



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 4, 2026 – 11:20 PM UTC

PDB ID : 11YO / pdb_000011yo
Title : Single-conformation model re-refinement of 2F/S3-rich PSII intermediate structure at 2.09 Angstrom resolution
Authors : Wang, J.; Armstrong, W.H.; Batista, V.S.
Deposited on : 2026-03-18
Resolution : 2.09 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

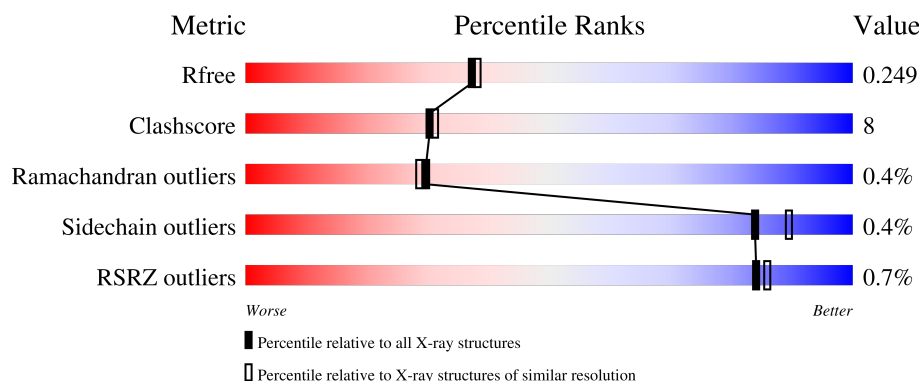
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.09 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.













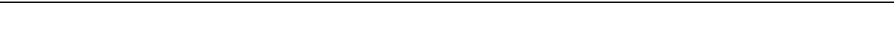

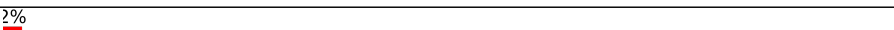
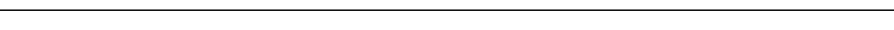









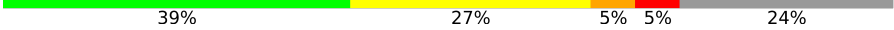

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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

Mol	Chain	Length	Quality of chain
1	A	344	
1	a	344	
2	B	510	
2	b	510	
3	C	461	







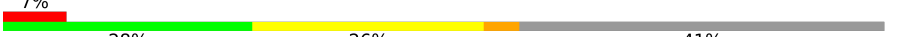



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Mol	Chain	Length	Quality of chain
3	c	461	 89% 8% ..
4	D	352	 82% 14% ..
4	d	352	 80% 16% .
5	E	84	 71% 26% .
5	e	84	 61% 33% ...
6	F	45	 51% 24% 24%
6	f	45	 60% 16% 24%
7	H	66	 82% 11% 5% ..
7	h	66	 74% 15% 5% . 5%
8	I	38	 87% 5% . 5%
8	i	38	 87% 8% 5%
9	J	40	 58% 32% 10%
9	j	40	 60% 30% 10%
10	K	46	 50% 26% . 20%
10	k	46	 54% 22% .. 20%
11	L	37	 92% 8%
11	l	37	 84% 11% ..
12	M	36	 78% 14% 8%
12	m	36	 61% 22% . . 11%
13	O	272	 71% 17% . 10%
13	o	272	 74% 12% . 10%
14	R	41	 44% 37% . 17%
14	r	41	 39% 27% 5% 5% 24%
15	T	32	 75% 16% . 6%
15	t	32	 84% 6% . 6%

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Mol	Chain	Length	Quality of chain
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	404	X	-	-	-
22	CLA	B	702	X	-	-	-
22	CLA	B	703	X	-	-	-
22	CLA	B	704	X	-	-	-
22	CLA	B	705	X	-	-	-
22	CLA	B	706	X	-	-	-
22	CLA	B	707	X	-	-	-
22	CLA	B	708	X	-	-	-
22	CLA	B	710	X	-	-	-
22	CLA	B	711	X	-	-	-
22	CLA	B	712	X	-	-	-
22	CLA	B	713	X	-	-	-
22	CLA	B	714	X	-	-	-
22	CLA	B	715	X	-	-	-
22	CLA	B	716	X	-	-	-
22	CLA	B	727	X	-	-	-
22	CLA	C	502	X	-	-	-
22	CLA	C	503	X	-	-	-
22	CLA	C	504	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	512	X	-	-	-
22	CLA	C	513	X	-	-	-
22	CLA	C	514	X	-	-	-
22	CLA	D	402	X	-	-	-
22	CLA	D	403	X	-	-	-
22	CLA	D	404	X	-	-	-
22	CLA	a	402	X	-	-	-
22	CLA	a	403	X	-	-	-
22	CLA	a	405	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	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	616	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	c	514	X	-	-	-
22	CLA	d	401	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	d	403	X	-	-	-
22	CLA	d	404	X	-	-	-
22	CLA	h	701	X	-	-	-

2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 52261 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	64	0
			2622	1717	431	459	15			
1	a	334	Total	C	N	O	S	0	64	0
			2619	1714	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	N	O	S	0	4	0
			4005	2631	666	695	13			
2	b	505	Total	C	N	O	S	0	0	0
			3978	2610	665	690	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	442	Total	C	N	O	S	0	11	0
			3426	2249	571	593	13			
3	c	451	Total	C	N	O	S	0	12	0
			3500	2290	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	N	O	S	0	2	0
			2717	1800	444	461	12			
4	d	341	Total	C	N	O	S	0	3	0
			2723	1804	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	N	O	0	1	0
			666	436	107	123			
5	e	82	Total	C	N	O	0	0	0
			664	434	108	122			

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	L	37	Total	C	N	O	S	0	0	0
			304	202	48	53	1			
11	l	36	Total	C	N	O		0	0	0
			296	197	47	52				

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	244	Total	C	N	O	S	0	1	0
			1870	1168	313	385	4			
13	o	244	Total	C	N	O	S	0	0	0
			1874	1170	317	383	4			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	R	34	Total	C	N	O	0	0	0
			271	184	47	40			
14	r	31	Total	C	N	O	0	0	0
			240	162	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	N	O	S	0	0	0
			258	181	36	39	2			
15	t	30	Total	C	N	O	S	0	0	0
			256	180	36	38	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
16	U	97	Total	C	N	O	0	0	0
			774	491	129	154			
16	u	97	Total	C	N	O	0	0	0
			774	491	129	154			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	V	137	Total	C	N	O	S	0	0	0
			1064	675	177	208	4			
17	v	137	Total	C	N	O	S	0	0	0
			1064	675	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	N	O	0	0	0
			281	188	45	48			
18	x	39	Total	C	N	O	0	0	0
			286	191	46	49			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Y	27	Total	C	N	O	S	0	0	0
			196	128	35	30	3			
19	y	30	Total	C	N	O	S	0	0	0
			218	144	35	36	3			

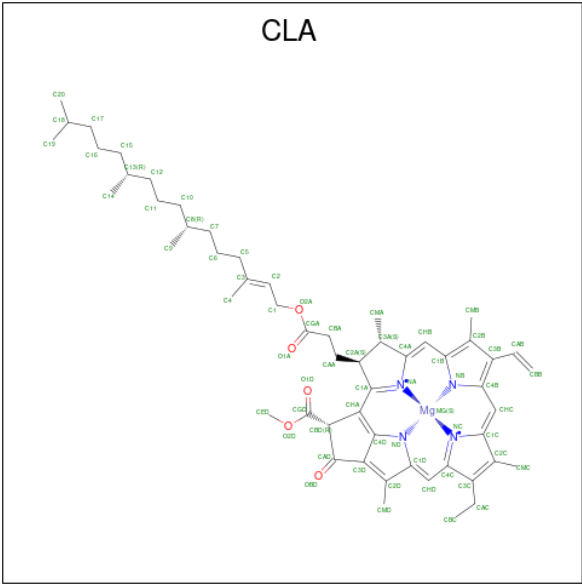
- Molecule 20 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	Z	62	Total	C	N	O	S	0	0	0
			479	328	72	77	2			
20	z	62	Total	C	N	O	S	0	0	0
			477	326	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: C₅₅H₇₂MgN₄O₅).



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

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

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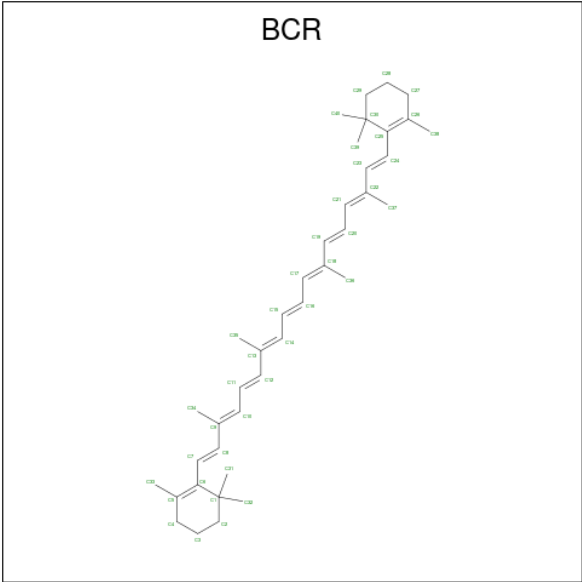
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total 65	C 55	Mg 1	N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

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

- Molecule 23 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



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

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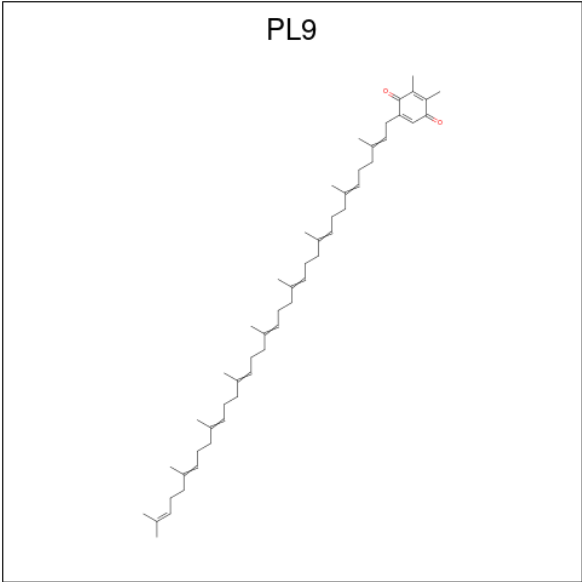
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	b	1	Total C 40 40	0	0
23	c	1	Total C 40 40	0	0
23	c	1	Total C 40 40	0	0
23	d	1	Total C 40 40	0	0
23	h	1	Total C 40 40	0	0
23	k	1	Total C 40 40	0	0
23	k	1	Total C 40 40	0	0
23	t	1	Total C 40 40	0	0

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

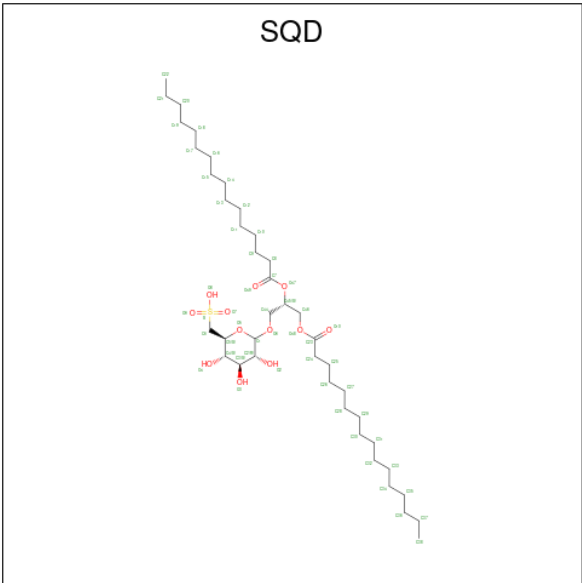
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	A	2	Total Cl 2 2	0	0
24	a	2	Total Cl 2 2	0	0

- Molecule 25 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: C₅₃H₈₀O₂).



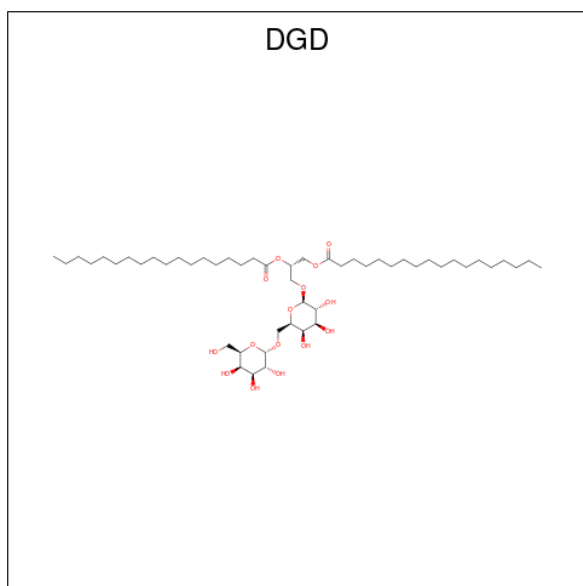
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	A	1	Total	C	O	0	0
			55	53	2		
25	D	1	Total	C	O	0	0
			55	53	2		
25	a	1	Total	C	O	0	0
			55	53	2		
25	d	1	Total	C	O	0	0
			55	53	2		

- Molecule 26 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
26	A	1	Total C O S 52 39 12 1	0	0
26	A	1	Total C O 39 35 4	0	0
26	B	1	Total C O S 54 41 12 1	0	0
26	D	1	Total C O S 36 25 10 1	0	0
26	a	1	Total C O S 54 41 12 1	0	0
26	a	1	Total C O 36 31 5	0	0
26	f	1	Total C O S 41 28 12 1	0	0
26	l	1	Total C O S 49 36 12 1	0	0

- Molecule 27 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



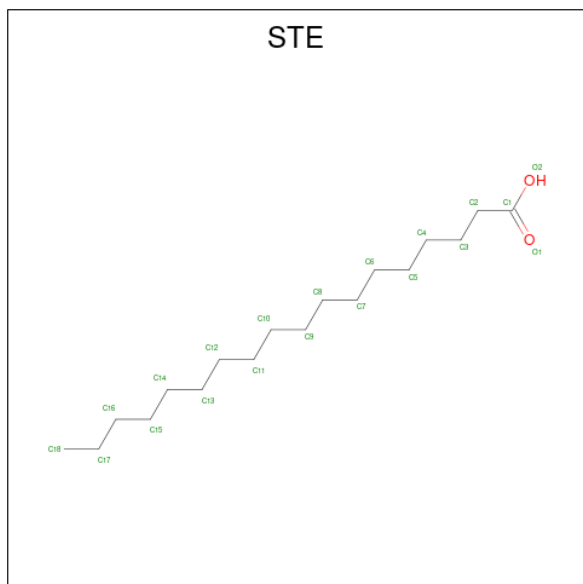
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	1	Total C O 66 51 15	0	0
27	C	1	Total C O 62 47 15	0	0
27	C	1	Total C O 62 47 15	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	C	1	Total C O 62 47 15	0	0
27	H	1	Total C O 62 47 15	0	0
27	c	1	Total C O 62 47 15	0	0
27	c	1	Total C O 62 47 15	0	0
27	c	1	Total C O 62 47 15	0	0
27	h	1	Total C O 62 47 15	0	0

- Molecule 28 is STEARIC ACID (CCD ID: STE) (formula: $C_{18}H_{36}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	A	1	Total C 5 5	0	0
28	B	1	Total C O 12 10 2	0	0
28	B	1	Total C O 17 15 2	0	0
28	B	1	Total C O 12 10 2	0	0
28	B	1	Total C O 18 16 2	0	0

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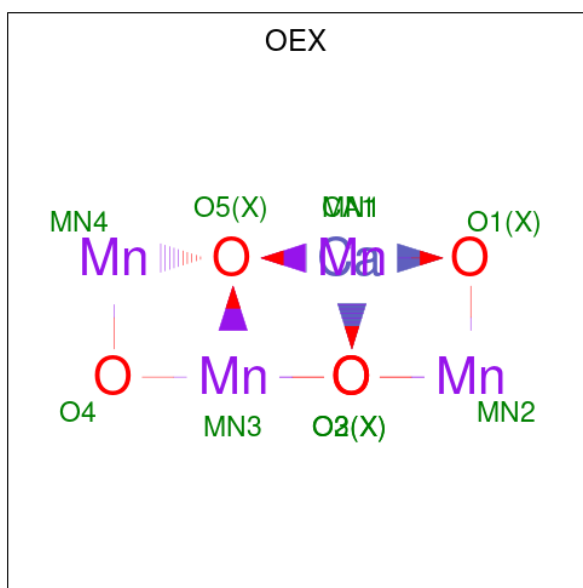
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	B	1	Total C 16 16	0	0
28	C	1	Total C O 12 10 2	0	0
28	C	1	Total C 16 16	0	0
28	C	1	Total C O 12 10 2	0	0
28	E	1	Total C O 12 10 2	0	0
28	E	1	Total C 7 7	0	0
28	H	1	Total C 18 18	0	0
28	H	1	Total C 8 8	0	0
28	I	1	Total C 15 15	0	0
28	J	1	Total C O 12 10 2	0	0
28	M	1	Total C O 15 13 2	0	0
28	M	1	Total C 10 10	0	0
28	T	1	Total C 15 15	0	0
28	X	1	Total C O 20 18 2	0	0
28	Z	1	Total C 8 8	0	0
28	a	1	Total C 10 10	0	0
28	a	1	Total C O 12 10 2	0	0
28	a	1	Total C 15 15	0	0
28	b	1	Total C 16 16	0	0
28	b	1	Total C O 20 18 2	0	0
28	b	1	Total C O 16 14 2	0	0

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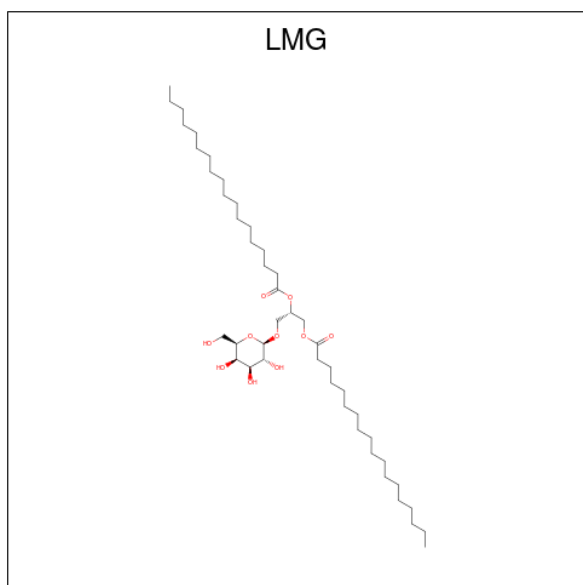
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	b	1	Total C O 20 18 2	0	0
28	b	1	Total C 10 10	0	0
28	c	1	Total C O 12 10 2	0	0
28	c	1	Total C O 20 18 2	0	0
28	d	1	Total C O 20 18 2	0	0
28	d	1	Total C O 17 15 2	0	0
28	h	1	Total C 14 14	0	0
28	j	1	Total C O 12 10 2	0	0
28	m	1	Total C 18 18	0	0
28	m	1	Total C O 12 10 2	0	0
28	t	1	Total C O 14 12 2	0	0
28	x	1	Total C O 20 18 2	0	0

- Molecule 29 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5).



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

- Molecule 30 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).



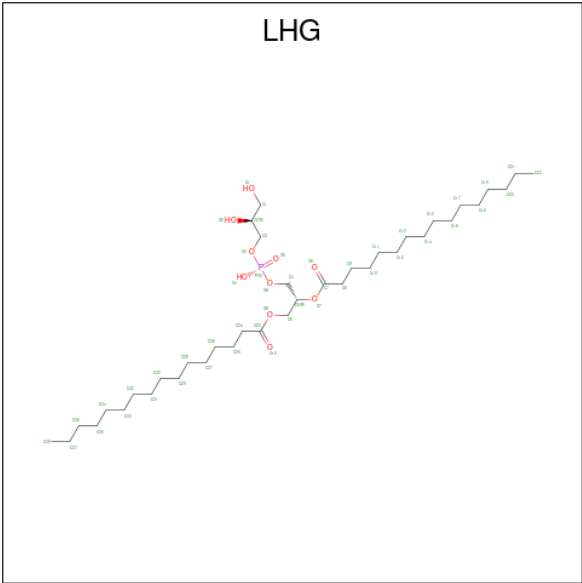
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	B	1	Total	C	O	0	0
			28	24	4		
30	C	1	Total	C	O	0	0
			48	38	10		
30	C	1	Total	C	O	0	0
			48	38	10		
30	D	1	Total	C	O	0	0
			51	41	10		
30	D	1	Total	C	O	0	0
			32	27	5		
30	M	1	Total	C	O	0	0
			51	41	10		
30	a	1	Total	C	O	0	0
			55	45	10		
30	b	1	Total	C	O	0	0
			51	41	10		
30	b	1	Total	C	O	0	0
			55	45	10		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	c	1	Total	C	O	0	0
			37	27	10		
30	c	1	Total	C	O	0	0
			48	38	10		
30	c	1	Total	C	O	0	0
			49	39	10		
30	d	1	Total	C	O	0	0
			44	34	10		

- Molecule 31 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



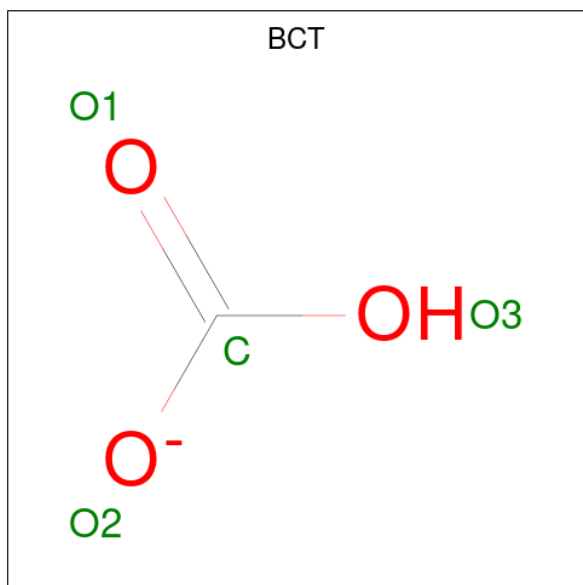
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	B	1	Total	C	O	P	0	0
			49	38	10	1		
31	D	1	Total	C	O	P	0	0
			49	38	10	1		
31	D	1	Total	C	O	P	0	0
			47	36	10	1		
31	E	1	Total	C	O	P	0	0
			49	38	10	1		
31	L	1	Total	C	O	P	0	0
			49	38	10	1		
31	a	1	Total	C	O	P	0	0
			49	38	10	1		
31	a	1	Total	C	O	P	0	0
			42	31	10	1		

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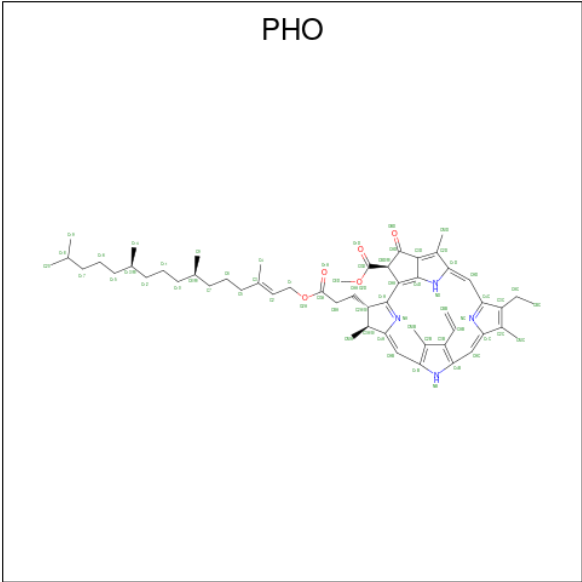
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	d	1	Total	C	O	P	0	0
			49	38	10	1		
31	d	1	Total	C	O	P	0	0
			39	28	10	1		
31	l	1	Total	C	O	P	0	0
			49	38	10	1		

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



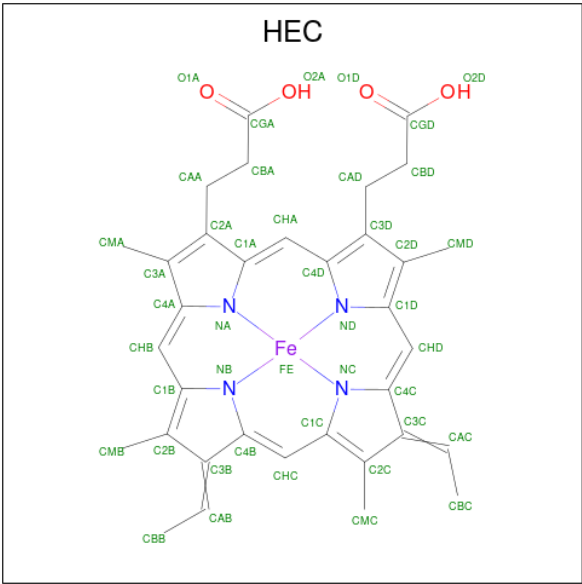
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	D	1	Total	C	O	0	0
			4	1	3		
32	a	1	Total	C	O	0	0
			4	1	3		

- Molecule 33 is PHEOPHYTIN A (CCD ID: PHO) (formula: $\text{C}_{55}\text{H}_{74}\text{N}_4\text{O}_5$).



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

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



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

- Molecule 35 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	A	137	Total 137	O 137	0	4
35	B	234	Total 234	O 234	0	0
35	C	167	Total 167	O 167	0	0
35	D	116	Total 116	O 116	0	0
35	E	37	Total 37	O 37	0	0
35	F	10	Total 10	O 10	0	0
35	H	34	Total 34	O 34	0	0
35	I	20	Total 20	O 20	0	0
35	J	14	Total 14	O 14	0	0
35	K	3	Total 3	O 3	0	0
35	L	10	Total 10	O 10	0	0
35	M	8	Total 8	O 8	0	0
35	O	105	Total 105	O 105	0	0
35	R	3	Total 3	O 3	0	0
35	T	9	Total 9	O 9	0	0
35	U	52	Total 52	O 52	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	V	64	Total O 64 64	0	0
35	X	17	Total O 17 17	0	0
35	Y	3	Total O 3 3	0	0
35	a	121	Total O 121 121	0	4
35	b	194	Total O 194 194	0	0
35	c	169	Total O 169 169	0	0
35	d	108	Total O 108 108	0	0
35	e	22	Total O 22 22	0	0
35	f	5	Total O 5 5	0	0
35	h	22	Total O 22 22	0	0
35	i	17	Total O 17 17	0	0
35	j	7	Total O 7 7	0	0
35	k	4	Total O 4 4	0	0
35	l	11	Total O 11 11	0	0
35	m	6	Total O 6 6	0	0
35	o	98	Total O 98 98	0	0
35	r	8	Total O 8 8	0	0
35	t	7	Total O 7 7	0	0
35	u	64	Total O 64 64	0	0
35	v	63	Total O 63 63	0	0
35	x	7	Total O 7 7	0	0

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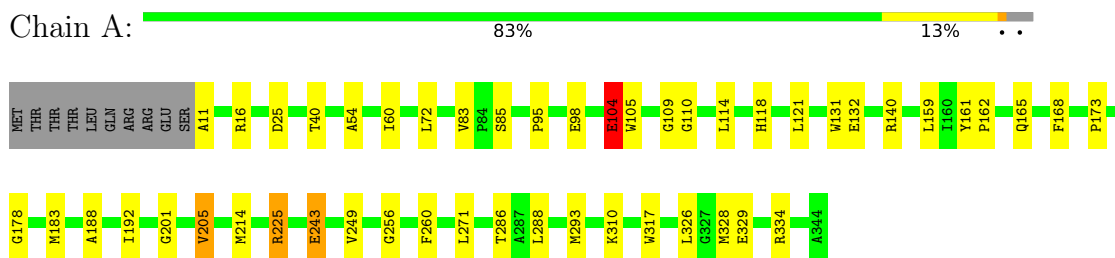
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	y	9	Total	O	0	0
			9	9		
35	z	9	Total	O	0	0
			9	9		

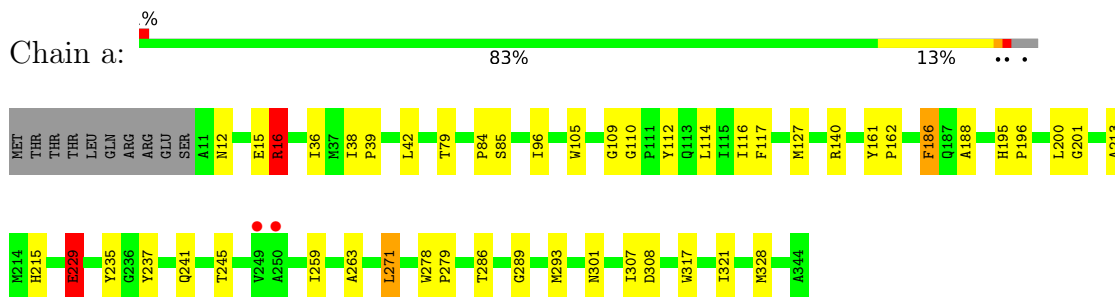
3 Residue-property plots [i](#)

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

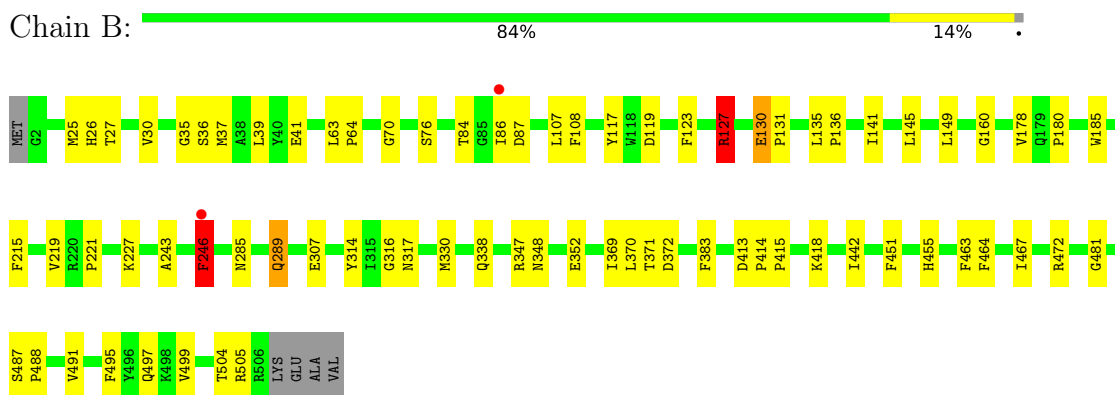
- Molecule 1: Photosystem II protein D1 1



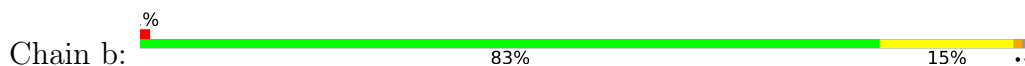
- Molecule 1: Photosystem II protein D1 1

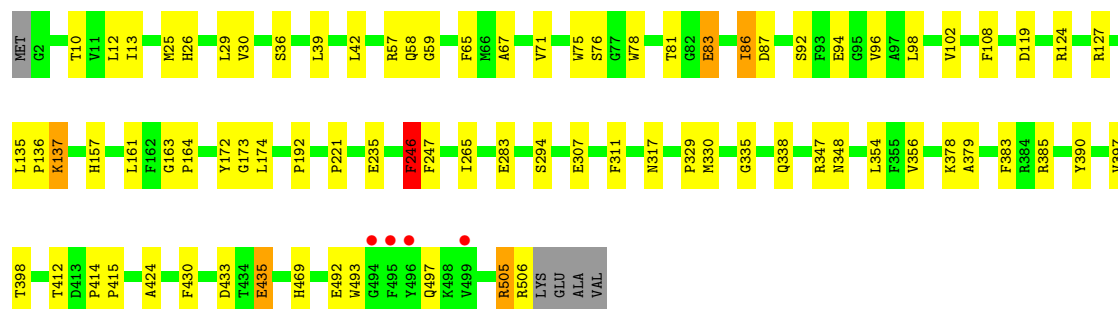


- Molecule 2: Photosystem II CP47 reaction center protein



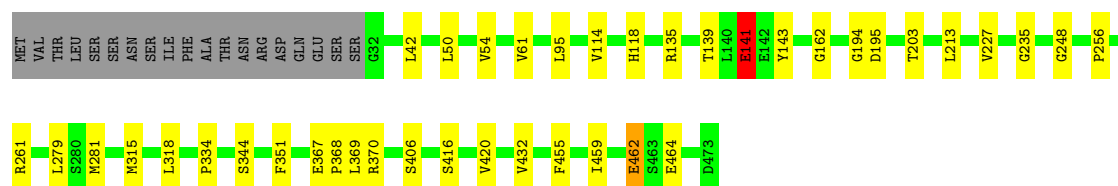
- Molecule 2: Photosystem II CP47 reaction center protein





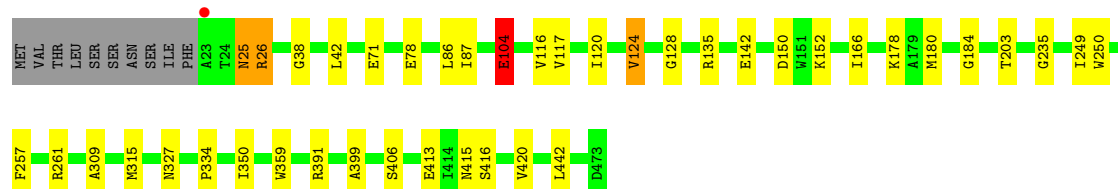
• Molecule 3: Photosystem II CP43 reaction center protein

Chain C: 87% 8% .



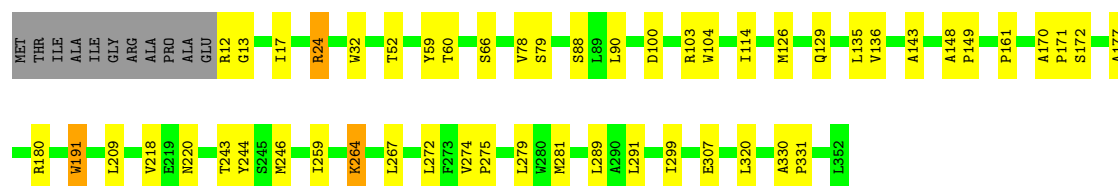
• Molecule 3: Photosystem II CP43 reaction center protein

Chain c: 89% 8% ..



• Molecule 4: Photosystem II D2 protein

Chain D: 82% 14% ..



• Molecule 4: Photosystem II D2 protein

Chain d: 80% 16% .

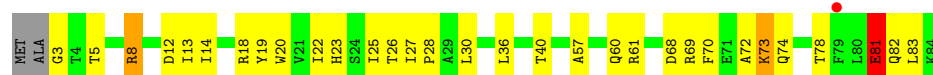




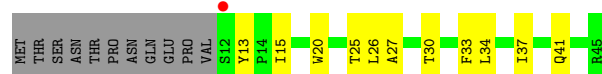
- Molecule 5: Cytochrome b559 subunit alpha



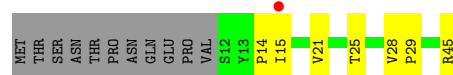
- Molecule 5: Cytochrome b559 subunit alpha



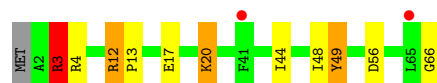
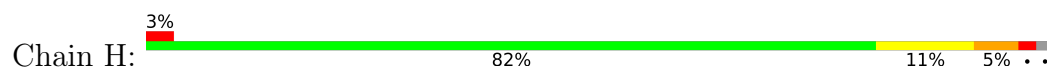
- Molecule 6: Cytochrome b559 subunit beta



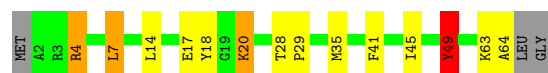
- Molecule 6: Cytochrome b559 subunit beta




- Molecule 7: Photosystem II reaction center protein H

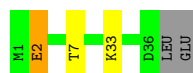


- Molecule 7: Photosystem II reaction center protein H




- Molecule 8: Photosystem II reaction center protein I

Chain I:  87% 5% • 5%



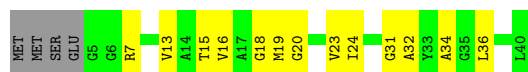
- Molecule 8: Photosystem II reaction center protein I

Chain i:  87% 8% 5%



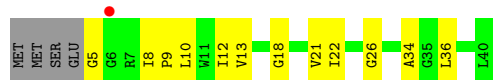
- Molecule 9: Photosystem II reaction center protein J

Chain J:  58% 32% 10%



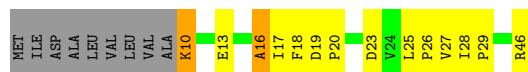
- Molecule 9: Photosystem II reaction center protein J

Chain j:  2% 60% 30% 10%



- Molecule 10: Photosystem II reaction center protein K

Chain K:  50% 26% • 20%



- Molecule 10: Photosystem II reaction center protein K

Chain k:  54% 22% • • 20%




- Molecule 11: Photosystem II reaction center protein L

Chain L:  92% 8%




- Molecule 11: Photosystem II reaction center protein L

Chain l:  84% 11% . .



- Molecule 12: Photosystem II reaction center protein M

Chain M:  78% 14% 8%



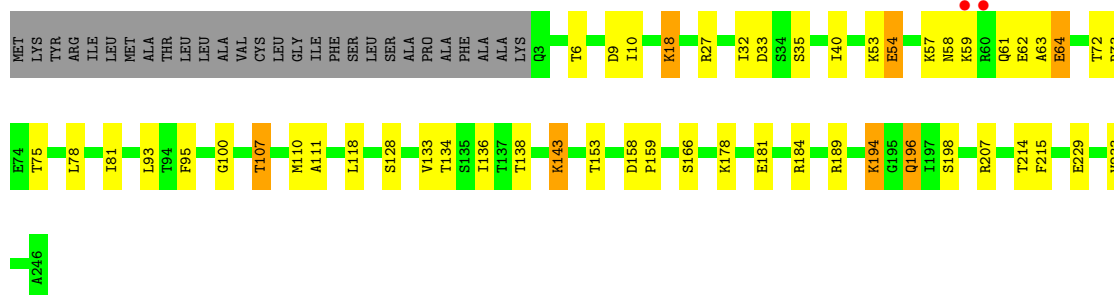
- Molecule 12: Photosystem II reaction center protein M

Chain m:  61% 22% . . 11%



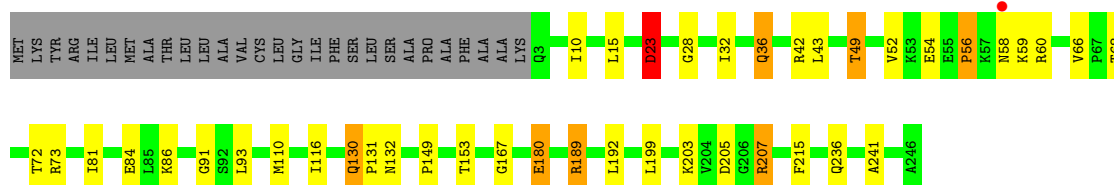
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:  71% 17% . 10%




- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:  74% 12% . 10%

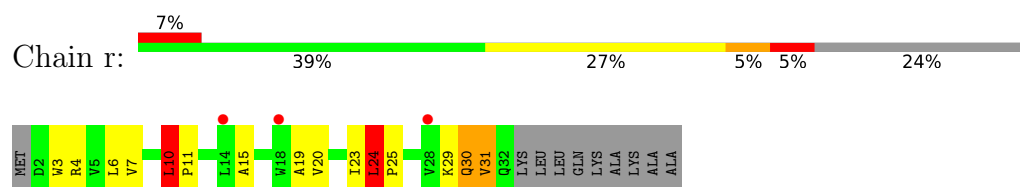


- Molecule 14: Photosystem II protein Y

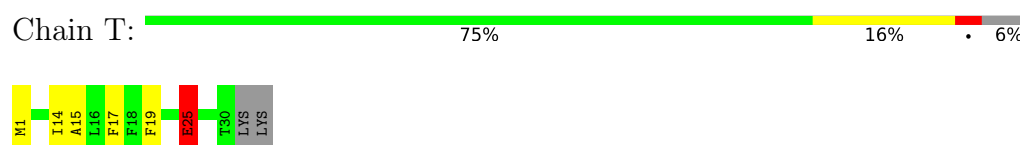
Chain R:  44% 37% . 17%



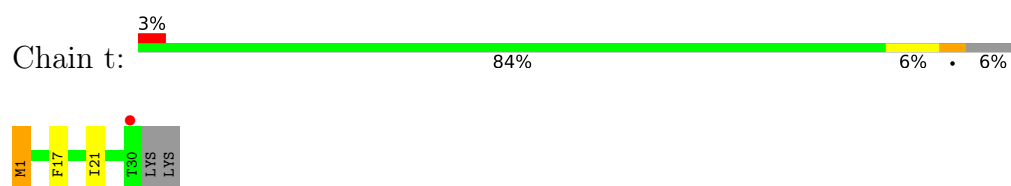
- Molecule 14: Photosystem II protein Y



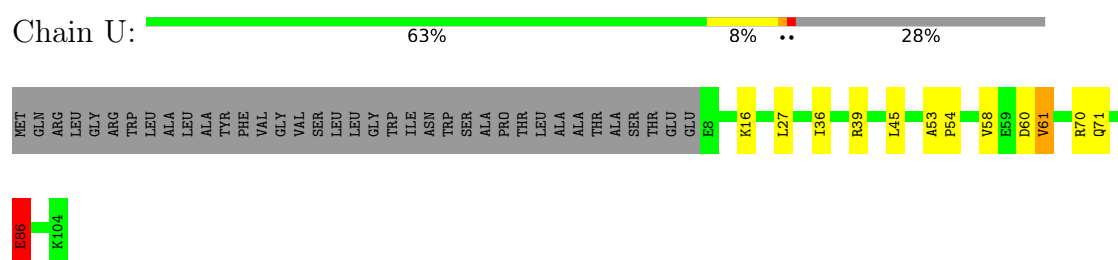
- Molecule 15: Photosystem II reaction center protein T



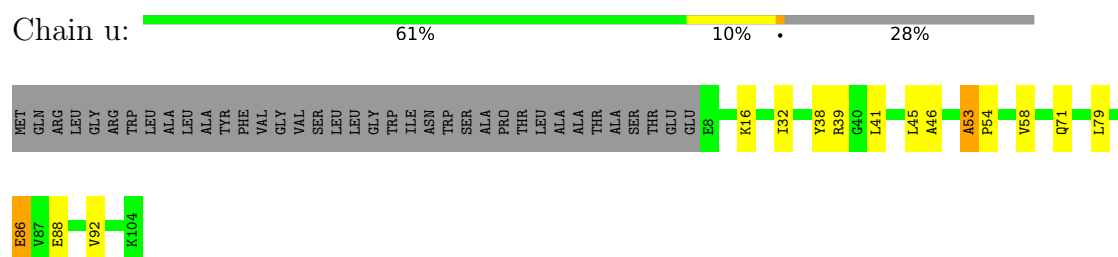
- Molecule 15: Photosystem II reaction center protein T



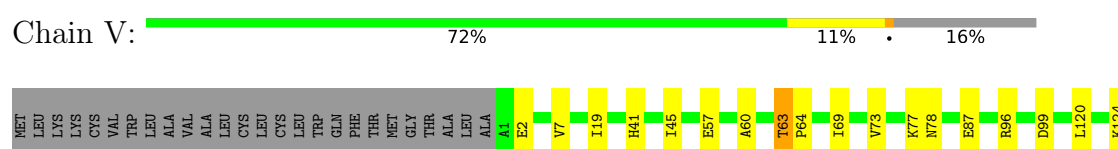
- Molecule 16: Photosystem II 12 kDa extrinsic protein



- Molecule 16: Photosystem II 12 kDa extrinsic protein



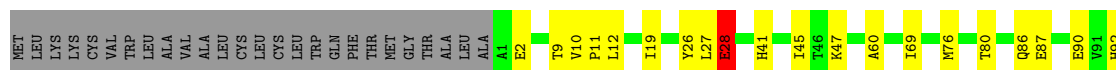
- Molecule 17: Cytochrome c-550





- Molecule 17: Cytochrome c-550

Chain v: 64% 19% 16%



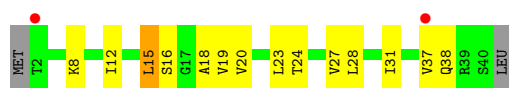
- Molecule 18: Photosystem II reaction center X protein

Chain X: 2% 73% 20% 7%



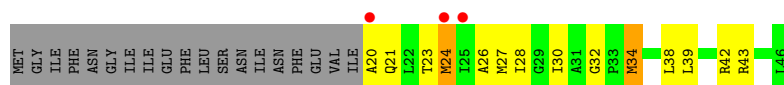
- Molecule 18: Photosystem II reaction center X protein

Chain x: 5% 61% 32% 5%



- Molecule 19: Photosystem II reaction center protein Ycf12

Chain Y: 7% 28% 26% 41%



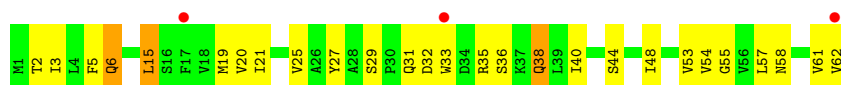
- Molecule 19: Photosystem II reaction center protein Ycf12

Chain y: 41% 17% 35%

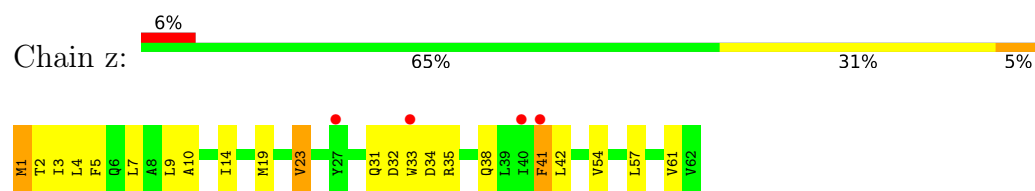


- Molecule 20: Photosystem II reaction center protein Z

Chain Z: 5% 56% 39% 5%



- 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 221.65Å 307.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.65 – 2.09 33.65 – 2.09	Depositor EDS
% Data completeness (in resolution range)	99.8 (33.65-2.09) 99.8 (33.65-2.09)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.23 (at 2.08Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.183 , 0.243 0.195 , 0.249	Depositor DCC
R_{free} test set	4162 reflections (0.89%)	wwPDB-VP
Wilson B-factor (Å ²)	31.5	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 60.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	52261	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.40% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.77	0/2707	0.87	8/3692 (0.2%)
1	a	0.81	3/2704 (0.1%)	1.00	14/3688 (0.4%)
2	B	0.81	7/4155 (0.2%)	1.03	19/5661 (0.3%)
2	b	0.78	3/4118 (0.1%)	0.88	15/5611 (0.3%)
3	C	0.78	4/3539 (0.1%)	0.85	6/4819 (0.1%)
3	c	0.69	4/3619 (0.1%)	0.88	6/4926 (0.1%)
4	D	0.78	2/2812 (0.1%)	0.84	3/3832 (0.1%)
4	d	0.76	2/2821 (0.1%)	0.97	16/3844 (0.4%)
5	E	0.56	0/688	0.74	1/940 (0.1%)
5	e	0.63	1/683 (0.1%)	1.04	6/932 (0.6%)
6	F	0.55	0/284	0.62	0/387
6	f	0.58	0/284	0.77	0/387
7	H	0.94	2/523 (0.4%)	1.11	6/713 (0.8%)
7	h	0.77	1/511 (0.2%)	1.07	3/697 (0.4%)
8	I	0.77	0/293	1.06	3/396 (0.8%)
8	i	0.70	0/293	0.75	0/396
9	J	0.61	0/263	0.90	0/356
9	j	0.56	0/263	0.76	0/356
10	K	0.81	1/303 (0.3%)	0.81	1/416 (0.2%)
10	k	0.85	2/303 (0.7%)	1.16	4/416 (1.0%)
11	L	0.76	0/311	0.83	0/422
11	l	0.83	0/303	0.90	1/412 (0.2%)
12	M	0.71	0/249	0.78	0/341
12	m	0.84	0/244	1.13	2/334 (0.6%)
13	O	0.81	3/1904 (0.2%)	1.09	17/2585 (0.7%)
13	o	0.72	0/1905	0.95	8/2583 (0.3%)
14	R	0.74	1/277 (0.4%)	1.25	2/380 (0.5%)
14	r	0.70	0/246	1.19	6/339 (1.8%)
15	T	0.79	0/257	1.11	3/349 (0.9%)
15	t	0.72	0/255	0.76	0/346
16	U	0.60	0/785	0.85	2/1064 (0.2%)
16	u	0.71	0/785	0.96	4/1064 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	V	0.67	0/1085	0.84	1/1473 (0.1%)
17	v	0.71	1/1085 (0.1%)	1.05	5/1473 (0.3%)
18	X	0.54	0/284	0.76	0/384
18	x	0.59	1/289 (0.3%)	1.09	3/391 (0.8%)
19	Y	0.80	0/197	1.17	2/264 (0.8%)
19	y	0.54	0/219	0.91	3/294 (1.0%)
20	Z	0.65	0/490	1.11	4/669 (0.6%)
20	z	0.72	3/488 (0.6%)	1.17	5/666 (0.8%)
All	All	0.75	41/42824 (0.1%)	0.94	179/58298 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	a	0	3
2	B	0	3
2	b	0	2
3	C	0	1
3	c	0	1
4	d	0	3
5	e	0	1
7	H	0	3
7	h	0	1
8	I	0	1
10	k	0	1
12	m	0	1
13	O	0	3
13	o	0	3
15	T	0	1
16	U	0	1
16	u	0	1
17	V	0	1
17	v	0	1
19	y	0	1
20	Z	0	1
20	z	0	1
All	All	0	37

The worst 5 of 41 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	b	435	GLU	CD-OE2	-15.11	0.96	1.25
3	C	462	GLU	CB-CG	-12.05	1.16	1.52
4	d	16	ASP	CG-OD1	10.70	1.45	1.25
7	H	3	ARG	CZ-NH1	10.54	1.47	1.32
2	b	435	GLU	CG-CD	10.05	1.77	1.52

The worst 5 of 179 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	130	GLU	CA-CB-CG	19.99	154.08	114.10
2	B	246	PHE	CB-CG-CD2	-15.71	93.99	120.70
4	d	16	ASP	N-CA-CB	-14.96	88.02	110.16
3	c	104	GLU	CG-CD-OE2	-14.84	84.28	118.40
7	h	20	LYS	CB-CG-CD	14.07	143.66	111.30

There are no chirality outliers.

5 of 37 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	104	GLU	Sidechain
1	A	243	GLU	Sidechain
2	B	127	ARG	Sidechain
2	B	130	GLU	Sidechain
2	B	246	PHE	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2622	0	2517	36	0
1	a	2619	0	2508	41	0
2	B	4005	0	3871	65	0
2	b	3978	0	3836	71	0
3	C	3426	0	3351	28	3
3	c	3500	0	3424	39	0
4	D	2717	0	2621	46	0
4	d	2723	0	2627	47	0
5	E	666	0	651	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	e	664	0	648	33	0
6	F	275	0	282	9	0
6	f	275	0	282	6	0
7	H	510	0	532	8	3
7	h	498	0	518	17	0
8	I	296	0	311	2	0
8	i	296	0	311	1	0
9	J	257	0	268	15	0
9	j	257	0	268	15	0
10	K	293	0	305	15	0
10	k	293	0	305	15	0
11	L	304	0	316	5	0
11	l	296	0	304	9	0
12	M	256	0	269	4	0
12	m	251	0	267	7	0
13	O	1870	0	1830	43	0
13	o	1874	0	1846	27	0
14	R	271	0	298	20	0
14	r	240	0	250	17	0
15	T	258	0	261	4	0
15	t	256	0	256	3	0
16	U	774	0	773	13	0
16	u	774	0	773	9	0
17	V	1064	0	1073	13	0
17	v	1064	0	1073	30	0
18	X	281	0	312	6	0
18	x	286	0	314	16	0
19	Y	196	0	217	13	0
19	y	218	0	241	10	0
20	Z	479	0	516	28	0
20	z	477	0	509	18	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	A	184	0	192	3	0
22	B	1035	0	1139	15	0
22	C	839	0	922	23	0
22	D	195	0	216	8	0
22	a	195	0	216	2	0
22	b	970	0	1067	21	0
22	c	839	0	919	12	0
22	d	195	0	216	5	0
22	h	65	0	72	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	A	40	0	56	2	0
23	B	120	0	168	13	0
23	C	120	0	168	3	0
23	D	40	0	56	3	0
23	H	40	0	56	2	0
23	T	40	0	56	4	0
23	Y	40	0	56	4	0
23	a	40	0	56	2	0
23	b	120	0	168	3	0
23	c	80	0	112	3	0
23	d	40	0	56	2	0
23	h	40	0	56	1	0
23	k	80	0	112	5	0
23	t	40	0	56	3	0
24	A	2	0	0	0	0
24	a	2	0	0	0	0
25	A	55	0	80	3	0
25	D	55	0	80	2	0
25	a	55	0	80	5	0
25	d	55	0	80	0	0
26	A	91	0	135	0	0
26	B	54	0	77	0	0
26	D	36	0	45	0	0
26	a	90	0	132	2	0
26	f	41	0	46	0	0
26	l	49	0	64	8	0
27	A	66	0	96	4	0
27	C	186	0	245	1	0
27	H	62	0	81	1	0
27	c	186	0	243	1	0
27	h	62	0	80	0	0
28	A	5	0	6	0	0
28	B	75	0	117	1	0
28	C	40	0	63	1	0
28	E	19	0	26	0	0
28	H	26	0	47	0	0
28	I	15	0	26	2	0
28	J	12	0	16	0	0
28	M	25	0	38	0	0
28	T	15	0	29	0	0
28	X	20	0	35	1	0
28	Z	8	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	a	37	0	58	1	0
28	b	82	0	141	2	0
28	c	32	0	51	1	0
28	d	37	0	61	2	0
28	h	14	0	27	1	0
28	j	12	0	16	1	0
28	m	30	0	51	0	0
28	t	14	0	20	0	0
28	x	20	0	35	2	0
29	A	10	0	0	0	0
29	a	10	0	0	0	0
30	B	28	0	40	0	0
30	C	96	0	132	2	0
30	D	83	0	117	3	0
30	M	51	0	72	0	0
30	a	55	0	86	5	0
30	b	106	0	158	2	0
30	c	134	0	181	2	0
30	d	44	0	58	0	0
31	B	49	0	74	2	0
31	D	96	0	140	1	0
31	E	49	0	74	1	0
31	L	49	0	74	0	0
31	a	91	0	131	4	0
31	d	88	0	125	6	0
31	l	49	0	74	1	0
32	D	4	0	1	0	0
32	a	4	0	1	0	0
33	D	128	0	148	5	0
33	a	64	0	74	0	0
33	d	64	0	74	2	0
34	F	43	0	32	6	0
34	V	43	0	30	2	0
34	f	43	0	32	9	0
34	v	43	0	30	0	0
35	A	137	0	0	5	0
35	B	234	0	0	2	1
35	C	167	0	0	0	1
35	D	116	0	0	1	0
35	E	37	0	0	2	0
35	F	10	0	0	0	0
35	H	34	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	I	20	0	0	0	0
35	J	14	0	0	6	0
35	K	3	0	0	2	0
35	L	10	0	0	0	0
35	M	8	0	0	0	0
35	O	105	0	0	6	0
35	R	3	0	0	0	0
35	T	9	0	0	1	0
35	U	52	0	0	5	0
35	V	64	0	0	3	0
35	X	17	0	0	0	0
35	Y	3	0	0	0	0
35	a	121	0	0	2	0
35	b	194	0	0	9	0
35	c	169	0	0	7	0
35	d	108	0	0	2	0
35	e	22	0	0	2	0
35	f	5	0	0	1	0
35	h	22	0	0	0	0
35	i	17	0	0	0	0
35	j	7	0	0	3	0
35	k	4	0	0	1	0
35	l	11	0	0	0	0
35	m	6	0	0	2	0
35	o	98	0	0	2	0
35	r	8	0	0	1	0
35	t	7	0	0	0	0
35	u	64	0	0	1	0
35	v	63	0	0	3	0
35	x	7	0	0	0	0
35	y	9	0	0	1	0
35	z	9	0	0	0	0
All	All	52261	0	51722	859	4

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 8.

The worst 5 of 859 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:194:LYS:CD	13:O:194:LYS:CG	1.75	1.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:127:ARG:CD	2:B:127:ARG:CG	1.75	1.61
3:c:104:GLU:CB	3:c:104:GLU:CG	1.76	1.60
2:B:127:ARG:CG	2:B:127:ARG:CB	1.81	1.57
10:K:10:LYS:CE	10:K:10:LYS:CD	1.77	1.57

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:462:GLU:OE1	7:H:3:ARG:NH2[4_557]	2.07	0.13
35:B:1027:HOH:O	35:C:762:HOH:O[1_455]	2.14	0.06
3:C:462:GLU:OE1	7:H:3:ARG:CZ[4_557]	2.17	0.03
3:C:462:GLU:OE1	7:H:3:ARG:NH1[4_557]	2.19	0.01

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	332/344 (96%)	323 (97%)	9 (3%)	0	100	100
1	a	332/344 (96%)	326 (98%)	5 (2%)	1 (0%)	36	36
2	B	507/510 (99%)	499 (98%)	8 (2%)	0	100	100
2	b	503/510 (99%)	490 (97%)	12 (2%)	1 (0%)	43	44
3	C	441/461 (96%)	428 (97%)	12 (3%)	1 (0%)	43	44
3	c	451/461 (98%)	433 (96%)	16 (4%)	2 (0%)	30	28
4	D	339/352 (96%)	332 (98%)	7 (2%)	0	100	100
4	d	340/352 (97%)	330 (97%)	10 (3%)	0	100	100
5	E	81/84 (96%)	79 (98%)	2 (2%)	0	100	100
5	e	80/84 (95%)	75 (94%)	5 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	32/45 (71%)	32 (100%)	0	0	100	100
6	f	32/45 (71%)	31 (97%)	1 (3%)	0	100	100
7	H	63/66 (96%)	59 (94%)	3 (5%)	1 (2%)	7	4
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%)	33 (97%)	1 (3%)	0	100	100
9	j	34/40 (85%)	33 (97%)	1 (3%)	0	100	100
10	K	35/46 (76%)	33 (94%)	1 (3%)	1 (3%)	3	1
10	k	35/46 (76%)	35 (100%)	0	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	34/37 (92%)	34 (100%)	0	0	100	100
12	M	31/36 (86%)	31 (100%)	0	0	100	100
12	m	30/36 (83%)	28 (93%)	2 (7%)	0	100	100
13	O	243/272 (89%)	230 (95%)	10 (4%)	3 (1%)	10	7
13	o	242/272 (89%)	227 (94%)	13 (5%)	2 (1%)	16	12
14	R	32/41 (78%)	25 (78%)	6 (19%)	1 (3%)	3	1
14	r	29/41 (71%)	26 (90%)	2 (7%)	1 (3%)	3	1
15	T	28/32 (88%)	28 (100%)	0	0	100	100
15	t	28/32 (88%)	28 (100%)	0	0	100	100
16	U	95/134 (71%)	92 (97%)	3 (3%)	0	100	100
16	u	95/134 (71%)	91 (96%)	3 (3%)	1 (1%)	11	8
17	V	135/163 (83%)	128 (95%)	6 (4%)	1 (1%)	18	15
17	v	135/163 (83%)	130 (96%)	5 (4%)	0	100	100
18	X	36/41 (88%)	35 (97%)	1 (3%)	0	100	100
18	x	37/41 (90%)	36 (97%)	1 (3%)	0	100	100
19	Y	25/46 (54%)	23 (92%)	1 (4%)	1 (4%)	2	0
19	y	28/46 (61%)	25 (89%)	1 (4%)	2 (7%)	1	0
20	Z	60/62 (97%)	55 (92%)	5 (8%)	0	100	100
20	z	60/62 (97%)	54 (90%)	5 (8%)	1 (2%)	7	3
All	All	5238/5700 (92%)	5054 (96%)	164 (3%)	20 (0%)	30	28

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
10	K	16	ALA
13	O	59	LYS
13	O	62	GLU
17	V	64	PRO

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	270/280 (96%)	269 (100%)	1 (0%)	84	89
1	a	269/280 (96%)	268 (100%)	1 (0%)	84	89
2	B	407/407 (100%)	407 (100%)	0	100	100
2	b	402/407 (99%)	401 (100%)	1 (0%)	87	93
3	C	345/362 (95%)	345 (100%)	0	100	100
3	c	354/362 (98%)	354 (100%)	0	100	100
4	D	276/283 (98%)	276 (100%)	0	100	100
4	d	277/283 (98%)	277 (100%)	0	100	100
5	E	72/73 (99%)	70 (97%)	2 (3%)	38	43
5	e	71/73 (97%)	71 (100%)	0	100	100
6	F	28/39 (72%)	28 (100%)	0	100	100
6	f	28/39 (72%)	28 (100%)	0	100	100
7	H	54/55 (98%)	54 (100%)	0	100	100
7	h	53/55 (96%)	52 (98%)	1 (2%)	50	58
8	I	32/34 (94%)	32 (100%)	0	100	100
8	i	32/34 (94%)	32 (100%)	0	100	100
9	J	24/28 (86%)	24 (100%)	0	100	100
9	j	24/28 (86%)	24 (100%)	0	100	100
10	K	30/37 (81%)	30 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	k	30/37 (81%)	29 (97%)	1 (3%)	33	37
11	L	35/35 (100%)	35 (100%)	0	100	100
11	l	34/35 (97%)	33 (97%)	1 (3%)	37	42
12	M	28/32 (88%)	28 (100%)	0	100	100
12	m	28/32 (88%)	26 (93%)	2 (7%)	13	11
13	O	206/228 (90%)	205 (100%)	1 (0%)	81	88
13	o	207/228 (91%)	206 (100%)	1 (0%)	81	88
14	R	28/33 (85%)	28 (100%)	0	100	100
14	r	23/33 (70%)	21 (91%)	2 (9%)	9	7
15	T	26/28 (93%)	26 (100%)	0	100	100
15	t	25/28 (89%)	25 (100%)	0	100	100
16	U	84/112 (75%)	83 (99%)	1 (1%)	63	72
16	u	84/112 (75%)	84 (100%)	0	100	100
17	V	117/138 (85%)	116 (99%)	1 (1%)	70	78
17	v	117/138 (85%)	116 (99%)	1 (1%)	70	78
18	X	31/34 (91%)	31 (100%)	0	100	100
18	x	31/34 (91%)	31 (100%)	0	100	100
19	Y	19/37 (51%)	19 (100%)	0	100	100
19	y	22/37 (60%)	22 (100%)	0	100	100
20	Z	52/52 (100%)	51 (98%)	1 (2%)	50	58
20	z	51/52 (98%)	51 (100%)	0	100	100
All	All	4326/4654 (93%)	4308 (100%)	18 (0%)	84	89

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	o	49	THR
17	v	107	LEU
14	r	24	LEU
2	b	246	PHE
12	m	16	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
14	r	30	GLN
16	u	78	ASN
18	x	33	GLN
12	M	32	GLN
5	E	82	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
12	FME	m	1	12	8,9,10	0.96	0	8,9,11	1.56	2 (25%)
12	FME	M	1	12	8,9,10	0.97	0	8,9,11	0.72	0
8	FME	i	1	8	8,9,10	1.01	1 (12%)	8,9,11	1.94	3 (37%)
8	FME	I	1	8	8,9,10	0.81	0	8,9,11	1.07	0
15	FME	t	1	15	8,9,10	1.53	1 (12%)	8,9,11	1.03	1 (12%)
15	FME	T	1	15	8,9,10	1.19	1 (12%)	8,9,11	1.50	2 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	FME	m	1	12	-	0/7/9/11	-
12	FME	M	1	12	-	1/7/9/11	-
8	FME	i	1	8	-	1/7/9/11	-
8	FME	I	1	8	-	1/7/9/11	-
15	FME	t	1	15	-	1/7/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	FME	T	1	15	-	3/7/9/11	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	t	1	FME	CA-N	-3.04	1.42	1.46
15	T	1	FME	CB-CA	2.45	1.58	1.53
8	i	1	FME	CA-N	-2.08	1.43	1.46

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	i	1	FME	CA-N-CN	-3.90	116.83	122.82
15	T	1	FME	C-CA-N	3.15	115.58	109.50
15	t	1	FME	CB-CA-N	2.63	115.30	110.52
12	m	1	FME	CA-N-CN	-2.39	119.14	122.82
12	m	1	FME	C-CA-N	-2.38	104.90	109.50

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	t	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 192 ligands modelled in this entry, 6 are monoatomic - leaving 186 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$
23	BCR	c	516	-	41,41,41	1.46	4 (9%)	56,56,56	1.59	14 (25%)
33	PHO	a	404	-	58,69,69	2.08	10 (17%)	55,99,99	1.74	14 (25%)
23	BCR	C	515	-	41,41,41	1.48	8 (19%)	56,56,56	1.34	6 (10%)
30	LMG	c	522	-	48,48,55	1.51	6 (12%)	56,56,63	1.31	11 (19%)
28	STE	x	101	-	19,19,19	0.79	0	19,19,19	0.77	1 (5%)
22	CLA	C	511	-	69,73,73	1.25	9 (13%)	82,113,113	1.17	6 (7%)
31	LHG	E	101	-	48,48,48	0.89	3 (6%)	51,54,54	1.26	6 (11%)
22	CLA	B	710	35	69,73,73	1.36	10 (14%)	82,113,113	1.51	12 (14%)
22	CLA	C	510	3	69,73,73	1.33	12 (17%)	82,113,113	1.57	17 (20%)
27	DGD	C	518	-	63,63,67	1.50	11 (17%)	77,77,81	1.61	14 (18%)
30	LMG	M	101	-	51,51,55	1.11	3 (5%)	59,59,63	1.50	11 (18%)
23	BCR	B	717	-	41,41,41	1.38	4 (9%)	56,56,56	1.32	5 (8%)
22	CLA	A	402	1	69,73,73	1.31	10 (14%)	82,113,113	1.32	9 (10%)
26	SQD	A	409	-	50,52,54	1.05	5 (10%)	60,63,65	2.09	16 (26%)
22	CLA	b	616	2	64,68,73	1.23	9 (14%)	76,107,113	1.41	9 (11%)
26	SQD	A	410	-	38,38,54	1.03	3 (7%)	40,40,65	1.28	4 (10%)
33	PHO	D	407	-	58,69,69	1.73	10 (17%)	55,99,99	1.65	12 (21%)
23	BCR	C	501	-	41,41,41	1.28	5 (12%)	56,56,56	1.15	3 (5%)
23	BCR	A	405	-	41,41,41	1.37	3 (7%)	56,56,56	1.55	13 (23%)
28	STE	M	102	-	14,14,19	0.75	0	14,14,19	1.02	0
23	BCR	t	701	-	41,41,41	1.23	4 (9%)	56,56,56	1.43	8 (14%)
26	SQD	a	412	-	52,54,54	1.01	5 (9%)	62,65,65	1.95	13 (20%)
28	STE	H	103	-	17,17,19	0.54	0	16,16,19	0.53	0
22	CLA	B	705	2	69,73,73	1.36	9 (13%)	82,113,113	1.62	12 (14%)
25	PL9	A	408	-	55,55,55	1.16	2 (3%)	68,69,69	1.64	15 (22%)
28	STE	h	704	-	13,13,19	0.45	0	12,12,19	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	SQD	l	101	-	47,49,54	1.10	3 (6%)	57,60,65	2.39	15 (26%)
29	OEX	a	419[A]	3,1,35	0,15,15	-	-	-		
27	DGD	h	703	-	63,63,67	1.30	9 (14%)	77,77,81	1.69	17 (22%)
30	LMG	a	418	-	55,55,55	1.50	8 (14%)	63,63,63	1.29	4 (6%)
22	CLA	A	403	35	69,73,73	1.28	6 (8%)	82,113,113	1.50	16 (19%)
22	CLA	B	727	35	69,73,73	1.43	13 (18%)	82,113,113	1.38	10 (12%)
22	CLA	C	507	3	69,73,73	1.20	9 (13%)	82,113,113	1.36	11 (13%)
22	CLA	c	504	3	69,73,73	1.13	6 (8%)	82,113,113	1.69	10 (12%)
23	BCR	D	405	-	41,41,41	1.32	5 (12%)	56,56,56	1.31	5 (8%)
25	PL9	D	406	-	55,55,55	1.49	8 (14%)	68,69,69	1.71	15 (22%)
28	STE	b	623	-	15,15,19	0.88	1 (6%)	15,15,19	0.91	1 (6%)
28	STE	d	411	-	16,16,19	0.78	0	16,16,19	1.35	2 (12%)
22	CLA	c	509	3	68,72,73	1.26	9 (13%)	80,111,113	1.74	17 (21%)
27	DGD	H	102	-	63,63,67	1.52	11 (17%)	77,77,81	1.54	16 (20%)
22	CLA	C	506	3	69,73,73	1.18	9 (13%)	82,113,113	1.42	8 (9%)
22	CLA	B	716	2	64,68,73	1.27	8 (12%)	76,107,113	1.35	11 (14%)
22	CLA	b	610	35	69,73,73	1.31	10 (14%)	82,113,113	1.48	12 (14%)
31	LHG	B	722	-	48,48,48	1.13	3 (6%)	51,54,54	1.45	7 (13%)
22	CLA	B	707	35	69,73,73	1.41	13 (18%)	82,113,113	1.34	7 (8%)
22	CLA	c	514	3	69,73,73	1.15	9 (13%)	82,113,113	1.53	10 (12%)
28	STE	C	522	-	15,15,19	0.47	0	14,14,19	0.78	0
26	SQD	D	410	-	34,36,54	1.09	3 (8%)	42,45,65	1.96	11 (26%)
31	LHG	D	412	-	46,46,48	1.30	6 (13%)	49,52,54	1.35	4 (8%)
28	STE	m	101	-	17,17,19	0.50	0	16,16,19	0.63	0
32	BCT	a	409	21	3,3,3	0.93	0	2,3,3	3.97	2 (100%)
27	DGD	c	518	-	63,63,67	1.27	9 (14%)	77,77,81	1.51	14 (18%)
30	LMG	C	516	-	48,48,55	1.26	7 (14%)	56,56,63	1.45	5 (8%)
30	LMG	D	413	-	31,31,55	1.69	4 (12%)	33,33,63	1.09	1 (3%)
31	LHG	L	101	-	48,48,48	0.98	4 (8%)	51,54,54	1.35	6 (11%)
22	CLA	B	714	2	69,73,73	1.19	12 (17%)	82,113,113	1.28	11 (13%)
22	CLA	C	502	3	69,73,73	1.19	8 (11%)	82,113,113	1.48	10 (12%)
23	BCR	b	617	-	41,41,41	1.39	4 (9%)	56,56,56	1.61	14 (25%)
28	STE	B	724	-	11,11,19	0.80	0	11,11,19	1.19	2 (18%)
22	CLA	c	512	3	69,73,73	1.35	11 (15%)	82,113,113	1.33	7 (8%)
22	CLA	b	612	2	69,73,73	1.11	5 (7%)	82,113,113	1.45	9 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	LHG	a	413	-	41,41,48	0.86	1 (2%)	44,47,54	1.27	3 (6%)
22	CLA	C	503	3	69,73,73	1.18	8 (11%)	82,113,113	1.24	8 (9%)
31	LHG	D	411	-	48,48,48	1.05	3 (6%)	51,54,54	1.27	6 (11%)
22	CLA	B	709	2	69,73,73	1.22	7 (10%)	82,113,113	1.36	7 (8%)
22	CLA	a	405	1	69,73,73	1.43	12 (17%)	82,113,113	1.34	7 (8%)
22	CLA	C	512	3	69,73,73	1.27	9 (13%)	82,113,113	1.08	4 (4%)
30	LMG	D	409	-	51,51,55	1.29	5 (9%)	59,59,63	1.37	7 (11%)
22	CLA	b	613	2	69,73,73	1.31	12 (17%)	82,113,113	1.56	14 (17%)
26	SQD	a	414	-	35,35,54	1.18	2 (5%)	37,37,65	1.40	5 (13%)
31	LHG	a	411	-	48,48,48	0.91	1 (2%)	51,54,54	1.47	6 (11%)
28	STE	m	102	-	11,11,19	0.78	0	11,11,19	1.56	2 (18%)
34	HEC	v	201	17	46,50,50	1.92	6 (13%)	58,82,82	1.84	6 (10%)
22	CLA	B	712	2	69,73,73	1.18	8 (11%)	82,113,113	1.54	11 (13%)
30	LMG	C	520	-	48,48,55	1.27	6 (12%)	56,56,63	1.47	10 (17%)
29	OEX	A	413[A]	3,1,35	0,15,15	-	-	-	-	-
22	CLA	c	502	3	69,73,73	1.18	9 (13%)	82,113,113	1.56	10 (12%)
28	STE	b	624	-	19,19,19	0.79	0	19,19,19	0.96	1 (5%)
33	PHO	d	407	-	58,69,69	2.09	12 (20%)	55,99,99	1.71	11 (20%)
23	BCR	h	702	-	41,41,41	1.24	4 (9%)	56,56,56	1.28	7 (12%)
22	CLA	b	614	2	69,73,73	1.30	11 (15%)	82,113,113	1.53	8 (9%)
22	CLA	c	510	3	69,73,73	1.22	6 (8%)	82,113,113	1.80	8 (9%)
28	STE	B	726	-	15,15,19	0.48	0	14,14,19	0.58	0
28	STE	a	417	-	14,14,19	0.45	0	13,13,19	0.71	0
22	CLA	B	711	2	69,73,73	1.28	8 (11%)	82,113,113	1.33	12 (14%)
30	LMG	b	620	-	51,51,55	1.19	5 (9%)	59,59,63	1.58	11 (18%)
22	CLA	b	603	2	69,73,73	1.27	9 (13%)	82,113,113	1.56	15 (18%)
23	BCR	d	405	-	41,41,41	1.30	5 (12%)	56,56,56	1.40	12 (21%)
27	DGD	A	411	-	67,67,67	1.47	9 (13%)	81,81,81	1.69	18 (22%)
23	BCR	k	101	-	41,41,41	1.26	4 (9%)	56,56,56	1.17	6 (10%)
23	BCR	c	515	-	41,41,41	1.43	5 (12%)	56,56,56	1.31	8 (14%)
22	CLA	c	513	3	69,73,73	1.22	11 (15%)	82,113,113	1.52	11 (13%)
28	STE	J	101	-	11,11,19	0.66	0	11,11,19	1.54	2 (18%)
28	STE	c	521	-	19,19,19	0.71	0	19,19,19	0.94	1 (5%)
22	CLA	C	505	35	63,67,73	1.29	7 (11%)	74,105,113	1.30	7 (9%)
28	STE	B	725	-	17,17,19	0.75	0	17,17,19	0.85	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	PL9	d	406	-	55,55,55	1.61	8 (14%)	68,69,69	1.74	16 (23%)
26	SQD	f	102	-	39,41,54	1.19	4 (10%)	49,52,65	1.74	11 (22%)
22	CLA	d	401	35	69,73,73	1.27	7 (10%)	82,113,113	1.53	14 (17%)
30	LMG	B	721	-	26,26,55	0.84	2 (7%)	26,26,63	1.35	2 (7%)
25	PL9	a	410	-	55,55,55	0.93	3 (5%)	68,69,69	1.70	15 (22%)
28	STE	H	104	-	7,7,19	0.43	0	6,6,19	0.55	0
22	CLA	d	403	4	69,73,73	1.21	7 (10%)	82,113,113	1.32	9 (10%)
22	CLA	B	713	2	69,73,73	1.15	7 (10%)	82,113,113	1.48	12 (14%)
22	CLA	h	701	35	69,73,73	1.39	9 (13%)	82,113,113	1.41	8 (9%)
23	BCR	b	619	-	41,41,41	1.33	4 (9%)	56,56,56	1.41	10 (17%)
23	BCR	b	618	-	41,41,41	1.42	4 (9%)	56,56,56	1.34	8 (14%)
22	CLA	C	508	35	69,73,73	1.24	12 (17%)	82,113,113	1.54	10 (12%)
23	BCR	C	524	-	41,41,41	1.34	4 (9%)	56,56,56	1.58	15 (26%)
28	STE	X	101	-	19,19,19	0.56	0	19,19,19	1.26	3 (15%)
28	STE	A	412	-	4,4,19	0.52	0	3,3,19	0.41	0
28	STE	c	501	-	11,11,19	0.80	0	11,11,19	1.06	1 (9%)
27	DGD	C	517	-	63,63,67	1.34	7 (11%)	77,77,81	1.36	11 (14%)
28	STE	C	523	-	11,11,19	0.81	0	11,11,19	1.03	1 (9%)
22	CLA	c	506	3	69,73,73	1.17	9 (13%)	82,113,113	1.37	6 (7%)
22	CLA	a	403	35	69,73,73	1.31	9 (13%)	82,113,113	1.60	11 (13%)
23	BCR	B	719	-	41,41,41	1.45	8 (19%)	56,56,56	1.55	11 (19%)
28	STE	E	103	-	6,6,19	0.43	0	5,5,19	0.52	0
22	CLA	b	605	2	69,73,73	1.20	7 (10%)	82,113,113	1.51	13 (15%)
22	CLA	b	604	2	69,73,73	1.31	9 (13%)	82,113,113	1.68	10 (12%)
34	HEC	V	201	17	46,50,50	1.82	7 (15%)	58,82,82	2.18	9 (15%)
34	HEC	f	101	5,6	46,50,50	1.86	7 (15%)	58,82,82	2.03	7 (12%)
22	CLA	D	404	4	69,73,73	1.35	14 (20%)	82,113,113	1.61	10 (12%)
28	STE	B	701	-	11,11,19	1.04	0	11,11,19	0.97	1 (9%)
22	CLA	B	708	2	69,73,73	1.31	10 (14%)	82,113,113	1.72	15 (18%)
31	LHG	d	408	-	48,48,48	0.78	0	51,54,54	1.17	5 (9%)
23	BCR	a	406	-	41,41,41	1.35	4 (9%)	56,56,56	1.57	13 (23%)
31	LHG	l	102	-	48,48,48	0.86	2 (4%)	51,54,54	1.16	6 (11%)
22	CLA	b	608	2	69,73,73	1.28	11 (15%)	82,113,113	1.61	12 (14%)
30	LMG	c	523	-	49,49,55	1.16	5 (10%)	57,57,63	1.34	9 (15%)
33	PHO	D	408	-	58,69,69	1.95	13 (22%)	55,99,99	1.80	12 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	C	504	3	69,73,73	1.30	10 (14%)	82,113,113	1.47	16 (19%)
30	LMG	c	520	-	37,37,55	1.45	6 (16%)	45,45,63	1.45	6 (13%)
22	CLA	B	715	2	69,73,73	1.37	10 (14%)	82,113,113	1.40	12 (14%)
23	BCR	T	701	-	41,41,41	1.27	6 (14%)	56,56,56	1.39	8 (14%)
32	BCT	D	401	21	3,3,3	0.81	0	2,3,3	5.42	2 (100%)
22	CLA	d	404	4	69,73,73	1.29	10 (14%)	82,113,113	1.34	9 (10%)
28	STE	t	702	-	13,13,19	0.57	0	13,13,19	1.33	2 (15%)
28	STE	C	521	-	11,11,19	0.91	0	11,11,19	1.46	3 (27%)
30	LMG	d	410	-	44,44,55	1.43	6 (13%)	52,52,63	1.56	8 (15%)
22	CLA	B	706	2	69,73,73	1.15	8 (11%)	82,113,113	1.51	7 (8%)
28	STE	a	415	-	9,9,19	0.57	0	8,8,19	0.38	0
28	STE	b	621	-	19,19,19	0.61	0	19,19,19	0.86	1 (5%)
22	CLA	c	511	3	69,73,73	1.16	6 (8%)	82,113,113	1.53	12 (14%)
23	BCR	B	718	-	41,41,41	1.37	5 (12%)	56,56,56	1.61	11 (19%)
28	STE	j	101	-	11,11,19	0.77	0	11,11,19	1.60	3 (27%)
22	CLA	B	704	2	69,73,73	1.18	7 (10%)	82,113,113	1.58	15 (18%)
22	CLA	C	514	3	69,73,73	1.27	8 (11%)	82,113,113	1.57	10 (12%)
22	CLA	c	503	3	69,73,73	1.20	9 (13%)	82,113,113	1.43	8 (9%)
26	SQD	B	723	-	52,54,54	1.00	3 (5%)	62,65,65	1.88	12 (19%)
28	STE	b	601	-	15,15,19	0.49	0	14,14,19	0.67	0
28	STE	E	102	-	11,11,19	0.94	0	11,11,19	0.77	0
22	CLA	a	402	1	69,73,73	1.28	9 (13%)	82,113,113	1.53	17 (20%)
22	CLA	b	602	2	69,73,73	1.19	7 (10%)	82,113,113	1.71	16 (19%)
27	DGD	c	519	-	63,63,67	1.32	8 (12%)	77,77,81	1.57	16 (20%)
22	CLA	C	509	3	69,73,73	1.24	9 (13%)	82,113,113	1.36	9 (10%)
22	CLA	D	402	4	69,73,73	1.27	9 (13%)	82,113,113	1.39	11 (13%)
23	BCR	Y	101	-	41,41,41	1.16	3 (7%)	56,56,56	1.26	5 (8%)
28	STE	Z	101	-	7,7,19	0.38	0	6,6,19	0.47	0
22	CLA	b	615	2	69,73,73	1.25	9 (13%)	82,113,113	1.35	10 (12%)
22	CLA	A	404	1	58,62,73	1.36	6 (10%)	68,99,113	1.66	11 (16%)
22	CLA	b	607	35	69,73,73	1.27	10 (14%)	82,113,113	1.44	13 (15%)
22	CLA	B	703	2	69,73,73	1.16	7 (10%)	82,113,113	1.55	9 (10%)
34	HEC	F	101	5,6	46,50,50	1.90	7 (15%)	58,82,82	1.95	7 (12%)
22	CLA	B	702	2	69,73,73	1.39	10 (14%)	82,113,113	1.48	15 (18%)
22	CLA	b	606	2	69,73,73	1.26	7 (10%)	82,113,113	1.61	15 (18%)
28	STE	T	702	-	14,14,19	0.48	0	13,13,19	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	STE	b	625	-	9,9,19	0.59	0	8,8,19	0.33	0
27	DGD	C	519	-	63,63,67	1.07	4 (6%)	77,77,81	1.44	10 (12%)
23	BCR	H	101	-	41,41,41	1.29	6 (14%)	56,56,56	1.40	10 (17%)
28	STE	M	103	-	9,9,19	0.51	0	8,8,19	0.55	0
28	STE	d	402	-	19,19,19	0.53	0	19,19,19	1.14	1 (5%)
28	STE	a	416	-	11,11,19	0.90	1 (9%)	11,11,19	0.88	0
22	CLA	c	508	35	69,73,73	1.21	8 (11%)	82,113,113	1.50	10 (12%)
22	CLA	c	505	35	64,68,73	1.33	10 (15%)	76,107,113	1.50	13 (17%)
22	CLA	D	403	35	69,73,73	1.30	8 (11%)	82,113,113	1.34	8 (9%)
28	STE	I	101	-	14,14,19	0.66	0	13,13,19	0.35	0
31	LHG	d	409	-	38,38,48	1.07	3 (7%)	41,44,54	1.14	2 (4%)
22	CLA	b	609	-	69,73,73	1.19	7 (10%)	82,113,113	1.53	13 (15%)
27	DGD	c	517	-	63,63,67	1.36	10 (15%)	77,77,81	1.45	10 (12%)
28	STE	B	720	-	16,16,19	0.66	0	16,16,19	1.39	2 (12%)
30	LMG	b	622	-	55,55,55	1.43	8 (14%)	63,63,63	1.55	12 (19%)
22	CLA	b	611	2	69,73,73	1.21	11 (15%)	82,113,113	1.52	13 (15%)
22	CLA	C	513	3	69,73,73	1.26	11 (15%)	82,113,113	1.49	14 (17%)
23	BCR	k	102	-	41,41,41	1.25	6 (14%)	56,56,56	1.18	4 (7%)
22	CLA	c	507	3	69,73,73	1.22	10 (14%)	82,113,113	1.53	10 (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
23	BCR	c	516	-	-	4/29/63/63	0/2/2/2
33	PHO	a	404	-	-	5/37/103/103	0/5/6/6
23	BCR	C	515	-	-	7/29/63/63	0/2/2/2
30	LMG	c	522	-	-	25/43/63/70	0/1/1/1
28	STE	x	101	-	-	11/17/17/17	-
22	CLA	C	511	-	-	10/39/115/115	-
31	LHG	E	101	-	-	27/53/53/53	-
22	CLA	B	710	35	1/1/15/20	5/39/115/115	-
22	CLA	C	510	3	1/1/15/20	13/39/115/115	-
27	DGD	C	518	-	-	14/51/91/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	LMG	M	101	-	-	24/46/66/70	0/1/1/1
23	BCR	B	717	-	-	7/29/63/63	0/2/2/2
22	CLA	A	402	1	1/1/15/20	7/39/115/115	-
26	SQD	A	409	-	-	22/47/67/69	0/1/1/1
22	CLA	b	616	2	1/1/14/20	11/33/109/115	-
26	SQD	A	410	-	-	15/39/39/69	-
33	PHO	D	407	-	-	6/37/103/103	0/5/6/6
23	BCR	C	501	-	-	13/29/63/63	0/2/2/2
23	BCR	A	405	-	-	8/29/63/63	0/2/2/2
28	STE	M	102	-	-	5/12/12/17	-
23	BCR	t	701	-	-	7/29/63/63	0/2/2/2
26	SQD	a	412	-	-	24/49/69/69	0/1/1/1
28	STE	H	103	-	-	6/15/15/17	-
22	CLA	B	705	2	1/1/15/20	8/39/115/115	-
25	PL9	A	408	-	-	25/53/73/73	0/1/1/1
28	STE	h	704	-	-	6/11/11/17	-
26	SQD	l	101	-	-	21/44/64/69	0/1/1/1
27	DGD	h	703	-	-	15/51/91/95	0/2/2/2
30	LMG	a	418	-	-	25/50/70/70	0/1/1/1
22	CLA	A	403	35	-	10/39/115/115	-
22	CLA	B	727	35	1/1/15/20	13/39/115/115	-
22	CLA	C	507	3	1/1/15/20	8/39/115/115	-
22	CLA	c	504	3	1/1/15/20	8/39/115/115	-
23	BCR	D	405	-	-	9/29/63/63	0/2/2/2
25	PL9	D	406	-	-	12/53/73/73	0/1/1/1
28	STE	b	623	-	-	11/13/13/17	-
28	STE	d	411	-	-	4/14/14/17	-
22	CLA	c	509	3	1/1/14/20	5/38/114/115	-
27	DGD	H	102	-	-	18/51/91/95	0/2/2/2
22	CLA	C	506	3	1/1/15/20	12/39/115/115	-
22	CLA	B	716	2	1/1/14/20	10/33/109/115	-
22	CLA	b	610	35	1/1/15/20	4/39/115/115	-
31	LHG	B	722	-	-	18/53/53/53	-
22	CLA	B	707	35	1/1/15/20	4/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	c	514	3	1/1/15/20	8/39/115/115	-
28	STE	C	522	-	-	2/13/13/17	-
26	SQD	D	410	-	-	7/28/48/69	0/1/1/1
31	LHG	D	412	-	-	24/51/51/53	-
28	STE	m	101	-	-	5/15/15/17	-
27	DGD	c	518	-	-	23/51/91/95	0/2/2/2
30	LMG	C	516	-	-	18/43/63/70	0/1/1/1
30	LMG	D	413	-	-	14/33/33/70	-
31	LHG	L	101	-	-	20/53/53/53	-
22	CLA	B	714	2	1/1/15/20	10/39/115/115	-
22	CLA	C	502	3	1/1/15/20	3/39/115/115	-
23	BCR	b	617	-	-	10/29/63/63	0/2/2/2
28	STE	B	724	-	-	4/9/9/17	-
22	CLA	c	512	3	1/1/15/20	12/39/115/115	-
22	CLA	b	612	2	1/1/15/20	4/39/115/115	-
31	LHG	a	413	-	-	19/46/46/53	-
22	CLA	C	503	3	1/1/15/20	9/39/115/115	-
31	LHG	D	411	-	-	17/53/53/53	-
22	CLA	B	709	2	-	3/39/115/115	-
22	CLA	a	405	1	1/1/15/20	11/39/115/115	-
22	CLA	C	512	3	1/1/15/20	3/39/115/115	-
30	LMG	D	409	-	-	16/46/66/70	0/1/1/1
22	CLA	b	613	2	1/1/15/20	5/39/115/115	-
26	SQD	a	414	-	-	19/37/37/69	-
31	LHG	a	411	-	-	25/53/53/53	-
28	STE	m	102	-	-	2/9/9/17	-
34	HEC	v	201	17	-	6/14/54/54	-
22	CLA	B	712	2	1/1/15/20	9/39/115/115	-
30	LMG	C	520	-	-	19/43/63/70	0/1/1/1
22	CLA	c	502	3	1/1/15/20	3/39/115/115	-
28	STE	b	624	-	-	8/17/17/17	-
33	PHO	d	407	-	-	5/37/103/103	0/5/6/6
23	BCR	h	702	-	-	5/29/63/63	0/2/2/2
22	CLA	b	614	2	1/1/15/20	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	c	510	3	1/1/15/20	10/39/115/115	-
28	STE	B	726	-	-	5/13/13/17	-
28	STE	a	417	-	-	4/12/12/17	-
22	CLA	B	711	2	1/1/15/20	8/39/115/115	-
30	LMG	b	620	-	-	15/46/66/70	0/1/1/1
22	CLA	b	603	2	1/1/15/20	8/39/115/115	-
23	BCR	d	405	-	-	10/29/63/63	0/2/2/2
27	DGD	A	411	-	-	25/55/95/95	0/2/2/2
23	BCR	k	101	-	-	13/29/63/63	0/2/2/2
23	BCR	c	515	-	-	10/29/63/63	0/2/2/2
22	CLA	c	513	3	1/1/15/20	21/39/115/115	-
28	STE	J	101	-	-	3/9/9/17	-
28	STE	c	521	-	-	7/17/17/17	-
22	CLA	C	505	35	1/1/13/20	4/32/108/115	-
28	STE	B	725	-	-	6/15/15/17	-
25	PL9	d	406	-	-	18/53/73/73	0/1/1/1
26	SQD	f	102	-	-	14/36/56/69	0/1/1/1
22	CLA	d	401	35	1/1/15/20	5/39/115/115	-
30	LMG	B	721	-	-	12/22/22/70	-
25	PL9	a	410	-	-	20/53/73/73	0/1/1/1
28	STE	H	104	-	-	3/5/5/17	-
22	CLA	d	403	4	1/1/15/20	10/39/115/115	-
22	CLA	B	713	2	1/1/15/20	13/39/115/115	-
22	CLA	h	701	35	1/1/15/20	11/39/115/115	-
23	BCR	b	619	-	-	6/29/63/63	0/2/2/2
23	BCR	b	618	-	-	1/29/63/63	0/2/2/2
22	CLA	C	508	35	1/1/15/20	9/39/115/115	-
23	BCR	C	524	-	-	8/29/63/63	0/2/2/2
28	STE	X	101	-	-	9/17/17/17	-
28	STE	A	412	-	-	1/2/2/17	-
28	STE	c	501	-	-	2/9/9/17	-
27	DGD	C	517	-	-	21/51/91/95	0/2/2/2
28	STE	C	523	-	-	6/9/9/17	-
22	CLA	c	506	3	1/1/15/20	11/39/115/115	-
22	CLA	a	403	35	1/1/15/20	1/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	BCR	B	719	-	-	1/29/63/63	0/2/2/2
28	STE	E	103	-	-	1/4/4/17	-
22	CLA	b	605	2	1/1/15/20	13/39/115/115	-
22	CLA	b	604	2	1/1/15/20	8/39/115/115	-
34	HEC	V	201	17	-	6/14/54/54	-
34	HEC	f	101	5,6	-	6/14/54/54	-
22	CLA	D	404	4	1/1/15/20	7/39/115/115	-
28	STE	B	701	-	-	3/9/9/17	-
22	CLA	B	708	2	1/1/15/20	2/39/115/115	-
31	LHG	d	408	-	-	14/53/53/53	-
23	BCR	a	406	-	-	3/29/63/63	0/2/2/2
31	LHG	l	102	-	-	24/53/53/53	-
22	CLA	b	608	2	1/1/15/20	7/39/115/115	-
30	LMG	c	523	-	-	20/44/64/70	0/1/1/1
33	PHO	D	408	-	-	2/37/103/103	0/5/6/6
22	CLA	C	504	3	1/1/15/20	8/39/115/115	-
30	LMG	c	520	-	-	12/31/51/70	0/1/1/1
22	CLA	B	715	2	1/1/15/20	7/39/115/115	-
23	BCR	T	701	-	-	3/29/63/63	0/2/2/2
22	CLA	d	404	4	1/1/15/20	9/39/115/115	-
28	STE	t	702	-	-	4/11/11/17	-
28	STE	C	521	-	-	2/9/9/17	-
30	LMG	d	410	-	-	12/39/59/70	0/1/1/1
22	CLA	B	706	2	1/1/15/20	6/39/115/115	-
28	STE	a	415	-	-	4/7/7/17	-
28	STE	b	621	-	-	10/17/17/17	-
22	CLA	c	511	3	1/1/15/20	9/39/115/115	-
23	BCR	B	718	-	-	7/29/63/63	0/2/2/2
28	STE	j	101	-	-	2/9/9/17	-
22	CLA	B	704	2	1/1/15/20	11/39/115/115	-
22	CLA	C	514	3	1/1/15/20	15/39/115/115	-
22	CLA	c	503	3	1/1/15/20	4/39/115/115	-
26	SQD	B	723	-	-	29/49/69/69	0/1/1/1
28	STE	b	601	-	-	8/13/13/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	STE	E	102	-	-	5/9/9/17	-
22	CLA	a	402	1	1/1/15/20	8/39/115/115	-
22	CLA	b	602	2	-	8/39/115/115	-
27	DGD	c	519	-	-	19/51/91/95	0/2/2/2
22	CLA	C	509	3	1/1/15/20	5/39/115/115	-
22	CLA	D	402	4	1/1/15/20	7/39/115/115	-
23	BCR	Y	101	-	-	7/29/63/63	0/2/2/2
28	STE	Z	101	-	-	3/5/5/17	-
22	CLA	b	615	2	-	10/39/115/115	-
22	CLA	A	404	1	1/1/12/20	4/26/102/115	-
22	CLA	b	607	35	1/1/15/20	16/39/115/115	-
22	CLA	B	703	2	1/1/15/20	11/39/115/115	-
34	HEC	F	101	5,6	-	4/14/54/54	-
22	CLA	B	702	2	1/1/15/20	8/39/115/115	-
22	CLA	b	606	2	1/1/15/20	8/39/115/115	-
28	STE	T	702	-	-	8/12/12/17	-
28	STE	b	625	-	-	4/7/7/17	-
27	DGD	C	519	-	-	17/51/91/95	0/2/2/2
23	BCR	H	101	-	-	6/29/63/63	0/2/2/2
28	STE	M	103	-	-	4/7/7/17	-
28	STE	d	402	-	-	9/17/17/17	-
28	STE	a	416	-	-	4/9/9/17	-
22	CLA	c	508	35	1/1/15/20	3/39/115/115	-
22	CLA	c	505	35	1/1/14/20	7/33/109/115	-
22	CLA	D	403	35	1/1/15/20	6/39/115/115	-
28	STE	I	101	-	-	4/12/12/17	-
31	LHG	d	409	-	-	10/43/43/53	-
22	CLA	b	609	-	1/1/15/20	7/39/115/115	-
27	DGD	c	517	-	-	21/51/91/95	0/2/2/2
28	STE	B	720	-	-	9/14/14/17	-
30	LMG	b	622	-	-	22/50/70/70	0/1/1/1
22	CLA	b	611	2	1/1/15/20	7/39/115/115	-
22	CLA	C	513	3	1/1/15/20	14/39/115/115	-
23	BCR	k	102	-	-	4/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	c	507	3	1/1/15/20	13/39/115/115	-

The worst 5 of 1034 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	d	407	PHO	C1B-C2B	9.97	1.50	1.39
33	a	404	PHO	C1B-C2B	8.14	1.48	1.39
33	D	408	PHO	C1B-C2B	8.14	1.48	1.39
33	D	408	PHO	C3B-C4B	7.18	1.48	1.41
33	D	407	PHO	C1B-C2B	7.09	1.47	1.39

The worst 5 of 1492 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	510	CLA	C4A-NA-C1A	12.08	112.19	106.68
34	F	101	HEC	CBC-CAC-C3C	-10.92	105.60	127.43
26	l	101	SQD	O6-C1-C2	10.85	124.75	108.27
34	V	201	HEC	CBB-CAB-C3B	-10.61	106.23	127.43
22	c	504	CLA	C4A-NA-C1A	9.62	111.07	106.68

5 of 65 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	A	402	CLA	ND
22	A	404	CLA	ND
22	B	702	CLA	ND
22	B	703	CLA	ND
22	B	704	CLA	ND

5 of 1794 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	B	705	CLA	C11-C12-C13-C14
22	B	714	CLA	CAD-CBD-CGD-O1D
22	B	714	CLA	CAD-CBD-CGD-O2D
22	B	714	CLA	C6-C7-C8-C9
22	B	727	CLA	CAD-CBD-CGD-O1D

There are no ring outliers.

