



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 03:40 PM UTC

PDB ID : 6W1P / pdb_00006w1p
Title : RT XFEL structure of the one-flash state of Photosystem II (1F, S2-rich) at 2.26 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 : 2.26 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)

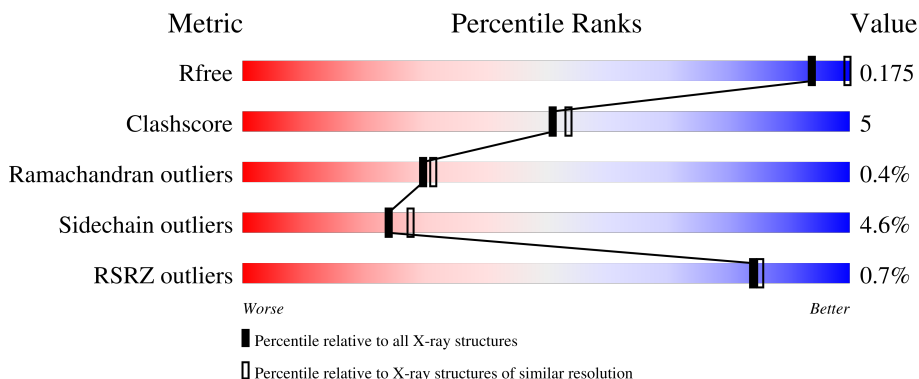
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.26 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	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

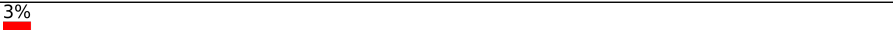
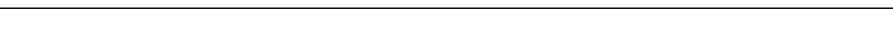
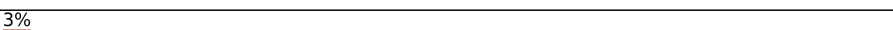
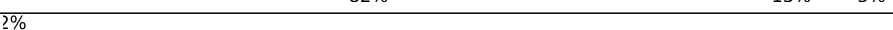
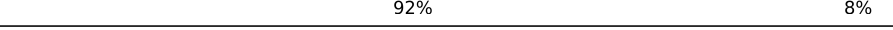
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively.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

Mol	Chain	Length	Quality of chain
1	A	334	 89% 11% .
1	a	334	 89% 10% .

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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	405	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	608	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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	B	616	X	-	-	-
22	CLA	B	617	X	-	-	-
22	CLA	C	502	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	508	X	-	-	-
22	CLA	C	509	X	-	-	-
22	CLA	C	510	X	-	-	-
22	CLA	C	511	X	-	-	-
22	CLA	C	512	X	-	-	-
22	CLA	C	513	X	-	-	-
22	CLA	D	402	X	-	-	-
22	CLA	D	403	X	-	-	-
22	CLA	D	404	X	-	-	-
22	CLA	a	402	X	-	-	-
22	CLA	a	405	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	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	502	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	508	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	c	509	X	-	-	-
22	CLA	c	510	X	-	-	-
22	CLA	c	511	X	-	-	-
22	CLA	c	512	X	-	-	-
22	CLA	c	513	X	-	-	-
22	CLA	d	403	X	-	-	-

2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 103385 atoms, of which 51555 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	334	Total	C	H	N	O	S	0	0	0
			5130	1717	2508	431	459	15			
1	a	334	Total	C	H	N	O	S	0	0	0
			5118	1714	2499	431	459	15			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	505	Total	C	H	N	O	S	0	5	0
			7864	2631	3859	666	695	13			
2	b	505	Total	C	H	N	O	S	0	0	0
			7800	2610	3822	665	690	13			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	442	Total	C	H	N	O	S	0	2	0
			6768	2249	3342	571	593	13			
3	c	451	Total	C	H	N	O	S	0	2	0
			6913	2290	3413	587	610	13			

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

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	K	37	Total	C	H	N	O	0	0	0
			598	204	305	43	46			
10	k	37	Total	C	H	N	O	0	0	0
			598	204	305	43	46			

- Molecule 11 is a protein called Photosystem II reaction center protein L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	L	37	Total	C	H	N	O	0	0	0
			620	202	316	48	53			
11	l	36	Total	C	H	N	O	0	0	0
			600	197	304	47	52			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	33	Total	C	H	N	O	0	0	0
			525	171	269	37	47			
12	m	32	Total	C	H	N	O	0	0	0
			518	168	267	36	46			

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

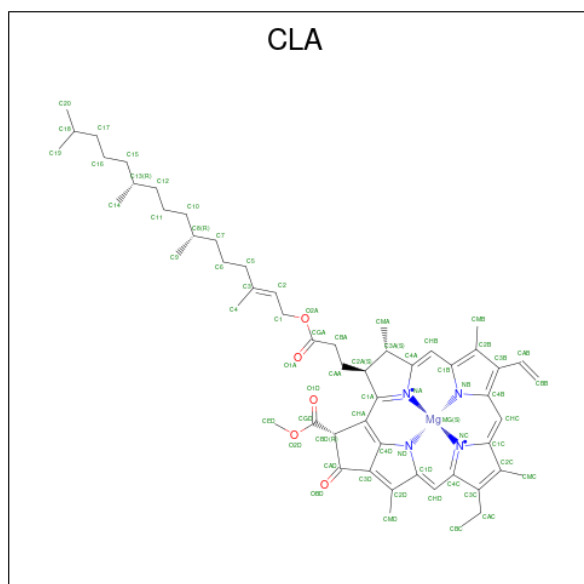
- Molecule 20 is a protein called Photosystem II reaction center protein Z.

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

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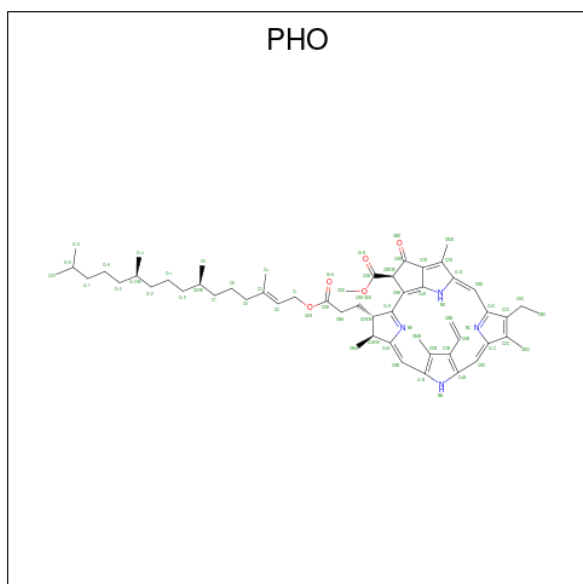
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total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

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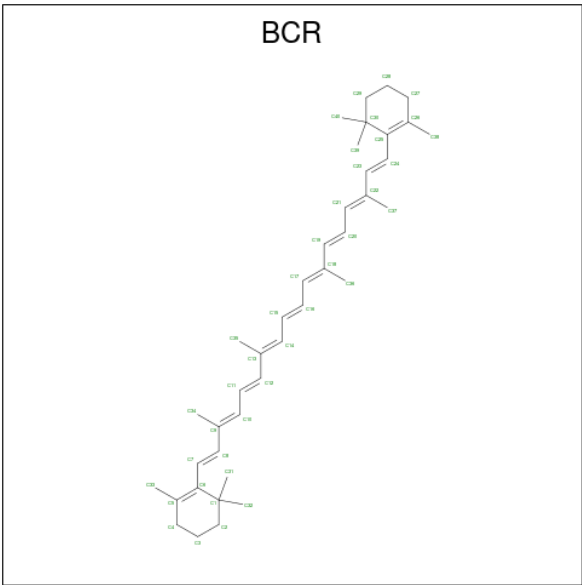
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	d	1	Total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

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



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

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



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

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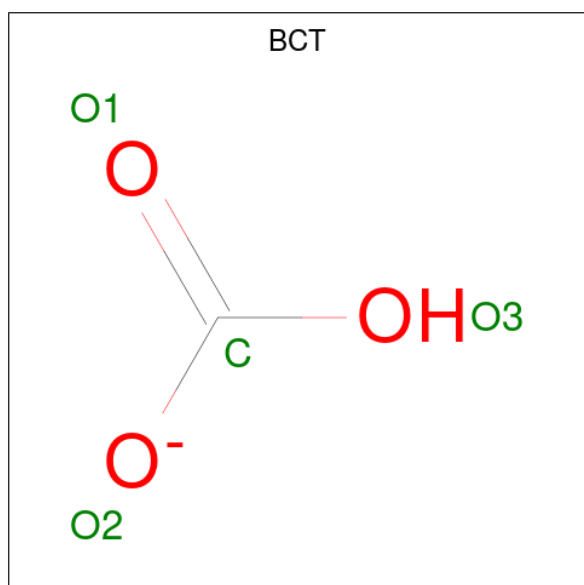
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	b	1	Total	C	H	0	0
			96	40	56		
24	c	1	Total	C	H	0	0
			96	40	56		
24	c	1	Total	C	H	0	0
			96	40	56		
24	d	1	Total	C	H	0	0
			96	40	56		
24	k	1	Total	C	H	0	0
			96	40	56		
24	k	1	Total	C	H	0	0
			96	40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

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

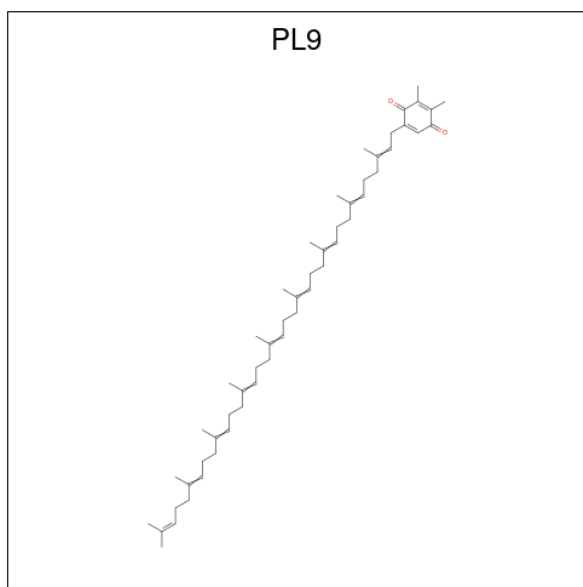
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	A	2	Total	Cl	0	0
			2	2		
25	a	2	Total	Cl	0	0
			2	2		

- Molecule 26 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



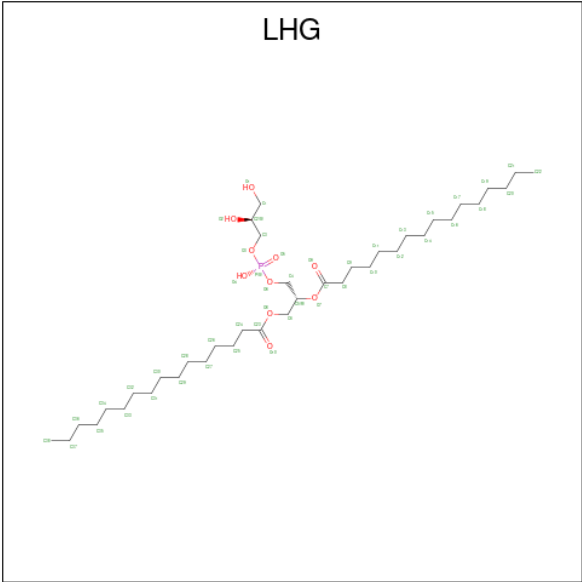
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	A	1	Total	C	H	O	0	0
			5	1	1	3		
26	a	1	Total	C	H	O	0	0
			5	1	1	3		

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



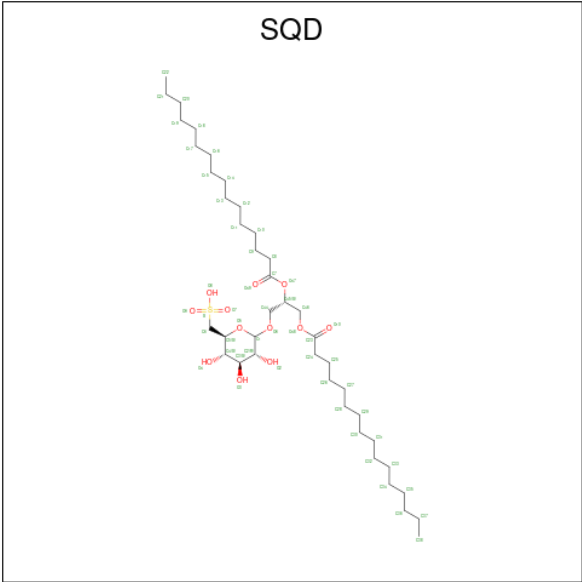
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	A	1	Total	C	H	O	0	0
			135	53	80	2		
27	D	1	Total	C	H	O	0	0
			135	53	80	2		
27	a	1	Total	C	H	O	0	0
			135	53	80	2		
27	d	1	Total	C	H	O	0	0
			135	53	80	2		

- Molecule 28 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



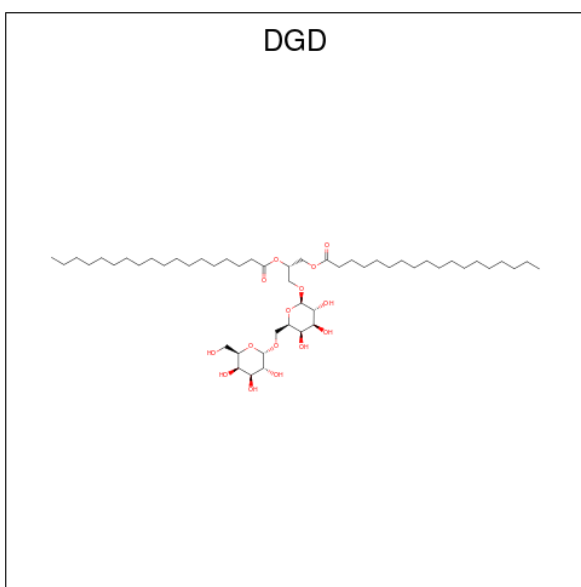
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
28	A	1	Total	C	H	O	P	0	0
			113	36	66	10	1		
28	A	1	Total	C	H	O	P	0	0
			122	38	73	10	1		
28	B	1	Total	C	H	O	P	0	0
			121	38	72	10	1		
28	D	1	Total	C	H	O	P	0	0
			121	38	72	10	1		
28	L	1	Total	C	H	O	P	0	0
			122	38	73	10	1		
28	a	1	Total	C	H	O	P	0	0
			97	31	55	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
			121	38	72	10	1		
28	d	1	Total	C	H	O	P	0	0
			88	28	49	10	1		
28	l	1	Total	C	H	O	P	0	0
			123	38	74	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).



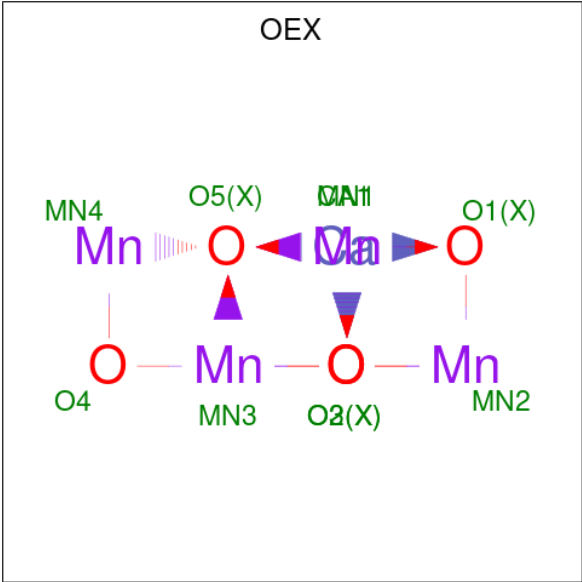
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
29	A	1	Total	C	H	O	S	0	0
			121	39	69	12	1		
29	A	1	Total	C	H	O		0	0
			104	35	65	4			
29	B	1	Total	C	H	O	S	0	0
			132	41	78	12	1		
29	F	1	Total	C	H	O	S	0	0
			81	25	45	10	1		
29	L	1	Total	C	H	O	S	0	0
			113	36	64	12	1		
29	a	1	Total	C	H	O	S	0	0
			131	41	77	12	1		
29	a	1	Total	C	H	O		0	0
			92	31	56	5			
29	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).



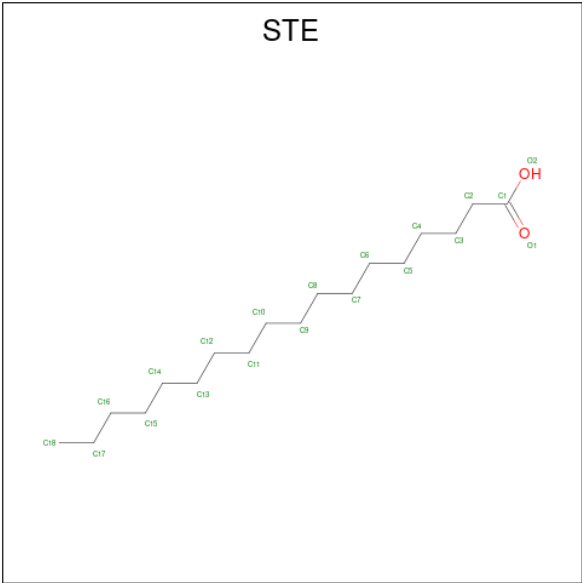
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	A	1	Total	C	H	O	0	0
			161	51	95	15		
30	C	1	Total	C	H	O	0	0
			141	47	79	15		
30	C	1	Total	C	H	O	0	0
			141	47	79	15		
30	C	1	Total	C	H	O	0	0
			141	47	79	15		
30	H	1	Total	C	H	O	0	0
			141	47	79	15		
30	c	1	Total	C	H	O	0	0
			141	47	79	15		
30	c	1	Total	C	H	O	0	0
			139	47	77	15		
30	c	1	Total	C	H	O	0	0
			139	47	77	15		
30	h	1	Total	C	H	O	0	0
			140	47	78	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	0
			10	1	4	5		
31	a	1	Total	Ca	Mn	O	0	0
			10	1	4	5		

- Molecule 32 is STEARIC ACID (CCD ID: STE) (formula: C₁₈H₃₆O₂).



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

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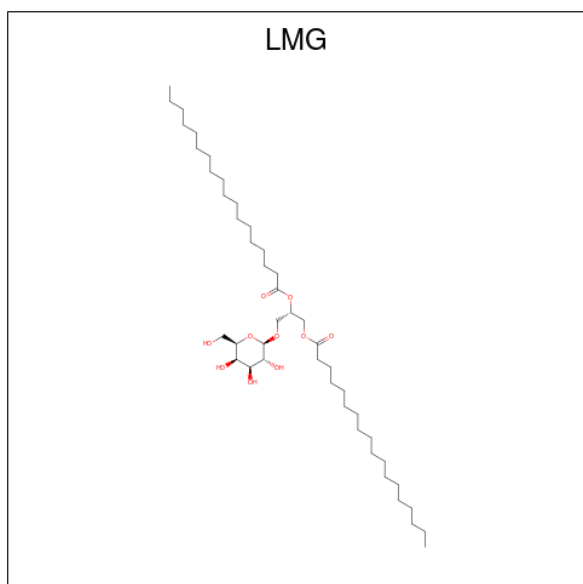
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	B	1	Total C H O 28 10 16 2	0	0
32	B	1	Total C H 47 16 31	0	0
32	B	1	Total C H 41 15 26	0	0
32	C	1	Total C H O 28 10 16 2	0	0
32	C	1	Total C H 47 16 31	0	0
32	C	1	Total C H O 28 10 16 2	0	0
32	D	1	Total C H O 55 18 35 2	0	0
32	E	1	Total C H O 28 10 16 2	0	0
32	H	1	Total C H 53 18 35	0	0
32	I	1	Total C H 41 15 26	0	0
32	J	1	Total C H O 28 10 16 2	0	0
32	L	1	Total C H O 28 10 16 2	0	0
32	M	1	Total C H O 37 13 22 2	0	0
32	M	1	Total C H 26 10 16	0	0
32	M	1	Total C H 53 18 35	0	0
32	T	1	Total C H 44 15 29	0	0
32	Z	1	Total C H 20 8 12	0	0
32	a	1	Total C H O 28 10 16 2	0	0
32	b	1	Total C H 47 16 31	0	0
32	b	1	Total C H O 55 18 35 2	0	0
32	b	1	Total C H O 40 14 24 2	0	0

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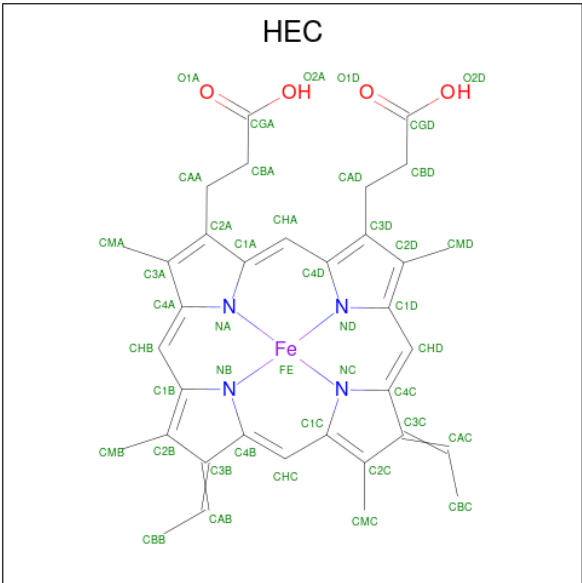
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	b	1	Total C H O 55 18 35 2	0	0
32	b	1	Total C H 26 10 16	0	0
32	b	1	Total C H O 55 18 35 2	0	0
32	c	1	Total C H O 55 18 35 2	0	0
32	d	1	Total C H O 43 15 26 2	0	0
32	h	1	Total C H 41 14 27	0	0
32	j	1	Total C H O 28 10 16 2	0	0
32	k	1	Total C H O 28 10 16 2	0	0
32	t	1	Total C H O 34 12 20 2	0	0
32	t	1	Total C H 26 10 16	0	0
32	t	1	Total C H O 46 16 28 2	0	0
32	x	1	Total C H O 55 18 35 2	0	0

- Molecule 33 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	B	1	Total	C	H	O	0	0
			141	45	86	10		
33	C	1	Total	C	H	O	0	0
			112	38	64	10		
33	D	1	Total	C	H	O	0	0
			122	41	71	10		
33	D	1	Total	C	H	O	0	0
			78	27	45	6		
33	D	1	Total	C	H	O	0	0
			68	24	40	4		
33	M	1	Total	C	H	O	0	0
			122	41	71	10		
33	Y	1	Total	C	H	O	0	0
			114	38	66	10		
33	b	1	Total	C	H	O	0	0
			140	45	85	10		
33	c	1	Total	C	H	O	0	0
			80	27	43	10		
33	c	1	Total	C	H	O	0	0
			117	38	69	10		
33	c	1	Total	C	H	O	0	0
			116	39	67	10		
33	d	1	Total	C	H	O	0	0
			100	34	56	10		
33	m	1	Total	C	H	O	0	0
			122	41	71	10		

- Molecule 34 is HEME C (CCD ID: HEC) (formula: C₃₄H₃₄FeN₄O₄).



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

- Molecule 35 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	A	132	Total	O	0	0
			132	132		
35	B	174	Total	O	0	0
			174	174		
35	C	139	Total	O	0	0
			139	139		
35	D	116	Total	O	0	0
			116	116		
35	E	26	Total	O	0	0
			26	26		
35	F	4	Total	O	0	0
			4	4		
35	H	16	Total	O	0	0
			16	16		
35	I	14	Total	O	0	0
			14	14		
35	J	9	Total	O	0	0
			9	9		
35	K	7	Total	O	0	0
			7	7		
35	L	9	Total	O	0	0
			9	9		
35	M	5	Total	O	0	0
			5	5		
35	O	78	Total	O	0	0
			78	78		
35	R	1	Total	O	0	0
			1	1		
35	T	9	Total	O	0	0
			9	9		
35	U	34	Total	O	0	0
			34	34		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	V	53	Total 53	O 53	0	0
35	X	12	Total 12	O 12	0	0
35	Y	6	Total 6	O 6	0	0
35	Z	1	Total 1	O 1	0	0
35	a	109	Total 109	O 109	0	0
35	b	134	Total 134	O 134	0	0
35	c	130	Total 130	O 130	0	0
35	d	91	Total 91	O 91	0	0
35	e	15	Total 15	O 15	0	0
35	f	8	Total 8	O 8	0	0
35	h	26	Total 26	O 26	0	0
35	i	7	Total 7	O 7	0	0
35	j	9	Total 9	O 9	0	0
35	k	6	Total 6	O 6	0	0
35	l	10	Total 10	O 10	0	0
35	m	3	Total 3	O 3	0	0
35	o	81	Total 81	O 81	0	0
35	r	7	Total 7	O 7	0	0
35	t	11	Total 11	O 11	0	0
35	u	43	Total 43	O 43	0	0
35	v	37	Total 37	O 37	0	0

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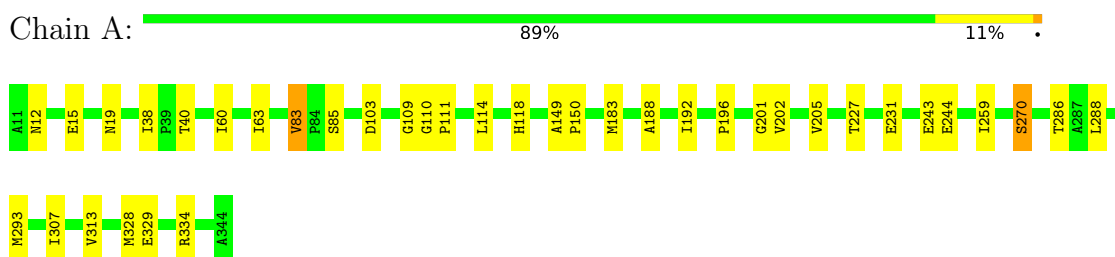
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	x	4	Total 4	O 4	0	0
35	y	2	Total 2	O 2	0	0
35	z	4	Total 4	O 4	0	0

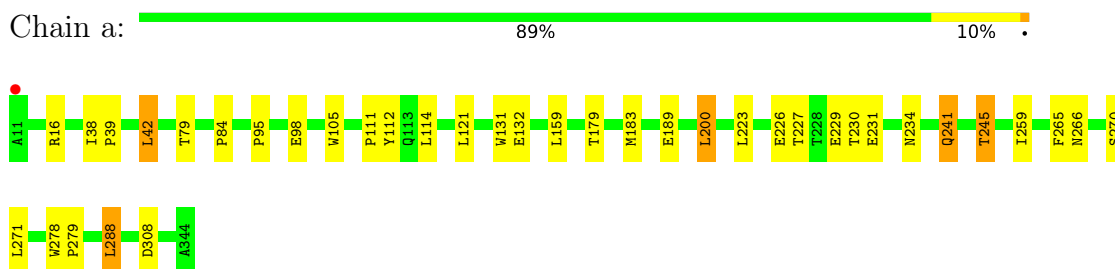
3 Residue-property plots

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

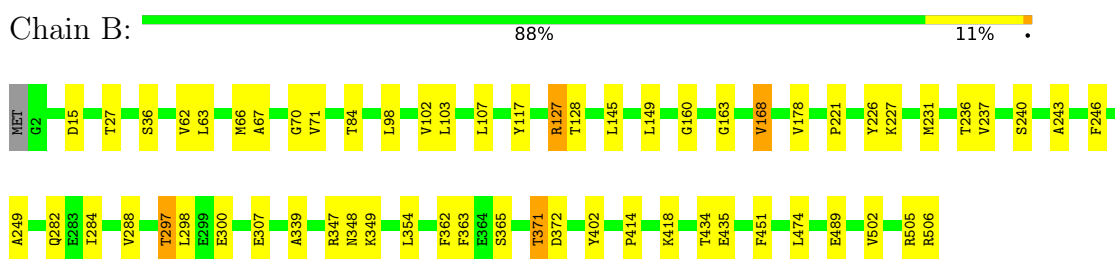
• Molecule 1: Photosystem II protein D1 1



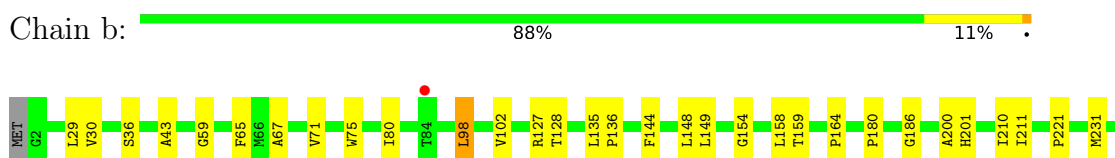
• Molecule 1: Photosystem II protein D1 1



• Molecule 2: Photosystem II CP47 reaction center protein



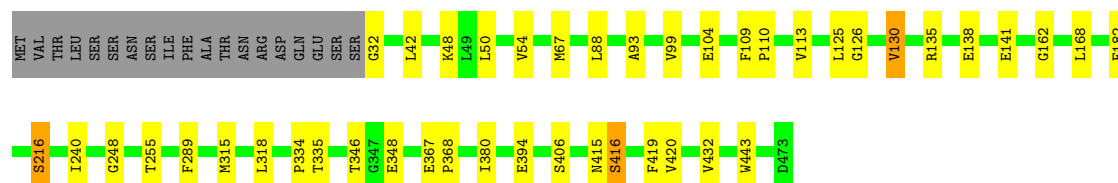
• Molecule 2: Photosystem II CP47 reaction center protein





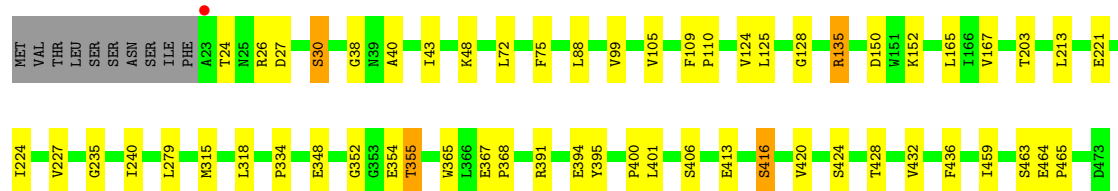
• Molecule 3: Photosystem II CP43 reaction center protein

Chain C: 86% 9% ..



• Molecule 3: Photosystem II CP43 reaction center protein

Chain c: 85% 12% ..



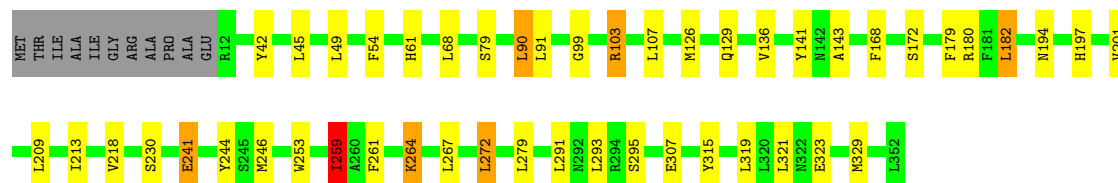
• Molecule 4: Photosystem II D2 protein

Chain D: 88% 8% .



• Molecule 4: Photosystem II D2 protein

Chain d: 83% 12% ..



• Molecule 5: Cytochrome b559 subunit alpha

Chain E: 86% 11% ..



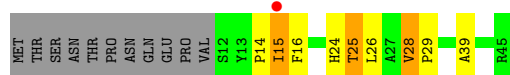
- Molecule 5: Cytochrome b559 subunit alpha



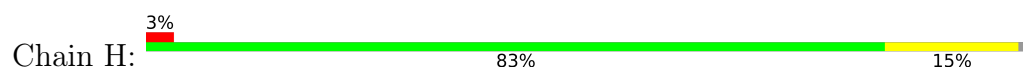
- Molecule 6: Cytochrome b559 subunit beta



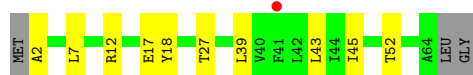
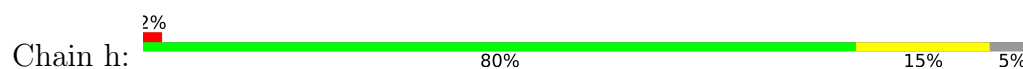
- Molecule 6: Cytochrome b559 subunit beta



- Molecule 7: Photosystem II reaction center protein H



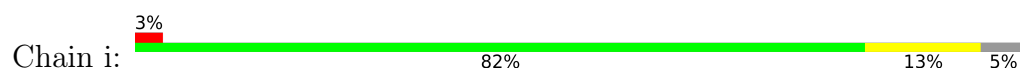
- Molecule 7: Photosystem II reaction center protein H



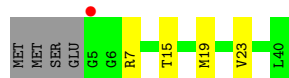
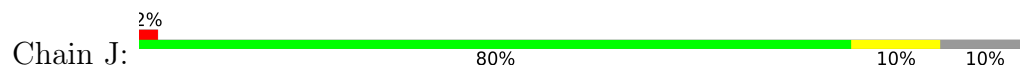
- Molecule 8: Photosystem II reaction center protein I



- Molecule 8: Photosystem II reaction center protein I



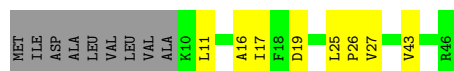
• Molecule 9: Photosystem II reaction center protein J



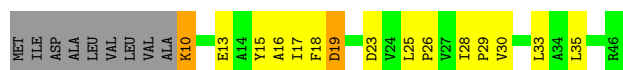
• Molecule 9: Photosystem II reaction center protein J



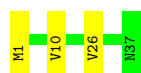
• Molecule 10: Photosystem II reaction center protein K



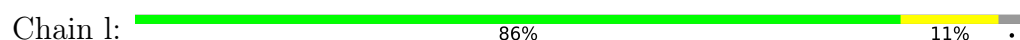
• Molecule 10: Photosystem II reaction center protein K



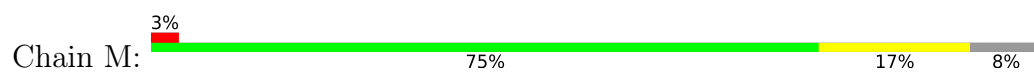
• Molecule 11: Photosystem II reaction center protein L



• Molecule 11: Photosystem II reaction center protein L



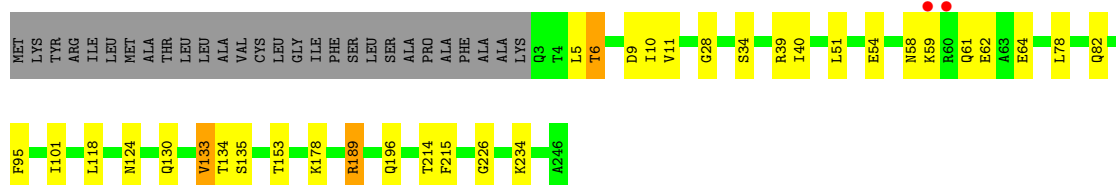
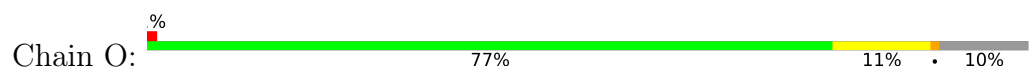
• Molecule 12: Photosystem II reaction center protein M



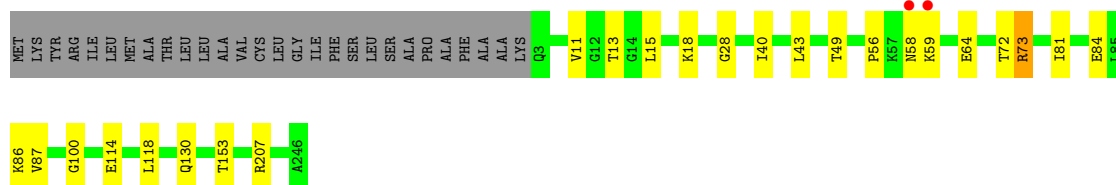
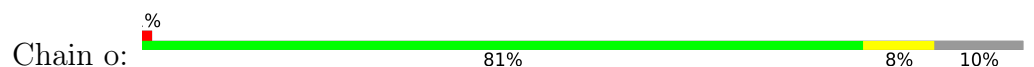
• Molecule 12: Photosystem II reaction center protein M



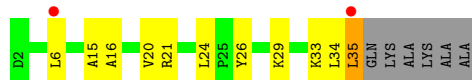
• Molecule 13: Photosystem II manganese-stabilizing polypeptide



• Molecule 13: Photosystem II manganese-stabilizing polypeptide



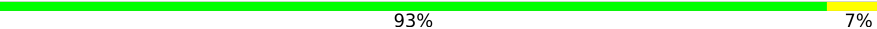
• Molecule 14: Photosystem II protein Y



• Molecule 14: Photosystem II protein Y



• Molecule 15: Photosystem II reaction center protein T

Chain T:  93% 7%



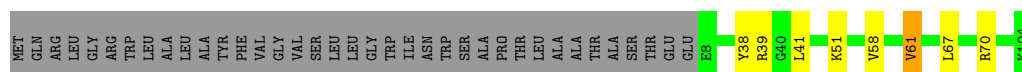
- Molecule 15: Photosystem II reaction center protein T

Chain t:  3% 87% 13%



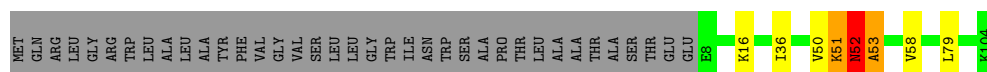
- Molecule 16: Photosystem II 12 kDa extrinsic protein

Chain U:  66% 5% 28%



- Molecule 16: Photosystem II 12 kDa extrinsic protein

Chain u:  66% 28%



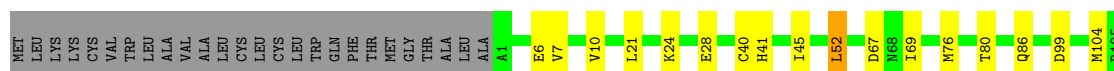
- Molecule 17: Cytochrome c-550

Chain V:  70% 13% 16%



- Molecule 17: Cytochrome c-550

Chain v:  71% 13% 16%

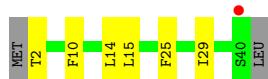
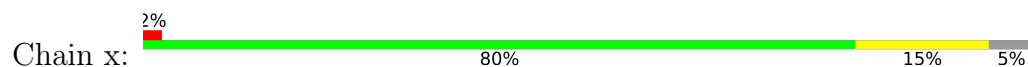


- Molecule 18: Photosystem II reaction center X protein

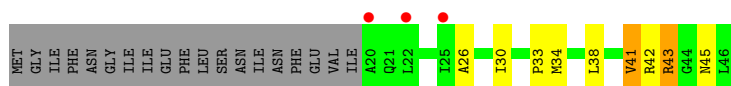
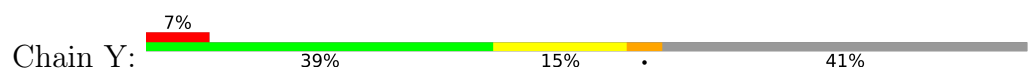
Chain X:  83% 10% 7%



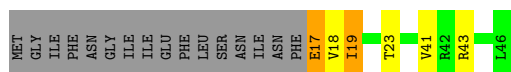
- Molecule 18: Photosystem II reaction center X protein



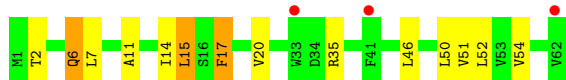
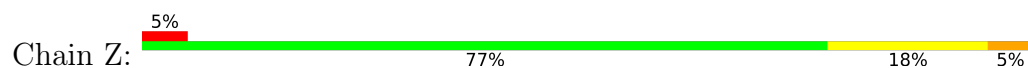
- Molecule 19: Photosystem II reaction center protein Ycf12



- Molecule 19: Photosystem II reaction center protein Ycf12



- Molecule 20: Photosystem II reaction center protein Z



- Molecule 20: Photosystem II reaction center protein Z



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	116.96Å 221.64Å 307.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.54 – 2.26 33.54 – 2.26	Depositor EDS
% Data completeness (in resolution range)	99.8 (33.54-2.26) 86.7 (33.54-2.26)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.83 (at 2.27Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.173 , 0.241 (Not available) , 0.175	Depositor DCC
R_{free} test set	3302 reflections (0.53%)	wwPDB-VP
Wilson B-factor (Å ²)	30.1	Xtriage
Anisotropy	0.248	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 51.1	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	103385	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.48% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CLA, HEC, PL9, SQD, LHG, CL, FE2, PHO, STE, BCT, FME, BCR, OEX, DGD, 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	0.65	0/2707	0.75	1/3692 (0.0%)
1	a	0.63	0/2704	0.71	0/3688
2	B	0.62	0/4161	0.70	0/5669
2	b	0.60	0/4118	0.70	0/5611
3	C	0.59	0/3547	0.66	0/4830
3	c	0.55	0/3619	0.68	0/4926
4	D	0.63	0/2812	0.69	0/3832
4	d	0.62	1/2821 (0.0%)	0.72	0/3844
5	E	0.51	0/688	0.62	0/940
5	e	0.49	0/683	0.64	0/932
6	F	0.53	0/284	0.68	0/387
6	f	0.55	0/284	0.67	0/387
7	H	0.68	0/523	0.67	0/713
7	h	0.54	0/511	0.66	0/697
8	I	0.59	0/293	0.73	0/396
8	i	0.61	0/293	0.65	0/396
9	J	0.52	0/263	0.63	0/356
9	j	0.49	0/263	0.60	0/356
10	K	0.46	0/303	0.66	0/416
10	k	0.45	0/303	0.60	0/416
11	L	0.67	0/311	0.69	0/422
11	l	0.63	0/303	0.68	0/412
12	M	0.67	0/249	0.77	0/341
12	m	0.63	0/244	0.71	0/334
13	O	0.60	0/1904	0.71	0/2585
13	o	0.59	0/1905	0.70	0/2583
14	R	0.47	0/277	0.61	0/380
14	r	0.42	0/246	0.56	0/339
15	T	0.62	0/257	0.69	0/349
15	t	0.64	0/255	0.65	0/346
16	U	0.56	0/785	0.65	0/1064
16	u	0.61	0/785	0.77	2/1064 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	V	0.60	0/1085	0.69	1/1473 (0.1%)
17	v	0.58	0/1085	0.67	0/1473
18	X	0.49	0/284	0.63	0/384
18	x	0.40	0/289	0.55	0/391
19	Y	0.51	0/197	0.62	0/264
19	y	0.42	0/219	0.56	0/294
20	Z	0.47	0/490	0.58	0/669
20	z	0.41	0/488	0.55	0/666
All	All	0.59	1/42838 (0.0%)	0.69	4/58317 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	b	0	1
17	V	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	d	259	ILE	CG1-CD1	-5.34	1.30	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	u	52	ASN	CA-C-N	6.34	133.12	121.70
16	u	52	ASN	C-N-CA	6.34	133.12	121.70
1	A	83	VAL	N-CA-C	5.97	113.76	108.63
17	V	63	THR	C-N-CD	-5.04	104.32	125.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
17	V	63	THR	Peptide
2	b	186	GLY	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2622	2508	2519	22	0
1	a	2619	2499	2510	24	0
2	B	4005	3859	3867	41	0
2	b	3978	3822	3836	40	0
3	C	3426	3342	3343	27	0
3	c	3500	3413	3426	42	0
4	D	2717	2613	2621	22	0
4	d	2723	2619	2627	33	0
5	E	666	650	651	7	0
5	e	664	647	648	19	0
6	F	275	281	282	3	0
6	f	275	281	282	8	0
7	H	510	532	532	6	0
7	h	498	518	518	6	0
8	I	296	311	311	3	0
8	i	296	311	311	2	0
9	J	257	268	268	2	0
9	j	257	268	268	4	0
10	K	293	305	305	2	0
10	k	293	305	305	12	0
11	L	304	316	316	2	0
11	l	296	304	304	0	0
12	M	256	269	269	6	0
12	m	251	267	267	4	0
13	O	1870	1828	1830	21	0
13	o	1874	1844	1846	11	0
14	R	271	298	298	5	0
14	r	240	253	250	10	0
15	T	258	261	261	0	0
15	t	256	256	256	1	0
16	U	774	772	773	4	0
16	u	774	772	773	12	0
17	V	1064	1068	1073	12	0
17	v	1064	1068	1073	16	0
18	X	281	312	312	2	0
18	x	286	316	314	2	0
19	Y	196	217	217	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	y	218	241	241	3	0
20	Z	479	516	516	6	0
20	z	477	509	509	15	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	A	184	192	192	4	0
22	B	1035	1139	1139	18	0
22	C	839	922	922	11	0
22	D	195	216	216	6	0
22	a	195	216	216	3	0
22	b	1035	1139	1139	18	0
22	c	839	919	919	19	0
22	d	195	216	216	1	0
23	A	64	74	74	0	0
23	D	64	74	74	2	0
23	a	64	74	74	3	0
23	d	64	74	74	4	0
24	A	40	56	56	1	0
24	B	120	168	168	6	0
24	C	80	112	112	3	0
24	D	40	56	56	3	0
24	H	40	56	56	4	0
24	K	40	56	56	1	0
24	T	40	56	56	1	0
24	Z	40	56	56	3	0
24	a	40	56	56	1	0
24	b	120	168	168	5	0
24	c	80	112	112	4	0
24	d	40	56	56	3	0
24	k	80	112	112	2	0
24	t	40	56	56	4	0
24	x	40	56	56	1	0
25	A	2	0	0	0	0
25	a	2	0	0	0	0
26	A	4	1	1	0	0
26	a	4	1	1	0	0
27	A	55	80	80	3	0
27	D	55	80	80	1	0
27	a	55	80	80	1	0
27	d	55	80	80	1	0
28	A	96	139	141	1	0
28	B	49	72	74	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	D	49	72	74	1	0
28	L	49	73	74	1	0
28	a	42	55	57	0	0
28	d	137	193	199	4	0
28	l	49	74	74	1	0
29	A	91	134	134	1	0
29	B	54	78	78	0	0
29	F	36	45	45	0	0
29	L	49	64	64	1	0
29	a	90	133	133	2	0
29	f	41	48	48	0	0
30	A	66	95	96	4	0
30	C	186	237	244	3	0
30	H	62	79	81	0	0
30	c	186	233	245	2	0
30	h	62	78	81	0	0
31	A	10	0	0	0	0
31	a	10	0	0	1	0
32	B	72	115	115	1	0
32	C	40	63	63	0	0
32	D	20	35	35	1	0
32	E	12	16	16	0	0
32	H	18	35	35	1	0
32	I	15	26	26	2	0
32	J	12	16	16	1	0
32	L	12	16	16	0	0
32	M	43	73	73	1	0
32	T	15	29	29	0	0
32	Z	8	12	12	0	0
32	a	12	16	16	2	0
32	b	102	176	176	3	0
32	c	20	35	35	0	0
32	d	17	26	26	0	0
32	h	14	27	27	0	0
32	j	12	16	16	0	0
32	k	12	16	16	0	0
32	t	42	64	64	0	0
32	x	20	35	35	1	0
33	B	55	86	86	1	0
33	C	48	64	66	1	0
33	D	112	156	156	4	0
33	M	51	71	72	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	Y	48	66	66	1	0
33	b	55	85	86	4	0
33	c	134	179	181	0	0
33	d	44	56	58	0	0
33	m	51	71	72	0	0
34	E	43	32	32	6	0
34	V	43	30	31	5	0
34	e	43	32	32	7	0
34	v	43	30	30	2	0
35	A	132	0	0	3	0
35	B	174	0	0	7	0
35	C	139	0	0	2	0
35	D	116	0	0	3	0
35	E	26	0	0	1	0
35	F	4	0	0	0	0
35	H	16	0	0	1	0
35	I	14	0	0	1	0
35	J	9	0	0	0	0
35	K	7	0	0	0	0
35	L	9	0	0	0	0
35	M	5	0	0	0	0
35	O	78	0	0	3	0
35	R	1	0	0	0	0
35	T	9	0	0	0	0
35	U	34	0	0	1	0
35	V	53	0	0	0	0
35	X	12	0	0	0	0
35	Y	6	0	0	0	0
35	Z	1	0	0	0	0
35	a	109	0	0	3	0
35	b	134	0	0	5	0
35	c	130	0	0	8	0
35	d	91	0	0	0	0
35	e	15	0	0	0	0
35	f	8	0	0	0	0
35	h	26	0	0	2	0
35	i	7	0	0	0	0
35	j	9	0	0	2	0
35	k	6	0	0	1	0
35	l	10	0	0	0	0
35	m	3	0	0	0	0
35	o	81	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	r	7	0	0	0	0
35	t	11	0	0	0	0
35	u	43	0	0	3	0
35	v	37	0	0	0	0
35	x	4	0	0	0	0
35	y	2	0	0	0	0
35	z	4	0	0	1	0
All	All	51830	51555	51694	528	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 528 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	34:V:201:HEC:CAC	2.02	1.46
17:v:40:CYS:SG	34:v:201:HEC:CAC	2.05	1.45
17:V:40:CYS:SG	34:V:201:HEC:HAC	1.95	1.03
3:c:315:MET:SD	35:c:711:HOH:O	2.28	0.89
1:A:244:GLU:OE1	35:A:501:HOH:O	1.95	0.84

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	332/334 (99%)	325 (98%)	6 (2%)	1 (0%)	36 40
1	a	332/334 (99%)	326 (98%)	5 (2%)	1 (0%)	36 40
2	B	508/506 (100%)	497 (98%)	11 (2%)	0	100 100
2	b	503/506 (99%)	491 (98%)	12 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	442/461 (96%)	428 (97%)	13 (3%)	1 (0%)	43	50
3	c	451/461 (98%)	435 (96%)	15 (3%)	1 (0%)	43	50
4	D	339/352 (96%)	330 (97%)	9 (3%)	0	100	100
4	d	340/352 (97%)	328 (96%)	12 (4%)	0	100	100
5	E	81/84 (96%)	80 (99%)	1 (1%)	0	100	100
5	e	80/84 (95%)	80 (100%)	0	0	100	100
6	F	32/45 (71%)	32 (100%)	0	0	100	100
6	f	32/45 (71%)	29 (91%)	3 (9%)	0	100	100
7	H	63/66 (96%)	58 (92%)	5 (8%)	0	100	100
7	h	61/66 (92%)	57 (93%)	4 (7%)	0	100	100
8	I	34/38 (90%)	33 (97%)	1 (3%)	0	100	100
8	i	34/38 (90%)	32 (94%)	2 (6%)	0	100	100
9	J	34/40 (85%)	32 (94%)	1 (3%)	1 (3%)	3	1
9	j	34/40 (85%)	33 (97%)	1 (3%)	0	100	100
10	K	35/46 (76%)	32 (91%)	2 (6%)	1 (3%)	3	1
10	k	35/46 (76%)	34 (97%)	1 (3%)	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	34/37 (92%)	34 (100%)	0	0	100	100
12	M	31/36 (86%)	31 (100%)	0	0	100	100
12	m	30/36 (83%)	28 (93%)	2 (7%)	0	100	100
13	O	243/272 (89%)	228 (94%)	12 (5%)	3 (1%)	10	7
13	o	242/272 (89%)	231 (96%)	9 (4%)	2 (1%)	16	14
14	R	32/40 (80%)	28 (88%)	3 (9%)	1 (3%)	3	1
14	r	29/40 (72%)	26 (90%)	1 (3%)	2 (7%)	1	0
15	T	28/30 (93%)	28 (100%)	0	0	100	100
15	t	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
16	U	95/134 (71%)	91 (96%)	4 (4%)	0	100	100
16	u	95/134 (71%)	91 (96%)	2 (2%)	2 (2%)	5	2
17	V	135/163 (83%)	130 (96%)	4 (3%)	1 (1%)	18	17
17	v	135/163 (83%)	130 (96%)	5 (4%)	0	100	100
18	X	36/41 (88%)	34 (94%)	2 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	x	37/41 (90%)	37 (100%)	0	0	100	100
19	Y	25/46 (54%)	23 (92%)	1 (4%)	1 (4%)	2	1
19	y	28/46 (61%)	25 (89%)	3 (11%)	0	100	100
20	Z	60/62 (97%)	55 (92%)	5 (8%)	0	100	100
20	z	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	7	3
All	All	5240/5666 (92%)	5062 (97%)	159 (3%)	19 (0%)	30	31

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
13	O	59	LYS
13	O	62	GLU
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	270/270 (100%)	265 (98%)	5 (2%)	50	61
1	a	269/270 (100%)	258 (96%)	11 (4%)	27	33
2	B	408/404 (101%)	397 (97%)	11 (3%)	39	49
2	b	402/404 (100%)	391 (97%)	11 (3%)	39	49
3	C	346/362 (96%)	336 (97%)	10 (3%)	37	47
3	c	354/362 (98%)	336 (95%)	18 (5%)	21	23
4	D	276/283 (98%)	270 (98%)	6 (2%)	45	56
4	d	277/283 (98%)	264 (95%)	13 (5%)	23	26
5	E	72/73 (99%)	69 (96%)	3 (4%)	26	31
5	e	71/73 (97%)	66 (93%)	5 (7%)	14	13
6	F	28/39 (72%)	27 (96%)	1 (4%)	31	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	f	28/39 (72%)	25 (89%)	3 (11%)	6	4
7	H	54/55 (98%)	51 (94%)	3 (6%)	19	20
7	h	53/55 (96%)	48 (91%)	5 (9%)	8	6
8	I	32/34 (94%)	30 (94%)	2 (6%)	16	16
8	i	32/34 (94%)	31 (97%)	1 (3%)	35	44
9	J	24/28 (86%)	24 (100%)	0	100	100
9	j	24/28 (86%)	20 (83%)	4 (17%)	2	0
10	K	30/37 (81%)	26 (87%)	4 (13%)	4	2
10	k	30/37 (81%)	26 (87%)	4 (13%)	4	2
11	L	35/35 (100%)	34 (97%)	1 (3%)	37	47
11	l	34/35 (97%)	30 (88%)	4 (12%)	5	3
12	M	28/32 (88%)	28 (100%)	0	100	100
12	m	28/32 (88%)	26 (93%)	2 (7%)	13	12
13	O	206/228 (90%)	195 (95%)	11 (5%)	20	22
13	o	207/228 (91%)	200 (97%)	7 (3%)	32	40
14	R	28/32 (88%)	24 (86%)	4 (14%)	3	1
14	r	23/32 (72%)	17 (74%)	6 (26%)	0	0
15	T	26/26 (100%)	24 (92%)	2 (8%)	12	10
15	t	25/26 (96%)	23 (92%)	2 (8%)	11	9
16	U	84/112 (75%)	80 (95%)	4 (5%)	23	25
16	u	84/112 (75%)	81 (96%)	3 (4%)	31	39
17	V	117/138 (85%)	109 (93%)	8 (7%)	14	14
17	v	117/138 (85%)	113 (97%)	4 (3%)	32	40
18	X	31/34 (91%)	29 (94%)	2 (6%)	15	14
18	x	31/34 (91%)	29 (94%)	2 (6%)	15	14
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%)	43 (83%)	9 (17%)	2	0
20	z	51/52 (98%)	45 (88%)	6 (12%)	5	3
All	All	4328/4622 (94%)	4126 (95%)	202 (5%)	24	26

5 of 202 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	c	124	VAL
5	e	63	ILE
20	z	32	ASP
3	c	221	GLU
4	d	182	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
2	b	409	GLN
16	u	78	ASN
4	d	350	ASN
13	o	61	GLN
20	z	38	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	FME	i	1	8	8,9,10	0.90	0	8,9,11	1.39	2 (25%)
15	FME	t	1	15	8,9,10	1.20	1 (12%)	8,9,11	0.74	0
15	FME	T	1	15	8,9,10	0.90	0	8,9,11	1.04	0
8	FME	I	1	8	8,9,10	1.12	1 (12%)	8,9,11	0.87	0
12	FME	m	1	12	8,9,10	1.02	1 (12%)	8,9,11	0.62	0
12	FME	M	1	12	8,9,10	1.04	0	8,9,11	1.29	1 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	FME	i	1	8	-	1/7/9/11	-
15	FME	t	1	15	-	2/7/9/11	-
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	-
12	FME	M	1	12	-	1/7/9/11	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	t	1	FME	CA-N	-2.68	1.42	1.46
12	m	1	FME	CA-N	-2.13	1.43	1.46
8	I	1	FME	CA-N	-2.05	1.43	1.46

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	i	1	FME	CA-N-CN	-2.38	119.17	122.82
8	i	1	FME	CB-CA-N	2.31	114.73	110.52
12	M	1	FME	CB-CA-N	2.23	114.58	110.52

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	T	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
12	M	1	FME	CA-CB-CG-SD

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 189 ligands modelled in this entry, 6 are monoatomic - leaving 183 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
22	CLA	b	606	-	69,73,73	1.46	5 (7%)	82,113,113	1.50	6 (7%)
32	STE	a	414	-	11,11,19	0.94	0	11,11,19	1.04	0
22	CLA	C	513	-	69,73,73	1.60	6 (8%)	82,113,113	1.50	13 (15%)
29	SQD	B	623	-	52,54,54	0.96	2 (3%)	62,65,65	1.84	11 (17%)
23	PHO	a	404	-	58,69,69	1.91	12 (20%)	55,99,99	1.76	13 (23%)
22	CLA	C	503	-	69,73,73	1.27	9 (13%)	82,113,113	1.48	12 (14%)
32	STE	E	102	-	11,11,19	0.96	0	11,11,19	1.04	0
22	CLA	D	402	-	69,73,73	1.33	7 (10%)	82,113,113	1.39	10 (12%)
24	BCR	k	102	-	41,41,41	1.13	4 (9%)	56,56,56	1.22	7 (12%)
22	CLA	c	509	-	69,73,73	1.57	9 (13%)	82,113,113	1.35	6 (7%)
30	DGD	C	517	-	63,63,67	1.41	9 (14%)	77,77,81	1.35	7 (9%)
32	STE	B	621	-	16,16,19	0.81	1 (6%)	16,16,19	0.92	1 (6%)
22	CLA	b	609	-	69,73,73	1.49	9 (13%)	82,113,113	1.39	11 (13%)
33	LMG	d	410	-	44,44,55	1.03	4 (9%)	52,52,63	1.47	7 (13%)
34	HEC	E	101	6,5	46,50,50	1.89	9 (19%)	58,82,82	1.85	8 (13%)
22	CLA	c	513	-	69,73,73	1.27	10 (14%)	82,113,113	1.25	6 (7%)
32	STE	B	624	-	11,11,19	1.02	1 (9%)	11,11,19	0.88	0
33	LMG	b	622	-	55,55,55	1.43	7 (12%)	63,63,63	1.51	8 (12%)
29	SQD	a	413	-	35,35,54	1.20	2 (5%)	37,37,65	1.40	7 (18%)
28	LHG	B	622	-	48,48,48	1.07	4 (8%)	51,54,54	1.35	6 (11%)
28	LHG	l	101	-	48,48,48	0.79	0	51,54,54	1.28	4 (7%)
22	CLA	c	505	-	69,73,73	1.11	7 (10%)	82,113,113	1.28	7 (8%)
24	BCR	A	406	-	41,41,41	1.03	3 (7%)	56,56,56	1.51	10 (17%)
22	CLA	b	605	-	69,73,73	1.19	8 (11%)	82,113,113	1.43	13 (15%)
24	BCR	c	514	-	41,41,41	1.02	2 (4%)	56,56,56	1.37	9 (16%)
33	LMG	c	522	-	49,49,55	0.99	3 (6%)	57,57,63	1.37	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	BCR	C	501	-	41,41,41	1.05	3 (7%)	56,56,56	1.28	6 (10%)
24	BCR	B	620	-	41,41,41	1.24	2 (4%)	56,56,56	1.45	7 (12%)
24	BCR	d	405	-	41,41,41	1.20	2 (4%)	56,56,56	1.29	7 (12%)
22	CLA	c	501	-	69,73,73	1.28	7 (10%)	82,113,113	1.46	10 (12%)
30	DGD	h	101	-	63,63,67	1.21	9 (14%)	77,77,81	1.50	14 (18%)
22	CLA	B	605	-	69,73,73	1.31	7 (10%)	82,113,113	1.66	12 (14%)
30	DGD	C	518	-	63,63,67	1.39	10 (15%)	77,77,81	1.44	10 (12%)
28	LHG	A	411	-	46,46,48	1.08	3 (6%)	49,52,54	1.22	3 (6%)
22	CLA	C	512	3	69,73,73	1.36	10 (14%)	82,113,113	1.35	7 (8%)
22	CLA	C	508	35	69,73,73	1.09	5 (7%)	82,113,113	1.30	6 (7%)
32	STE	b	624	-	19,19,19	0.94	0	19,19,19	0.82	1 (5%)
22	CLA	b	603	-	69,73,73	1.27	10 (14%)	82,113,113	1.46	14 (17%)
24	BCR	H	101	-	41,41,41	1.13	1 (2%)	56,56,56	1.49	8 (14%)
33	LMG	Y	101	-	48,48,55	1.05	4 (8%)	56,56,63	1.37	7 (12%)
33	LMG	B	627	-	55,55,55	1.51	7 (12%)	63,63,63	1.61	9 (14%)
26	BCT	A	409	21	3,3,3	1.10	0	2,3,3	2.67	1 (50%)
22	CLA	B	616	-	69,73,73	1.20	6 (8%)	82,113,113	1.28	9 (10%)
22	CLA	B	607	-	69,73,73	1.53	6 (8%)	82,113,113	1.61	8 (9%)
32	STE	h	102	-	13,13,19	0.52	0	12,12,19	0.54	0
22	CLA	b	608	-	69,73,73	1.30	10 (14%)	82,113,113	1.13	7 (8%)
34	HEC	V	201	17	46,50,50	1.77	5 (10%)	58,82,82	2.30	12 (20%)
23	PHO	D	401	-	58,69,69	2.05	12 (20%)	55,99,99	1.43	10 (18%)
24	BCR	K	101	-	41,41,41	1.04	2 (4%)	56,56,56	1.27	4 (7%)
29	SQD	A	414	-	38,38,54	1.17	3 (7%)	40,40,65	1.36	4 (10%)
24	BCR	b	619	-	41,41,41	1.19	2 (4%)	56,56,56	1.38	11 (19%)
32	STE	M	104	-	17,17,19	0.44	0	16,16,19	0.84	0
22	CLA	B	617	-	64,68,73	1.37	9 (14%)	76,107,113	1.66	9 (11%)
27	PL9	D	406	-	55,55,55	1.66	7 (12%)	68,69,69	1.77	16 (23%)
32	STE	j	101	-	11,11,19	1.09	0	11,11,19	0.79	0
22	CLA	C	510	-	69,73,73	1.11	8 (11%)	82,113,113	1.32	9 (10%)
22	CLA	b	602	-	69,73,73	1.29	9 (13%)	82,113,113	1.48	9 (10%)
33	LMG	C	516	-	48,48,55	0.96	2 (4%)	56,56,63	1.27	6 (10%)
32	STE	t	102	-	13,13,19	0.69	0	13,13,19	1.29	1 (7%)
22	CLA	b	614	-	69,73,73	1.53	12 (17%)	82,113,113	1.34	10 (12%)
22	CLA	b	615	-	69,73,73	1.60	9 (13%)	82,113,113	1.32	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	STE	t	104	-	17,17,19	0.75	0	17,17,19	1.15	1 (5%)
30	DGD	H	102	-	63,63,67	1.49	14 (22%)	77,77,81	1.42	11 (14%)
24	BCR	x	101	-	41,41,41	1.13	2 (4%)	56,56,56	1.28	8 (14%)
27	PL9	A	410	-	55,55,55	1.20	3 (5%)	68,69,69	1.44	12 (17%)
22	CLA	D	403	35	69,73,73	1.09	3 (4%)	82,113,113	1.27	5 (6%)
22	CLA	b	610	35	69,73,73	1.31	8 (11%)	82,113,113	1.34	12 (14%)
33	LMG	m	101	-	51,51,55	1.18	6 (11%)	59,59,63	1.49	9 (15%)
22	CLA	C	505	35	63,67,73	1.31	11 (17%)	74,105,113	1.34	7 (9%)
22	CLA	A	405	-	58,62,73	1.74	10 (17%)	68,99,113	1.38	12 (17%)
24	BCR	B	618	-	41,41,41	1.31	3 (7%)	56,56,56	1.32	9 (16%)
22	CLA	c	512	-	69,73,73	1.24	9 (13%)	82,113,113	1.46	11 (13%)
22	CLA	B	611	35	69,73,73	1.39	8 (11%)	82,113,113	1.32	9 (10%)
22	CLA	c	508	-	68,72,73	1.58	11 (16%)	80,111,113	1.37	8 (10%)
29	SQD	L	101	-	47,49,54	0.97	2 (4%)	57,60,65	2.25	15 (26%)
30	DGD	c	516	-	63,63,67	1.16	6 (9%)	77,77,81	1.40	9 (11%)
22	CLA	B	602	35	69,73,73	1.73	11 (15%)	82,113,113	1.30	5 (6%)
22	CLA	d	402	-	69,73,73	1.36	9 (13%)	82,113,113	1.40	9 (10%)
32	STE	b	621	-	19,19,19	0.79	1 (5%)	19,19,19	1.05	2 (10%)
32	STE	k	101	-	11,11,19	0.84	0	11,11,19	0.87	0
22	CLA	B	610	-	69,73,73	1.33	10 (14%)	82,113,113	1.28	9 (10%)
28	LHG	d	408	-	48,48,48	0.75	1 (2%)	51,54,54	1.21	4 (7%)
22	CLA	b	607	35	69,73,73	1.21	6 (8%)	82,113,113	1.40	8 (9%)
22	CLA	B	604	-	69,73,73	1.74	8 (11%)	82,113,113	1.37	12 (14%)
32	STE	C	522	-	11,11,19	0.87	0	11,11,19	0.83	0
28	LHG	a	412	-	41,41,48	1.08	4 (9%)	44,47,54	1.32	3 (6%)
24	BCR	k	103	-	41,41,41	1.02	2 (4%)	56,56,56	1.30	6 (10%)
32	STE	b	623	-	15,15,19	0.79	0	15,15,19	0.86	0
32	STE	H	103	-	17,17,19	0.58	0	16,16,19	0.53	0
32	STE	b	626	-	19,19,19	0.74	0	19,19,19	1.12	0
33	LMG	D	410	-	26,26,55	1.08	1 (3%)	26,26,63	1.13	1 (3%)
22	CLA	B	613	-	69,73,73	1.05	5 (7%)	82,113,113	1.40	10 (12%)
32	STE	C	521	-	15,15,19	0.71	0	14,14,19	0.40	0
31	OEX	A	416	3,35,1	0,15,15	-	-	-	-	-
24	BCR	Z	101	-	41,41,41	1.10	2 (4%)	56,56,56	1.47	11 (19%)
32	STE	L	103	-	11,11,19	0.81	0	11,11,19	1.25	1 (9%)
32	STE	b	620	-	15,15,19	0.65	0	14,14,19	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	SQD	a	411	-	52,54,54	0.95	5 (9%)	62,65,65	1.87	14 (22%)
33	LMG	D	409	-	31,31,55	1.08	4 (12%)	33,33,63	1.09	0
23	PHO	A	404	-	58,69,69	1.92	11 (18%)	55,99,99	1.58	10 (18%)
30	DGD	c	517	-	63,63,67	1.19	7 (11%)	77,77,81	1.37	9 (11%)
24	BCR	B	619	-	41,41,41	1.11	2 (4%)	56,56,56	1.27	9 (16%)
24	BCR	a	406	-	41,41,41	1.05	3 (7%)	56,56,56	1.16	4 (7%)
22	CLA	C	506	-	69,73,73	1.36	8 (11%)	82,113,113	1.29	8 (9%)
22	CLA	d	404	-	69,73,73	1.33	10 (14%)	82,113,113	1.25	10 (12%)
22	CLA	b	616	-	64,68,73	1.17	5 (7%)	76,107,113	1.39	9 (11%)
30	DGD	c	518	-	63,63,67	1.22	6 (9%)	77,77,81	1.40	9 (11%)
22	CLA	b	601	35	69,73,73	1.53	10 (14%)	82,113,113	1.35	7 (8%)
33	LMG	c	519	-	37,37,55	1.18	4 (10%)	45,45,63	1.32	6 (13%)
24	BCR	t	101	-	41,41,41	1.21	2 (4%)	56,56,56	1.29	5 (8%)
22	CLA	C	507	-	69,73,73	1.14	4 (5%)	82,113,113	1.11	7 (8%)
24	BCR	C	515	-	41,41,41	1.27	5 (12%)	56,56,56	1.36	6 (10%)
22	CLA	B	612	-	69,73,73	1.21	9 (13%)	82,113,113	1.38	8 (9%)
22	CLA	B	609	-	69,73,73	1.45	8 (11%)	82,113,113	1.43	13 (15%)
32	STE	B	625	-	15,15,19	0.60	0	14,14,19	0.48	0
23	PHO	d	401	-	58,69,69	2.05	12 (20%)	55,99,99	1.68	12 (21%)
32	STE	B	601	-	11,11,19	0.82	0	11,11,19	1.31	1 (9%)
32	STE	Z	102	-	7,7,19	0.53	0	6,6,19	0.56	0
30	DGD	C	519	-	63,63,67	1.16	6 (9%)	77,77,81	1.35	10 (12%)
22	CLA	C	502	-	69,73,73	1.59	11 (15%)	82,113,113	1.33	13 (15%)
32	STE	C	520	-	11,11,19	0.79	0	11,11,19	1.37	2 (18%)
22	CLA	c	504	35	64,68,73	1.24	11 (17%)	76,107,113	1.32	8 (10%)
27	PL9	d	406	-	55,55,55	1.63	9 (16%)	68,69,69	1.77	15 (22%)
22	CLA	C	511	-	69,73,73	1.46	11 (15%)	82,113,113	1.39	8 (9%)
28	LHG	L	102	-	48,48,48	0.90	2 (4%)	51,54,54	1.25	3 (5%)
22	CLA	A	403	35	69,73,73	1.32	9 (13%)	82,113,113	1.15	6 (7%)
28	LHG	D	408	-	48,48,48	0.81	1 (2%)	51,54,54	1.36	6 (11%)
32	STE	J	101	-	11,11,19	0.69	0	11,11,19	1.32	2 (18%)
32	STE	d	411	-	16,16,19	0.79	0	16,16,19	1.01	1 (6%)
29	SQD	f	101	-	39,41,54	1.12	3 (7%)	49,52,65	1.85	11 (22%)
32	STE	D	411	-	19,19,19	0.77	1 (5%)	19,19,19	1.26	3 (15%)
33	LMG	c	521	-	48,48,55	1.17	4 (8%)	56,56,63	1.25	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	c	506	-	69,73,73	1.23	9 (13%)	82,113,113	1.18	7 (8%)
22	CLA	a	402	-	69,73,73	1.41	11 (15%)	82,113,113	1.25	8 (9%)
24	BCR	b	618	-	41,41,41	1.29	3 (7%)	56,56,56	1.32	9 (16%)
22	CLA	b	611	-	69,73,73	1.20	9 (13%)	82,113,113	1.51	13 (15%)
32	STE	B	626	-	14,14,19	0.59	0	13,13,19	0.40	0
33	LMG	D	407	-	51,51,55	1.14	4 (7%)	59,59,63	1.31	6 (10%)
22	CLA	c	503	-	69,73,73	1.28	7 (10%)	82,113,113	1.55	9 (10%)
27	PL9	a	410	-	55,55,55	0.94	3 (5%)	68,69,69	1.58	11 (16%)
28	LHG	A	413	-	48,48,48	1.12	5 (10%)	51,54,54	1.26	6 (11%)
22	CLA	B	615	-	69,73,73	1.52	8 (11%)	82,113,113	1.45	8 (9%)
22	CLA	b	604	-	69,73,73	1.19	7 (10%)	82,113,113	1.56	13 (15%)
22	CLA	a	403	35	69,73,73	1.27	7 (10%)	82,113,113	1.43	15 (18%)
32	STE	M	102	-	14,14,19	0.80	0	14,14,19	0.95	0
29	SQD	A	412	-	50,52,54	1.08	4 (8%)	60,63,65	1.95	13 (21%)
22	CLA	c	507	35	69,73,73	1.26	8 (11%)	82,113,113	1.40	8 (9%)
22	CLA	C	504	-	69,73,73	1.52	10 (14%)	82,113,113	1.79	12 (14%)
22	CLA	d	403	35	69,73,73	1.28	11 (15%)	82,113,113	1.40	10 (12%)
24	BCR	c	515	-	41,41,41	1.12	4 (9%)	56,56,56	1.40	7 (12%)
24	BCR	T	101	-	41,41,41	1.19	4 (9%)	56,56,56	1.31	4 (7%)
24	BCR	D	405	-	41,41,41	1.17	3 (7%)	56,56,56	1.22	6 (10%)
22	CLA	A	402	-	69,73,73	1.49	10 (14%)	82,113,113	1.17	6 (7%)
30	DGD	A	415	-	67,67,67	1.34	8 (11%)	81,81,81	1.40	14 (17%)
32	STE	M	103	-	9,9,19	0.47	0	8,8,19	0.74	0
22	CLA	b	613	-	69,73,73	1.28	10 (14%)	82,113,113	1.41	11 (13%)
28	LHG	d	409	-	38,38,48	0.95	1 (2%)	41,44,54	1.29	3 (7%)
22	CLA	C	509	-	69,73,73	1.44	10 (14%)	82,113,113	1.34	10 (12%)
32	STE	x	102	-	19,19,19	0.73	0	19,19,19	0.80	1 (5%)
31	OEX	a	415	3,35,1	0,15,15	-	-	-	-	-
22	CLA	c	502	-	69,73,73	1.21	8 (11%)	82,113,113	1.25	9 (10%)
32	STE	c	520	-	19,19,19	0.77	0	19,19,19	1.01	1 (5%)
32	STE	t	103	-	9,9,19	0.54	0	8,8,19	0.47	0
34	HEC	v	201	17	46,50,50	1.79	6 (13%)	58,82,82	2.04	9 (15%)
22	CLA	B	606	-	69,73,73	1.26	8 (11%)	82,113,113	1.34	9 (10%)
22	CLA	c	511	3	69,73,73	1.78	11 (15%)	82,113,113	1.41	7 (8%)
22	CLA	D	404	-	69,73,73	1.57	6 (8%)	82,113,113	1.43	15 (18%)
29	SQD	F	101	-	34,36,54	1.04	2 (5%)	42,45,65	1.76	9 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	B	608	35	69,73,73	1.28	9 (13%)	82,113,113	1.51	10 (12%)
22	CLA	c	510	-	69,73,73	1.44	10 (14%)	82,113,113	1.39	8 (9%)
32	STE	I	101	-	14,14,19	0.65	0	13,13,19	0.44	0
22	CLA	C	514	-	69,73,73	1.31	8 (11%)	82,113,113	1.42	8 (9%)
22	CLA	B	603	-	69,73,73	1.31	10 (14%)	82,113,113	1.27	11 (13%)
22	CLA	a	405	-	69,73,73	1.46	12 (17%)	82,113,113	1.39	8 (9%)
34	HEC	e	101	6,5	46,50,50	1.83	6 (13%)	58,82,82	1.90	9 (15%)
33	LMG	M	101	-	51,51,55	0.99	4 (7%)	59,59,63	1.43	8 (13%)
32	STE	T	102	-	14,14,19	0.45	0	13,13,19	0.78	0
28	LHG	d	407	-	48,48,48	1.08	4 (8%)	51,54,54	1.32	5 (9%)
24	BCR	b	617	-	41,41,41	1.19	3 (7%)	56,56,56	1.48	8 (14%)
22	CLA	B	614	-	69,73,73	1.35	8 (11%)	82,113,113	1.37	9 (10%)
22	CLA	b	612	-	69,73,73	1.10	7 (10%)	82,113,113	1.22	8 (9%)
26	BCT	a	409	21	3,3,3	1.35	0	2,3,3	4.10	2 (100%)
32	STE	b	625	-	9,9,19	0.56	0	8,8,19	0.52	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
22	CLA	b	606	-	1/1/20/20	8/39/115/115	-
32	STE	a	414	-	-	3/9/9/17	-
22	CLA	C	513	-	1/1/20/20	20/39/115/115	-
29	SQD	B	623	-	-	20/49/69/69	0/1/1/1
23	PHO	a	404	-	-	6/37/103/103	0/5/6/6
22	CLA	C	503	-	1/1/20/20	7/39/115/115	-
32	STE	E	102	-	-	5/9/9/17	-
22	CLA	D	402	-	1/1/20/20	5/39/115/115	-
24	BCR	k	102	-	-	9/29/63/63	0/2/2/2
22	CLA	c	509	-	1/1/20/20	14/39/115/115	-
30	DGD	C	517	-	-	22/51/91/95	0/2/2/2
32	STE	B	621	-	-	6/14/14/17	-
22	CLA	b	609	-	1/1/20/20	4/39/115/115	-
33	LMG	d	410	-	-	14/39/59/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	HEC	E	101	6,5	-	6/14/54/54	-
22	CLA	c	513	-	1/1/20/20	10/39/115/115	-
32	STE	B	624	-	-	5/9/9/17	-
33	LMG	b	622	-	-	28/50/70/70	0/1/1/1
29	SQD	a	413	-	-	12/37/37/69	-
28	LHG	B	622	-	-	20/53/53/53	-
28	LHG	l	101	-	-	20/53/53/53	-
22	CLA	c	505	-	1/1/20/20	13/39/115/115	-
24	BCR	A	406	-	-	11/29/63/63	0/2/2/2
22	CLA	b	605	-	1/1/20/20	10/39/115/115	-
24	BCR	c	514	-	-	15/29/63/63	0/2/2/2
33	LMG	c	522	-	-	16/44/64/70	0/1/1/1
24	BCR	C	501	-	-	7/29/63/63	0/2/2/2
24	BCR	B	620	-	-	4/29/63/63	0/2/2/2
24	BCR	d	405	-	-	6/29/63/63	0/2/2/2
22	CLA	c	501	-	1/1/20/20	3/39/115/115	-
30	DGD	h	101	-	-	17/51/91/95	0/2/2/2
22	CLA	B	605	-	1/1/20/20	7/39/115/115	-
30	DGD	C	518	-	-	20/51/91/95	0/2/2/2
28	LHG	A	411	-	-	23/51/51/53	-
22	CLA	C	512	3	1/1/20/20	4/39/115/115	-
22	CLA	C	508	35	1/1/20/20	7/39/115/115	-
32	STE	b	624	-	-	7/17/17/17	-
22	CLA	b	603	-	1/1/20/20	10/39/115/115	-
24	BCR	H	101	-	-	6/29/63/63	0/2/2/2
33	LMG	Y	101	-	-	20/43/63/70	0/1/1/1
33	LMG	B	627	-	-	29/50/70/70	0/1/1/1
22	CLA	B	616	-	1/1/20/20	8/39/115/115	-
22	CLA	B	607	-	1/1/20/20	9/39/115/115	-
32	STE	h	102	-	-	7/11/11/17	-
22	CLA	b	608	-	-	4/39/115/115	-
34	HEC	V	201	17	-	6/14/54/54	-
23	PHO	D	401	-	-	4/37/103/103	0/5/6/6
24	BCR	K	101	-	-	12/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	SQD	A	414	-	-	15/39/39/69	-
24	BCR	b	619	-	-	11/29/63/63	0/2/2/2
32	STE	M	104	-	-	8/15/15/17	-
22	CLA	B	617	-	1/1/19/20	8/33/109/115	-
27	PL9	D	406	-	-	7/53/73/73	0/1/1/1
32	STE	j	101	-	-	1/9/9/17	-
22	CLA	C	510	-	1/1/20/20	18/39/115/115	-
22	CLA	b	602	-	1/1/20/20	11/39/115/115	-
33	LMG	C	516	-	-	23/43/63/70	0/1/1/1
32	STE	t	102	-	-	5/11/11/17	-
22	CLA	b	614	-	1/1/20/20	18/39/115/115	-
22	CLA	b	615	-	1/1/20/20	8/39/115/115	-
32	STE	t	104	-	-	8/15/15/17	-
30	DGD	H	102	-	-	18/51/91/95	0/2/2/2
24	BCR	x	101	-	-	4/29/63/63	0/2/2/2
27	PL9	A	410	-	-	25/53/73/73	0/1/1/1
22	CLA	D	403	35	1/1/20/20	5/39/115/115	-
22	CLA	b	610	35	1/1/20/20	5/39/115/115	-
33	LMG	m	101	-	-	21/46/66/70	0/1/1/1
22	CLA	C	505	35	1/1/18/20	9/32/108/115	-
22	CLA	A	405	-	1/1/17/20	4/26/102/115	-
24	BCR	B	618	-	-	6/29/63/63	0/2/2/2
22	CLA	c	512	-	1/1/20/20	24/39/115/115	-
22	CLA	B	611	35	1/1/20/20	4/39/115/115	-
22	CLA	c	508	-	1/1/19/20	16/38/114/115	-
29	SQD	L	101	-	-	21/44/64/69	0/1/1/1
30	DGD	c	516	-	-	20/51/91/95	0/2/2/2
22	CLA	B	602	35	1/1/20/20	20/39/115/115	-
22	CLA	d	402	-	-	6/39/115/115	-
32	STE	b	621	-	-	7/17/17/17	-
32	STE	k	101	-	-	3/9/9/17	-
22	CLA	B	610	-	-	3/39/115/115	-
28	LHG	d	408	-	-	20/53/53/53	-
22	CLA	b	607	35	1/1/20/20	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	B	604	-	1/1/20/20	11/39/115/115	-
32	STE	C	522	-	-	3/9/9/17	-
28	LHG	a	412	-	-	25/46/46/53	-
24	BCR	k	103	-	-	5/29/63/63	0/2/2/2
32	STE	b	623	-	-	5/13/13/17	-
32	STE	H	103	-	-	10/15/15/17	-
32	STE	b	626	-	-	7/17/17/17	-
33	LMG	D	410	-	-	8/22/22/70	-
22	CLA	B	613	-	1/1/20/20	5/39/115/115	-
32	STE	C	521	-	-	5/13/13/17	-
24	BCR	Z	101	-	-	8/29/63/63	0/2/2/2
32	STE	L	103	-	-	5/9/9/17	-
32	STE	b	620	-	-	6/13/13/17	-
29	SQD	a	411	-	-	21/49/69/69	0/1/1/1
33	LMG	D	409	-	-	16/33/33/70	-
23	PHO	A	404	-	-	2/37/103/103	0/5/6/6
30	DGD	c	517	-	-	17/51/91/95	0/2/2/2
24	BCR	B	619	-	-	9/29/63/63	0/2/2/2
24	BCR	a	406	-	-	5/29/63/63	0/2/2/2
22	CLA	C	506	-	1/1/20/20	8/39/115/115	-
22	CLA	d	404	-	-	5/39/115/115	-
22	CLA	b	616	-	1/1/19/20	8/33/109/115	-
30	DGD	c	518	-	-	19/51/91/95	0/2/2/2
22	CLA	b	601	35	1/1/20/20	16/39/115/115	-
33	LMG	c	519	-	-	7/31/51/70	0/1/1/1
24	BCR	t	101	-	-	8/29/63/63	0/2/2/2
22	CLA	C	507	-	1/1/20/20	11/39/115/115	-
24	BCR	C	515	-	-	7/29/63/63	0/2/2/2
22	CLA	B	612	-	1/1/20/20	7/39/115/115	-
22	CLA	B	609	-	-	5/39/115/115	-
32	STE	B	625	-	-	6/13/13/17	-
23	PHO	d	401	-	-	5/37/103/103	0/5/6/6
32	STE	B	601	-	-	2/9/9/17	-
32	STE	Z	102	-	-	3/5/5/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	DGD	C	519	-	-	12/51/91/95	0/2/2/2
22	CLA	C	502	-	1/1/20/20	3/39/115/115	-
32	STE	C	520	-	-	4/9/9/17	-
22	CLA	c	504	35	1/1/19/20	6/33/109/115	-
27	PL9	d	406	-	-	17/53/73/73	0/1/1/1
22	CLA	C	511	-	1/1/20/20	11/39/115/115	-
28	LHG	L	102	-	-	20/53/53/53	-
22	CLA	A	403	35	1/1/20/20	2/39/115/115	-
28	LHG	D	408	-	-	16/53/53/53	-
32	STE	J	101	-	-	8/9/9/17	-
32	STE	d	411	-	-	8/14/14/17	-
29	SQD	f	101	-	-	12/36/56/69	0/1/1/1
32	STE	D	411	-	-	11/17/17/17	-
33	LMG	c	521	-	-	23/43/63/70	0/1/1/1
22	CLA	c	506	-	1/1/20/20	18/39/115/115	-
22	CLA	a	402	-	1/1/20/20	3/39/115/115	-
24	BCR	b	618	-	-	1/29/63/63	0/2/2/2
22	CLA	b	611	-	1/1/20/20	6/39/115/115	-
32	STE	B	626	-	-	11/12/12/17	-
33	LMG	D	407	-	-	15/46/66/70	0/1/1/1
22	CLA	c	503	-	1/1/20/20	11/39/115/115	-
27	PL9	a	410	-	-	25/53/73/73	0/1/1/1
28	LHG	A	413	-	-	29/53/53/53	-
22	CLA	B	615	-	1/1/20/20	12/39/115/115	-
22	CLA	b	604	-	1/1/20/20	4/39/115/115	-
22	CLA	a	403	35	-	14/39/115/115	-
32	STE	M	102	-	-	5/12/12/17	-
29	SQD	A	412	-	-	18/47/67/69	0/1/1/1
22	CLA	c	507	35	1/1/20/20	14/39/115/115	-
22	CLA	C	504	-	1/1/20/20	3/39/115/115	-
22	CLA	d	403	35	1/1/20/20	9/39/115/115	-
24	BCR	c	515	-	-	5/29/63/63	0/2/2/2
24	BCR	T	101	-	-	10/29/63/63	0/2/2/2
24	BCR	D	405	-	-	5/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	A	402	-	1/1/20/20	2/39/115/115	-
30	DGD	A	415	-	-	27/55/95/95	0/2/2/2
32	STE	M	103	-	-	3/7/7/17	-
22	CLA	b	613	-	1/1/20/20	6/39/115/115	-
28	LHG	d	409	-	-	12/43/43/53	-
22	CLA	C	509	-	1/1/20/20	3/39/115/115	-
32	STE	x	102	-	-	14/17/17/17	-
22	CLA	c	502	-	1/1/20/20	6/39/115/115	-
32	STE	c	520	-	-	7/17/17/17	-
32	STE	t	103	-	-	5/7/7/17	-
34	HEC	v	201	17	-	6/14/54/54	-
22	CLA	B	606	-	1/1/20/20	10/39/115/115	-
22	CLA	c	511	3	1/1/20/20	14/39/115/115	-
22	CLA	D	404	-	1/1/20/20	9/39/115/115	-
29	SQD	F	101	-	-	10/28/48/69	0/1/1/1
22	CLA	B	608	35	1/1/20/20	5/39/115/115	-
22	CLA	c	510	-	1/1/20/20	12/39/115/115	-
32	STE	I	101	-	-	6/12/12/17	-
22	CLA	C	514	-	-	13/39/115/115	-
22	CLA	B	603	-	1/1/20/20	9/39/115/115	-
22	CLA	a	405	-	1/1/20/20	8/39/115/115	-
34	HEC	e	101	6,5	-	3/14/54/54	-
33	LMG	M	101	-	-	23/46/66/70	0/1/1/1
32	STE	T	102	-	-	8/12/12/17	-
28	LHG	d	407	-	-	18/53/53/53	-
24	BCR	b	617	-	-	6/29/63/63	0/2/2/2
22	CLA	B	614	-	1/1/20/20	16/39/115/115	-
22	CLA	b	612	-	1/1/20/20	10/39/115/115	-
32	STE	b	625	-	-	3/7/7/17	-

The worst 5 of 932 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	401	PHO	C1B-C2B	9.12	1.49	1.39
22	B	607	CLA	MG-NA	8.88	2.27	2.06
22	B	604	CLA	MG-ND	8.83	2.23	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	405	CLA	MG-NB	-8.54	1.88	2.05
22	D	404	CLA	MG-NB	-8.49	1.89	2.05

The worst 5 of 1266 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	V	201	HEC	CBB-CAB-C3B	-11.30	104.85	127.43
22	C	504	CLA	C4A-NA-C1A	10.72	111.57	106.68
34	v	201	HEC	CBB-CAB-C3B	-10.00	107.45	127.43
22	B	617	CLA	C4A-NA-C1A	9.84	111.17	106.68
29	L	101	SQD	O6-C1-C2	9.63	122.90	108.27

5 of 63 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	A	402	CLA	ND
22	A	403	CLA	ND
22	A	405	CLA	ND
22	B	602	CLA	ND
22	B	603	CLA	ND

5 of 1858 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	B	602	CLA	C1A-C2A-CAA-CBA
22	B	602	CLA	C3A-C2A-CAA-CBA
22	B	602	CLA	CAD-CBD-CGD-O1D
22	B	602	CLA	CAD-CBD-CGD-O2D
22	B	615	CLA	CAD-CBD-CGD-O1D

There are no ring outliers.

