



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 20, 2026 – 04:20 PM UTC

PDB ID : 6DHF / pdb_00006dhf
Title : RT XFEL structure of the one-flash state of Photosystem II (1F, S2-rich) at 2.08 Angstrom resolution
Authors : Kern, J.; Chatterjee, R.; Young, I.D.; Fuller, F.D.; Lassalle, L.; Ibrahim, M.; Gul, S.; Fransson, T.; Brewster, A.S.; Alonso-Mori, R.; Hussein, R.; Zhang, M.; Douthit, L.; de Lichtenberg, C.; Cheah, M.H.; Shevela, D.; Wersig, J.; Seufert, I.; Sokaras, D.; Pastor, E.; Weninger, C.; Kroll, T.; Sierra, R.G.; Aller, P.; Butryn, A.; Orville, A.M.; Liang, M.; Batyuk, A.; Koglin, J.E.; Carbajo, S.; Boutet, S.; Moriarty, N.W.; Holton, J.M.; Dobbek, H.; Adams, P.D.; Bergmann, U.; Sauter, N.K.; Zouni, A.; Messinger, J.; Yano, J.; Yachandra, V.K.
Deposited on : 2018-05-20
Resolution : 2.08 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

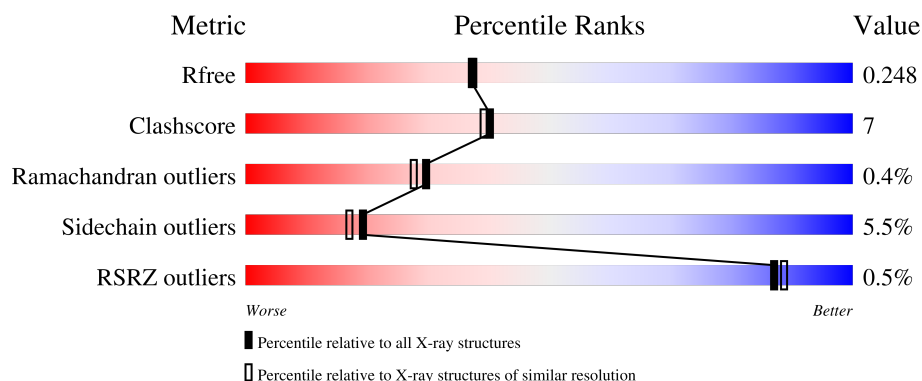
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.08 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	8172 (2.10-2.06)
Clashscore	190562	8714 (2.10-2.06)
Ramachandran outliers	187476	8641 (2.10-2.06)
Sidechain outliers	187428	8642 (2.10-2.06)
RSRZ outliers	180081	8177 (2.10-2.06)

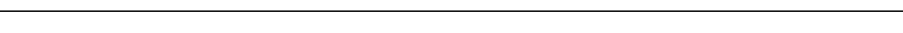
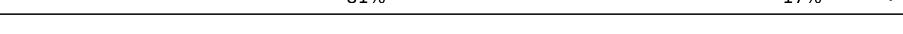
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively.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

Mol	Chain	Length	Quality of chain
1	A	334	

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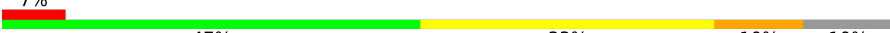
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
 Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
 CCP4 : 9.0.010 (Gargrove)
 Density-Fitness : 1.0.12
 Ideal geometry (proteins) : Engh & Huber (2001)
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
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

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Mol	Chain	Length	Quality of chain
1	a	334	 82% 17% .
2	B	505	 82% 16% .
2	b	505	 84% 15% .
3	C	451	 84% 14% .
3	c	451	 84% 16% .
4	D	341	 85% 15% .
4	d	341	 86% 13% .
5	E	82	 60% 35% . .
5	e	82	 79% 20% .
6	F	34	 3% 76% 24% .
6	f	34	 59% 32% 9% .
7	H	65	 2% 85% 14% .
7	h	65	 75% 20% . .
8	I	36	 83% 14% .
8	i	36	 81% 17% .
9	J	36	 69% 28% .
9	j	36	 3% 72% 25% .
10	K	37	 3% 68% 24% 8% .
10	k	37	 3% 65% 30% 5% .
11	L	37	 86% 14% .
11	l	37	 76% 22% .
12	M	33	 76% 21% .
12	m	33	 79% 18% .
13	O	244	 81% 17% .
13	o	244	 84% 14% . .

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Mol	Chain	Length	Quality of chain
14	T	30	
14	t	30	
15	U	97	
15	u	97	
16	V	137	
16	v	137	
17	Y	30	
17	y	30	
18	X	38	
18	x	38	
19	Z	62	
19	z	62	
20	R	34	
20	r	34	

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
24	CLA	A	405	X	-	-	-
24	CLA	A	406	X	-	-	-
24	CLA	A	408	X	-	-	-
24	CLA	B	601	X	-	-	-
24	CLA	B	602	X	-	-	-
24	CLA	B	604	X	-	-	-
24	CLA	B	605	X	-	-	-
24	CLA	B	606	X	-	-	-
24	CLA	B	607	X	-	-	-
24	CLA	B	610	X	-	-	-
24	CLA	B	612	X	-	-	-
24	CLA	B	613	X	-	-	-
24	CLA	B	614	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	B	615	X	-	-	-
24	CLA	B	616	X	-	-	-
24	CLA	C	502	X	-	-	-
24	CLA	C	503	X	-	-	-
24	CLA	C	504	X	-	-	-
24	CLA	C	505	X	-	-	-
24	CLA	C	506	X	-	-	-
24	CLA	C	508	X	-	-	-
24	CLA	C	510	X	-	-	-
24	CLA	C	511	X	-	-	-
24	CLA	C	512	X	-	-	-
24	CLA	C	513	X	-	-	-
24	CLA	C	514	X	-	-	-
24	CLA	D	402	X	-	-	-
24	CLA	D	403	X	-	-	-
24	CLA	a	404	X	-	-	-
24	CLA	a	407	X	-	-	-
24	CLA	b	603	X	-	-	-
24	CLA	b	604	X	-	-	-
24	CLA	b	605	X	-	-	-
24	CLA	b	606	X	-	-	-
24	CLA	b	607	X	-	-	-
24	CLA	b	608	X	-	-	-
24	CLA	b	609	X	-	-	-
24	CLA	b	610	X	-	-	-
24	CLA	b	611	X	-	-	-
24	CLA	b	612	X	-	-	-
24	CLA	b	613	X	-	-	-
24	CLA	b	614	X	-	-	-
24	CLA	b	615	X	-	-	-
24	CLA	b	616	X	-	-	-
24	CLA	b	617	X	-	-	-
24	CLA	c	501	X	-	-	-
24	CLA	c	502	X	-	-	-
24	CLA	c	503	X	-	-	-
24	CLA	c	504	X	-	-	-
24	CLA	c	505	X	-	-	-
24	CLA	c	506	X	-	-	-
24	CLA	c	507	X	-	-	-
24	CLA	c	509	X	-	-	-
24	CLA	c	510	X	-	-	-
24	CLA	c	511	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	c	512	X	-	-	-
24	CLA	c	513	X	-	-	-
24	CLA	d	403	X	-	-	-
24	CLA	d	404	X	-	-	-
24	CLA	d	405	X	-	-	-
24	CLA	h	101	X	-	-	-
31	UNL	x	101	-	-	X	-

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 103698 atoms, of which 51491 are hydrogens and 0 are deuteriums.

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

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

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

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	505	Total	C	H	N	O	S	0	5	0
			7849	2631	3845	666	694	13			
2	b	505	Total	C	H	N	O	S	0	0	0
			7789	2610	3811	665	690	13			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	442	Total	C	H	N	O	S	0	1	0
			6768	2249	3346	570	590	13			
3	c	451	Total	C	H	N	O	S	0	2	0
			6911	2290	3411	587	610	13			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	81	Total	C	H	N	O	0	1	0
			1309	434	647	106	122			
5	e	82	Total	C	H	N	O	0	0	0
			1311	434	647	108	122			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	65	Total	C	H	N	O	0	0	0
			1030	338	523	82	85			
7	h	63	Total	C	H	N	O	0	0	0
			1016	333	518	80	83			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	36	Total	C	H	N	O	0	0	0
			525	174	268	40	42			
9	j	36	Total	C	H	N	O	0	0	0
			516	172	261	40	42			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	K	37	Total	C	H	N	O	0	1	0
			620	209	318	46	47			

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	244	Total	C	H	N	O	0	1	0
			3730	1174	1850	317	385			
13	o	244	Total	C	H	N	O	0	0	0
			3718	1170	1844	317	383			

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

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

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

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

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
16	V	137	Total	C	H	N	O	S	0	0	0
			2134	675	1070	177	208	4			
16	v	137	Total	C	H	N	O	S	0	0	0
			2134	675	1070	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	H	N	O	S	0	0	0
			404	128	208	35	30	3			
17	y	30	Total	C	H	N	O	S	0	0	0
			459	144	241	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	H	N	O		0	0	0
			593	188	312	45	48				
18	x	38	Total	C	H	N	O		0	0	0
			593	188	312	45	48				

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
19	Z	62	Total	C	H	N	O	S	0	0	0
			988	328	509	72	77	2			
19	z	62	Total	C	H	N	O	S	0	0	0
			986	326	509	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	H	N	O		0	0	0
			569	184	298	47	40				
20	r	31	Total	C	H	N	O		0	0	0
			461	154	234	40	33				

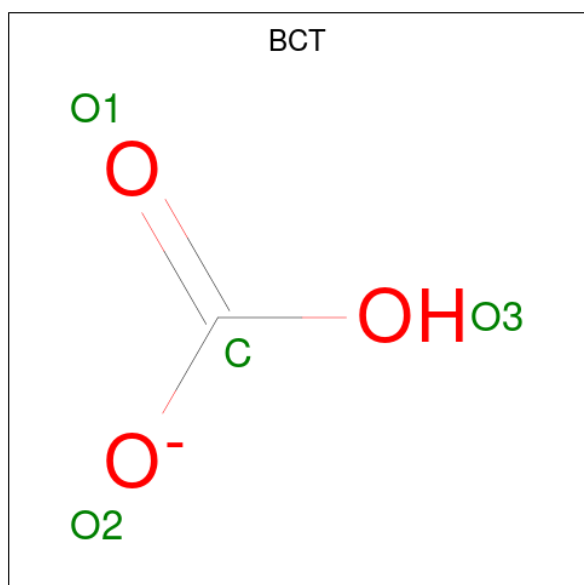
- Molecule 21 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

- Molecule 22 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

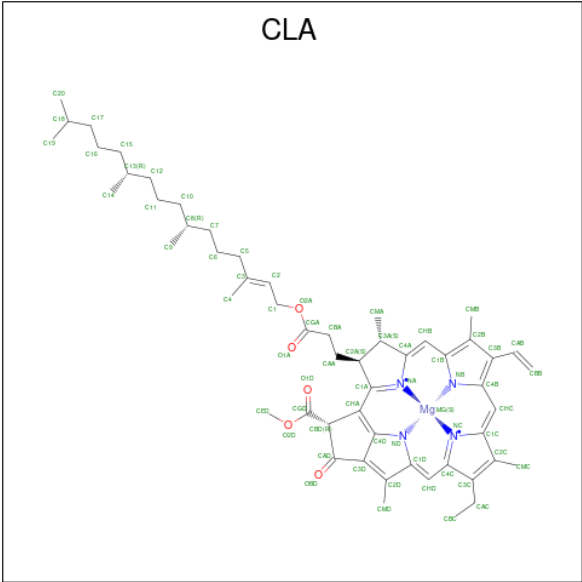
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	2	Total	Cl	0	0
			2	2		
22	a	2	Total	Cl	0	0
			2	2		

- Molecule 23 is BICARBONATE ION (CCD ID: BCT) (formula: CHO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
23	A	1	Total	C	H	O	0	0
			5	1	1	3		
23	d	1	Total	C	H	O	0	0
			5	1	1	3		

- Molecule 24 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
24	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	A	1	Total	C	H	Mg	N	O	0	0
			102	44	48	1	4	5		
24	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
24	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	B	1	Total	C	H	Mg	N	O	0	0
			119	50	59	1	4	5		
24	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	C	1	Total	C	H	Mg	N	O	0	0
			117	49	58	1	4	5		
24	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	D	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	D	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	D	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

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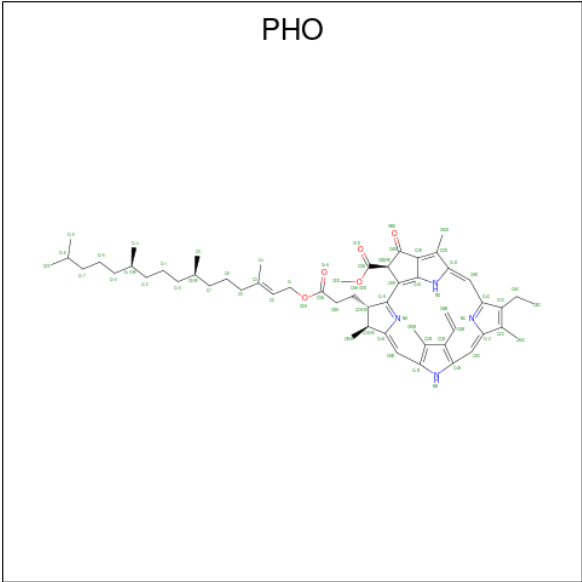
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
24	a	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	a	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	a	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	b	1	Total 137	C 55	H 72	Mg 1	N 4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

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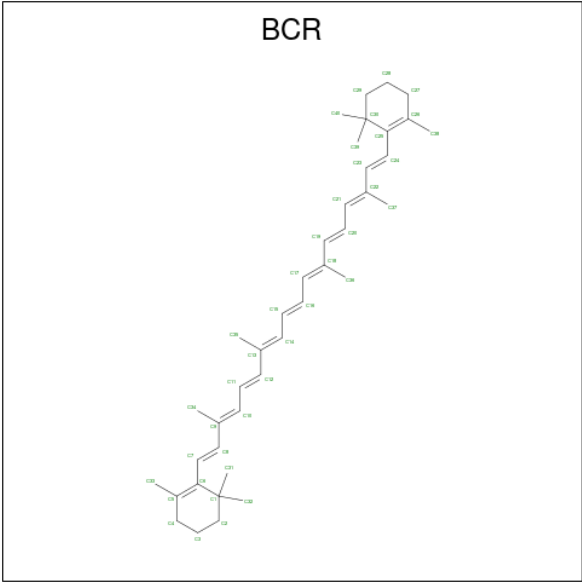
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
24	c	1	Total 119	C 50	H 59	Mg 1	N 4	O 5	0	0
24	c	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	c	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	c	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	c	1	Total 132	C 54	H 68	Mg 1	N 4	O 5	0	0
24	c	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	c	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	c	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	c	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	c	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	d	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	d	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	d	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	h	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0

- Molecule 25 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



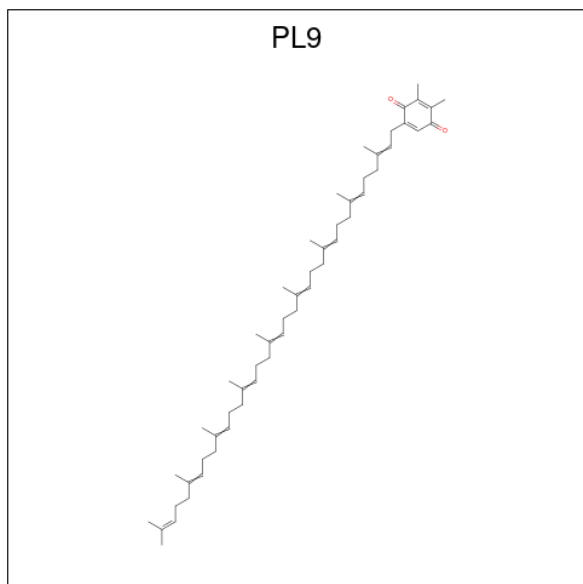
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	A	1	Total	C	H	N	O	0	0
			138	55	74	4	5		
25	D	1	Total	C	H	N	O	0	0
			138	55	74	4	5		
25	a	1	Total	C	H	N	O	0	0
			138	55	74	4	5		
25	d	1	Total	C	H	N	O	0	0
			138	55	74	4	5		

- Molecule 26 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



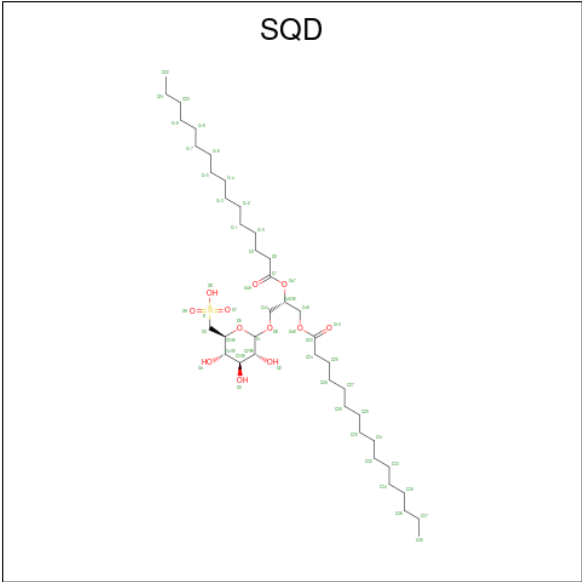
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	A	1	Total	C	H	0	0
			96	40	56		
26	B	1	Total	C	H	0	0
			96	40	56		
26	B	1	Total	C	H	0	0
			96	40	56		
26	B	1	Total	C	H	0	0
			96	40	56		
26	C	1	Total	C	H	0	0
			96	40	56		
26	C	1	Total	C	H	0	0
			96	40	56		
26	D	1	Total	C	H	0	0
			96	40	56		
26	H	1	Total	C	H	0	0
			96	40	56		
26	K	1	Total	C	H	0	0
			96	40	56		
26	Y	1	Total	C	H	0	0
			96	40	56		
26	a	1	Total	C	H	0	0
			96	40	56		
26	b	1	Total	C	H	0	0
			96	40	56		
26	b	1	Total	C	H	0	0
			96	40	56		
26	b	1	Total	C	H	0	0
			96	40	56		
26	b	1	Total	C	H	0	0
			96	40	56		
26	c	1	Total	C	H	0	0
			96	40	56		
26	c	1	Total	C	H	0	0
			96	40	56		
26	c	1	Total	C	H	0	0
			96	40	56		
26	d	1	Total	C	H	0	0
			96	40	56		
26	h	1	Total	C	H	0	0
			96	40	56		
26	k	1	Total	C	H	0	0
			96	40	56		
26	t	1	Total	C	H	0	0
			96	40	56		

- Molecule 27 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: $C_{53}H_{80}O_2$).



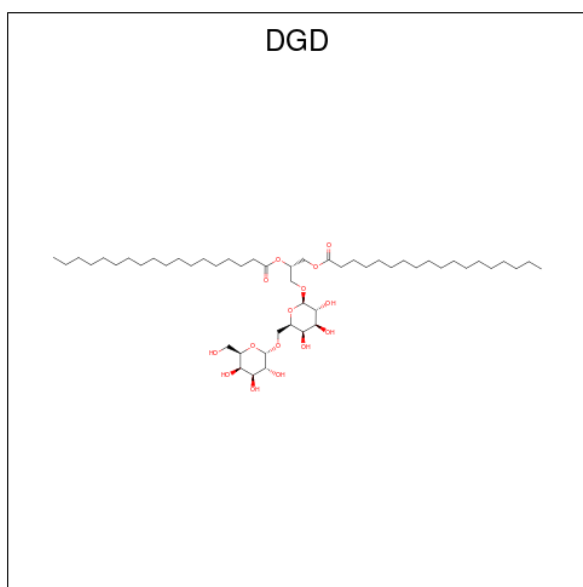
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	A	1	Total	C	H	O	0	0
			135	53	80	2		
27	D	1	Total	C	H	O	0	0
			135	53	80	2		
27	a	1	Total	C	H	O	0	0
			135	53	80	2		
27	d	1	Total	C	H	O	0	0
			135	53	80	2		

- Molecule 28 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



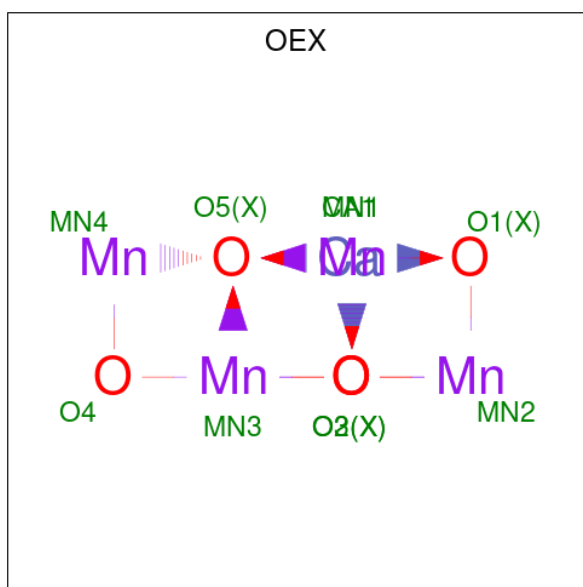
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
28	A	1	Total	C	H	O	S	0	0
			122	39	70	12	1		
28	A	1	Total	C	H	O		0	0
			104	35	65	4			
28	B	1	Total	C	H	O	S	0	0
			132	41	78	12	1		
28	F	1	Total	C	H	O	S	0	0
			81	25	45	10	1		
28	a	1	Total	C	H	O	S	0	0
			132	41	78	12	1		
28	a	1	Total	C	H	O		0	0
			92	31	56	5			
28	b	1	Total	C	H	O	S	0	0
			114	36	65	12	1		
28	f	1	Total	C	H	O	S	0	0
			90	28	49	12	1		

- Molecule 29 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: C₅₁H₉₆O₁₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	A	1	Total	C	H	O	0	0
			162	51	96	15		
29	C	1	Total	C	H	O	0	0
			144	47	82	15		
29	C	1	Total	C	H	O	0	0
			144	47	82	15		
29	C	1	Total	C	H	O	0	0
			144	47	82	15		
29	H	1	Total	C	H	O	0	0
			144	47	82	15		
29	a	1	Total	C	H	O	0	0
			119	39	75	5		
29	c	1	Total	C	H	O	0	0
			144	47	82	15		
29	c	1	Total	C	H	O	0	0
			144	47	82	15		
29	c	1	Total	C	H	O	0	0
			144	47	82	15		
29	h	1	Total	C	H	O	0	0
			144	47	82	15		

- Molecule 30 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5).



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

- Molecule 31 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

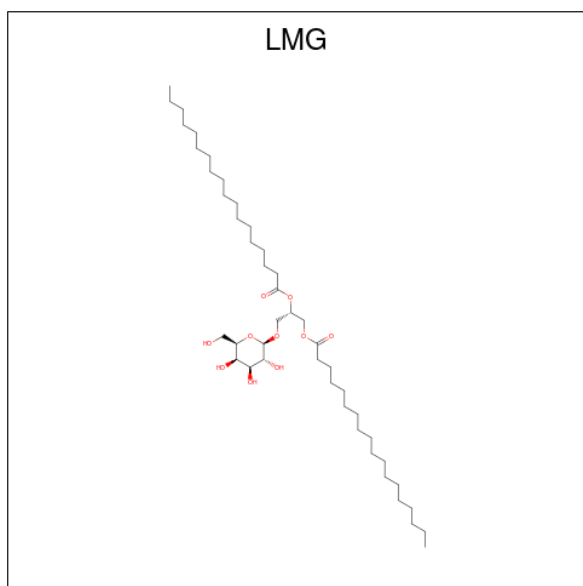
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	B	5	Total	C	H	O	0	0
			192	67	117	8		
31	C	3	Total	C	H	O	0	0
			103	36	63	4		
31	E	1	Total	C	H	O	0	0
			28	10	16	2		
31	H	1	Total	C	H		0	0
			53	18	35			
31	I	1	Total	C	H		0	0
			41	15	26			
31	J	1	Total	C	H	O	0	0
			28	10	16	2		
31	M	3	Total	C	H	O	0	0
			116	41	73	2		
31	T	2	Total	C	H		0	0
			91	31	60			
31	X	1	Total	C	H	O	0	0
			55	18	35	2		
31	a	1	Total	C	H	O	0	0
			28	10	16	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	b	4	Total	C	H	O	0	0
			176	60	110	6		
31	c	2	Total	C	H	O	0	0
			83	28	51	4		
31	d	1	Total	C	H	O	0	0
			43	15	26	2		
31	j	1	Total	C	H	O	0	0
			28	10	16	2		
31	m	1	Total	C	H	O	0	0
			28	10	16	2		
31	t	2	Total	C	H	O	0	0
			60	22	36	2		
31	x	1	Total	C	H	O	0	0
			55	18	35	2		

- Molecule 32 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



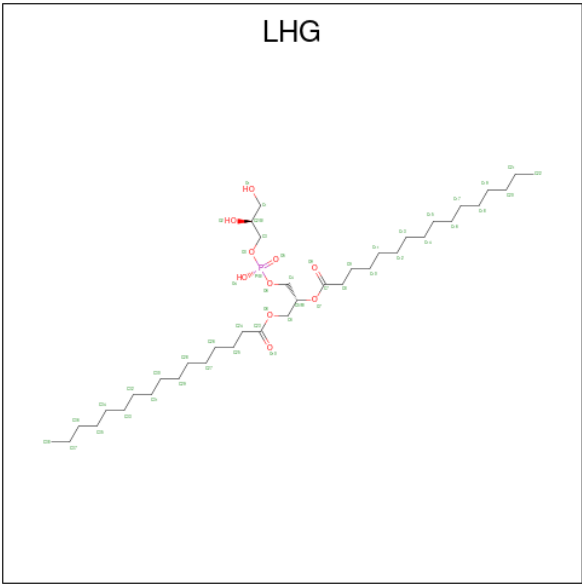
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	B	1	Total	C	H	O	0	0
			68	24	40	4		
32	C	1	Total	C	H	O	0	0
			114	38	66	10		
32	D	1	Total	C	H	O	0	0
			123	41	72	10		
32	D	1	Total	C	H	O	0	0
			78	27	45	6		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	K	1	Total	C	H	O	0	0
			114	38	66	10		
32	M	1	Total	C	H	O	0	0
			123	41	72	10		
32	b	1	Total	C	H	O	0	0
			123	41	72	10		
32	b	1	Total	C	H	O	0	0
			141	45	86	10		
32	c	1	Total	C	H	O	0	0
			81	27	44	10		
32	c	1	Total	C	H	O	0	0
			117	38	69	10		
32	c	1	Total	C	H	O	0	0
			117	39	68	10		
32	d	1	Total	C	H	O	0	0
			102	34	58	10		
32	h	1	Total	C	H	O	0	0
			57	21	34	2		

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



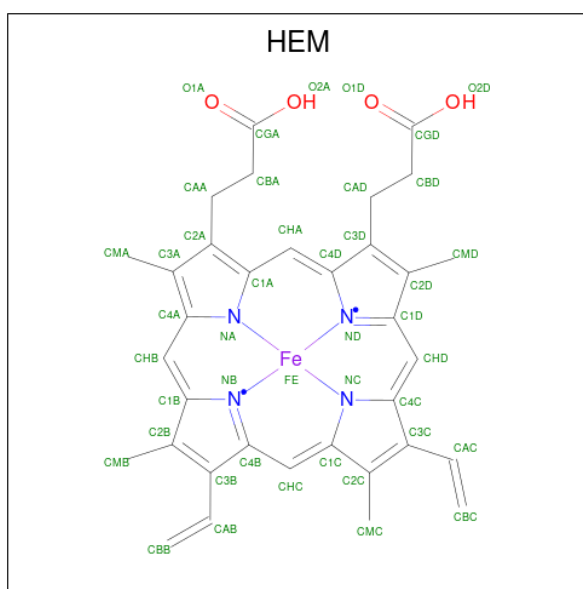
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
33	D	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
33	D	1	Total	C	H	O	P	0	0
			114	36	67	10	1		

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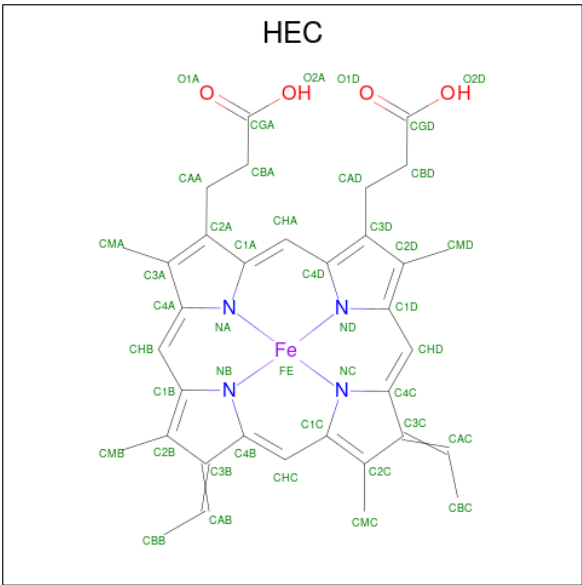
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
33	D	1	Total 123	C 38	H 74	O 10	P 1	0	0
33	E	1	Total 123	C 38	H 74	O 10	P 1	0	0
33	L	1	Total 123	C 38	H 74	O 10	P 1	0	0
33	d	1	Total 123	C 38	H 74	O 10	P 1	0	0
33	d	1	Total 123	C 38	H 74	O 10	P 1	0	0
33	d	1	Total 90	C 28	H 51	O 10	P 1	0	0
33	e	1	Total 99	C 31	H 57	O 10	P 1	0	0
33	l	1	Total 123	C 38	H 74	O 10	P 1	0	0

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



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
34	F	1	Total 73	C 34	Fe 1	H 30	N 4	O 4	0	0
34	e	1	Total 73	C 34	Fe 1	H 30	N 4	O 4	0	0

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



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

- Molecule 36 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	A	141	Total	O	0	0
			141	141		
36	B	218	Total	O	0	0
			218	218		
36	C	197	Total	O	0	0
			197	197		
36	D	138	Total	O	0	0
			138	138		
36	E	29	Total	O	0	0
			29	29		
36	F	14	Total	O	0	0
			14	14		
36	H	26	Total	O	0	0
			26	26		
36	I	16	Total	O	0	0
			16	16		
36	J	12	Total	O	0	0
			12	12		
36	K	2	Total	O	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	L	9	Total 9	O 9	0	0
36	M	5	Total 5	O 5	0	0
36	O	125	Total 125	O 125	0	0
36	T	11	Total 11	O 11	0	0
36	U	52	Total 52	O 52	0	0
36	V	68	Total 68	O 68	0	0
36	Y	5	Total 5	O 5	0	0
36	X	6	Total 6	O 6	0	0
36	Z	3	Total 3	O 3	0	0
36	R	4	Total 4	O 4	0	0
36	a	121	Total 121	O 121	0	0
36	b	187	Total 187	O 187	0	0
36	c	156	Total 156	O 156	0	0
36	d	123	Total 123	O 123	0	0
36	e	22	Total 22	O 22	0	0
36	f	2	Total 2	O 2	0	0
36	h	19	Total 19	O 19	0	0
36	i	10	Total 10	O 10	0	0
36	j	10	Total 10	O 10	0	0
36	k	5	Total 5	O 5	0	0
36	l	9	Total 9	O 9	0	0

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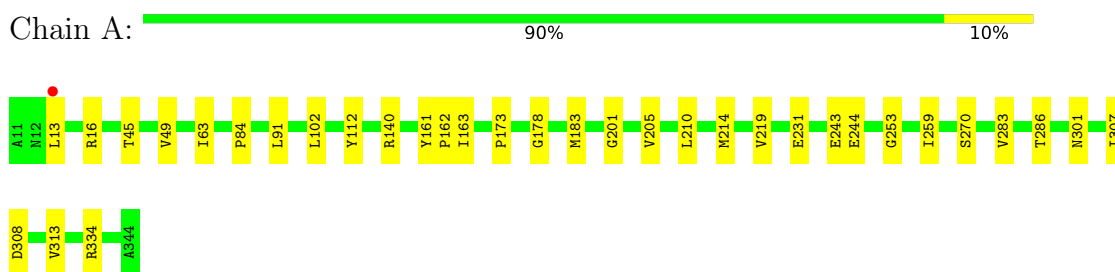
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	m	7	Total 7	O 7	0	0
36	o	113	Total 113	O 113	0	0
36	t	11	Total 11	O 11	0	0
36	u	57	Total 57	O 57	0	0
36	v	62	Total 62	O 62	0	0
36	y	4	Total 4	O 4	0	0
36	x	12	Total 12	O 12	0	0
36	z	1	Total 1	O 1	0	0
36	r	5	Total 5	O 5	0	0

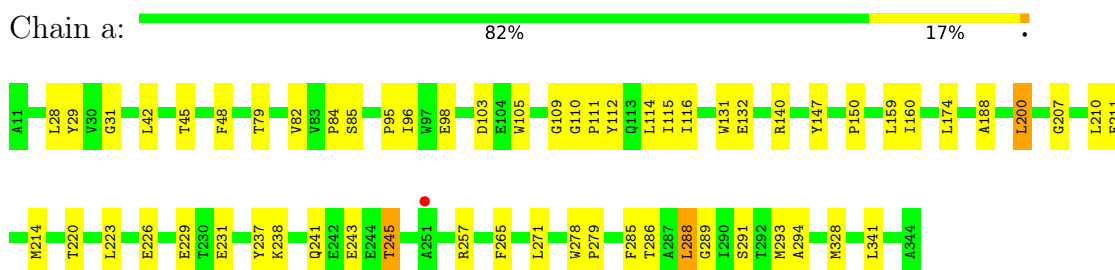
3 Residue-property plots

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

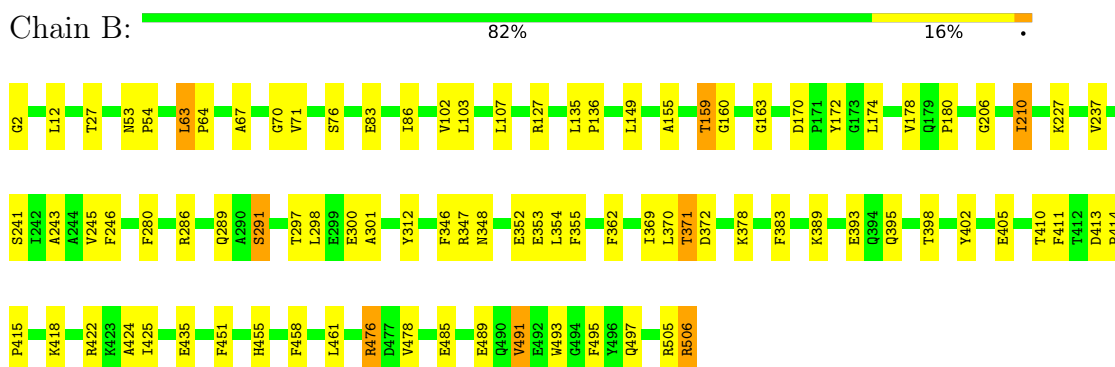
- Molecule 1: Photosystem II protein D1 1



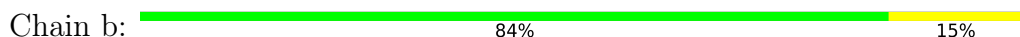
- Molecule 1: Photosystem II protein D1 1

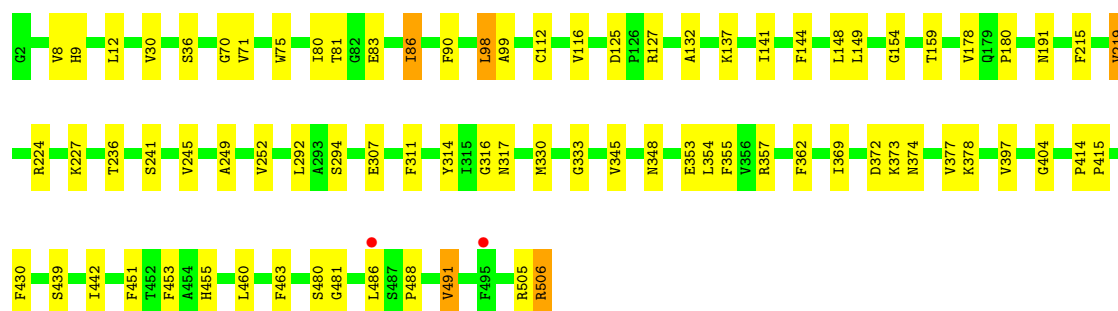


- Molecule 2: Photosystem II CP47 reaction center protein

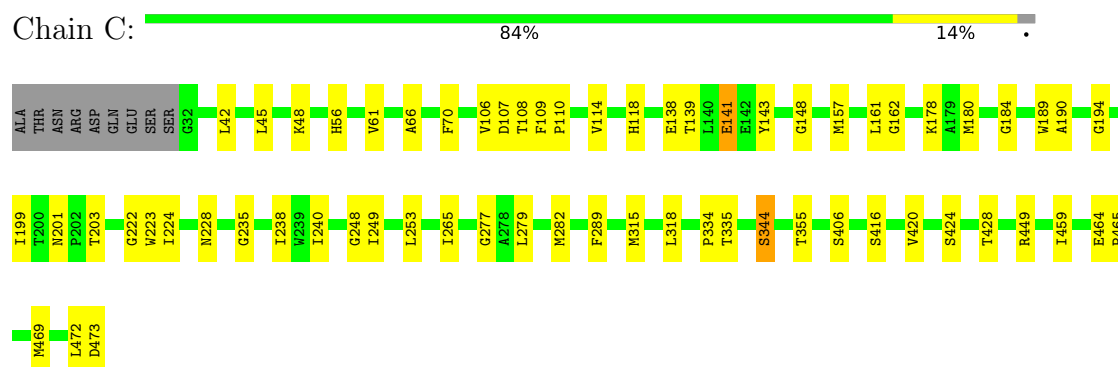


- Molecule 2: Photosystem II CP47 reaction center protein

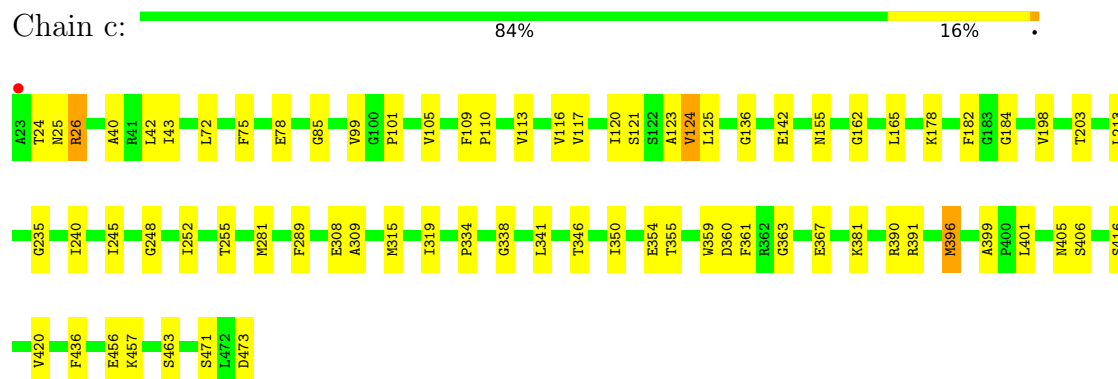




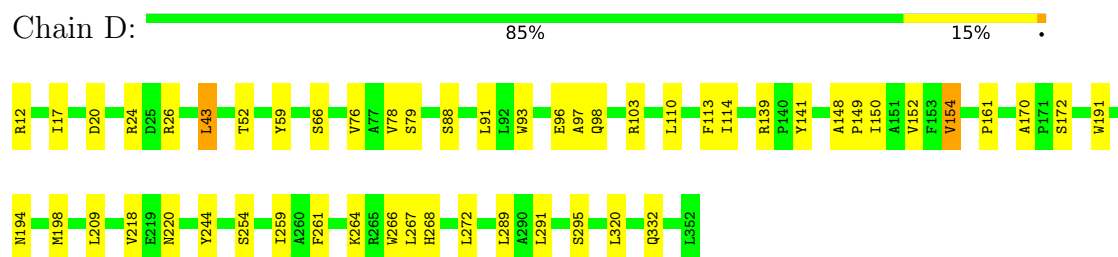
- Molecule 3: Photosystem II CP43 reaction center protein



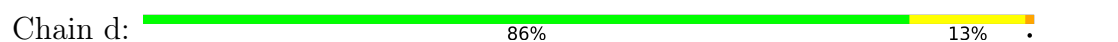
- Molecule 3: Photosystem II CP43 reaction center protein

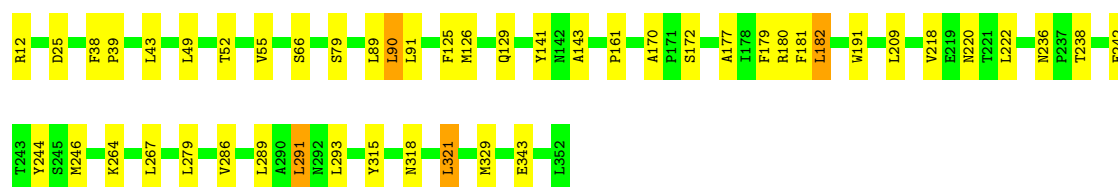


- Molecule 4: Photosystem II D2 protein



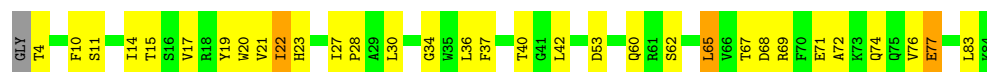
- Molecule 4: Photosystem II D2 protein





- Molecule 5: Cytochrome b559 subunit alpha

Chain E: 60% 35% ..



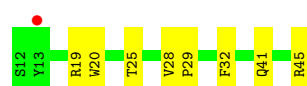
- Molecule 5: Cytochrome b559 subunit alpha

Chain e: 79% 20% .



- Molecule 6: Cytochrome b559 subunit beta

Chain F: 3% 76% 24%



- Molecule 6: Cytochrome b559 subunit beta

Chain f: 59% 32% 9%



- Molecule 7: Photosystem II reaction center protein H

Chain H: 2% 85% 14% .



- Molecule 7: Photosystem II reaction center protein H

Chain h: 75% 20% ..



- Molecule 8: Photosystem II reaction center protein I

Chain I:  83% 14% .



- Molecule 8: Photosystem II reaction center protein I

Chain i:  81% 17% .



- Molecule 9: Photosystem II reaction center protein J

Chain J:  69% 28% .



- Molecule 9: Photosystem II reaction center protein J

Chain j:  3% 72% 25% .



- Molecule 10: Photosystem II reaction center protein K

Chain K:  3% 68% 24% 8% .



- Molecule 10: Photosystem II reaction center protein K

Chain k:  3% 65% 30% 5% .



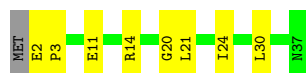
- Molecule 11: Photosystem II reaction center protein L

Chain L:  86% 14% .



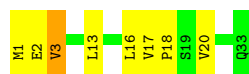
- Molecule 11: Photosystem II reaction center protein L

Chain l:  76% 22% .



- Molecule 12: Photosystem II reaction center protein M

Chain M:  76% 21% .



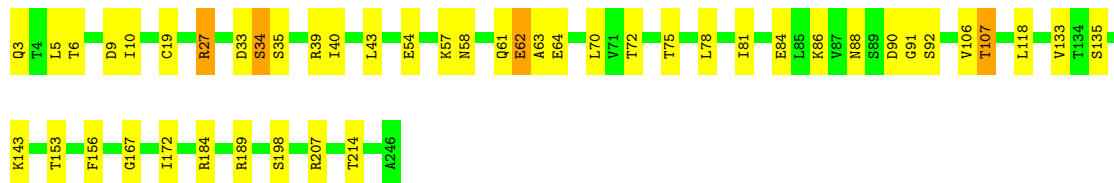
- Molecule 12: Photosystem II reaction center protein M

Chain m:  79% 18% .



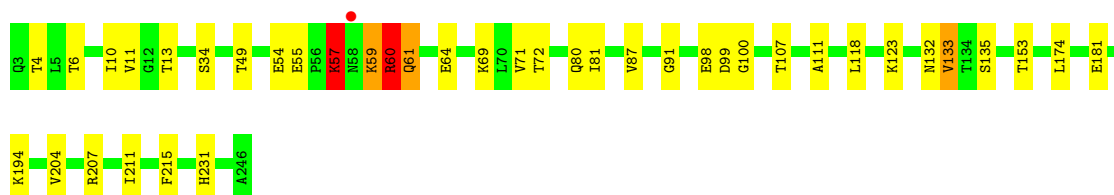
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:  81% 17% .



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:  84% 14% ..



- Molecule 14: Photosystem II reaction center protein T

Chain T:  83% 13% .



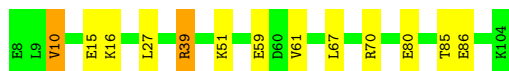
- Molecule 14: Photosystem II reaction center protein T

Chain t:  3% 83% 17%



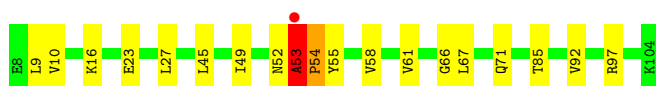
- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U: 87% 11% .



- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u: 80% 18% ..



- Molecule 16: Cytochrome c-550

Chain V: 79% 19% .



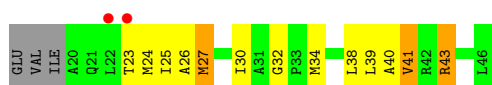
- Molecule 16: Cytochrome c-550

Chain v: 77% 22% .



- Molecule 17: Photosystem II reaction center protein Ycf12

Chain Y: 7% 47% 33% 10% 10%



- Molecule 17: Photosystem II reaction center protein Ycf12

Chain y: 60% 37% .