118 monomers are involved in 227 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	c	516	BCR	1	0
23	C	515	BCR	1	0
30	c	522	LMG	1	0
28	x	101	STE	2	0
22	C	511	CLA	2	0
31	E	101	LHG	1	0
22	C	510	CLA	4	0
27	C	518	DGD	1	0
23	B	717	BCR	1	0
22	A	402	CLA	3	0
22	b	616	CLA	2	0
33	D	407	PHO	2	0
23	A	405	BCR	2	0
23	t	701	BCR	3	0
22	B	705	CLA	2	0
25	A	408	PL9	3	0
28	h	704	STE	1	0
26	l	101	SQD	8	0
30	a	418	LMG	5	0
22	B	727	CLA	2	0
22	C	507	CLA	1	0
22	c	504	CLA	1	0
23	D	405	BCR	3	0
25	D	406	PL9	2	0
22	c	509	CLA	1	0
27	H	102	DGD	1	0
22	C	506	CLA	2	0
22	B	716	CLA	1	0
31	B	722	LHG	2	0
22	B	707	CLA	1	0
22	c	514	CLA	1	0
28	C	522	STE	1	0
30	C	516	LMG	1	0
30	D	413	LMG	1	0
22	B	714	CLA	2	0
22	C	502	CLA	3	0
28	B	724	STE	1	0
22	c	512	CLA	2	0
22	b	612	CLA	1	0
31	a	413	LHG	1	0
22	C	503	CLA	2	0
31	D	411	LHG	1	0
22	B	709	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	a	405	CLA	2	0
22	C	512	CLA	2	0
30	D	409	LMG	2	0
22	b	613	CLA	2	0
26	a	414	SQD	2	0
31	a	411	LHG	3	0
30	C	520	LMG	1	0
22	c	502	CLA	1	0
28	b	624	STE	1	0
33	d	407	PHO	2	0
23	h	702	BCR	1	0
22	b	614	CLA	1	0
22	c	510	CLA	2	0
22	B	711	CLA	1	0
30	b	620	LMG	1	0
23	d	405	BCR	2	0
27	A	411	DGD	4	0
23	k	101	BCR	2	0
23	c	515	BCR	2	0
22	c	513	CLA	1	0
28	c	521	STE	1	0
22	d	401	CLA	2	0
25	a	410	PL9	5	0
22	d	403	CLA	2	0
22	B	713	CLA	1	0
22	h	701	CLA	6	0
23	b	619	BCR	1	0
23	b	618	BCR	2	0
23	C	524	BCR	2	0
28	X	101	STE	1	0
22	c	506	CLA	1	0
23	B	719	BCR	8	0
22	b	605	CLA	1	0
22	b	604	CLA	2	0
34	V	201	HEC	2	0
34	f	101	HEC	9	0
22	D	404	CLA	3	0
22	B	708	CLA	3	0
31	d	408	LHG	5	0
23	a	406	BCR	2	0
31	l	102	LHG	1	0
30	c	523	LMG	1	0

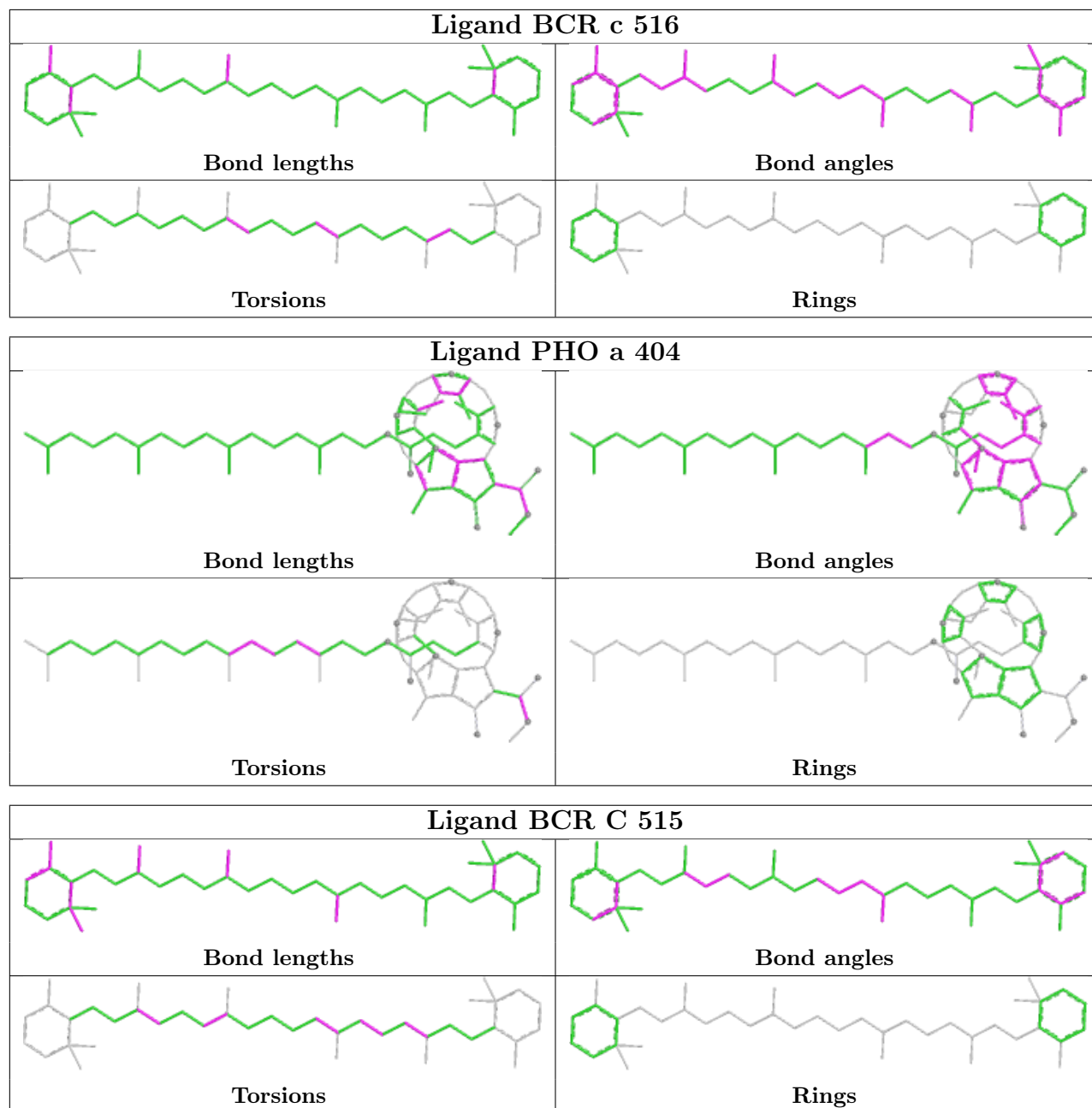
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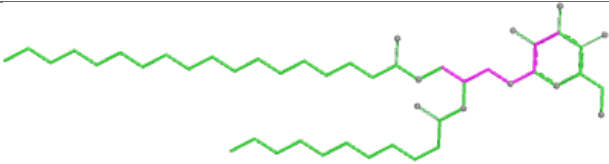
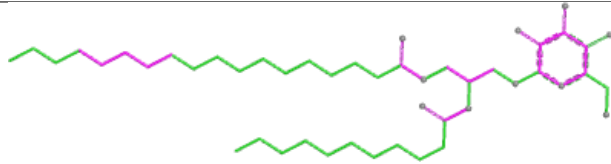
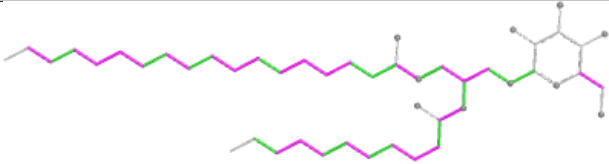
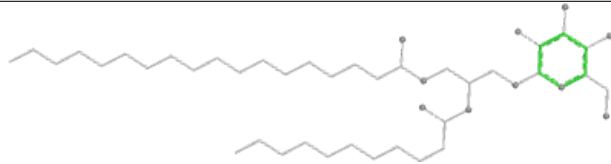
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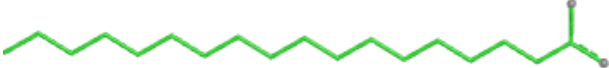
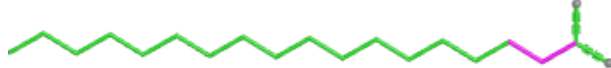
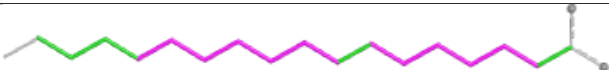
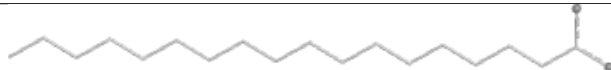
Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	D	408	PHO	3	0
22	C	504	CLA	1	0
22	B	715	CLA	1	0
23	T	701	BCR	4	0
22	d	404	CLA	1	0
22	B	706	CLA	1	0
28	b	621	STE	1	0
22	c	511	CLA	1	0
23	B	718	BCR	4	0
28	j	101	STE	1	0
22	B	704	CLA	3	0
22	C	514	CLA	3	0
22	c	503	CLA	2	0
22	b	602	CLA	2	0
27	c	519	DGD	1	0
22	C	509	CLA	2	0
22	D	402	CLA	2	0
23	Y	101	BCR	4	0
22	b	615	CLA	3	0
22	b	607	CLA	1	0
34	F	101	HEC	6	0
22	b	606	CLA	7	0
23	H	101	BCR	2	0
28	d	402	STE	2	0
28	a	416	STE	1	0
22	c	508	CLA	1	0
22	D	403	CLA	3	0
28	I	101	STE	2	0
31	d	409	LHG	1	0
22	b	609	CLA	1	0
30	b	622	LMG	1	0
22	C	513	CLA	5	0
23	k	102	BCR	3	0

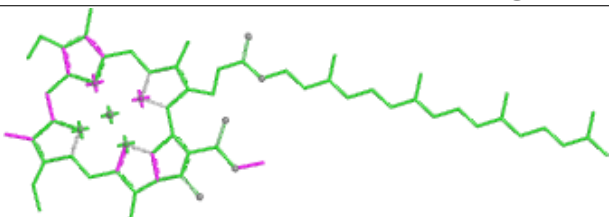
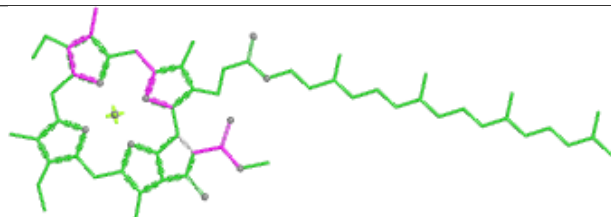
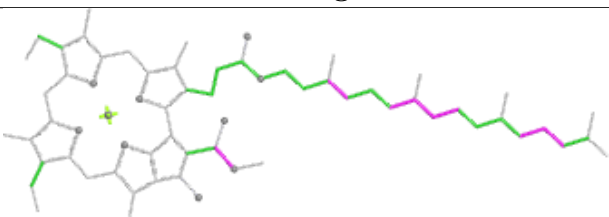
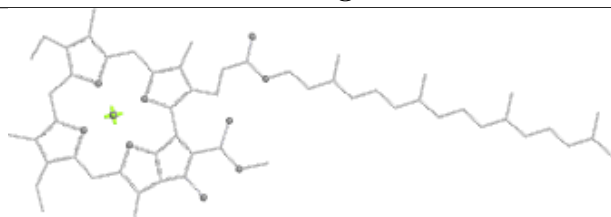
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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

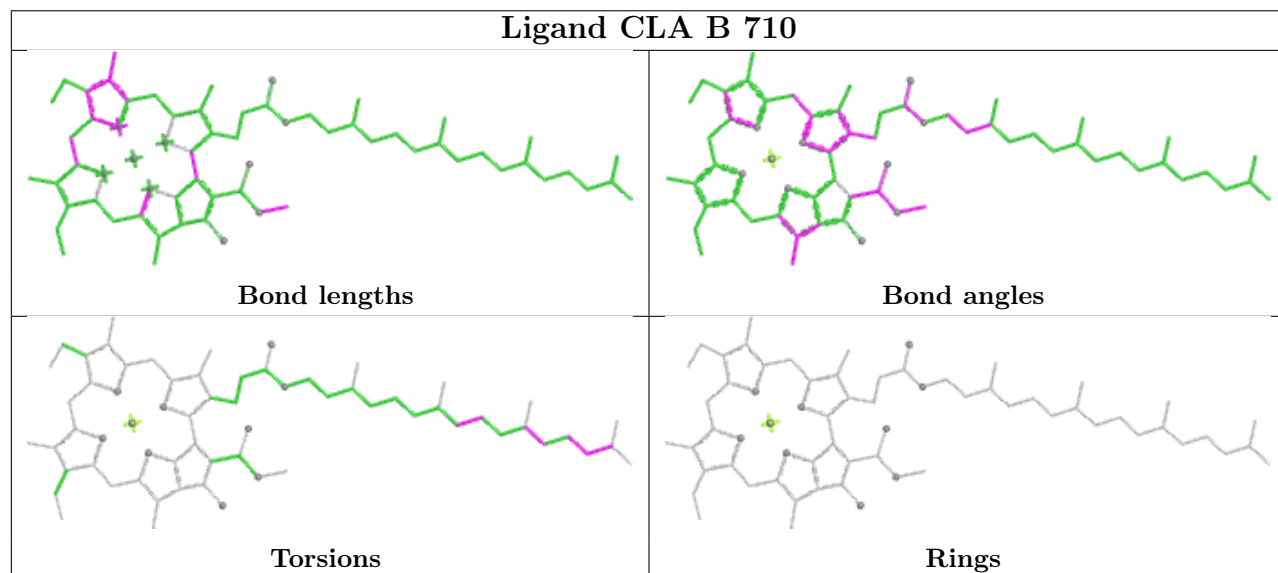
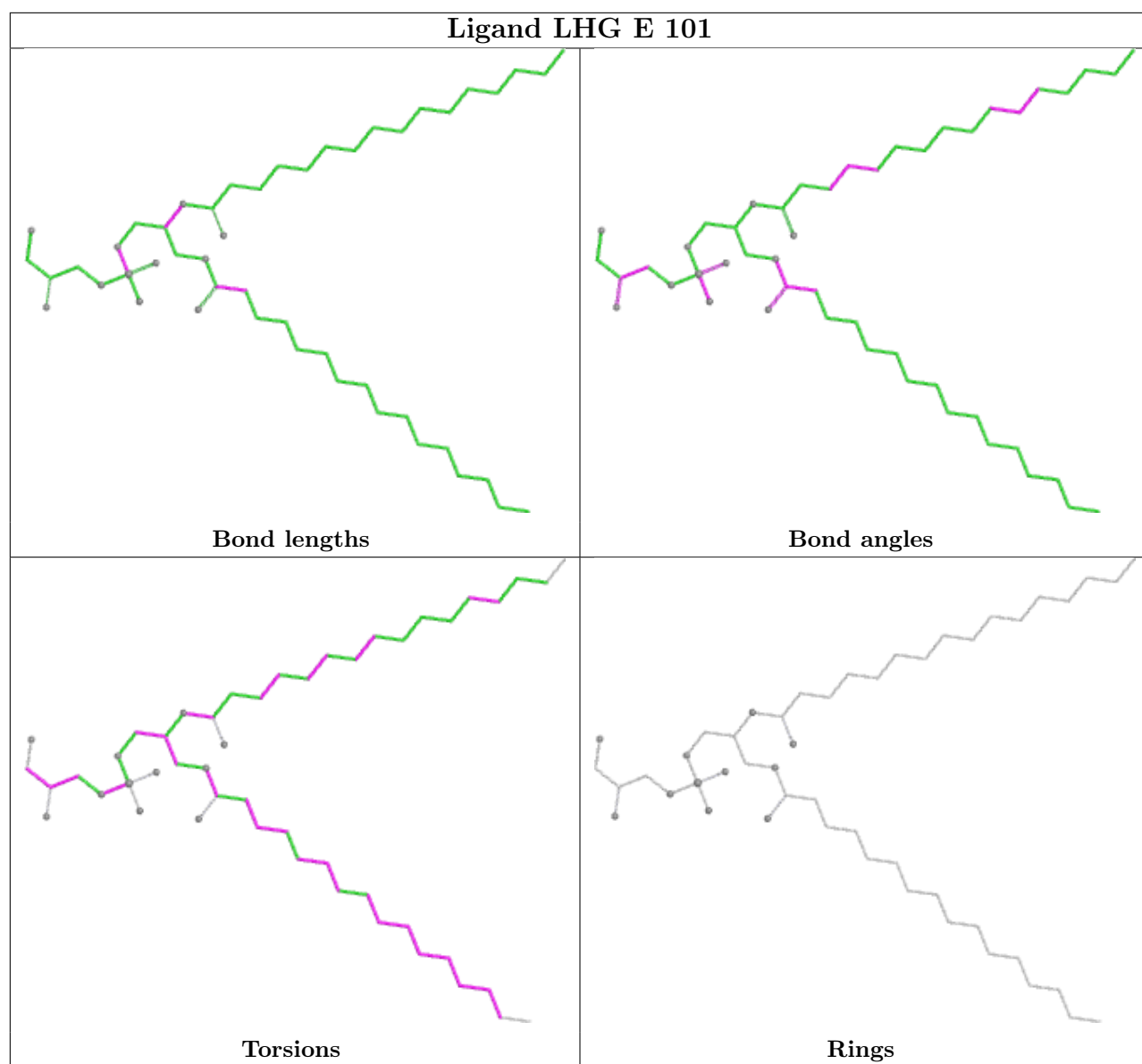
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

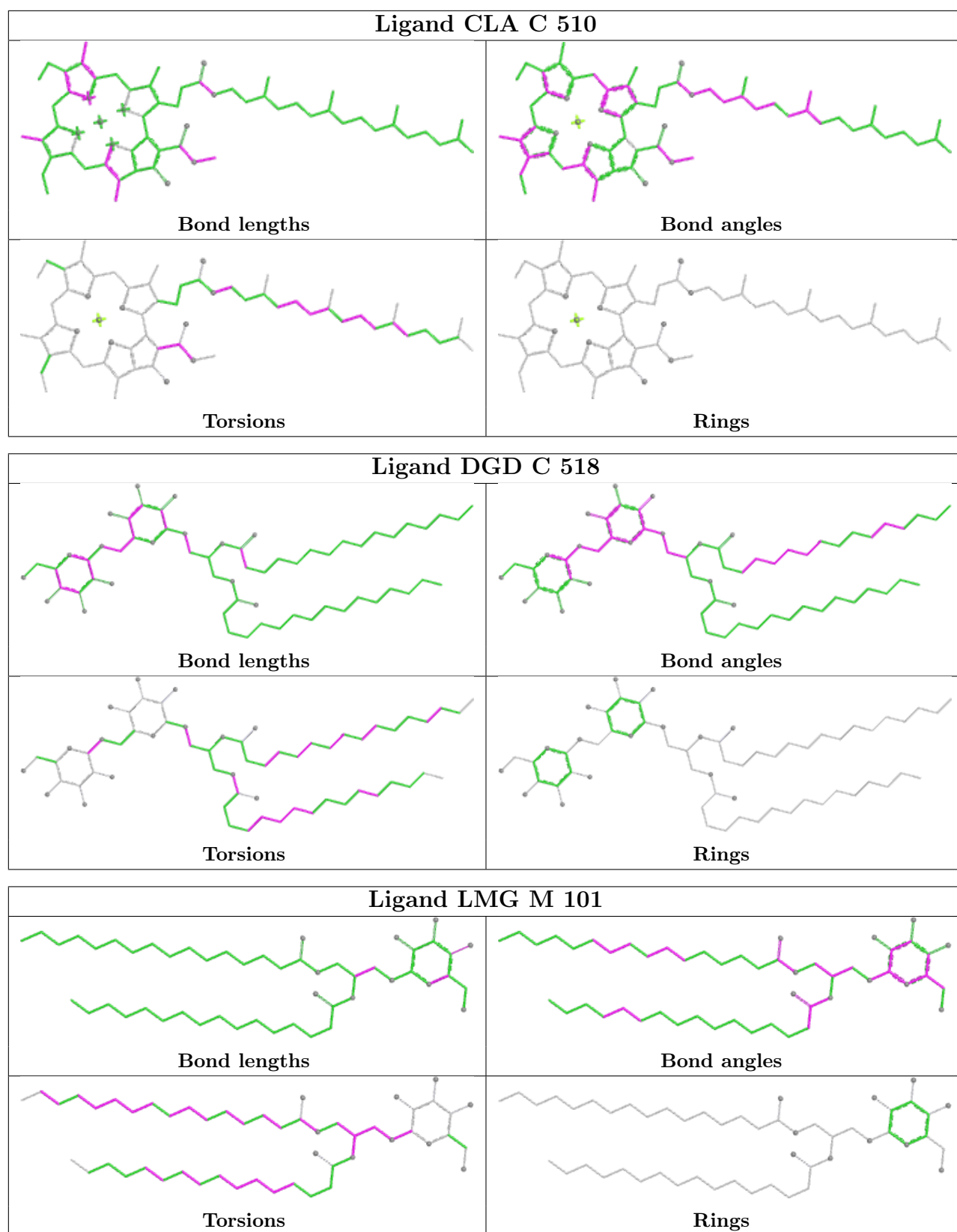


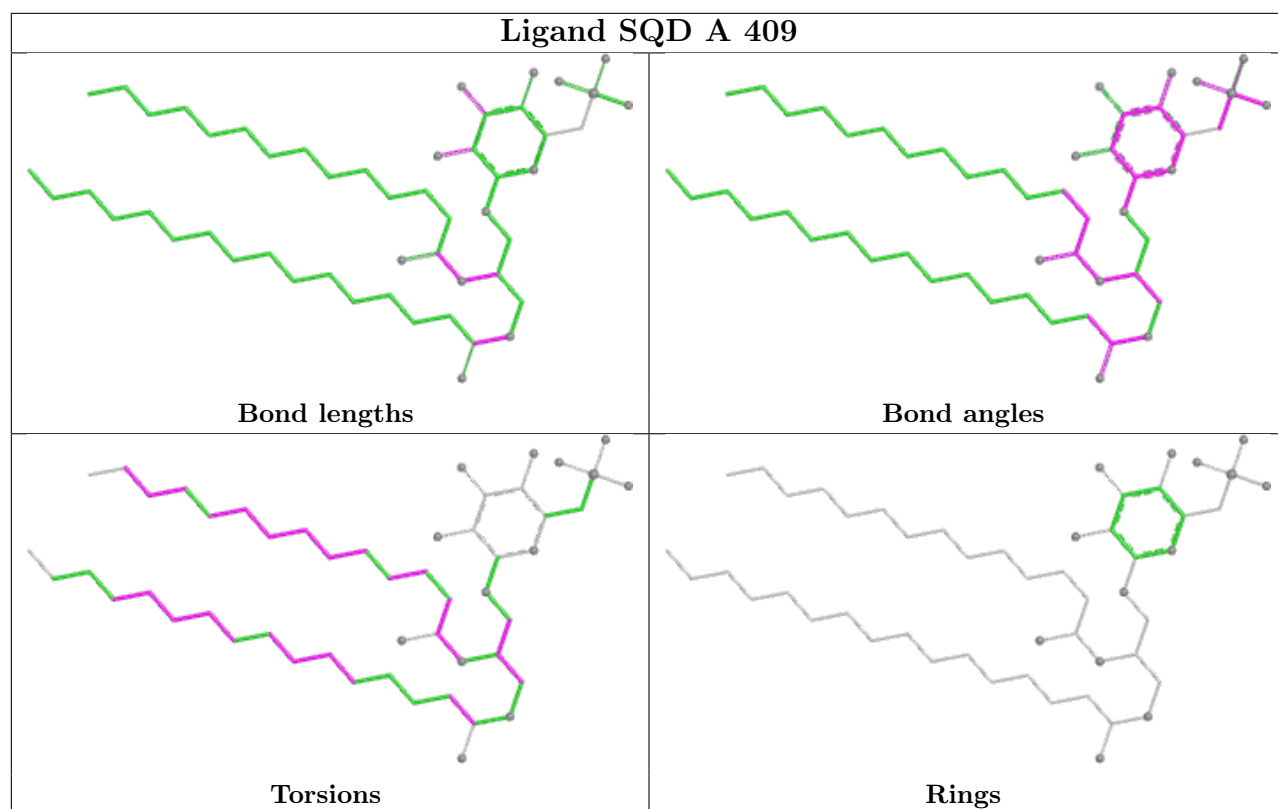
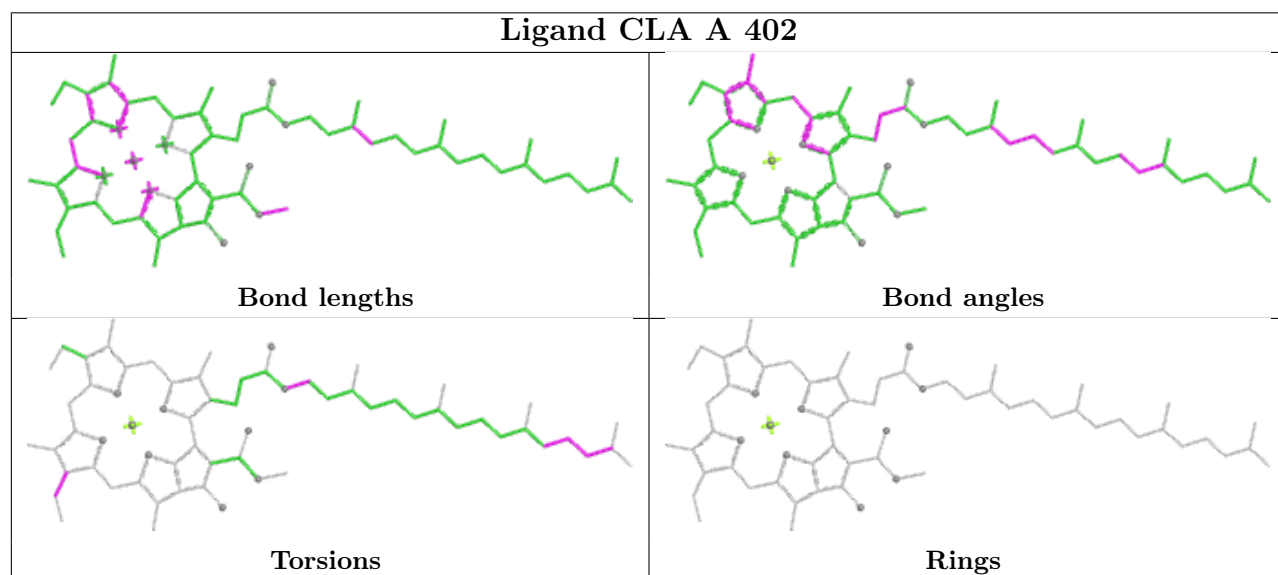
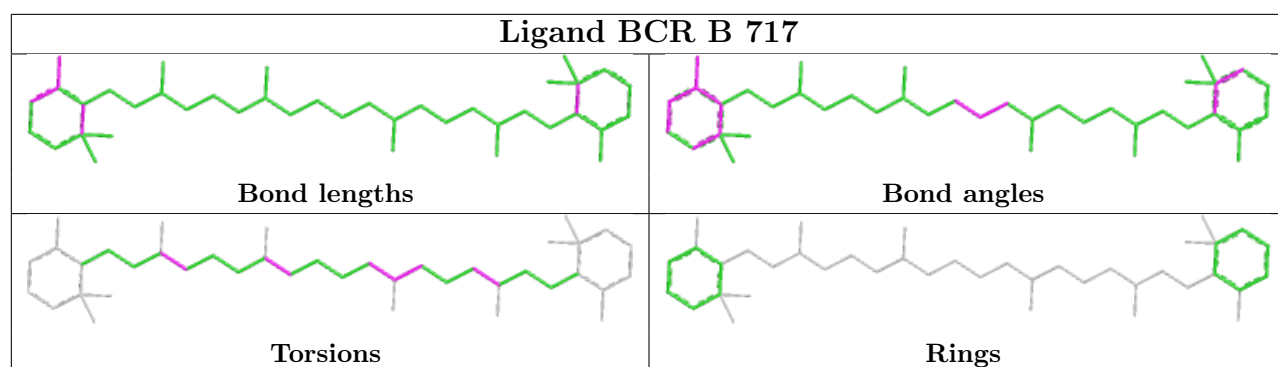
Ligand LMG c 522	
	
Bond lengths	Bond angles
	
Torsions	Rings

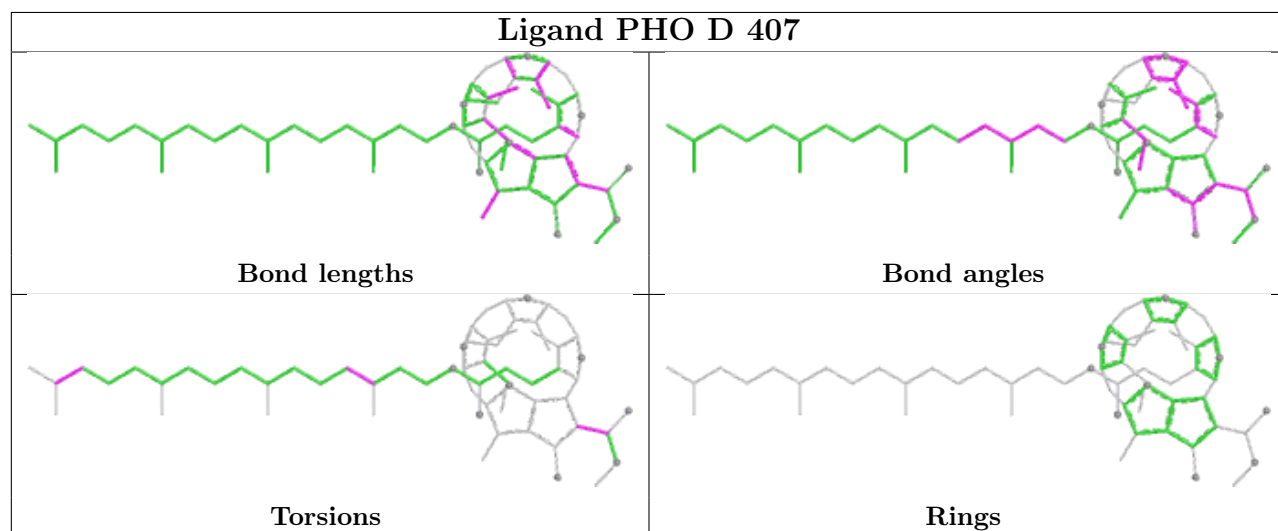
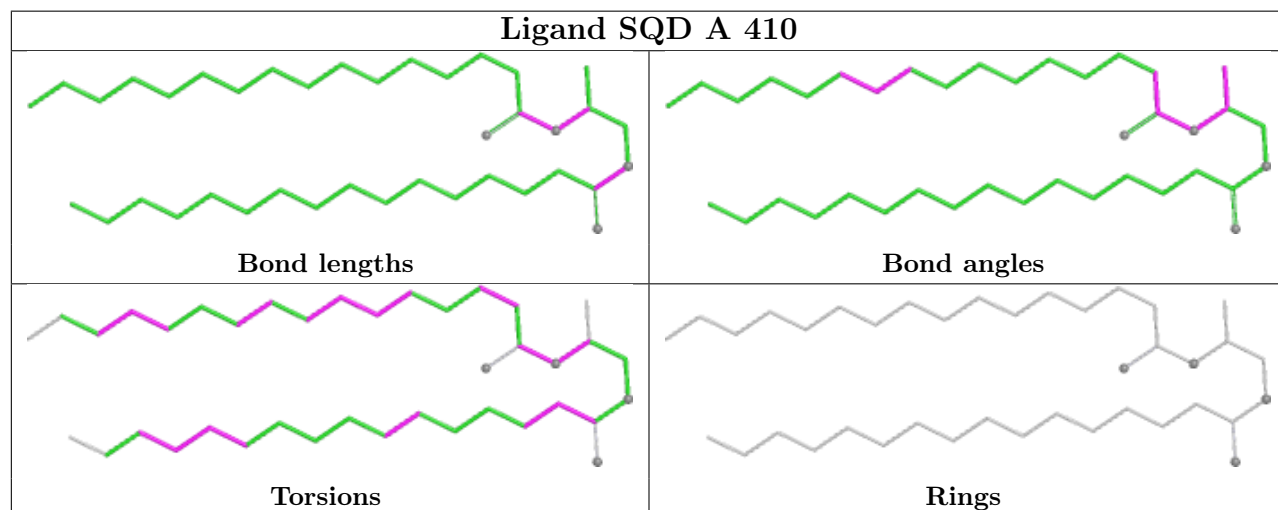
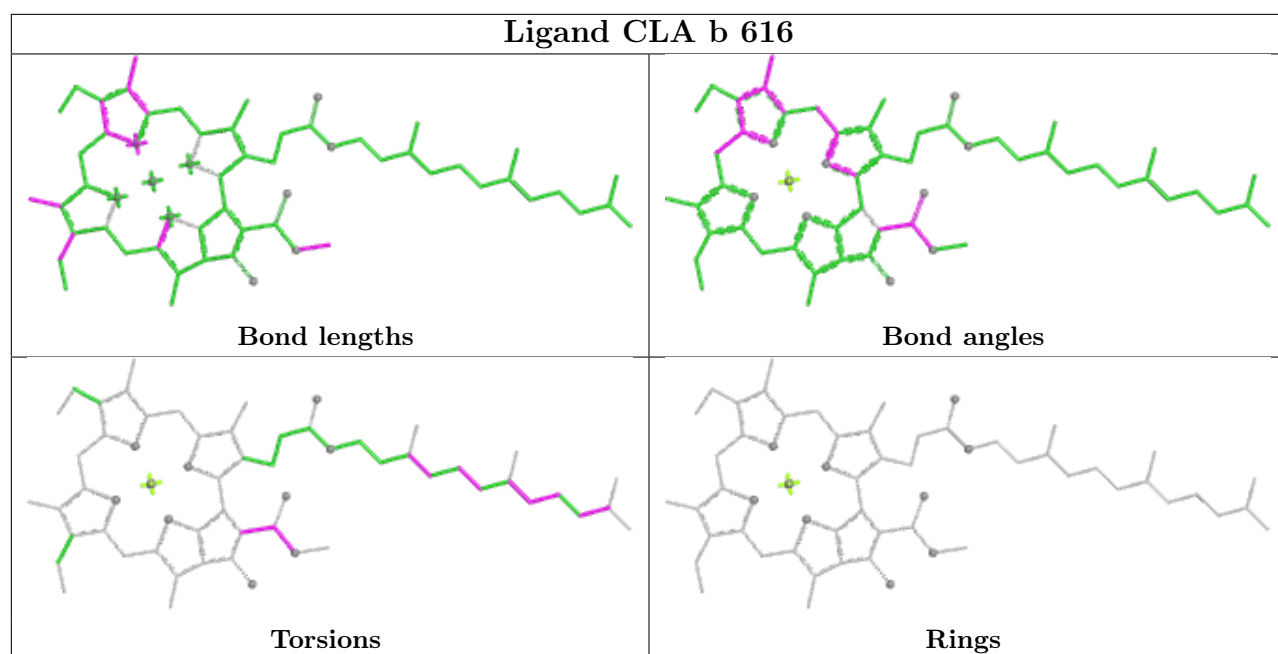
Ligand STE x 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

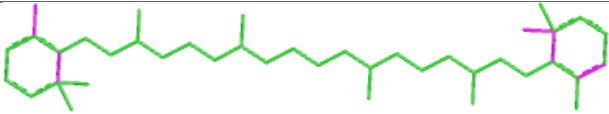
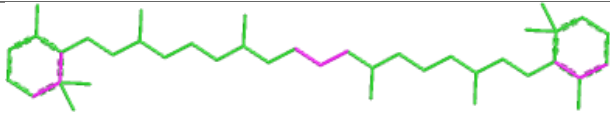
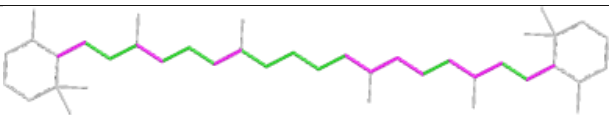
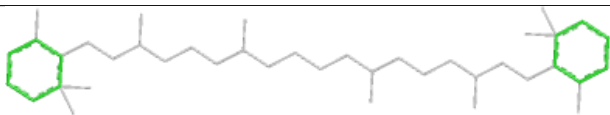
Ligand CLA C 511	
	
Bond lengths	Bond angles
	
Torsions	Rings


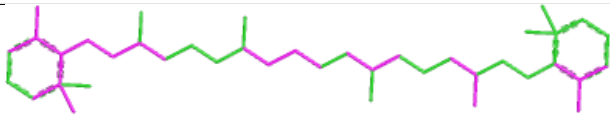
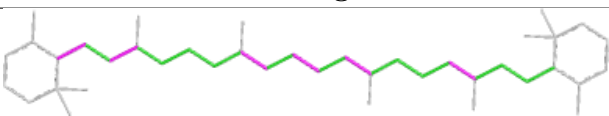
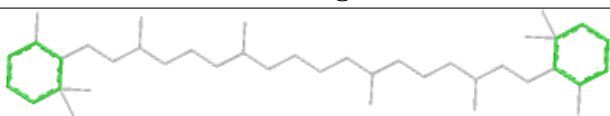


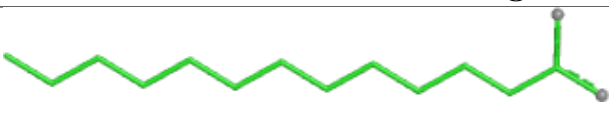
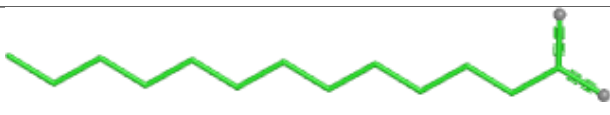
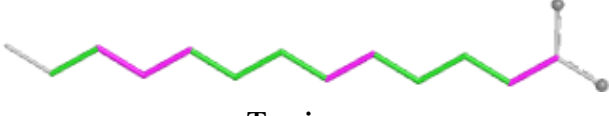
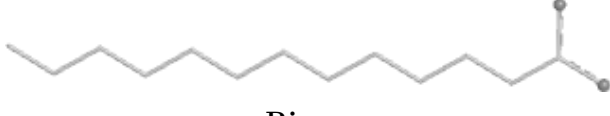


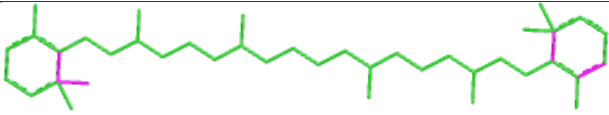
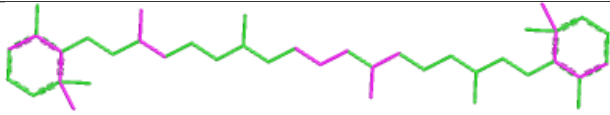

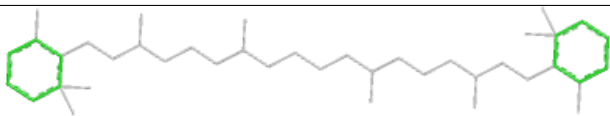


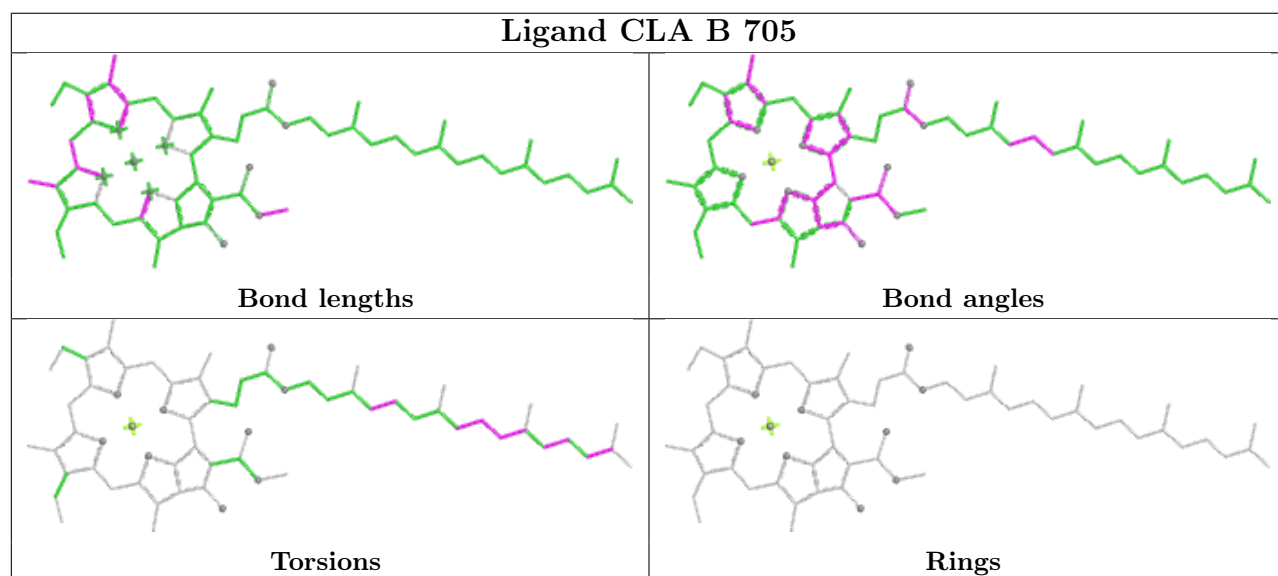
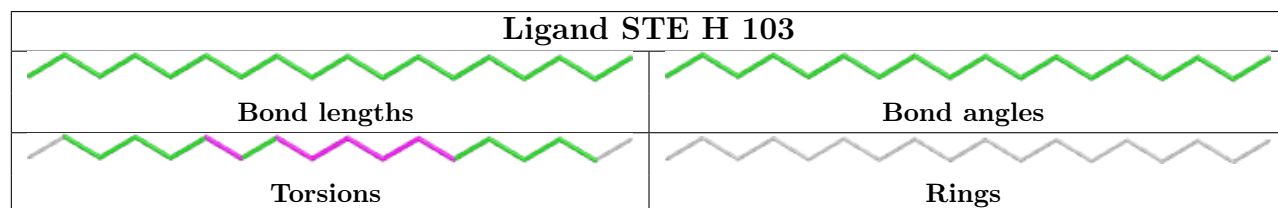
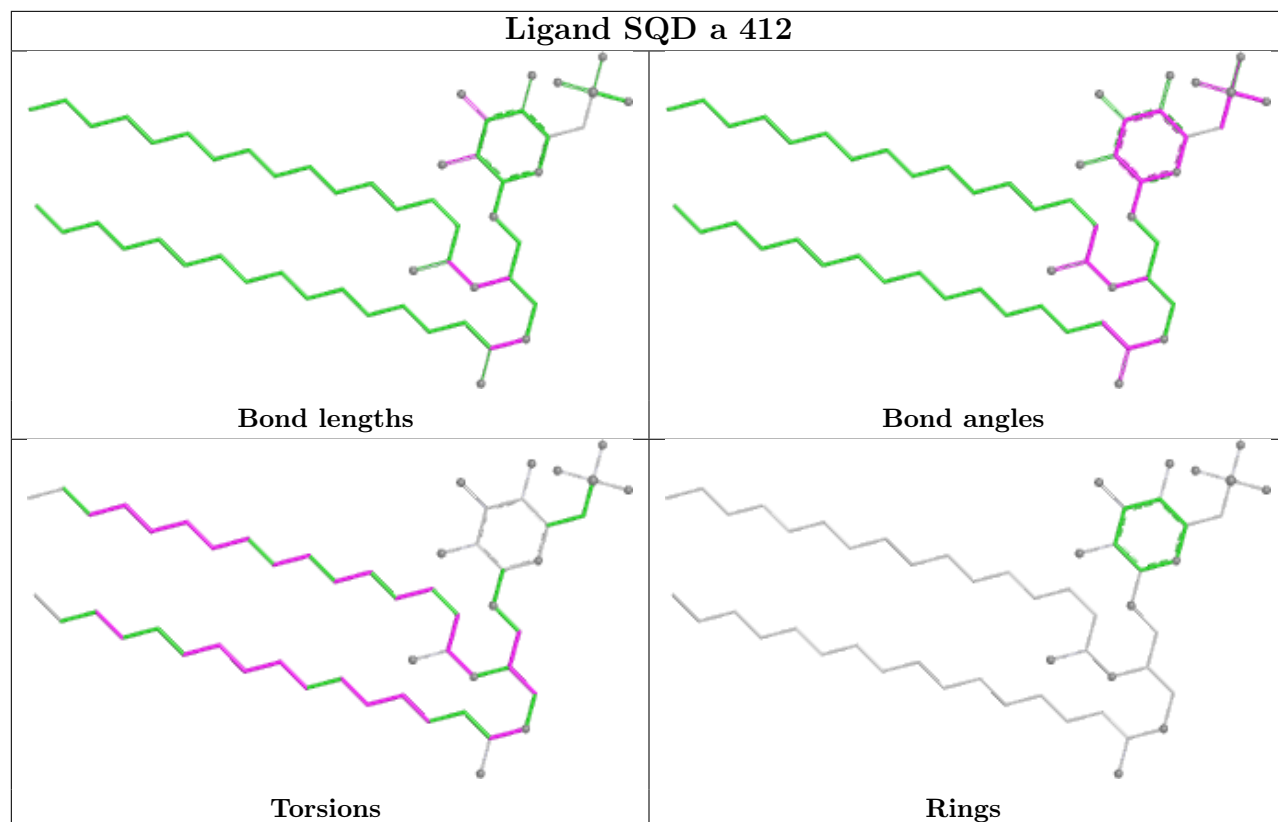


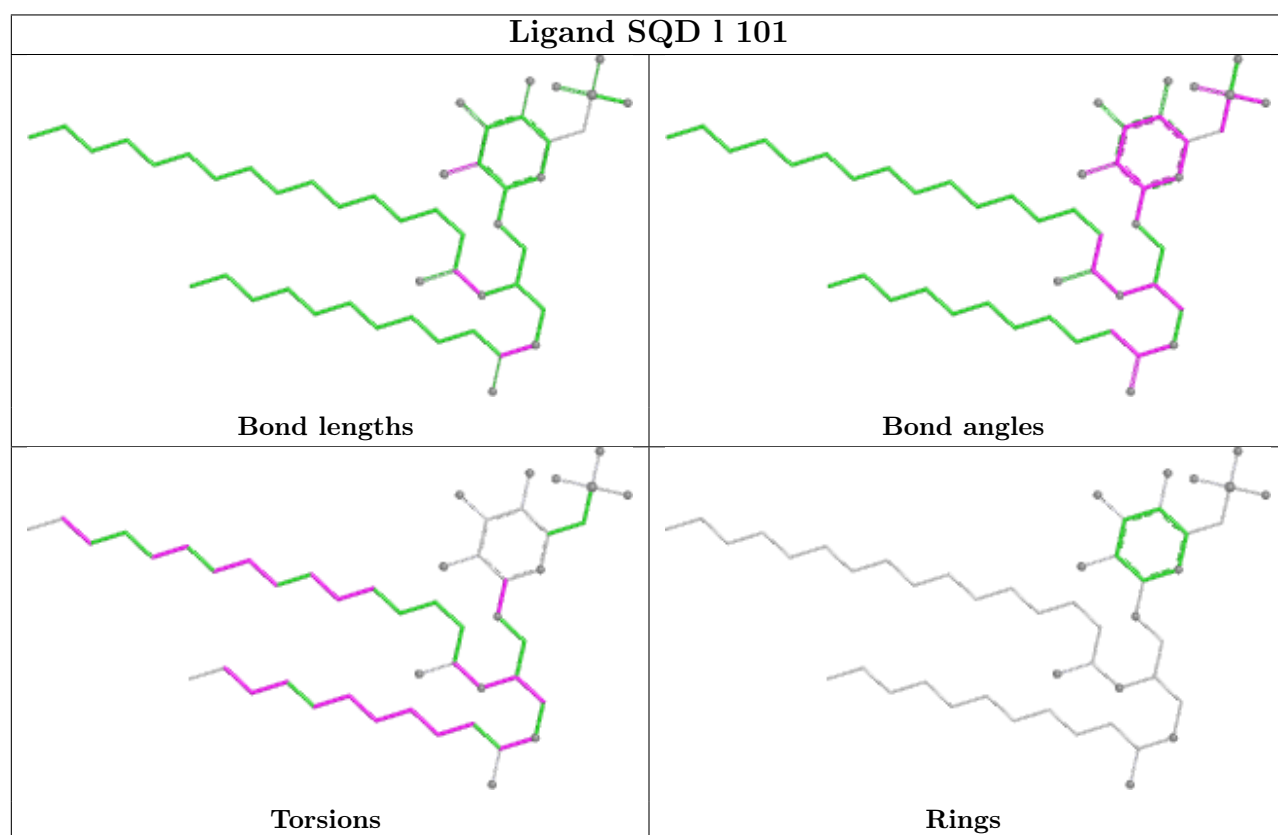
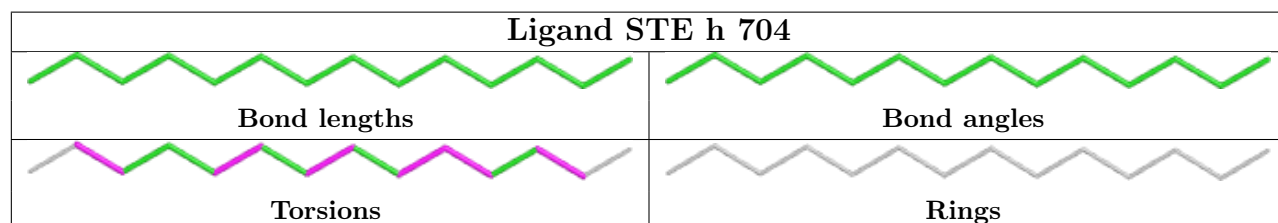
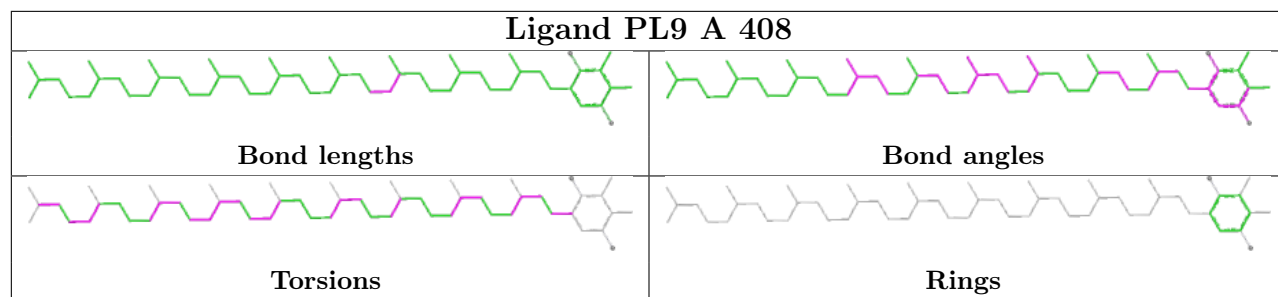
Ligand BCR C 501	
	
Bond lengths	Bond angles
	
Torsions	Rings

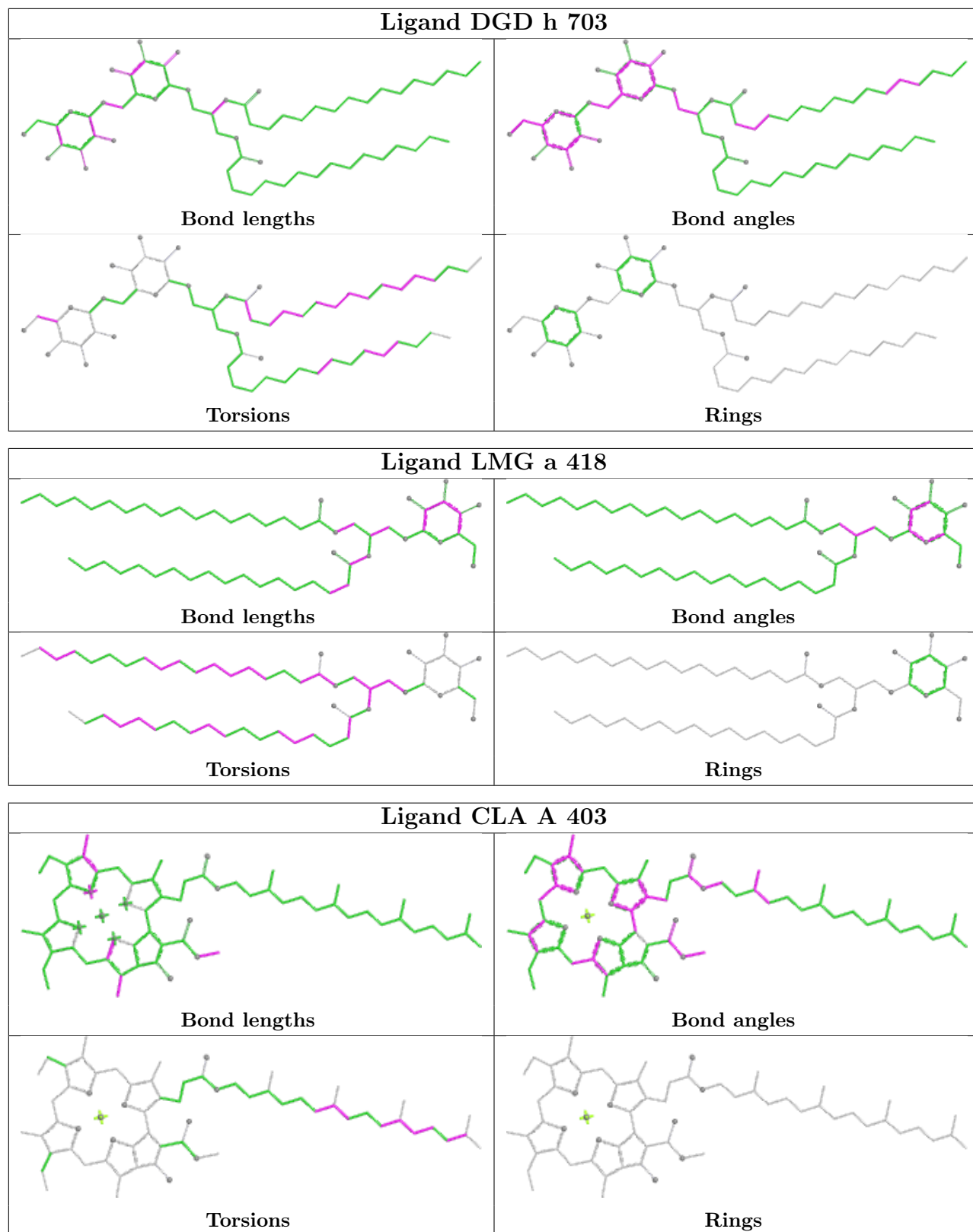
Ligand BCR A 405	
	
Bond lengths	Bond angles
	
Torsions	Rings

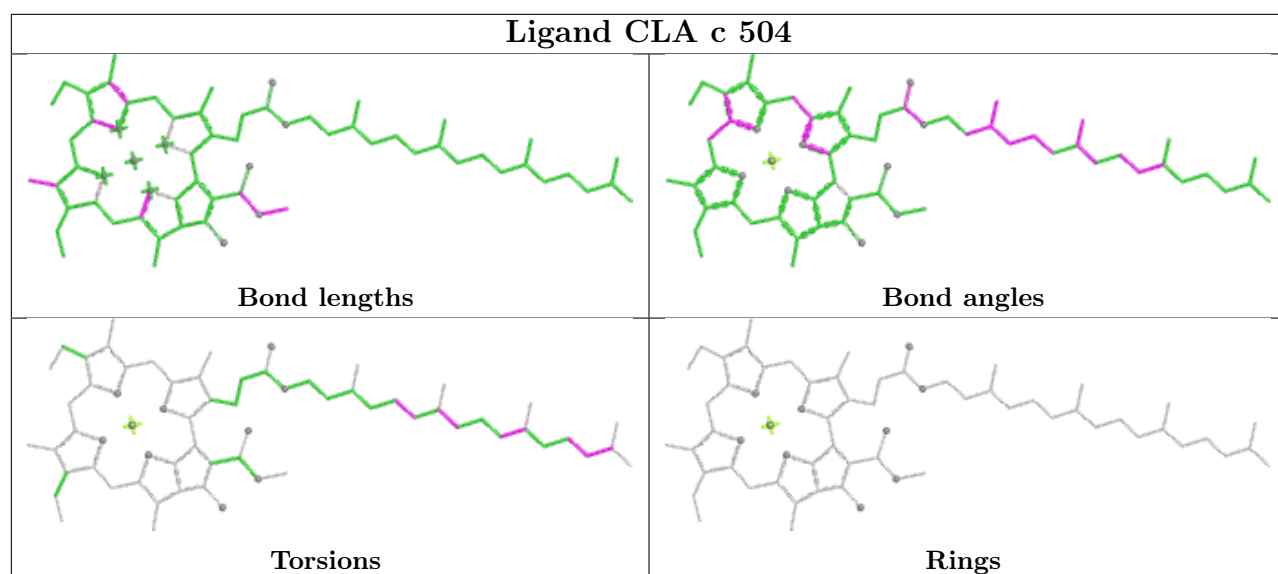
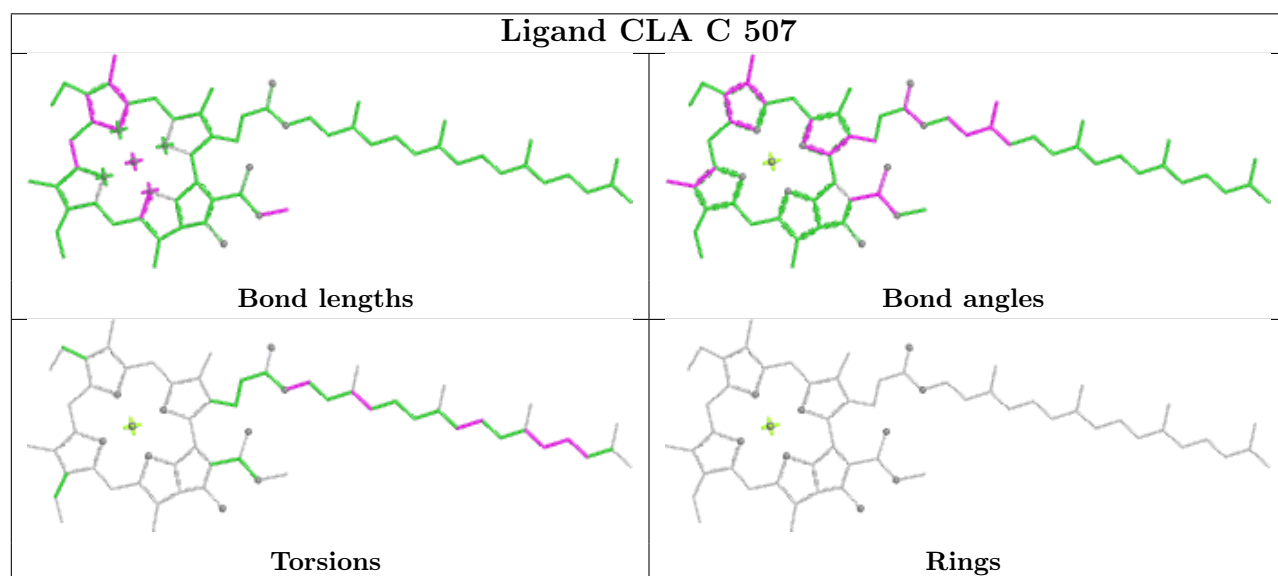
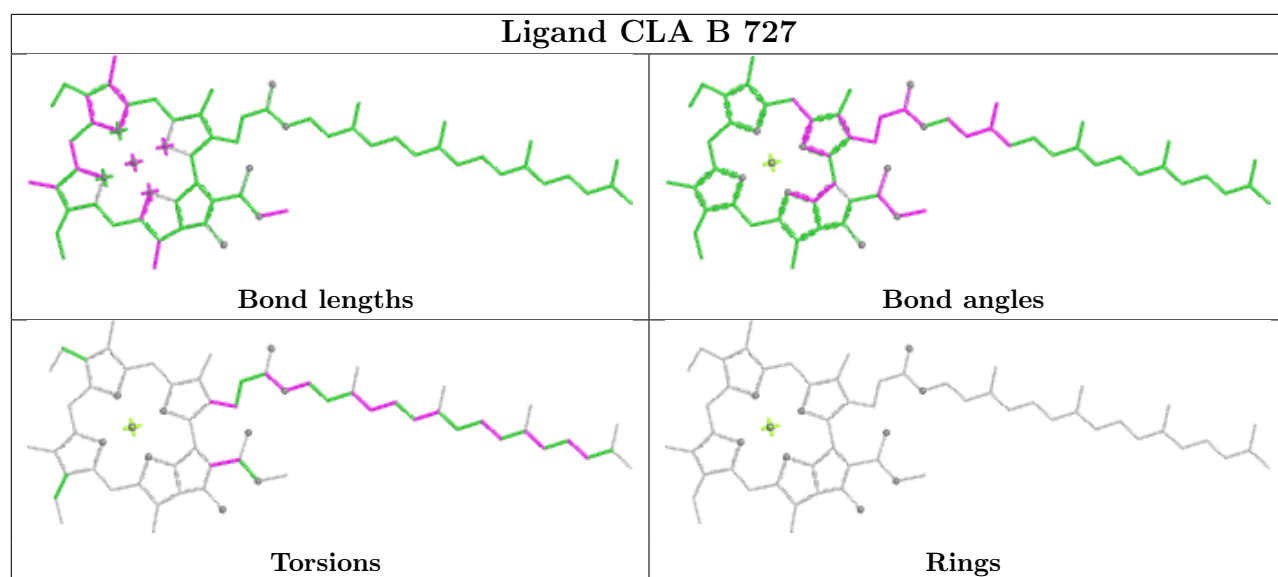
Ligand STE M 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

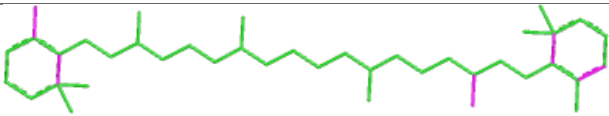
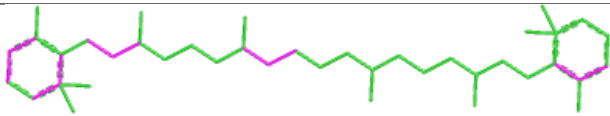
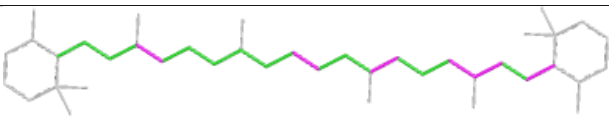
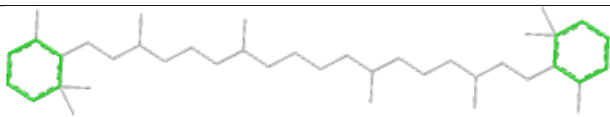
Ligand BCR t 701	
	
Bond lengths	Bond angles
	
Torsions	Rings

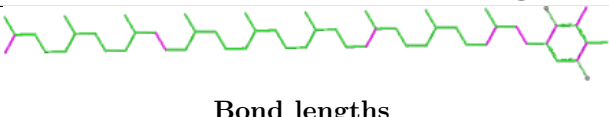
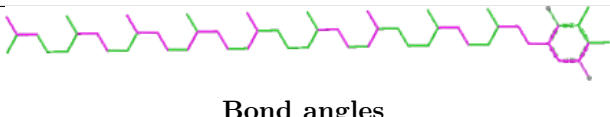
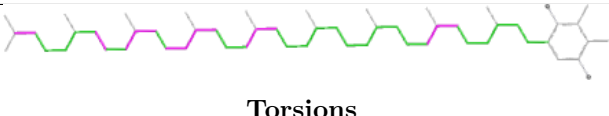



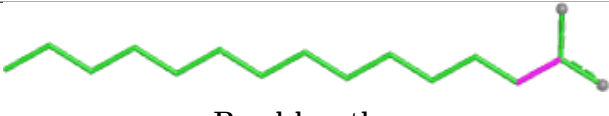
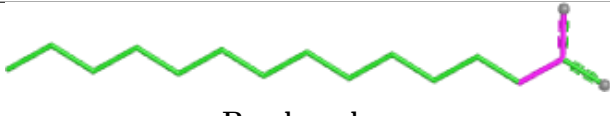
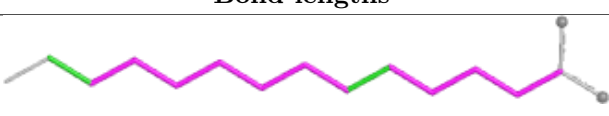
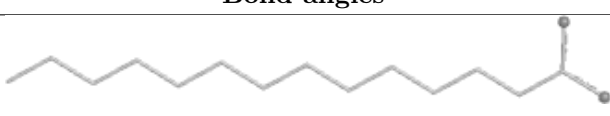


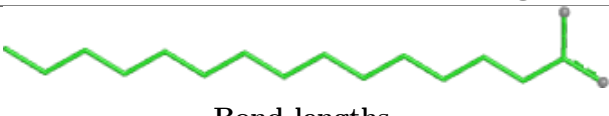
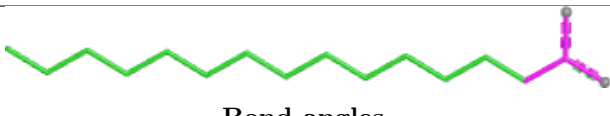
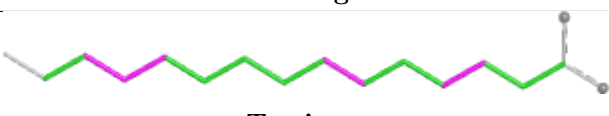
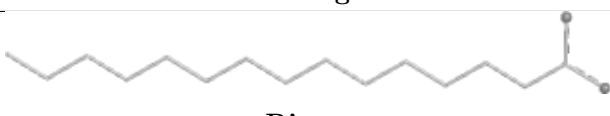


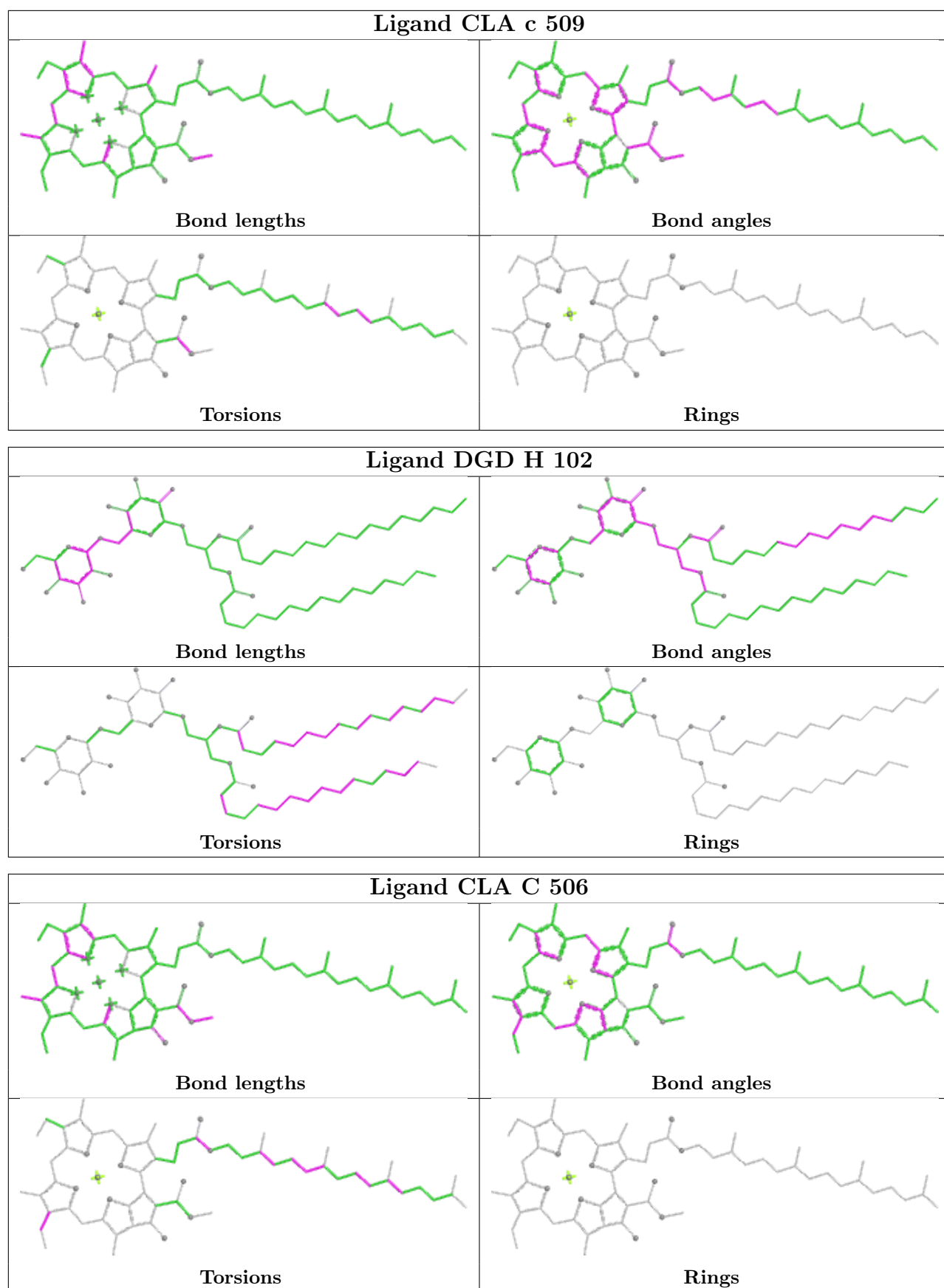


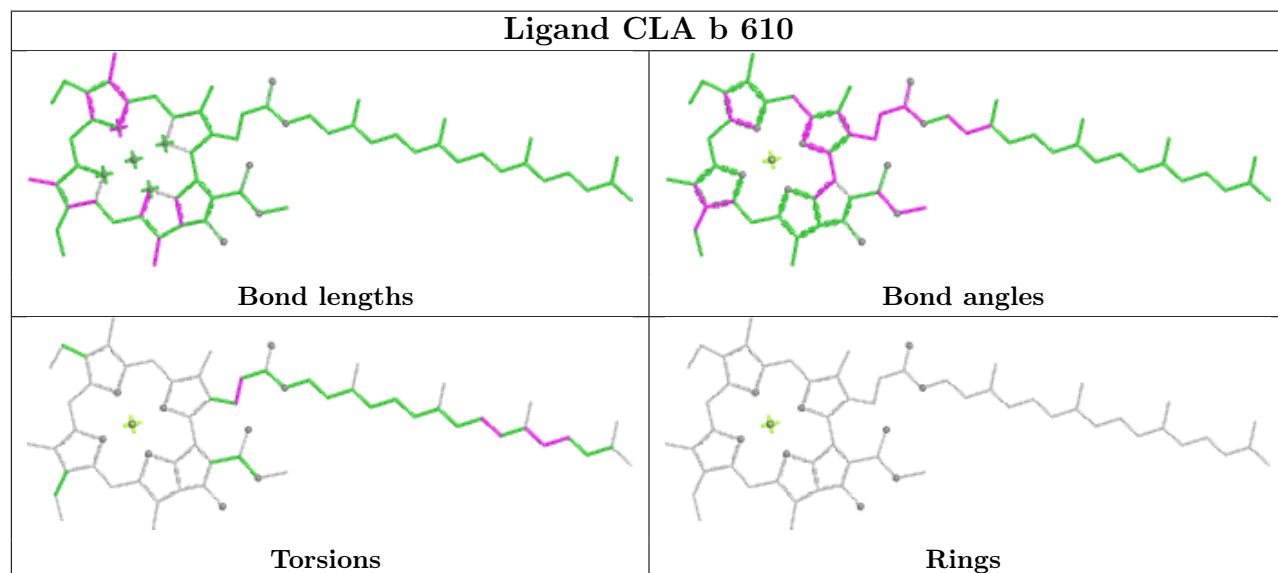
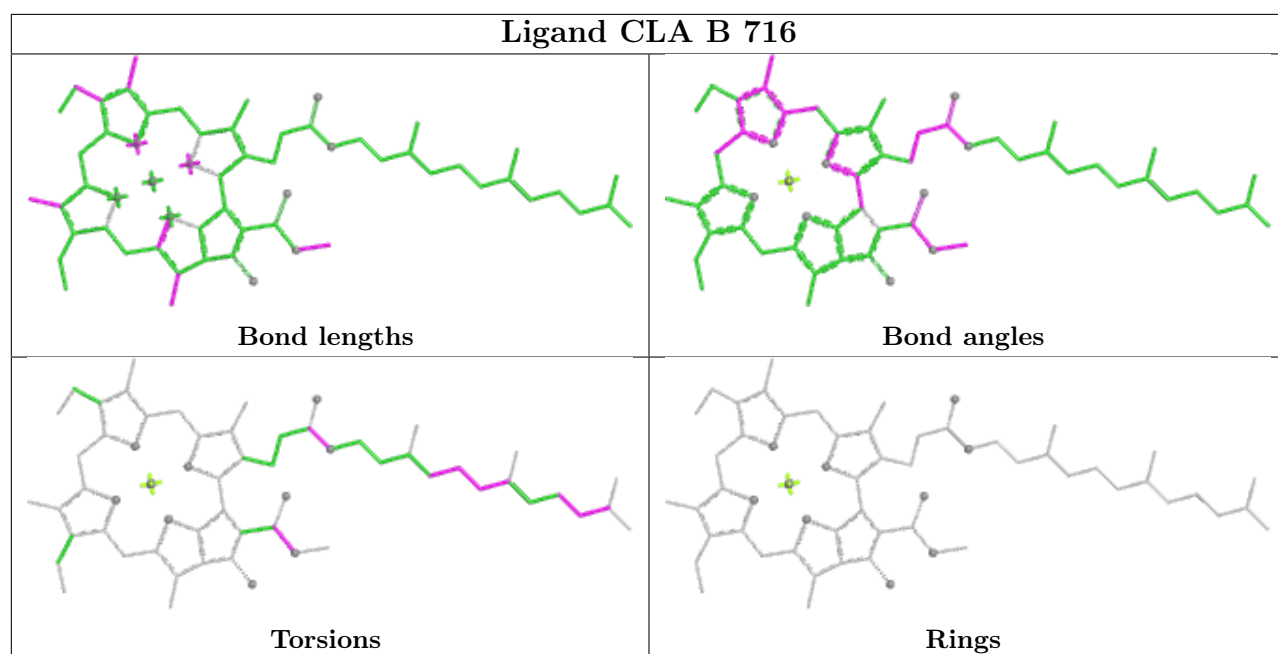
Ligand BCR D 405	
	