115 monomers are involved in 190 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	b	606	CLA	3	0
32	a	414	STE	2	0
22	C	513	CLA	3	0
23	a	404	PHO	3	0
22	C	503	CLA	3	0
22	D	402	CLA	3	0
24	k	102	BCR	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	c	509	CLA	2	0
32	B	621	STE	1	0
22	b	609	CLA	3	0
34	E	101	HEC	6	0
22	c	513	CLA	1	0
33	b	622	LMG	4	0
29	a	413	SQD	1	0
28	B	622	LHG	3	0
28	l	101	LHG	1	0
22	c	505	CLA	1	0
24	A	406	BCR	1	0
22	b	605	CLA	3	0
24	B	620	BCR	1	0
24	d	405	BCR	3	0
22	c	501	CLA	2	0
22	B	605	CLA	4	0
30	C	518	DGD	2	0
22	C	512	CLA	2	0
32	b	624	STE	1	0
22	b	603	CLA	1	0
24	H	101	BCR	4	0
33	Y	101	LMG	1	0
33	B	627	LMG	1	0
22	B	616	CLA	4	0
22	B	607	CLA	1	0
34	V	201	HEC	5	0
23	D	401	PHO	2	0
24	K	101	BCR	1	0
24	b	619	BCR	1	0
32	M	104	STE	1	0
22	B	617	CLA	1	0
27	D	406	PL9	1	0
22	C	510	CLA	2	0
22	b	602	CLA	2	0
33	C	516	LMG	1	0
22	b	615	CLA	2	0
24	x	101	BCR	1	0
27	A	410	PL9	3	0
22	D	403	CLA	2	0
22	b	610	CLA	1	0
24	B	618	BCR	1	0
22	c	512	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	c	508	CLA	4	0
29	L	101	SQD	1	0
22	B	602	CLA	1	0
22	d	402	CLA	1	0
22	B	610	CLA	1	0
28	d	408	LHG	2	0
22	b	607	CLA	1	0
22	B	604	CLA	1	0
24	k	103	BCR	1	0
32	b	623	STE	1	0
32	H	103	STE	1	0
22	B	613	CLA	1	0
24	Z	101	BCR	3	0
29	a	411	SQD	1	0
33	D	409	LMG	2	0
30	c	517	DGD	1	0
24	B	619	BCR	4	0
24	a	406	BCR	1	0
22	C	506	CLA	1	0
22	b	616	CLA	1	0
30	c	518	DGD	1	0
24	t	101	BCR	4	0
24	C	515	BCR	3	0
22	B	612	CLA	1	0
23	d	401	PHO	4	0
30	C	519	DGD	1	0
22	c	504	CLA	1	0
27	d	406	PL9	1	0
28	L	102	LHG	1	0
22	A	403	CLA	1	0
28	D	408	LHG	1	0
32	J	101	STE	1	0
32	D	411	STE	1	0
22	c	506	CLA	1	0
22	a	402	CLA	1	0
24	b	618	BCR	3	0
33	D	407	LMG	2	0
22	c	503	CLA	2	0
27	a	410	PL9	1	0
28	A	413	LHG	1	0
22	b	604	CLA	3	0
22	a	403	CLA	1	0

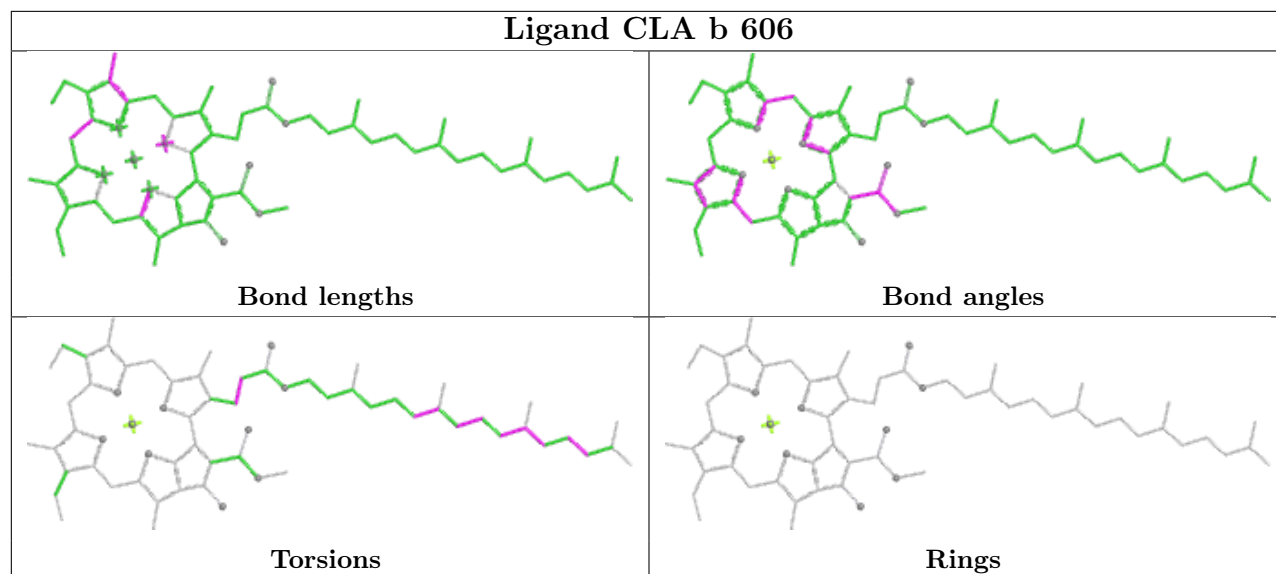
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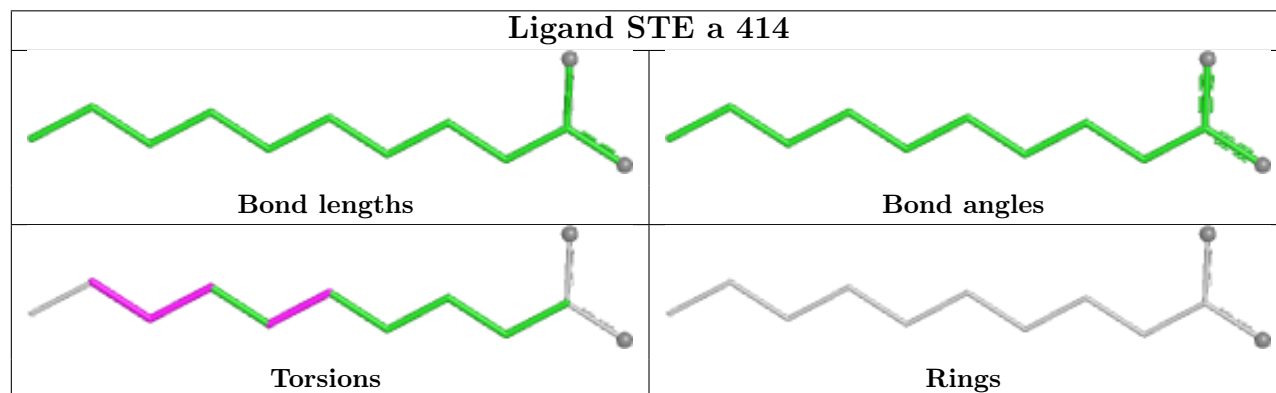
Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	A	412	SQD	1	0
22	c	507	CLA	2	0
24	c	515	BCR	4	0
24	T	101	BCR	1	0
24	D	405	BCR	3	0
22	A	402	CLA	3	0
30	A	415	DGD	4	0
22	C	509	CLA	1	0
32	x	102	STE	1	0
31	a	415	OEX	1	0
34	v	201	HEC	2	0
22	B	606	CLA	3	0
22	c	511	CLA	3	0
22	D	404	CLA	1	0
22	B	608	CLA	1	0
22	c	510	CLA	5	0
32	I	101	STE	2	0
22	B	603	CLA	1	0
22	a	405	CLA	1	0
34	e	101	HEC	7	0
28	d	407	LHG	2	0
24	b	617	BCR	1	0
22	B	614	CLA	2	0
32	b	625	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.

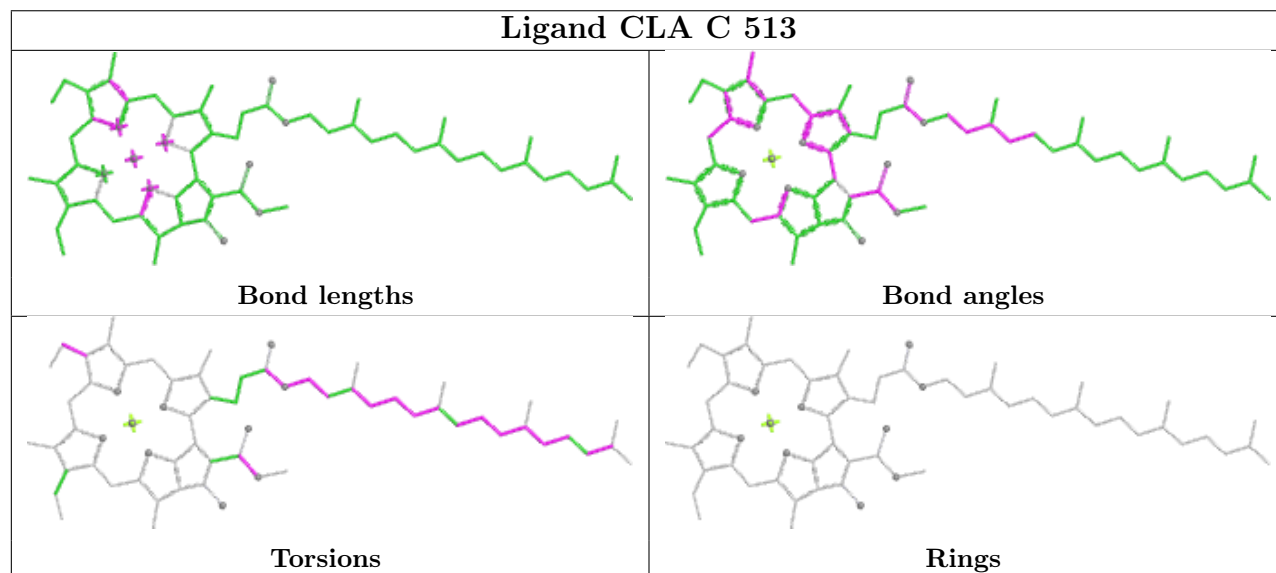
Ligand CLA b 606

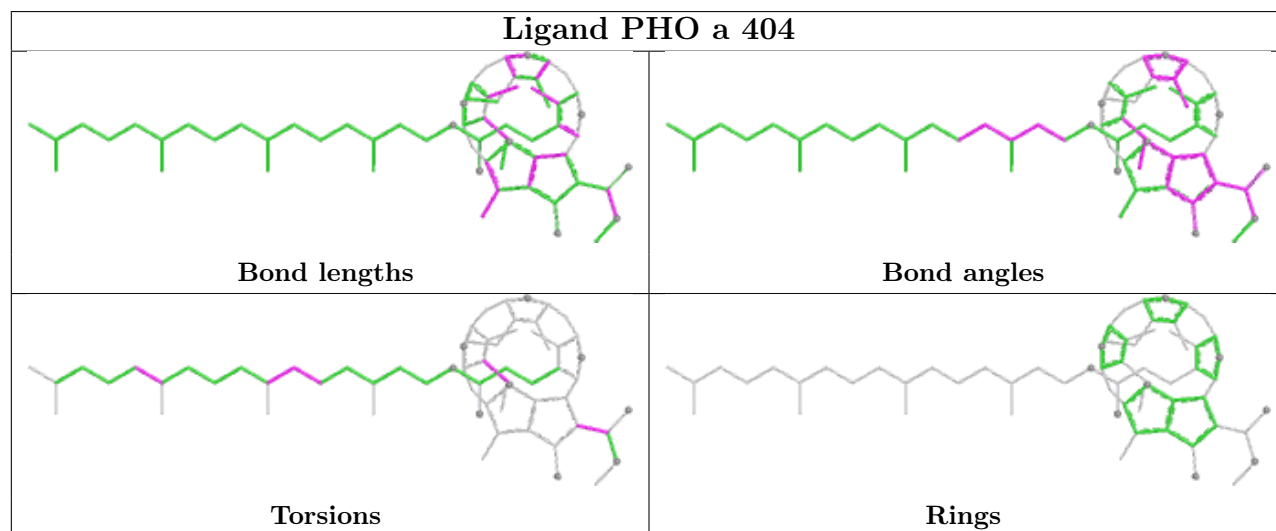
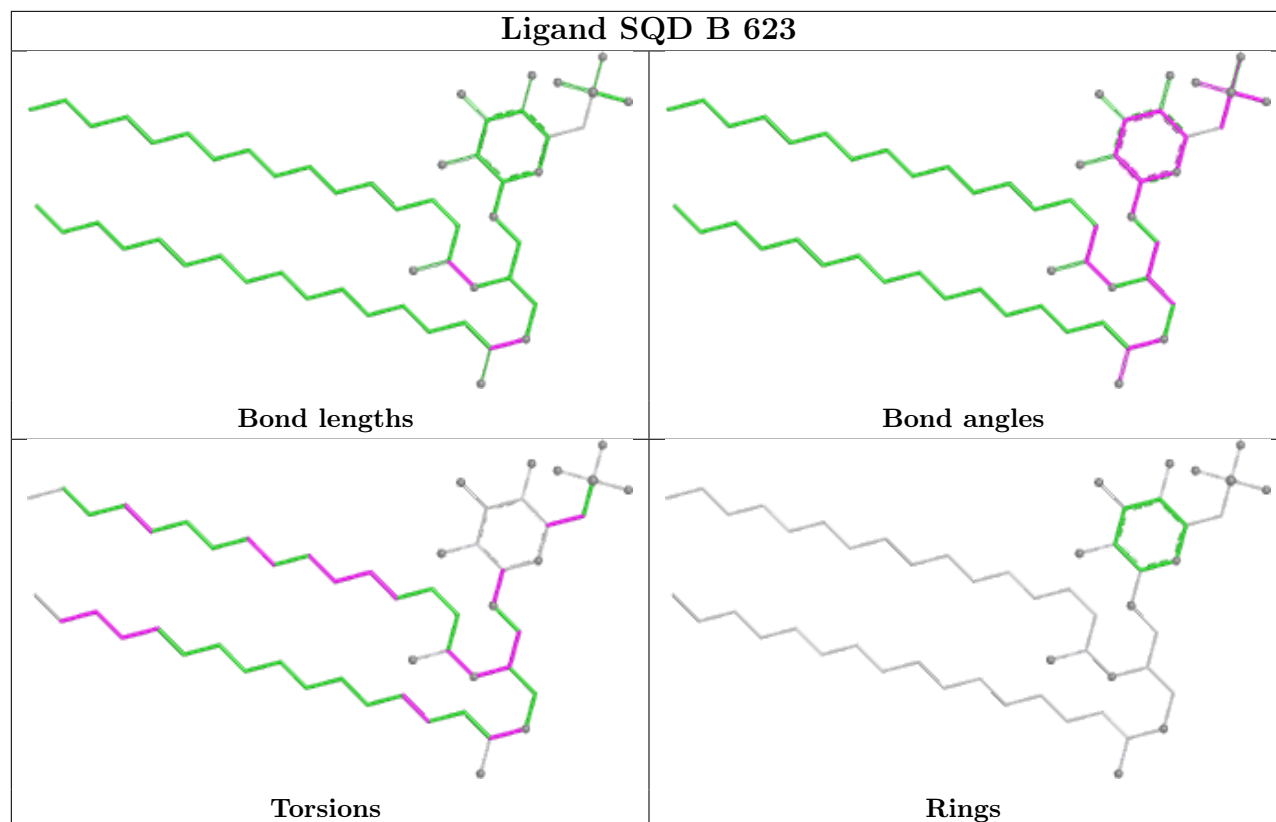


Ligand STE a 414

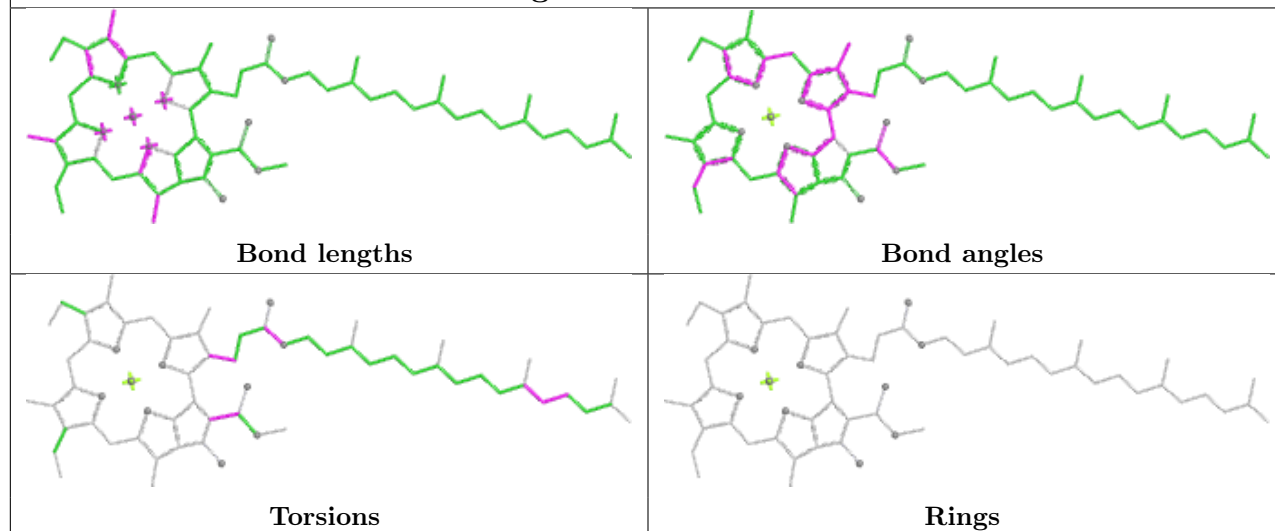


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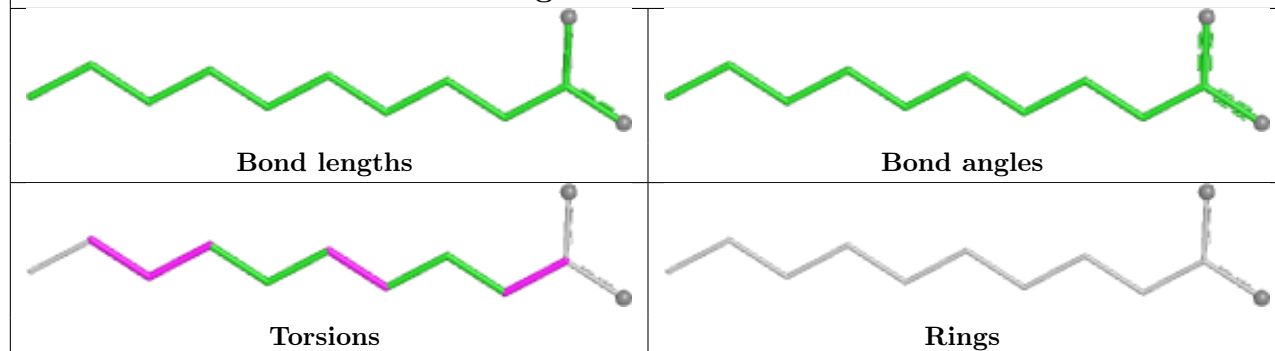




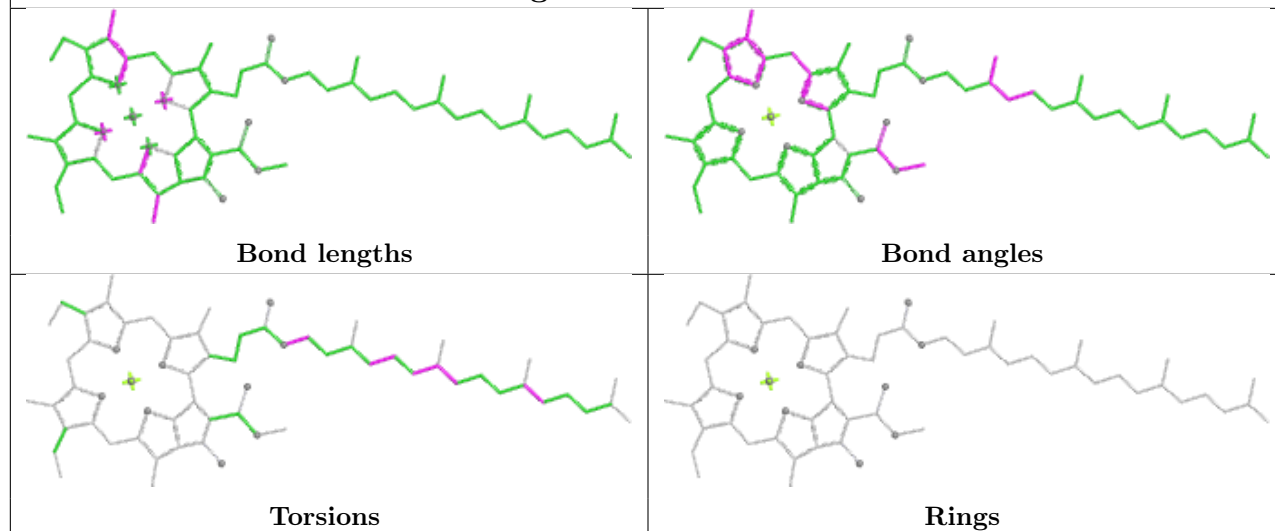
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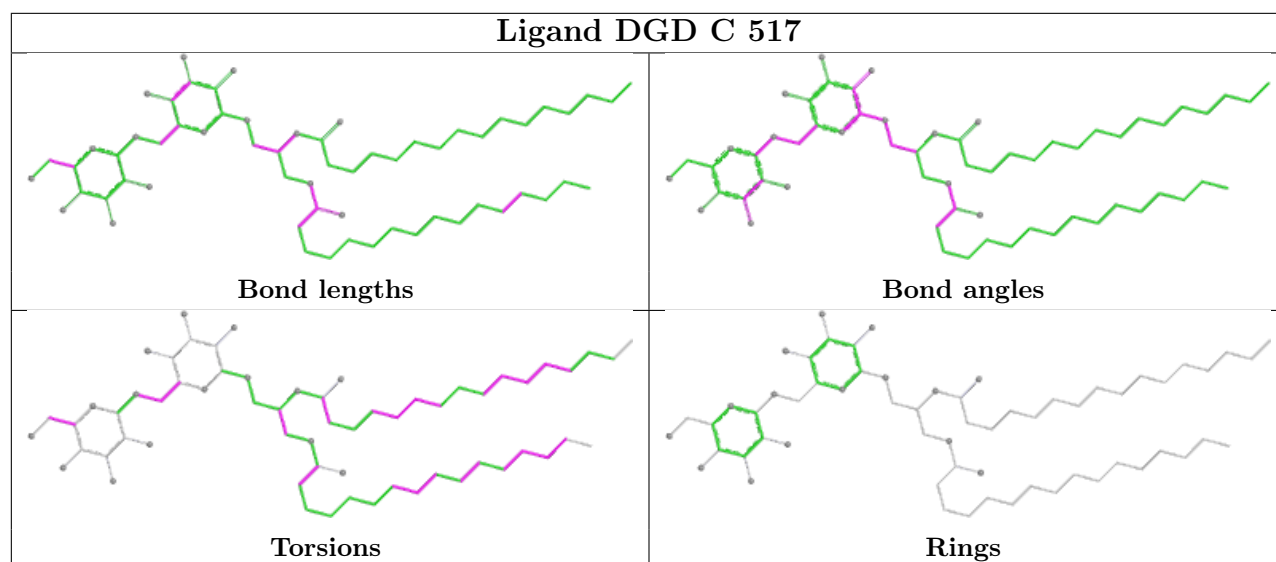
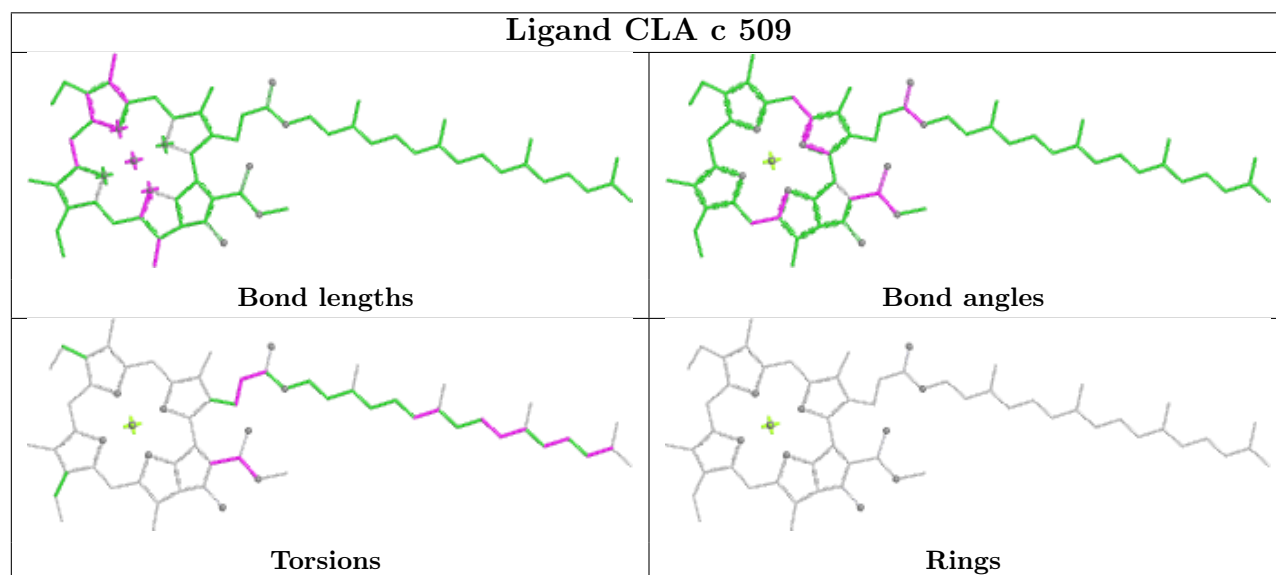
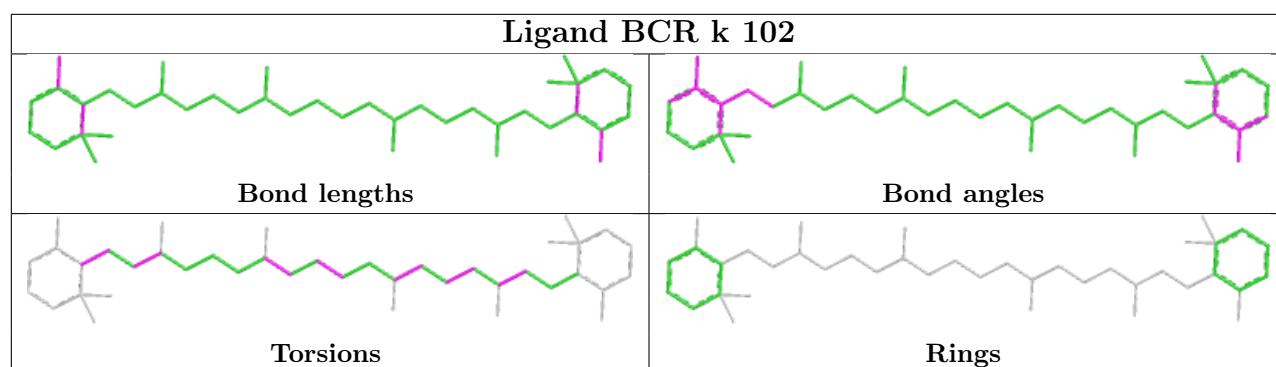


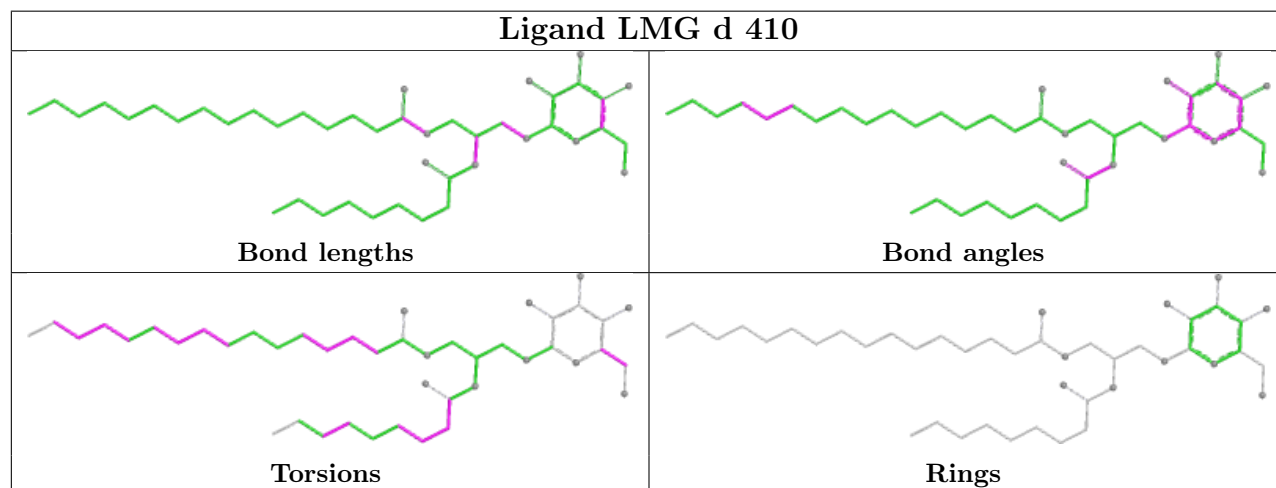
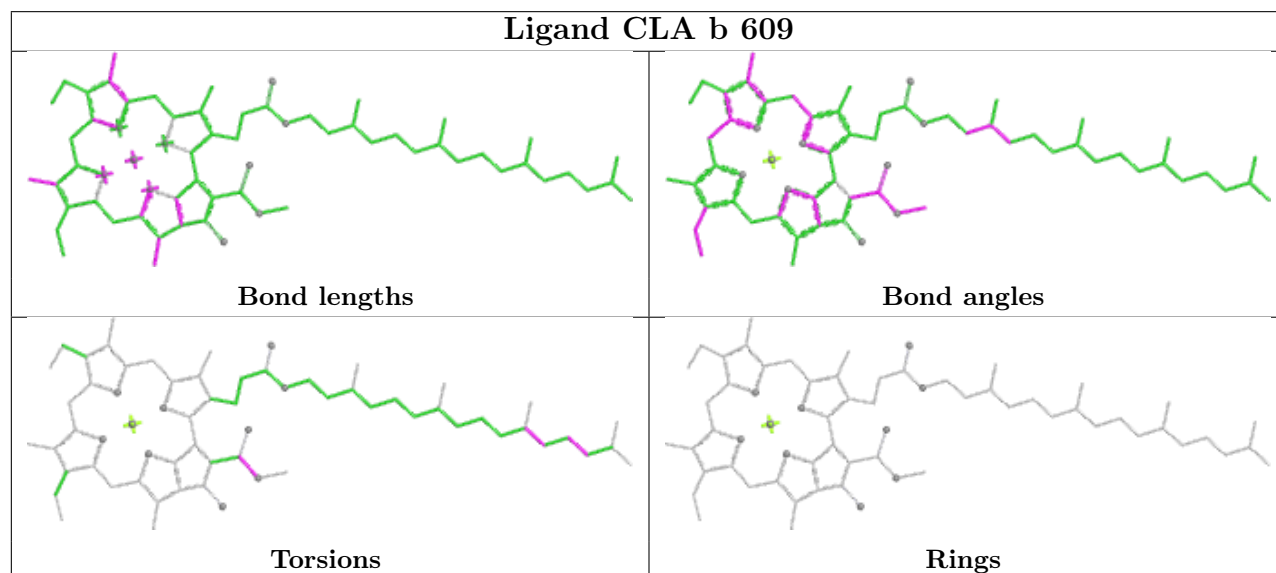
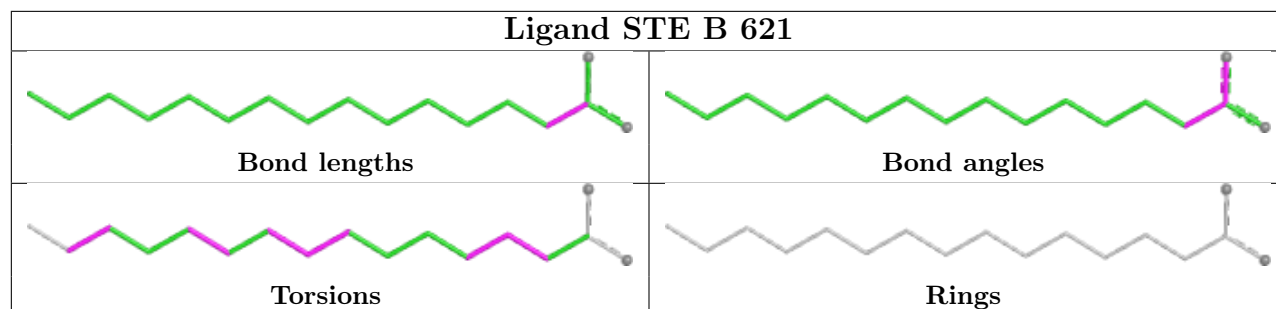
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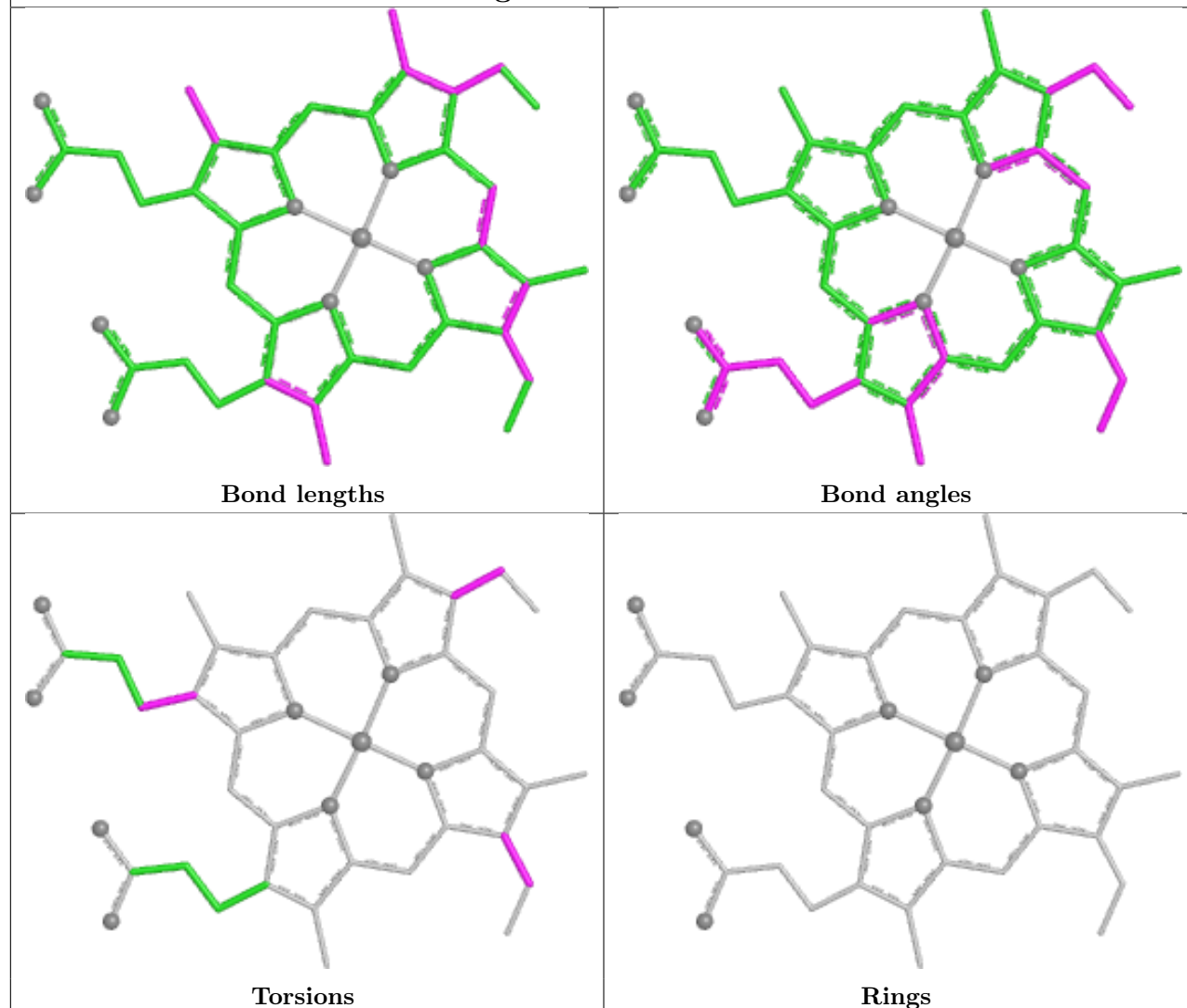
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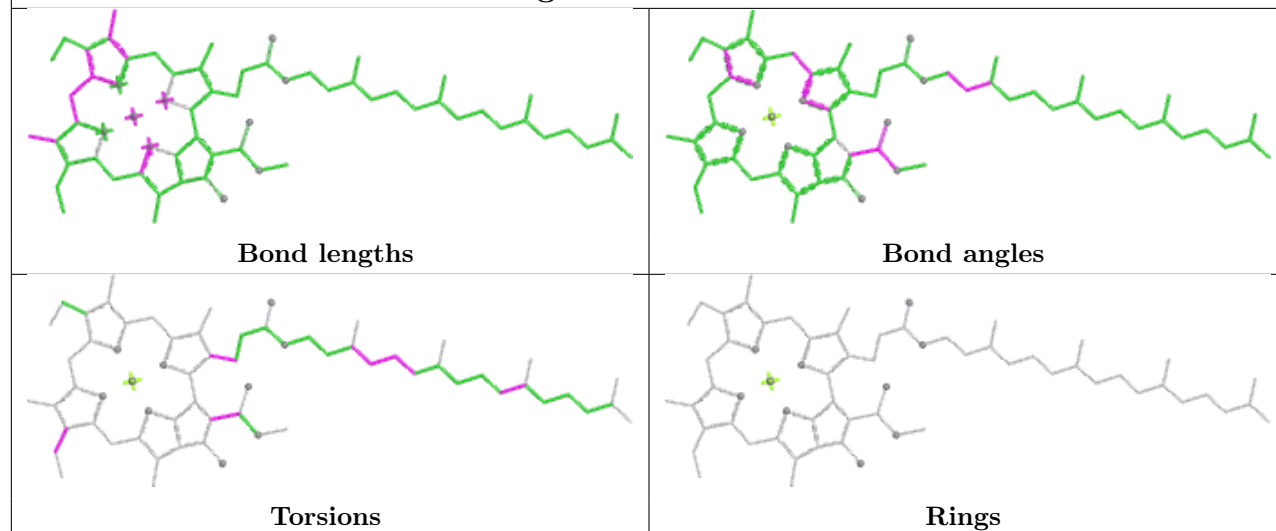


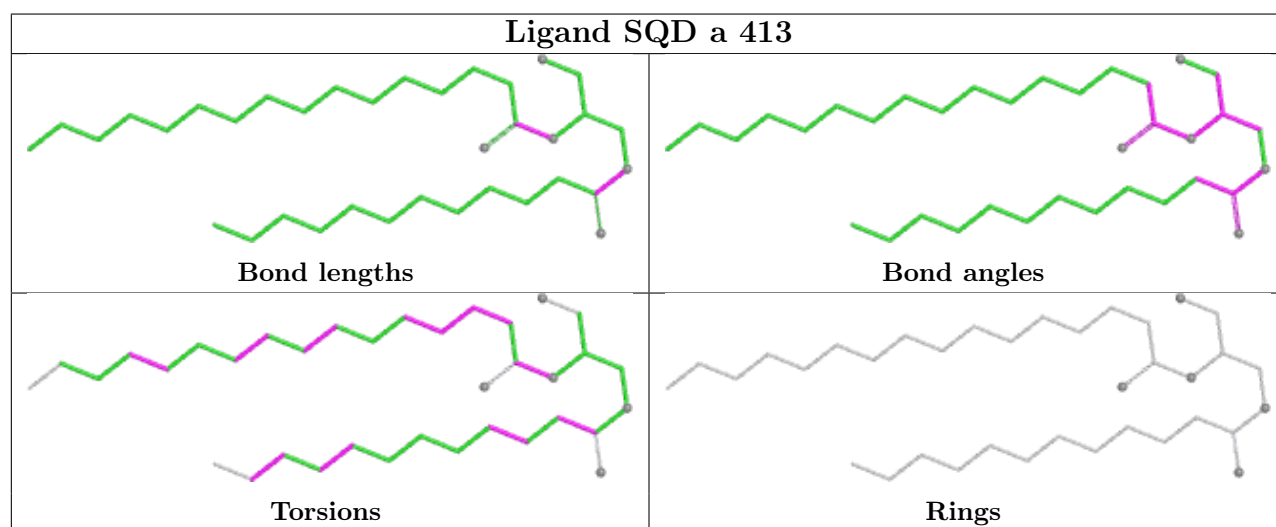
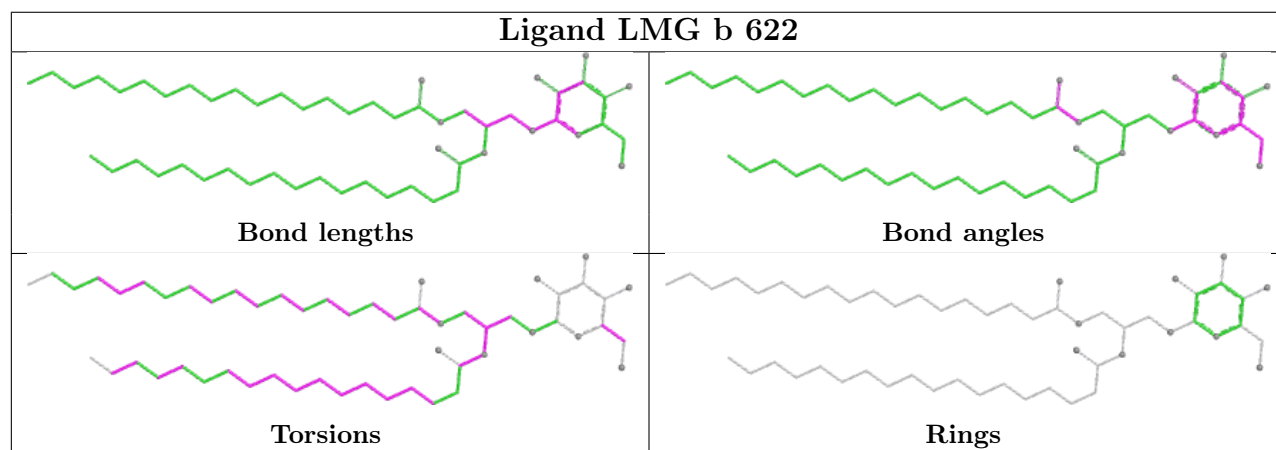
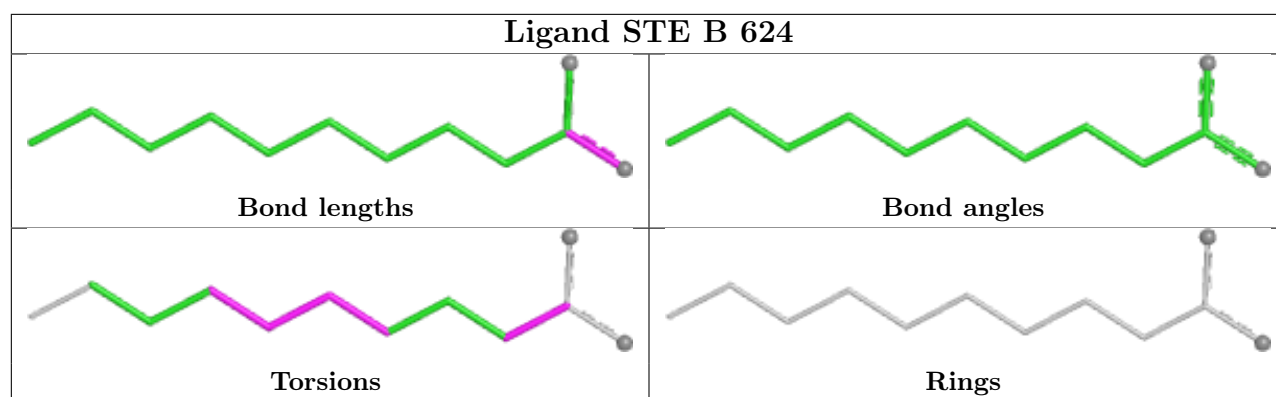


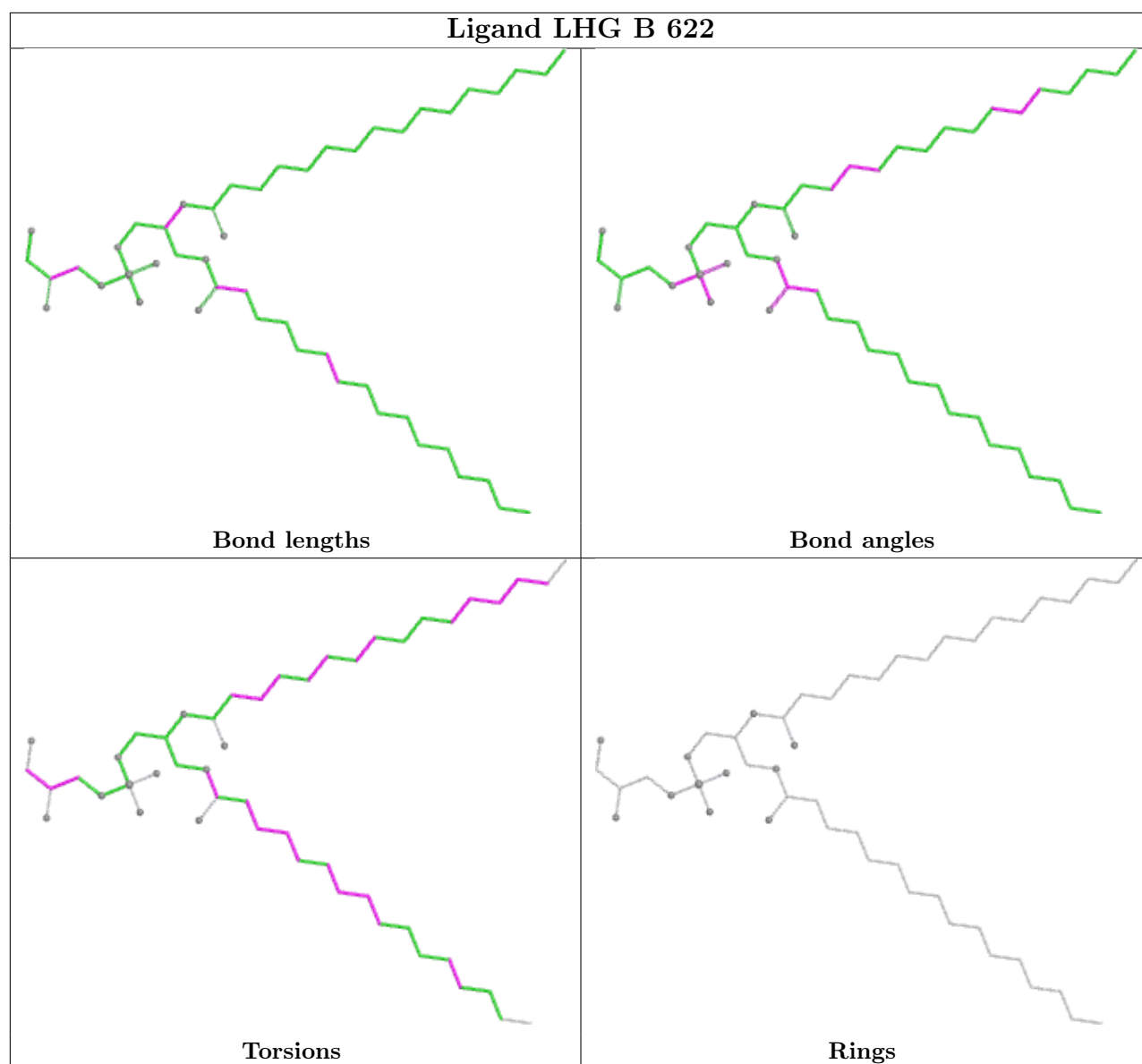
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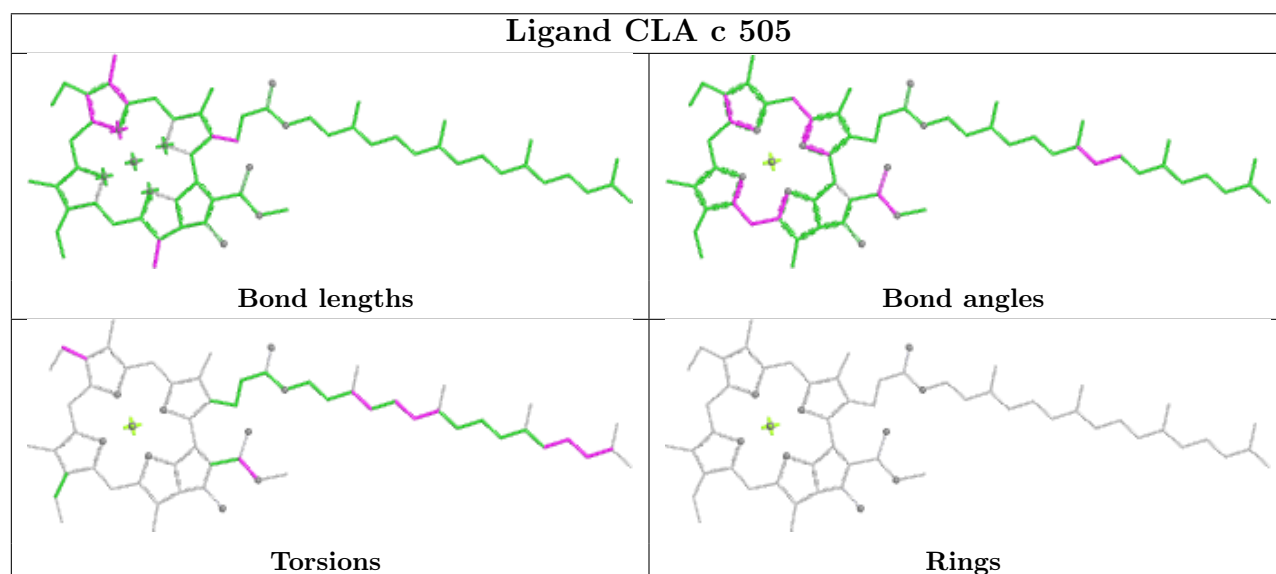
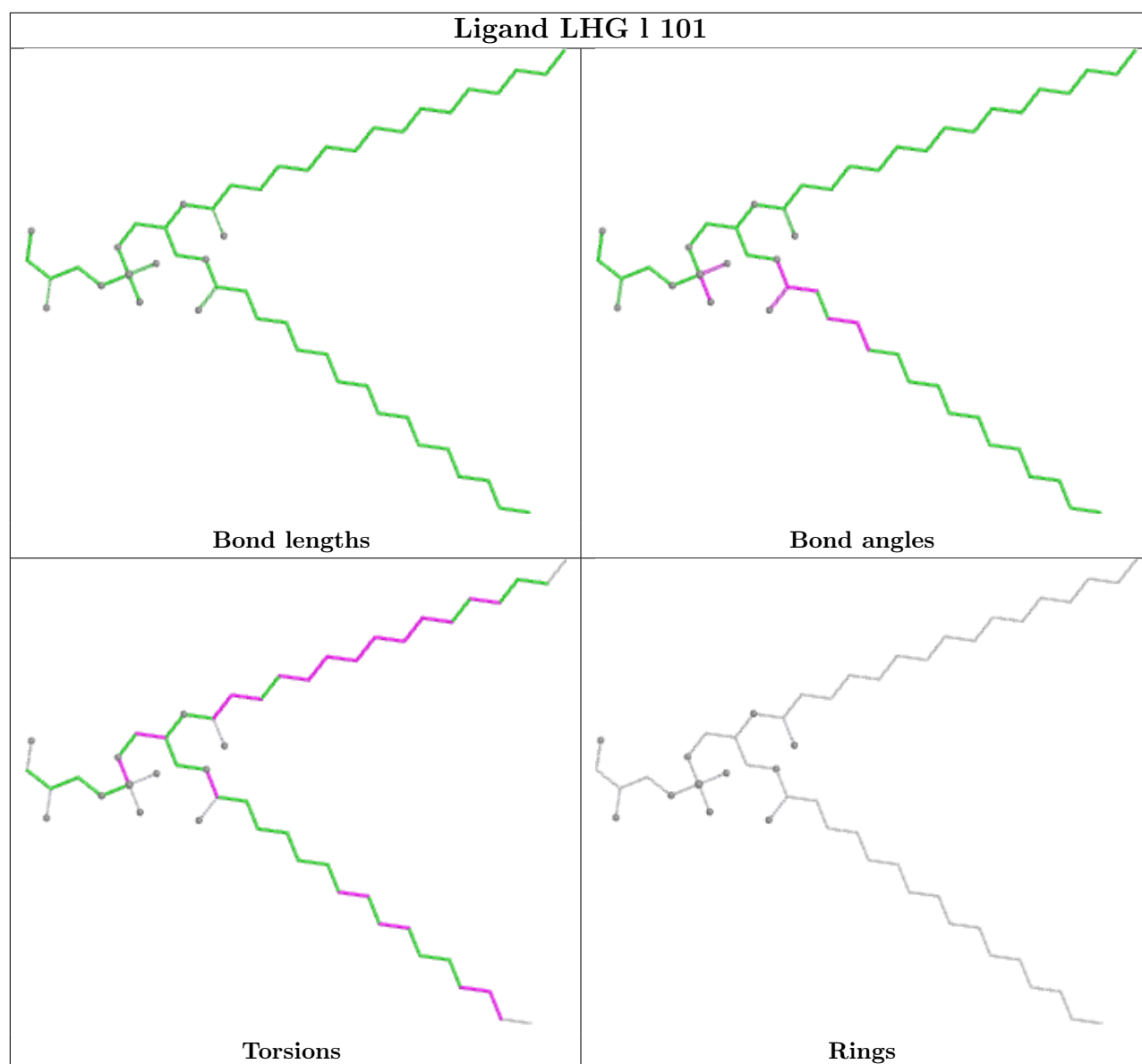


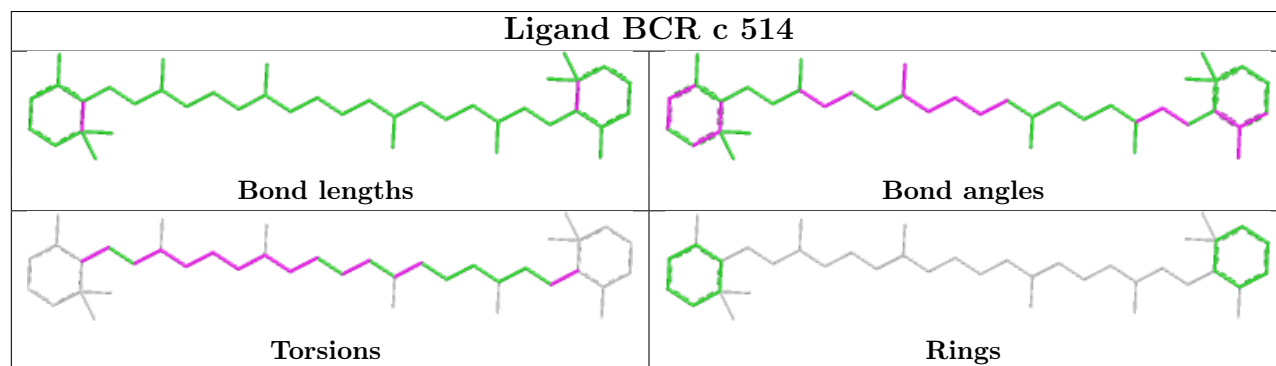
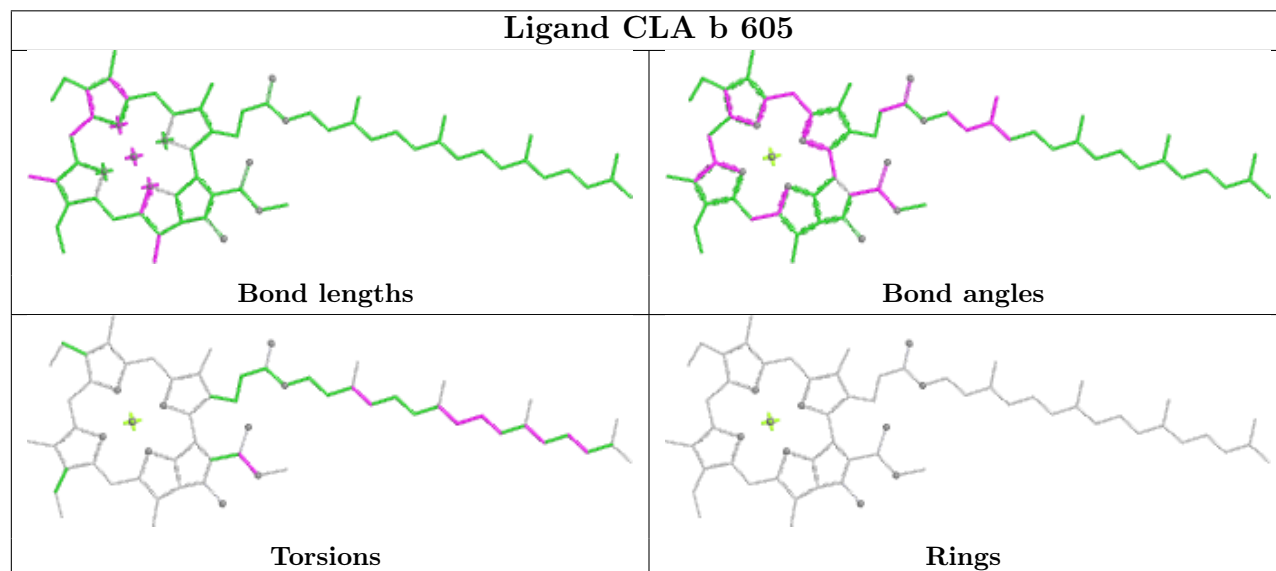
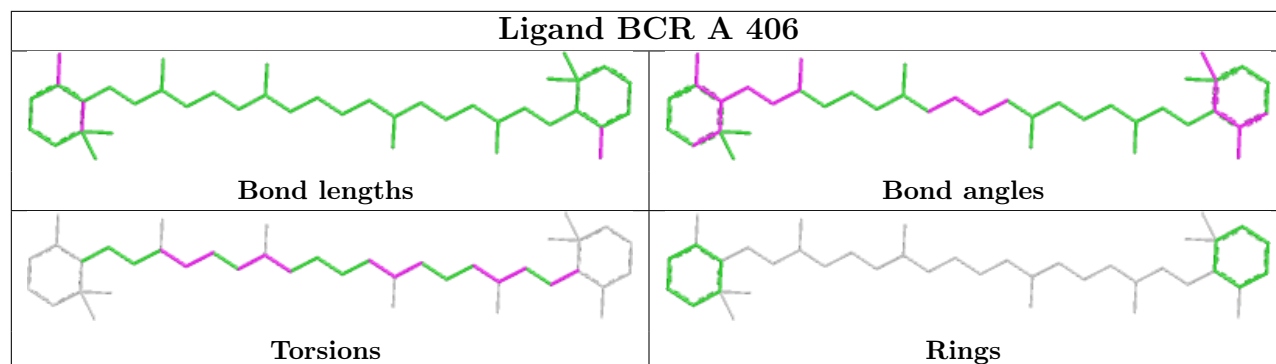
Ligand CLA c 513

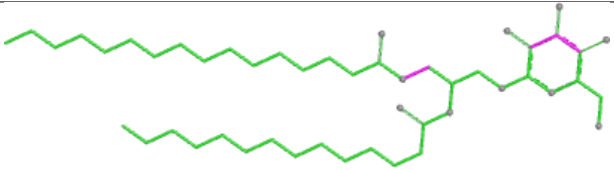
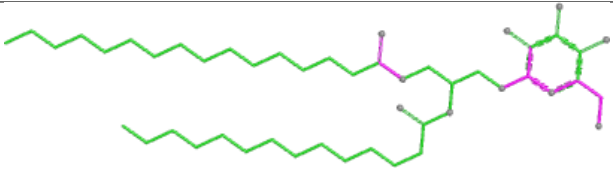
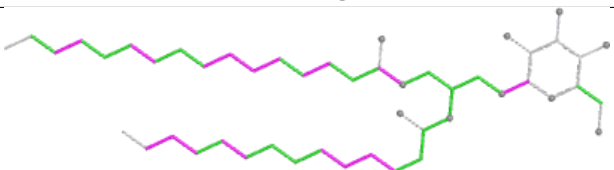
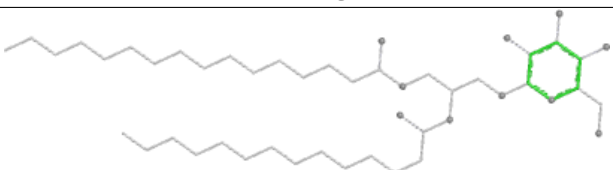


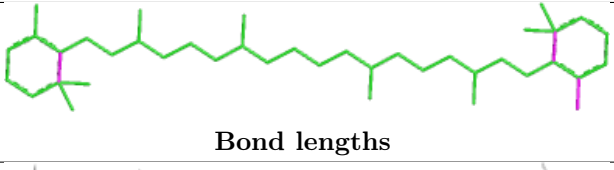
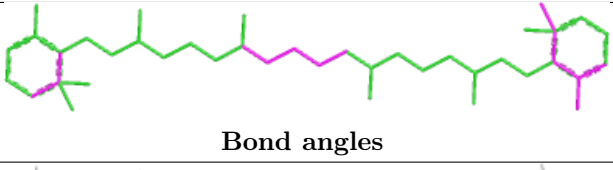
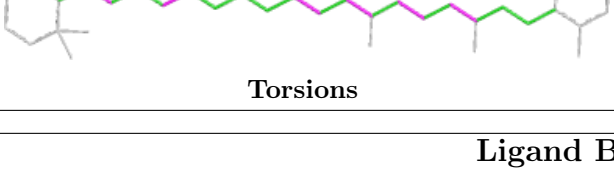
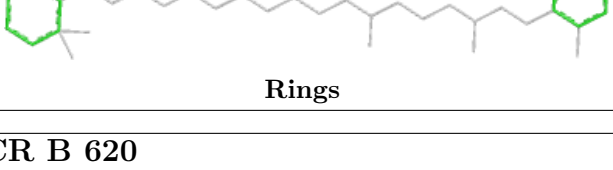


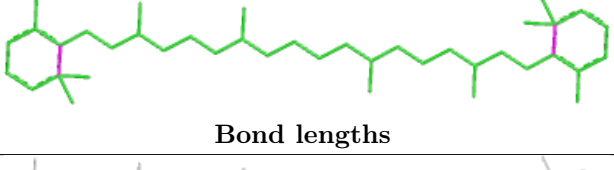
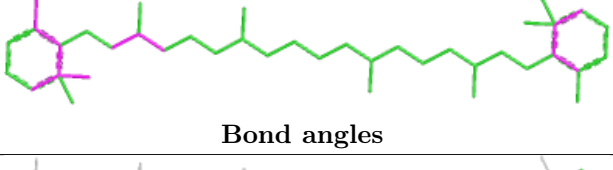


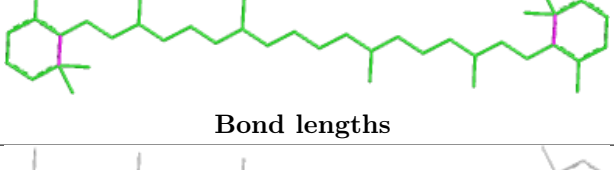
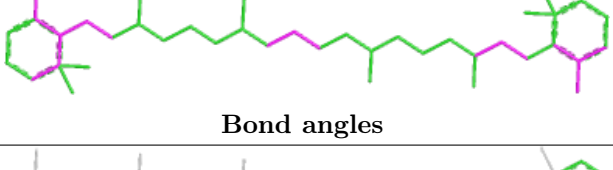


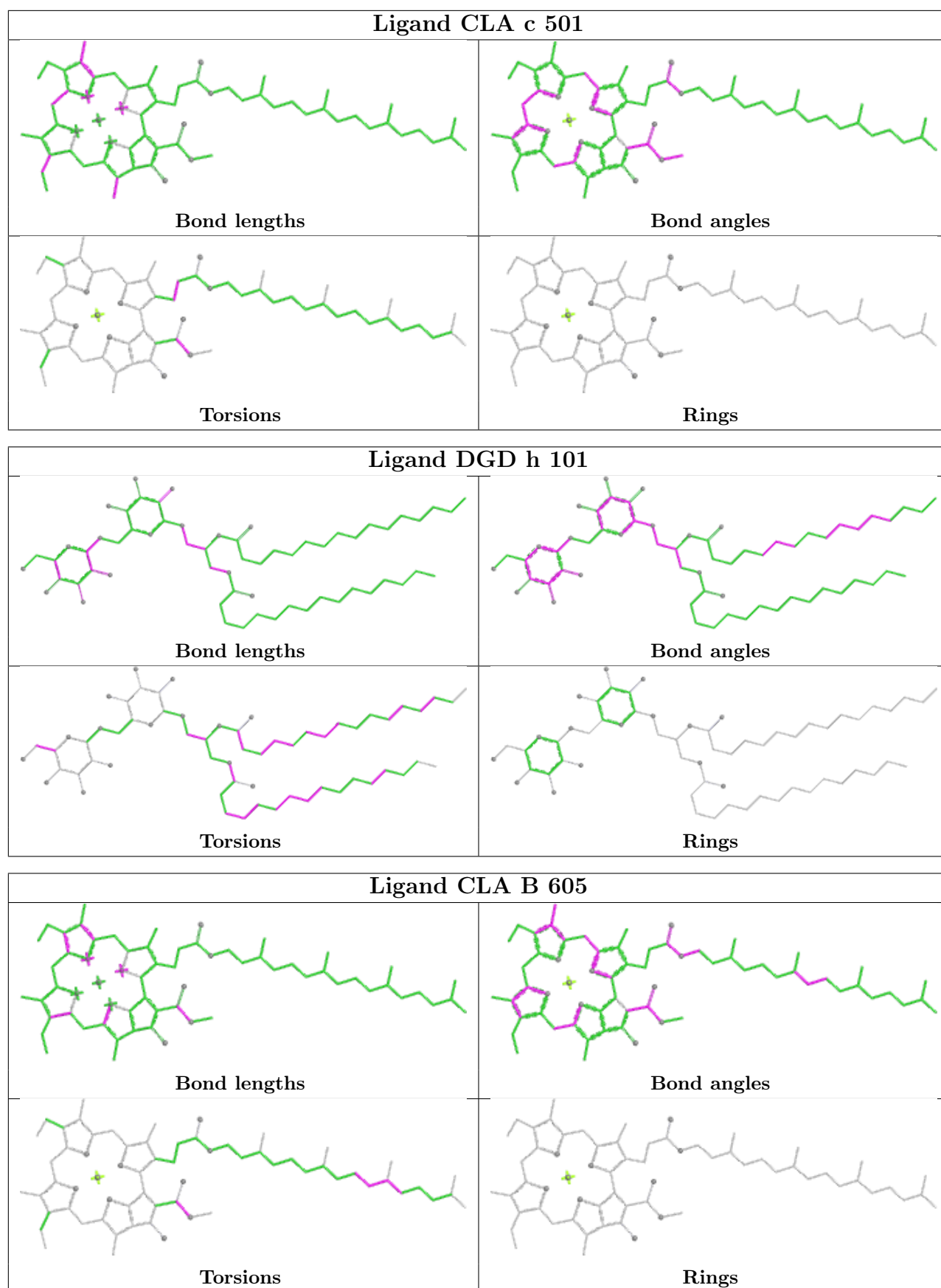


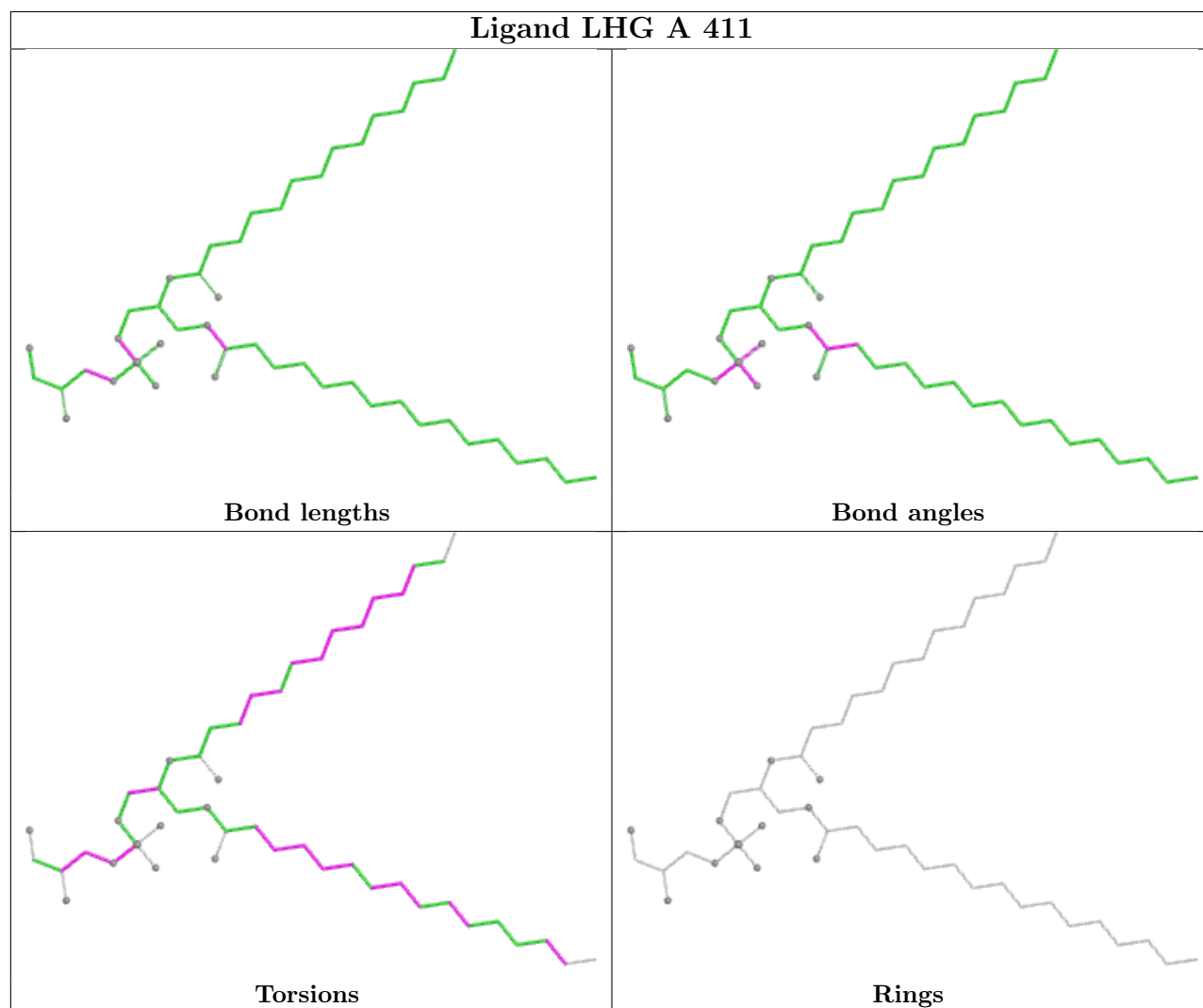
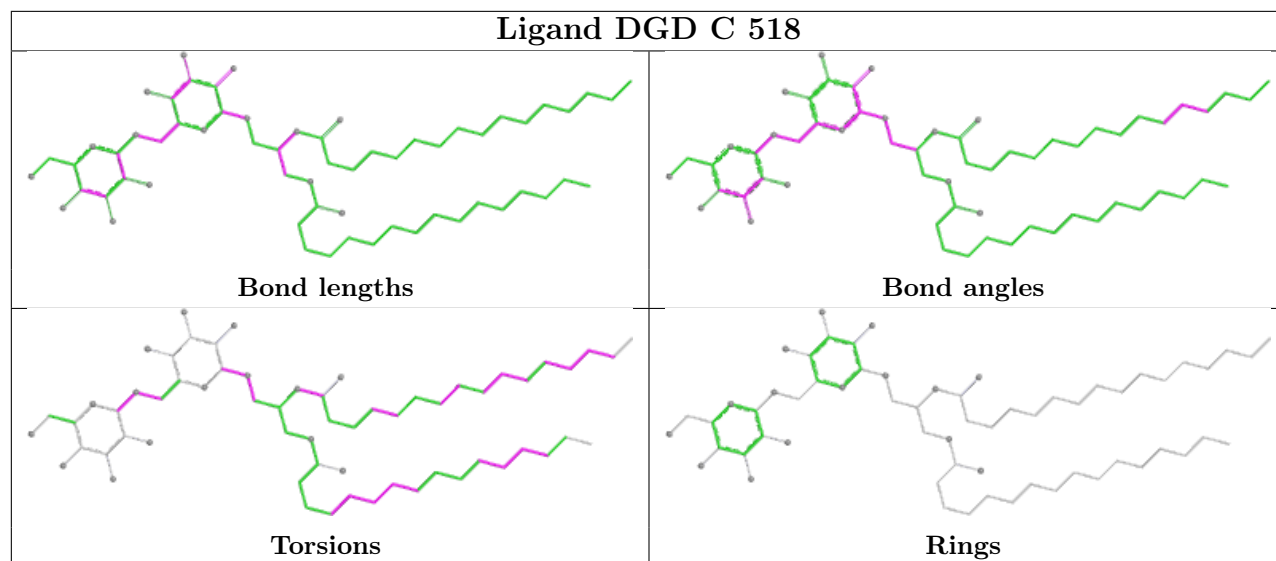
Ligand LMG c 522	
	
Bond lengths	Bond angles
	
Torsions	Rings

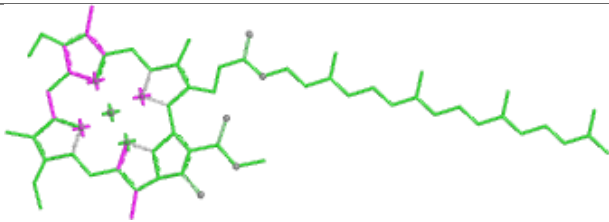
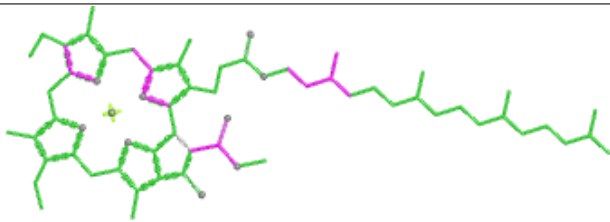
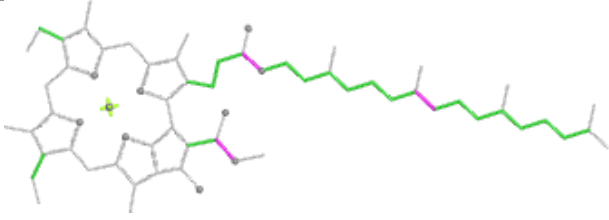
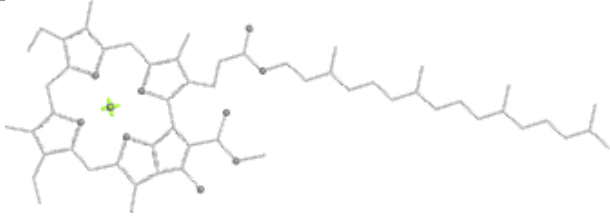
Ligand BCR C 501	
	
Bond lengths	Bond angles
	
Torsions	Rings

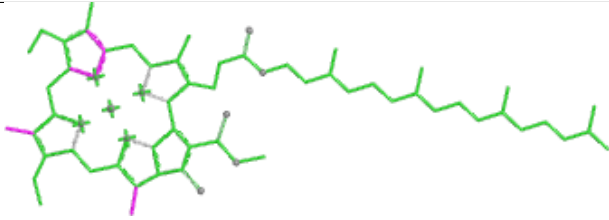
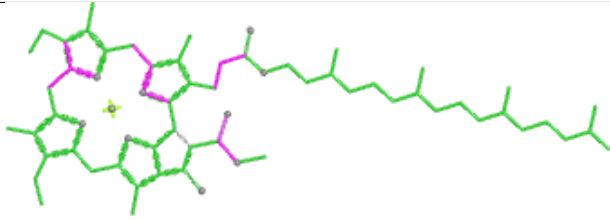
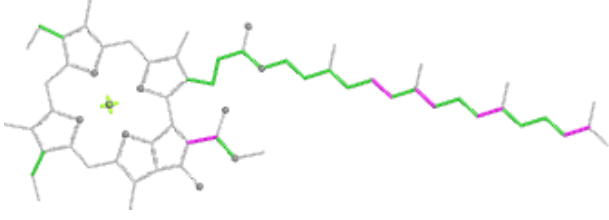
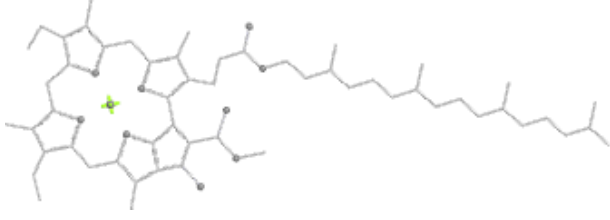
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Bond lengths	Bond angles
	
Torsions	Rings

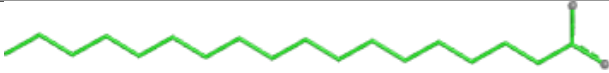
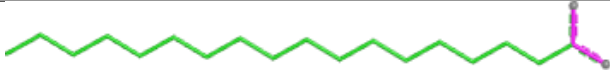
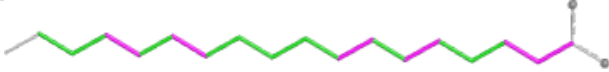
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Bond lengths	Bond angles
	
Torsions	Rings

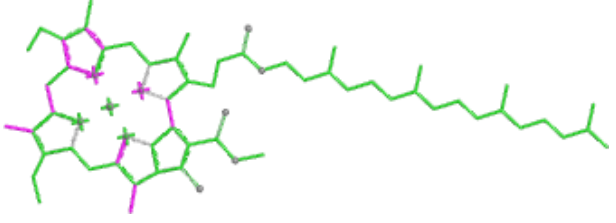
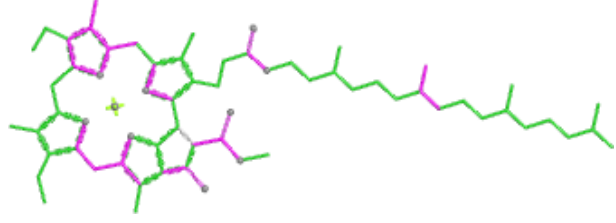
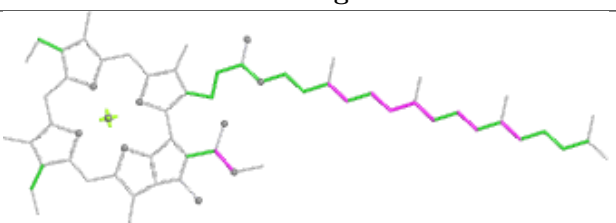
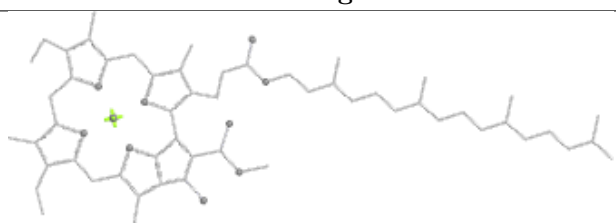
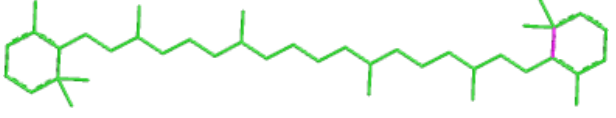
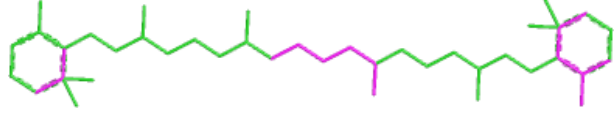
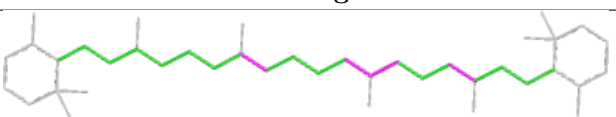
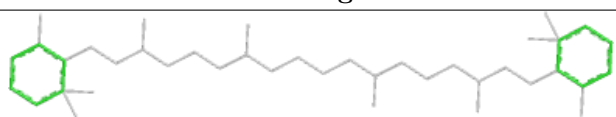
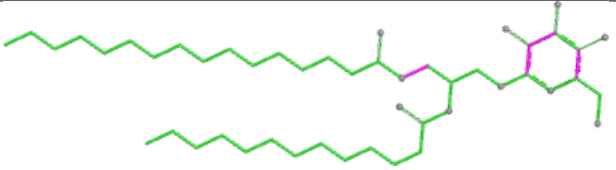
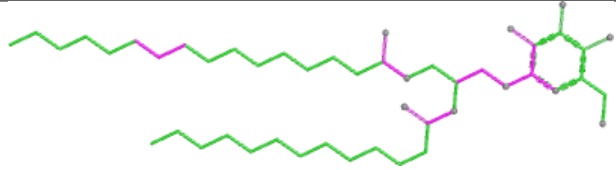
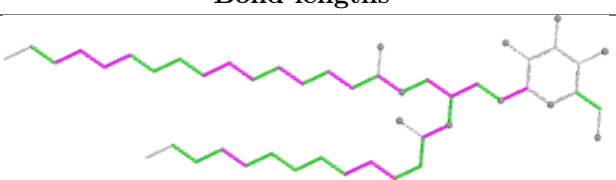
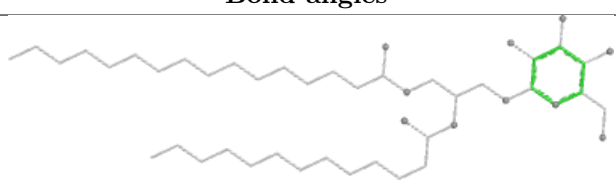