- Molecule 18: Photosystem II reaction center X protein

Chain X: 3% 84% 16%

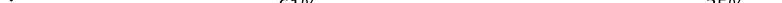


- Molecule 18: Photosystem II reaction center X protein

Chain x: 82% 18%

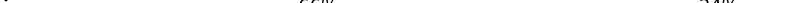


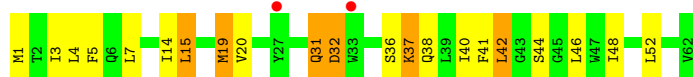
- Molecule 19: Photosystem II reaction center protein Z

Chain Z:  3% 61% 35%

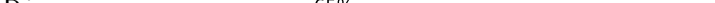


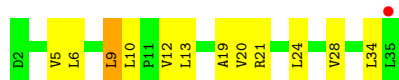
- Molecule 19: Photosystem II reaction center protein Z

Chain z:  3% 66% 24% 10%

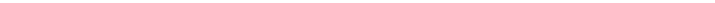


- Molecule 20: Photosystem II protein Y

Chain R:  3% 65% 32%



- Molecule 20: Photosystem II protein Y

Chain r: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	116.82Å 220.89Å 307.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.43 – 2.08 30.43 – 2.08	Depositor EDS
% Data completeness (in resolution range)	99.7 (30.43-2.08) 86.9 (30.43-2.08)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.56 (at 2.08Å)	Xtriage
Refinement program	PHENIX dev_svn	Depositor
R, R_{free}	0.189 , 0.247 0.189 , 0.248	Depositor DCC
R_{free} test set	4194 reflections (0.71%)	wwPDB-VP
Wilson B-factor (Å ²)	27.1	Xtriage
Anisotropy	0.298	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 62.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	103698	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.59% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.64	0/2707	0.73	0/3692
1	a	0.63	0/2704	0.73	1/3688 (0.0%)
2	B	0.60	0/4160	0.68	0/5668
2	b	0.57	0/4118	0.67	0/5611
3	C	0.59	0/3538	0.66	0/4818
3	c	0.53	0/3619	0.65	0/4926
4	D	0.63	0/2812	0.71	0/3832
4	d	0.57	0/2821	0.67	0/3844
5	E	0.43	0/684	0.61	0/935
5	e	0.41	0/683	0.57	0/932
6	F	0.47	0/284	0.59	0/387
6	f	0.42	0/284	0.63	0/387
7	H	0.58	0/520	0.70	0/709
7	h	0.51	0/511	0.61	0/697
8	I	0.60	0/293	0.74	0/396
8	i	0.67	0/293	0.72	0/396
9	J	0.45	0/263	0.65	0/356
9	j	0.40	0/261	0.54	0/353
10	K	0.44	0/314	0.58	0/427
10	k	0.38	0/303	0.50	0/416
11	L	0.65	0/311	0.67	0/422
11	l	0.66	0/303	0.68	0/412
12	M	0.57	0/249	0.69	0/341
12	m	0.64	0/244	0.67	0/334
13	O	0.56	0/1914	0.69	0/2596
13	o	0.55	0/1905	0.70	0/2583
14	T	0.63	0/257	0.76	0/349
14	t	0.63	0/255	0.67	0/346
15	U	0.51	0/785	0.63	0/1064
15	u	0.58	0/785	0.69	0/1064
16	V	0.54	0/1085	0.64	0/1473
16	v	0.49	0/1085	0.62	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	Y	0.40	0/197	0.60	0/264
17	y	0.29	0/219	0.47	0/294
18	X	0.46	0/284	0.59	0/384
18	x	0.35	0/284	0.48	0/384
19	Z	0.43	0/490	0.55	0/669
19	z	0.32	0/488	0.48	0/666
20	R	0.37	0/277	0.53	0/380
20	r	0.32	0/233	0.51	0/323
All	All	0.56	0/42822	0.67	1/58291 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
15	u	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	110	GLY	O-C-N	9.17	124.37	121.07

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
15	u	53	ALA	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2622	2508	2519	22	0
1	a	2619	2499	2510	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	4004	3845	3864	56	0
2	b	3978	3811	3836	52	0
3	C	3422	3346	3359	38	0
3	c	3500	3411	3426	42	0
4	D	2717	2613	2621	37	0
4	d	2723	2619	2627	35	0
5	E	662	647	648	24	0
5	e	664	647	648	14	0
6	F	275	281	282	7	0
6	f	275	281	282	12	0
7	H	507	523	523	5	0
7	h	498	518	518	9	0
8	I	296	311	311	2	0
8	i	296	311	311	4	0
9	J	257	268	268	10	0
9	j	255	261	261	10	0
10	K	302	318	318	12	0
10	k	293	305	305	10	0
11	L	304	316	316	5	0
11	l	296	304	304	3	0
12	M	256	269	269	6	0
12	m	251	267	267	5	0
13	O	1880	1850	1852	30	0
13	o	1874	1844	1846	23	0
14	T	258	261	261	3	0
14	t	256	256	256	4	0
15	U	774	772	773	6	0
15	u	774	772	773	11	0
16	V	1064	1070	1073	15	0
16	v	1064	1070	1073	17	0
17	Y	196	208	217	9	0
17	y	218	241	241	5	0
18	X	281	312	312	4	0
18	x	281	312	312	5	0
19	Z	479	509	516	12	0
19	z	477	509	509	10	0
20	R	271	298	298	6	0
20	r	227	234	224	11	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	A	2	0	0	0	0
22	a	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	A	4	1	1	0	0
23	d	4	1	1	0	0
24	A	184	192	192	1	0
24	B	1035	1139	1139	18	0
24	C	839	922	922	12	0
24	D	195	216	216	3	0
24	a	195	216	216	2	0
24	b	970	1067	1067	26	0
24	c	839	919	919	7	0
24	d	195	216	216	3	0
24	h	65	72	72	4	0
25	A	64	74	74	0	0
25	D	64	74	74	1	0
25	a	64	74	74	1	0
25	d	64	74	74	1	0
26	A	40	56	56	1	0
26	B	120	168	168	8	0
26	C	80	112	112	3	0
26	D	40	56	56	5	0
26	H	40	56	56	1	0
26	K	40	56	56	4	0
26	Y	40	56	56	3	0
26	a	40	56	56	1	0
26	b	160	224	224	11	0
26	c	120	168	168	4	0
26	d	40	56	56	2	0
26	h	40	56	56	4	0
26	k	40	56	56	0	0
26	t	40	56	56	6	0
27	A	55	80	80	0	0
27	D	55	80	80	1	0
27	a	55	80	80	3	0
27	d	55	80	80	0	0
28	A	91	135	135	2	0
28	B	54	78	78	3	0
28	F	36	45	46	1	0
28	a	90	134	133	3	0
28	b	49	65	65	0	0
28	f	41	49	48	4	0
29	A	66	96	96	2	0
29	C	186	246	245	0	0
29	H	62	82	82	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	a	44	75	75	1	0
29	c	186	246	244	1	0
29	h	62	82	82	1	0
30	A	10	0	0	0	0
30	a	10	0	0	0	0
31	B	75	117	0	2	0
31	C	40	63	0	0	0
31	E	12	16	0	0	0
31	H	18	35	0	0	0
31	I	15	26	0	0	0
31	J	12	16	0	0	0
31	M	43	73	0	0	0
31	T	31	60	0	0	0
31	X	20	35	0	0	0
31	a	12	16	0	0	0
31	b	66	110	0	0	0
31	c	32	51	0	1	0
31	d	17	26	0	1	0
31	j	12	16	0	0	0
31	m	12	16	0	0	0
31	t	24	36	0	0	0
31	x	20	35	0	2	0
32	B	28	40	40	0	0
32	C	48	66	66	0	0
32	D	84	117	116	0	0
32	K	48	66	66	0	0
32	M	51	72	72	1	0
32	b	106	158	158	2	0
32	c	134	181	181	4	0
32	d	44	58	58	0	0
32	h	23	34	34	0	0
33	D	145	215	215	5	0
33	E	49	74	74	2	0
33	L	49	74	74	1	0
33	d	137	199	199	5	0
33	e	42	57	57	0	0
33	l	49	74	74	1	0
34	F	43	30	30	4	0
34	e	43	30	30	5	0
35	V	43	30	30	1	0
35	v	43	30	30	2	0
36	A	141	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	B	218	0	0	9	0
36	C	197	0	0	4	0
36	D	138	0	0	6	0
36	E	29	0	0	0	0
36	F	14	0	0	1	0
36	H	26	0	0	0	0
36	I	16	0	0	0	0
36	J	12	0	0	2	0
36	K	2	0	0	0	0
36	L	9	0	0	2	0
36	M	5	0	0	0	0
36	O	125	0	0	11	0
36	R	4	0	0	0	0
36	T	11	0	0	0	0
36	U	52	0	0	2	0
36	V	68	0	0	2	0
36	X	6	0	0	0	0
36	Y	5	0	0	0	0
36	Z	3	0	0	0	0
36	a	121	0	0	1	0
36	b	187	0	0	10	0
36	c	156	0	0	7	0
36	d	123	0	0	5	0
36	e	22	0	0	1	0
36	f	2	0	0	1	0
36	h	19	0	0	0	0
36	i	10	0	0	1	0
36	j	10	0	0	1	0
36	k	5	0	0	2	0
36	l	9	0	0	0	0
36	m	7	0	0	1	0
36	o	113	0	0	5	0
36	r	5	0	0	2	0
36	t	11	0	0	1	0
36	u	57	0	0	1	0
36	v	62	0	0	1	0
36	x	12	0	0	0	0
36	y	4	0	0	0	0
36	z	1	0	0	0	0
All	All	52207	51491	50871	668	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 7.

The worst 5 of 668 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)
2:B:497:GLN:OE1	36:B:701:HOH:O	1.85	0.94
2:B:2:GLY:N	36:L:201:HOH:O	2.01	0.94
4:D:332:GLN:NE2	36:D:501:HOH:O	2.04	0.90
4:d:12:ARG:N	36:d:501:HOH:O	2.04	0.90
2:B:410:THR:O	36:B:702:HOH:O	1.91	0.89

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	332/334 (99%)	325 (98%)	6 (2%)	1 (0%)	36	36
1	a	332/334 (99%)	324 (98%)	8 (2%)	0	100	100
2	B	508/505 (101%)	494 (97%)	14 (3%)	0	100	100
2	b	503/505 (100%)	491 (98%)	10 (2%)	2 (0%)	30	28
3	C	441/451 (98%)	428 (97%)	12 (3%)	1 (0%)	43	44
3	c	451/451 (100%)	433 (96%)	15 (3%)	3 (1%)	18	14
4	D	339/341 (99%)	328 (97%)	11 (3%)	0	100	100
4	d	340/341 (100%)	325 (96%)	15 (4%)	0	100	100
5	E	80/82 (98%)	76 (95%)	4 (5%)	0	100	100
5	e	80/82 (98%)	77 (96%)	3 (4%)	0	100	100
6	F	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
6	f	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
7	H	63/65 (97%)	58 (92%)	5 (8%)	0	100	100
7	h	61/65 (94%)	55 (90%)	5 (8%)	1 (2%)	7	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	I	34/36 (94%)	32 (94%)	2 (6%)	0	100	100
8	i	34/36 (94%)	31 (91%)	3 (9%)	0	100	100
9	J	34/36 (94%)	31 (91%)	2 (6%)	1 (3%)	3	1
9	j	34/36 (94%)	31 (91%)	3 (9%)	0	100	100
10	K	35/37 (95%)	34 (97%)	0	1 (3%)	3	1
10	k	35/37 (95%)	35 (100%)	0	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	34/37 (92%)	33 (97%)	1 (3%)	0	100	100
12	M	31/33 (94%)	31 (100%)	0	0	100	100
12	m	30/33 (91%)	29 (97%)	1 (3%)	0	100	100
13	O	243/244 (100%)	228 (94%)	13 (5%)	2 (1%)	16	12
13	o	242/244 (99%)	228 (94%)	11 (4%)	3 (1%)	10	6
14	T	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
14	t	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
15	U	95/97 (98%)	92 (97%)	3 (3%)	0	100	100
15	u	95/97 (98%)	89 (94%)	4 (4%)	2 (2%)	5	2
16	V	135/137 (98%)	130 (96%)	5 (4%)	0	100	100
16	v	135/137 (98%)	126 (93%)	9 (7%)	0	100	100
17	Y	25/30 (83%)	20 (80%)	3 (12%)	2 (8%)	1	0
17	y	28/30 (93%)	25 (89%)	3 (11%)	0	100	100
18	X	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
18	x	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	54 (90%)	6 (10%)	0	100	100
19	z	60/62 (97%)	53 (88%)	6 (10%)	1 (2%)	7	3
20	R	32/34 (94%)	30 (94%)	2 (6%)	0	100	100
20	r	29/34 (85%)	23 (79%)	5 (17%)	1 (3%)	3	1
All	All	5237/5326 (98%)	5019 (96%)	197 (4%)	21 (0%)	30	28

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
10	K	16	ALA

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Mol	Chain	Res	Type
13	O	62	GLU
17	Y	41	VAL
3	c	416	SER

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	270/270 (100%)	264 (98%)	6 (2%)	45	51
1	a	269/270 (100%)	257 (96%)	12 (4%)	24	24
2	B	407/403 (101%)	385 (95%)	22 (5%)	20	17
2	b	402/403 (100%)	387 (96%)	15 (4%)	30	31
3	C	345/352 (98%)	335 (97%)	10 (3%)	37	40
3	c	354/352 (101%)	336 (95%)	18 (5%)	21	20
4	D	276/276 (100%)	271 (98%)	5 (2%)	51	58
4	d	277/276 (100%)	270 (98%)	7 (2%)	42	46
5	E	72/72 (100%)	63 (88%)	9 (12%)	4	2
5	e	71/72 (99%)	68 (96%)	3 (4%)	26	26
6	F	28/28 (100%)	27 (96%)	1 (4%)	31	32
6	f	28/28 (100%)	23 (82%)	5 (18%)	2	1
7	H	53/54 (98%)	50 (94%)	3 (6%)	18	16
7	h	53/54 (98%)	51 (96%)	2 (4%)	29	30
8	I	32/32 (100%)	29 (91%)	3 (9%)	8	5
8	i	32/32 (100%)	31 (97%)	1 (3%)	35	38
9	J	24/24 (100%)	23 (96%)	1 (4%)	26	26
9	j	23/24 (96%)	20 (87%)	3 (13%)	4	2
10	K	31/30 (103%)	28 (90%)	3 (10%)	8	5
10	k	30/30 (100%)	25 (83%)	5 (17%)	2	1
11	L	35/35 (100%)	34 (97%)	1 (3%)	37	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	l	34/35 (97%)	31 (91%)	3 (9%)	9	6
12	M	28/29 (97%)	24 (86%)	4 (14%)	3	1
12	m	28/29 (97%)	27 (96%)	1 (4%)	31	32
13	O	208/207 (100%)	194 (93%)	14 (7%)	15	11
13	o	207/207 (100%)	193 (93%)	14 (7%)	14	11
14	T	26/26 (100%)	23 (88%)	3 (12%)	5	3
14	t	25/26 (96%)	25 (100%)	0	100	100
15	U	84/84 (100%)	78 (93%)	6 (7%)	13	10
15	u	84/84 (100%)	82 (98%)	2 (2%)	43	47
16	V	117/117 (100%)	109 (93%)	8 (7%)	14	11
16	v	117/117 (100%)	109 (93%)	8 (7%)	14	11
17	Y	19/23 (83%)	16 (84%)	3 (16%)	2	1
17	y	22/23 (96%)	18 (82%)	4 (18%)	2	1
18	X	31/31 (100%)	29 (94%)	2 (6%)	15	12
18	x	31/31 (100%)	29 (94%)	2 (6%)	15	12
19	Z	52/52 (100%)	45 (86%)	7 (14%)	4	2
19	z	51/52 (98%)	39 (76%)	12 (24%)	1	0
20	R	28/29 (97%)	22 (79%)	6 (21%)	1	0
20	r	19/29 (66%)	13 (68%)	6 (32%)	0	0
All	All	4323/4348 (99%)	4083 (94%)	240 (6%)	19	16

5 of 240 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
20	R	20	VAL
18	x	15	LEU
2	b	506	ARG
17	y	45	ASN
20	r	7	VAL

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

Mol	Chain	Res	Type
13	o	124	ASN

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Mol	Chain	Res	Type
13	o	200	ASN
16	V	86	GLN
15	U	81	HIS
18	x	33	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	FME	i	1	8	8,9,10	1.12	0	8,9,11	0.93	0
12	FME	m	1	12	8,9,10	1.22	1 (12%)	8,9,11	1.00	1 (12%)
14	FME	T	1	14	8,9,10	1.08	1 (12%)	8,9,11	1.56	2 (25%)
14	FME	t	1	14	8,9,10	1.43	1 (12%)	8,9,11	1.32	1 (12%)
12	FME	M	1	12	8,9,10	1.27	1 (12%)	8,9,11	1.01	0
8	FME	I	1	8	8,9,10	1.00	0	8,9,11	1.54	1 (12%)

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	FME	I	1	8	-	0/7/9/11	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	t	1	FME	CA-N	-3.62	1.41	1.46
12	M	1	FME	CA-N	-2.93	1.42	1.46
12	m	1	FME	CA-N	-2.65	1.42	1.46
14	T	1	FME	CA-N	-2.37	1.43	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	I	1	FME	C-CA-N	3.83	116.89	109.50
14	T	1	FME	CA-N-CN	-2.56	118.89	122.82
14	t	1	FME	C-CA-N	2.43	114.18	109.50
14	T	1	FME	O1-CN-N	-2.29	119.39	125.32
12	m	1	FME	CB-CA-N	2.00	114.16	110.52

There are no chirality outliers.

All (5) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 186 ligands modelled in this entry, 6 are monoatomic and 31 are unknown - leaving 149 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
29	DGD	H	102	-	63,63,67	1.29	8 (12%)	77,77,81	1.45	9 (11%)
30	OEX	A	414	3,36,1	0,15,15	-	-	-		
32	LMG	C	501	-	48,48,55	0.91	2 (4%)	56,56,63	1.39	9 (16%)
23	BCT	A	404	21	3,3,3	1.06	0	2,3,3	3.25	1 (50%)
24	CLA	B	612	-	69,73,73	0.96	4 (5%)	82,113,113	1.32	10 (12%)
32	LMG	c	522	-	48,48,55	1.19	6 (12%)	56,56,63	1.34	7 (12%)
28	SQD	a	411	-	35,35,54	1.12	2 (5%)	37,37,65	1.36	4 (10%)
24	CLA	C	512	3	69,73,73	1.35	10 (14%)	82,113,113	1.48	8 (9%)
24	CLA	b	603	-	69,73,73	1.21	9 (13%)	82,113,113	1.52	12 (14%)
33	LHG	l	101	-	48,48,48	0.86	2 (4%)	51,54,54	1.28	7 (13%)
32	LMG	c	519	-	37,37,55	1.10	3 (8%)	45,45,63	1.25	5 (11%)
24	CLA	B	613	-	69,73,73	1.37	11 (15%)	82,113,113	1.58	11 (13%)
25	PHO	A	407	-	58,69,69	1.81	11 (18%)	55,99,99	1.37	7 (12%)
24	CLA	c	512	-	69,73,73	1.20	9 (13%)	82,113,113	1.31	8 (9%)
24	CLA	B	615	-	69,73,73	1.29	8 (11%)	82,113,113	1.41	9 (10%)
24	CLA	b	616	-	69,73,73	1.52	10 (14%)	82,113,113	1.56	10 (12%)
29	DGD	h	104	-	63,63,67	1.07	5 (7%)	77,77,81	1.40	8 (10%)
24	CLA	b	612	-	69,73,73	1.57	8 (11%)	82,113,113	1.25	10 (12%)
24	CLA	b	604	-	69,73,73	1.22	8 (11%)	82,113,113	1.48	11 (13%)
26	BCR	B	619	-	41,41,41	1.30	3 (7%)	56,56,56	1.52	12 (21%)
32	LMG	h	102	-	21,21,55	0.84	1 (4%)	20,20,63	1.01	1 (5%)
24	CLA	b	614	-	69,73,73	1.56	11 (15%)	82,113,113	1.37	13 (15%)
32	LMG	b	621	-	51,51,55	0.83	0	59,59,63	1.53	9 (15%)
35	HEC	V	201	16	46,50,50	1.88	7 (15%)	58,82,82	1.35	3 (5%)
24	CLA	a	407	-	69,73,73	1.66	13 (18%)	82,113,113	1.31	10 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	c	510	-	69,73,73	1.31	7 (10%)	82,113,113	1.44	7 (8%)
24	CLA	d	405	-	69,73,73	1.59	8 (11%)	82,113,113	1.42	17 (20%)
24	CLA	C	506	-	69,73,73	1.28	9 (13%)	82,113,113	1.27	10 (12%)
24	CLA	c	504	36	64,68,73	1.29	10 (15%)	76,107,113	1.33	8 (10%)
26	BCR	b	618	-	41,41,41	1.19	3 (7%)	56,56,56	1.44	11 (19%)
32	LMG	K	102	-	48,48,55	1.06	4 (8%)	56,56,63	1.33	5 (8%)
24	CLA	B	607	36	69,73,73	1.59	6 (8%)	82,113,113	1.34	8 (9%)
24	CLA	B	614	-	69,73,73	1.44	9 (13%)	82,113,113	1.16	5 (6%)
26	BCR	c	521	-	41,41,41	0.98	3 (7%)	56,56,56	1.27	6 (10%)
26	BCR	B	618	-	41,41,41	1.18	2 (4%)	56,56,56	1.35	8 (14%)
24	CLA	B	605	-	69,73,73	1.48	9 (13%)	82,113,113	1.50	12 (14%)
26	BCR	C	519	-	41,41,41	1.05	2 (4%)	56,56,56	1.39	8 (14%)
29	DGD	c	516	-	63,63,67	1.12	3 (4%)	77,77,81	1.39	9 (11%)
24	CLA	c	501	-	69,73,73	1.35	13 (18%)	82,113,113	1.56	10 (12%)
25	PHO	d	402	-	58,69,69	2.09	9 (15%)	55,99,99	1.74	12 (21%)
33	LHG	d	409	-	48,48,48	0.72	0	51,54,54	1.26	5 (9%)
24	CLA	B	602	-	69,73,73	1.42	9 (13%)	82,113,113	1.30	12 (14%)
24	CLA	c	505	-	69,73,73	1.18	7 (10%)	82,113,113	1.39	10 (12%)
24	CLA	A	408	-	58,62,73	1.46	12 (20%)	68,99,113	1.50	11 (16%)
24	CLA	D	402	36	69,73,73	1.27	10 (14%)	82,113,113	1.35	8 (9%)
32	LMG	b	623	-	55,55,55	0.96	5 (9%)	63,63,63	1.43	7 (11%)
33	LHG	D	411	-	48,48,48	1.07	6 (12%)	51,54,54	1.44	8 (15%)
24	CLA	B	604	-	69,73,73	1.31	6 (8%)	82,113,113	1.54	8 (9%)
26	BCR	a	408	-	41,41,41	1.19	4 (9%)	56,56,56	1.43	8 (14%)
33	LHG	D	408	-	48,48,48	1.08	5 (10%)	51,54,54	1.27	5 (9%)
26	BCR	d	406	-	41,41,41	1.17	2 (4%)	56,56,56	1.25	6 (10%)
26	BCR	b	602	-	41,41,41	1.20	3 (7%)	56,56,56	1.33	7 (12%)
33	LHG	L	101	-	48,48,48	0.71	1 (2%)	51,54,54	1.18	4 (7%)
26	BCR	h	103	-	41,41,41	1.16	1 (2%)	56,56,56	1.48	13 (23%)
24	CLA	c	507	36	69,73,73	1.16	8 (11%)	82,113,113	1.47	13 (15%)
24	CLA	b	606	-	69,73,73	1.28	9 (13%)	82,113,113	1.49	16 (19%)
24	CLA	b	617	-	64,68,73	1.30	9 (14%)	76,107,113	1.52	9 (11%)
28	SQD	b	601	-	47,49,54	0.95	2 (4%)	57,60,65	1.97	14 (24%)
26	BCR	c	515	-	41,41,41	1.41	4 (9%)	56,56,56	1.42	10 (17%)
26	BCR	Y	101	-	41,41,41	1.13	2 (4%)	56,56,56	1.18	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	LHG	e	101	-	41,41,48	0.76	0	44,47,54	1.32	3 (6%)
27	PL9	D	406	-	55,55,55	1.92	9 (16%)	68,69,69	1.45	13 (19%)
24	CLA	C	502	-	69,73,73	1.59	11 (15%)	82,113,113	1.32	9 (10%)
33	LHG	d	408	-	48,48,48	0.73	0	51,54,54	1.24	5 (9%)
26	BCR	b	619	-	41,41,41	1.29	2 (4%)	56,56,56	1.46	10 (17%)
30	OEX	a	414	3,36,1	0,15,15	-	-	-	-	-
33	LHG	d	410	-	38,38,48	0.80	2 (5%)	41,44,54	1.17	3 (7%)
24	CLA	C	510	-	69,73,73	1.20	7 (10%)	82,113,113	1.20	6 (7%)
33	LHG	E	101	-	48,48,48	0.92	3 (6%)	51,54,54	1.14	2 (3%)
24	CLA	c	502	-	69,73,73	1.28	7 (10%)	82,113,113	1.24	11 (13%)
24	CLA	c	503	-	69,73,73	1.28	4 (5%)	82,113,113	1.41	7 (8%)
25	PHO	a	406	-	58,69,69	2.07	9 (15%)	55,99,99	1.49	8 (14%)
29	DGD	c	517	-	63,63,67	1.23	9 (14%)	77,77,81	1.42	11 (14%)
24	CLA	C	509	-	69,73,73	1.46	8 (11%)	82,113,113	1.47	13 (15%)
24	CLA	h	101	36	69,73,73	1.50	10 (14%)	82,113,113	1.43	11 (13%)
24	CLA	b	607	-	69,73,73	1.70	7 (10%)	82,113,113	1.58	14 (17%)
35	HEC	v	201	16	46,50,50	1.85	8 (17%)	58,82,82	1.32	9 (15%)
24	CLA	b	608	36	69,73,73	1.26	6 (8%)	82,113,113	1.26	5 (6%)
34	HEM	F	102	5,6	50,50,50	1.42	7 (14%)	67,82,82	1.02	3 (4%)
32	LMG	M	101	-	51,51,55	1.13	6 (11%)	59,59,63	1.59	14 (23%)
26	BCR	c	514	-	41,41,41	1.19	2 (4%)	56,56,56	1.36	8 (14%)
26	BCR	D	405	-	41,41,41	1.10	2 (4%)	56,56,56	1.17	3 (5%)
29	DGD	a	412	-	43,43,67	1.24	3 (6%)	45,45,81	1.34	8 (17%)
24	CLA	C	503	-	69,73,73	1.31	7 (10%)	82,113,113	1.50	11 (13%)
24	CLA	B	606	-	69,73,73	1.51	9 (13%)	82,113,113	1.37	11 (13%)
24	CLA	d	404	-	69,73,73	1.14	8 (11%)	82,113,113	1.31	8 (9%)
32	LMG	D	410	-	31,31,55	1.17	3 (9%)	33,33,63	1.10	0
33	LHG	D	409	-	46,46,48	1.13	3 (6%)	49,52,54	1.43	7 (14%)
24	CLA	C	511	-	69,73,73	1.37	11 (15%)	82,113,113	1.28	5 (6%)
24	CLA	a	405	36	69,73,73	1.10	7 (10%)	82,113,113	1.29	8 (9%)
24	CLA	D	404	-	69,73,73	1.60	11 (15%)	82,113,113	1.07	6 (7%)
24	CLA	A	406	36	69,73,73	1.21	9 (13%)	82,113,113	1.32	10 (12%)
27	PL9	a	409	-	55,55,55	1.15	4 (7%)	68,69,69	1.46	11 (16%)
24	CLA	C	513	-	69,73,73	1.20	9 (13%)	82,113,113	1.36	10 (12%)
26	BCR	H	101	-	41,41,41	1.12	3 (7%)	56,56,56	1.30	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	b	611	36	69,73,73	1.22	9 (13%)	82,113,113	1.36	12 (14%)
24	CLA	d	403	36	69,73,73	1.44	9 (13%)	82,113,113	1.41	12 (14%)
24	CLA	C	508	36	69,73,73	1.74	5 (7%)	82,113,113	1.36	8 (9%)
24	CLA	b	610	-	69,73,73	1.14	5 (7%)	82,113,113	1.30	9 (10%)
24	CLA	B	601	36	69,73,73	1.96	9 (13%)	82,113,113	1.46	9 (10%)
24	CLA	c	508	-	68,72,73	1.28	11 (16%)	80,111,113	1.09	4 (5%)
29	DGD	A	413	-	67,67,67	1.24	7 (10%)	81,81,81	1.47	11 (13%)
28	SQD	F	101	-	34,36,54	1.01	1 (2%)	42,45,65	1.71	12 (28%)
24	CLA	B	608	-	69,73,73	1.22	8 (11%)	82,113,113	1.21	7 (8%)
29	DGD	C	517	-	63,63,67	1.16	6 (9%)	77,77,81	1.46	13 (16%)
24	CLA	C	505	36	63,67,73	1.15	5 (7%)	74,105,113	1.43	15 (20%)
24	CLA	C	504	-	69,73,73	1.42	12 (17%)	82,113,113	1.48	11 (13%)
24	CLA	b	613	-	69,73,73	1.37	6 (8%)	82,113,113	1.31	11 (13%)
24	CLA	c	506	-	69,73,73	2.02	10 (14%)	82,113,113	1.33	10 (12%)
28	SQD	f	101	-	39,41,54	1.13	5 (12%)	49,52,65	1.57	7 (14%)
32	LMG	D	407	-	51,51,55	1.13	4 (7%)	59,59,63	1.24	4 (6%)
24	CLA	b	609	-	69,73,73	1.20	7 (10%)	82,113,113	1.35	12 (14%)
23	BCT	d	401	21	3,3,3	1.22	0	2,3,3	3.08	2 (100%)
24	CLA	b	605	-	69,73,73	1.28	10 (14%)	82,113,113	1.53	13 (15%)
24	CLA	C	514	-	69,73,73	1.21	7 (10%)	82,113,113	1.37	10 (12%)
24	CLA	B	603	-	69,73,73	1.15	6 (8%)	82,113,113	1.39	11 (13%)
34	HEM	e	102	5,6	50,50,50	1.56	8 (16%)	67,82,82	1.09	3 (4%)
32	LMG	d	411	-	44,44,55	1.09	3 (6%)	52,52,63	1.35	5 (9%)
28	SQD	A	412	-	38,38,54	1.09	3 (7%)	40,40,65	1.33	4 (10%)
24	CLA	B	611	-	69,73,73	1.16	7 (10%)	82,113,113	1.48	11 (13%)
28	SQD	B	622	-	52,54,54	0.94	2 (3%)	62,65,65	1.79	14 (22%)
28	SQD	A	411	-	50,52,54	1.01	4 (8%)	60,63,65	2.31	14 (23%)
26	BCR	C	515	-	41,41,41	1.48	4 (9%)	56,56,56	1.37	10 (17%)
24	CLA	A	405	-	69,73,73	1.37	10 (14%)	82,113,113	1.24	7 (8%)
24	CLA	C	507	-	69,73,73	1.52	10 (14%)	82,113,113	1.15	8 (9%)
32	LMG	c	524	-	49,49,55	0.83	2 (4%)	57,57,63	1.37	4 (7%)
24	CLA	B	616	-	64,68,73	1.53	10 (15%)	76,107,113	1.39	11 (14%)
28	SQD	a	410	-	52,54,54	1.01	5 (9%)	62,65,65	1.97	12 (19%)
26	BCR	A	409	-	41,41,41	1.09	3 (7%)	56,56,56	1.33	8 (14%)
26	BCR	K	101	-	41,41,41	1.17	2 (4%)	56,56,56	1.57	12 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	B	609	-	69,73,73	1.43	9 (13%)	82,113,113	1.31	11 (13%)
26	BCR	b	620	-	41,41,41	1.14	2 (4%)	56,56,56	1.29	9 (16%)
24	CLA	a	404	-	69,73,73	1.35	12 (17%)	82,113,113	1.50	9 (10%)
24	CLA	c	511	3	69,73,73	1.63	7 (10%)	82,113,113	1.25	7 (8%)
26	BCR	B	617	-	41,41,41	1.25	3 (7%)	56,56,56	1.47	7 (12%)
29	DGD	C	518	-	63,63,67	1.09	6 (9%)	77,77,81	1.47	13 (16%)
24	CLA	B	610	36	69,73,73	1.43	10 (14%)	82,113,113	1.45	12 (14%)
24	CLA	D	403	-	69,73,73	1.30	10 (14%)	82,113,113	1.25	9 (10%)
24	CLA	b	615	-	69,73,73	1.42	9 (13%)	82,113,113	1.50	12 (14%)
32	LMG	B	621	-	26,26,55	0.83	1 (3%)	26,26,63	1.17	2 (7%)
27	PL9	A	410	-	55,55,55	1.37	5 (9%)	68,69,69	1.43	11 (16%)
26	BCR	t	101	-	41,41,41	1.15	3 (7%)	56,56,56	1.40	8 (14%)
27	PL9	d	407	-	55,55,55	1.43	5 (9%)	68,69,69	1.77	20 (29%)
24	CLA	c	513	-	69,73,73	1.31	10 (14%)	82,113,113	1.09	6 (7%)
24	CLA	c	509	-	69,73,73	1.38	9 (13%)	82,113,113	1.46	10 (12%)
25	PHO	D	401	-	58,69,69	2.03	11 (18%)	55,99,99	1.54	8 (14%)
29	DGD	c	518	-	63,63,67	1.10	4 (6%)	77,77,81	1.42	10 (12%)
29	DGD	C	516	-	63,63,67	1.20	6 (9%)	77,77,81	1.32	12 (15%)
26	BCR	k	101	-	41,41,41	1.13	3 (7%)	56,56,56	1.15	3 (5%)

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
29	DGD	H	102	-	-	17/51/91/95	0/2/2/2
32	LMG	C	501	-	-	23/43/63/70	0/1/1/1
24	CLA	B	612	-	1/1/20/20	11/39/115/115	-
32	LMG	c	522	-	-	24/43/63/70	0/1/1/1
28	SQD	a	411	-	-	23/37/37/69	-
24	CLA	C	512	3	1/1/20/20	5/39/115/115	-
24	CLA	b	603	-	1/1/20/20	9/39/115/115	-
33	LHG	l	101	-	-	17/53/53/53	-
32	LMG	c	519	-	-	13/31/51/70	0/1/1/1
24	CLA	B	613	-	1/1/20/20	10/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	PHO	A	407	-	-	6/37/103/103	0/5/6/6
24	CLA	c	512	-	1/1/20/20	22/39/115/115	-
24	CLA	B	615	-	1/1/20/20	13/39/115/115	-
24	CLA	b	616	-	1/1/20/20	9/39/115/115	-
29	DGD	h	104	-	-	18/51/91/95	0/2/2/2
24	CLA	b	612	-	1/1/20/20	7/39/115/115	-
24	CLA	b	604	-	1/1/20/20	6/39/115/115	-
26	BCR	B	619	-	-	7/29/63/63	0/2/2/2
32	LMG	h	102	-	-	13/17/17/70	-
24	CLA	b	614	-	1/1/20/20	6/39/115/115	-
32	LMG	b	621	-	-	20/46/66/70	0/1/1/1
35	HEC	V	201	16	-	6/14/54/54	-
24	CLA	a	407	-	1/1/20/20	8/39/115/115	-
24	CLA	c	510	-	1/1/20/20	15/39/115/115	-
24	CLA	d	405	-	1/1/20/20	4/39/115/115	-
24	CLA	C	506	-	1/1/20/20	9/39/115/115	-
24	CLA	c	504	36	1/1/19/20	7/33/109/115	-
26	BCR	b	618	-	-	6/29/63/63	0/2/2/2
32	LMG	K	102	-	-	11/43/63/70	0/1/1/1
24	CLA	B	607	36	1/1/20/20	10/39/115/115	-
24	CLA	B	614	-	1/1/20/20	10/39/115/115	-
26	BCR	c	521	-	-	14/29/63/63	0/2/2/2
26	BCR	B	618	-	-	1/29/63/63	0/2/2/2
24	CLA	B	605	-	1/1/20/20	11/39/115/115	-
26	BCR	C	519	-	-	11/29/63/63	0/2/2/2
29	DGD	c	516	-	-	27/51/91/95	0/2/2/2
24	CLA	c	501	-	1/1/20/20	6/39/115/115	-
25	PHO	d	402	-	-	5/37/103/103	0/5/6/6
33	LHG	d	409	-	-	16/53/53/53	-
24	CLA	B	602	-	1/1/20/20	4/39/115/115	-
24	CLA	c	505	-	1/1/20/20	9/39/115/115	-
24	CLA	A	408	-	1/1/17/20	4/26/102/115	-
24	CLA	D	402	36	1/1/20/20	1/39/115/115	-
32	LMG	b	623	-	-	18/50/70/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	LHG	D	411	-	-	16/53/53/53	-
24	CLA	B	604	-	1/1/20/20	12/39/115/115	-
26	BCR	a	408	-	-	3/29/63/63	0/2/2/2
33	LHG	D	408	-	-	20/53/53/53	-
26	BCR	d	406	-	-	11/29/63/63	0/2/2/2
26	BCR	b	602	-	-	11/29/63/63	0/2/2/2
33	LHG	L	101	-	-	21/53/53/53	-
26	BCR	h	103	-	-	10/29/63/63	0/2/2/2
24	CLA	c	507	36	1/1/20/20	11/39/115/115	-
24	CLA	b	606	-	1/1/20/20	10/39/115/115	-
24	CLA	b	617	-	1/1/19/20	7/33/109/115	-
28	SQD	b	601	-	-	21/44/64/69	0/1/1/1
26	BCR	c	515	-	-	8/29/63/63	0/2/2/2
26	BCR	Y	101	-	-	6/29/63/63	0/2/2/2
33	LHG	e	101	-	-	29/46/46/53	-
27	PL9	D	406	-	-	10/53/73/73	0/1/1/1
24	CLA	C	502	-	1/1/20/20	4/39/115/115	-
33	LHG	d	408	-	-	20/53/53/53	-
26	BCR	b	619	-	-	5/29/63/63	0/2/2/2
33	LHG	d	410	-	-	11/43/43/53	-
24	CLA	C	510	-	1/1/20/20	10/39/115/115	-
33	LHG	E	101	-	-	25/53/53/53	-
24	CLA	c	502	-	1/1/20/20	3/39/115/115	-
24	CLA	c	503	-	1/1/20/20	7/39/115/115	-
25	PHO	a	406	-	-	2/37/103/103	0/5/6/6
29	DGD	c	517	-	-	15/51/91/95	0/2/2/2
24	CLA	C	509	-	-	9/39/115/115	-
24	CLA	h	101	36	1/1/20/20	20/39/115/115	-
24	CLA	b	607	-	1/1/20/20	8/39/115/115	-
35	HEC	v	201	16	-	6/14/54/54	-
24	CLA	b	608	36	1/1/20/20	12/39/115/115	-
34	HEM	F	102	5,6	-	3/14/54/54	-
32	LMG	M	101	-	-	21/46/66/70	0/1/1/1
26	BCR	c	514	-	-	9/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	BCR	D	405	-	-	5/29/63/63	0/2/2/2
29	DGD	a	412	-	-	21/45/45/95	-
24	CLA	C	503	-	1/1/20/20	11/39/115/115	-
24	CLA	B	606	-	1/1/20/20	6/39/115/115	-
24	CLA	d	404	-	1/1/20/20	6/39/115/115	-
32	LMG	D	410	-	-	19/33/33/70	-
33	LHG	D	409	-	-	25/51/51/53	-
24	CLA	C	511	-	1/1/20/20	13/39/115/115	-
24	CLA	a	405	36	-	13/39/115/115	-
24	CLA	D	404	-	-	11/39/115/115	-
24	CLA	A	406	36	1/1/20/20	5/39/115/115	-
27	PL9	a	409	-	-	22/53/73/73	0/1/1/1
24	CLA	C	513	-	1/1/20/20	11/39/115/115	-
26	BCR	H	101	-	-	6/29/63/63	0/2/2/2
24	CLA	b	611	36	1/1/20/20	9/39/115/115	-
24	CLA	d	403	36	1/1/20/20	1/39/115/115	-
24	CLA	C	508	36	1/1/20/20	7/39/115/115	-
24	CLA	b	610	-	1/1/20/20	11/39/115/115	-
24	CLA	B	601	36	1/1/20/20	15/39/115/115	-
24	CLA	c	508	-	-	7/38/114/115	-
29	DGD	A	413	-	-	25/55/95/95	0/2/2/2
28	SQD	F	101	-	-	13/28/48/69	0/1/1/1
24	CLA	B	608	-	-	5/39/115/115	-
29	DGD	C	517	-	-	19/51/91/95	0/2/2/2
24	CLA	C	505	36	1/1/18/20	8/32/108/115	-
24	CLA	C	504	-	1/1/20/20	4/39/115/115	-
24	CLA	b	613	-	1/1/20/20	5/39/115/115	-
24	CLA	c	506	-	1/1/20/20	15/39/115/115	-
28	SQD	f	101	-	-	18/36/56/69	0/1/1/1
32	LMG	D	407	-	-	17/46/66/70	0/1/1/1
24	CLA	b	609	-	1/1/20/20	5/39/115/115	-
24	CLA	b	605	-	1/1/20/20	10/39/115/115	-
24	CLA	C	514	-	1/1/20/20	11/39/115/115	-
24	CLA	B	603	-	-	11/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	HEM	e	102	5,6	-	4/14/54/54	-
32	LMG	d	411	-	-	11/39/59/70	0/1/1/1
28	SQD	A	412	-	-	17/39/39/69	-
24	CLA	B	611	-	-	9/39/115/115	-
28	SQD	B	622	-	-	21/49/69/69	0/1/1/1
28	SQD	A	411	-	-	23/47/67/69	0/1/1/1
26	BCR	C	515	-	-	2/29/63/63	0/2/2/2
24	CLA	A	405	-	1/1/20/20	3/39/115/115	-
24	CLA	C	507	-	-	9/39/115/115	-
32	LMG	c	524	-	-	25/44/64/70	0/1/1/1
24	CLA	B	616	-	1/1/19/20	9/33/109/115	-
28	SQD	a	410	-	-	22/49/69/69	0/1/1/1
26	BCR	A	409	-	-	6/29/63/63	0/2/2/2
26	BCR	K	101	-	-	11/29/63/63	0/2/2/2
24	CLA	B	609	-	-	5/39/115/115	-
26	BCR	b	620	-	-	8/29/63/63	0/2/2/2
24	CLA	a	404	-	1/1/20/20	6/39/115/115	-
24	CLA	c	511	3	1/1/20/20	6/39/115/115	-
26	BCR	B	617	-	-	5/29/63/63	0/2/2/2
29	DGD	C	518	-	-	13/51/91/95	0/2/2/2
24	CLA	B	610	36	1/1/20/20	5/39/115/115	-
24	CLA	D	403	-	1/1/20/20	7/39/115/115	-
24	CLA	b	615	-	1/1/20/20	13/39/115/115	-
32	LMG	B	621	-	-	8/22/22/70	-
27	PL9	A	410	-	-	24/53/73/73	0/1/1/1
26	BCR	t	101	-	-	12/29/63/63	0/2/2/2
27	PL9	d	407	-	-	18/53/73/73	0/1/1/1
24	CLA	c	513	-	1/1/20/20	11/39/115/115	-
24	CLA	c	509	-	1/1/20/20	14/39/115/115	-
25	PHO	D	401	-	-	2/37/103/103	0/5/6/6
29	DGD	c	518	-	-	14/51/91/95	0/2/2/2
29	DGD	C	516	-	-	17/51/91/95	0/2/2/2
26	BCR	k	101	-	-	9/29/63/63	0/2/2/2

The worst 5 of 899 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	506	CLA	MG-ND	-12.77	1.80	2.05
24	C	508	CLA	MG-NA	10.07	2.30	2.06
24	b	607	CLA	MG-NA	9.96	2.29	2.06
25	d	402	PHO	C1B-C2B	9.78	1.50	1.39
25	a	406	PHO	C1B-C2B	9.34	1.49	1.39

The worst 5 of 1286 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	A	411	SQD	O6-C1-C2	9.81	123.17	108.27
28	a	410	SQD	O6-C1-C2	9.43	122.59	108.27
24	b	607	CLA	C4A-NA-C1A	8.39	110.51	106.68
24	a	404	CLA	C4A-NA-C1A	8.36	110.49	106.68
28	b	601	SQD	O6-C1-C2	8.22	120.75	108.27

5 of 61 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	A	405	CLA	ND
24	A	406	CLA	ND
24	A	408	CLA	ND
24	B	601	CLA	ND
24	B	602	CLA	ND

5 of 1647 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	A	408	CLA	C4-C3-C5-C6
24	B	606	CLA	C4B-C3B-CAB-CBB
24	B	616	CLA	CBD-CGD-O2D-CED
24	C	508	CLA	CHA-CBD-CGD-O1D
24	C	508	CLA	CHA-CBD-CGD-O2D

There are no ring outliers.