Bond lengths	Bond angles
	
Torsions	Rings

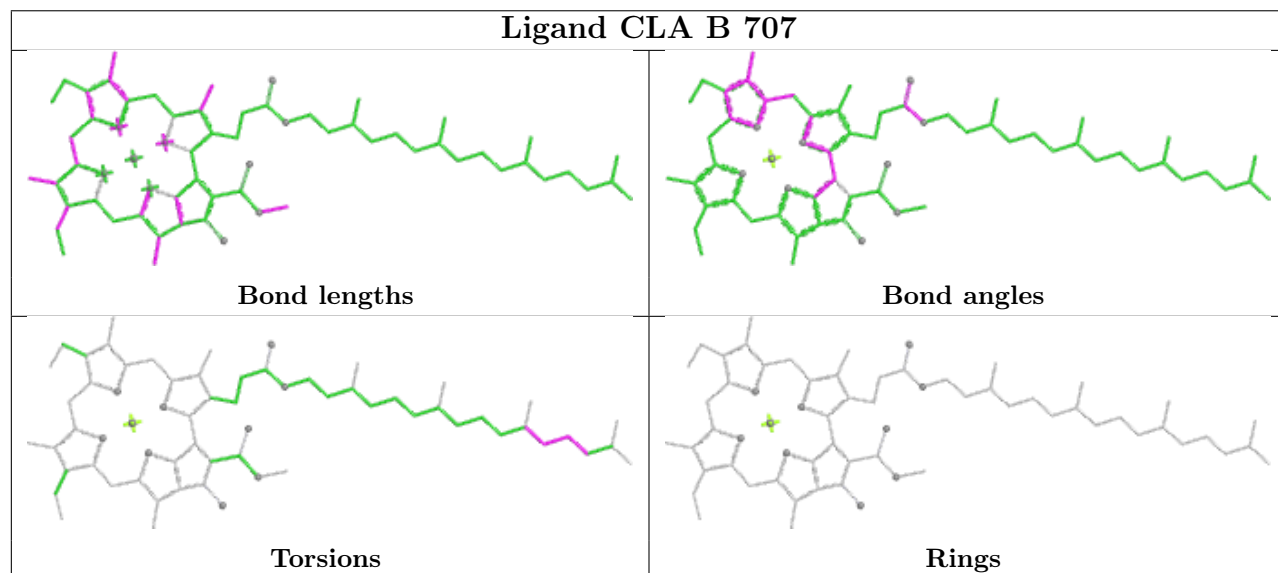
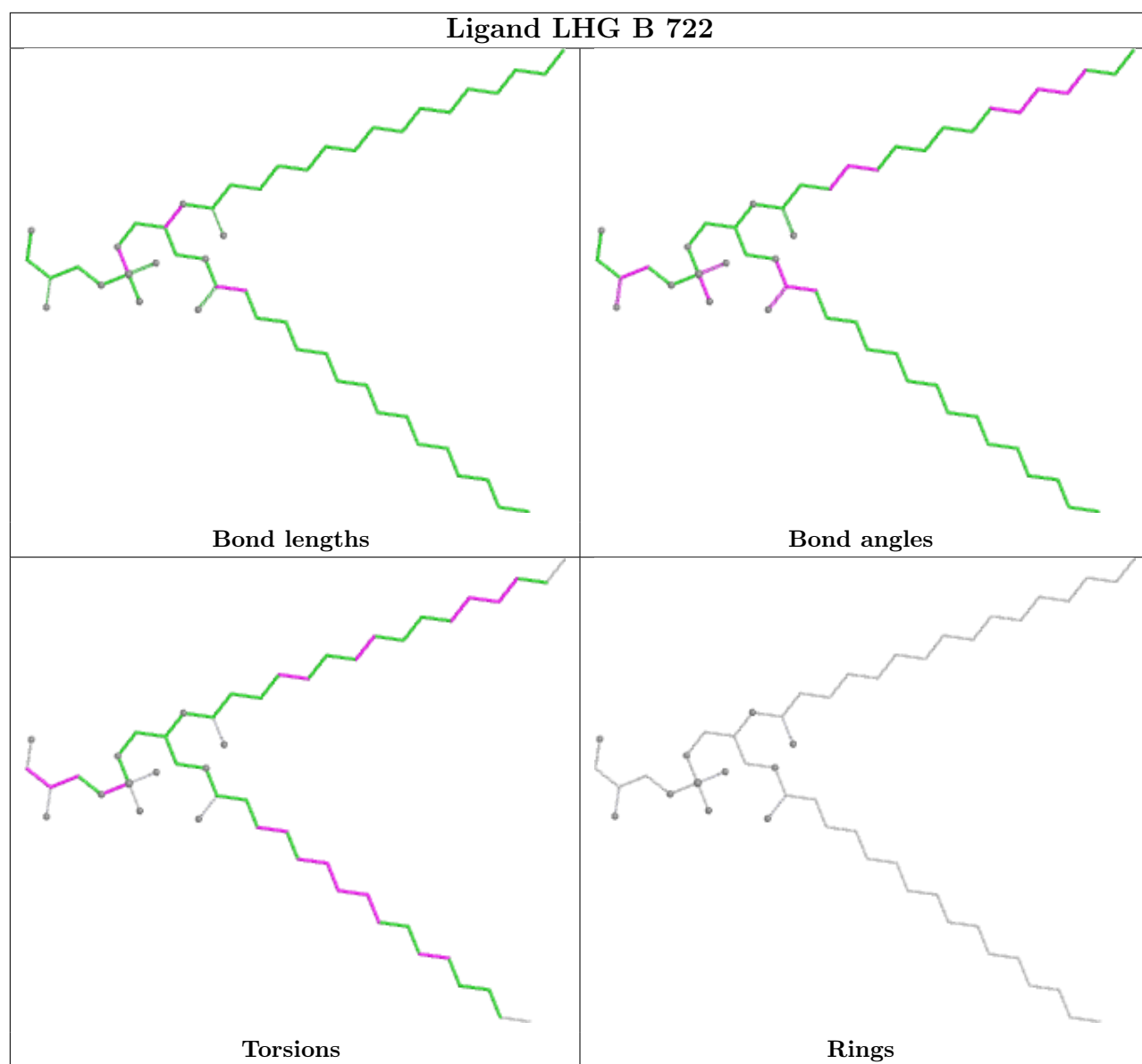
Ligand PL9 D 406	
	
Bond lengths	Bond angles
	
Torsions	Rings

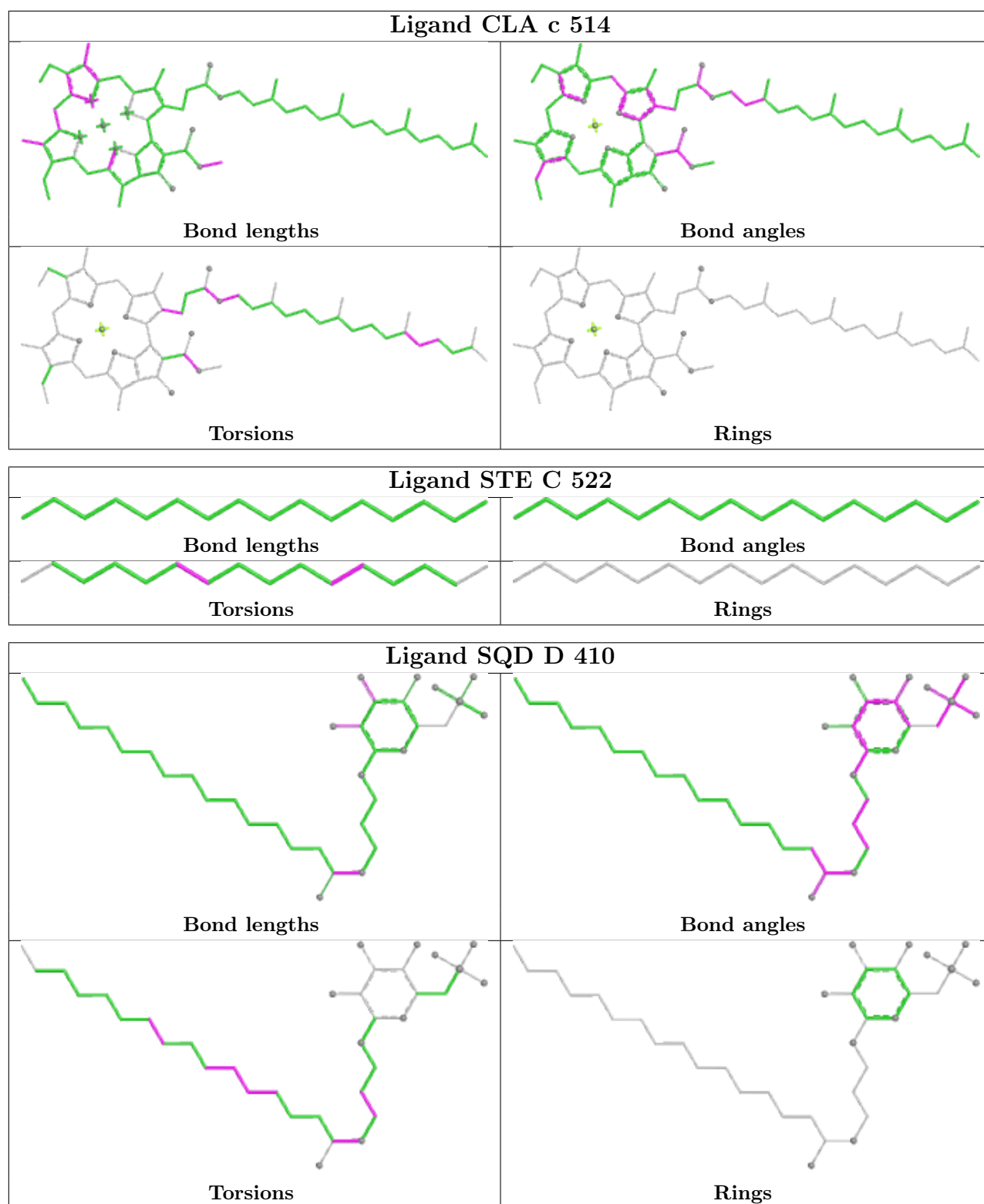
Ligand STE b 623	
	
Bond lengths	Bond angles
	
Torsions	Rings

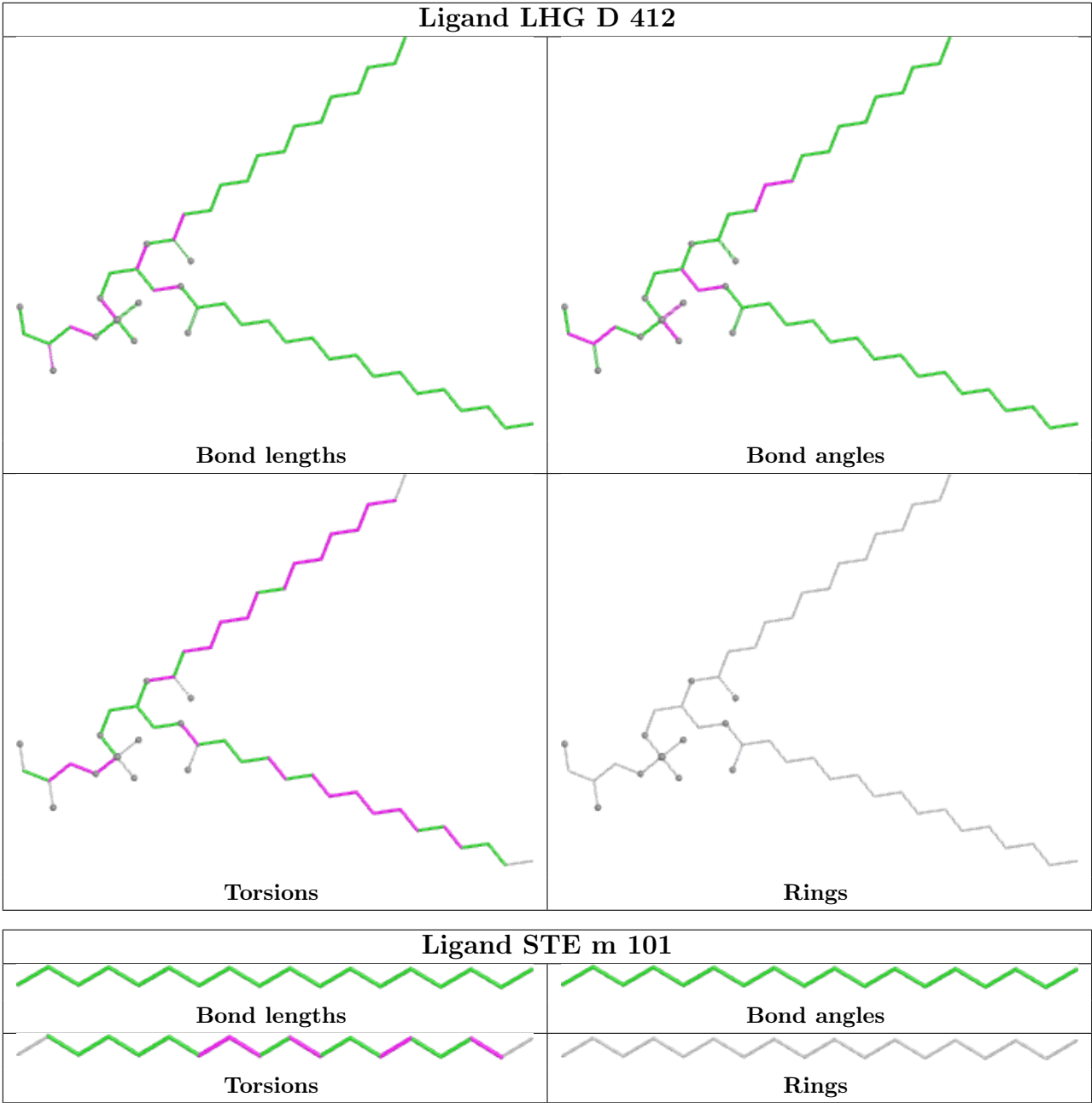
Ligand STE d 411	
	
Bond lengths	Bond angles
	
Torsions	Rings

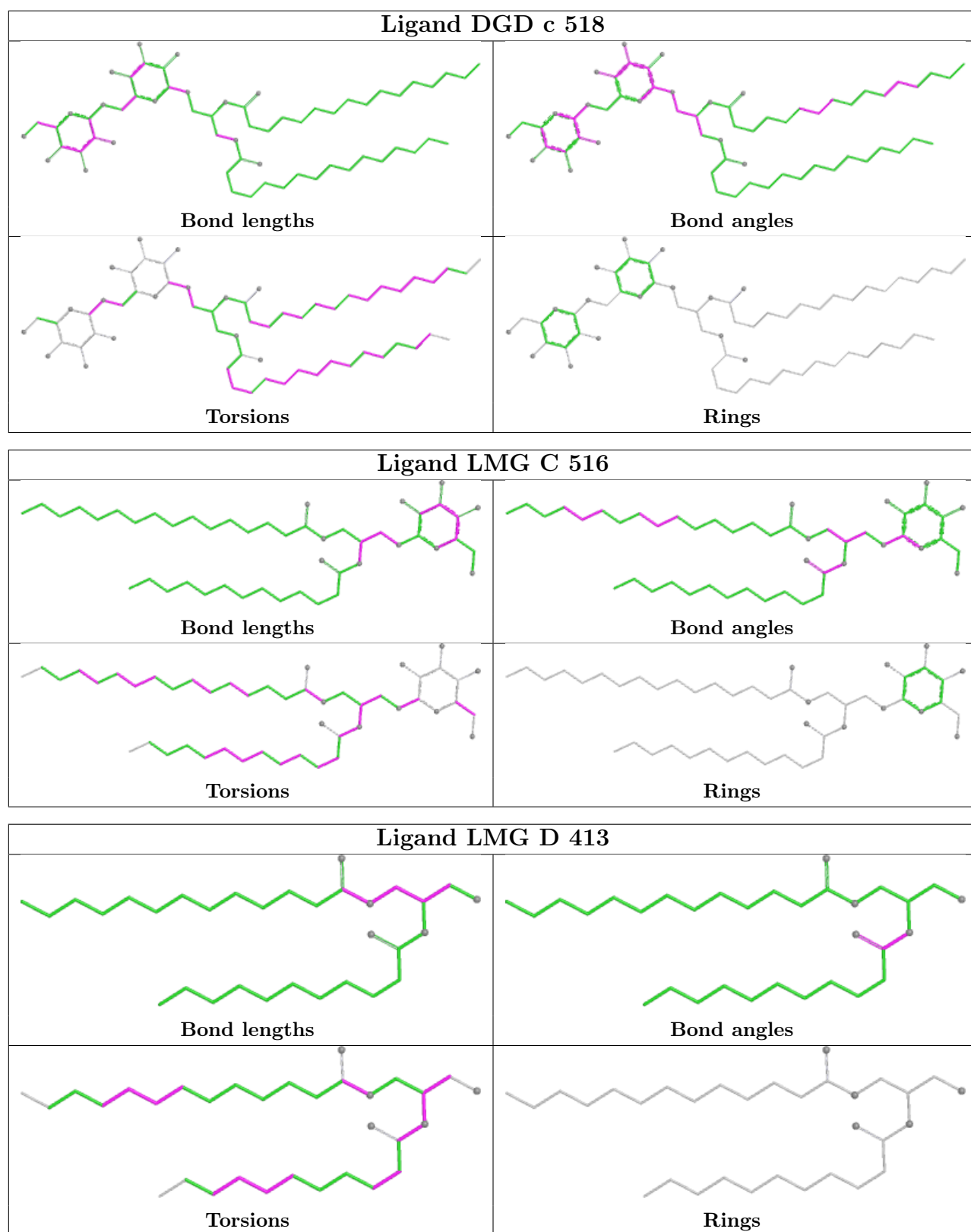


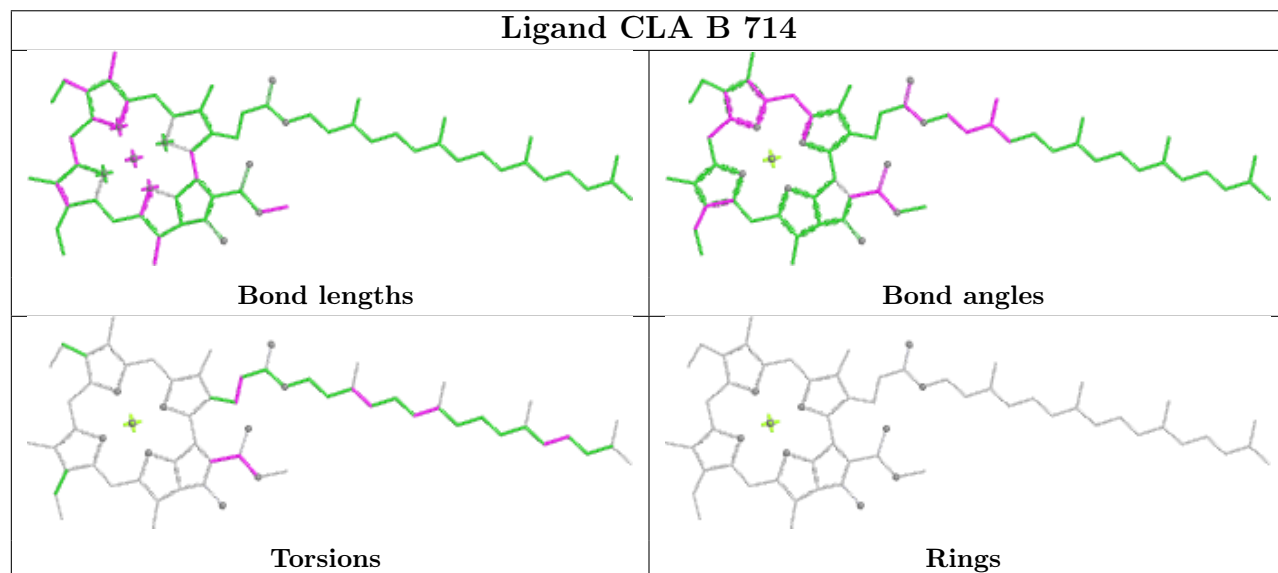
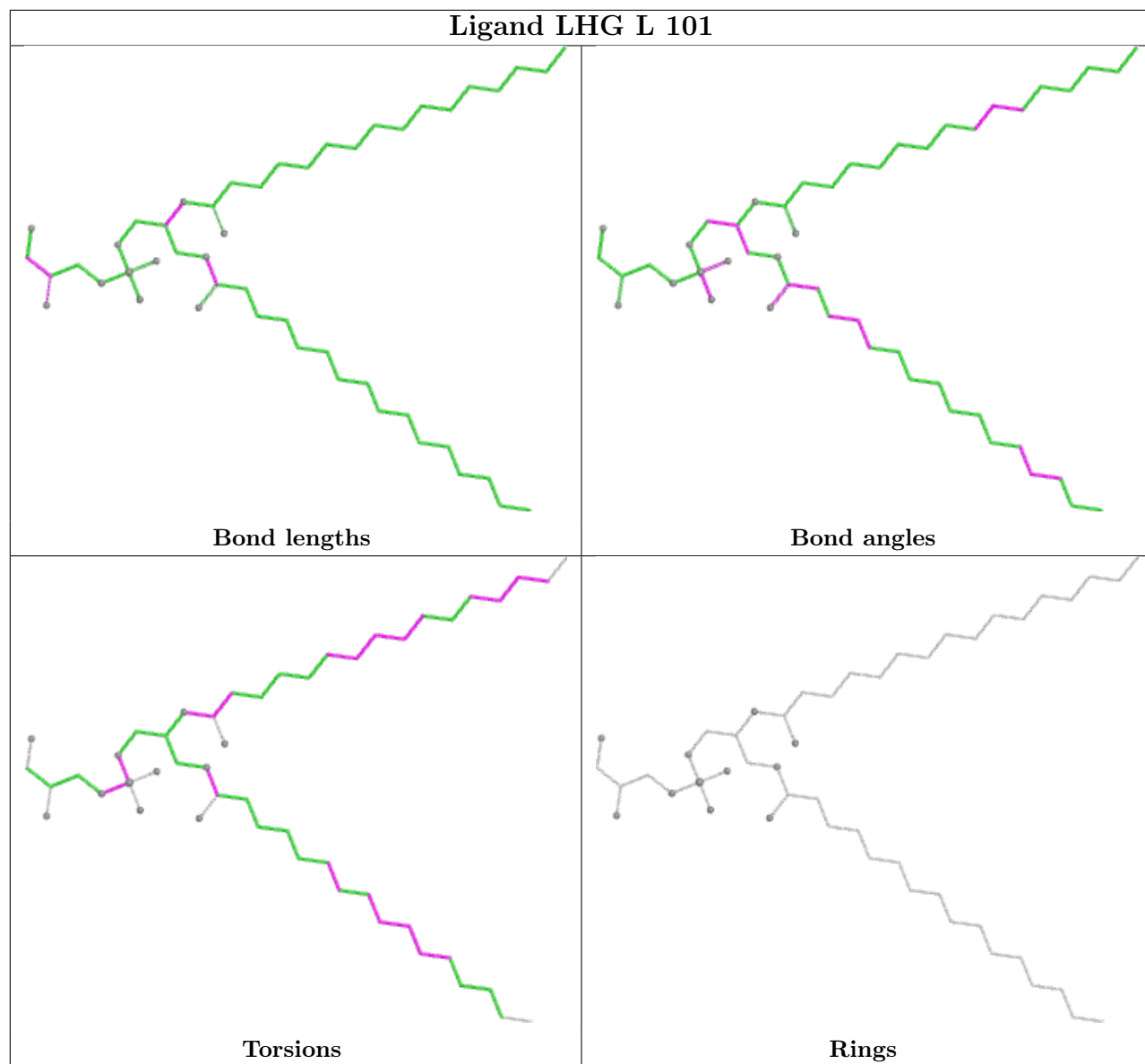


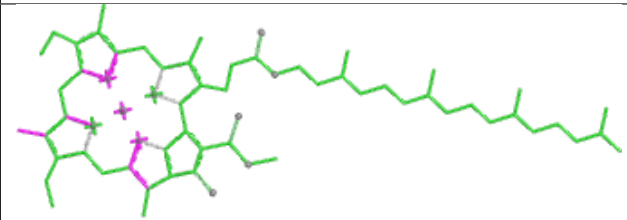
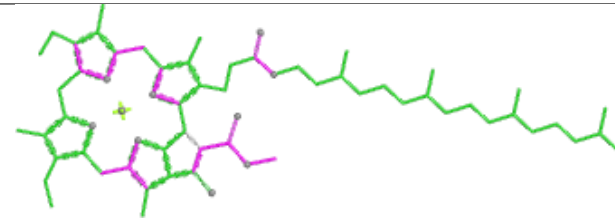
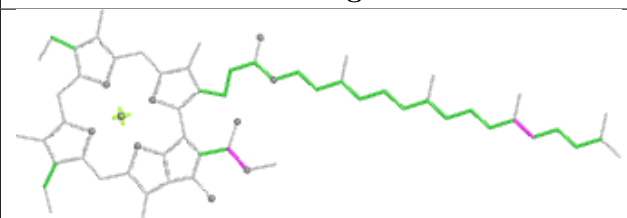
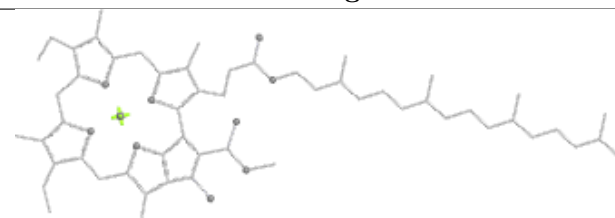


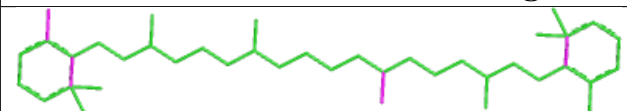
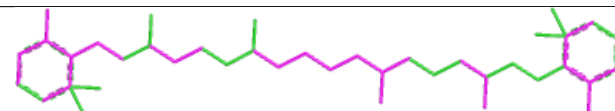
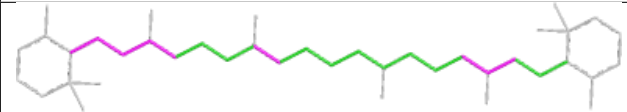
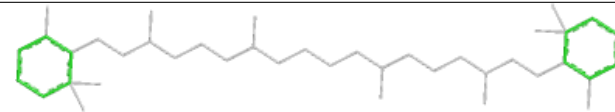


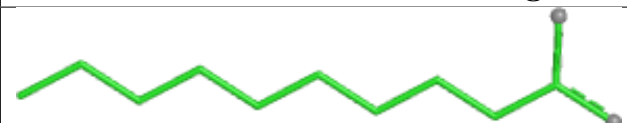
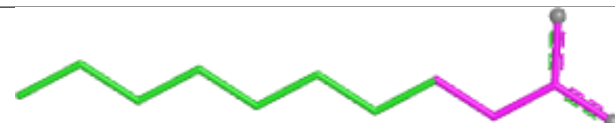
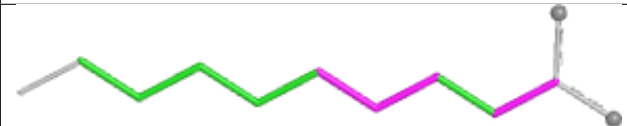
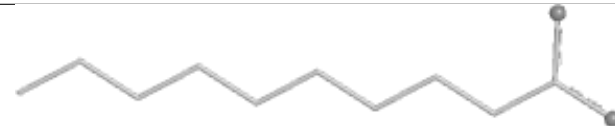


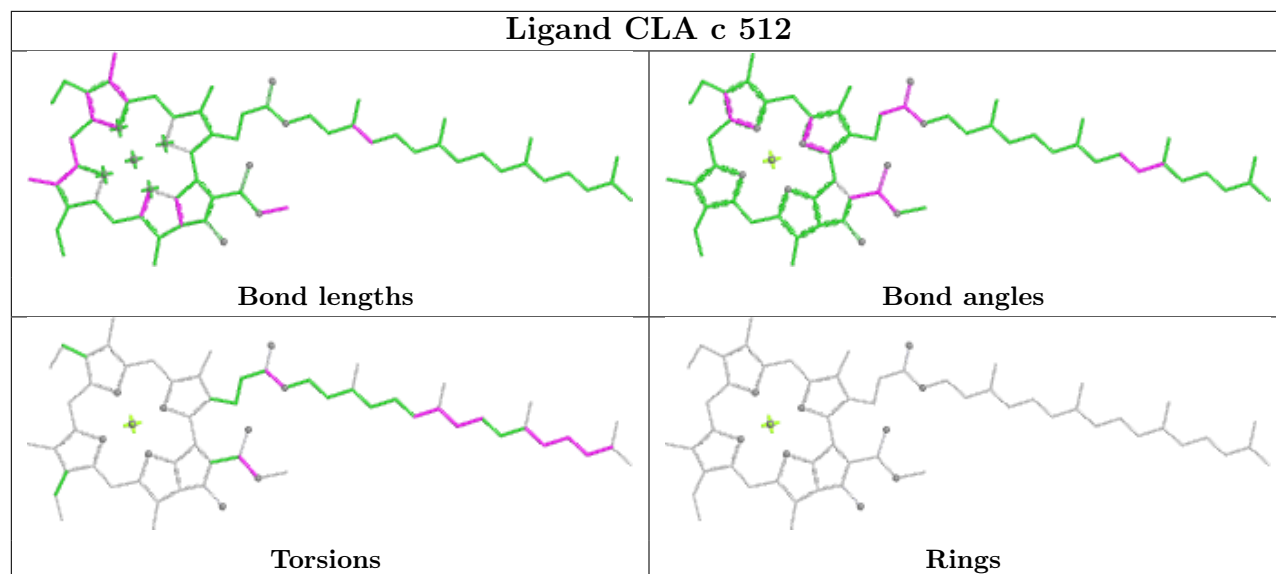
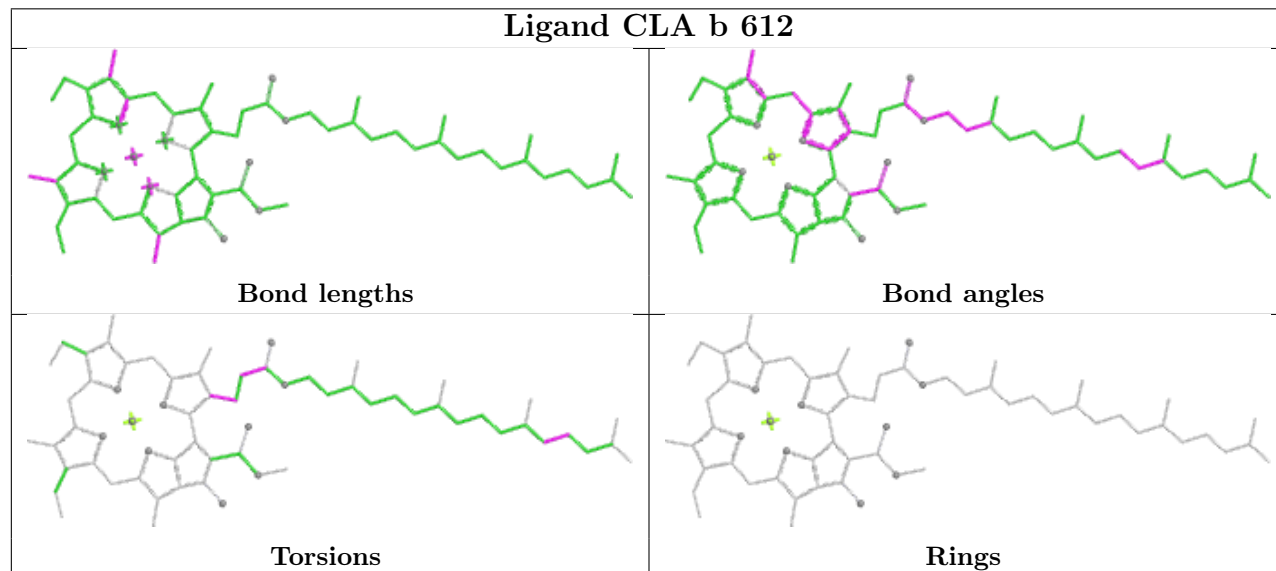


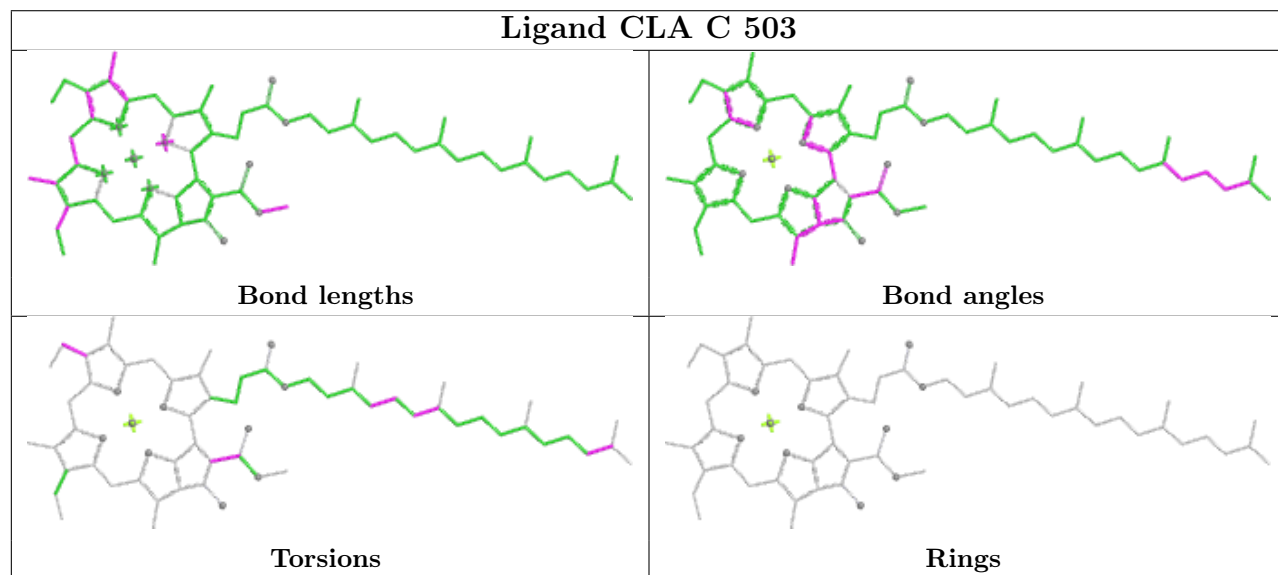
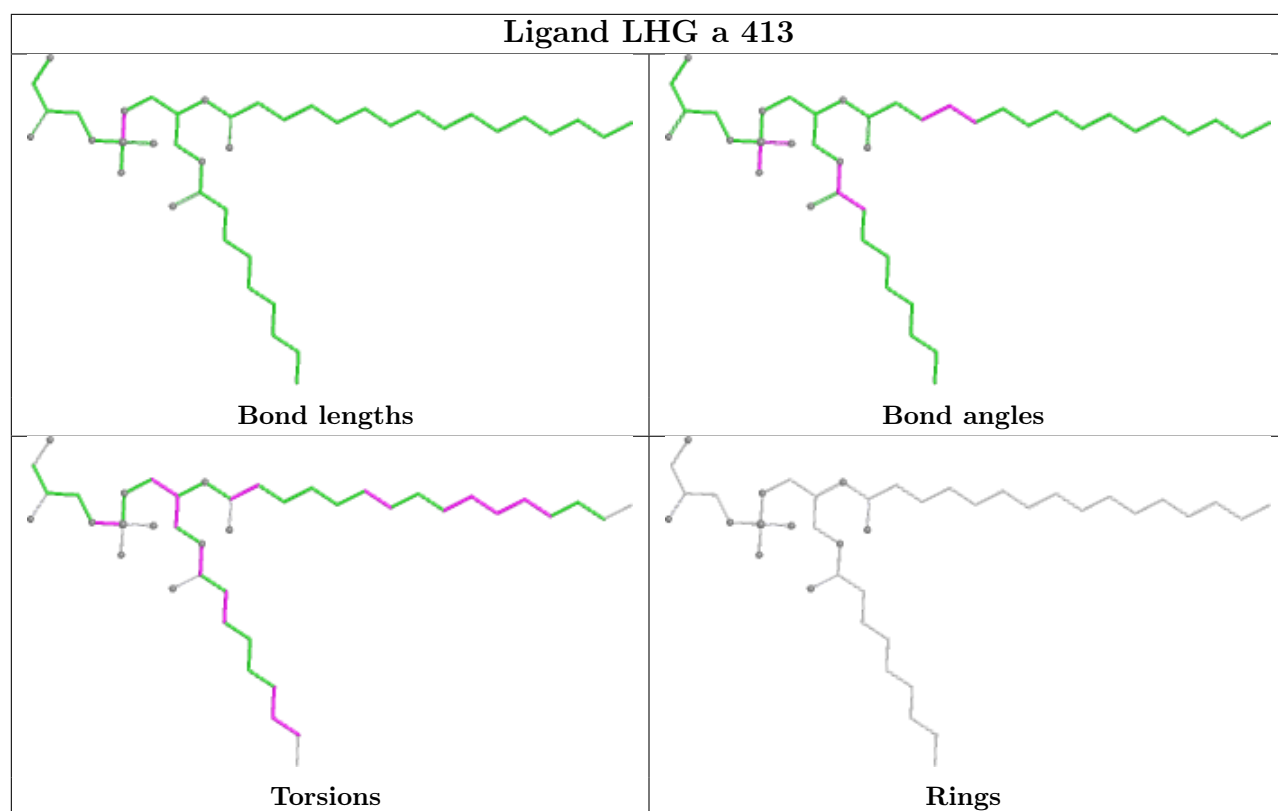


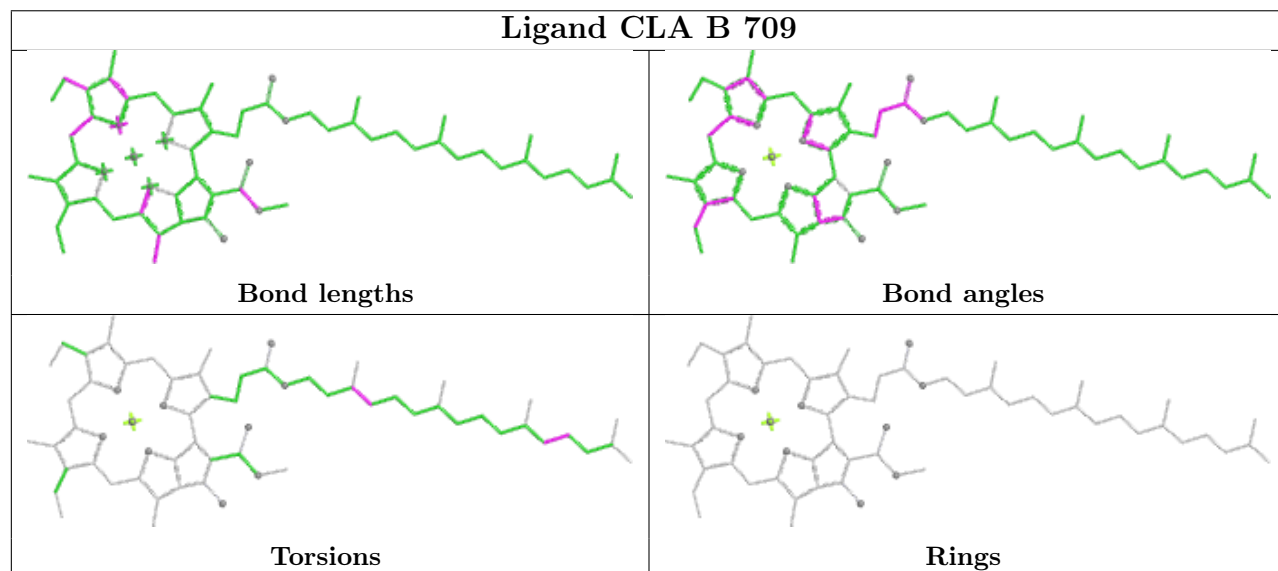
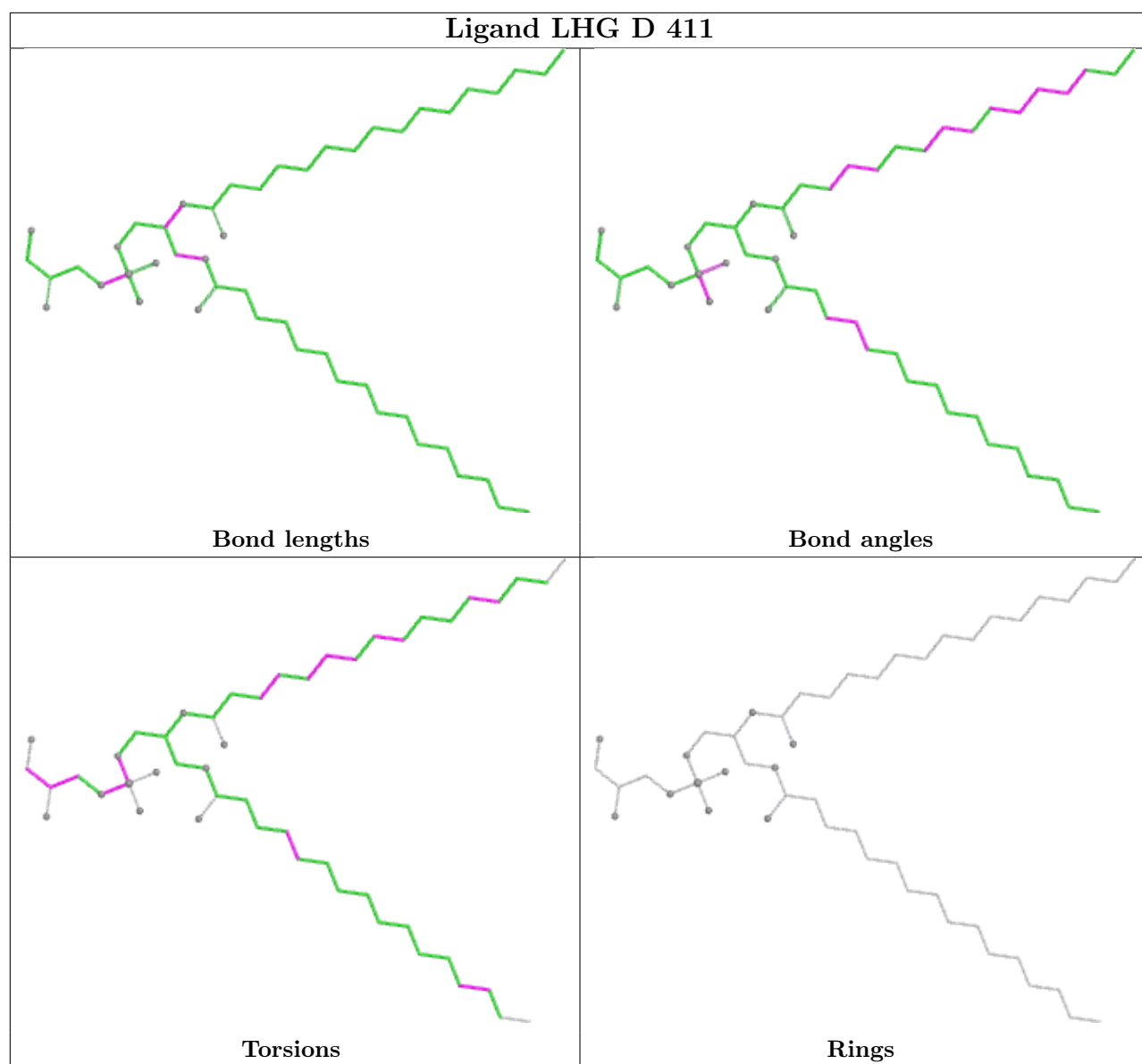
Ligand CLA C 502	
	
Bond lengths	Bond angles
	
Torsions	Rings

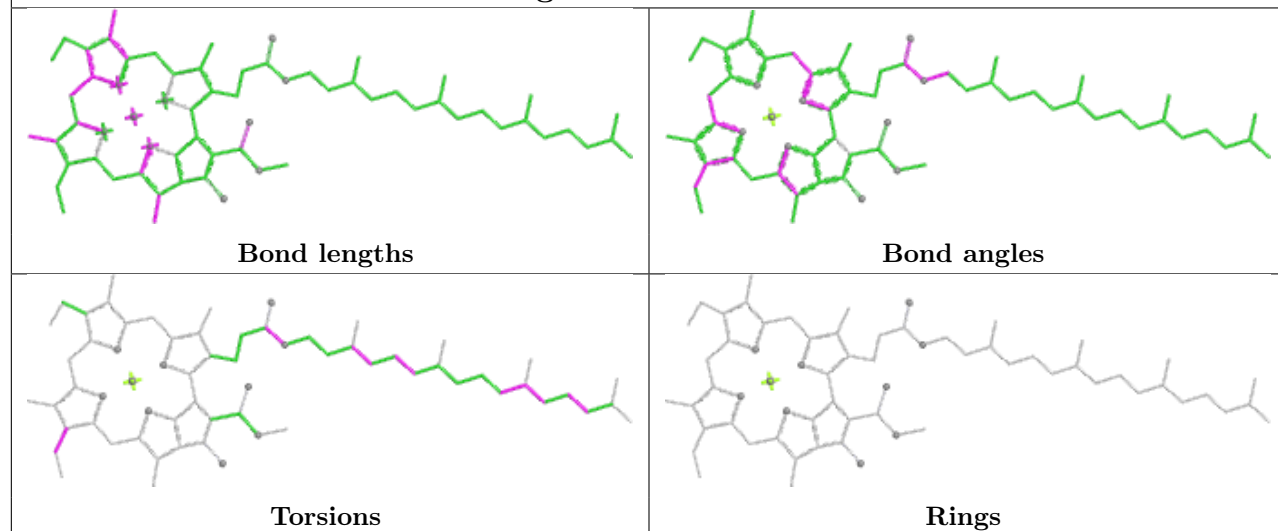
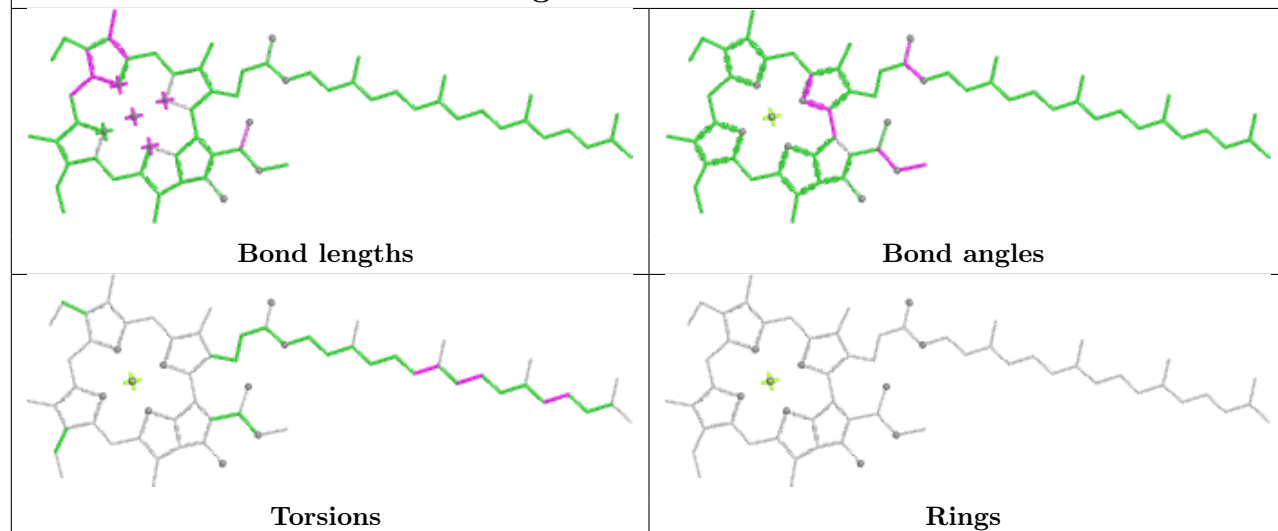
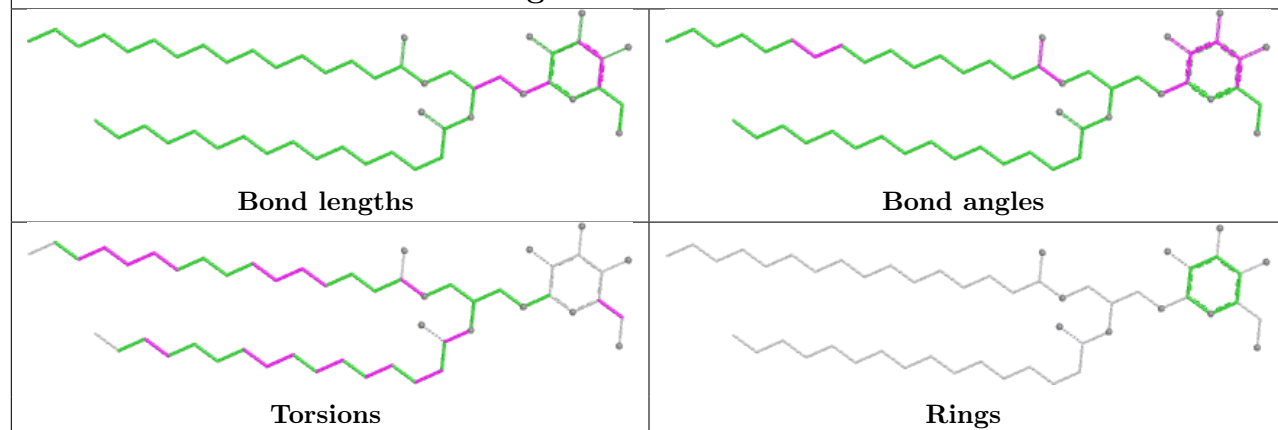
Ligand BCR b 617	
	
Bond lengths	Bond angles
	
Torsions	Rings

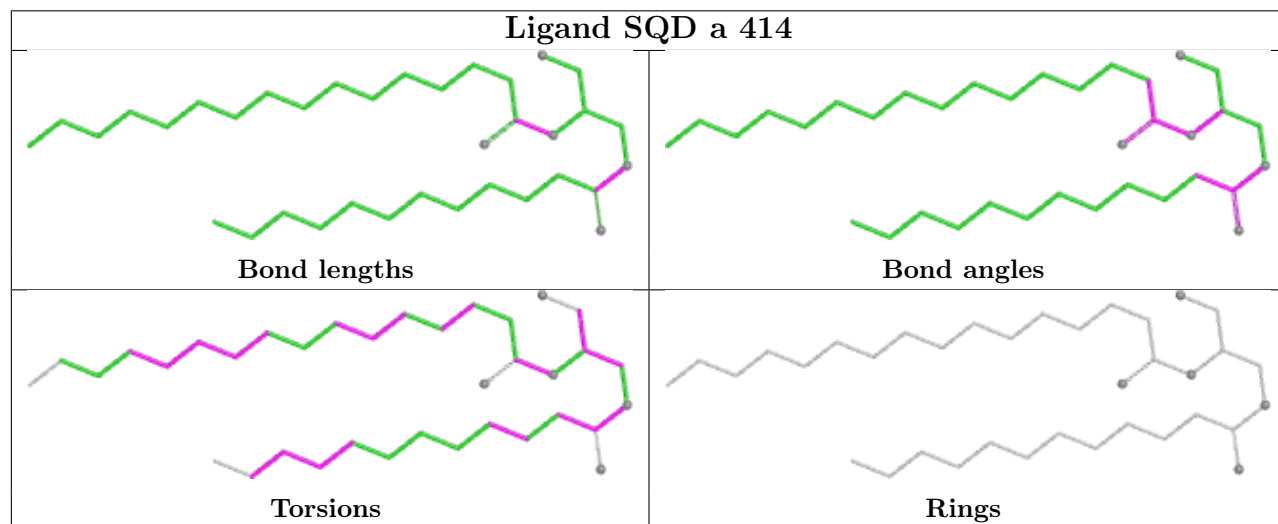
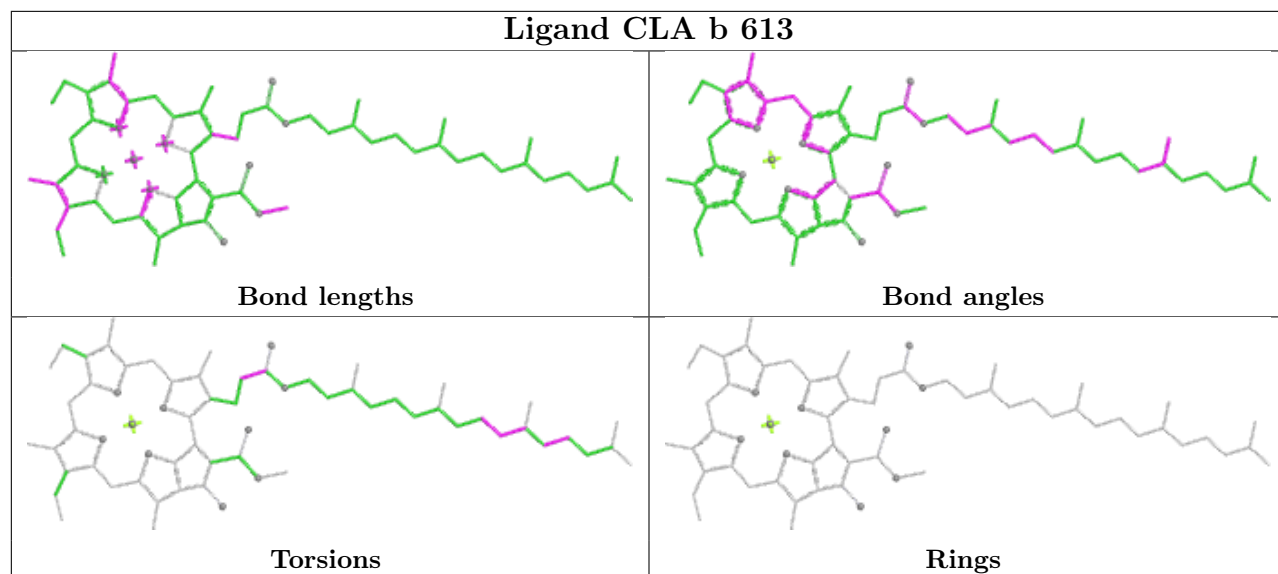
Ligand STE B 724	
	
Bond lengths	Bond angles
	
Torsions	Rings

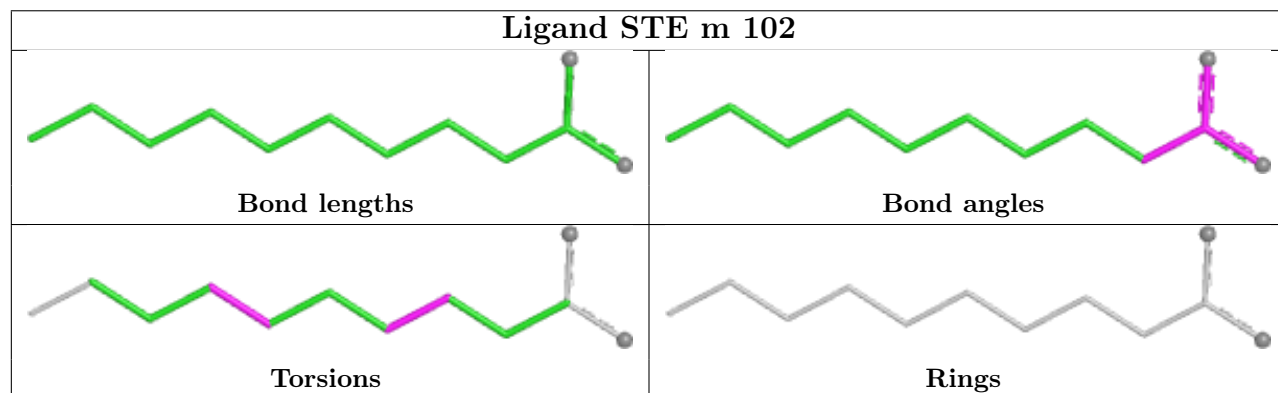
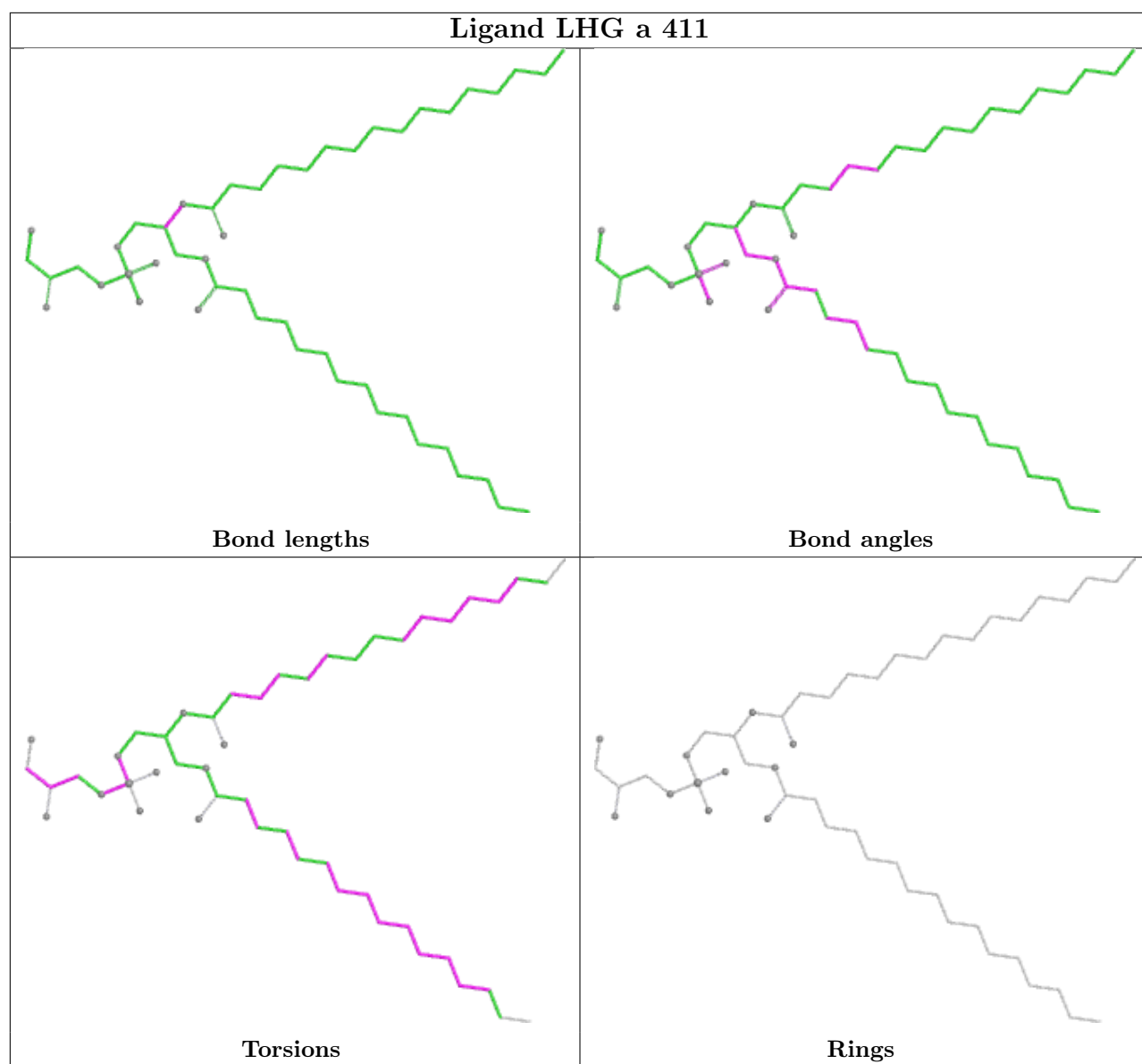
Ligand CLA c 512**Ligand CLA b 612**



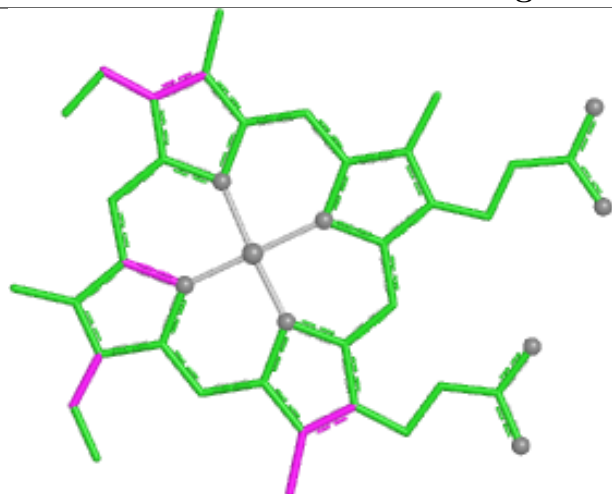


Ligand CLA a 405**Ligand CLA C 512****Ligand LMG D 409**

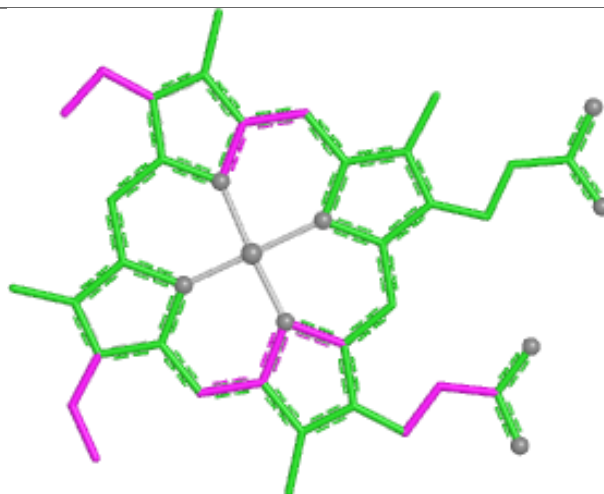




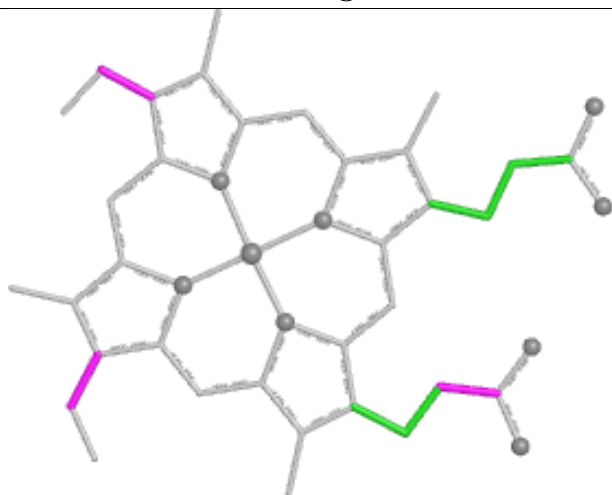
Ligand HEC v 201



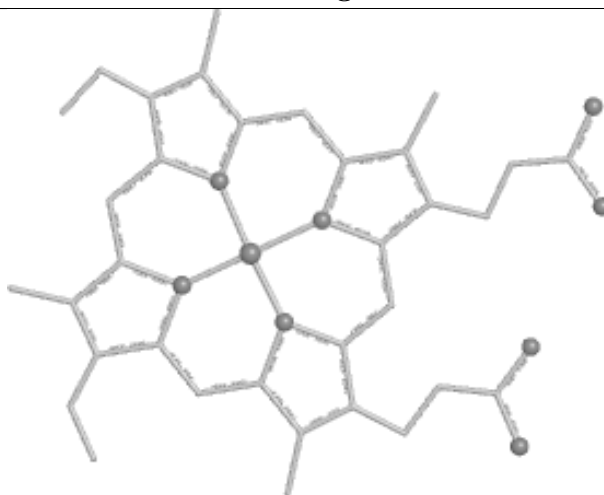
Bond lengths



Bond angles

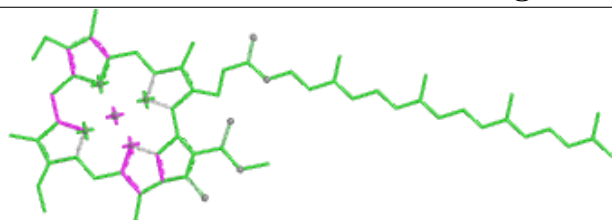


Torsions

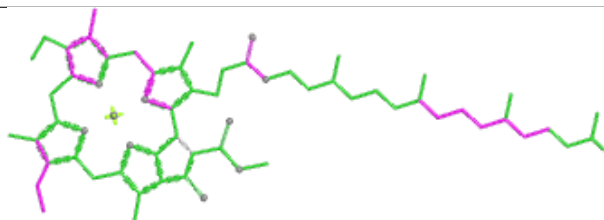


Rings

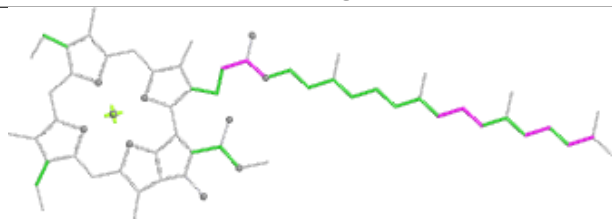
Ligand CLA B 712



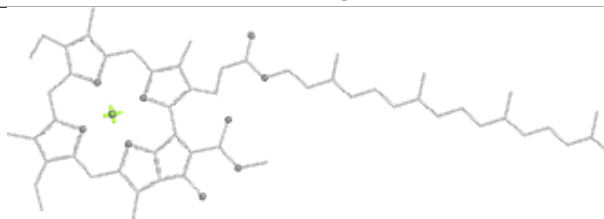
Bond lengths



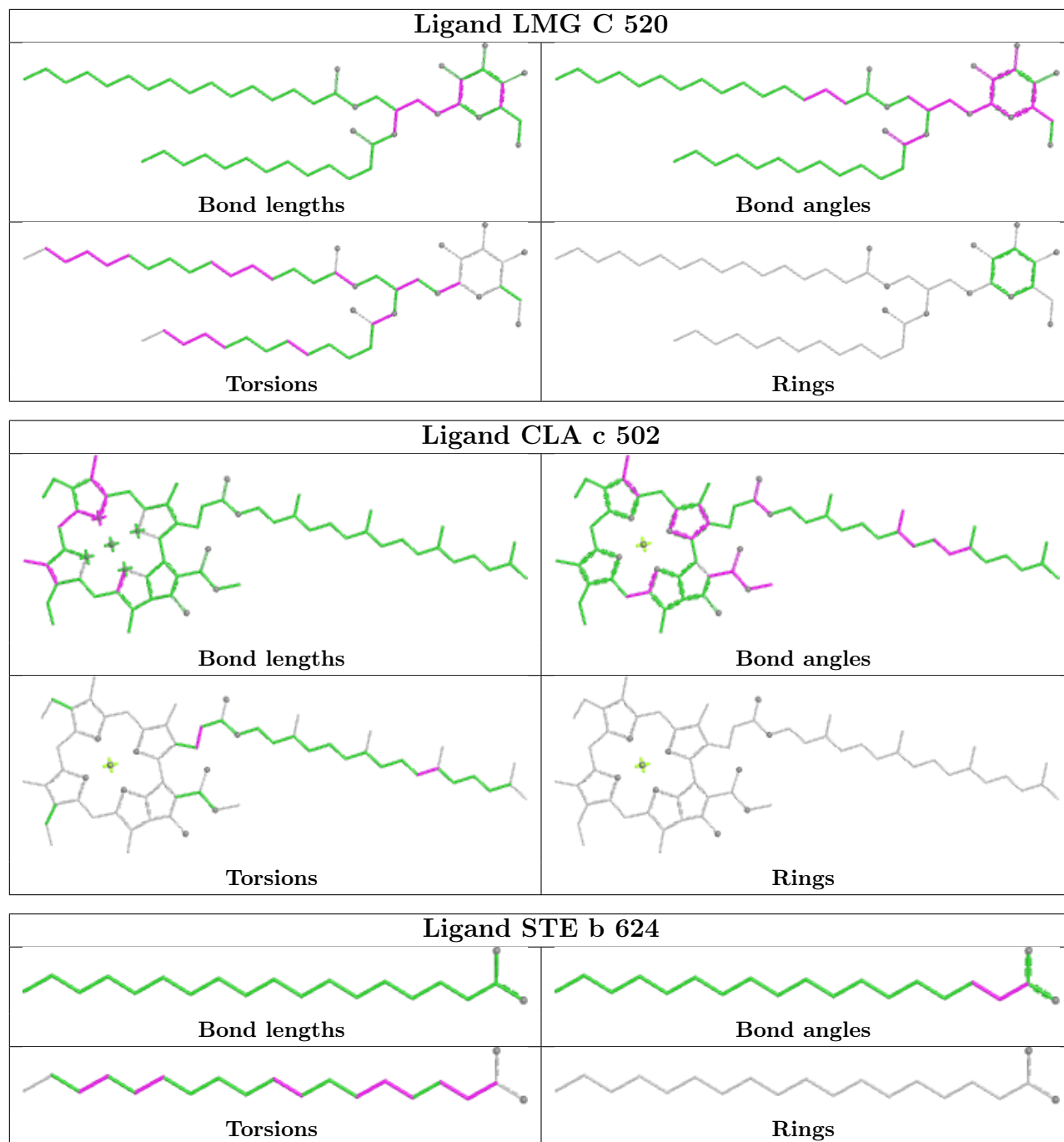
Bond angles

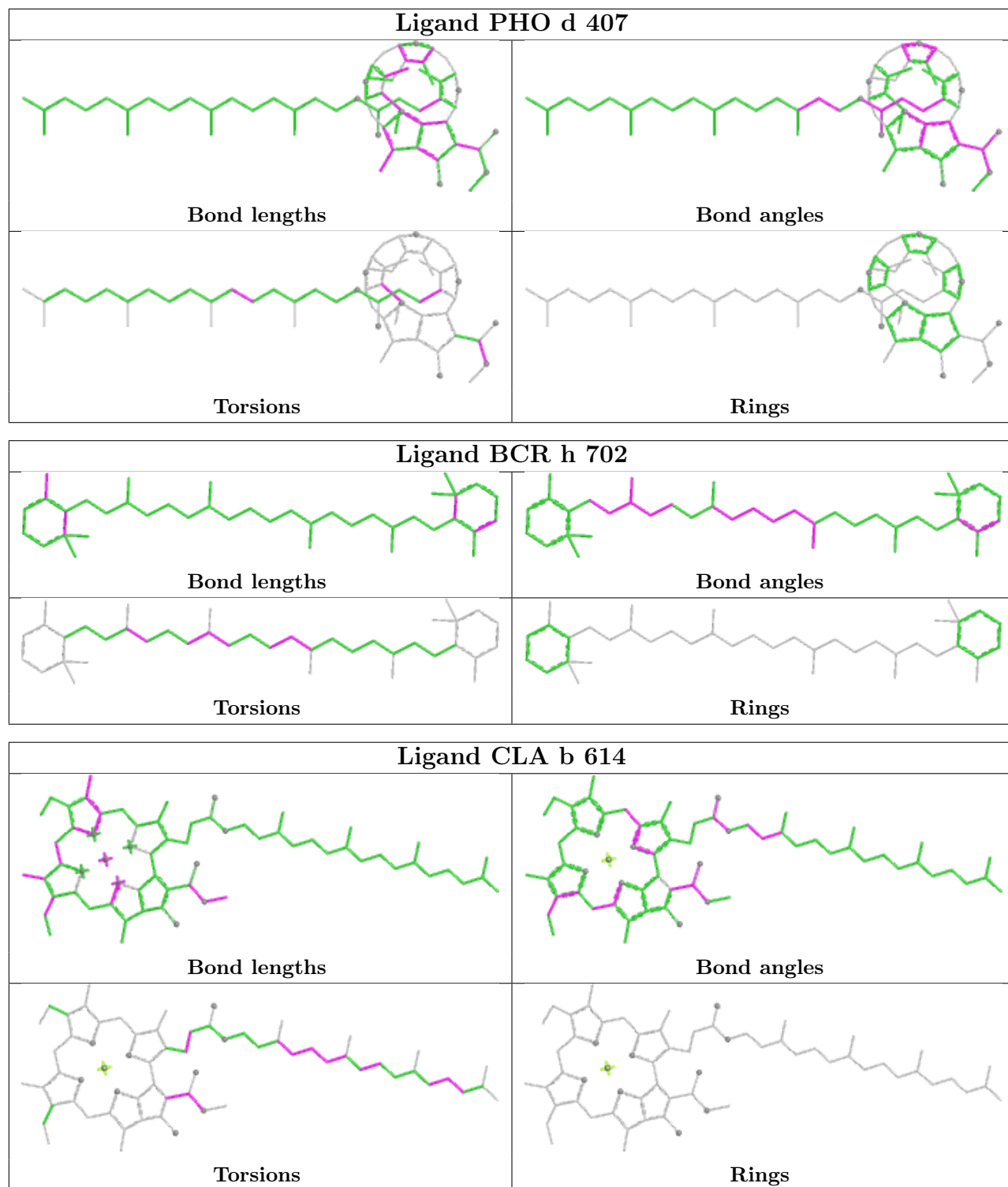


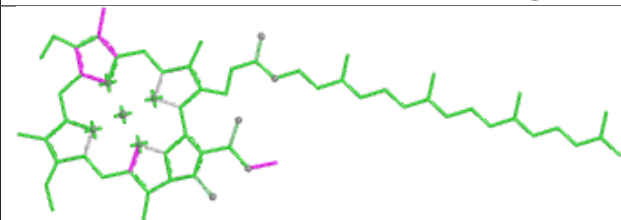
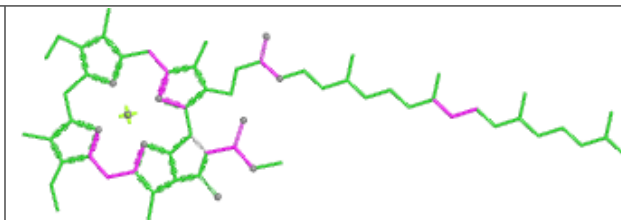
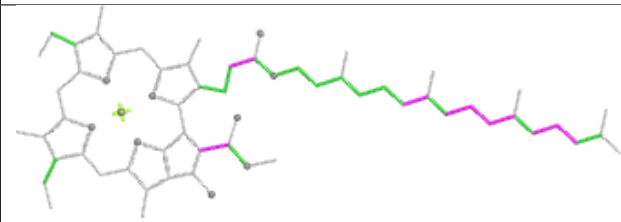
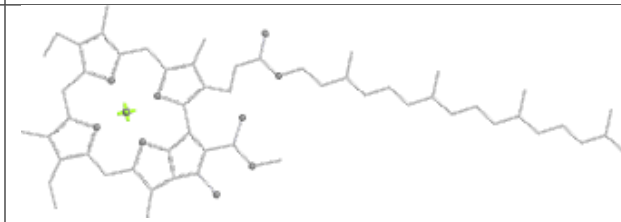
Torsions



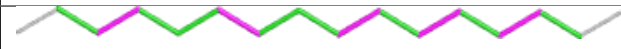







Rings

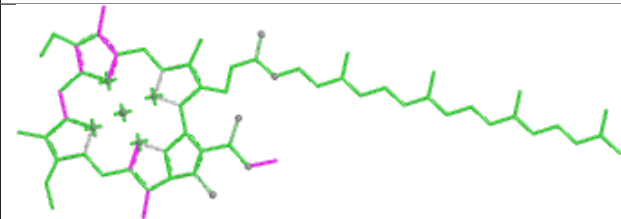
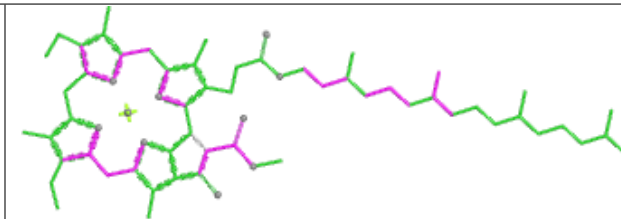
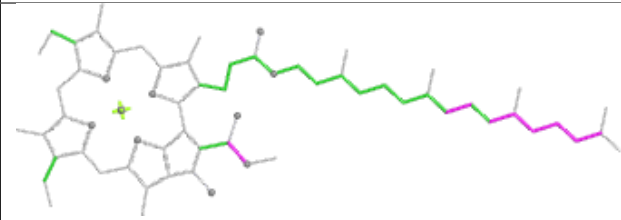
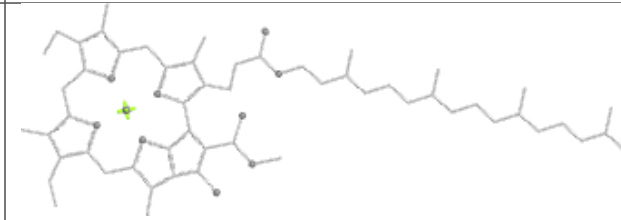


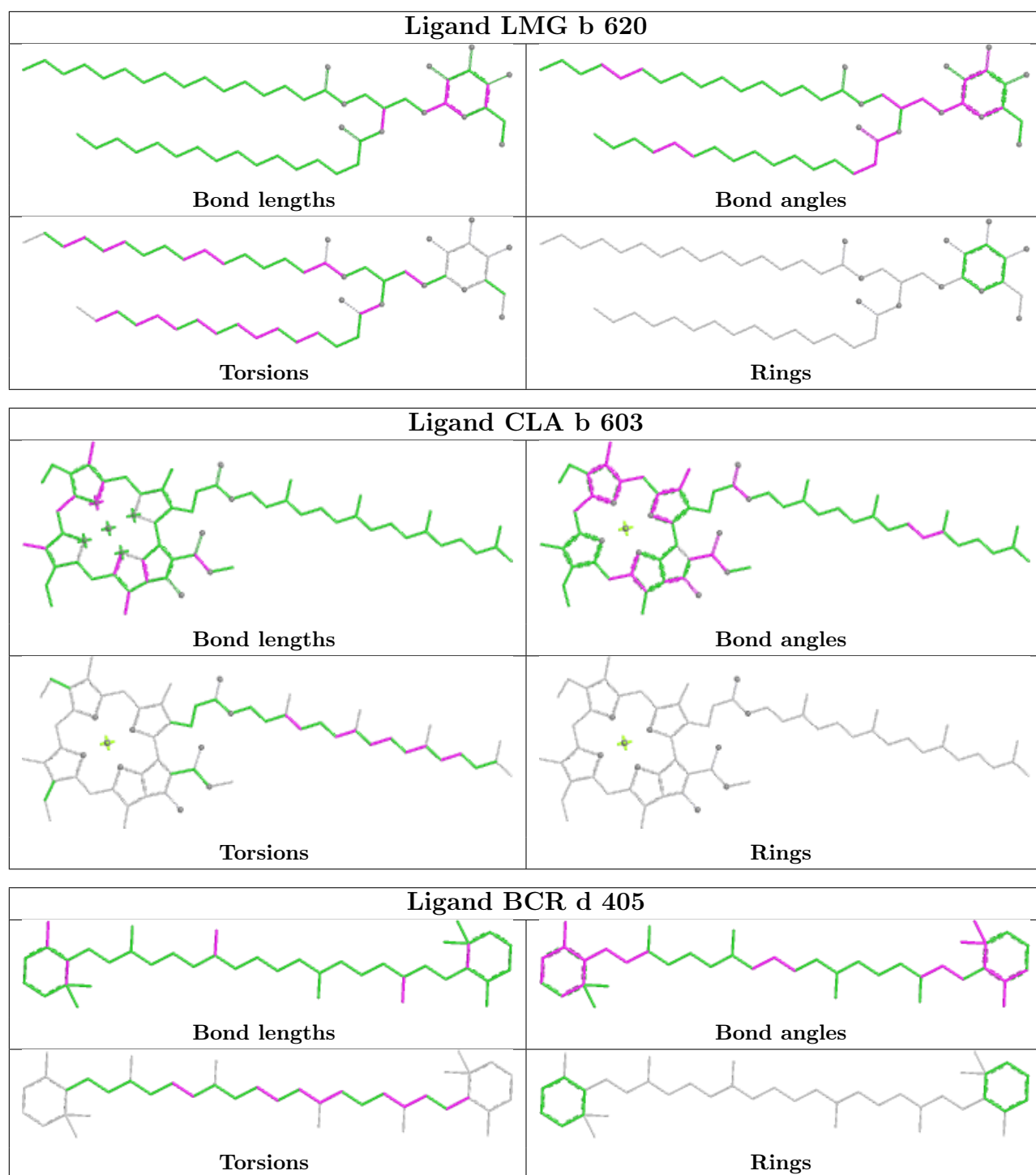


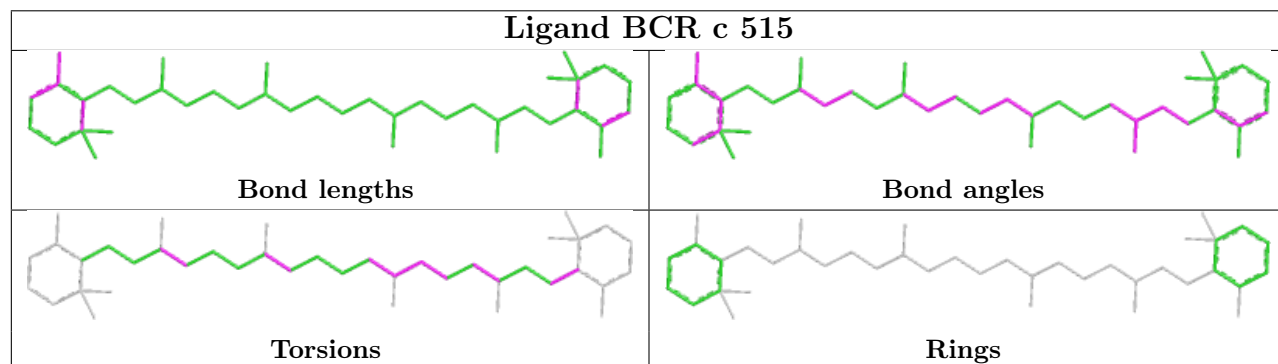
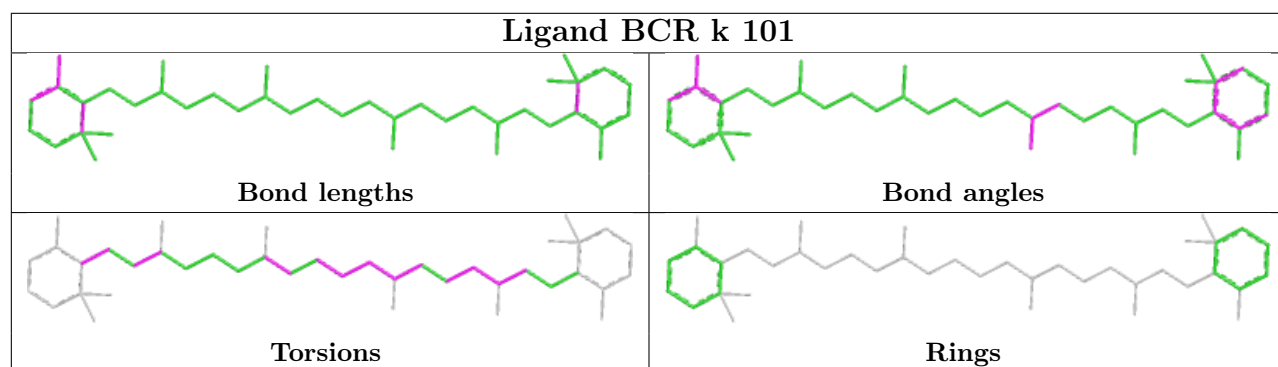
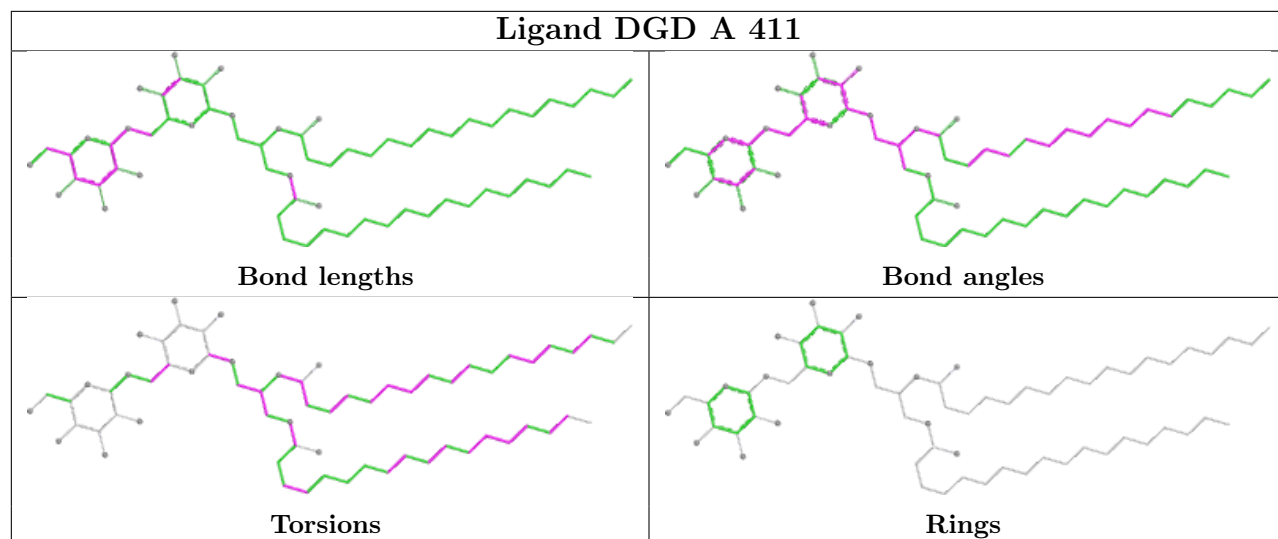
Ligand CLA c 510	
	Bond lengths
	Bond angles
	Torsions
	Rings

