



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 7, 2026 – 12:39 AM UTC

PDB ID : 8F4I / pdb_00008f4i
Title : RT XFEL structure of Photosystem II 2000 microseconds after the third illumination 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

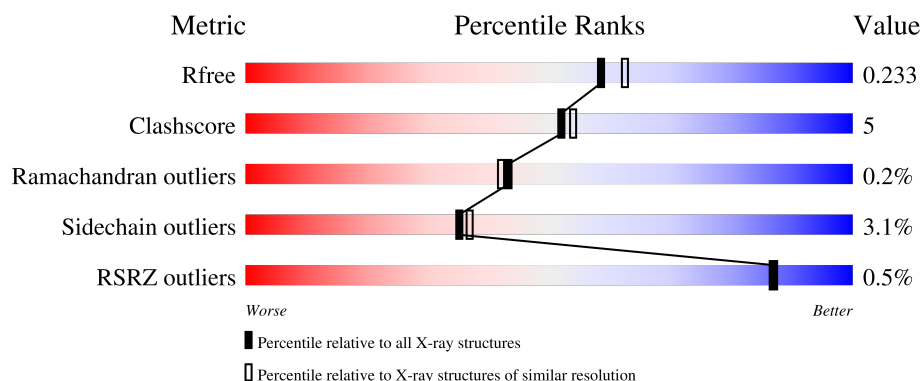
1 Overall quality at a glance

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)

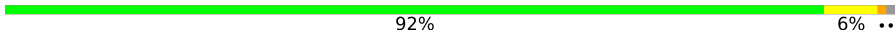
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	

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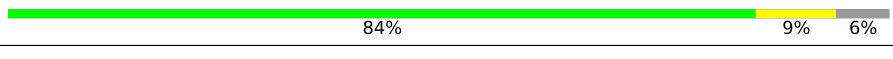
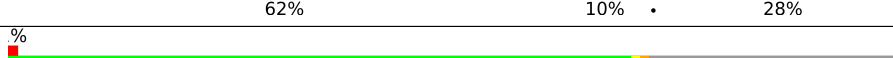
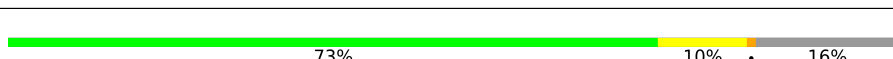
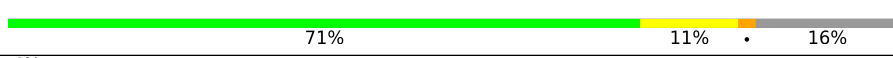
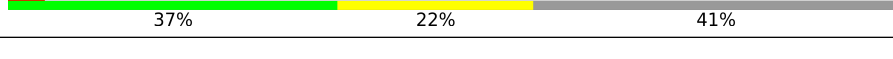
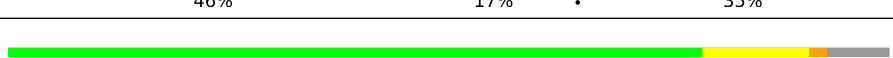
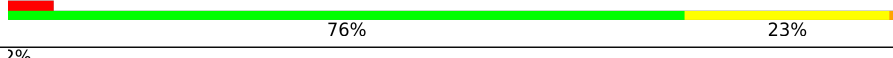
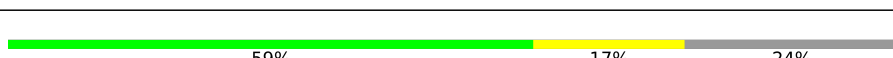
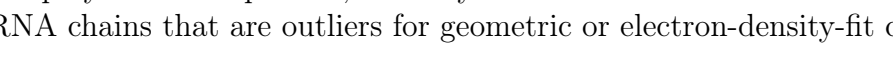
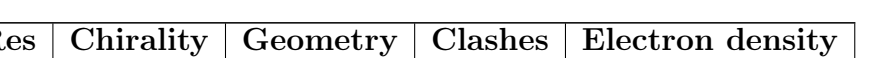
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
 Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
 CCP4 : 9.0.010 (Gargrove)
 Density-Fitness : 1.0.12
 Ideal geometry (proteins) : Engh & Huber (2001)
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
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

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Mol	Chain	Length	Quality of chain
1	a	344	 84% 13% .
2	B	510	 92% 6% ..
2	b	510	 91% 7% .
3	C	461	 88% 8% .
3	c	461	 88% 9% ..
4	D	352	 88% 9% .
4	d	352	 89% 7% ..
5	E	84	 % 86% 12% .
5	e	84	 % 74% 24% .
6	F	45	 2% 69% . 24%
6	f	45	 60% 11% . 24%
7	H	66	 3% 91% 8% .
7	h	66	 83% 12% 5%
8	I	38	 79% 13% . 5%
8	i	38	 82% 13% 5%
9	J	40	 78% 10% . 10%
9	j	40	 72% 15% . 10%
10	K	46	 72% 9% 20%
10	k	46	 59% 15% 7% 20%
11	L	37	 86% 14%
11	l	37	 89% 8% .
12	M	36	 67% 25% 8%
12	m	36	 64% 19% 6% 11%
13	O	272	 % 75% 13% . 10%
13	o	272	 % 79% 10% 10%

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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	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	610	X	-	-	-
25	CLA	B	611	X	-	-	-
25	CLA	B	612	X	-	-	-
25	CLA	B	613	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	B	614	X	-	-	-
25	CLA	B	615	X	-	-	-
25	CLA	B	616	X	-	-	-
25	CLA	C	501	X	-	-	-
25	CLA	C	504	X	-	-	-
25	CLA	C	505	X	-	-	-
25	CLA	C	506	X	-	-	-
25	CLA	C	507	X	-	-	-
25	CLA	C	508	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	403	X	-	-	-
25	CLA	a	606	X	-	-	-
25	CLA	a	607	X	-	-	-
25	CLA	a	609	X	-	-	-
25	CLA	a	612	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	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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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 54640 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
			3604	2343	595	643	23			
1	a	334	Total	C	N	O	S	0	64	0
			3601	2340	595	643	23			

- 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
			3592	2355	601	621	15			
3	c	451	Total	C	N	O	S	0	12	0
			3666	2396	617	638	15			

- 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
			2745	1818	448	467	12			
4	d	341	Total	C	N	O	S	0	3	0
			2751	1822	448	469	12			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	82	Total	C	N	O	0	1	0
			666	436	107	123			
5	e	82	Total	C	N	O	0	0	0
			664	434	108	122			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 14 is a protein called Photosystem II 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			

- 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				

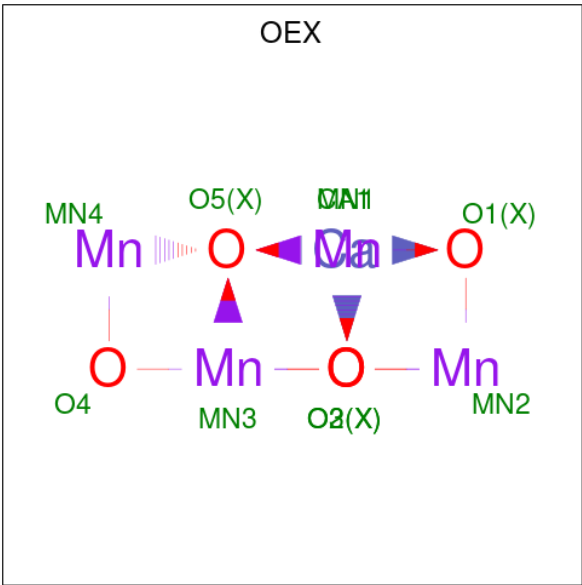
- Molecule 19 is a protein called Photosystem II reaction center protein Z.

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.

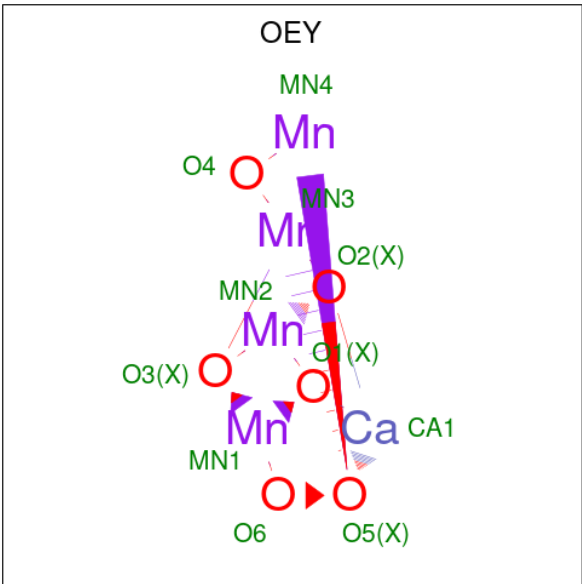
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	R	34	Total	C	N	O		0	0	0
			271	184	47	40				
20	r	31	Total	C	N	O		0	0	0
			246	166	43	37				

- Molecule 21 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
21	A	1	Total	Ca	Mn	O	0	1
			20	2	8	10		
21	a	1	Total	Ca	Mn	O	0	1
			20	2	8	10		

- Molecule 22 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
22	A	1	Total	Ca	Mn	O	0	1
			11	1	4	6		

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

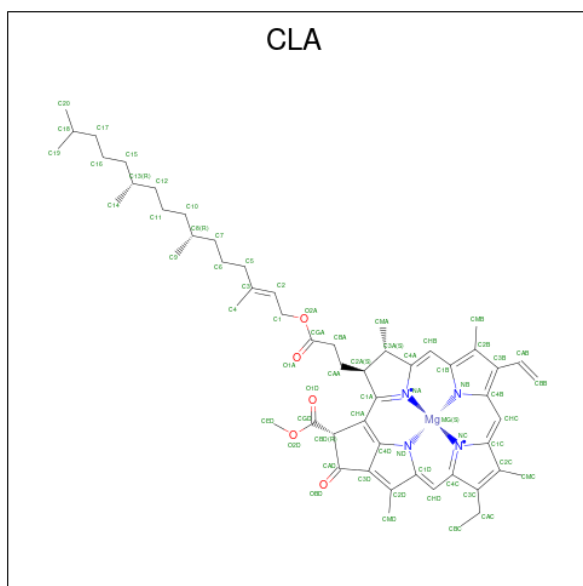
- Molecule 23 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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).



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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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		
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
			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		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	C	1	Total	C	Mg	N	O	0	0
			59	49	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	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		
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
			65	55	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		

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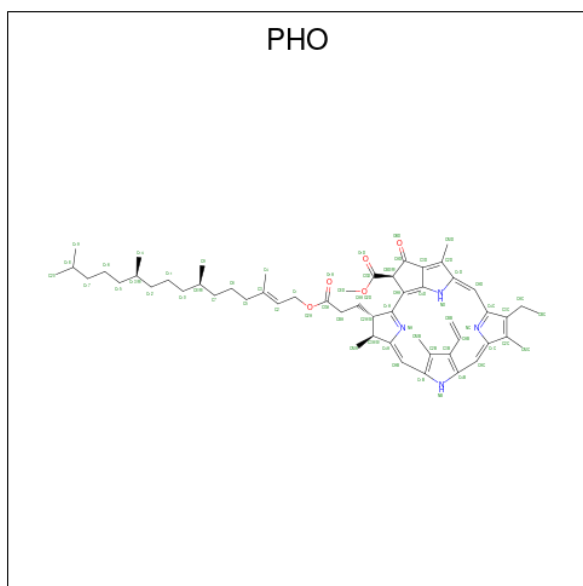
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N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

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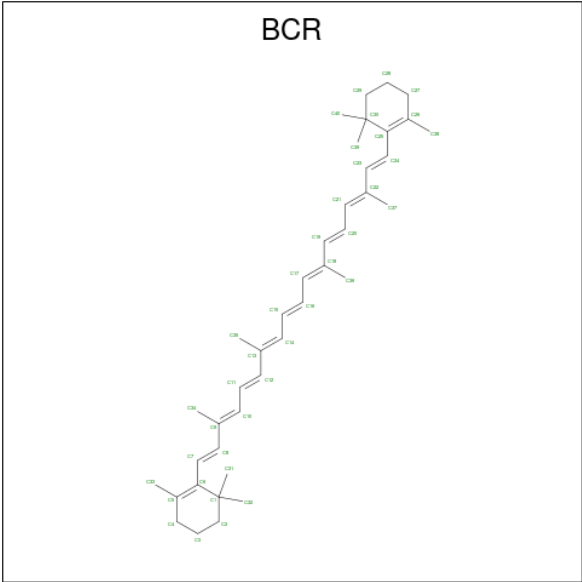
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 26 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



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

- Molecule 27 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



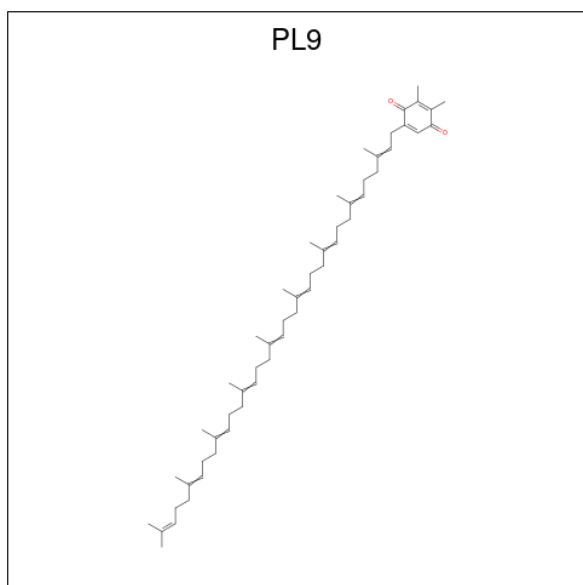
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	C	1	Total C 40 40	0	0
27	C	1	Total C 40 40	0	0
27	C	1	Total C 40 40	0	0
27	D	1	Total C 40 40	0	0
27	H	1	Total C 40 40	0	0
27	K	1	Total C 40 40	0	0
27	T	1	Total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

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

- Molecule 28 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).



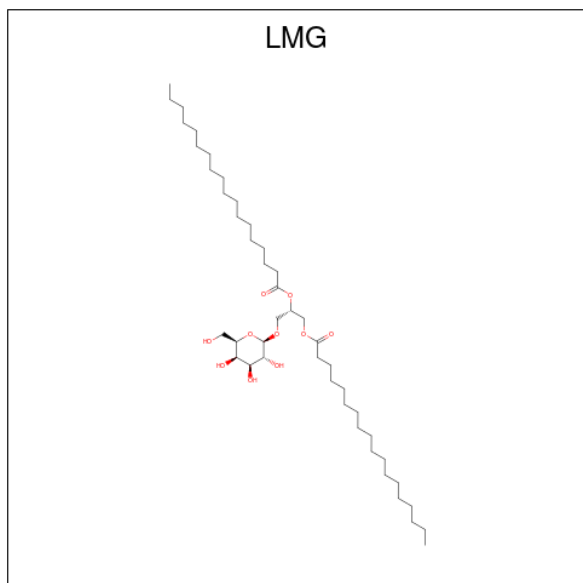
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	A	1	Total C O 55 53 2	0	0
28	D	1	Total C O 55 53 2	0	0

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

- Molecule 29 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



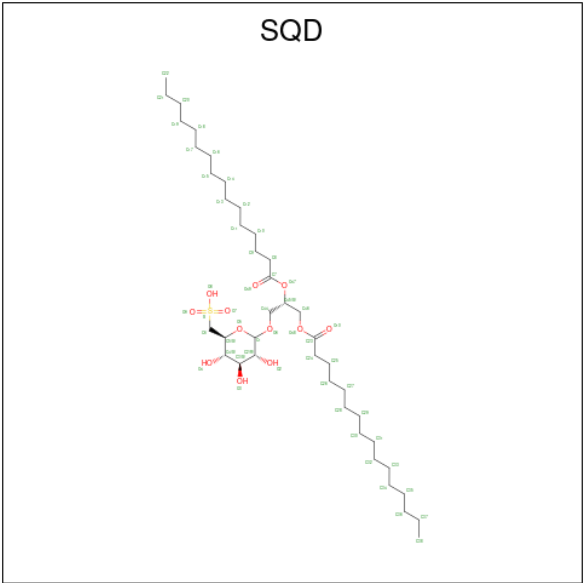
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	A	1	Total	C	O	0	0
			48	38	10		
29	B	1	Total	C	O	0	0
			51	41	10		
29	B	1	Total	C	O	0	0
			28	24	4		
29	C	1	Total	C	O	0	0
			48	38	10		
29	D	1	Total	C	O	0	0
			51	41	10		
29	D	1	Total	C	O	0	0
			33	27	6		
29	b	1	Total	C	O	0	0
			55	45	10		
29	c	1	Total	C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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	c	1	Total	C	O	0	0
			49	39	10		
29	d	1	Total	C	O	0	0
			23	21	2		
29	d	1	Total	C	O	0	0
			44	34	10		
29	m	1	Total	C	O	0	0
			51	41	10		

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



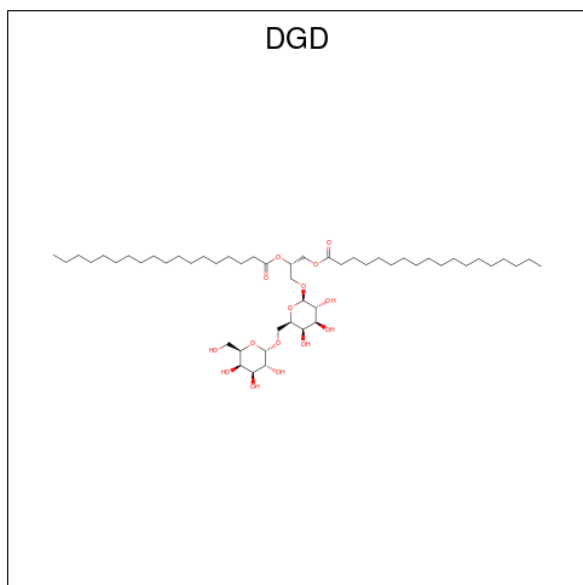
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	A	1	Total	C	O	S	0	0
			52	39	12	1		
30	A	1	Total	C	O		0	0
			39	35	4			
30	B	1	Total	C	O	S	0	0
			54	41	12	1		
30	D	1	Total	C	O	S	0	0
			36	25	10	1		
30	a	1	Total	C	O	S	0	0
			54	41	12	1		
30	a	1	Total	C	O		0	0
			36	31	5			
30	b	1	Total	C	O	S	0	0
			49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

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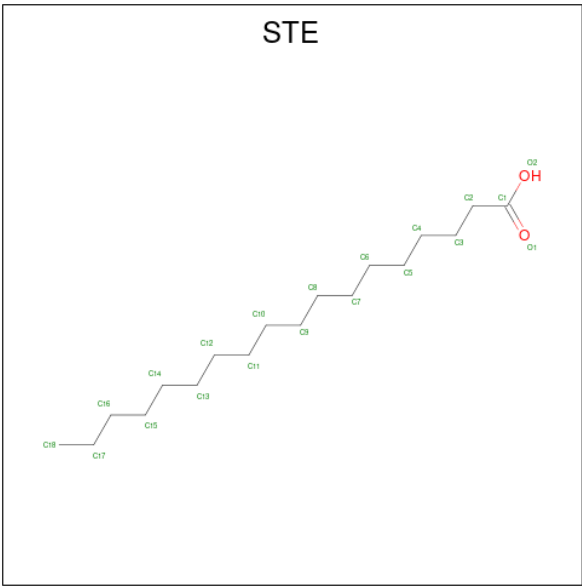
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	f	1	Total	C	O	S	0	0
			41	28	12	1		

- 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	a	1	Total	C	O	0	0
			44	39	5		
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		

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



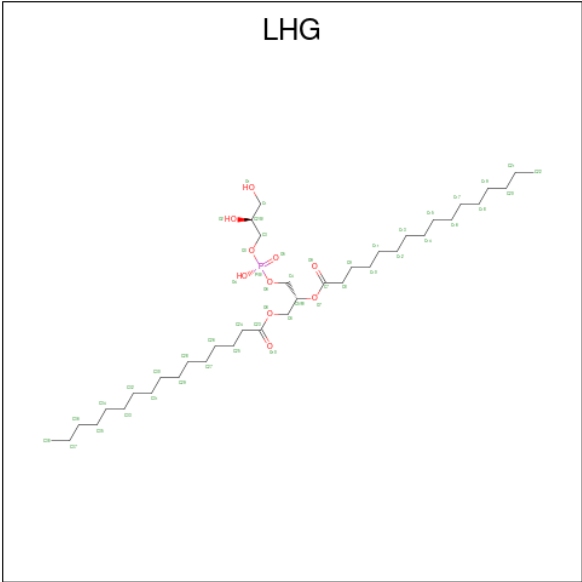
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	B	1	Total	C	O	0	0
			17	15	2		
32	B	1	Total	C	O	0	0
			14	12	2		
32	B	1	Total	C	O	0	0
			12	10	2		
32	B	1	Total	C	O	0	0
			18	16	2		
32	B	1	Total	C	O	0	0
			12	10	2		
32	B	1	Total	C		0	0
			16	16			
32	C	1	Total	C	O	0	0
			12	10	2		
32	C	1	Total	C	O	0	0
			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		

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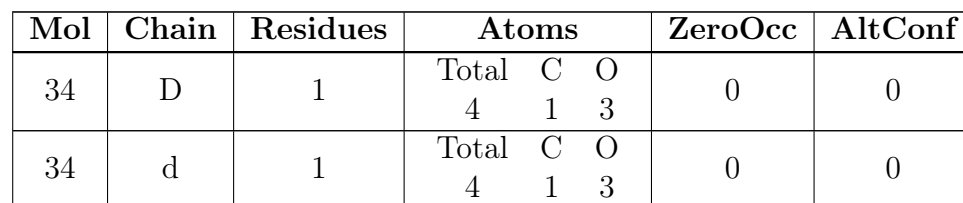
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	M	1	Total C O 15 13 2	0	0
32	M	1	Total C 10 10	0	0
32	T	1	Total C 16 16	0	0
32	T	1	Total C 15 15	0	0
32	X	1	Total C O 20 18 2	0	0
32	a	1	Total C O 12 10 2	0	0
32	b	1	Total C O 20 18 2	0	0
32	b	1	Total C O 16 14 2	0	0
32	b	1	Total C O 20 18 2	0	0
32	b	1	Total 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 10 10	0	0

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	B	1	Total	C	O	P	0	0
			49	38	10	1		
33	D	1	Total	C	O	P	0	0
			49	38	10	1		
33	D	1	Total	C	O	P	0	0
			47	36	10	1		
33	D	1	Total	C	O	P	0	0
			49	38	10	1		
33	E	1	Total	C	O	P	0	0
			49	38	10	1		
33	a	1	Total	C	O	P	0	0
			49	38	10	1		
33	d	1	Total	C	O	P	0	0
			49	38	10	1		
33	d	1	Total	C	O	P	0	0
			39	28	10	1		
33	e	1	Total	C	O	P	0	0
			42	31	10	1		
33	l	1	Total	C	O	P	0	0
			49	38	10	1		

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



- # HEM

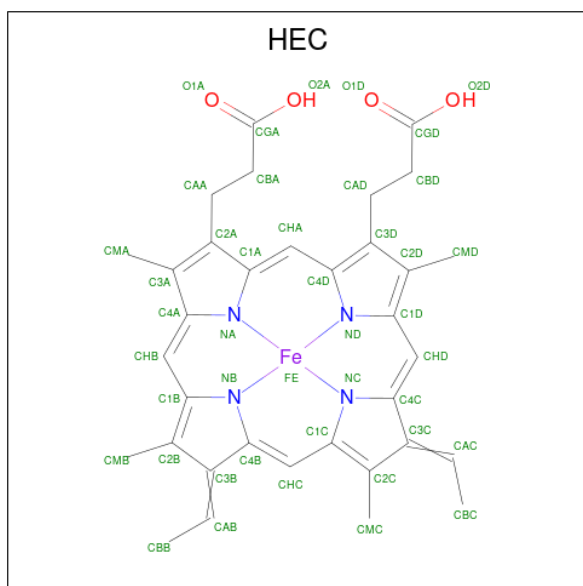
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
35	F	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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

- Molecule 36 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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	144	Total	O	0	4
			152	152		
37	B	218	Total	O	0	0
			218	218		
37	C	183	Total	O	0	0
			183	183		
37	D	124	Total	O	0	0
			124	124		
37	E	37	Total	O	0	0
			37	37		
37	F	6	Total	O	0	0
			6	6		

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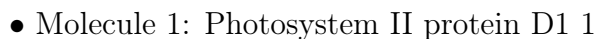
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	H	30	Total 30	O 30	0	0
37	I	8	Total 8	O 8	0	0
37	J	8	Total 8	O 8	0	0
37	K	6	Total 6	O 6	0	0
37	L	10	Total 10	O 10	0	0
37	M	6	Total 6	O 6	0	0
37	O	97	Total 97	O 97	0	0
37	T	15	Total 15	O 15	0	0
37	U	47	Total 47	O 47	0	0
37	V	67	Total 67	O 67	0	0
37	Y	2	Total 2	O 2	0	0
37	X	8	Total 8	O 8	0	0
37	Z	9	Total 9	O 9	0	0
37	R	5	Total 5	O 5	0	0
37	a	133	Total 141	O 141	0	4
37	b	221	Total 221	O 221	0	0
37	c	182	Total 182	O 182	0	0
37	d	123	Total 123	O 123	0	0
37	e	24	Total 24	O 24	0	0
37	f	10	Total 10	O 10	0	0
37	h	19	Total 19	O 19	0	0

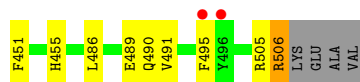
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	i	9	Total 9	O 9	0	0
37	j	10	Total 10	O 10	0	0
37	k	3	Total 3	O 3	0	0
37	l	7	Total 7	O 7	0	0
37	m	9	Total 9	O 9	0	0
37	o	88	Total 88	O 88	0	0
37	t	9	Total 9	O 9	0	0
37	u	61	Total 61	O 61	0	0
37	v	68	Total 68	O 68	0	0
37	y	3	Total 3	O 3	0	0
37	x	5	Total 5	O 5	0	0
37	z	7	Total 7	O 7	0	0

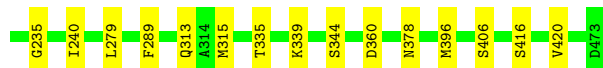
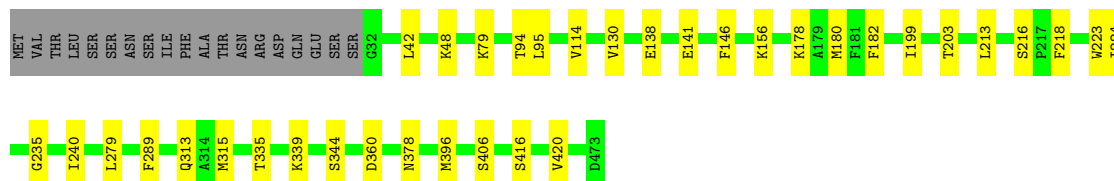
- Molecule 1: Photosystem II protein D1 1





- Molecule 3: Photosystem II CP43 reaction center protein

Chain C: 88% 8% .



- Molecule 3: Photosystem II CP43 reaction center protein

Chain c: 88% 9% ..



- Molecule 4: Photosystem II D2 protein

Chain D: 88% 9% .



- Molecule 4: Photosystem II D2 protein

Chain d: 89% 7% ..

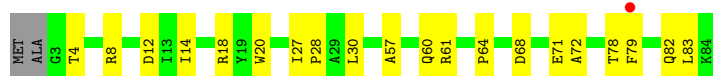
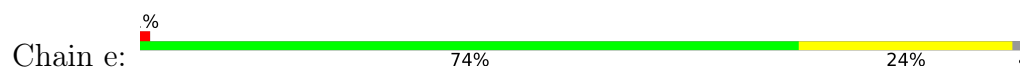


- Molecule 5: Cytochrome b559 subunit alpha

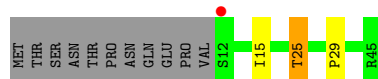
Chain E: 86% 12% .



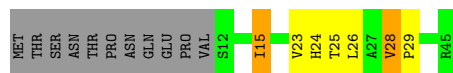
- Molecule 5: Cytochrome b559 subunit alpha



- Molecule 6: Cytochrome b559 subunit beta



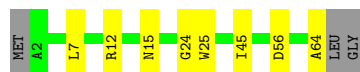
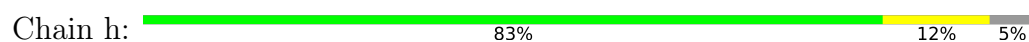
- Molecule 6: Cytochrome b559 subunit beta



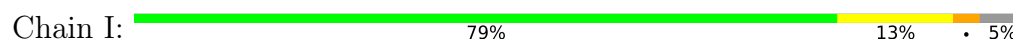
- Molecule 7: Photosystem II reaction center protein H



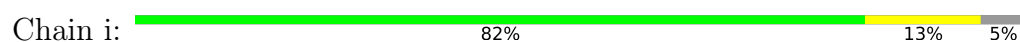
- Molecule 7: Photosystem II reaction center protein H



- Molecule 8: Photosystem II reaction center protein I

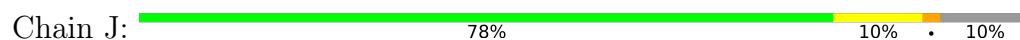


- Molecule 8: Photosystem II reaction center protein I





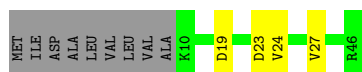
- Molecule 9: Photosystem II reaction center protein J



- Molecule 9: Photosystem II reaction center protein J



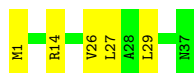
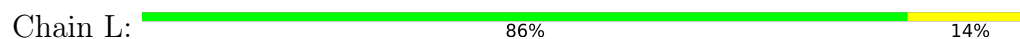
- Molecule 10: Photosystem II reaction center protein K



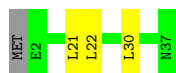
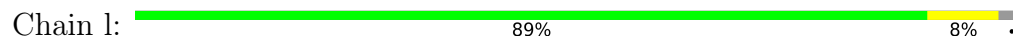
- Molecule 10: Photosystem II reaction center protein K



- Molecule 11: Photosystem II reaction center protein L

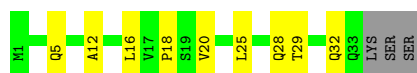


- Molecule 11: Photosystem II reaction center protein L

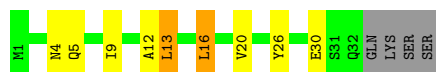


- Molecule 12: Photosystem II reaction center protein M

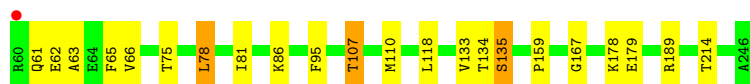
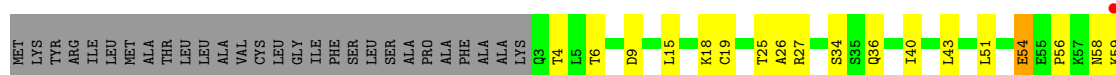
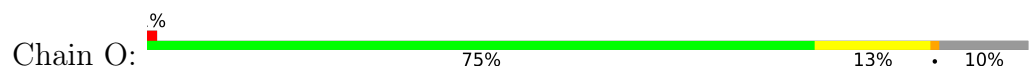




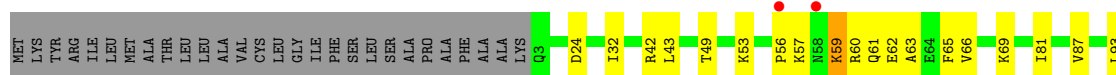
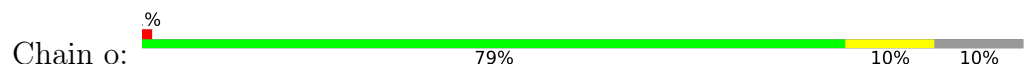
- Molecule 12: Photosystem II reaction center protein M



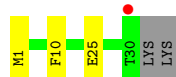
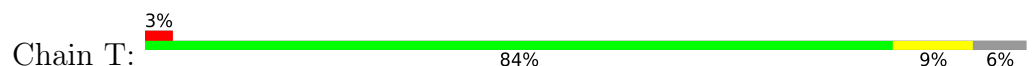
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



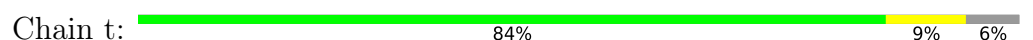
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



- Molecule 14: Photosystem II reaction center protein T

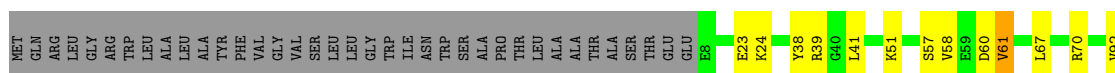


- Molecule 14: Photosystem II reaction center protein T

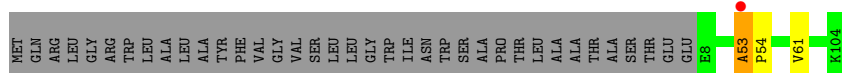


- Molecule 15: Photosystem II 12 kDa extrinsic protein





- Molecule 15: Photosystem II 12 kDa extrinsic protein



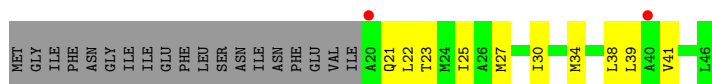
- Molecule 16: Cytochrome c-550



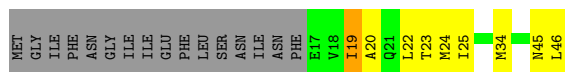
- Molecule 16: Cytochrome c-550



- Molecule 17: Photosystem II reaction center protein Ycf12



- Molecule 17: Photosystem II reaction center protein Ycf12



- Molecule 18: Photosystem II reaction center X protein

Chain X:  78% 12% 7%



- Molecule 18: Photosystem II reaction center X protein

Chain x:  5% 85% 10% 5%



- Molecule 19: Photosystem II reaction center protein Z

Chain Z:  5% 76% 23%



- Molecule 19: Photosystem II reaction center protein Z

Chain z:  2% 84% 16%



- Molecule 20: Photosystem II protein Y

Chain R:  2% 59% 15% 10% 17%



- Molecule 20: Photosystem II protein Y

Chain r:  59% 17% 24%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	117.31Å 222.59Å 308.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.72 – 2.00 19.72 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.72-2.00) 87.7 (19.72-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.47 (at 2.01Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.186 , 0.232 0.186 , 0.233	Depositor DCC
R_{free} test set	4797 reflections (0.76%)	wwPDB-VP
Wilson B-factor (Å ²)	28.7	Xtriage
Anisotropy	0.284	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 50.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	54640	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% 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: LHG, FME, FE2, DGD, STE, PHO, PL9, OEX, BCT, HEC, BCR, OEY, CL, LMG, HEM, SQD, CLA

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	0.28	0/3717	0.45	0/5060
1	a	0.27	0/3714	0.44	0/5056
2	B	0.31	0/4155	0.47	0/5661
2	b	0.31	0/4118	0.49	0/5611
3	C	0.30	0/3711	0.46	0/5051
3	c	0.28	0/3791	0.45	0/5158
4	D	0.34	0/2838	0.50	0/3862
4	d	0.32	0/2847	0.49	0/3874
5	E	0.24	0/688	0.44	0/940
5	e	0.22	0/683	0.42	0/932
6	F	0.27	0/284	0.42	0/387
6	f	0.25	0/284	0.46	0/387
7	H	0.31	0/523	0.45	0/713
7	h	0.28	0/511	0.44	0/697
8	I	0.29	0/293	0.48	0/396
8	i	0.31	0/293	0.42	0/396
9	J	0.25	0/263	0.43	0/356
9	j	0.22	0/263	0.42	0/356
10	K	0.24	0/303	0.39	0/416
10	k	0.24	0/303	0.39	0/416
11	L	0.34	0/311	0.45	0/422
11	l	0.37	0/303	0.50	0/412
12	M	0.29	0/249	0.50	0/341
12	m	0.30	0/244	0.51	0/334
13	O	0.30	0/1904	0.50	0/2585
13	o	0.30	0/1905	0.49	0/2583
14	T	0.34	0/257	0.50	0/349
14	t	0.30	0/255	0.41	0/346
15	U	0.28	0/785	0.47	0/1064
15	u	0.31	0/785	0.49	0/1064
16	V	0.29	0/1085	0.46	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.27	0/1085	0.42	0/1473
17	Y	0.20	0/197	0.34	0/264
17	y	0.19	0/219	0.40	0/294
18	X	0.22	0/284	0.35	0/384
18	x	0.19	0/289	0.27	0/391
19	Z	0.19	0/490	0.41	0/669
19	z	0.15	0/488	0.30	0/666
20	R	0.25	0/277	0.43	0/380
20	r	0.22	0/252	0.35	0/347
All	All	0.29	0/45246	0.46	0/61566

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	3604	0	3445	24	0
1	a	3601	0	3436	27	0
2	B	4005	0	3871	29	0
2	b	3978	0	3836	30	0
3	C	3592	0	3501	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	c	3666	0	3574	26	0
4	D	2745	0	2653	25	0
4	d	2751	0	2659	22	0
5	E	666	0	651	6	0
5	e	664	0	648	16	0
6	F	275	0	282	4	0
6	f	275	0	282	6	0
7	H	510	0	532	4	0
7	h	498	0	518	5	0
8	I	296	0	311	3	0
8	i	296	0	311	4	0
9	J	257	0	268	3	0
9	j	257	0	268	6	0
10	K	293	0	305	3	0
10	k	293	0	305	5	0
11	L	304	0	316	7	0
11	l	296	0	304	1	0
12	M	256	0	269	7	0
12	m	251	0	267	7	0
13	O	1870	0	1830	27	0
13	o	1874	0	1846	17	0
14	T	258	0	261	2	0
14	t	256	0	256	1	0
15	U	774	0	773	6	0
15	u	774	0	773	1	0
16	V	1064	0	1073	12	0
16	v	1064	0	1073	16	0
17	Y	196	0	217	5	0
17	y	218	0	241	4	0
18	X	281	0	312	8	0
18	x	286	0	314	3	0
19	Z	479	0	516	9	0
19	z	477	0	509	4	0
20	R	271	0	298	7	0
20	r	246	0	263	1	0
21	A	20	0	0	0	0
21	a	20	0	0	0	0
22	A	11	0	0	1	0
22	a	11	0	0	1	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	37	0
25	C	839	0	922	18	0
25	D	130	0	144	7	0
25	a	260	0	288	11	0
25	b	1035	0	1139	32	0
25	c	839	0	919	24	0
25	d	130	0	144	2	0
26	A	64	0	74	1	0
26	D	64	0	74	2	0
26	a	64	0	74	0	0
26	d	64	0	74	2	0
27	A	40	0	56	3	0
27	B	120	0	168	7	0
27	C	120	0	168	7	0
27	D	40	0	56	2	0
27	H	40	0	56	2	0
27	K	40	0	56	0	0
27	T	40	0	56	2	0
27	a	40	0	56	1	0
27	b	120	0	168	5	0
27	c	40	0	56	3	0
27	d	40	0	56	1	0
27	k	120	0	168	3	0
27	t	40	0	56	2	0
27	x	40	0	56	2	0
28	A	55	0	80	5	0
28	D	55	0	80	1	0
28	a	55	0	80	7	0
28	d	55	0	80	2	0
29	A	48	0	66	4	0
29	B	79	0	112	2	0
29	C	48	0	66	2	0
29	D	84	0	117	3	0
29	b	55	0	86	1	0
29	c	134	0	181	3	0
29	d	67	0	92	2	0
29	m	51	0	72	3	0
30	A	91	0	136	2	0
30	B	54	0	78	0	0
30	D	36	0	46	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	a	90	0	134	3	0
30	b	49	0	65	1	0
30	f	41	0	49	1	0
31	A	66	0	96	5	0
31	C	186	0	246	4	0
31	H	62	0	82	2	0
31	a	44	0	75	6	0
31	c	186	0	246	6	0
31	h	62	0	82	1	0
32	B	89	0	137	4	0
32	C	40	0	63	1	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	1	0
32	M	25	0	38	1	0
32	T	31	0	60	0	0
32	X	20	0	35	2	0
32	a	12	0	16	0	0
32	b	66	0	110	10	0
32	c	32	0	51	1	0
32	d	37	0	61	2	0
32	j	12	0	16	0	0
32	l	18	0	35	1	0
32	m	12	0	16	0	0
32	t	10	0	16	0	0
33	B	49	0	74	2	0
33	D	145	0	215	5	0
33	E	49	0	74	3	0
33	a	49	0	74	1	0
33	d	88	0	125	5	0
33	e	42	0	57	1	0
33	l	49	0	74	1	0
34	D	4	0	1	1	0
34	d	4	0	1	0	0
35	F	43	0	30	2	0
35	e	43	0	30	4	0
36	V	43	0	30	0	0
36	v	43	0	30	2	0
37	A	152	0	0	3	0
37	B	218	0	0	2	0
37	C	183	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	D	124	0	0	1	0
37	E	37	0	0	1	0
37	F	6	0	0	0	0
37	H	30	0	0	1	0
37	I	8	0	0	0	0
37	J	8	0	0	0	0
37	K	6	0	0	1	0
37	L	10	0	0	0	0
37	M	6	0	0	1	0
37	O	97	0	0	5	0
37	R	5	0	0	0	0
37	T	15	0	0	0	0
37	U	47	0	0	0	0
37	V	67	0	0	2	0
37	X	8	0	0	1	0
37	Y	2	0	0	0	0
37	Z	9	0	0	2	0
37	a	141	0	0	2	0
37	b	221	0	0	0	0
37	c	182	0	0	4	0
37	d	123	0	0	1	0
37	e	24	0	0	0	0
37	f	10	0	0	0	0
37	h	19	0	0	2	0
37	i	9	0	0	1	0
37	j	10	0	0	1	0
37	k	3	0	0	1	0
37	l	7	0	0	0	0
37	m	9	0	0	0	0
37	o	88	0	0	0	0
37	t	9	0	0	0	0
37	u	61	0	0	0	0
37	v	68	0	0	1	0
37	x	5	0	0	0	0
37	y	3	0	0	0	0
37	z	7	0	0	0	0
All	All	54640	0	53863	547	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 547 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)
25:c:501:CLA:H192	25:c:507:CLA:HBB1	1.54	0.90
1:a:102:LEU:HD12	31:a:616:DGD:HB22	1.59	0.81
22:a:602[A]:OEY:O6	22:a:602[A]:OEY:O5	1.97	0.81
13:O:178:LYS:NZ	37:O:301:HOH:O	2.16	0.77
31:A:616:DGD:HE4	2:b:76:SER:HB3	1.67	0.76

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	458/344 (133%)	455 (99%)	2 (0%)	1 (0%)	43	42
1	a	458/344 (133%)	452 (99%)	5 (1%)	1 (0%)	43	42
2	B	507/510 (99%)	500 (99%)	7 (1%)	0	100	100
2	b	503/510 (99%)	492 (98%)	11 (2%)	0	100	100
3	C	461/461 (100%)	453 (98%)	7 (2%)	1 (0%)	43	42
3	c	471/461 (102%)	462 (98%)	8 (2%)	1 (0%)	43	42
4	D	341/352 (97%)	329 (96%)	12 (4%)	0	100	100
4	d	342/352 (97%)	332 (97%)	10 (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%)	60 (95%)	3 (5%)	0	100	100
7	h	61/66 (92%)	57 (93%)	4 (7%)	0	100	100
8	I	34/38 (90%)	32 (94%)	2 (6%)	0	100	100
8	i	34/38 (90%)	32 (94%)	2 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	J	34/40 (85%)	33 (97%)	1 (3%)	0	100	100
9	j	34/40 (85%)	32 (94%)	2 (6%)	0	100	100
10	K	35/46 (76%)	34 (97%)	1 (3%)	0	100	100
10	k	35/46 (76%)	35 (100%)	0	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	34/37 (92%)	34 (100%)	0	0	100	100
12	M	31/36 (86%)	31 (100%)	0	0	100	100
12	m	30/36 (83%)	29 (97%)	1 (3%)	0	100	100
13	O	243/272 (89%)	232 (96%)	7 (3%)	4 (2%)	7	3
13	o	242/272 (89%)	230 (95%)	11 (4%)	1 (0%)	30	27
14	T	28/32 (88%)	28 (100%)	0	0	100	100
14	t	28/32 (88%)	26 (93%)	2 (7%)	0	100	100
15	U	95/134 (71%)	92 (97%)	3 (3%)	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%)	25 (100%)	0	0	100	100
17	y	28/46 (61%)	27 (96%)	1 (4%)	0	100	100
18	X	36/41 (88%)	34 (94%)	2 (6%)	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%)	57 (95%)	3 (5%)	0	100	100
20	R	32/41 (78%)	30 (94%)	2 (6%)	0	100	100
20	r	29/41 (71%)	28 (97%)	0	1 (3%)	3	1
All	All	5534/5700 (97%)	5398 (98%)	124 (2%)	12 (0%)	43	42

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	V	64	PRO
3	C	416	SER
3	c	416	SER
15	u	53	ALA
13	O	59	LYS

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	374/280 (134%)	369 (99%)	5 (1%)	61	68
1	a	373/280 (133%)	362 (97%)	11 (3%)	37	40
2	B	407/407 (100%)	401 (98%)	6 (2%)	57	64
2	b	402/407 (99%)	397 (99%)	5 (1%)	63	70
3	C	361/362 (100%)	356 (99%)	5 (1%)	59	66
3	c	370/362 (102%)	357 (96%)	13 (4%)	32	32
4	D	278/283 (98%)	275 (99%)	3 (1%)	65	73
4	d	279/283 (99%)	272 (98%)	7 (2%)	42	45
5	E	72/73 (99%)	69 (96%)	3 (4%)	26	25
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%)	25 (89%)	3 (11%)	6	4
7	H	54/55 (98%)	54 (100%)	0	100	100
7	h	53/55 (96%)	51 (96%)	2 (4%)	29	29
8	I	32/34 (94%)	30 (94%)	2 (6%)	16	13
8	i	32/34 (94%)	32 (100%)	0	100	100
9	J	24/28 (86%)	23 (96%)	1 (4%)	26	25
9	j	24/28 (86%)	23 (96%)	1 (4%)	26	25
10	K	30/37 (81%)	29 (97%)	1 (3%)	33	34
10	k	30/37 (81%)	24 (80%)	6 (20%)	1	0
11	L	35/35 (100%)	35 (100%)	0	100	100
11	l	34/35 (97%)	32 (94%)	2 (6%)	18	14
12	M	28/32 (88%)	27 (96%)	1 (4%)	31	31
12	m	28/32 (88%)	25 (89%)	3 (11%)	6	4
13	O	206/228 (90%)	198 (96%)	8 (4%)	28	28
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%)	83 (99%)	1 (1%)	63	70
16	V	117/138 (85%)	115 (98%)	2 (2%)	53	60
16	v	117/138 (85%)	113 (97%)	4 (3%)	32	33
17	Y	19/37 (51%)	17 (90%)	2 (10%)	6	4
17	y	22/37 (60%)	18 (82%)	4 (18%)	2	1
18	X	31/34 (91%)	30 (97%)	1 (3%)	34	35
18	x	31/34 (91%)	30 (97%)	1 (3%)	34	35
19	Z	52/52 (100%)	47 (90%)	5 (10%)	8	5
19	z	51/52 (98%)	45 (88%)	6 (12%)	5	3
20	R	28/33 (85%)	23 (82%)	5 (18%)	2	1
20	r	25/33 (76%)	21 (84%)	4 (16%)	2	1
All	All	4572/4654 (98%)	4434 (97%)	138 (3%)	35	38

5 of 138 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	o	118	LEU
16	v	19	ILE
19	z	20	VAL
19	Z	46	LEU
19	Z	35	ARG

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

Mol	Chain	Res	Type
12	m	5	GLN
13	o	231	HIS
20	r	30	GLN
18	X	38	GLN
16	V	86	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	FME	M	1	12	8,9,10	1.05	0	8,9,11	1.03	0
8	FME	i	1	8	8,9,10	1.05	0	8,9,11	1.16	1 (12%)
12	FME	m	1	12	8,9,10	0.99	0	8,9,11	0.69	0
14	FME	t	1	14	8,9,10	0.97	0	8,9,11	1.27	1 (12%)
14	FME	T	1	14	8,9,10	1.16	1 (12%)	8,9,11	1.06	0
8	FME	I	1	8	8,9,10	1.01	0	8,9,11	1.13	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	FME	M	1	12	-	5/7/9/11	-
8	FME	i	1	8	-	0/7/9/11	-
12	FME	m	1	12	-	0/7/9/11	-
14	FME	t	1	14	-	2/7/9/11	-
14	FME	T	1	14	-	2/7/9/11	-
8	FME	I	1	8	-	0/7/9/11	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	T	1	FME	CA-N	-2.24	1.43	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	i	1	FME	CA-N-CN	-2.39	119.14	122.82
14	t	1	FME	CB-CA-N	2.22	114.56	110.52

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 190 ligands modelled in this entry, 6 are monoatomic - leaving 184 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	604	-	69,73,73	1.08	6 (8%)	82,113,113	1.43	11 (13%)
25	CLA	C	510	-	69,73,73	1.16	7 (10%)	82,113,113	1.35	8 (9%)
25	CLA	B	604	-	69,73,73	1.31	7 (10%)	82,113,113	1.51	10 (12%)
33	LHG	B	623	-	48,48,48	0.75	1 (2%)	51,54,54	1.17	3 (5%)
27	BCR	t	101	-	41,41,41	1.01	2 (4%)	56,56,56	1.37	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	OEX	a	601[C]	1,37,3	0,15,15	-	-	-		
31	DGD	C	519	-	63,63,67	0.81	2 (3%)	77,77,81	1.36	7 (9%)
32	STE	B	625	-	13,13,19	0.69	0	13,13,19	1.26	2 (15%)
33	LHG	E	101	-	48,48,48	0.75	2 (4%)	51,54,54	1.23	6 (11%)
25	CLA	c	510	-	69,73,73	1.33	7 (10%)	82,113,113	1.25	5 (6%)
29	LMG	c	520	-	48,48,55	0.91	3 (6%)	56,56,63	1.29	8 (14%)
22	OEY	a	602[A]	1,37,3	0,16,16	-	-	-		
32	STE	E	102	-	11,11,19	0.76	0	11,11,19	1.13	1 (9%)
27	BCR	d	405	-	41,41,41	1.06	2 (4%)	56,56,56	1.22	6 (10%)
32	STE	I	101	-	14,14,19	0.36	0	13,13,19	0.83	0
32	STE	j	101	-	11,11,19	0.73	0	11,11,19	1.23	2 (18%)
30	SQD	a	615	-	35,35,54	1.73	5 (14%)	37,37,65	1.46	5 (13%)
25	CLA	b	615	-	69,73,73	1.40	7 (10%)	82,113,113	1.28	8 (9%)
21	OEX	A	601[C]	1,37,3	0,15,15	-	-	-		
27	BCR	x	101	-	41,41,41	0.97	2 (4%)	56,56,56	1.25	6 (10%)
32	STE	B	629	-	15,15,19	0.34	0	14,14,19	0.80	0
27	BCR	k	102	-	41,41,41	1.09	3 (7%)	56,56,56	1.07	3 (5%)
27	BCR	b	617	-	41,41,41	0.95	2 (4%)	56,56,56	1.29	6 (10%)
21	OEX	a	601[B]	1,37,3	0,15,15	-	-	-		
33	LHG	D	412	-	48,48,48	0.80	1 (2%)	51,54,54	1.32	6 (11%)
25	CLA	c	504	37	64,68,73	1.25	7 (10%)	76,107,113	1.25	8 (10%)
25	CLA	B	605	-	69,73,73	1.21	6 (8%)	82,113,113	1.29	7 (8%)
32	STE	B	627	-	17,17,19	0.64	0	17,17,19	1.21	1 (5%)
27	BCR	B	618	-	41,41,41	1.04	2 (4%)	56,56,56	1.19	4 (7%)
25	CLA	B	602	-	69,73,73	1.25	6 (8%)	82,113,113	1.36	10 (12%)
27	BCR	C	515	-	41,41,41	1.07	2 (4%)	56,56,56	1.17	4 (7%)
29	LMG	b	622	-	55,55,55	0.71	2 (3%)	63,63,63	1.36	9 (14%)
32	STE	C	522	-	11,11,19	0.69	0	11,11,19	1.22	1 (9%)
32	STE	b	624	-	19,19,19	0.64	0	19,19,19	1.09	1 (5%)
25	CLA	b	610	37	69,73,73	1.23	7 (10%)	82,113,113	1.41	7 (8%)
26	PHO	D	402	-	58,69,69	2.03	10 (17%)	55,99,99	1.46	9 (16%)
25	CLA	C	504	37	63,67,73	1.22	7 (11%)	74,105,113	1.29	7 (9%)
30	SQD	B	624	-	52,54,54	1.58	10 (19%)	62,65,65	1.70	10 (16%)
33	LHG	d	408	-	38,38,48	0.81	1 (2%)	41,44,54	1.19	4 (9%)
27	BCR	C	514	-	41,41,41	1.02	2 (4%)	56,56,56	1.22	6 (10%)
30	SQD	A	614	-	50,52,54	1.59	7 (14%)	60,63,65	1.91	12 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	OEX	A	601[B]	1,37,3	0,15,15	-	-	-		
25	CLA	C	505	-	69,73,73	1.37	8 (11%)	82,113,113	1.42	9 (10%)
32	STE	J	101	-	11,11,19	0.74	0	11,11,19	1.13	0
29	LMG	m	101	-	51,51,55	0.73	0	59,59,63	1.41	9 (15%)
32	STE	T	102	-	15,15,19	0.33	0	14,14,19	0.91	0
31	DGD	c	515	-	63,63,67	0.95	3 (4%)	77,77,81	1.42	11 (14%)
28	PL9	a	611	-	55,55,55	0.78	2 (3%)	68,69,69	1.60	11 (16%)
31	DGD	C	518	-	63,63,67	1.06	4 (6%)	77,77,81	1.35	10 (12%)
36	HEC	v	201	16	46,50,50	1.91	7 (15%)	58,82,82	1.88	7 (12%)
27	BCR	D	405	-	41,41,41	1.07	3 (7%)	56,56,56	1.19	4 (7%)
25	CLA	c	501	-	69,73,73	1.20	8 (11%)	82,113,113	1.35	9 (10%)
25	CLA	c	506	-	69,73,73	1.18	7 (10%)	82,113,113	1.27	4 (4%)
25	CLA	B	601	37	69,73,73	1.37	8 (11%)	82,113,113	1.39	7 (8%)
33	LHG	e	102	-	41,41,48	0.72	1 (2%)	44,47,54	1.30	6 (13%)
31	DGD	C	517	-	63,63,67	1.00	5 (7%)	77,77,81	1.36	9 (11%)
25	CLA	B	606	-	69,73,73	1.38	6 (8%)	82,113,113	1.43	6 (7%)
25	CLA	c	503	-	69,73,73	1.24	10 (14%)	82,113,113	1.38	7 (8%)
25	CLA	C	506	-	69,73,73	1.43	9 (13%)	82,113,113	1.24	7 (8%)
25	CLA	A	612	37	69,73,73	1.38	7 (10%)	82,113,113	1.24	7 (8%)
32	STE	B	621	-	16,16,19	0.70	0	16,16,19	1.06	0
36	HEC	V	201	16	46,50,50	1.86	6 (13%)	58,82,82	2.01	8 (13%)
25	CLA	B	612	-	69,73,73	1.09	5 (7%)	82,113,113	1.35	11 (13%)
28	PL9	d	406	-	55,55,55	1.05	3 (5%)	68,69,69	1.64	13 (19%)
25	CLA	C	503	-	69,73,73	1.53	9 (13%)	82,113,113	1.44	5 (6%)
25	CLA	B	610	37	69,73,73	1.13	7 (10%)	82,113,113	1.28	7 (8%)
25	CLA	C	502	-	69,73,73	1.21	7 (10%)	82,113,113	1.20	7 (8%)
32	STE	c	521	-	11,11,19	0.77	0	11,11,19	1.08	0
26	PHO	a	608	-	58,69,69	2.12	10 (17%)	55,99,99	1.43	9 (16%)
30	SQD	f	101	-	39,41,54	1.67	7 (17%)	49,52,65	1.66	10 (20%)
31	DGD	c	517	-	63,63,67	0.86	2 (3%)	77,77,81	1.30	6 (7%)
25	CLA	b	608	-	69,73,73	1.36	8 (11%)	82,113,113	1.41	11 (13%)
30	SQD	a	614	-	52,54,54	1.59	7 (13%)	62,65,65	1.78	11 (17%)
29	LMG	d	410	-	44,44,55	0.82	1 (2%)	52,52,63	1.30	6 (11%)
29	LMG	c	522	-	49,49,55	0.88	4 (8%)	57,57,63	1.28	6 (10%)
29	LMG	B	622	-	26,26,55	0.69	2 (7%)	26,26,63	1.27	1 (3%)
25	CLA	C	513	-	69,73,73	1.31	7 (10%)	82,113,113	1.40	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	b	607	37	69,73,73	1.19	5 (7%)	82,113,113	1.19	7 (8%)
25	CLA	D	403	-	69,73,73	1.07	5 (7%)	82,113,113	1.20	11 (13%)
32	STE	b	623	-	15,15,19	0.72	0	15,15,19	0.99	0
27	BCR	k	103	-	41,41,41	1.05	2 (4%)	56,56,56	1.14	5 (8%)
35	HEM	F	101	6,5	50,50,50	1.42	8 (16%)	67,82,82	1.09	2 (2%)
25	CLA	B	603	-	69,73,73	1.10	7 (10%)	82,113,113	1.31	9 (10%)
25	CLA	C	512	-	69,73,73	1.29	9 (13%)	82,113,113	1.30	9 (10%)
31	DGD	A	616	-	67,67,67	0.97	4 (5%)	81,81,81	1.32	12 (14%)
32	STE	c	519	-	19,19,19	0.61	0	19,19,19	1.00	0
27	BCR	a	610	-	41,41,41	0.98	2 (4%)	56,56,56	1.15	2 (3%)
25	CLA	b	602	-	69,73,73	1.13	7 (10%)	82,113,113	1.29	6 (7%)
25	CLA	c	508	-	68,72,73	1.30	8 (11%)	80,111,113	1.25	6 (7%)
32	STE	d	412	-	19,19,19	0.56	0	19,19,19	1.21	1 (5%)
32	STE	a	617	-	11,11,19	0.81	0	11,11,19	0.99	0
25	CLA	c	502	-	69,73,73	1.20	8 (11%)	82,113,113	1.28	8 (9%)
35	HEM	e	101	6,5	50,50,50	1.47	8 (16%)	67,82,82	1.30	8 (11%)
25	CLA	b	612	-	69,73,73	1.13	9 (13%)	82,113,113	1.31	11 (13%)
25	CLA	C	507	37	69,73,73	1.15	7 (10%)	82,113,113	1.42	7 (8%)
25	CLA	a	612	37	69,73,73	1.28	6 (8%)	82,113,113	1.32	9 (10%)
29	LMG	D	407	-	51,51,55	0.80	3 (5%)	59,59,63	1.38	6 (10%)
31	DGD	H	102	-	63,63,67	1.05	4 (6%)	77,77,81	1.39	10 (12%)
29	LMG	B	620	-	51,51,55	0.81	1 (1%)	59,59,63	1.38	7 (11%)
32	STE	l	102	-	17,17,19	0.29	0	16,16,19	0.96	0
27	BCR	b	619	-	41,41,41	0.97	2 (4%)	56,56,56	1.16	3 (5%)
32	STE	d	411	-	16,16,19	0.54	0	16,16,19	1.34	2 (12%)
32	STE	T	103	-	14,14,19	0.36	0	13,13,19	0.82	0
27	BCR	c	514	-	41,41,41	1.15	2 (4%)	56,56,56	1.22	6 (10%)
27	BCR	b	618	-	41,41,41	1.11	3 (7%)	56,56,56	1.17	5 (8%)
27	BCR	B	619	-	41,41,41	1.00	2 (4%)	56,56,56	1.26	4 (7%)
29	LMG	C	520	-	48,48,55	0.74	2 (4%)	56,56,63	1.38	8 (14%)
33	LHG	l	101	-	48,48,48	0.60	0	51,54,54	1.18	6 (11%)
25	CLA	B	616	-	64,68,73	1.40	6 (9%)	76,107,113	1.40	6 (7%)
32	STE	C	523	-	15,15,19	0.34	0	14,14,19	0.87	0
32	STE	C	521	-	11,11,19	0.67	0	11,11,19	1.59	2 (18%)
32	STE	B	626	-	11,11,19	0.79	0	11,11,19	1.11	0
25	CLA	b	609	-	69,73,73	1.28	9 (13%)	82,113,113	1.32	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	c	513	-	69,73,73	1.22	8 (11%)	82,113,113	1.25	8 (9%)
25	CLA	b	601	37	69,73,73	1.29	7 (10%)	82,113,113	1.39	7 (8%)
32	STE	B	628	-	11,11,19	0.77	0	11,11,19	1.17	1 (9%)
26	PHO	d	402	-	58,69,69	2.14	11 (18%)	55,99,99	1.48	8 (14%)
25	CLA	b	603	-	69,73,73	1.13	7 (10%)	82,113,113	1.39	10 (12%)
34	BCT	D	401	23	3,3,3	1.13	0	2,3,3	3.21	1 (50%)
25	CLA	b	611	-	69,73,73	1.30	6 (8%)	82,113,113	1.37	9 (10%)
26	PHO	A	608	-	58,69,69	1.94	8 (13%)	55,99,99	1.47	8 (14%)
25	CLA	c	505	-	69,73,73	1.08	7 (10%)	82,113,113	1.19	6 (7%)
25	CLA	A	606	-	69,73,73	1.22	8 (11%)	82,113,113	1.27	5 (6%)
28	PL9	A	611	-	55,55,55	0.64	0	68,69,69	1.53	10 (14%)
33	LHG	d	407	-	48,48,48	0.70	2 (4%)	51,54,54	1.24	6 (11%)
25	CLA	A	609	-	58,62,73	1.23	5 (8%)	68,99,113	1.40	6 (8%)
25	CLA	c	507	37	69,73,73	1.28	9 (13%)	82,113,113	1.35	9 (10%)
32	STE	M	102	-	9,9,19	0.34	0	8,8,19	0.86	0
25	CLA	b	606	-	69,73,73	1.40	7 (10%)	82,113,113	1.48	6 (7%)
25	CLA	b	613	-	69,73,73	1.26	6 (8%)	82,113,113	1.44	11 (13%)
32	STE	b	625	-	9,9,19	0.31	0	8,8,19	0.80	0
29	LMG	c	518	-	37,37,55	0.93	2 (5%)	45,45,63	1.35	6 (13%)
25	CLA	a	607	37	69,73,73	1.24	8 (11%)	82,113,113	1.24	6 (7%)
29	LMG	d	409	-	21,21,55	0.53	1 (4%)	20,20,63	1.26	2 (10%)
22	OEY	A	602[A]	1,37,3	0,16,16	-	-	-	-	-
25	CLA	B	607	37	69,73,73	1.32	8 (11%)	82,113,113	1.16	6 (7%)
30	SQD	D	408	-	34,36,54	1.49	5 (14%)	42,45,65	1.58	9 (21%)
25	CLA	B	613	-	69,73,73	1.31	8 (11%)	82,113,113	1.35	7 (8%)
27	BCR	H	101	-	41,41,41	0.97	1 (2%)	56,56,56	1.23	6 (10%)
25	CLA	a	606	-	69,73,73	1.38	9 (13%)	82,113,113	1.20	9 (10%)
27	BCR	B	617	-	41,41,41	1.01	3 (7%)	56,56,56	1.18	6 (10%)
32	STE	b	621	-	19,19,19	0.59	0	19,19,19	1.06	0
32	STE	X	101	-	19,19,19	0.57	0	19,19,19	1.16	0
32	STE	M	101	-	14,14,19	0.72	0	14,14,19	1.02	0
34	BCT	d	401	23	3,3,3	1.14	0	2,3,3	3.17	1 (50%)
27	BCR	K	101	-	41,41,41	1.05	2 (4%)	56,56,56	1.11	4 (7%)
31	DGD	h	101	-	63,63,67	0.93	5 (7%)	77,77,81	1.42	13 (16%)
25	CLA	d	404	-	69,73,73	1.15	6 (8%)	82,113,113	1.15	4 (4%)
25	CLA	B	609	-	69,73,73	1.29	10 (14%)	82,113,113	1.37	9 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	b	605	-	69,73,73	1.22	6 (8%)	82,113,113	1.32	6 (7%)
25	CLA	c	511	3	69,73,73	1.44	6 (8%)	82,113,113	1.46	4 (4%)
25	CLA	c	512	-	69,73,73	1.25	7 (10%)	82,113,113	1.34	7 (8%)
27	BCR	T	101	-	41,41,41	0.97	2 (4%)	56,56,56	1.26	8 (14%)
31	DGD	a	616	-	43,43,67	0.71	2 (4%)	45,45,81	1.37	7 (15%)
25	CLA	b	614	-	69,73,73	1.21	6 (8%)	82,113,113	1.25	7 (8%)
32	STE	H	103	-	17,17,19	0.36	0	16,16,19	0.76	0
32	STE	m	102	-	11,11,19	0.71	0	11,11,19	1.41	2 (18%)
33	LHG	a	613	-	48,48,48	0.75	3 (6%)	51,54,54	1.31	7 (13%)
29	LMG	D	411	-	31,31,55	0.63	1 (3%)	33,33,63	1.26	2 (6%)
31	DGD	c	516	-	63,63,67	1.01	5 (7%)	77,77,81	1.31	9 (11%)
25	CLA	B	614	-	69,73,73	1.24	5 (7%)	82,113,113	1.32	6 (7%)
25	CLA	C	511	3	69,73,73	1.29	6 (8%)	82,113,113	1.44	7 (8%)
25	CLA	d	403	-	69,73,73	1.19	7 (10%)	82,113,113	1.30	9 (10%)
25	CLA	C	509	-	69,73,73	1.22	8 (11%)	82,113,113	1.31	7 (8%)
27	BCR	A	610	-	41,41,41	0.96	3 (7%)	56,56,56	1.20	3 (5%)
29	LMG	A	613	-	48,48,55	0.75	0	56,56,63	1.37	6 (10%)
25	CLA	a	609	-	69,73,73	1.18	6 (8%)	82,113,113	1.26	6 (7%)
25	CLA	c	509	-	69,73,73	1.12	4 (5%)	82,113,113	1.41	7 (8%)
25	CLA	C	501	-	69,73,73	1.29	7 (10%)	82,113,113	1.32	6 (7%)
33	LHG	D	409	-	48,48,48	0.75	2 (4%)	51,54,54	1.25	7 (13%)
30	SQD	A	615	-	38,38,54	1.76	5 (13%)	40,40,65	1.22	2 (5%)
30	SQD	b	620	-	47,49,54	1.60	8 (17%)	57,60,65	1.71	10 (17%)
28	PL9	D	406	-	55,55,55	0.98	1 (1%)	68,69,69	1.55	13 (19%)
25	CLA	C	508	-	69,73,73	1.17	8 (11%)	82,113,113	1.42	9 (10%)
25	CLA	B	615	-	69,73,73	1.45	8 (11%)	82,113,113	1.30	6 (7%)
25	CLA	D	404	-	69,73,73	1.24	7 (10%)	82,113,113	1.29	7 (8%)
25	CLA	A	607	37	69,73,73	1.12	8 (11%)	82,113,113	1.28	8 (9%)
32	STE	t	102	-	9,9,19	0.37	0	8,8,19	0.74	0
27	BCR	C	516	-	41,41,41	1.05	2 (4%)	56,56,56	1.10	3 (5%)
27	BCR	k	101	-	41,41,41	1.09	2 (4%)	56,56,56	1.31	10 (17%)
25	CLA	B	608	-	69,73,73	1.13	6 (8%)	82,113,113	1.31	9 (10%)
33	LHG	D	410	-	46,46,48	0.95	2 (4%)	49,52,54	1.31	5 (10%)
25	CLA	B	611	-	69,73,73	1.22	6 (8%)	82,113,113	1.31	5 (6%)
25	CLA	b	616	-	64,68,73	1.19	6 (9%)	76,107,113	1.31	8 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	b	604	-	1/1/15/20	9/39/115/115	-
25	CLA	C	510	-	1/1/15/20	5/39/115/115	-
25	CLA	B	604	-	1/1/15/20	8/39/115/115	-
33	LHG	B	623	-	-	25/53/53/53	-
27	BCR	t	101	-	-	5/29/63/63	0/2/2/2
31	DGD	C	519	-	-	16/51/91/95	0/2/2/2
32	STE	B	625	-	-	3/11/11/17	-
33	LHG	E	101	-	-	18/53/53/53	-
25	CLA	c	510	-	1/1/15/20	9/39/115/115	-
29	LMG	c	520	-	-	23/43/63/70	0/1/1/1
32	STE	E	102	-	-	3/9/9/17	-
27	BCR	d	405	-	-	4/29/63/63	0/2/2/2
32	STE	I	101	-	-	4/12/12/17	-
32	STE	j	101	-	-	5/9/9/17	-
30	SQD	a	615	-	-	16/37/37/69	-
25	CLA	b	615	-	1/1/15/20	11/39/115/115	-
27	BCR	x	101	-	-	7/29/63/63	0/2/2/2
32	STE	B	629	-	-	7/13/13/17	-
27	BCR	k	102	-	-	6/29/63/63	0/2/2/2
27	BCR	b	617	-	-	3/29/63/63	0/2/2/2
33	LHG	D	412	-	-	13/53/53/53	-
25	CLA	c	504	37	1/1/14/20	7/33/109/115	-
25	CLA	B	605	-	1/1/15/20	6/39/115/115	-
32	STE	B	627	-	-	8/15/15/17	-
27	BCR	B	618	-	-	3/29/63/63	0/2/2/2
25	CLA	B	602	-	1/1/15/20	6/39/115/115	-
27	BCR	C	515	-	-	4/29/63/63	0/2/2/2
29	LMG	b	622	-	-	28/50/70/70	0/1/1/1
32	STE	C	522	-	-	4/9/9/17	-
32	STE	b	624	-	-	8/17/17/17	-
25	CLA	b	610	37	1/1/15/20	5/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PHO	D	402	-	-	2/37/103/103	0/5/6/6
25	CLA	C	504	37	1/1/13/20	9/32/108/115	-
30	SQD	B	624	-	-	23/49/69/69	0/1/1/1
33	LHG	d	408	-	-	13/43/43/53	-
27	BCR	C	514	-	-	0/29/63/63	0/2/2/2
30	SQD	A	614	-	-	20/47/67/69	0/1/1/1
25	CLA	C	505	-	1/1/15/20	13/39/115/115	-
32	STE	J	101	-	-	5/9/9/17	-
29	LMG	m	101	-	-	18/46/66/70	0/1/1/1
32	STE	T	102	-	-	8/13/13/17	-
31	DGD	c	515	-	-	28/51/91/95	0/2/2/2
28	PL9	a	611	-	-	22/53/73/73	0/1/1/1
31	DGD	C	518	-	-	19/51/91/95	0/2/2/2
36	HEC	v	201	16	-	6/14/54/54	-
27	BCR	D	405	-	-	5/29/63/63	0/2/2/2
25	CLA	c	501	-	1/1/15/20	4/39/115/115	-
25	CLA	c	506	-	1/1/15/20	14/39/115/115	-
25	CLA	B	601	37	1/1/15/20	17/39/115/115	-
33	LHG	e	102	-	-	27/46/46/53	-
31	DGD	C	517	-	-	22/51/91/95	0/2/2/2
25	CLA	B	606	-	1/1/15/20	15/39/115/115	-
25	CLA	c	503	-	1/1/15/20	9/39/115/115	-
25	CLA	C	506	-	1/1/15/20	11/39/115/115	-
25	CLA	A	612	37	-	4/39/115/115	-
32	STE	B	621	-	-	6/14/14/17	-
36	HEC	V	201	16	-	6/14/54/54	-
25	CLA	B	612	-	1/1/15/20	7/39/115/115	-
28	PL9	d	406	-	-	8/53/73/73	0/1/1/1
25	CLA	C	503	-	-	3/39/115/115	-
25	CLA	B	610	37	1/1/15/20	6/39/115/115	-
25	CLA	C	502	-	-	9/39/115/115	-
32	STE	c	521	-	-	4/9/9/17	-
26	PHO	a	608	-	-	2/37/103/103	0/5/6/6
30	SQD	f	101	-	-	17/36/56/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	DGD	c	517	-	-	17/51/91/95	0/2/2/2
25	CLA	b	608	-	1/1/15/20	4/39/115/115	-
30	SQD	a	614	-	-	21/49/69/69	0/1/1/1
29	LMG	d	410	-	-	9/39/59/70	0/1/1/1
29	LMG	c	522	-	-	26/44/64/70	0/1/1/1
29	LMG	B	622	-	-	10/22/22/70	-
25	CLA	C	513	-	1/1/15/20	12/39/115/115	-
25	CLA	b	607	37	1/1/15/20	13/39/115/115	-
25	CLA	D	403	-	1/1/15/20	8/39/115/115	-
32	STE	b	623	-	-	6/13/13/17	-
27	BCR	k	103	-	-	4/29/63/63	0/2/2/2
35	HEM	F	101	6,5	-	3/14/54/54	-
25	CLA	B	603	-	1/1/15/20	10/39/115/115	-
25	CLA	C	512	-	1/1/15/20	13/39/115/115	-
31	DGD	A	616	-	-	27/55/95/95	0/2/2/2
32	STE	c	519	-	-	9/17/17/17	-
27	BCR	a	610	-	-	0/29/63/63	0/2/2/2
25	CLA	b	602	-	1/1/15/20	4/39/115/115	-
25	CLA	c	508	-	-	4/38/114/115	-
32	STE	d	412	-	-	9/17/17/17	-
32	STE	a	617	-	-	4/9/9/17	-
25	CLA	c	502	-	-	3/39/115/115	-
35	HEM	e	101	6,5	-	5/14/54/54	-
25	CLA	b	612	-	1/1/15/20	5/39/115/115	-
25	CLA	C	507	37	1/1/15/20	9/39/115/115	-
25	CLA	a	612	37	1/1/15/20	0/39/115/115	-
29	LMG	D	407	-	-	14/46/66/70	0/1/1/1
31	DGD	H	102	-	-	20/51/91/95	0/2/2/2
29	LMG	B	620	-	-	25/46/66/70	0/1/1/1
32	STE	l	102	-	-	6/15/15/17	-
27	BCR	b	619	-	-	2/29/63/63	0/2/2/2
32	STE	d	411	-	-	8/14/14/17	-
32	STE	T	103	-	-	9/12/12/17	-
27	BCR	c	514	-	-	3/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	BCR	b	618	-	-	2/29/63/63	0/2/2/2
27	BCR	B	619	-	-	6/29/63/63	0/2/2/2
29	LMG	C	520	-	-	19/43/63/70	0/1/1/1
33	LHG	l	101	-	-	19/53/53/53	-
25	CLA	B	616	-	1/1/14/20	10/33/109/115	-
32	STE	C	523	-	-	2/13/13/17	-
32	STE	C	521	-	-	3/9/9/17	-
32	STE	B	626	-	-	6/9/9/17	-
25	CLA	c	513	-	1/1/15/20	10/39/115/115	-
25	CLA	b	609	-	-	6/39/115/115	-
25	CLA	b	601	37	1/1/15/20	16/39/115/115	-
32	STE	B	628	-	-	5/9/9/17	-
26	PHO	d	402	-	-	4/37/103/103	0/5/6/6
25	CLA	b	603	-	1/1/15/20	10/39/115/115	-
25	CLA	b	611	-	1/1/15/20	10/39/115/115	-
26	PHO	A	608	-	-	2/37/103/103	0/5/6/6
25	CLA	c	505	-	1/1/15/20	8/39/115/115	-
25	CLA	A	606	-	1/1/15/20	5/39/115/115	-
28	PL9	A	611	-	-	28/53/73/73	0/1/1/1
33	LHG	d	407	-	-	17/53/53/53	-
25	CLA	A	609	-	1/1/12/20	4/26/102/115	-
25	CLA	c	507	37	1/1/15/20	7/39/115/115	-
32	STE	M	102	-	-	2/7/7/17	-
25	CLA	b	606	-	1/1/15/20	10/39/115/115	-
25	CLA	b	613	-	1/1/15/20	7/39/115/115	-
32	STE	b	625	-	-	3/7/7/17	-
29	LMG	c	518	-	-	10/31/51/70	0/1/1/1
25	CLA	a	607	37	1/1/15/20	9/39/115/115	-
29	LMG	d	409	-	-	7/17/17/70	-
25	CLA	B	607	37	1/1/15/20	7/39/115/115	-
30	SQD	D	408	-	-	13/28/48/69	0/1/1/1
25	CLA	B	613	-	1/1/15/20	5/39/115/115	-
27	BCR	H	101	-	-	2/29/63/63	0/2/2/2
25	CLA	a	606	-	1/1/15/20	4/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	BCR	B	617	-	-	2/29/63/63	0/2/2/2
32	STE	b	621	-	-	13/17/17/17	-
32	STE	X	101	-	-	10/17/17/17	-
32	STE	M	101	-	-	7/12/12/17	-
27	BCR	K	101	-	-	4/29/63/63	0/2/2/2
31	DGD	h	101	-	-	17/51/91/95	0/2/2/2
25	CLA	d	404	-	1/1/15/20	8/39/115/115	-
25	CLA	B	609	-	-	2/39/115/115	-
25	CLA	b	605	-	1/1/15/20	9/39/115/115	-
25	CLA	c	511	3	1/1/15/20	4/39/115/115	-
25	CLA	c	512	-	1/1/15/20	19/39/115/115	-
27	BCR	T	101	-	-	7/29/63/63	0/2/2/2
31	DGD	a	616	-	-	31/45/45/95	-
25	CLA	b	614	-	1/1/15/20	10/39/115/115	-
32	STE	H	103	-	-	10/15/15/17	-
32	STE	m	102	-	-	3/9/9/17	-
33	LHG	a	613	-	-	21/53/53/53	-
29	LMG	D	411	-	-	16/33/33/70	-
31	DGD	c	516	-	-	17/51/91/95	0/2/2/2
25	CLA	B	614	-	1/1/15/20	11/39/115/115	-
25	CLA	C	511	3	1/1/15/20	4/39/115/115	-
25	CLA	d	403	-	1/1/15/20	4/39/115/115	-
25	CLA	C	509	-	1/1/15/20	13/39/115/115	-
27	BCR	A	610	-	-	3/29/63/63	0/2/2/2
29	LMG	A	613	-	-	18/43/63/70	0/1/1/1
25	CLA	a	609	-	1/1/15/20	8/39/115/115	-
25	CLA	c	509	-	1/1/15/20	13/39/115/115	-
25	CLA	C	501	-	1/1/15/20	4/39/115/115	-
33	LHG	D	409	-	-	18/53/53/53	-
30	SQD	A	615	-	-	16/39/39/69	-
30	SQD	b	620	-	-	22/44/64/69	0/1/1/1
28	PL9	D	406	-	-	6/53/73/73	0/1/1/1
25	CLA	C	508	-	1/1/15/20	6/39/115/115	-
25	CLA	B	615	-	1/1/15/20	9/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	D	404	-	-	7/39/115/115	-
25	CLA	A	607	37	-	13/39/115/115	-
32	STE	t	102	-	-	3/7/7/17	-
27	BCR	C	516	-	-	7/29/63/63	0/2/2/2
27	BCR	k	101	-	-	10/29/63/63	0/2/2/2
25	CLA	B	608	-	-	3/39/115/115	-
33	LHG	D	410	-	-	23/51/51/53	-
25	CLA	B	611	-	1/1/15/20	2/39/115/115	-
25	CLA	b	616	-	1/1/14/20	7/33/109/115	-

The worst 5 of 744 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	a	608	PHO	C1B-C2B	10.09	1.50	1.39
26	d	402	PHO	C1B-C2B	9.43	1.49	1.39
26	D	402	PHO	C1B-C2B	9.09	1.49	1.39
26	d	402	PHO	C3B-C4B	9.06	1.50	1.41
26	A	608	PHO	C1B-C2B	8.74	1.49	1.39

The worst 5 of 1052 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	V	201	HEC	CBB-CAB-C3B	-9.33	108.80	127.43
25	c	511	CLA	C4A-NA-C1A	8.79	110.69	106.68
25	b	606	CLA	C4A-NA-C1A	8.71	110.66	106.68
36	v	201	HEC	CBC-CAC-C3C	-8.68	110.09	127.43
25	B	604	CLA	C4A-NA-C1A	8.48	110.55	106.68

5 of 60 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
25	A	606	CLA	ND
25	A	609	CLA	ND
25	B	601	CLA	ND
25	B	602	CLA	ND
25	B	603	CLA	ND

5 of 1701 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	A	607	CLA	C2B-C3B-CAB-CBB
25	A	607	CLA	C4B-C3B-CAB-CBB
25	A	612	CLA	C14-C13-C15-C16
25	B	601	CLA	C1A-C2A-CAA-CBA
25	B	614	CLA	CAD-CBD-CGD-O1D

There are no ring outliers.

