



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 1, 2026 – 12:46 PM UTC

PDB ID : 8F4C / pdb_00008f4c
Title : RT XFEL structure of the two-flash state of Photosystem II (2F, S3-rich) at 2.00 Angstrom resolution
Authors : Bhowmick, A.; Hussein, R.; Bogacz, I.; Simon, P.S.; Ibrahim, M.; Chatterjee, R.; Doyle, M.D.; Cheah, M.H.; Fransson, T.; Chernev, P.; Kim, I.-S.; Makita, H.; Dasgupta, M.; Kaminsky, C.J.; Zhang, M.; Gatcke, J.; Haupt, S.; Nangca, I.I.; Keable, S.M.; Aydin, O.; Tono, K.; Owada, S.; Gee, L.B.; Fuller, F.D.; Batyuk, A.; Alonso-Mori, R.; Holton, J.M.; Paley, D.W.; Moriarty, N.W.; Mamedov, F.; Adams, P.D.; Brewster, A.S.; Dobbek, H.; Sauter, N.K.; Bergmann, U.; Zouni, A.; Messinger, J.; Kern, J.; Yano, J.; Yachandra, V.K.
Deposited on : 2022-11-10
Resolution : 2.00 Å(reported)

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

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

A user guide is available at
<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0

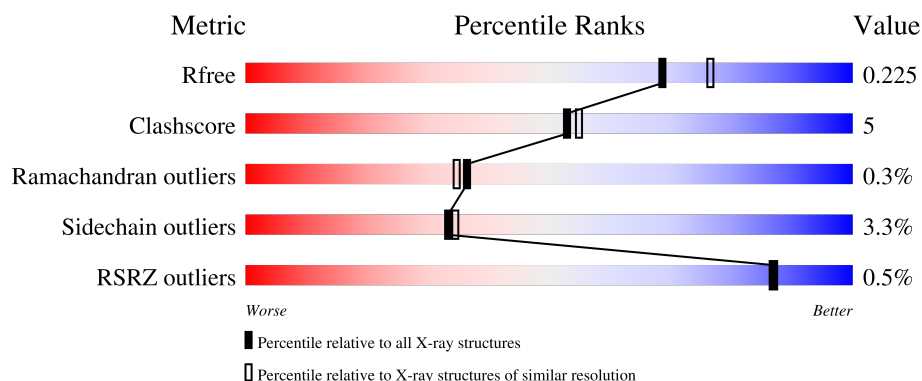
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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

Mol	Chain	Length	Quality of chain
1	A	344	 88% 9% .

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Buster-report : wwPDB partial adaption of 1.1.7 (2018)
 Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
 CCP4 : 9.0.010 (Gargrove)
 Density-Fitness : 1.0.12
 Ideal geometry (proteins) : Engh & Huber (2001)
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Chain	Length	Quality of chain
1	a	344	
2	B	510	
2	b	510	
3	C	461	
3	c	461	
4	D	352	
4	d	352	
5	E	84	
5	e	84	
6	F	45	
6	f	45	
7	H	66	
7	h	66	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	46	
10	k	46	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	272	
13	o	272	

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Mol	Chain	Length	Quality of chain
14	T	32	
14	t	32	
15	U	134	
15	u	134	
16	V	163	
16	v	163	
17	Y	46	
17	y	46	
18	X	41	
18	x	41	
19	Z	62	
19	z	62	
20	R	41	
20	r	41	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	A	606	X	-	-	-
25	CLA	A	607	X	-	-	-
25	CLA	A	608	X	-	-	-
25	CLA	A	611	X	-	-	-
25	CLA	B	601	X	-	-	-
25	CLA	B	602	X	-	-	-
25	CLA	B	603	X	-	-	-
25	CLA	B	604	X	-	-	-
25	CLA	B	605	X	-	-	-
25	CLA	B	606	X	-	-	-
25	CLA	B	607	X	-	-	-
25	CLA	B	608	X	-	-	-
25	CLA	B	610	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	B	611	X	-	-	-
25	CLA	B	612	X	-	-	-
25	CLA	B	613	X	-	-	-
25	CLA	B	614	X	-	-	-
25	CLA	B	615	X	-	-	-
25	CLA	B	616	X	-	-	-
25	CLA	C	501	X	-	-	-
25	CLA	C	503	X	-	-	-
25	CLA	C	504	X	-	-	-
25	CLA	C	505	X	-	-	-
25	CLA	C	506	X	-	-	-
25	CLA	C	507	X	-	-	-
25	CLA	C	509	X	-	-	-
25	CLA	C	510	X	-	-	-
25	CLA	C	511	X	-	-	-
25	CLA	C	512	X	-	-	-
25	CLA	C	513	X	-	-	-
25	CLA	D	404	X	-	-	-
25	CLA	a	607	X	-	-	-
25	CLA	a	609	X	-	-	-
25	CLA	b	601	X	-	-	-
25	CLA	b	602	X	-	-	-
25	CLA	b	603	X	-	-	-
25	CLA	b	604	X	-	-	-
25	CLA	b	605	X	-	-	-
25	CLA	b	606	X	-	-	-
25	CLA	b	607	X	-	-	-
25	CLA	b	608	X	-	-	-
25	CLA	b	610	X	-	-	-
25	CLA	b	611	X	-	-	-
25	CLA	b	612	X	-	-	-
25	CLA	b	613	X	-	-	-
25	CLA	b	614	X	-	-	-
25	CLA	b	615	X	-	-	-
25	CLA	b	616	X	-	-	-
25	CLA	c	501	X	-	-	-
25	CLA	c	502	X	-	-	-
25	CLA	c	503	X	-	-	-
25	CLA	c	504	X	-	-	-
25	CLA	c	505	X	-	-	-
25	CLA	c	506	X	-	-	-
25	CLA	c	507	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	c	509	X	-	-	-
25	CLA	c	510	X	-	-	-
25	CLA	c	511	X	-	-	-
25	CLA	c	512	X	-	-	-
25	CLA	c	513	X	-	-	-
25	CLA	d	403	X	-	-	-
25	CLA	d	404	X	-	-	-

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 53435 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
			3113	2030	513	551	19			
1	a	334	Total	C	N	O	S	0	64	0
			3110	2027	513	551	19			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	505	Total	C	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
			3509	2302	586	607	14			
3	c	451	Total	C	N	O	S	0	12	0
			3583	2343	602	624	14			

- 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
			2731	1809	446	464	12			
4	d	341	Total	C	N	O	S	0	3	0
			2737	1813	446	466	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			

There are 2 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	36	Total	C	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			
10	k	37	Total	C	N	O	0	0	0
			293	204	43	46			

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

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

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

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

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

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

- Molecule 14 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	30	Total	C	N	O	S	0	0	0
			258	181	36	39	2			
14	t	30	Total	C	N	O	S	0	0	0
			256	180	36	38	2			

There are 2 discrepancies between the modelled and reference sequences:

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

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

- Molecule 15 is a protein called Photosystem II 12 kDa extrinsic protein.

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

- Molecule 16 is a protein called Cytochrome c-550.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total	C	N	O	S	0	0	0
			1064	675	177	208	4			
16	v	137	Total	C	N	O	S	0	0	0
			1064	675	177	208	4			

- Molecule 17 is a protein called Photosystem II reaction center protein Ycf12.

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	X	38	Total	C	N	O	0	0	0
			281	188	45	48			
18	x	39	Total	C	N	O	0	0	0
			286	191	46	49			

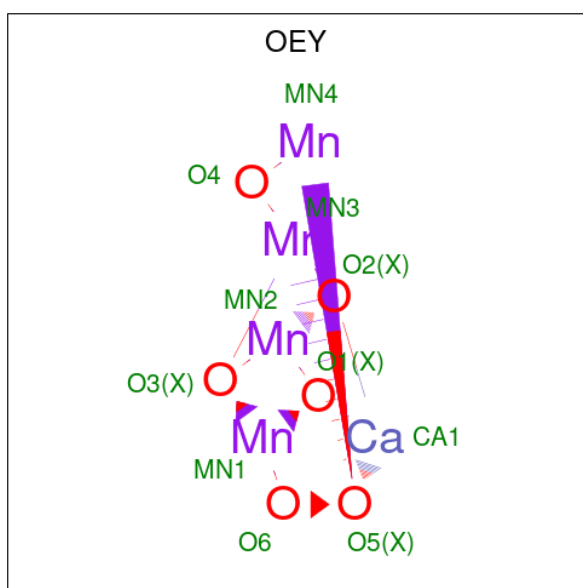
- Molecule 19 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Z	62	Total	C	N	O	S	0	0	0
			479	328	72	77	2			
19	z	62	Total	C	N	O	S	0	0	0
			477	326	72	77	2			

- Molecule 20 is a protein called Photosystem II protein Y.

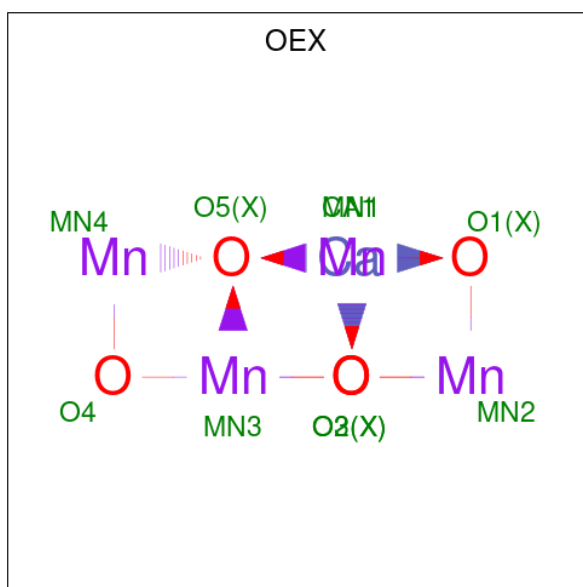
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	R	34	Total	C	N	O	0	0	0
			271	184	47	40			
20	r	31	Total	C	N	O	0	0	0
			246	166	43	37			

- Molecule 21 is CA-MN4-O6 CLUSTER (CCD ID: OEY) (formula: CaMn_4O_6) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 22 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5) (labeled as "Ligand of Interest" by depositor).



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

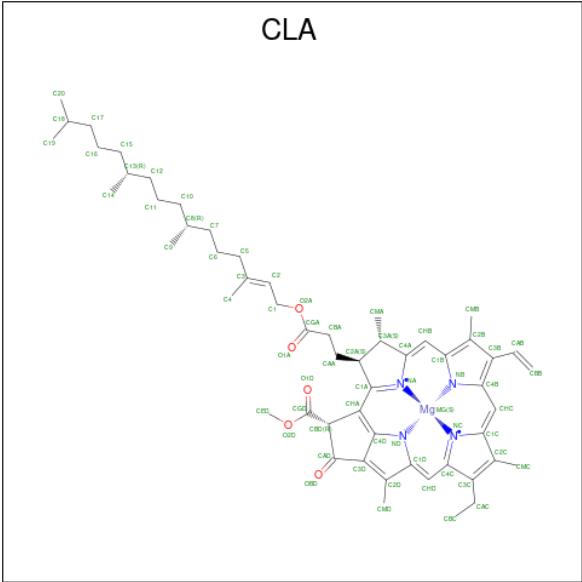
- Molecule 23 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

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

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

- Molecule 25 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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

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

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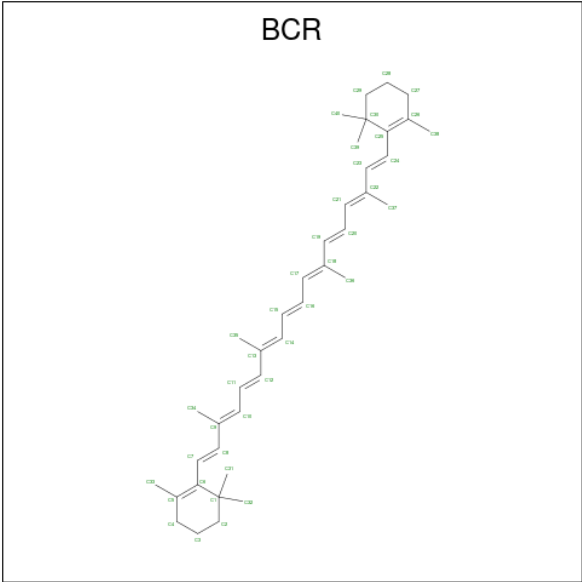
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N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

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

- Molecule 26 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



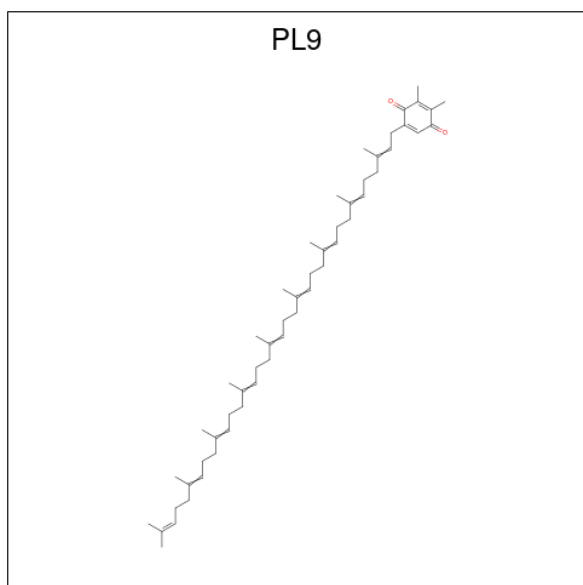
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	D	1	Total C 40 40	0	0
26	H	1	Total C 40 40	0	0
26	K	1	Total C 40 40	0	0
26	K	1	Total C 40 40	0	0
26	T	1	Total C 40 40	0	0
26	Z	1	Total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

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

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



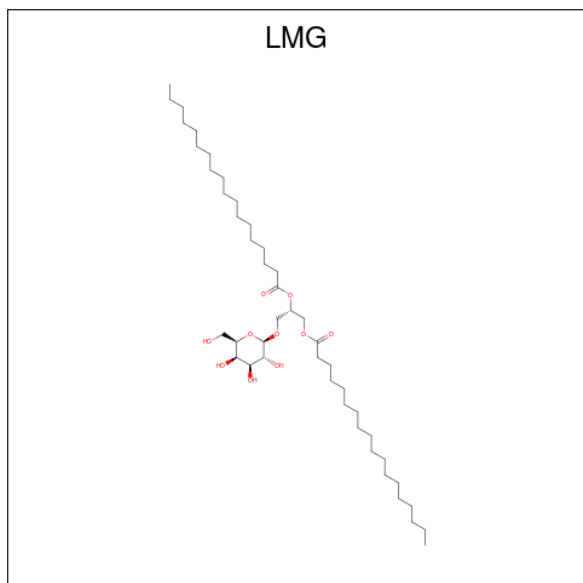
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	1	Total C O 55 53 2	0	0
27	D	1	Total C O 55 53 2	0	0

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

- Molecule 28 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



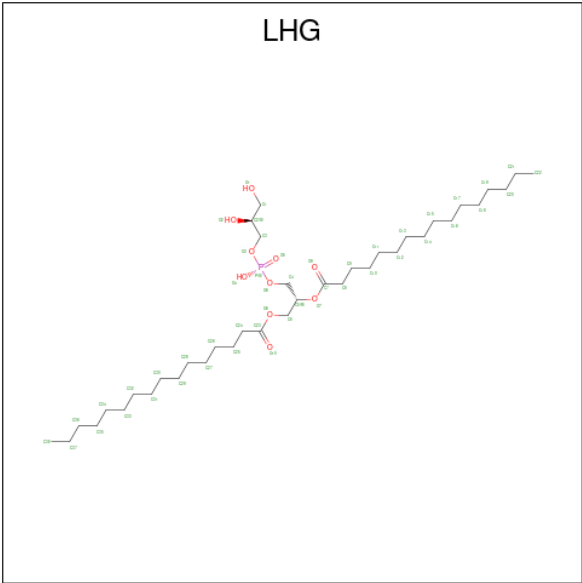
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	A	1	Total	C	O	0	0
			48	38	10		
28	B	1	Total	C	O	0	0
			28	24	4		
28	C	1	Total	C	O	0	0
			48	38	10		
28	D	1	Total	C	O	0	0
			51	41	10		
28	D	1	Total	C	O	0	0
			33	27	6		
28	M	1	Total	C	O	0	0
			51	41	10		
28	b	1	Total	C	O	0	0
			51	41	10		
28	b	1	Total	C	O	0	0
			55	45	10		
28	c	1	Total	C	O	0	0
			37	27	10		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	c	1	Total	C	O	0	0
			48	38	10		
28	c	1	Total	C	O	0	0
			49	39	10		
28	d	1	Total	C	O	0	0
			23	21	2		
28	d	1	Total	C	O	0	0
			44	34	10		

- Molecule 29 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



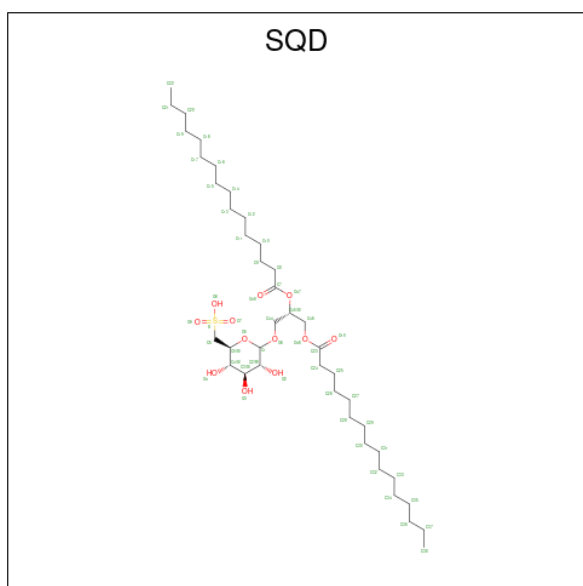
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	A	1	Total	C	O	P	0	0
			47	36	10	1		
29	B	1	Total	C	O	P	0	0
			49	38	10	1		
29	D	1	Total	C	O	P	0	0
			49	38	10	1		
29	E	1	Total	C	O	P	0	0
			49	38	10	1		
29	L	1	Total	C	O	P	0	0
			49	38	10	1		
29	d	1	Total	C	O	P	0	0
			49	38	10	1		
29	d	1	Total	C	O	P	0	0
			49	38	10	1		

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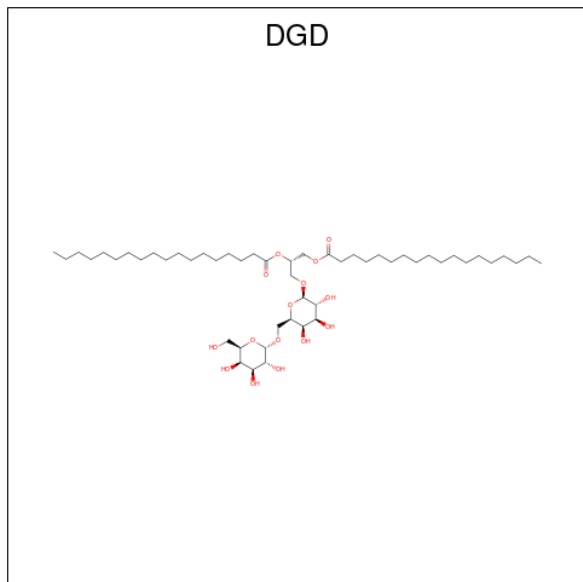
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	d	1	Total	C	O	P	0	0
			39	28	10	1		
29	e	1	Total	C	O	P	0	0
			42	31	10	1		
29	l	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 30 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



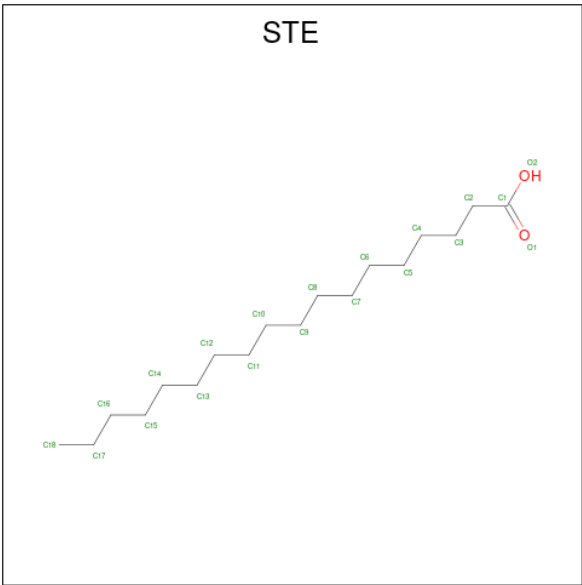
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	A	1	Total	C	O	S	0	0
			52	39	12	1		
30	A	1	Total	C	O		0	0
			39	35	4			
30	B	1	Total	C	O	S	0	0
			54	41	12	1		
30	D	1	Total	C	O	S	0	0
			36	25	10	1		
30	a	1	Total	C	O	S	0	0
			54	41	12	1		
30	a	1	Total	C	O		0	0
			36	31	5			
30	b	1	Total	C	O	S	0	0
			49	36	12	1		
30	f	1	Total	C	O	S	0	0
			41	28	12	1		

- Molecule 31 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



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

- Molecule 32 is STEARIC ACID (CCD ID: STE) (formula: $C_{18}H_{36}O_2$).



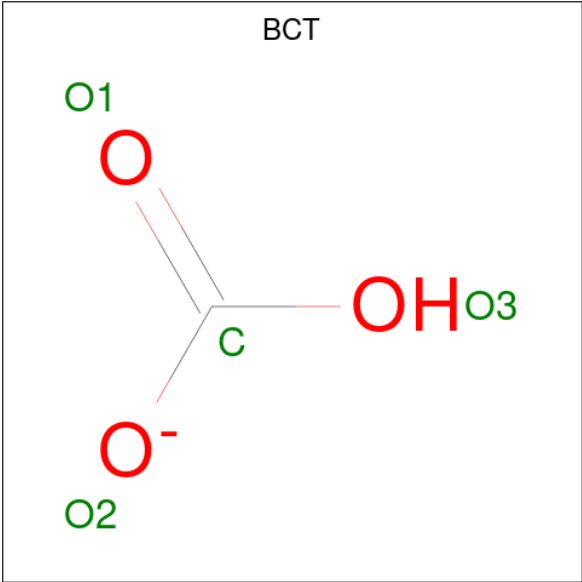
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	B	1	Total	C	O	0	0
			17	15	2		
32	B	1	Total	C	O	0	0
			12	10	2		
32	B	1	Total	C	O	0	0
			18	16	2		
32	B	1	Total	C	O	0	0
			12	10	2		
32	B	1	Total	C		0	0
			16	16			
32	C	1	Total	C	O	0	0
			12	10	2		
32	C	1	Total	C	O	0	0
			12	10	2		
32	C	1	Total	C		0	0
	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

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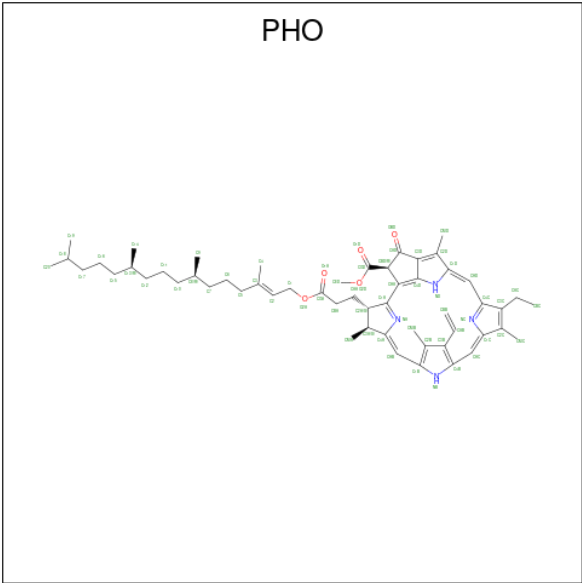
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	T	1	Total C 15 15	0	0
32	T	1	Total C O 20 18 2	0	0
32	X	1	Total C O 20 18 2	0	0
32	a	1	Total C O 12 10 2	0	0
32	b	1	Total C 16 16	0	0
32	b	1	Total C O 20 18 2	0	0
32	b	1	Total C O 16 14 2	0	0
32	b	1	Total C 10 10	0	0
32	c	1	Total C O 20 18 2	0	0
32	c	1	Total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

- Molecule 33 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



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

- Molecule 34 is PHEOPHYTIN A (CCD ID: PHO) (formula: C₅₅H₇₄N₄O₅).



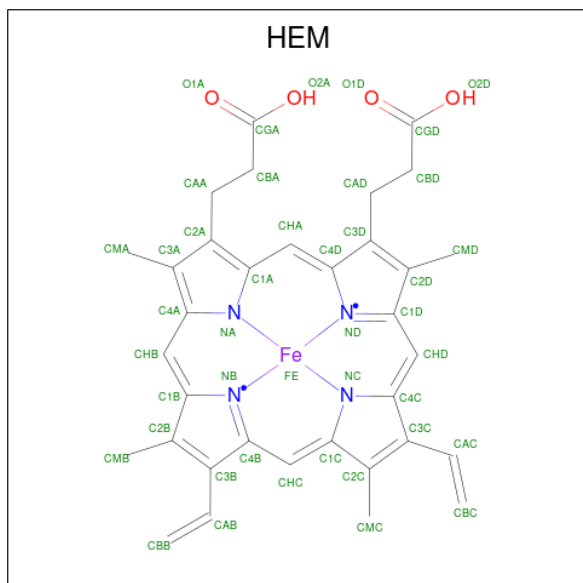
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	D	1	Total	C	N	O	0	0
			64	55	4	5		
34	D	1	Total	C	N	O	0	0
			64	55	4	5		

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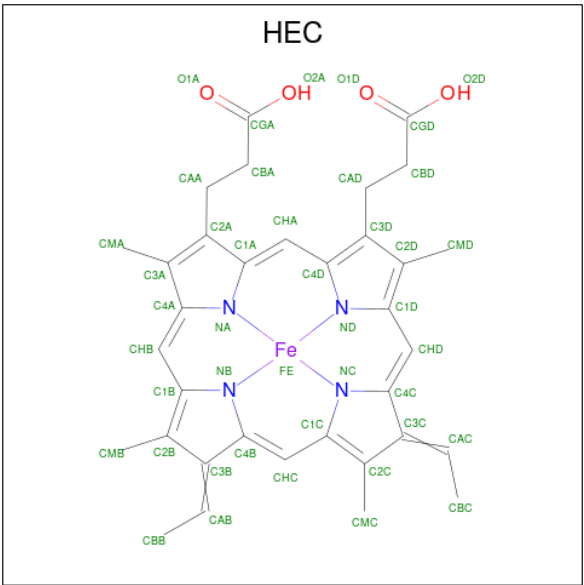
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	d	1	Total 64	C 55	N 4	O 5	0	0
34	d	1	Total 64	C 55	N 4	O 5	0	0

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



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

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



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

- Molecule 37 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	A	140	Total	O	0	4
			144	144		
37	B	208	Total	O	0	0
			208	208		
37	C	199	Total	O	0	0
			199	199		
37	D	134	Total	O	0	0
			134	134		
37	E	31	Total	O	0	0
			31	31		
37	F	8	Total	O	0	0
			8	8		
37	H	30	Total	O	0	0
			30	30		
37	I	16	Total	O	0	0
			16	16		
37	J	12	Total	O	0	0
			12	12		
37	K	5	Total	O	0	0
			5	5		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	L	9	Total 9	O 9	0	0
37	M	11	Total 11	O 11	0	0
37	O	85	Total 85	O 85	0	0
37	T	12	Total 12	O 12	0	0
37	U	41	Total 41	O 41	0	0
37	V	71	Total 71	O 71	0	0
37	Y	5	Total 5	O 5	0	0
37	X	9	Total 9	O 9	0	0
37	Z	5	Total 5	O 5	0	0
37	R	10	Total 10	O 10	0	0
37	a	133	Total 137	O 137	0	4
37	b	199	Total 199	O 199	0	0
37	c	172	Total 172	O 172	0	0
37	d	119	Total 119	O 119	0	0
37	e	32	Total 32	O 32	0	0
37	f	6	Total 6	O 6	0	0
37	h	27	Total 27	O 27	0	0
37	i	15	Total 15	O 15	0	0
37	j	9	Total 9	O 9	0	0
37	k	6	Total 6	O 6	0	0
37	l	9	Total 9	O 9	0	0

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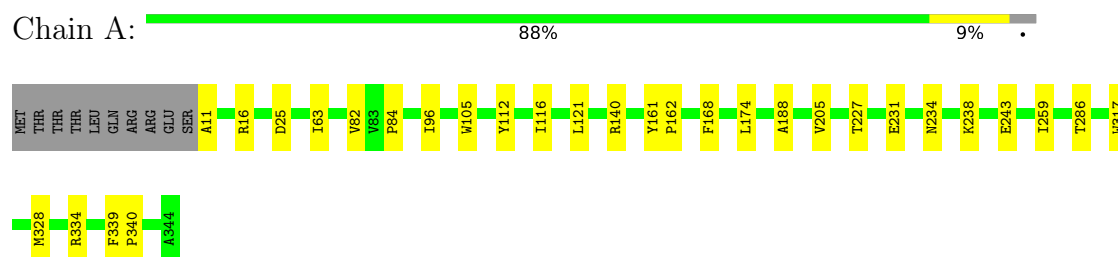
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	m	10	Total 10	O 10	0	0
37	o	102	Total 102	O 102	0	0
37	t	9	Total 9	O 9	0	0
37	u	53	Total 53	O 53	0	0
37	v	57	Total 57	O 57	0	0
37	y	5	Total 5	O 5	0	0
37	x	9	Total 9	O 9	0	0
37	z	3	Total 3	O 3	0	0
37	r	4	Total 4	O 4	0	0

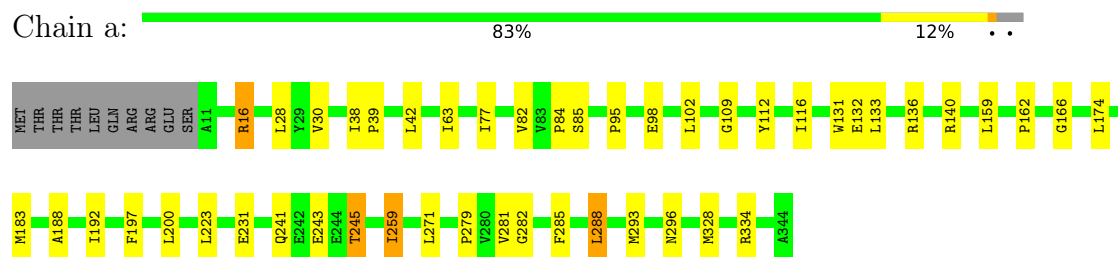
3 Residue-property plots [i](#)

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

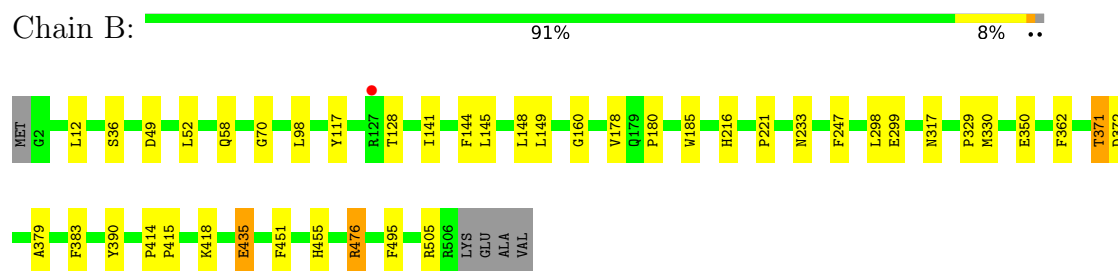
- Molecule 1: Photosystem II protein D1 1



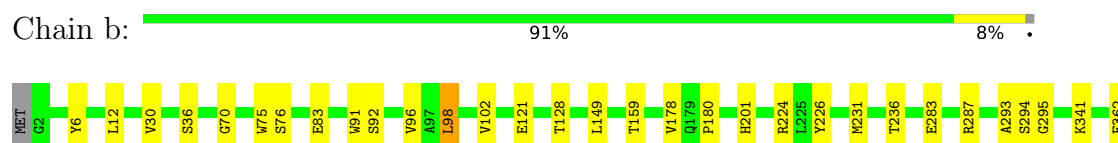
- Molecule 1: Photosystem II protein D1 1



- Molecule 2: Photosystem II CP47 reaction center protein

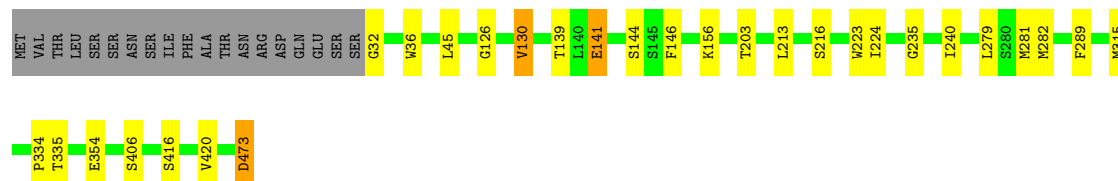
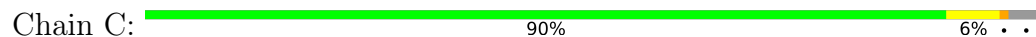


- Molecule 2: Photosystem II CP47 reaction center protein

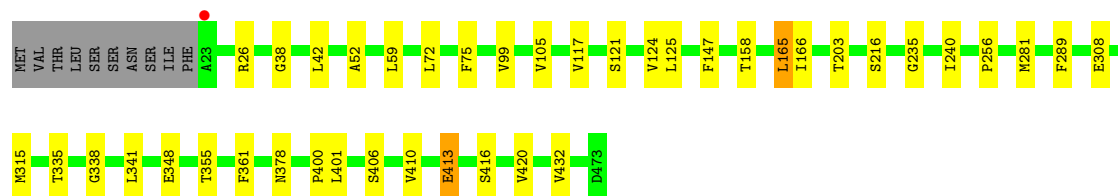
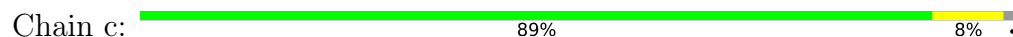




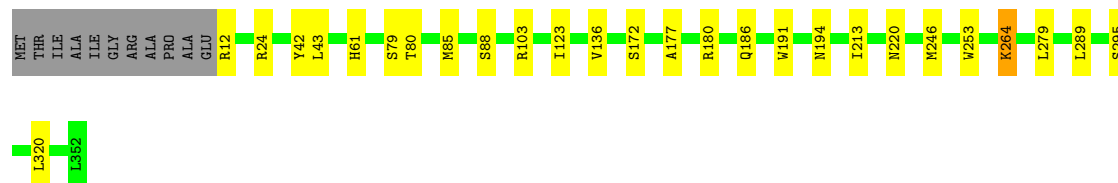
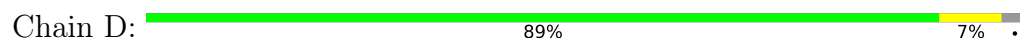
• Molecule 3: Photosystem II CP43 reaction center protein



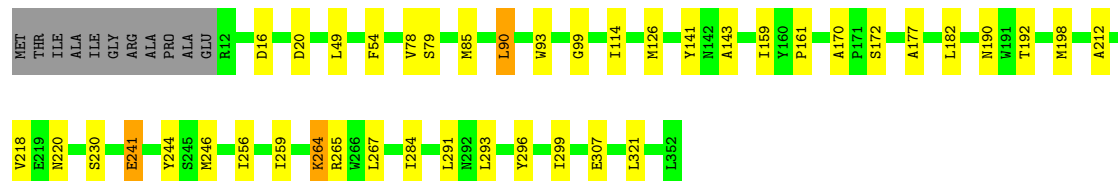
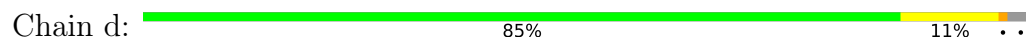
• Molecule 3: Photosystem II CP43 reaction center protein



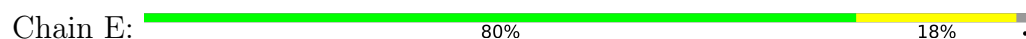
• Molecule 4: Photosystem II D2 protein



• Molecule 4: Photosystem II D2 protein

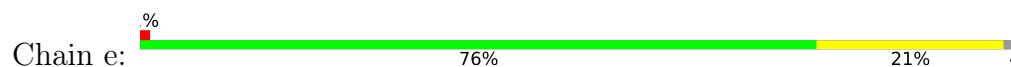


• Molecule 5: Cytochrome b559 subunit alpha





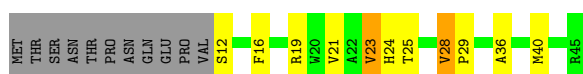
- Molecule 5: Cytochrome b559 subunit alpha



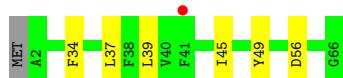
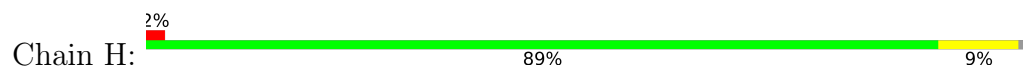
- Molecule 6: Cytochrome b559 subunit beta



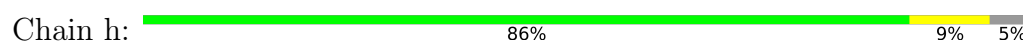
- Molecule 6: Cytochrome b559 subunit beta



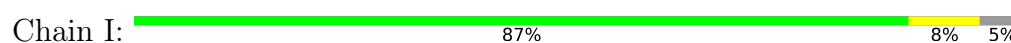
- Molecule 7: Photosystem II reaction center protein H



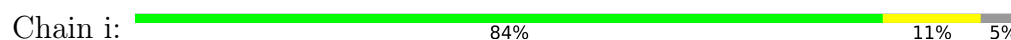
- Molecule 7: Photosystem II reaction center protein H



- Molecule 8: Photosystem II reaction center protein I



- Molecule 8: Photosystem II reaction center protein I





- Molecule 9: Photosystem II reaction center protein J

Chain J: 72% 18% 10%



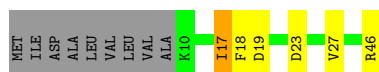
- Molecule 9: Photosystem II reaction center protein J

Chain j: 68% 20% 10%



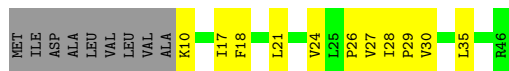
- Molecule 10: Photosystem II reaction center protein K

Chain K: 67% 11% 20%



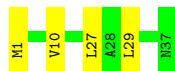
- Molecule 10: Photosystem II reaction center protein K

Chain k: 57% 24% 20%



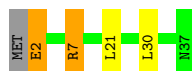
- Molecule 11: Photosystem II reaction center protein L

Chain L: 89% 11%



- Molecule 11: Photosystem II reaction center protein L

Chain l: 86% 5% 5% 5%



- Molecule 12: Photosystem II reaction center protein M

Chain M: 75% 17% 8%



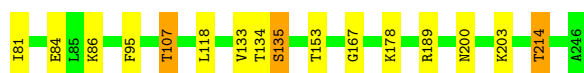
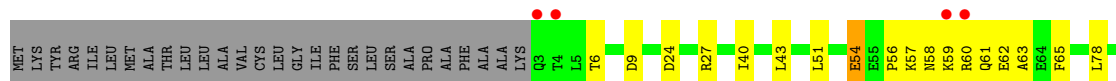
- Molecule 12: Photosystem II reaction center protein M

Chain m: 81% 8% 11%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O: 77% 11% 10%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o: 80% 10% 10%



- Molecule 14: Photosystem II reaction center protein T

Chain T: 3% 81% 12% 6%



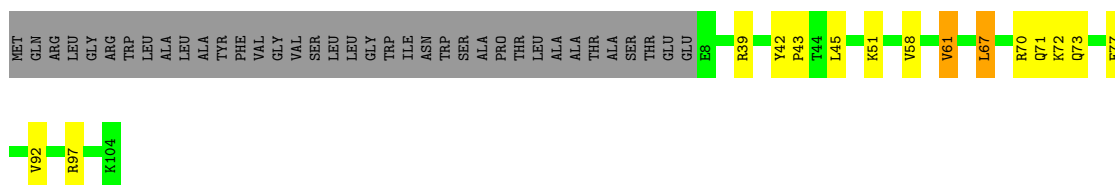
- Molecule 14: Photosystem II reaction center protein T

Chain t: 78% 16% 6%

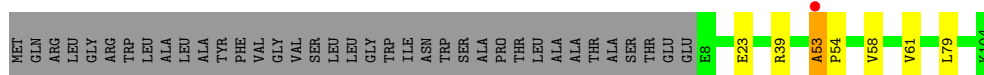


- Molecule 15: Photosystem II 12 kDa extrinsic protein

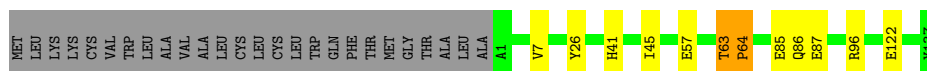
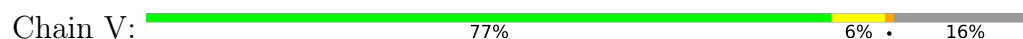
Chain U: 61% 10% 28%



- Molecule 15: Photosystem II 12 kDa extrinsic protein



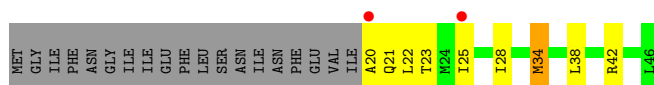
- Molecule 16: Cytochrome c-550



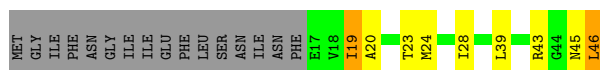
- Molecule 16: Cytochrome c-550



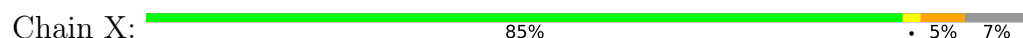
- Molecule 17: Photosystem II reaction center protein Ycf12



- Molecule 17: Photosystem II reaction center protein Ycf12

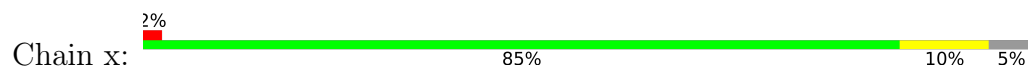


- Molecule 18: Photosystem II reaction center X protein

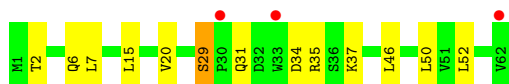
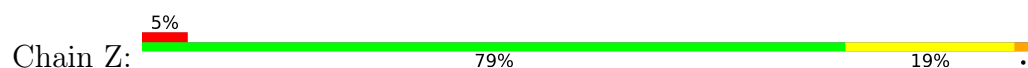




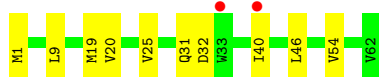
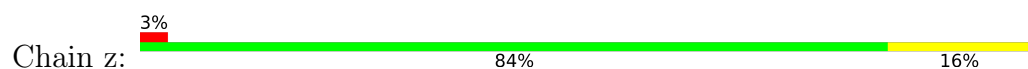
• Molecule 18: Photosystem II reaction center X protein



• Molecule 19: Photosystem II reaction center protein Z



• Molecule 19: Photosystem II reaction center protein Z



• Molecule 20: Photosystem II protein Y



• Molecule 20: Photosystem II protein Y



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	117.33Å 222.79Å 309.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.80 – 2.00 19.80 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (19.80-2.00) 85.5 (19.80-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.39 (at 2.01Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.180 , 0.224 0.180 , 0.225	Depositor DCC
R_{free} test set	4804 reflections (0.76%)	wwPDB-VP
Wilson B-factor (Å ²)	27.6	Xtriage
Anisotropy	0.236	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 47.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	53435	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.31	0/3212	0.49	0/4376
1	a	0.29	0/3209	0.47	0/4372
2	B	0.31	0/4155	0.48	0/5661
2	b	0.30	0/4118	0.45	0/5611
3	C	0.30	0/3625	0.44	0/4935
3	c	0.28	0/3705	0.44	0/5042
4	D	0.33	0/2825	0.49	0/3847
4	d	0.31	0/2834	0.48	0/3859
5	E	0.25	0/688	0.43	0/940
5	e	0.24	0/683	0.43	0/932
6	F	0.26	0/284	0.42	0/387
6	f	0.23	0/284	0.48	0/387
7	H	0.31	0/523	0.46	0/713
7	h	0.26	0/511	0.44	0/697
8	I	0.31	0/293	0.43	0/396
8	i	0.31	0/293	0.41	0/396
9	J	0.25	0/263	0.46	0/356
9	j	0.23	0/263	0.37	0/356
10	K	0.26	0/303	0.41	0/416
10	k	0.26	0/303	0.41	0/416
11	L	0.33	0/311	0.46	0/422
11	l	0.32	0/303	0.47	0/412
12	M	0.30	0/249	0.48	0/341
12	m	0.30	0/244	0.50	0/334
13	O	0.31	0/1904	0.52	0/2585
13	o	0.30	0/1905	0.46	0/2583
14	T	0.34	0/257	0.52	0/349
14	t	0.30	0/255	0.45	0/346
15	U	0.25	0/785	0.47	0/1064
15	u	0.28	0/785	0.48	0/1064
16	V	0.28	0/1085	0.50	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.26	0/1085	0.42	0/1473
17	Y	0.22	0/197	0.35	0/264
17	y	0.20	0/219	0.37	0/294
18	X	0.24	0/284	0.37	0/384
18	x	0.22	0/289	0.28	0/391
19	Z	0.24	0/490	0.44	0/669
19	z	0.30	0/488	0.31	0/666
20	R	0.27	0/277	0.45	0/380
20	r	0.21	0/252	0.37	0/347
All	All	0.30	0/44038	0.46	0/59936

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

Mol	Chain	#Chirality outliers	#Planarity outliers
16	V	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	V	63	THR	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3113	0	2981	21	0
1	a	3110	0	2972	34	0
2	B	4005	0	3871	30	0
2	b	3978	0	3836	34	0
3	C	3509	0	3426	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	c	3583	0	3499	24	0
4	D	2731	0	2637	23	0
4	d	2737	0	2643	29	0
5	E	666	0	651	9	0
5	e	664	0	648	17	0
6	F	275	0	282	4	0
6	f	275	0	282	9	0
7	H	510	0	532	6	0
7	h	498	0	518	5	0
8	I	296	0	311	2	0
8	i	296	0	311	2	0
9	J	257	0	268	4	0
9	j	257	0	268	7	0
10	K	293	0	305	4	0
10	k	293	0	305	5	0
11	L	304	0	316	3	0
11	l	296	0	304	2	0
12	M	256	0	269	4	0
12	m	251	0	267	2	0
13	O	1870	0	1830	21	0
13	o	1874	0	1846	15	0
14	T	258	0	261	4	0
14	t	256	0	256	4	0
15	U	774	0	773	8	0
15	u	774	0	773	3	0
16	V	1064	0	1073	5	0
16	v	1064	0	1073	12	0
17	Y	196	0	217	7	0
17	y	218	0	241	7	0
18	X	281	0	312	3	0
18	x	286	0	314	1	0
19	Z	479	0	516	6	0
19	z	477	0	509	3	0
20	R	271	0	298	3	0
20	r	246	0	263	8	0
21	A	11	0	0	1	0
21	a	11	0	0	1	0
22	A	10	0	0	0	0
22	a	10	0	0	0	0
23	A	1	0	0	0	0
23	a	1	0	0	0	0
24	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	a	2	0	0	0	0
25	A	249	0	264	6	0
25	B	1035	0	1139	38	0
25	C	839	0	922	16	0
25	D	130	0	144	2	0
25	a	260	0	288	7	0
25	b	1035	0	1139	32	0
25	c	839	0	919	26	0
25	d	130	0	144	3	0
26	A	40	0	56	1	0
26	B	120	0	168	6	0
26	C	40	0	56	3	0
26	D	40	0	56	1	0
26	H	40	0	56	0	0
26	K	80	0	112	3	0
26	T	40	0	56	5	0
26	Z	40	0	56	2	0
26	a	40	0	56	1	0
26	b	120	0	168	5	0
26	c	40	0	56	2	0
26	d	40	0	56	3	0
26	k	120	0	168	6	0
26	t	40	0	56	3	0
26	x	40	0	56	2	0
27	A	55	0	80	5	0
27	D	55	0	80	1	0
27	a	55	0	80	4	0
27	d	55	0	80	1	0
28	A	48	0	66	2	0
28	B	28	0	40	0	0
28	C	48	0	66	0	0
28	D	84	0	117	3	0
28	M	51	0	72	2	0
28	b	106	0	158	2	0
28	c	134	0	181	9	0
28	d	67	0	92	0	0
29	A	47	0	67	5	0
29	B	49	0	74	3	0
29	D	49	0	74	1	0
29	E	49	0	74	4	0
29	L	49	0	74	2	0
29	d	137	0	199	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	e	42	0	57	1	0
29	l	49	0	74	1	0
30	A	91	0	136	4	0
30	B	54	0	78	3	0
30	D	36	0	46	2	0
30	a	90	0	134	4	0
30	b	49	0	65	1	0
30	f	41	0	49	2	0
31	A	66	0	96	7	0
31	C	186	0	246	3	0
31	H	62	0	81	3	0
31	c	186	0	246	3	0
31	h	62	0	82	0	0
31	o	44	0	75	3	0
32	B	75	0	117	2	0
32	C	40	0	63	0	0
32	E	12	0	16	0	0
32	H	18	0	35	1	0
32	I	15	0	26	2	0
32	J	12	0	16	0	0
32	M	25	0	38	0	0
32	T	35	0	64	3	0
32	X	20	0	35	1	0
32	a	12	0	16	0	0
32	b	62	0	106	4	0
32	c	32	0	51	3	0
32	d	37	0	61	4	0
32	j	12	0	16	1	0
32	l	18	0	35	2	0
32	m	12	0	16	0	0
32	t	24	0	36	0	0
33	D	4	0	1	1	0
33	a	4	0	1	0	0
34	D	128	0	148	2	0
34	d	128	0	148	2	0
35	F	43	0	30	2	0
35	f	43	0	30	5	0
36	V	43	0	30	0	0
36	v	43	0	30	1	0
37	A	144	0	0	4	0
37	B	208	0	0	0	0
37	C	199	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	D	134	0	0	2	0
37	E	31	0	0	0	0
37	F	8	0	0	0	0
37	H	30	0	0	0	0
37	I	16	0	0	0	0
37	J	12	0	0	1	0
37	K	5	0	0	2	0
37	L	9	0	0	0	0
37	M	11	0	0	0	0
37	O	85	0	0	4	0
37	R	10	0	0	0	0
37	T	12	0	0	0	0
37	U	41	0	0	0	0
37	V	71	0	0	0	0
37	X	9	0	0	0	0
37	Y	5	0	0	0	0
37	Z	5	0	0	0	0
37	a	137	0	0	2	0
37	b	199	0	0	3	0
37	c	172	0	0	1	0
37	d	119	0	0	1	0
37	e	32	0	0	2	0
37	f	6	0	0	1	0
37	h	27	0	0	1	0
37	i	15	0	0	0	0
37	j	9	0	0	0	0
37	k	6	0	0	0	0
37	l	9	0	0	1	0
37	m	10	0	0	1	0
37	o	102	0	0	0	0
37	r	4	0	0	2	0
37	t	9	0	0	0	0
37	u	53	0	0	0	0
37	v	57	0	0	0	0
37	x	9	0	0	0	0
37	y	5	0	0	1	0
37	z	3	0	0	0	0
All	All	53435	0	52752	525	0

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

The worst 5 of 525 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)
4:d:246:MET:HE3	4:d:264:LYS:HD2	1.53	0.91
27:A:610:PL9:H361	6:F:25:THR:HG21	1.53	0.89
25:c:501:CLA:H192	25:c:507:CLA:HBB1	1.57	0.85
5:e:57:ALA:H	5:e:60:GLN:HE21	1.22	0.83
21:a:601[B]:OEY:O6	21:a:601[B]:OEY:O5	1.97	0.81

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	395/344 (115%)	389 (98%)	5 (1%)	1 (0%)	36	35
1	a	395/344 (115%)	388 (98%)	5 (1%)	2 (0%)	24	21
2	B	507/510 (99%)	498 (98%)	9 (2%)	0	100	100
2	b	503/510 (99%)	494 (98%)	8 (2%)	1 (0%)	43	42
3	C	451/461 (98%)	443 (98%)	7 (2%)	1 (0%)	43	42
3	c	461/461 (100%)	453 (98%)	7 (2%)	1 (0%)	43	42
4	D	340/352 (97%)	331 (97%)	9 (3%)	0	100	100
4	d	341/352 (97%)	332 (97%)	9 (3%)	0	100	100
5	E	81/84 (96%)	80 (99%)	1 (1%)	0	100	100
5	e	80/84 (95%)	80 (100%)	0	0	100	100
6	F	32/45 (71%)	32 (100%)	0	0	100	100
6	f	32/45 (71%)	32 (100%)	0	0	100	100
7	H	63/66 (96%)	61 (97%)	2 (3%)	0	100	100
7	h	61/66 (92%)	58 (95%)	3 (5%)	0	100	100
8	I	34/38 (90%)	33 (97%)	1 (3%)	0	100	100
8	i	34/38 (90%)	31 (91%)	3 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	J	34/40 (85%)	32 (94%)	1 (3%)	1 (3%)	3	1
9	j	34/40 (85%)	33 (97%)	1 (3%)	0	100	100
10	K	35/46 (76%)	35 (100%)	0	0	100	100
10	k	35/46 (76%)	35 (100%)	0	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	34/37 (92%)	34 (100%)	0	0	100	100
12	M	31/36 (86%)	31 (100%)	0	0	100	100
12	m	30/36 (83%)	29 (97%)	1 (3%)	0	100	100
13	O	243/272 (89%)	231 (95%)	8 (3%)	4 (2%)	7	3
13	o	242/272 (89%)	236 (98%)	5 (2%)	1 (0%)	30	27
14	T	28/32 (88%)	28 (100%)	0	0	100	100
14	t	28/32 (88%)	28 (100%)	0	0	100	100
15	U	95/134 (71%)	93 (98%)	2 (2%)	0	100	100
15	u	95/134 (71%)	91 (96%)	3 (3%)	1 (1%)	11	7
16	V	135/163 (83%)	131 (97%)	3 (2%)	1 (1%)	18	14
16	v	135/163 (83%)	129 (96%)	6 (4%)	0	100	100
17	Y	25/46 (54%)	24 (96%)	1 (4%)	0	100	100
17	y	28/46 (61%)	28 (100%)	0	0	100	100
18	X	36/41 (88%)	35 (97%)	1 (3%)	0	100	100
18	x	37/41 (90%)	37 (100%)	0	0	100	100
19	Z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
19	z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
20	R	32/41 (78%)	31 (97%)	1 (3%)	0	100	100
20	r	29/41 (71%)	28 (97%)	1 (3%)	0	100	100
All	All	5386/5700 (94%)	5265 (98%)	107 (2%)	14 (0%)	36	35

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
16	V	64	PRO
3	c	416	SER
9	J	7	ARG
13	O	60	ARG

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	322/280 (115%)	319 (99%)	3 (1%)	70	78
1	a	321/280 (115%)	310 (97%)	11 (3%)	32	33
2	B	407/407 (100%)	401 (98%)	6 (2%)	57	64
2	b	402/407 (99%)	395 (98%)	7 (2%)	53	60
3	C	353/362 (98%)	344 (98%)	9 (2%)	42	45
3	c	362/362 (100%)	349 (96%)	13 (4%)	31	31
4	D	277/283 (98%)	274 (99%)	3 (1%)	65	73
4	d	278/283 (98%)	269 (97%)	9 (3%)	34	35
5	E	72/73 (99%)	66 (92%)	6 (8%)	10	7
5	e	71/73 (97%)	68 (96%)	3 (4%)	26	25
6	F	28/39 (72%)	27 (96%)	1 (4%)	31	31
6	f	28/39 (72%)	26 (93%)	2 (7%)	13	10
7	H	54/55 (98%)	53 (98%)	1 (2%)	50	56
7	h	53/55 (96%)	52 (98%)	1 (2%)	50	56
8	I	32/34 (94%)	31 (97%)	1 (3%)	35	37
8	i	32/34 (94%)	30 (94%)	2 (6%)	16	13
9	J	24/28 (86%)	24 (100%)	0	100	100
9	j	24/28 (86%)	23 (96%)	1 (4%)	26	25
10	K	30/37 (81%)	27 (90%)	3 (10%)	7	4
10	k	30/37 (81%)	27 (90%)	3 (10%)	7	4
11	L	35/35 (100%)	34 (97%)	1 (3%)	37	40
11	l	34/35 (97%)	30 (88%)	4 (12%)	5	3
12	M	28/32 (88%)	26 (93%)	2 (7%)	13	10
12	m	28/32 (88%)	27 (96%)	1 (4%)	31	31
13	O	206/228 (90%)	199 (97%)	7 (3%)	32	33
13	o	207/228 (91%)	201 (97%)	6 (3%)	37	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	T	26/28 (93%)	26 (100%)	0	100	100
14	t	25/28 (89%)	24 (96%)	1 (4%)	28	27
15	U	84/112 (75%)	80 (95%)	4 (5%)	23	21
15	u	84/112 (75%)	82 (98%)	2 (2%)	43	47
16	V	117/138 (85%)	114 (97%)	3 (3%)	40	44
16	v	117/138 (85%)	114 (97%)	3 (3%)	40	44
17	Y	19/37 (51%)	18 (95%)	1 (5%)	20	18
17	y	22/37 (60%)	19 (86%)	3 (14%)	3	2
18	X	31/34 (91%)	29 (94%)	2 (6%)	15	12
18	x	31/34 (91%)	28 (90%)	3 (10%)	8	5
19	Z	52/52 (100%)	45 (86%)	7 (14%)	4	2
19	z	51/52 (98%)	45 (88%)	6 (12%)	5	3
20	R	28/33 (85%)	26 (93%)	2 (7%)	13	10
20	r	25/33 (76%)	21 (84%)	4 (16%)	2	1
All	All	4450/4654 (96%)	4303 (97%)	147 (3%)	33	34

5 of 147 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	l	7	ARG
20	r	9	LEU
13	o	49	THR
16	v	107	LEU
16	V	57	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
1	a	19	ASN
13	o	155	ASN
2	b	394	GLN
19	z	31	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	$\# Z > 2$
8	FME	i	1	8	8,9,10	0.95	0	8,9,11	0.94	0
14	FME	t	1	14	8,9,10	1.09	0	8,9,11	1.01	0
12	FME	M	1	12	8,9,10	1.01	0	8,9,11	0.82	0
14	FME	T	1	14	8,9,10	1.07	0	8,9,11	0.77	0
12	FME	m	1	12	8,9,10	0.95	0	8,9,11	0.85	0
8	FME	I	1	8	8,9,10	0.99	0	8,9,11	0.89	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	FME	i	1	8	-	0/7/9/11	-
14	FME	t	1	14	-	4/7/9/11	-
12	FME	M	1	12	-	0/7/9/11	-
14	FME	T	1	14	-	1/7/9/11	-
12	FME	m	1	12	-	0/7/9/11	-
8	FME	I	1	8	-	0/7/9/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 188 ligands modelled in this entry, 6 are monoatomic - leaving 182 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	$\# Z > 2$
25	CLA	B	615	-	69,73,73	1.41	9 (13%)	82,113,113	1.23	7 (8%)
26	BCR	k	102	-	41,41,41	1.04	2 (4%)	56,56,56	1.06	2 (3%)
25	CLA	b	613	-	69,73,73	1.29	7 (10%)	82,113,113	1.54	14 (17%)
29	LHG	d	407	-	48,48,48	0.76	2 (4%)	51,54,54	1.34	6 (11%)
25	CLA	B	603	-	69,73,73	1.21	7 (10%)	82,113,113	1.39	9 (10%)
25	CLA	C	504	37	63,67,73	1.20	8 (12%)	74,105,113	1.28	9 (12%)
25	CLA	c	507	37	69,73,73	1.25	8 (11%)	82,113,113	1.42	8 (9%)
25	CLA	B	616	-	64,68,73	1.29	6 (9%)	76,107,113	1.32	5 (6%)
25	CLA	C	506	-	69,73,73	1.24	8 (11%)	82,113,113	1.16	6 (7%)
25	CLA	a	608	37	69,73,73	1.17	6 (8%)	82,113,113	1.23	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	LMG	d	411	-	44,44,55	0.81	1 (2%)	52,52,63	1.33	6 (11%)
36	HEC	v	201	16	46,50,50	1.90	6 (13%)	58,82,82	1.75	6 (10%)
32	STE	E	102	-	11,11,19	0.74	0	11,11,19	1.16	1 (9%)
26	BCR	B	618	-	41,41,41	1.01	2 (4%)	56,56,56	1.20	6 (10%)
34	PHO	D	403	-	58,69,69	2.14	9 (15%)	55,99,99	1.39	8 (14%)
29	LHG	A	613	-	46,46,48	0.86	2 (4%)	49,52,54	1.24	4 (8%)
25	CLA	a	607	-	69,73,73	1.50	11 (15%)	82,113,113	1.37	6 (7%)
26	BCR	B	619	-	41,41,41	1.04	2 (4%)	56,56,56	1.25	4 (7%)
32	STE	I	101	-	14,14,19	0.35	0	13,13,19	0.80	0
25	CLA	B	604	-	69,73,73	1.24	7 (10%)	82,113,113	1.45	7 (8%)
25	CLA	B	612	-	69,73,73	1.07	6 (8%)	82,113,113	1.41	12 (14%)
27	PL9	d	406	-	55,55,55	1.20	4 (7%)	68,69,69	1.63	14 (20%)
25	CLA	C	505	-	69,73,73	1.31	6 (8%)	82,113,113	1.35	9 (10%)
26	BCR	a	610	-	41,41,41	0.91	1 (2%)	56,56,56	1.28	6 (10%)
31	DGD	o	301	-	43,43,67	0.80	3 (6%)	45,45,81	1.43	6 (13%)
36	HEC	V	201	16	46,50,50	1.81	5 (10%)	58,82,82	1.82	6 (10%)
25	CLA	c	502	-	69,73,73	1.30	7 (10%)	82,113,113	1.26	9 (10%)
32	STE	t	102	-	13,13,19	0.68	0	13,13,19	1.20	1 (7%)
28	LMG	C	518	-	48,48,55	0.80	1 (2%)	56,56,63	1.33	8 (14%)
25	CLA	b	616	-	64,68,73	1.21	7 (10%)	76,107,113	1.42	10 (13%)
30	SQD	a	613	-	52,54,54	1.57	7 (13%)	62,65,65	1.83	12 (19%)
32	STE	C	520	-	11,11,19	0.72	0	11,11,19	1.19	1 (9%)
32	STE	T	102	-	14,14,19	0.31	0	13,13,19	0.99	0
26	BCR	b	619	-	41,41,41	0.99	2 (4%)	56,56,56	1.12	3 (5%)
32	STE	b	625	-	15,15,19	0.73	0	15,15,19	0.93	0
25	CLA	B	608	-	69,73,73	1.20	7 (10%)	82,113,113	1.36	10 (12%)
26	BCR	t	101	-	41,41,41	0.99	2 (4%)	56,56,56	1.30	6 (10%)
25	CLA	C	503	-	69,73,73	1.33	10 (14%)	82,113,113	1.61	9 (10%)
29	LHG	d	409	-	38,38,48	0.82	1 (2%)	41,44,54	1.09	2 (4%)
32	STE	B	627	-	15,15,19	0.37	0	14,14,19	0.78	0
26	BCR	C	514	-	41,41,41	1.06	2 (4%)	56,56,56	1.15	6 (10%)
31	DGD	C	515	-	63,63,67	1.00	4 (6%)	77,77,81	1.36	8 (10%)
25	CLA	a	609	-	69,73,73	1.23	7 (10%)	82,113,113	1.24	6 (7%)
26	BCR	k	101	-	41,41,41	1.09	2 (4%)	56,56,56	1.26	5 (8%)
25	CLA	D	405	-	69,73,73	1.33	8 (11%)	82,113,113	1.21	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	c	505	-	69,73,73	1.27	9 (13%)	82,113,113	1.21	8 (9%)
25	CLA	c	508	-	68,72,73	1.24	8 (11%)	80,111,113	1.36	8 (10%)
25	CLA	C	512	-	69,73,73	1.41	10 (14%)	82,113,113	1.29	7 (8%)
25	CLA	b	607	37	69,73,73	1.19	6 (8%)	82,113,113	1.24	5 (6%)
33	BCT	D	401	23	3,3,3	1.00	0	2,3,3	3.32	1 (50%)
27	PL9	D	407	-	55,55,55	0.93	3 (5%)	68,69,69	1.66	14 (20%)
31	DGD	c	515	-	63,63,67	1.00	4 (6%)	77,77,81	1.40	12 (15%)
29	LHG	E	101	-	48,48,48	0.77	2 (4%)	51,54,54	1.26	6 (11%)
25	CLA	b	611	-	69,73,73	1.24	5 (7%)	82,113,113	1.31	7 (8%)
26	BCR	T	101	-	41,41,41	0.94	2 (4%)	56,56,56	1.25	7 (12%)
28	LMG	b	622	-	51,51,55	0.87	1 (1%)	59,59,63	1.42	7 (11%)
25	CLA	c	504	37	64,68,73	1.13	5 (7%)	76,107,113	1.30	9 (11%)
25	CLA	b	608	-	69,73,73	1.33	9 (13%)	82,113,113	1.36	14 (17%)
25	CLA	A	607	37	69,73,73	1.31	7 (10%)	82,113,113	1.38	9 (10%)
26	BCR	b	618	-	41,41,41	1.15	2 (4%)	56,56,56	1.14	5 (8%)
30	SQD	D	409	-	34,36,54	1.51	5 (14%)	42,45,65	3.17	12 (28%)
32	STE	t	103	-	9,9,19	0.36	0	8,8,19	0.78	0
25	CLA	B	610	37	69,73,73	1.34	11 (15%)	82,113,113	1.28	9 (10%)
25	CLA	B	601	37	69,73,73	1.37	9 (13%)	82,113,113	1.42	8 (9%)
32	STE	m	101	-	11,11,19	0.71	0	11,11,19	1.19	1 (9%)
25	CLA	c	506	-	69,73,73	1.35	9 (13%)	82,113,113	1.27	7 (8%)
26	BCR	D	406	-	41,41,41	1.03	2 (4%)	56,56,56	1.08	3 (5%)
32	STE	M	103	-	9,9,19	0.36	0	8,8,19	0.76	0
25	CLA	A	608	-	58,62,73	1.21	6 (10%)	68,99,113	1.32	5 (7%)
29	LHG	l	101	-	48,48,48	0.70	1 (2%)	51,54,54	1.22	4 (7%)
35	HEM	f	101	5,6	50,50,50	1.59	8 (16%)	67,82,82	1.29	8 (11%)
32	STE	j	101	-	11,11,19	0.77	0	11,11,19	1.07	0
26	BCR	K	102	-	41,41,41	1.01	2 (4%)	56,56,56	1.06	3 (5%)
25	CLA	b	603	-	69,73,73	1.24	9 (13%)	82,113,113	1.35	10 (12%)
25	CLA	B	602	-	69,73,73	1.22	8 (11%)	82,113,113	1.30	10 (12%)
25	CLA	c	513	-	69,73,73	1.23	7 (10%)	82,113,113	1.22	7 (8%)
28	LMG	D	408	-	51,51,55	0.85	2 (3%)	59,59,63	1.32	5 (8%)
32	STE	T	103	-	19,19,19	0.59	0	19,19,19	1.07	1 (5%)
26	BCR	d	405	-	41,41,41	1.10	2 (4%)	56,56,56	1.23	5 (8%)
25	CLA	b	615	-	69,73,73	1.44	9 (13%)	82,113,113	1.41	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	SQD	B	623	-	52,54,54	1.59	9 (17%)	62,65,65	1.65	11 (17%)
25	CLA	B	613	-	69,73,73	1.18	8 (11%)	82,113,113	1.40	9 (10%)
25	CLA	a	612	37	69,73,73	1.50	9 (13%)	82,113,113	1.36	9 (10%)
25	CLA	d	403	-	69,73,73	1.21	6 (8%)	82,113,113	1.22	5 (6%)
35	HEM	F	101	5,6	50,50,50	1.46	7 (14%)	67,82,82	1.15	3 (4%)
25	CLA	b	609	-	69,73,73	1.29	9 (13%)	82,113,113	1.32	6 (7%)
32	STE	c	521	-	11,11,19	0.73	0	11,11,19	1.15	1 (9%)
25	CLA	b	610	37	69,73,73	1.27	7 (10%)	82,113,113	1.37	11 (13%)
25	CLA	c	501	-	69,73,73	1.13	4 (5%)	82,113,113	1.33	6 (7%)
26	BCR	b	617	-	41,41,41	1.02	3 (7%)	56,56,56	1.27	4 (7%)
25	CLA	B	607	37	69,73,73	1.15	6 (8%)	82,113,113	1.34	8 (9%)
32	STE	B	624	-	11,11,19	0.76	0	11,11,19	1.27	0
26	BCR	K	101	-	41,41,41	1.04	2 (4%)	56,56,56	1.16	5 (8%)
31	DGD	C	517	-	63,63,67	0.92	2 (3%)	77,77,81	1.38	10 (12%)
29	LHG	D	410	-	48,48,48	0.82	2 (4%)	51,54,54	1.24	7 (13%)
25	CLA	b	601	37	69,73,73	1.25	7 (10%)	82,113,113	1.37	5 (6%)
30	SQD	b	620	-	47,49,54	1.63	9 (19%)	57,60,65	1.75	10 (17%)
25	CLA	c	510	-	69,73,73	1.35	8 (11%)	82,113,113	1.31	8 (9%)
32	STE	H	103	-	17,17,19	0.36	0	16,16,19	0.88	0
25	CLA	B	609	-	69,73,73	1.21	6 (8%)	82,113,113	1.34	8 (9%)
33	BCT	a	606	23	3,3,3	1.12	0	2,3,3	3.07	1 (50%)
25	CLA	c	503	-	69,73,73	1.26	10 (14%)	82,113,113	1.44	7 (8%)
21	OEY	A	601[B]	3,37,1	0,16,16	-	-	-	-	-
32	STE	b	621	-	15,15,19	0.35	0	14,14,19	0.82	0
29	LHG	d	408	-	48,48,48	0.70	1 (2%)	51,54,54	1.24	6 (11%)
22	OEX	A	602[A]	3,37,1	0,15,15	-	-	-	-	-
25	CLA	b	602	-	69,73,73	1.09	6 (8%)	82,113,113	1.33	10 (12%)
30	SQD	f	102	-	39,41,54	1.69	8 (20%)	49,52,65	1.69	11 (22%)
28	LMG	B	621	-	26,26,55	0.68	1 (3%)	26,26,63	1.23	2 (7%)
25	CLA	B	605	-	69,73,73	1.13	6 (8%)	82,113,113	1.28	7 (8%)
25	CLA	d	404	-	69,73,73	1.26	10 (14%)	82,113,113	1.18	4 (4%)
31	DGD	h	101	-	63,63,67	0.97	3 (4%)	77,77,81	1.40	11 (14%)
32	STE	B	625	-	17,17,19	0.61	0	17,17,19	1.16	0
28	LMG	b	624	-	55,55,55	0.78	3 (5%)	63,63,63	1.41	10 (15%)
25	CLA	C	511	3	69,73,73	1.31	6 (8%)	82,113,113	1.40	8 (9%)
32	STE	J	101	-	11,11,19	0.73	0	11,11,19	1.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	b	604	-	69,73,73	1.13	7 (10%)	82,113,113	1.46	10 (12%)
25	CLA	C	509	-	69,73,73	1.20	7 (10%)	82,113,113	1.25	8 (9%)
32	STE	c	519	-	19,19,19	0.60	0	19,19,19	1.01	0
25	CLA	C	501	-	69,73,73	1.46	10 (14%)	82,113,113	1.34	5 (6%)
29	LHG	L	101	-	48,48,48	0.76	1 (2%)	51,54,54	1.19	4 (7%)
32	STE	d	413	-	19,19,19	0.65	0	19,19,19	1.03	1 (5%)
32	STE	b	623	-	19,19,19	0.65	0	19,19,19	0.99	0
34	PHO	d	401	-	58,69,69	2.07	10 (17%)	55,99,99	1.31	5 (9%)
31	DGD	C	516	-	63,63,67	1.06	6 (9%)	77,77,81	1.36	14 (18%)
25	CLA	c	509	-	69,73,73	1.14	6 (8%)	82,113,113	1.40	8 (9%)
26	BCR	H	101	-	41,41,41	0.98	2 (4%)	56,56,56	1.20	5 (8%)
26	BCR	c	514	-	41,41,41	1.15	3 (7%)	56,56,56	1.22	6 (10%)
28	LMG	M	101	-	51,51,55	0.86	3 (5%)	59,59,63	1.36	5 (8%)
32	STE	d	412	-	16,16,19	0.58	0	16,16,19	1.23	1 (6%)
30	SQD	A	614	-	50,52,54	1.57	8 (16%)	60,63,65	1.91	11 (18%)
28	LMG	c	520	-	48,48,55	0.98	5 (10%)	56,56,63	1.29	7 (12%)
31	DGD	c	516	-	63,63,67	1.01	2 (3%)	77,77,81	1.37	10 (12%)
25	CLA	c	511	3	69,73,73	1.50	7 (10%)	82,113,113	1.42	6 (7%)
25	CLA	b	605	-	69,73,73	1.34	7 (10%)	82,113,113	1.41	9 (10%)
29	LHG	B	622	-	48,48,48	0.80	1 (2%)	51,54,54	1.32	7 (13%)
32	STE	X	101	-	19,19,19	0.59	0	19,19,19	1.17	0
26	BCR	x	101	-	41,41,41	1.00	2 (4%)	56,56,56	1.23	5 (8%)
32	STE	l	102	-	17,17,19	0.31	0	16,16,19	0.95	0
26	BCR	Z	101	-	41,41,41	1.06	2 (4%)	56,56,56	1.13	4 (7%)
26	BCR	A	609	-	41,41,41	0.94	2 (4%)	56,56,56	1.29	6 (10%)
25	CLA	B	611	-	69,73,73	1.29	7 (10%)	82,113,113	1.33	5 (6%)
25	CLA	b	614	-	69,73,73	1.20	7 (10%)	82,113,113	1.25	8 (9%)
34	PHO	D	402	-	58,69,69	1.94	11 (18%)	55,99,99	1.38	6 (10%)
25	CLA	C	513	-	69,73,73	1.14	7 (10%)	82,113,113	1.41	7 (8%)
25	CLA	b	606	-	69,73,73	1.45	5 (7%)	82,113,113	1.42	7 (8%)
31	DGD	H	102	-	63,63,67	1.20	7 (11%)	77,77,81	1.37	10 (12%)
32	STE	B	626	-	11,11,19	0.69	0	11,11,19	1.34	1 (9%)
30	SQD	A	615	-	38,38,54	1.75	5 (13%)	40,40,65	1.24	3 (7%)
22	OEX	a	602[A]	3,37,1	0,15,15	-	-	-	-	-
25	CLA	B	614	-	69,73,73	1.13	6 (8%)	82,113,113	1.43	9 (10%)
28	LMG	c	518	-	37,37,55	0.99	3 (8%)	45,45,63	1.34	5 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	A	606	-	69,73,73	1.36	9 (13%)	82,113,113	1.19	6 (7%)
25	CLA	C	510	-	69,73,73	1.15	7 (10%)	82,113,113	1.35	8 (9%)
32	STE	a	615	-	11,11,19	0.80	0	11,11,19	1.16	1 (9%)
31	DGD	c	517	-	63,63,67	0.86	1 (1%)	77,77,81	1.34	7 (9%)
34	PHO	d	402	-	58,69,69	2.16	9 (15%)	55,99,99	1.51	8 (14%)
30	SQD	a	614	-	35,35,54	1.69	5 (14%)	37,37,65	1.51	6 (16%)
27	PL9	a	611	-	55,55,55	0.68	1 (1%)	68,69,69	1.53	10 (14%)
25	CLA	C	508	-	69,73,73	1.21	8 (11%)	82,113,113	1.40	13 (15%)
28	LMG	d	410	-	21,21,55	0.52	0	20,20,63	1.28	3 (15%)
28	LMG	c	522	-	49,49,55	0.89	4 (8%)	57,57,63	1.27	3 (5%)
25	CLA	b	612	-	69,73,73	1.32	10 (14%)	82,113,113	1.40	10 (12%)
32	STE	B	620	-	16,16,19	0.69	0	16,16,19	1.09	0
32	STE	C	519	-	11,11,19	0.69	0	11,11,19	1.44	1 (9%)
25	CLA	D	404	-	69,73,73	1.18	6 (8%)	82,113,113	1.35	9 (10%)
26	BCR	k	103	-	41,41,41	1.05	2 (4%)	56,56,56	1.17	4 (7%)
26	BCR	B	617	-	41,41,41	1.02	3 (7%)	56,56,56	1.20	5 (8%)
25	CLA	C	507	37	69,73,73	1.21	6 (8%)	82,113,113	1.37	10 (12%)
21	OEY	a	601[B]	3,37,1	0,16,16	-	-	-	-	-
27	PL9	A	610	-	55,55,55	0.85	1 (1%)	68,69,69	1.47	12 (17%)
25	CLA	B	606	-	69,73,73	1.47	8 (11%)	82,113,113	1.40	6 (7%)
25	CLA	A	611	37	69,73,73	1.43	10 (14%)	82,113,113	1.35	6 (7%)
31	DGD	A	616	-	67,67,67	1.10	7 (10%)	81,81,81	1.31	8 (9%)
32	STE	b	626	-	9,9,19	0.35	0	8,8,19	0.72	0
32	STE	C	521	-	15,15,19	0.31	0	14,14,19	0.93	0
29	LHG	e	101	-	41,41,48	0.76	1 (2%)	44,47,54	1.35	6 (13%)
32	STE	M	102	-	14,14,19	0.76	0	14,14,19	1.05	0
28	LMG	A	612	-	48,48,55	0.95	4 (8%)	56,56,63	1.23	3 (5%)
28	LMG	D	411	-	31,31,55	0.71	1 (3%)	33,33,63	1.25	3 (9%)
25	CLA	C	502	-	69,73,73	1.16	7 (10%)	82,113,113	1.25	5 (6%)
25	CLA	c	512	-	69,73,73	1.21	7 (10%)	82,113,113	1.31	7 (8%)

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
25	CLA	B	615	-	1/1/15/20	11/39/115/115	-
26	BCR	k	102	-	-	7/29/63/63	0/2/2/2
25	CLA	b	613	-	1/1/15/20	14/39/115/115	-
29	LHG	d	407	-	-	18/53/53/53	-
25	CLA	B	603	-	1/1/15/20	5/39/115/115	-
25	CLA	C	504	37	1/1/13/20	6/32/108/115	-
25	CLA	c	507	37	1/1/15/20	8/39/115/115	-
25	CLA	B	616	-	1/1/14/20	7/33/109/115	-
25	CLA	C	506	-	1/1/15/20	11/39/115/115	-
25	CLA	a	608	37	-	10/39/115/115	-
28	LMG	d	411	-	-	13/39/59/70	0/1/1/1
36	HEC	v	201	16	-	6/14/54/54	-
32	STE	E	102	-	-	6/9/9/17	-
26	BCR	B	618	-	-	2/29/63/63	0/2/2/2
34	PHO	D	403	-	-	1/37/103/103	0/5/6/6
29	LHG	A	613	-	-	18/51/51/53	-
25	CLA	a	607	-	1/1/15/20	3/39/115/115	-
26	BCR	B	619	-	-	6/29/63/63	0/2/2/2
32	STE	I	101	-	-	3/12/12/17	-
25	CLA	B	604	-	1/1/15/20	11/39/115/115	-
25	CLA	B	612	-	1/1/15/20	9/39/115/115	-
27	PL9	d	406	-	-	13/53/73/73	0/1/1/1
25	CLA	C	505	-	1/1/15/20	10/39/115/115	-
26	BCR	a	610	-	-	1/29/63/63	0/2/2/2
31	DGD	o	301	-	-	19/45/45/95	-
36	HEC	V	201	16	-	6/14/54/54	-
25	CLA	c	502	-	1/1/15/20	2/39/115/115	-
32	STE	t	102	-	-	3/11/11/17	-
28	LMG	C	518	-	-	20/43/63/70	0/1/1/1
25	CLA	b	616	-	1/1/14/20	5/33/109/115	-
30	SQD	a	613	-	-	24/49/69/69	0/1/1/1
32	STE	C	520	-	-	4/9/9/17	-
32	STE	T	102	-	-	9/12/12/17	-
26	BCR	b	619	-	-	1/29/63/63	0/2/2/2
32	STE	b	625	-	-	6/13/13/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	B	608	-	1/1/15/20	6/39/115/115	-
26	BCR	t	101	-	-	8/29/63/63	0/2/2/2
25	CLA	C	503	-	1/1/15/20	3/39/115/115	-
29	LHG	d	409	-	-	9/43/43/53	-
32	STE	B	627	-	-	7/13/13/17	-
26	BCR	C	514	-	-	1/29/63/63	0/2/2/2
31	DGD	C	515	-	-	24/51/91/95	0/2/2/2
25	CLA	a	609	-	1/1/15/20	7/39/115/115	-
26	BCR	k	101	-	-	8/29/63/63	0/2/2/2
25	CLA	c	505	-	1/1/15/20	8/39/115/115	-
25	CLA	D	405	-	-	6/39/115/115	-
25	CLA	c	508	-	-	3/38/114/115	-
25	CLA	C	512	-	1/1/15/20	17/39/115/115	-
25	CLA	b	607	37	1/1/15/20	13/39/115/115	-
27	PL9	D	407	-	-	13/53/73/73	0/1/1/1
31	DGD	c	515	-	-	26/51/91/95	0/2/2/2
29	LHG	E	101	-	-	23/53/53/53	-
25	CLA	b	611	-	1/1/15/20	4/39/115/115	-
26	BCR	T	101	-	-	6/29/63/63	0/2/2/2
28	LMG	b	622	-	-	17/46/66/70	0/1/1/1
25	CLA	c	504	37	1/1/14/20	7/33/109/115	-
25	CLA	b	608	-	1/1/15/20	6/39/115/115	-
25	CLA	A	607	37	1/1/15/20	12/39/115/115	-
26	BCR	b	618	-	-	1/29/63/63	0/2/2/2
30	SQD	D	409	-	-	13/28/48/69	0/1/1/1
32	STE	t	103	-	-	3/7/7/17	-
25	CLA	B	610	37	1/1/15/20	5/39/115/115	-
25	CLA	B	601	37	1/1/15/20	20/39/115/115	-
32	STE	m	101	-	-	4/9/9/17	-
25	CLA	c	506	-	1/1/15/20	15/39/115/115	-
26	BCR	D	406	-	-	6/29/63/63	0/2/2/2
32	STE	M	103	-	-	5/7/7/17	-
25	CLA	A	608	-	1/1/12/20	3/26/102/115	-
29	LHG	l	101	-	-	15/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	HEM	f	101	5,6	-	4/14/54/54	-
32	STE	j	101	-	-	5/9/9/17	-
26	BCR	K	102	-	-	7/29/63/63	0/2/2/2
25	CLA	b	603	-	1/1/15/20	15/39/115/115	-
25	CLA	B	602	-	1/1/15/20	8/39/115/115	-
25	CLA	c	513	-	1/1/15/20	5/39/115/115	-
28	LMG	D	408	-	-	18/46/66/70	0/1/1/1
32	STE	T	103	-	-	8/17/17/17	-
26	BCR	d	405	-	-	6/29/63/63	0/2/2/2
25	CLA	b	615	-	1/1/15/20	9/39/115/115	-
30	SQD	B	623	-	-	21/49/69/69	0/1/1/1
25	CLA	B	613	-	1/1/15/20	11/39/115/115	-
25	CLA	d	403	-	1/1/15/20	8/39/115/115	-
25	CLA	a	612	37	-	2/39/115/115	-
35	HEM	F	101	5,6	-	2/14/54/54	-
25	CLA	b	609	-	-	6/39/115/115	-
32	STE	c	521	-	-	4/9/9/17	-
25	CLA	b	610	37	1/1/15/20	6/39/115/115	-
25	CLA	c	501	-	1/1/15/20	5/39/115/115	-
26	BCR	b	617	-	-	4/29/63/63	0/2/2/2
25	CLA	B	607	37	1/1/15/20	5/39/115/115	-
32	STE	B	624	-	-	5/9/9/17	-
26	BCR	K	101	-	-	3/29/63/63	0/2/2/2
31	DGD	C	517	-	-	16/51/91/95	0/2/2/2
29	LHG	D	410	-	-	20/53/53/53	-
25	CLA	b	601	37	1/1/15/20	15/39/115/115	-
30	SQD	b	620	-	-	20/44/64/69	0/1/1/1
25	CLA	c	510	-	1/1/15/20	9/39/115/115	-
32	STE	H	103	-	-	10/15/15/17	-
25	CLA	B	609	-	-	2/39/115/115	-
25	CLA	c	503	-	1/1/15/20	7/39/115/115	-
32	STE	b	621	-	-	10/13/13/17	-
29	LHG	d	408	-	-	21/53/53/53	-
25	CLA	b	602	-	1/1/15/20	9/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	SQD	f	102	-	-	17/36/56/69	0/1/1/1
28	LMG	B	621	-	-	5/22/22/70	-
25	CLA	B	605	-	1/1/15/20	10/39/115/115	-
25	CLA	d	404	-	1/1/15/20	7/39/115/115	-
31	DGD	h	101	-	-	14/51/91/95	0/2/2/2
32	STE	B	625	-	-	9/15/15/17	-
28	LMG	b	624	-	-	24/50/70/70	0/1/1/1
25	CLA	C	511	3	1/1/15/20	4/39/115/115	-
32	STE	J	101	-	-	7/9/9/17	-
25	CLA	b	604	-	1/1/15/20	7/39/115/115	-
25	CLA	C	509	-	1/1/15/20	14/39/115/115	-
32	STE	c	519	-	-	10/17/17/17	-
25	CLA	C	501	-	1/1/15/20	4/39/115/115	-
29	LHG	L	101	-	-	18/53/53/53	-
32	STE	d	413	-	-	10/17/17/17	-
32	STE	b	623	-	-	12/17/17/17	-
34	PHO	d	401	-	-	0/37/103/103	0/5/6/6
31	DGD	C	516	-	-	21/51/91/95	0/2/2/2
25	CLA	c	509	-	1/1/15/20	12/39/115/115	-
26	BCR	H	101	-	-	2/29/63/63	0/2/2/2
26	BCR	c	514	-	-	5/29/63/63	0/2/2/2
28	LMG	M	101	-	-	23/46/66/70	0/1/1/1
32	STE	d	412	-	-	10/14/14/17	-
30	SQD	A	614	-	-	22/47/67/69	0/1/1/1
28	LMG	c	520	-	-	21/43/63/70	0/1/1/1
31	DGD	c	516	-	-	18/51/91/95	0/2/2/2
25	CLA	c	511	3	1/1/15/20	7/39/115/115	-
25	CLA	b	605	-	1/1/15/20	12/39/115/115	-
29	LHG	B	622	-	-	18/53/53/53	-
32	STE	X	101	-	-	10/17/17/17	-
26	BCR	x	101	-	-	3/29/63/63	0/2/2/2
32	STE	l	102	-	-	9/15/15/17	-
26	BCR	Z	101	-	-	3/29/63/63	0/2/2/2
26	BCR	A	609	-	-	1/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	B	611	-	1/1/15/20	5/39/115/115	-
25	CLA	b	614	-	1/1/15/20	20/39/115/115	-
34	PHO	D	402	-	-	2/37/103/103	0/5/6/6
25	CLA	C	513	-	1/1/15/20	11/39/115/115	-
25	CLA	b	606	-	1/1/15/20	5/39/115/115	-
31	DGD	H	102	-	-	17/51/91/95	0/2/2/2
32	STE	B	626	-	-	6/9/9/17	-
30	SQD	A	615	-	-	12/39/39/69	-
25	CLA	B	614	-	1/1/15/20	7/39/115/115	-
28	LMG	c	518	-	-	12/31/51/70	0/1/1/1
25	CLA	A	606	-	1/1/15/20	4/39/115/115	-
25	CLA	C	510	-	1/1/15/20	3/39/115/115	-
32	STE	a	615	-	-	6/9/9/17	-
31	DGD	c	517	-	-	23/51/91/95	0/2/2/2
34	PHO	d	402	-	-	4/37/103/103	0/5/6/6
30	SQD	a	614	-	-	18/37/37/69	-
27	PL9	a	611	-	-	15/53/73/73	0/1/1/1
25	CLA	C	508	-	-	6/39/115/115	-
28	LMG	d	410	-	-	13/17/17/70	-
28	LMG	c	522	-	-	24/44/64/70	0/1/1/1
25	CLA	b	612	-	1/1/15/20	3/39/115/115	-
32	STE	B	620	-	-	8/14/14/17	-
32	STE	C	519	-	-	1/9/9/17	-
25	CLA	D	404	-	1/1/15/20	3/39/115/115	-
26	BCR	k	103	-	-	2/29/63/63	0/2/2/2
26	BCR	B	617	-	-	4/29/63/63	0/2/2/2
25	CLA	C	507	37	1/1/15/20	10/39/115/115	-
27	PL9	A	610	-	-	26/53/73/73	0/1/1/1
25	CLA	B	606	-	1/1/15/20	15/39/115/115	-
25	CLA	A	611	37	1/1/15/20	5/39/115/115	-
31	DGD	A	616	-	-	28/55/95/95	0/2/2/2
32	STE	b	626	-	-	5/7/7/17	-
32	STE	C	521	-	-	5/13/13/17	-
29	LHG	e	101	-	-	26/46/46/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	STE	M	102	-	-	6/12/12/17	-
28	LMG	A	612	-	-	17/43/63/70	0/1/1/1
28	LMG	D	411	-	-	14/33/33/70	-
25	CLA	C	502	-	-	7/39/115/115	-
25	CLA	c	512	-	1/1/15/20	22/39/115/115	-

The worst 5 of 782 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	d	401	PHO	C1B-C2B	9.75	1.50	1.39
34	d	402	PHO	C1B-C2B	9.70	1.50	1.39
34	D	403	PHO	C3B-C4B	9.56	1.51	1.41
34	d	402	PHO	C3B-C4B	9.03	1.50	1.41
34	D	403	PHO	C1B-C2B	8.96	1.49	1.39

The worst 5 of 1061 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	D	409	SQD	O6-C1-C2	12.90	127.87	108.27
25	C	503	CLA	C4A-NA-C1A	9.31	110.92	106.68
25	c	511	CLA	C4A-NA-C1A	8.54	110.58	106.68
36	v	201	HEC	CBB-CAB-C3B	-8.46	110.52	127.43
25	C	511	CLA	C4A-NA-C1A	8.24	110.44	106.68

5 of 62 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
25	A	606	CLA	ND
25	A	607	CLA	ND
25	A	608	CLA	ND
25	A	611	CLA	ND
25	B	601	CLA	ND

5 of 1717 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	A	607	CLA	C4B-C3B-CAB-CBB
25	B	601	CLA	C1A-C2A-CAA-CBA
25	B	602	CLA	C14-C13-C15-C16
25	B	606	CLA	C2B-C3B-CAB-CBB
25	B	606	CLA	C4B-C3B-CAB-CBB

There are no ring outliers.