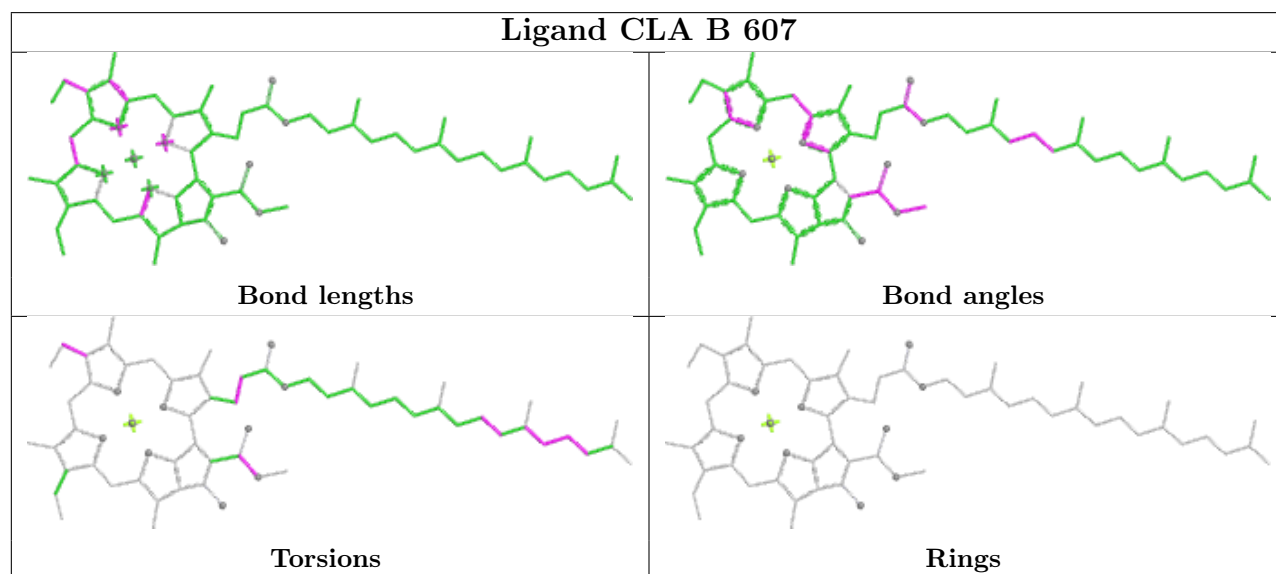
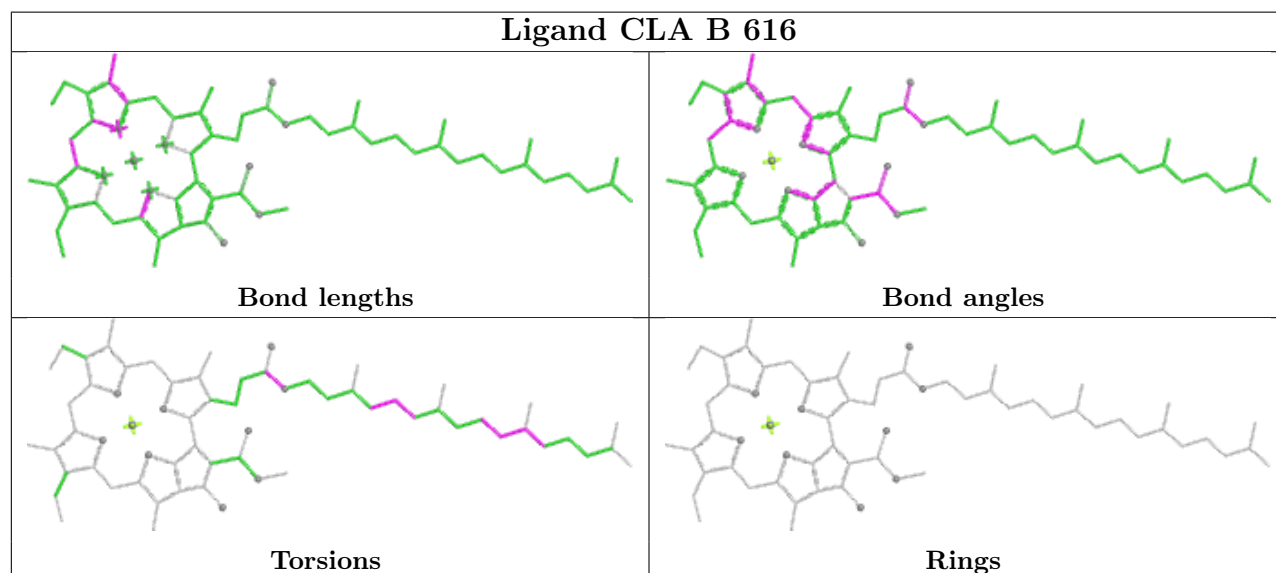
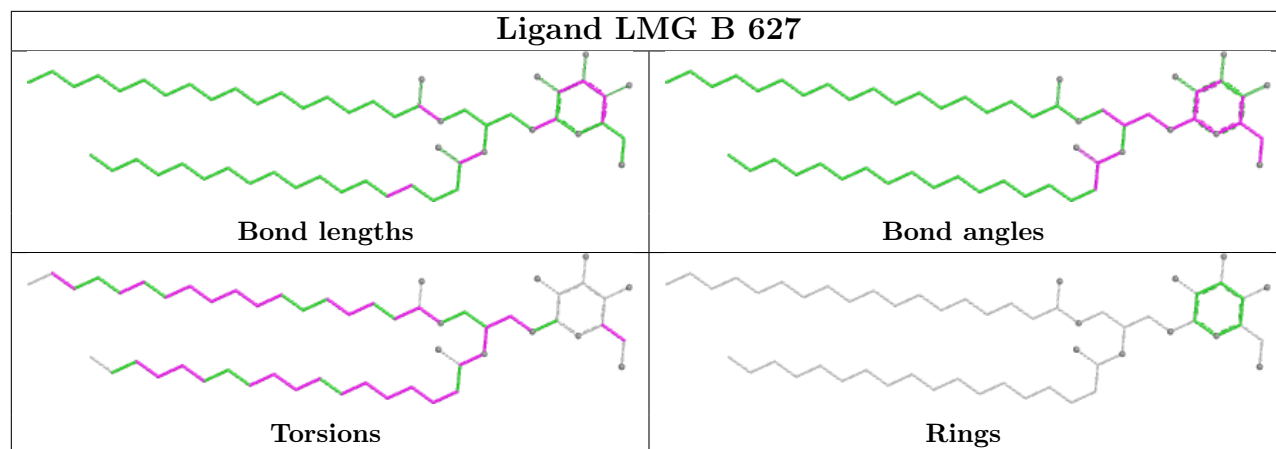


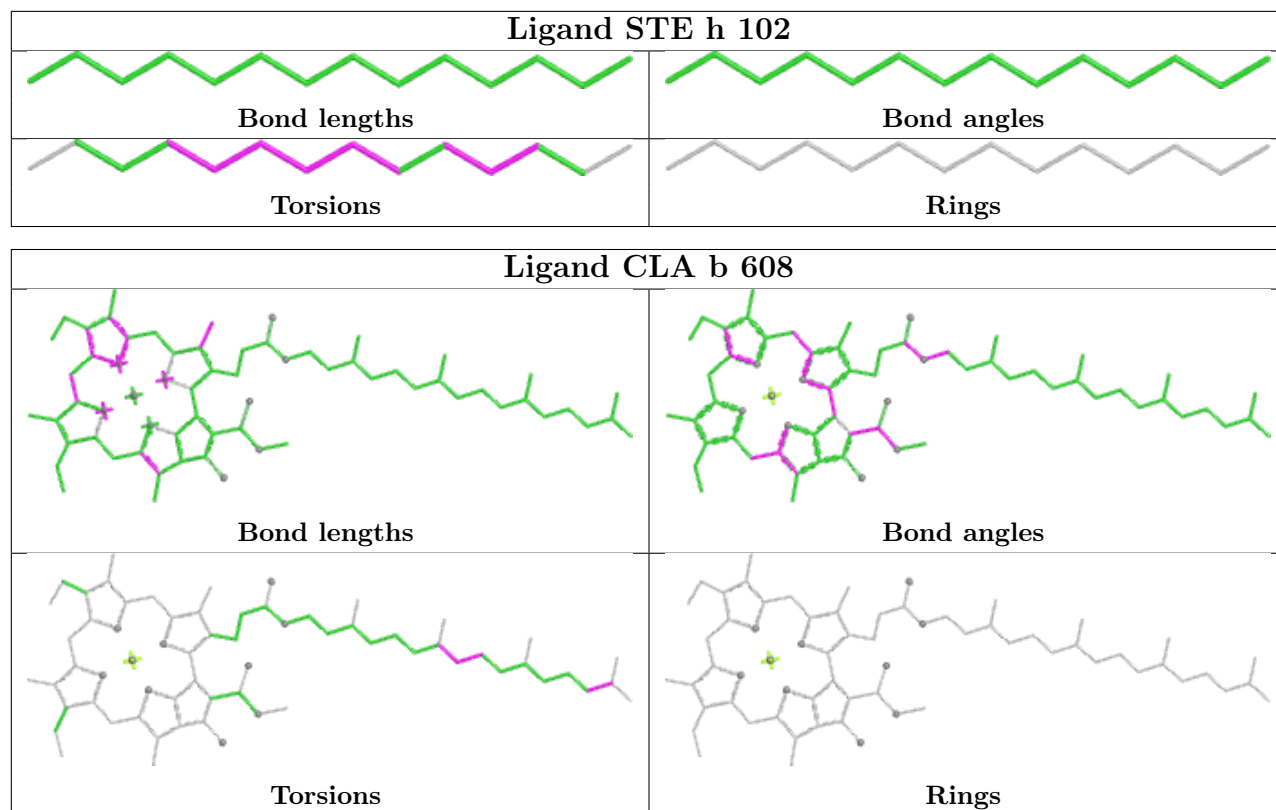
Ligand CLA C 512	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA C 508	
	
Bond lengths	Bond angles
	
Torsions	Rings

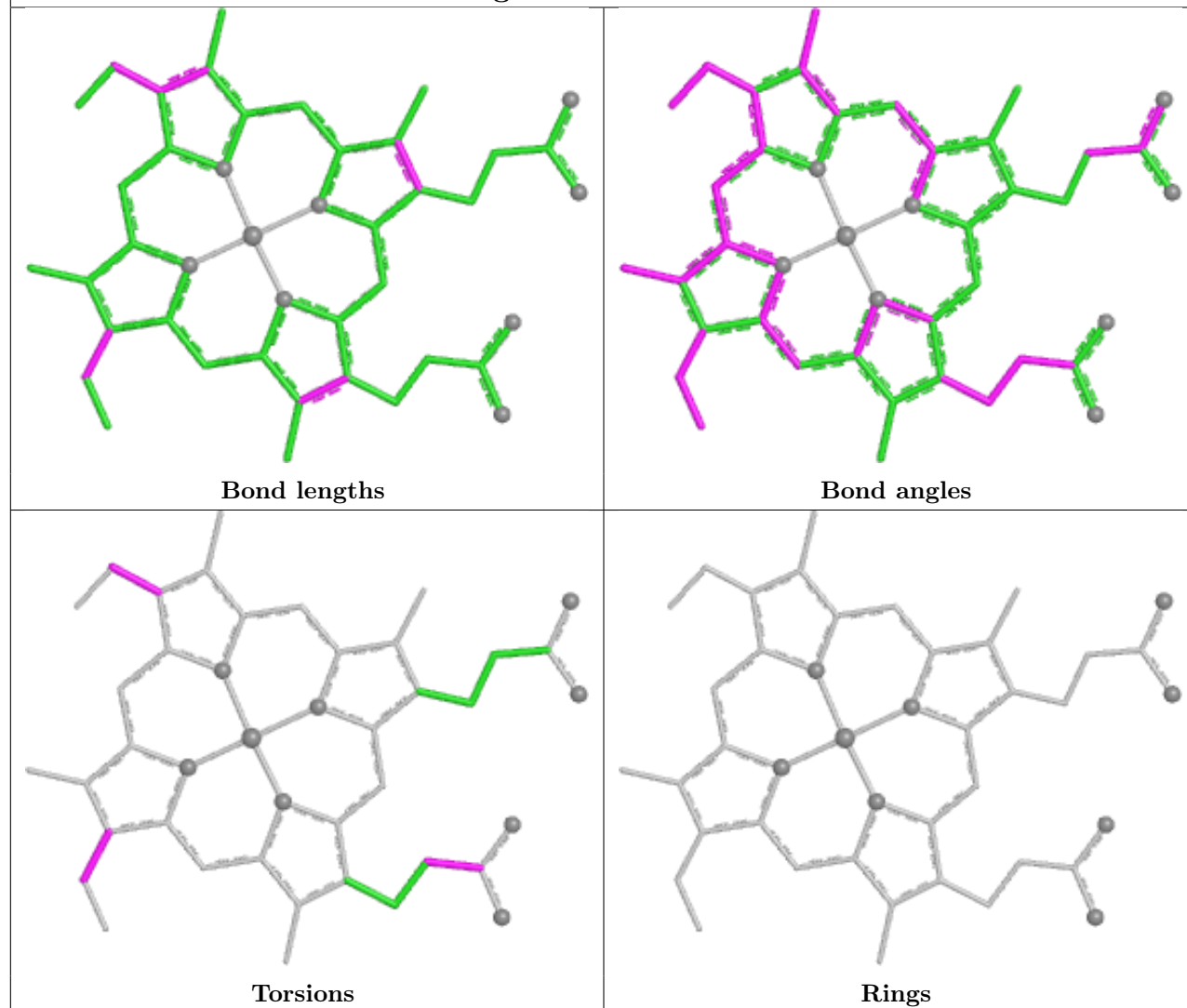
Ligand STE b 624	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 603	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR H 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG Y 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

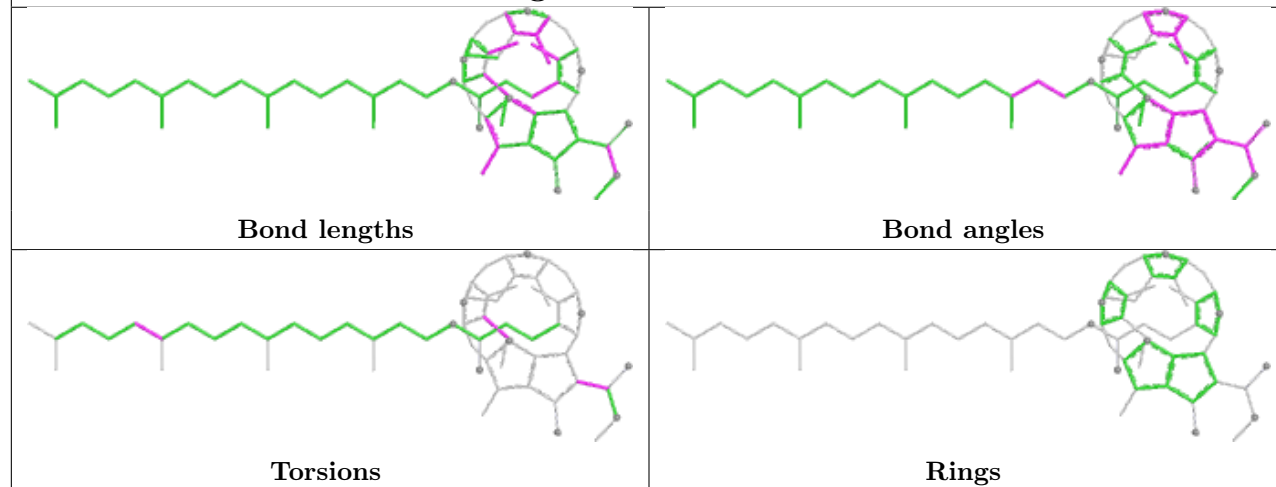


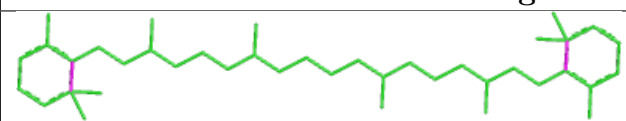
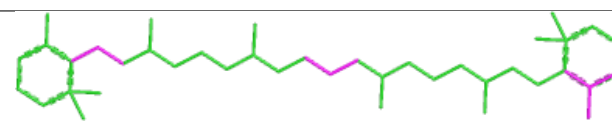
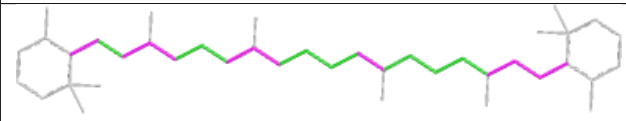
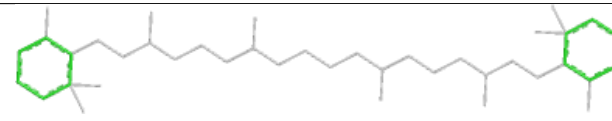


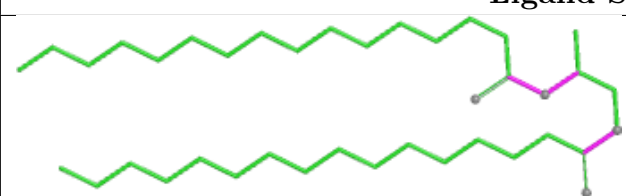
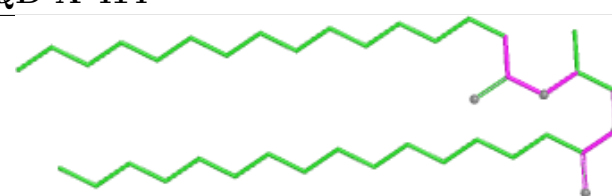
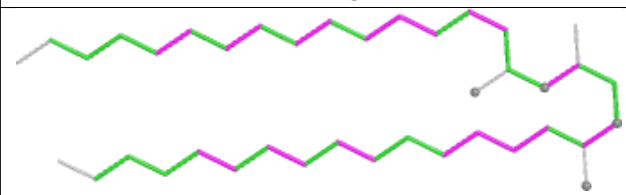
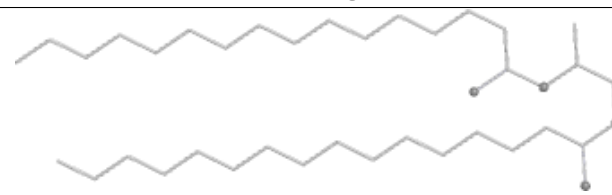
Ligand HEC V 201

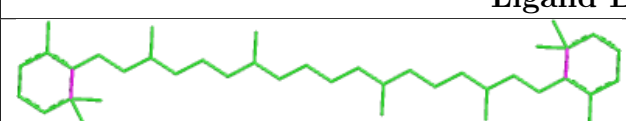
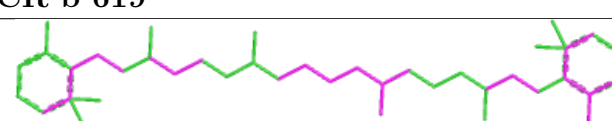
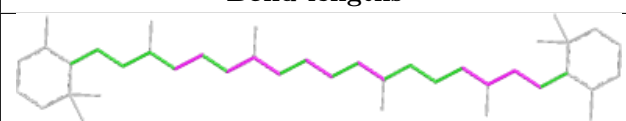
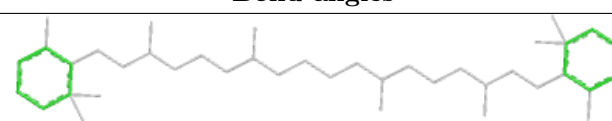


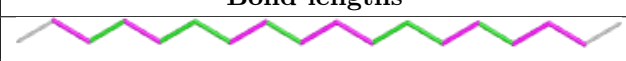
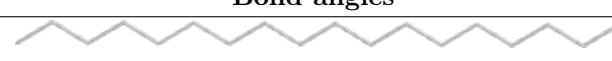
Ligand PHO D 401

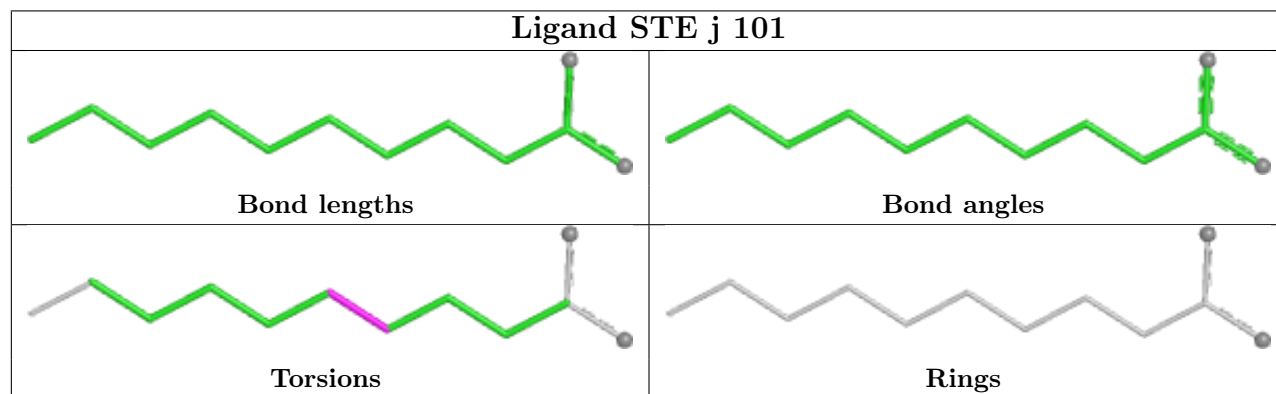
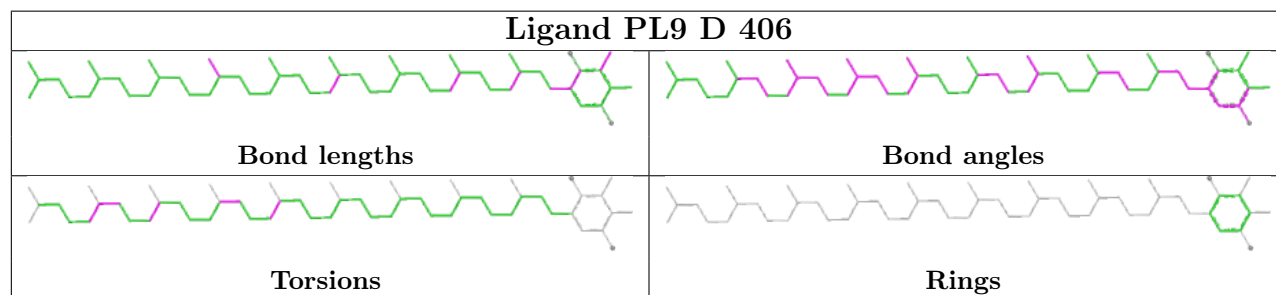
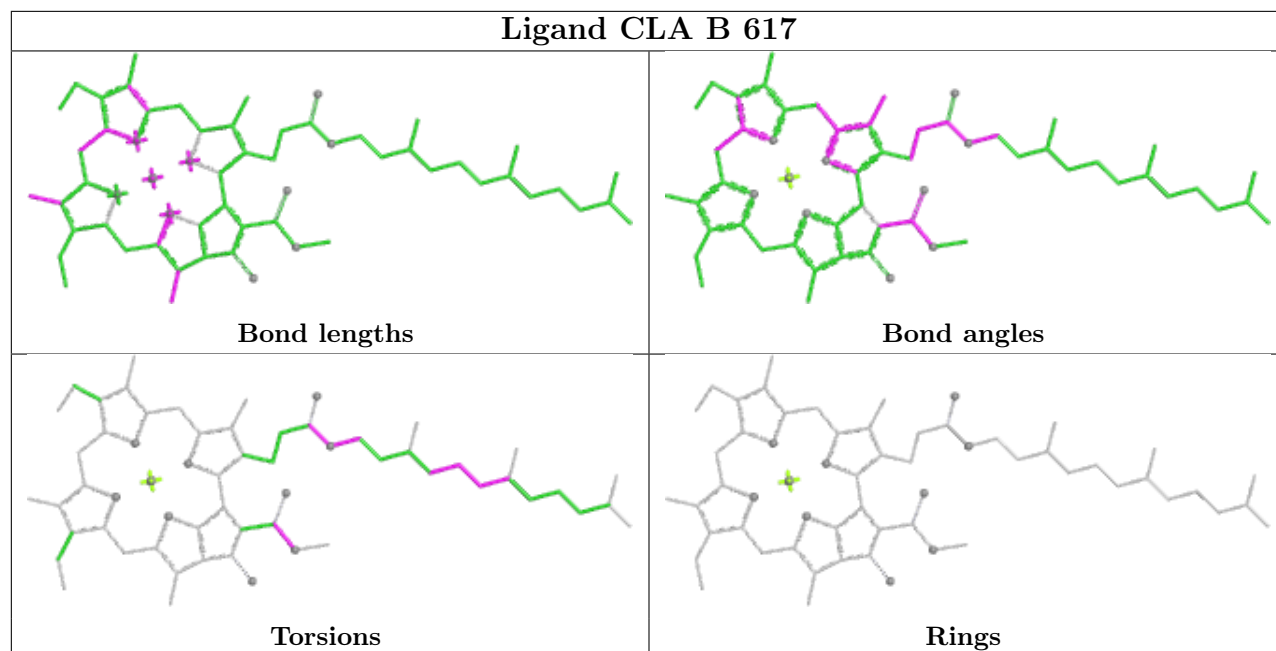


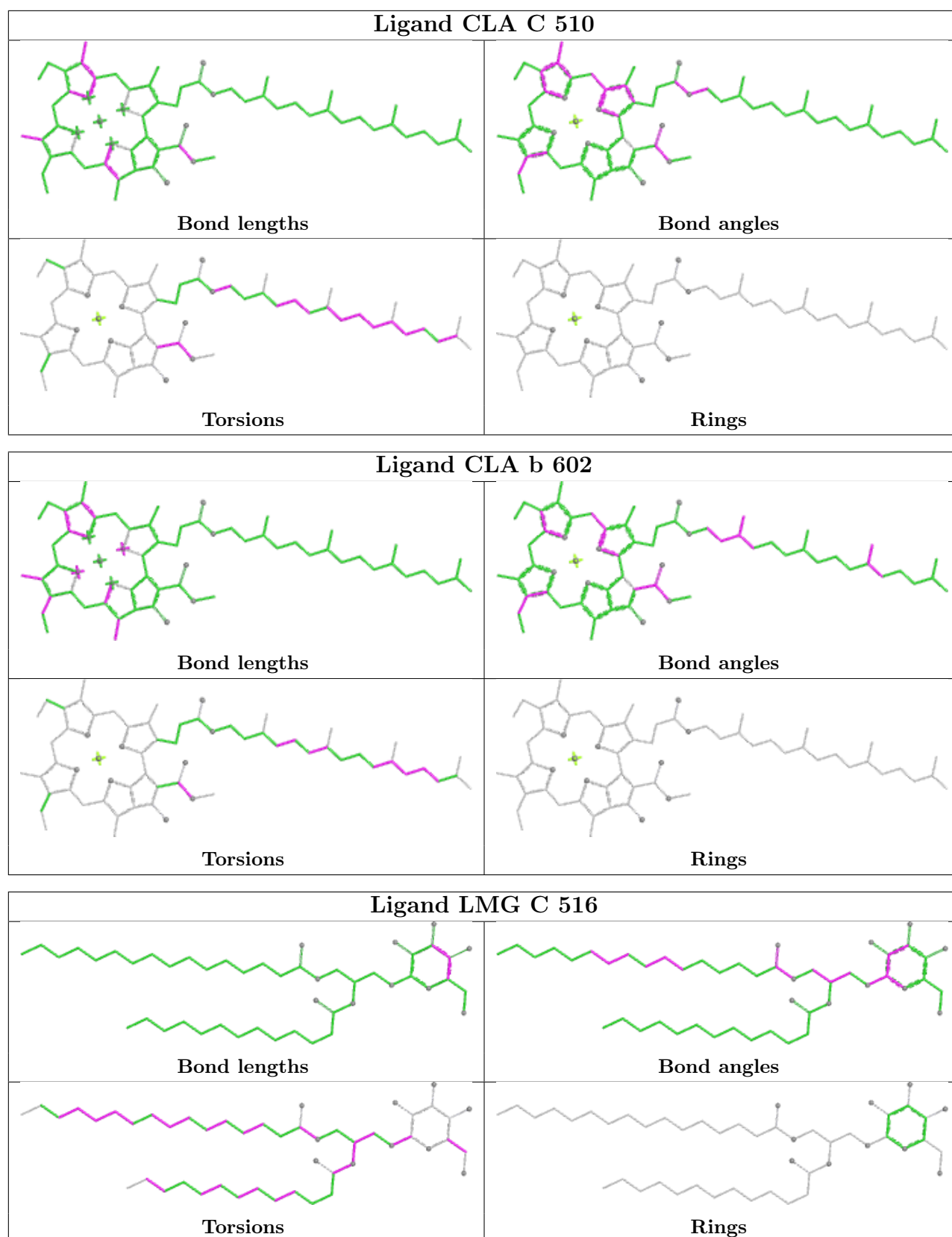
Ligand BCR K 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

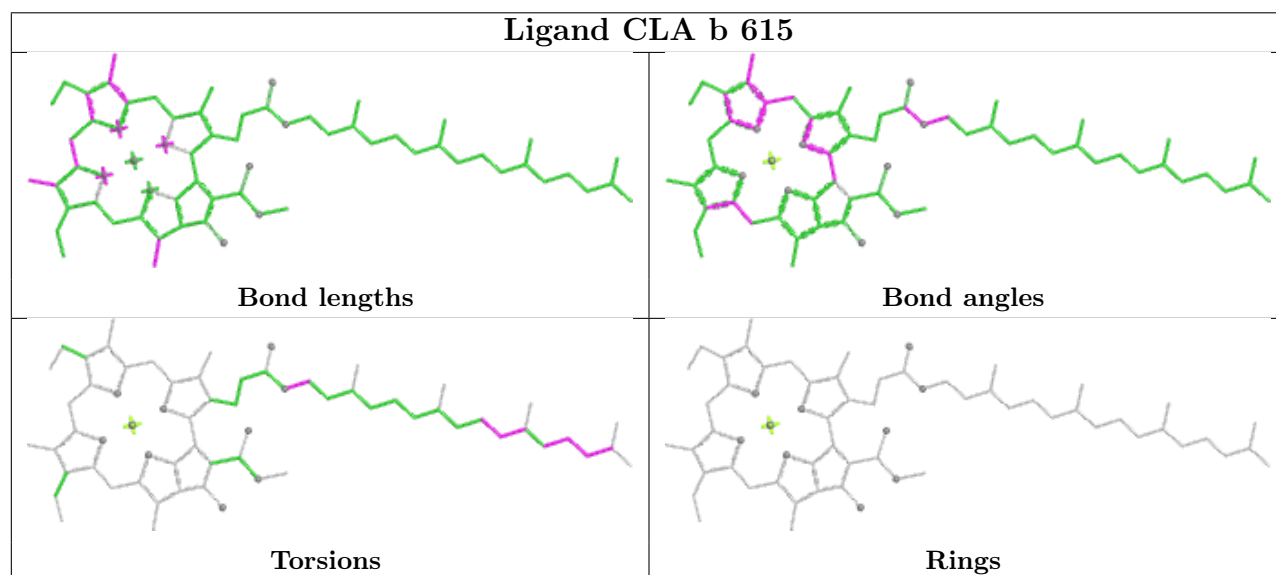
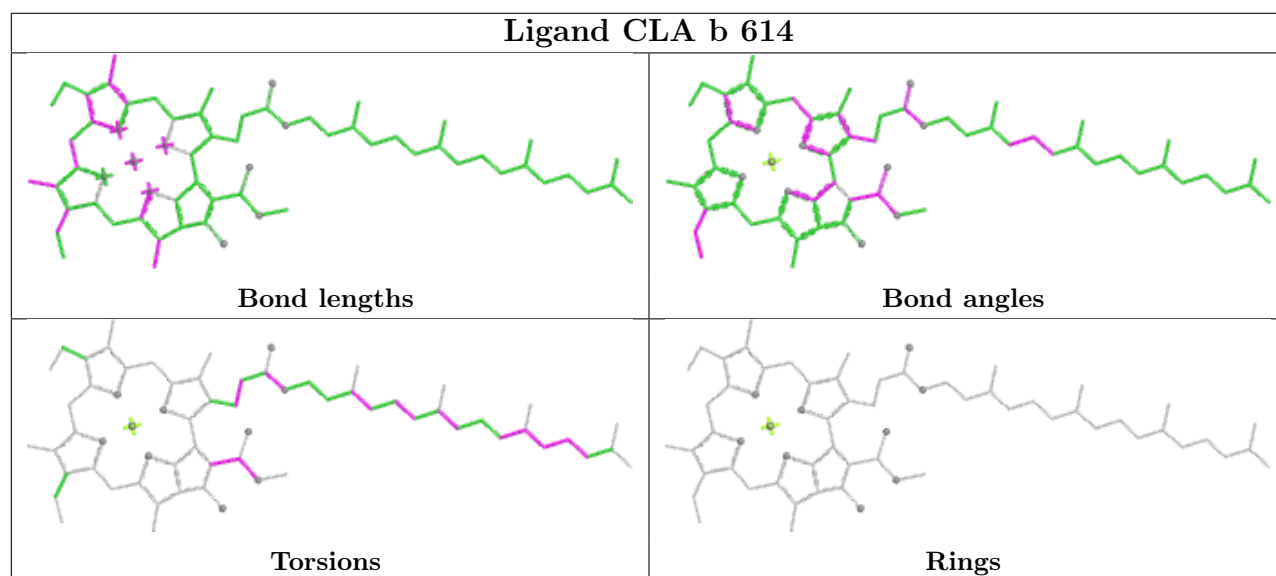
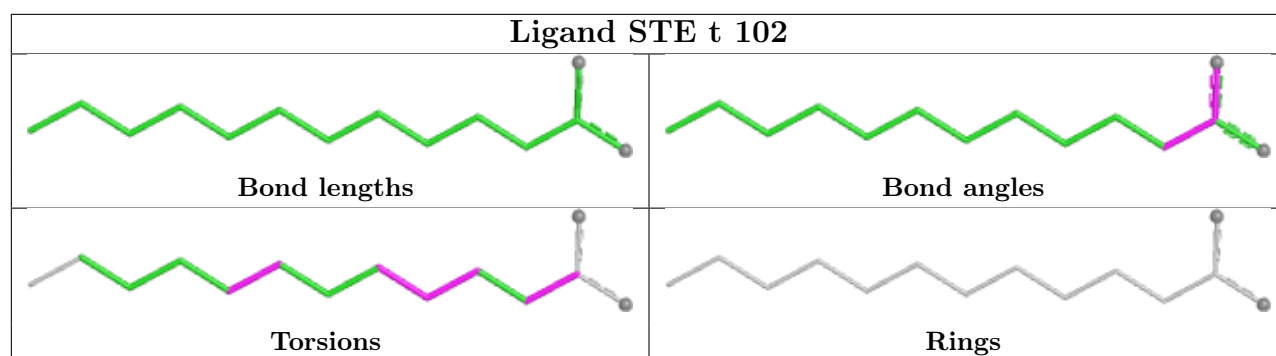
Ligand SQD A 414	
	
Bond lengths	Bond angles
	
Torsions	Rings

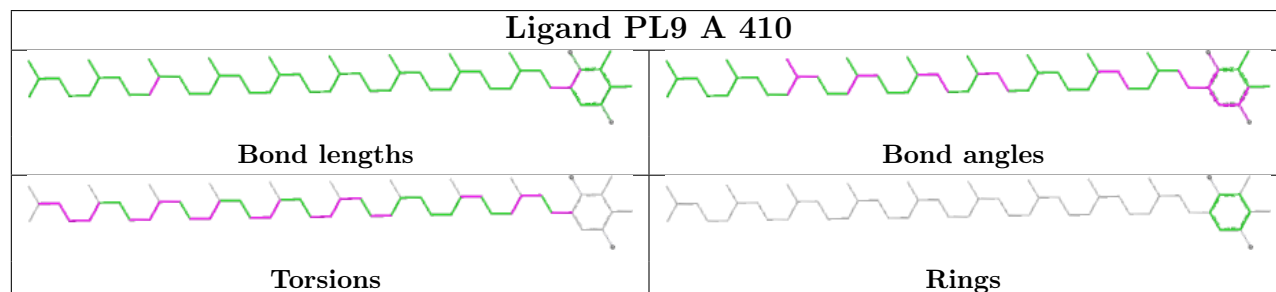
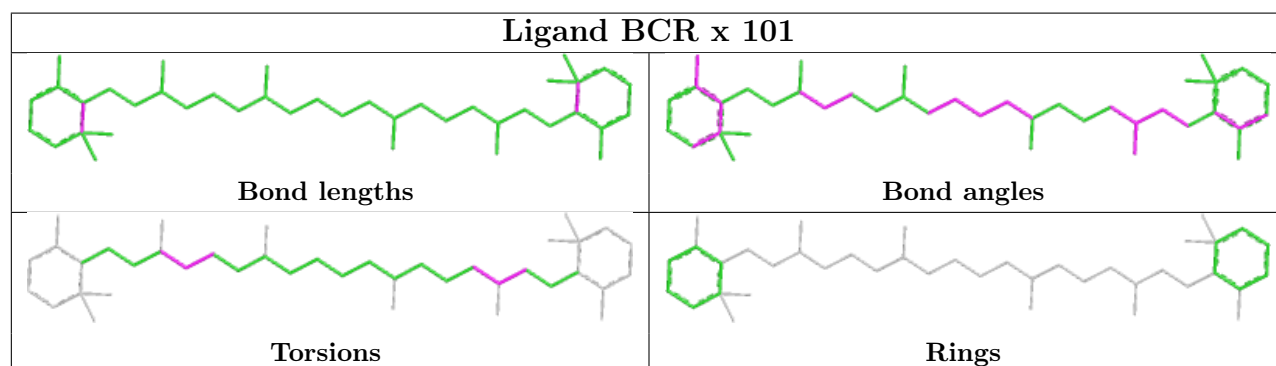
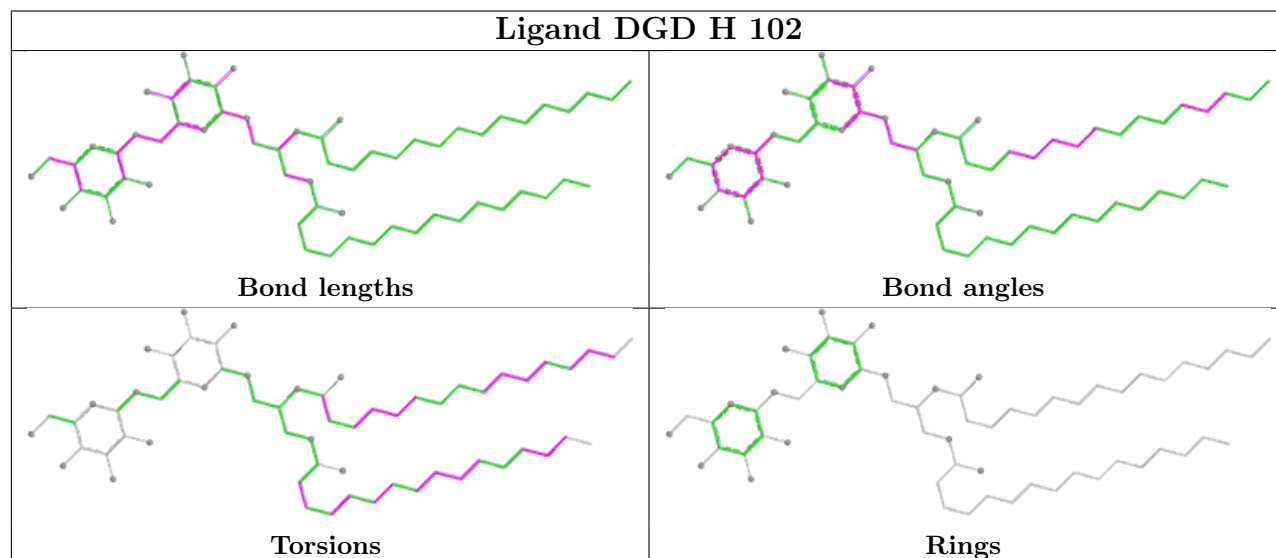
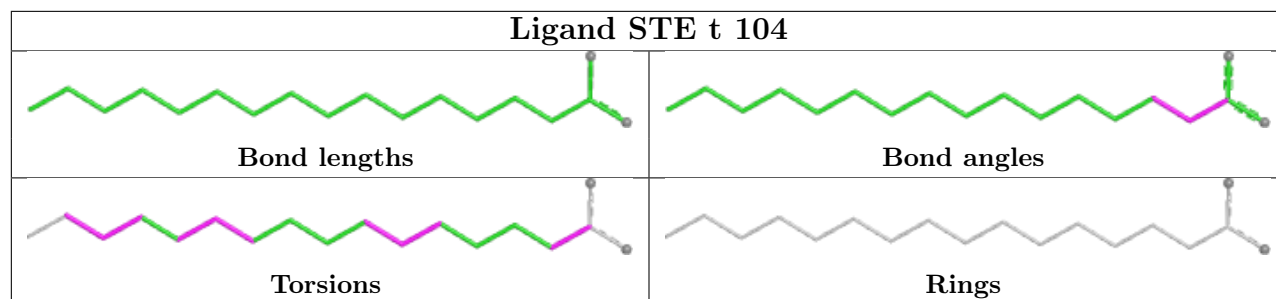
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Bond lengths	Bond angles
	
Torsions	Rings

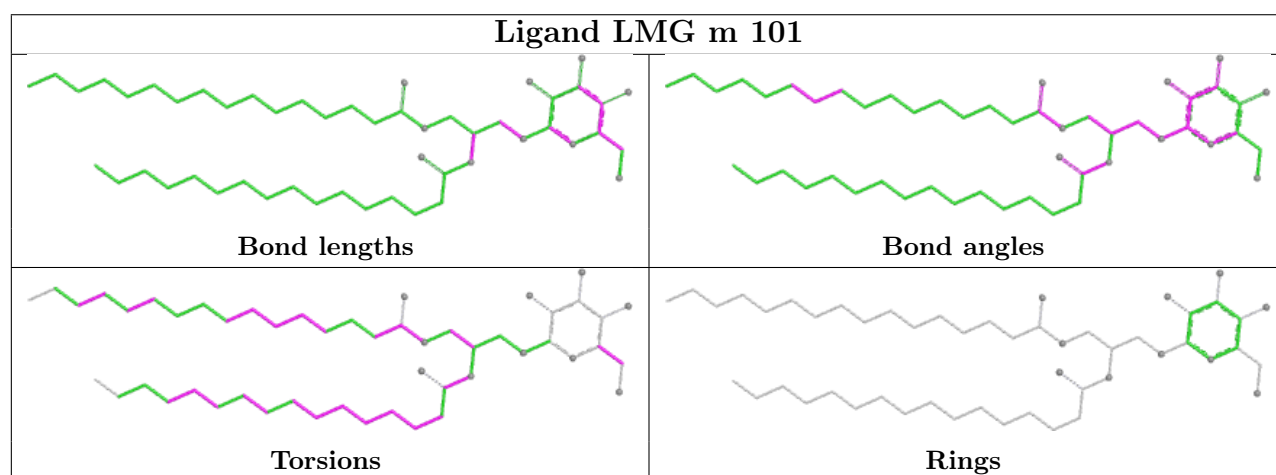
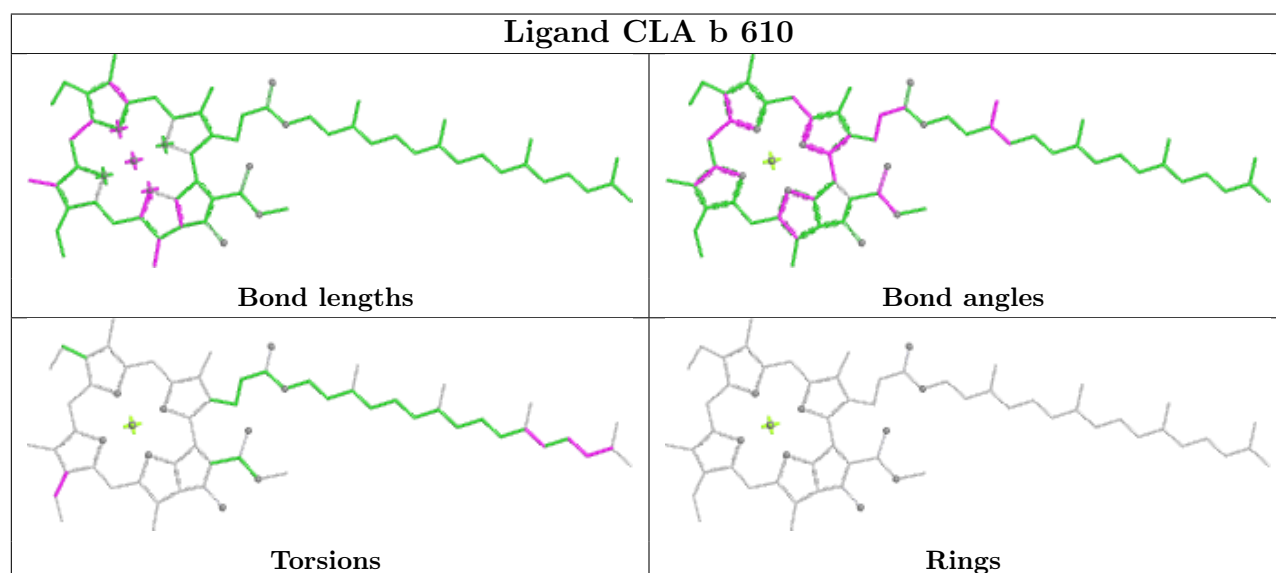
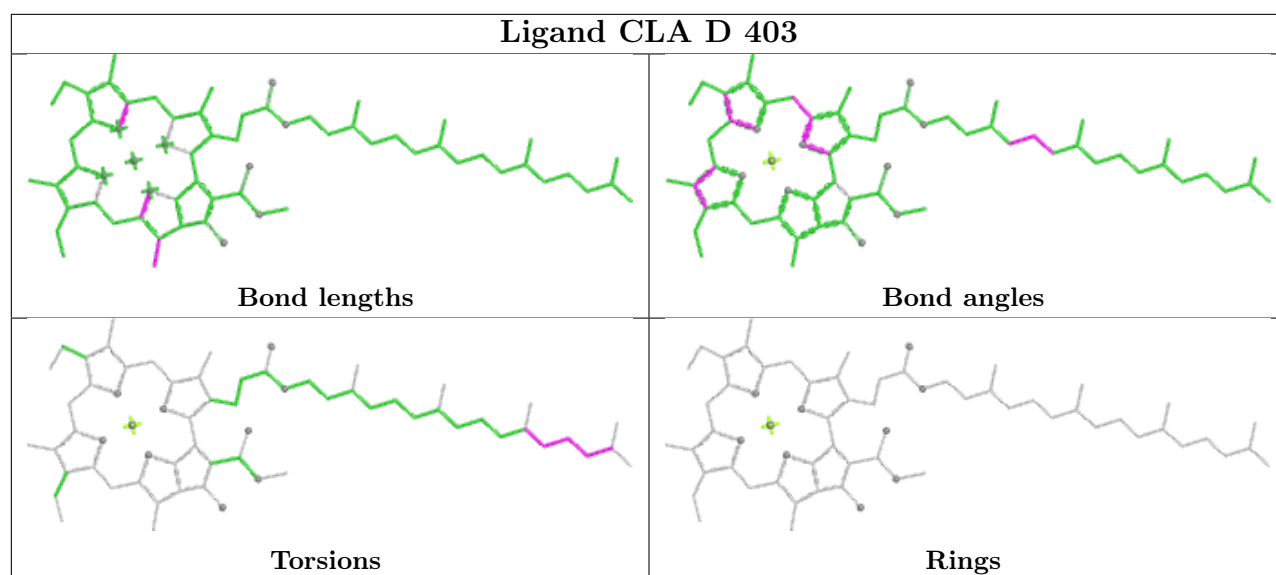
Ligand STE M 104	
	
Bond lengths	Bond angles
	
Torsions	Rings



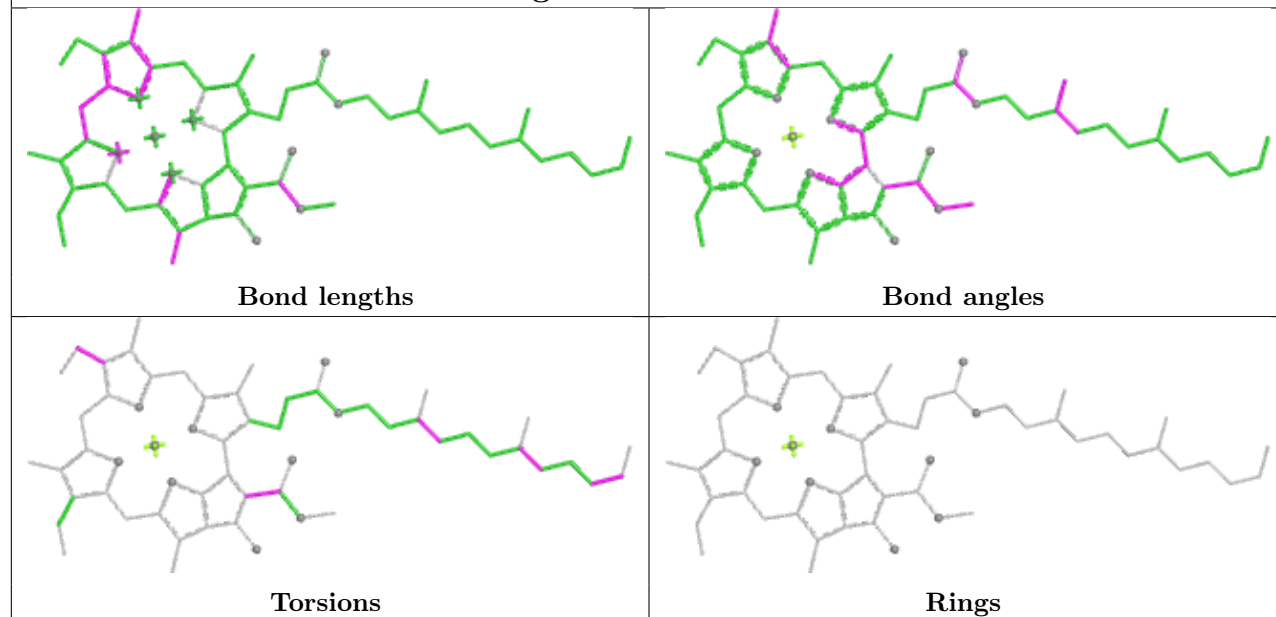




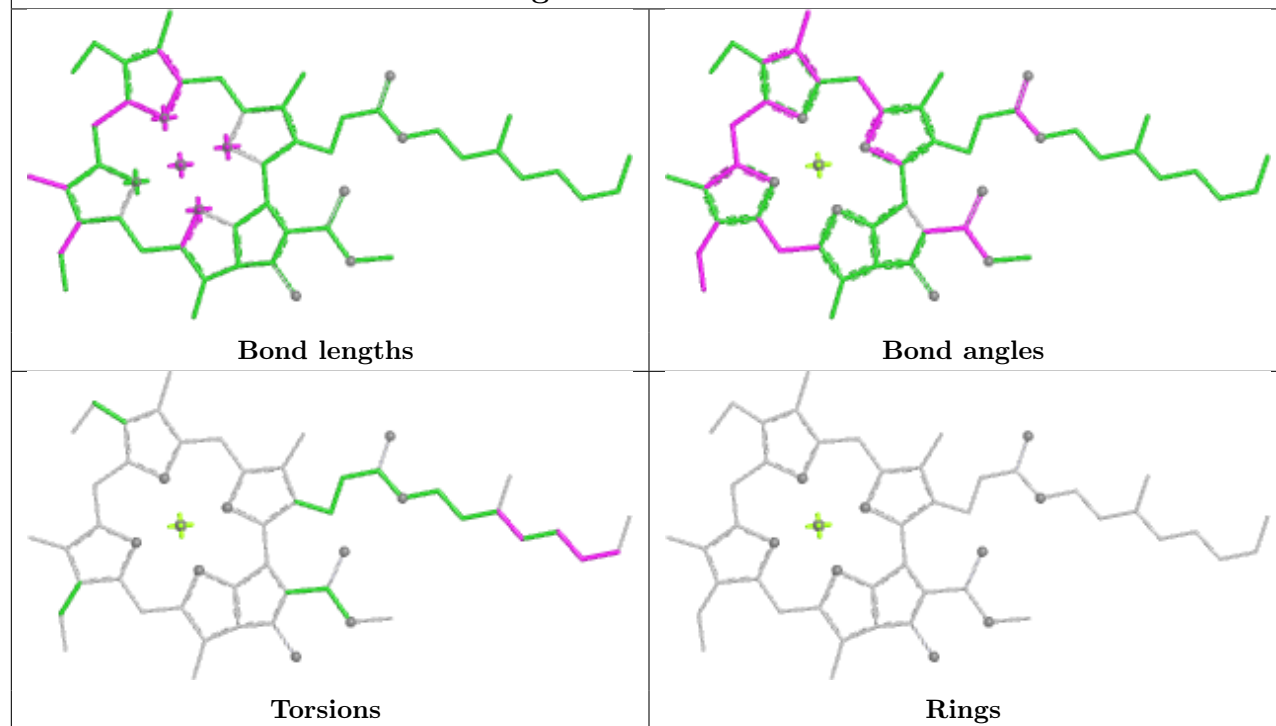


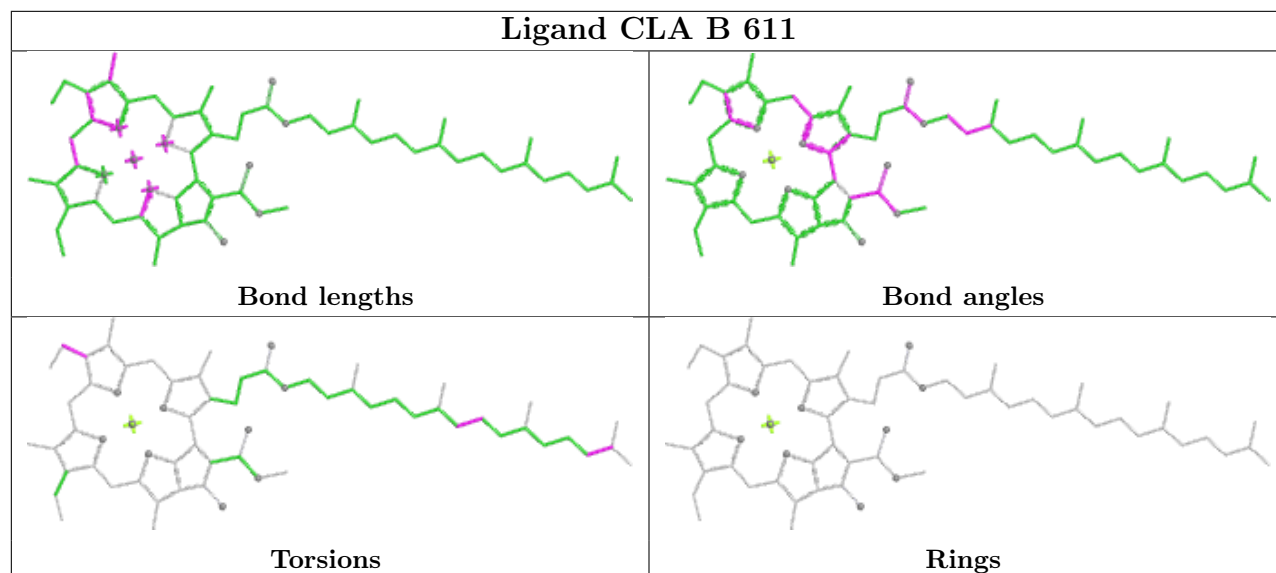
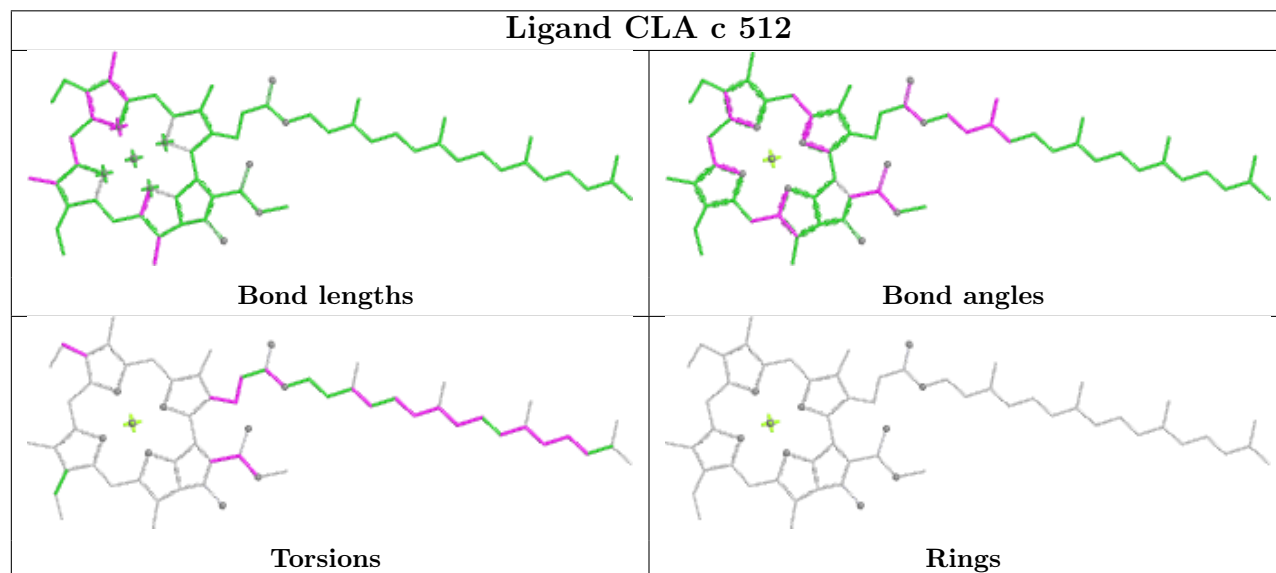
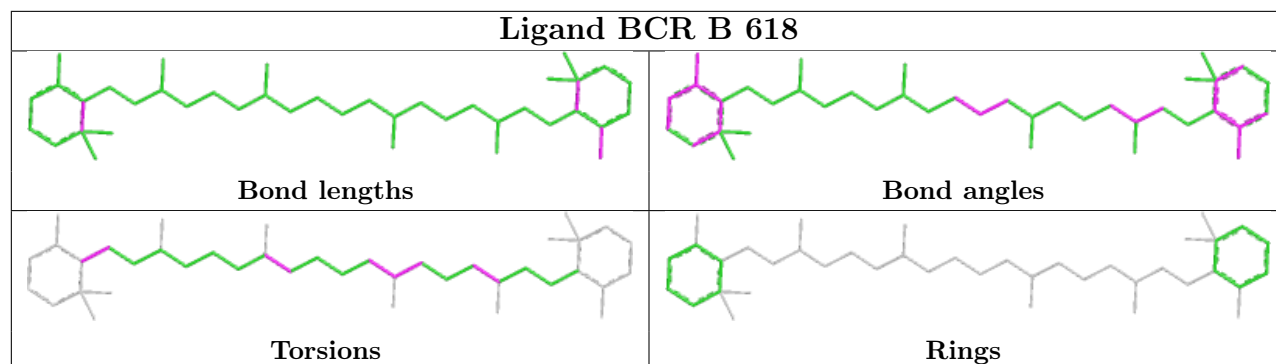


Ligand CLA C 505

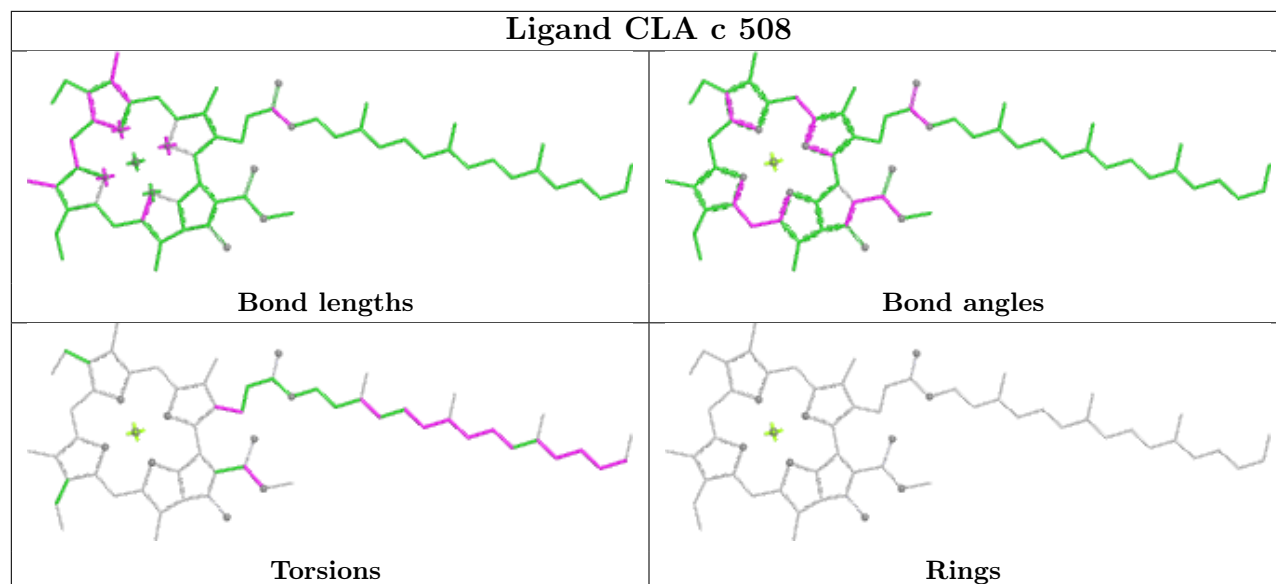


Ligand CLA A 405

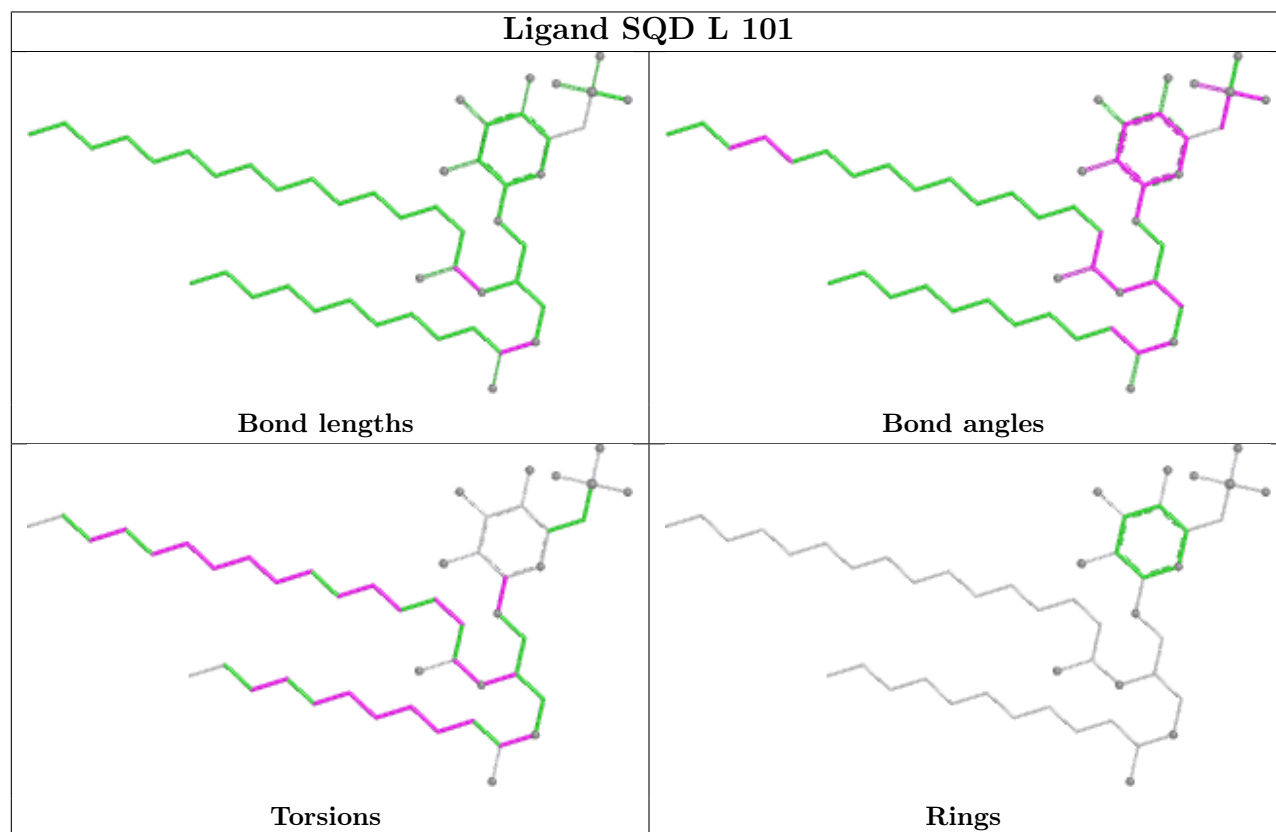


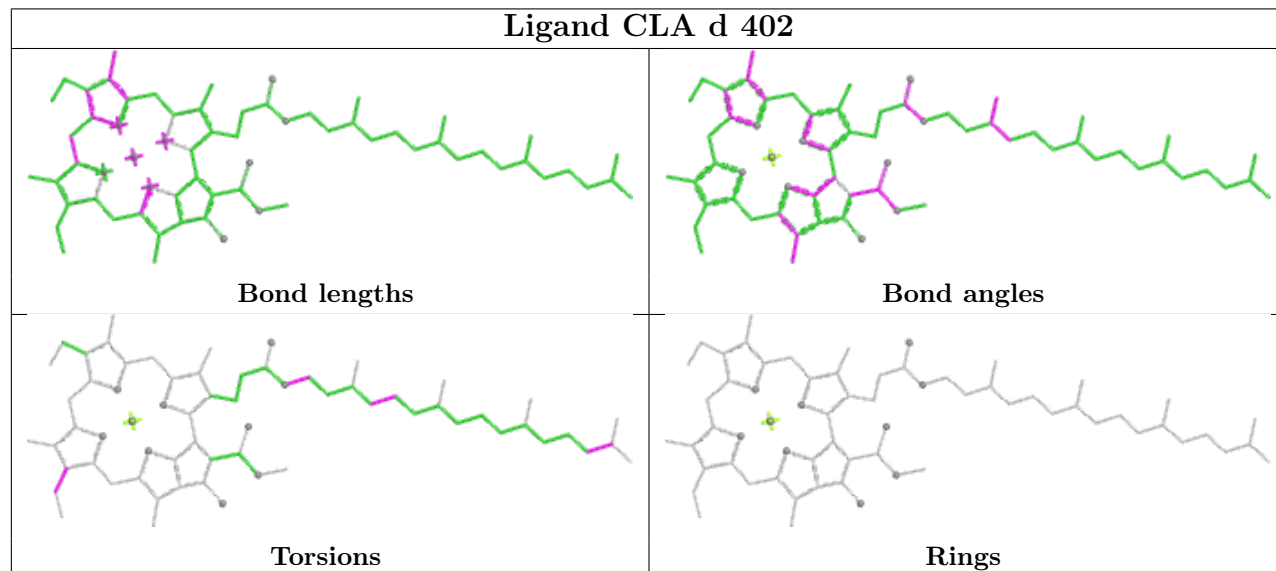
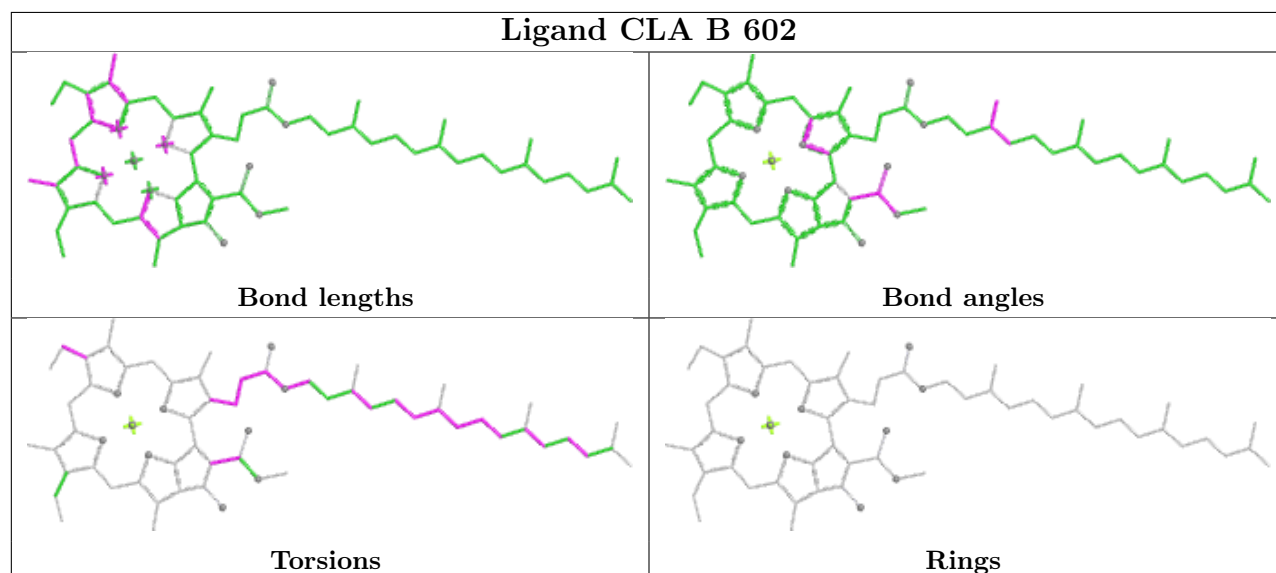
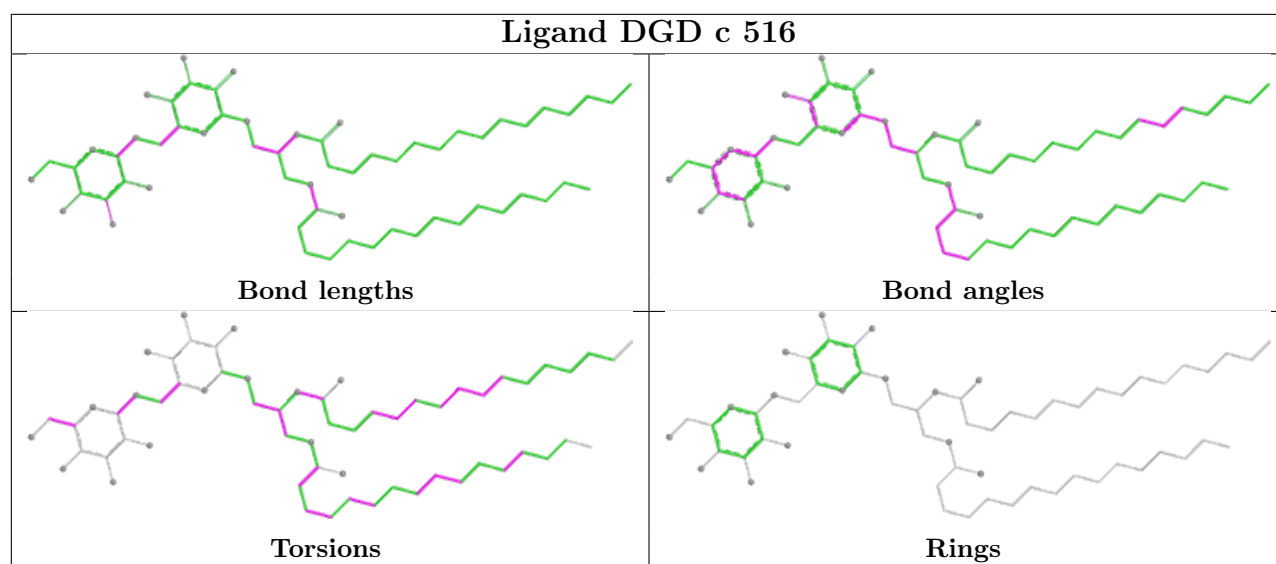


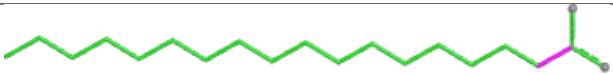
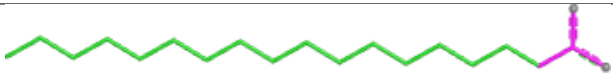
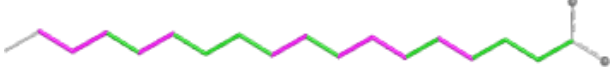
Ligand CLA c 508



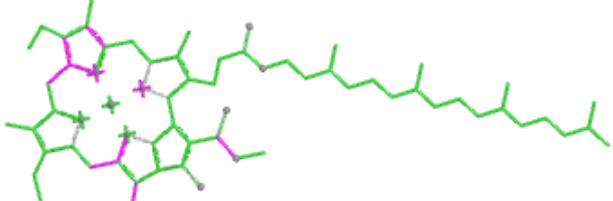
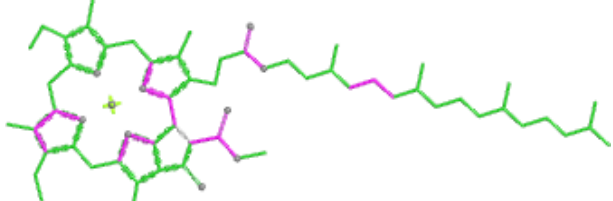
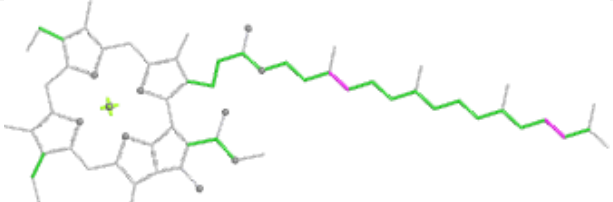
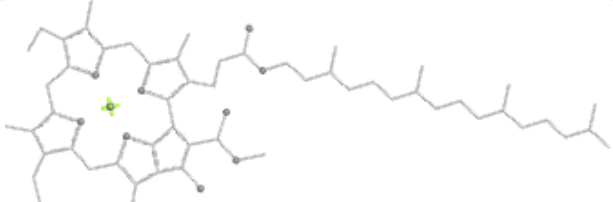
Ligand SQD L 101



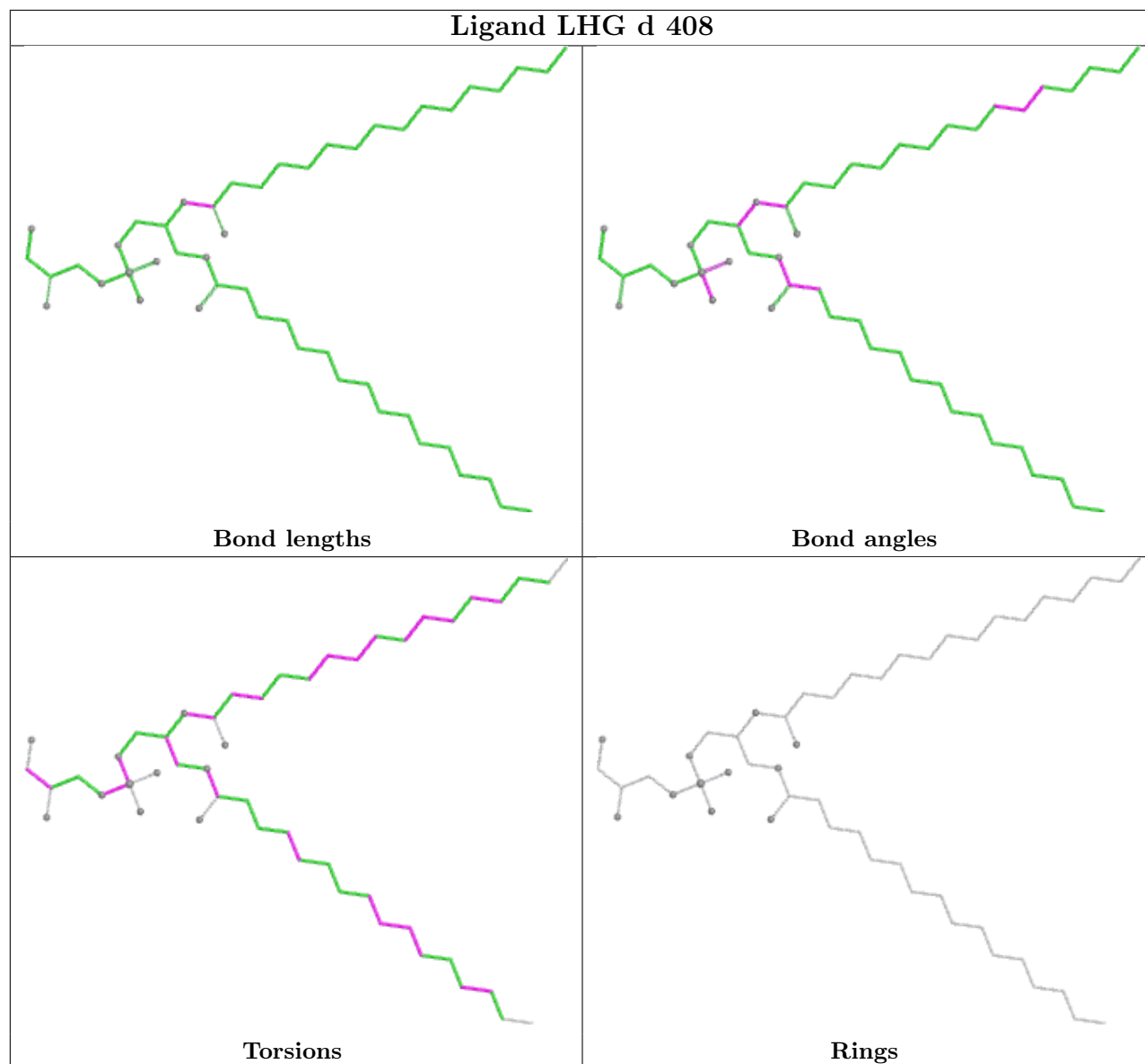


Ligand STE b 621	
 Bond lengths	 Bond angles
 Torsions	 Rings

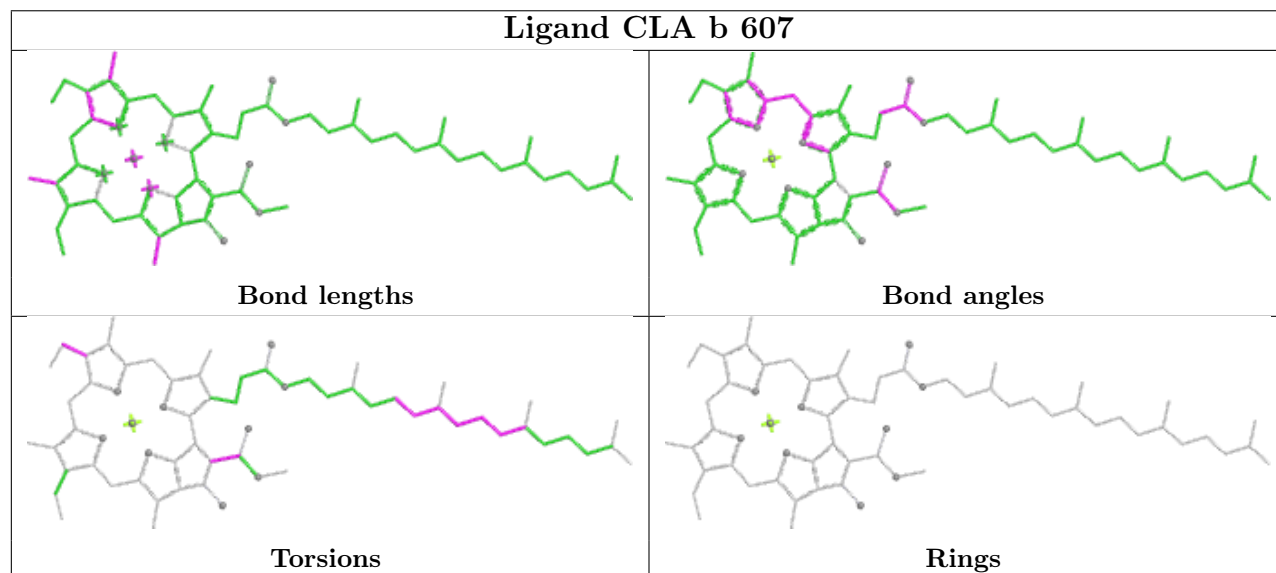
Ligand STE k 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

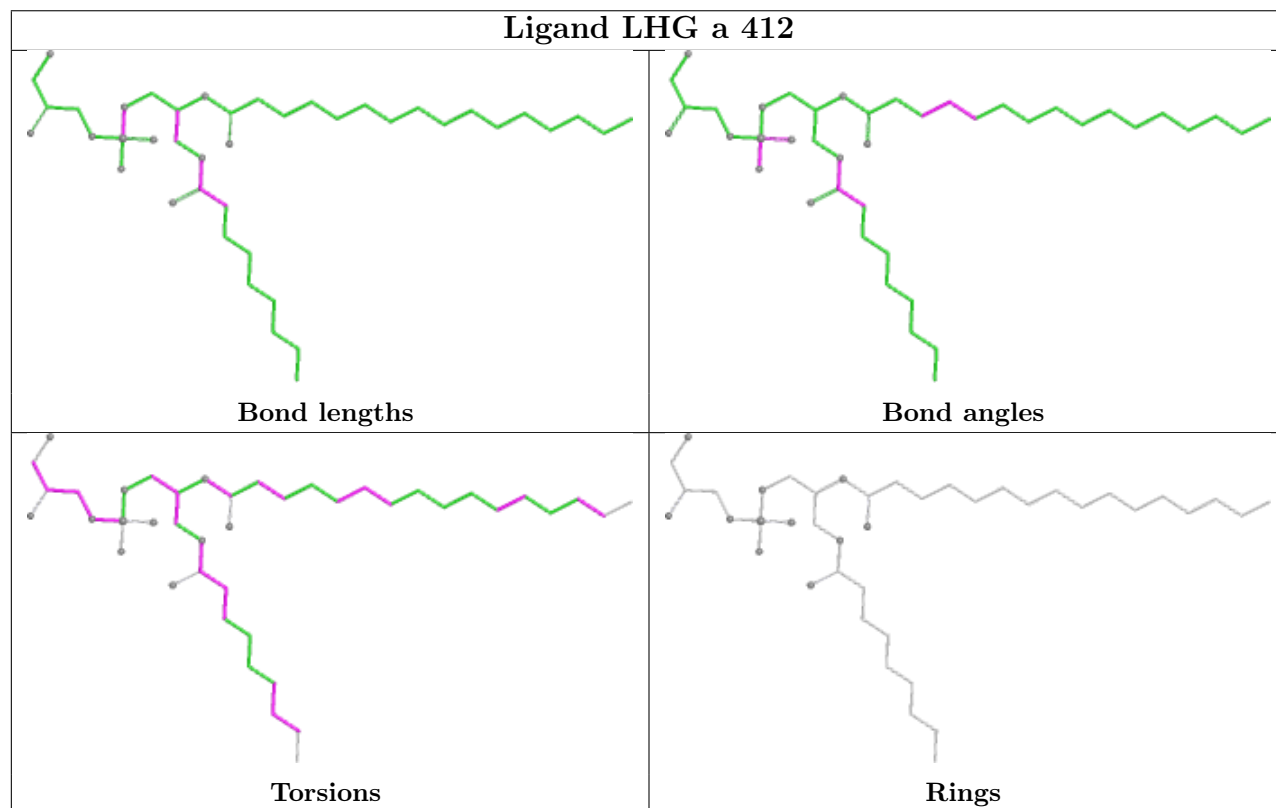
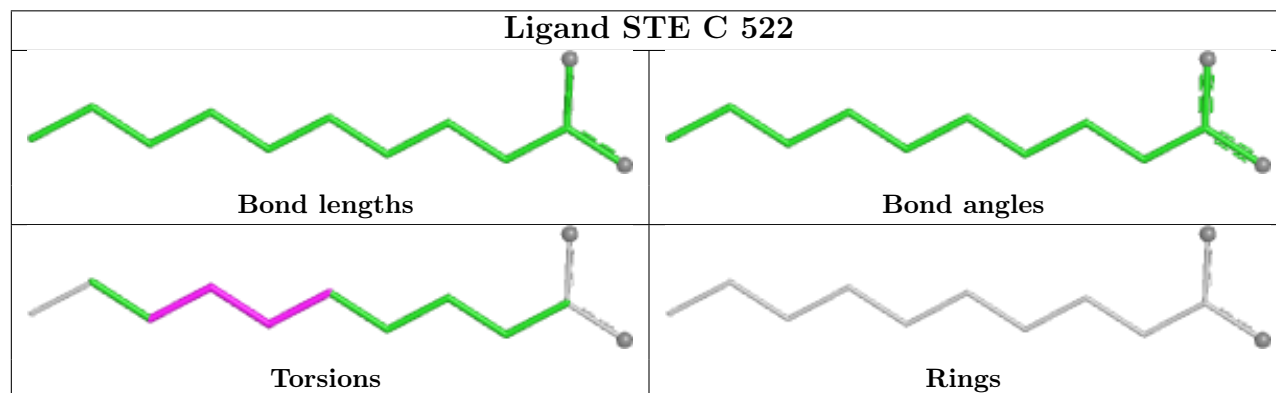
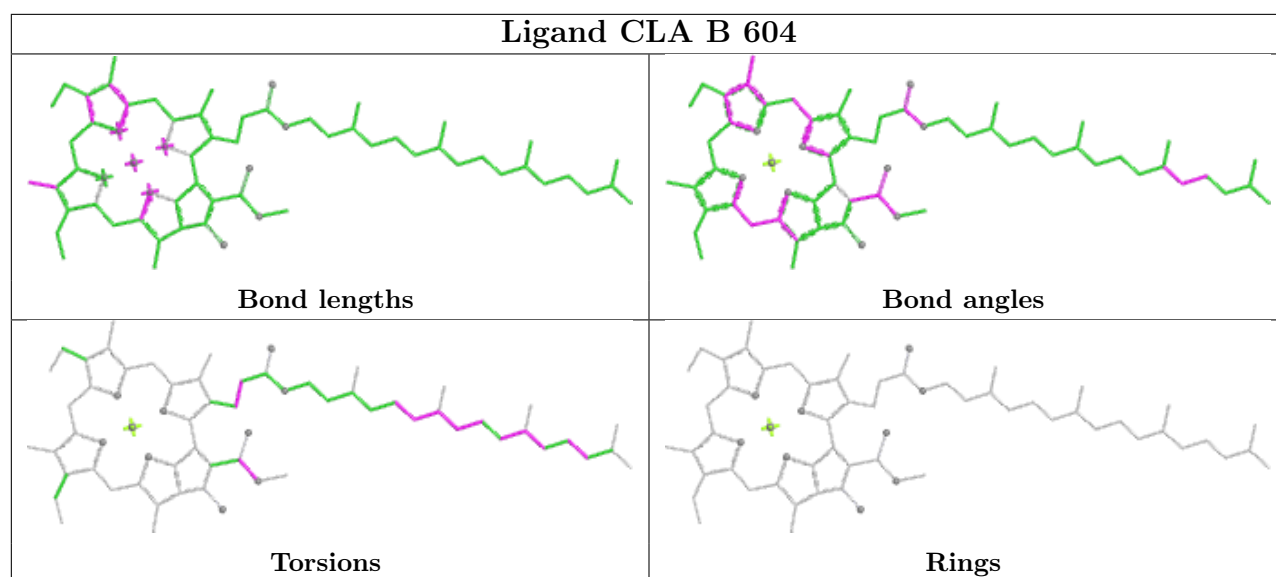
Ligand CLA B 610	
 Bond lengths	 Bond angles
 Torsions	 Rings

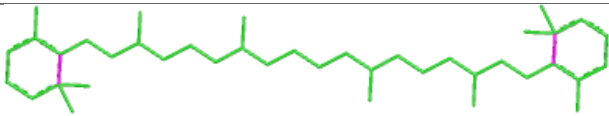
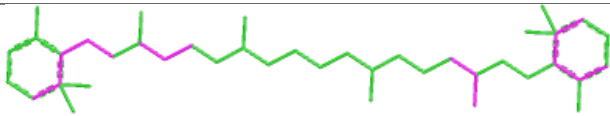
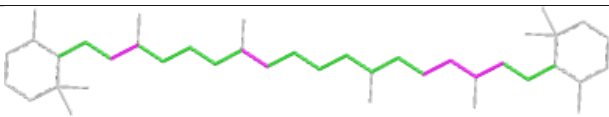
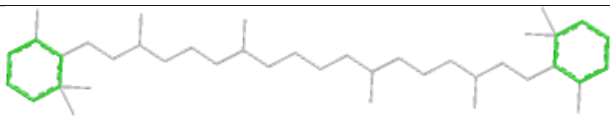
Ligand LHG d 408

