65	0.97	0.06	21,32,55,60	0
22	CLA	B	607	65/65	0.97	0.07	16,31,62,74	0
28	LHG	B	621	49/49	0.97	0.07	25,39,58,66	0
23	PHO	A	404	64/64	0.97	0.05	17,27,36,43	0
28	LHG	D	409	49/49	0.97	0.06	22,39,51,55	0
22	CLA	b	613	65/65	0.97	0.06	16,33,71,82	0
22	CLA	B	608	65/65	0.97	0.06	17,32,54,58	0
28	LHG	d	408	49/49	0.97	0.06	25,40,51,57	0
22	CLA	B	602	65/65	0.97	0.06	22,35,55,61	0
22	CLA	D	402	65/65	0.97	0.06	15,28,52,62	0
28	LHG	l	101	49/49	0.97	0.06	27,42,52,59	0
34	BCT	D	401	4/4	0.97	0.06	29,31,31,37	0
22	CLA	D	403	65/65	0.97	0.05	18,27,44,55	0
35	HEC	F	101	43/43	0.97	0.08	31,45,59,61	0
35	HEC	f	101	43/43	0.97	0.08	36,52,70,71	0
22	CLA	A	406	54/65	0.98	0.05	17,32,63,66	0
35	HEC	v	201	43/43	0.98	0.06	25,36,44,46	0
21	FE2	a	401	1/1	0.99	0.02	29,29,29,29	0
25	CL	A	408	1/1	0.99	0.03	28,28,28,28	0
25	CL	A	409	1/1	0.99	0.04	27,27,27,27	0
25	CL	a	406	1/1	0.99	0.03	26,26,26,26	0
31	OEX	A	416[A]	10/10	0.99	0.03	28,31,34,36	10
31	OEX	a	417[A]	10/10	0.99	0.03	25,31,35,35	10
35	HEC	V	201	43/43	0.99	0.05	22,31,40,41	0
32	OEY	A	417[B]	11/11	0.99	0.03	18,21,25,25	11
32	OEY	a	418[B]	11/11	0.99	0.03	16,21,24,25	11
25	CL	a	407	1/1	1.00	0.04	26,26,26,26	0
21	FE2	A	401	1/1	1.00	0.04	29,29,29,29	0

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

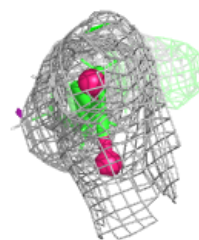
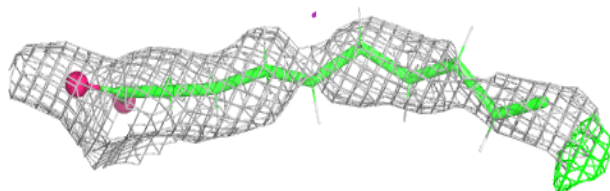
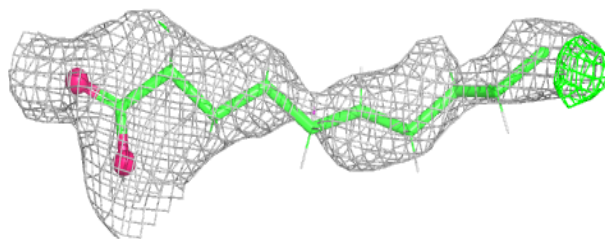
Electron density around STE H 103:

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

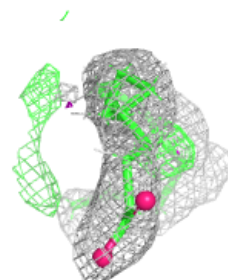
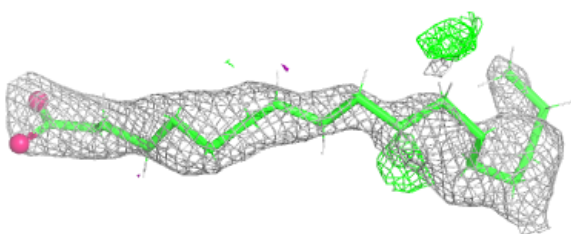
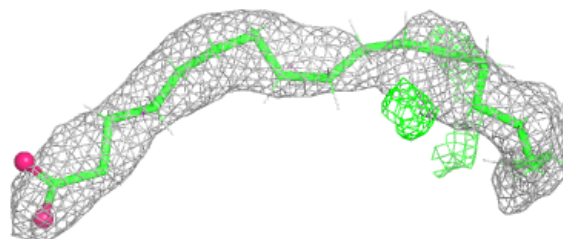


Electron density around STE a 414:

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

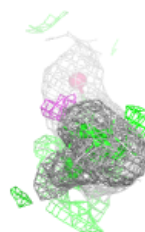
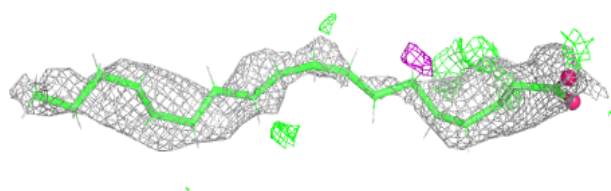
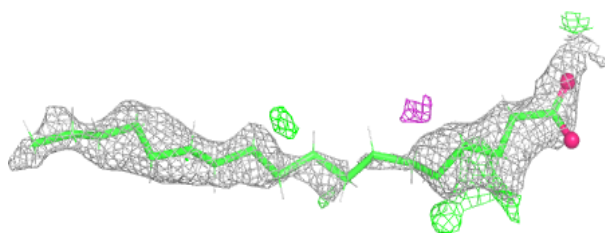
**Electron density around STE d 413:**

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

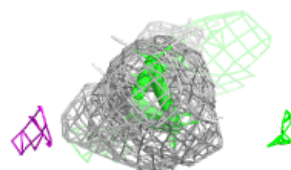
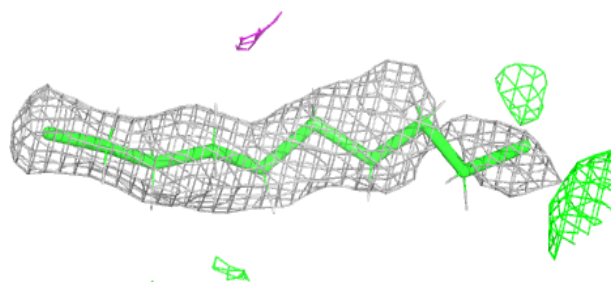
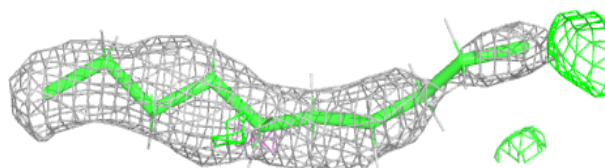


Electron density around STE b 625:

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

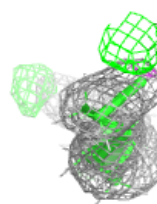
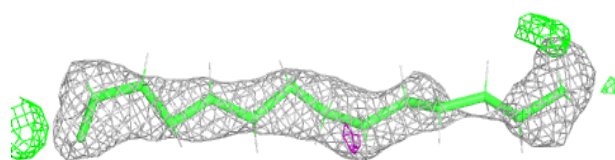
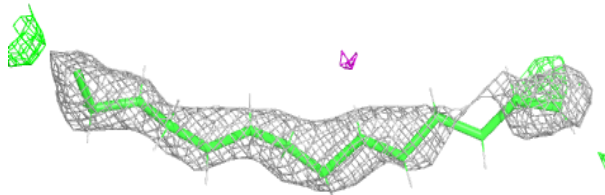
**Electron density around STE a 413:**

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

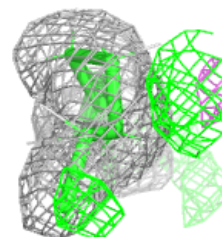
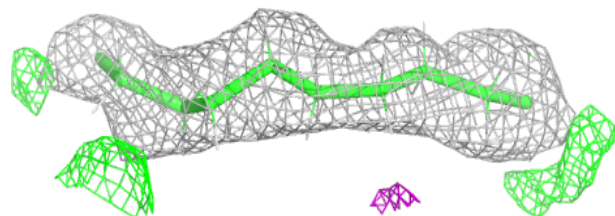
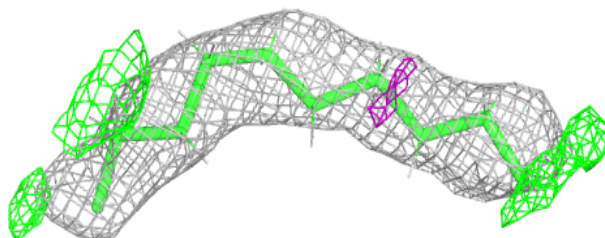


Electron density around STE b 627:

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

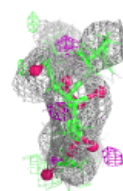
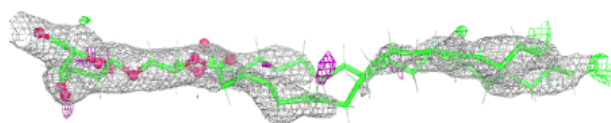
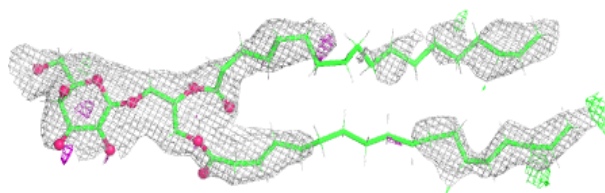
**Electron density around STE b 626:**

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

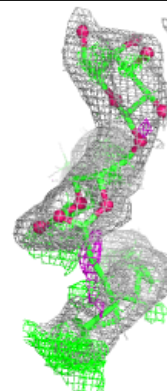
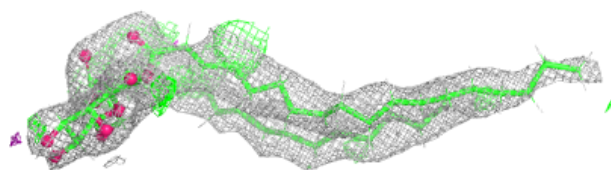
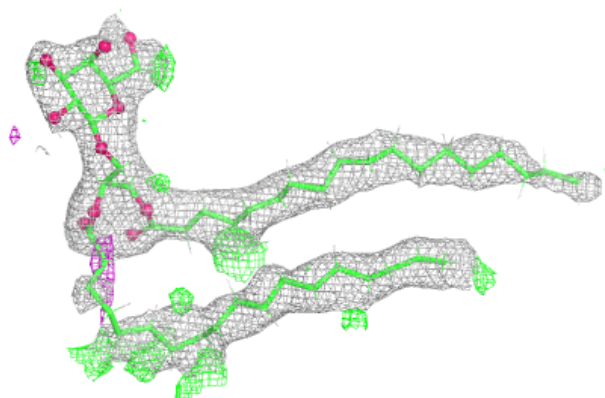


Electron density around LMG b 623:

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and green (positive)

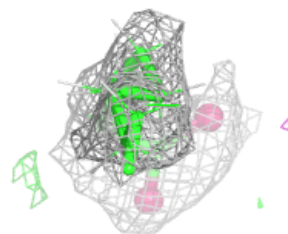
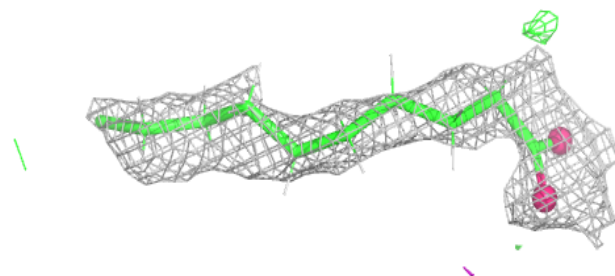
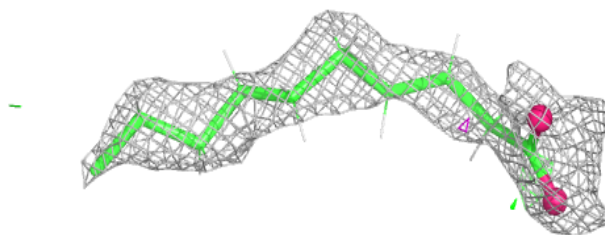
**Electron density around LMG a 416:**

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

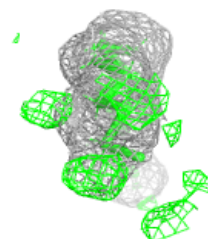
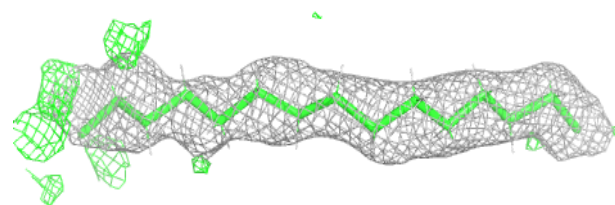
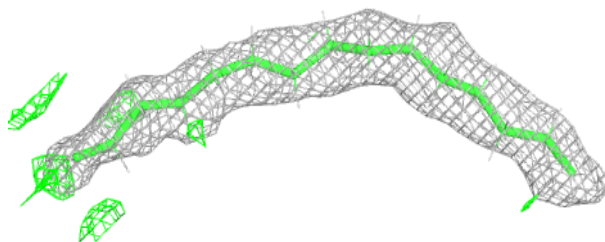


Electron density around STE R 101:

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

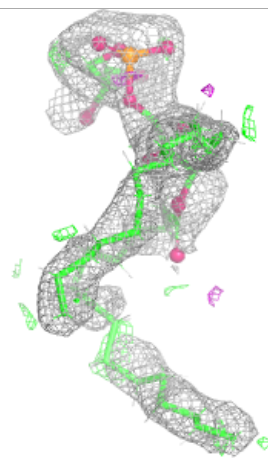
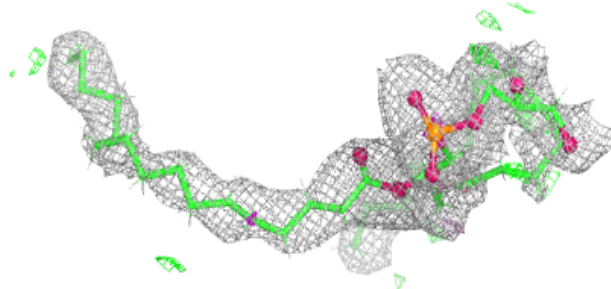
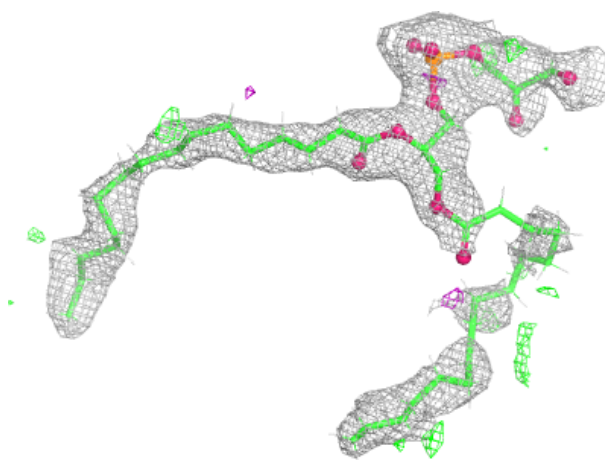
**Electron density around STE I 101:**

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



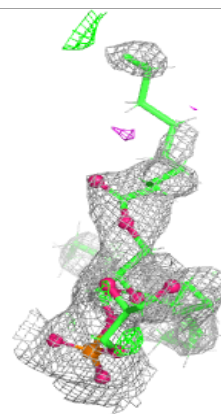
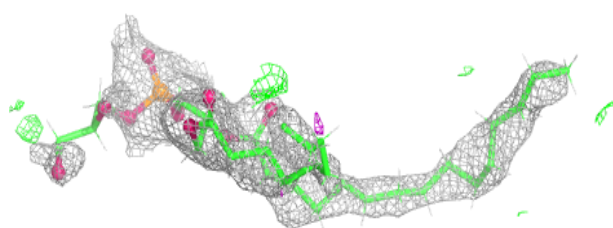
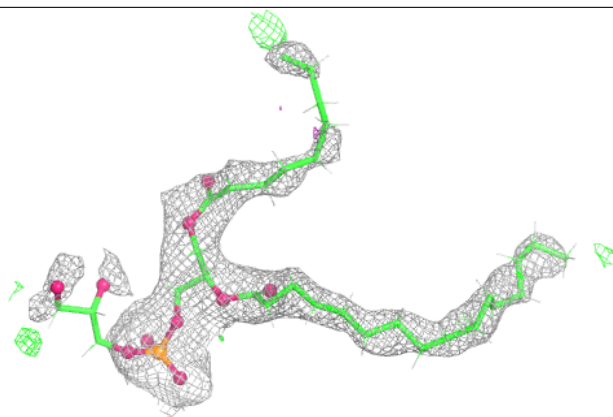
Electron density around LHG E 101:

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and green (positive)

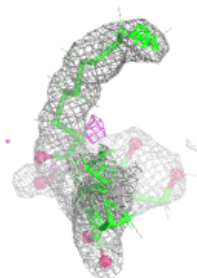
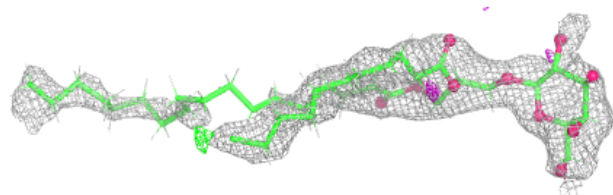
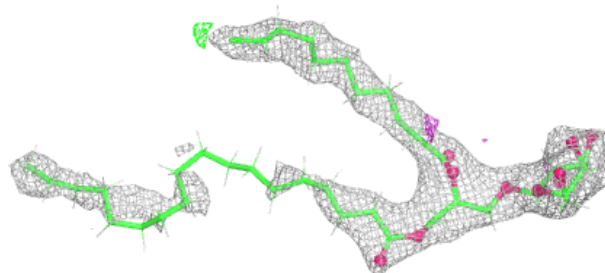


Electron density around LHG e 101:

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

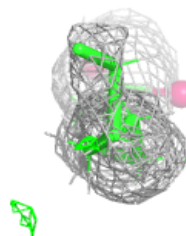
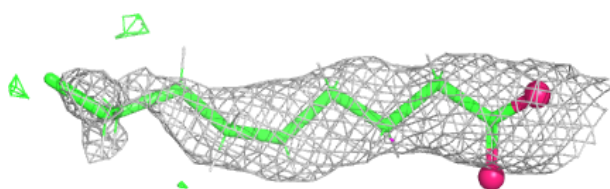
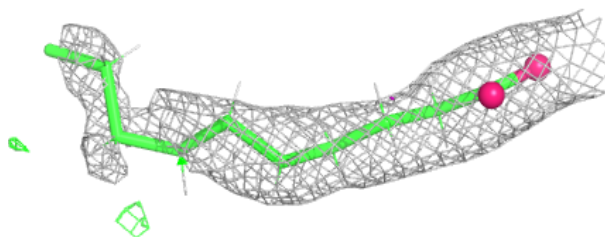
**Electron density around LMG c 522:**

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

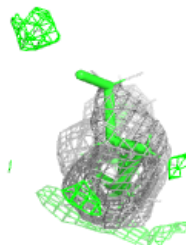
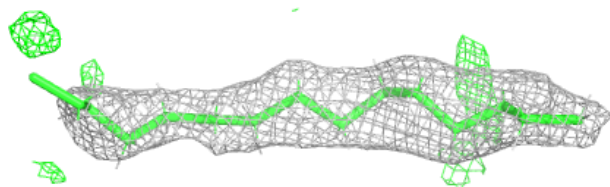
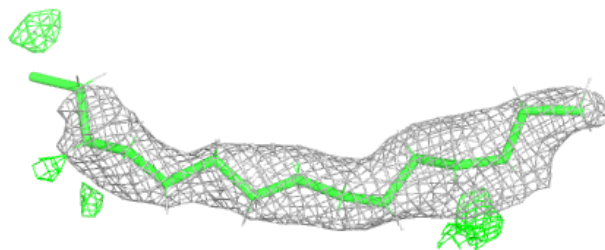


Electron density around STE m 102:

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

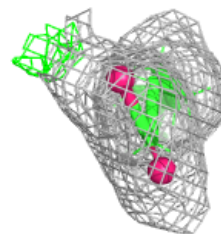
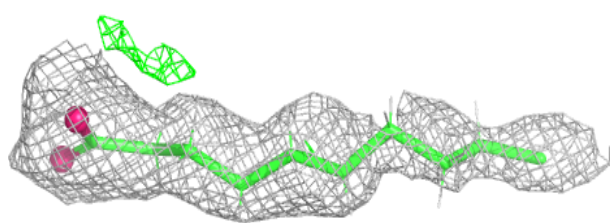
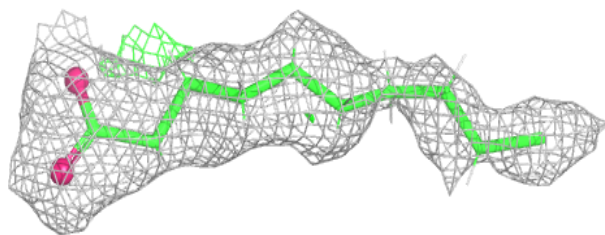
**Electron density around STE T 102:**

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

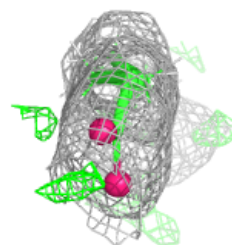
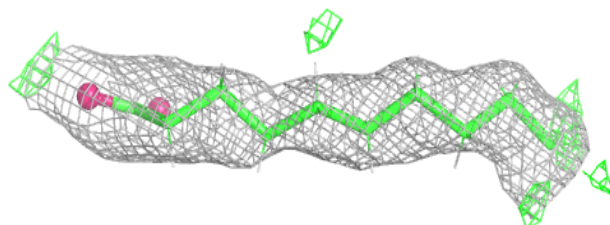
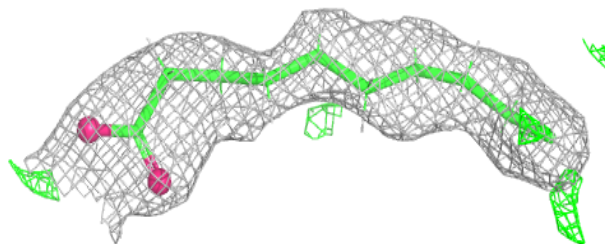


Electron density around STE k 102:

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

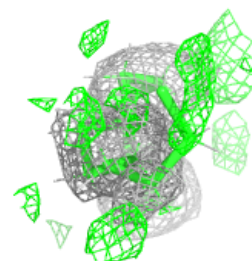
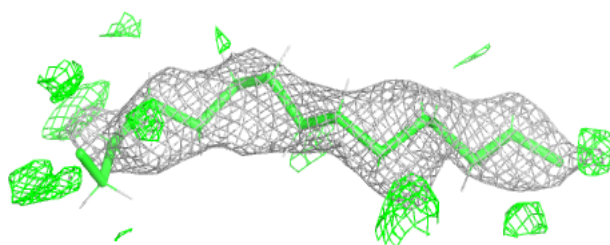
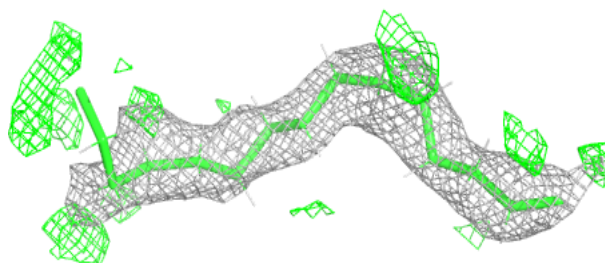
**Electron density around STE C 521:**

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

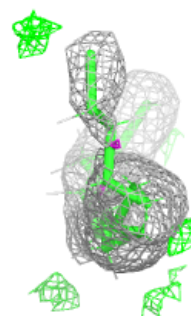
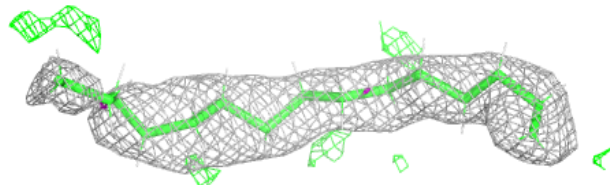
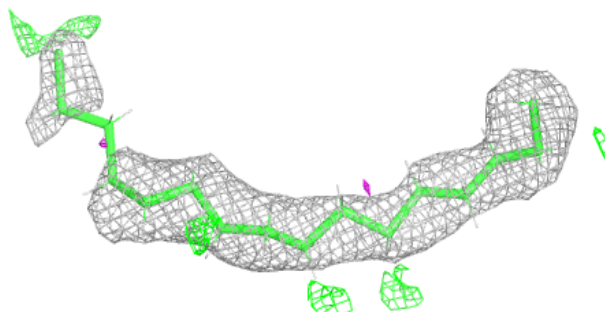


Electron density around STE a 415:

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

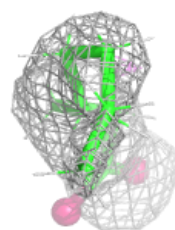
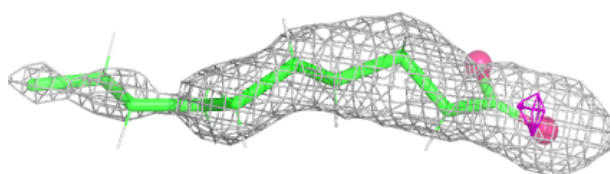
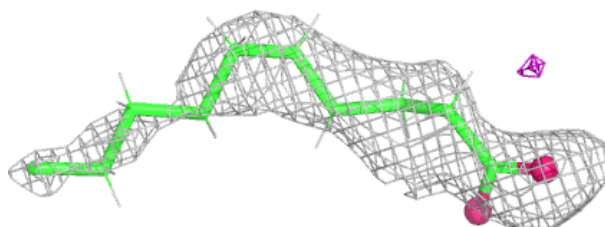
**Electron density around STE b 621:**

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

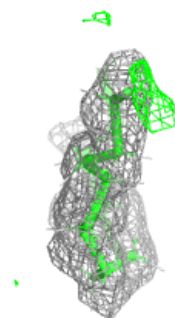
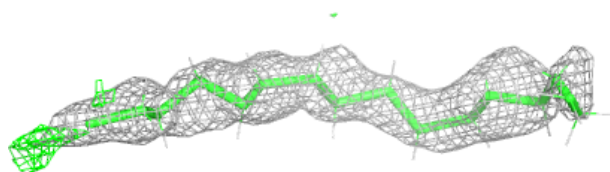
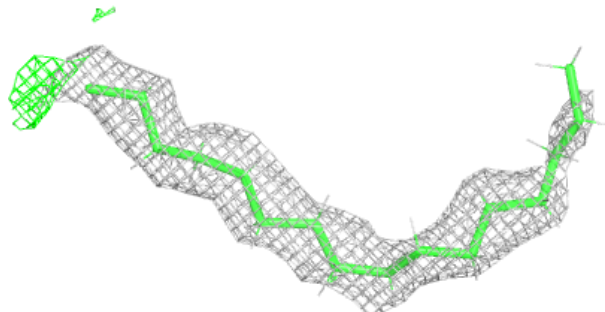


Electron density around STE B 626:

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

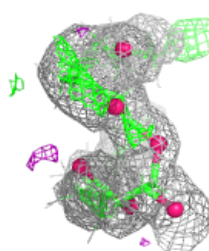
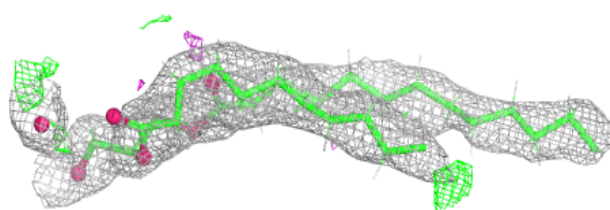
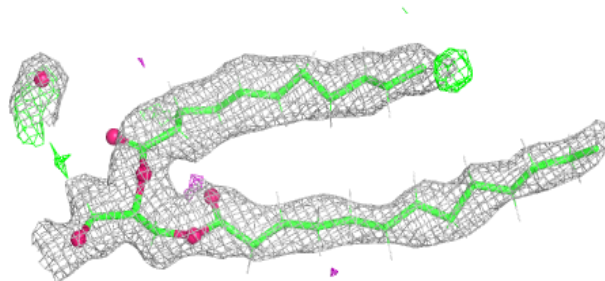
**Electron density around STE B 625:**

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

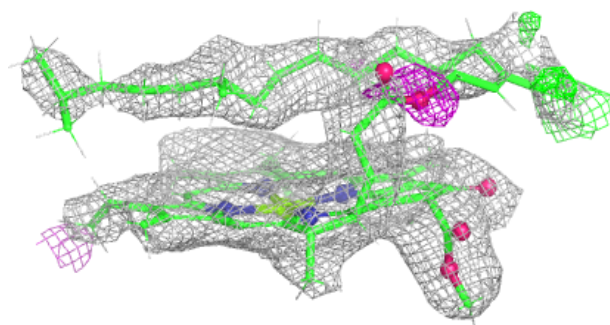
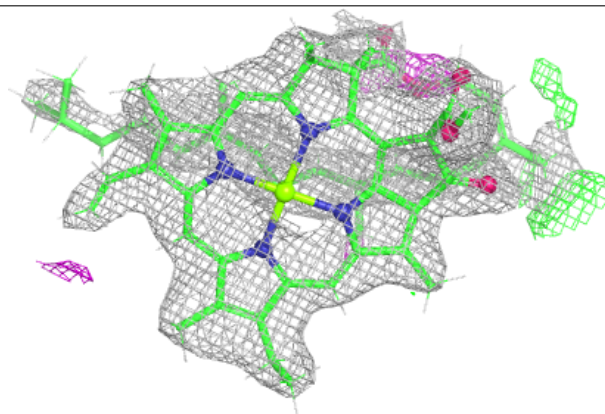


Electron density around LMG D 410:

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

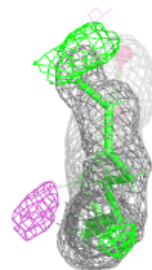
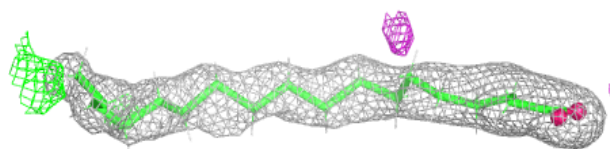
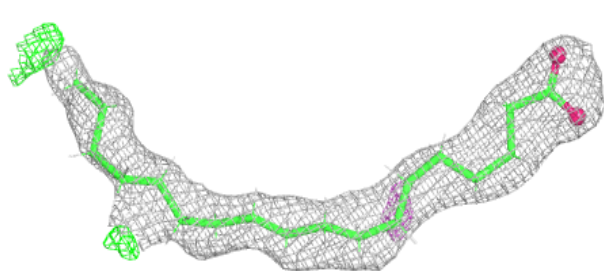
**Electron density around CLA b 601:**

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



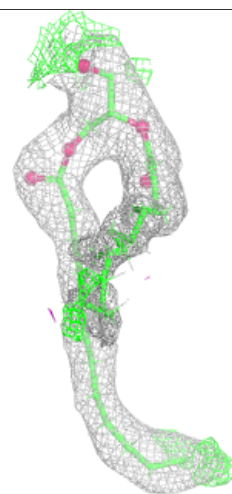
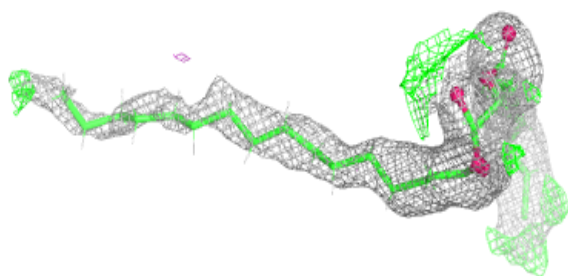
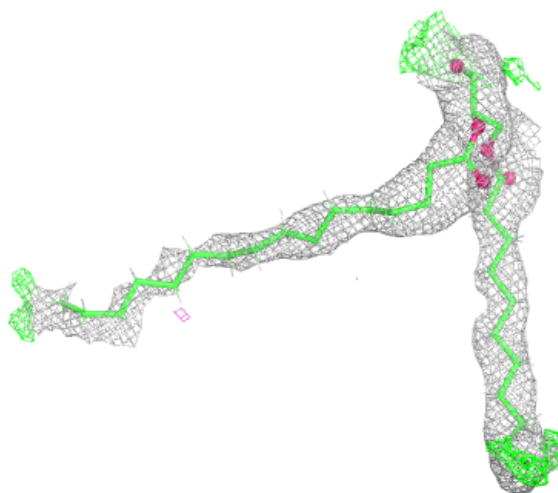
Electron density around STE d 412:

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



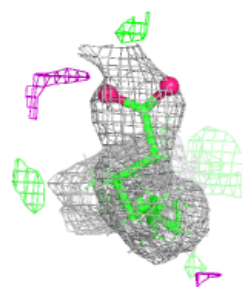
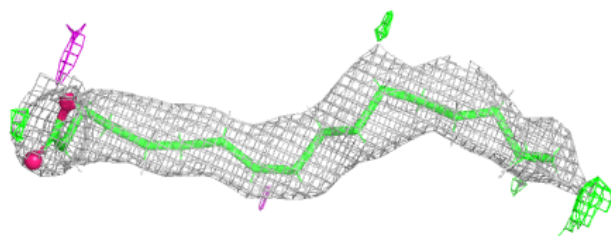
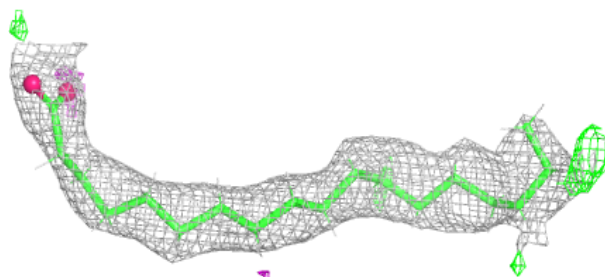
Electron density around SQD a 412:

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

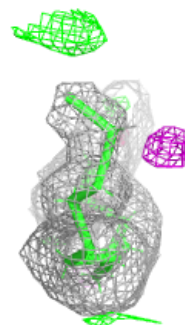
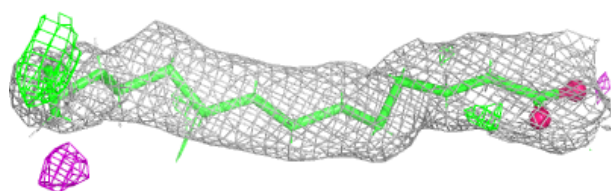
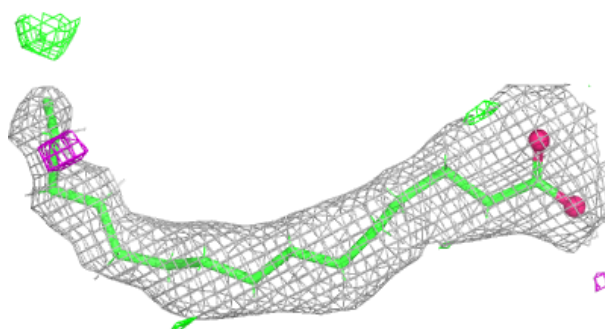


Electron density around STE b 622:

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

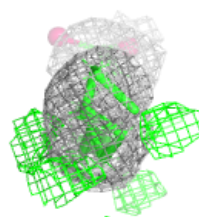
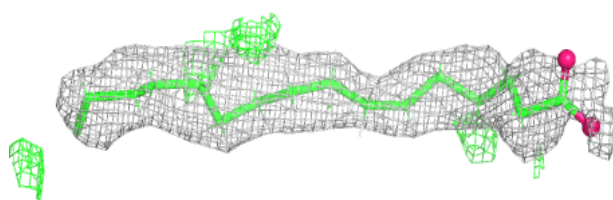
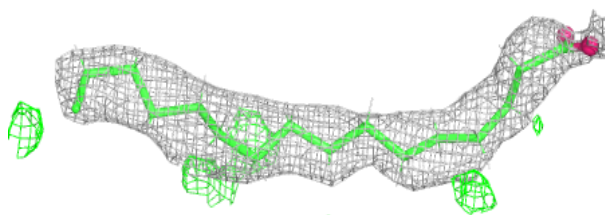
**Electron density around STE B 620:**

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

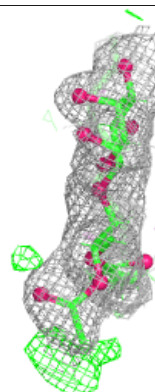
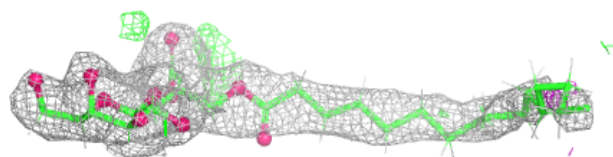
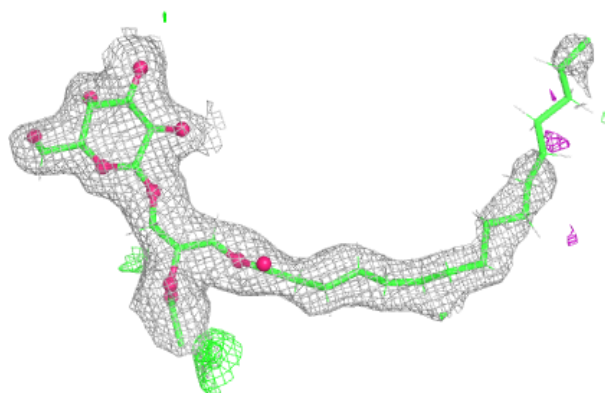


Electron density around STE t 103:

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

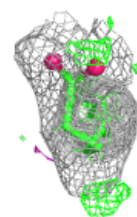
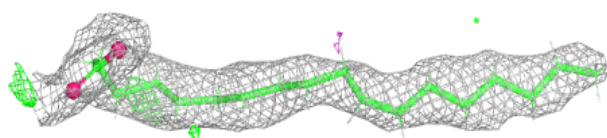
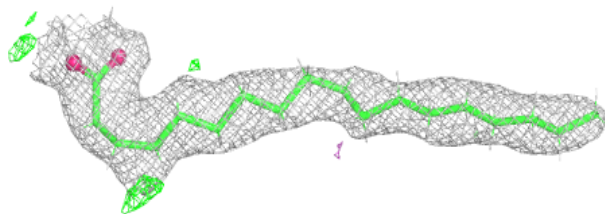
**Electron density around LMG c 520:**

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

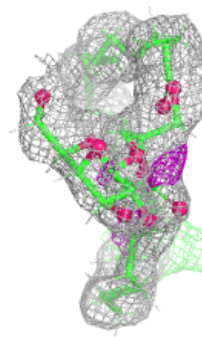
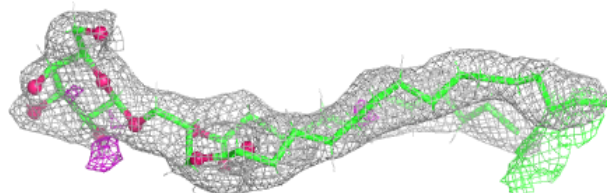
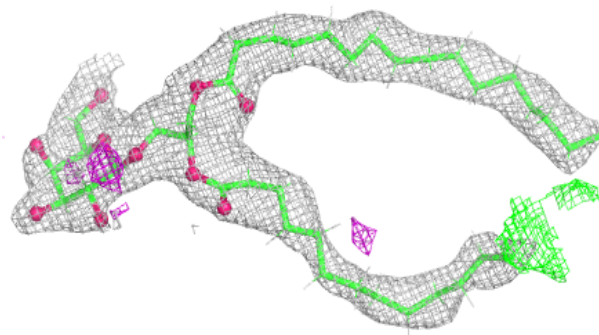


Electron density around STE c 521:

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

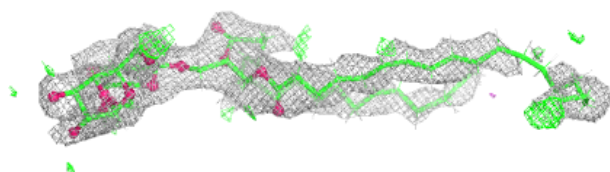
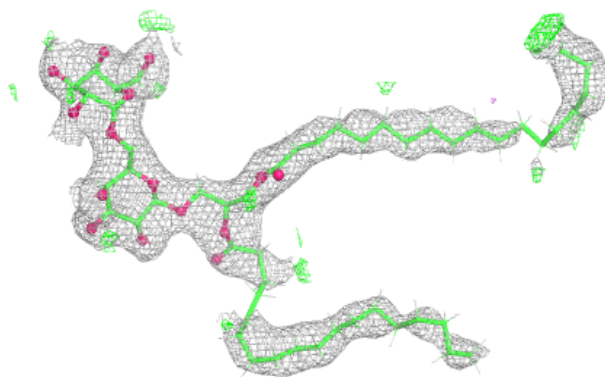
**Electron density around LMG A 411:**

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

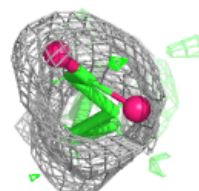
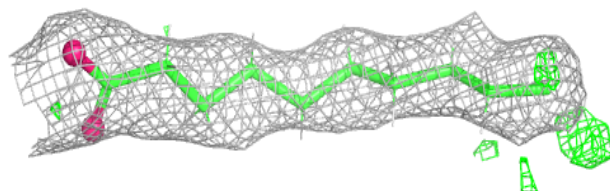
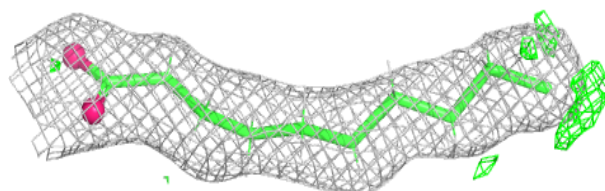


Electron density around DGD A 415:

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

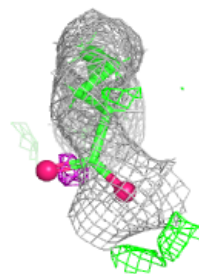
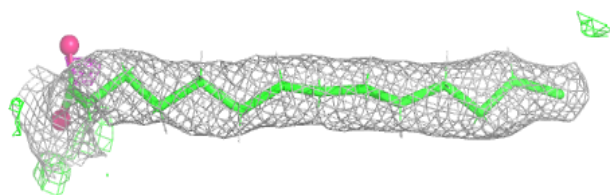
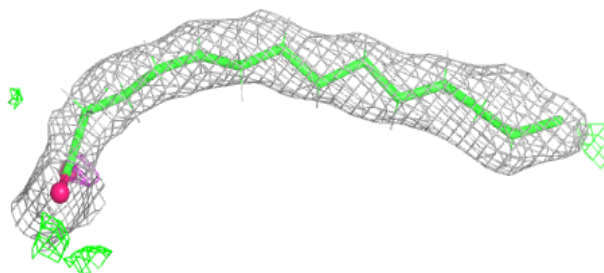
**Electron density around STE j 101:**

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

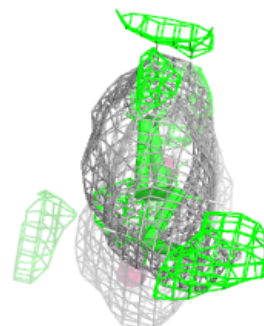
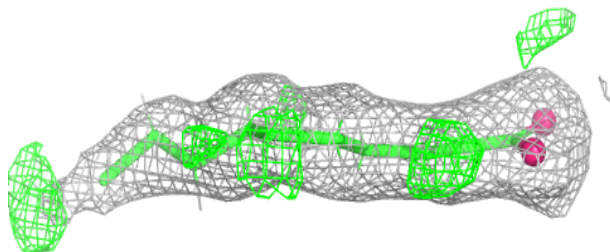
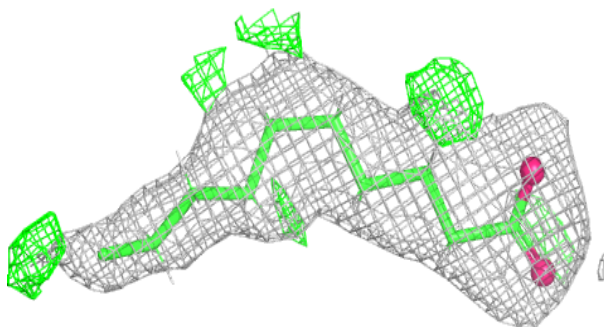


Electron density around STE b 624:

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

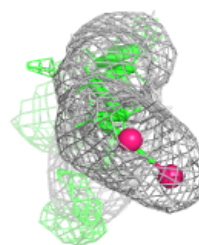
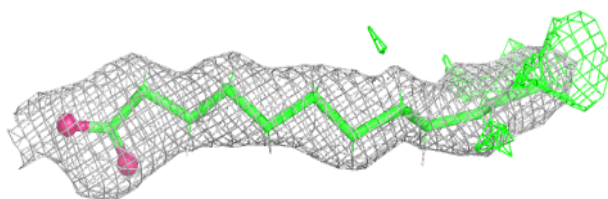
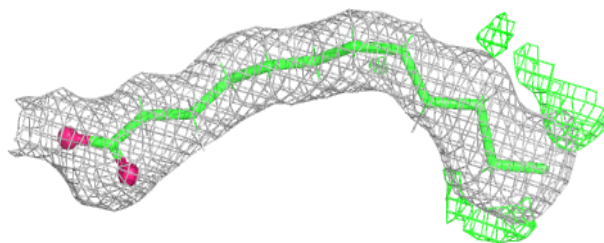
**Electron density around STE C 523:**

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

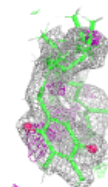
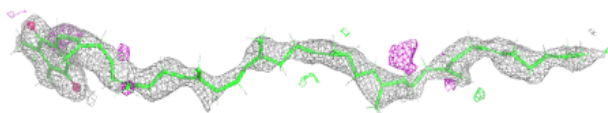
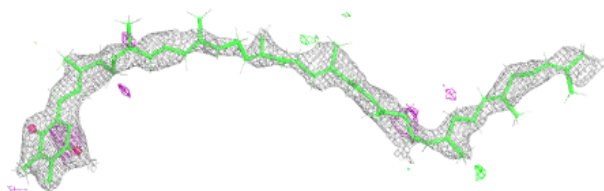


Electron density around STE t 102:

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

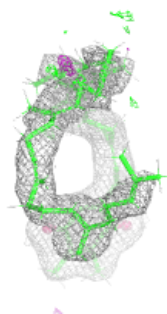
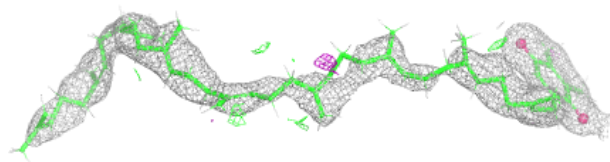
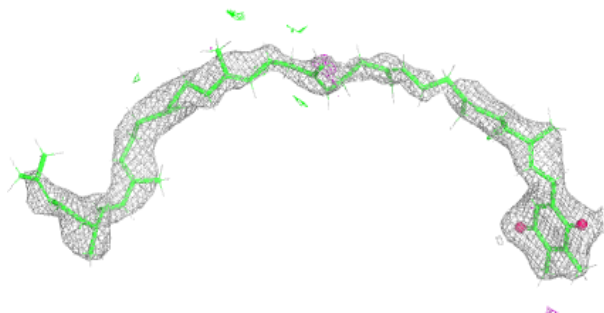
**Electron density around PL9 A 410:**

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

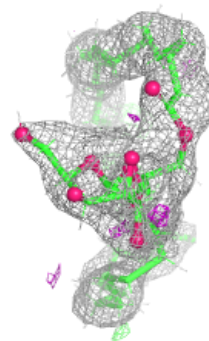
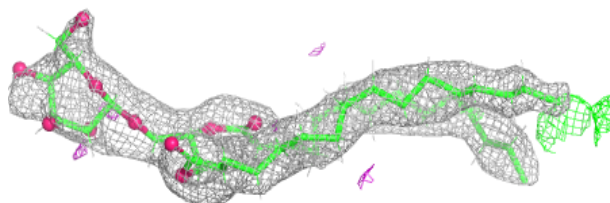
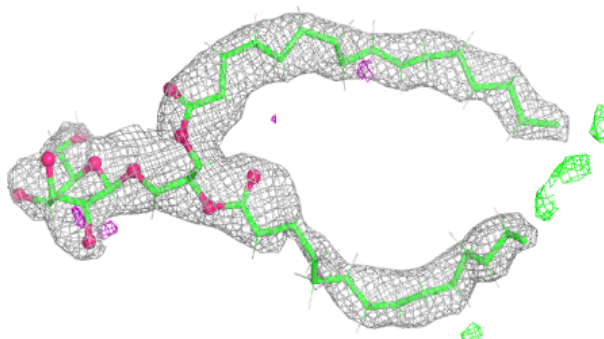


Electron density around PL9 a 409:

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

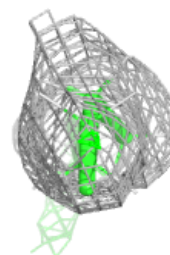
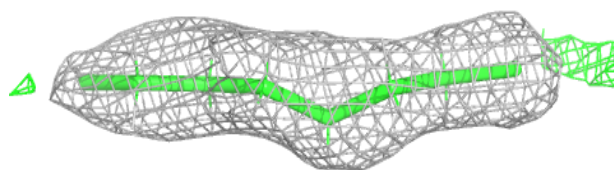
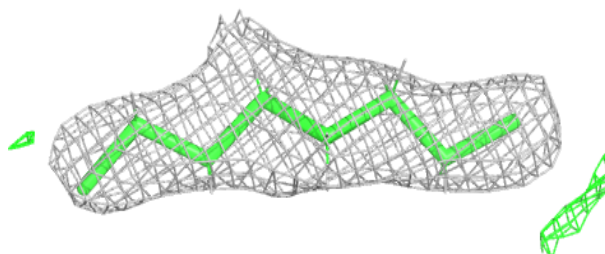
**Electron density around LMG c 523:**

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

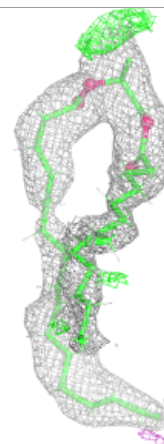
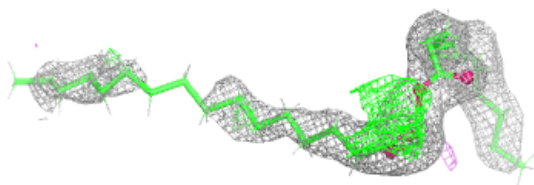
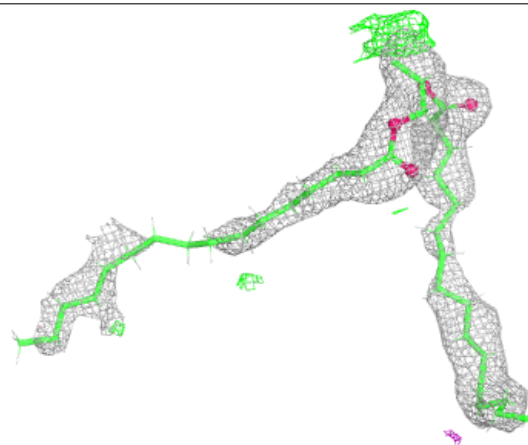


Electron density around STE Z 101:

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

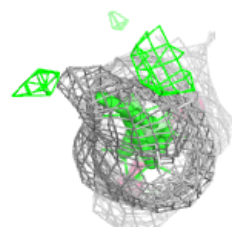
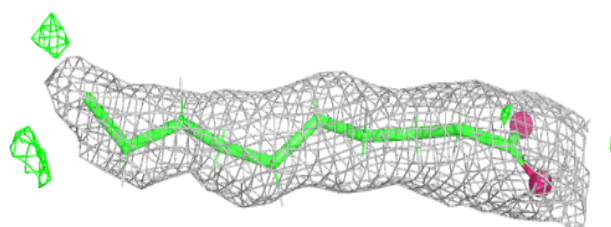
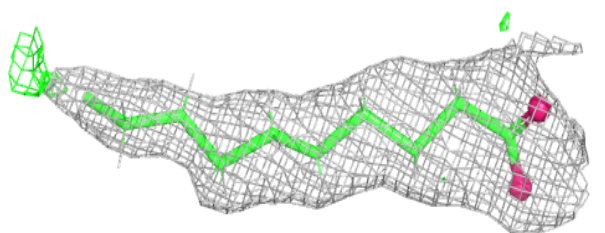
**Electron density around SQD A 414:**

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

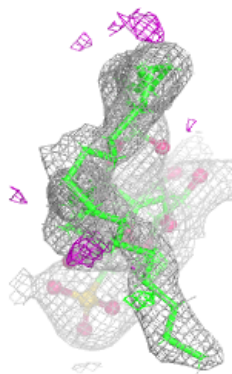
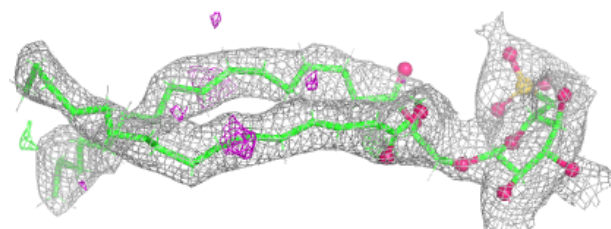
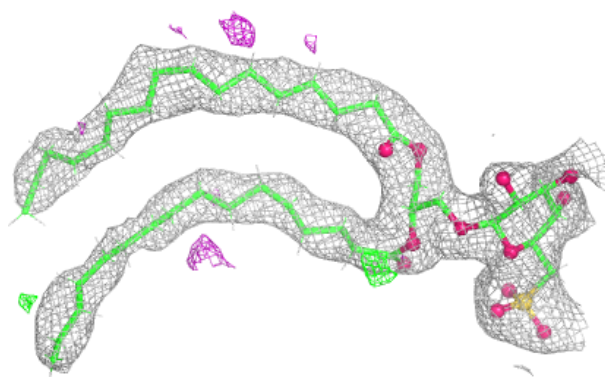


Electron density around STE J 101:

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

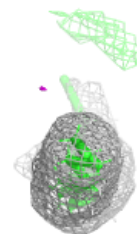
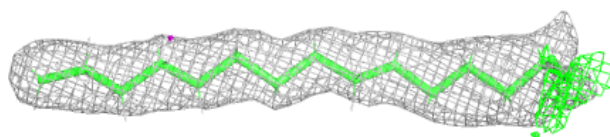
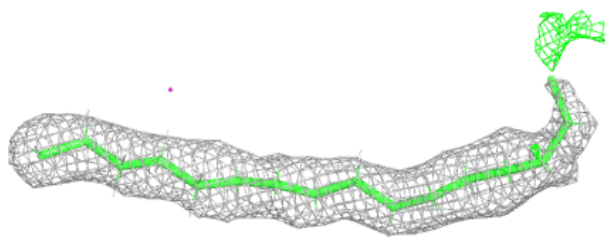
**Electron density around SQD B 623:**

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

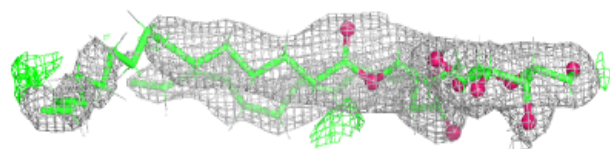
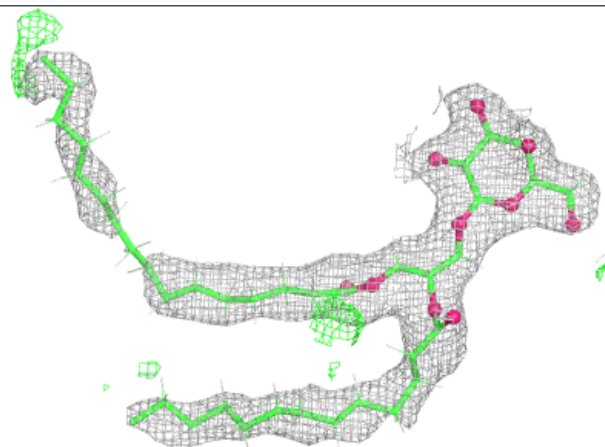


Electron density around STE C 522:

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

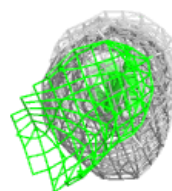
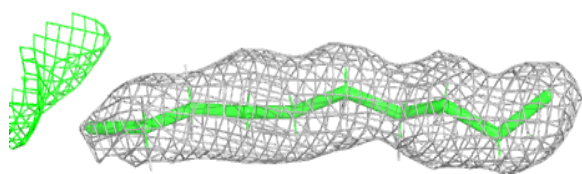
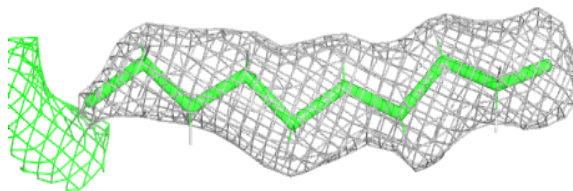
**Electron density around LMG C 520:**

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

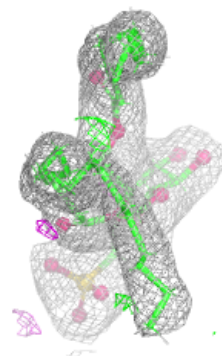
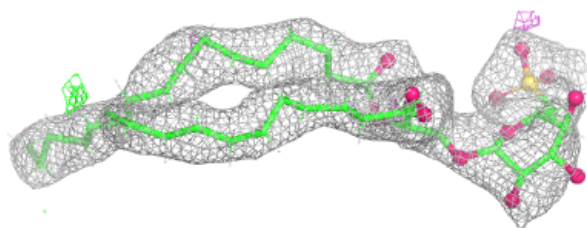
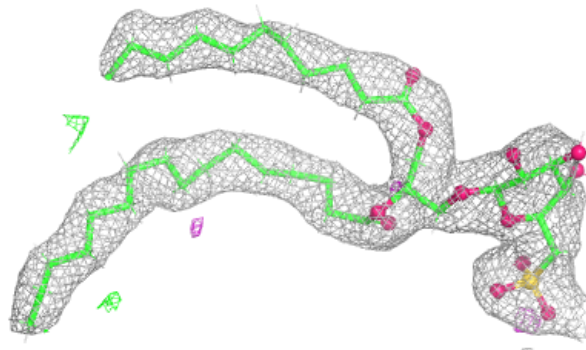


Electron density around STE M 103:

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

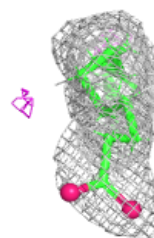
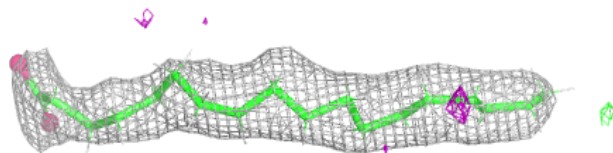
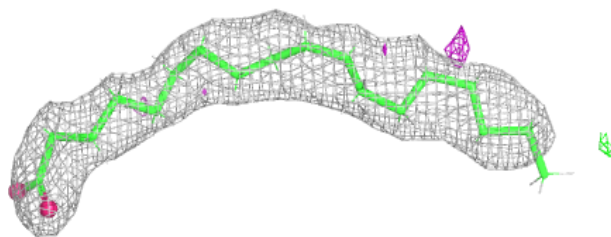
**Electron density around SQD b 620:**

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

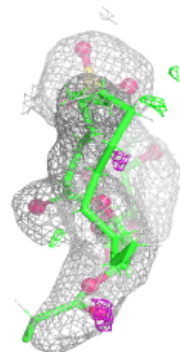
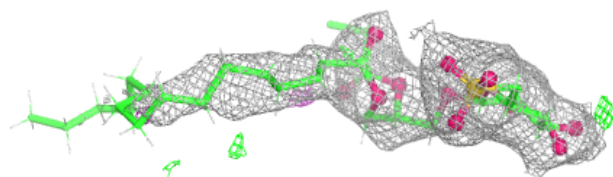
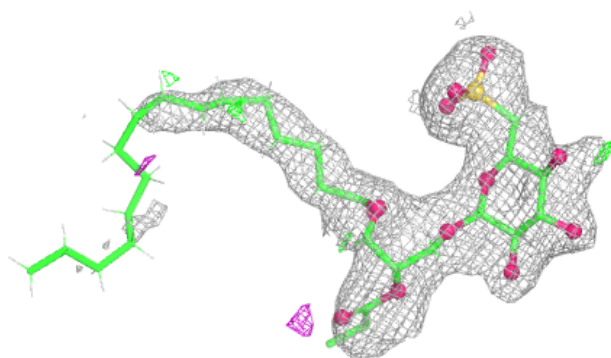


Electron density around STE D 412:

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

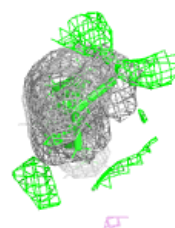
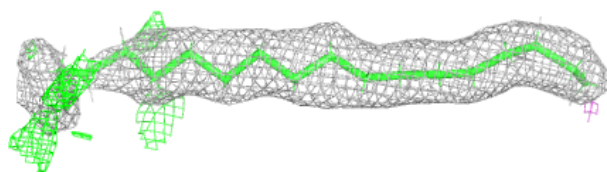
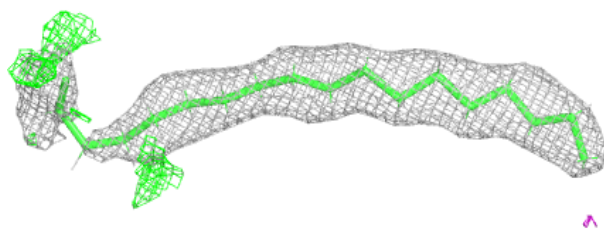
**Electron density around SQD f 102:**

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

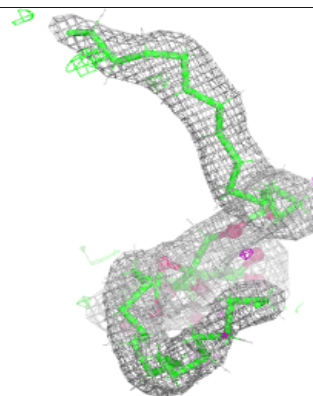
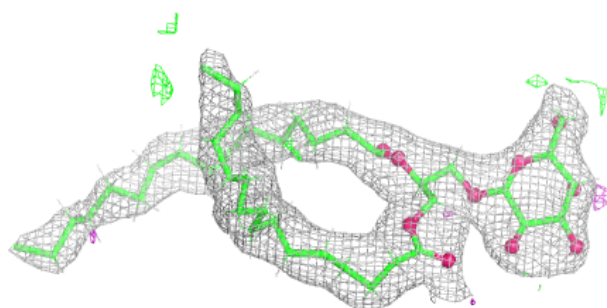
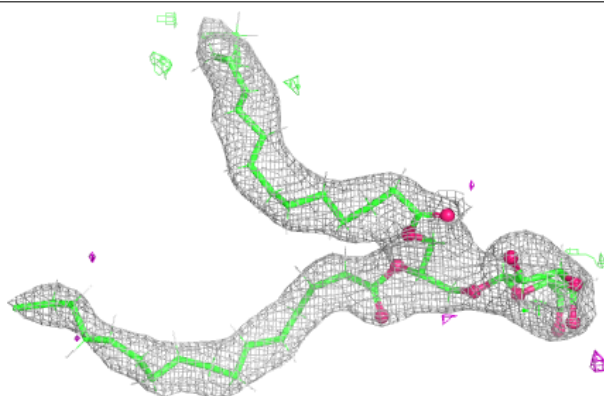


Electron density around STE l 102:

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

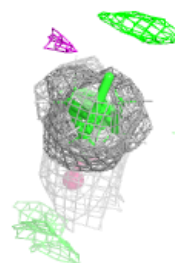
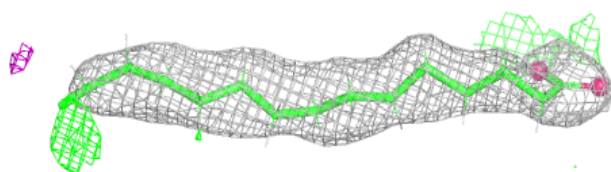
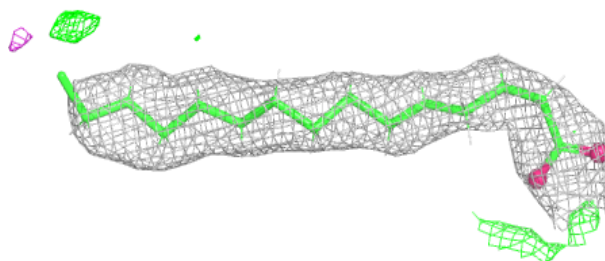
**Electron density around LMG m 101:**

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

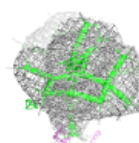
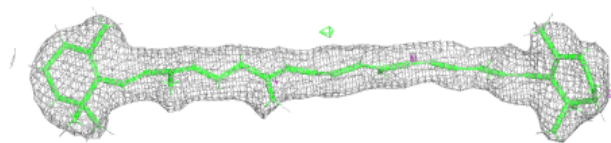
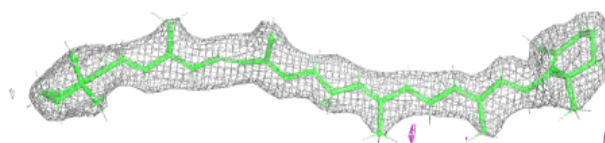