142 monomers are involved in 268 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	B	615	CLA	3	0
26	k	102	BCR	2	0
25	b	613	CLA	1	0
29	d	407	LHG	3	0
25	B	603	CLA	3	0
25	C	504	CLA	3	0
25	c	507	CLA	3	0
25	B	616	CLA	3	0
25	C	506	CLA	2	0
25	a	608	CLA	2	0
36	v	201	HEC	1	0
26	B	618	BCR	2	0
34	D	403	PHO	1	0
29	A	613	LHG	5	0
25	a	607	CLA	2	0
26	B	619	BCR	1	0
32	I	101	STE	2	0
25	B	604	CLA	2	0
25	B	612	CLA	3	0
27	d	406	PL9	1	0
25	C	505	CLA	1	0
26	a	610	BCR	1	0
31	o	301	DGD	3	0
25	b	616	CLA	5	0
30	a	613	SQD	4	0
32	T	102	STE	2	0
26	b	619	BCR	1	0
26	t	101	BCR	3	0
29	d	409	LHG	1	0
26	C	514	BCR	3	0
31	C	515	DGD	1	0
25	a	609	CLA	2	0
26	k	101	BCR	1	0
25	D	405	CLA	1	0
25	c	505	CLA	5	0
25	c	508	CLA	2	0
25	C	512	CLA	2	0
33	D	401	BCT	1	0
27	D	407	PL9	1	0
29	E	101	LHG	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	b	611	CLA	2	0
26	T	101	BCR	5	0
28	b	622	LMG	1	0
25	c	504	CLA	1	0
25	b	608	CLA	1	0
25	A	607	CLA	3	0
26	b	618	BCR	2	0
30	D	409	SQD	2	0
25	B	610	CLA	3	0
25	B	601	CLA	3	0
26	D	406	BCR	1	0
25	A	608	CLA	1	0
29	l	101	LHG	1	0
35	f	101	HEM	5	0
32	j	101	STE	1	0
26	K	102	BCR	1	0
25	b	603	CLA	2	0
25	B	602	CLA	3	0
25	c	513	CLA	3	0
28	D	408	LMG	2	0
32	T	103	STE	1	0
26	d	405	BCR	3	0
25	b	615	CLA	2	0
30	B	623	SQD	3	0
25	B	613	CLA	3	0
25	a	612	CLA	2	0
25	d	403	CLA	2	0
35	F	101	HEM	2	0
25	b	609	CLA	1	0
32	c	521	STE	1	0
25	b	610	CLA	2	0
25	c	501	CLA	3	0
26	b	617	BCR	2	0
25	B	607	CLA	2	0
26	K	101	BCR	2	0
31	C	517	DGD	2	0
29	D	410	LHG	1	0
25	b	601	CLA	1	0
30	b	620	SQD	1	0
25	c	510	CLA	2	0
32	H	103	STE	1	0
25	B	609	CLA	3	0

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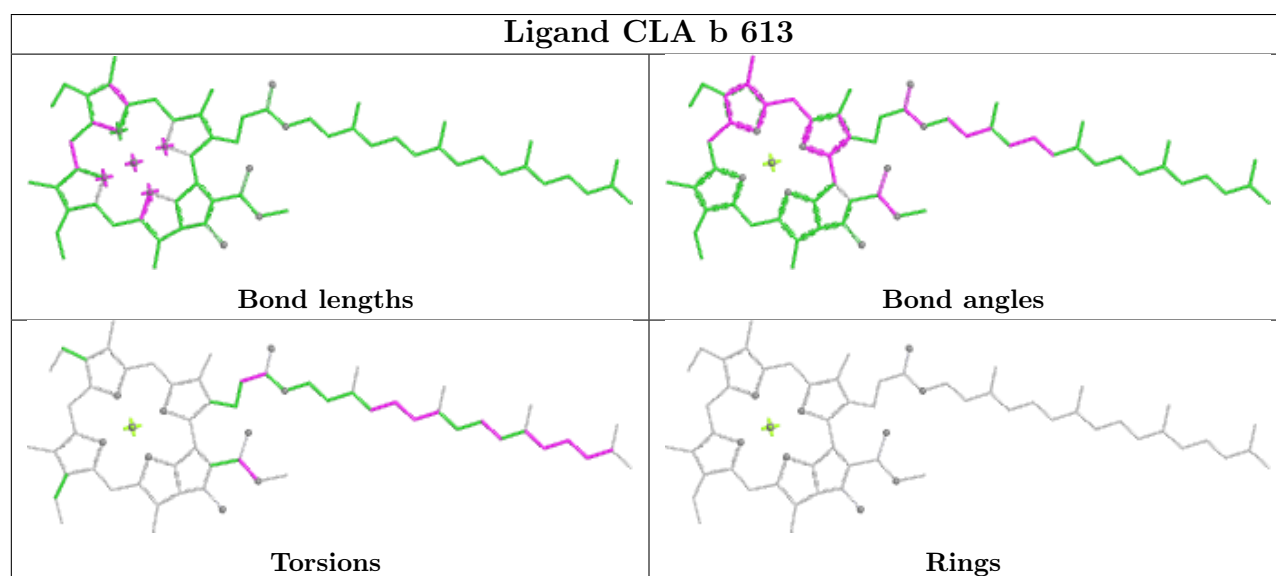
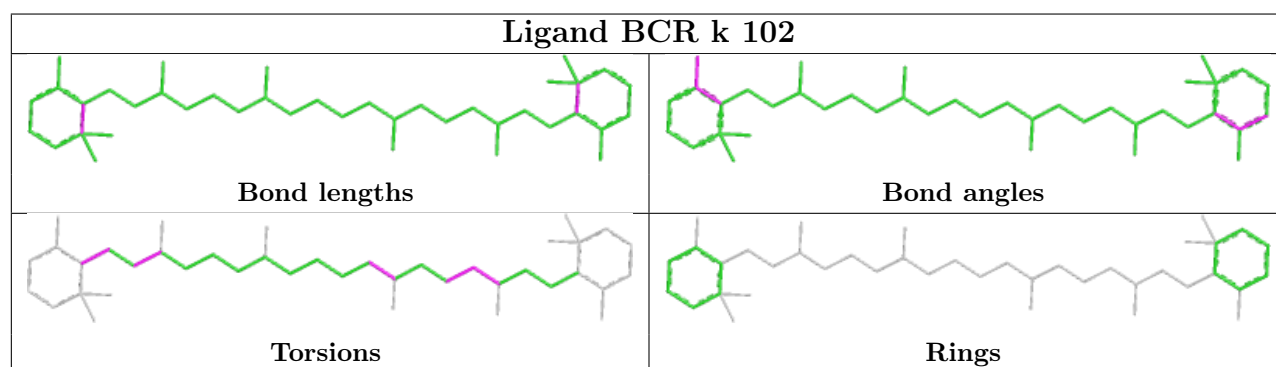
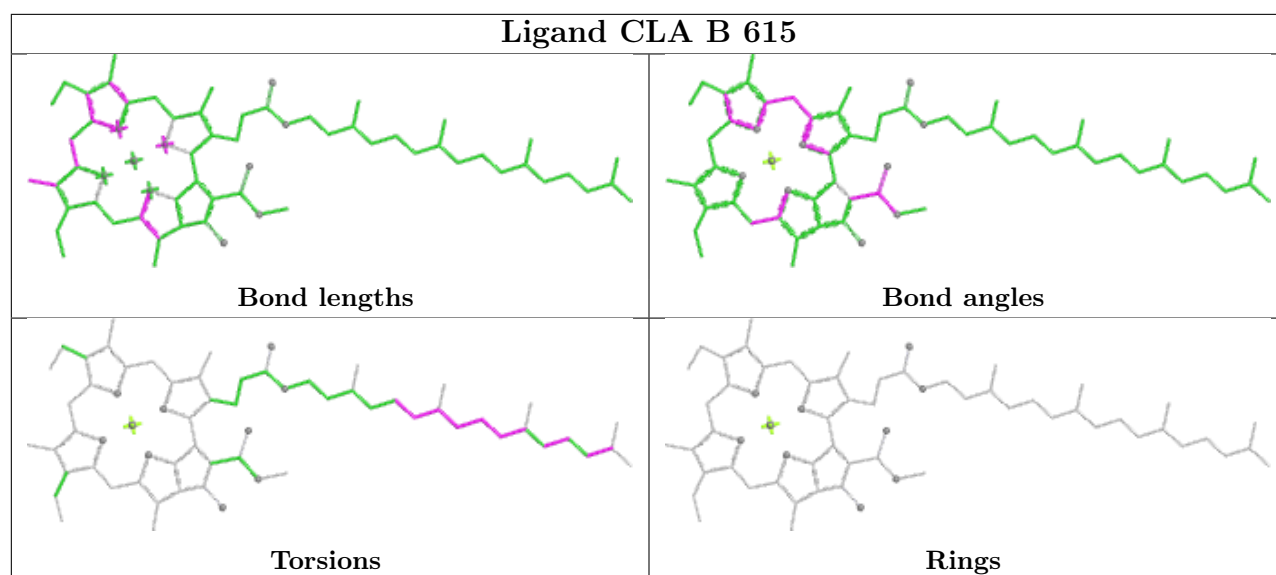
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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21	A	601[B]	OEY	1	0
29	d	408	LHG	2	0
25	b	602	CLA	4	0
30	f	102	SQD	2	0
25	B	605	CLA	4	0
25	d	404	CLA	1	0
32	B	625	STE	2	0
28	b	624	LMG	1	0
25	C	511	CLA	1	0
25	b	604	CLA	2	0
32	c	519	STE	2	0
25	C	501	CLA	1	0
29	L	101	LHG	2	0
32	d	413	STE	4	0
32	b	623	STE	4	0
25	c	509	CLA	1	0
26	c	514	BCR	2	0
28	M	101	LMG	2	0
30	A	614	SQD	2	0
28	c	520	LMG	5	0
31	c	516	DGD	1	0
25	c	511	CLA	5	0
25	b	605	CLA	4	0
29	B	622	LHG	3	0
32	X	101	STE	1	0
26	x	101	BCR	2	0
32	l	102	STE	2	0
26	Z	101	BCR	2	0
26	A	609	BCR	1	0
25	B	611	CLA	2	0
25	b	614	CLA	5	0
34	D	402	PHO	1	0
25	C	513	CLA	3	0
25	b	606	CLA	3	0
31	H	102	DGD	3	0
30	A	615	SQD	2	0
25	B	614	CLA	4	0
28	c	518	LMG	1	0
25	A	606	CLA	2	0
25	C	510	CLA	1	0
31	c	517	DGD	2	0

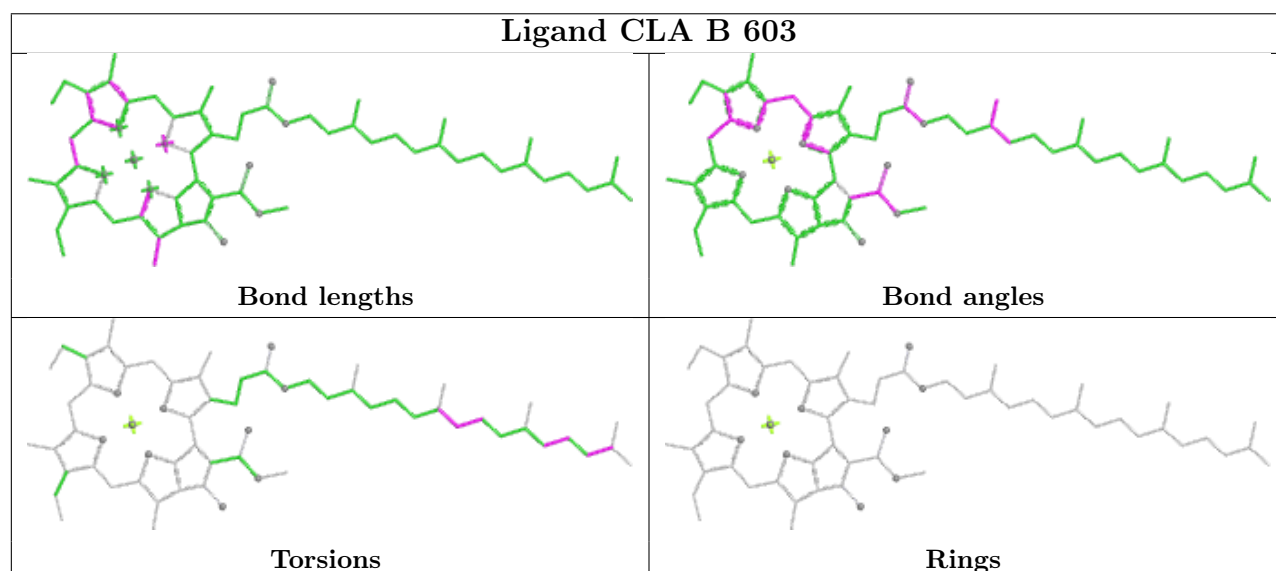
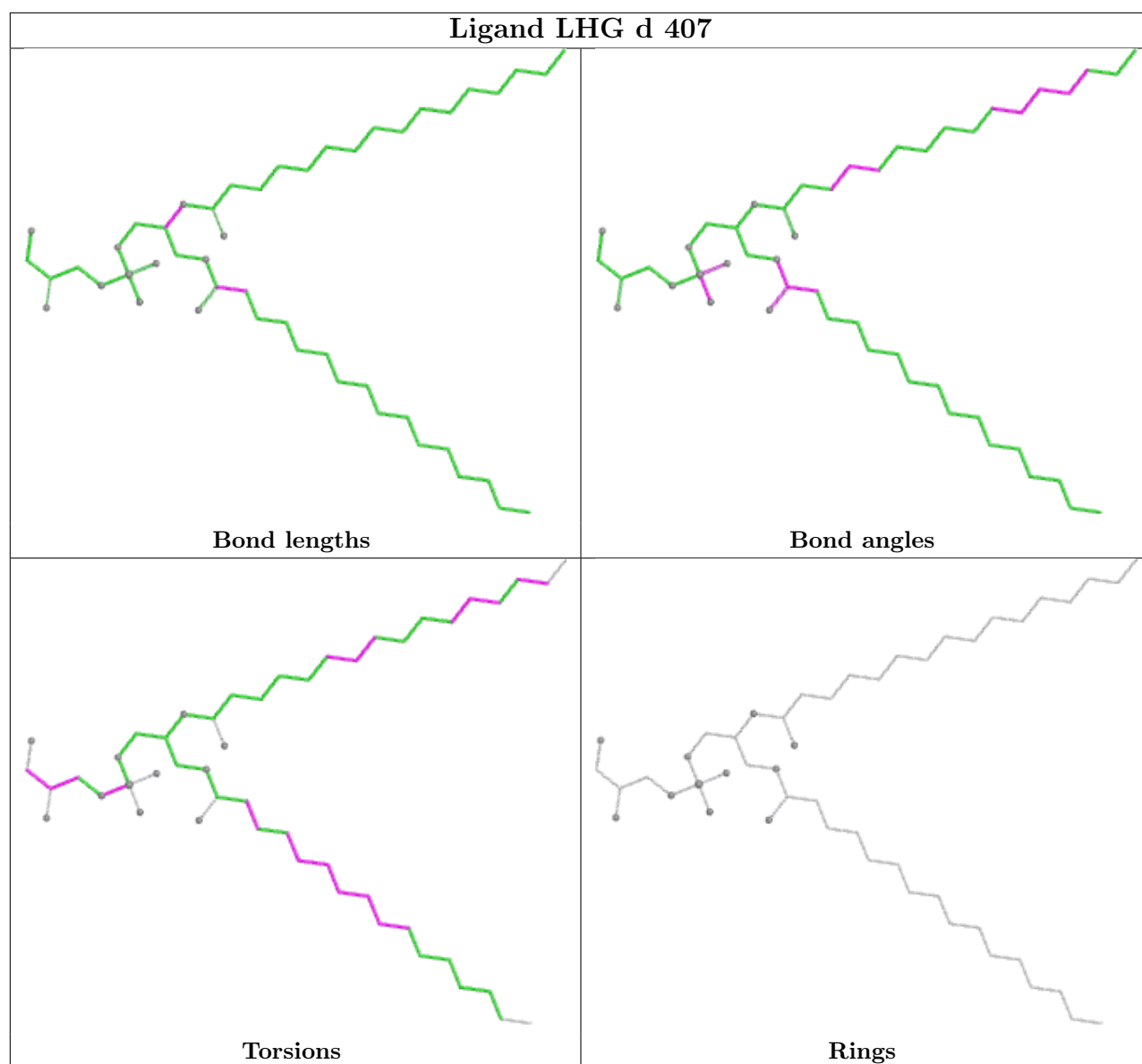
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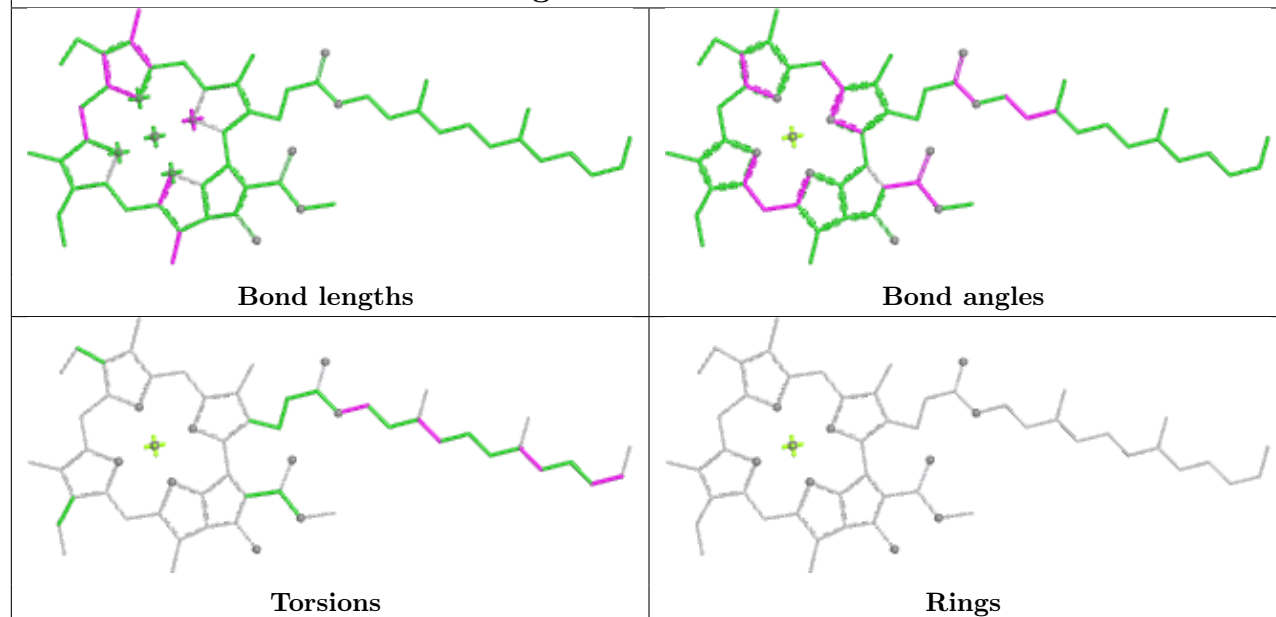
Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	d	402	PHO	2	0
27	a	611	PL9	4	0
25	C	508	CLA	2	0
28	c	522	LMG	3	0
25	b	612	CLA	2	0
25	D	404	CLA	1	0
26	k	103	BCR	3	0
26	B	617	BCR	3	0
25	C	507	CLA	1	0
21	a	601[B]	OEY	1	0
27	A	610	PL9	5	0
25	B	606	CLA	3	0
31	A	616	DGD	7	0
29	e	101	LHG	1	0
28	A	612	LMG	2	0
28	D	411	LMG	1	0
25	C	502	CLA	1	0
25	c	512	CLA	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.

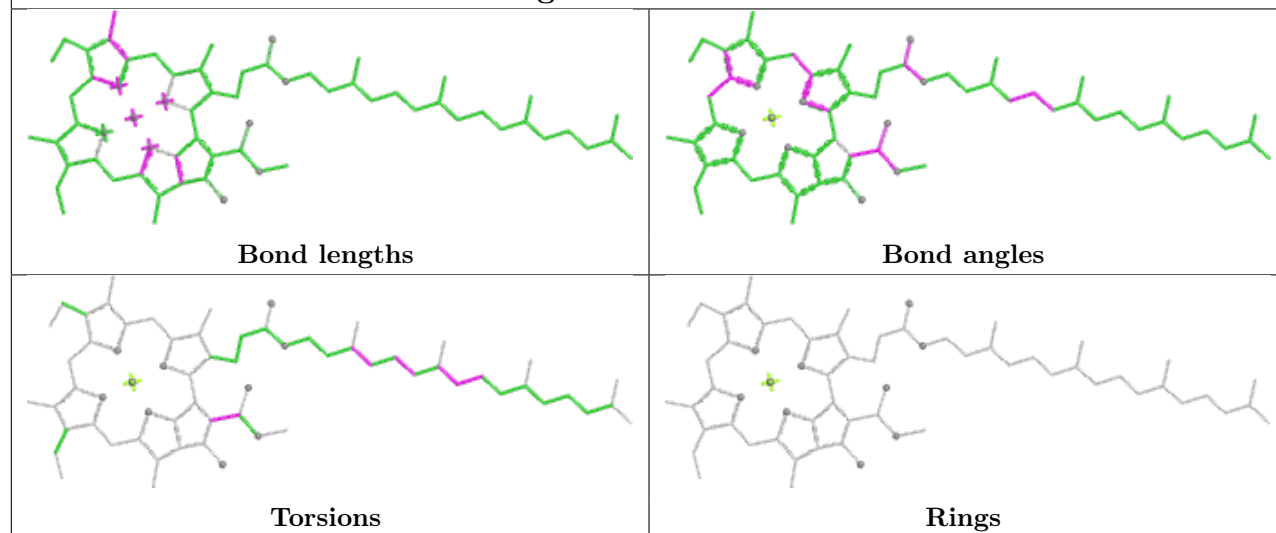


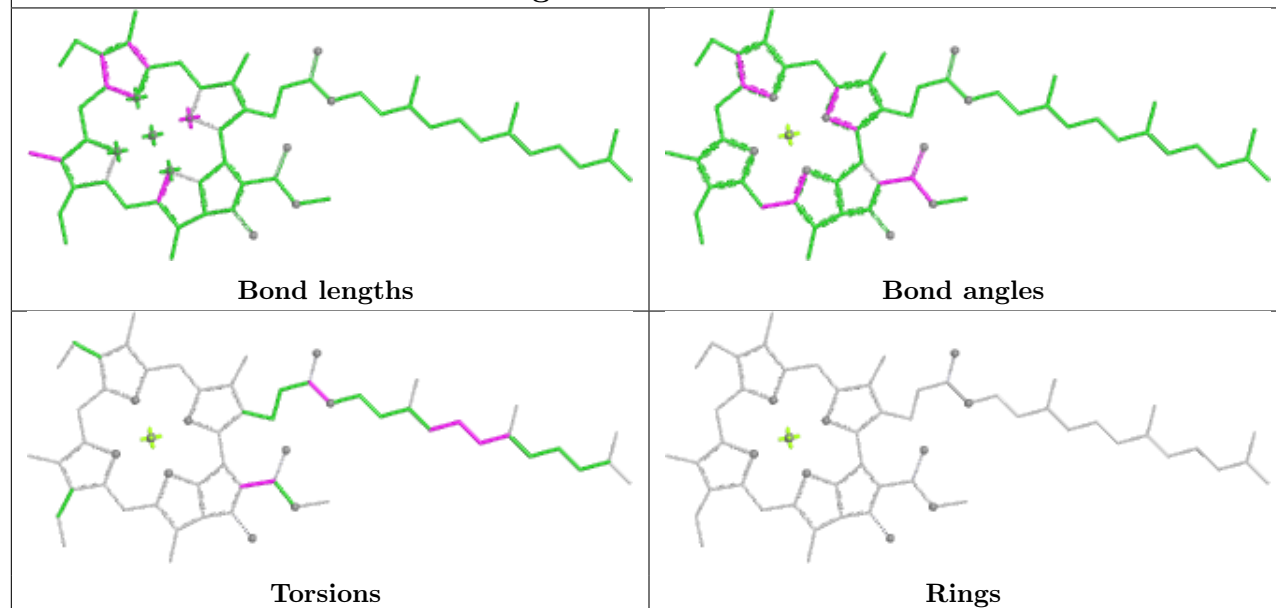
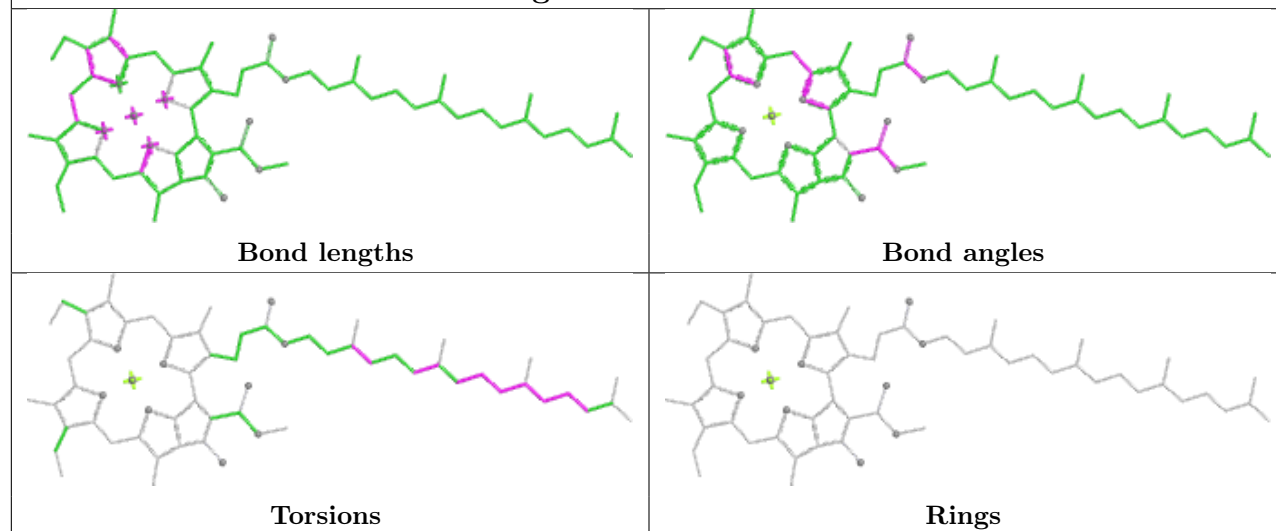


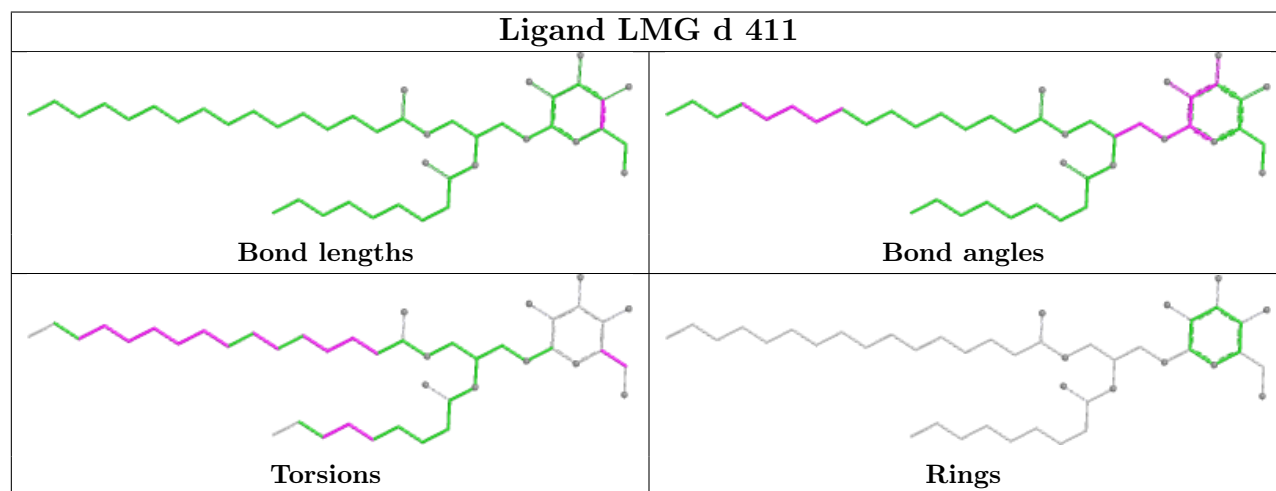
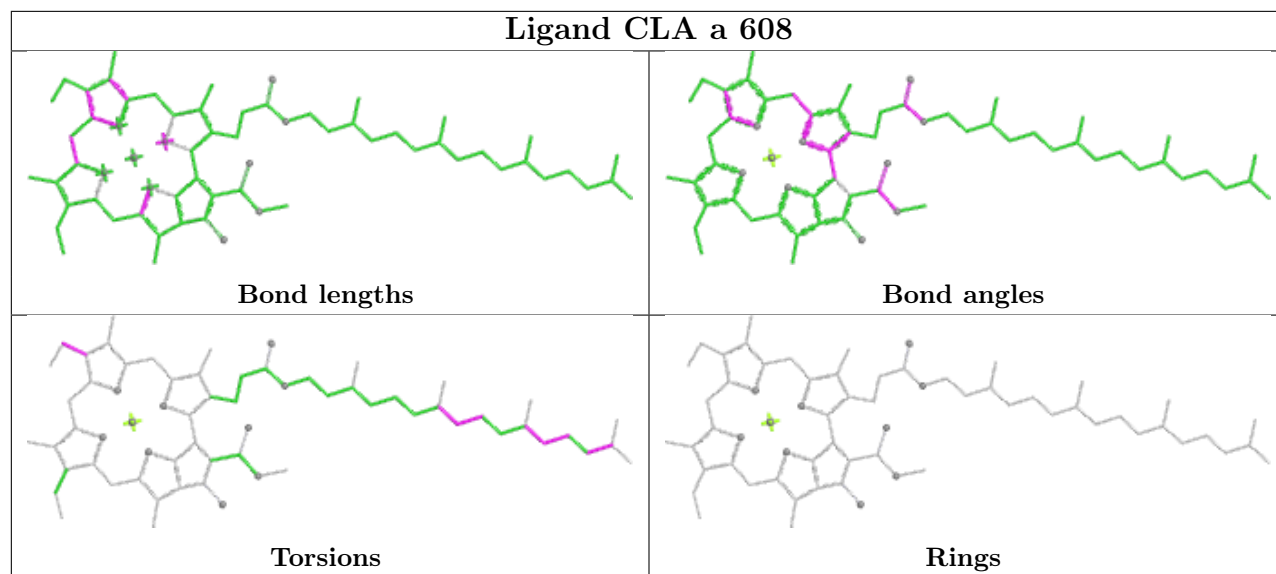
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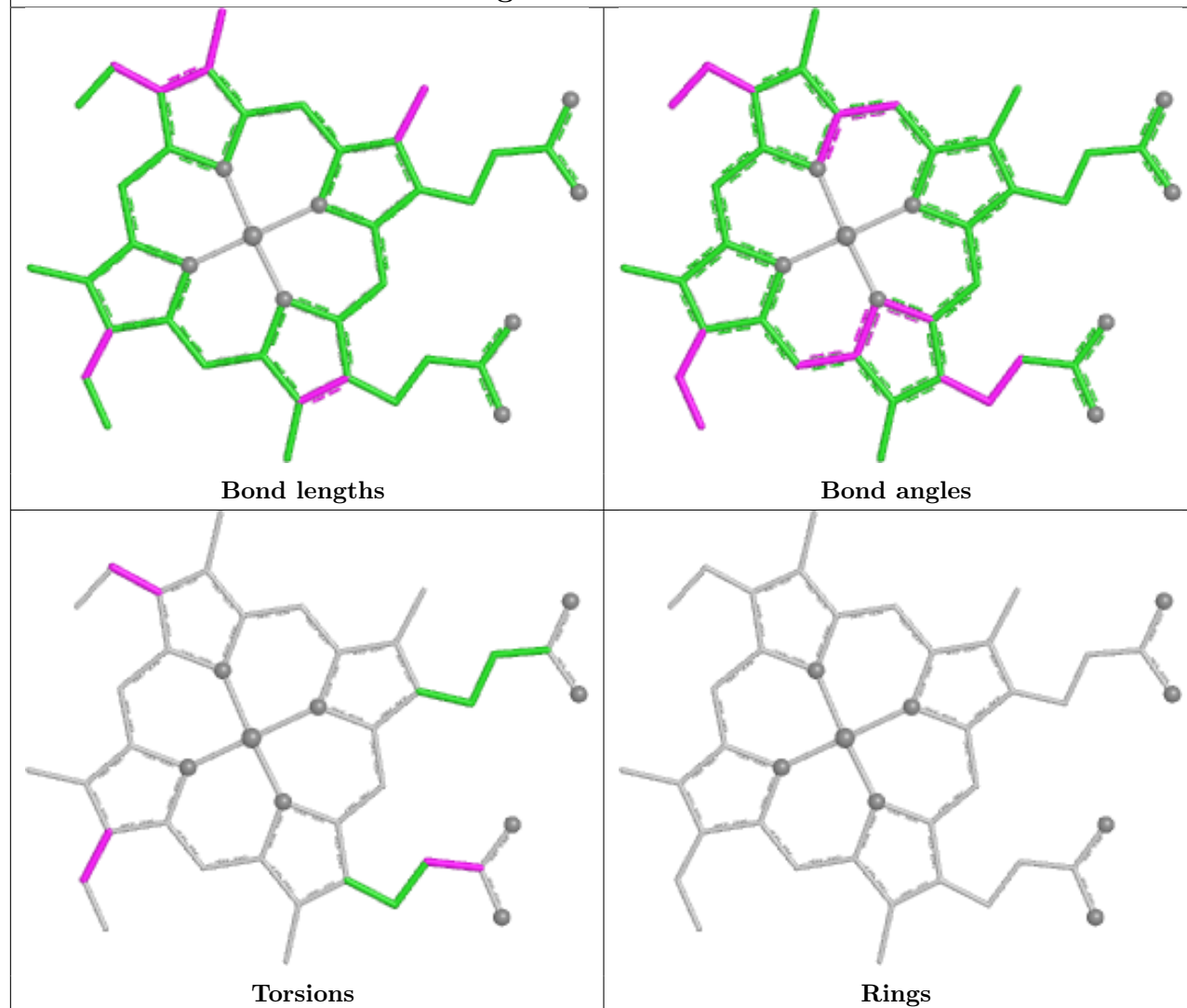
Ligand CLA c 507



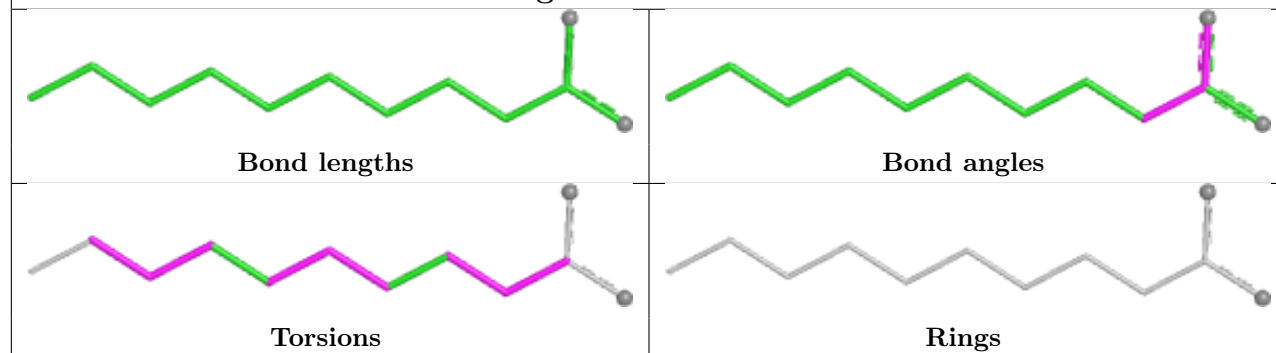
Ligand CLA B 616**Ligand CLA C 506**

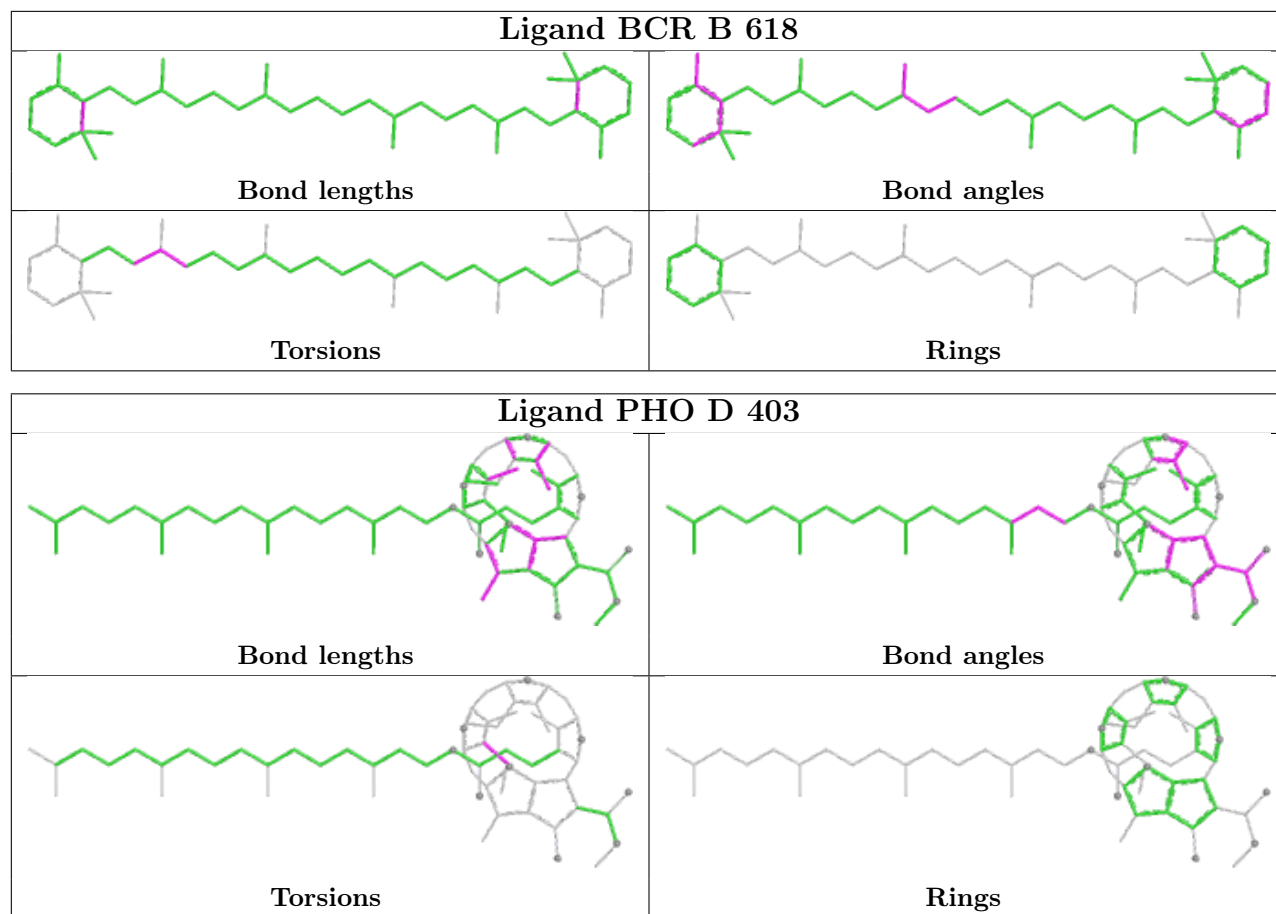


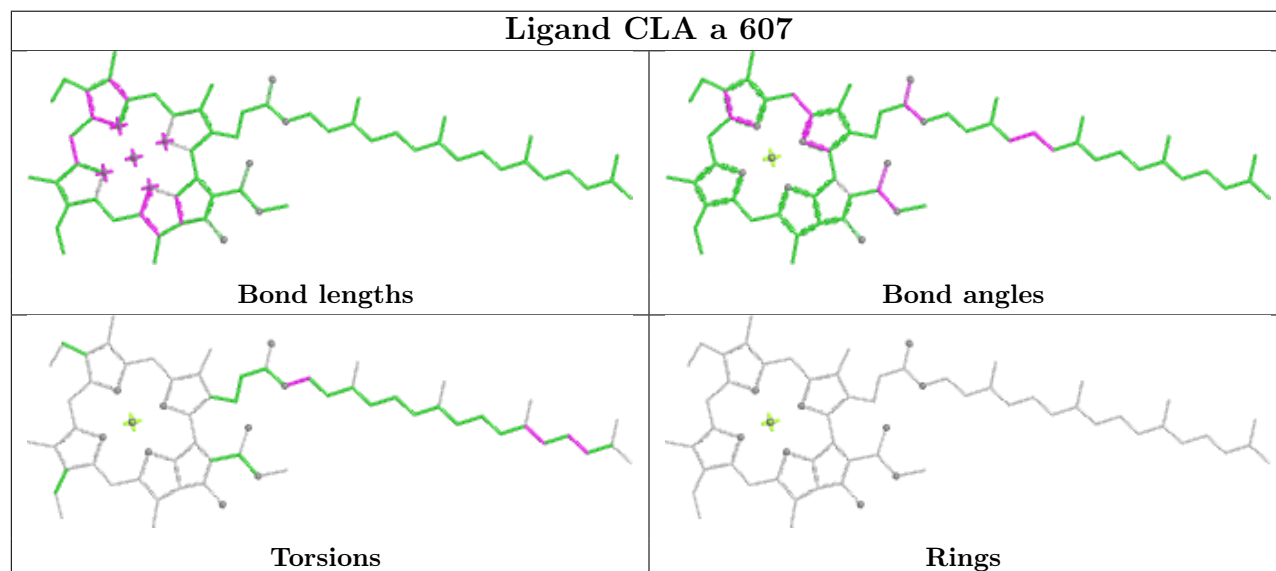
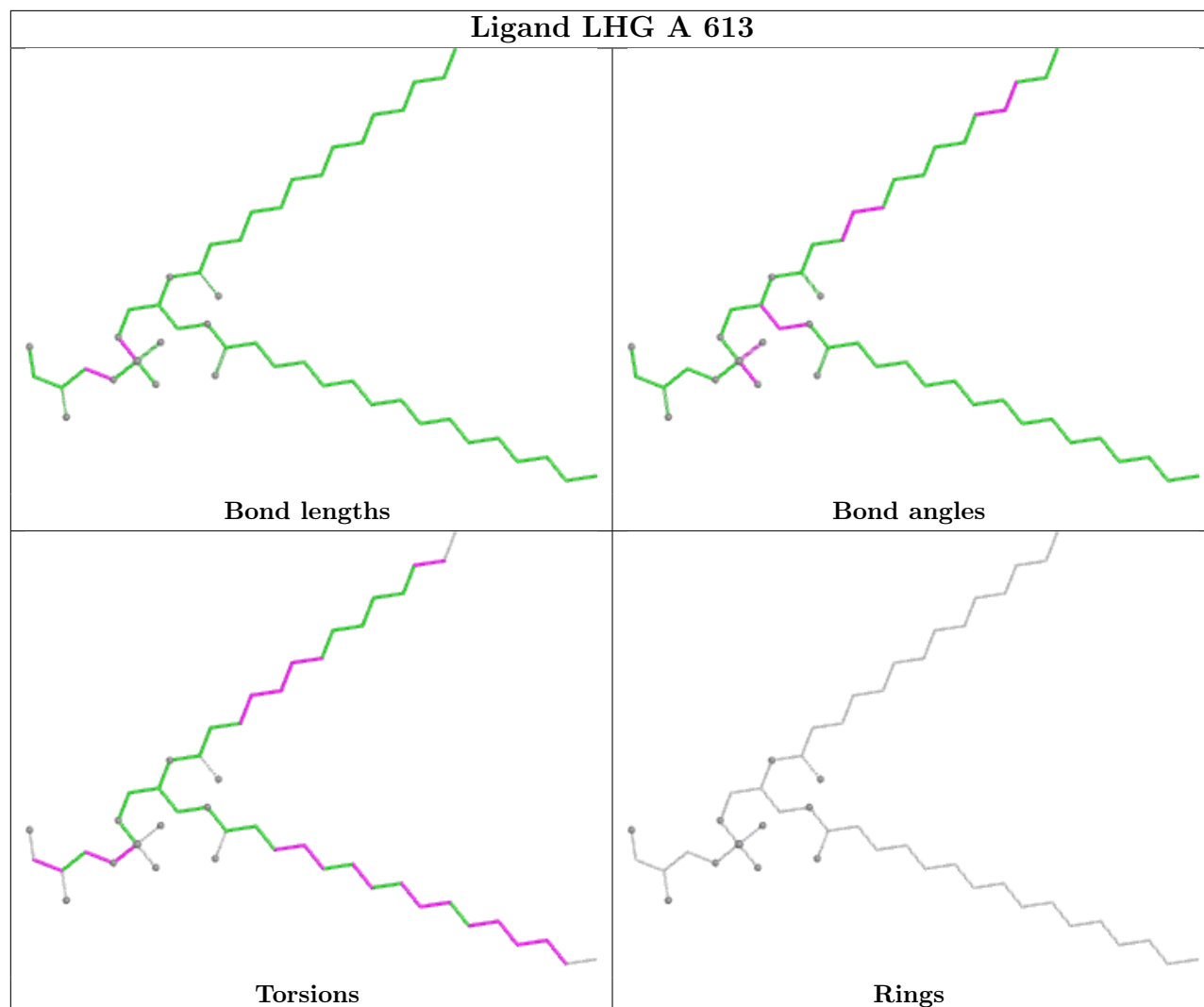
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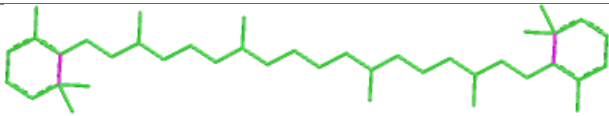
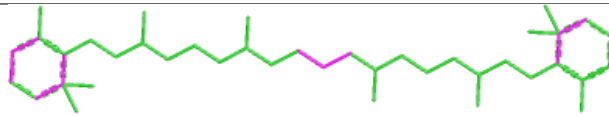
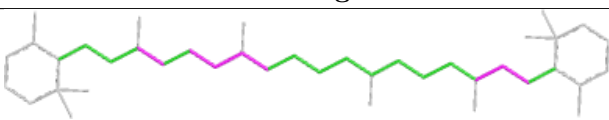
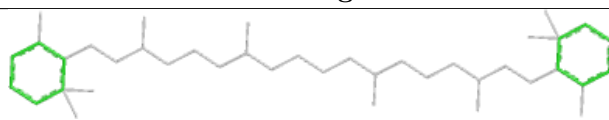


Ligand STE E 102

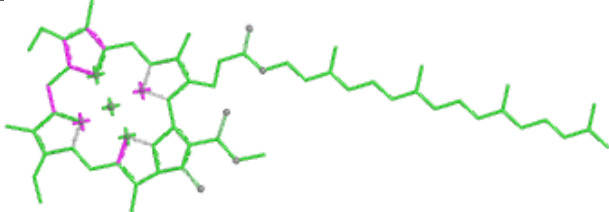
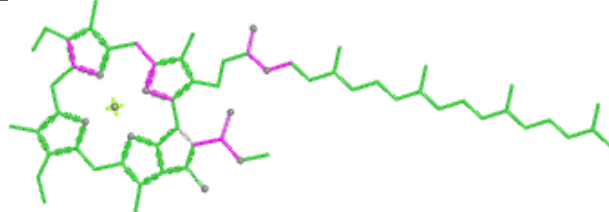
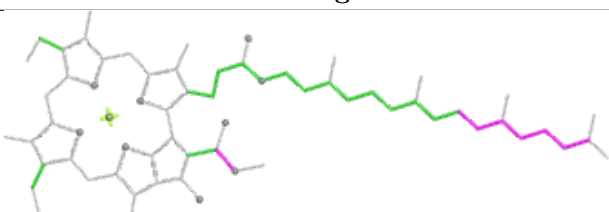
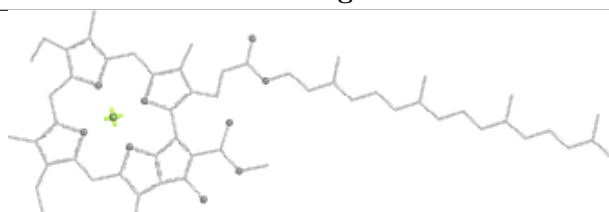


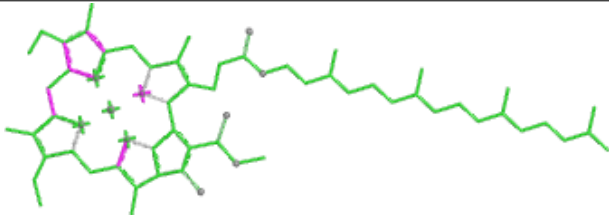
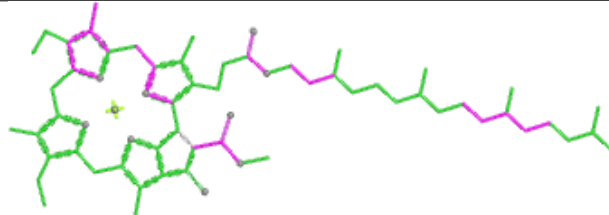
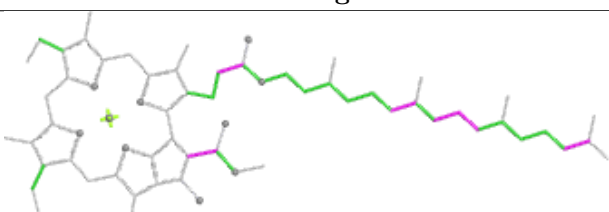
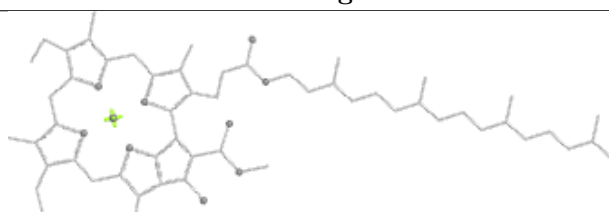


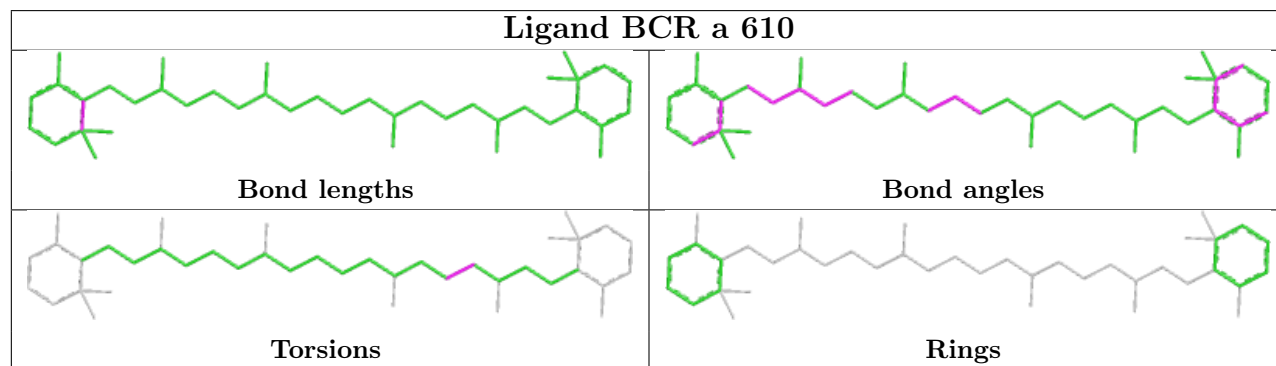
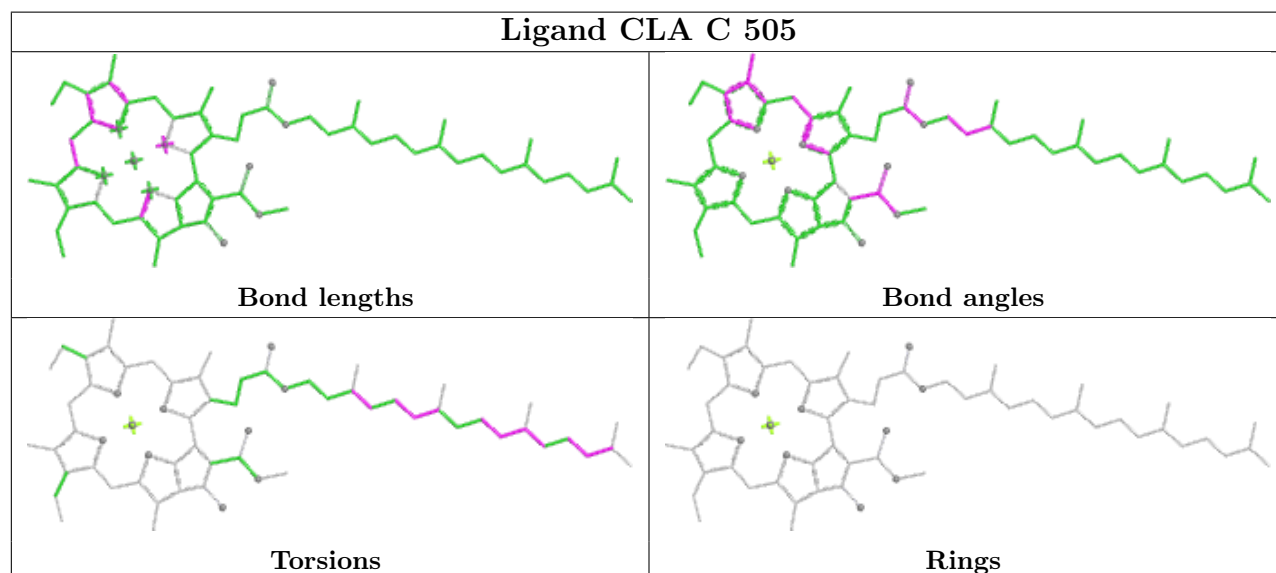
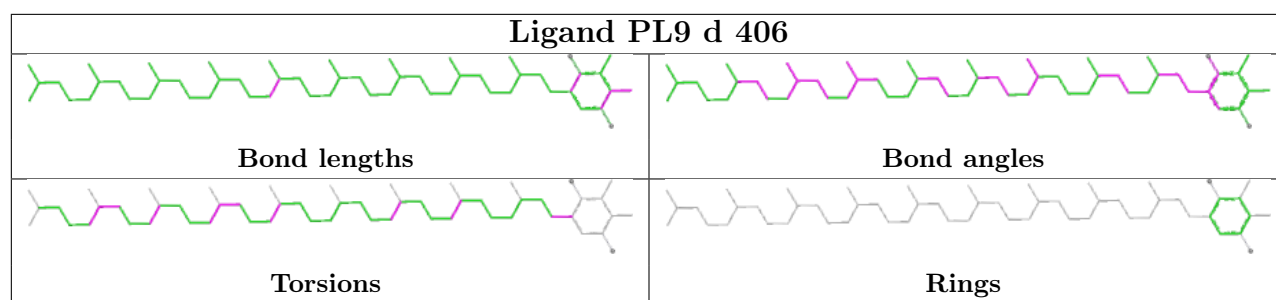


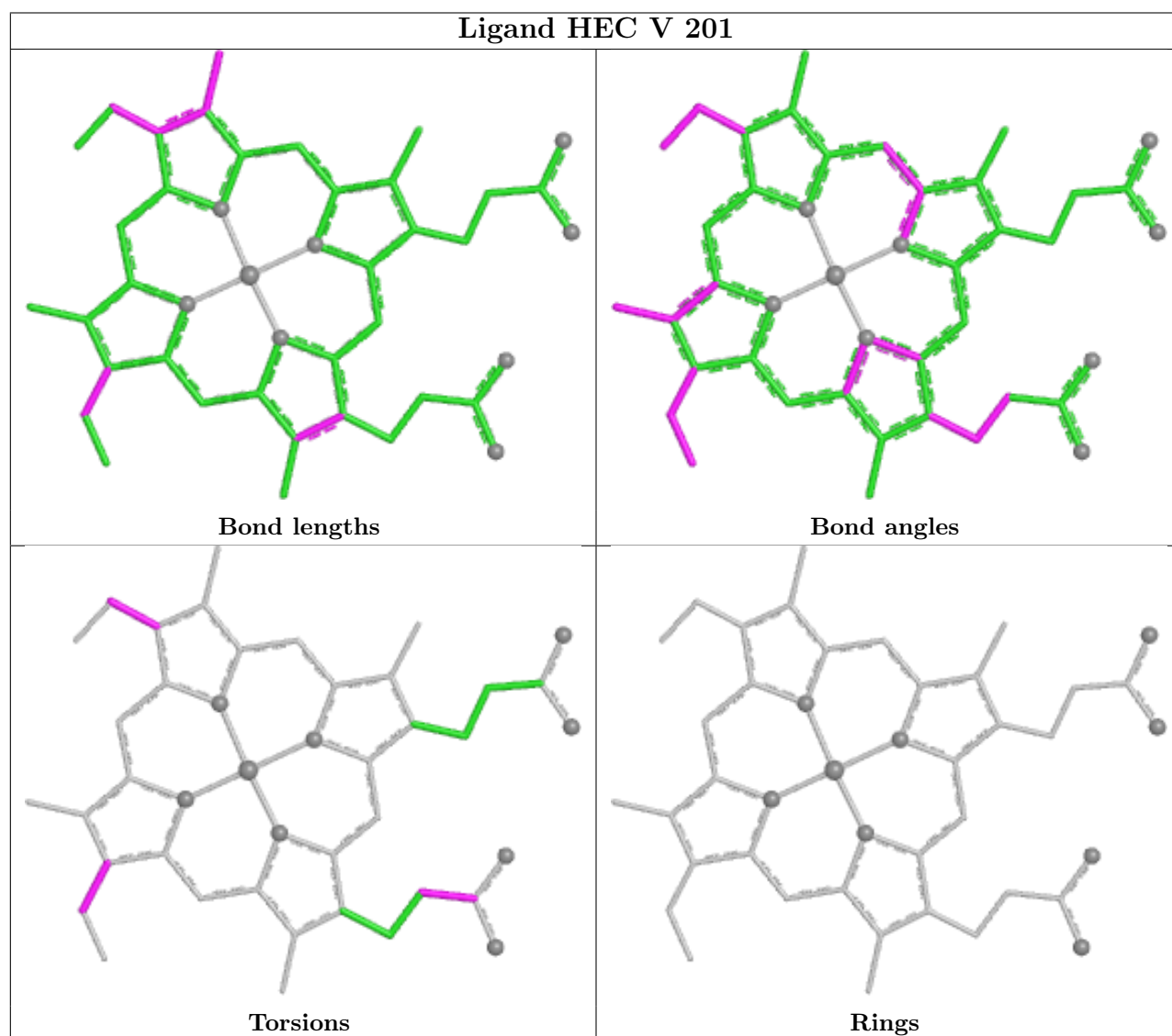
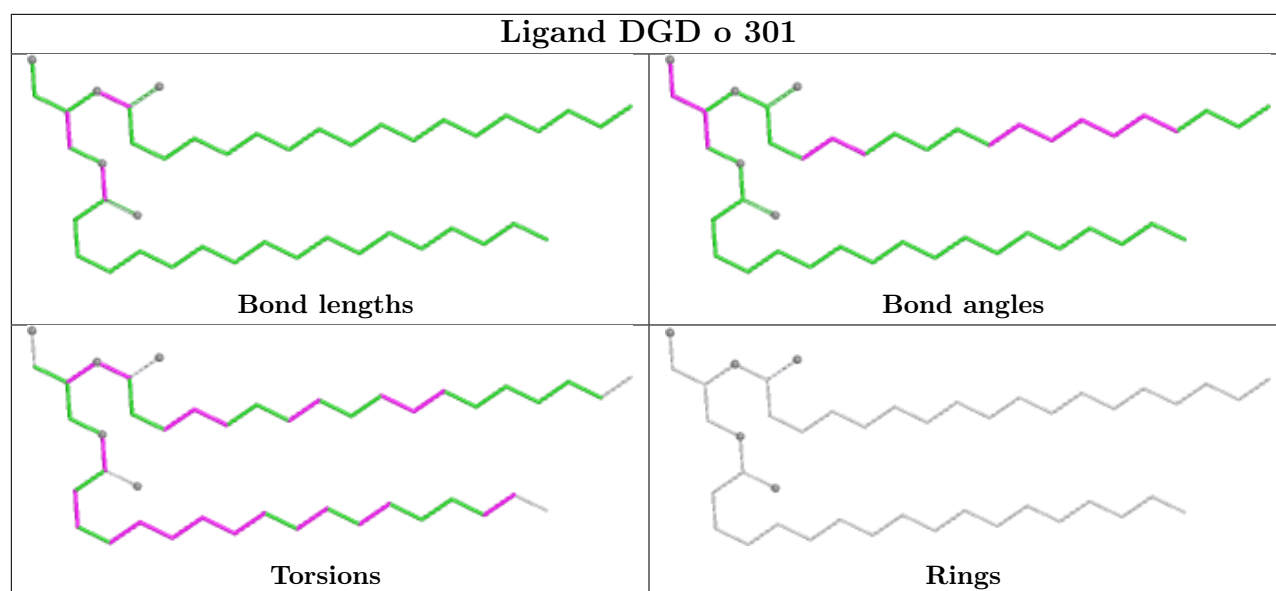
Ligand BCR B 619	
	
Bond lengths	Bond angles
	
Torsions	Rings

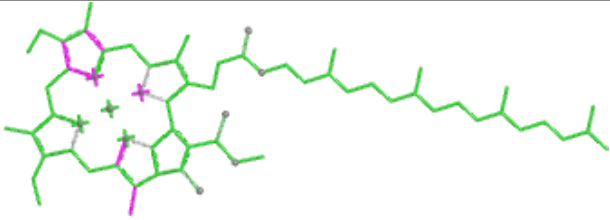
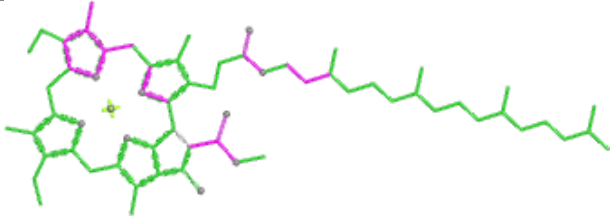
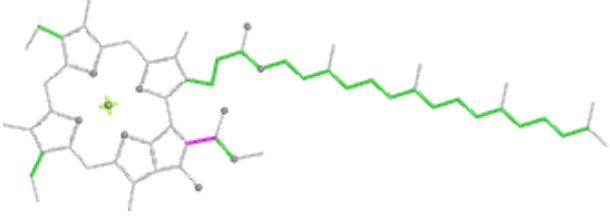
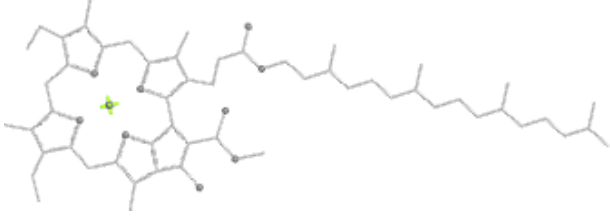
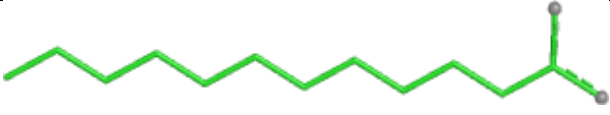
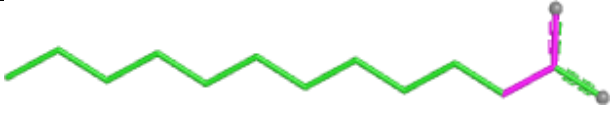
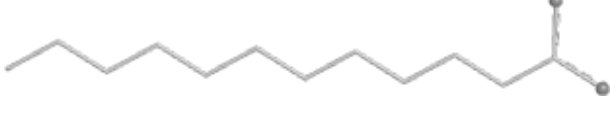
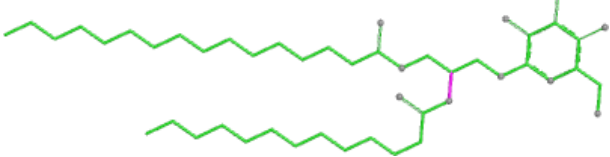
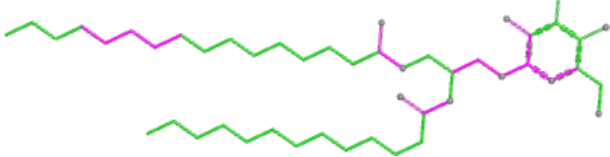
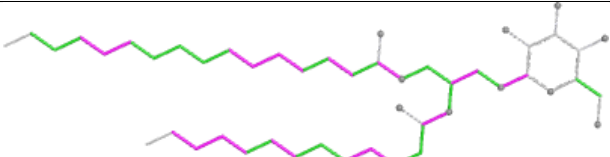
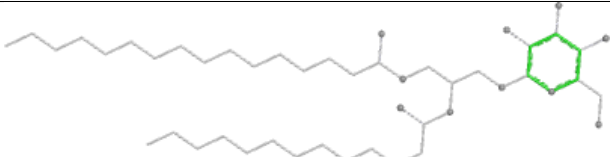
Ligand STE I 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 604	
	
Bond lengths	Bond angles
	
Torsions	Rings

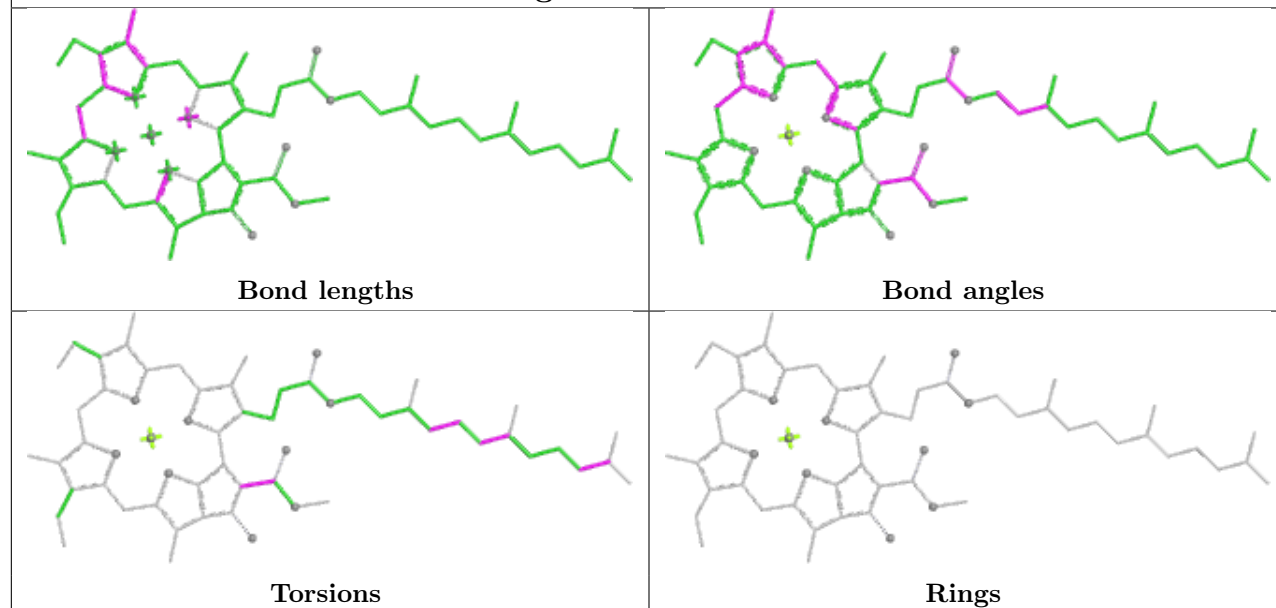
Ligand CLA B 612	
	
Bond lengths	Bond angles
	
Torsions	Rings



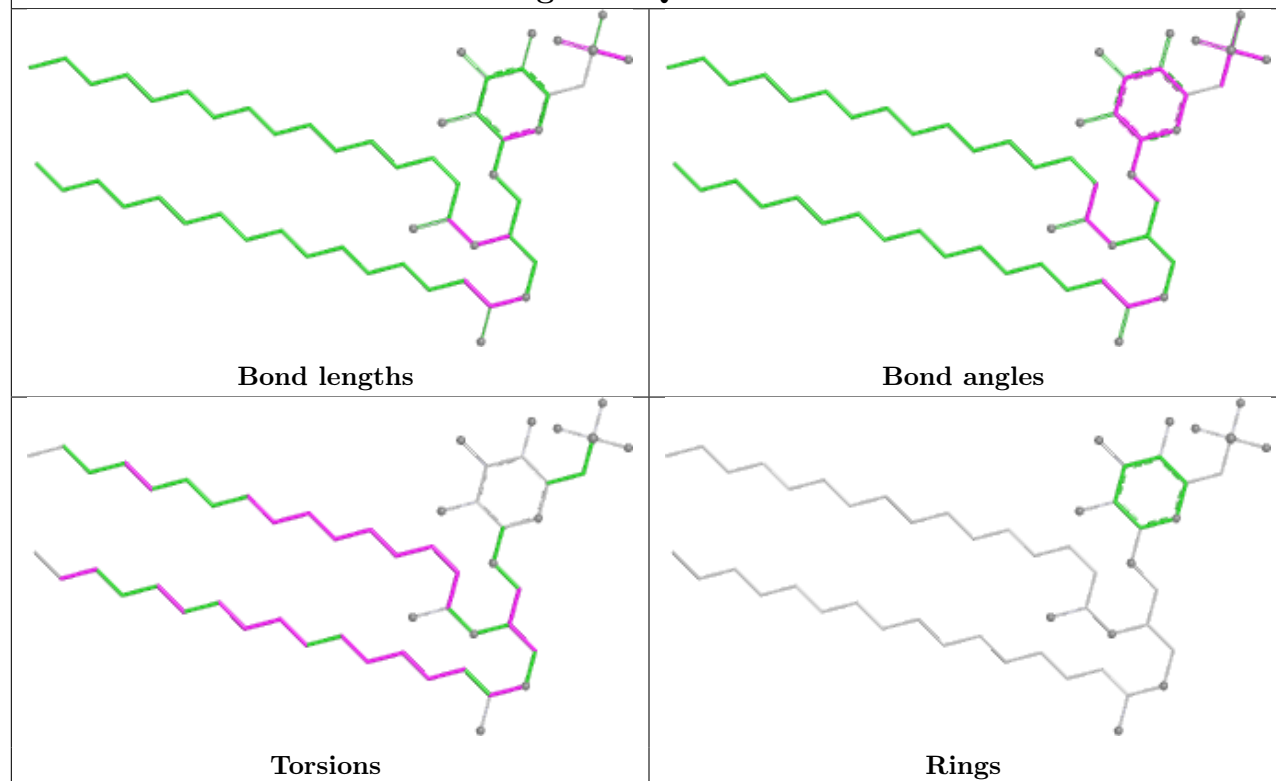


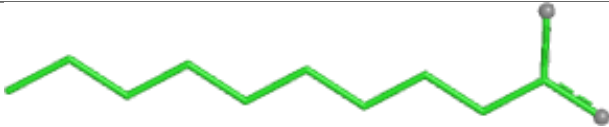
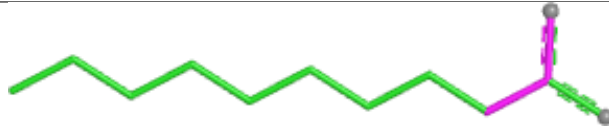
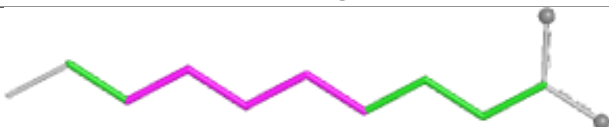
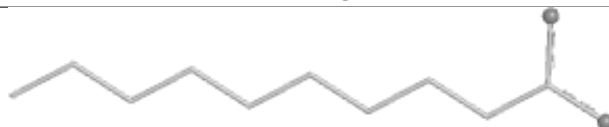
Ligand CLA c 502	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand STE t 102	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG C 518	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA b 616

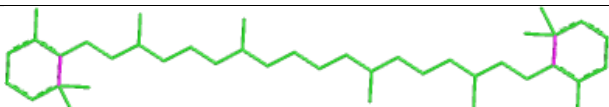
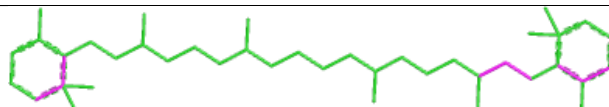
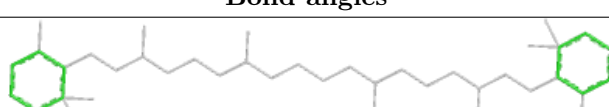


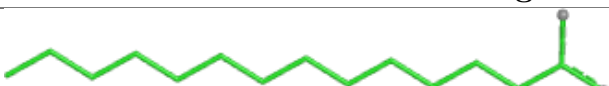
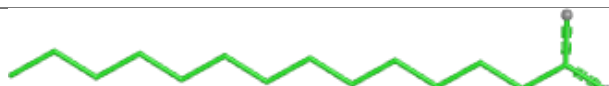
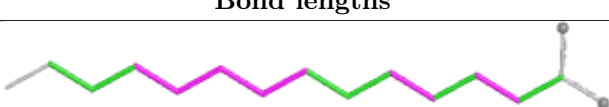
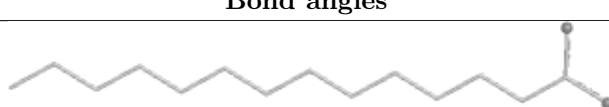
Ligand SQD a 613

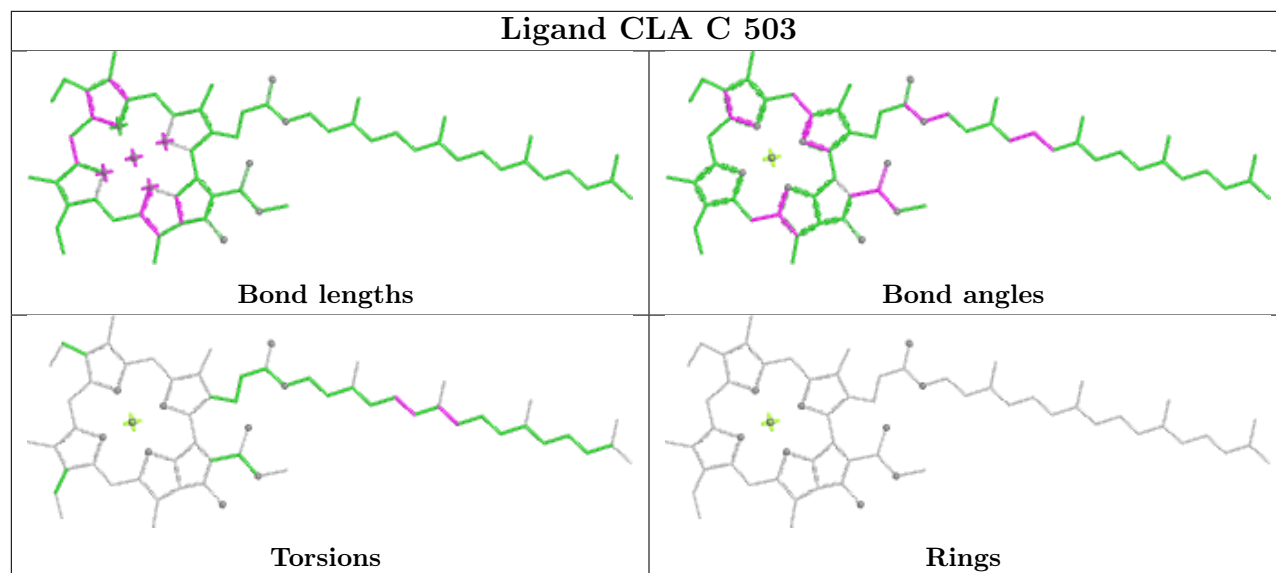
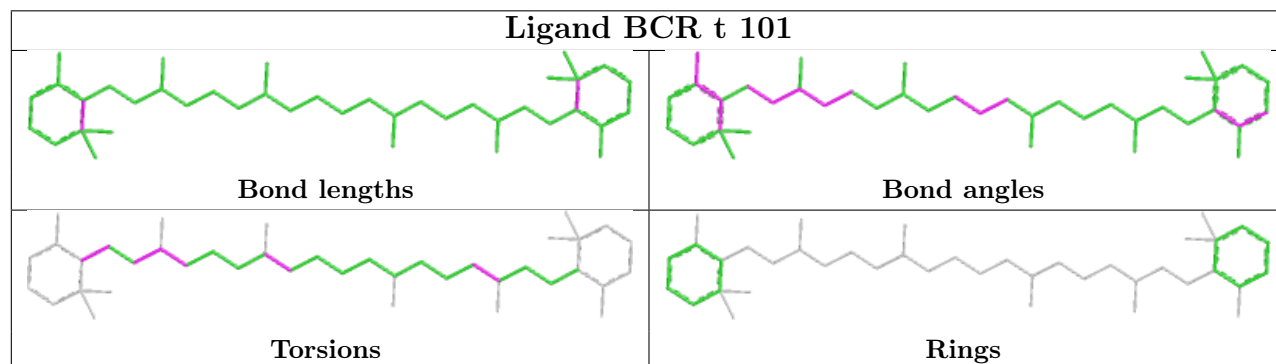
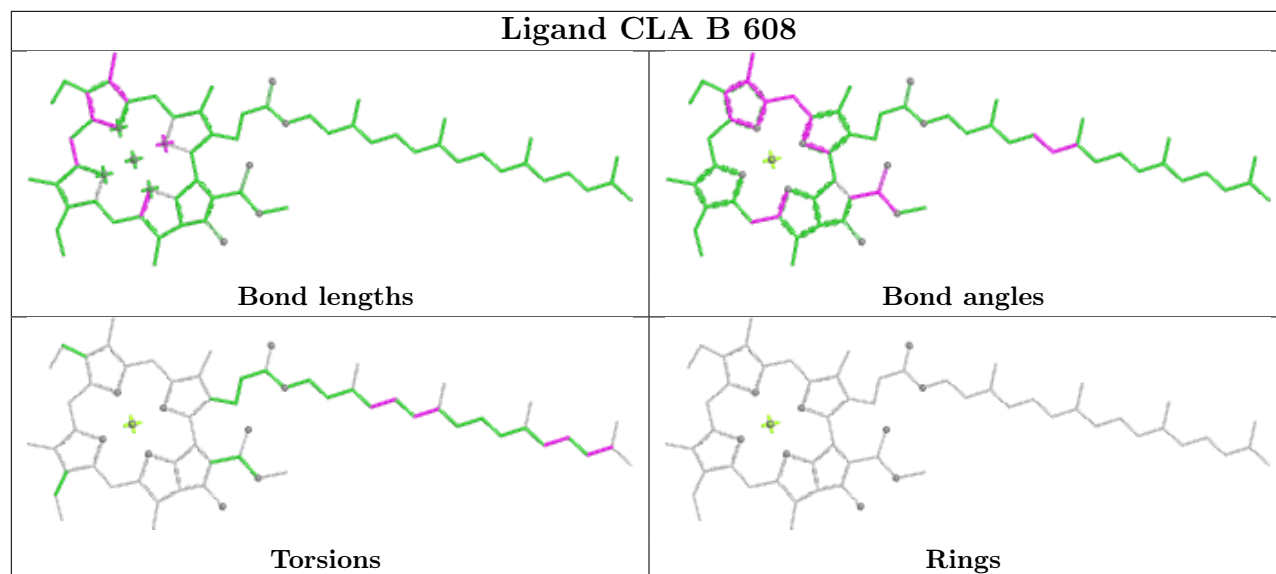


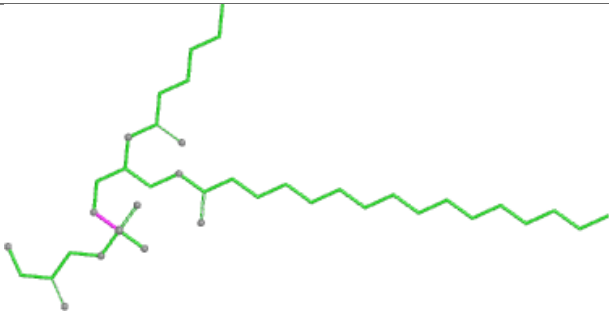
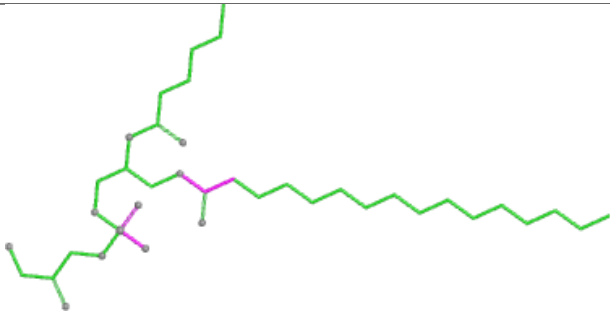
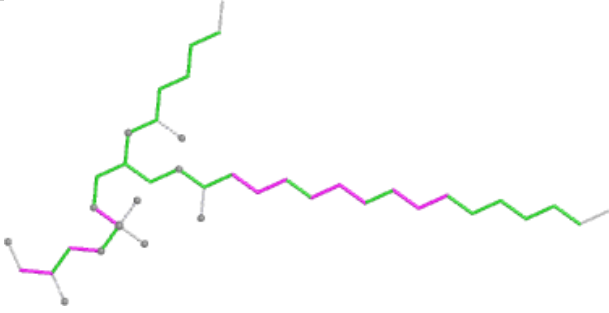
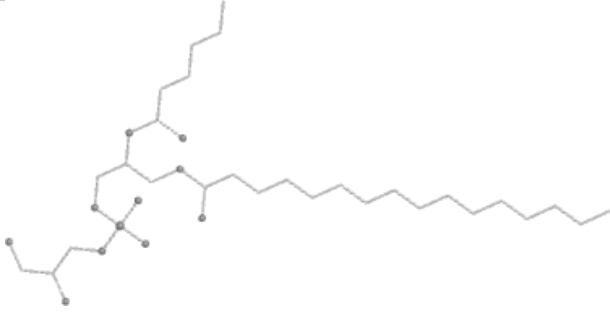
Ligand STE C 520	
	
Bond lengths	Bond angles
	
Torsions	Rings

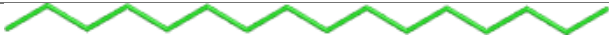
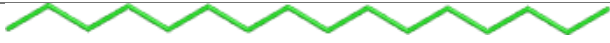
Ligand STE T 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

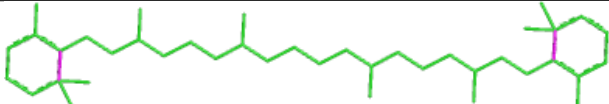
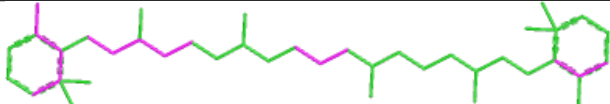
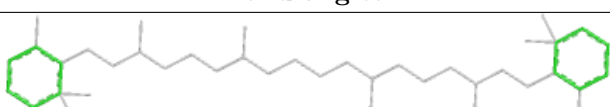
Ligand BCR b 619	
	