97 monomers are involved in 174 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	H	102	DGD	1	0
24	B	612	CLA	1	0
32	c	522	LMG	1	0
28	a	411	SQD	1	0
24	C	512	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	b	603	CLA	1	0
33	l	101	LHG	1	0
24	B	613	CLA	1	0
24	B	615	CLA	1	0
24	b	616	CLA	1	0
29	h	104	DGD	1	0
24	b	604	CLA	1	0
26	B	619	BCR	3	0
24	b	614	CLA	1	0
32	b	621	LMG	1	0
35	V	201	HEC	1	0
24	C	506	CLA	2	0
24	c	504	CLA	1	0
26	b	618	BCR	3	0
24	B	614	CLA	1	0
26	c	521	BCR	4	0
26	B	618	BCR	5	0
24	B	605	CLA	2	0
24	c	501	CLA	2	0
25	d	402	PHO	1	0
33	d	409	LHG	1	0
24	B	602	CLA	1	0
24	D	402	CLA	1	0
32	b	623	LMG	1	0
33	D	411	LHG	2	0
24	B	604	CLA	3	0
26	a	408	BCR	1	0
33	D	408	LHG	2	0
26	d	406	BCR	2	0
26	b	602	BCR	2	0
33	L	101	LHG	1	0
26	h	103	BCR	4	0
24	c	507	CLA	1	0
24	b	606	CLA	4	0
26	Y	101	BCR	3	0
27	D	406	PL9	1	0
33	d	408	LHG	4	0
26	b	619	BCR	3	0
24	C	510	CLA	2	0
33	E	101	LHG	2	0
24	c	503	CLA	1	0
25	a	406	PHO	1	0

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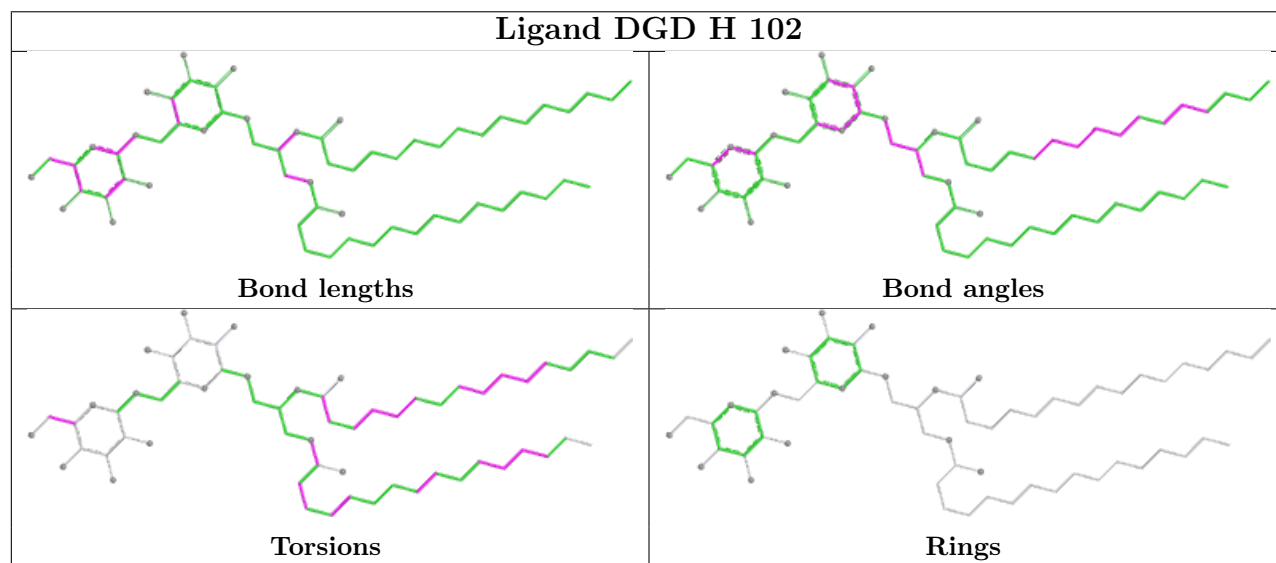
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24	h	101	CLA	4	0
24	b	607	CLA	5	0
35	v	201	HEC	2	0
24	b	608	CLA	1	0
34	F	102	HEM	4	0
32	M	101	LMG	1	0
26	D	405	BCR	5	0
29	a	412	DGD	1	0
24	C	503	CLA	1	0
24	B	606	CLA	6	0
24	d	404	CLA	1	0
33	D	409	LHG	1	0
27	a	409	PL9	3	0
24	C	513	CLA	2	0
26	H	101	BCR	1	0
24	b	611	CLA	1	0
24	d	403	CLA	2	0
24	b	610	CLA	1	0
24	B	601	CLA	2	0
24	c	508	CLA	1	0
29	A	413	DGD	2	0
28	F	101	SQD	1	0
24	B	608	CLA	1	0
24	b	613	CLA	3	0
24	c	506	CLA	1	0
28	f	101	SQD	4	0
24	b	609	CLA	3	0
24	b	605	CLA	4	0
24	C	514	CLA	4	0
24	B	603	CLA	1	0
34	e	102	HEM	5	0
28	A	412	SQD	2	0
28	B	622	SQD	3	0
26	C	515	BCR	3	0
24	A	405	CLA	1	0
32	c	524	LMG	3	0
28	a	410	SQD	2	0
26	A	409	BCR	1	0
26	K	101	BCR	4	0
24	B	609	CLA	1	0
26	b	620	BCR	3	0
24	a	404	CLA	2	0

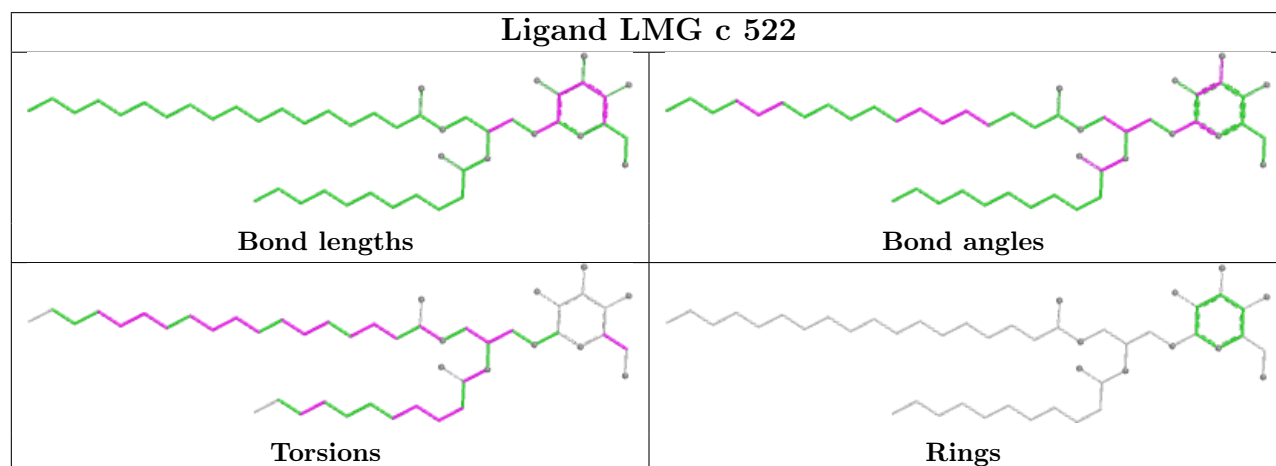
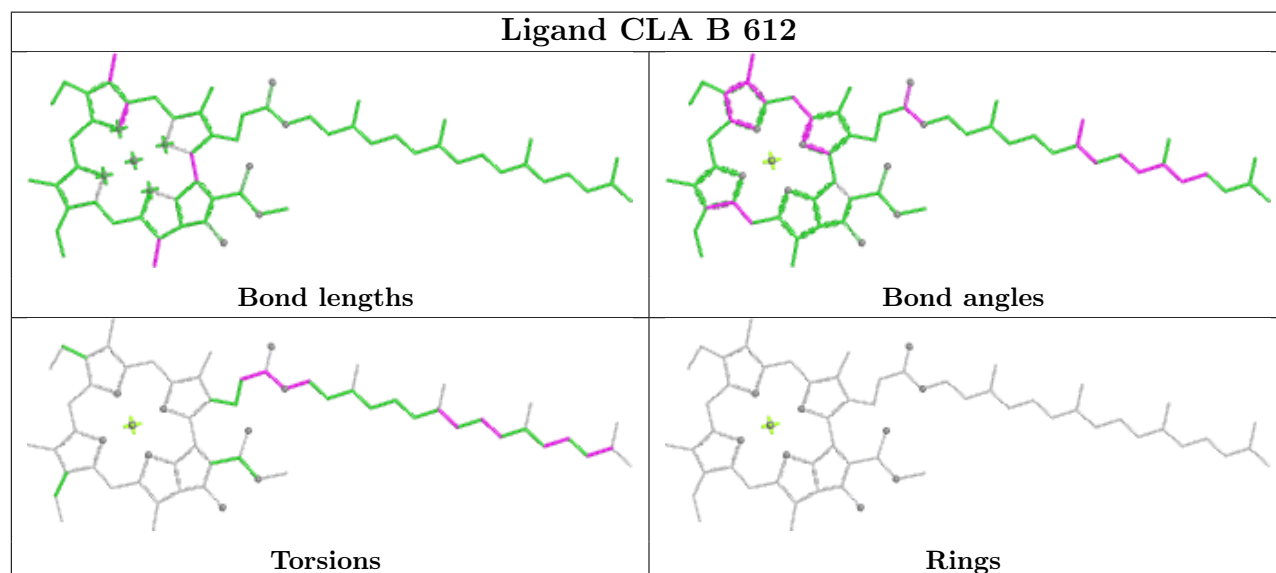
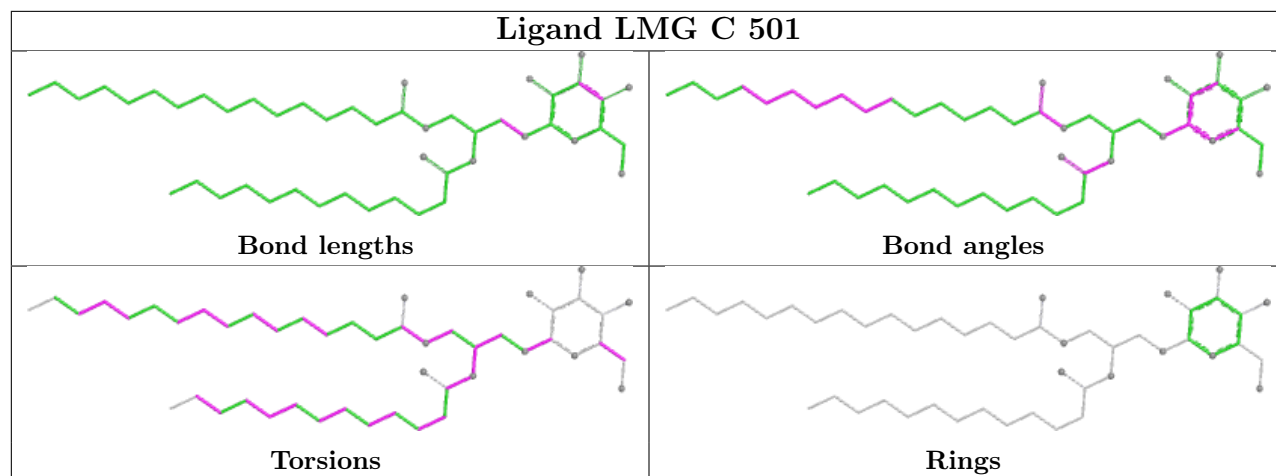
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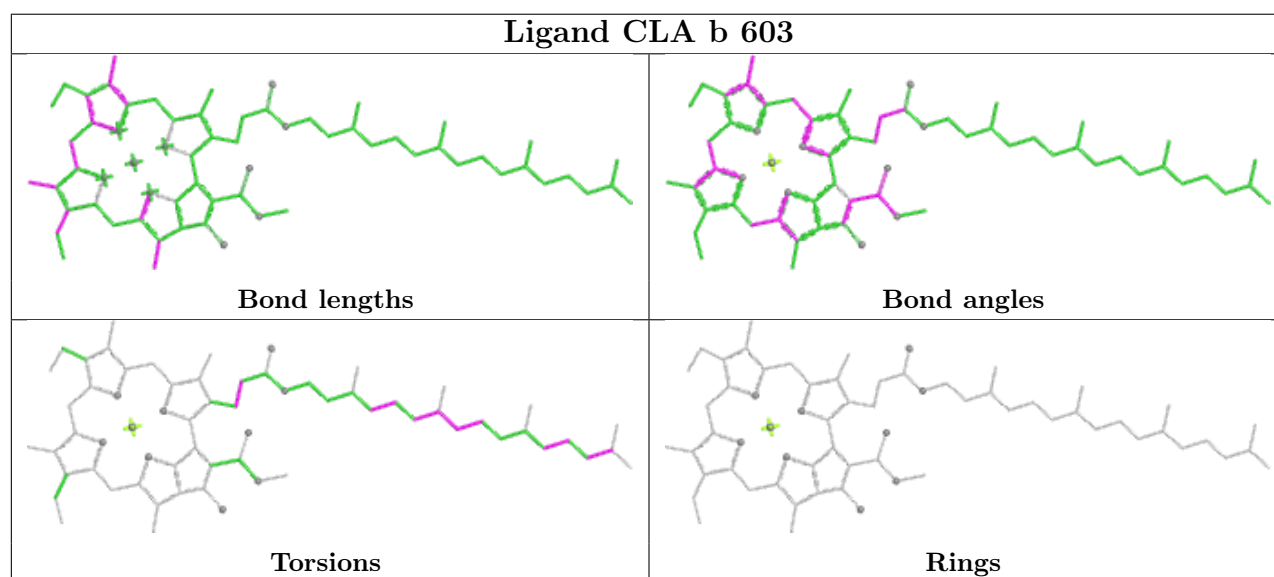
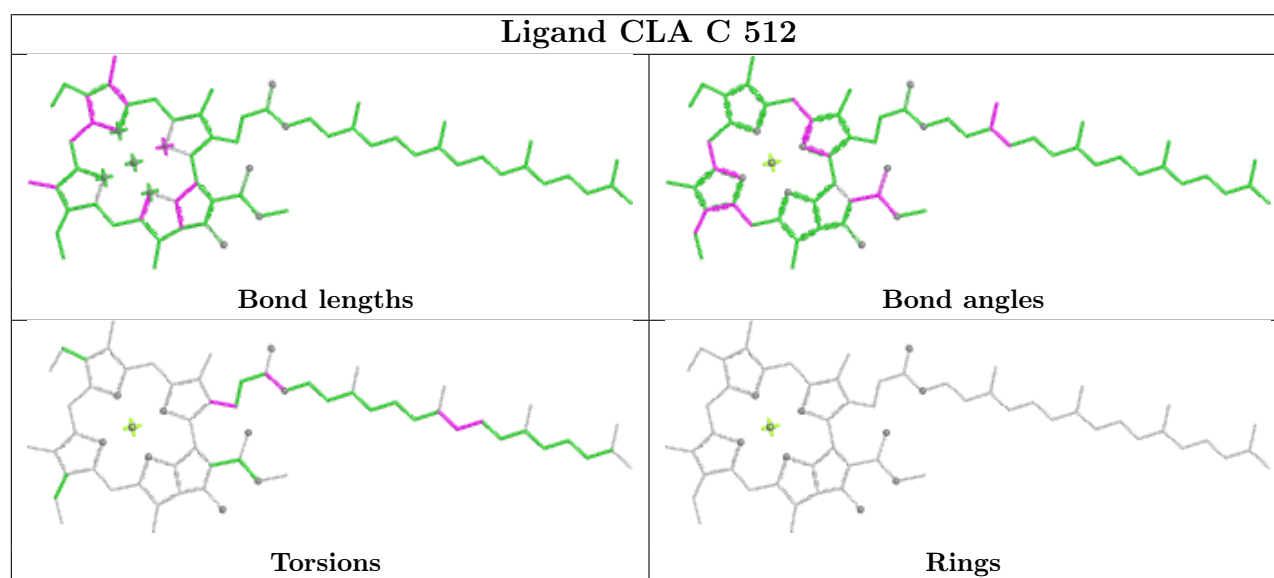
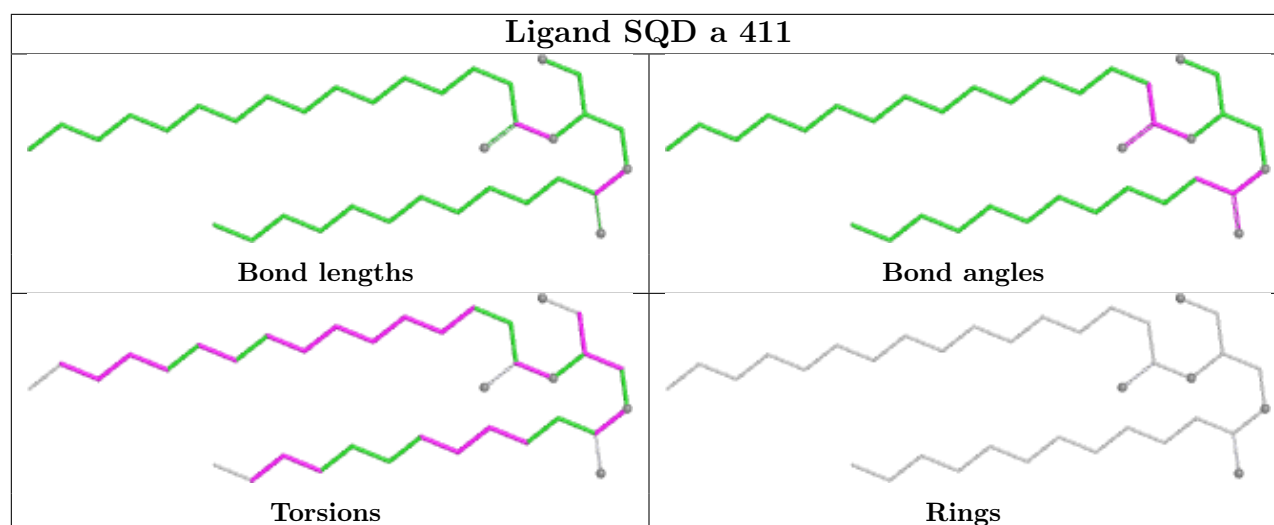
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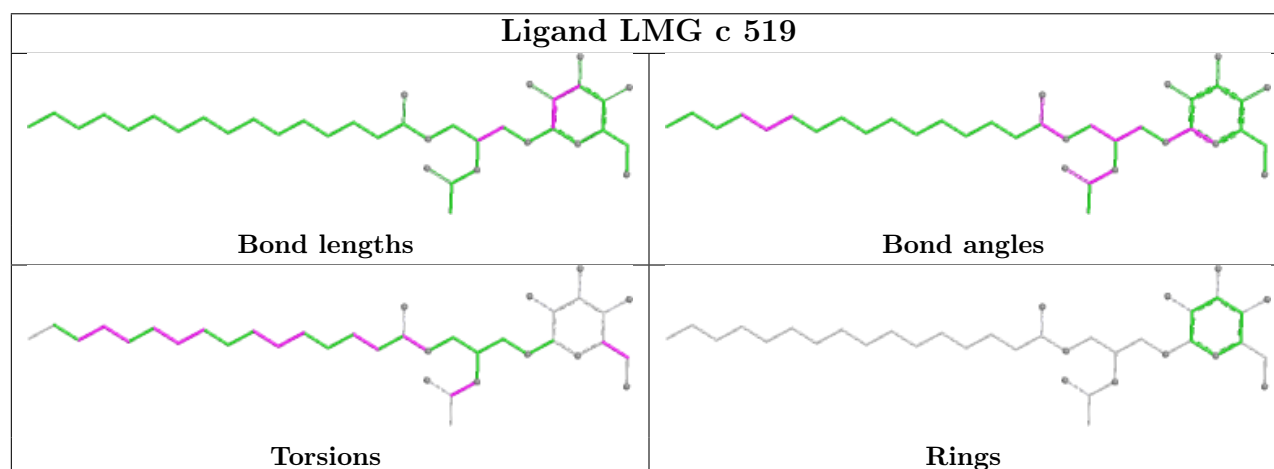
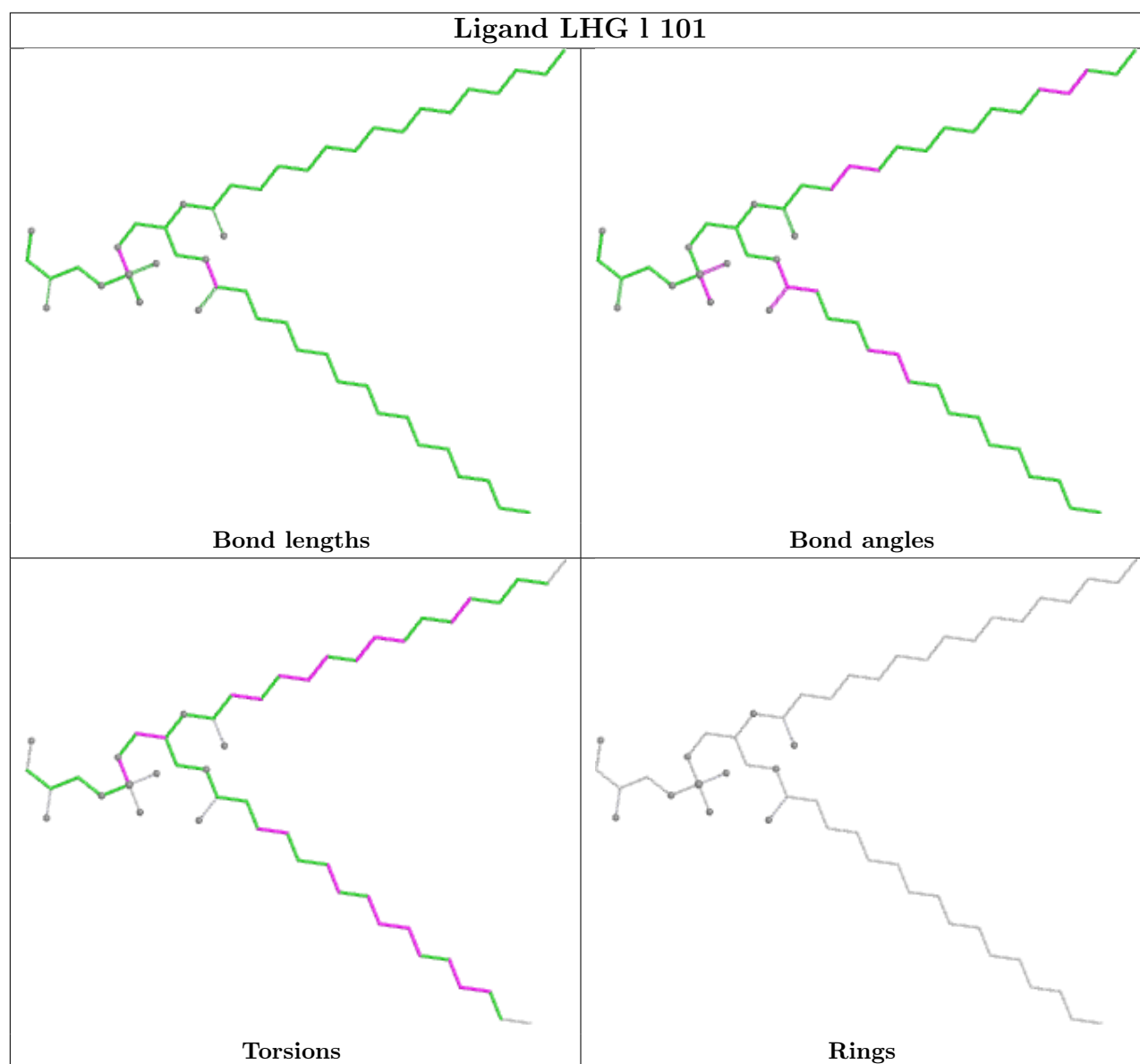
Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	c	511	CLA	1	0
24	B	610	CLA	1	0
24	D	403	CLA	2	0
24	b	615	CLA	3	0
26	t	101	BCR	6	0
24	c	513	CLA	1	0
25	D	401	PHO	1	0
29	c	518	DGD	1	0

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

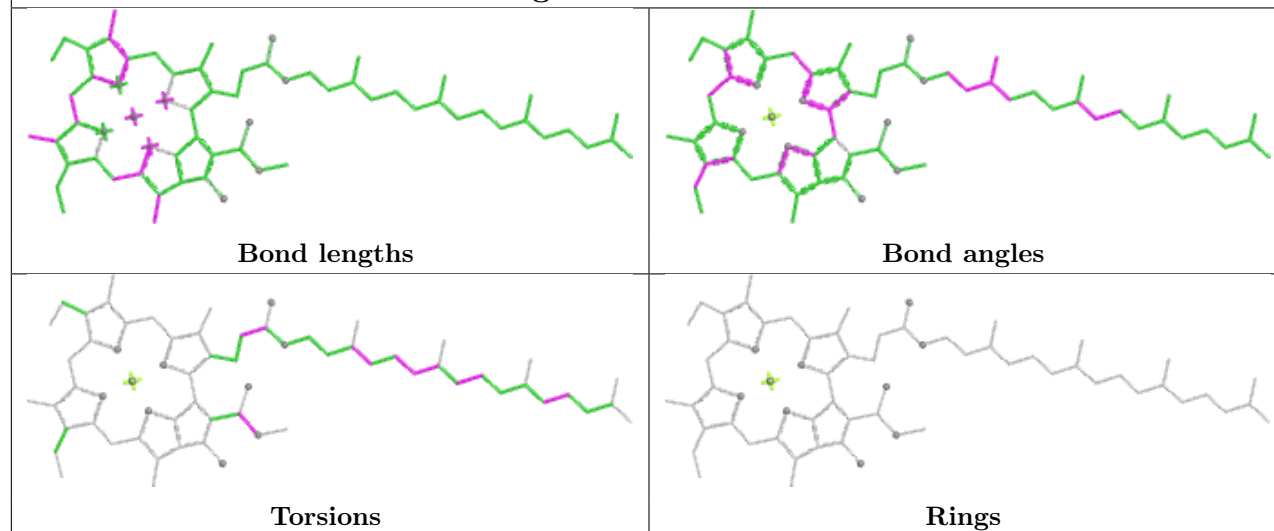




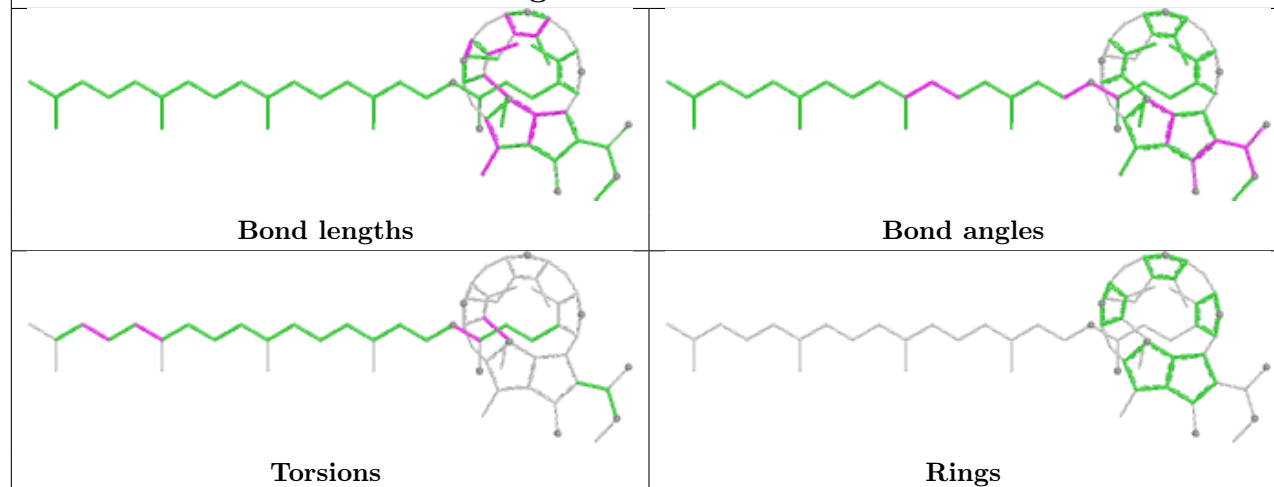




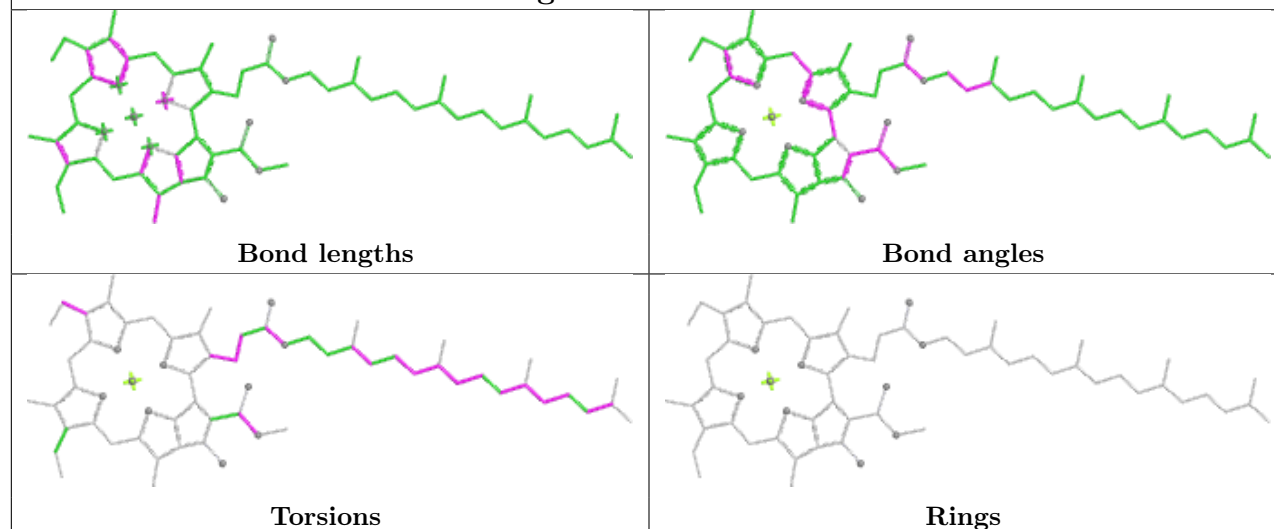
Ligand CLA B 613

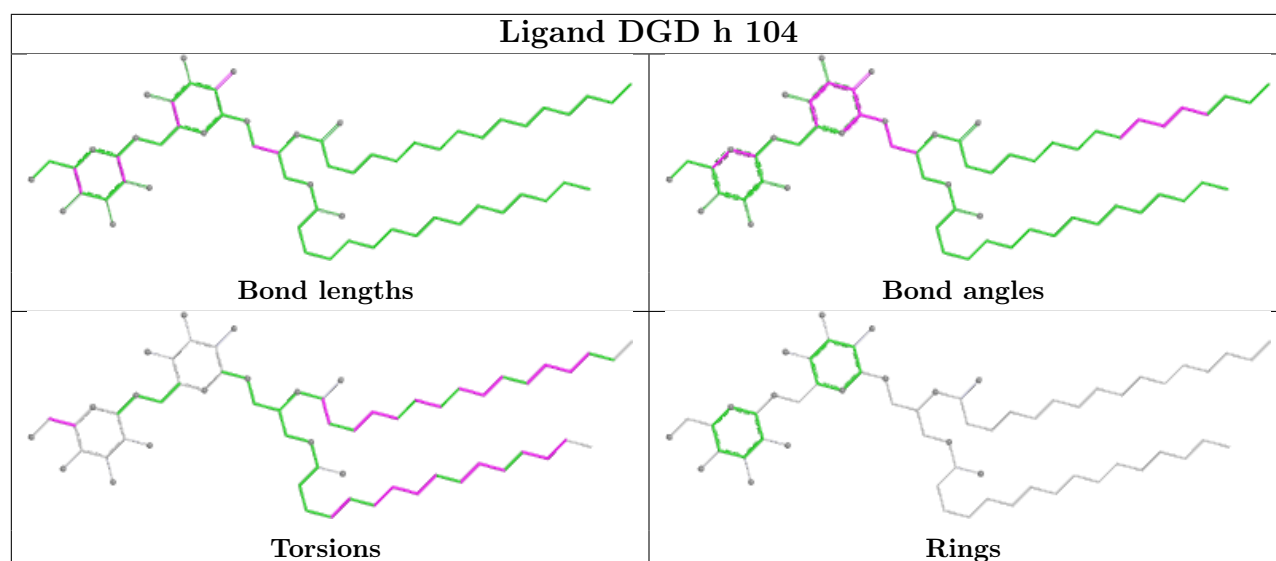
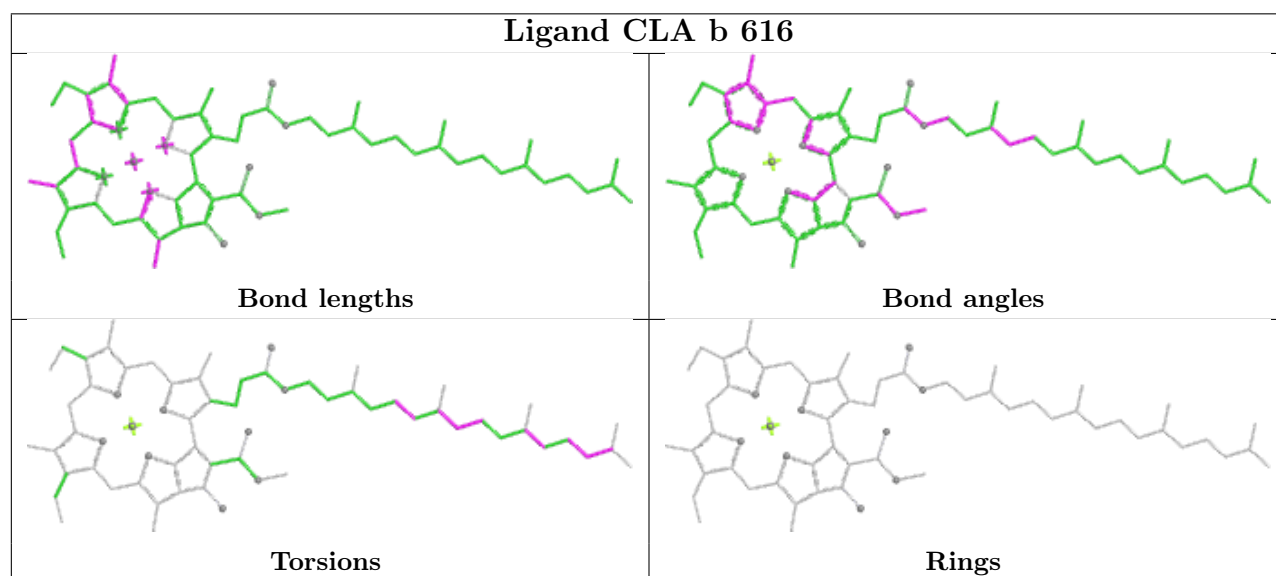
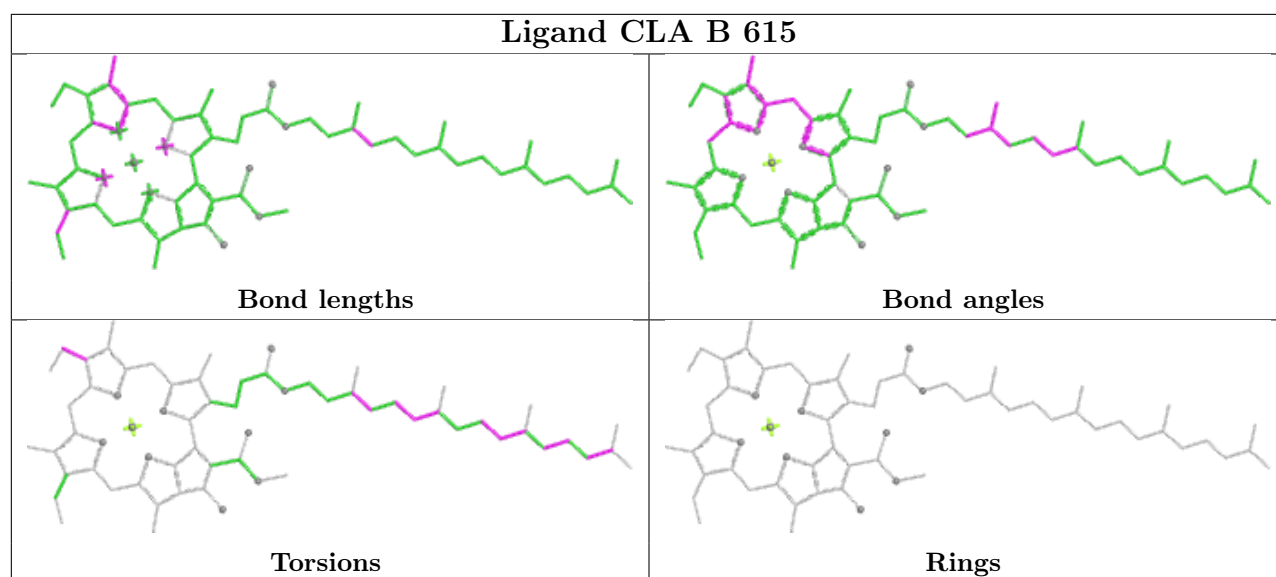


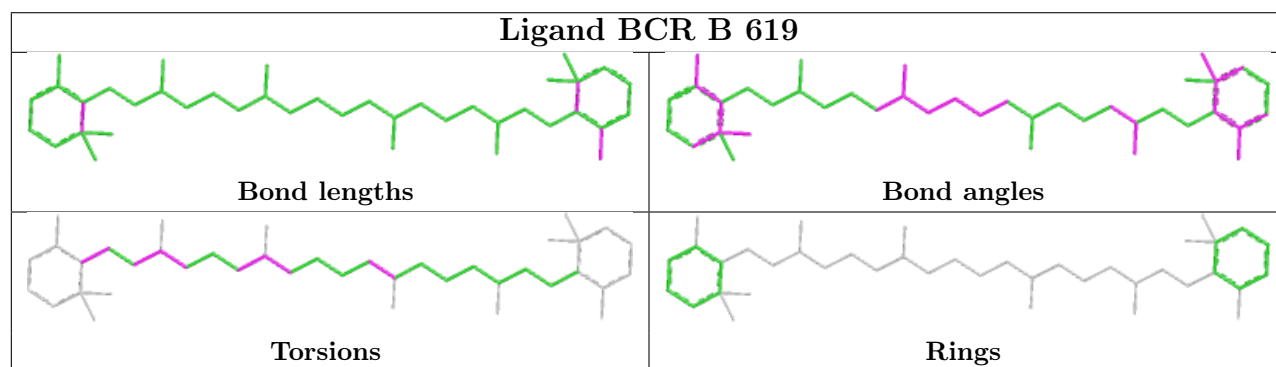
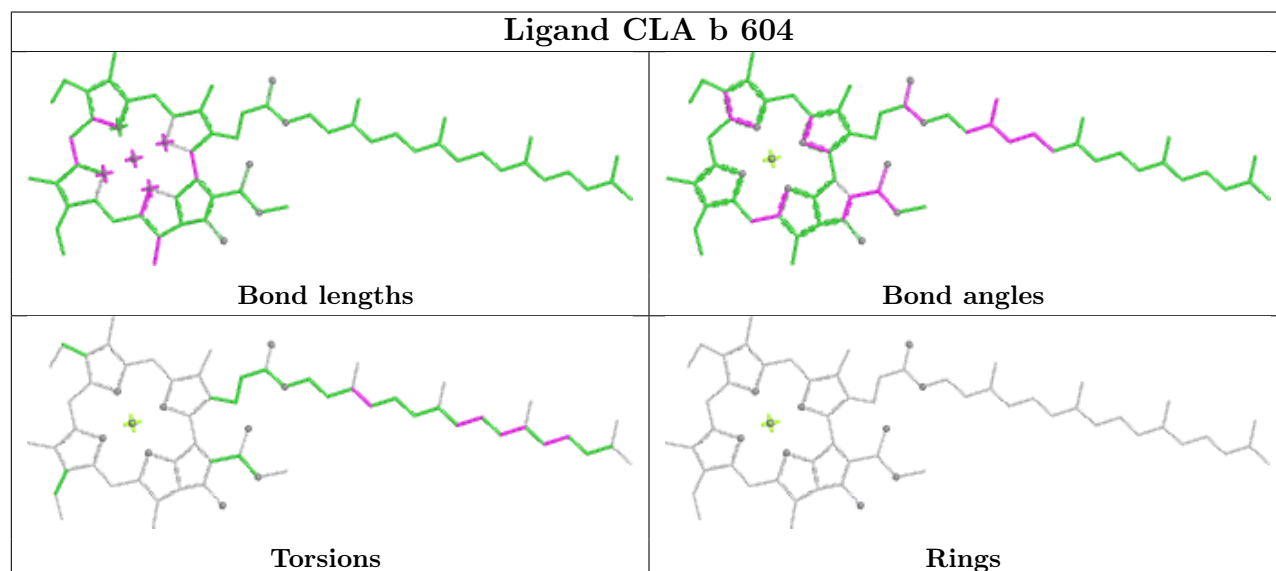
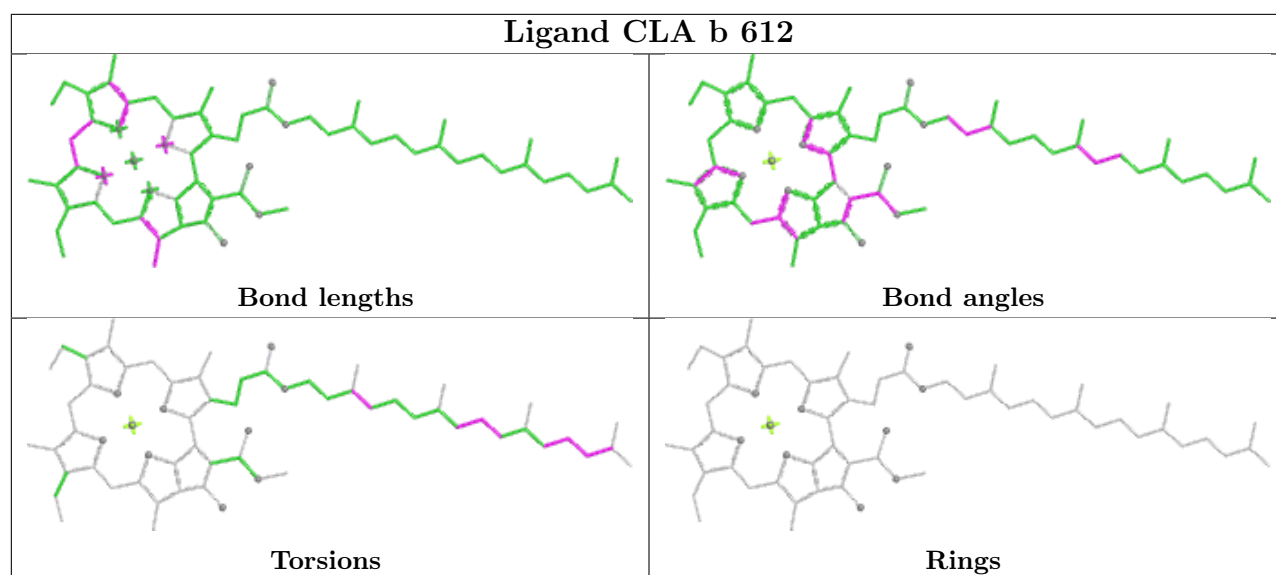
Ligand PHO A 407

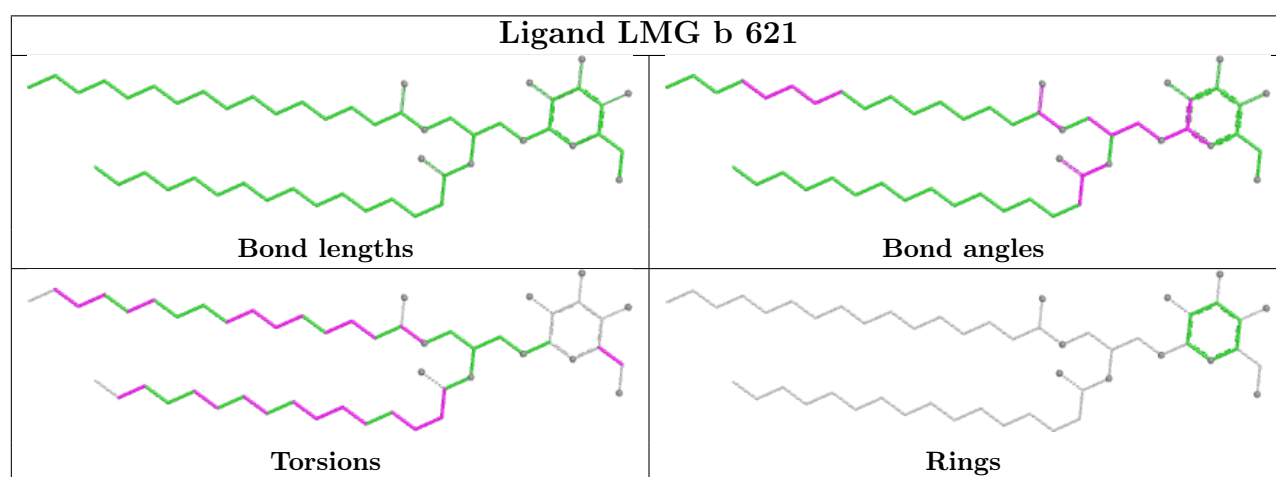
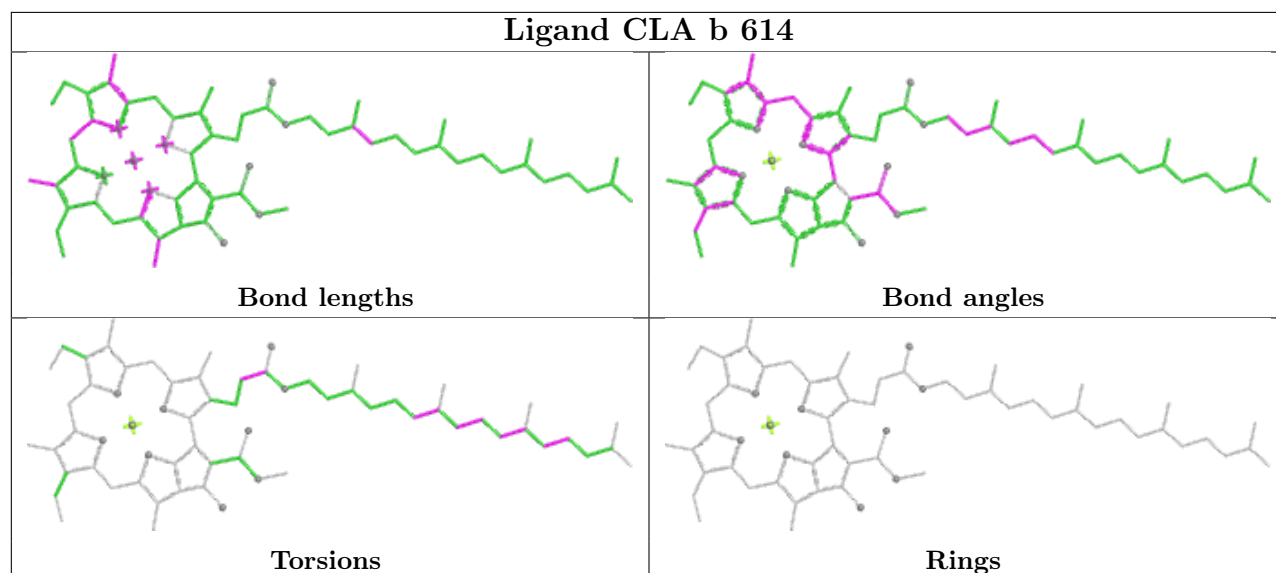
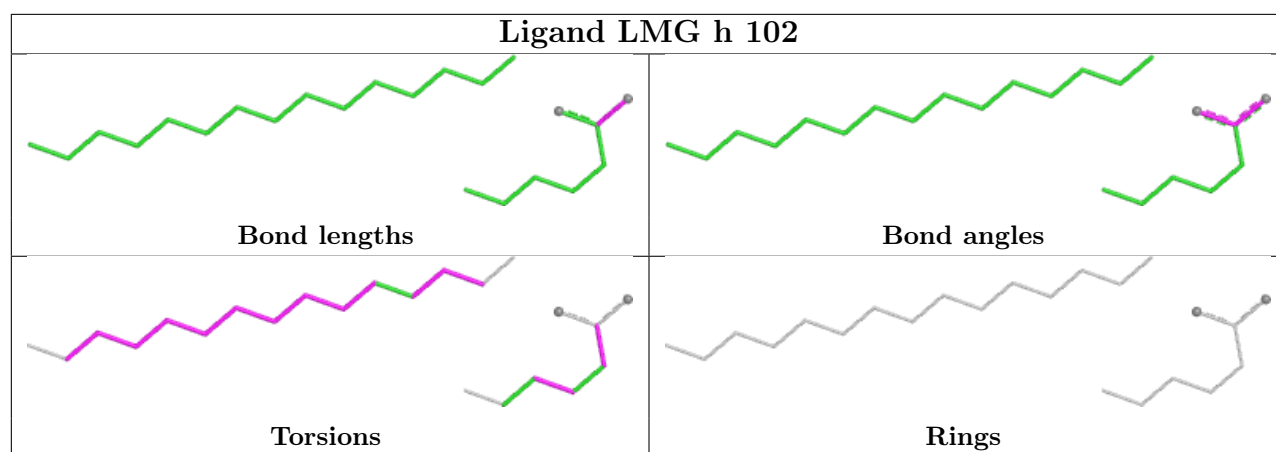


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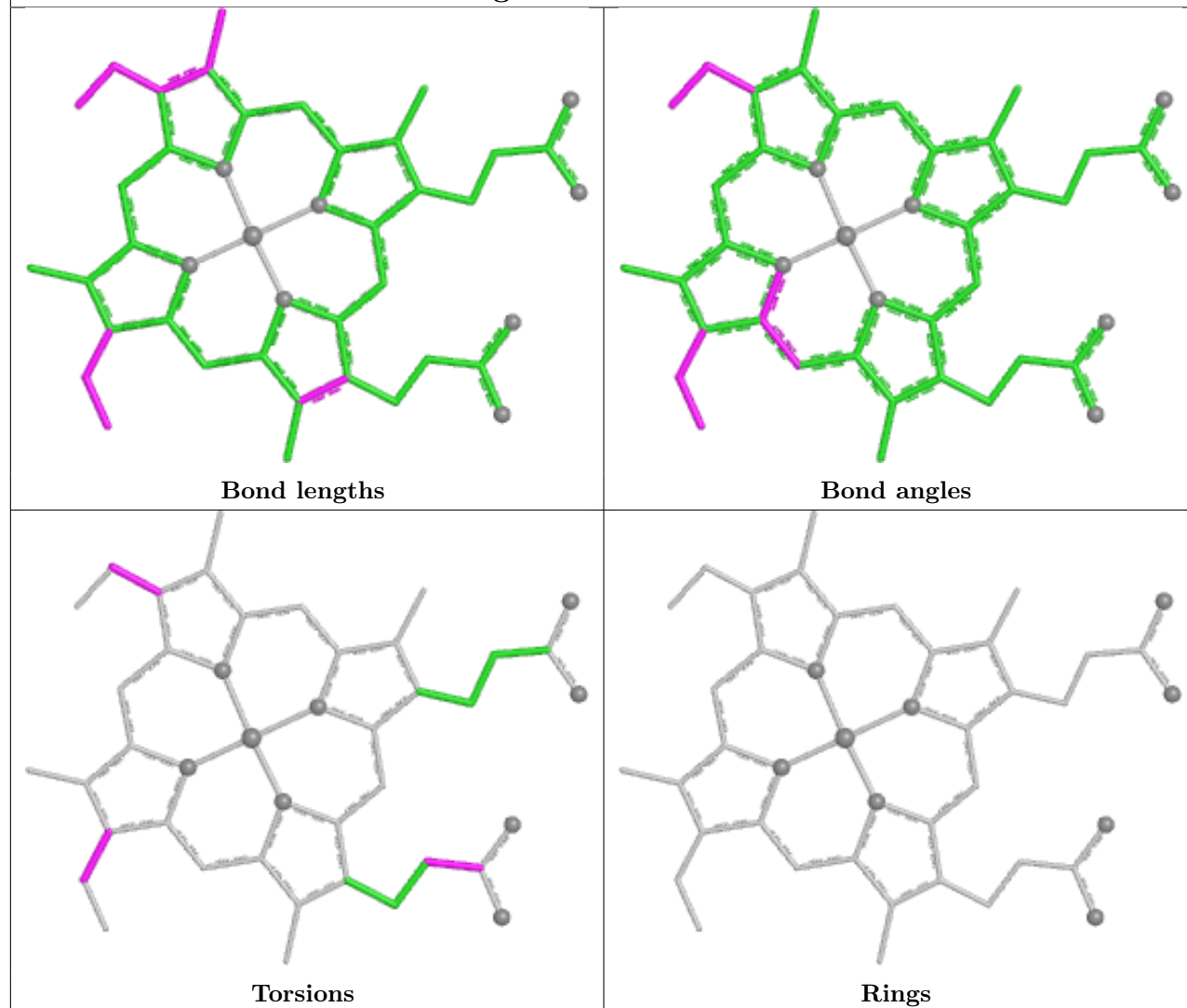