Ligand STE B 726	
	Bond lengths
	Bond angles
	Torsions
	Rings

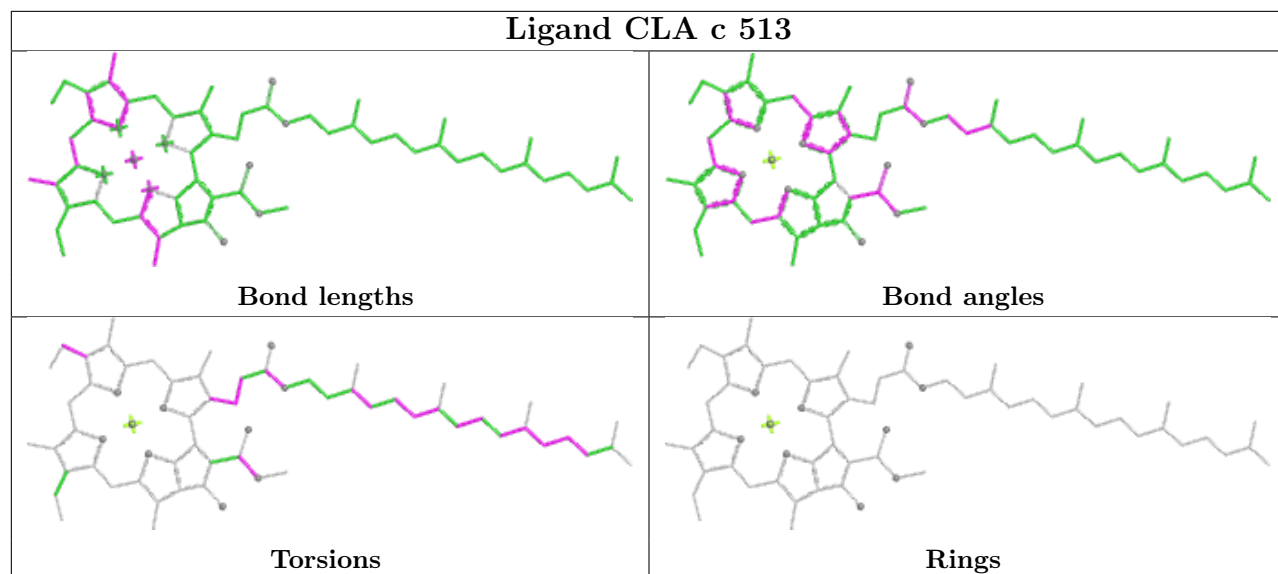
Ligand STE a 417	
	Bond lengths
	Bond angles
	Torsions
	Rings

Ligand CLA B 711	
	Bond lengths
	Bond angles
	Torsions
	Rings

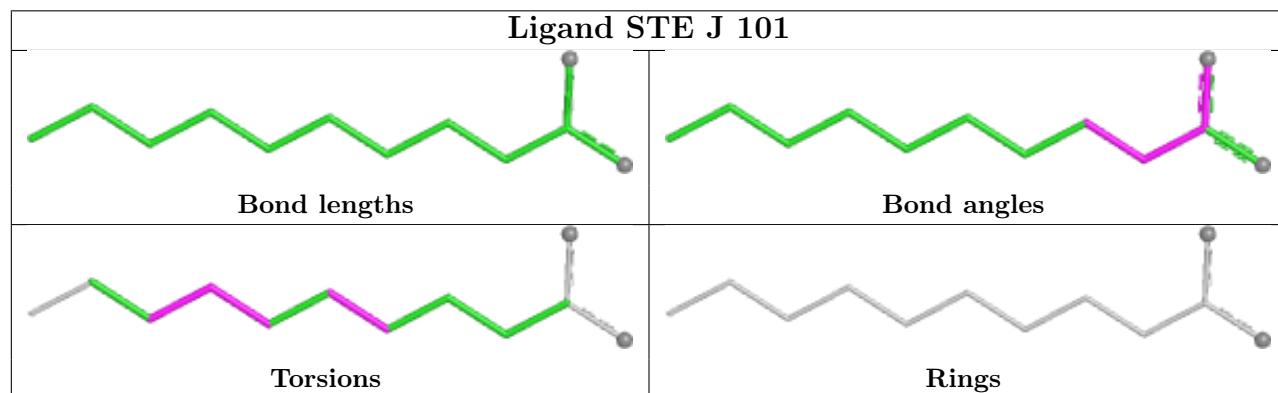




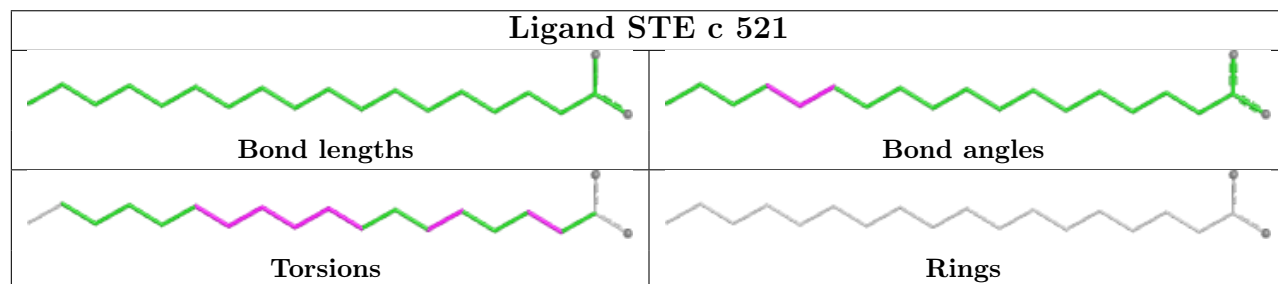
Ligand CLA c 513

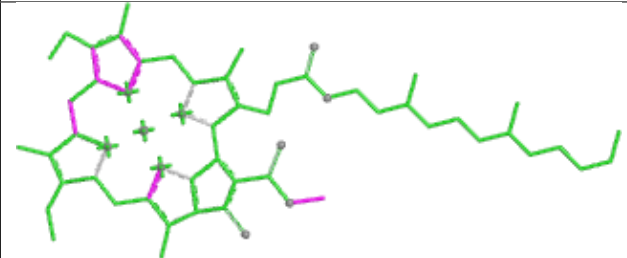
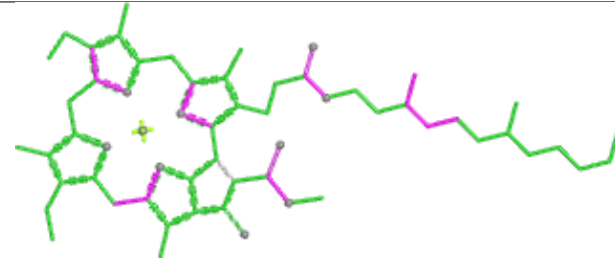
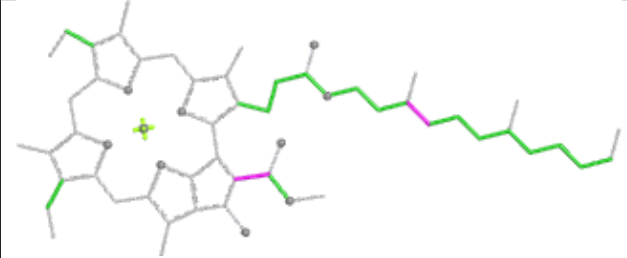
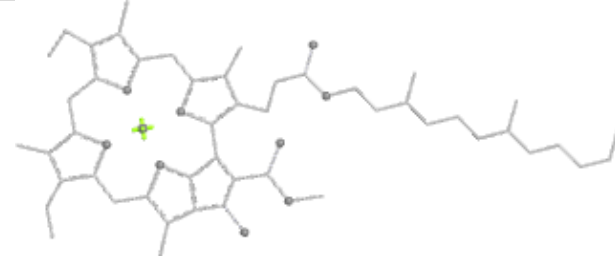


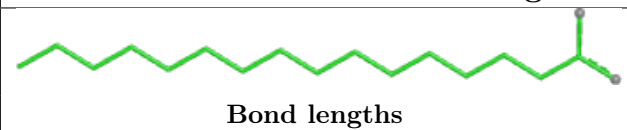
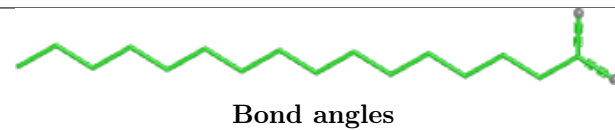
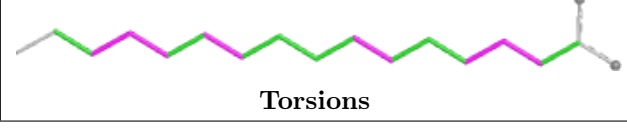
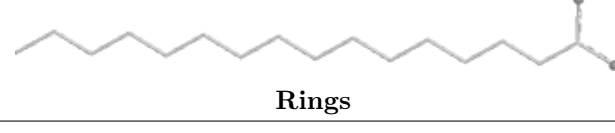
Ligand STE J 101

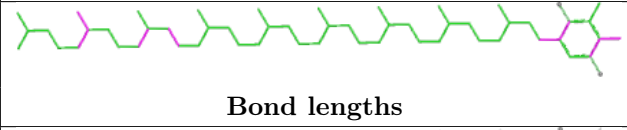
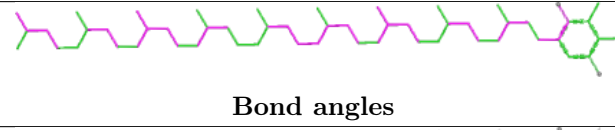

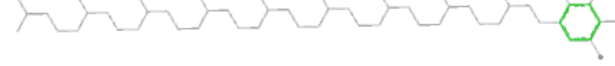


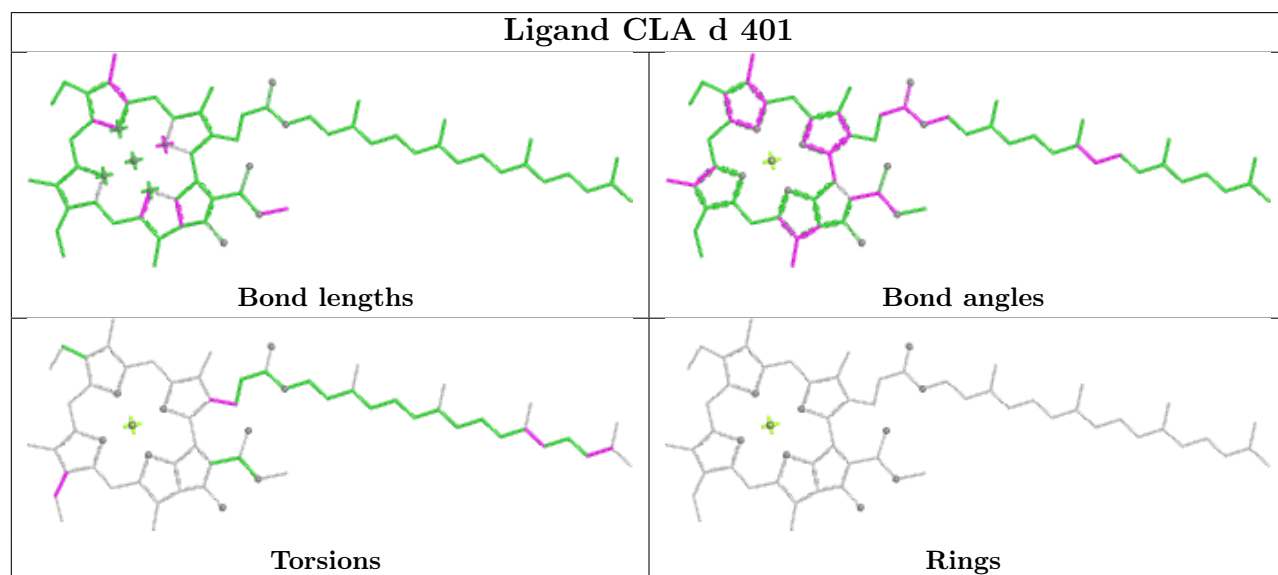
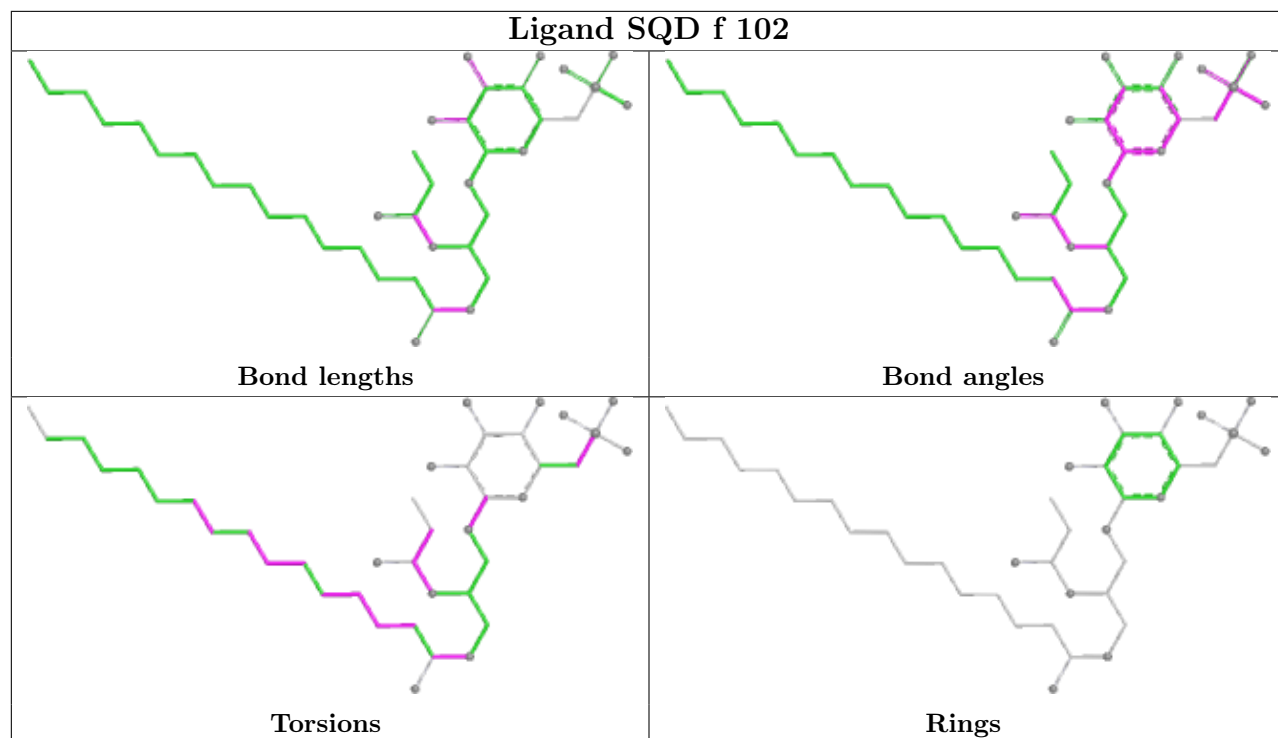
Ligand STE c 521

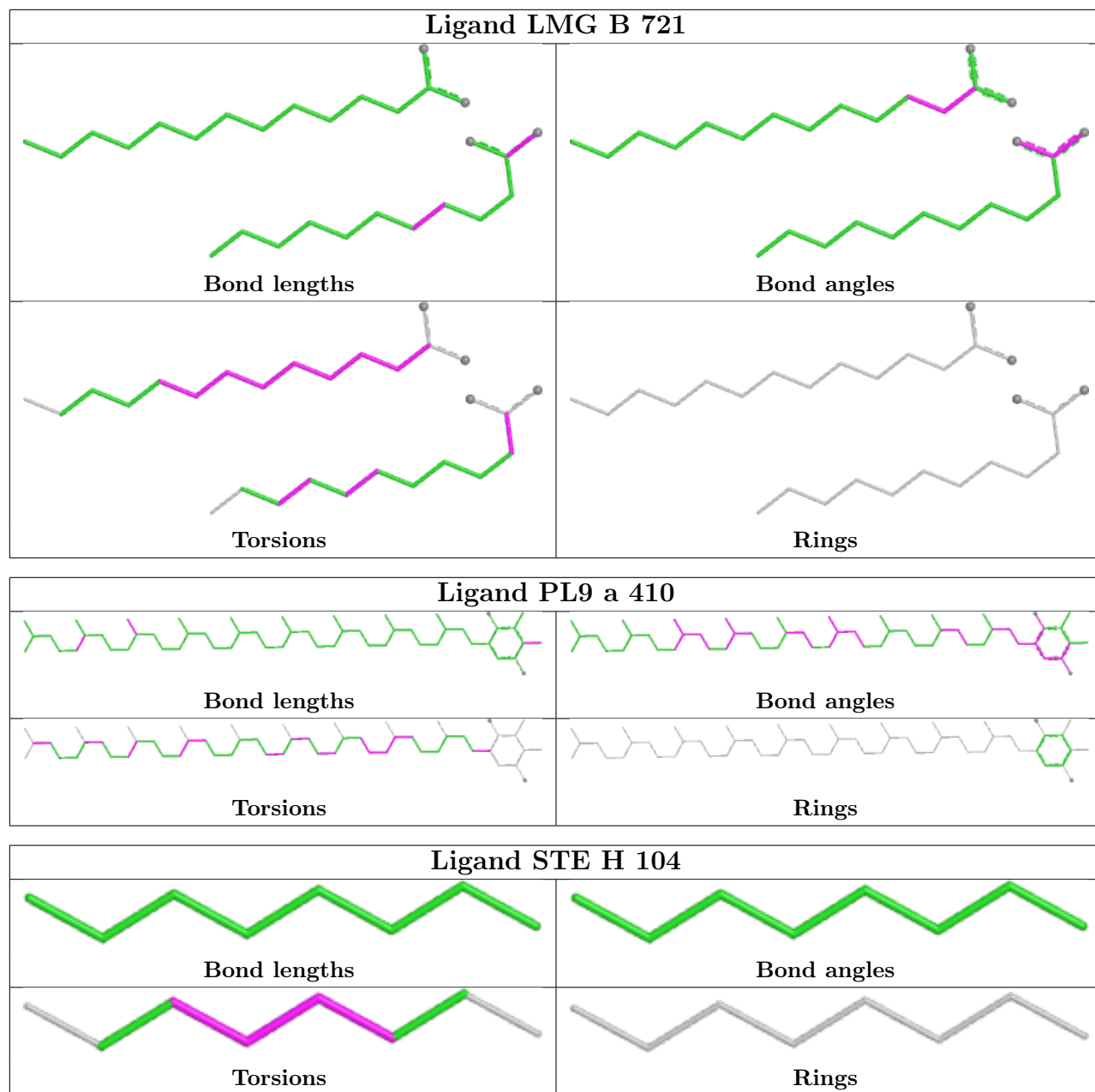


Ligand CLA C 505	
	
Bond lengths	Bond angles
	
Torsions	Rings

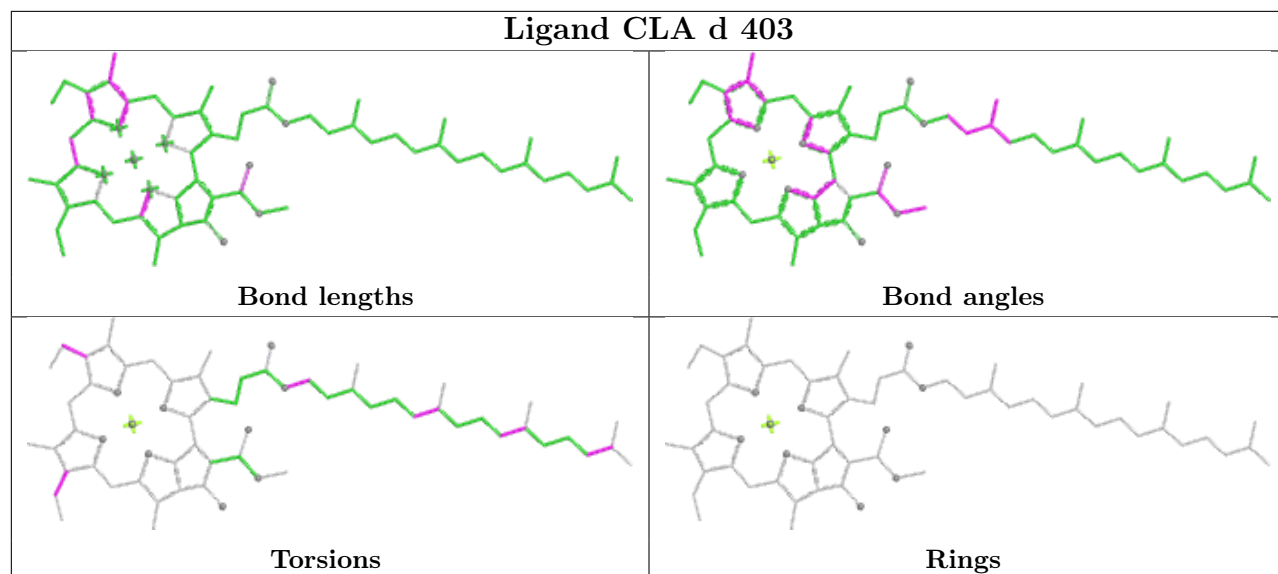
Ligand STE B 725	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PL9 d 406	
	
Bond lengths	Bond angles
	
Torsions	Rings

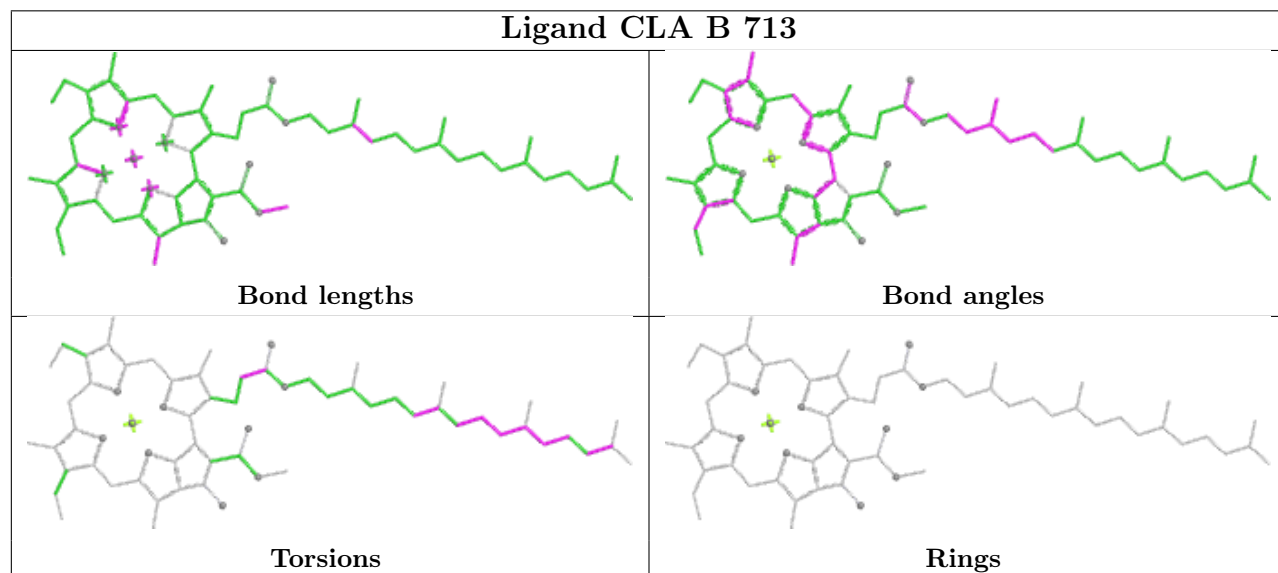




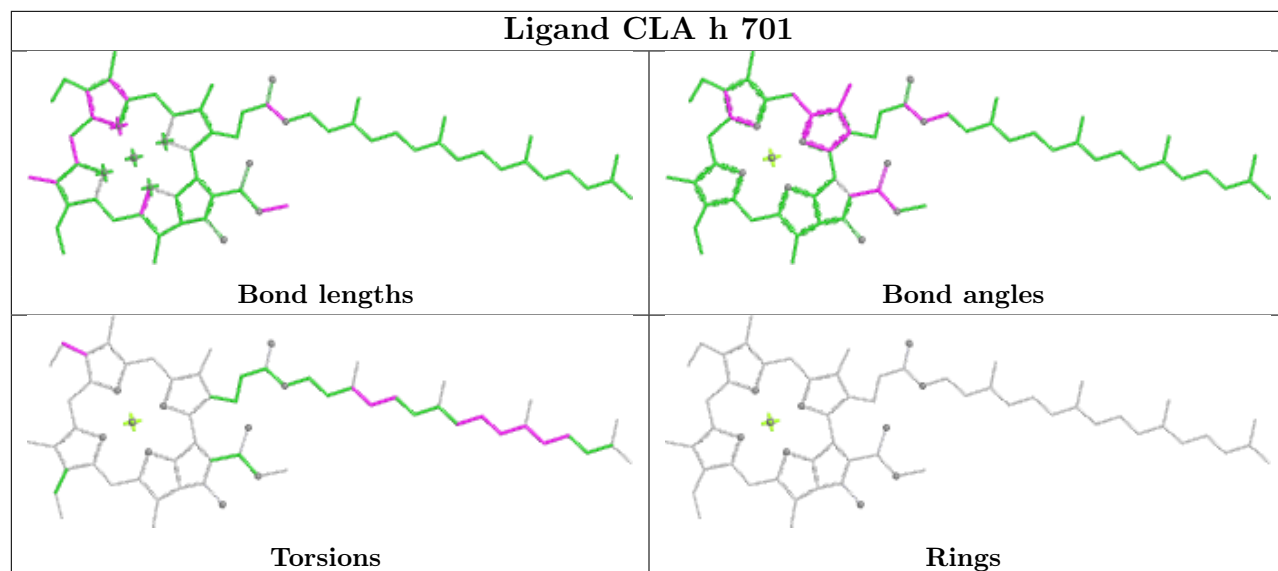
Ligand CLA d 403

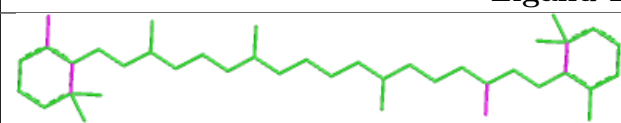
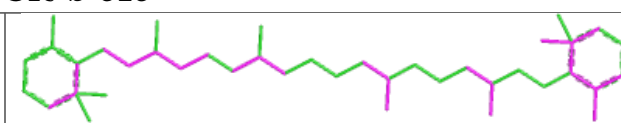
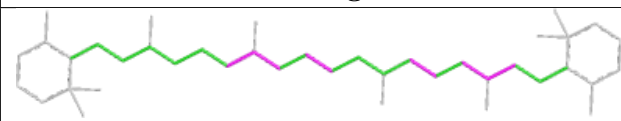
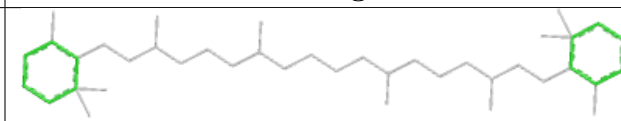



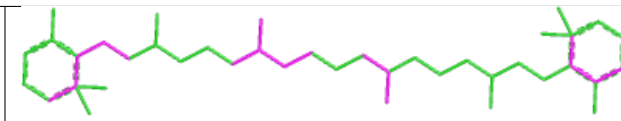
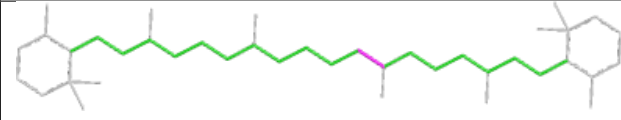
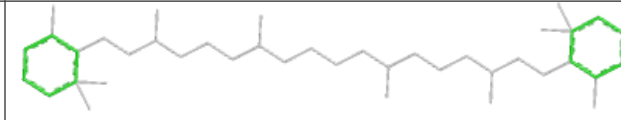
Ligand CLA B 713

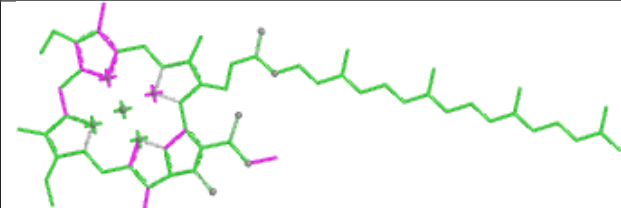
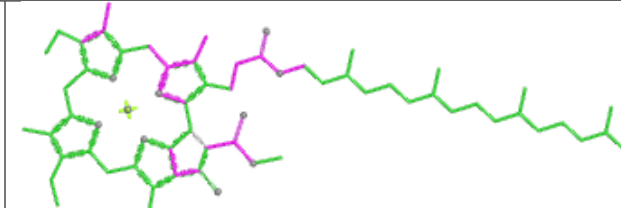
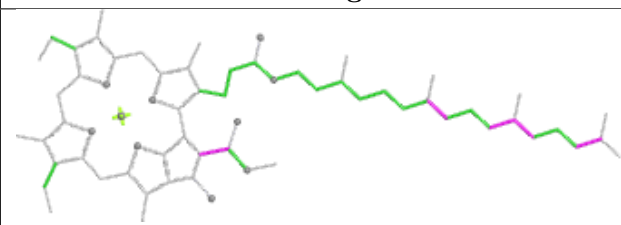
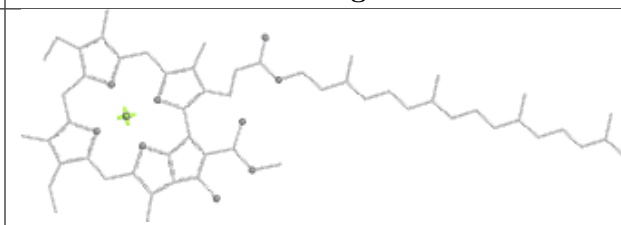



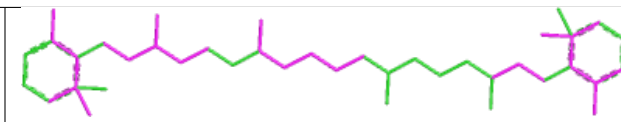
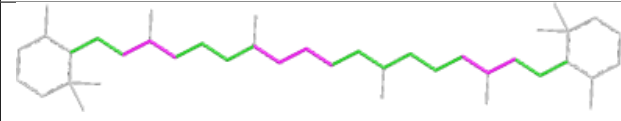
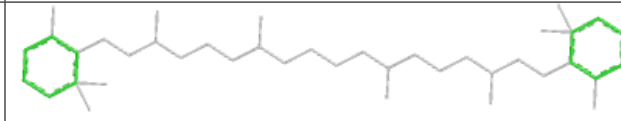
Ligand CLA h 701

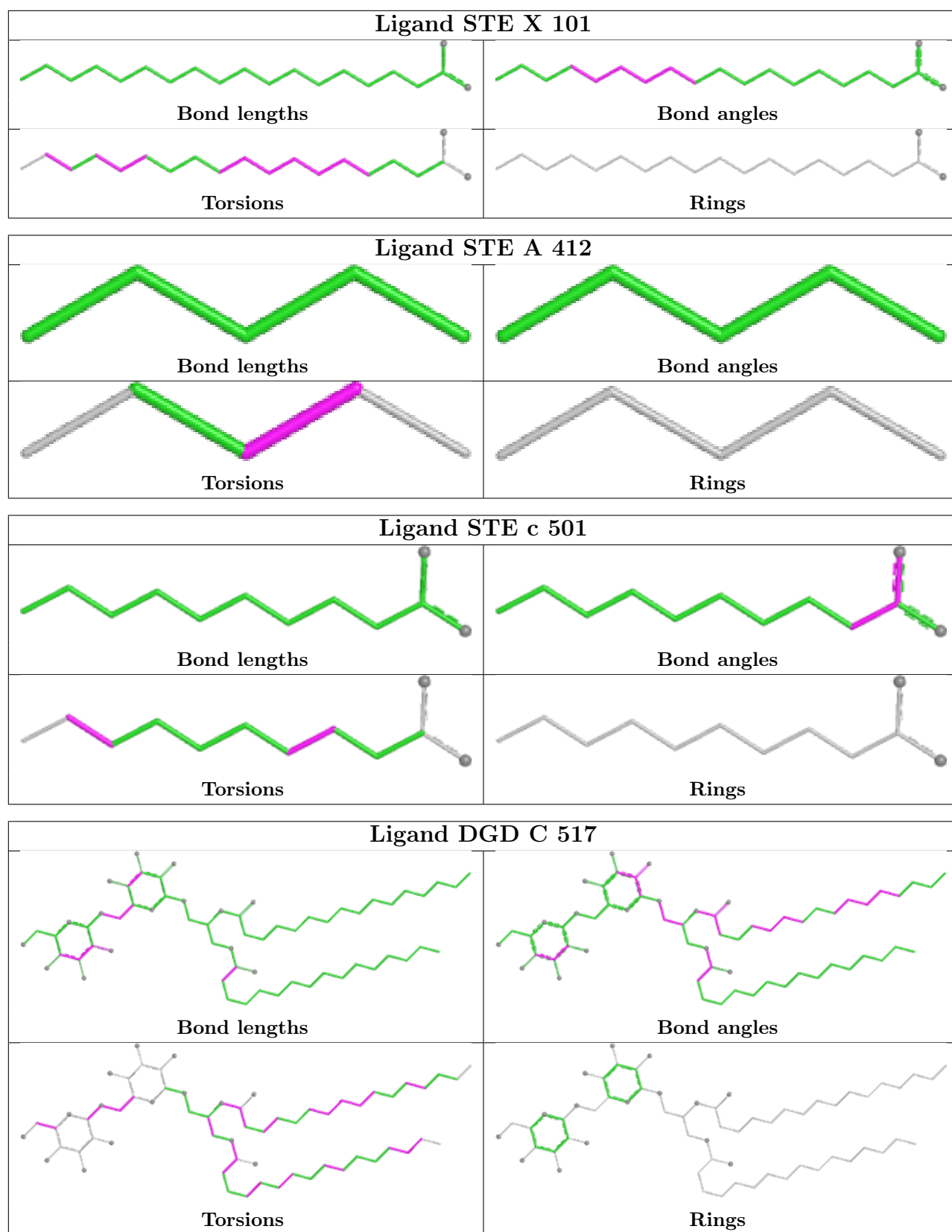


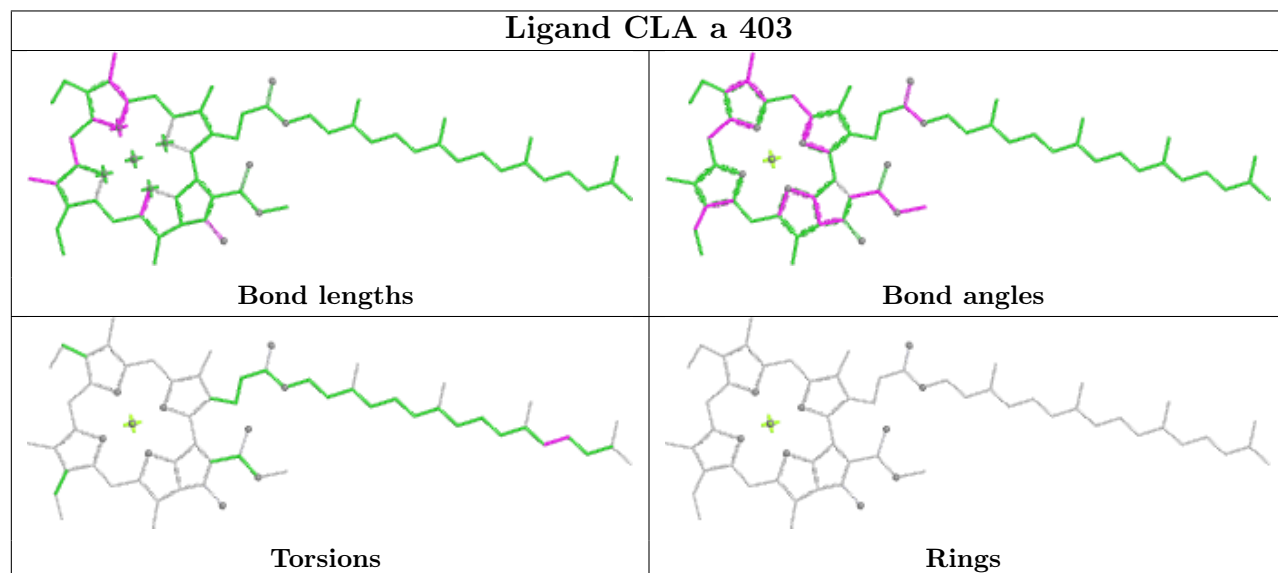
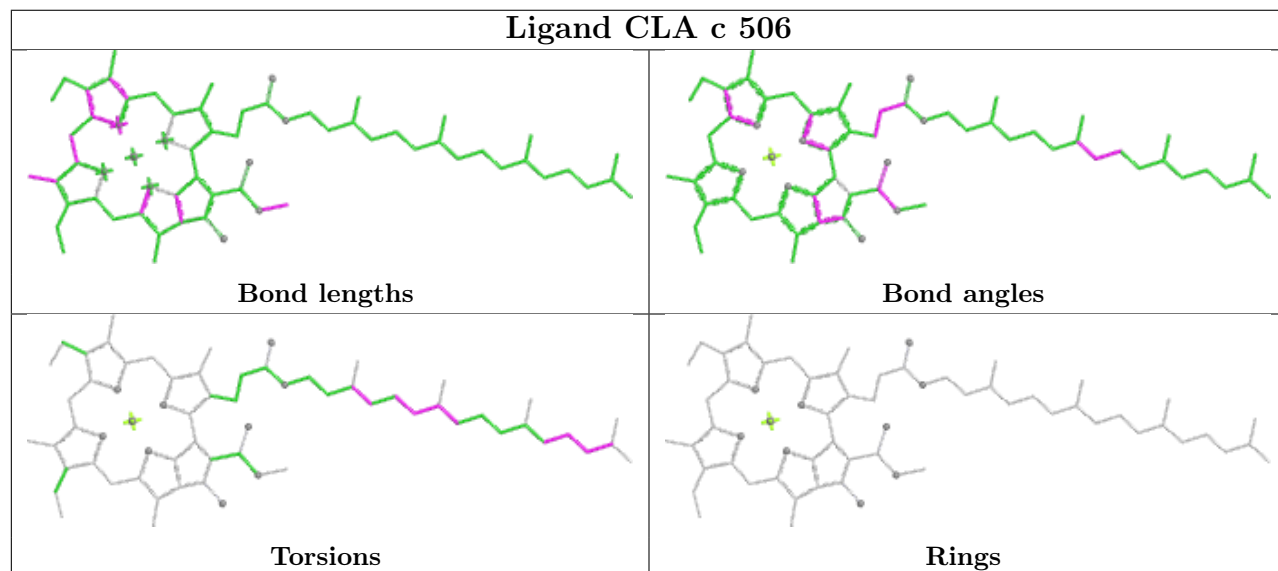
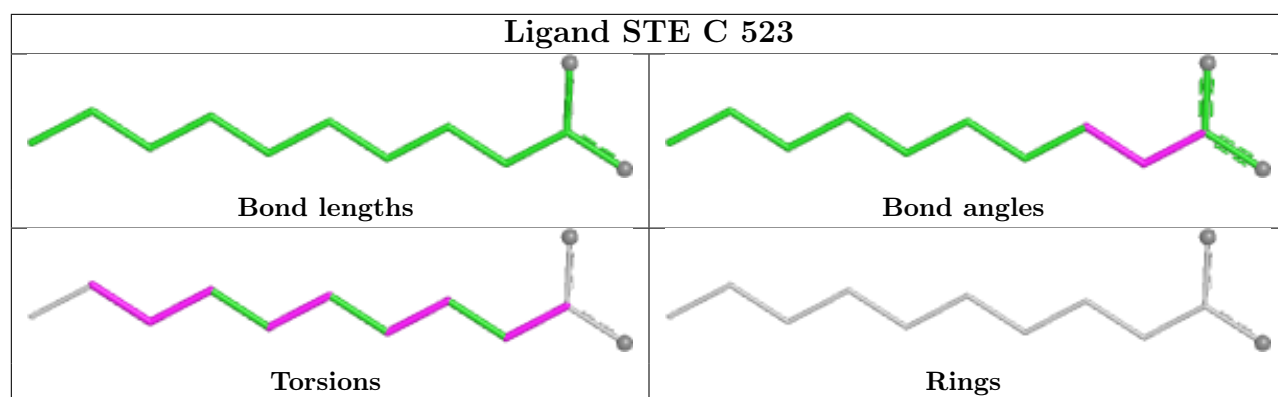
Ligand BCR b 619	
	
Bond lengths	Bond angles
	
Torsions	Rings

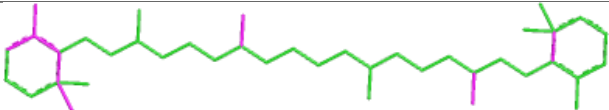
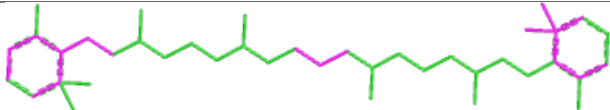
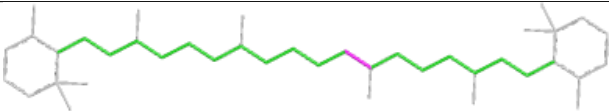
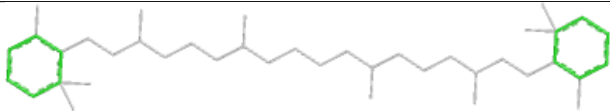
Ligand BCR b 618	
	
Bond lengths	Bond angles
	
Torsions	Rings





Ligand CLA C 508	
	
Bond lengths	Bond angles
	
Torsions	Rings

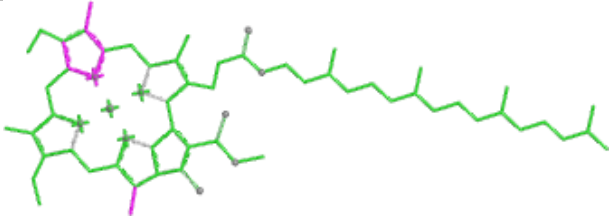
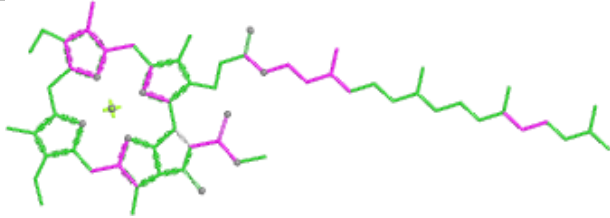
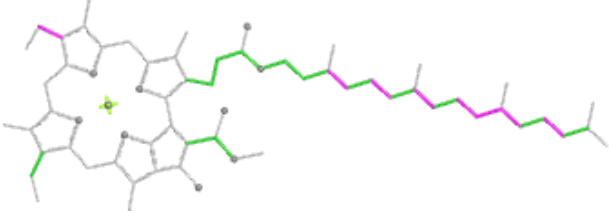
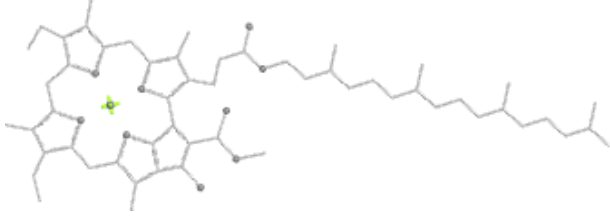
Ligand BCR C 524	
	
Bond lengths	Bond angles
	
Torsions	Rings



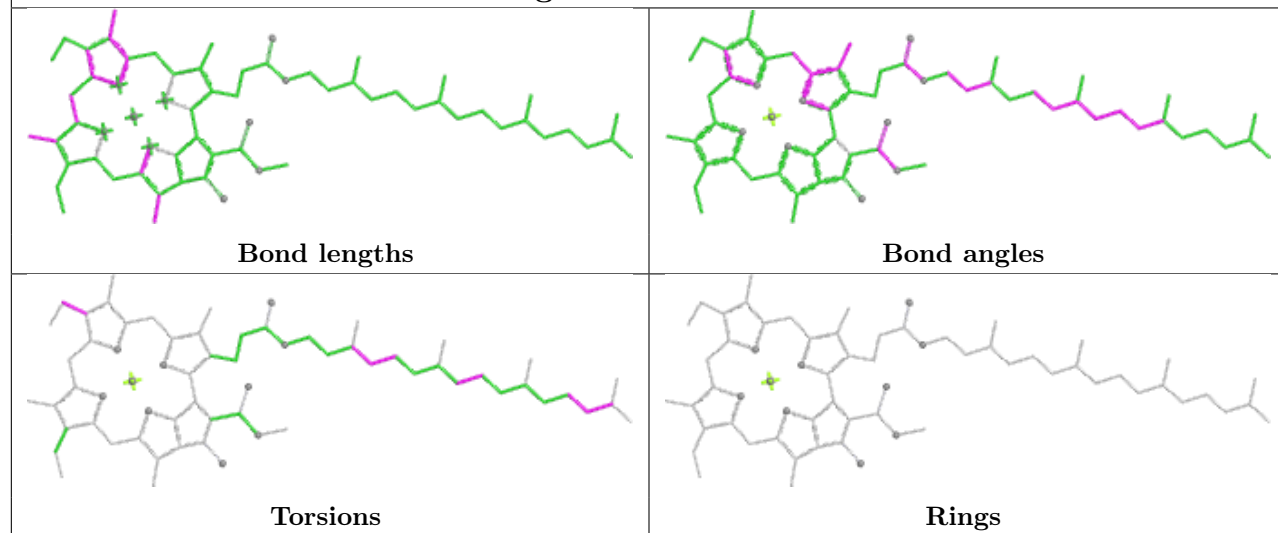


Ligand BCR B 719	
	
Bond lengths	Bond angles
	
Torsions	Rings

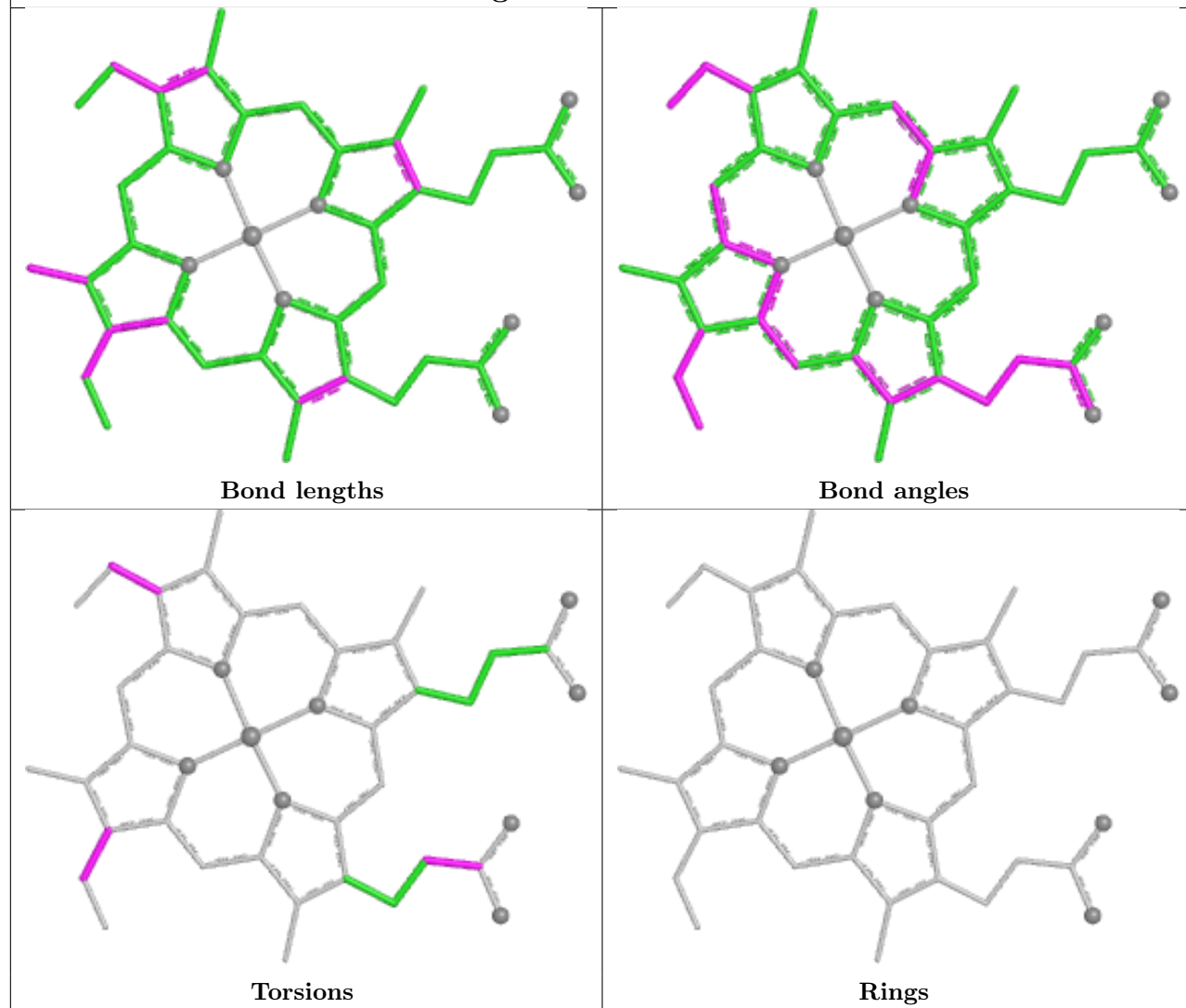
Ligand STE E 103	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 605	
	
Bond lengths	Bond angles
	
Torsions	Rings

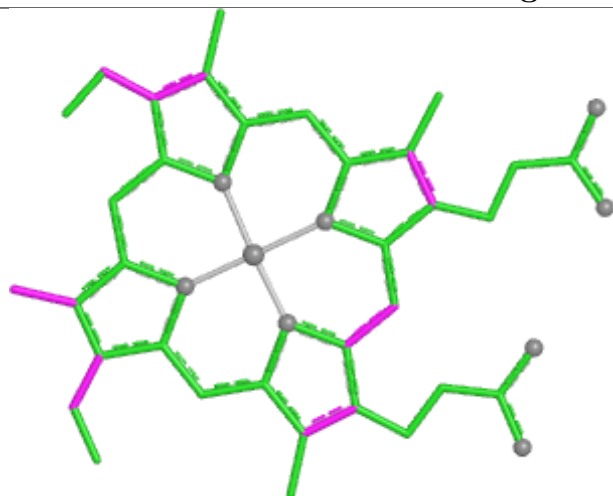
Ligand CLA b 604



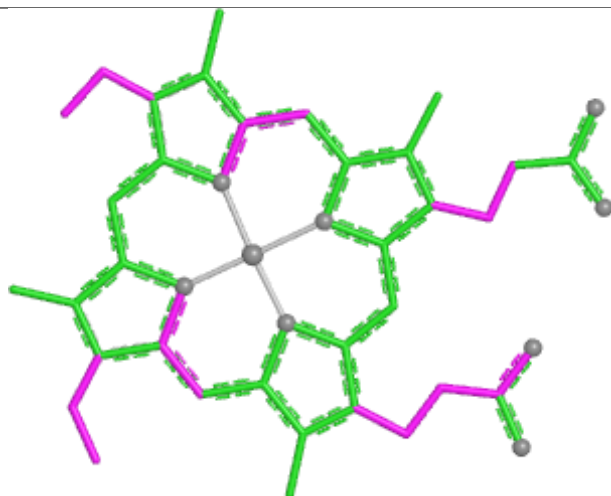
Ligand HEC V 201



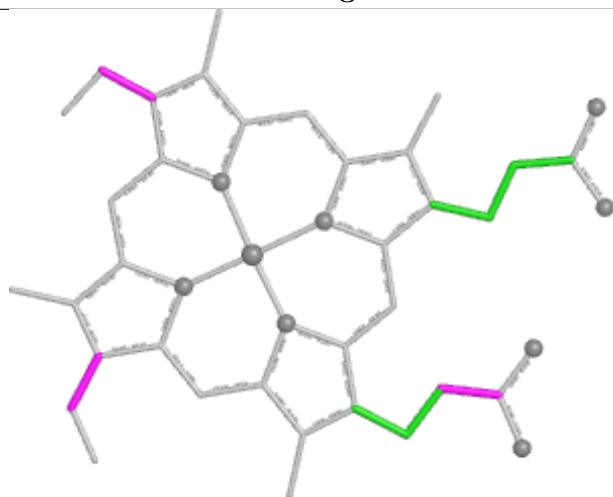
Ligand HEC f 101



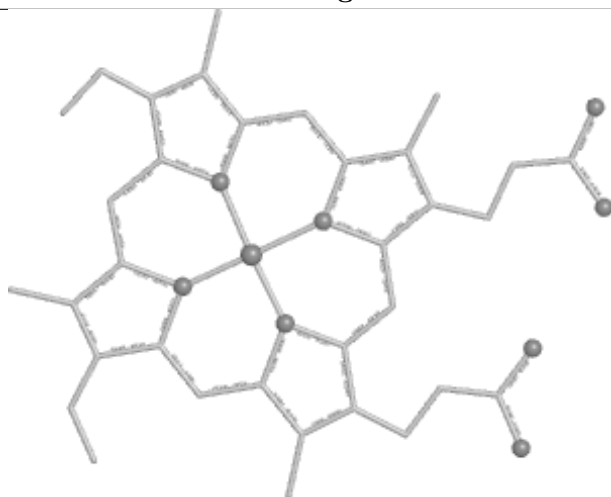
Bond lengths



Bond angles

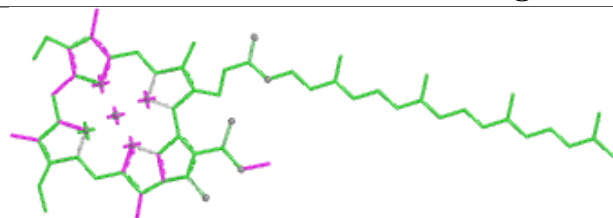


Torsions

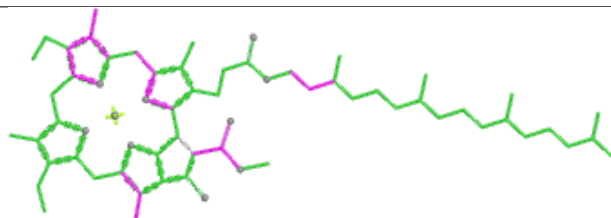


Rings

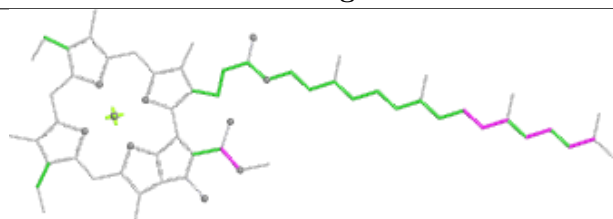
Ligand CLA D 404



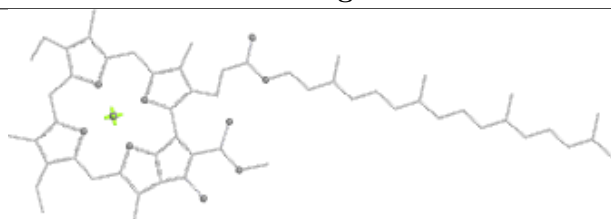
Bond lengths



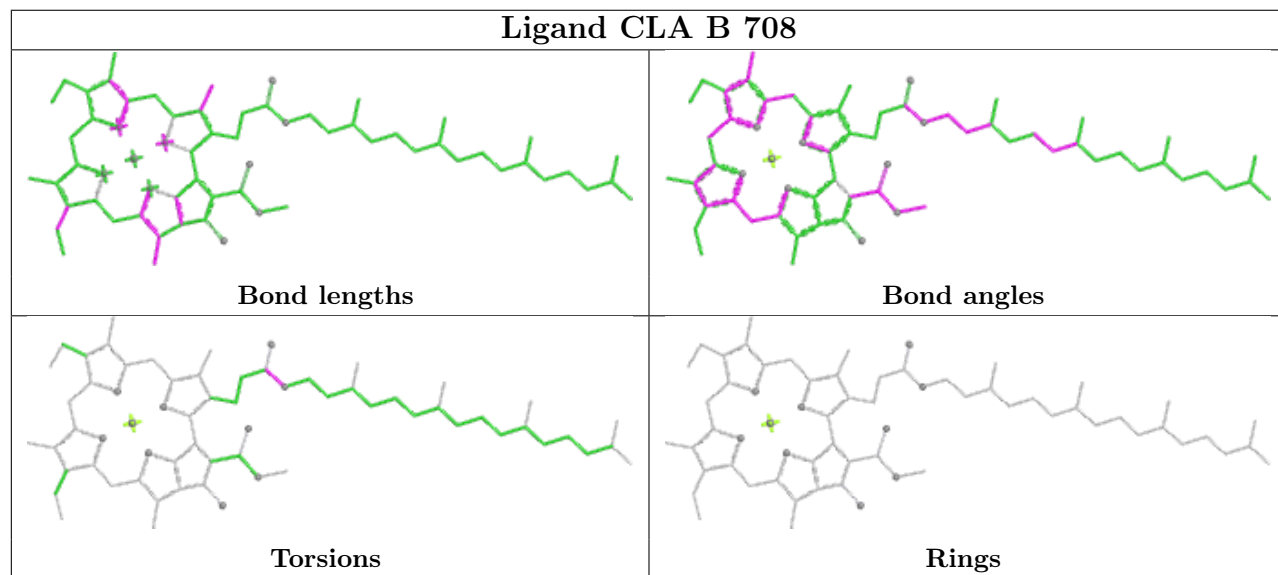
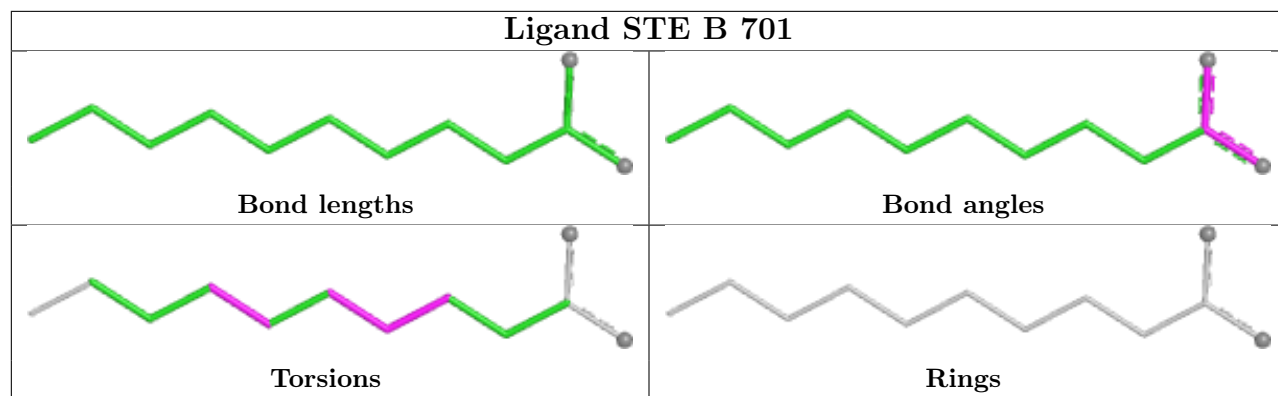
Bond angles



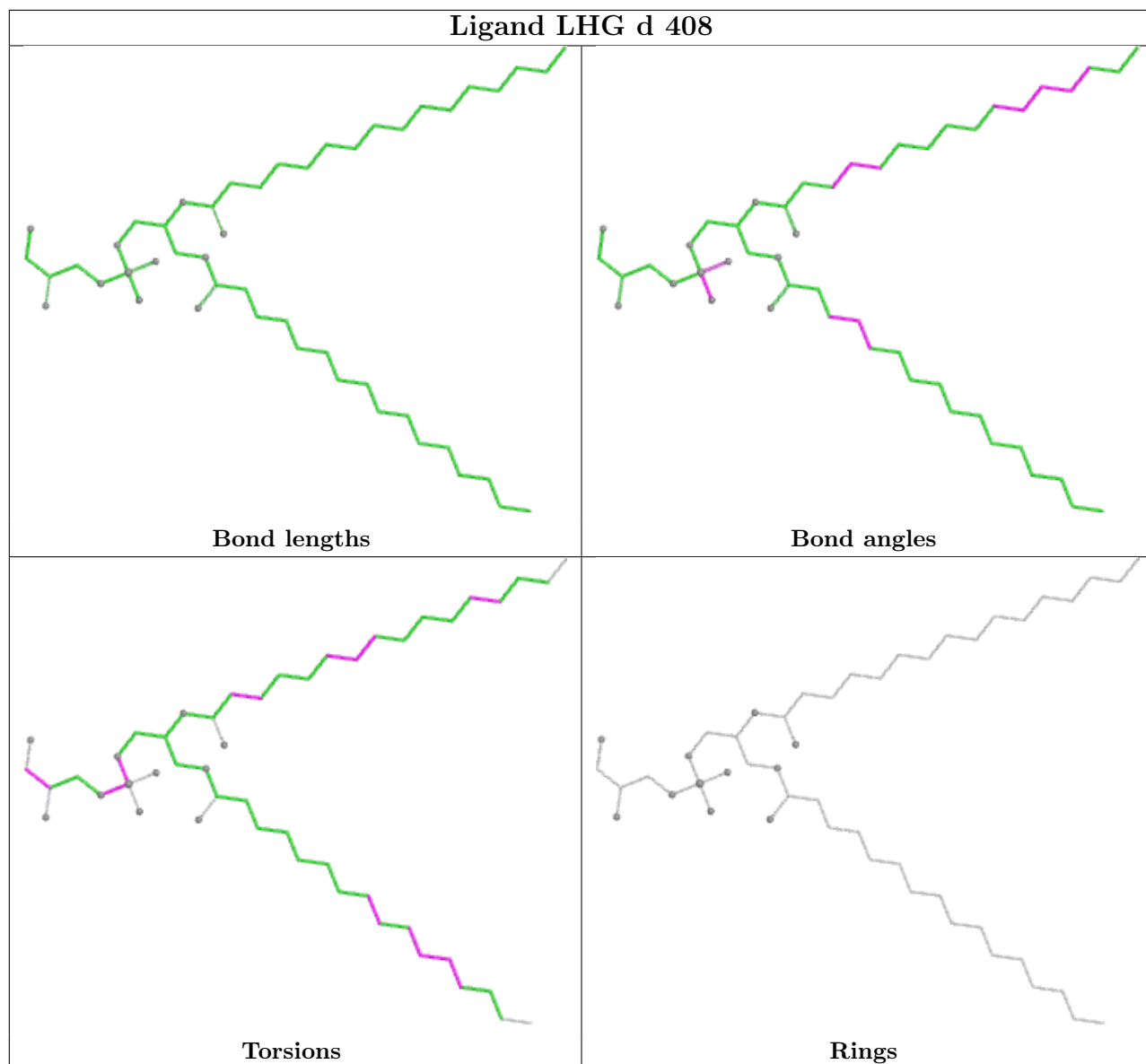
Torsions



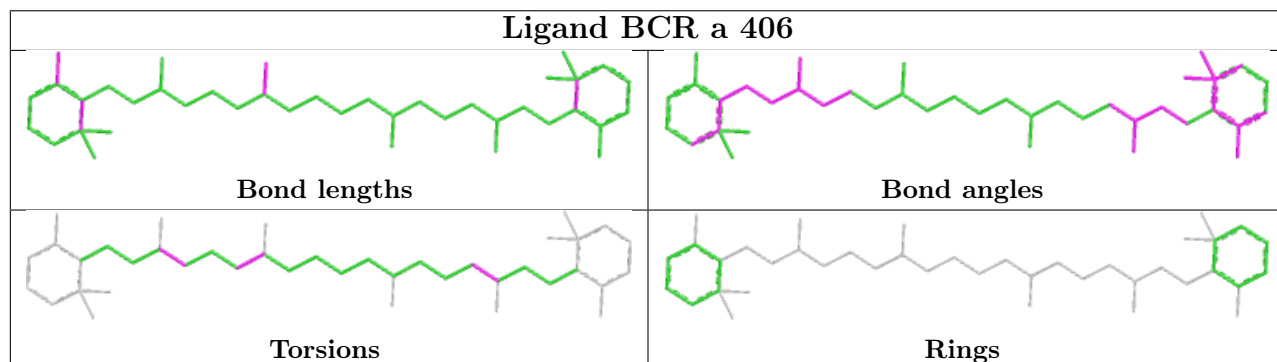
Rings

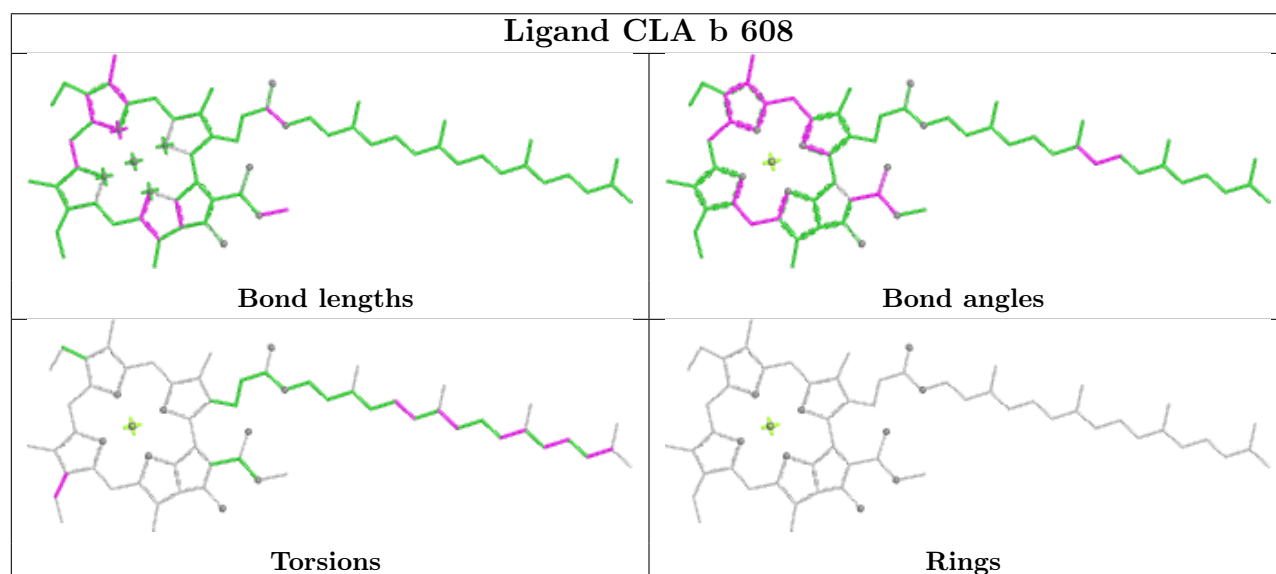
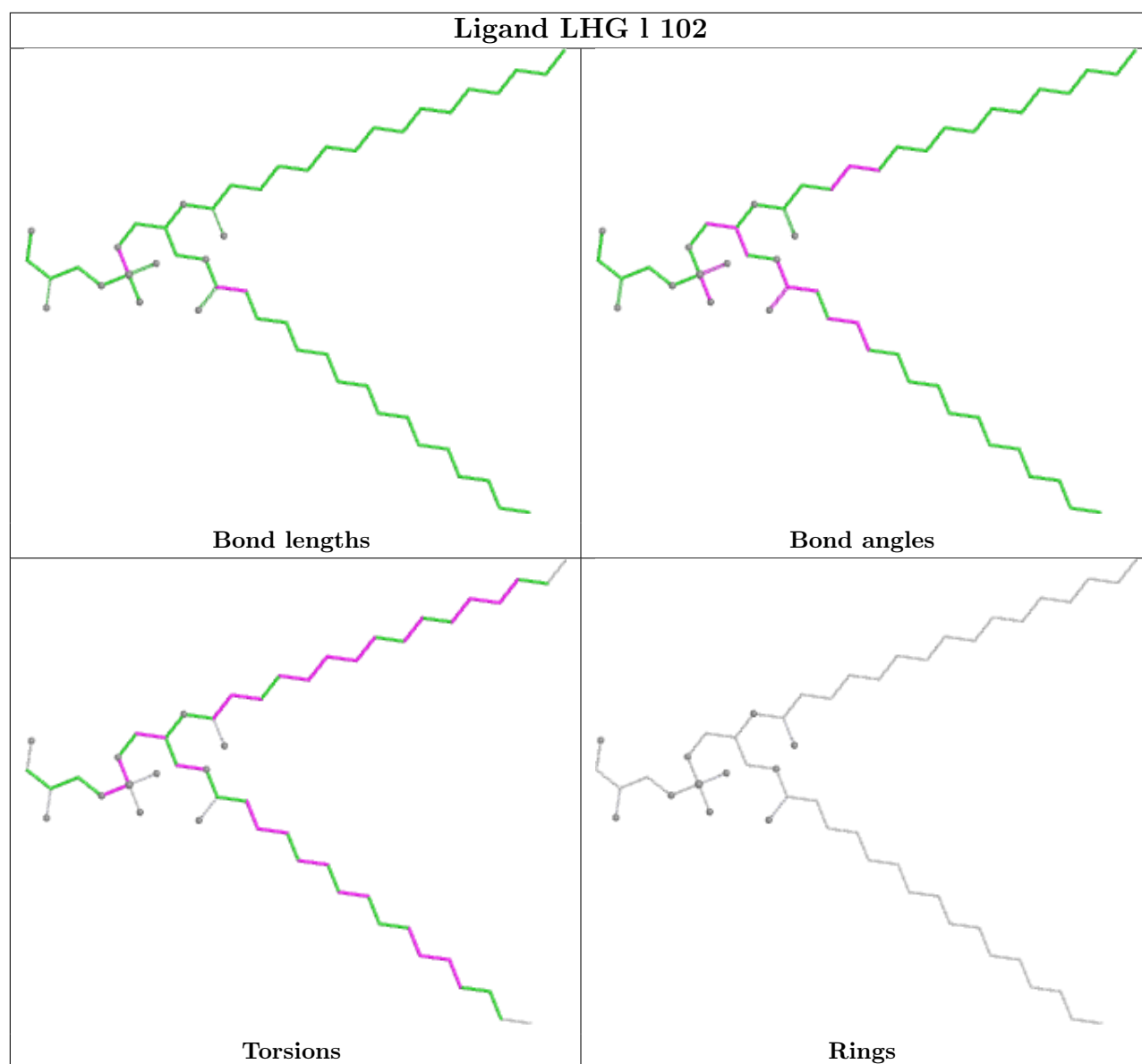


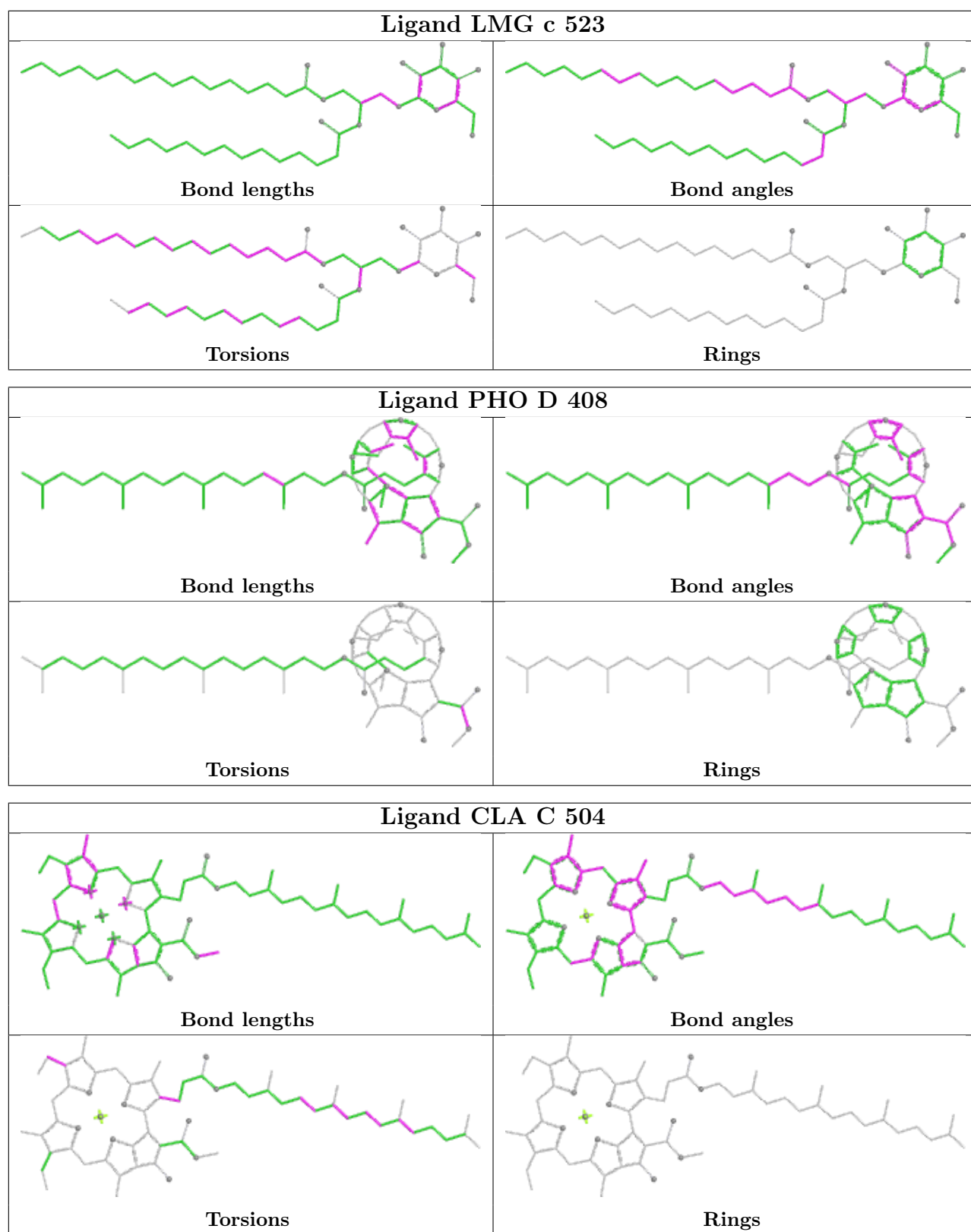
Ligand LHG d 408

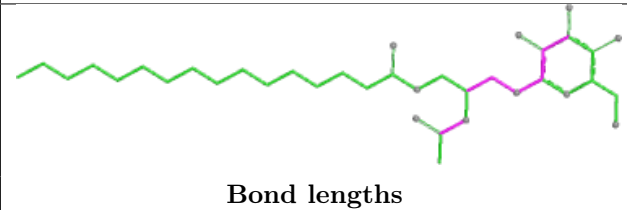
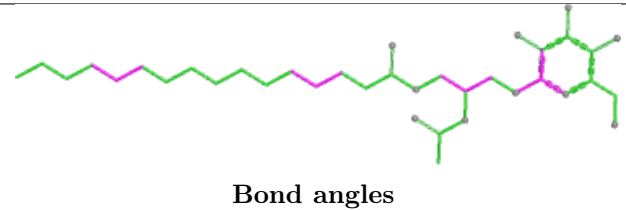
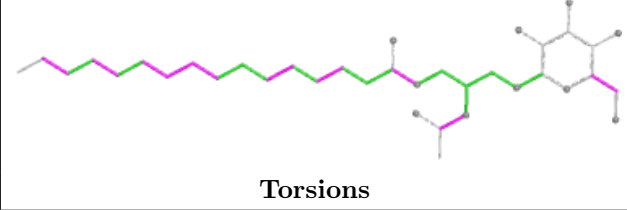
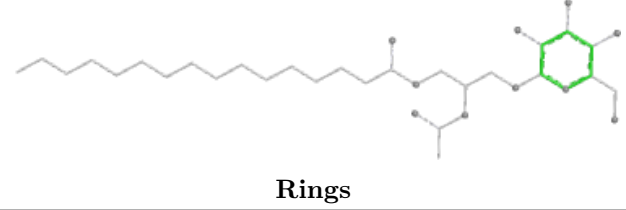


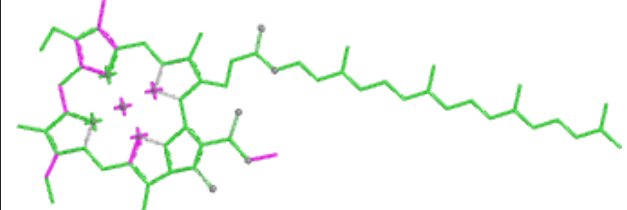
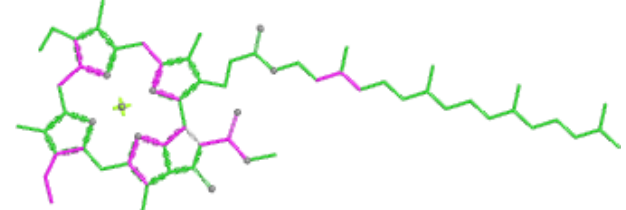
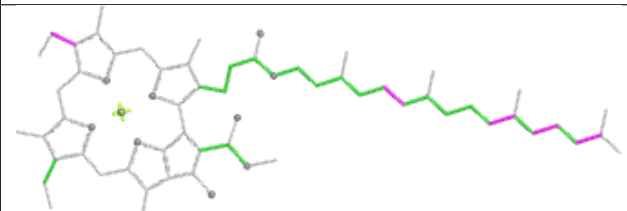
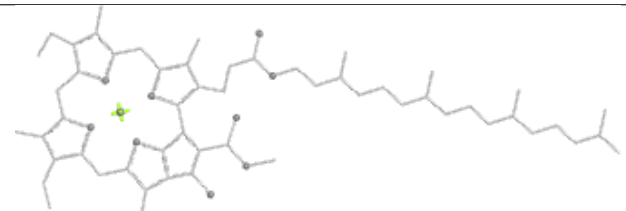
Ligand BCR a 406

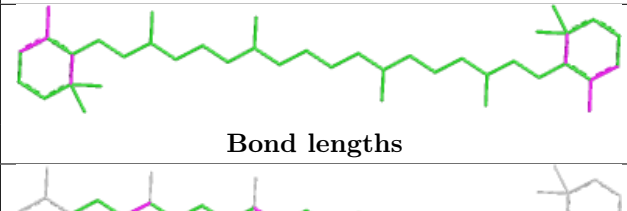
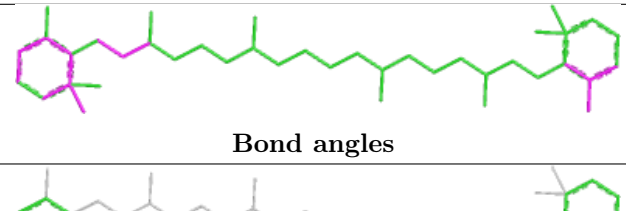
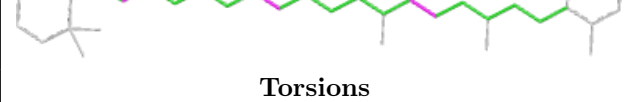



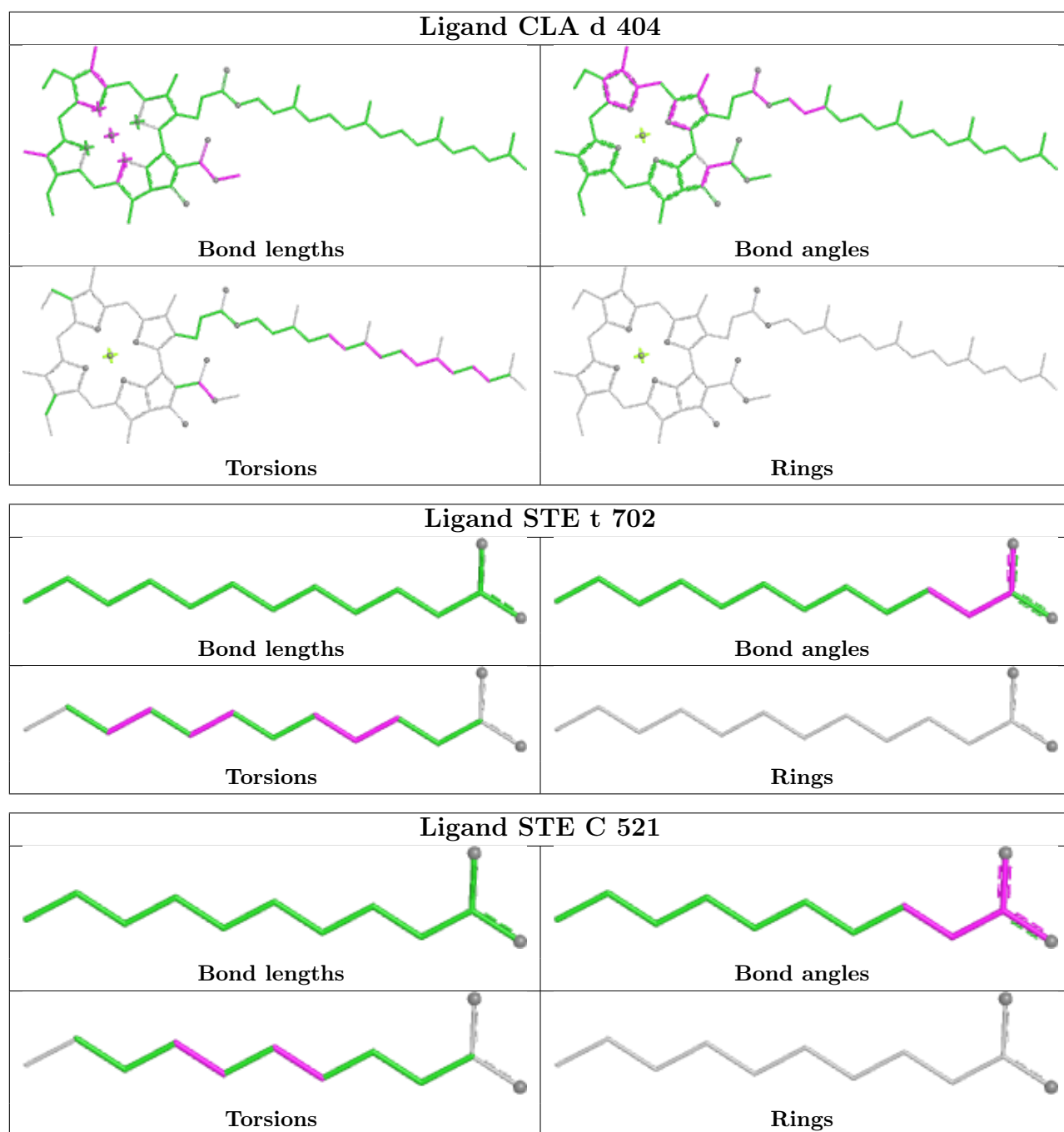


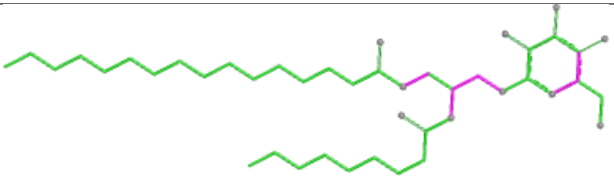
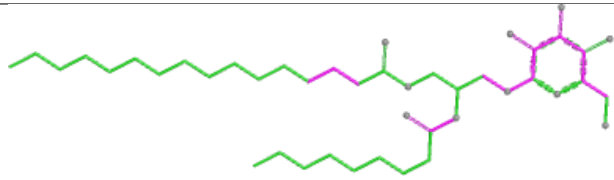
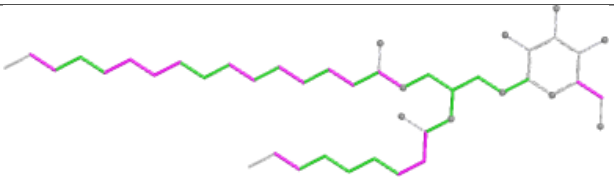
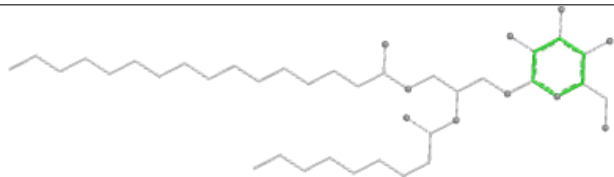


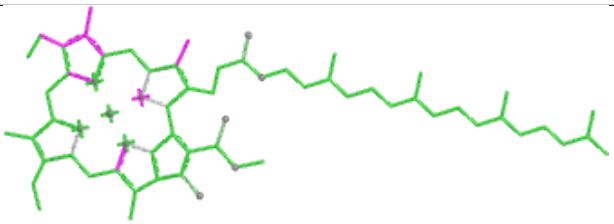
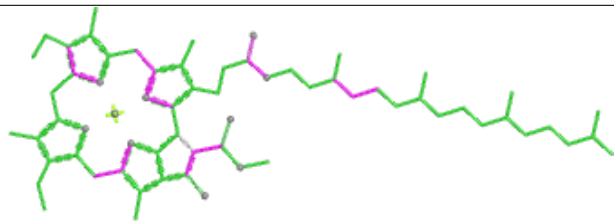
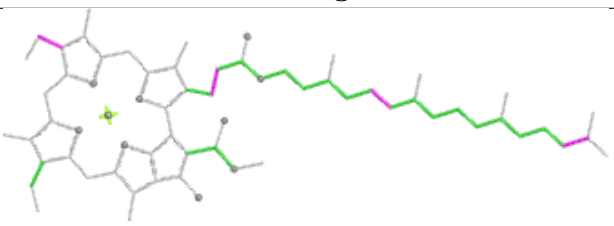
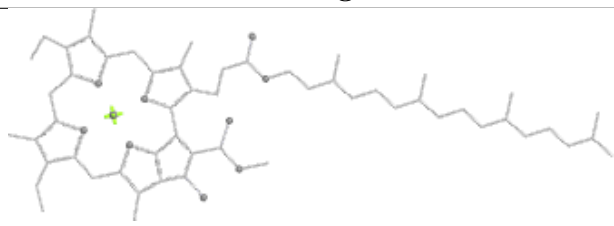
Ligand LMG c 520	
	