Bond lengths	Bond angles
	
Torsions	Rings

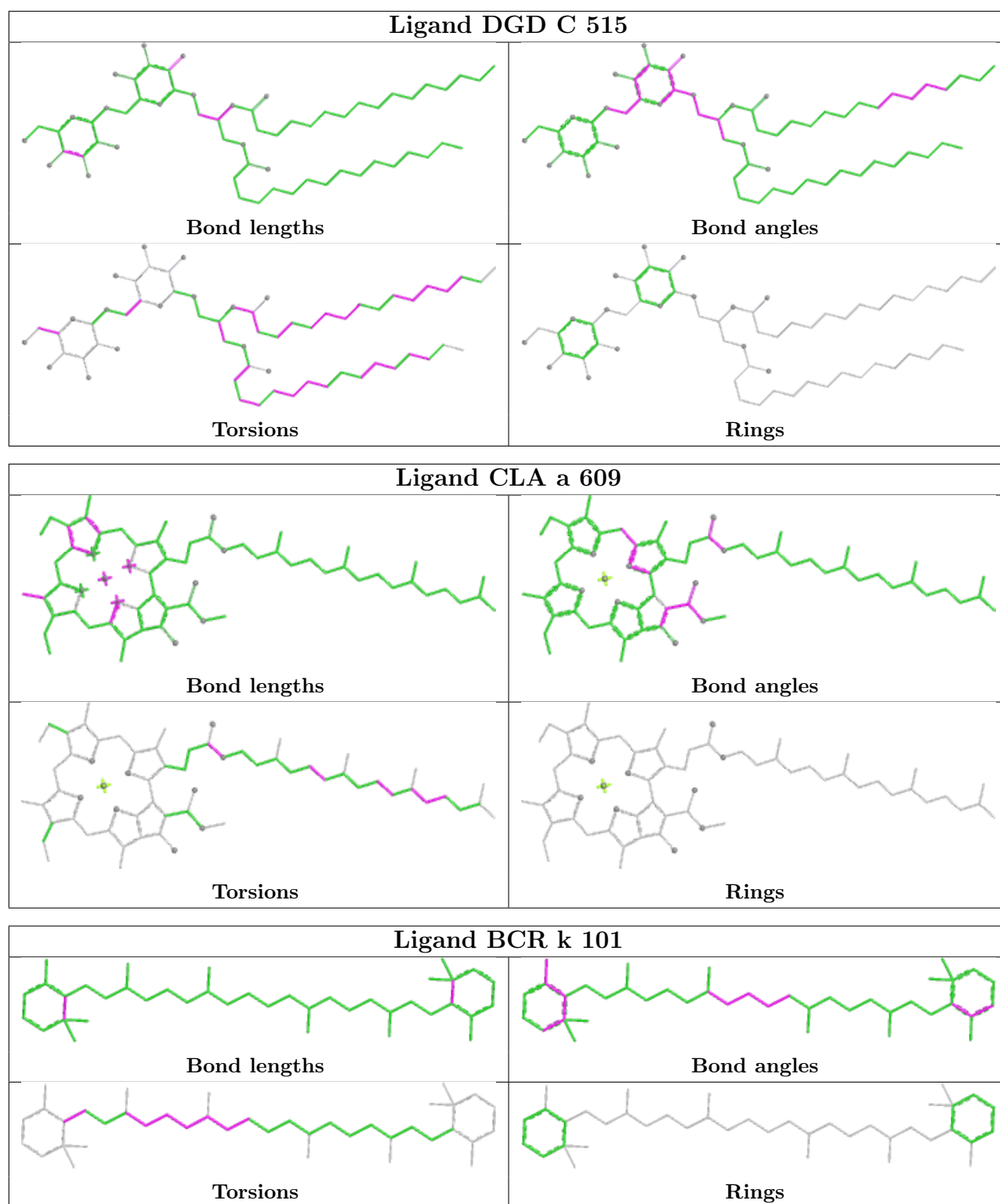
Ligand STE b 625	
	
Bond lengths	Bond angles
	
Torsions	Rings

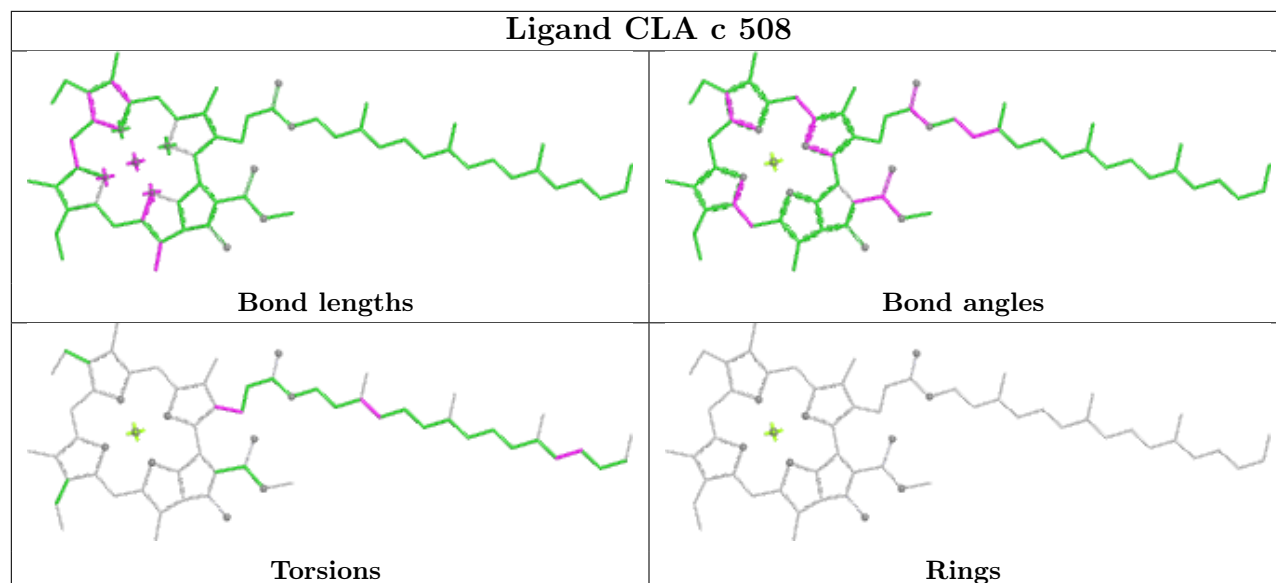
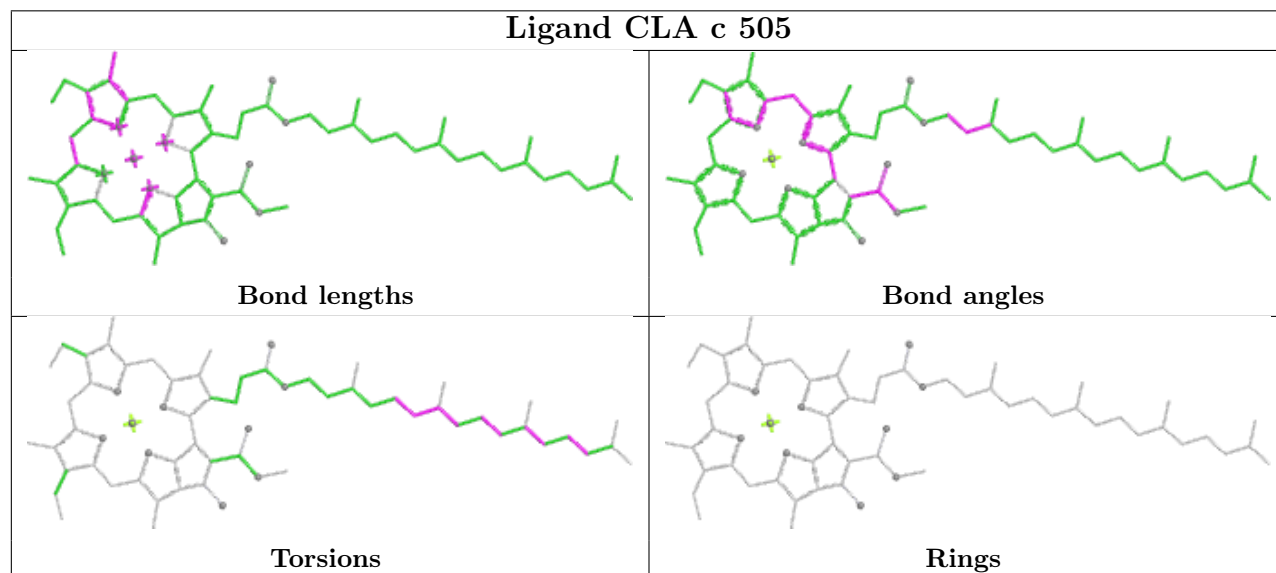
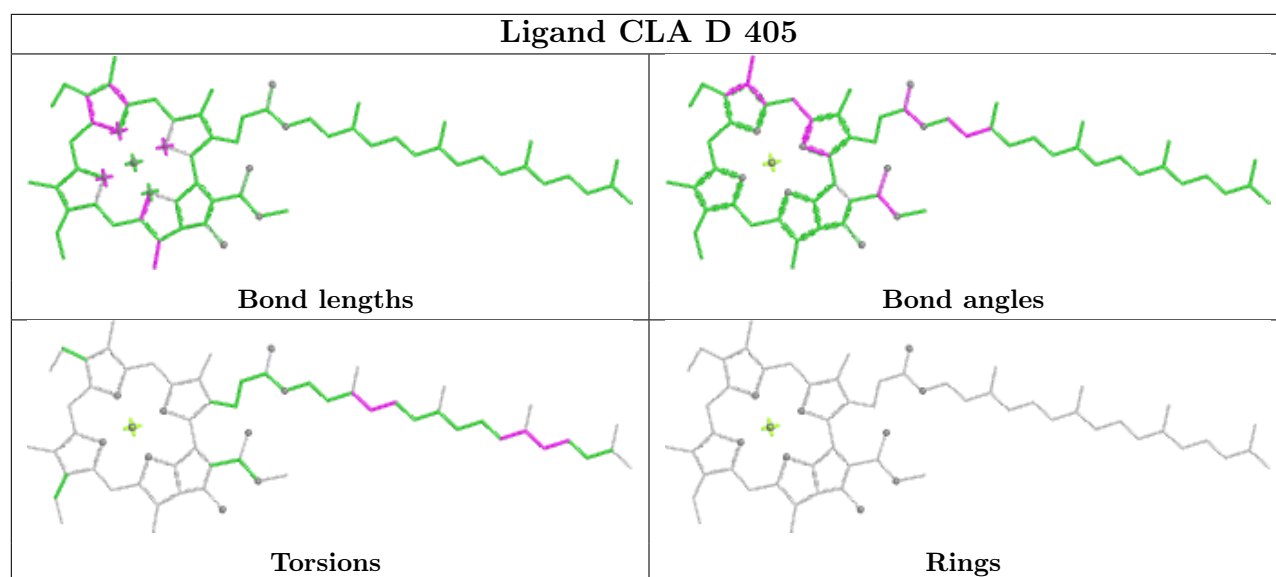


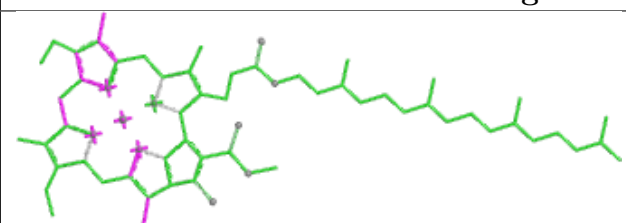
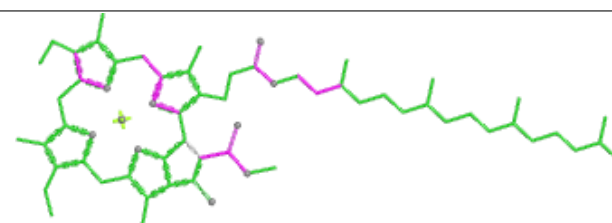
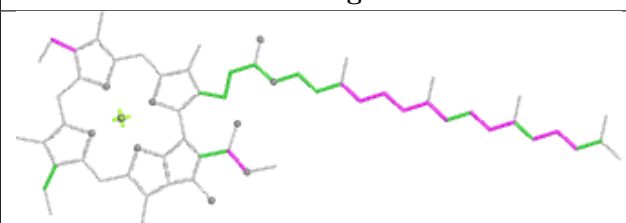
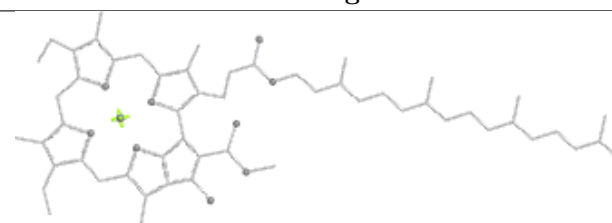
Ligand LHG d 409	
	
Bond lengths	Bond angles
	
Torsions	Rings

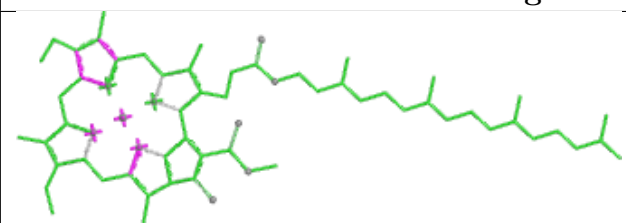
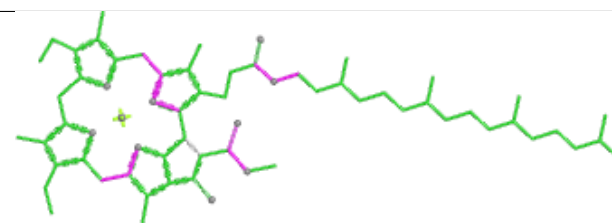
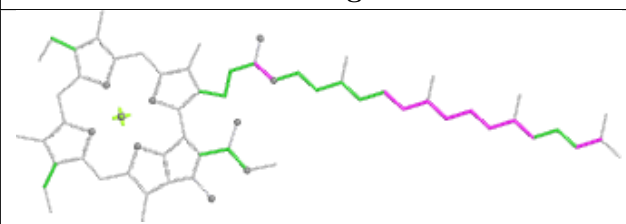
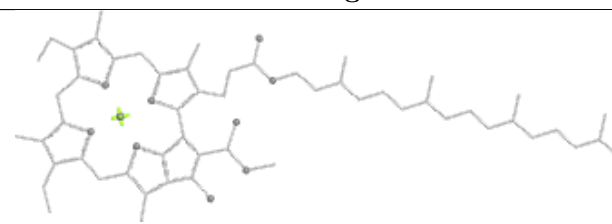
Ligand STE B 627	
	
Bond lengths	Bond angles
	
Torsions	Rings

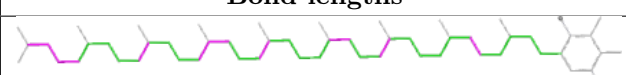
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Bond lengths	Bond angles
	
Torsions	Rings

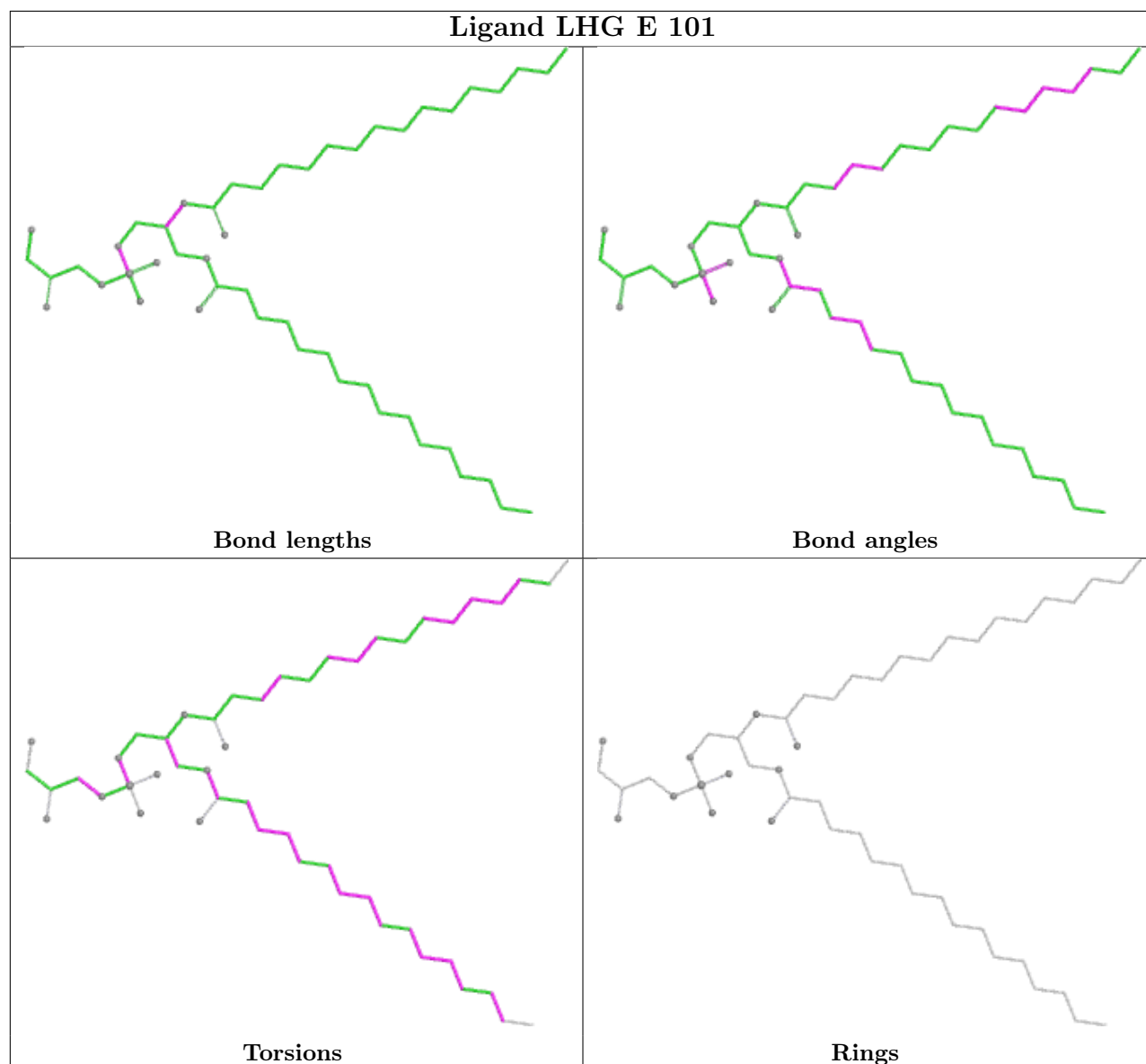
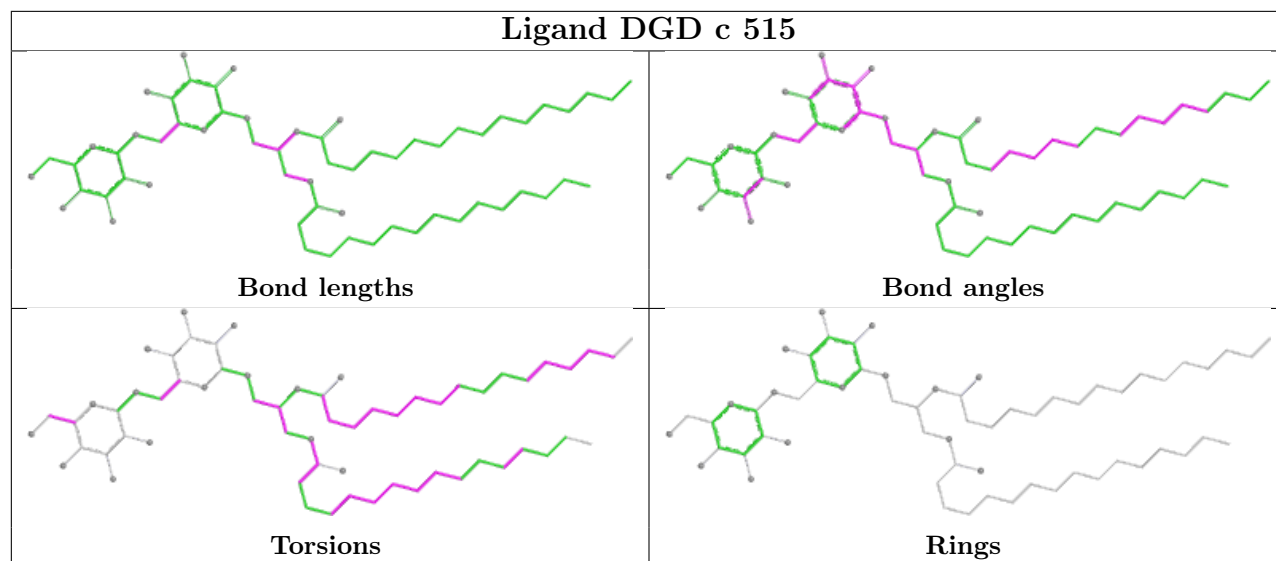


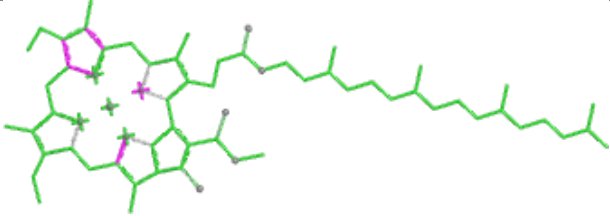
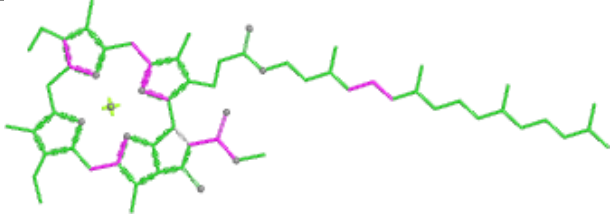
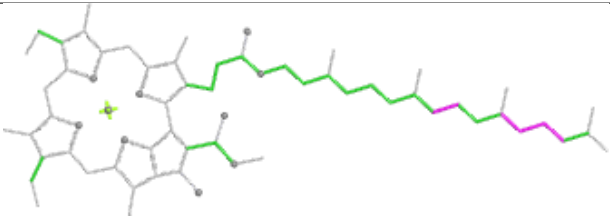
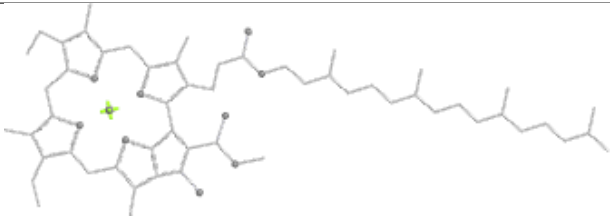
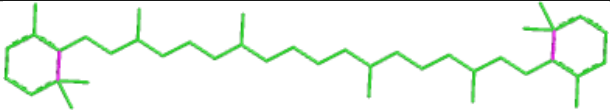
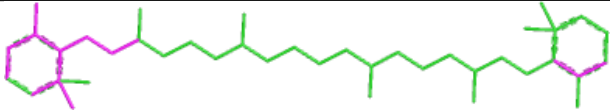
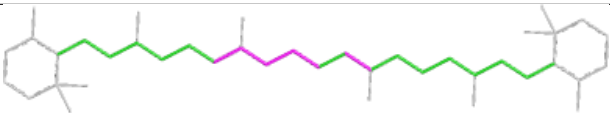
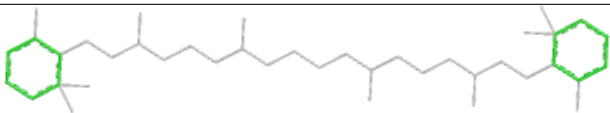
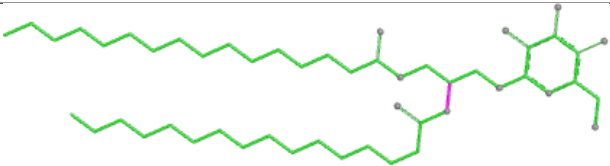
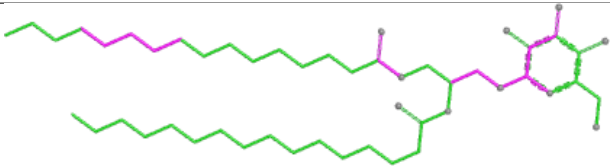
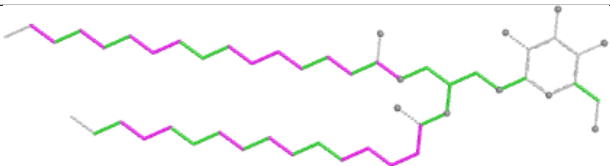
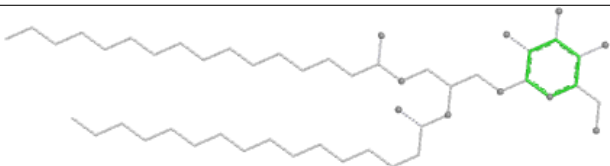


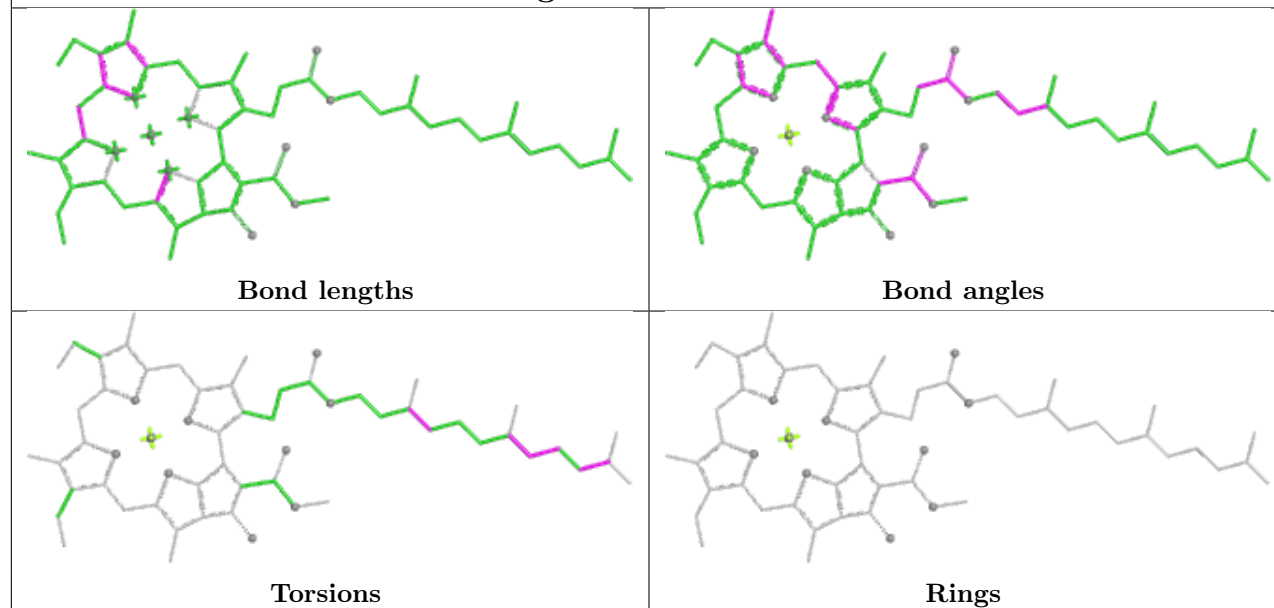
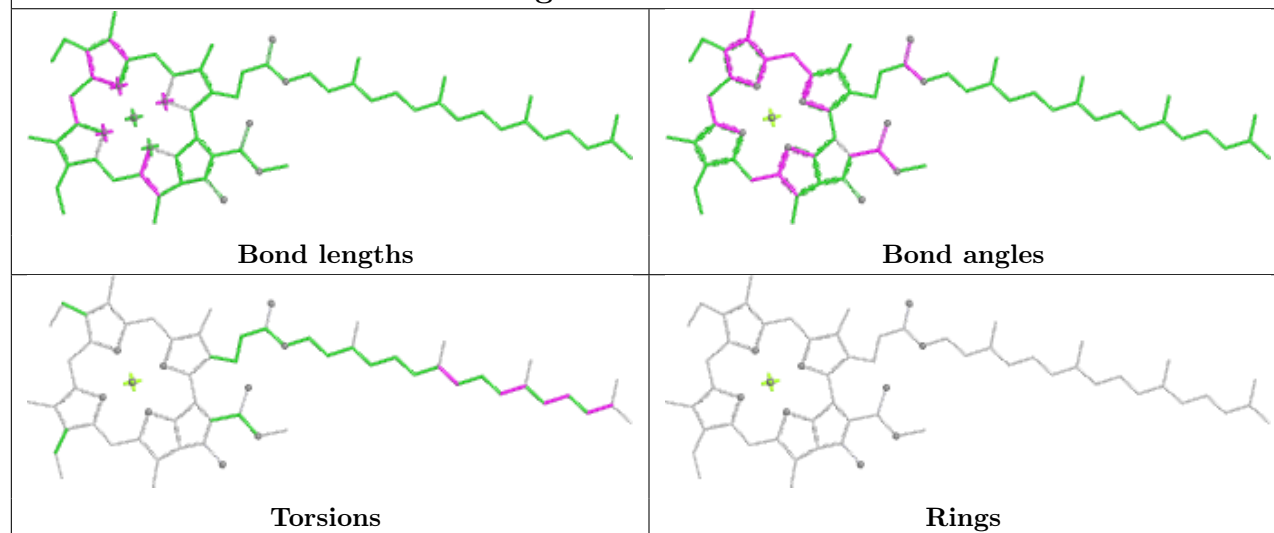
Ligand CLA C 512	
	
Bond lengths	Bond angles
	
Torsions	Rings

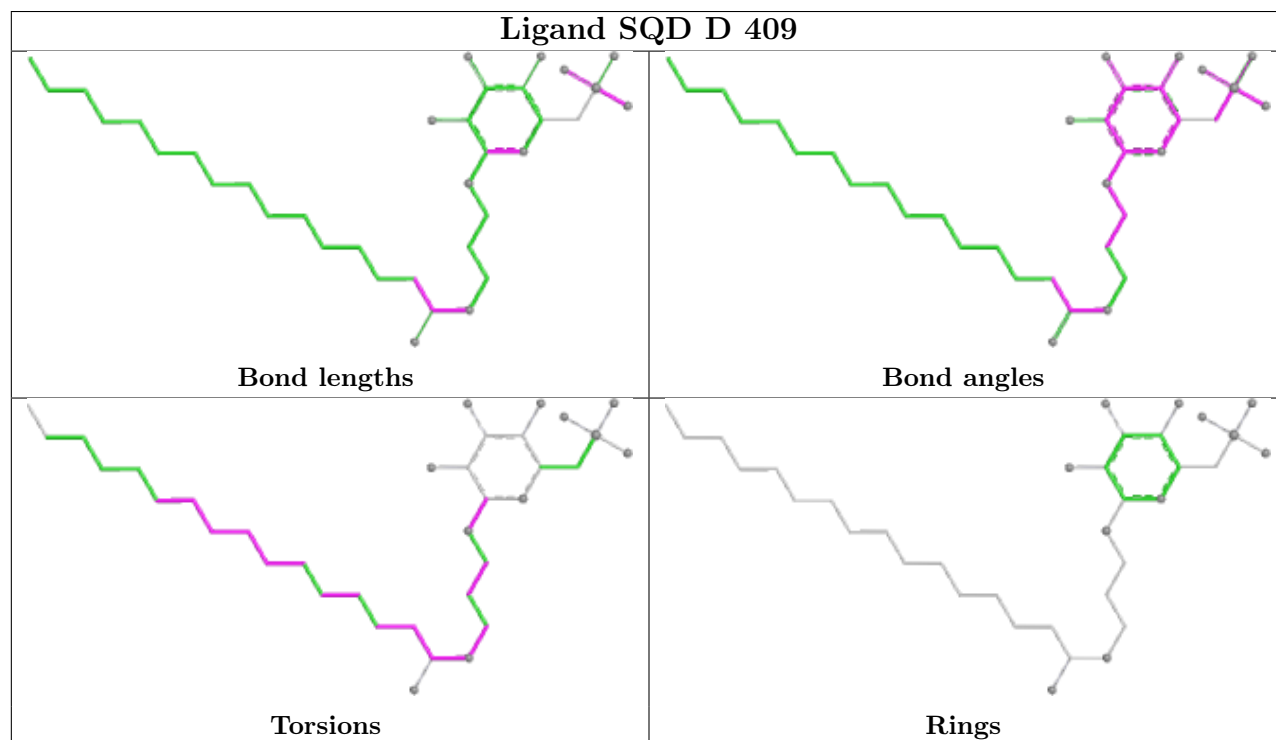
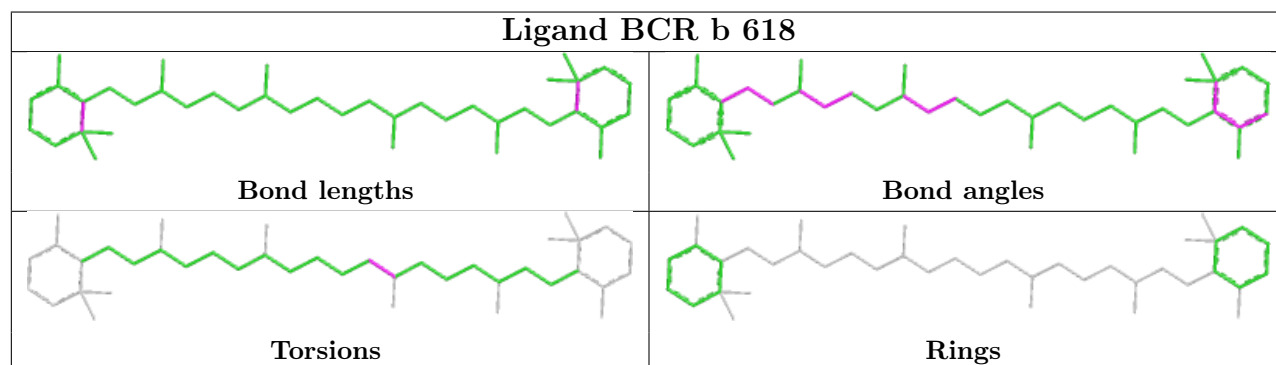
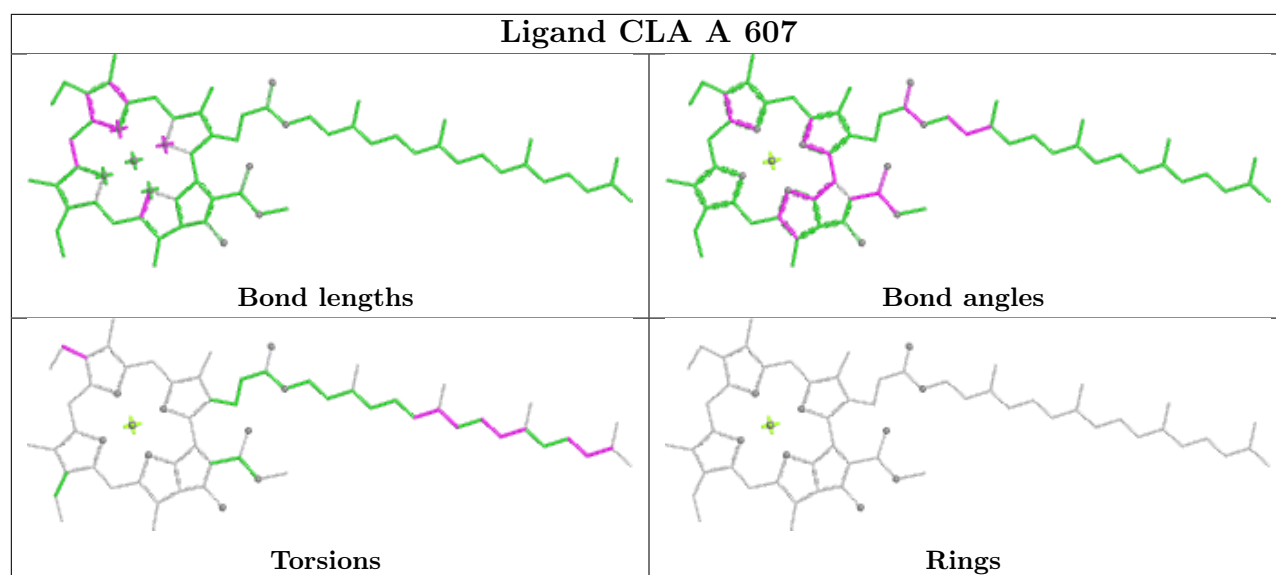
Ligand CLA b 607	
	
Bond lengths	Bond angles
	
Torsions	Rings

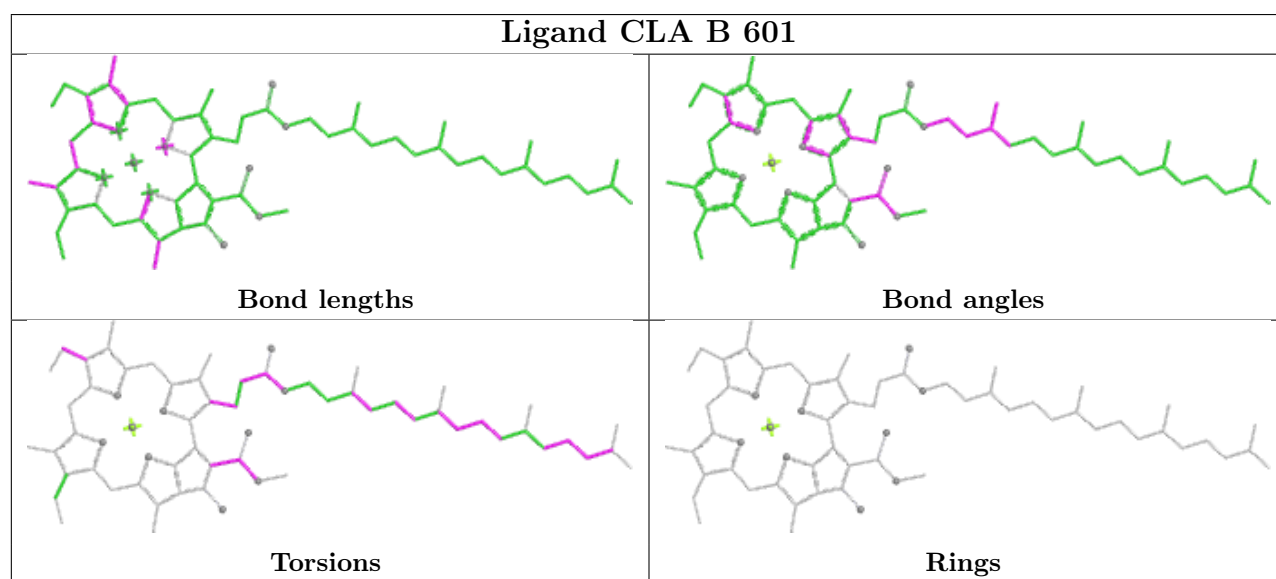
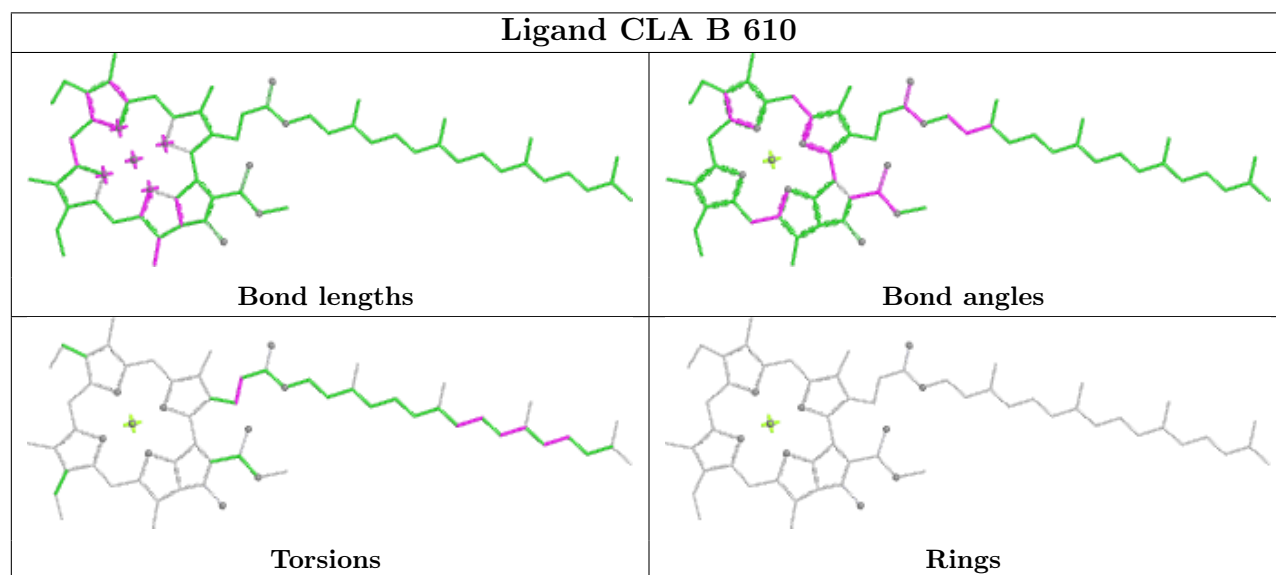
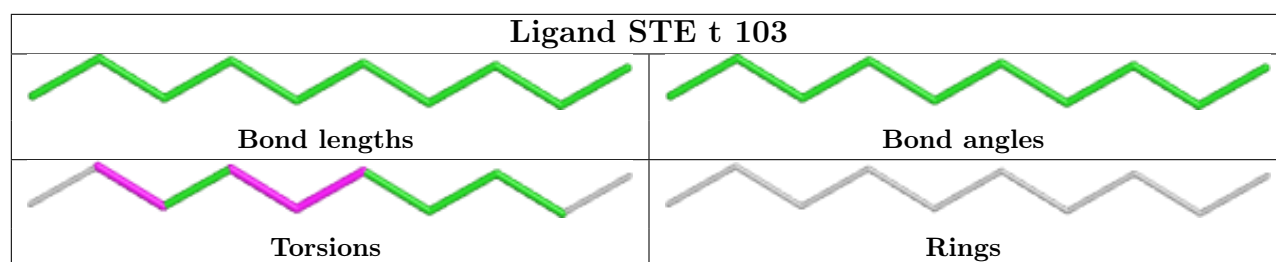
Ligand PL9 D 407	
	
Bond lengths	Bond angles
	
Torsions	Rings

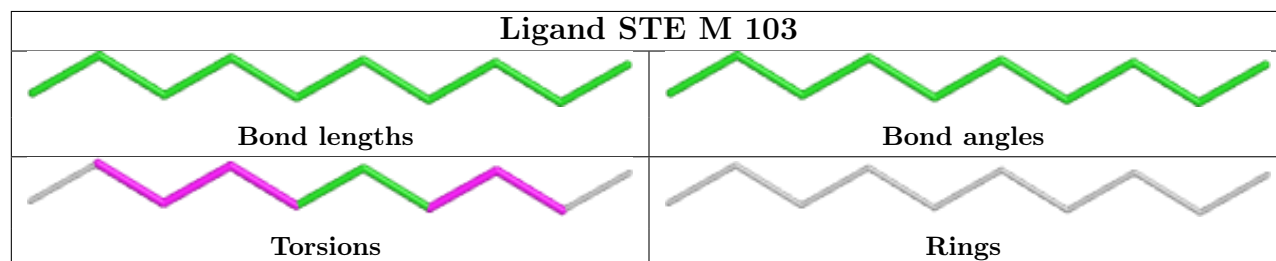
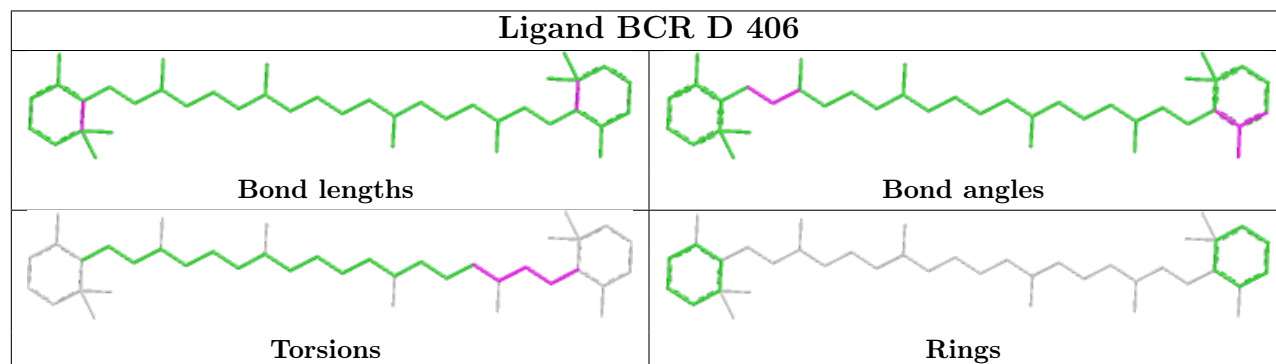
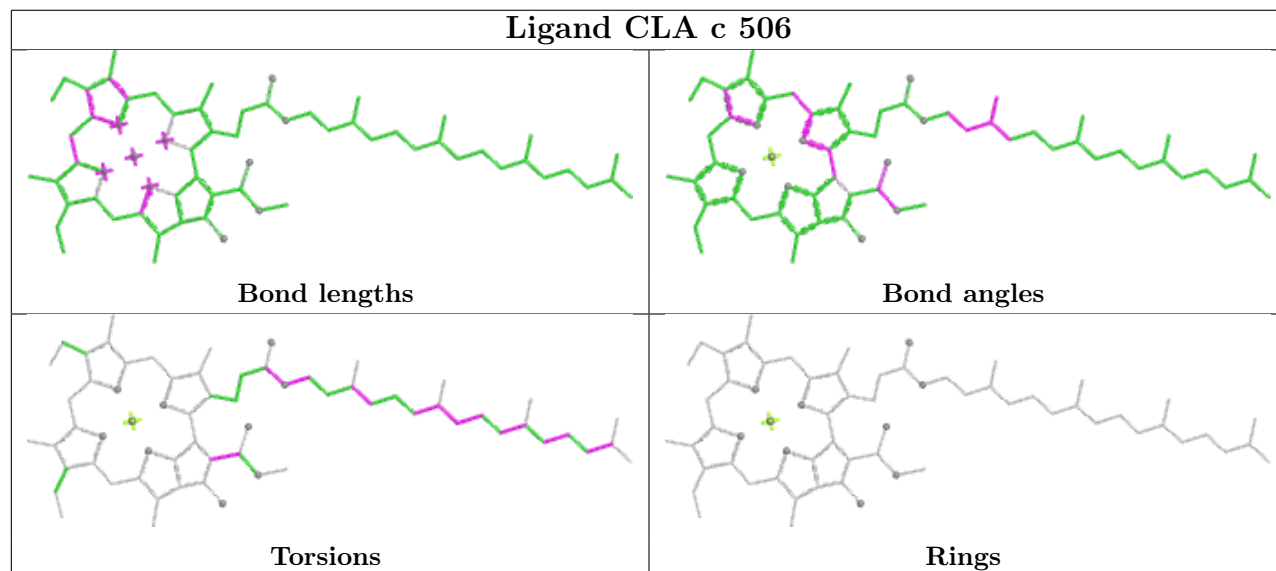
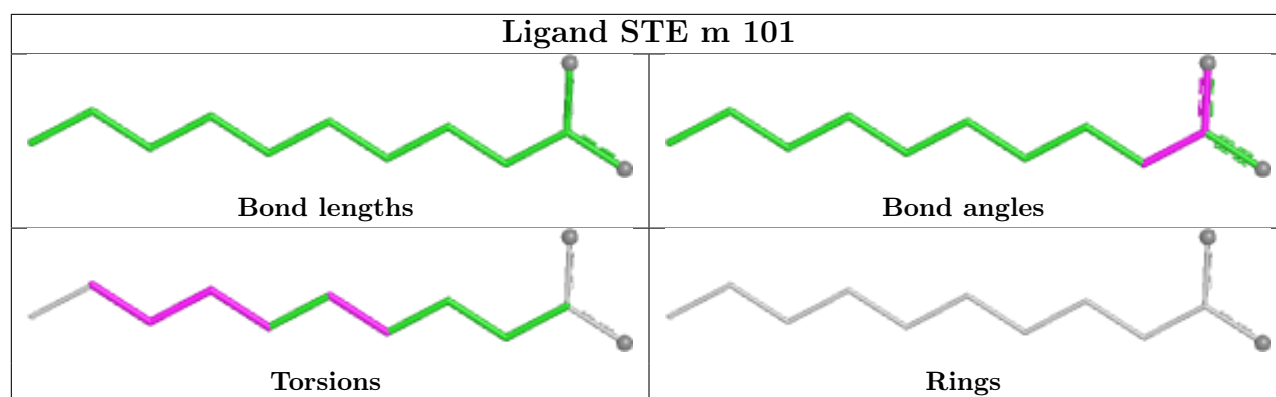


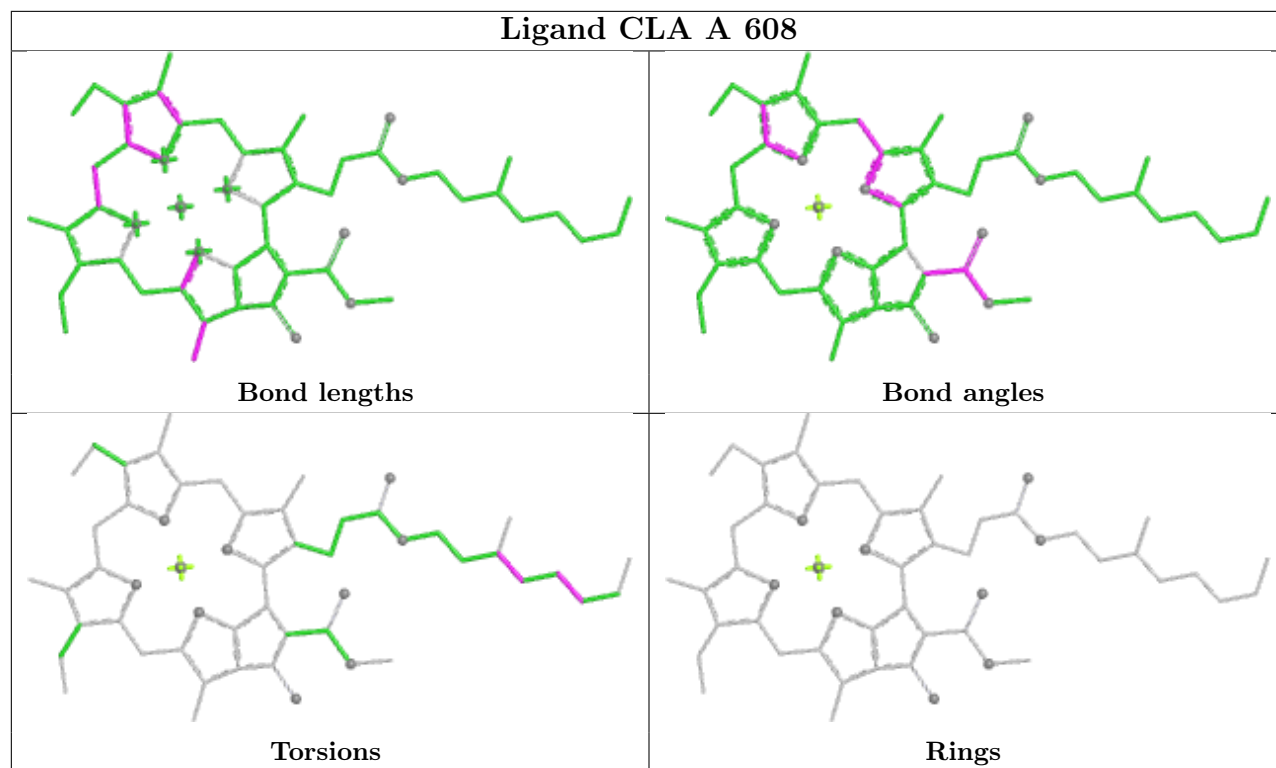
Ligand CLA b 611	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR T 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG b 622	
 Bond lengths	 Bond angles
 Torsions	 Rings

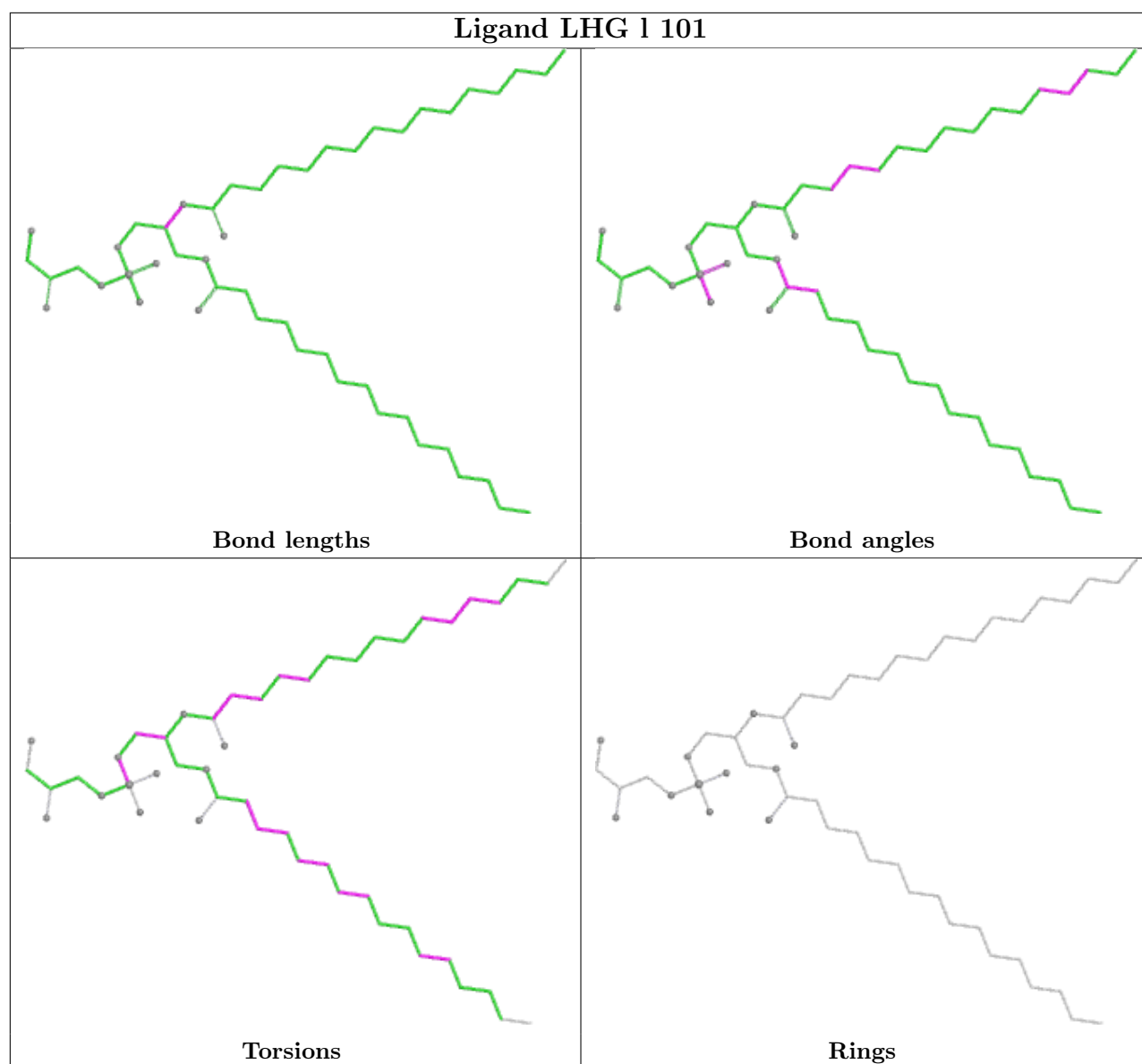
Ligand CLA c 504**Ligand CLA b 608**



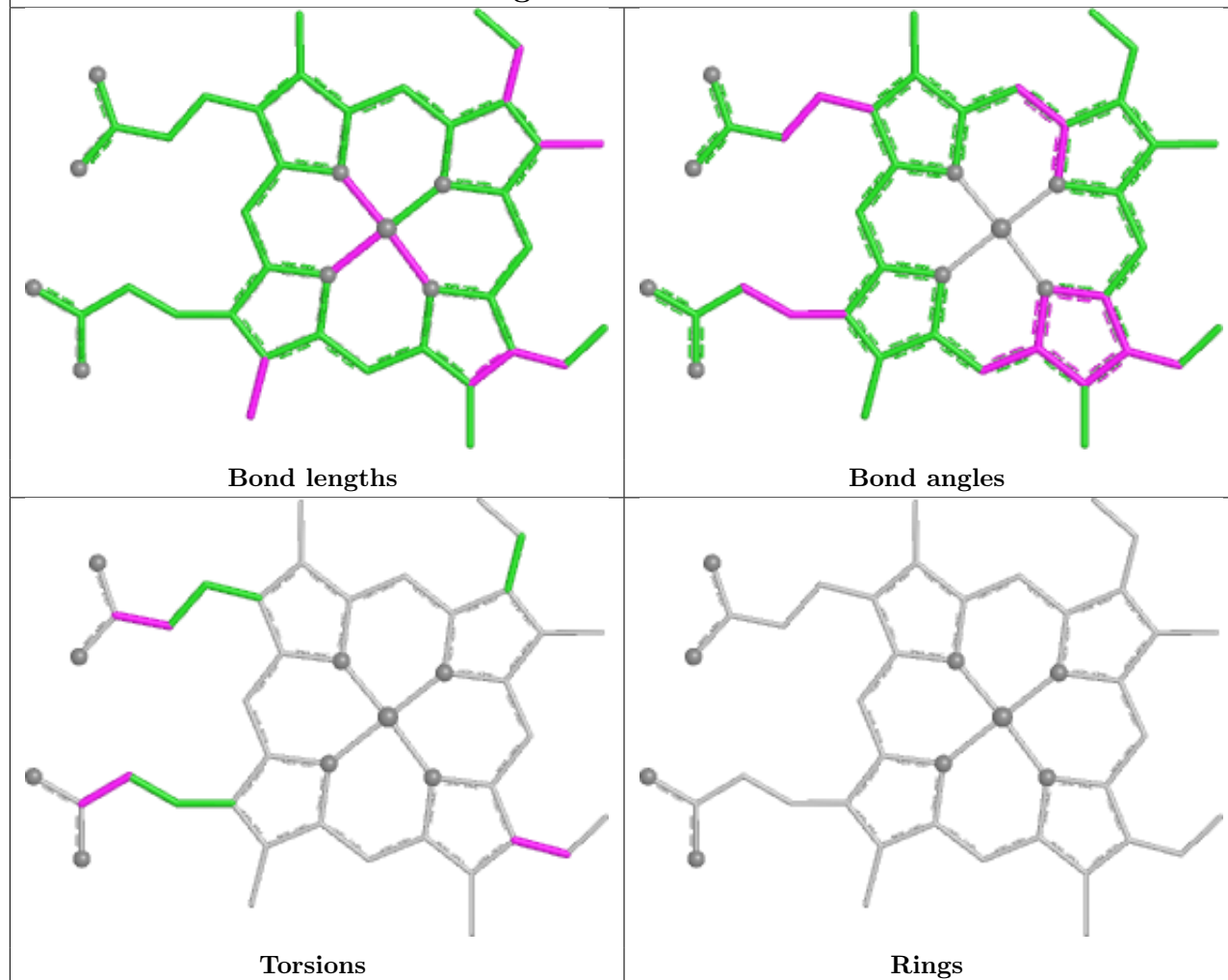




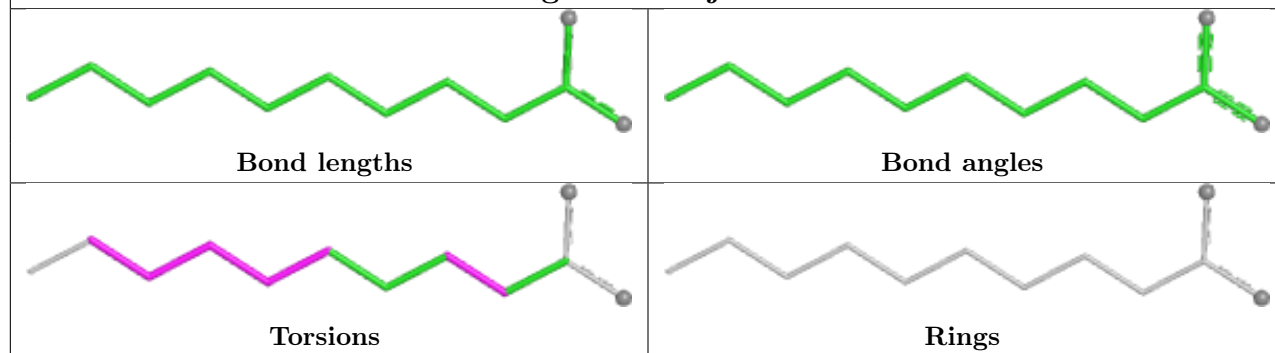


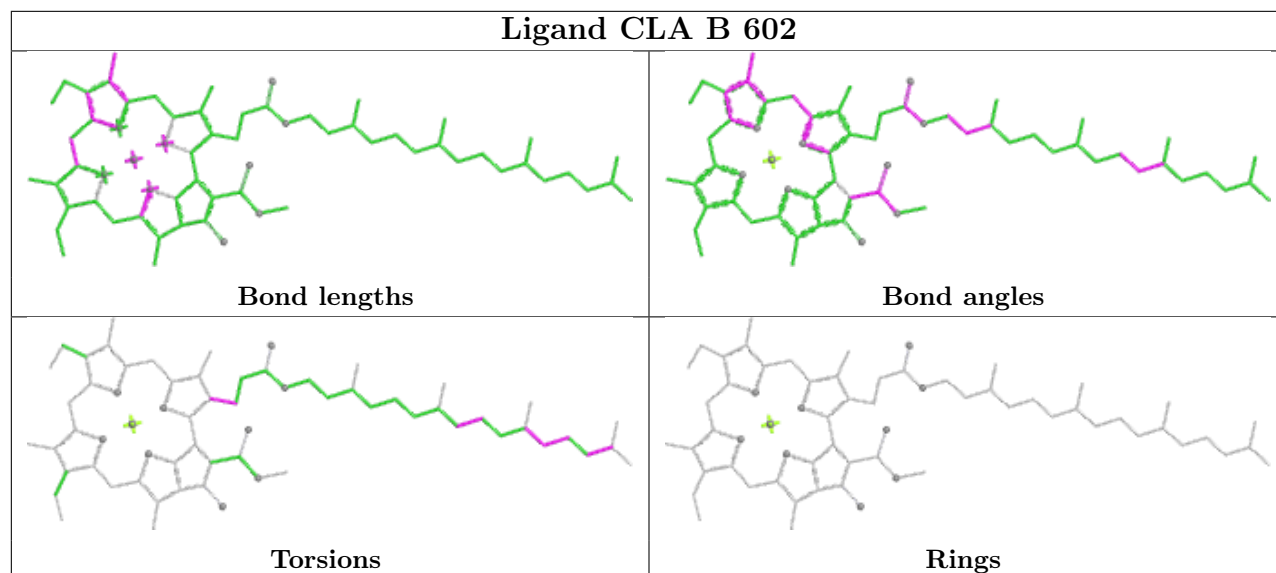
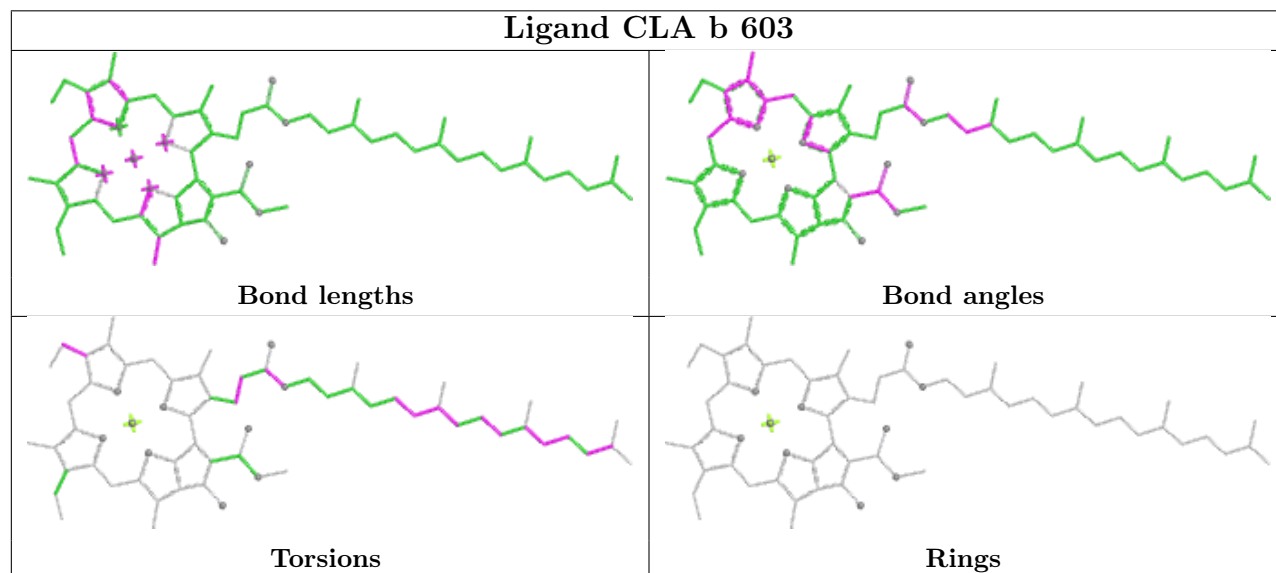
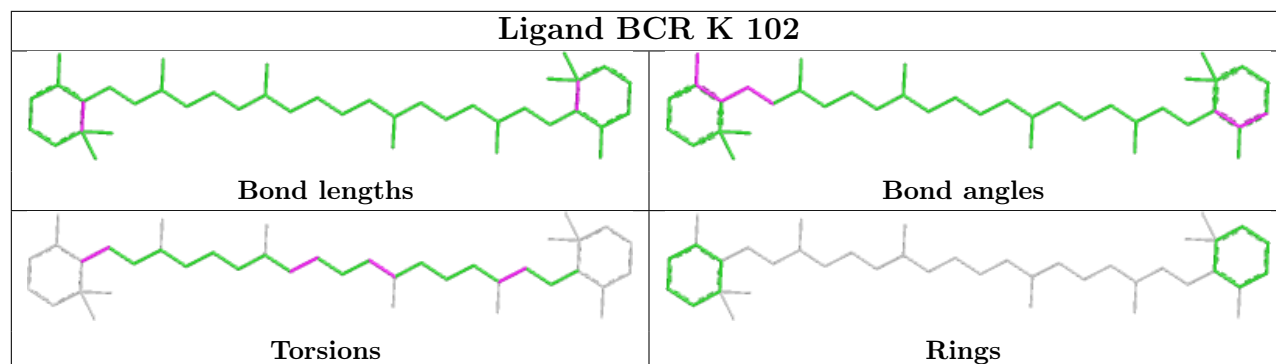


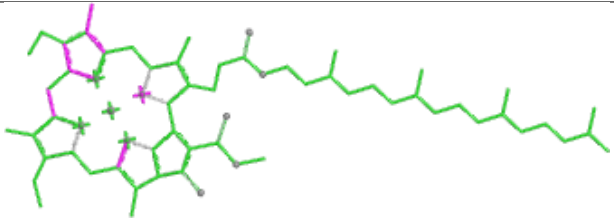
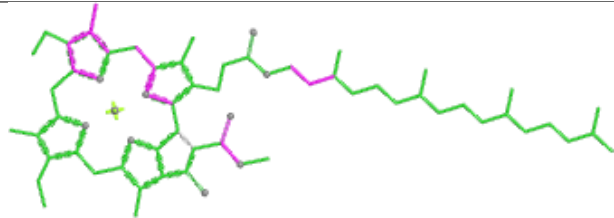
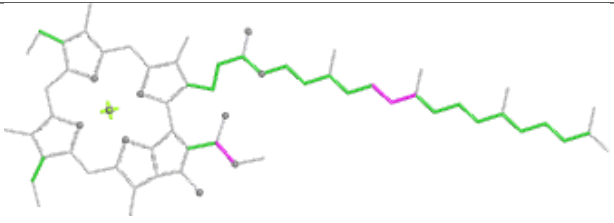
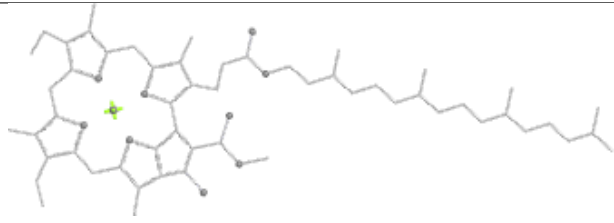
Ligand HEM f 101

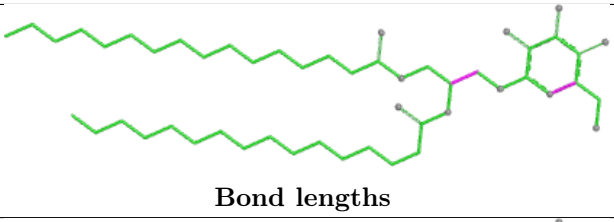
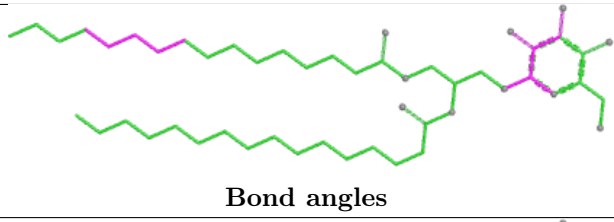
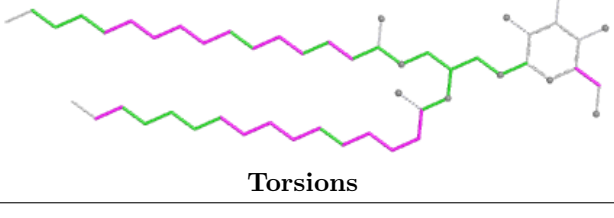
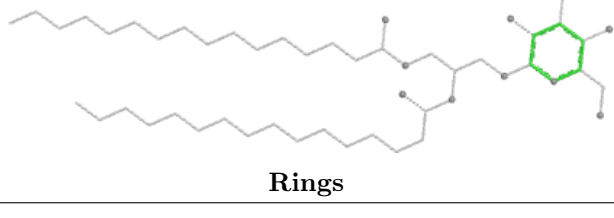


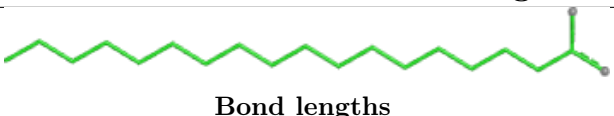
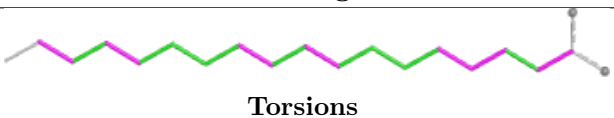
Ligand STE j 101

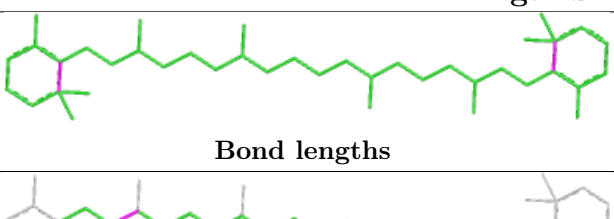
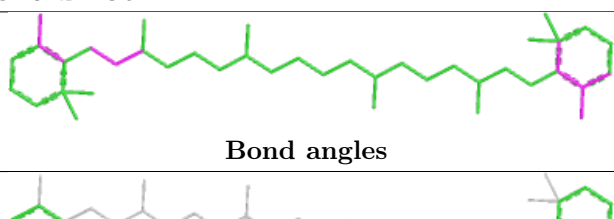


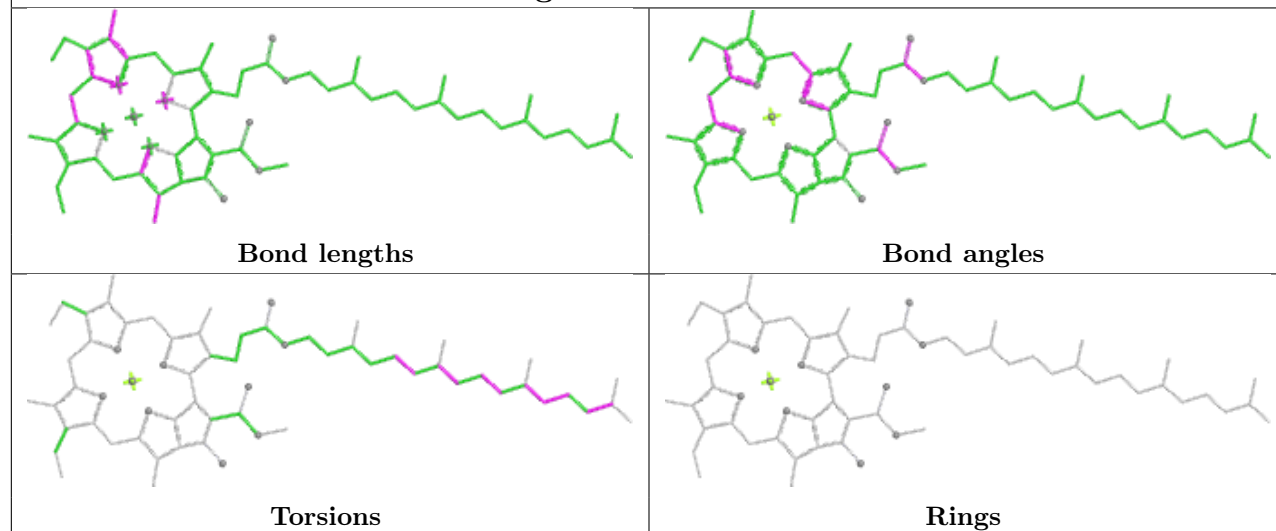
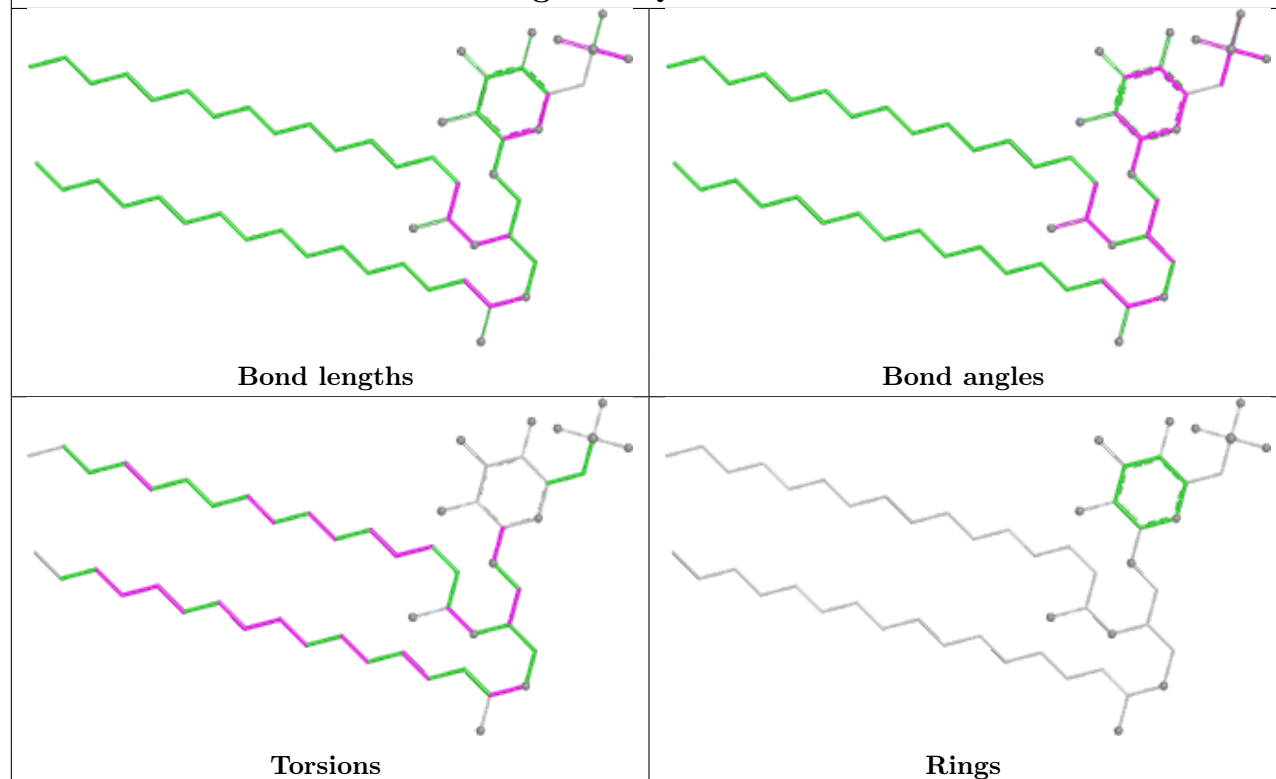


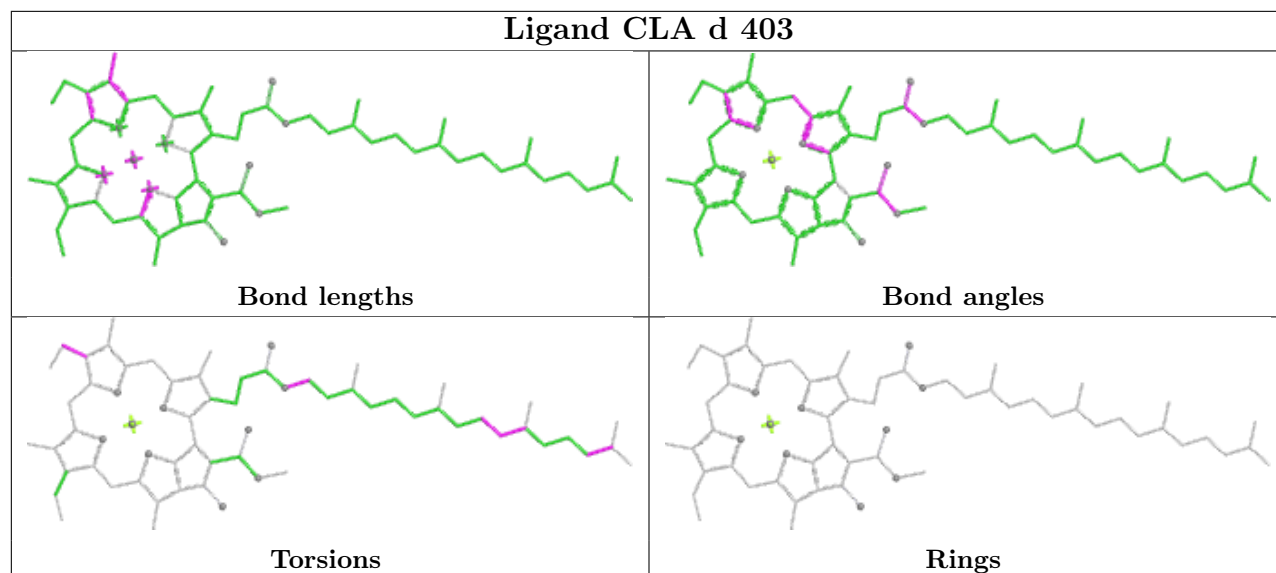
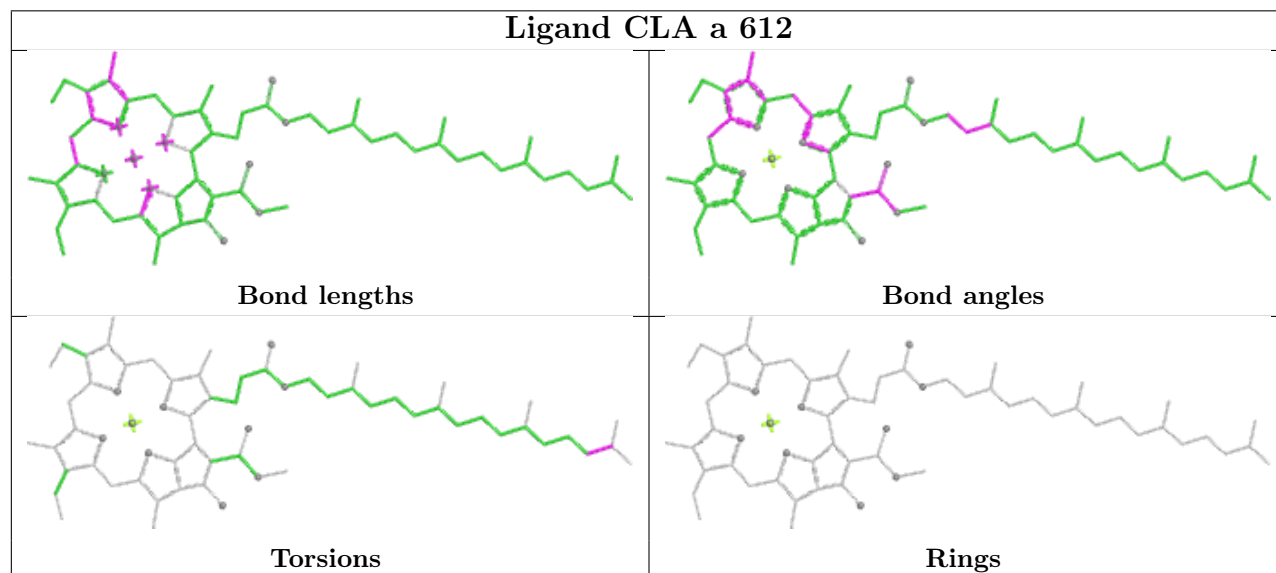
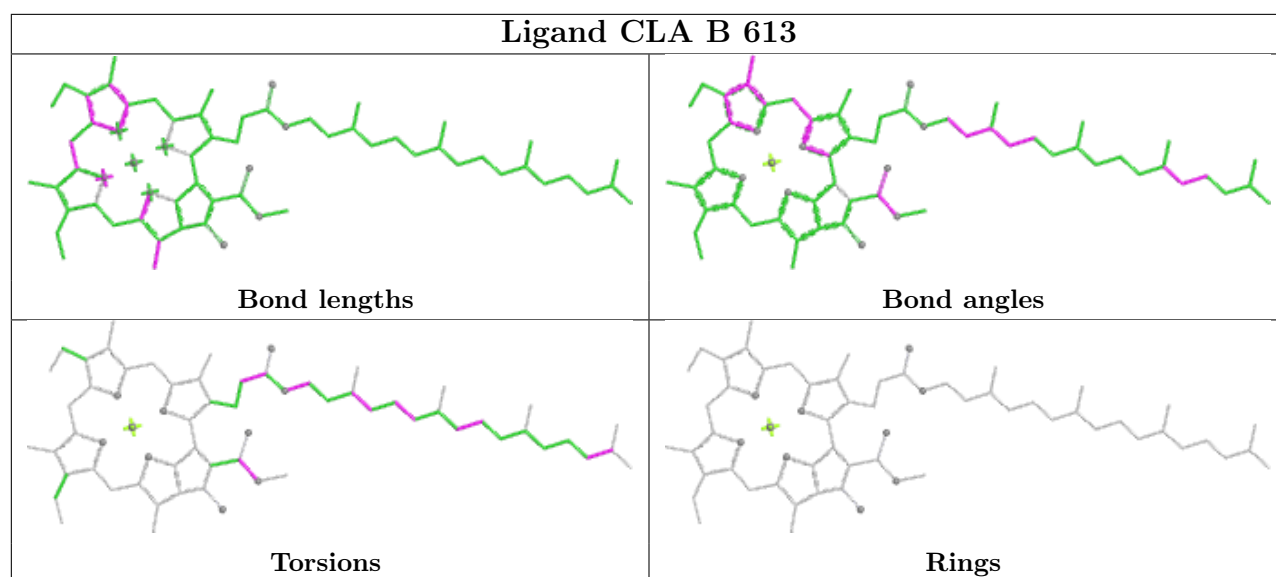
Ligand CLA c 513	
	
Bond lengths	Bond angles
	
Torsions	Rings

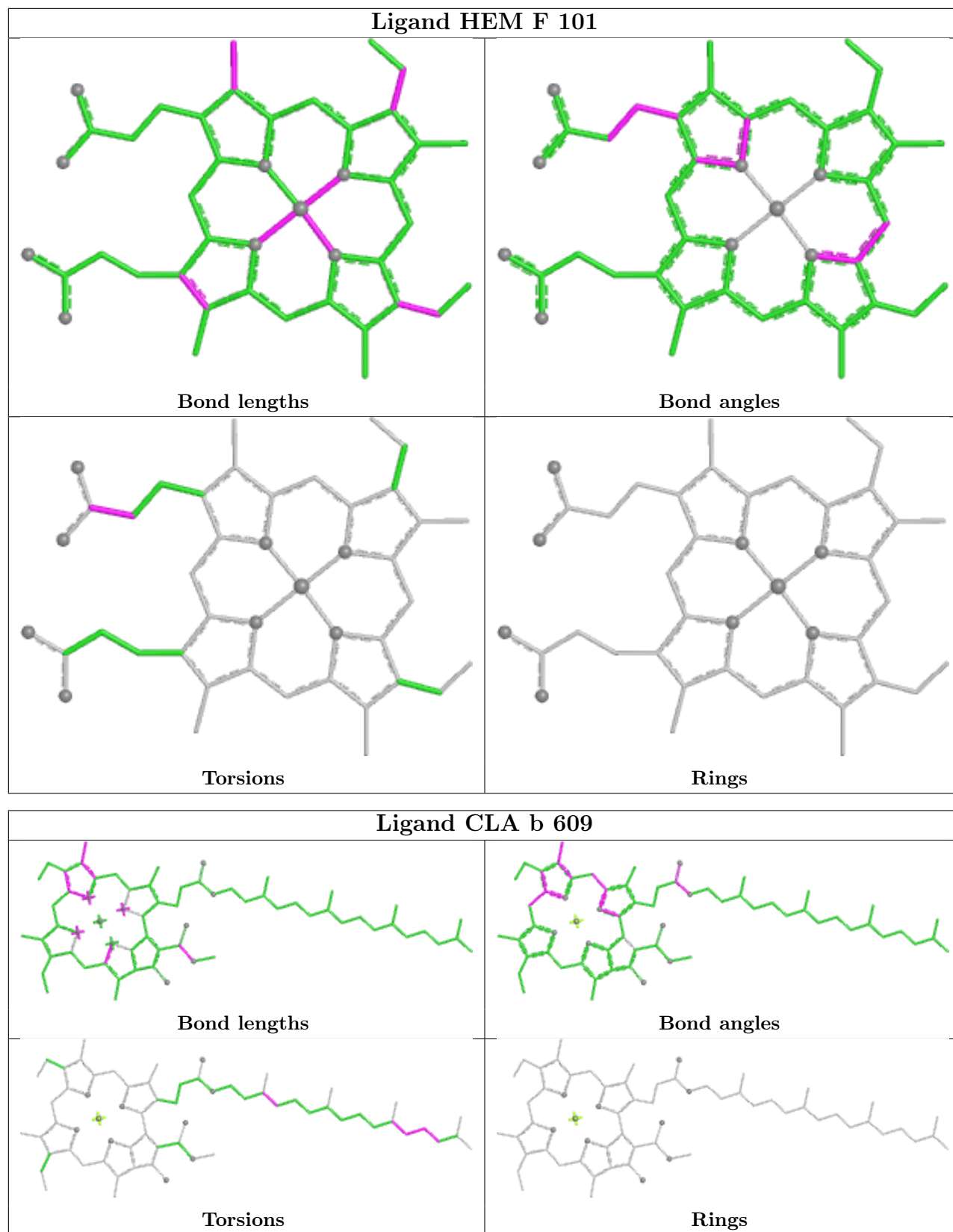
Ligand LMG D 408	
	
Bond lengths	Bond angles
	
Torsions	Rings

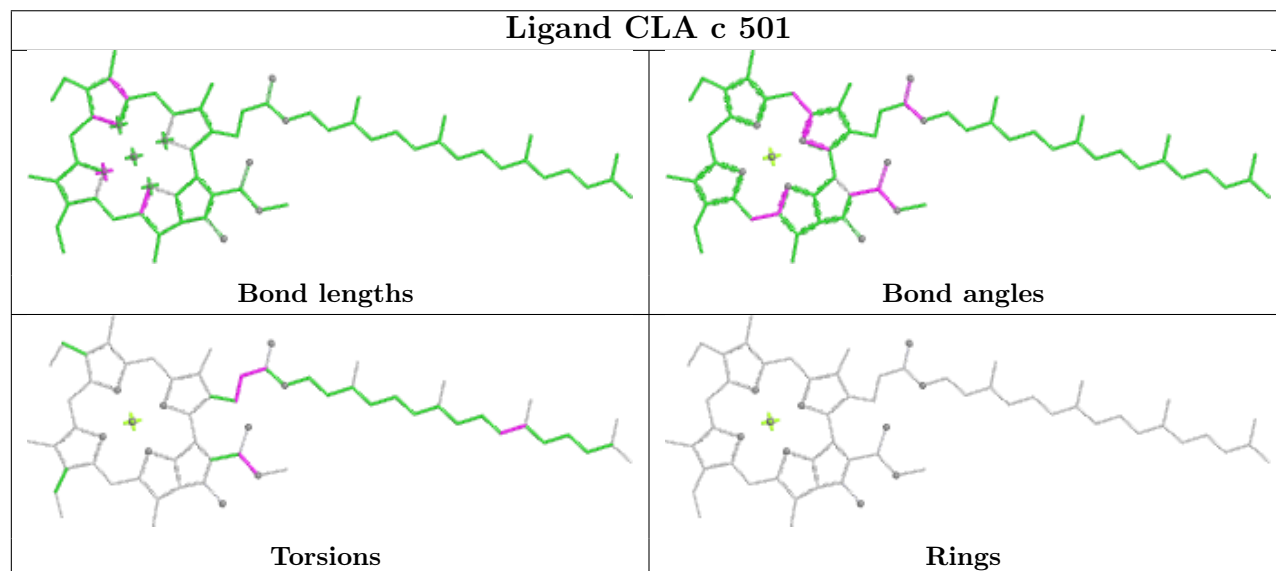
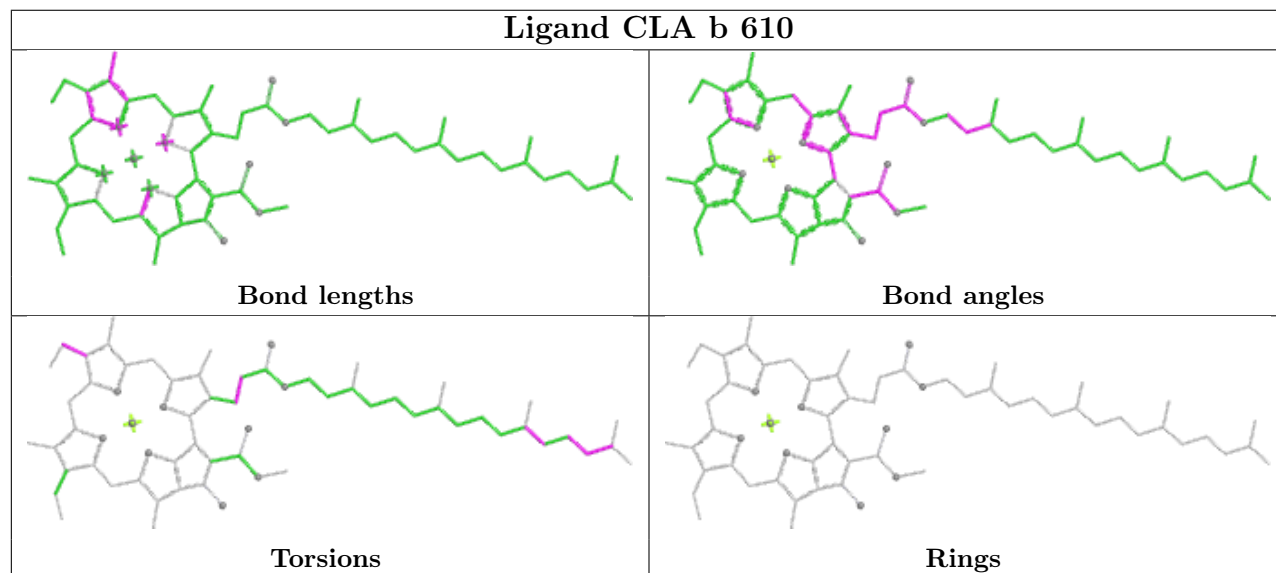
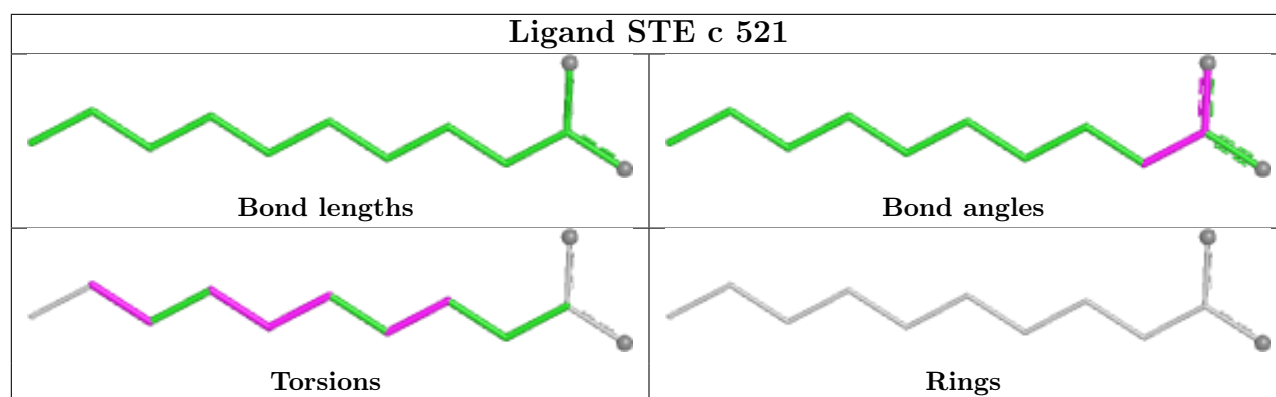
Ligand STE T 103	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR d 405	
	