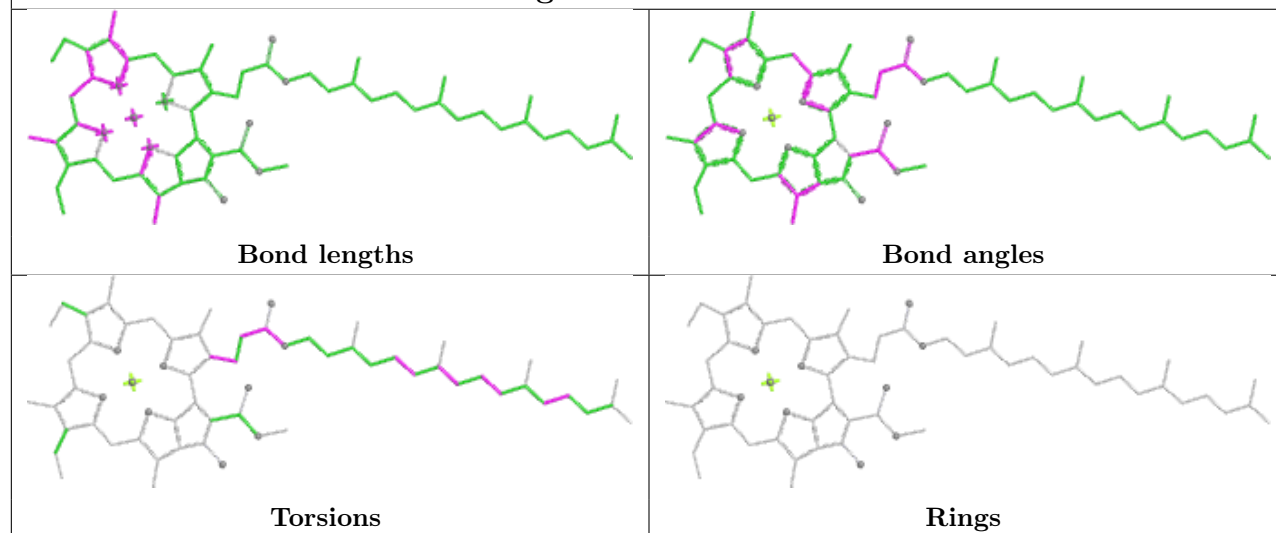




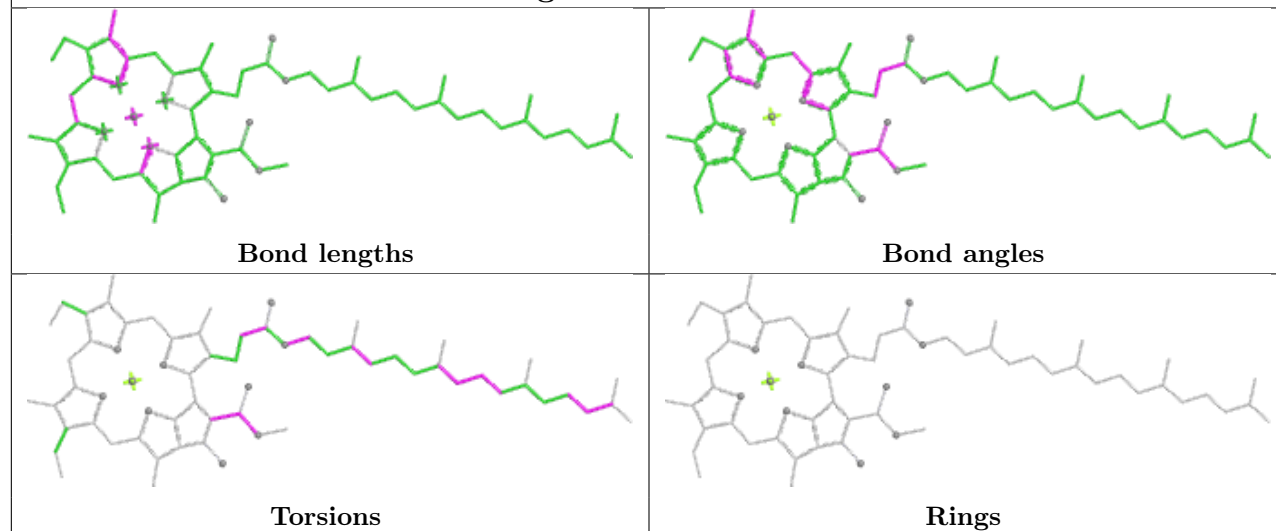
Ligand HEC V 201



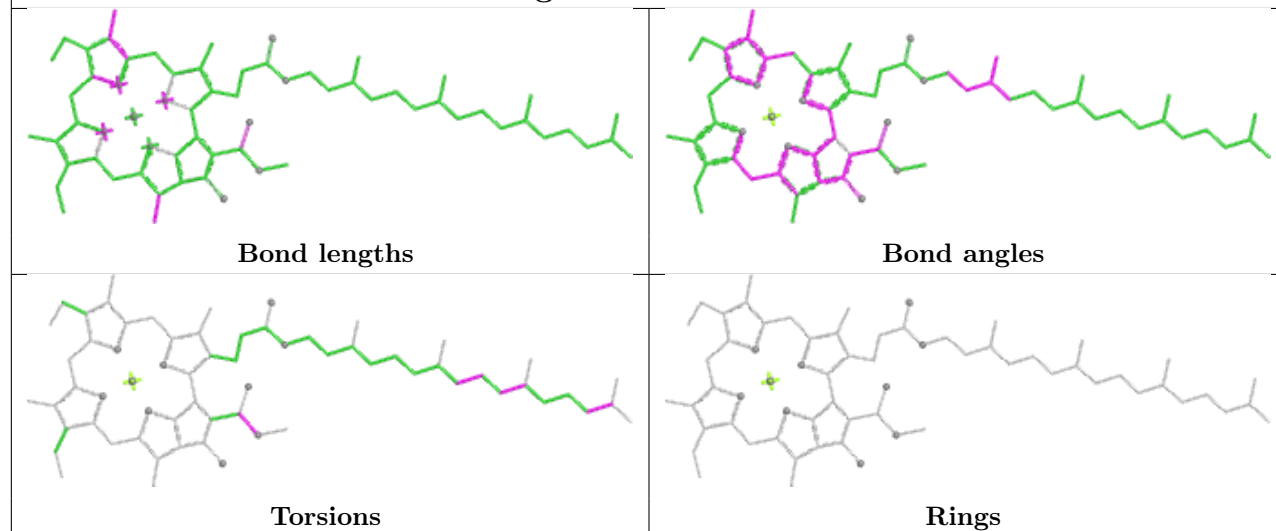
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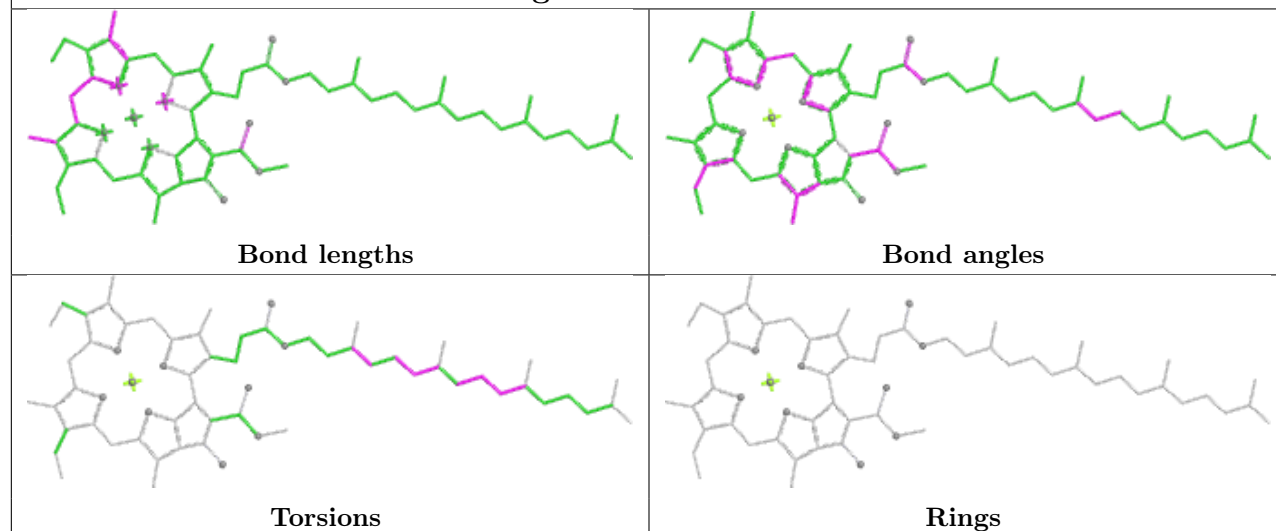
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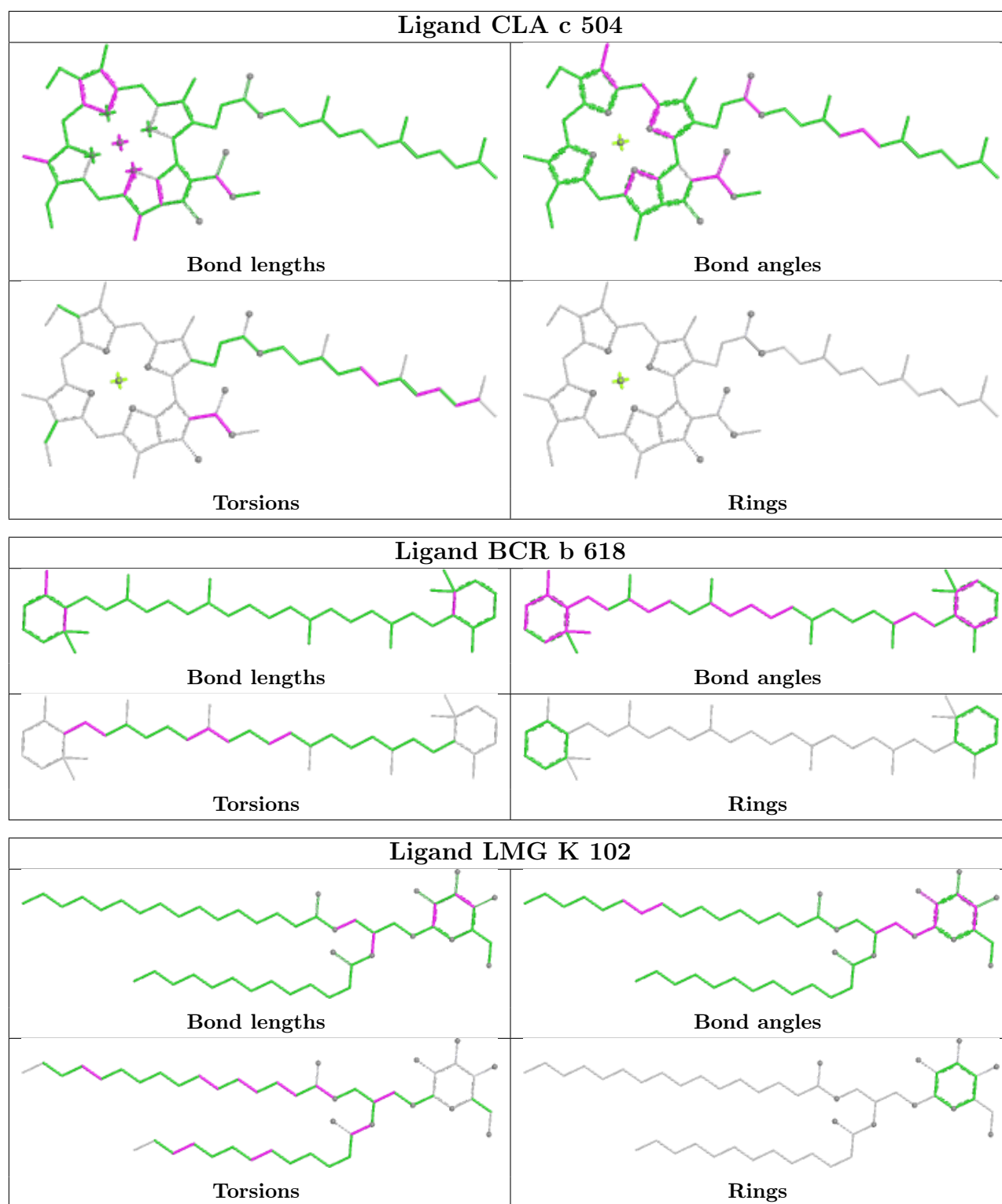


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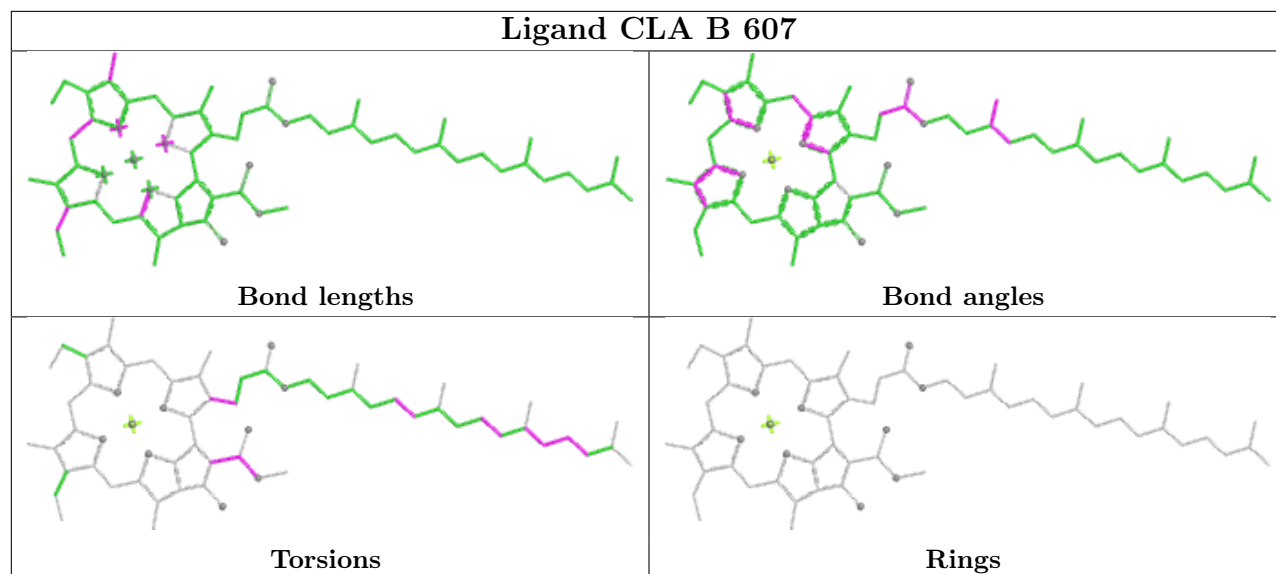


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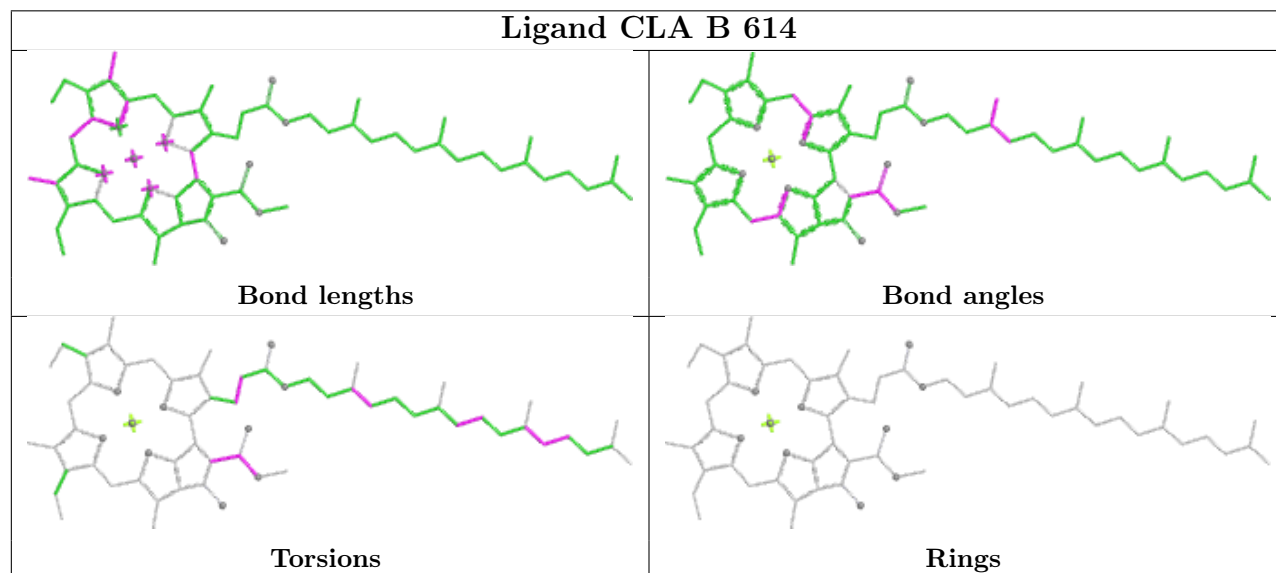




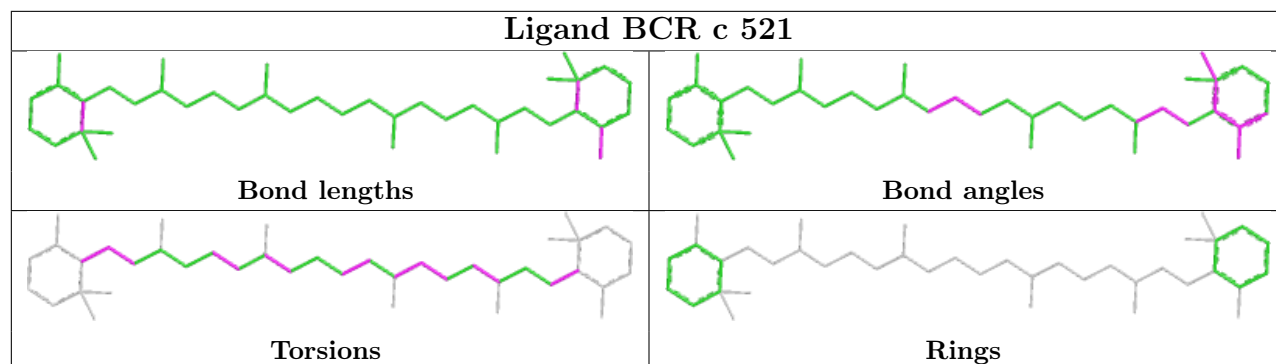
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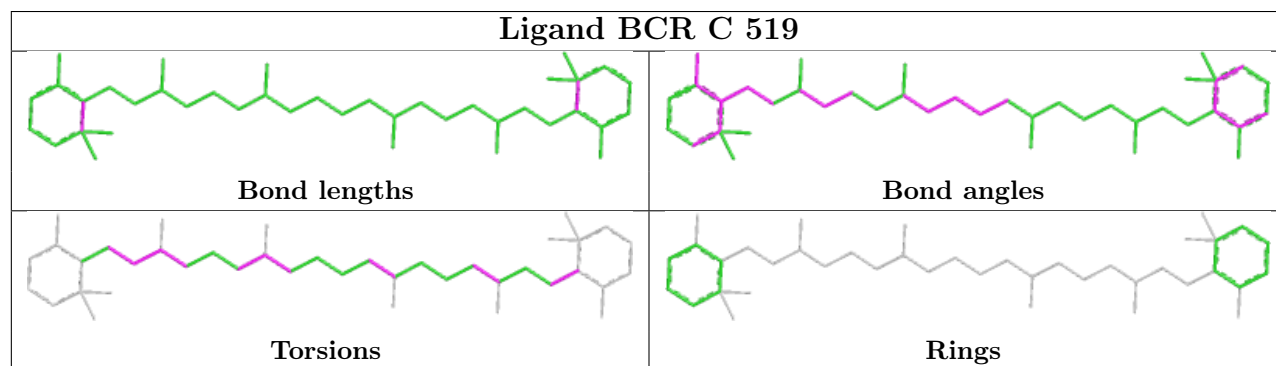
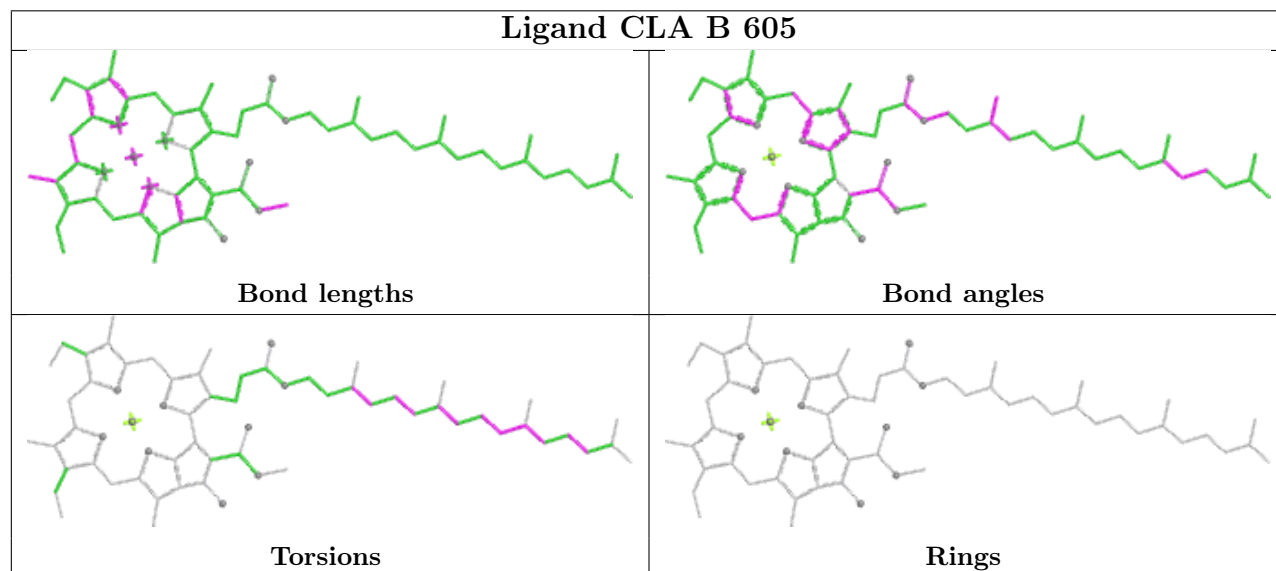
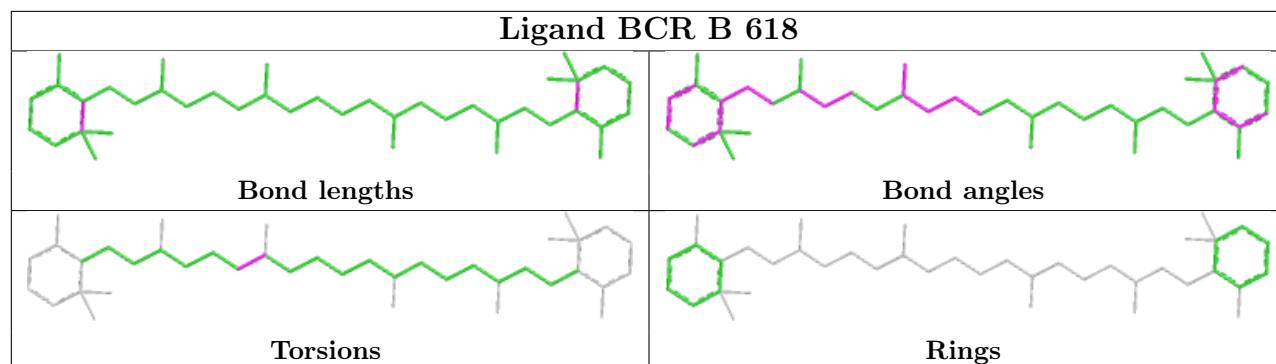


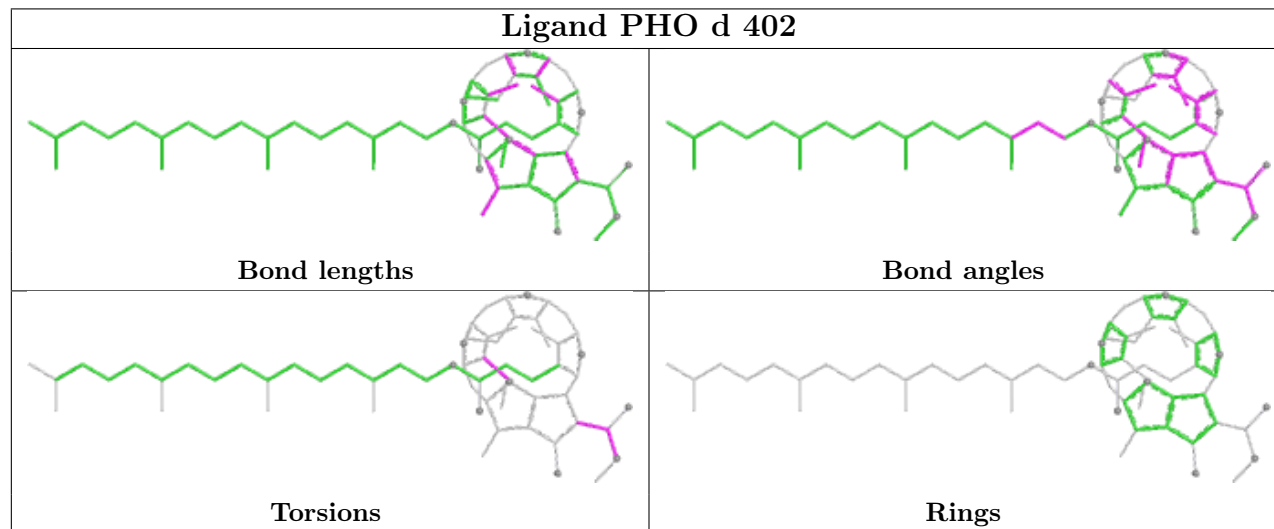
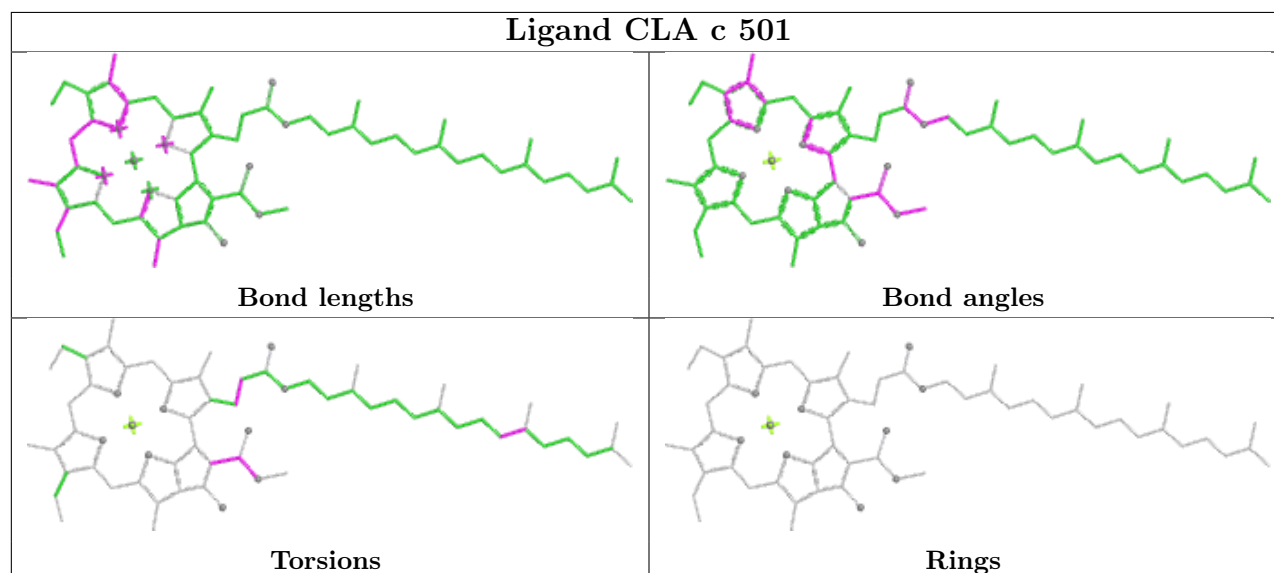
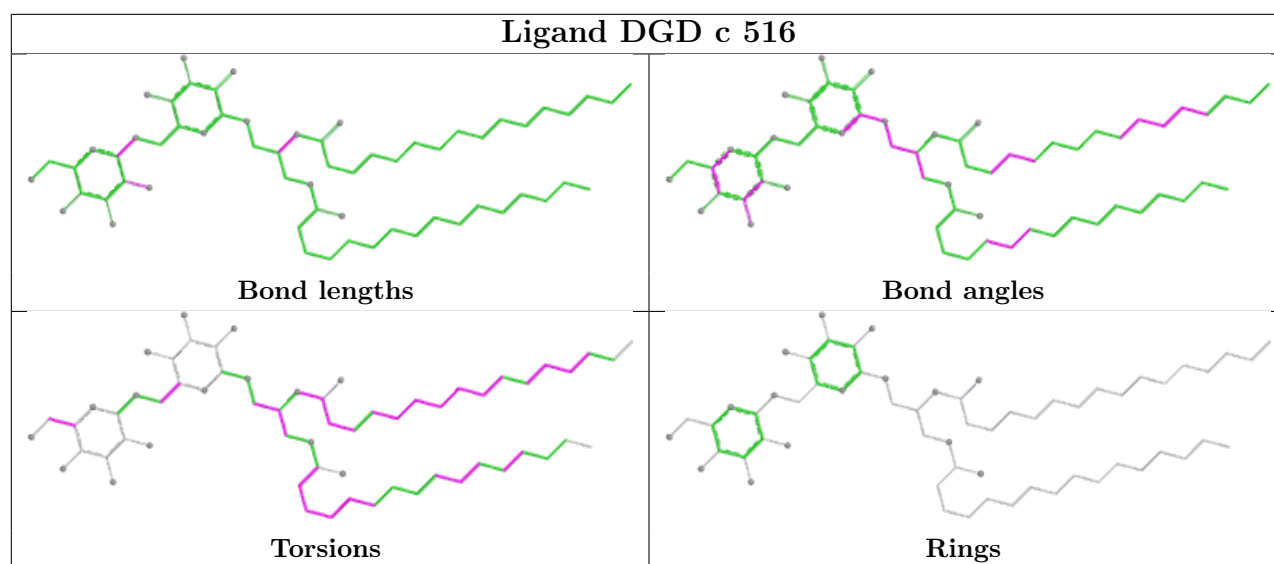
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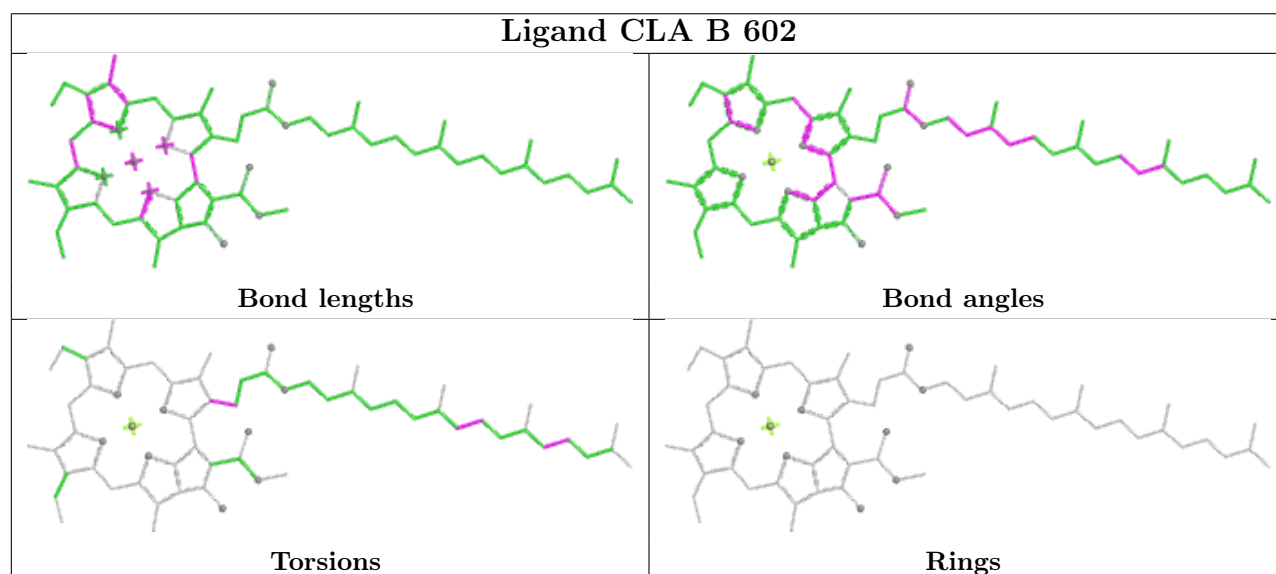
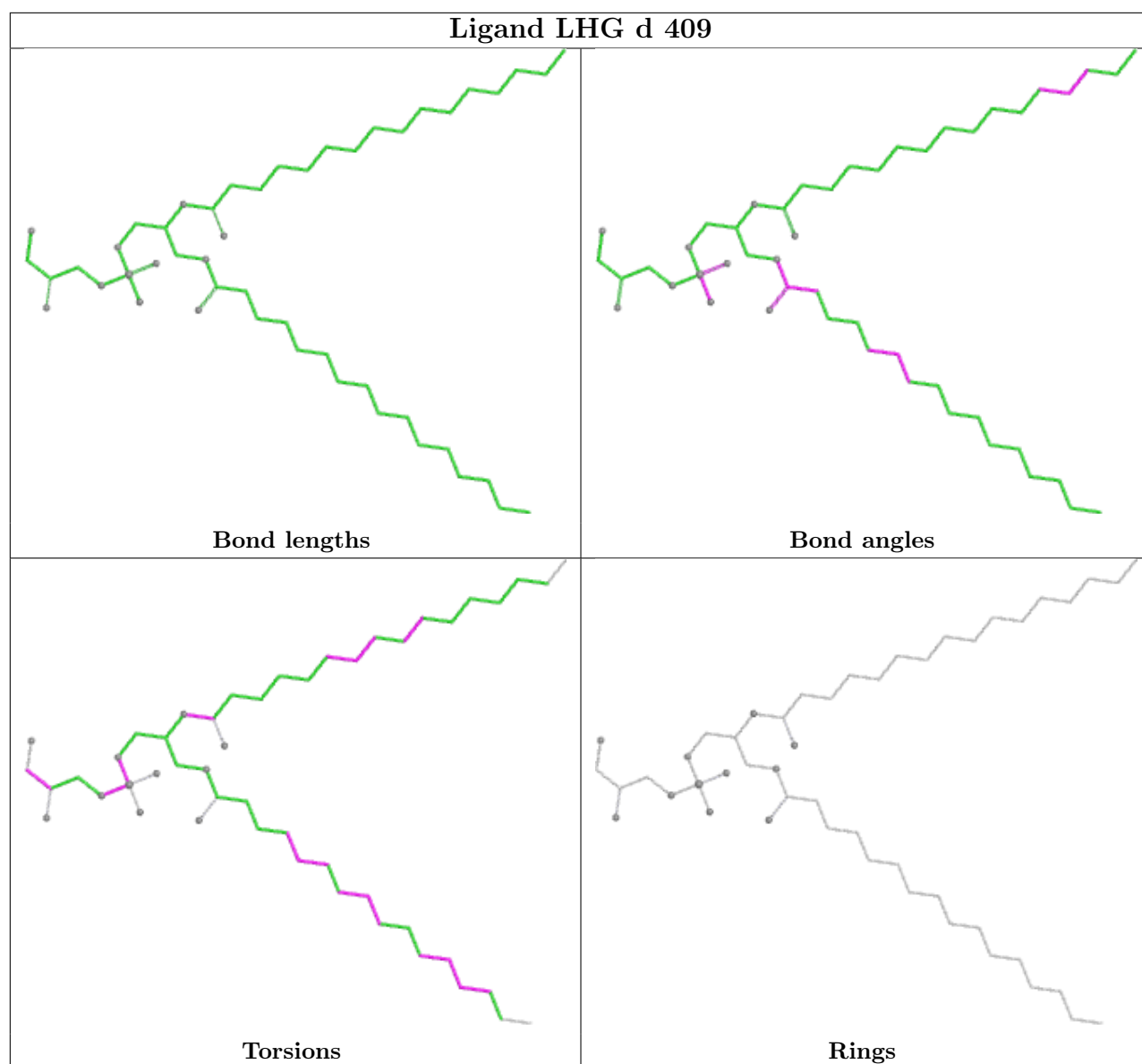


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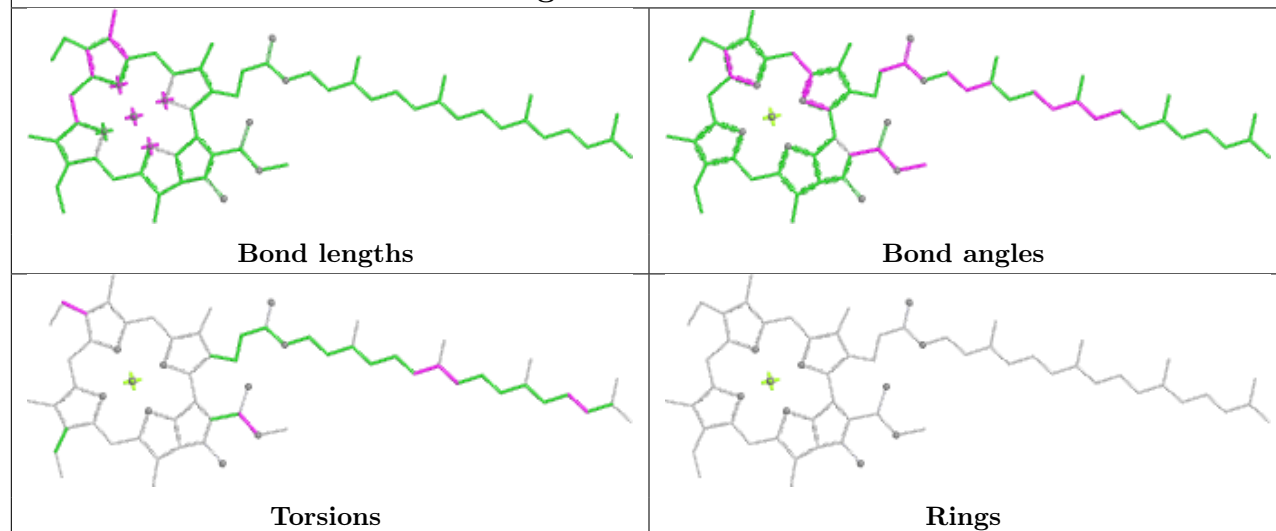