Electron density around STE d 411:

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

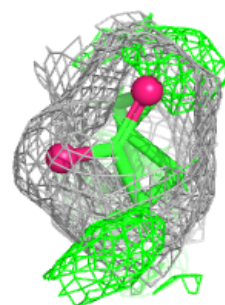
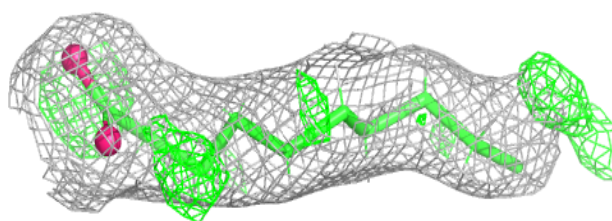
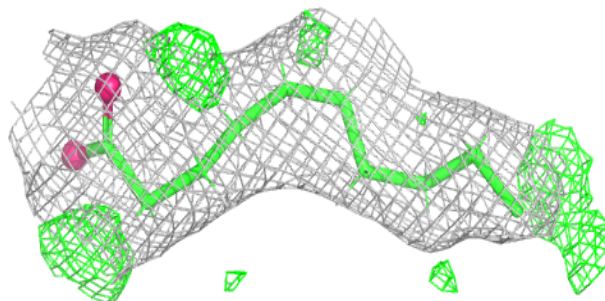
**Electron density around BCR C 514:**

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

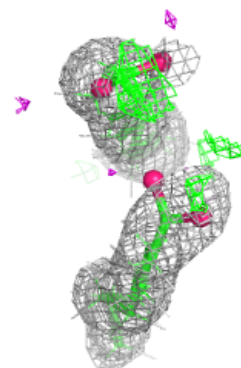
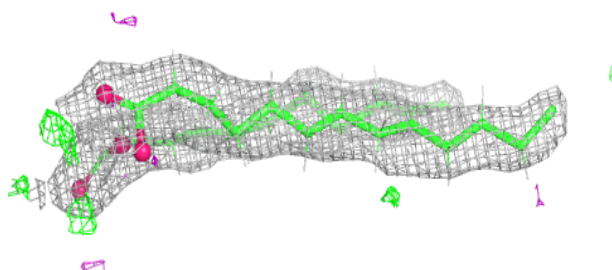
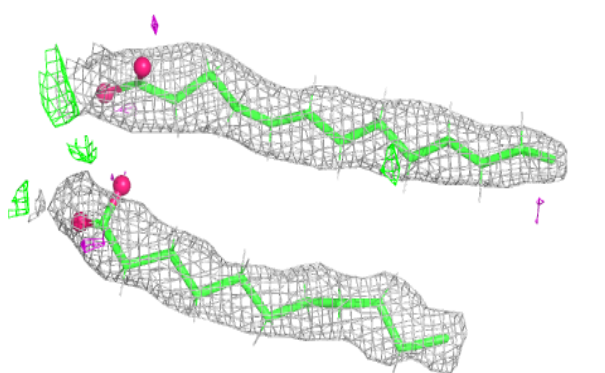


Electron density around STE B 624:

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

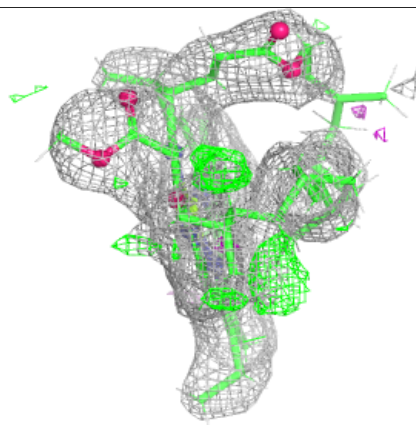
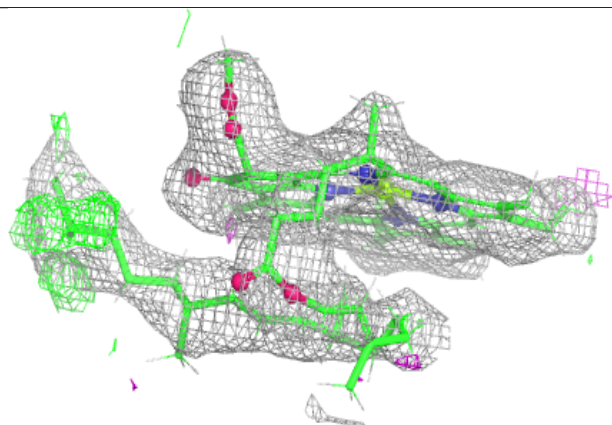
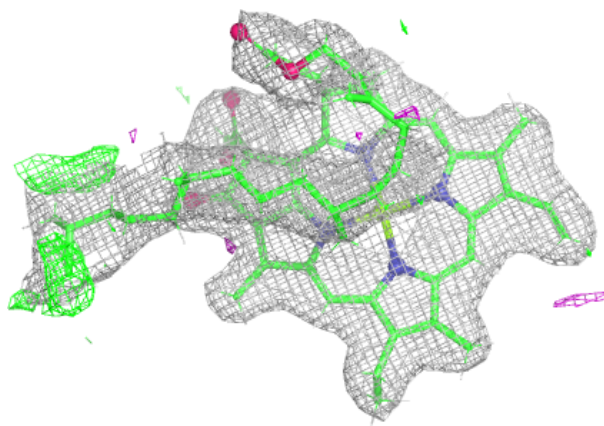
**Electron density around LMG D 411:**

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

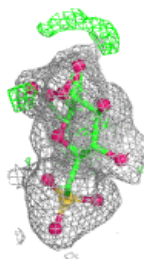
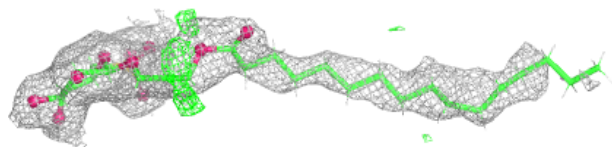
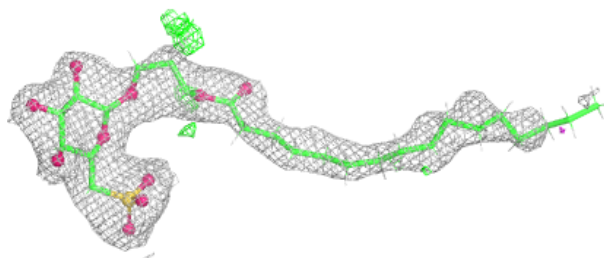


Electron density around CLA B 601:

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

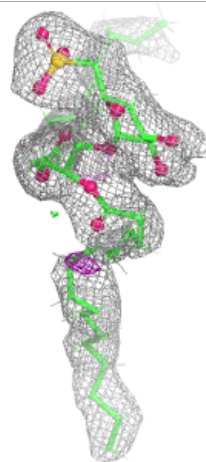
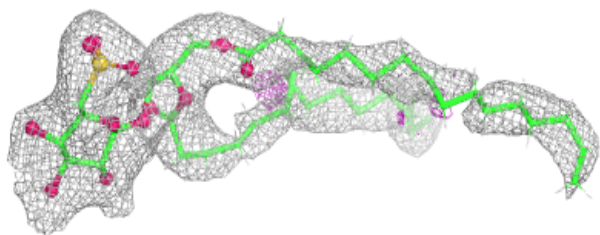
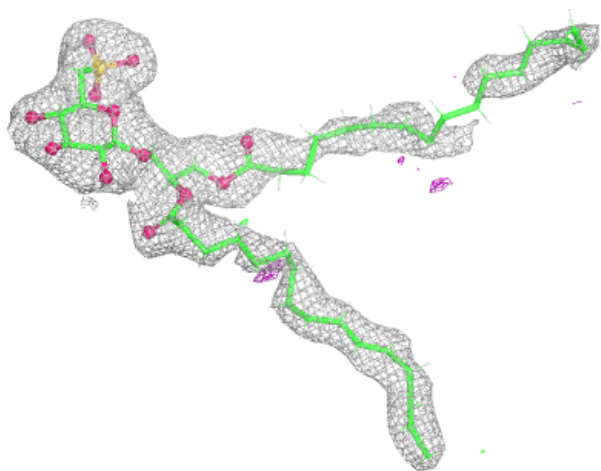
**Electron density around SQD D 408:**

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



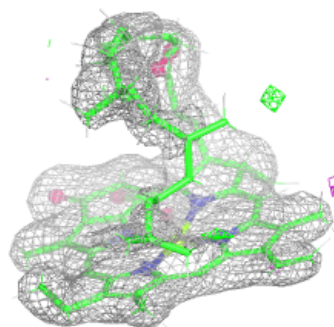
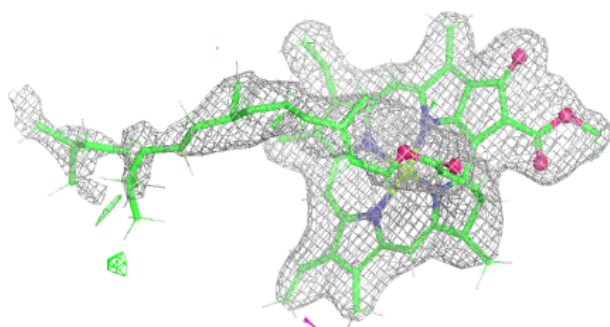
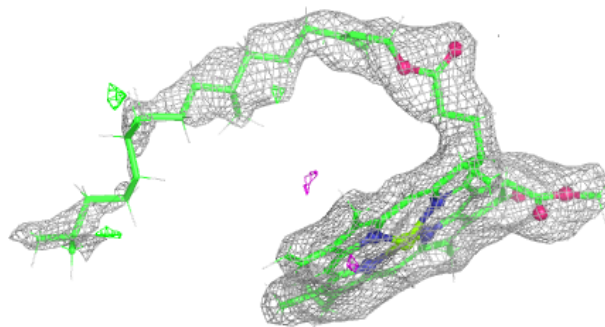
Electron density around SQD a 411:

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

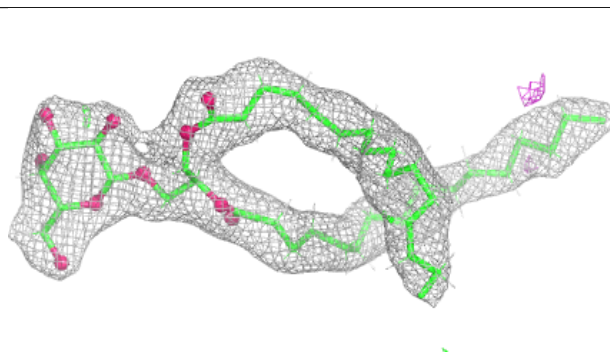
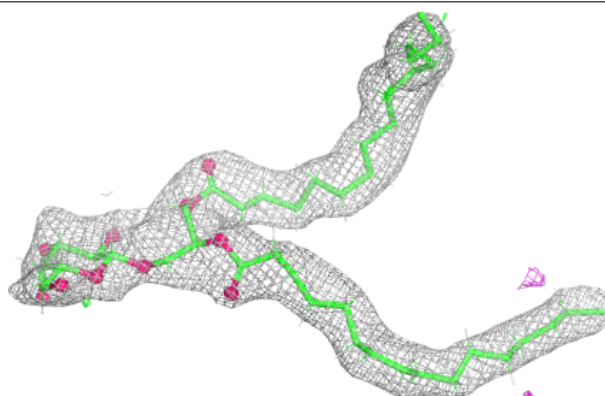


Electron density around CLA C 513:

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

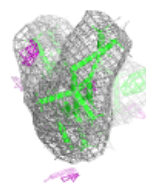
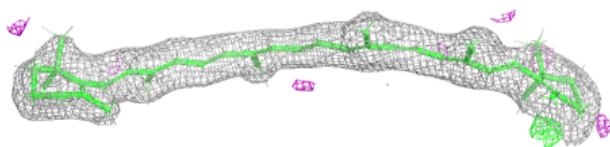
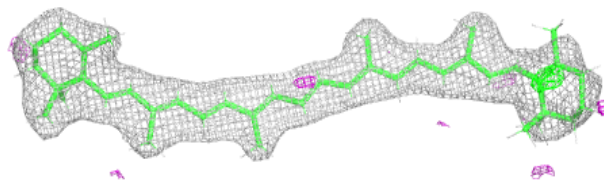
**Electron density around LMG M 101:**

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

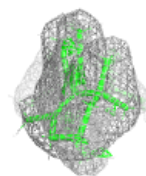
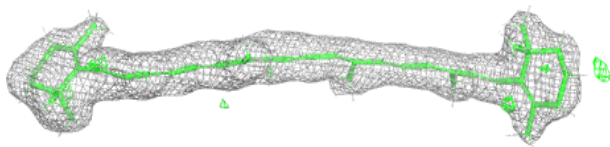


Electron density around BCR D 405:

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

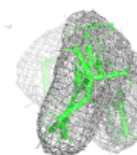
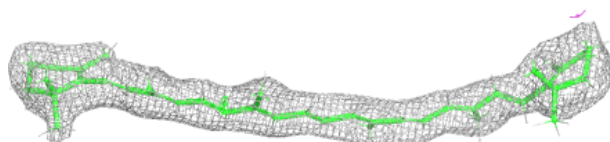
**Electron density around BCR Y 101:**

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

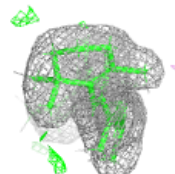
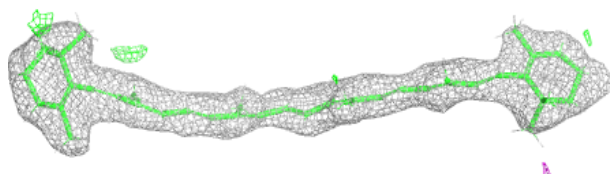
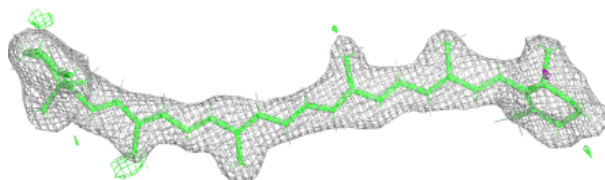


Electron density around BCR d 406:

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

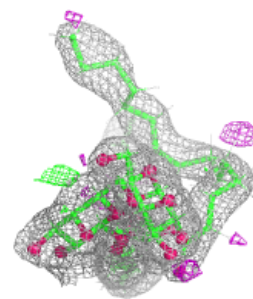
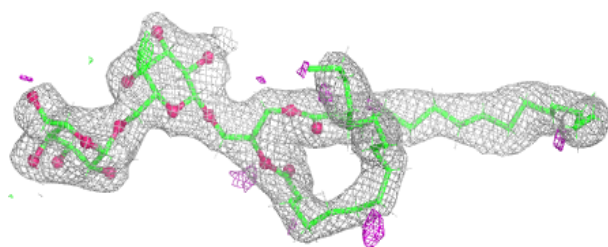
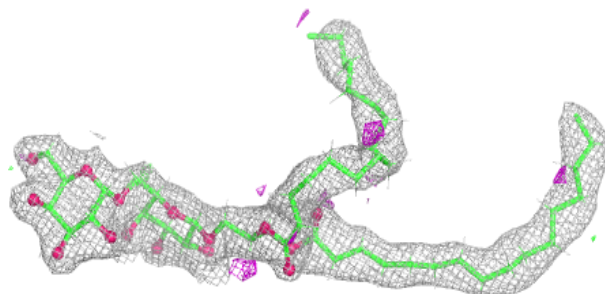
**Electron density around BCR x 101:**

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

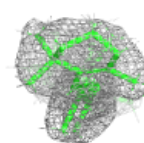
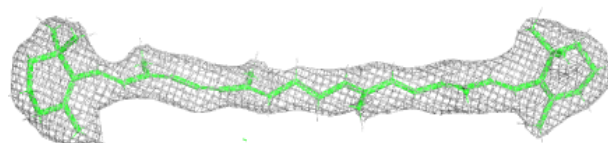
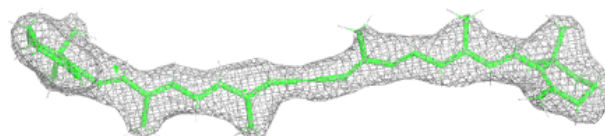


Electron density around DGD h 101:

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

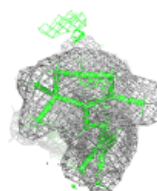
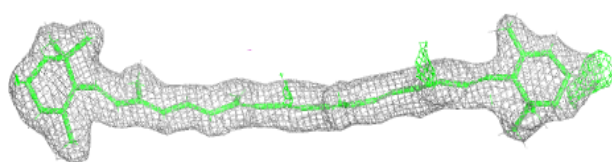
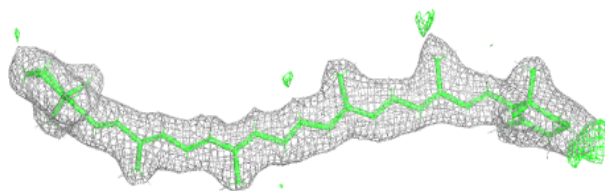
**Electron density around BCR c 514:**

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

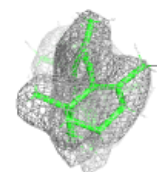
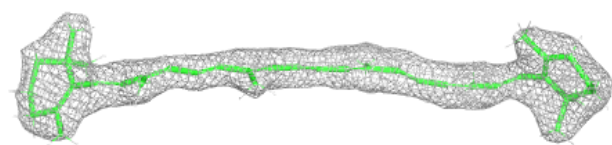
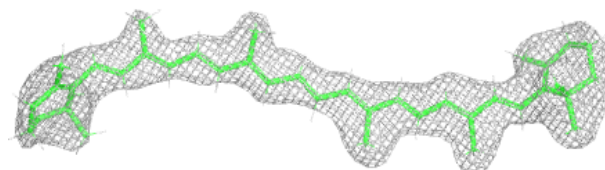


Electron density around BCR H 101:

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

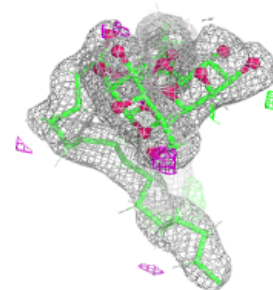
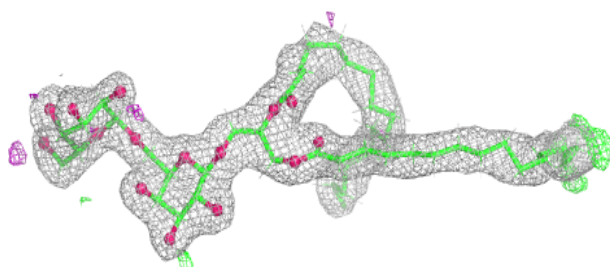
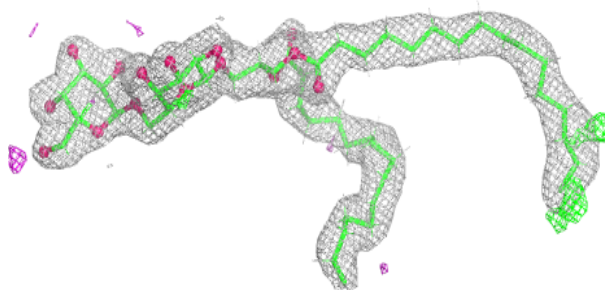
**Electron density around BCR k 101:**

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

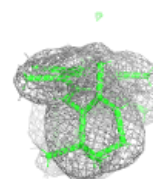
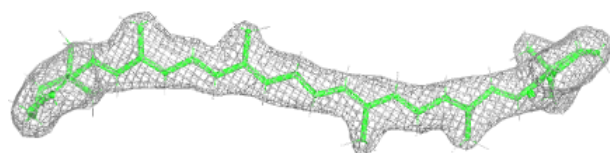
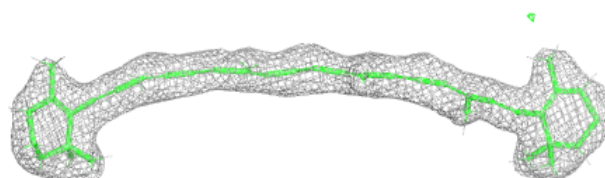


Electron density around DGD H 102:

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

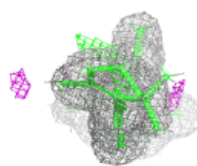
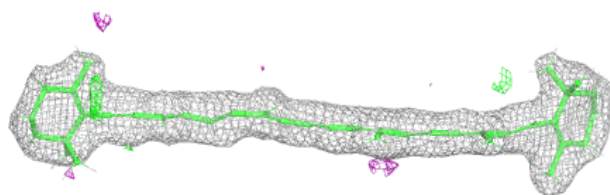
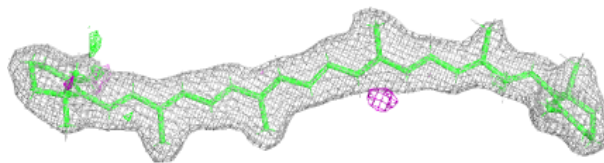
**Electron density around BCR c 516:**

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



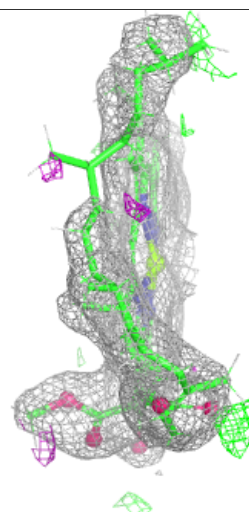
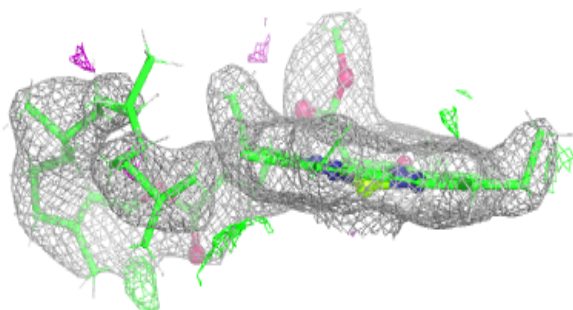
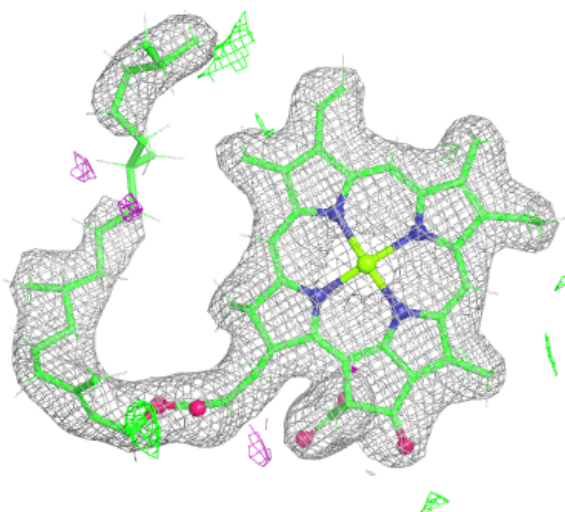
Electron density around BCR C 515:

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



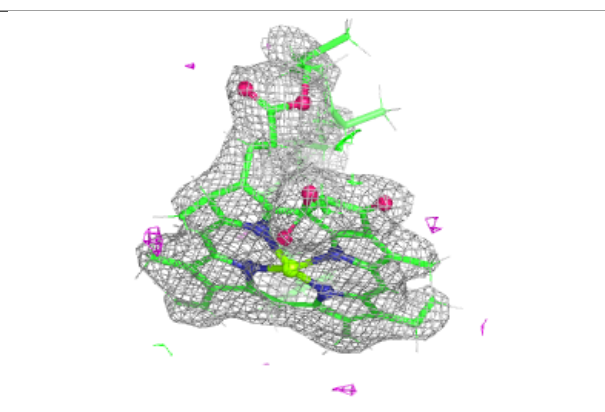
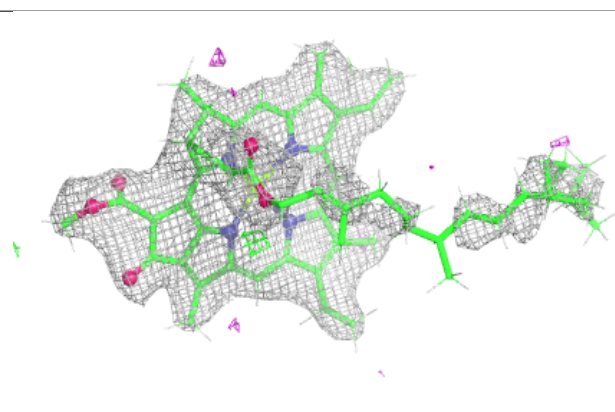
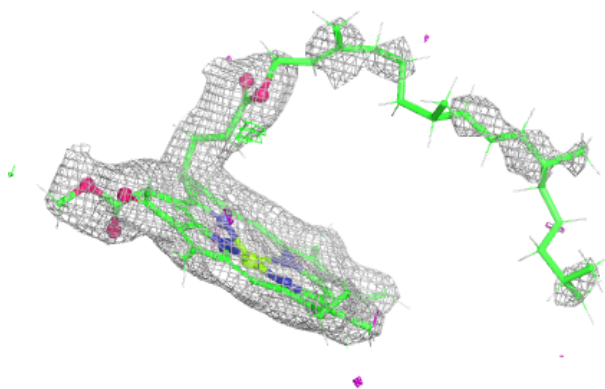
Electron density around CLA c 512:

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

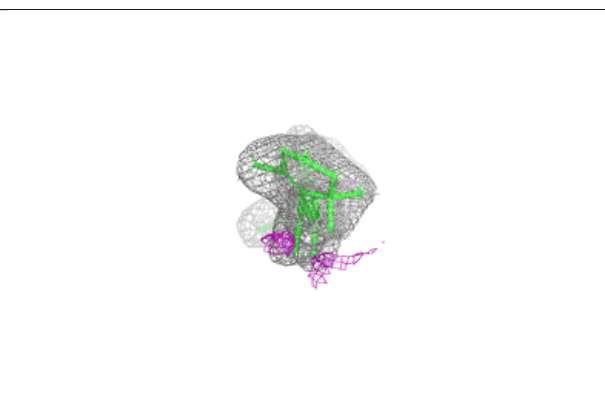
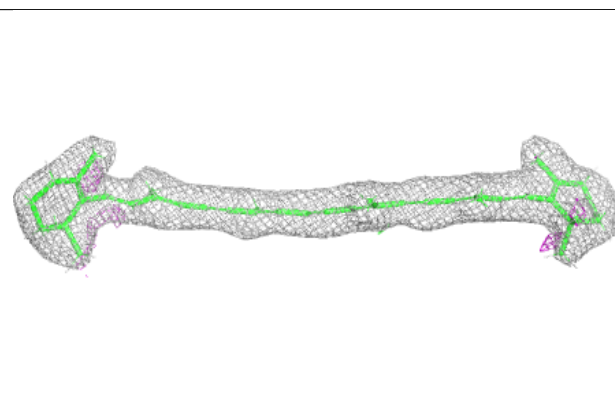
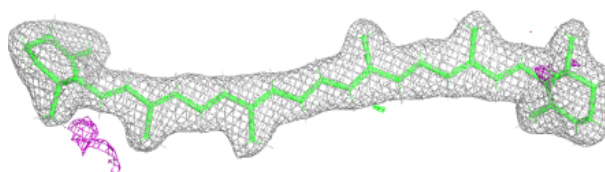


Electron density around CLA c 513:

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

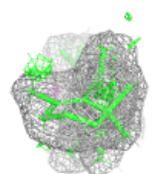
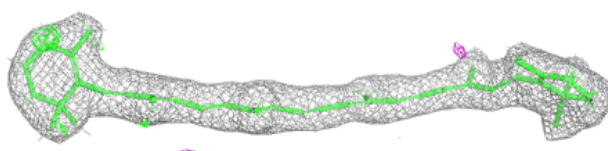
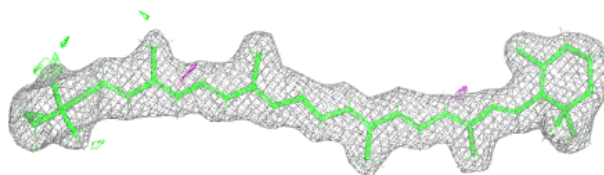
**Electron density around BCR B 618:**

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

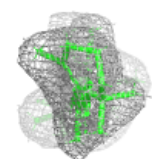
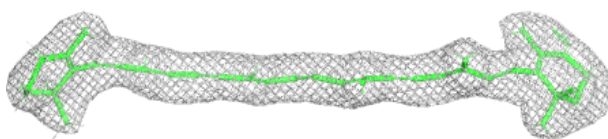
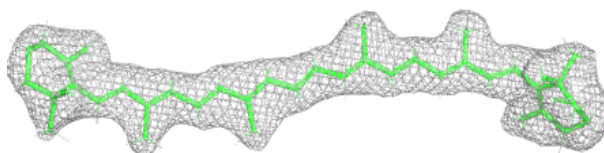


Electron density around BCR b 617:

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

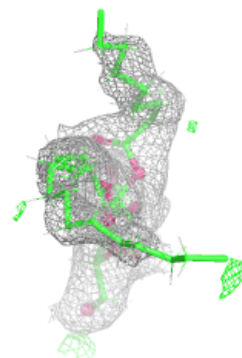
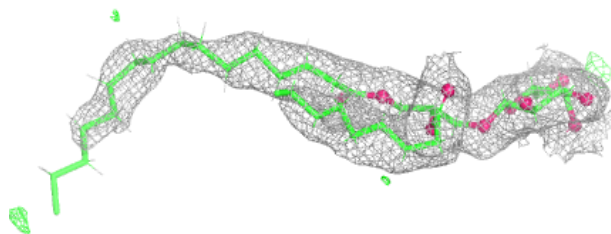
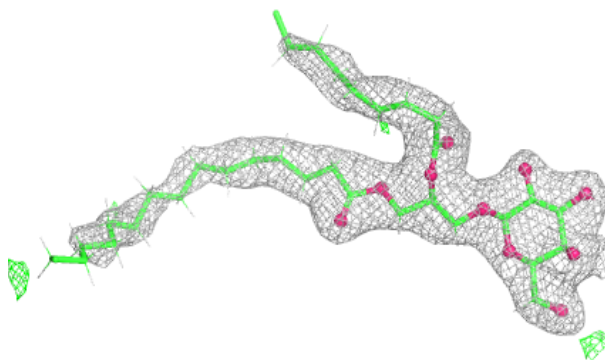
**Electron density around BCR b 618:**

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

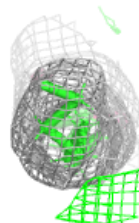
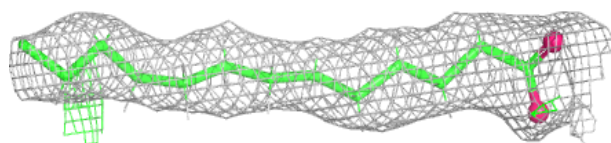
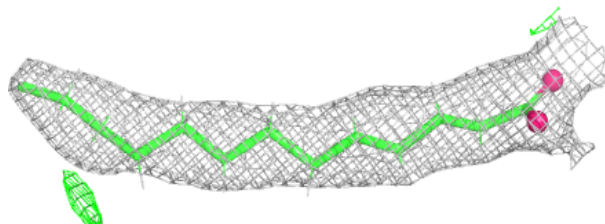


Electron density around LMG d 410:

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

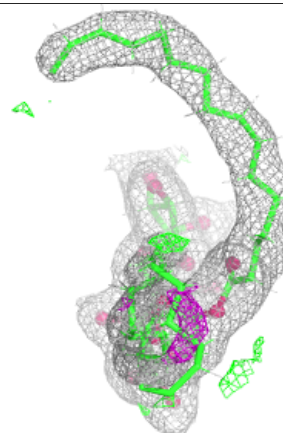
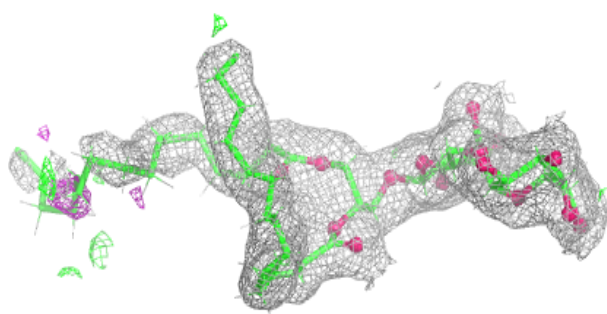
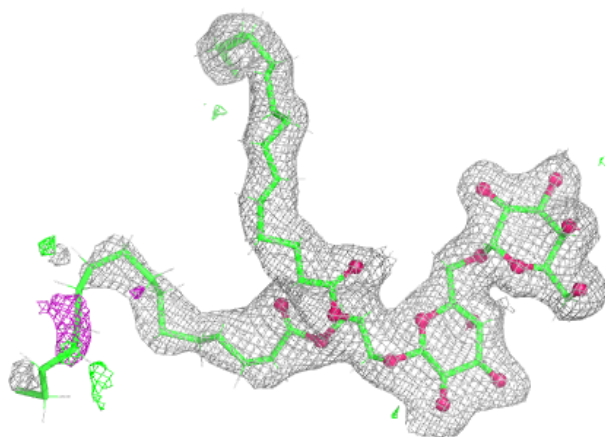
**Electron density around STE M 102:**