Bond lengths	Bond angles
	
Torsions	Rings

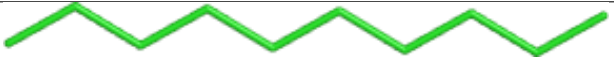



Ligand CLA B 715	
	
Bond lengths	Bond angles
	
Torsions	Rings





Ligand BCR T 701	
	
Bond lengths	Bond angles
	
Torsions	Rings

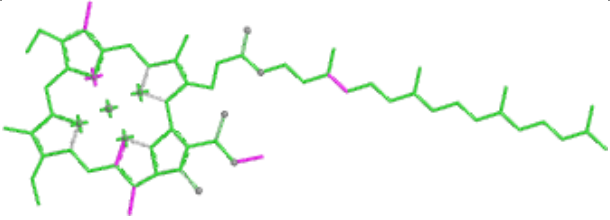
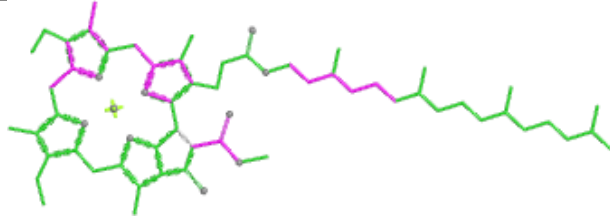
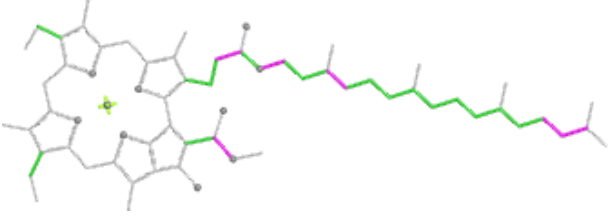
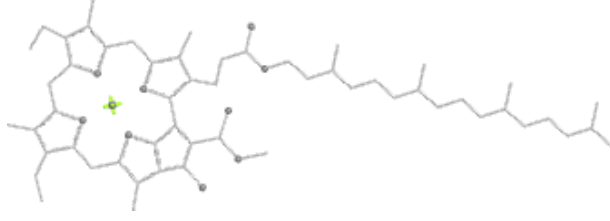
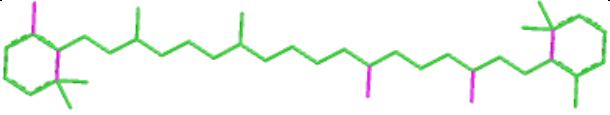
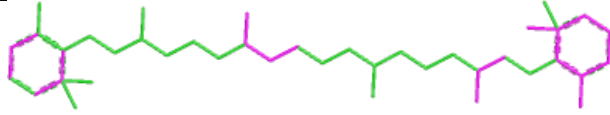
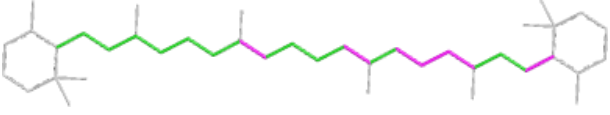
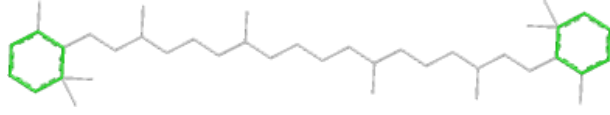
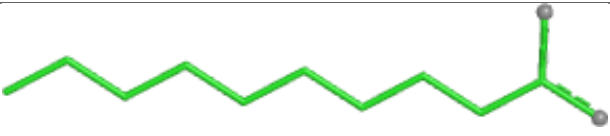
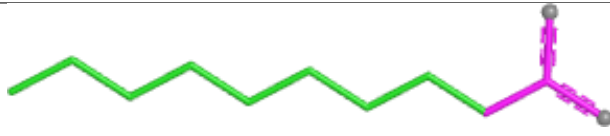
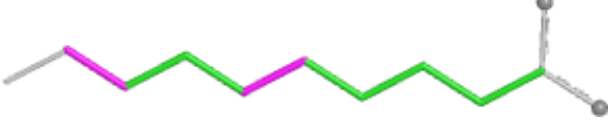
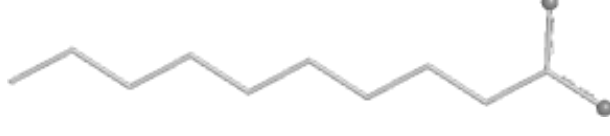


Ligand LMG d 410	
	
Bond lengths	Bond angles
	
Torsions	Rings

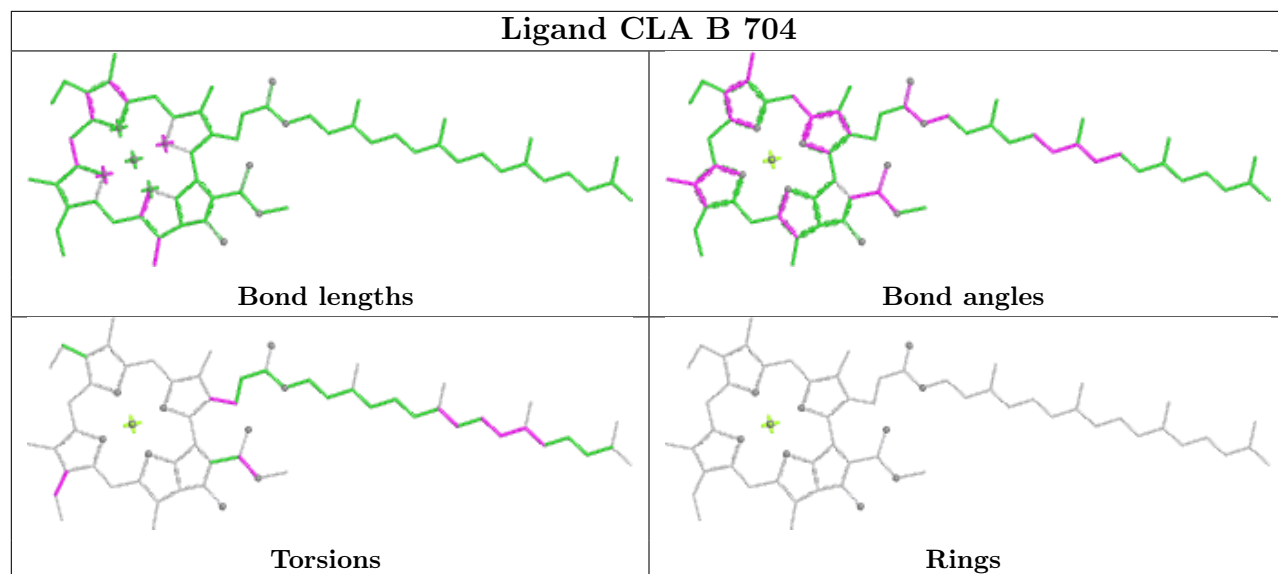
Ligand CLA B 706	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand STE a 415	
	
Bond lengths	Bond angles
	
Torsions	Rings

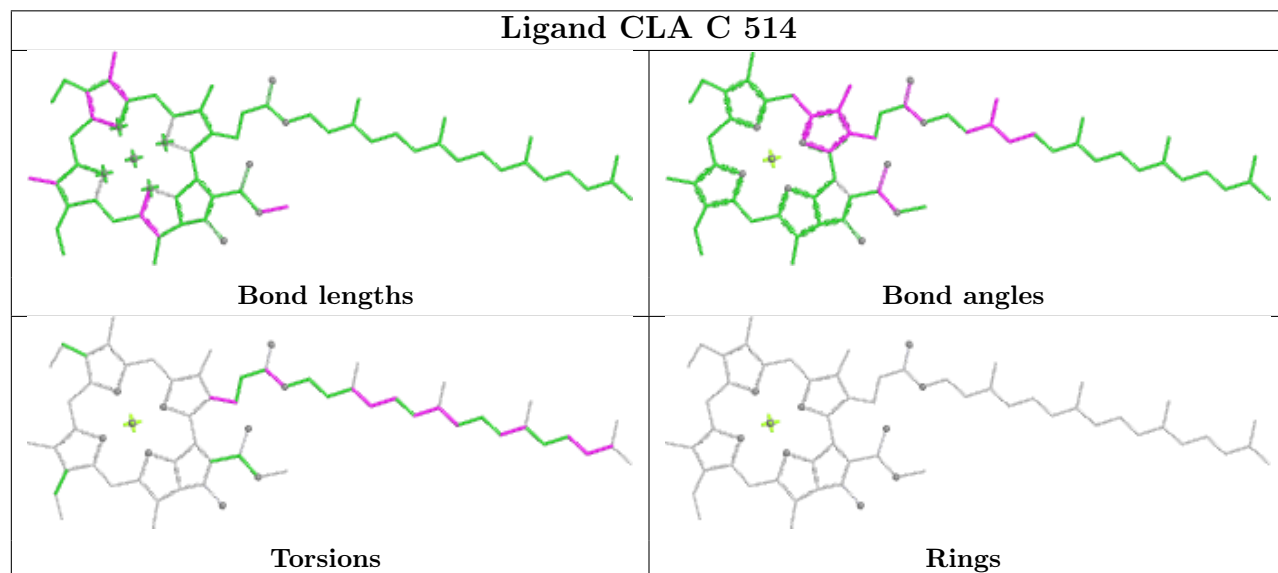
Ligand STE b 621	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA c 511	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR B 718	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand STE j 101	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

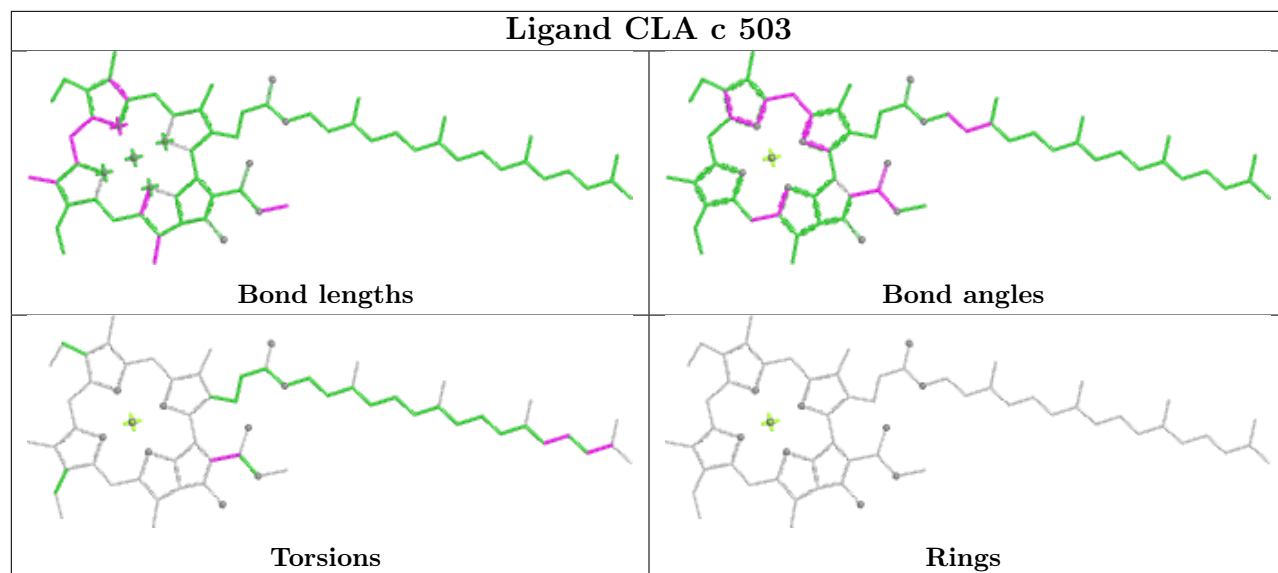
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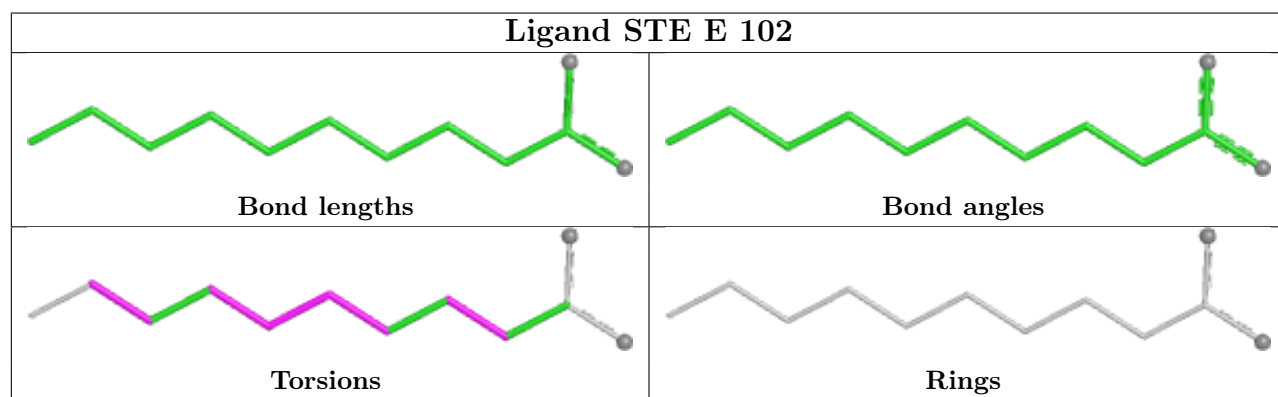
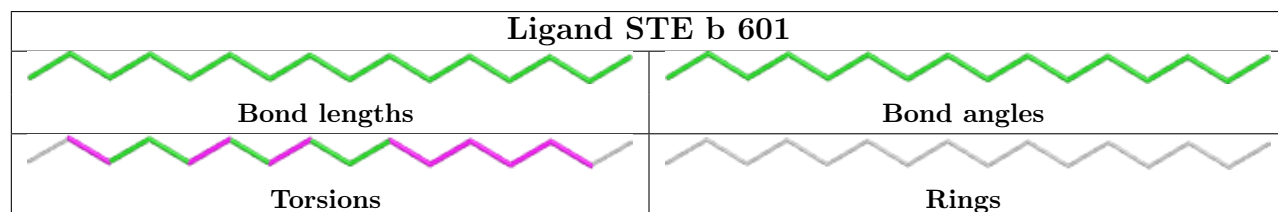
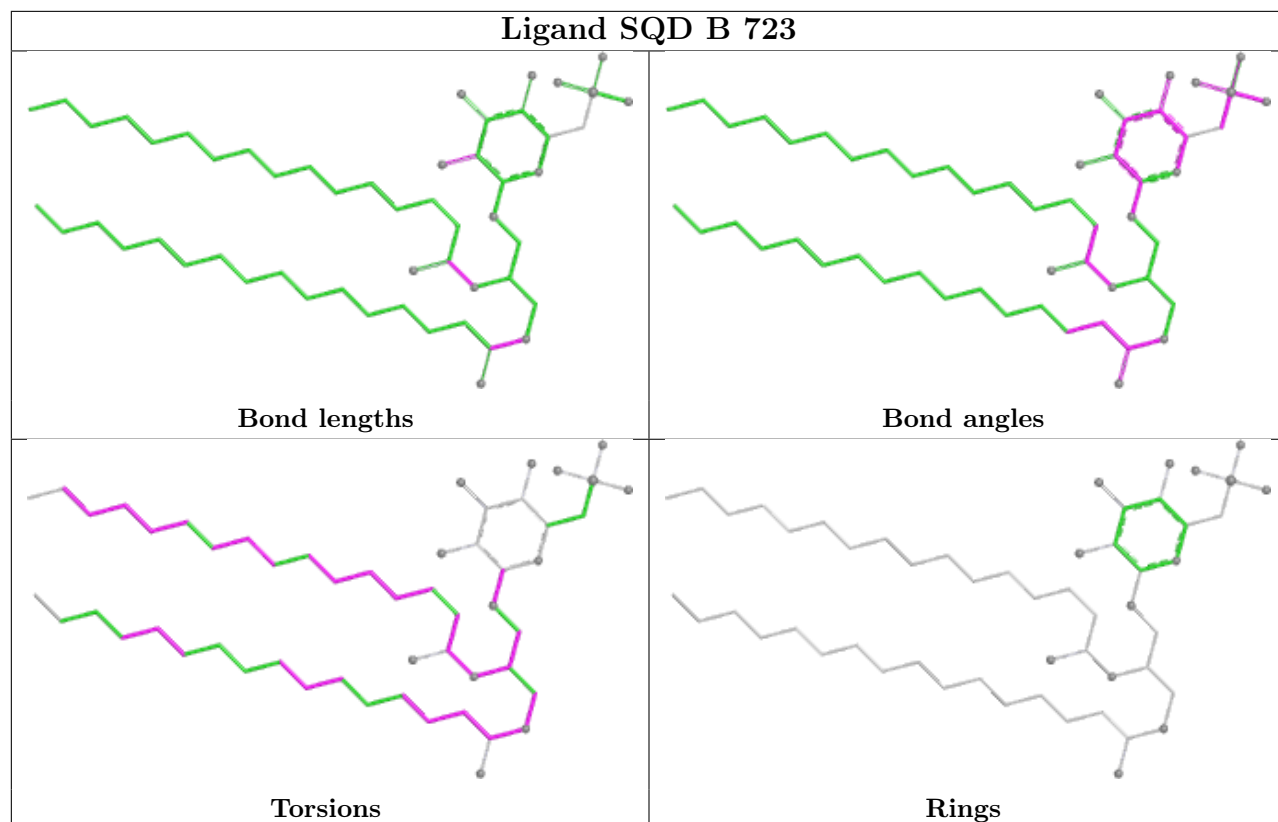


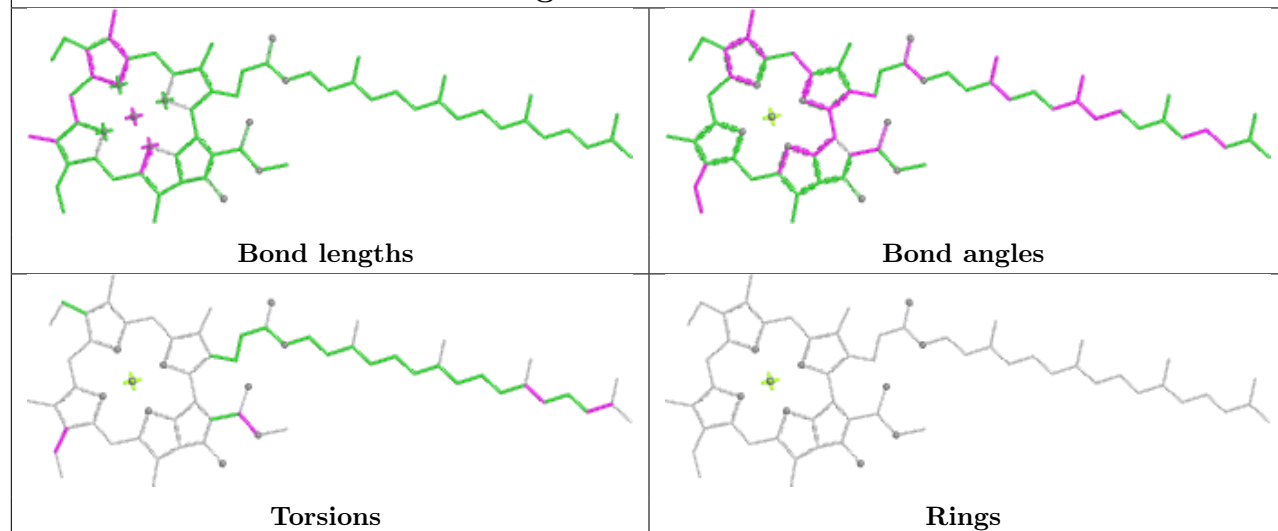
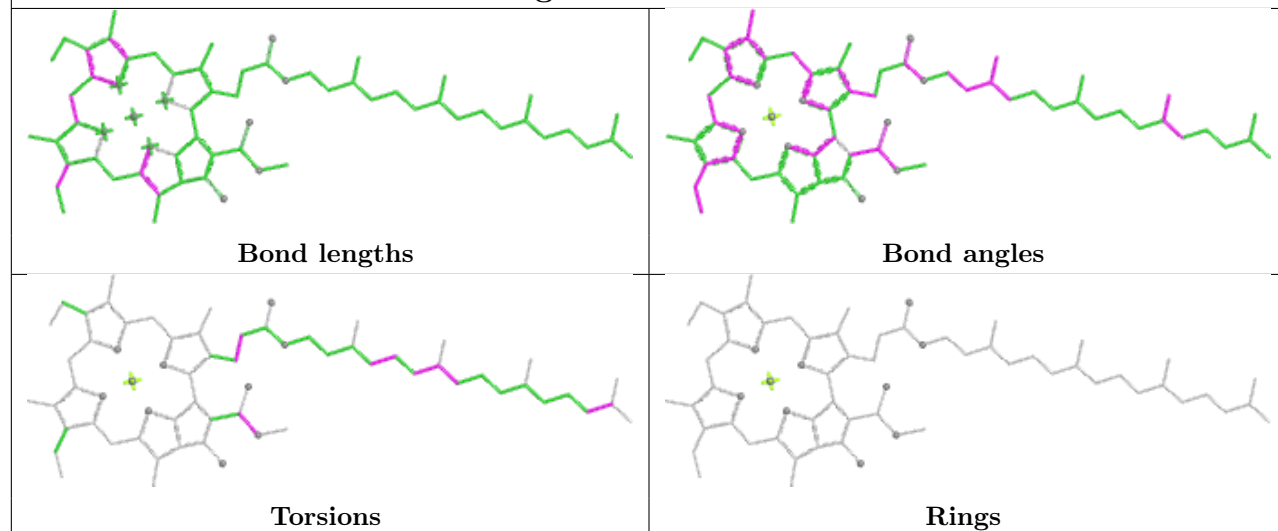
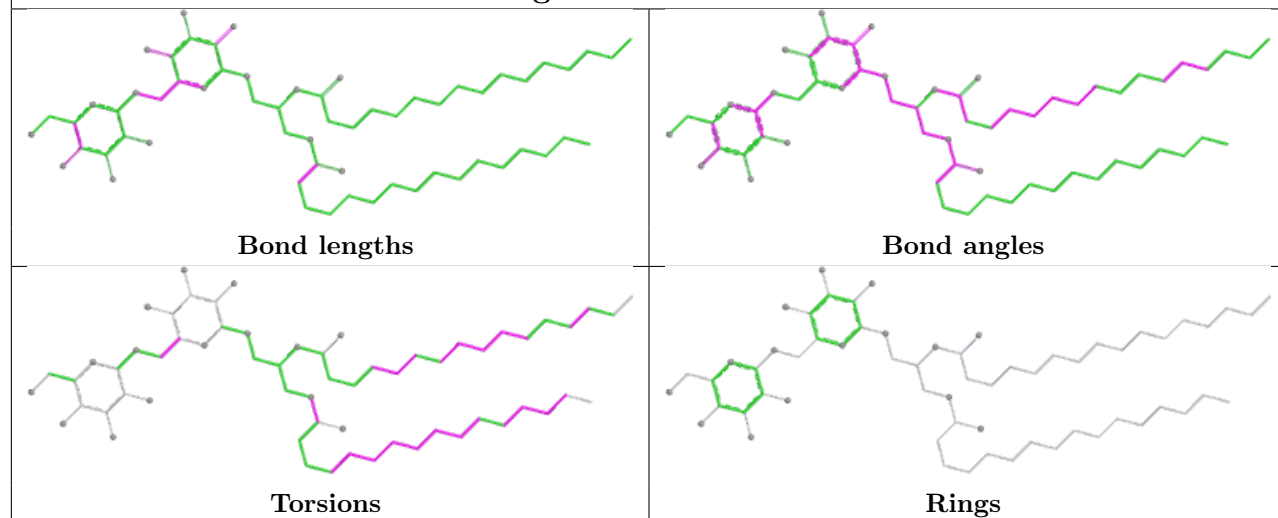
Ligand CLA C 514

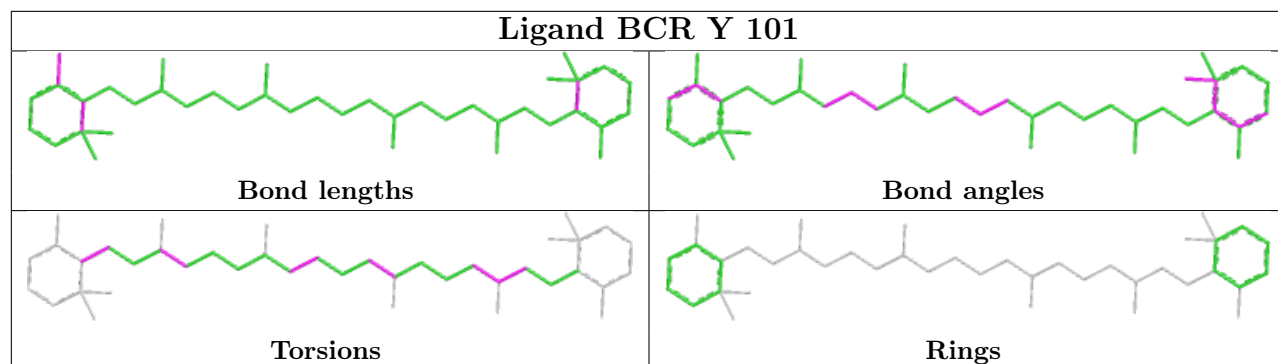
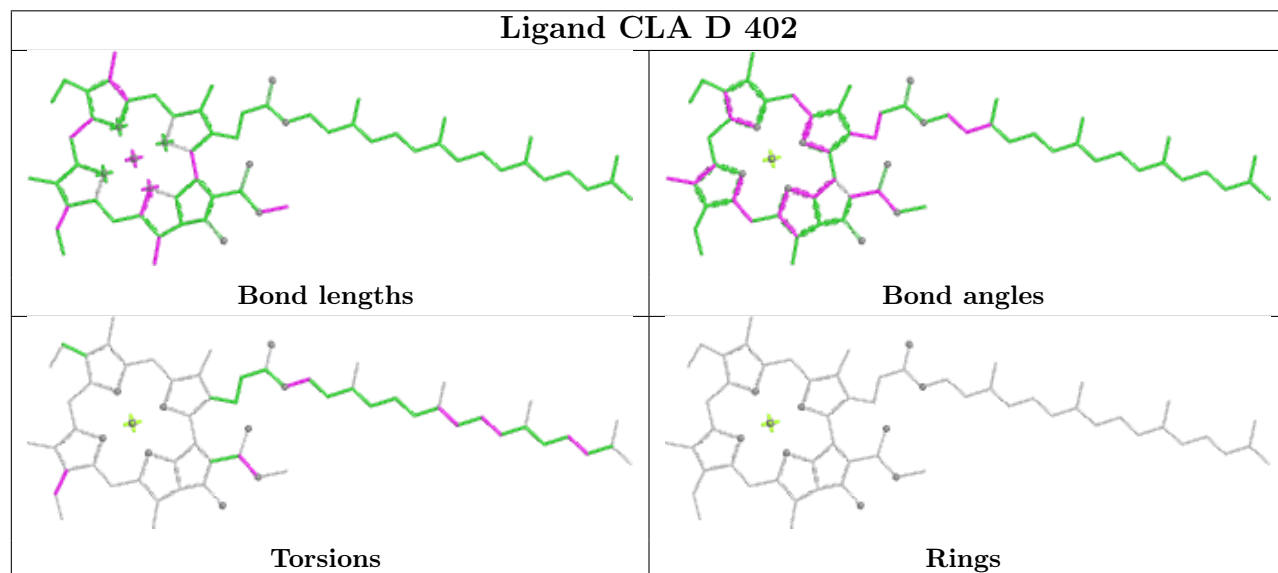
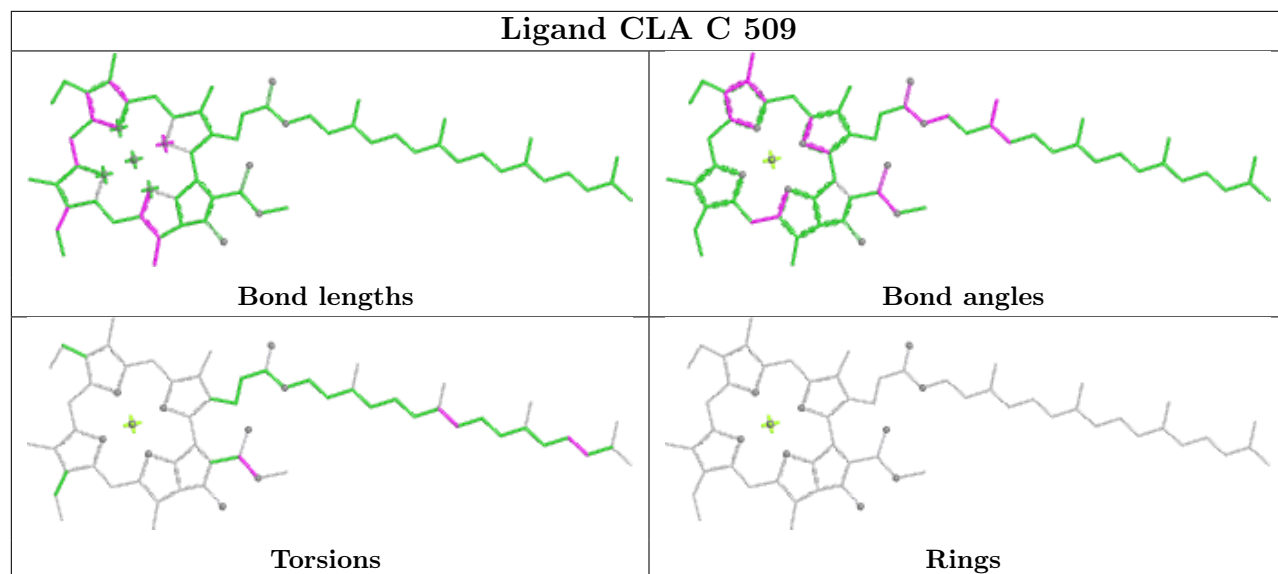


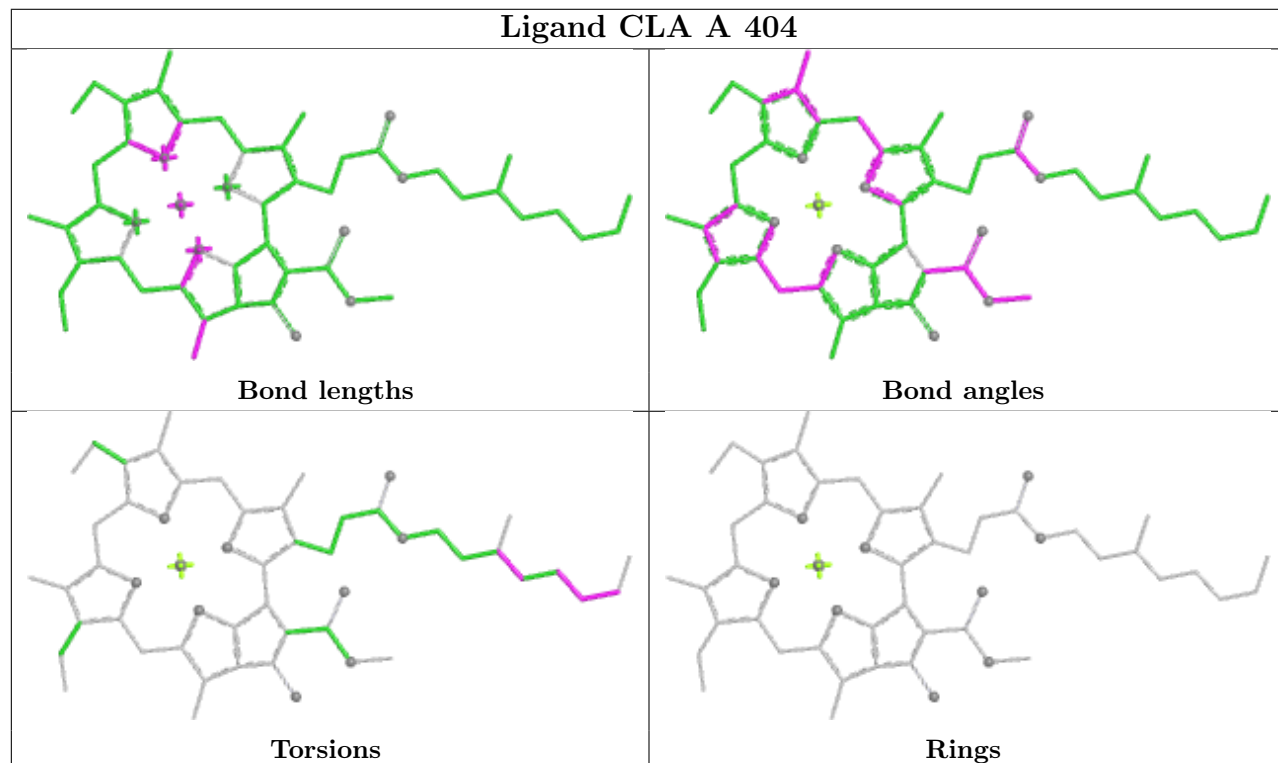
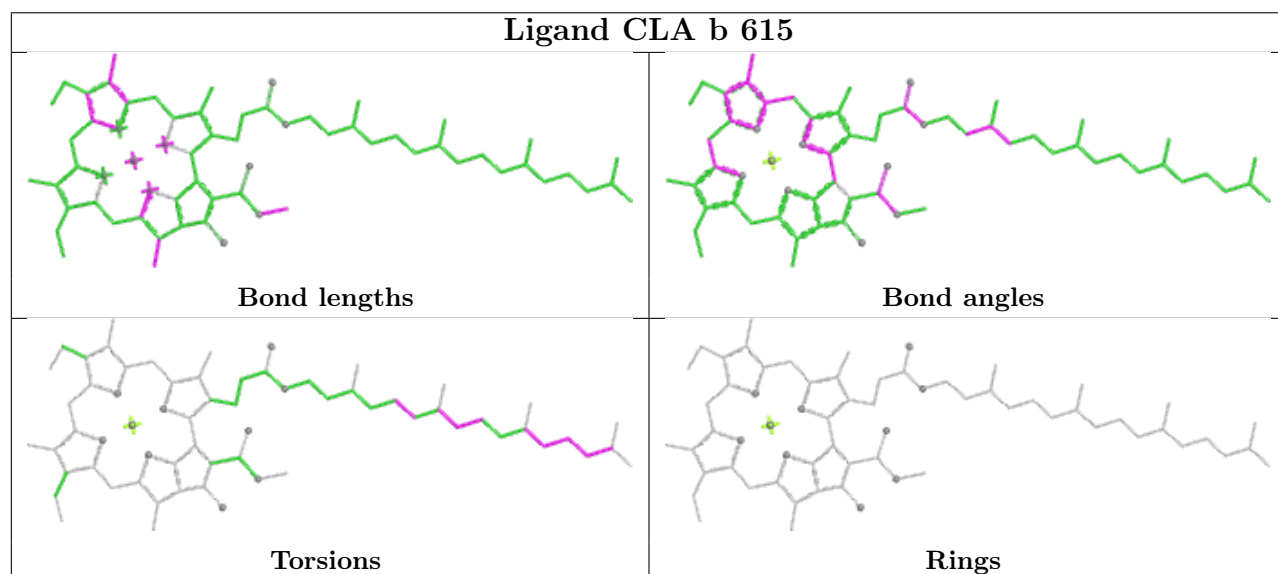
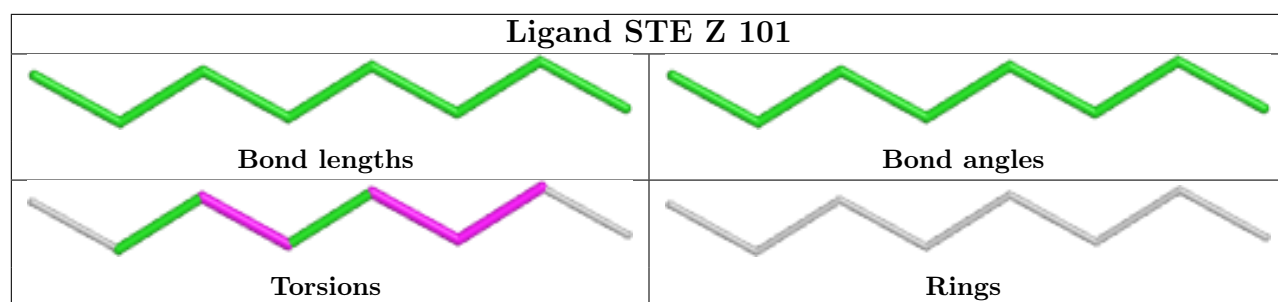
Ligand CLA c 503

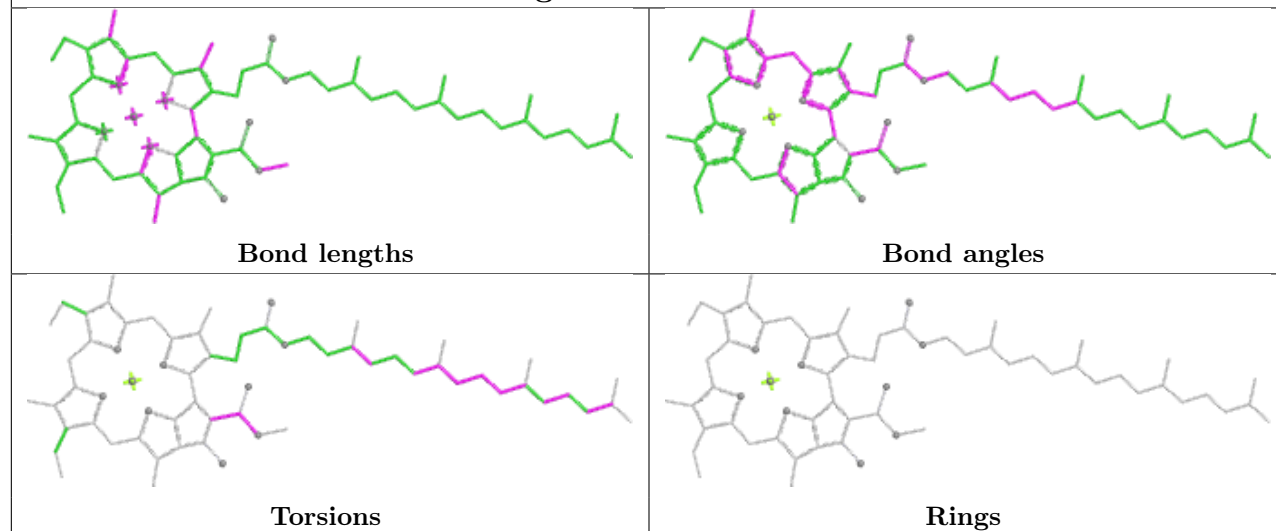
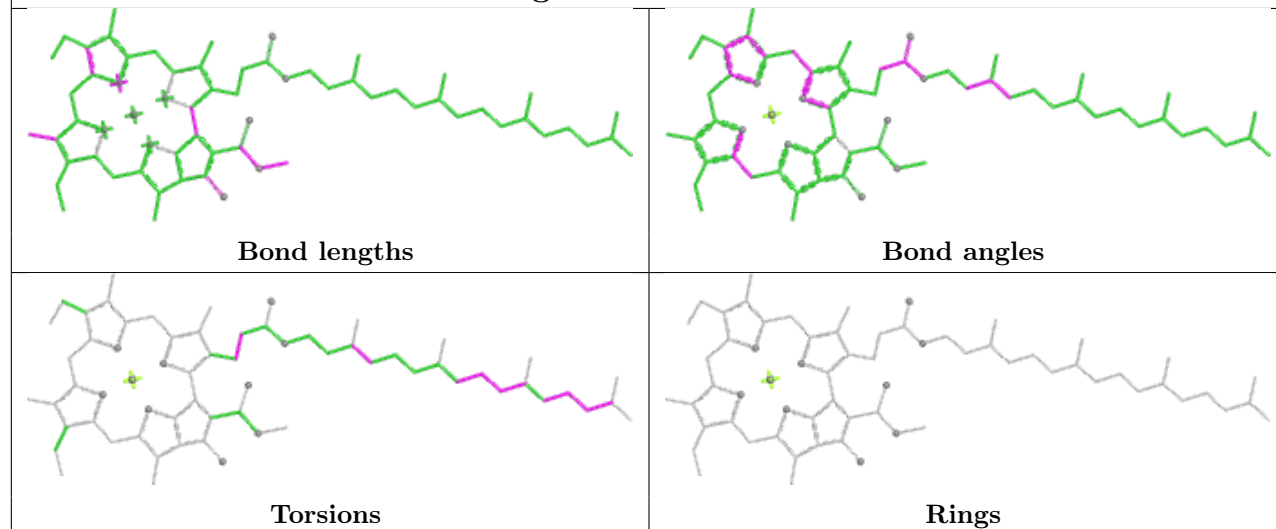




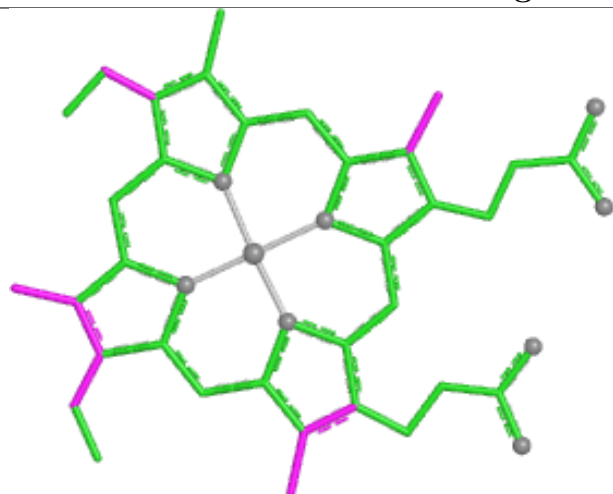
Ligand CLA a 402**Ligand CLA b 602****Ligand DGD c 519**



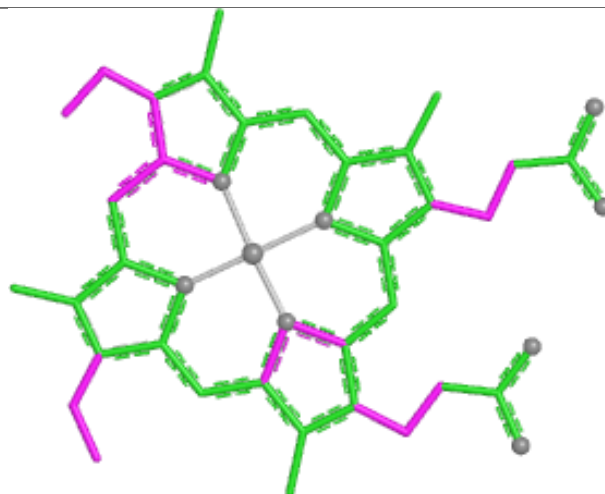


Ligand CLA b 607**Ligand CLA B 703**

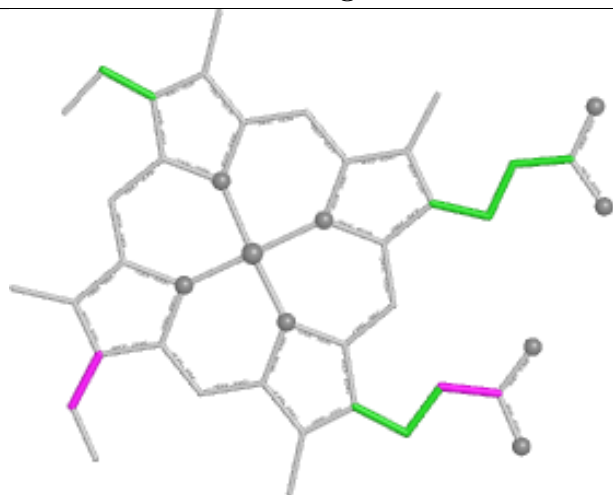
Ligand HEC F 101



Bond lengths



Bond angles

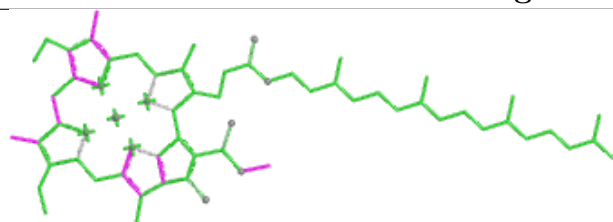


Torsions

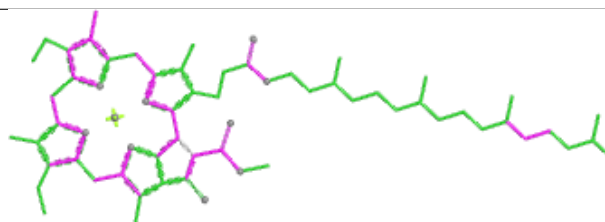


Rings

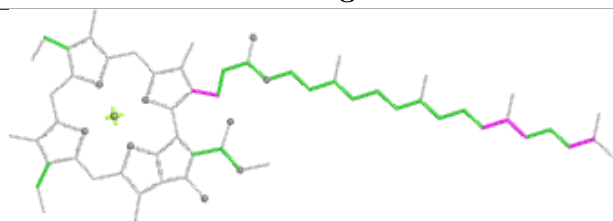
Ligand CLA B 702



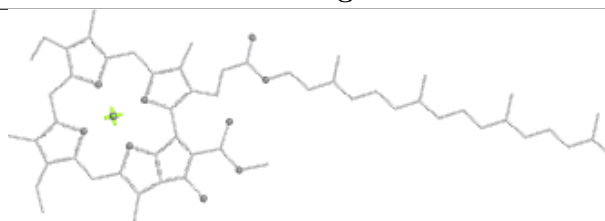
Bond lengths



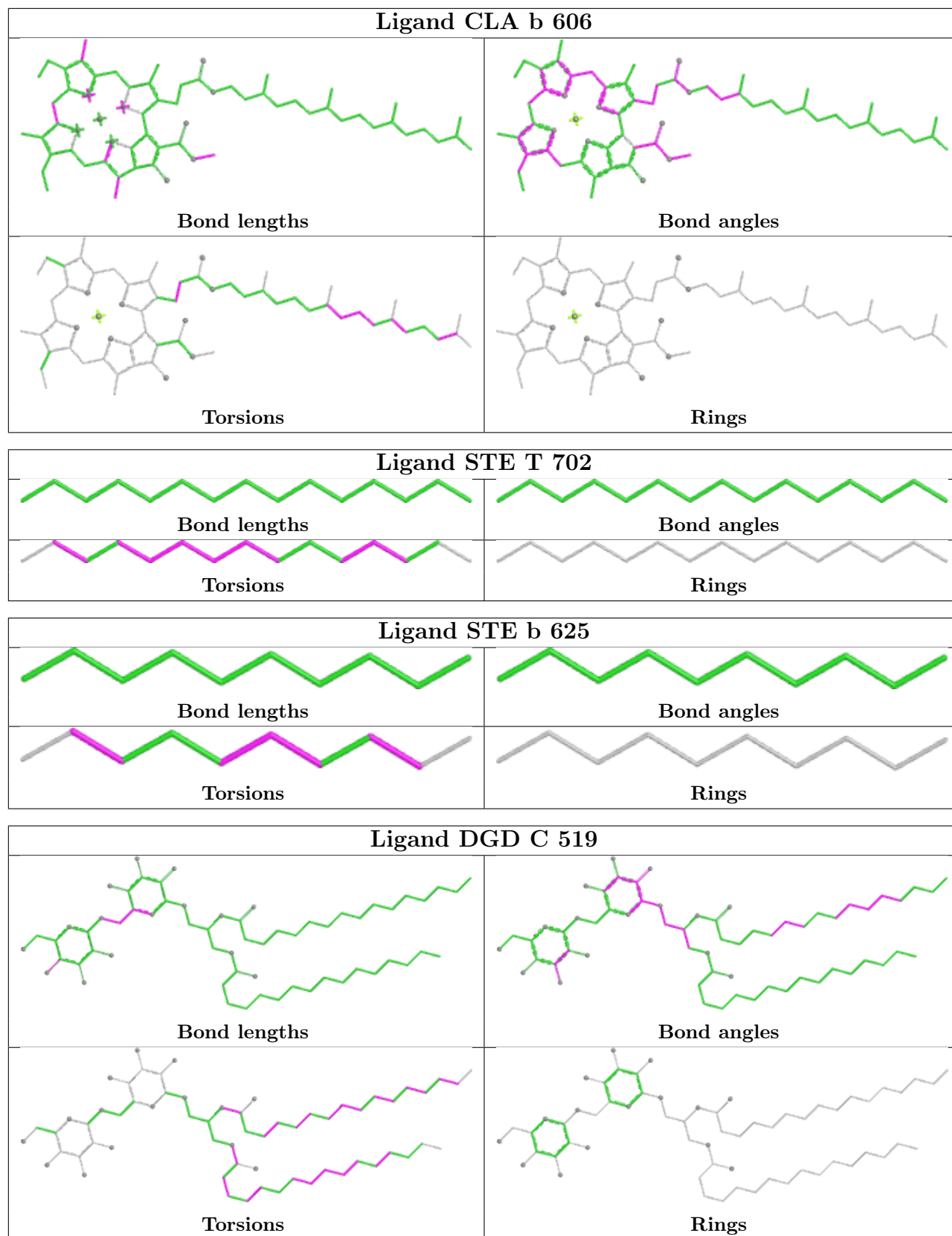
Bond angles

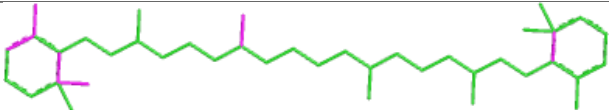
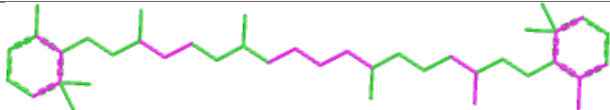
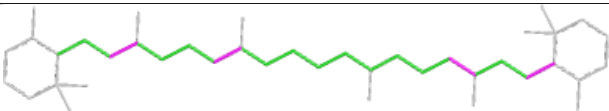
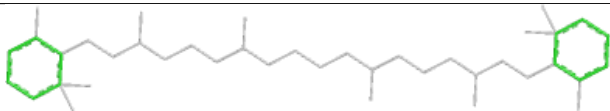






Torsions







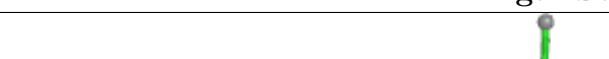
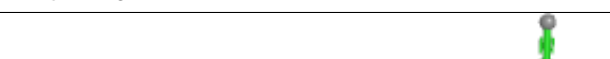
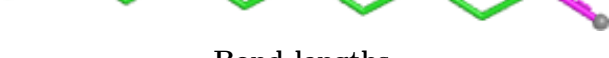
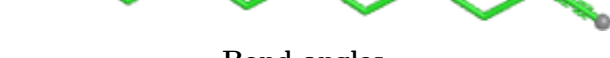
Rings



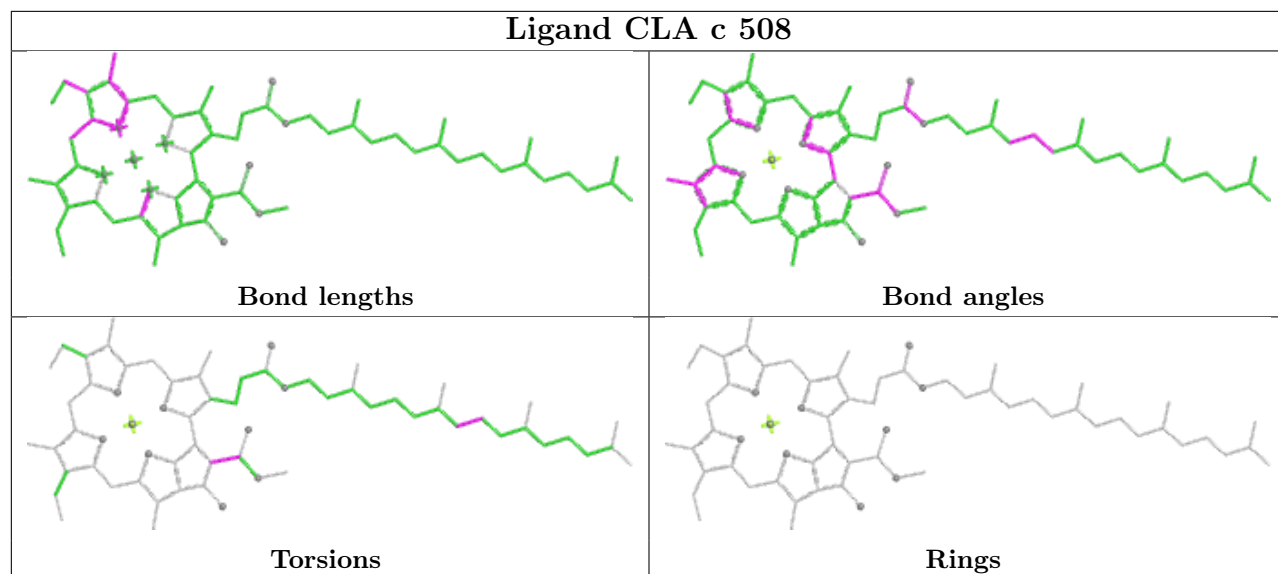
Ligand BCR H 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand STE M 103	
	
Bond lengths	Bond angles
	
Torsions	Rings

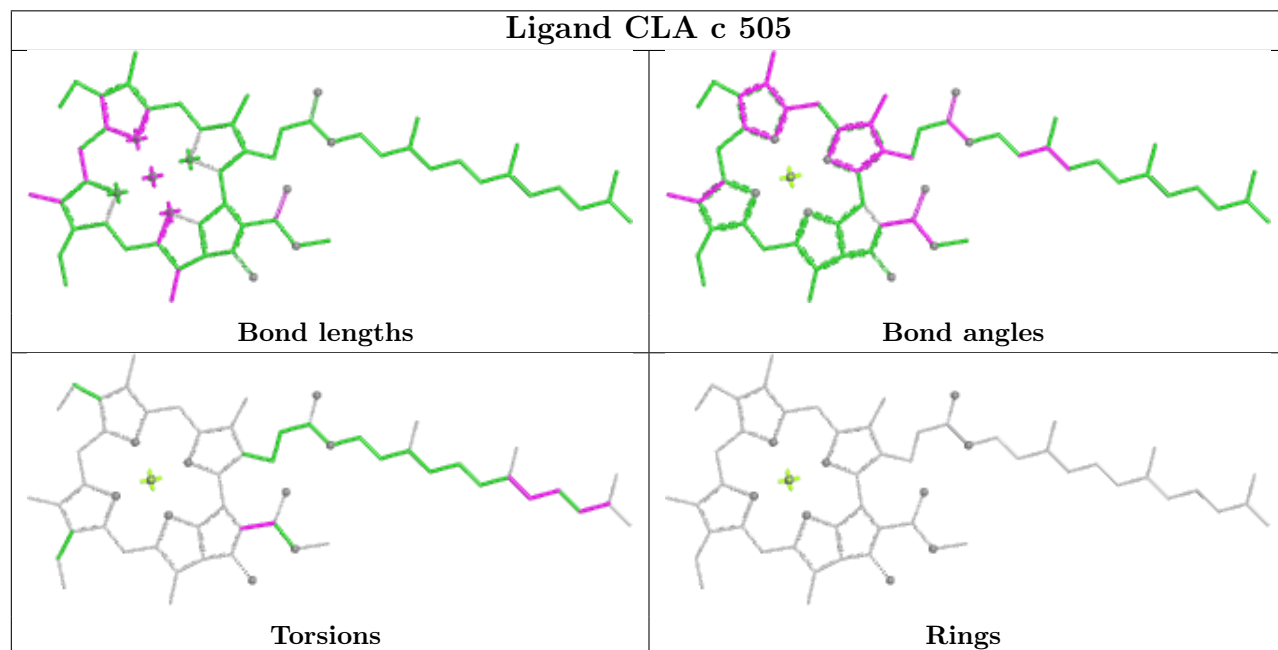
Ligand STE d 402	
	
Bond lengths	Bond angles
	
Torsions	Rings

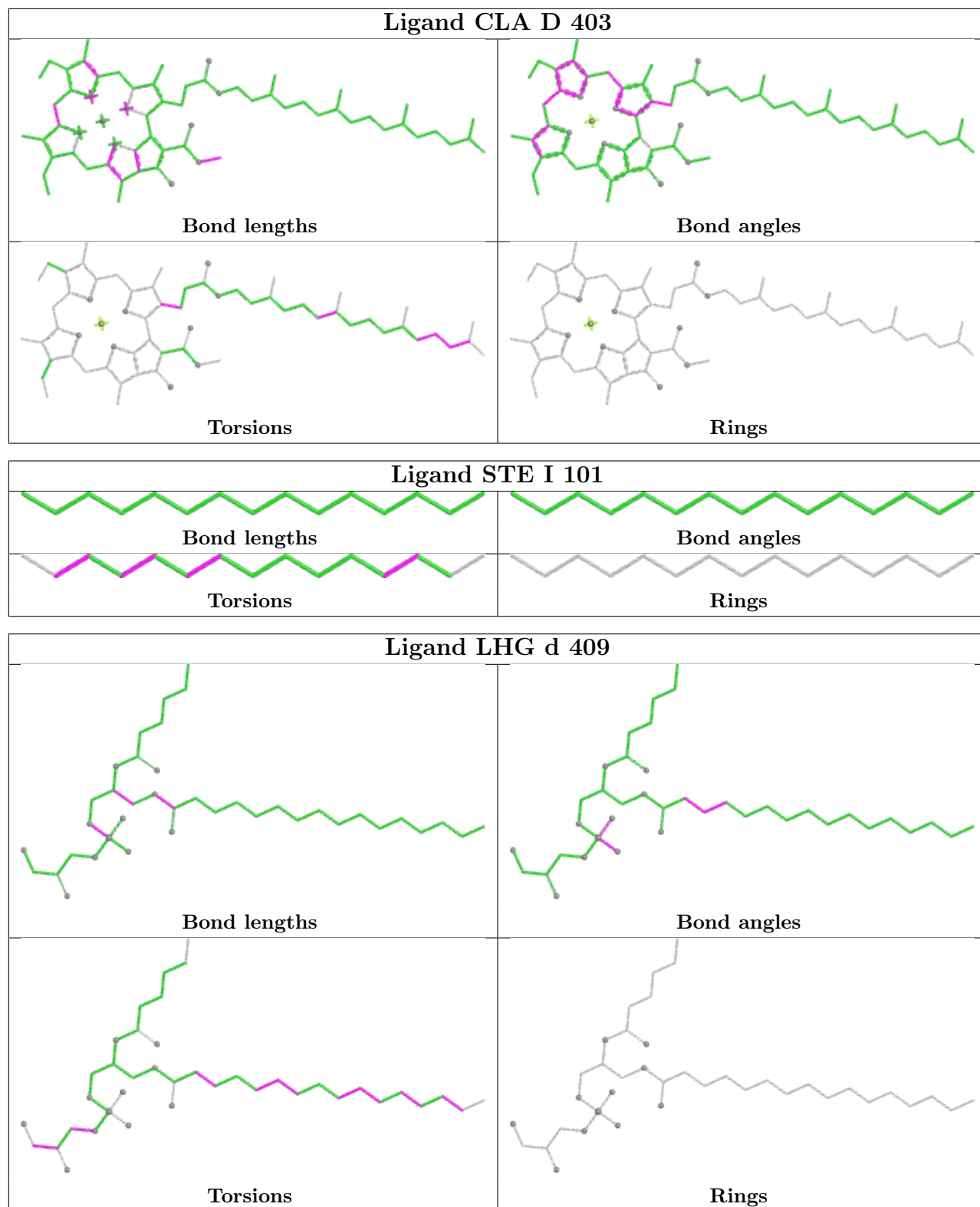
Ligand STE a 416	
	
Bond lengths	Bond angles
	
Torsions	Rings

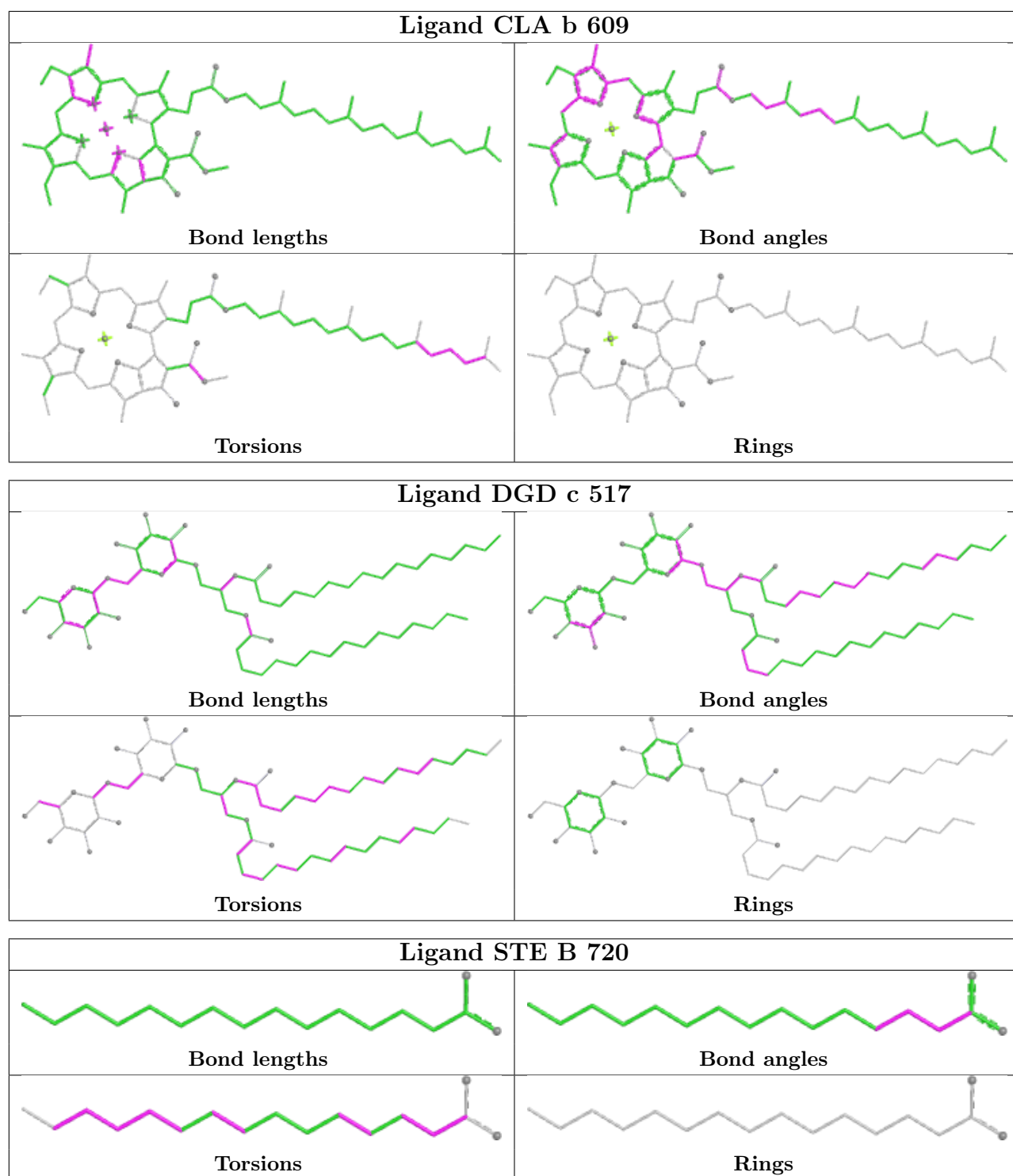
Ligand CLA c 508

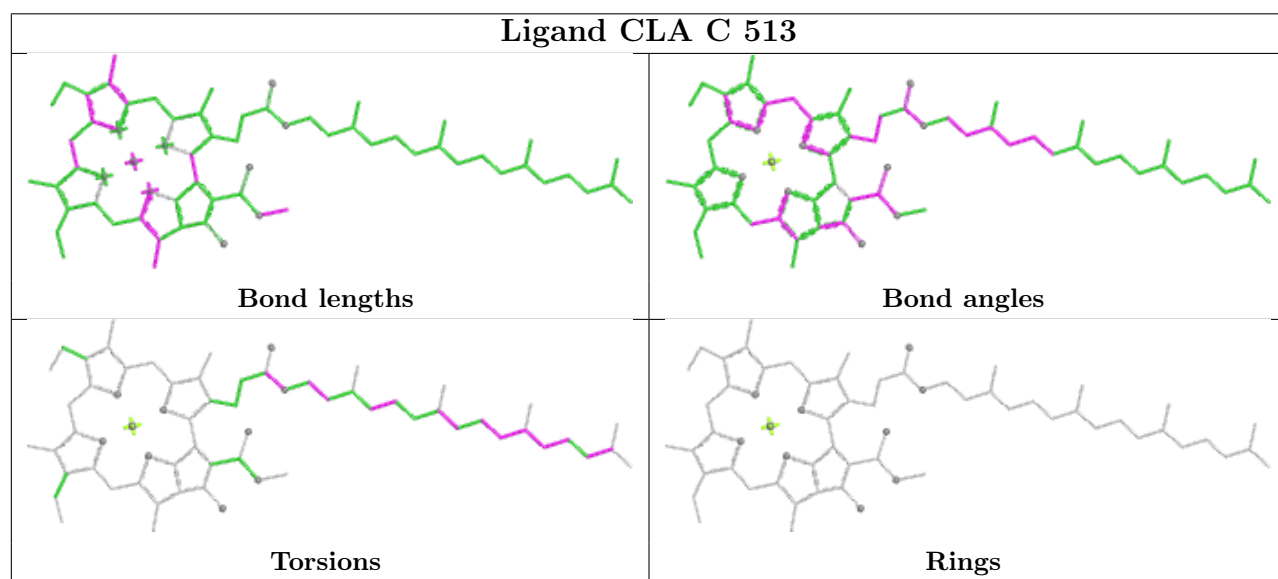
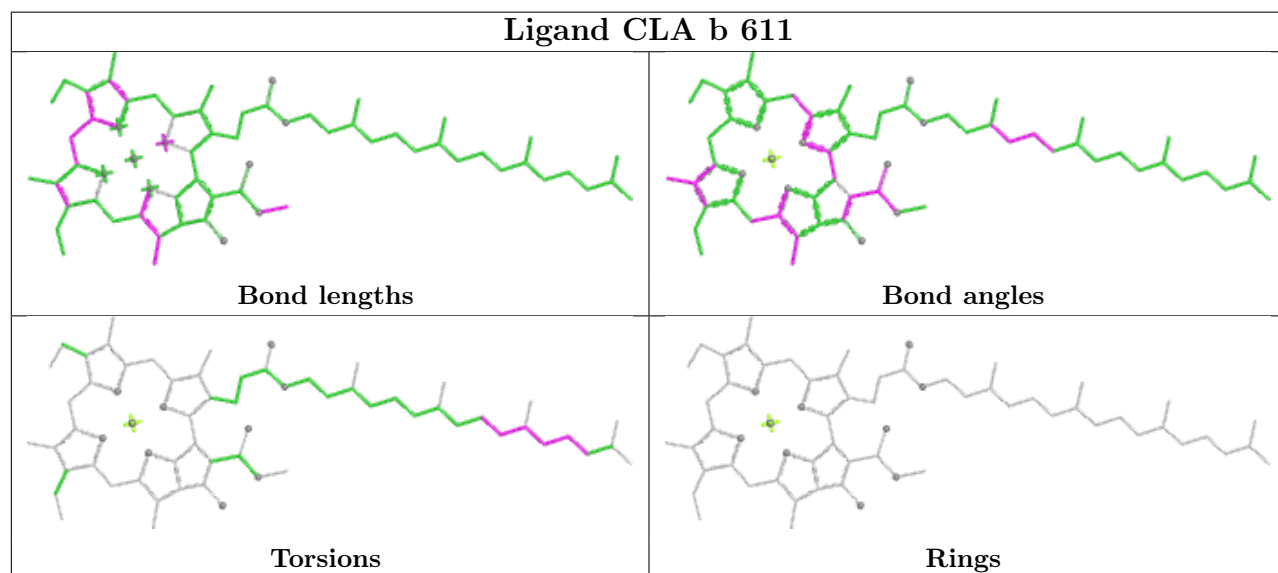
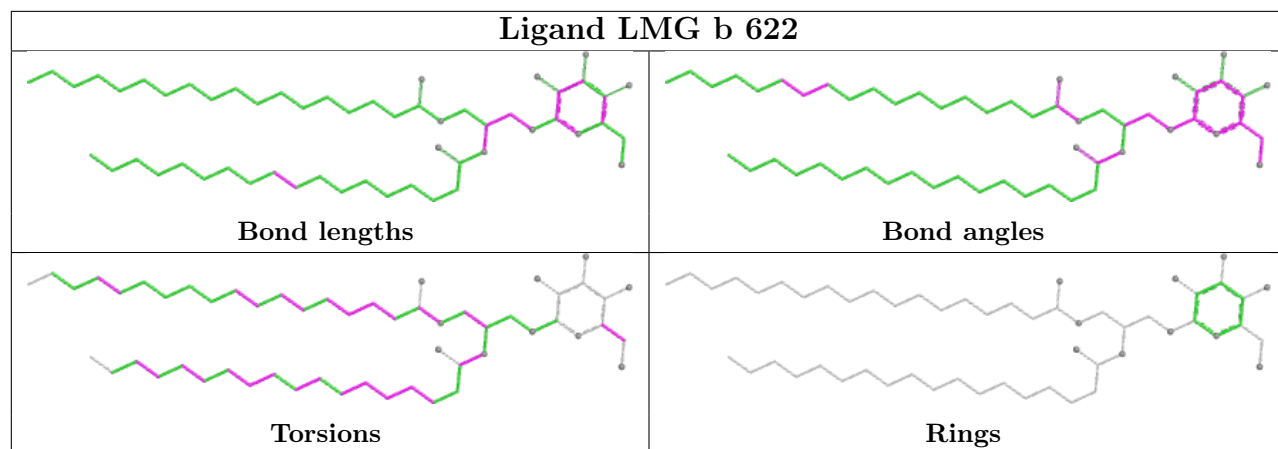


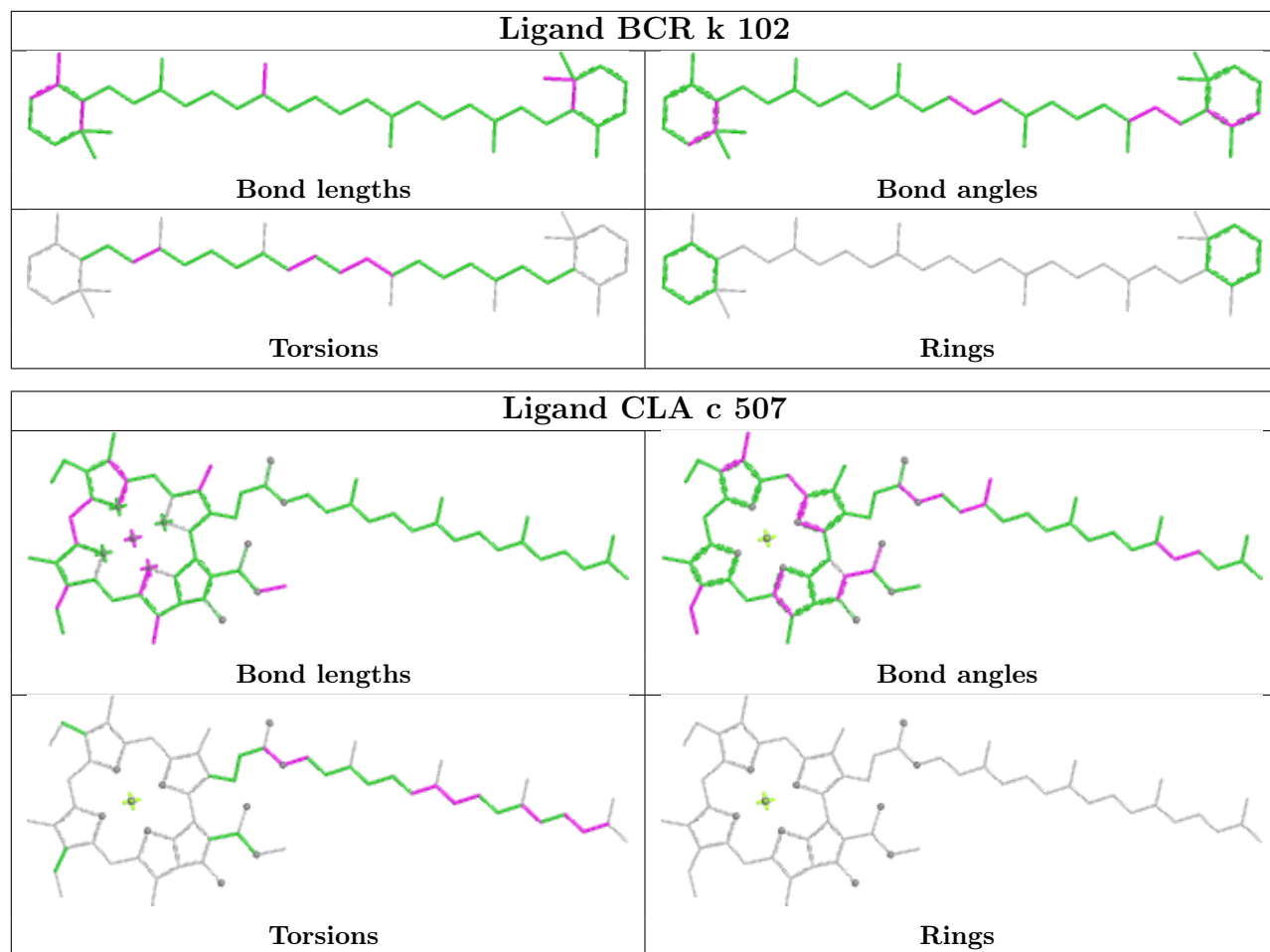
Ligand CLA c 505











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	334/344 (97%)	-0.52	0 100 100	22, 30, 51, 82	0
1	a	334/344 (97%)	-0.42	2 (0%) 85 87	22, 31, 58, 86	0
2	B	505/510 (99%)	-0.36	2 (0%) 88 90	17, 33, 62, 90	4 (0%)
2	b	505/510 (99%)	-0.23	4 (0%) 82 84	23, 36, 72, 104	0
3	C	442/461 (95%)	-0.29	0 100 100	16, 37, 54, 82	1 (0%)
3	c	451/461 (97%)	-0.21	1 (0%) 91 92	21, 40, 62, 95	2 (0%)
4	D	341/352 (96%)	-0.48	0 100 100	23, 31, 49, 77	0
4	d	341/352 (96%)	-0.34	1 (0%) 90 91	25, 34, 58, 77	1 (0%)
5	E	82/84 (97%)	0.27	1 (1%) 76 78	34, 52, 70, 81	1 (1%)
5	e	82/84 (97%)	0.30	1 (1%) 76 78	37, 59, 77, 80	0
6	F	34/45 (75%)	0.01	1 (2%) 53 56	39, 44, 65, 86	0
6	f	34/45 (75%)	0.23	1 (2%) 53 56	39, 49, 78, 93	0
7	H	65/66 (98%)	-0.11	2 (3%) 51 54	33, 41, 61, 69	0
7	h	63/66 (95%)	0.10	0 100 100	40, 50, 63, 73	0
8	I	35/38 (92%)	-0.26	0 100 100	31, 38, 73, 80	0
8	i	35/38 (92%)	-0.19	0 100 100	31, 40, 71, 80	0
9	J	36/40 (90%)	0.01	0 100 100	32, 50, 77, 90	0
9	j	36/40 (90%)	0.26	1 (2%) 55 57	41, 50, 85, 94	0
10	K	37/46 (80%)	0.20	0 100 100	44, 53, 69, 85	0
10	k	37/46 (80%)	0.15	0 100 100	47, 55, 67, 83	0
11	L	37/37 (100%)	-0.50	0 100 100	26, 31, 64, 72	0
11	l	36/37 (97%)	-0.48	0 100 100	24, 31, 75, 88	0
12	M	32/36 (88%)	-0.48	0 100 100	28, 35, 65, 70	0
12	m	31/36 (86%)	-0.50	0 100 100	25, 34, 53, 69	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/272 (89%)	-0.16	2 (0%) 82 84	24, 42, 83, 131	1 (0%)
13	o	244/272 (89%)	-0.19	1 (0%) 88 90	25, 41, 78, 122	0
14	R	34/41 (82%)	1.14	2 (5%) 28 30	64, 78, 93, 110	0
14	r	31/41 (75%)	1.29	3 (9%) 13 14	83, 102, 116, 126	0
15	T	29/32 (90%)	-0.56	0 100 100	26, 31, 61, 77	0
15	t	29/32 (90%)	-0.50	1 (3%) 48 50	27, 33, 82, 88	0
16	U	97/134 (72%)	-0.20	0 100 100	31, 43, 69, 89	0
16	u	97/134 (72%)	-0.26	0 100 100	31, 40, 59, 80	0
17	V	137/163 (84%)	-0.28	0 100 100	31, 40, 57, 83	0
17	v	137/163 (84%)	-0.07	0 100 100	30, 46, 69, 87	0
18	X	38/41 (92%)	0.05	1 (2%) 57 60	42, 51, 71, 82	0
18	x	39/41 (95%)	0.22	2 (5%) 33 35	47, 59, 90, 105	0
19	Y	27/46 (58%)	1.05	3 (11%) 10 10	53, 73, 89, 94	0
19	y	30/46 (65%)	0.55	0 100 100	59, 72, 86, 96	0
20	Z	62/62 (100%)	0.67	3 (4%) 35 38	53, 66, 109, 130	0
20	z	62/62 (100%)	0.66	4 (6%) 25 26	54, 70, 105, 115	0
All	All	5302/5700 (93%)	-0.21	39 (0%) 84 86	16, 38, 74, 131	10 (0%)

The worst 5 of 39 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
14	R	35	LEU	4.4
13	O	60	ARG	3.4
9	j	6	GLY	3.2
3	c	23	ALA	3.1
7	H	41	PHE	3.1

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
15	FME	t	1	10/11	0.92	0.09	28,34,63,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
12	FME	M	1	10/11	0.93	0.10	39,46,55,65	0
8	FME	I	1	10/11	0.93	0.09	37,47,57,58	0
8	FME	i	1	10/11	0.96	0.11	38,45,49,49	0
15	FME	T	1	10/11	0.96	0.08	25,36,51,65	0
12	FME	m	1	10/11	0.97	0.07	30,44,66,70	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
28	STE	H	103	18/20	0.80	0.17	44,67,73,79	0
28	STE	d	402	20/20	0.80	0.17	42,66,78,82	0
28	STE	b	624	20/20	0.81	0.15	44,56,69,71	0
31	LHG	E	101	49/49	0.82	0.13	50,72,92,97	0
28	STE	A	412	5/20	0.83	0.20	39,52,56,64	0
28	STE	I	101	15/20	0.83	0.14	39,52,65,72	0
30	LMG	b	622	55/55	0.83	0.15	47,68,82,90	0
28	STE	J	101	12/20	0.83	0.14	46,57,69,70	0
28	STE	a	415	10/20	0.84	0.13	34,52,54,55	0
28	STE	m	102	12/20	0.84	0.14	44,53,61,64	0
30	LMG	a	418	55/55	0.84	0.13	33,55,90,109	0
28	STE	E	102	12/20	0.84	0.15	60,69,80,86	0
28	STE	c	501	12/20	0.84	0.11	53,60,76,82	0
31	LHG	a	413	42/49	0.84	0.14	49,78,98,103	0
28	STE	b	623	16/20	0.85	0.14	50,56,87,90	0
28	STE	x	101	20/20	0.85	0.13	46,53,63,67	0
28	STE	C	523	12/20	0.85	0.14	34,45,53,59	0
28	STE	b	625	10/20	0.85	0.13	43,52,58,63	0
30	LMG	c	522	48/55	0.85	0.13	37,71,94,102	0
25	PL9	A	408	55/55	0.85	0.15	47,61,72,82	0
28	STE	B	726	16/20	0.85	0.14	48,58,69,70	0
28	STE	B	724	12/20	0.86	0.12	40,48,56,67	0
27	DGD	A	411	66/66	0.86	0.11	40,56,71,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
30	LMG	D	413	32/55	0.86	0.13	36,51,68,73	0
22	CLA	h	701	65/65	0.86	0.12	46,63,79,82	0
28	STE	B	720	17/20	0.86	0.13	31,46,61,68	0
28	STE	c	521	20/20	0.86	0.11	41,50,65,74	0
28	STE	a	416	12/20	0.86	0.11	49,57,62,65	0
28	STE	h	704	14/20	0.86	0.16	42,56,74,77	0
30	LMG	C	516	48/55	0.87	0.11	40,55,71,82	0
28	STE	a	417	15/20	0.87	0.14	37,54,66,66	0
28	STE	C	522	16/20	0.87	0.12	38,48,57,67	0
26	SQD	a	414	36/54	0.87	0.12	31,56,74,81	0
28	STE	j	101	12/20	0.87	0.12	46,50,59,64	0
25	PL9	a	410	55/55	0.87	0.14	40,62,77,84	0
26	SQD	B	723	54/54	0.87	0.11	37,58,81,90	0
28	STE	b	601	16/20	0.88	0.14	32,43,66,68	0
26	SQD	f	102	41/54	0.89	0.13	54,82,91,98	0
26	SQD	D	410	36/54	0.89	0.12	51,68,82,84	0
30	LMG	C	520	48/55	0.89	0.11	42,62,74,77	0
28	STE	B	725	18/20	0.89	0.11	41,48,76,79	0
26	SQD	A	410	39/54	0.89	0.12	37,55,87,89	0
28	STE	d	411	17/20	0.89	0.11	41,49,58,64	0
30	LMG	c	520	37/55	0.89	0.10	41,61,73,77	0
28	STE	b	621	20/20	0.89	0.10	35,48,65,74	0
28	STE	B	701	12/20	0.89	0.13	45,59,73,79	0
28	STE	X	101	20/20	0.89	0.11	33,43,71,82	0
28	STE	E	103	7/20	0.90	0.12	47,58,62,63	0
28	STE	C	521	12/20	0.90	0.11	40,46,54,55	0
30	LMG	b	620	51/55	0.90	0.10	33,48,69,76	0
28	STE	H	104	8/20	0.90	0.12	46,51,57,60	0
28	STE	t	702	14/20	0.90	0.11	38,49,59,61	0
23	BCR	h	702	40/40	0.90	0.11	34,53,64,75	0
23	BCR	c	515	40/40	0.90	0.10	43,53,63,69	0
23	BCR	d	405	40/40	0.90	0.11	37,48,77,91	0
30	LMG	B	721	28/55	0.91	0.12	34,47,60,68	0
28	STE	m	101	18/20	0.91	0.11	34,41,65,69	0
22	CLA	C	514	65/65	0.91	0.09	40,56,83,93	0
26	SQD	l	101	49/54	0.91	0.09	34,57,82,95	0
30	LMG	c	523	49/55	0.91	0.10	35,57,74,86	0
30	LMG	M	101	51/55	0.91	0.09	31,45,63,66	0
23	BCR	k	101	40/40	0.91	0.11	36,55,72,73	0
23	BCR	Y	101	40/40	0.92	0.09	41,49,62,66	0
22	CLA	B	727	65/65	0.92	0.09	30,50,80,96	0
27	DGD	H	102	62/66	0.92	0.09	25,41,51,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
26	SQD	a	412	54/54	0.92	0.10	41,58,79,87	0
23	BCR	C	524	40/40	0.92	0.10	44,52,58,66	0
23	BCR	D	405	40/40	0.92	0.10	27,40,76,83	0
28	STE	M	102	15/20	0.92	0.11	32,44,71,80	0
28	STE	T	702	15/20	0.92	0.11	39,46,66,71	0
23	BCR	k	102	40/40	0.93	0.10	39,48,54,60	0
22	CLA	c	513	65/65	0.93	0.10	40,51,79,95	0
27	DGD	h	703	62/66	0.93	0.09	31,43,53,62	0
28	STE	Z	101	8/20	0.93	0.12	49,51,56,59	0
22	CLA	C	504	65/65	0.93	0.09	30,42,48,52	0
23	BCR	H	101	40/40	0.93	0.08	35,41,51,65	0
23	BCR	B	718	40/40	0.93	0.08	23,33,46,47	0
23	BCR	b	618	40/40	0.94	0.06	26,35,45,48	0
23	BCR	b	619	40/40	0.94	0.07	32,44,55,64	0
22	CLA	C	511	65/65	0.94	0.08	30,43,54,66	0
23	BCR	c	516	40/40	0.94	0.08	29,39,48,60	0
22	CLA	c	514	65/65	0.94	0.09	43,60,91,95	0
30	LMG	D	409	51/55	0.94	0.10	34,44,69,78	0
22	CLA	C	512	65/65	0.94	0.09	28,47,57,71	0
27	DGD	C	518	62/66	0.94	0.09	32,46,80,101	0
22	CLA	C	513	65/65	0.94	0.09	33,49,82,87	0
27	DGD	c	518	62/66	0.94	0.08	30,49,74,79	0
22	CLA	B	706	65/65	0.94	0.08	22,32,62,68	0
22	CLA	c	509	64/65	0.94	0.09	33,42,73,93	0
22	CLA	c	510	65/65	0.94	0.09	34,43,53,61	0
26	SQD	A	409	52/54	0.94	0.09	29,55,73,82	0
31	LHG	B	722	49/49	0.94	0.10	30,42,61,64	0
22	CLA	c	512	65/65	0.94	0.10	37,50,58,63	0
23	BCR	b	617	40/40	0.94	0.07	29,37,45,47	0
22	CLA	b	616	60/65	0.95	0.09	28,41,80,84	0
23	BCR	A	405	40/40	0.95	0.07	22,31,41,44	0
27	DGD	C	519	62/66	0.95	0.08	30,41,61,74	0
28	STE	M	103	10/20	0.95	0.07	35,42,45,48	0
23	BCR	B	717	40/40	0.95	0.07	26,35,50,53	0
22	CLA	c	504	65/65	0.95	0.07	21,42,50,52	0
23	BCR	B	719	40/40	0.95	0.06	23,36,48,54	0
23	BCR	C	501	40/40	0.95	0.09	35,49,62,65	0
23	BCR	t	701	40/40	0.95	0.07	22,33,45,46	0
23	BCR	C	515	40/40	0.95	0.07	24,36,44,46	0
25	PL9	D	406	55/55	0.95	0.07	22,30,43,47	0
22	CLA	c	507	65/65	0.95	0.08	29,42,82,90	0
22	CLA	c	508	65/65	0.95	0.07	25,39,51,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	CLA	C	503	65/65	0.95	0.07	29,38,47,52	0
23	BCR	T	701	40/40	0.95	0.06	28,35,50,51	0
22	CLA	C	509	65/65	0.95	0.08	27,37,88,99	0
23	BCR	a	406	40/40	0.95	0.06	20,30,44,46	0
22	CLA	b	606	65/65	0.95	0.07	23,37,61,70	0
31	LHG	D	412	47/49	0.95	0.09	23,39,70,84	0
22	CLA	b	609	65/65	0.95	0.07	28,41,55,68	0
31	LHG	a	411	49/49	0.95	0.10	30,44,66,71	0
22	CLA	b	614	65/65	0.95	0.08	21,35,60,70	0
31	LHG	l	102	49/49	0.95	0.08	31,41,49,53	0
22	CLA	d	404	65/65	0.96	0.08	26,37,75,92	0
22	CLA	B	716	60/65	0.96	0.09	22,32,81,86	0
22	CLA	a	402	65/65	0.96	0.06	20,28,36,51	0
22	CLA	a	403	65/65	0.96	0.08	27,36,86,96	0
22	CLA	a	405	65/65	0.96	0.08	17,28,64,69	0
27	DGD	C	517	62/66	0.96	0.09	21,35,66,73	0
22	CLA	b	602	65/65	0.96	0.07	24,36,52,55	0
22	CLA	b	604	65/65	0.96	0.08	21,32,71,85	0
22	CLA	b	605	65/65	0.96	0.07	20,30,42,48	0
22	CLA	B	704	65/65	0.96	0.08	21,27,63,69	0
27	DGD	c	519	62/66	0.96	0.07	28,44,72,86	0
22	CLA	b	608	65/65	0.96	0.07	28,39,54,61	0
22	CLA	C	502	65/65	0.96	0.06	22,32,44,54	0
22	CLA	b	610	65/65	0.96	0.07	23,33,42,51	0
22	CLA	b	612	65/65	0.96	0.07	23,31,43,48	0
22	CLA	A	403	65/65	0.96	0.08	21,30,76,84	0
22	CLA	b	615	65/65	0.96	0.07	28,38,51,53	0
22	CLA	B	709	65/65	0.96	0.06	24,34,44,50	0
22	CLA	c	502	65/65	0.96	0.07	27,36,46,51	0
22	CLA	c	503	65/65	0.96	0.07	28,40,53,61	0
22	CLA	C	505	59/65	0.96	0.07	27,38,63,73	0
22	CLA	c	505	60/65	0.96	0.07	32,42,65,70	0
22	CLA	c	506	65/65	0.96	0.07	26,36,61,65	0
22	CLA	C	507	65/65	0.96	0.08	24,39,70,83	0
22	CLA	C	508	65/65	0.96	0.07	25,35,49,53	0
22	CLA	B	710	65/65	0.96	0.07	19,30,39,44	0
22	CLA	C	510	65/65	0.96	0.08	25,40,52,64	0
22	CLA	c	511	65/65	0.96	0.07	32,45,52,61	0
30	LMG	d	410	44/55	0.96	0.07	34,43,70,71	0
22	CLA	B	711	65/65	0.96	0.06	18,27,43,50	0
31	LHG	D	411	49/49	0.96	0.07	21,37,44,56	0
25	PL9	d	406	55/55	0.96	0.06	21,31,38,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	CLA	B	712	65/65	0.96	0.07	21,28,39,44	0
22	CLA	B	715	65/65	0.96	0.07	24,33,56,65	0
22	CLA	d	401	65/65	0.96	0.06	20,29,35,44	0
31	LHG	d	409	39/49	0.96	0.08	34,43,60,64	0
22	CLA	d	403	65/65	0.96	0.07	21,31,47,53	0
32	BCT	a	409	4/4	0.96	0.07	31,32,40,49	0
33	PHO	D	408	64/64	0.96	0.06	22,30,36,43	0
33	PHO	a	404	64/64	0.96	0.06	19,28,35,37	0
33	PHO	d	407	64/64	0.96	0.06	26,36,44,51	0
22	CLA	B	702	65/65	0.97	0.06	25,33,45,54	0
27	DGD	c	517	62/66	0.97	0.07	23,35,70,72	0
22	CLA	B	713	65/65	0.97	0.06	20,29,57,63	0
22	CLA	D	402	65/65	0.97	0.06	14,26,49,59	0
22	CLA	b	611	65/65	0.97	0.06	23,30,50,56	0
22	CLA	D	403	65/65	0.97	0.05	19,24,40,47	0
22	CLA	b	613	65/65	0.97	0.06	18,29,59,68	0
22	CLA	D	404	65/65	0.97	0.07	22,34,93,105	0
22	CLA	C	506	65/65	0.97	0.07	22,34,60,69	0
31	LHG	L	101	49/49	0.97	0.07	31,36,48,55	0
22	CLA	B	714	65/65	0.97	0.07	19,31,63,79	0
22	CLA	B	707	65/65	0.97	0.06	16,28,51,59	0
31	LHG	d	408	49/49	0.97	0.07	25,39,49,54	0
22	CLA	B	708	65/65	0.97	0.06	20,30,46,53	0
22	CLA	b	603	65/65	0.97	0.07	22,31,57,63	0
32	BCT	D	401	4/4	0.97	0.06	25,31,34,37	0
22	CLA	B	703	65/65	0.97	0.06	19,28,48,52	0
33	PHO	D	407	64/64	0.97	0.05	16,25,33,38	0
22	CLA	A	402	65/65	0.97	0.06	16,25,38,48	0
22	CLA	B	705	65/65	0.97	0.06	18,27,41,44	0
22	CLA	b	607	65/65	0.97	0.07	18,31,55,65	0
34	HEC	F	101	43/43	0.97	0.08	31,46,60,69	0
34	HEC	f	101	43/43	0.97	0.08	39,53,74,84	0
34	HEC	V	201	43/43	0.98	0.06	17,30,40,44	0
22	CLA	A	404	54/65	0.98	0.05	16,26,57,59	0
34	HEC	v	201	43/43	0.98	0.06	26,34,43,48	0
29	OEX	A	413[A]	10/10	0.99	0.04	21,28,37,37	0
29	OEX	a	419[A]	10/10	0.99	0.03	23,30,33,40	0
24	CL	a	407	1/1	0.99	0.05	29,29,29,29	0
21	FE2	a	401	1/1	0.99	0.07	44,44,44,44	0
24	CL	A	406	1/1	0.99	0.04	30,30,30,30	0
21	FE2	A	401	1/1	1.00	0.01	28,28,28,28	0
24	CL	a	408	1/1	1.00	0.06	28,28,28,28	0