147 monomers are involved in 267 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	b	604	CLA	1	0
25	B	604	CLA	3	0
33	B	623	LHG	2	0
27	t	101	BCR	2	0
31	C	519	DGD	2	0
32	B	625	STE	1	0
33	E	101	LHG	3	0
25	c	510	CLA	3	0
29	c	520	LMG	1	0
22	a	602[A]	OEY	1	0
27	d	405	BCR	1	0
32	I	101	STE	2	0
30	a	615	SQD	2	0
25	b	615	CLA	2	0
27	x	101	BCR	2	0
27	k	102	BCR	1	0
27	b	617	BCR	1	0
33	D	412	LHG	4	0
25	c	504	CLA	2	0
25	B	605	CLA	3	0
32	B	627	STE	1	0
27	B	618	BCR	2	0
25	B	602	CLA	6	0
27	C	515	BCR	5	0
29	b	622	LMG	1	0
32	b	624	STE	2	0
25	b	610	CLA	2	0
26	D	402	PHO	2	0
33	d	408	LHG	1	0
27	C	514	BCR	2	0
30	A	614	SQD	1	0
25	C	505	CLA	3	0
32	J	101	STE	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	m	101	LMG	3	0
31	c	515	DGD	3	0
28	a	611	PL9	7	0
31	C	518	DGD	2	0
36	v	201	HEC	2	0
27	D	405	BCR	2	0
25	c	501	CLA	2	0
25	c	506	CLA	1	0
25	B	601	CLA	4	0
33	e	102	LHG	1	0
25	B	606	CLA	4	0
25	c	503	CLA	4	0
25	C	506	CLA	4	0
25	A	612	CLA	3	0
32	B	621	STE	2	0
25	B	612	CLA	2	0
28	d	406	PL9	2	0
25	B	610	CLA	2	0
25	C	502	CLA	1	0
32	c	521	STE	1	0
30	f	101	SQD	1	0
31	c	517	DGD	2	0
25	b	608	CLA	2	0
30	a	614	SQD	1	0
29	c	522	LMG	2	0
25	C	513	CLA	2	0
25	b	607	CLA	2	0
25	D	403	CLA	3	0
32	b	623	STE	2	0
27	k	103	BCR	2	0
35	F	101	HEM	2	0
25	B	603	CLA	3	0
25	C	512	CLA	4	0
31	A	616	DGD	5	0
27	a	610	BCR	1	0
25	b	602	CLA	1	0
25	c	508	CLA	1	0
32	d	412	STE	2	0
25	c	502	CLA	1	0
35	e	101	HEM	4	0
25	C	507	CLA	1	0
25	a	612	CLA	2	0

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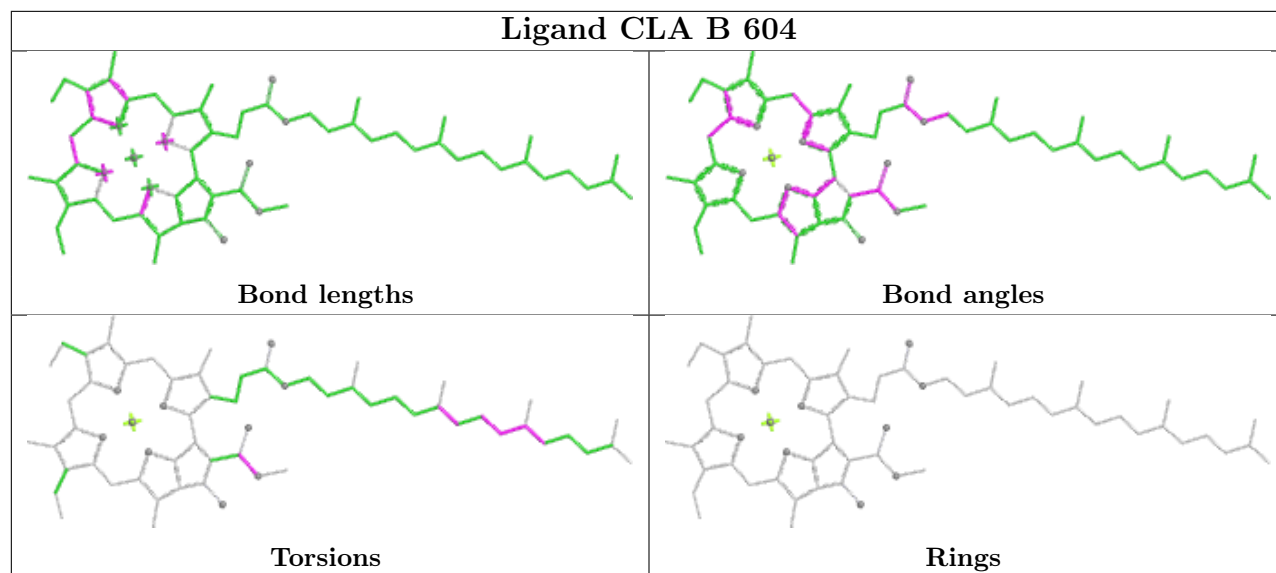
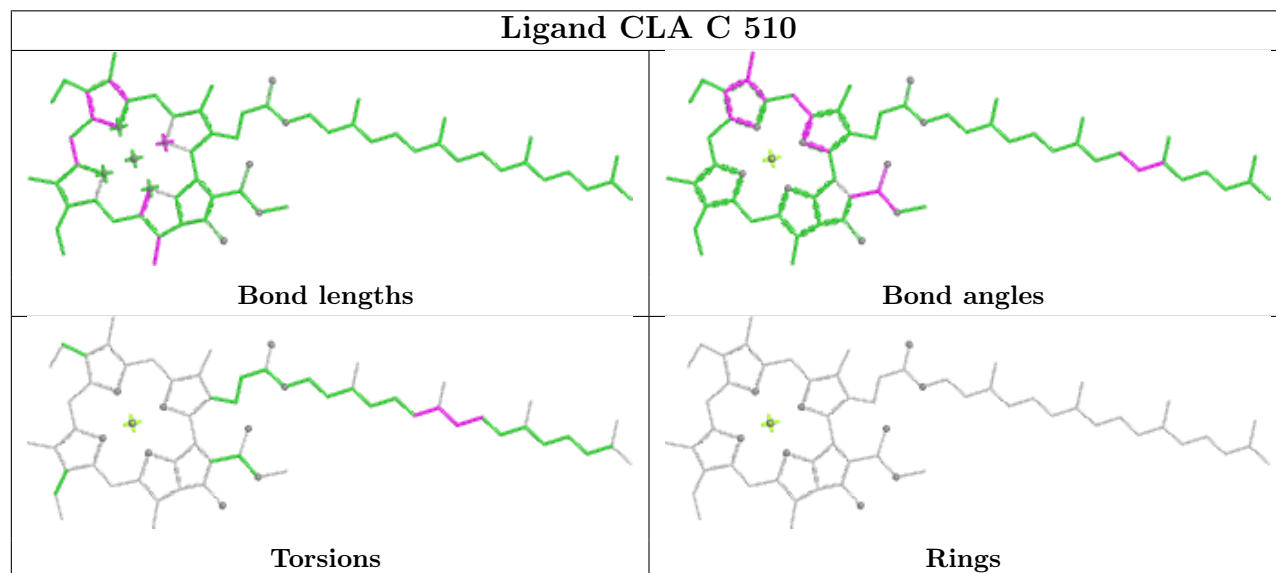
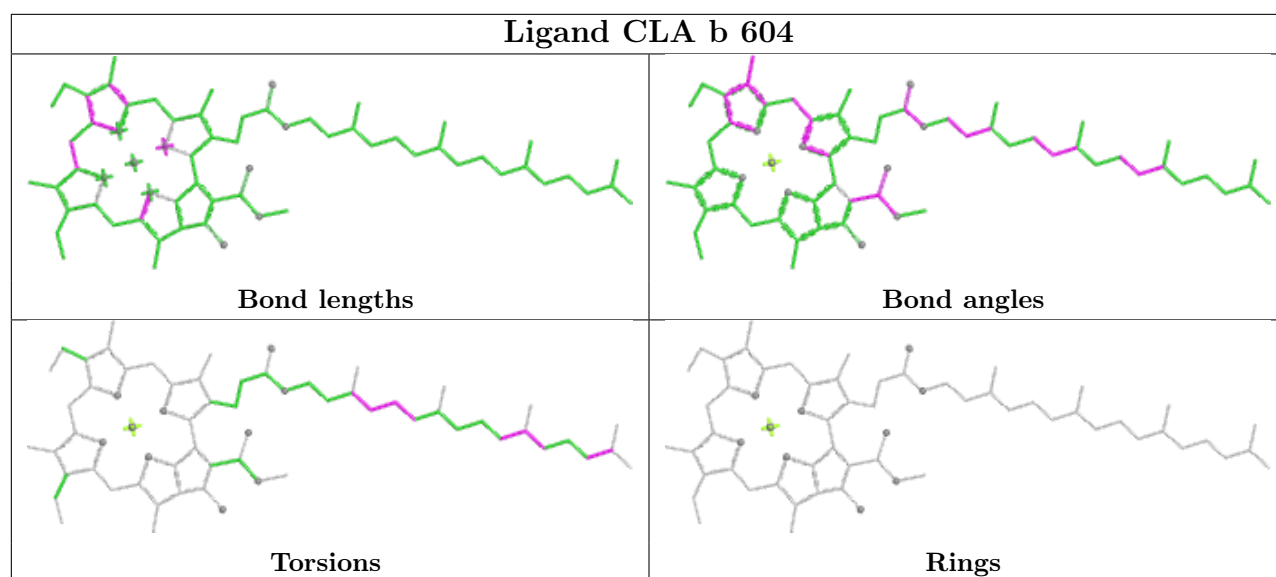
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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29	B	620	LMG	2	0
32	l	102	STE	1	0
27	b	619	BCR	2	0
27	c	514	BCR	3	0
27	b	618	BCR	2	0
27	B	619	BCR	4	0
29	C	520	LMG	2	0
33	l	101	LHG	1	0
25	B	616	CLA	1	0
32	C	523	STE	1	0
25	b	609	CLA	3	0
25	c	513	CLA	2	0
25	b	601	CLA	3	0
26	d	402	PHO	2	0
25	b	603	CLA	1	0
34	D	401	BCT	1	0
25	b	611	CLA	2	0
26	A	608	PHO	1	0
25	c	505	CLA	4	0
25	A	606	CLA	1	0
28	A	611	PL9	5	0
33	d	407	LHG	4	0
25	A	609	CLA	1	0
25	c	507	CLA	2	0
25	b	606	CLA	3	0
25	b	613	CLA	3	0
32	b	625	STE	1	0
25	a	607	CLA	2	0
29	d	409	LMG	2	0
22	A	602[A]	OEY	1	0
25	B	607	CLA	4	0
30	D	408	SQD	1	0
25	B	613	CLA	3	0
27	H	101	BCR	2	0
25	a	606	CLA	3	0
27	B	617	BCR	1	0
32	b	621	STE	5	0
32	X	101	STE	2	0
32	M	101	STE	1	0
31	h	101	DGD	1	0

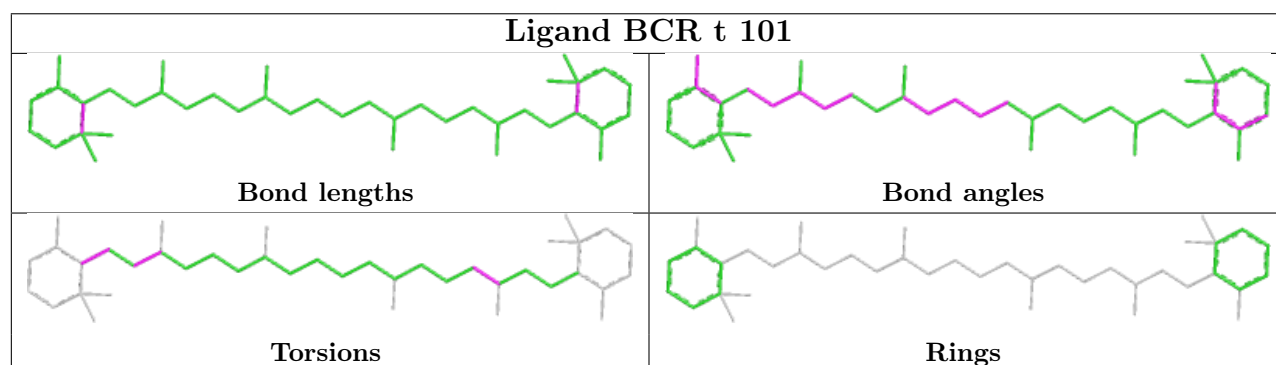
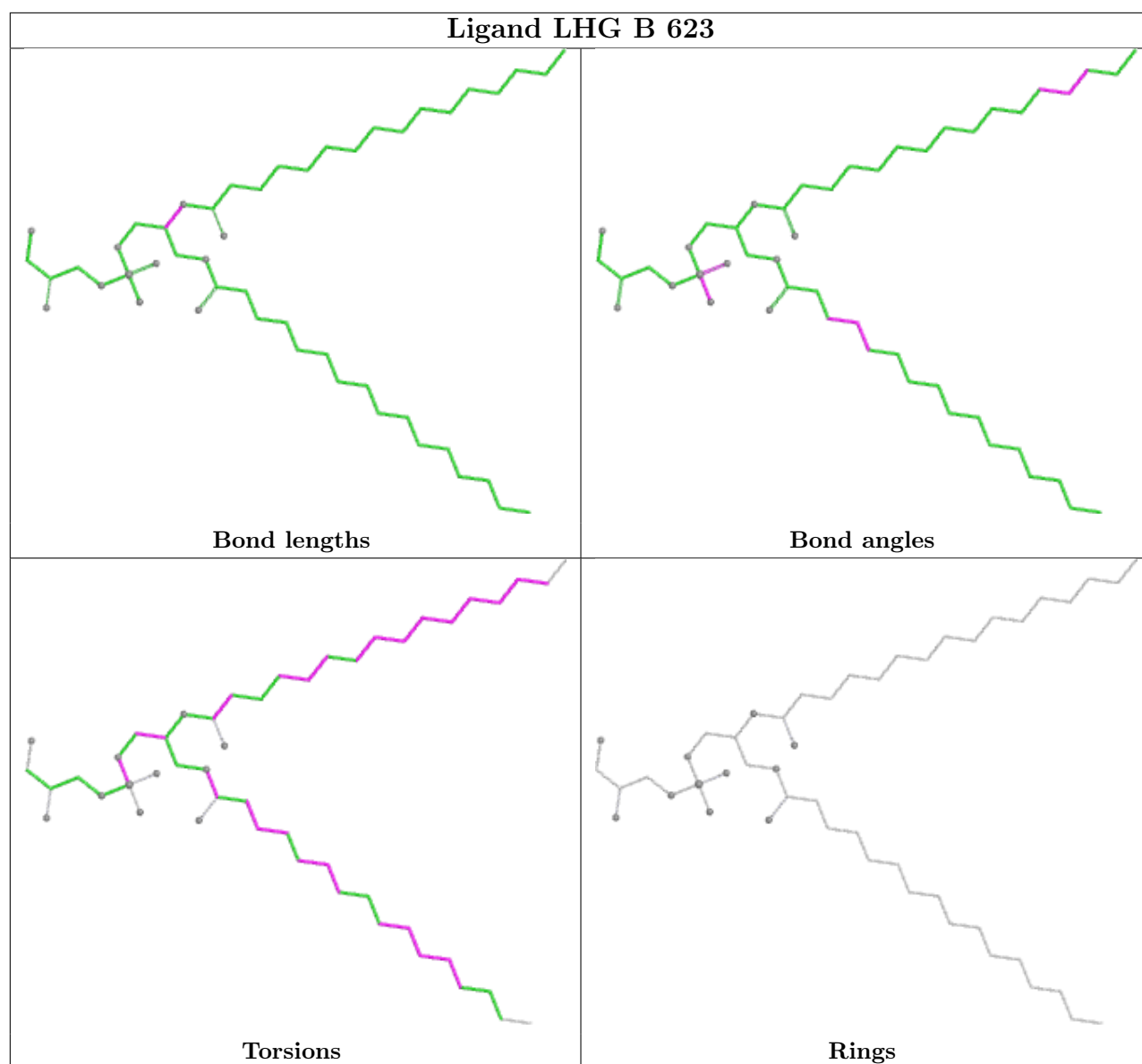
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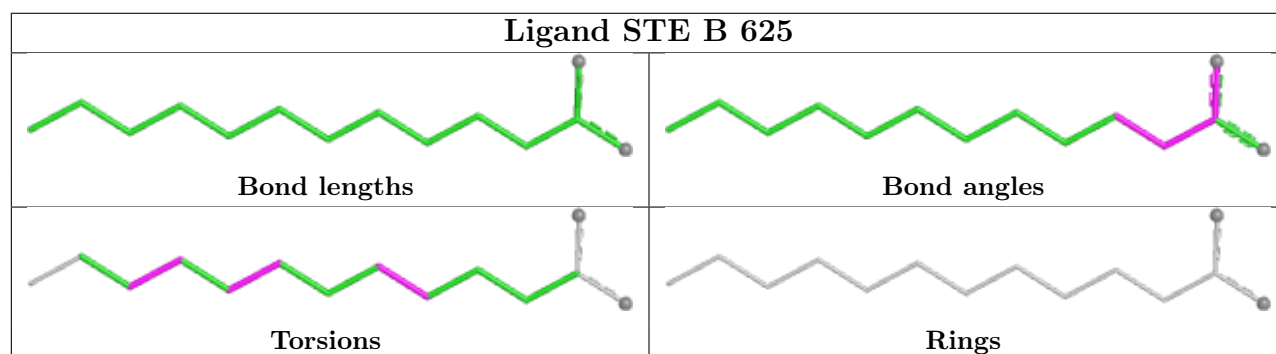
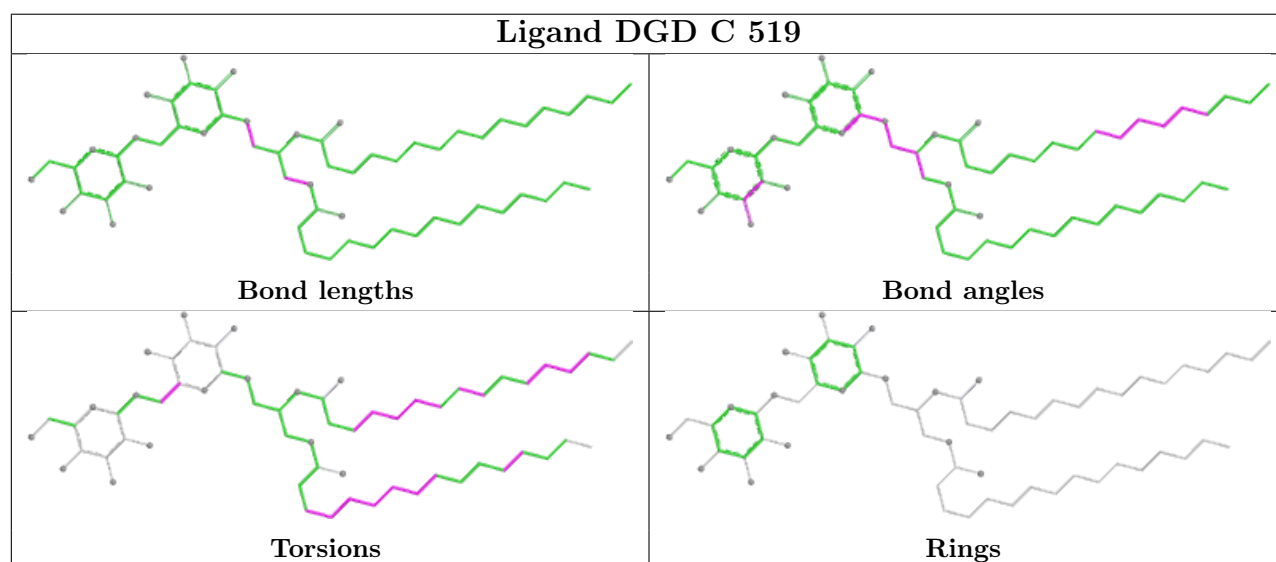
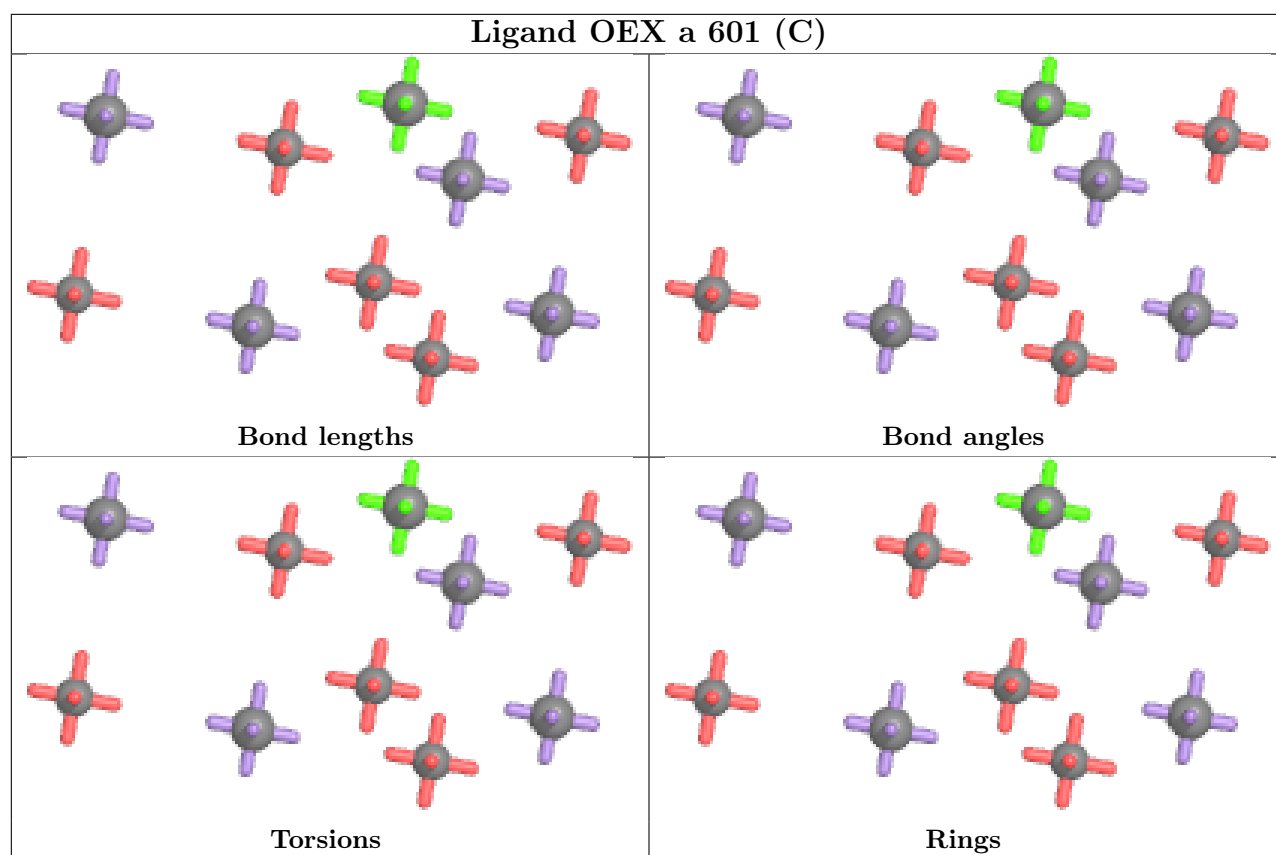
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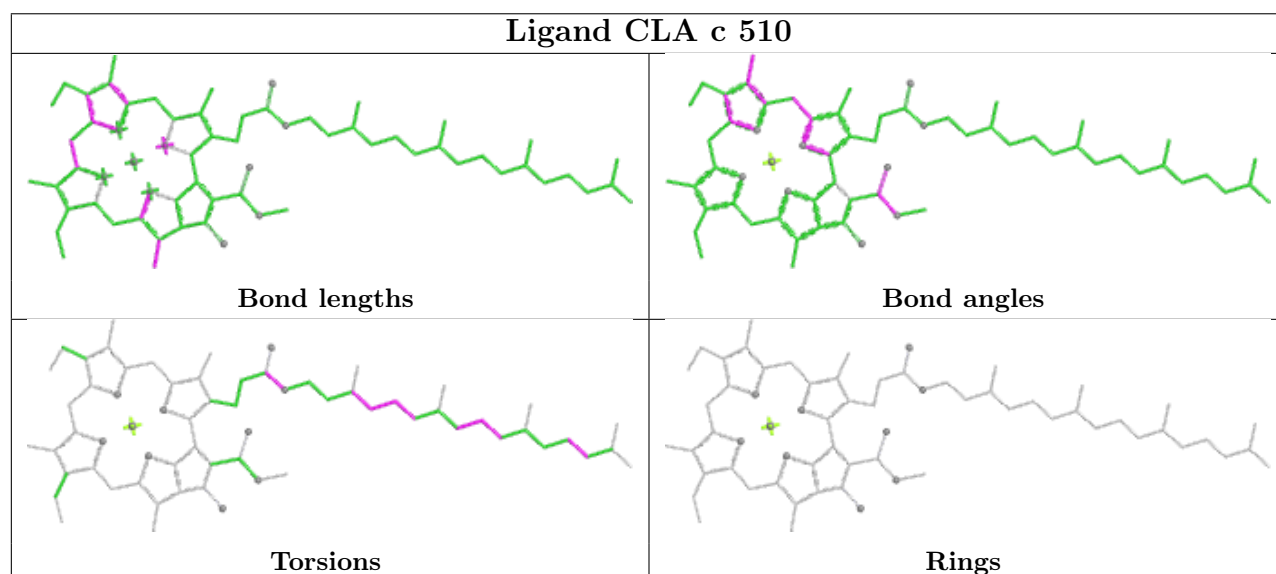
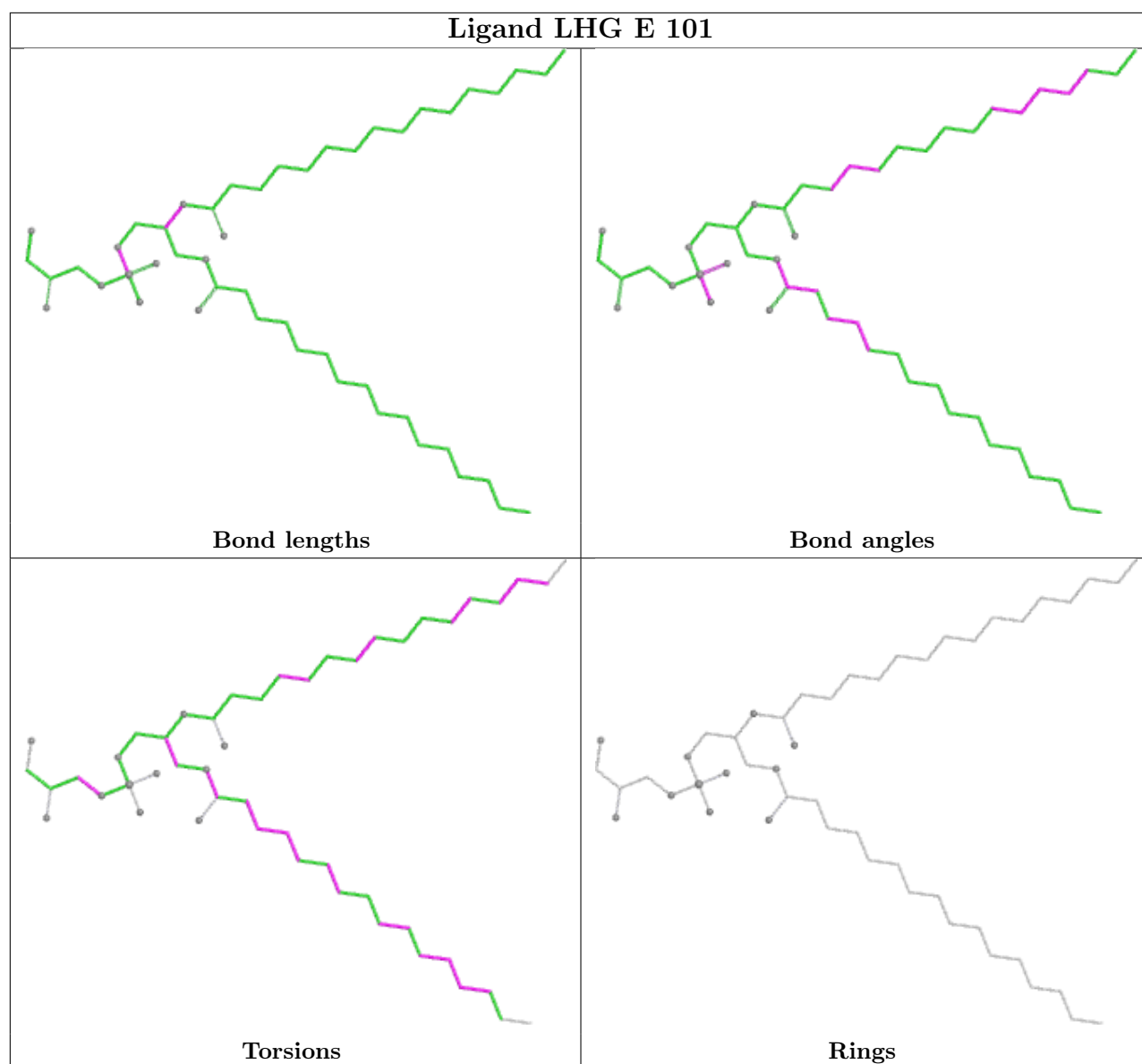
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25	b	605	CLA	2	0
25	c	511	CLA	4	0
25	c	512	CLA	1	0
27	T	101	BCR	2	0
31	a	616	DGD	6	0
25	b	614	CLA	5	0
32	H	103	STE	1	0
33	a	613	LHG	1	0
29	D	411	LMG	1	0
31	c	516	DGD	2	0
25	B	614	CLA	2	0
25	C	511	CLA	1	0
25	d	403	CLA	2	0
25	C	509	CLA	1	0
27	A	610	BCR	3	0
29	A	613	LMG	4	0
25	a	609	CLA	5	0
25	c	509	CLA	2	0
25	C	501	CLA	2	0
33	D	409	LHG	1	0
30	A	615	SQD	1	0
30	b	620	SQD	1	0
28	D	406	PL9	1	0
25	C	508	CLA	1	0
25	B	615	CLA	2	0
25	D	404	CLA	4	0
25	A	607	CLA	2	0
25	B	611	CLA	1	0
25	b	616	CLA	2	0

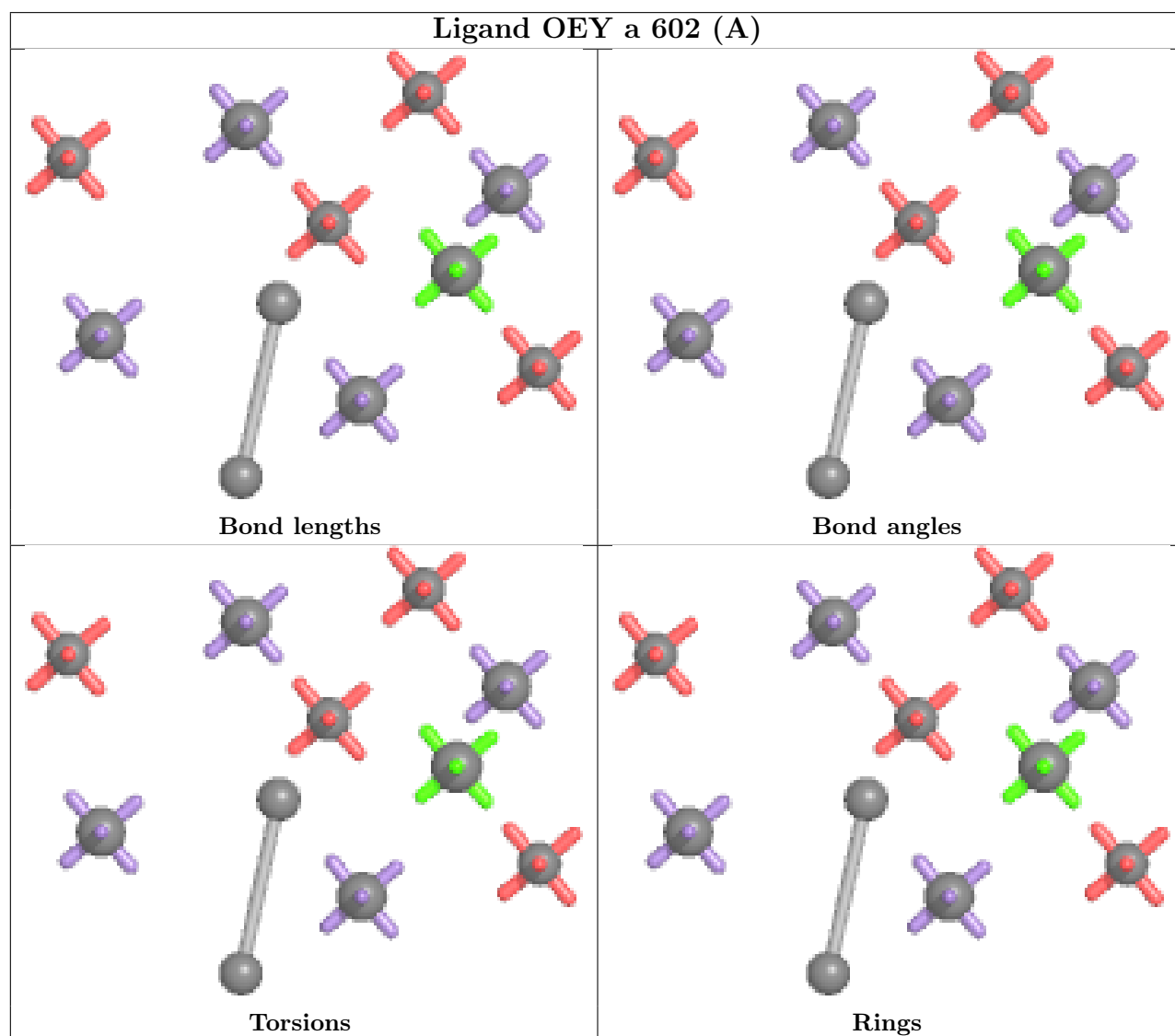
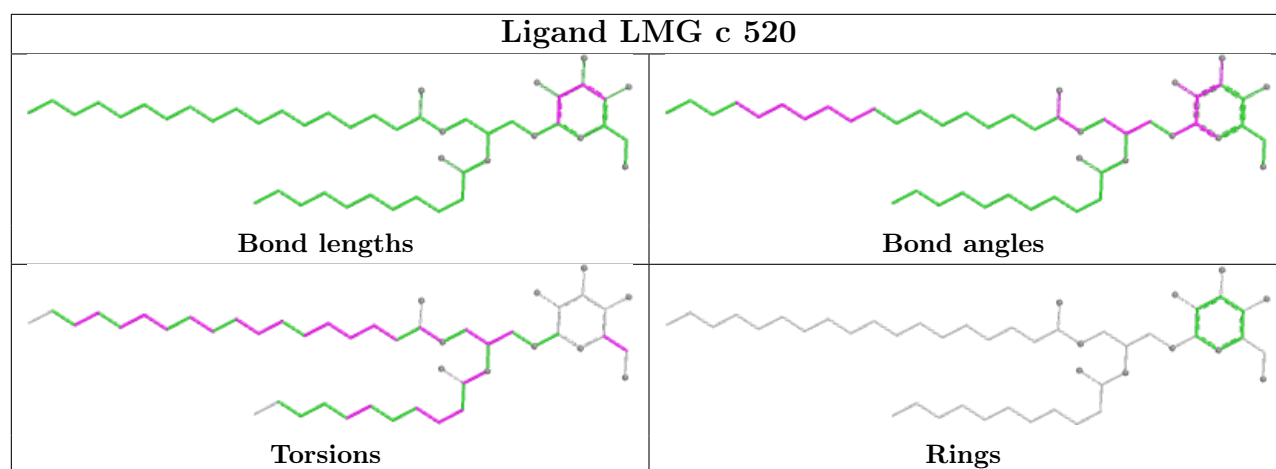
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

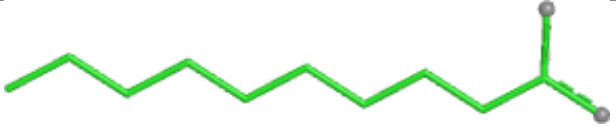
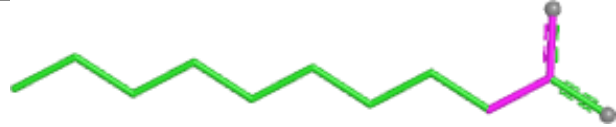
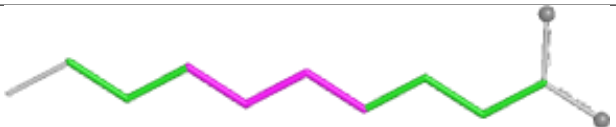
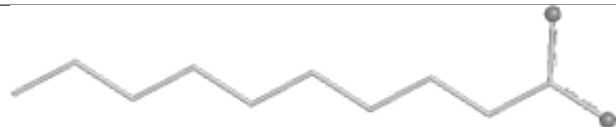


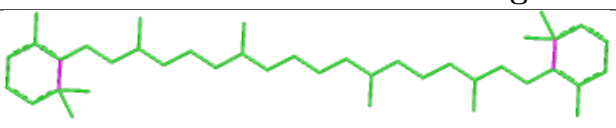
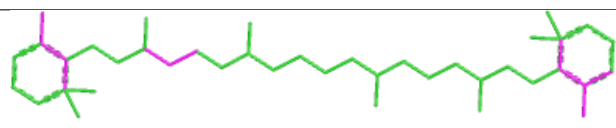
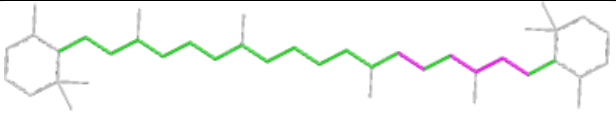
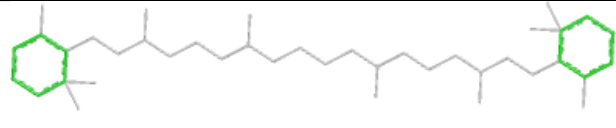


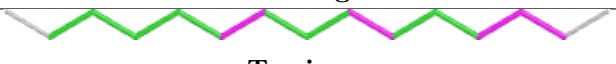


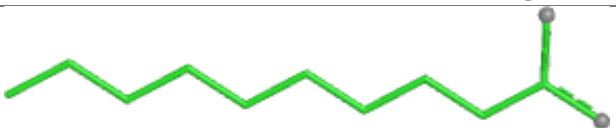
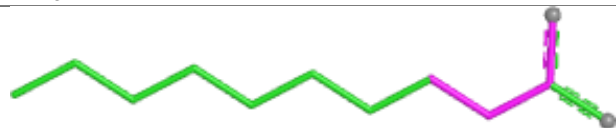
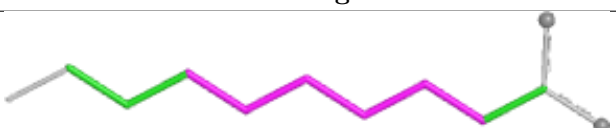
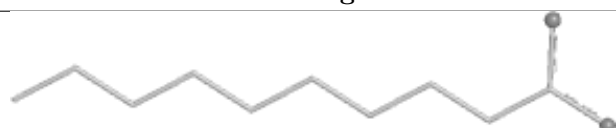


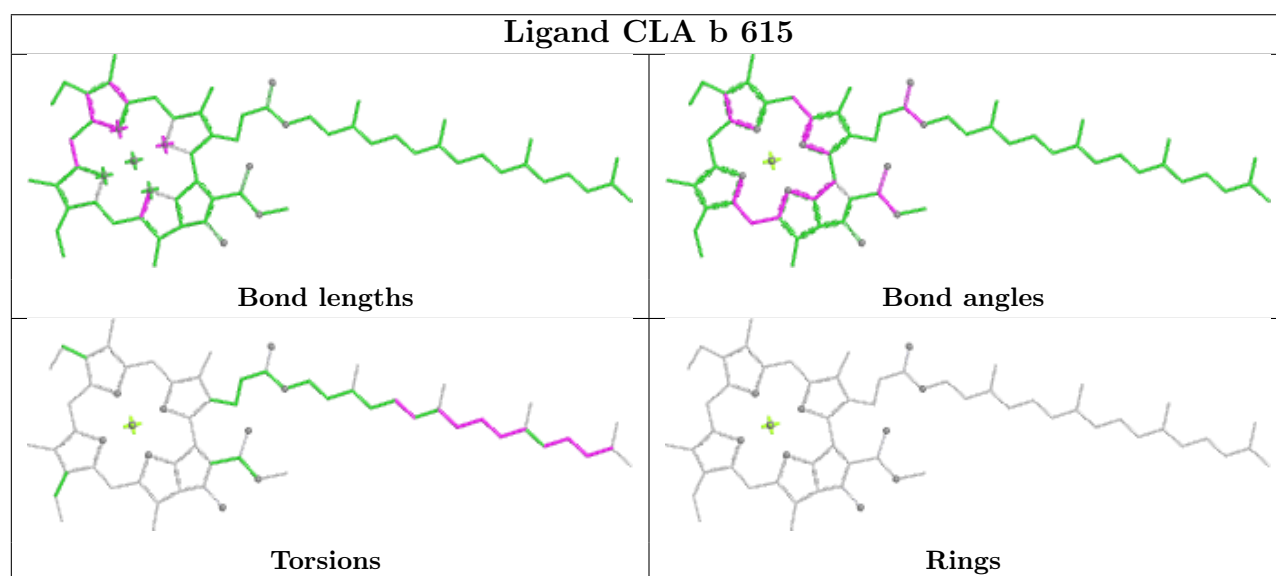
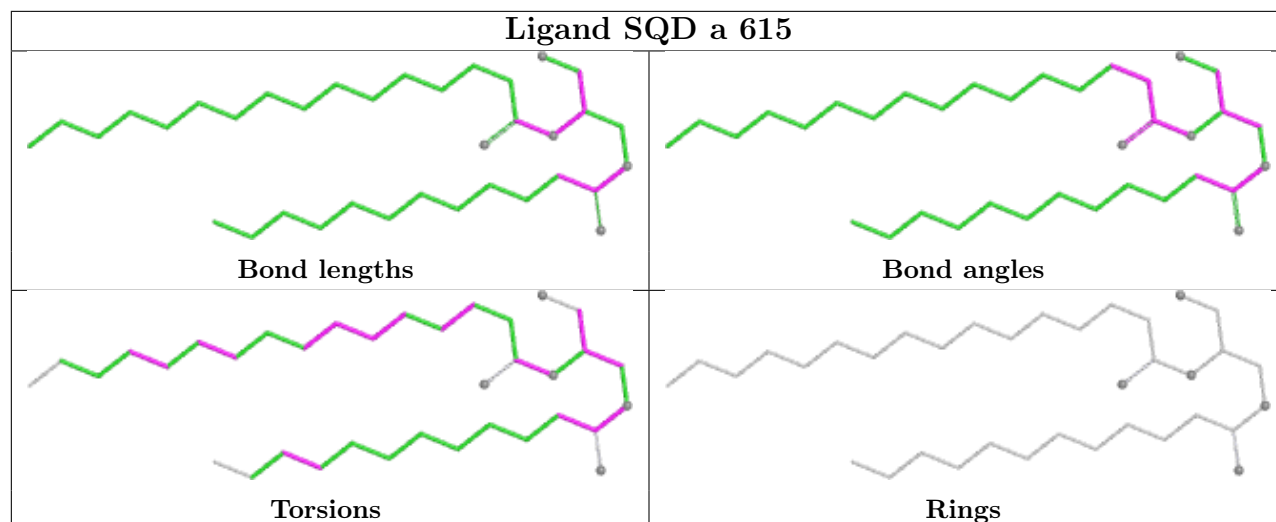


Ligand STE E 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

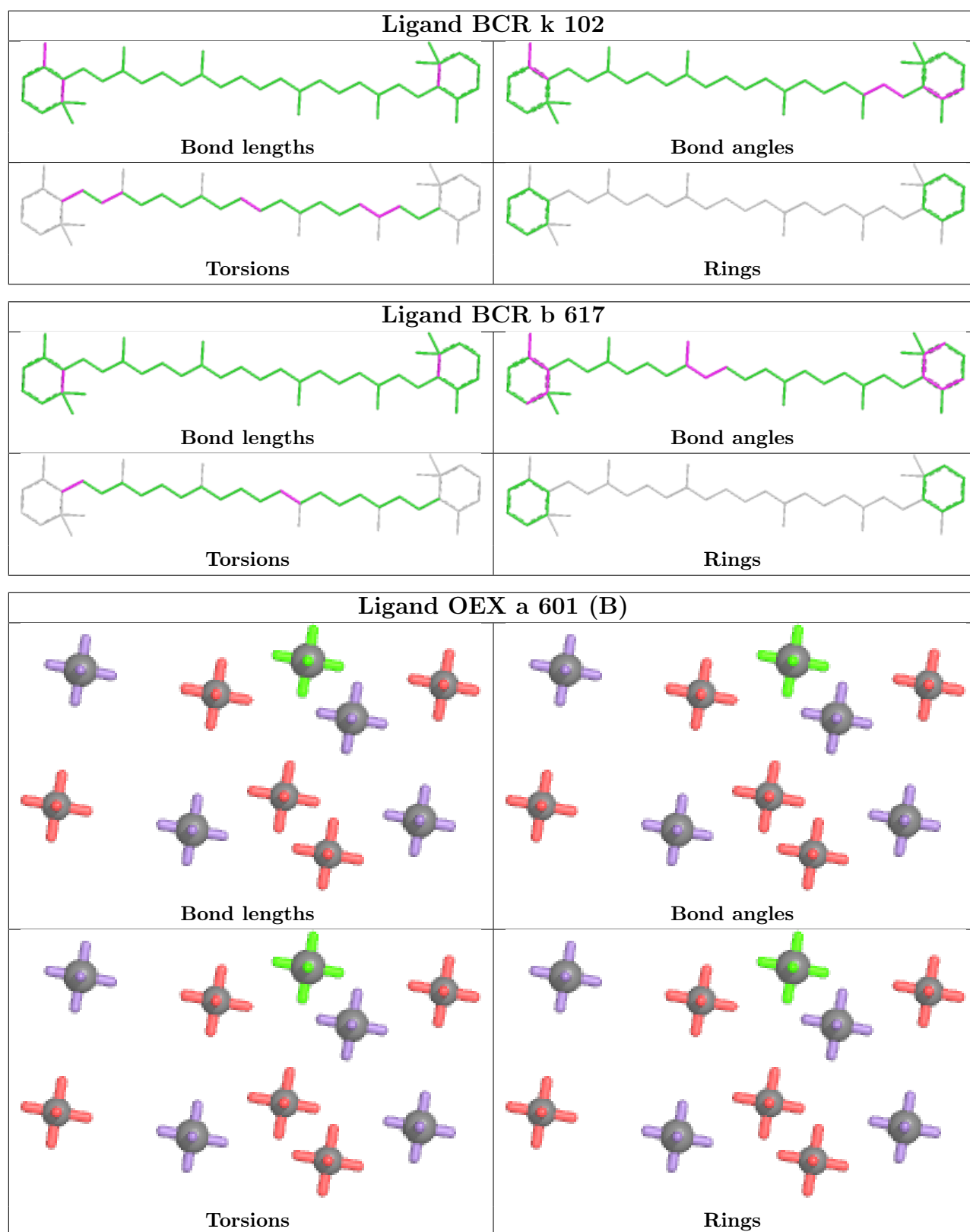
Ligand BCR d 405	
	
Bond lengths	Bond angles
	
Torsions	Rings

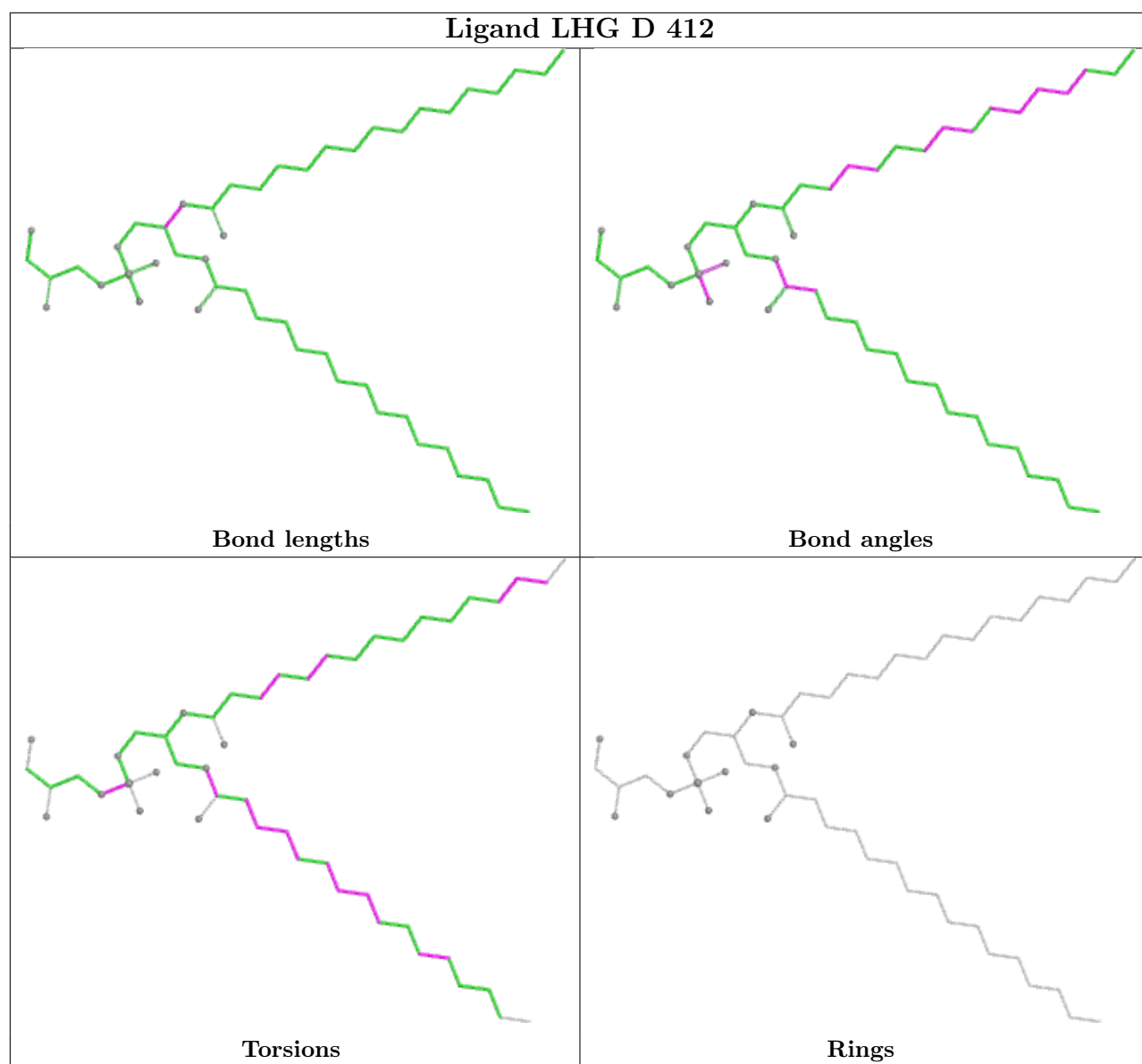
Ligand STE I 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

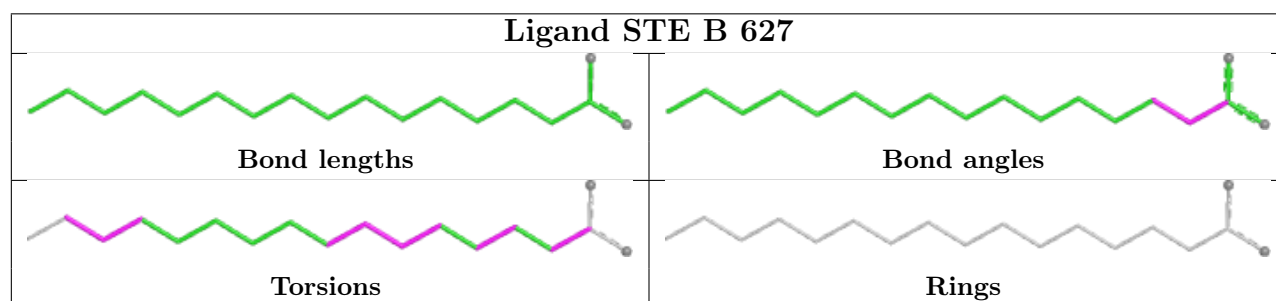
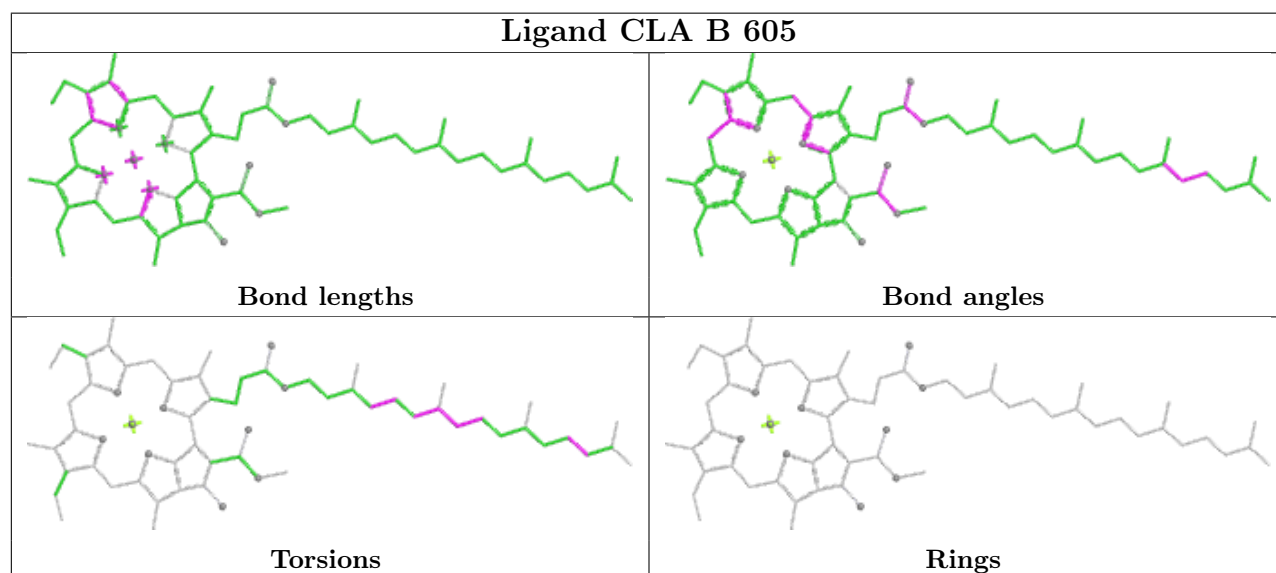
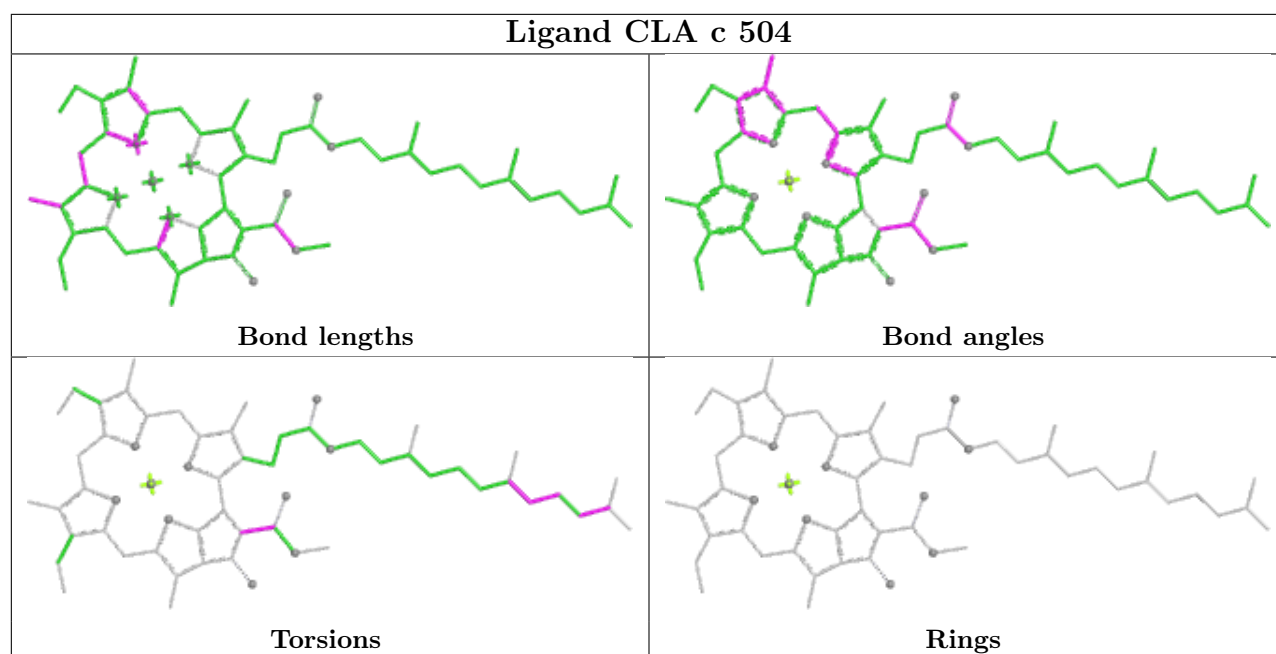
Ligand STE j 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

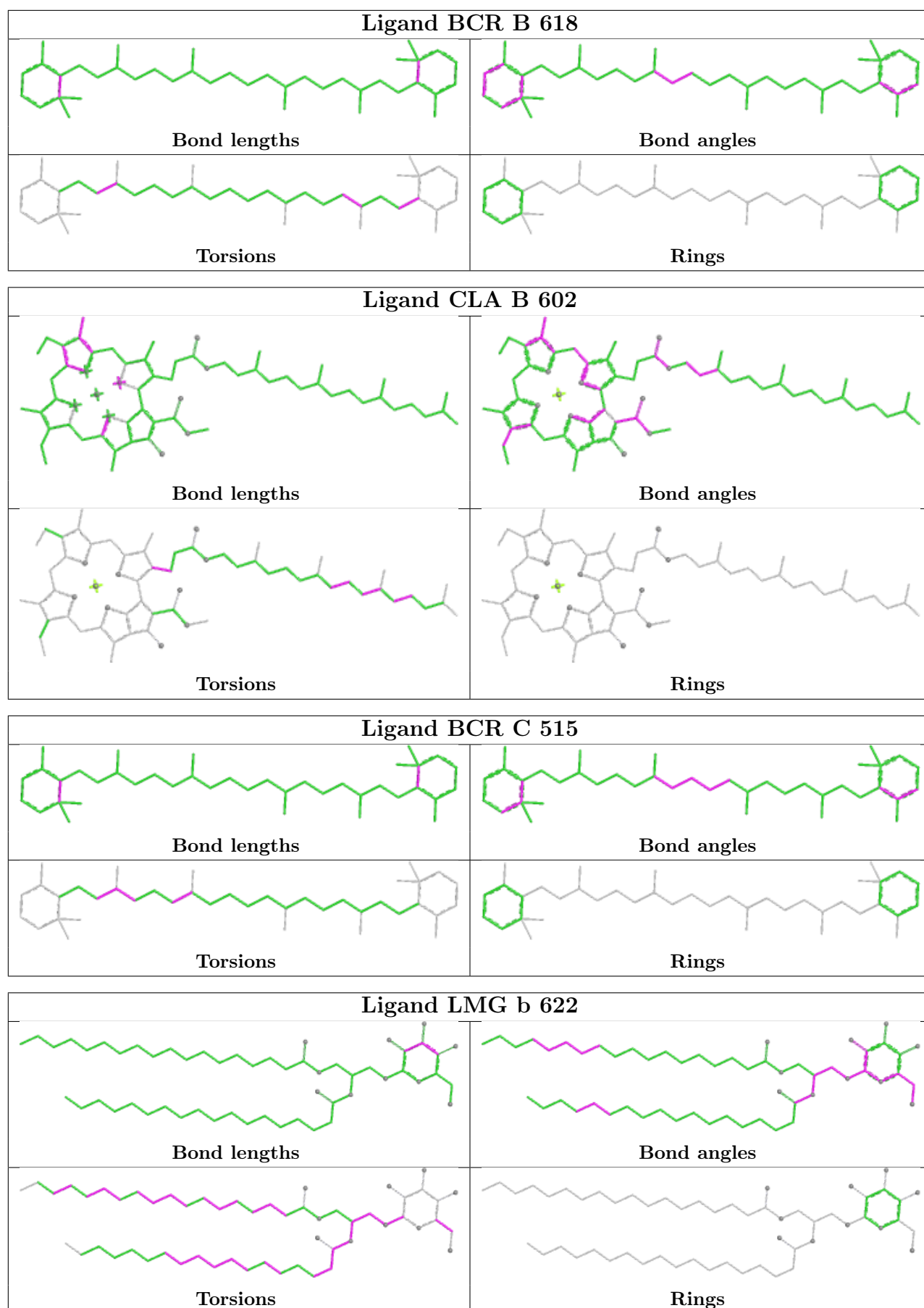


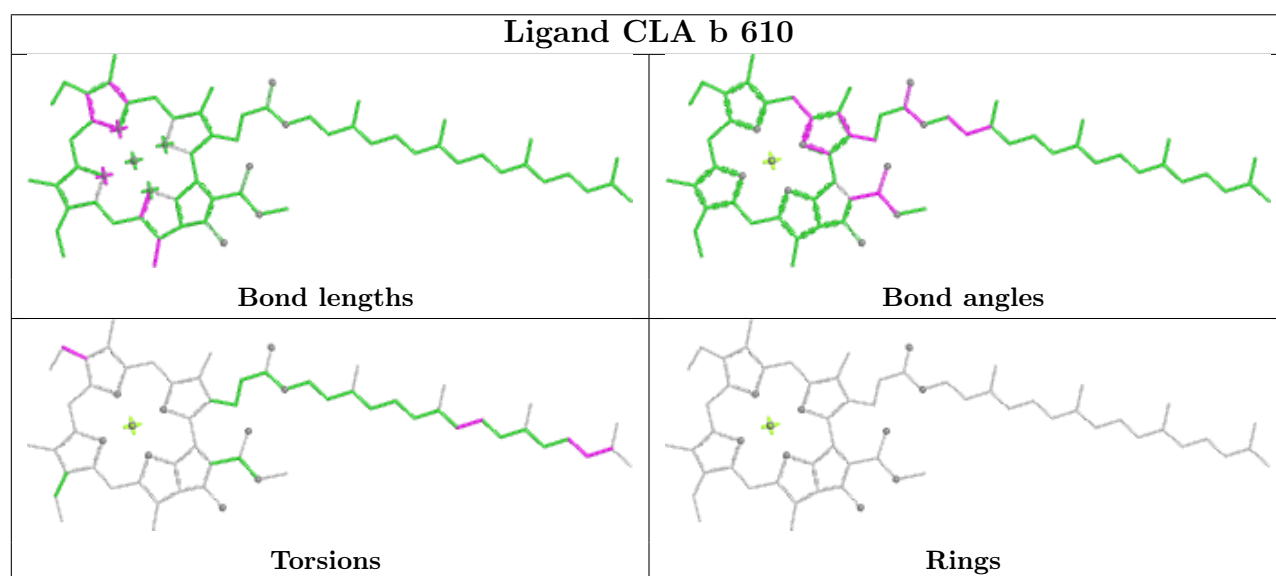
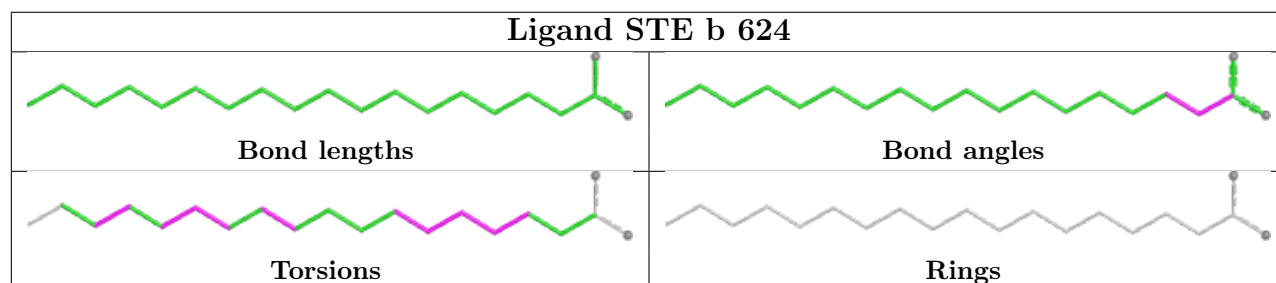
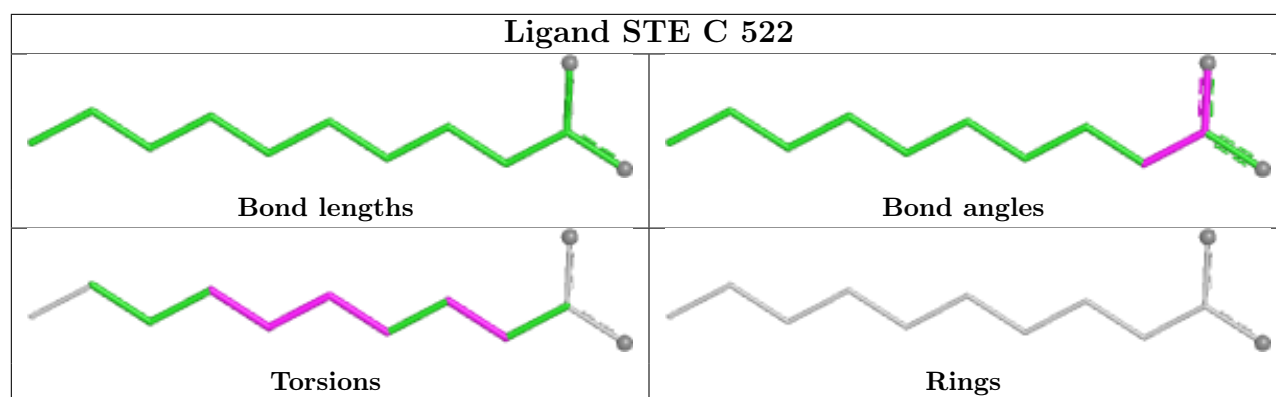
Ligand OEX A 601 (C)			
Bond lengths		Bond angles	
Torsions		Rings	
Ligand BCR x 101			
Bond lengths		Bond angles	
Torsions		Rings	
Ligand STE B 629			
Bond lengths		Bond angles	
Torsions		Rings	

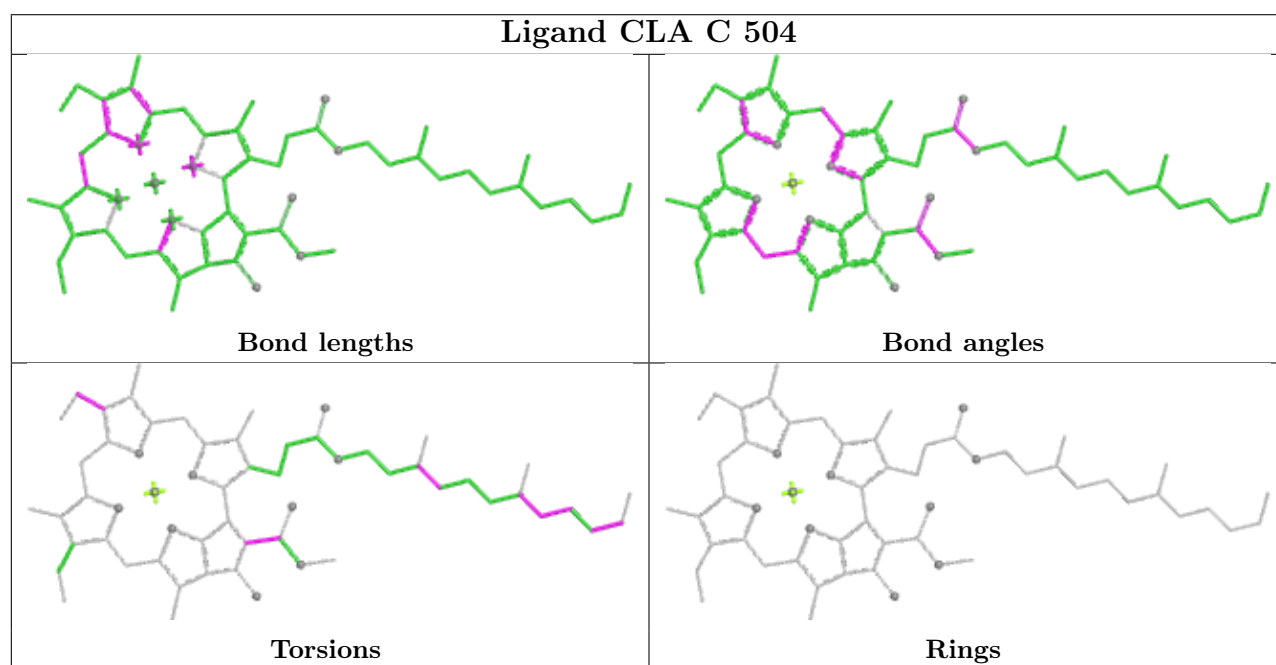
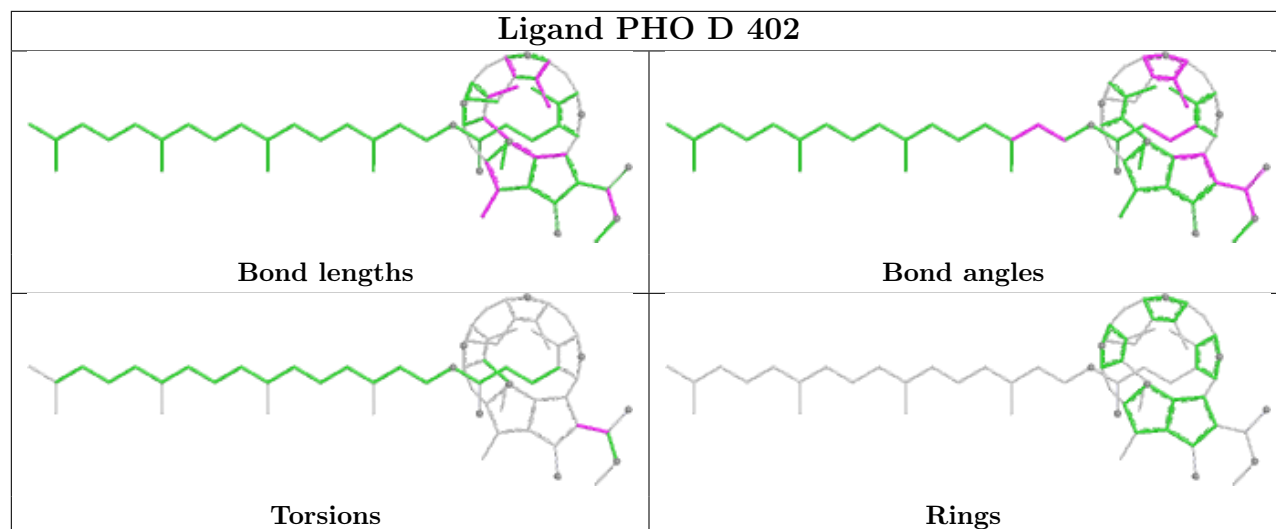


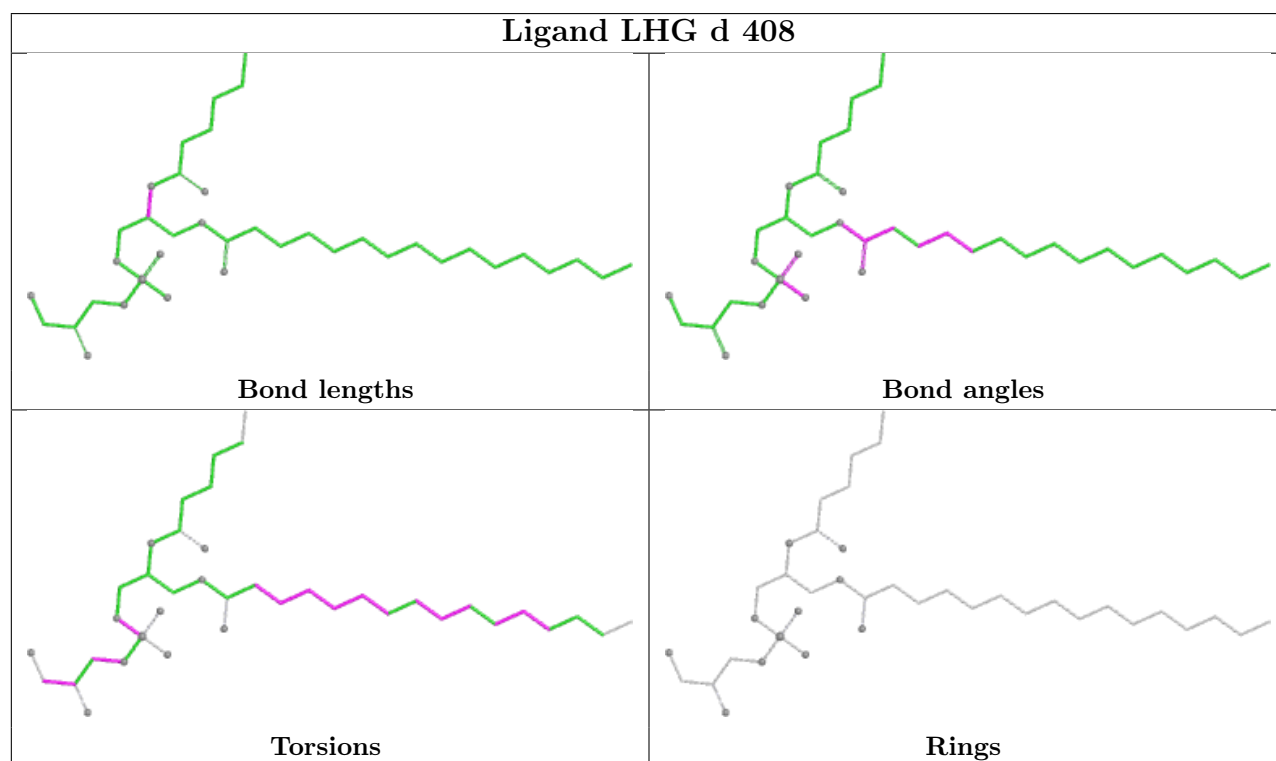
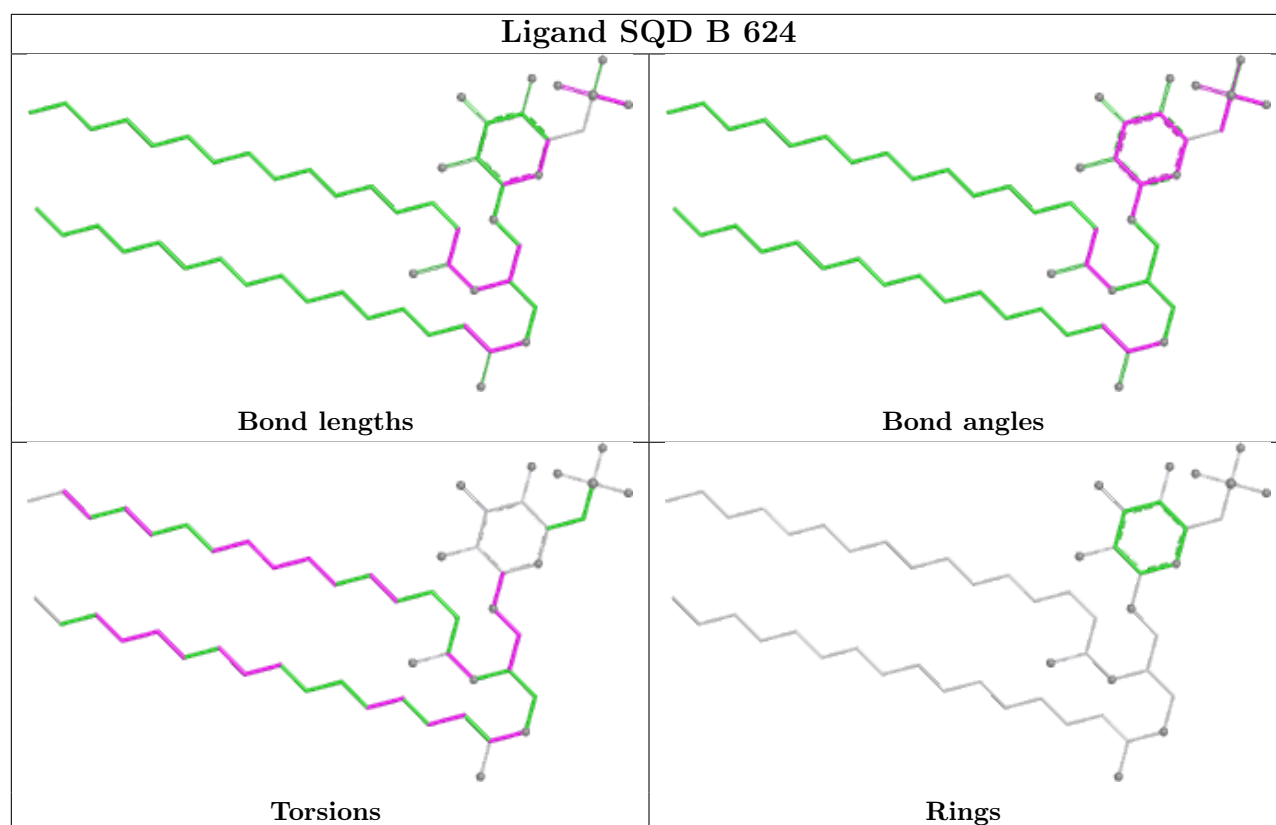


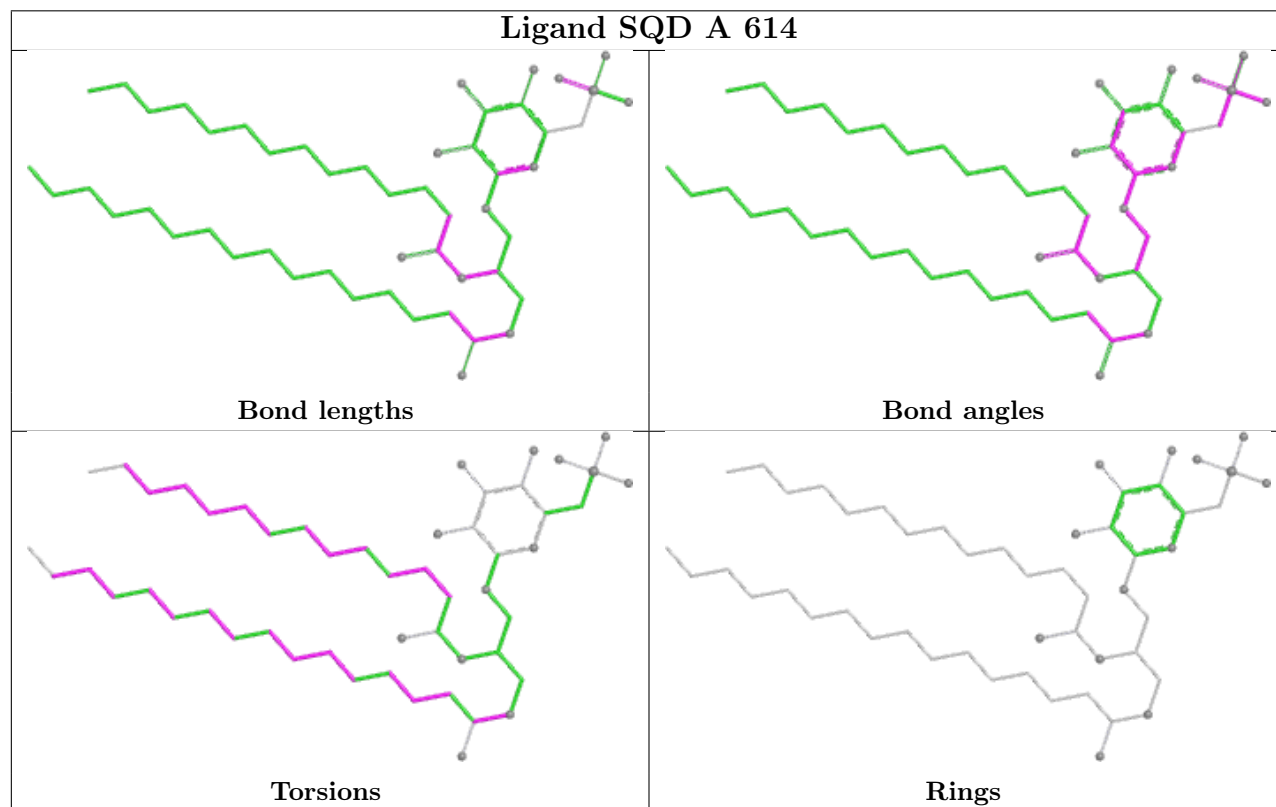
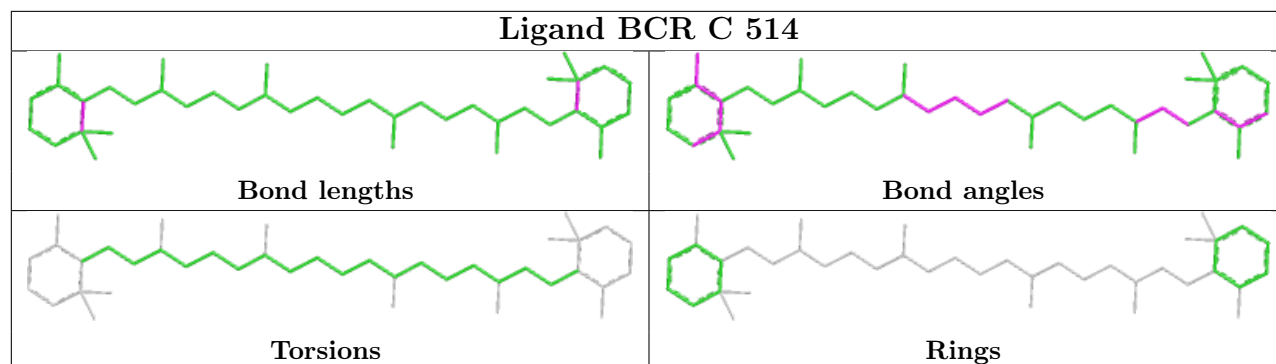




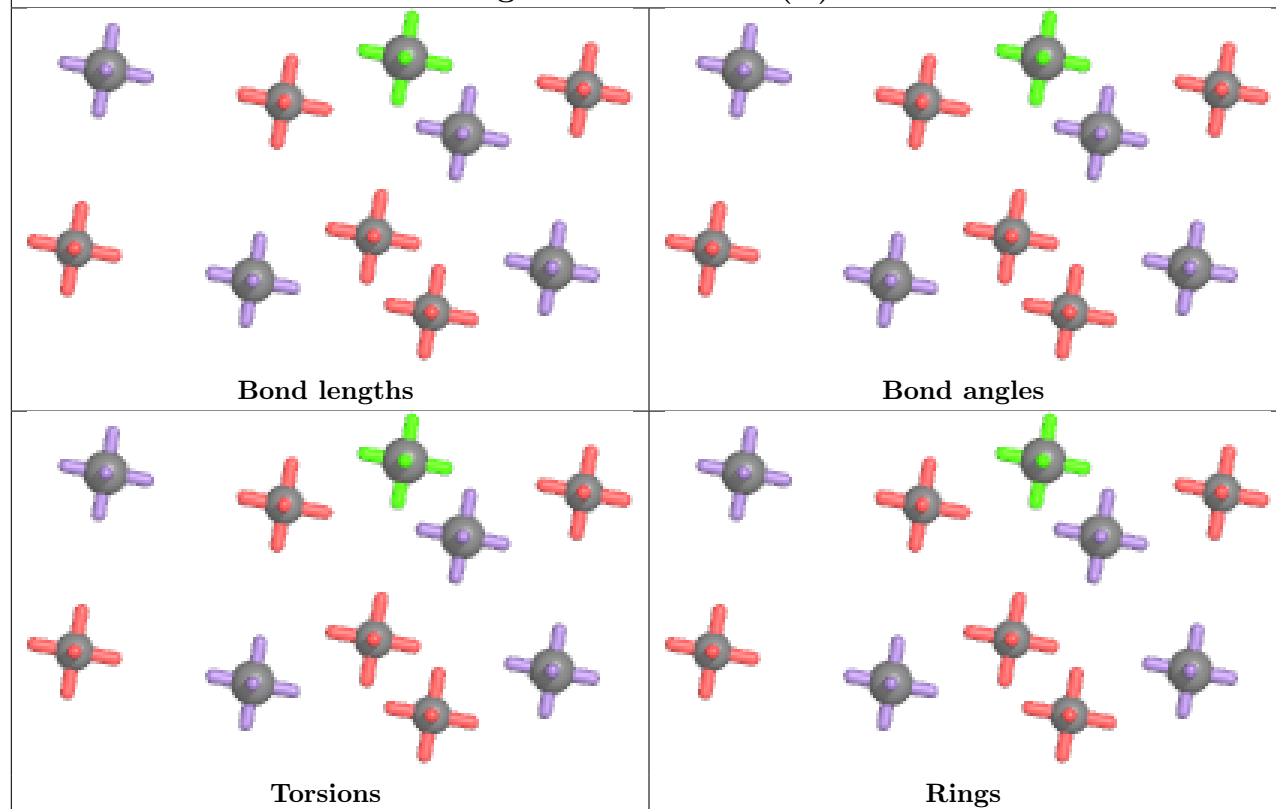




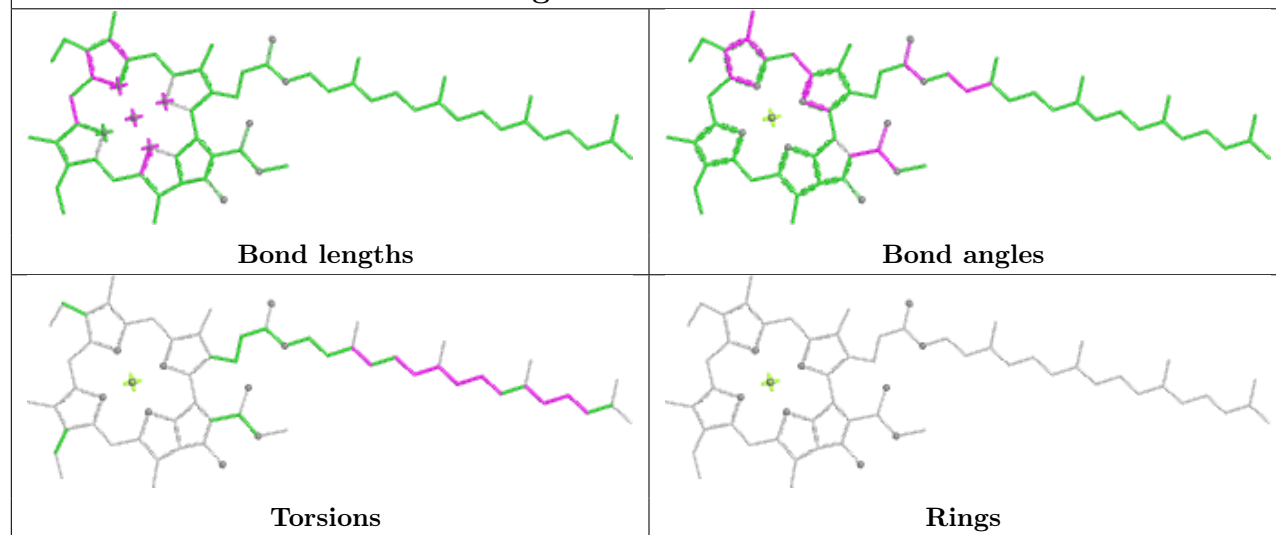


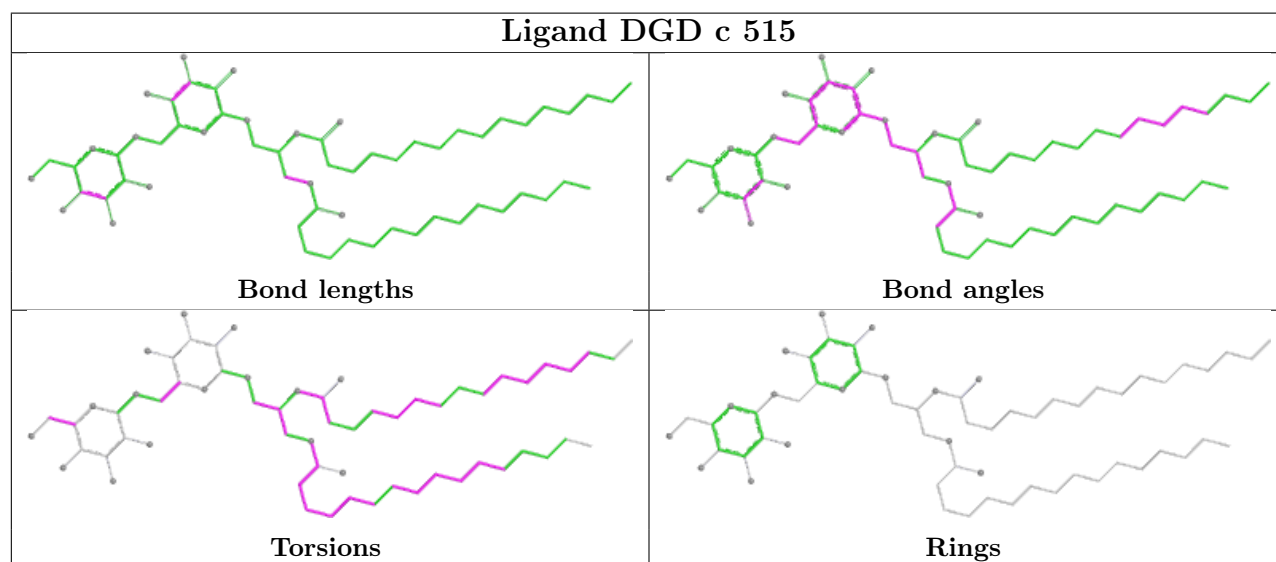
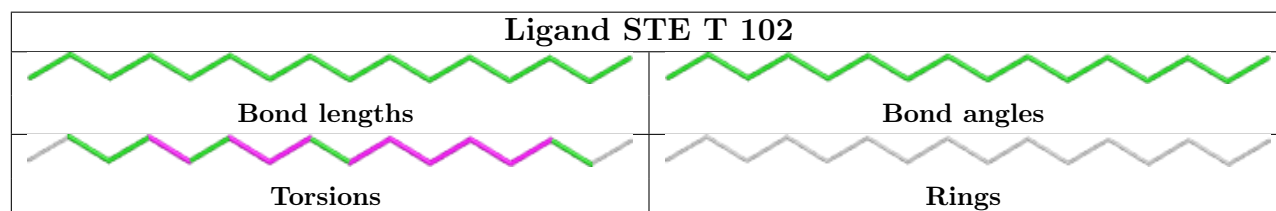
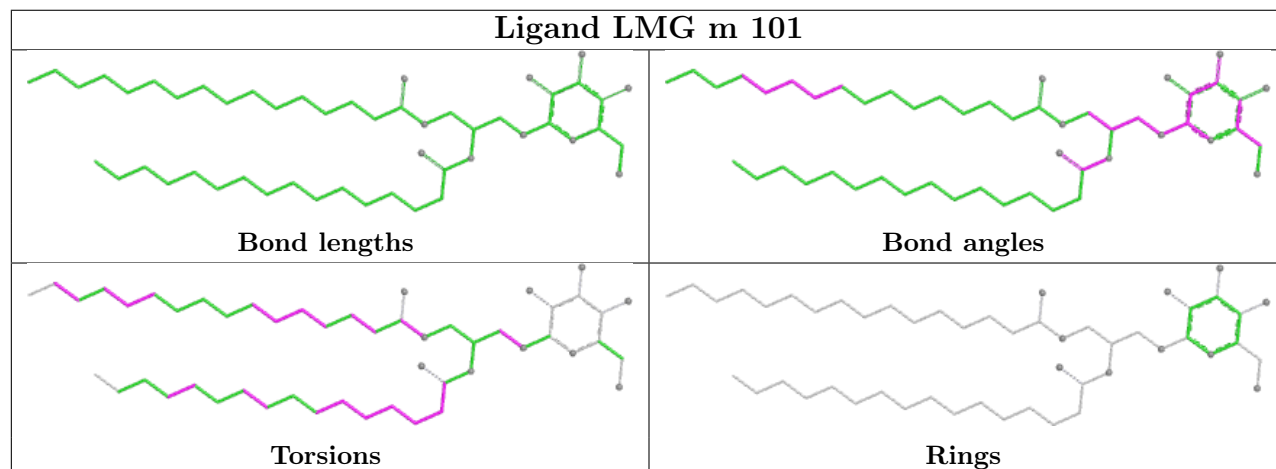
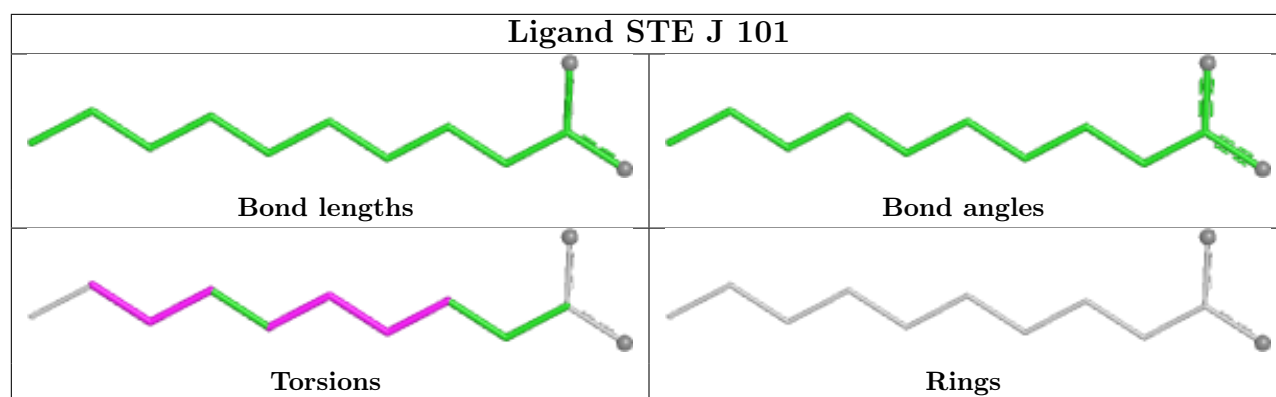