Bond lengths	Bond angles
	
Torsions	Rings

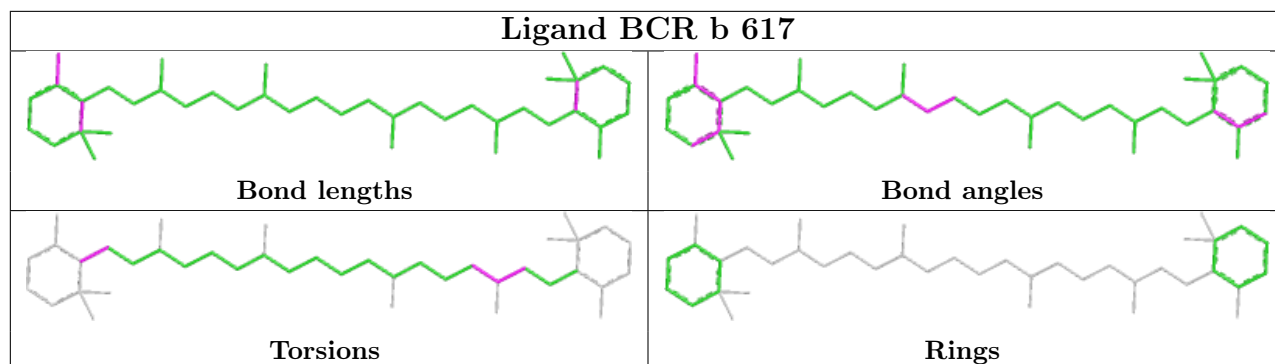
Ligand CLA b 615**Ligand SQD B 623**



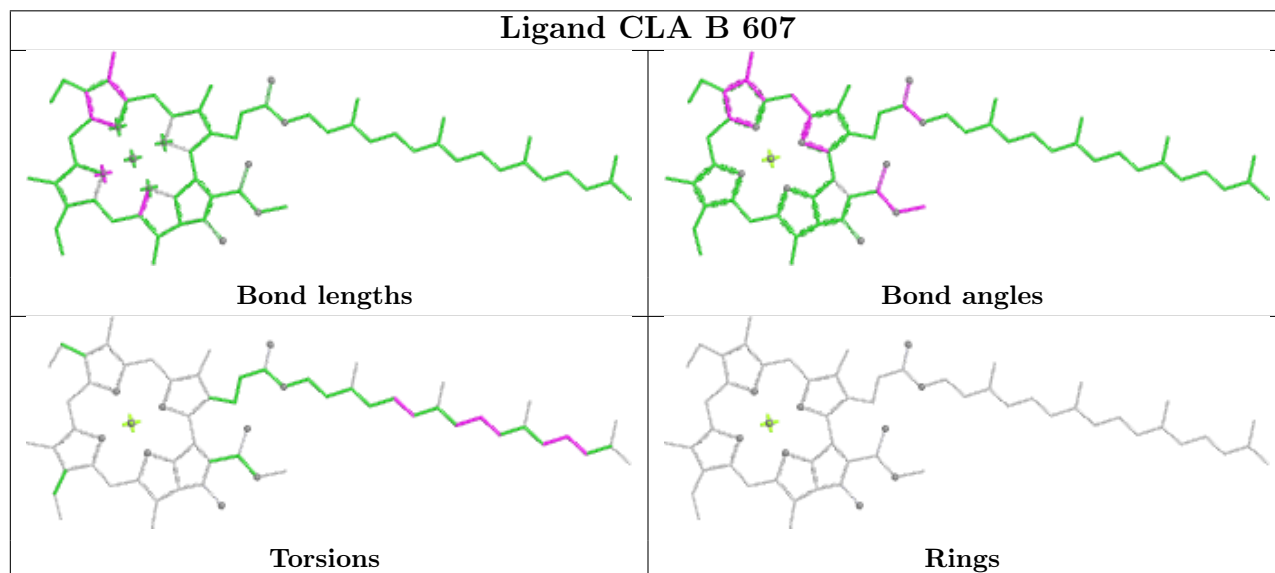




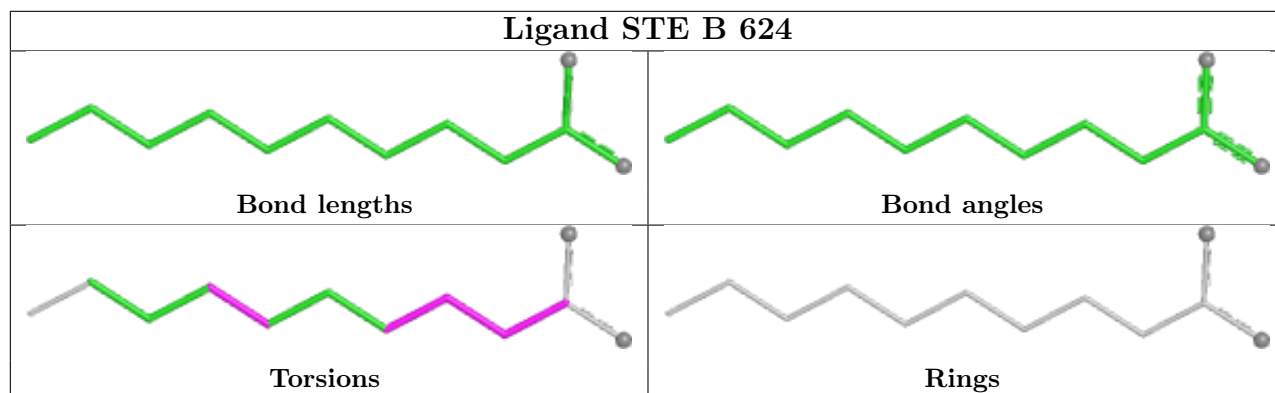
Ligand BCR b 617



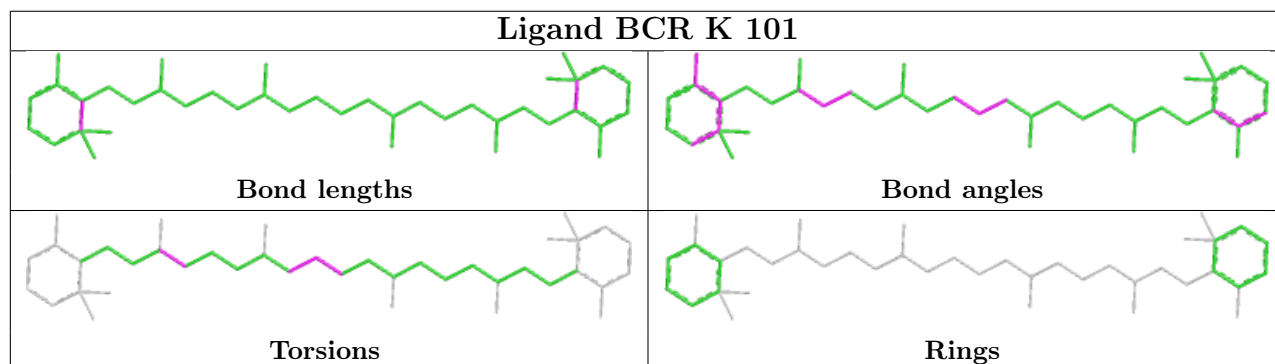
Ligand CLA B 607

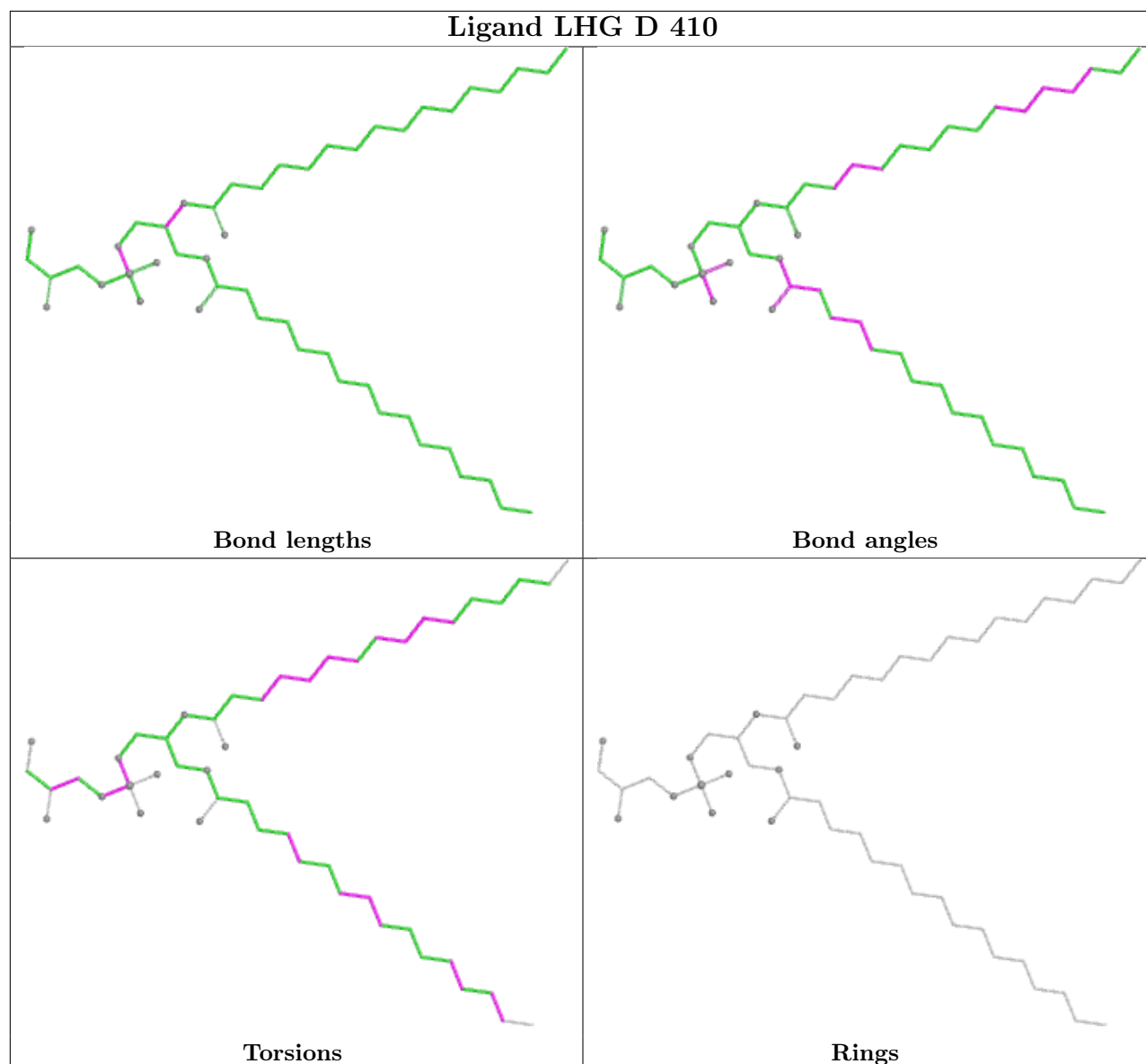
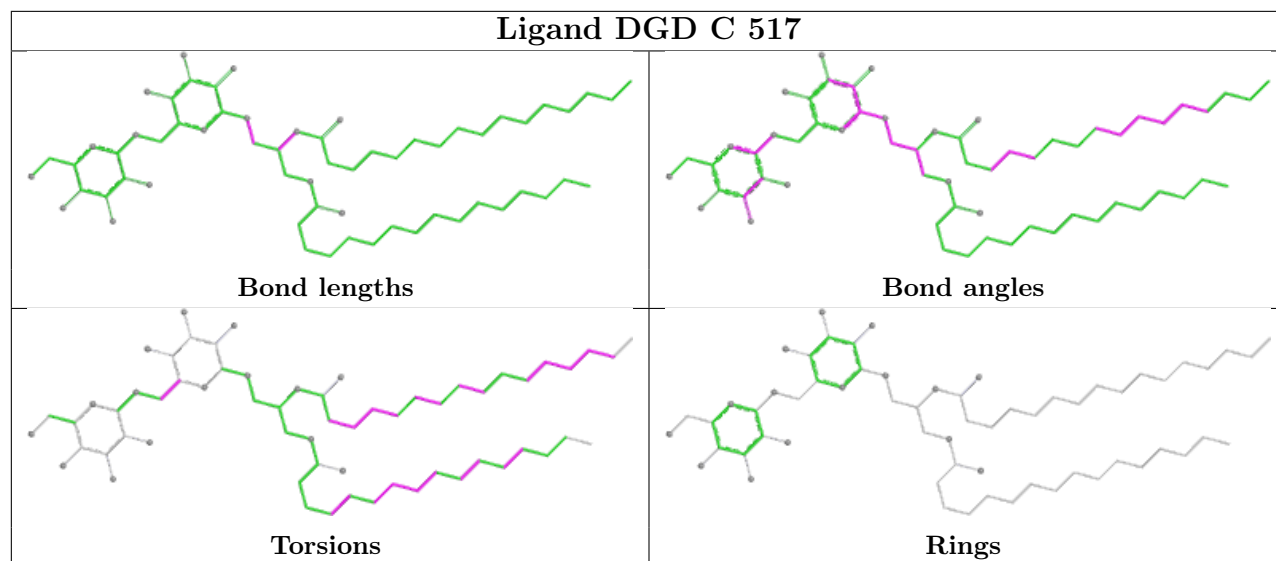


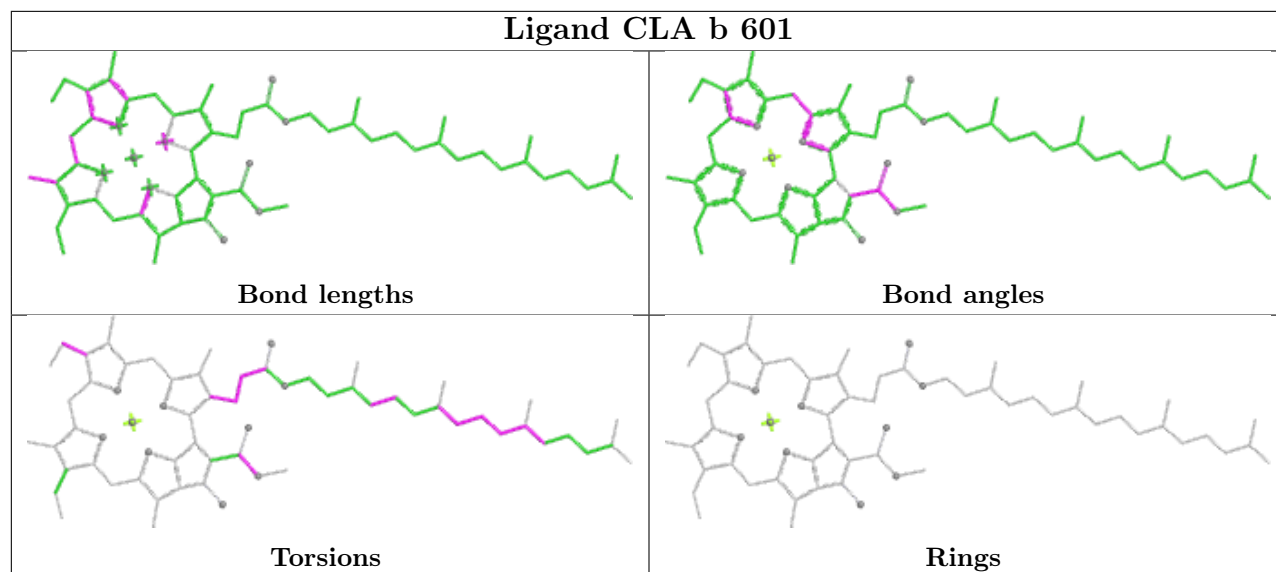
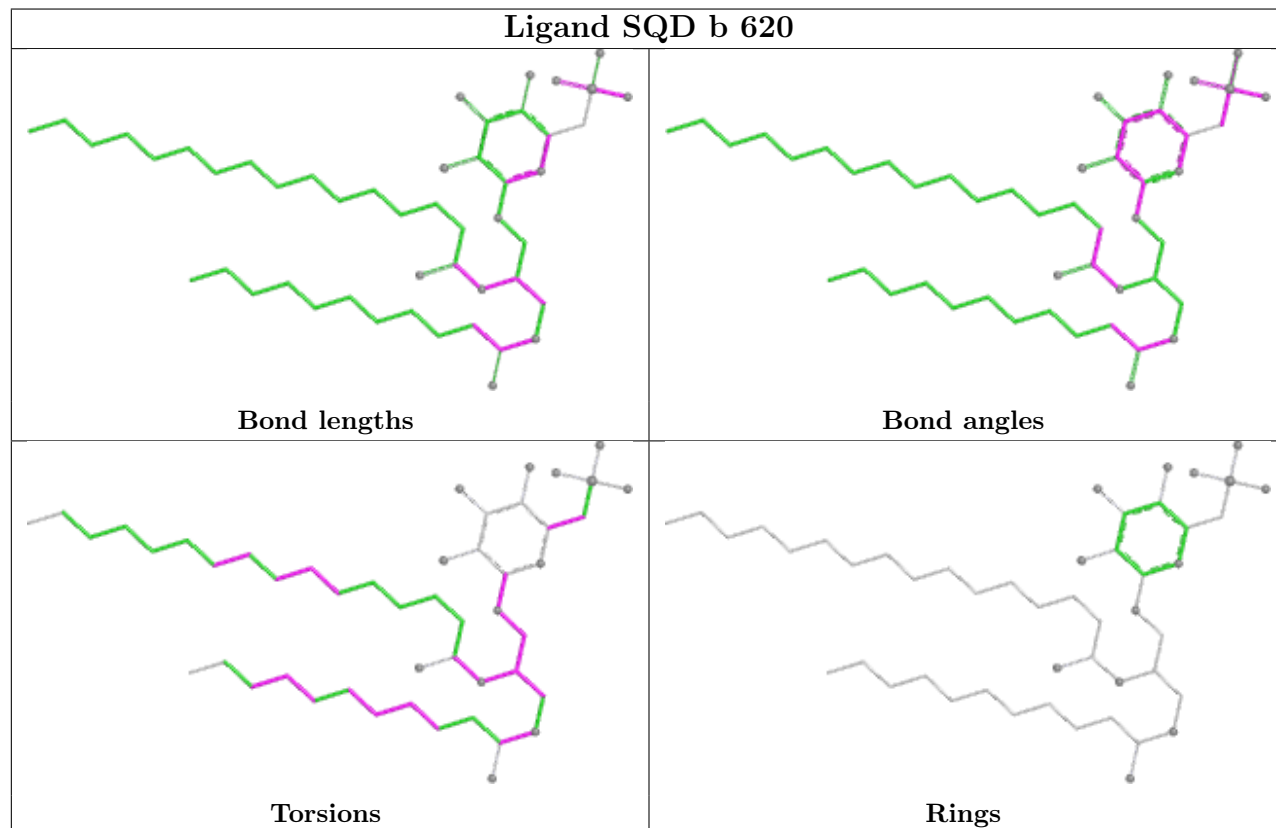
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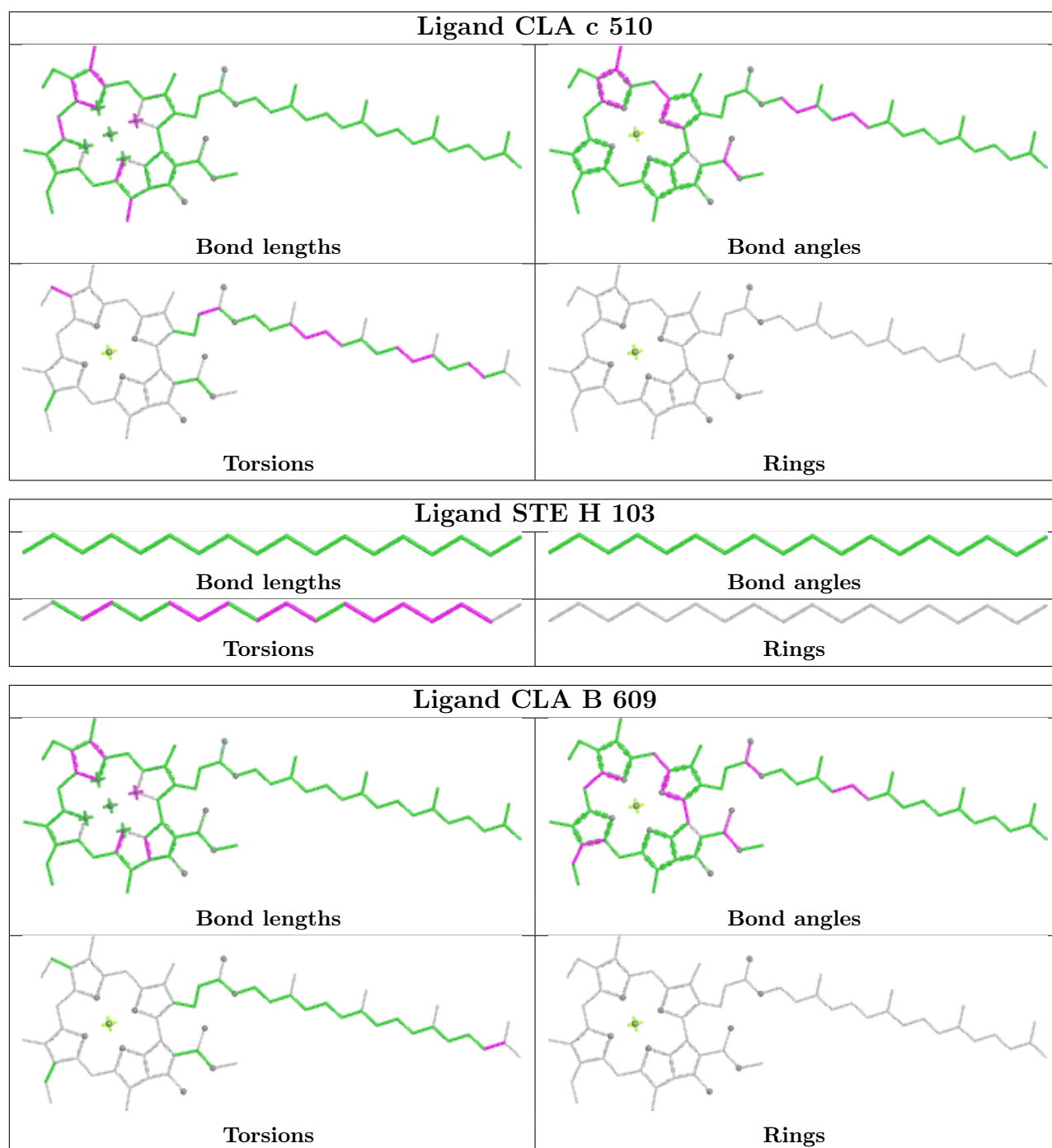


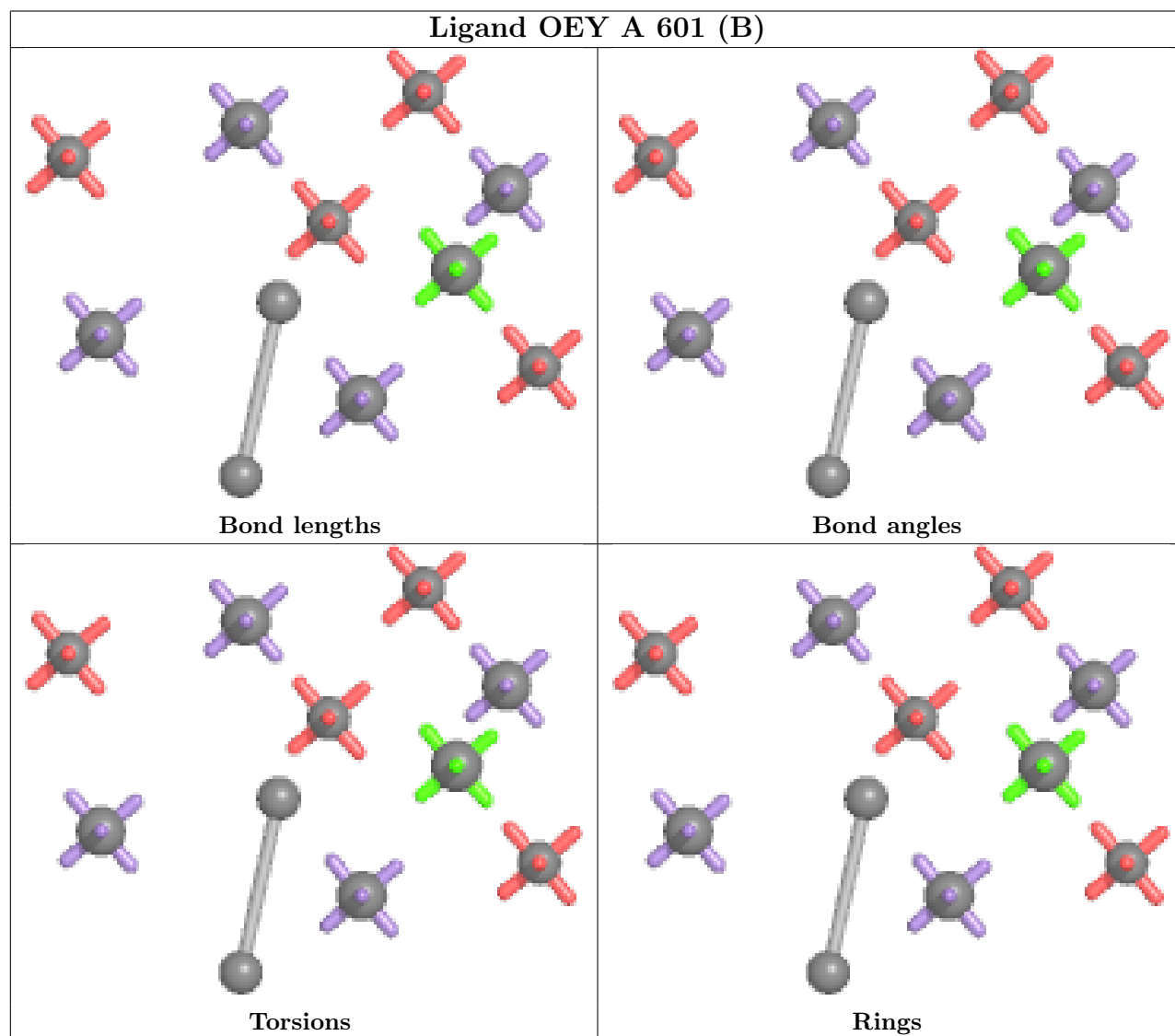
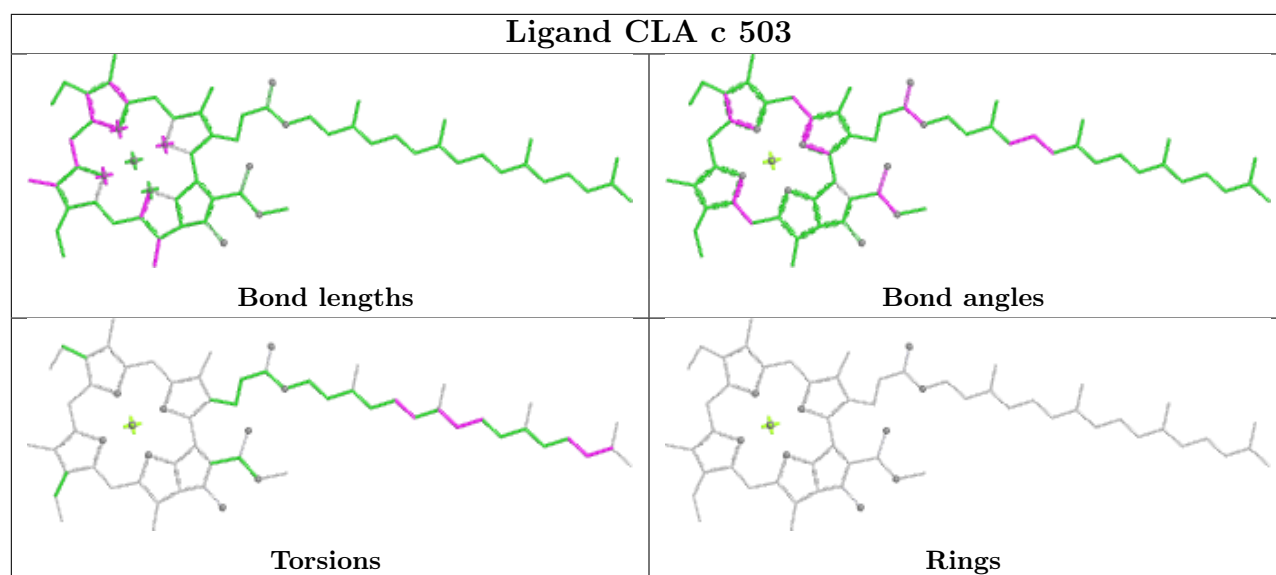
Ligand BCR K 101

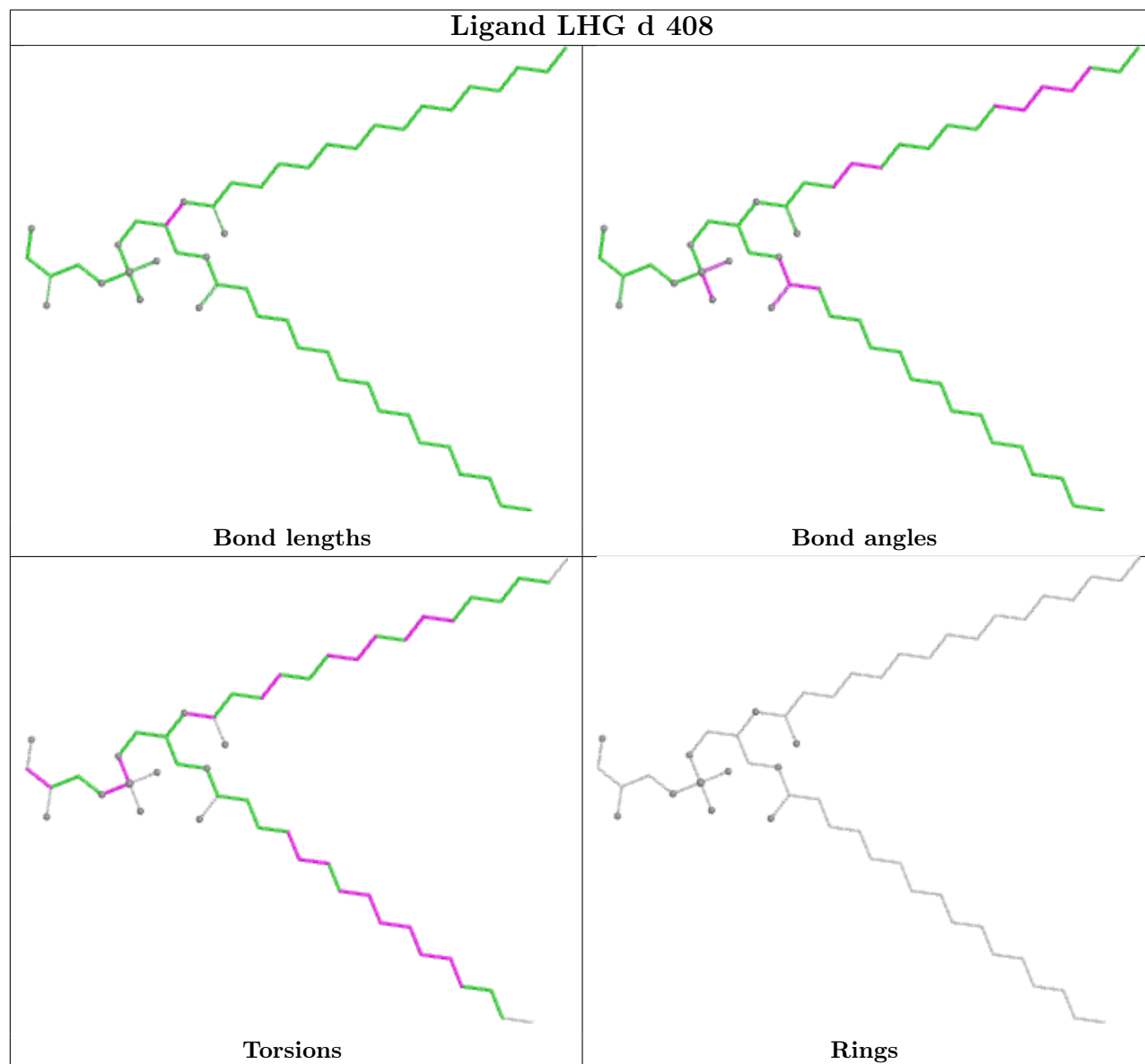
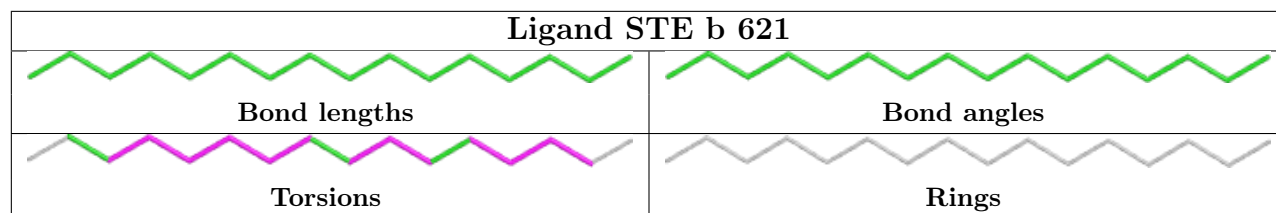


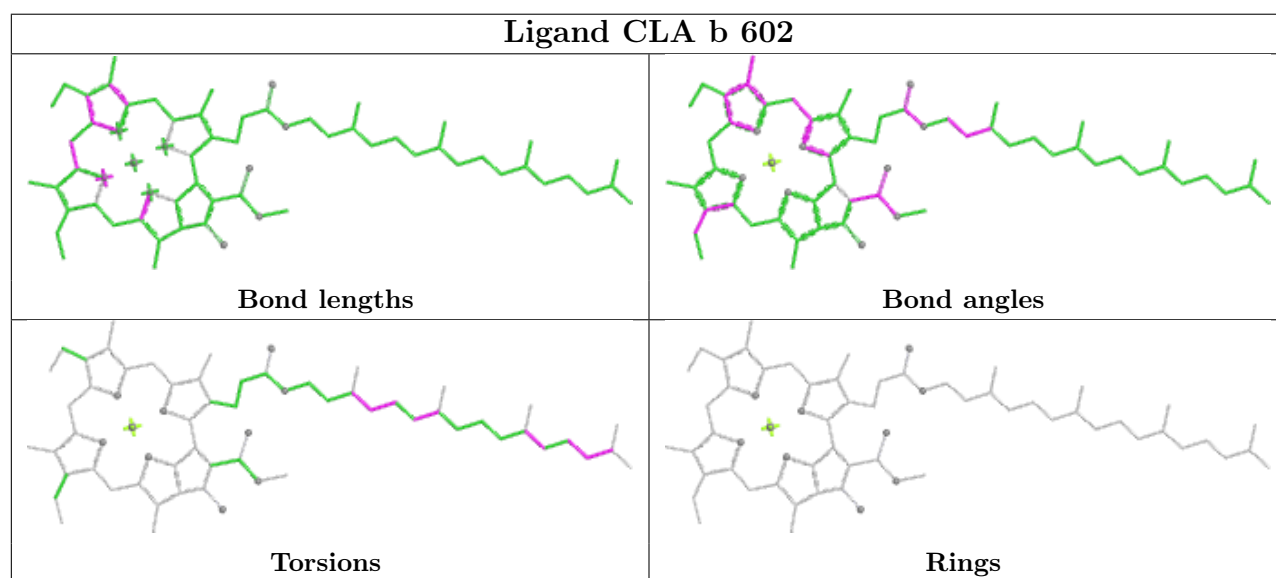
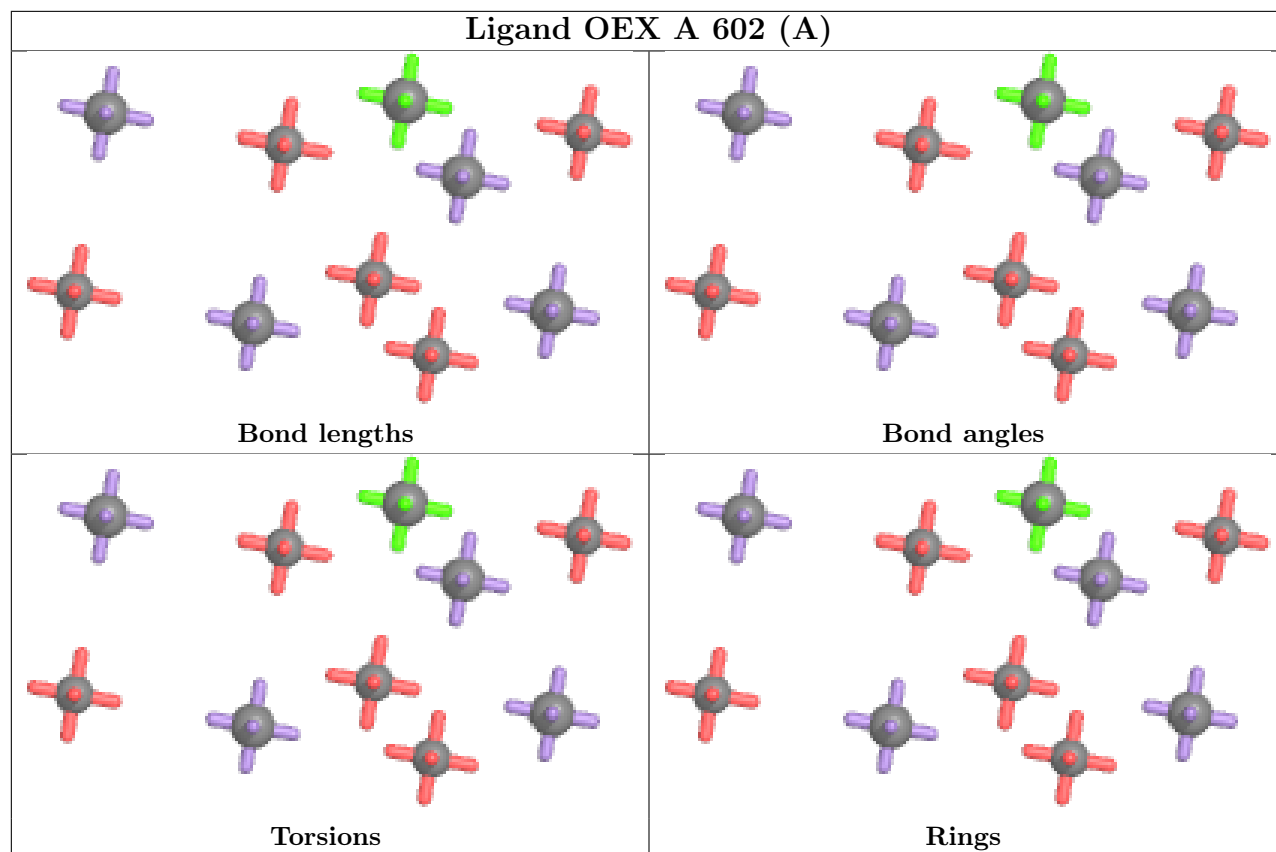


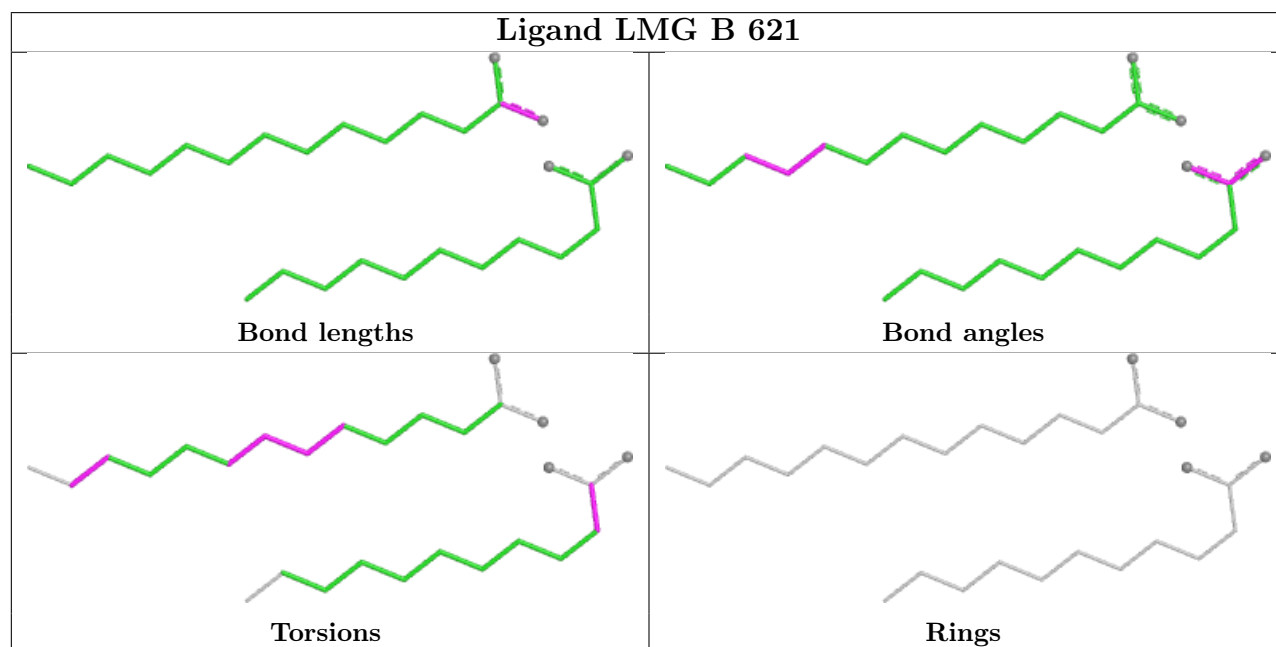
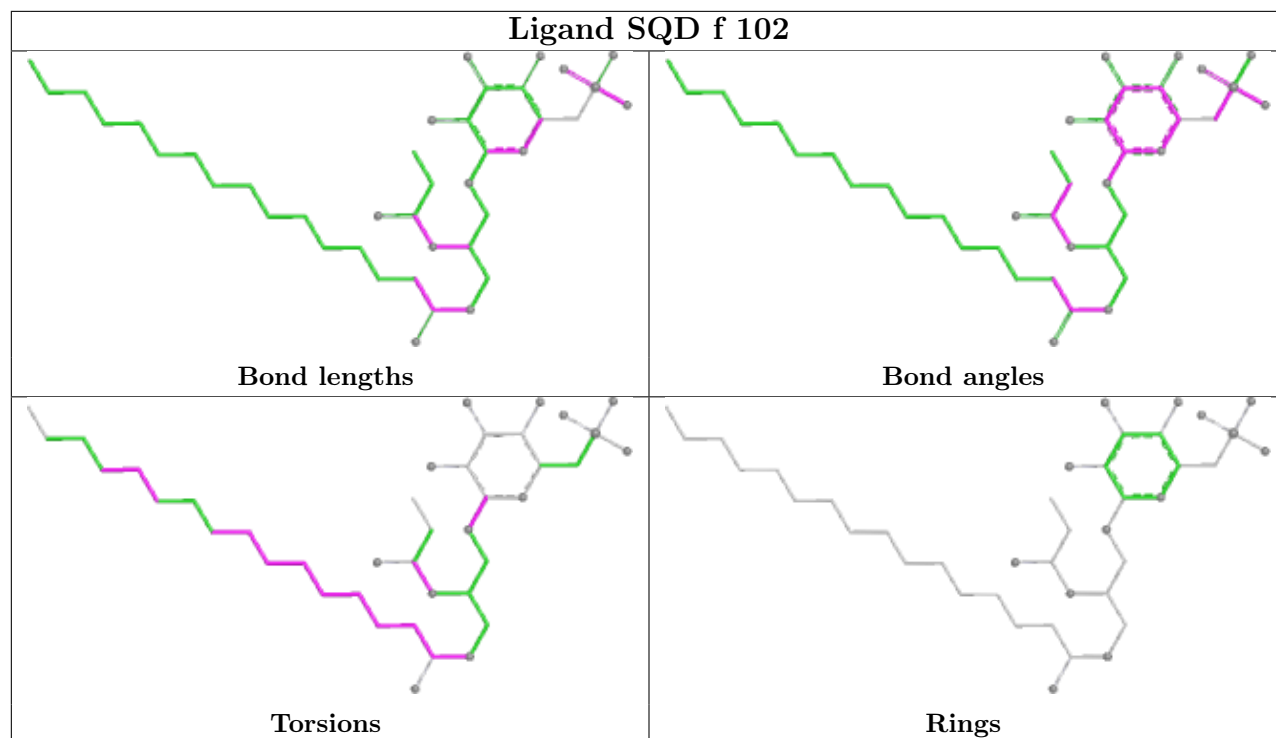
Ligand CLA b 601**Ligand SQD b 620**

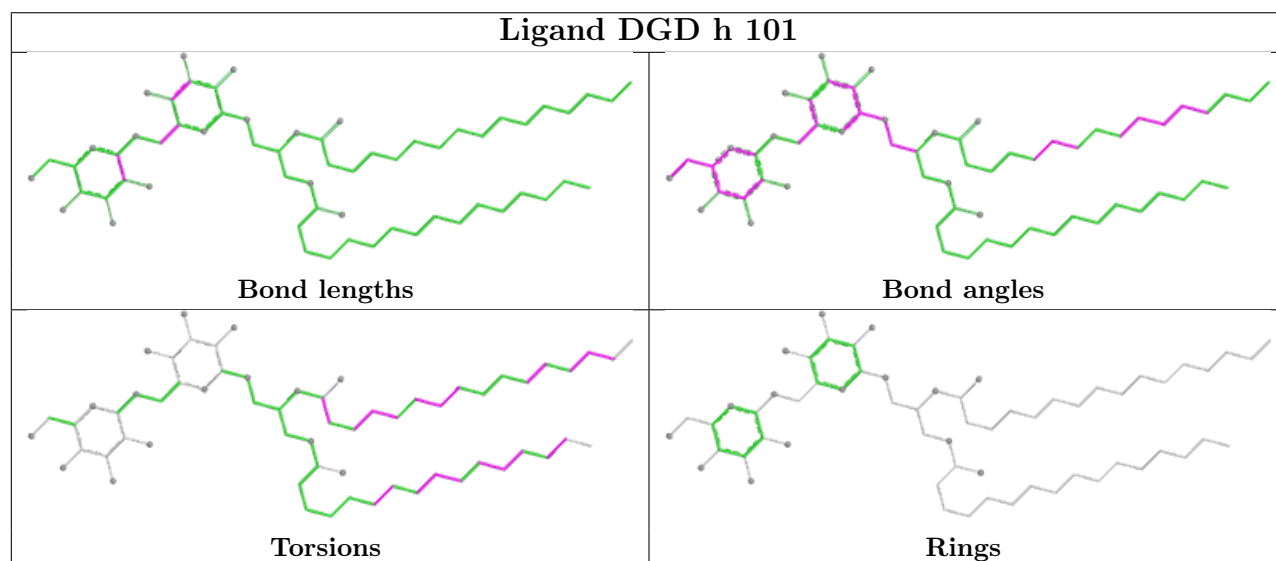
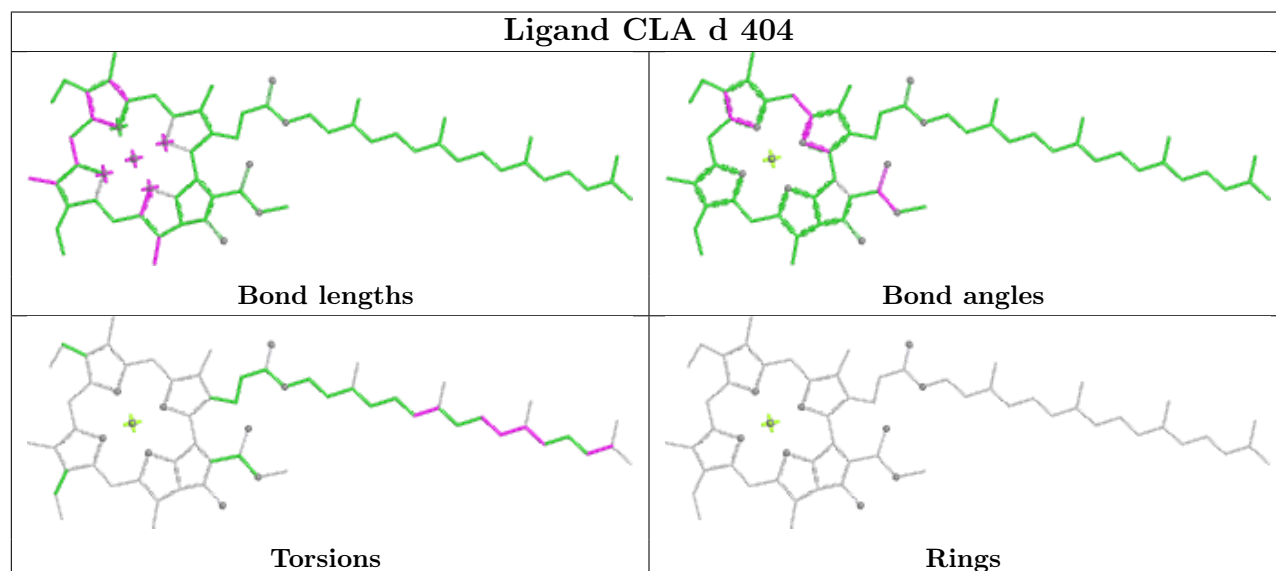
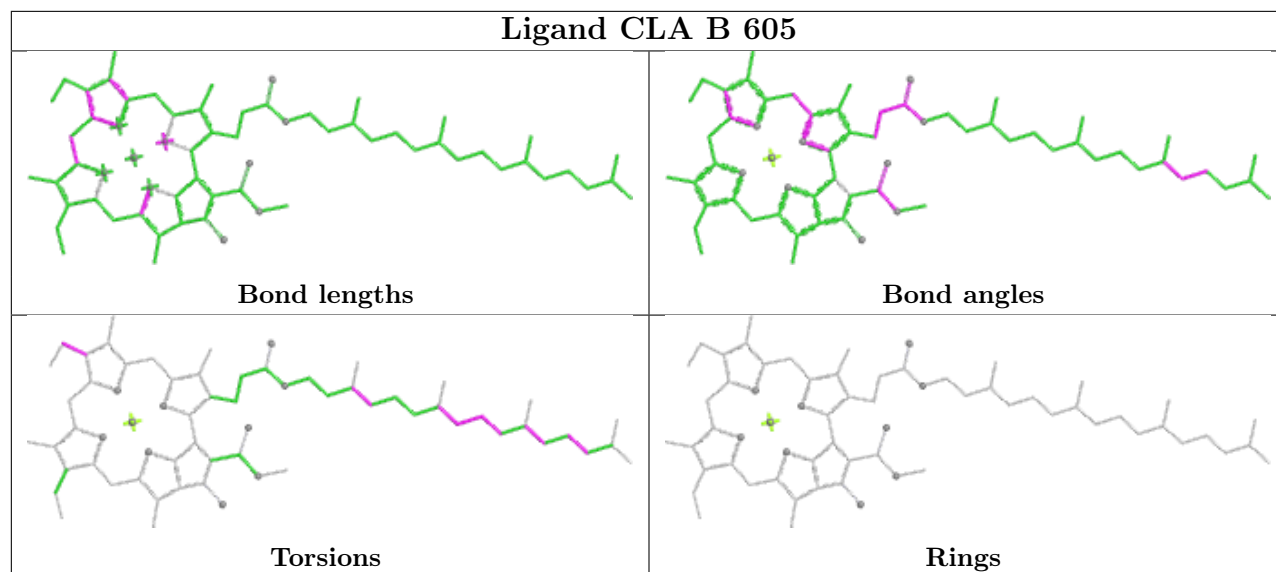


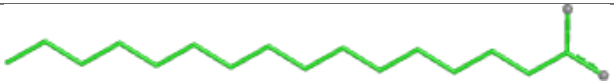
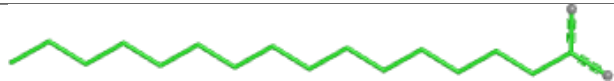
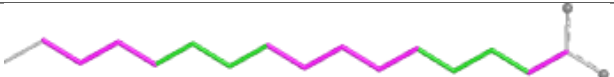
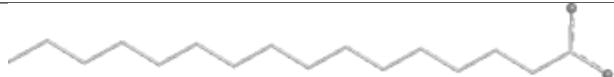


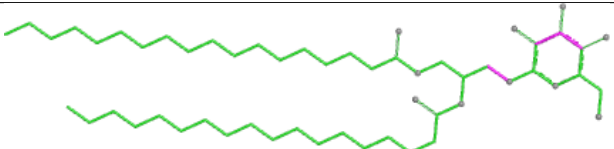
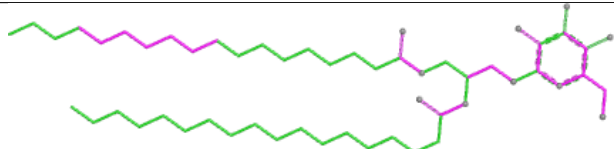


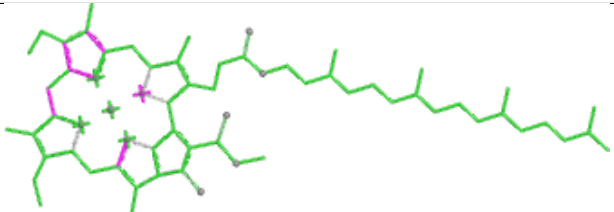
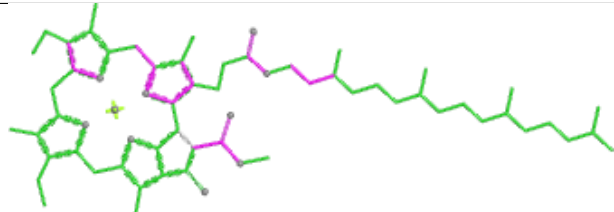
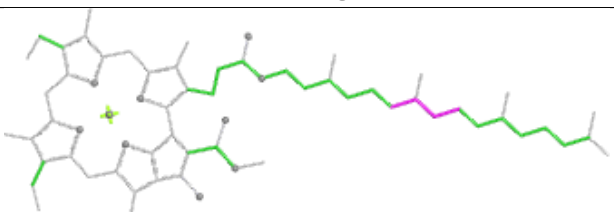
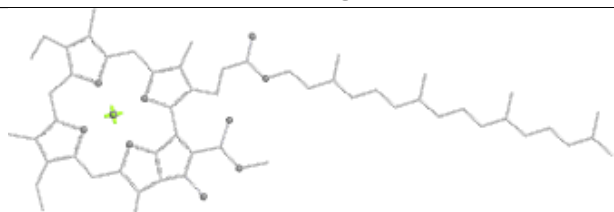


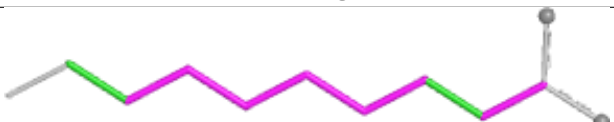
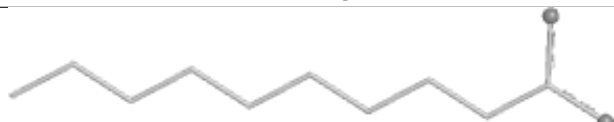


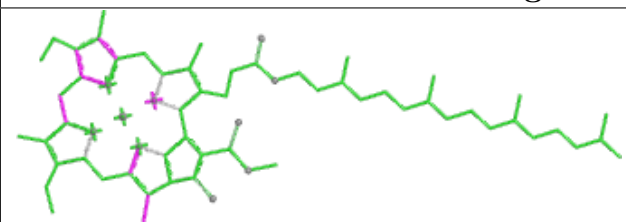
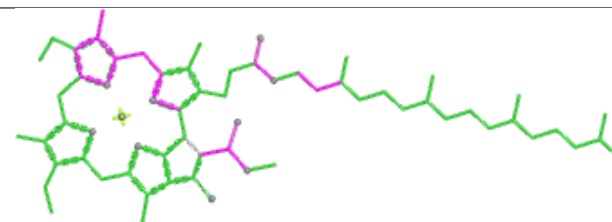
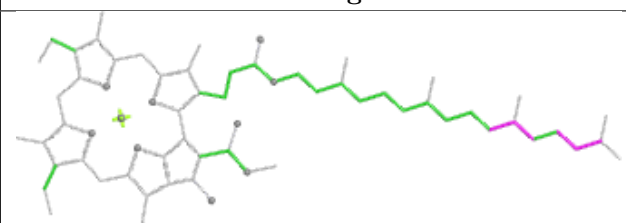
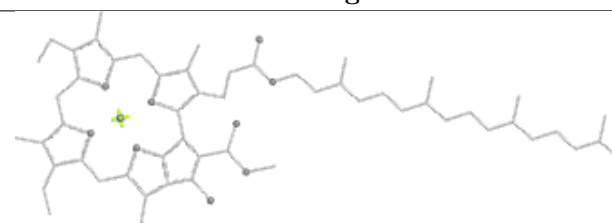


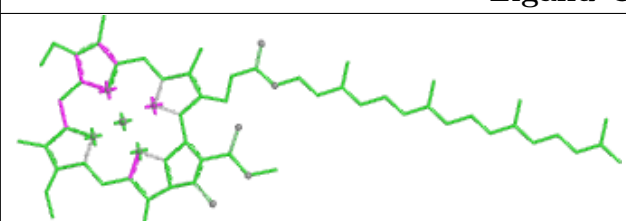
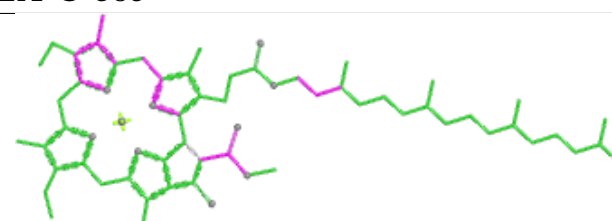
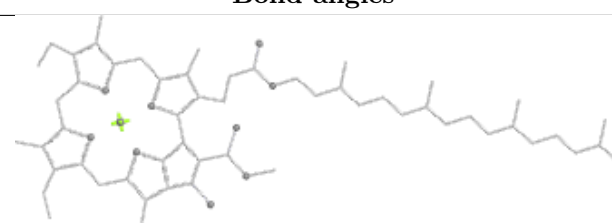
Ligand STE B 625	
 Bond lengths	 Bond angles
 Torsions	 Rings

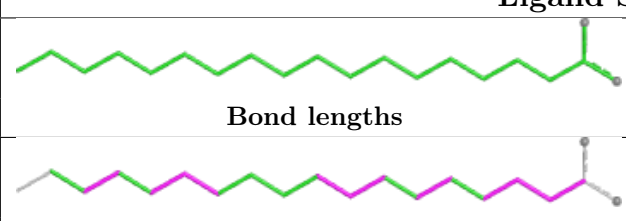
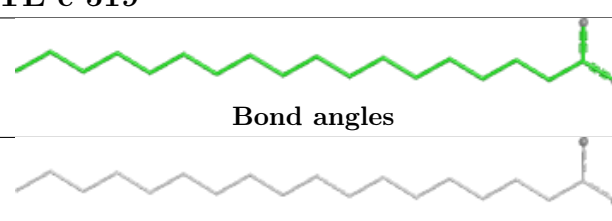
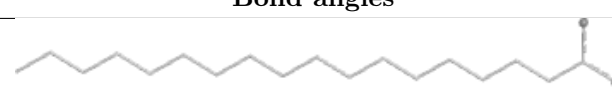
Ligand LMG b 624	
 Bond lengths	 Bond angles
 Torsions	 Rings

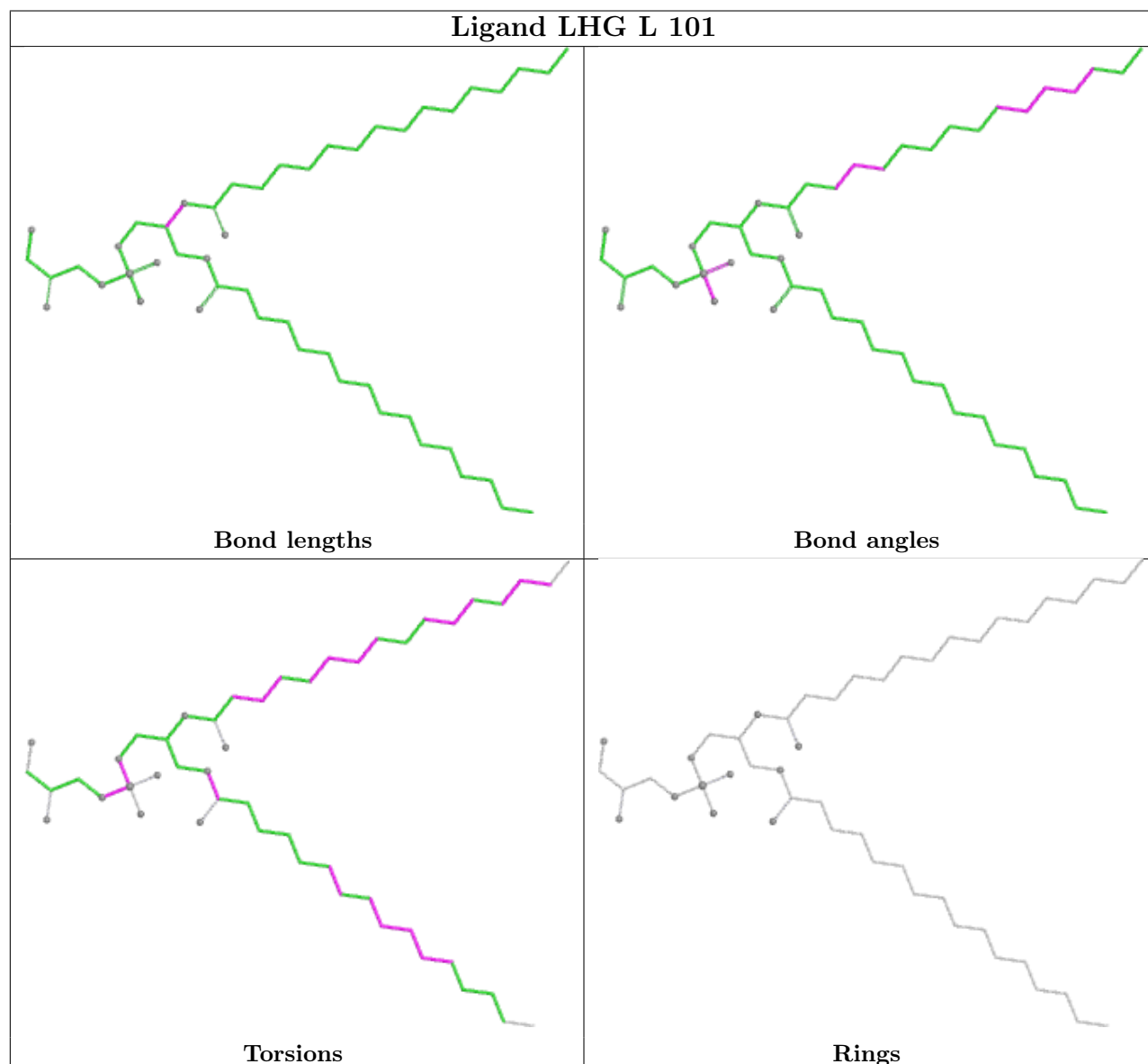
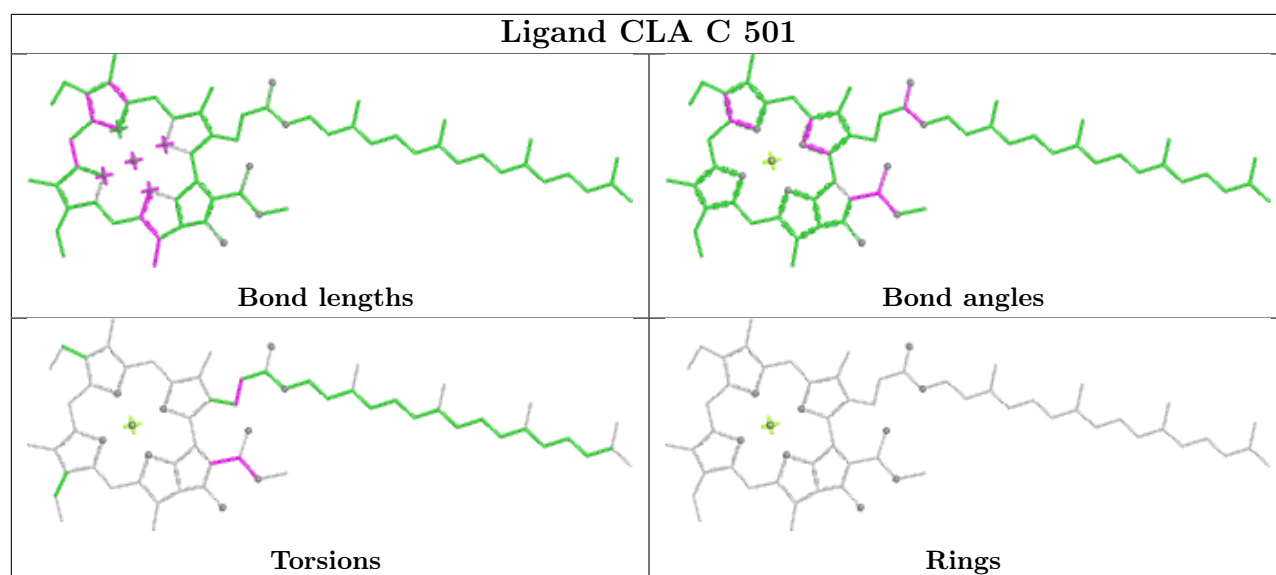
Ligand CLA C 511	
 Bond lengths	 Bond angles
 Torsions	 Rings

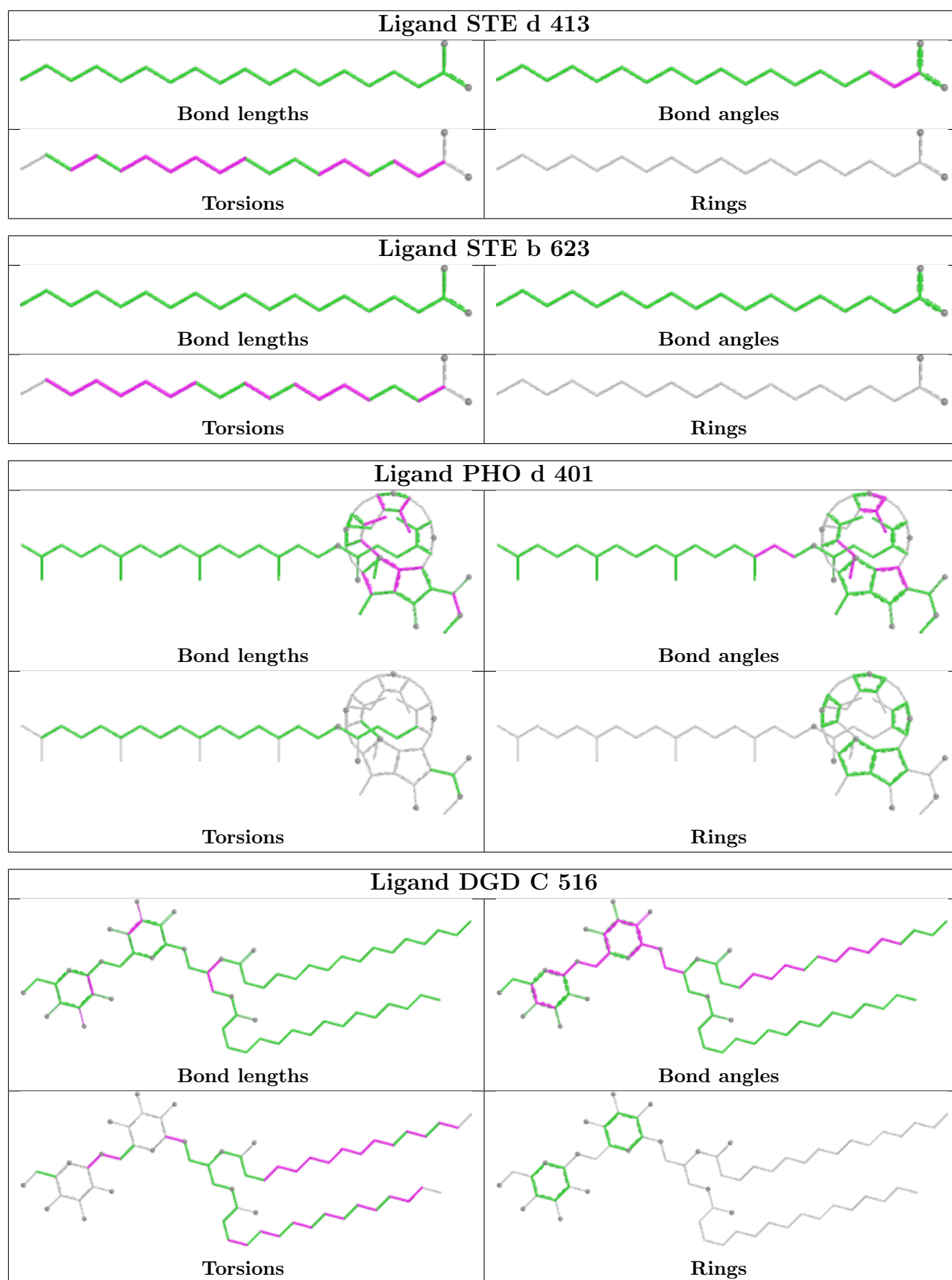
Ligand STE J 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

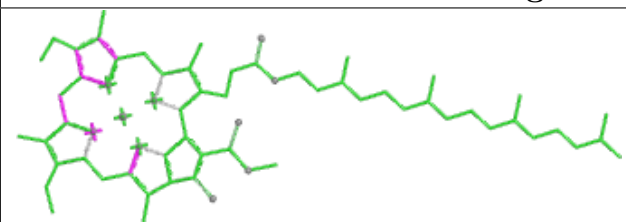
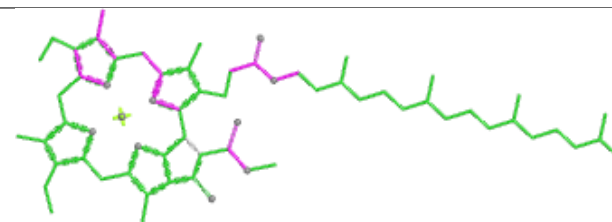
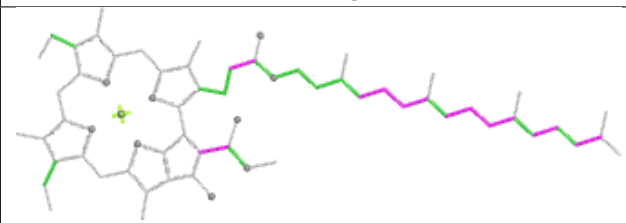
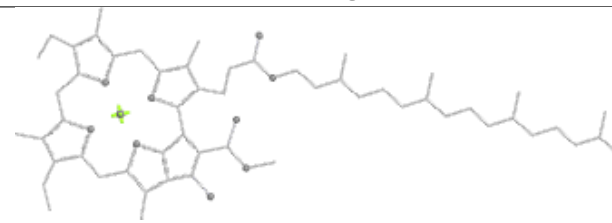
Ligand CLA b 604	
	
Bond lengths	Bond angles
	
Torsions	Rings

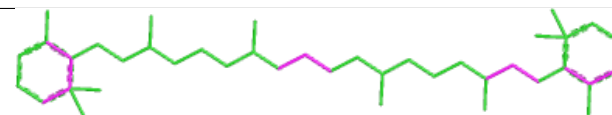
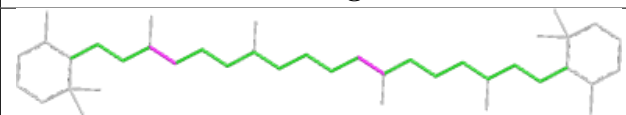
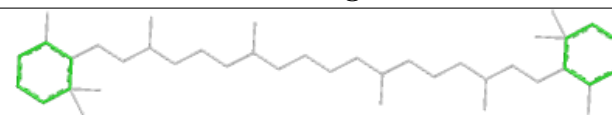
Ligand CLA C 509	
	
Bond lengths	Bond angles
	
Torsions	Rings

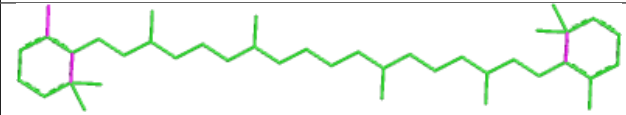
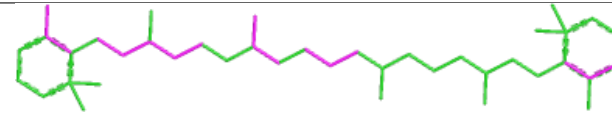
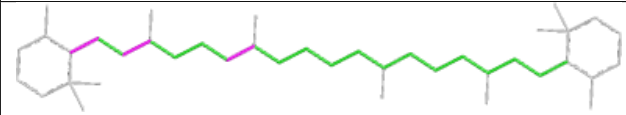
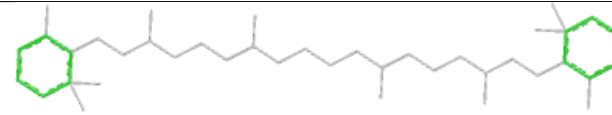
Ligand STE c 519	
	
Bond lengths	Bond angles
	
Torsions	Rings

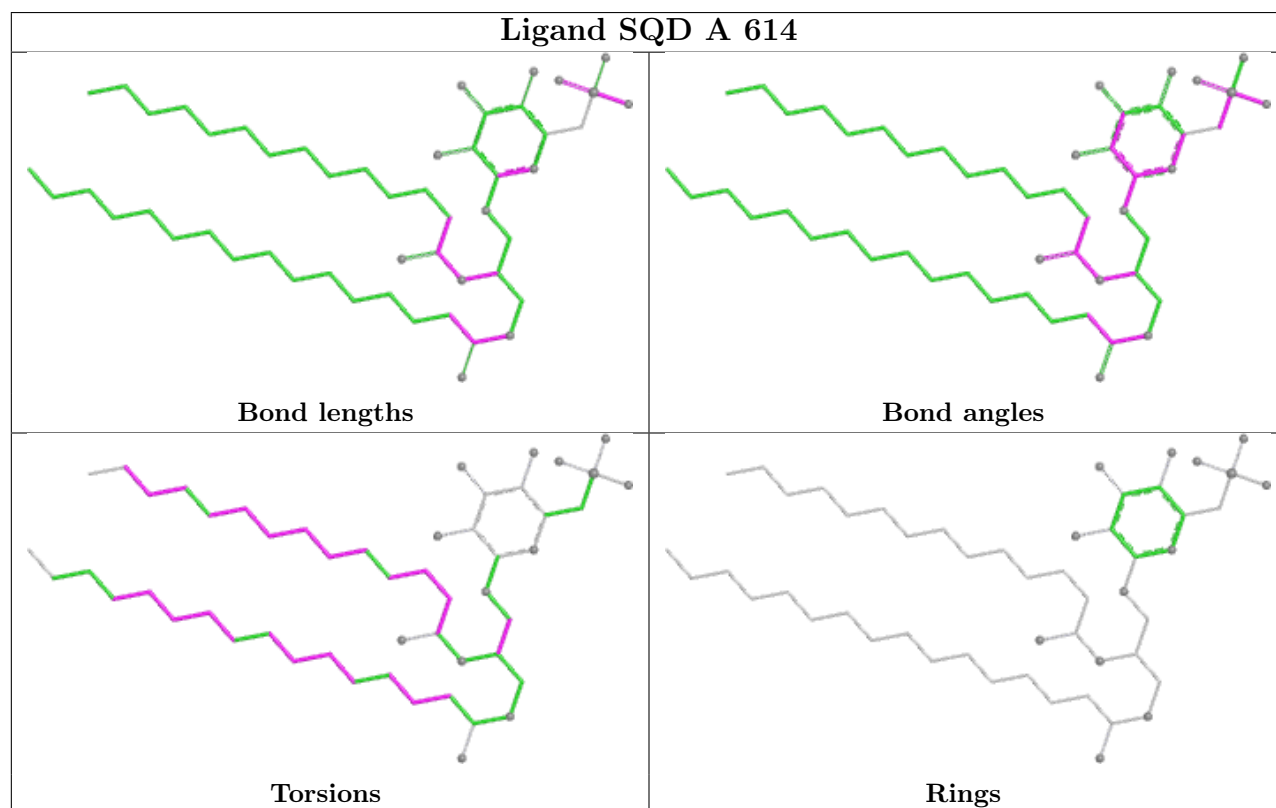
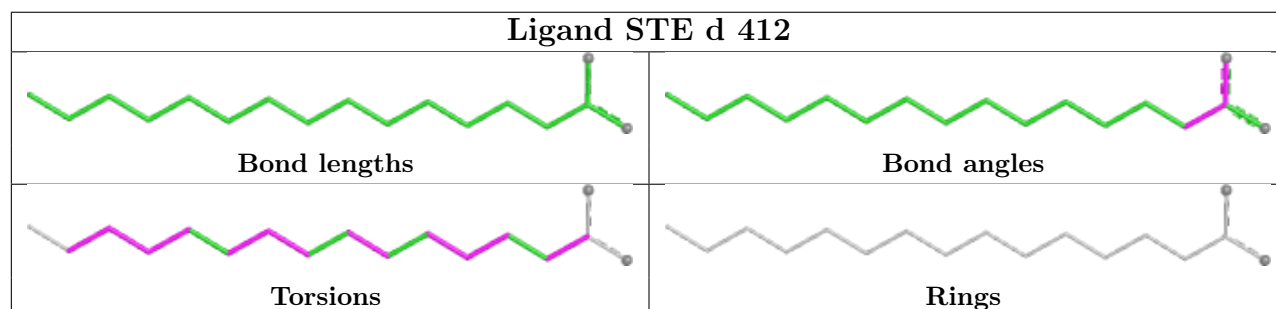
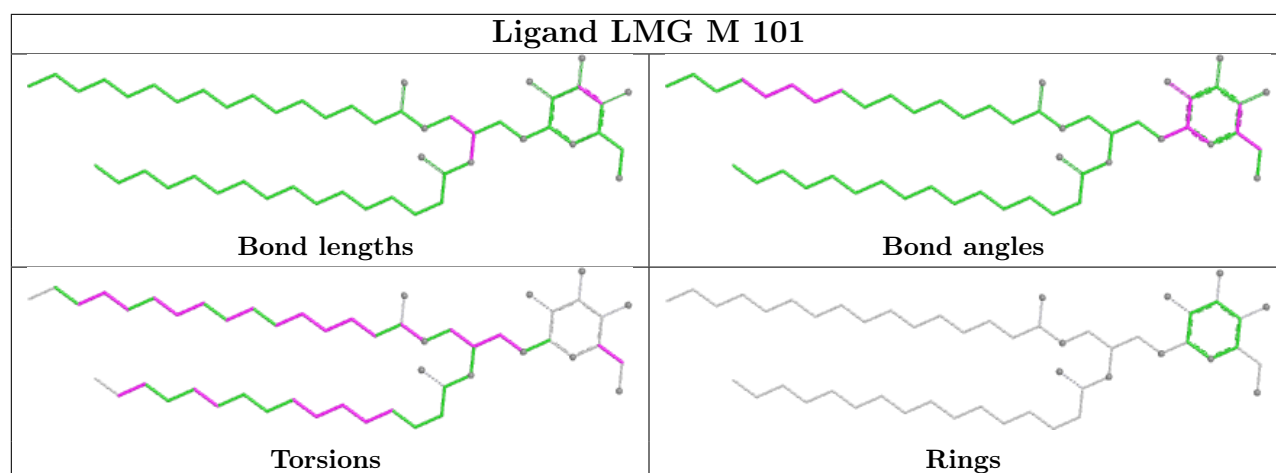


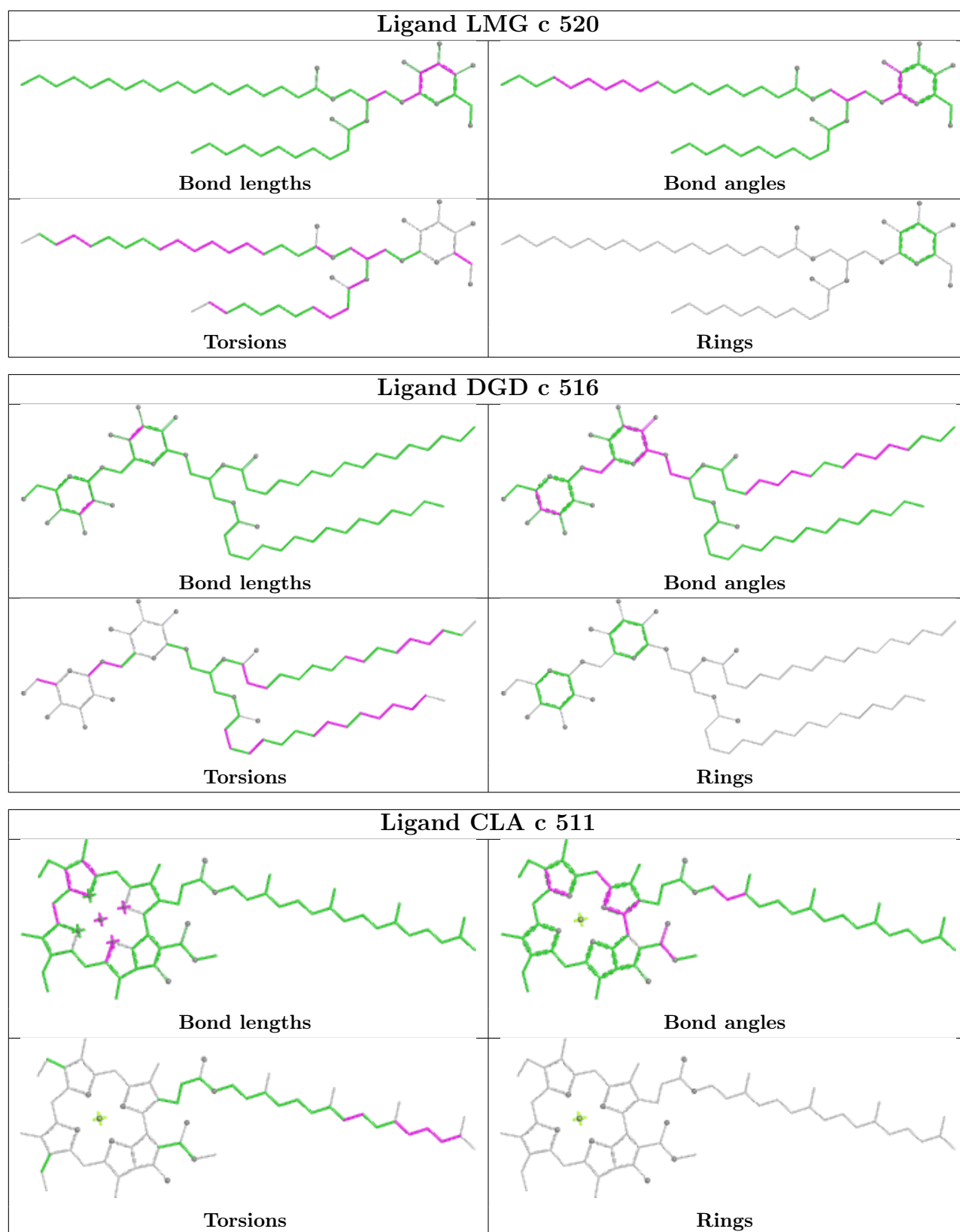


Ligand CLA c 509	
	
Bond lengths	Bond angles
	
Torsions	Rings

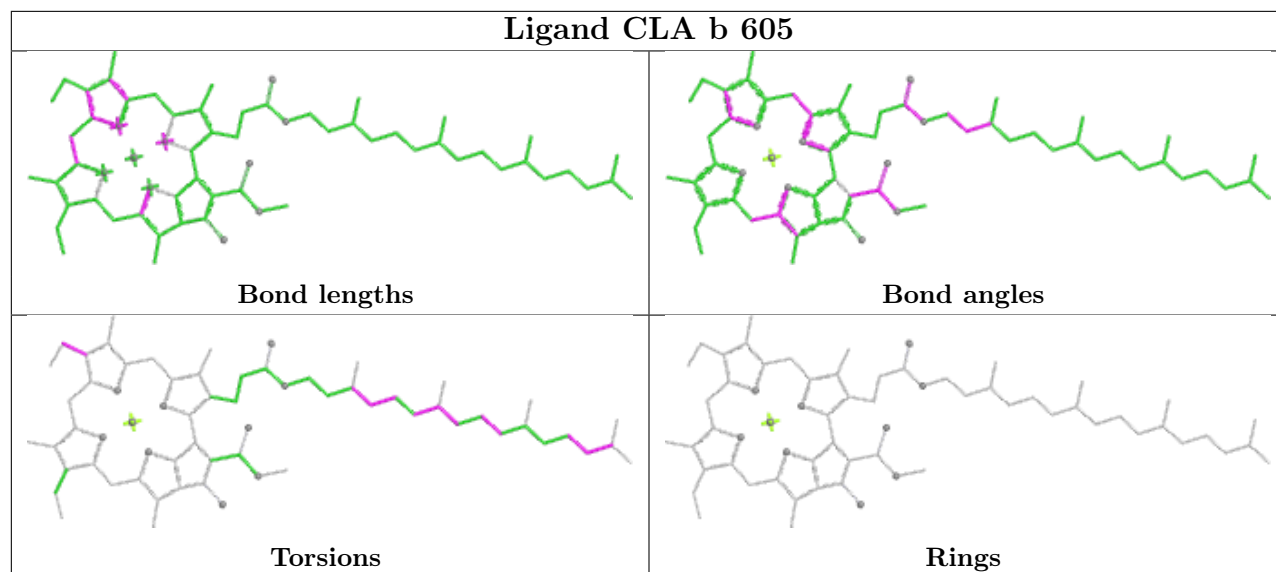
Ligand BCR H 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR c 514	
	
Bond lengths	Bond angles
	
Torsions	Rings

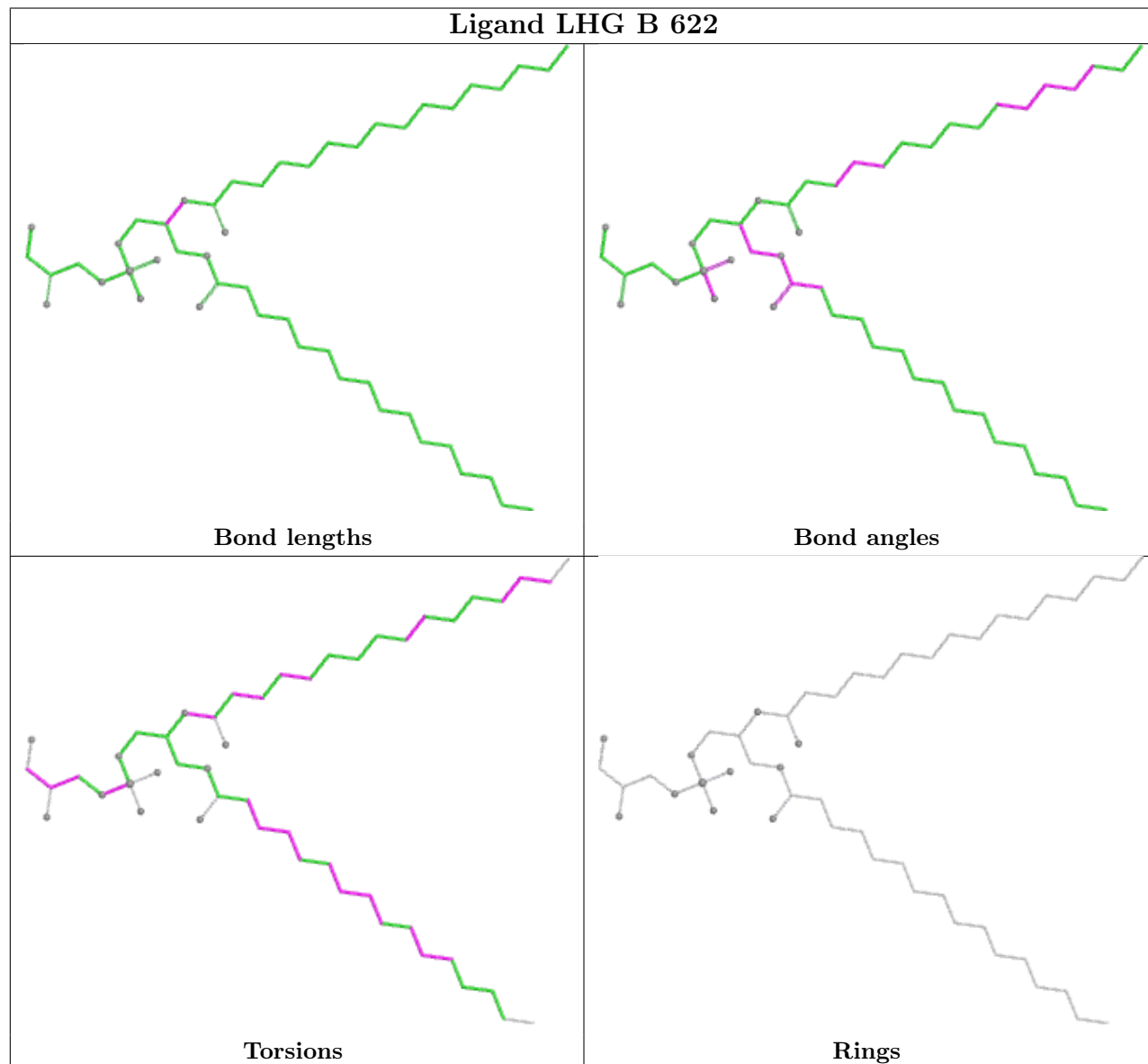


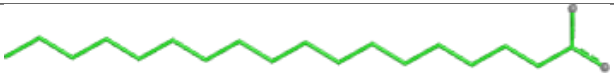
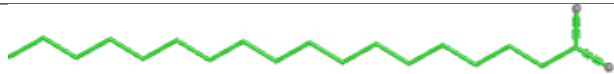
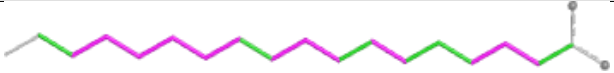