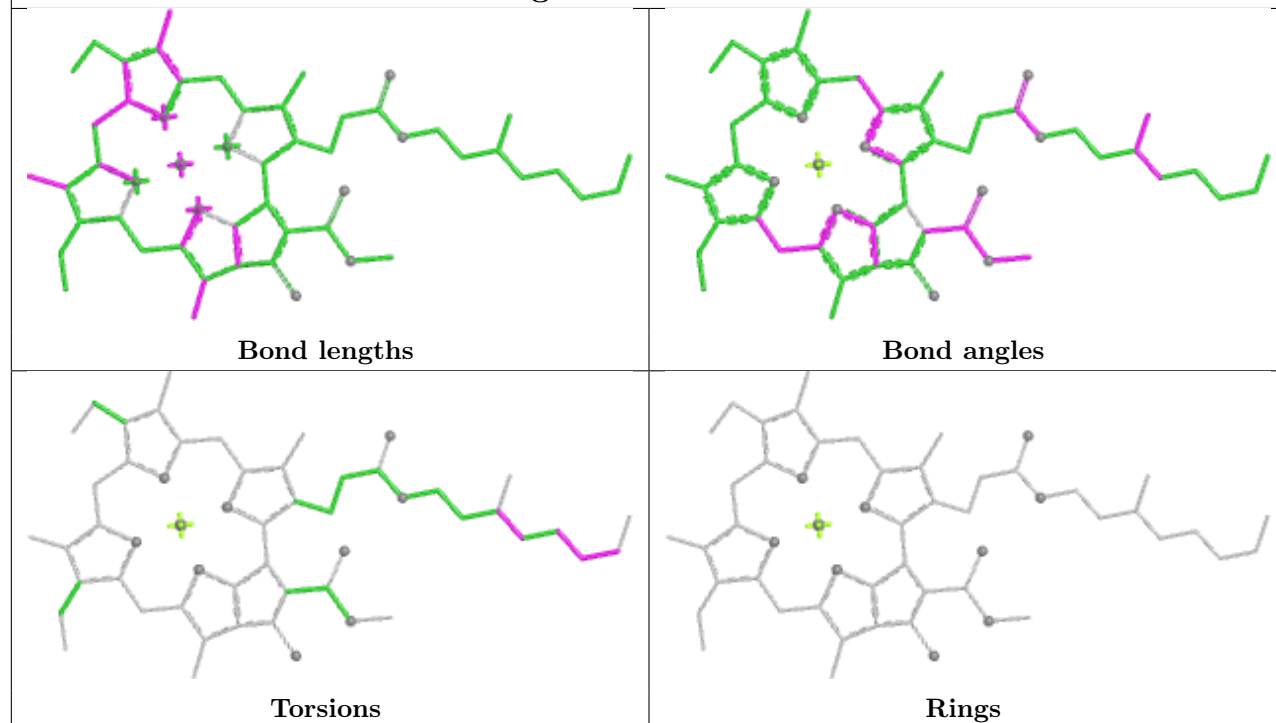


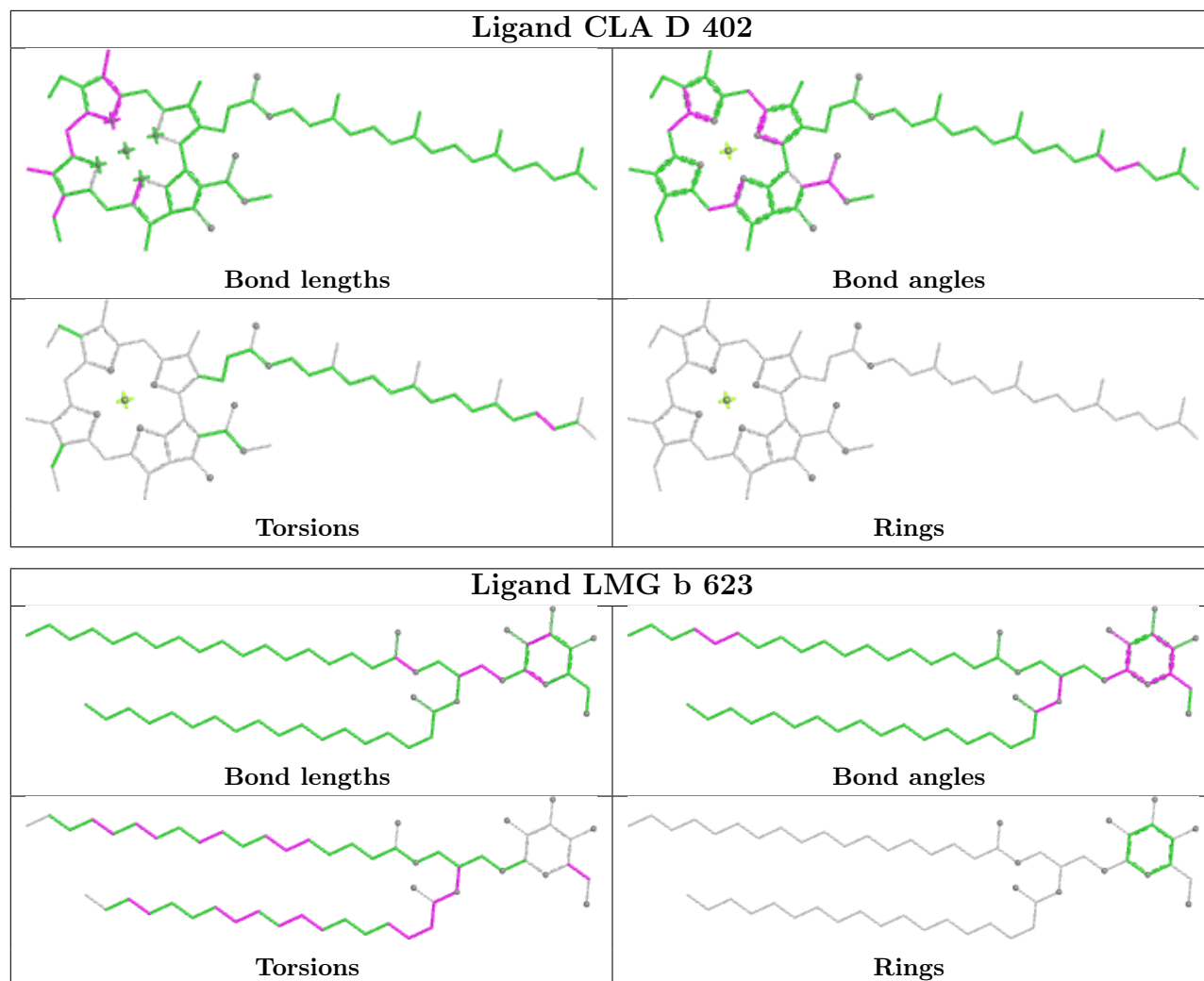


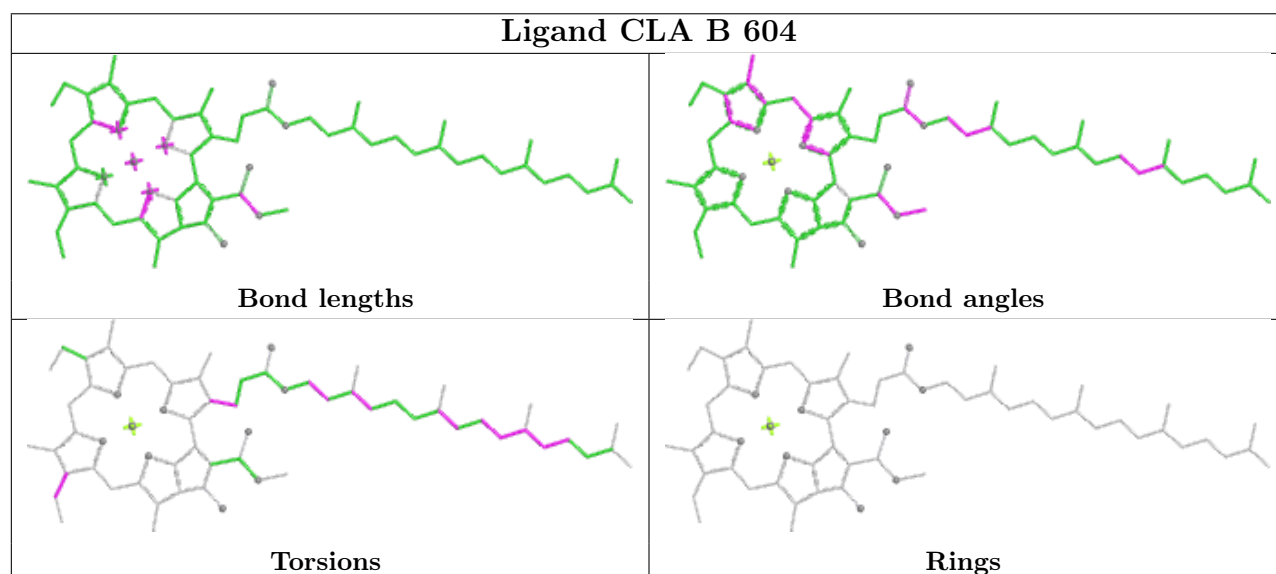
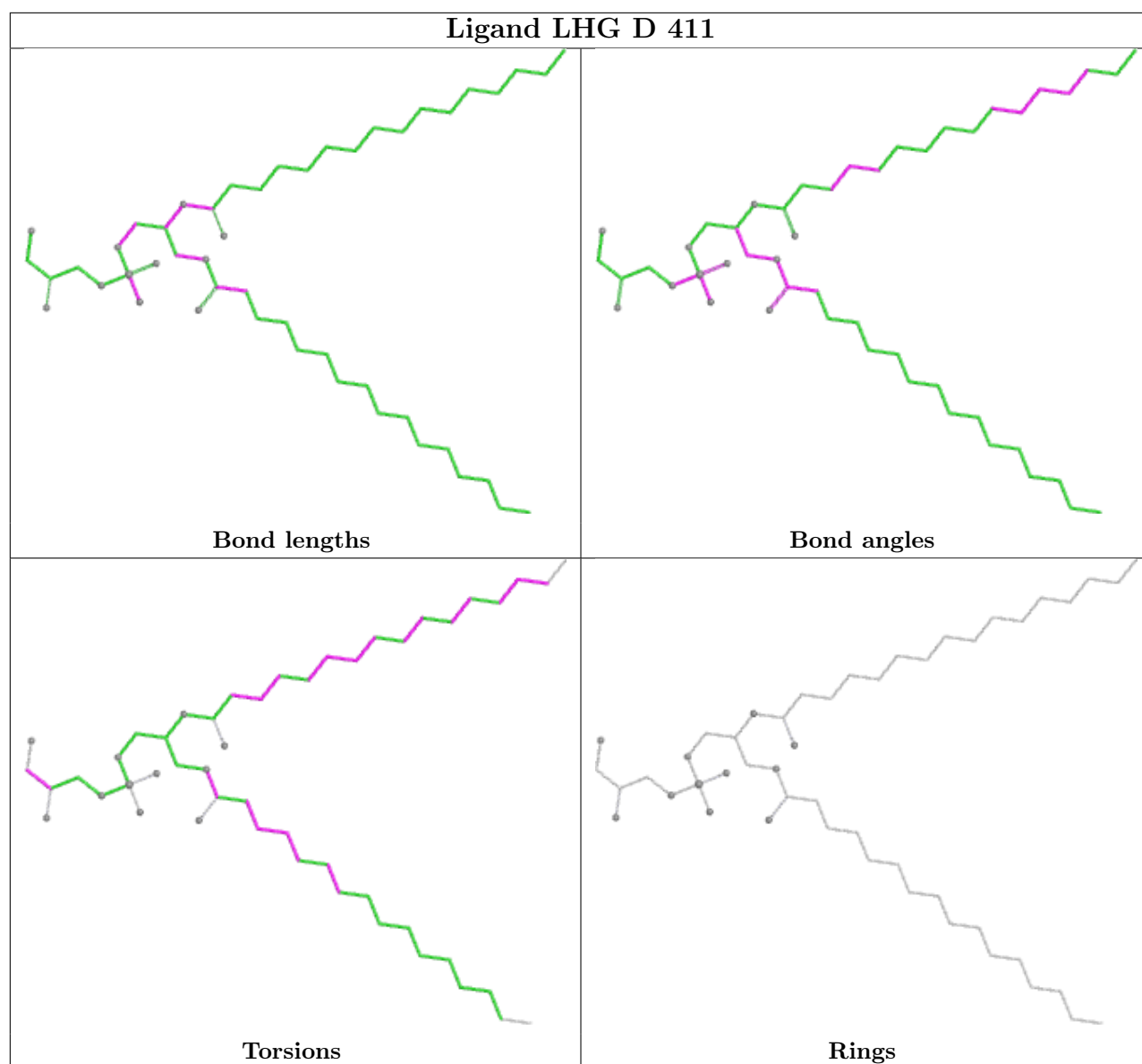
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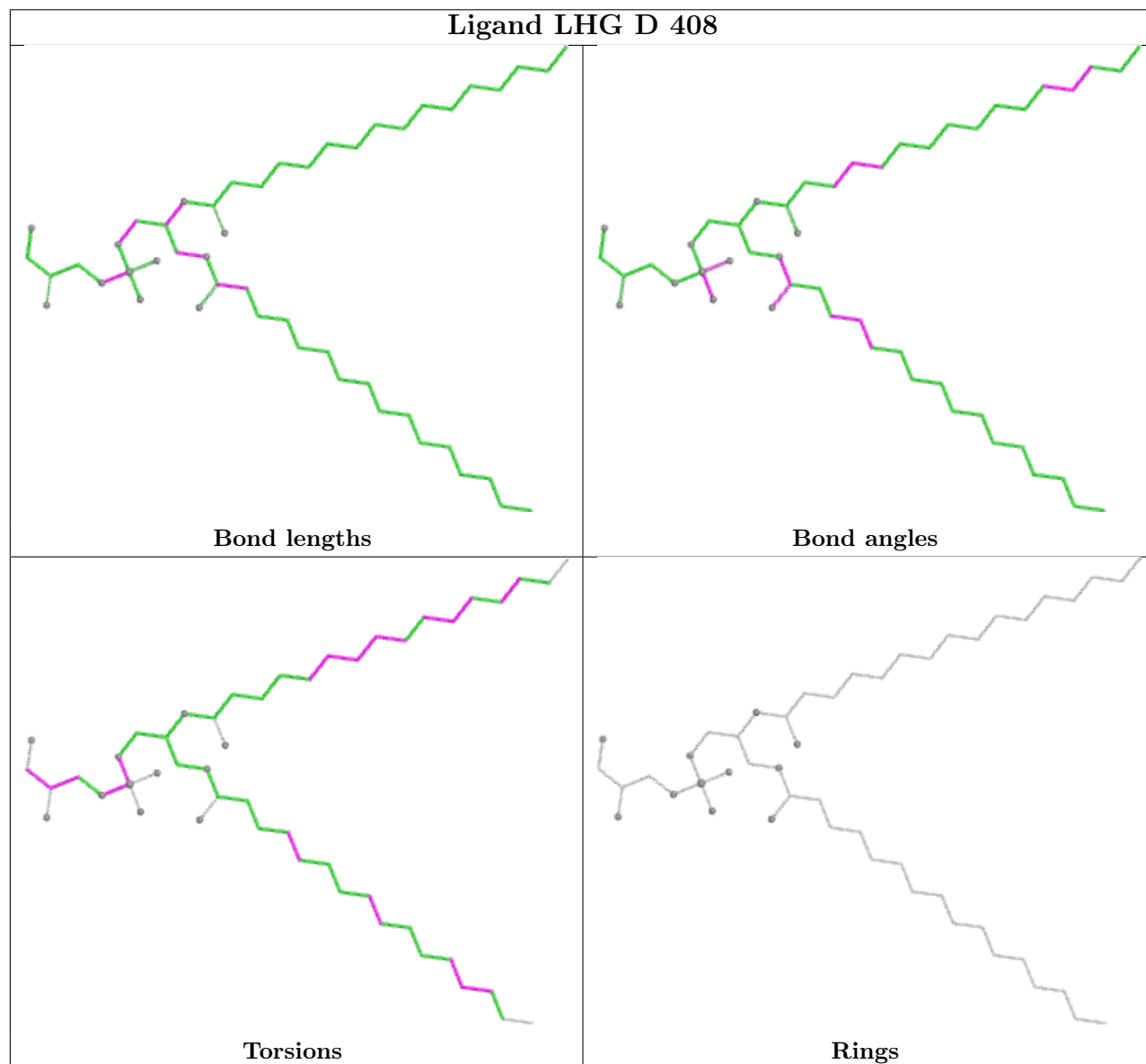
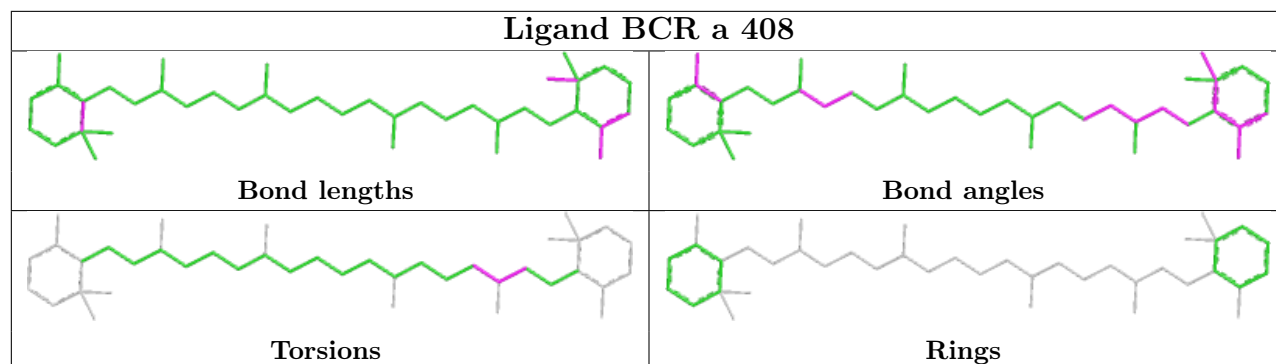


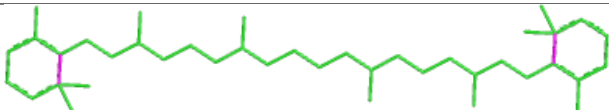
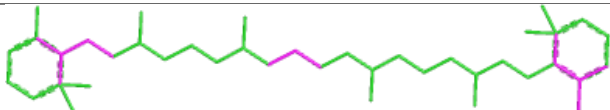
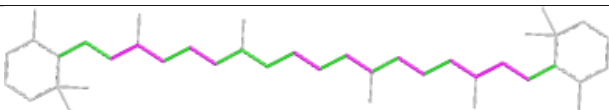
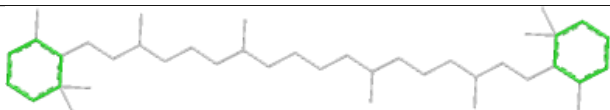
Ligand CLA A 408

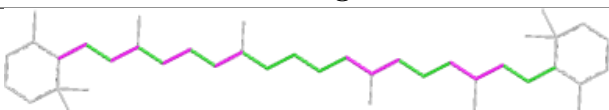
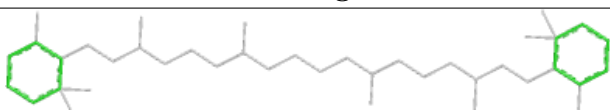


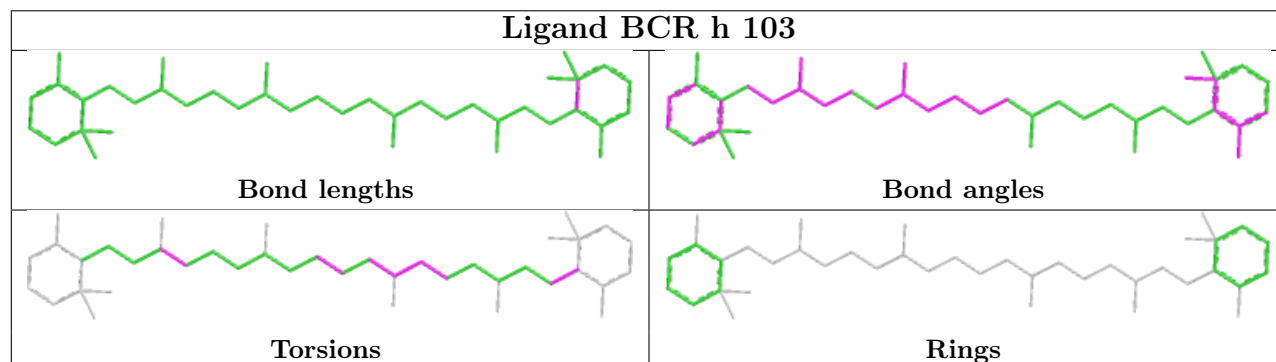
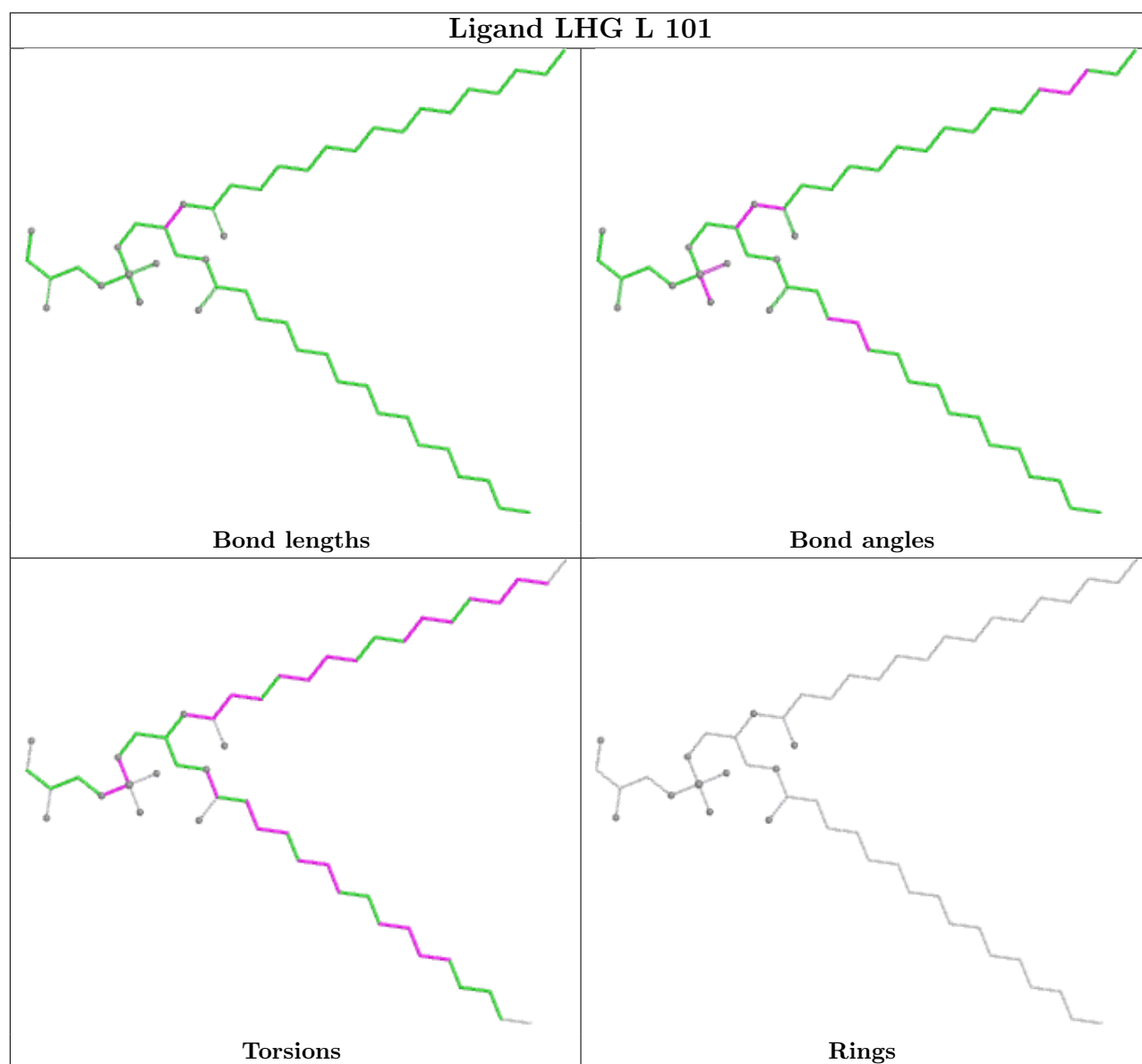


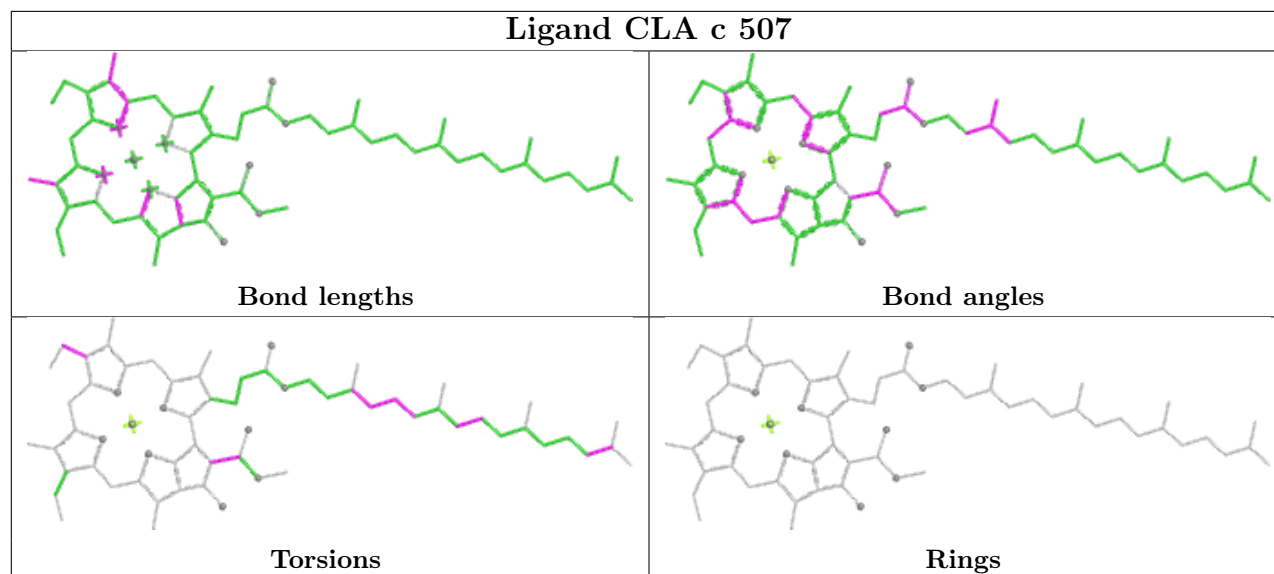
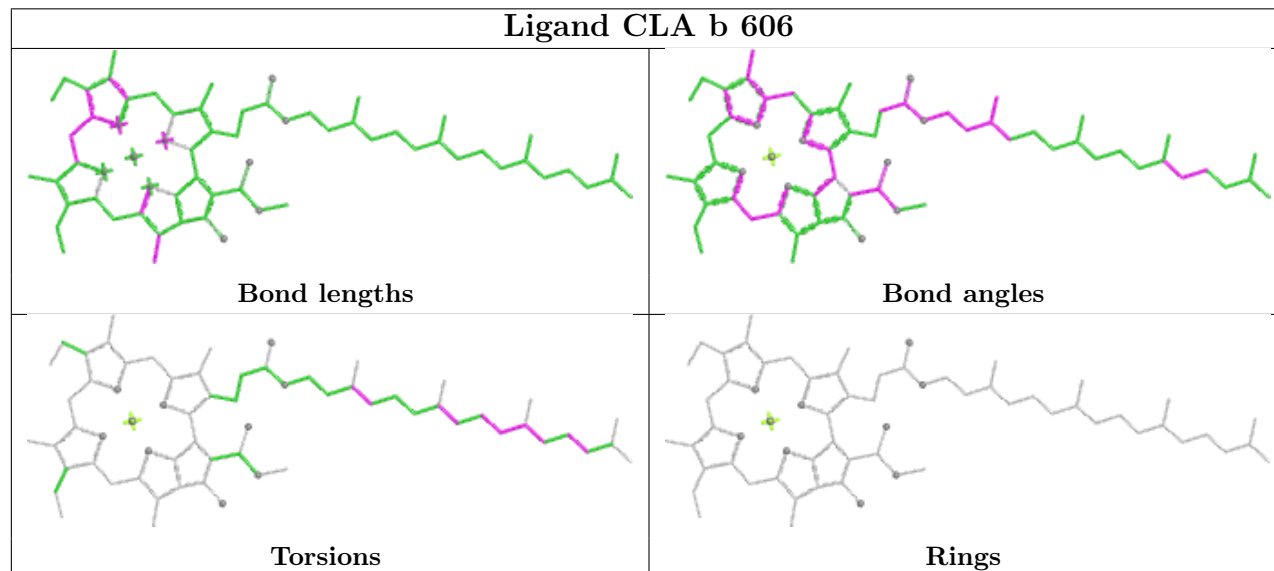




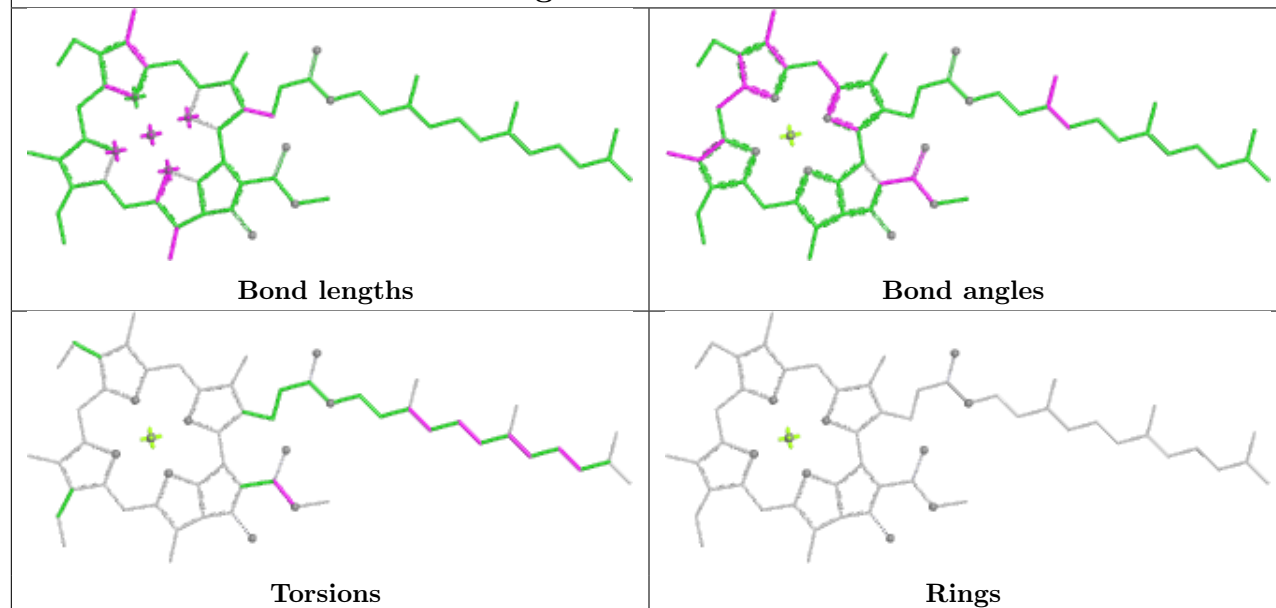
Ligand BCR d 406	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR b 602	
	
Bond lengths	Bond angles
	
Torsions	Rings

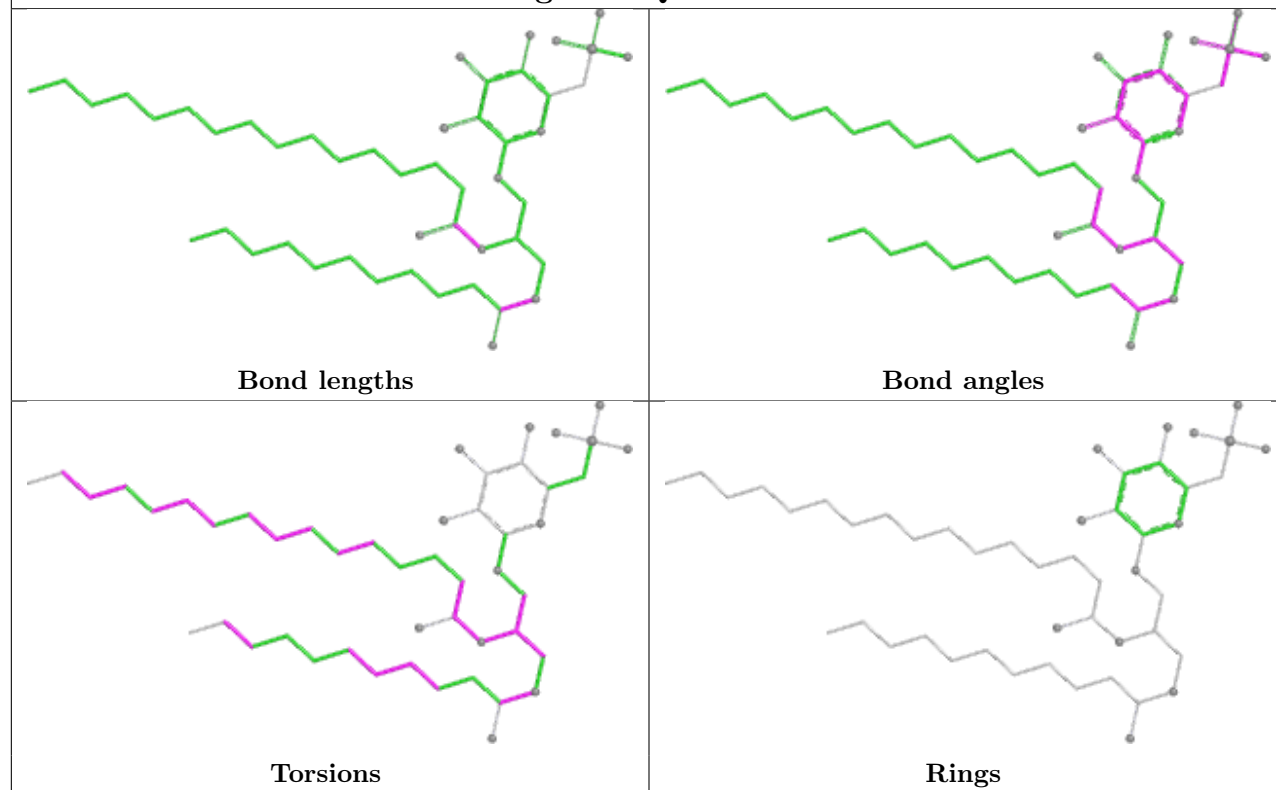


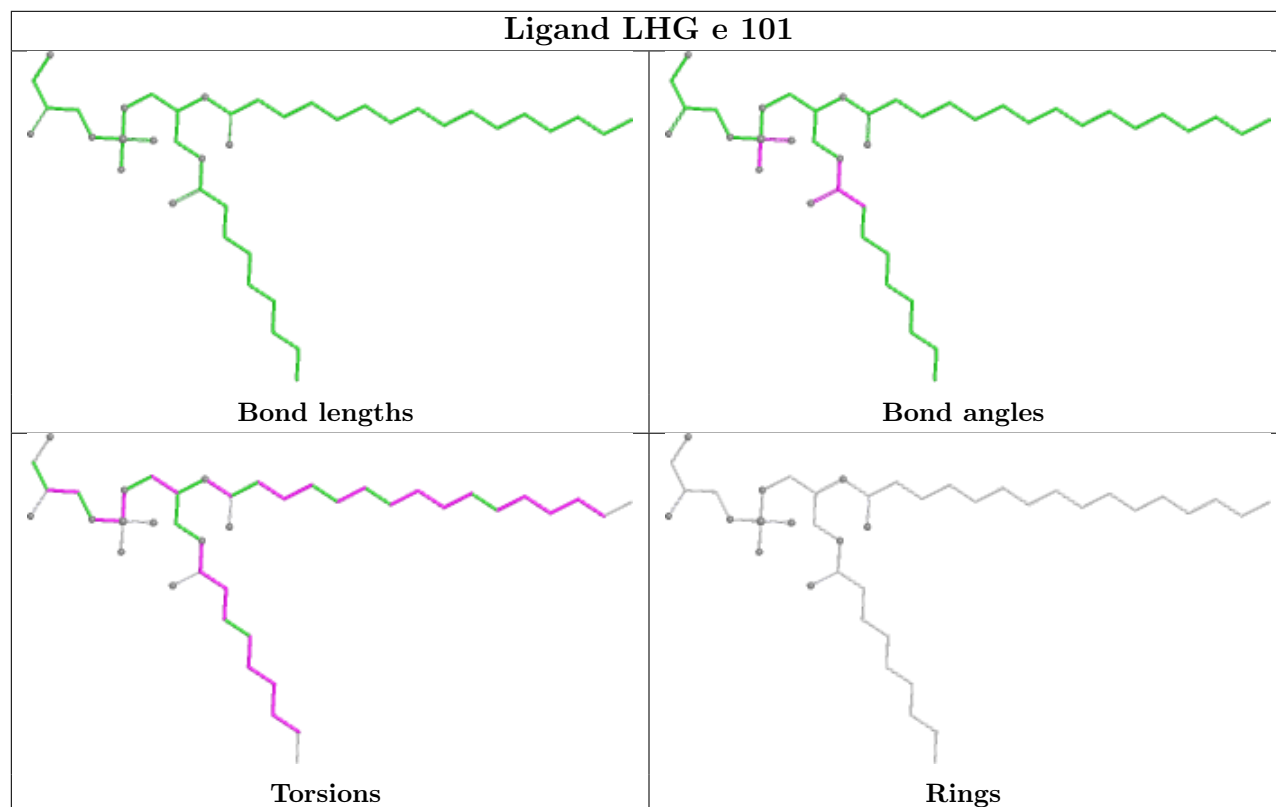
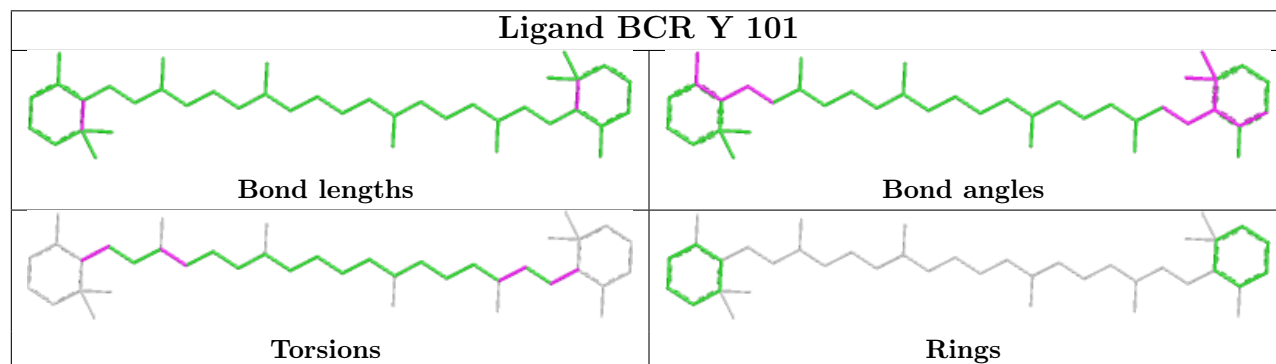
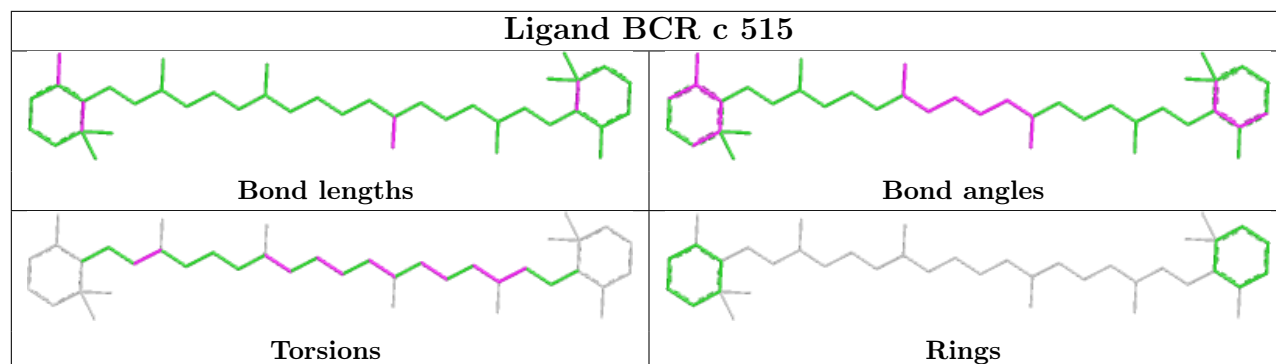
Ligand CLA c 507**Ligand CLA b 606**

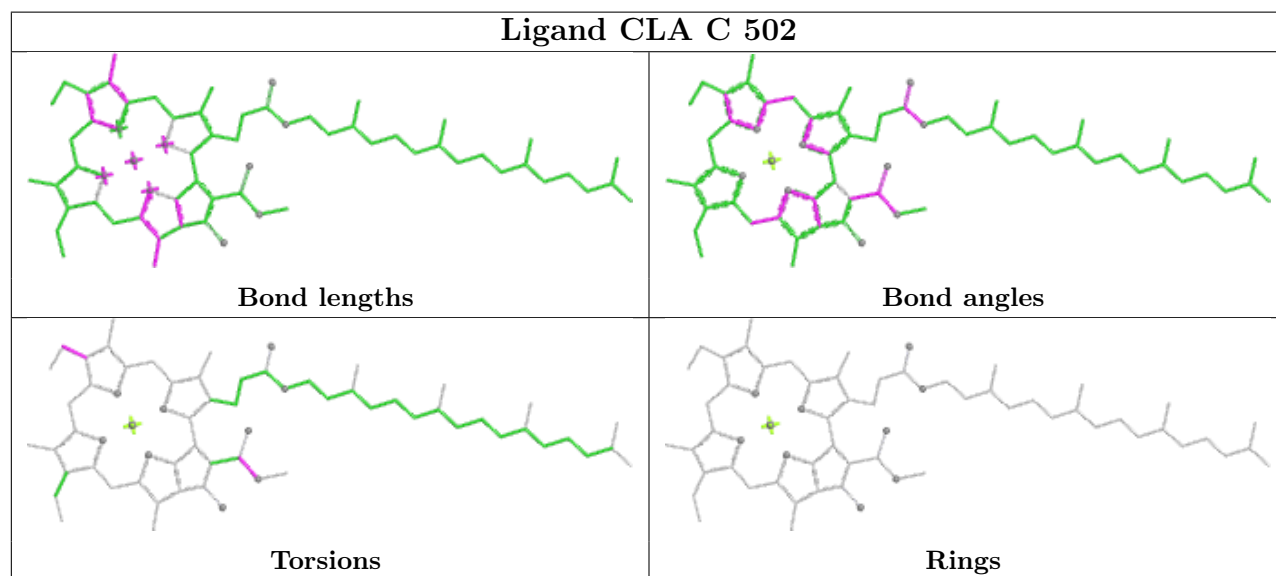
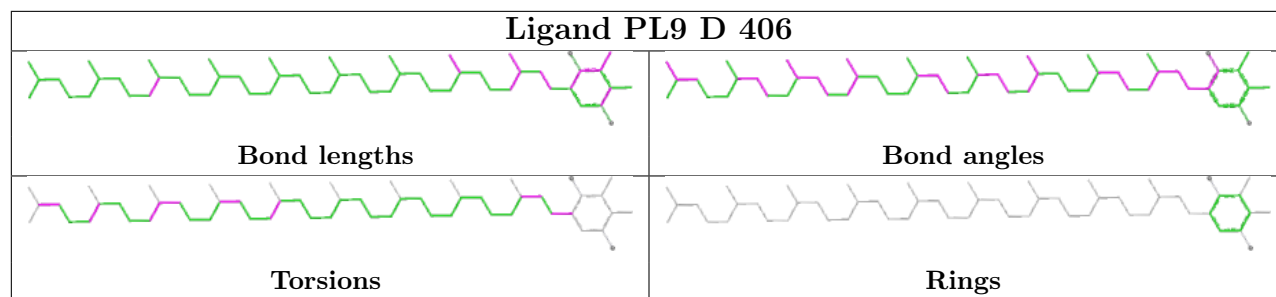
Ligand CLA b 617



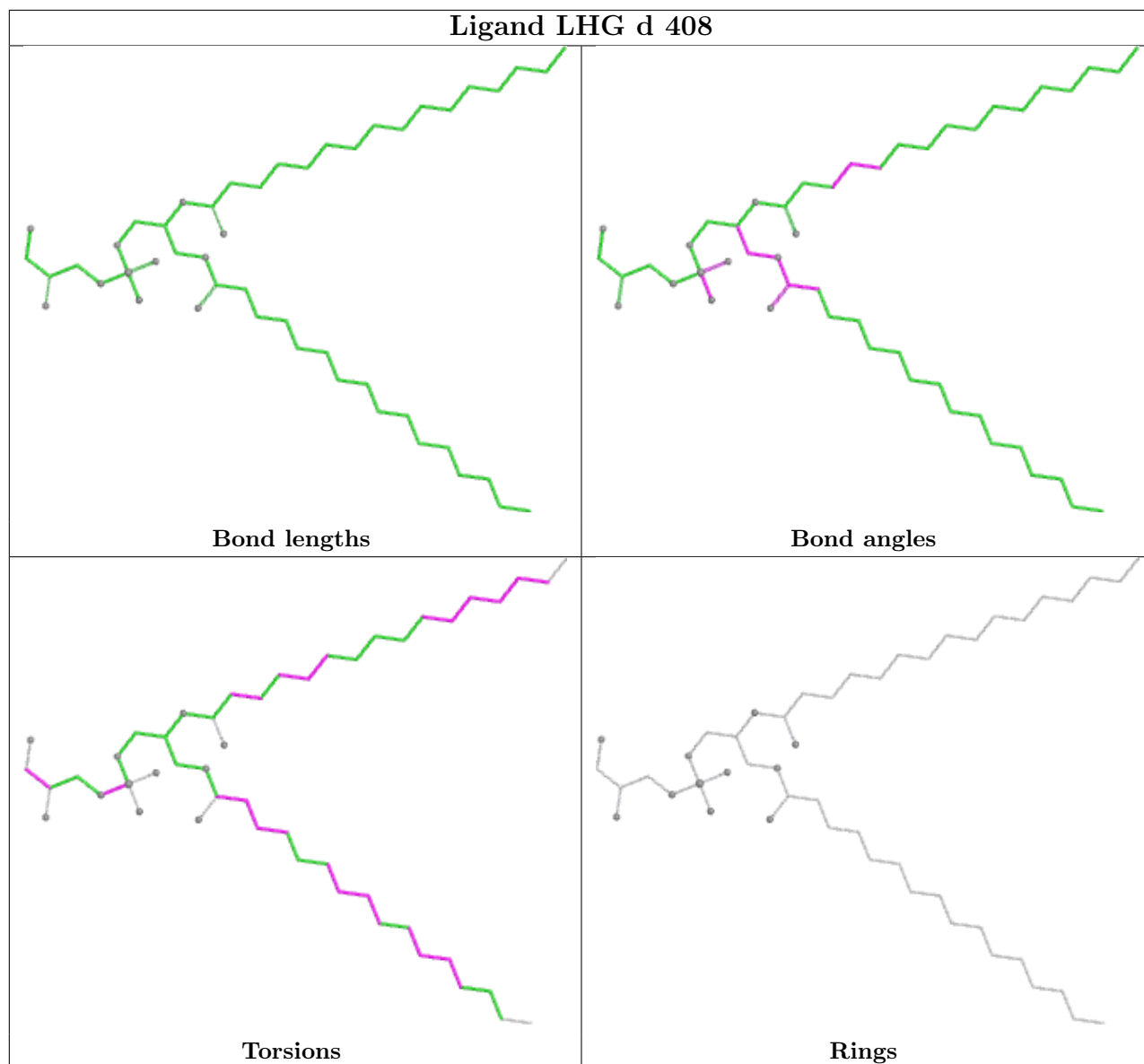
Ligand SQD b 601



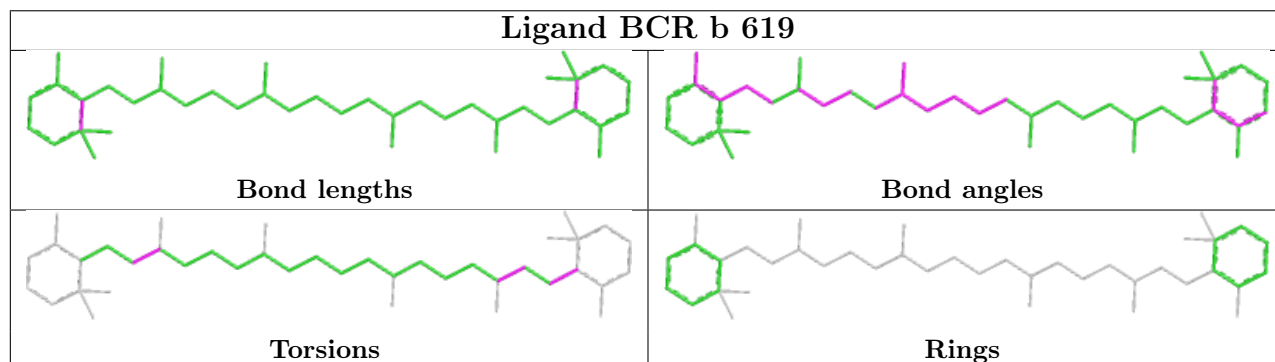


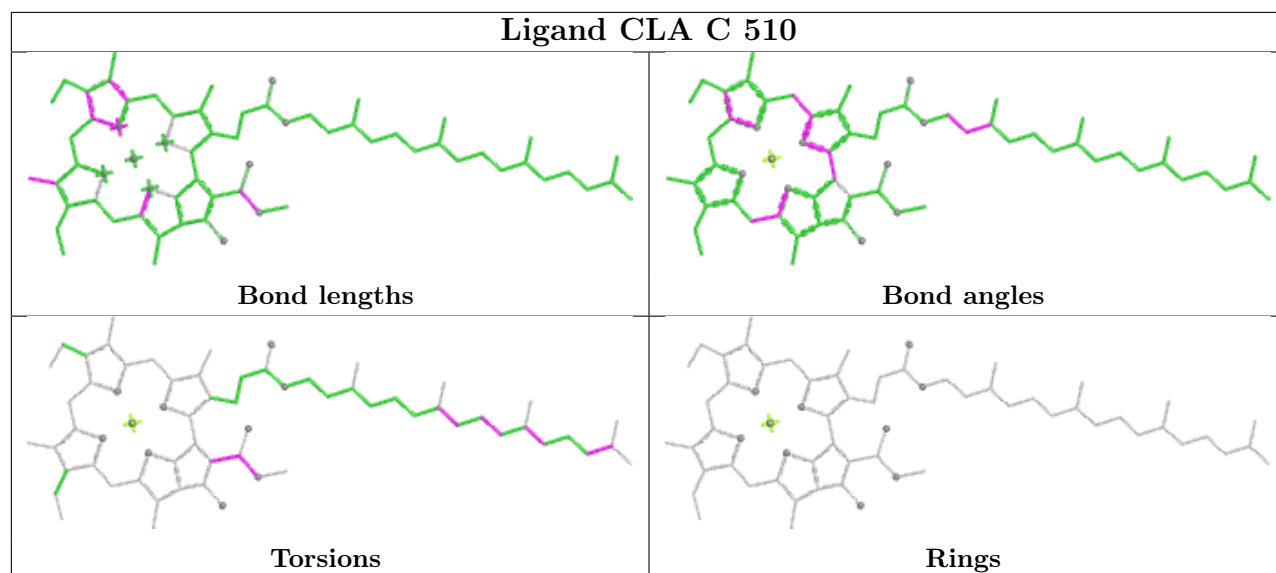
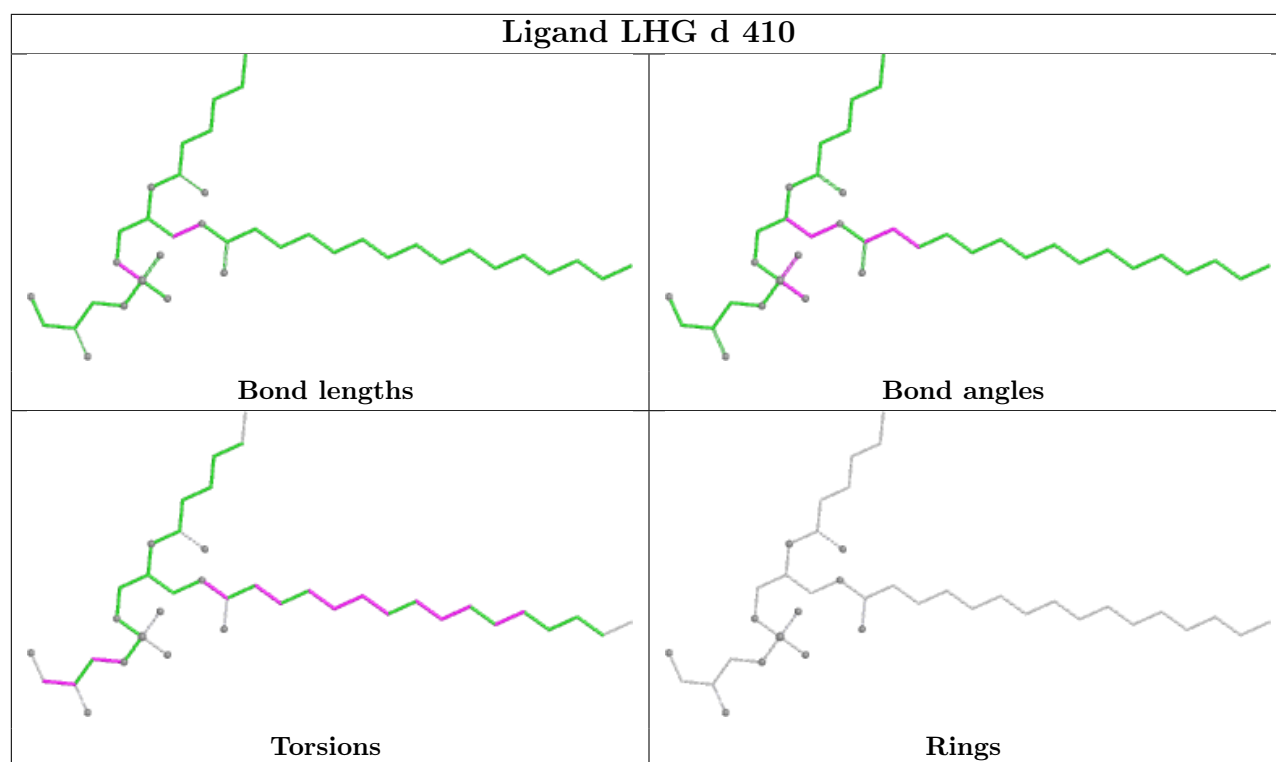