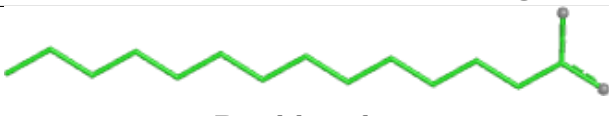
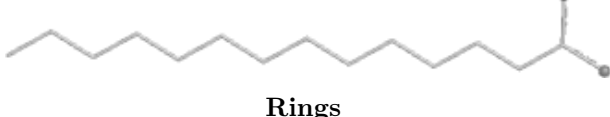


Ligand CLA b 607

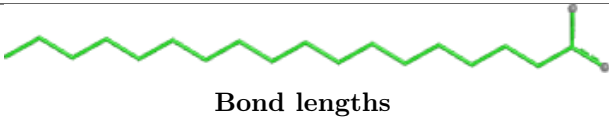
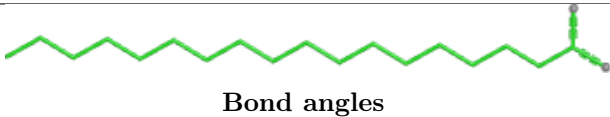


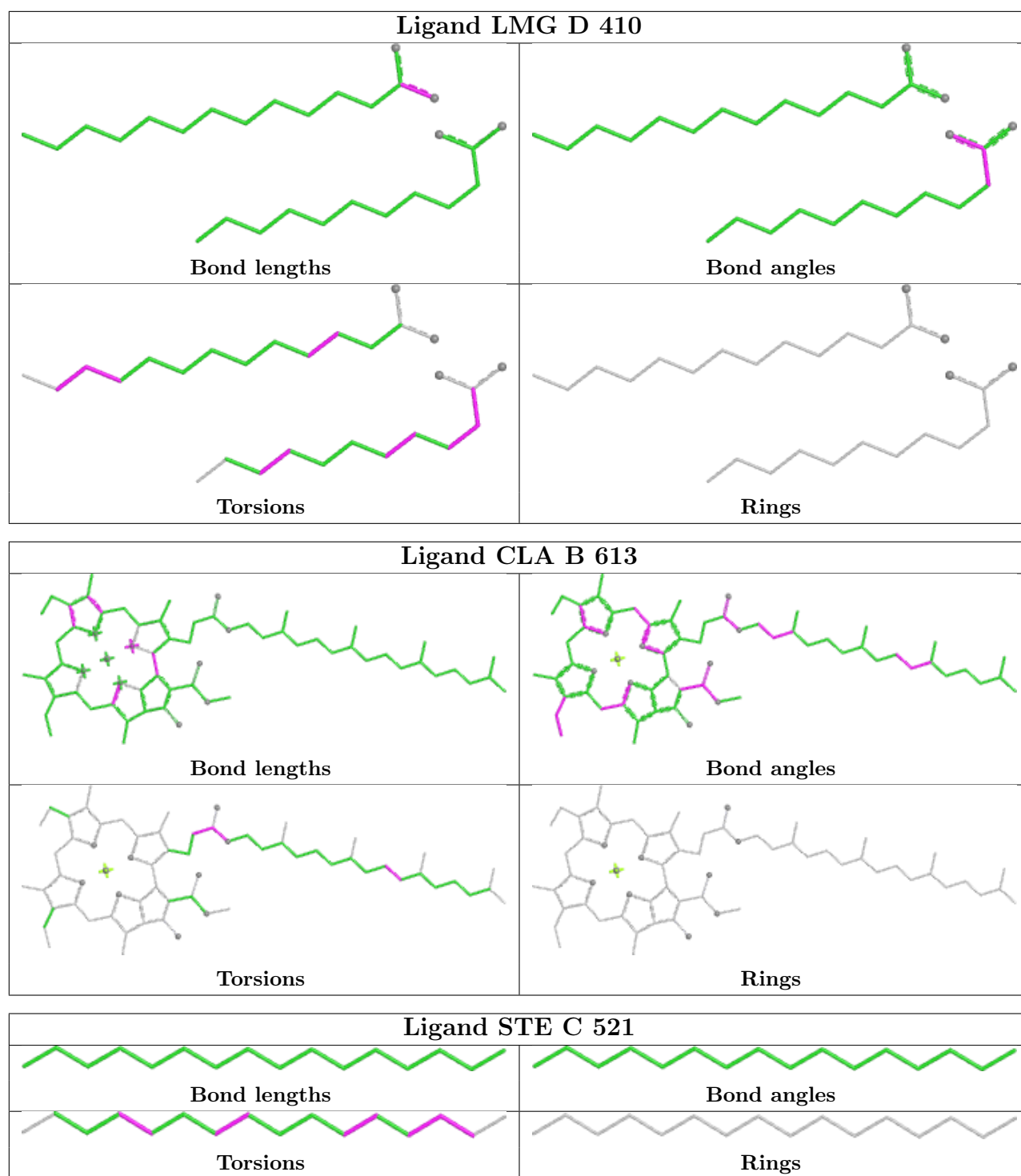


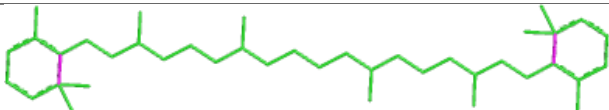
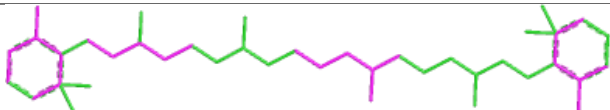
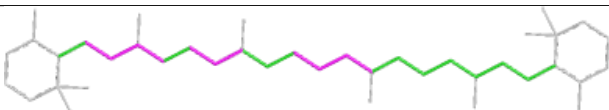
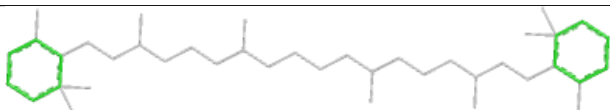
Ligand BCR k 103	
	
Bond lengths	Bond angles
	
Torsions	Rings

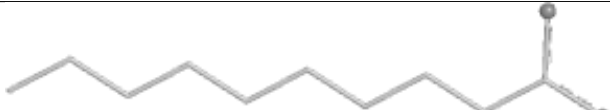
Ligand STE b 623	
	
Bond lengths	Bond angles
	
Torsions	Rings

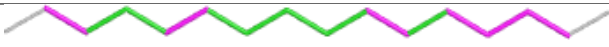
Ligand STE H 103	
	
Bond lengths	Bond angles
	
Torsions	Rings

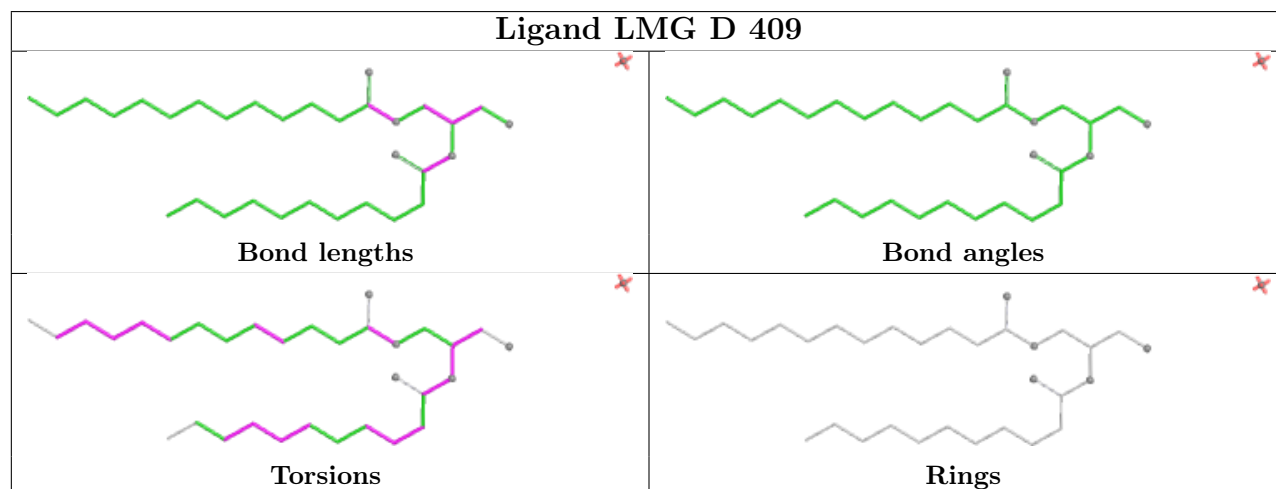
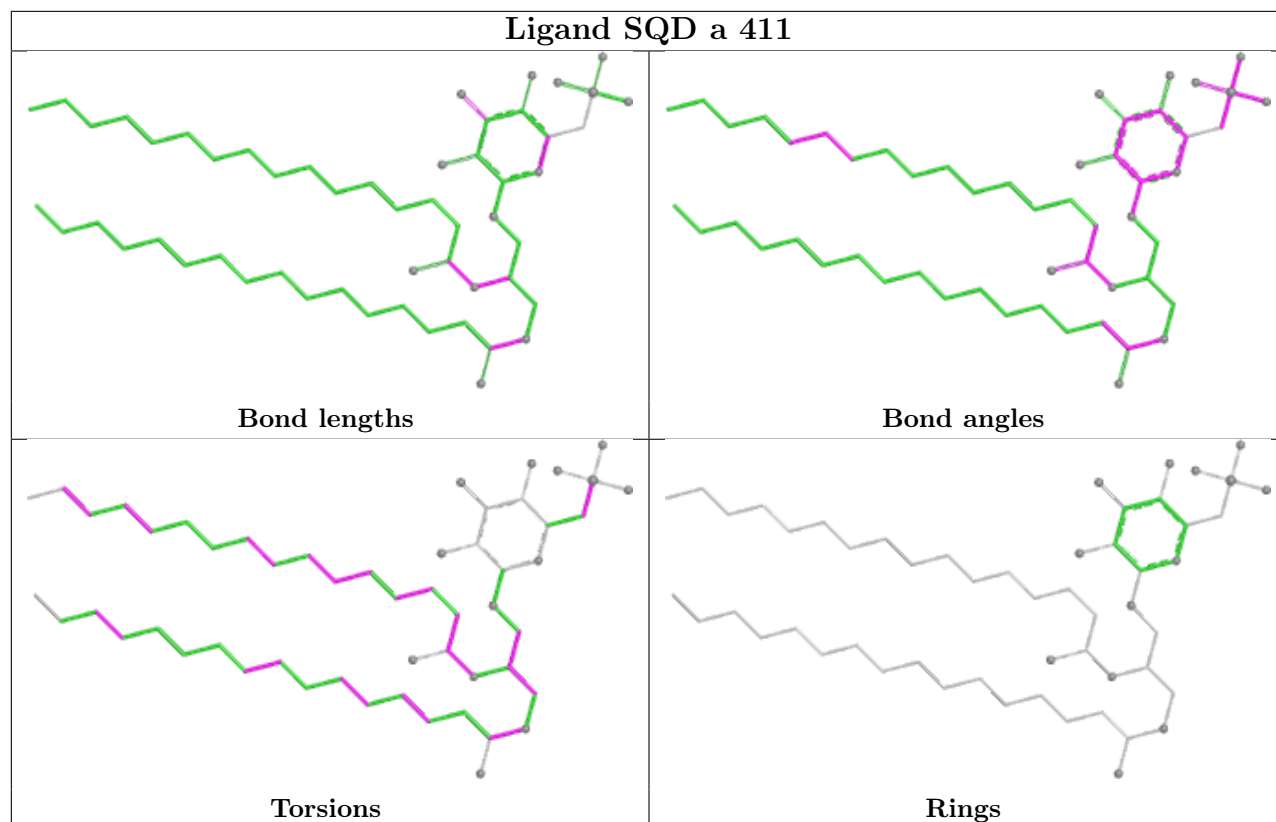
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Bond lengths	Bond angles
	
Torsions	Rings

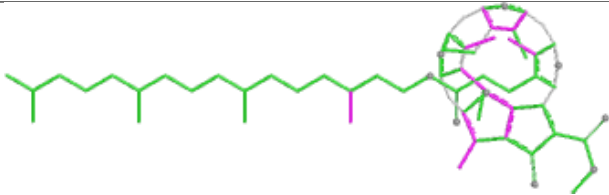
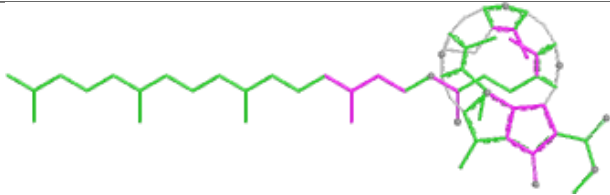
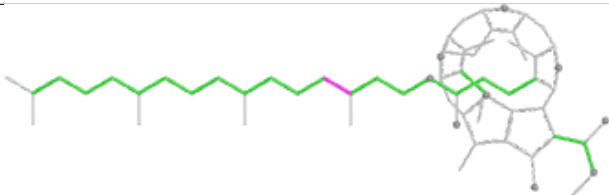
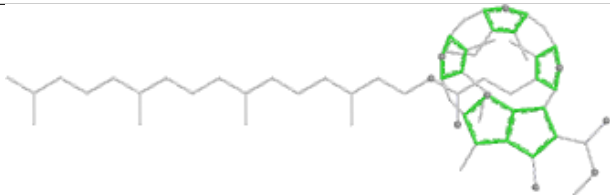


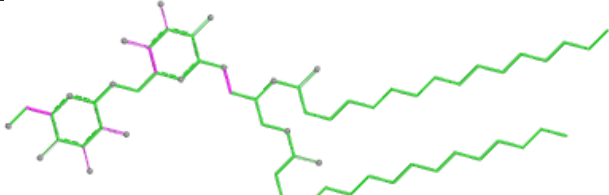
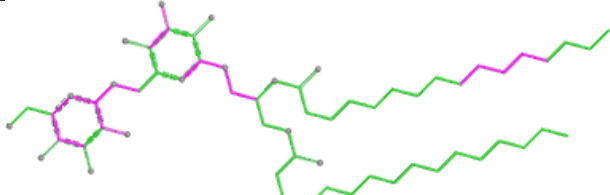
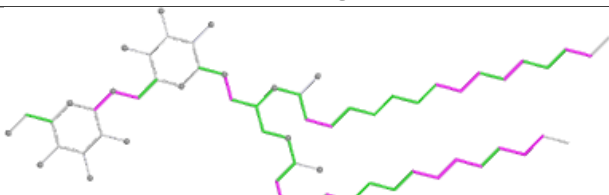
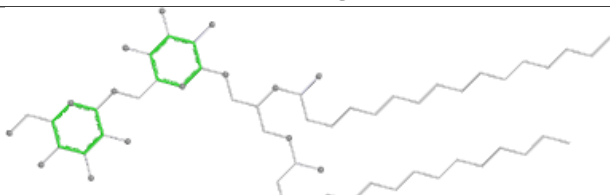
Ligand BCR Z 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

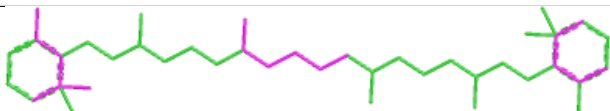
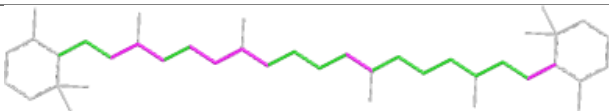
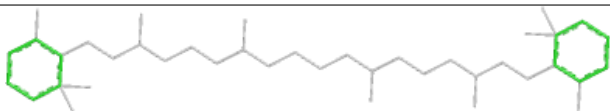
Ligand STE L 103	
	
Bond lengths	Bond angles
	
Torsions	Rings

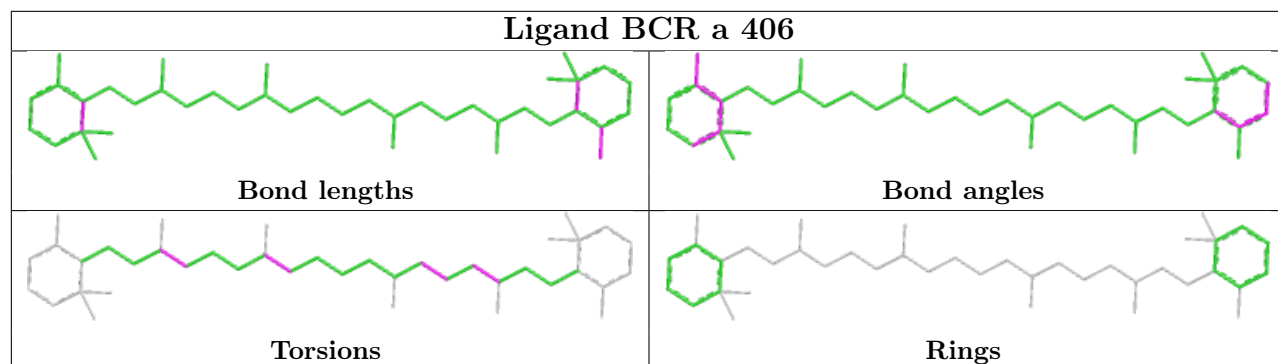
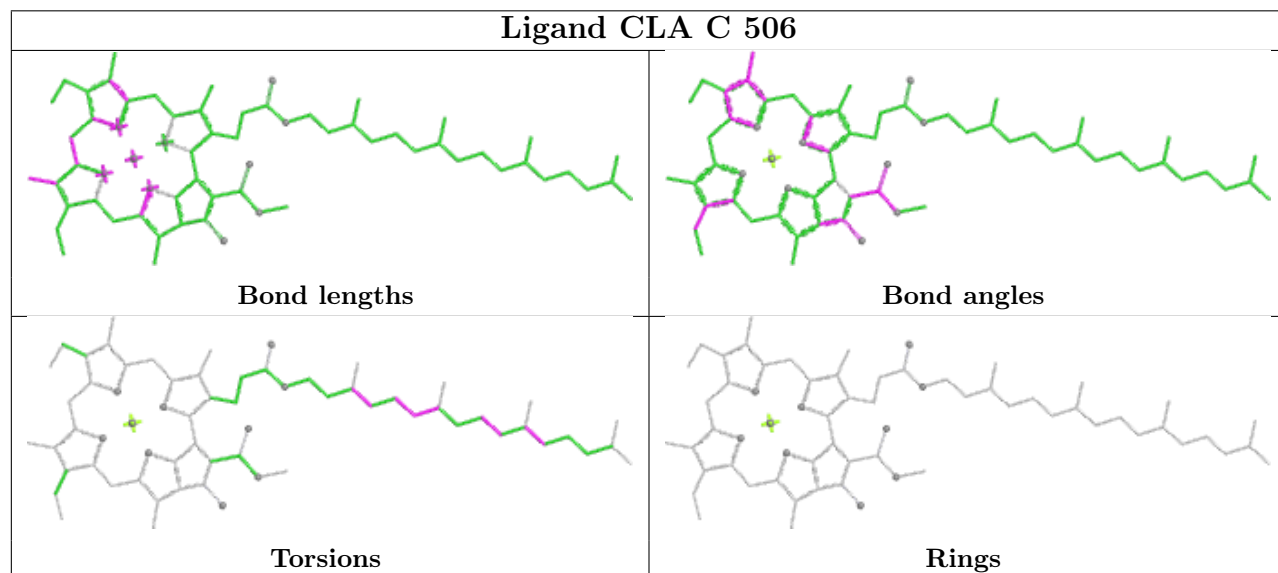
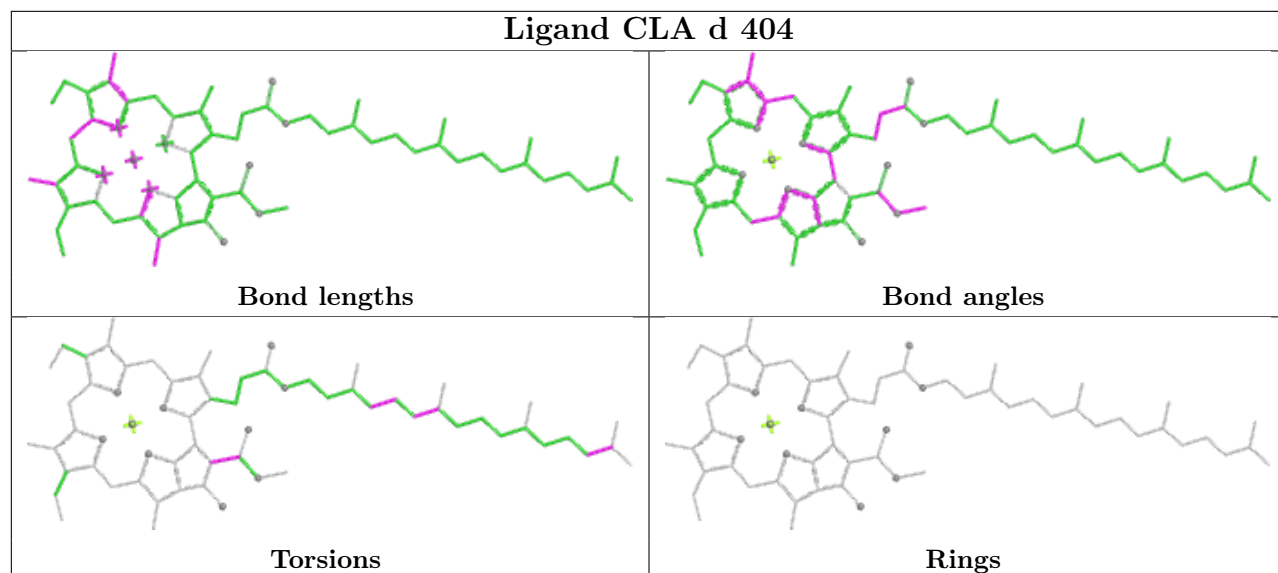
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Bond lengths	Bond angles
	
Torsions	Rings



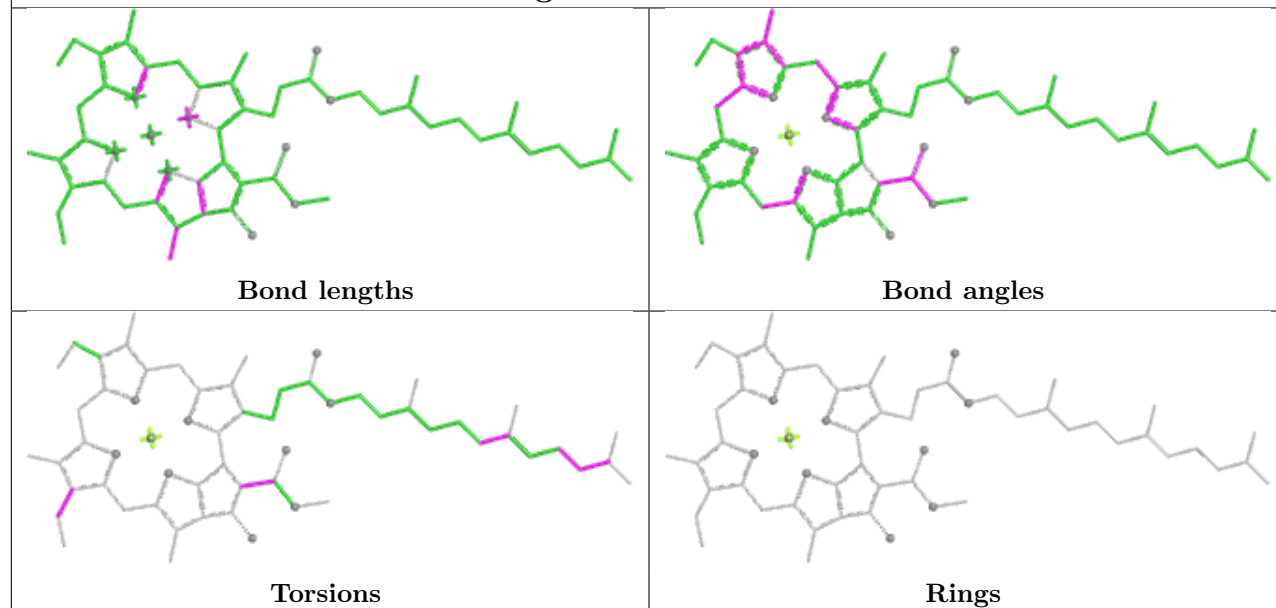
Ligand PHO A 404	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand DGD c 517	
	
Bond lengths	Bond angles
	
Torsions	Rings

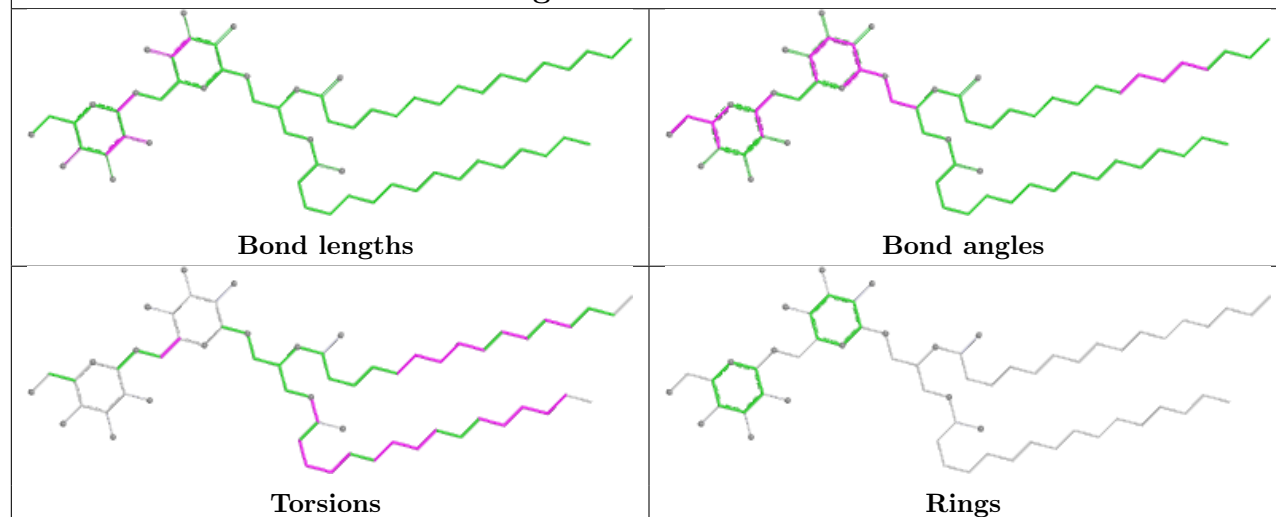
Ligand BCR B 619	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR a 406**Ligand CLA C 506****Ligand CLA d 404**

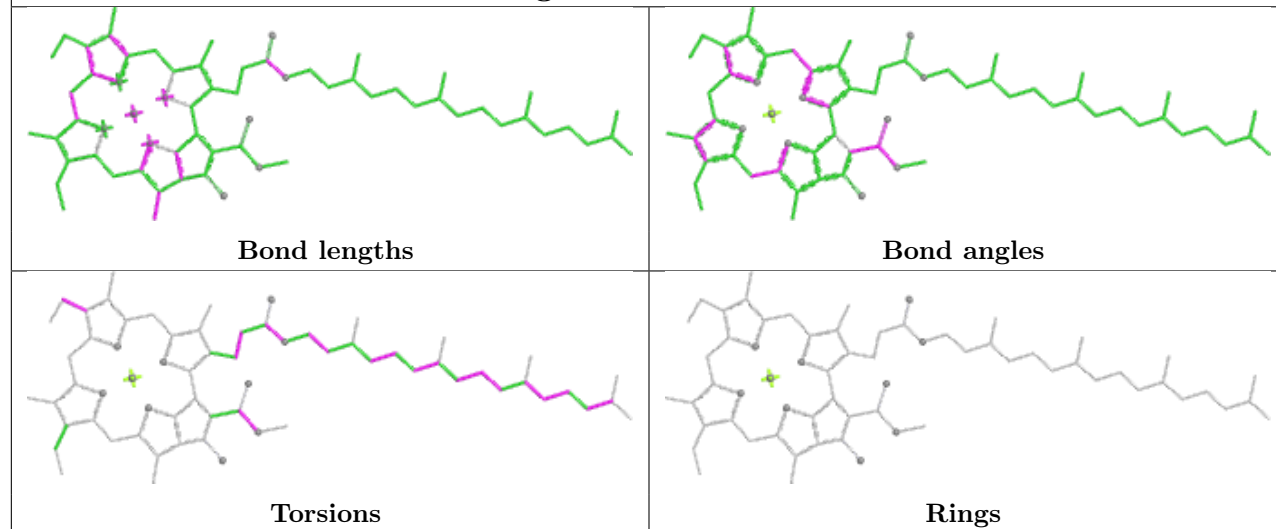
Ligand CLA b 616

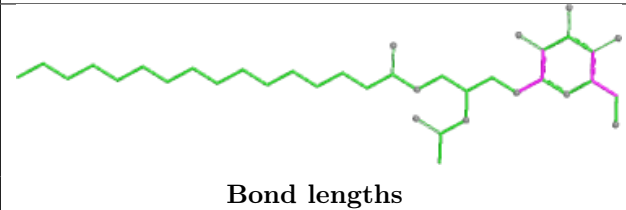
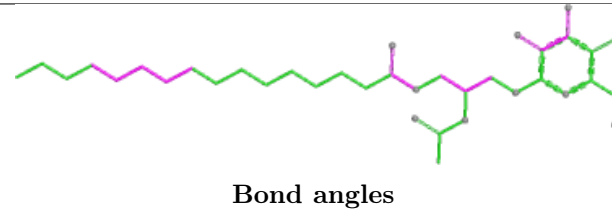
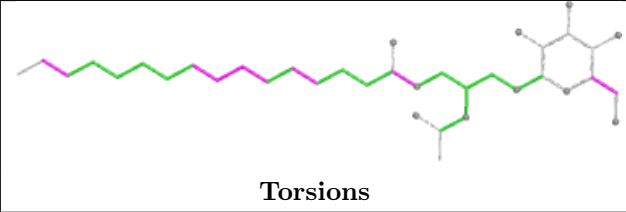
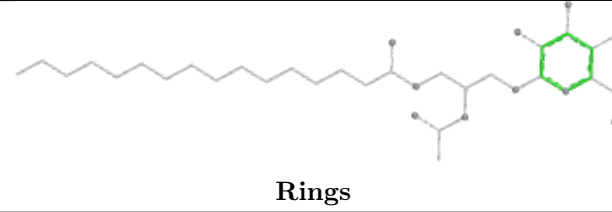


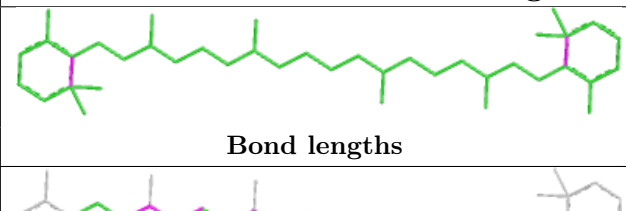
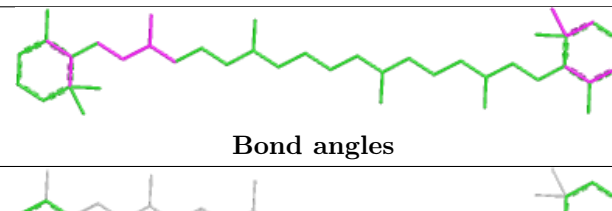
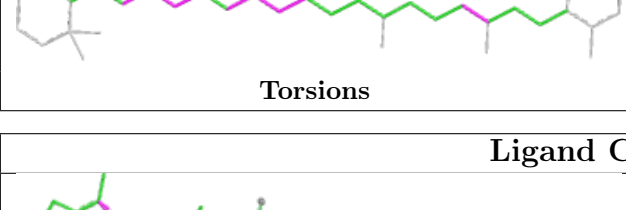
Ligand DGD c 518

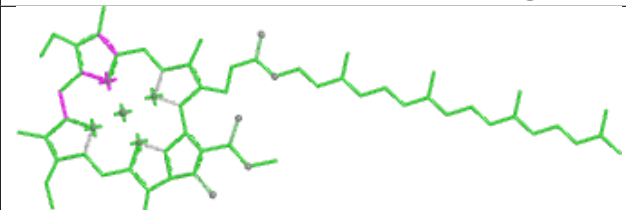
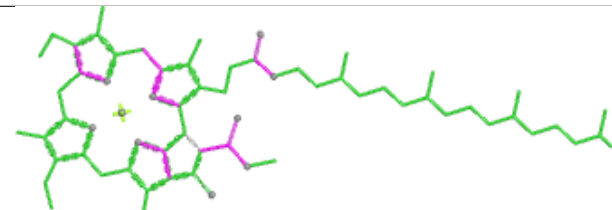
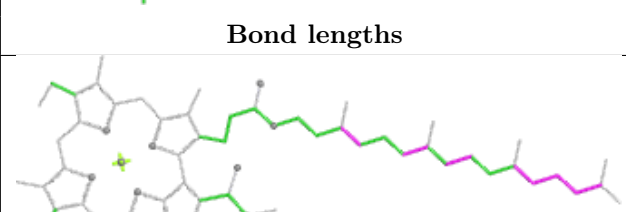
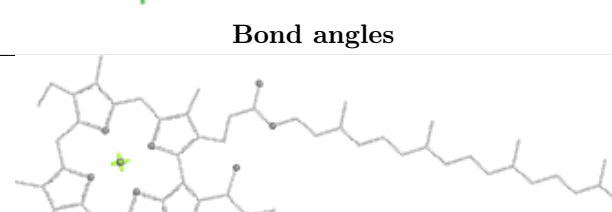


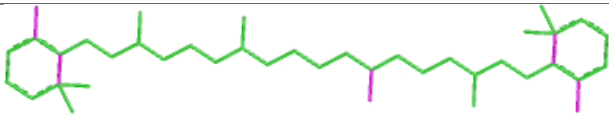
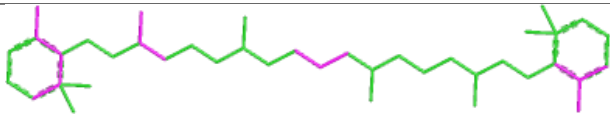
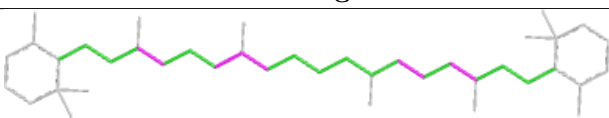
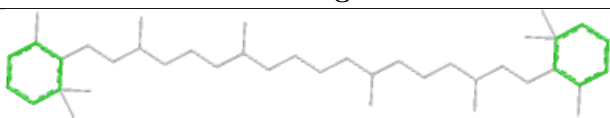
Ligand CLA b 601

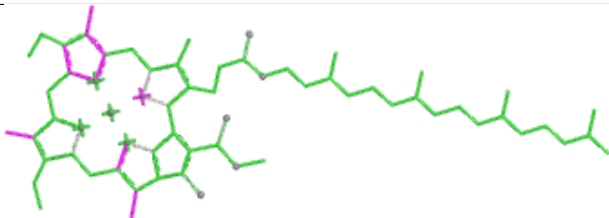
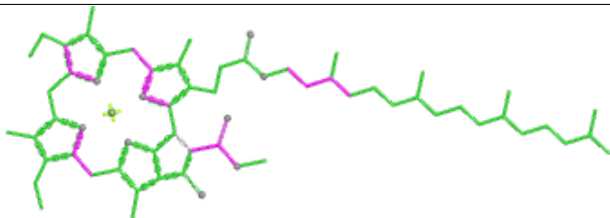
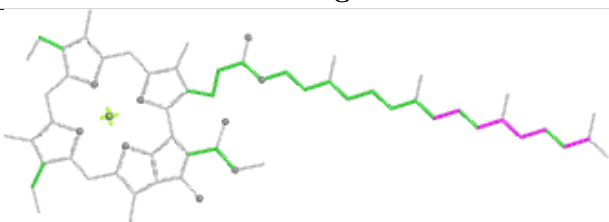
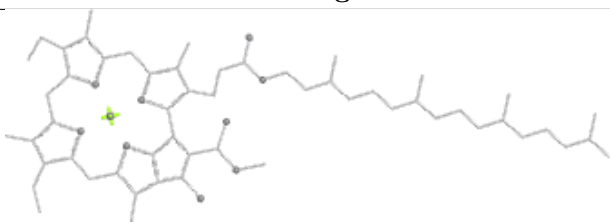


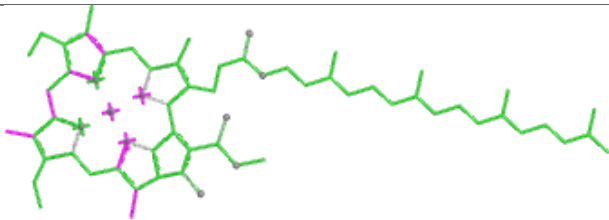
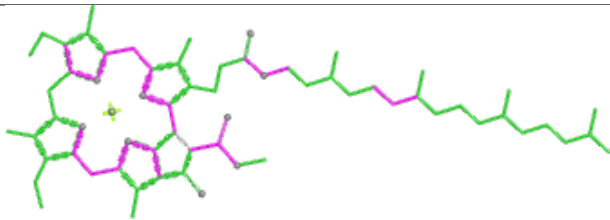
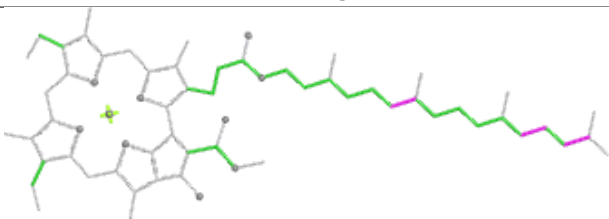
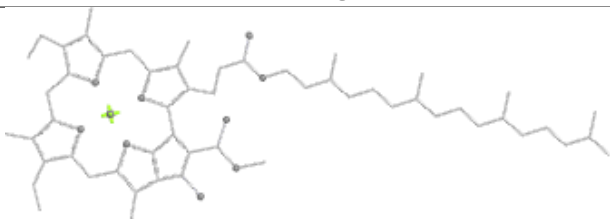
Ligand LMG c 519	
	
Bond lengths	Bond angles
	
Torsions	Rings

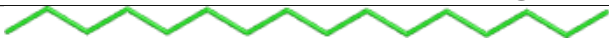
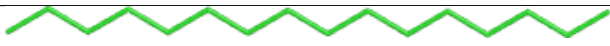
Ligand BCR t 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

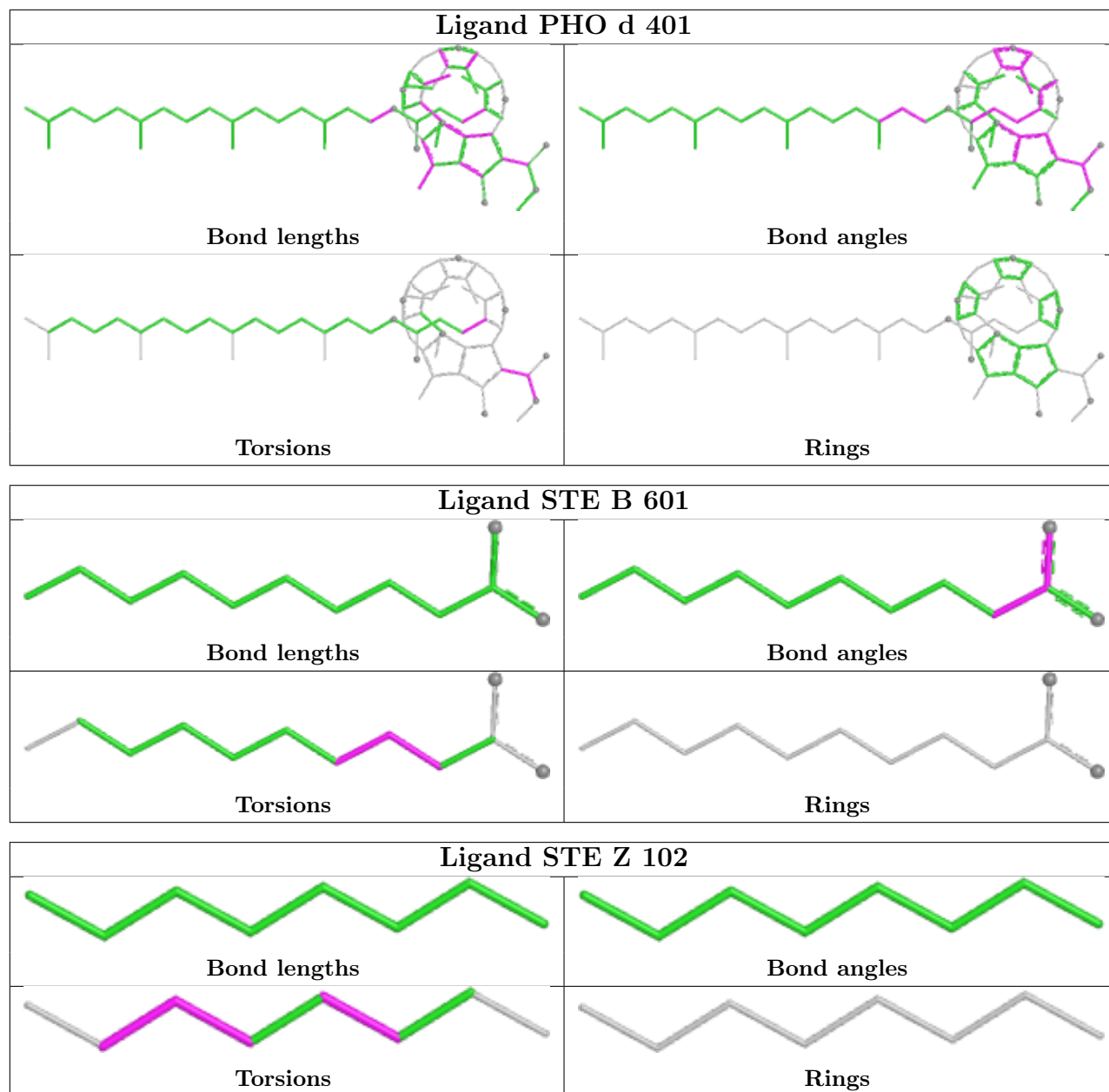
Ligand CLA C 507	
	
Bond lengths	Bond angles
	
Torsions	Rings

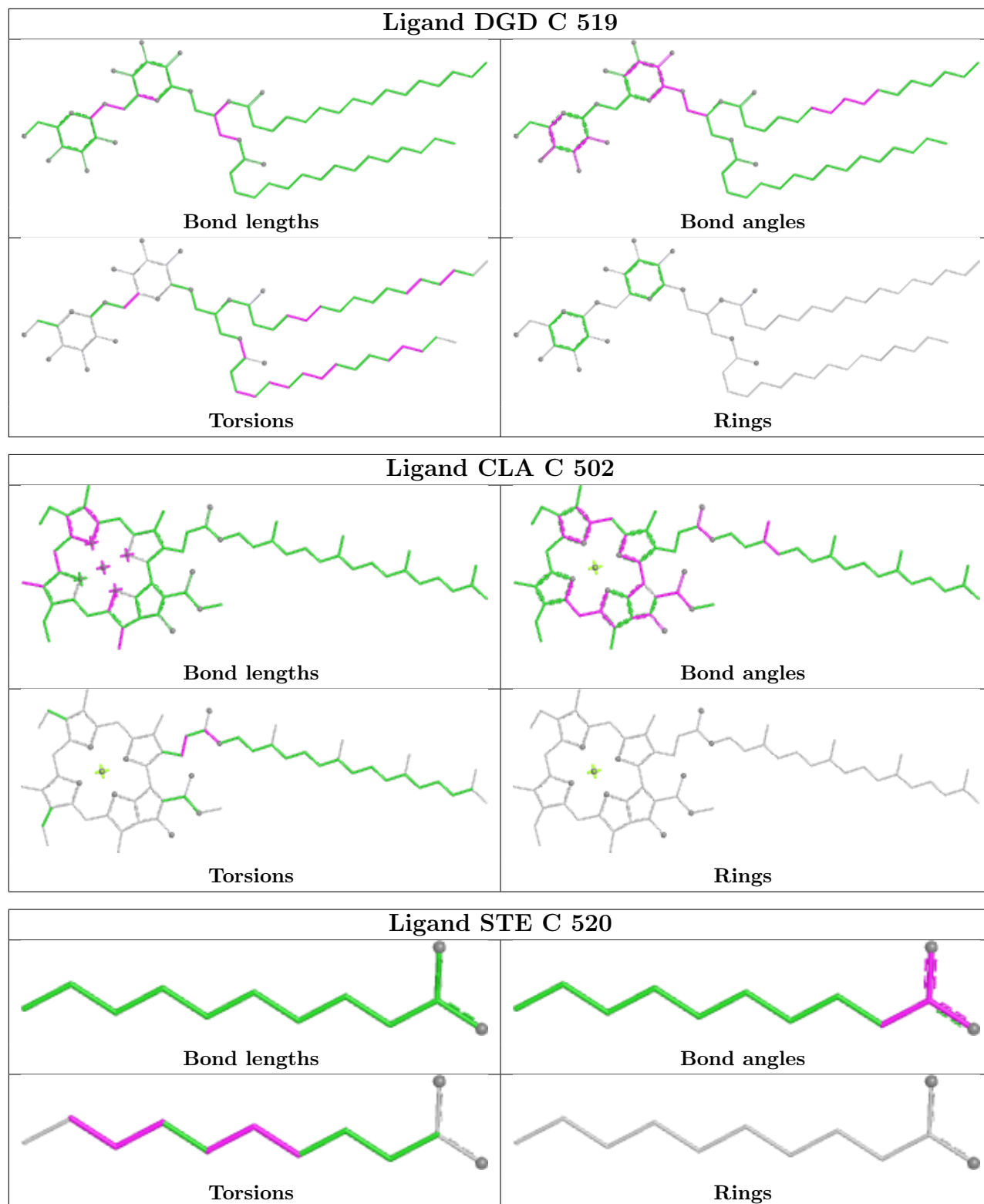
Ligand BCR C 515	
	
Bond lengths	Bond angles
	
Torsions	Rings

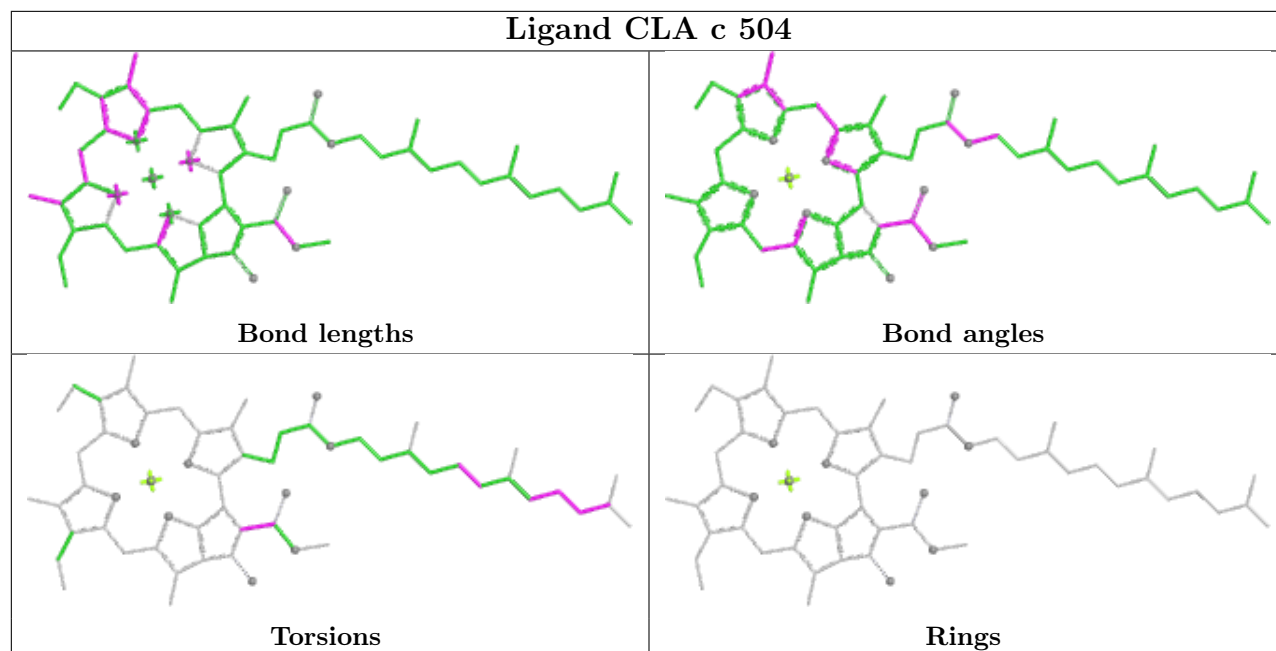
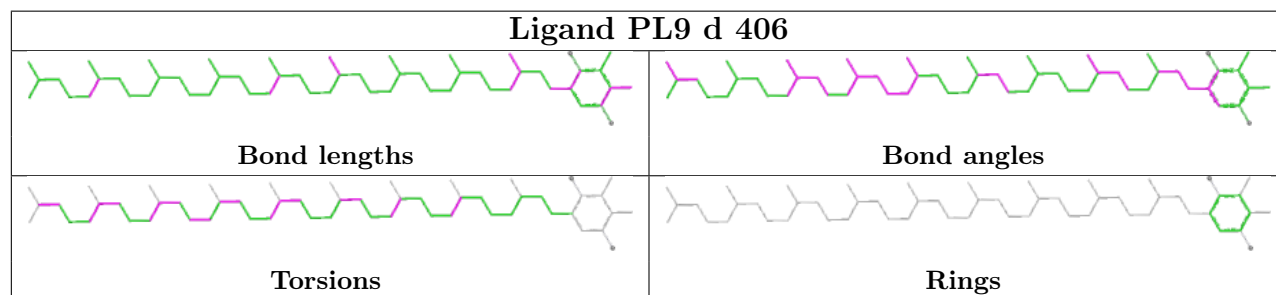
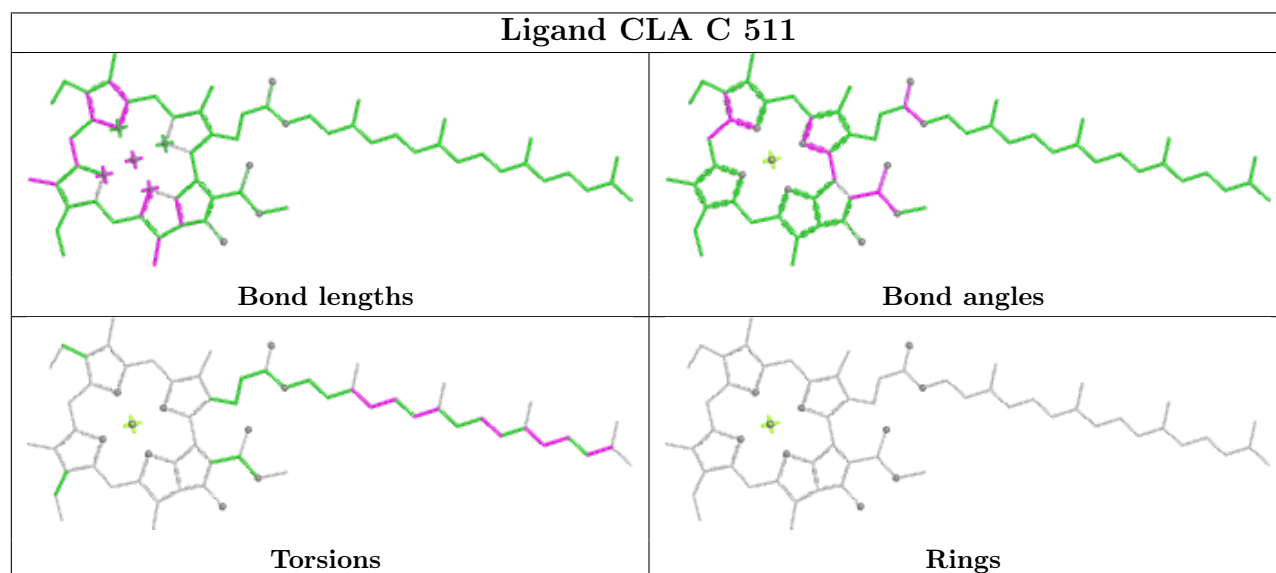
Ligand CLA B 612	
	
Bond lengths	Bond angles
	
Torsions	Rings

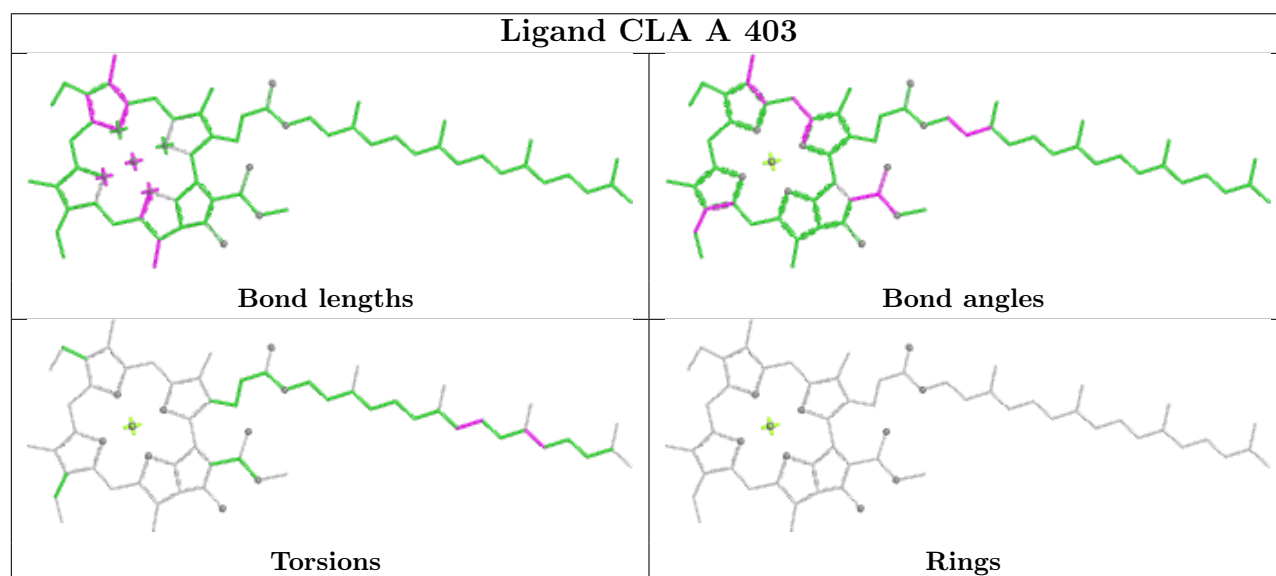
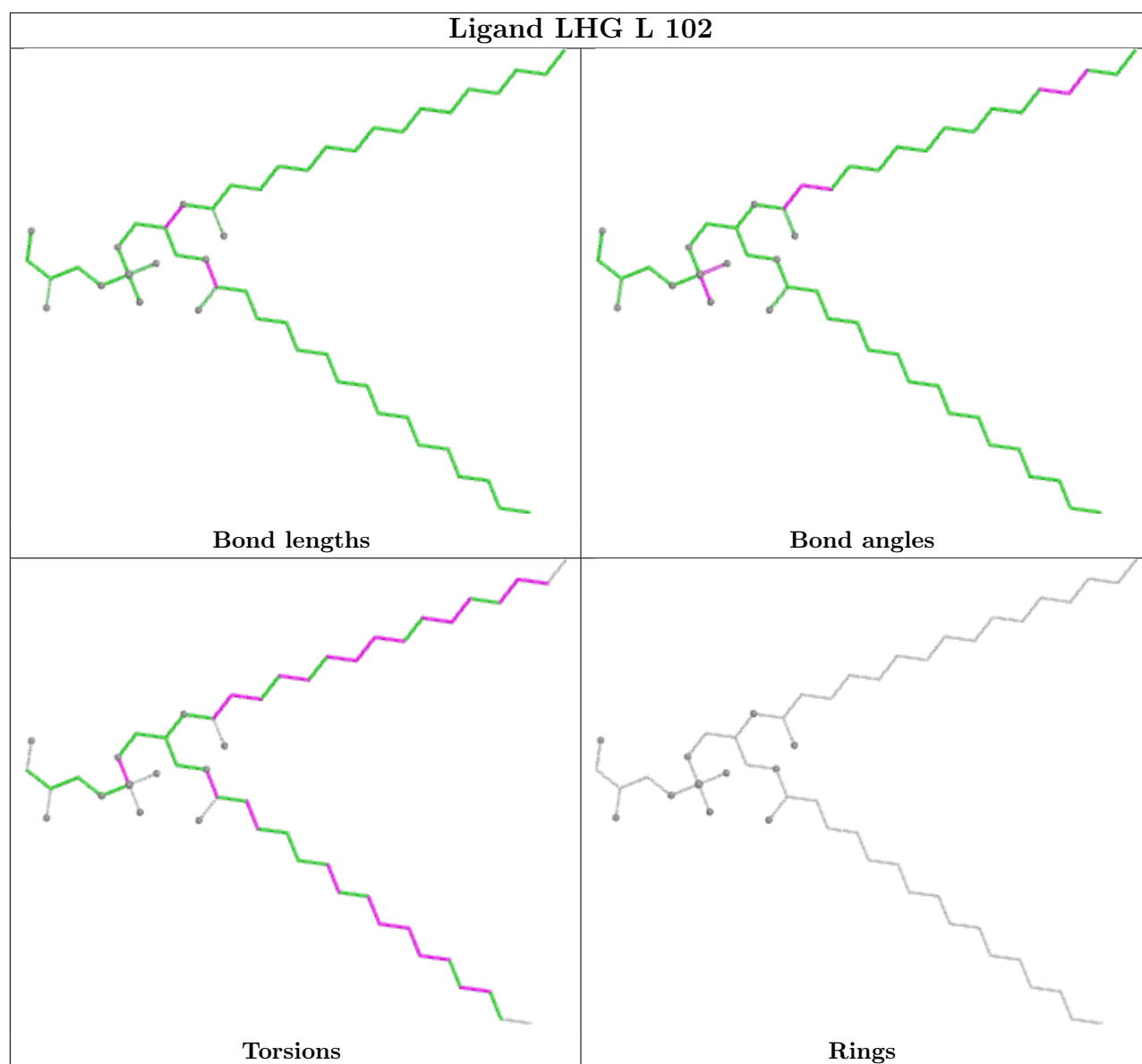
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Bond lengths	Bond angles
	
Torsions	Rings

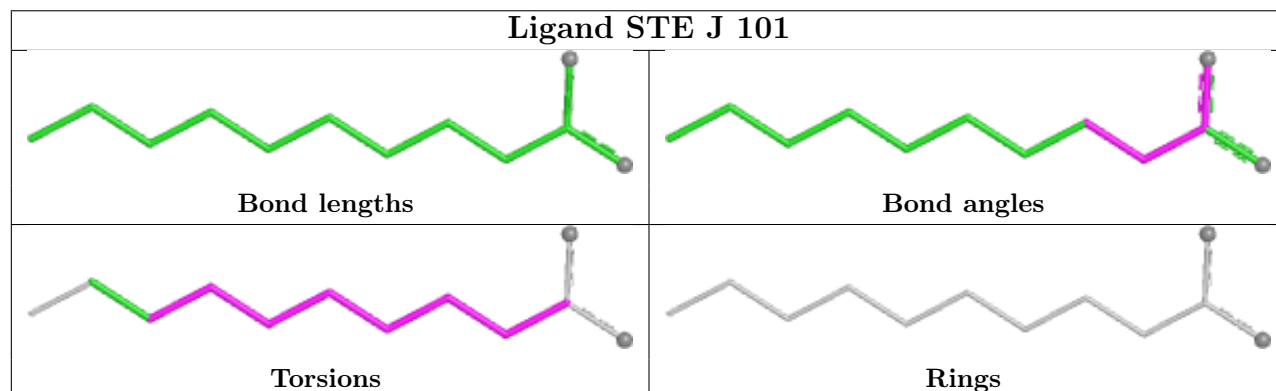
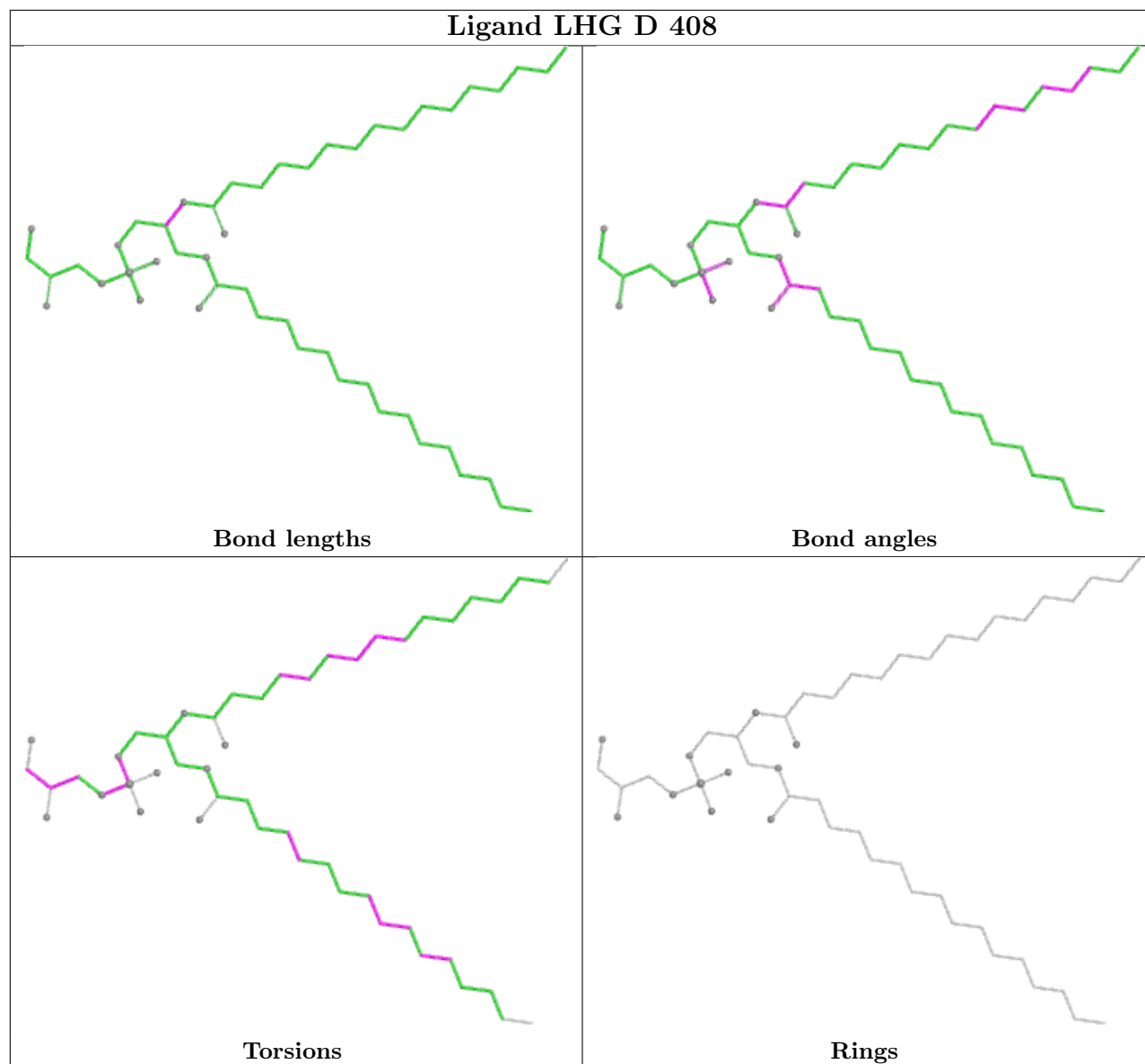
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Bond lengths	Bond angles
	
Torsions	Rings

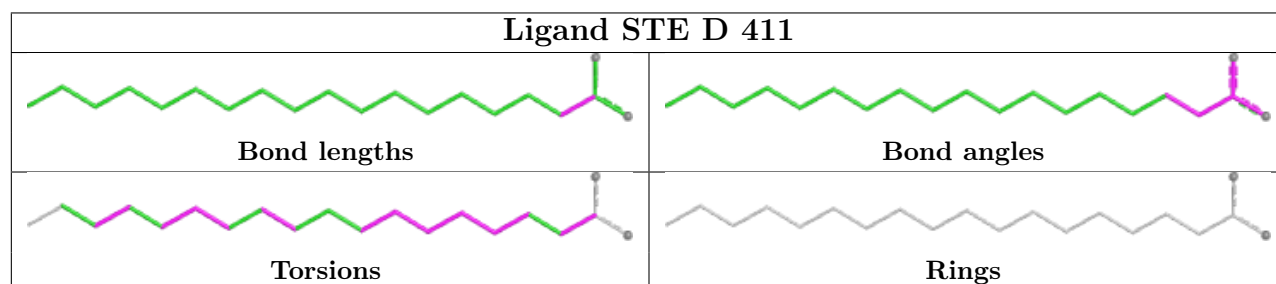
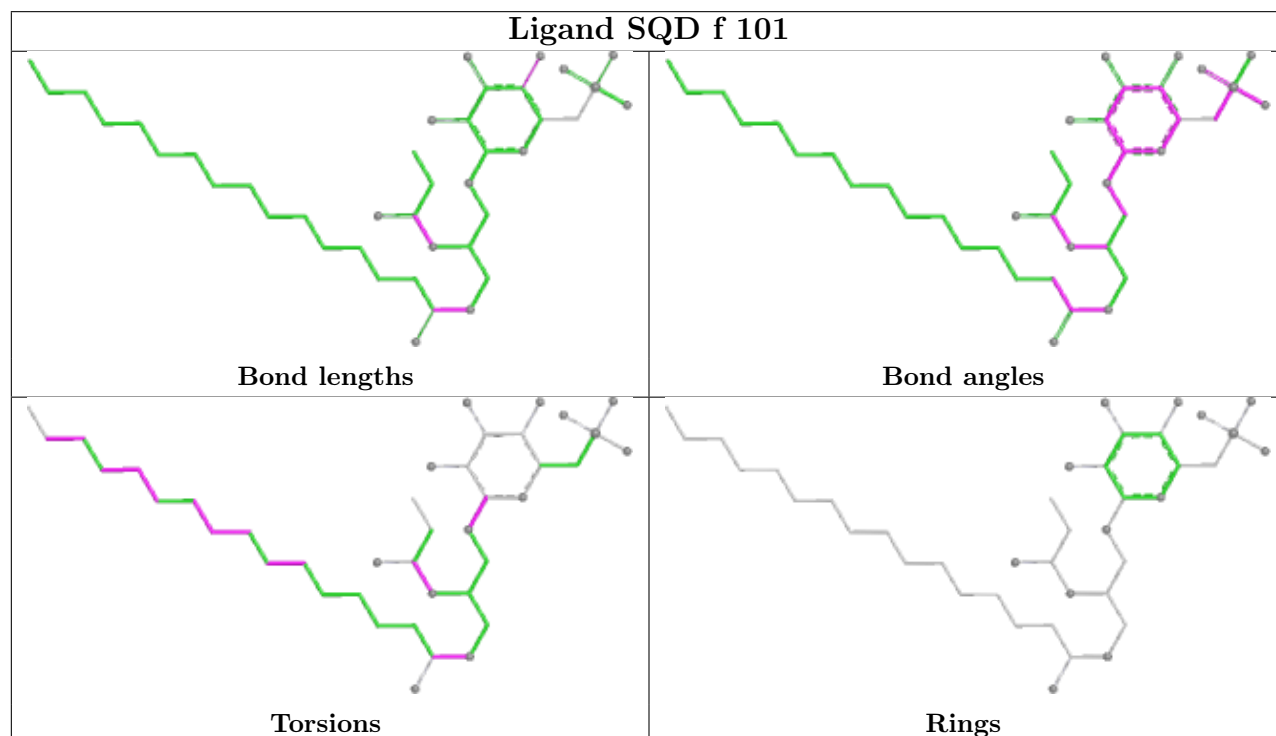
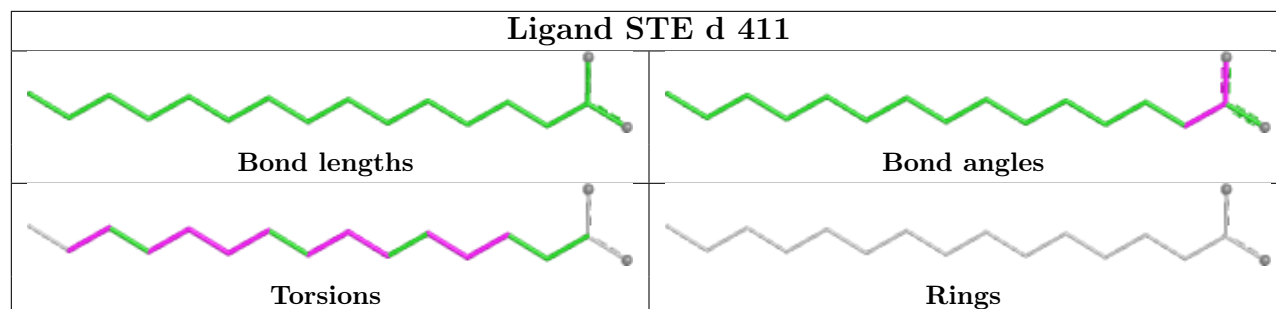


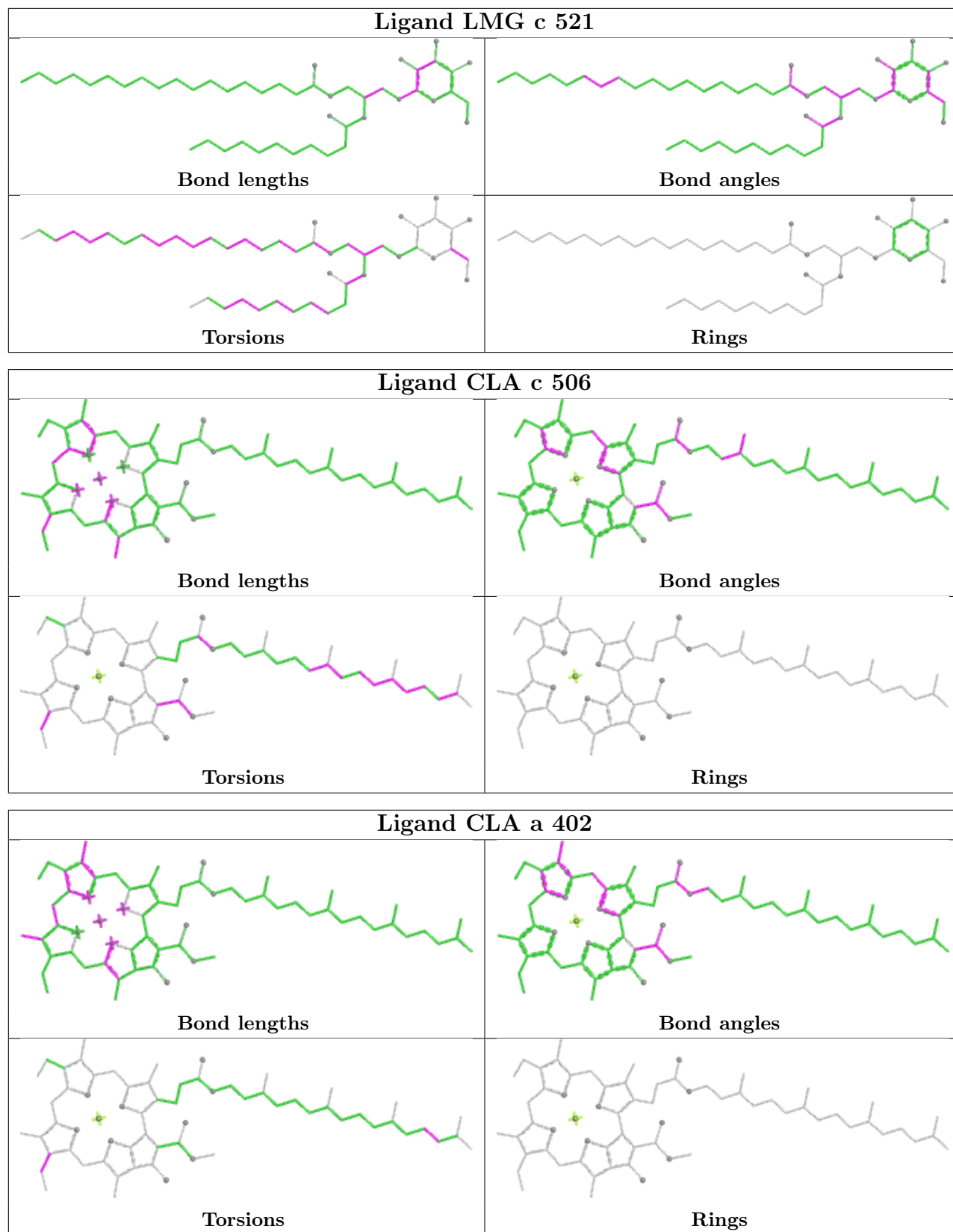


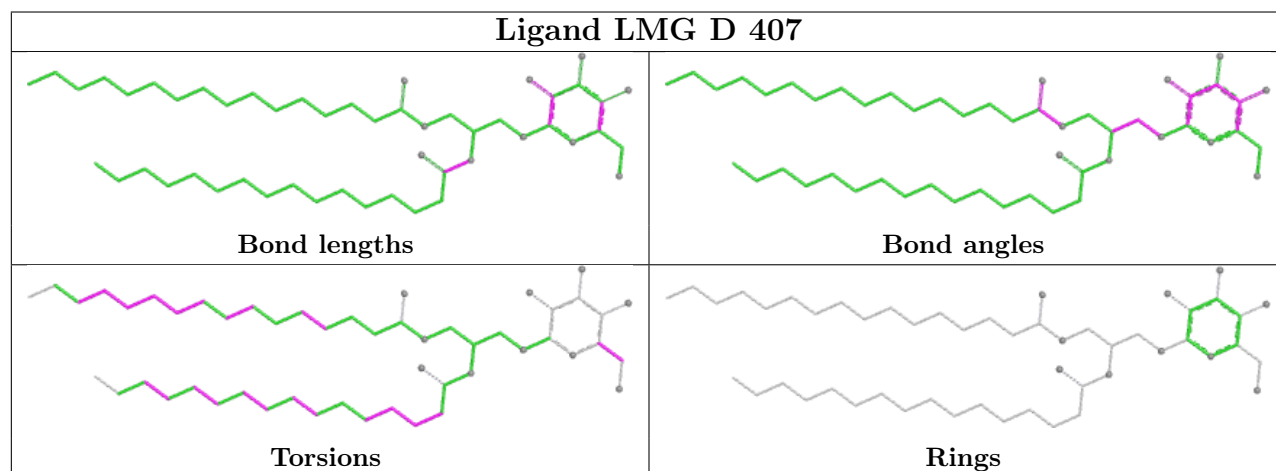
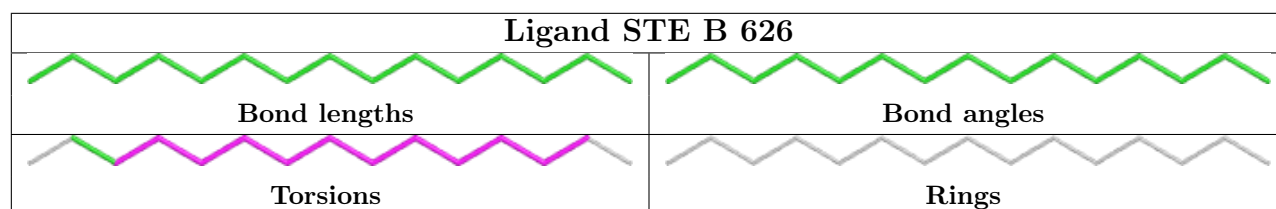
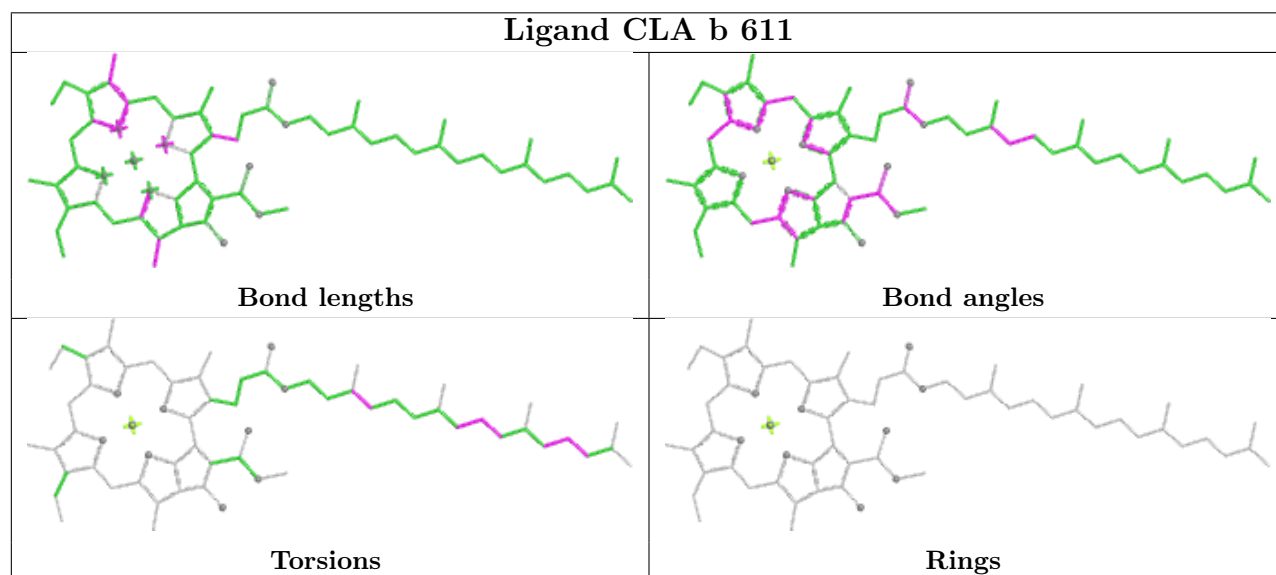
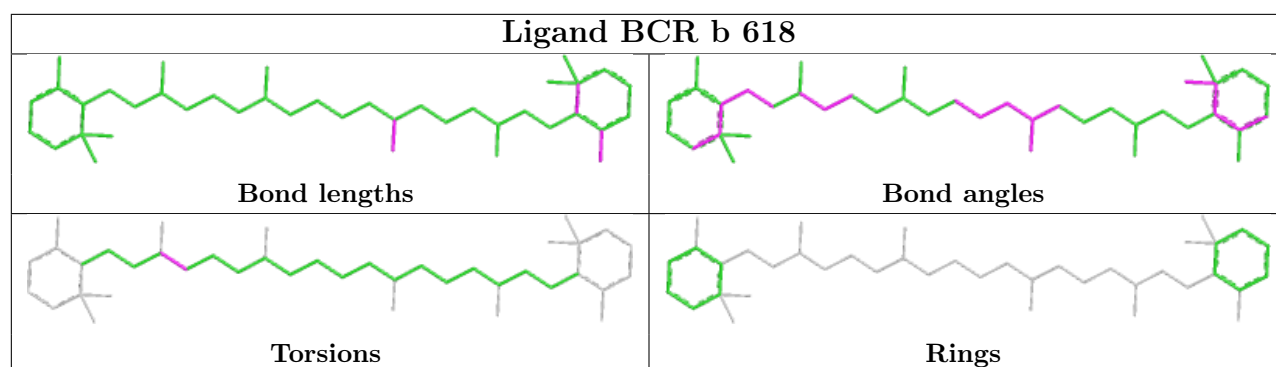
Ligand CLA c 504**Ligand PL9 d 406****Ligand CLA C 511**

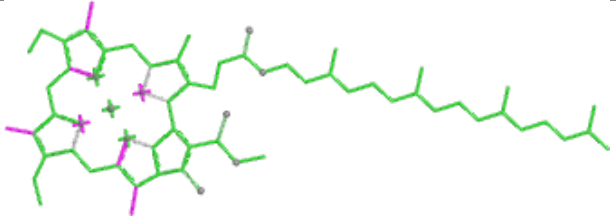
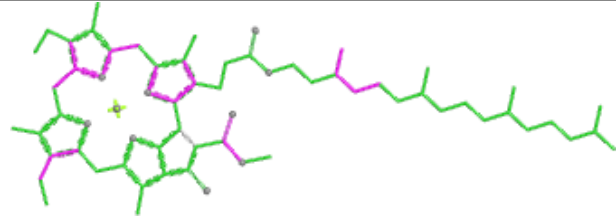
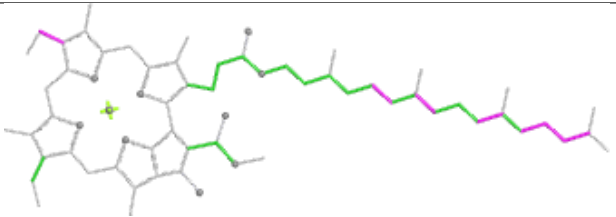
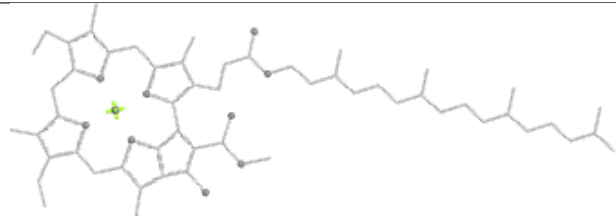


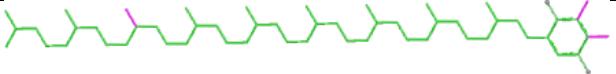
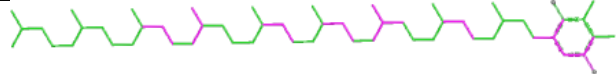
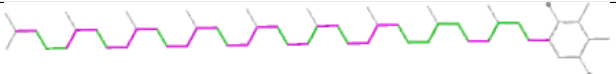
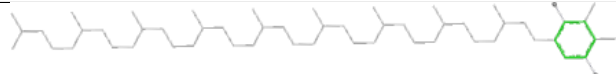


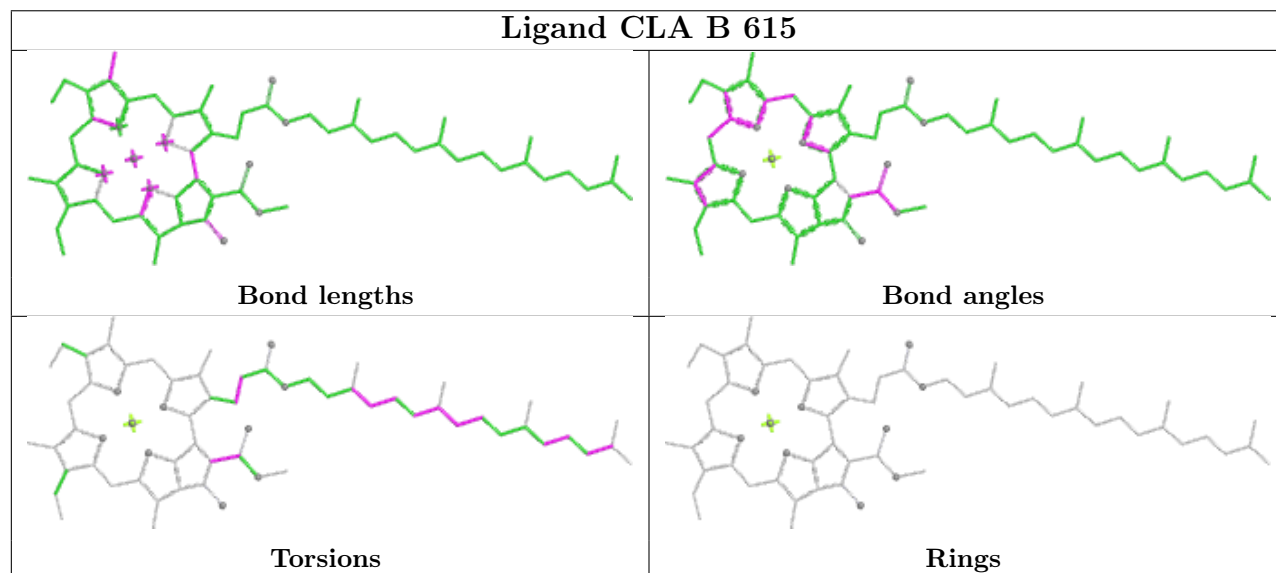
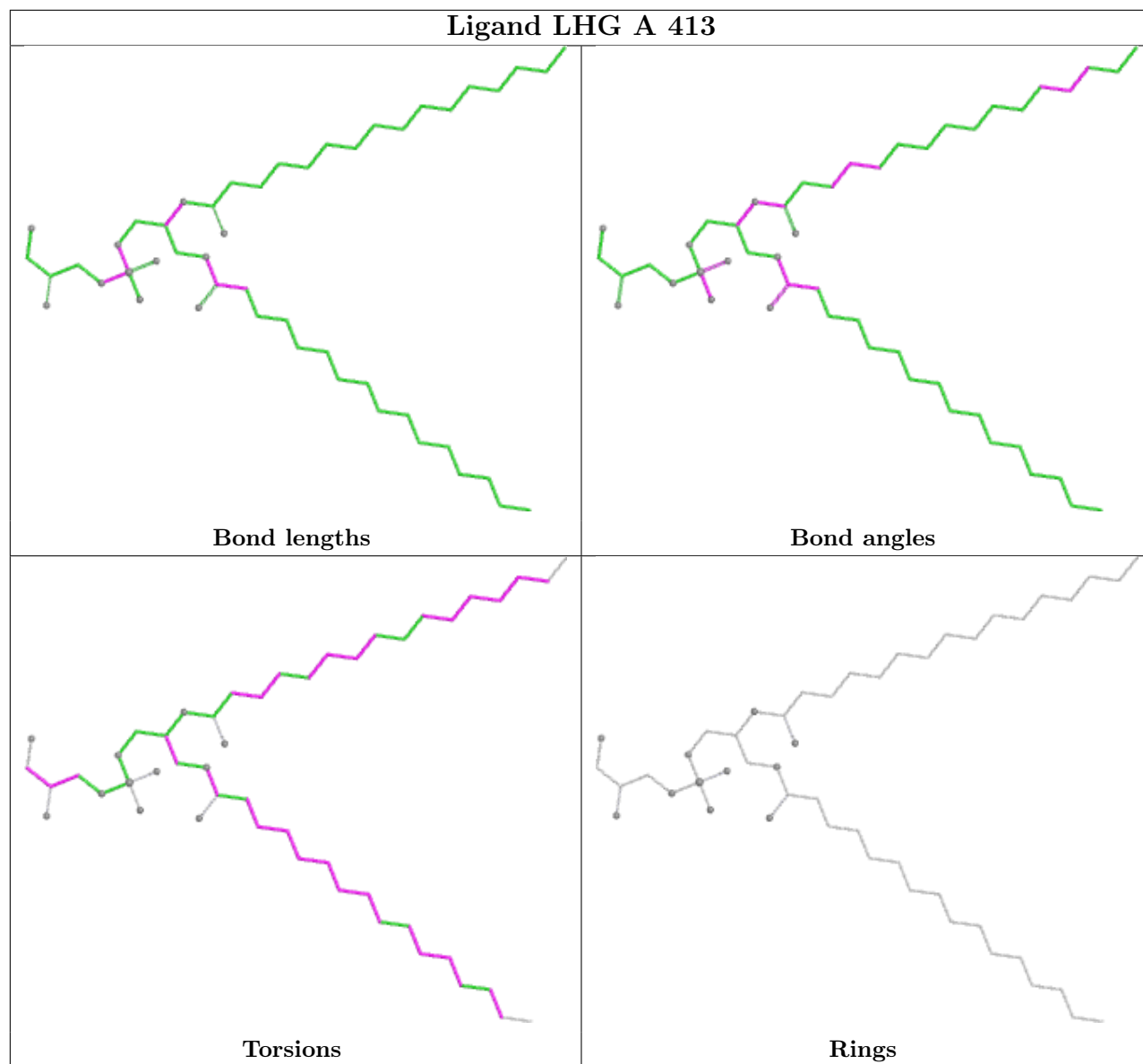