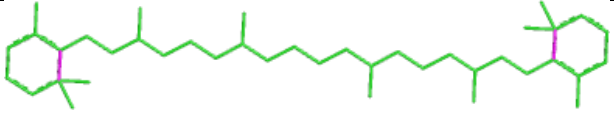
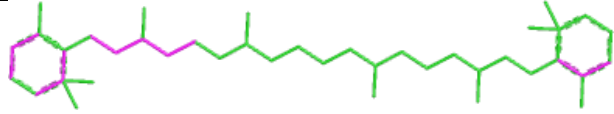
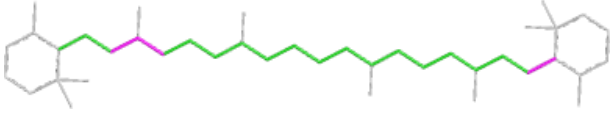
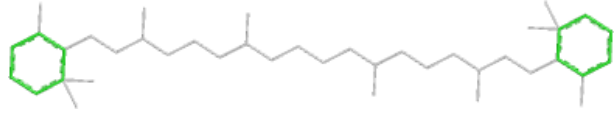
Ligand CLA b 605



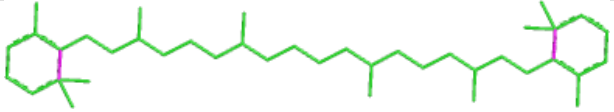
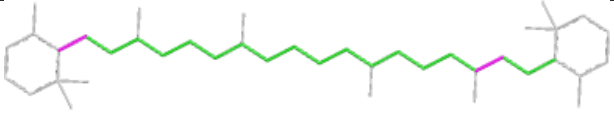
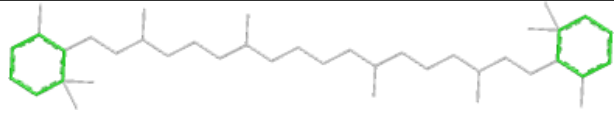
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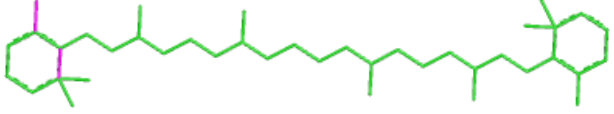
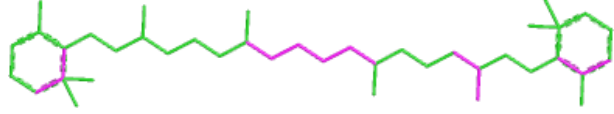
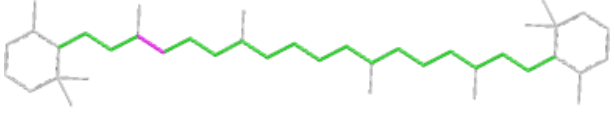
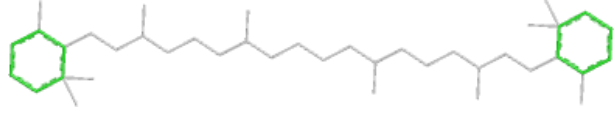


Ligand STE X 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

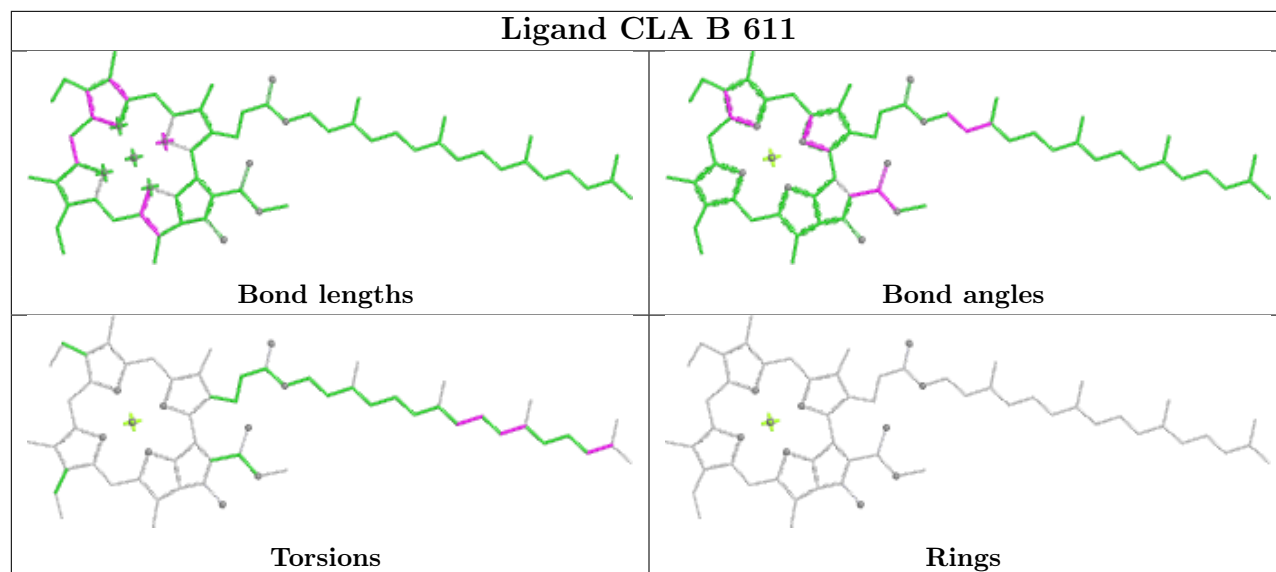
Ligand BCR x 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand STE l 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

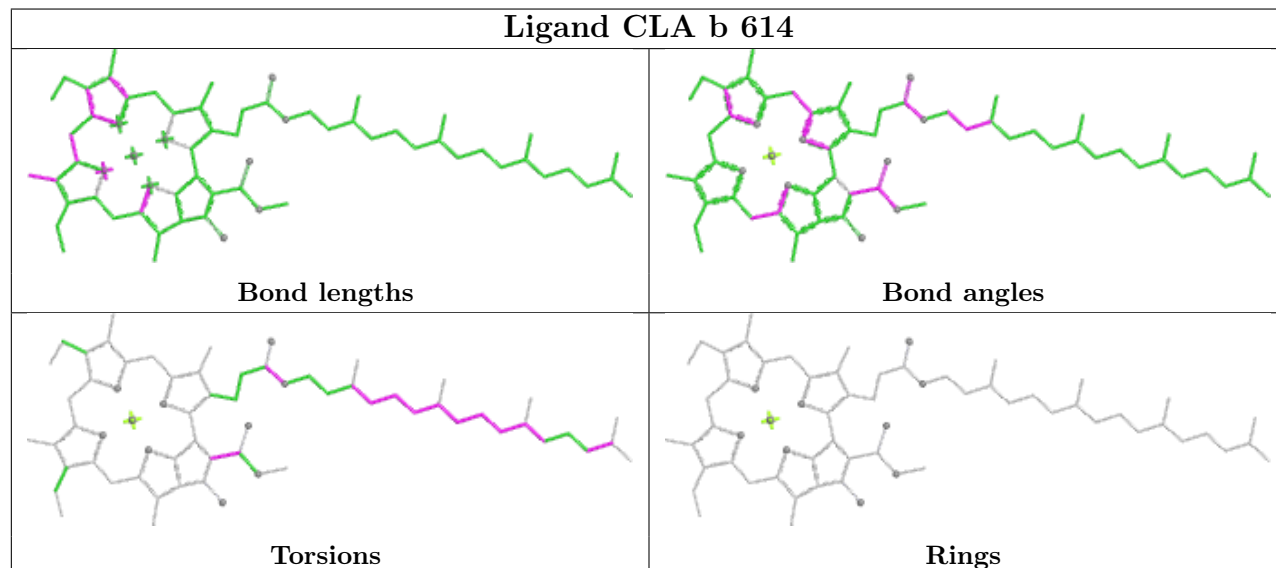
Ligand BCR Z 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR A 609	
 Bond lengths	 Bond angles
 Torsions	 Rings

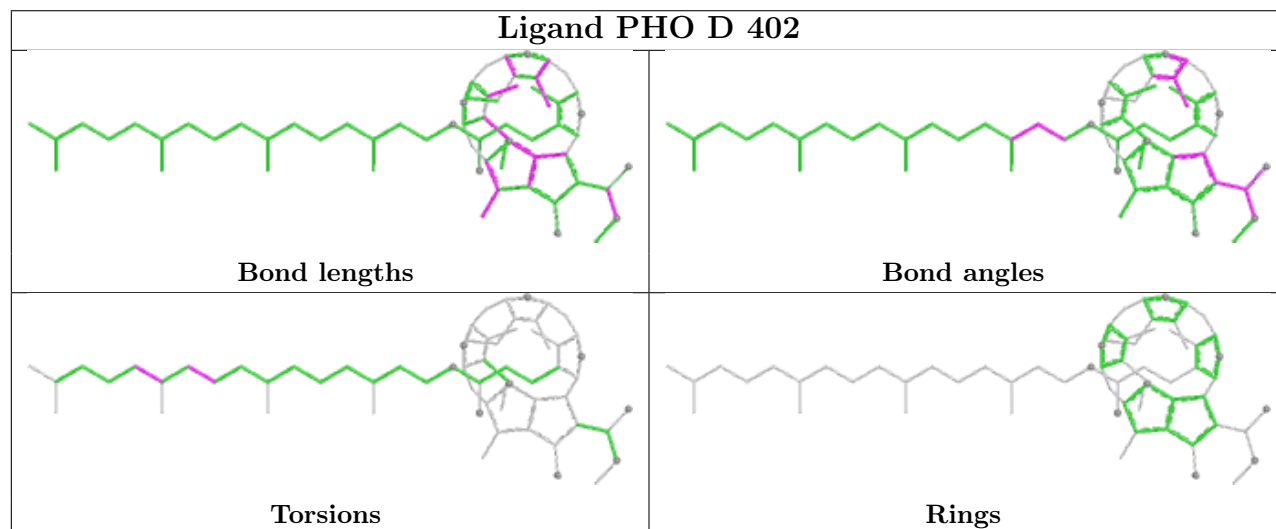
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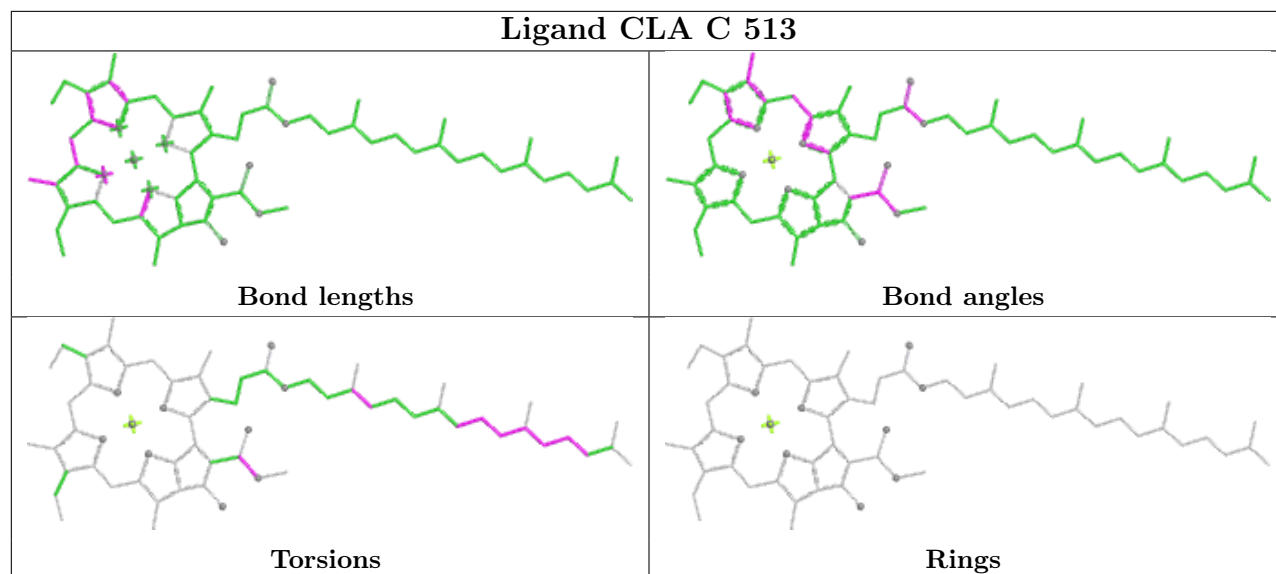
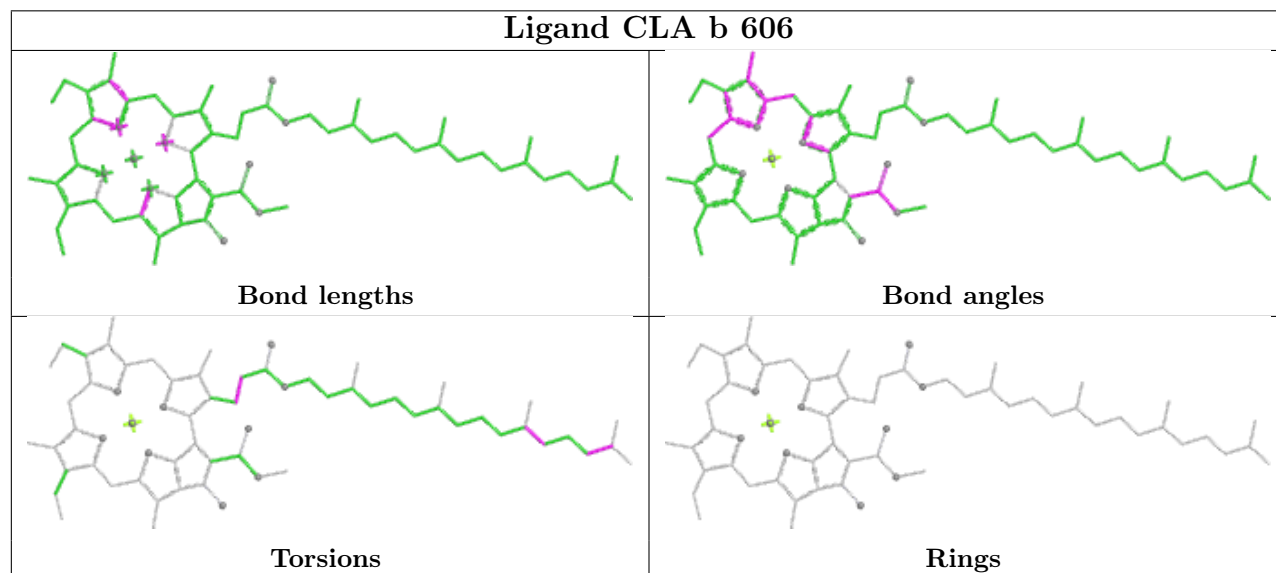
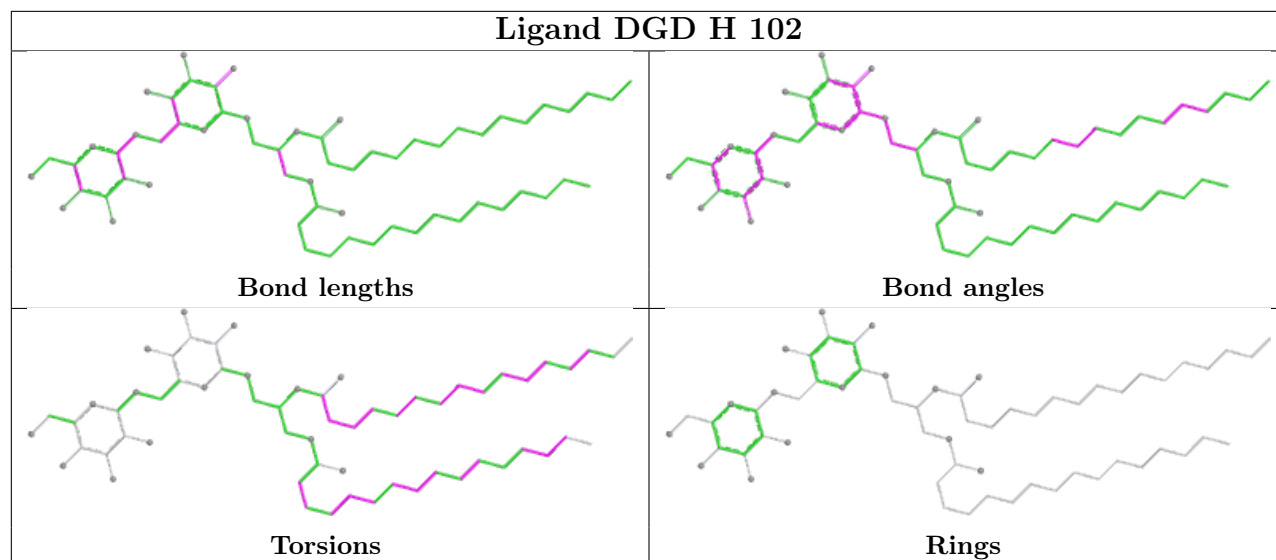


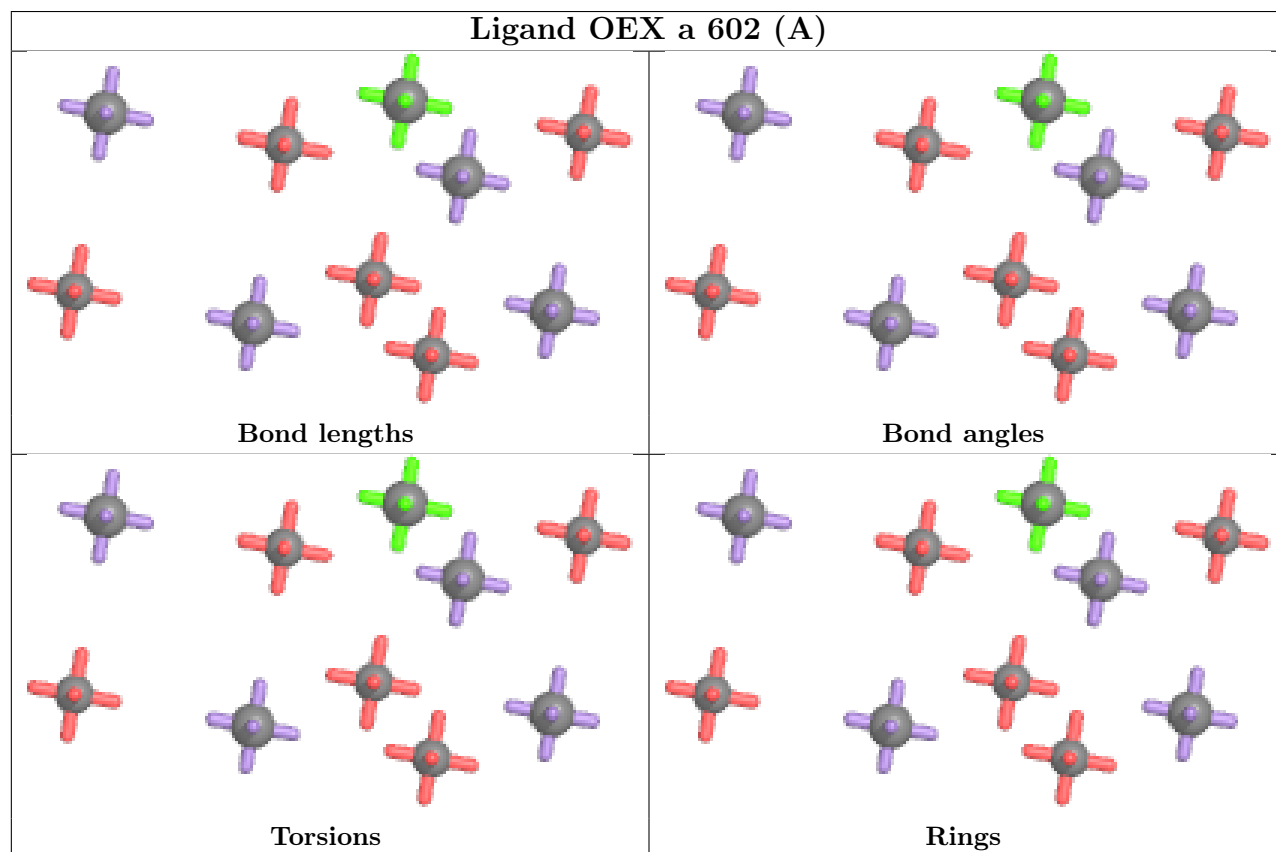
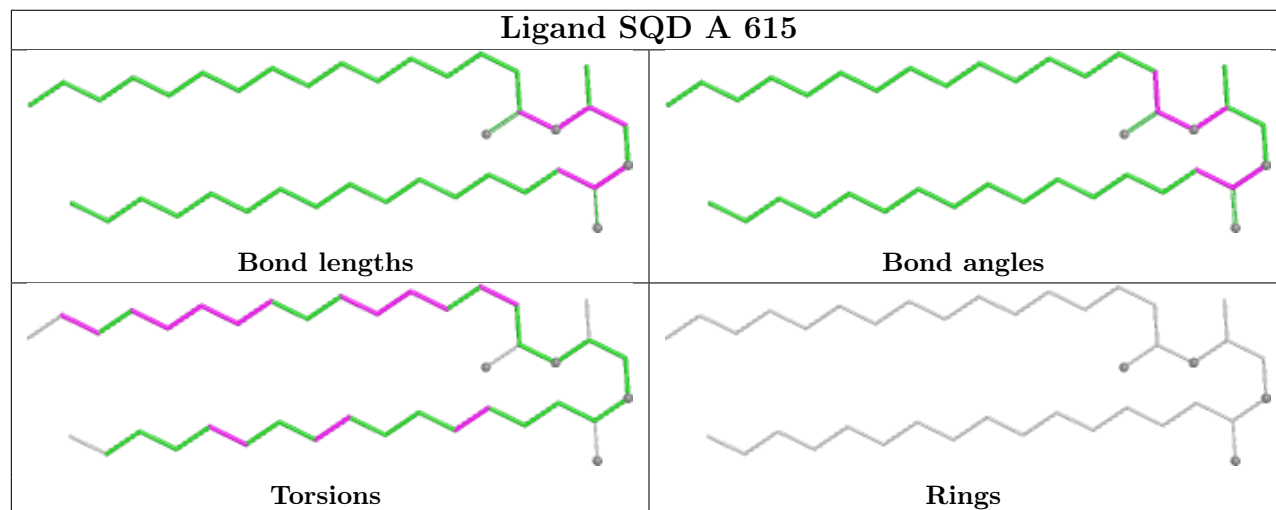
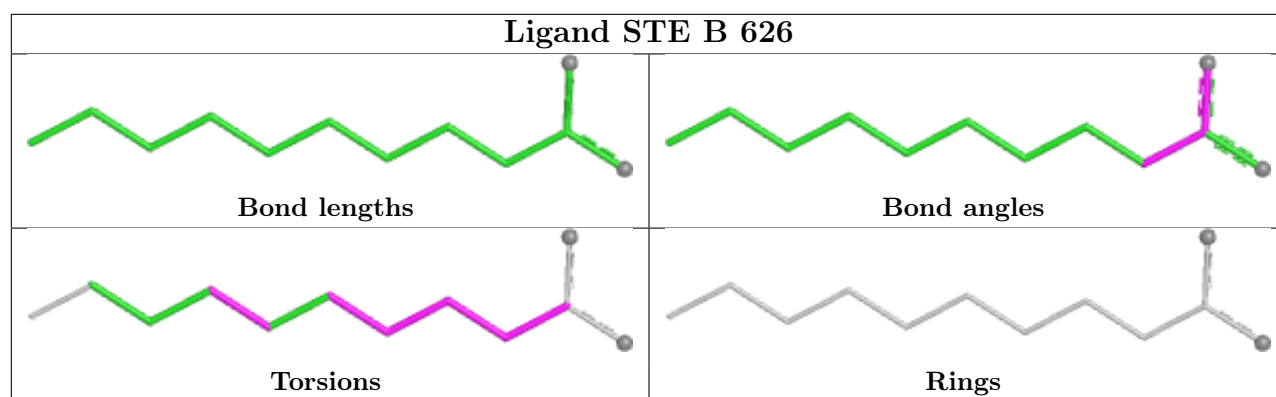
Ligand CLA b 614



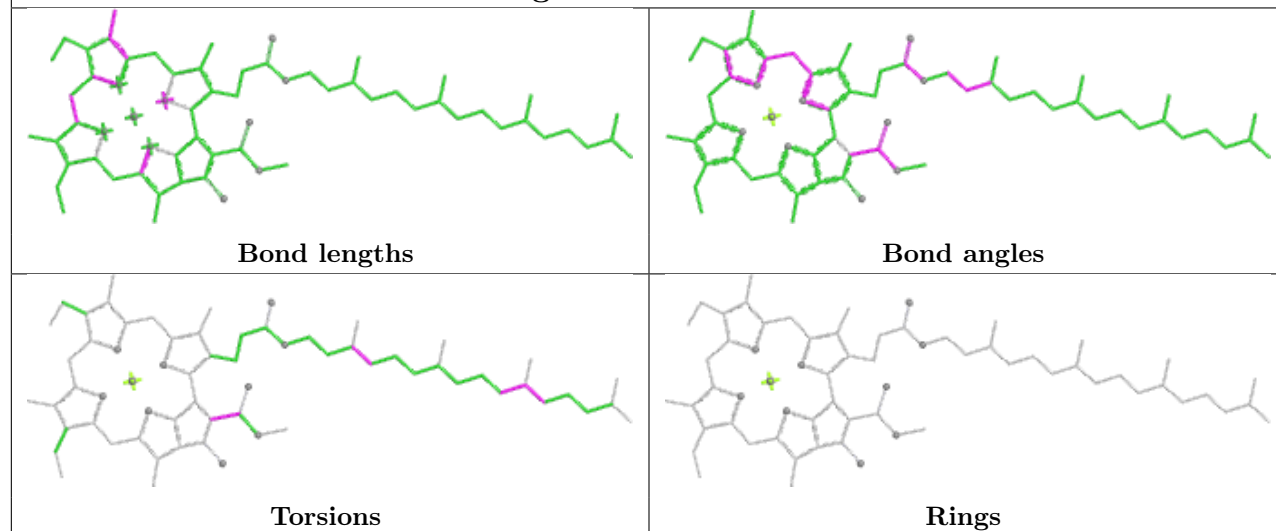
Ligand PHO D 402



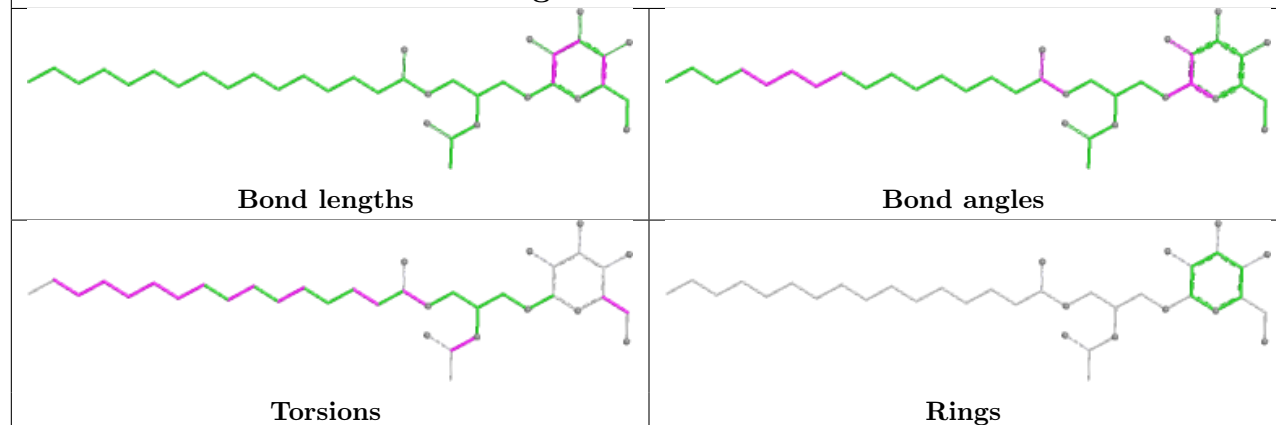
Ligand CLA C 513**Ligand CLA b 606****Ligand DGD H 102**



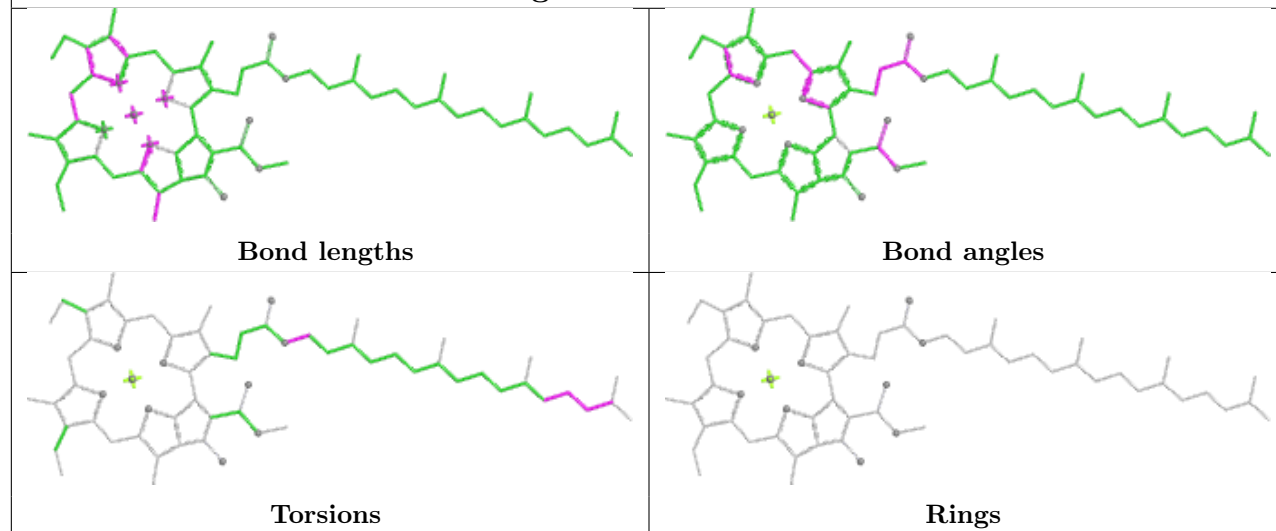
Ligand CLA B 614

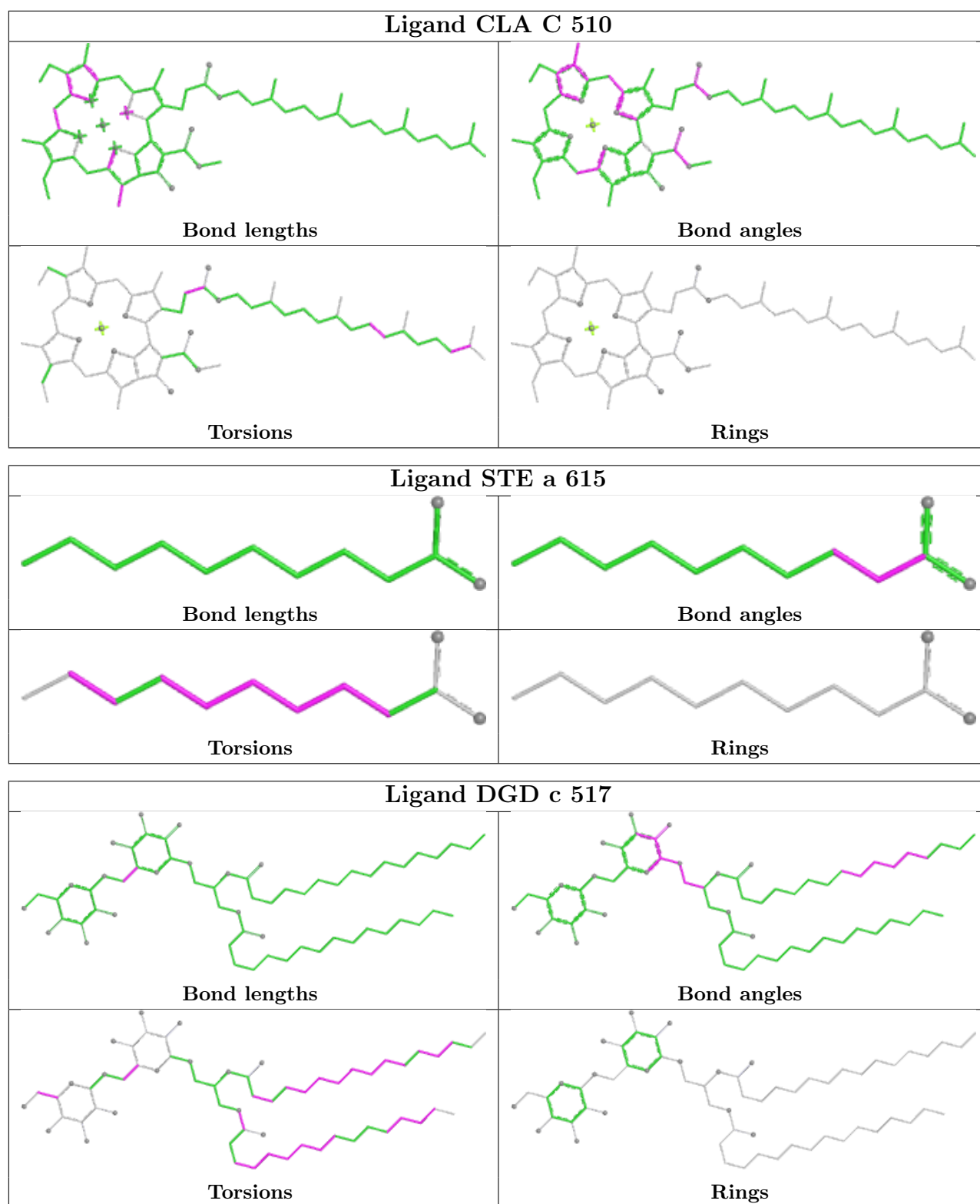


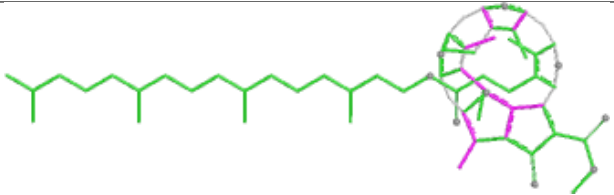
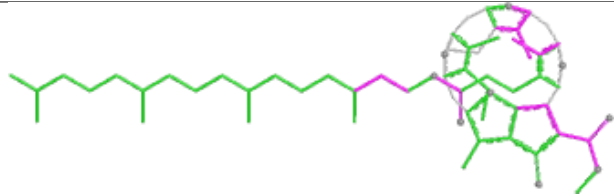
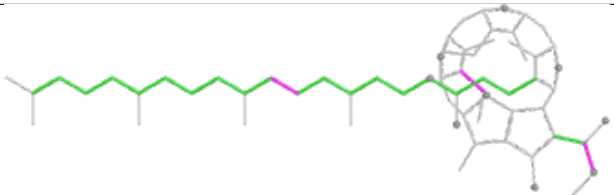
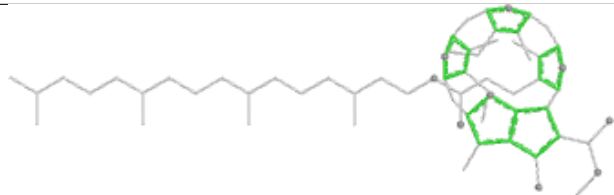
Ligand LMG c 518

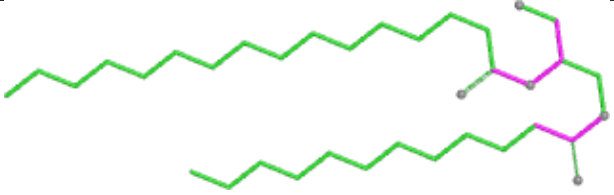
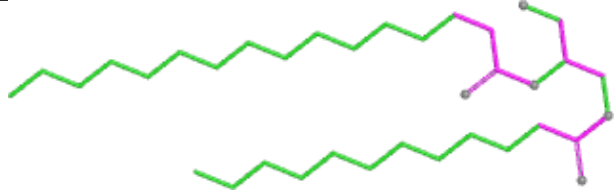
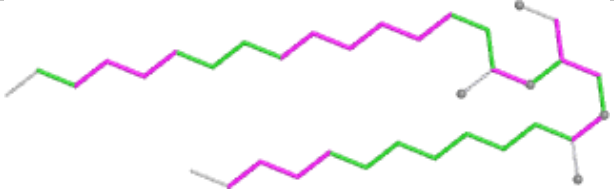


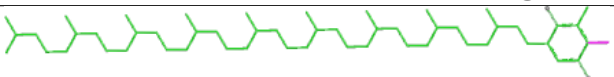
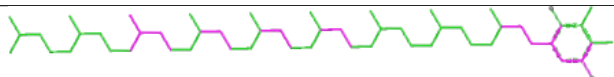
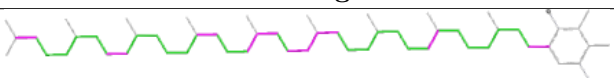
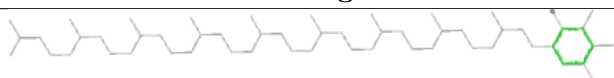
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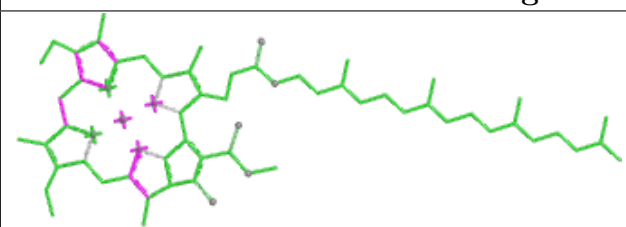
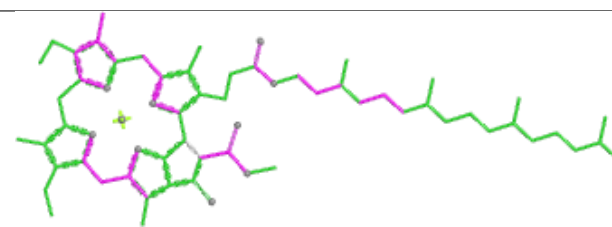
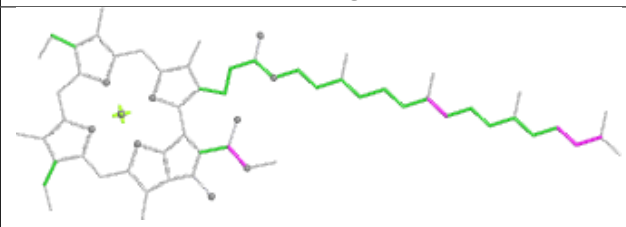
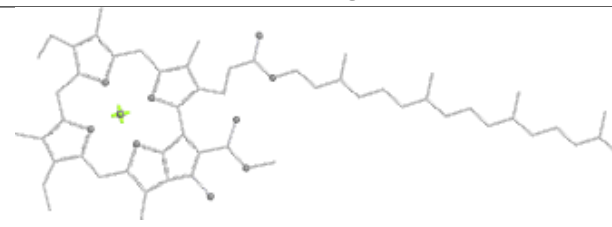


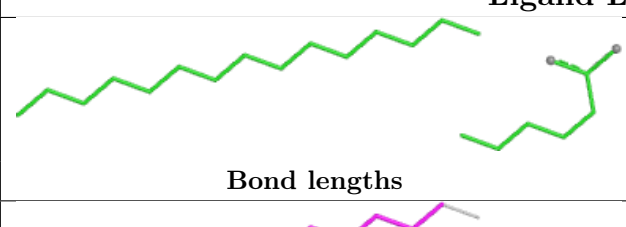
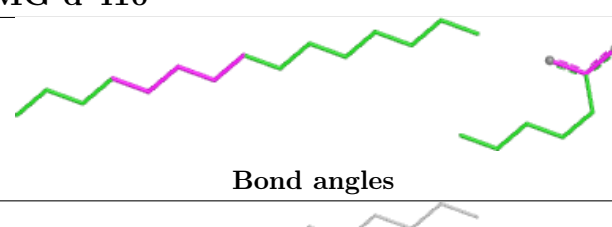
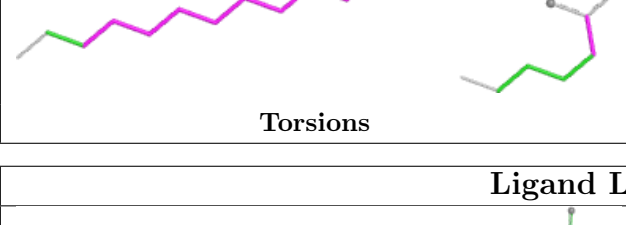


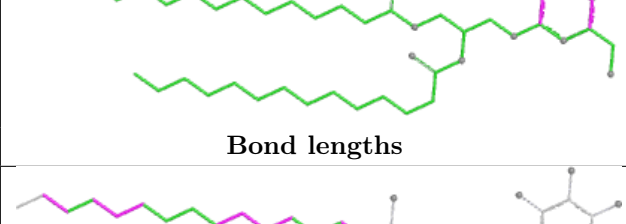
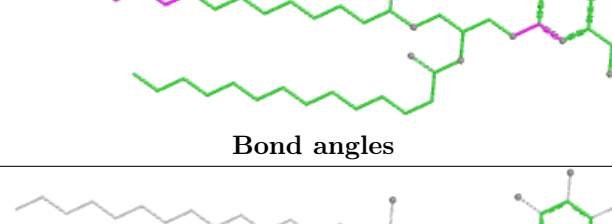
Ligand PHO d 402	
	
Bond lengths	Bond angles
	
Torsions	Rings

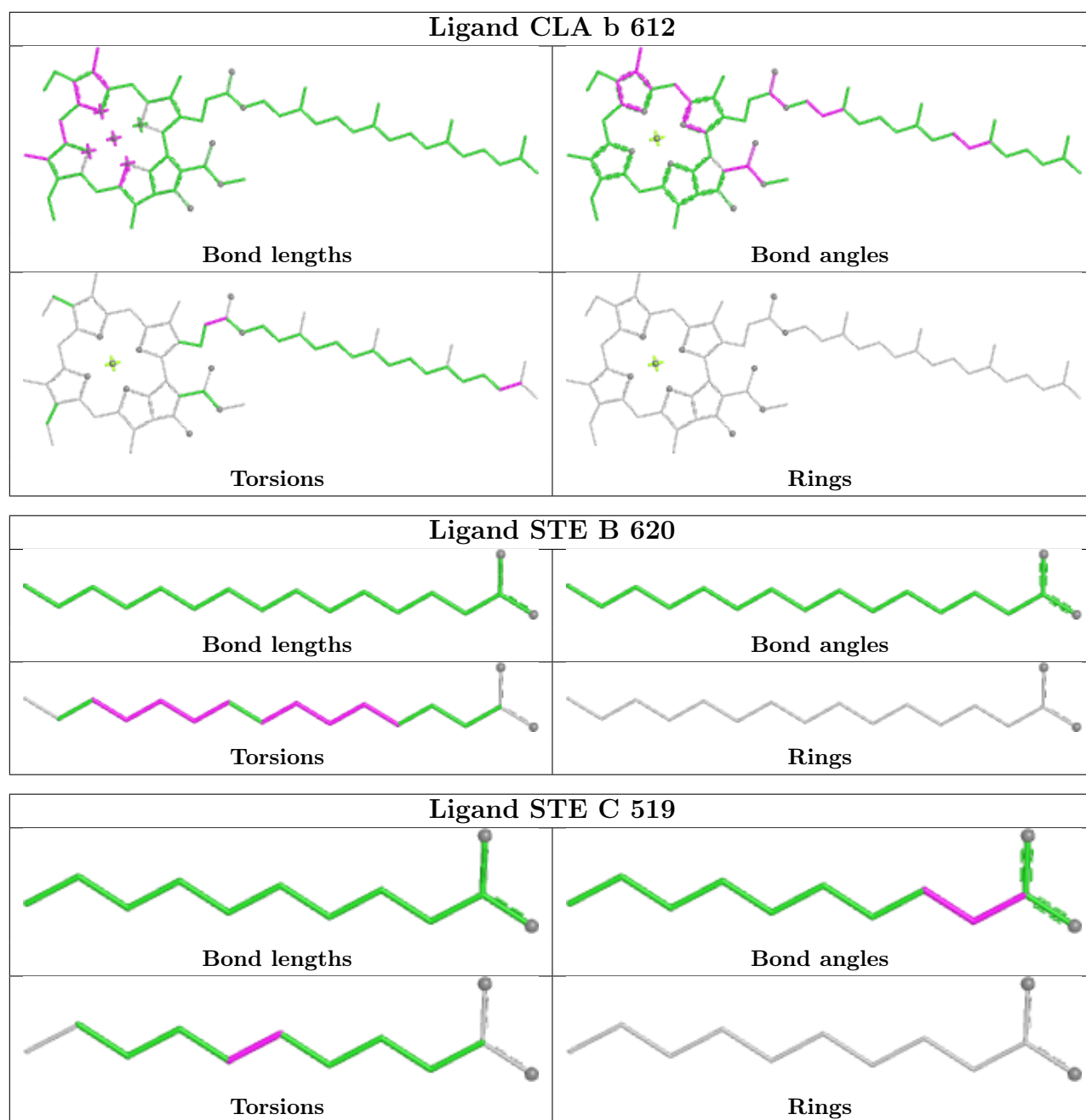
Ligand SQD a 614	
	
Bond lengths	Bond angles
	
Torsions	Rings

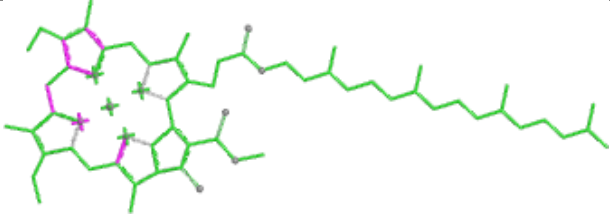
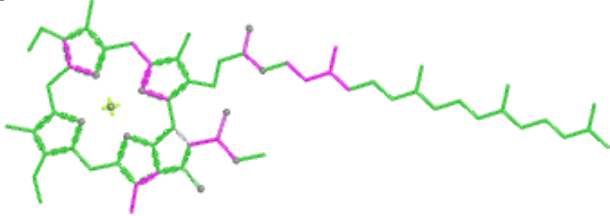
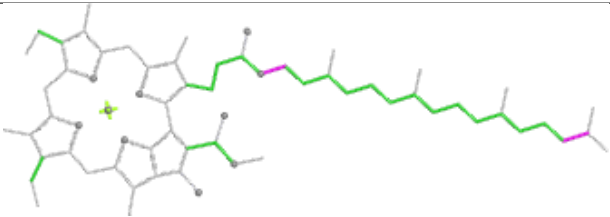
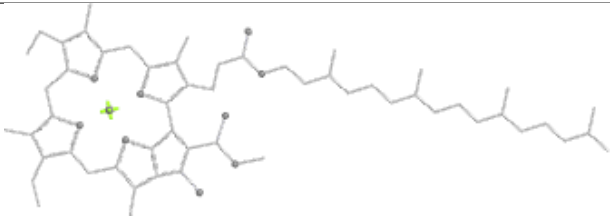
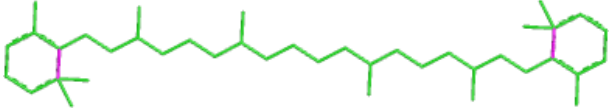
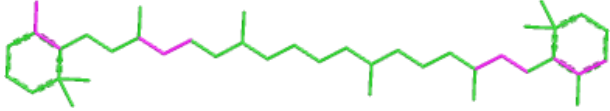
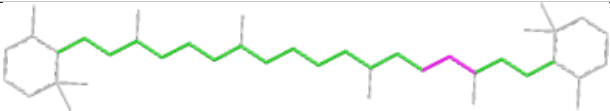
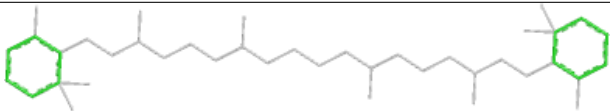
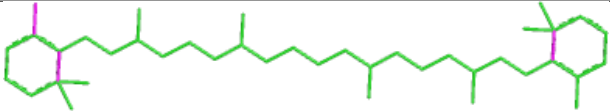
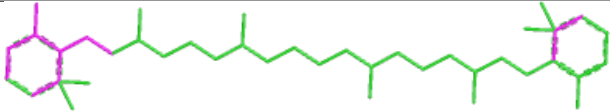
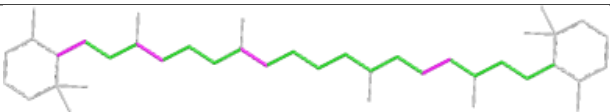
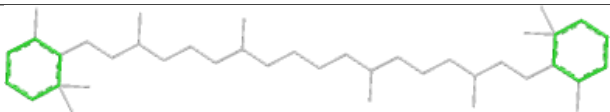
Ligand PL9 a 611	
	
Bond lengths	Bond angles
	
Torsions	Rings

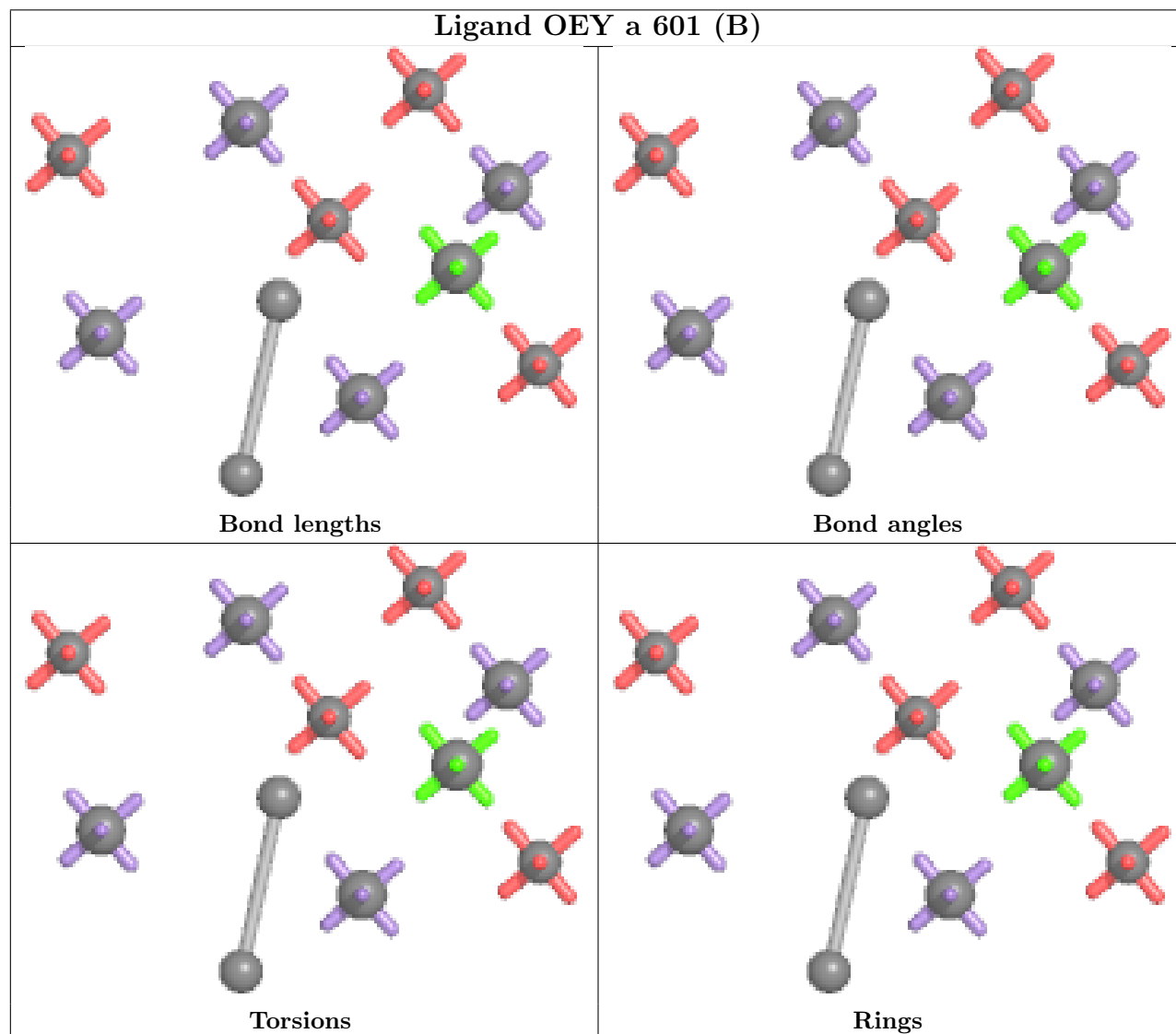
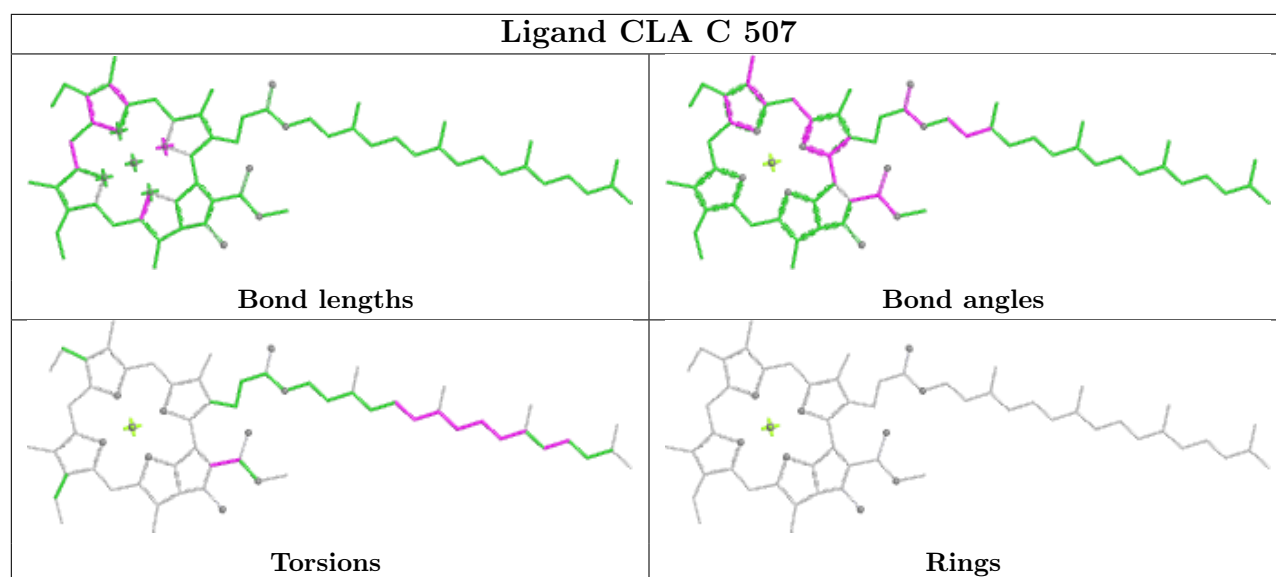
Ligand CLA C 508	
	
Bond lengths	Bond angles
	
Torsions	Rings

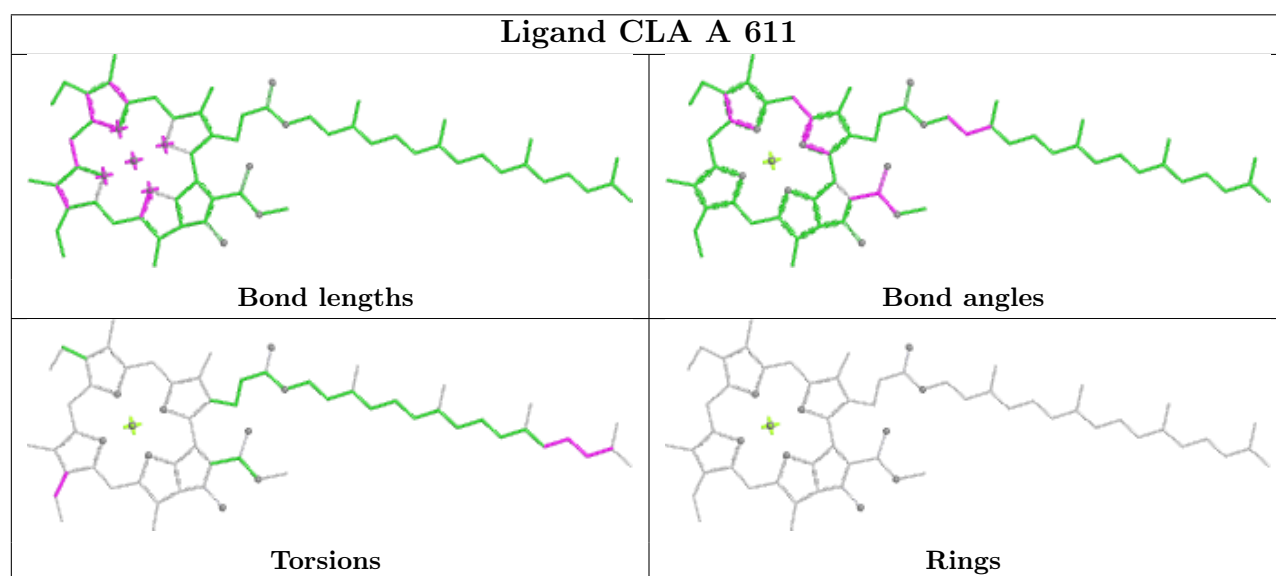
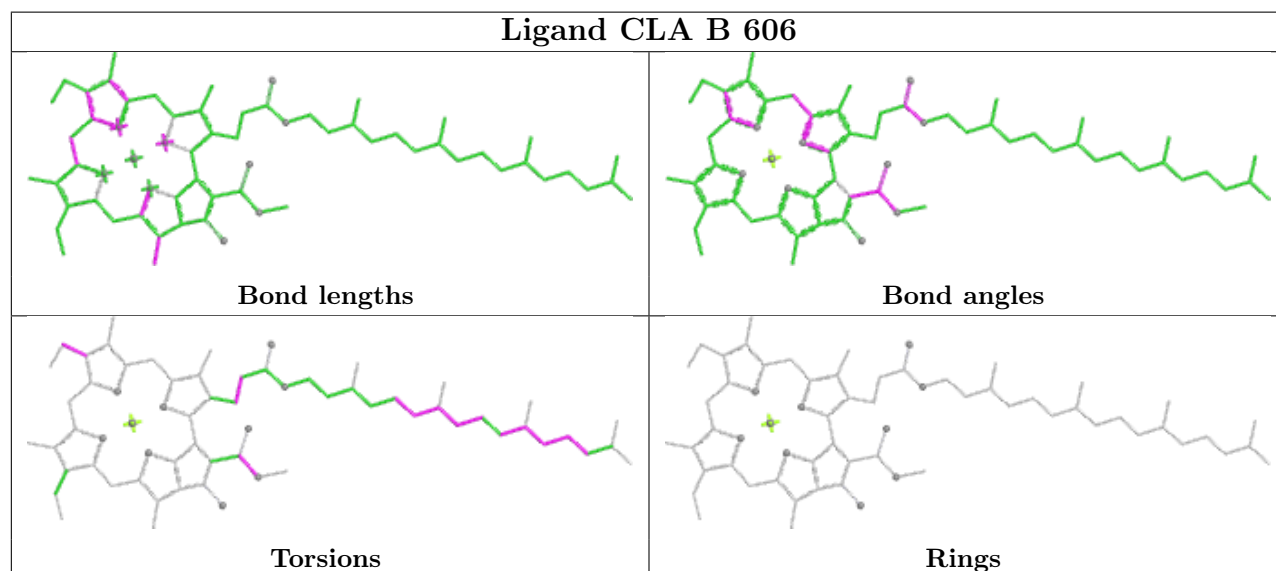
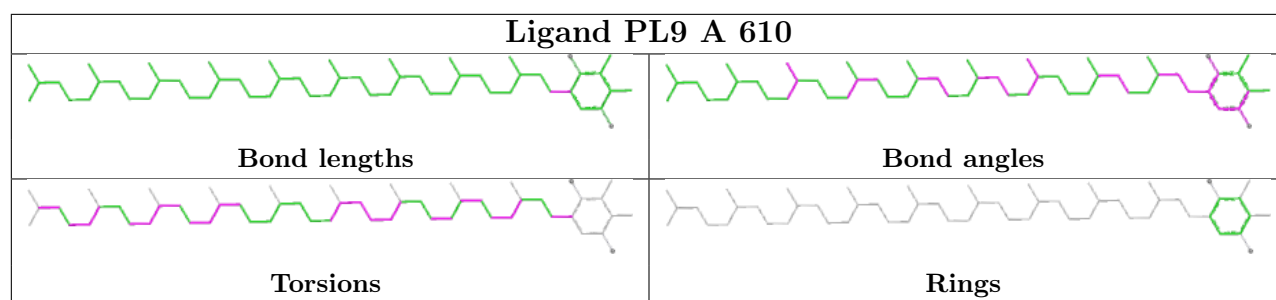
Ligand LMG d 410	
	
Bond lengths	Bond angles
	
Torsions	Rings

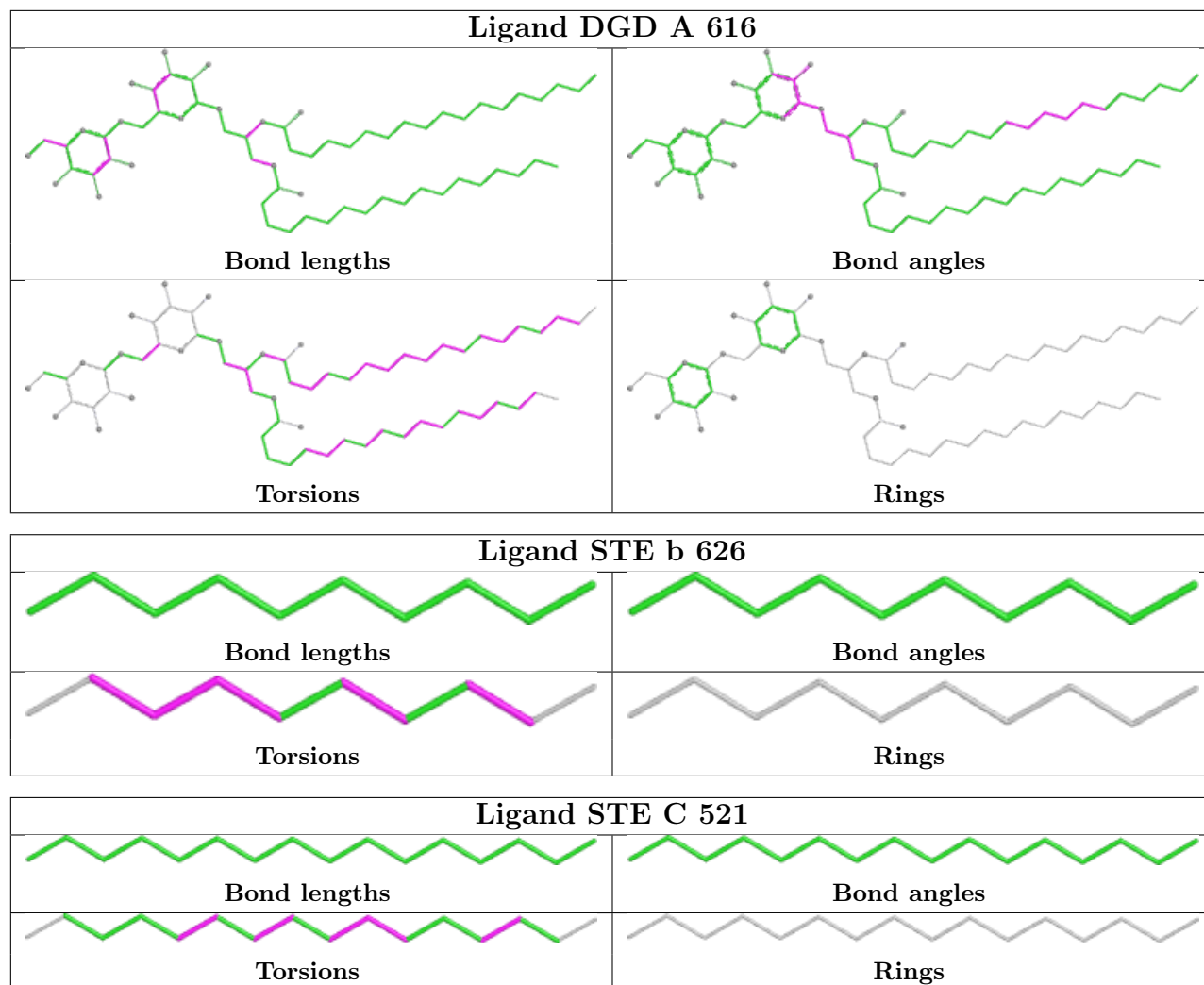
Ligand LMG c 522	
	
Bond lengths	Bond angles
	
Torsions	Rings

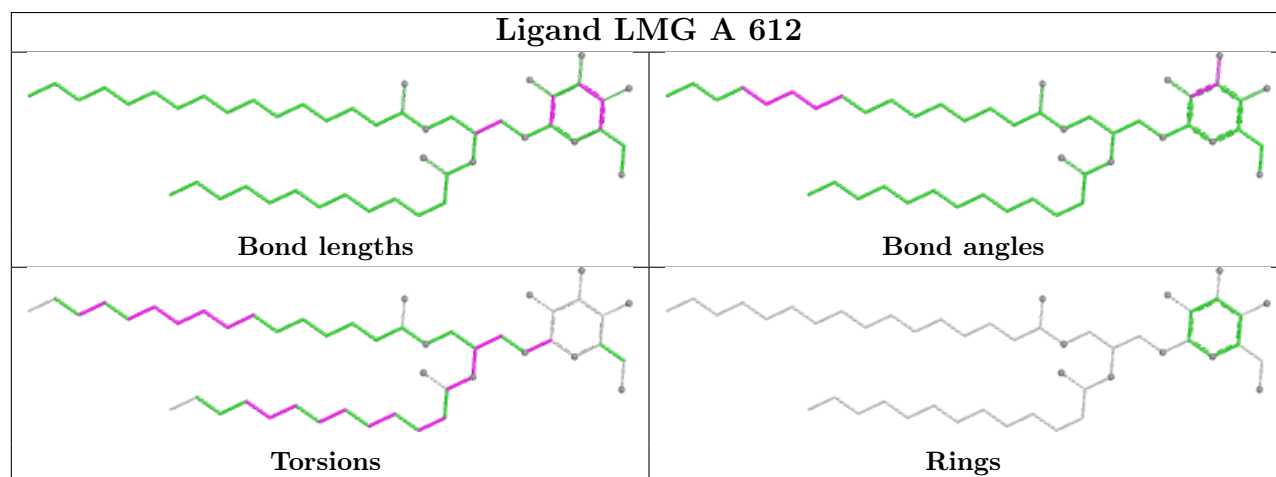
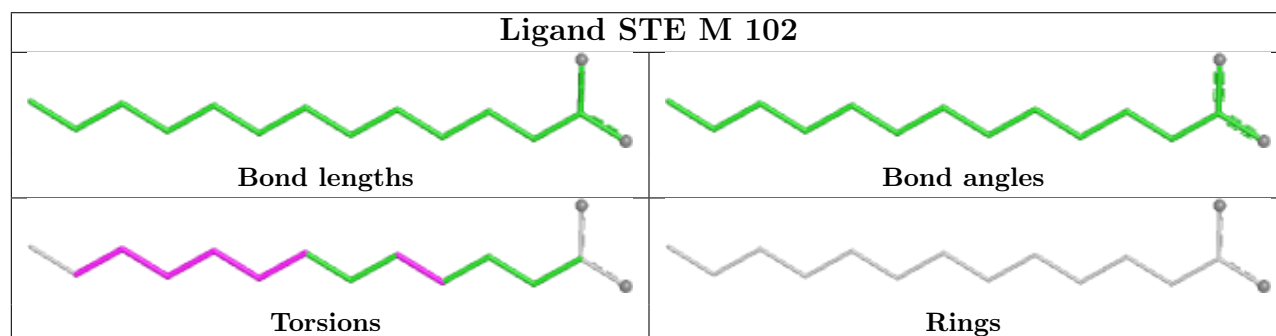
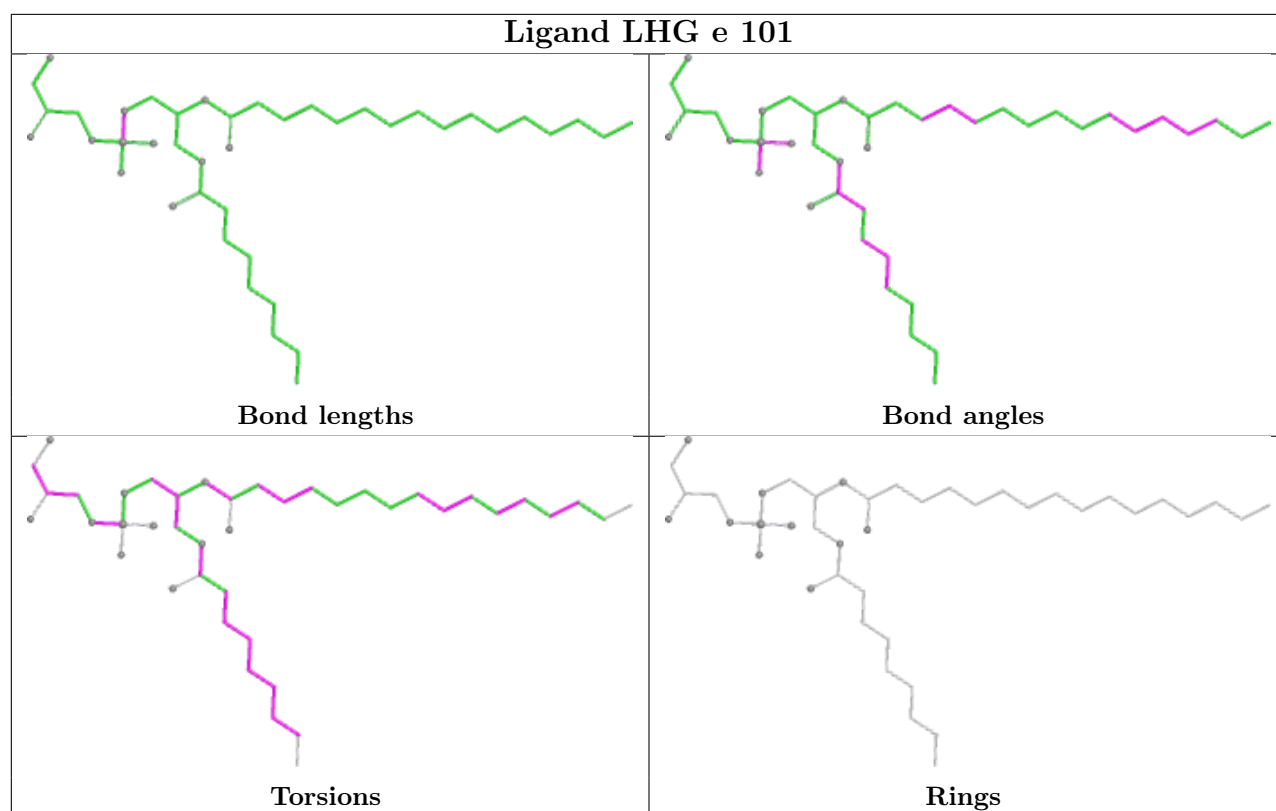


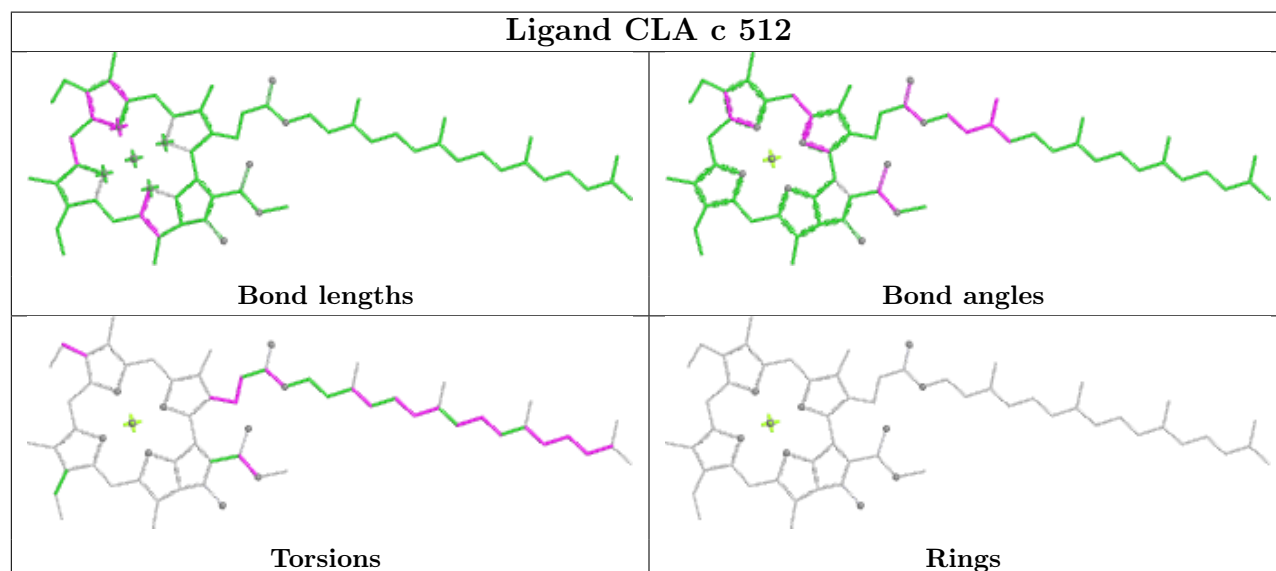
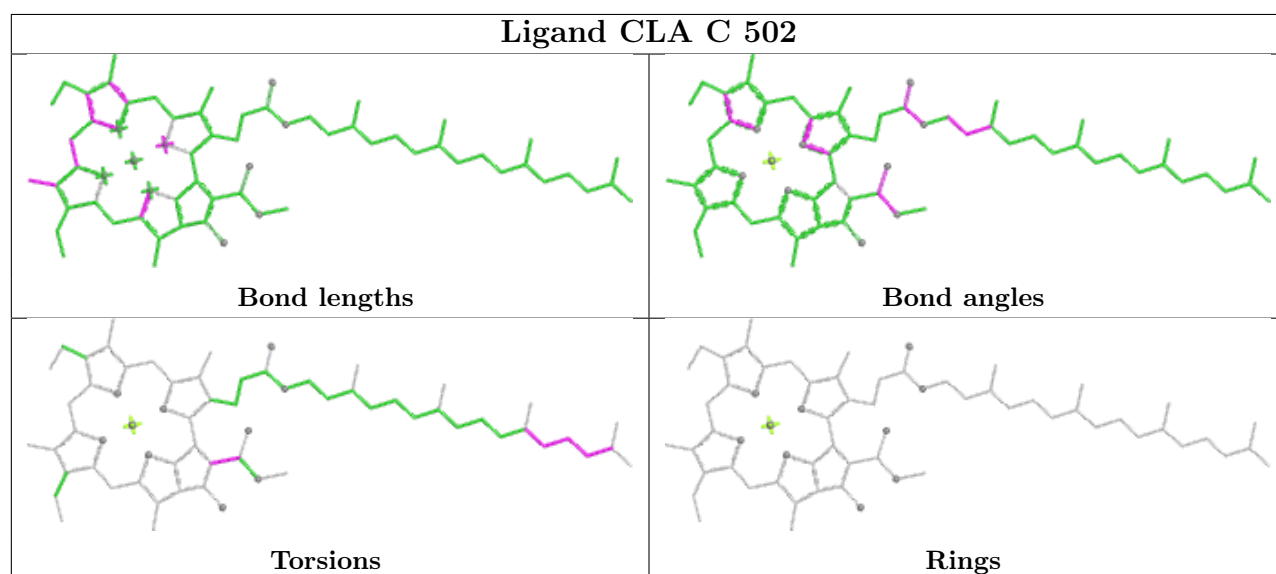
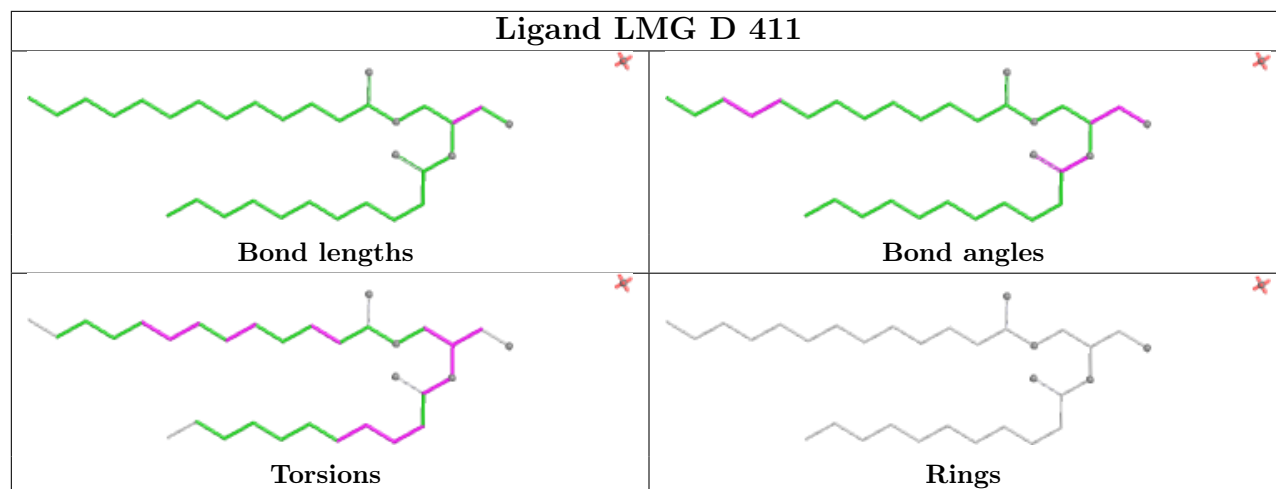
Ligand CLA D 404	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR k 103	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR B 617	
 Bond lengths	 Bond angles
 Torsions	 Rings











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [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%)	-0.71	0 100 100	11, 28, 45, 75	64 (19%)
1	a	334/344 (97%)	-0.65	0 100 100	11, 29, 54, 72	64 (19%)
2	B	505/510 (99%)	-0.57	1 (0%) 91 90	17, 32, 57, 88	4 (0%)
2	b	505/510 (99%)	-0.47	1 (0%) 91 90	25, 35, 67, 99	0
3	C	442/461 (95%)	-0.60	0 100 100	13, 34, 50, 69	11 (2%)
3	c	451/461 (97%)	-0.46	1 (0%) 91 90	13, 38, 57, 93	12 (2%)
4	D	341/352 (96%)	-0.74	0 100 100	14, 29, 44, 72	2 (0%)
4	d	341/352 (96%)	-0.62	0 100 100	14, 33, 55, 79	3 (0%)
5	E	82/84 (97%)	-0.05	0 100 100	31, 47, 66, 79	1 (1%)
5	e	82/84 (97%)	0.11	1 (1%) 76 76	39, 54, 73, 84	0
6	F	34/45 (75%)	-0.26	0 100 100	34, 42, 57, 87	0
6	f	34/45 (75%)	-0.11	0 100 100	39, 48, 76, 83	0
7	H	65/66 (98%)	-0.30	1 (1%) 72 71	32, 39, 54, 68	0
7	h	63/66 (95%)	-0.10	0 100 100	38, 49, 58, 61	0
8	I	35/38 (92%)	-0.42	0 100 100	33, 39, 62, 81	0
8	i	35/38 (92%)	-0.38	0 100 100	32, 39, 68, 86	0
9	J	36/40 (90%)	-0.25	0 100 100	32, 46, 70, 78	0
9	j	36/40 (90%)	-0.12	0 100 100	36, 51, 83, 93	0
10	K	37/46 (80%)	-0.34	0 100 100	38, 46, 61, 67	0
10	k	37/46 (80%)	-0.10	0 100 100	44, 52, 66, 74	0
11	L	37/37 (100%)	-0.59	0 100 100	25, 29, 59, 67	0
11	l	36/37 (97%)	-0.60	0 100 100	26, 29, 61, 80	0
12	M	32/36 (88%)	-0.60	0 100 100	27, 32, 57, 67	0
12	m	31/36 (86%)	-0.54	0 100 100	29, 34, 48, 61	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/272 (89%)	-0.34	4 (1%) 70 70	26, 40, 75, 127	1 (0%)
13	o	244/272 (89%)	-0.34	2 (0%) 82 82	26, 40, 76, 115	0
14	T	29/32 (90%)	-0.64	1 (3%) 48 47	27, 30, 56, 71	0
14	t	29/32 (90%)	-0.60	0 100 100	26, 32, 68, 81	0
15	U	97/134 (72%)	-0.43	0 100 100	32, 41, 65, 91	0
15	u	97/134 (72%)	-0.43	1 (1%) 79 79	30, 38, 54, 83	0
16	V	137/163 (84%)	-0.49	0 100 100	29, 38, 52, 71	0
16	v	137/163 (84%)	-0.33	0 100 100	34, 45, 63, 79	0
17	Y	27/46 (58%)	0.53	2 (7%) 20 19	49, 64, 79, 87	0
17	y	30/46 (65%)	0.27	0 100 100	56, 66, 76, 90	0
18	X	38/41 (92%)	-0.16	0 100 100	40, 48, 64, 71	0
18	x	39/41 (95%)	0.16	1 (2%) 57 56	47, 59, 79, 91	0
19	Z	62/62 (100%)	0.51	3 (4%) 35 34	48, 62, 100, 113	0
19	z	62/62 (100%)	0.33	2 (3%) 50 49	55, 64, 104, 112	0
20	R	34/41 (82%)	0.57	1 (2%) 53 52	56, 65, 78, 79	0
20	r	31/41 (75%)	1.04	2 (6%) 25 23	67, 81, 97, 101	0
All	All	5302/5700 (93%)	-0.44	24 (0%) 87 87	11, 36, 68, 127	162 (3%)

The worst 5 of 24 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
20	R	35	LEU	4.3
18	x	37	VAL	3.4
19	Z	62	VAL	3.3
20	r	31	VAL	3.1
13	o	58	ASN	3.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
14	FME	t	1	10/11	0.92	0.07	31,38,52,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
12	FME	M	1	10/11	0.93	0.09	36,46,59,62	0
14	FME	T	1	10/11	0.94	0.08	30,36,56,60	0
8	FME	I	1	10/11	0.95	0.06	38,44,50,50	0
12	FME	m	1	10/11	0.97	0.06	35,44,61,62	0
8	FME	i	1	10/11	0.98	0.06	37,45,47,48	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	STE	H	103	18/20	0.68	0.13	55,64,72,72	0
32	STE	a	615	12/20	0.75	0.10	51,57,70,73	0
32	STE	T	103	20/20	0.76	0.12	42,52,69,75	0
28	LMG	b	624	55/55	0.76	0.14	50,63,76,77	0
32	STE	b	625	16/20	0.77	0.11	49,56,68,71	0
29	LHG	e	101	42/49	0.78	0.12	56,75,91,95	0
32	STE	m	101	12/20	0.78	0.13	51,58,64,67	0
28	LMG	d	410	23/55	0.79	0.12	47,61,65,68	0
32	STE	c	521	12/20	0.79	0.12	57,66,70,71	0
29	LHG	E	101	49/49	0.79	0.12	40,69,89,97	0
32	STE	B	625	18/20	0.80	0.12	42,52,76,82	0
32	STE	B	627	16/20	0.80	0.12	46,56,68,68	0
28	LMG	c	520	48/55	0.80	0.12	52,68,80,83	0
31	DGD	o	301	44/66	0.80	0.12	36,50,67,70	0
32	STE	b	626	10/20	0.81	0.11	48,53,60,60	0
32	STE	T	102	15/20	0.81	0.13	43,50,65,66	0
32	STE	E	102	12/20	0.81	0.11	57,67,81,82	0
27	PL9	A	610	55/55	0.82	0.12	35,57,67,71	0
32	STE	B	626	12/20	0.82	0.10	50,54,67,69	0
31	DGD	A	616	66/66	0.82	0.10	45,55,63,68	0
28	LMG	D	411	33/55	0.82	0.10	38,51,70,71	0
32	STE	X	101	20/20	0.83	0.14	36,48,61,65	0
30	SQD	a	614	36/54	0.83	0.10	38,54,64,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	CLA	b	601	65/65	0.83	0.10	45,61,78,84	0
30	SQD	f	102	41/54	0.84	0.11	58,72,82,85	0
32	STE	J	101	12/20	0.84	0.10	46,52,61,63	0
30	SQD	A	615	39/54	0.84	0.10	41,51,74,77	0
27	PL9	a	611	55/55	0.84	0.12	39,60,70,76	0
32	STE	d	413	20/20	0.84	0.12	43,50,57,58	0
32	STE	B	620	17/20	0.84	0.11	36,47,60,64	0
32	STE	t	103	10/20	0.84	0.10	44,53,60,61	0
30	SQD	B	623	54/54	0.85	0.10	36,56,72,80	0
28	LMG	c	518	37/55	0.85	0.10	43,57,68,69	0
32	STE	I	101	15/20	0.85	0.10	42,50,56,56	0
28	LMG	A	612	48/55	0.85	0.09	41,54,62,65	0
32	STE	b	621	16/20	0.85	0.11	34,45,55,61	0
32	STE	t	102	14/20	0.85	0.09	40,44,57,58	0
32	STE	b	623	20/20	0.85	0.11	37,49,67,69	0
28	LMG	c	522	49/55	0.86	0.09	40,50,70,76	0
30	SQD	b	620	49/54	0.86	0.09	41,50,73,78	0
28	LMG	b	622	51/55	0.87	0.09	33,49,60,63	0
32	STE	C	519	12/20	0.87	0.10	39,44,58,59	0
32	STE	C	520	12/20	0.87	0.09	43,49,53,54	0
28	LMG	B	621	28/55	0.87	0.10	38,45,59,69	0
26	BCR	k	102	40/40	0.87	0.10	43,52,58,60	0
25	CLA	B	601	65/65	0.88	0.10	38,51,72,80	0
32	STE	j	101	12/20	0.88	0.09	46,52,58,58	0
32	STE	c	519	20/20	0.88	0.09	40,49,80,81	0
32	STE	B	624	12/20	0.88	0.11	44,53,58,60	0
32	STE	d	412	17/20	0.88	0.10	42,47,61,64	0
28	LMG	M	101	51/55	0.89	0.08	33,47,59,61	0
32	STE	M	103	10/20	0.89	0.09	40,43,49,51	0
28	LMG	C	518	48/55	0.89	0.09	38,59,70,72	0
26	BCR	x	101	40/40	0.90	0.09	38,50,63,64	0
26	BCR	K	102	40/40	0.90	0.09	38,44,53,55	0
32	STE	C	521	16/20	0.90	0.08	36,44,51,58	0
26	BCR	D	406	40/40	0.91	0.08	32,40,68,75	0
32	STE	l	102	18/20	0.91	0.09	35,45,60,62	0
30	SQD	a	613	54/54	0.91	0.10	37,54,73,77	0
25	CLA	C	513	65/65	0.91	0.08	41,51,72,76	0
26	BCR	d	405	40/40	0.91	0.08	38,44,70,72	0
31	DGD	c	516	62/66	0.92	0.07	34,45,68,72	0
26	BCR	k	101	40/40	0.92	0.08	42,52,57,60	0
32	STE	M	102	15/20	0.92	0.07	36,44,54,63	0
26	BCR	H	101	40/40	0.92	0.07	34,40,53,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	SQD	D	409	36/54	0.92	0.09	43,60,66,69	0
26	BCR	K	101	40/40	0.92	0.08	41,48,54,56	0
31	DGD	H	102	62/66	0.92	0.08	29,40,46,53	0
31	DGD	C	516	62/66	0.93	0.07	32,42,75,84	0
25	CLA	c	512	65/65	0.93	0.08	39,50,70,74	0
26	BCR	b	618	40/40	0.93	0.06	25,34,45,50	0
31	DGD	h	101	62/66	0.93	0.08	35,45,52,57	0
26	BCR	A	609	40/40	0.93	0.06	26,31,37,41	0
29	LHG	d	407	49/49	0.93	0.07	33,44,58,66	0
28	LMG	D	408	51/55	0.93	0.09	28,42,67,71	0
30	SQD	A	614	52/54	0.93	0.09	33,47,67,69	0
26	BCR	B	619	40/40	0.93	0.07	29,39,48,52	0
33	BCT	a	606	4/4	0.93	0.08	32,35,39,44	0
31	DGD	C	517	62/66	0.94	0.07	26,38,62,70	0
26	BCR	B	618	40/40	0.94	0.06	24,34,44,46	0
26	BCR	k	103	40/40	0.94	0.08	41,47,55,58	0
31	DGD	c	517	62/66	0.94	0.07	29,44,64,76	0
28	LMG	d	411	44/55	0.94	0.07	34,43,71,73	0
25	CLA	C	506	65/65	0.94	0.07	28,37,68,69	0
26	BCR	C	514	40/40	0.94	0.07	29,36,47,47	0
25	CLA	b	616	60/65	0.94	0.08	29,37,77,79	0
25	CLA	c	506	65/65	0.94	0.07	32,40,70,76	0
25	CLA	c	508	64/65	0.94	0.07	32,38,74,85	0
25	CLA	C	512	65/65	0.94	0.08	35,44,66,69	0
26	BCR	a	610	40/40	0.94	0.06	22,30,38,41	0
26	BCR	b	617	40/40	0.94	0.06	29,36,44,44	0
25	CLA	c	513	65/65	0.94	0.08	38,53,79,85	0
26	BCR	b	619	40/40	0.94	0.06	30,40,53,56	0
26	BCR	c	514	40/40	0.94	0.06	31,40,48,51	0
25	CLA	B	606	65/65	0.94	0.07	25,33,58,63	0
31	DGD	C	515	62/66	0.94	0.07	25,34,63,67	0
26	BCR	B	617	40/40	0.94	0.06	27,33,42,44	0
34	PHO	d	402	64/64	0.94	0.06	23,35,40,43	0
26	BCR	T	101	40/40	0.95	0.05	28,34,45,47	0
26	BCR	Z	101	40/40	0.95	0.07	34,42,53,54	0
25	CLA	C	508	65/65	0.95	0.06	28,34,75,82	0
29	LHG	A	613	47/49	0.95	0.08	27,39,64,68	0
29	LHG	B	622	49/49	0.95	0.07	30,39,53,55	0
25	CLA	c	503	65/65	0.95	0.06	31,39,43,50	0
25	CLA	c	504	60/65	0.95	0.06	29,38,70,72	0
25	CLA	C	510	65/65	0.95	0.06	27,35,46,51	0
29	LHG	l	101	49/49	0.95	0.06	32,39,46,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	CLA	c	507	65/65	0.95	0.07	29,37,46,49	0
25	CLA	C	511	65/65	0.95	0.07	30,41,54,56	0
25	CLA	c	509	65/65	0.95	0.07	31,38,52,55	0
25	CLA	c	510	65/65	0.95	0.07	32,40,51,53	0
25	CLA	c	511	65/65	0.95	0.07	36,47,58,62	0
26	BCR	t	101	40/40	0.95	0.05	25,36,46,48	0
25	CLA	C	501	65/65	0.95	0.06	26,31,43,47	0
25	CLA	C	503	65/65	0.95	0.06	30,36,40,48	0
25	CLA	d	403	65/65	0.95	0.07	22,29,47,56	0
27	PL9	d	406	55/55	0.95	0.06	25,31,36,38	0
25	CLA	d	404	65/65	0.95	0.08	30,38,76,78	0
25	CLA	a	607	65/65	0.95	0.06	21,27,37,45	0
25	CLA	a	608	65/65	0.95	0.07	27,34,72,79	0
31	DGD	c	515	62/66	0.95	0.07	22,35,58,66	0
25	CLA	B	609	65/65	0.95	0.06	27,34,47,54	0
25	CLA	b	602	65/65	0.95	0.07	29,36,49,55	0
25	CLA	b	606	65/65	0.95	0.07	29,35,61,64	0
25	CLA	b	608	65/65	0.95	0.06	27,36,53,59	0
25	CLA	b	609	65/65	0.95	0.07	29,38,56,66	0
33	BCT	D	401	4/4	0.95	0.06	29,32,34,35	0
25	CLA	b	610	65/65	0.95	0.07	27,34,41,47	0
25	CLA	b	614	65/65	0.95	0.06	26,35,62,66	0
29	LHG	L	101	49/49	0.96	0.06	28,35,46,55	0
25	CLA	D	405	65/65	0.96	0.07	27,33,74,84	0
29	LHG	d	408	49/49	0.96	0.06	30,37,48,50	0
29	LHG	d	409	39/49	0.96	0.07	33,38,53,55	0
25	CLA	B	616	60/65	0.96	0.07	25,33,69,74	0
25	CLA	B	602	65/65	0.96	0.06	24,32,47,50	0
25	CLA	a	609	65/65	0.96	0.08	22,28,62,68	0
25	CLA	a	612	65/65	0.96	0.05	22,27,38,44	0
25	CLA	C	502	65/65	0.96	0.06	26,32,44,50	0
25	CLA	B	604	65/65	0.96	0.06	22,28,57,59	0
27	PL9	D	407	55/55	0.96	0.05	22,28,37,39	0
25	CLA	b	603	65/65	0.96	0.06	26,31,52,61	0
25	CLA	C	504	59/65	0.96	0.06	28,34,67,70	0
25	CLA	b	607	65/65	0.96	0.06	23,30,54,57	0
25	CLA	C	505	65/65	0.96	0.06	26,35,56,62	0
25	CLA	A	607	65/65	0.96	0.06	22,28,73,79	0
25	CLA	B	607	65/65	0.96	0.06	21,28,49,55	0
25	CLA	b	611	65/65	0.96	0.05	25,30,43,50	0
25	CLA	b	612	65/65	0.96	0.06	23,30,38,45	0
25	CLA	b	613	65/65	0.96	0.06	19,28,60,65	0

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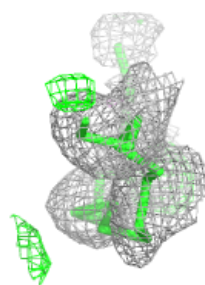
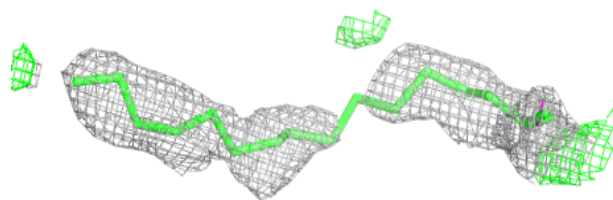
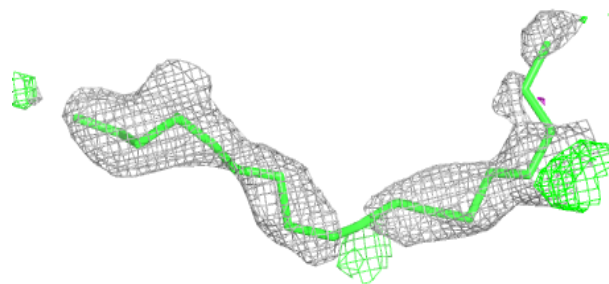
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	CLA	C	509	65/65	0.96	0.07	24,33,50,54	0
25	CLA	b	615	65/65	0.96	0.06	28,36,50,57	0
25	CLA	A	606	65/65	0.96	0.05	18,25,38,47	0
25	CLA	c	501	65/65	0.96	0.06	29,35,45,52	0
25	CLA	c	502	65/65	0.96	0.06	25,35,47,51	0
25	CLA	B	610	65/65	0.96	0.06	23,29,36,39	0
25	CLA	B	613	65/65	0.96	0.06	21,26,55,61	0
25	CLA	c	505	65/65	0.96	0.06	29,35,56,65	0
34	PHO	D	402	64/64	0.96	0.05	19,26,33,37	0
34	PHO	D	403	64/64	0.96	0.05	22,30,34,37	0
25	CLA	B	614	65/65	0.96	0.06	20,32,57,62	0
25	CLA	C	507	65/65	0.97	0.06	25,34,47,50	0
25	CLA	B	605	65/65	0.97	0.05	22,27,37,39	0
25	CLA	B	603	65/65	0.97	0.06	21,27,50,56	0
25	CLA	B	611	65/65	0.97	0.05	21,27,41,47	0
25	CLA	B	612	65/65	0.97	0.06	21,27,37,42	0
25	CLA	A	611	65/65	0.97	0.05	21,25,40,46	0
25	CLA	B	608	65/65	0.97	0.05	25,30,46,53	0
25	CLA	b	604	65/65	0.97	0.06	24,29,65,75	0
25	CLA	b	605	65/65	0.97	0.05	23,30,42,45	0
25	CLA	D	404	65/65	0.97	0.05	20,24,43,50	0
29	LHG	D	410	49/49	0.97	0.06	27,34,44,48	0
34	PHO	d	401	64/64	0.97	0.05	24,28,33,36	0
25	CLA	B	615	65/65	0.97	0.05	23,32,52,60	0
35	HEM	F	101	43/43	0.97	0.08	39,44,55,61	0
35	HEM	f	101	43/43	0.97	0.08	46,52,65,78	0
25	CLA	A	608	54/65	0.98	0.05	21,26,53,57	0
24	CL	A	604	1/1	0.98	0.03	28,28,28,28	0
36	HEC	V	201	43/43	0.98	0.05	25,29,36,40	0
22	OEX	A	602[A]	10/10	0.99	0.04	21,29,33,33	10
22	OEX	a	602[A]	10/10	0.99	0.03	24,28,31,31	10
23	FE2	a	603	1/1	0.99	0.02	33,33,33,33	0
21	OEY	A	601[B]	11/11	0.99	0.03	24,27,30,30	11
24	CL	A	605	1/1	0.99	0.05	29,29,29,29	0
24	CL	a	604	1/1	0.99	0.04	30,30,30,30	0
24	CL	a	605	1/1	0.99	0.06	30,30,30,30	0
21	OEY	a	601[B]	11/11	0.99	0.03	26,29,32,32	11
36	HEC	v	201	43/43	0.99	0.05	29,33,40,44	0
23	FE2	A	603	1/1	1.00	0.01	27,27,27,27	0

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

orientation to approximate a three-dimensional view.