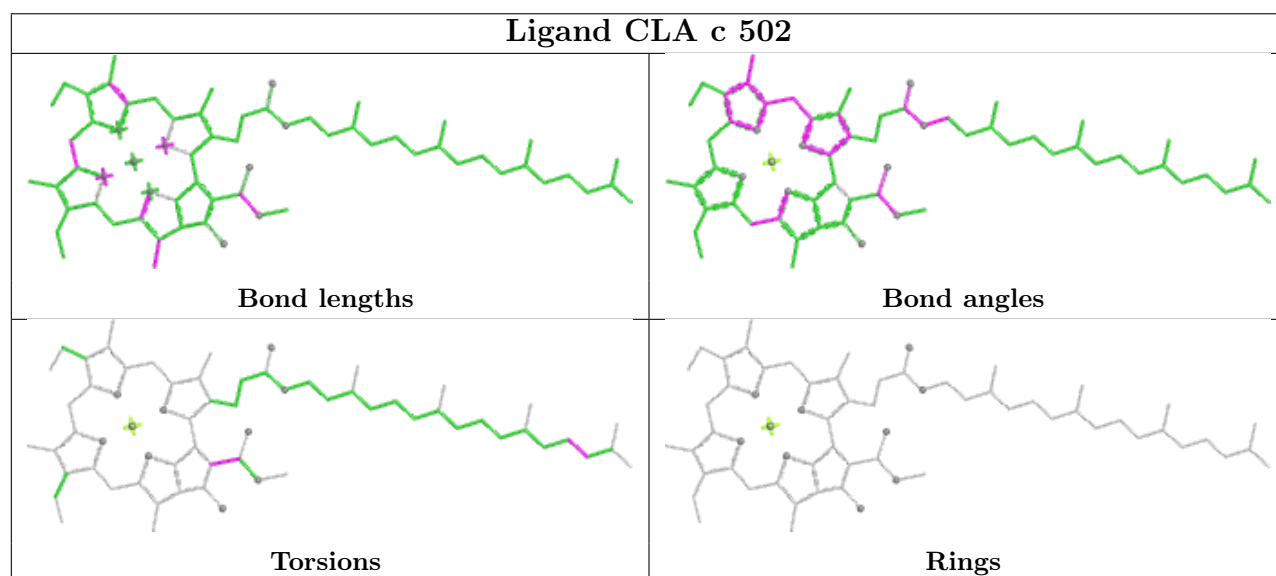
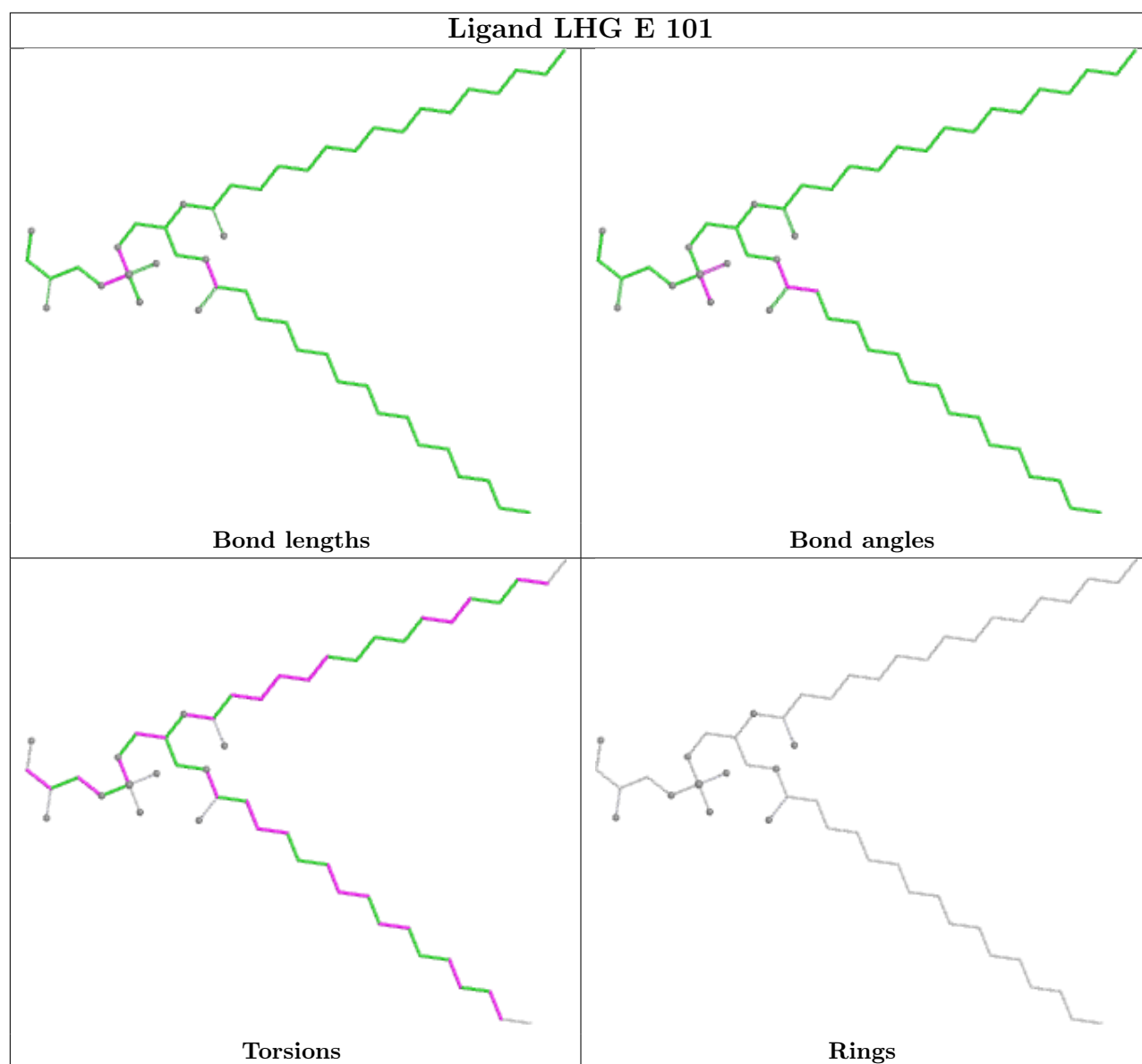
Ligand LHG d 408

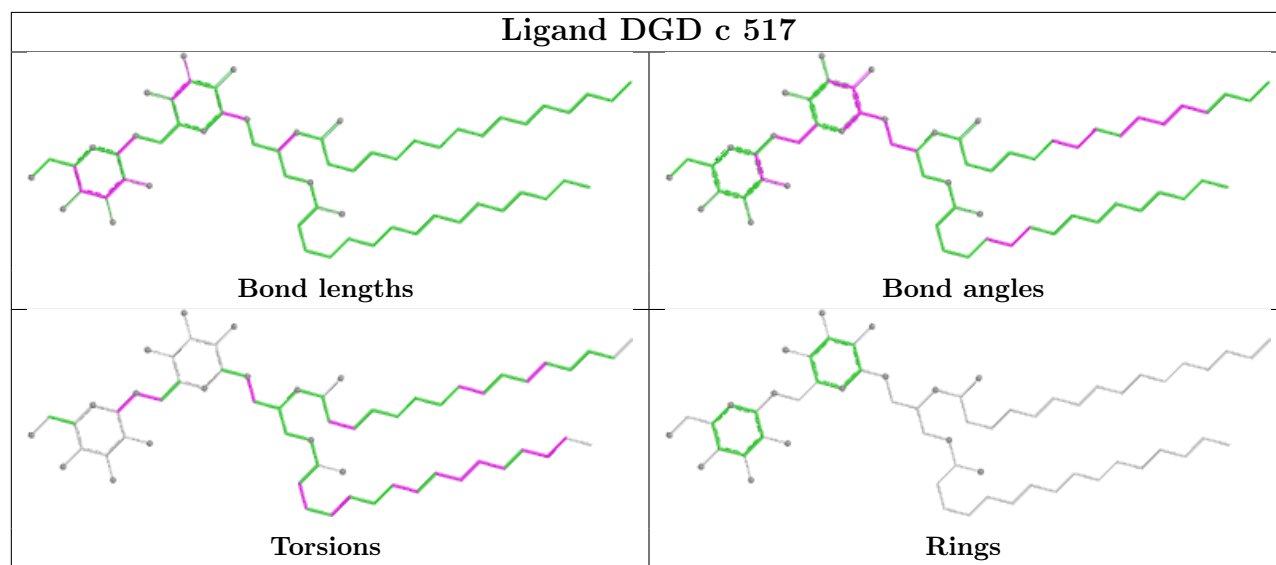
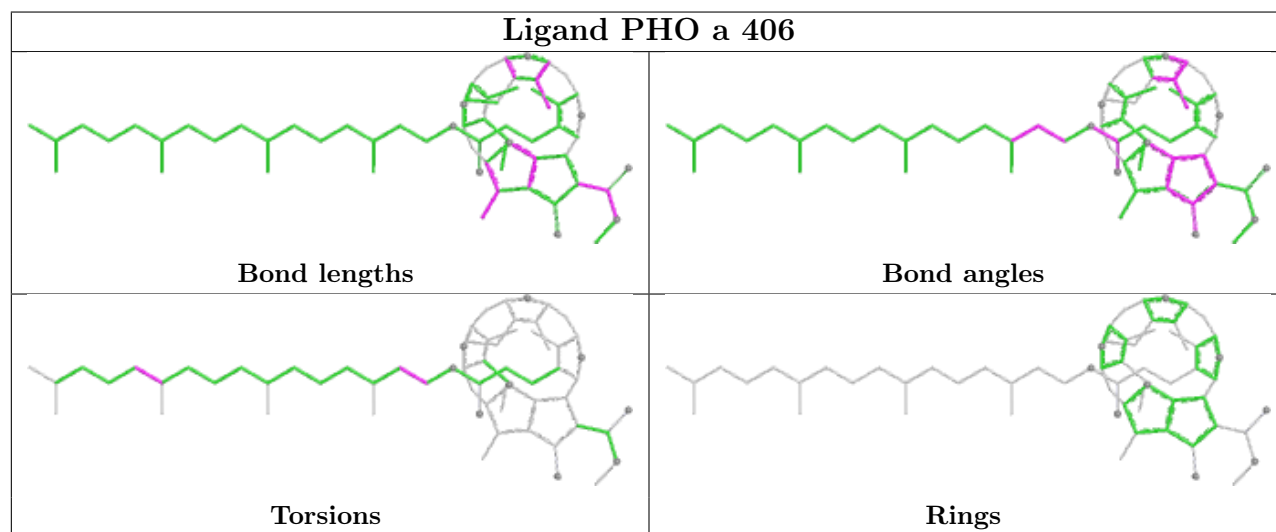
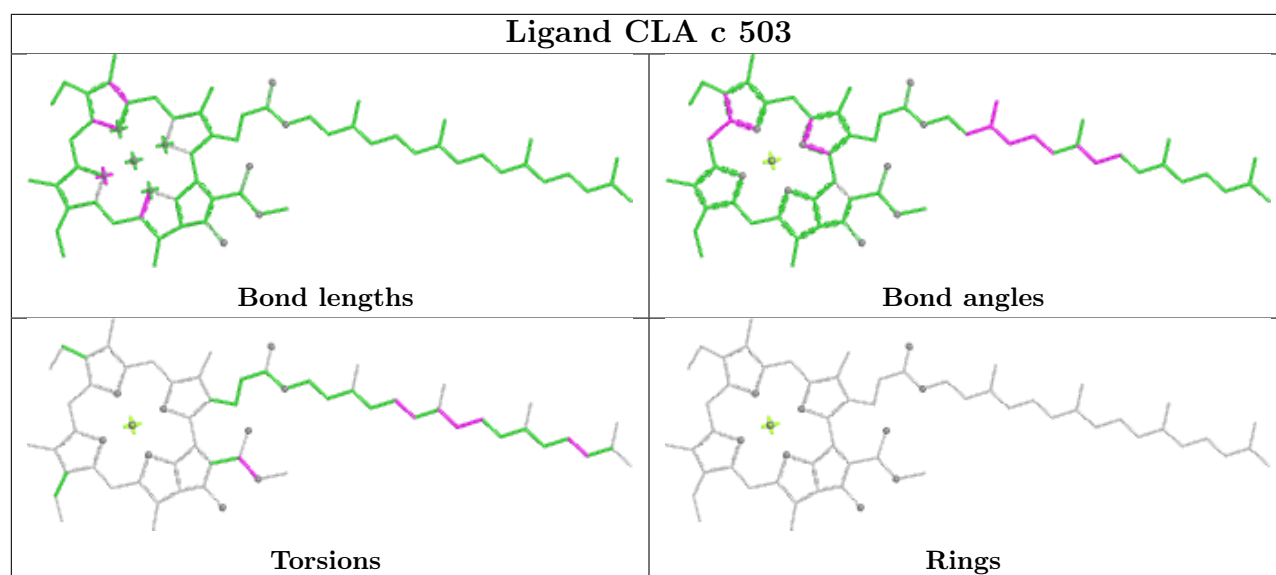


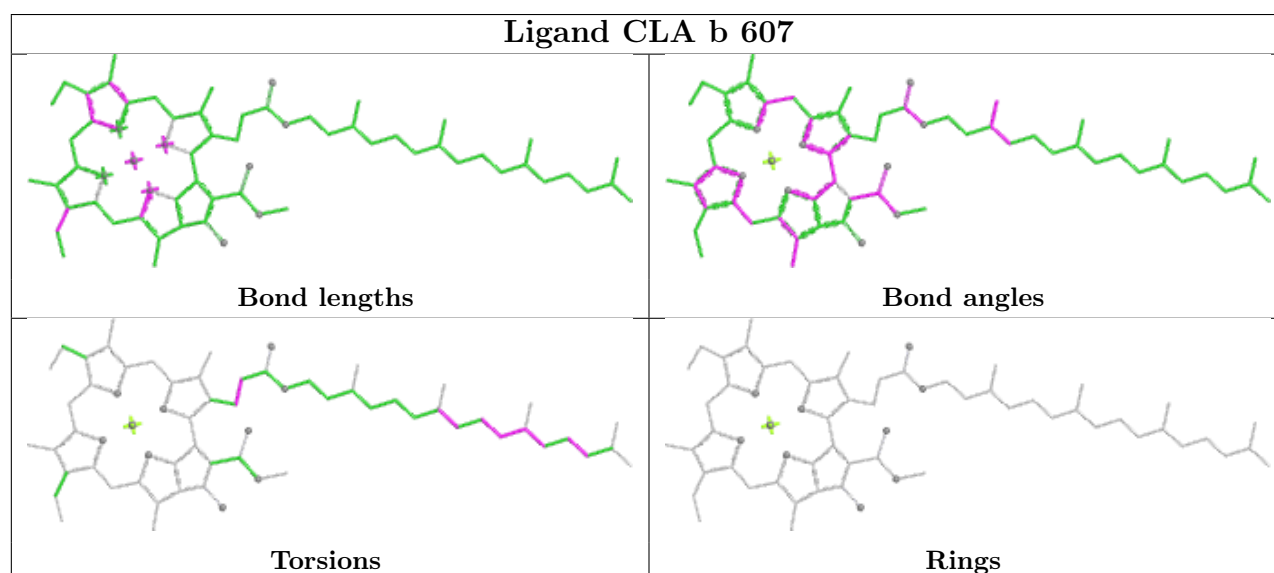
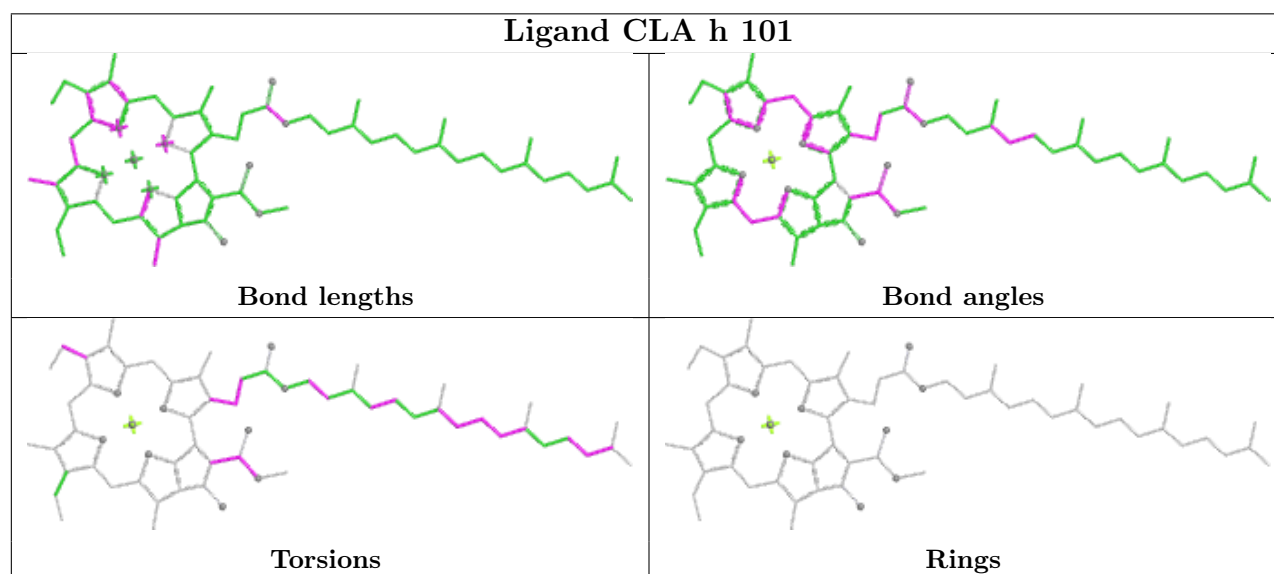
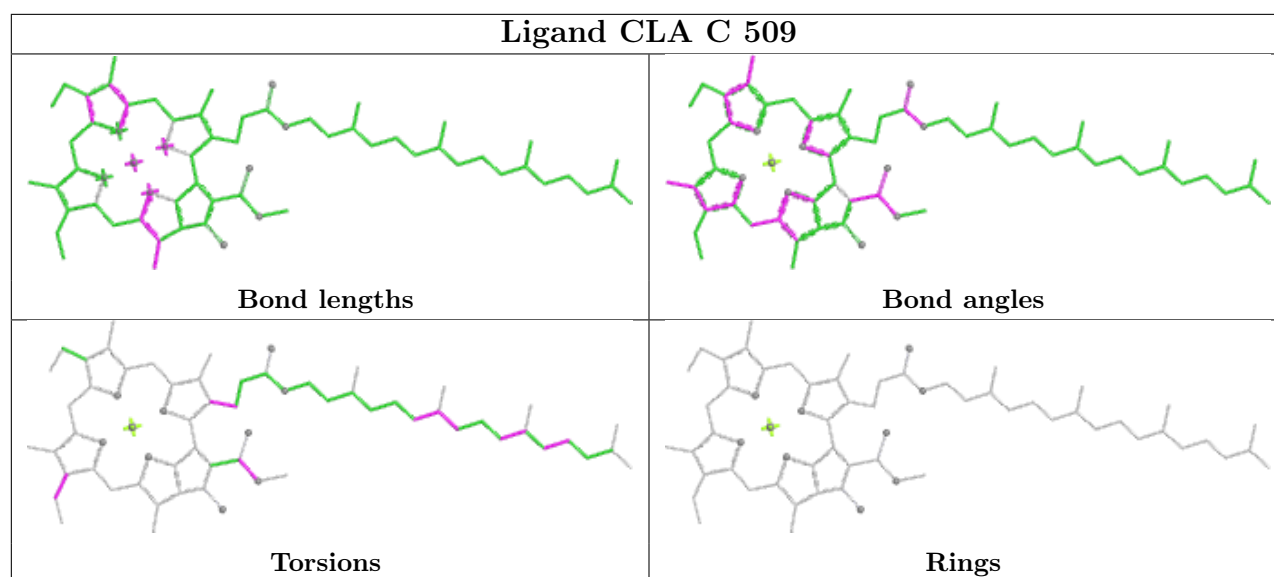
Ligand BCR b 619



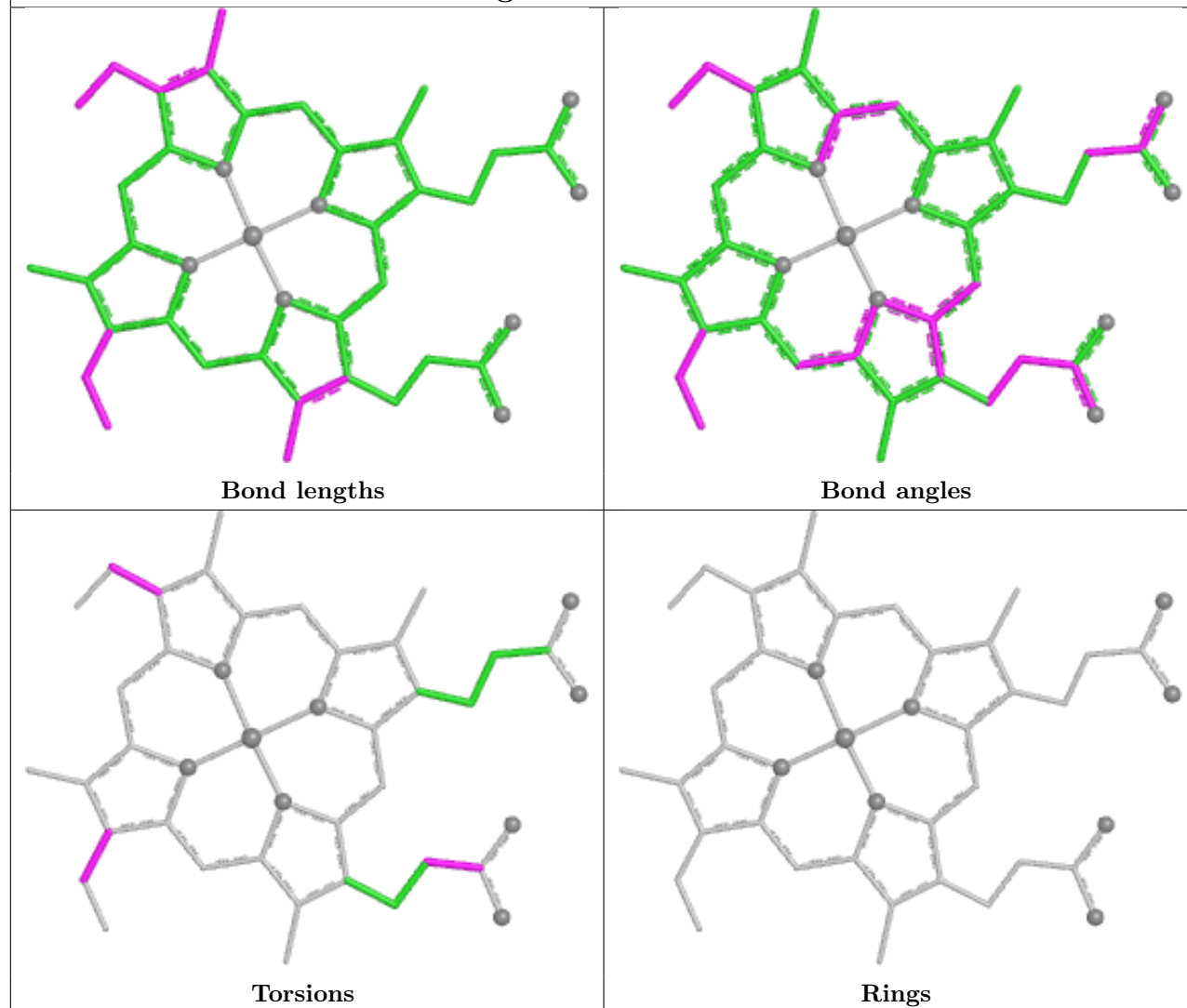




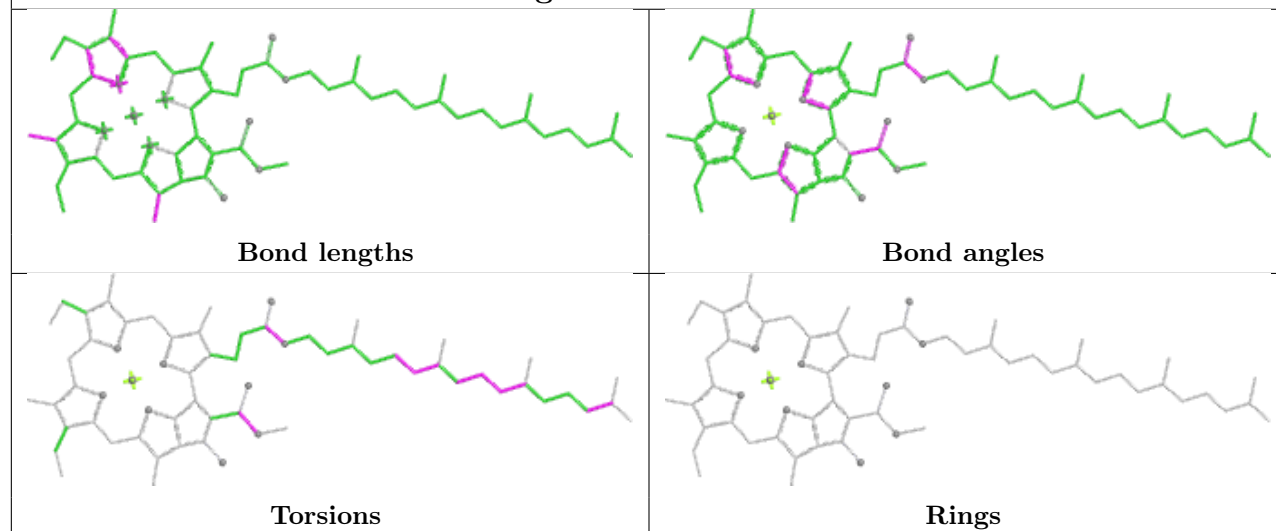


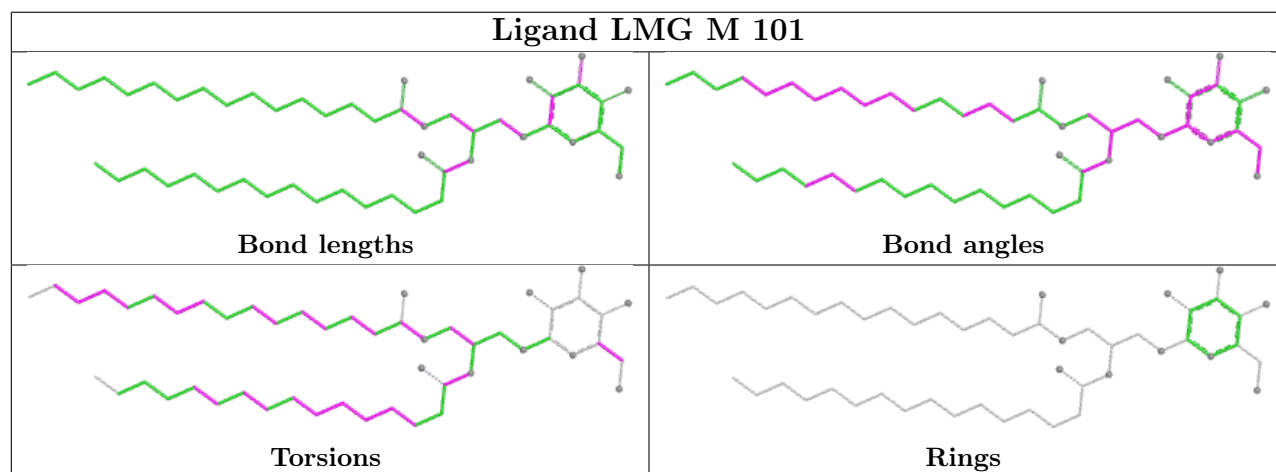
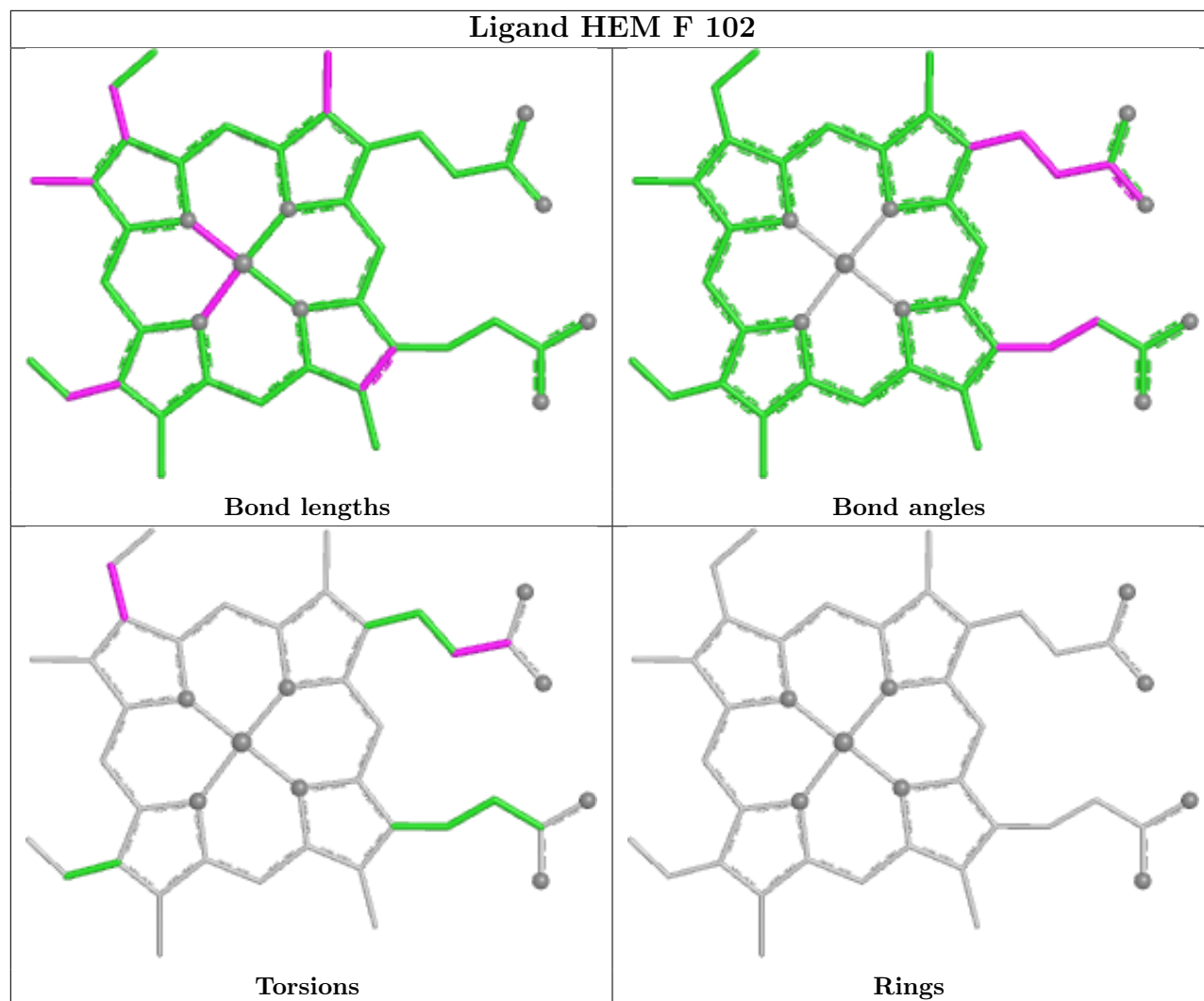


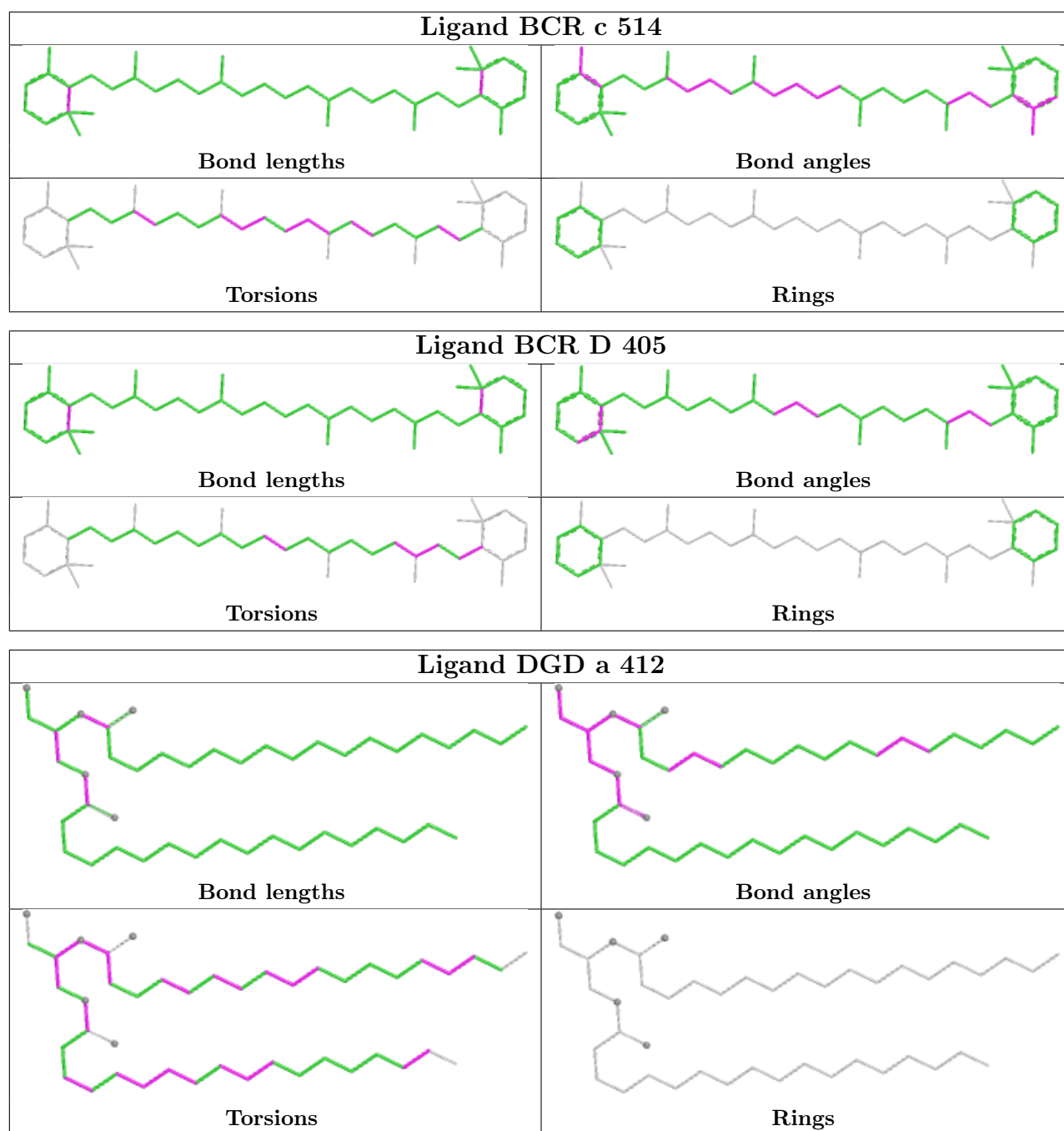
Ligand HEC v 201

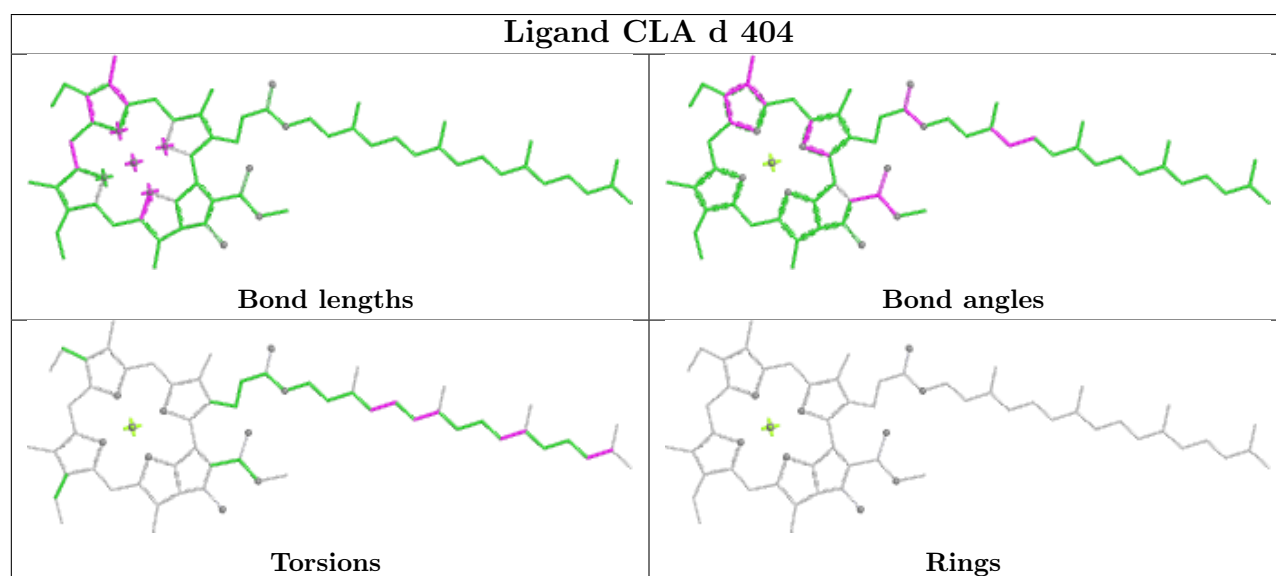
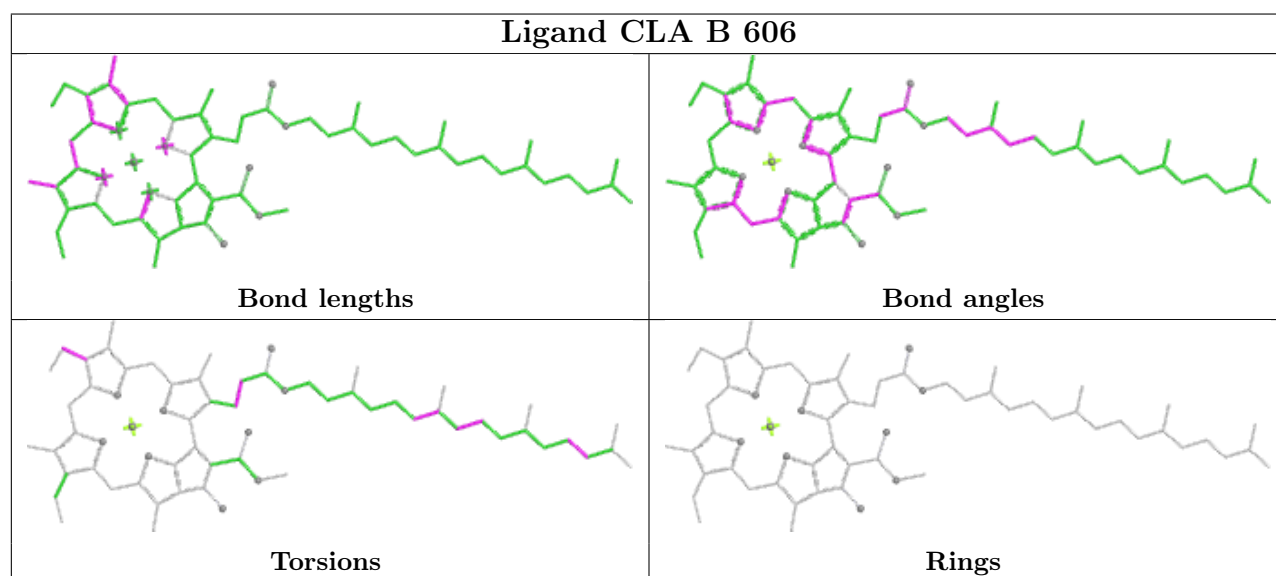
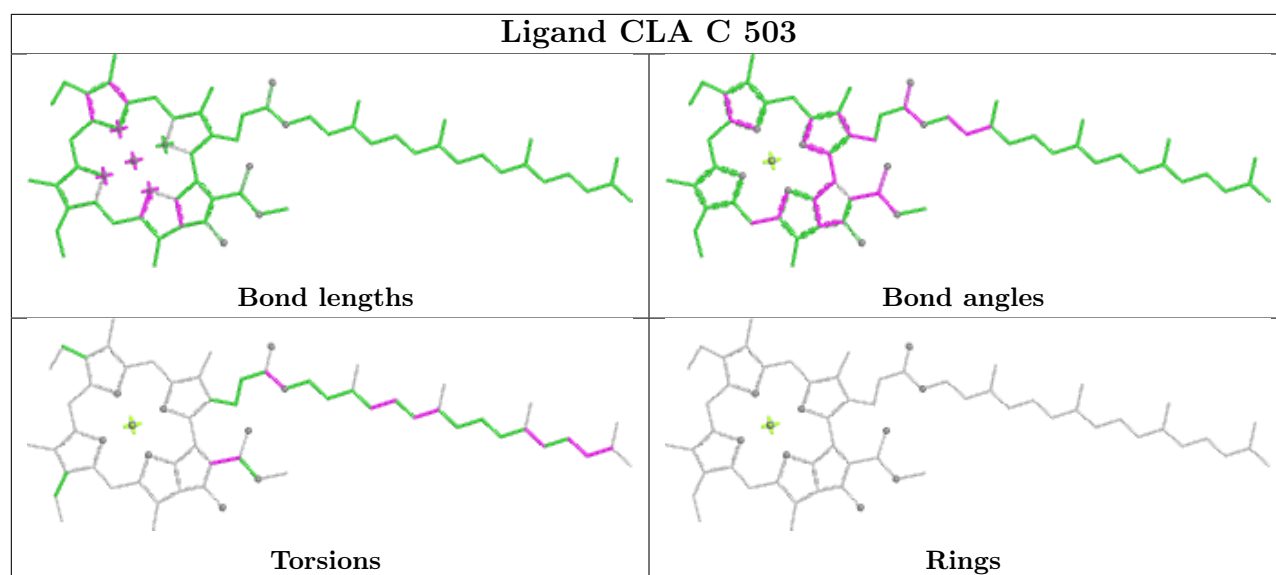


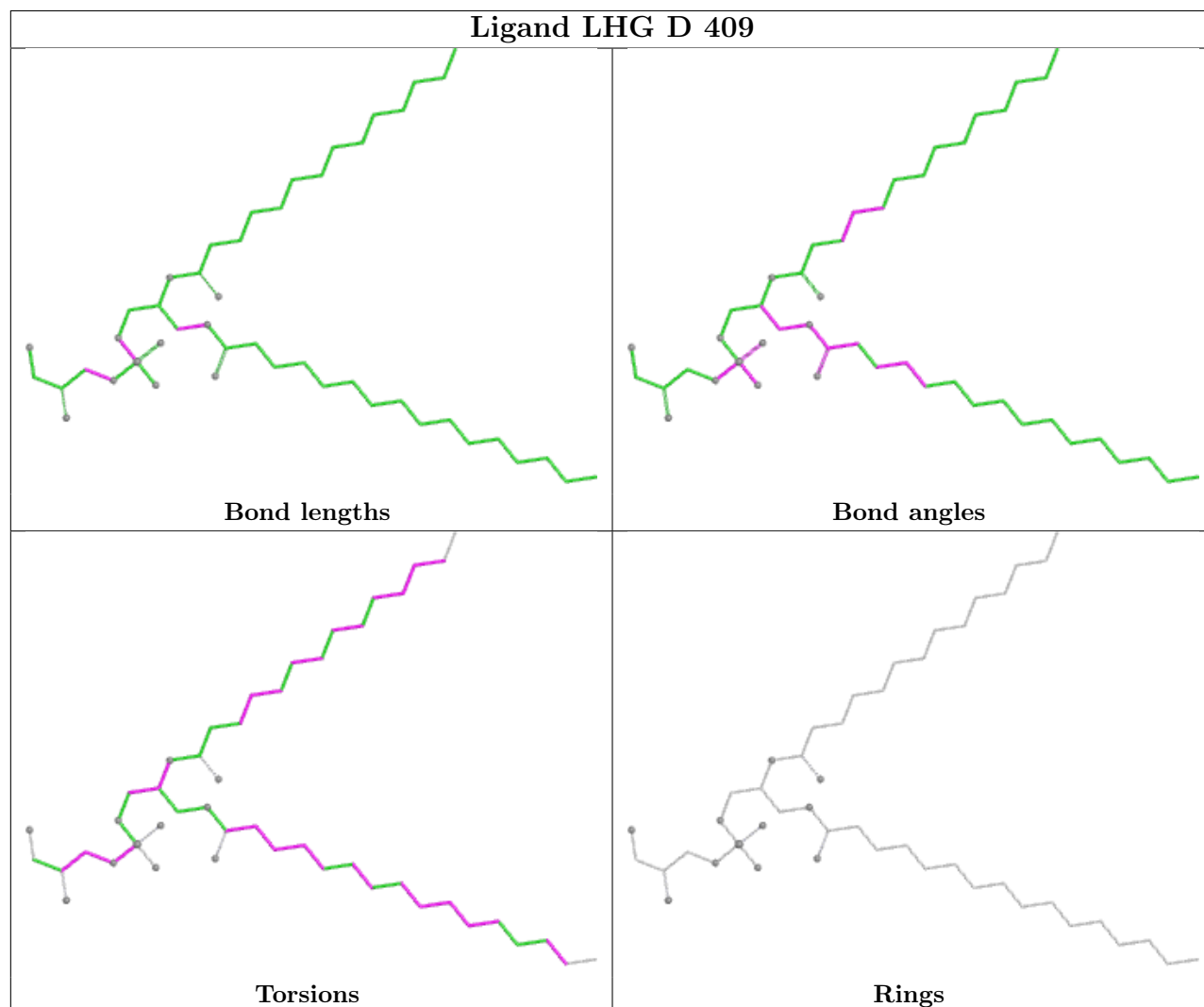
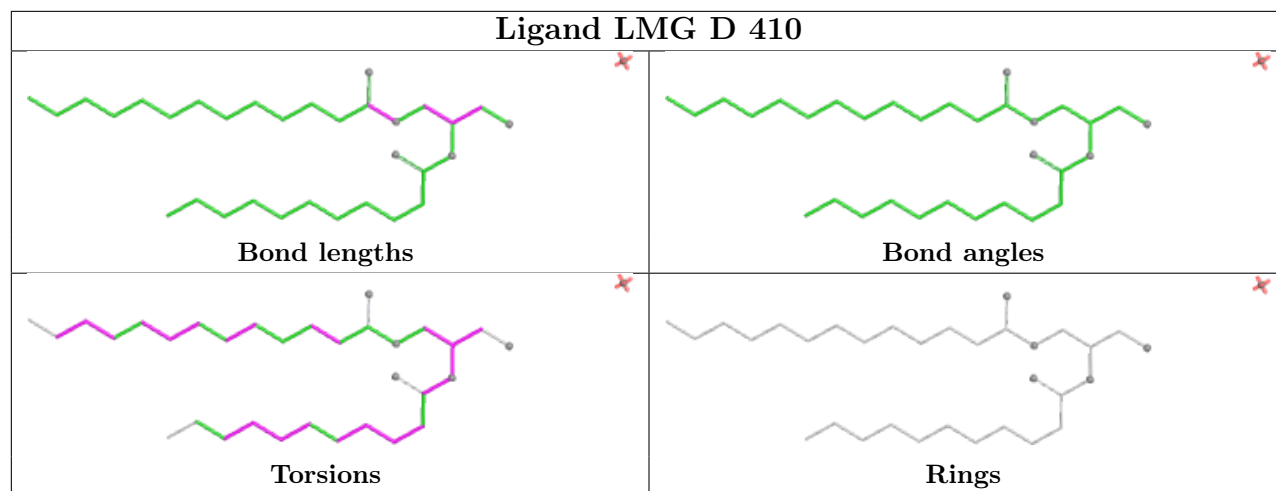
Ligand CLA b 608