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

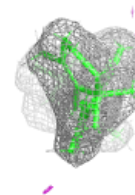
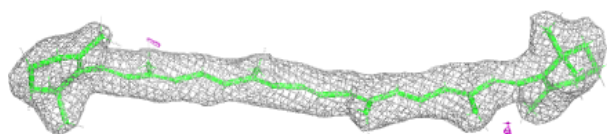
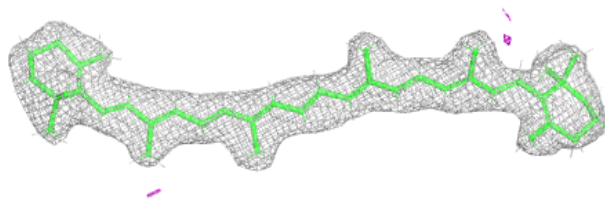


Electron density around DGD C 518:

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

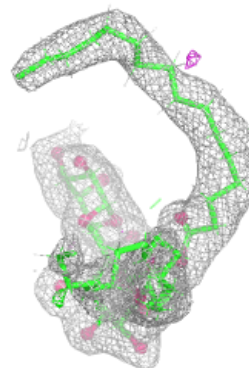
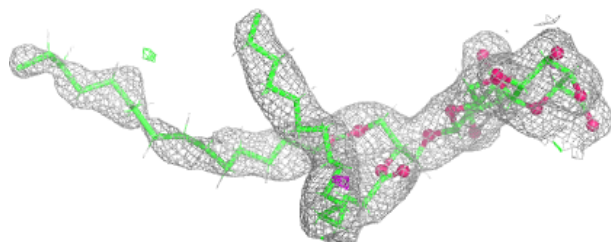
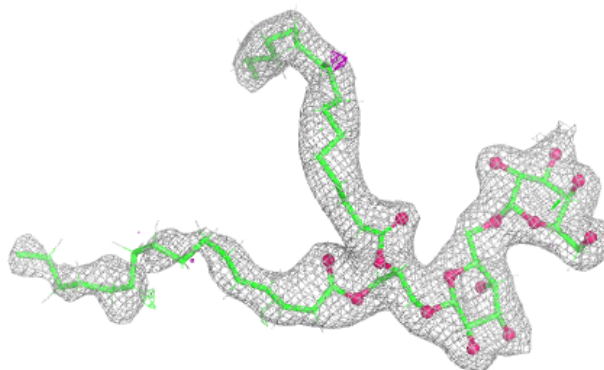
**Electron density around BCR b 619:**

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

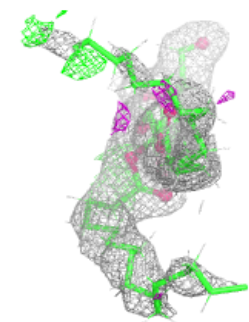
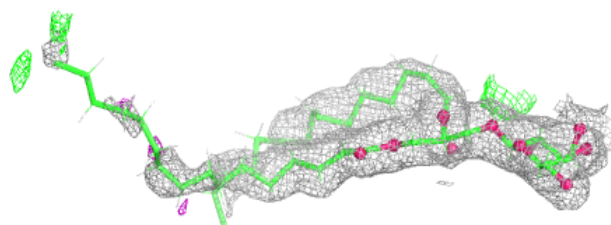
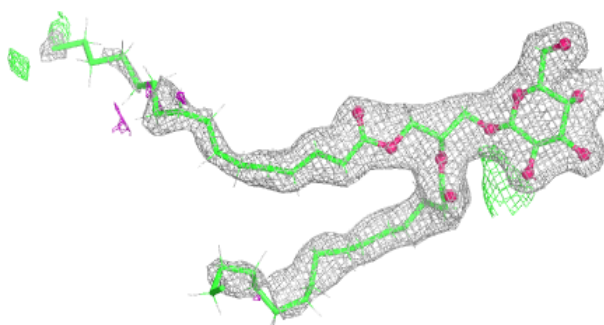


Electron density around DGD c 518:

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

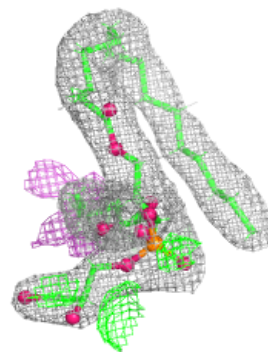
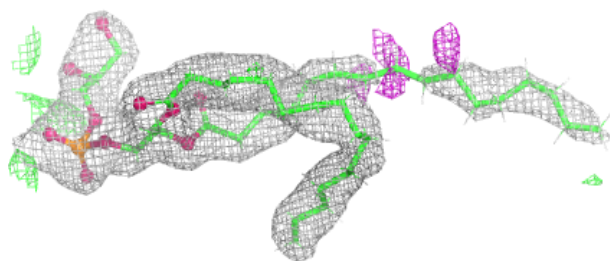
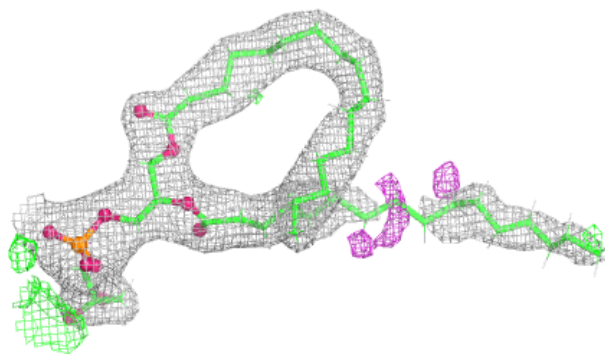
**Electron density around LMG D 407:**

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



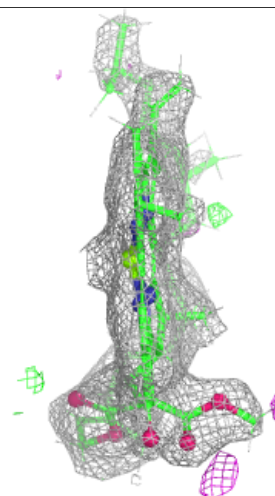
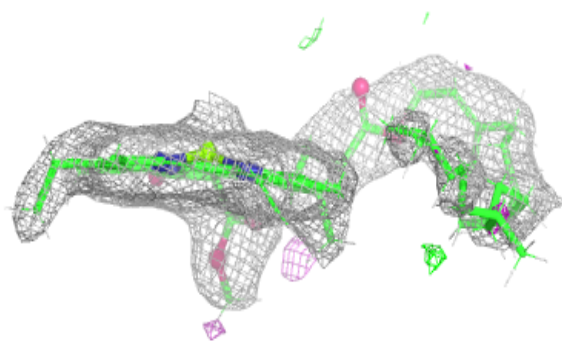
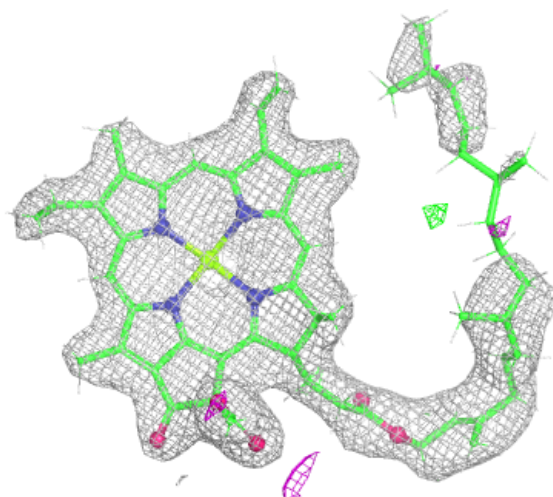
Electron density around LHG a 410:

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



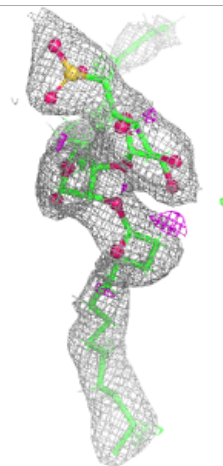
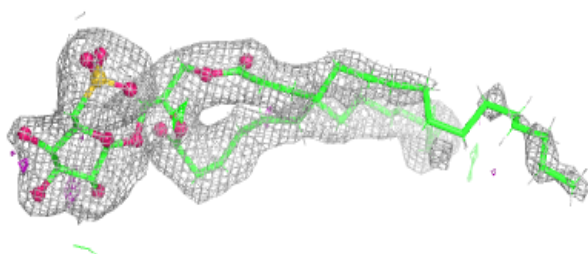
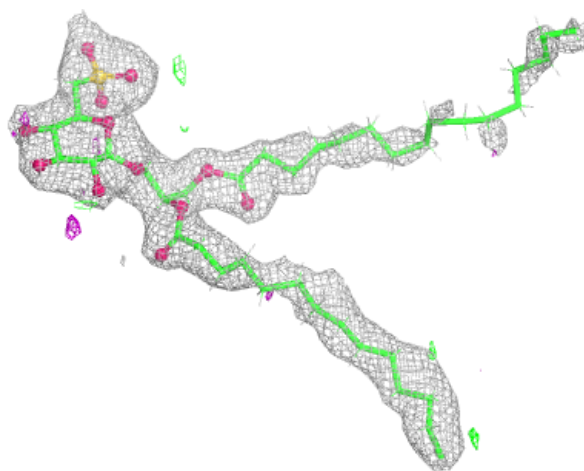
Electron density around CLA C 512:

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



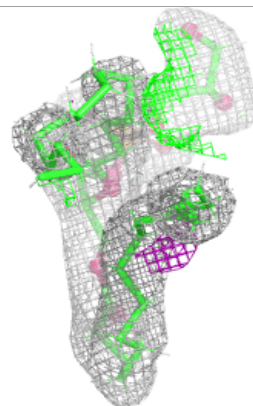
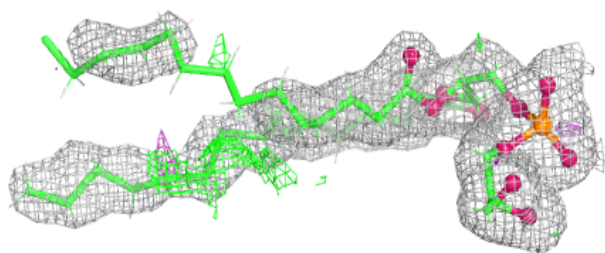
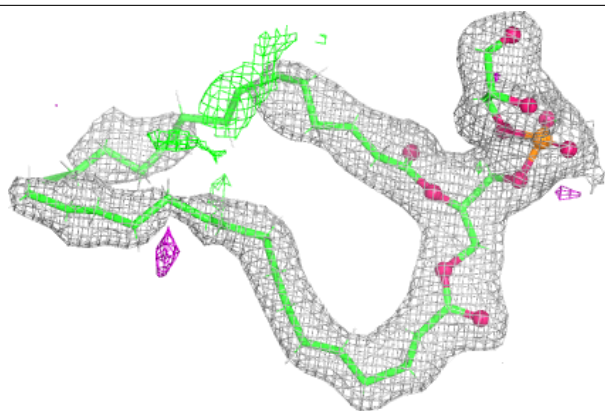
Electron density around SQD A 413:

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

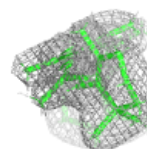
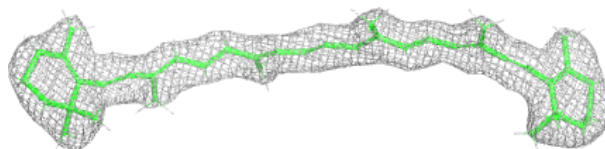


Electron density around LHG A 412:

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

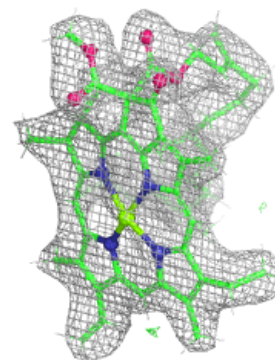
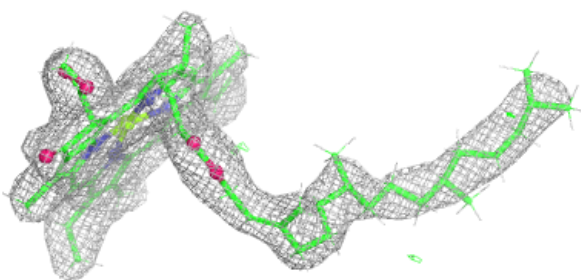
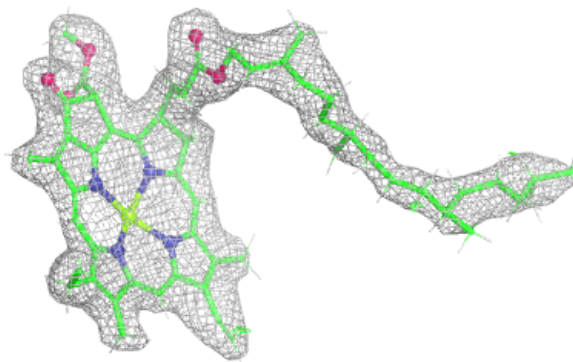
**Electron density around BCR C 516:**

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

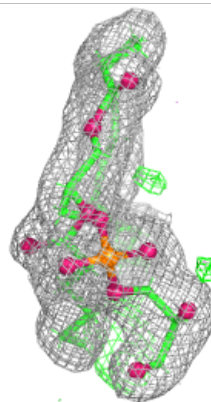
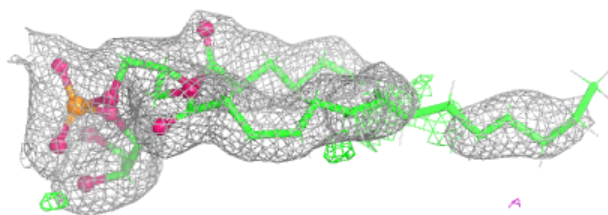
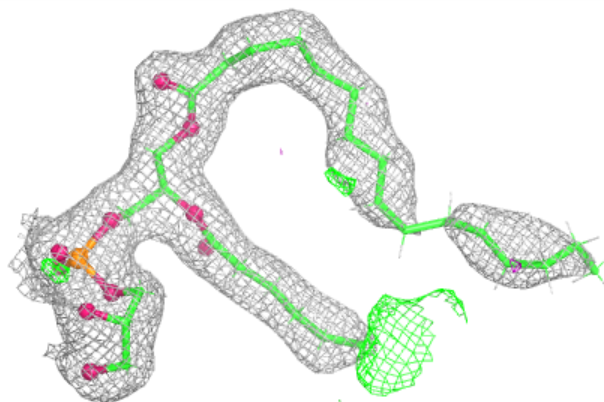


Electron density around CLA c 511:

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

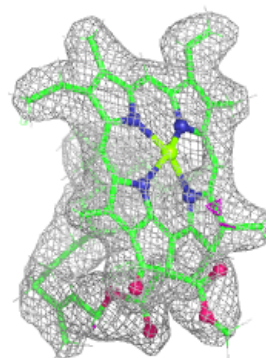
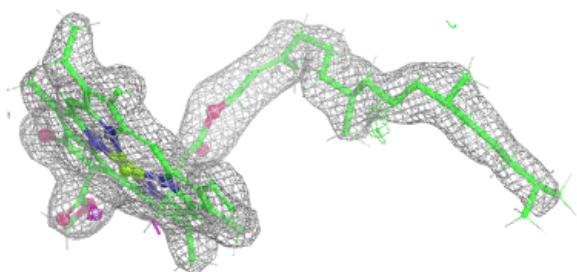
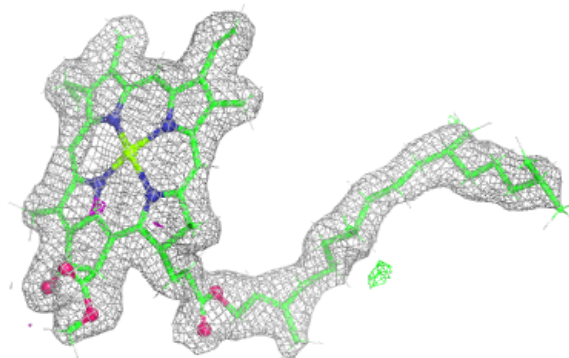
**Electron density around LHG d 409:**

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

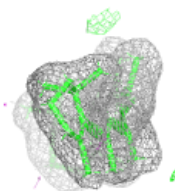
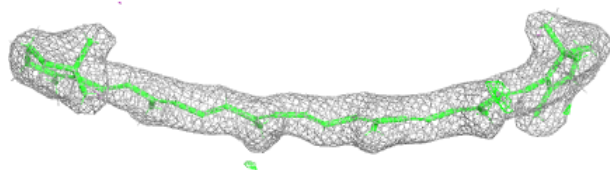
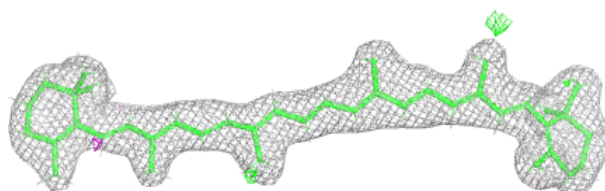


Electron density around CLA C 511:

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

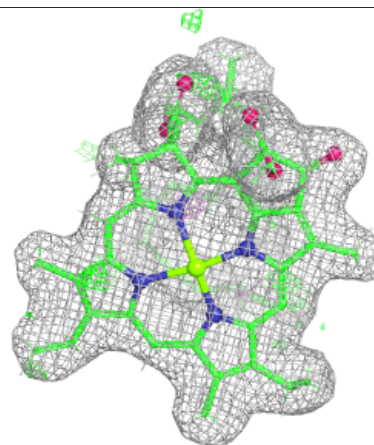
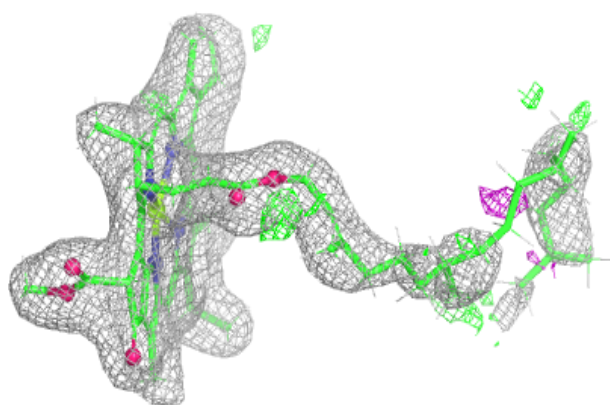
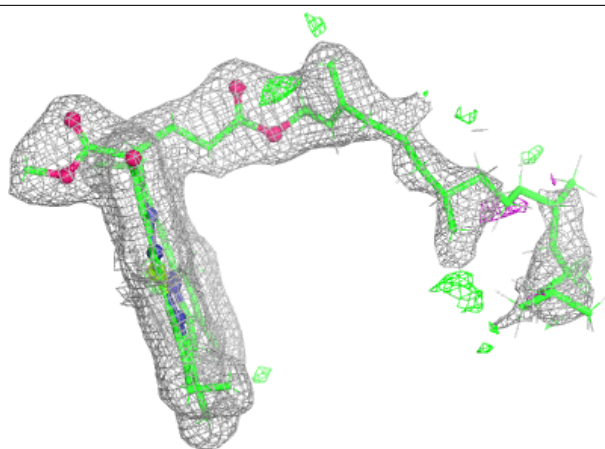
**Electron density around BCR T 101:**

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

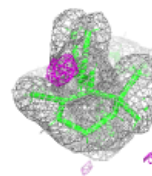
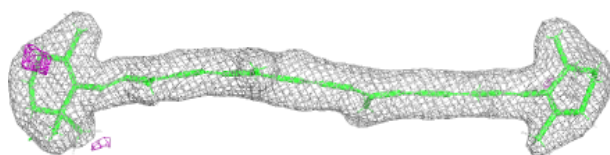
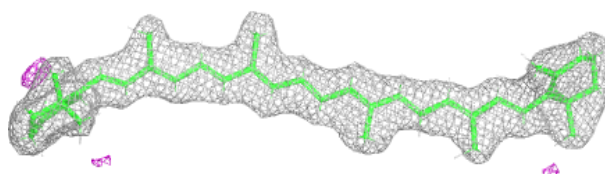


Electron density around CLA C 506:

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

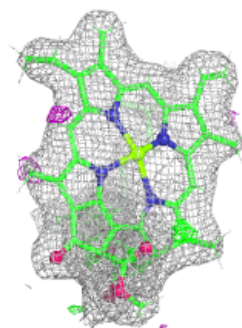
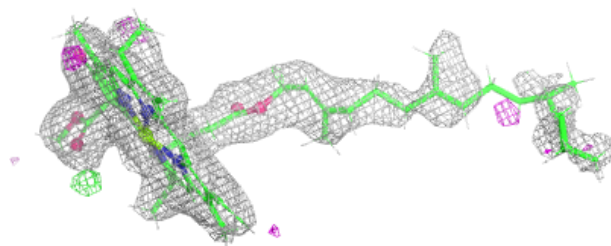
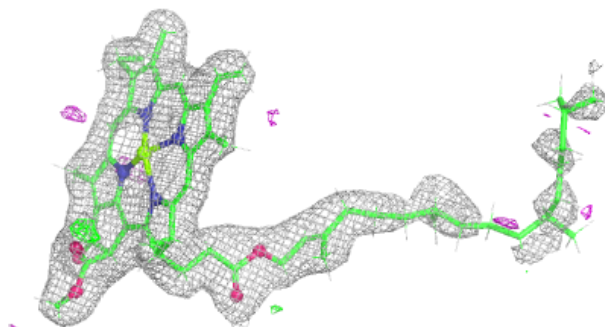
**Electron density around BCR a 405:**

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

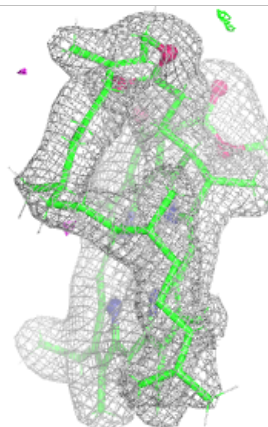
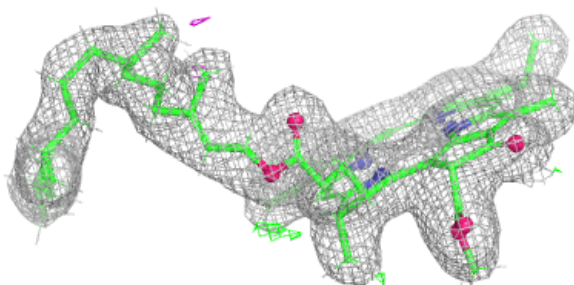
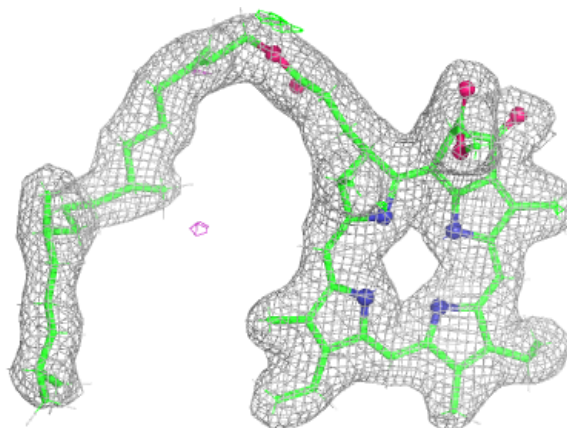


Electron density around CLA d 405:

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

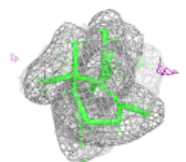
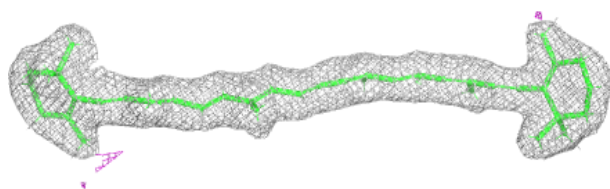
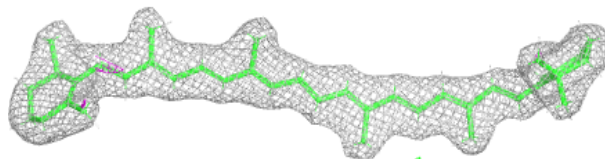
**Electron density around PHO d 402:**

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

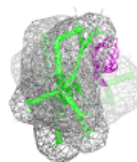
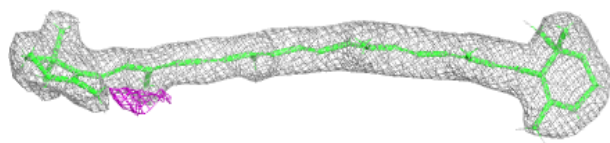
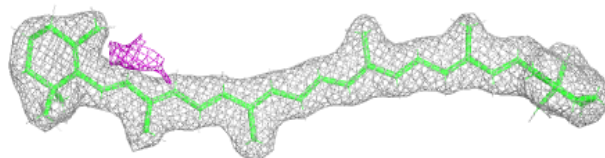


Electron density around BCR A 407:

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

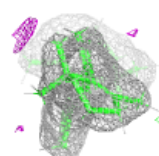
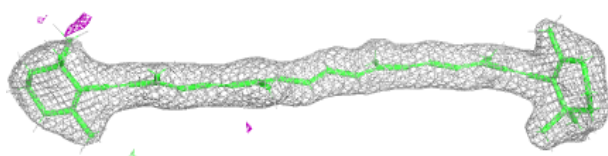
**Electron density around BCR B 617:**

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

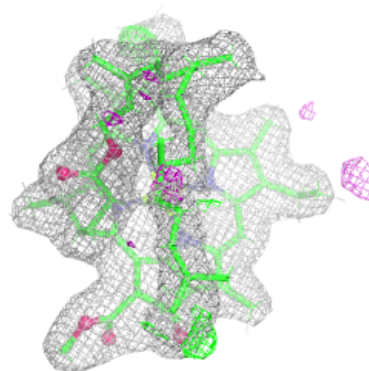
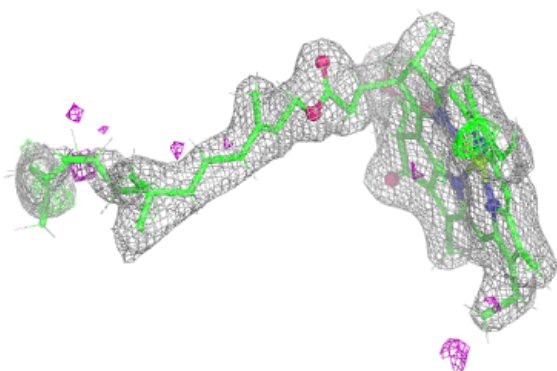
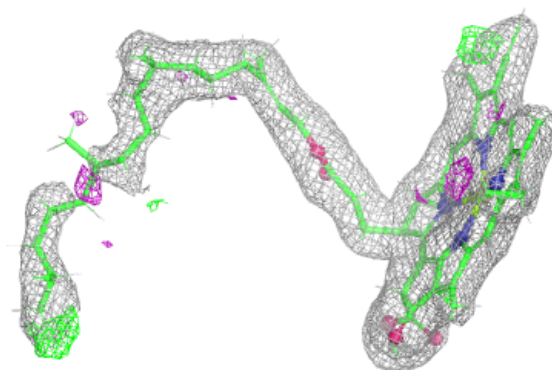


Electron density around BCR c 515:

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

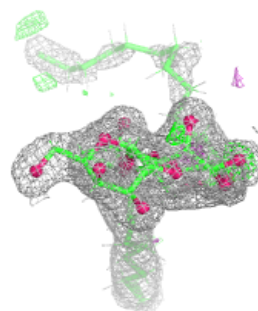
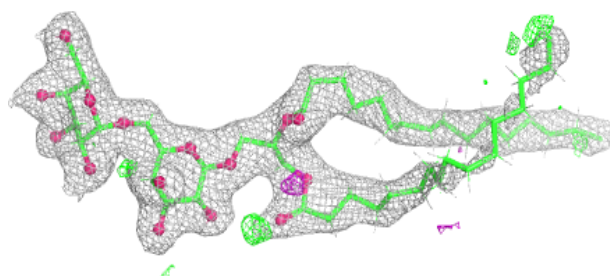
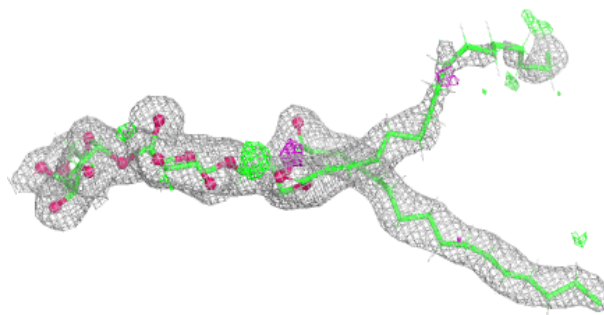
**Electron density around CLA b 606:**

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

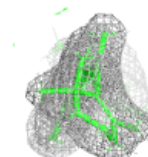
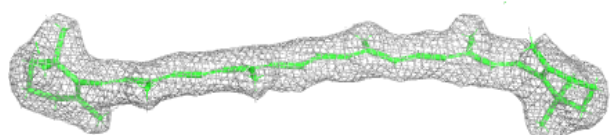
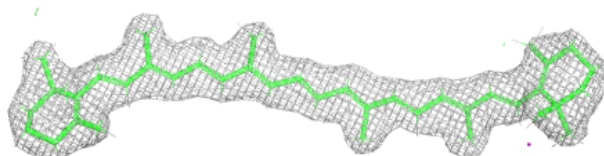


Electron density around DGD C 517:

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

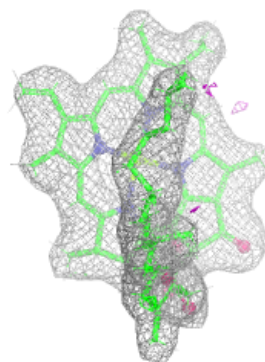
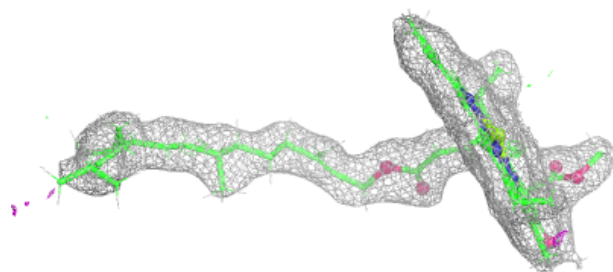
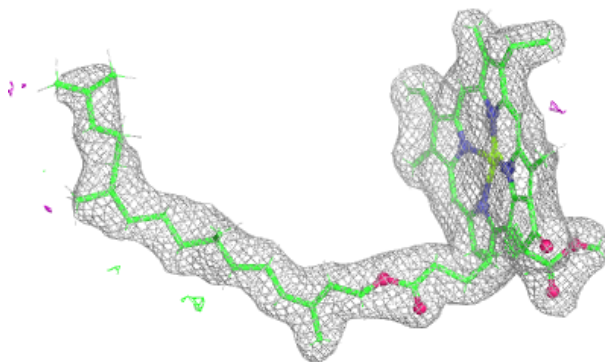
**Electron density around BCR B 619:**

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



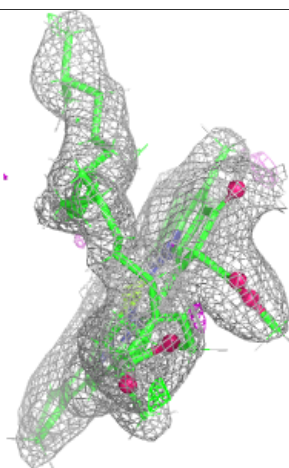
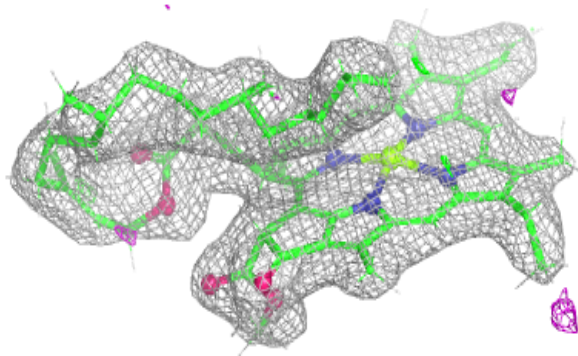
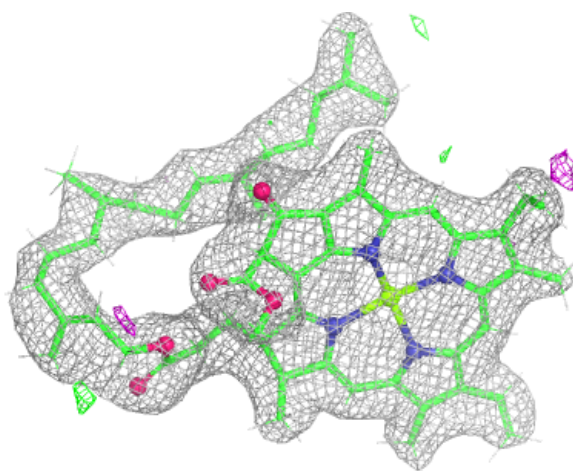
Electron density around CLA b 609:

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



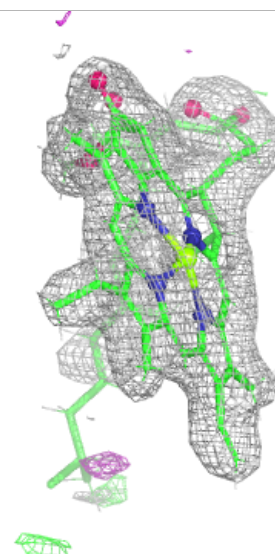
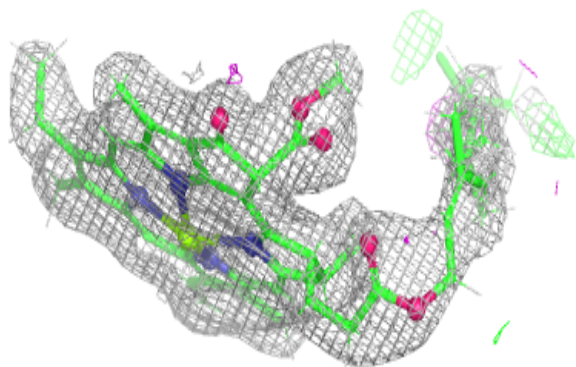
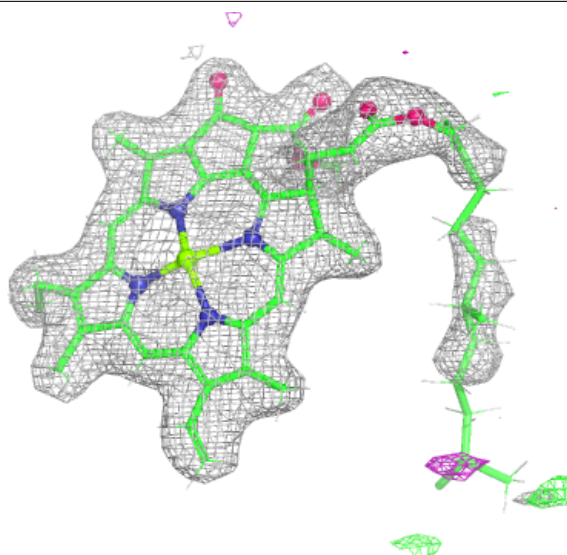
Electron density around CLA c 509:

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



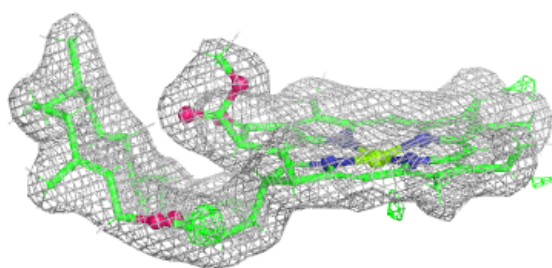
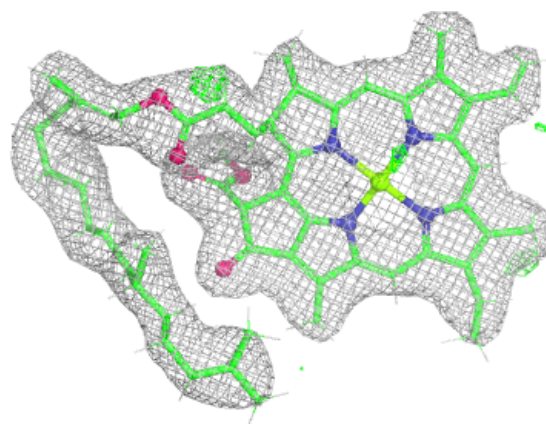
Electron density around CLA B 616:

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

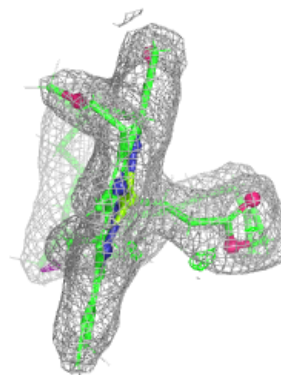
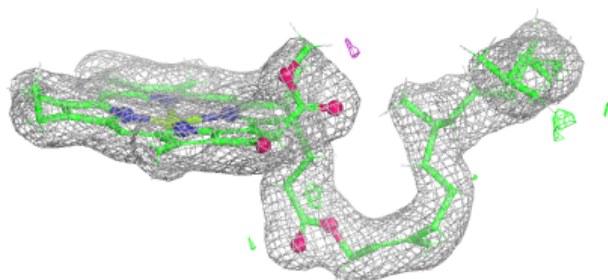
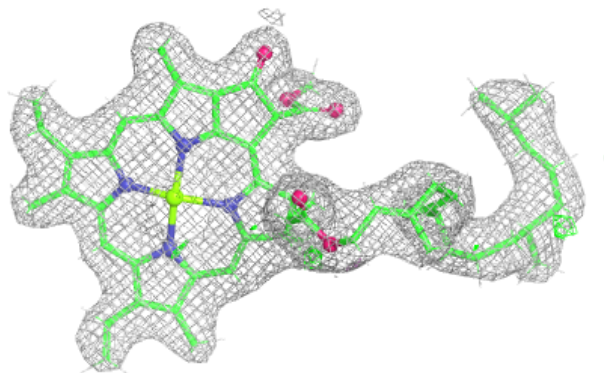


Electron density around CLA b 610:

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

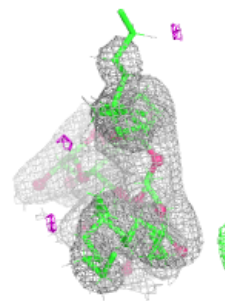
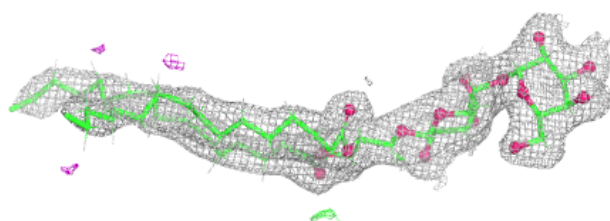
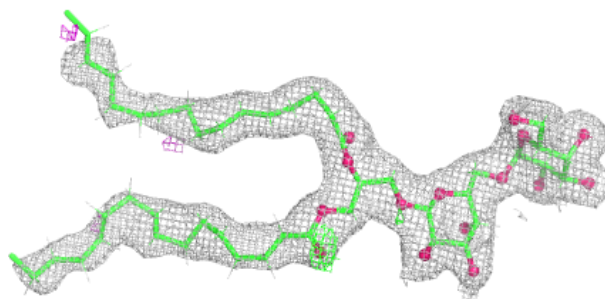
**Electron density around CLA b 612:**

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

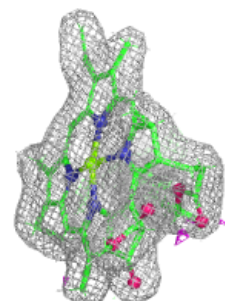
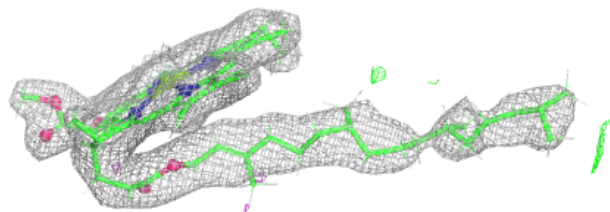
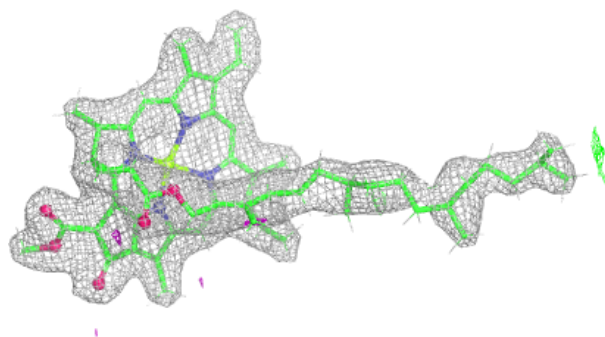


Electron density around DGD C 519:

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

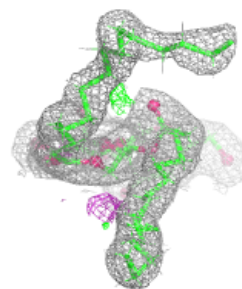
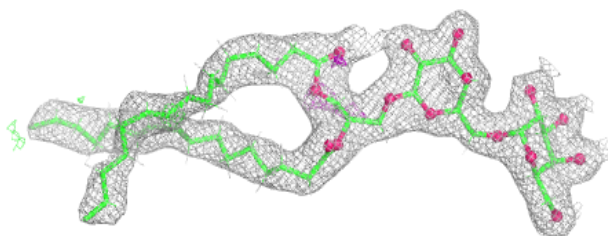
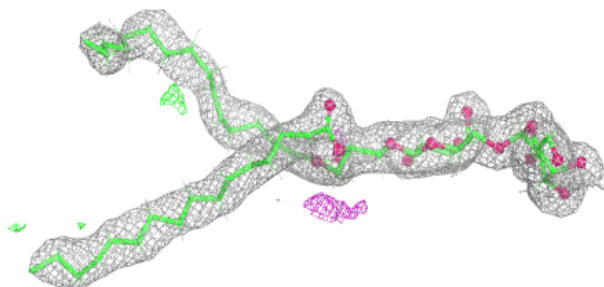
**Electron density around CLA b 614:**

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



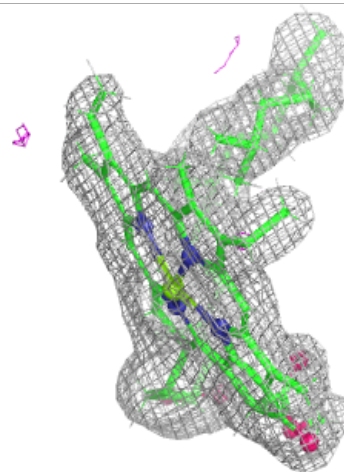
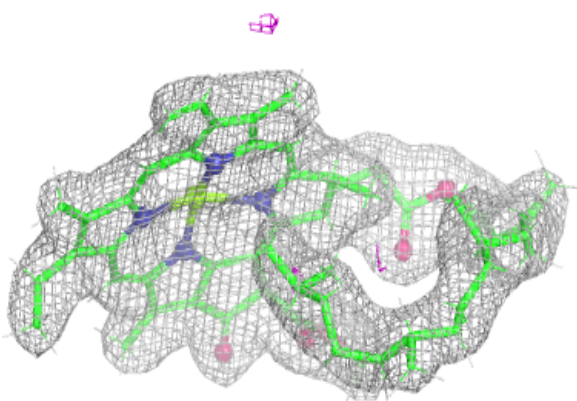
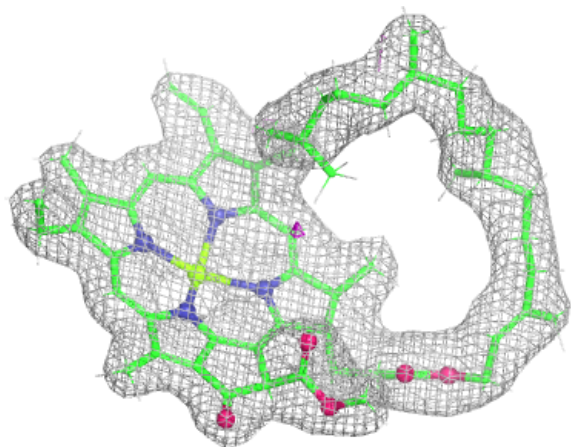
Electron density around DGD c 517:

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



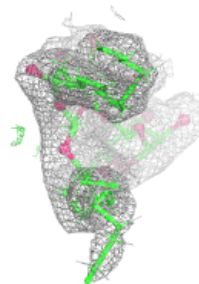
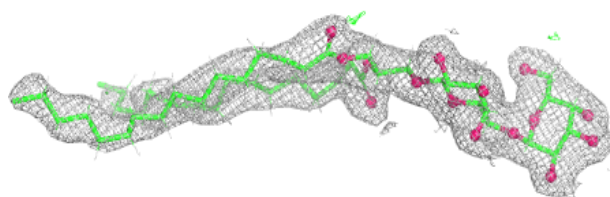
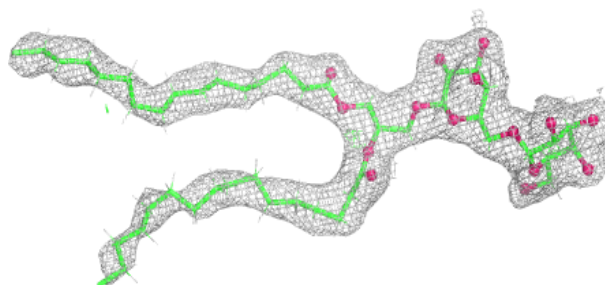
Electron density around CLA b 615:

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



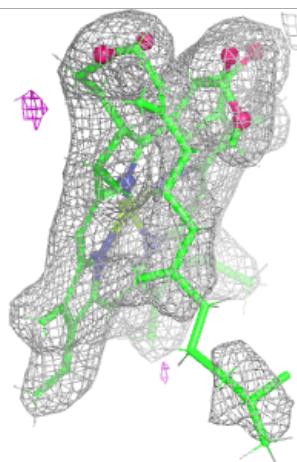
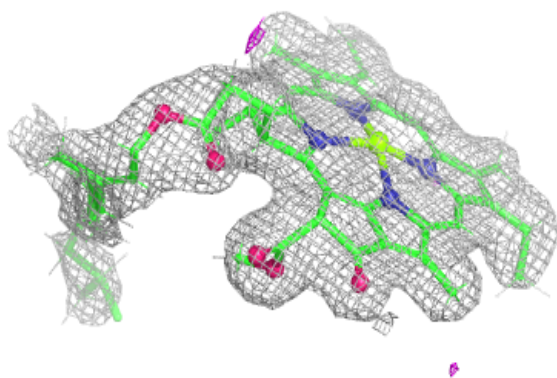
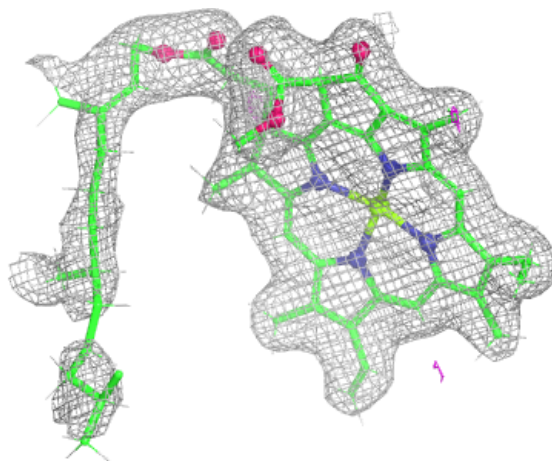
Electron density around DGD c 519:

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



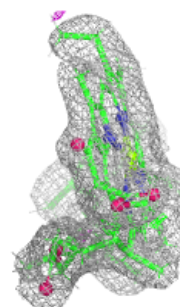
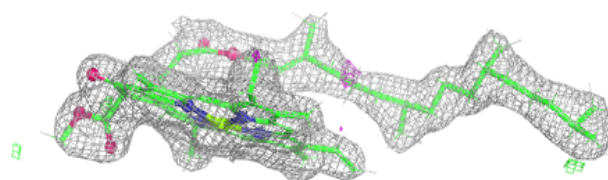
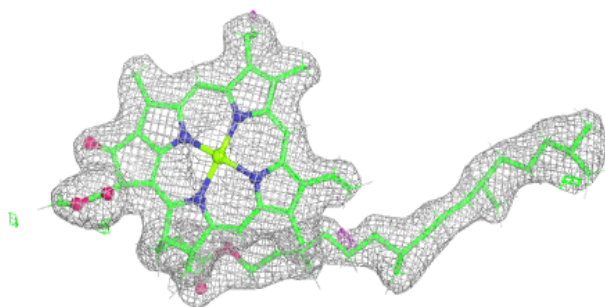
Electron density around CLA b 616:

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

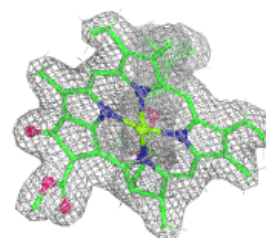
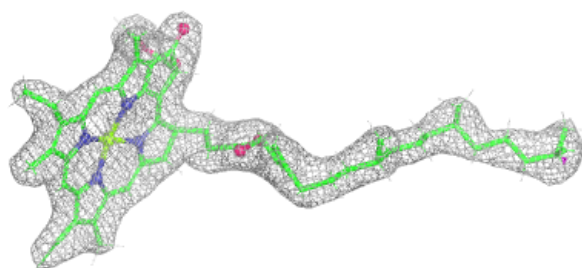
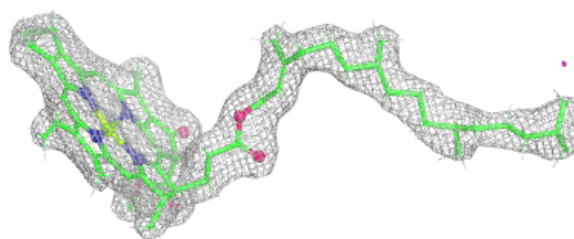


Electron density around CLA c 501:

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

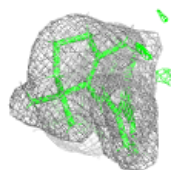
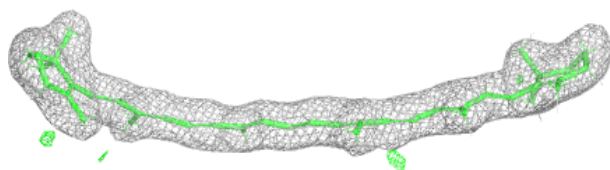
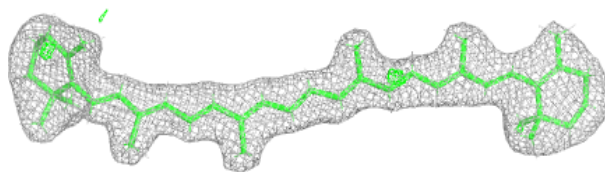
**Electron density around CLA c 502:**

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



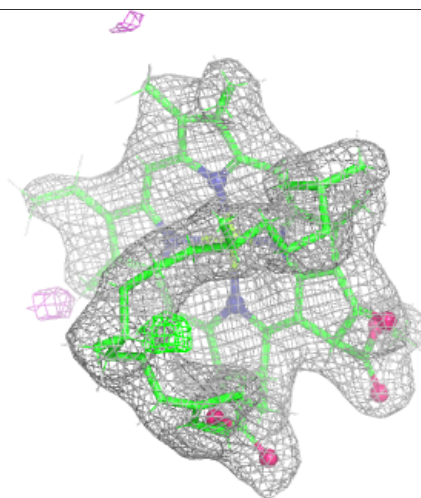
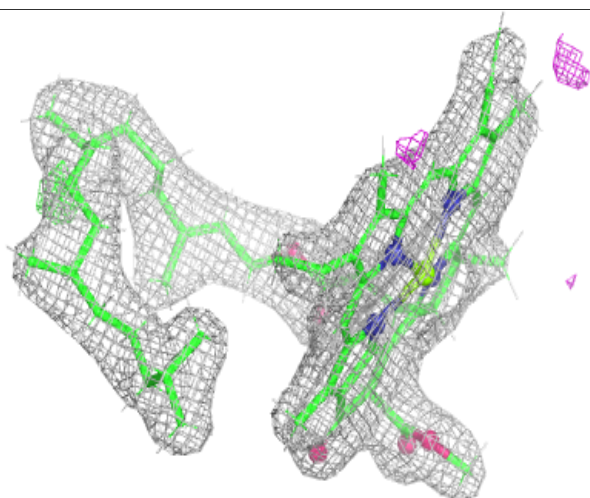
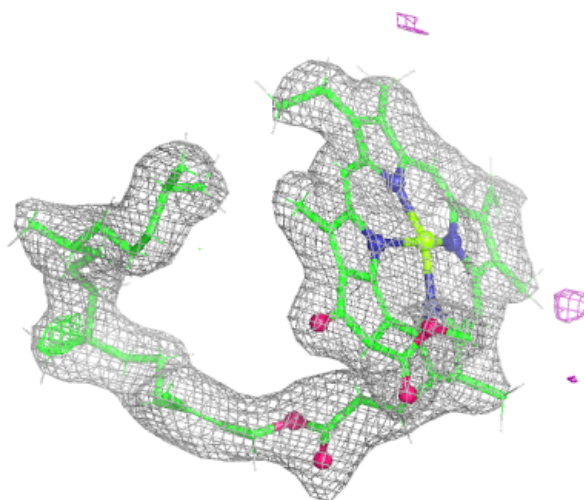
Electron density around BCR t 101:

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



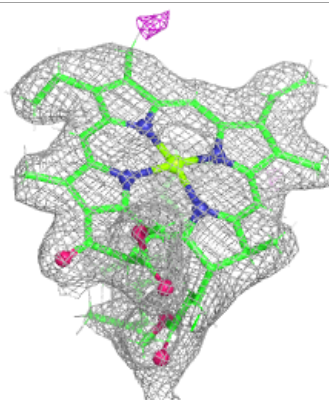
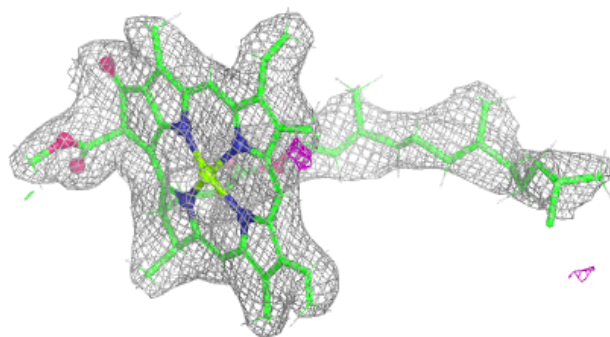
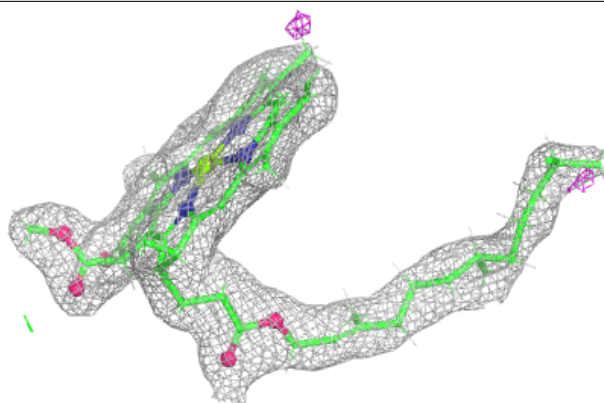
Electron density around CLA c 503:

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

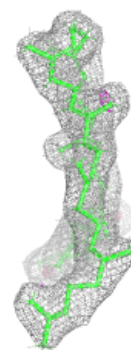
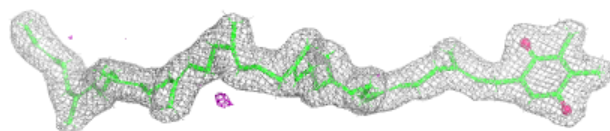
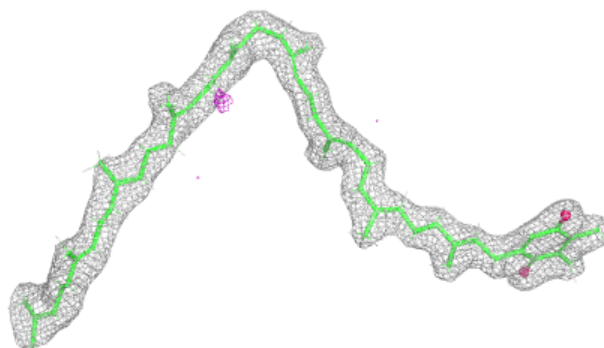


Electron density around CLA c 504:

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

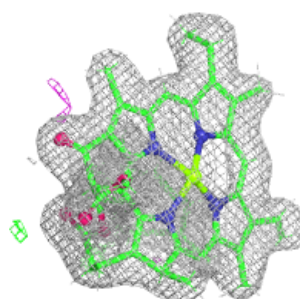
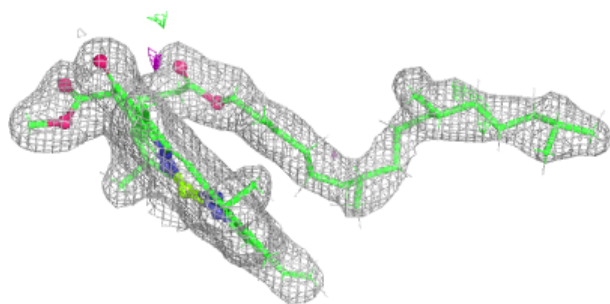
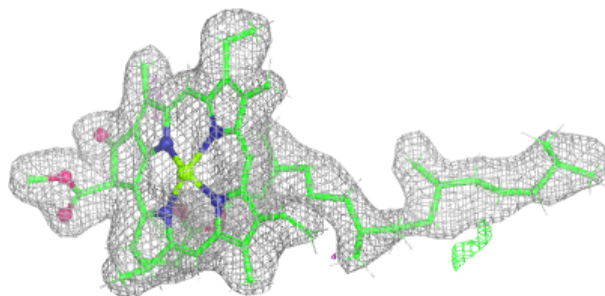
**Electron density around PL9 D 406:**

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

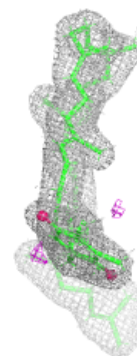
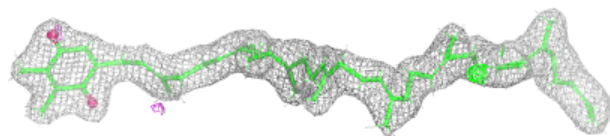
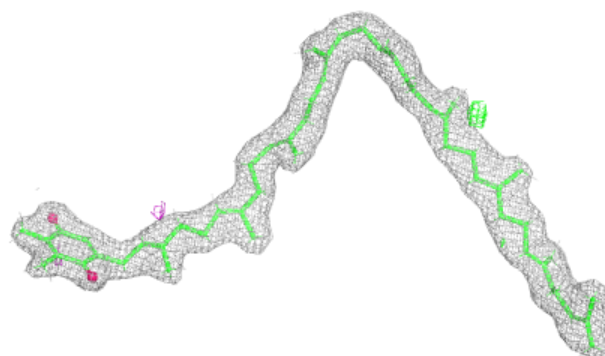


Electron density around CLA c 505:

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

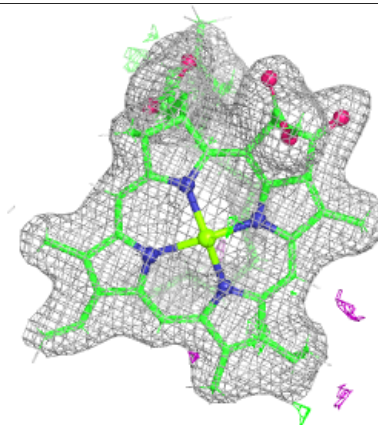
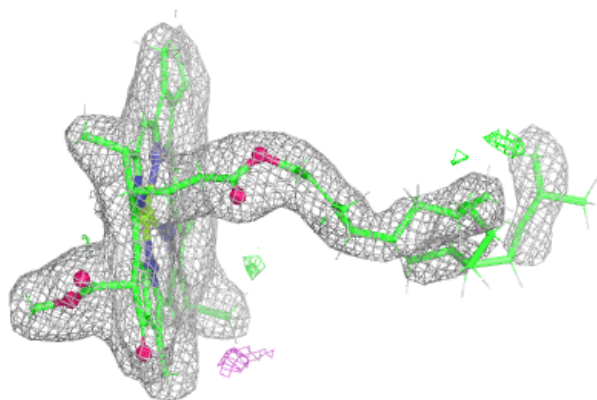
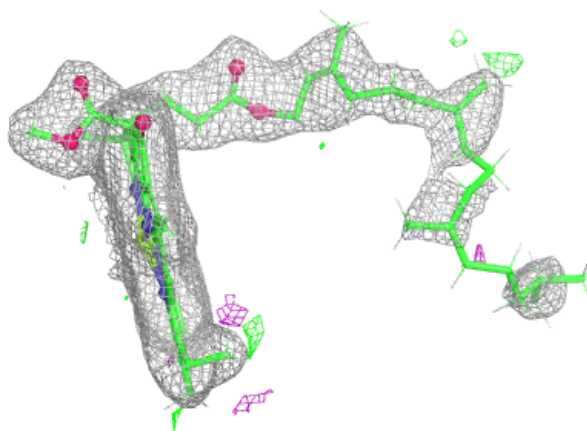
**Electron density around PL9 d 407:**

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



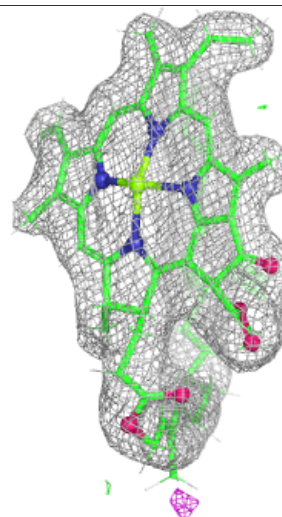
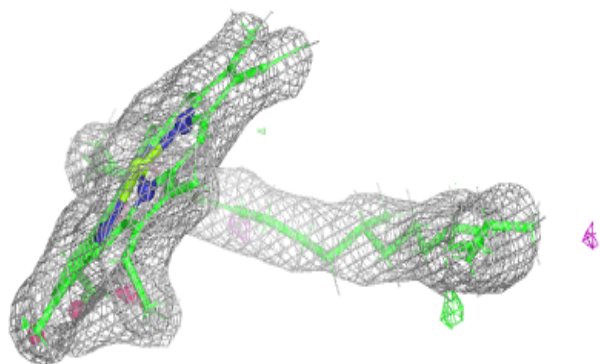
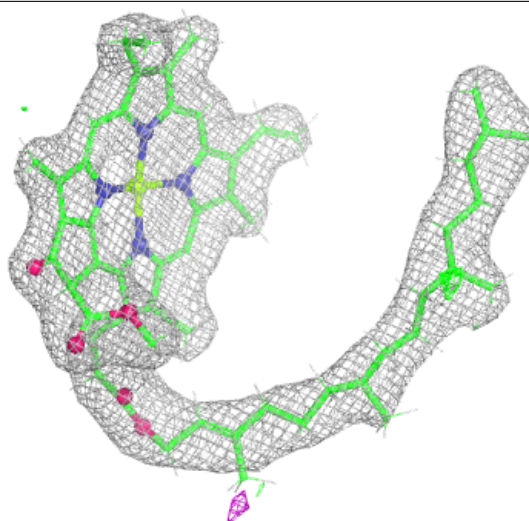
Electron density around CLA c 506:

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



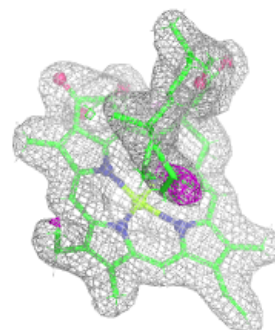
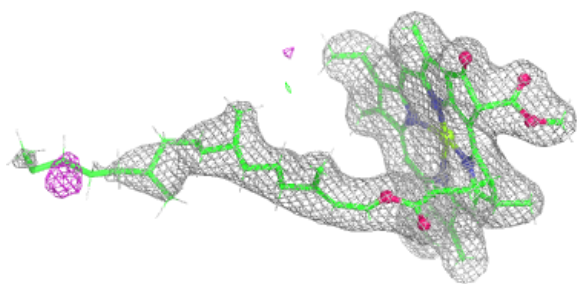
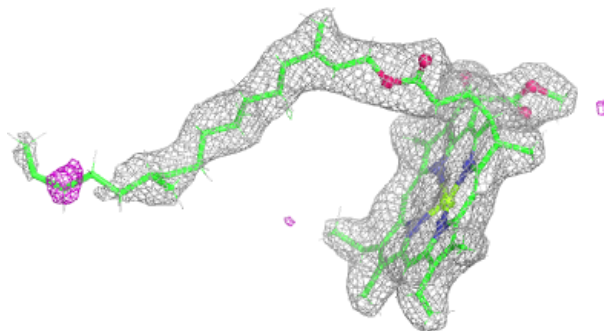
Electron density around CLA c 507:

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

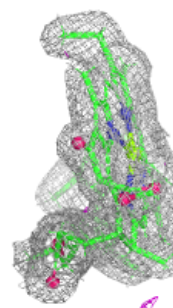
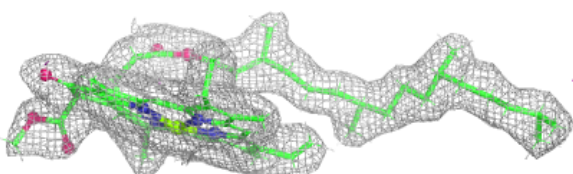
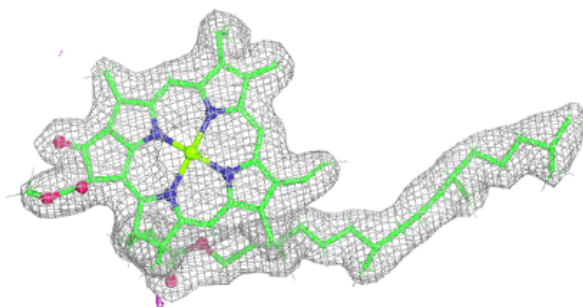


Electron density around CLA c 508:

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

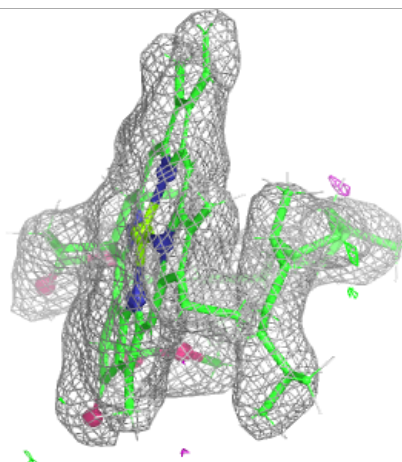
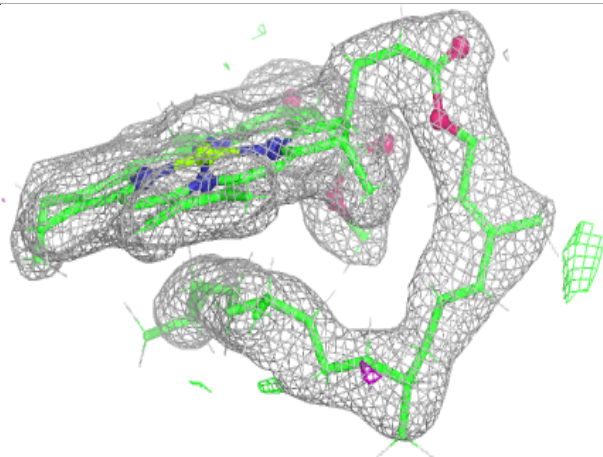
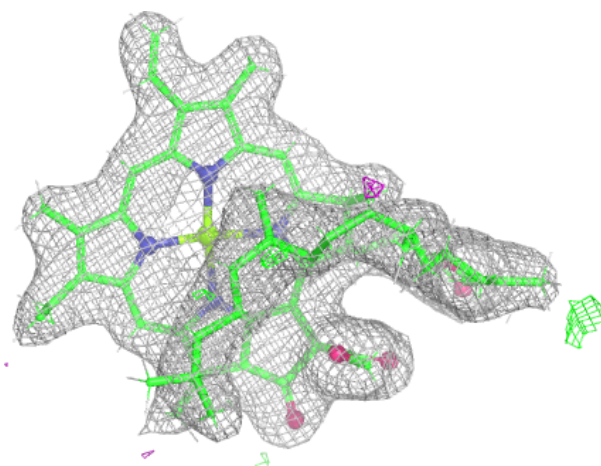
**Electron density around CLA C 501:**

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



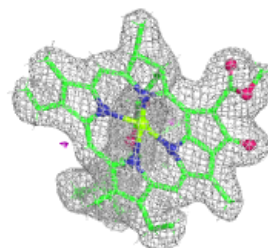
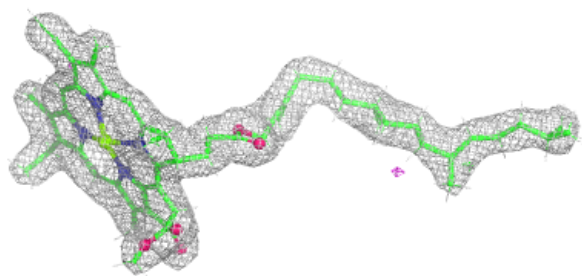
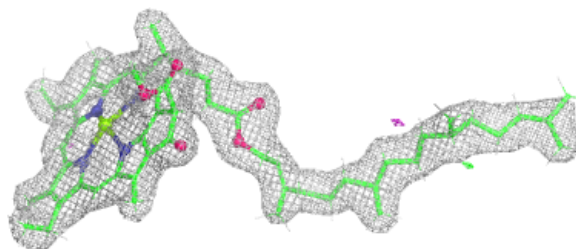
Electron density around CLA c 510:

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



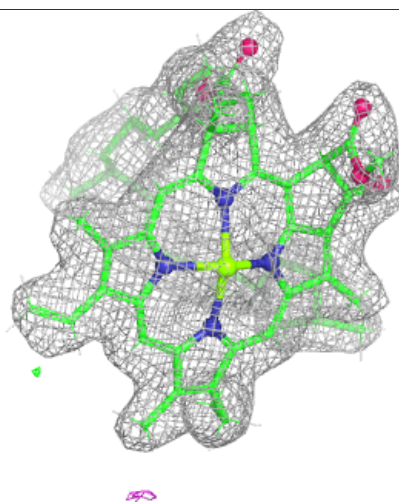
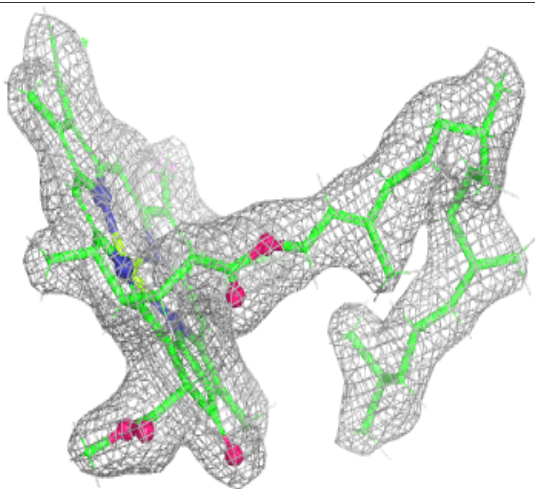
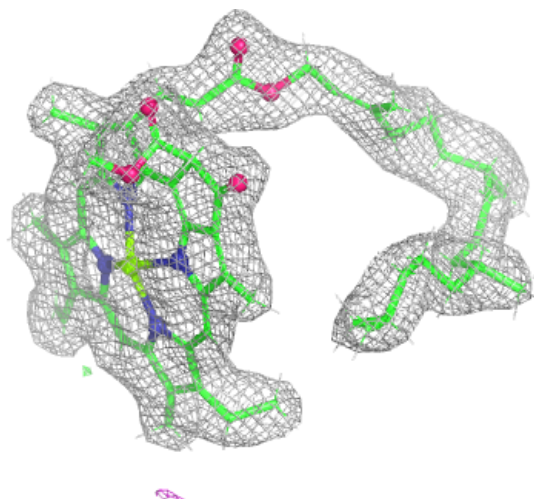
Electron density around CLA C 502:

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



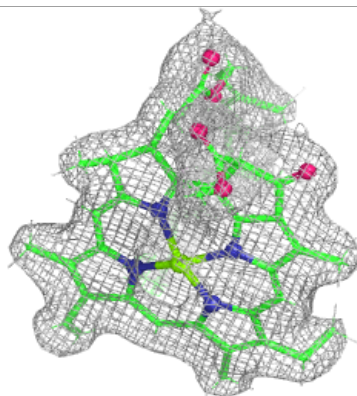
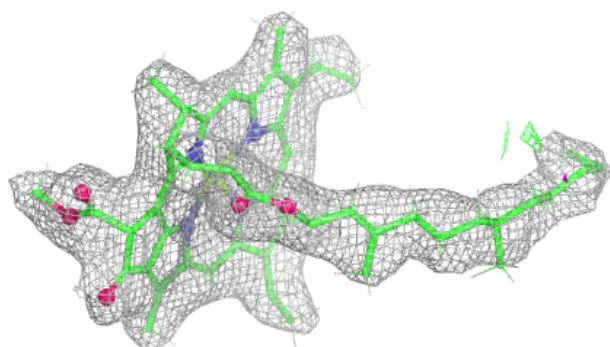
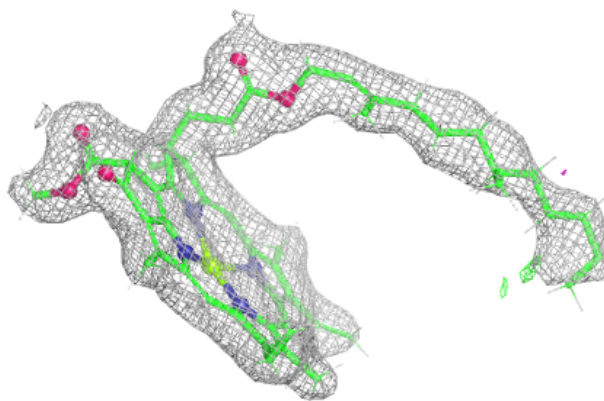
Electron density around CLA C 503:

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

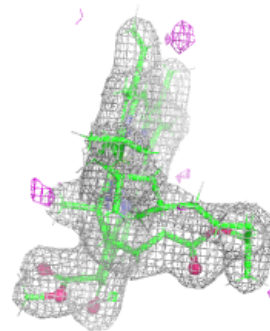
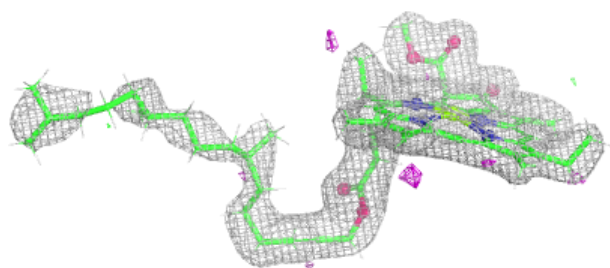
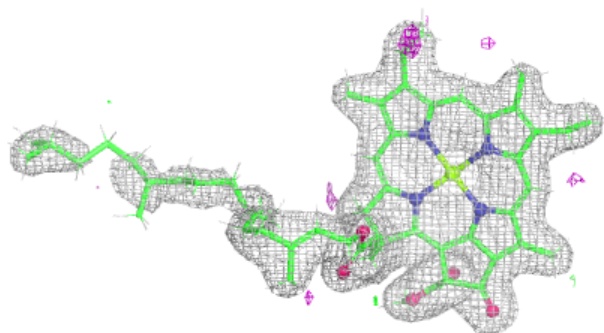


Electron density around CLA C 504:

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

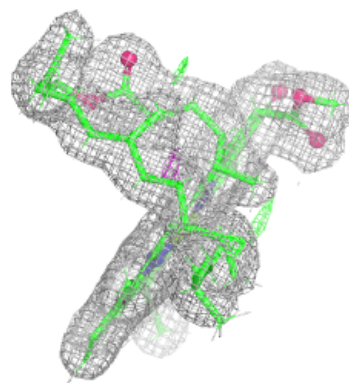
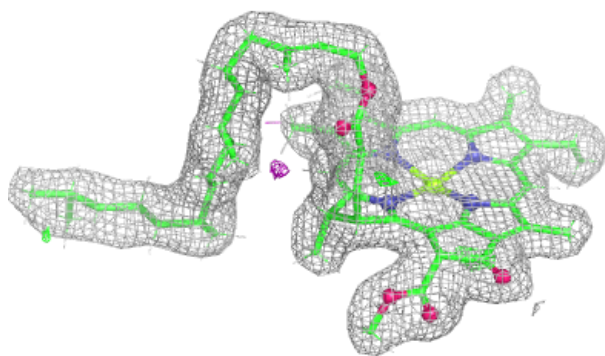
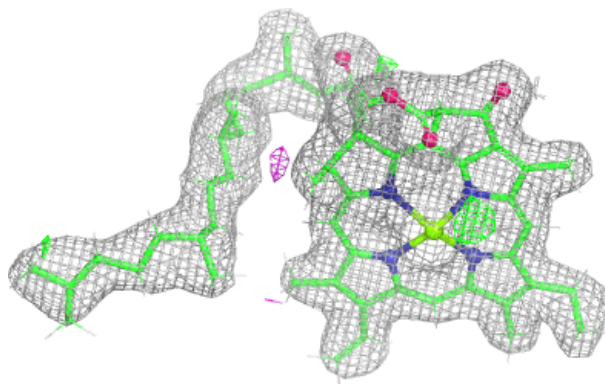
**Electron density around CLA d 401:**

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

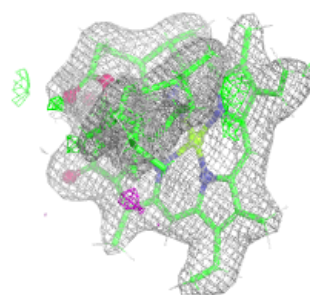
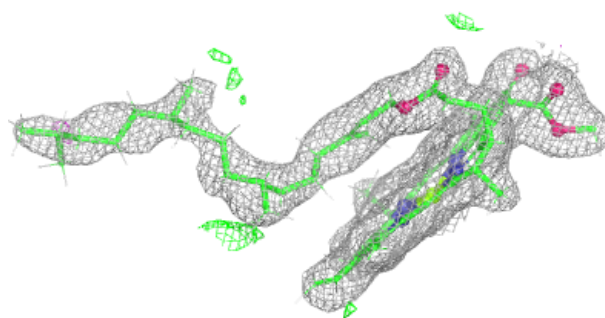
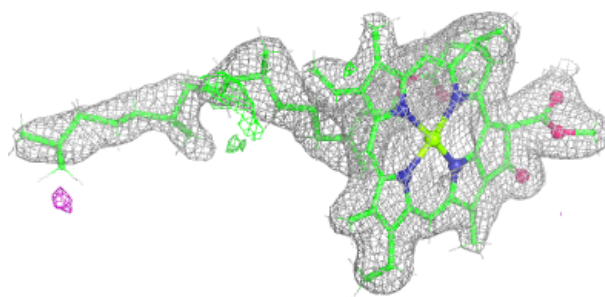


Electron density around CLA d 404:

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

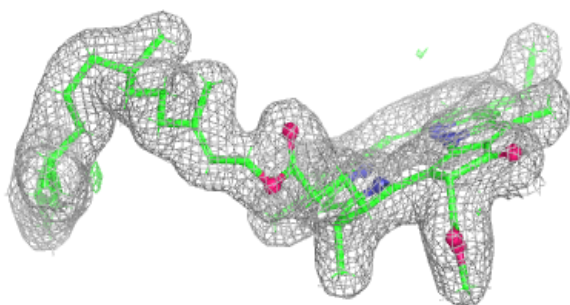
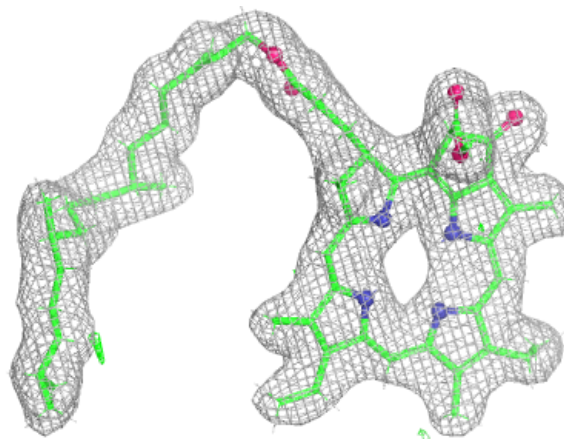
**Electron density around CLA C 505:**

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



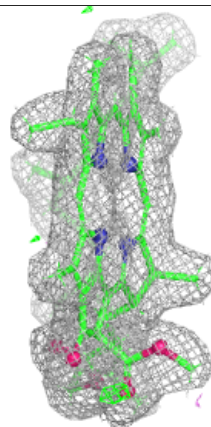
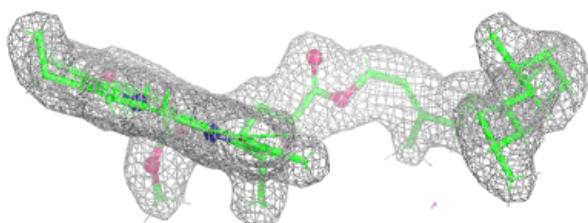
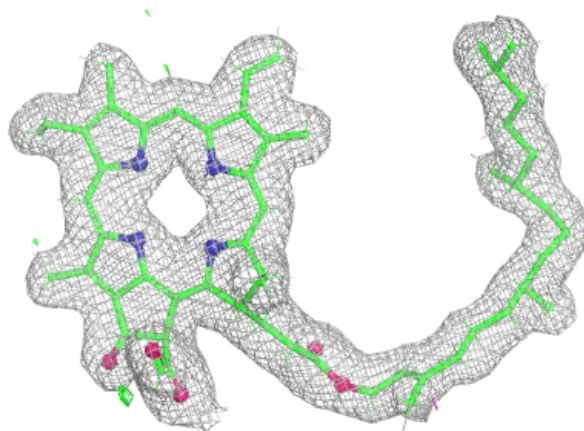
Electron density around PHO A 405:

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

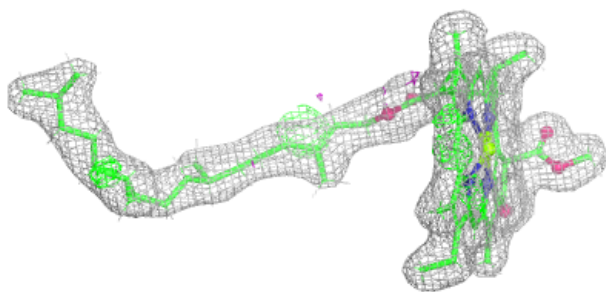
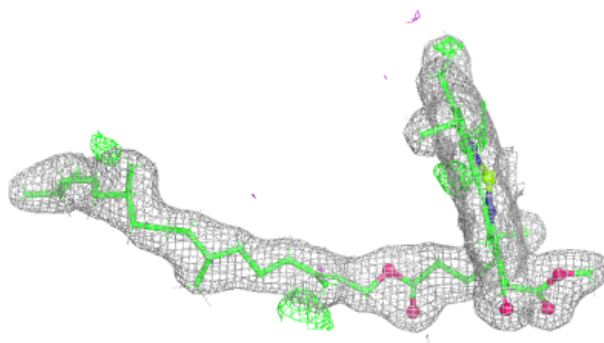


Electron density around PHO a 403:

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

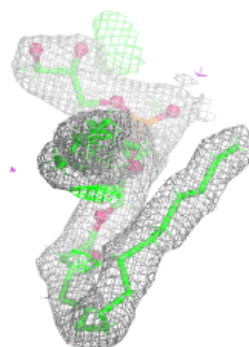
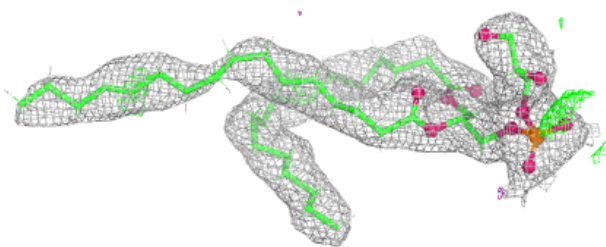
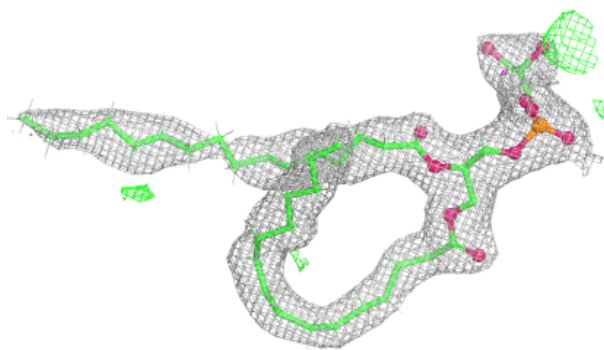
**Electron density around CLA B 605:**

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



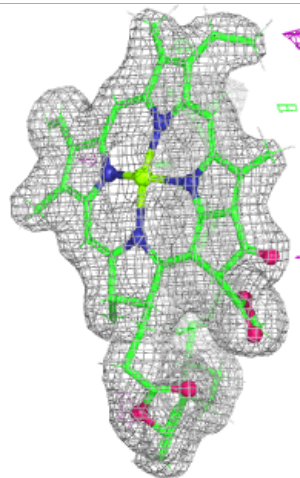
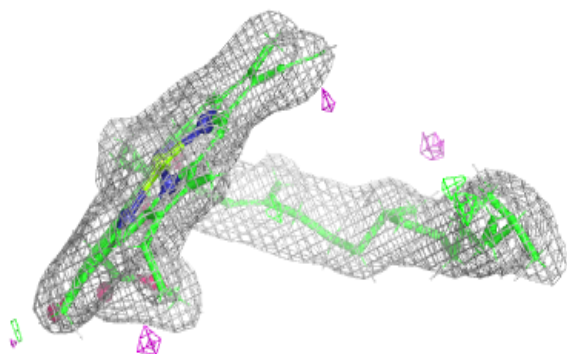
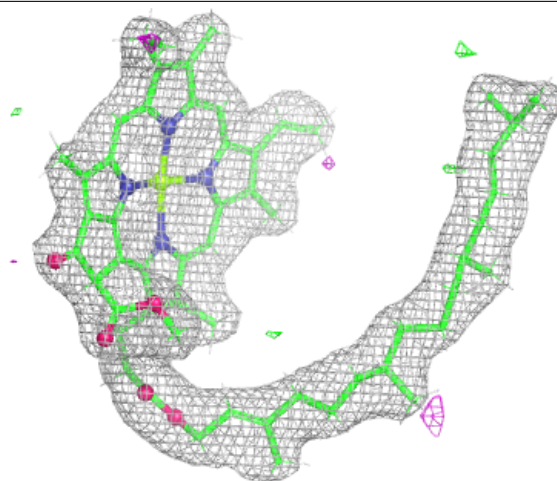
Electron density around LHG B 622:

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



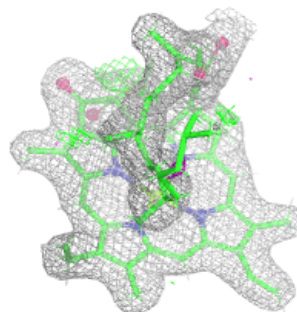
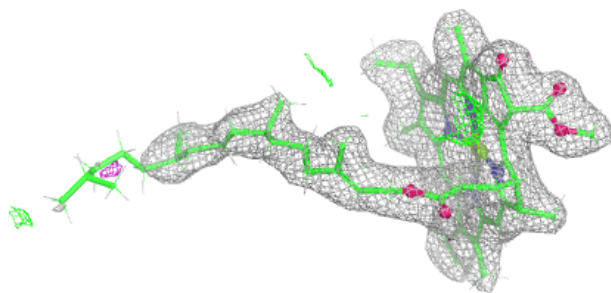
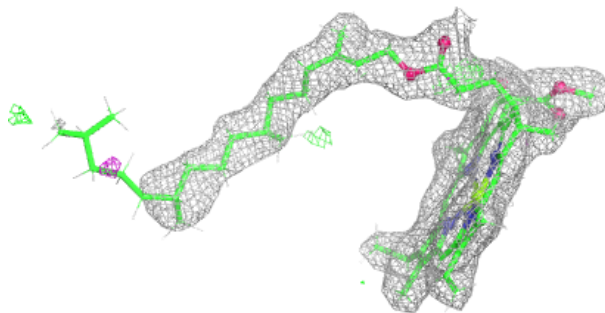
Electron density around CLA C 507:

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



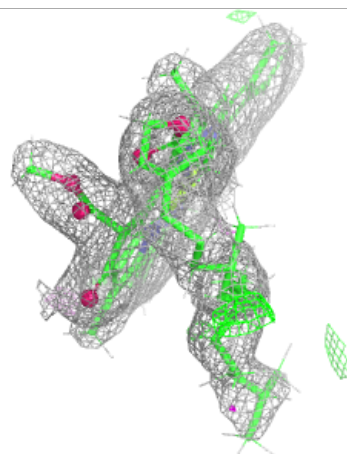
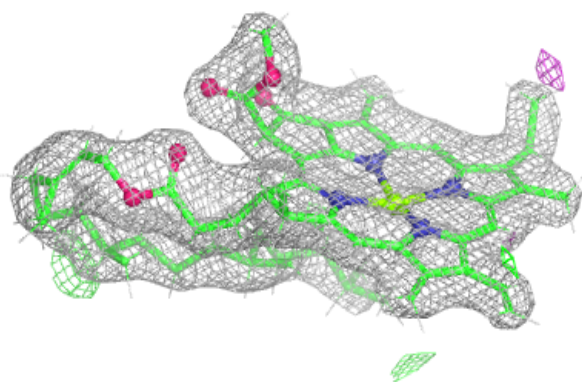
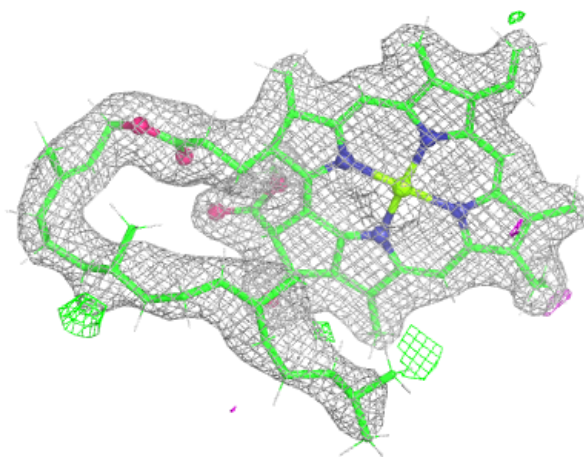
Electron density around CLA C 508:

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



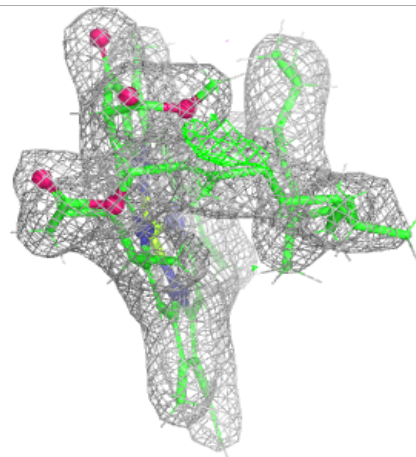
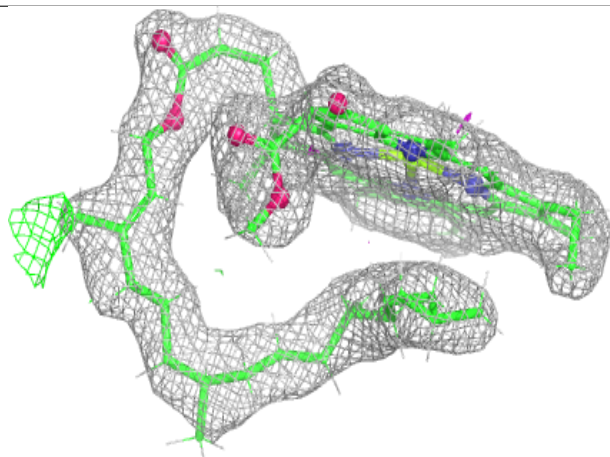
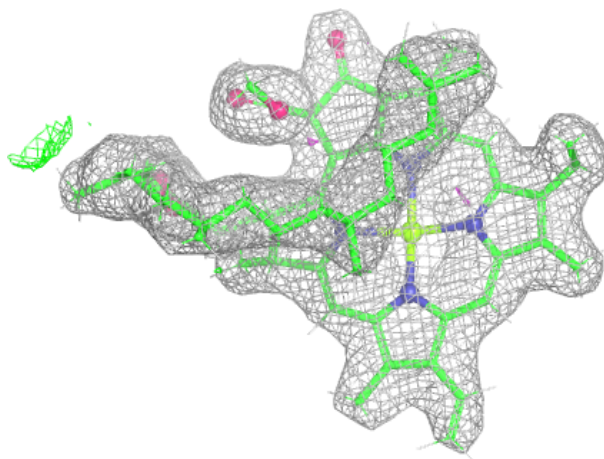
Electron density around CLA C 509:

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



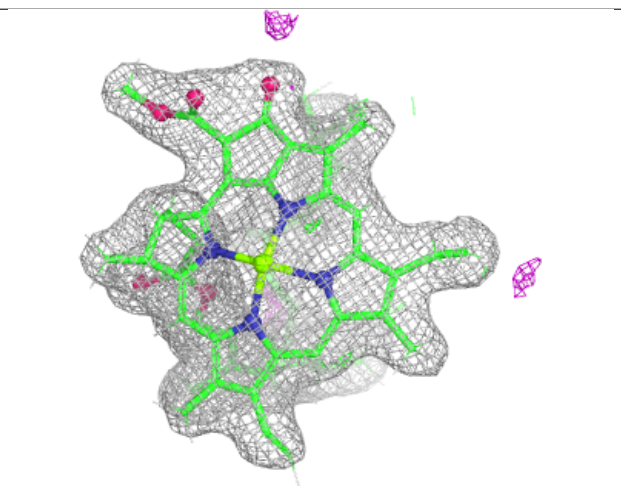
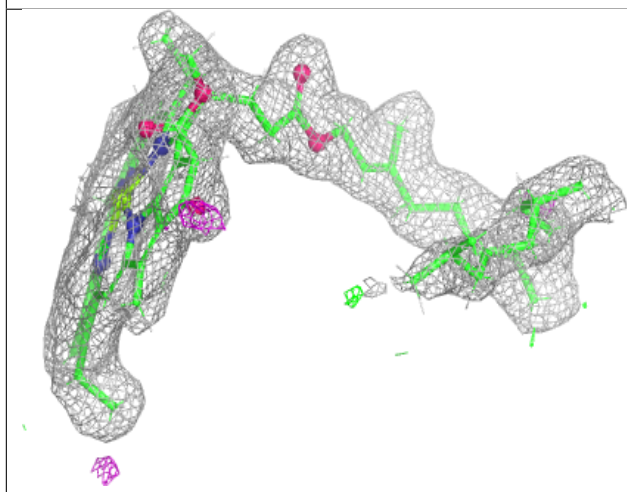
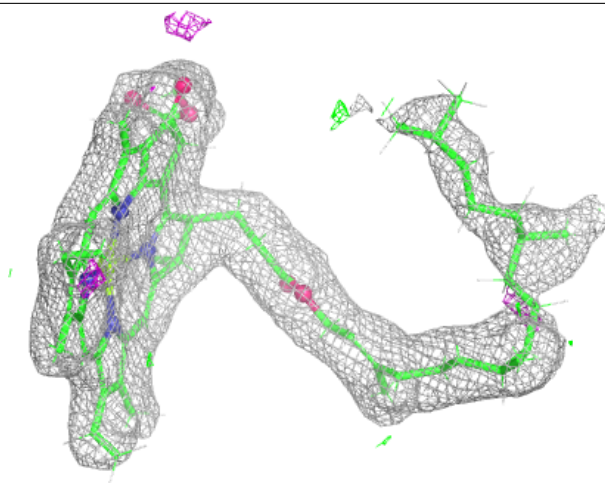
Electron density around CLA C 510:

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



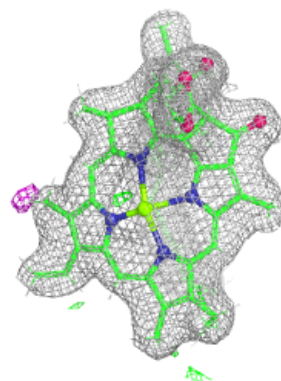
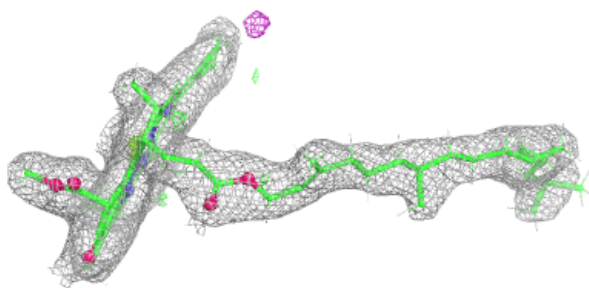
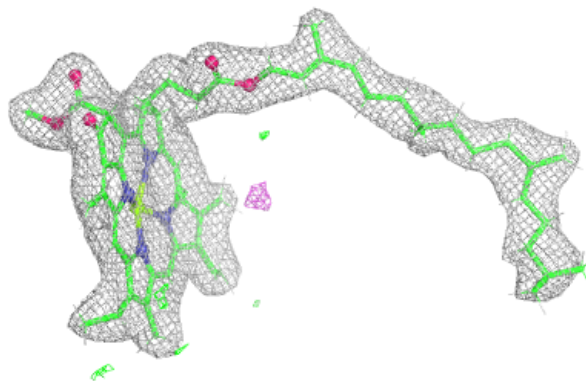
Electron density around CLA B 606:

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



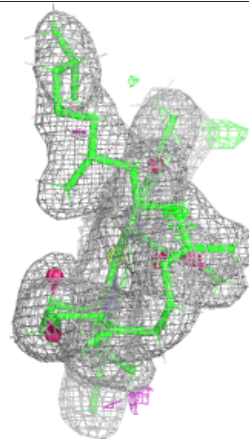
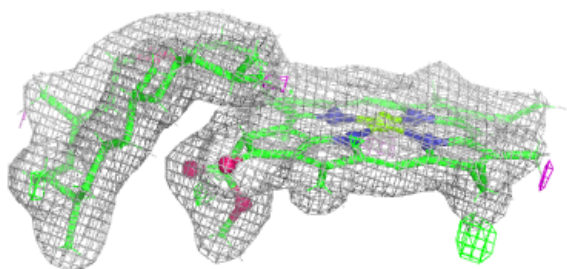
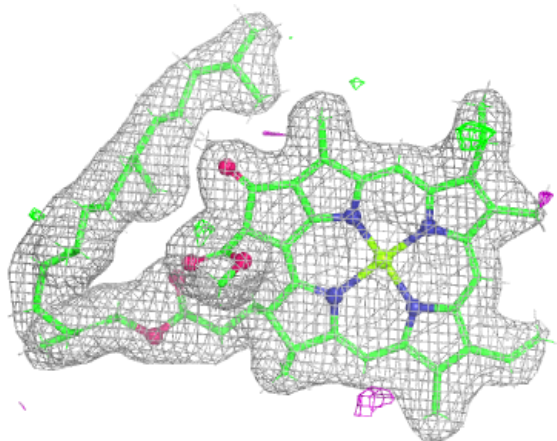
Electron density around CLA B 609:

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



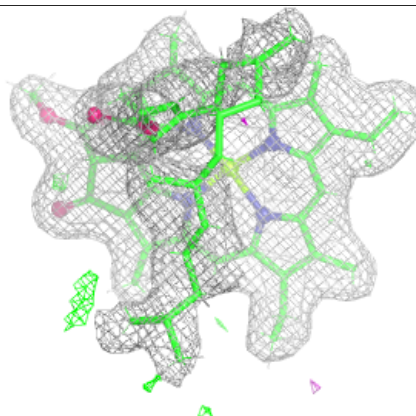
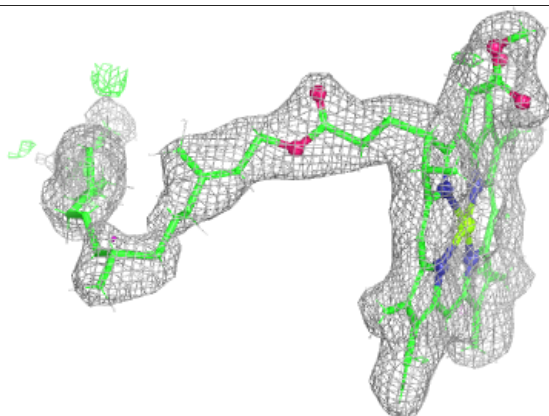
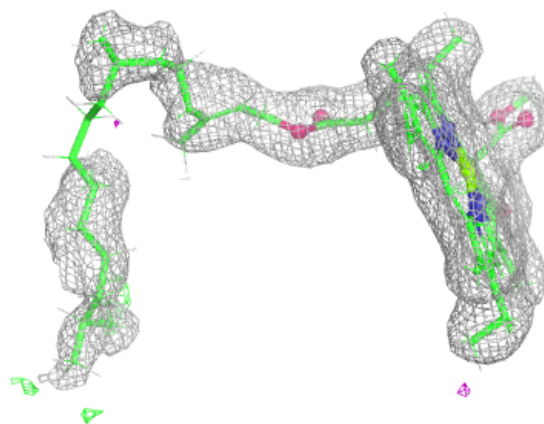
Electron density around CLA B 610:

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

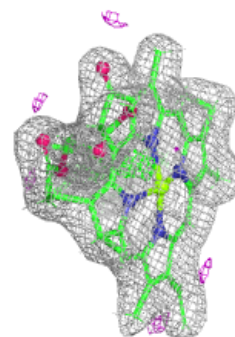
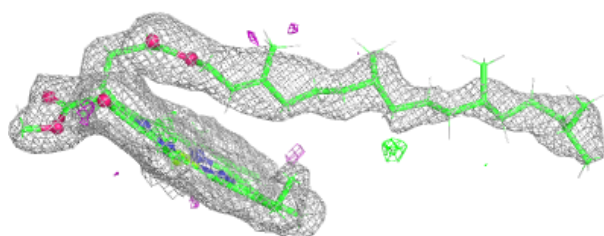
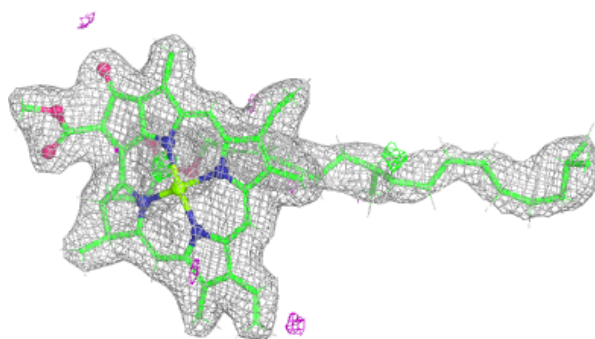


Electron density around CLA a 404:

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

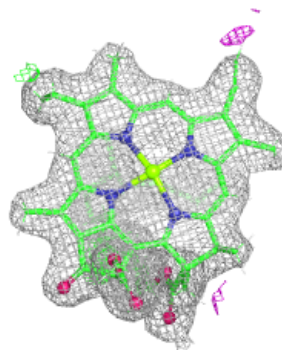
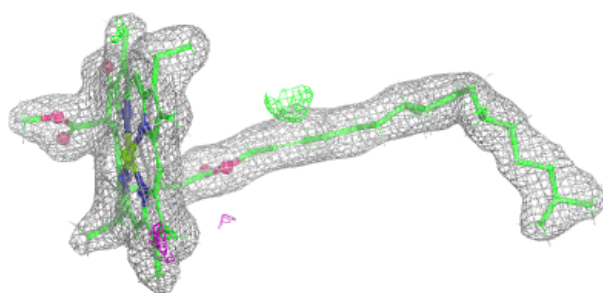
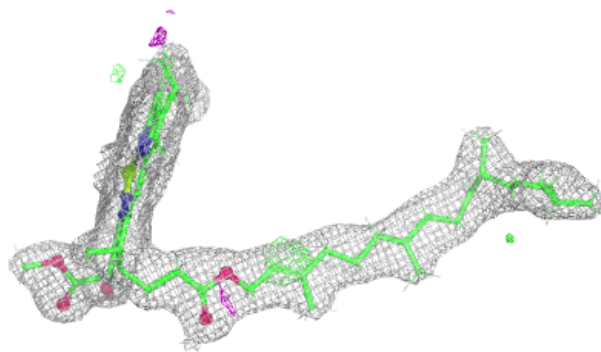
**Electron density around CLA B 614:**

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



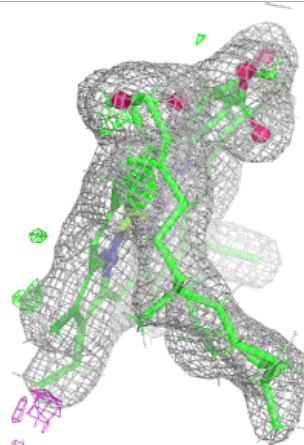
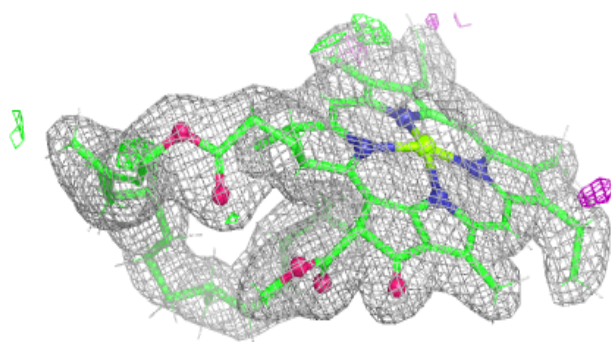
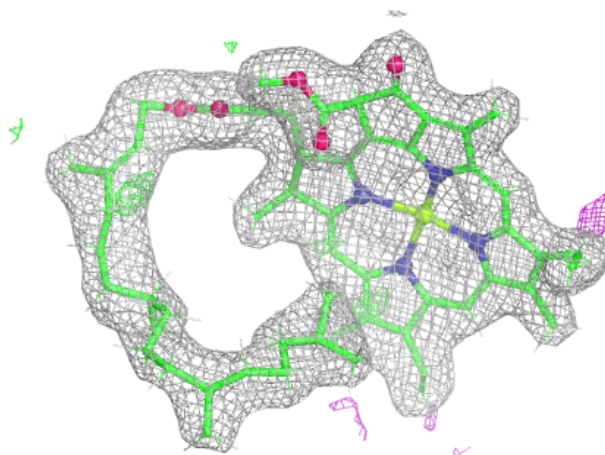
Electron density around CLA b 605:

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



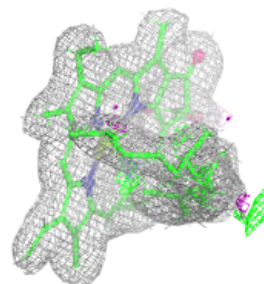
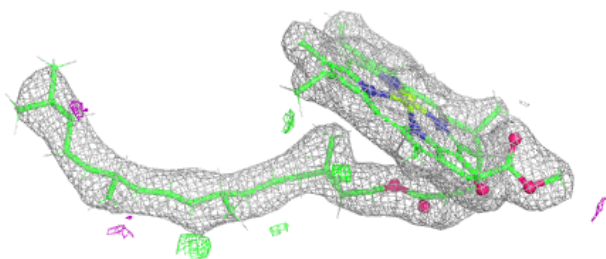
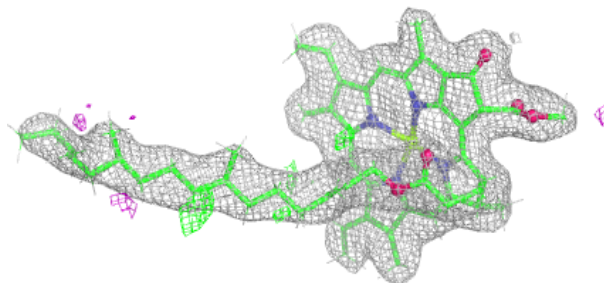
Electron density around CLA B 615:

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

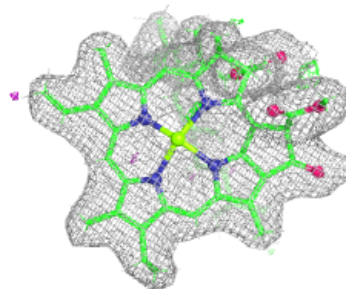
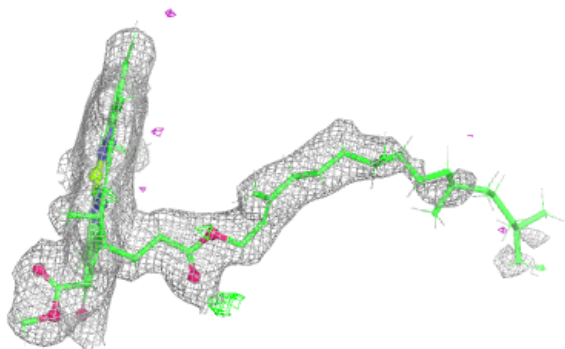
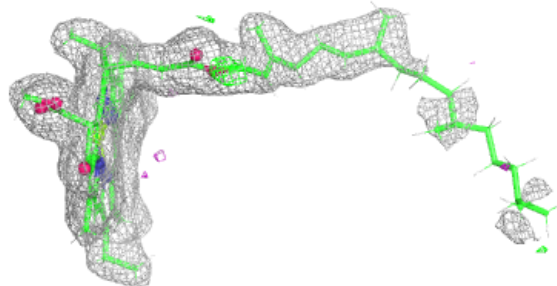


Electron density around CLA b 608:

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

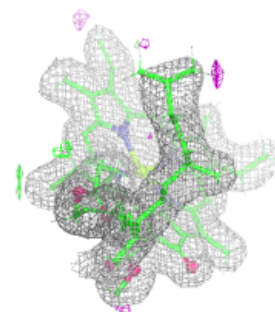
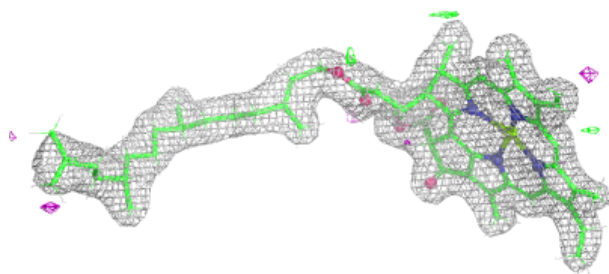
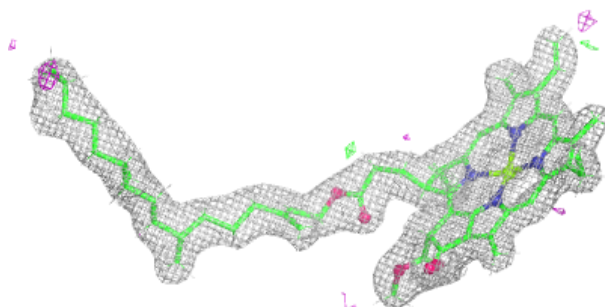
**Electron density around CLA D 404:**

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

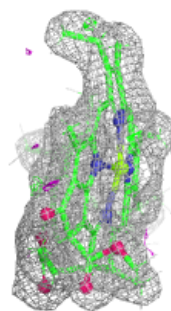
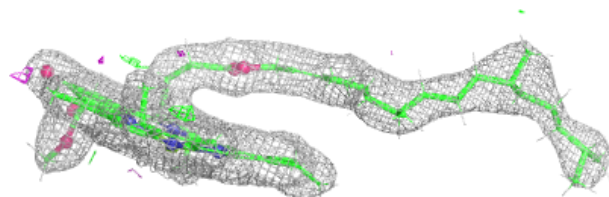
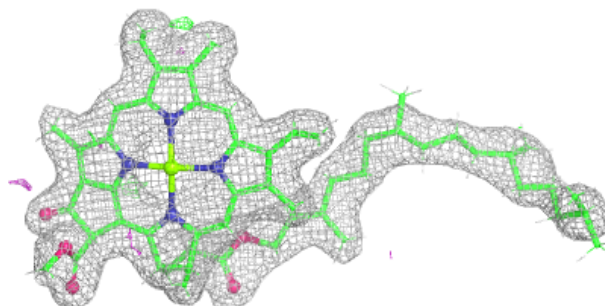


Electron density around CLA a 402:

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

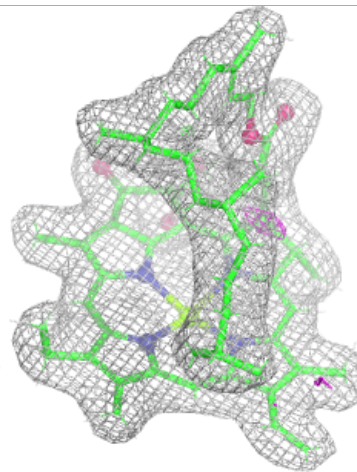
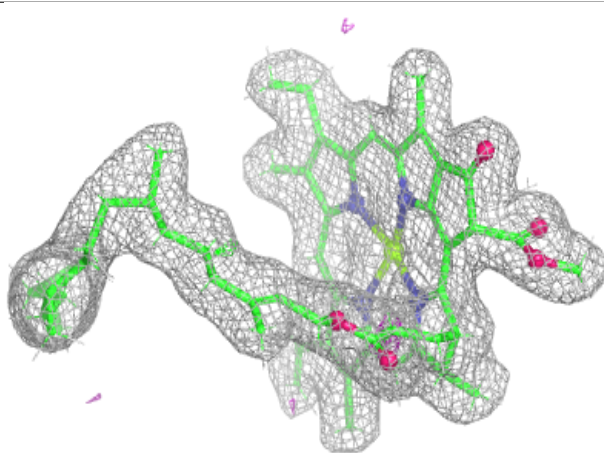
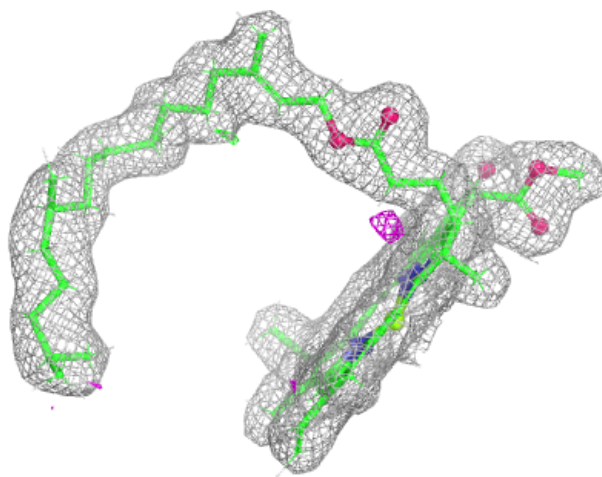
**Electron density around CLA B 603:**

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



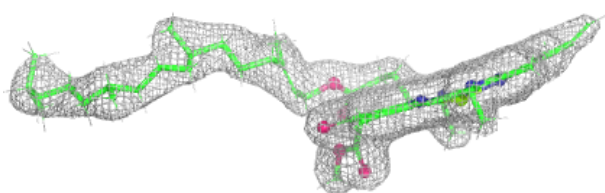
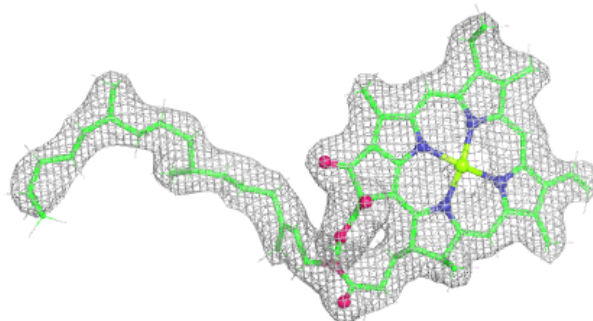
Electron density around CLA B 611:

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

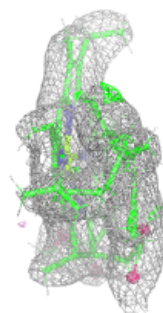
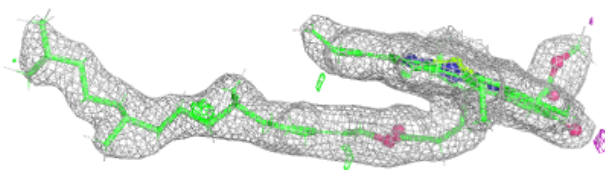
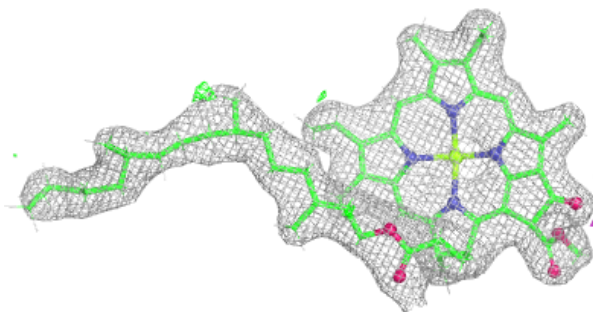


Electron density around CLA b 602:

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

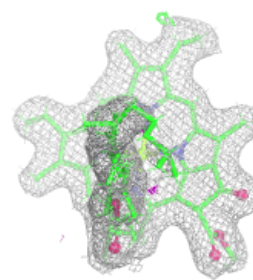
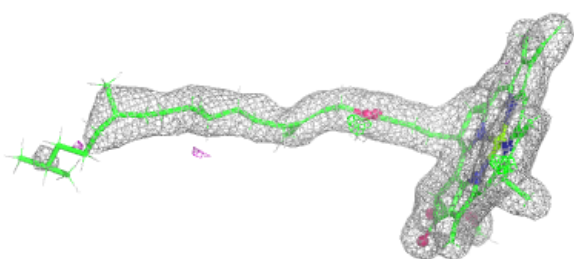
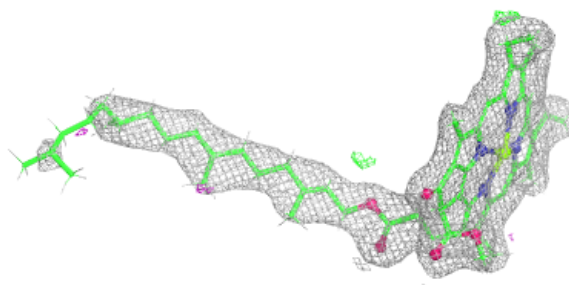
**Electron density around CLA b 603:**

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

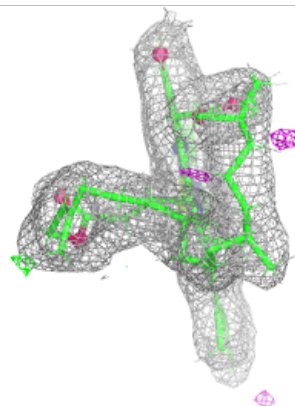
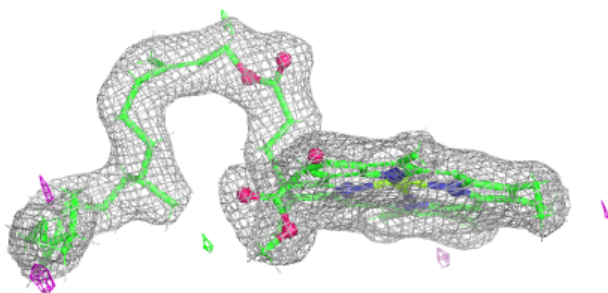
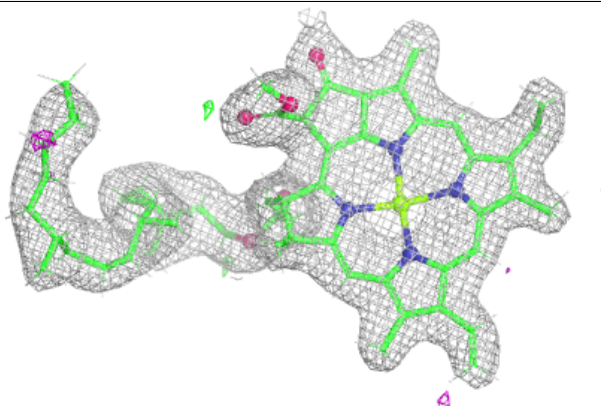


Electron density around CLA b 604:

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

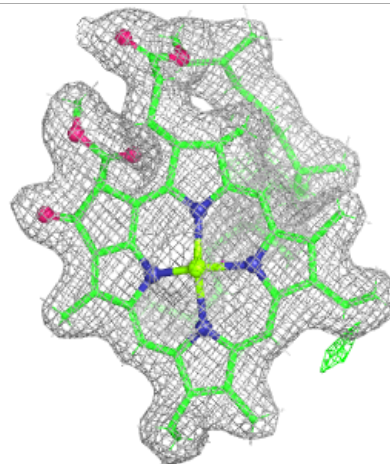
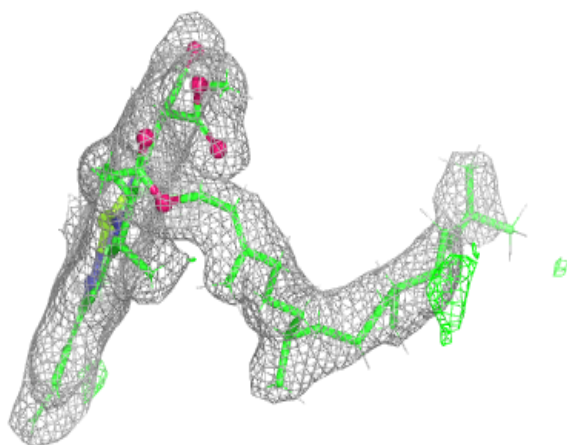
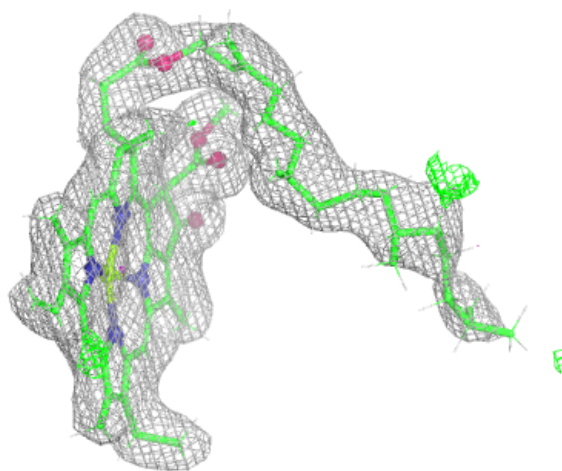
**Electron density around CLA B 612:**

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



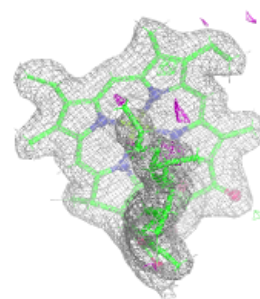
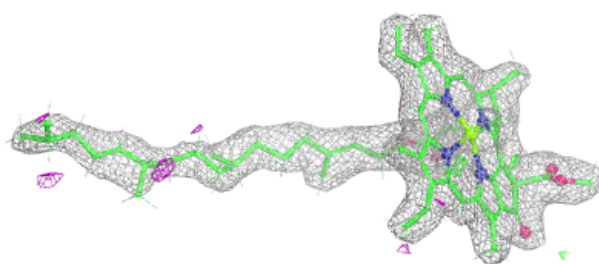
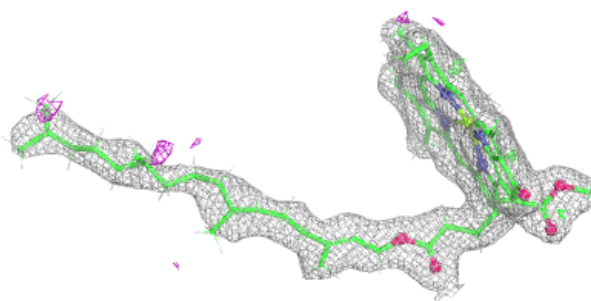
Electron density around CLA B 613:

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

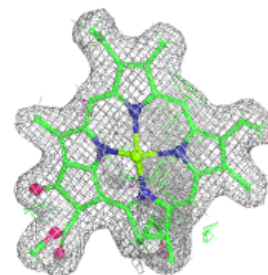
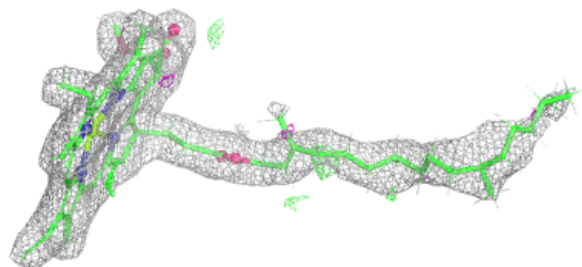
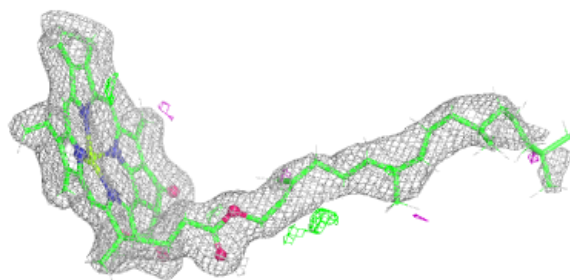


Electron density around CLA b 607:

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

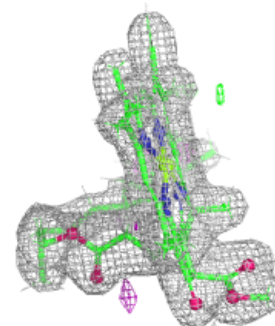
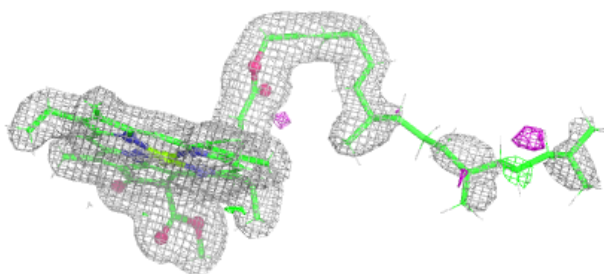
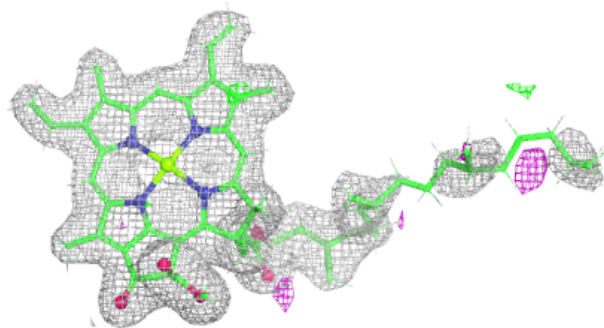
**Electron density around CLA B 604:**

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

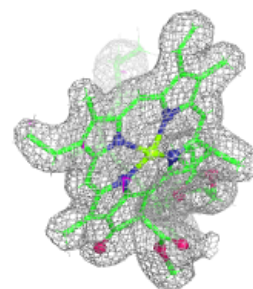
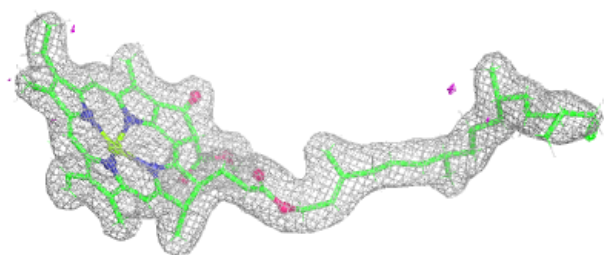
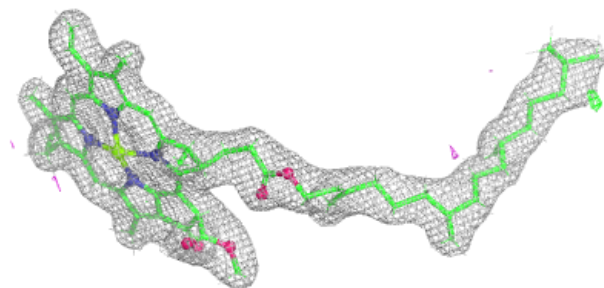


Electron density around CLA A 403:

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

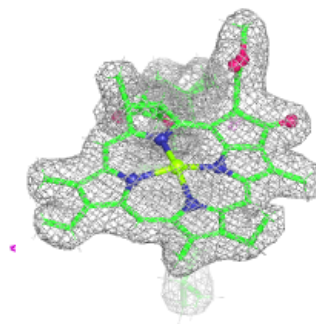
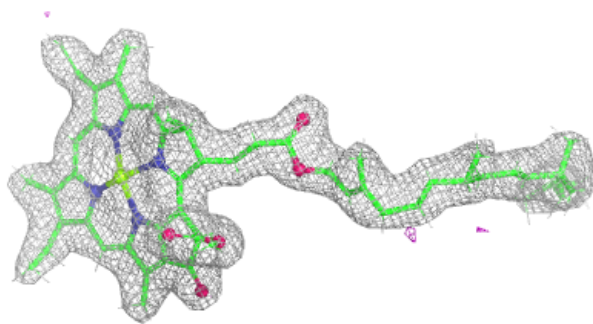
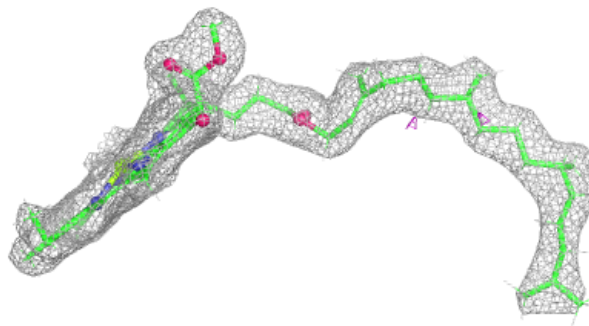
**Electron density around CLA A 402:**