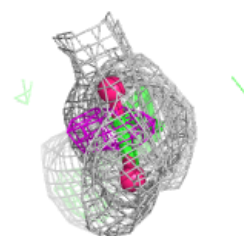
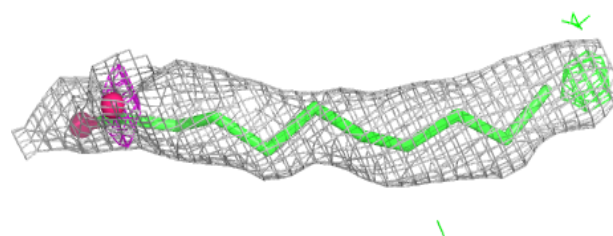
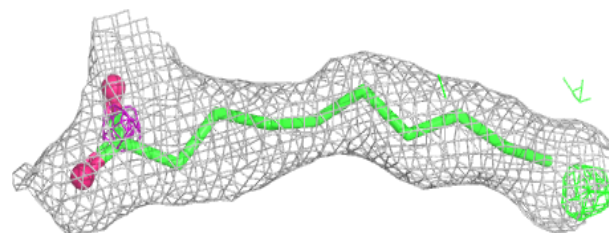
Electron density around STE H 103:

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



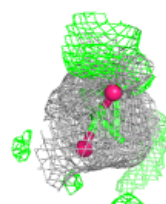
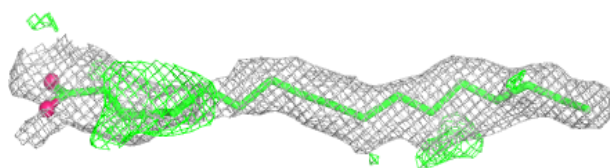
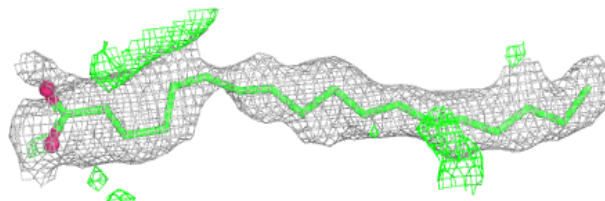
Electron density around STE a 615:

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and green (positive)

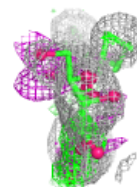
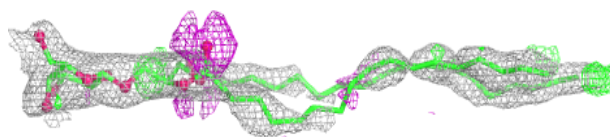
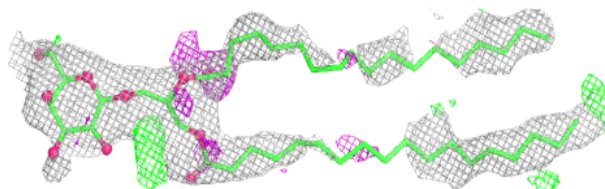


Electron density around STE T 103:

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

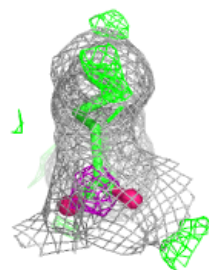
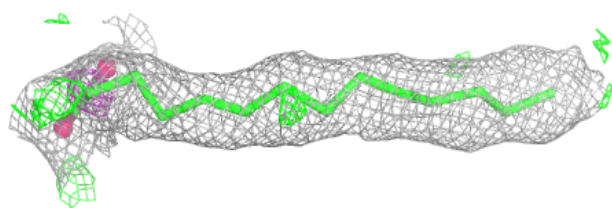
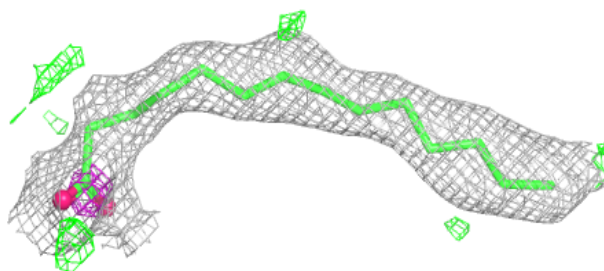
**Electron density around LMG b 624:**

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

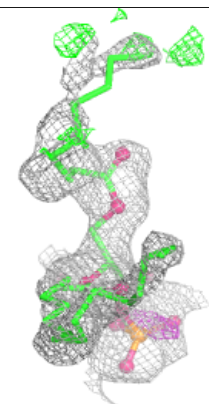
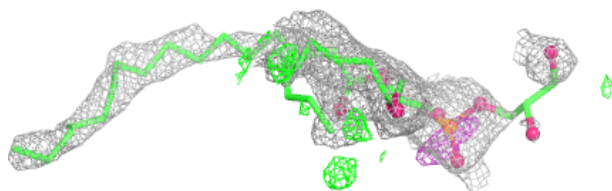
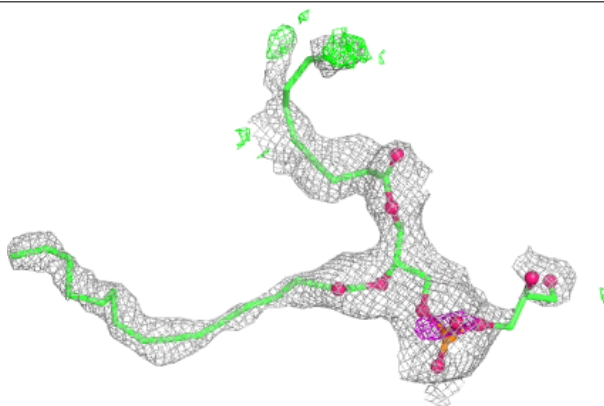


Electron density around STE b 625:

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

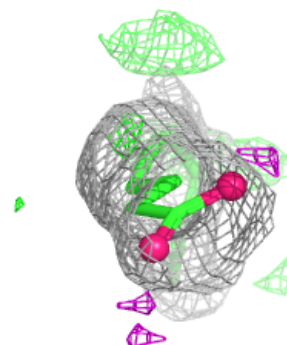
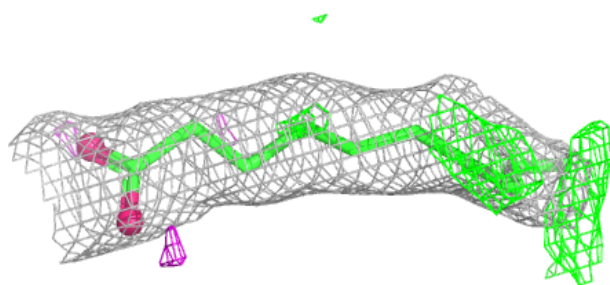
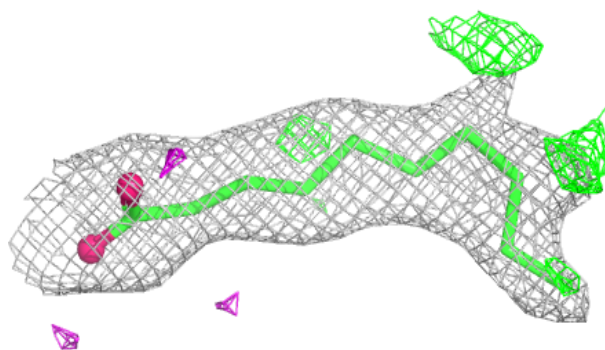
**Electron density around LHG e 101:**

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

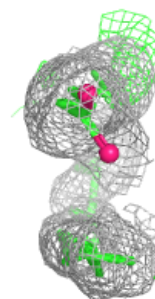
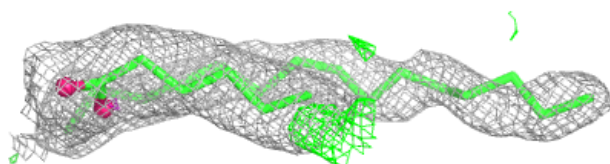
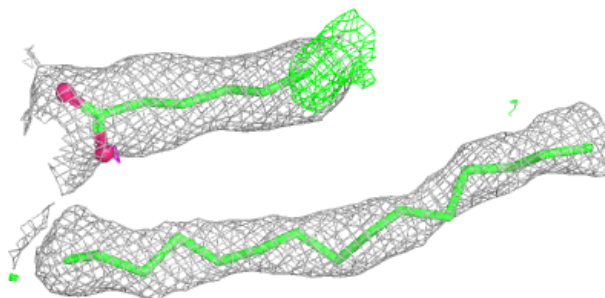


Electron density around STE m 101:

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

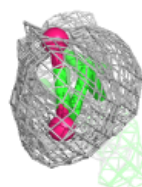
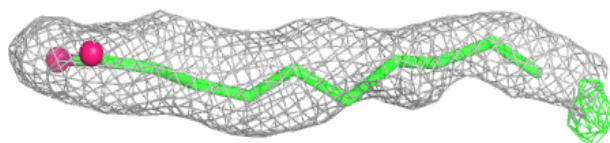
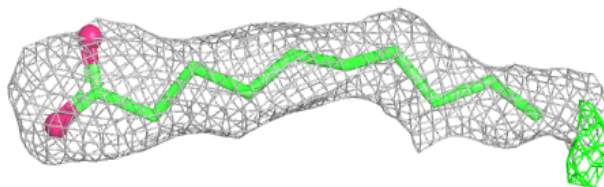
**Electron density around LMG d 410:**

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



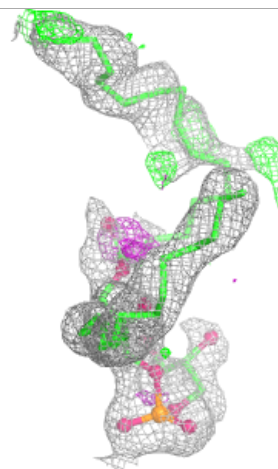
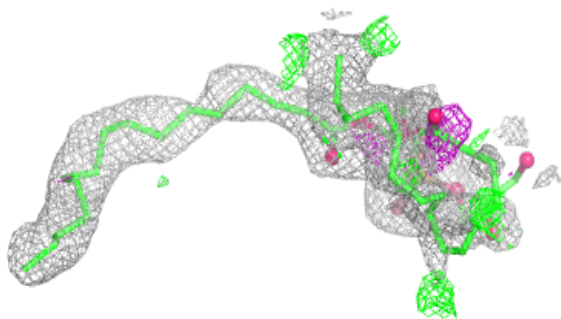
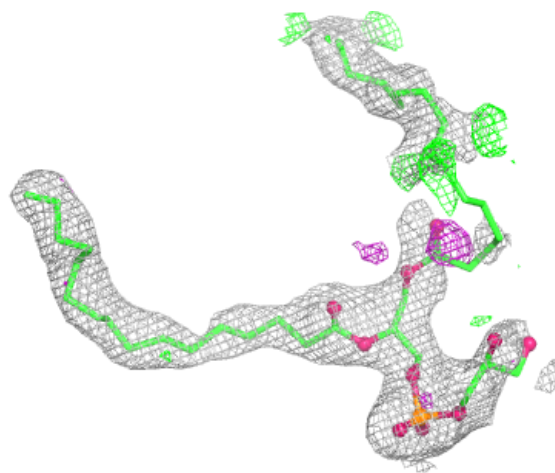
Electron density around STE c 521:

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and green (positive)



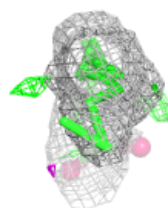
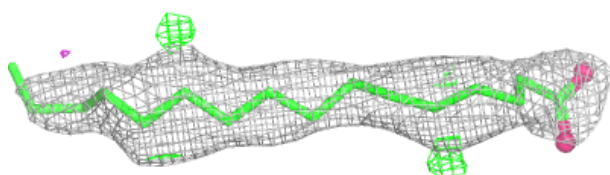
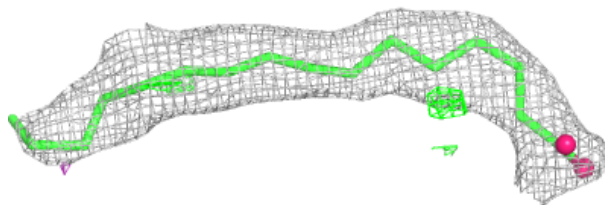
Electron density around LHG E 101:

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

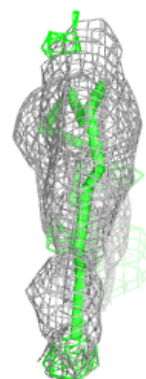
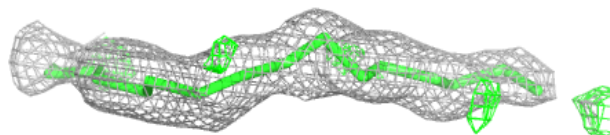


Electron density around STE B 625:

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and green (positive)

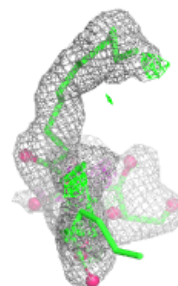
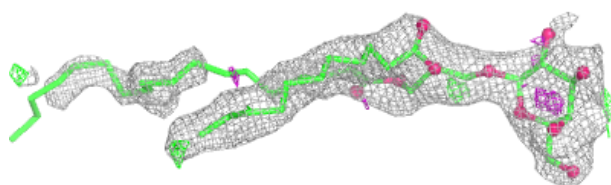
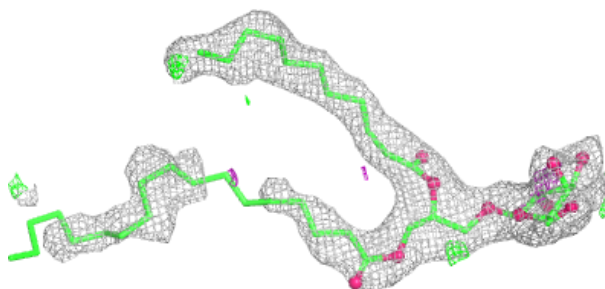
**Electron density around STE B 627:**

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and green (positive)

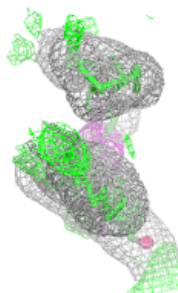
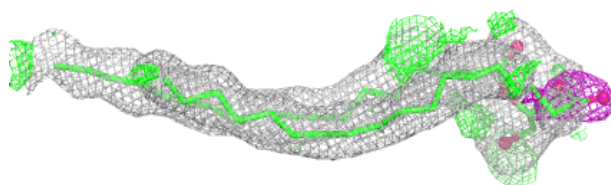
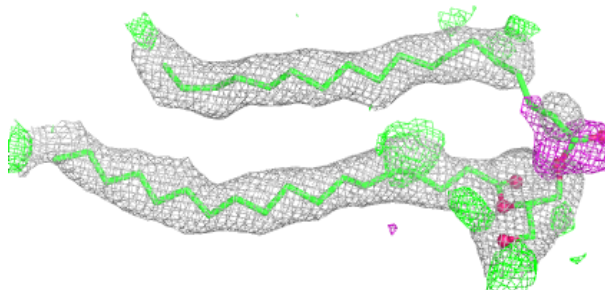


Electron density around LMG c 520:

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and green (positive)

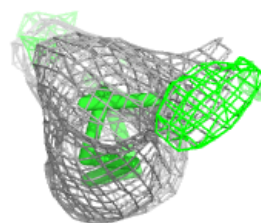
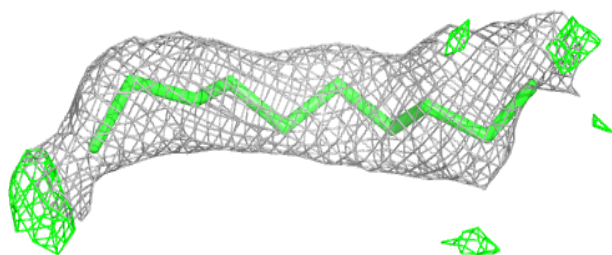
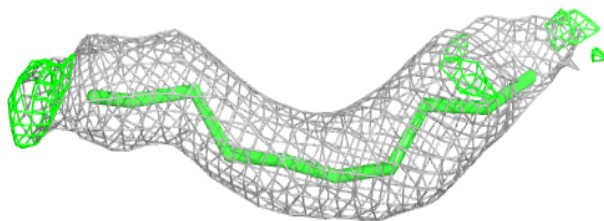
**Electron density around DGD o 301:**

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

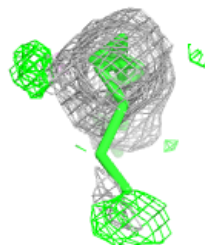
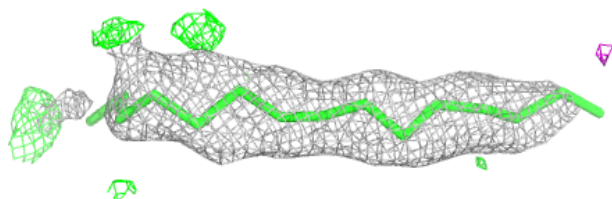
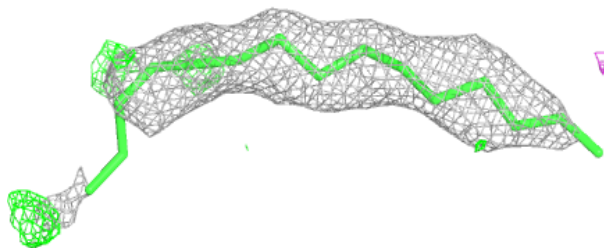


Electron density around STE b 626:

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

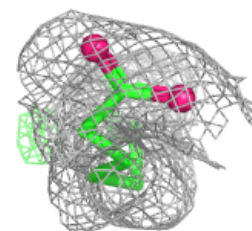
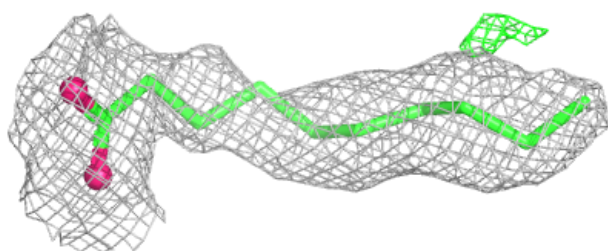
**Electron density around STE T 102:**

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

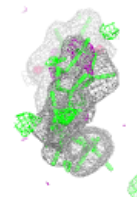
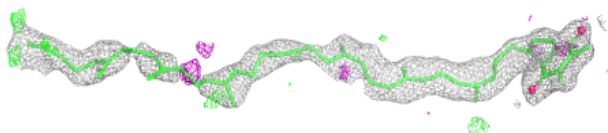
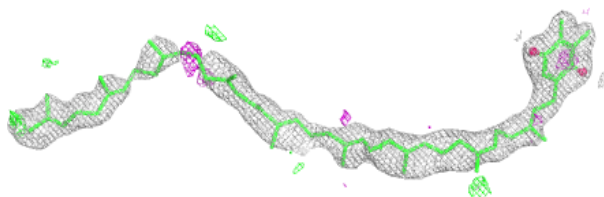


Electron density around STE E 102:

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and green (positive)

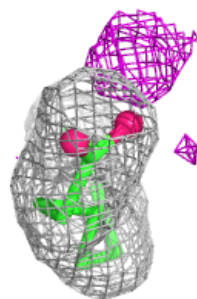
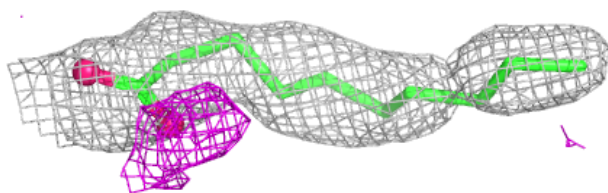
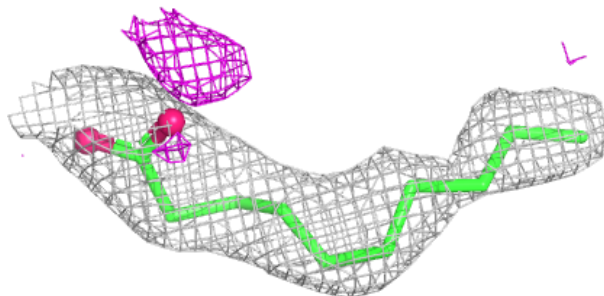
**Electron density around PL9 A 610:**

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

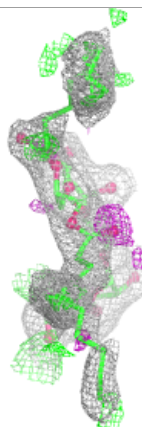
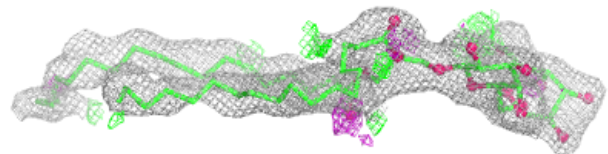
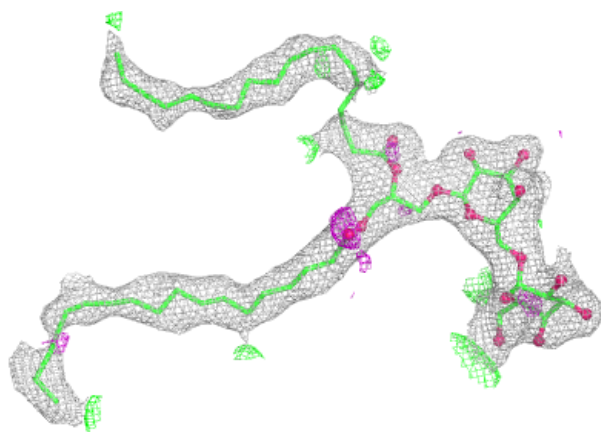


Electron density around STE B 626:

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and green (positive)

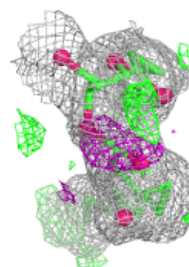
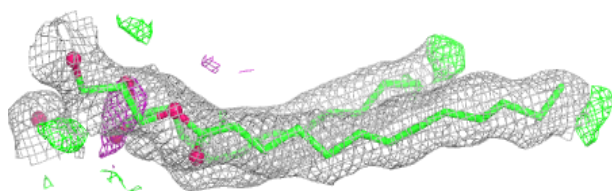
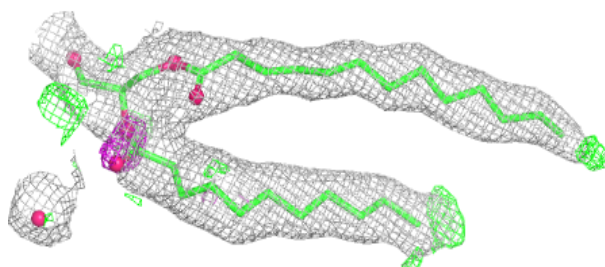
**Electron density around DGD A 616:**

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and green (positive)

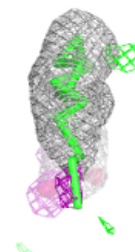
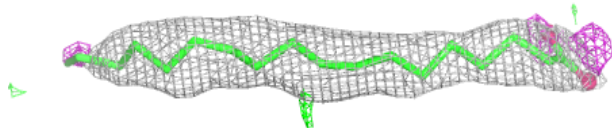
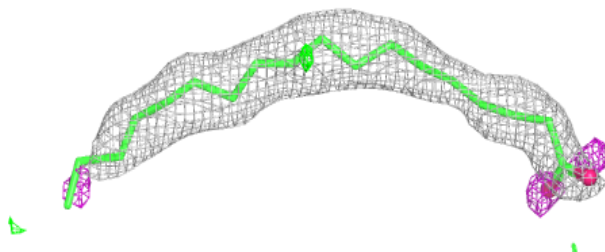


Electron density around LMG D 411:

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and green (positive)

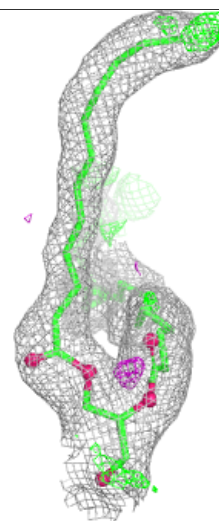
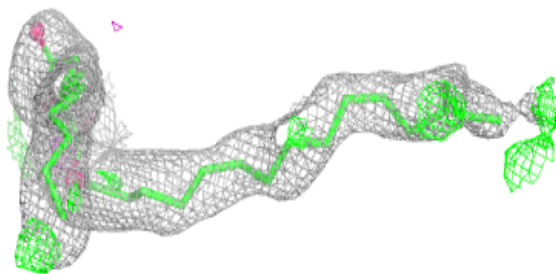
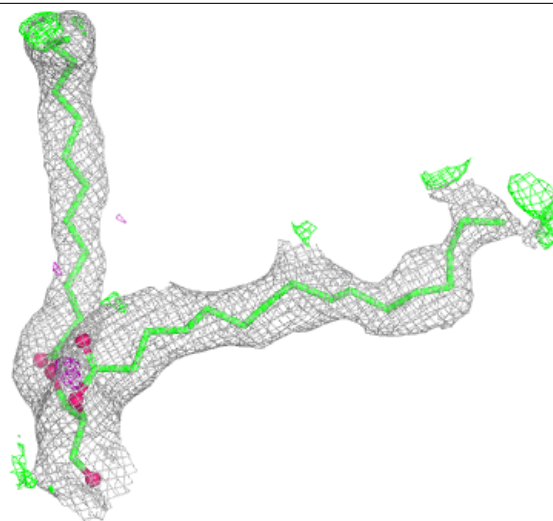
**Electron density around STE X 101:**

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



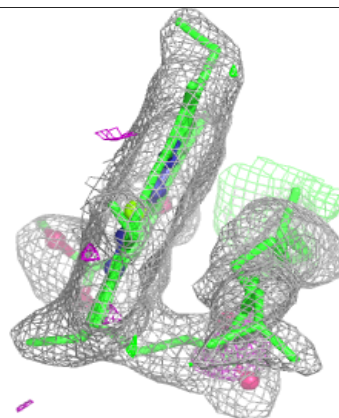
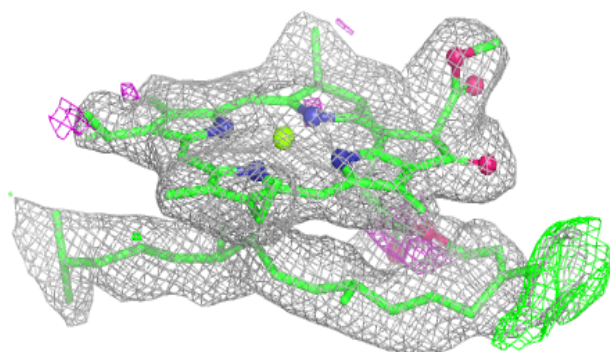
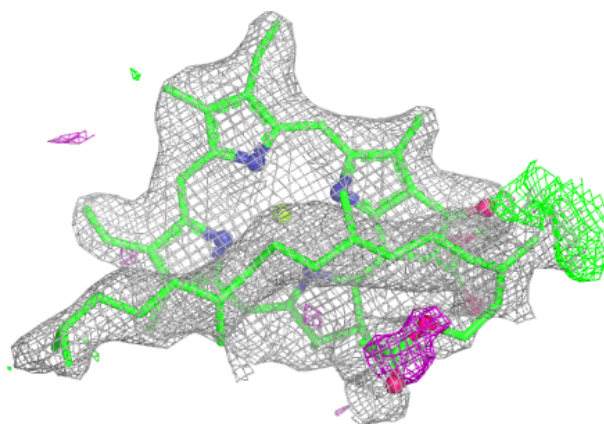
Electron density around SQD a 614:

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

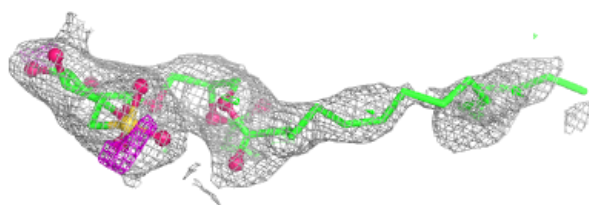
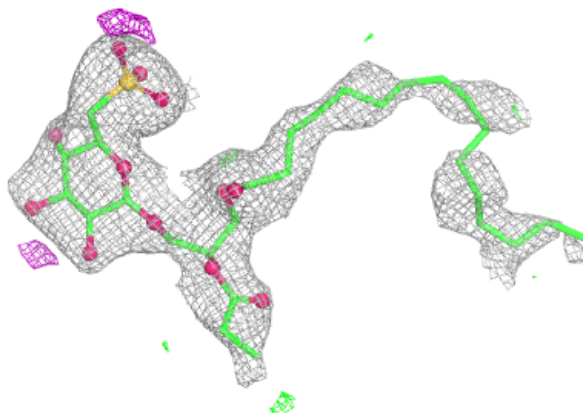


Electron density around CLA b 601:

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

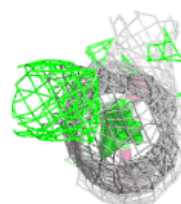
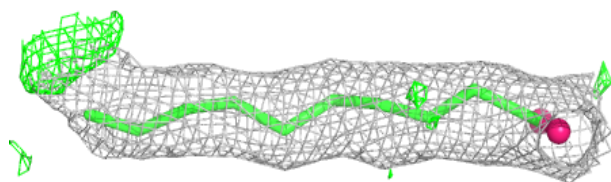
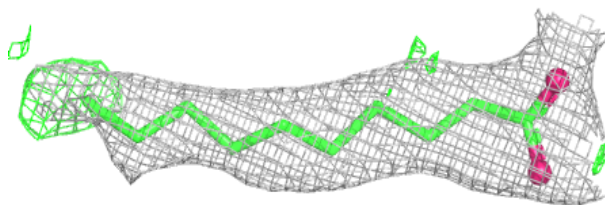
**Electron density around SQD f 102:**

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



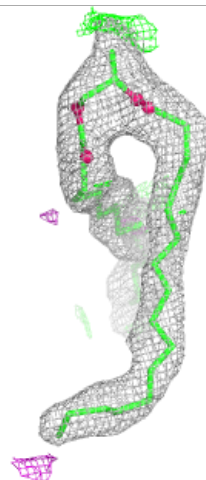
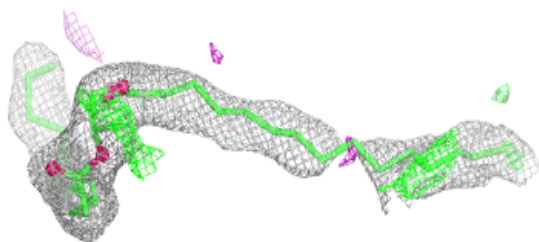
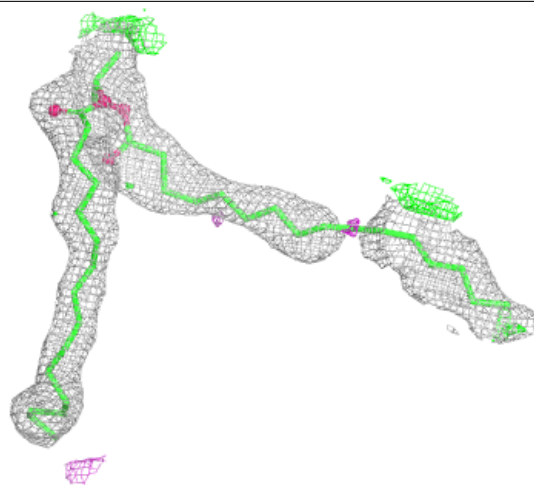
Electron density around STE J 101:

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



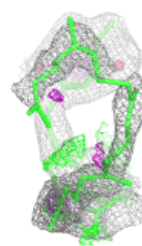
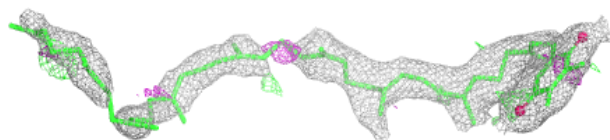
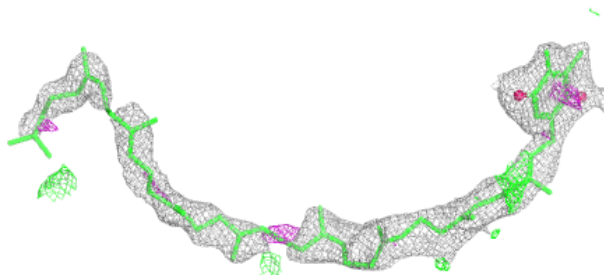
Electron density around SQD A 615:

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

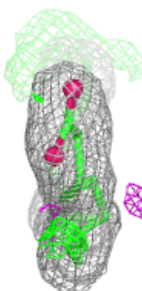
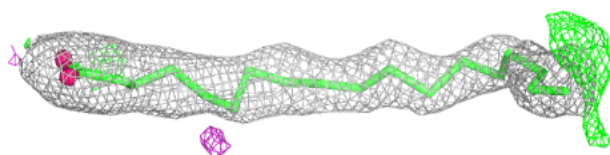
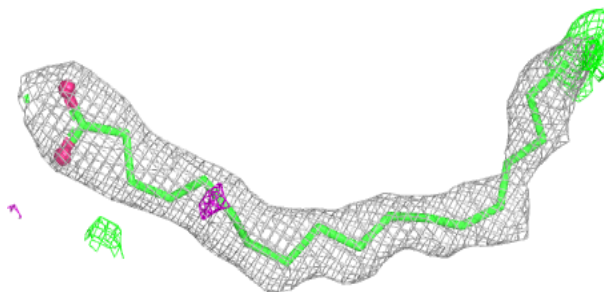


Electron density around PL9 a 611:

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

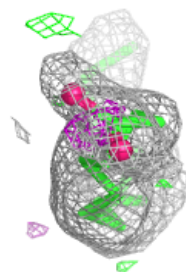
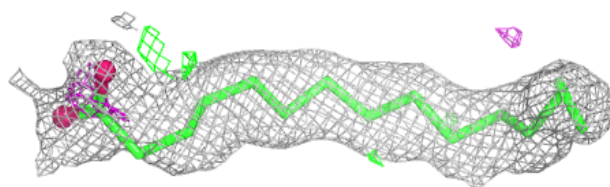
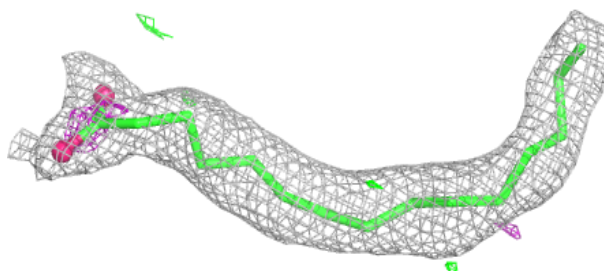
**Electron density around STE d 413:**

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

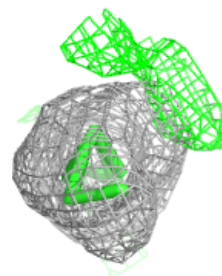
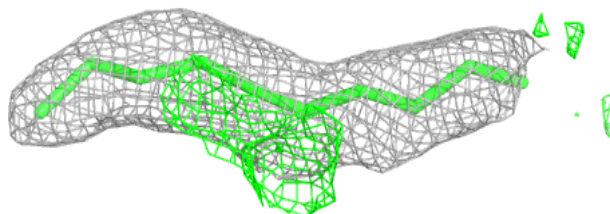
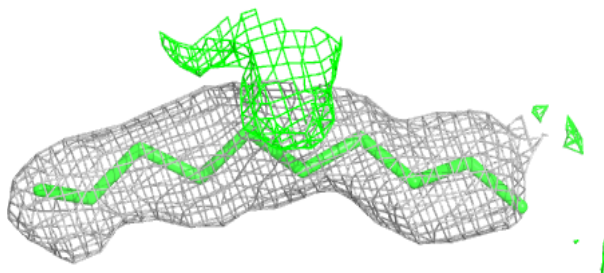


Electron density around STE B 620:

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

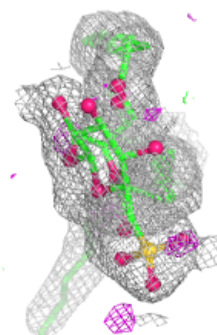
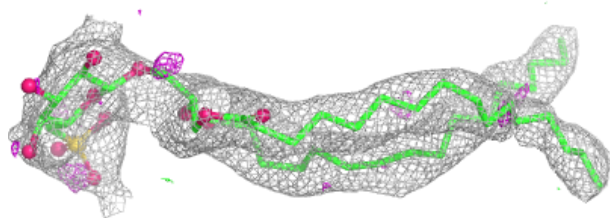
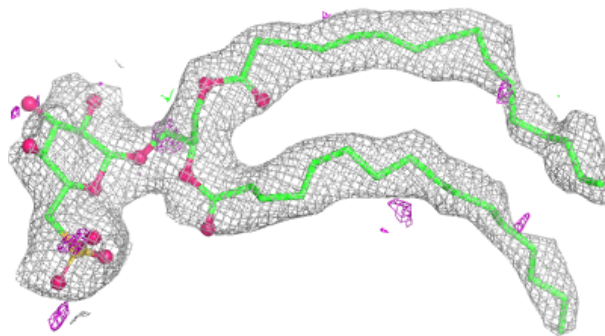
**Electron density around STE t 103:**

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

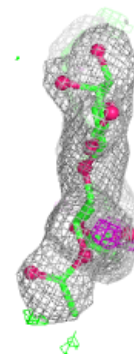
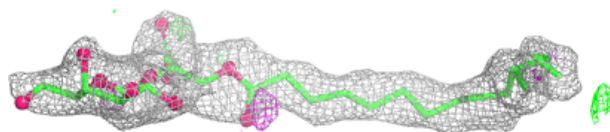
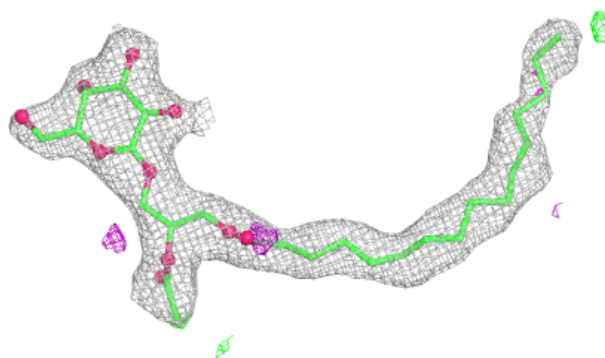


Electron density around SQD B 623:

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

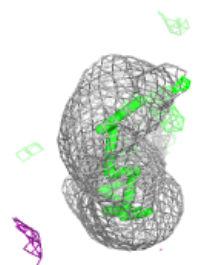
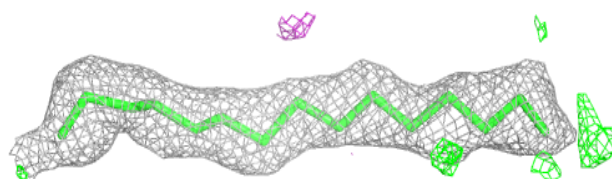
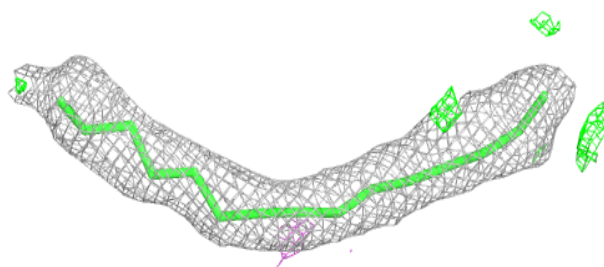
**Electron density around LMG c 518:**

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

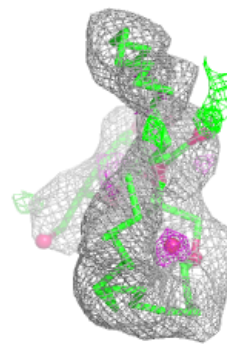
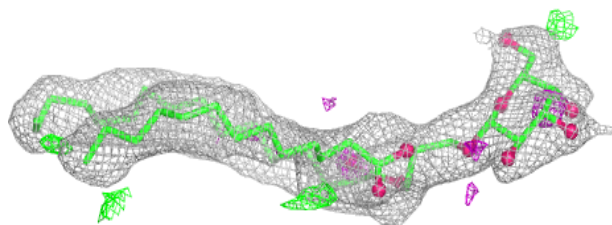
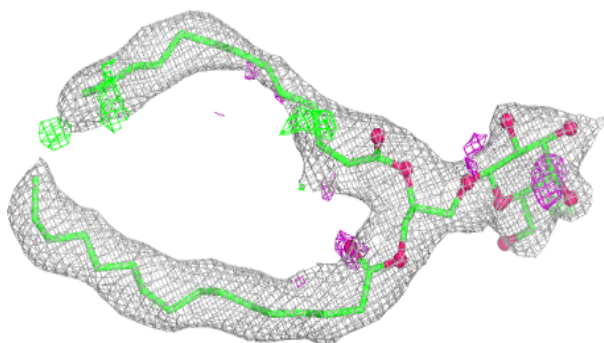


Electron density around STE I 101:

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

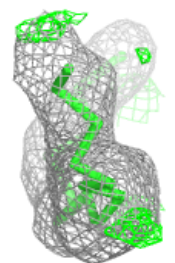
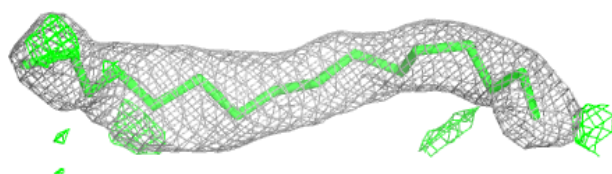
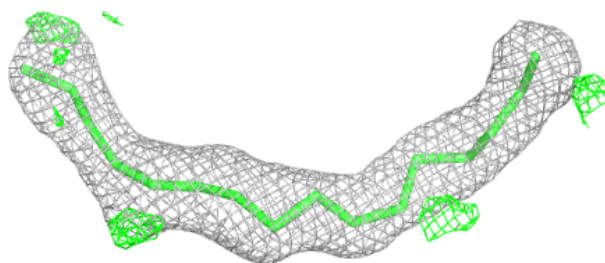
**Electron density around LMG A 612:**

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

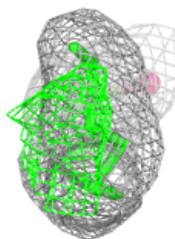
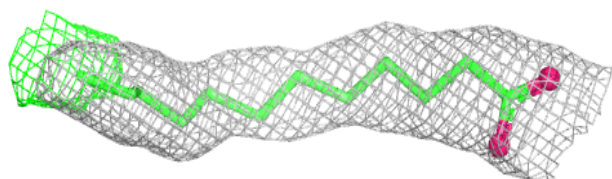
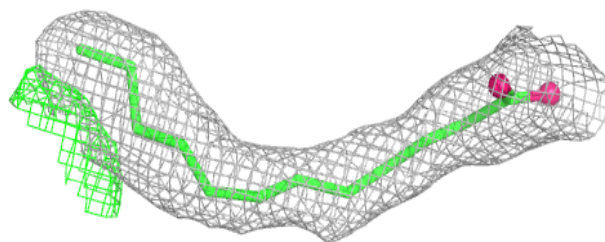


Electron density around STE b 621:

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

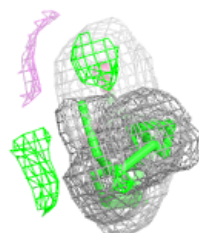
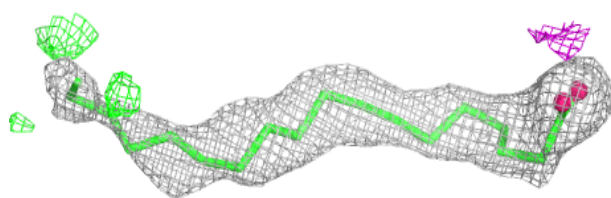
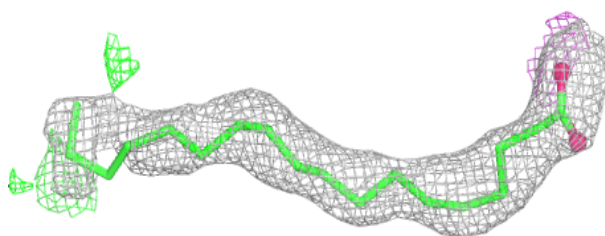
**Electron density around STE t 102:**

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

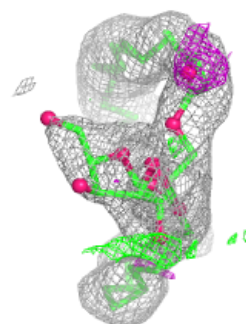
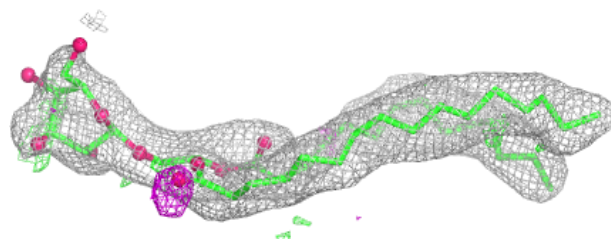
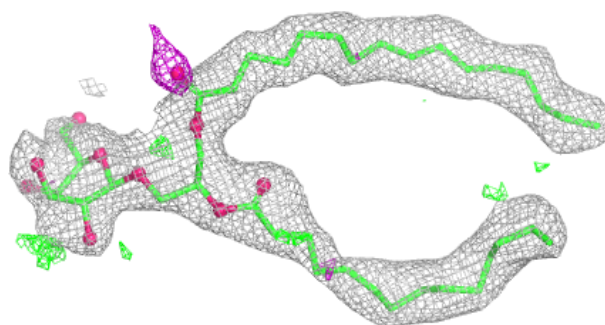


Electron density around STE b 623:

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

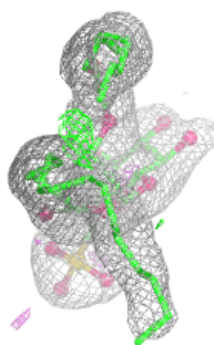
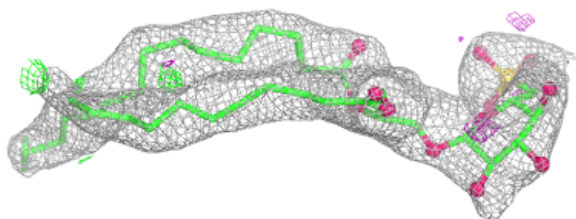
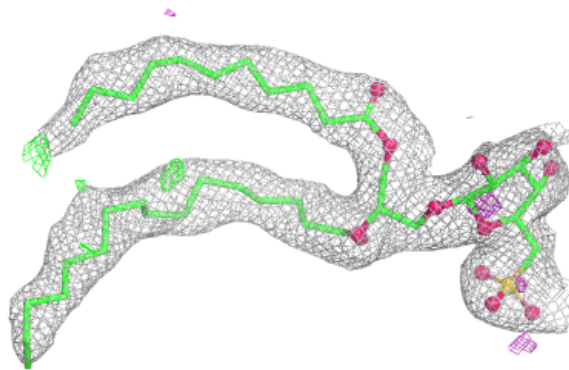
**Electron density around LMG c 522:**

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

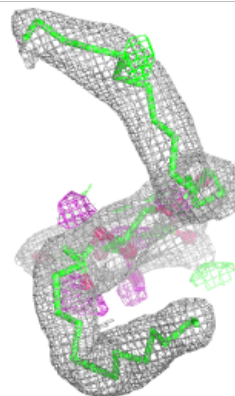
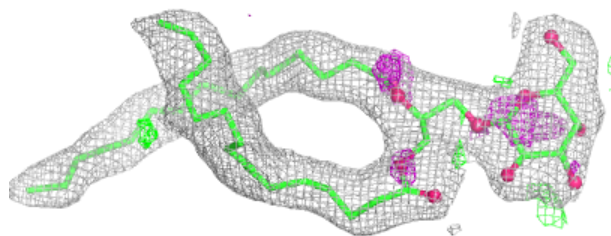
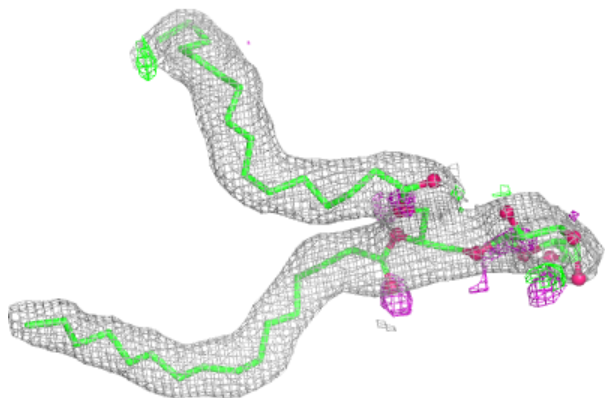


Electron density around SQD b 620:

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

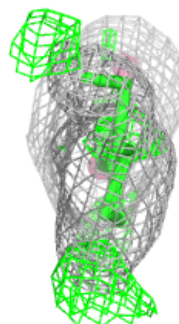
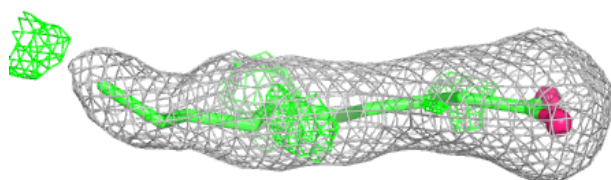
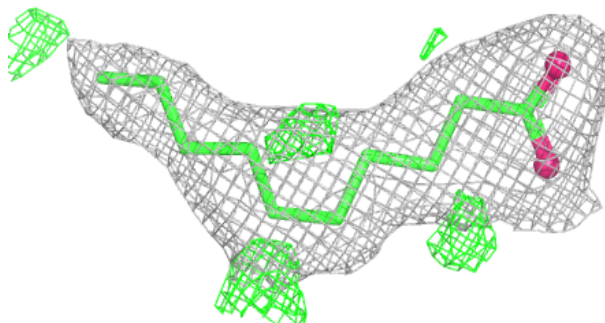
**Electron density around LMG b 622:**

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

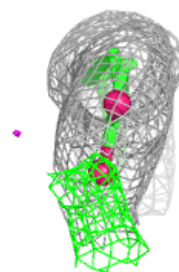
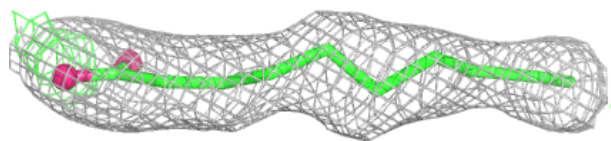
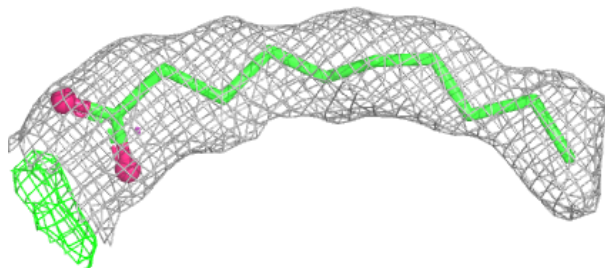


Electron density around STE C 519:

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

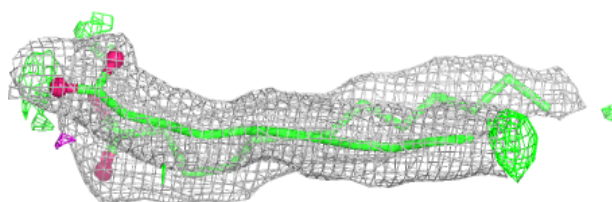
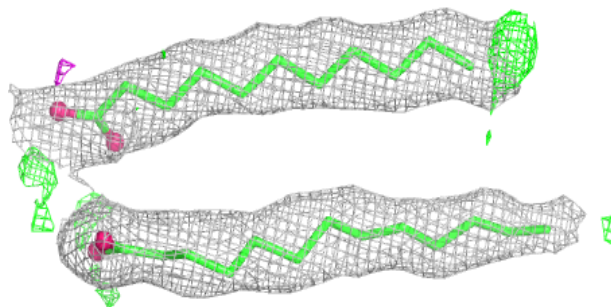
**Electron density around STE C 520:**

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

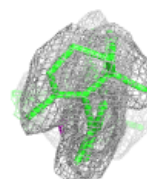
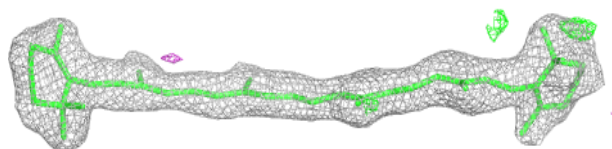
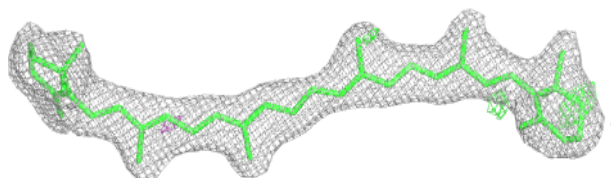


Electron density around LMG B 621:

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

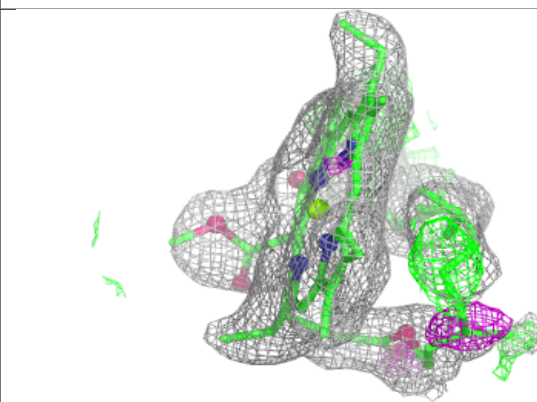
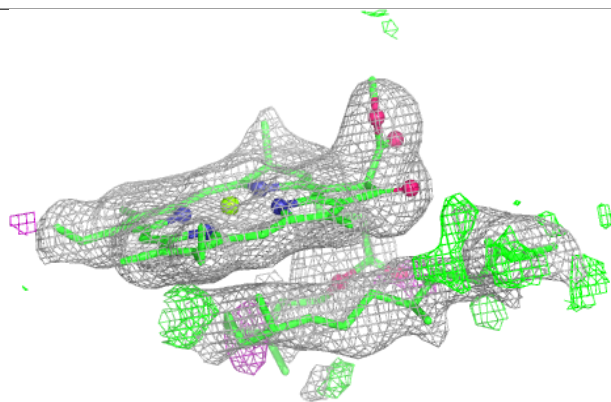
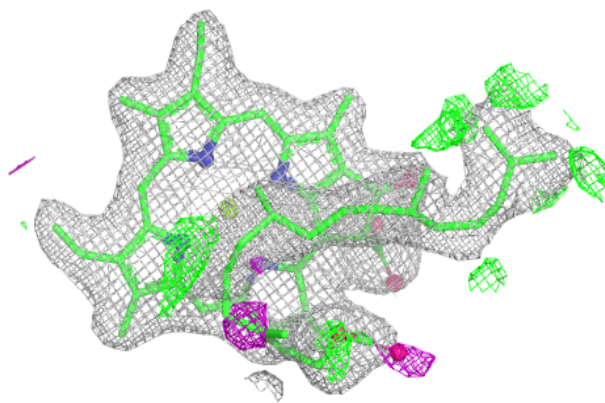
**Electron density around BCR k 102:**

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

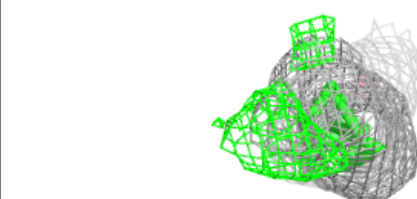
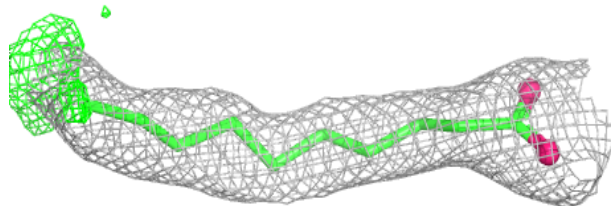
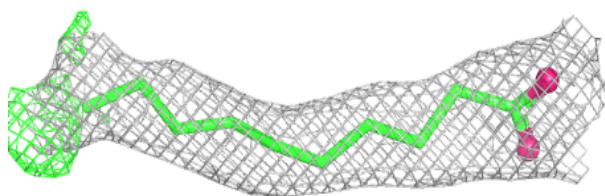


Electron density around CLA B 601:

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

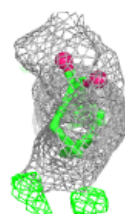
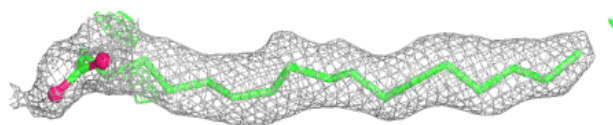
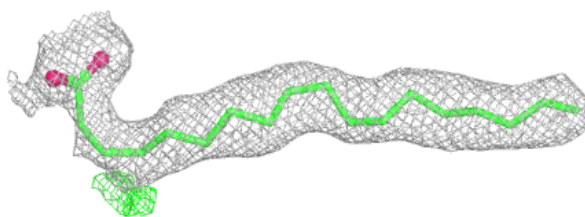
**Electron density around STE j 101:**

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

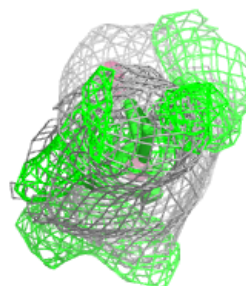
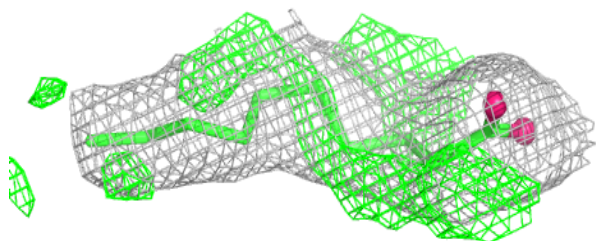
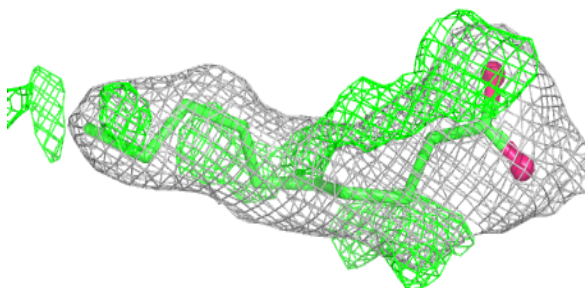


Electron density around STE c 519:

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

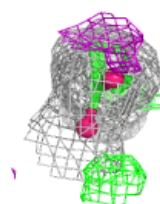
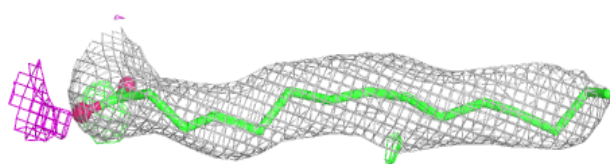
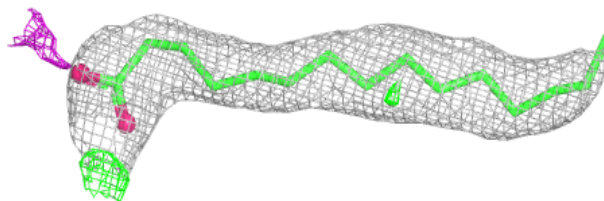
**Electron density around STE B 624:**

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

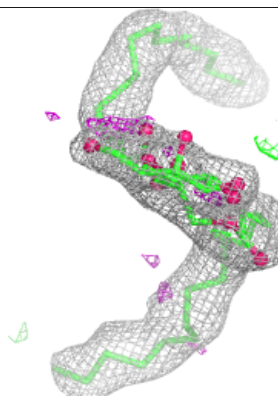
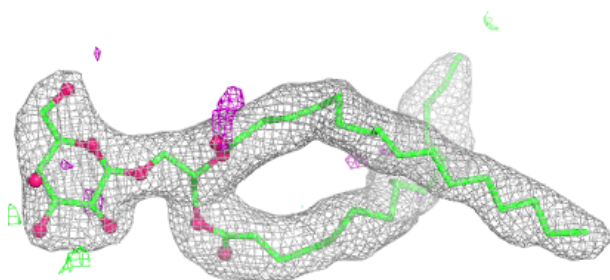
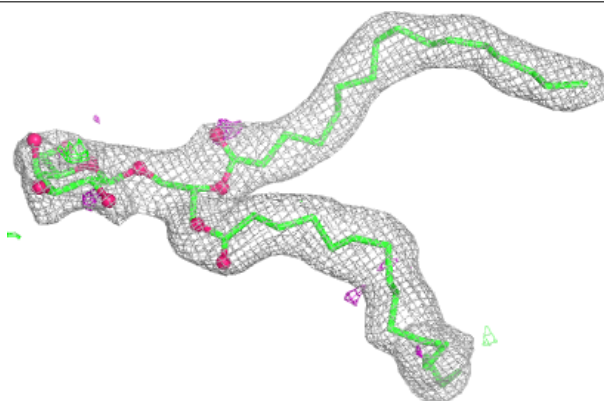


Electron density around STE d 412:

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

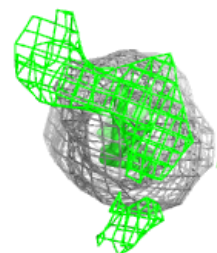
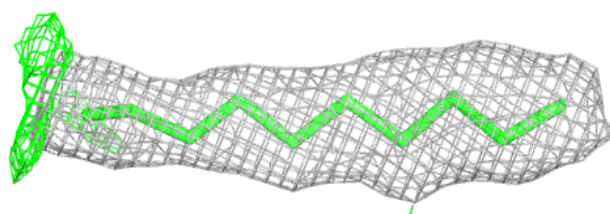
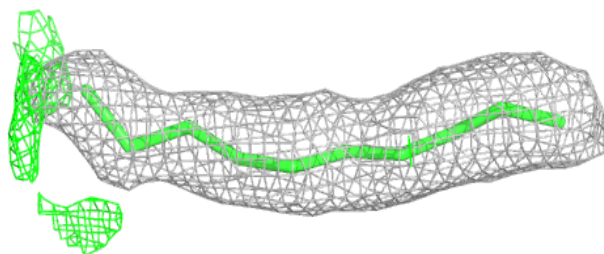
**Electron density around LMG M 101:**

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

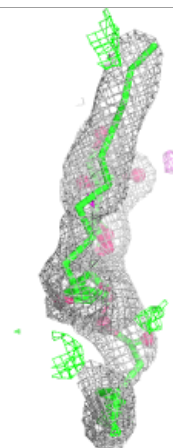
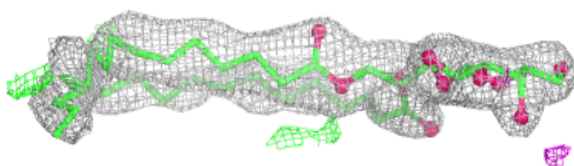
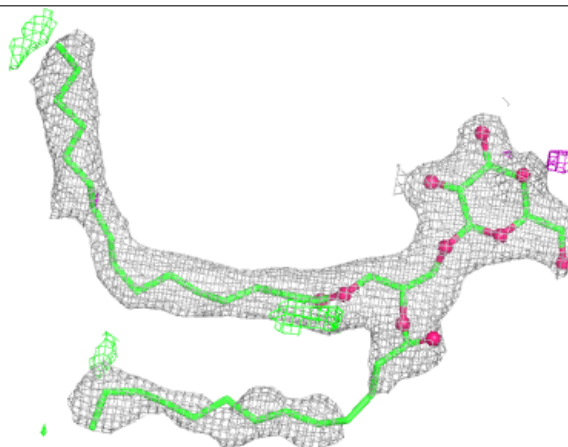


Electron density around STE M 103:

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

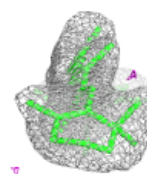
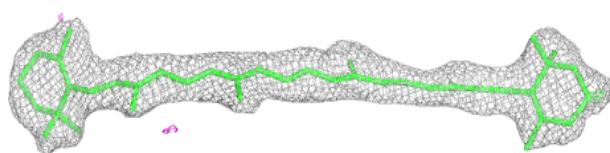
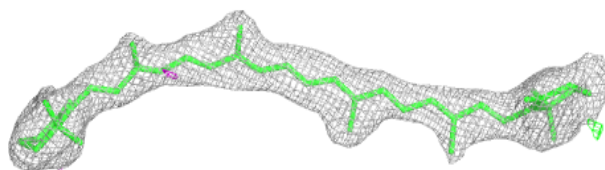
**Electron density around LMG C 518:**

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

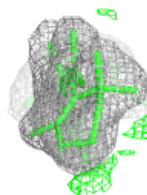
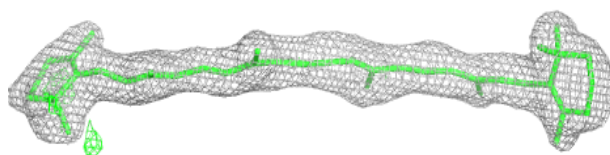
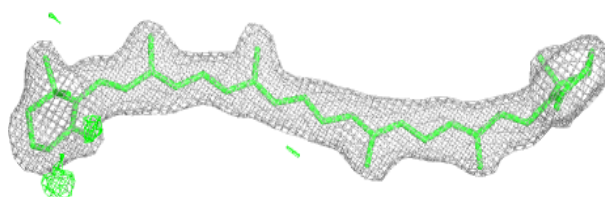


Electron density around BCR x 101:

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

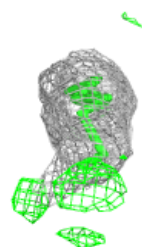
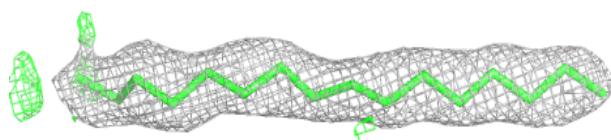
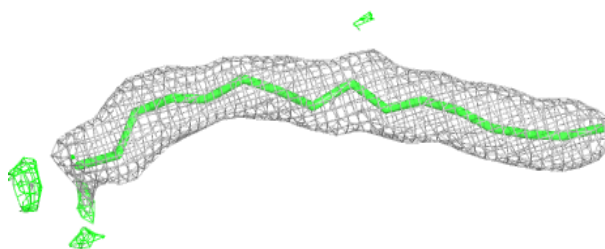
**Electron density around BCR K 102:**

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

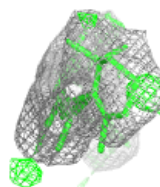
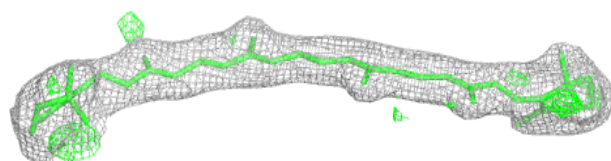
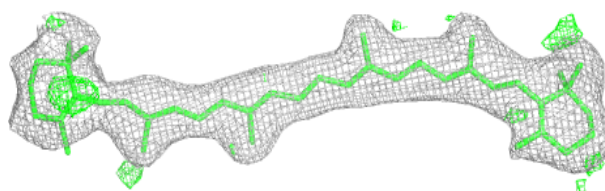


Electron density around STE C 521:

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

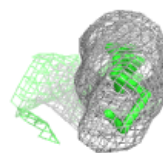
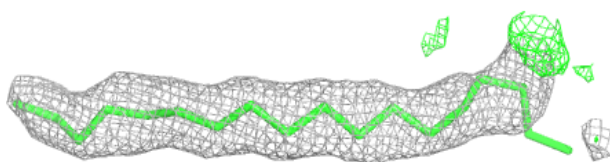
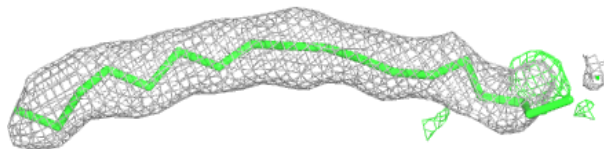
**Electron density around BCR D 406:**

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



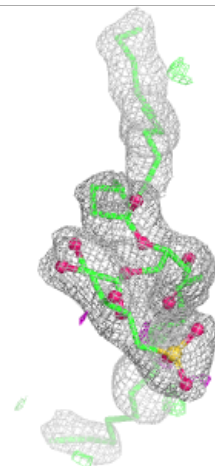
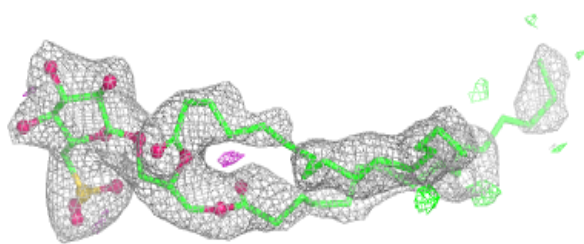
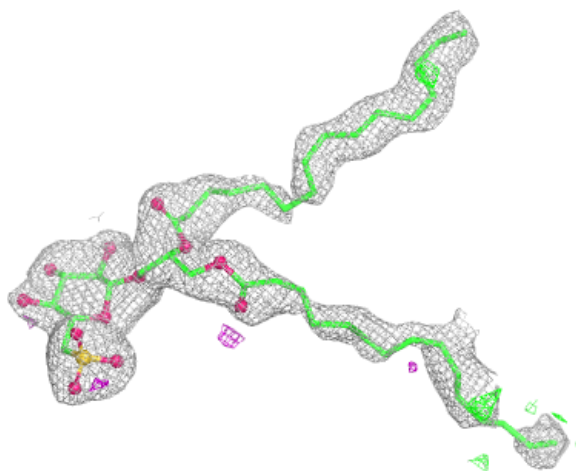
Electron density around STE I 102:

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



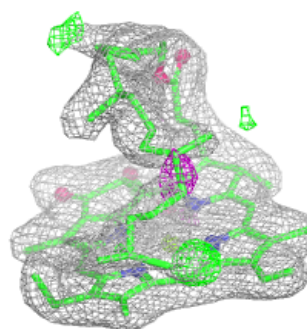
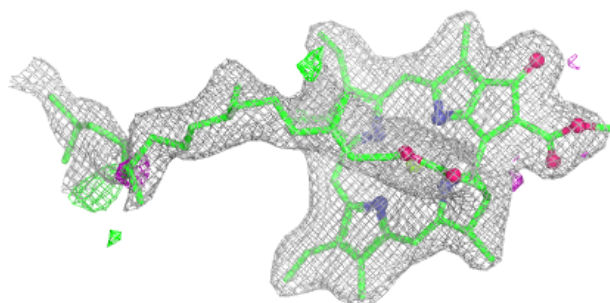
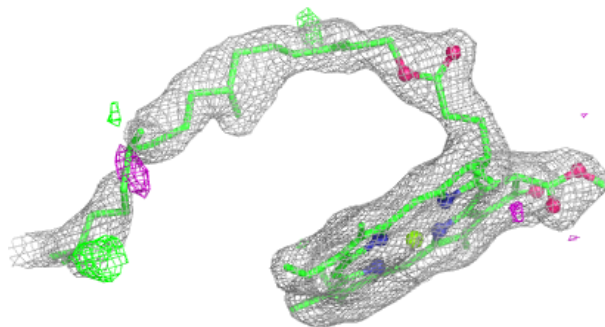
Electron density around SQD a 613:

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

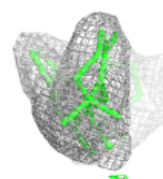
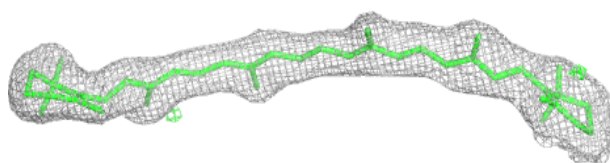
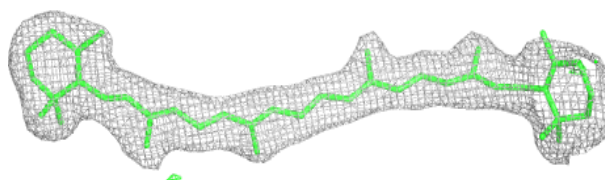


Electron density around CLA C 513:

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

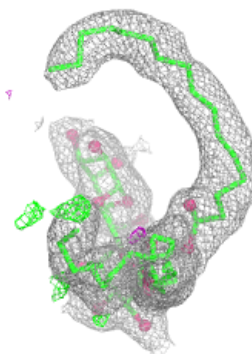
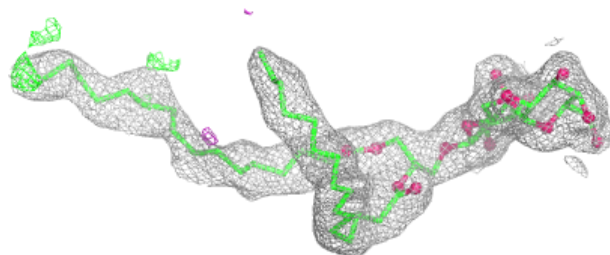
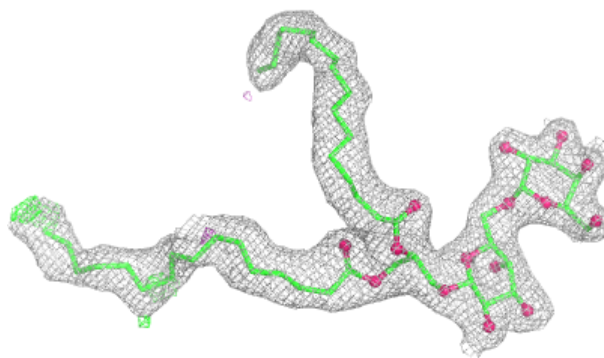
**Electron density around BCR d 405:**

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

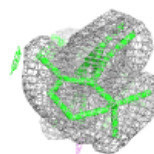
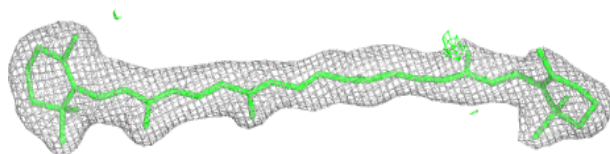
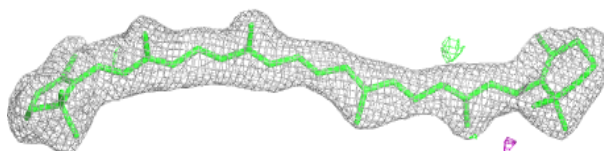


Electron density around DGD c 516:

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

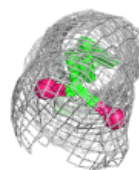
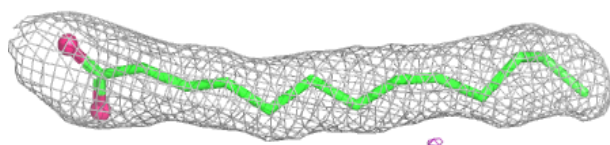
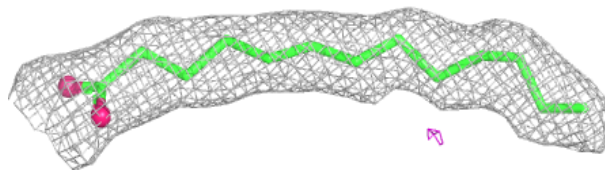
**Electron density around BCR k 101:**

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

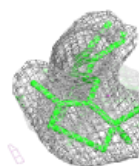
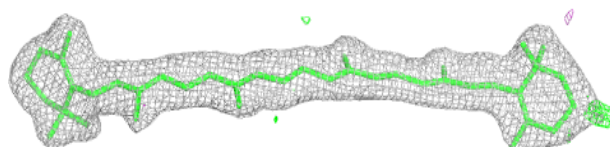
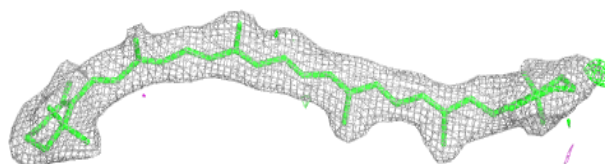


Electron density around STE M 102:

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

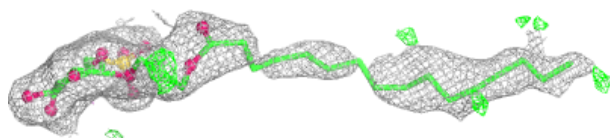
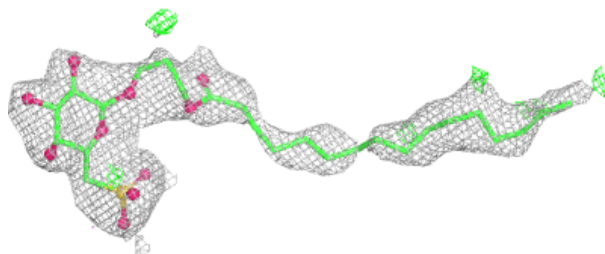
**Electron density around BCR H 101:**

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

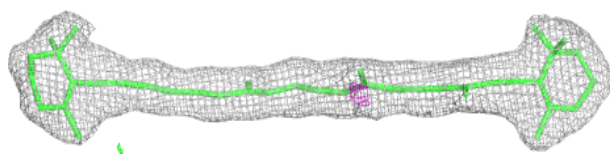
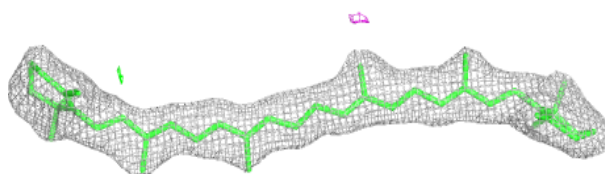


Electron density around SQD D 409:

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

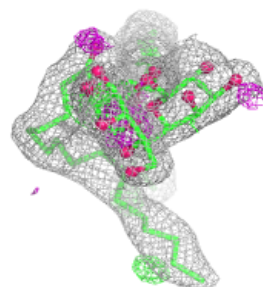
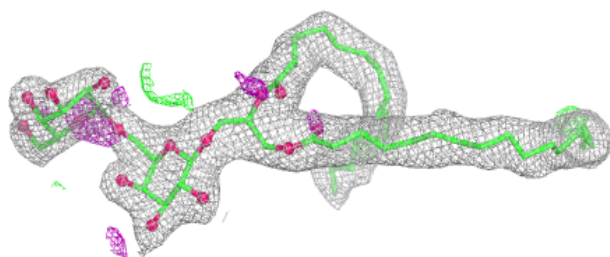
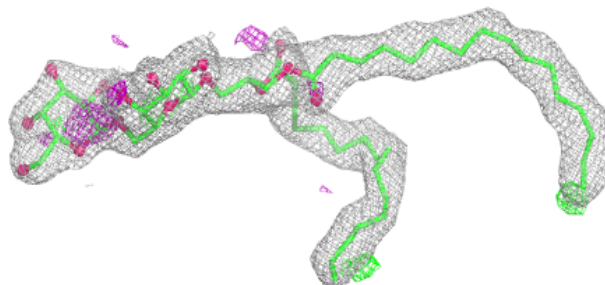
**Electron density around BCR K 101:**