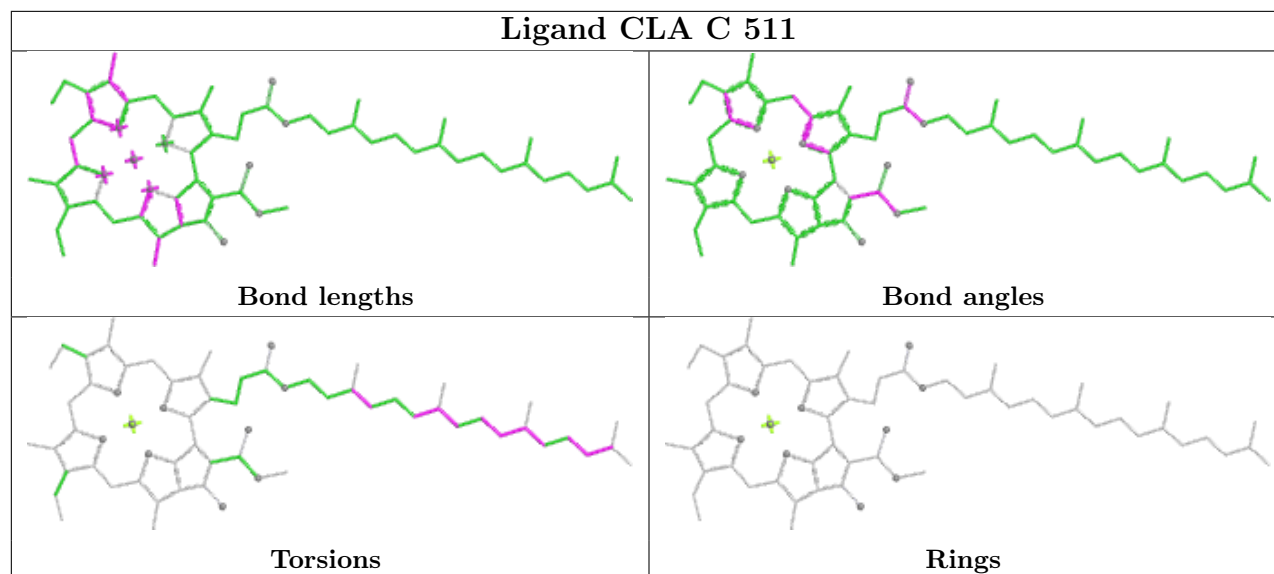




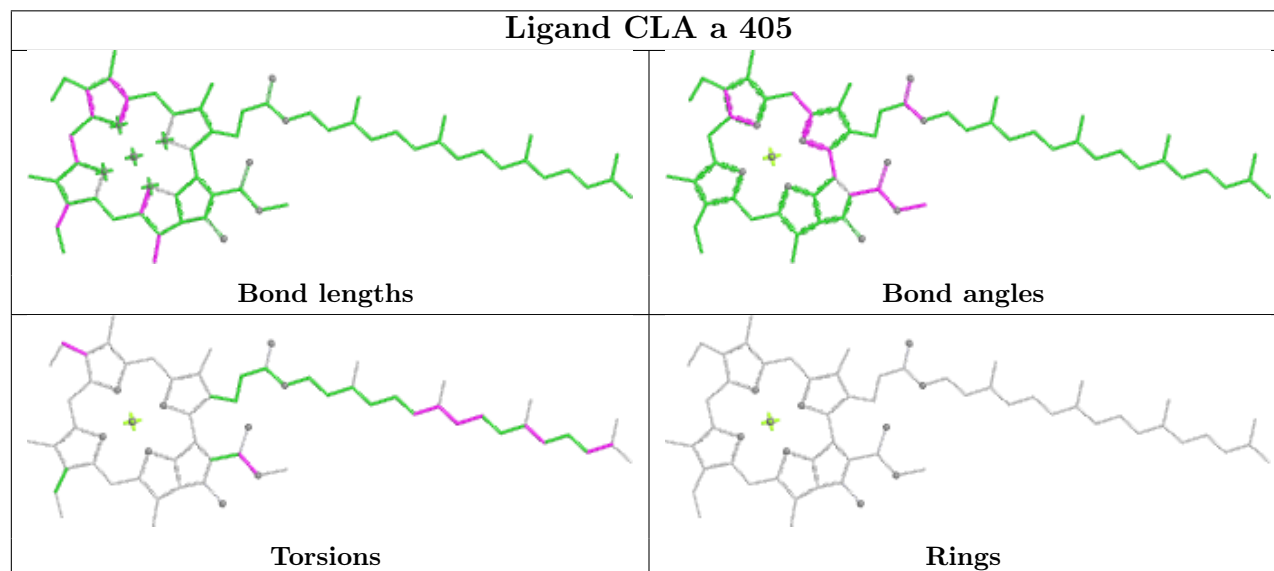




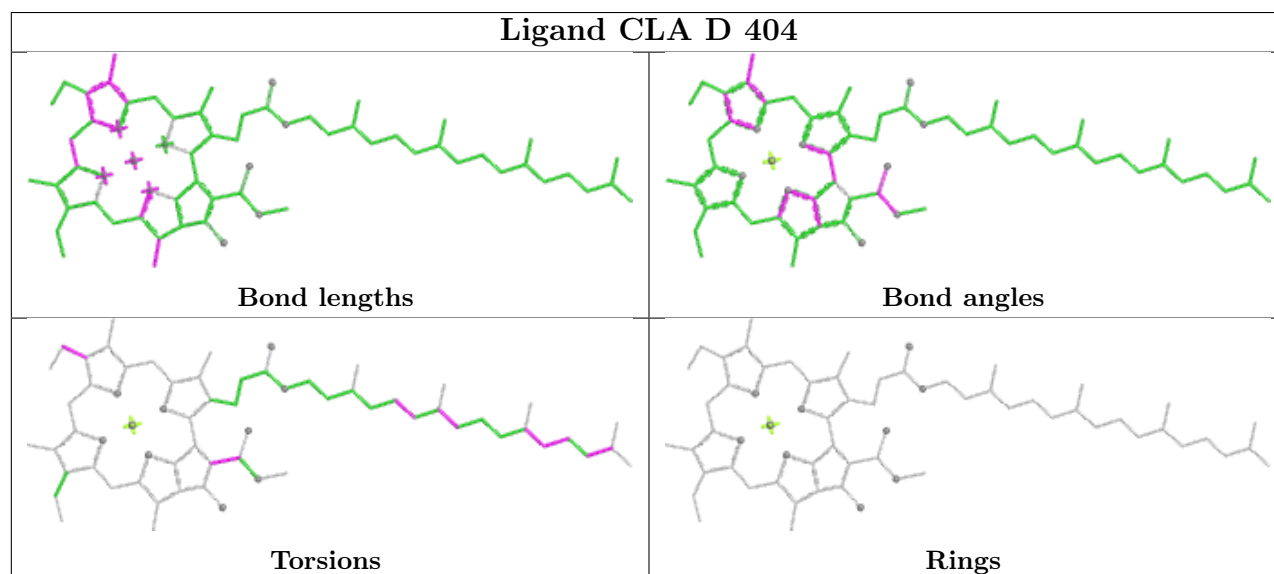
Ligand CLA C 511

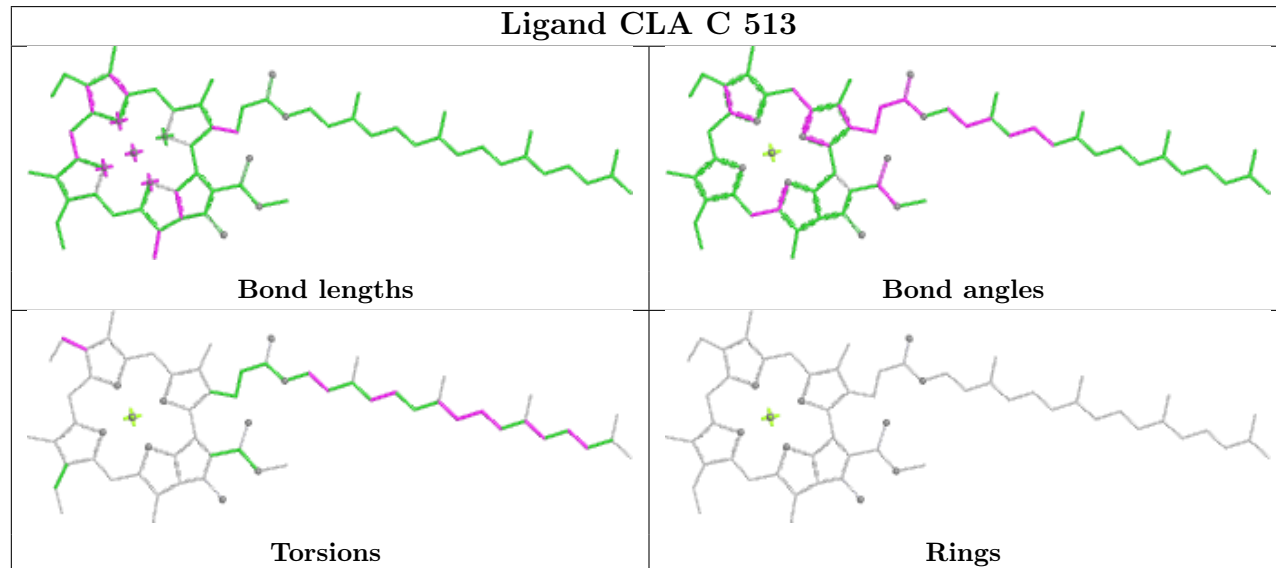
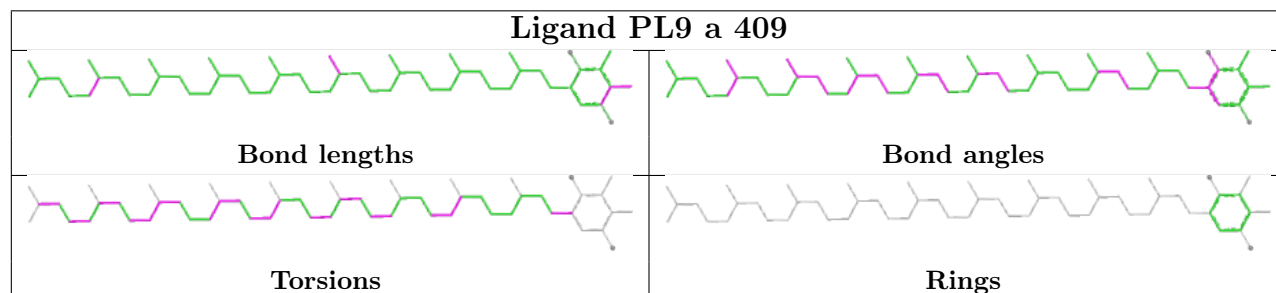
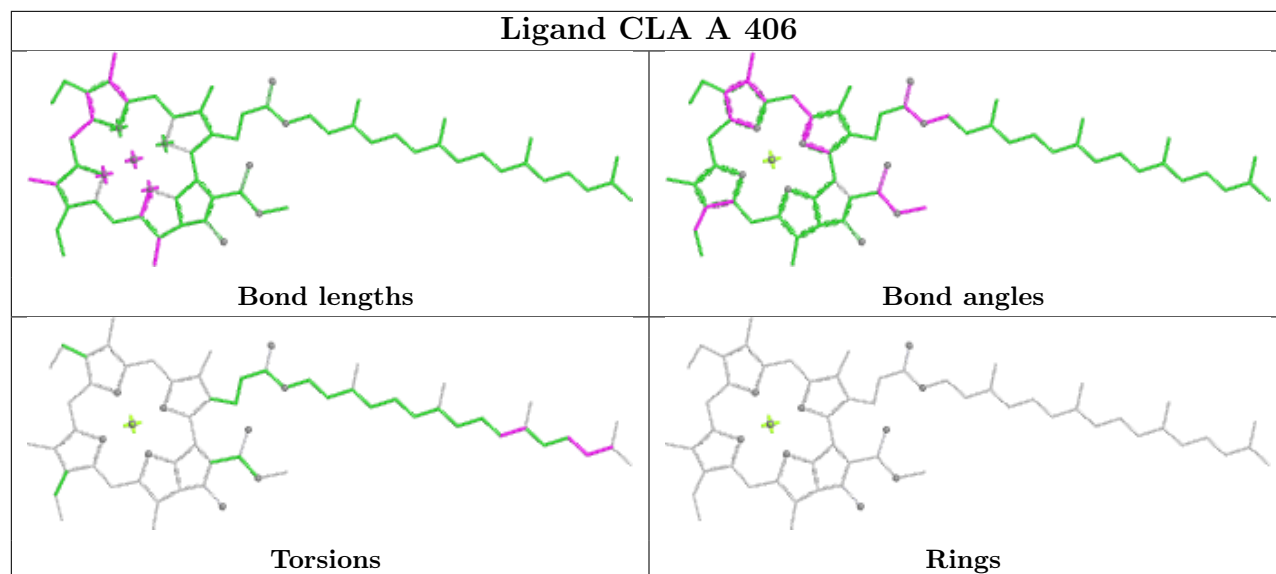


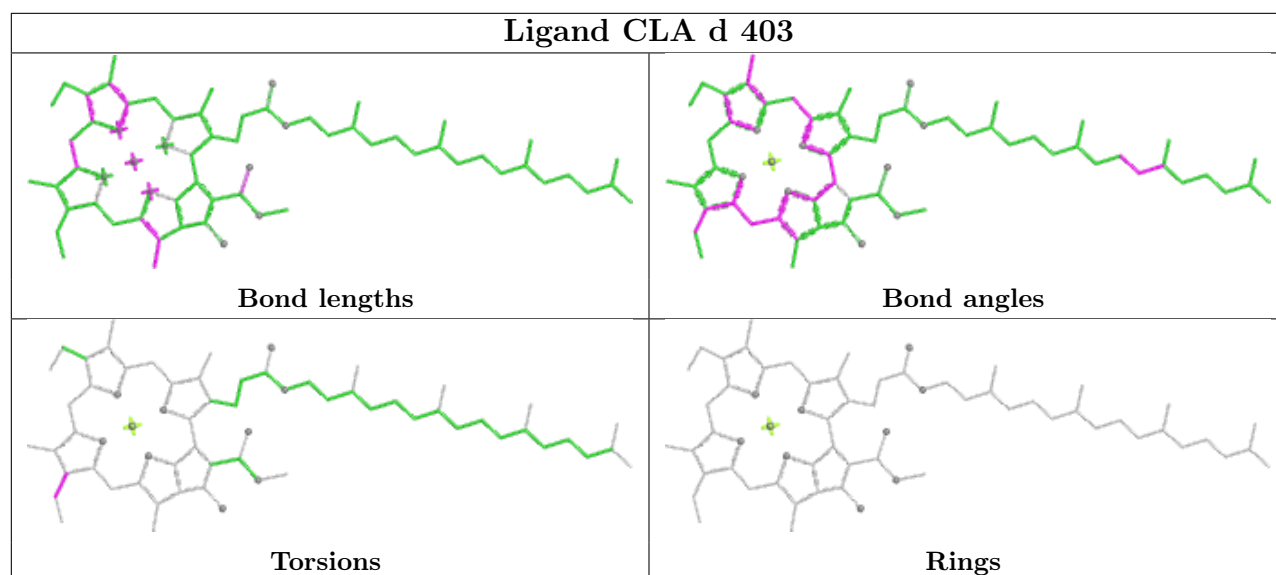
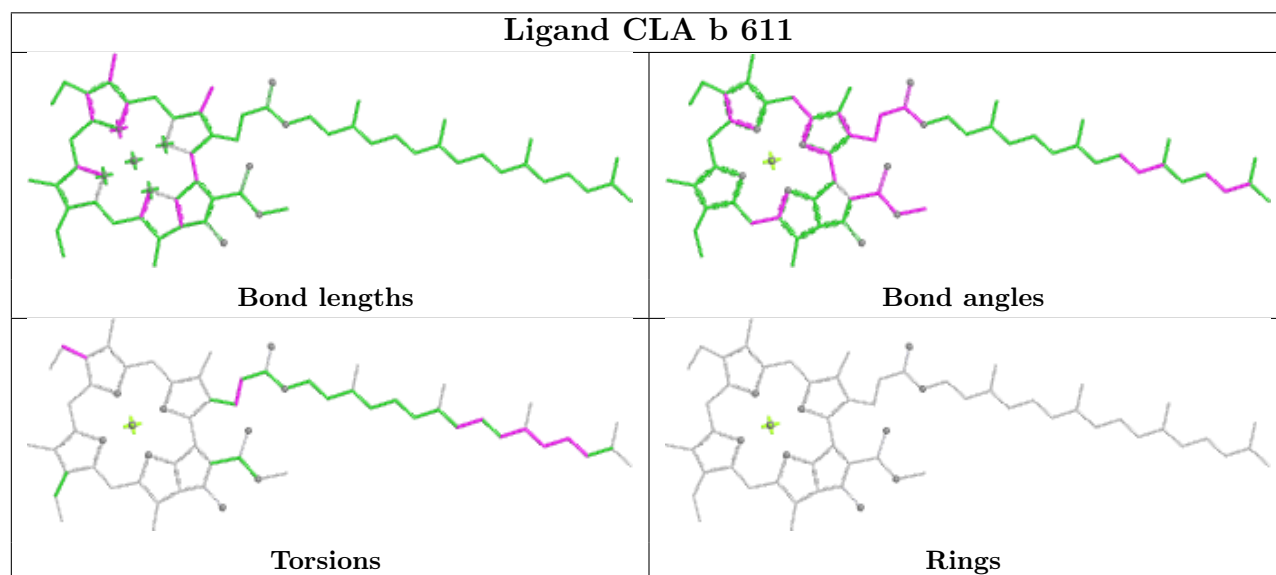
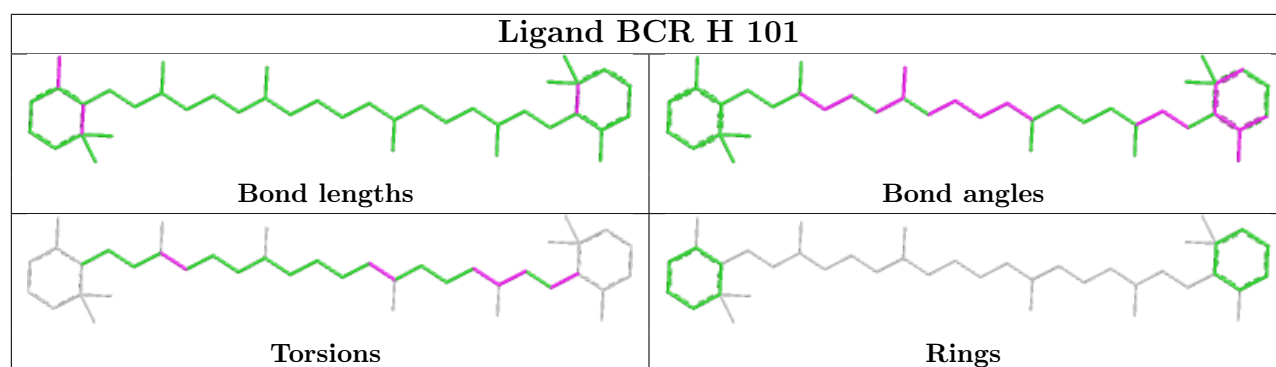
Ligand CLA a 405

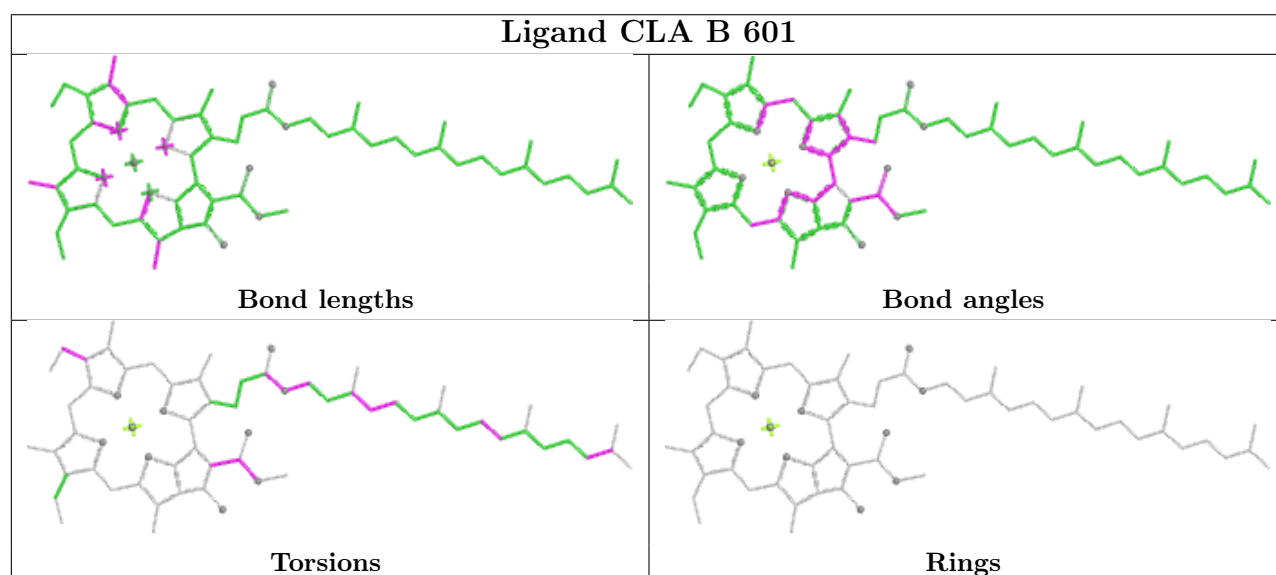
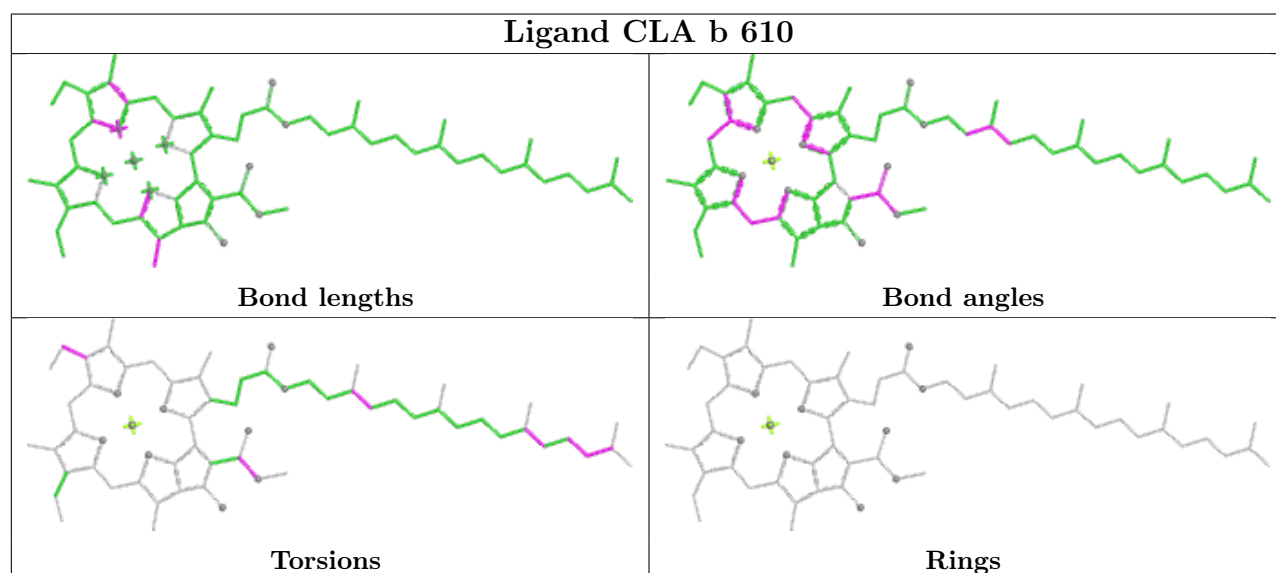
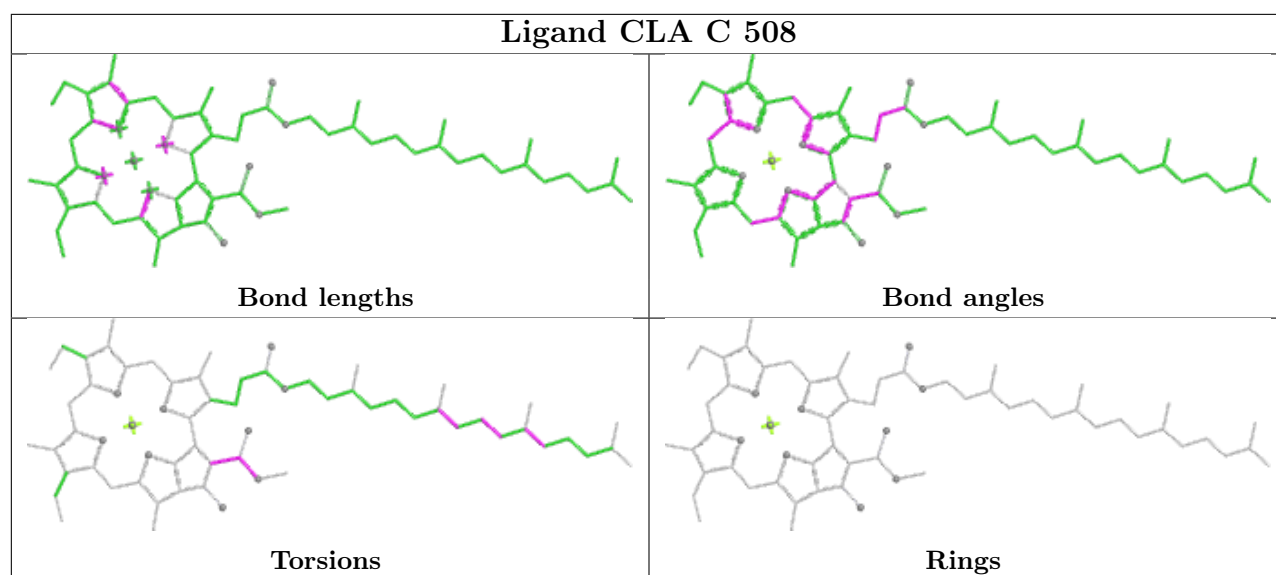


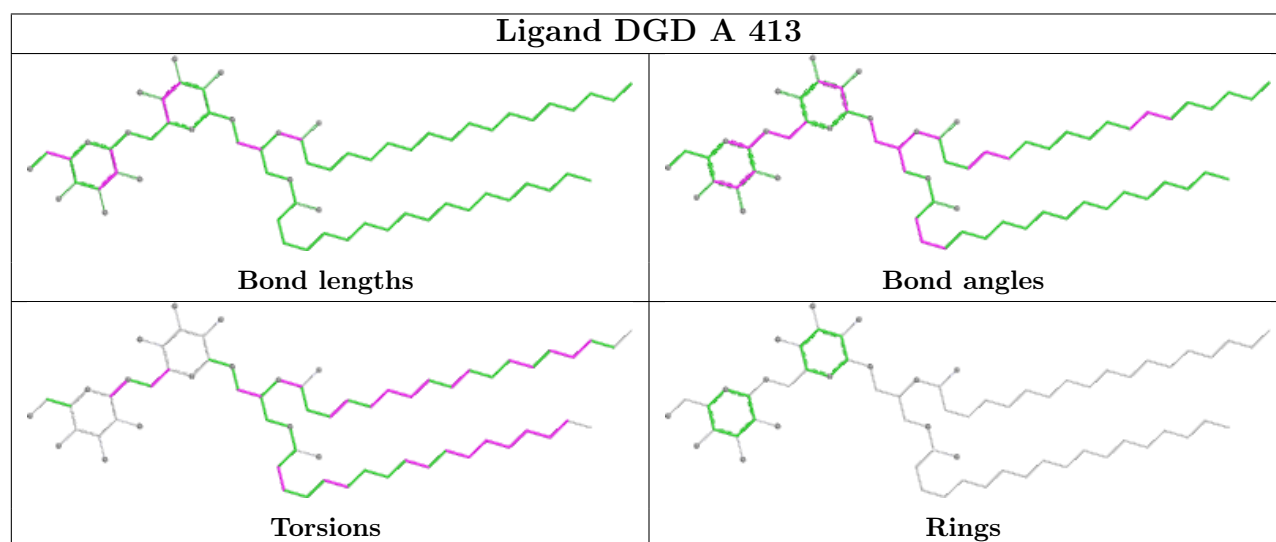
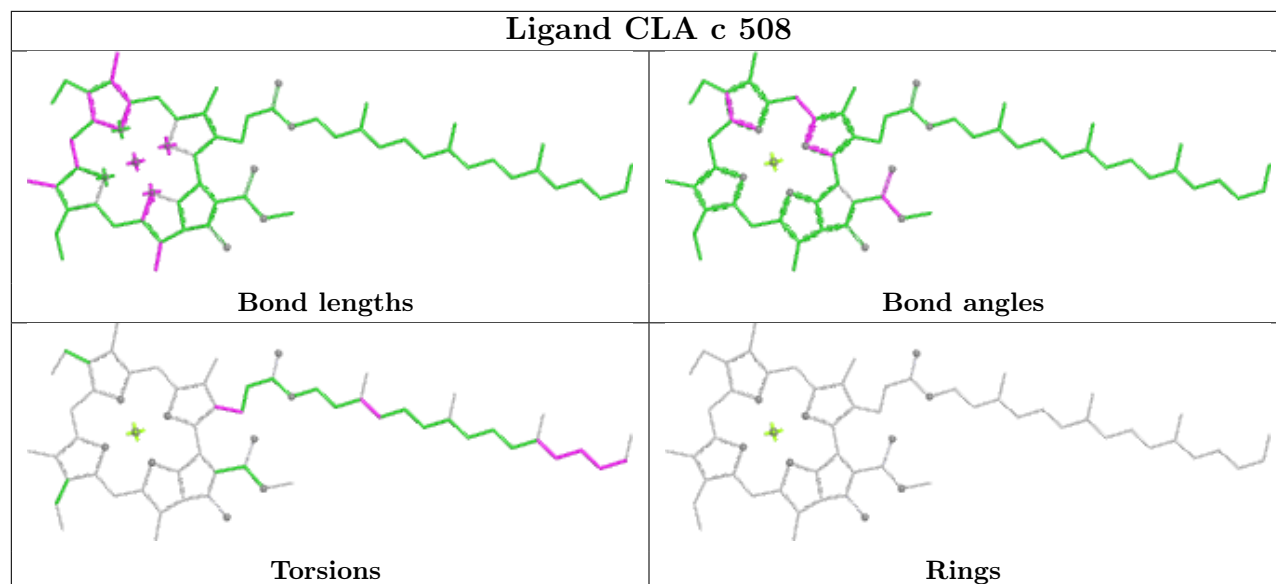
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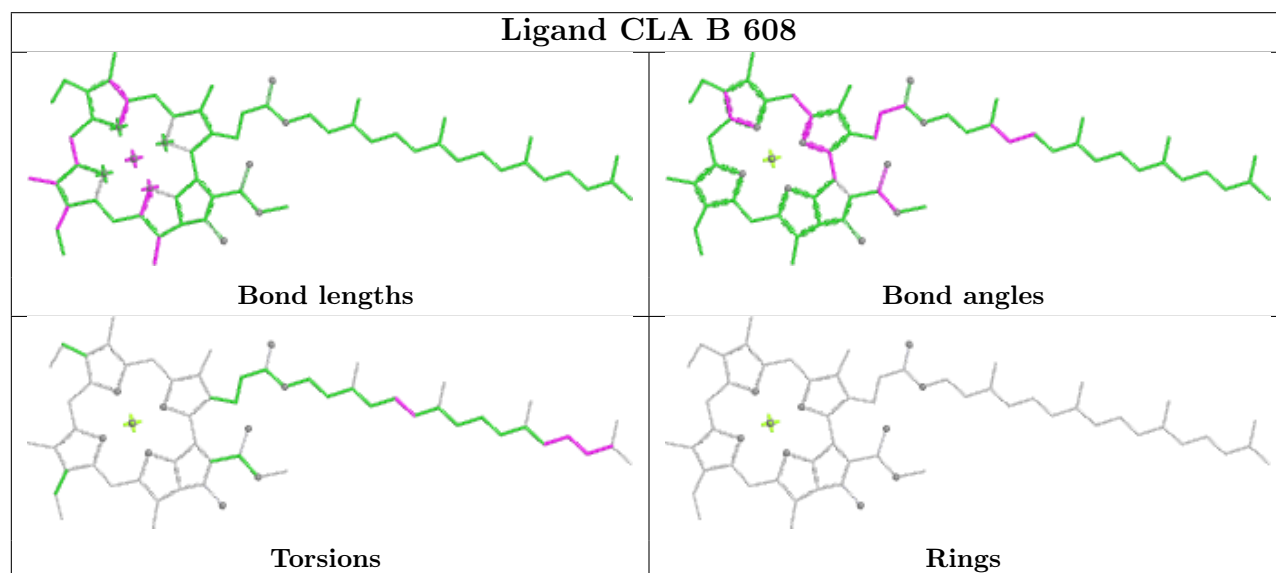
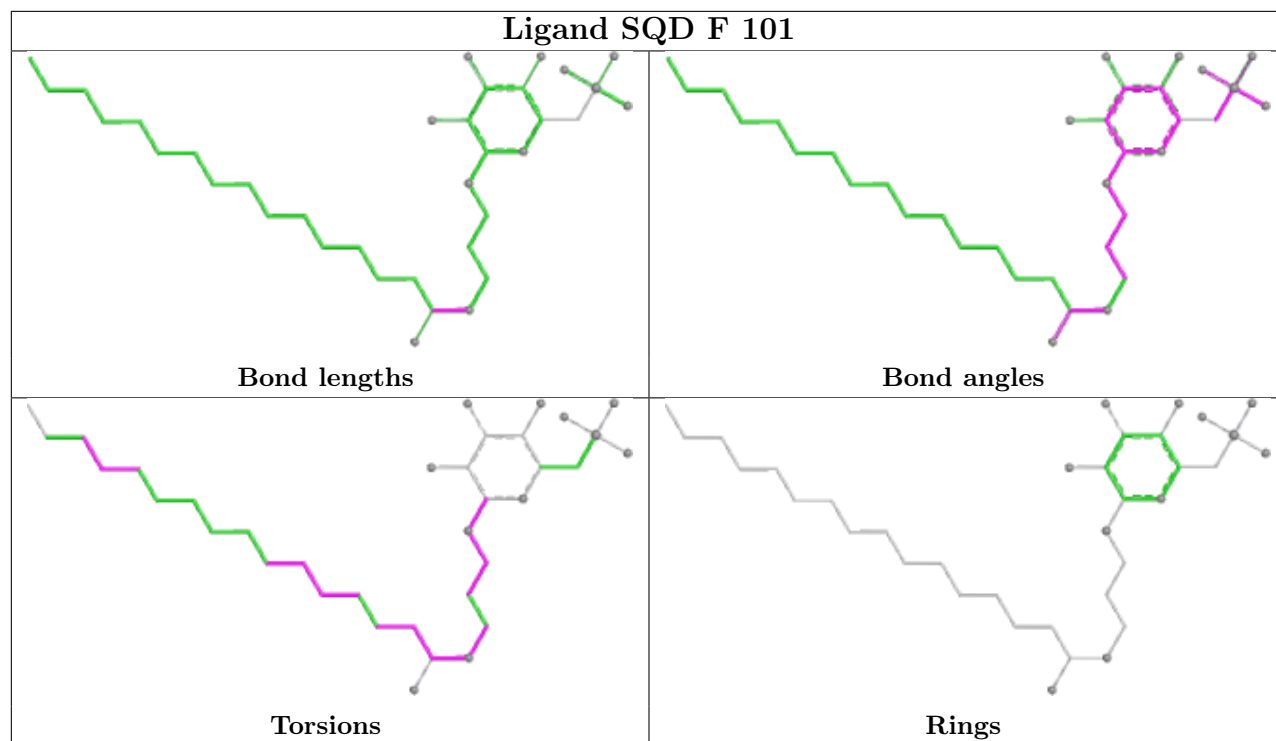


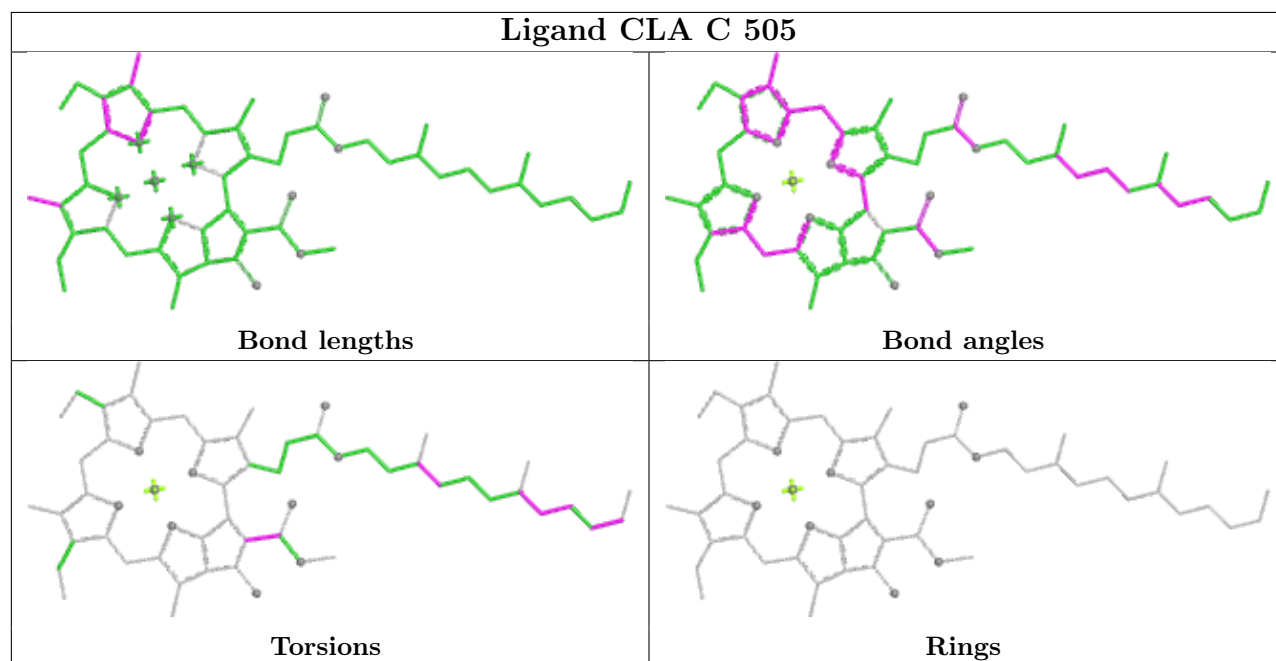
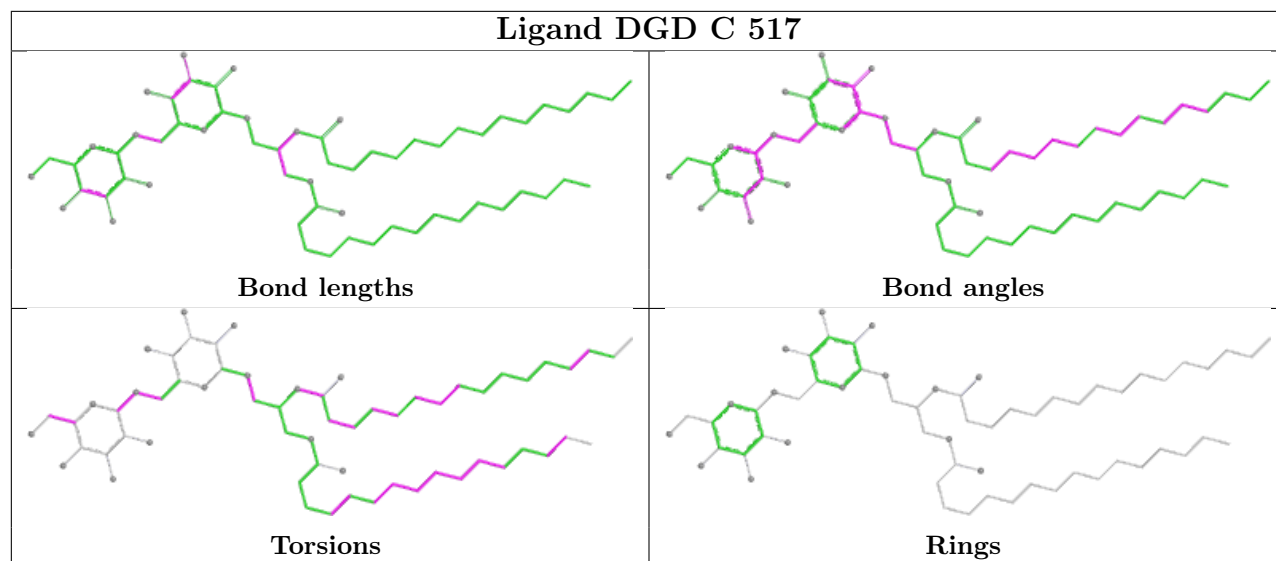