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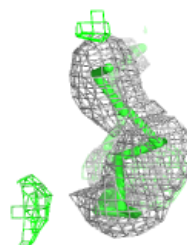
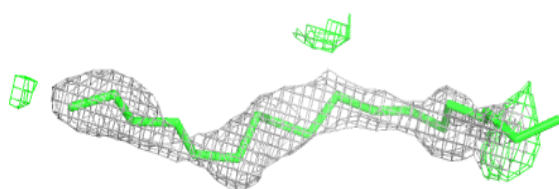
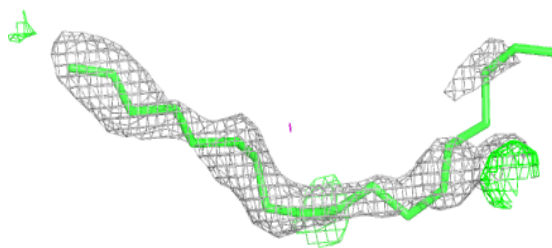
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
24	CL	A	407	1/1	1.00	0.08	28,28,28,28	0

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

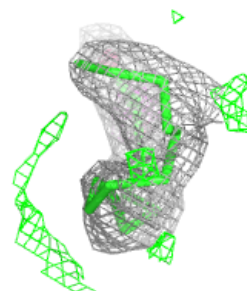
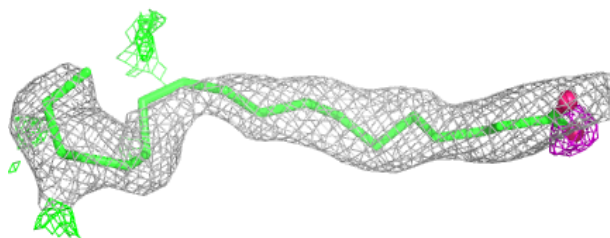
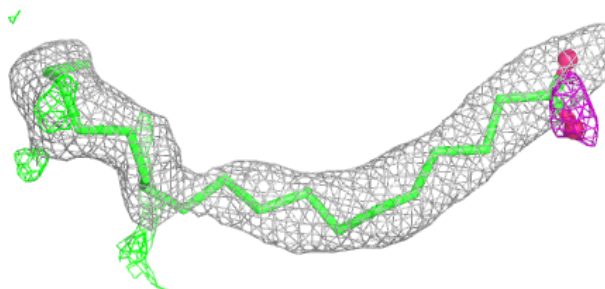
Electron density around STE H 103:

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

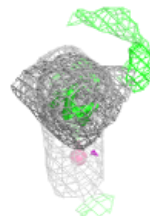
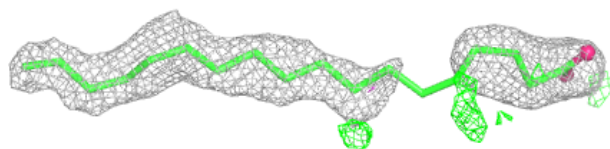
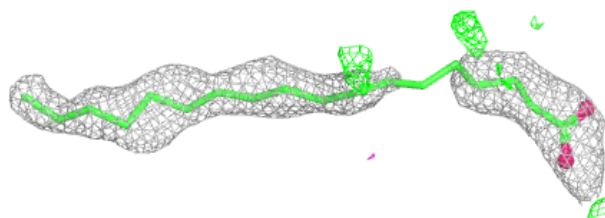


Electron density around STE d 402:

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

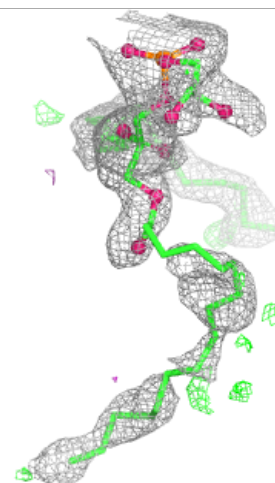
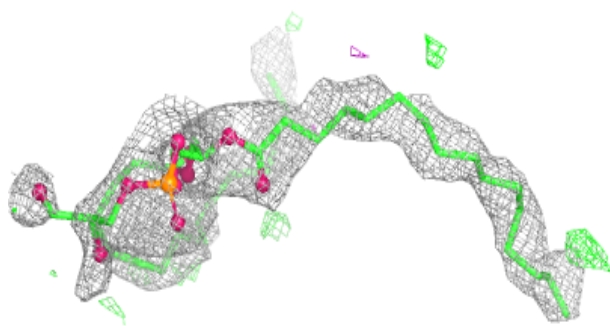
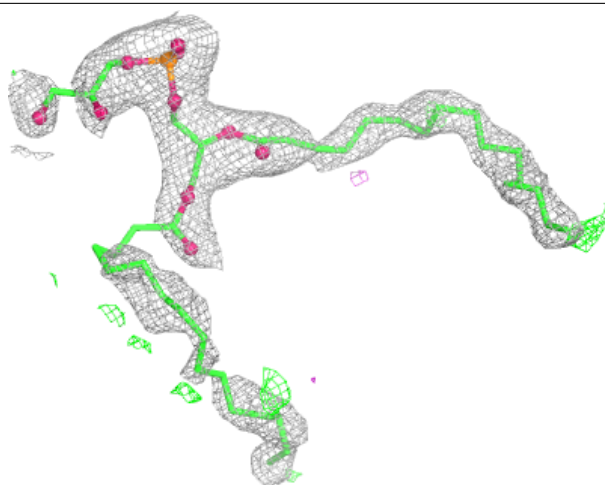
**Electron density around STE b 624:**

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



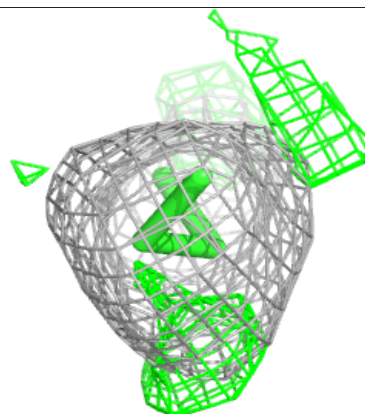
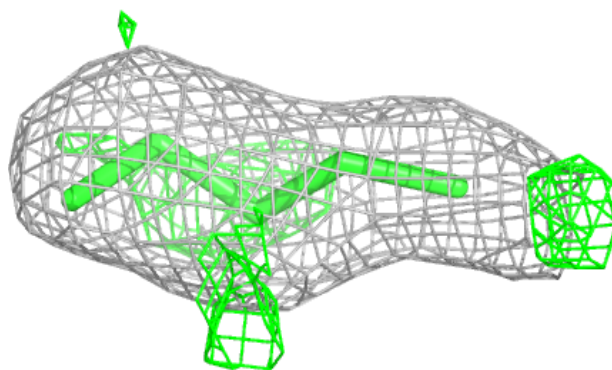
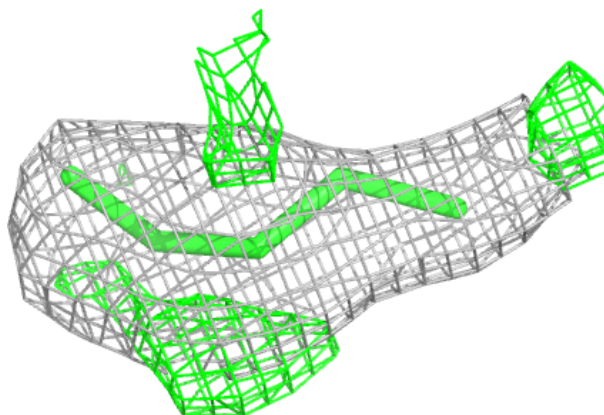
Electron density around LHG E 101:

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

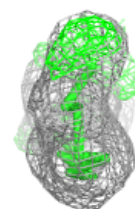
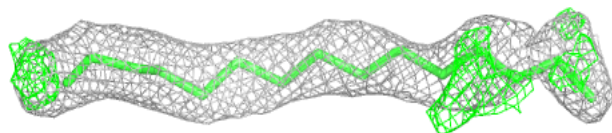
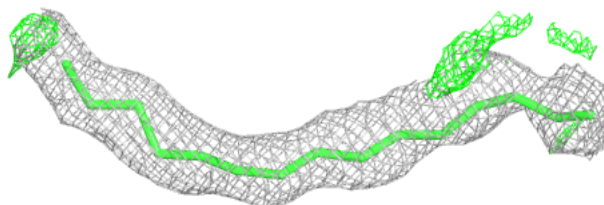


Electron density around STE A 412:

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

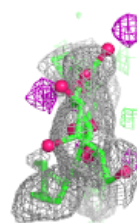
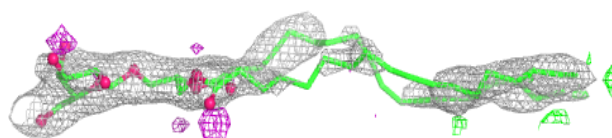
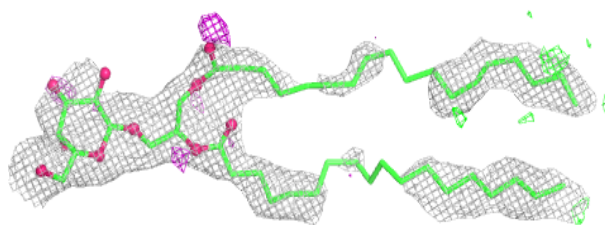
**Electron density around STE I 101:**

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

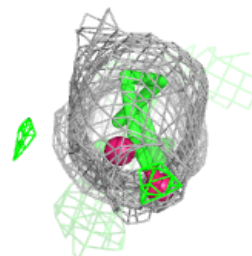
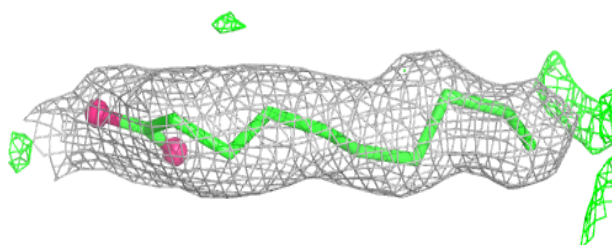
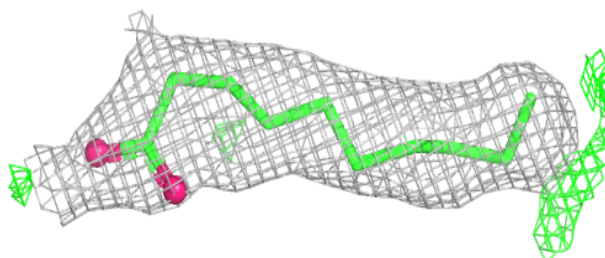


Electron density around LMG b 622:

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

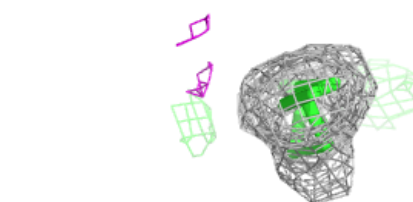
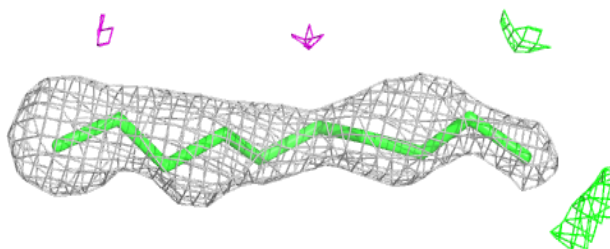
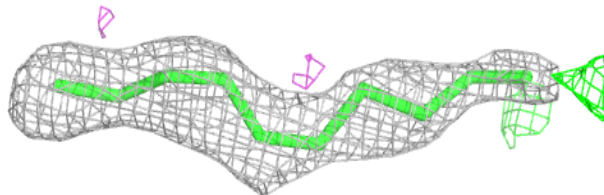
**Electron density around STE J 101:**

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

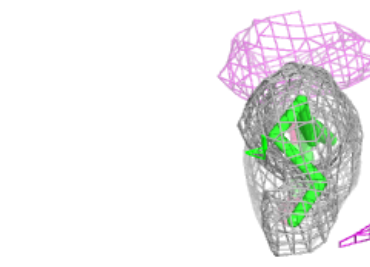
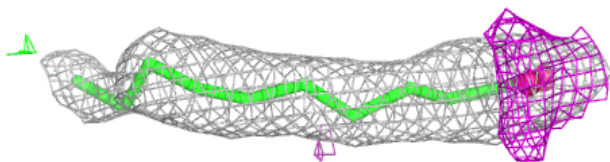
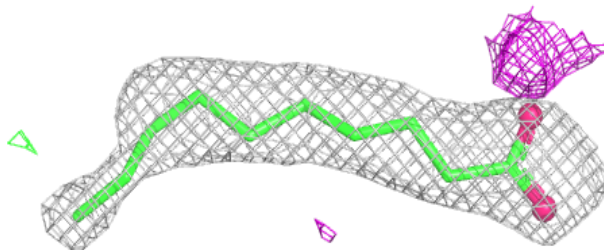


Electron density around STE a 415:

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

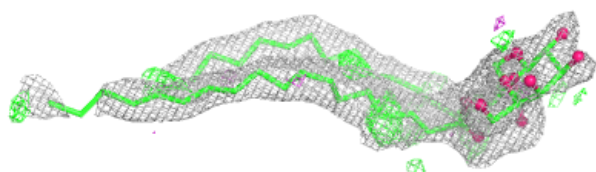
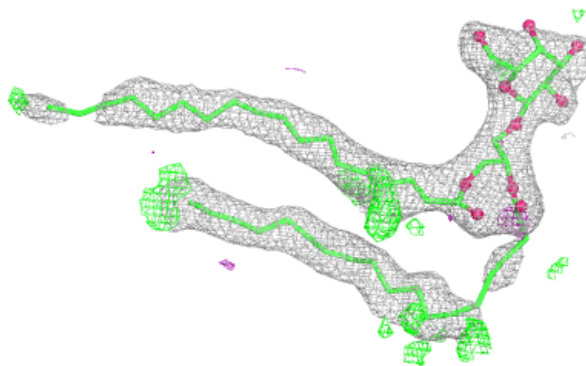
**Electron density around STE m 102:**

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

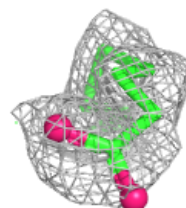
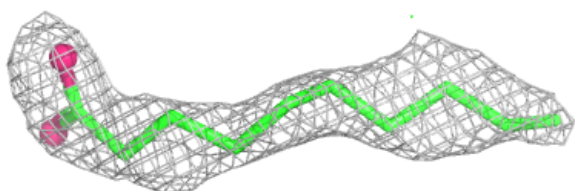
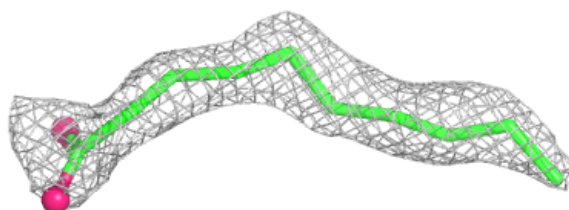


Electron density around LMG a 418:

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

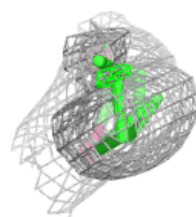
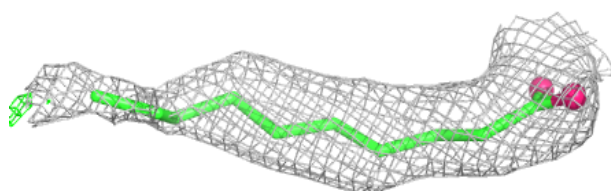
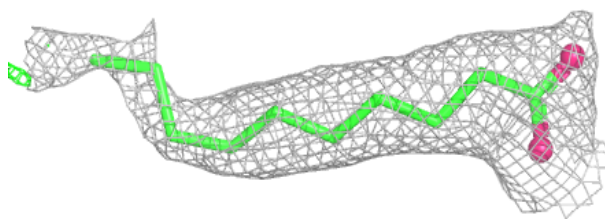
**Electron density around STE E 102:**

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

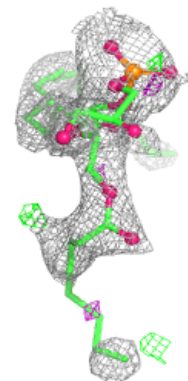
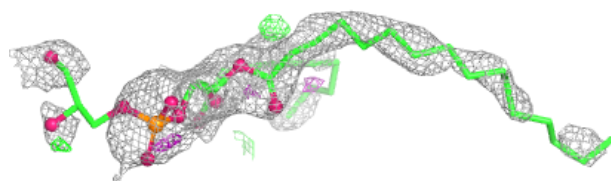
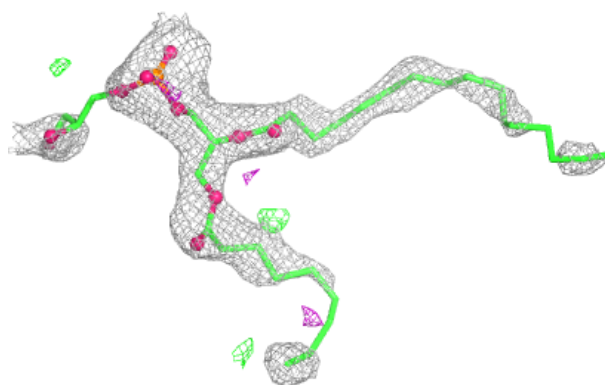


Electron density around STE c 501:

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

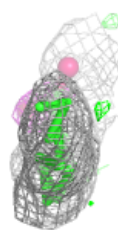
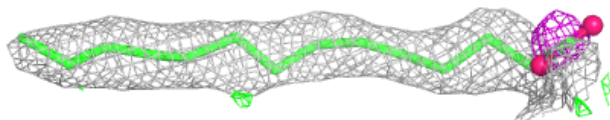
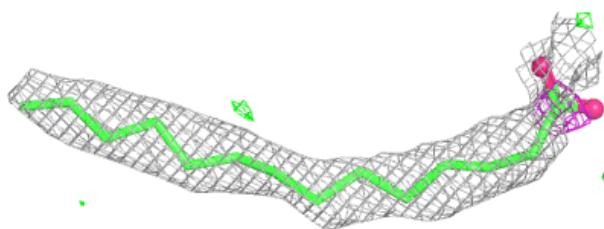
**Electron density around LHG a 413:**

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

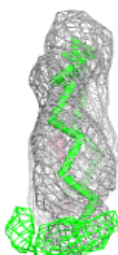
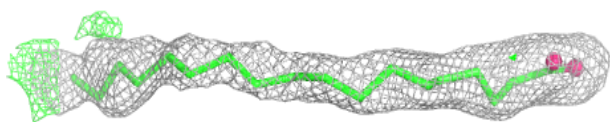
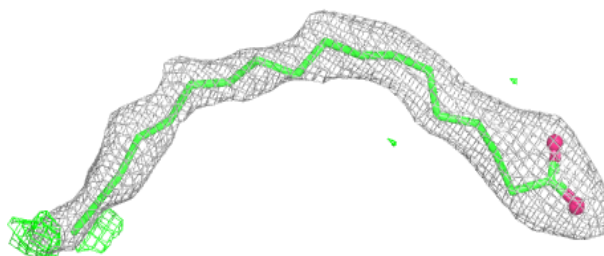


Electron density around STE b 623:

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

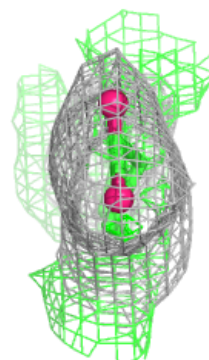
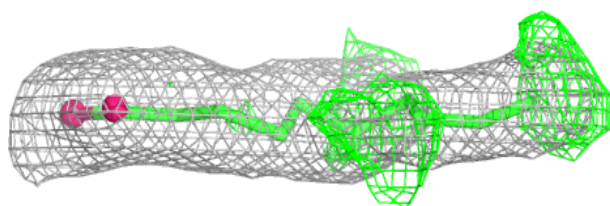
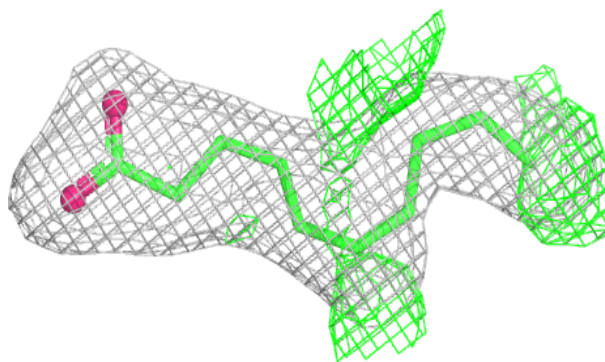
**Electron density around STE x 101:**

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

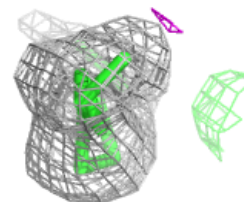
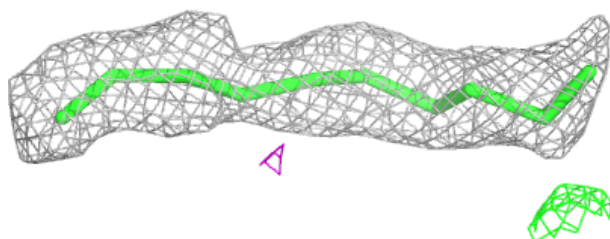
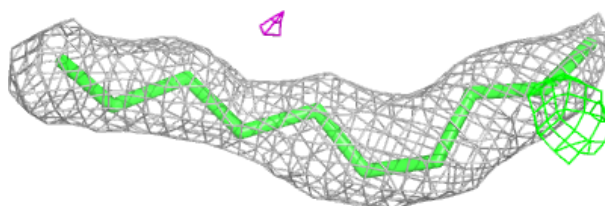


Electron density around STE C 523:

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and green (positive)

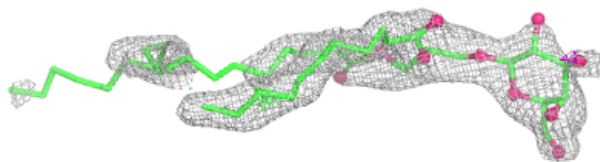
**Electron density around STE b 625:**

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and green (positive)

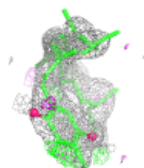
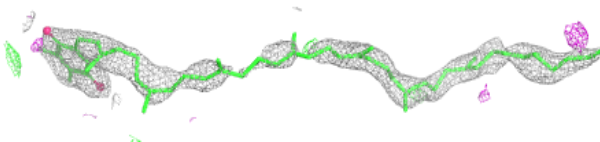
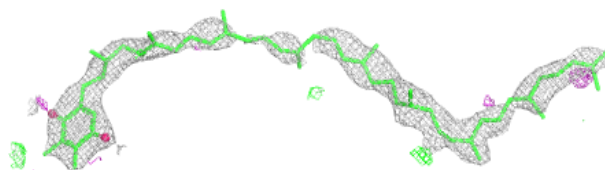


Electron density around LMG c 522:

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

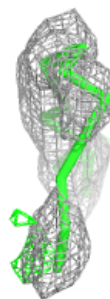
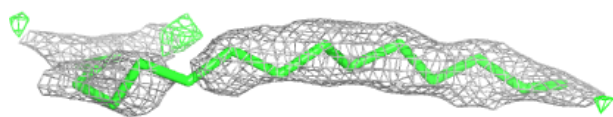
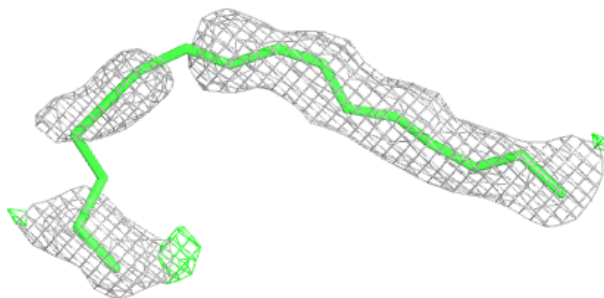
**Electron density around PL9 A 408:**

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

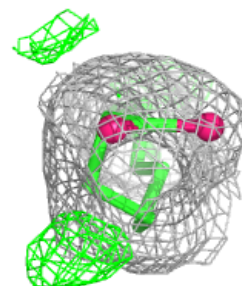
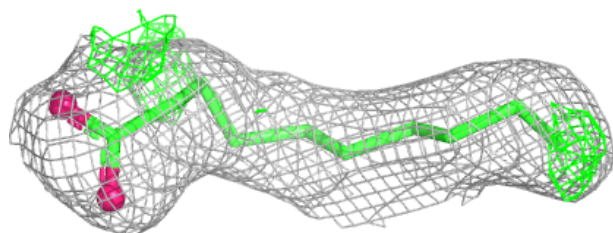
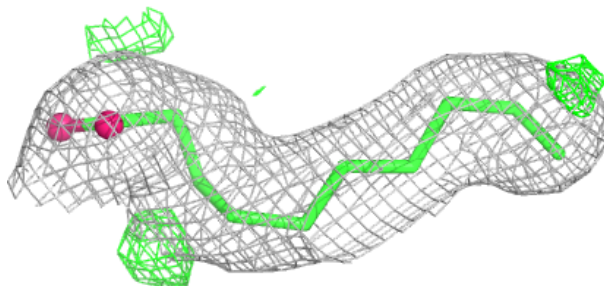


Electron density around STE B 726:

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

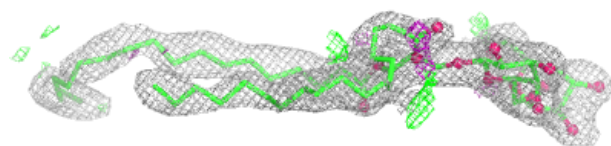
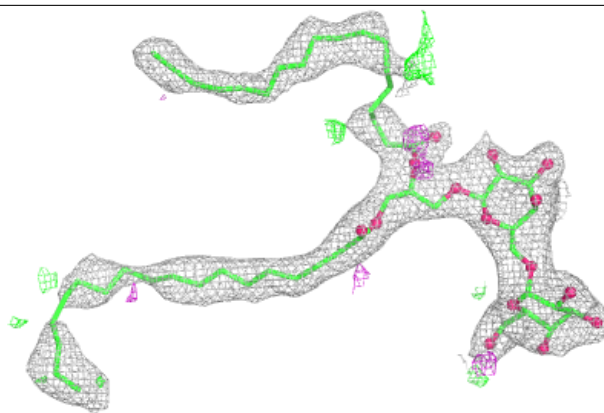
**Electron density around STE B 724:**

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

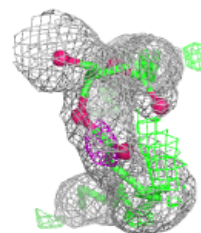
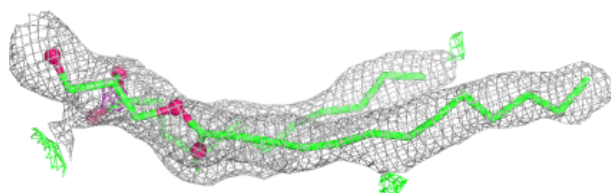
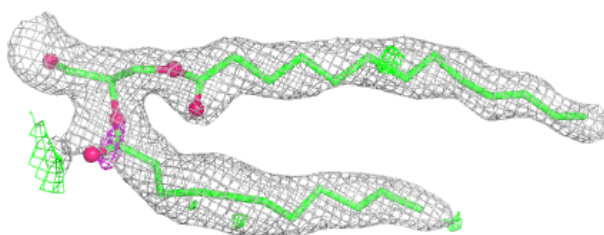


Electron density around DGD A 411:

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

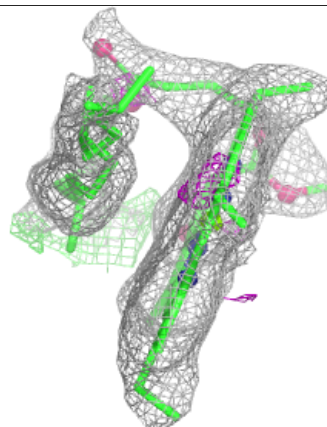
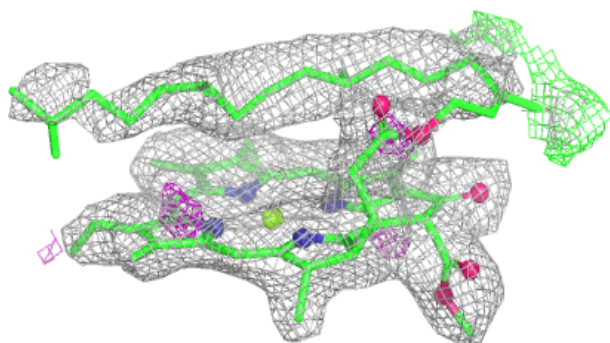
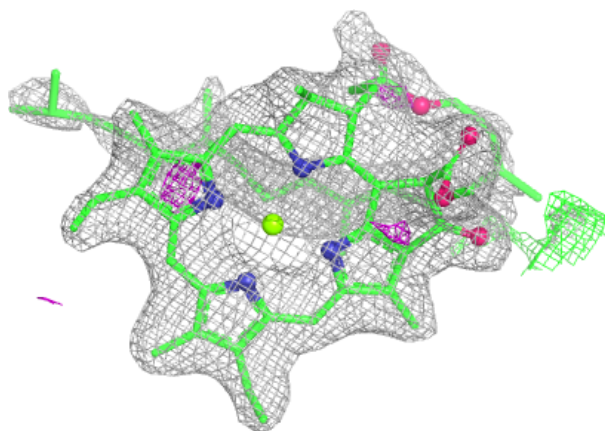
**Electron density around LMG D 413:**

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

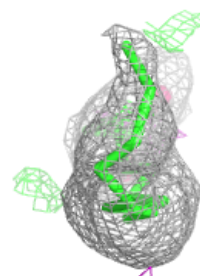
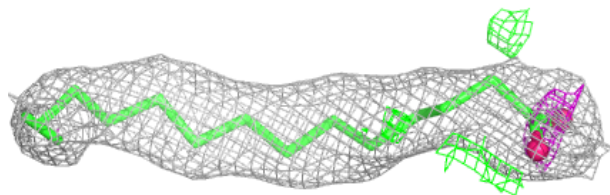
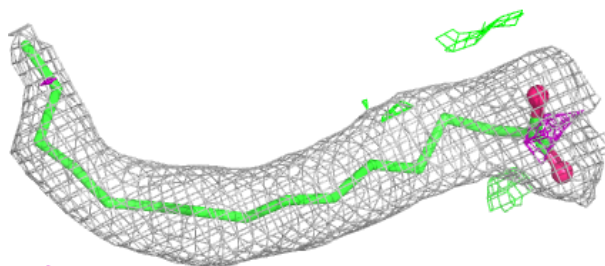


Electron density around CLA h 701:

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

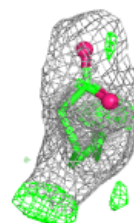
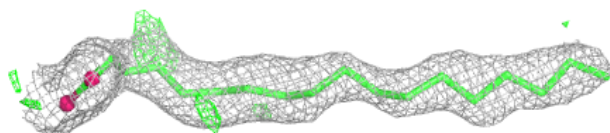
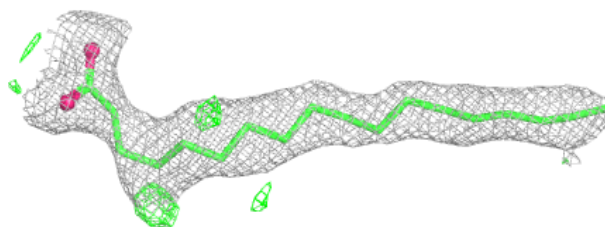
**Electron density around STE B 720:**

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

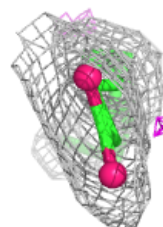
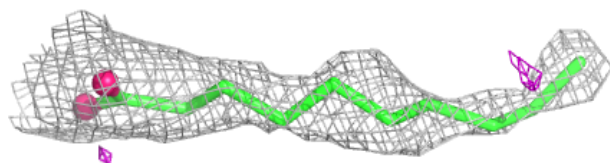
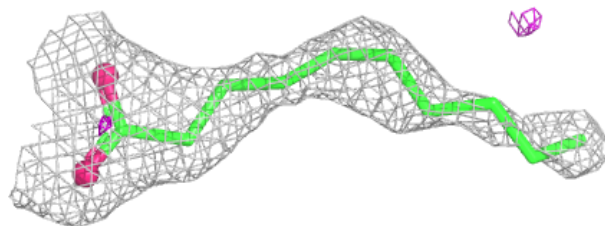


Electron density around STE c 521:

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

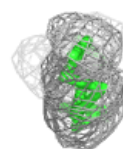
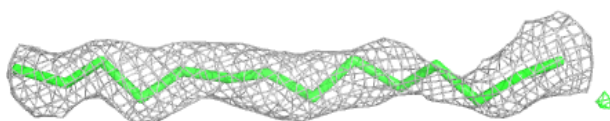
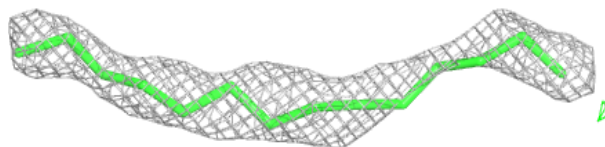
**Electron density around STE a 416:**

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

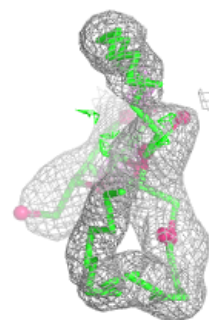
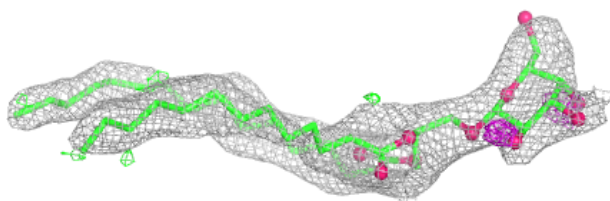
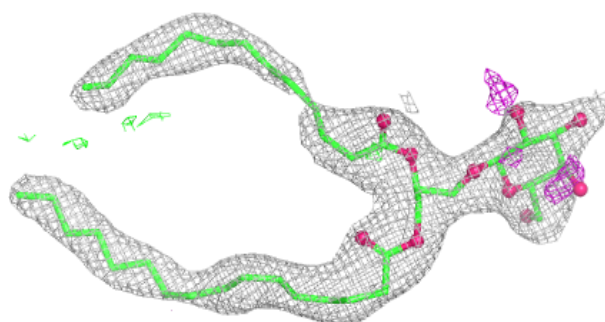


Electron density around STE h 704:

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

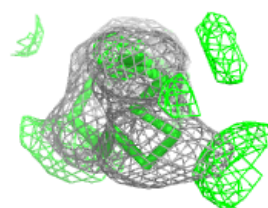
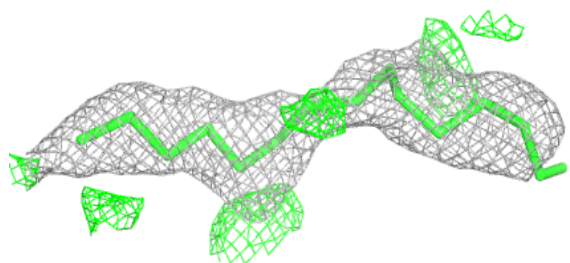
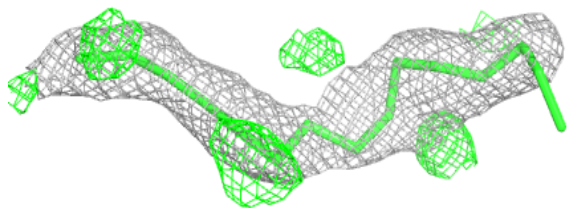
**Electron density around LMG C 516:**

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

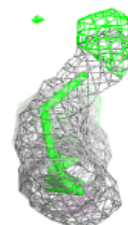
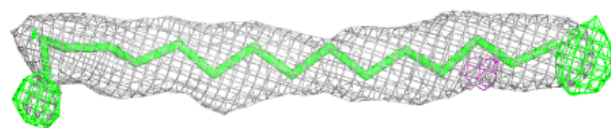
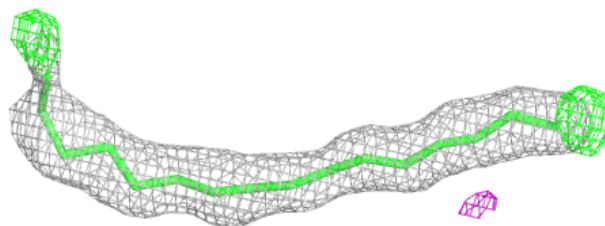


Electron density around STE a 417:

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

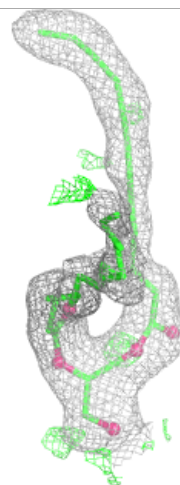
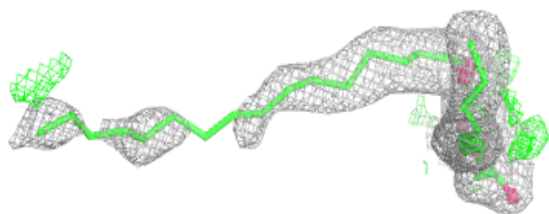
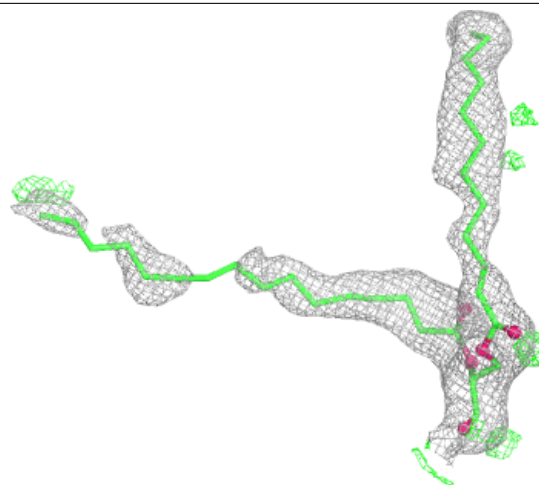
**Electron density around STE C 522:**

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



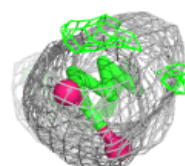
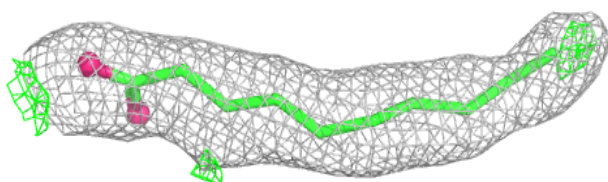
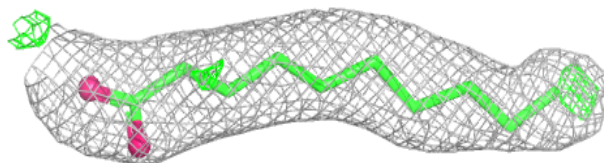
Electron density around SQD a 414:

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

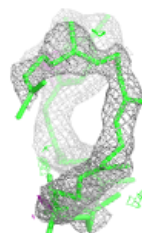
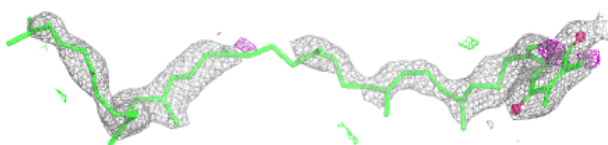
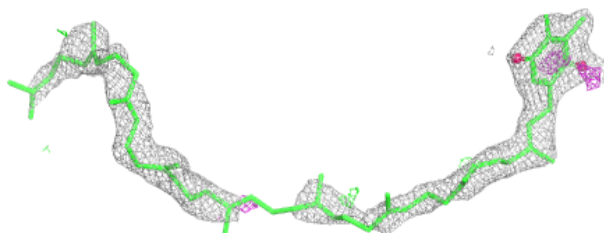


Electron density around STE j 101:

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

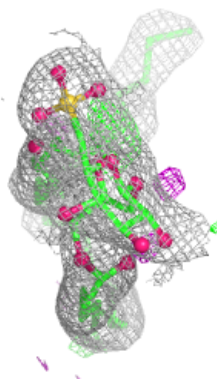
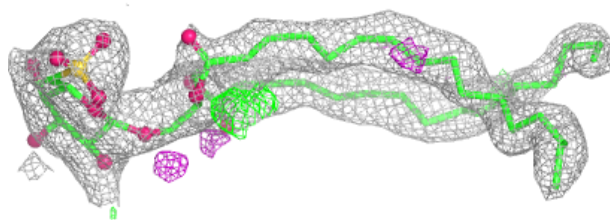
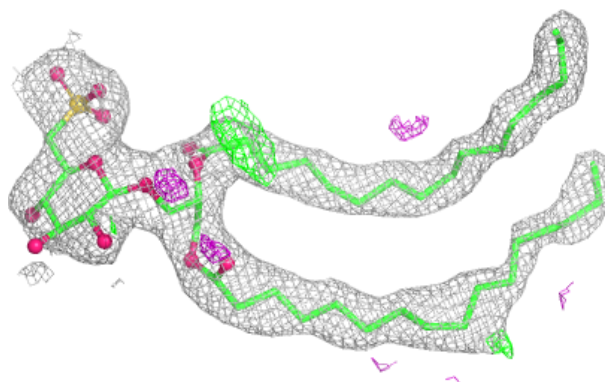
**Electron density around PL9 a 410:**

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

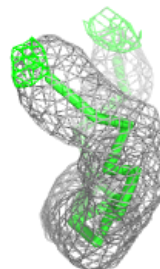
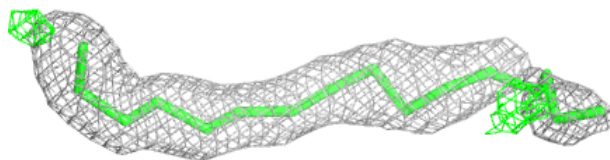
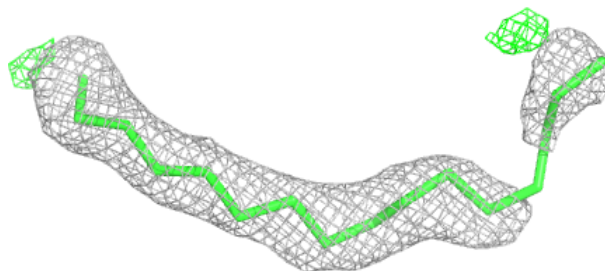


Electron density around SQD B 723:

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

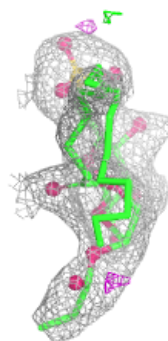
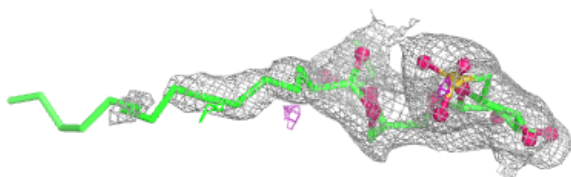
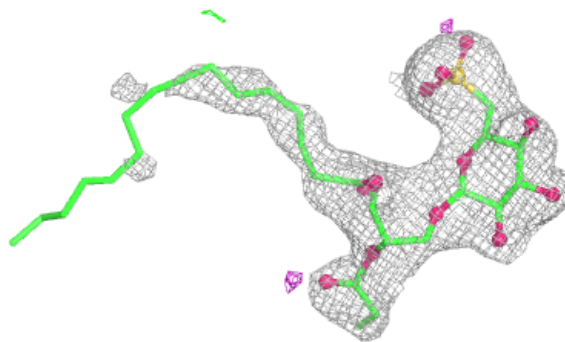
**Electron density around STE b 601:**

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

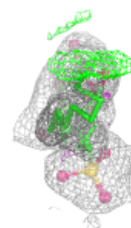
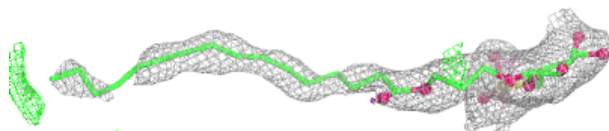
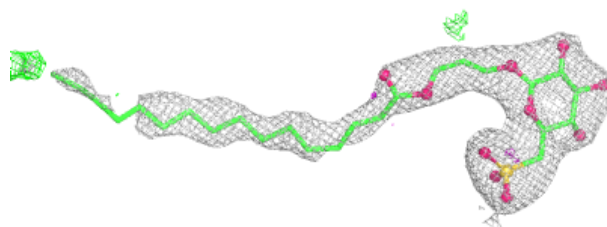


Electron density around SQD f 102:

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

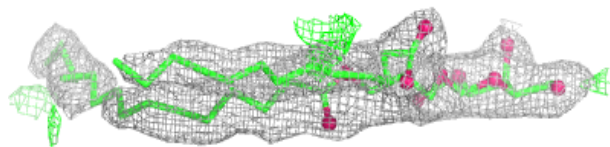
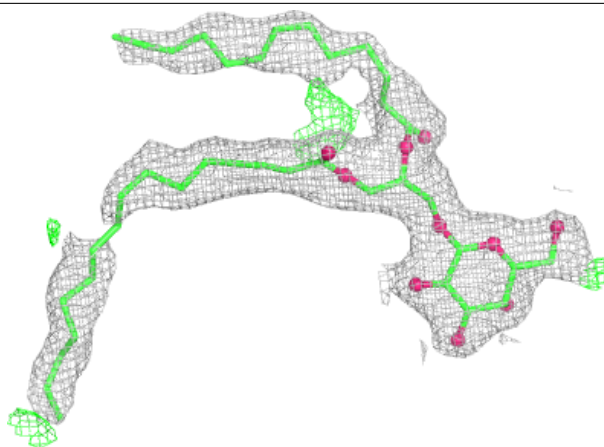
**Electron density around SQD D 410:**

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

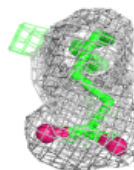
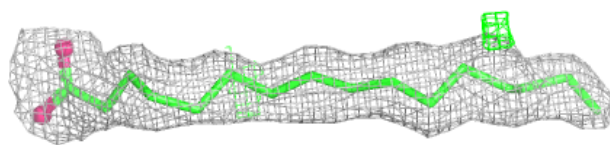
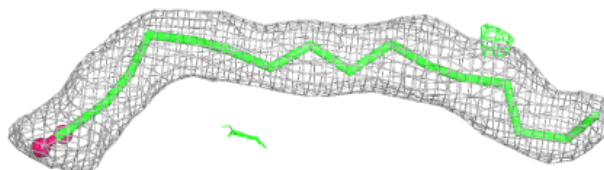


Electron density around LMG C 520:

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

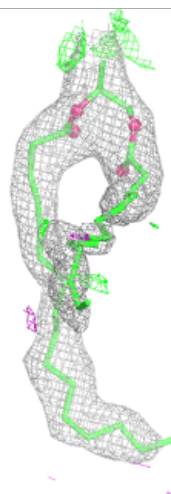
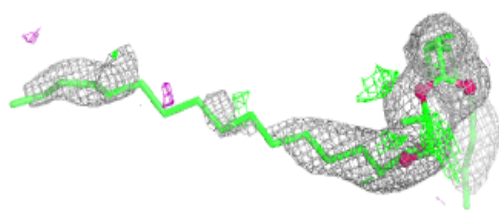
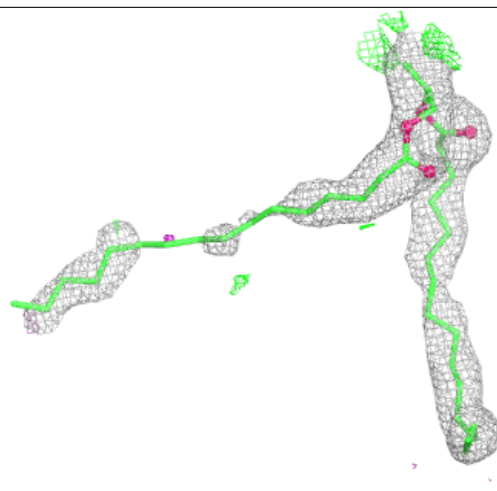
**Electron density around STE B 725:**

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



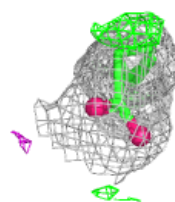
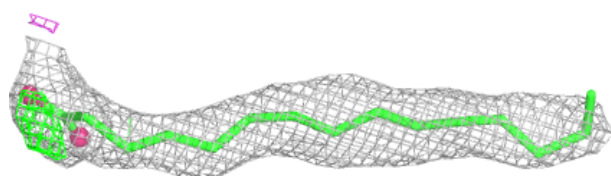
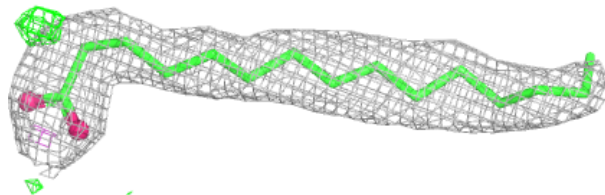
Electron density around SQD A 410:

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

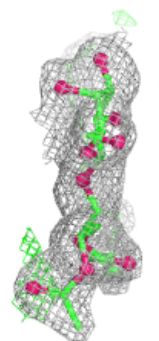
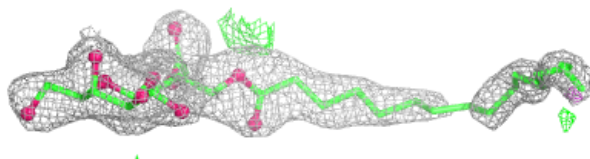


Electron density around STE d 411:

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

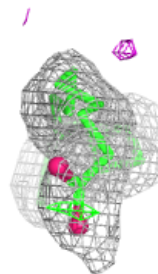
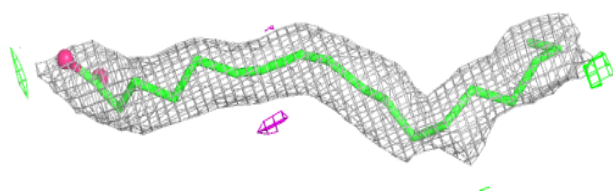
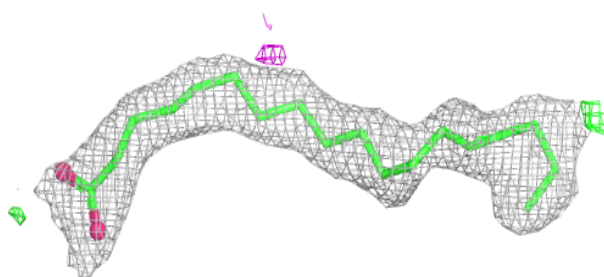
**Electron density around LMG c 520:**

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

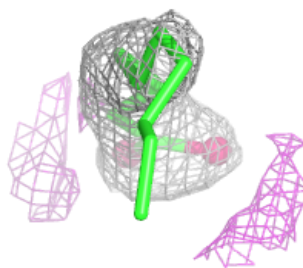
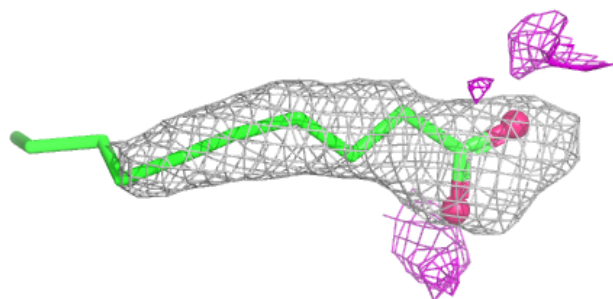
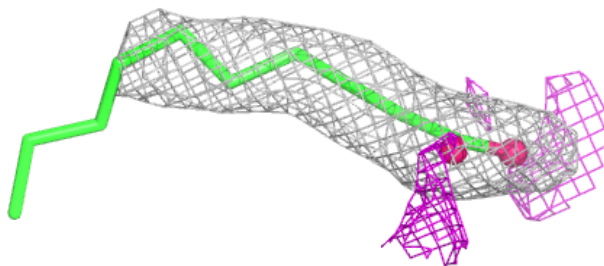


Electron density around STE b 621:

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

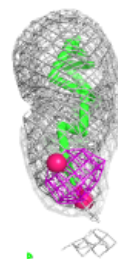
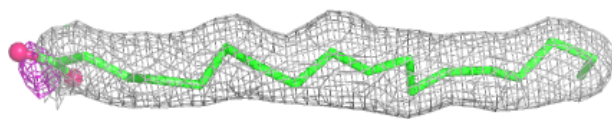
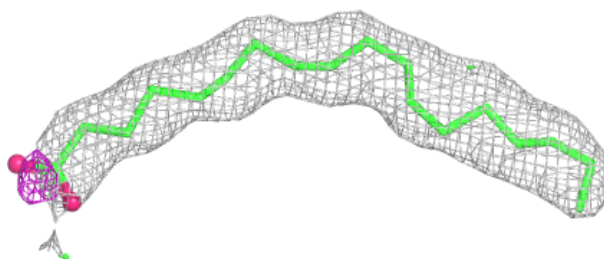
**Electron density around STE B 701:**

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

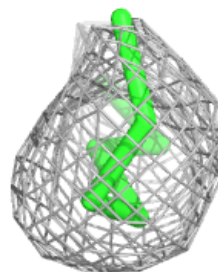
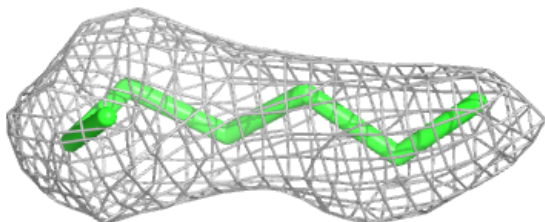
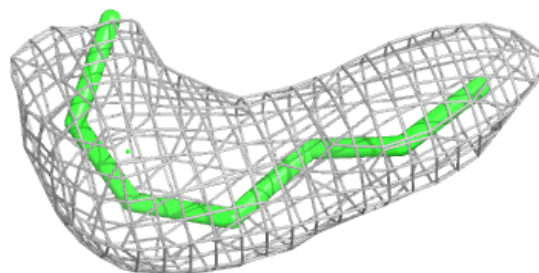


Electron density around STE X 101:

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

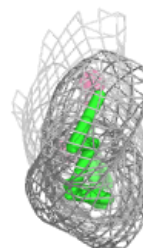
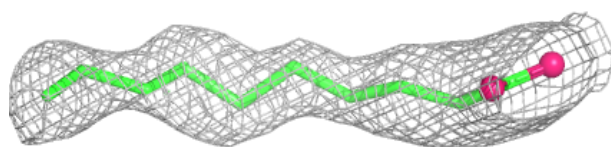
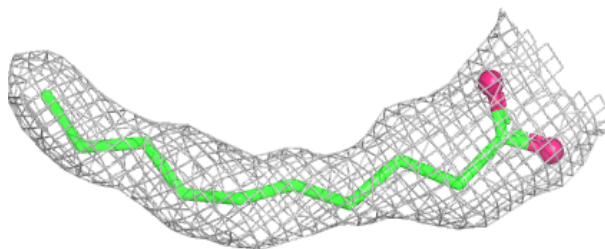
**Electron density around STE E 103:**

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

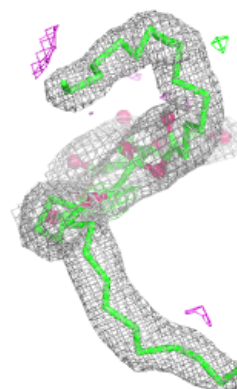
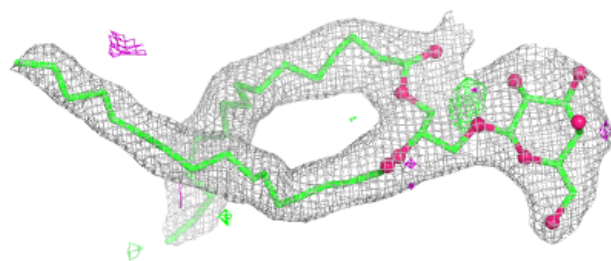
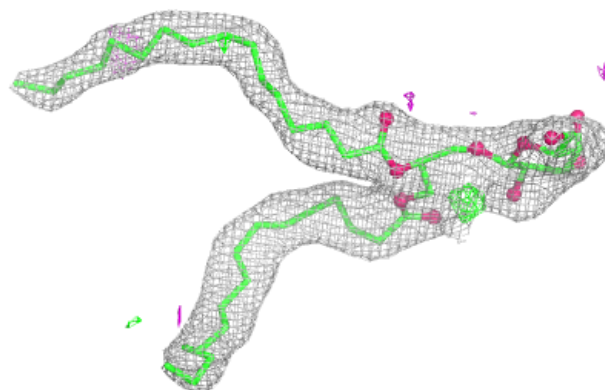


Electron density around STE C 521:

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

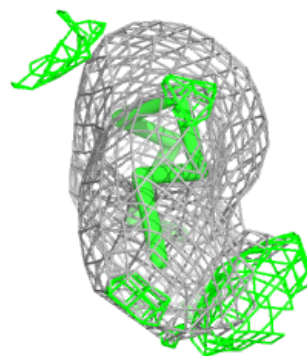
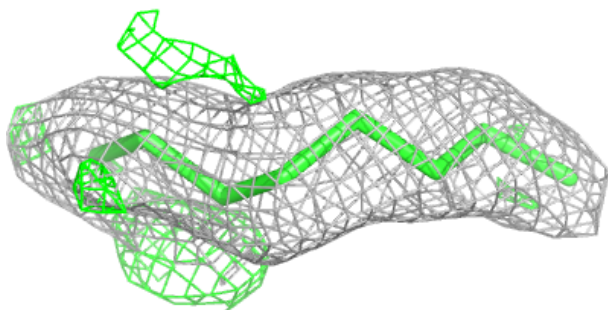
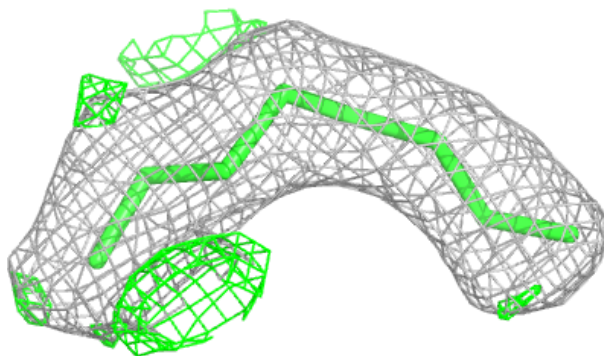
**Electron density around LMG b 620:**

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

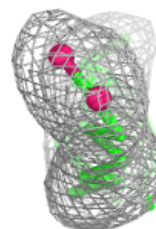
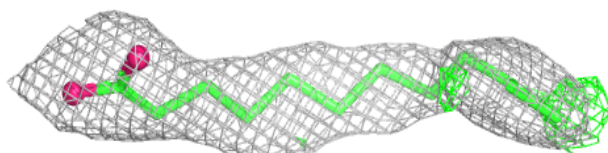
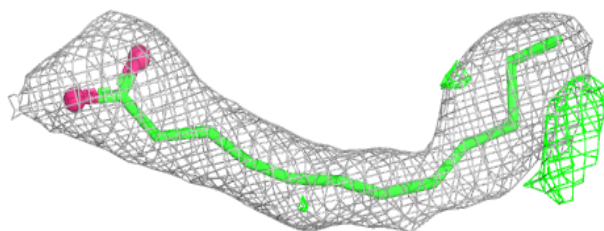


Electron density around STE H 104:

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

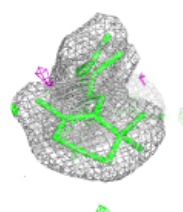
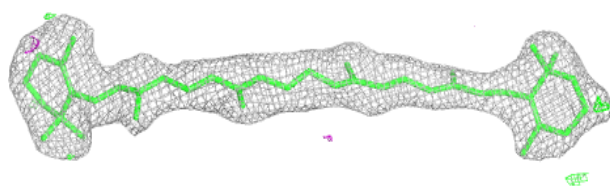
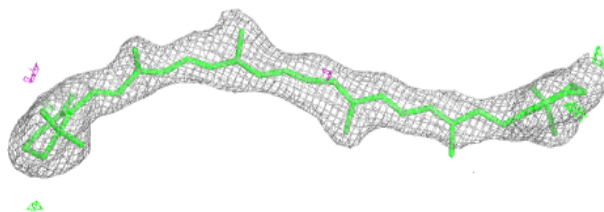
**Electron density around STE t 702:**

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

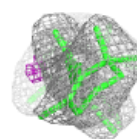
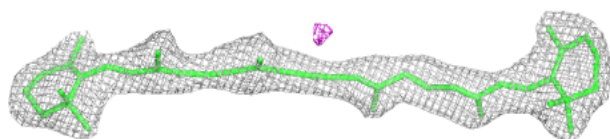
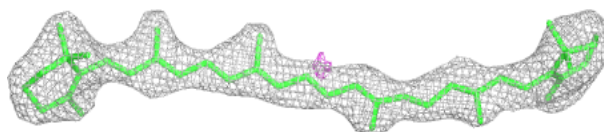


Electron density around BCR h 702:

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

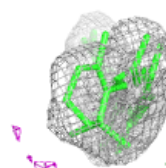
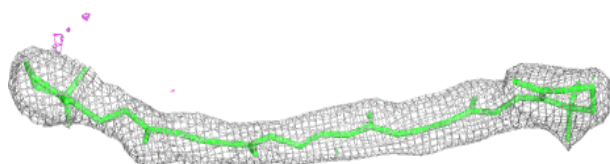
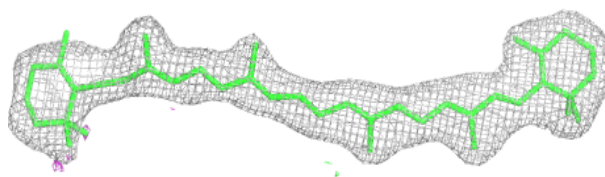
**Electron density around BCR c 515:**

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

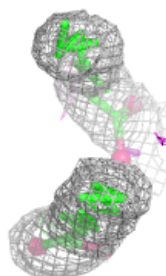
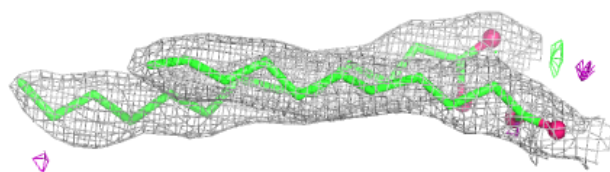
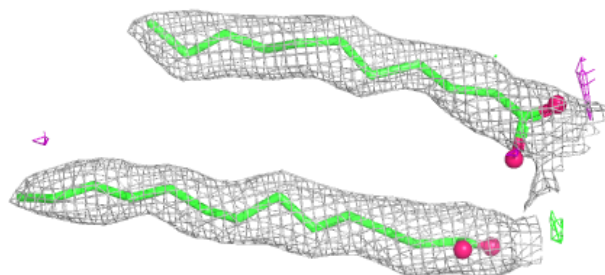


Electron density around BCR d 405:

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

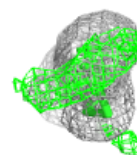
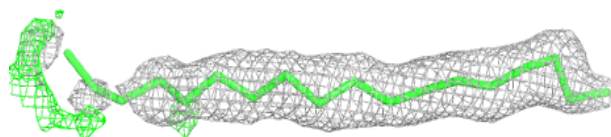
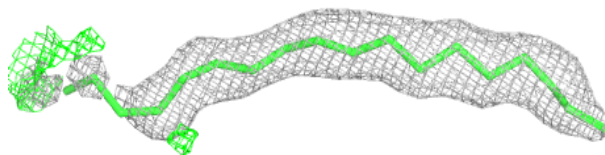
**Electron density around LMG B 721:**

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

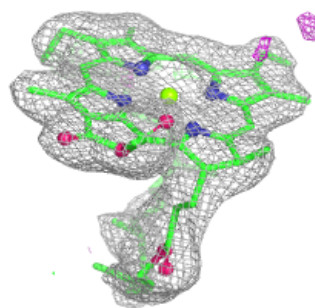
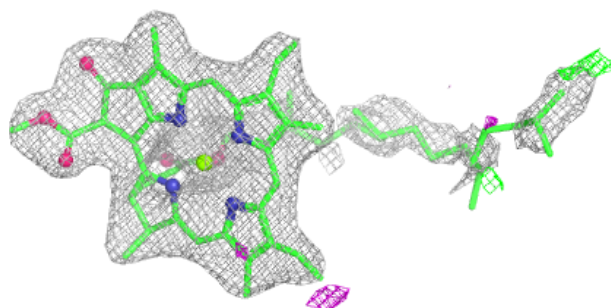
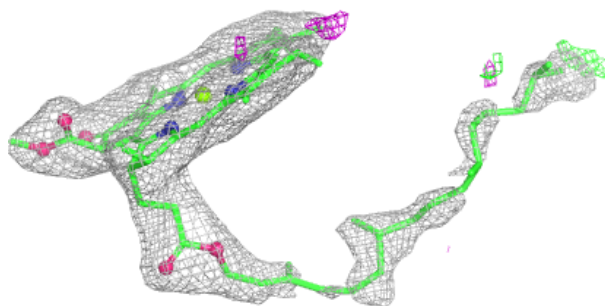


Electron density around STE m 101:

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

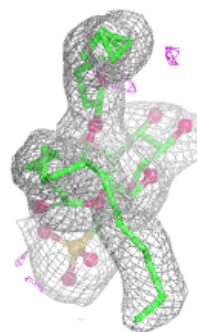
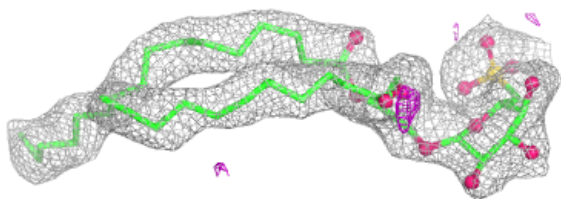
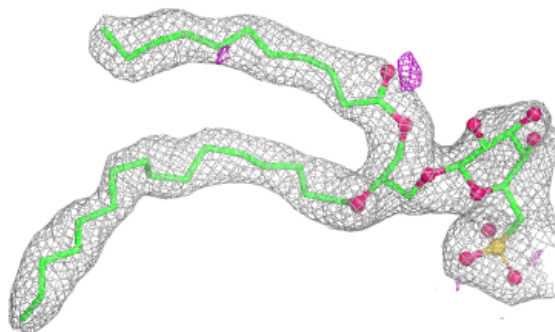
**Electron density around CLA C 514:**

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

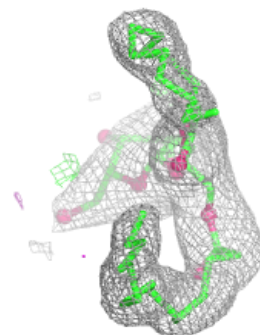
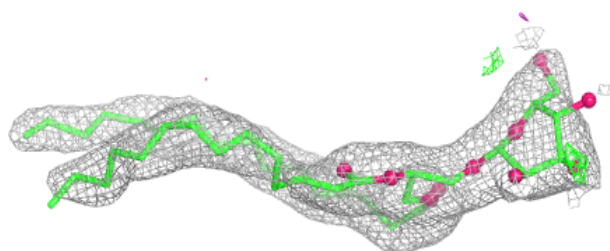
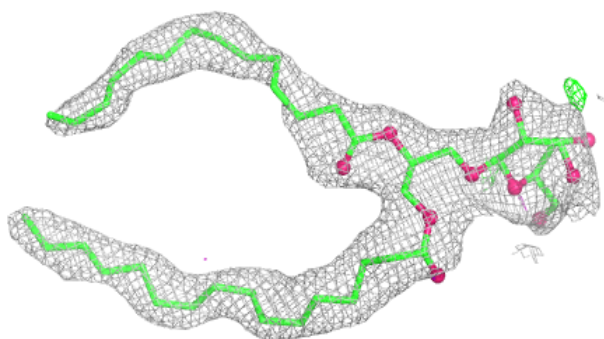


Electron density around SQD 1 101:

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

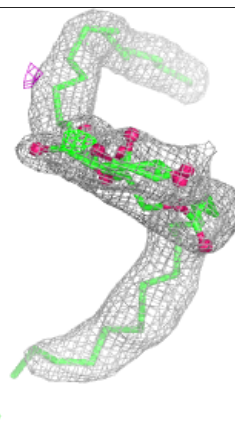
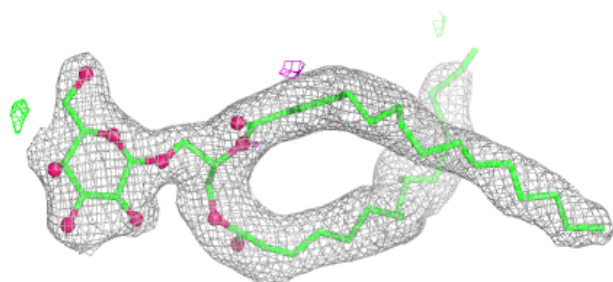
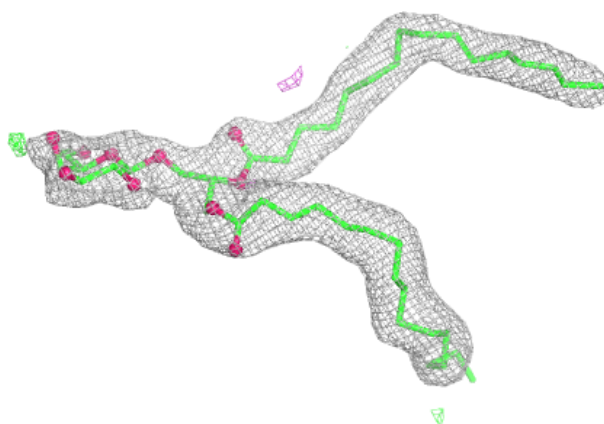
**Electron density around LMG c 523:**

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

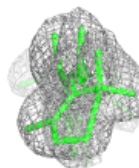
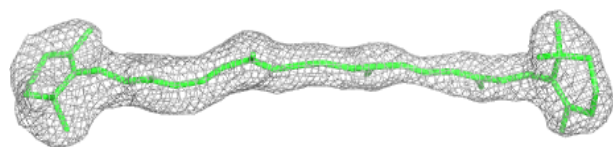
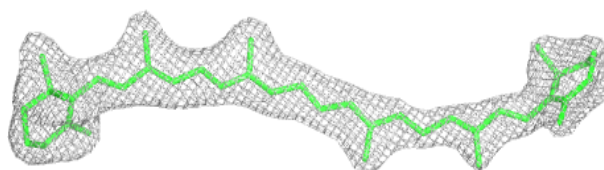


Electron density around LMG M 101:

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

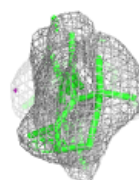
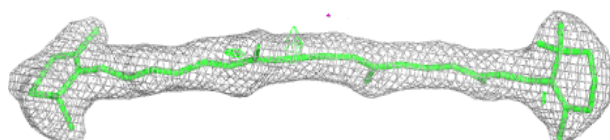
**Electron density around BCR k 101:**

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

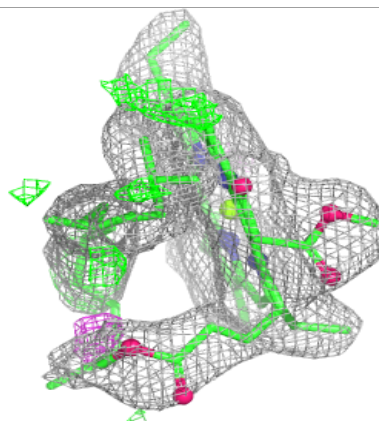
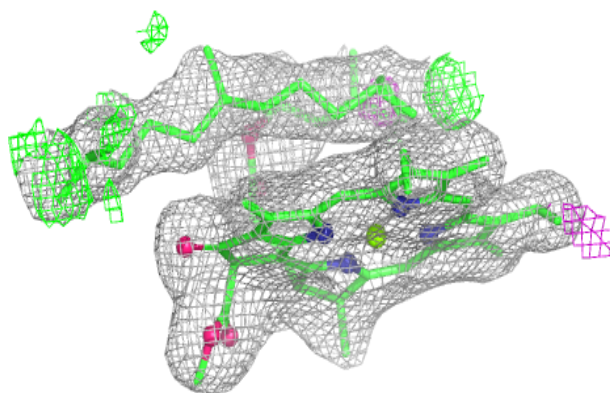
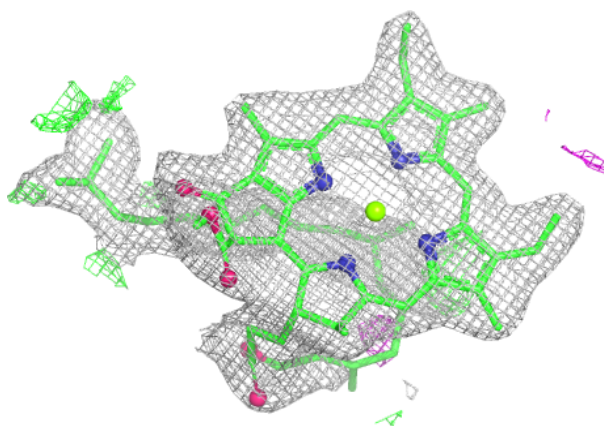


Electron density around BCR Y 101:

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

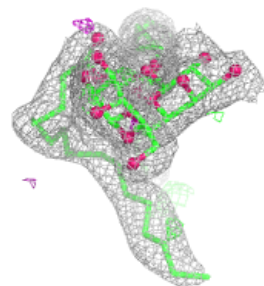
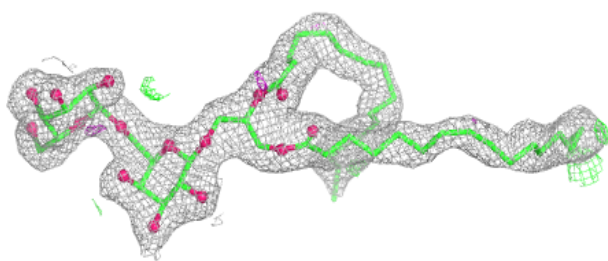
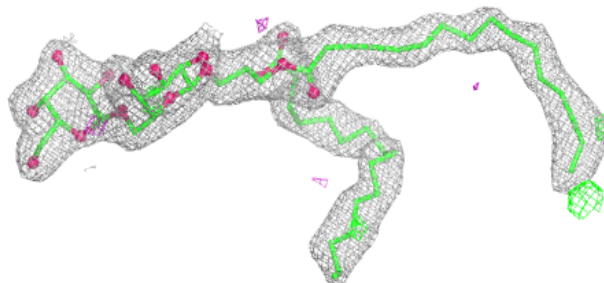
**Electron density around CLA B 727:**

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

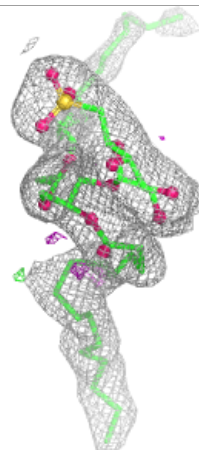
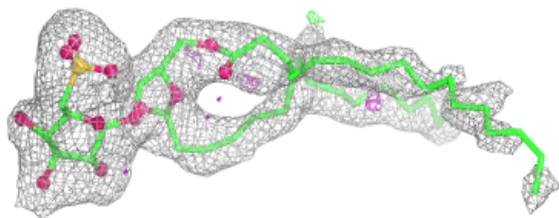
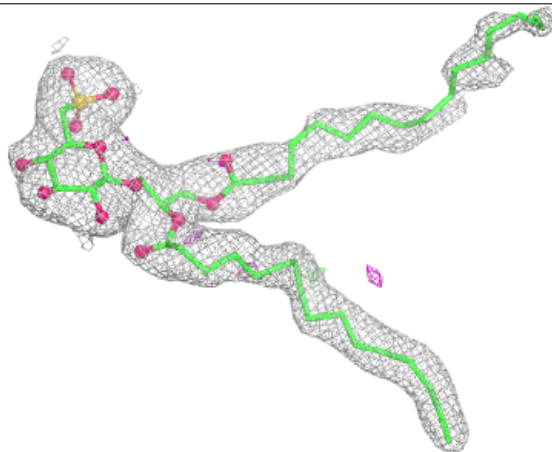


Electron density around DGD H 102:

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

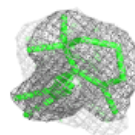
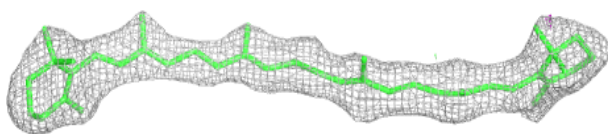
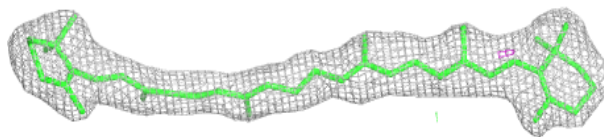
**Electron density around SQD a 412:**

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

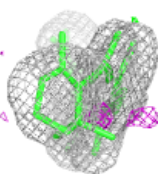
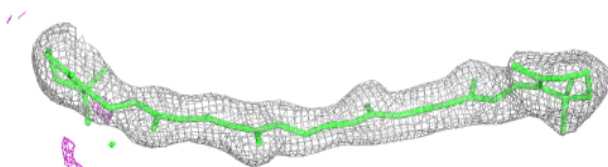
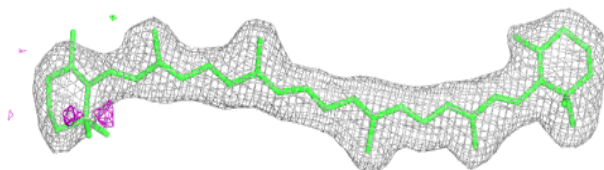


Electron density around BCR C 524:

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

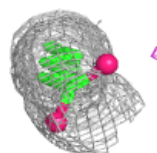
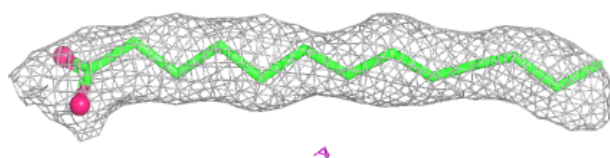
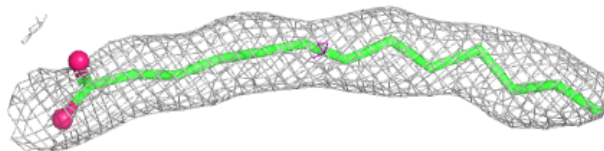
**Electron density around BCR D 405:**