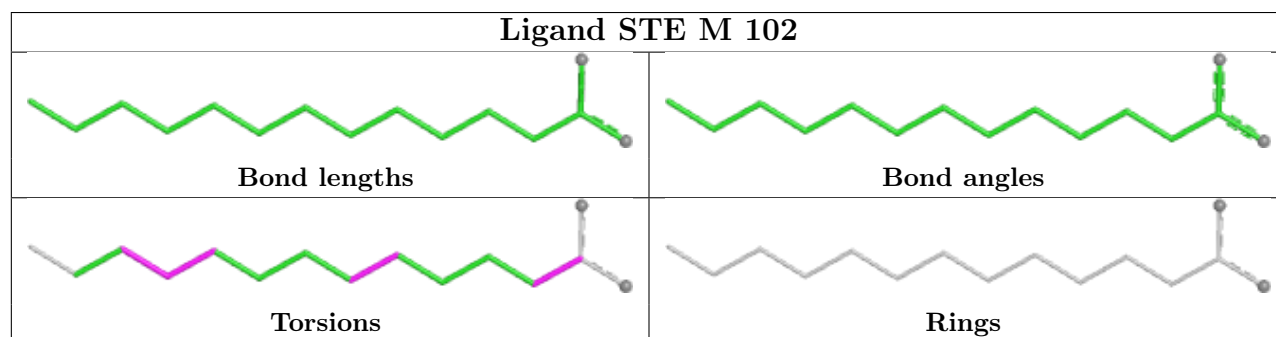
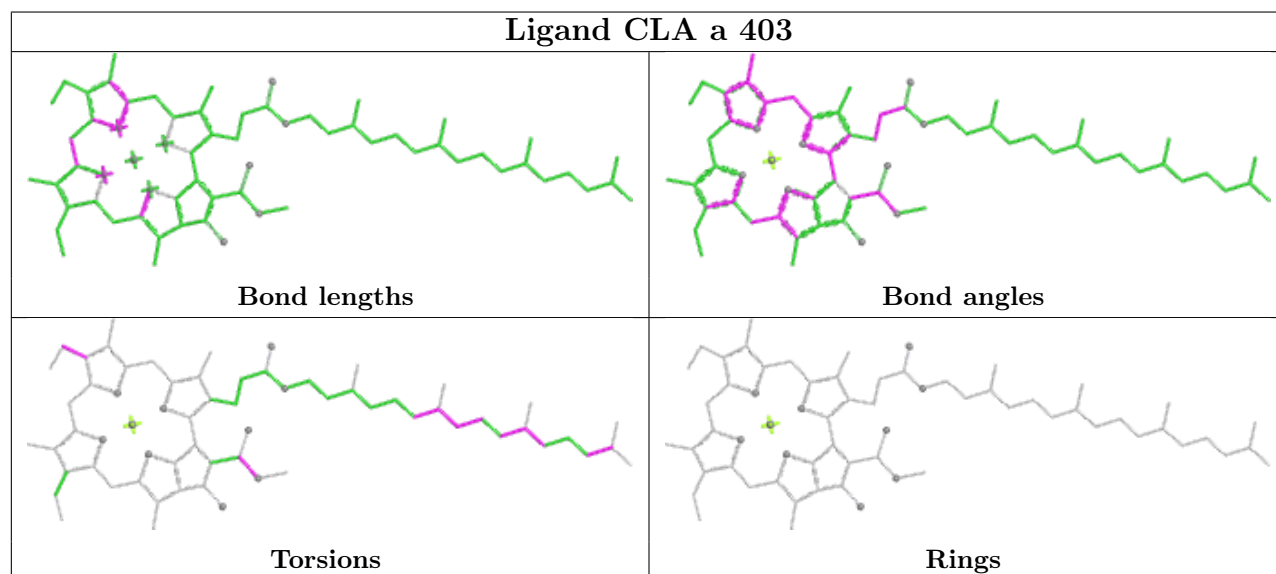
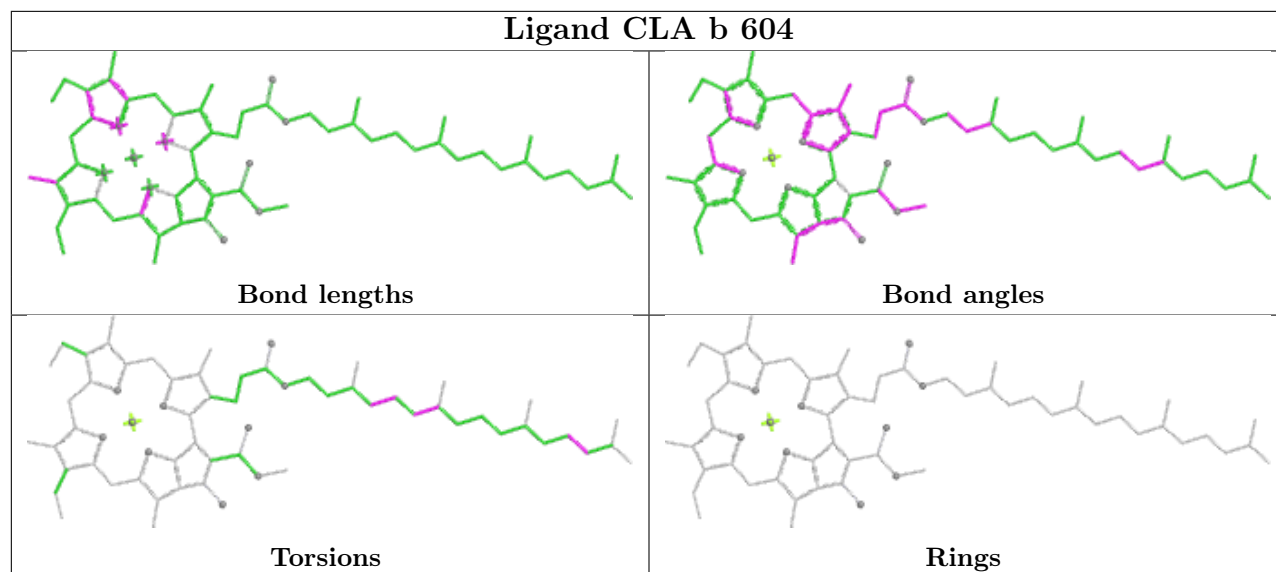


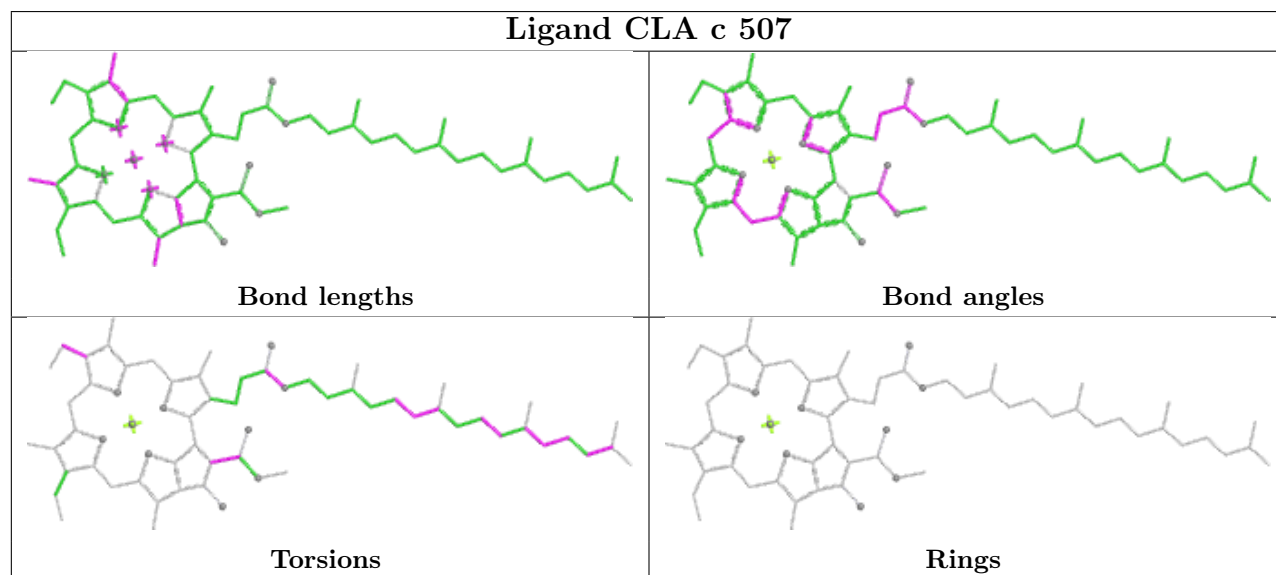
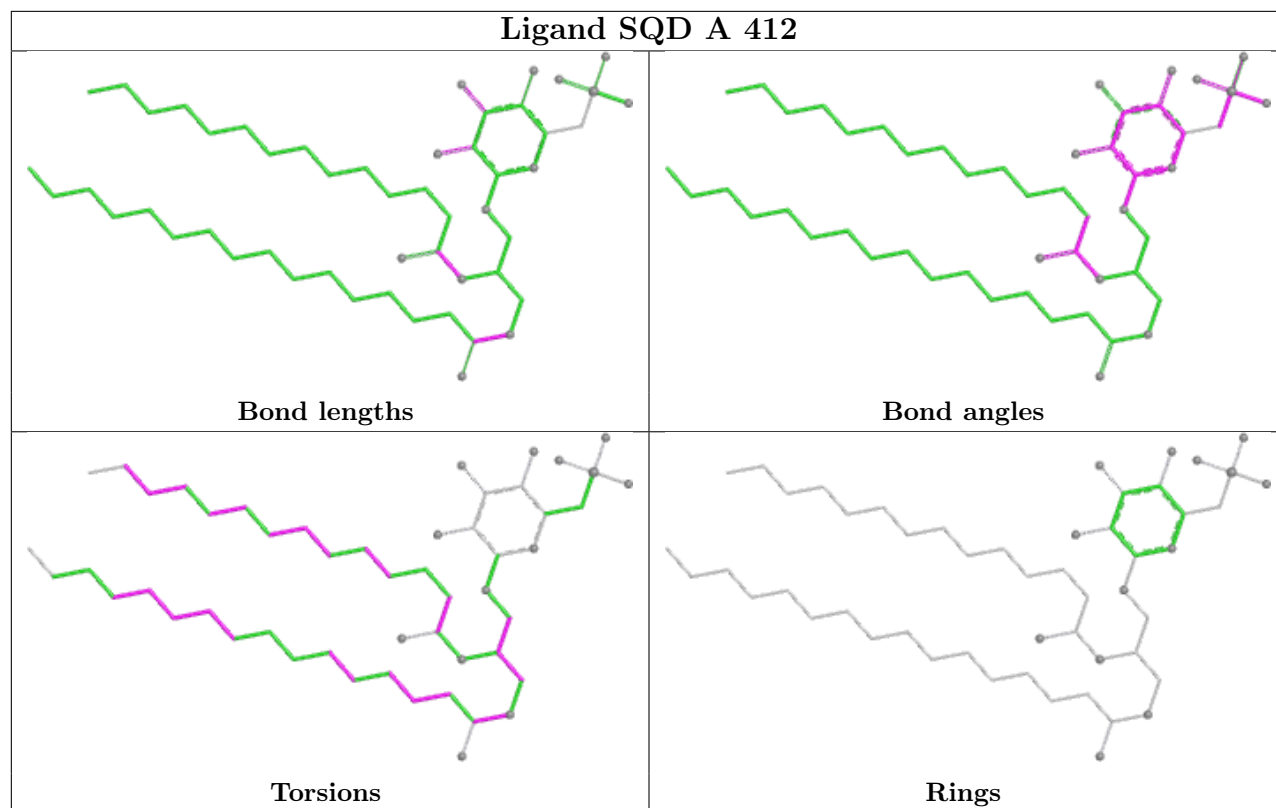


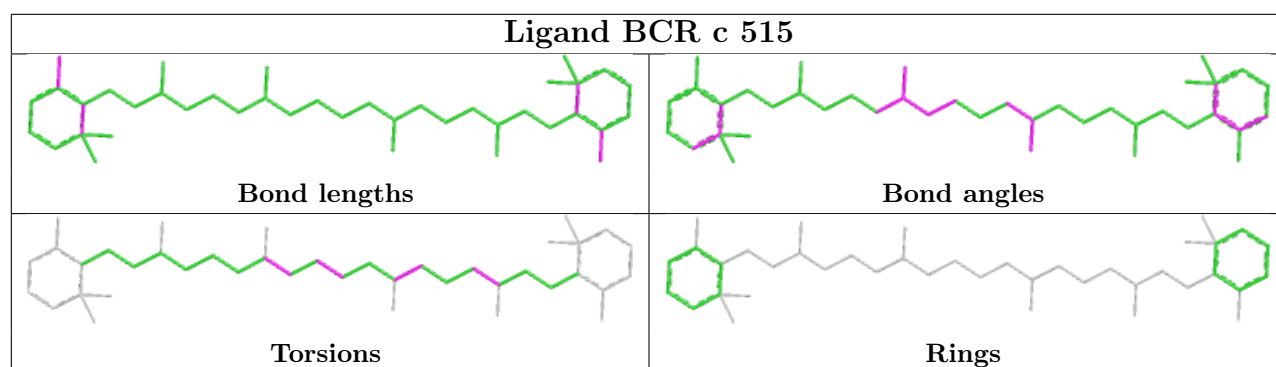
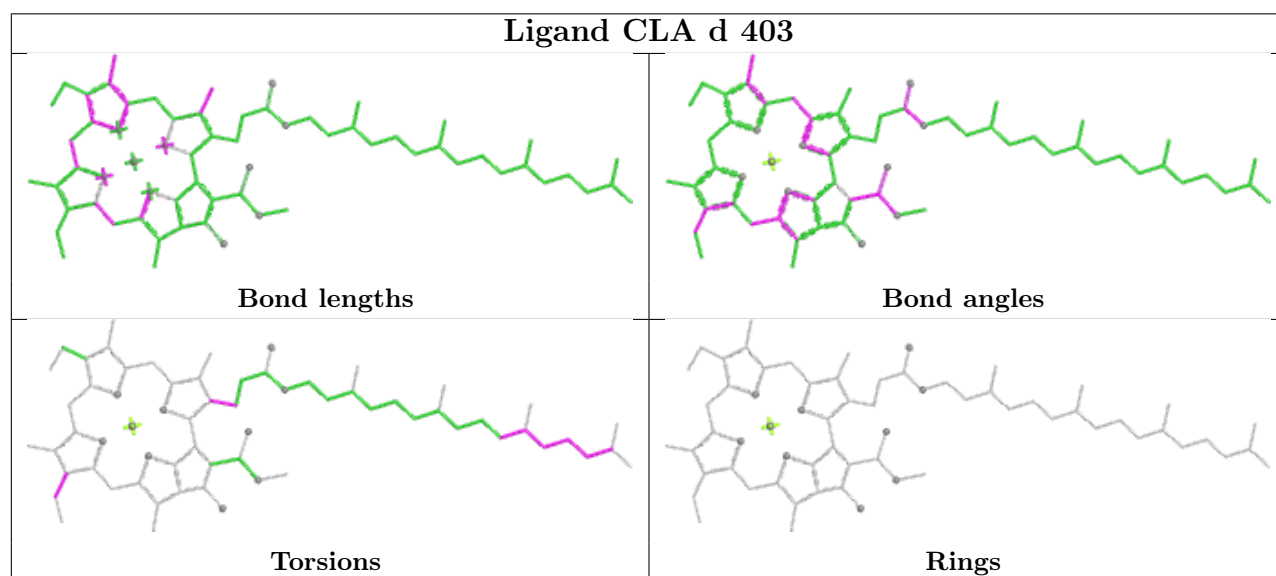
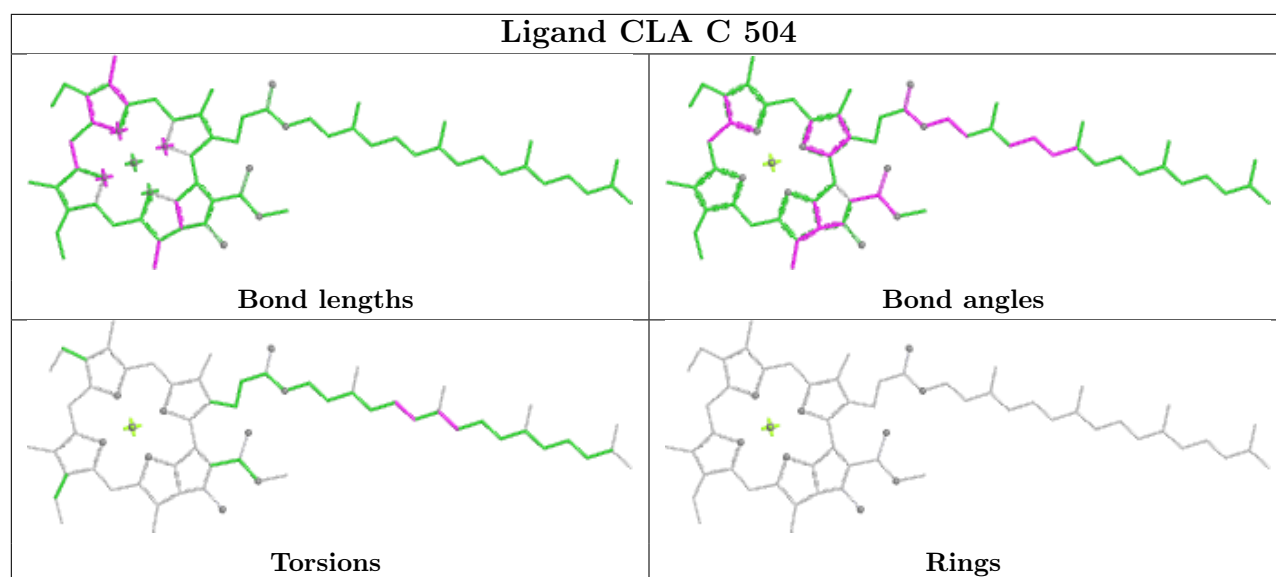
Ligand CLA c 503	
	
Bond lengths	Bond angles
	
Torsions	Rings

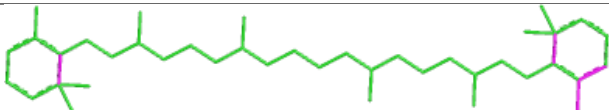
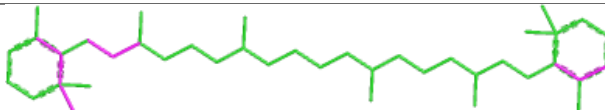
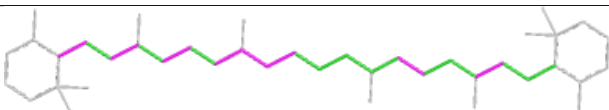
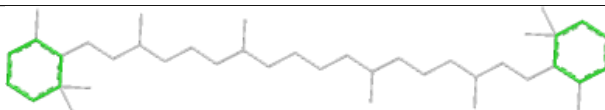
Ligand PL9 a 410	
	
Bond lengths	Bond angles
	
Torsions	Rings

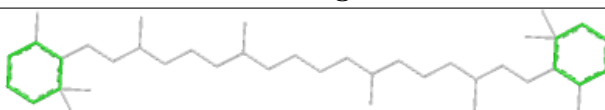


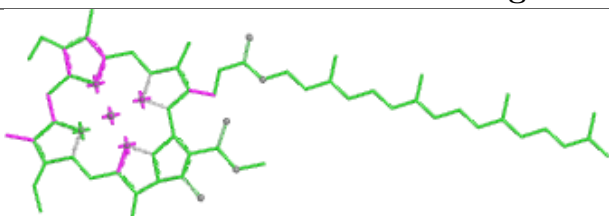
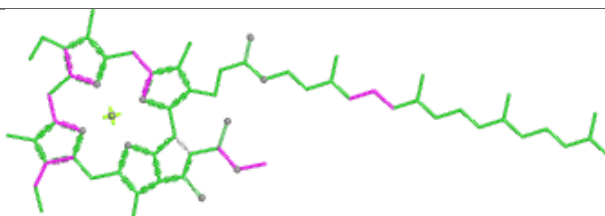
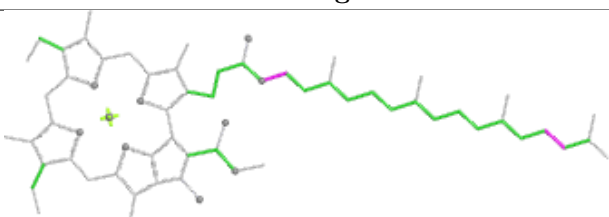
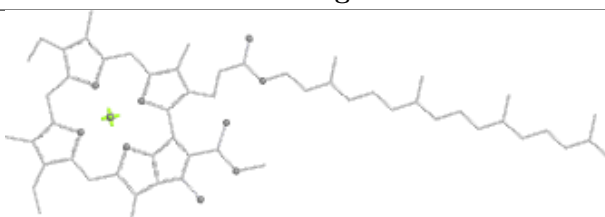


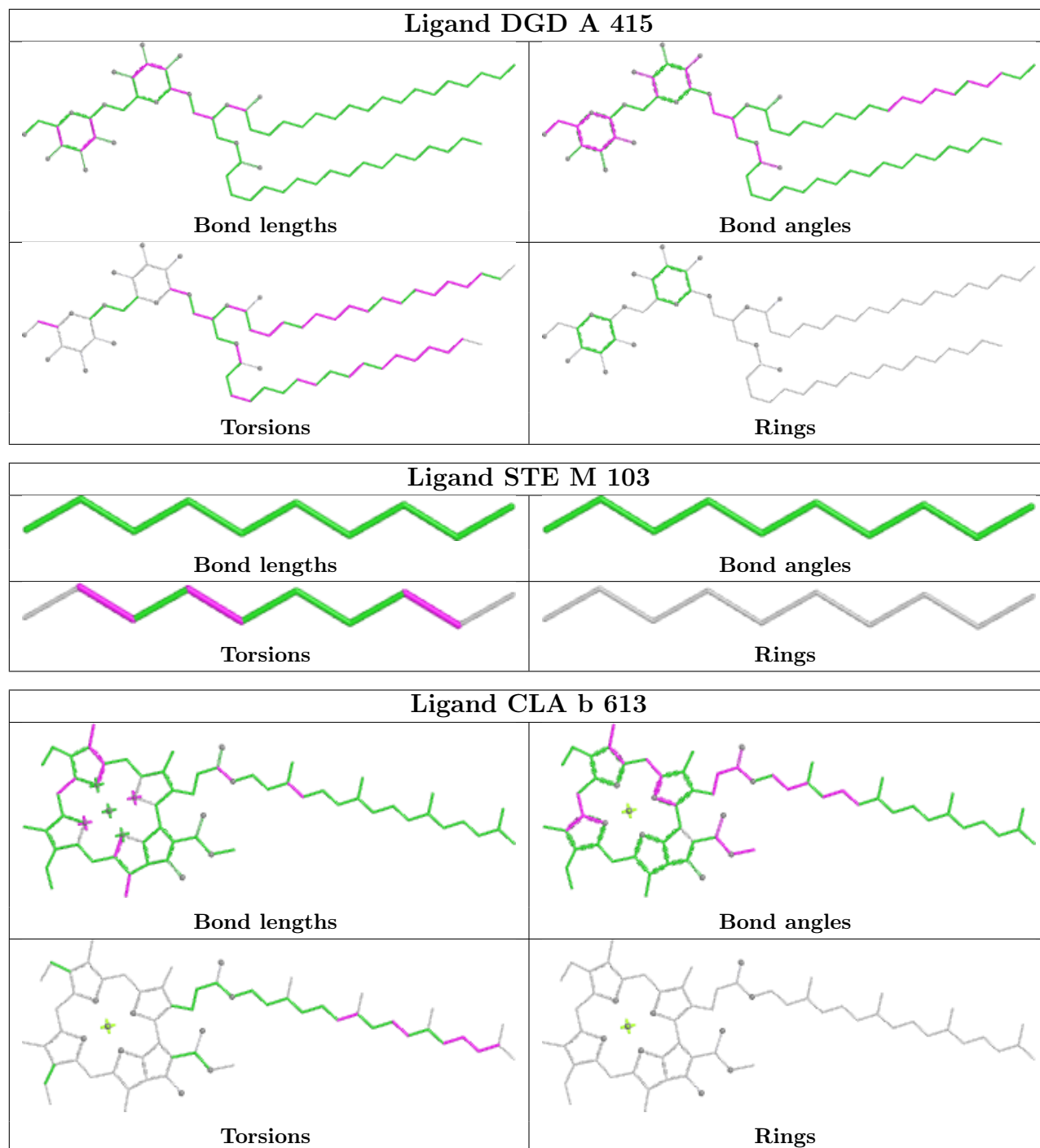


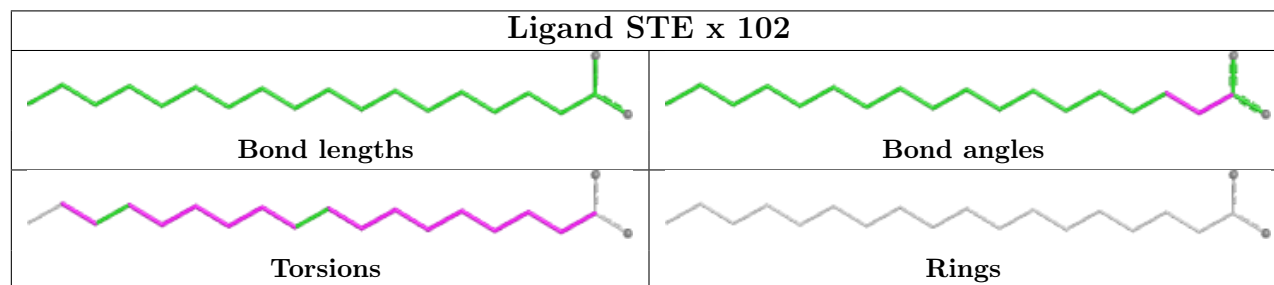
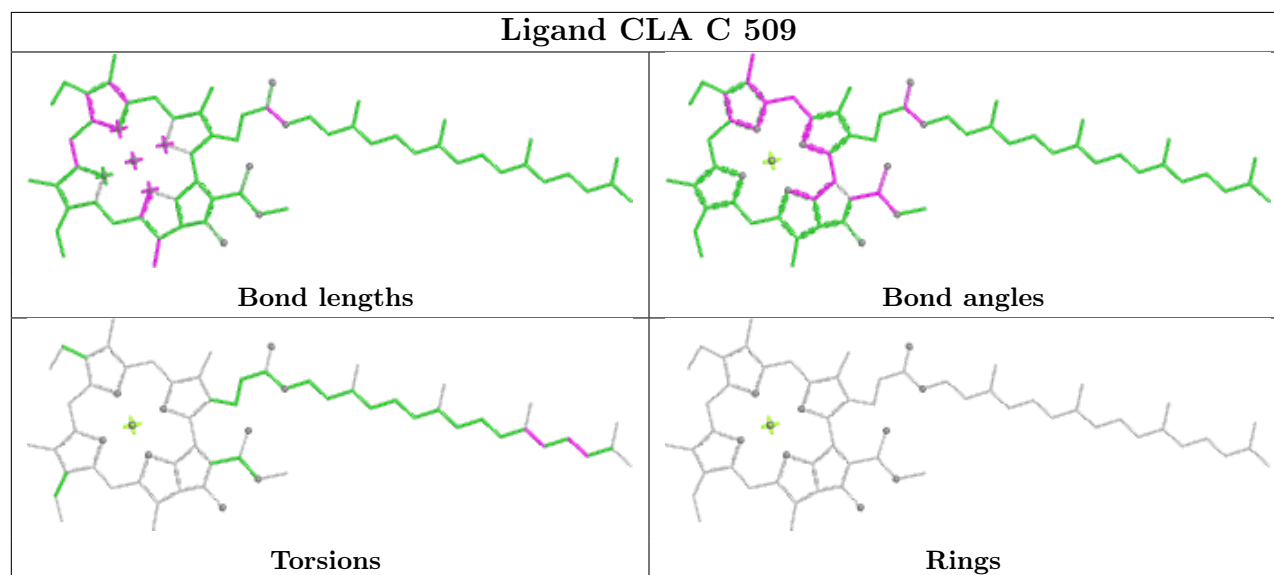
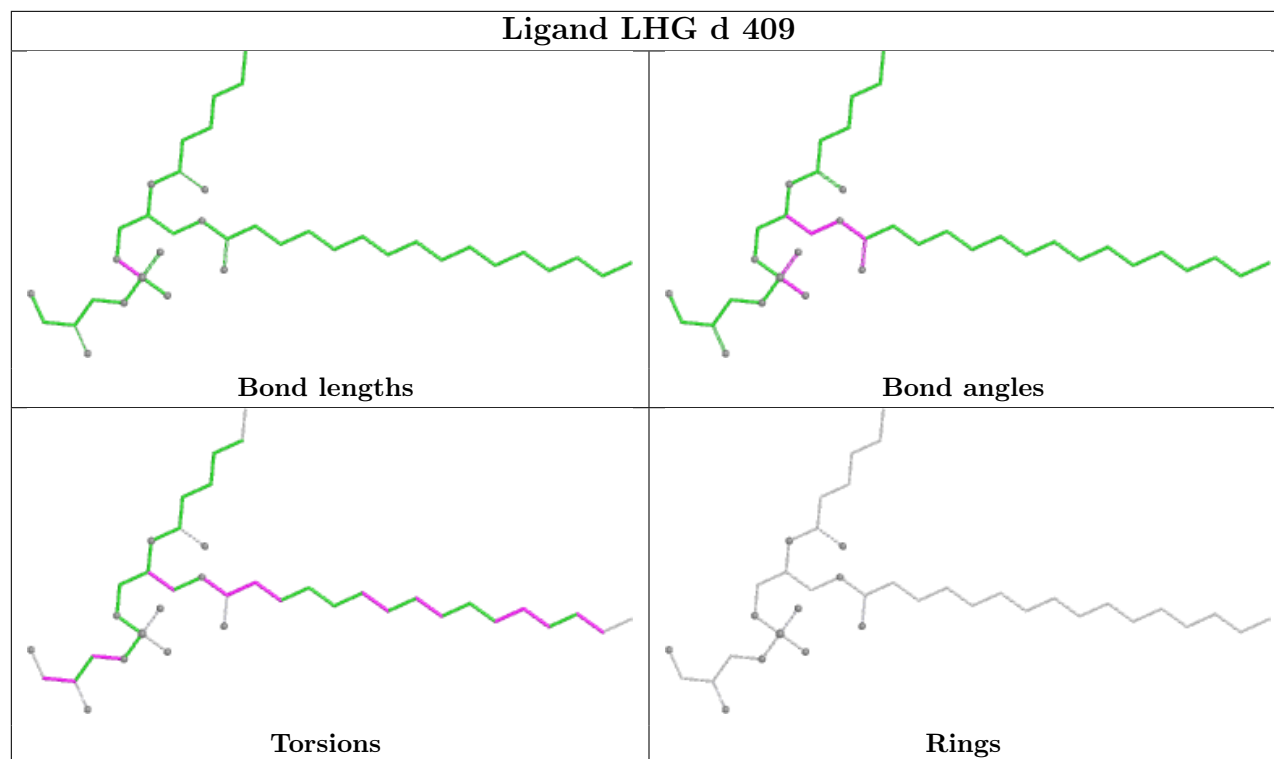


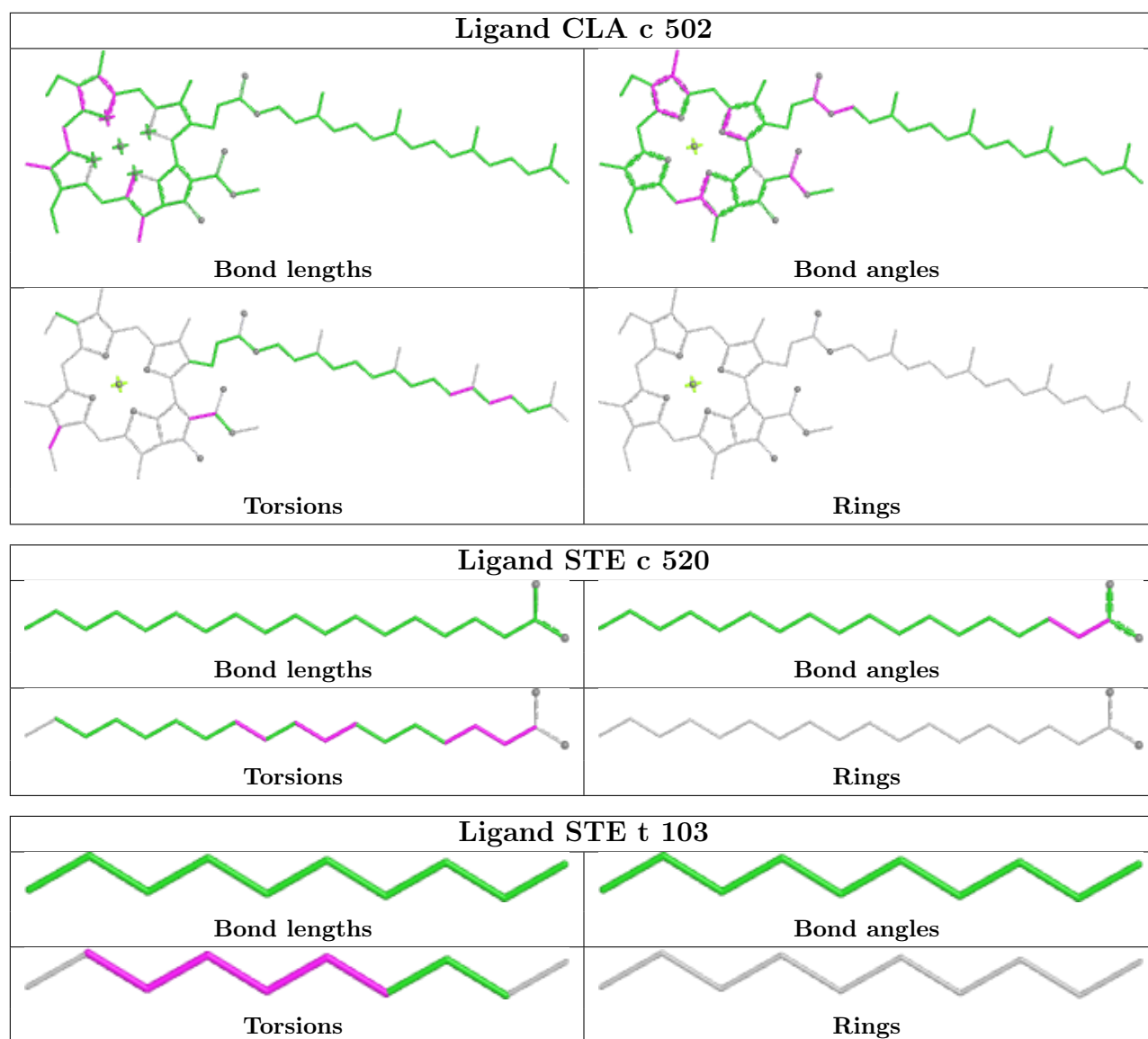
Ligand BCR T 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR D 405	
	
Bond lengths	Bond angles
	
Torsions	Rings

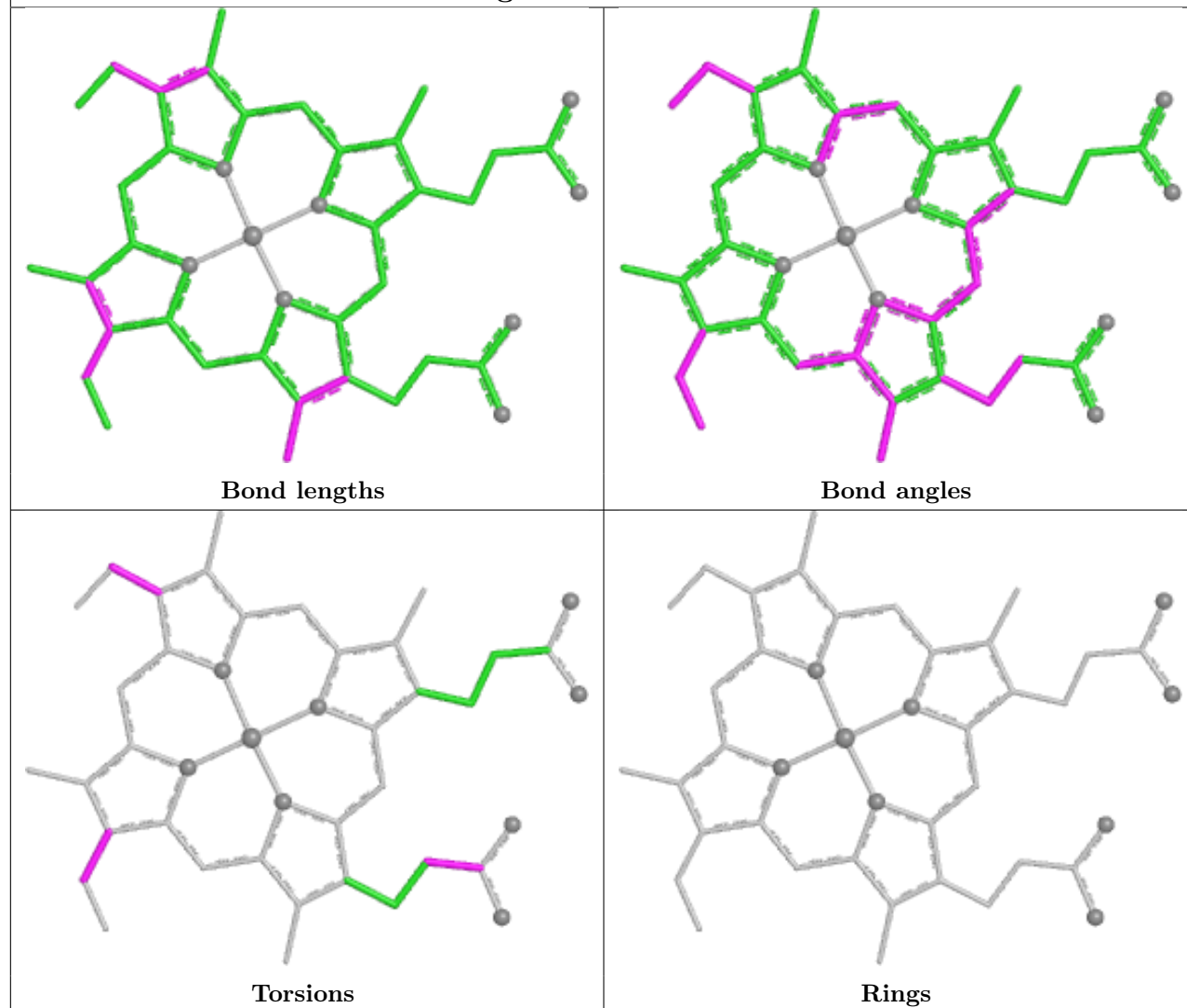
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Bond lengths	Bond angles
	
Torsions	Rings



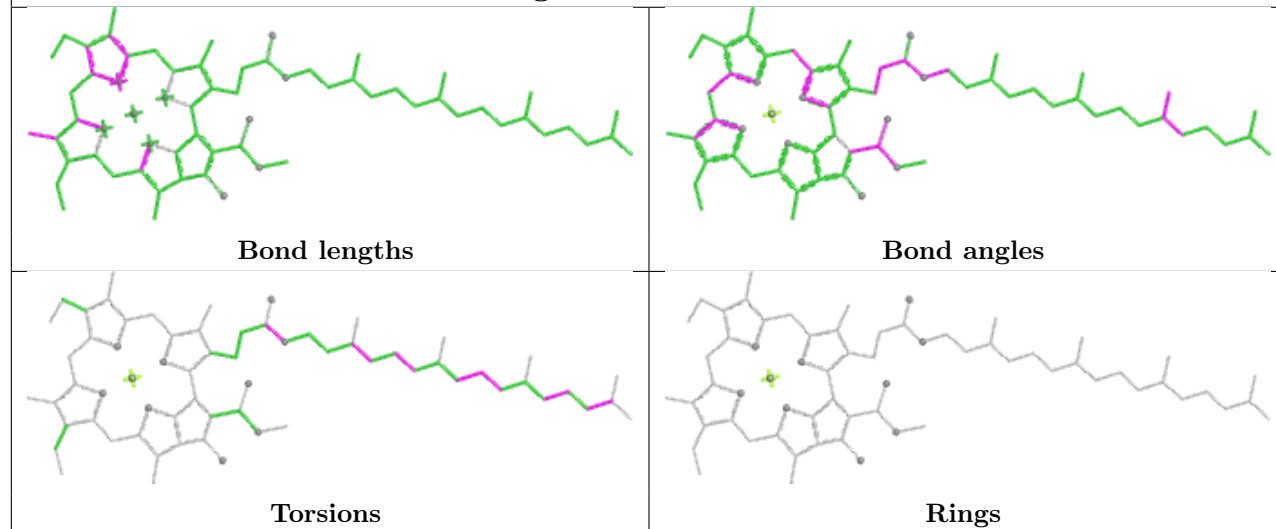


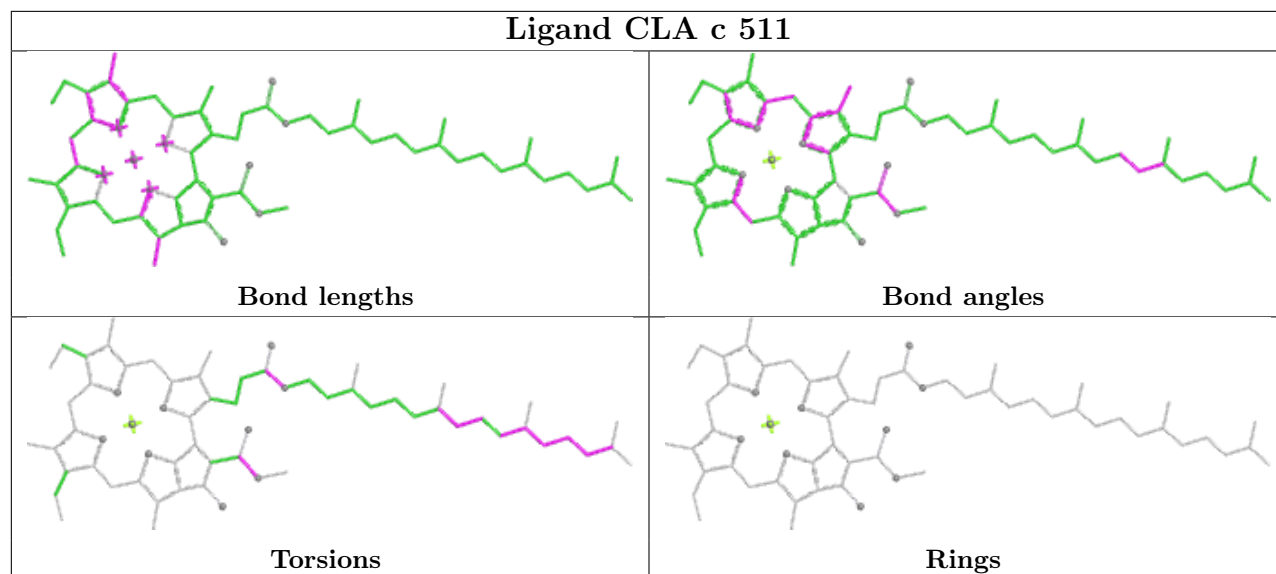
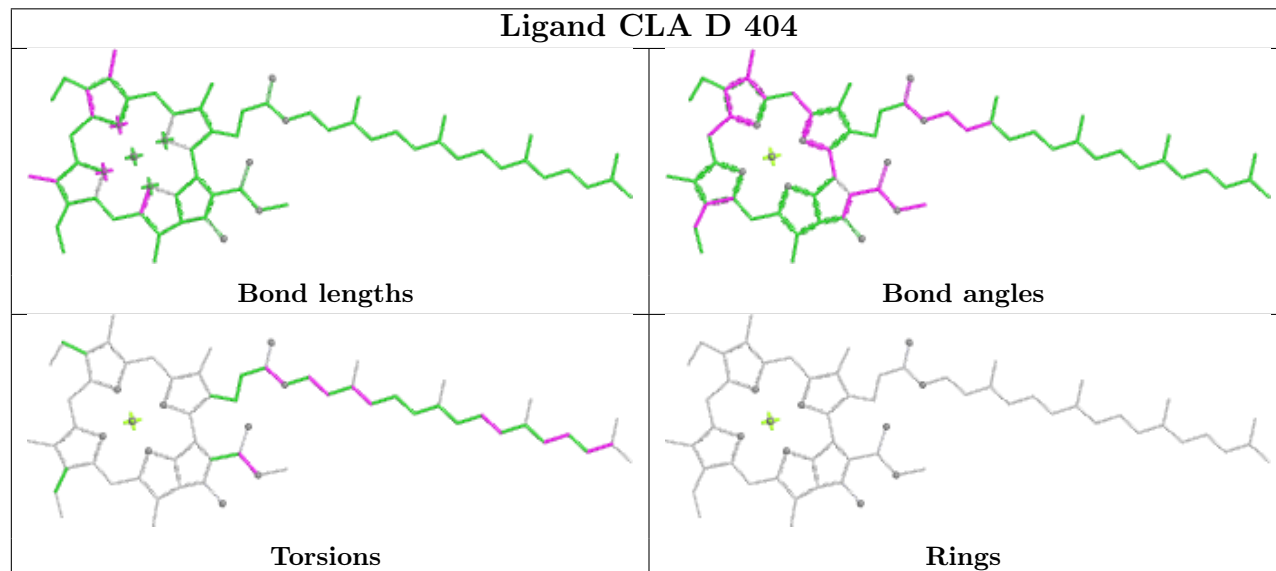


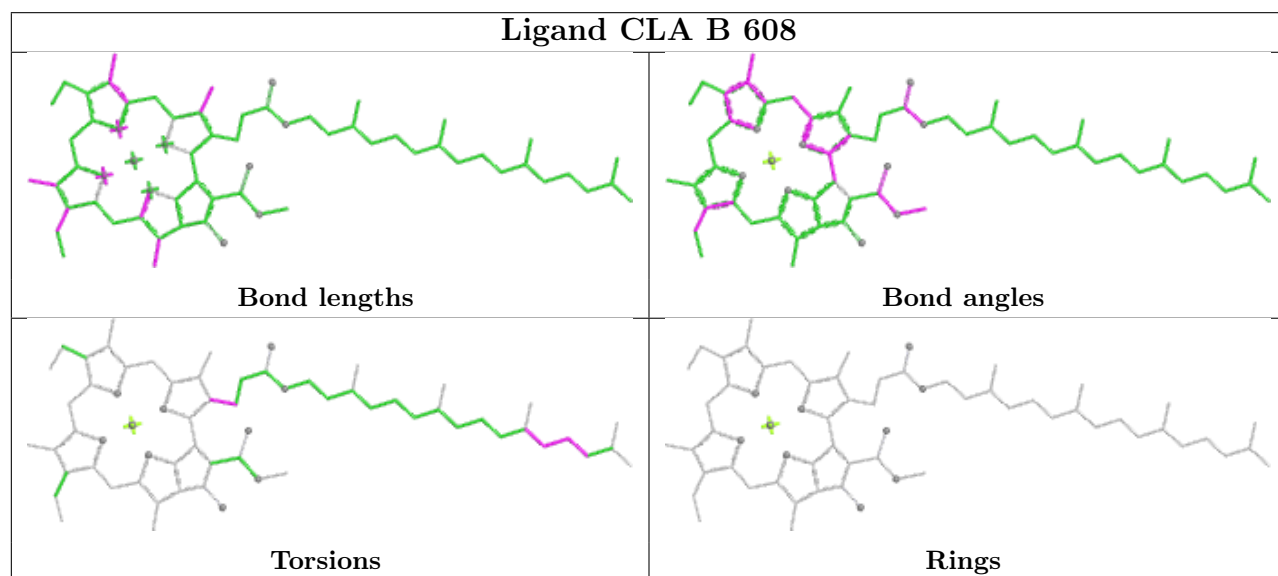
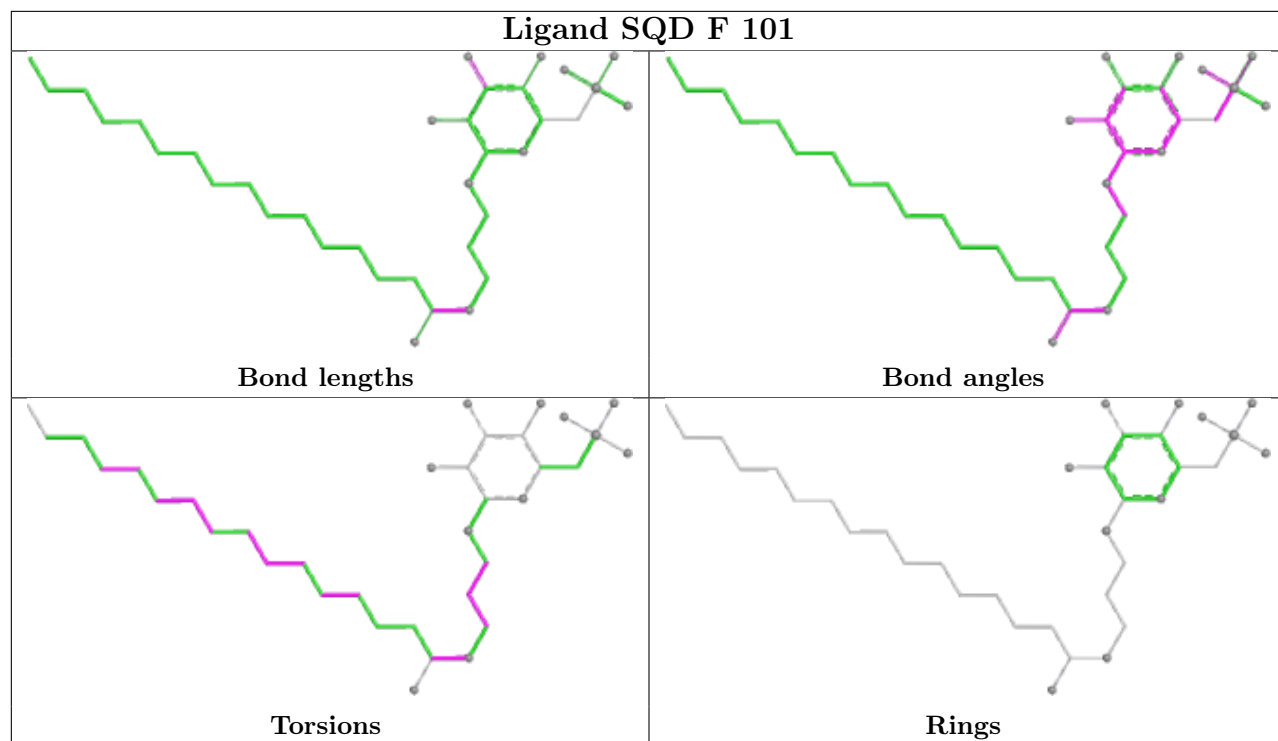
Ligand HEC v 201

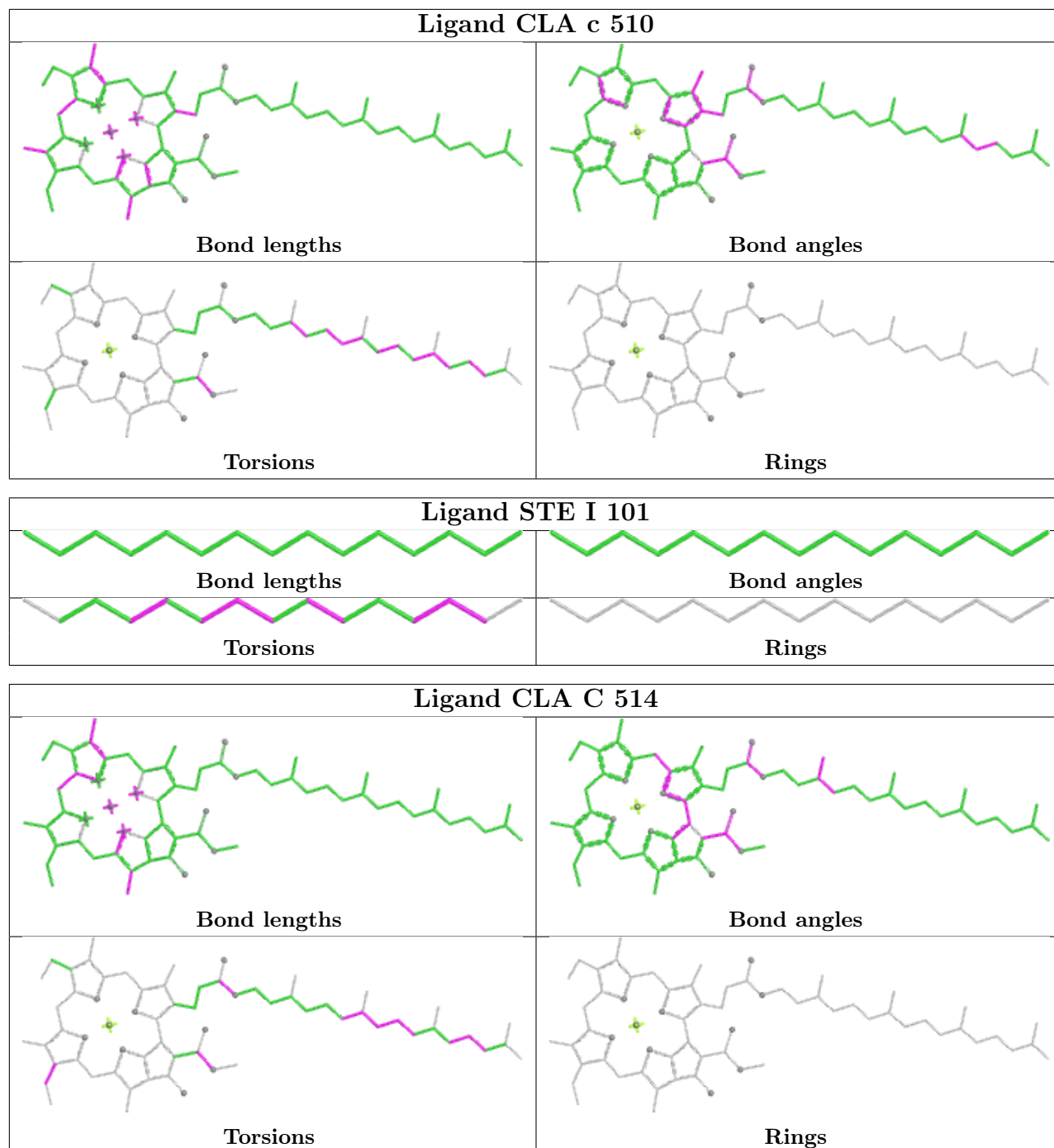


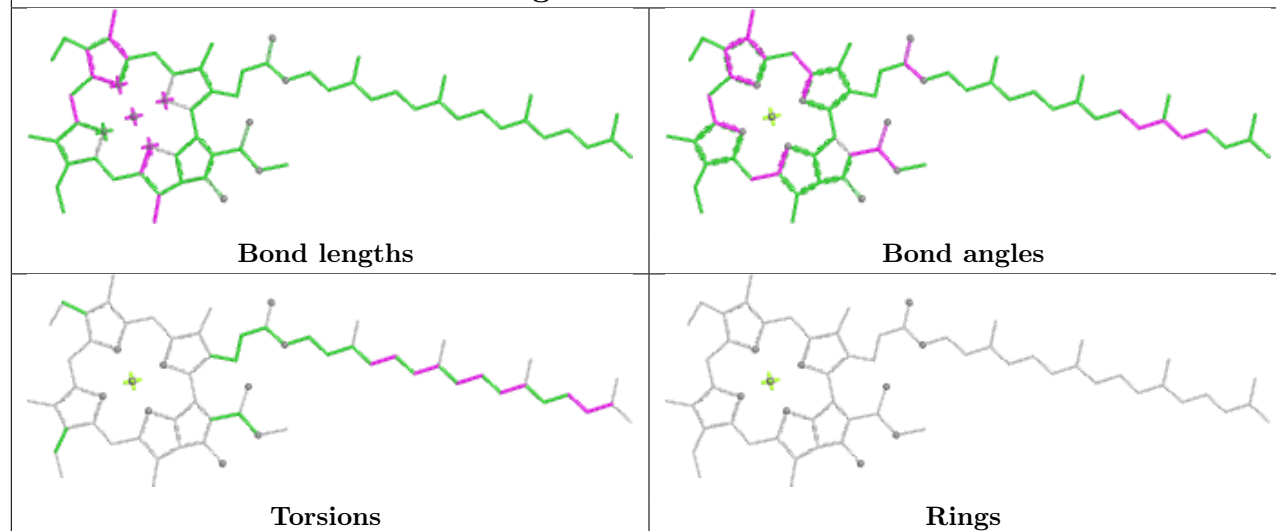
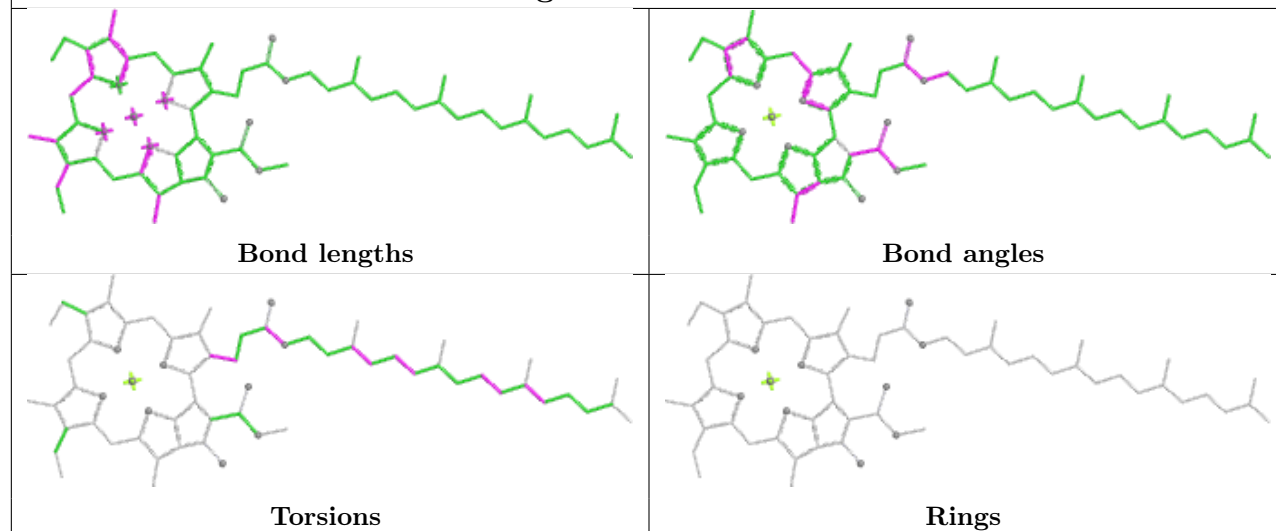
Ligand CLA B 606



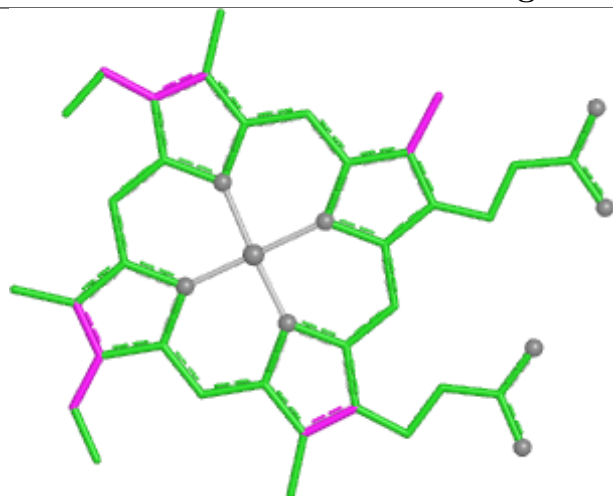
Ligand CLA c 511**Ligand CLA D 404**



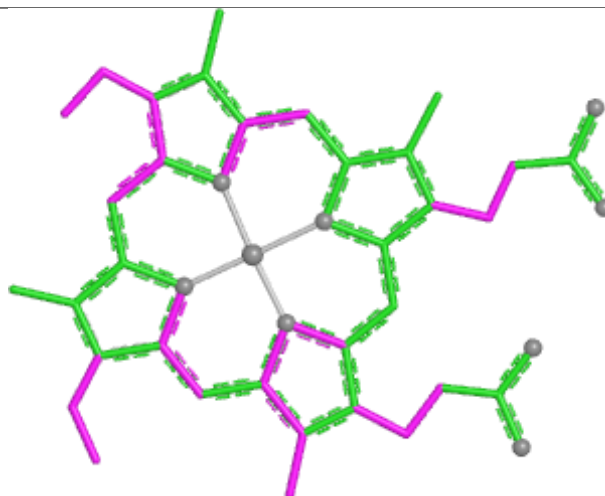


Ligand CLA B 603**Ligand CLA a 405**

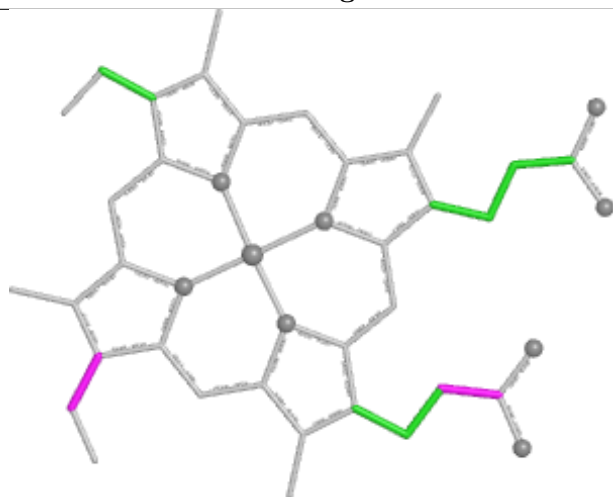
Ligand HEC e 101



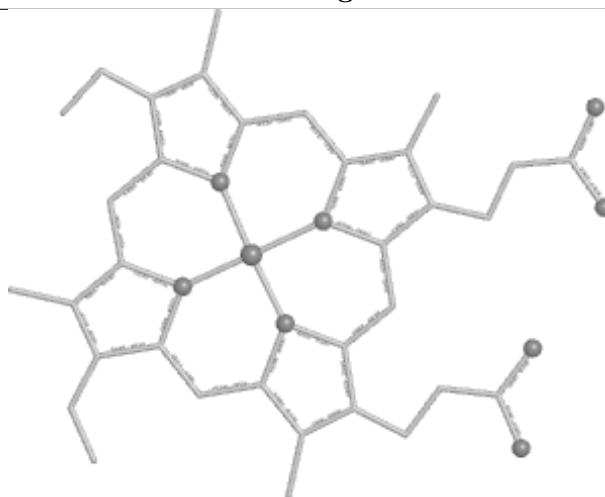
Bond lengths



Bond angles

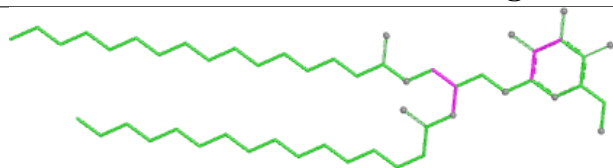


Torsions

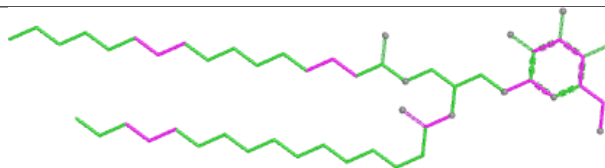


Rings

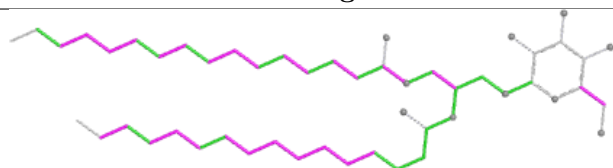
Ligand LMG M 101



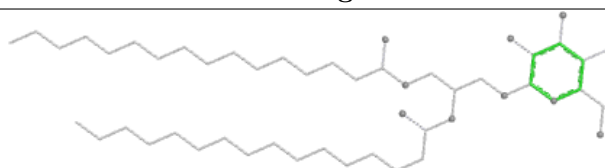
Bond lengths



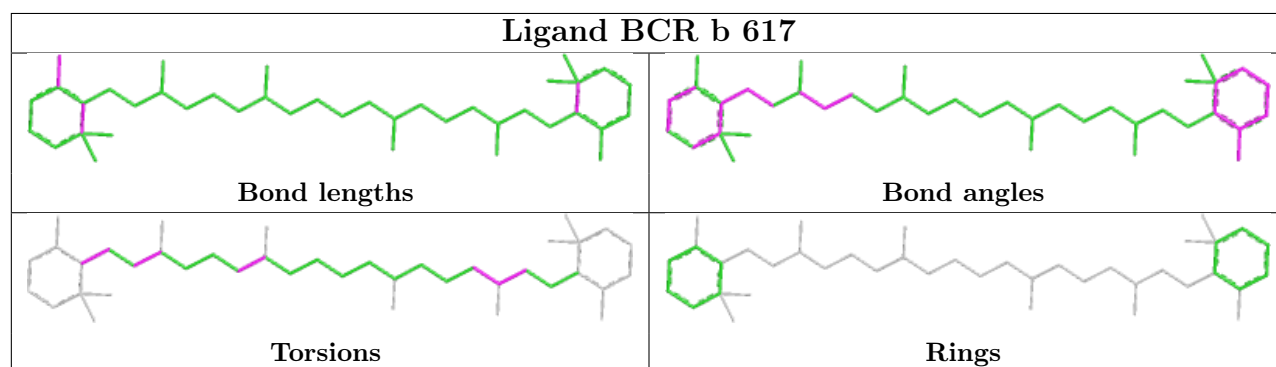
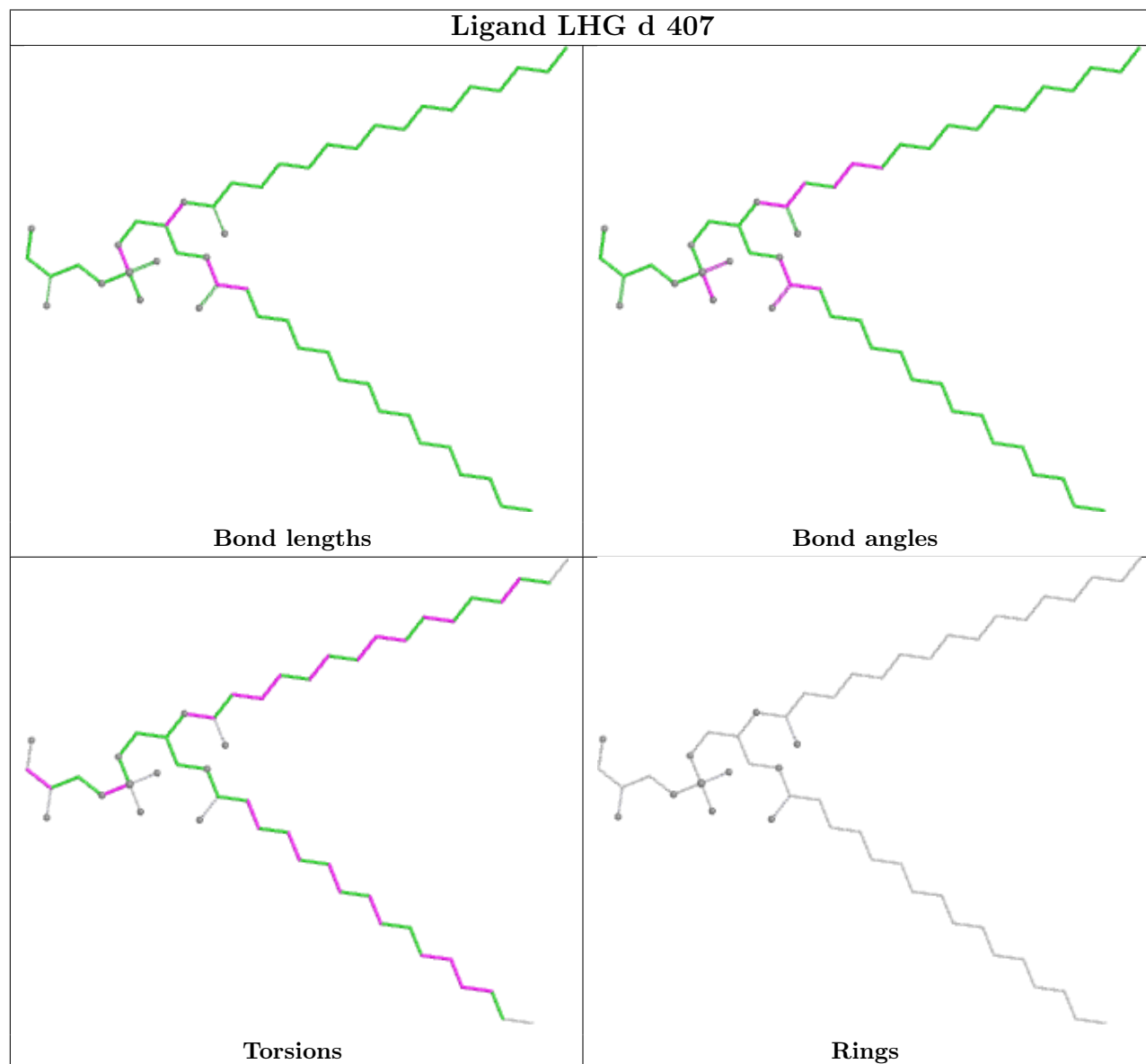
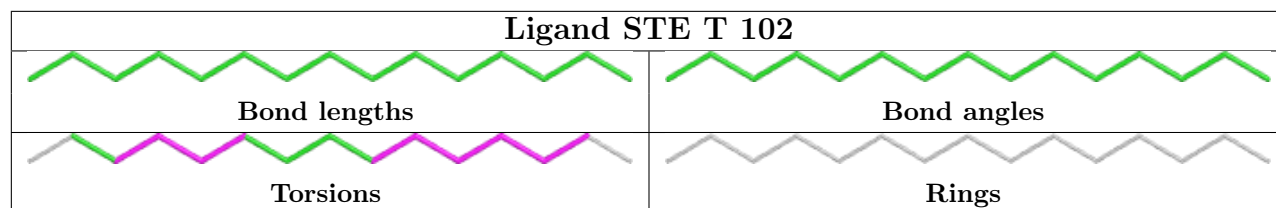
Bond angles

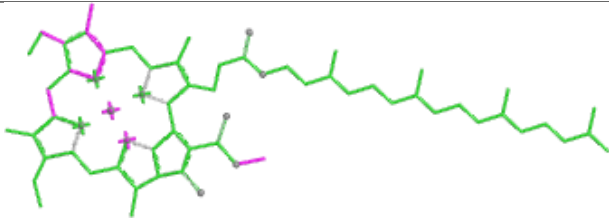
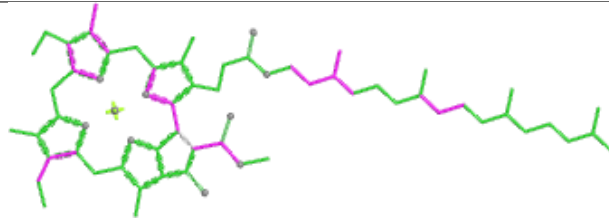
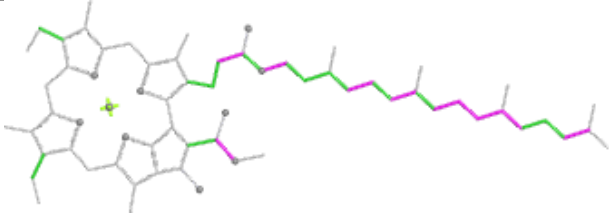
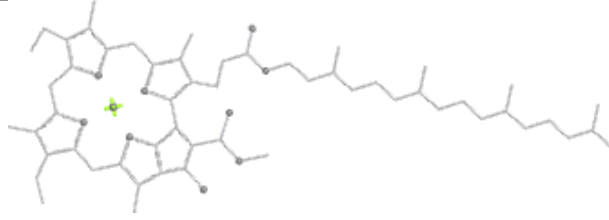


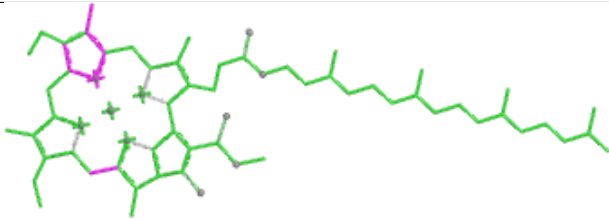
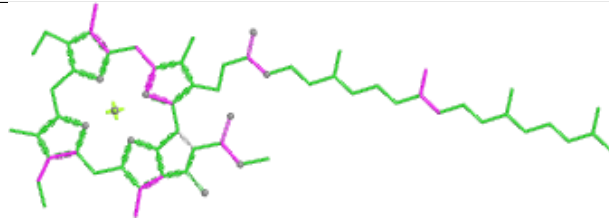
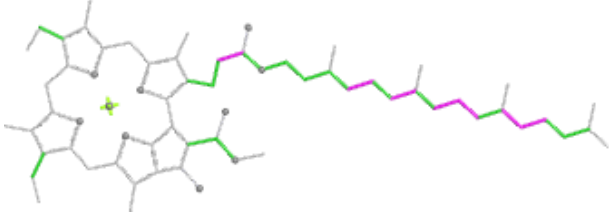
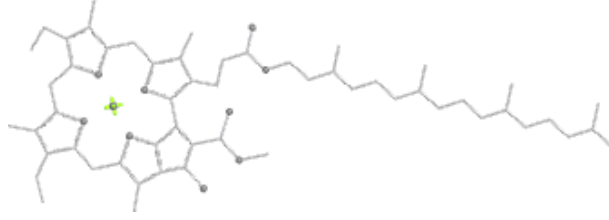
Torsions



Rings



Ligand CLA B 614	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 612	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand STE b 625	
	
Bond lengths	Bond angles
	
Torsions	Rings

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	334/334 (100%)	-0.67	0 100 100	27, 34, 54, 81	0
1	a	334/334 (100%)	-0.56	1 (0%) 90 90	27, 36, 63, 91	0
2	B	505/506 (99%)	-0.52	0 100 100	19, 39, 66, 95	4 (0%)
2	b	505/506 (99%)	-0.38	2 (0%) 88 89	29, 42, 77, 117	0
3	C	442/461 (95%)	-0.46	0 100 100	18, 42, 60, 90	1 (0%)
3	c	451/461 (97%)	-0.39	1 (0%) 91 92	21, 46, 67, 98	2 (0%)
4	D	341/352 (96%)	-0.65	0 100 100	26, 36, 52, 93	0
4	d	341/352 (96%)	-0.50	0 100 100	27, 40, 64, 94	1 (0%)
5	E	82/84 (97%)	-0.05	1 (1%) 76 77	34, 56, 75, 89	1 (1%)
5	e	82/84 (97%)	0.18	1 (1%) 76 77	47, 65, 84, 94	0
6	F	34/45 (75%)	-0.31	0 100 100	39, 49, 70, 77	0
6	f	34/45 (75%)	-0.11	1 (2%) 53 54	46, 55, 84, 91	0
7	H	65/66 (98%)	-0.37	2 (3%) 51 51	37, 46, 66, 89	0
7	h	63/66 (95%)	-0.07	1 (1%) 70 71	46, 59, 70, 79	0
8	I	35/38 (92%)	-0.39	0 100 100	38, 45, 75, 84	0
8	i	35/38 (92%)	-0.17	1 (2%) 53 54	37, 48, 88, 99	0
9	J	36/40 (90%)	-0.16	1 (2%) 55 55	40, 55, 79, 97	0
9	j	36/40 (90%)	-0.02	2 (5%) 30 28	44, 57, 92, 105	0
10	K	37/46 (80%)	-0.15	0 100 100	50, 58, 82, 84	0
10	k	37/46 (80%)	-0.02	0 100 100	51, 61, 74, 87	0
11	L	37/37 (100%)	-0.66	0 100 100	28, 35, 72, 85	0
11	l	36/37 (97%)	-0.56	0 100 100	30, 37, 76, 89	0
12	M	32/36 (88%)	-0.47	1 (3%) 51 51	32, 41, 64, 78	0
12	m	31/36 (86%)	-0.57	0 100 100	32, 41, 58, 82	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/272 (89%)	-0.29	2 (0%) 82 84	27, 48, 89, 134	1 (0%)
13	o	244/272 (89%)	-0.32	2 (0%) 82 84	30, 45, 85, 128	0
14	R	34/40 (85%)	0.77	2 (5%) 28 26	61, 80, 102, 112	0
14	r	31/40 (77%)	1.42	6 (19%) 3 2	79, 102, 118, 137	0
15	T	29/30 (96%)	-0.64	0 100 100	30, 38, 71, 84	0
15	t	29/30 (96%)	-0.46	1 (3%) 48 48	32, 39, 90, 98	0
16	U	97/134 (72%)	-0.32	0 100 100	36, 50, 75, 92	0
16	u	97/134 (72%)	-0.38	0 100 100	34, 46, 63, 88	0
17	V	137/163 (84%)	-0.47	0 100 100	34, 46, 62, 81	0
17	v	137/163 (84%)	-0.25	0 100 100	36, 52, 75, 86	0
18	X	38/41 (92%)	-0.19	0 100 100	45, 56, 79, 86	0
18	x	39/41 (95%)	0.10	1 (2%) 57 58	54, 66, 94, 110	0
19	Y	27/46 (58%)	0.85	3 (11%) 10 9	59, 77, 100, 106	0
19	y	30/46 (65%)	0.50	0 100 100	63, 79, 92, 108	0
20	Z	62/62 (100%)	0.57	3 (4%) 35 35	57, 73, 117, 133	0
20	z	62/62 (100%)	0.53	4 (6%) 25 23	55, 78, 115, 124	0
All	All	5302/5666 (93%)	-0.37	39 (0%) 84 85	18, 44, 80, 137	10 (0%)

The worst 5 of 39 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	o	58	ASN	4.8
7	H	66	GLY	4.1
20	z	33	TRP	3.9
14	r	32	GLN	3.9
14	R	35	LEU	3.8

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
15	FME	t	1	10/11	0.94	0.08	36,49,70,70	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	0.95	0.07	33,45,71,71	0
12	FME	m	1	10/11	0.96	0.08	36,55,70,84	0
8	FME	i	1	10/11	0.96	0.07	45,57,75,77	0
12	FME	M	1	10/11	0.96	0.09	45,54,77,86	0
8	FME	I	1	10/11	0.97	0.07	42,54,64,72	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
32	STE	H	103	18/20	0.73	0.19	42,77,99,99	0
32	STE	I	101	15/20	0.76	0.18	44,58,80,81	0
32	STE	b	626	20/20	0.76	0.17	46,73,96,101	0
32	STE	B	625	16/20	0.78	0.15	47,64,74,78	0
28	LHG	A	413	49/49	0.78	0.16	56,78,116,120	0
32	STE	k	101	12/20	0.78	0.13	49,73,89,92	0
32	STE	b	625	10/20	0.80	0.15	44,54,67,68	0
32	STE	E	102	12/20	0.80	0.16	50,78,89,94	0
32	STE	a	414	12/20	0.80	0.13	45,68,75,81	0
33	LMG	c	521	48/55	0.80	0.15	40,79,111,123	0
28	LHG	a	412	42/49	0.81	0.14	54,83,108,130	0
33	LMG	b	622	55/55	0.81	0.16	47,74,101,110	0
32	STE	b	624	20/20	0.81	0.15	46,70,82,93	0
32	STE	B	626	15/20	0.82	0.18	42,65,83,83	0
32	STE	J	101	12/20	0.83	0.15	48,62,72,84	0
32	STE	T	102	15/20	0.83	0.14	42,58,81,89	0
32	STE	j	101	12/20	0.83	0.14	39,61,75,80	0
32	STE	C	521	16/20	0.83	0.13	43,59,70,71	0
32	STE	b	620	16/20	0.83	0.15	33,55,75,78	0
32	STE	B	601	12/20	0.83	0.17	48,70,94,97	0
29	SQD	a	413	36/54	0.84	0.14	27,65,92,100	0
30	DGD	A	415	66/66	0.84	0.12	44,65,85,95	0
33	LMG	B	627	55/55	0.84	0.13	34,60,84,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
33	LMG	D	409	33/55	0.84	0.13	34,56,86,94	0
32	STE	c	520	20/20	0.84	0.12	42,61,83,84	0
32	STE	h	102	14/20	0.84	0.15	47,67,84,84	0
32	STE	L	103	12/20	0.85	0.17	52,64,88,89	0
27	PL9	A	410	55/55	0.85	0.14	37,69,85,95	0
29	SQD	A	414	39/54	0.85	0.13	37,66,87,95	0
32	STE	b	623	16/20	0.86	0.13	49,62,84,86	0
33	LMG	Y	101	48/55	0.86	0.12	43,75,97,104	0
22	CLA	b	601	65/65	0.87	0.11	46,71,90,108	0
32	STE	d	411	17/20	0.87	0.13	44,58,70,77	0
32	STE	t	104	18/20	0.88	0.11	42,62,76,80	0
32	STE	x	102	20/20	0.88	0.12	36,63,81,81	0
32	STE	C	522	12/20	0.88	0.11	33,45,57,61	0
27	PL9	a	410	55/55	0.88	0.13	41,70,89,102	0
33	LMG	D	410	28/55	0.88	0.12	31,51,69,73	0
32	STE	C	520	12/20	0.88	0.11	37,53,65,75	0
32	STE	Z	102	8/20	0.88	0.13	43,60,72,72	0
33	LMG	c	519	37/55	0.88	0.11	43,67,84,87	0
29	SQD	B	623	54/54	0.88	0.10	34,65,92,110	0
32	STE	b	621	20/20	0.89	0.10	37,58,76,81	0
33	LMG	C	516	48/55	0.89	0.10	36,58,77,83	0
33	LMG	c	522	49/55	0.89	0.10	32,58,90,114	0
32	STE	t	102	14/20	0.90	0.09	35,53,60,65	0
32	STE	M	104	18/20	0.90	0.11	37,54,88,89	0
29	SQD	f	101	41/54	0.90	0.12	60,81,107,111	0
29	SQD	L	101	49/54	0.90	0.10	45,61,96,100	0
32	STE	D	411	20/20	0.90	0.10	35,55,70,74	0
24	BCR	Z	101	40/40	0.90	0.11	38,60,75,77	0
32	STE	t	103	10/20	0.91	0.10	41,58,70,73	0
29	SQD	F	101	36/54	0.91	0.11	46,73,94,100	0
24	BCR	c	514	40/40	0.91	0.09	45,58,79,80	0
32	STE	B	621	17/20	0.91	0.09	35,53,68,75	0
32	STE	M	103	10/20	0.91	0.11	35,45,55,66	0
32	STE	B	624	12/20	0.91	0.10	35,53,67,74	0
24	BCR	D	405	40/40	0.92	0.09	28,47,85,101	0
29	SQD	a	411	54/54	0.92	0.10	41,67,95,97	0
24	BCR	K	101	40/40	0.92	0.09	40,56,73,77	0
22	CLA	C	514	65/65	0.92	0.10	44,64,100,106	0
22	CLA	B	602	65/65	0.92	0.10	34,60,89,98	0
33	LMG	M	101	51/55	0.92	0.09	33,52,76,86	0
30	DGD	C	518	62/66	0.92	0.10	34,53,108,130	0
30	DGD	h	101	62/66	0.92	0.09	33,51,67,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	BCR	d	405	40/40	0.92	0.10	31,52,87,102	0
24	BCR	k	102	40/40	0.92	0.10	46,63,80,82	0
24	BCR	x	101	40/40	0.92	0.09	37,56,74,79	0
22	CLA	c	513	65/65	0.93	0.10	44,68,109,121	0
22	CLA	c	512	65/65	0.93	0.10	45,61,100,112	0
24	BCR	b	617	40/40	0.93	0.08	27,45,60,60	0
24	BCR	H	101	40/40	0.93	0.08	32,48,64,73	0
30	DGD	c	517	62/66	0.93	0.09	33,55,98,104	0
32	STE	M	102	15/20	0.93	0.10	36,49,63,72	0
33	LMG	m	101	51/55	0.93	0.08	34,54,73,90	0
29	SQD	A	412	52/54	0.94	0.09	36,61,94,98	0
24	BCR	B	618	40/40	0.94	0.08	26,43,64,65	0
24	BCR	b	619	40/40	0.94	0.08	33,50,65,70	0
24	BCR	B	619	40/40	0.94	0.07	23,39,54,57	0
24	BCR	B	620	40/40	0.94	0.08	24,47,67,76	0
24	BCR	C	501	40/40	0.94	0.09	40,53,72,81	0
33	LMG	D	407	51/55	0.94	0.10	31,58,97,101	0
24	BCR	k	103	40/40	0.94	0.09	39,55,69,76	0
24	BCR	C	515	40/40	0.94	0.08	27,45,58,67	0
22	CLA	c	511	65/65	0.94	0.09	38,56,77,82	0
22	CLA	C	513	65/65	0.94	0.10	38,56,101,105	0
30	DGD	H	102	62/66	0.94	0.08	29,47,62,66	0
22	CLA	b	606	65/65	0.94	0.07	28,43,79,93	0
30	DGD	c	518	62/66	0.94	0.09	28,56,95,100	0
24	BCR	A	406	40/40	0.94	0.07	24,38,47,56	0
33	LMG	d	410	44/55	0.94	0.10	36,55,89,104	0
28	LHG	d	407	49/49	0.94	0.10	34,52,74,84	0
22	CLA	c	506	65/65	0.95	0.09	30,54,101,105	0
24	BCR	a	406	40/40	0.95	0.06	23,38,49,54	0
22	CLA	c	508	64/65	0.95	0.08	32,46,83,100	0
24	BCR	b	618	40/40	0.95	0.06	27,42,54,58	0
30	DGD	C	517	62/66	0.95	0.09	22,43,84,95	0
22	CLA	c	509	65/65	0.95	0.09	33,51,70,75	0
30	DGD	C	519	62/66	0.95	0.09	28,54,75,83	0
22	CLA	c	510	65/65	0.95	0.08	33,51,65,73	0
30	DGD	c	516	62/66	0.95	0.09	23,45,81,92	0
24	BCR	c	515	40/40	0.95	0.07	30,44,65,69	0
22	CLA	C	508	65/65	0.95	0.07	26,45,61,66	0
22	CLA	C	510	65/65	0.95	0.08	28,48,68,74	0
22	CLA	C	512	65/65	0.95	0.09	35,55,72,85	0
24	BCR	t	101	40/40	0.95	0.06	29,42,56,57	0
22	CLA	d	404	65/65	0.95	0.08	32,52,97,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
26	BCT	A	409	4/4	0.95	0.08	26,33,35,42	0
22	CLA	B	607	65/65	0.95	0.07	22,38,76,83	0
27	PL9	D	406	55/55	0.95	0.07	23,37,53,55	0
22	CLA	B	617	60/65	0.95	0.09	26,43,92,113	0
28	LHG	A	411	47/49	0.95	0.09	31,52,79,95	0
22	CLA	a	405	65/65	0.95	0.08	22,42,90,105	0
22	CLA	C	506	65/65	0.95	0.08	23,41,72,82	0
22	CLA	C	507	65/65	0.95	0.08	27,48,95,114	0
28	LHG	d	409	39/49	0.95	0.08	32,51,66,69	0
28	LHG	l	101	49/49	0.95	0.08	25,48,61,78	0
22	CLA	b	616	60/65	0.95	0.08	29,48,91,98	0
22	CLA	c	503	65/65	0.95	0.08	35,48,61,67	0
22	CLA	c	504	60/65	0.95	0.07	33,48,83,88	0
22	CLA	c	505	65/65	0.95	0.08	30,45,72,77	0
24	BCR	T	101	40/40	0.95	0.06	28,44,60,68	0
22	CLA	A	403	65/65	0.96	0.08	22,37,87,101	0
22	CLA	C	509	65/65	0.96	0.07	34,46,105,121	0
27	PL9	d	406	55/55	0.96	0.06	19,37,48,56	0
22	CLA	B	610	65/65	0.96	0.06	26,38,61,72	0
22	CLA	C	511	65/65	0.96	0.07	29,48,70,77	0
28	LHG	B	622	49/49	0.96	0.08	31,47,68,81	0
28	LHG	L	102	49/49	0.96	0.06	27,42,59,71	0
22	CLA	B	611	65/65	0.96	0.07	21,34,48,55	0
22	CLA	B	614	65/65	0.96	0.07	22,36,73,83	0
22	CLA	d	402	65/65	0.96	0.07	21,37,65,68	0
22	CLA	d	403	65/65	0.96	0.07	20,34,52,56	0
22	CLA	B	615	65/65	0.96	0.08	26,41,84,94	0
23	PHO	a	404	64/64	0.96	0.06	21,33,41,46	0
23	PHO	d	401	64/64	0.96	0.06	26,42,52,62	0
22	CLA	D	402	65/65	0.96	0.06	17,32,59,66	0
22	CLA	D	404	65/65	0.96	0.08	24,46,105,117	0
22	CLA	a	403	65/65	0.96	0.08	25,43,98,116	0
22	CLA	B	616	65/65	0.96	0.07	27,40,69,86	0
22	CLA	A	402	65/65	0.96	0.06	21,29,43,61	0
22	CLA	b	602	65/65	0.96	0.07	24,46,67,75	0
22	CLA	b	604	65/65	0.96	0.07	23,40,82,97	0
22	CLA	b	605	65/65	0.96	0.07	23,38,53,61	0
22	CLA	C	502	65/65	0.96	0.06	25,37,54,57	0
22	CLA	b	608	65/65	0.96	0.07	27,44,70,75	0
22	CLA	b	609	65/65	0.96	0.07	27,47,81,86	0
22	CLA	b	610	65/65	0.96	0.07	27,40,52,62	0
22	CLA	b	611	65/65	0.96	0.06	21,36,56,68	0

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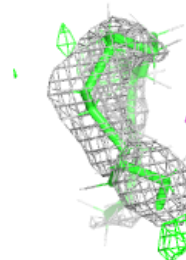
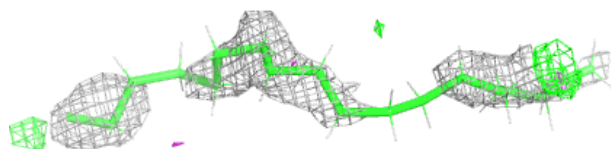
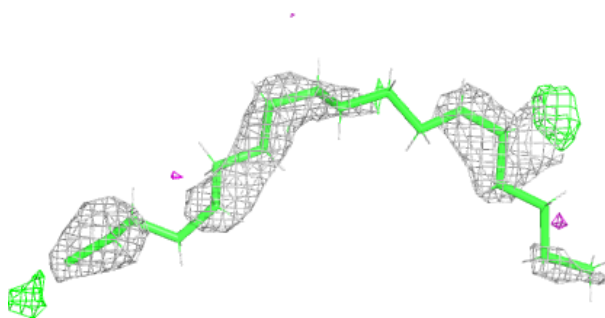
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	CLA	b	612	65/65	0.96	0.07	22,36,52,56	0
22	CLA	b	614	65/65	0.96	0.07	23,42,80,89	0
22	CLA	b	615	65/65	0.96	0.07	28,43,64,70	0
22	CLA	C	503	65/65	0.96	0.07	32,45,65,79	0
22	CLA	c	501	65/65	0.96	0.07	28,44,56,68	0
22	CLA	c	502	65/65	0.96	0.07	32,47,64,70	0
22	CLA	C	504	65/65	0.96	0.06	33,47,56,61	0
22	CLA	C	505	59/65	0.96	0.07	28,45,82,99	0
22	CLA	B	605	65/65	0.96	0.07	23,36,74,84	0
22	CLA	B	606	65/65	0.96	0.07	22,36,52,56	0
22	CLA	c	507	65/65	0.96	0.07	28,48,63,65	0
34	HEC	e	101	43/43	0.96	0.09	44,61,79,83	0
22	CLA	B	609	65/65	0.97	0.05	23,36,56,62	0
22	CLA	A	405	54/65	0.97	0.06	20,36,63,73	0
22	CLA	D	403	65/65	0.97	0.06	20,33,54,61	0
22	CLA	b	607	65/65	0.97	0.07	21,39,70,81	0
26	BCT	a	409	4/4	0.97	0.07	31,31,44,52	0
22	CLA	B	603	65/65	0.97	0.07	23,41,59,61	0
23	PHO	A	404	64/64	0.97	0.06	21,30,42,45	0
23	PHO	D	401	64/64	0.97	0.05	22,35,45,50	0
22	CLA	a	402	65/65	0.97	0.05	19,33,47,55	0
22	CLA	B	612	65/65	0.97	0.05	22,34,50,54	0
22	CLA	B	613	65/65	0.97	0.06	20,34,53,58	0
22	CLA	B	604	65/65	0.97	0.07	23,36,64,67	0
28	LHG	D	408	49/49	0.97	0.06	24,41,54,60	0
22	CLA	b	613	65/65	0.97	0.07	23,37,82,87	0
22	CLA	B	608	65/65	0.97	0.06	20,36,65,71	0
22	CLA	b	603	65/65	0.97	0.07	24,40,71,82	0
34	HEC	E	101	43/43	0.97	0.07	36,50,69,75	0
28	LHG	d	408	49/49	0.97	0.07	27,43,59,66	0
34	HEC	V	201	43/43	0.98	0.07	25,37,45,53	0
34	HEC	v	201	43/43	0.98	0.06	32,39,52,59	0
25	CL	A	408	1/1	0.99	0.03	32,32,32,32	0
25	CL	a	407	1/1	0.99	0.03	32,32,32,32	0
25	CL	a	408	1/1	0.99	0.10	32,32,32,32	0
25	CL	A	407	1/1	0.99	0.03	32,32,32,32	0
21	FE2	a	401	1/1	1.00	0.02	38,38,38,38	0
21	FE2	A	401	1/1	1.00	0.01	30,30,30,30	0
31	OEX	A	416	10/10	1.00	0.03	25,31,33,37	0
31	OEX	a	415	10/10	1.00	0.03	22,30,32,33	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.