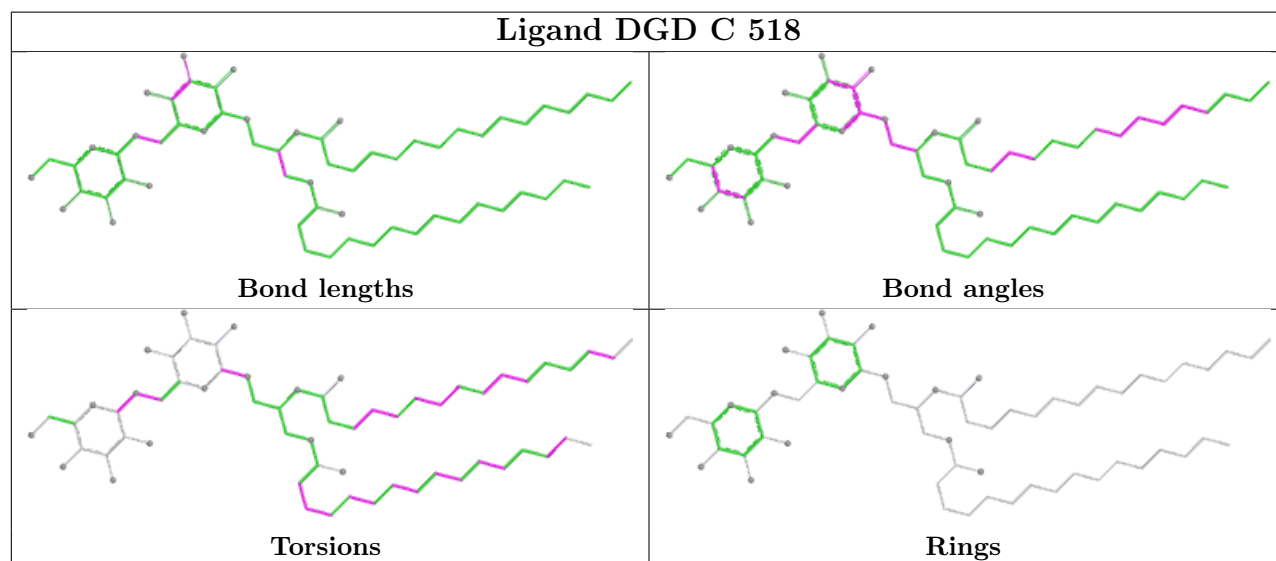
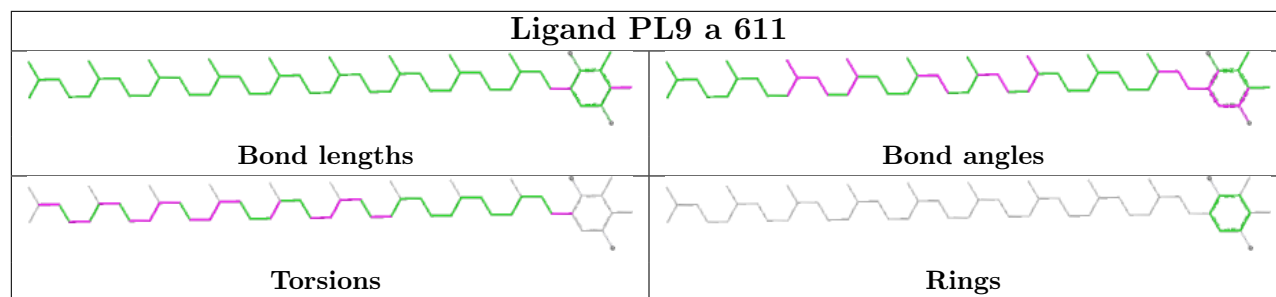
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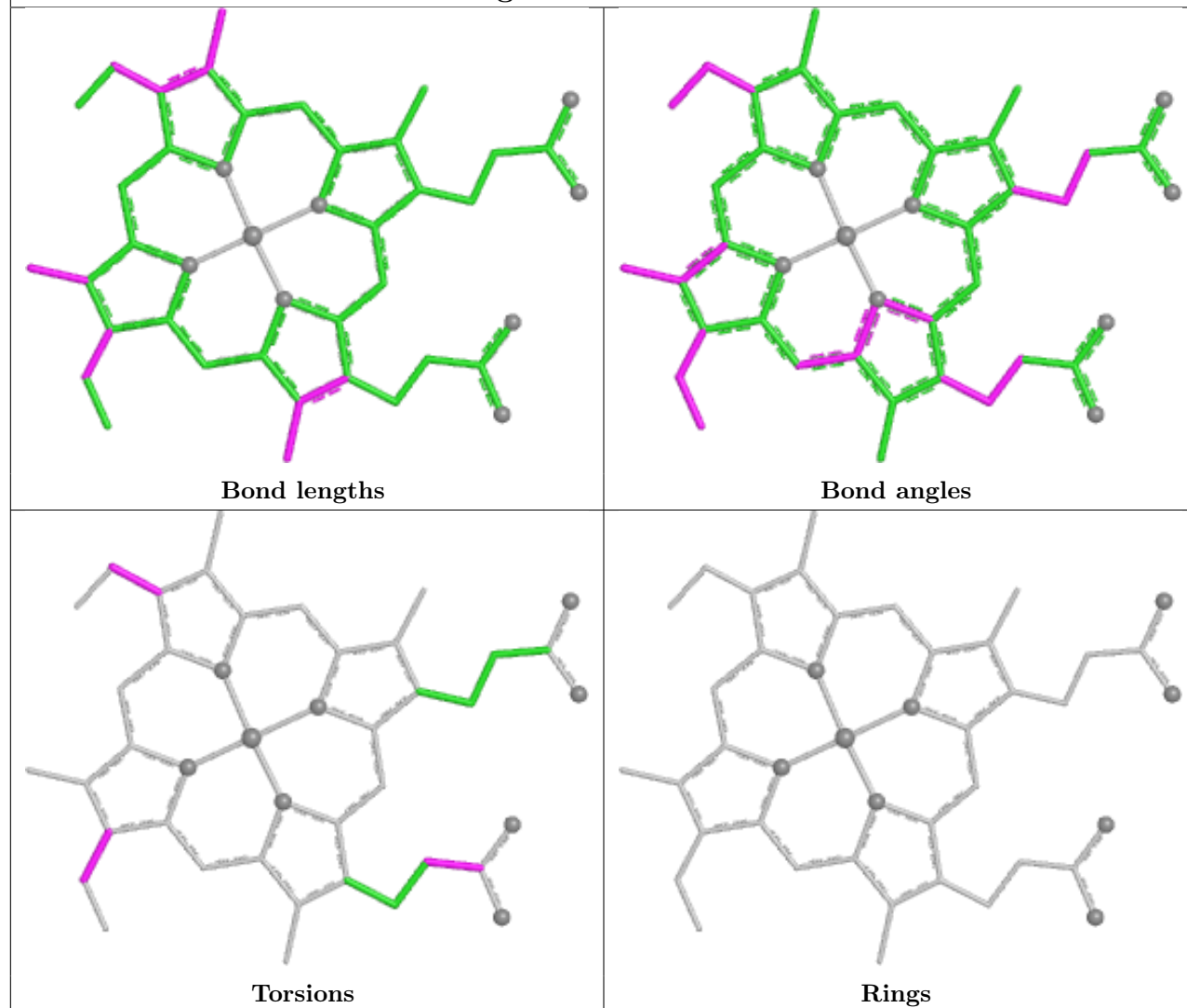
Ligand CLA C 505



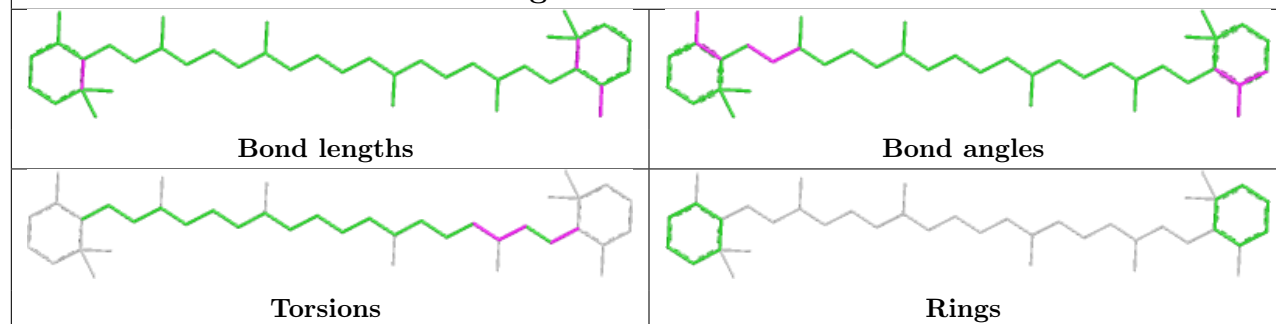


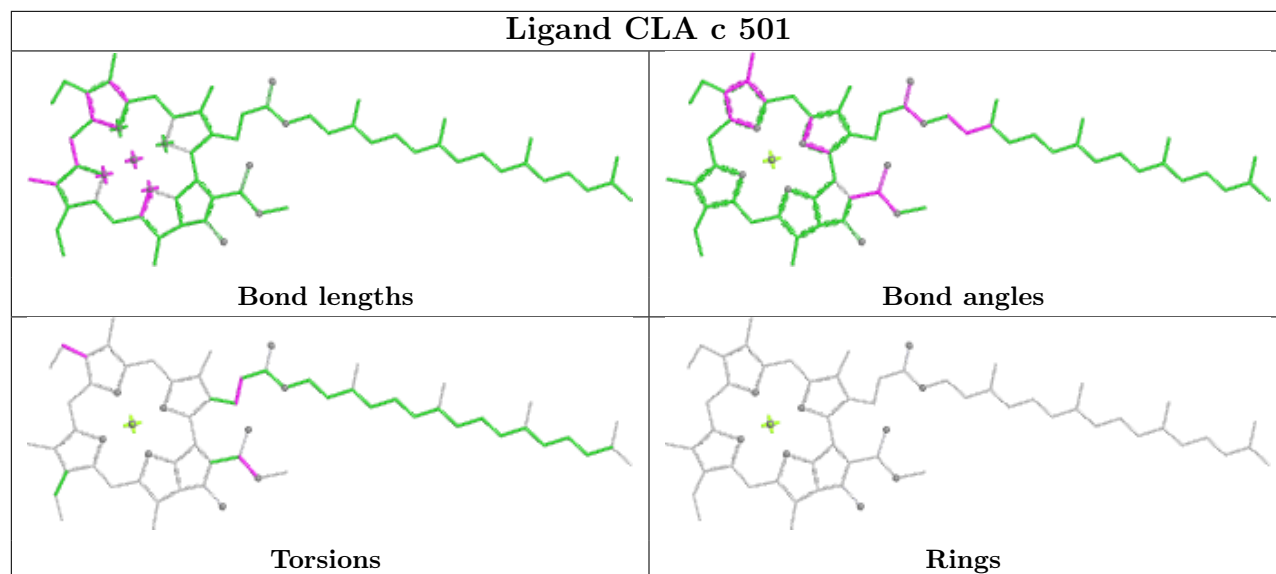
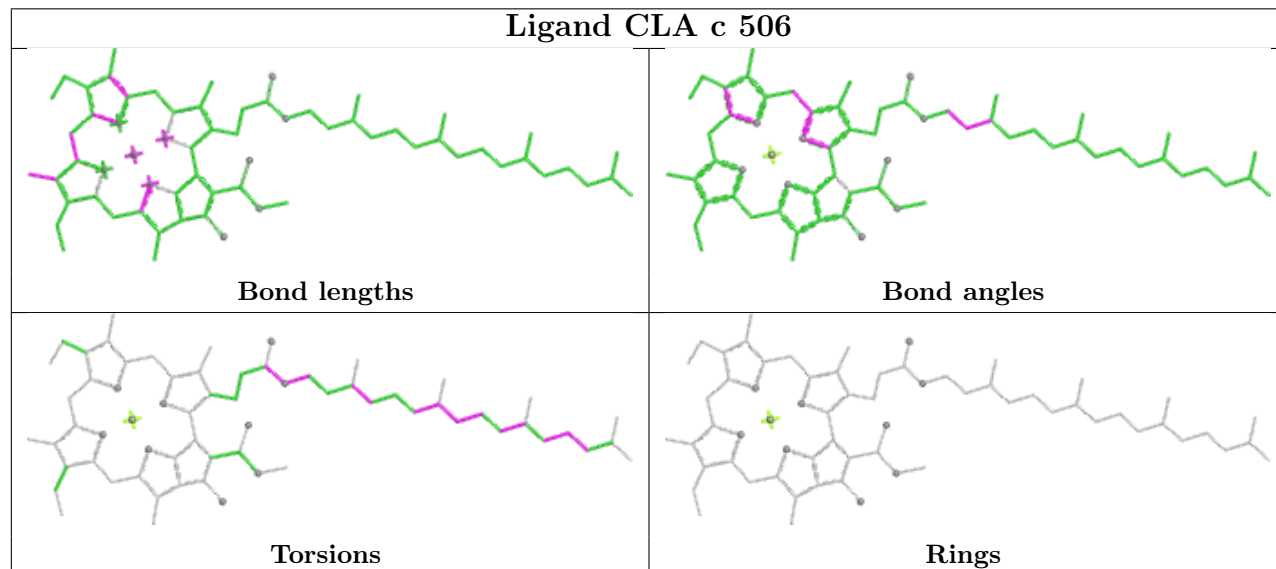
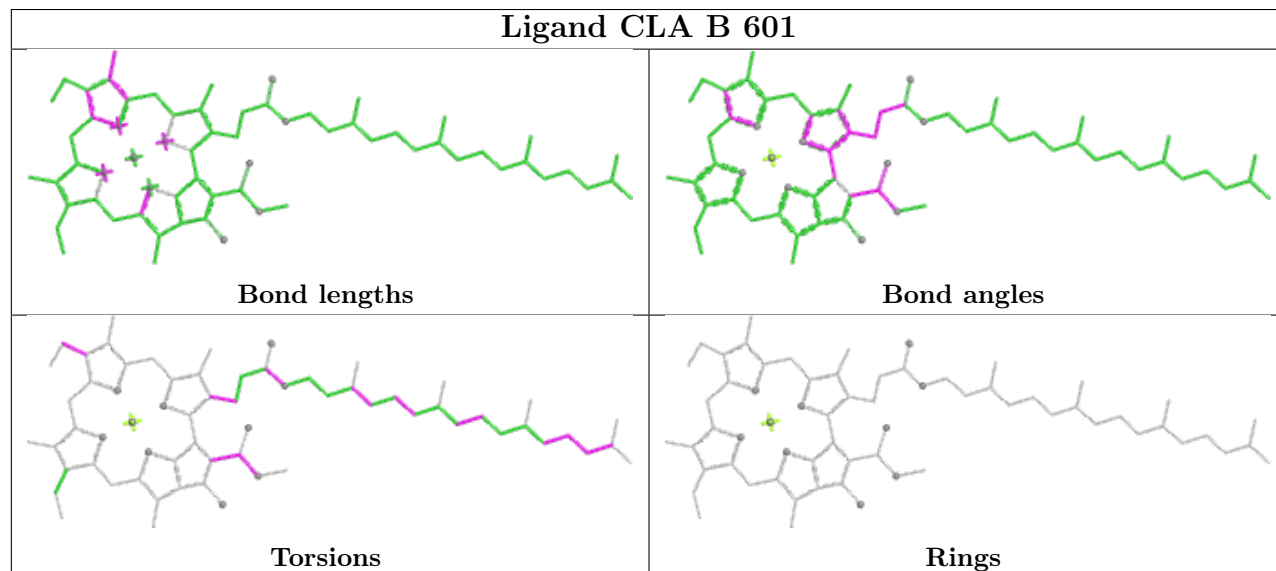


Ligand HEC v 201

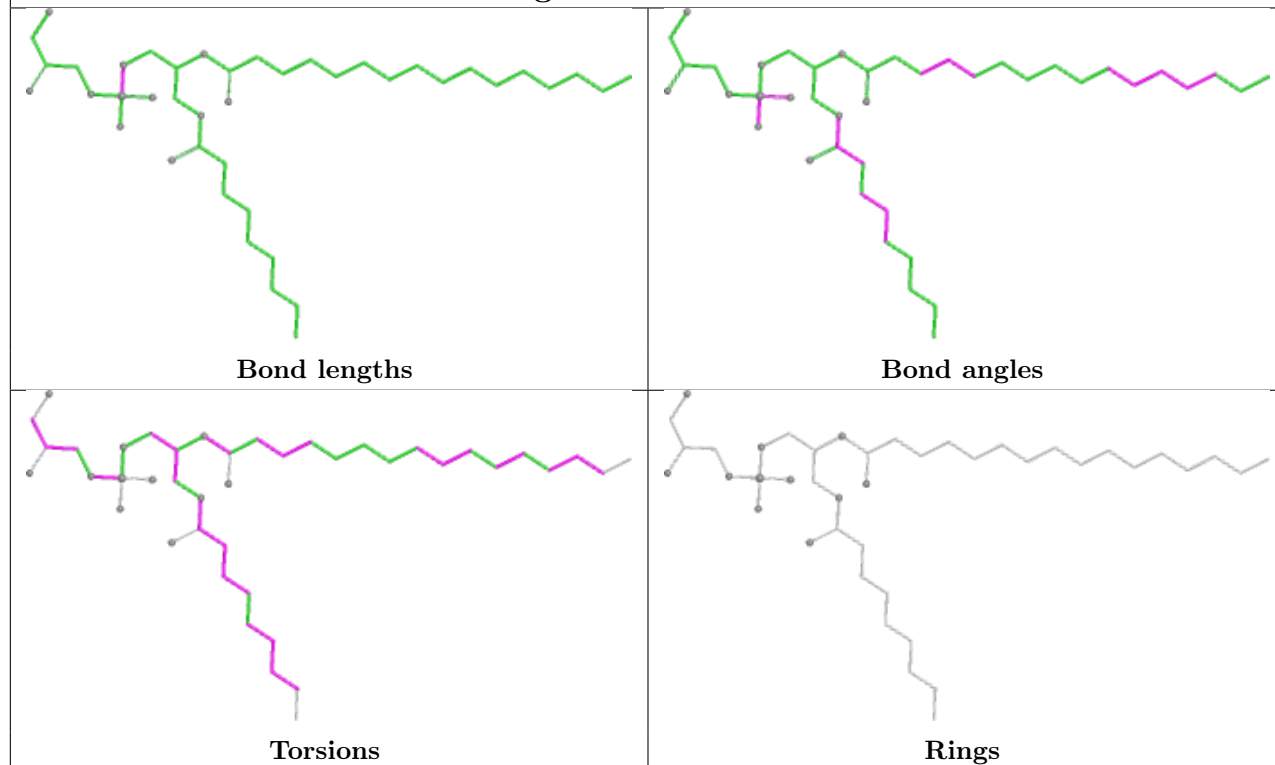


Ligand BCR D 405

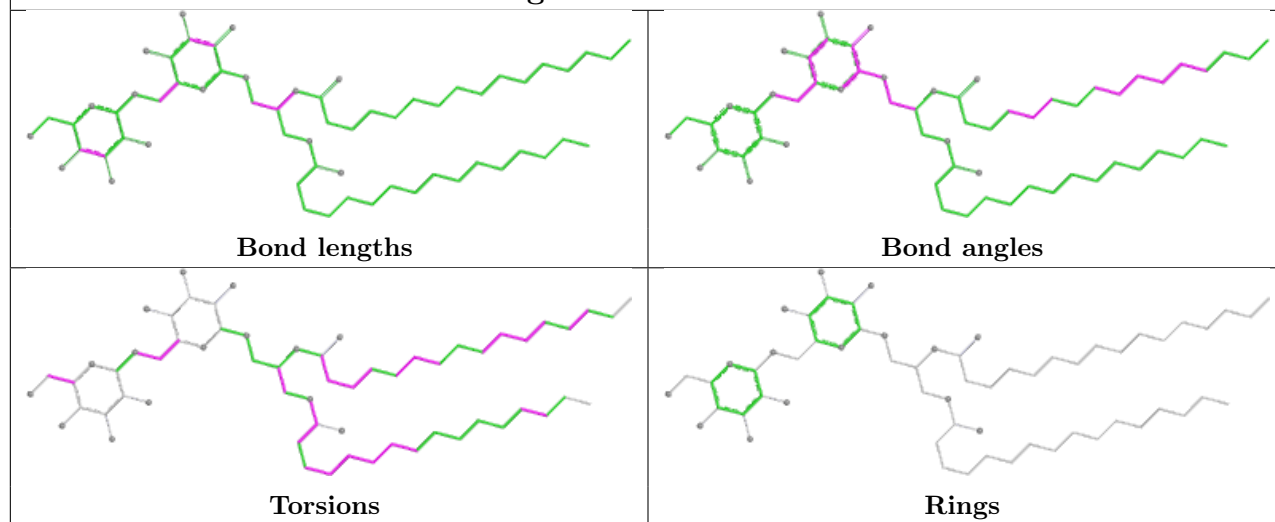


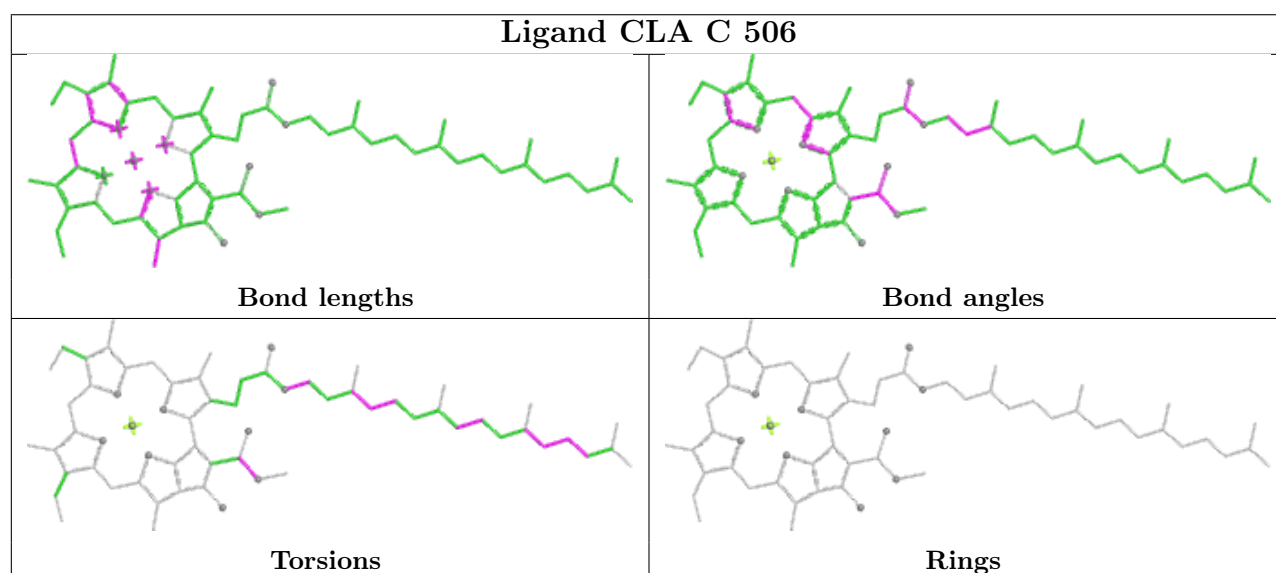
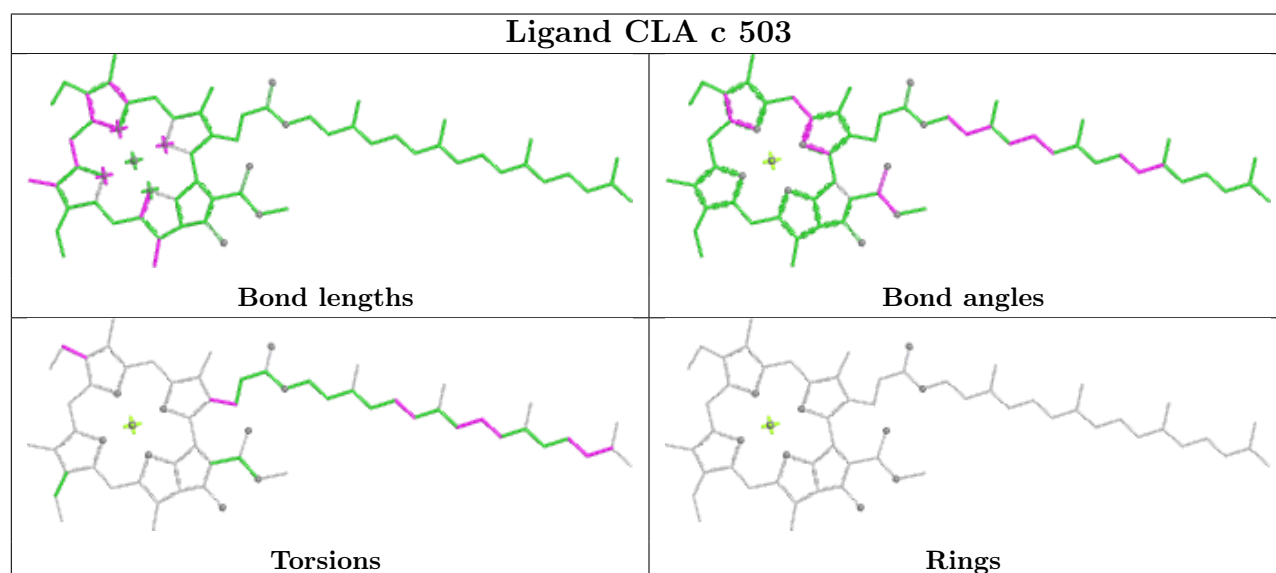
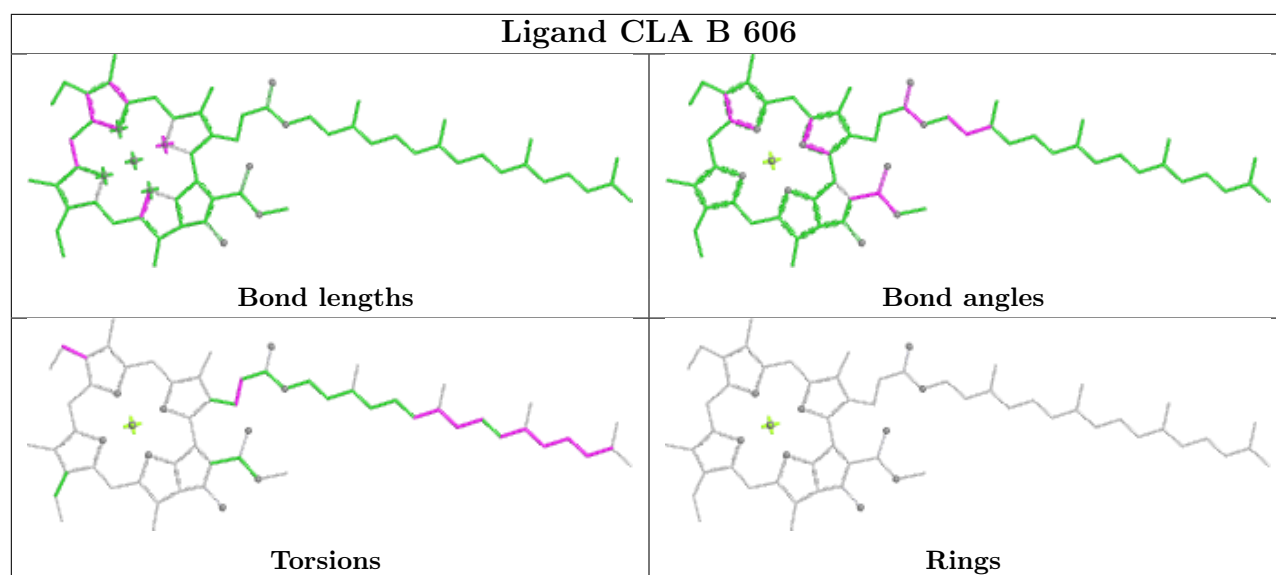
Ligand CLA c 501**Ligand CLA c 506****Ligand CLA B 601**

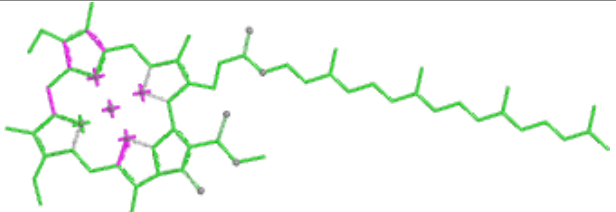
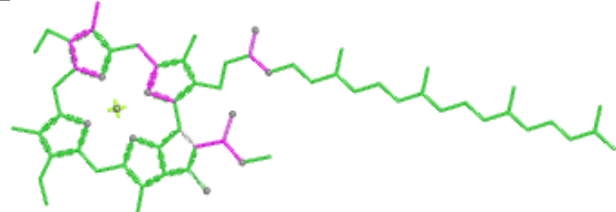
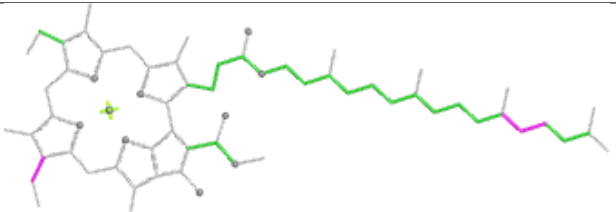
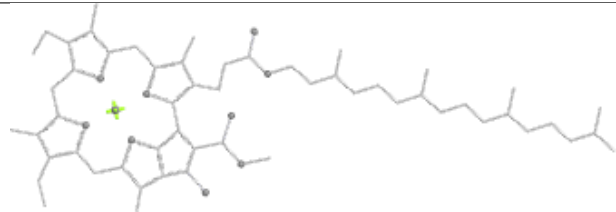
Ligand LHG e 102

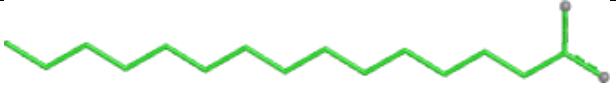
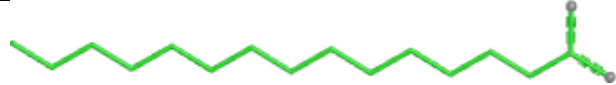
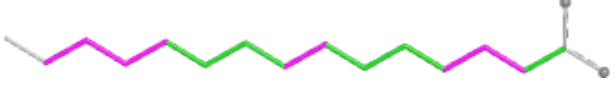
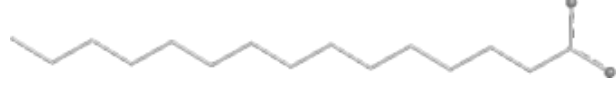


Ligand DGD C 517

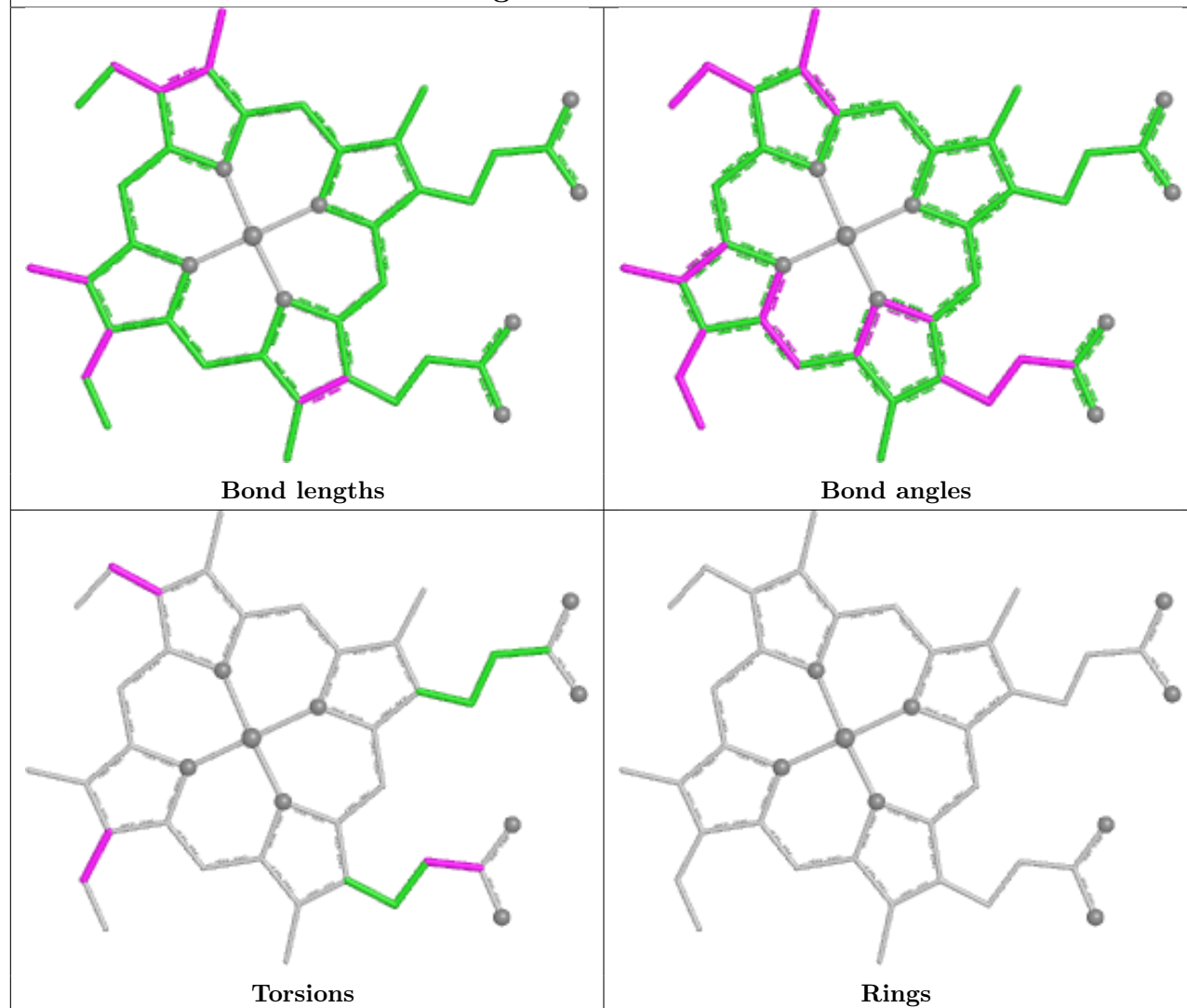




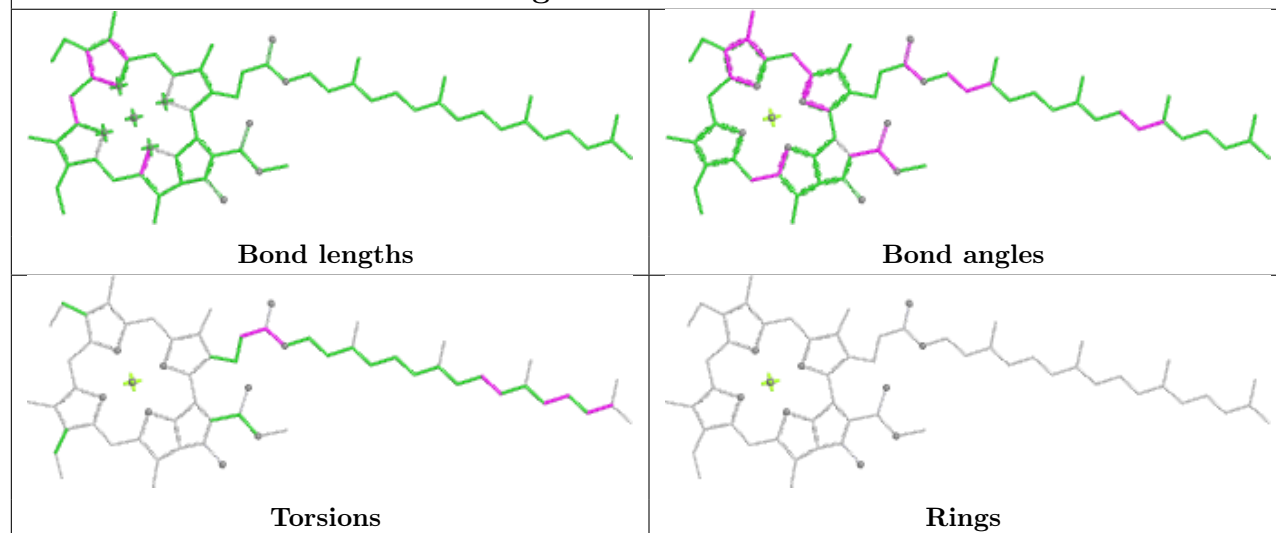
Ligand CLA A 612	
	
Bond lengths	Bond angles
	
Torsions	Rings

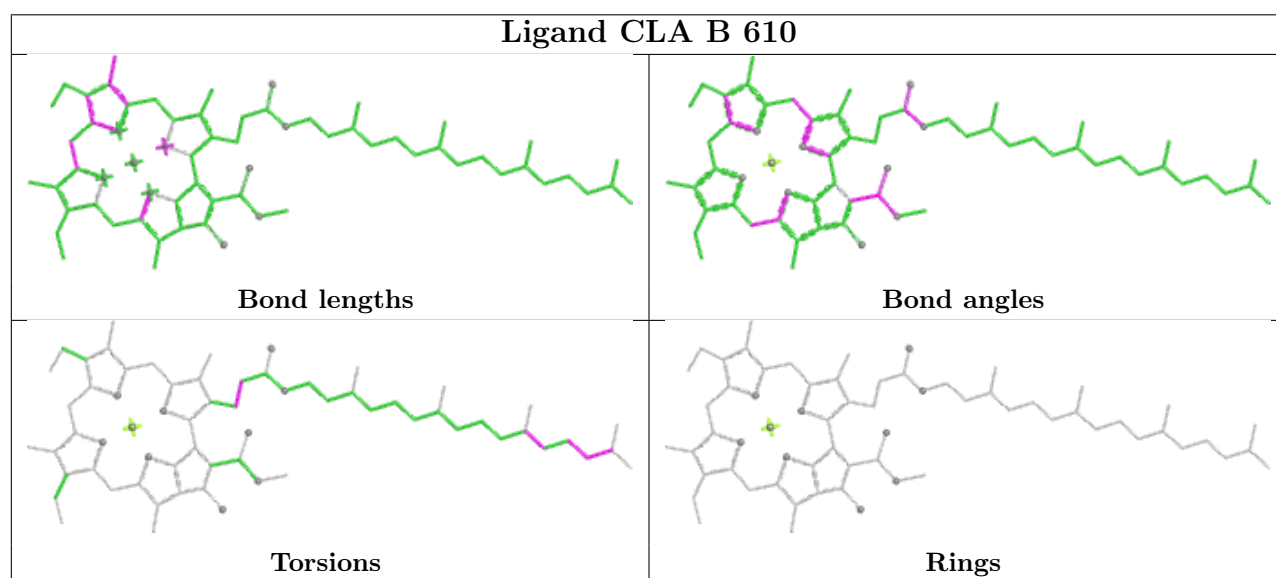
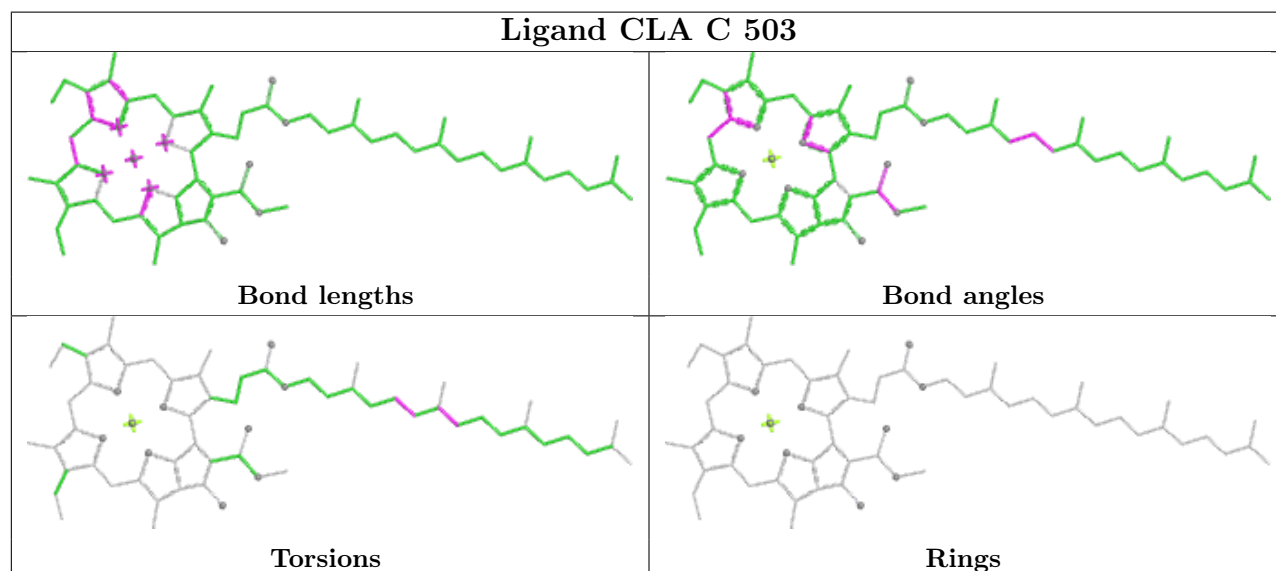
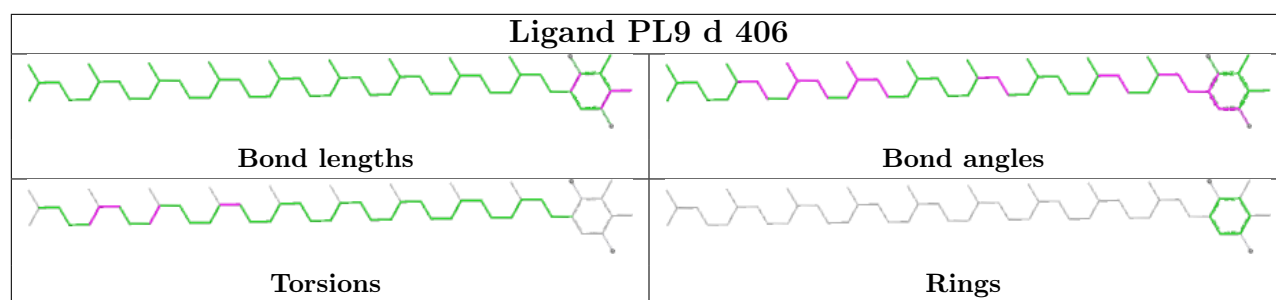
Ligand STE B 621	
	
Bond lengths	Bond angles
	
Torsions	Rings

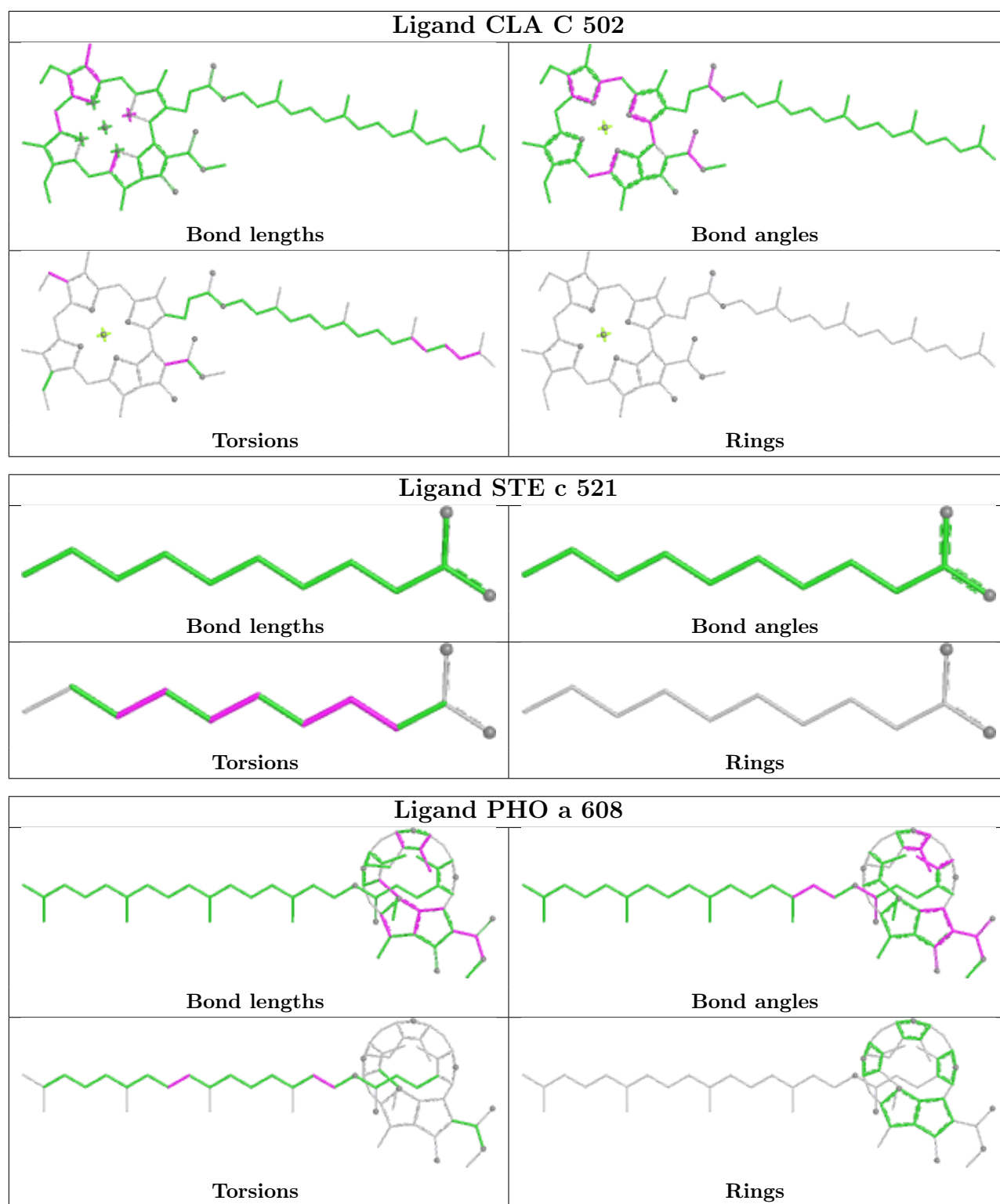
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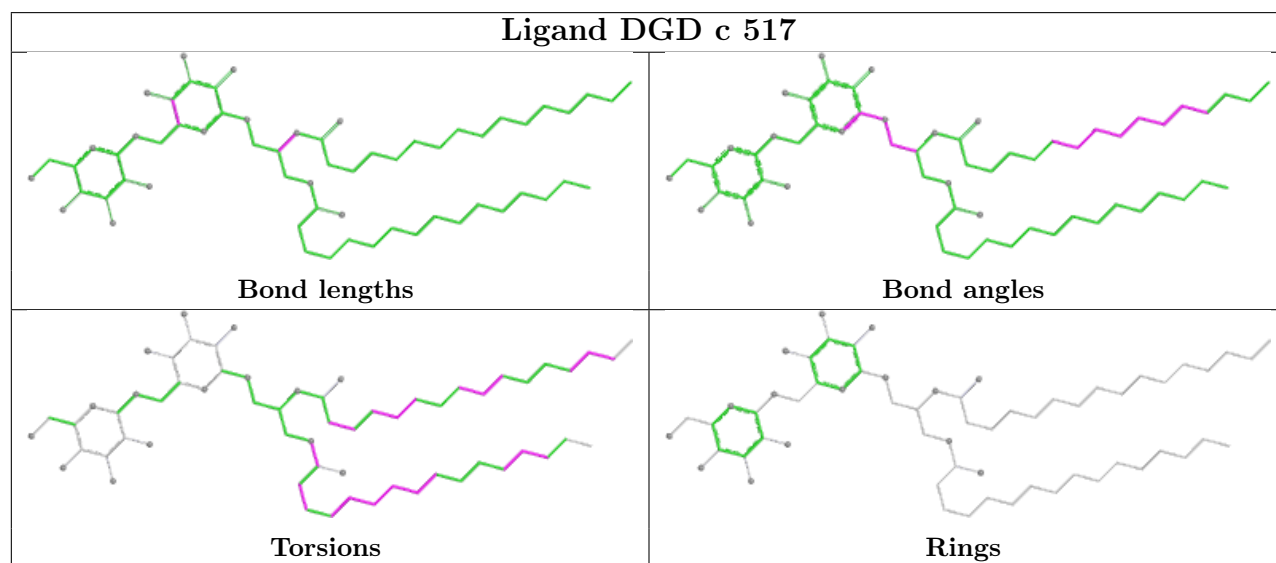
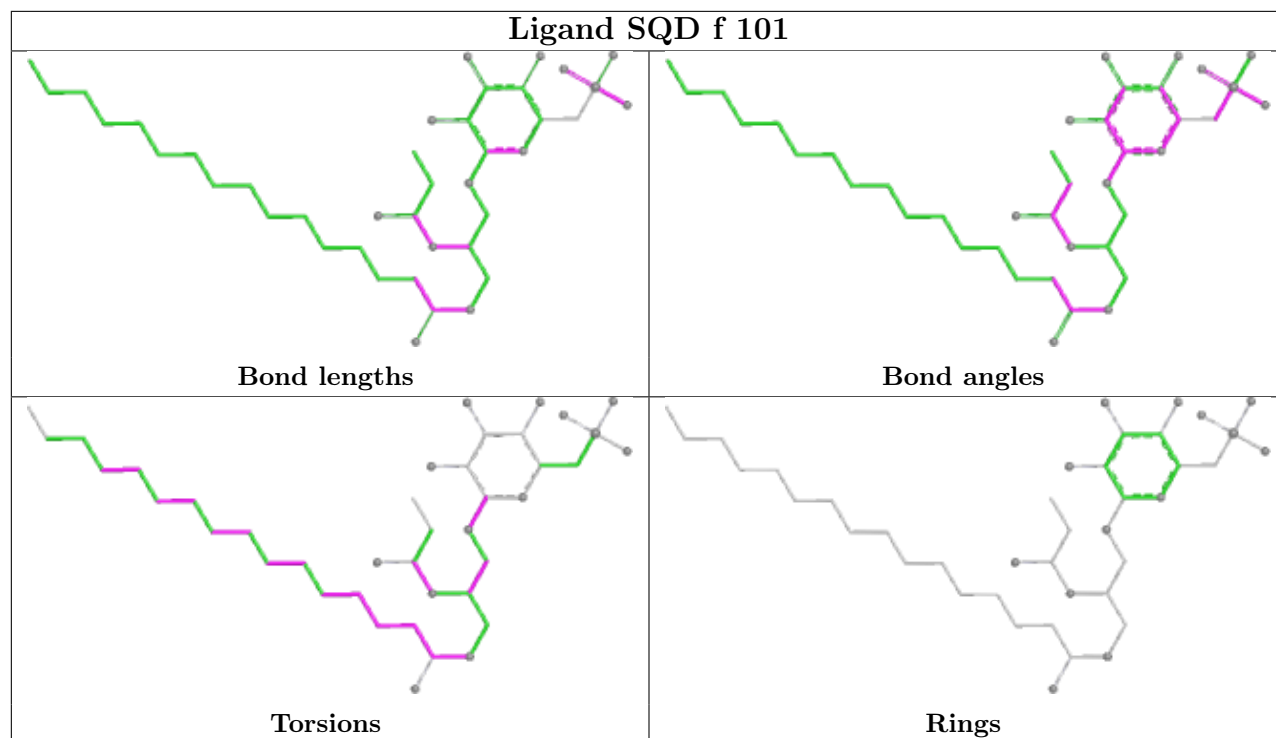


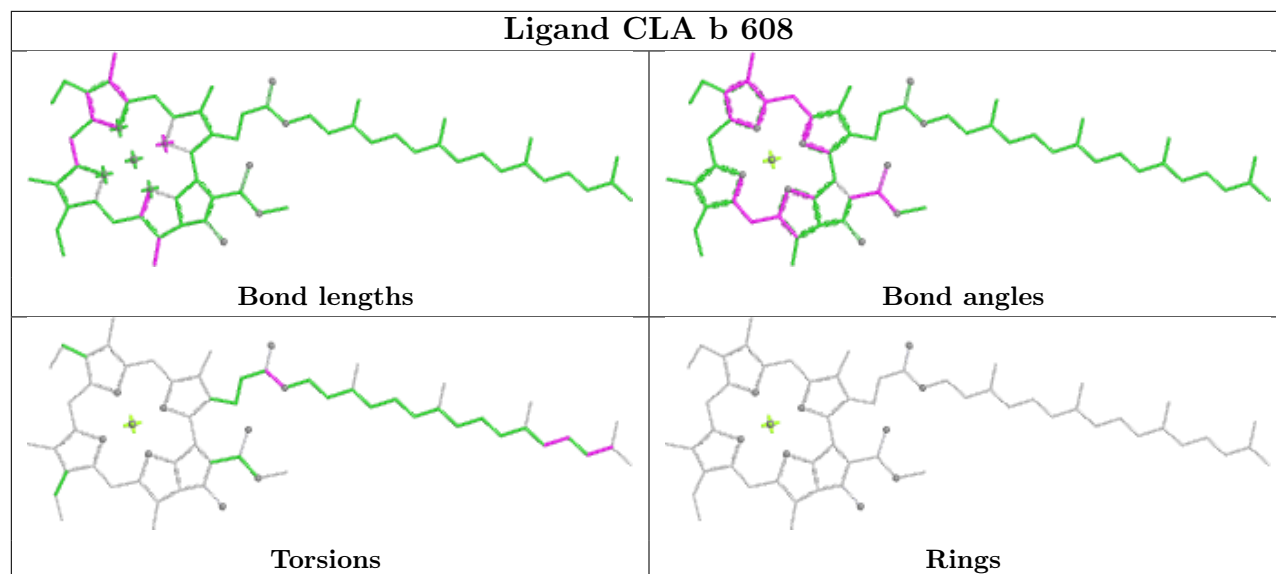
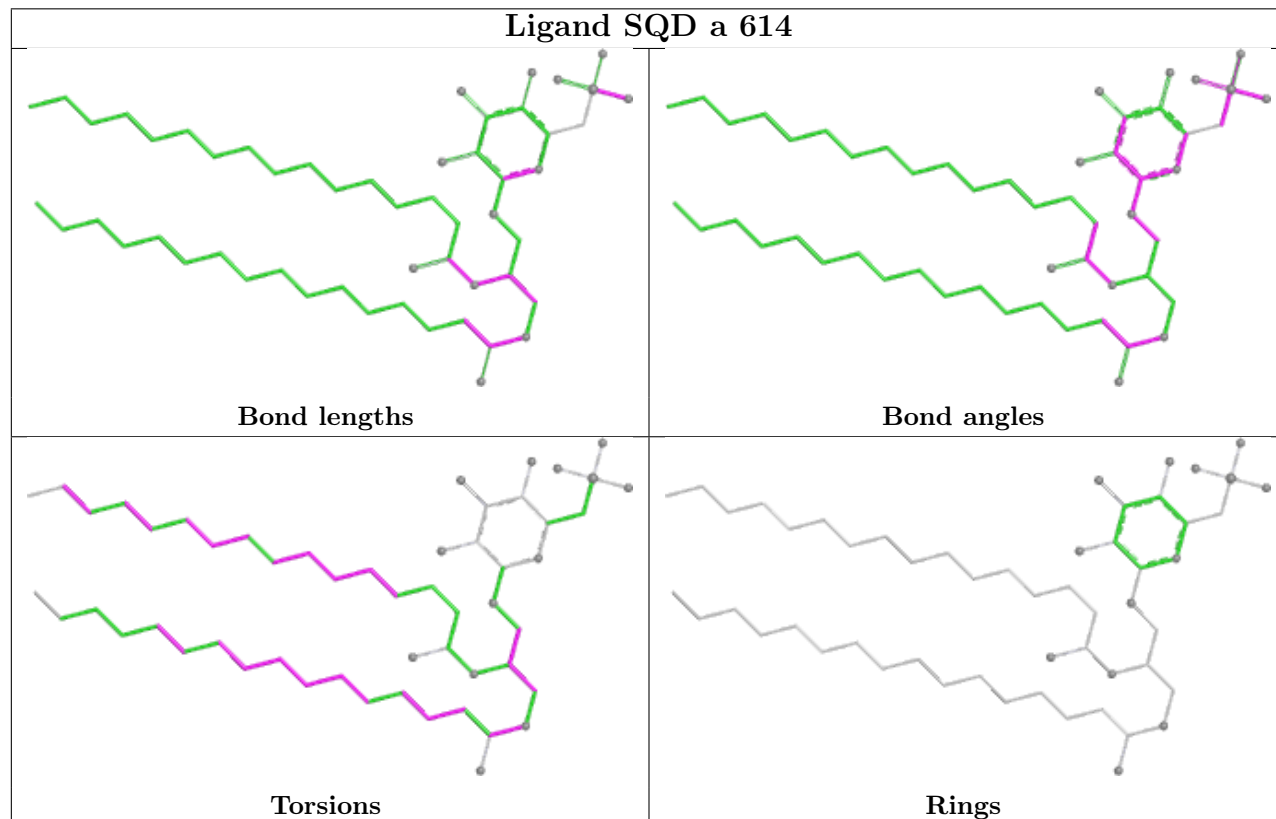
Ligand CLA B 612

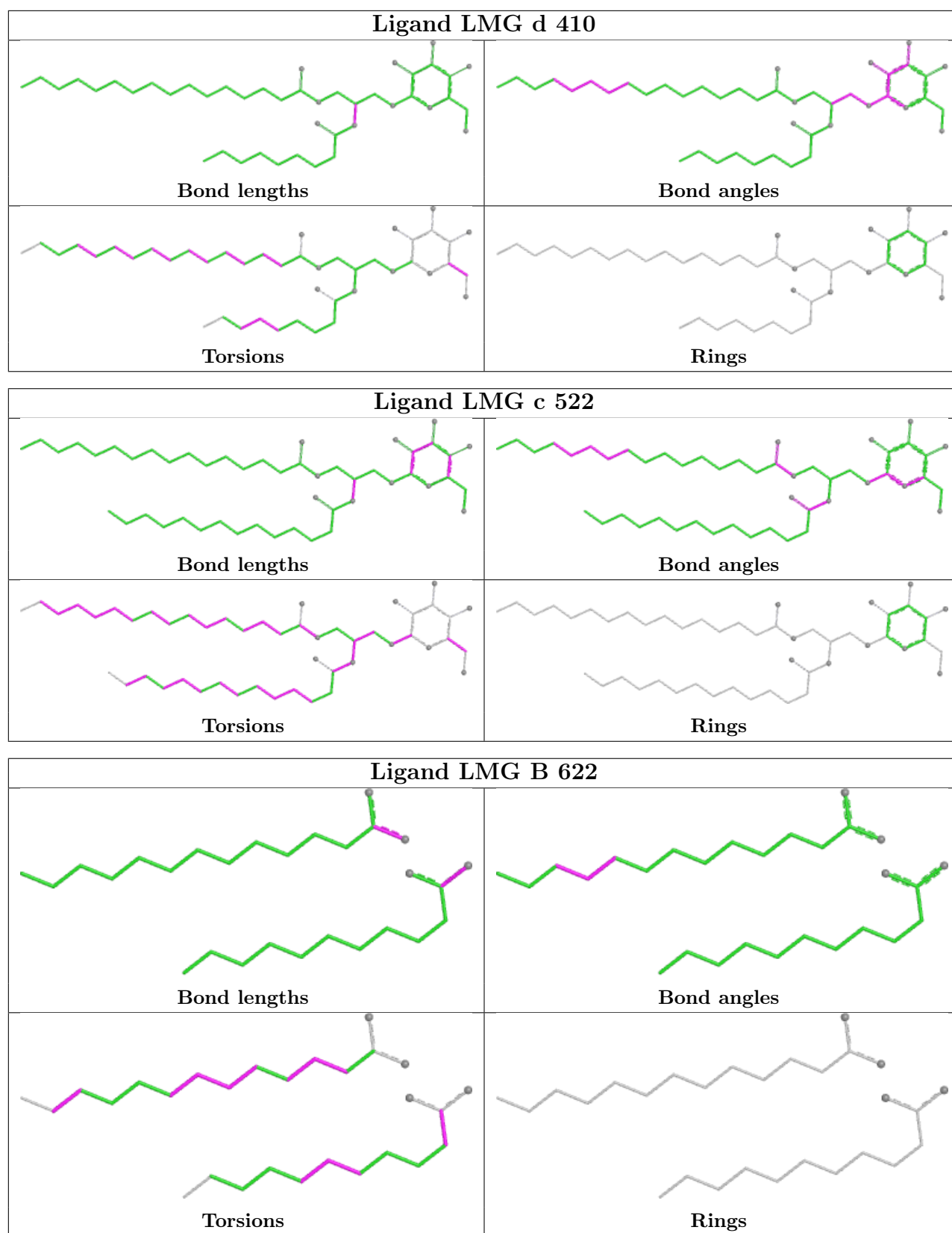


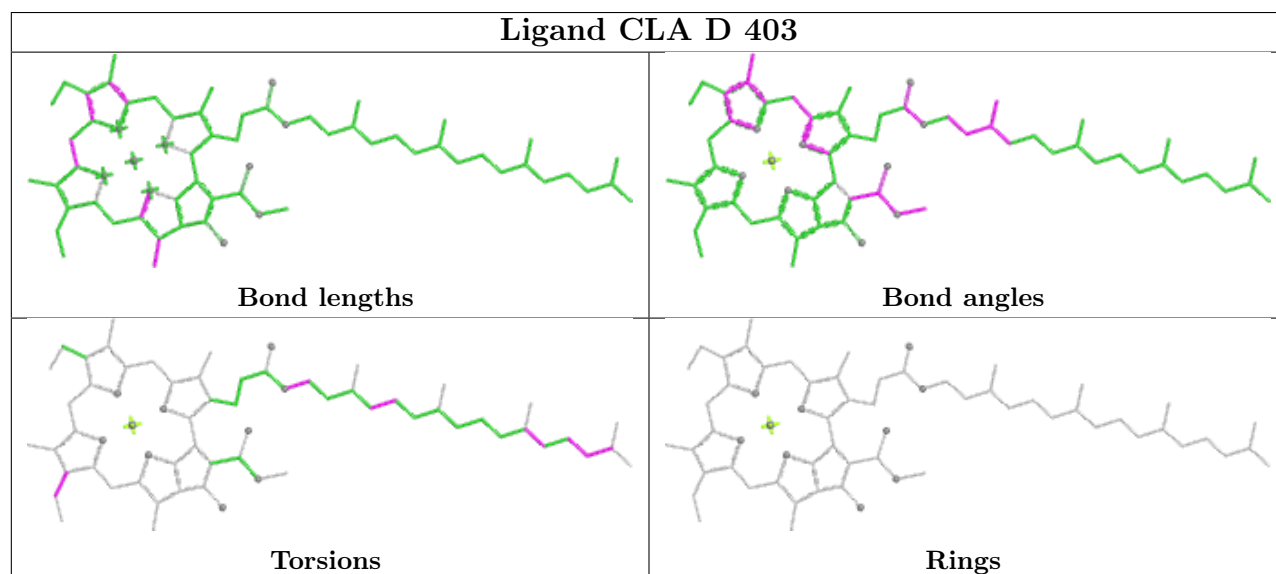
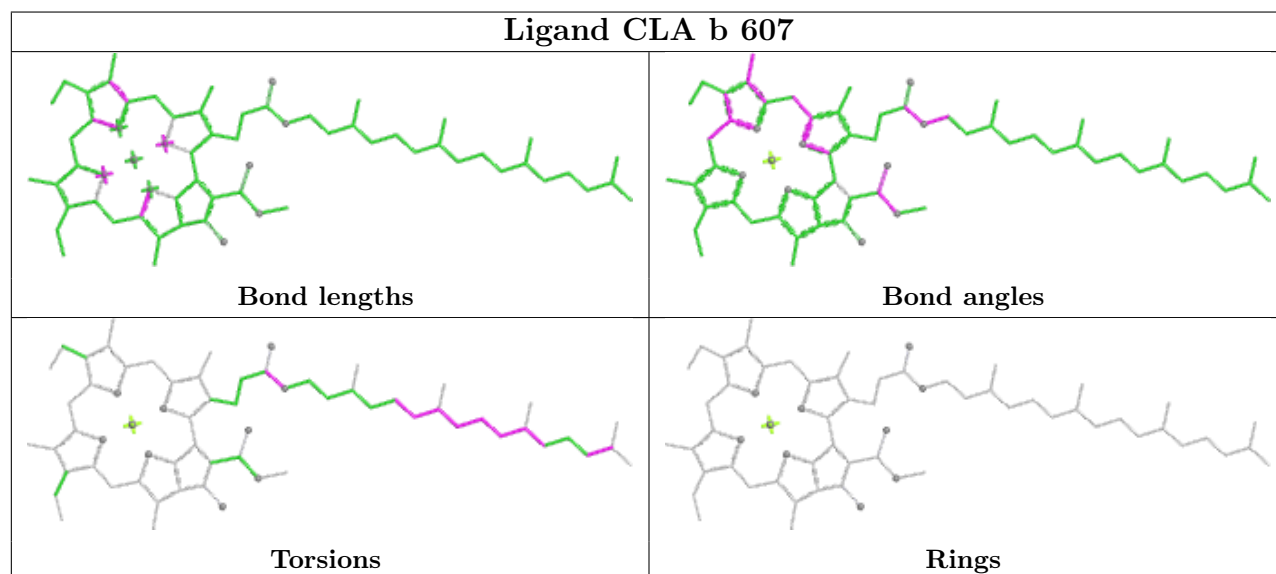
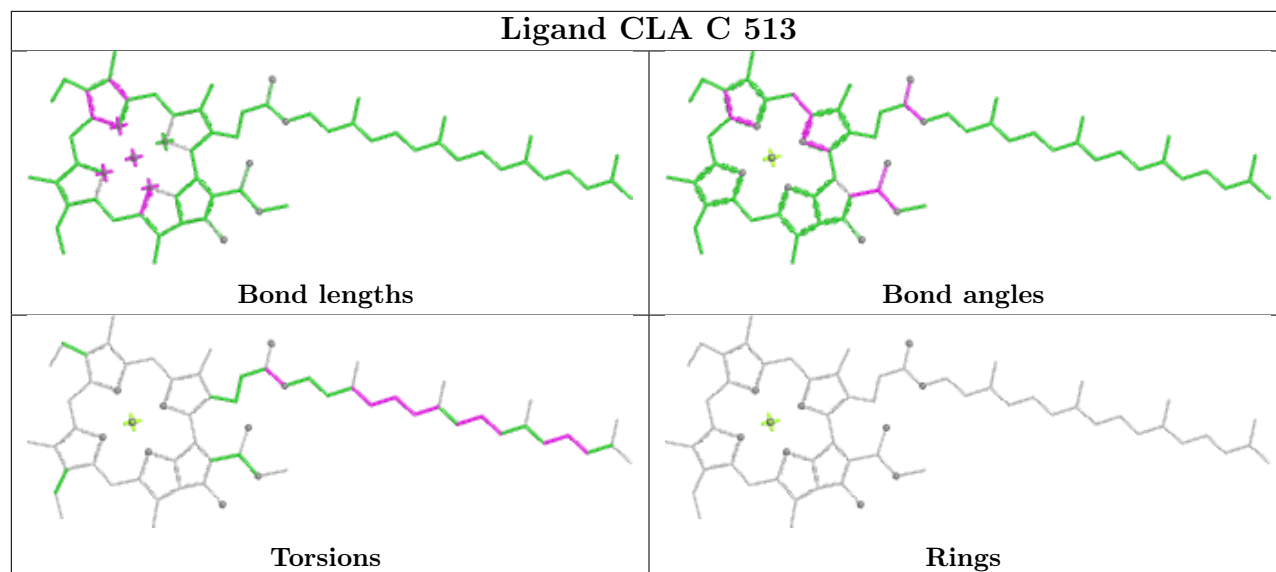


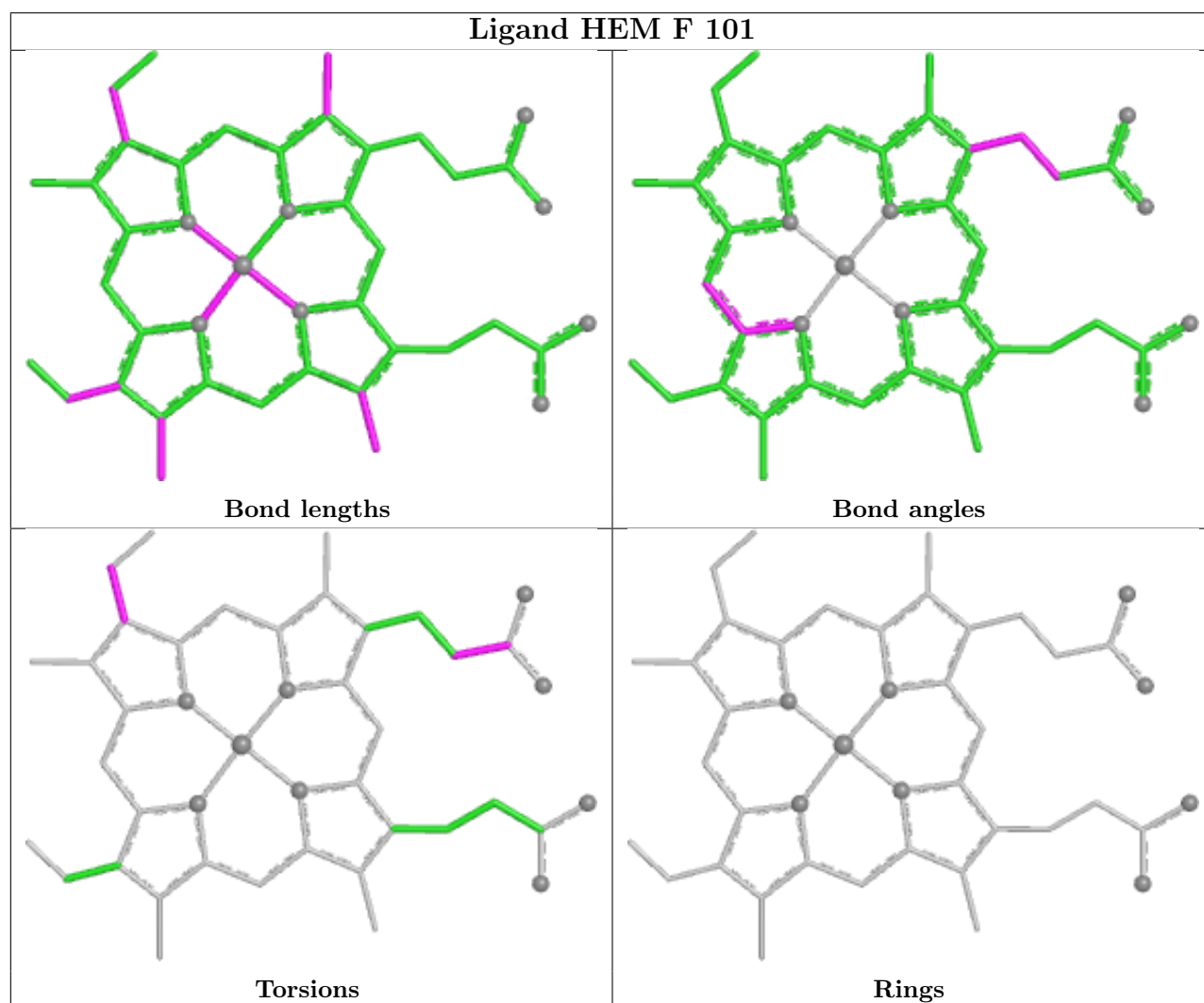
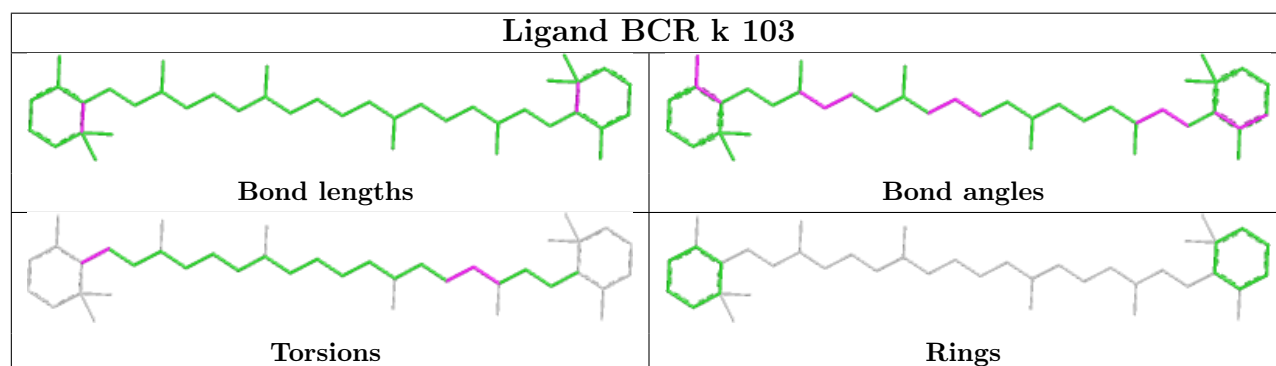
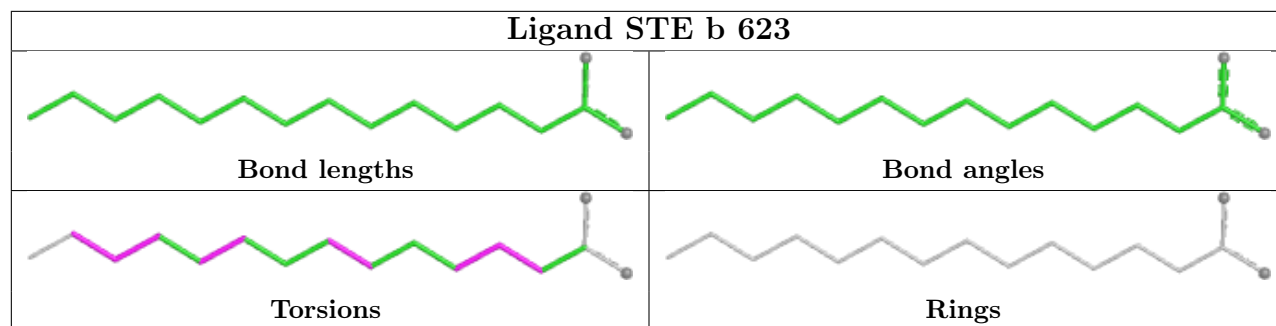


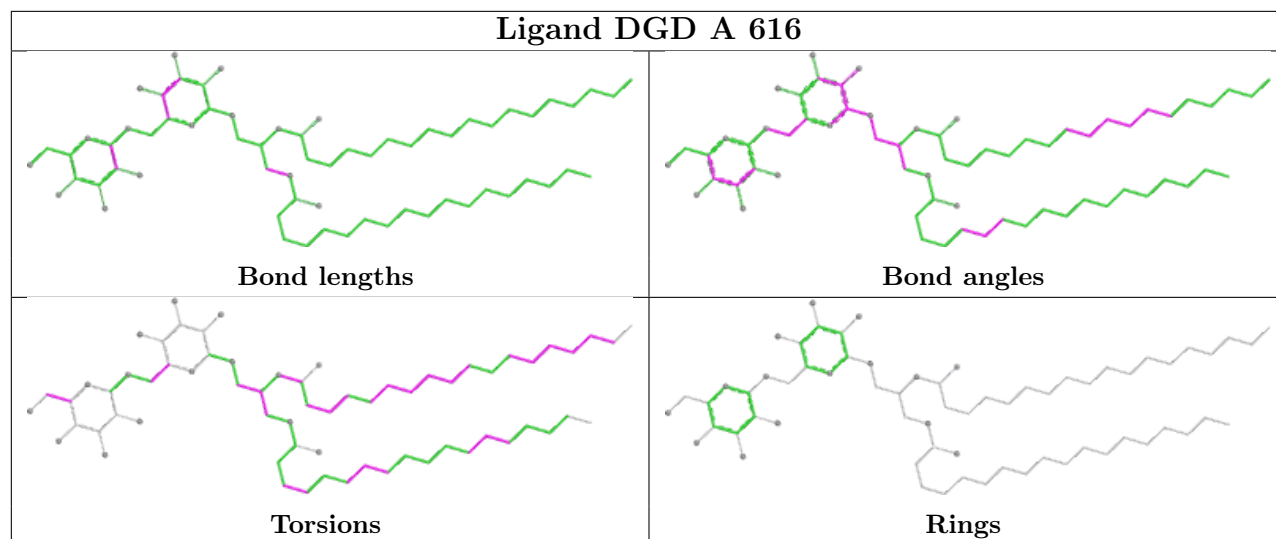
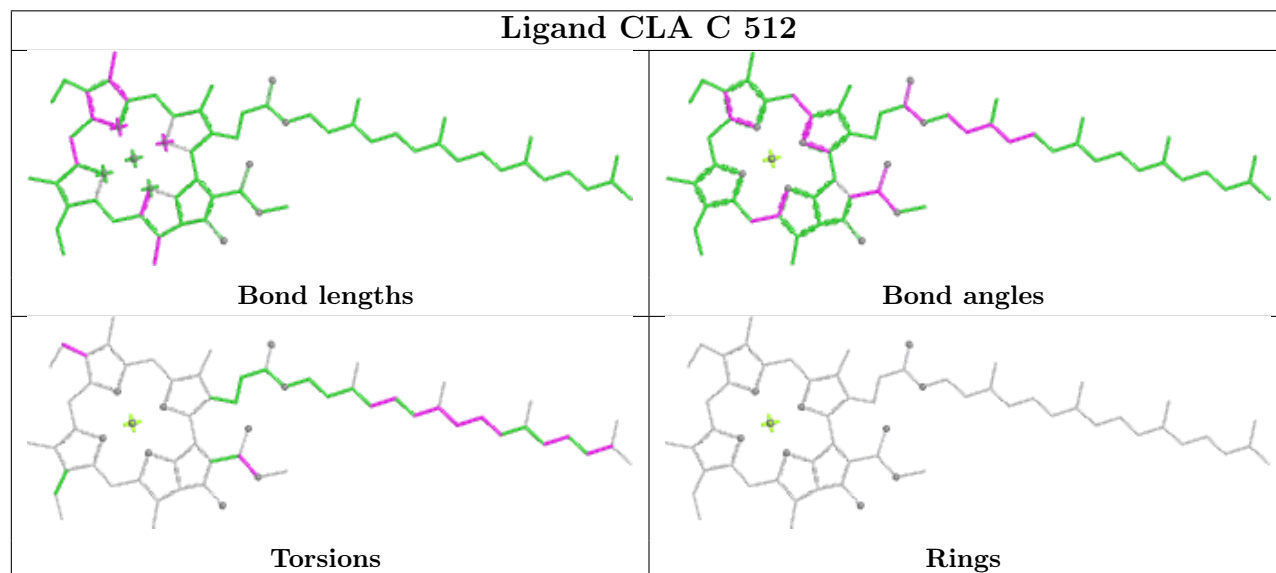
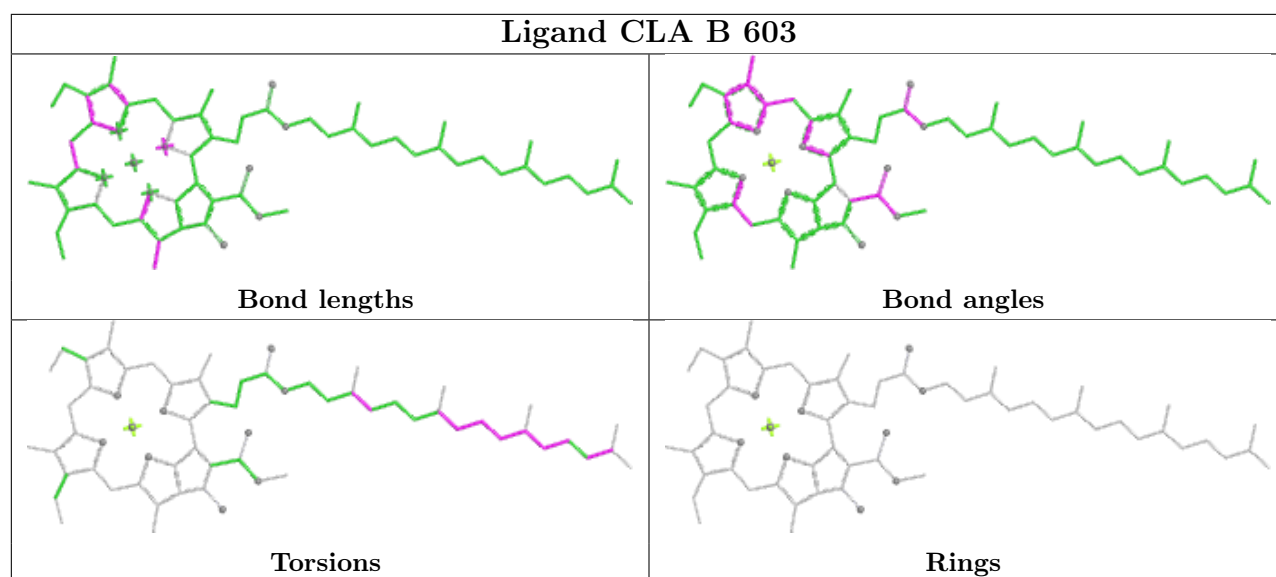


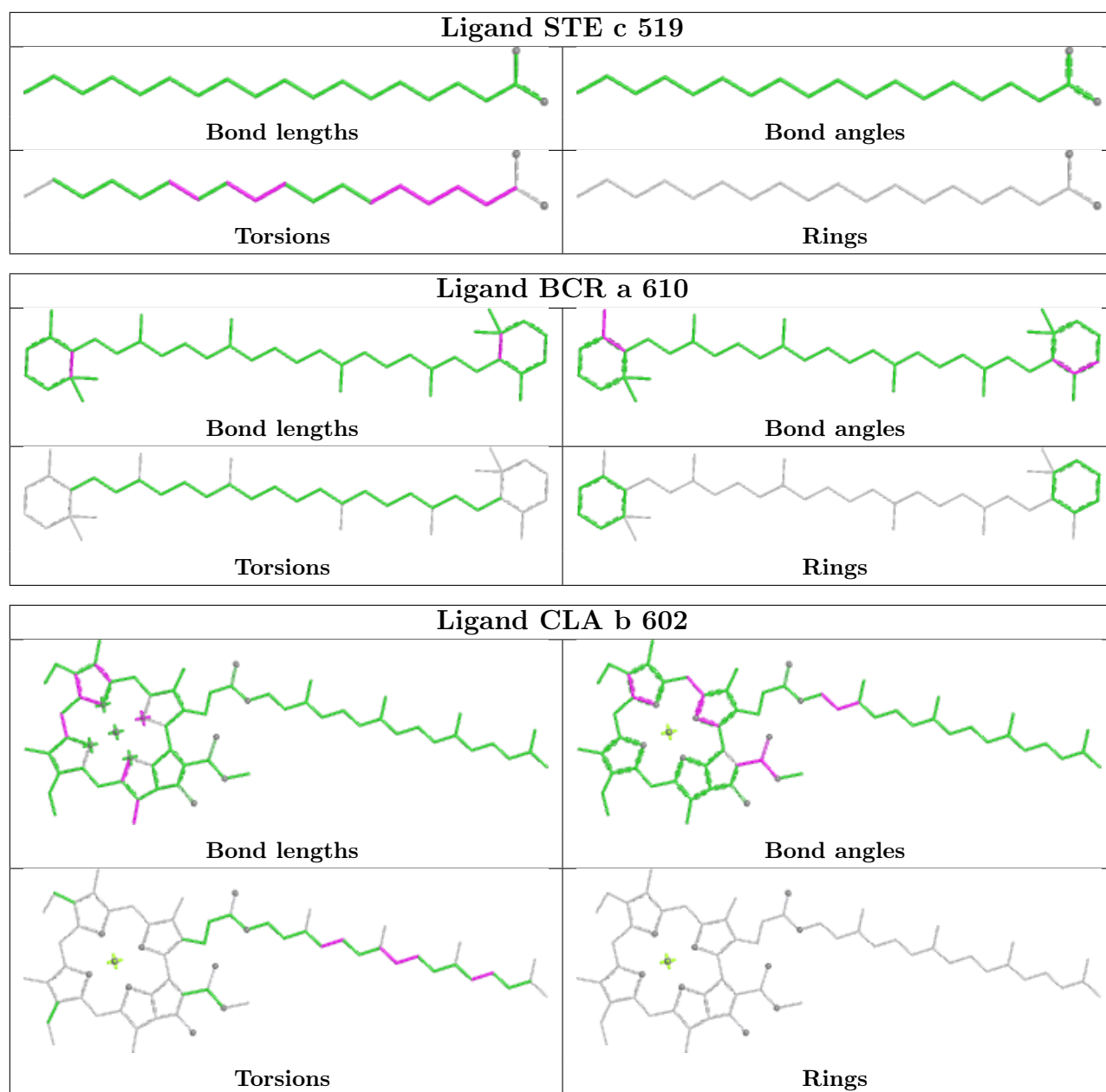
Ligand CLA b 608**Ligand SQD a 614**

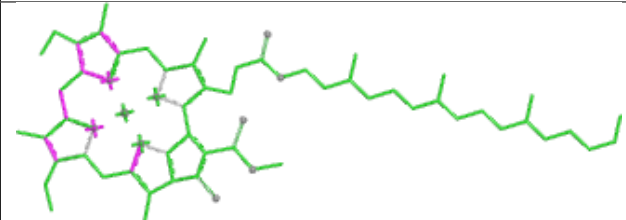
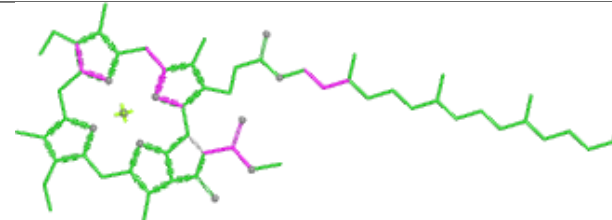
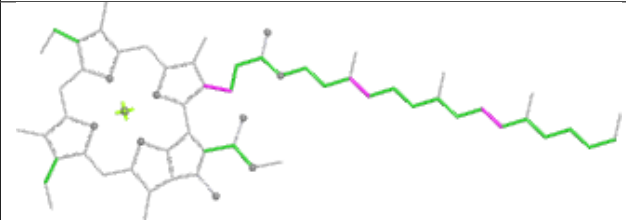
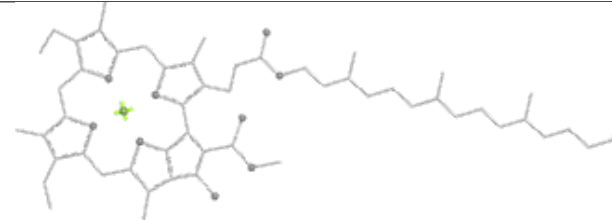
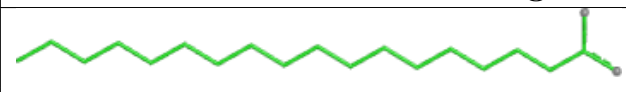
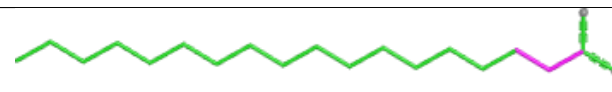
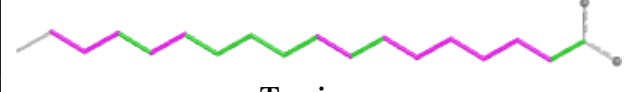
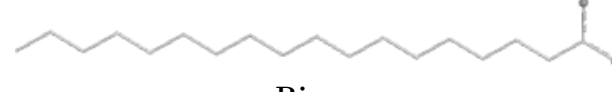
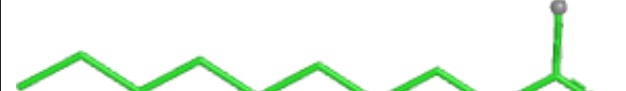




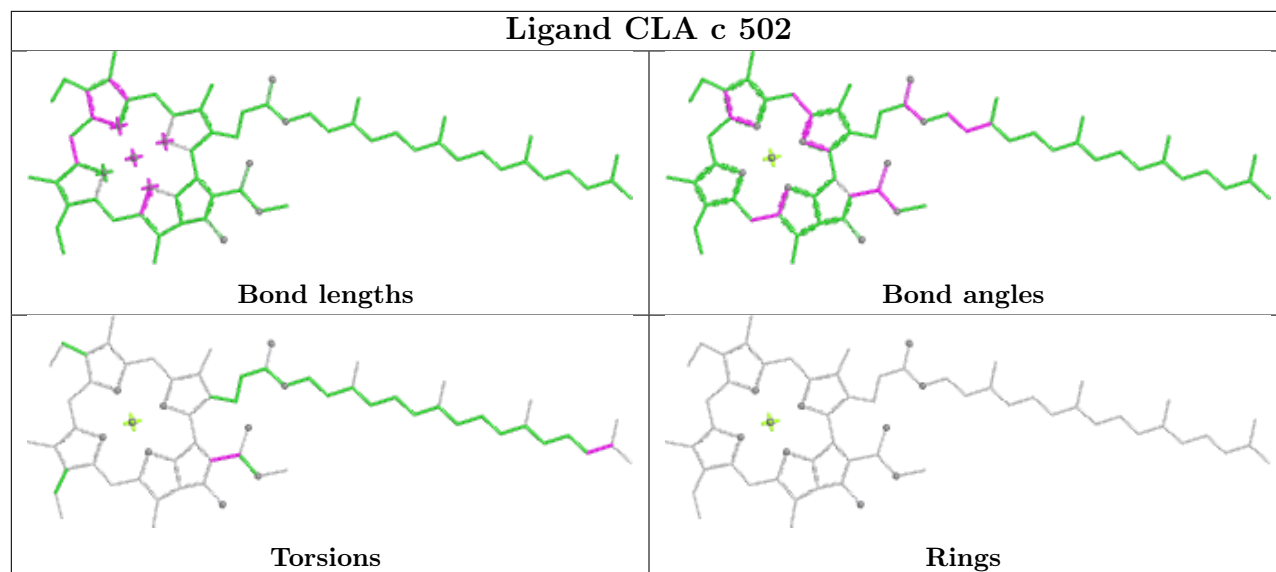




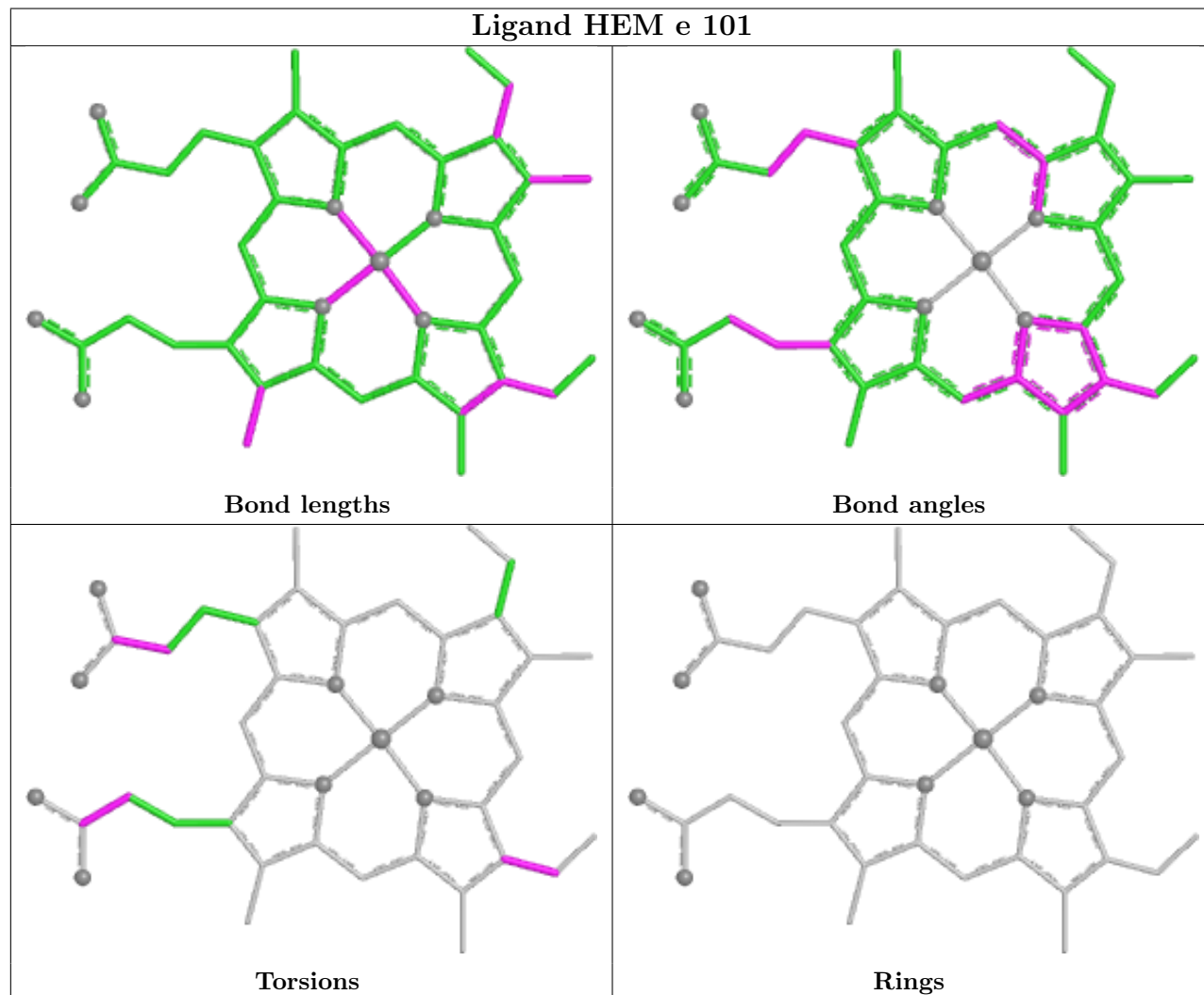


Ligand CLA c 508	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand STE d 412	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand STE a 617	
 Bond lengths	 Bond angles
 Torsions	 Rings