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



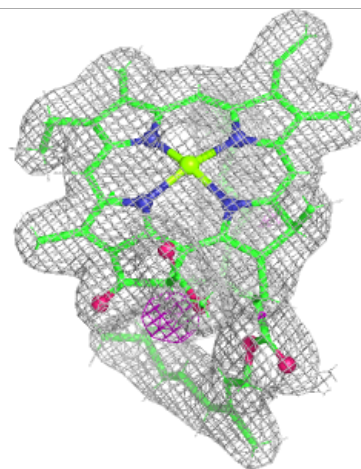
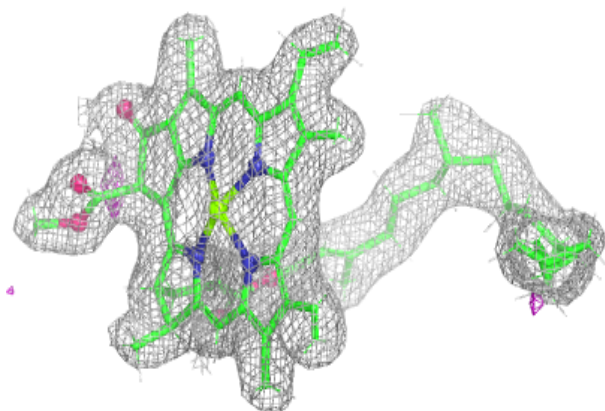
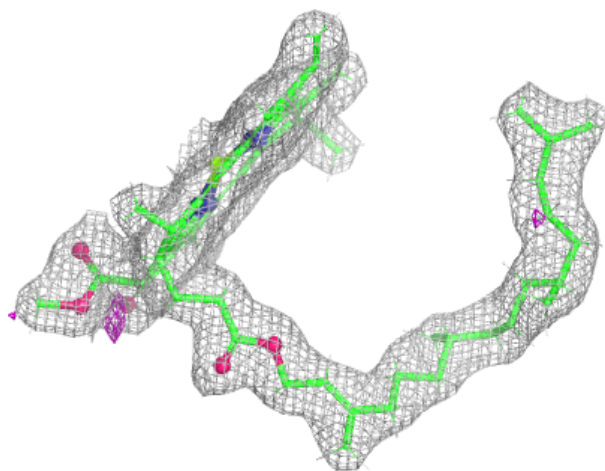
Electron density around CLA d 403:

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



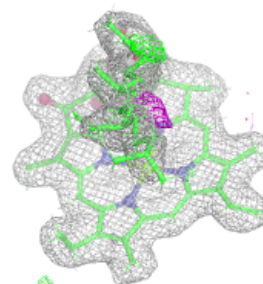
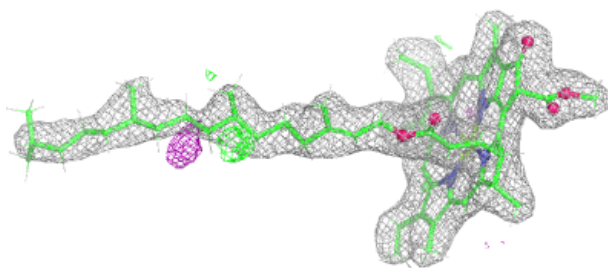
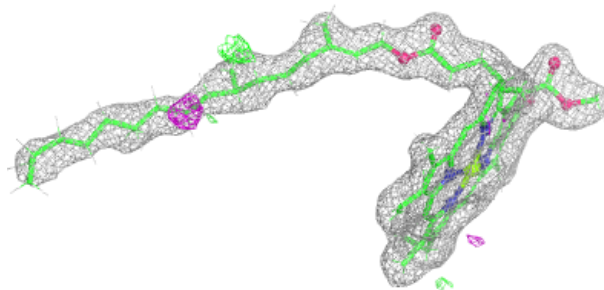
Electron density around CLA b 611:

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



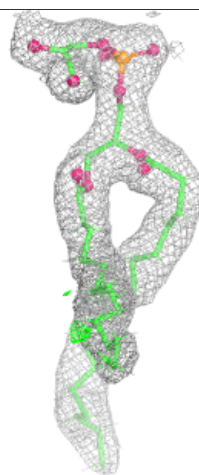
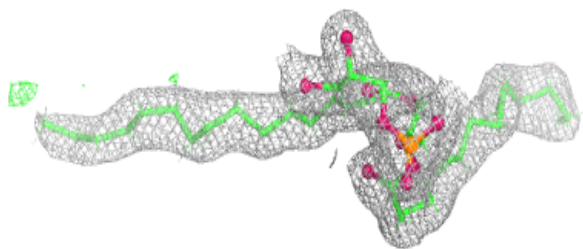
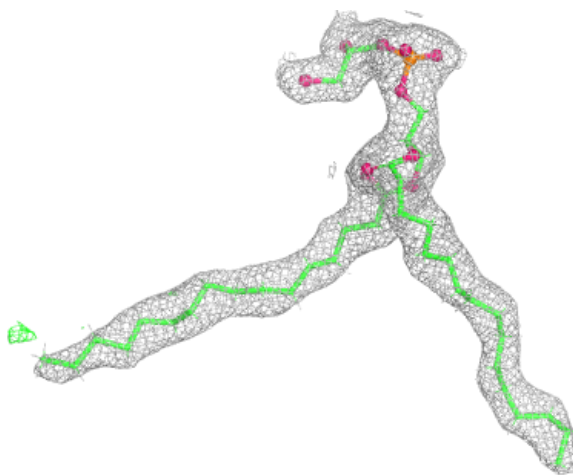
Electron density around CLA B 607:

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



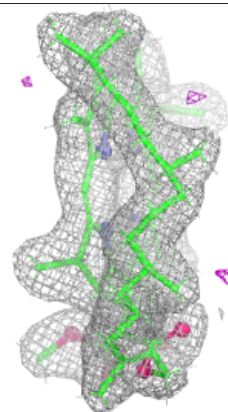
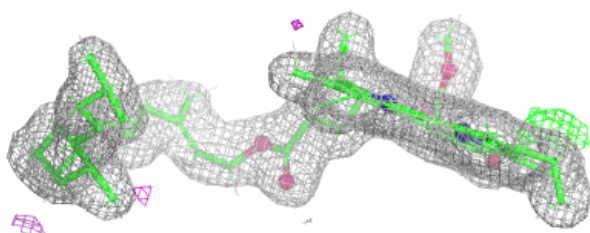
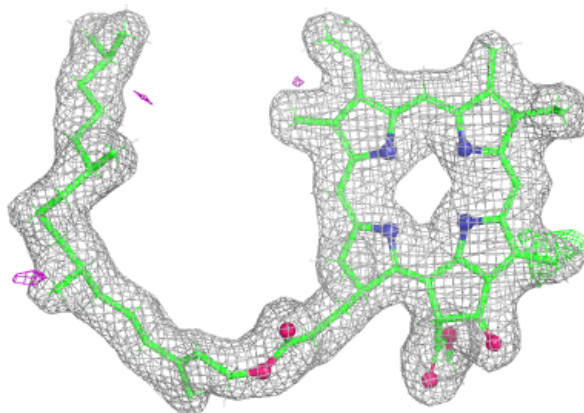
Electron density around LHG B 621:

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

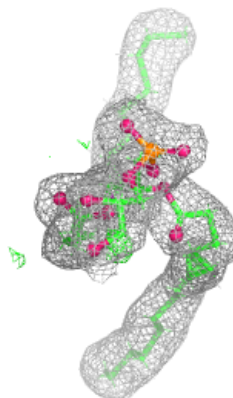
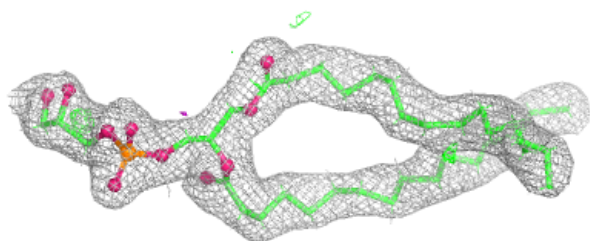
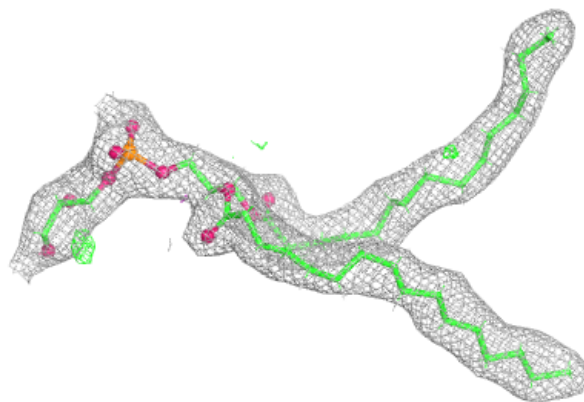


Electron density around PHO A 404:

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

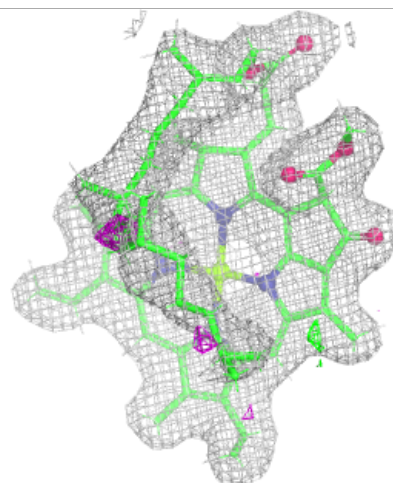
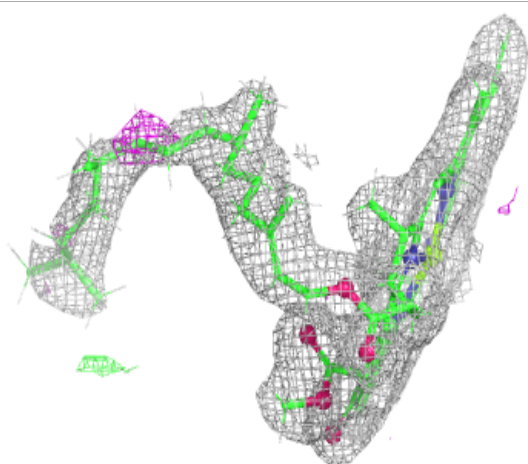
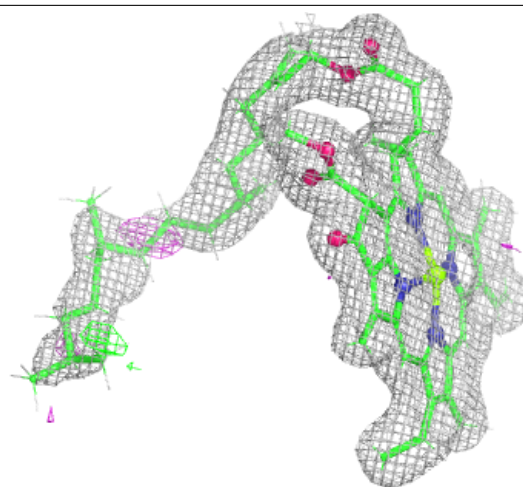
**Electron density around LHG D 409:**

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



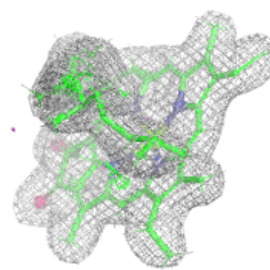
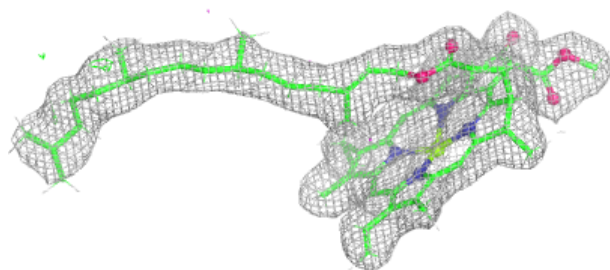
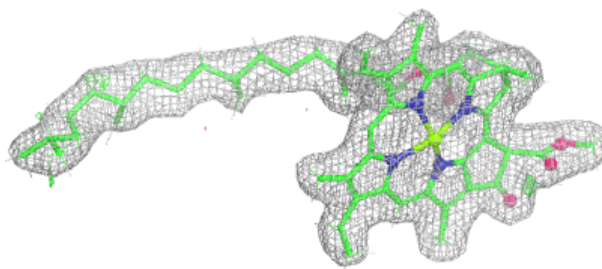
Electron density around CLA b 613:

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

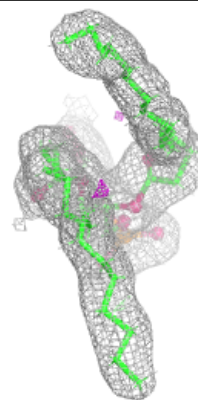
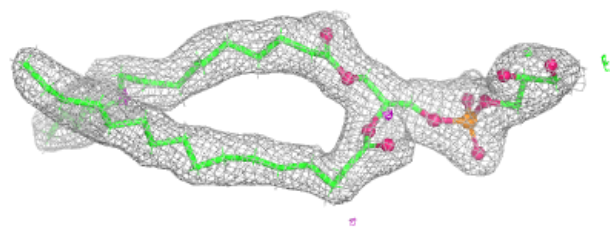
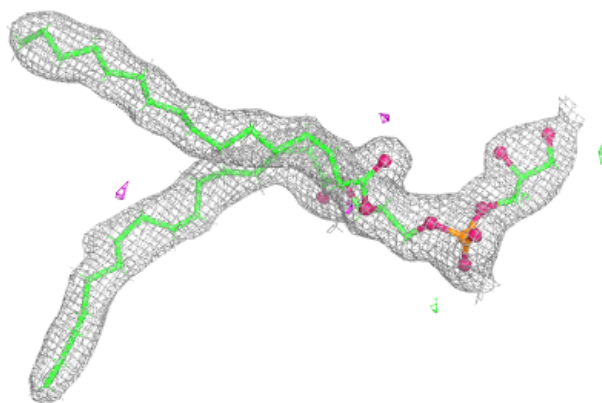


Electron density around CLA B 608:

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

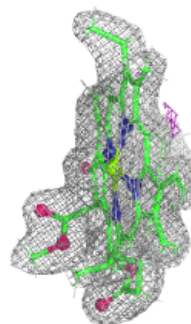
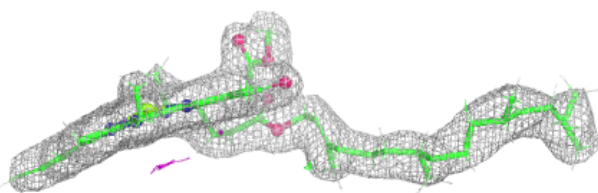
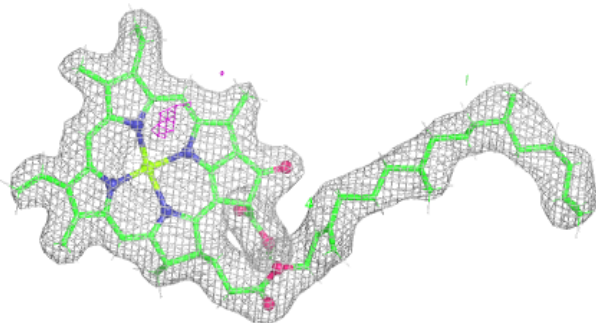
**Electron density around LHG d 408:**

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

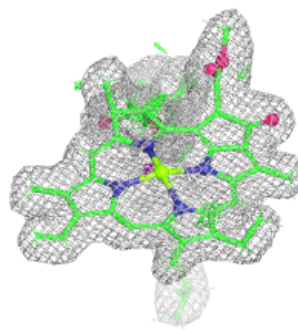
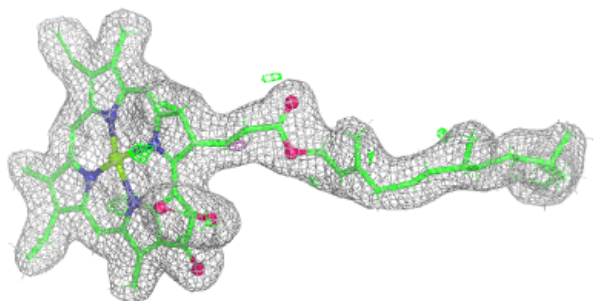
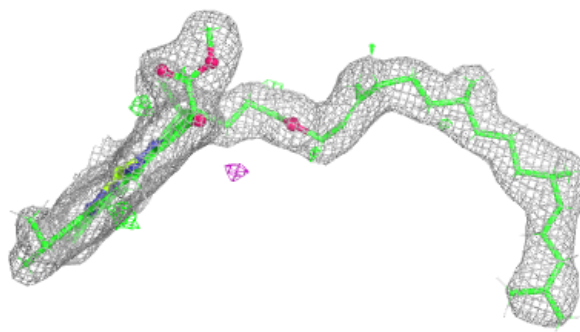


Electron density around CLA B 602:

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

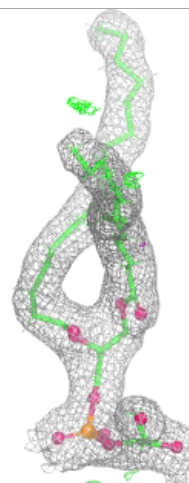
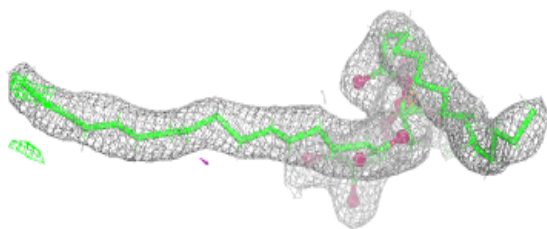
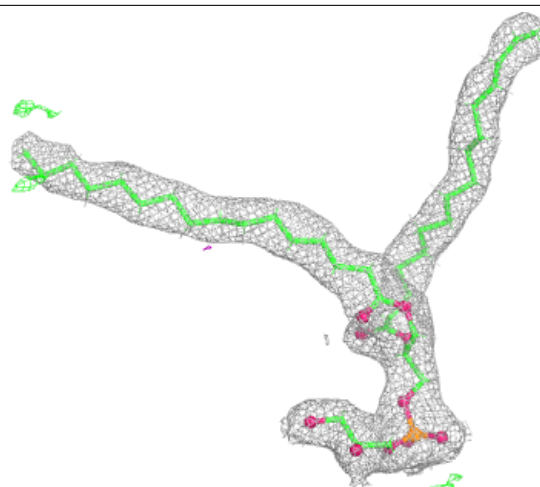
**Electron density around CLA D 402:**

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



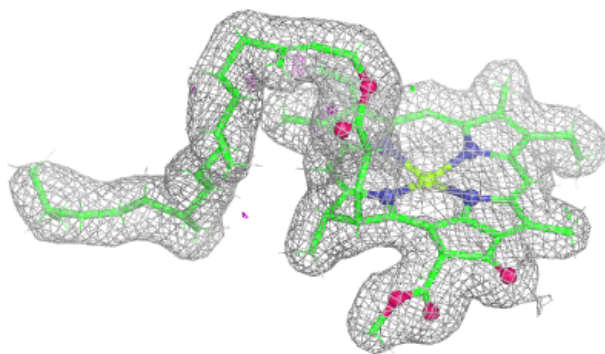
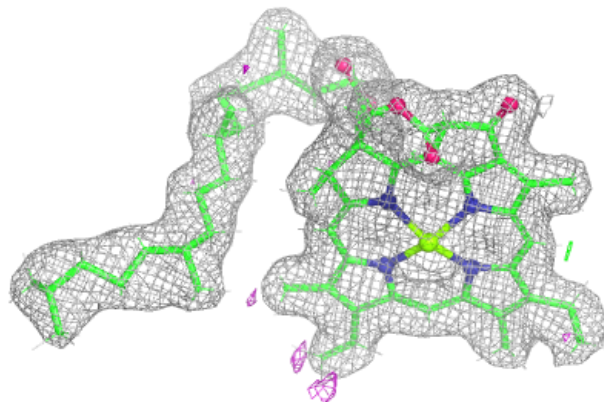
Electron density around LHG 1 101:

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



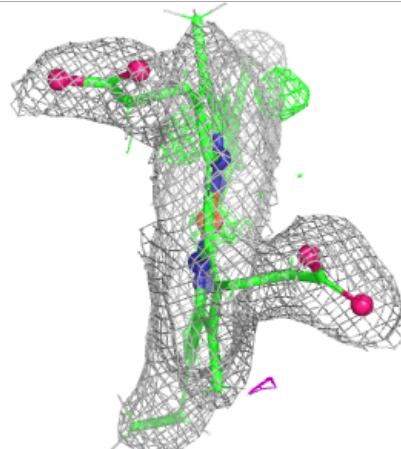
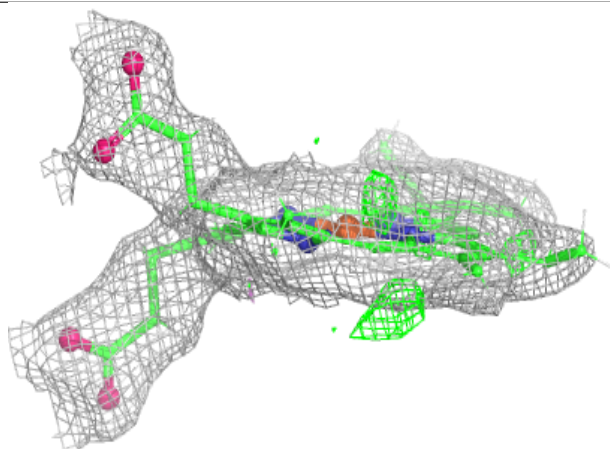
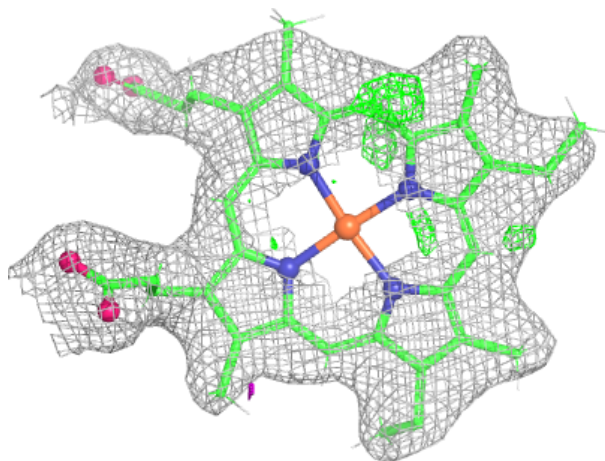
Electron density around CLA D 403:

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



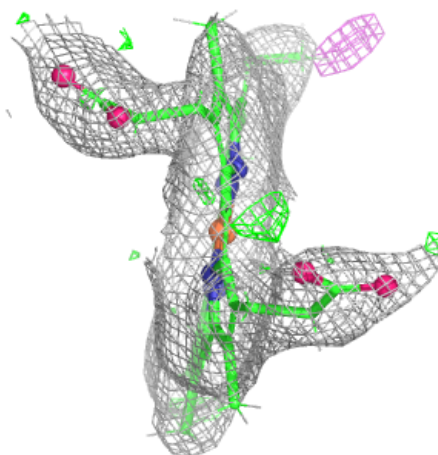
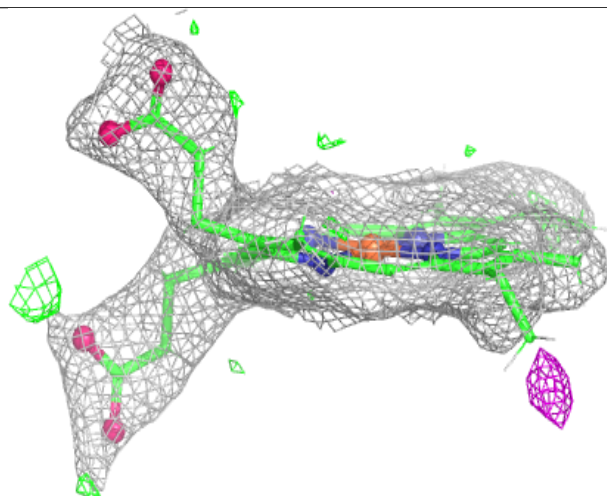
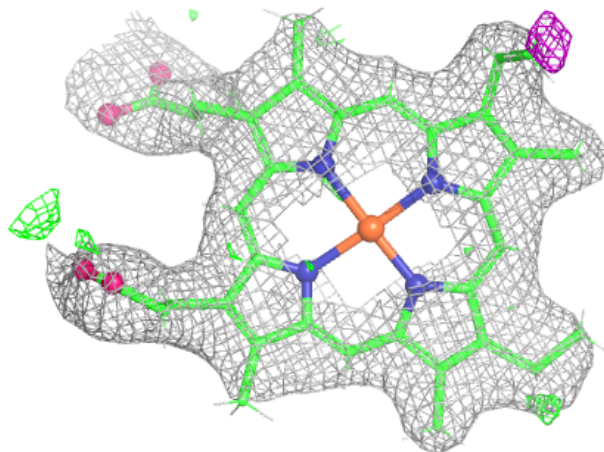
Electron density around HEC F 101:

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



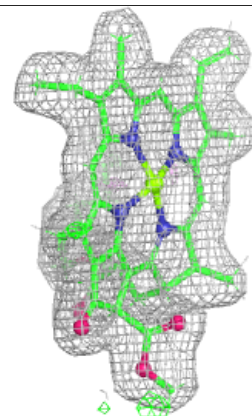
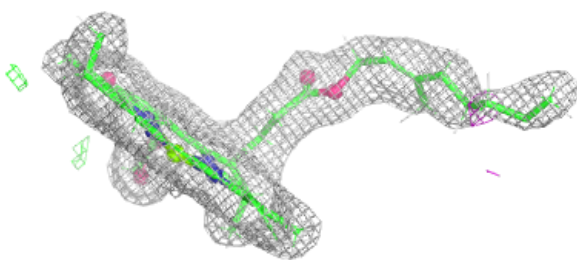
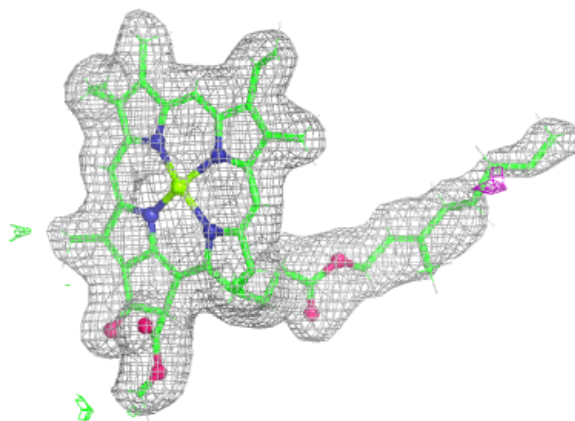
Electron density around HEC f 101:

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



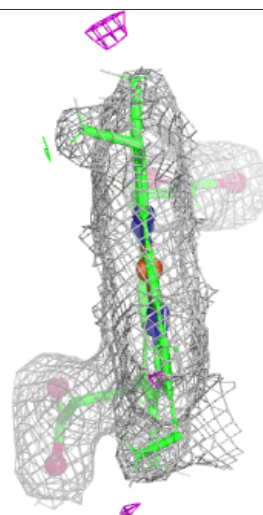
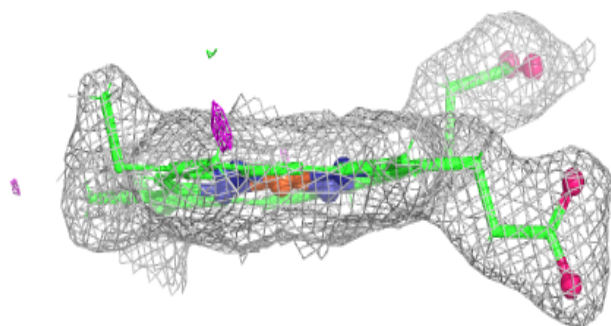
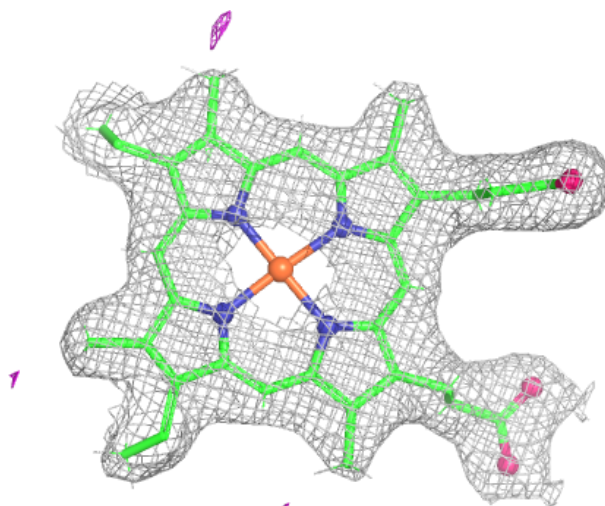
Electron density around CLA A 406:

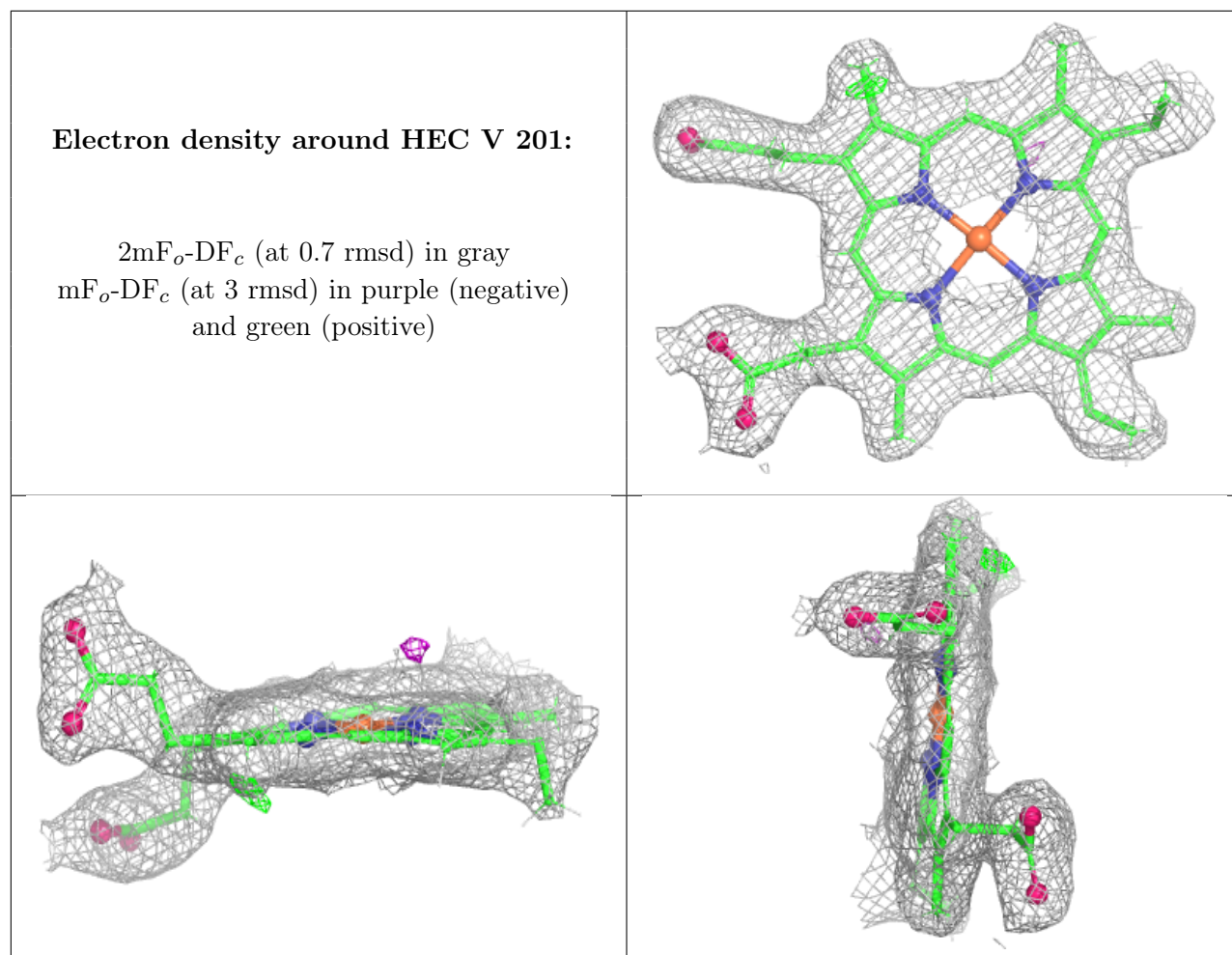
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 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.