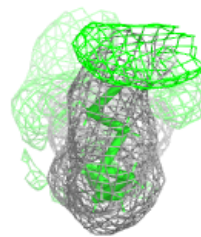
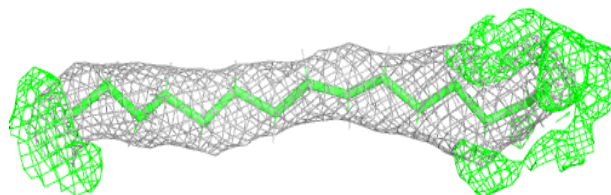
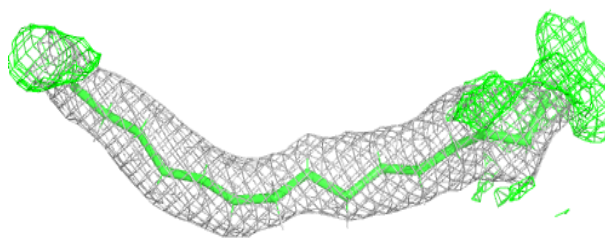
Electron density around STE H 103:

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



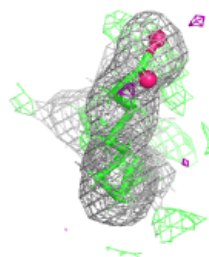
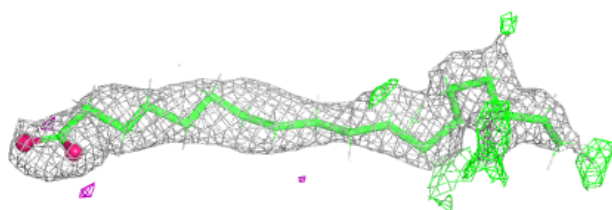
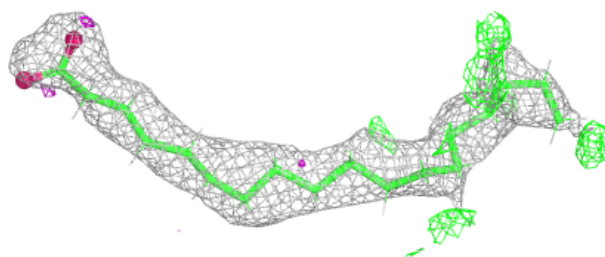
Electron density around STE I 101:

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

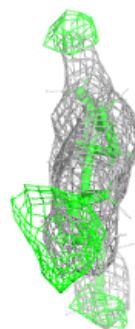
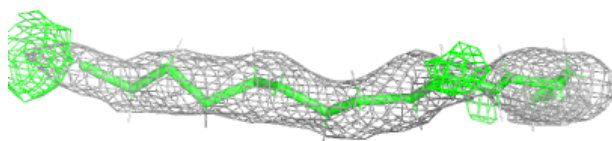
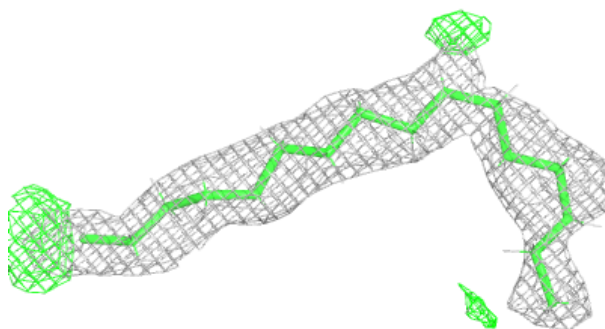


Electron density around STE b 626:

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

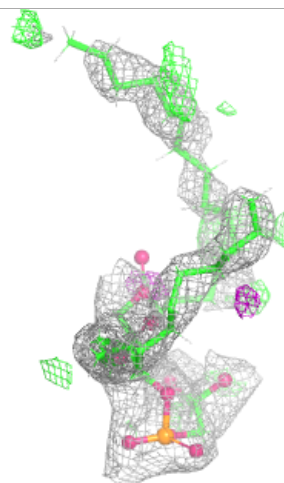
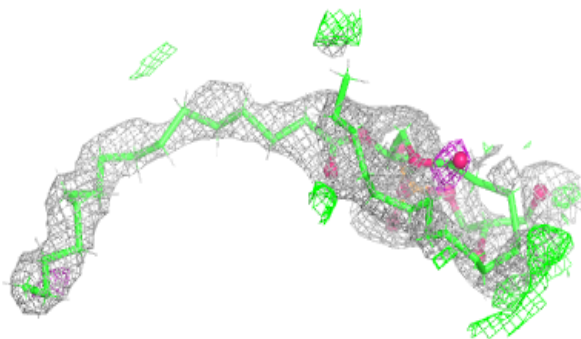
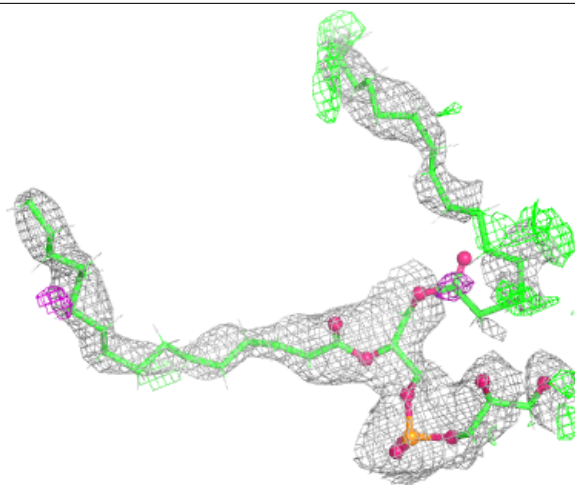
**Electron density around STE B 625:**

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



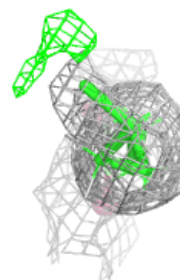
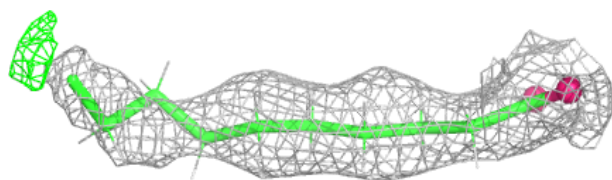
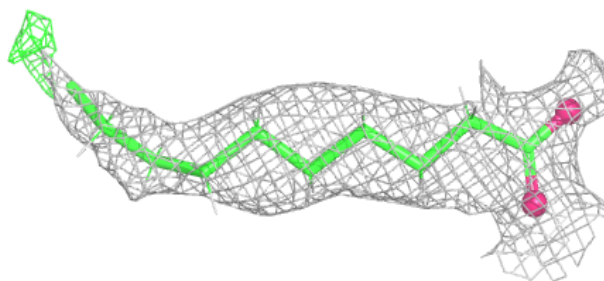
Electron density around LHG A 413:

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

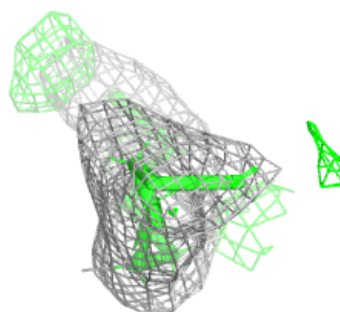
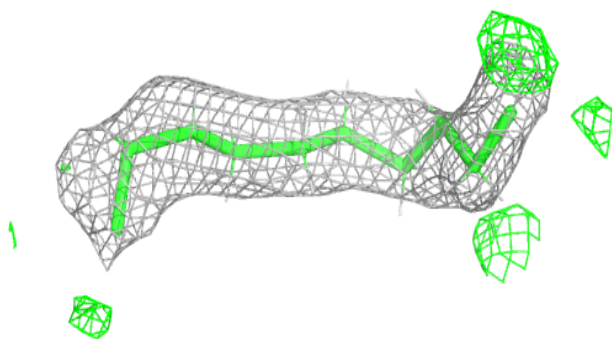
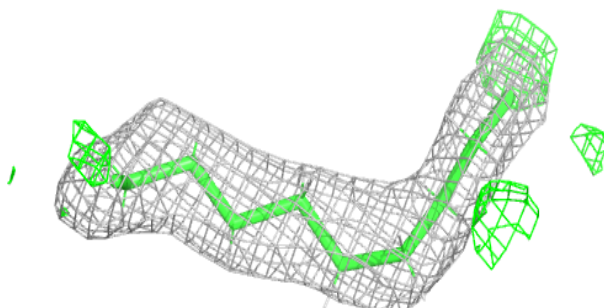


Electron density around STE k 101:

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and green (positive)

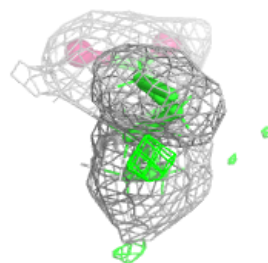
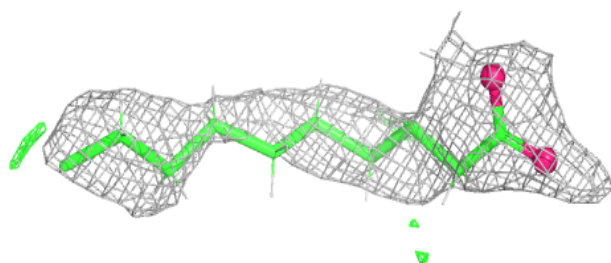
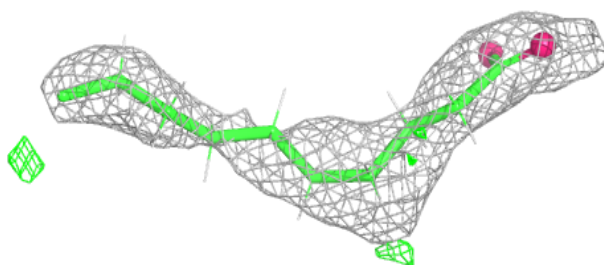
**Electron density around STE b 625:**

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

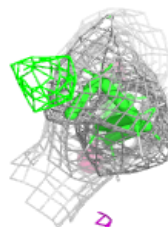
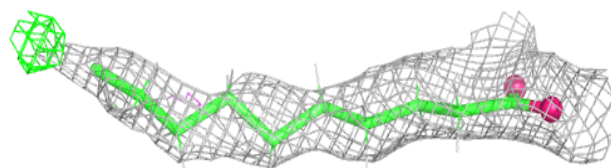
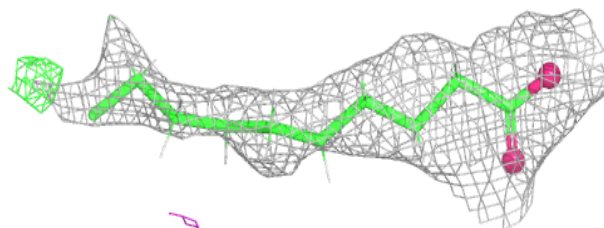


Electron density around STE E 102:

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

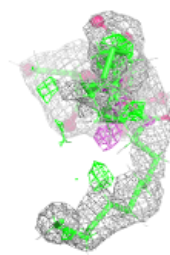
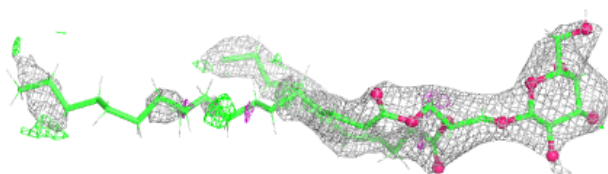
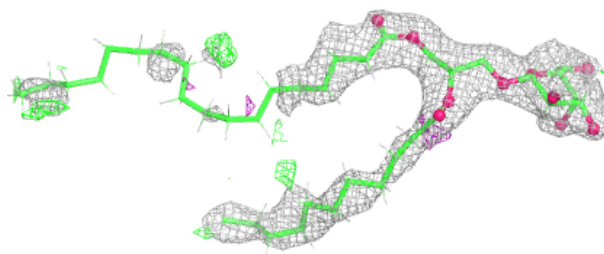
**Electron density around STE a 414:**

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and green (positive)

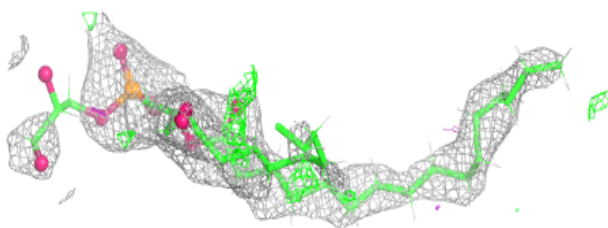
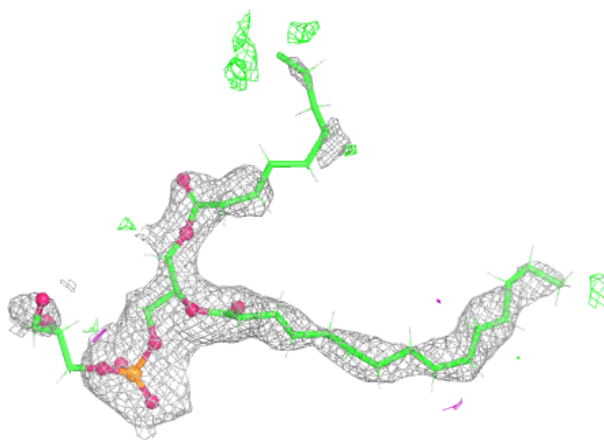


Electron density around LMG c 521:

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

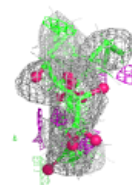
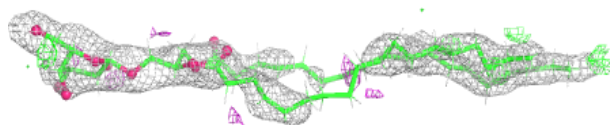
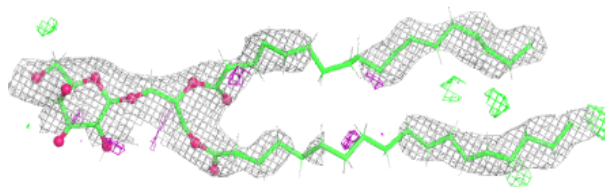
**Electron density around LHG a 412:**

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

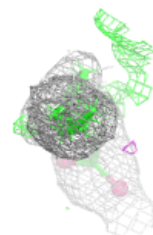
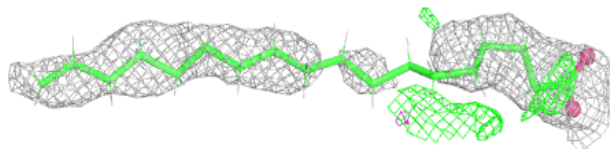
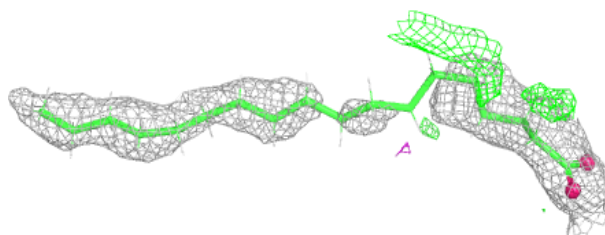


Electron density around LMG b 622:

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

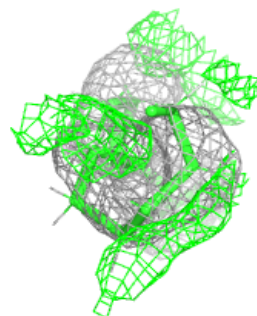
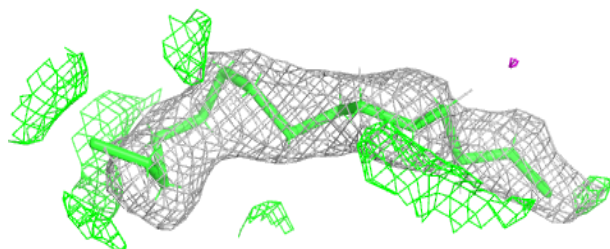
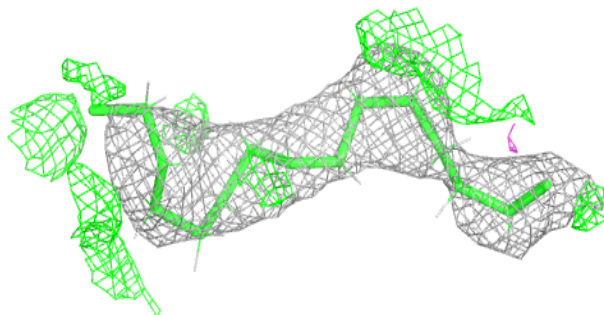
**Electron density around STE b 624:**

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

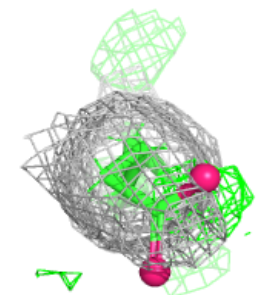
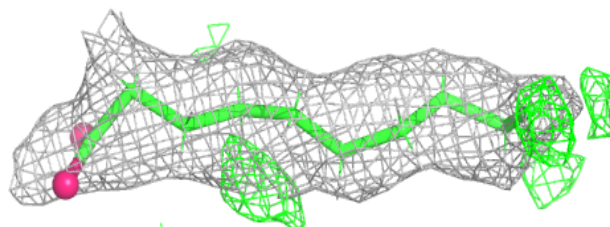
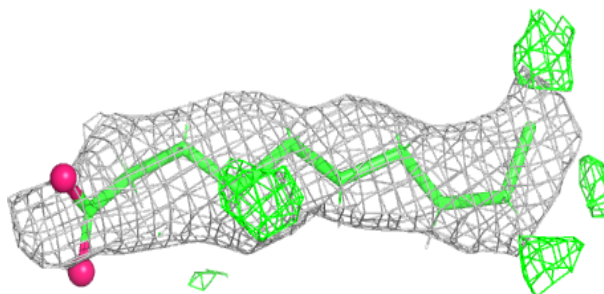


Electron density around STE B 626:

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

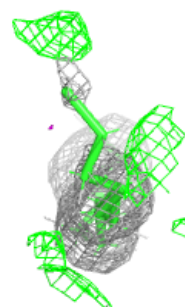
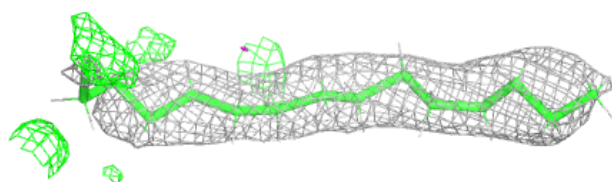
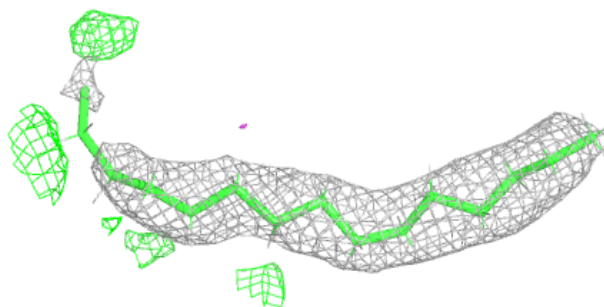
**Electron density around STE J 101:**

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

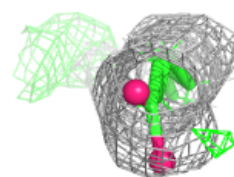
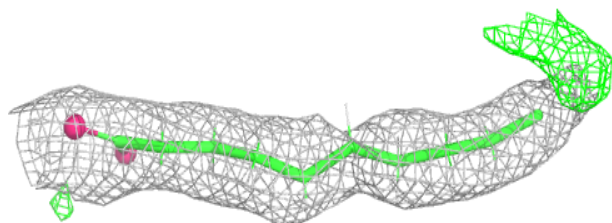
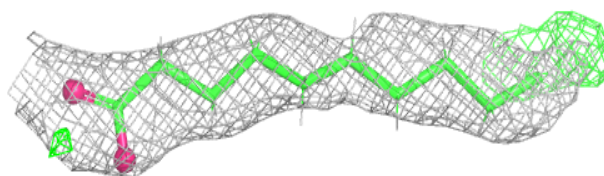


Electron density around STE T 102:

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and green (positive)

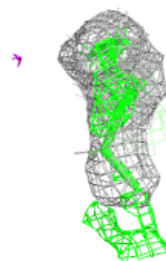
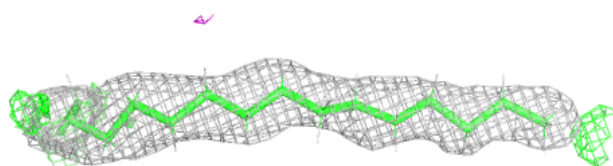
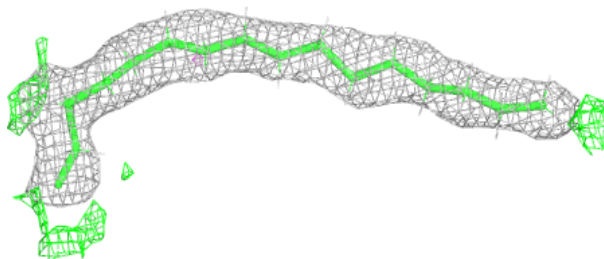
**Electron density around STE j 101:**

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and green (positive)

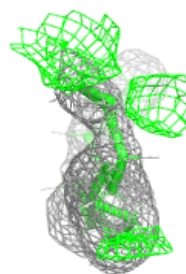
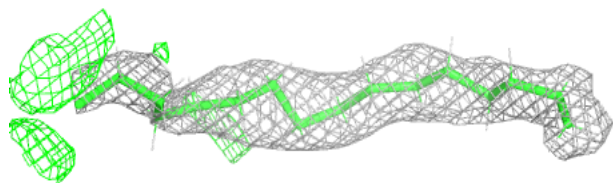
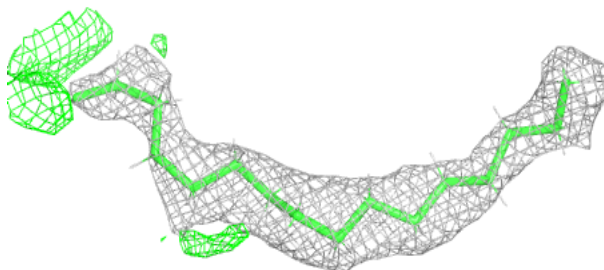


Electron density around STE C 521:

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and green (positive)

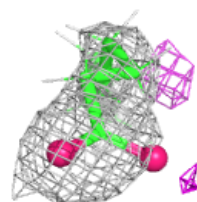
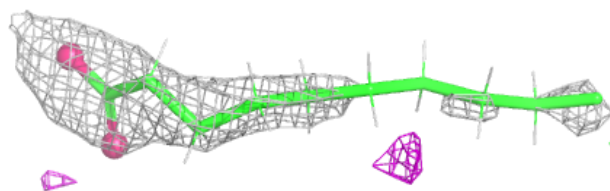
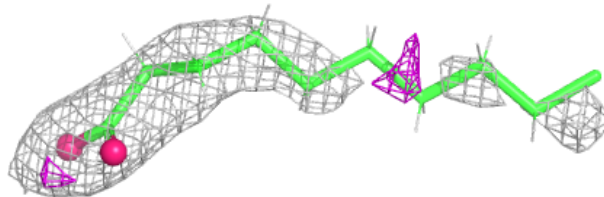
**Electron density around STE b 620:**

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and green (positive)



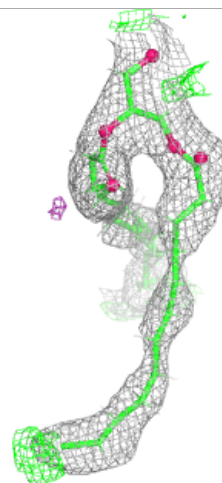
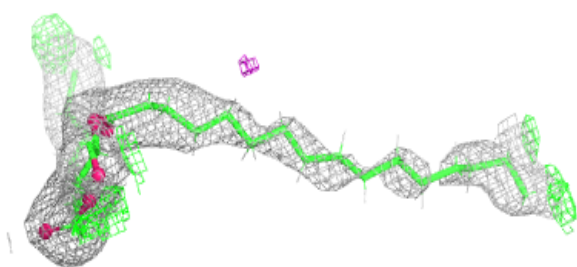
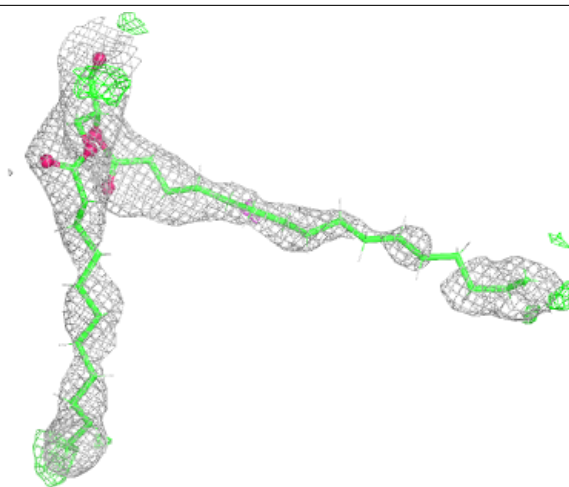
Electron density around STE B 601:

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and green (positive)



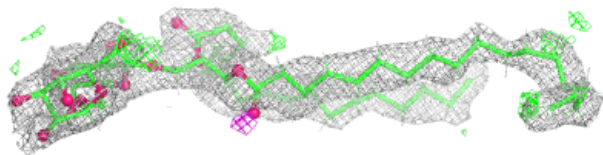
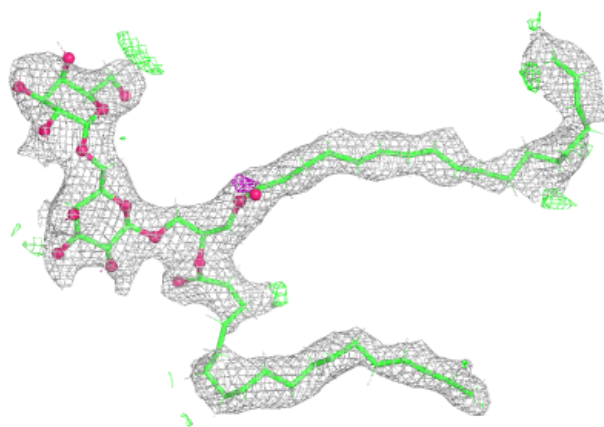
Electron density around SQD a 413:

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and green (positive)

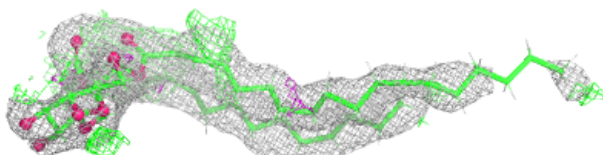
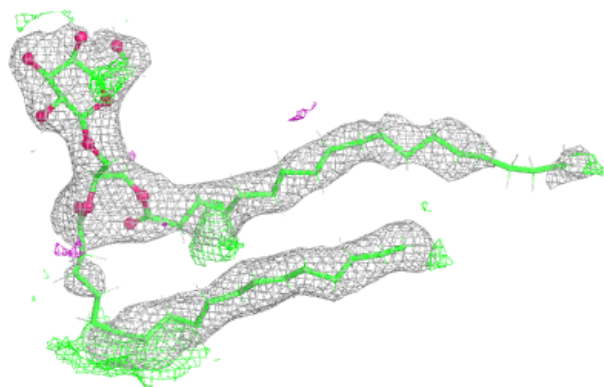


Electron density around DGD A 415:

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and green (positive)

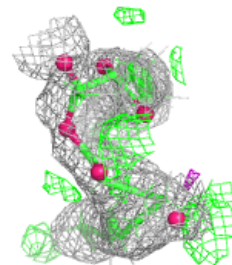
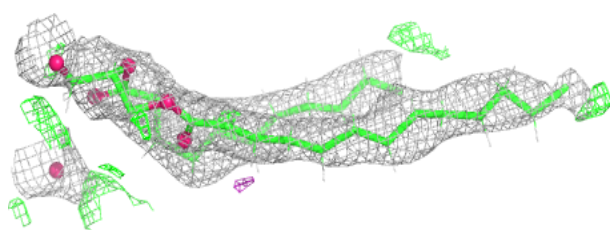
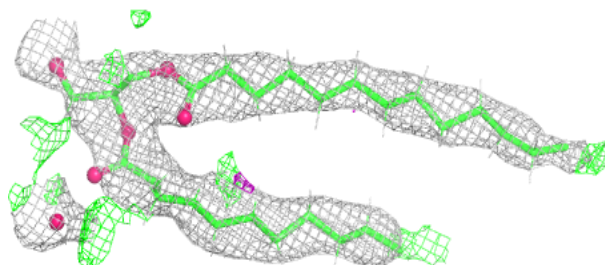
**Electron density around LMG B 627:**

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

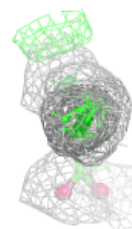
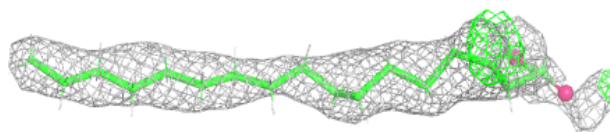
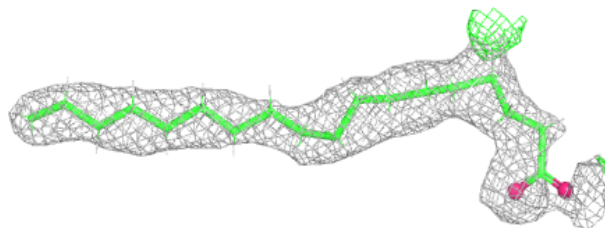


Electron density around LMG D 409:

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

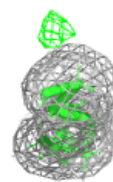
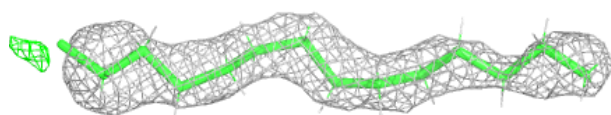
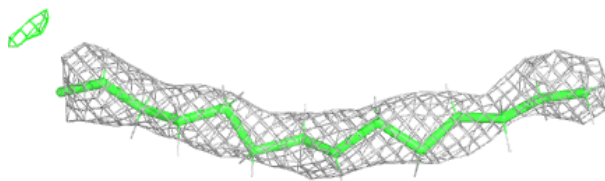
**Electron density around STE c 520:**

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

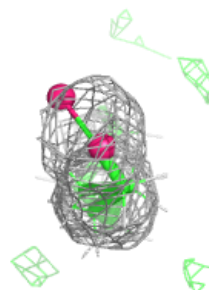
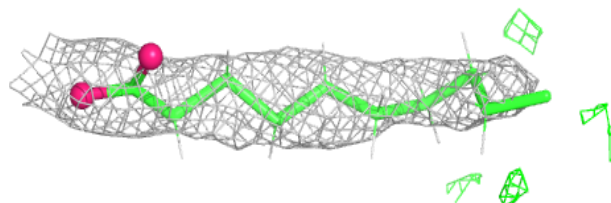
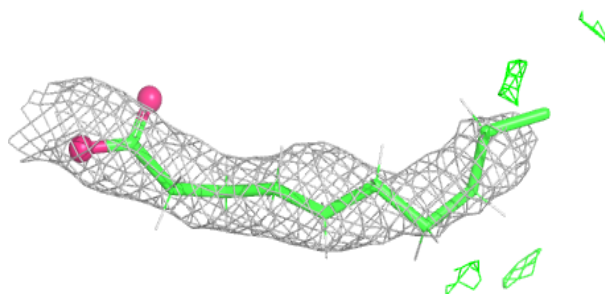


Electron density around STE h 102:

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

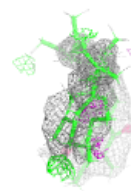
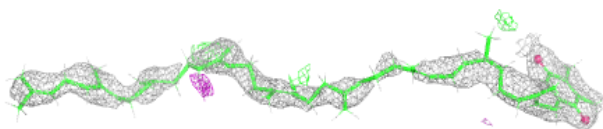
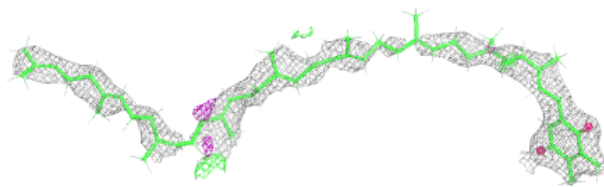
**Electron density around STE L 103:**

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



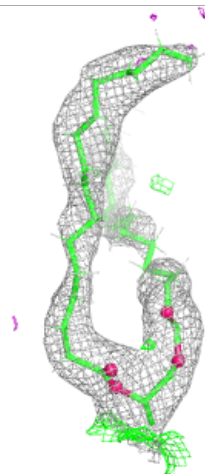
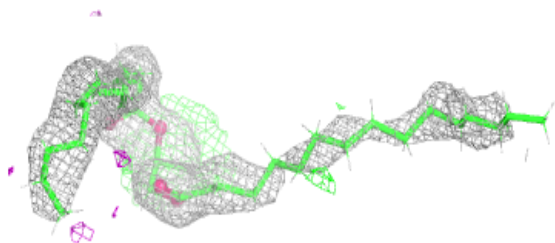
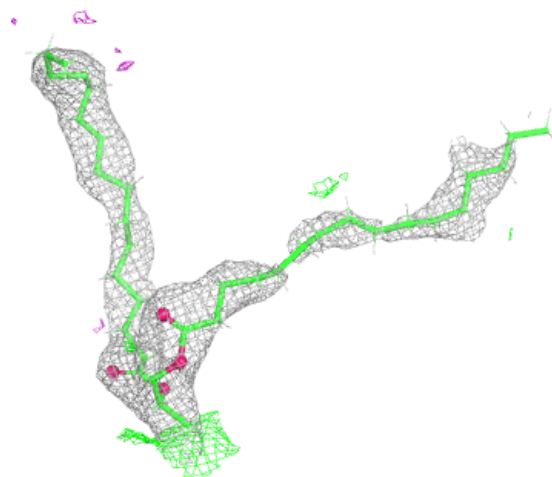
Electron density around PL9 A 410:

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



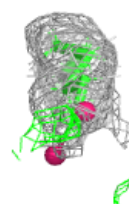
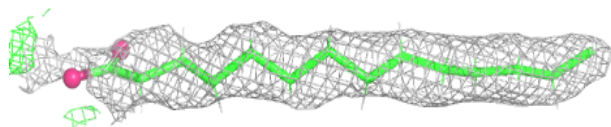
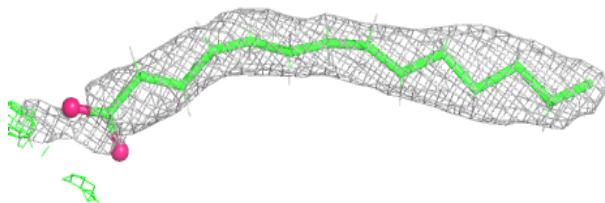
Electron density around SQD A 414:

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



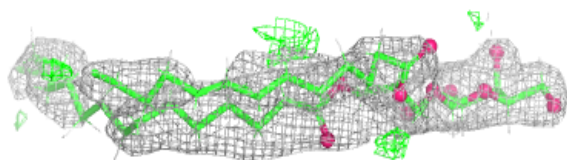
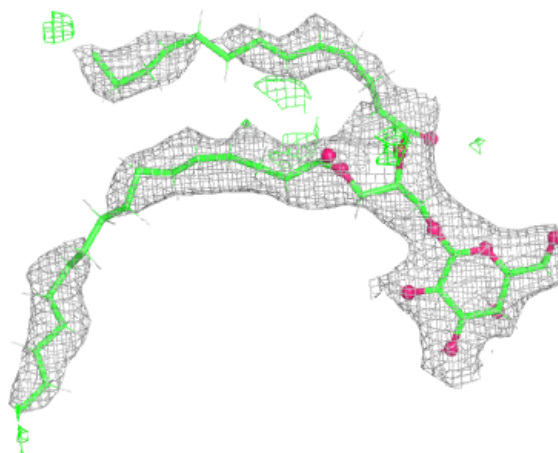
Electron density around STE b 623:

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



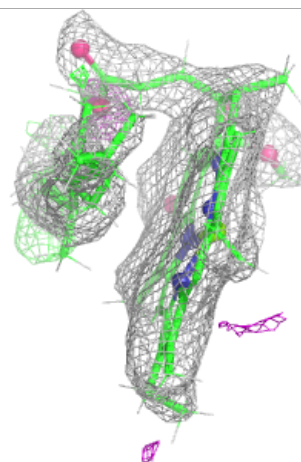
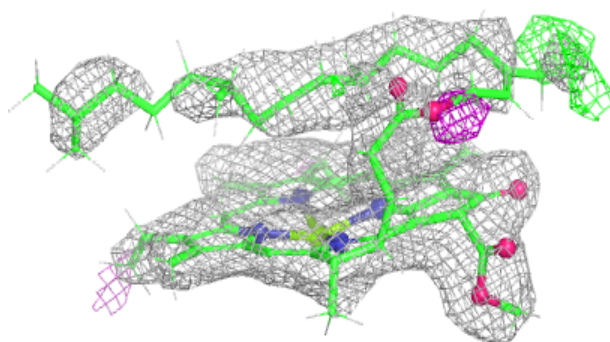
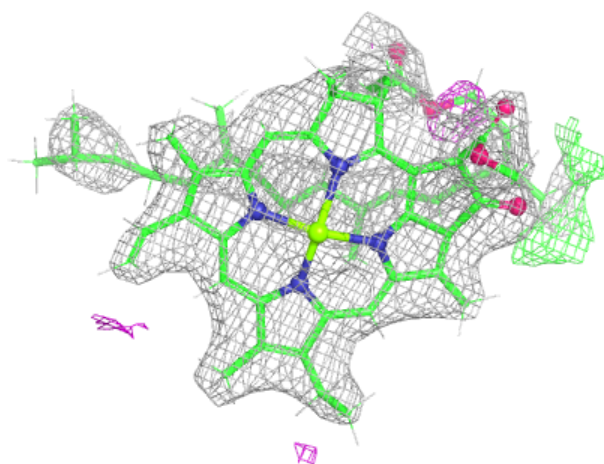
Electron density around LMG Y 101:

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



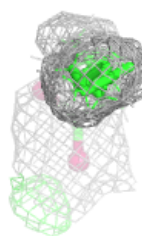
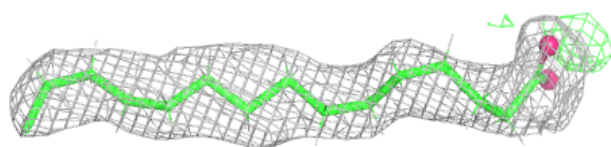
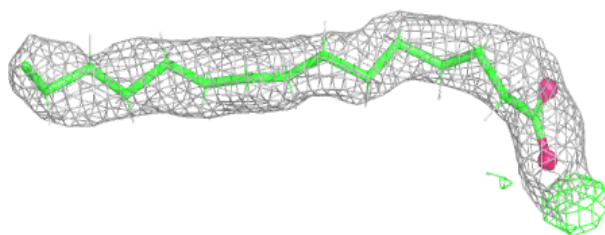
Electron density around CLA b 601:

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

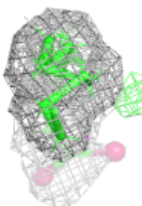
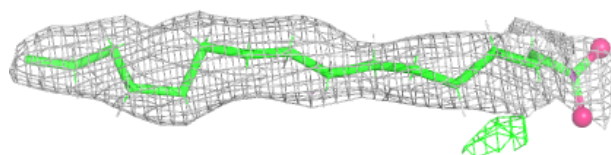
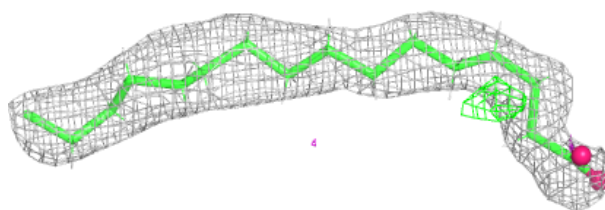


Electron density around STE d 411:

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

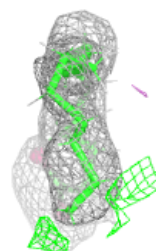
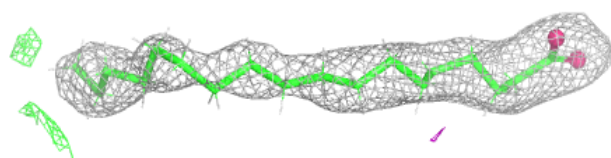
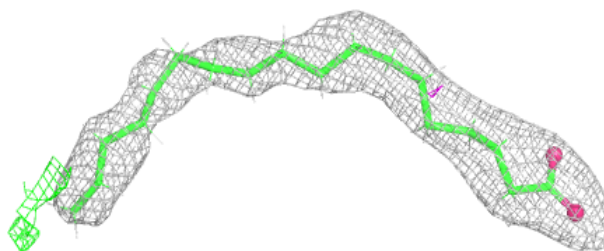
**Electron density around STE t 104:**

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

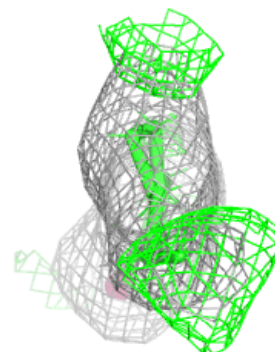
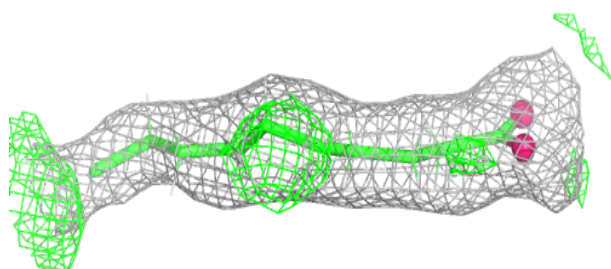
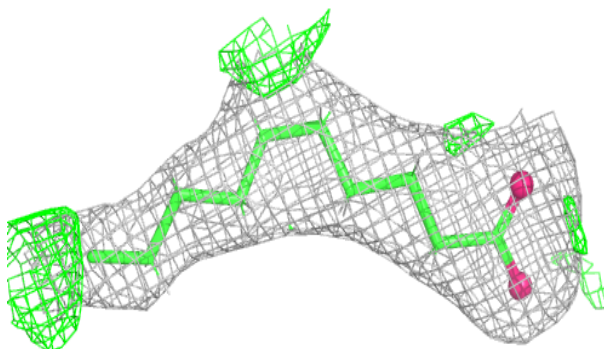


Electron density around STE x 102:

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

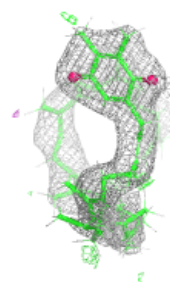
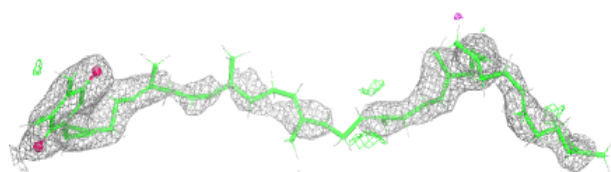
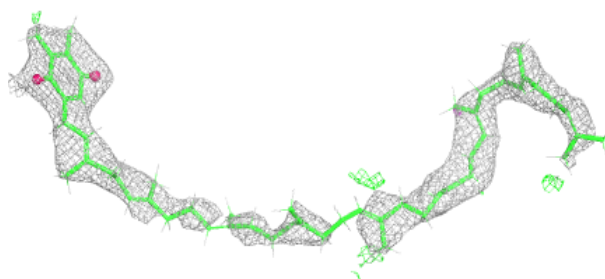
**Electron density around STE C 522:**

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

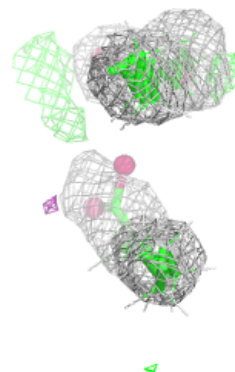
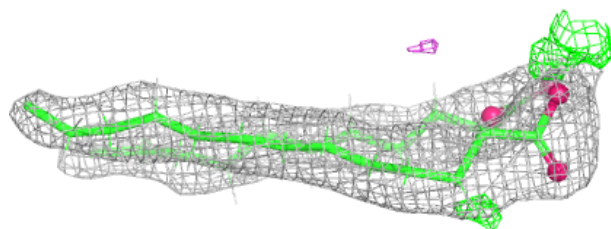
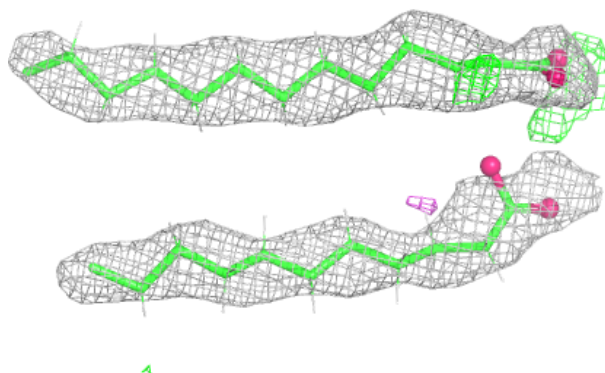


Electron density around PL9 a 410:

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

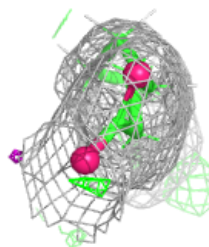
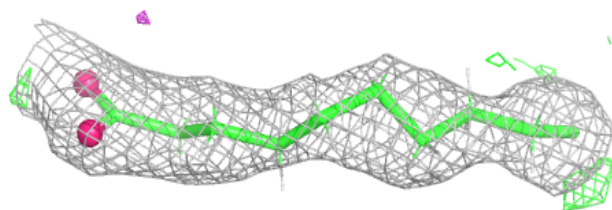
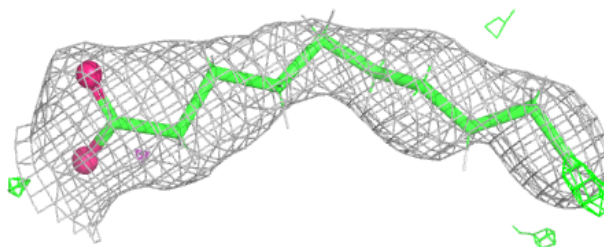
**Electron density around LMG D 410:**

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

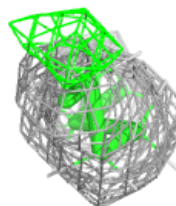
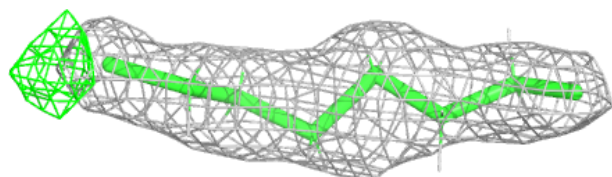
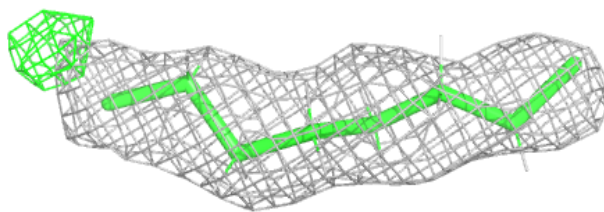


Electron density around STE C 520:

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

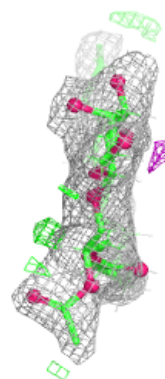
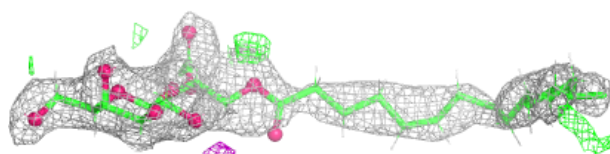
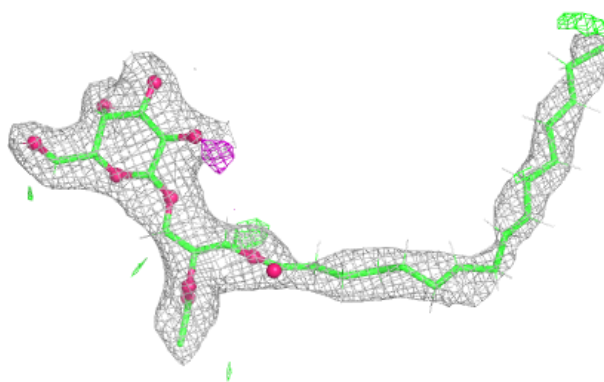
**Electron density around STE Z 102:**

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

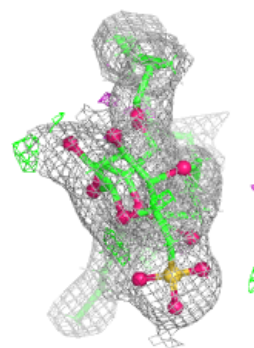
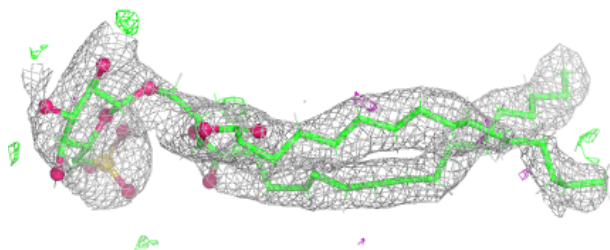
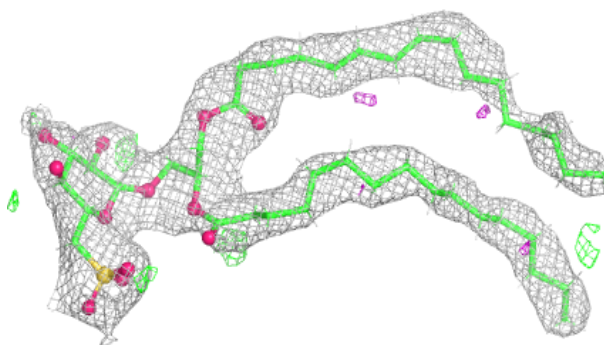


Electron density around LMG c 519:

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

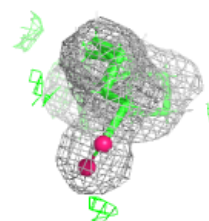
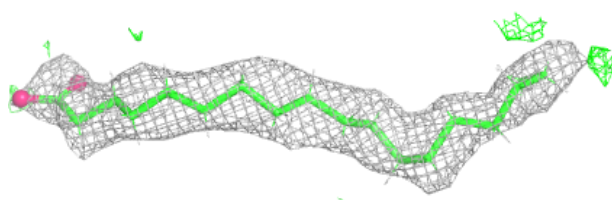
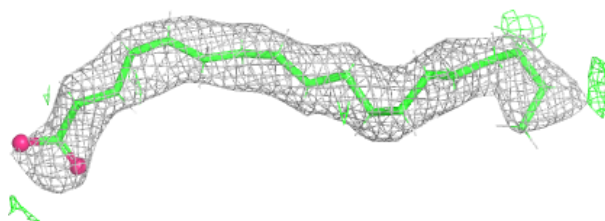
**Electron density around SQD B 623:**

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

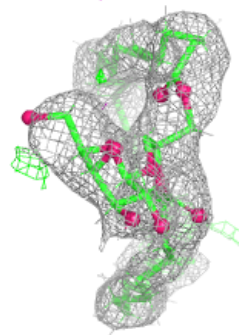
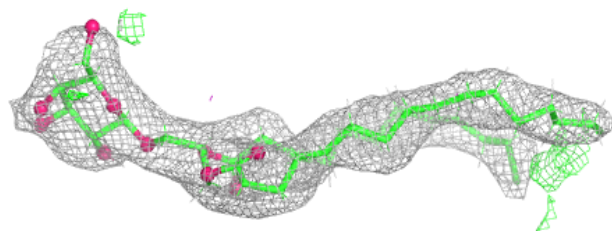
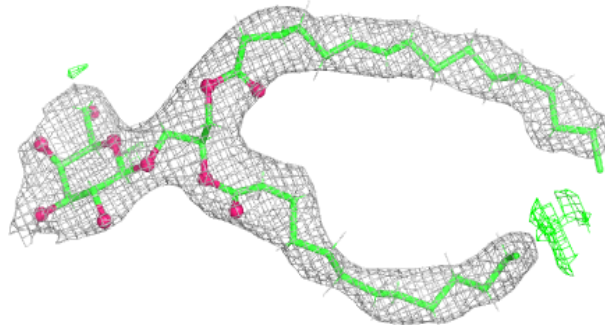


Electron density around STE b 621:

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

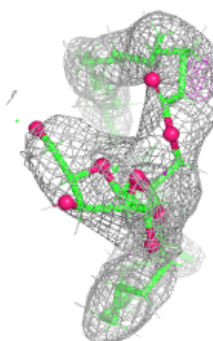
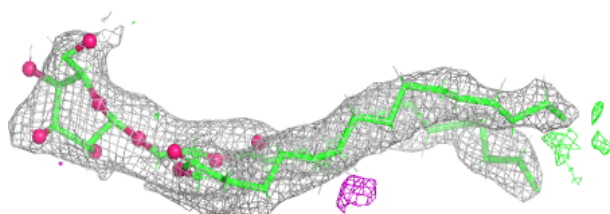
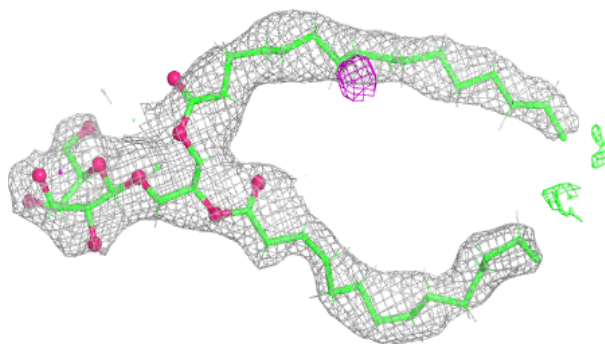
**Electron density around LMG C 516:**

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

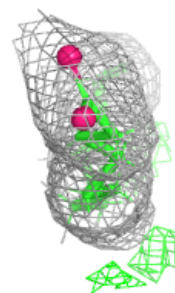
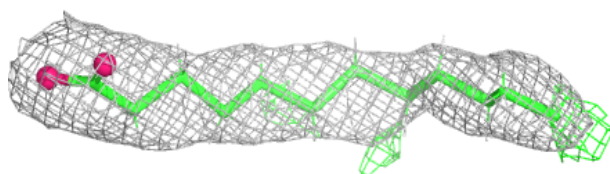
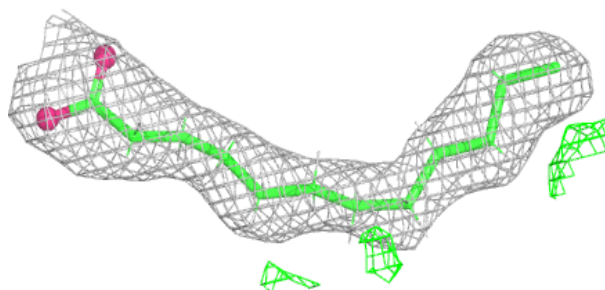


Electron density around LMG c 522:

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

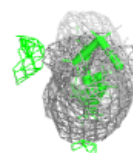
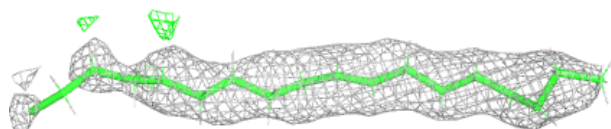
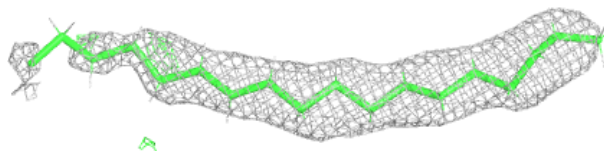
**Electron density around STE t 102:**

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

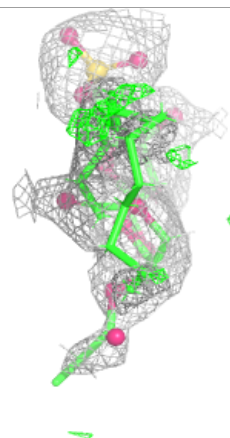
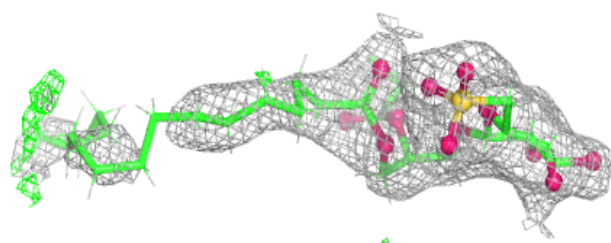
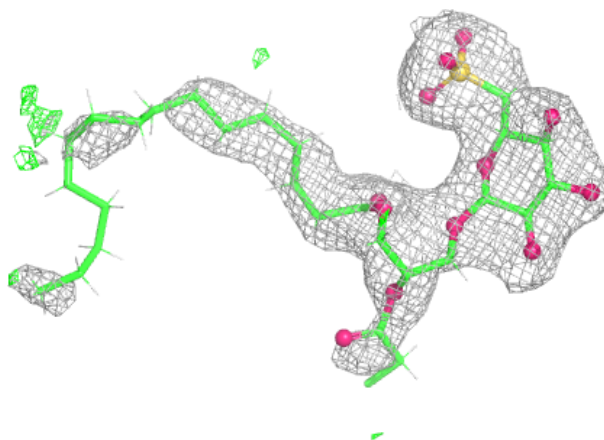


Electron density around STE M 104:

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

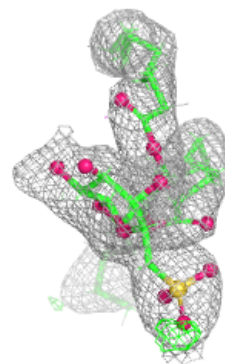
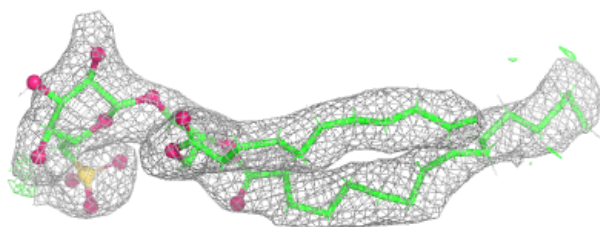
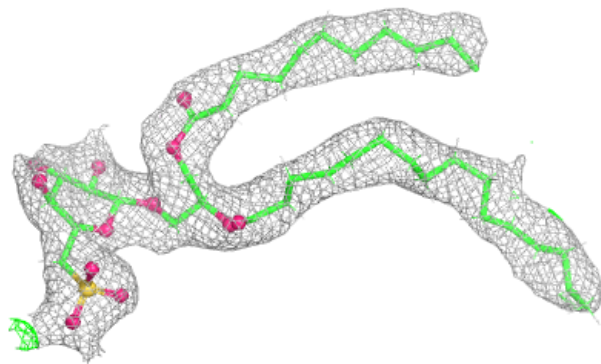
**Electron density around SQD f 101:**

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

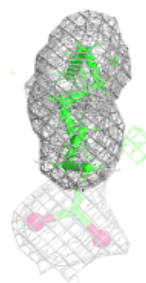
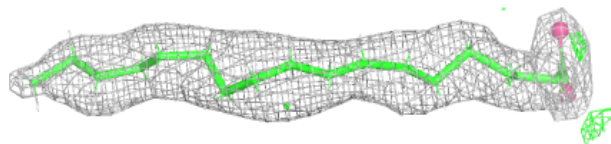
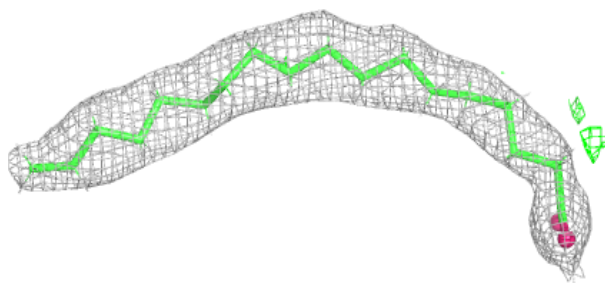


Electron density around SQD L 101:

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

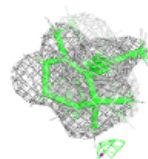
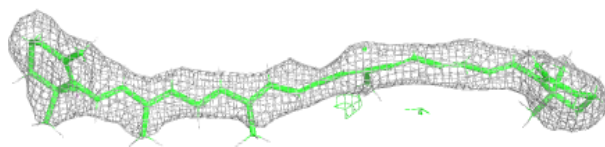
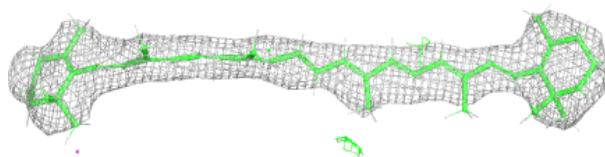
**Electron density around STE D 411:**

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

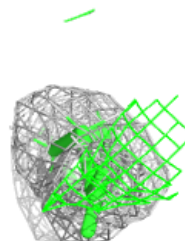
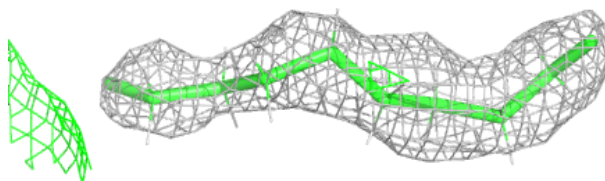
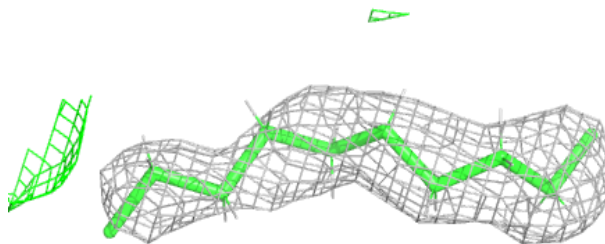


Electron density around BCR Z 101:

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

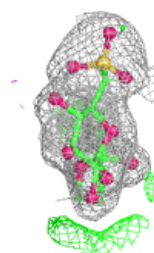
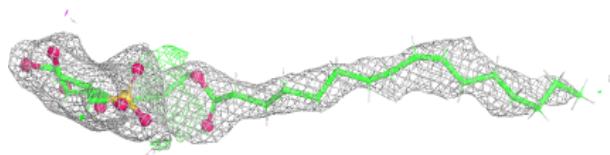
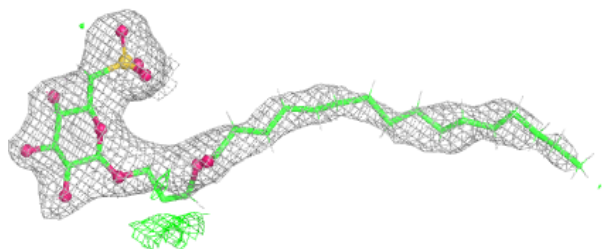
**Electron density around STE t 103:**

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

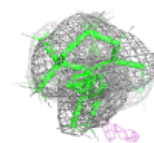
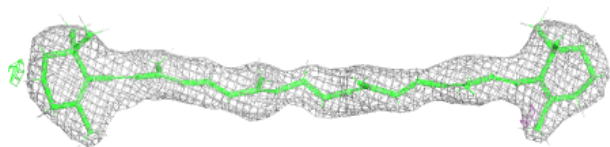


Electron density around SQD F 101:

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

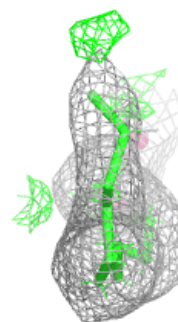
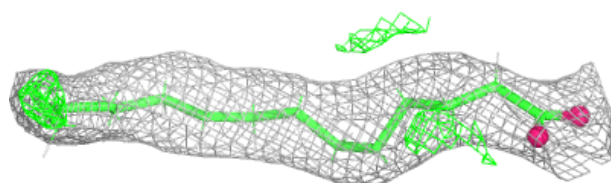
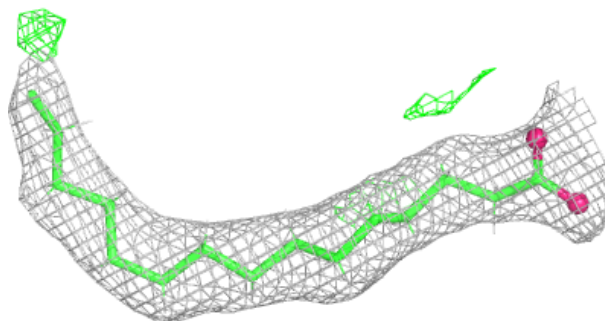
**Electron density around BCR c 514:**

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

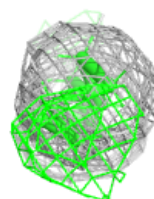
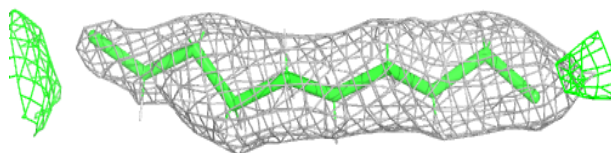
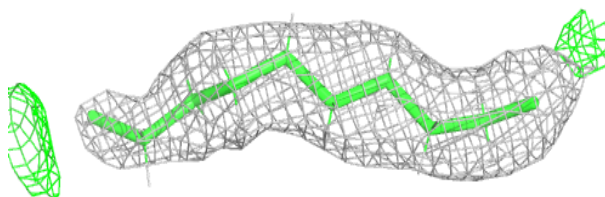


Electron density around STE B 621:

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

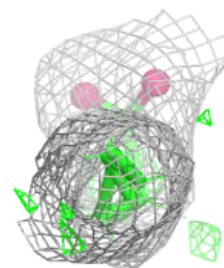
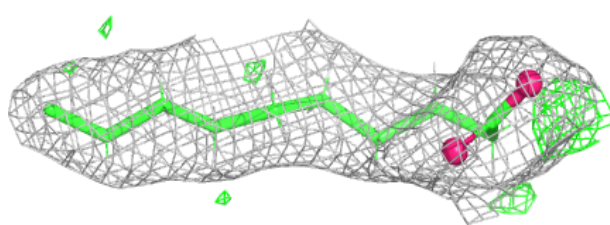
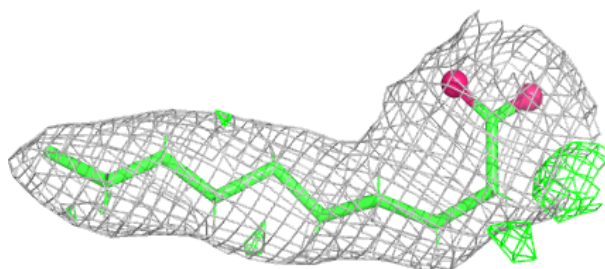
**Electron density around STE M 103:**

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

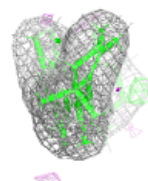
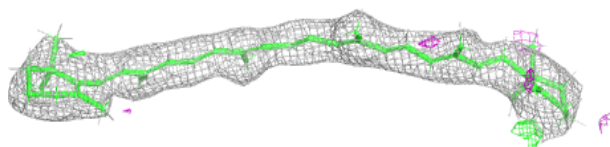
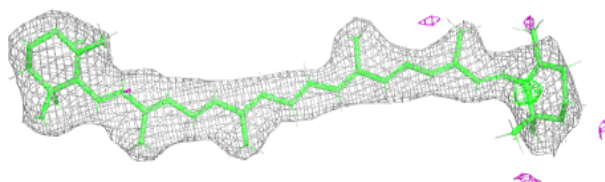


Electron density around STE B 624:

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

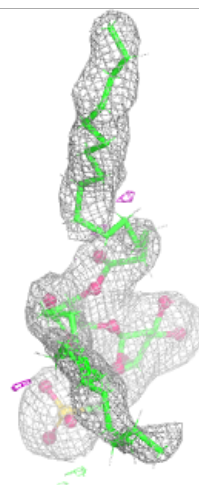
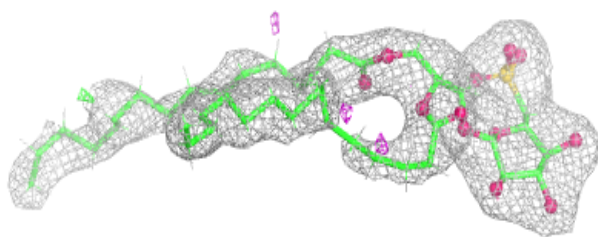
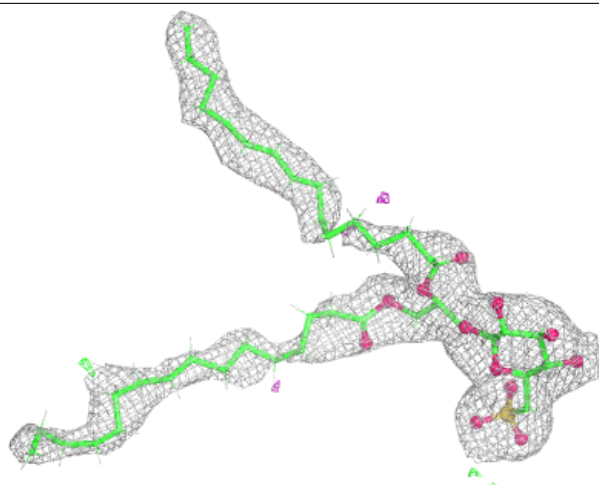
**Electron density around BCR D 405:**

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



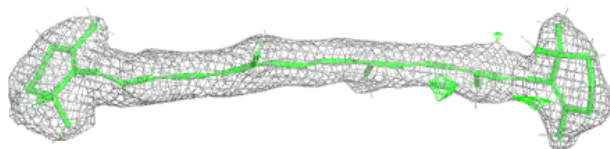
Electron density around SQD a 411:

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

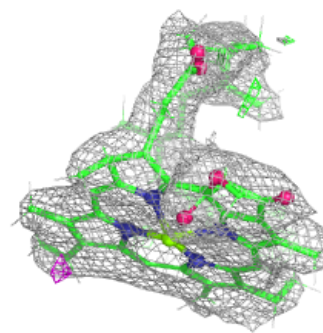
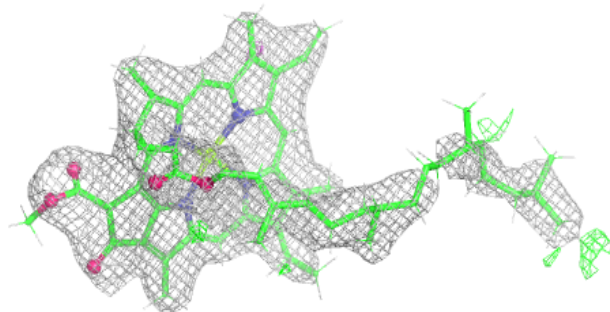
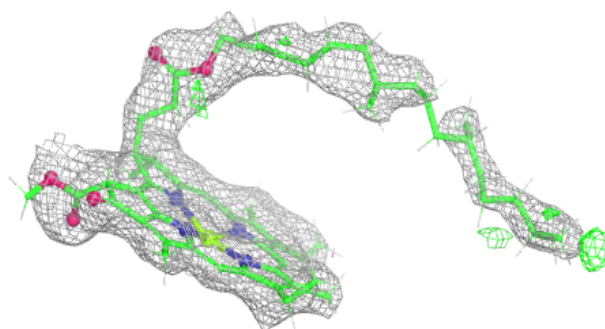


Electron density around BCR K 101:

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

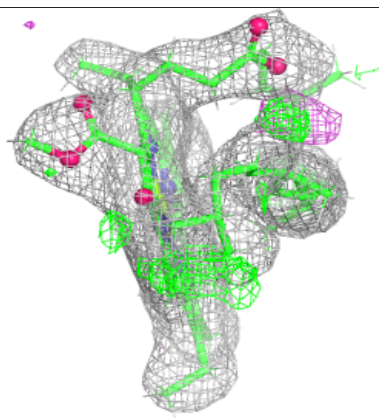
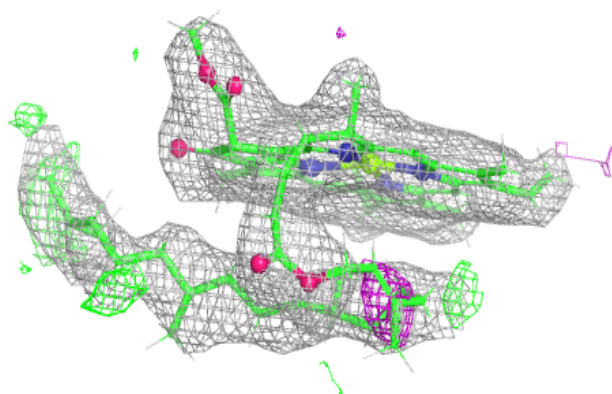
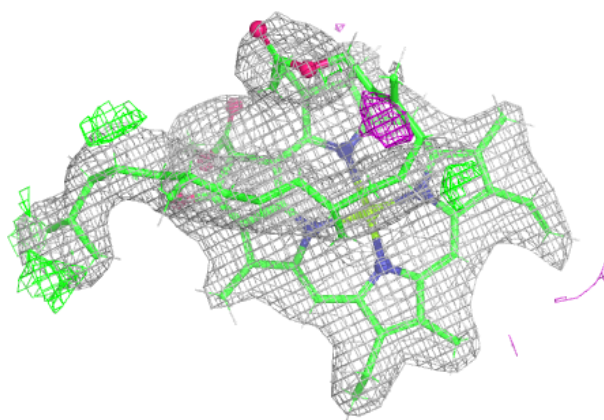
**Electron density around CLA C 514:**

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

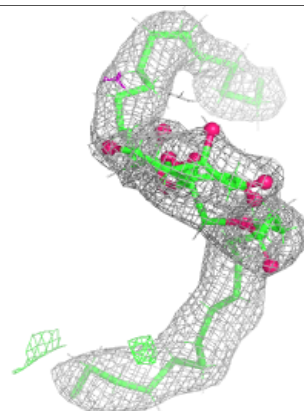
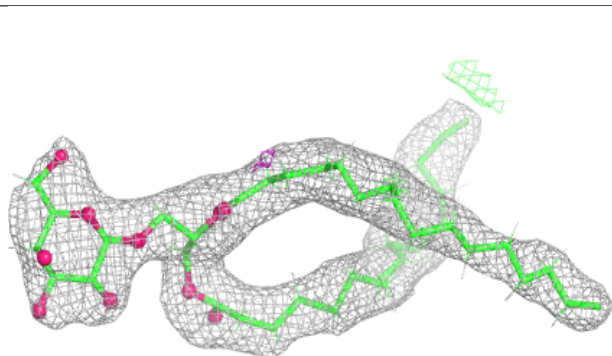
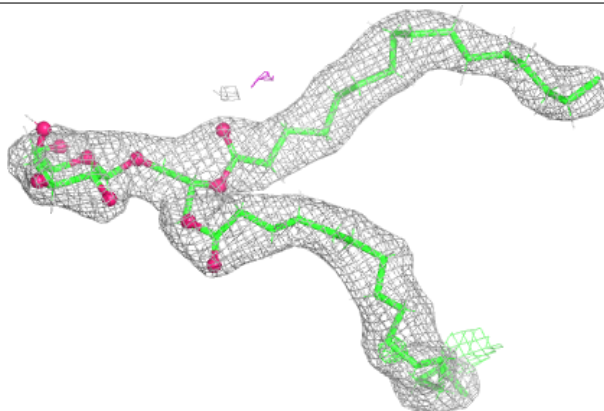


Electron density around CLA B 602:

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

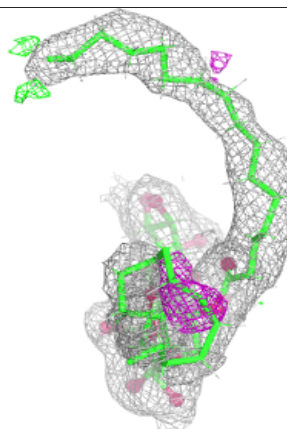
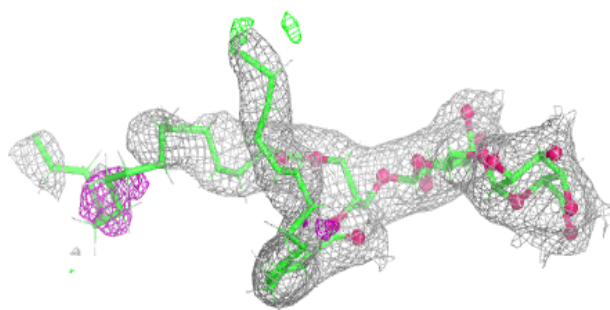
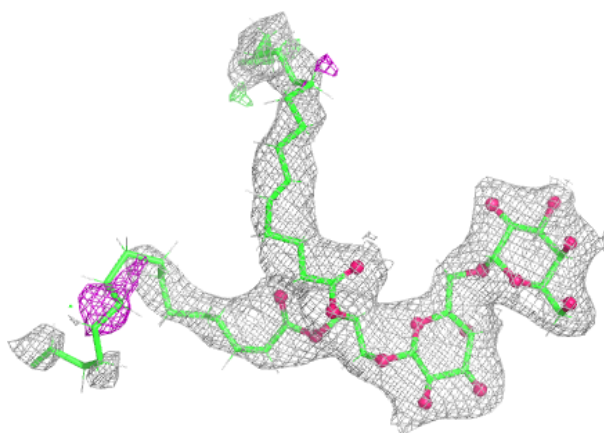
**Electron density around LMG M 101:**