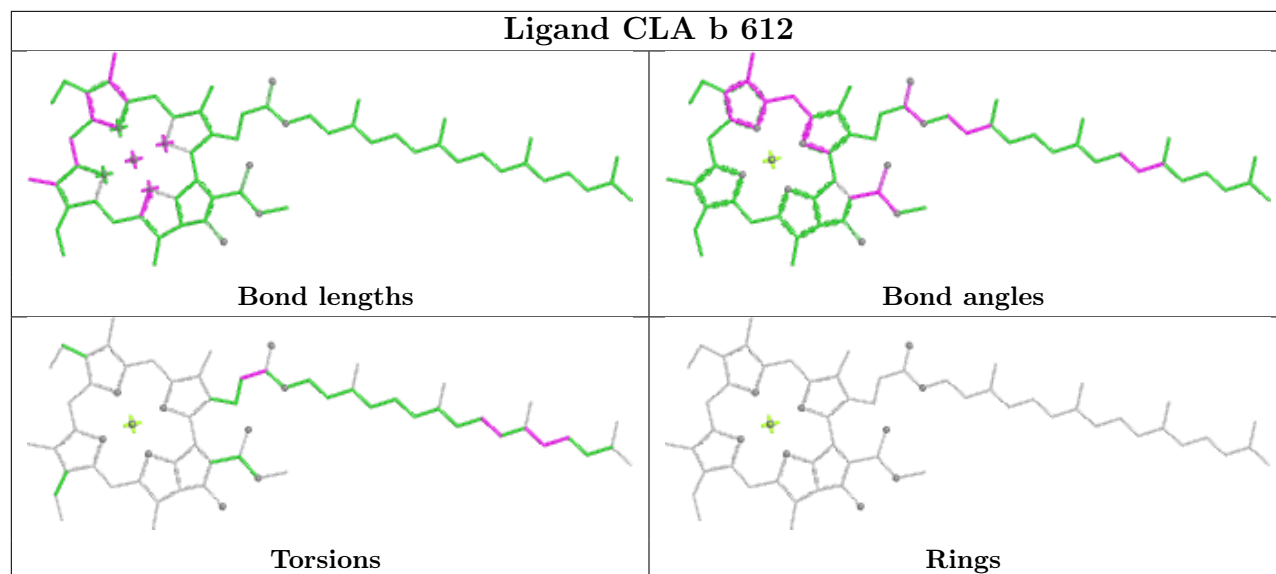
Ligand CLA c 502



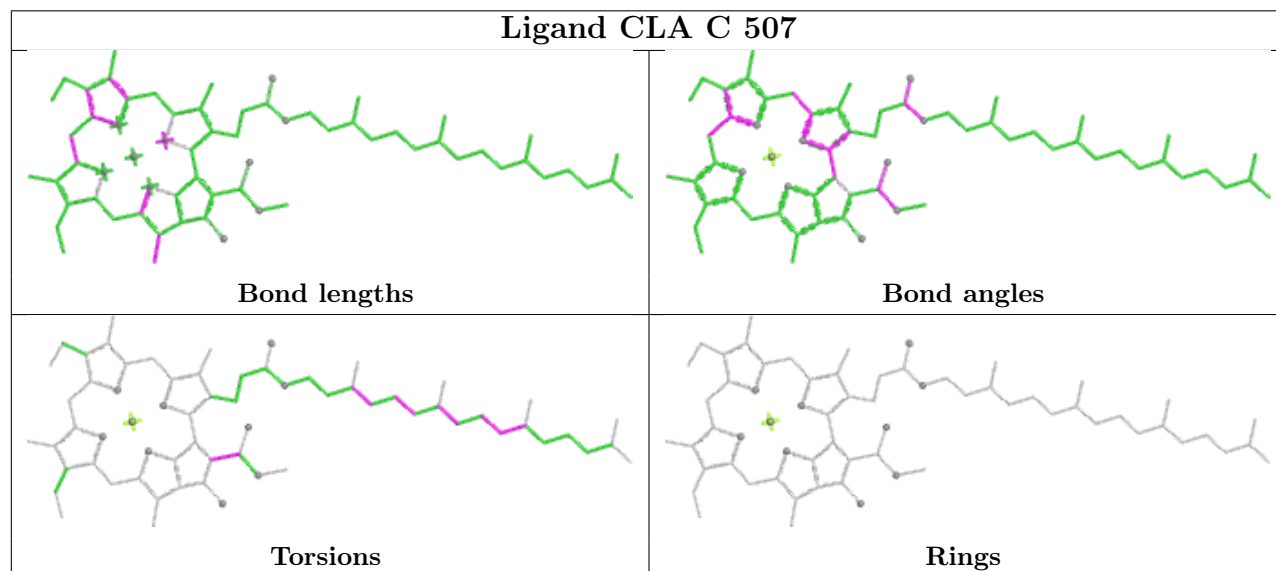
Ligand HEM e 101



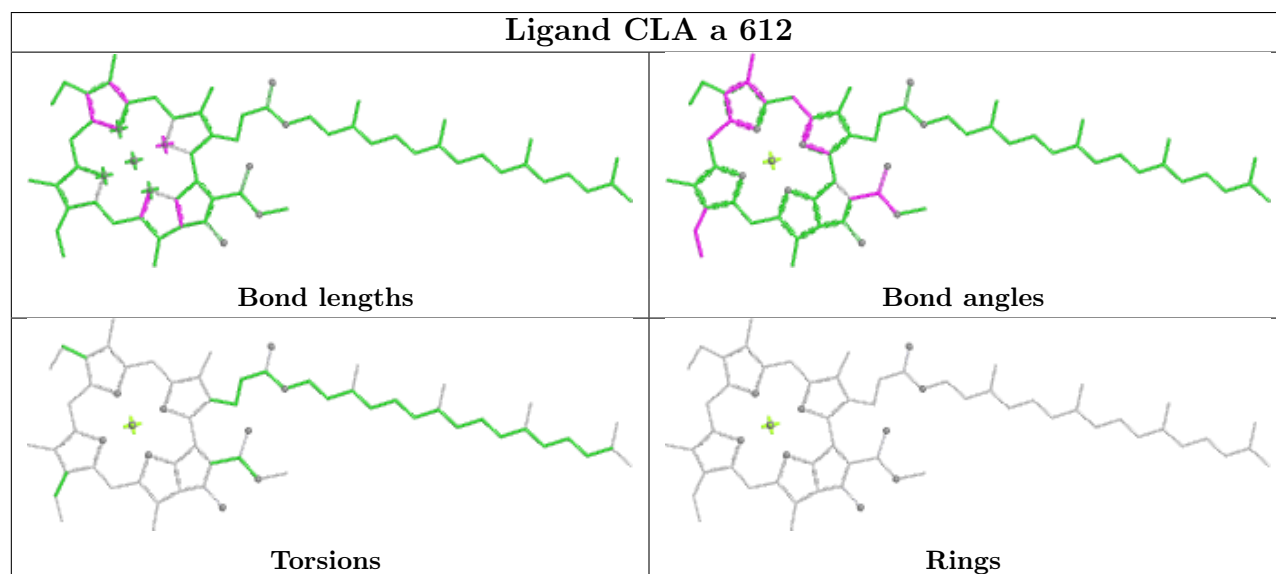
Ligand CLA b 612

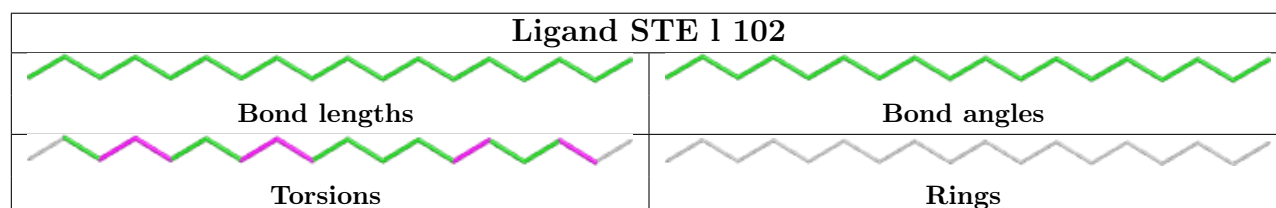
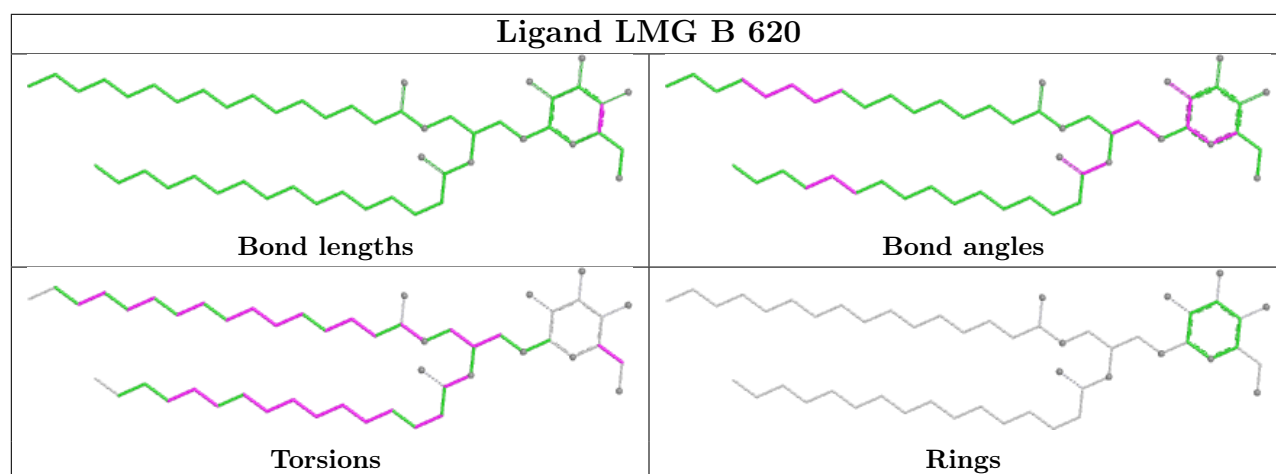
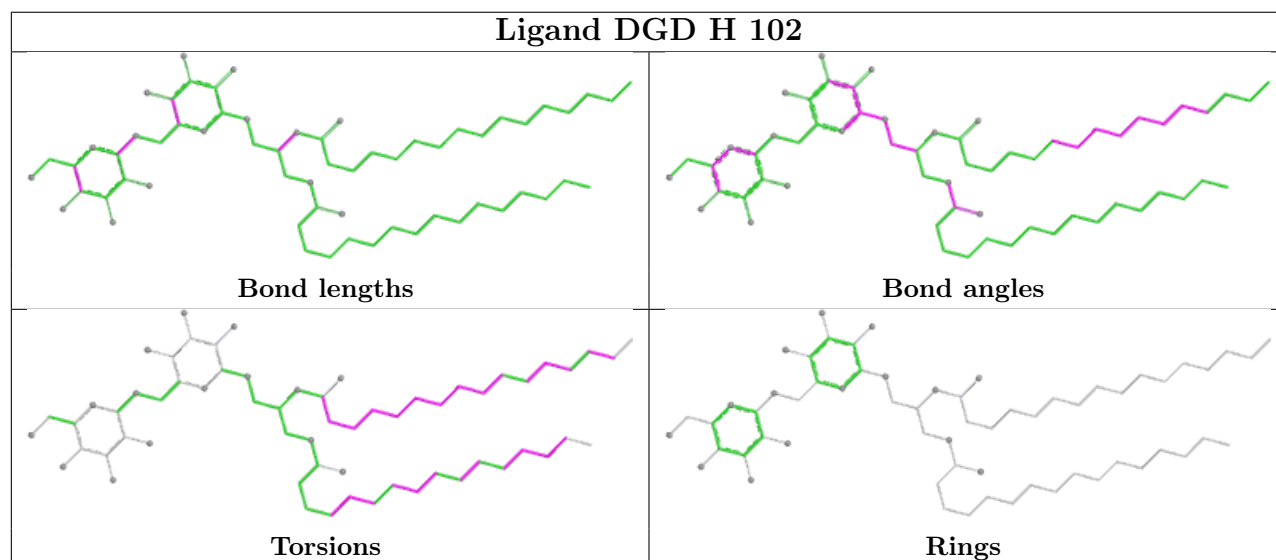
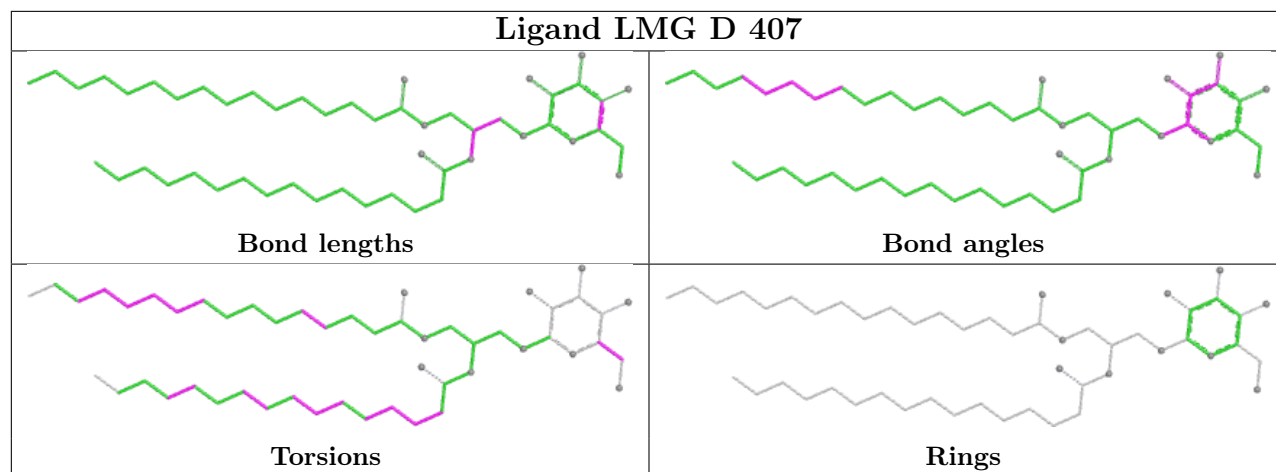


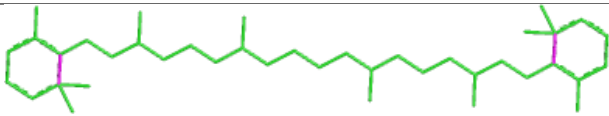
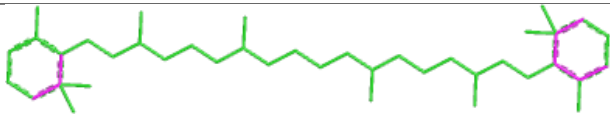
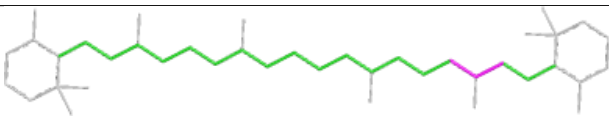
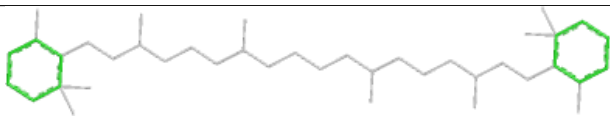
Ligand CLA C 507

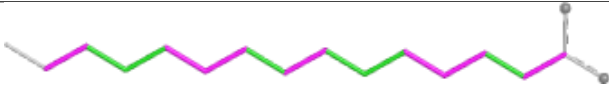
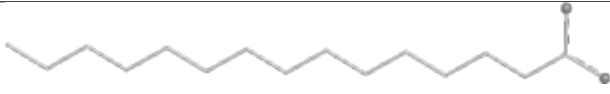


Ligand CLA a 612

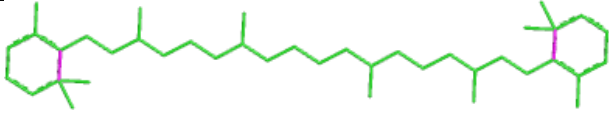
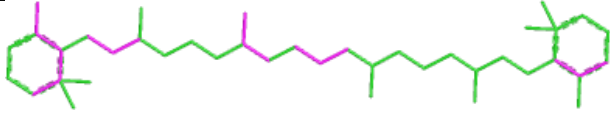
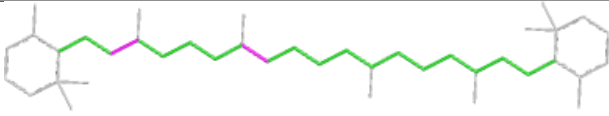
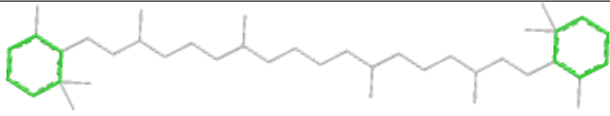


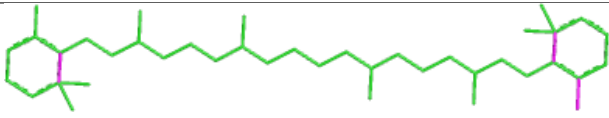
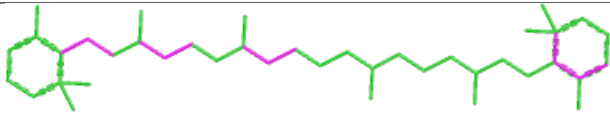
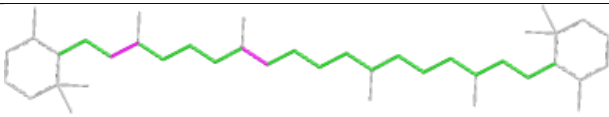
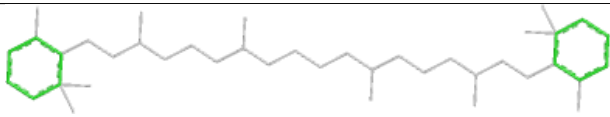


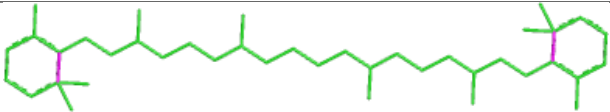
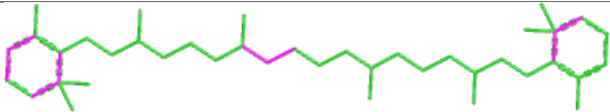
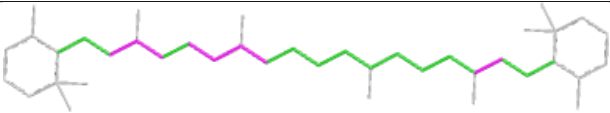
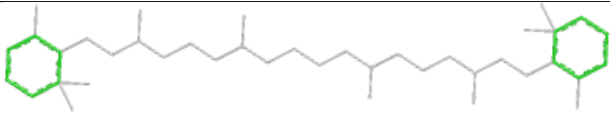
Ligand BCR b 619	
	
Bond lengths	Bond angles
	
Torsions	Rings

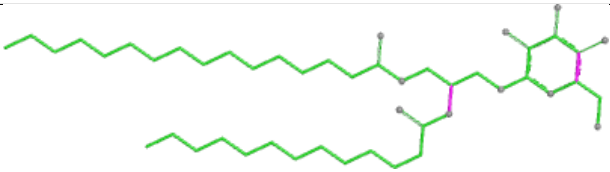
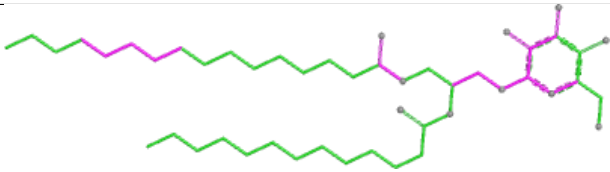
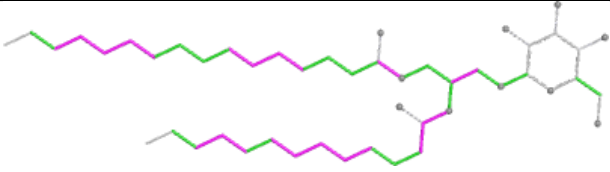
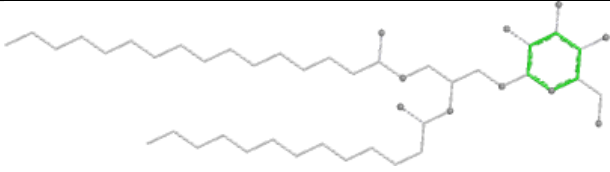
Ligand STE d 411	
	
Bond lengths	Bond angles
	
Torsions	Rings

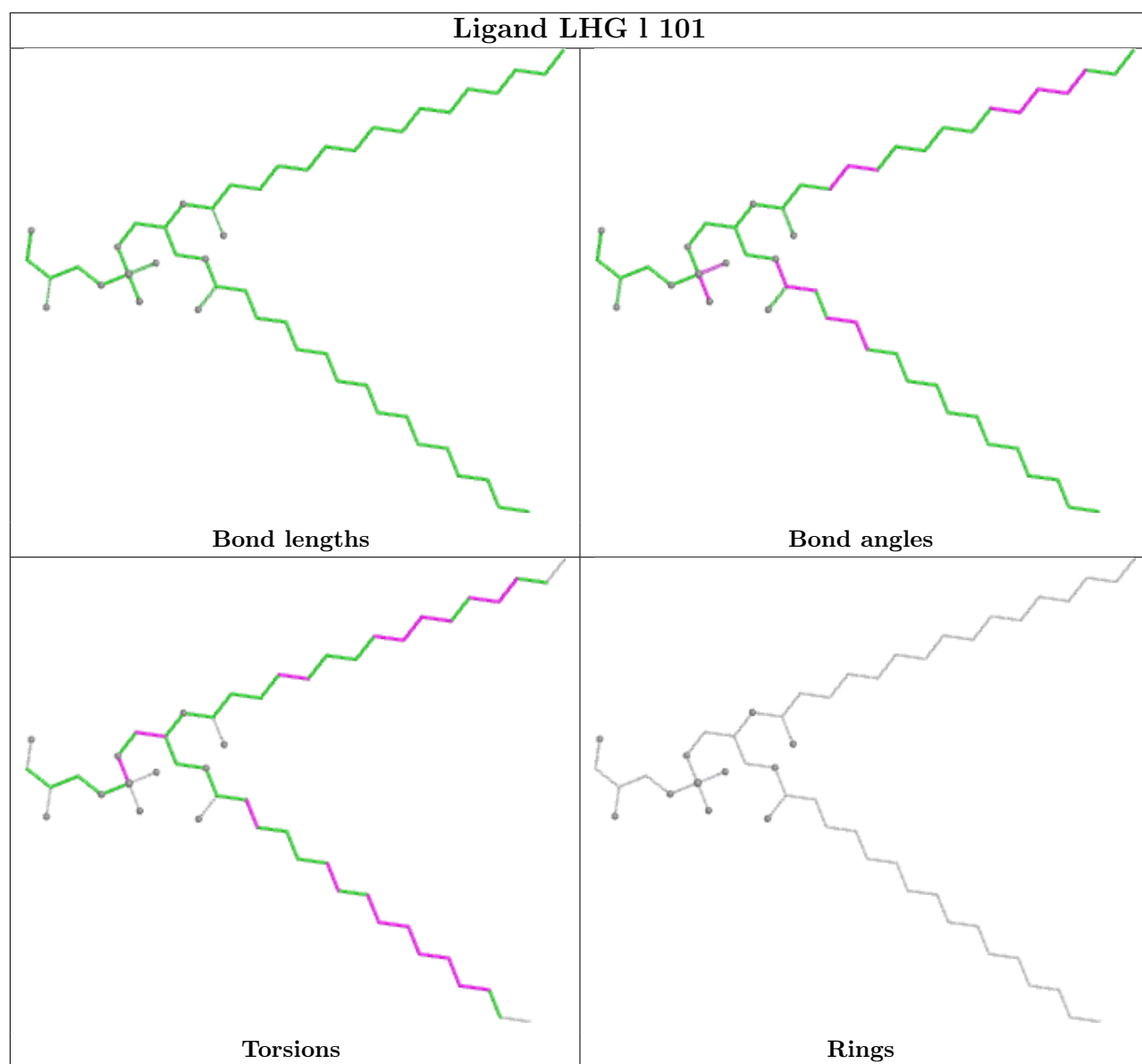
Ligand STE T 103	
	
Bond lengths	Bond angles
	
Torsions	Rings

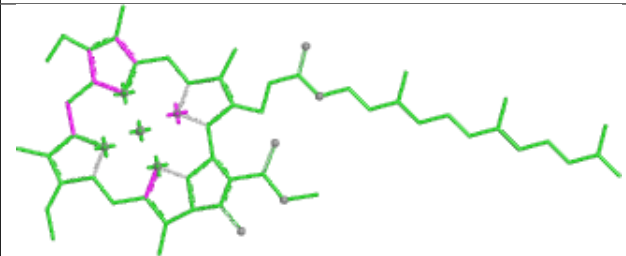
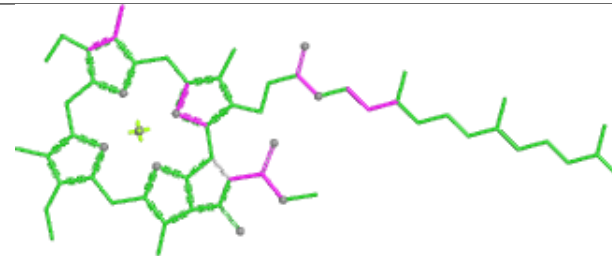
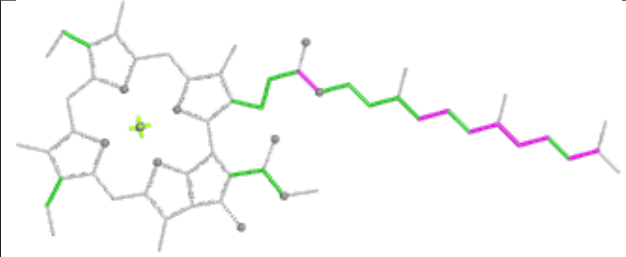
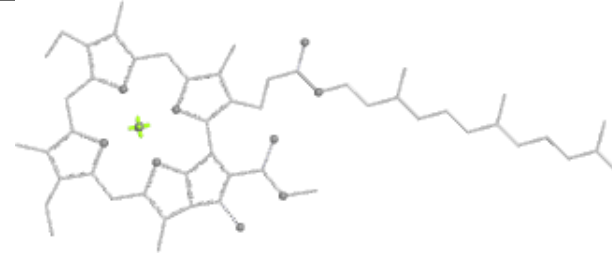
Ligand BCR c 514	
	
Bond lengths	Bond angles
	
Torsions	Rings

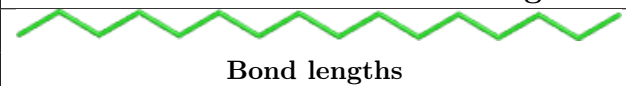
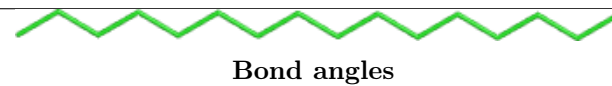
Ligand BCR b 618	
	
Bond lengths	Bond angles
	
Torsions	Rings

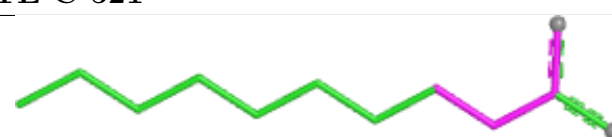
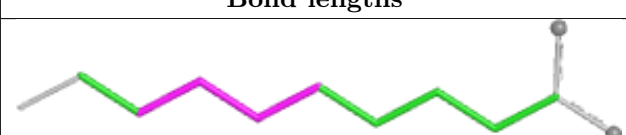
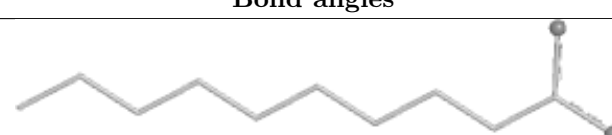
Ligand BCR B 619			
			
Bond lengths	Bond angles		
			
Torsions	Rings		

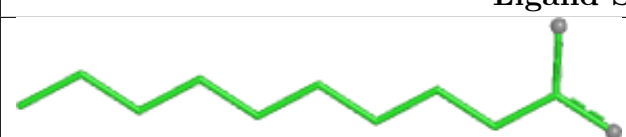
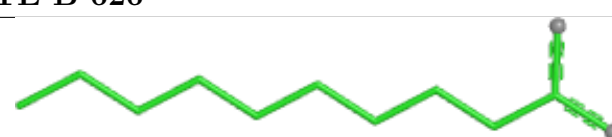
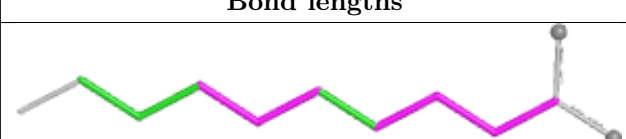
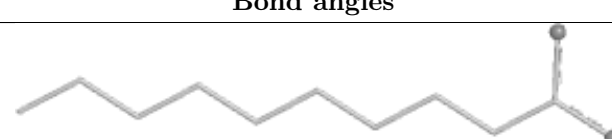
Ligand LMG C 520			
			
Bond lengths	Bond angles		
			
Torsions	Rings		



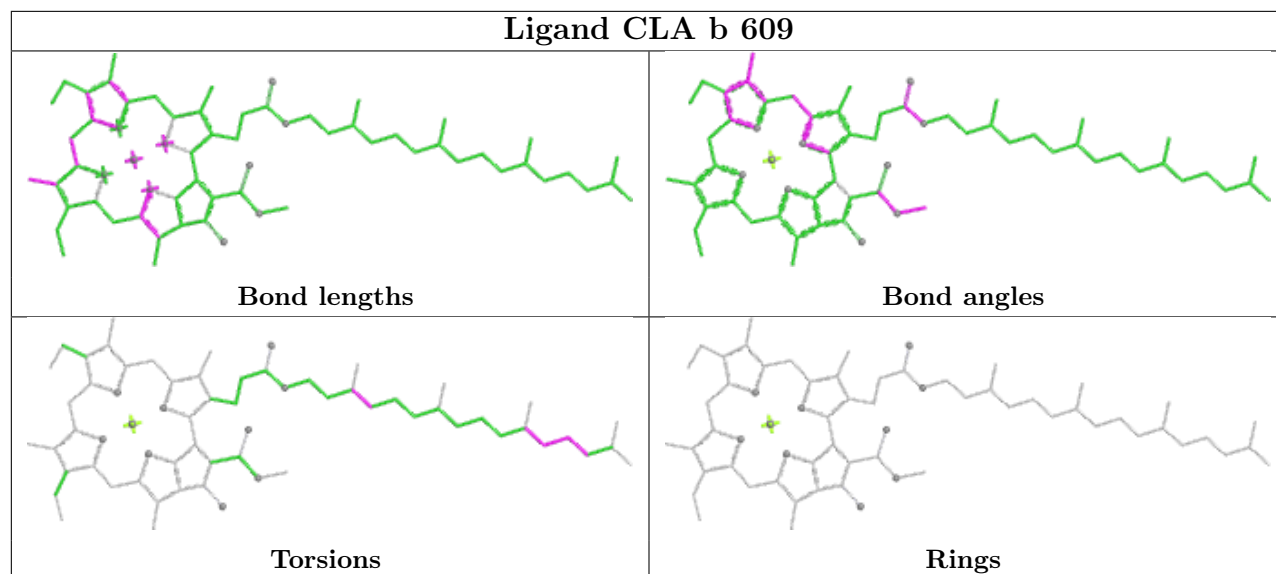
Ligand CLA B 616	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand STE C 523	
	
Bond lengths	Bond angles
	
Torsions	Rings

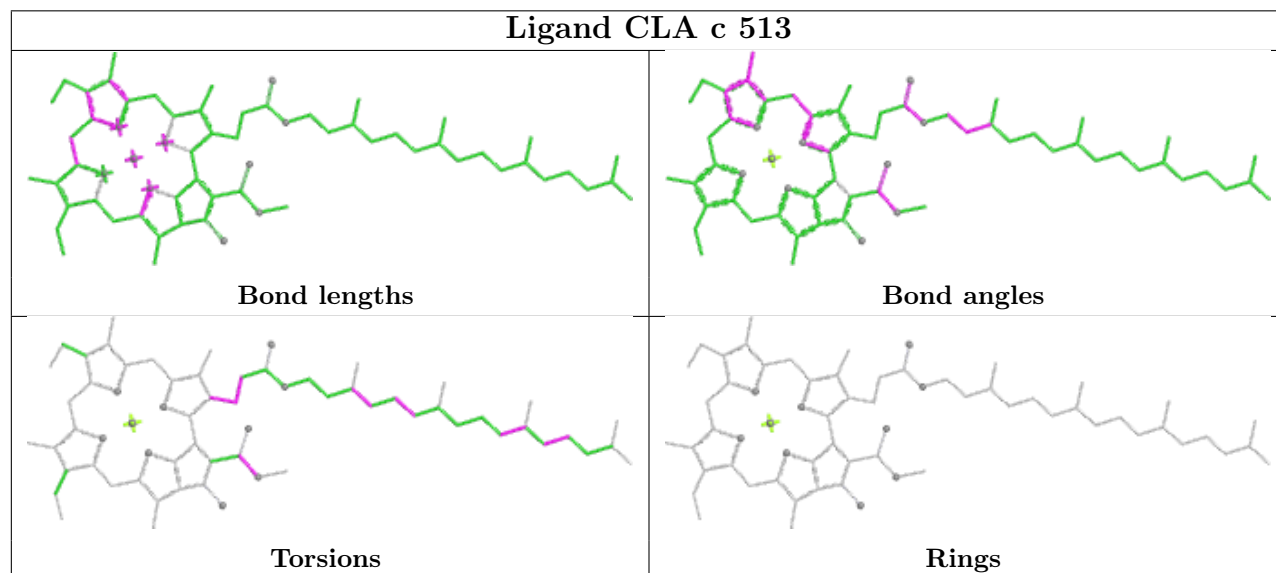
Ligand STE C 521	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand STE B 626	
	
Bond lengths	Bond angles
	
Torsions	Rings

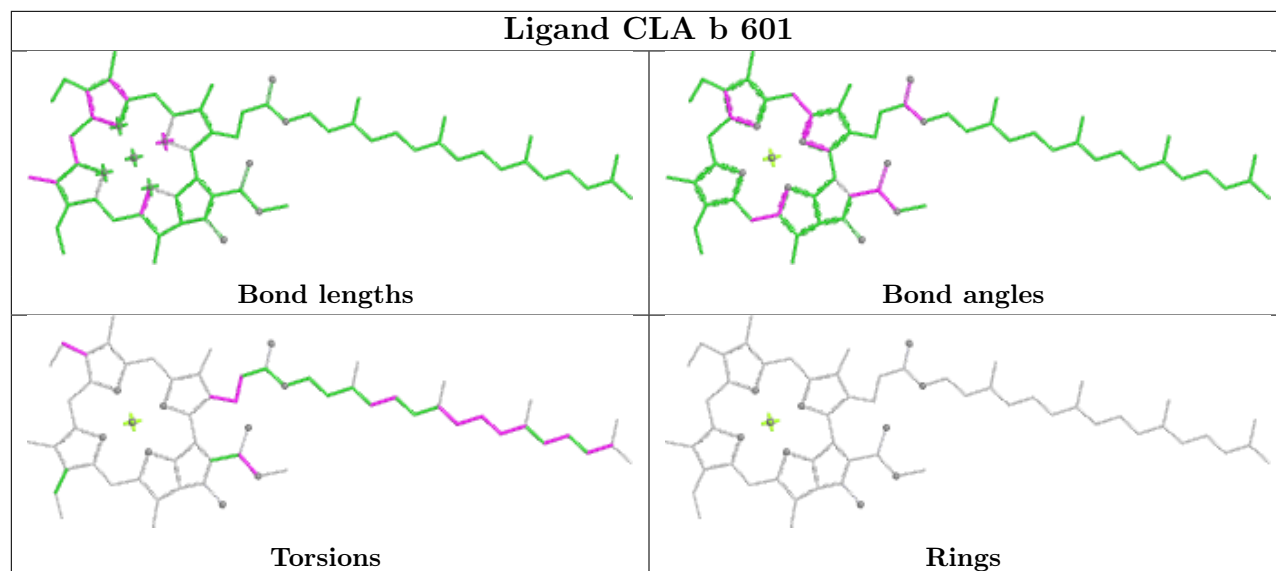
Ligand CLA b 609

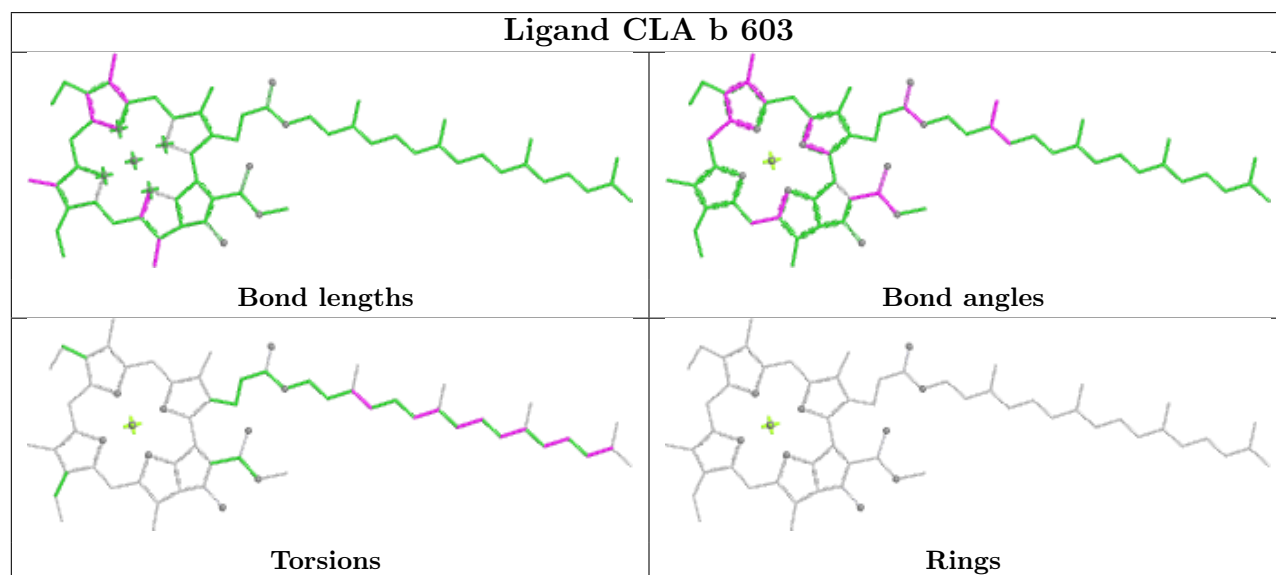
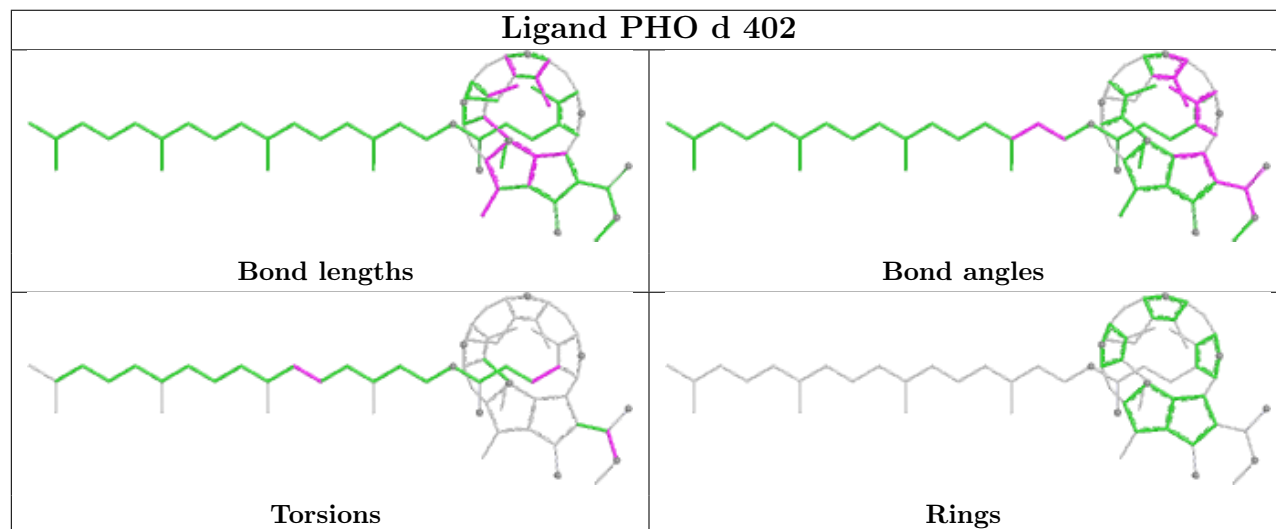
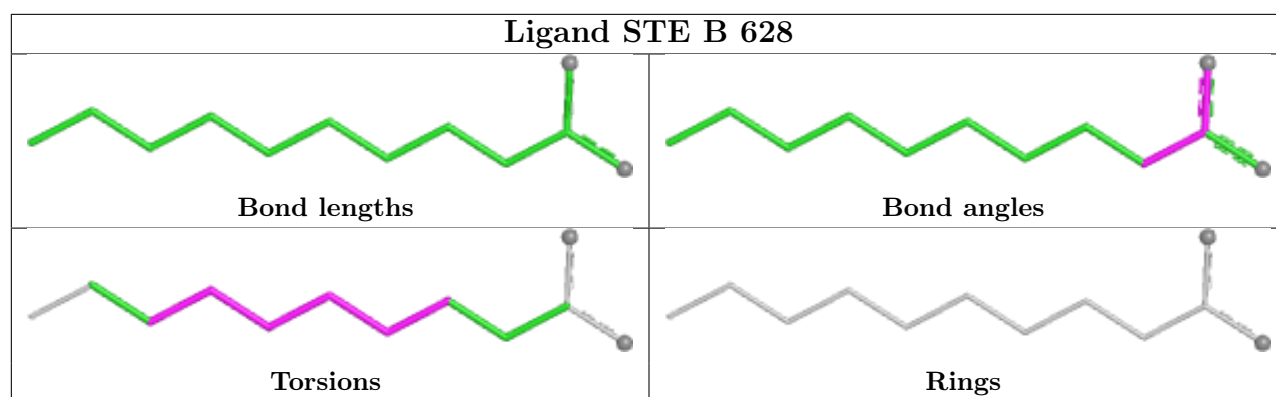


Ligand CLA c 513

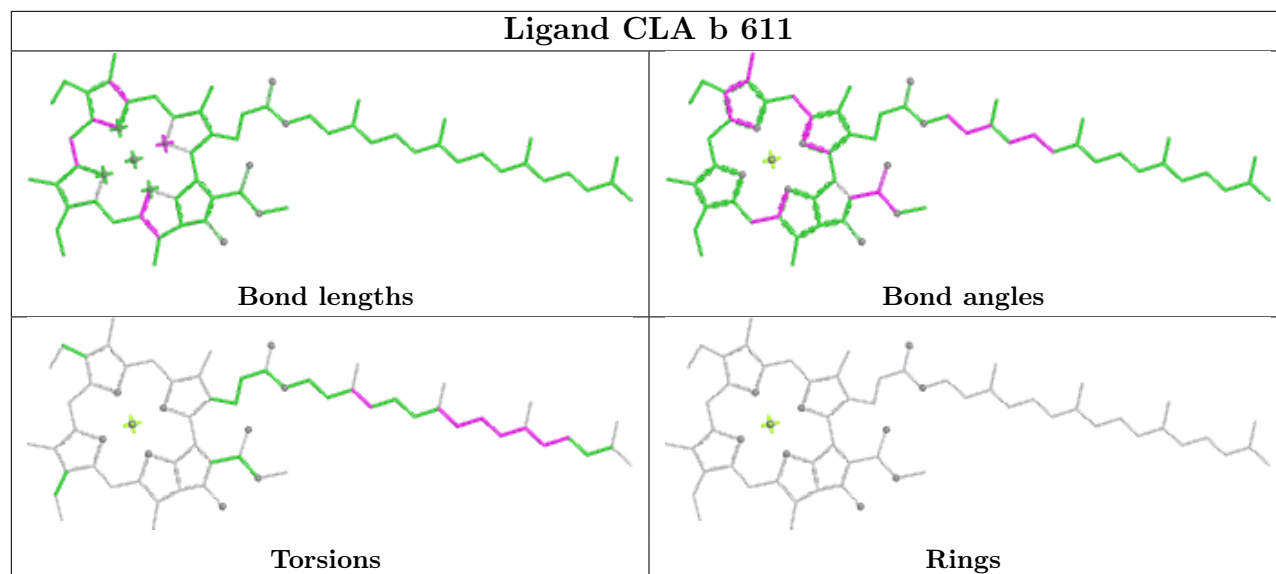


Ligand CLA b 601

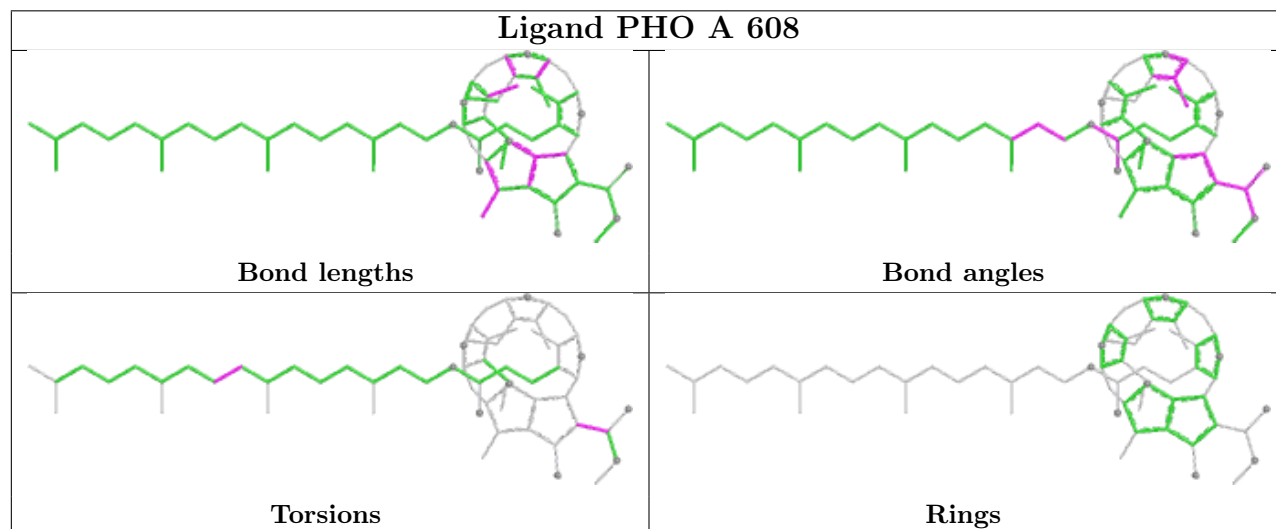




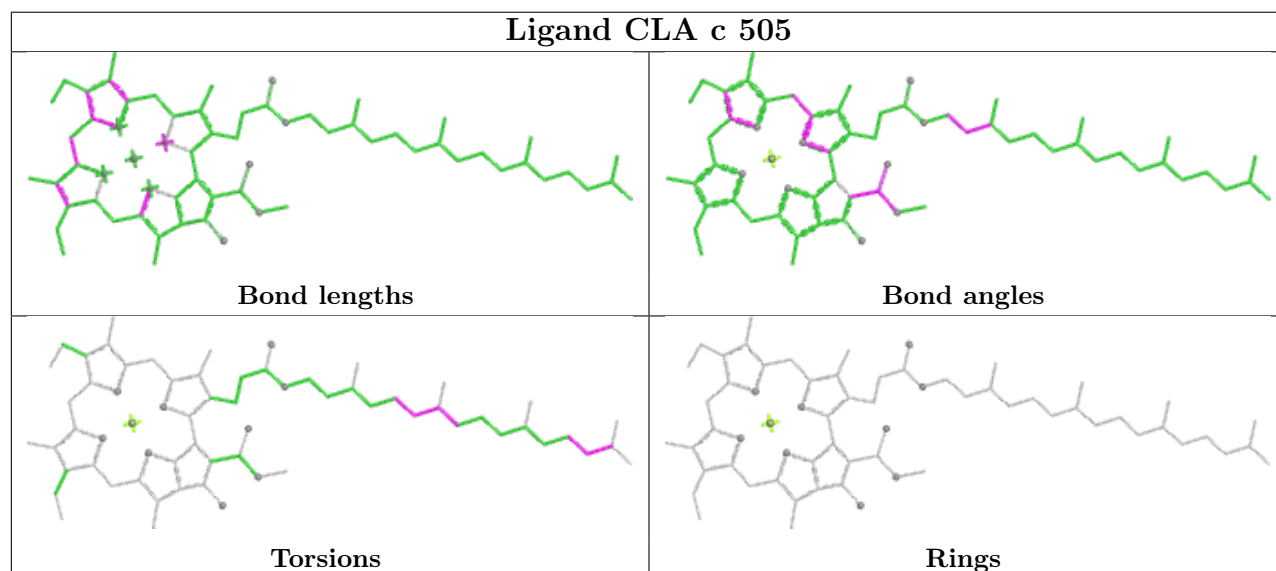
Ligand CLA b 611

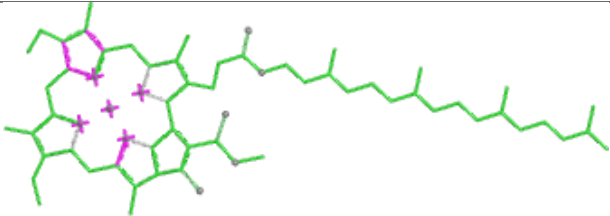
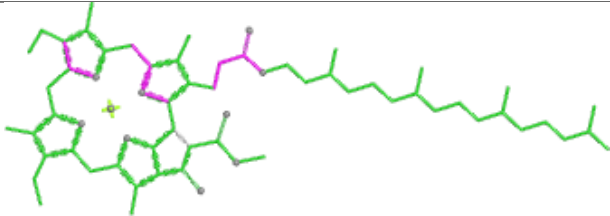
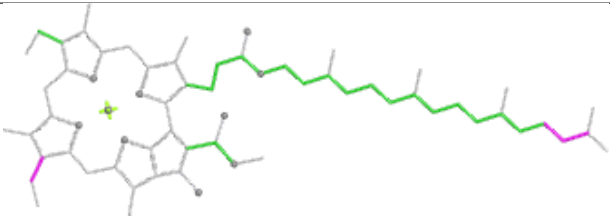
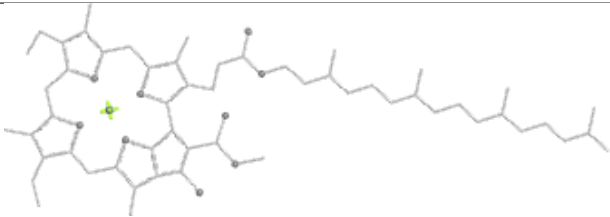
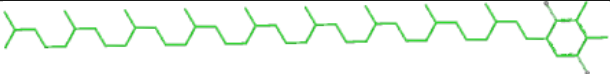
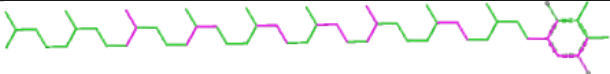
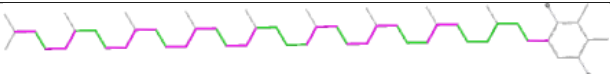
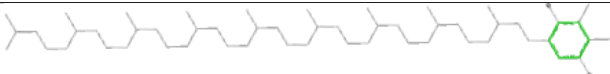


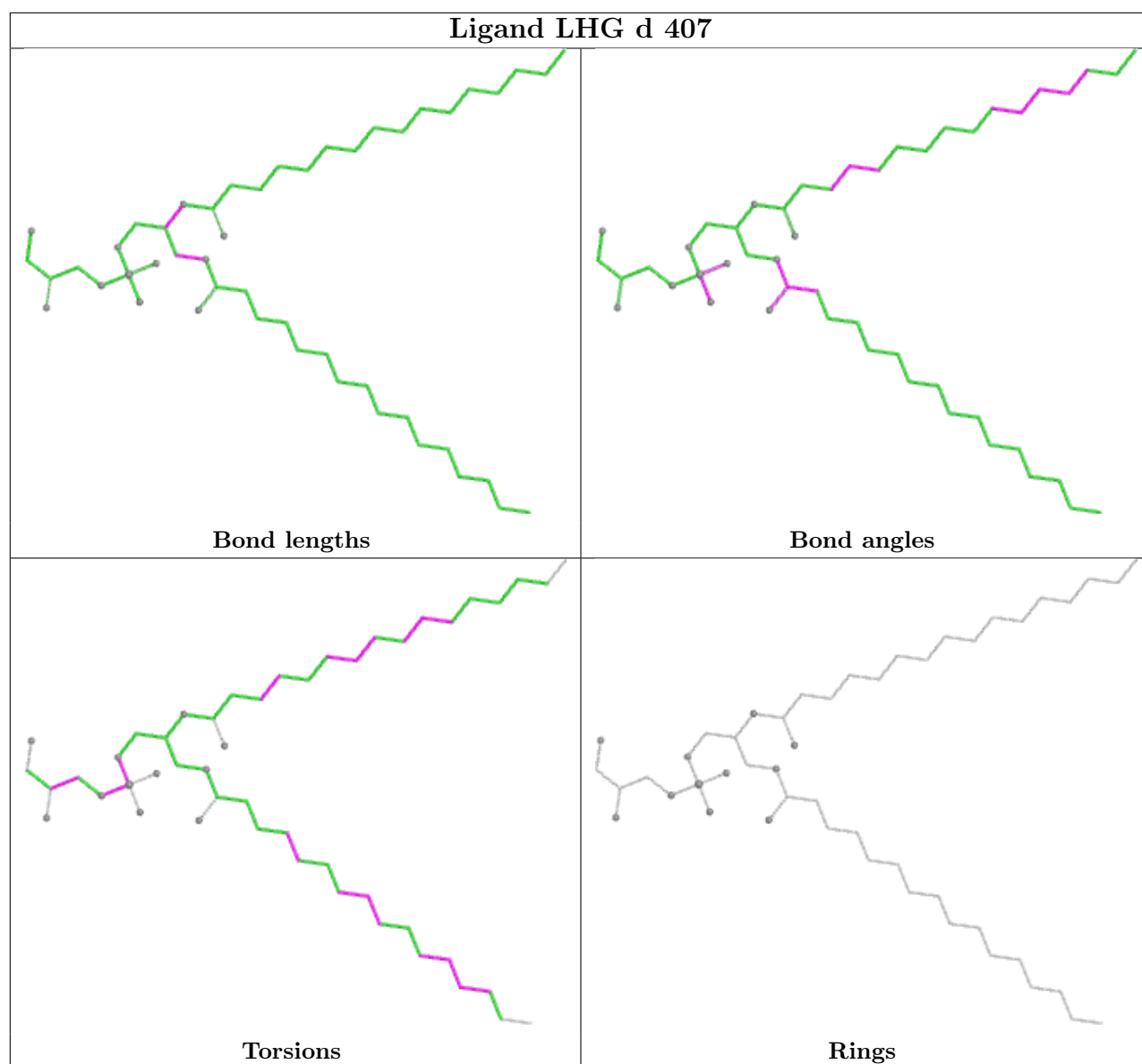
Ligand PHO A 608

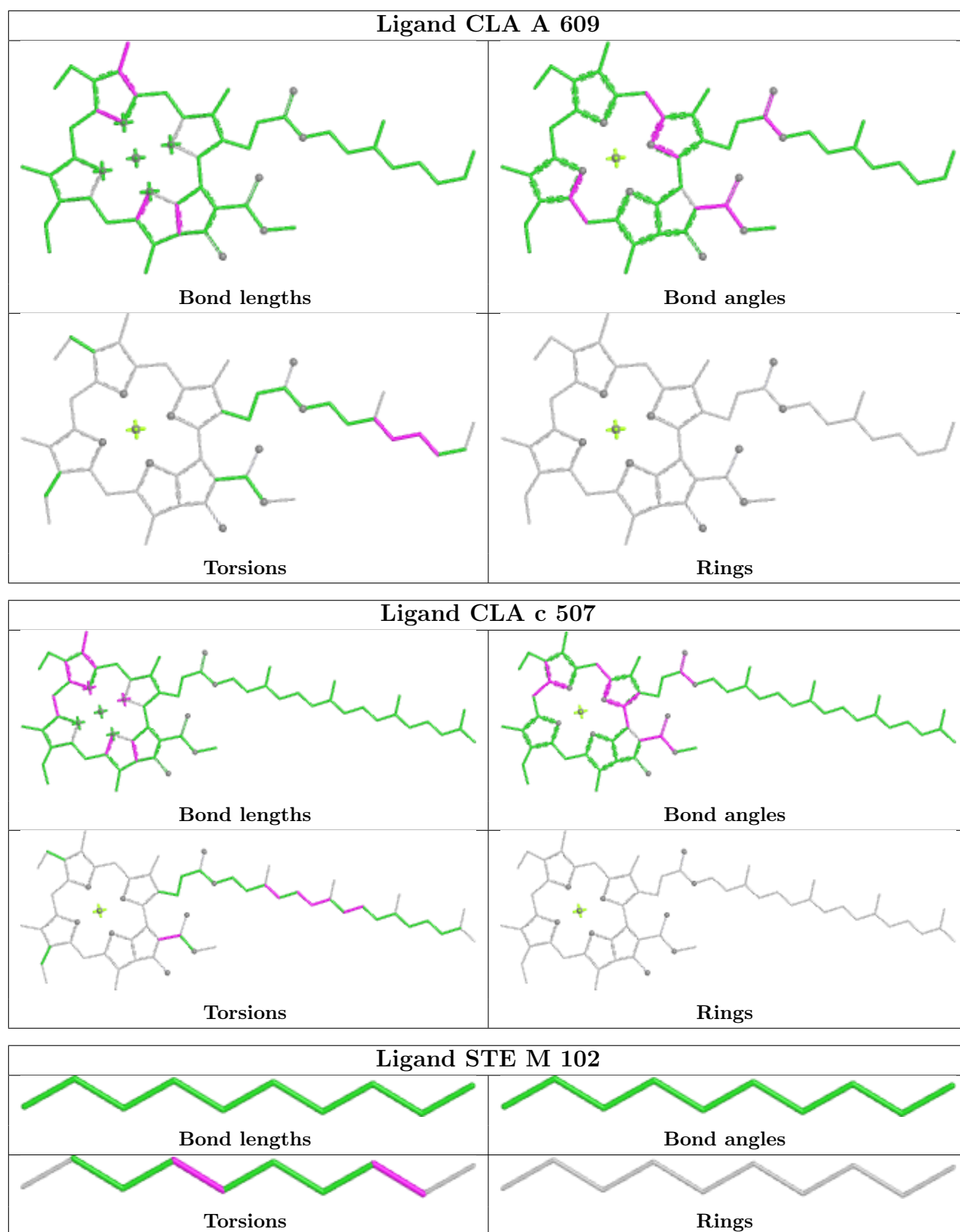


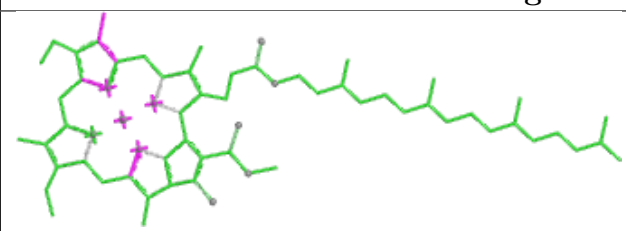
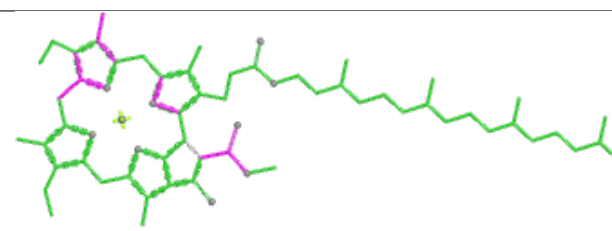
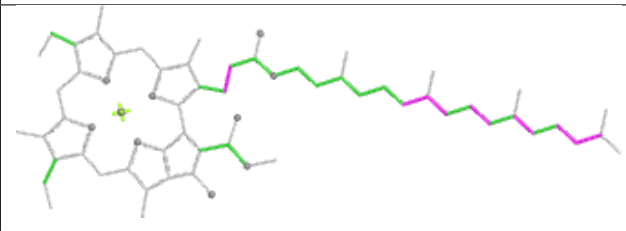
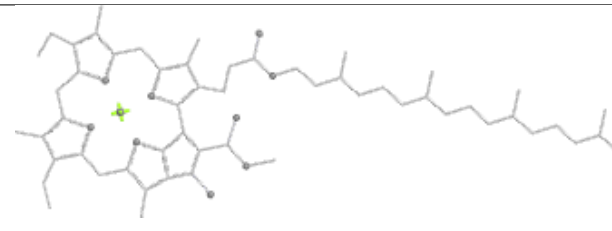
Ligand CLA c 505

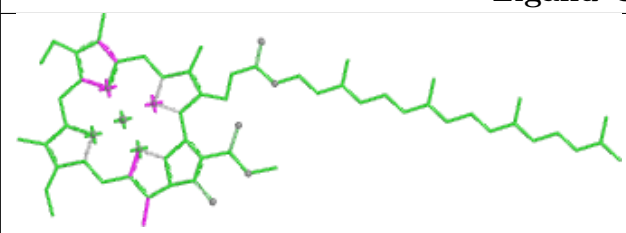
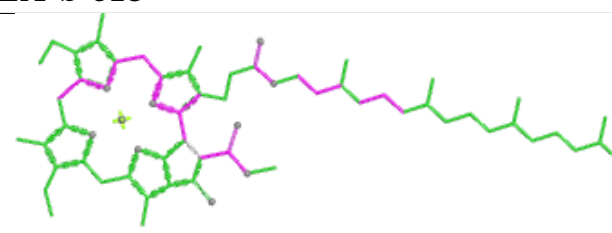
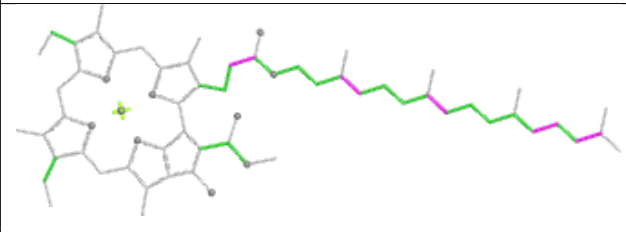
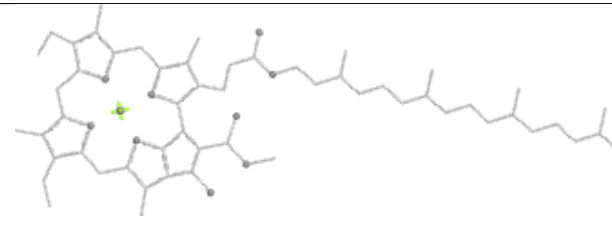


Ligand CLA A 606	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PL9 A 611	
 Bond lengths	 Bond angles
 Torsions	 Rings

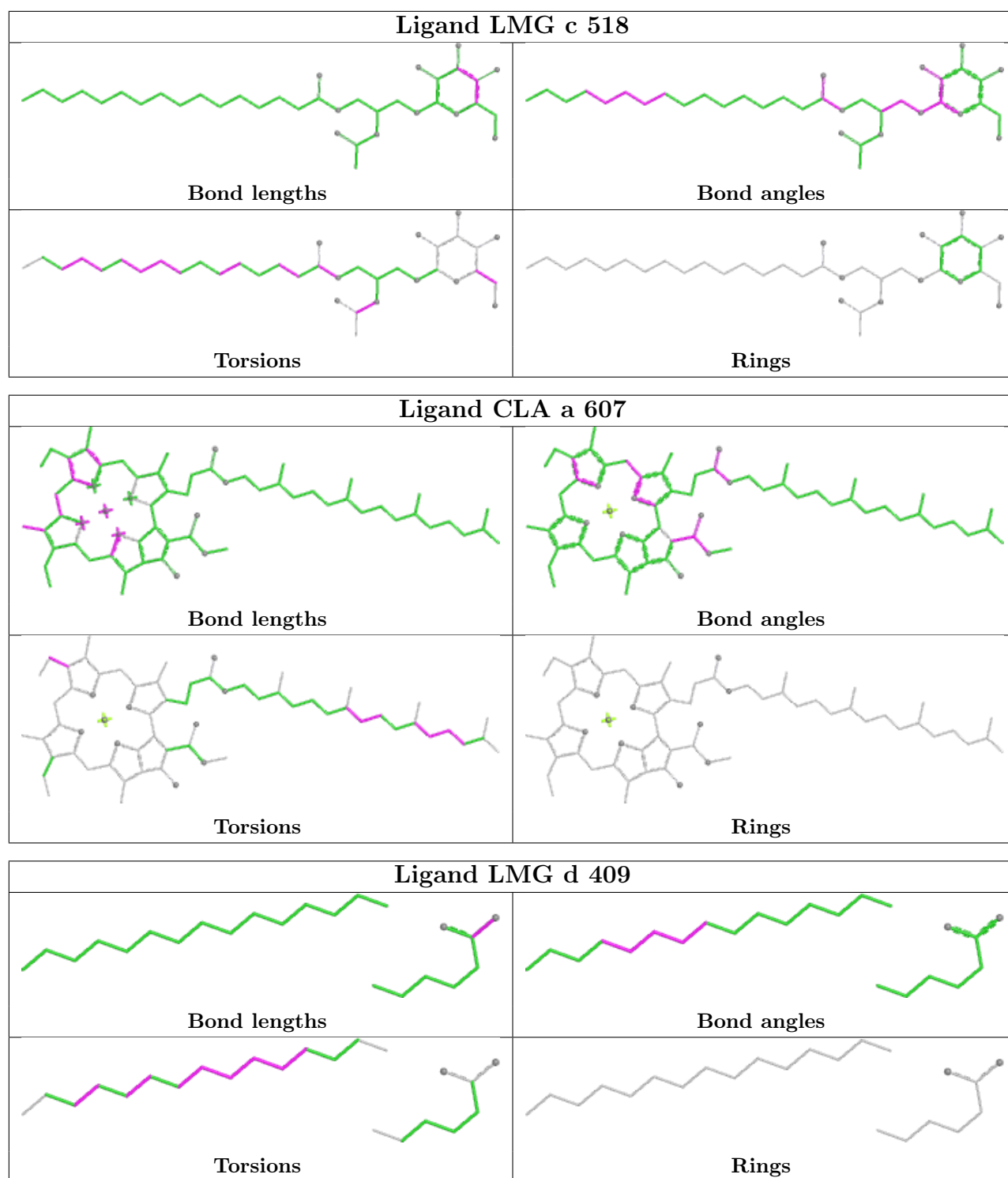


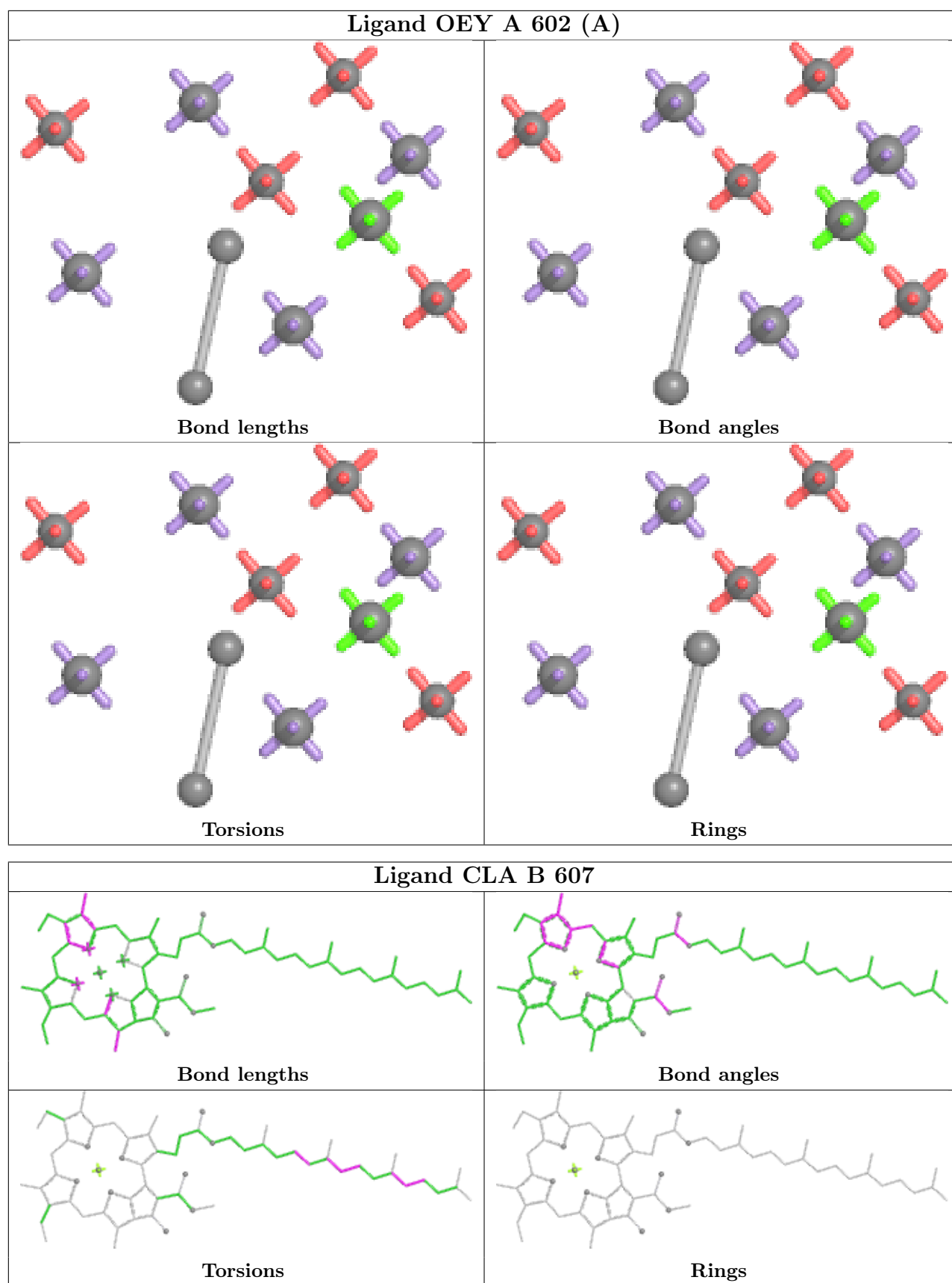


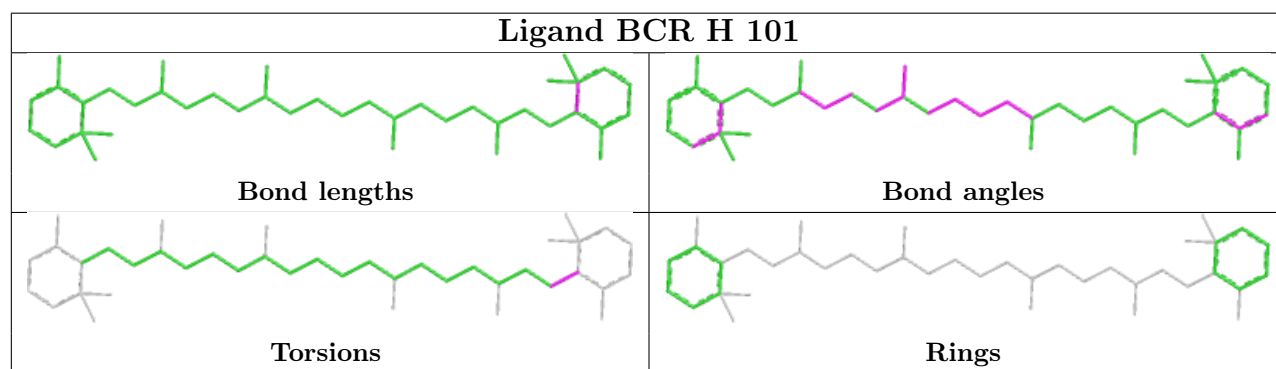
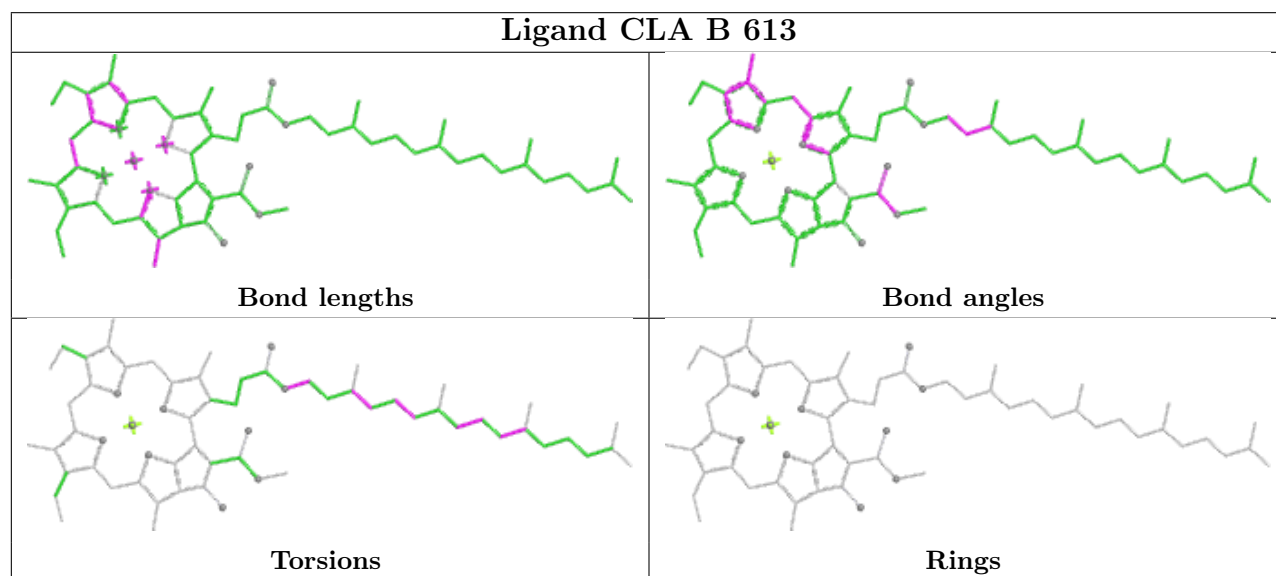
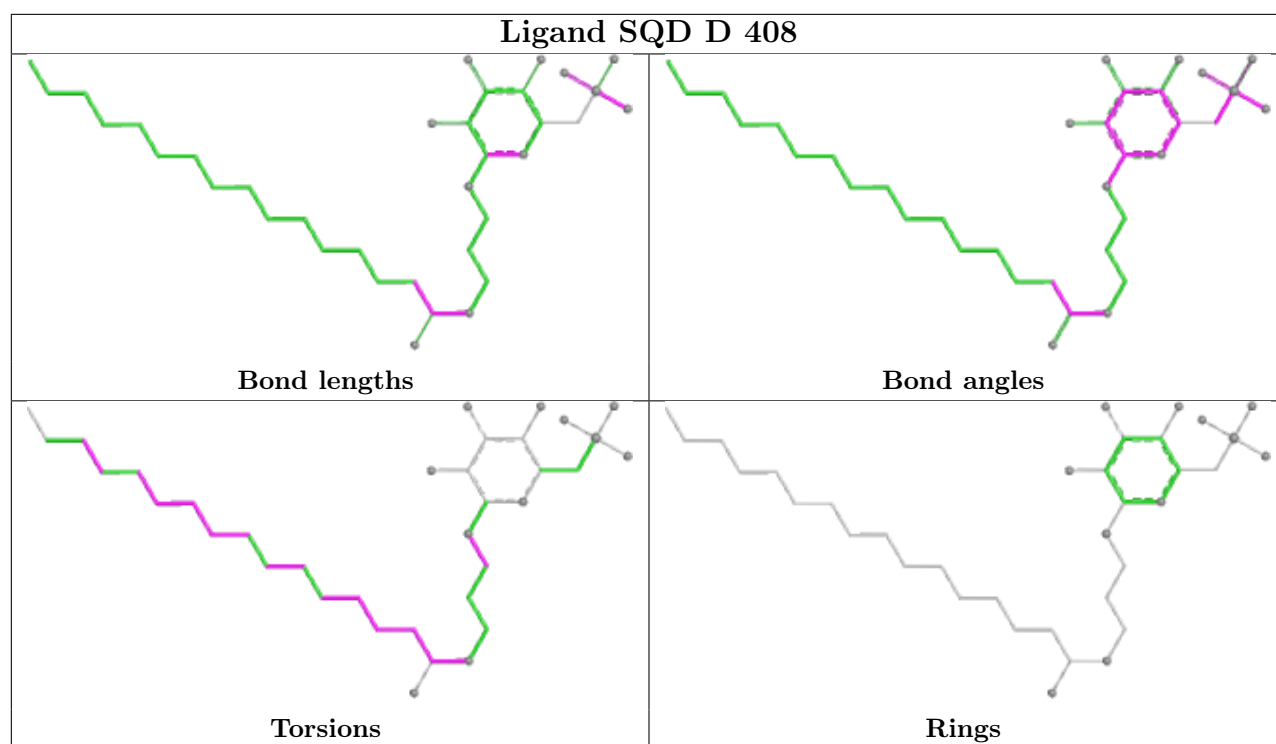
Ligand CLA b 606	
	
Bond lengths	Bond angles
	
Torsions	Rings

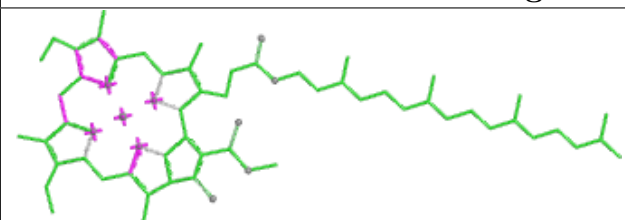
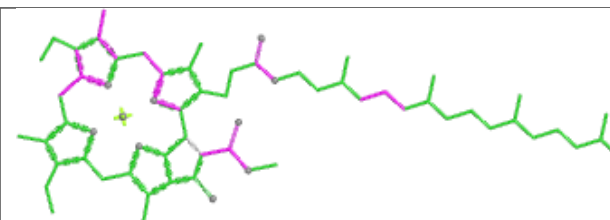
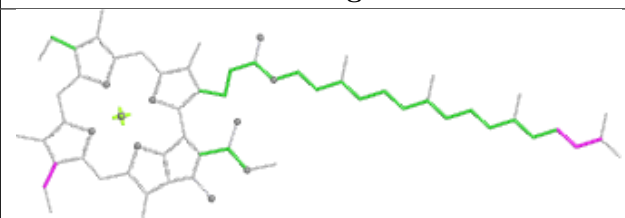
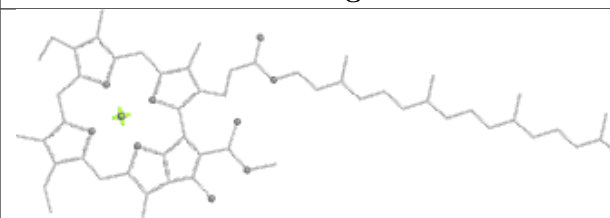
Ligand CLA b 613	
	
Bond lengths	Bond angles
	
Torsions	Rings

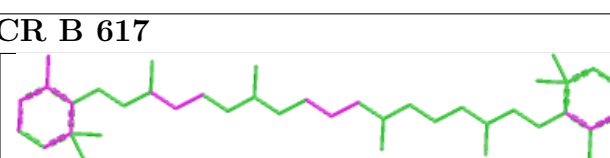
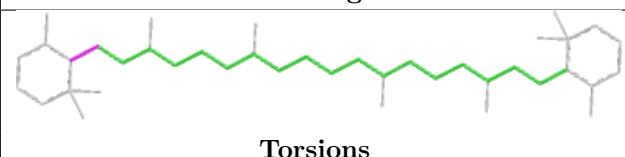
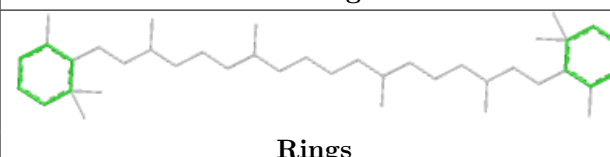
Ligand STE b 625	
	
Bond lengths	Bond angles
	
Torsions	Rings

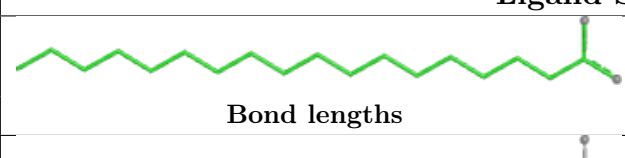
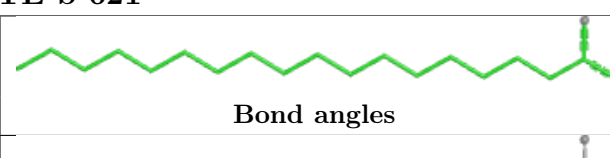
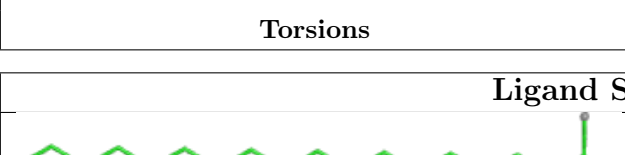
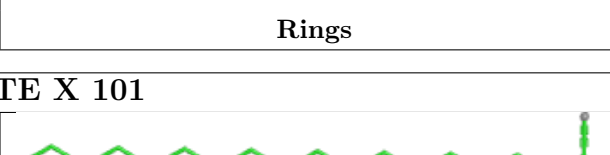


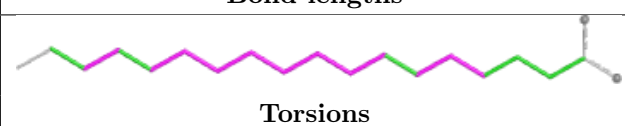
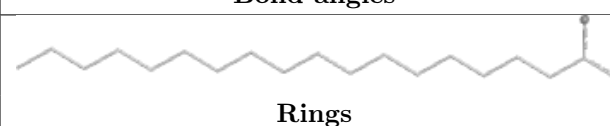


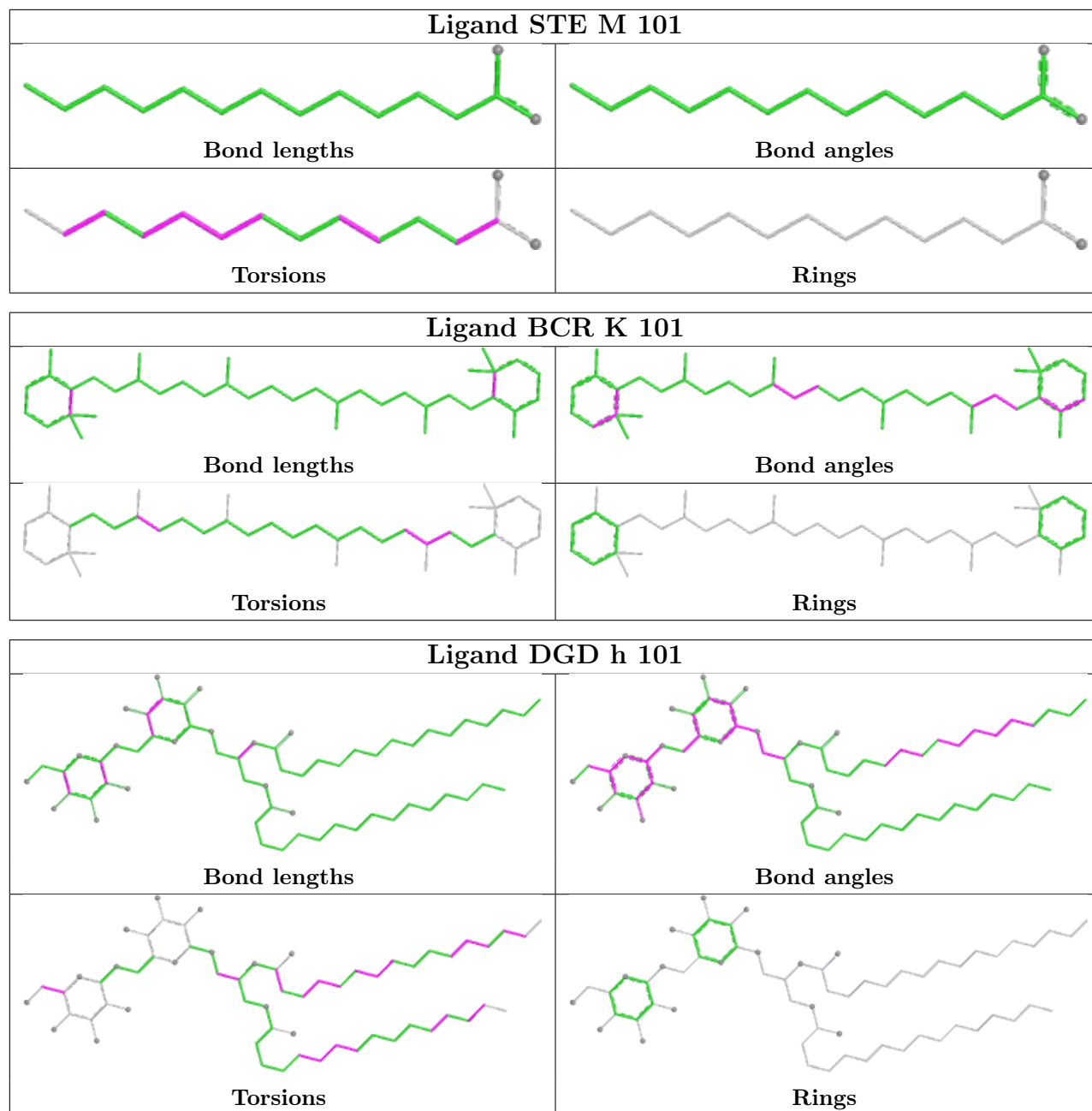


Ligand CLA a 606	
	
Bond lengths	Bond angles
	
Torsions	Rings

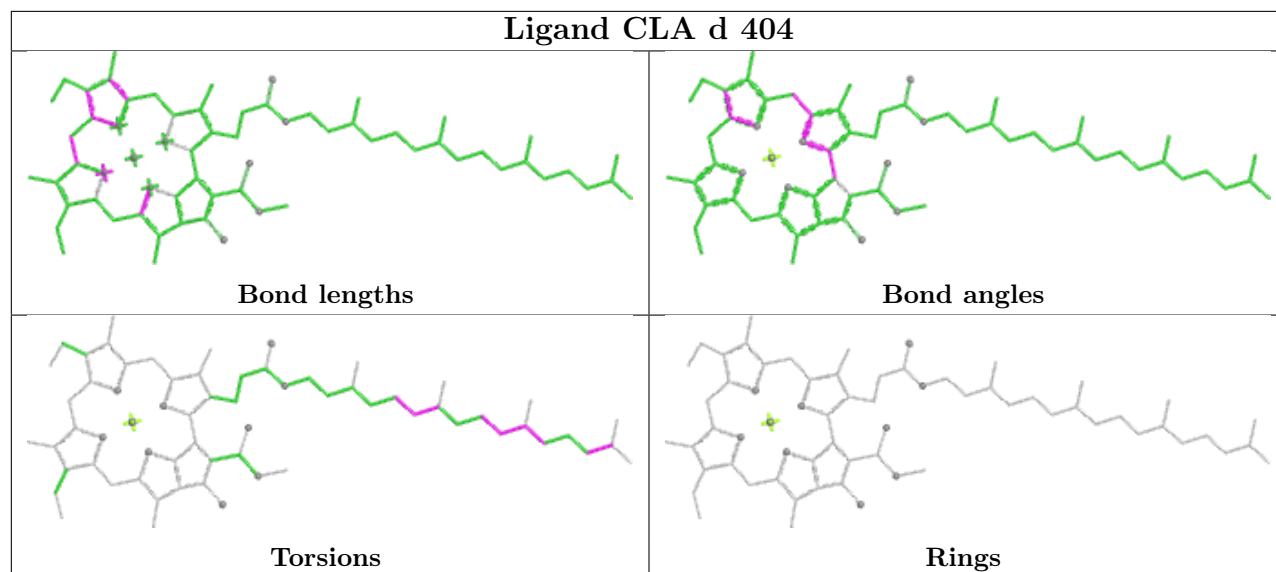
Ligand BCR B 617	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand STE b 621	
	