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

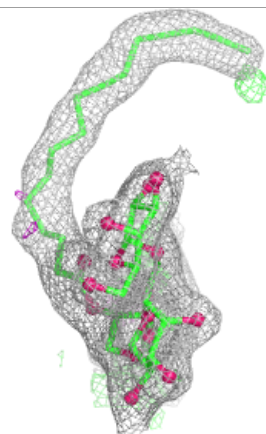
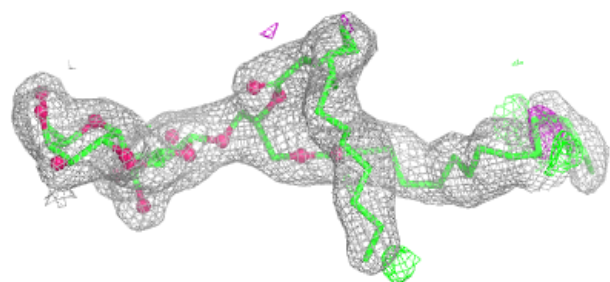
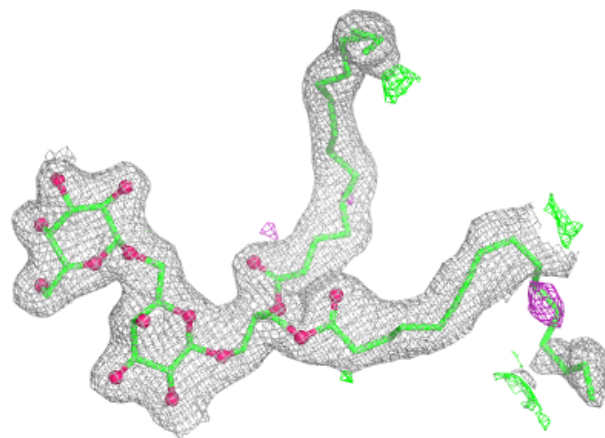


Electron density around DGD H 102:

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

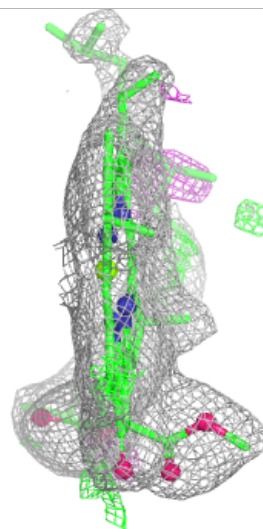
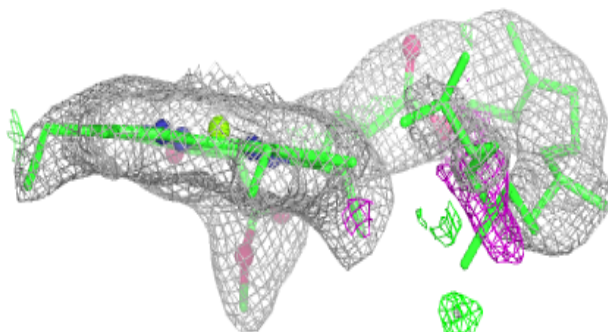
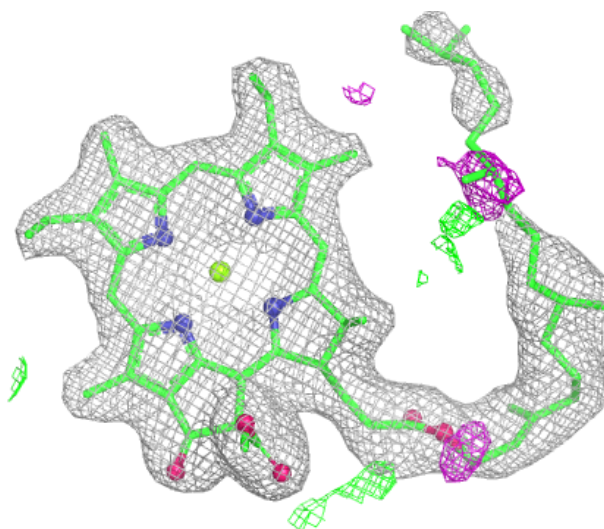
**Electron density around DGD C 516:**

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



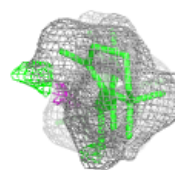
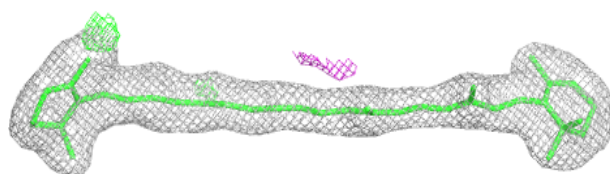
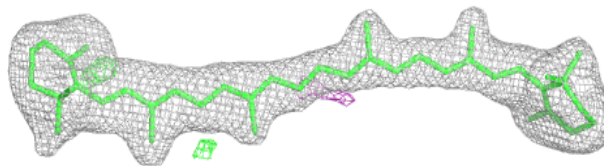
Electron density around CLA c 512:

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

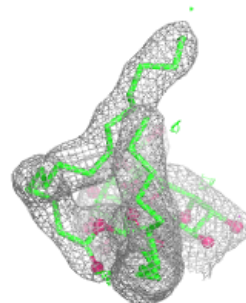
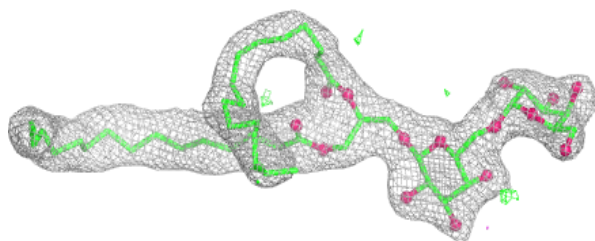
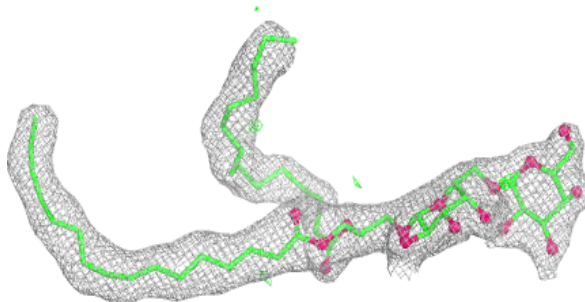


Electron density around BCR b 618:

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

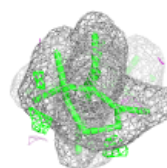
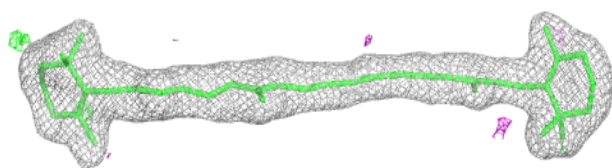
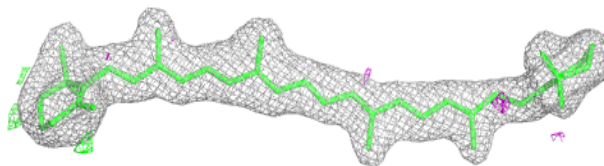
**Electron density around DGD h 101:**

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

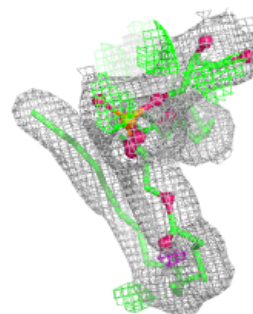
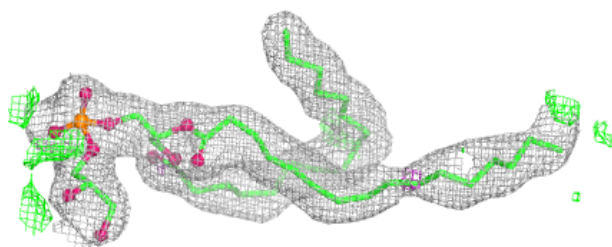
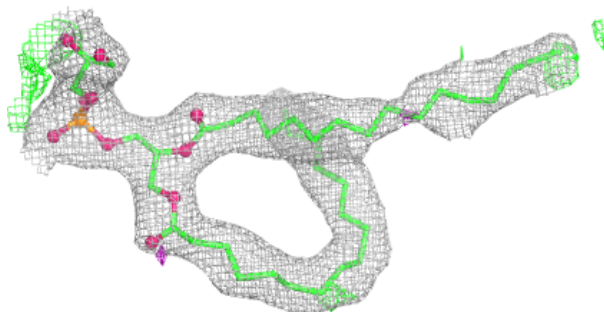


Electron density around BCR A 609:

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

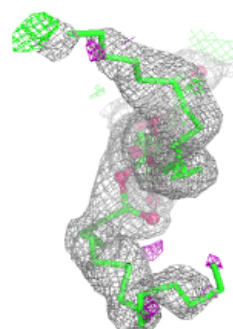
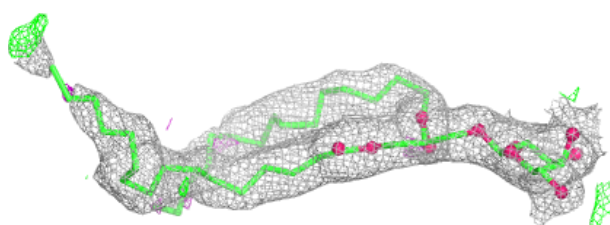
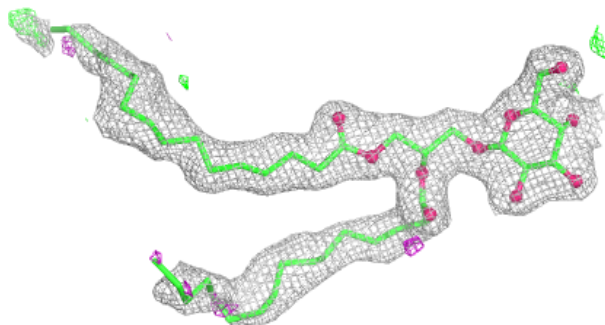
**Electron density around LHG d 407:**

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

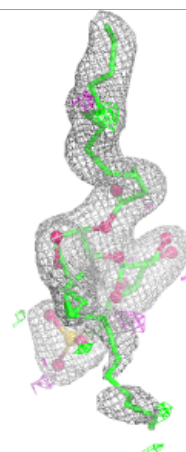
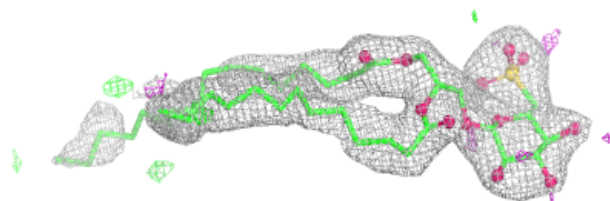
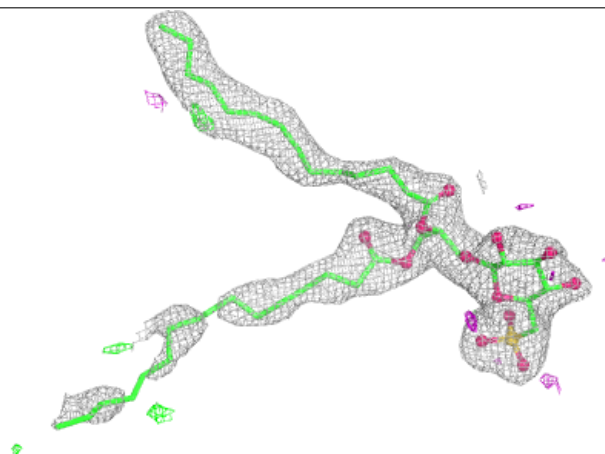


Electron density around LMG D 408:

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

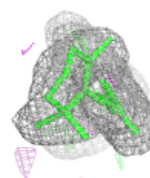
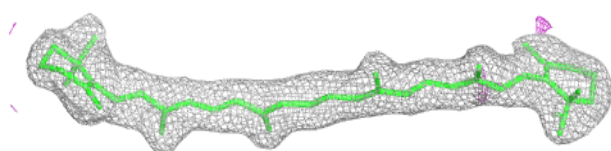
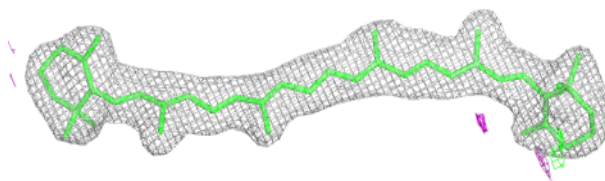
**Electron density around SQD A 614:**

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

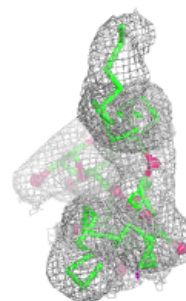
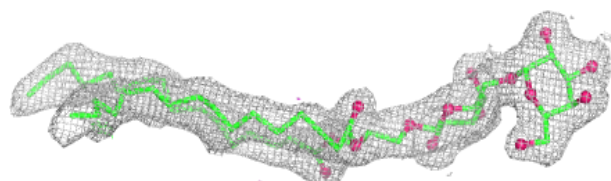
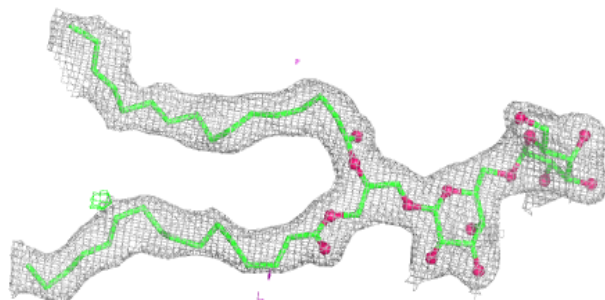


Electron density around BCR B 619:

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

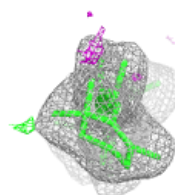
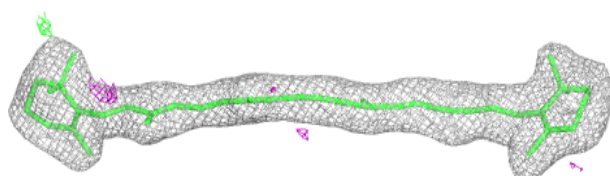
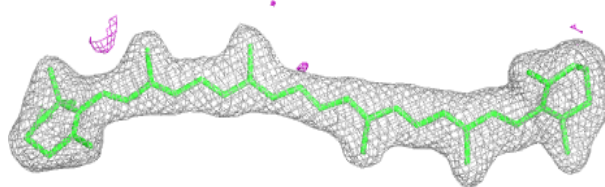
**Electron density around DGD C 517:**

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

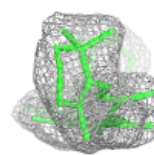
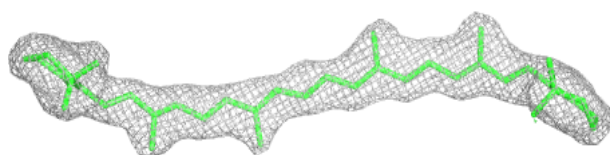
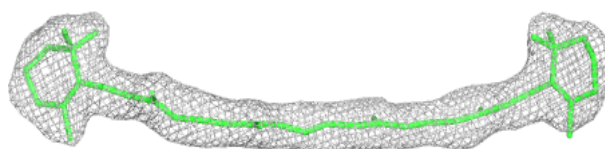


Electron density around BCR B 618:

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

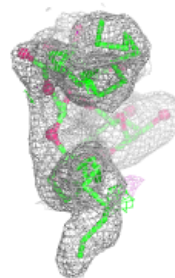
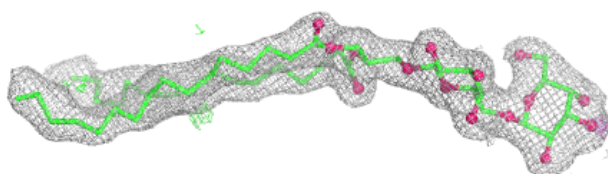
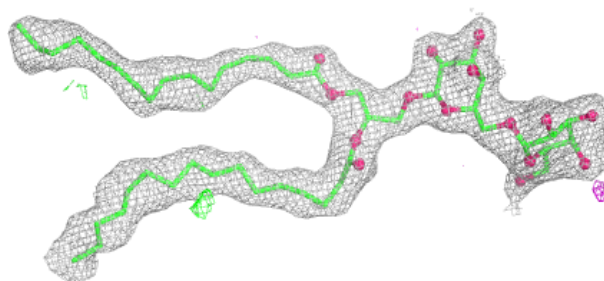
**Electron density around BCR k 103:**

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

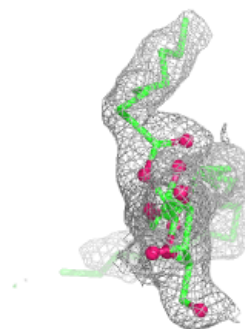
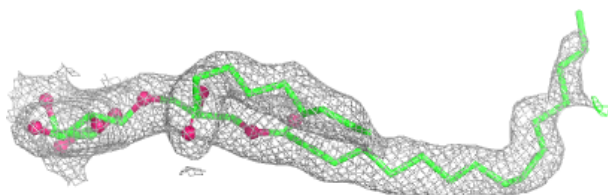
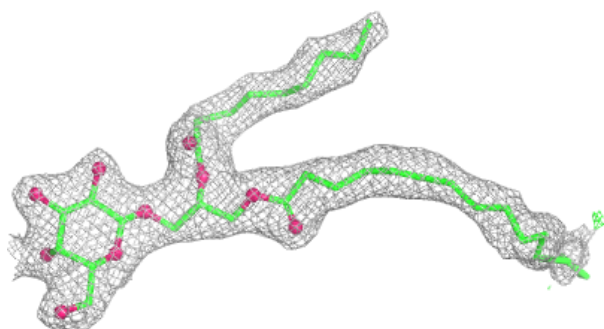


Electron density around DGD c 517:

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

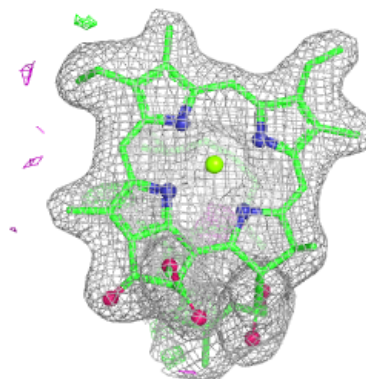
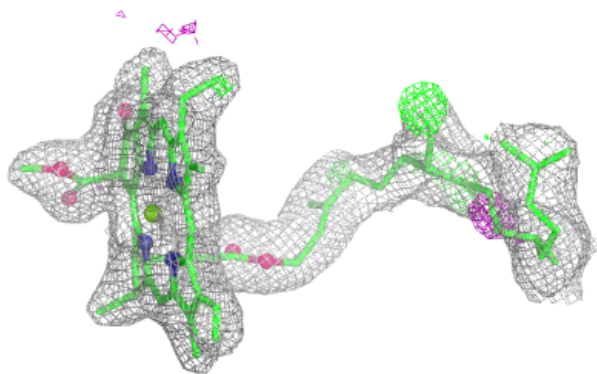
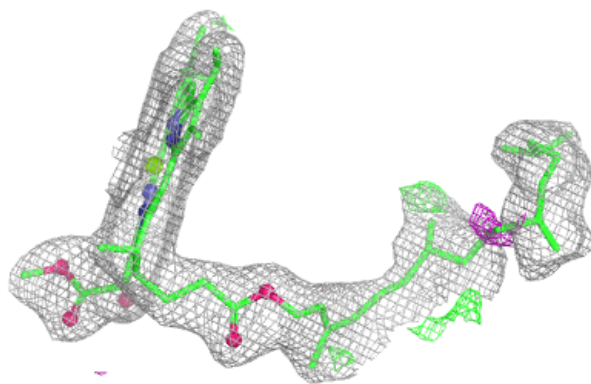
**Electron density around LMG d 411:**

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

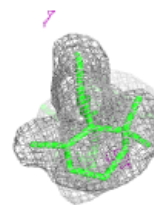
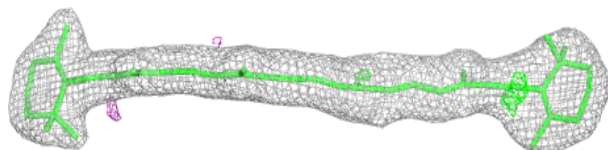
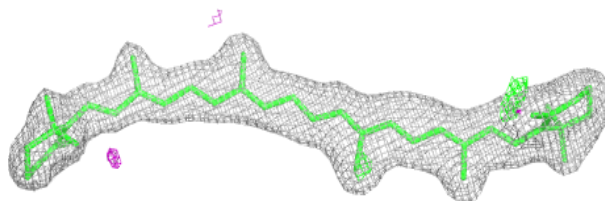


Electron density around CLA C 506:

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

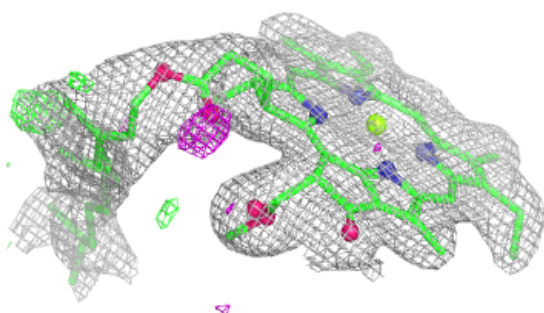
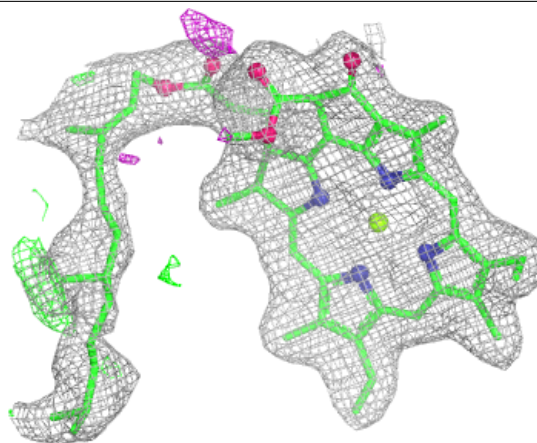
**Electron density around BCR C 514:**

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



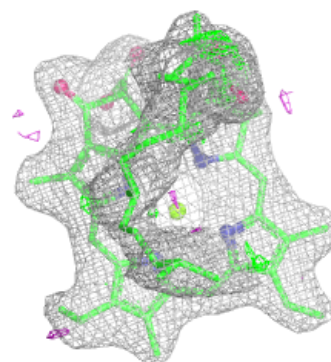
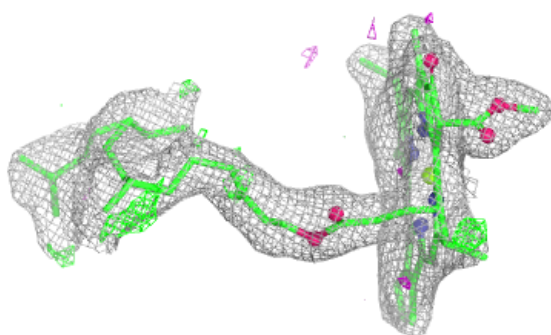
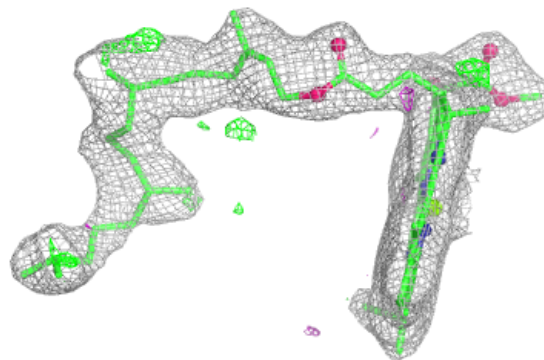
Electron density around CLA b 616:

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

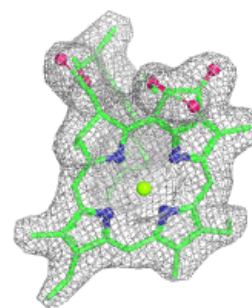
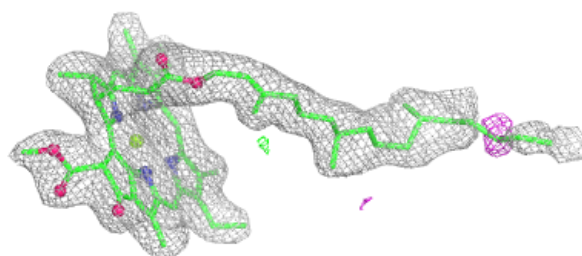
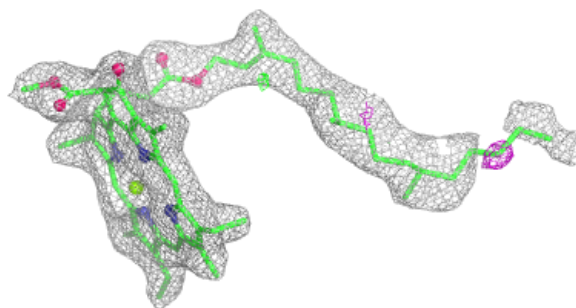


Electron density around CLA c 506:

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

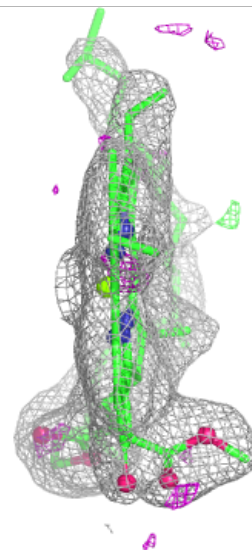
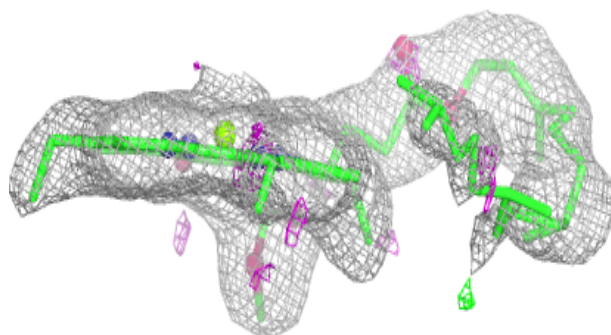
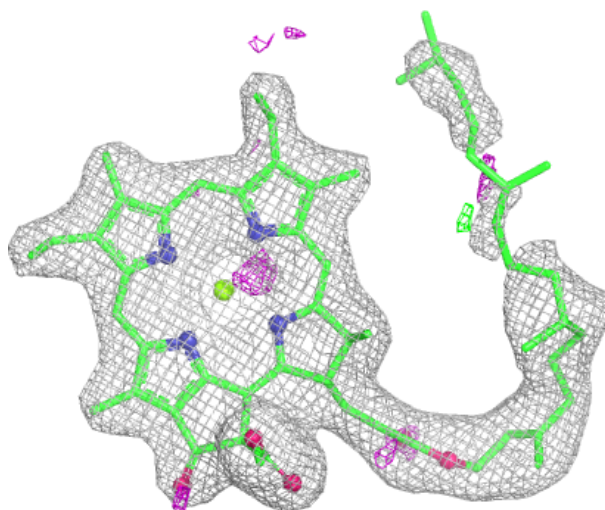
**Electron density around CLA c 508:**

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



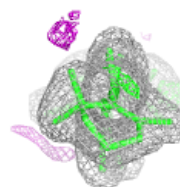
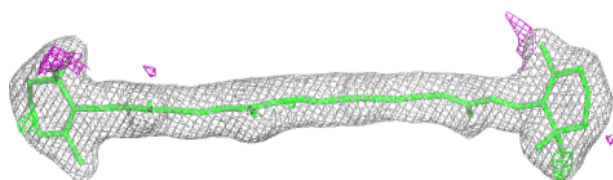
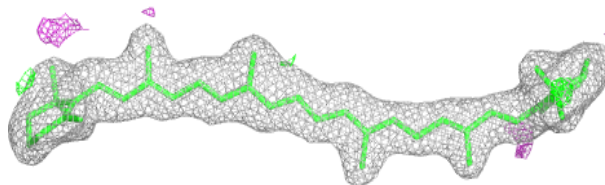
Electron density around CLA C 512:

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

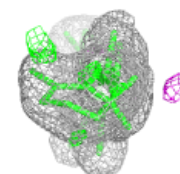
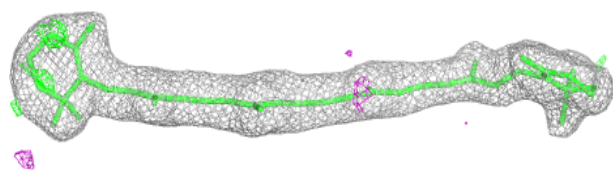
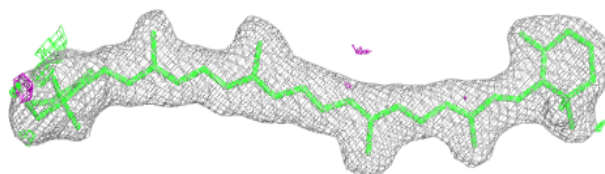


Electron density around BCR a 610:

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

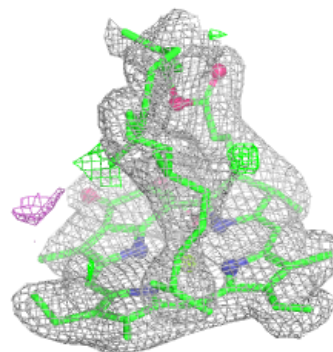
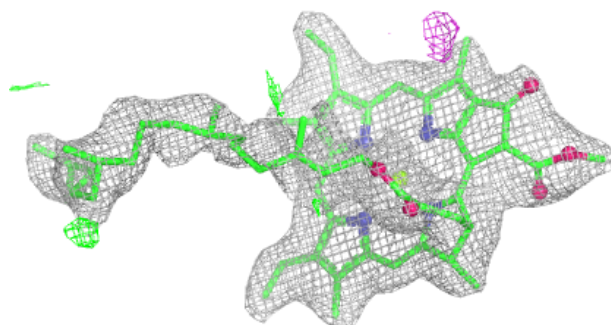
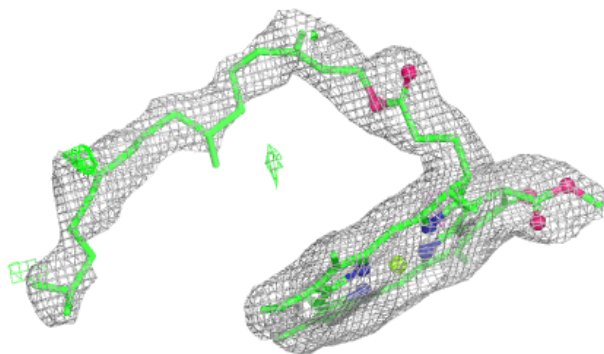
**Electron density around BCR b 617:**

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

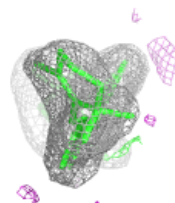
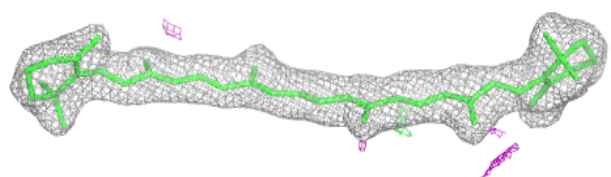
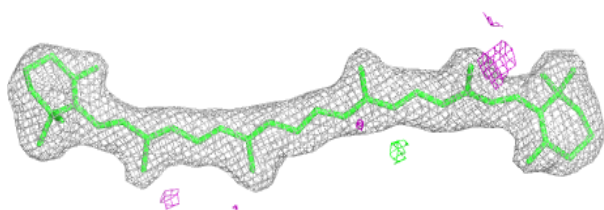


Electron density around CLA c 513:

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

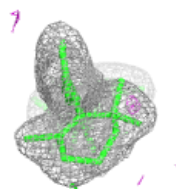
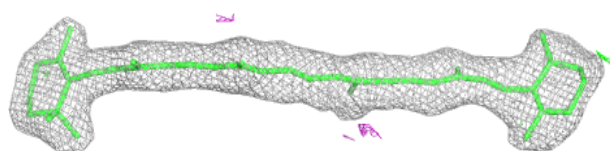
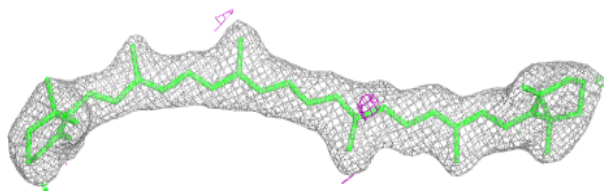
**Electron density around BCR b 619:**

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



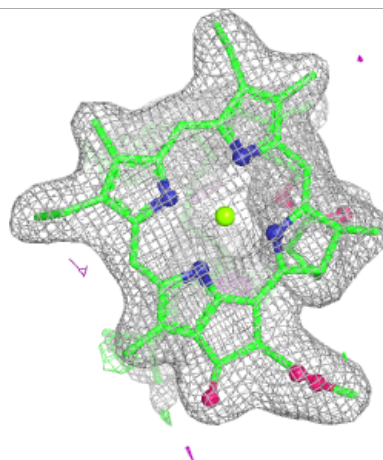
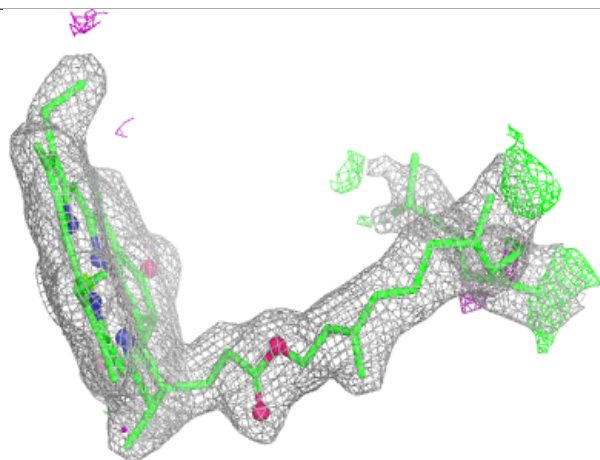
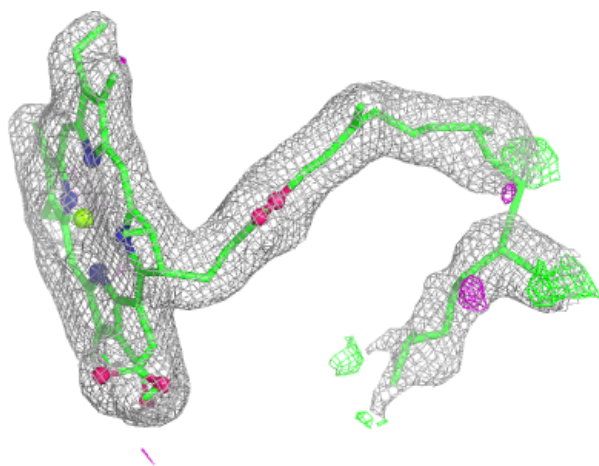
Electron density around BCR c 514:

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



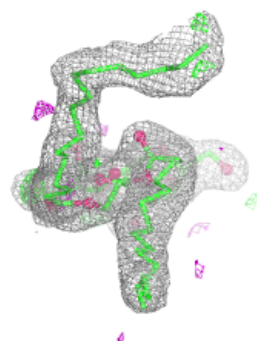
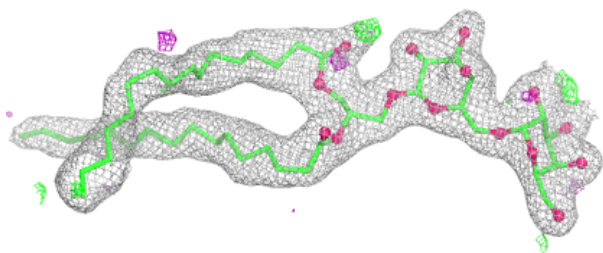
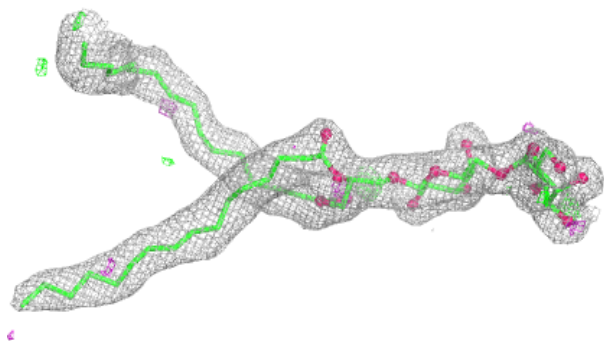
Electron density around CLA B 606:

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

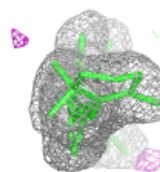
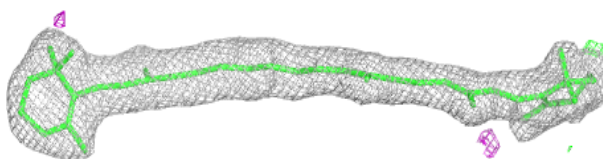
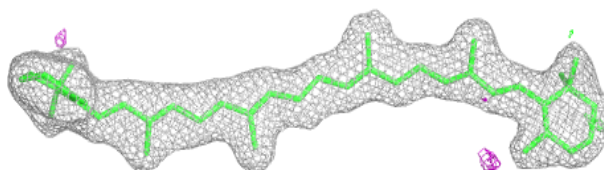


Electron density around DGD C 515:

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

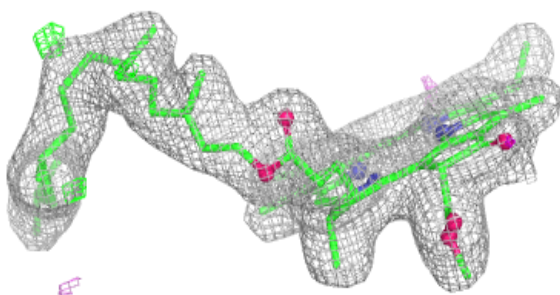
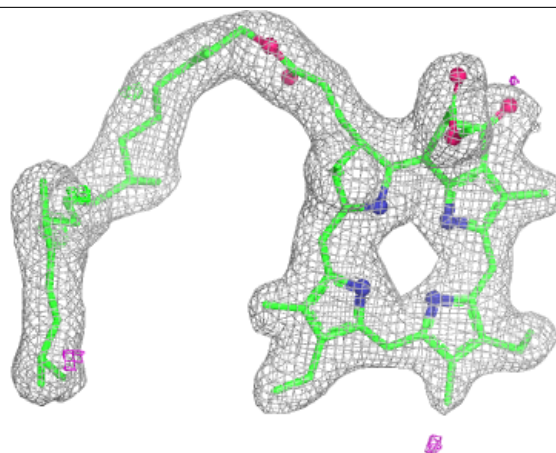
**Electron density around BCR B 617:**

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

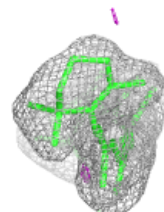
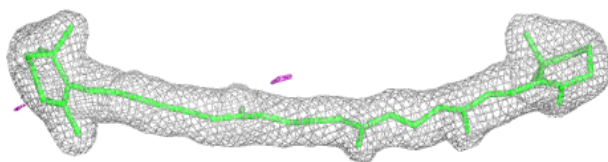
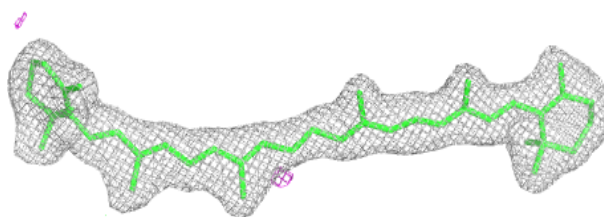


Electron density around PHO d 402:

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

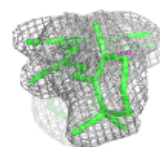
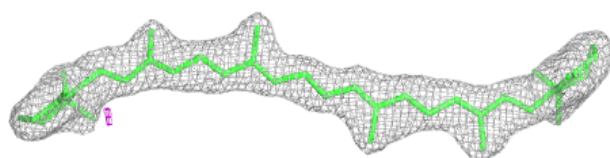
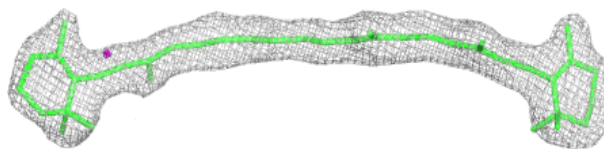
**Electron density around BCR T 101:**

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

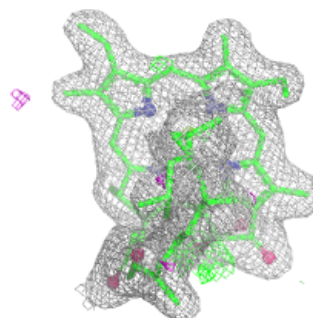
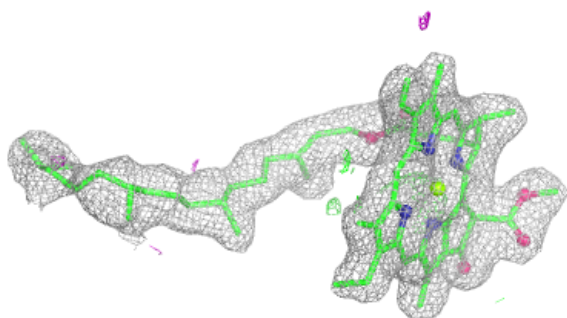
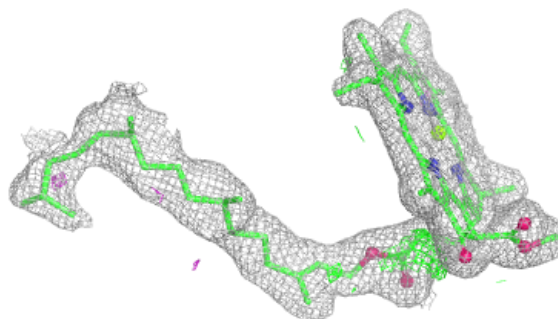


Electron density around BCR Z 101:

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

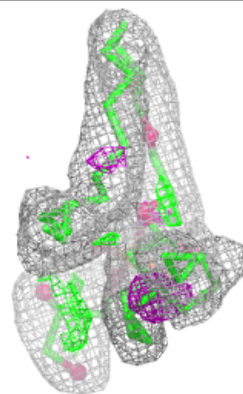
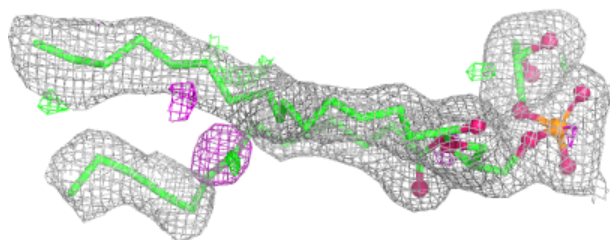
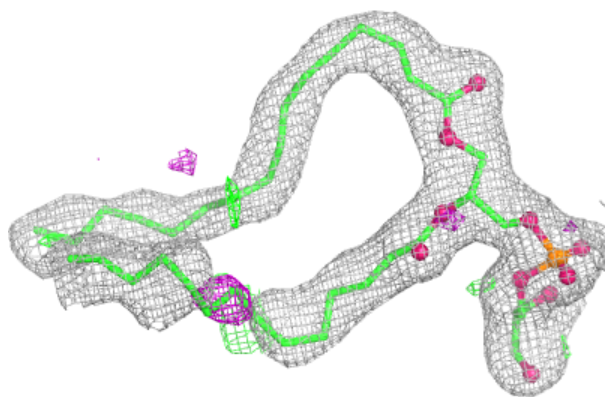
**Electron density around CLA C 508:**

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

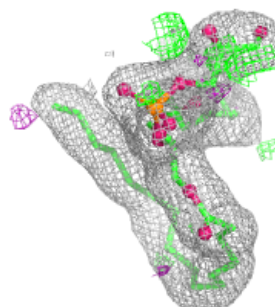
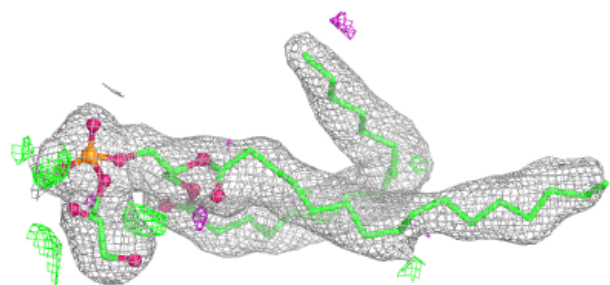
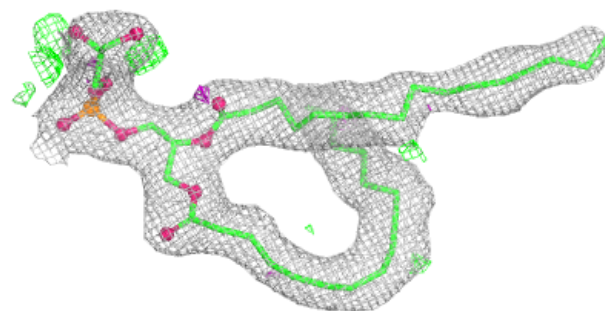


Electron density around LHG A 613:

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

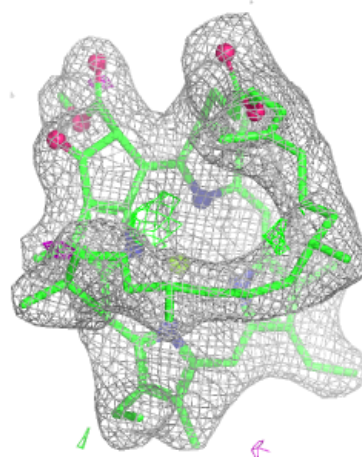
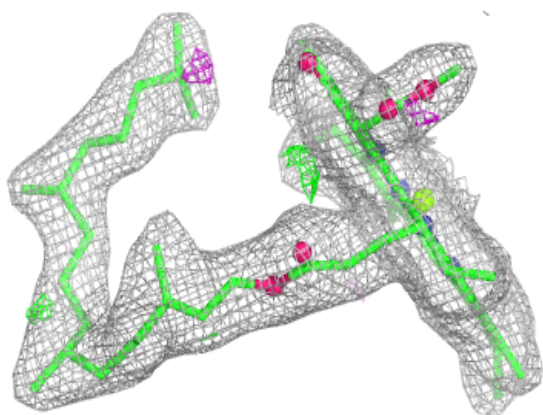
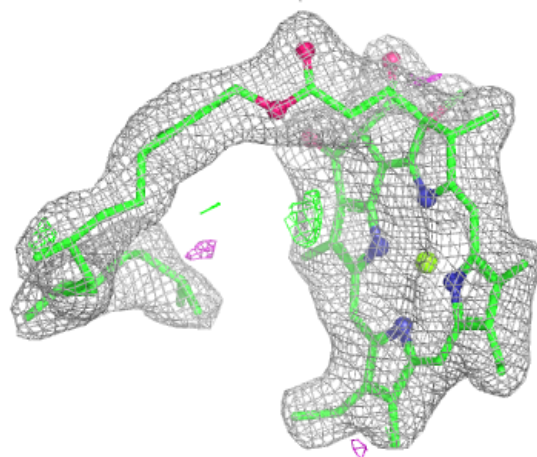
**Electron density around LHG B 622:**

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



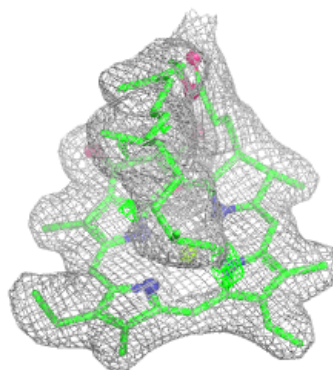
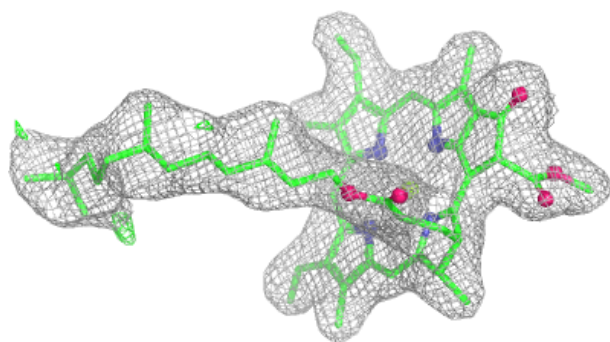
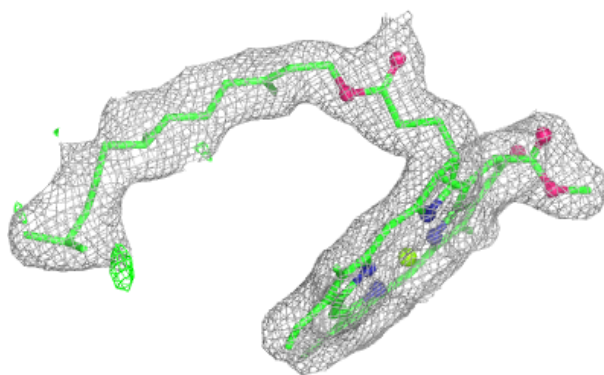
Electron density around CLA c 503:

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

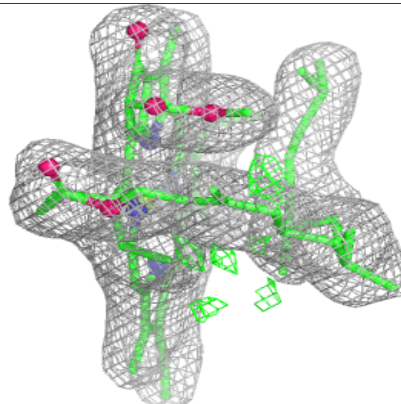
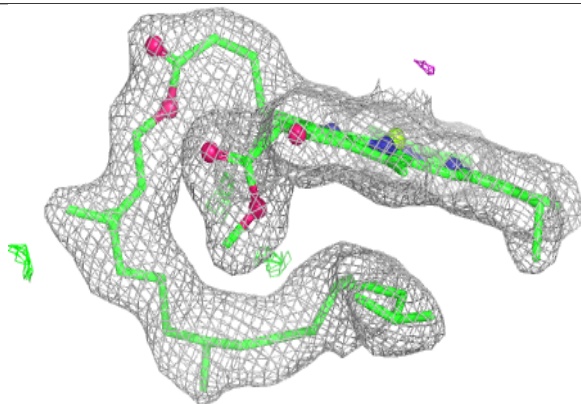
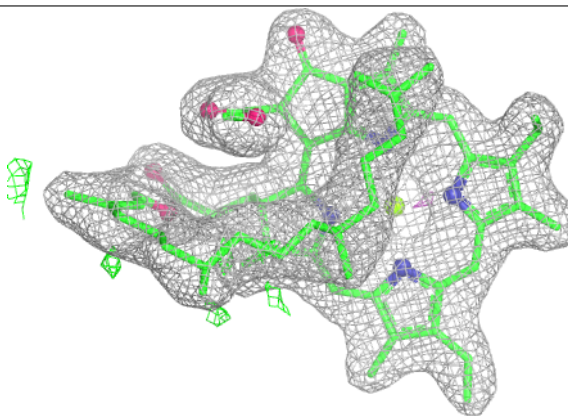


Electron density around CLA c 504:

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

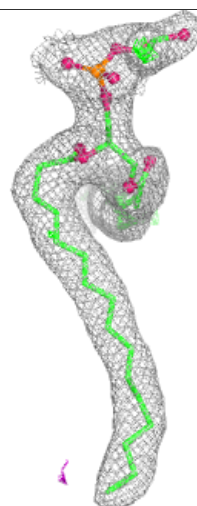
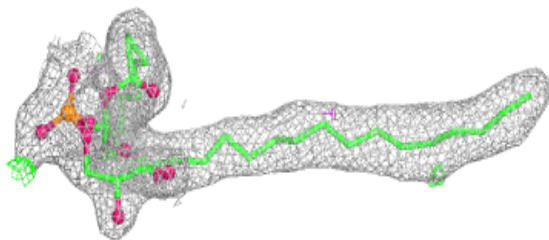
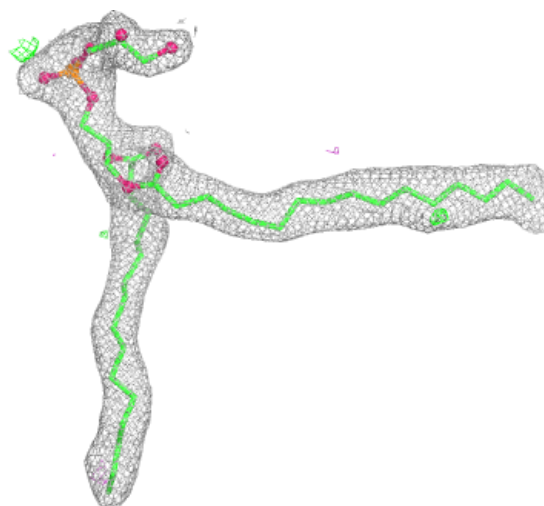
**Electron density around CLA C 510:**

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



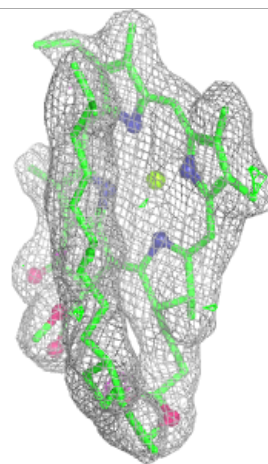
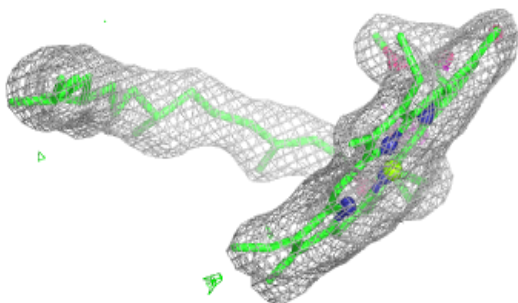
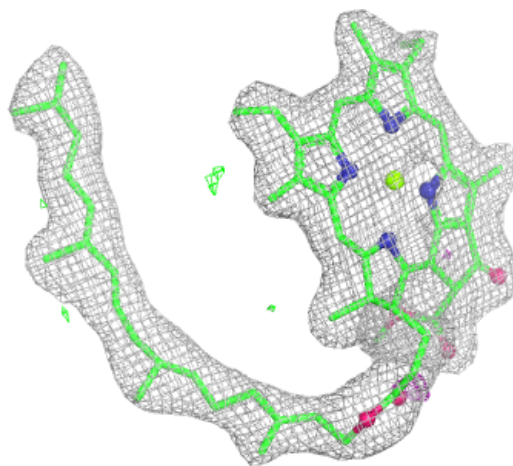
Electron density around LHG 1 101:

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



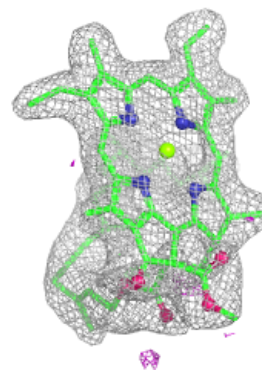
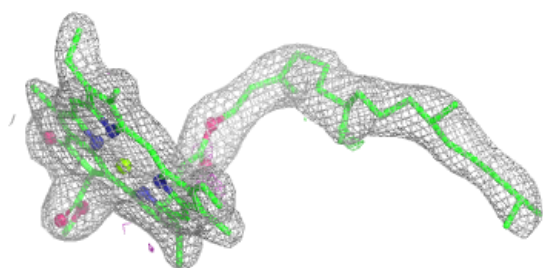
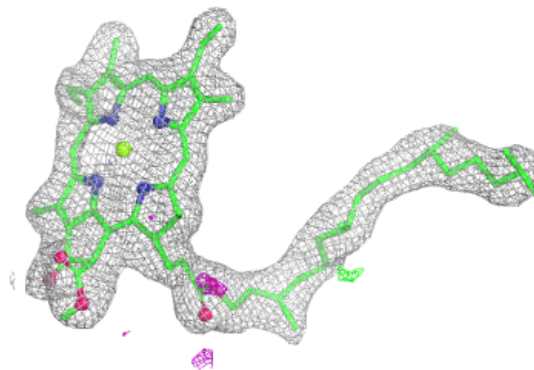
Electron density around CLA c 507:

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



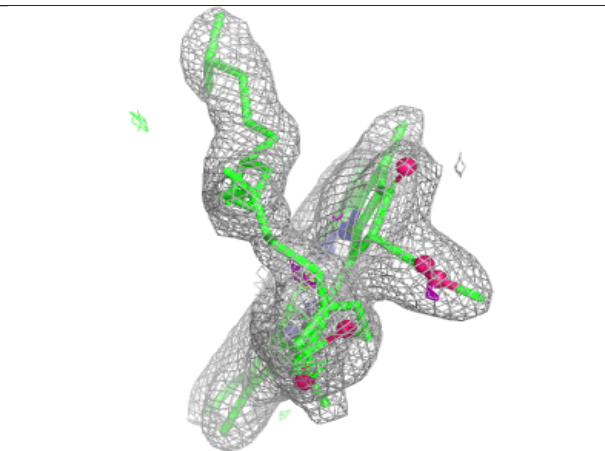
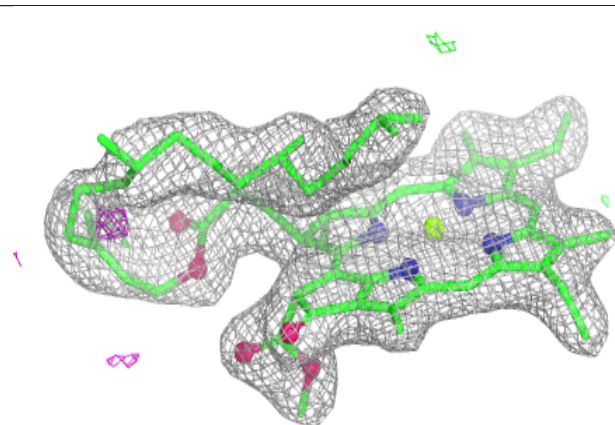
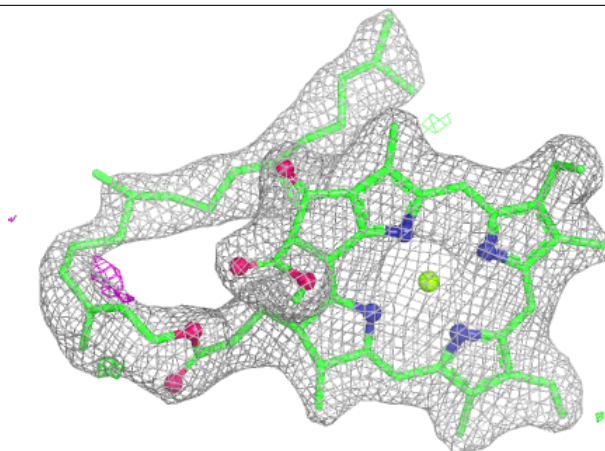
Electron density around CLA C 511:

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



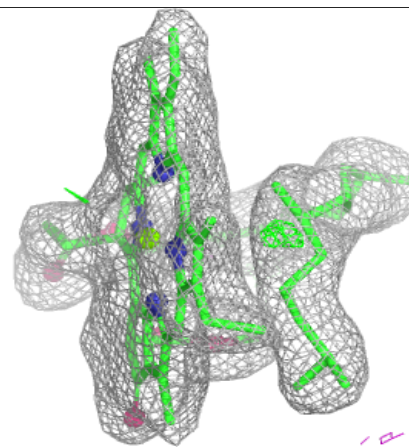
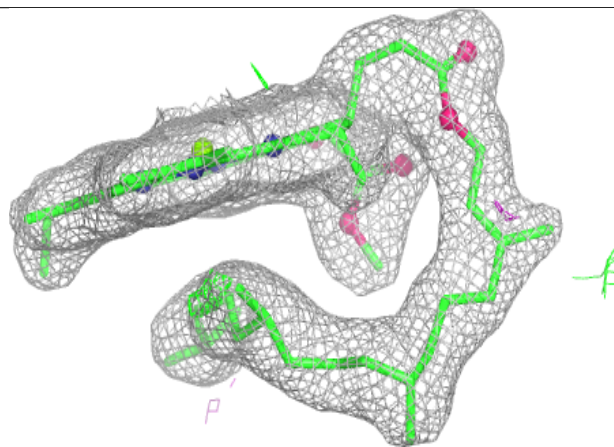
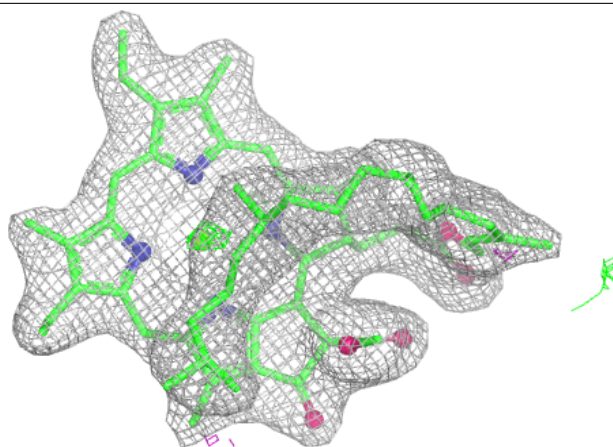
Electron density around CLA c 509:

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



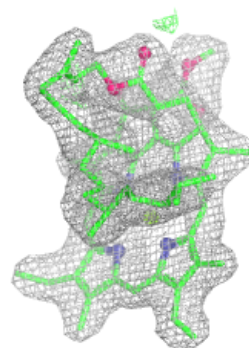
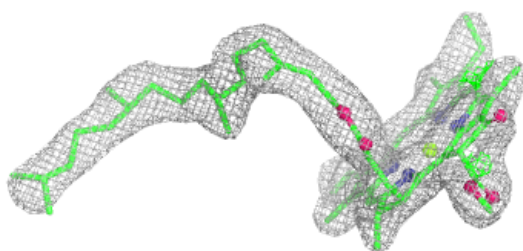
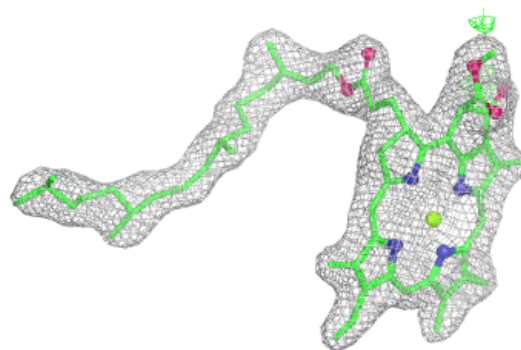
Electron density around CLA c 510:

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

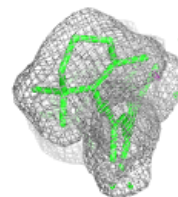
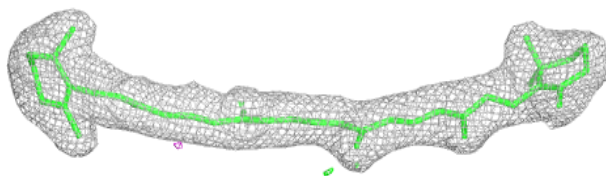
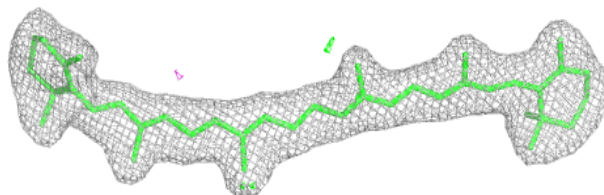


Electron density around CLA c 511:

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

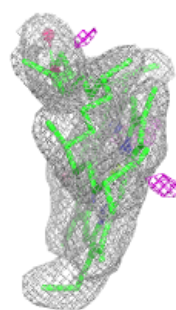
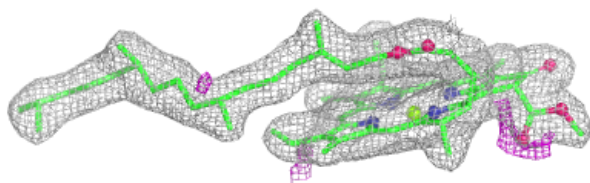
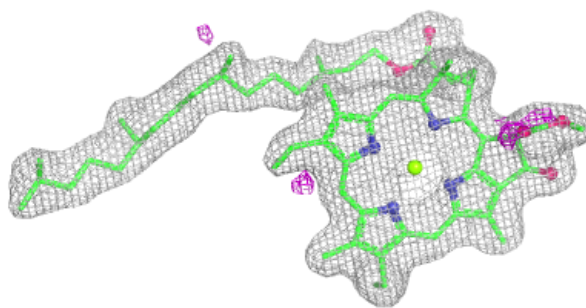
**Electron density around BCR t 101:**

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



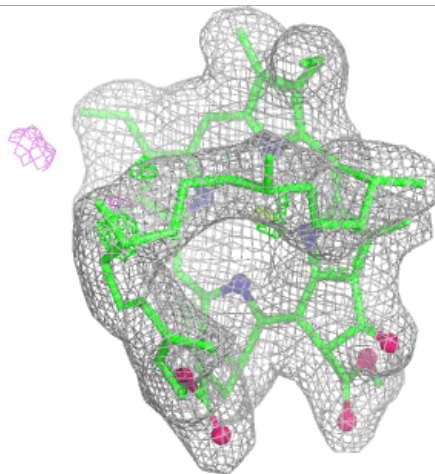
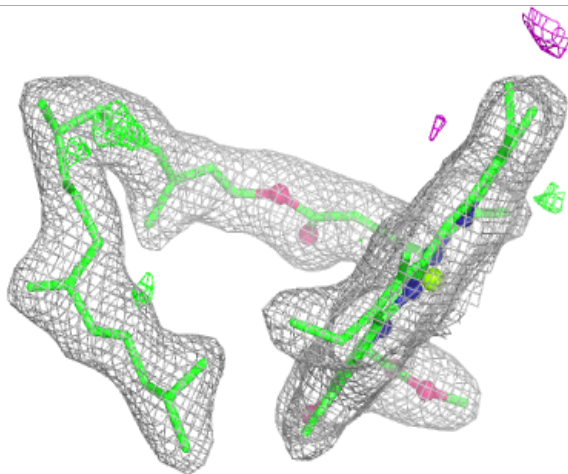
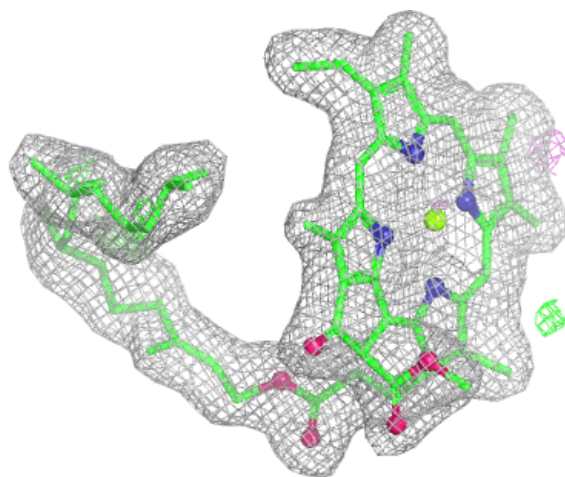
Electron density around CLA C 501:

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



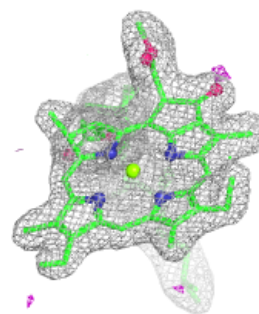
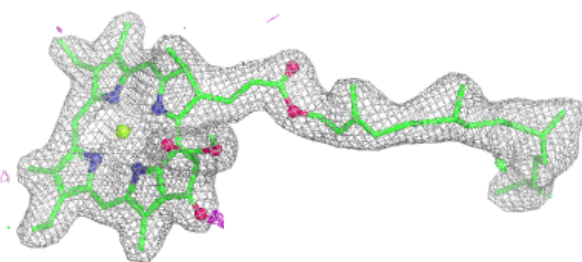
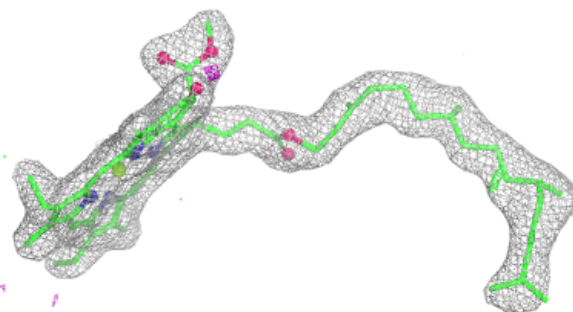
Electron density around CLA C 503:

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

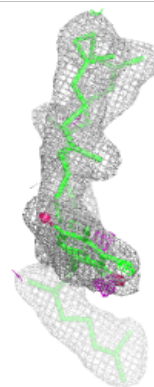
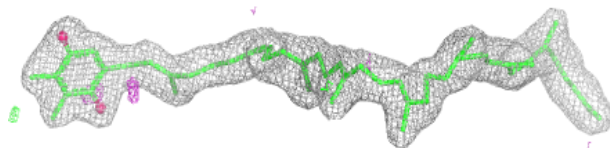
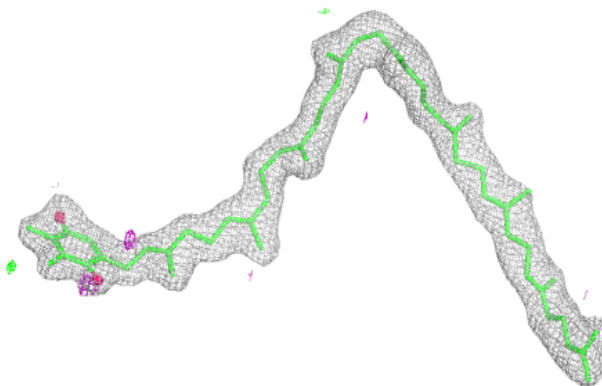


Electron density around CLA d 403:

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

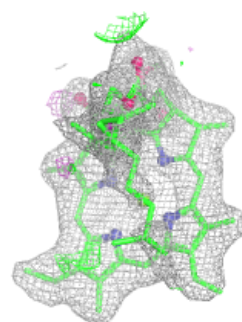
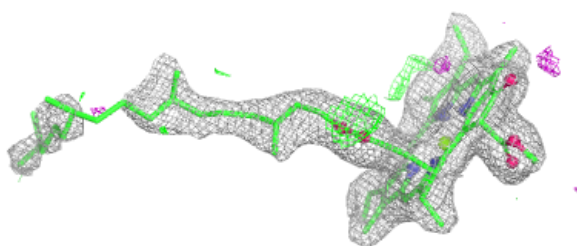
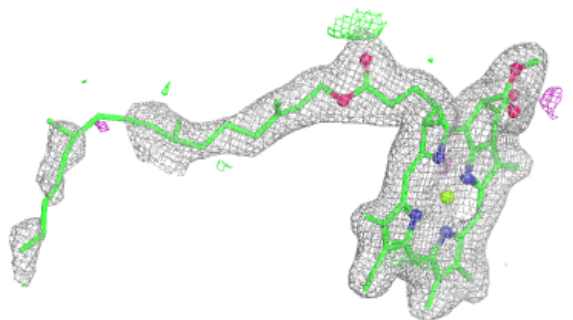
**Electron density around PL9 d 406:**

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

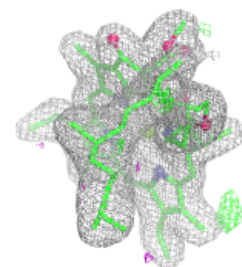
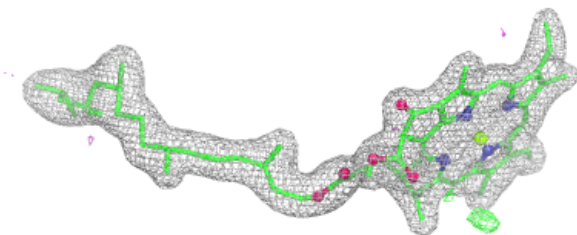
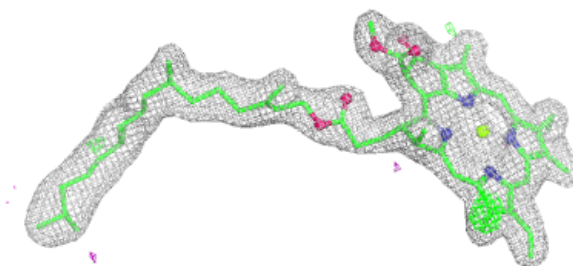


Electron density around CLA d 404:

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

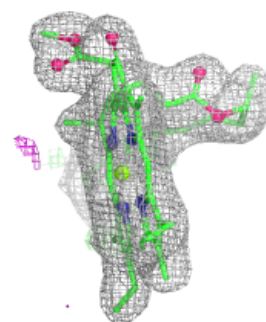
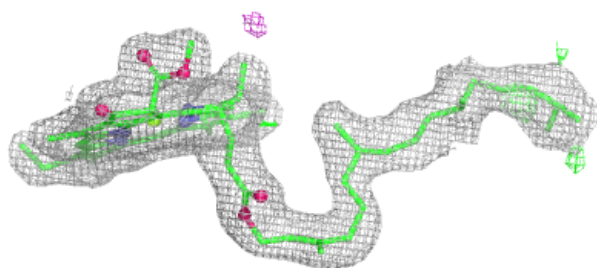
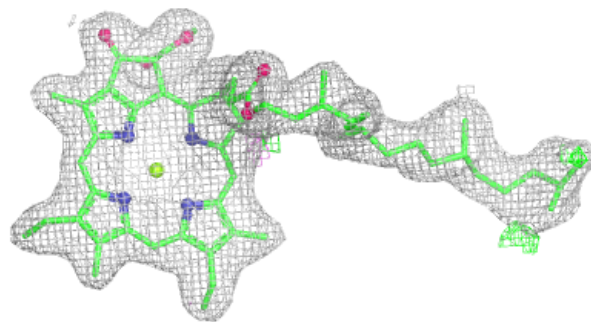
**Electron density around CLA a 607:**

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

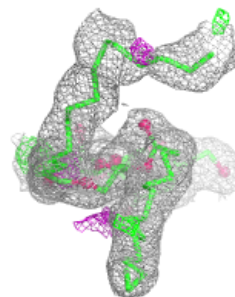
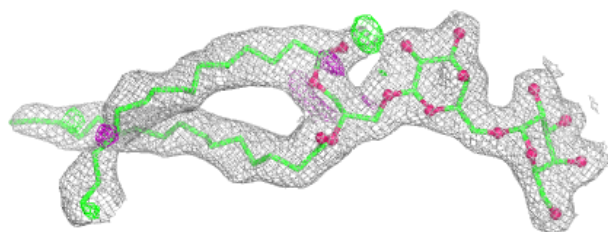
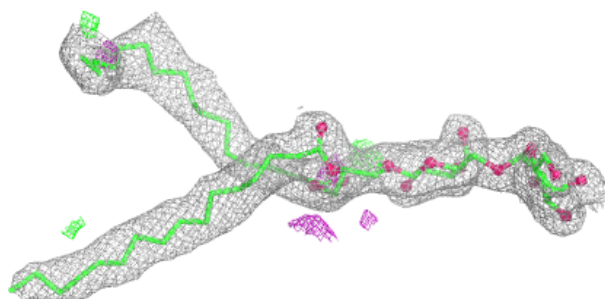


Electron density around CLA a 608:

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

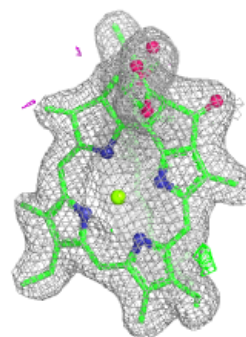
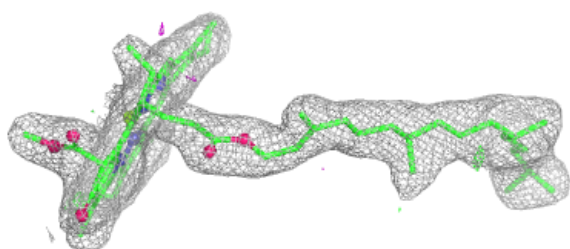
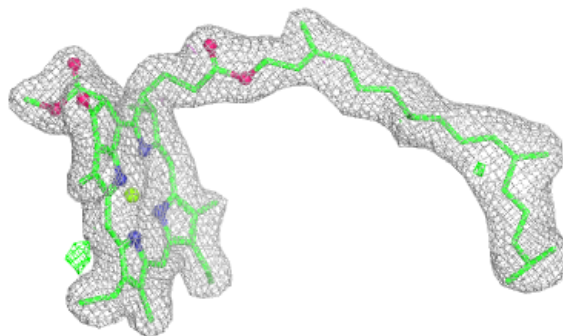
**Electron density around DGD c 515:**

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

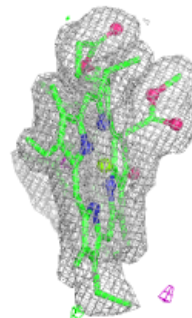
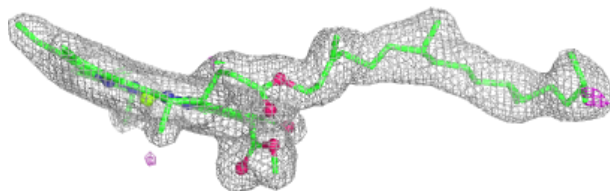
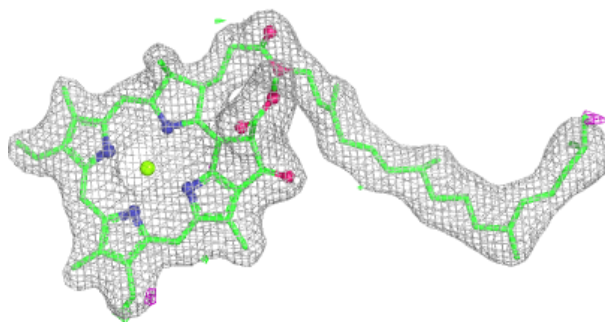


Electron density around CLA B 609:

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

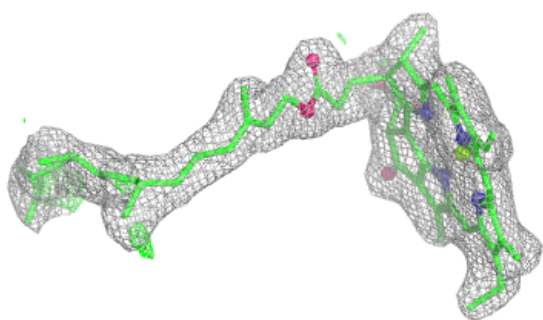
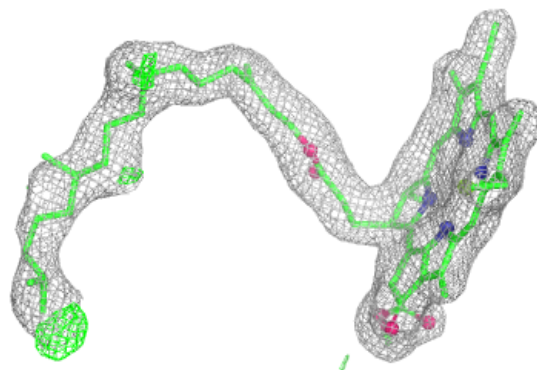
**Electron density around CLA b 602:**

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

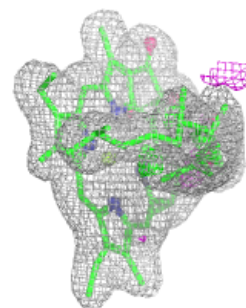
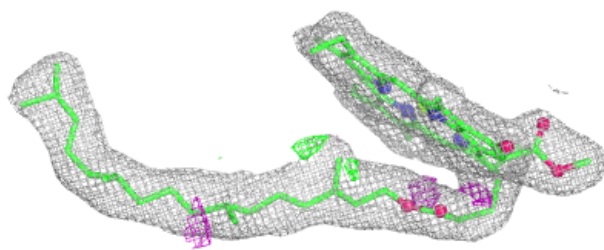
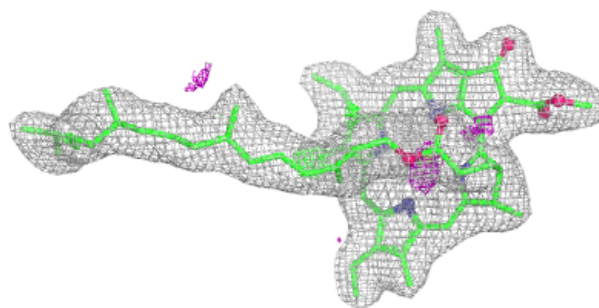


Electron density around CLA b 606:

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

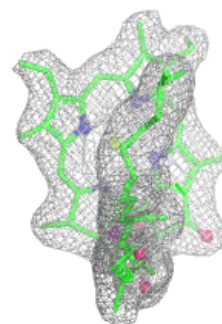
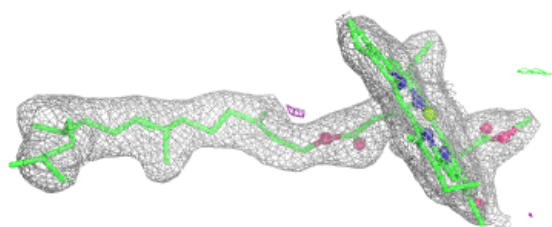
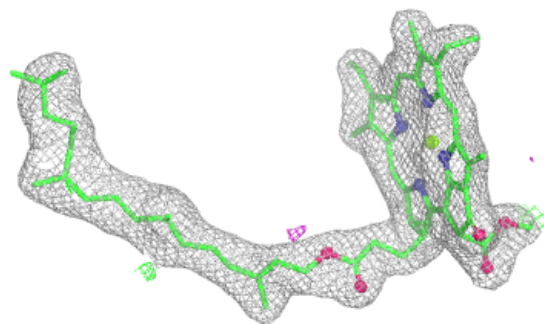
**Electron density around CLA b 608:**

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

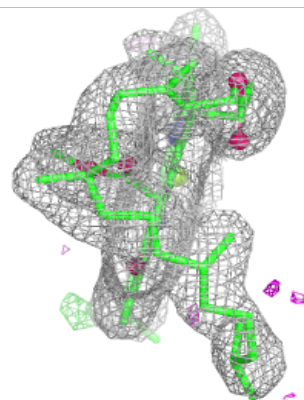
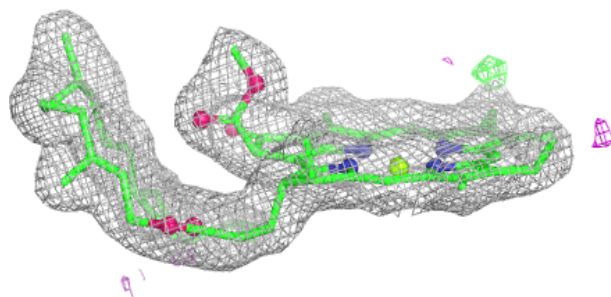
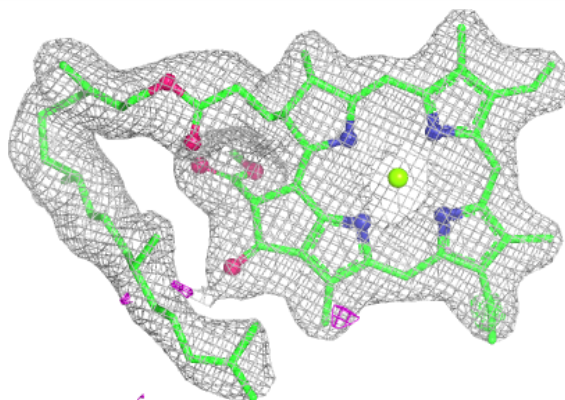


Electron density around CLA b 609:

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

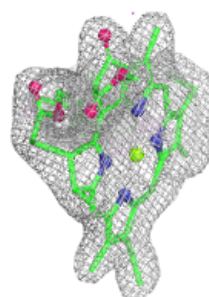
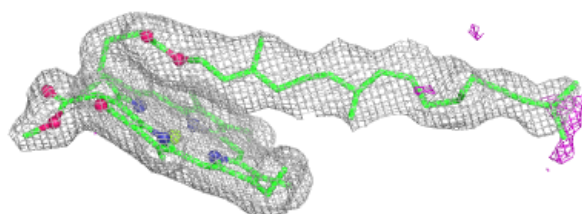
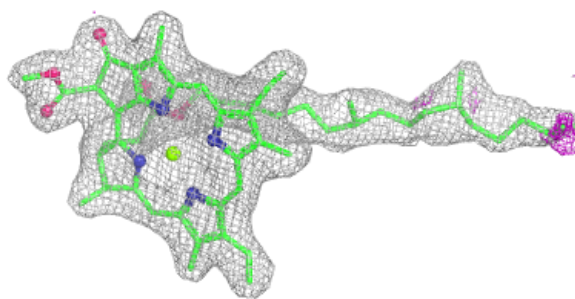
**Electron density around CLA b 610:**

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



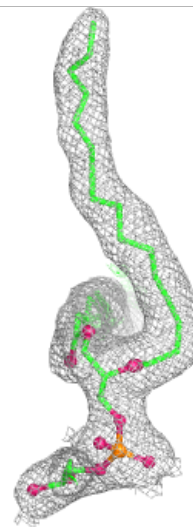
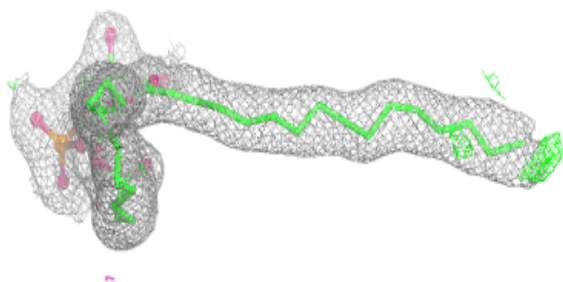
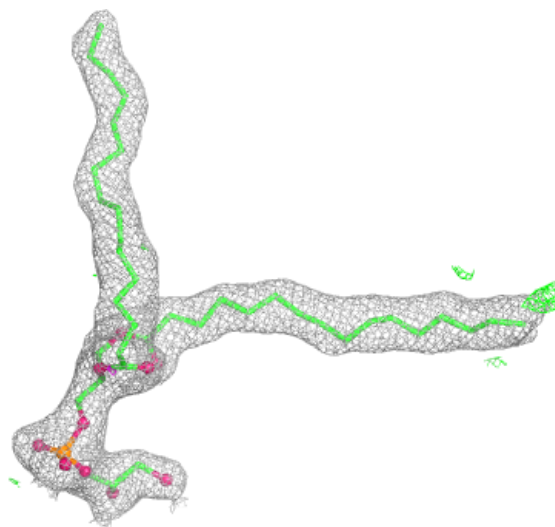
Electron density around CLA b 614:

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



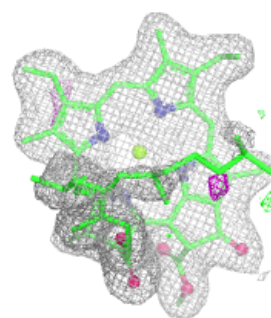
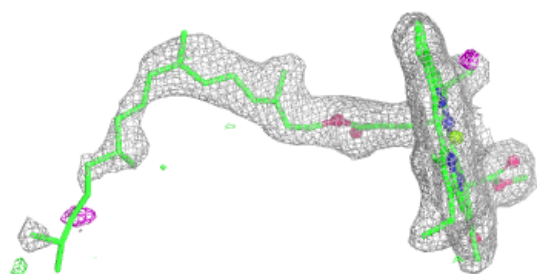
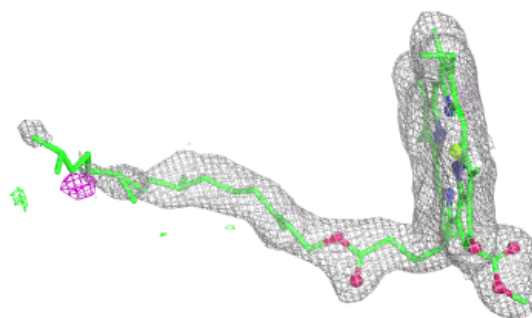
Electron density around LHG L 101:

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

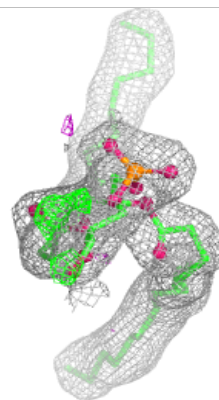
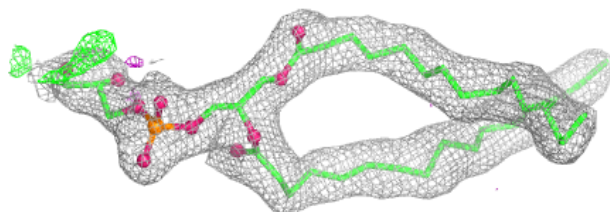
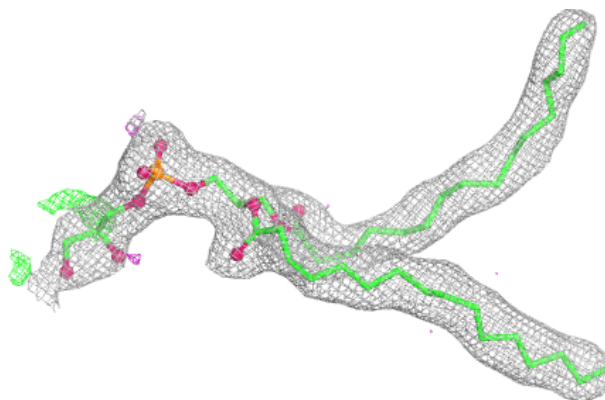