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

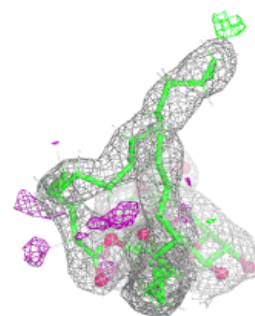
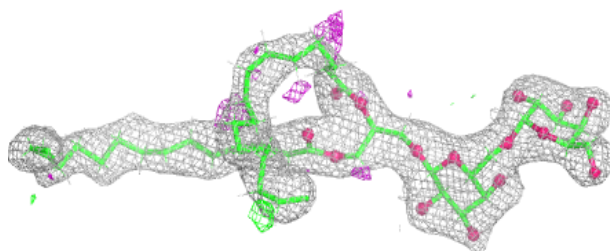
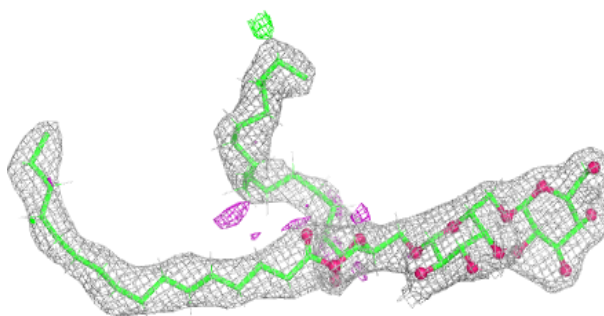


Electron density around DGD C 518:

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

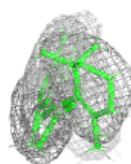
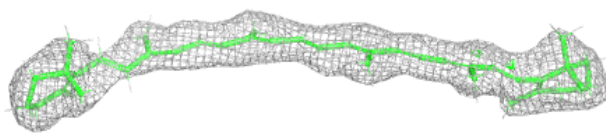
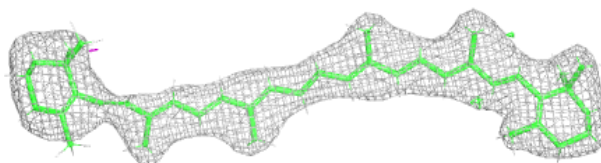
**Electron density around DGD h 101:**

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

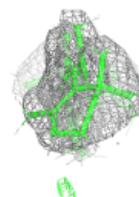
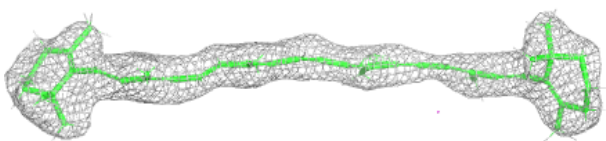
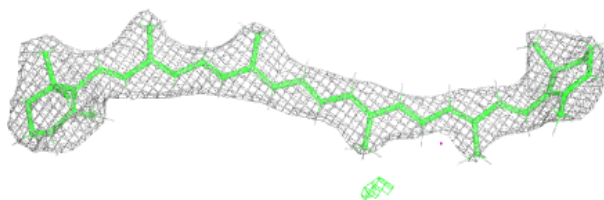


Electron density around BCR d 405:

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

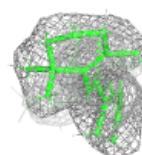
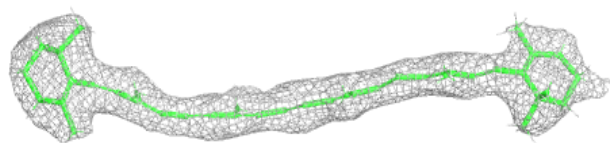
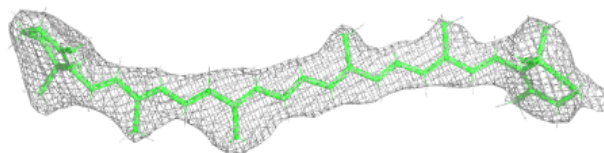
**Electron density around BCR k 102:**

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

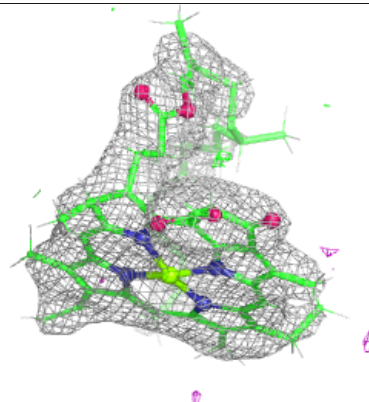
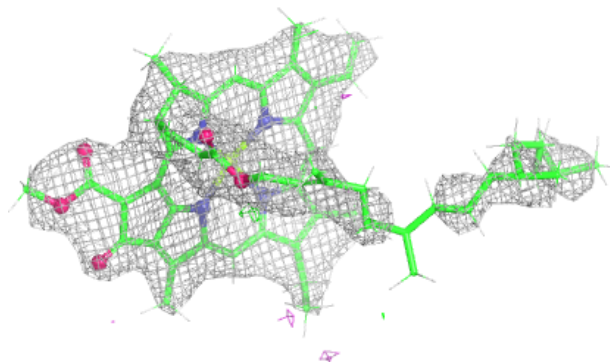
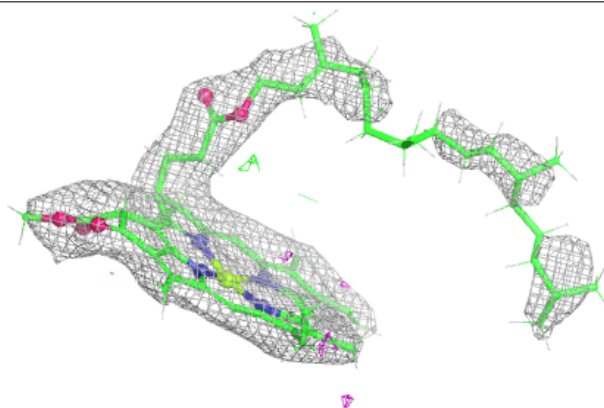


Electron density around BCR x 101:

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

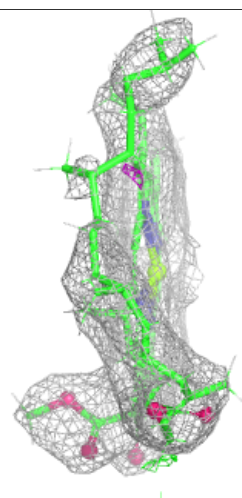
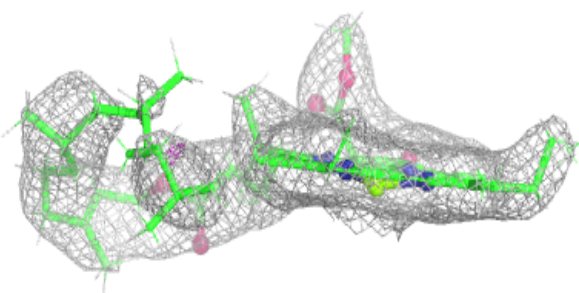
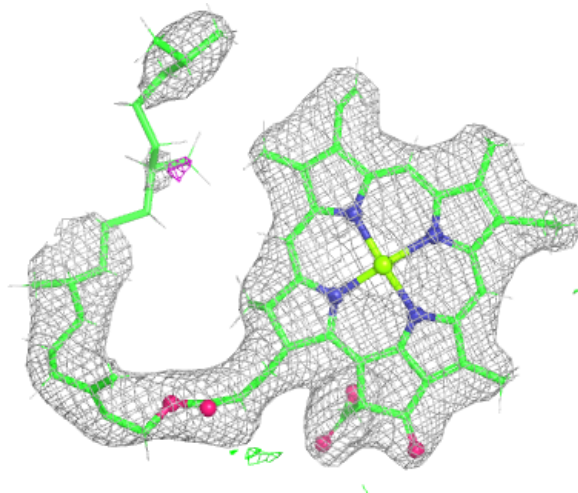
**Electron density around CLA c 513:**

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



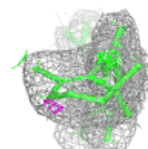
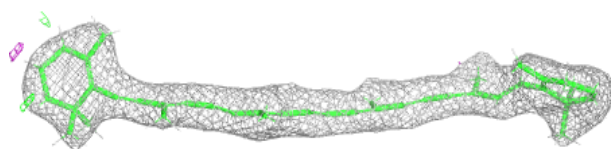
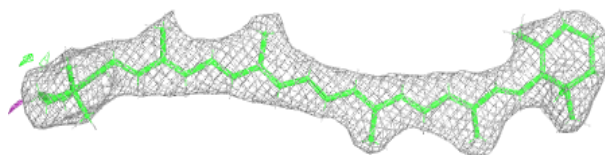
Electron density around CLA c 512:

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

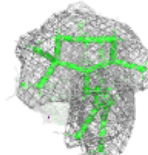
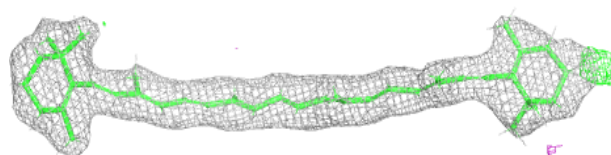
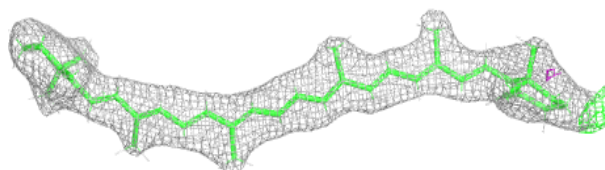


Electron density around BCR b 617:

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

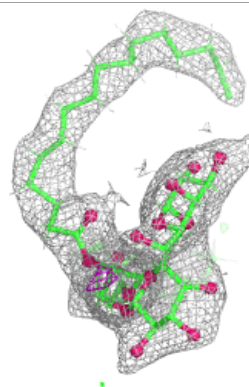
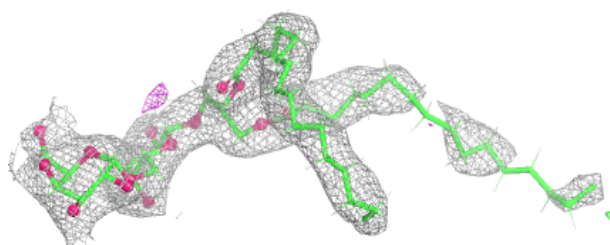
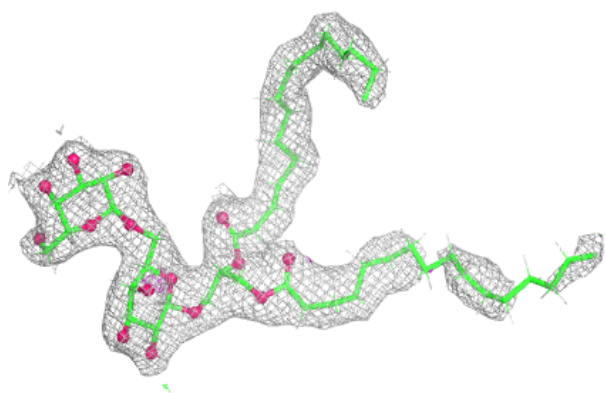
**Electron density around BCR H 101:**

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

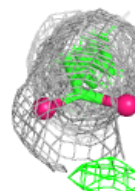
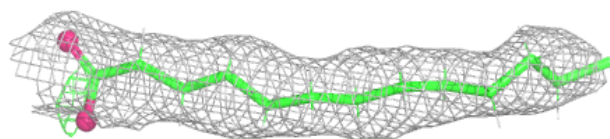
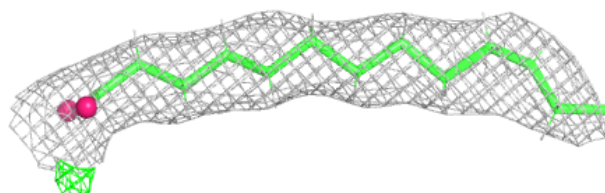


Electron density around DGD c 517:

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

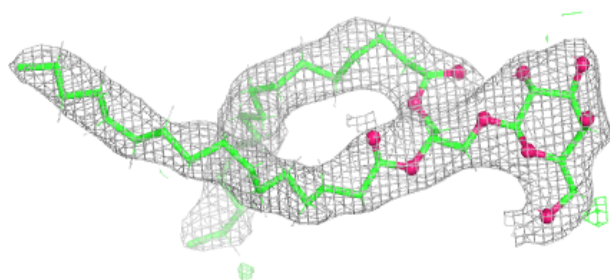
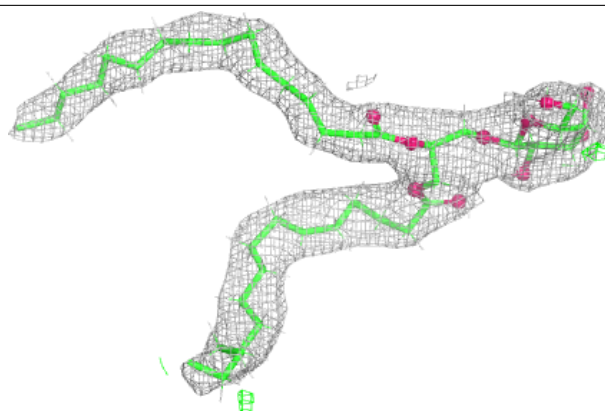
**Electron density around STE M 102:**

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



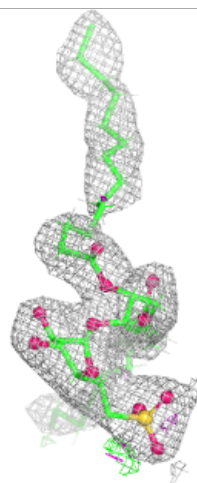
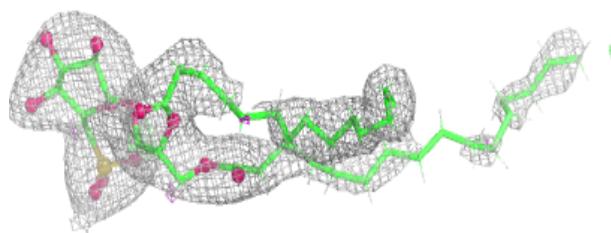
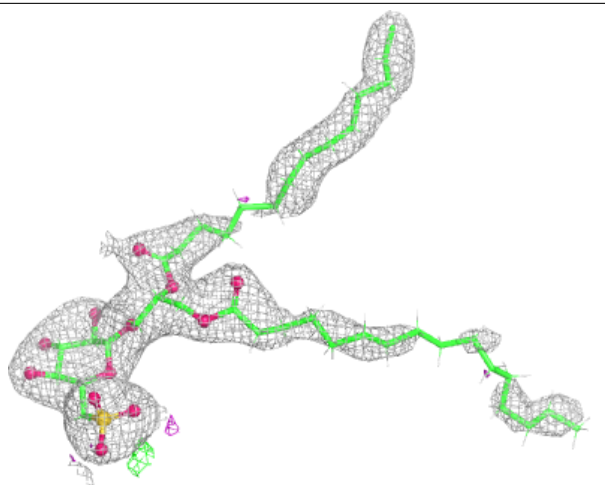
Electron density around LMG m 101:

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



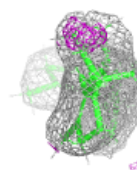
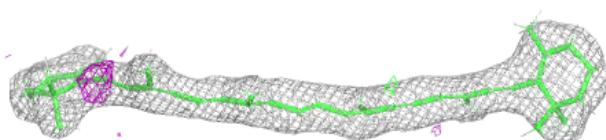
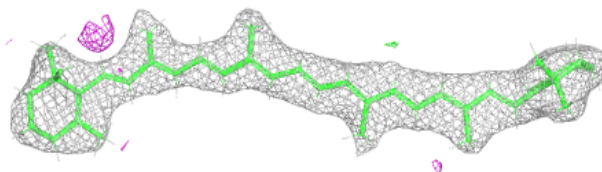
Electron density around SQD A 412:

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

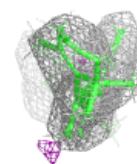
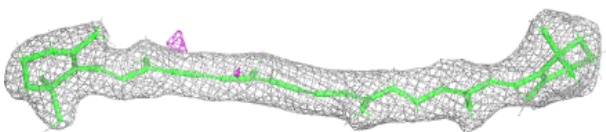
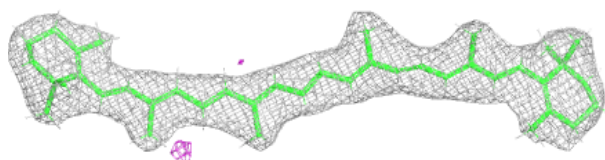


Electron density around BCR B 618:

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

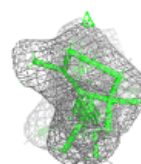
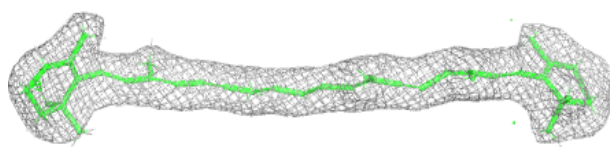
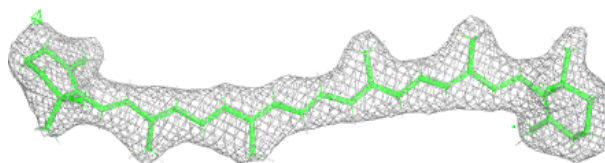
**Electron density around BCR b 619:**

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

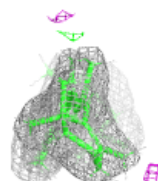
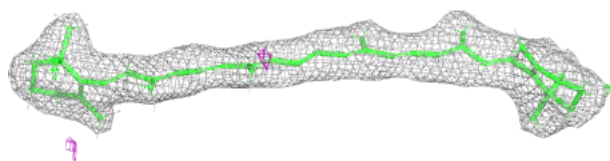


Electron density around BCR B 619:

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

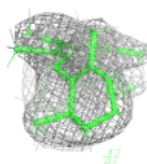
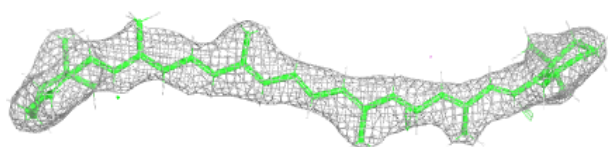
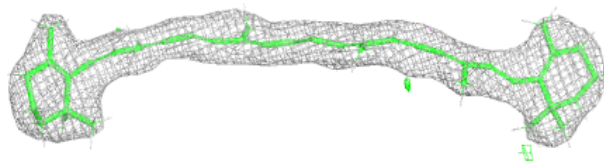
**Electron density around BCR B 620:**

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

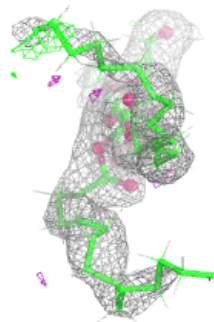
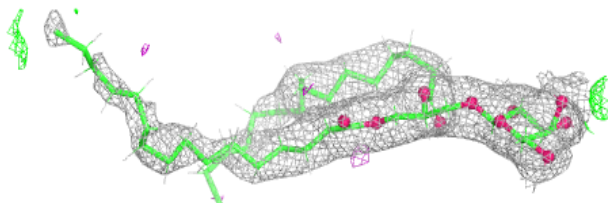
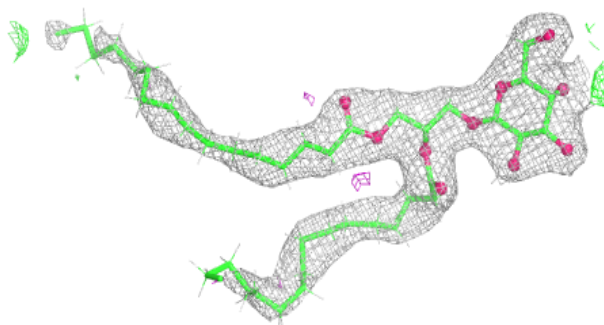


Electron density around BCR C 501:

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

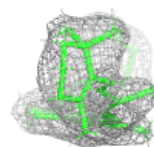
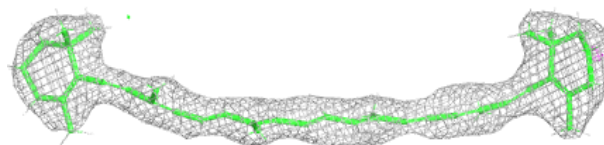
**Electron density around LMG D 407:**

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

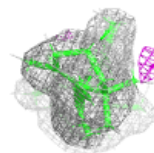
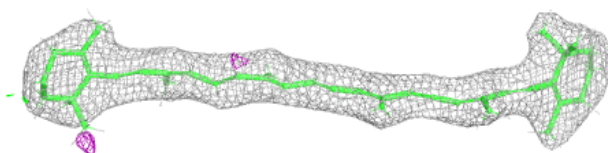


Electron density around BCR k 103:

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

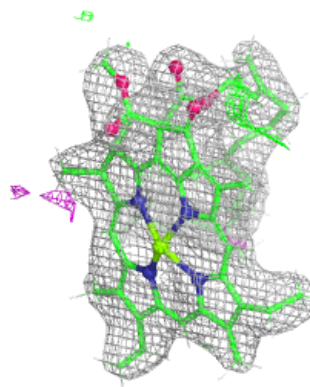
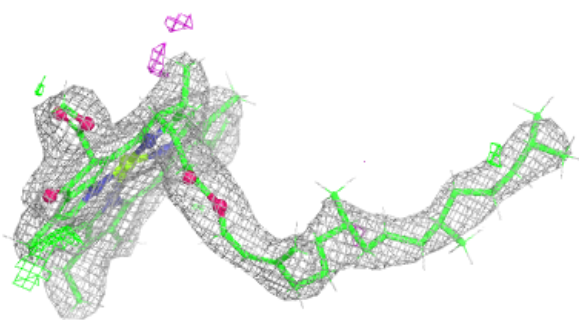
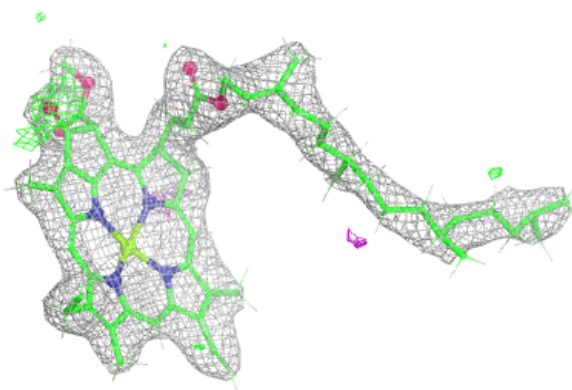
**Electron density around BCR C 515:**

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



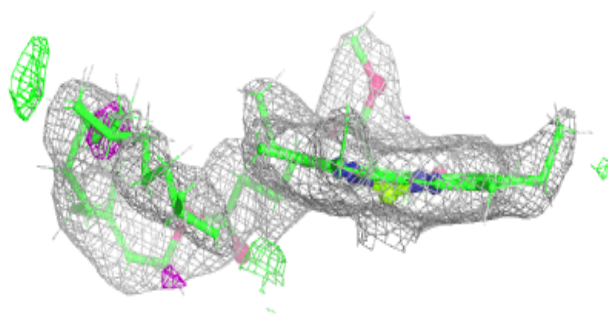
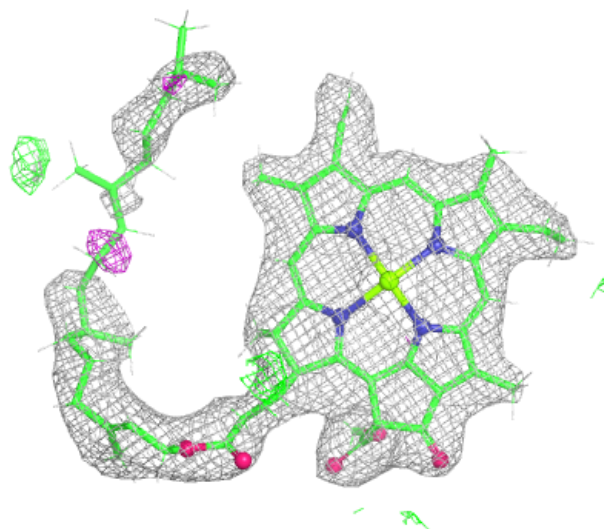
Electron density around CLA c 511:

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



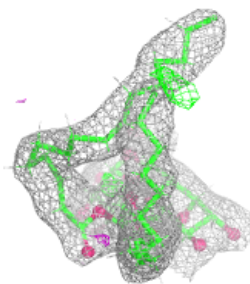
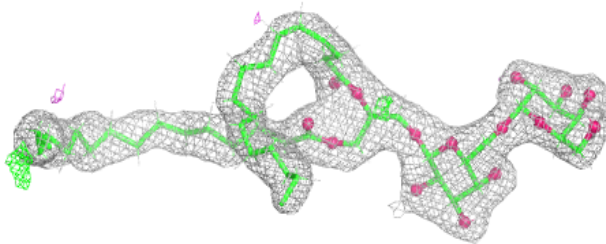
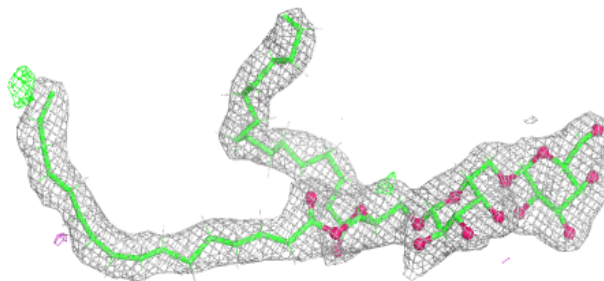
Electron density around CLA C 513:

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

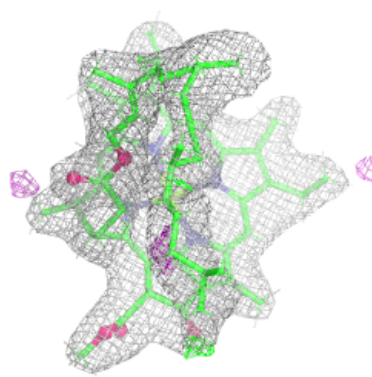
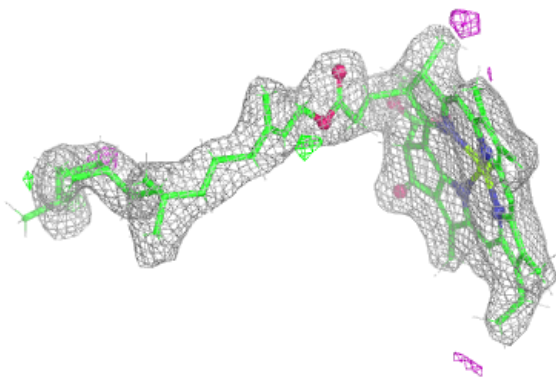
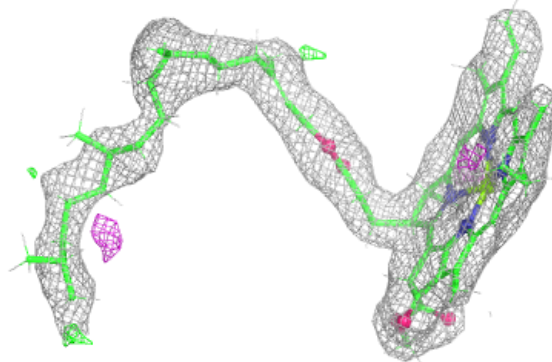


Electron density around DGD H 102:

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

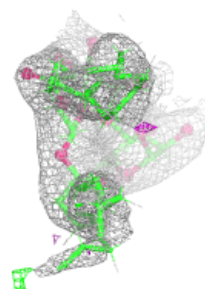
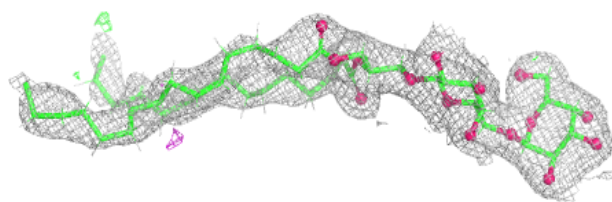
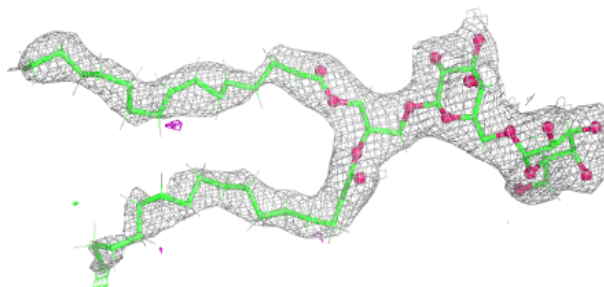
**Electron density around CLA b 606:**

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

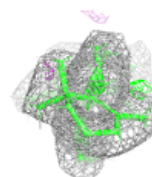
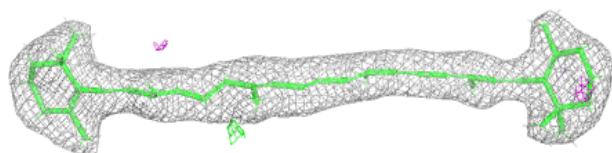
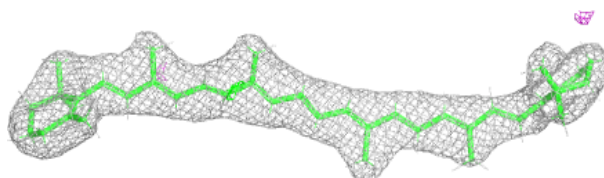


Electron density around DGD c 518:

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

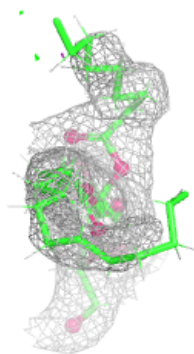
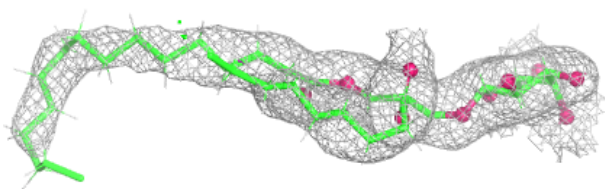
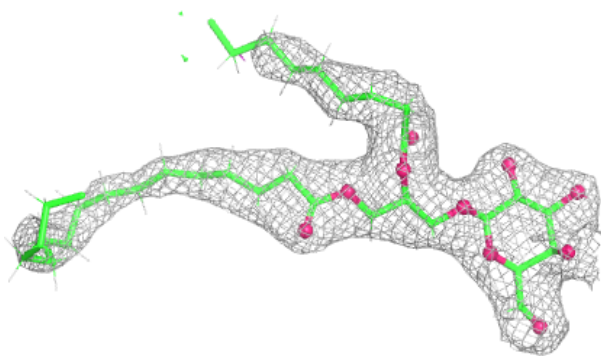
**Electron density around BCR A 406:**

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

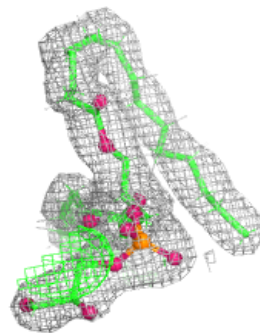
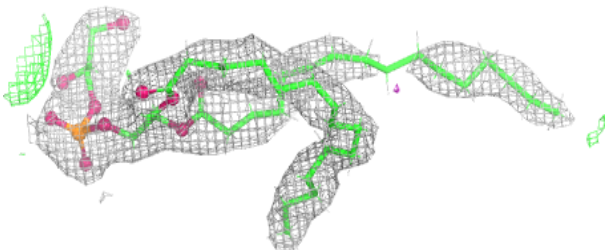
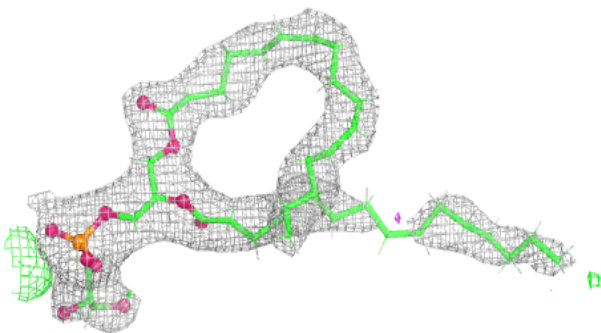


Electron density around LMG d 410:

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

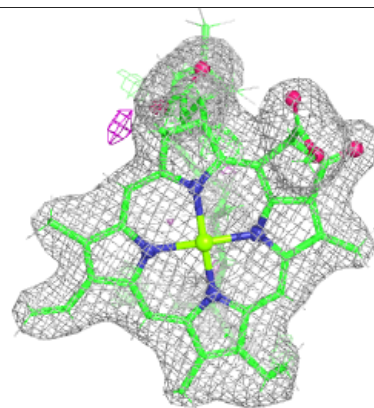
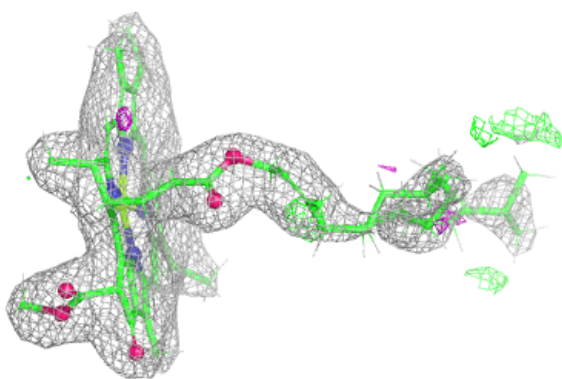
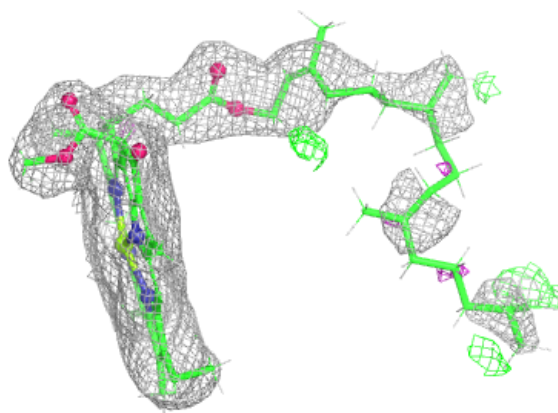
**Electron density around LHG d 407:**

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

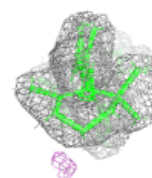
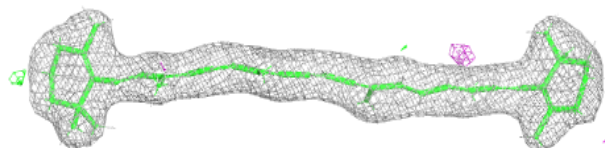
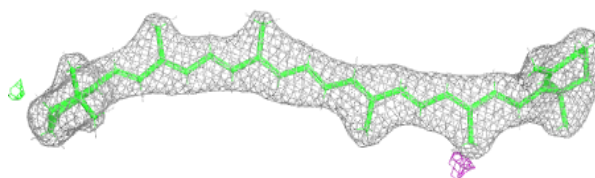


Electron density around CLA c 506:

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

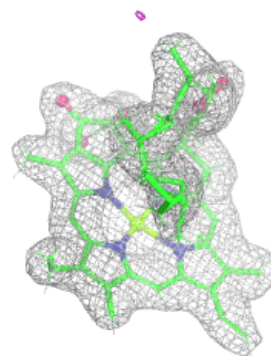
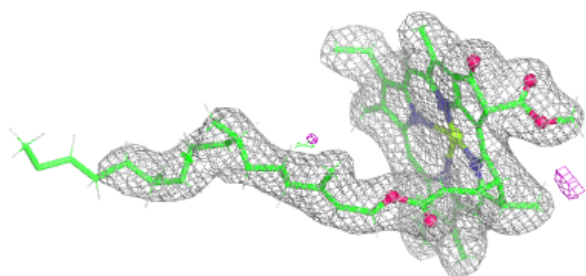
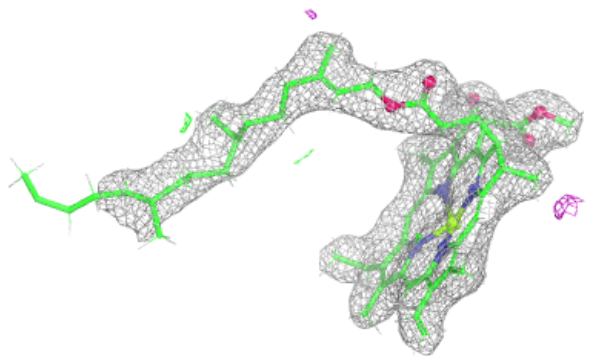
**Electron density around BCR a 406:**

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

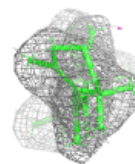
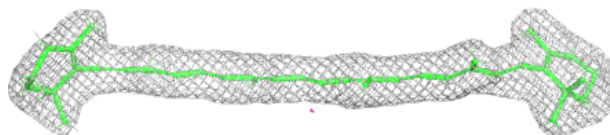
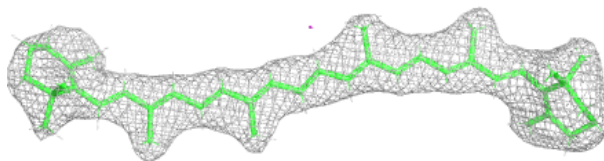


Electron density around CLA c 508:

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

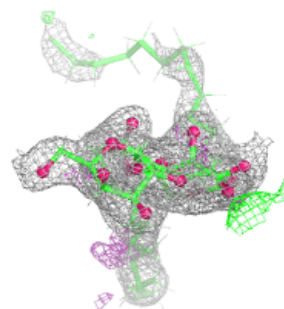
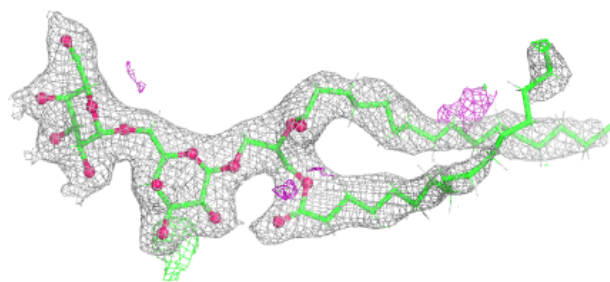
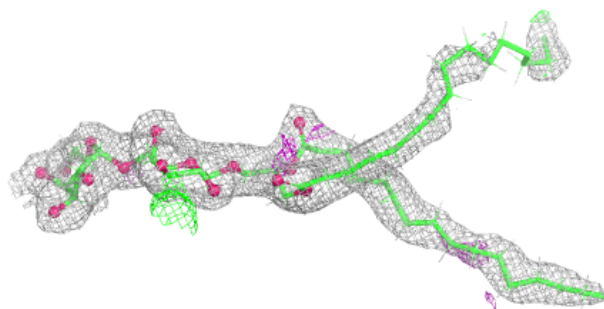
**Electron density around BCR b 618:**

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



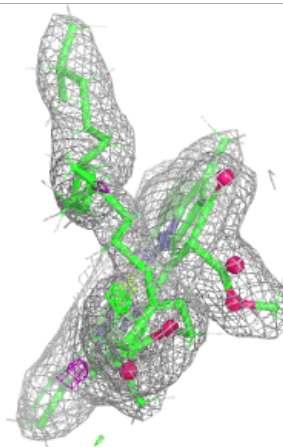
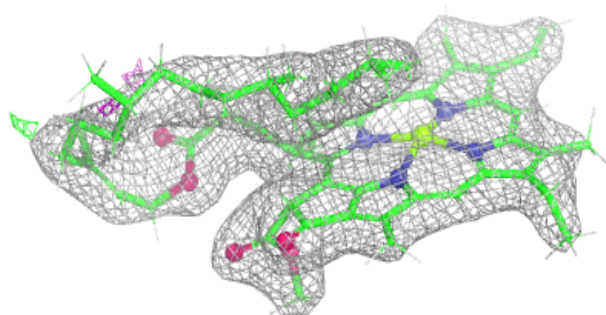
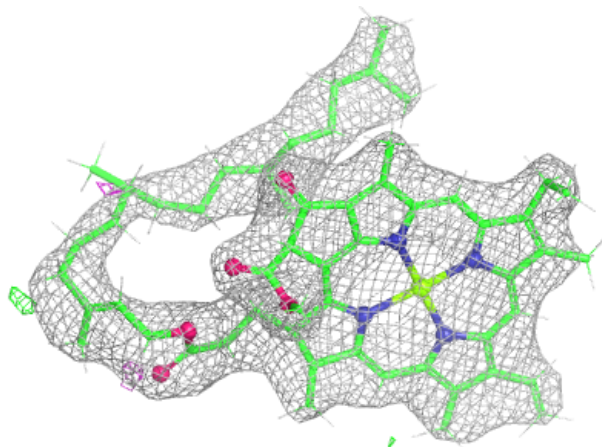
Electron density around DGD C 517:

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



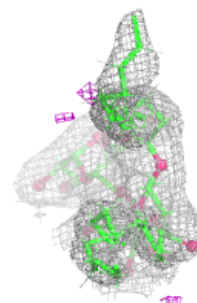
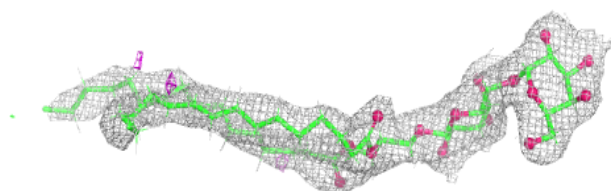
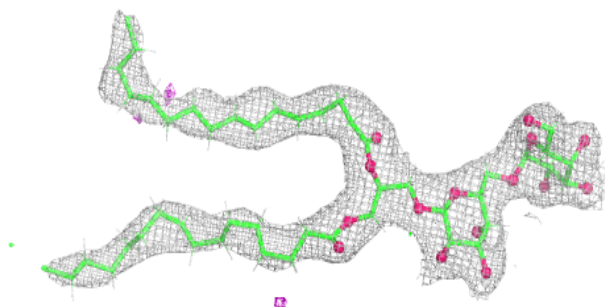
Electron density around CLA c 509:

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



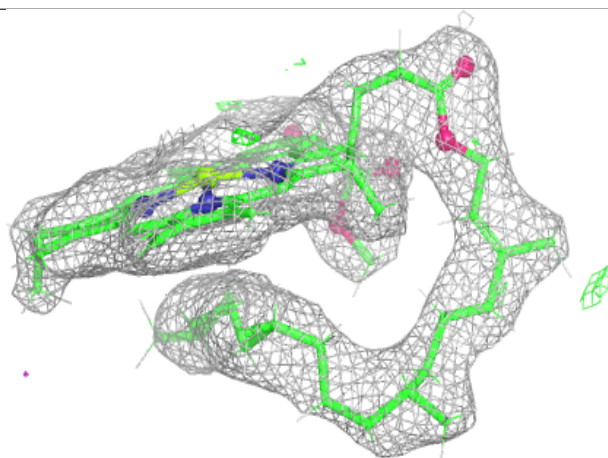
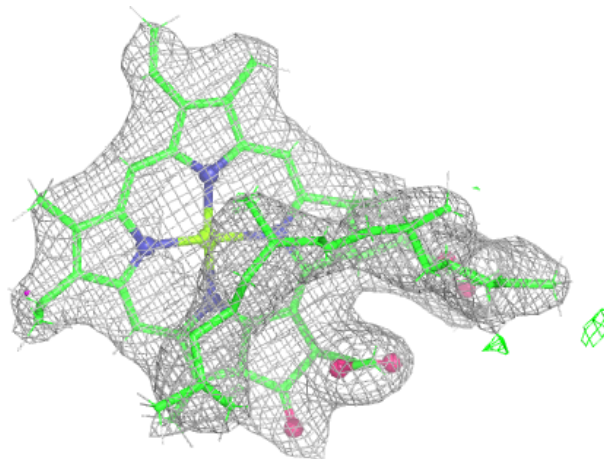
Electron density around DGD C 519:

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



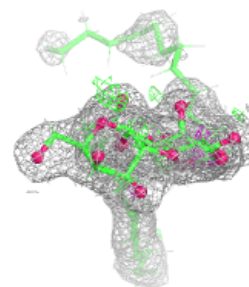
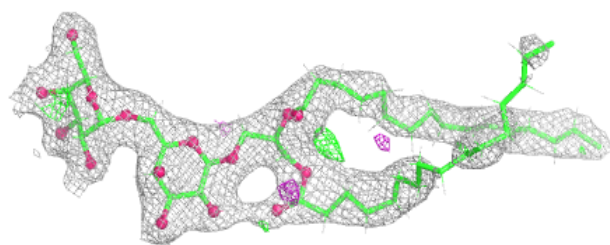
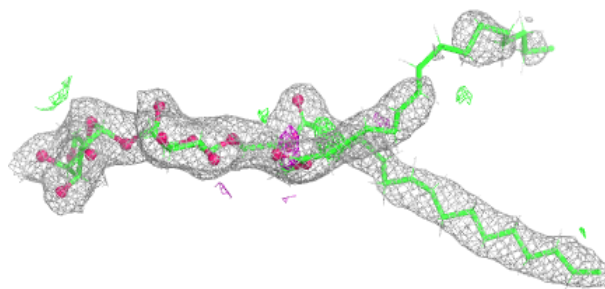
Electron density around CLA c 510:

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

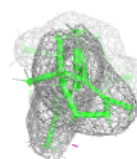
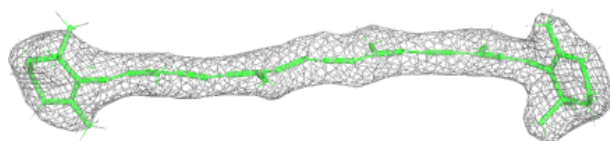
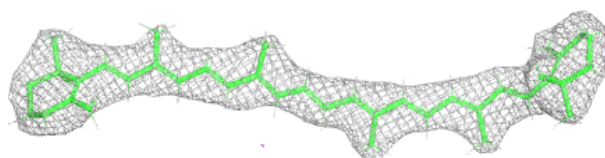


Electron density around DGD c 516:

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

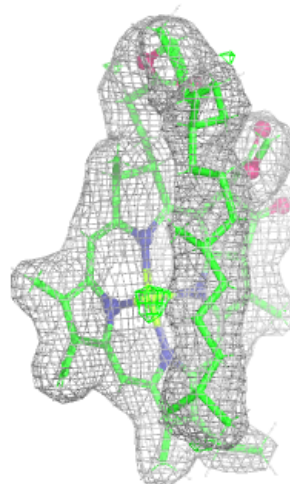
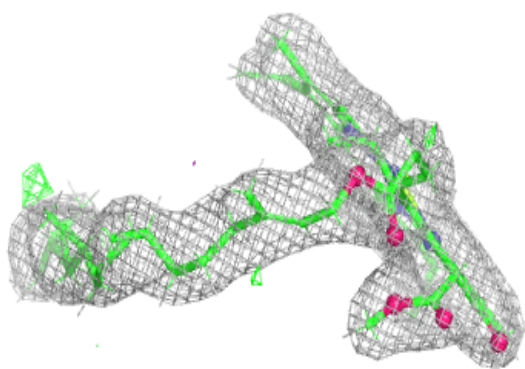
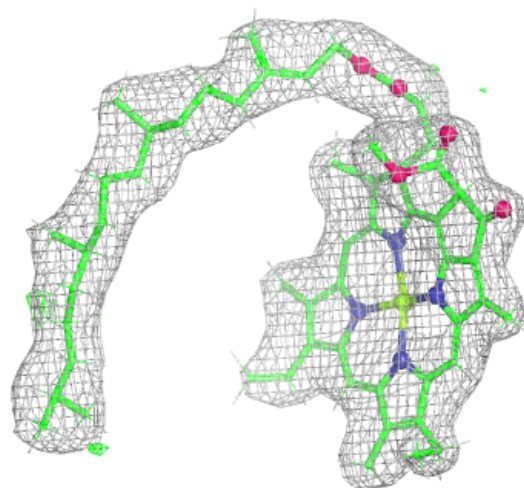
**Electron density around BCR c 515:**

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



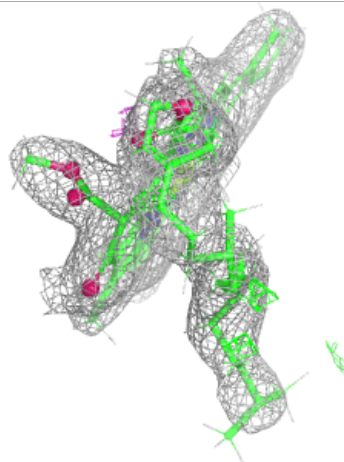
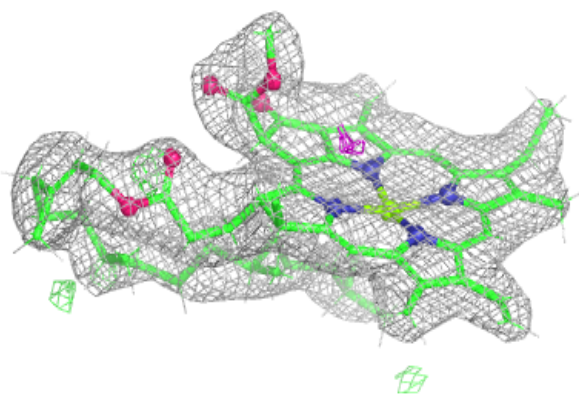
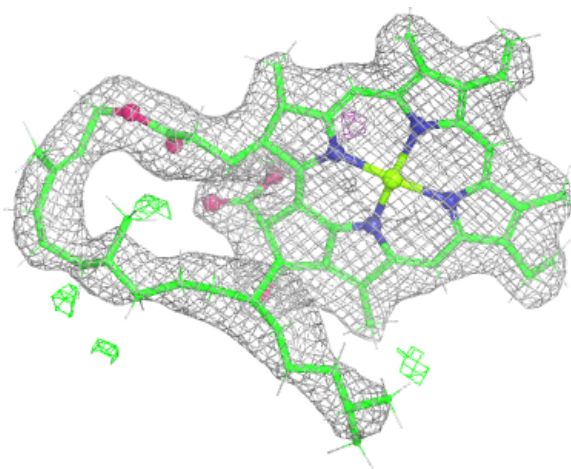
Electron density around CLA C 508:

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



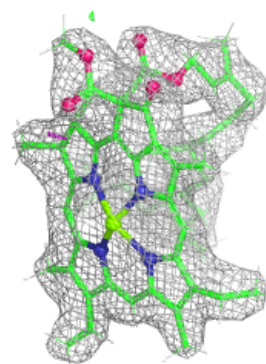
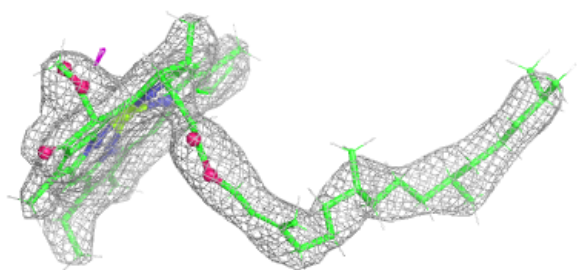
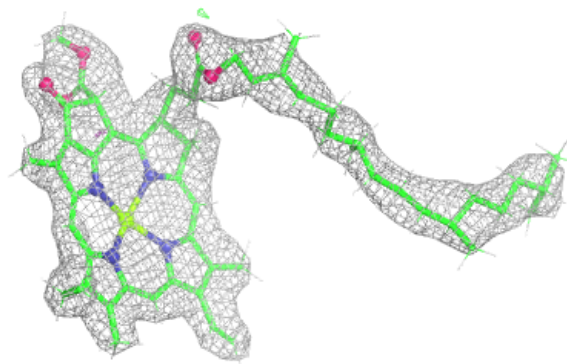
Electron density around CLA C 510:

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

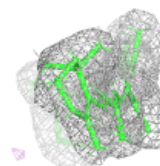
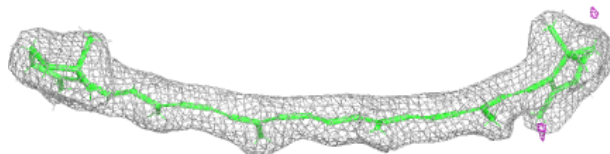
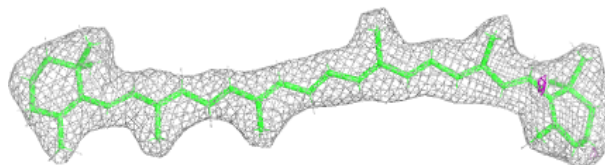


Electron density around CLA C 512:

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

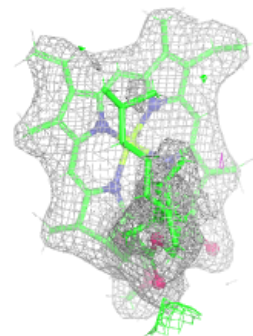
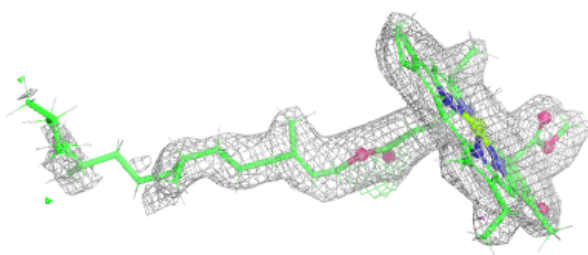
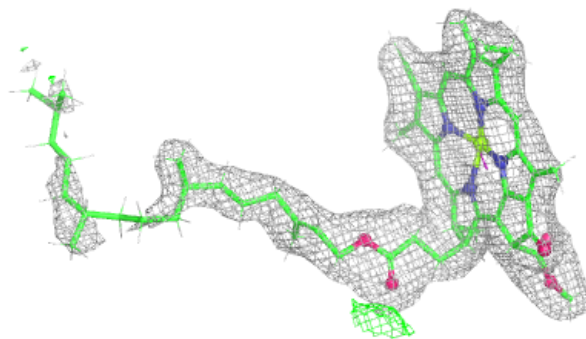
**Electron density around BCR t 101:**

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



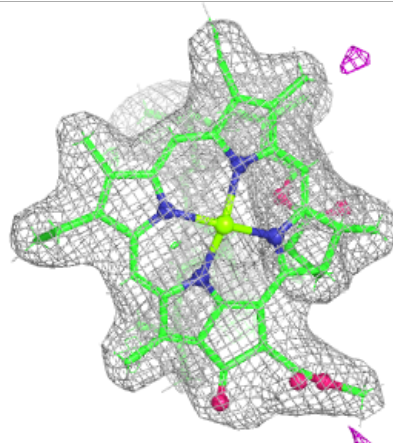
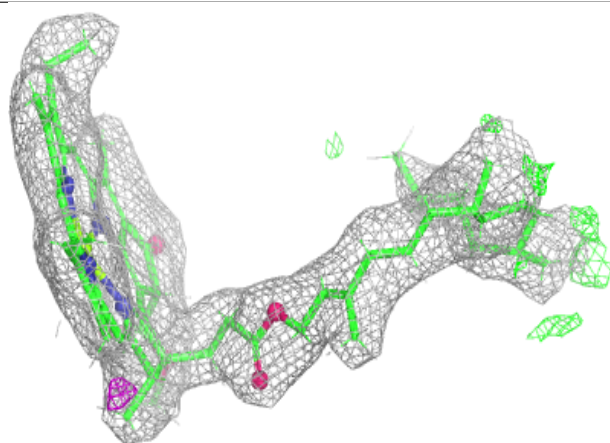
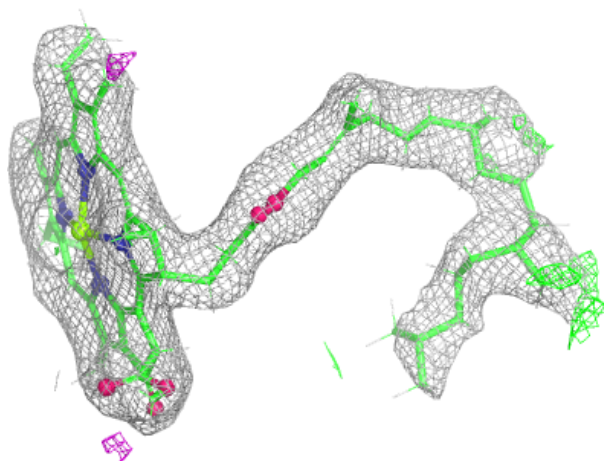
Electron density around CLA d 404:

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



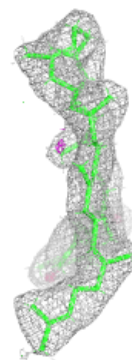
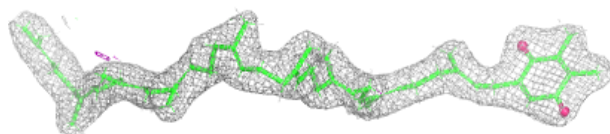
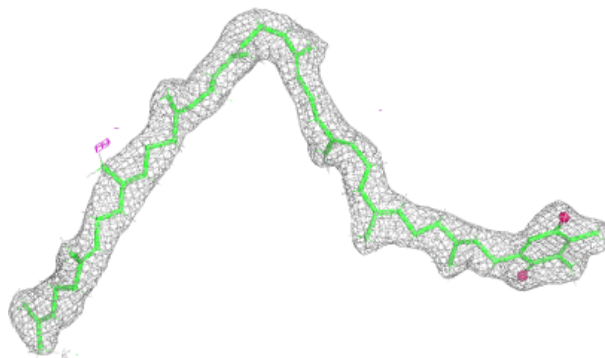
Electron density around CLA B 607:

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



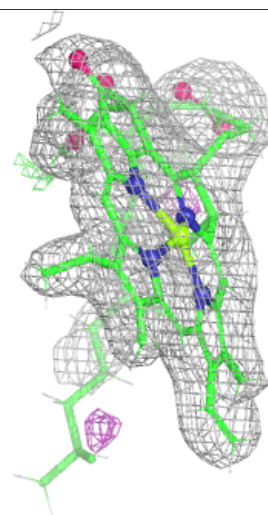
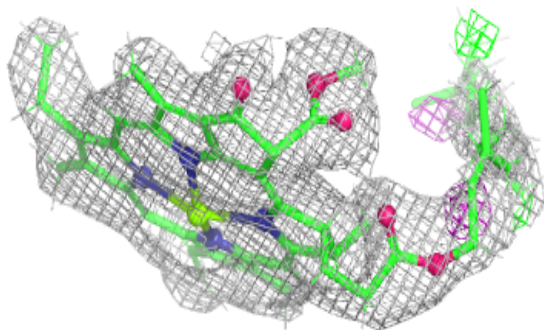
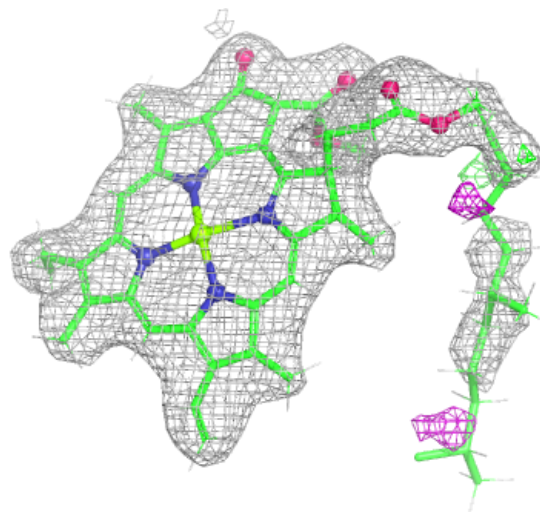
Electron density around PL9 D 406:

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



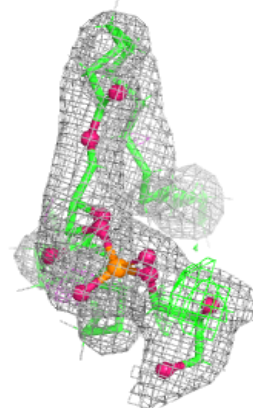
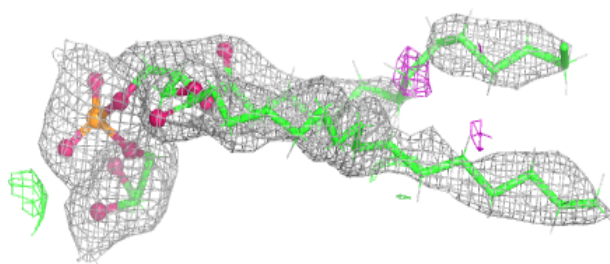
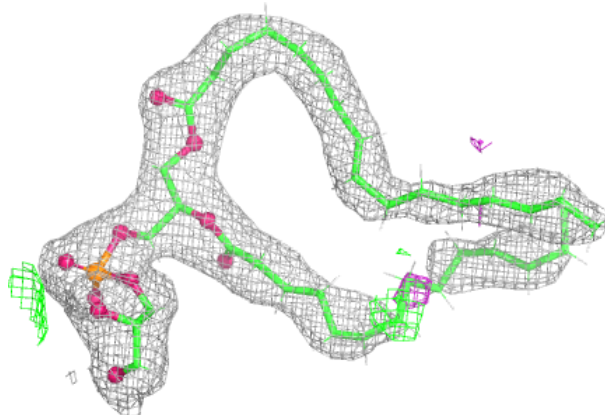
Electron density around CLA B 617:

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

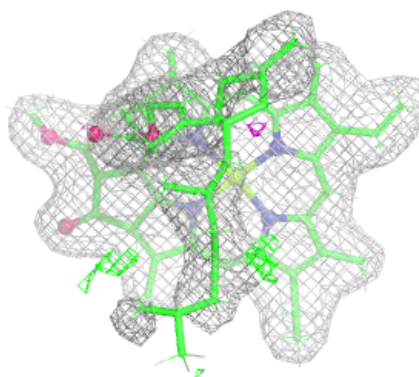
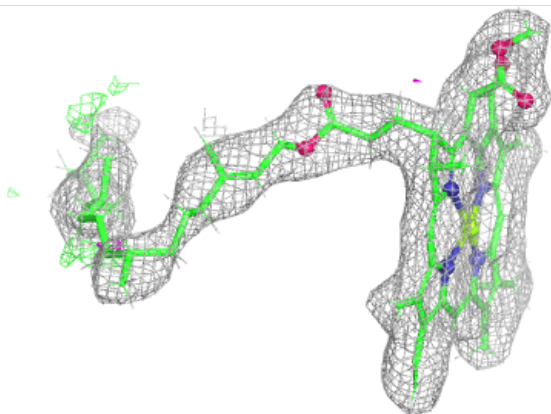
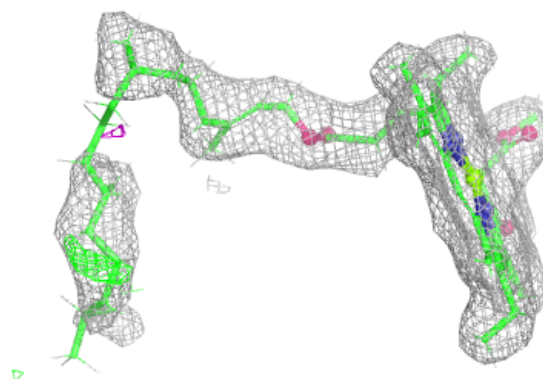


Electron density around LHG A 411:

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

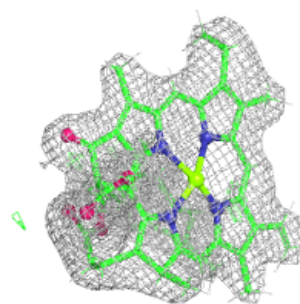
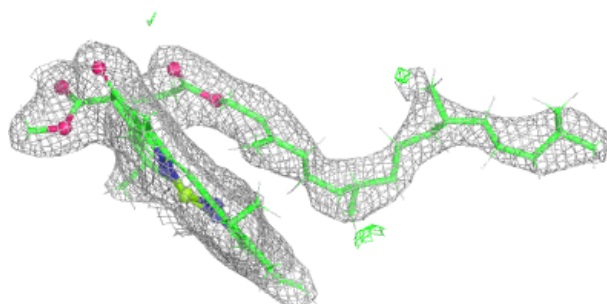
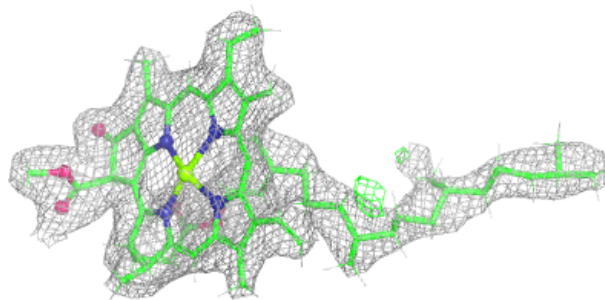
**Electron density around CLA a 405:**

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

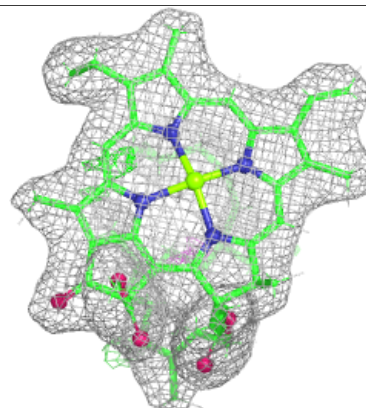
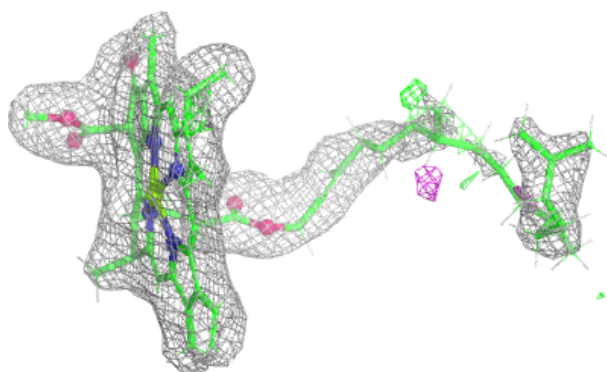
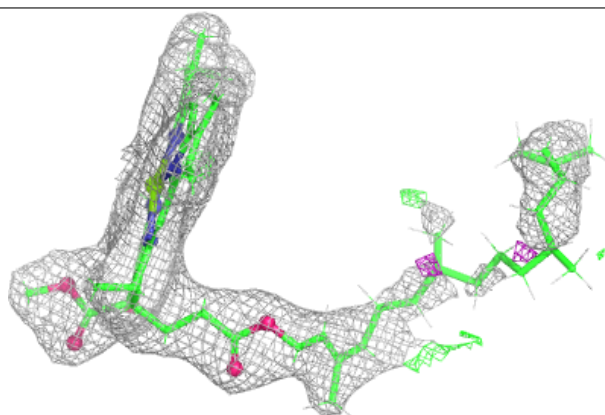


Electron density around CLA C 506:

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

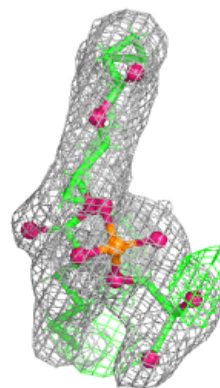
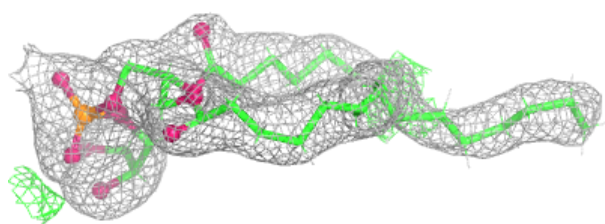
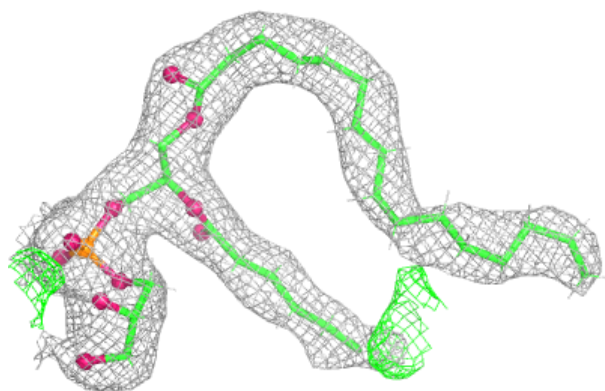
**Electron density around CLA C 507:**

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



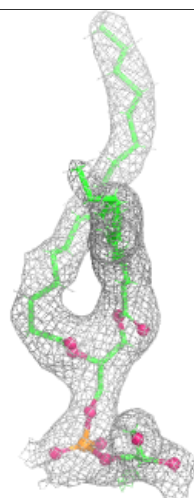
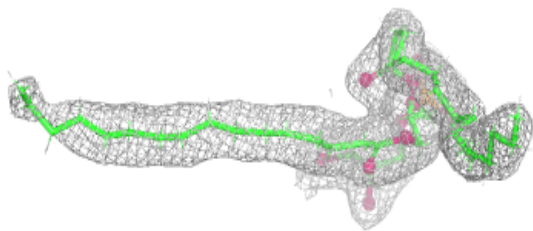
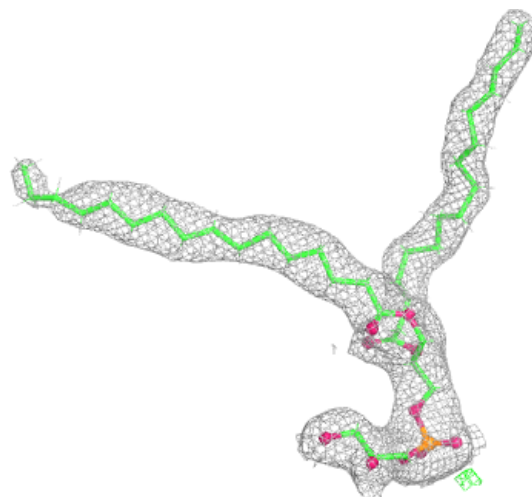
Electron density around LHG d 409:

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



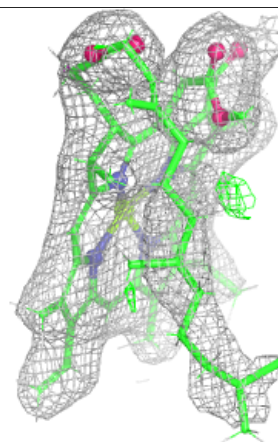
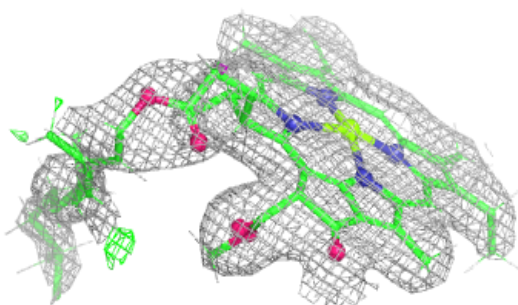
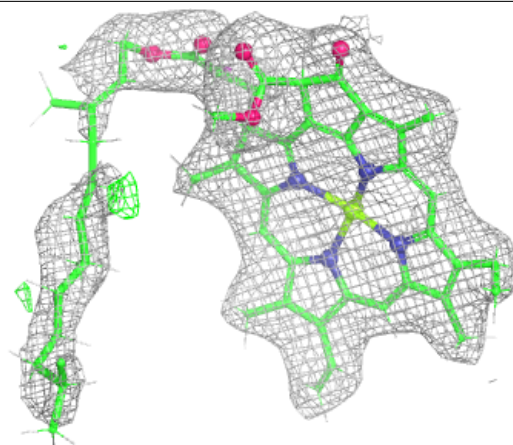
Electron density around LHG 1 101:

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



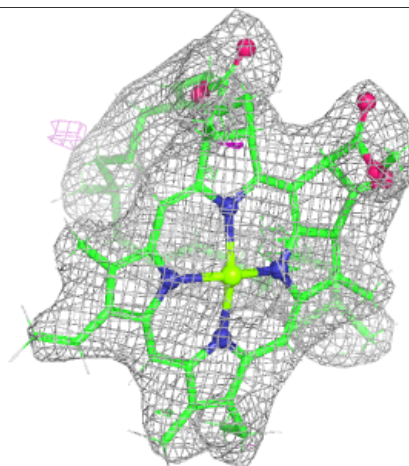
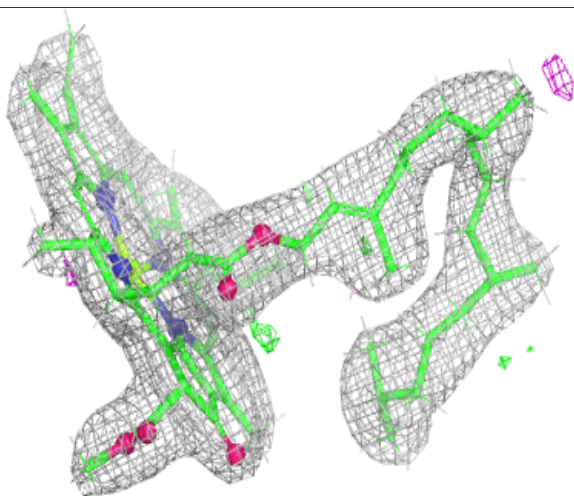
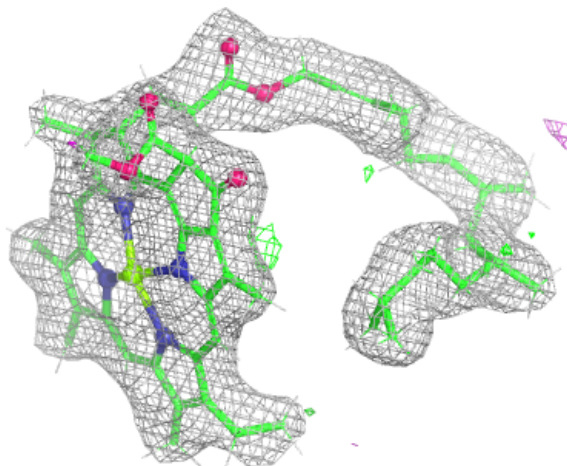
Electron density around CLA b 616:

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



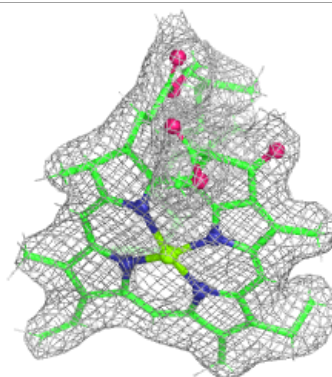
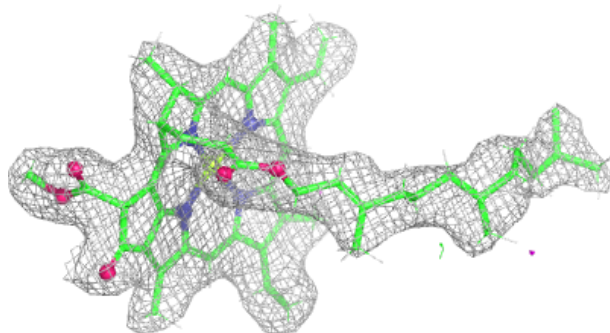
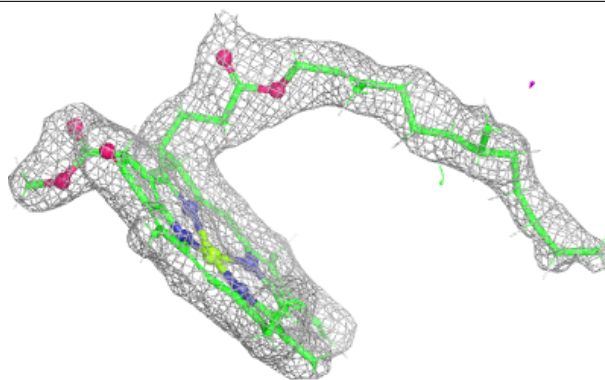
Electron density around CLA c 503:

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

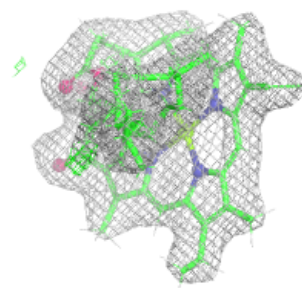
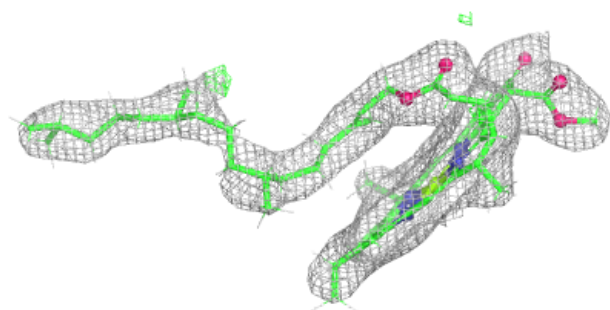
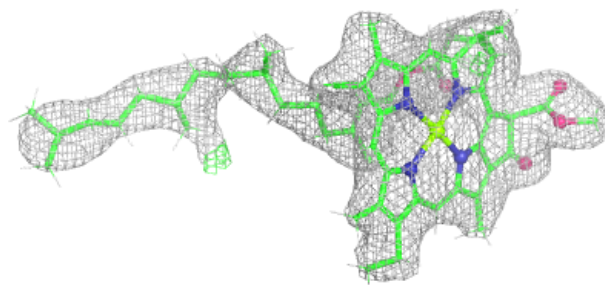


Electron density around CLA c 504:

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

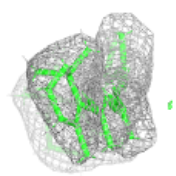
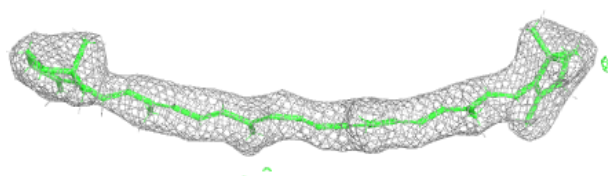
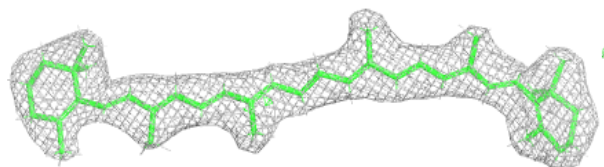
**Electron density around CLA c 505:**

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

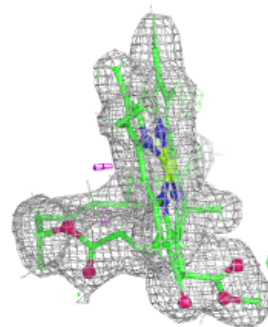
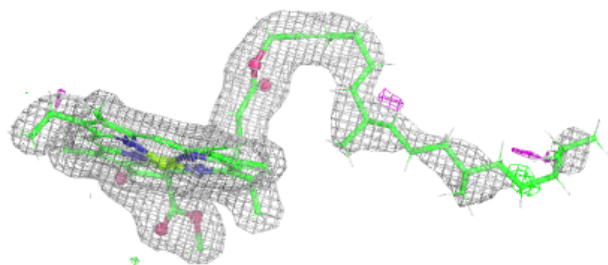
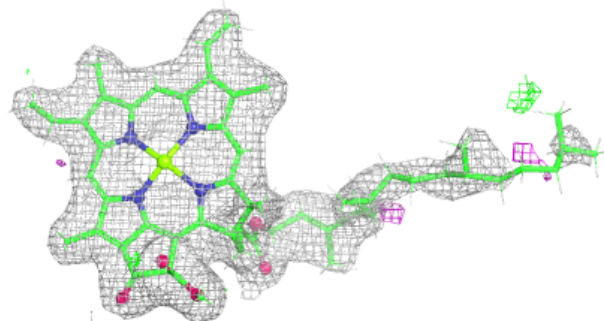


Electron density around BCR T 101:

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

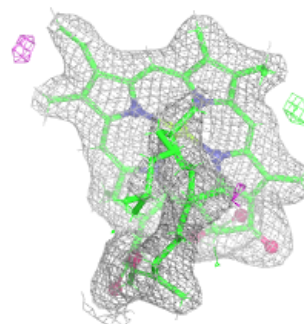
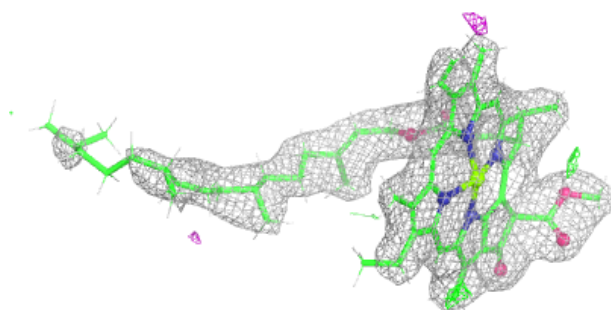
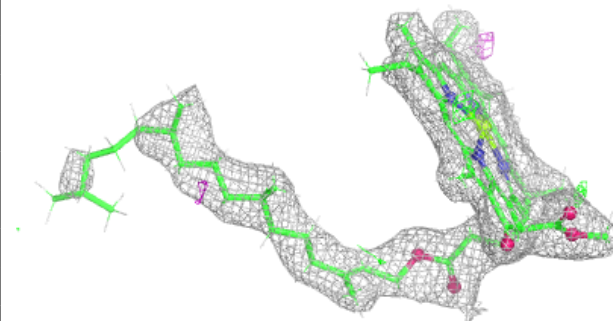
**Electron density around CLA A 403:**

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

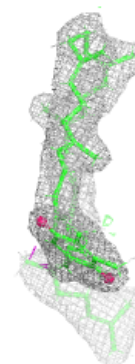
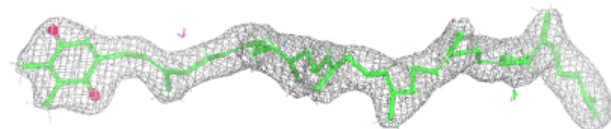
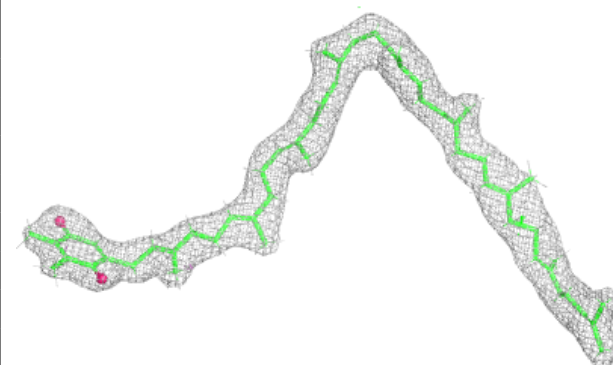


Electron density around CLA C 509:

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

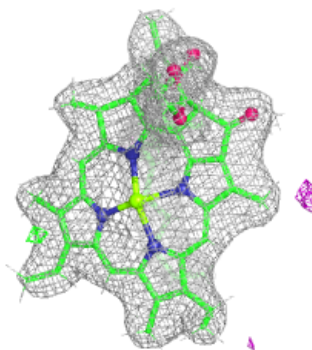
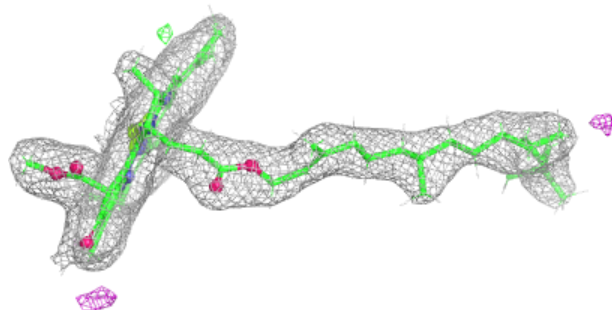
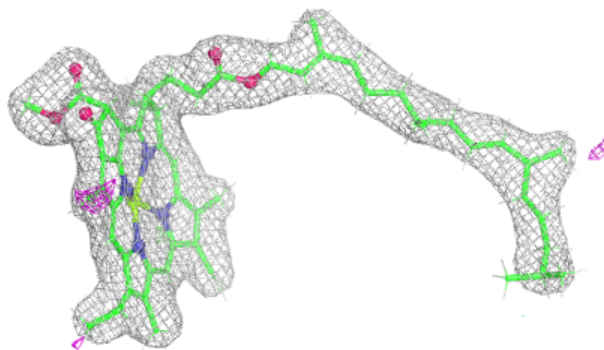
**Electron density around PL9 d 406:**

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



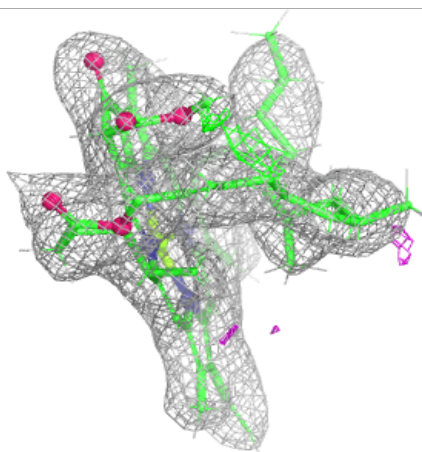
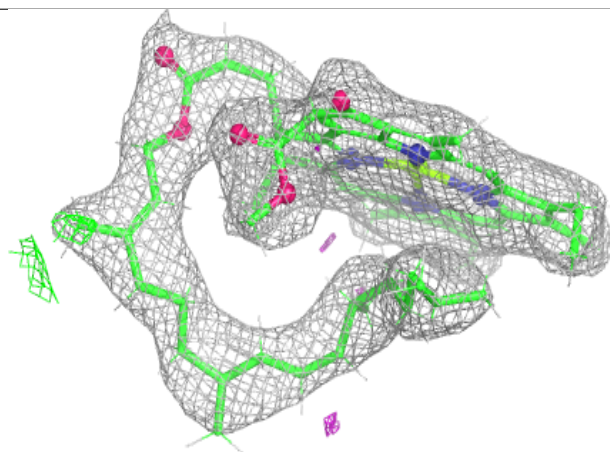
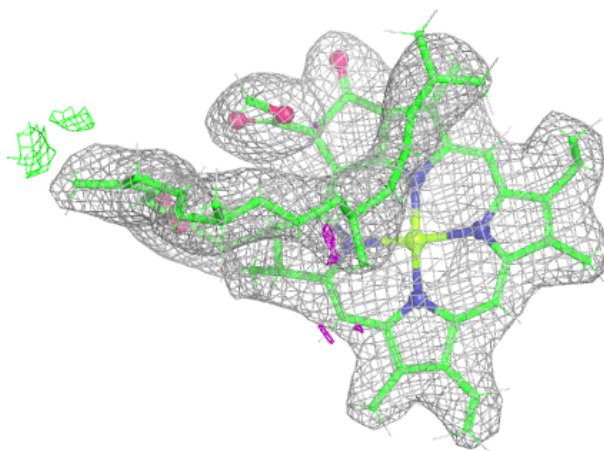
Electron density around CLA B 610:

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



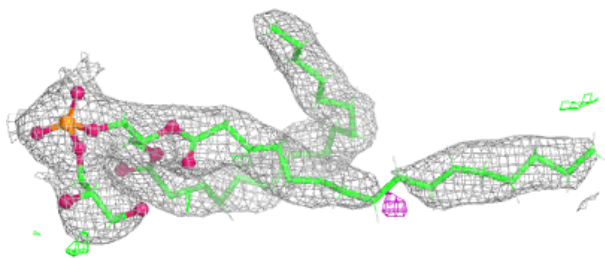
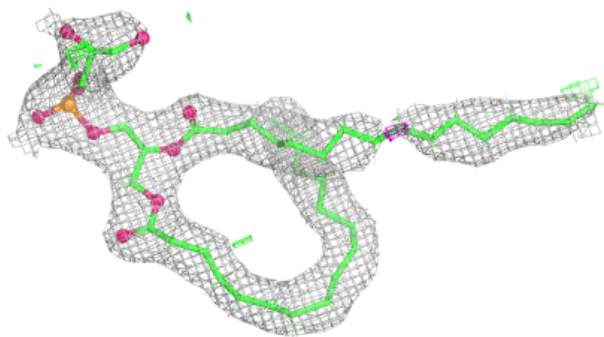
Electron density around CLA C 511:

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



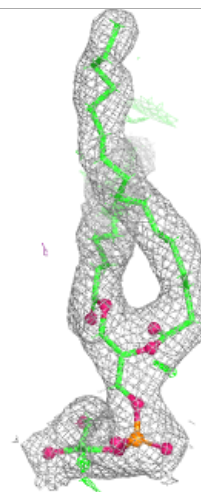
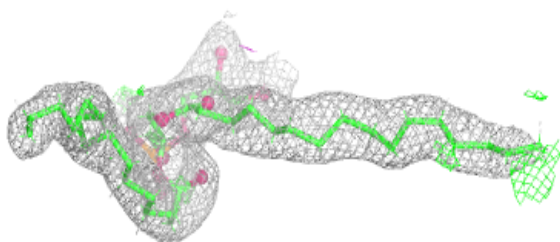
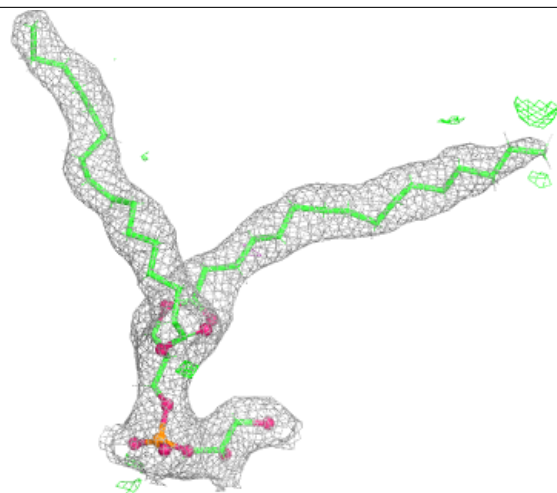
Electron density around LHG B 622:

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



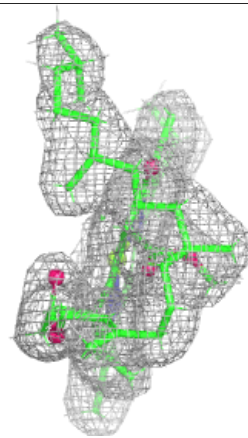
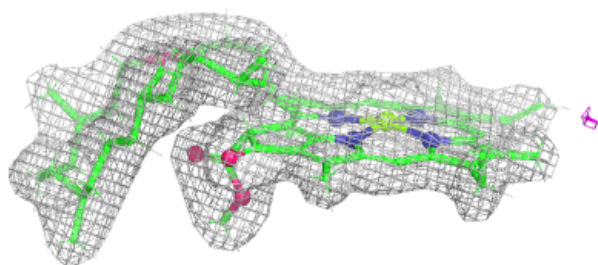
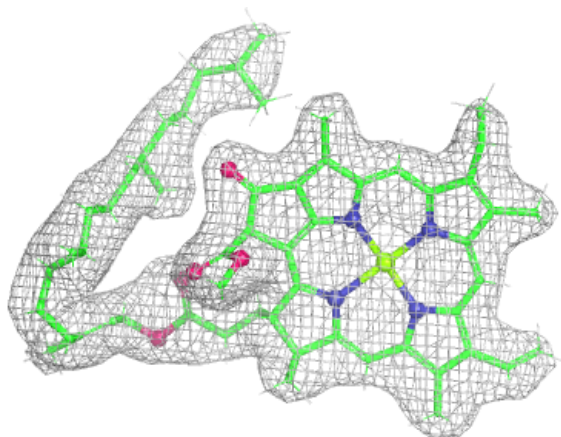
Electron density around LHG L 102:

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



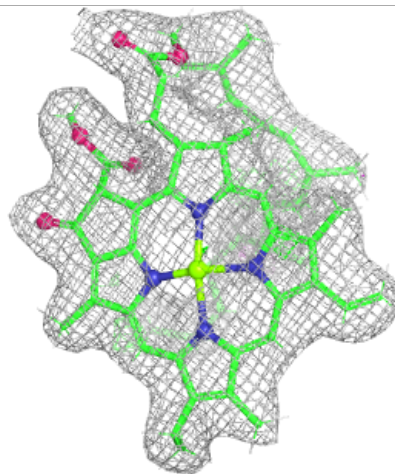
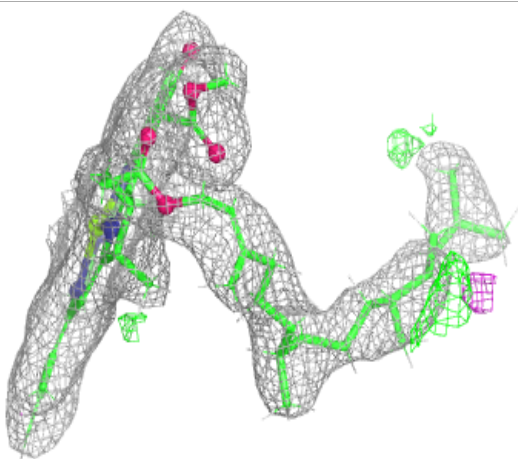
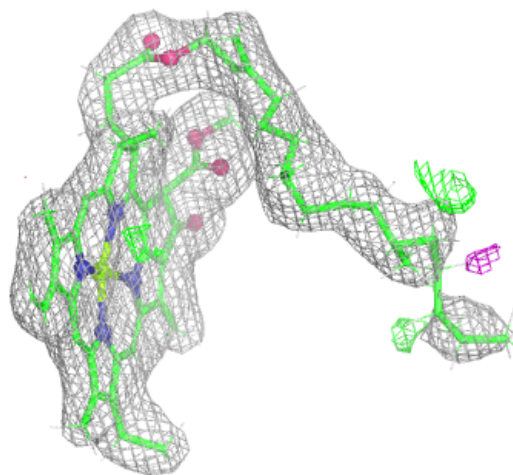
Electron density around CLA B 611:

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



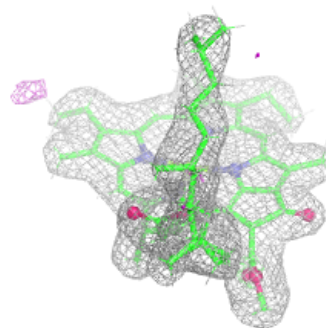
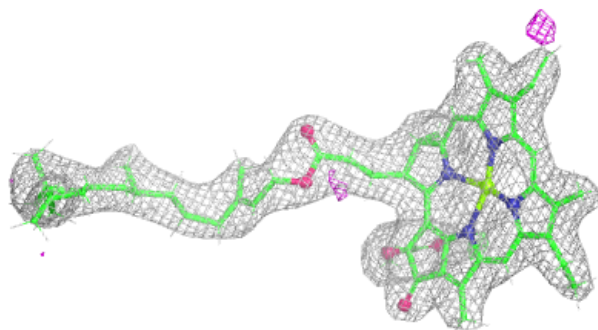
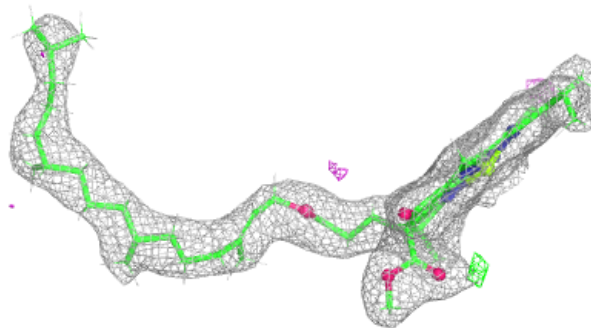
Electron density around CLA B 614:

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

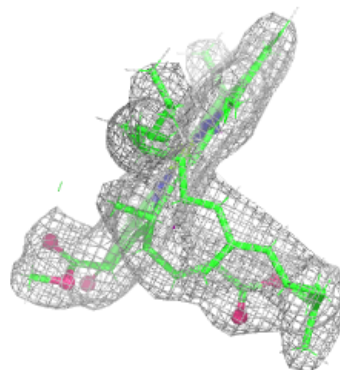
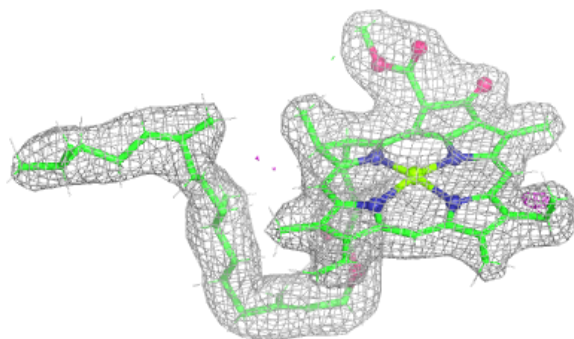
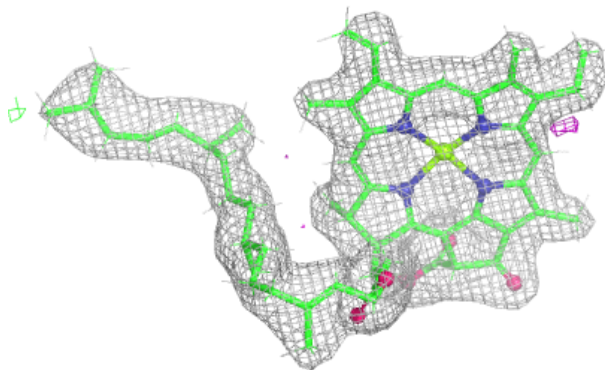


Electron density around CLA d 402:

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

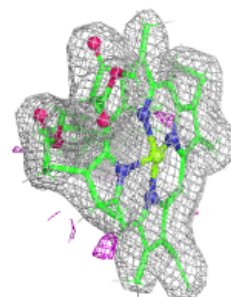
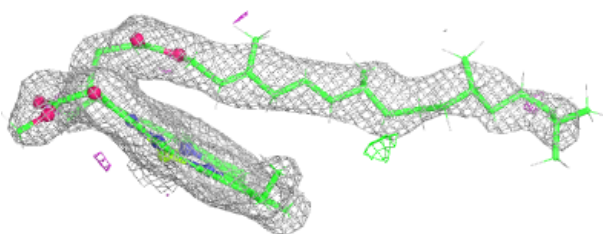
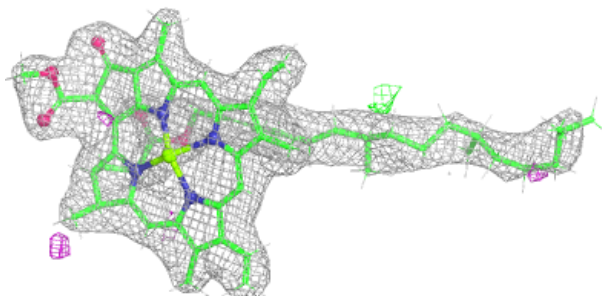
**Electron density around CLA d 403:**

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

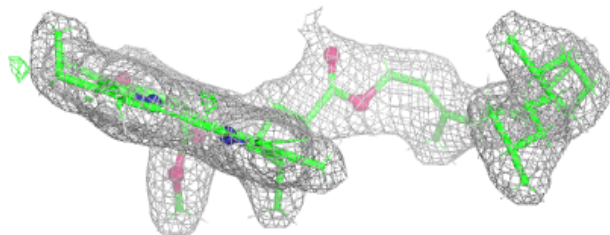
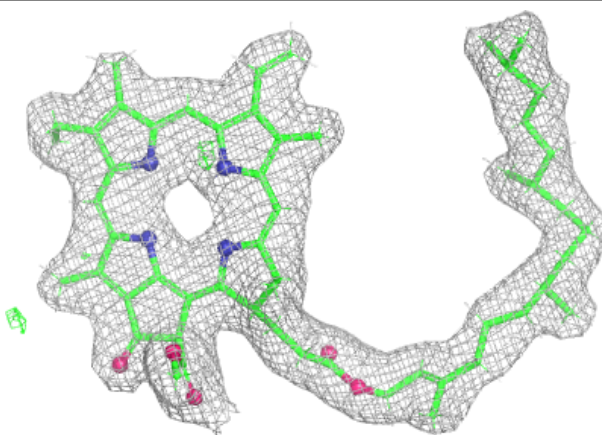


Electron density around CLA B 615:

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

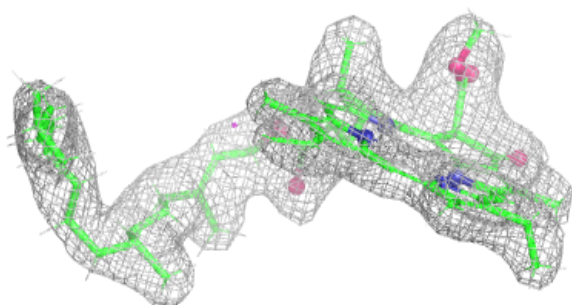
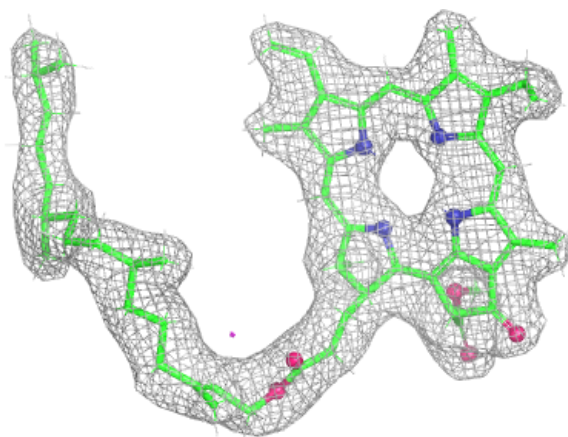
**Electron density around PHO a 404:**

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



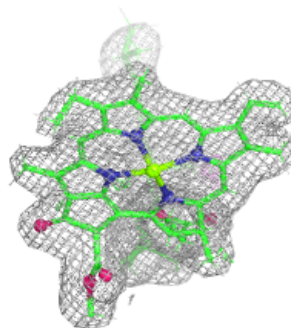
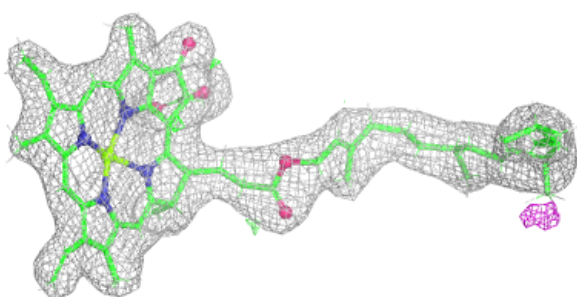
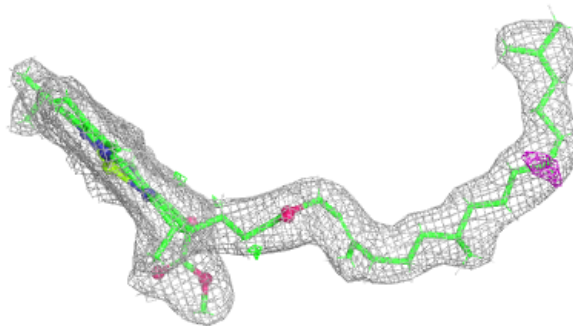
Electron density around PHO d 401:

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

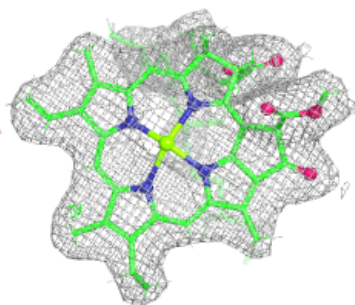
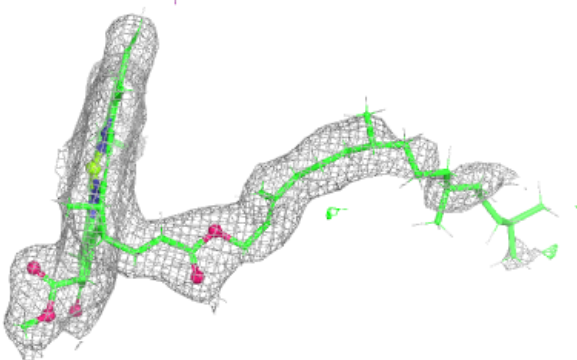
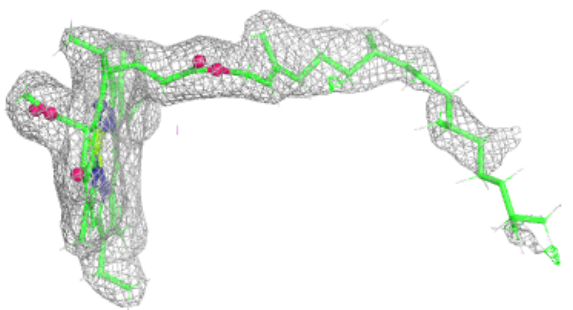


Electron density around CLA D 402:

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

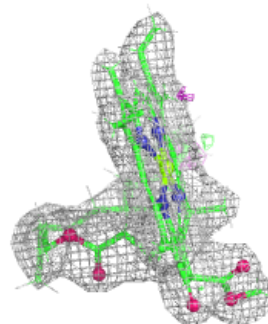
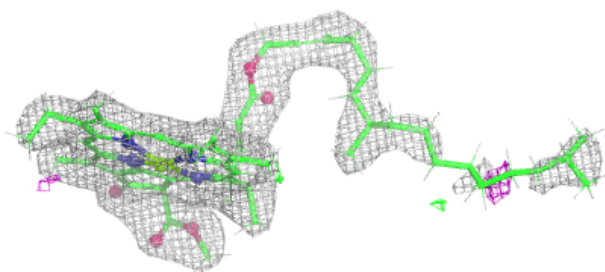
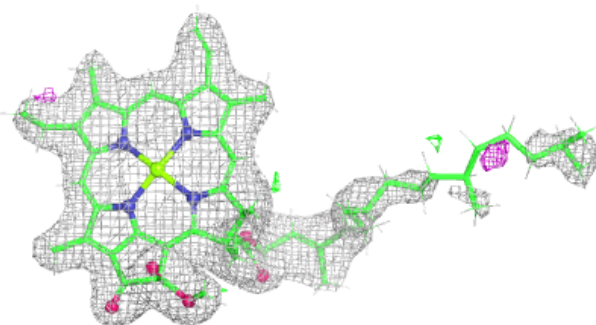
**Electron density around CLA D 404:**

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



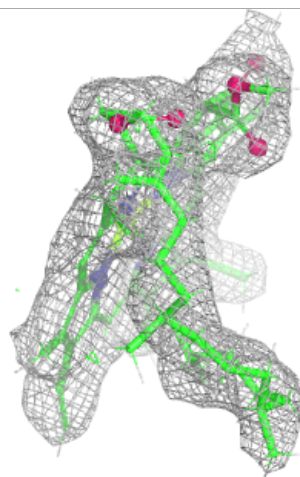
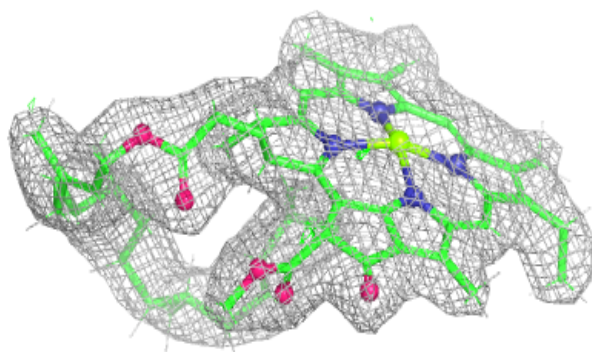
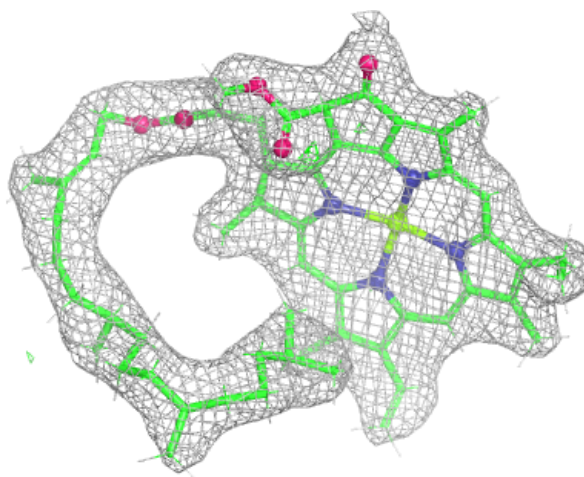
Electron density around CLA a 403:

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



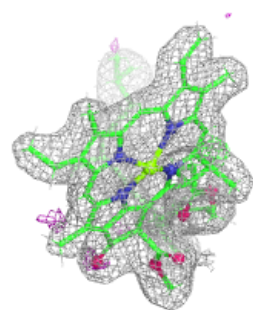
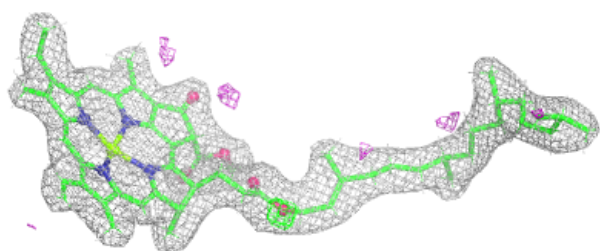
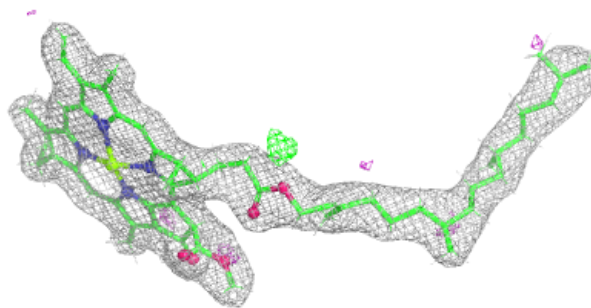
Electron density around CLA B 616:

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

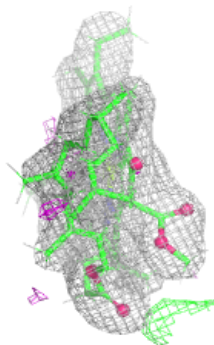
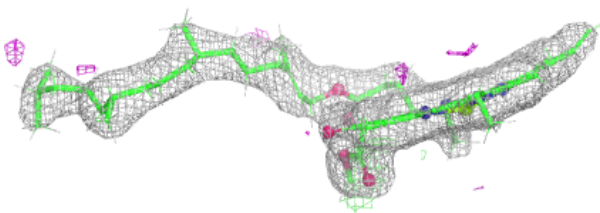
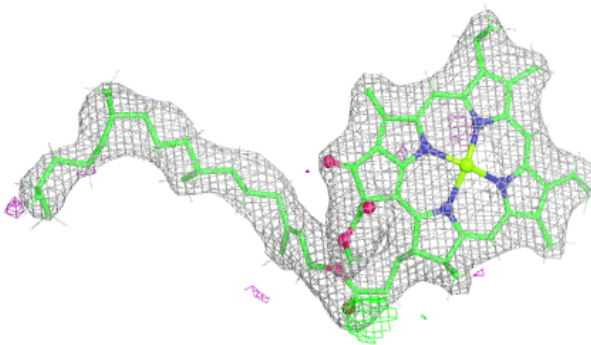


Electron density around CLA A 402:

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

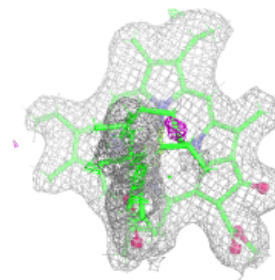
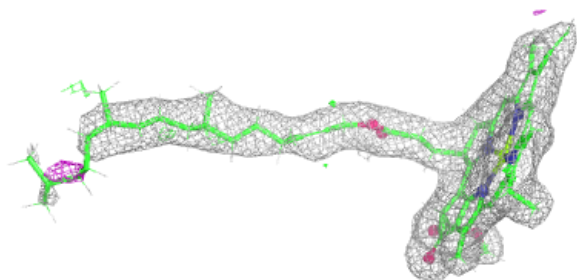
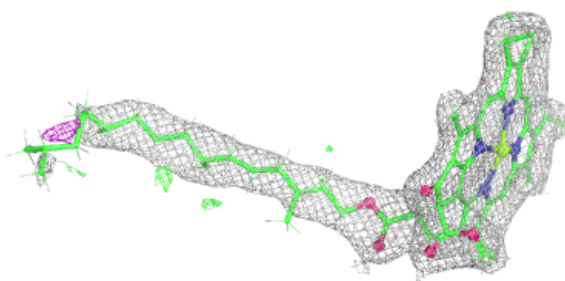
**Electron density around CLA b 602:**

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

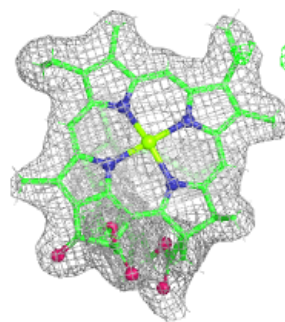
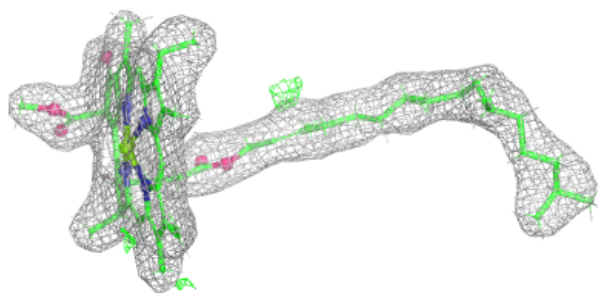
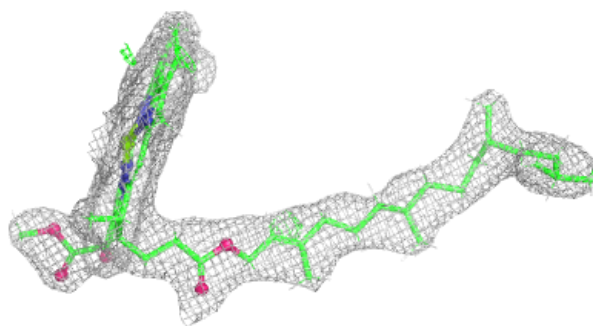


Electron density around CLA b 604:

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

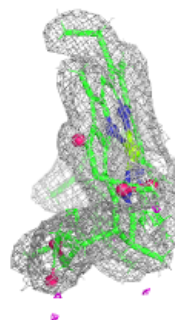
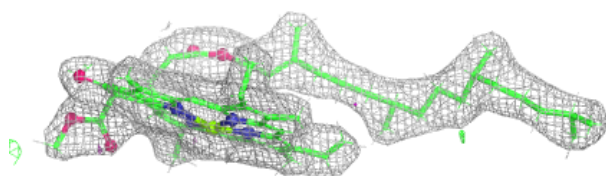
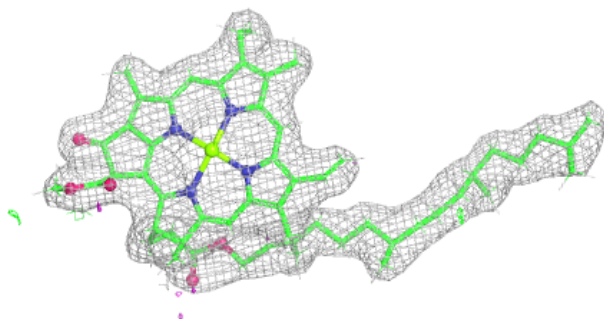
**Electron density around CLA b 605:**

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

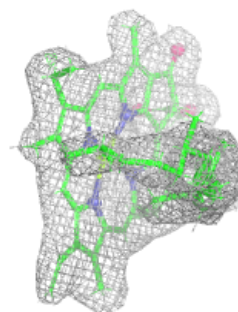
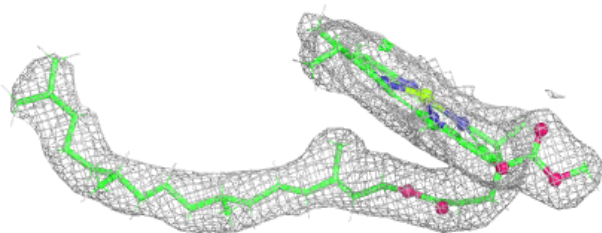
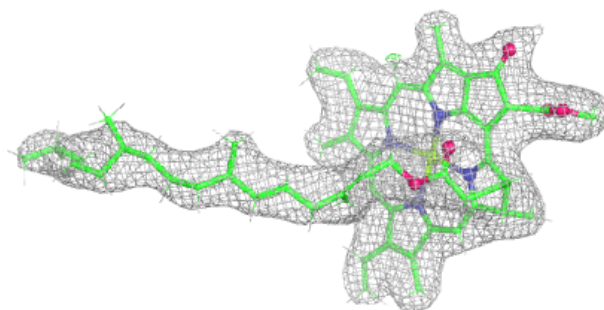


Electron density around CLA C 502:

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

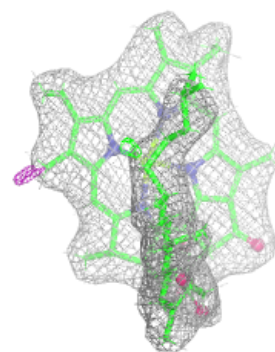
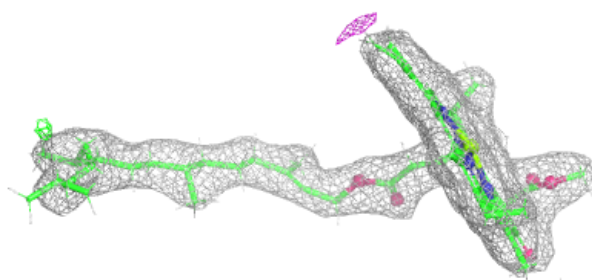
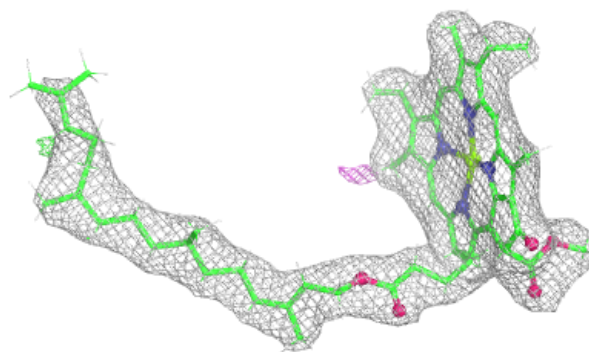
**Electron density around CLA b 608:**

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

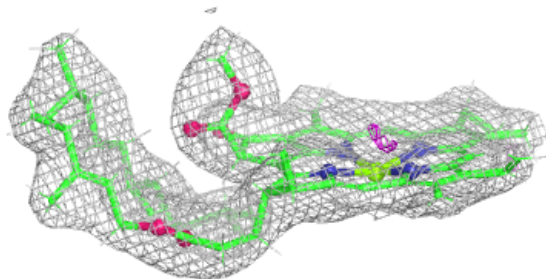
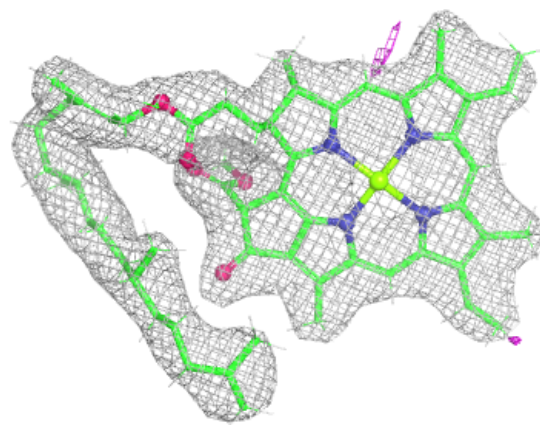


Electron density around CLA b 609:

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

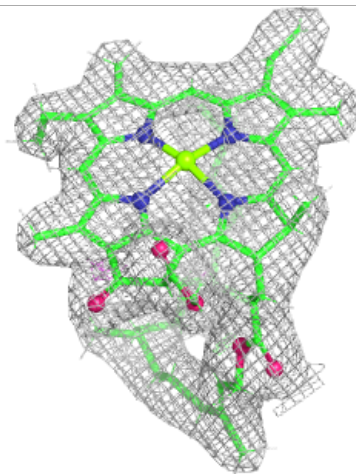
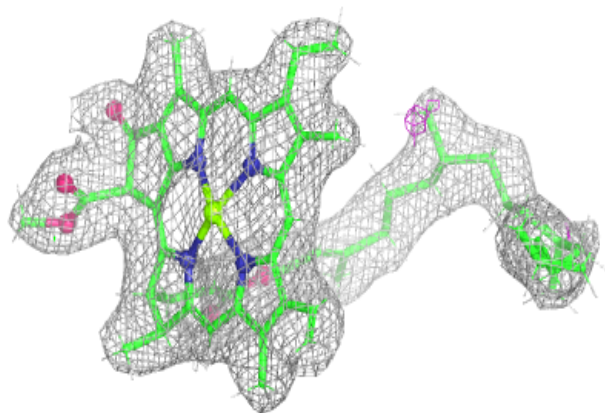
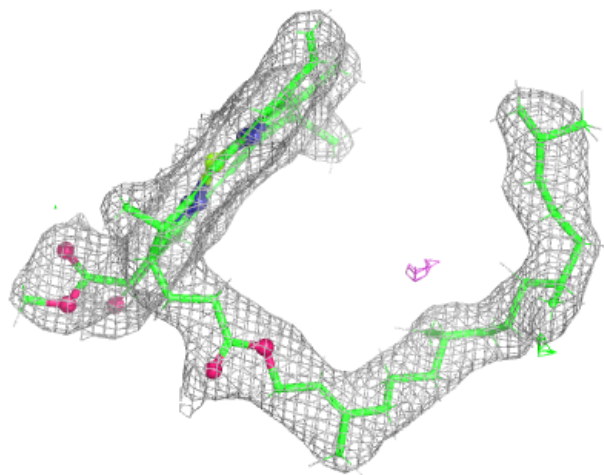
**Electron density around CLA b 610:**

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



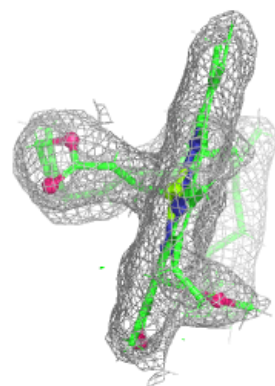
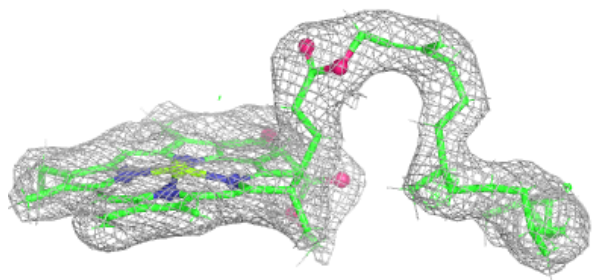
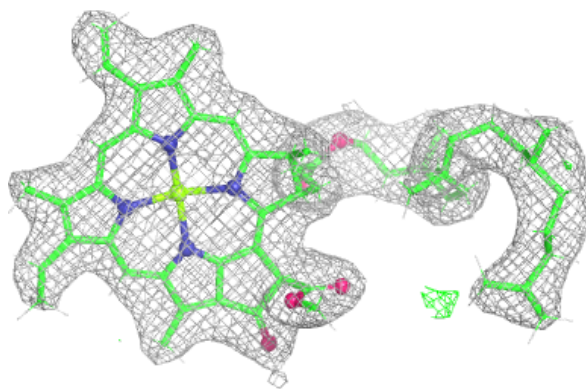
Electron density around CLA b 611:

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

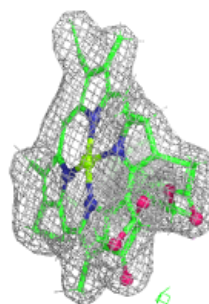
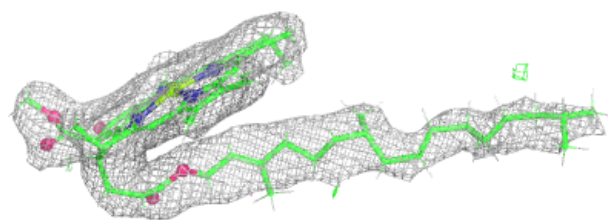
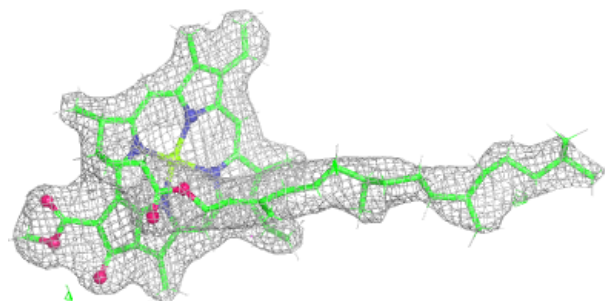


Electron density around CLA b 612:

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

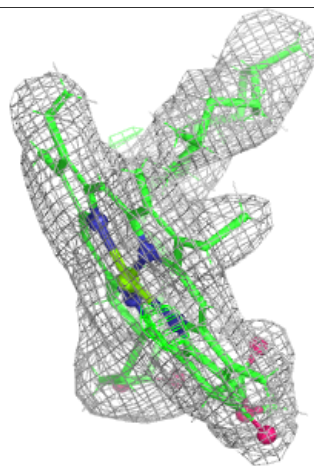
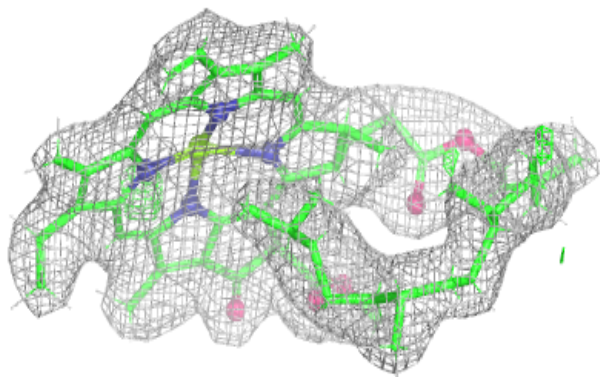
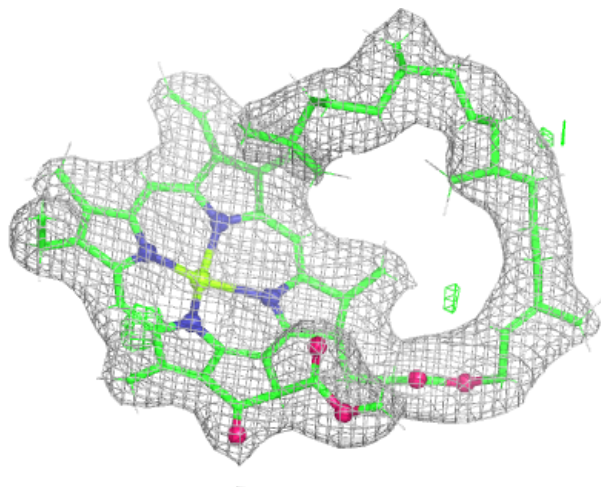
**Electron density around CLA b 614:**

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



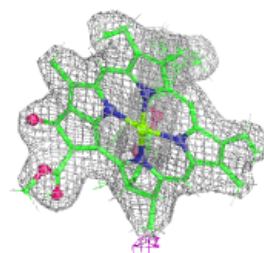
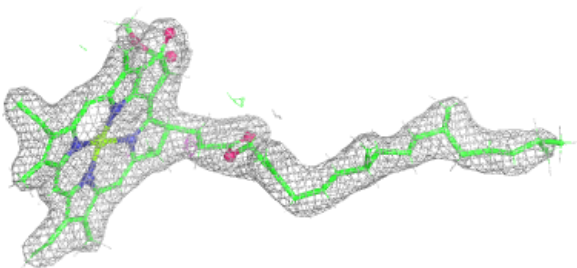
Electron density around CLA b 615:

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

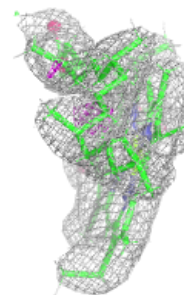
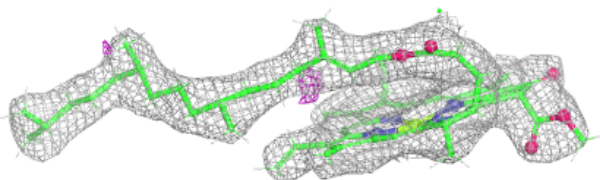
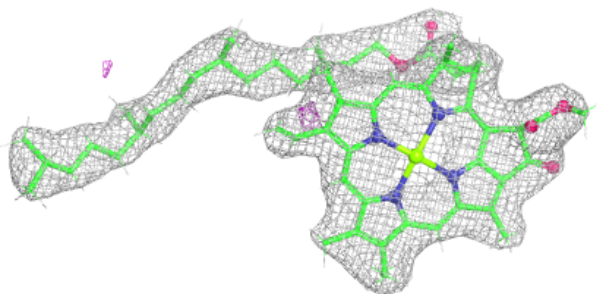


Electron density around CLA C 503:

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

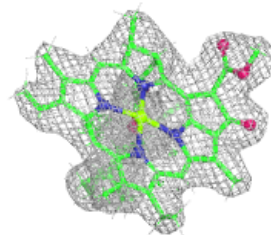
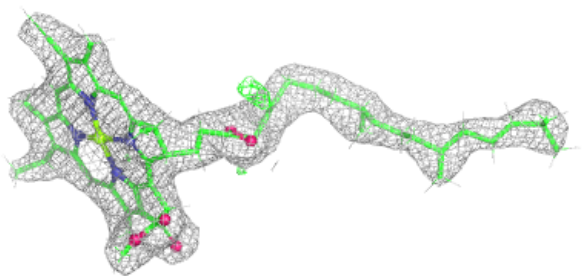
**Electron density around CLA c 501:**

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



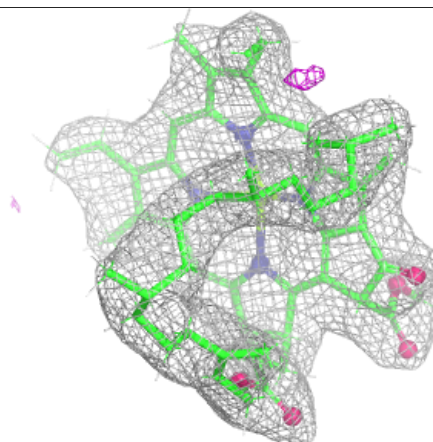
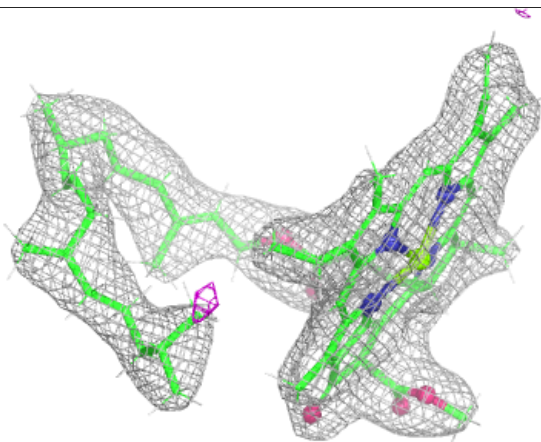
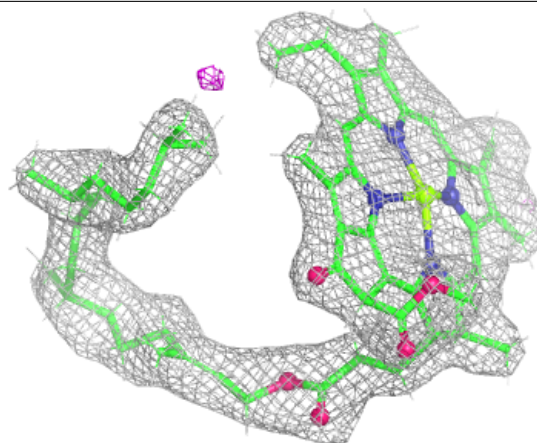
Electron density around CLA c 502:

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

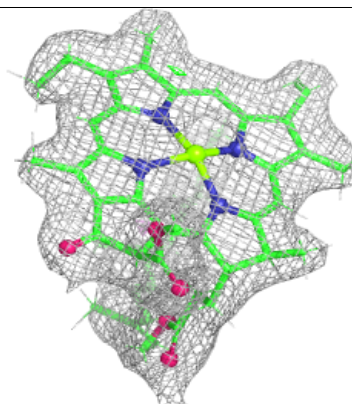
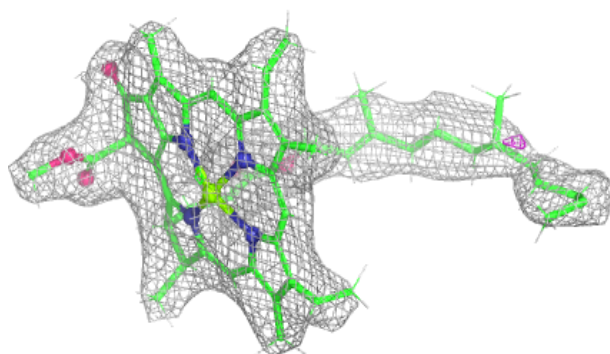
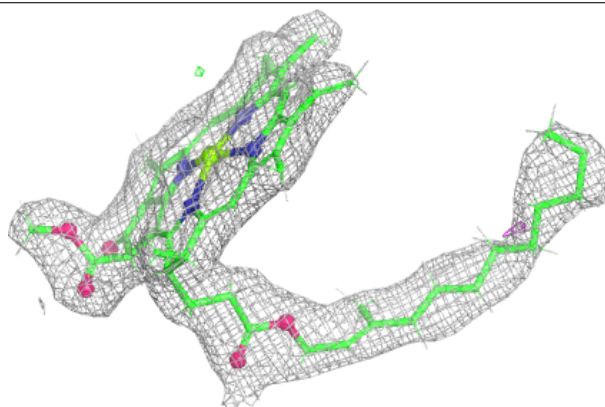


Electron density around CLA C 504:

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

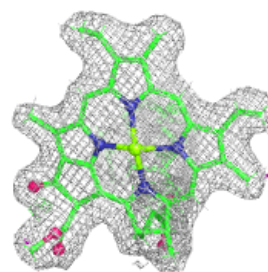
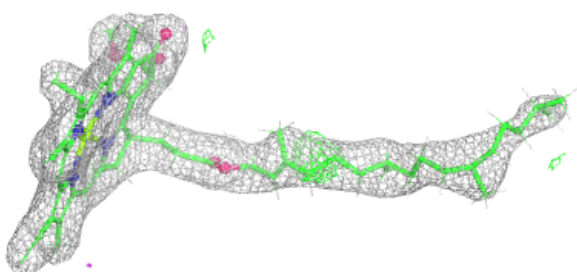
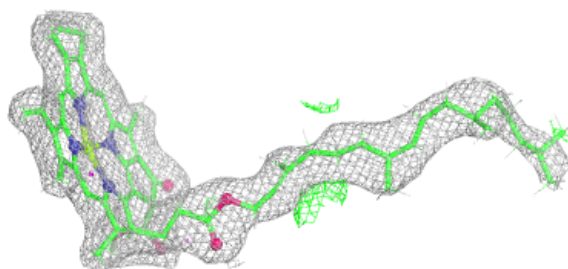
**Electron density around CLA C 505:**

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

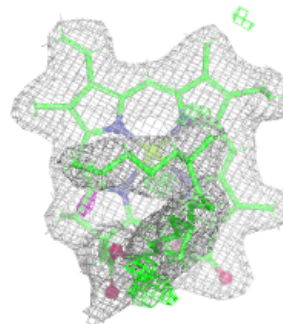
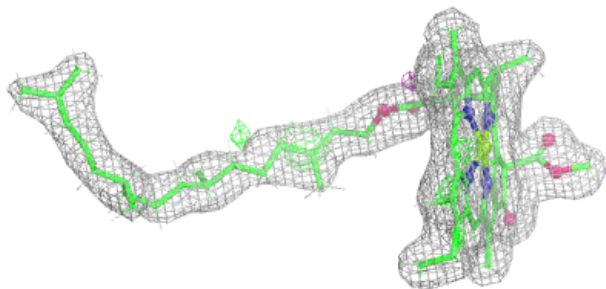
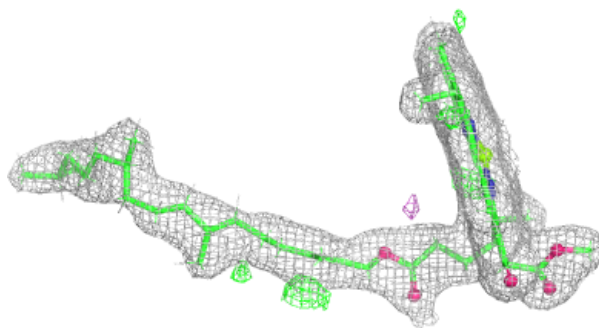


Electron density around CLA B 605:

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

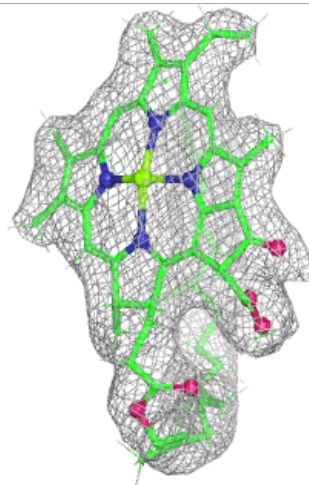
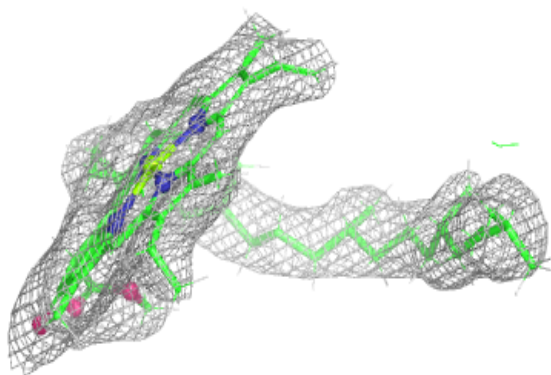
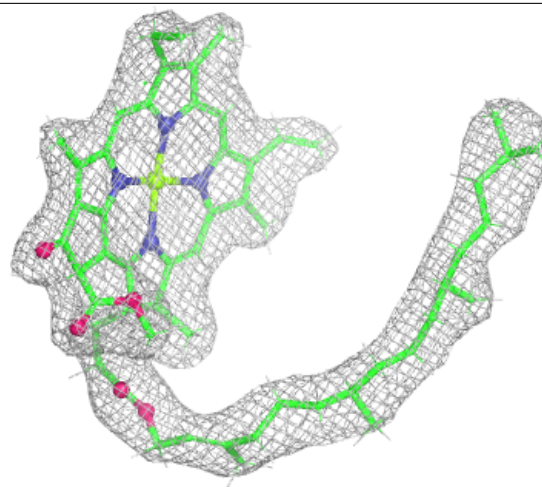
**Electron density around CLA B 606:**

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



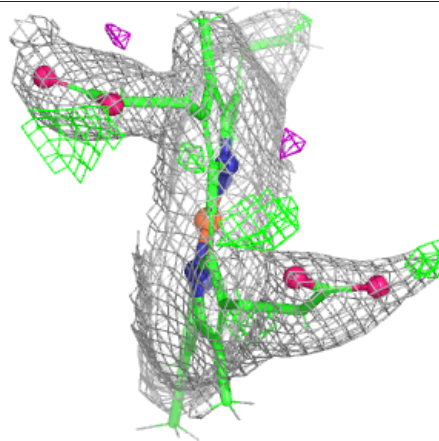
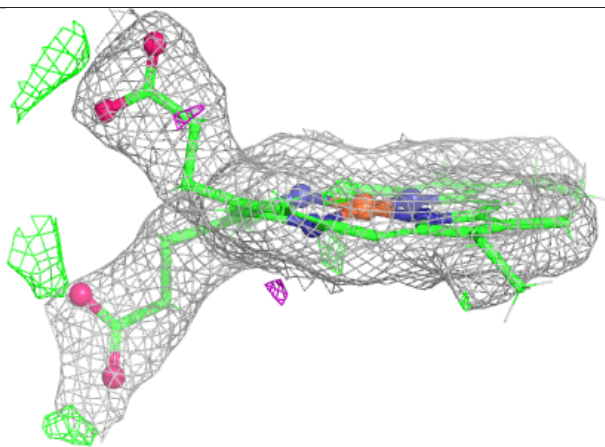
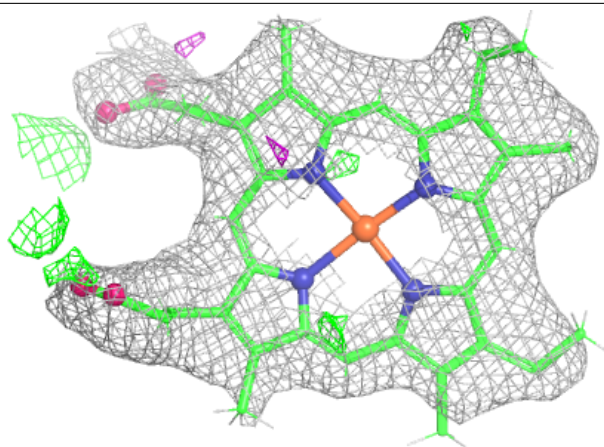
Electron density around CLA c 507:

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

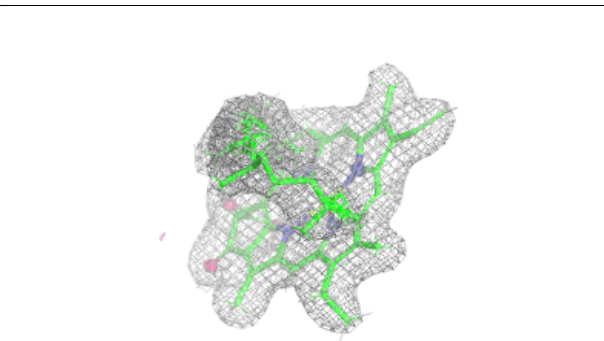
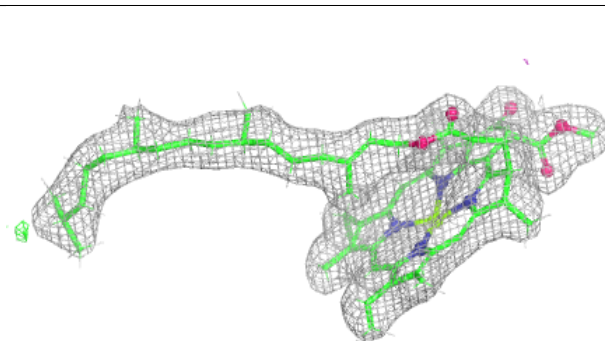
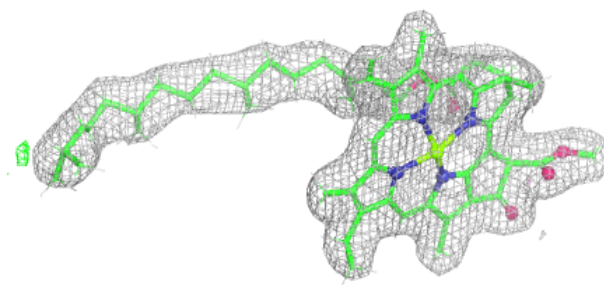


Electron density around HEC e 101:

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

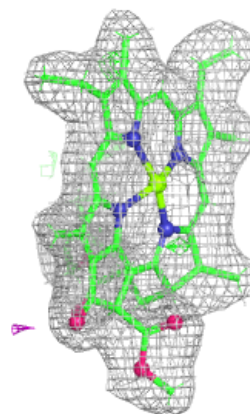
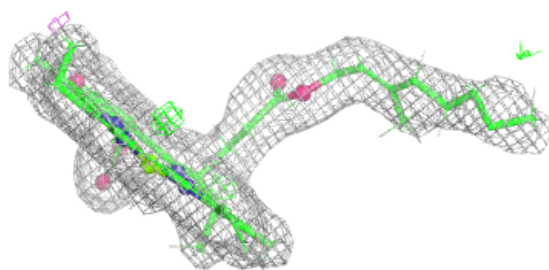
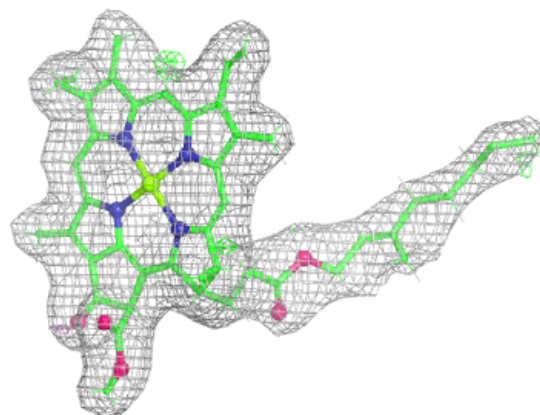
**Electron density around CLA B 609:**

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

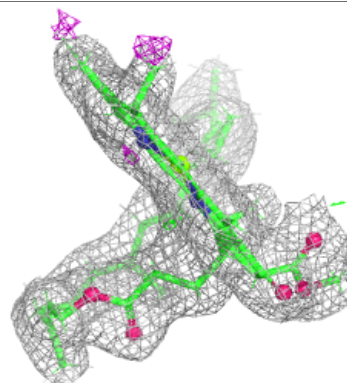
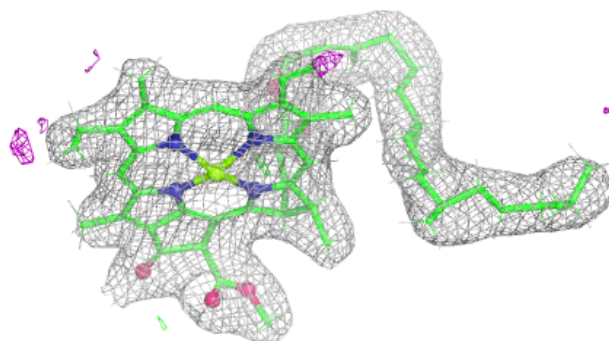
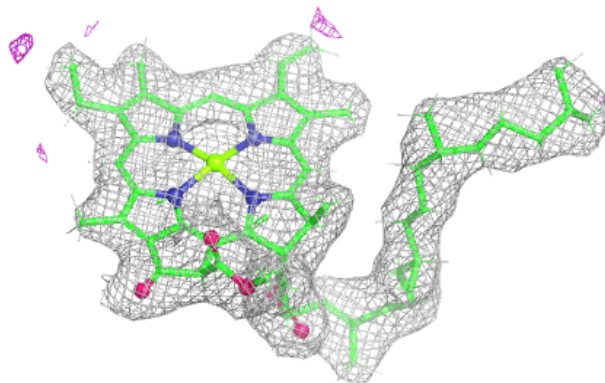


Electron density around CLA A 405:

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

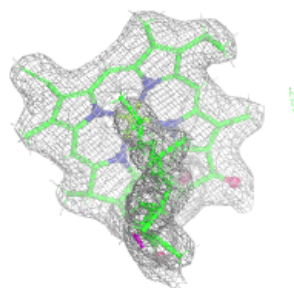
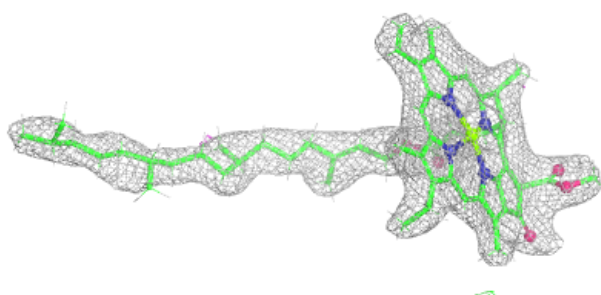
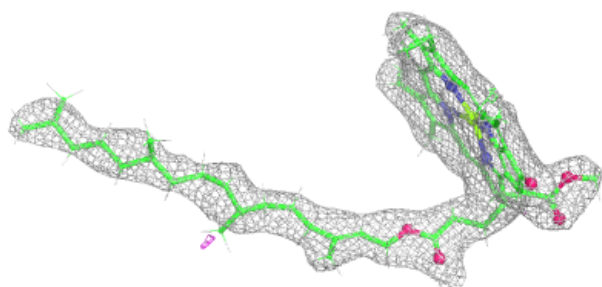
**Electron density around CLA D 403:**

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

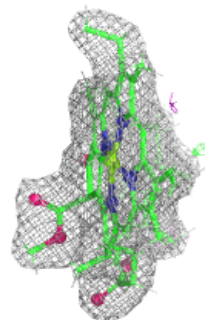
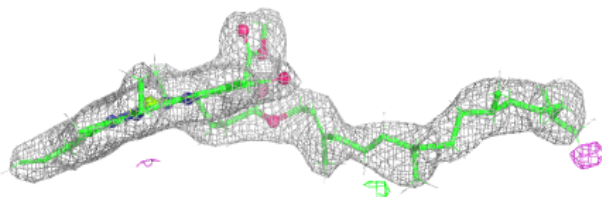
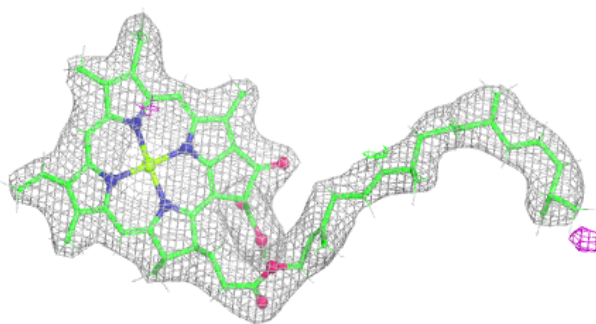


Electron density around CLA b 607:

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

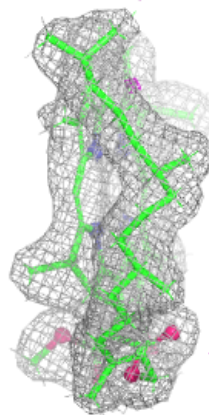
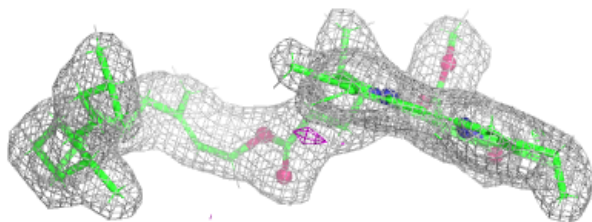
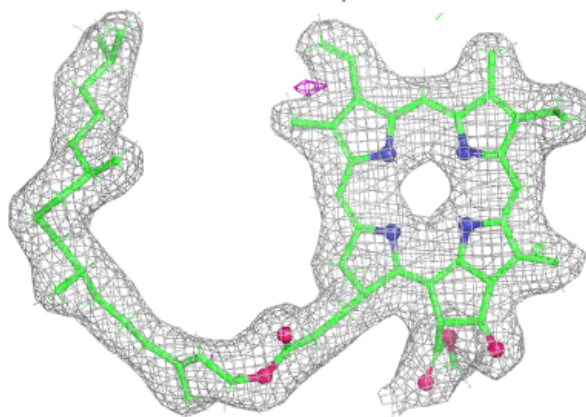
**Electron density around CLA B 603:**

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



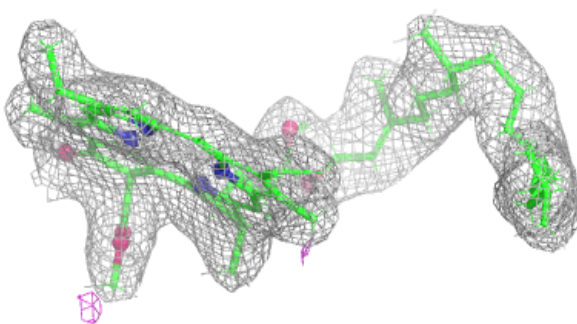
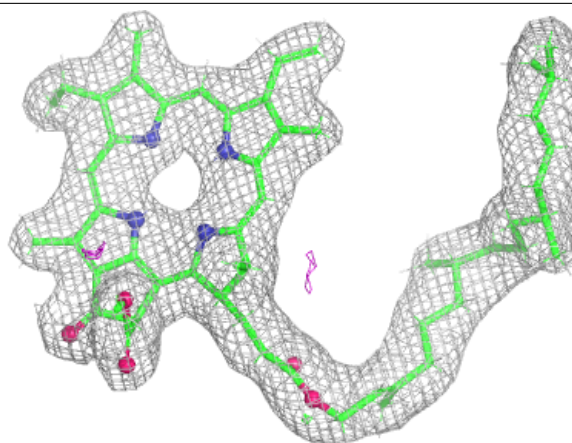
Electron density around PHO A 404:

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

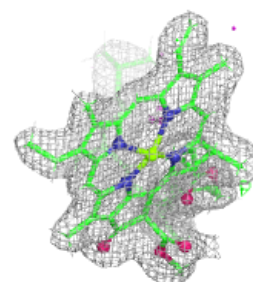
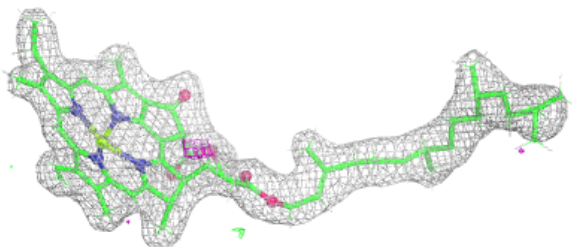
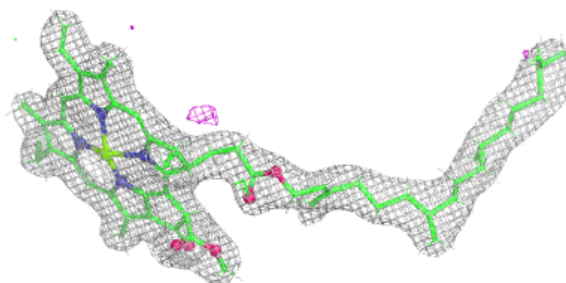


Electron density around PHO D 401:

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

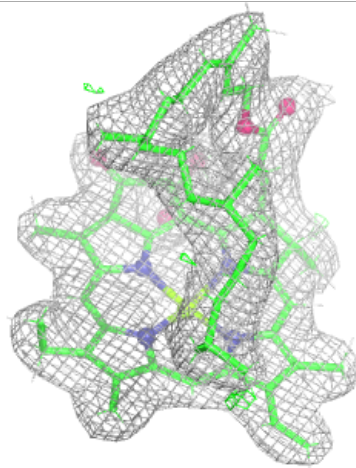
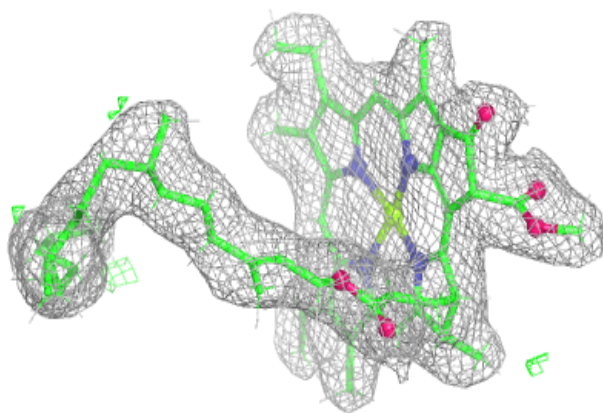
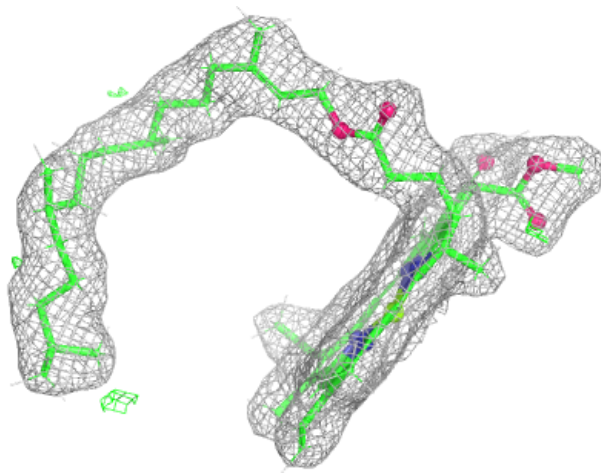
**Electron density around CLA a 402:**

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



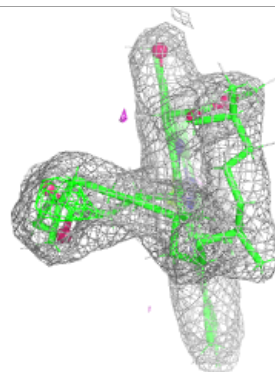
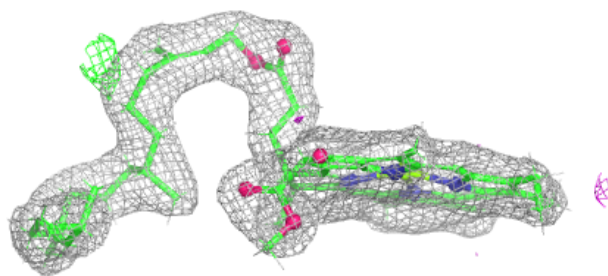
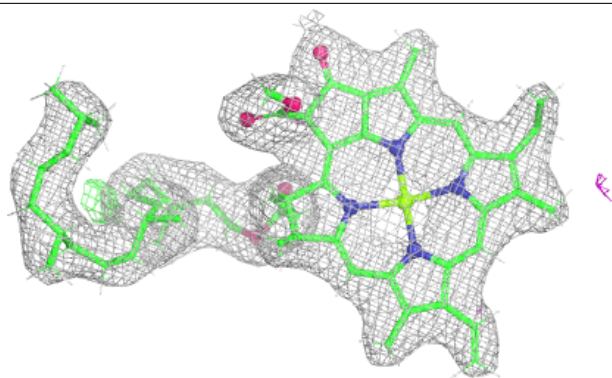
Electron density around CLA B 612:

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

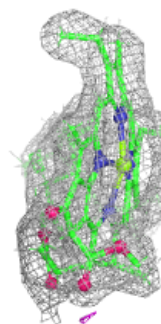
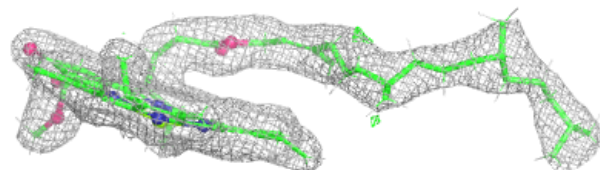
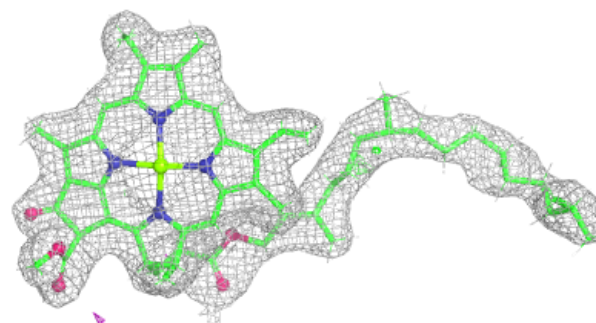


Electron density around CLA B 613:

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

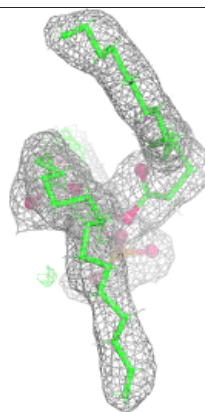
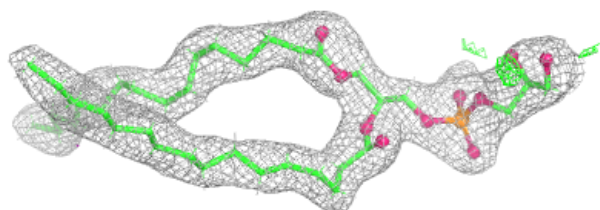
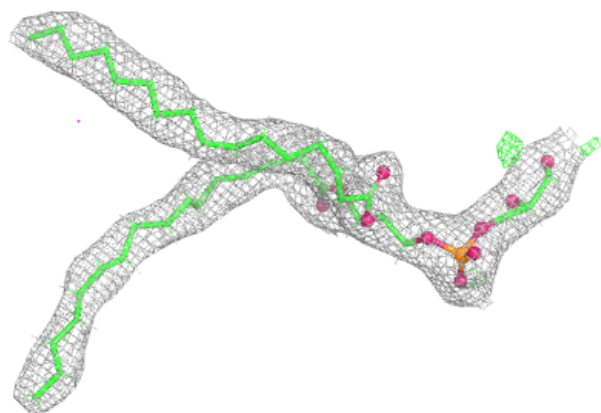
**Electron density around CLA B 604:**

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



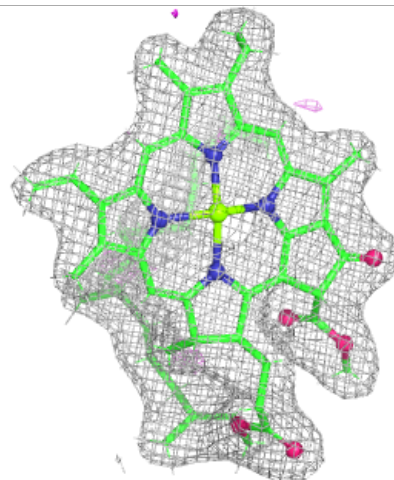
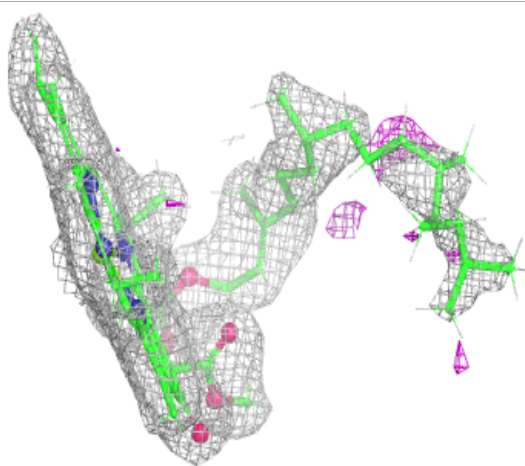
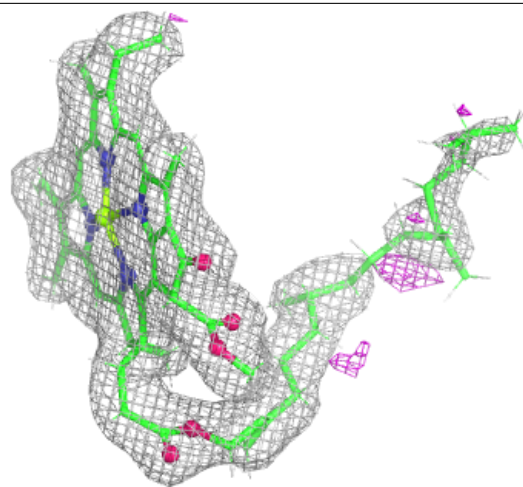
Electron density around LHG D 408:

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



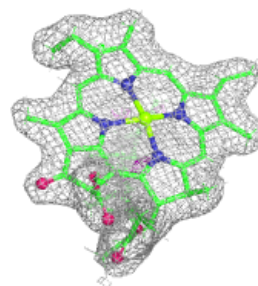
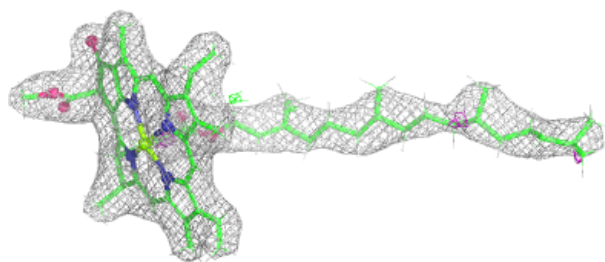
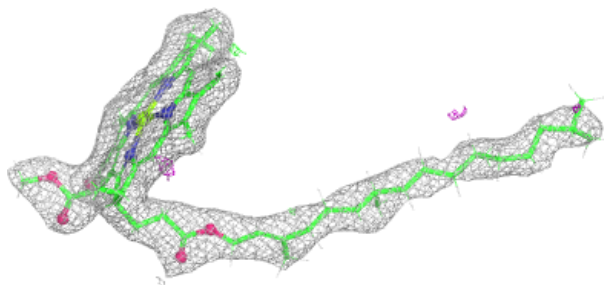
Electron density around CLA b 613:

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

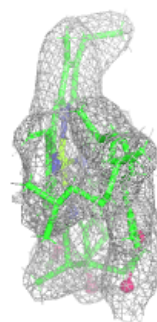
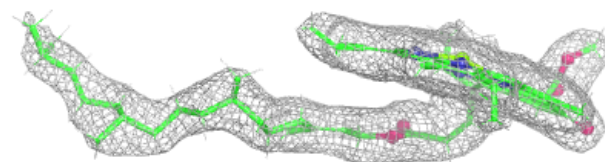
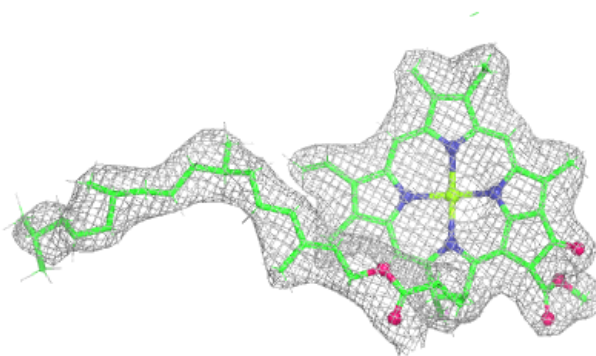


Electron density around CLA B 608:

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

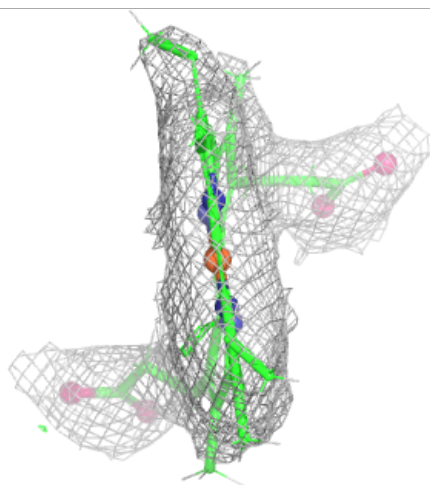
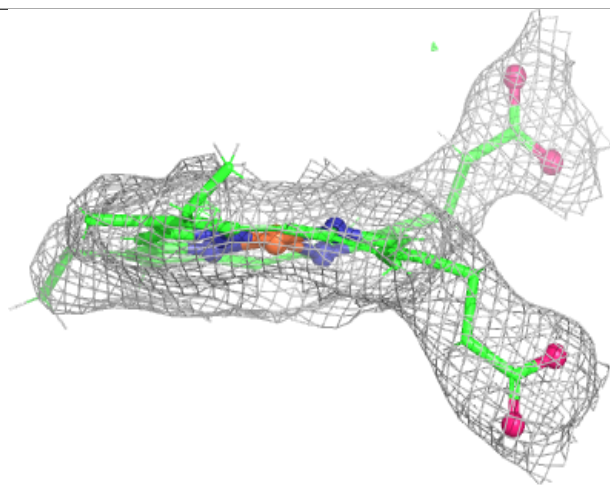
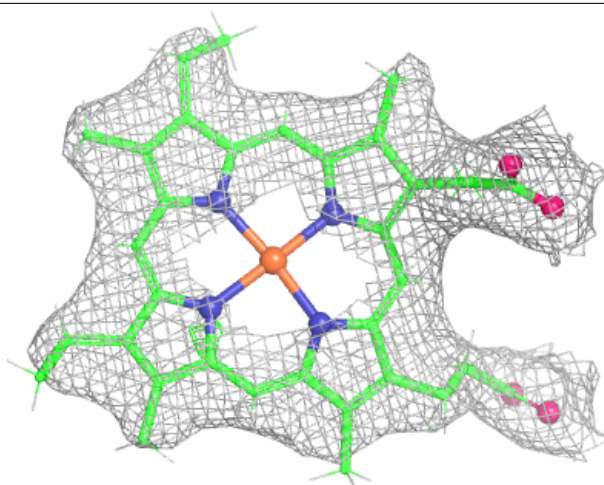
**Electron density around CLA b 603:**

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



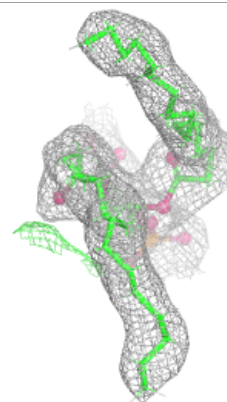
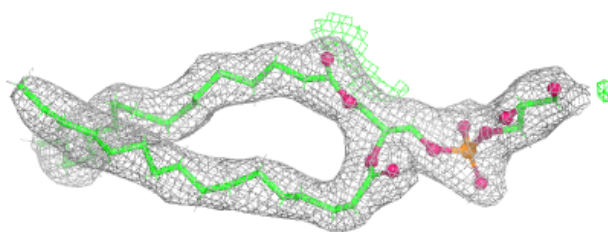
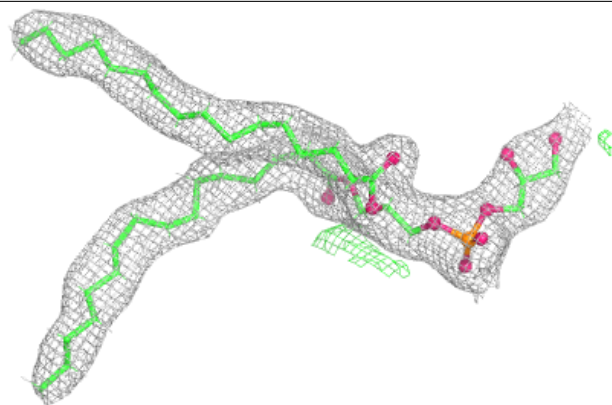
Electron density around HEC E 101:

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



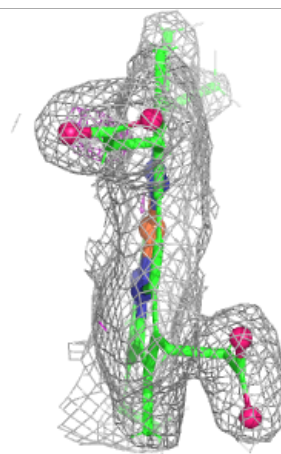
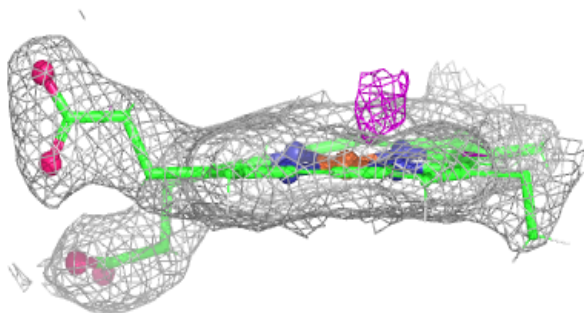
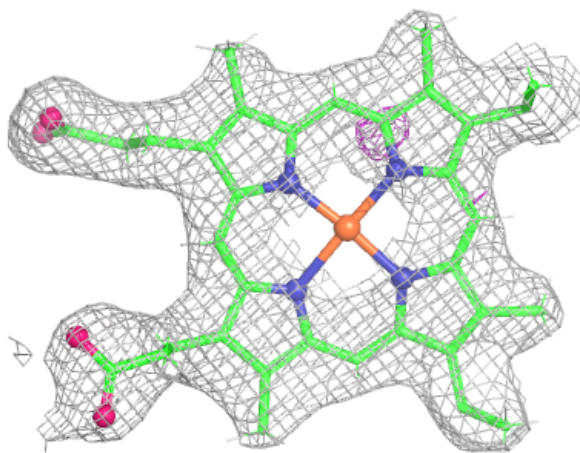
Electron density around LHG d 408:

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



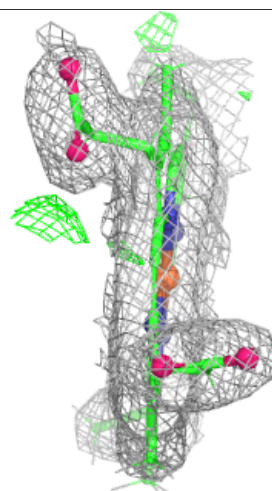
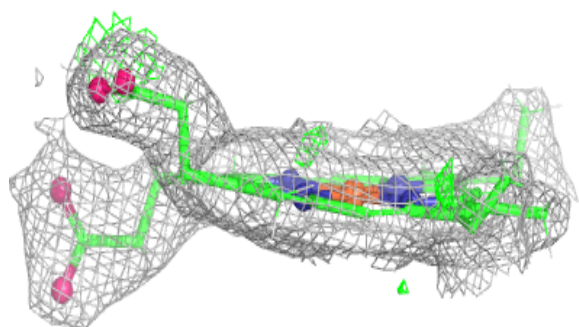
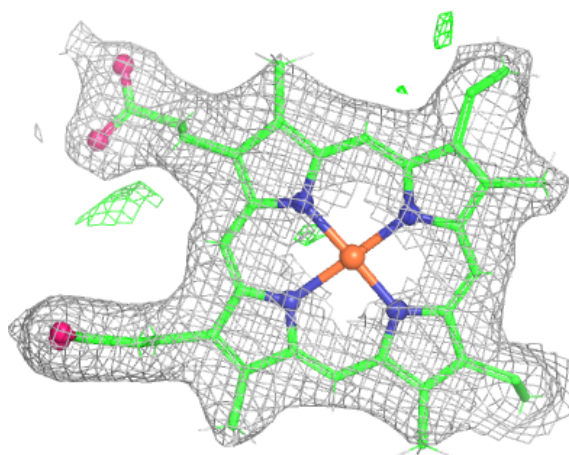
Electron density around HEC V 201:

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



Electron density around HEC v 201:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.