Bond lengths	Bond angles
	
Torsions	Rings

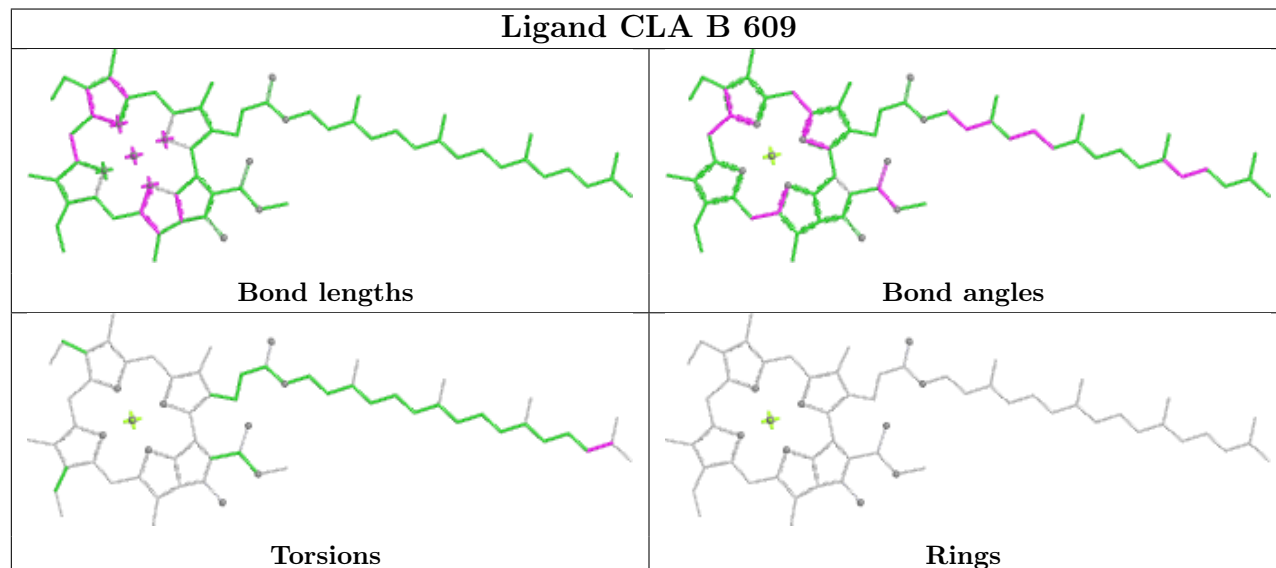
Ligand STE X 101	
	
Bond lengths	Bond angles
	
Torsions	Rings



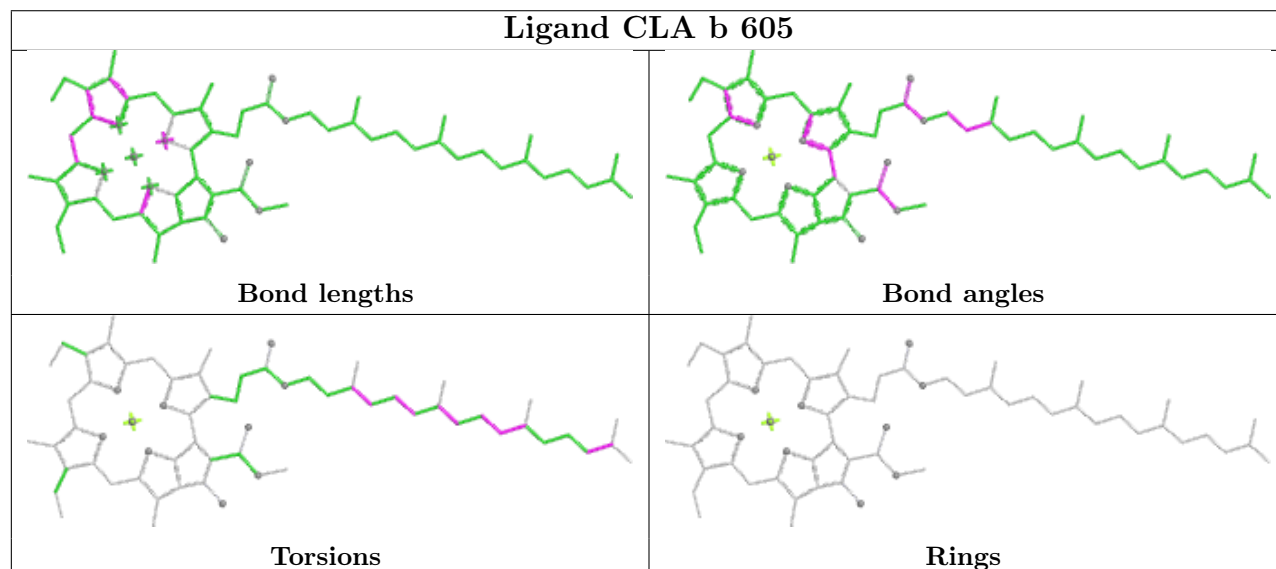
Ligand CLA d 404

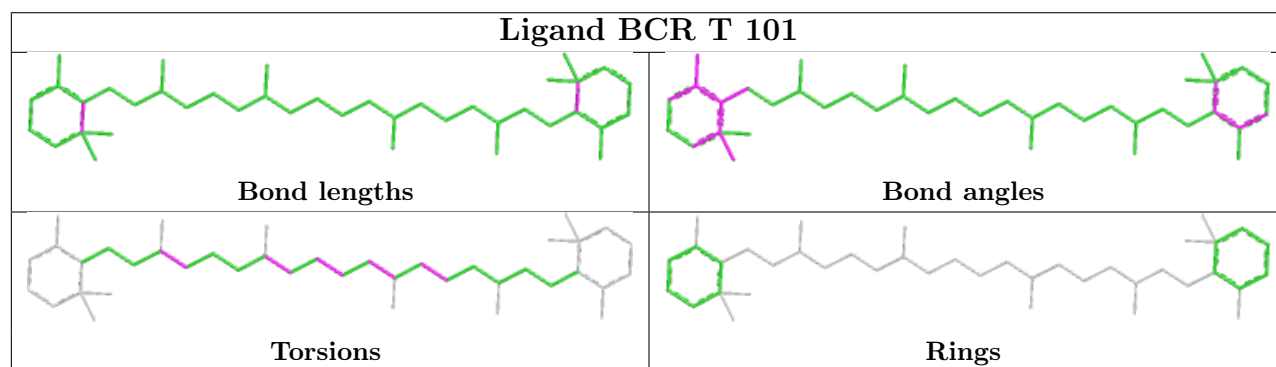
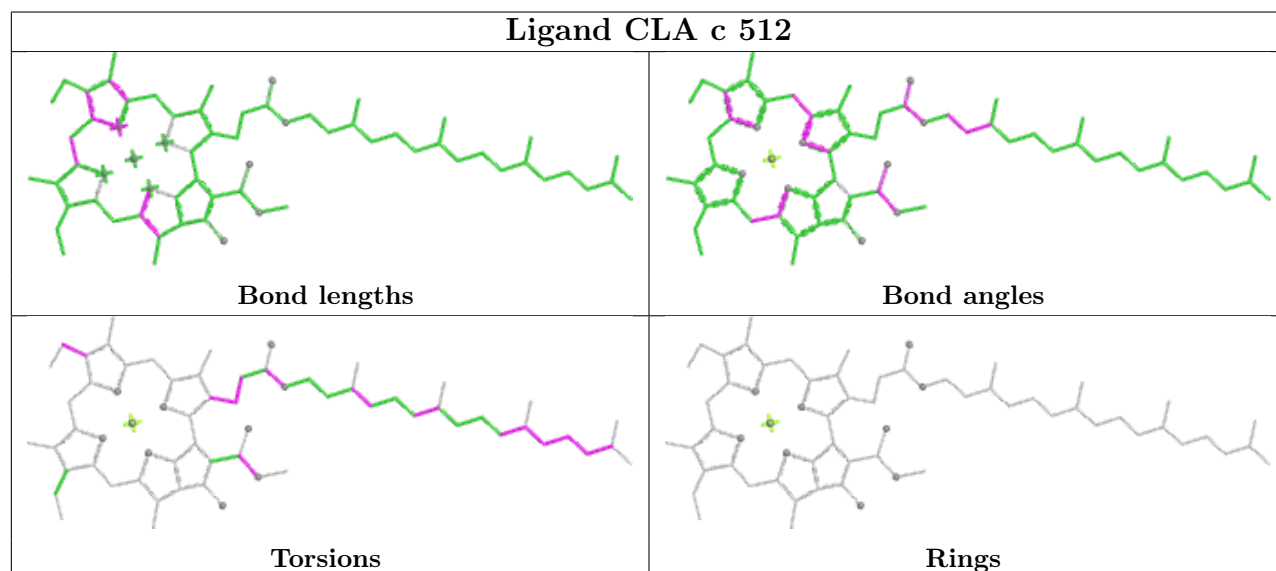
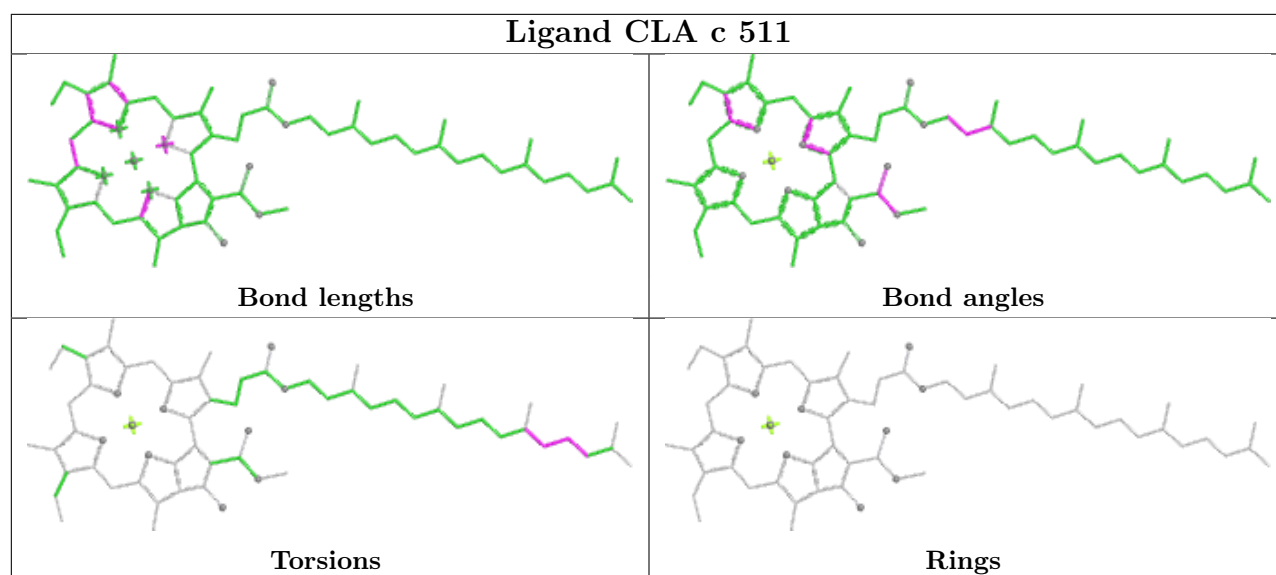


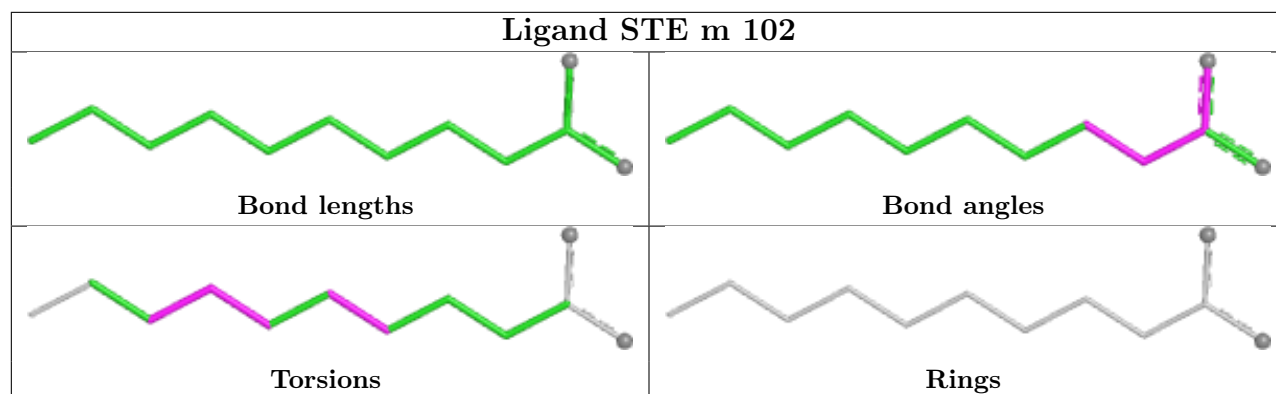
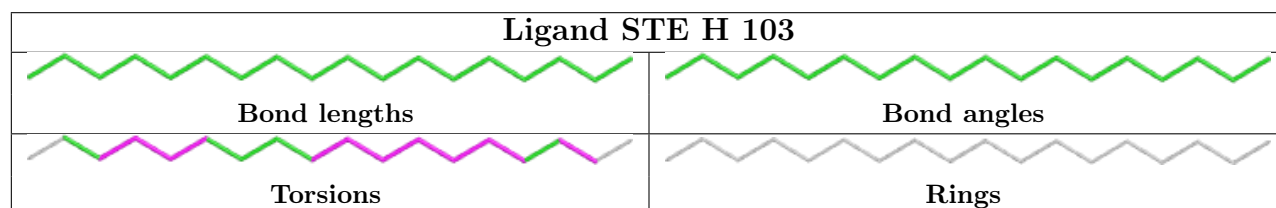
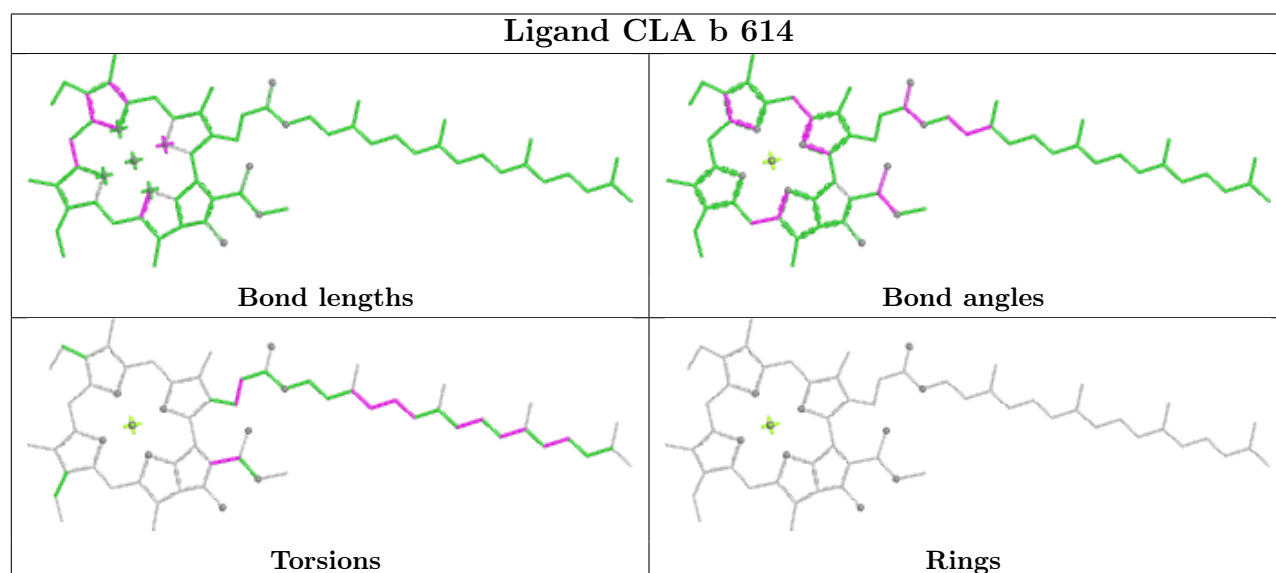
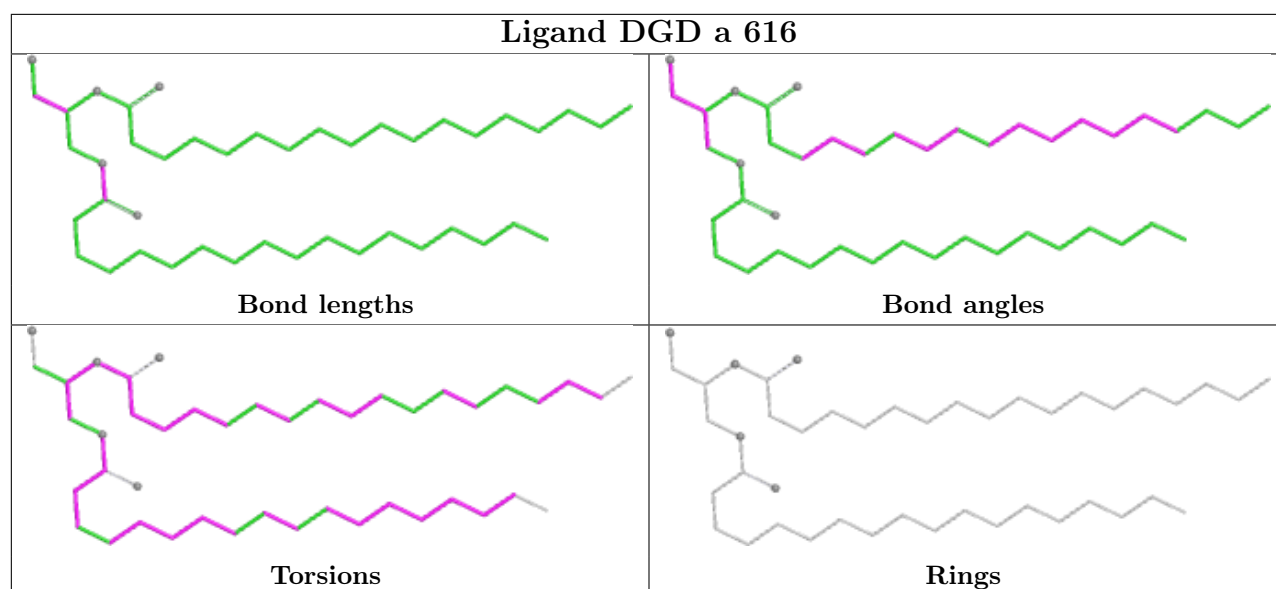
Ligand CLA B 609

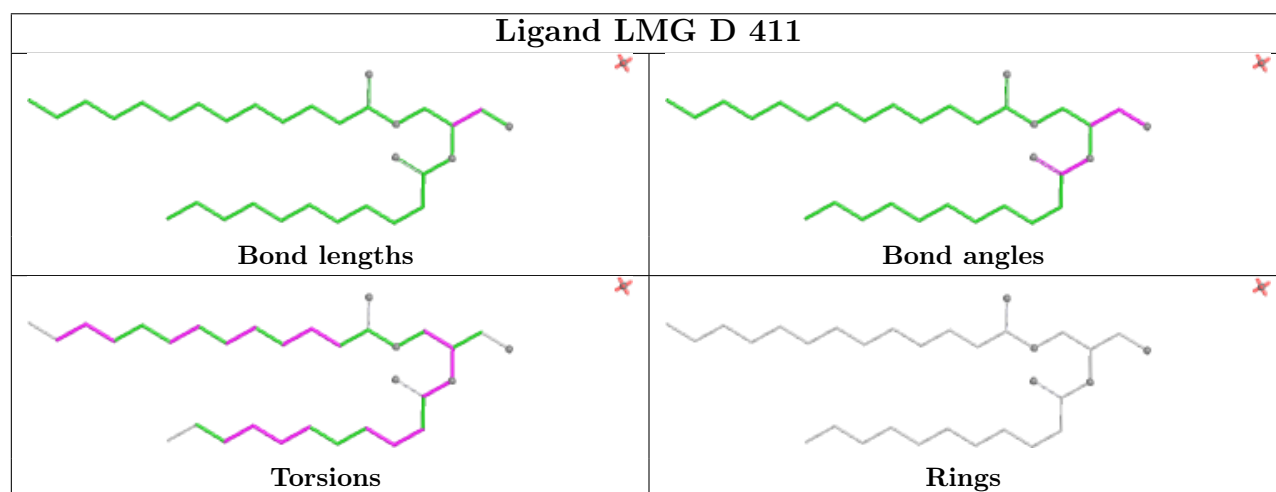
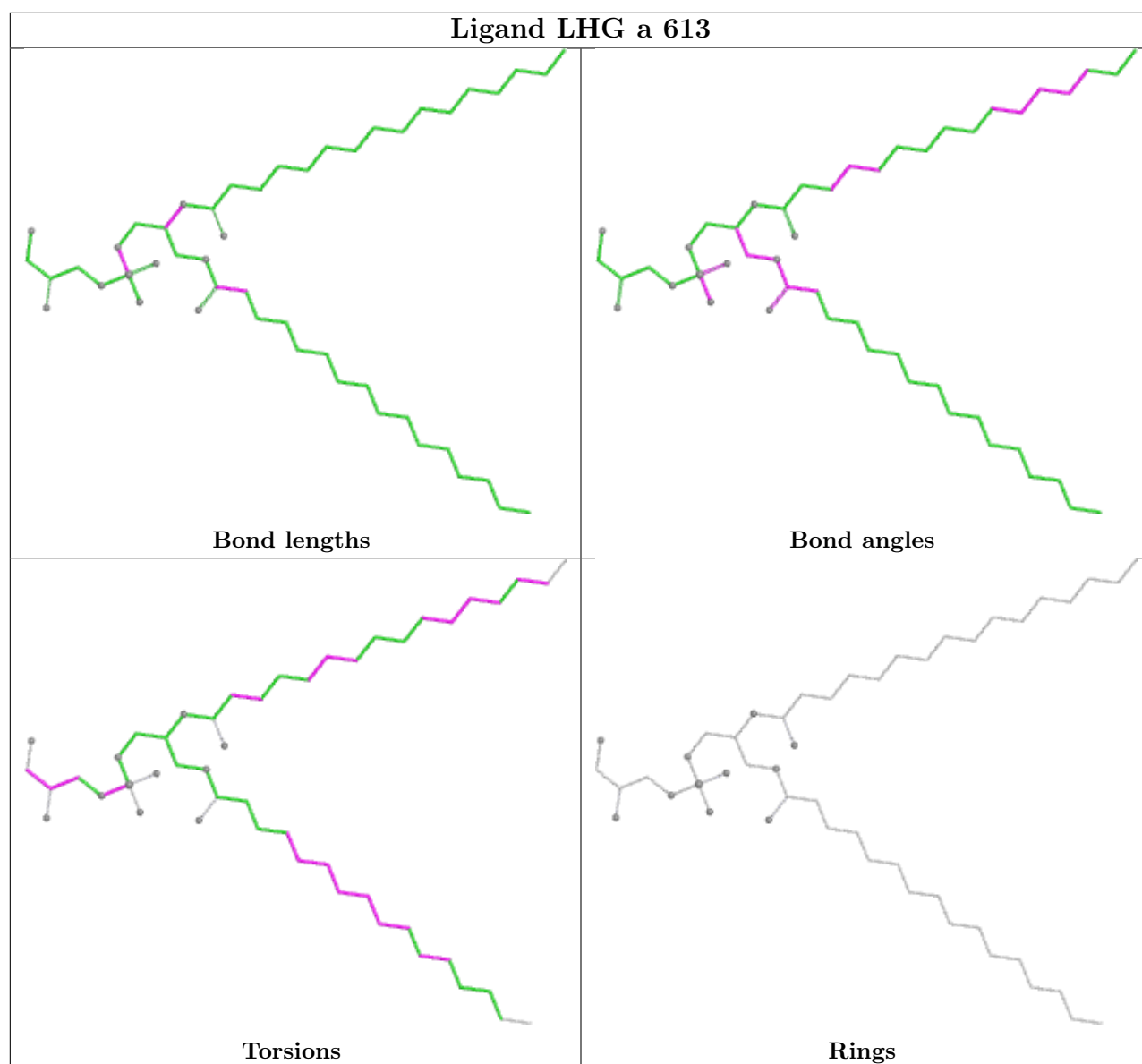


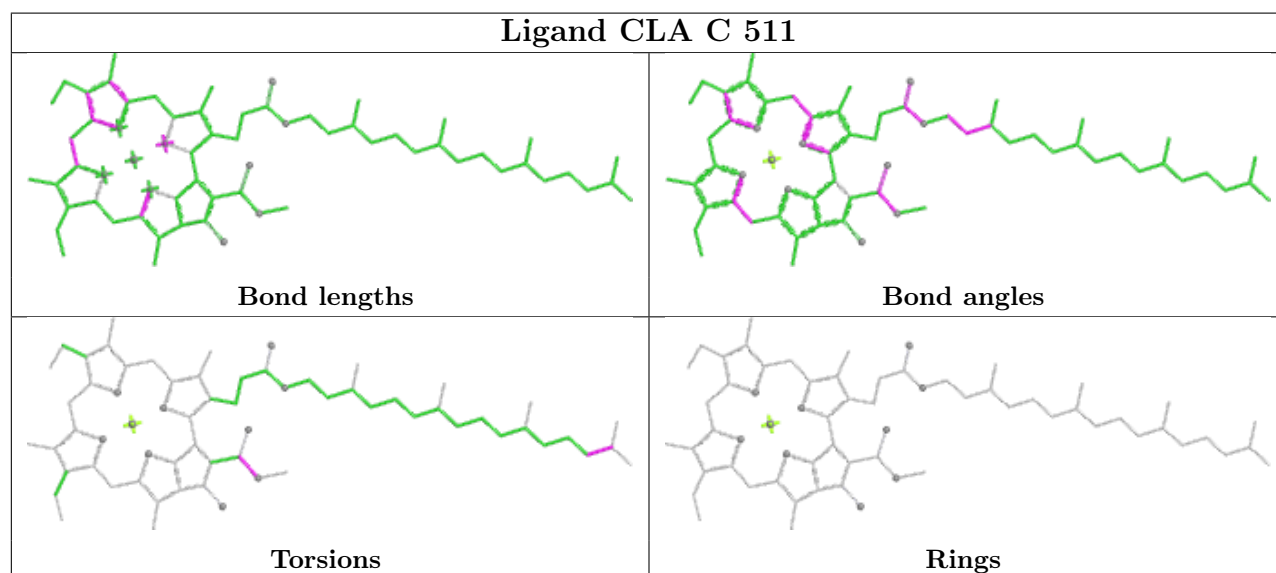
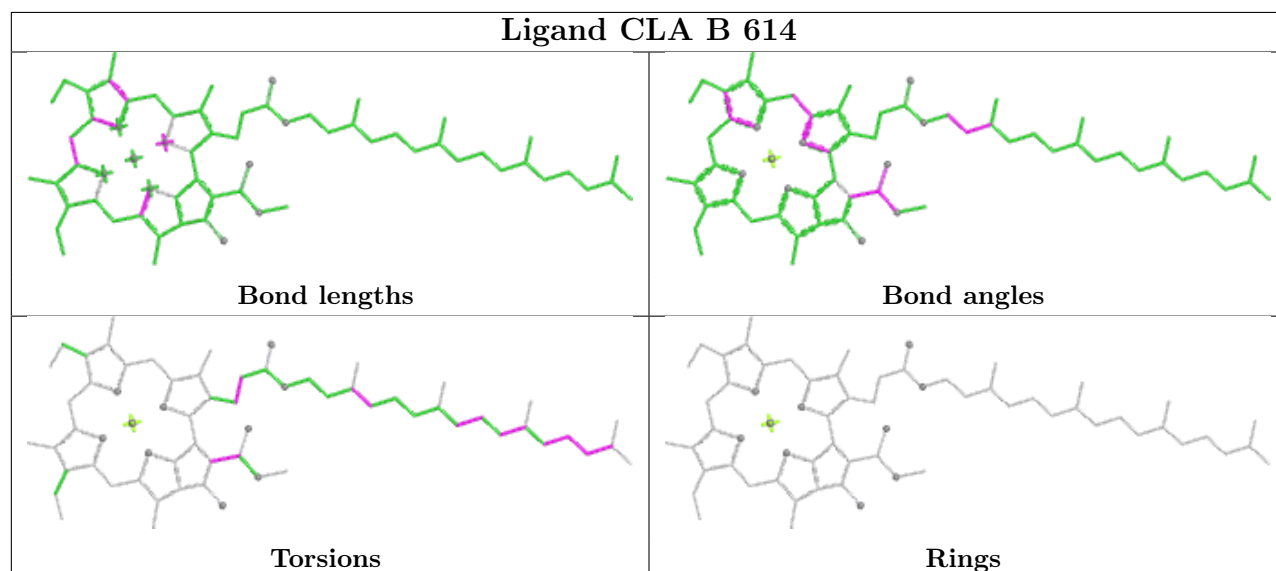
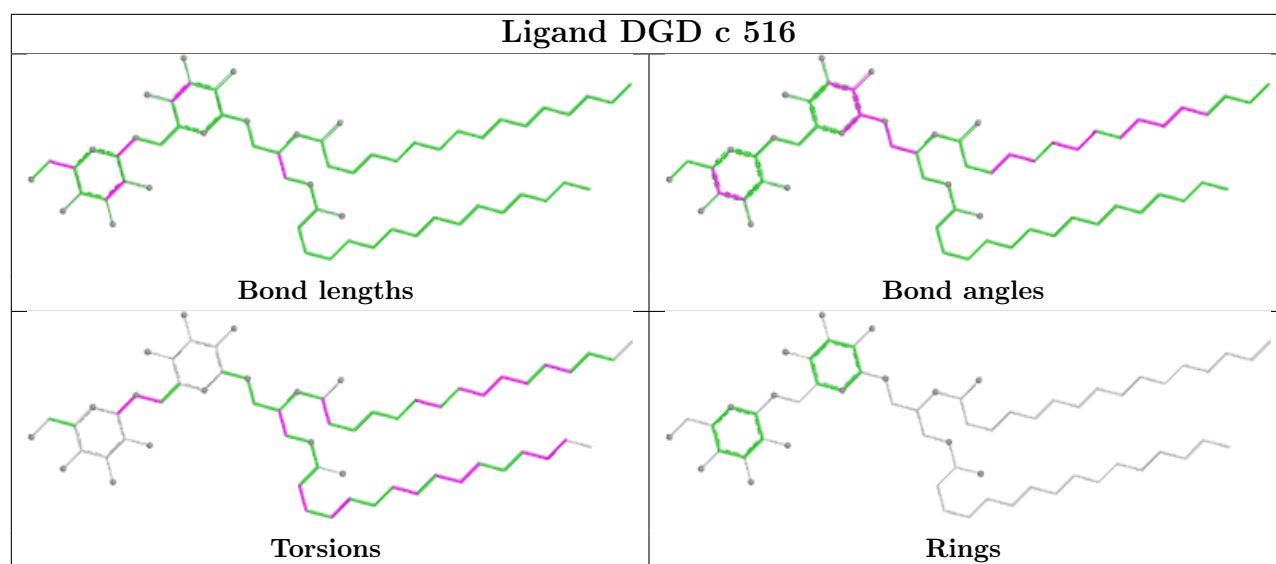
Ligand CLA b 605



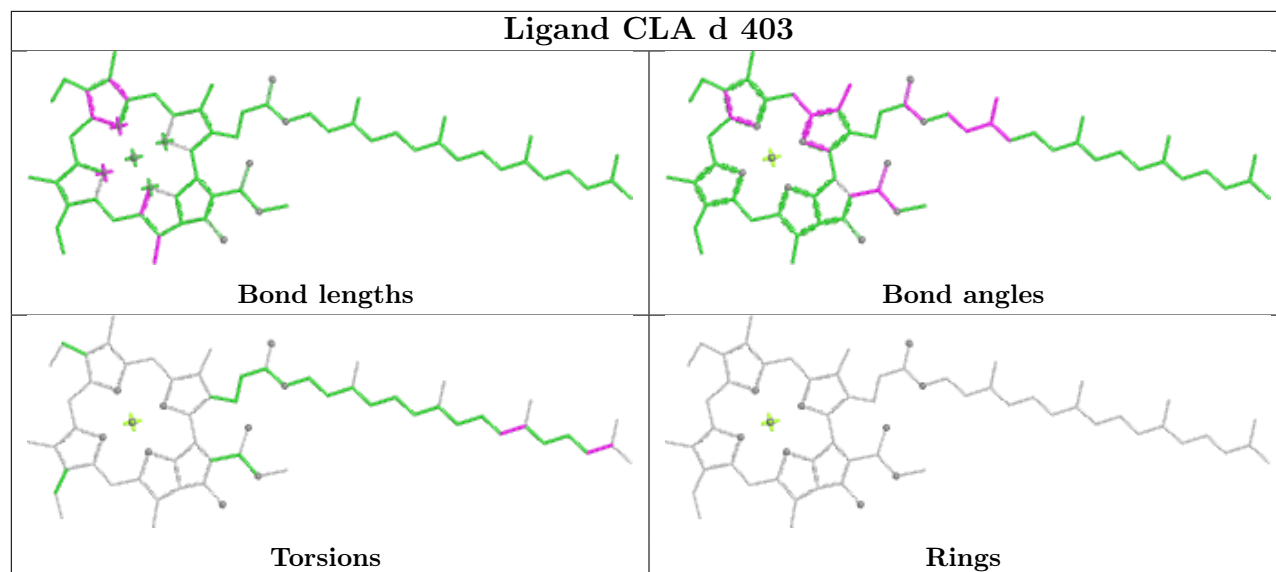




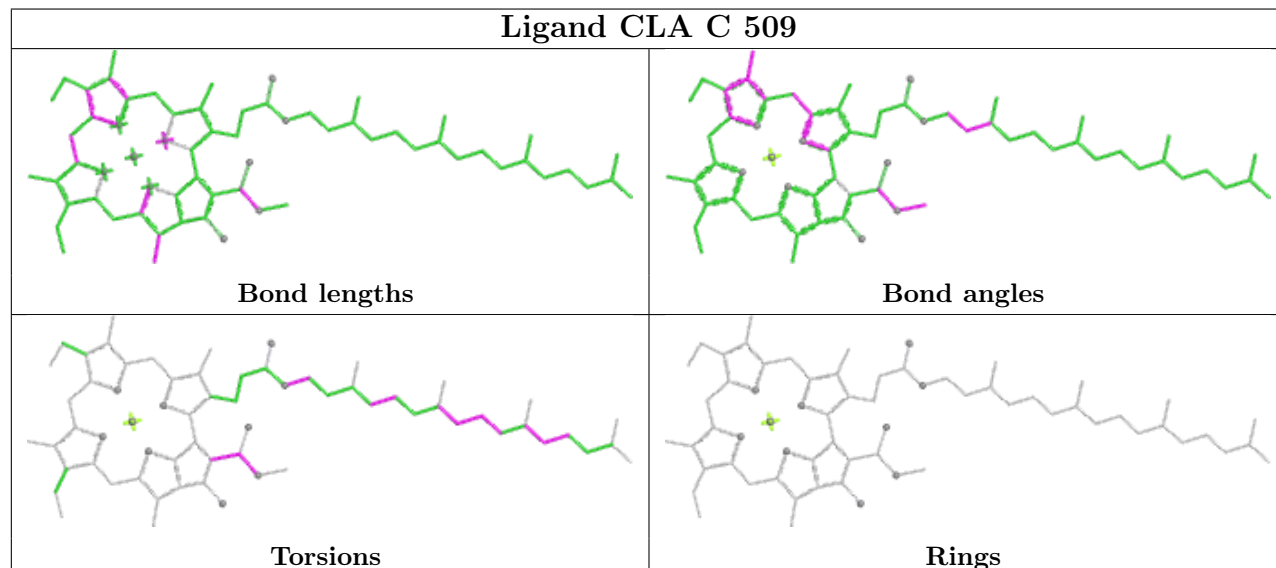




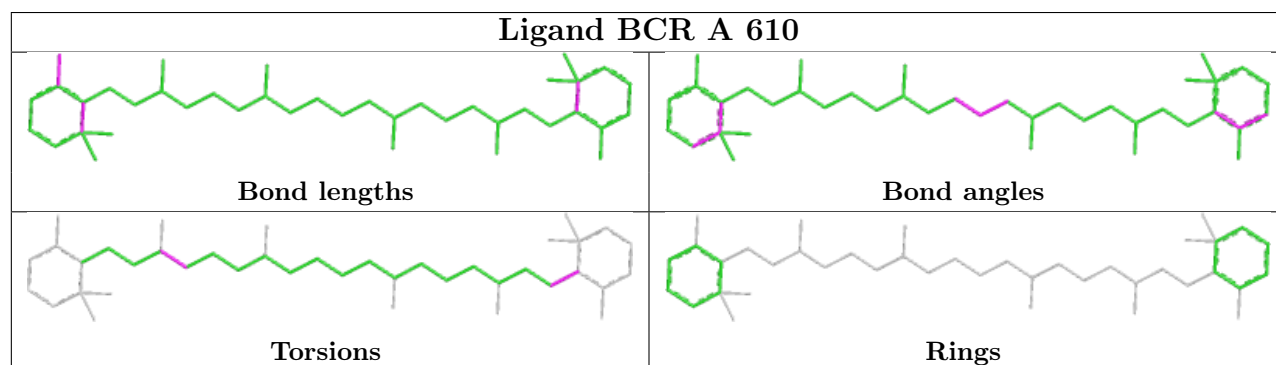
Ligand CLA d 403

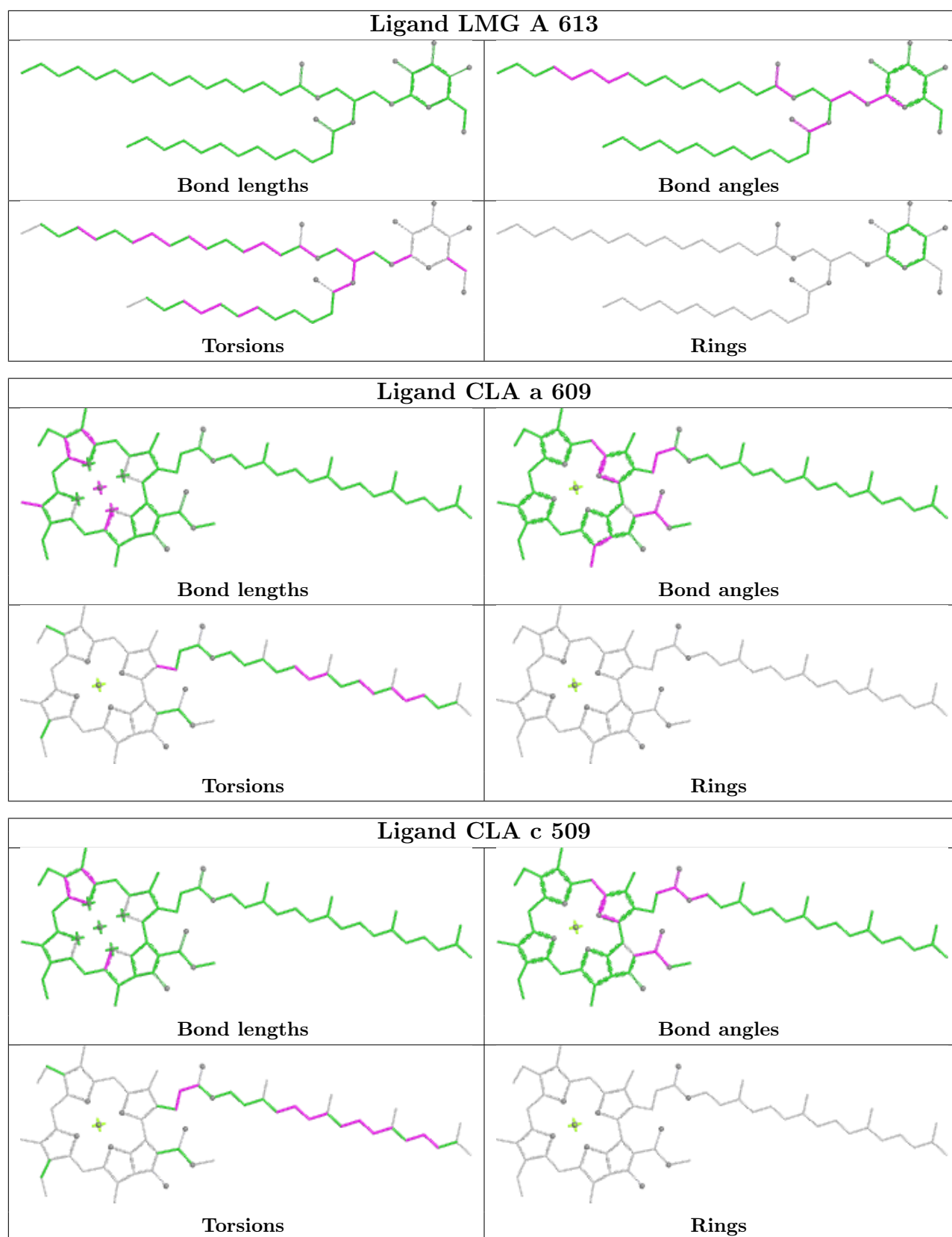


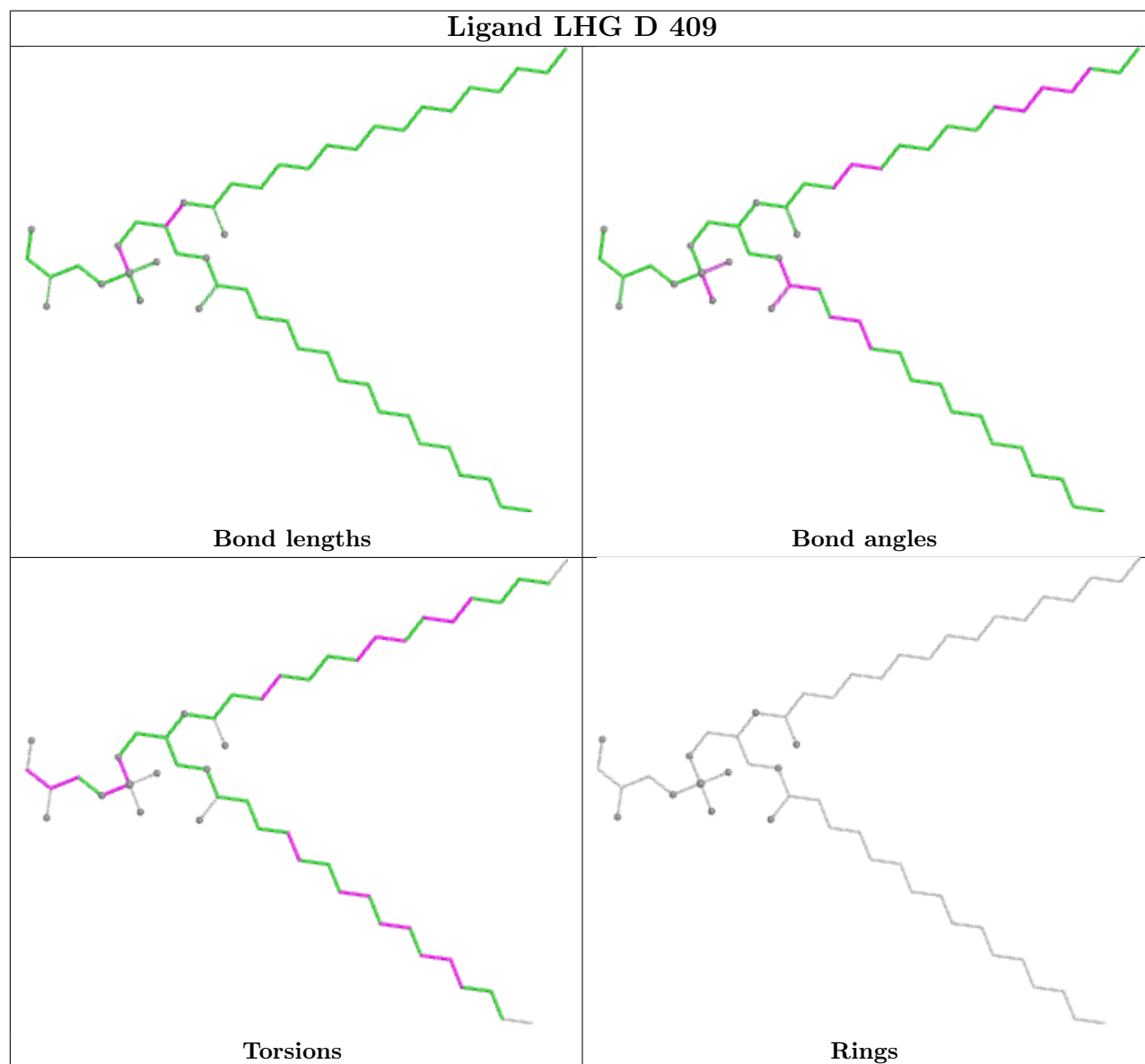
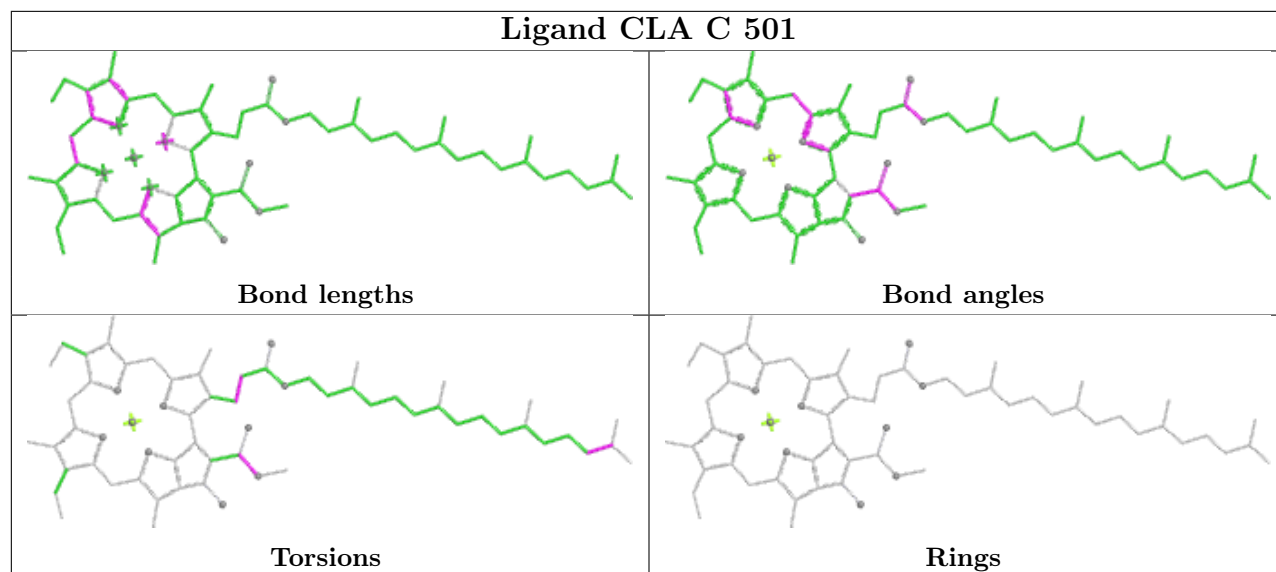
Ligand CLA C 509

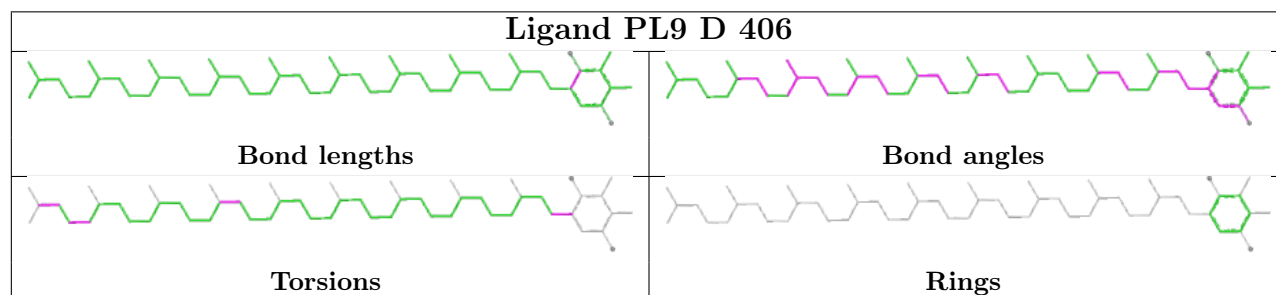
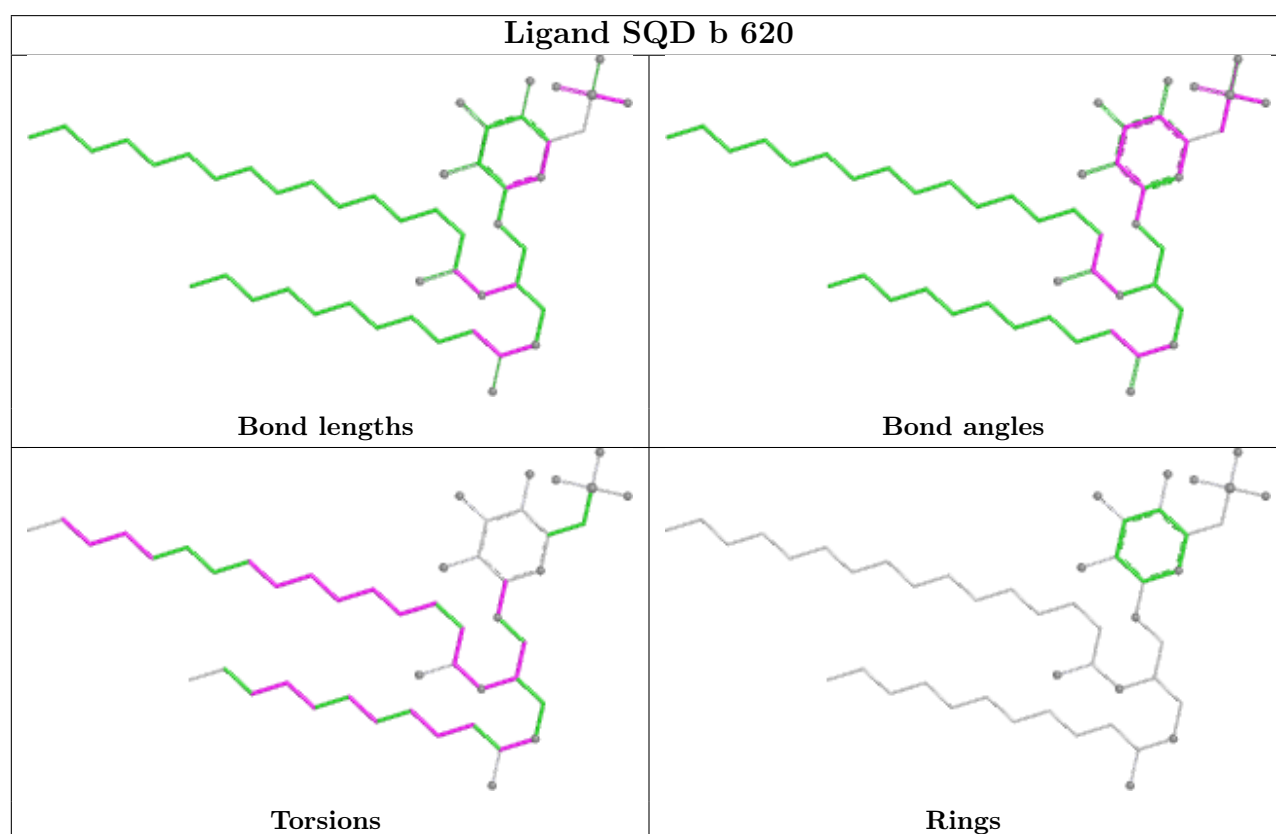
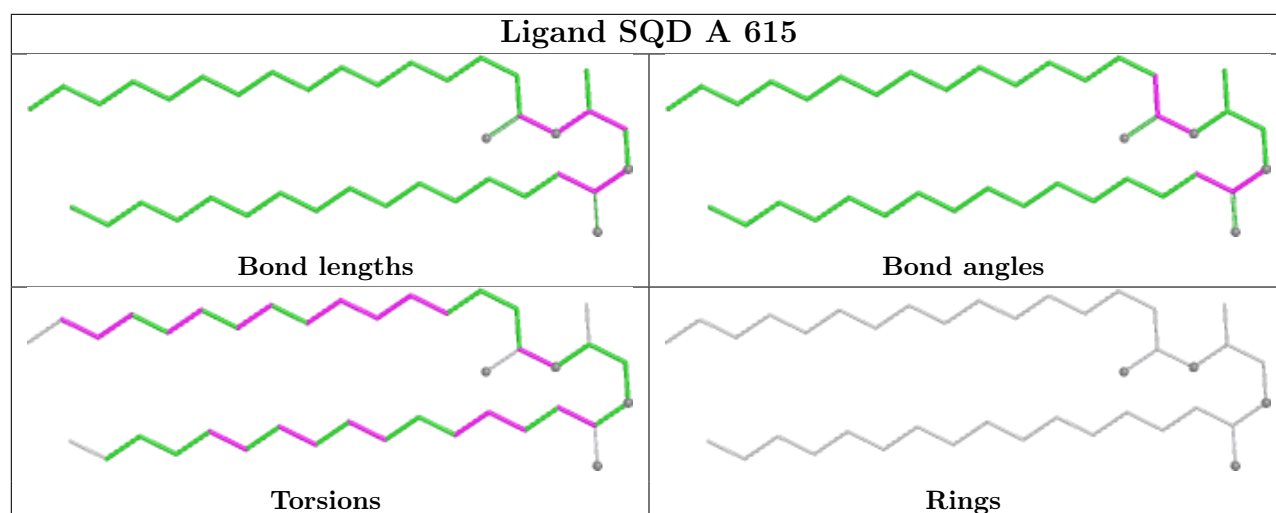


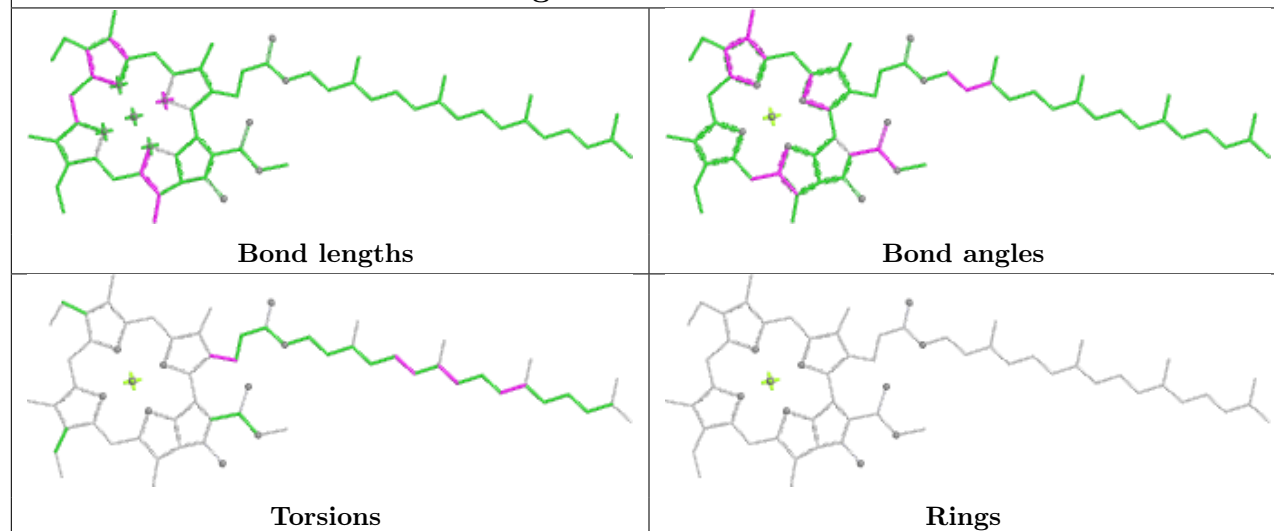
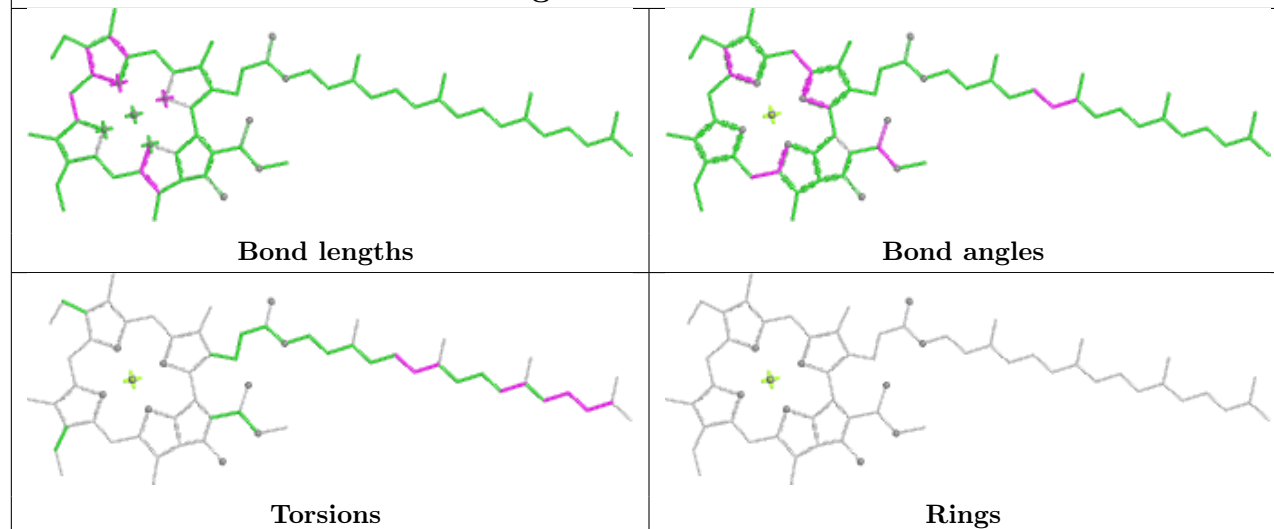
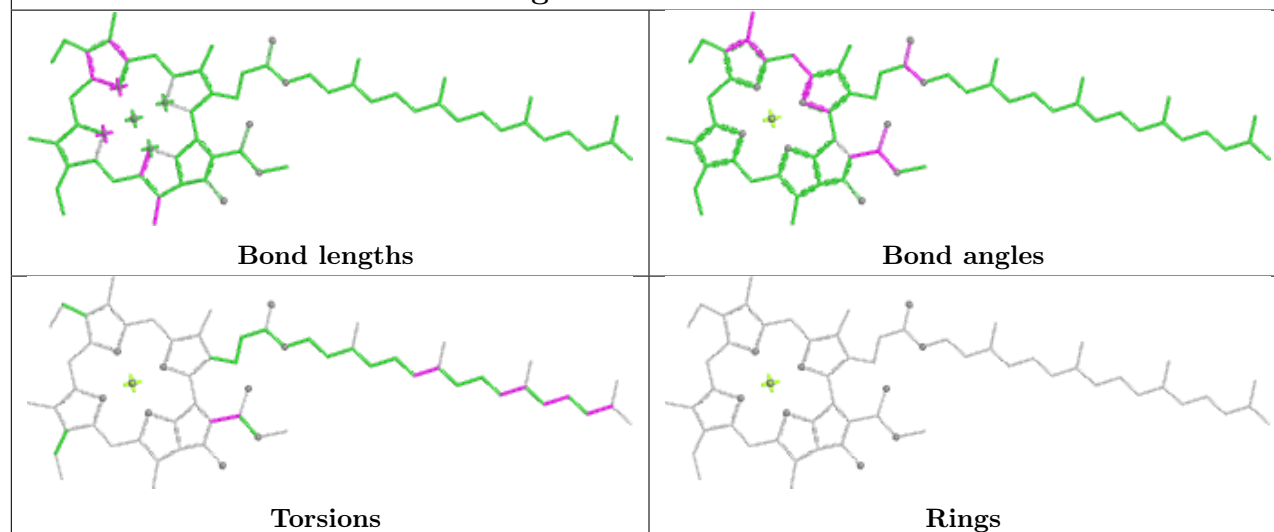
Ligand BCR A 610

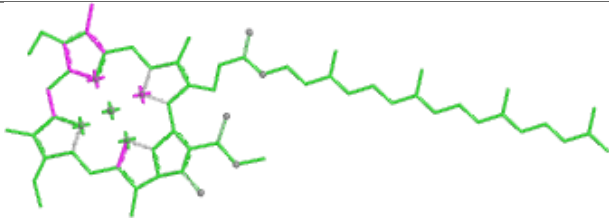
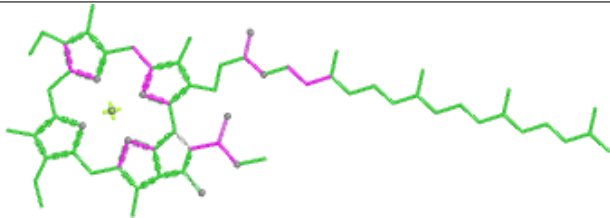
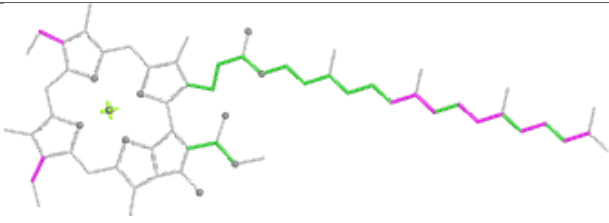
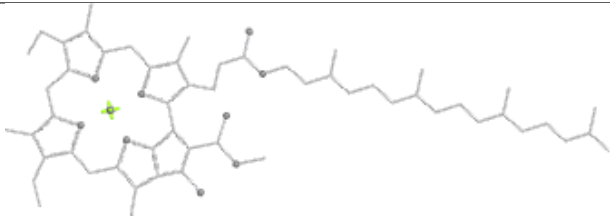




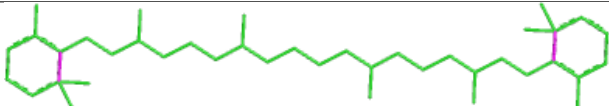
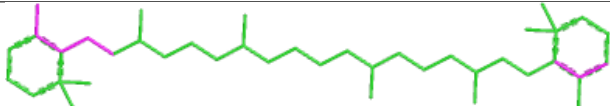
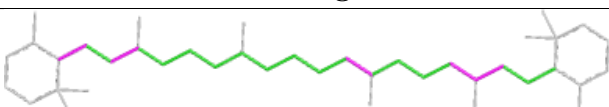
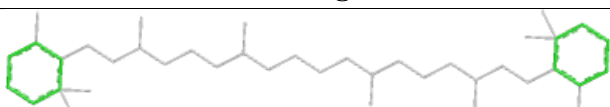


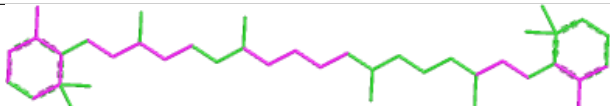
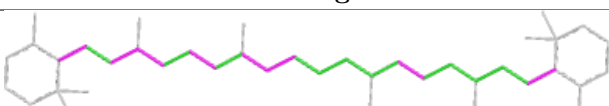
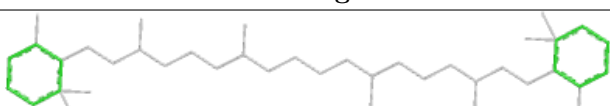


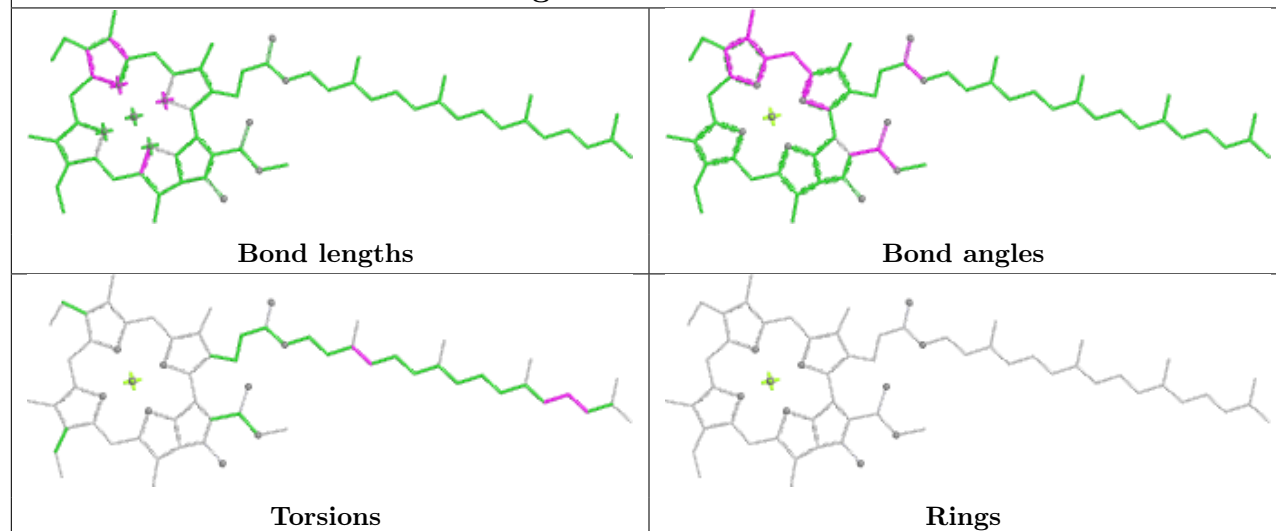
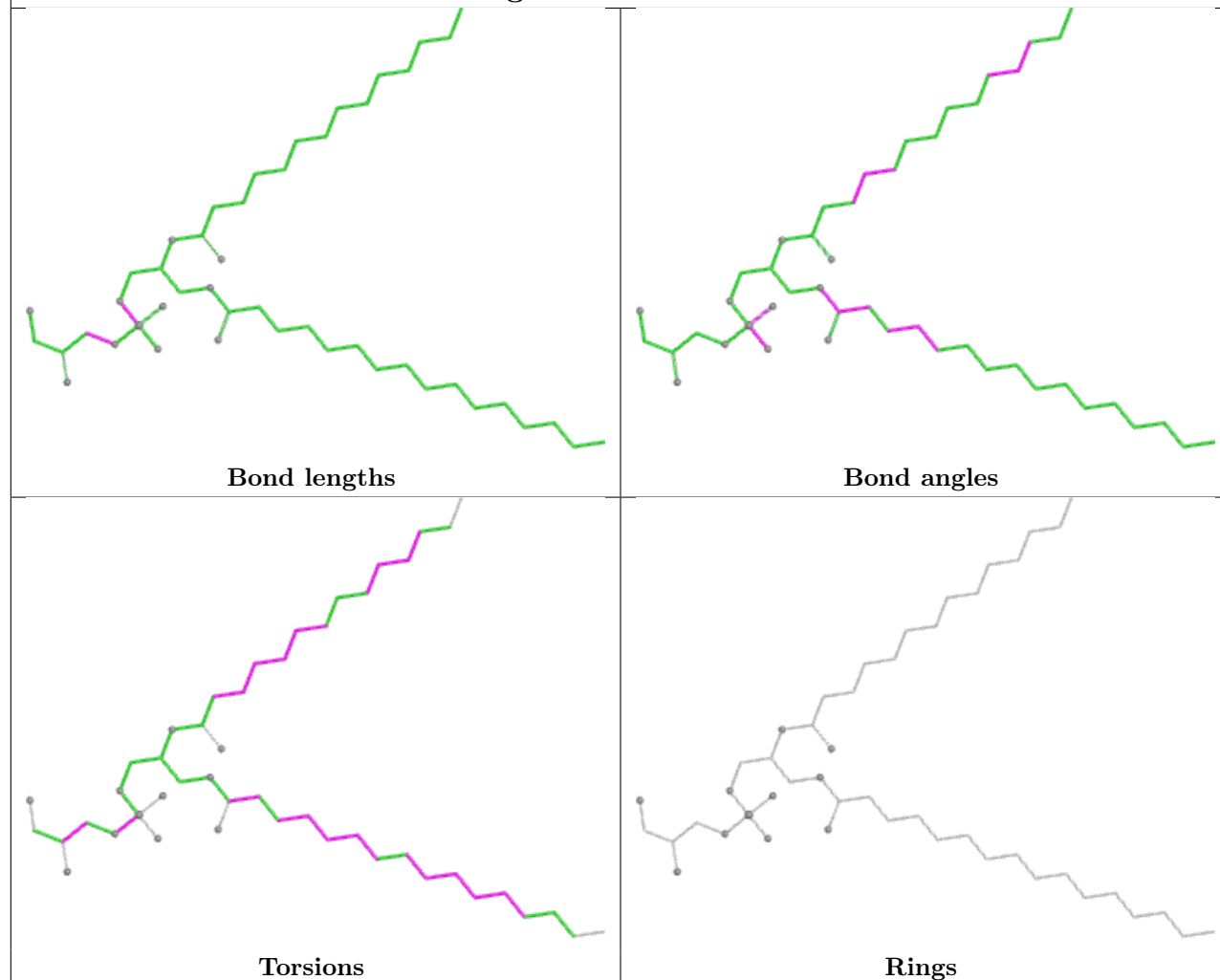
Ligand CLA C 508**Ligand CLA B 615****Ligand CLA D 404**

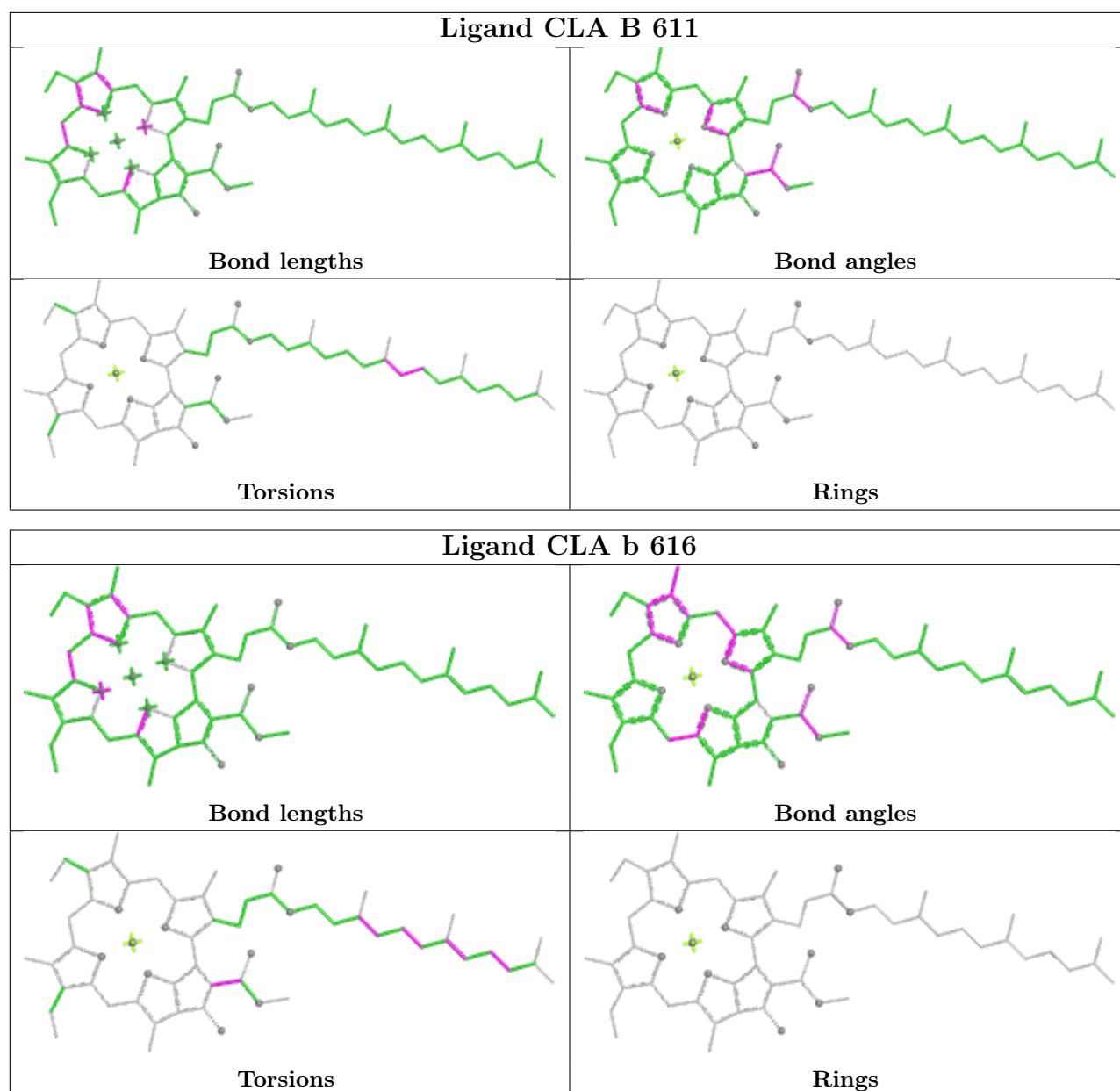
Ligand CLA A 607	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand STE t 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR C 516	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR k 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 608**Ligand LHG D 410**



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%)	-0.57	0 100 100	7, 26, 45, 71	64 (19%)
1	a	334/344 (97%)	-0.48	0 100 100	8, 28, 52, 74	64 (19%)
2	B	505/510 (99%)	-0.46	2 (0%) 88 88	17, 31, 58, 85	4 (0%)
2	b	505/510 (99%)	-0.35	2 (0%) 88 88	24, 35, 64, 100	0
3	C	442/461 (95%)	-0.47	0 100 100	9, 34, 49, 66	11 (2%)
3	c	451/461 (97%)	-0.33	2 (0%) 88 88	9, 37, 57, 93	12 (2%)
4	D	341/352 (96%)	-0.62	0 100 100	10, 28, 44, 74	2 (0%)
4	d	341/352 (96%)	-0.46	0 100 100	9, 32, 53, 76	3 (0%)
5	E	82/84 (97%)	0.11	1 (1%) 76 76	30, 48, 70, 85	1 (1%)
5	e	82/84 (97%)	0.22	1 (1%) 76 76	38, 55, 72, 85	0
6	F	34/45 (75%)	-0.18	1 (2%) 53 52	34, 41, 58, 81	0
6	f	34/45 (75%)	0.03	0 100 100	38, 48, 72, 79	0
7	H	65/66 (98%)	-0.23	2 (3%) 51 50	33, 40, 54, 64	0
7	h	63/66 (95%)	-0.03	0 100 100	37, 48, 59, 63	0
8	I	35/38 (92%)	-0.36	0 100 100	31, 38, 62, 78	0
8	i	35/38 (92%)	-0.33	0 100 100	31, 38, 66, 76	0
9	J	36/40 (90%)	-0.08	0 100 100	33, 47, 68, 84	0
9	j	36/40 (90%)	-0.02	0 100 100	37, 50, 82, 86	0
10	K	37/46 (80%)	-0.18	0 100 100	40, 47, 62, 69	0
10	k	37/46 (80%)	0.02	0 100 100	43, 51, 64, 76	0
11	L	37/37 (100%)	-0.44	0 100 100	23, 28, 60, 62	0
11	l	36/37 (97%)	-0.45	0 100 100	25, 29, 61, 78	0
12	M	32/36 (88%)	-0.46	0 100 100	26, 32, 55, 63	0
12	m	31/36 (86%)	-0.45	0 100 100	27, 32, 51, 61	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/272 (89%)	-0.27	2 (0%) 82 82	23, 40, 78, 122	1 (0%)
13	o	244/272 (89%)	-0.22	2 (0%) 82 82	25, 39, 73, 108	0
14	T	29/32 (90%)	-0.60	1 (3%) 48 47	25, 30, 52, 64	0
14	t	29/32 (90%)	-0.56	0 100 100	26, 30, 62, 79	0
15	U	97/134 (72%)	-0.22	0 100 100	30, 40, 66, 83	0
15	u	97/134 (72%)	-0.28	1 (1%) 79 79	28, 38, 52, 78	0
16	V	137/163 (84%)	-0.36	0 100 100	28, 38, 53, 68	0
16	v	137/163 (84%)	-0.22	0 100 100	32, 44, 63, 78	0
17	Y	27/46 (58%)	0.59	2 (7%) 20 19	47, 63, 77, 83	0
17	y	30/46 (65%)	0.32	0 100 100	55, 64, 75, 92	0
18	X	38/41 (92%)	-0.10	0 100 100	41, 48, 66, 71	0
18	x	39/41 (95%)	0.30	2 (5%) 33 32	46, 56, 79, 93	0
19	Z	62/62 (100%)	0.68	3 (4%) 35 34	52, 63, 100, 109	0
19	z	62/62 (100%)	0.43	1 (1%) 70 70	54, 65, 106, 112	0
20	R	34/41 (82%)	0.55	1 (2%) 53 52	56, 63, 72, 78	0
20	r	31/41 (75%)	0.83	0 100 100	66, 77, 93, 94	0
All	All	5302/5700 (93%)	-0.32	26 (0%) 87 87	7, 36, 67, 122	162 (3%)

The worst 5 of 26 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
19	Z	33	TRP	3.4
19	Z	62	VAL	3.4
18	x	37	VAL	3.0
19	Z	4	LEU	2.9
13	o	58	ASN	2.8

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
14	FME	T	1	10/11	0.91	0.10	30,35,53,62	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	0.92	0.10	36,47,61,62	0
14	FME	t	1	10/11	0.93	0.07	30,33,53,58	0
8	FME	I	1	10/11	0.95	0.07	38,44,53,54	0
12	FME	m	1	10/11	0.96	0.07	31,46,60,64	0
8	FME	i	1	10/11	0.96	0.06	41,46,49,50	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	0.67	0.14	55,61,68,71	0
32	STE	b	624	20/20	0.71	0.14	42,54,64,65	0
29	LMG	d	409	23/55	0.75	0.14	44,59,65,67	0
32	STE	c	521	12/20	0.75	0.13	51,62,67,72	0
32	STE	B	628	12/20	0.77	0.12	50,58,67,68	0
29	LMG	b	622	55/55	0.77	0.13	47,60,69,72	0
32	STE	a	617	12/20	0.77	0.11	55,60,65,66	0
28	PL9	a	611	55/55	0.77	0.14	40,60,76,79	0
31	DGD	a	616	44/66	0.77	0.12	39,50,65,71	0
32	STE	b	623	16/20	0.78	0.11	53,56,72,73	0
33	LHG	E	101	49/49	0.78	0.13	42,70,88,94	0
32	STE	B	627	18/20	0.79	0.12	40,49,70,74	0
28	PL9	A	611	55/55	0.79	0.12	37,57,70,73	0
32	STE	B	621	17/20	0.80	0.13	33,44,61,62	0
29	LMG	D	411	33/55	0.80	0.11	38,52,70,74	0
29	LMG	c	520	48/55	0.80	0.12	50,63,77,80	0
33	LHG	e	102	42/49	0.80	0.11	55,75,89,97	0
32	STE	b	621	20/20	0.81	0.11	36,46,66,70	0
31	DGD	A	616	66/66	0.81	0.10	46,55,64,69	0
25	CLA	b	601	65/65	0.82	0.11	43,60,76,81	0
32	STE	m	102	12/20	0.82	0.12	48,54,60,63	0
32	STE	T	103	15/20	0.82	0.12	44,50,65,66	0
32	STE	E	102	12/20	0.82	0.11	58,65,68,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
29	LMG	A	613	48/55	0.83	0.10	38,53,64,69	0
32	STE	I	101	15/20	0.83	0.12	41,50,61,61	0
32	STE	J	101	12/20	0.83	0.12	45,52,57,59	0
32	STE	d	412	20/20	0.83	0.13	41,53,59,60	0
32	STE	B	629	16/20	0.83	0.11	42,55,68,70	0
32	STE	t	102	10/20	0.83	0.11	44,55,62,65	0
32	STE	C	522	12/20	0.83	0.10	45,52,60,61	0
30	SQD	a	615	36/54	0.83	0.10	38,53,64,68	0
32	STE	j	101	12/20	0.84	0.10	45,53,57,60	0
32	STE	C	521	12/20	0.85	0.11	38,42,54,55	0
30	SQD	B	624	54/54	0.85	0.10	37,54,77,83	0
32	STE	B	625	14/20	0.85	0.09	39,43,52,55	0
29	LMG	c	522	49/55	0.85	0.09	38,50,69,76	0
29	LMG	c	518	37/55	0.85	0.09	40,55,66,66	0
30	SQD	A	615	39/54	0.85	0.10	42,51,72,78	0
30	SQD	f	101	41/54	0.86	0.11	57,70,83,85	0
29	LMG	B	622	28/55	0.86	0.10	39,49,57,63	0
32	STE	T	102	16/20	0.86	0.10	37,44,53,55	0
30	SQD	b	620	49/54	0.86	0.09	35,51,73,77	0
32	STE	b	625	10/20	0.86	0.10	46,52,56,61	0
32	STE	X	101	20/20	0.86	0.12	35,47,61,70	0
32	STE	c	519	20/20	0.87	0.10	39,48,73,74	0
27	BCR	d	405	40/40	0.87	0.10	38,46,72,72	0
25	CLA	B	601	65/65	0.88	0.10	37,53,73,86	0
32	STE	B	626	12/20	0.88	0.12	43,50,55,57	0
29	LMG	m	101	51/55	0.88	0.08	37,48,58,60	0
27	BCR	k	102	40/40	0.89	0.09	41,51,56,62	0
32	STE	l	102	18/20	0.89	0.10	33,43,60,63	0
31	DGD	H	102	62/66	0.89	0.09	29,40,49,53	0
29	LMG	B	620	51/55	0.89	0.08	31,47,57,60	0
32	STE	M	102	10/20	0.89	0.09	42,45,48,49	0
27	BCR	x	101	40/40	0.89	0.09	38,48,62,64	0
29	LMG	C	520	48/55	0.90	0.09	39,57,65,70	0
31	DGD	h	101	62/66	0.90	0.09	31,43,49,55	0
32	STE	M	101	15/20	0.90	0.09	34,43,54,57	0
27	BCR	C	514	40/40	0.90	0.09	41,49,54,55	0
32	STE	d	411	17/20	0.90	0.09	45,50,60,61	0
27	BCR	C	516	40/40	0.90	0.09	39,48,55,57	0
25	CLA	c	512	65/65	0.91	0.09	42,51,72,74	0
27	BCR	k	103	40/40	0.91	0.10	41,47,54,57	0
27	BCR	D	405	40/40	0.91	0.09	31,39,67,71	0
27	BCR	H	101	40/40	0.91	0.08	33,43,55,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	DGD	C	518	62/66	0.91	0.08	30,41,77,86	0
30	SQD	A	614	52/54	0.91	0.10	31,46,68,75	0
25	CLA	C	513	65/65	0.91	0.08	41,49,71,74	0
27	BCR	k	101	40/40	0.91	0.09	41,51,55,57	0
30	SQD	D	408	36/54	0.91	0.10	43,61,66,70	0
30	SQD	a	614	54/54	0.91	0.09	38,54,66,69	0
31	DGD	c	516	62/66	0.92	0.08	32,44,69,73	0
29	LMG	D	407	51/55	0.92	0.08	28,44,67,69	0
32	STE	C	523	16/20	0.92	0.08	37,47,54,55	0
31	DGD	c	515	62/66	0.93	0.07	23,35,57,67	0
27	BCR	B	619	40/40	0.93	0.07	28,37,49,52	0
25	CLA	C	506	65/65	0.93	0.07	29,37,61,65	0
25	CLA	c	508	64/65	0.93	0.07	30,38,71,85	0
25	CLA	B	606	65/65	0.93	0.07	25,32,55,63	0
25	CLA	c	513	65/65	0.93	0.08	42,52,83,86	0
27	BCR	b	617	40/40	0.93	0.07	28,36,44,47	0
27	BCR	b	618	40/40	0.93	0.07	25,36,46,47	0
31	DGD	C	517	62/66	0.93	0.08	23,34,67,72	0
27	BCR	b	619	40/40	0.93	0.07	30,41,55,58	0
33	LHG	D	412	49/49	0.93	0.07	30,38,56,56	0
27	BCR	c	514	40/40	0.93	0.07	26,40,50,52	0
33	LHG	a	613	49/49	0.93	0.07	34,44,57,62	0
27	BCR	A	610	40/40	0.93	0.06	23,31,39,40	0
34	BCT	d	401	4/4	0.93	0.08	32,38,41,47	0
25	CLA	C	503	65/65	0.94	0.07	30,37,41,49	0
27	BCR	t	101	40/40	0.94	0.06	26,33,44,47	0
25	CLA	d	404	65/65	0.94	0.08	30,40,72,76	0
25	CLA	a	606	65/65	0.94	0.07	18,26,37,46	0
28	PL9	D	406	55/55	0.94	0.06	22,28,37,38	0
27	BCR	B	617	40/40	0.94	0.06	27,34,42,44	0
28	PL9	d	406	55/55	0.94	0.06	24,30,35,39	0
31	DGD	C	519	62/66	0.94	0.07	29,37,65,68	0
27	BCR	B	618	40/40	0.94	0.06	24,35,42,45	0
25	CLA	C	508	65/65	0.94	0.07	27,33,74,81	0
25	CLA	b	606	65/65	0.94	0.07	28,34,61,68	0
27	BCR	C	515	40/40	0.94	0.07	28,37,45,50	0
31	DGD	c	517	62/66	0.94	0.08	27,42,64,68	0
25	CLA	b	608	65/65	0.94	0.07	30,36,49,55	0
25	CLA	b	610	65/65	0.94	0.07	24,33,40,42	0
25	CLA	b	614	65/65	0.94	0.07	22,33,56,66	0
27	BCR	K	101	40/40	0.94	0.08	35,42,55,57	0
27	BCR	T	101	40/40	0.94	0.06	28,33,43,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	CLA	b	616	60/65	0.94	0.08	26,37,78,82	0
25	CLA	c	503	65/65	0.94	0.07	34,38,44,50	0
33	LHG	D	410	47/49	0.94	0.08	27,39,70,76	0
25	CLA	c	506	65/65	0.94	0.08	32,40,77,79	0
25	CLA	C	510	65/65	0.94	0.07	30,38,48,51	0
25	CLA	c	509	65/65	0.94	0.08	32,38,51,56	0
25	CLA	c	511	65/65	0.94	0.08	37,46,56,62	0
25	CLA	C	512	65/65	0.94	0.08	38,45,70,82	0
29	LMG	d	410	44/55	0.95	0.07	36,44,65,71	0
25	CLA	c	501	65/65	0.95	0.06	28,35,42,47	0
25	CLA	c	502	65/65	0.95	0.06	28,34,45,49	0
25	CLA	a	607	65/65	0.95	0.07	27,33,71,74	0
25	CLA	c	504	60/65	0.95	0.06	28,38,64,66	0
25	CLA	c	505	65/65	0.95	0.07	31,35,55,65	0
25	CLA	B	609	65/65	0.95	0.06	24,33,44,49	0
25	CLA	c	507	65/65	0.95	0.07	26,36,48,51	0
25	CLA	B	610	65/65	0.95	0.06	21,27,35,37	0
25	CLA	C	511	65/65	0.95	0.07	33,42,51,54	0
25	CLA	c	510	65/65	0.95	0.07	29,39,50,54	0
27	BCR	a	610	40/40	0.95	0.06	23,31,40,42	0
25	CLA	b	609	65/65	0.95	0.07	28,40,55,65	0
33	LHG	B	623	49/49	0.95	0.07	27,35,44,51	0
25	CLA	C	502	65/65	0.95	0.06	27,32,44,48	0
25	CLA	b	612	65/65	0.95	0.07	23,29,41,48	0
25	CLA	d	403	65/65	0.95	0.06	22,28,49,54	0
25	CLA	A	606	65/65	0.95	0.06	18,24,39,43	0
33	LHG	d	408	39/49	0.95	0.07	31,39,57,58	0
26	PHO	d	402	64/64	0.95	0.06	27,35,40,43	0
33	LHG	l	101	49/49	0.95	0.07	29,39,46,54	0
25	CLA	A	607	65/65	0.95	0.07	22,29,78,81	0
25	CLA	C	501	65/65	0.96	0.06	26,32,41,47	0
25	CLA	b	602	65/65	0.96	0.06	29,36,50,53	0
25	CLA	b	604	65/65	0.96	0.06	22,28,59,72	0
25	CLA	b	605	65/65	0.96	0.06	22,29,39,45	0
26	PHO	D	402	64/64	0.96	0.05	22,29,34,39	0
26	PHO	a	608	64/64	0.96	0.05	19,27,32,40	0
25	CLA	A	612	65/65	0.96	0.06	18,24,38,48	0
25	CLA	B	607	65/65	0.96	0.06	19,27,52,54	0
25	CLA	C	504	59/65	0.96	0.06	28,34,60,63	0
25	CLA	C	505	65/65	0.96	0.06	25,34,51,60	0
25	CLA	B	608	65/65	0.96	0.06	22,29,47,54	0
25	CLA	b	613	65/65	0.96	0.06	21,28,59,61	0