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

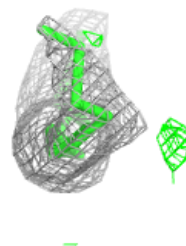
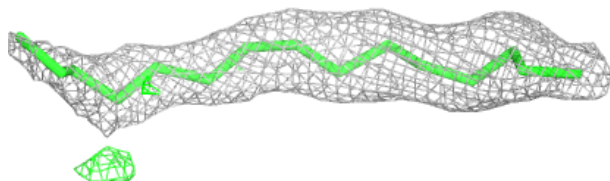
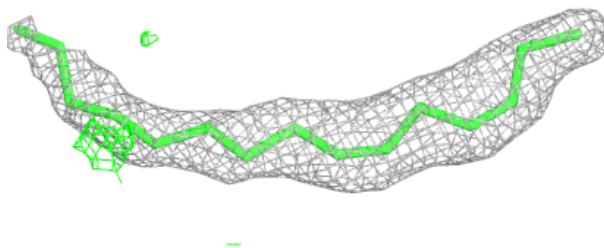


Electron density around STE M 102:

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

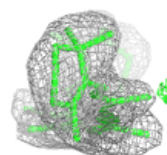
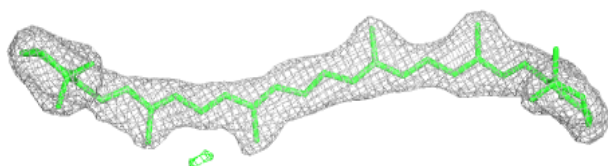
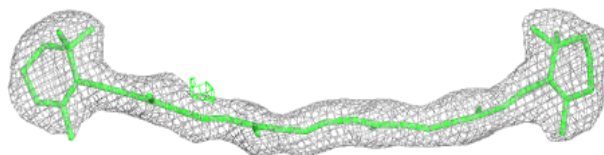
**Electron density around STE T 702:**

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



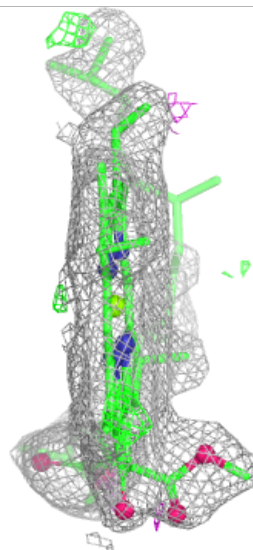
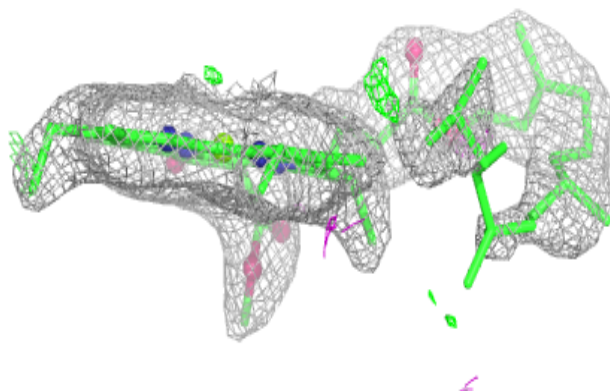
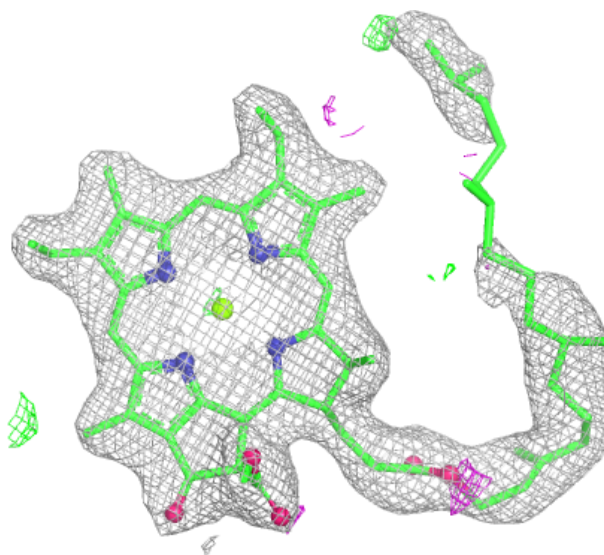
Electron density around BCR k 102:

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



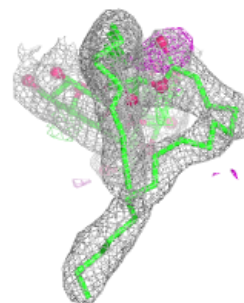
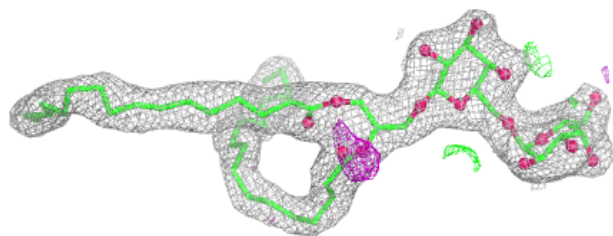
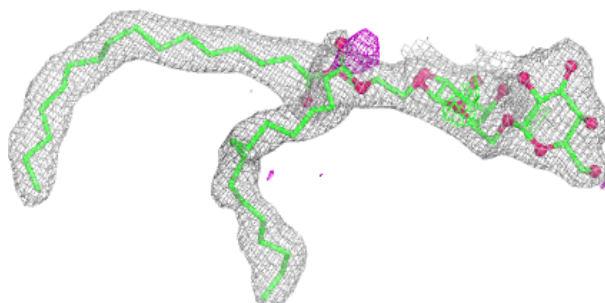
Electron density around CLA c 513:

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

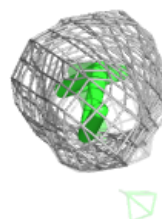
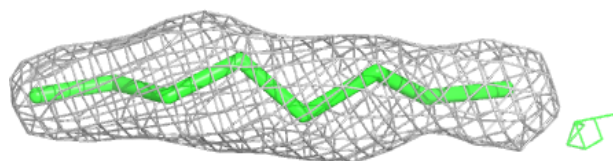
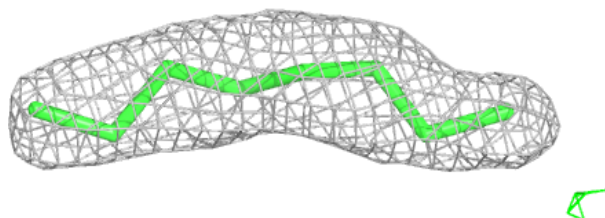


Electron density around DGD h 703:

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

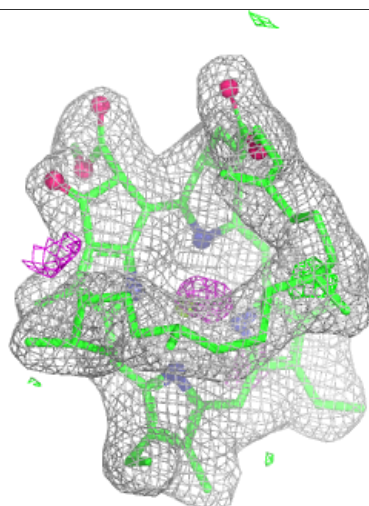
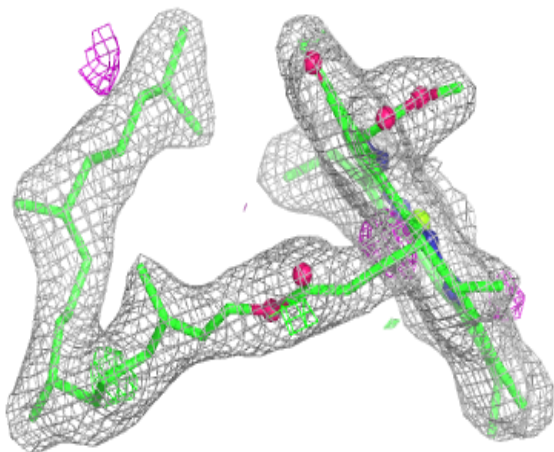
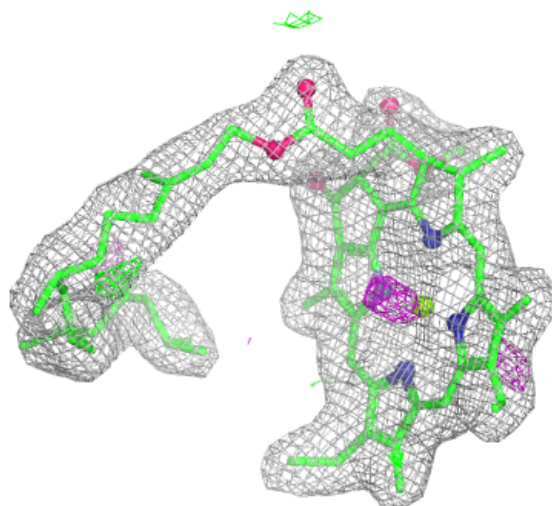
**Electron density around STE Z 101:**

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



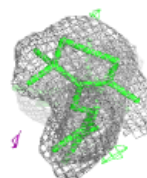
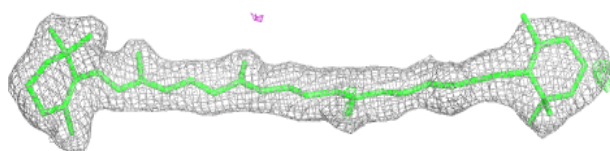
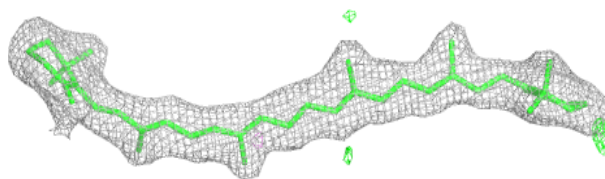
Electron density around CLA C 504:

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

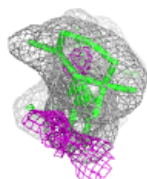
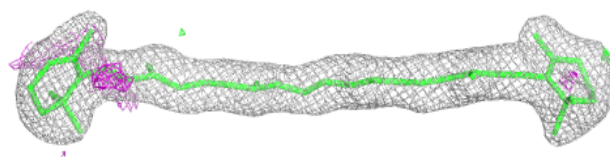
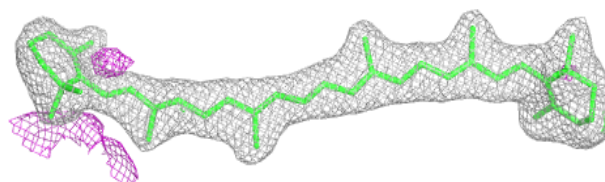


Electron density around BCR H 101:

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

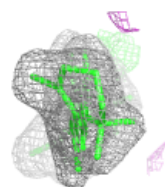
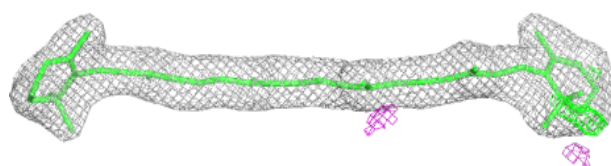
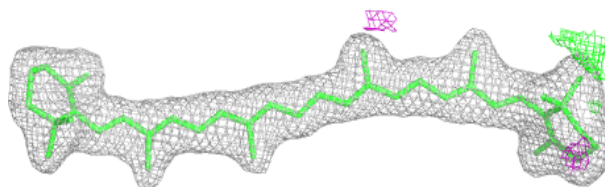
**Electron density around BCR B 718:**

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

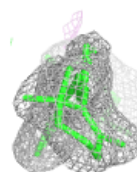
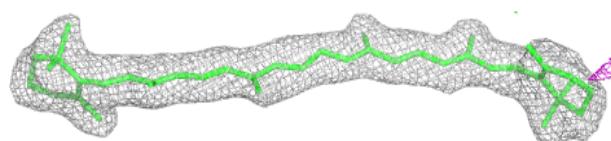
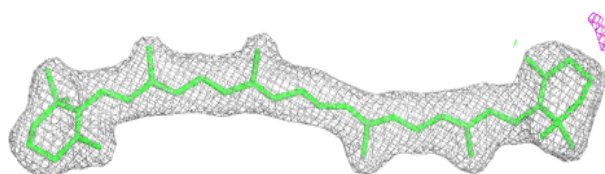


Electron density around BCR b 618:

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

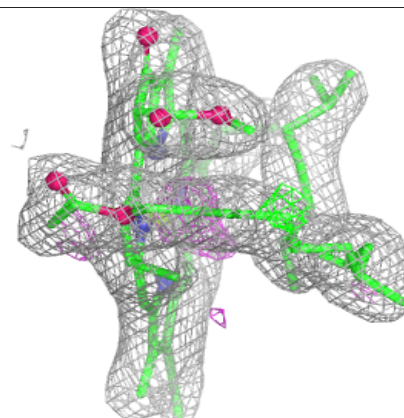
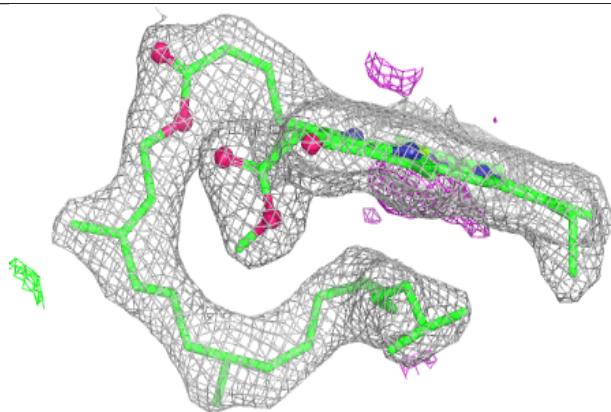
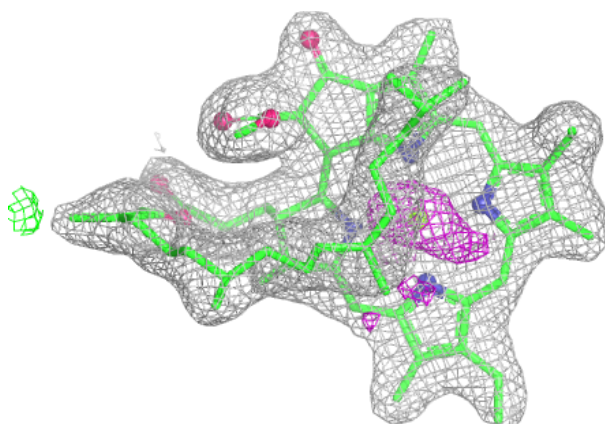
**Electron density around BCR b 619:**

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

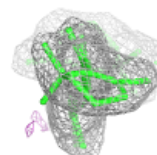
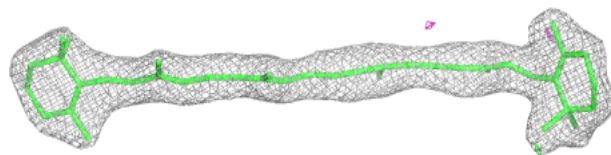
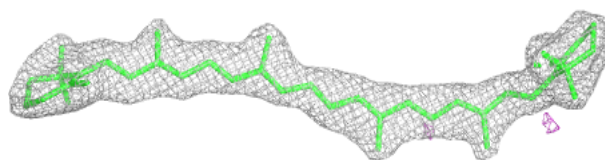


Electron density around CLA C 511:

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

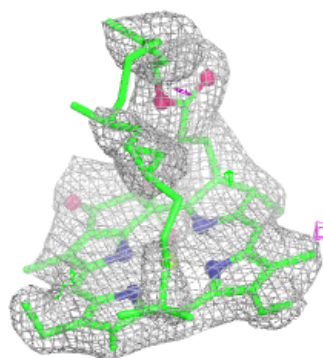
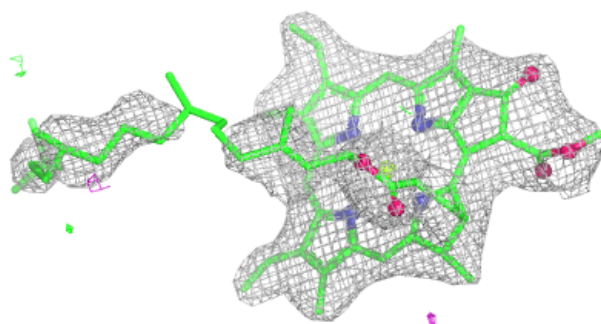
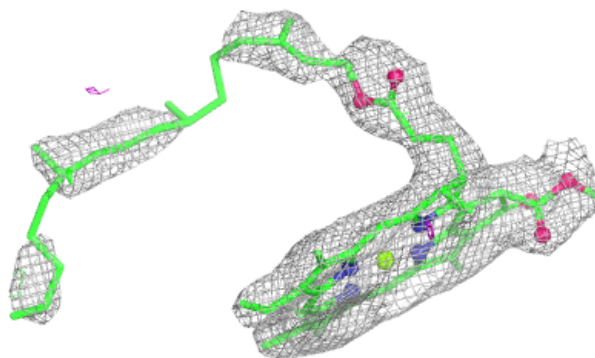
**Electron density around BCR c 516:**

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

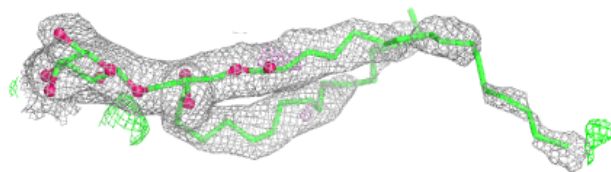


Electron density around CLA c 514:

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

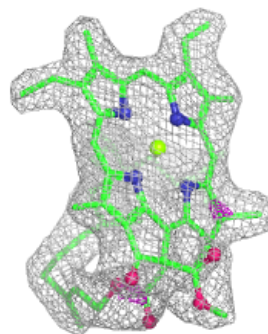
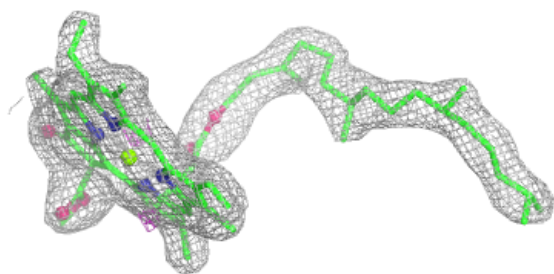
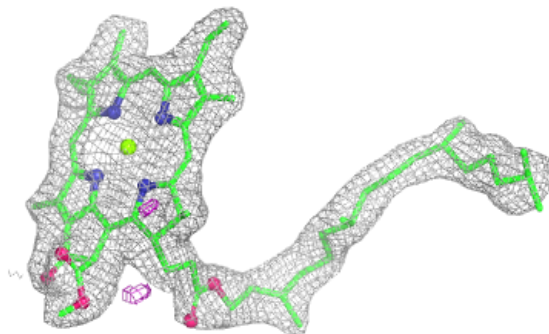
**Electron density around LMG D 409:**

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



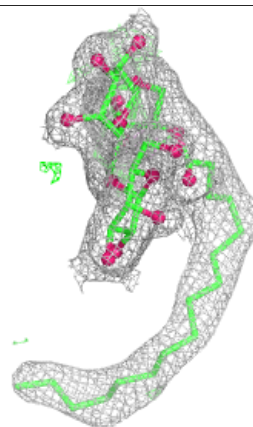
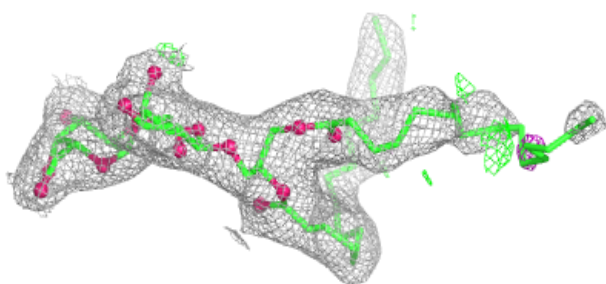
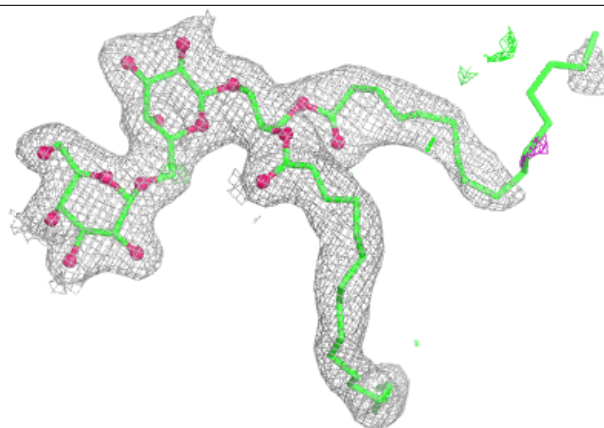
Electron density around CLA C 512:

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



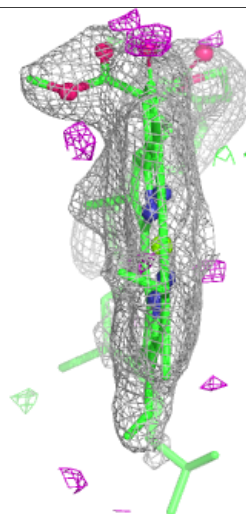
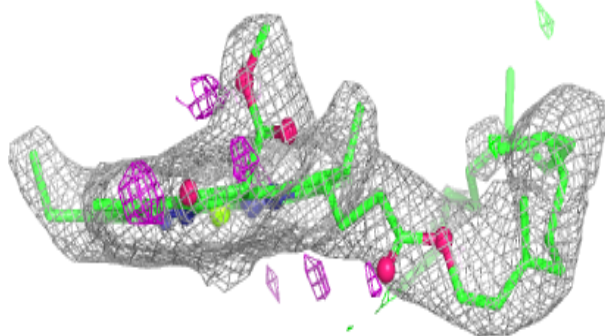
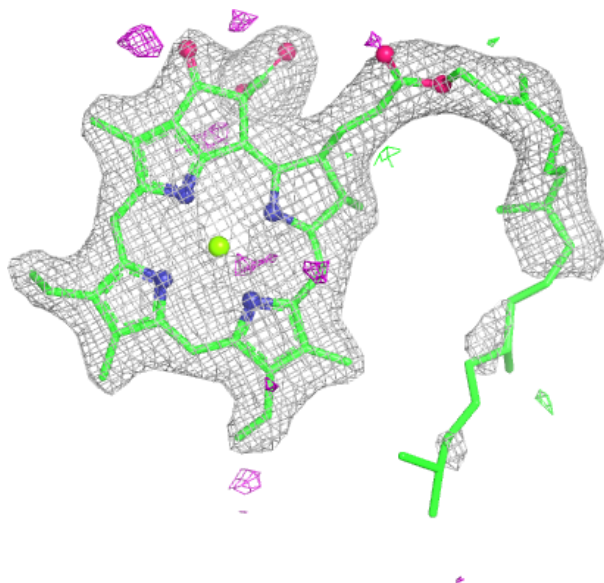
Electron density around DGD C 518:

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



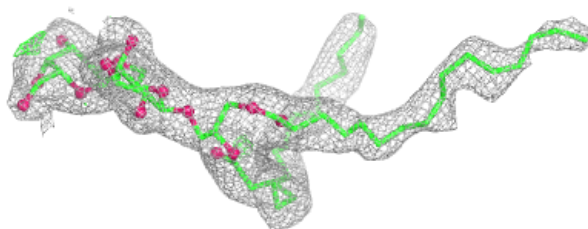
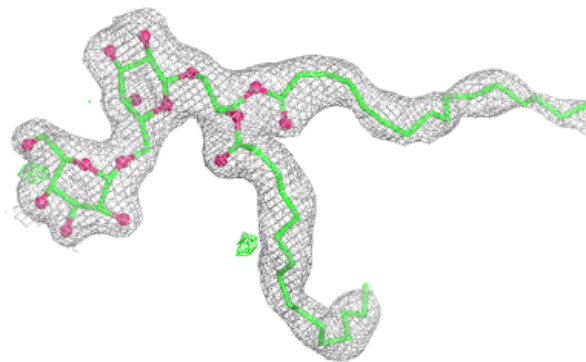
Electron density around CLA C 513:

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



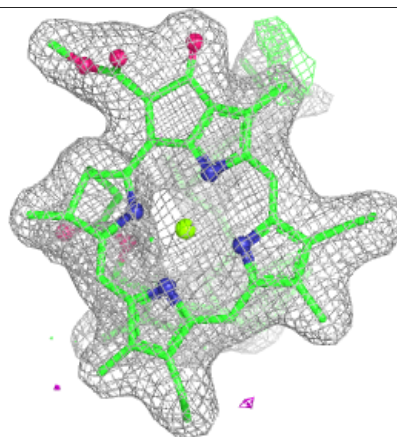
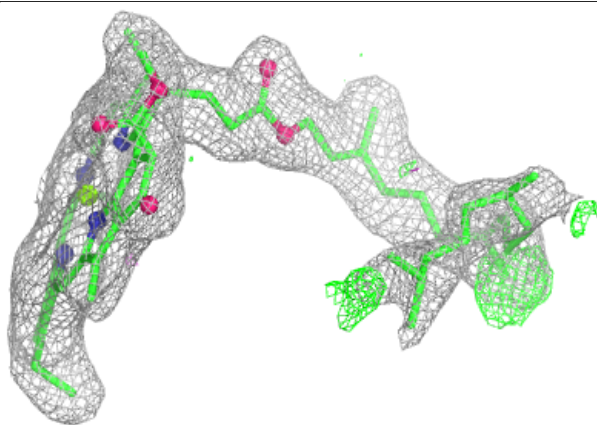
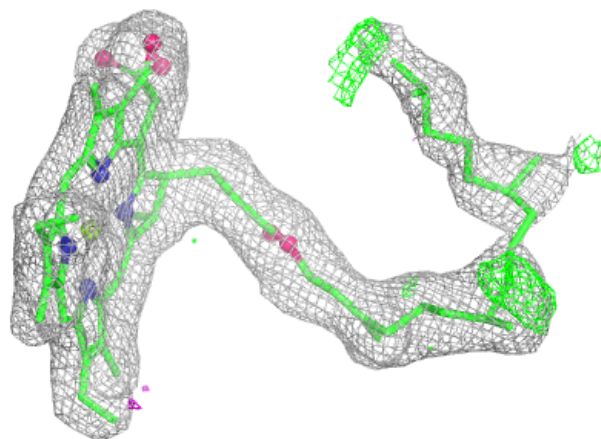
Electron density around DGD c 518:

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



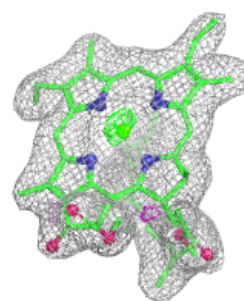
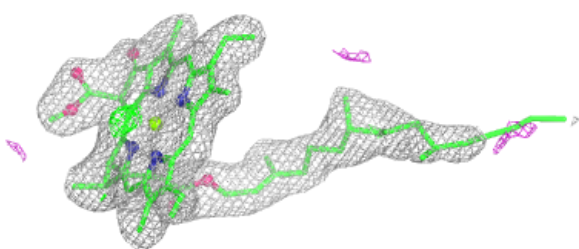
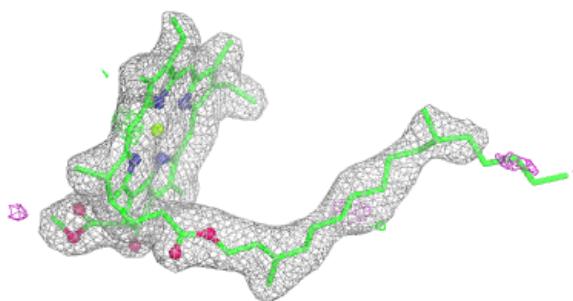
Electron density around CLA B 706:

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



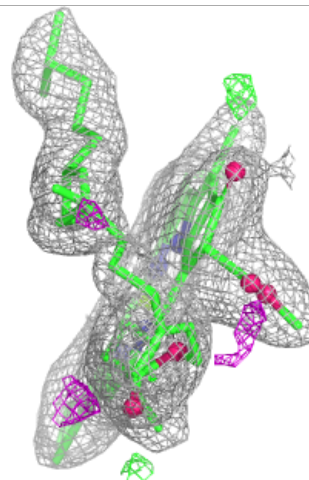
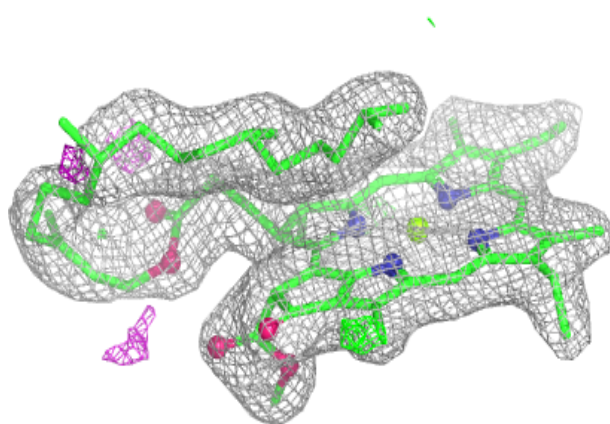
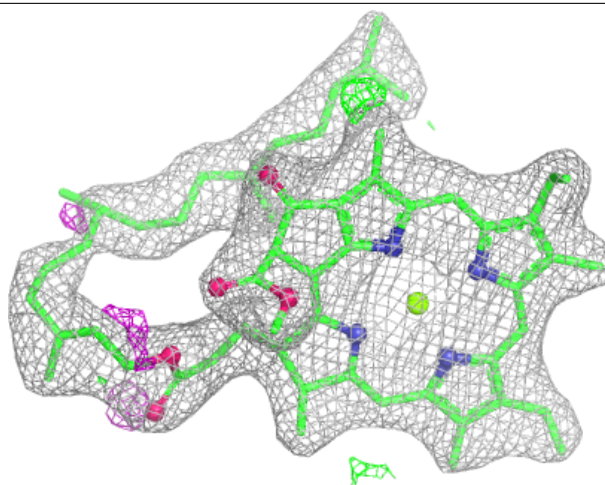
Electron density around CLA c 509:

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



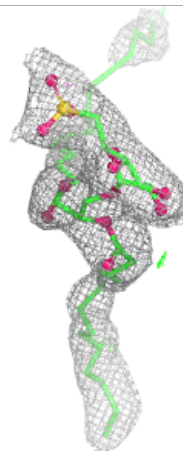
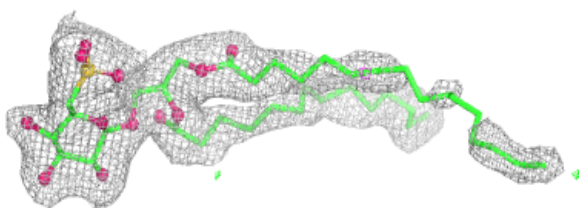
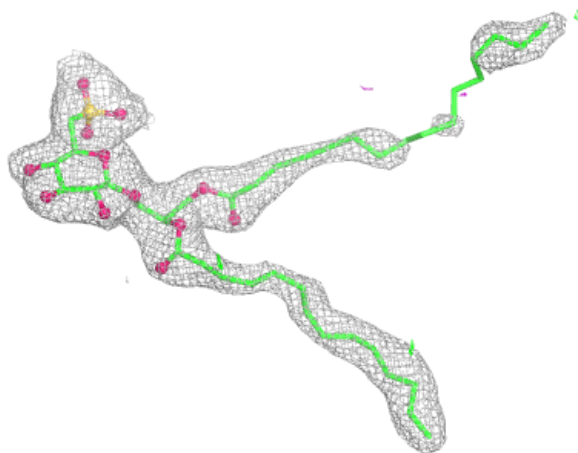
Electron density around CLA c 510:

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



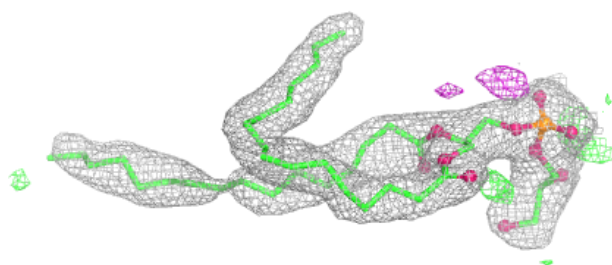
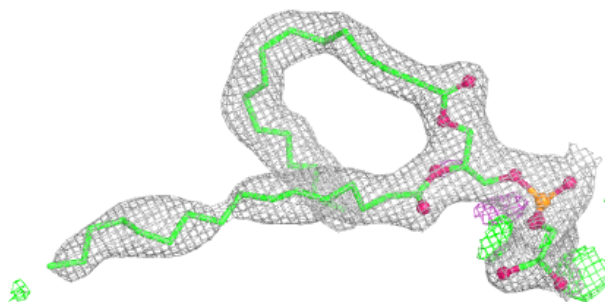
Electron density around SQD A 409:

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

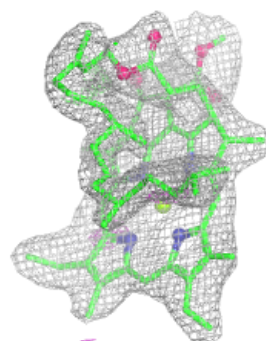
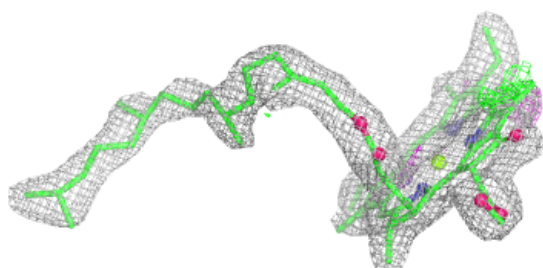
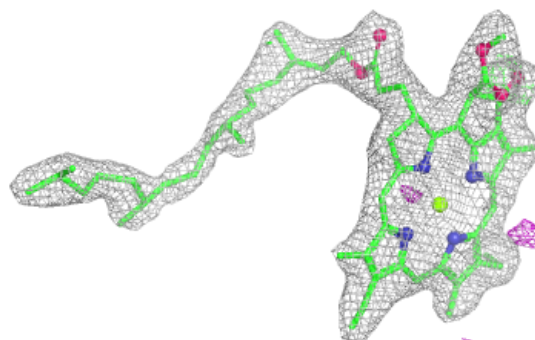


Electron density around LHG B 722:

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

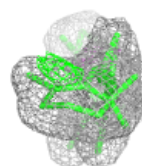
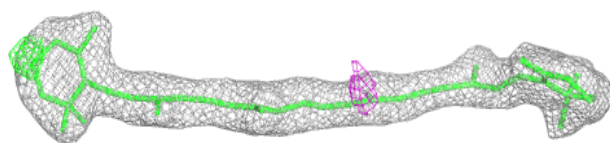
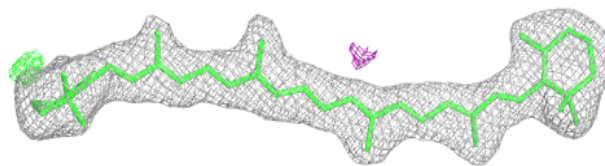
**Electron density around CLA c 512:**

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



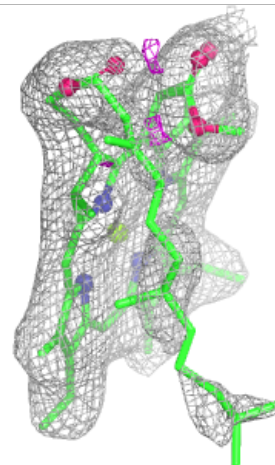
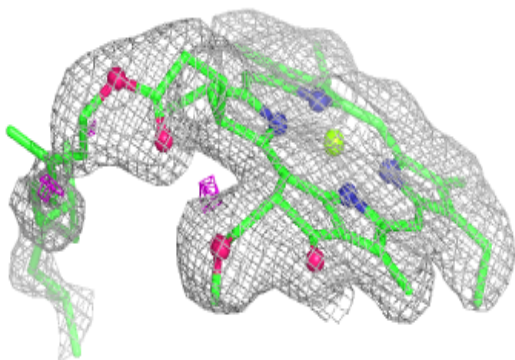
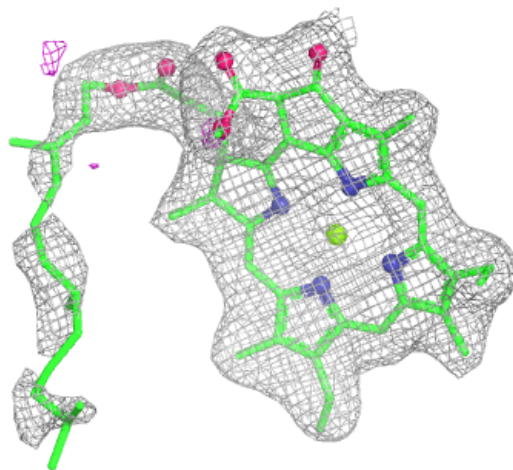
Electron density around BCR b 617:

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



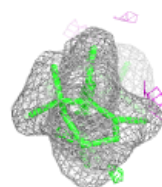
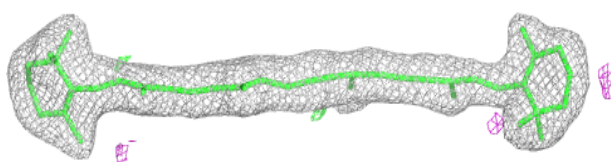
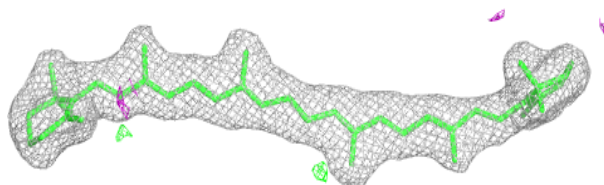
Electron density around CLA b 616:

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

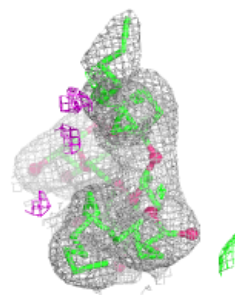
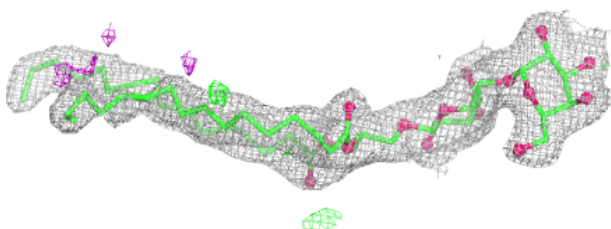
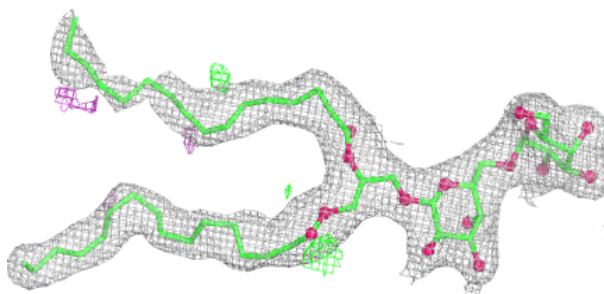


Electron density around BCR A 405:

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

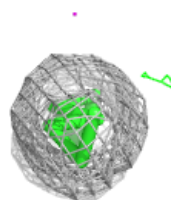
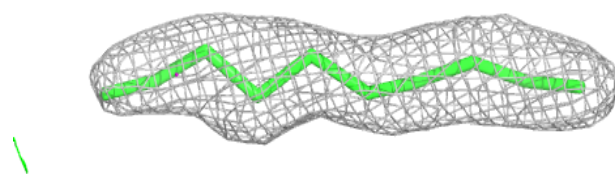
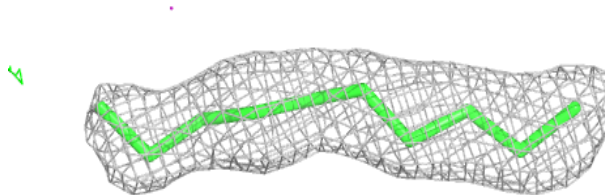
**Electron density around DGD C 519:**

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

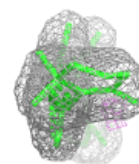
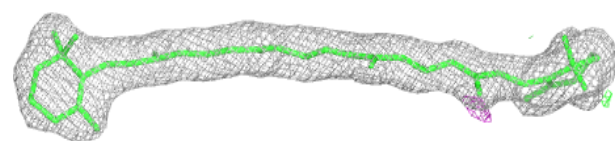
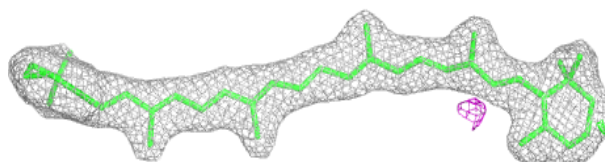


Electron density around STE M 103:

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

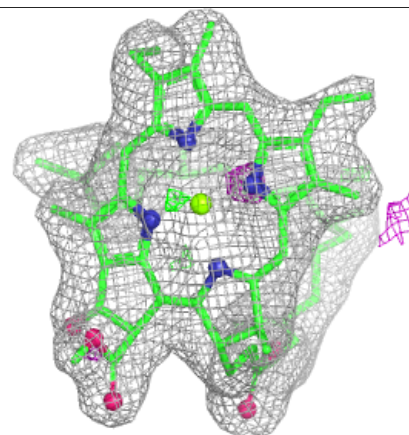
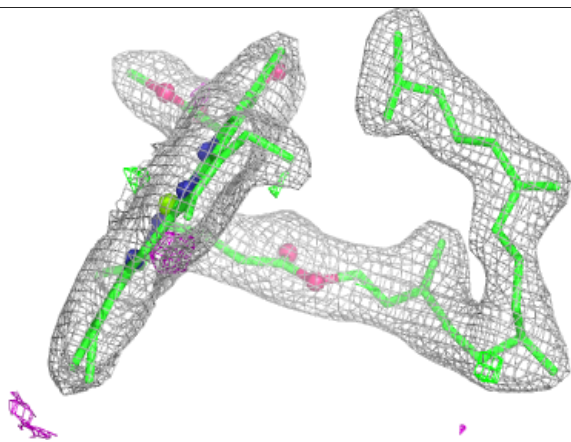
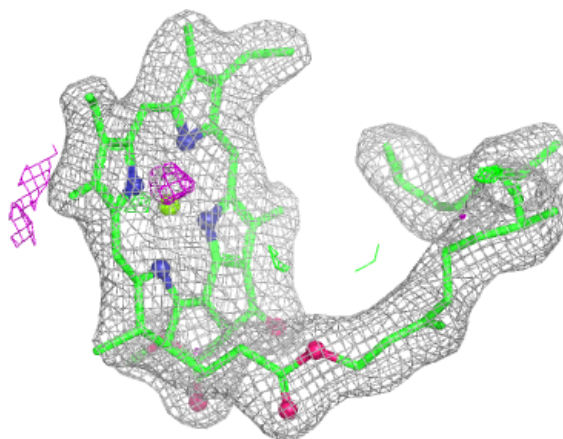
**Electron density around BCR B 717:**

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

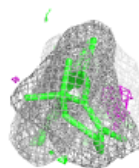
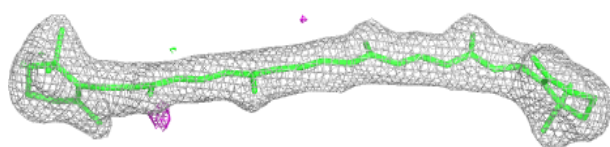
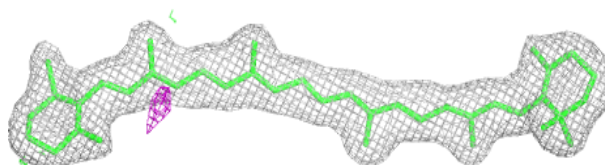


Electron density around CLA c 504:

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

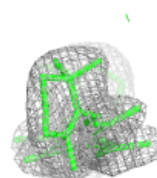
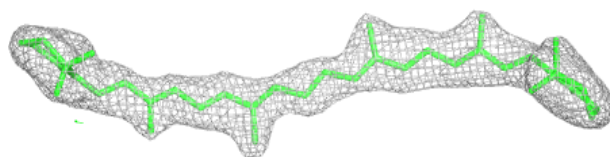
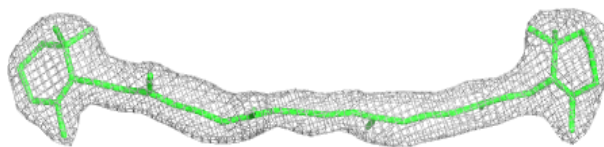
**Electron density around BCR B 719:**

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

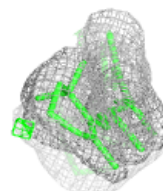
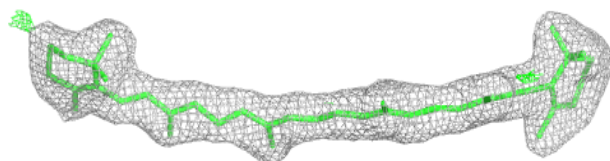
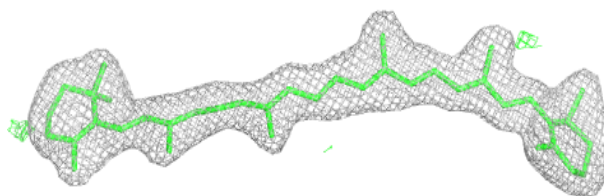


Electron density around BCR C 501:

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

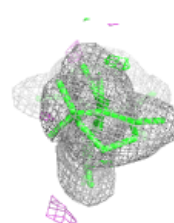
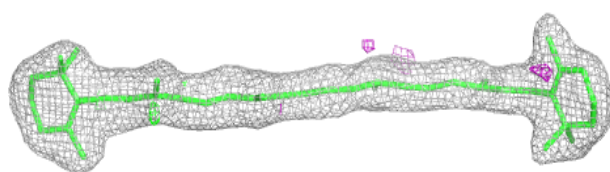
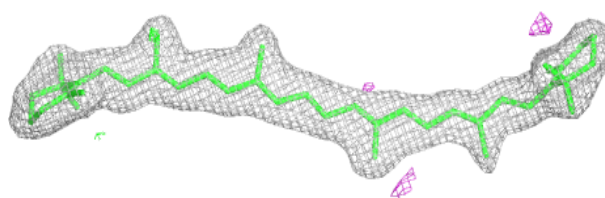
**Electron density around BCR t 701:**

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

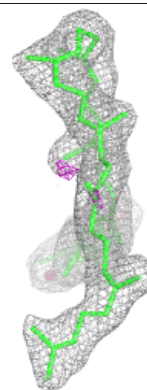
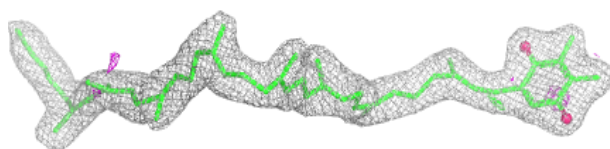
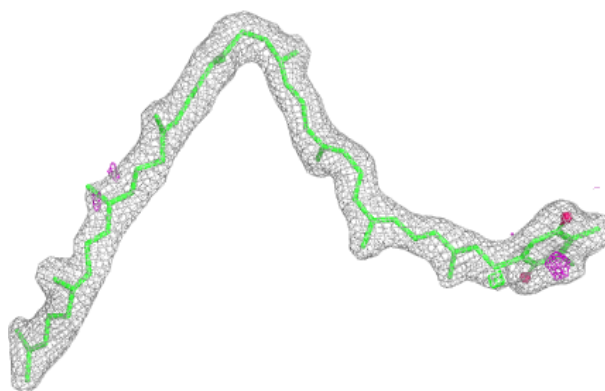


Electron density around BCR C 515:

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

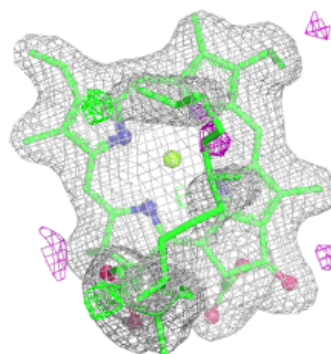
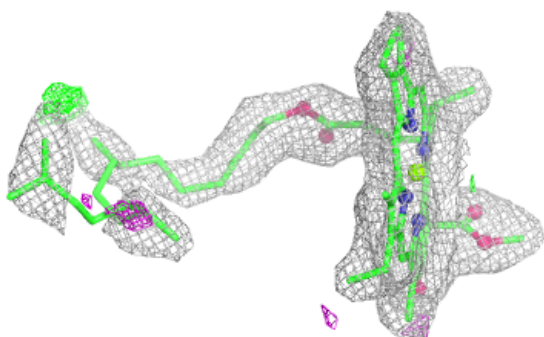
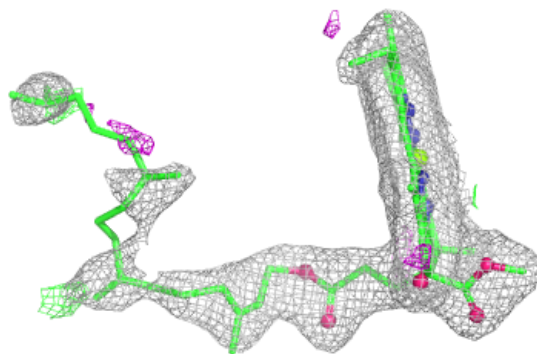
**Electron density around PL9 D 406:**

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



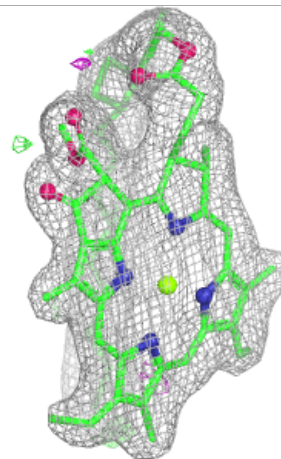
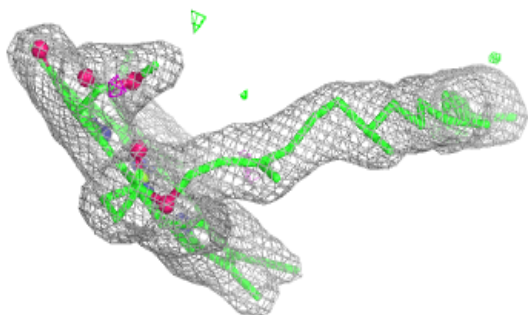
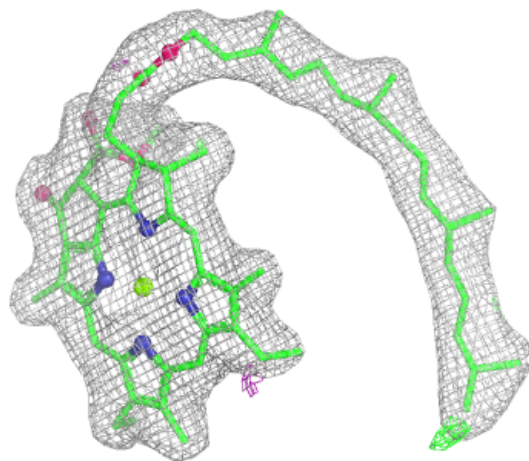
Electron density around CLA c 507:

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



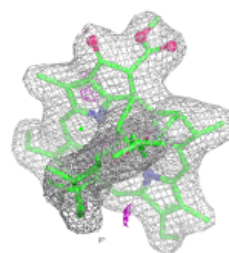
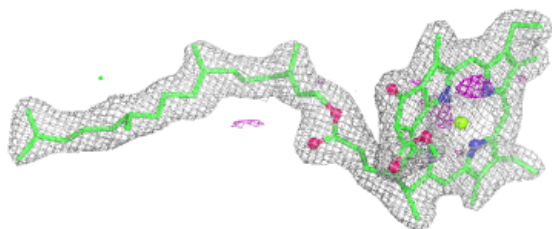
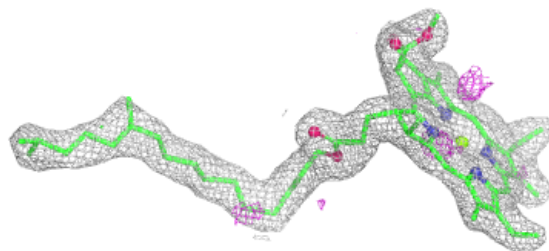
Electron density around CLA c 508:

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

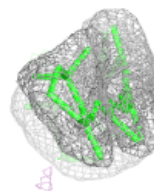
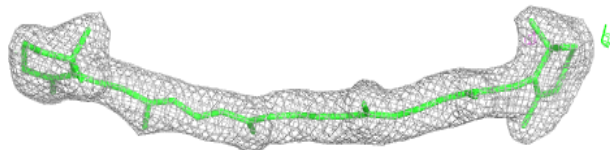
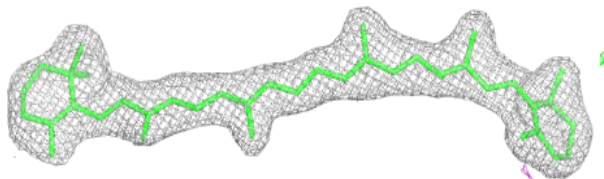


Electron density around CLA C 503:

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

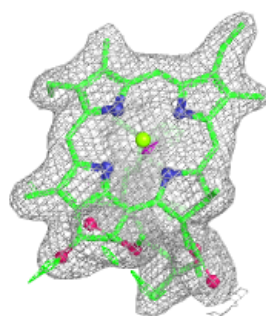
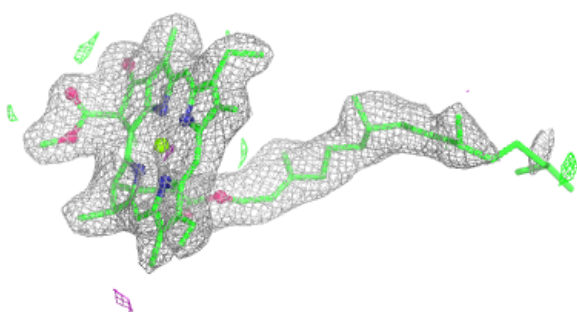
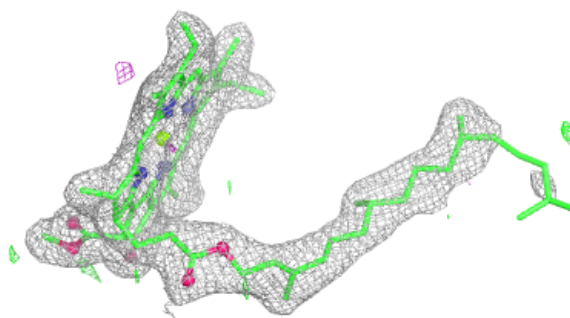
**Electron density around BCR T 701:**

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

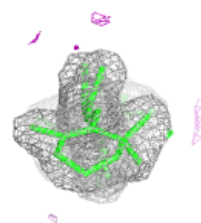
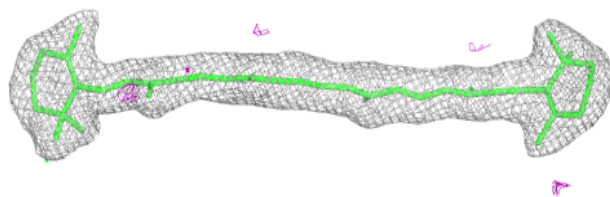
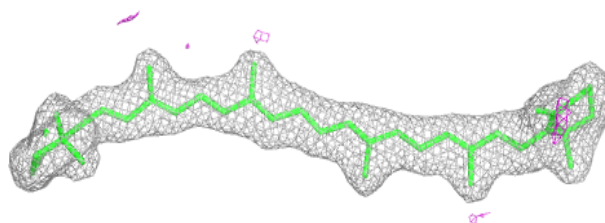


Electron density around CLA C 509:

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

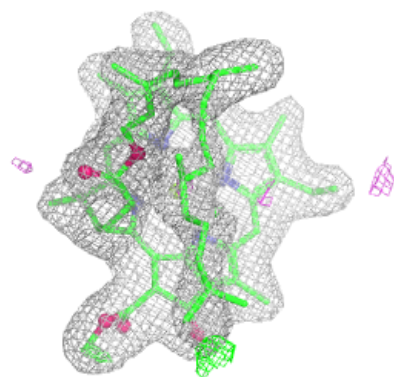
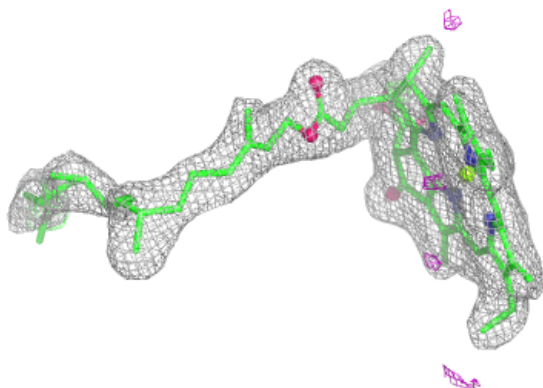
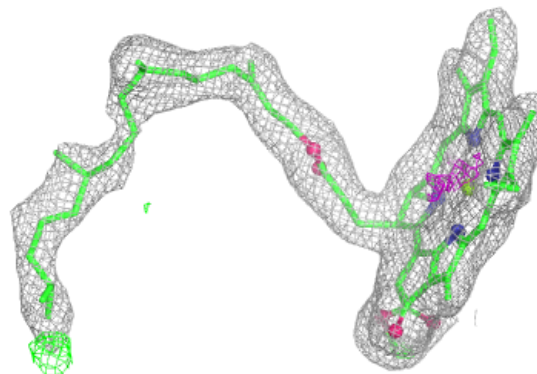
**Electron density around BCR a 406:**

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

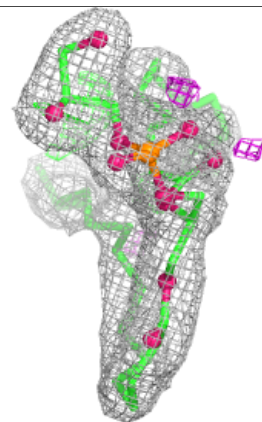
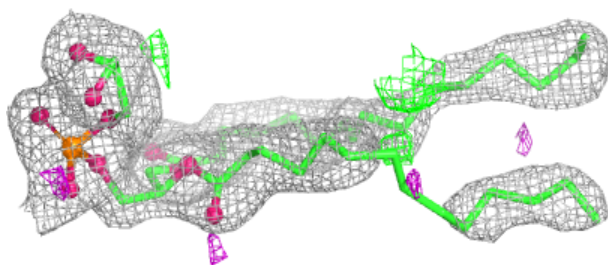
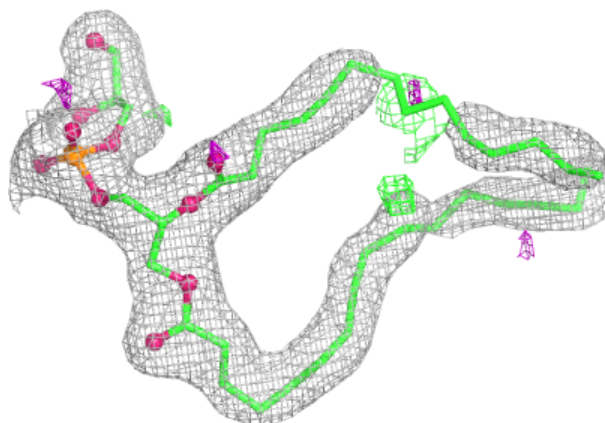


Electron density around CLA b 606:

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

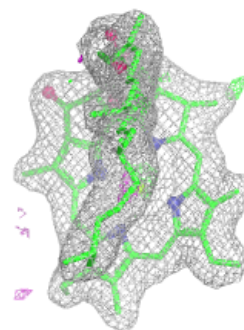
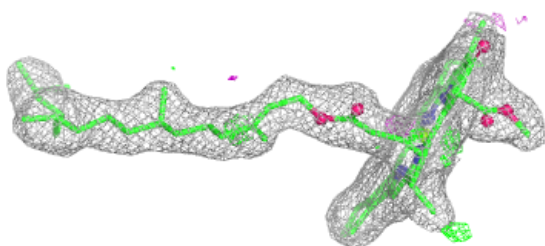
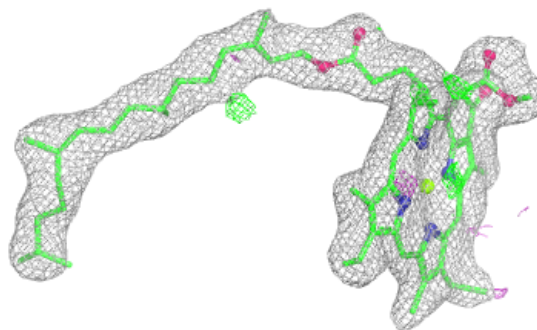
**Electron density around LHG D 412:**

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

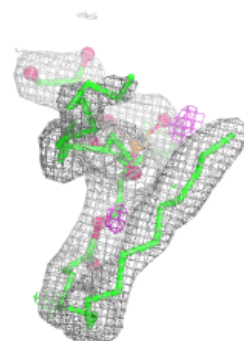
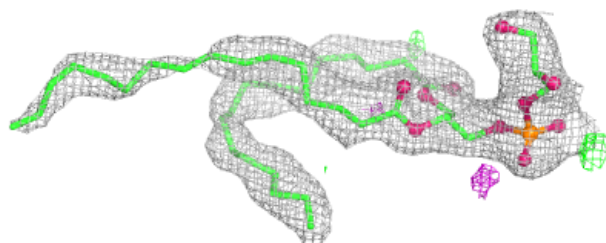
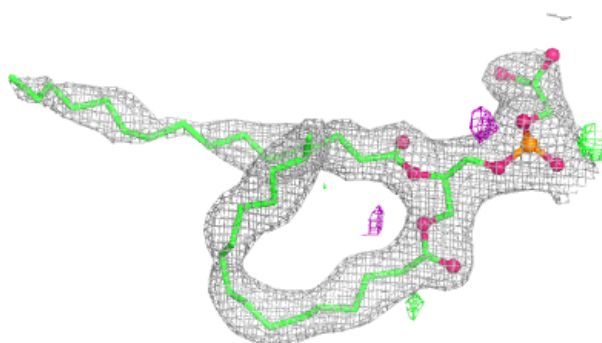


Electron density around CLA b 609:

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

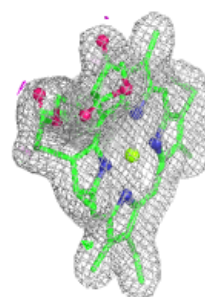
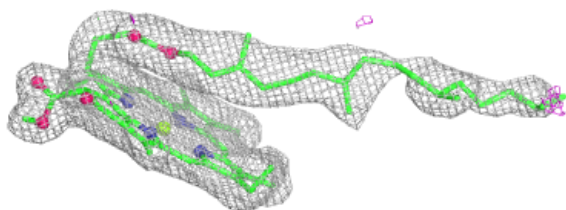
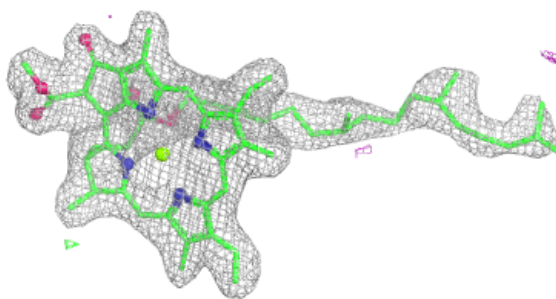
**Electron density around LHG a 411:**

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



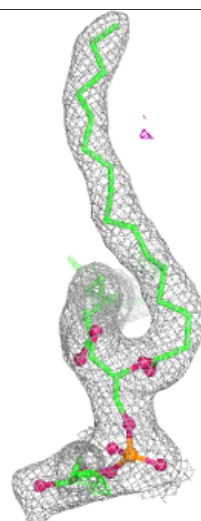
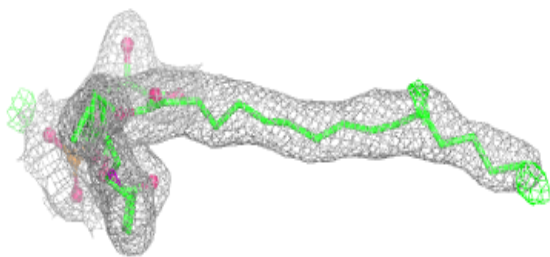
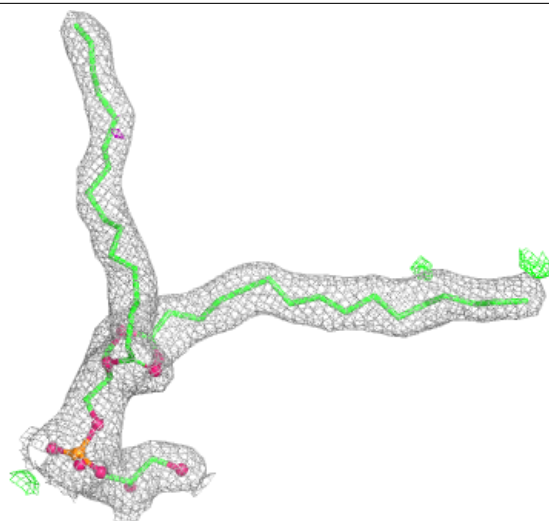
Electron density around CLA b 614:

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



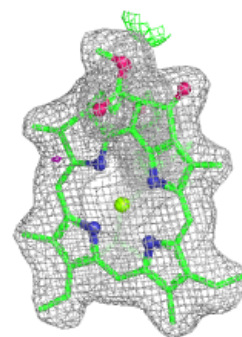
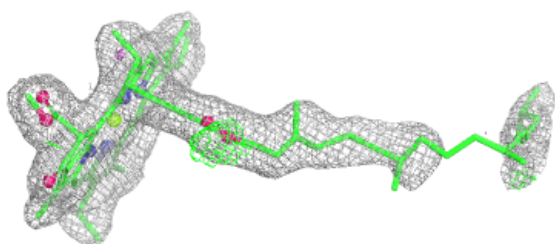
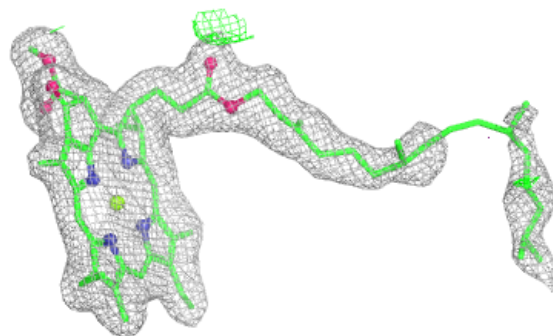
Electron density around LHG 1 102:

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



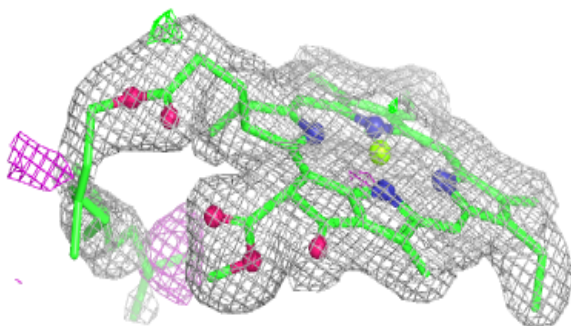
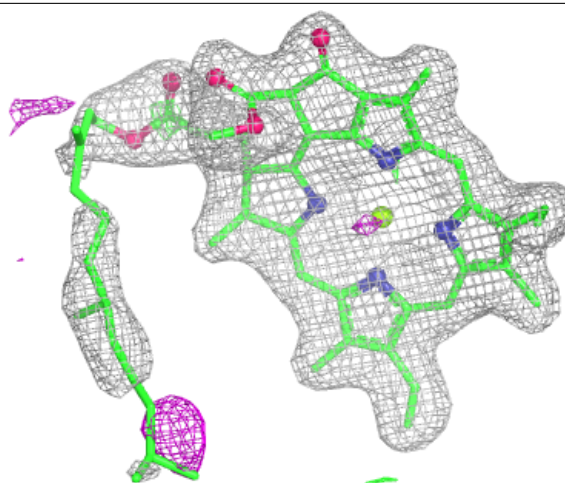
Electron density around CLA d 404:

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



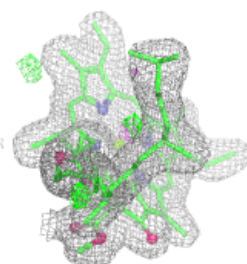
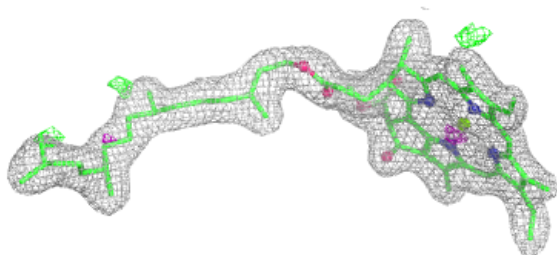
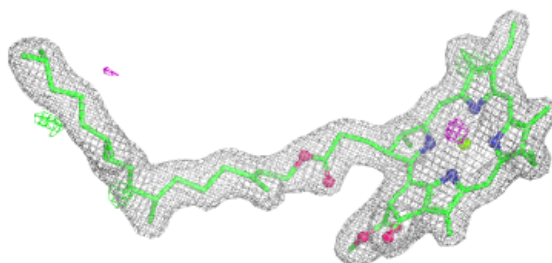
Electron density around CLA B 716:

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

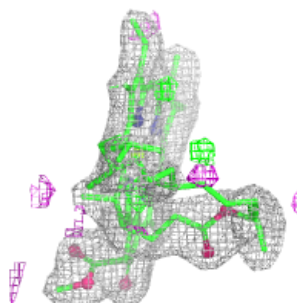
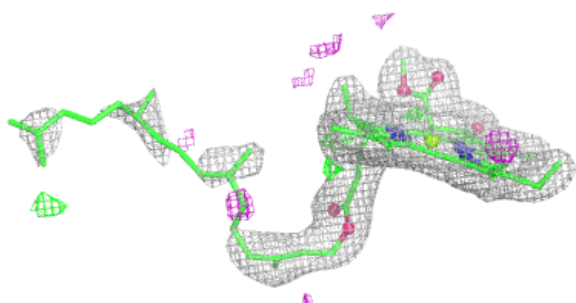
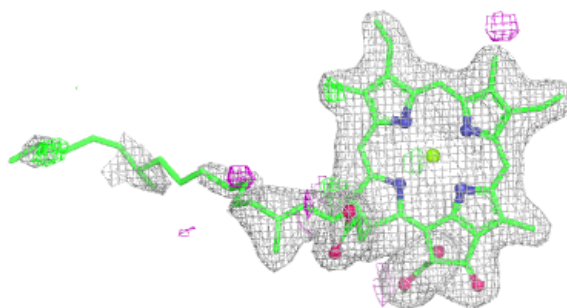


Electron density around CLA a 402:

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

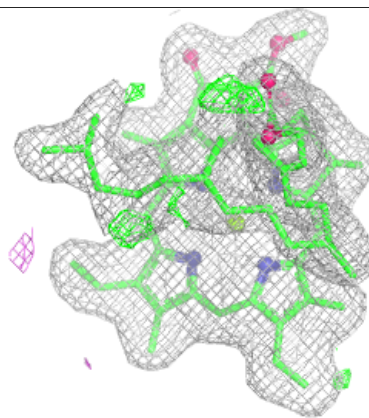
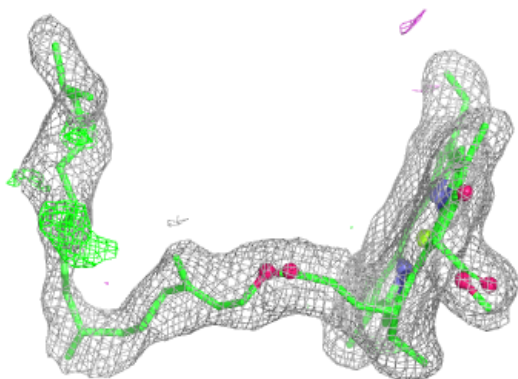
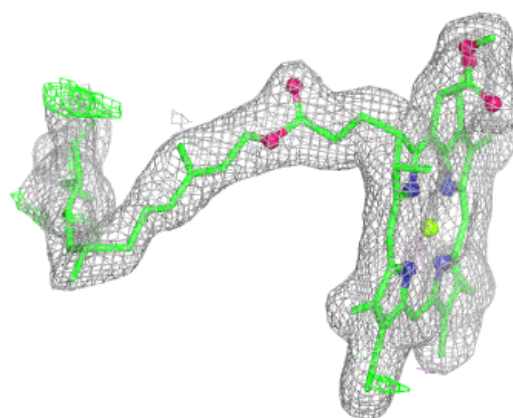
**Electron density around CLA a 403:**

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

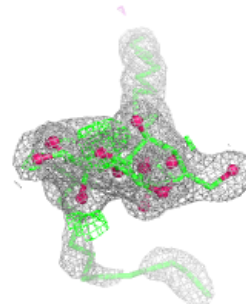
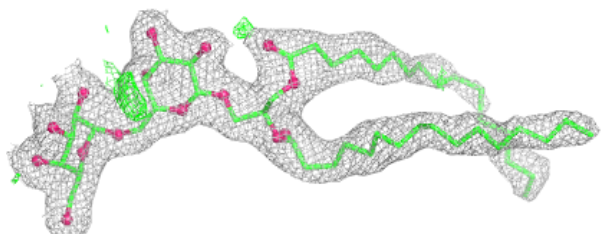
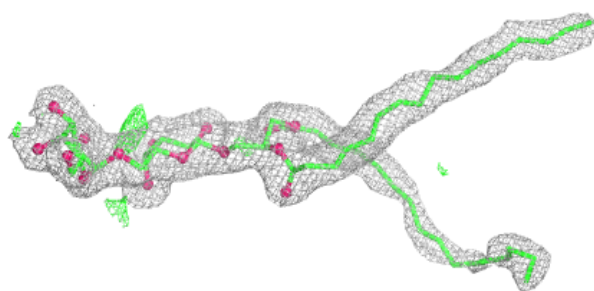


Electron density around CLA a 405:

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

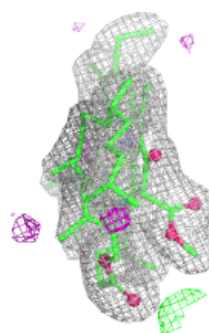
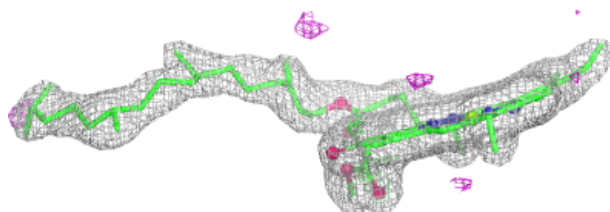
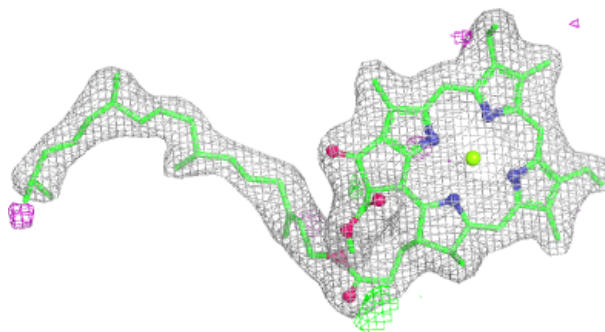
**Electron density around DGD C 517:**

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

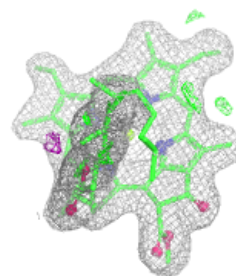
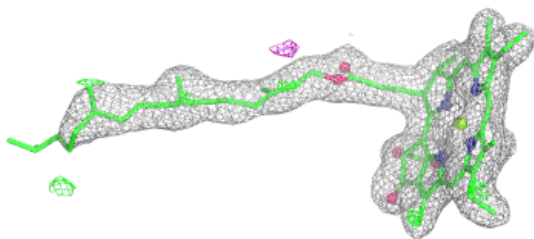
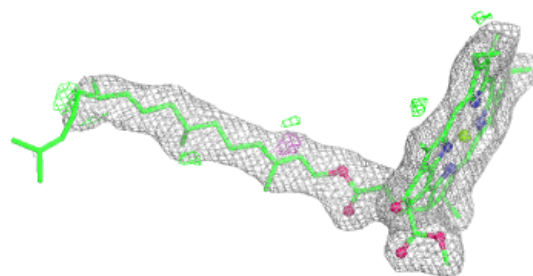


Electron density around CLA b 602:

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

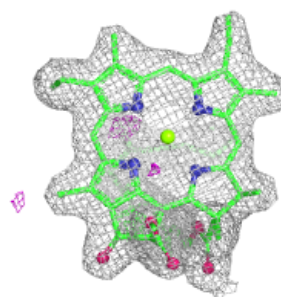
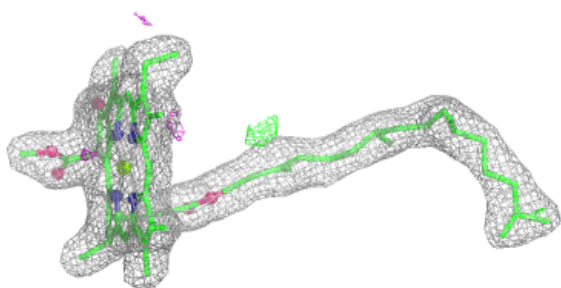
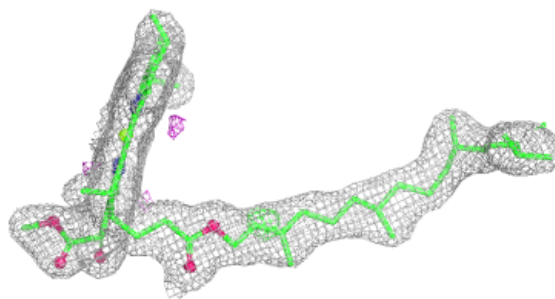
**Electron density around CLA b 604:**

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

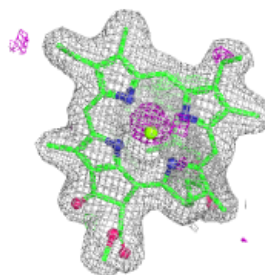
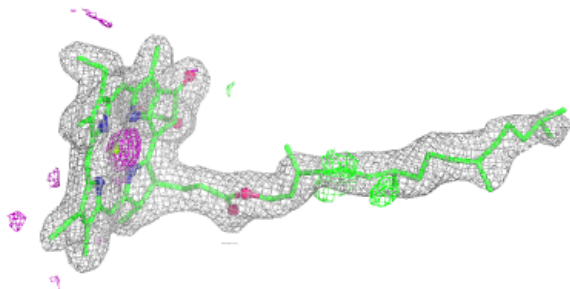
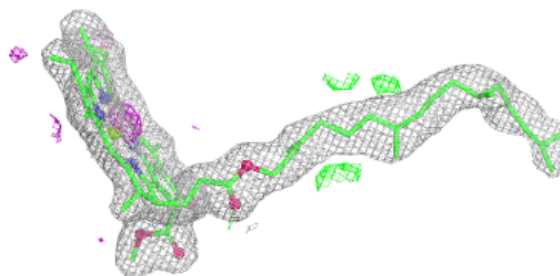


Electron density around CLA b 605:

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

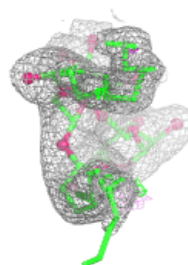
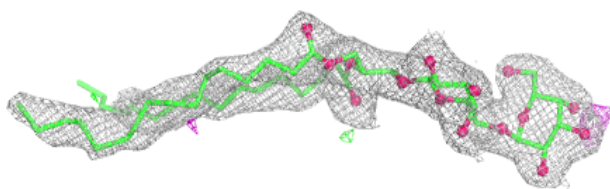
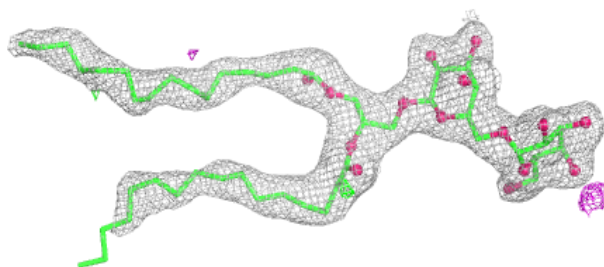
**Electron density around CLA B 704:**

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

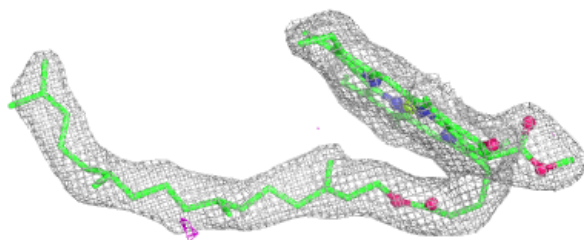
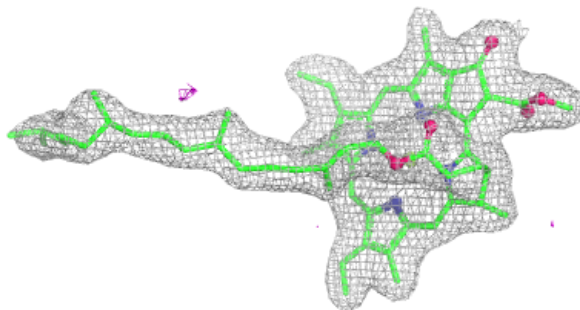


Electron density around DGD c 519:

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

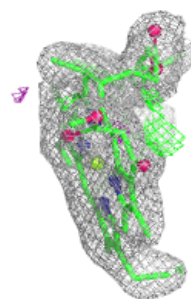
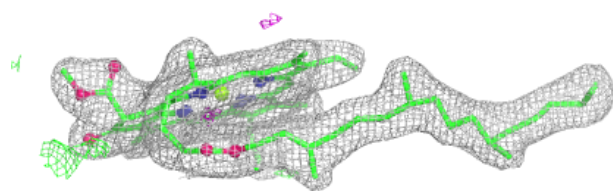
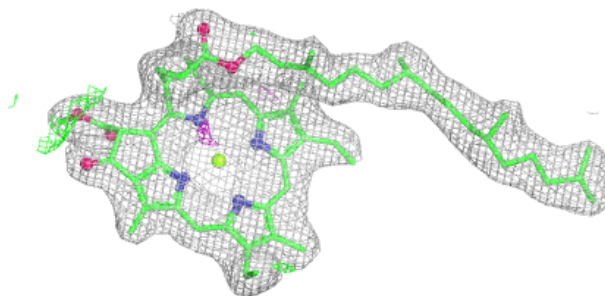
**Electron density around CLA b 608:**

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



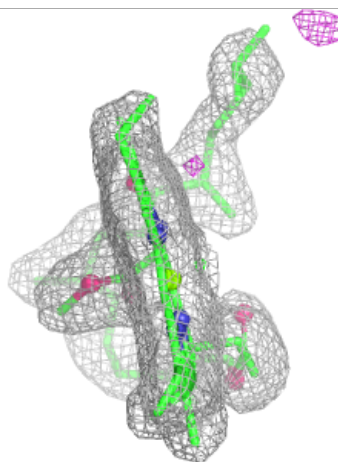
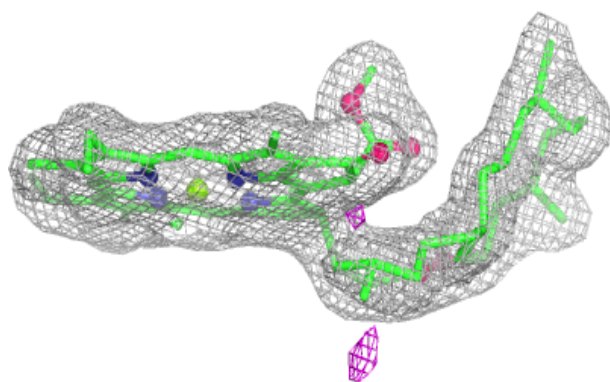
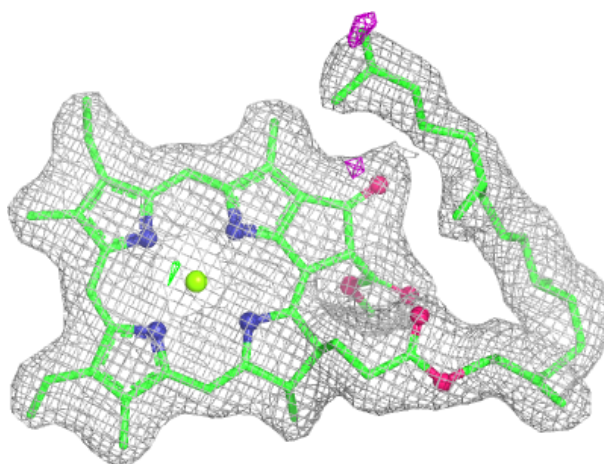
Electron density around CLA C 502:

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



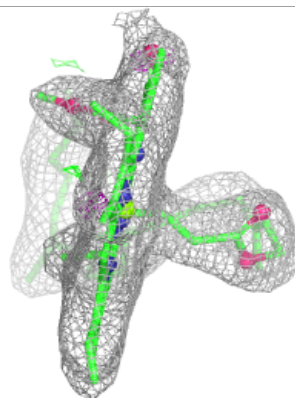
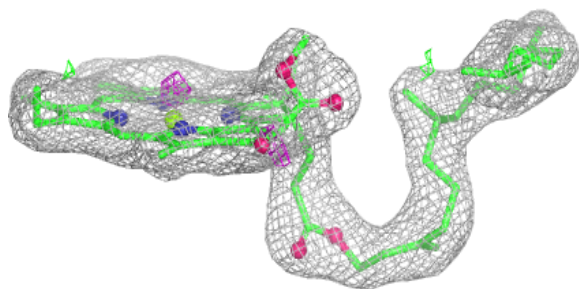
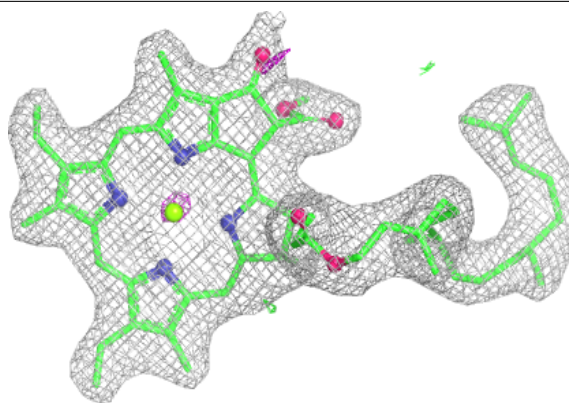
Electron density around CLA b 610:

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

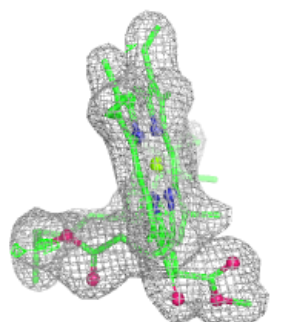
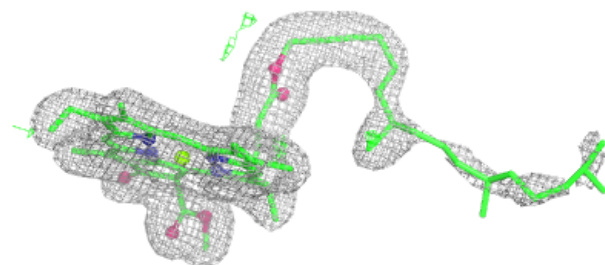
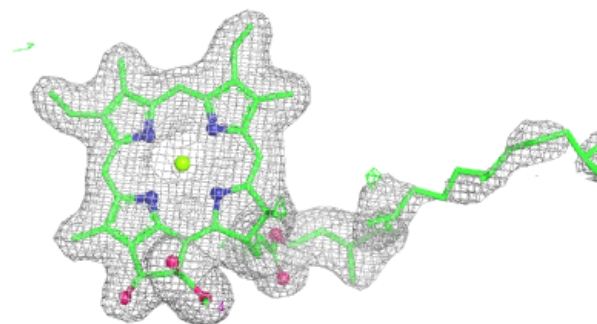


Electron density around CLA b 612:

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

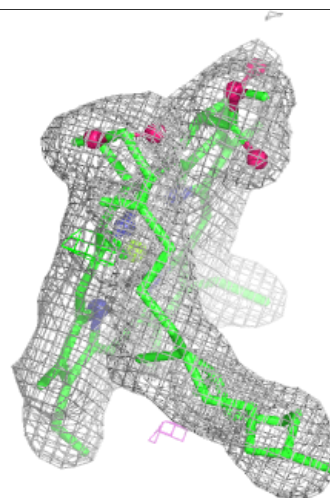
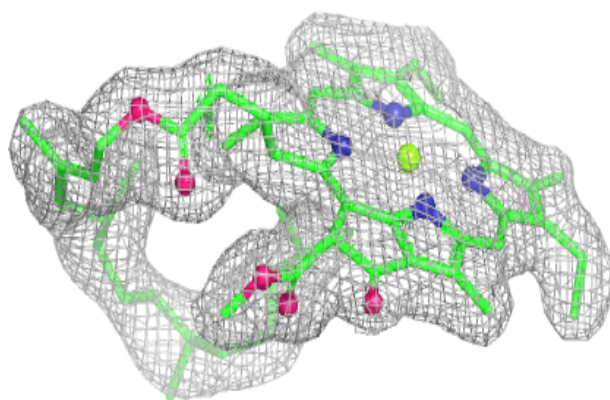
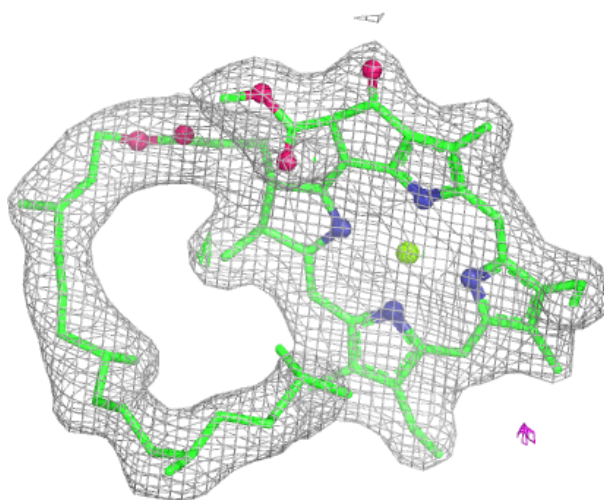
**Electron density around CLA A 403:**

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



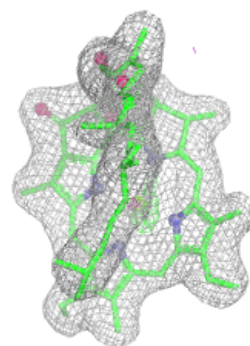
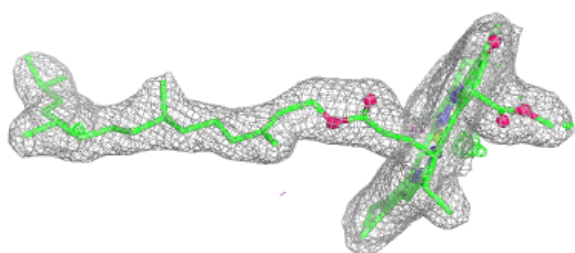
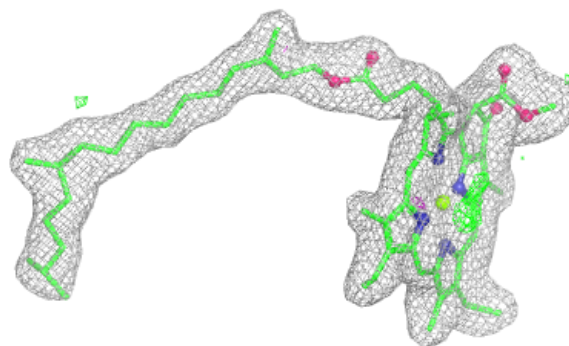
Electron density around CLA b 615:

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

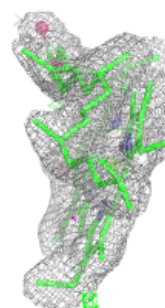
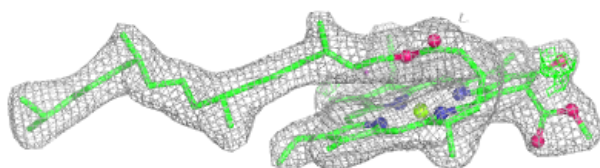
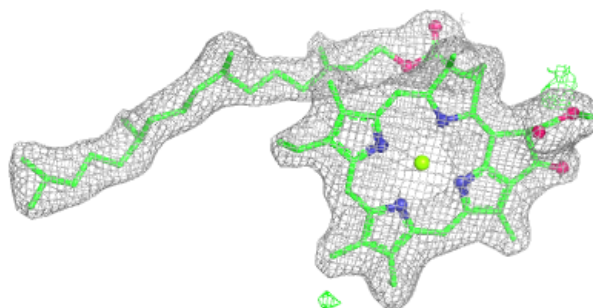


Electron density around CLA B 709:

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

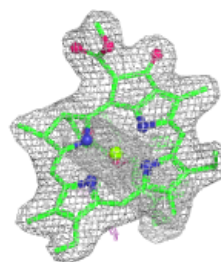
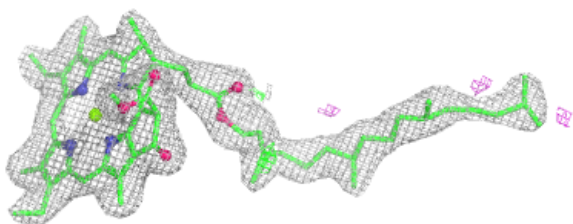
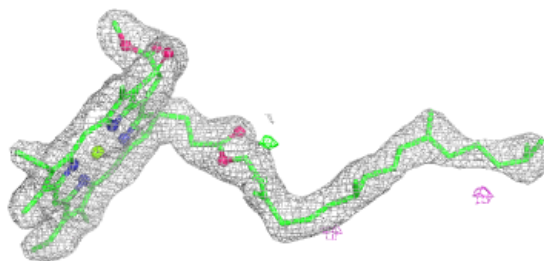
**Electron density around CLA c 502:**

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

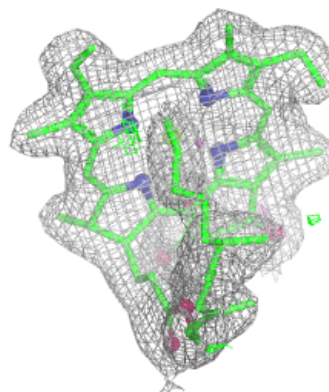
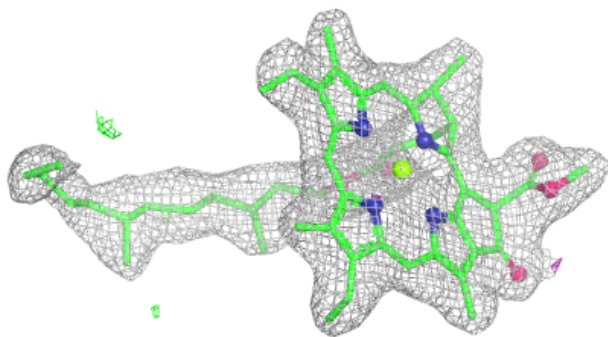
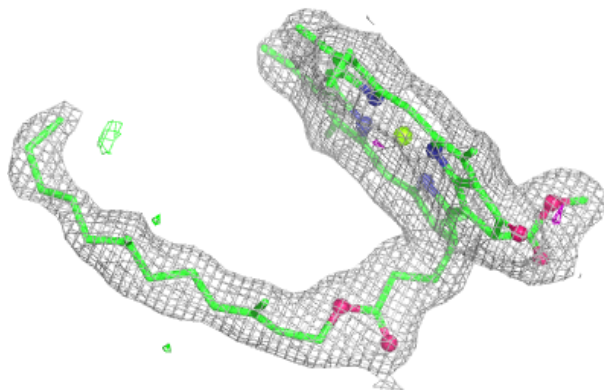


Electron density around CLA c 503:

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

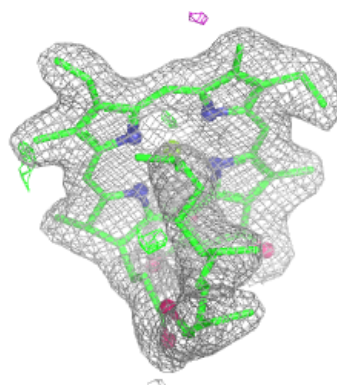
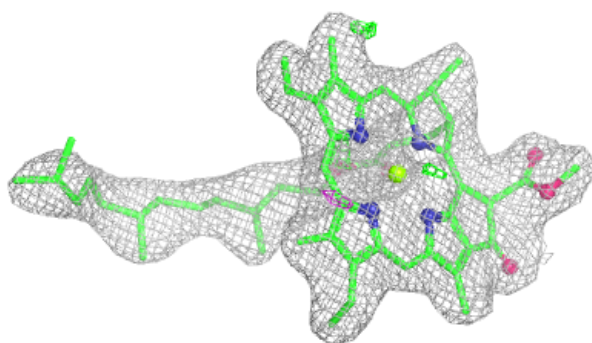
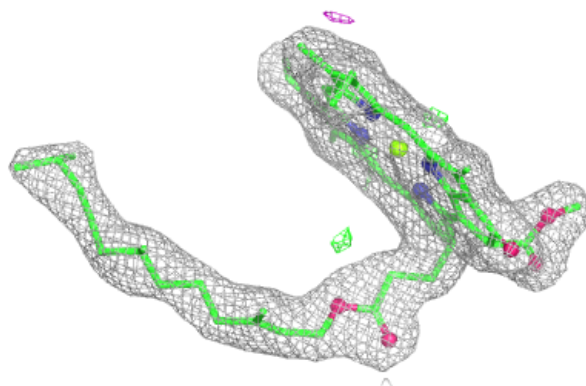
**Electron density around CLA C 505:**

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

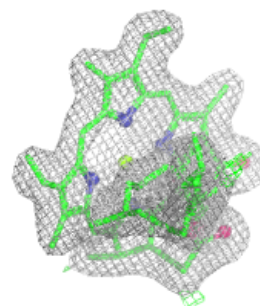
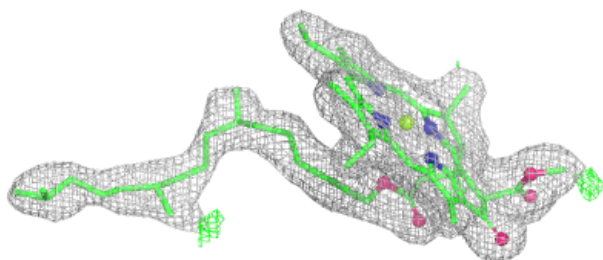
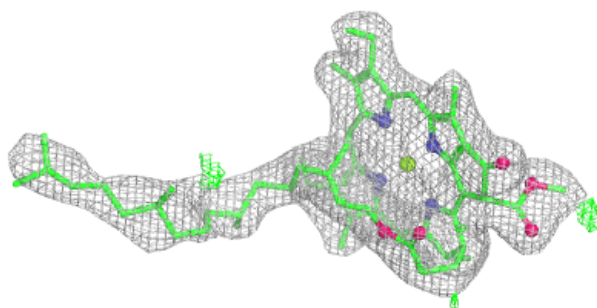


Electron density around CLA c 505:

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

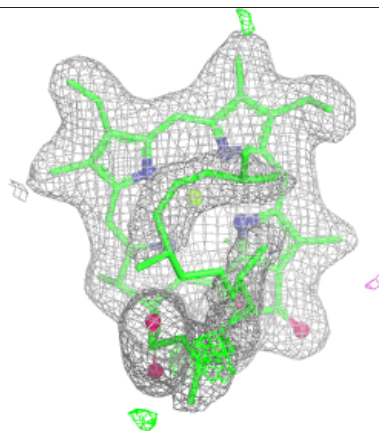
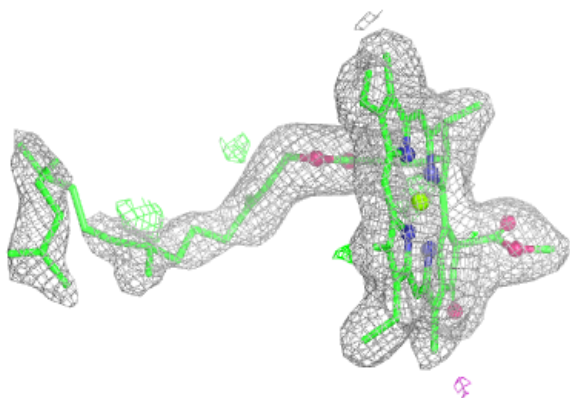
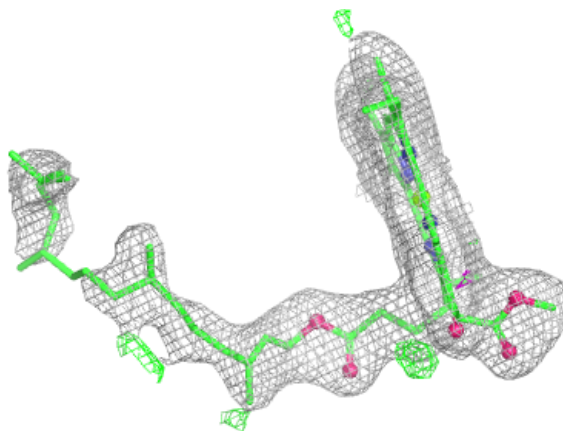
**Electron density around CLA c 506:**

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



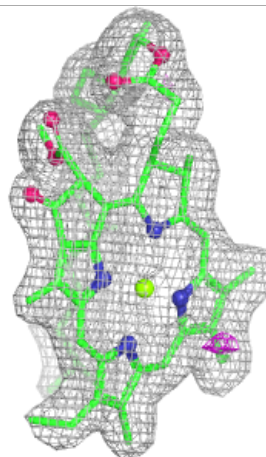
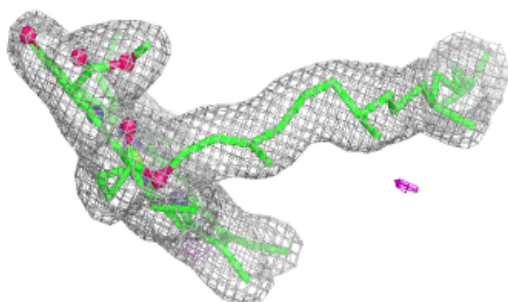
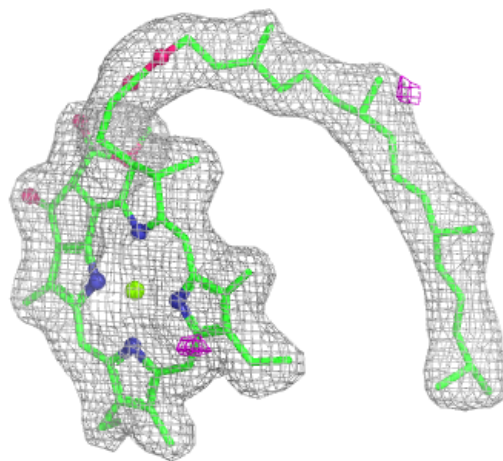
Electron density around CLA C 507:

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



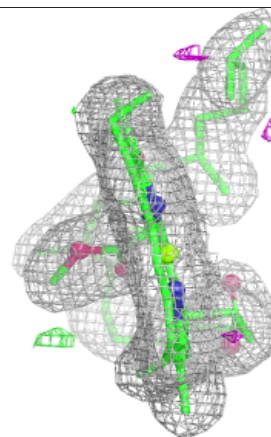
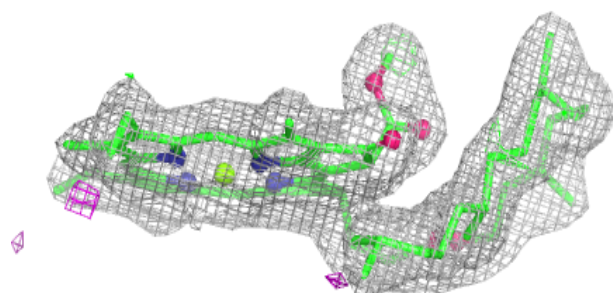
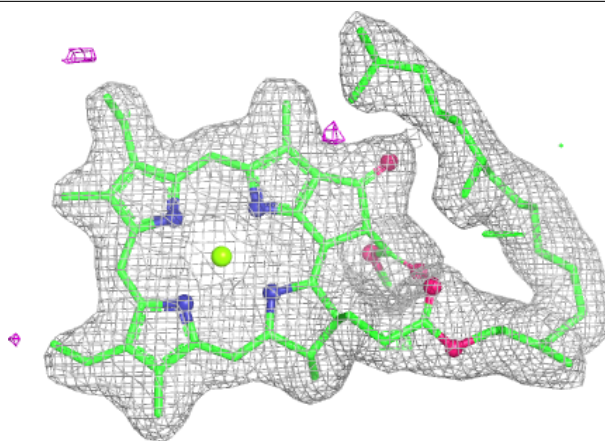
Electron density around CLA C 508:

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



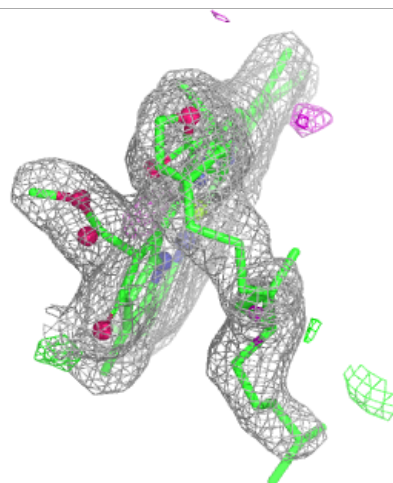
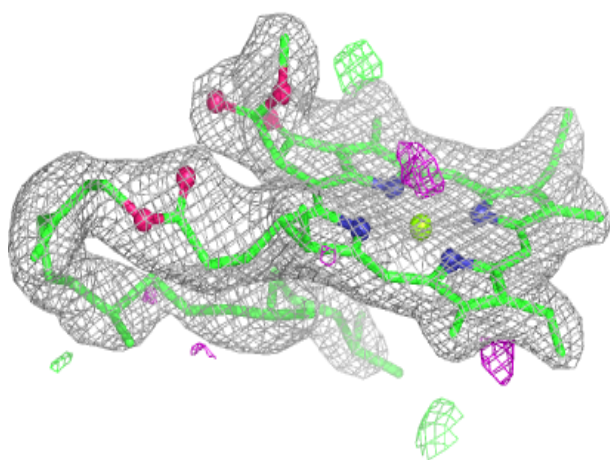
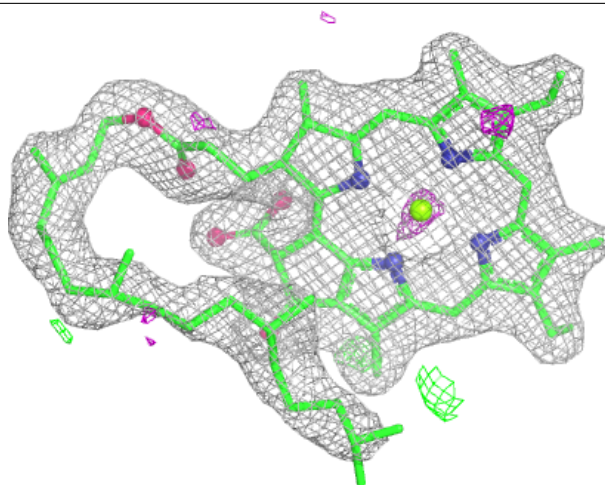
Electron density around CLA B 710:

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



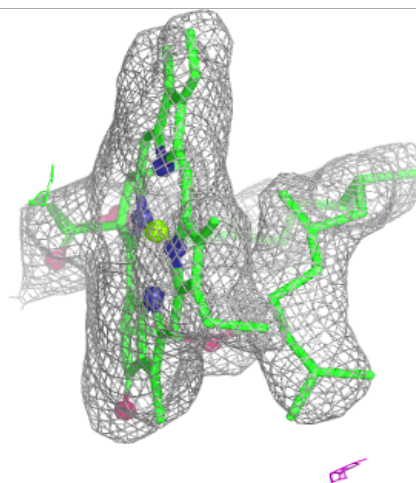
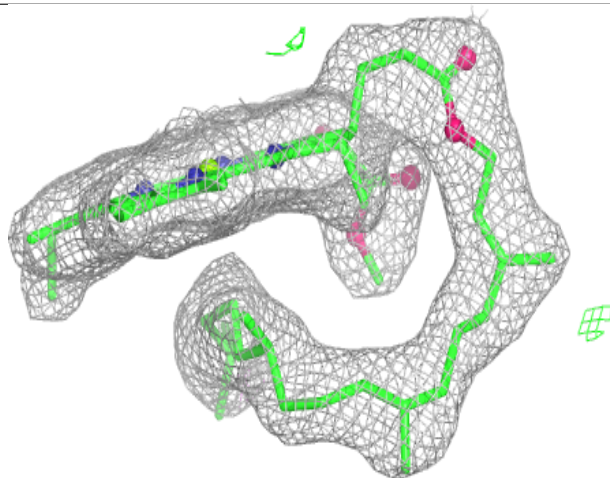
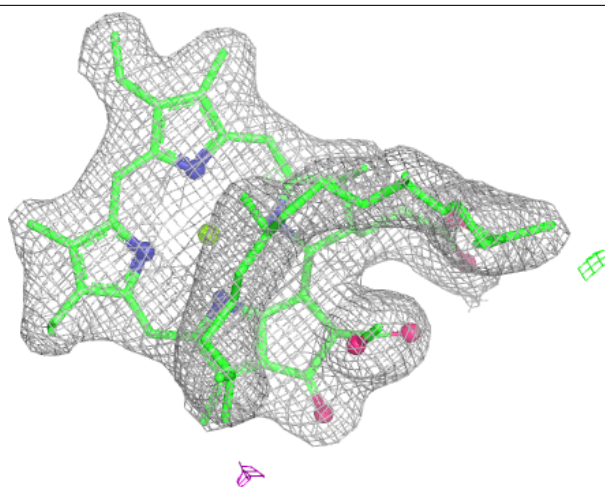
Electron density around CLA C 510:

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



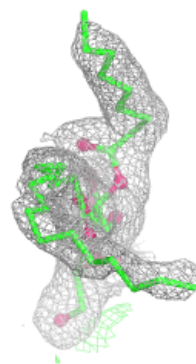
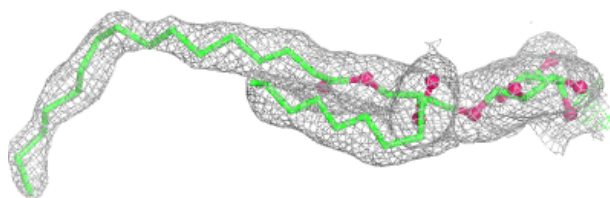
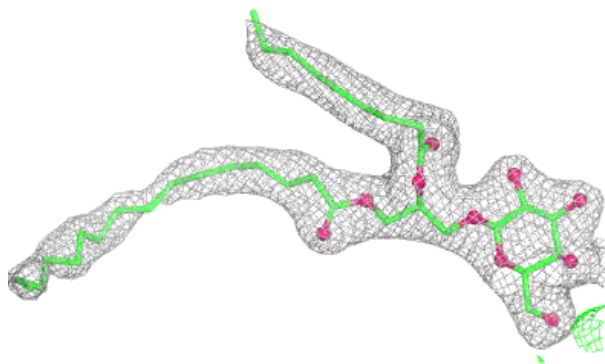
Electron density around CLA c 511:

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



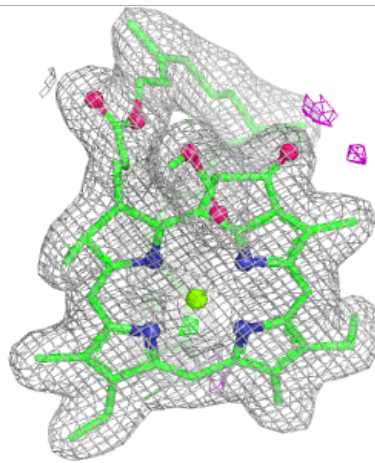
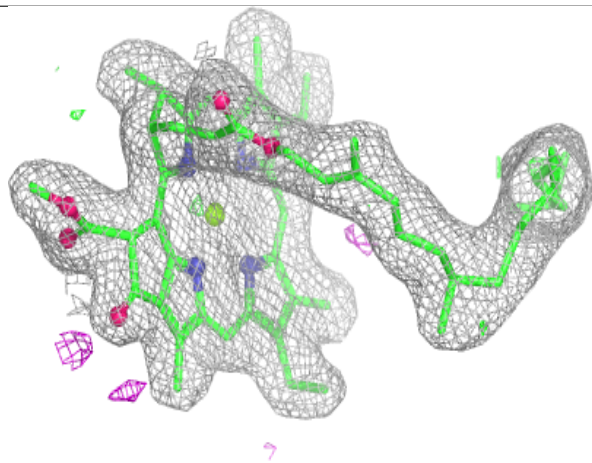
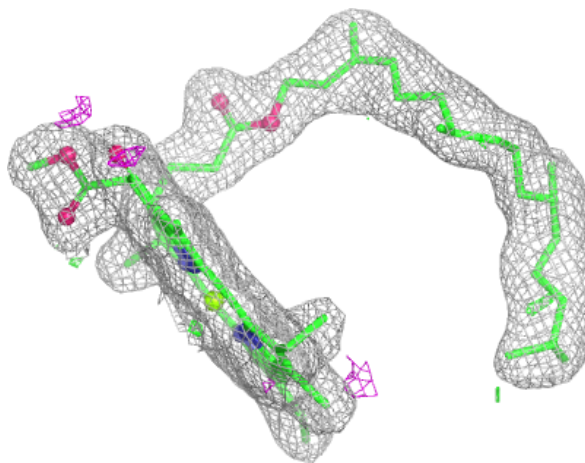
Electron density around LMG d 410:

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



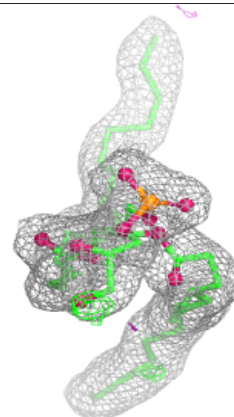
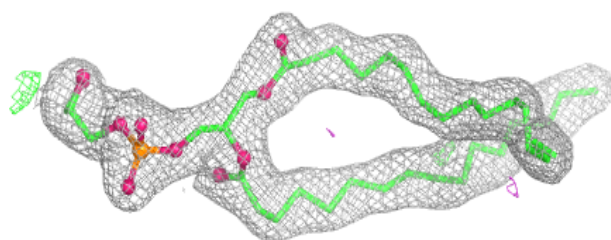
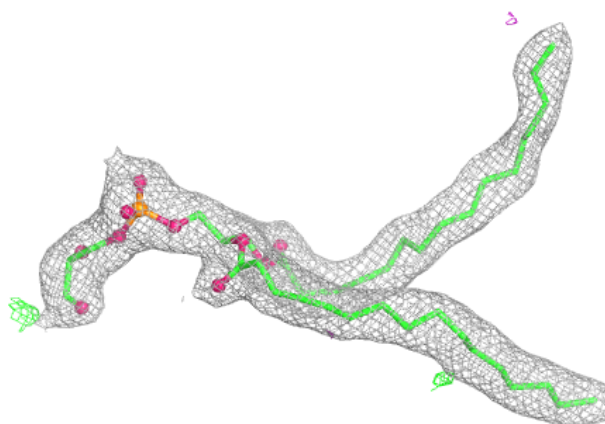
Electron density around CLA B 711:

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

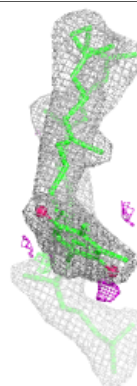
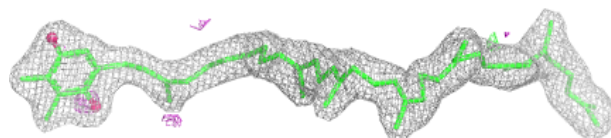
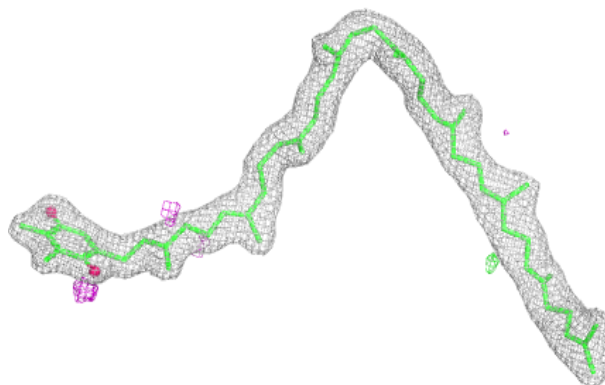


Electron density around LHG D 411:

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

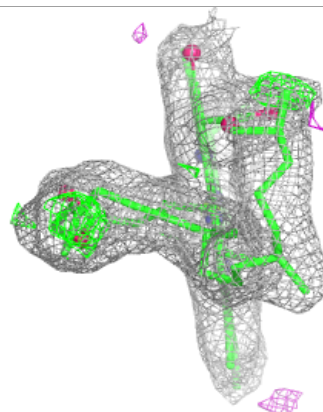
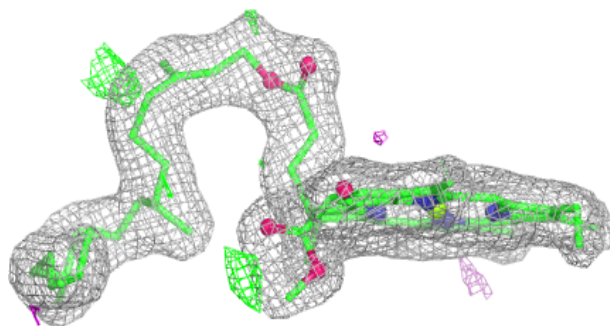
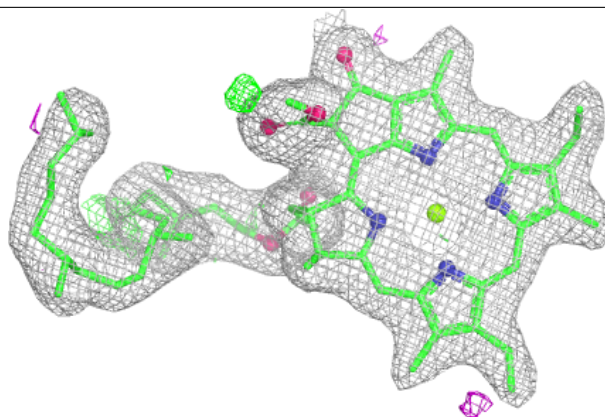
**Electron density around PL9 d 406:**

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



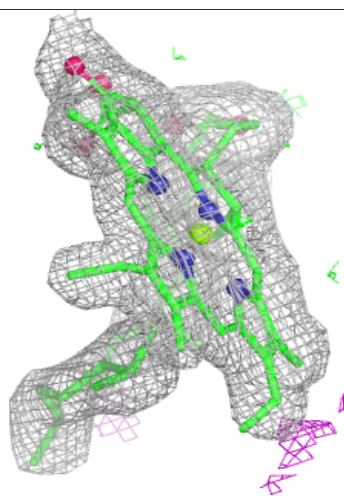
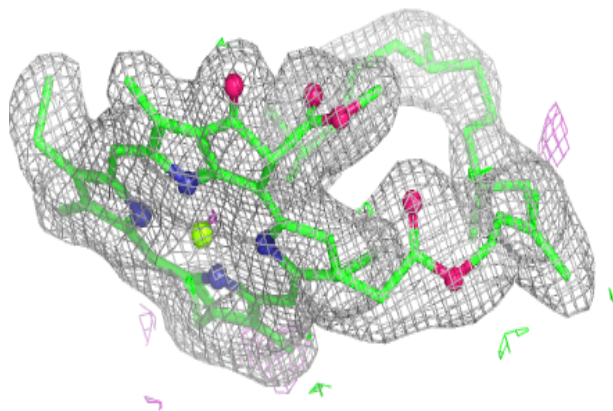
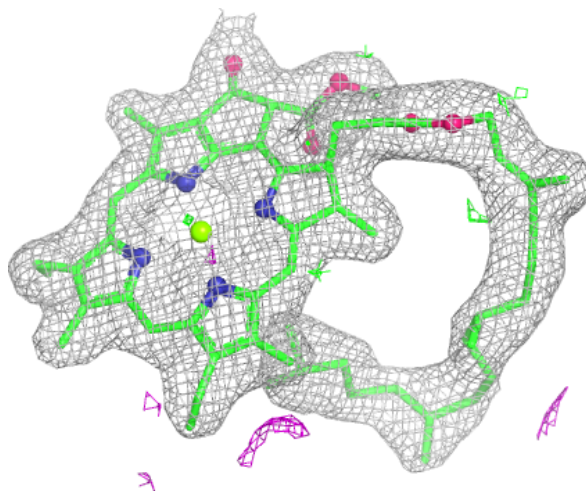
Electron density around CLA B 712:

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



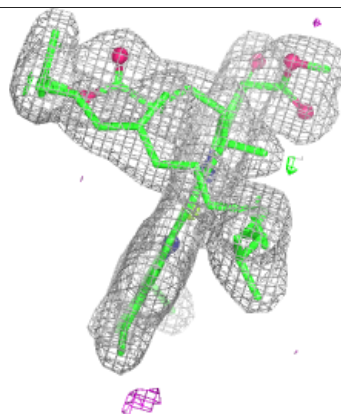
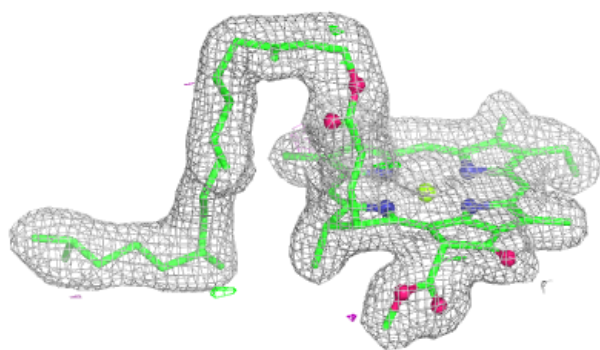
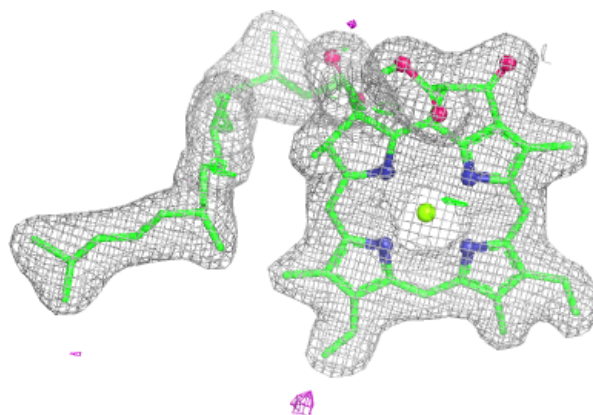
Electron density around CLA B 715:

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

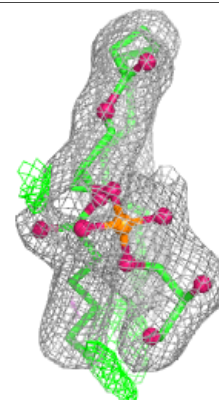
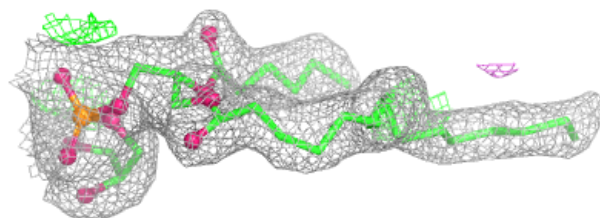
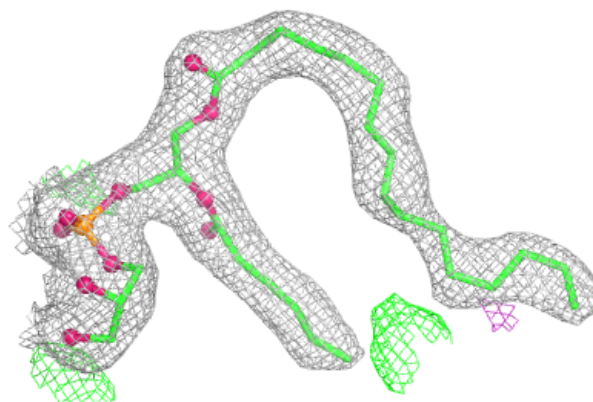


Electron density around CLA d 401:

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

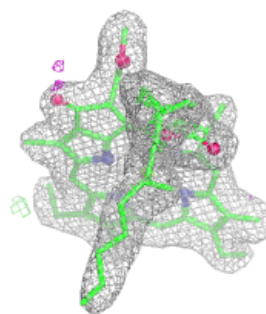
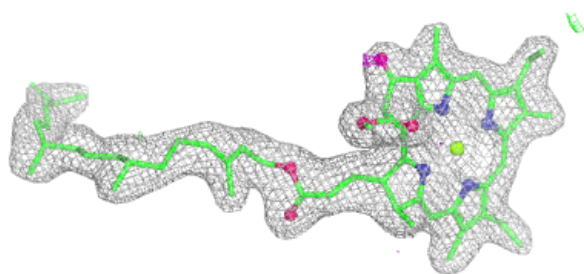
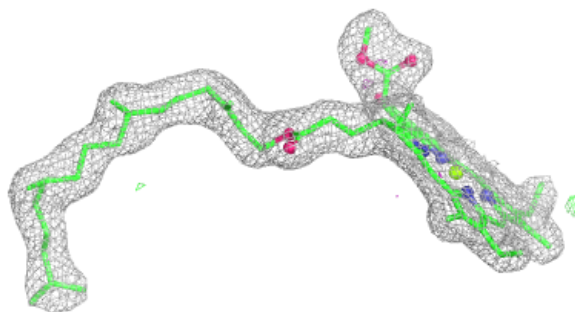
**Electron density around LHG d 409:**

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



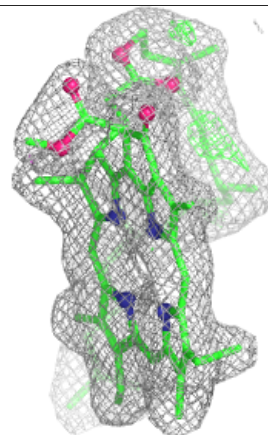
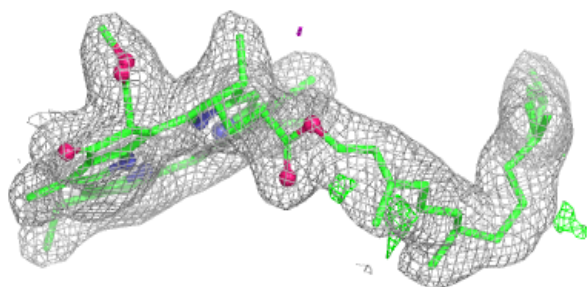
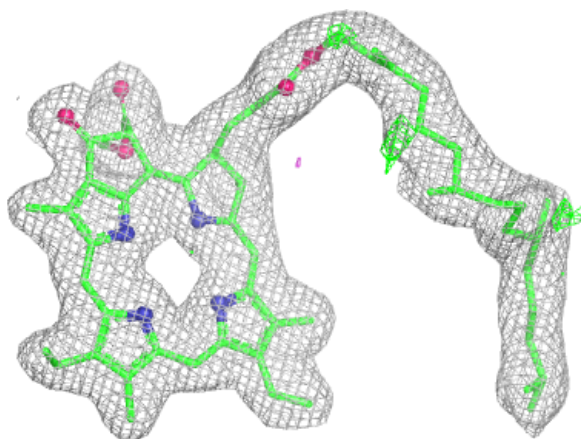
Electron density around CLA d 403:

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



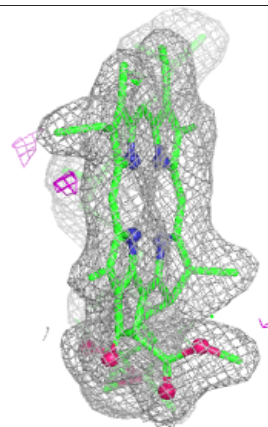
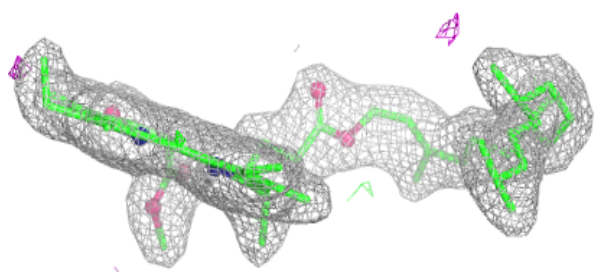
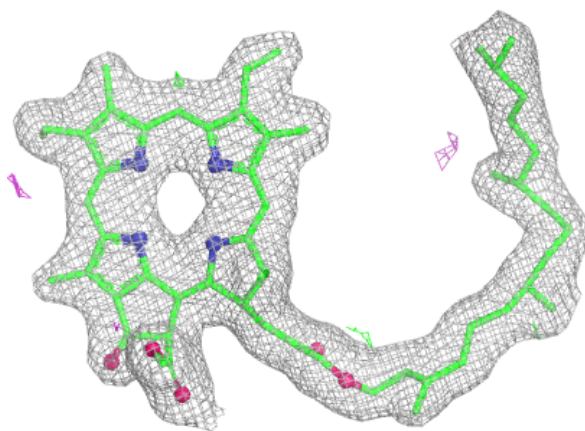
Electron density around PHO D 408:

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



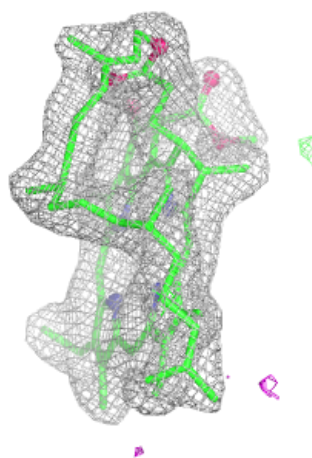
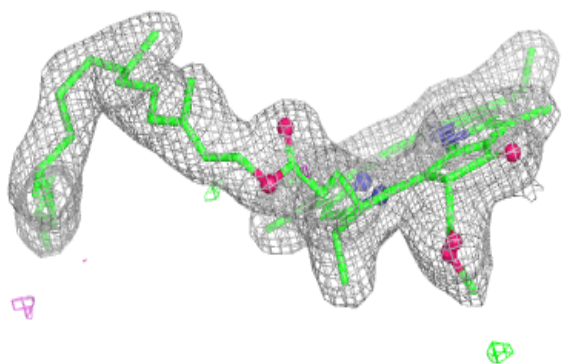
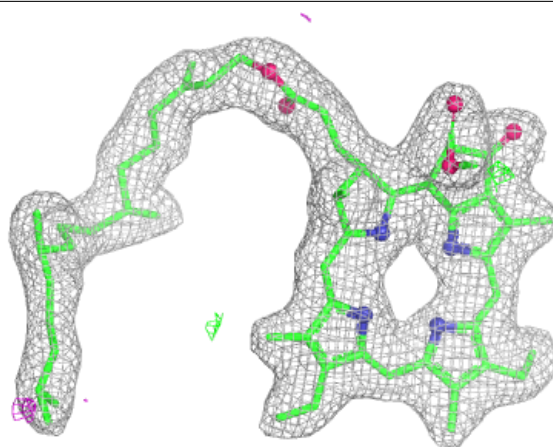
Electron density around PHO a 404:

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



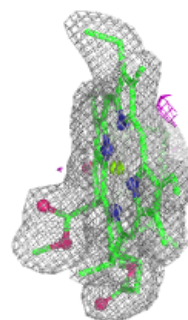
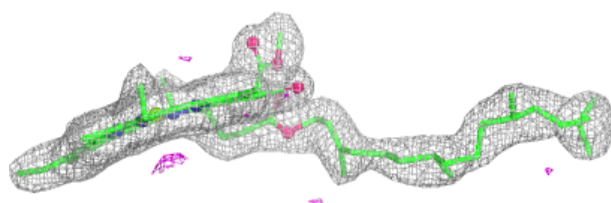
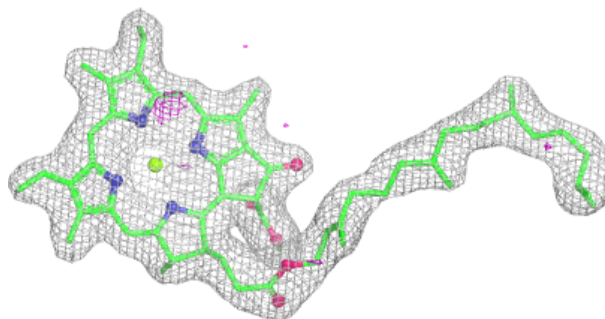
Electron density around PHO d 407:

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

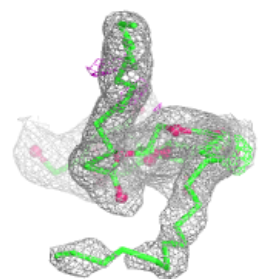
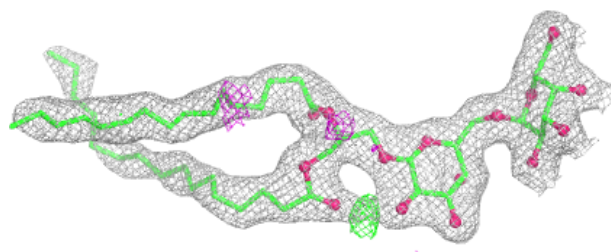
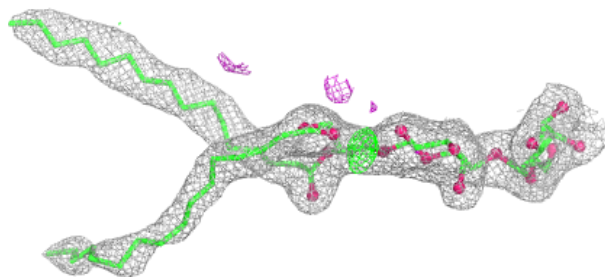


Electron density around CLA B 702:

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

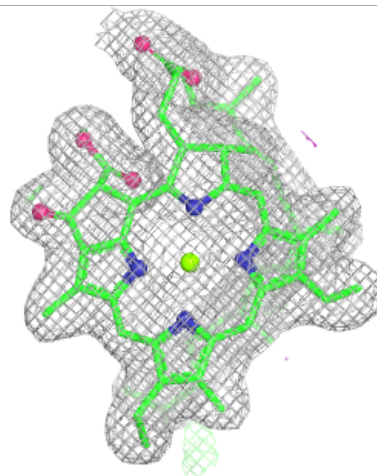
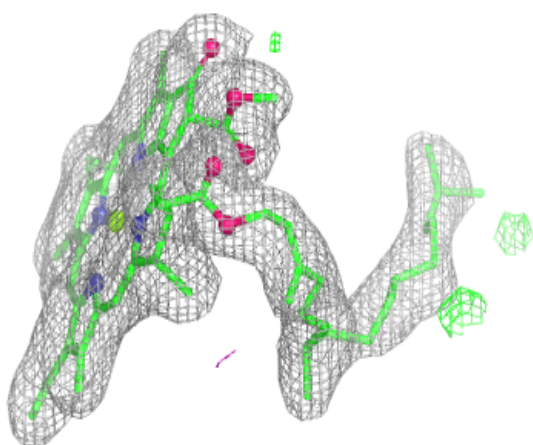
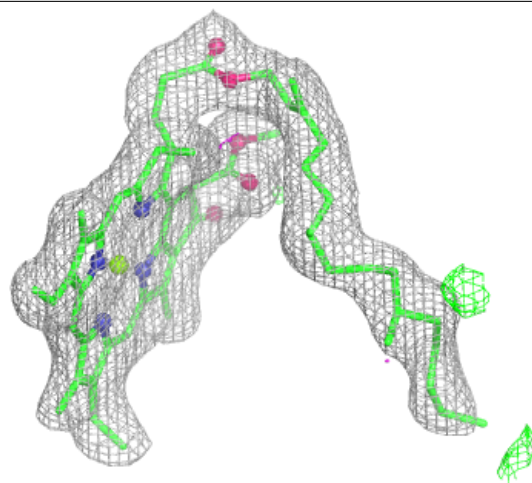
**Electron density around DGD c 517:**

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



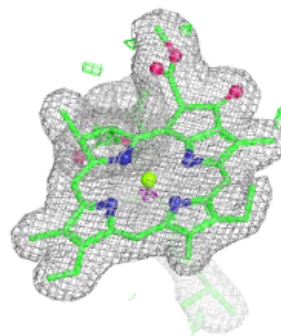
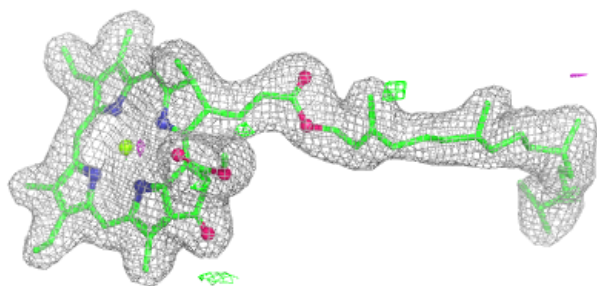
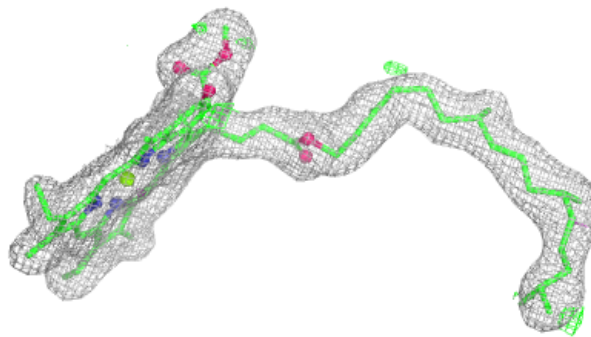
Electron density around CLA B 713:

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



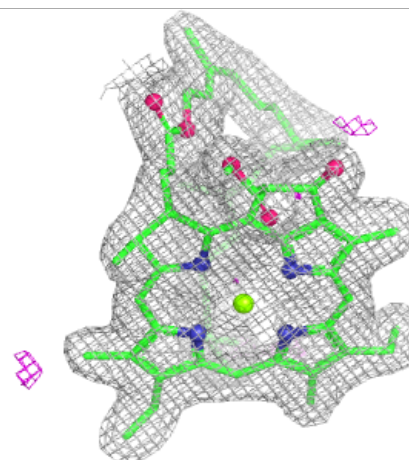
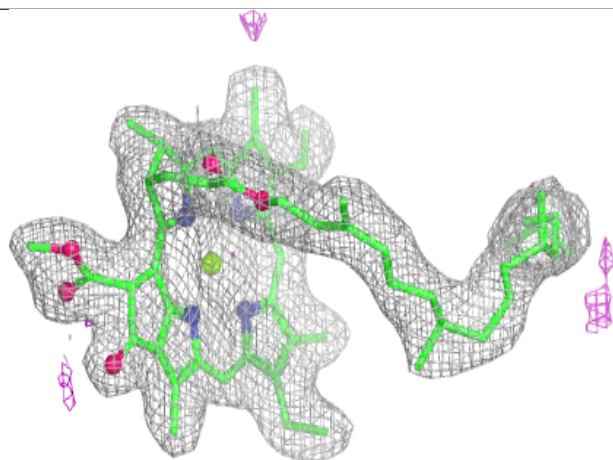
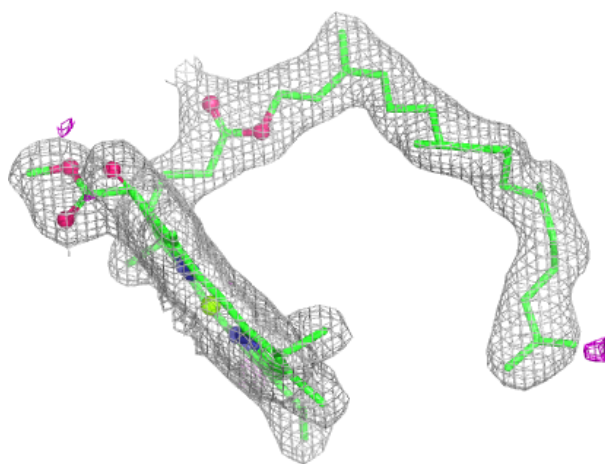
Electron density around CLA D 402:

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



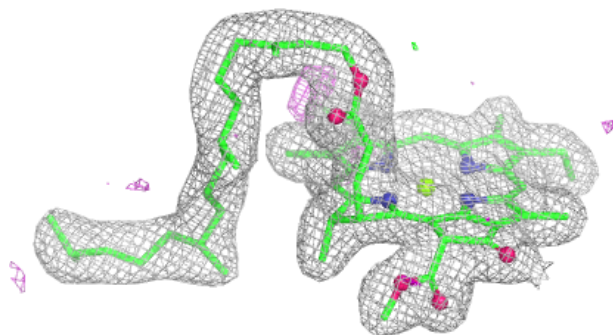
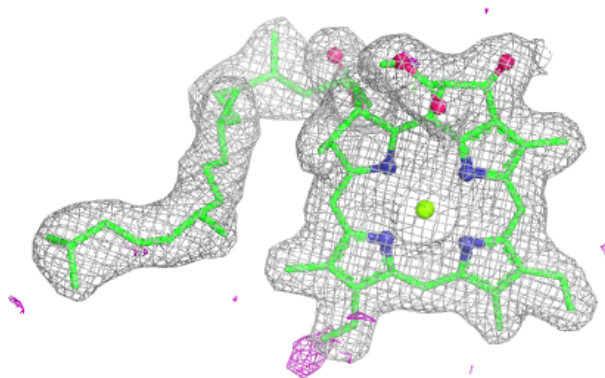
Electron density around CLA b 611:

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



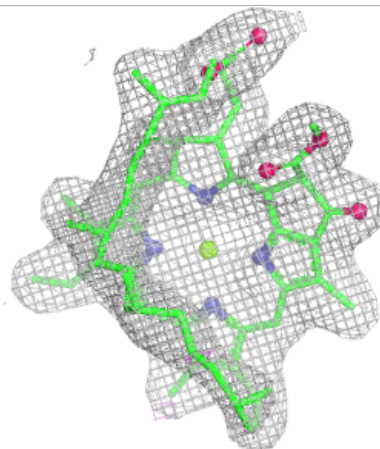
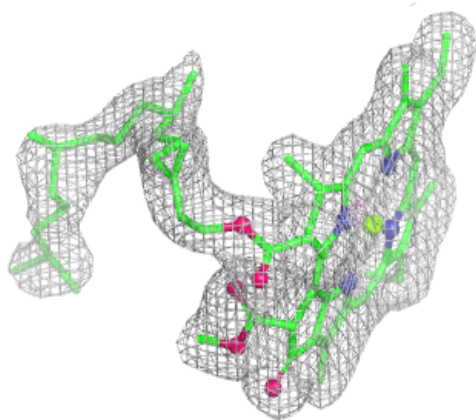
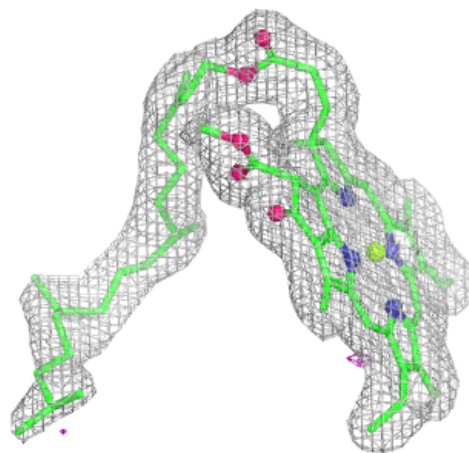
Electron density around CLA D 403:

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



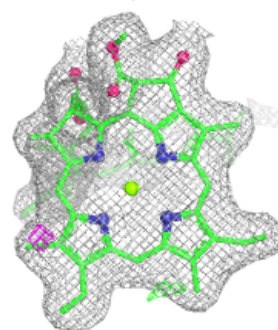
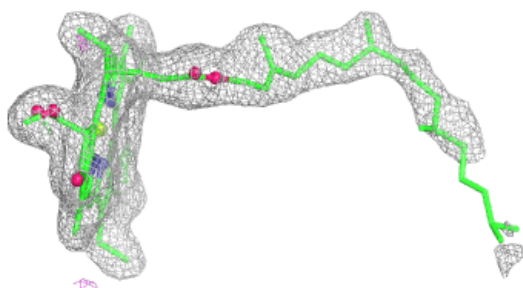
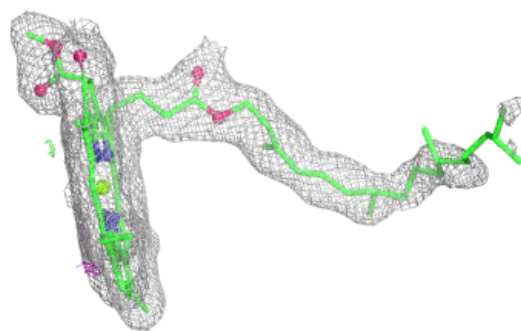
Electron density around CLA b 613:

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

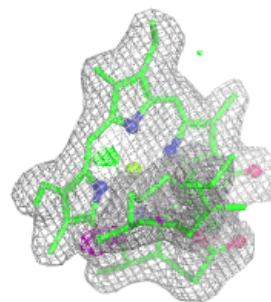
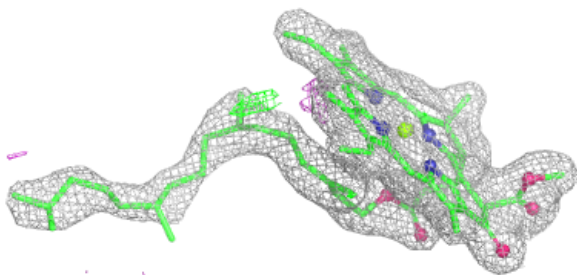
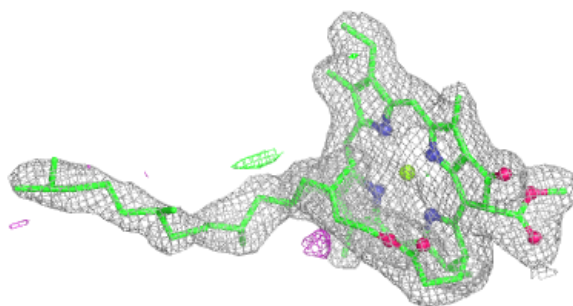


Electron density around CLA D 404:

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

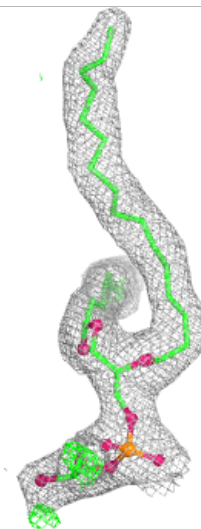
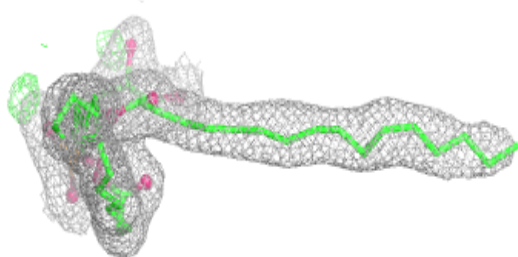
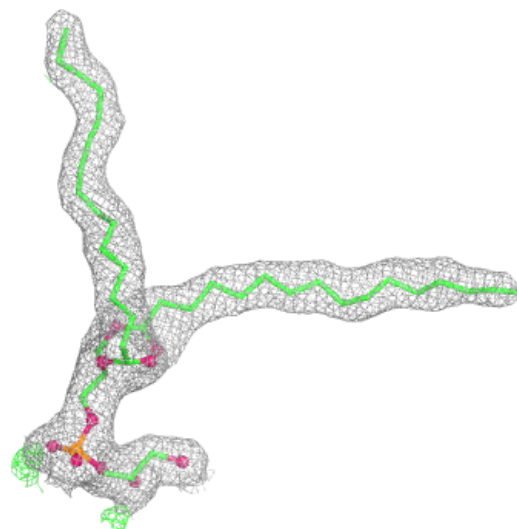
**Electron density around CLA C 506:**

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



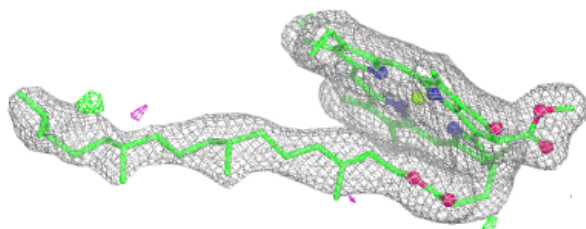
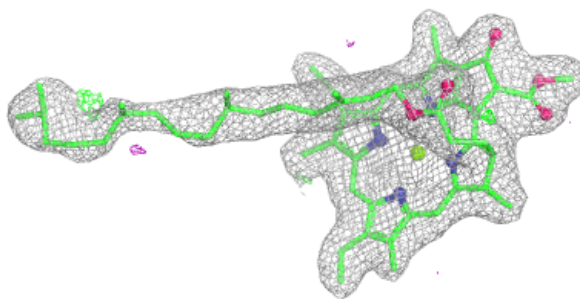
Electron density around LHG L 101:

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

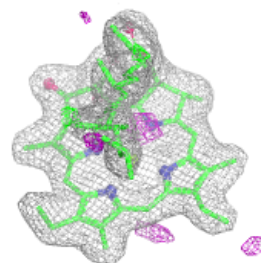
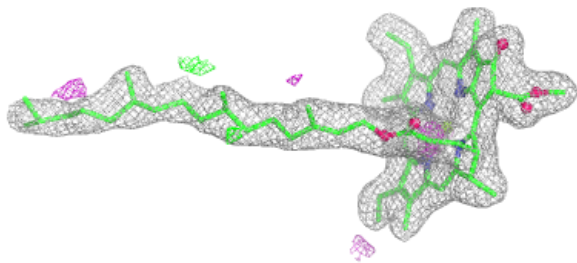
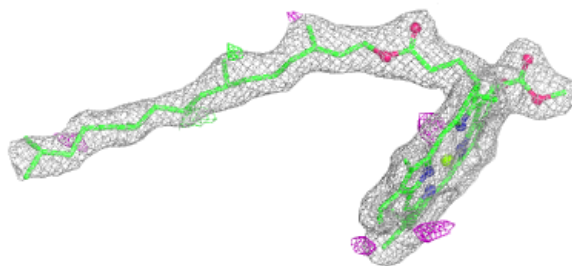


Electron density around CLA B 714:

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

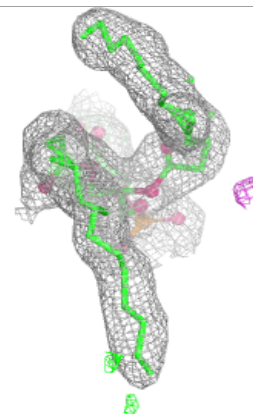
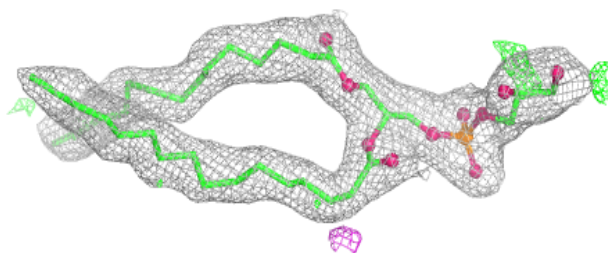
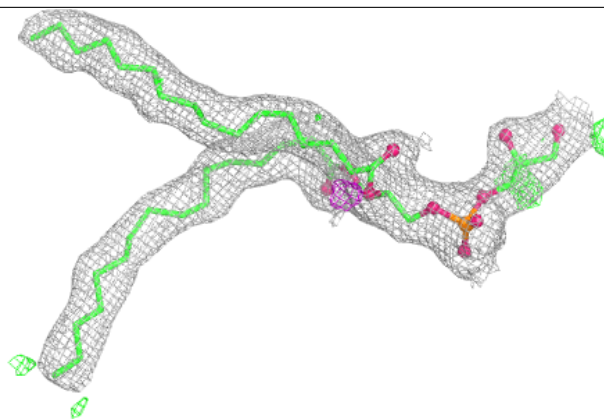
**Electron density around CLA B 707:**

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

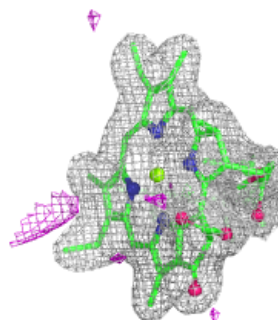
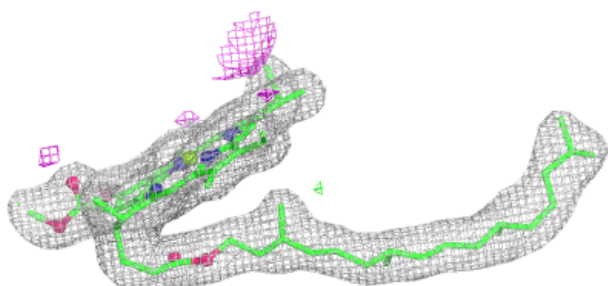
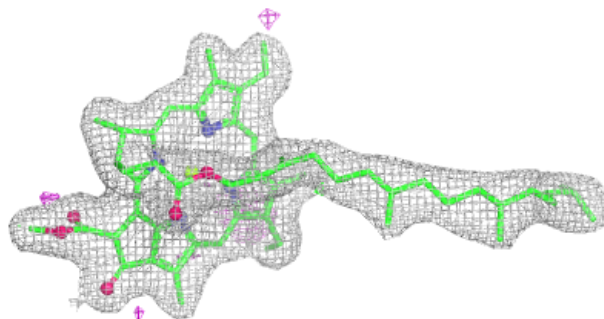


Electron density around LHG d 408:

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

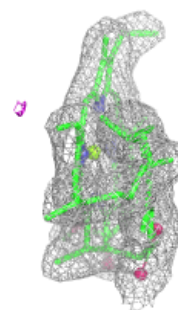
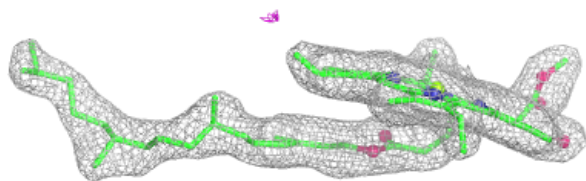
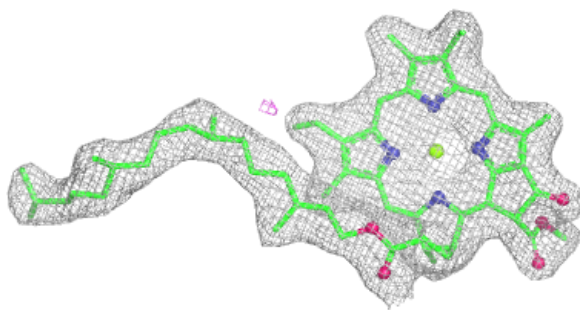
**Electron density around CLA B 708:**

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

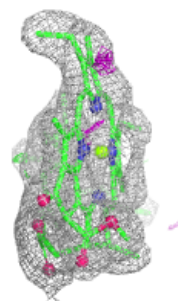
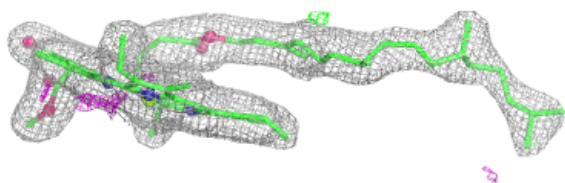
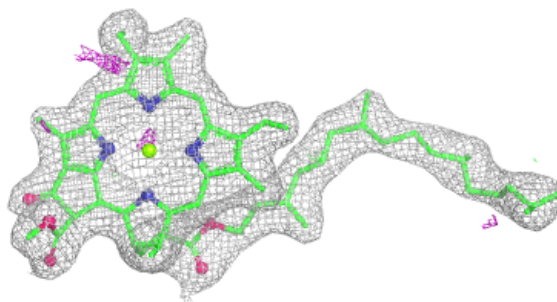


Electron density around CLA b 603:

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

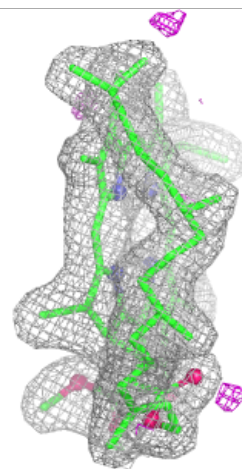
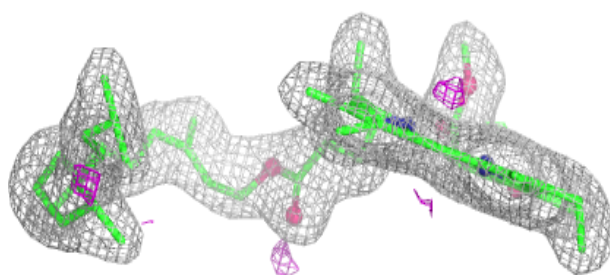
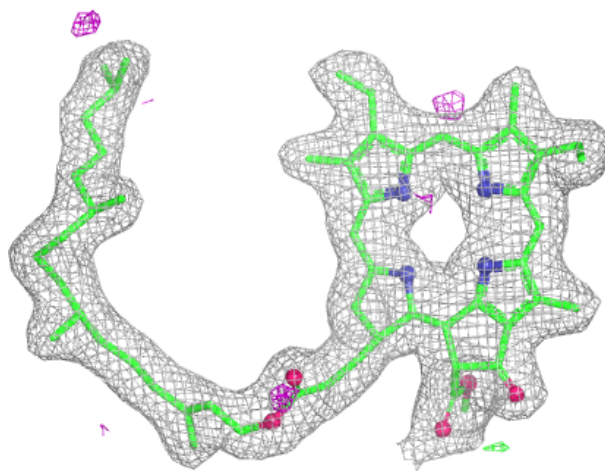
**Electron density around CLA B 703:**

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



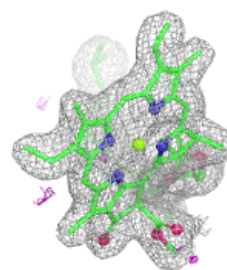
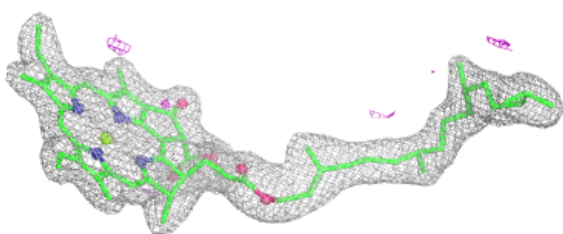
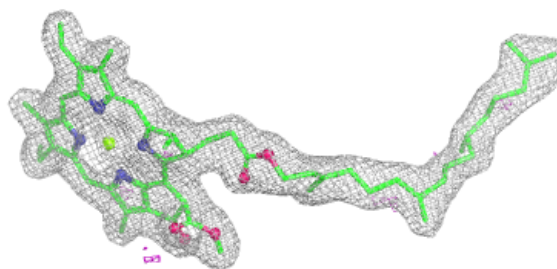
Electron density around PHO D 407:

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

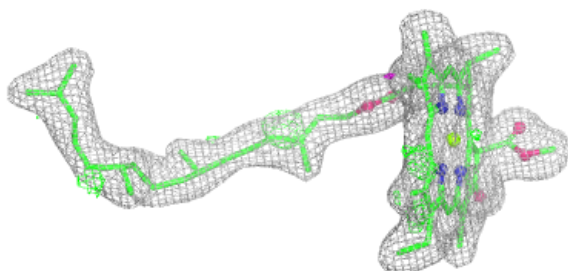
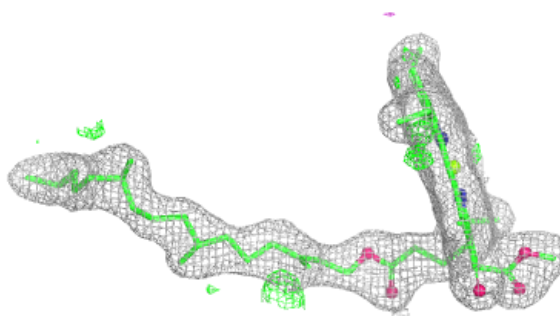


Electron density around CLA A 402:

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

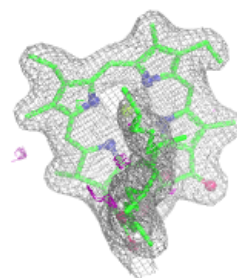
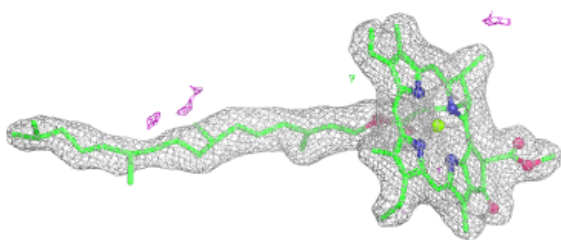
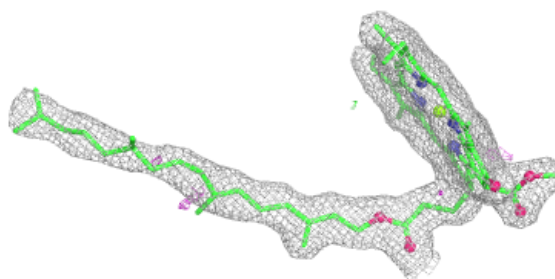
**Electron density around CLA B 705:**

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



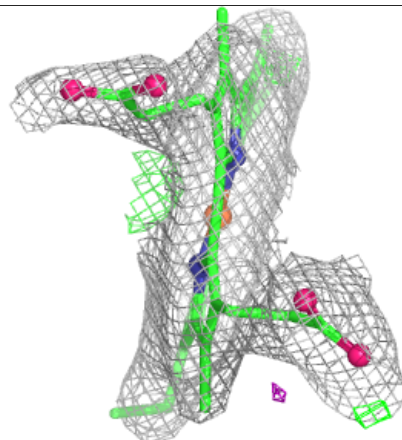
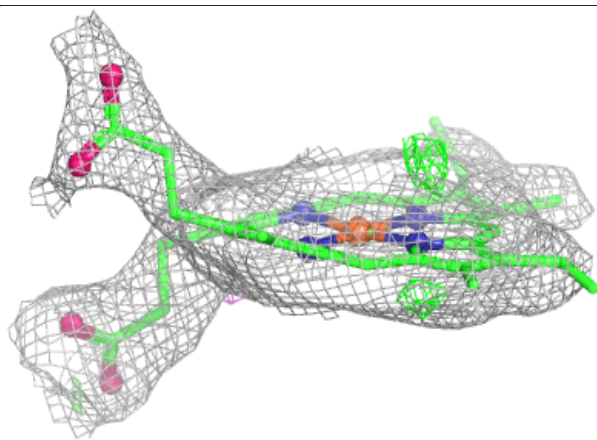
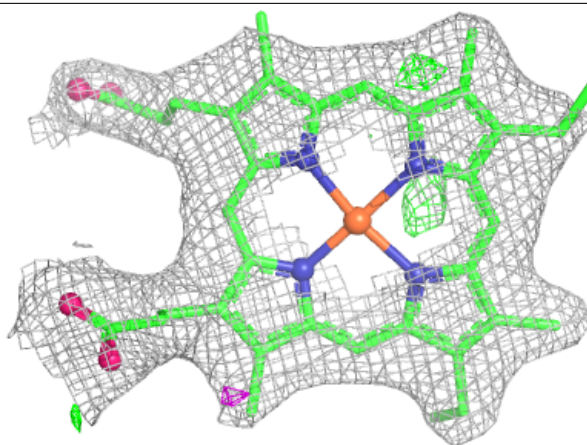
Electron density around CLA b 607:

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



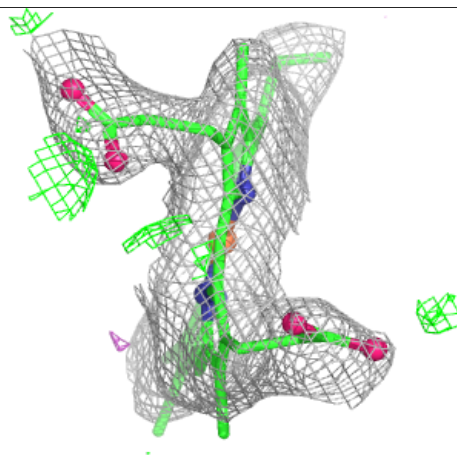
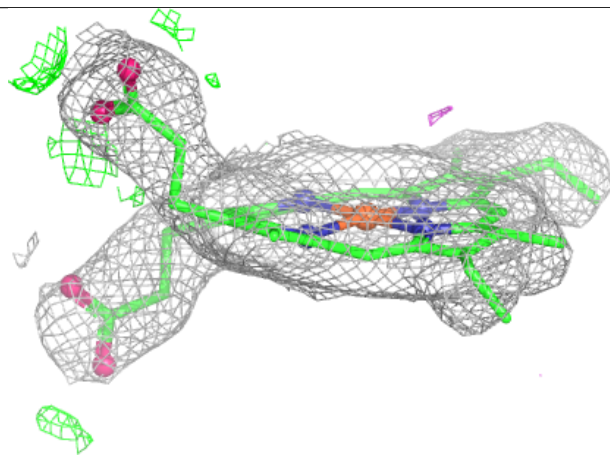
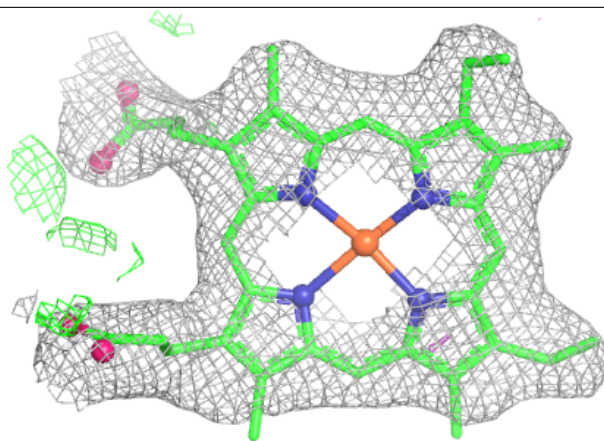
Electron density around HEC F 101:

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



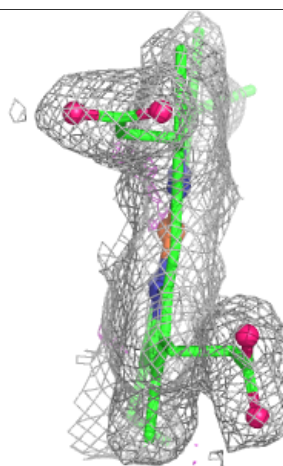
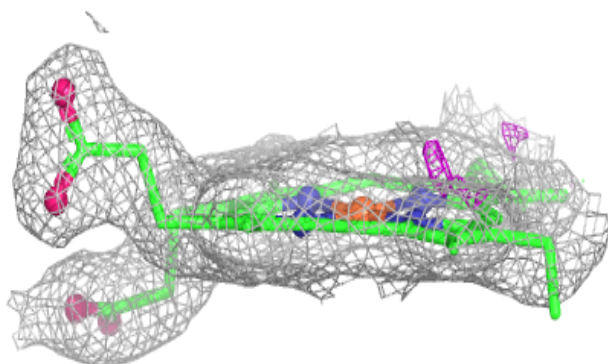
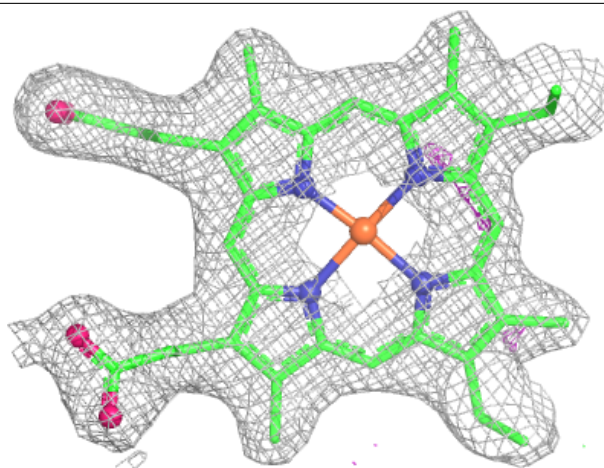
Electron density around HEC f 101:

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



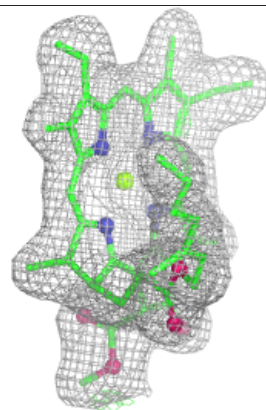
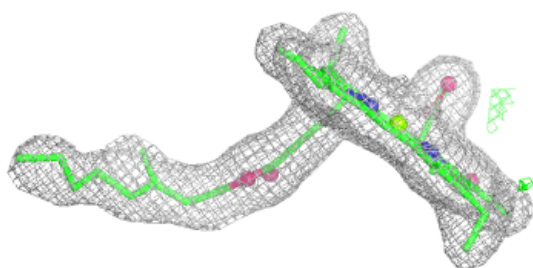
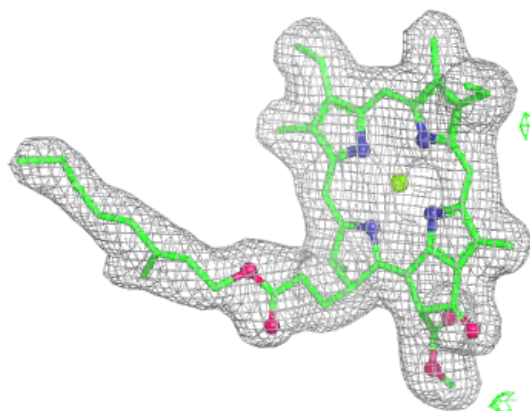
Electron density around HEC V 201:

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



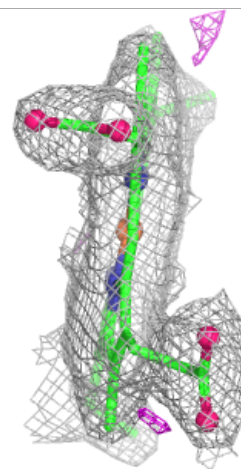
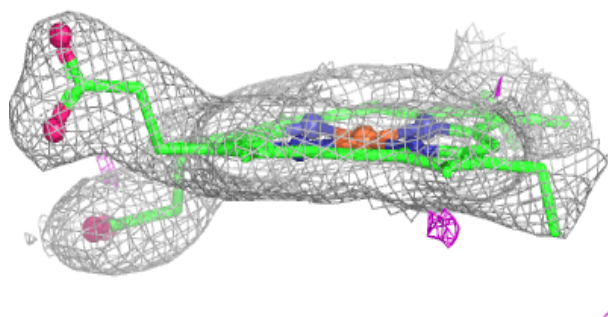
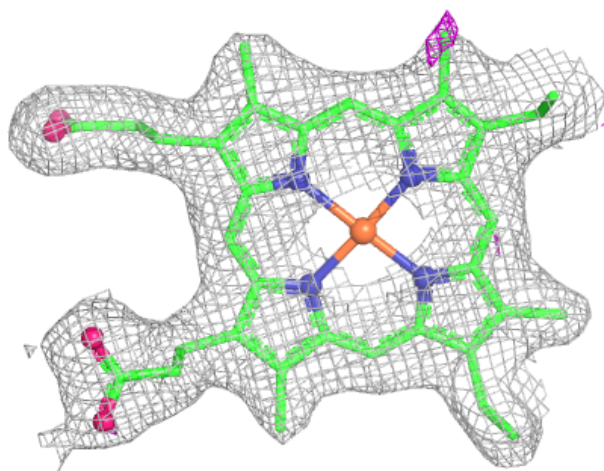
Electron density around CLA A 404:

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



Electron density around 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.