Electron density around CLA D 405:

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

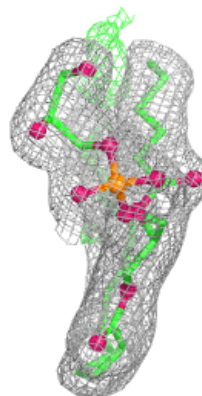
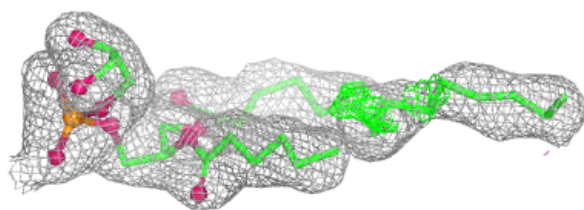
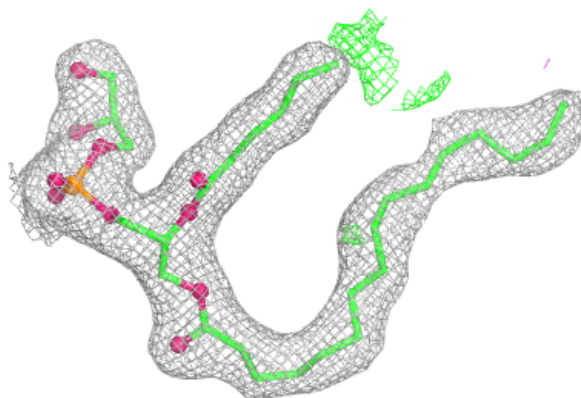
**Electron density around LHG d 408:**

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



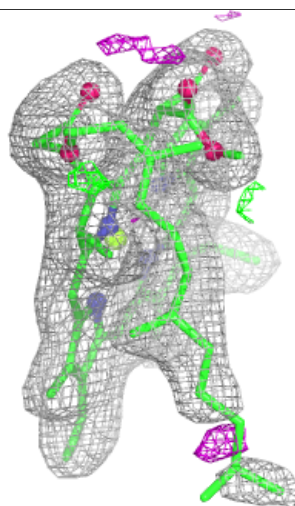
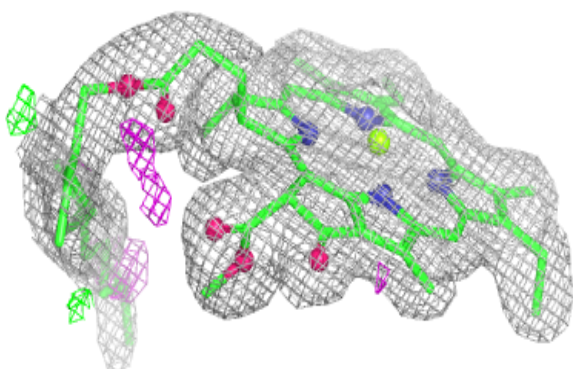
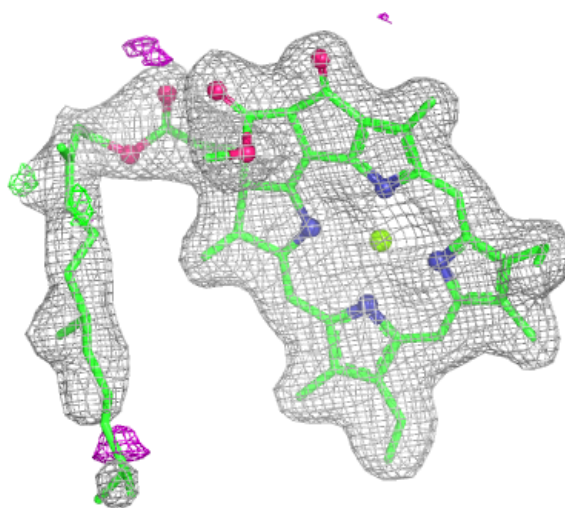
Electron density around LHG d 409:

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



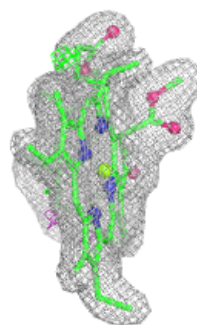
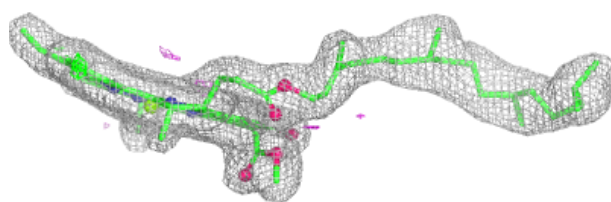
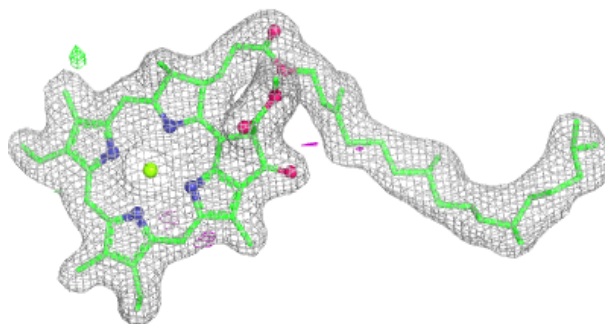
Electron density around CLA B 616:

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

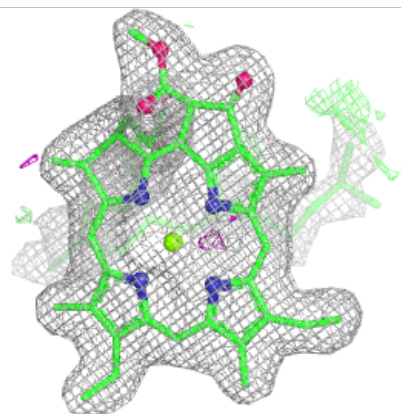
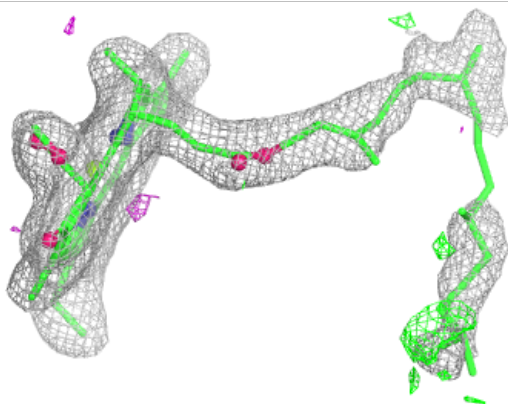
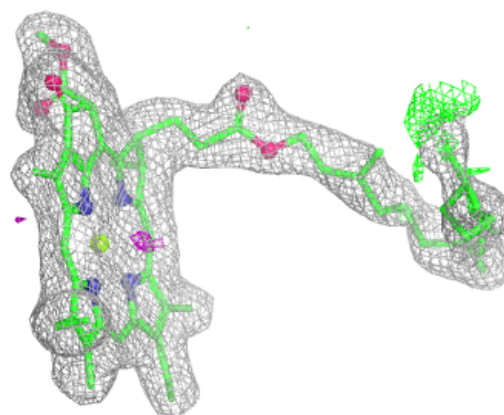


Electron density around CLA B 602:

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

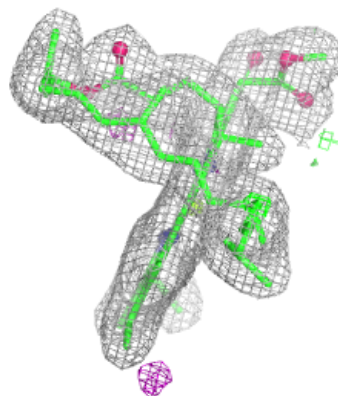
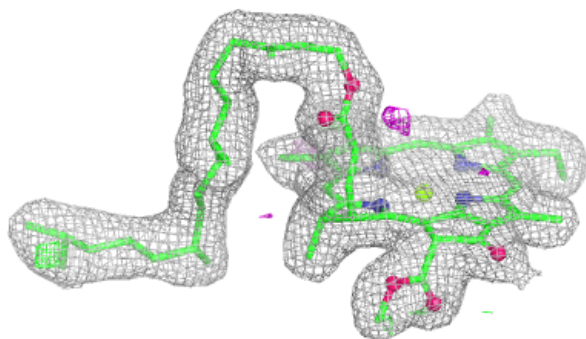
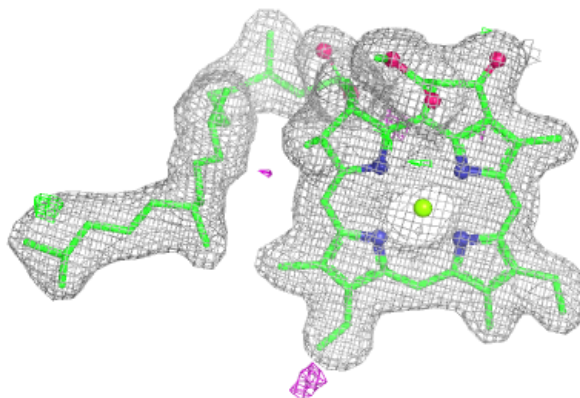
**Electron density around CLA a 609:**

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

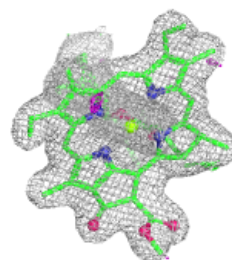
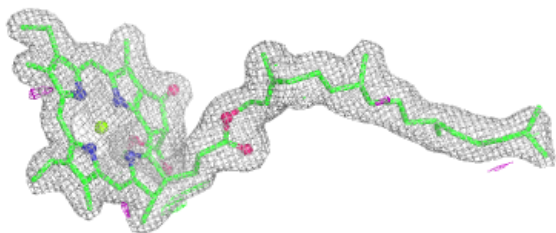
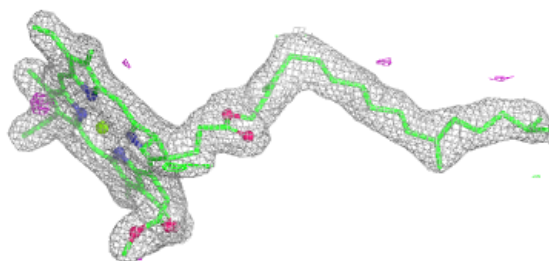


Electron density around CLA a 612:

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

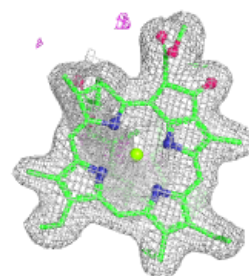
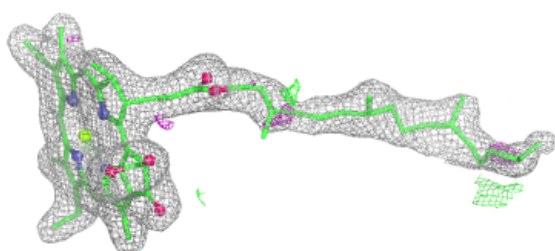
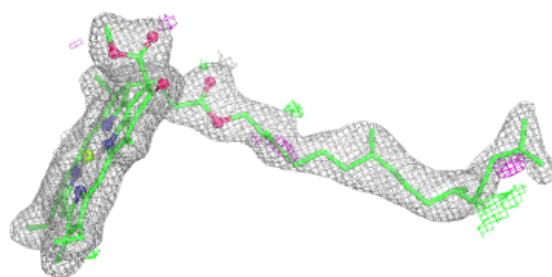
**Electron density around CLA C 502:**

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

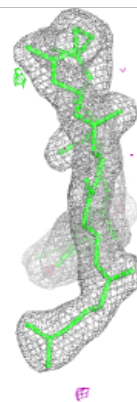
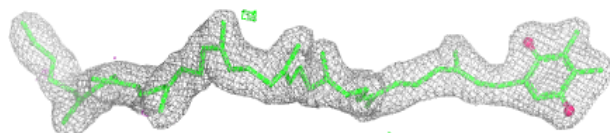
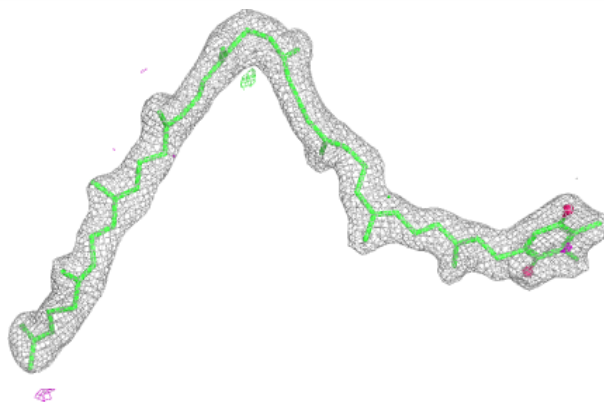


Electron density around CLA B 604:

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

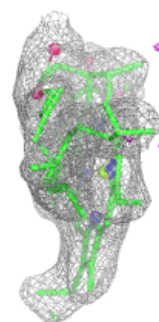
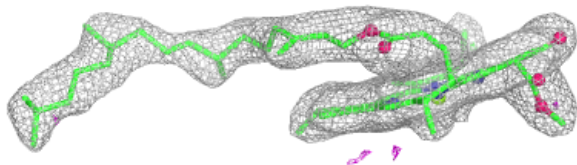
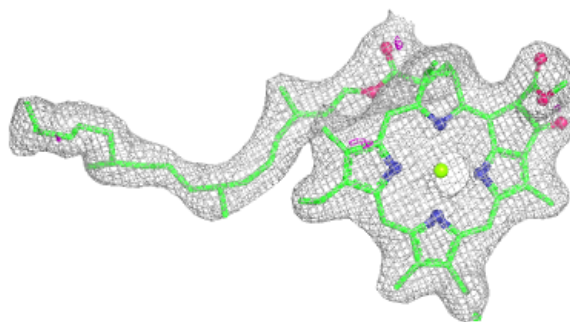
**Electron density around PL9 D 407:**

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

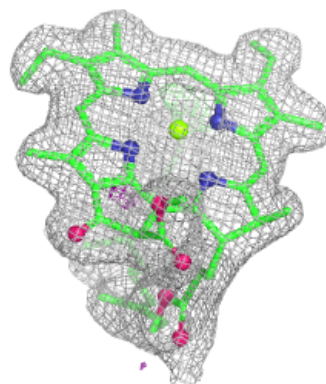
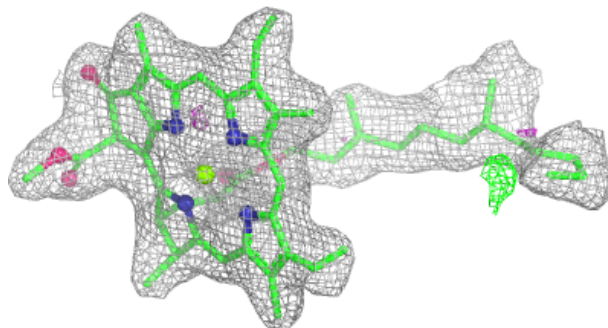
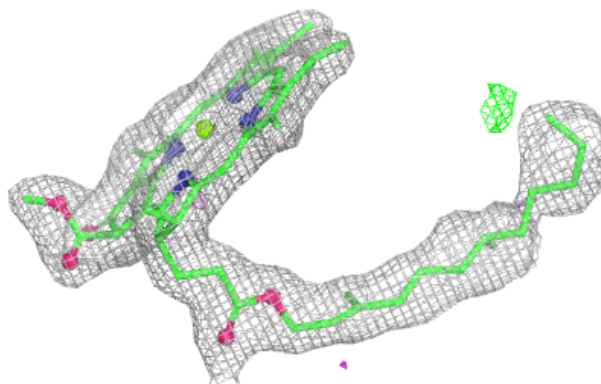


Electron density around CLA b 603:

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

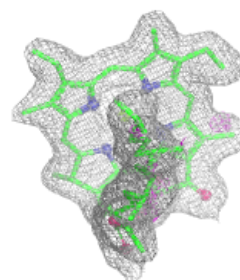
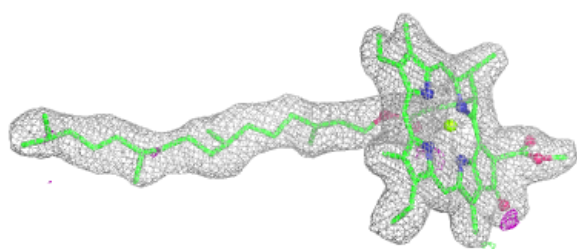
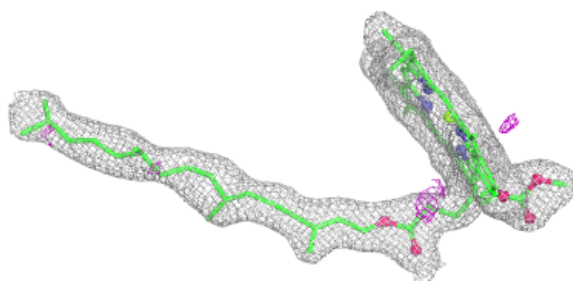
**Electron density around CLA C 504:**

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

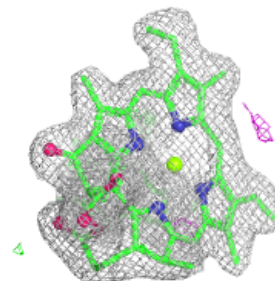
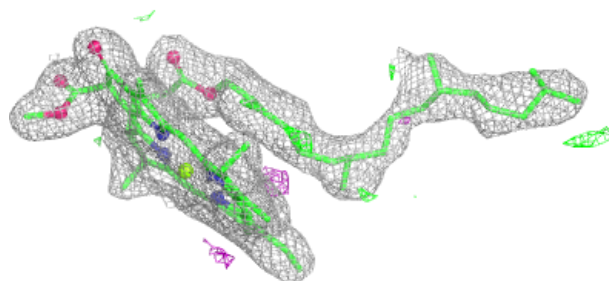
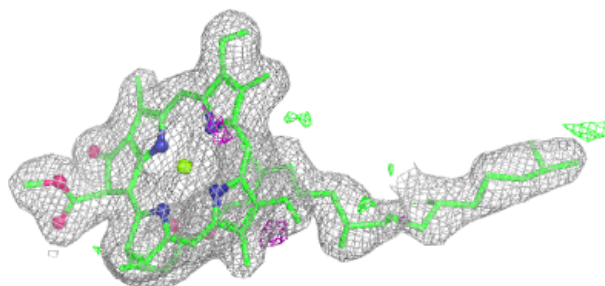


Electron density around CLA b 607:

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

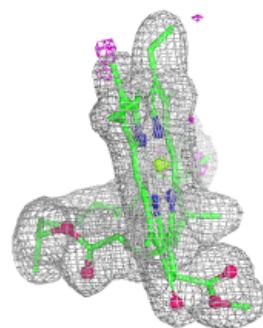
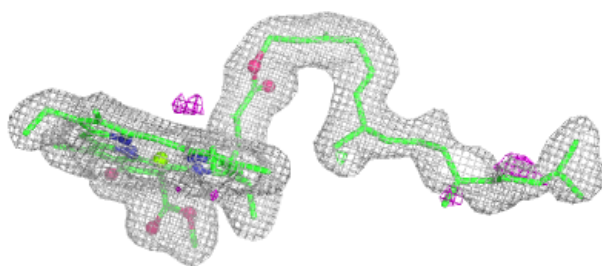
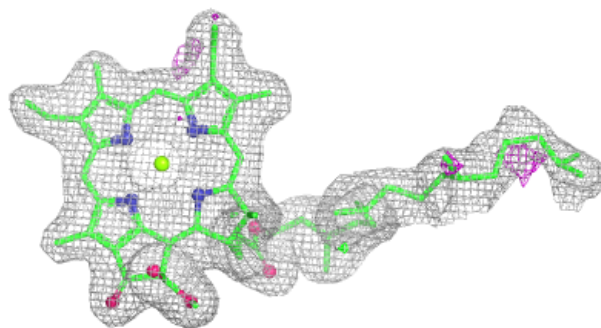
**Electron density around CLA C 505:**

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

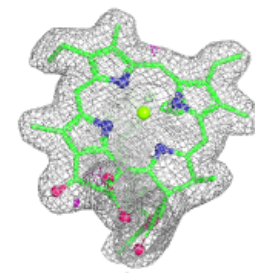
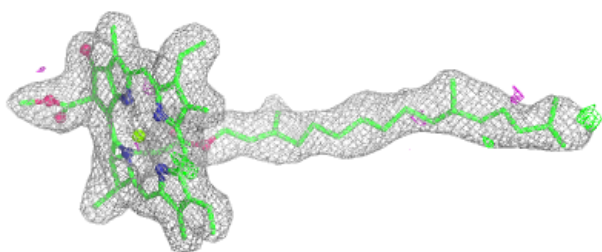
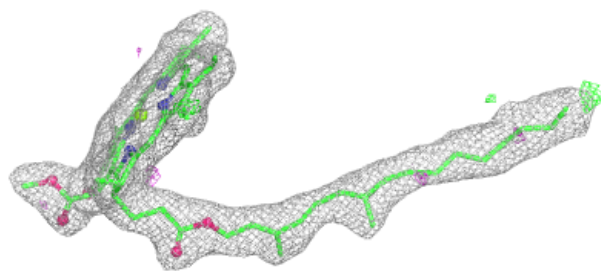


Electron density around CLA A 607:

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

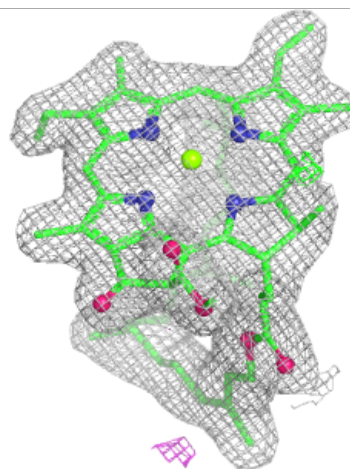
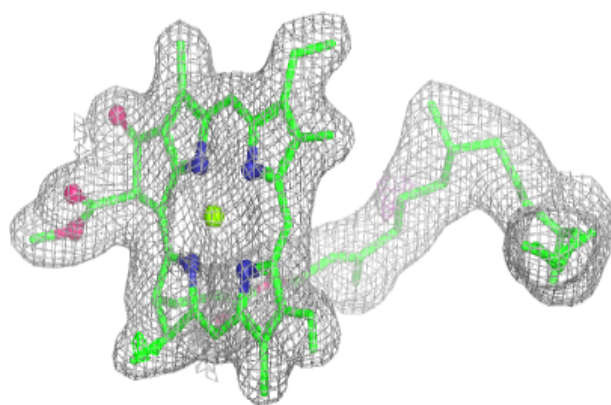
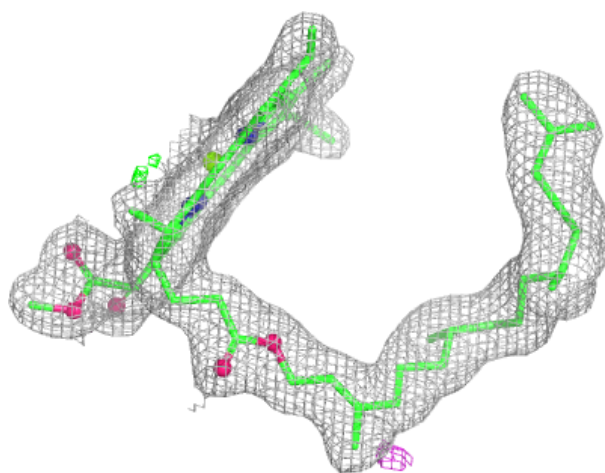
**Electron density around CLA B 607:**

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



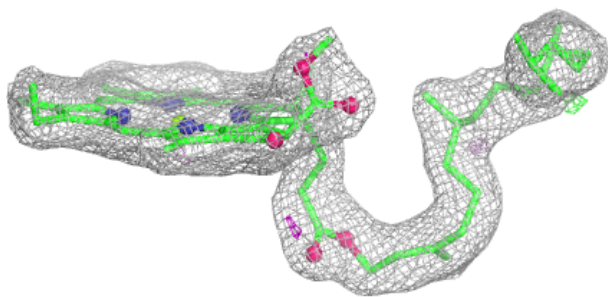
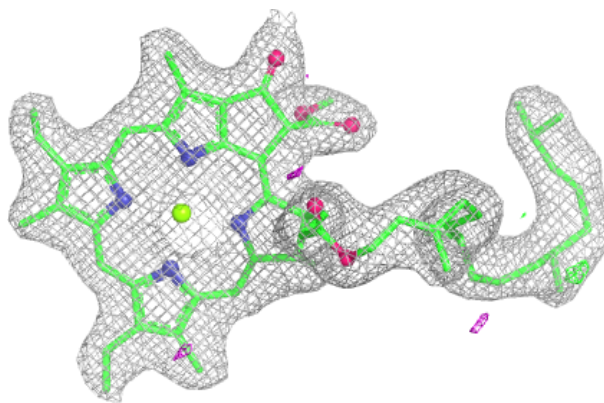
Electron density around CLA b 611:

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

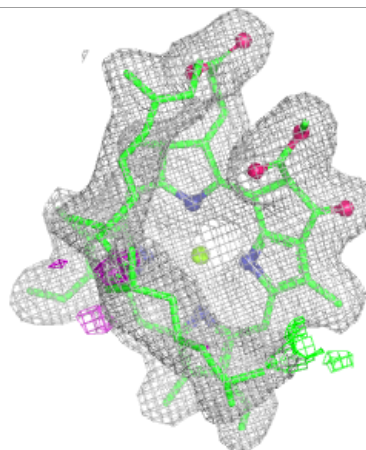
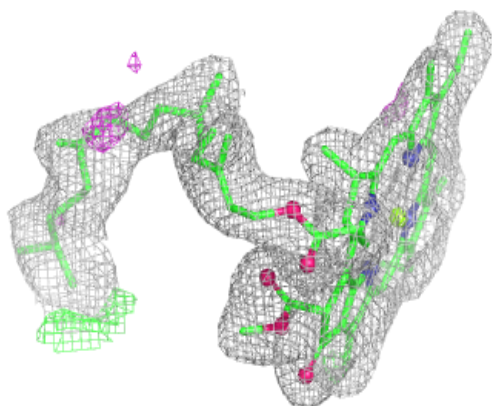
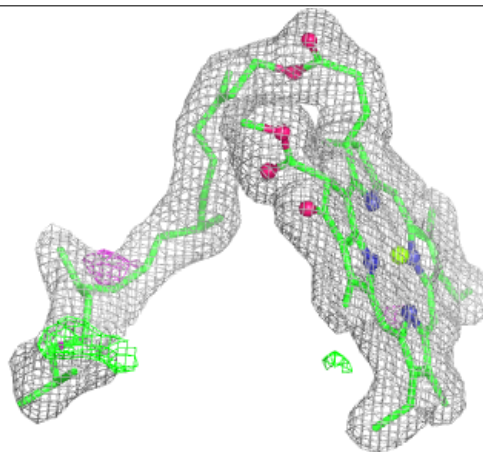


Electron density around CLA b 612:

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

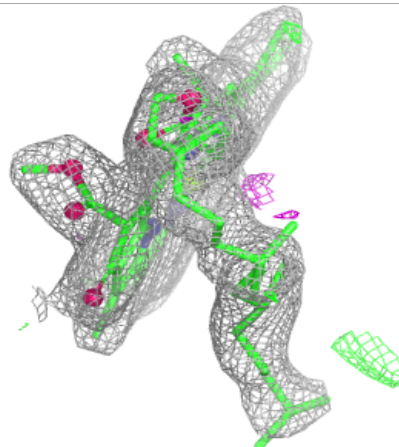
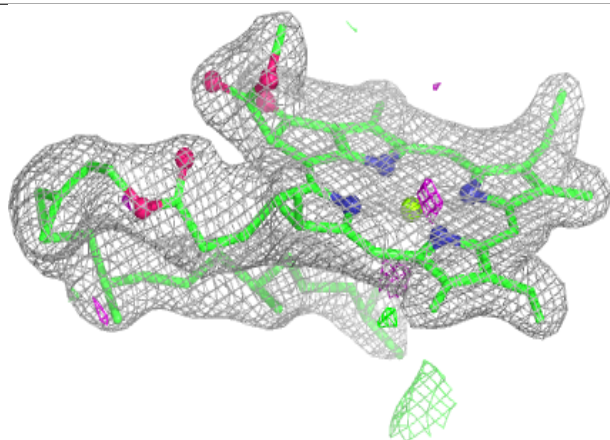
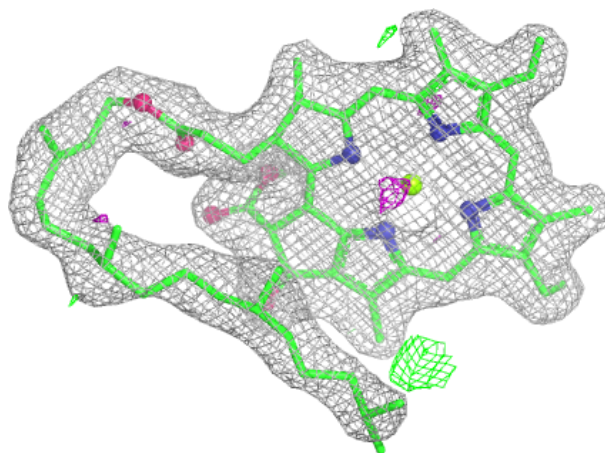
**Electron density around CLA b 613:**

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



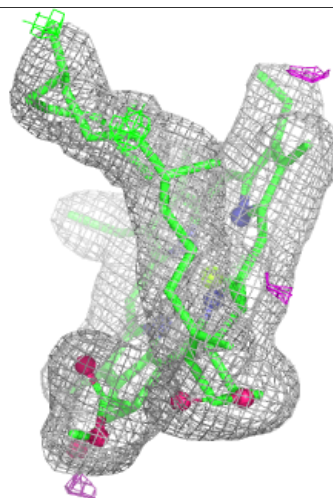
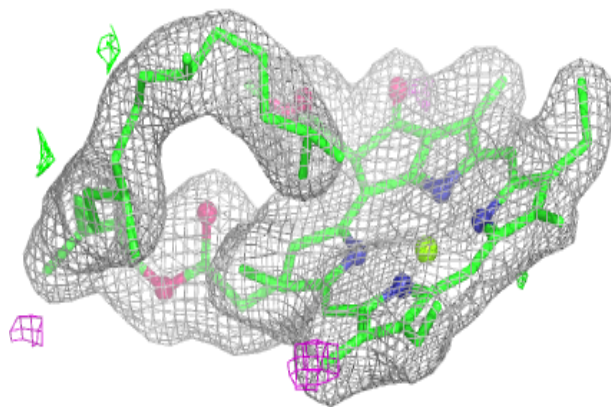
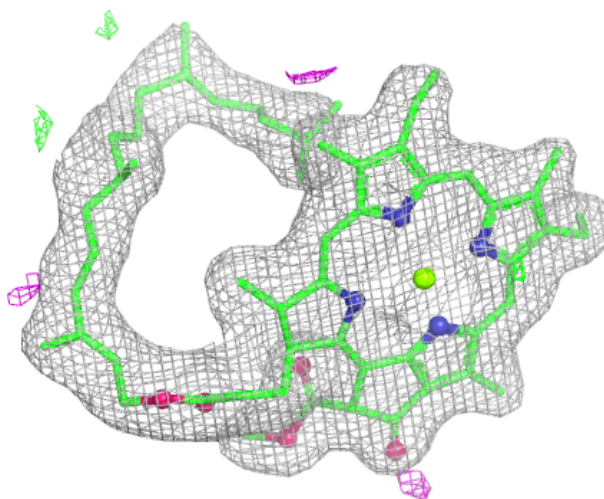
Electron density around CLA C 509:

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



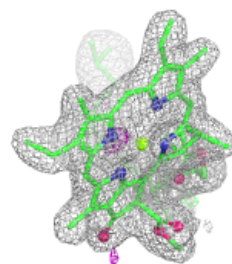
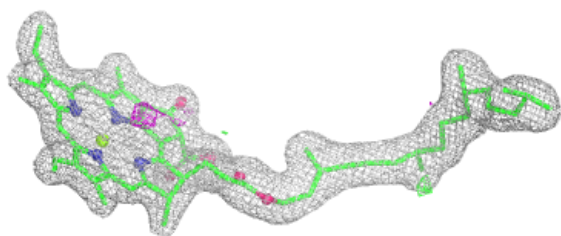
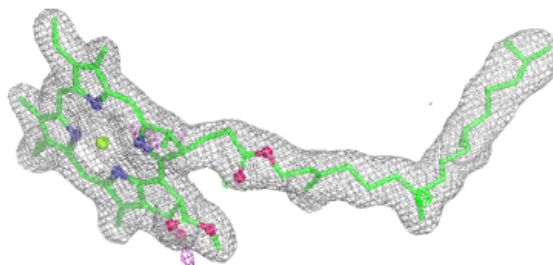
Electron density around CLA b 615:

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

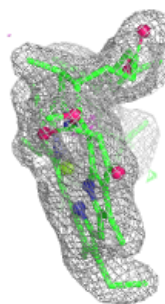
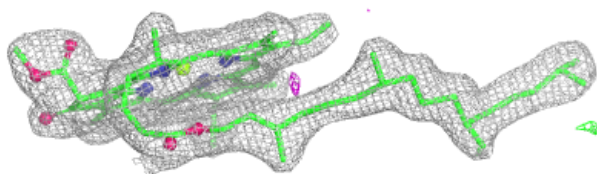
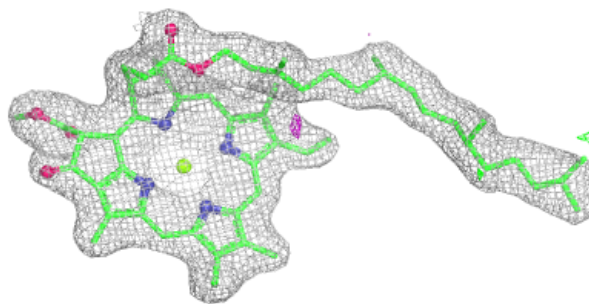


Electron density around CLA A 606:

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

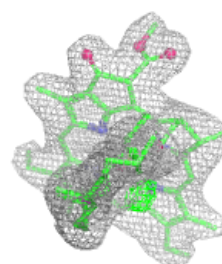
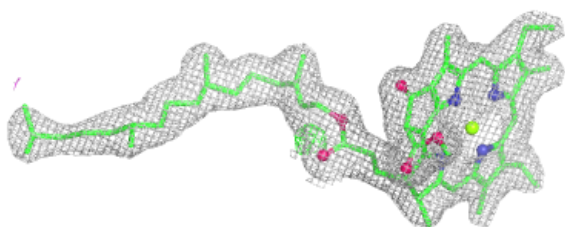
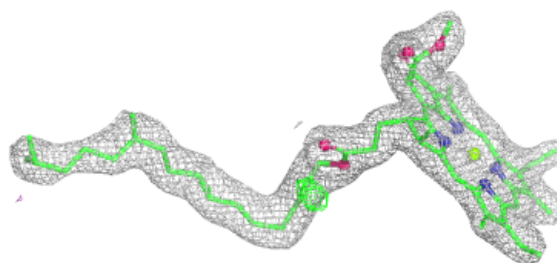
**Electron density around CLA c 501:**

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



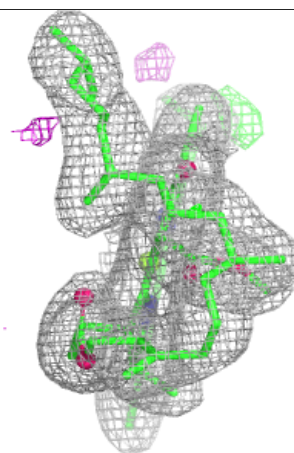
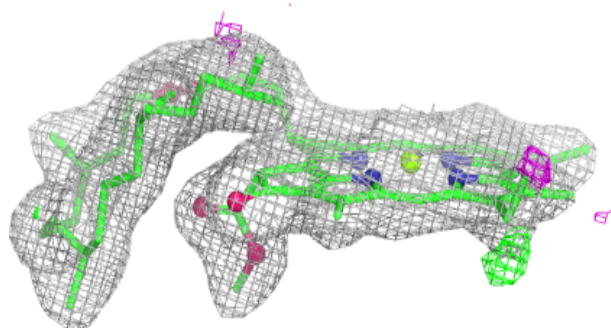
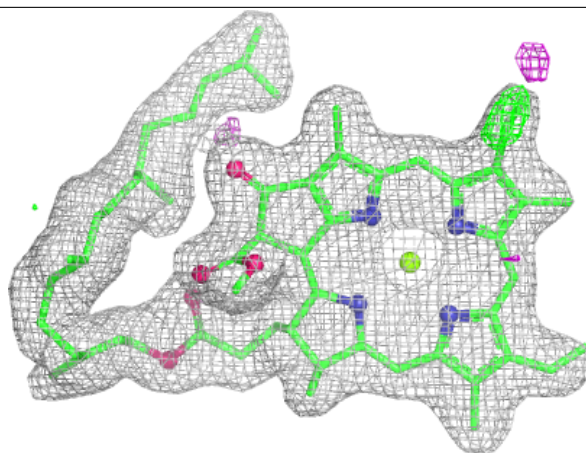
Electron density around CLA c 502:

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



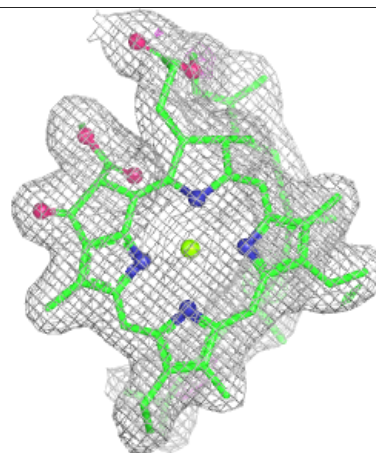
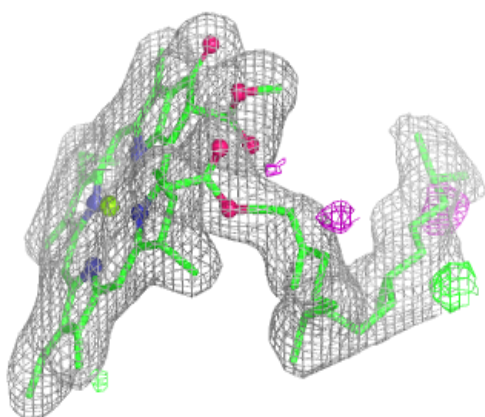
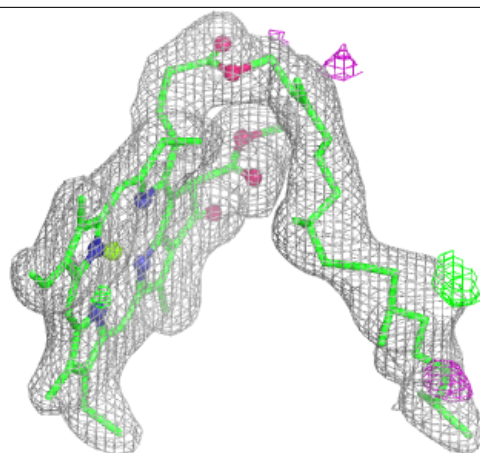
Electron density around CLA B 610:

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

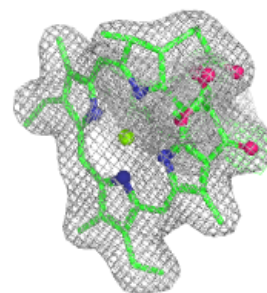
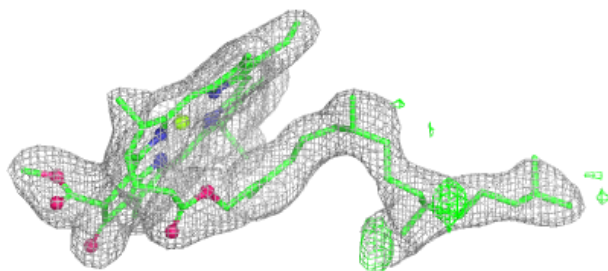
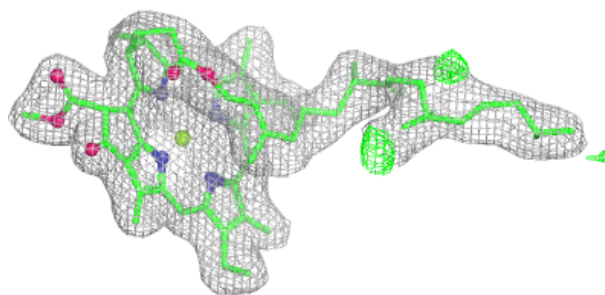


Electron density around CLA B 613:

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

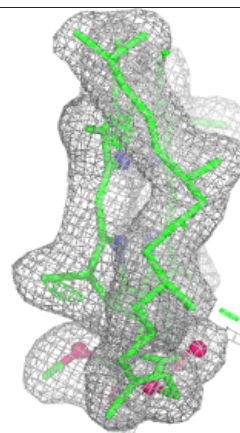
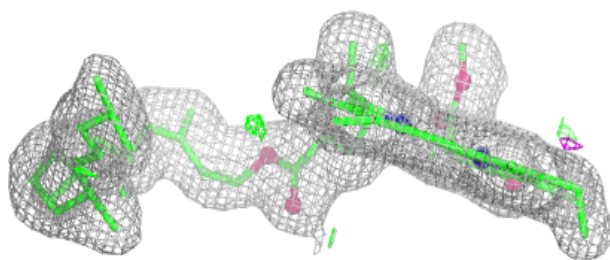
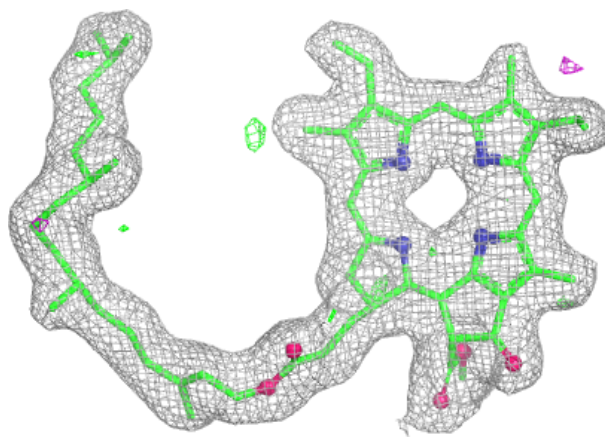
**Electron density around CLA c 505:**

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



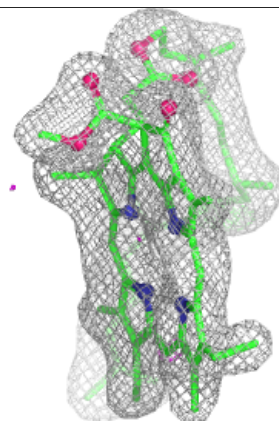
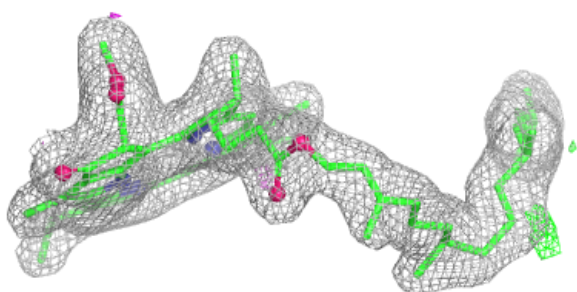
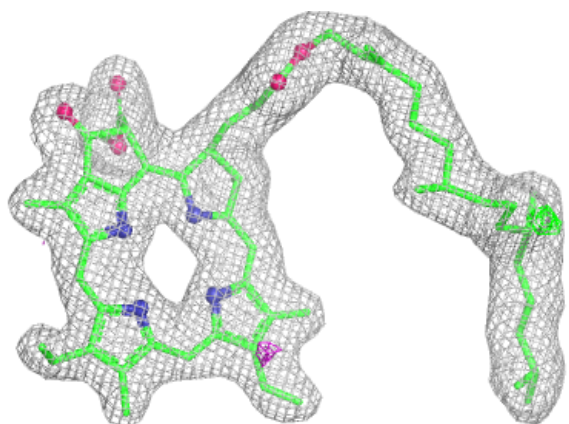
Electron density around PHO D 402:

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

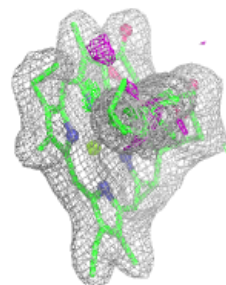
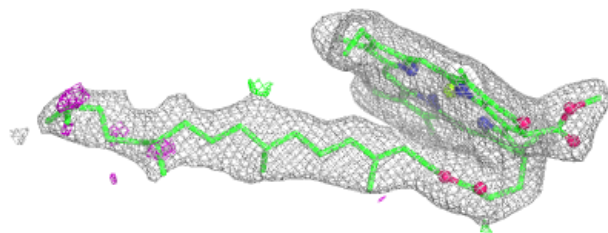
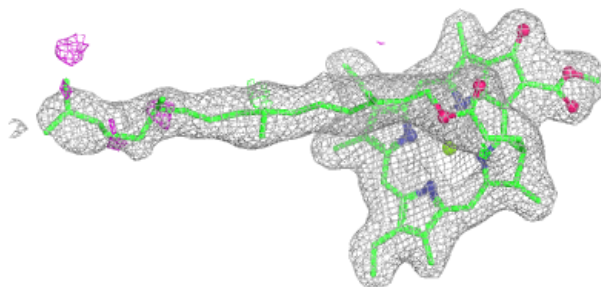


Electron density around PHO D 403:

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

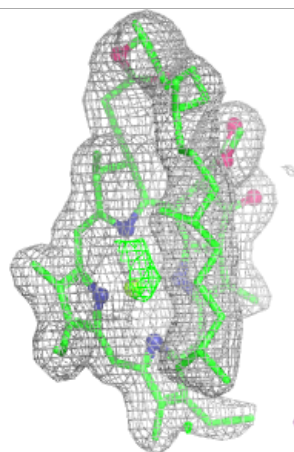
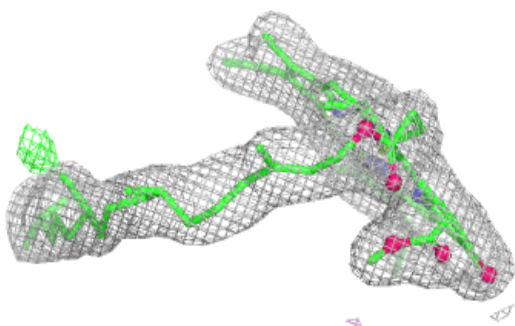
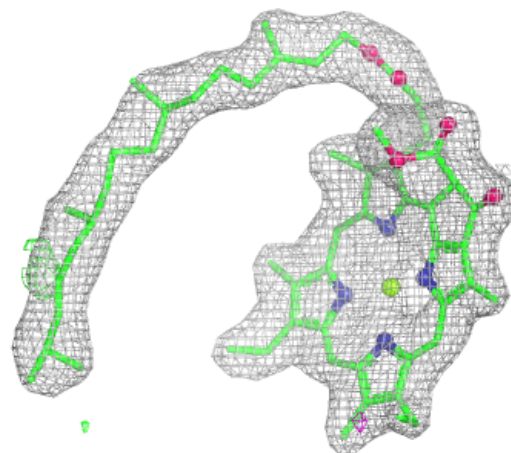
**Electron density around CLA B 614:**

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



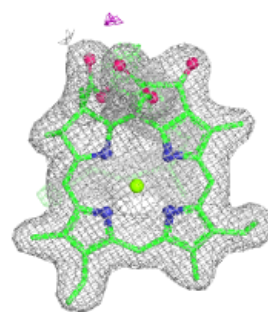
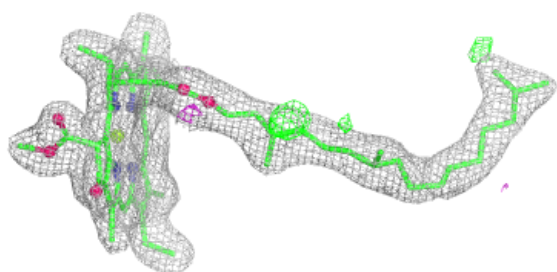
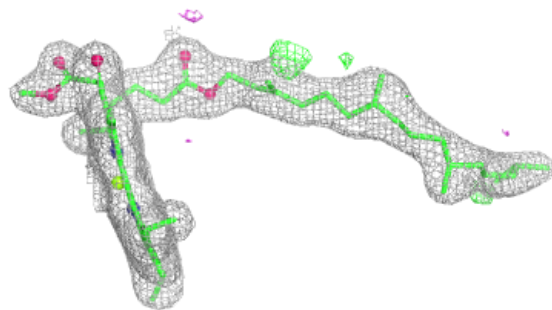
Electron density around CLA C 507:

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

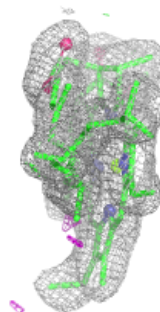
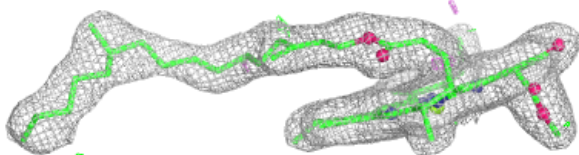
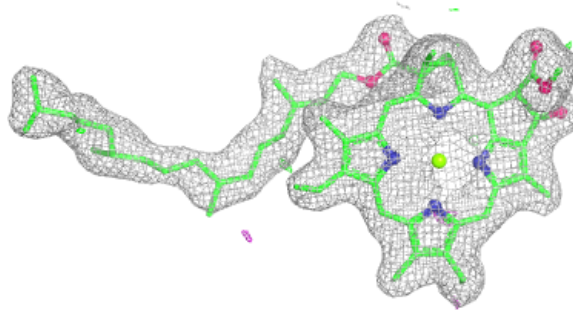


Electron density around CLA B 605:

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

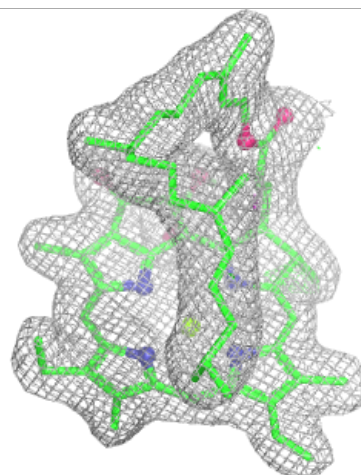
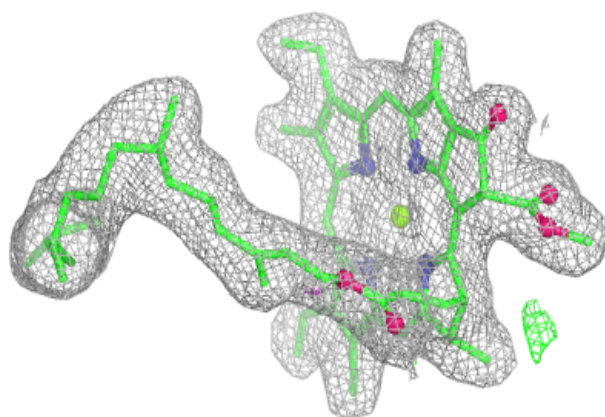
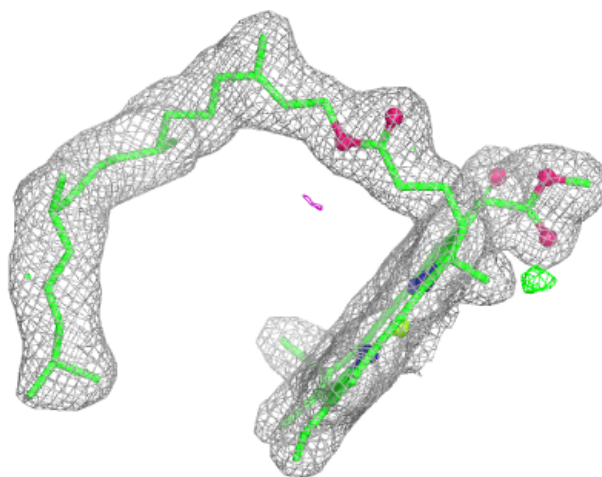
**Electron density around CLA B 603:**

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



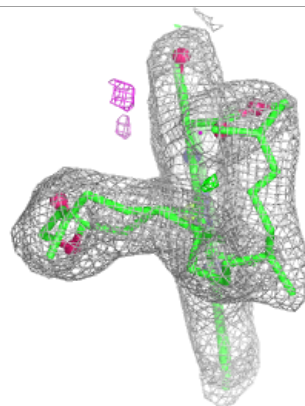
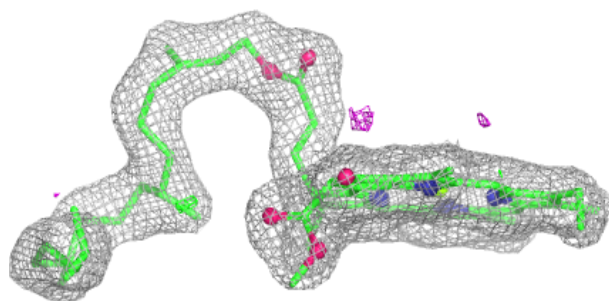
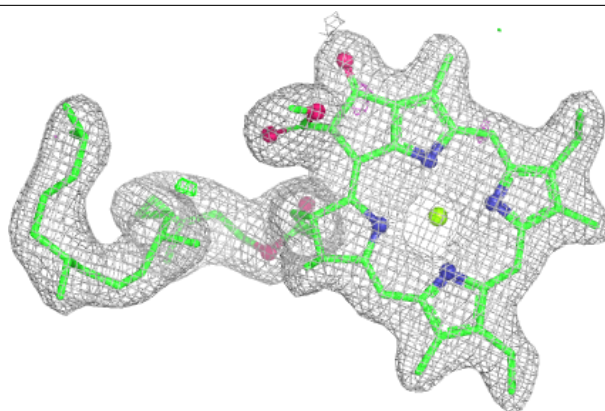
Electron density around CLA B 611:

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

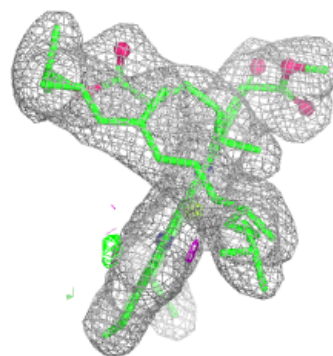
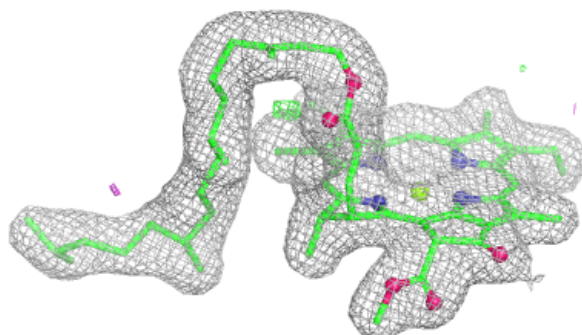
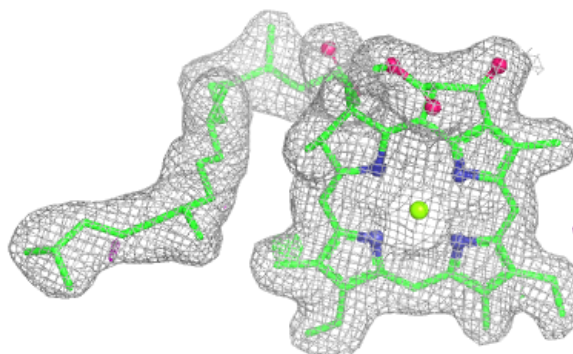


Electron density around CLA B 612:

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

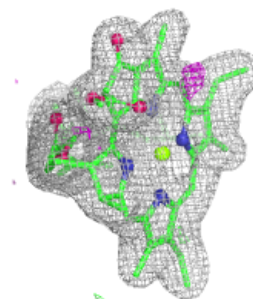
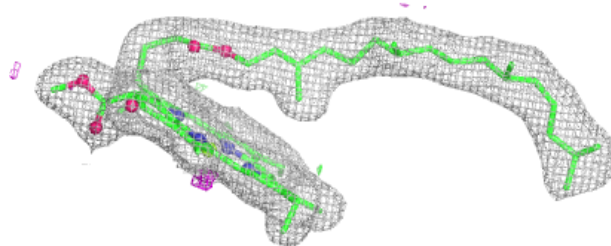
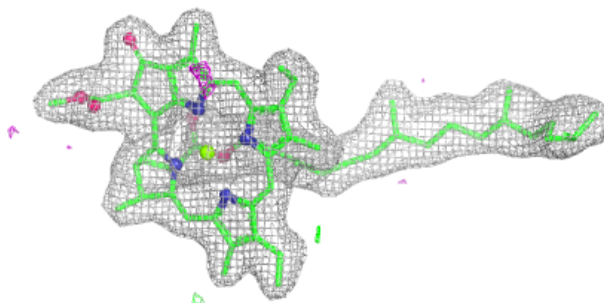
**Electron density around CLA A 611:**

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

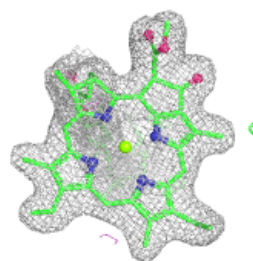
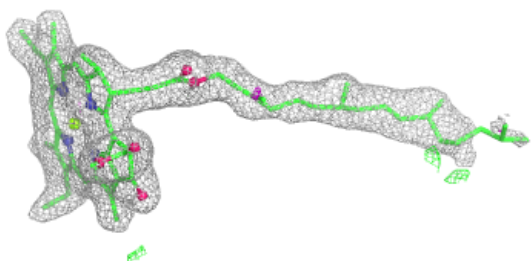
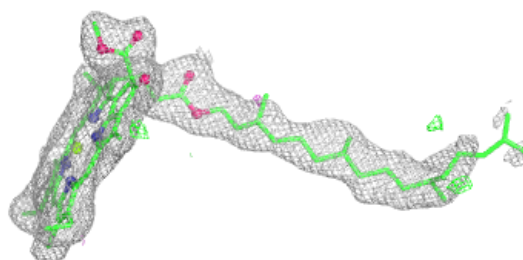


Electron density around CLA B 608:

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

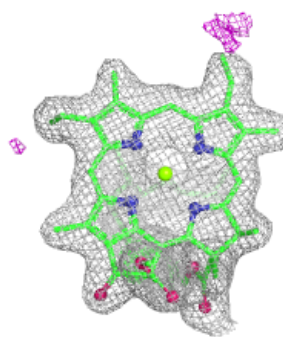
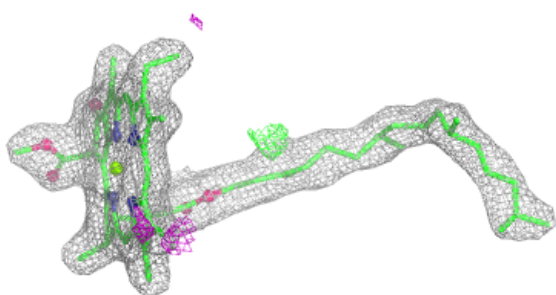
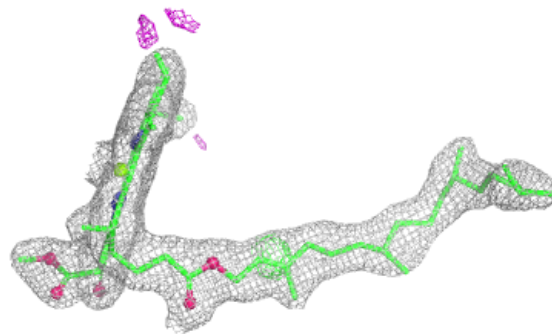
**Electron density around CLA b 604:**

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

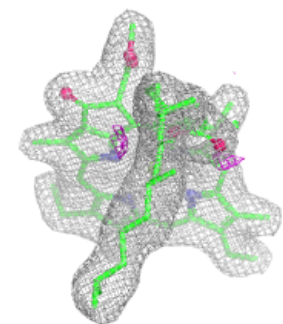
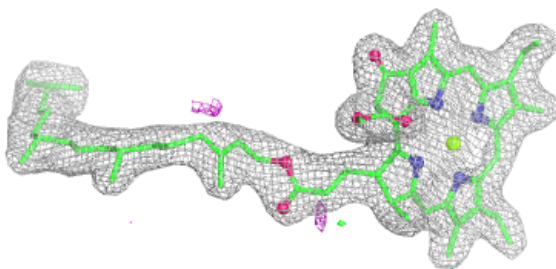
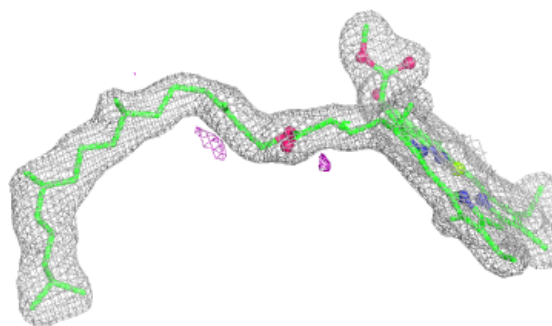


Electron density around CLA b 605:

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

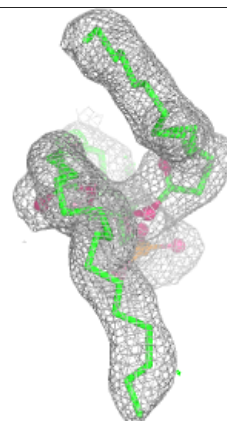
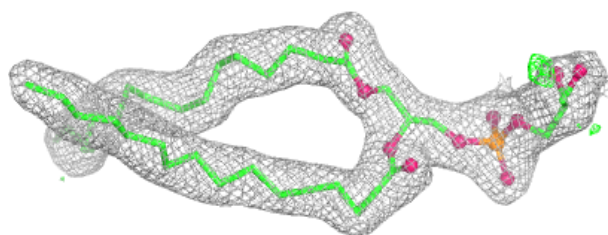
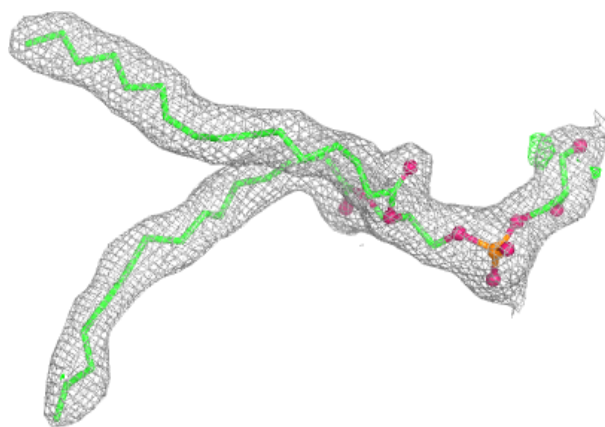
**Electron density around CLA D 404:**

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



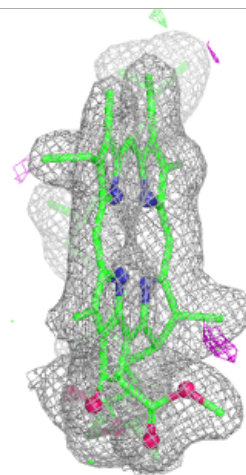
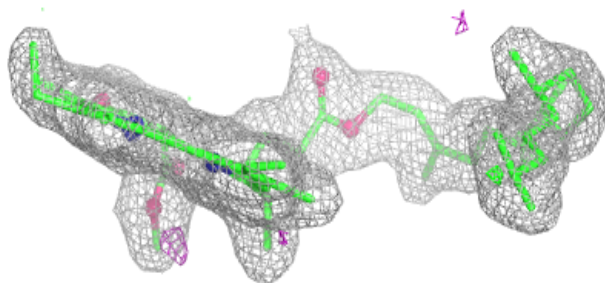
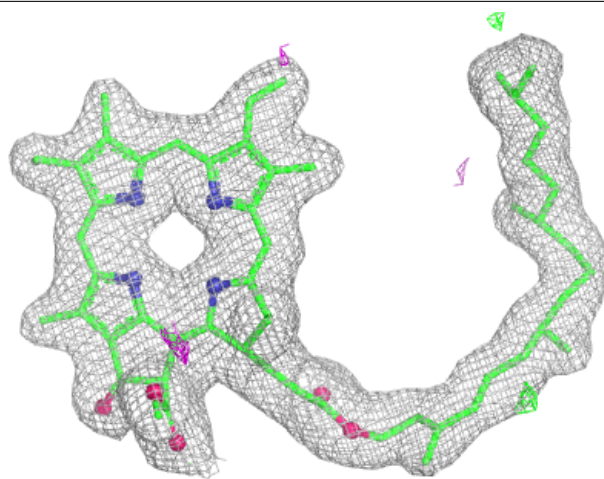
Electron density around LHG D 410:

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



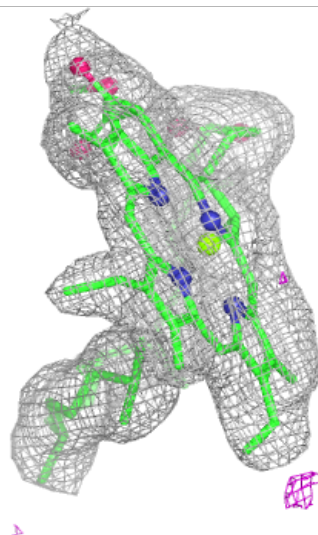
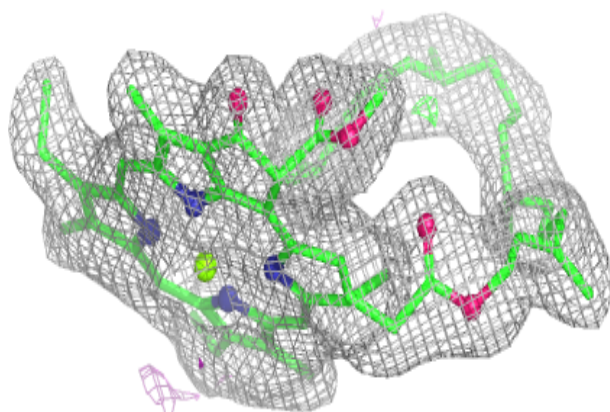
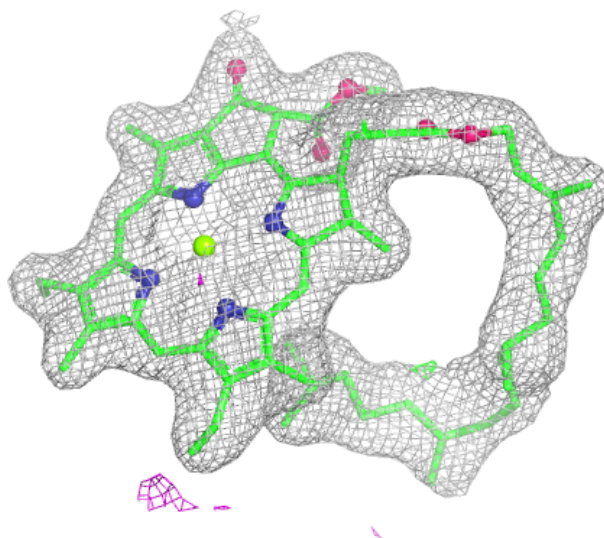
Electron density around PHO d 401:

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



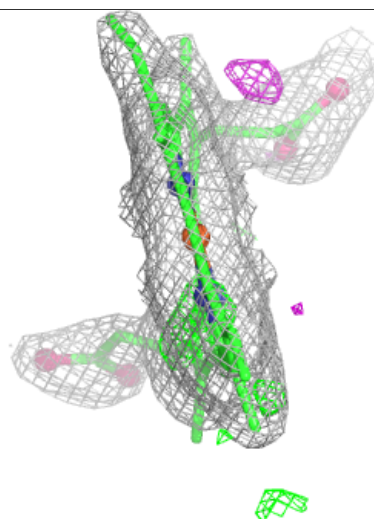
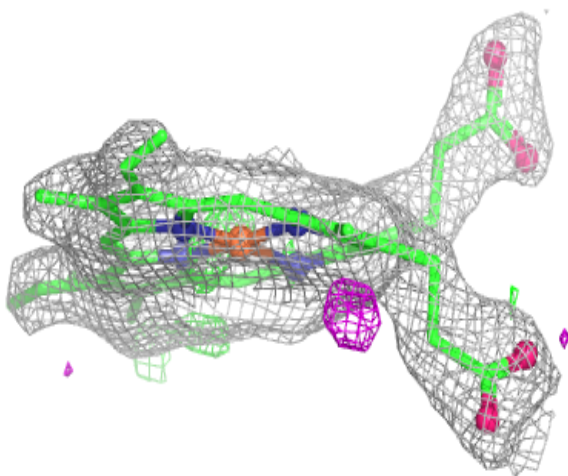
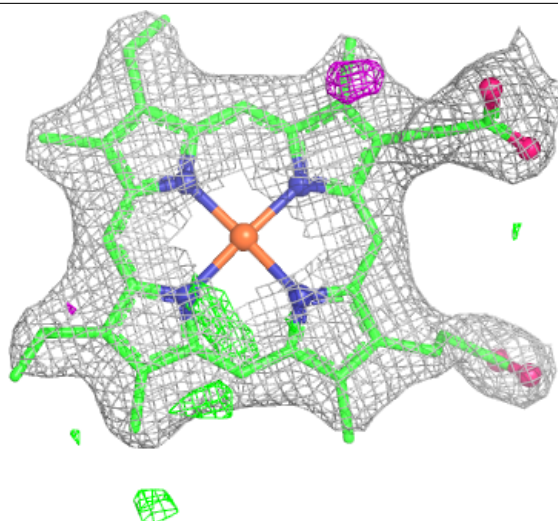
Electron density around CLA B 615:

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



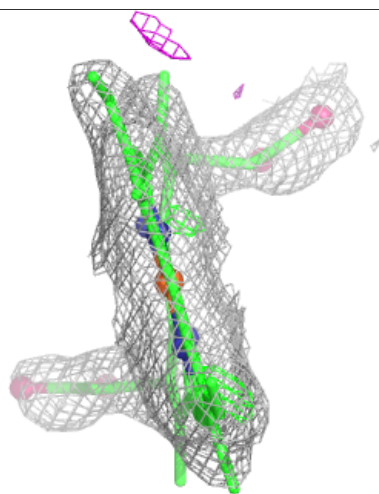
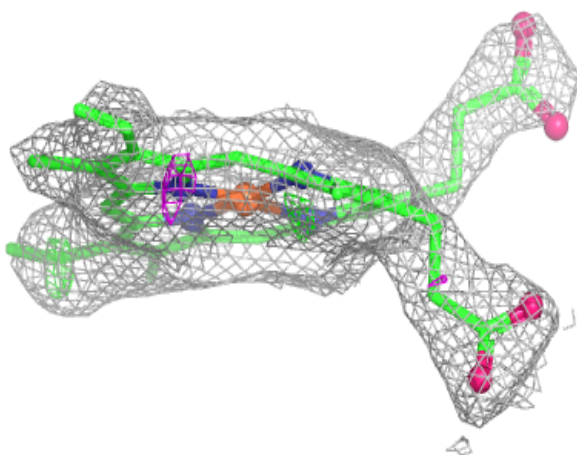
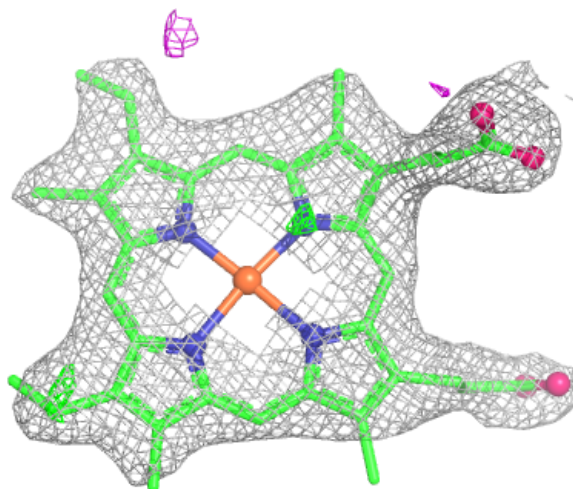
Electron density around HEM F 101:

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



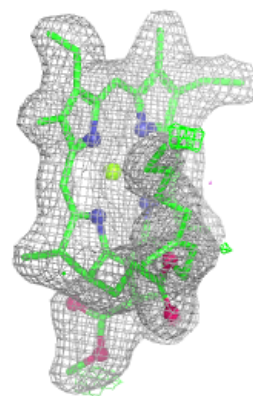
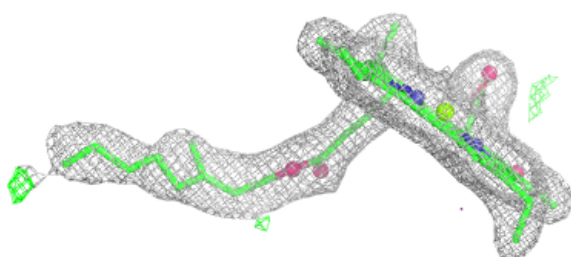
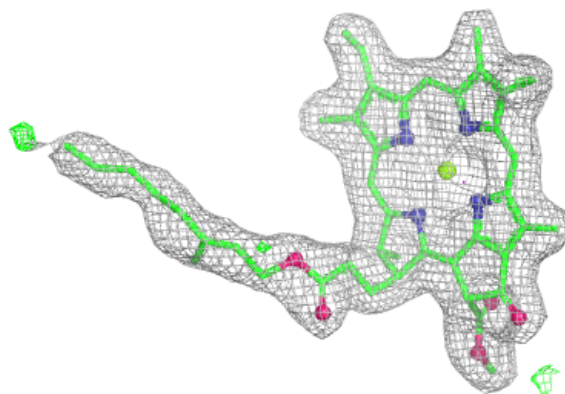
Electron density around HEM f 101:

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



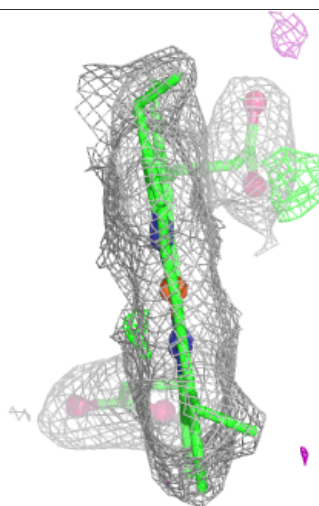
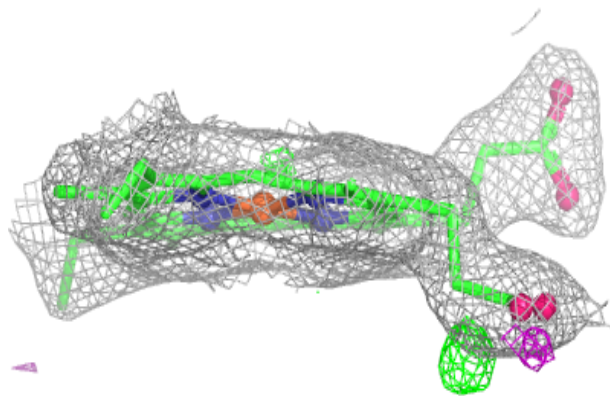
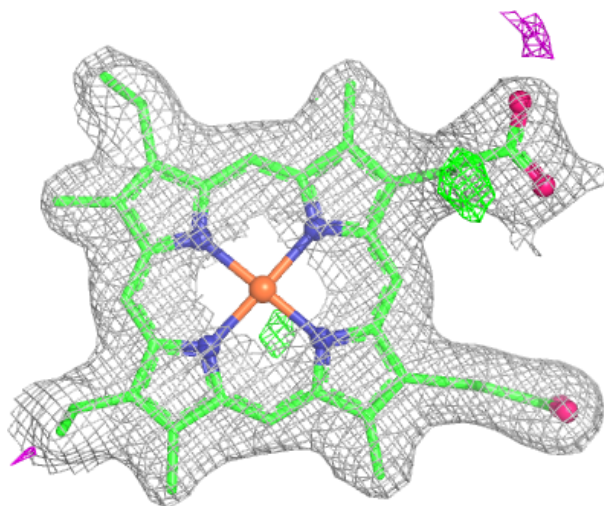
Electron density around CLA A 608:

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



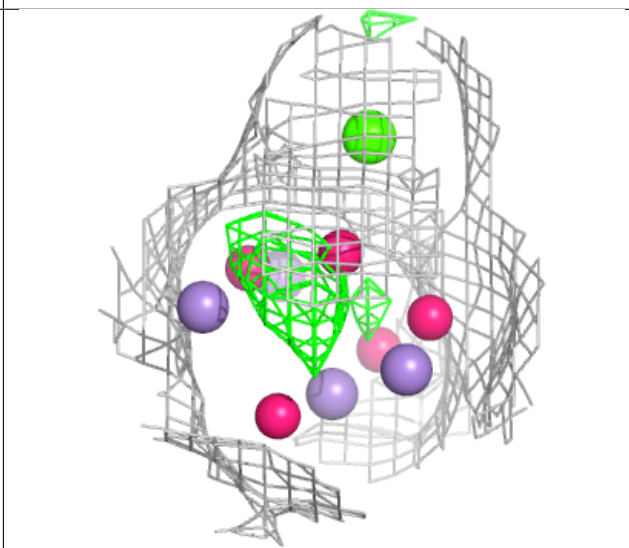
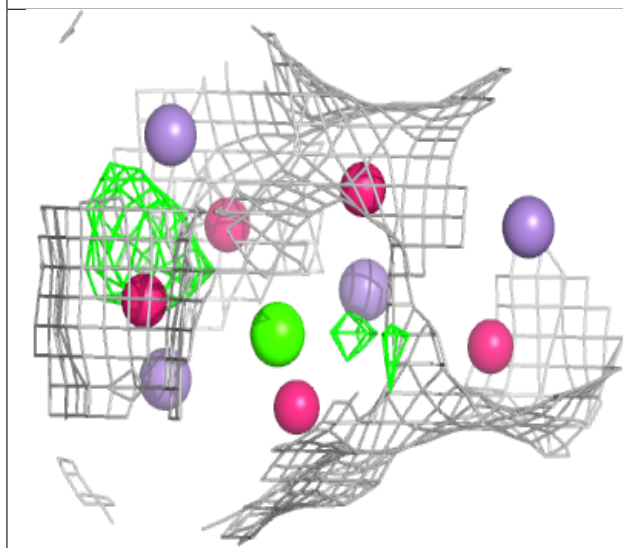
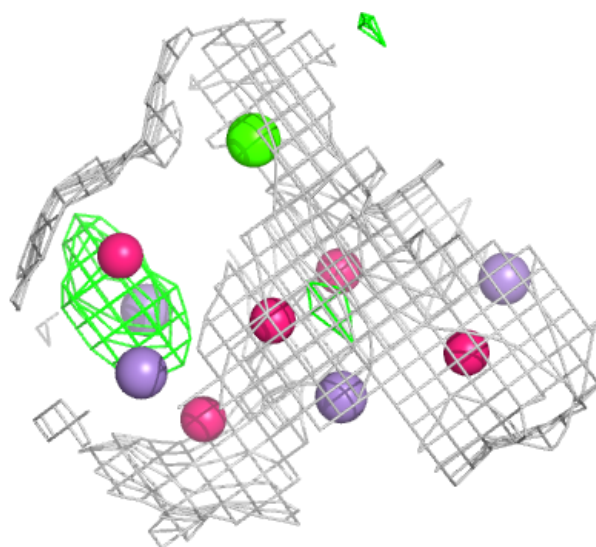
Electron density around HEC V 201:

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



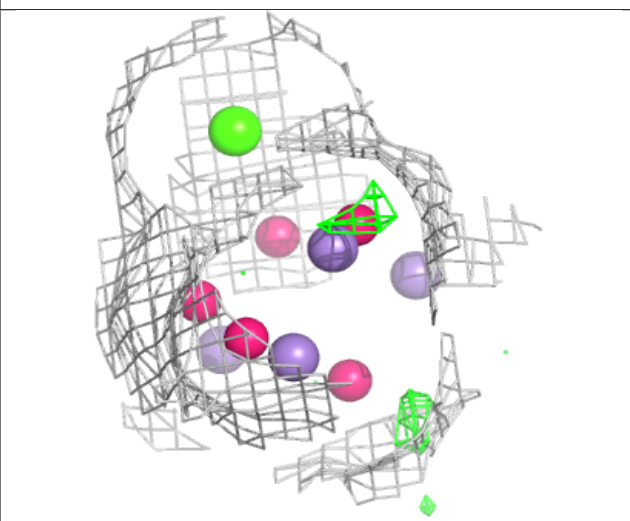
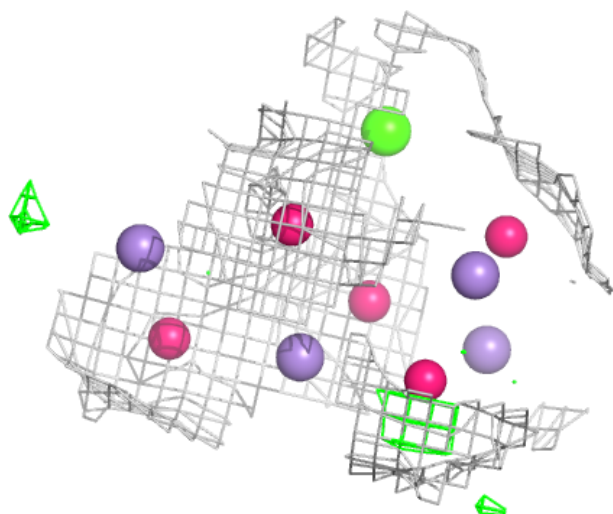
Electron density around OEX A 602 (A):

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



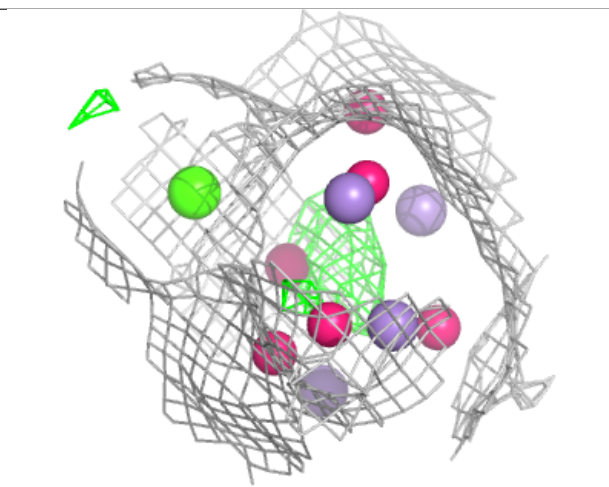
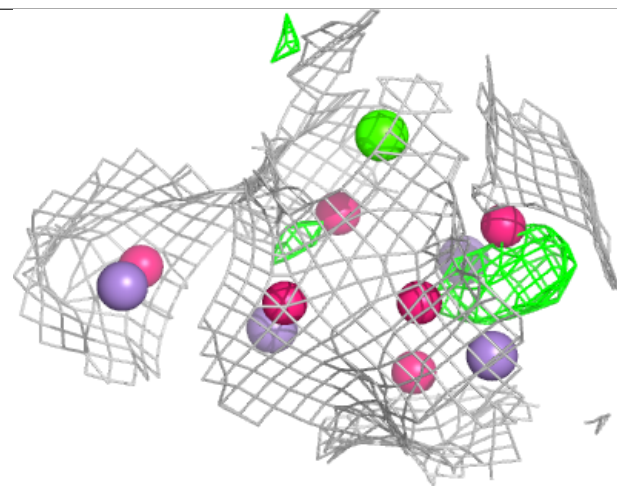
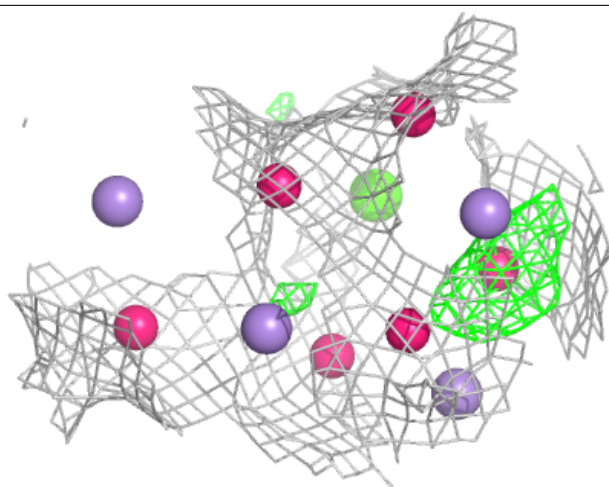
Electron density around OEX a 602 (A):

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



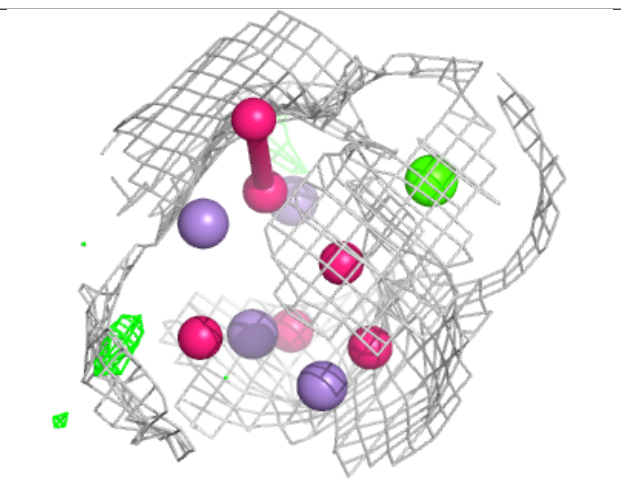
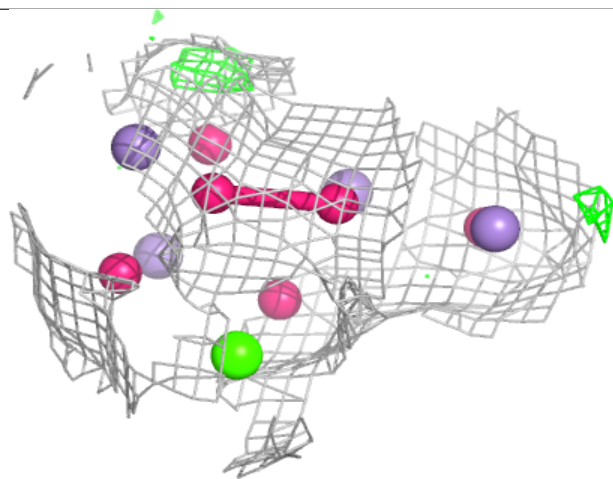
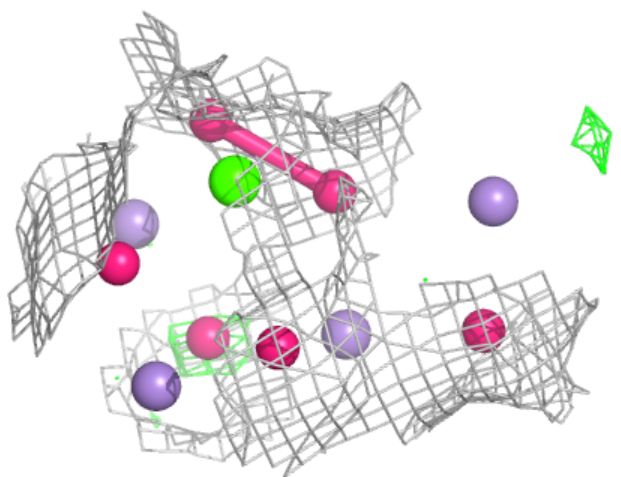
Electron density around OEY A 601 (B):

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



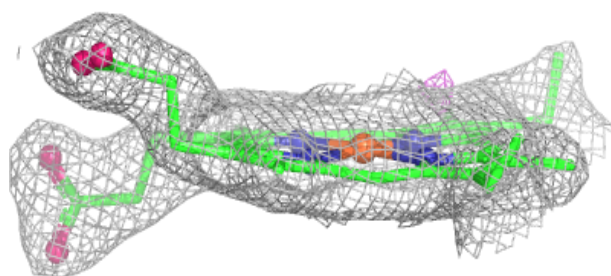
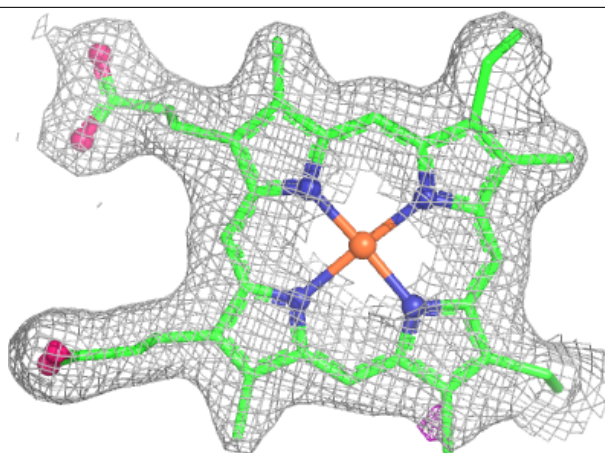
Electron density around OEY a 601 (B):

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



Electron density around 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.