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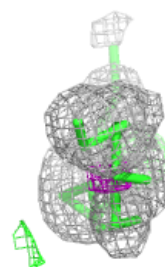
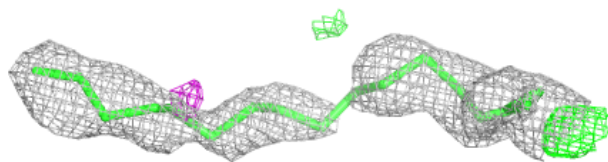
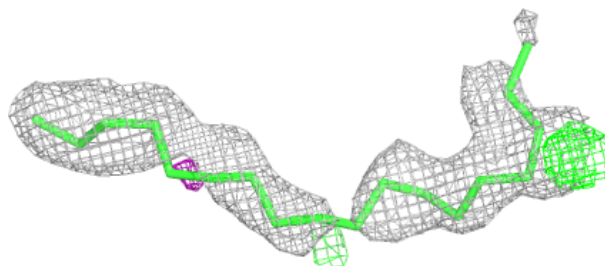
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	CLA	C	507	65/65	0.96	0.06	25,33,46,48	0
25	CLA	b	615	65/65	0.96	0.06	26,35,47,53	0
25	CLA	B	602	65/65	0.96	0.06	24,32,46,50	0
25	CLA	C	509	65/65	0.96	0.07	26,35,50,54	0
25	CLA	B	604	65/65	0.96	0.07	21,26,56,61	0
25	CLA	B	611	65/65	0.96	0.05	19,26,40,44	0
33	LHG	D	409	49/49	0.96	0.06	26,34,42,46	0
25	CLA	B	613	65/65	0.96	0.06	19,25,55,64	0
25	CLA	B	614	65/65	0.96	0.06	22,32,55,63	0
25	CLA	D	403	65/65	0.96	0.06	18,24,44,52	0
25	CLA	D	404	65/65	0.96	0.07	26,32,76,85	0
33	LHG	d	407	49/49	0.96	0.06	29,37,46,53	0
25	CLA	B	615	65/65	0.96	0.06	23,30,48,58	0
25	CLA	B	616	60/65	0.96	0.07	24,32,71,76	0
25	CLA	a	609	65/65	0.96	0.09	21,28,62,66	0
34	BCT	D	401	4/4	0.96	0.06	29,29,31,34	0
25	CLA	a	612	65/65	0.96	0.05	21,27,39,44	0
26	PHO	A	608	64/64	0.97	0.05	20,25,30,35	0
25	CLA	b	611	65/65	0.97	0.05	23,29,44,50	0
25	CLA	B	605	65/65	0.97	0.05	20,27,37,41	0
25	CLA	B	612	65/65	0.97	0.06	20,27,36,41	0
25	CLA	b	607	65/65	0.97	0.06	23,30,56,61	0
25	CLA	B	603	65/65	0.97	0.06	20,28,50,52	0
25	CLA	b	603	65/65	0.97	0.06	23,30,55,63	0
25	CLA	A	609	54/65	0.97	0.06	20,25,57,61	0
35	HEM	F	101	43/43	0.97	0.08	39,44,53,58	0
35	HEM	e	101	43/43	0.97	0.09	45,53,66,78	0
36	HEC	V	201	43/43	0.98	0.06	24,29,37,44	0
36	HEC	v	201	43/43	0.98	0.06	27,33,36,41	0
24	CL	A	605	1/1	0.99	0.04	27,27,27,27	0
24	CL	a	604	1/1	0.99	0.06	26,26,26,26	0
21	OEX	A	601[B]	10/10	0.99	0.03	24,28,32,32	10
21	OEX	A	601[C]	10/10	0.99	0.03	18,22,26,27	10
21	OEX	a	601[B]	10/10	0.99	0.02	25,29,31,31	10
21	OEX	a	601[C]	10/10	0.99	0.02	17,24,26,28	10
22	OXY	A	602[A]	11/11	0.99	0.04	25,28,31,31	11
22	OXY	a	602[A]	11/11	0.99	0.03	27,29,33,33	11
23	FE2	a	603	1/1	0.99	0.02	33,33,33,33	0
24	CL	A	604	1/1	0.99	0.03	27,27,27,27	0
23	FE2	A	603	1/1	1.00	0.02	26,26,26,26	0
24	CL	a	605	1/1	1.00	0.07	28,28,28,28	0

The following is a graphical depiction of the model fit to experimental electron density of all

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

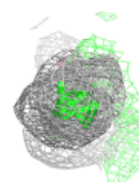
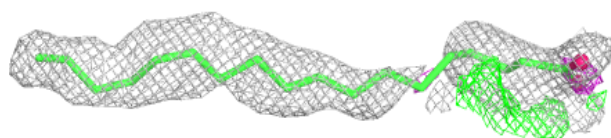
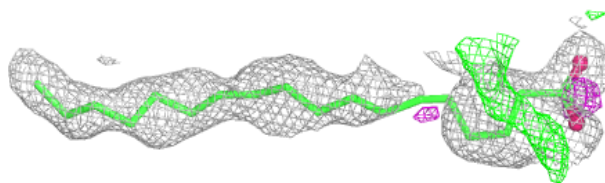
Electron density around STE H 103:

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

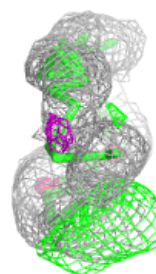
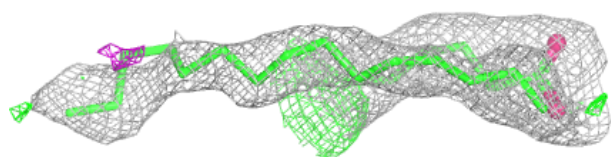
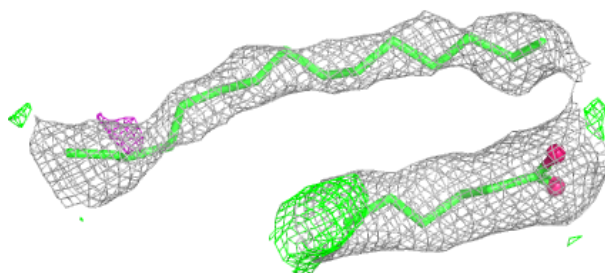


Electron density around STE b 624:

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

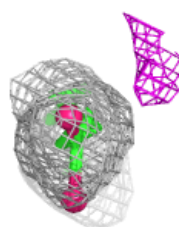
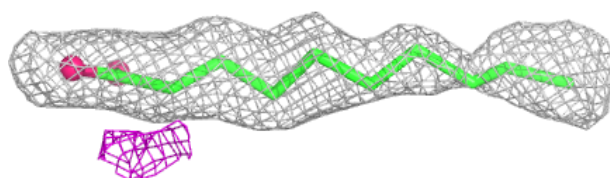
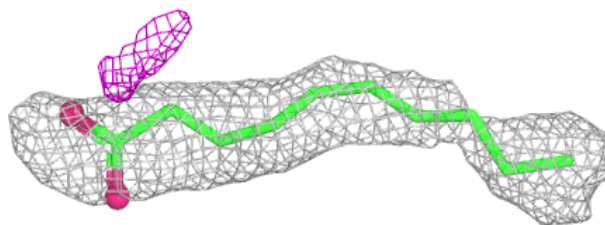
**Electron density around LMG d 409:**

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

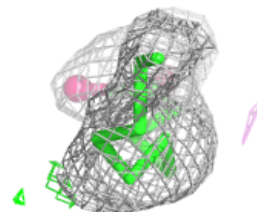
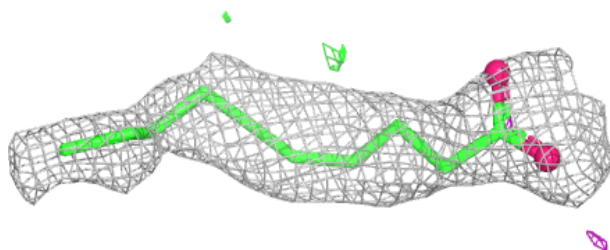
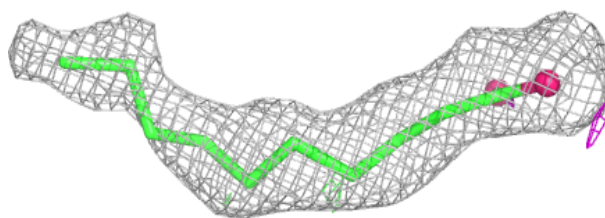


Electron density around STE c 521:

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

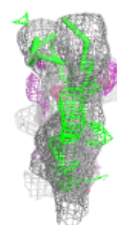
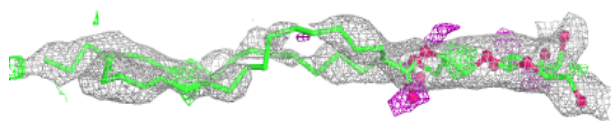
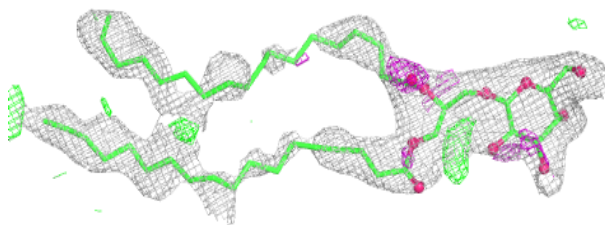
**Electron density around STE B 628:**

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

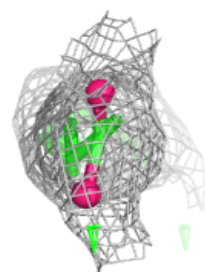
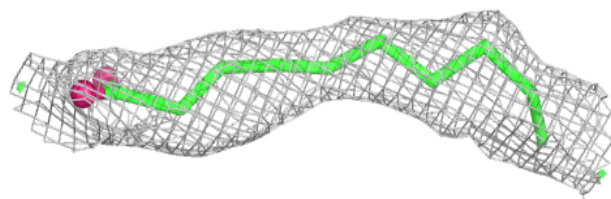
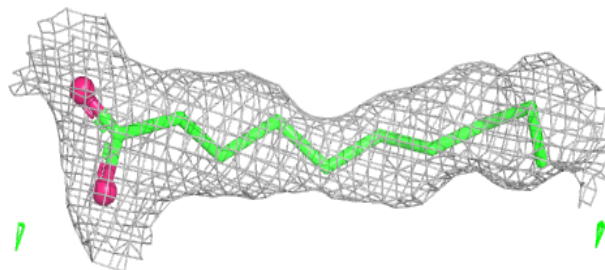


Electron density around LMG b 622:

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

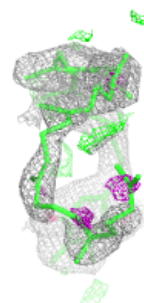
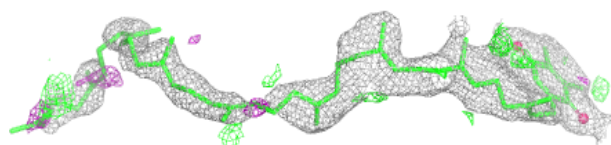
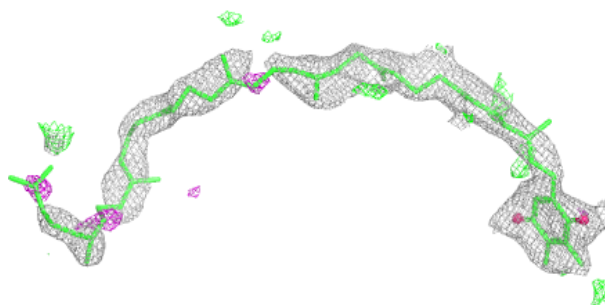
**Electron density around STE a 617:**

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

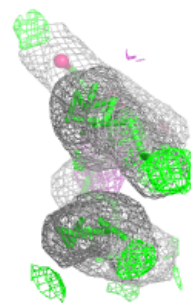
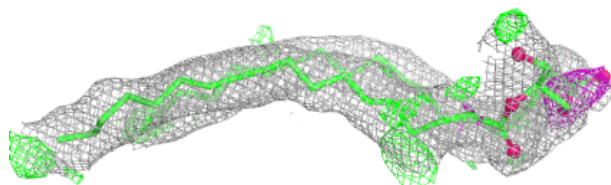
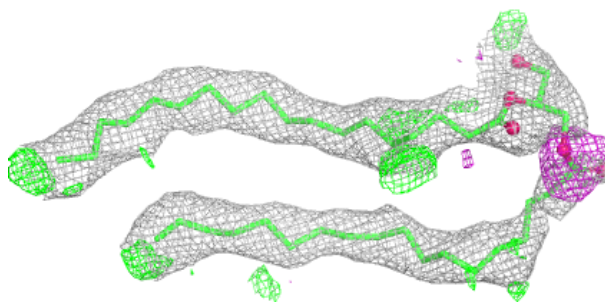


Electron density around PL9 a 611:

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

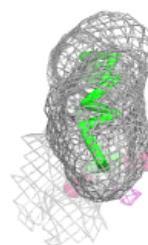
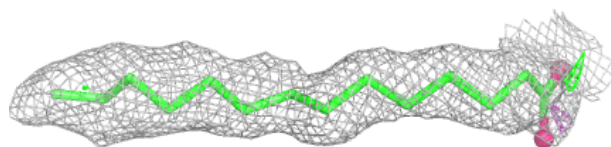
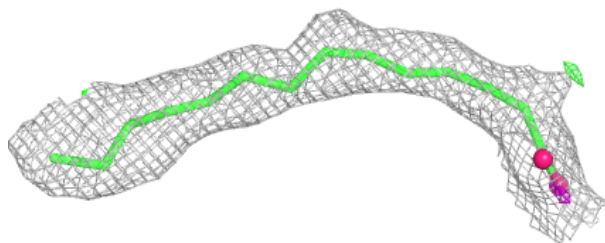
**Electron density around DGD a 616:**

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



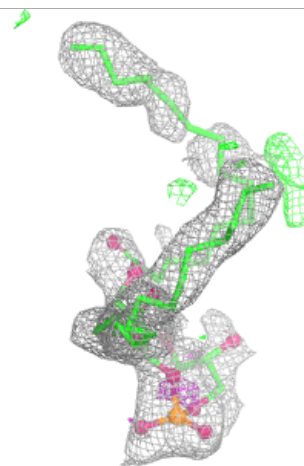
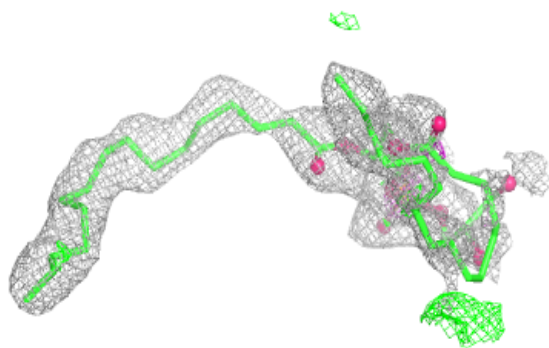
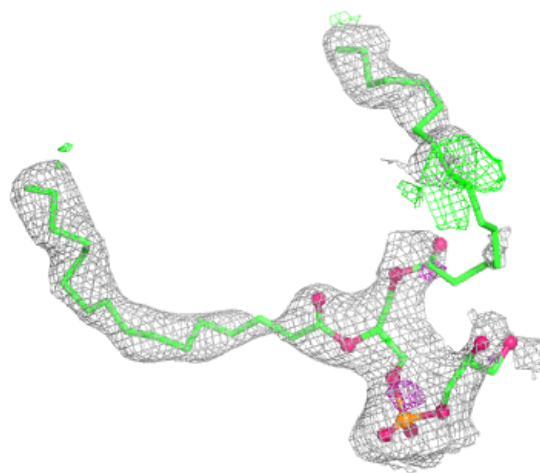
Electron density around STE b 623:

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



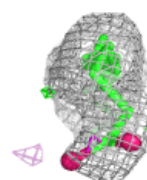
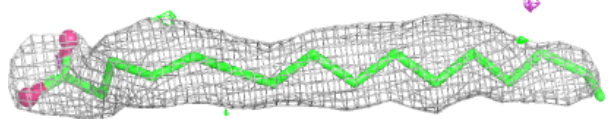
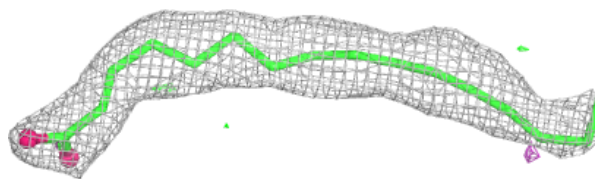
Electron density around LHG E 101:

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

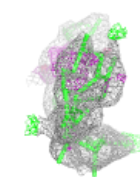
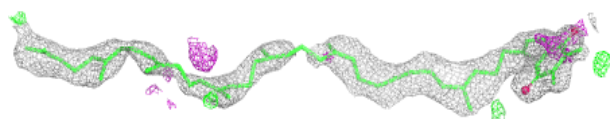
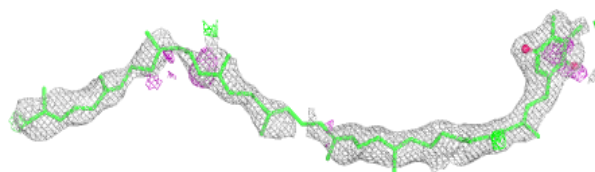


Electron density around STE B 627:

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

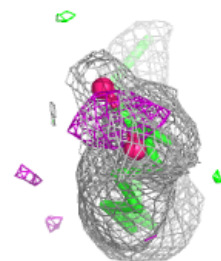
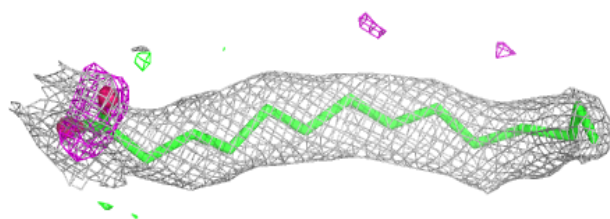
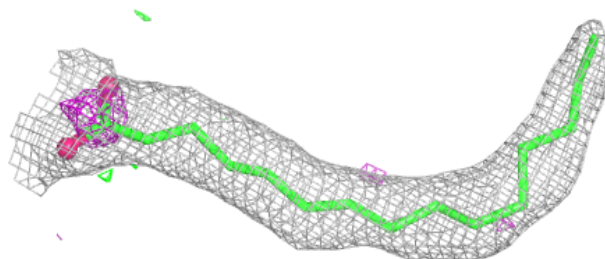
**Electron density around PL9 A 611:**

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

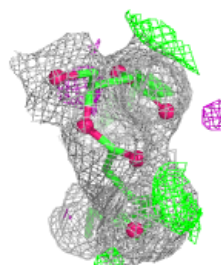
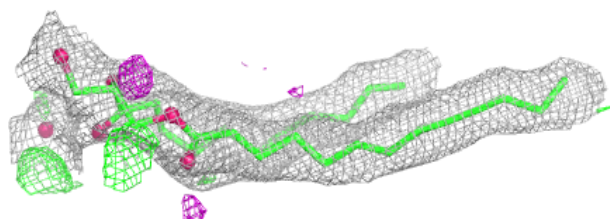
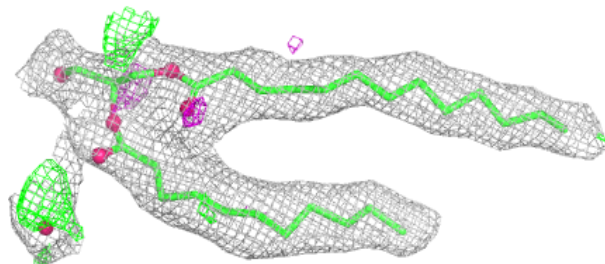


Electron density around STE B 621:

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

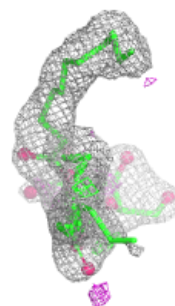
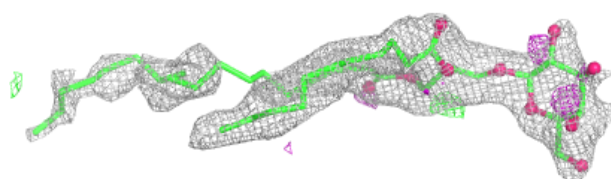
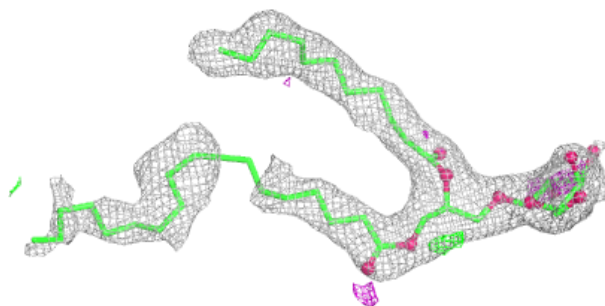
**Electron density around LMG D 411:**

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

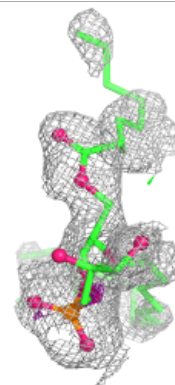
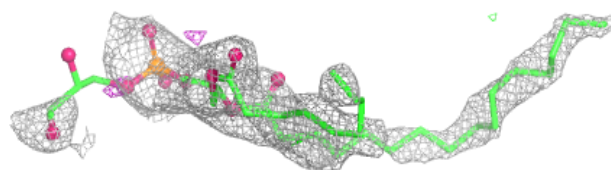
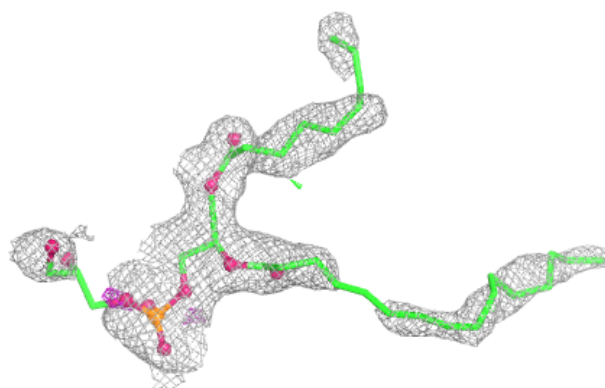


Electron density around LMG c 520:

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

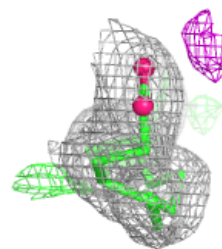
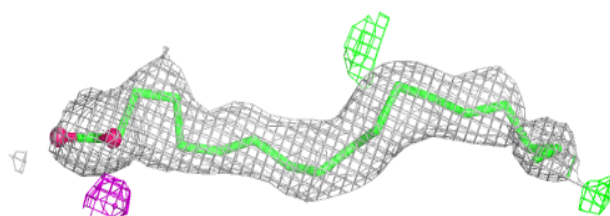
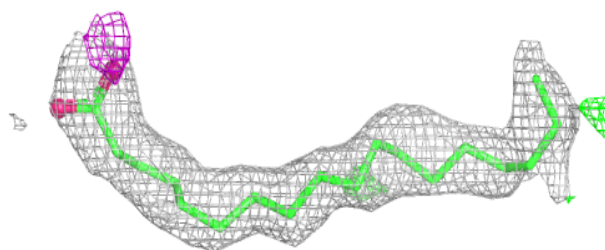
**Electron density around LHG e 102:**

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

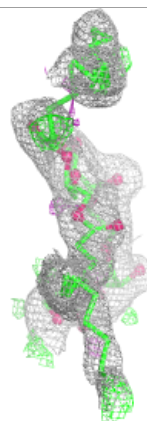
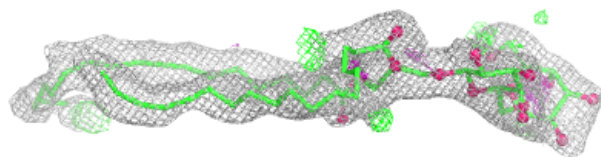
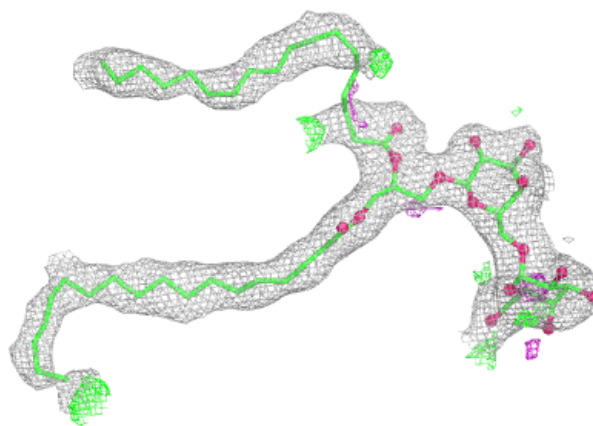


Electron density around STE b 621:

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

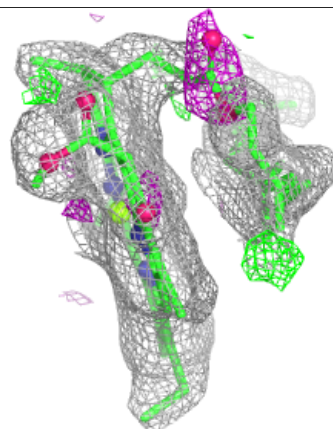
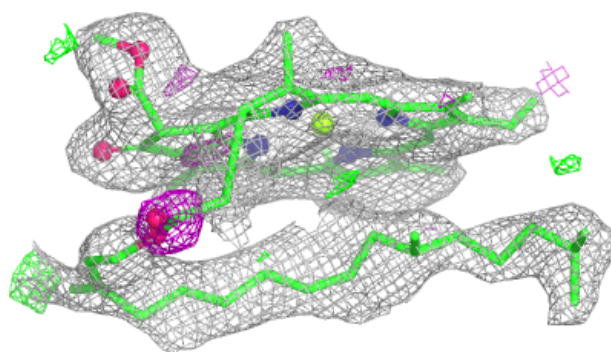
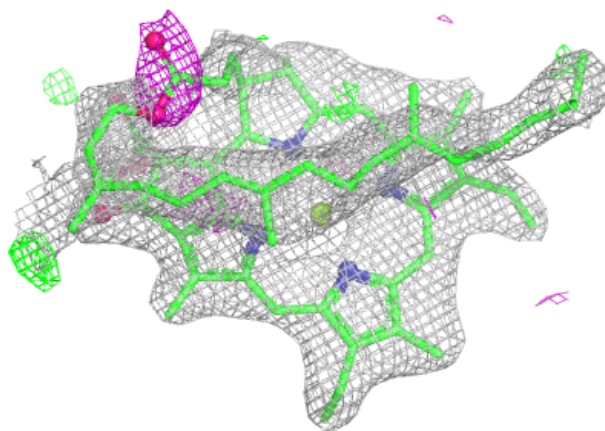
**Electron density around DGD A 616:**

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

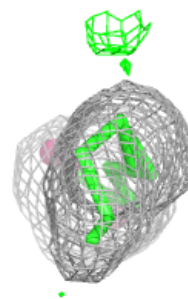
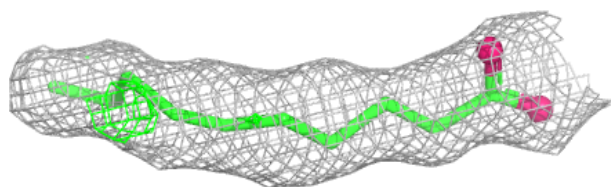
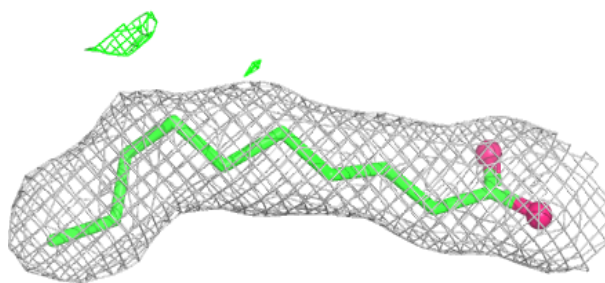


Electron density around CLA b 601:

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

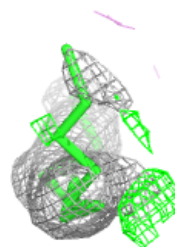
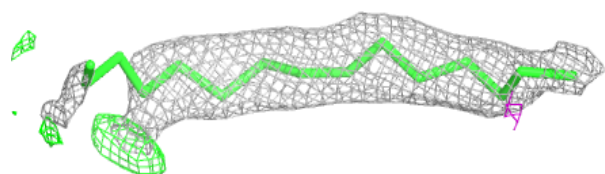
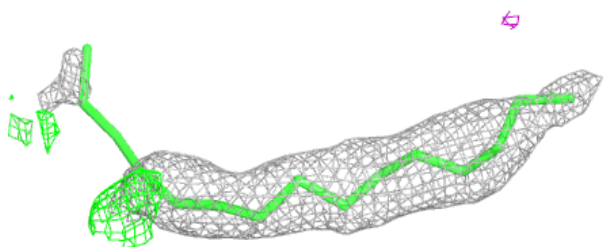
**Electron density around STE m 102:**

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

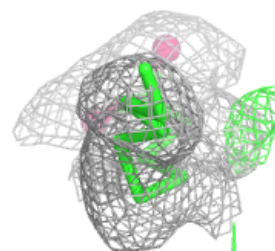
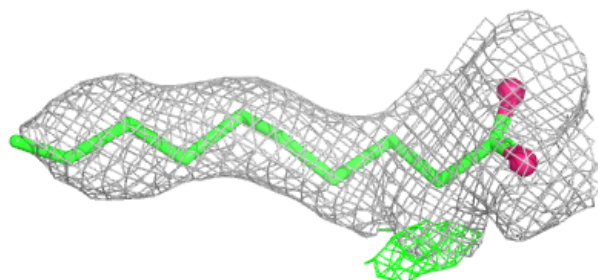
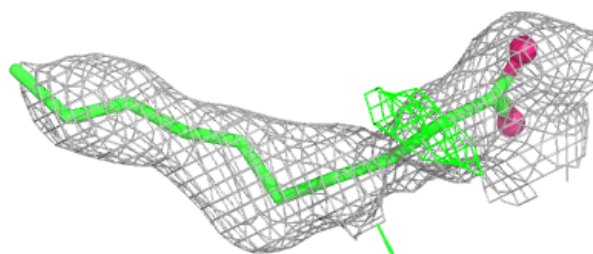


Electron density around STE T 103:

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

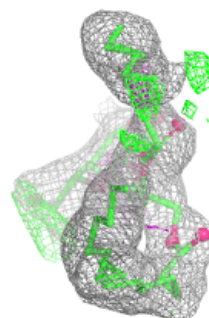
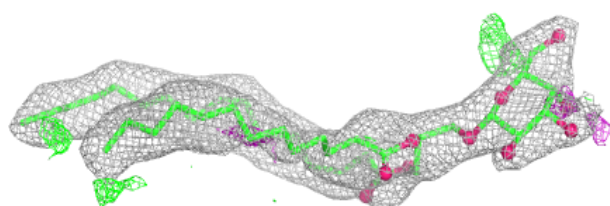
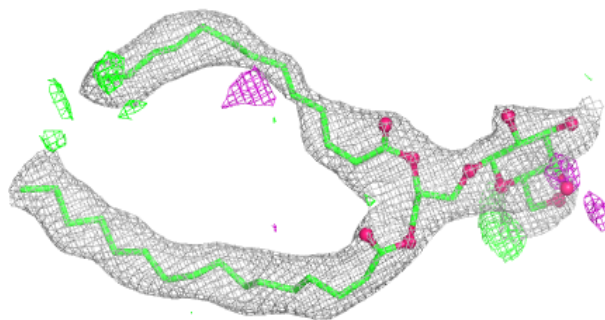
**Electron density around STE E 102:**

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

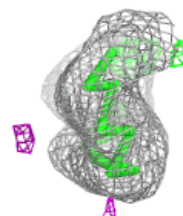
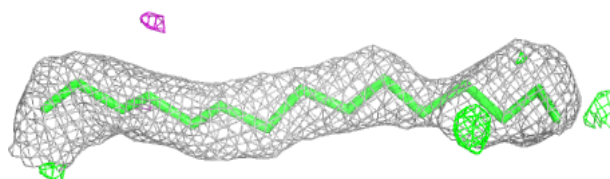
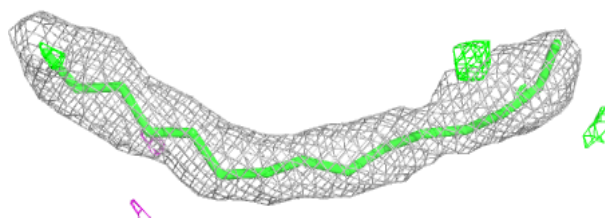


Electron density around LMG A 613:

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

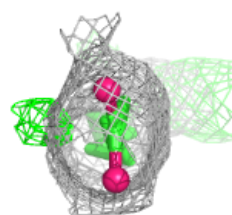
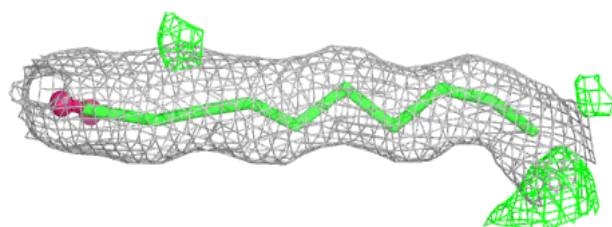
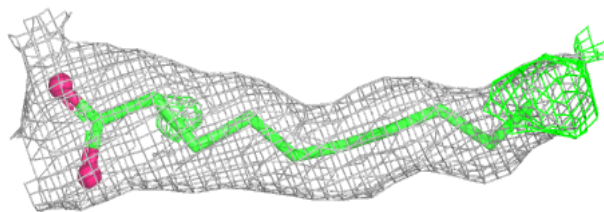
**Electron density around STE I 101:**

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

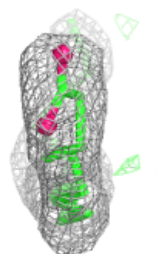
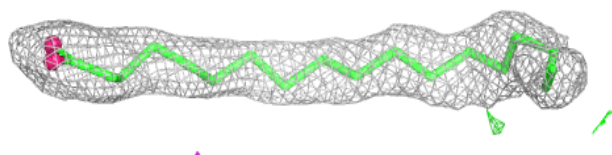
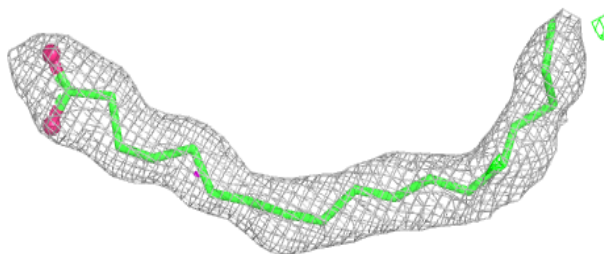


Electron density around STE J 101:

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

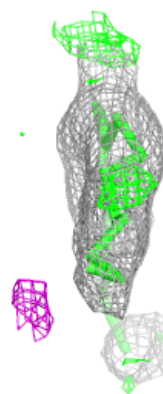
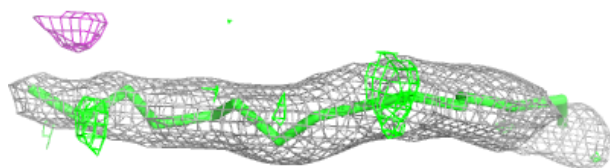
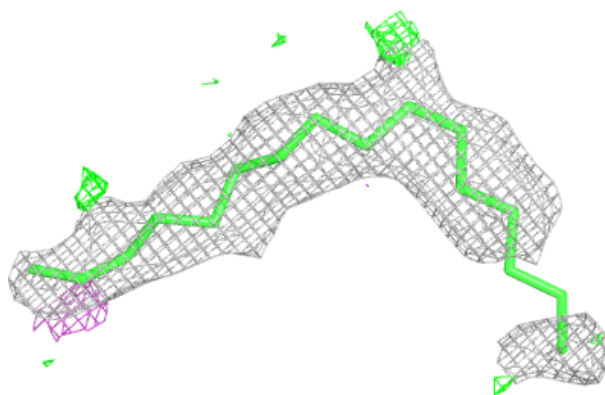
**Electron density around STE d 412:**

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

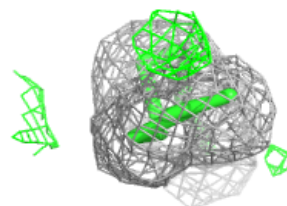
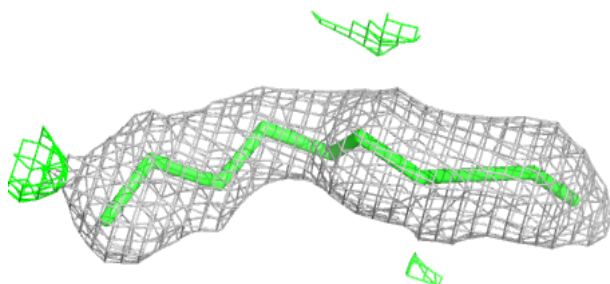
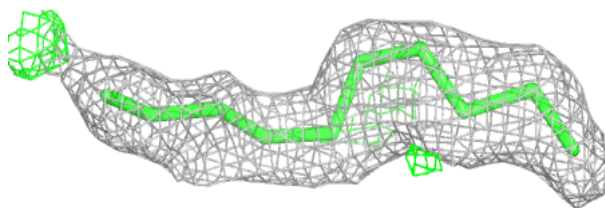


Electron density around STE B 629:

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

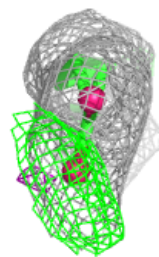
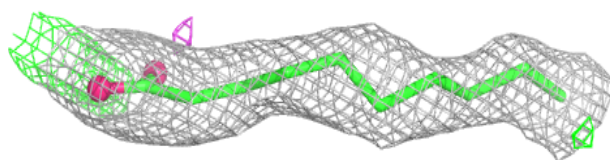
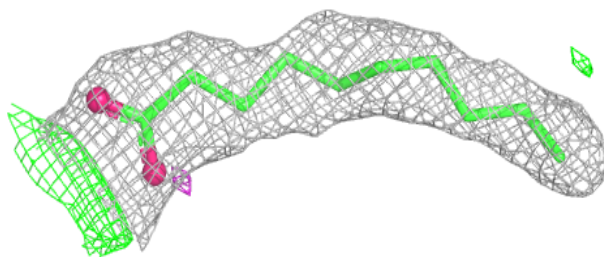
**Electron density around STE t 102:**

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



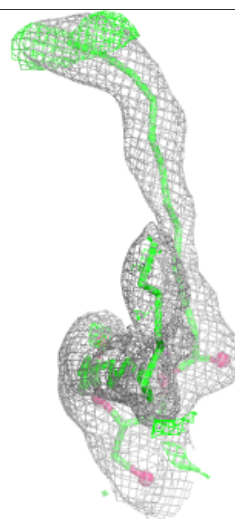
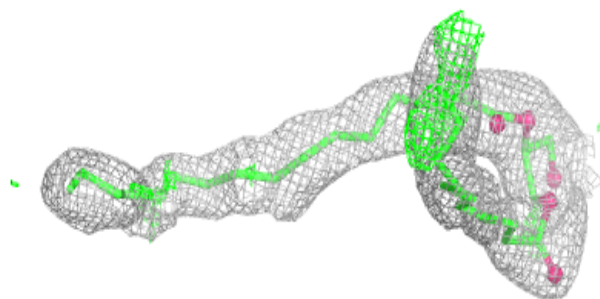
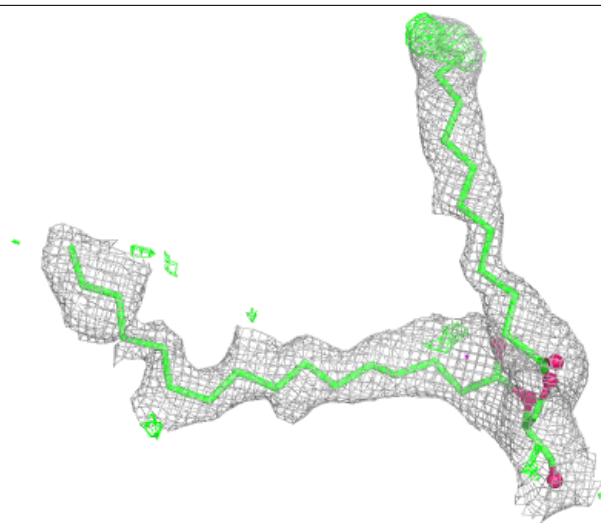
Electron density around STE C 522:

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



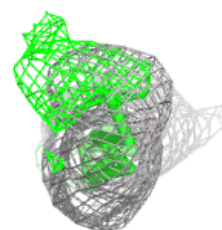
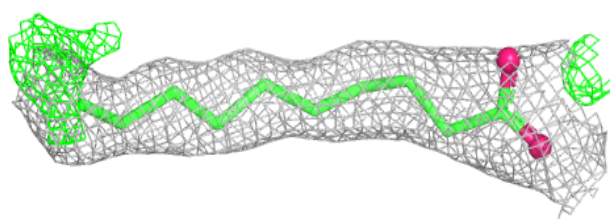
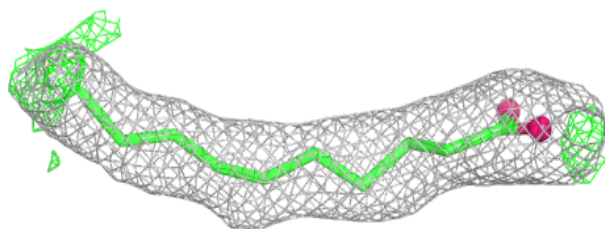
Electron density around SQD a 615:

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

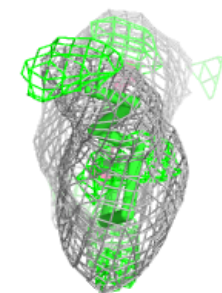
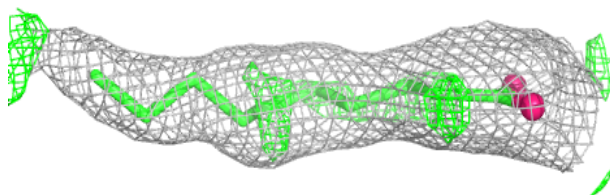
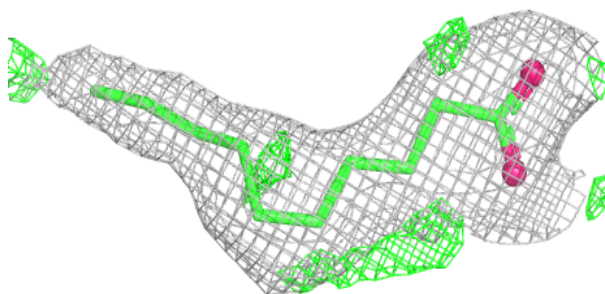


Electron density around STE j 101:

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

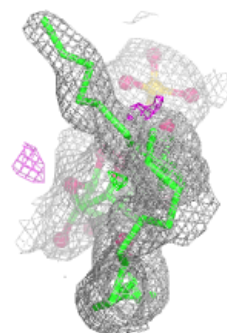
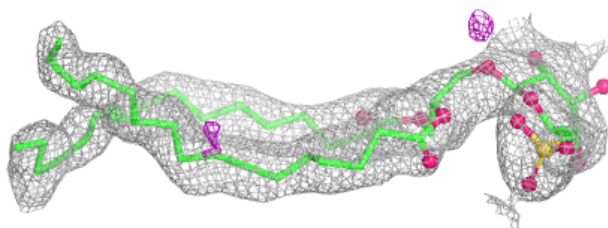
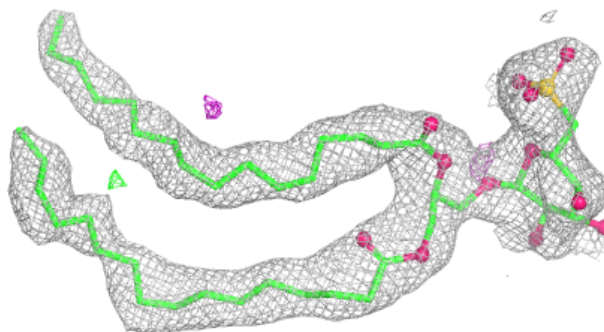
**Electron density around STE C 521:**

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

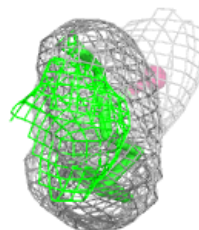
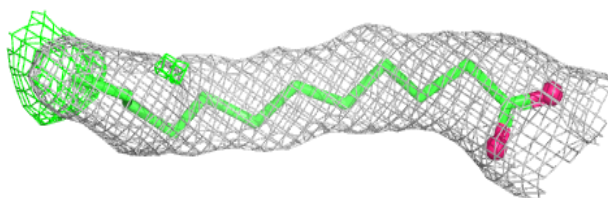
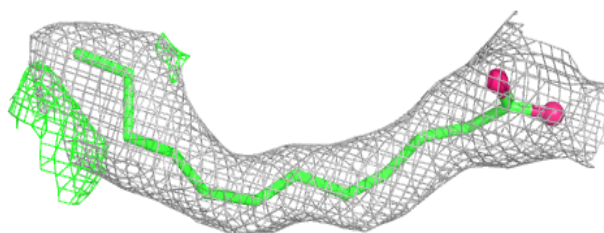


Electron density around SQD B 624:

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

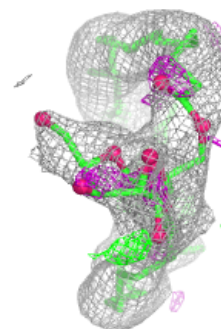
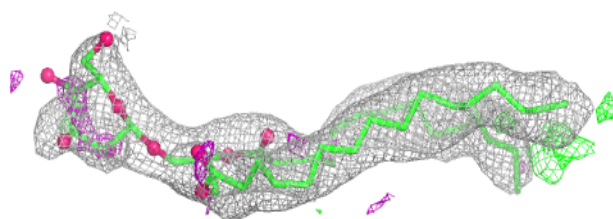
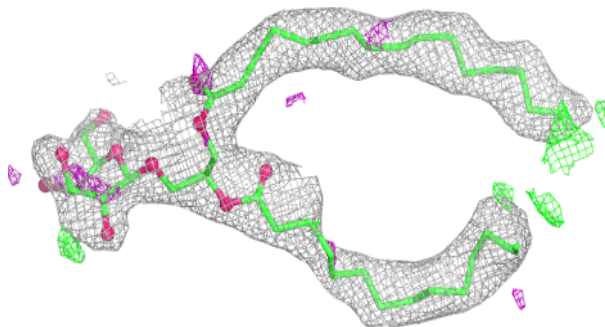
**Electron density around STE B 625:**

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

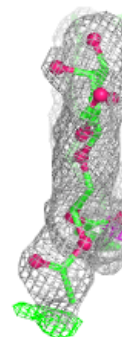
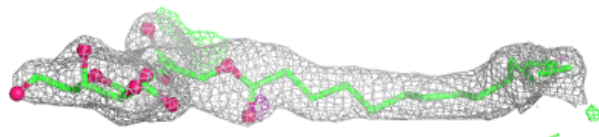
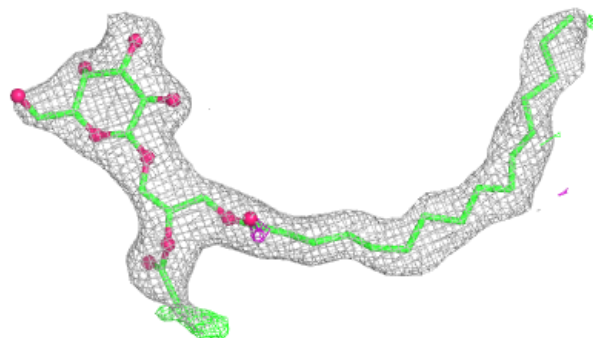


Electron density around LMG c 522:

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

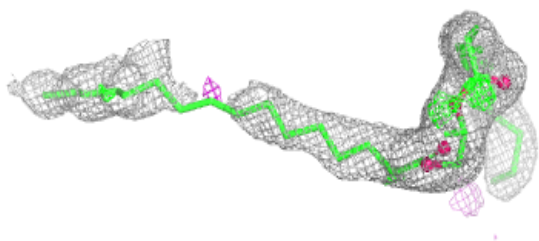
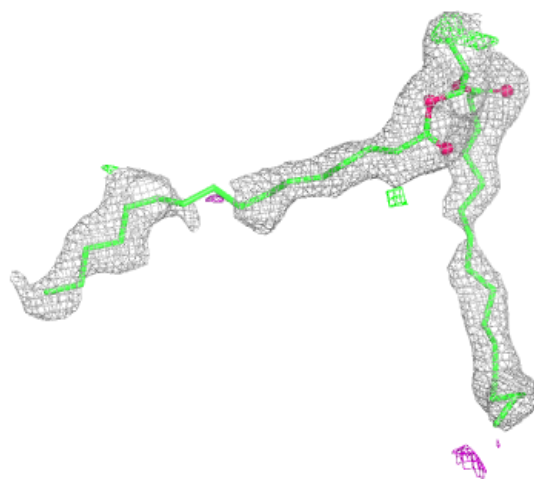
**Electron density around LMG c 518:**

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



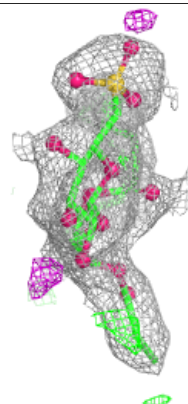
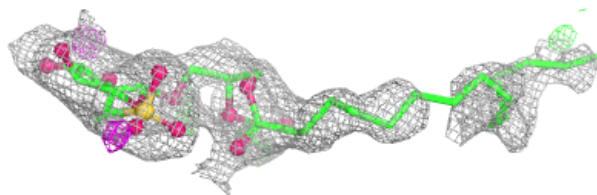
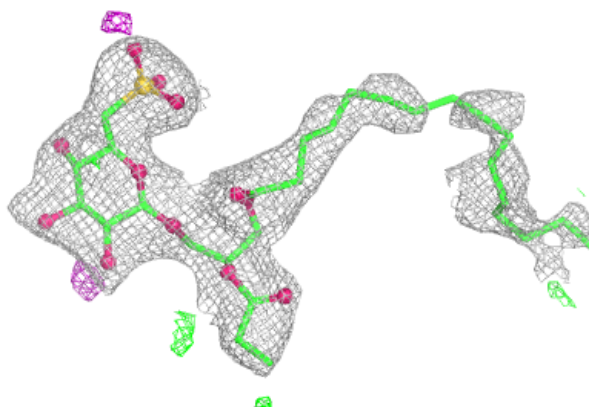
Electron density around SQD A 615:

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

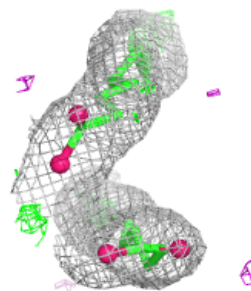
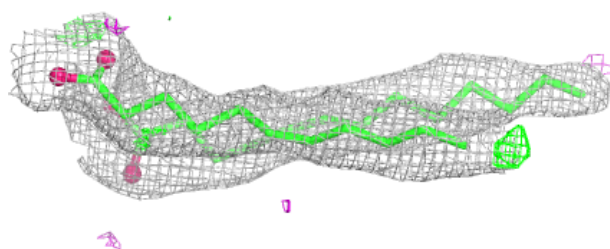
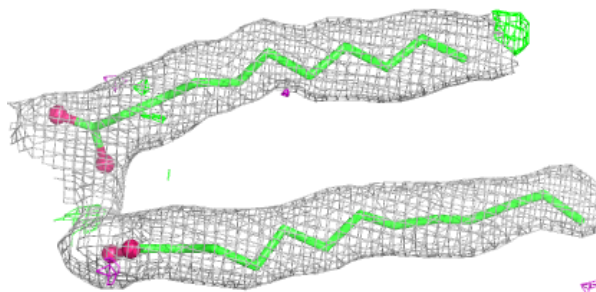


Electron density around SQD f 101:

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

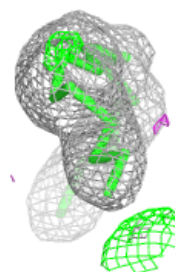
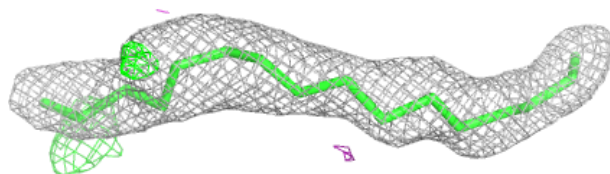
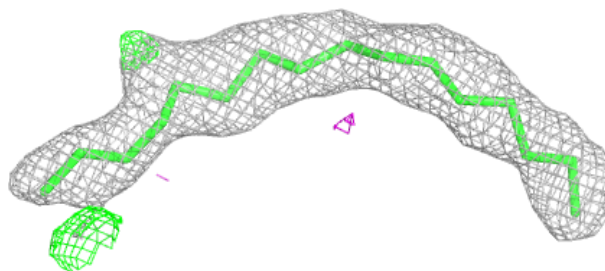
**Electron density around LMG B 622:**

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

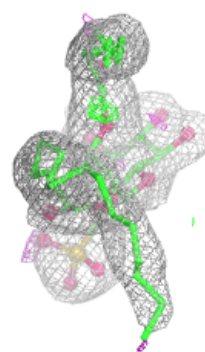
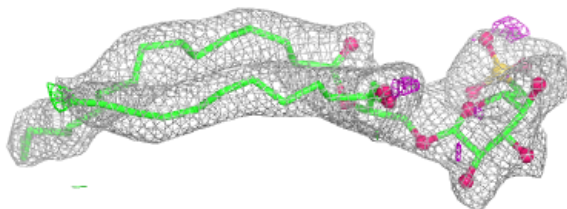
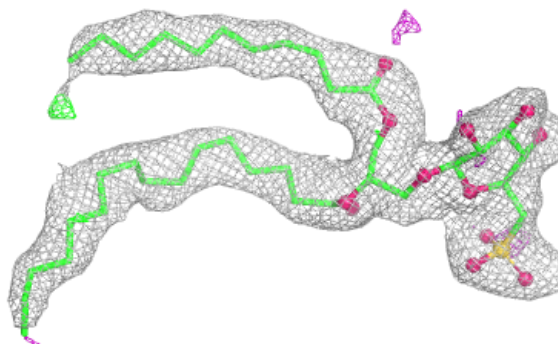


Electron density around STE T 102:

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

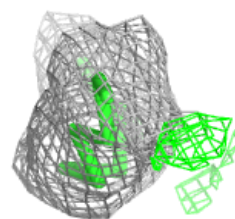
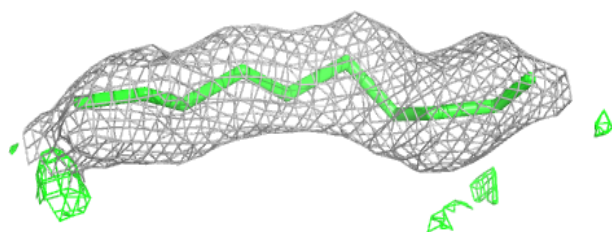
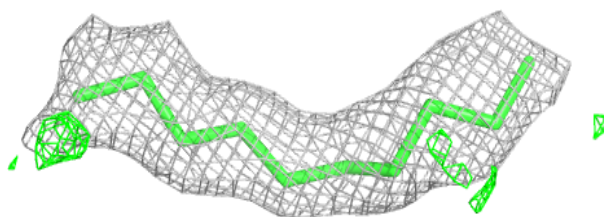
**Electron density around SQD b 620:**

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

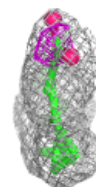
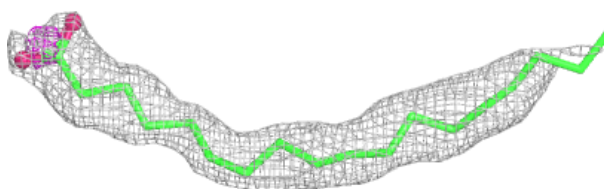


Electron density around STE b 625:

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

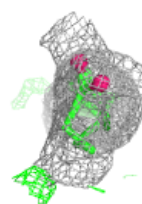
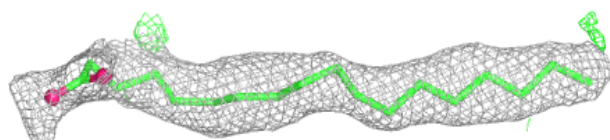
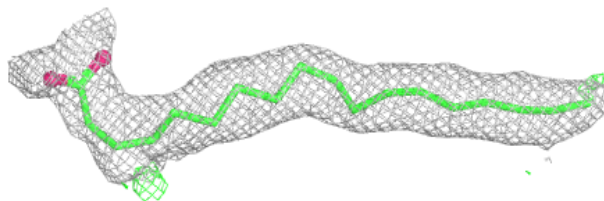
**Electron density around STE X 101:**

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

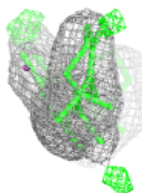
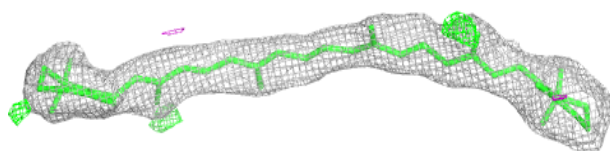
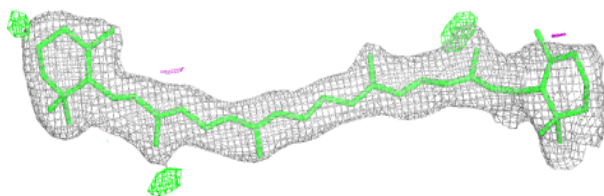


Electron density around STE c 519:

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

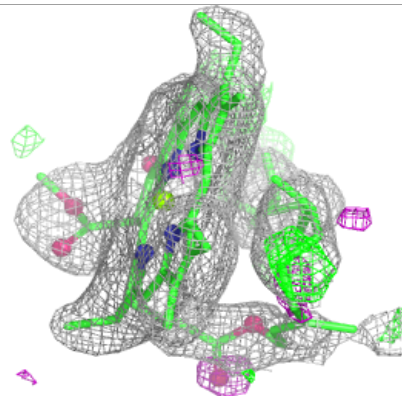
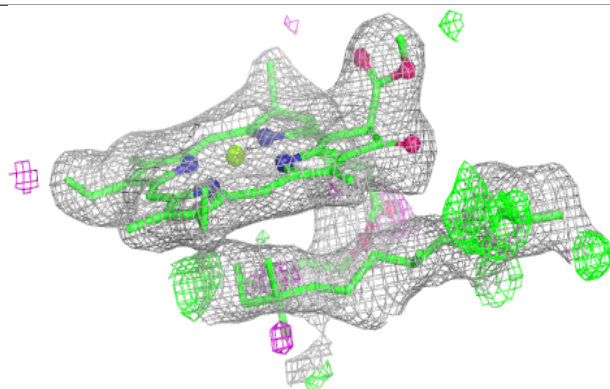
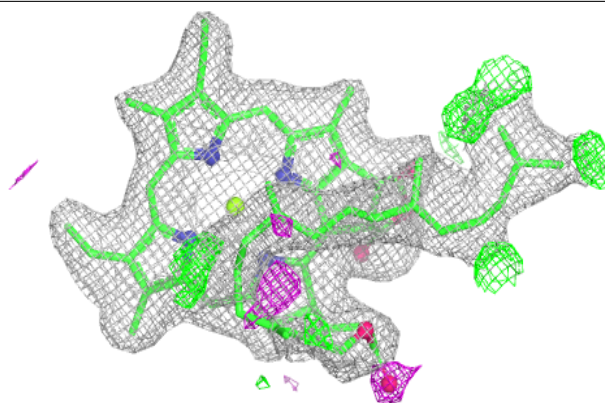
**Electron density around BCR d 405:**

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

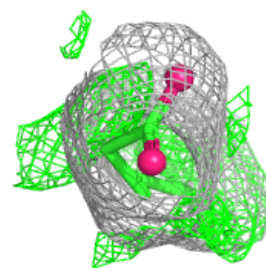
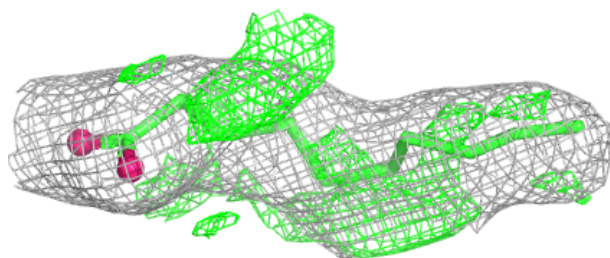
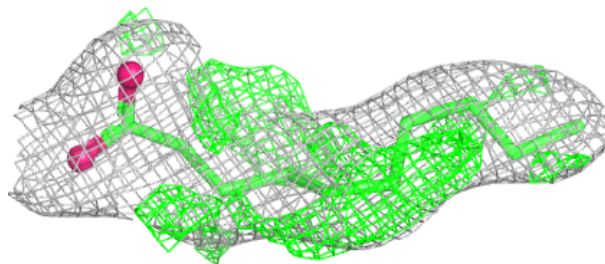


Electron density around CLA B 601:

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

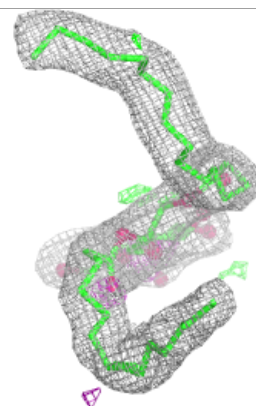
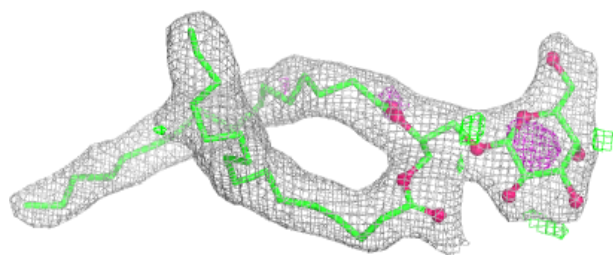
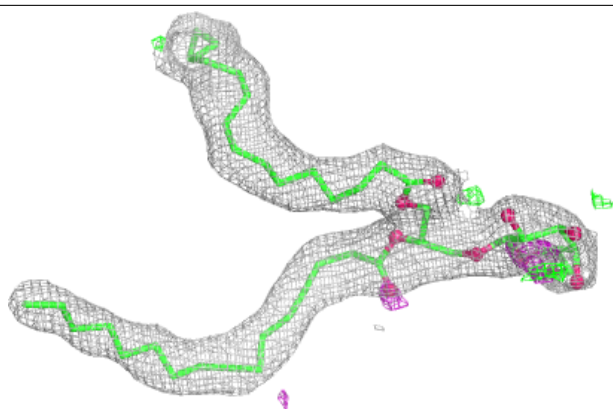
**Electron density around STE B 626:**

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

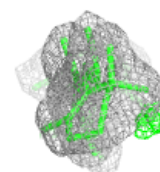
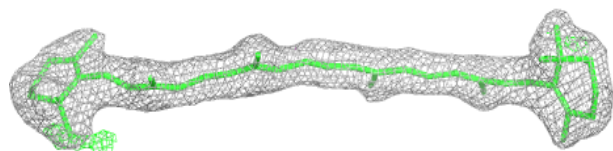
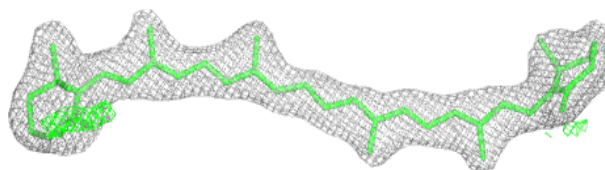


Electron density around LMG m 101:

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

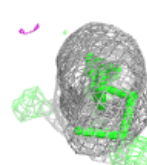
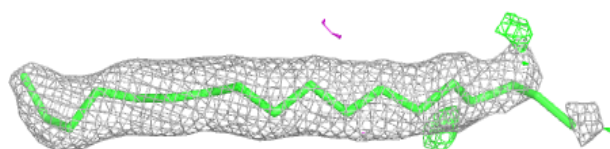
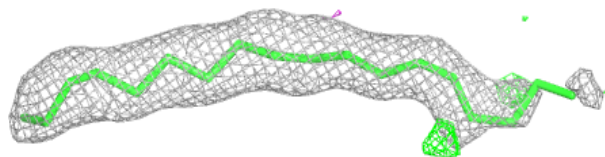
**Electron density around BCR k 102:**

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

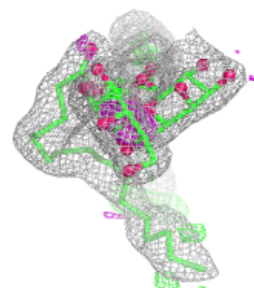
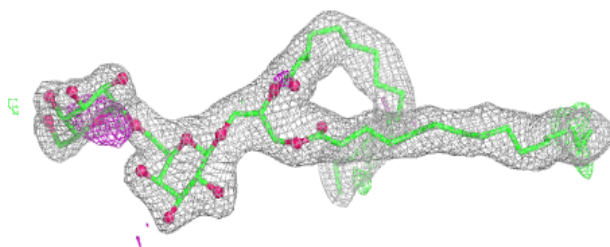
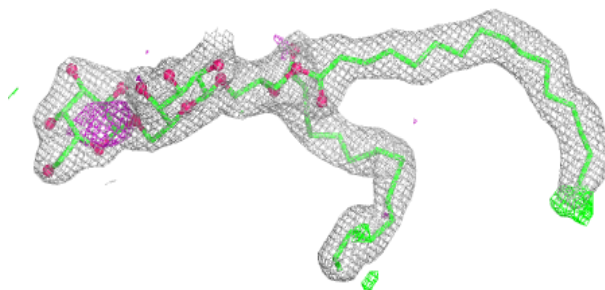


Electron density around STE I 102:

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

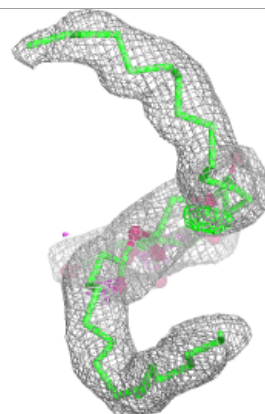
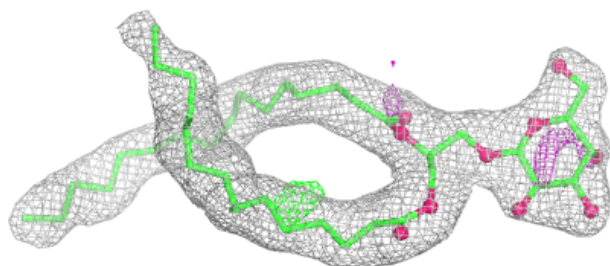
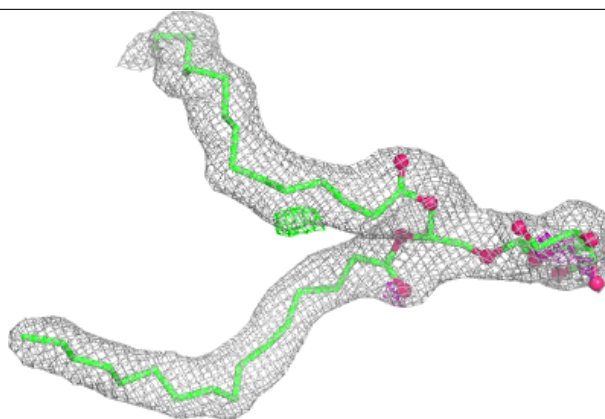
**Electron density around DGD H 102:**

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

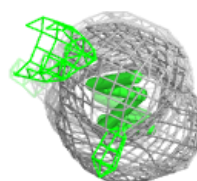
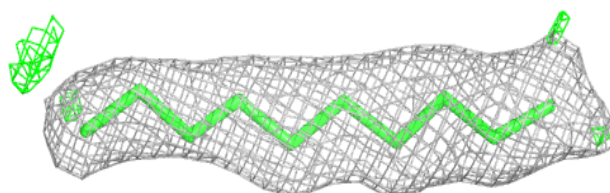
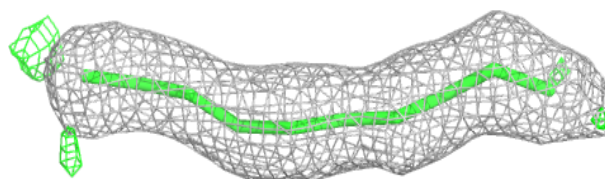


Electron density around LMG B 620:

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

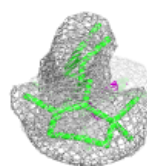
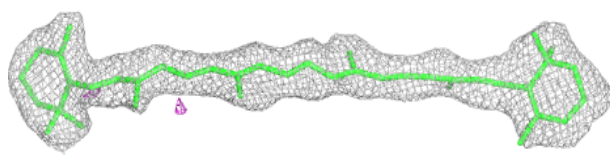
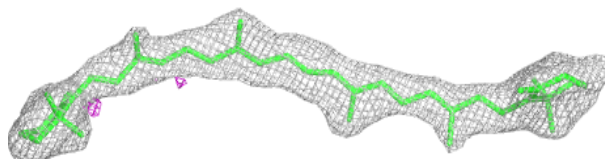
**Electron density around STE M 102:**

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

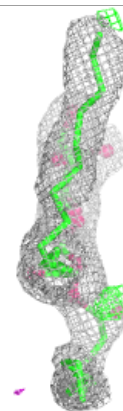
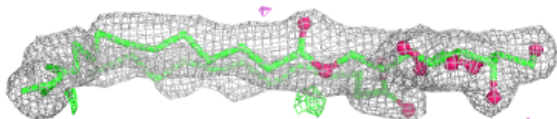
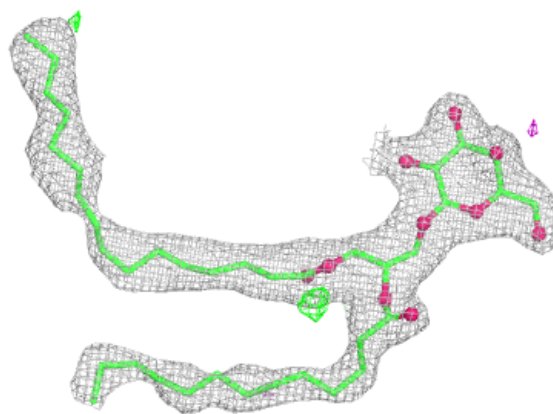


Electron density around BCR x 101:

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

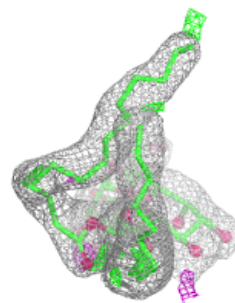
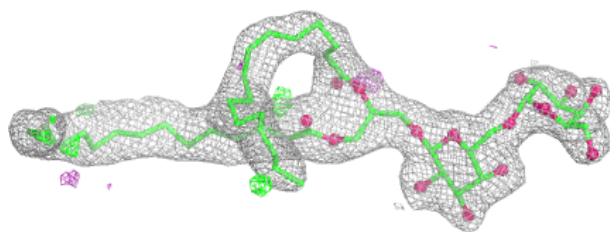
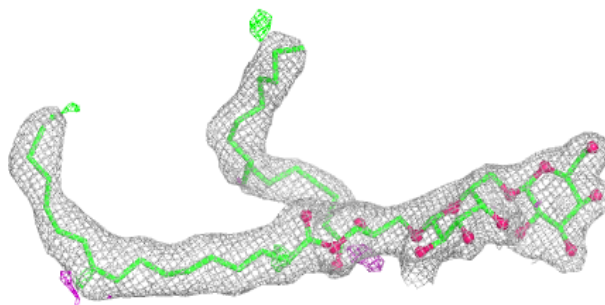
**Electron density around LMG C 520:**

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

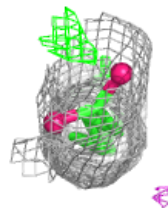
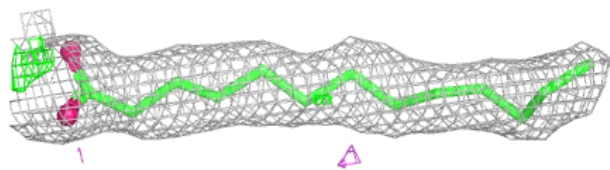
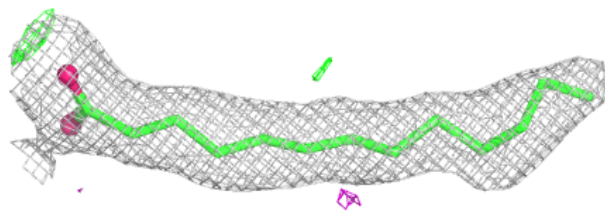


Electron density around DGD h 101:

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

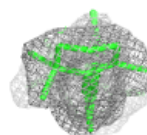
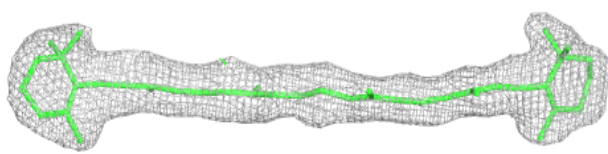
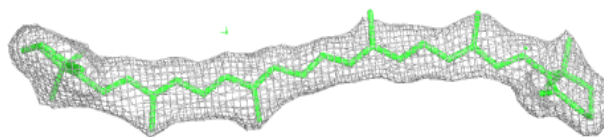
**Electron density around STE M 101:**

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

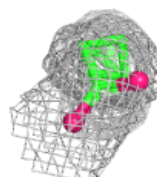
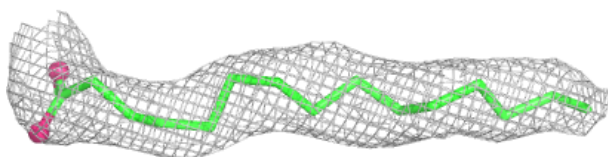
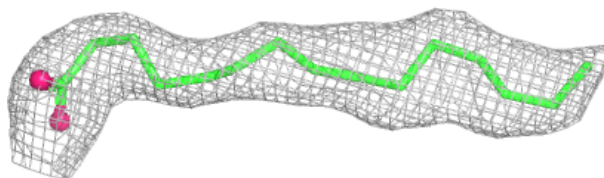


Electron density around BCR C 514:

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

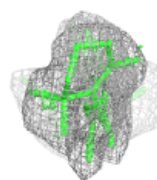
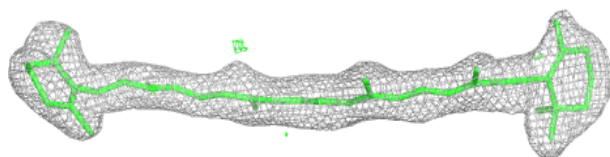
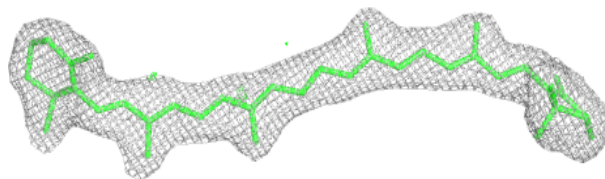
**Electron density around STE d 411:**

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



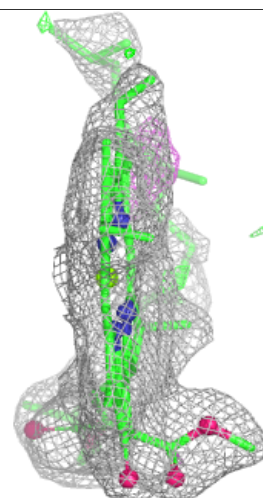
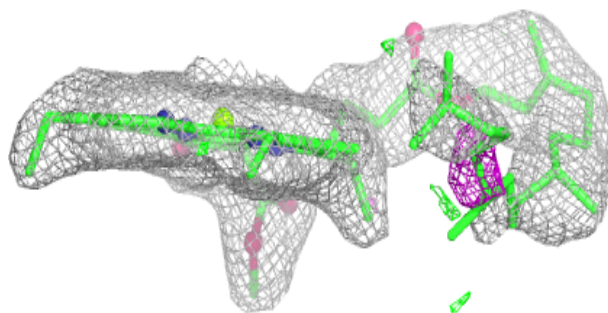
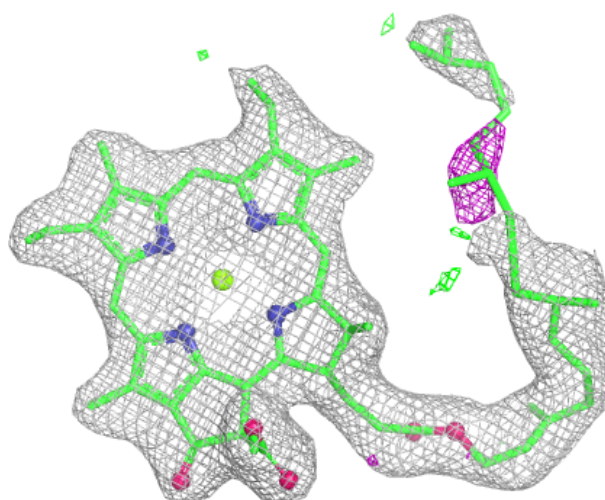
Electron density around BCR C 516:

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



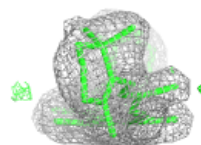
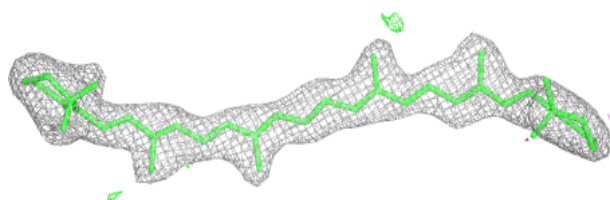
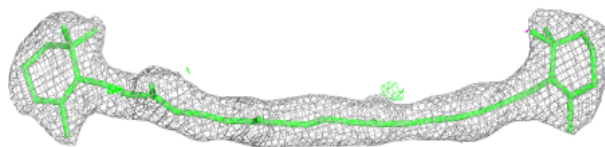
Electron density around CLA c 512:

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

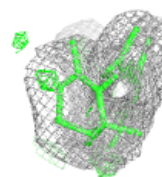
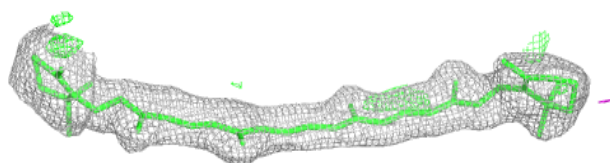
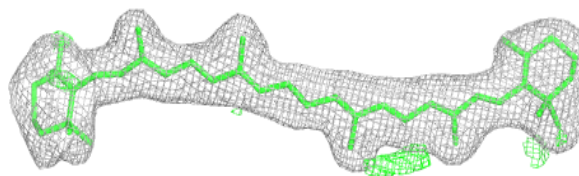


Electron density around BCR k 103:

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

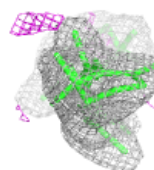
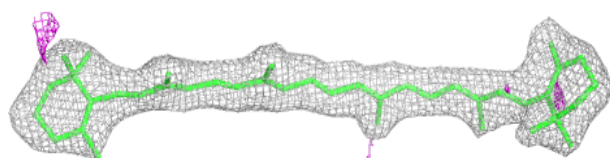
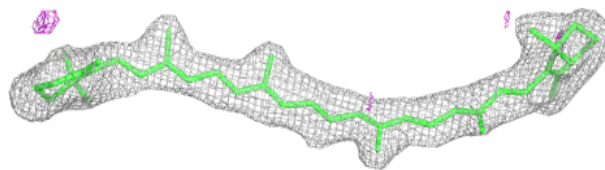
**Electron density around BCR D 405:**

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

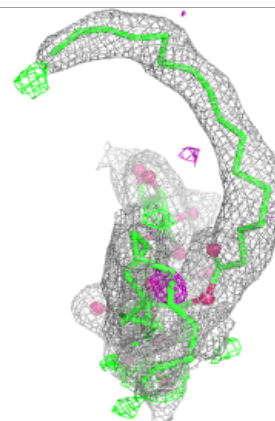
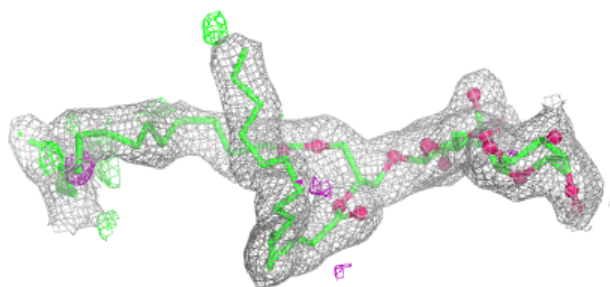
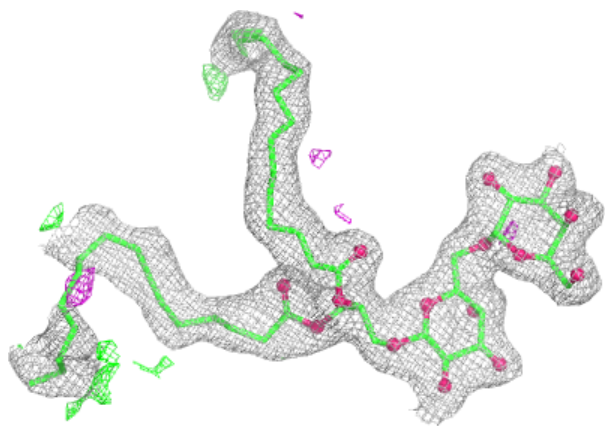


Electron density around BCR H 101:

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

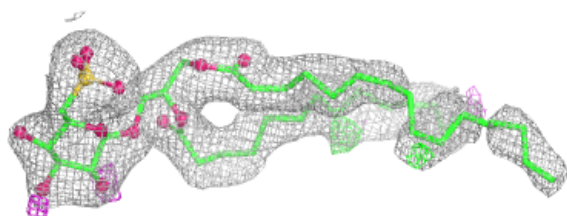
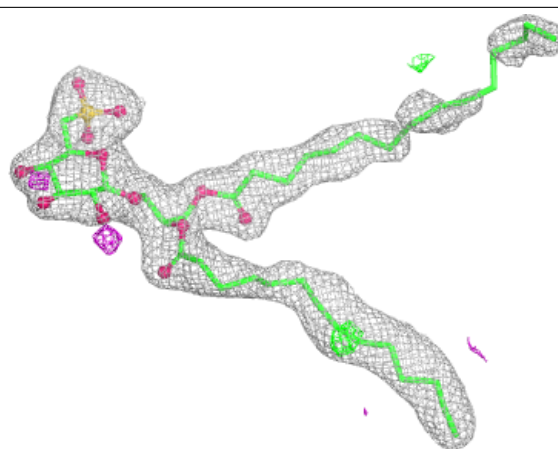
**Electron density around DGD C 518:**

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

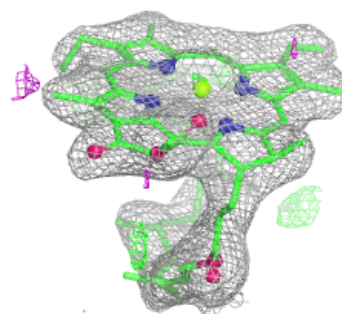
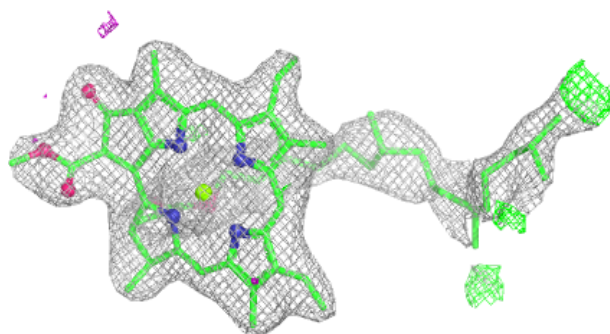
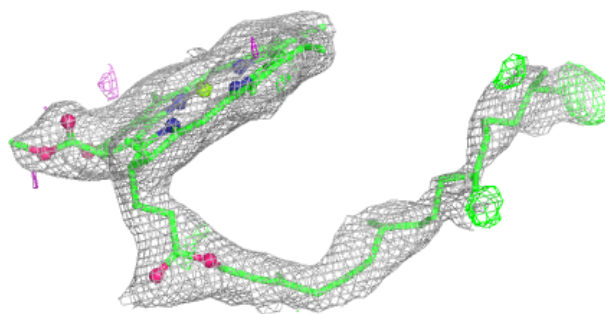


Electron density around SQD A 614:

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

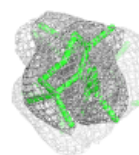
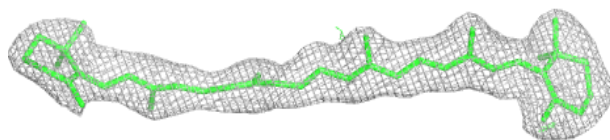
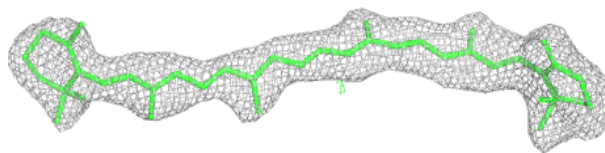
**Electron density around CLA C 513:**

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

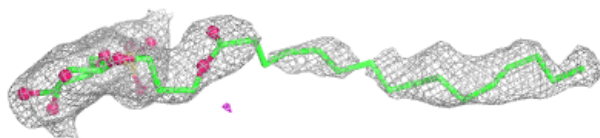
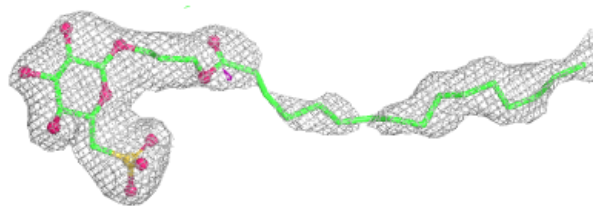


Electron density around BCR k 101:

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

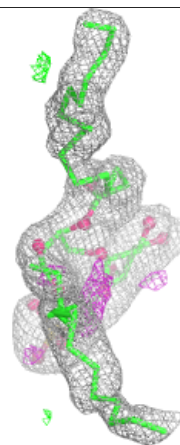
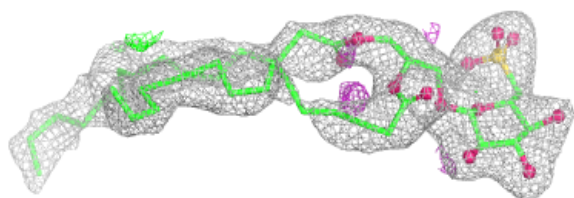
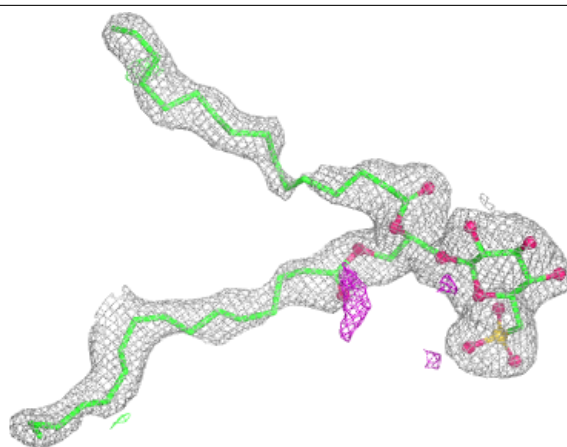
**Electron density around SQD D 408:**

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

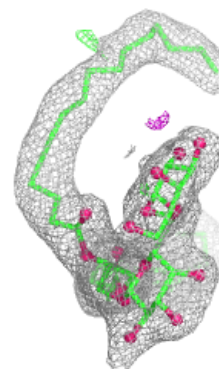
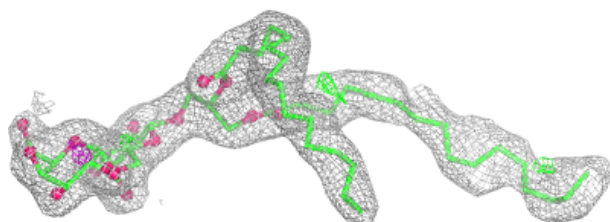
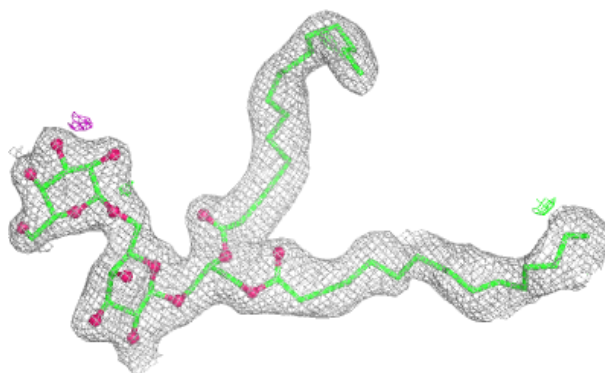


Electron density around SQD a 614:

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

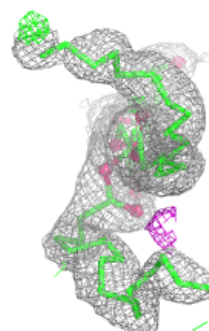
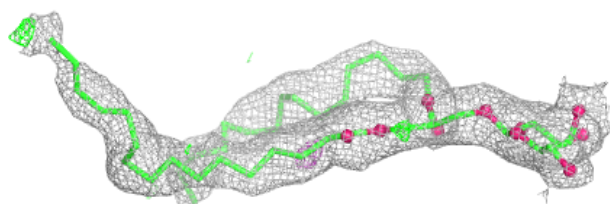
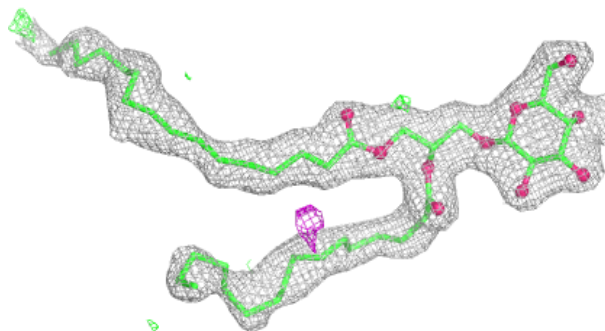
**Electron density around DGD c 516:**

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

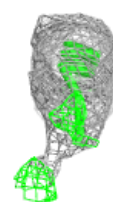
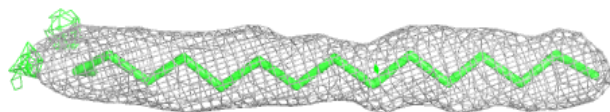
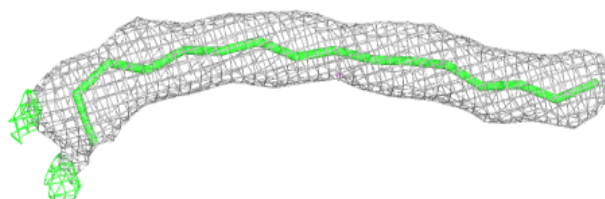


Electron density around LMG D 407:

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

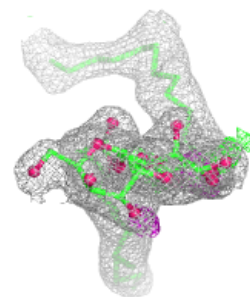
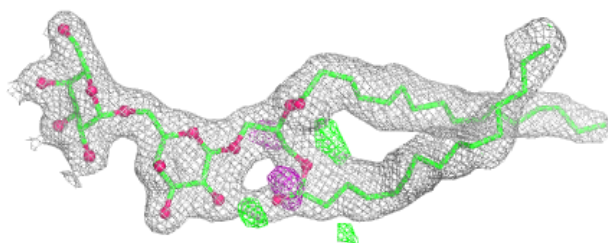
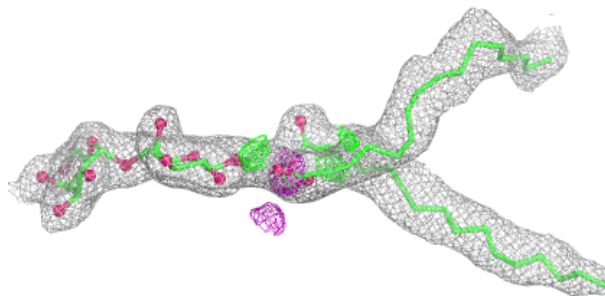
**Electron density around STE C 523:**

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

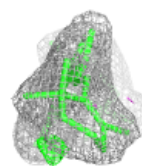
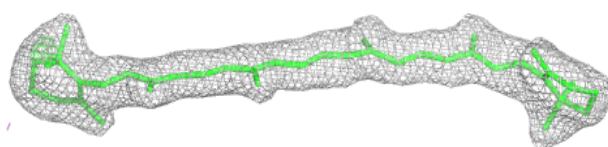
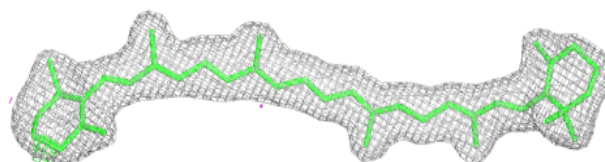


Electron density around DGD c 515:

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

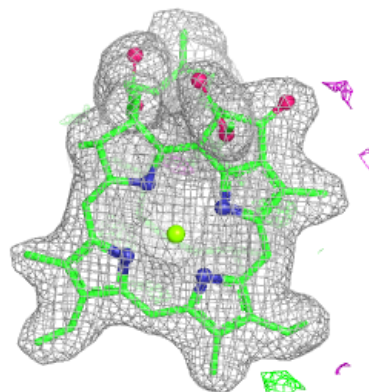
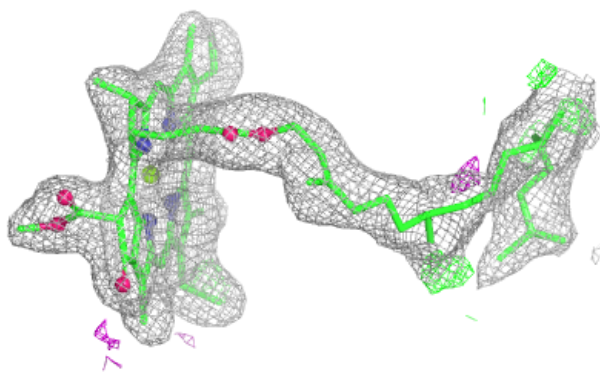
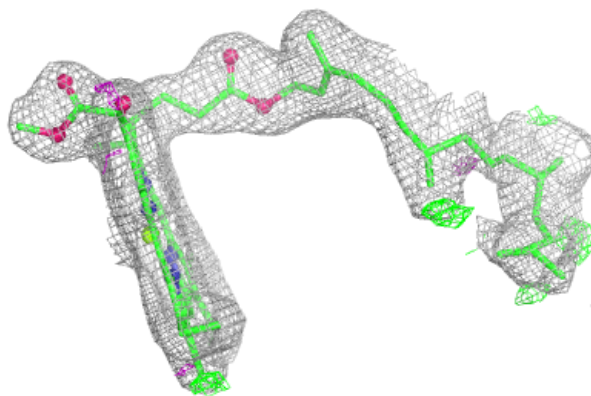
**Electron density around BCR B 619:**

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

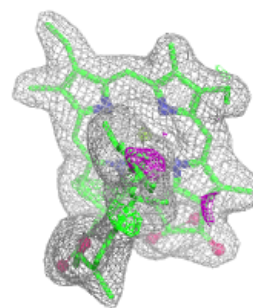
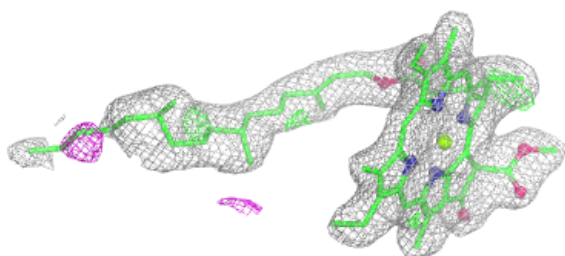
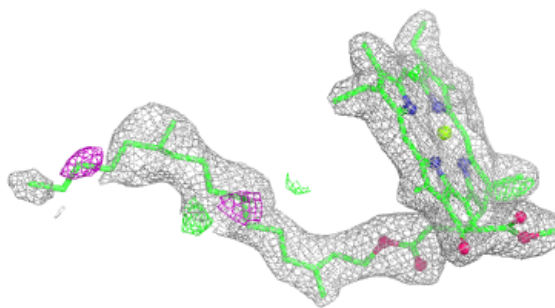


Electron density around CLA C 506:

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

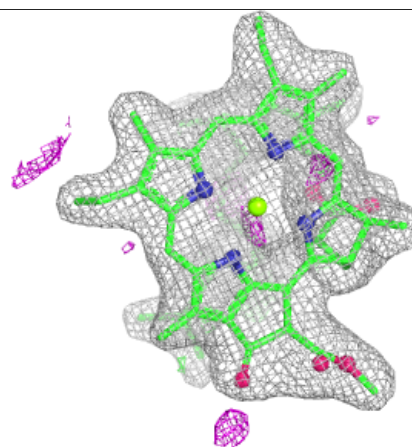
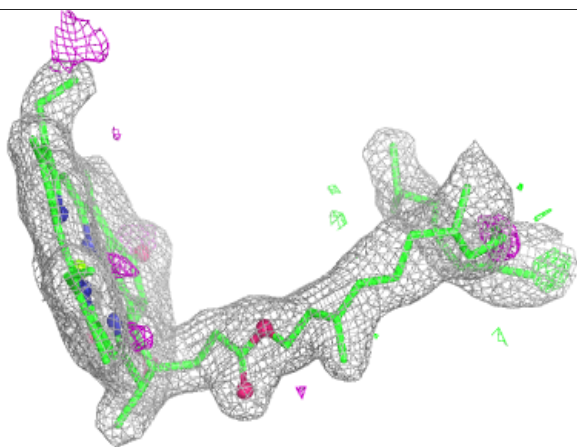
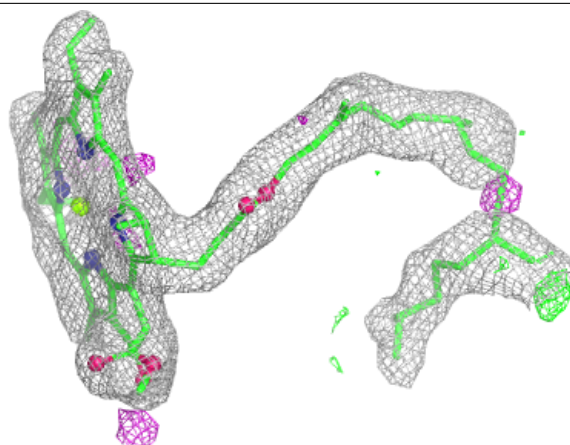
**Electron density around CLA c 508:**

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

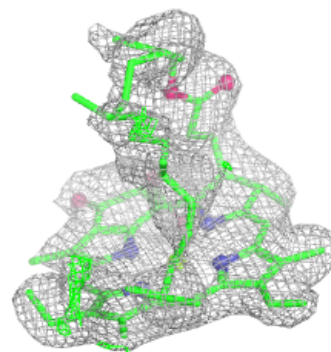
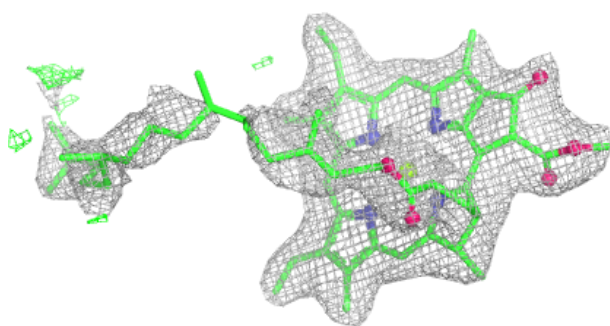
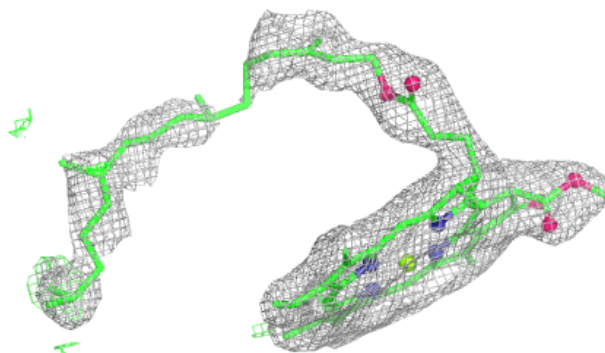


Electron density around CLA B 606:

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

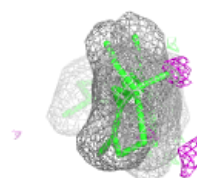
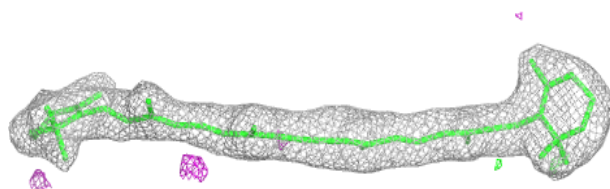
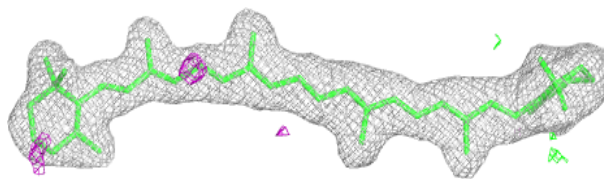
**Electron density around CLA c 513:**

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

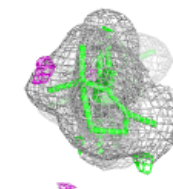
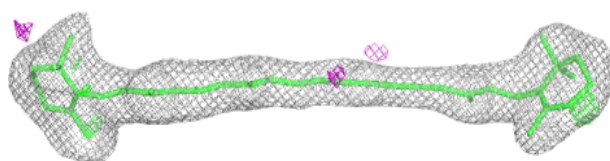
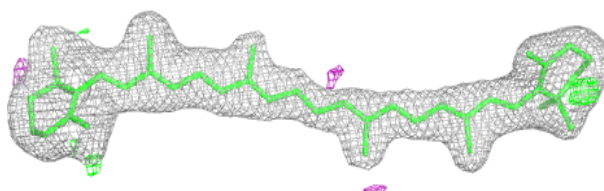


Electron density around BCR b 617:

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

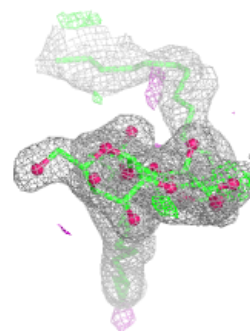
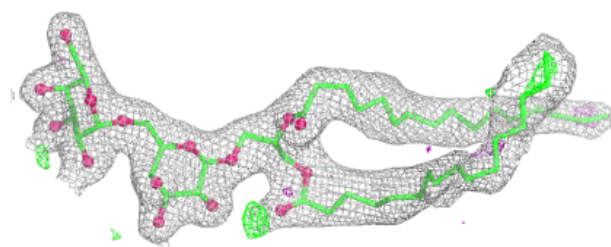
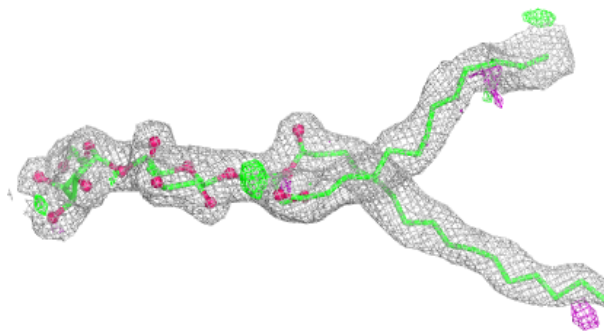
**Electron density around BCR b 618:**

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

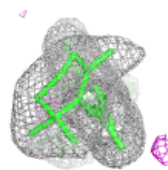
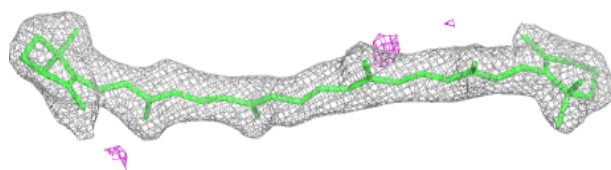
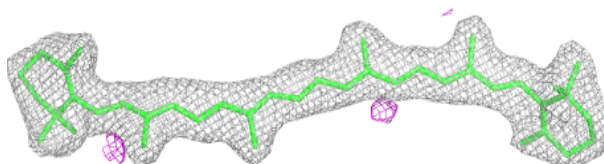


Electron density around DGD C 517:

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

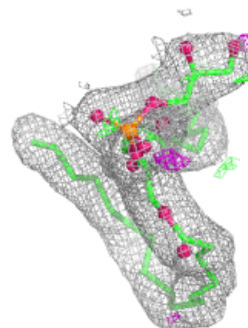
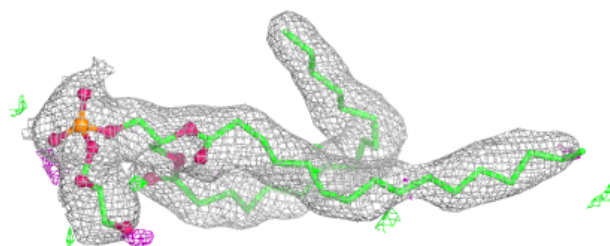
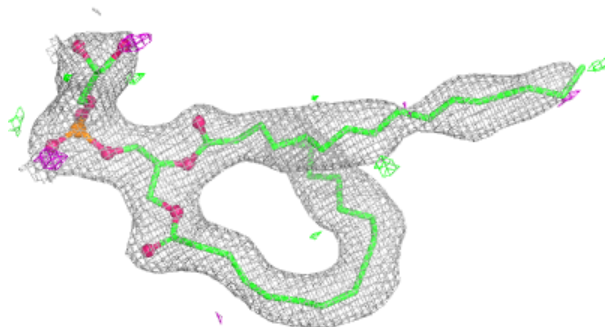
**Electron density around BCR b 619:**

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

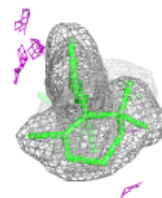
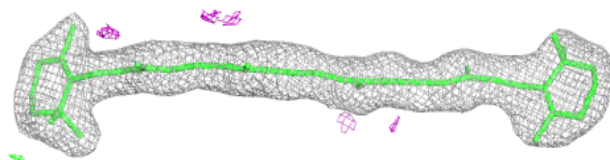
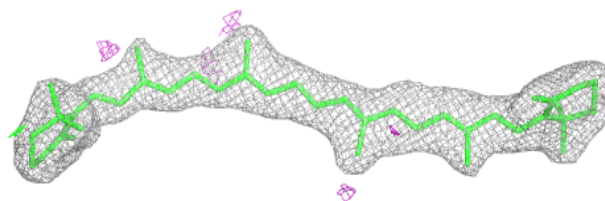


Electron density around LHG D 412:

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

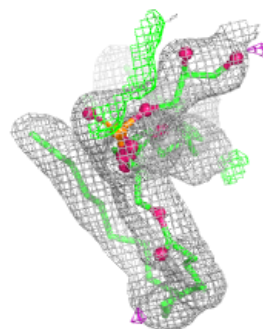
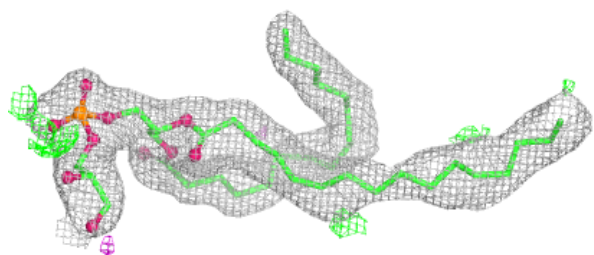
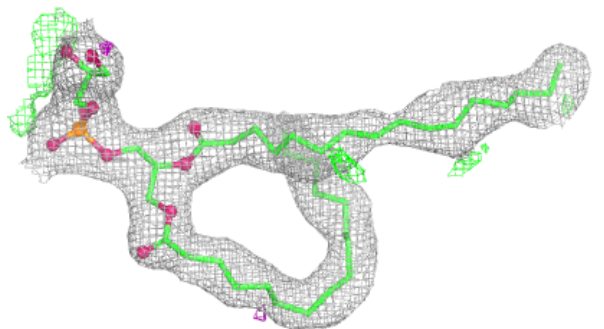
**Electron density around BCR c 514:**

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

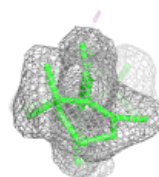
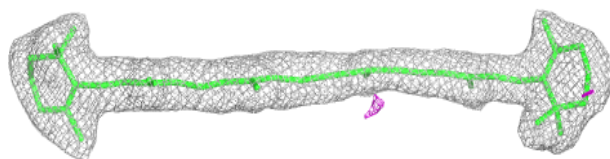
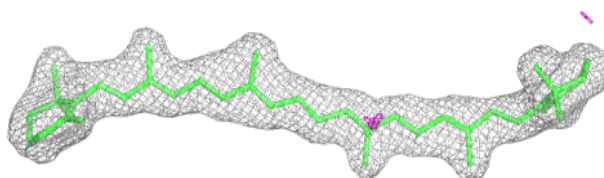


Electron density around LHG a 613:

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

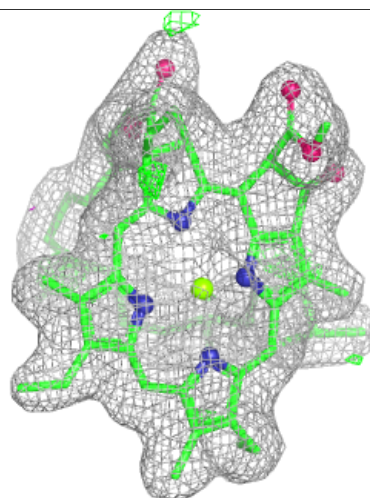
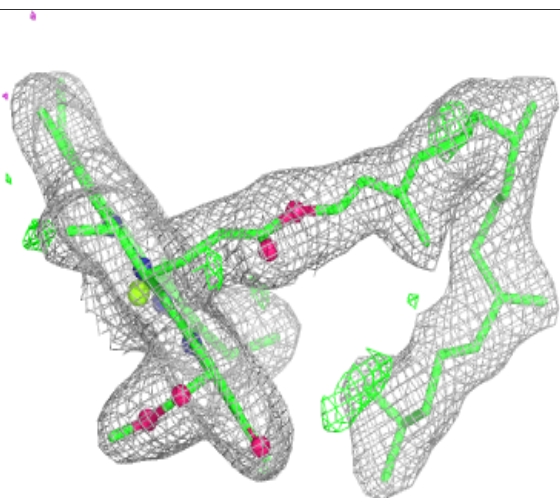
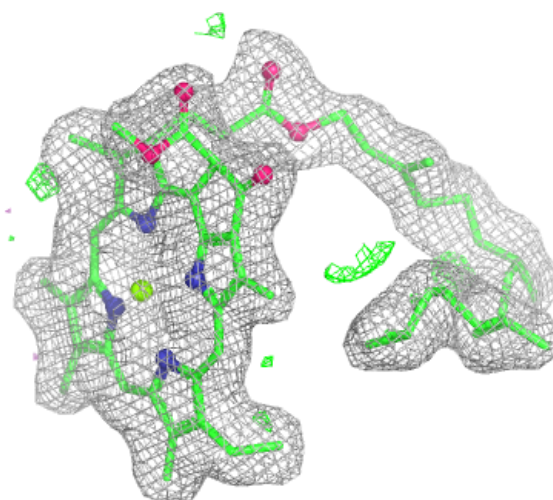
**Electron density around BCR A 610:**

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



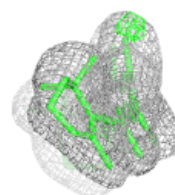
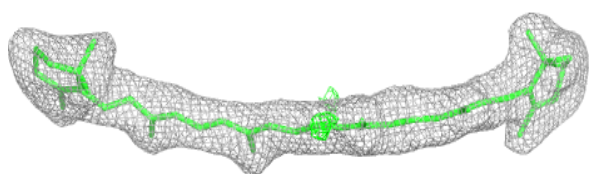
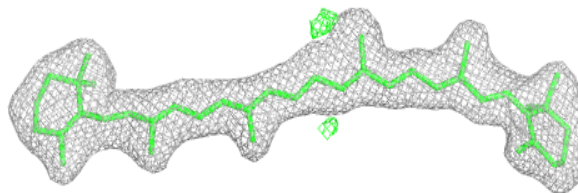
Electron density around CLA C 503:

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

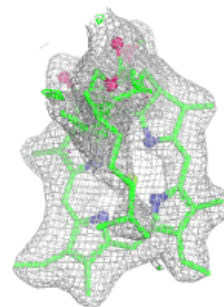
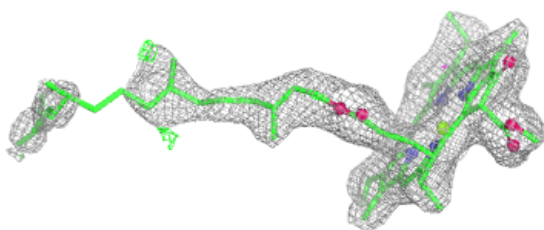
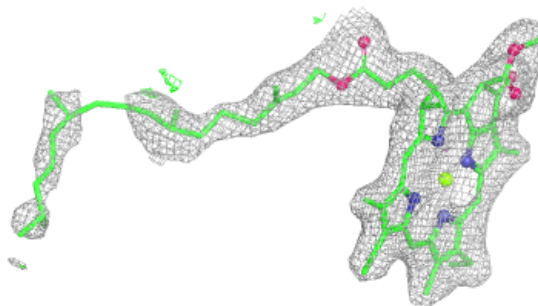


Electron density around BCR t 101:

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

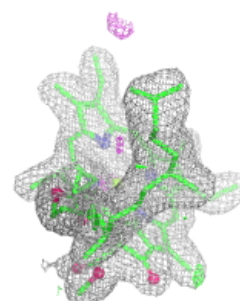
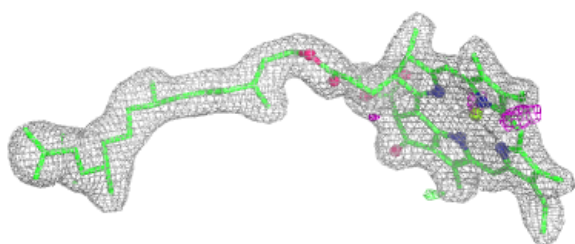
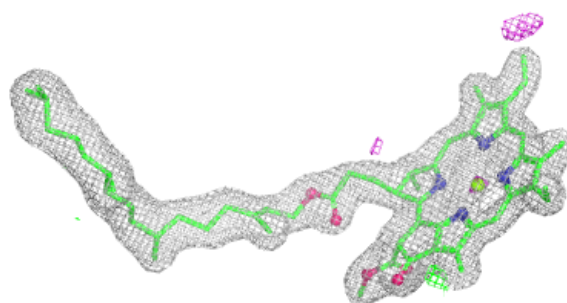
**Electron density around CLA d 404:**

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

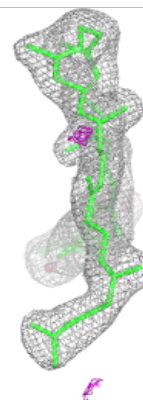
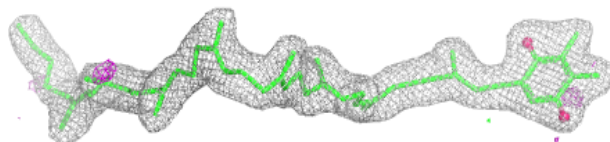
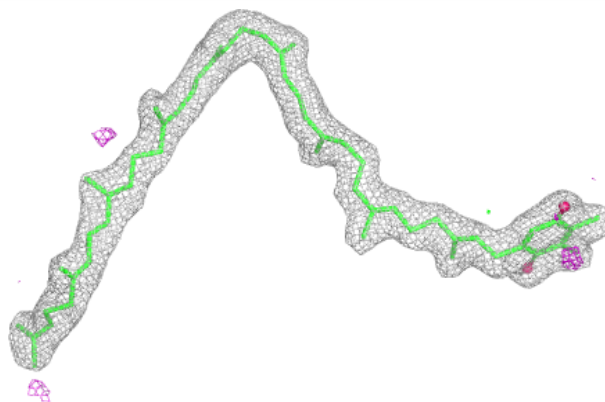


Electron density around CLA a 606:

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

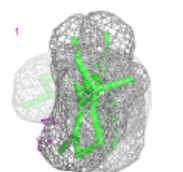
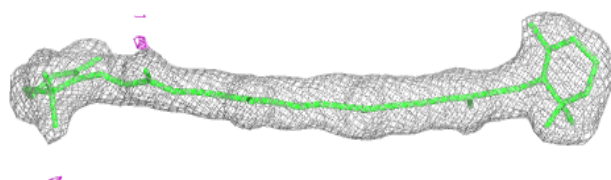
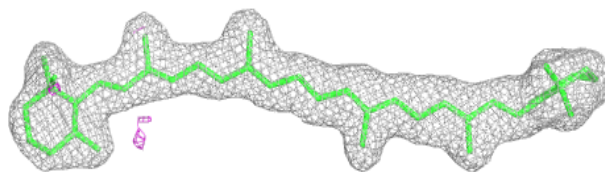
**Electron density around PL9 D 406:**

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

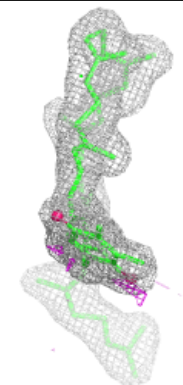
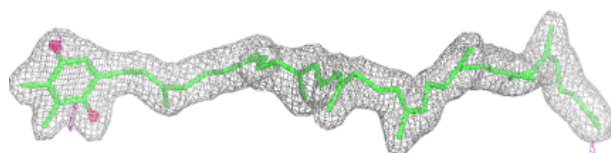
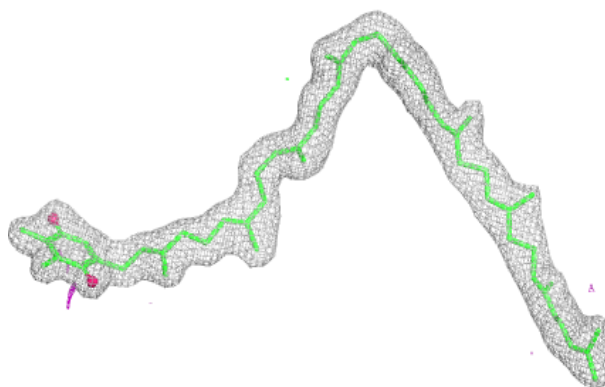


Electron density around BCR B 617:

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

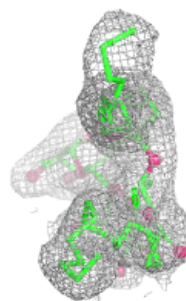
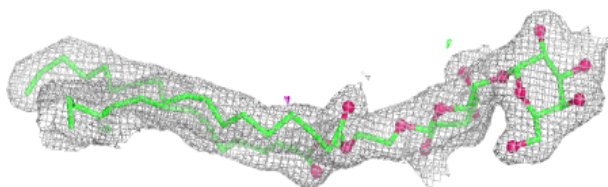
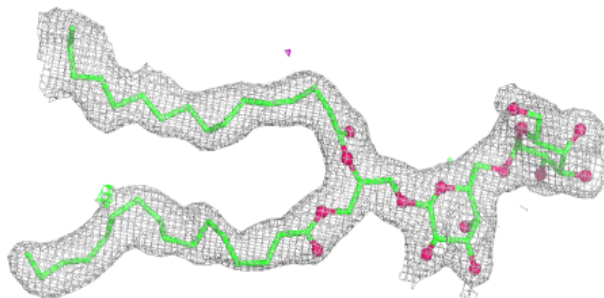
**Electron density around PL9 d 406:**

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

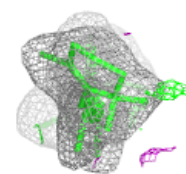
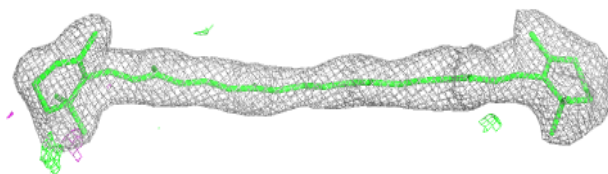
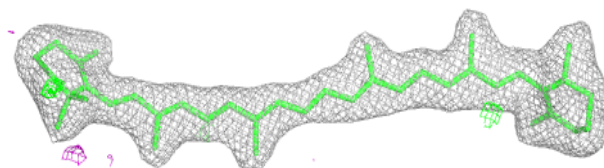


Electron density around DGD C 519:

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

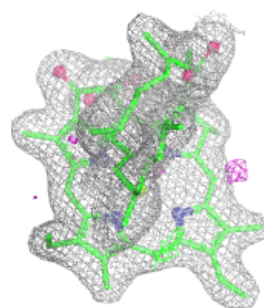
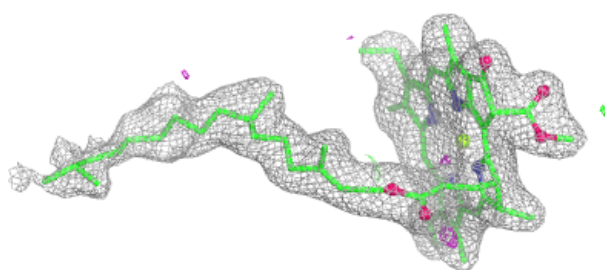
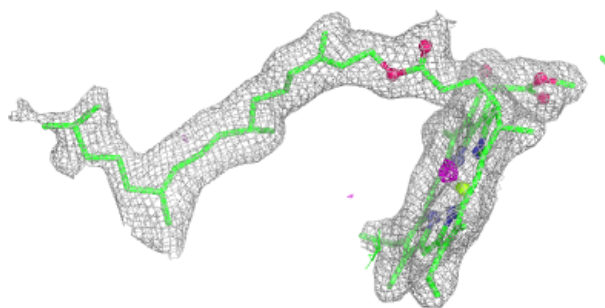
**Electron density around BCR B 618:**

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

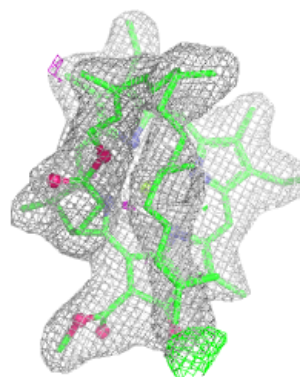
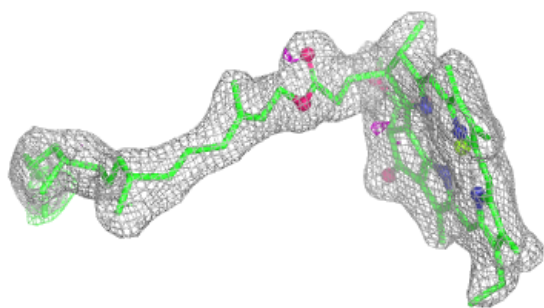
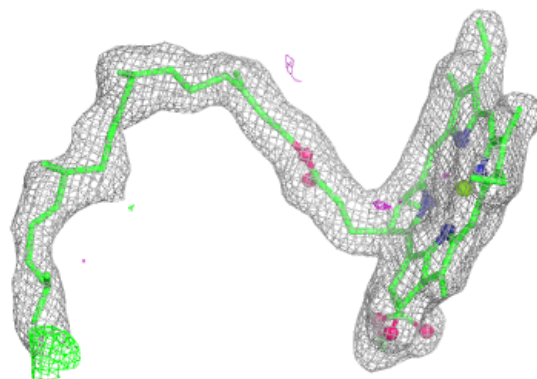


Electron density around CLA C 508:

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

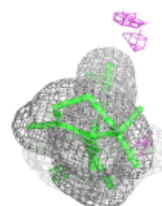
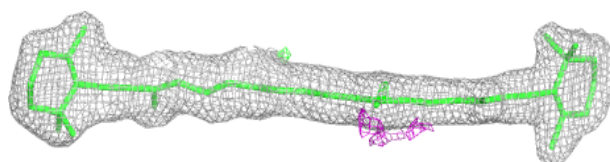
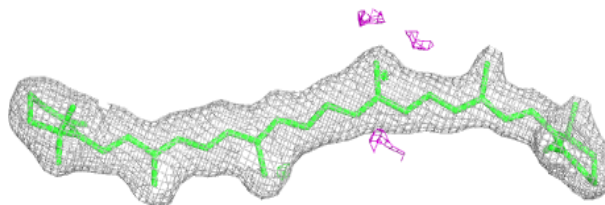
**Electron density around CLA b 606:**

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

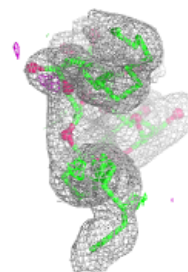
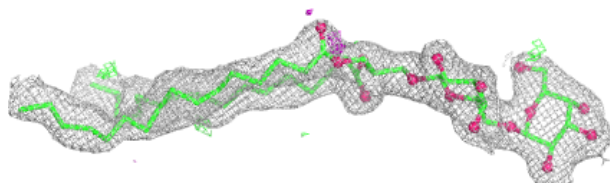
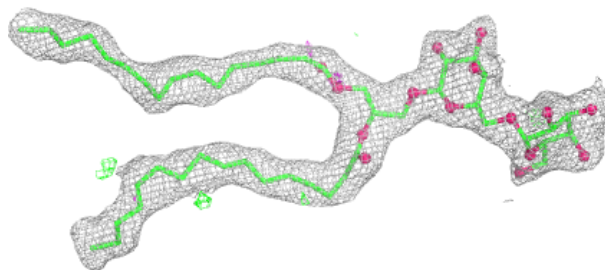


Electron density around BCR C 515:

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

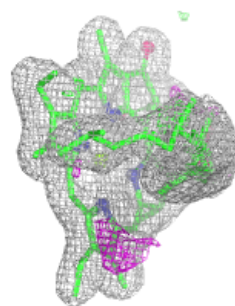
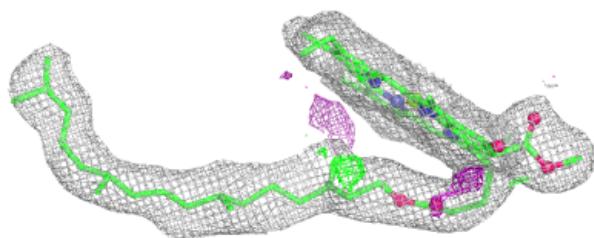
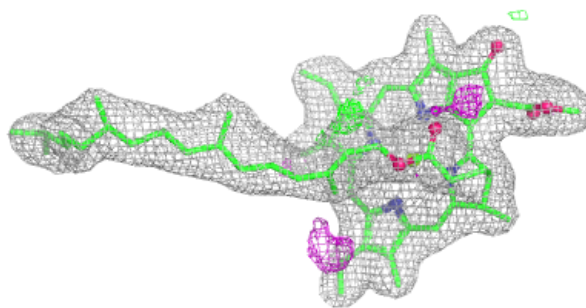
**Electron density around DGD c 517:**

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



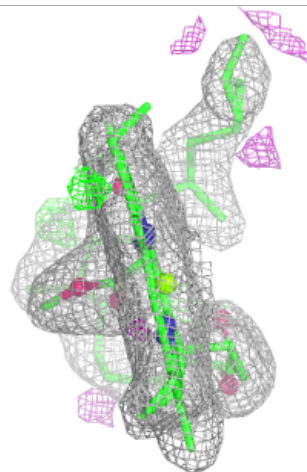
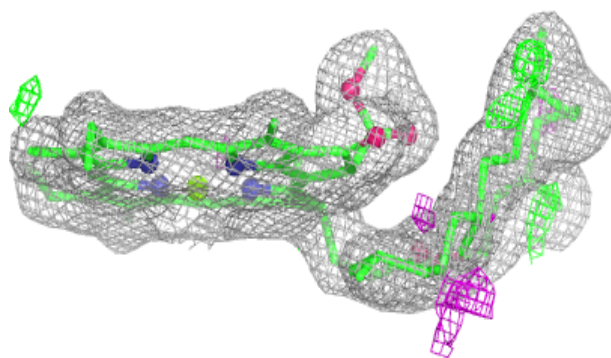
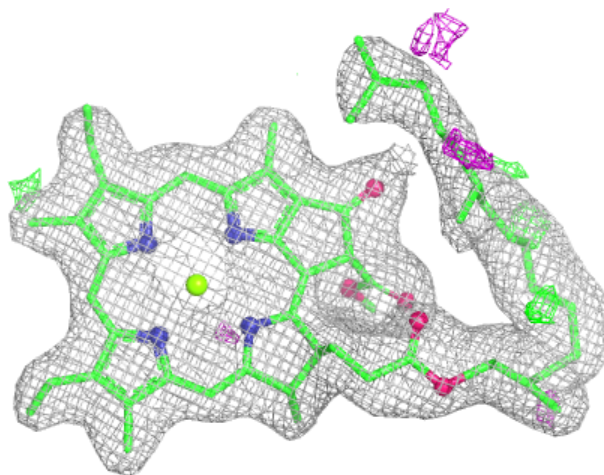
Electron density around CLA b 608:

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



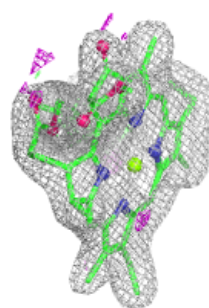
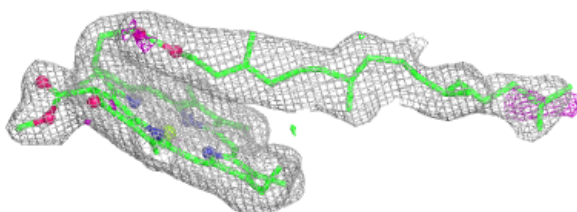
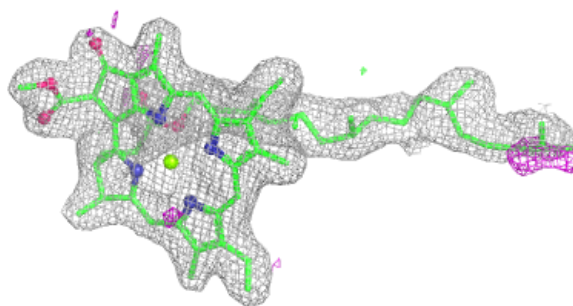
Electron density around CLA b 610:

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

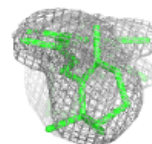
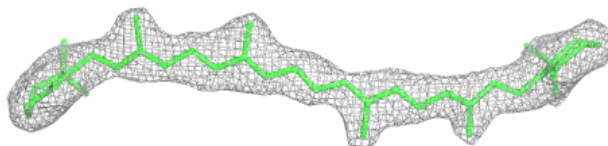
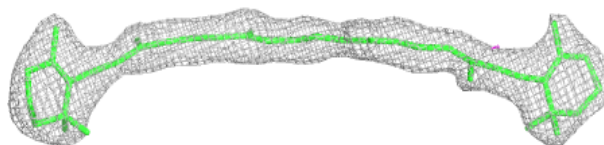


Electron density around CLA b 614:

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

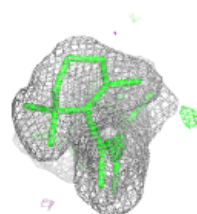
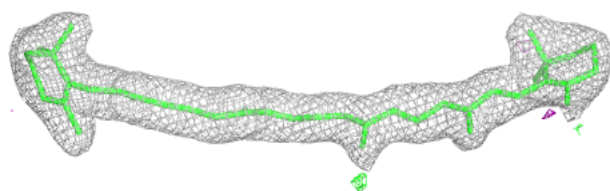
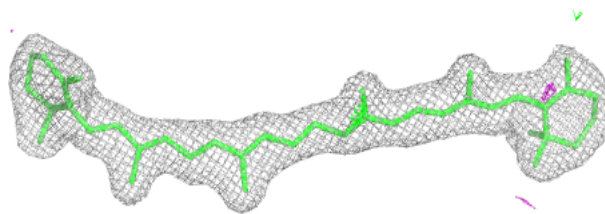
**Electron density around BCR K 101:**

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



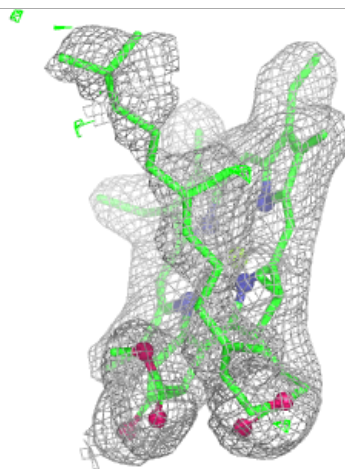
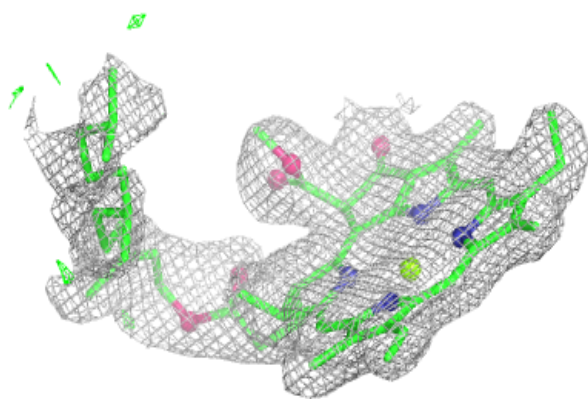
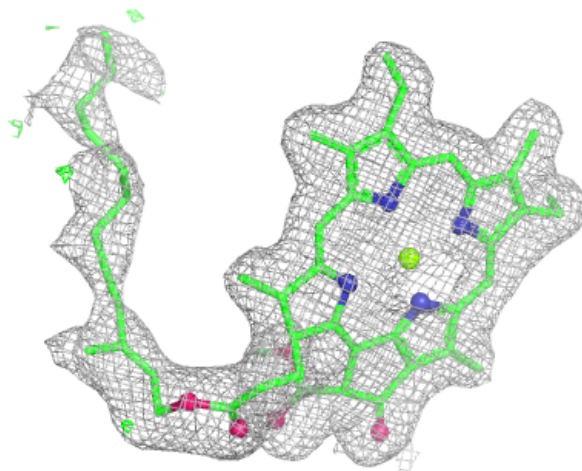
Electron density around BCR T 101:

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



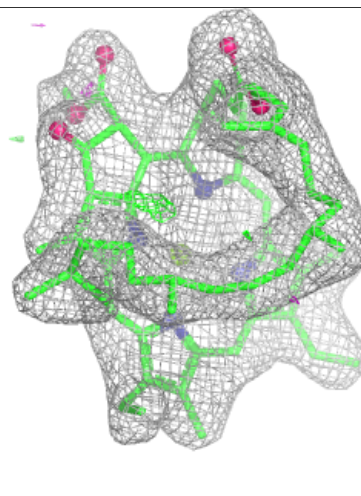
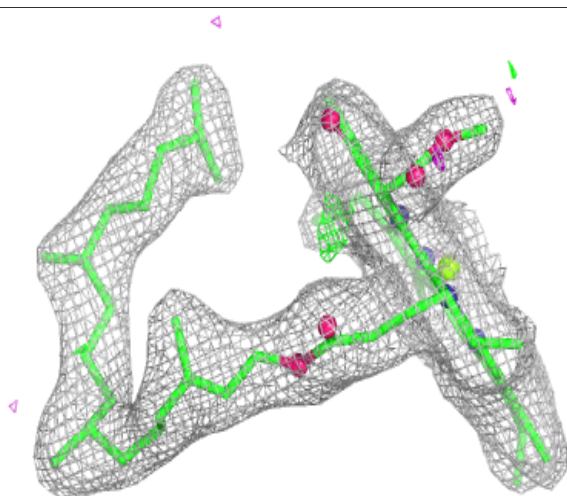
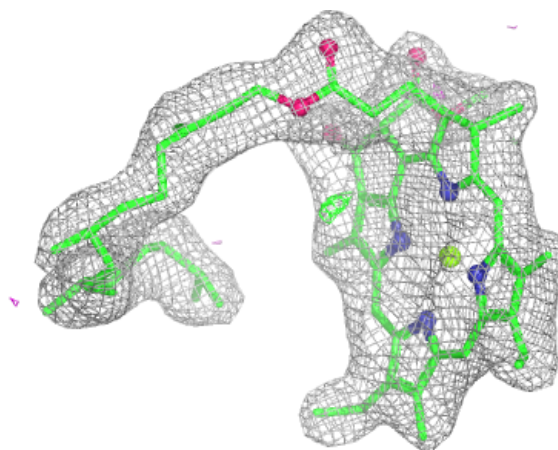
Electron density around CLA b 616:

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



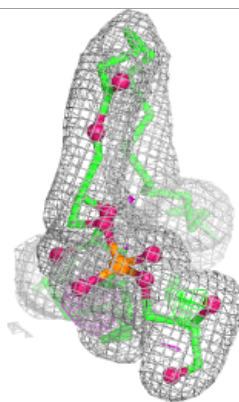
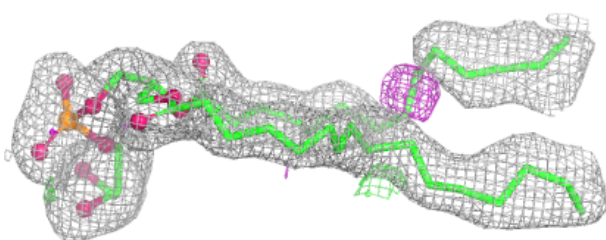
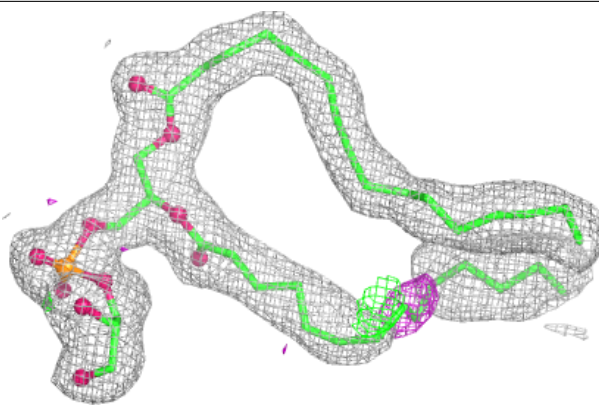
Electron density around CLA c 503:

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

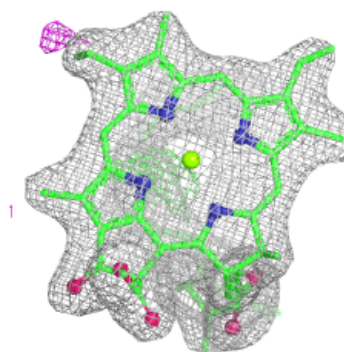
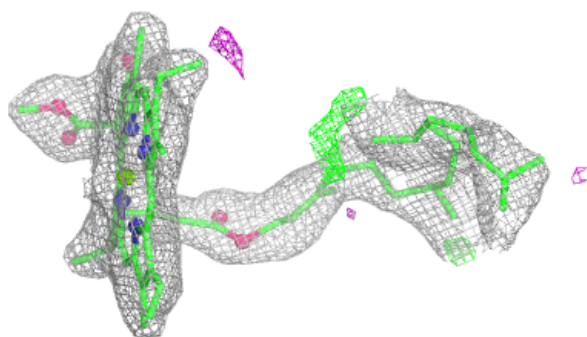
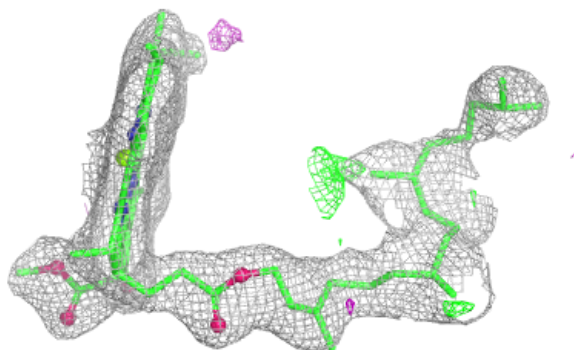


Electron density around LHG D 410:

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

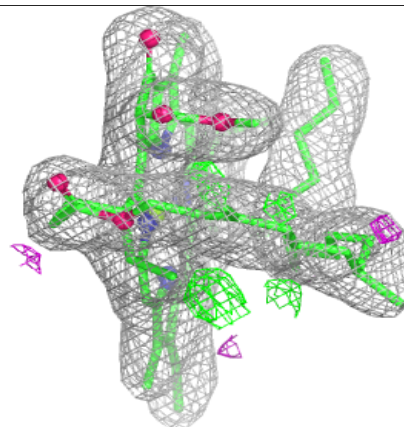
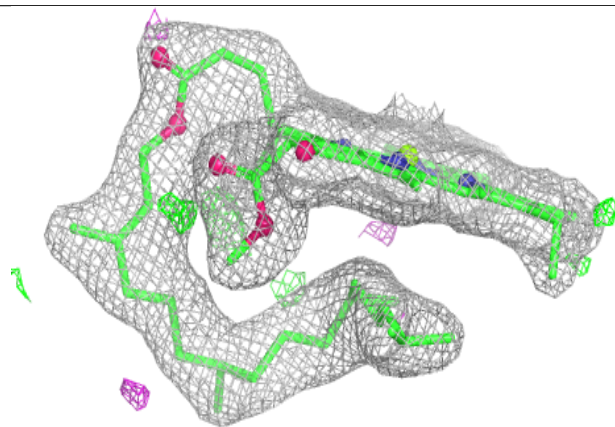
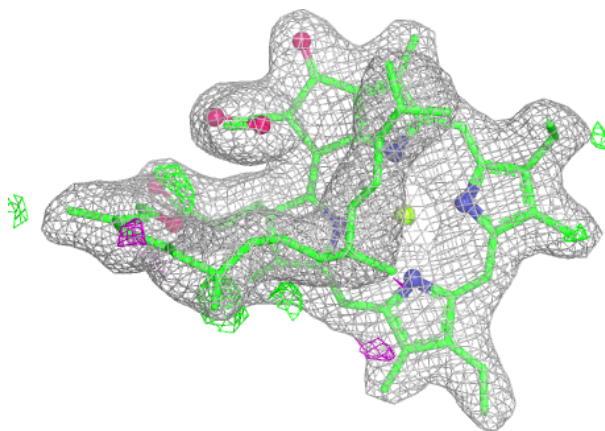
**Electron density around CLA c 506:**

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



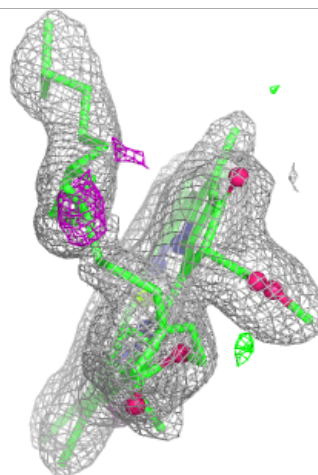
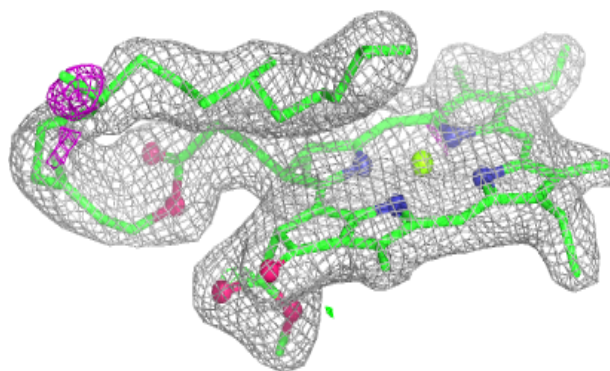
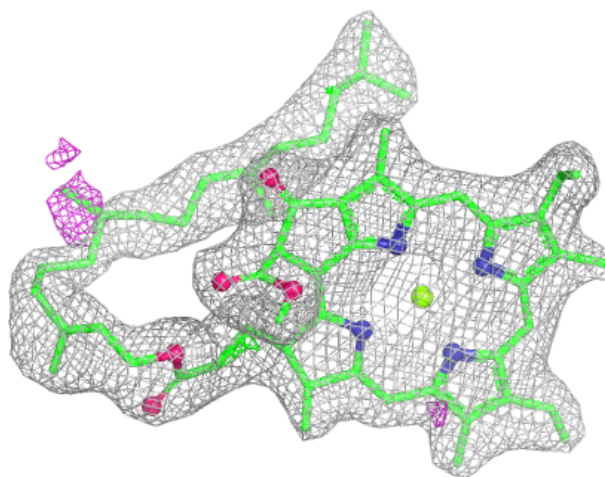
Electron density around CLA C 510:

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



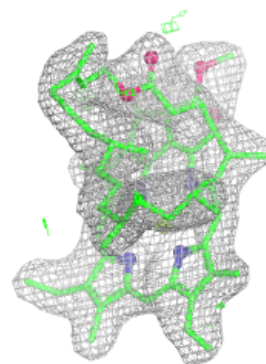
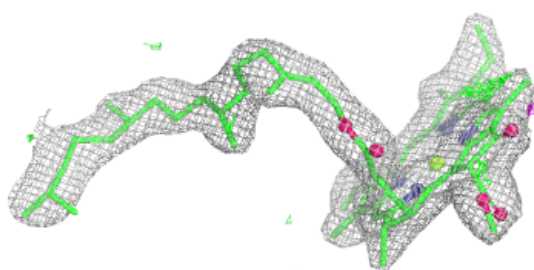
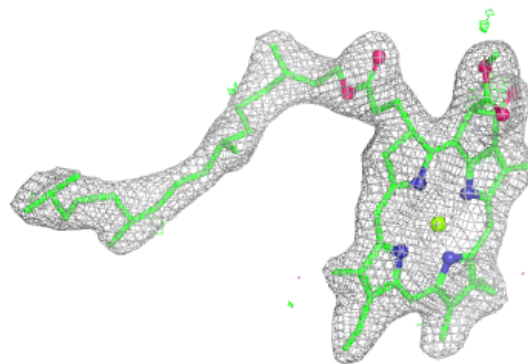
Electron density around CLA c 509:

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



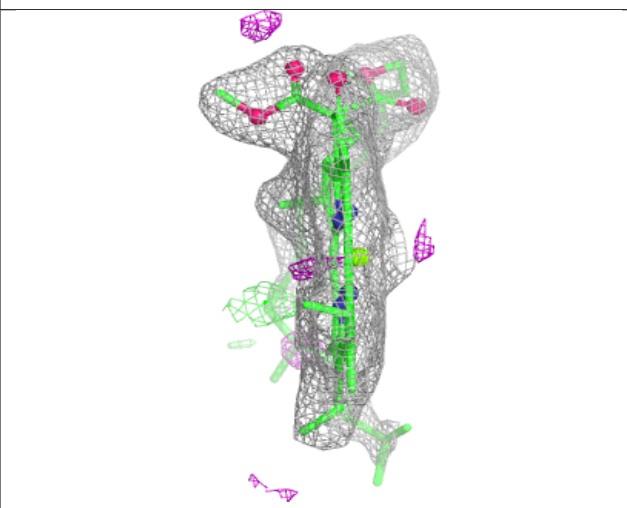
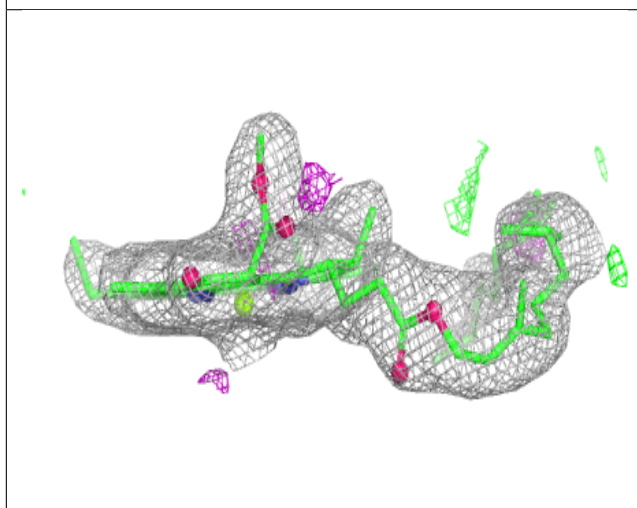
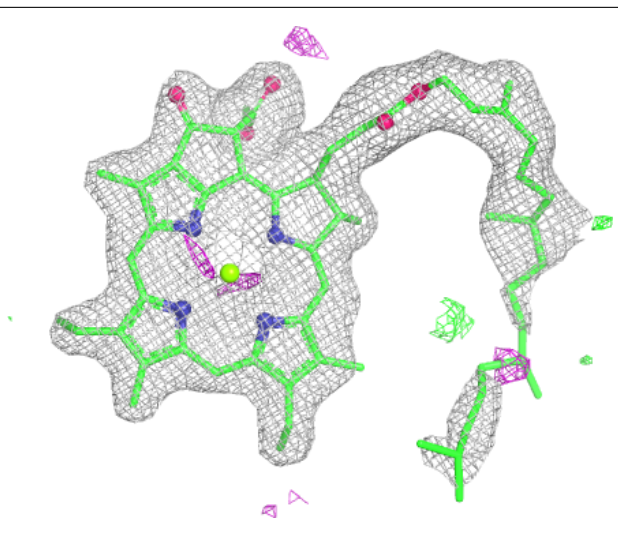
Electron density around CLA c 511:

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



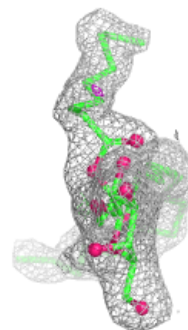
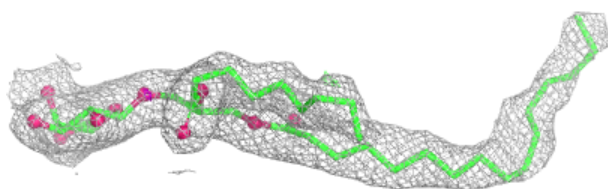
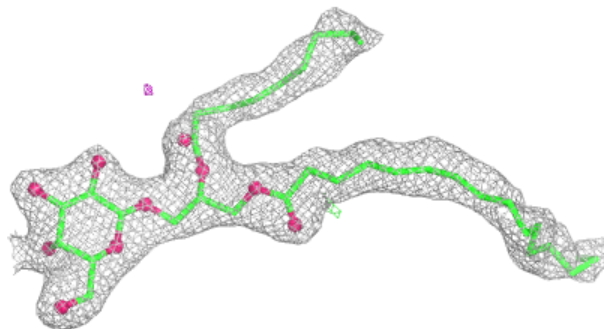
Electron density around CLA C 512:

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

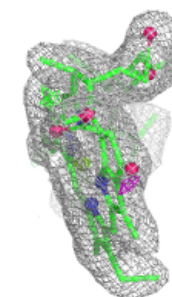
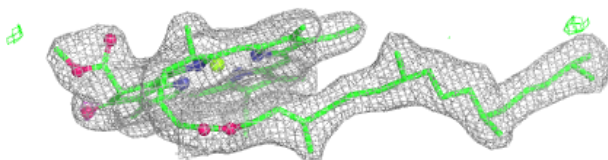
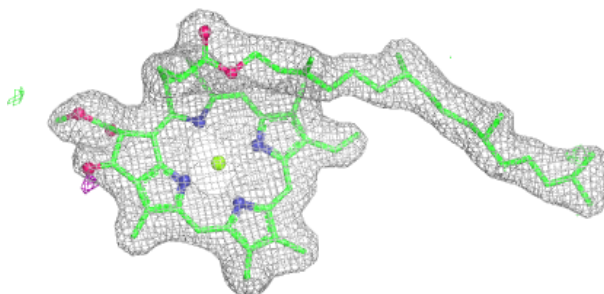


Electron density around LMG d 410:

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

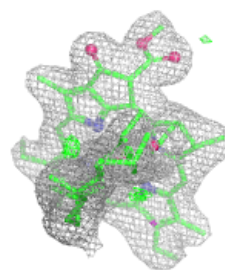
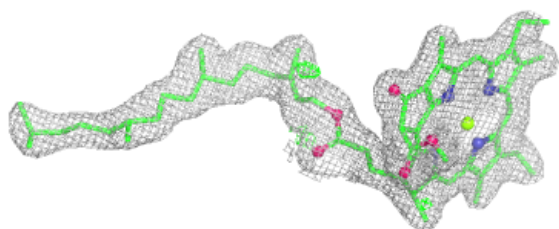
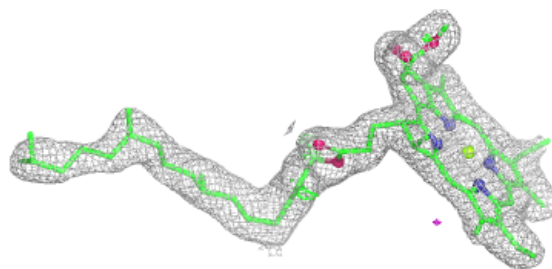
**Electron density around CLA c 501:**

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

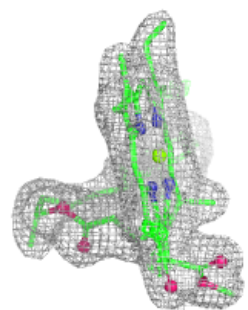
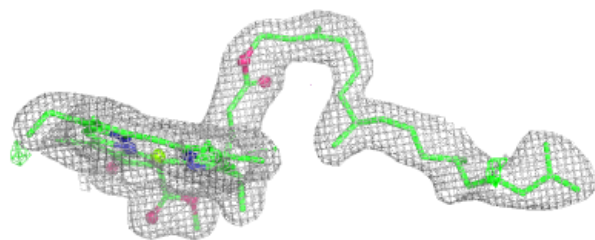
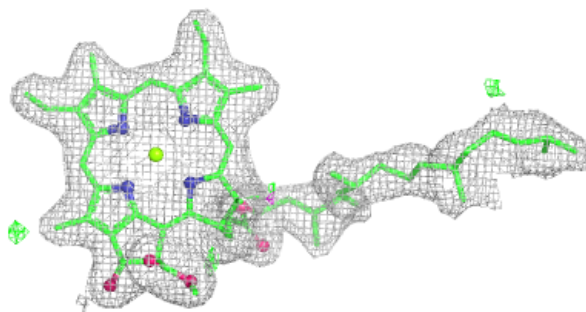


Electron density around CLA c 502:

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

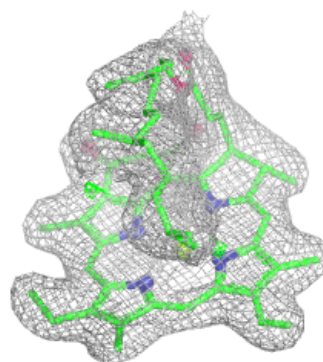
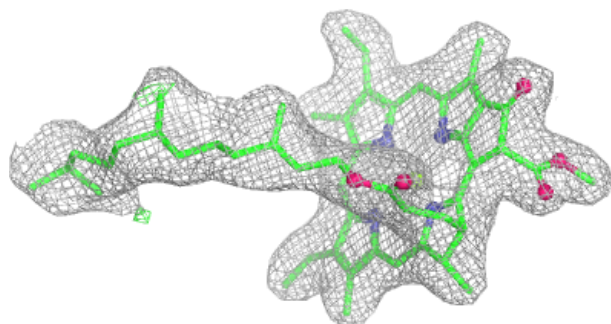
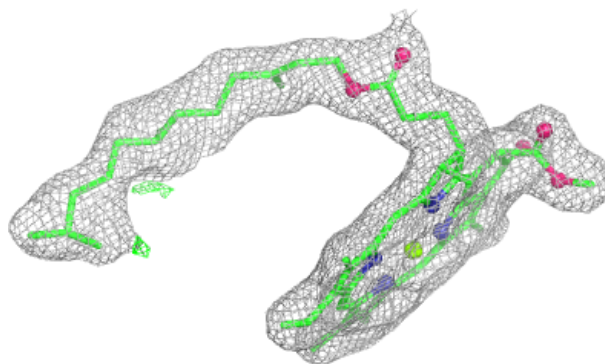
**Electron density around CLA a 607:**

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

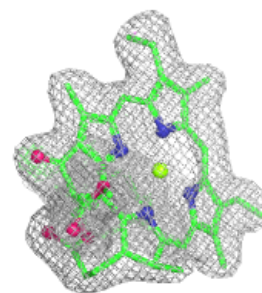
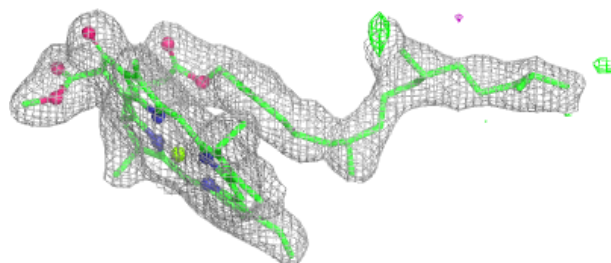
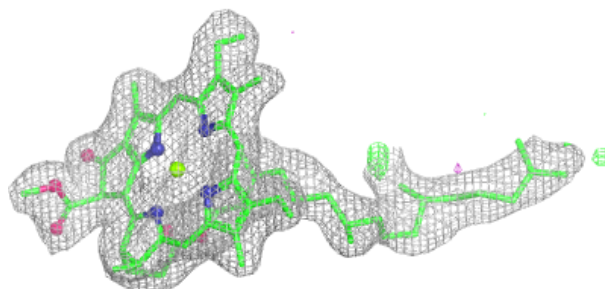


Electron density around CLA c 504:

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

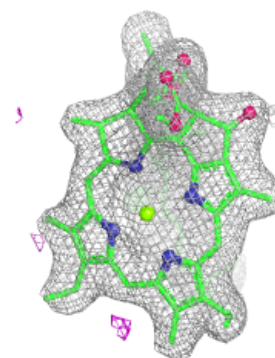
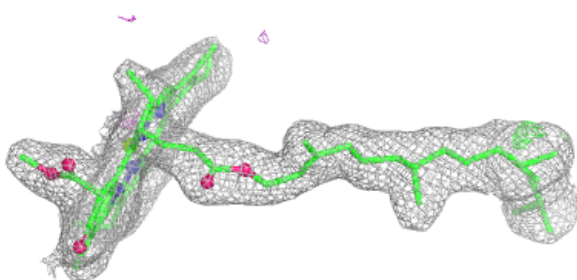
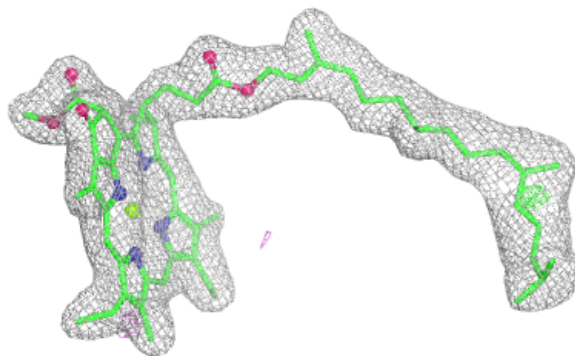
**Electron density around CLA c 505:**

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



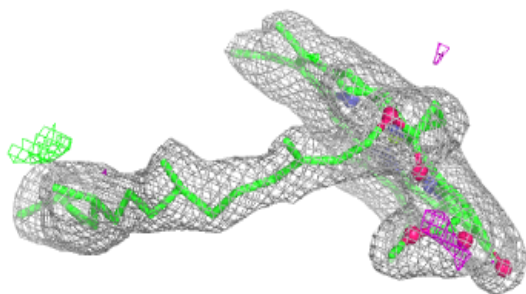
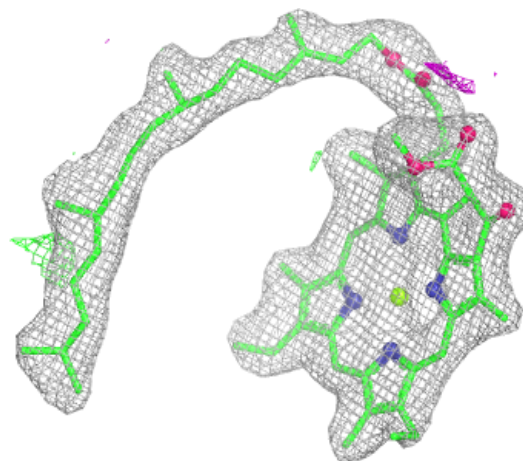
Electron density around CLA B 609:

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



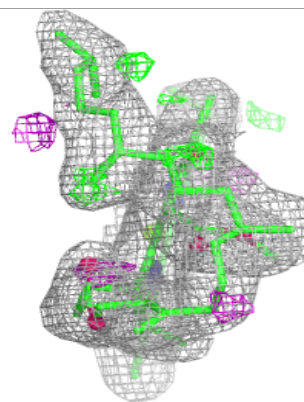
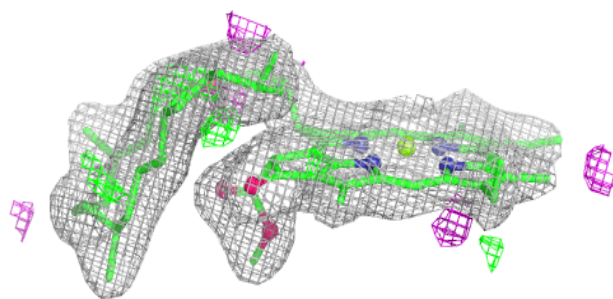
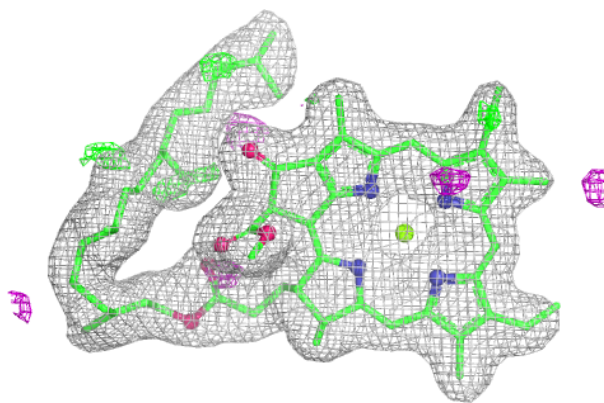
Electron density around CLA c 507:

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

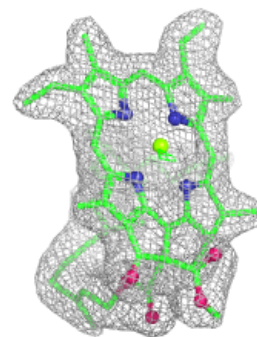
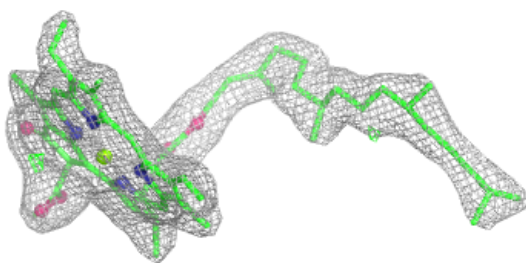
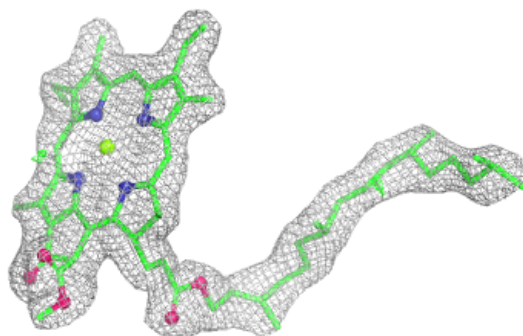


Electron density around CLA B 610:

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

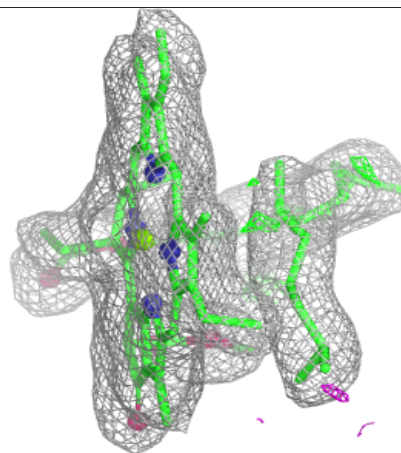
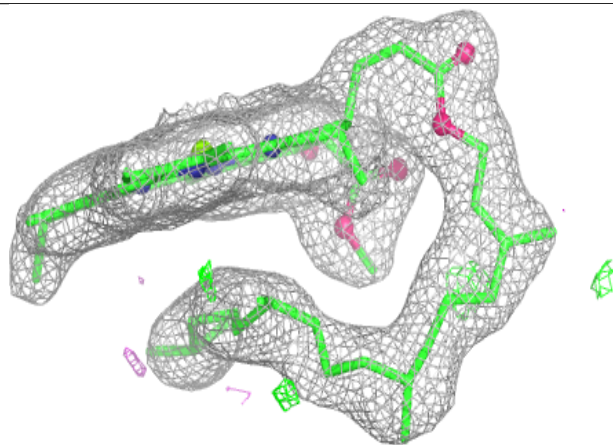
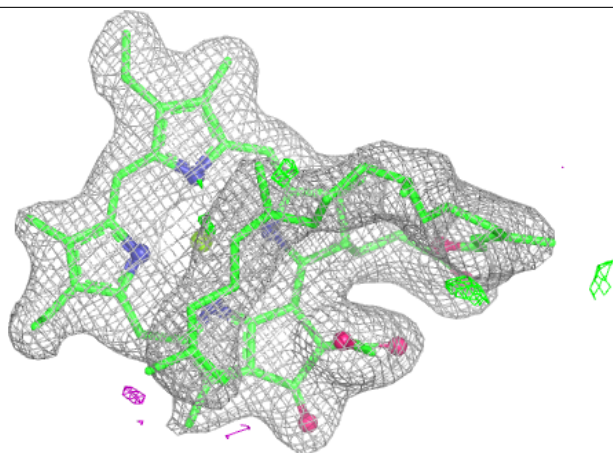
**Electron density around CLA C 511:**

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

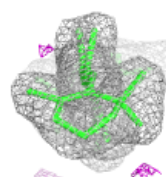
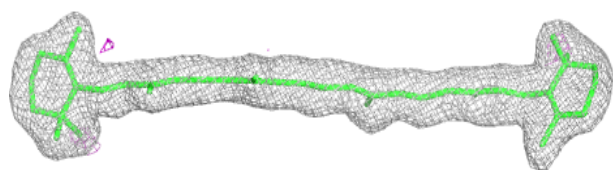
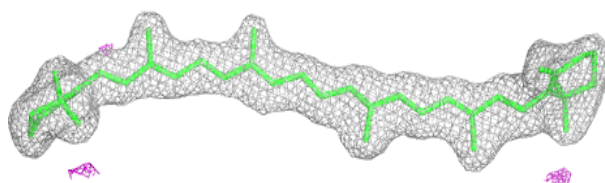


Electron density around CLA c 510:

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

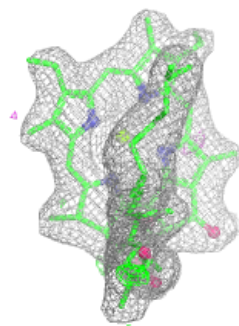
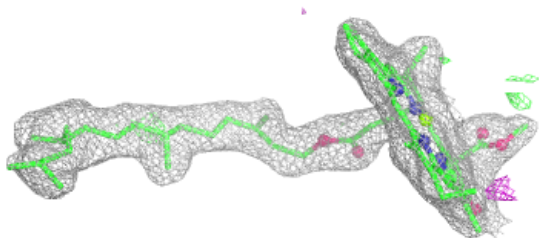
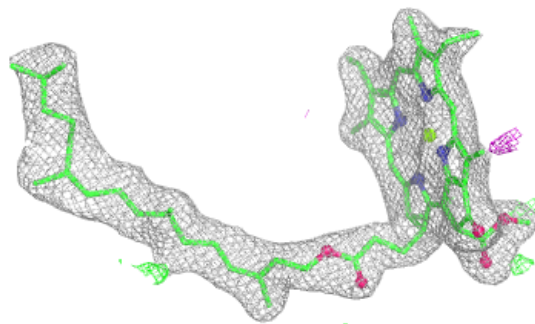
**Electron density around BCR a 610:**

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



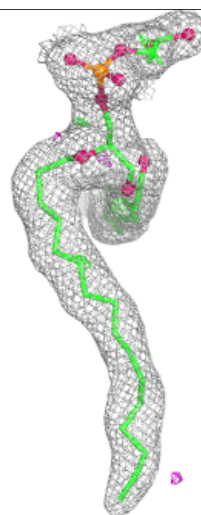
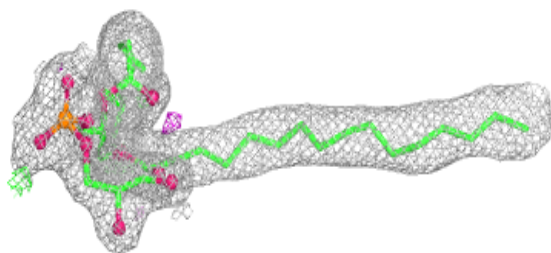
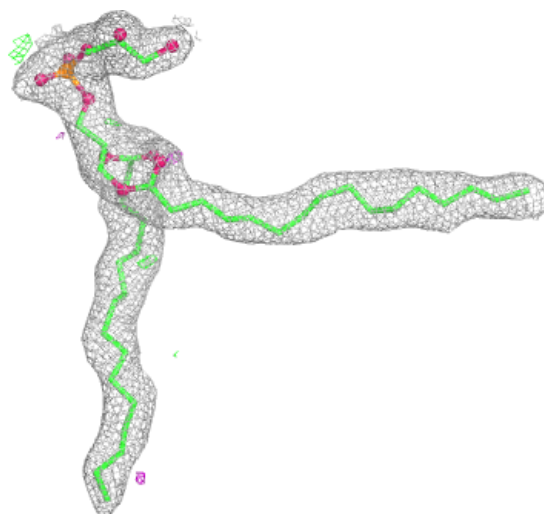
Electron density around CLA b 609:

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



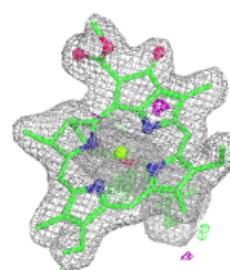
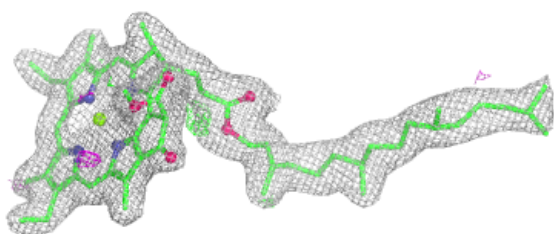
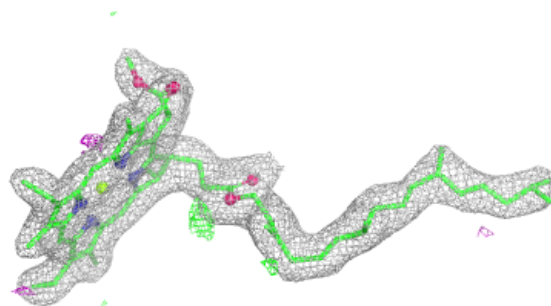
Electron density around LHG B 623:

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



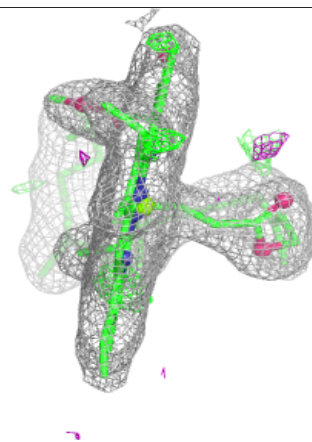
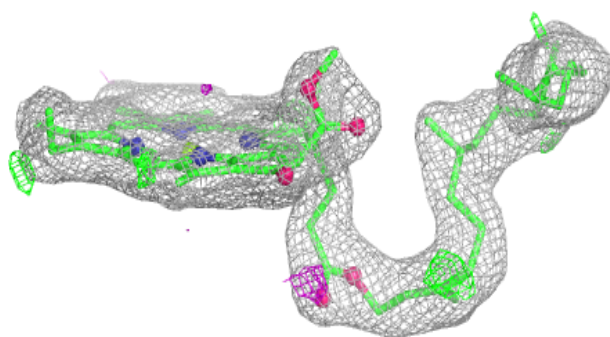
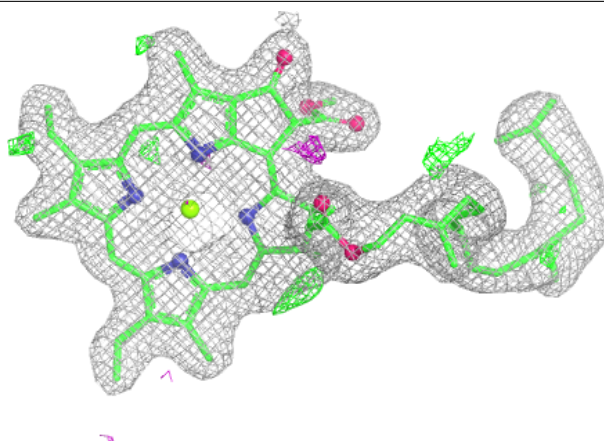
Electron density around CLA C 502:

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



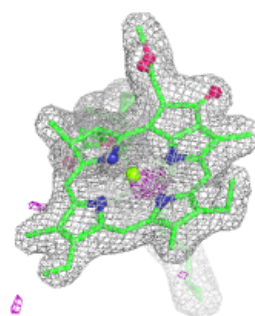
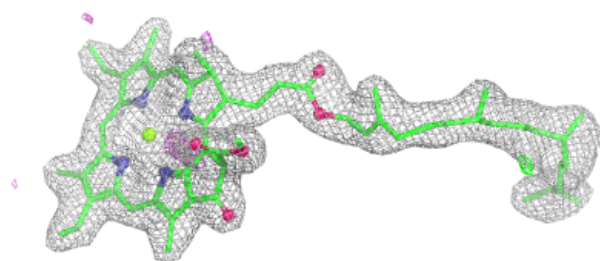
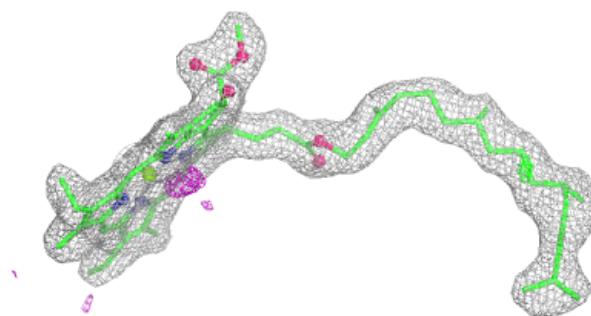
Electron density around CLA b 612:

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

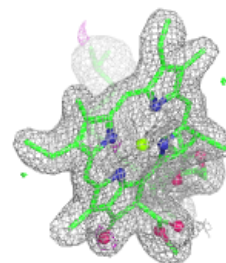
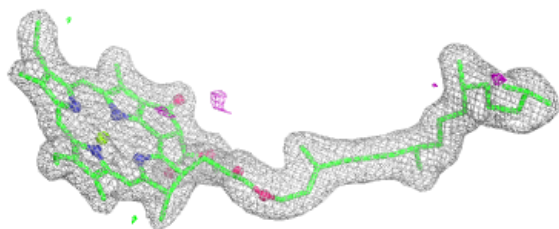
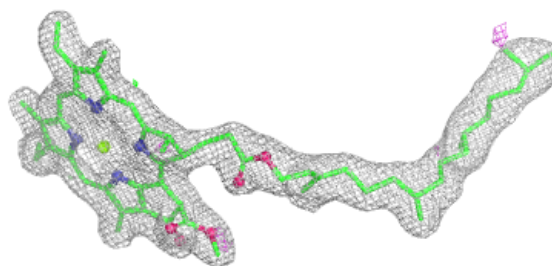


Electron density around CLA d 403:

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

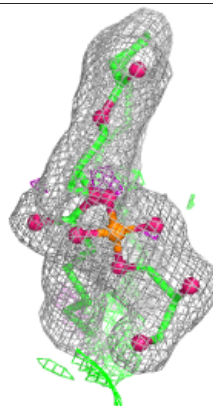
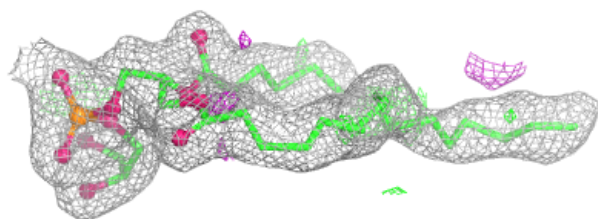
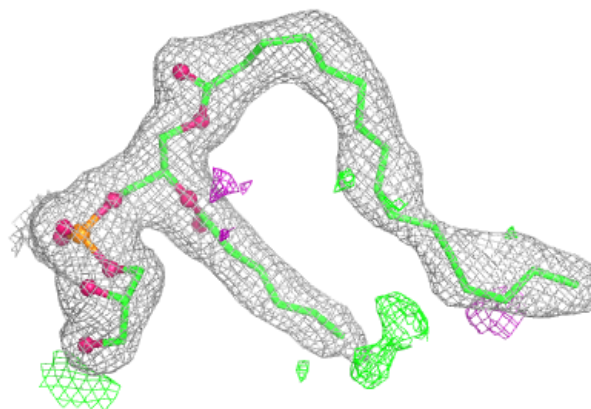
**Electron density around CLA A 606:**

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

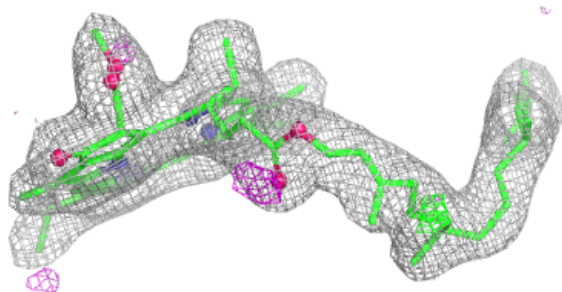
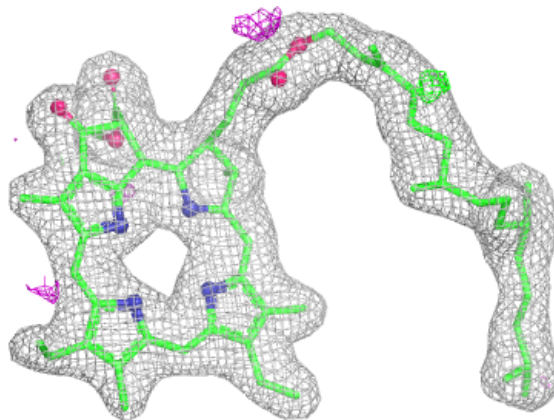


Electron density around LHG d 408:

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

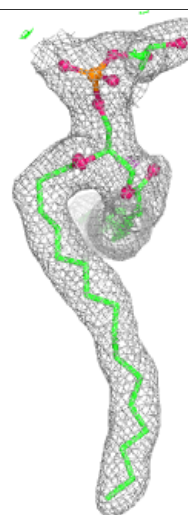
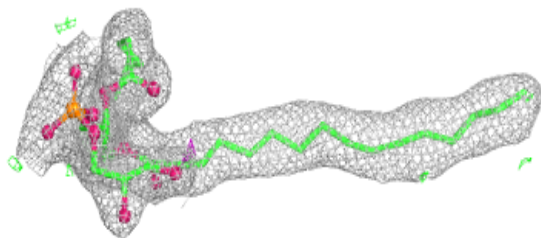
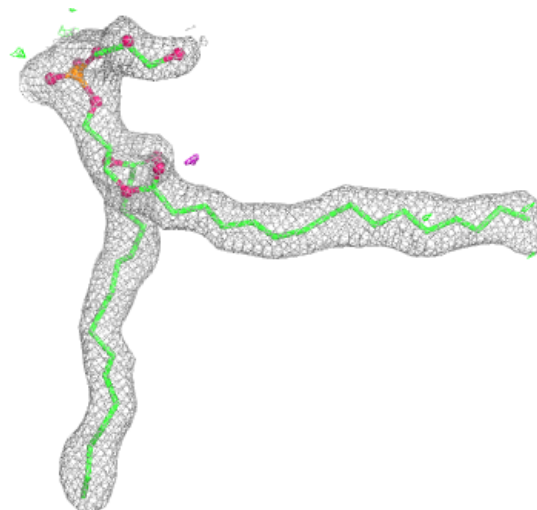
**Electron density around PHO d 402:**

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



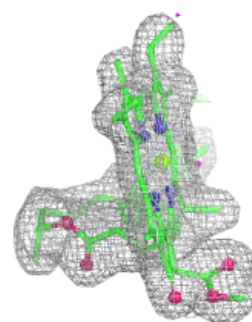
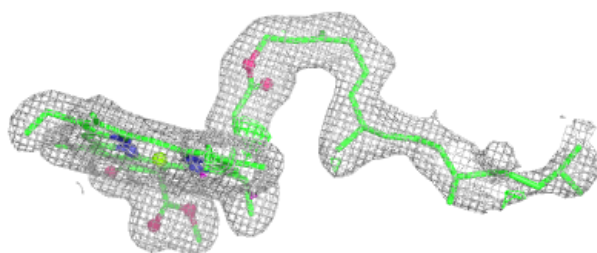
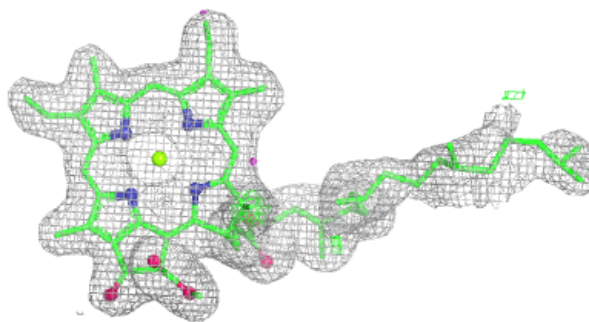
Electron density around LHG 1 101:

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

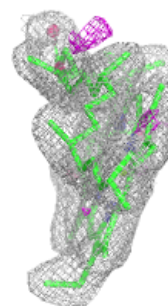
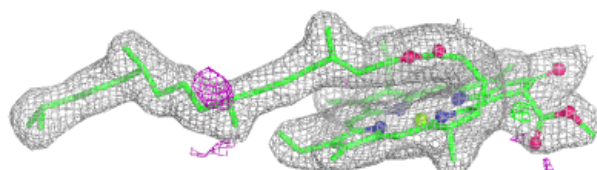
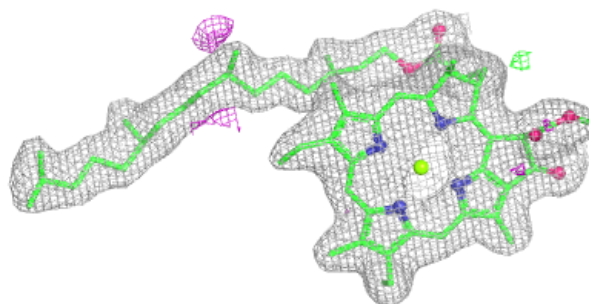


Electron density around CLA A 607:

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

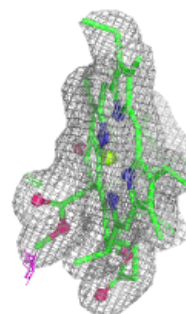
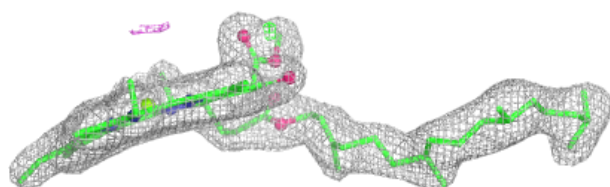
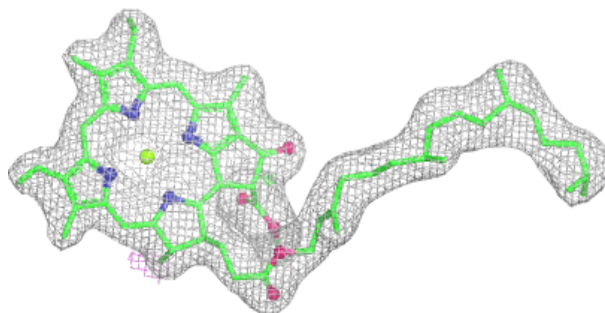
**Electron density around CLA C 501:**

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

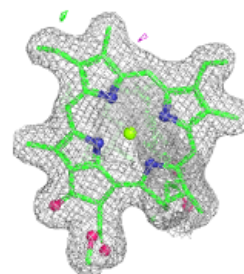
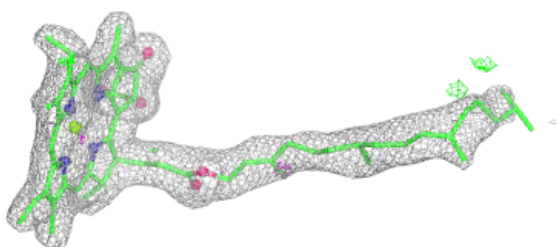
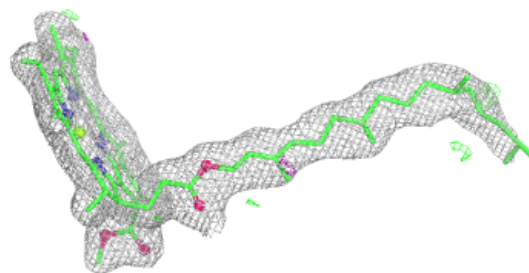


Electron density around CLA b 602:

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

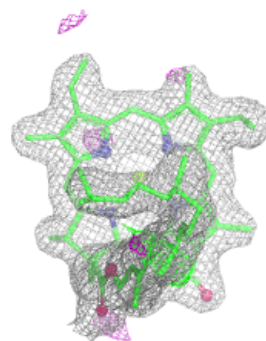
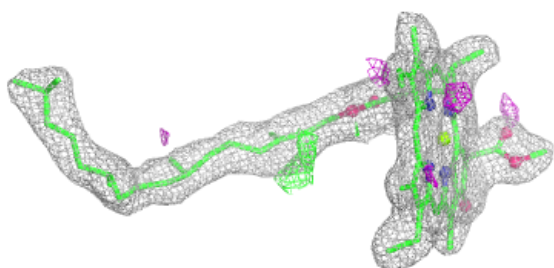
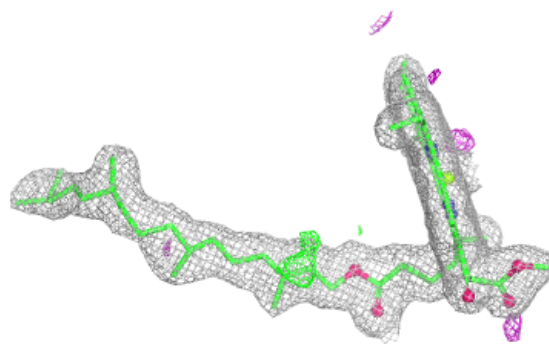
**Electron density around CLA b 604:**

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

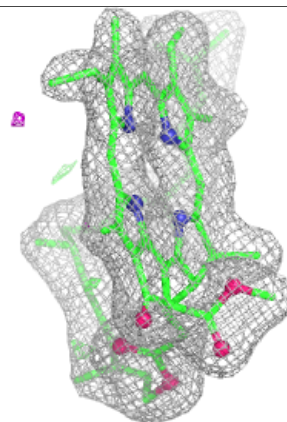
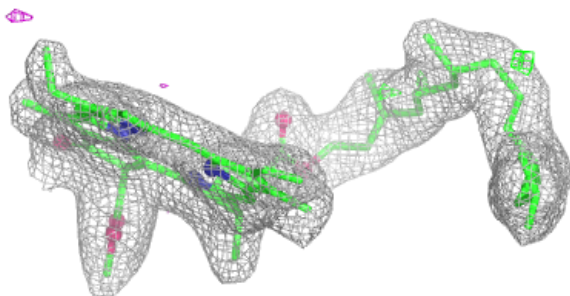
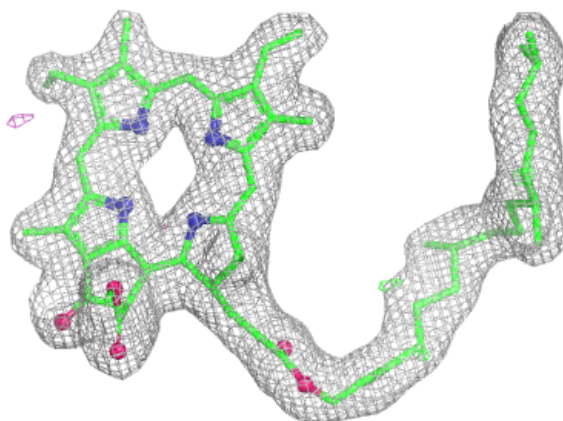


Electron density around CLA b 605:

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

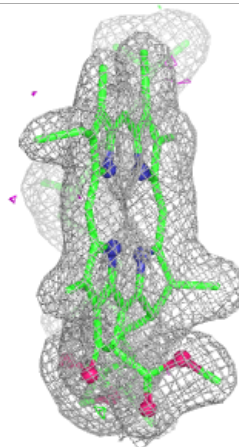
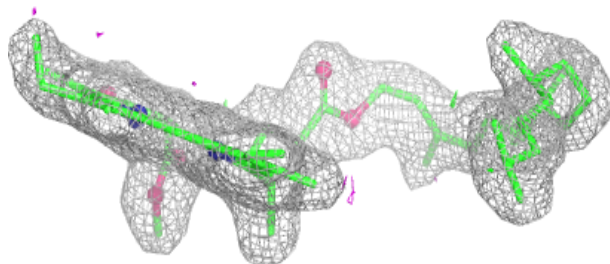
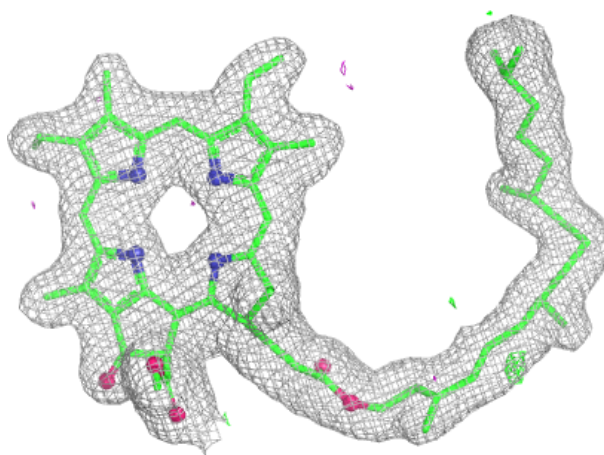
**Electron density around PHO D 402:**

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



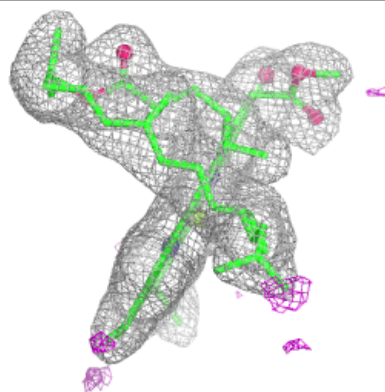
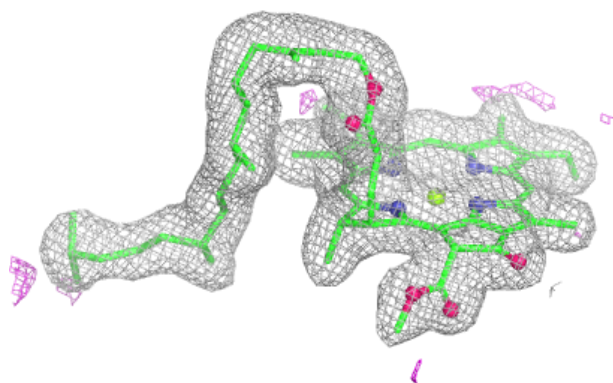
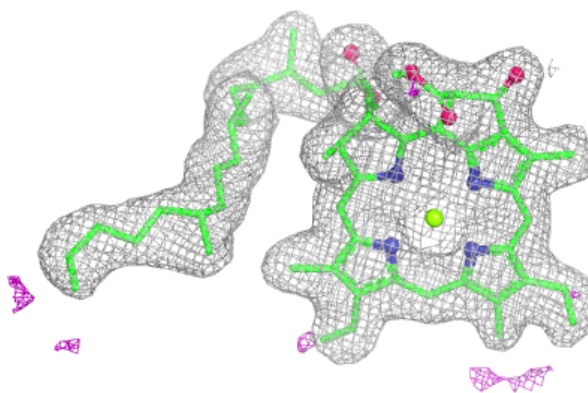
Electron density around PHO a 608:

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

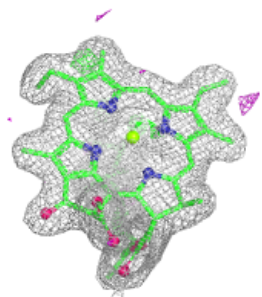
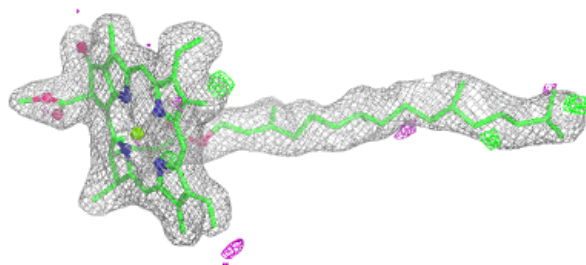
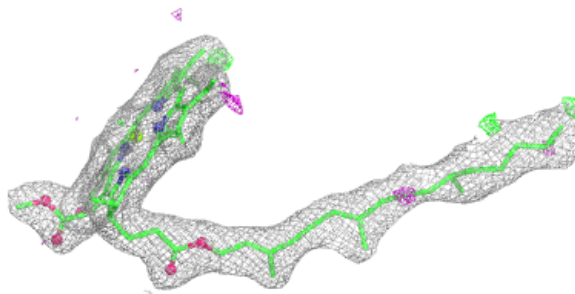


Electron density around CLA A 612:

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

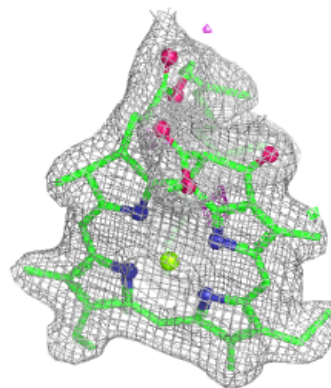
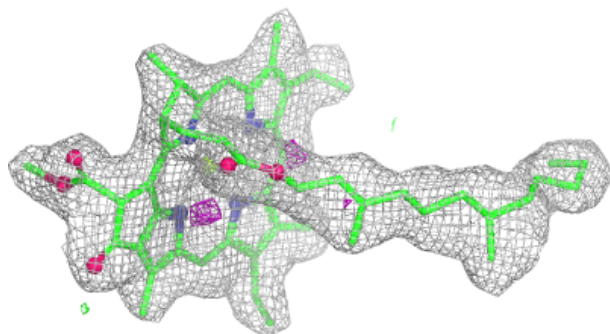
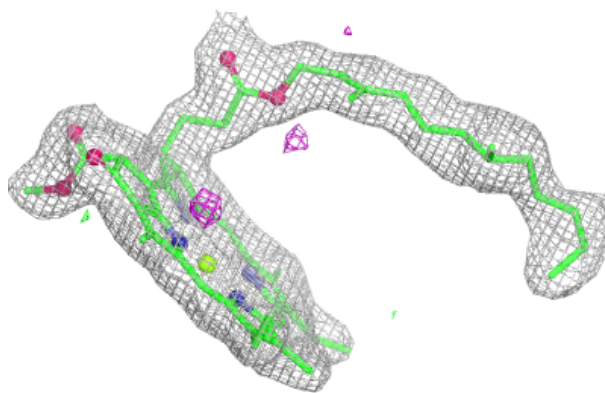
**Electron density around CLA B 607:**

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

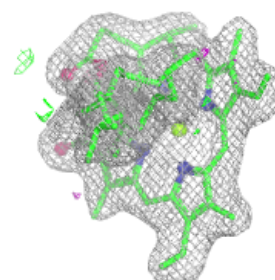
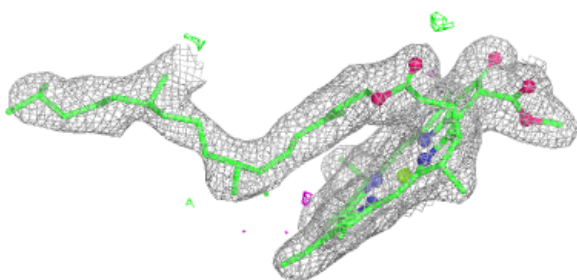
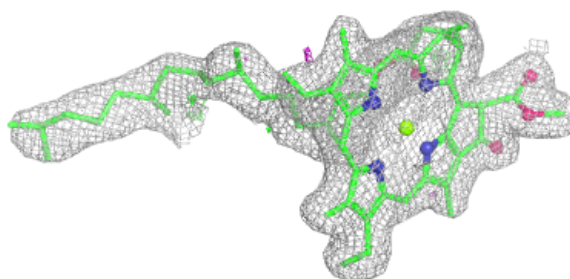


Electron density around CLA C 504:

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

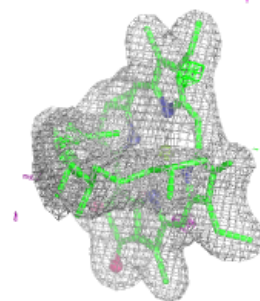
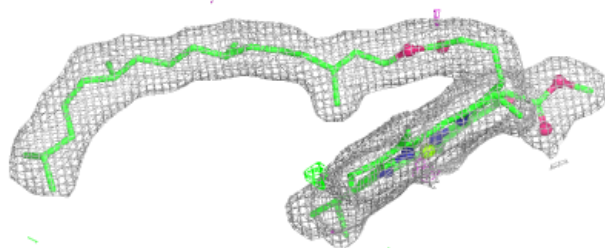
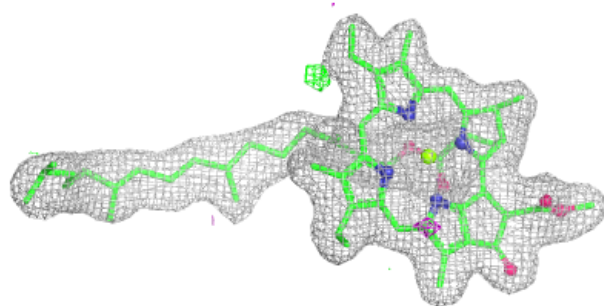
**Electron density around CLA C 505:**

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



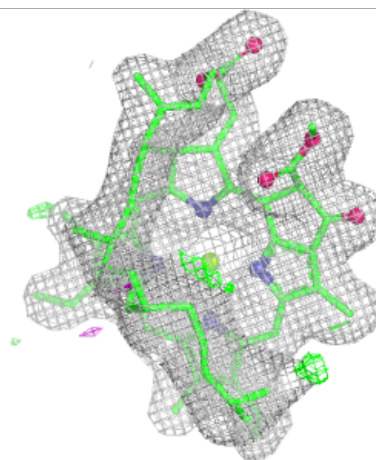
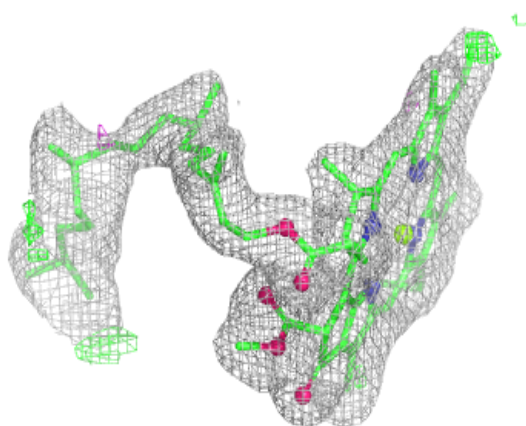
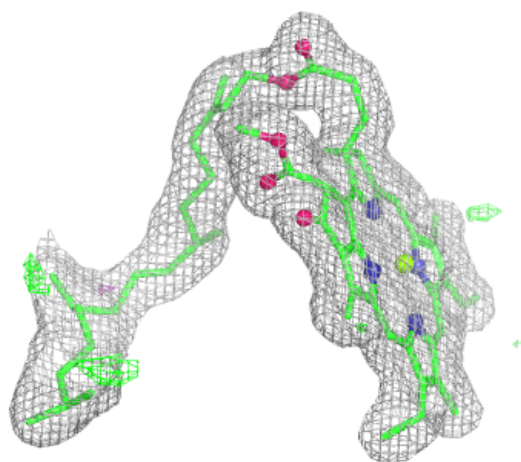
Electron density around CLA B 608:

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



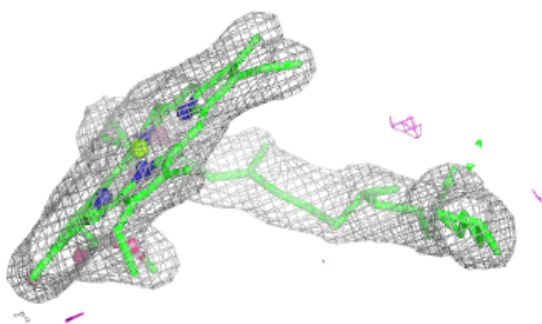
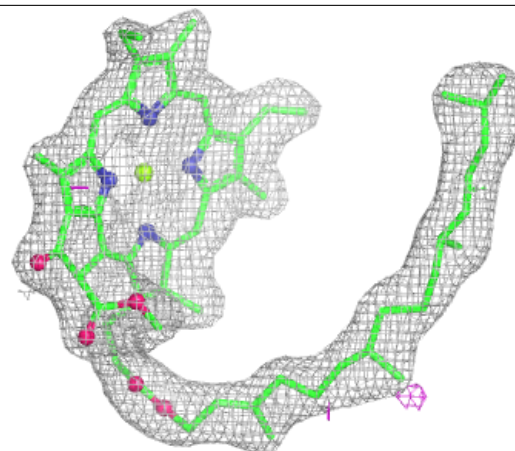
Electron density around CLA b 613:

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



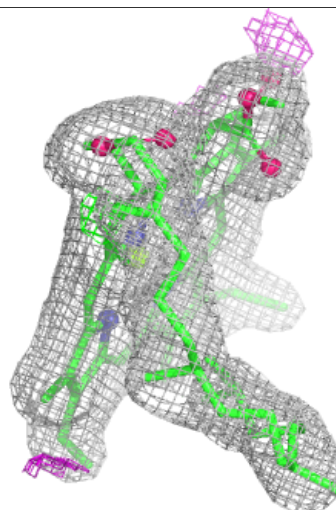
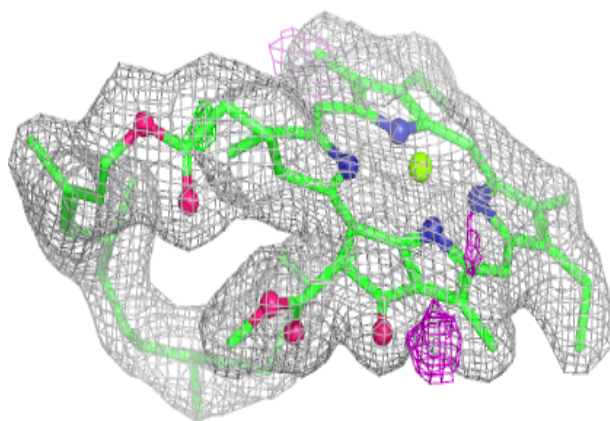
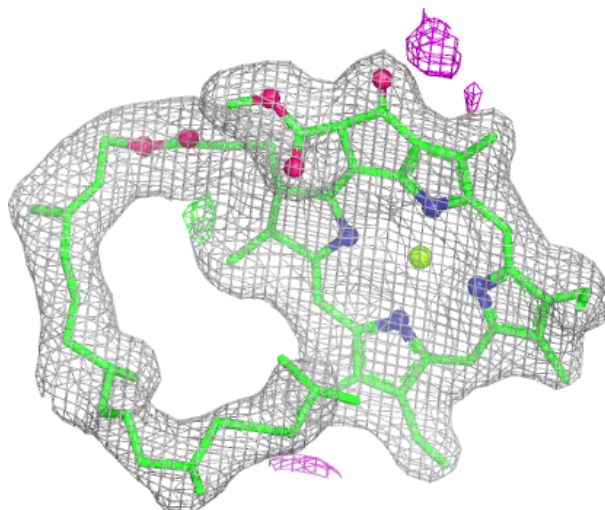
Electron density around CLA C 507:

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



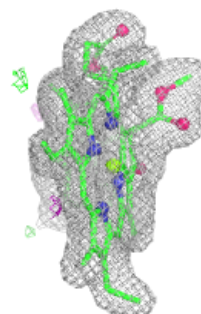
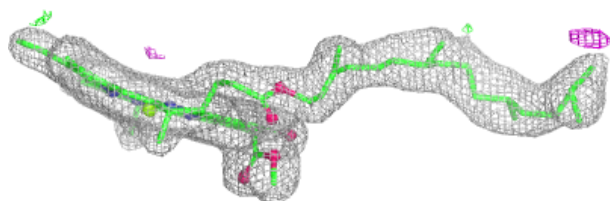
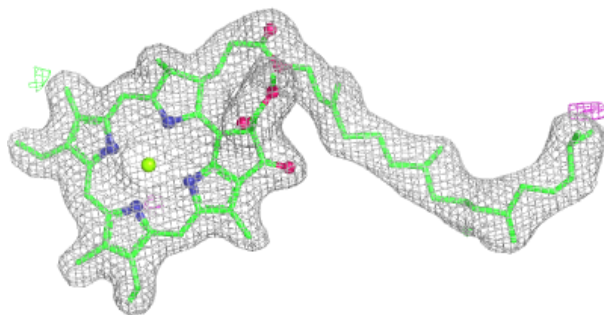
Electron density around CLA b 615:

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



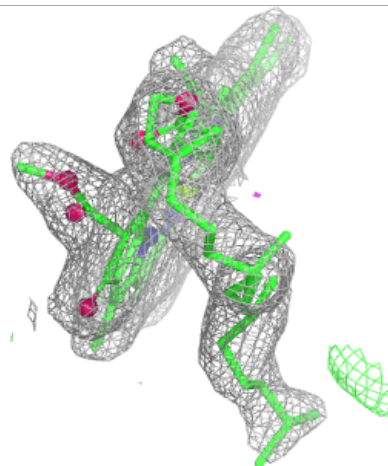
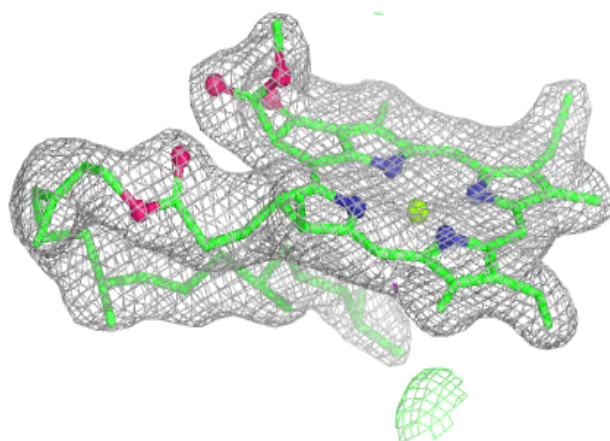
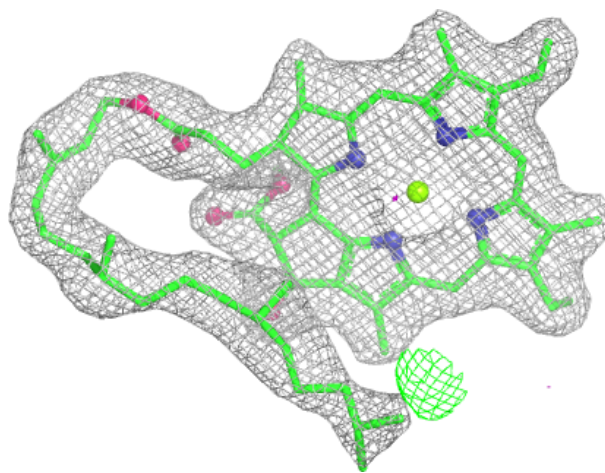
Electron density around CLA B 602:

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



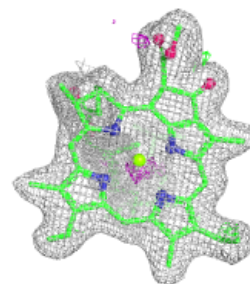
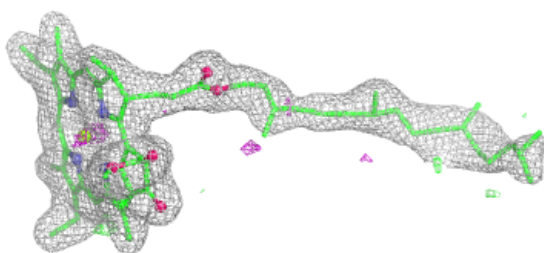
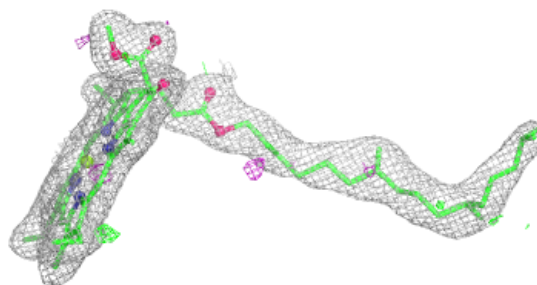
Electron density around CLA C 509:

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



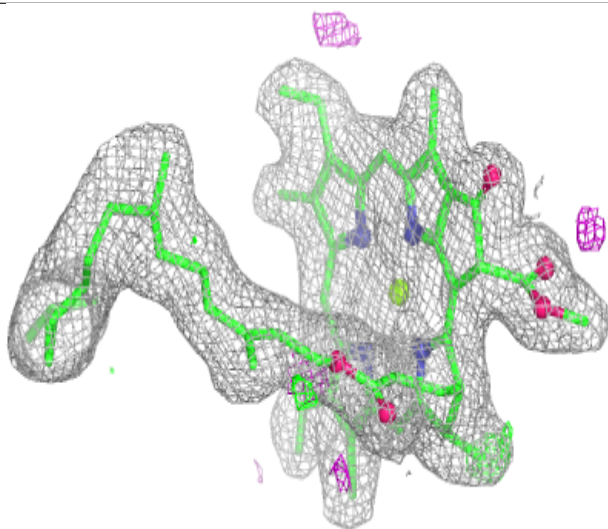
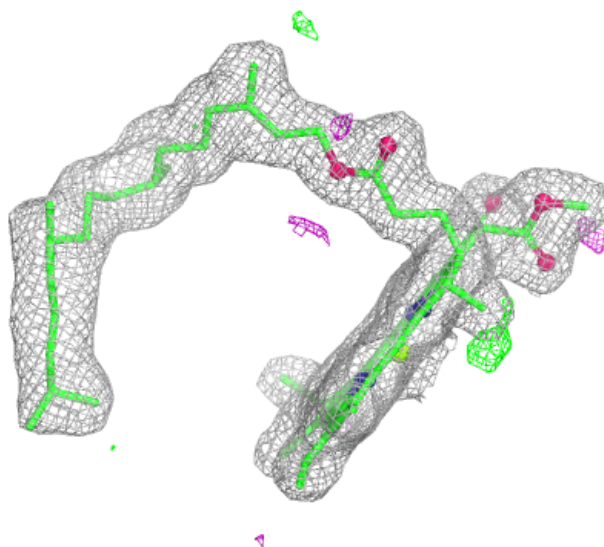
Electron density around CLA B 604:

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



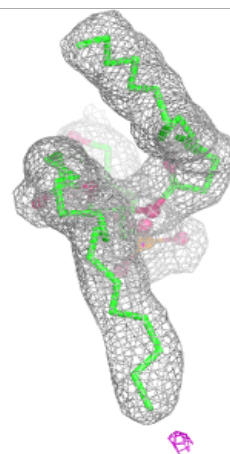
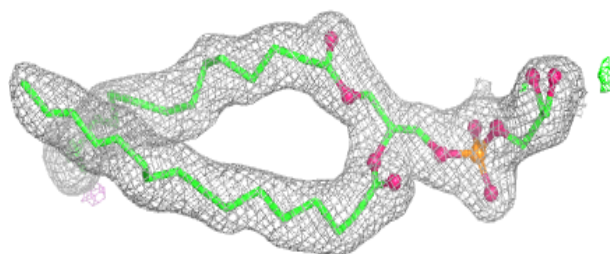
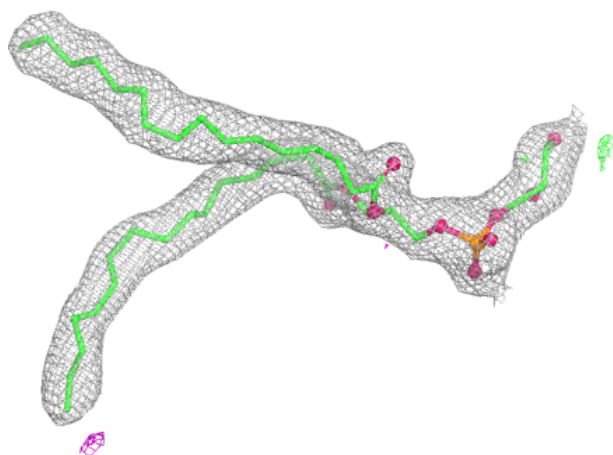
Electron density around CLA B 611:

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



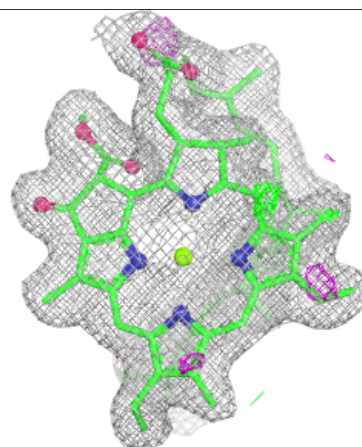
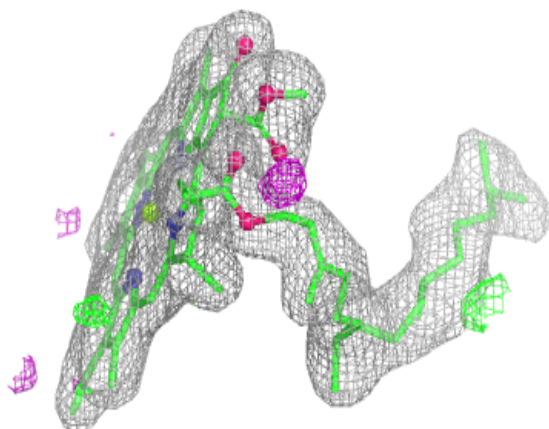
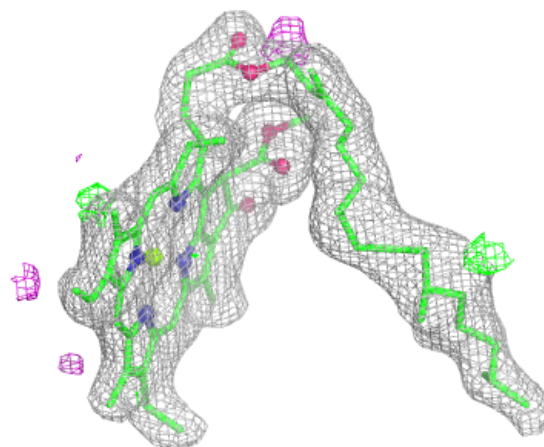
Electron density around LHG D 409:

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



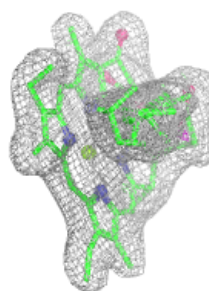
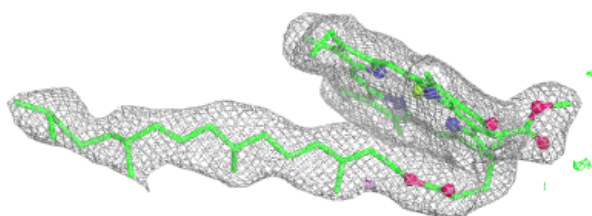
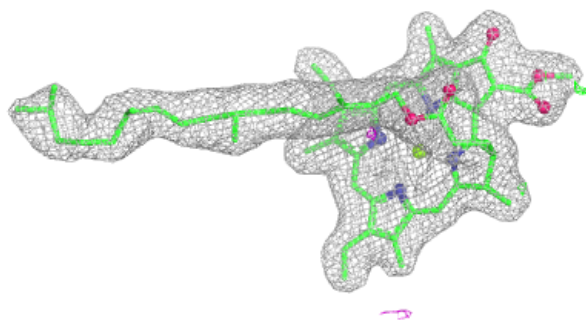
Electron density around CLA B 613:

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

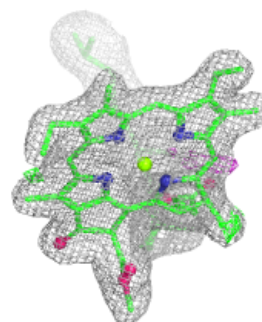
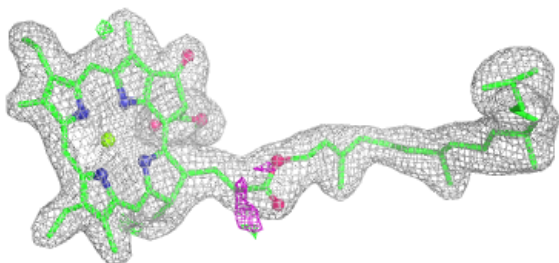
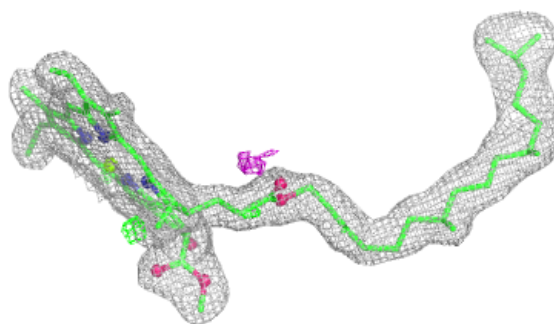


Electron density around CLA B 614:

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

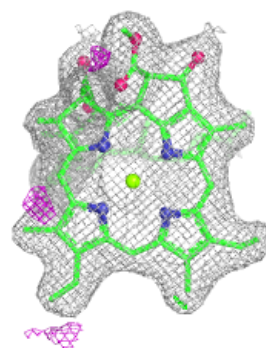
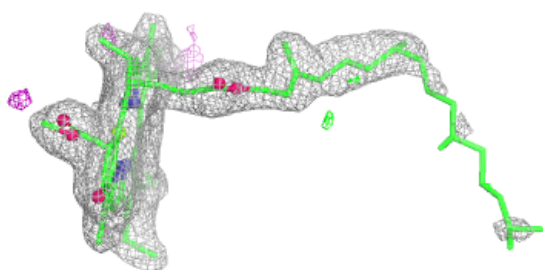
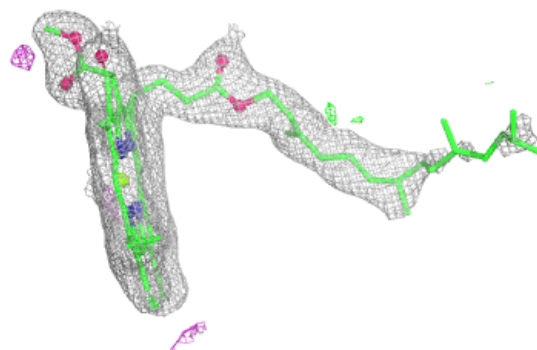
**Electron density around CLA D 403:**

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

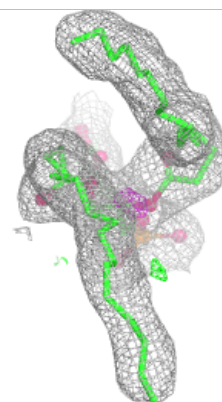
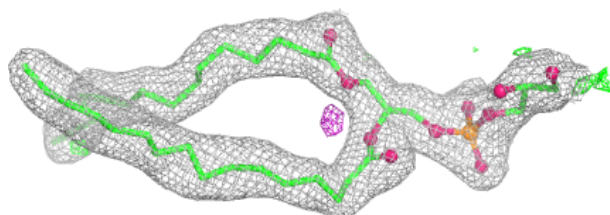
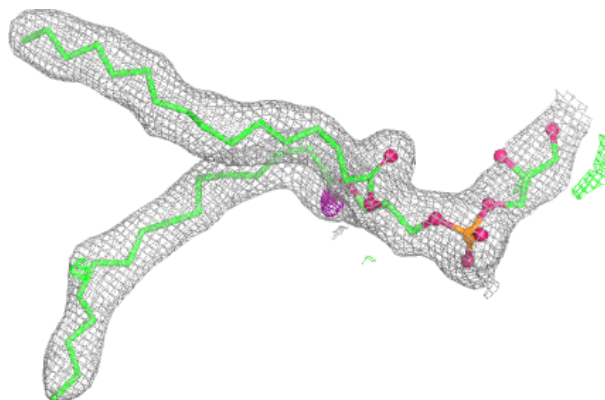


Electron density around CLA D 404:

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

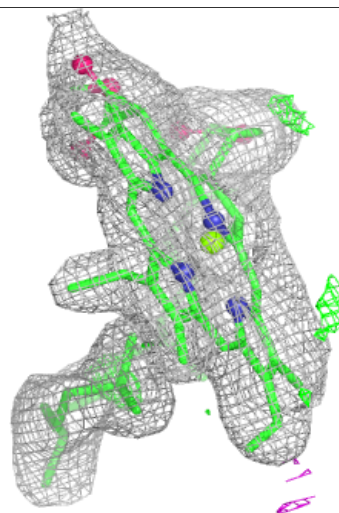
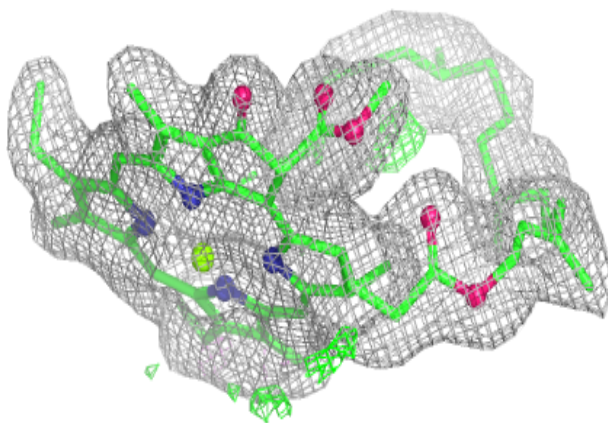
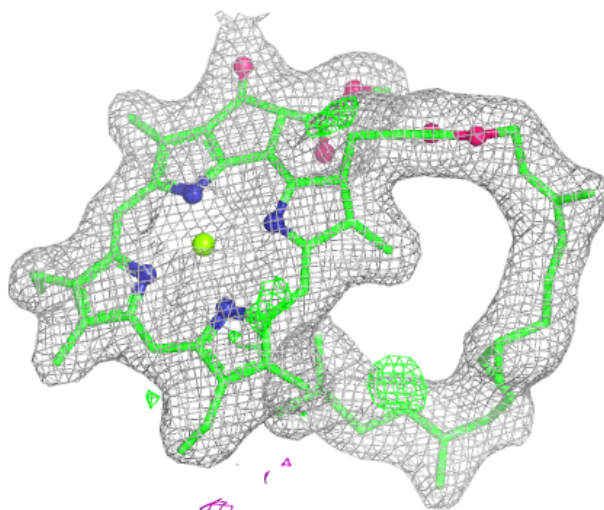
**Electron density around LHG d 407:**

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



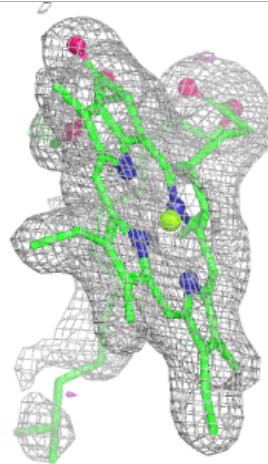
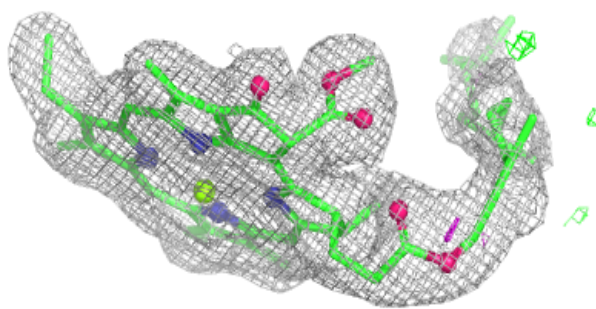
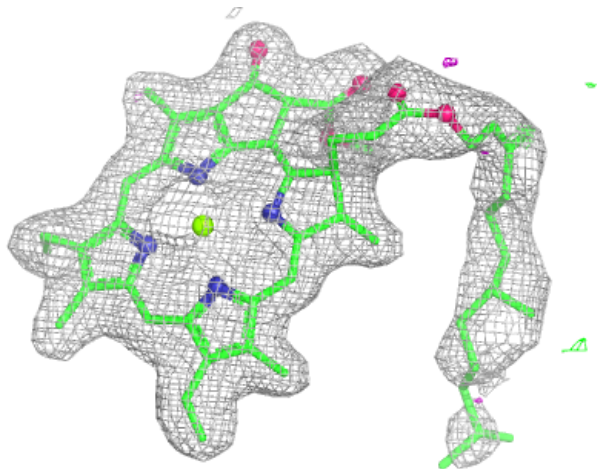
Electron density around CLA B 615:

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



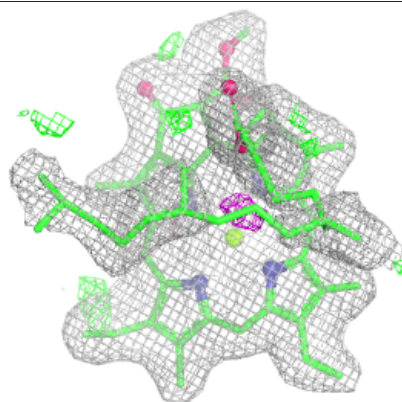
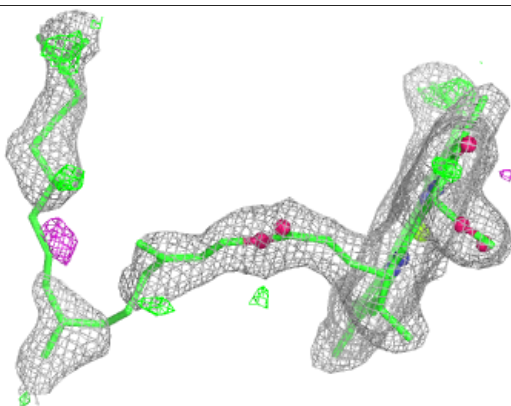
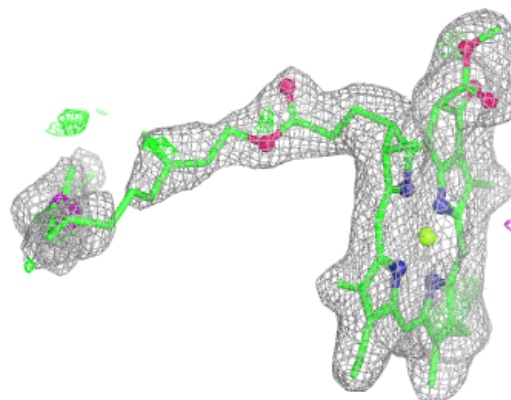
Electron density around CLA B 616:

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

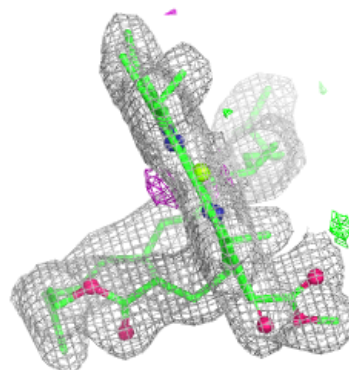
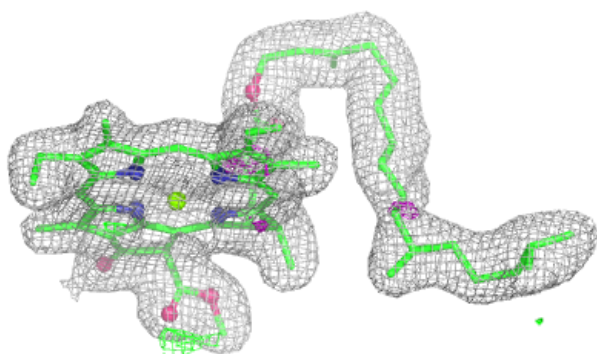
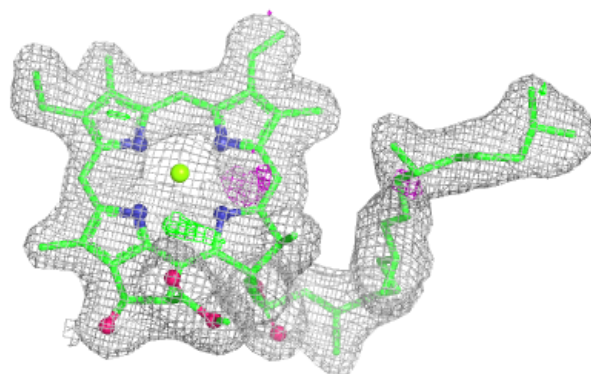


Electron density around CLA a 609:

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

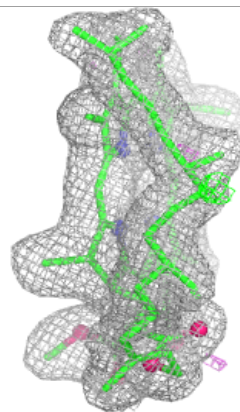
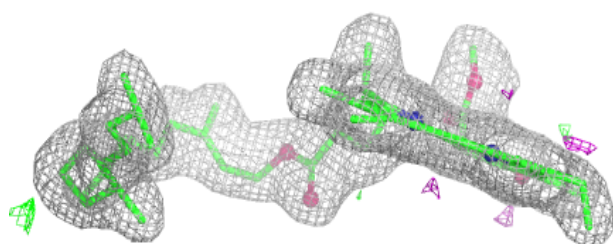
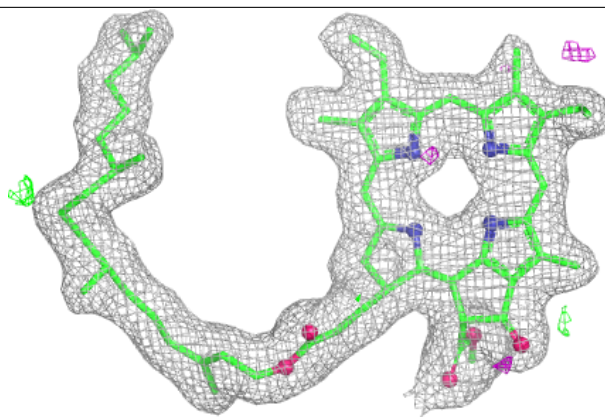
**Electron density around CLA a 612:**

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



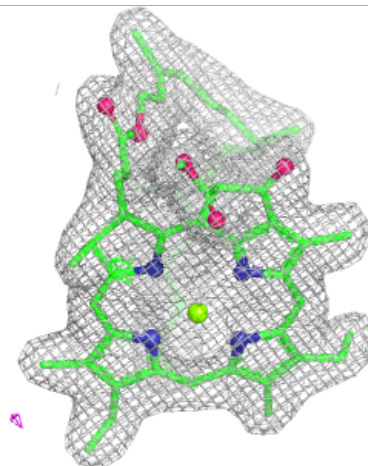
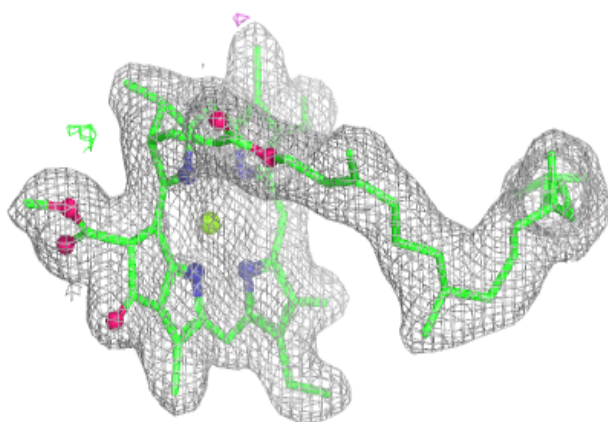
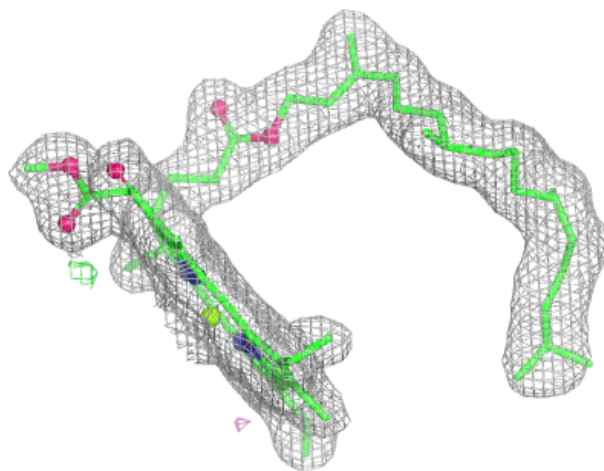
Electron density around PHO A 608:

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



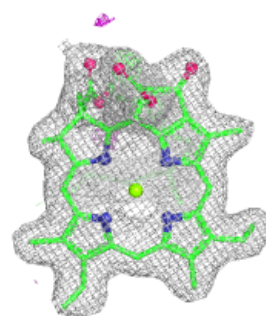
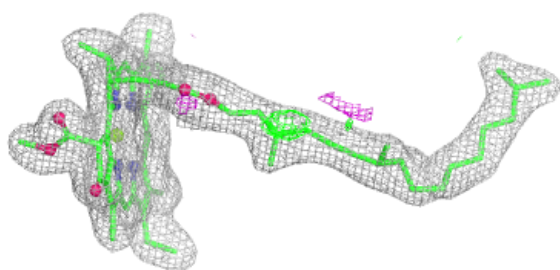
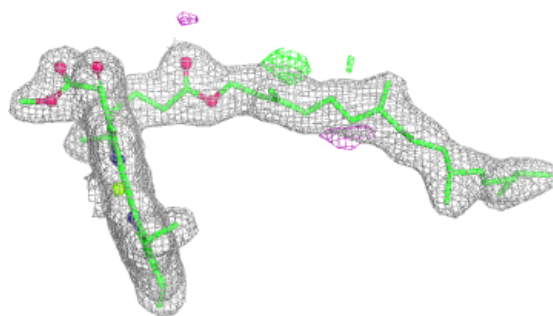
Electron density around CLA b 611:

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

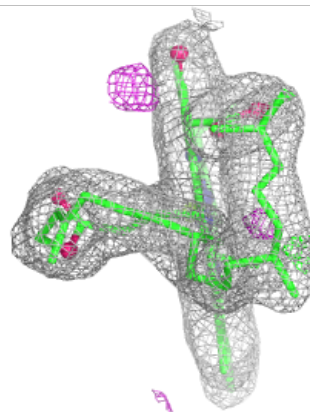
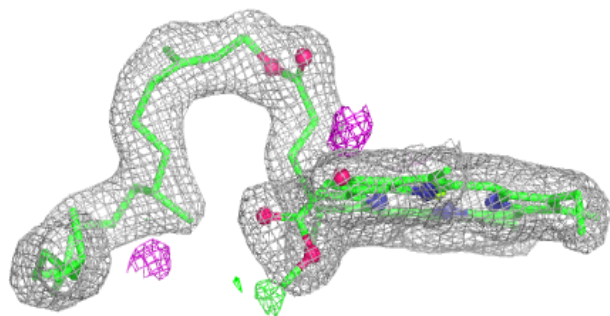
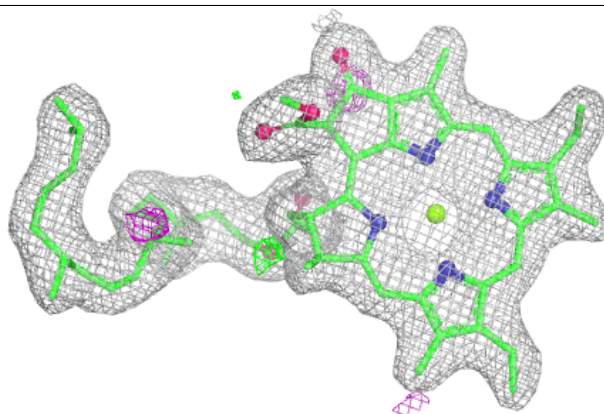


Electron density around CLA B 605:

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

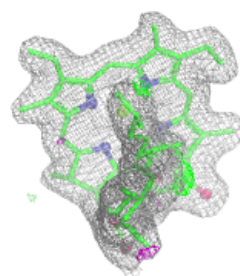
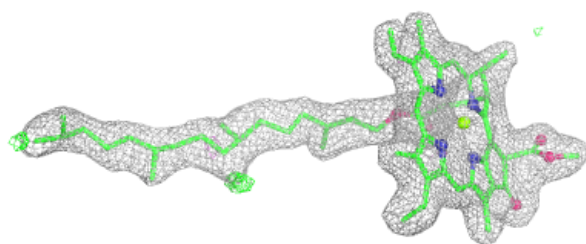
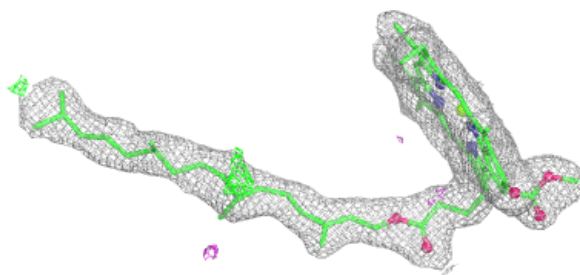
**Electron density around CLA B 612:**

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

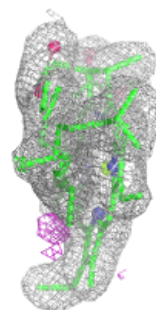
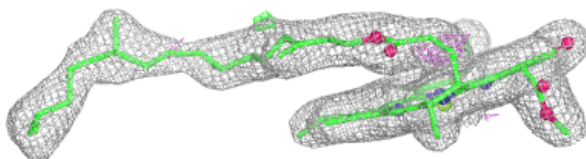
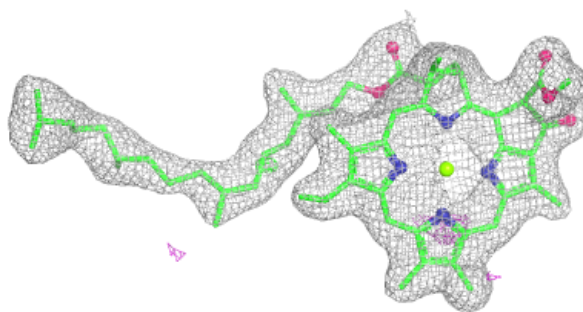


Electron density around CLA b 607:

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

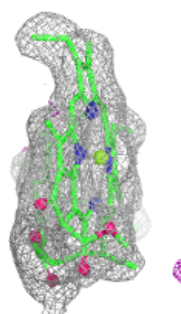
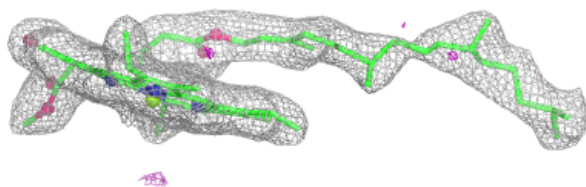
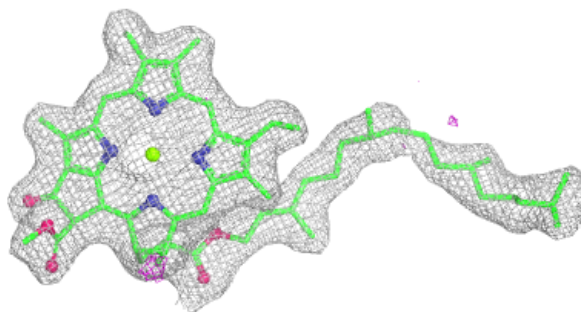
**Electron density around CLA B 603:**

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

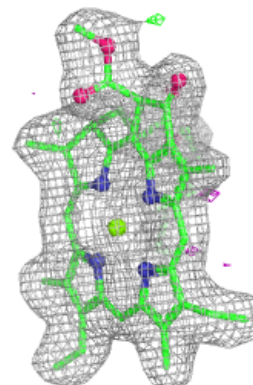
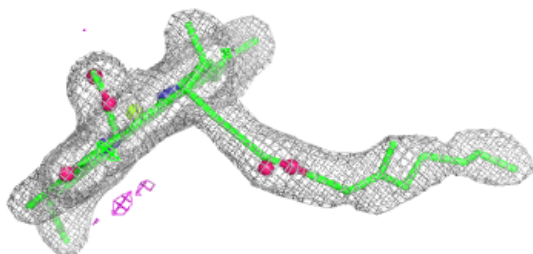
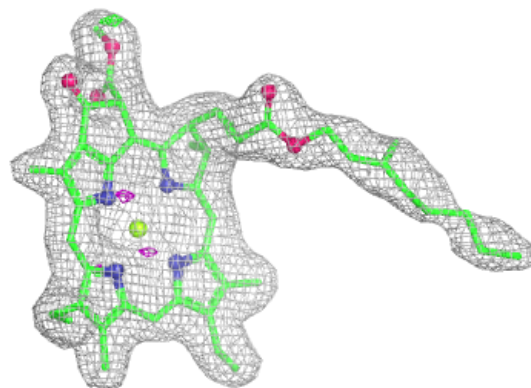


Electron density around CLA b 603:

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

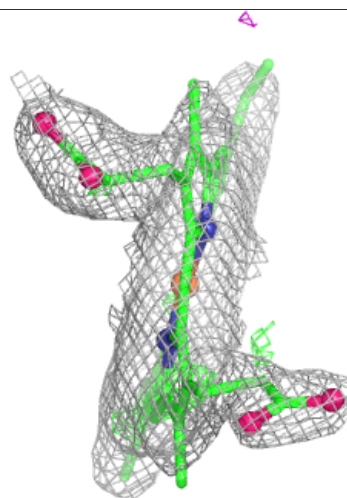
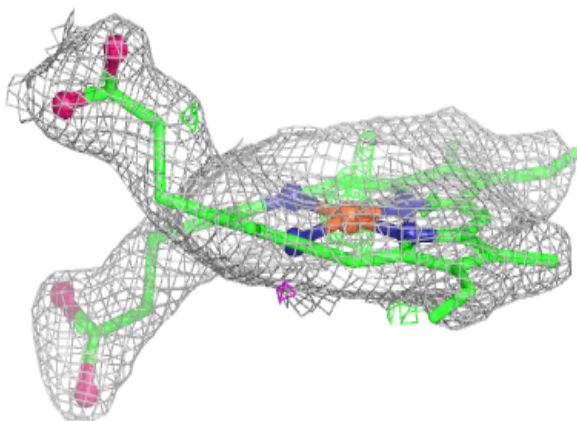
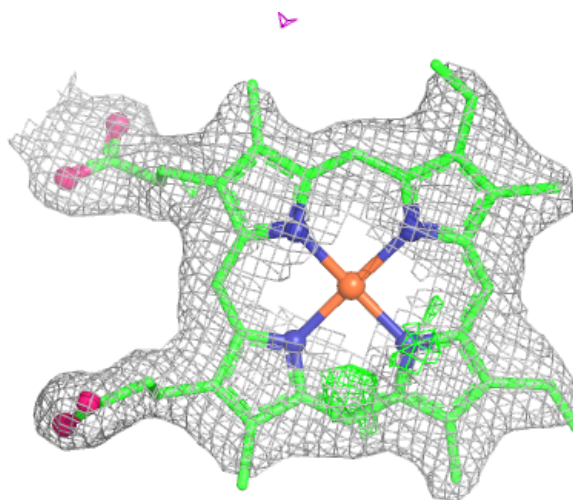
**Electron density around CLA A 609:**

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



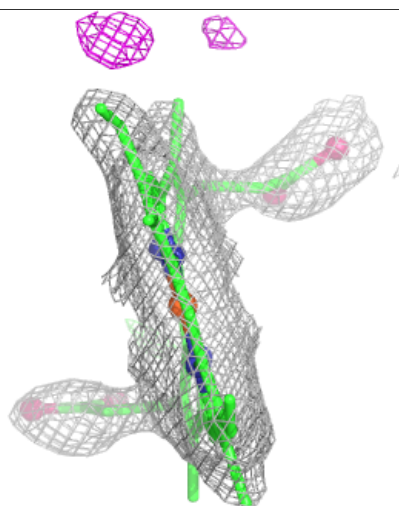
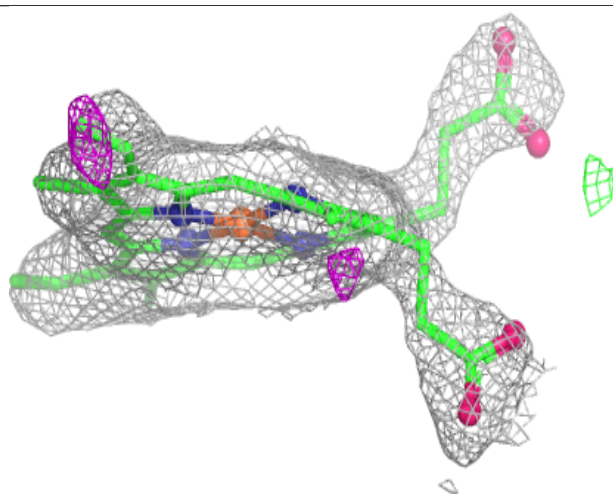
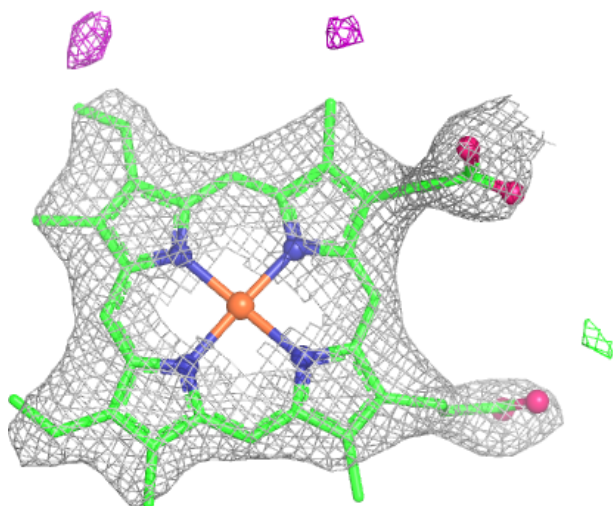
Electron density around HEM F 101:

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



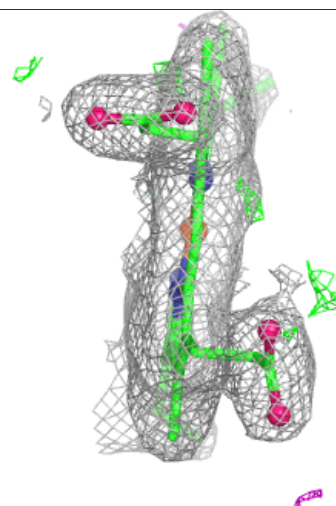
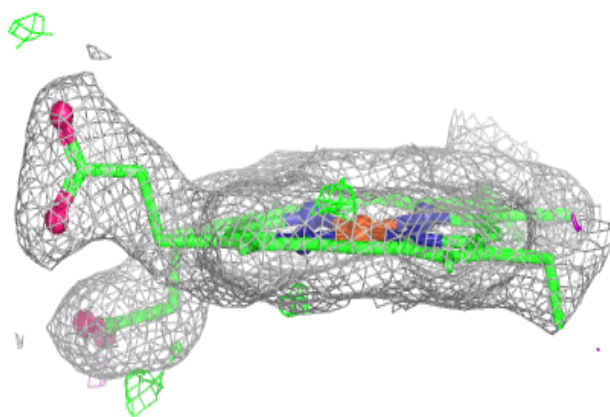
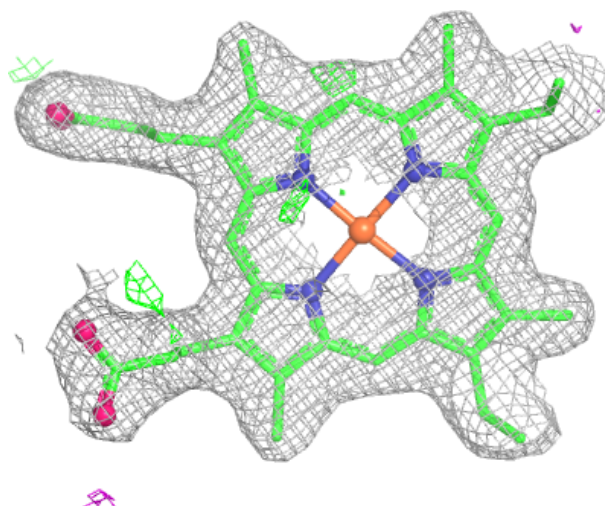
Electron density around HEM e 101:

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



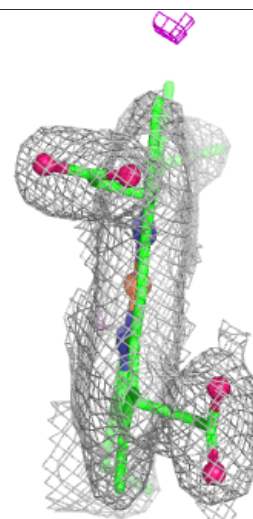
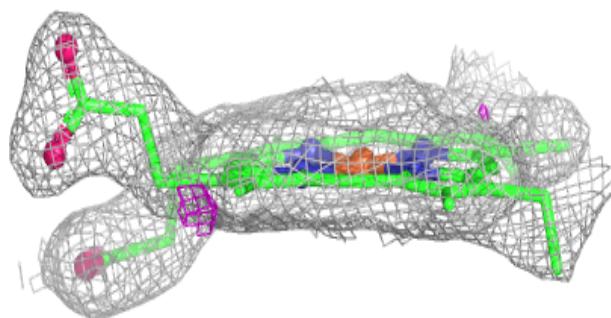
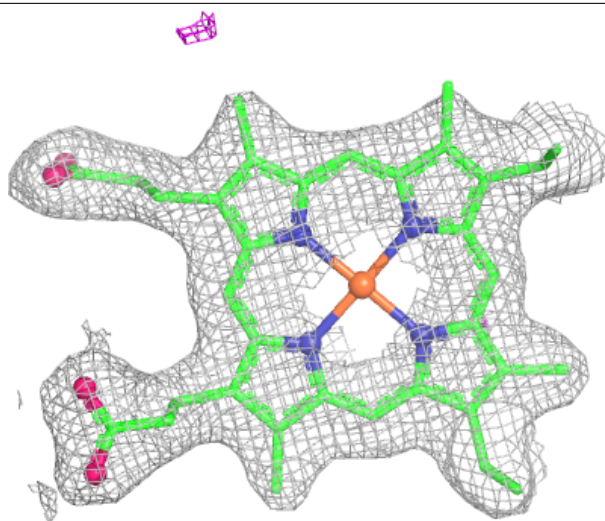
Electron density around HEC V 201:

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



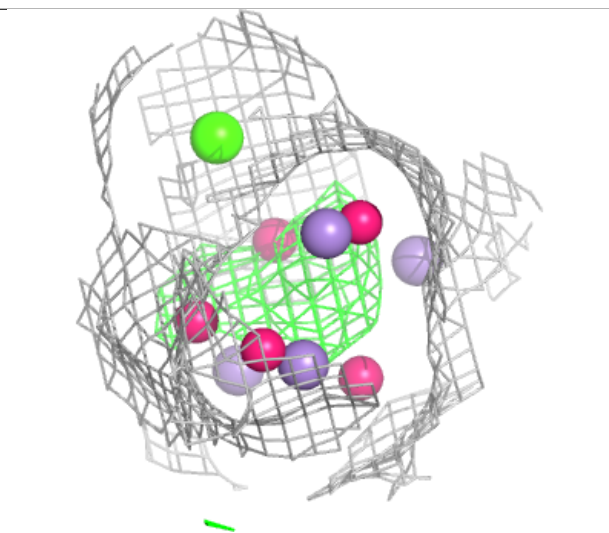
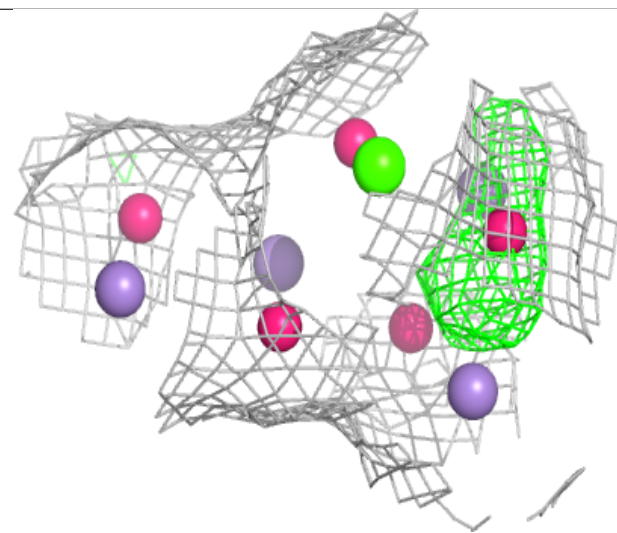
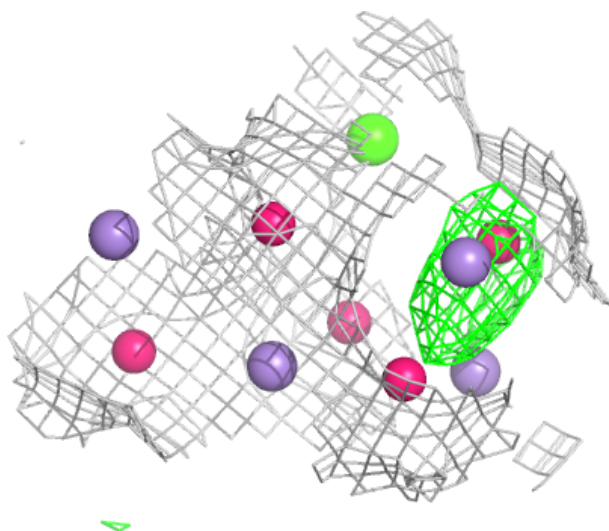
Electron density around HEC v 201:

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



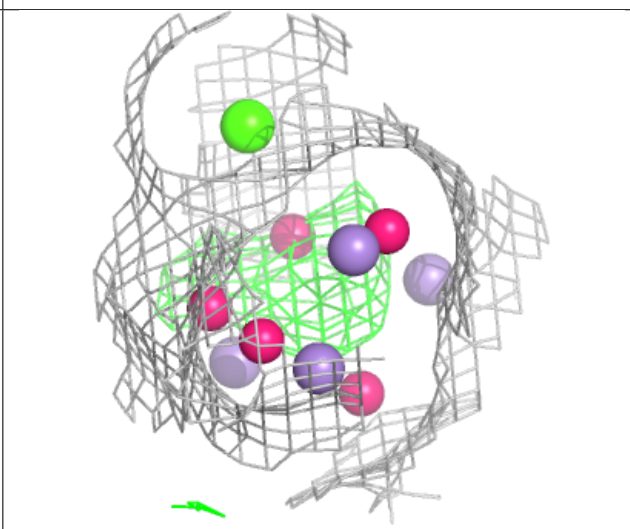
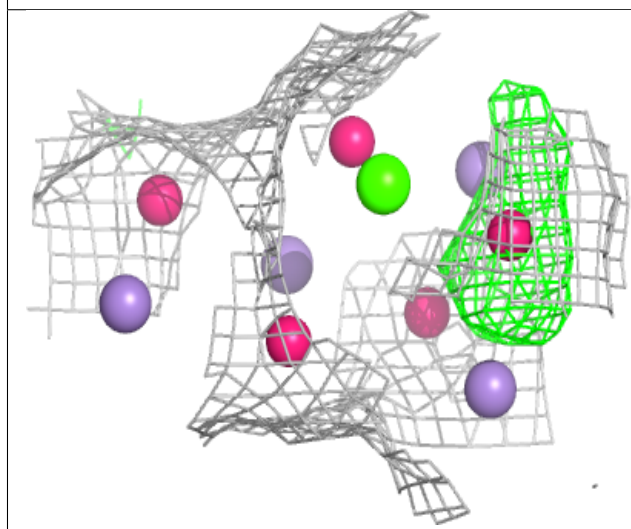
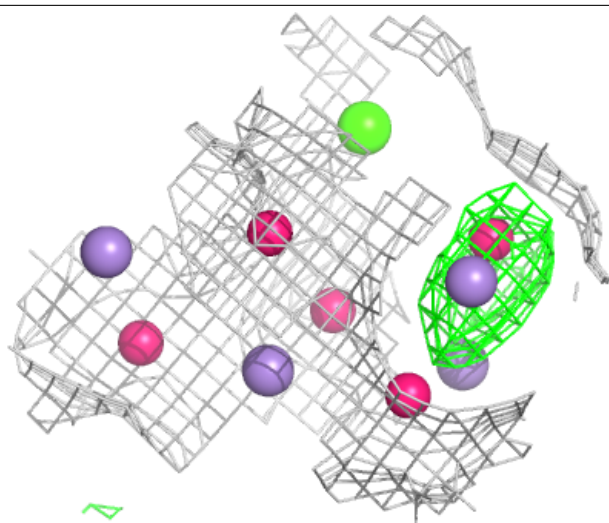
Electron density around OEX A 601 (B):

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



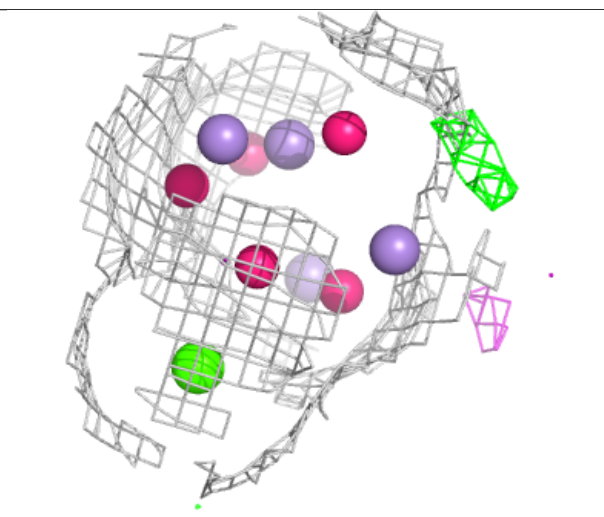
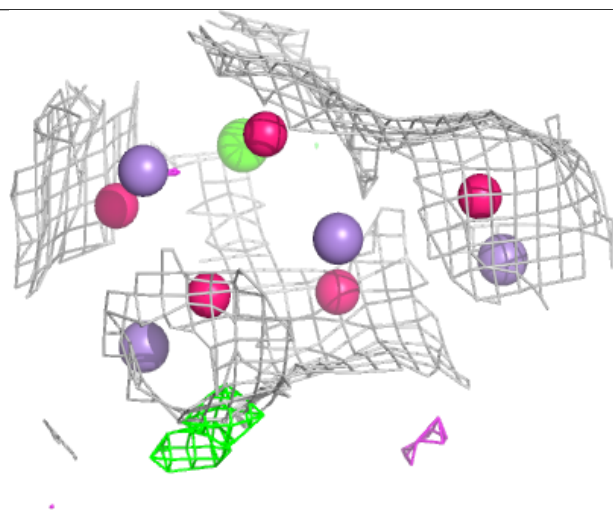
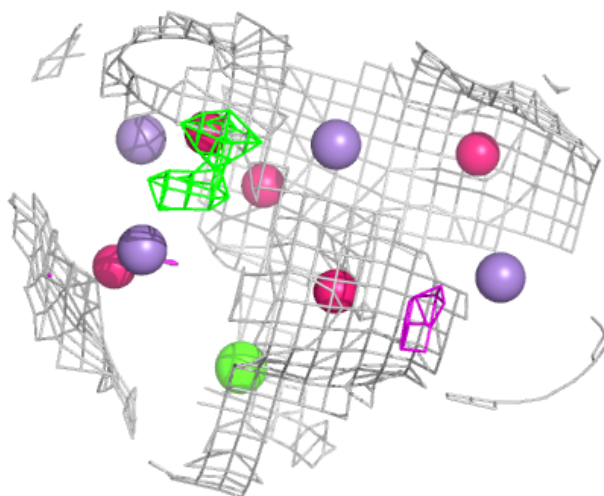
Electron density around OEX A 601 (C):

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



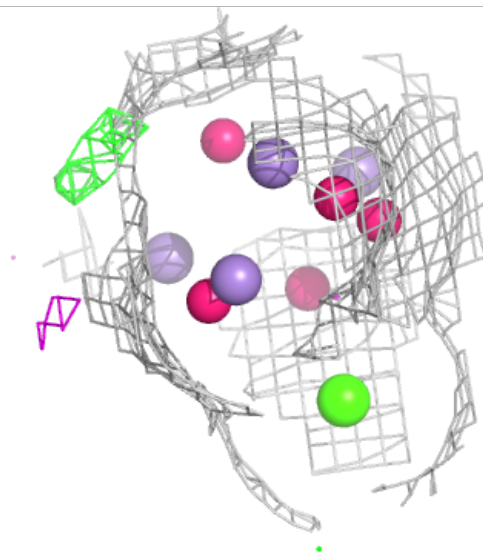
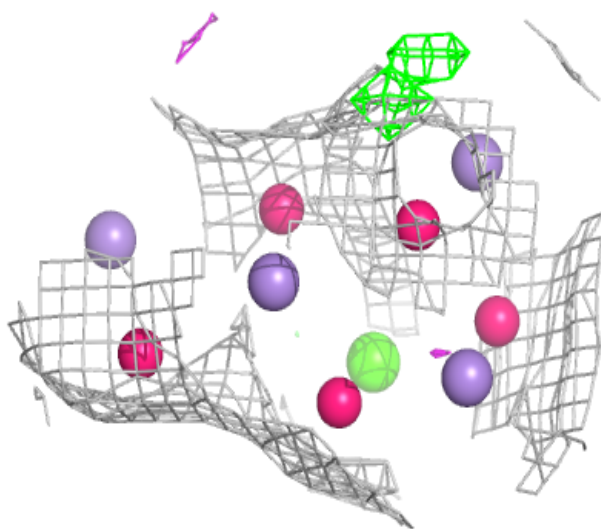
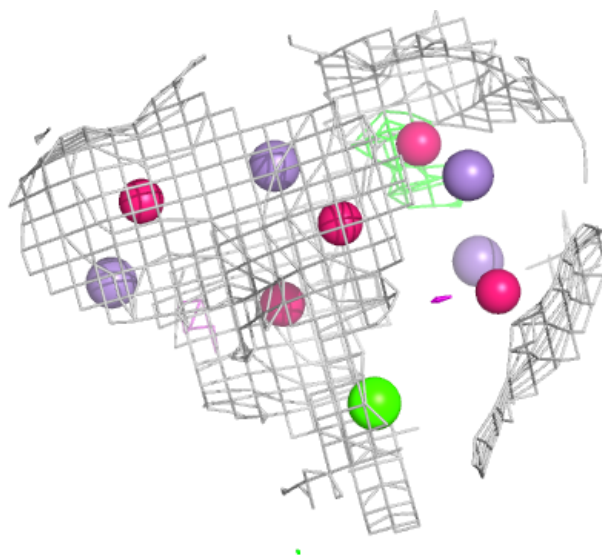
Electron density around OEX a 601 (B):

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



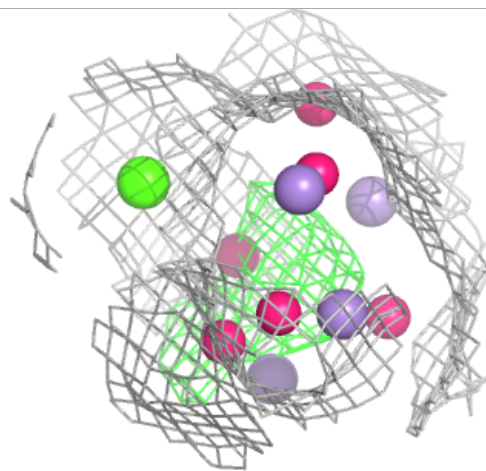
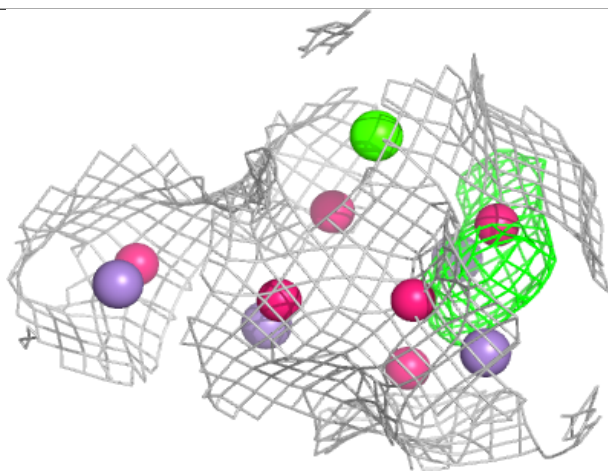
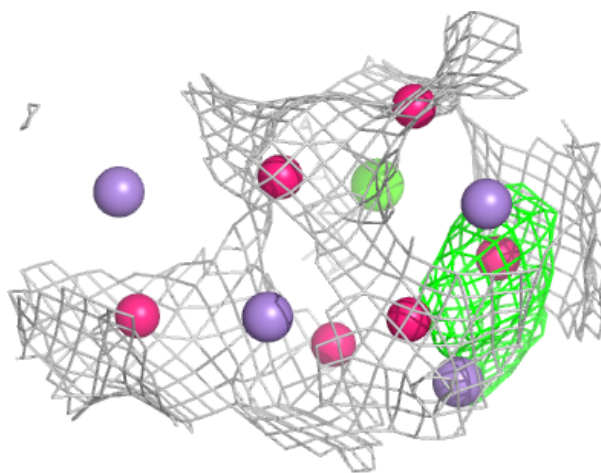
Electron density around OEX a 601 (C):

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



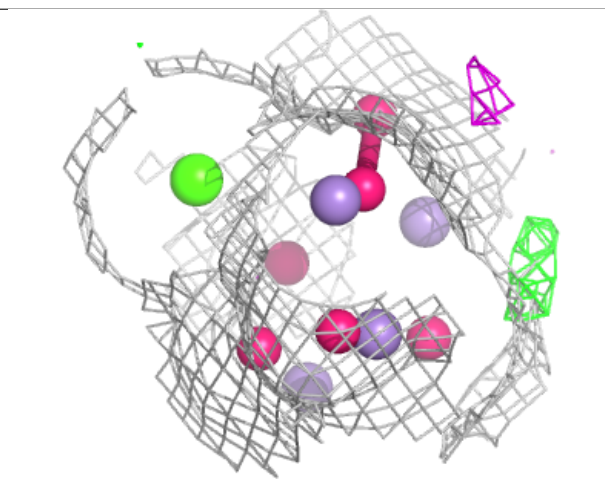
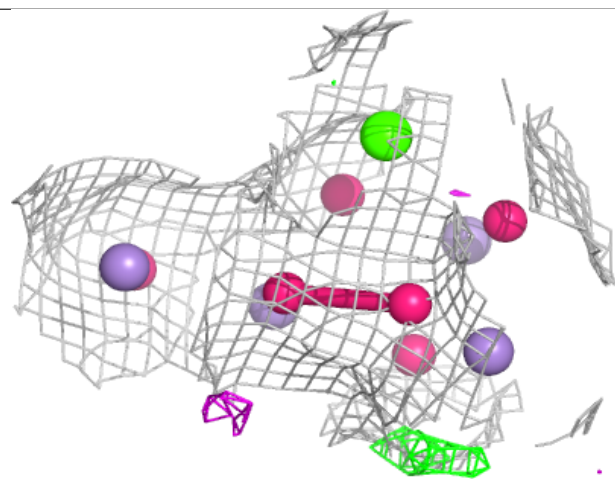
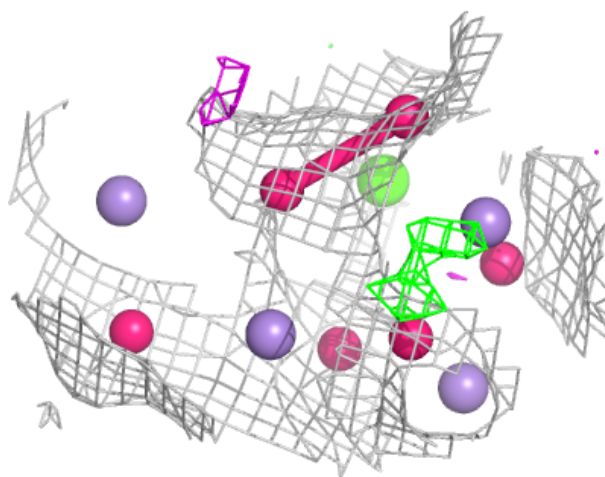
Electron density around OEY A 602 (A):

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



Electron density around OEY a 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.