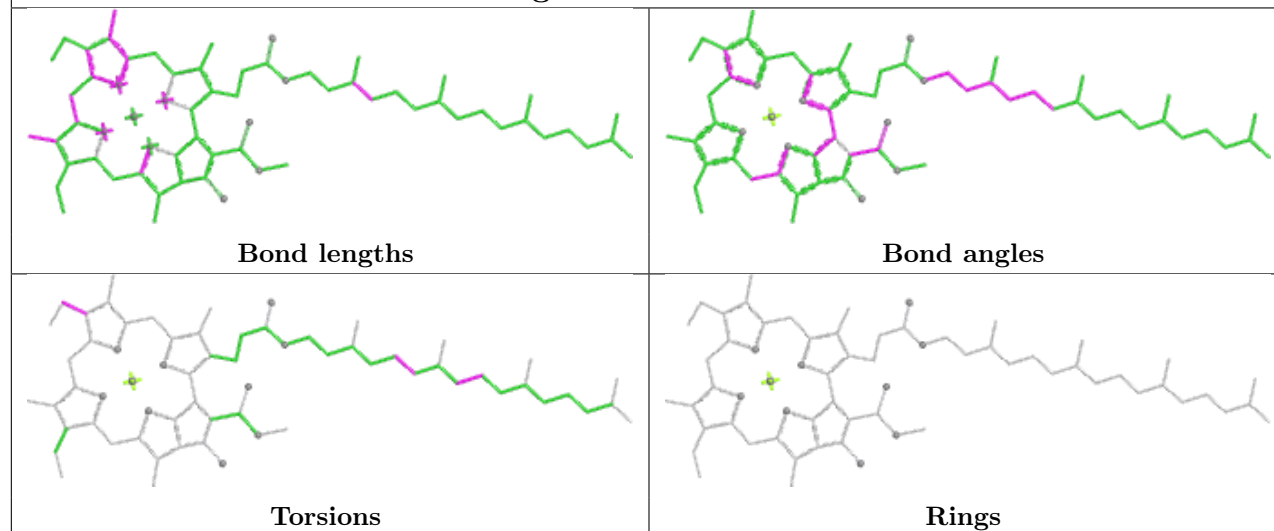




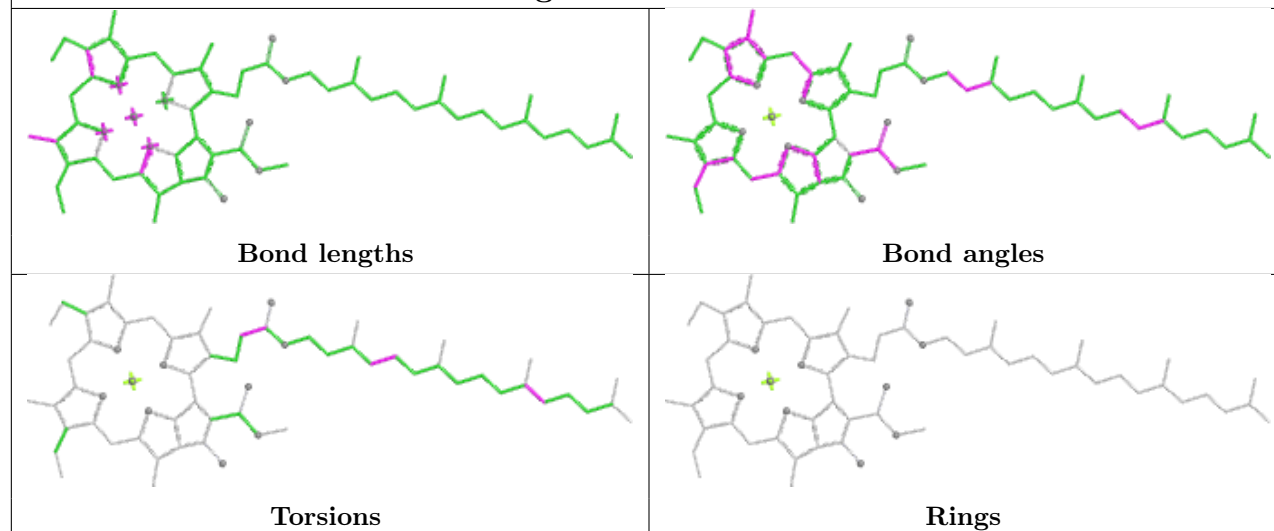




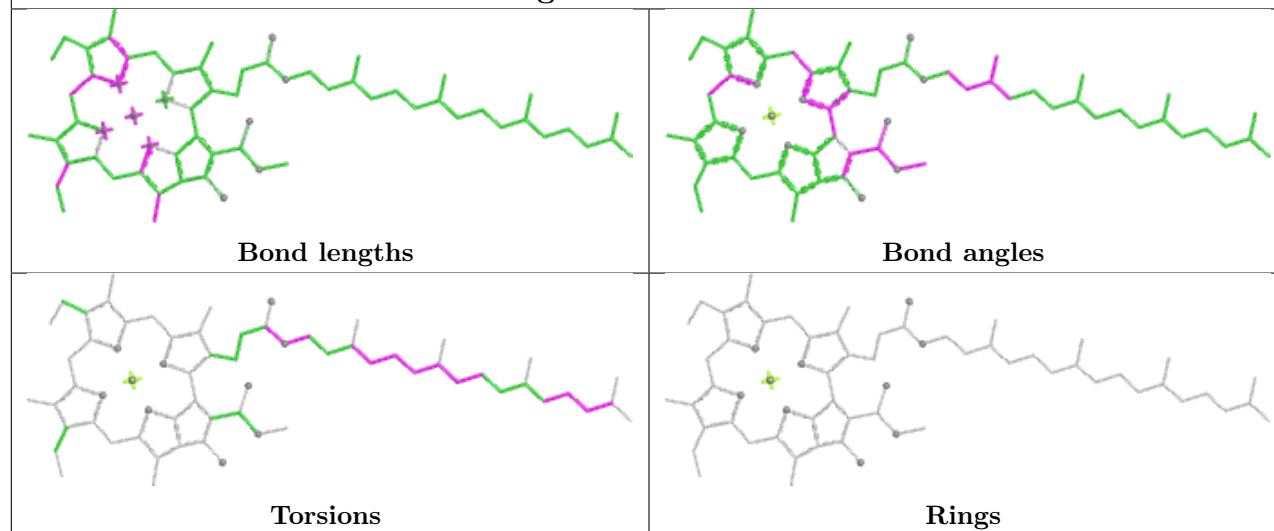
Ligand CLA C 504

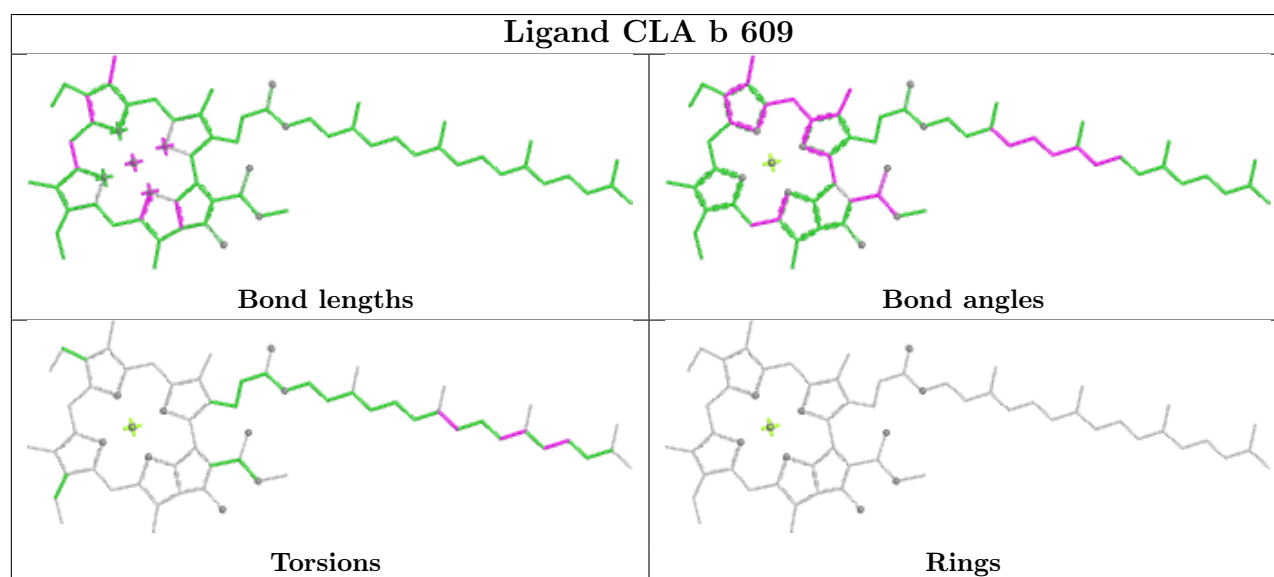
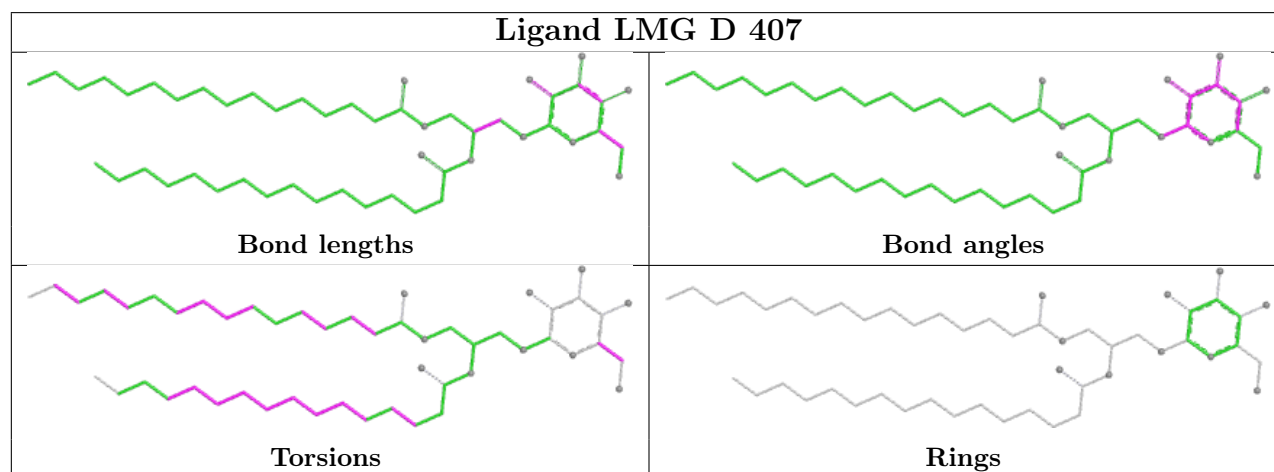
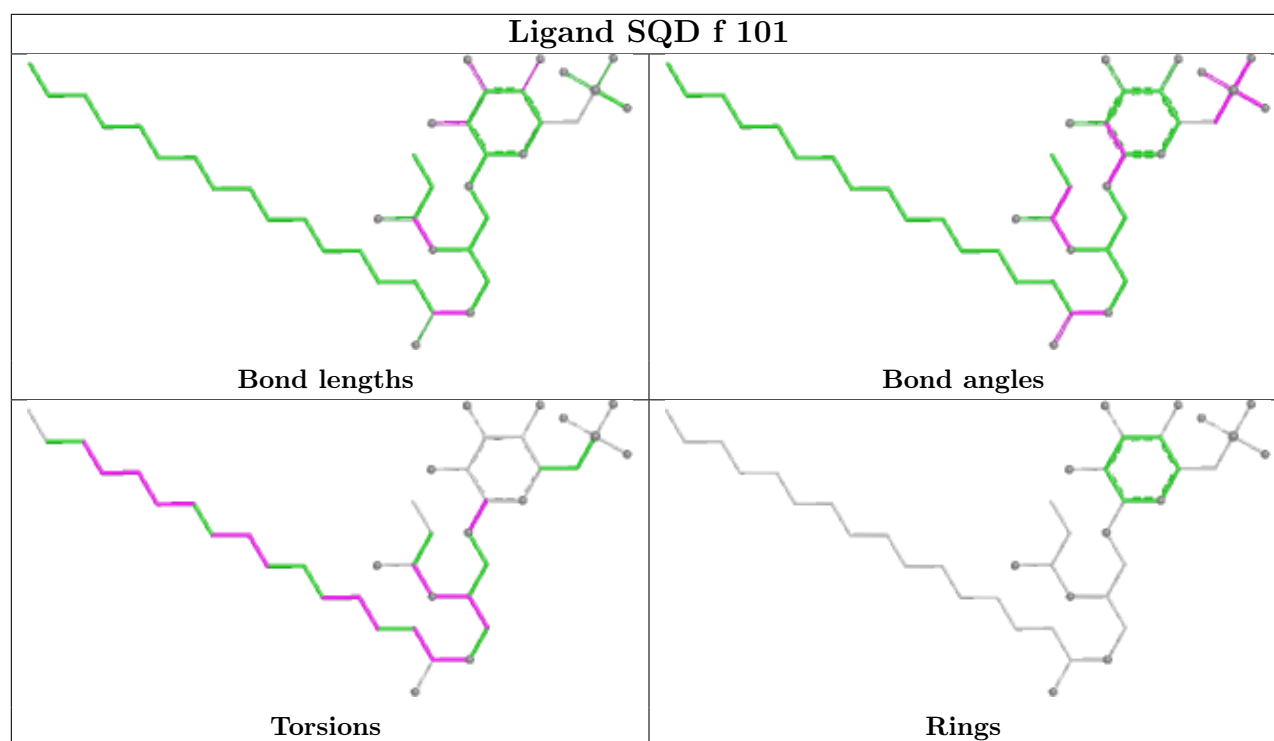


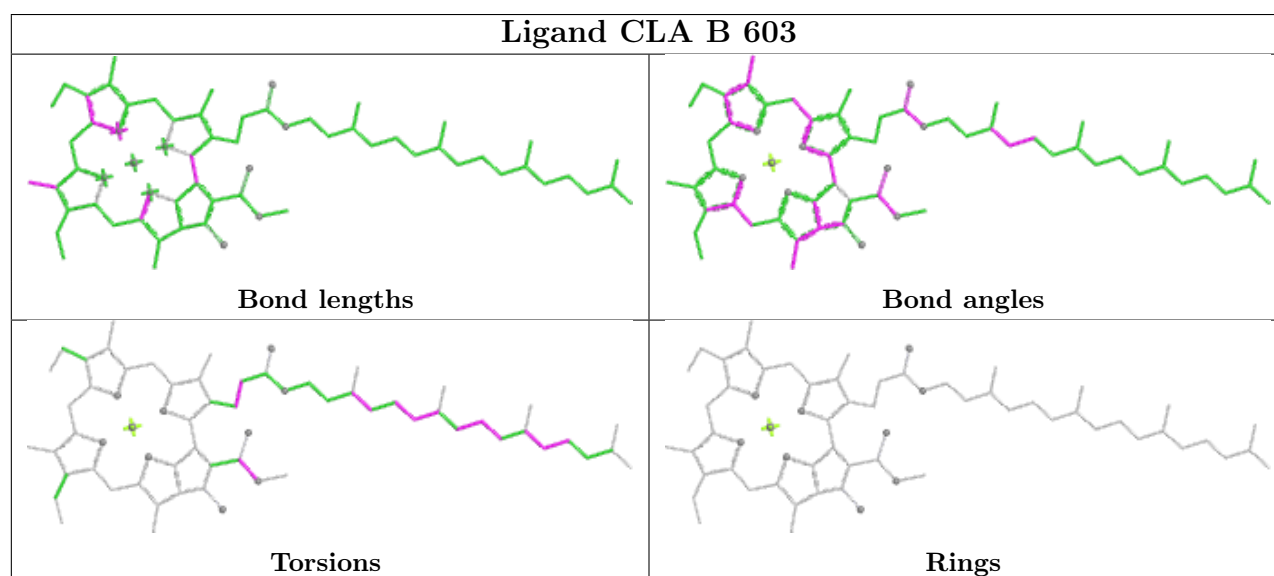
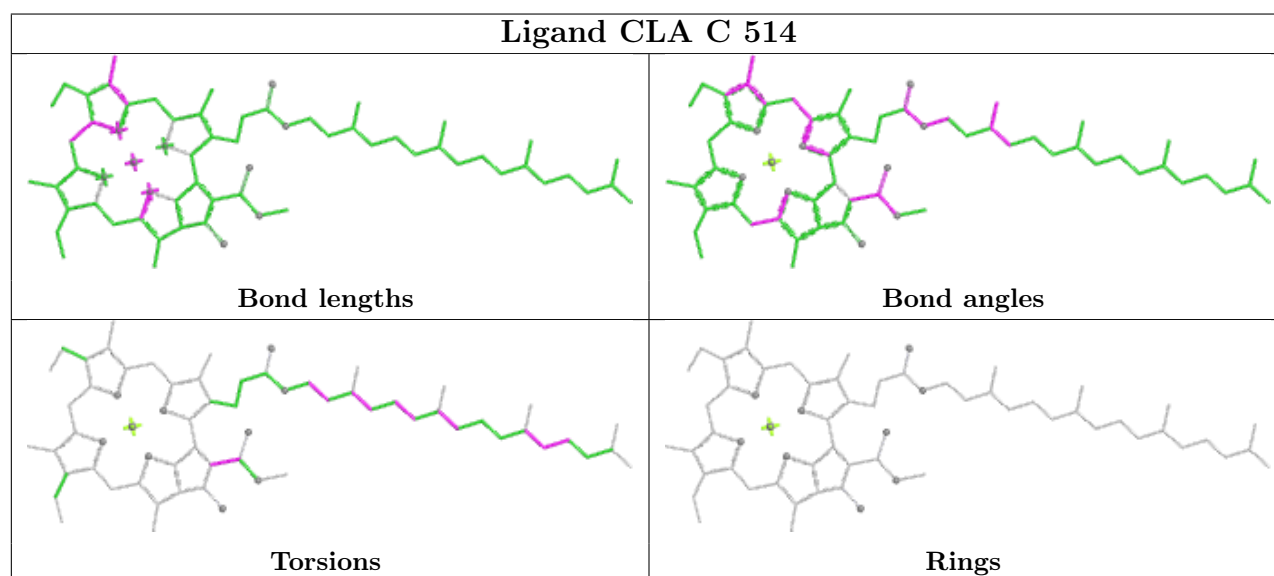
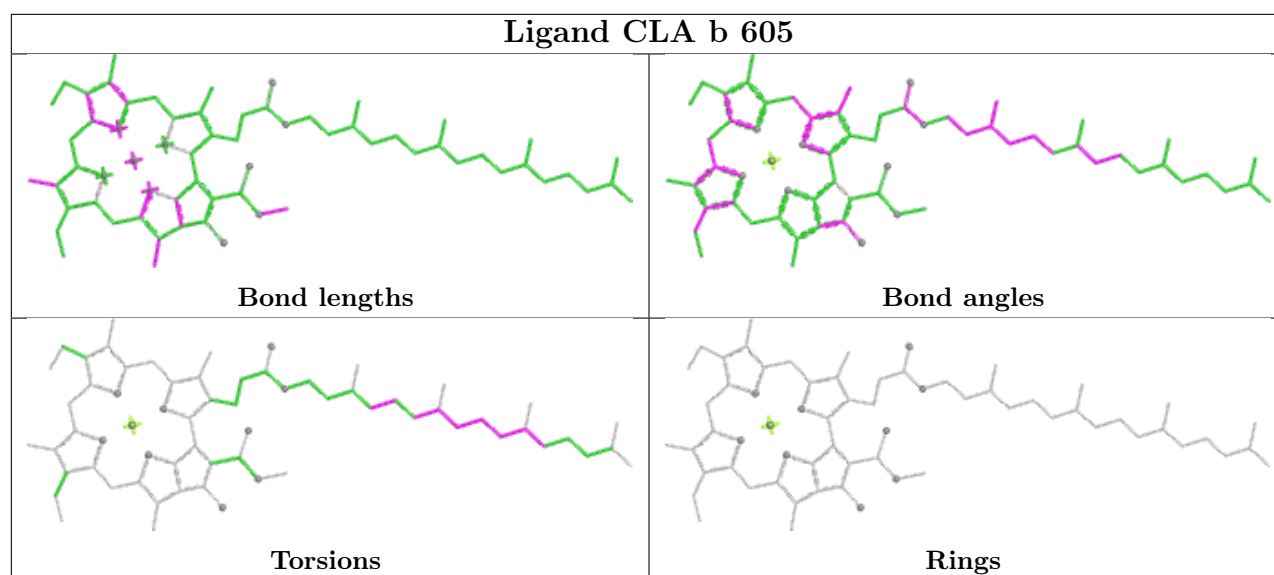
Ligand CLA b 613



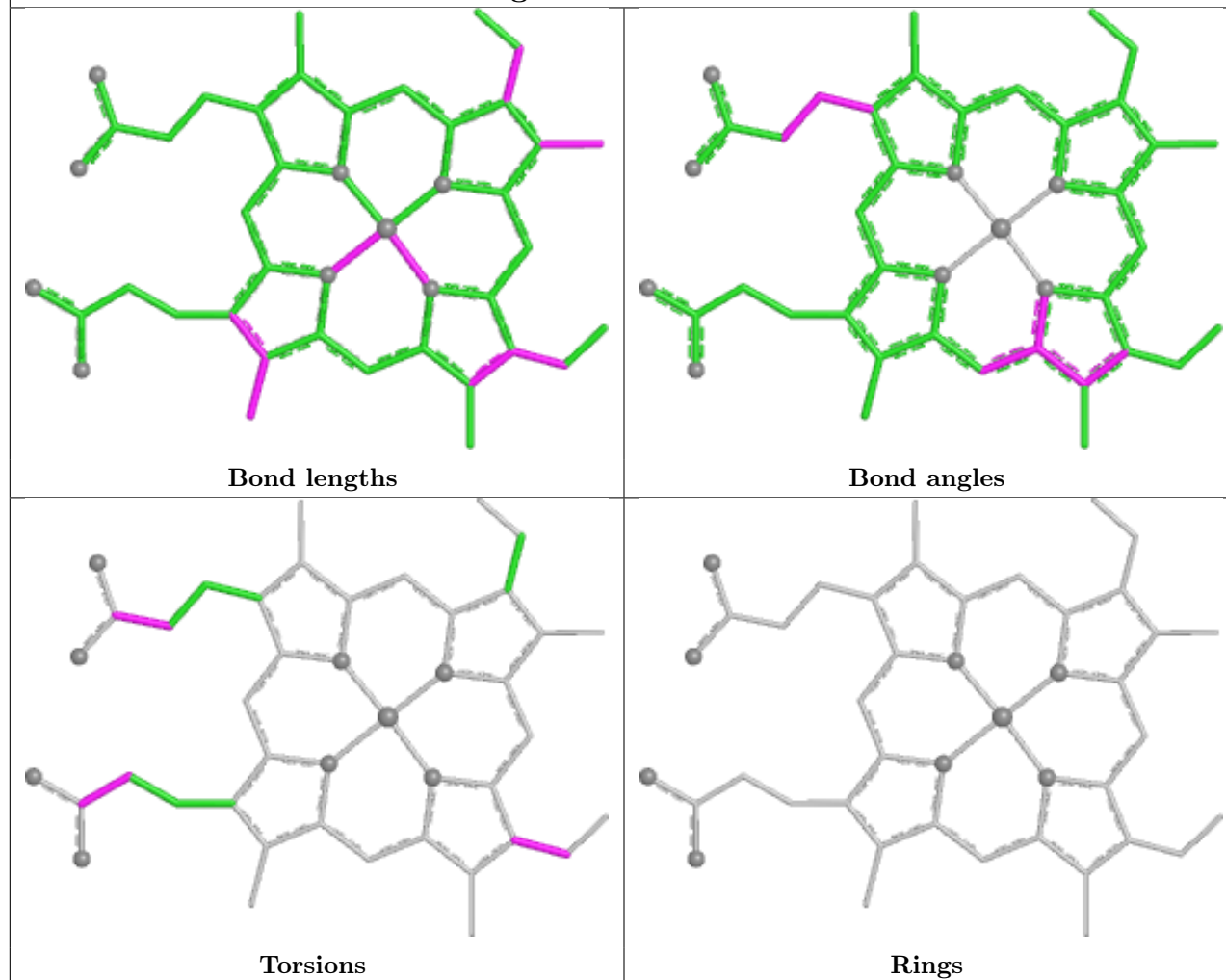
Ligand CLA c 506



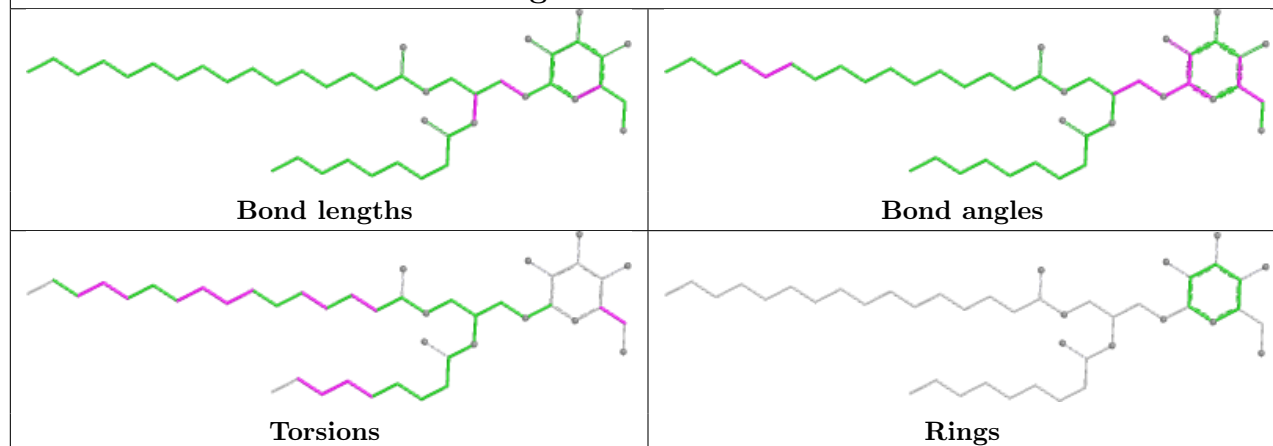


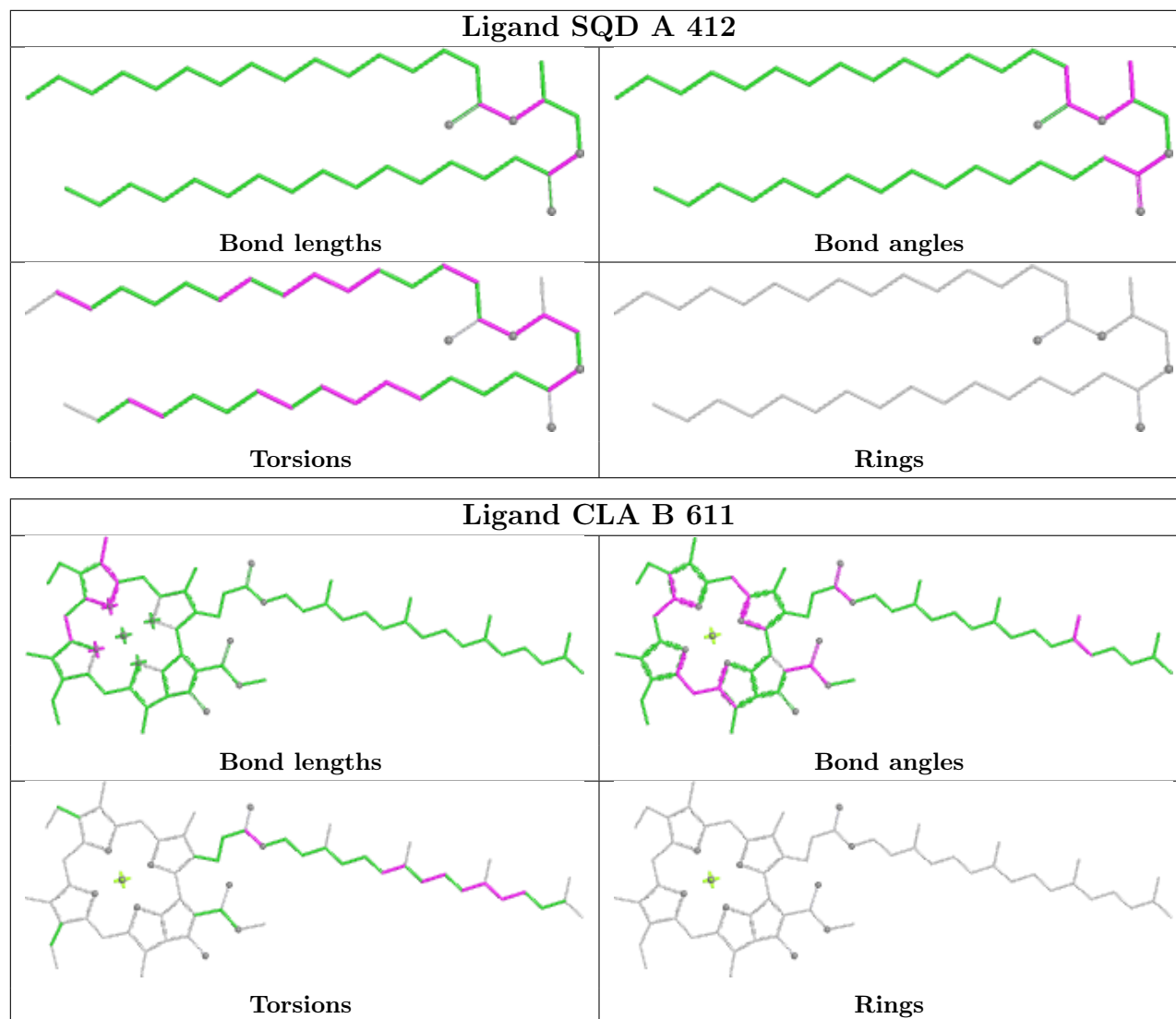


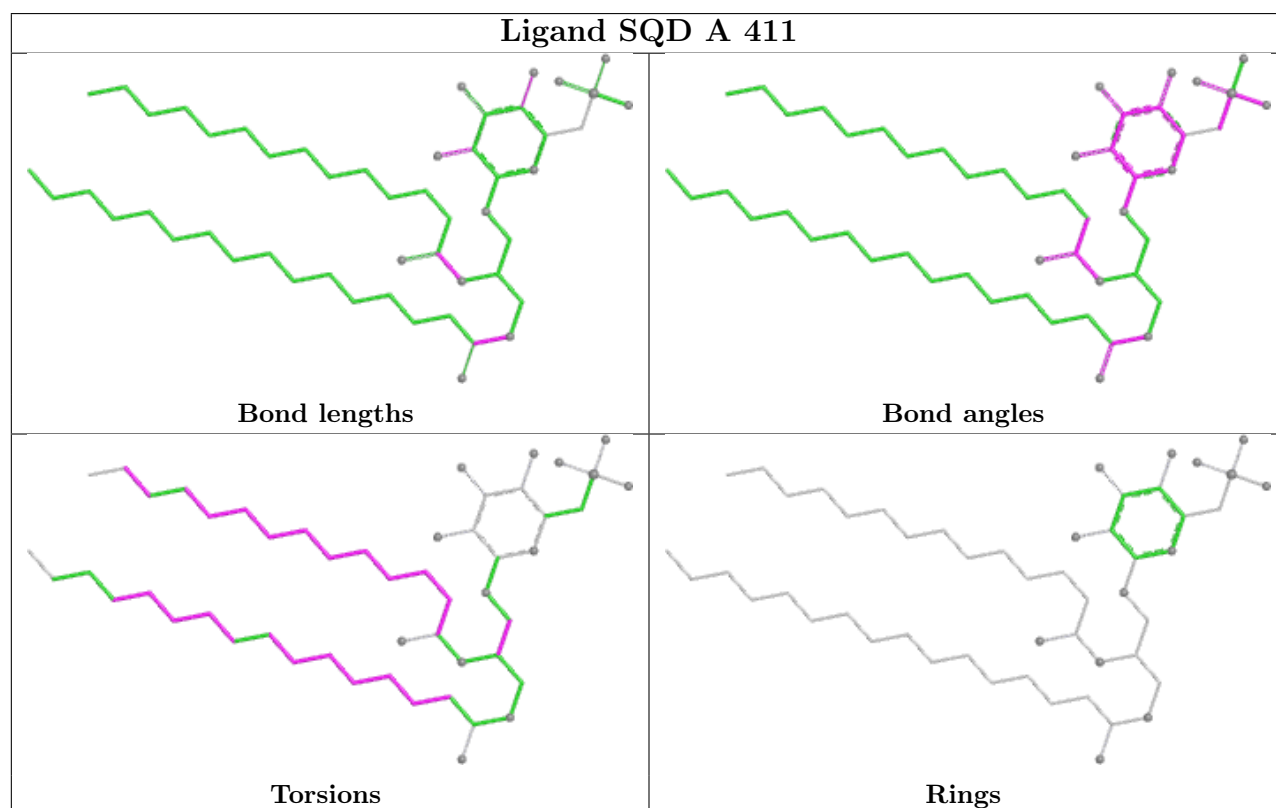
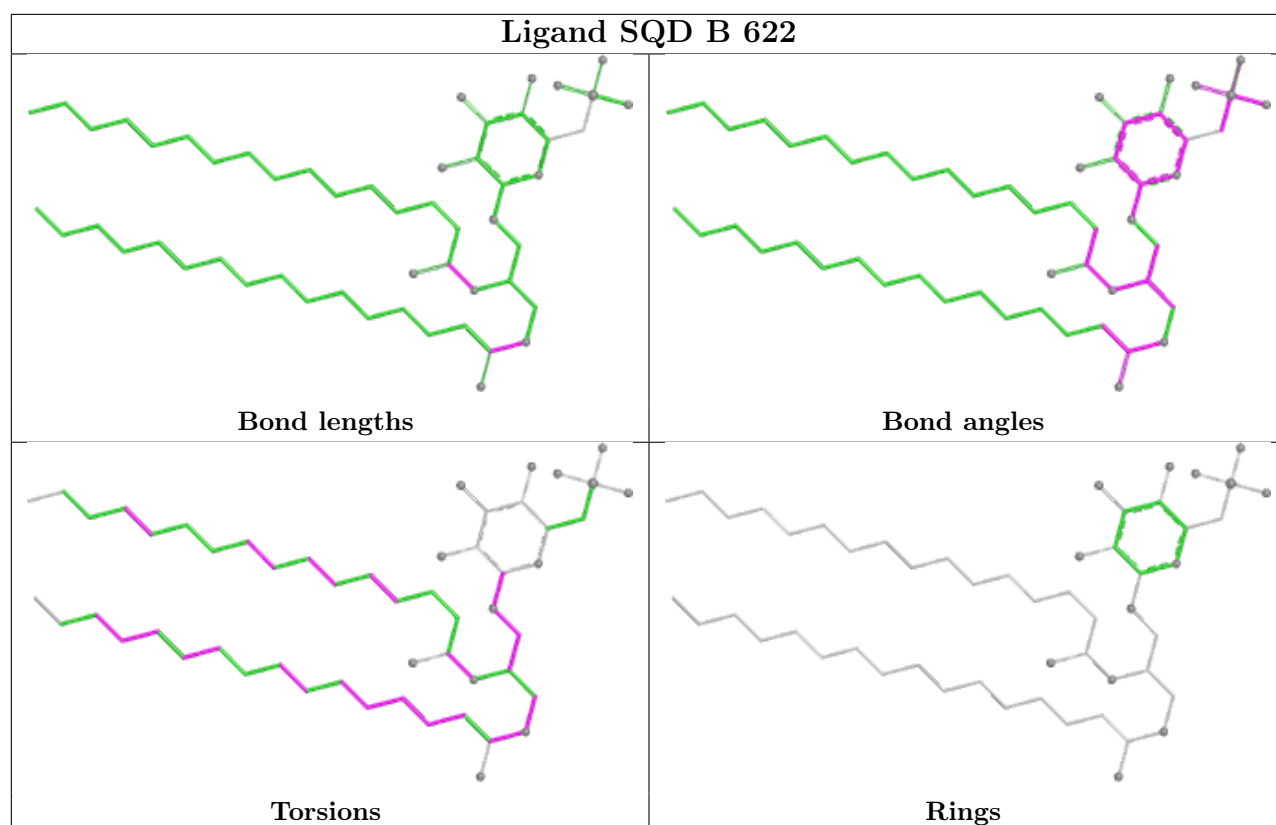
Ligand HEM e 102

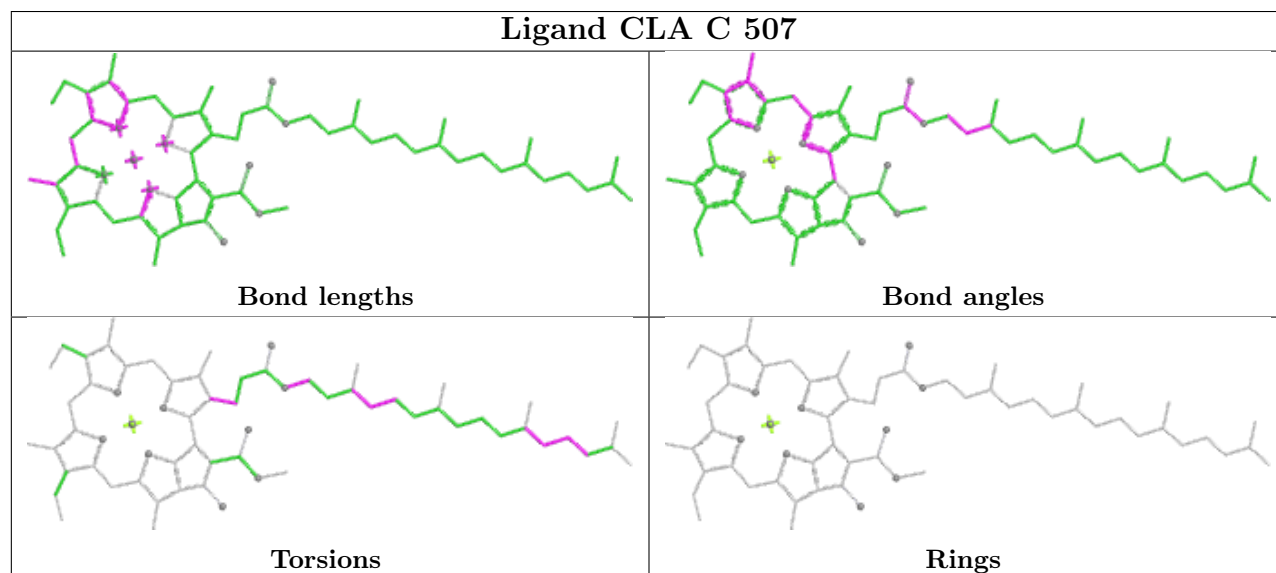
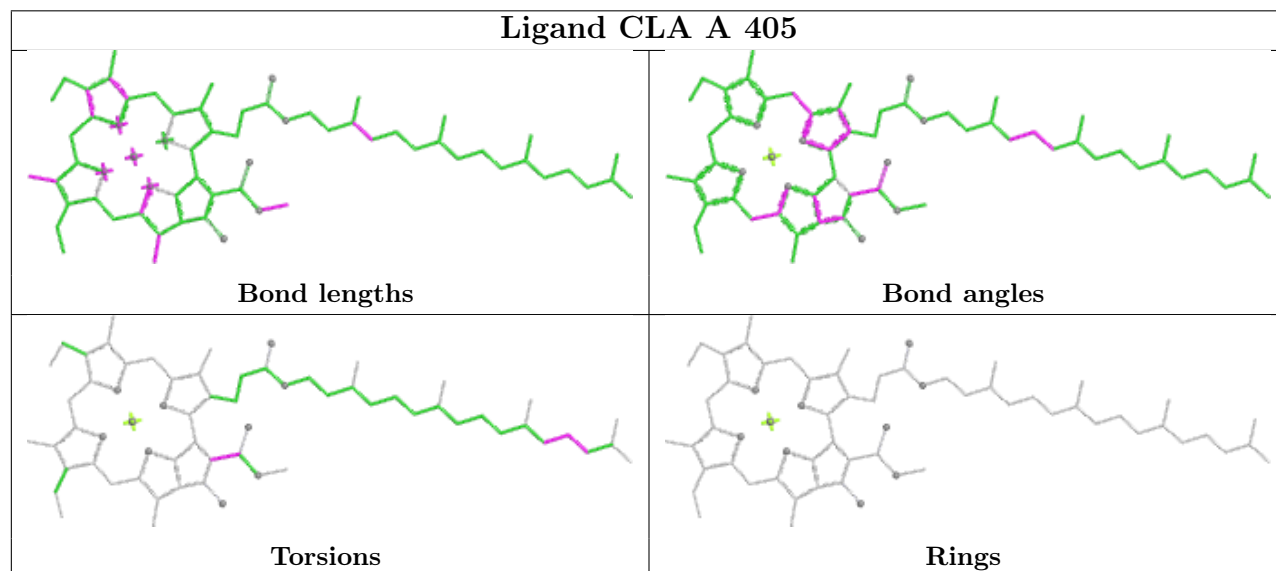
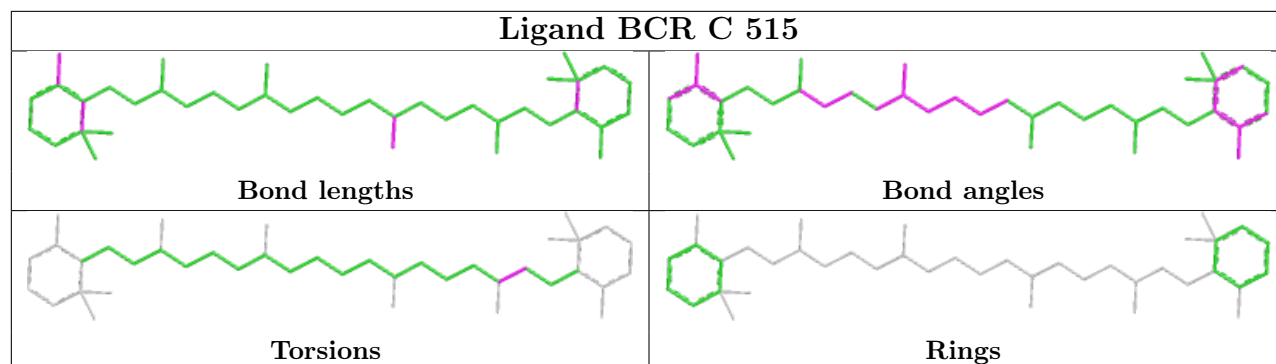


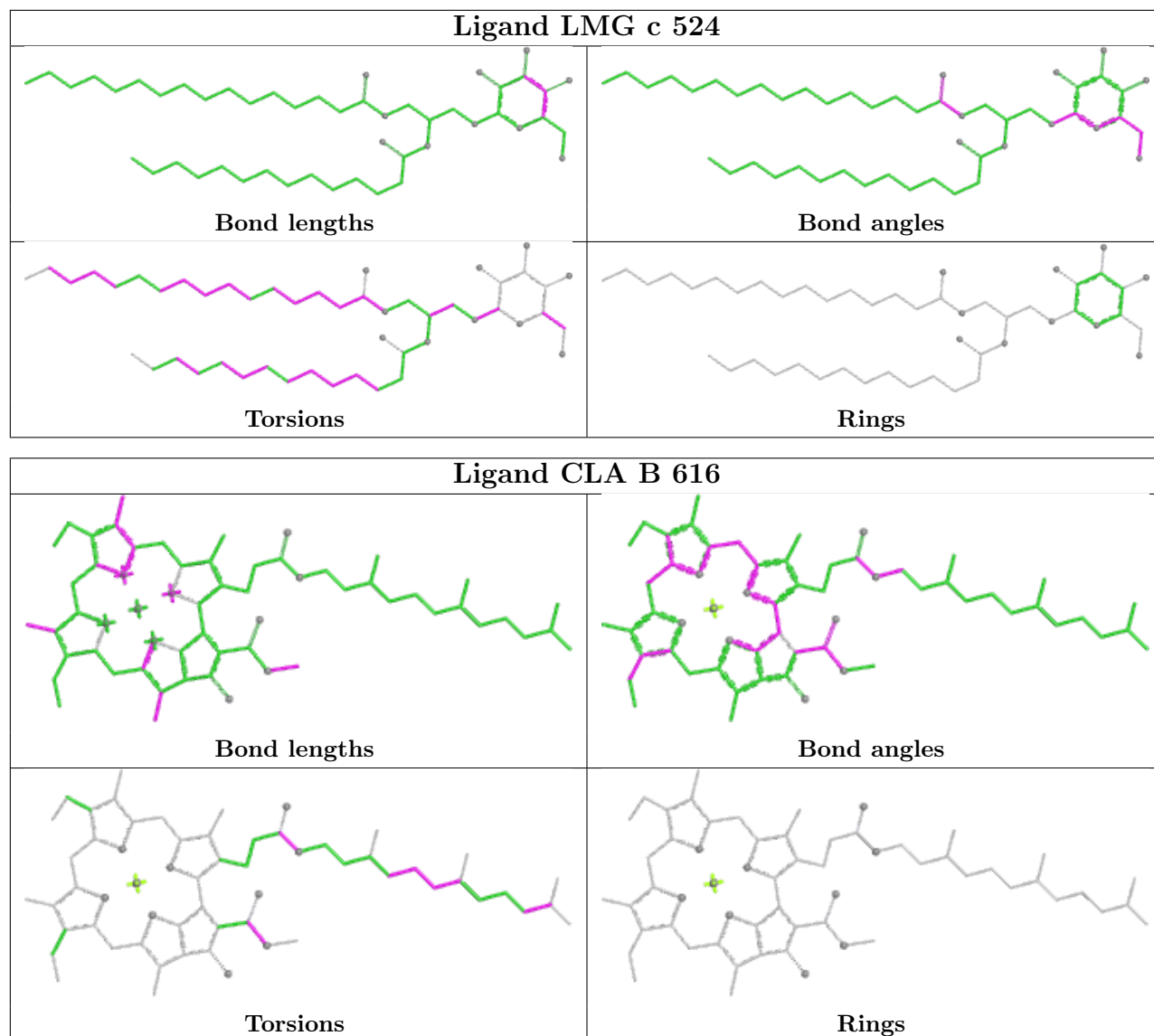
Ligand LMG d 411

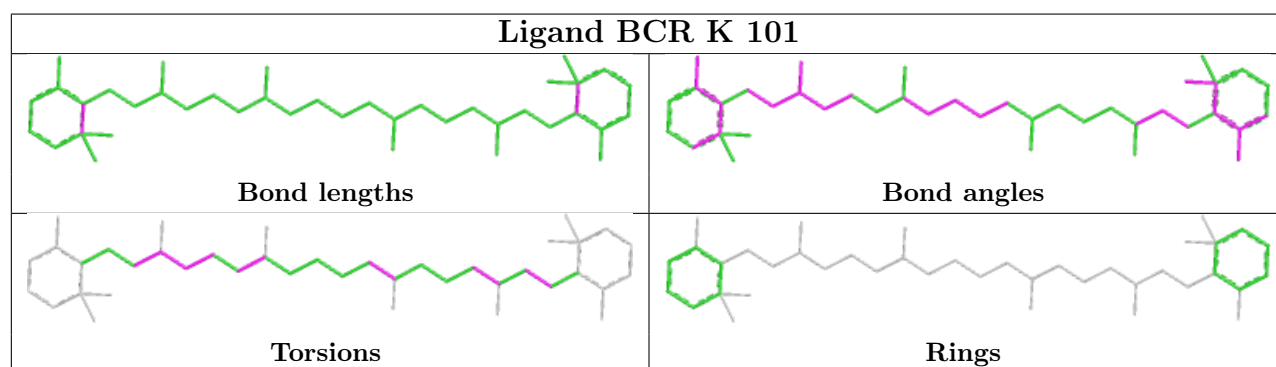
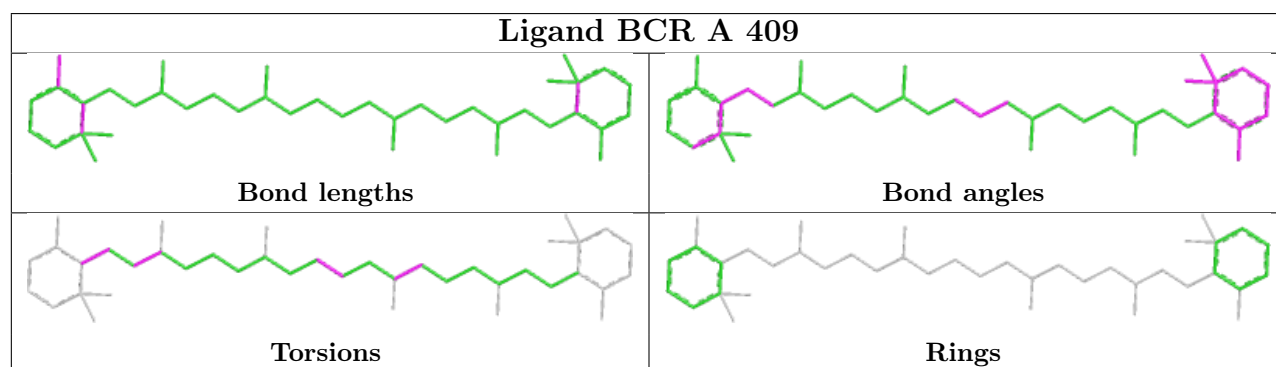
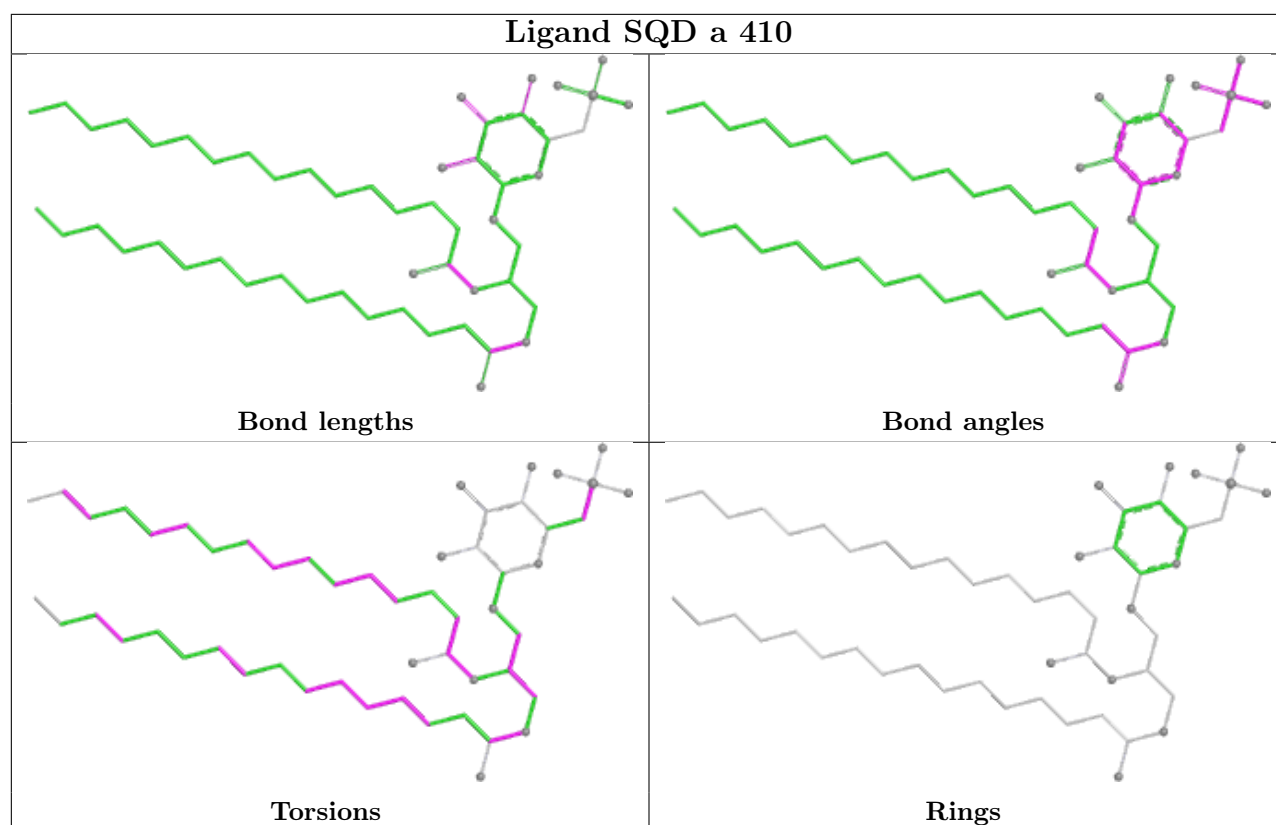


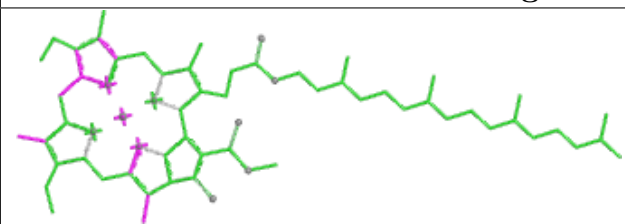
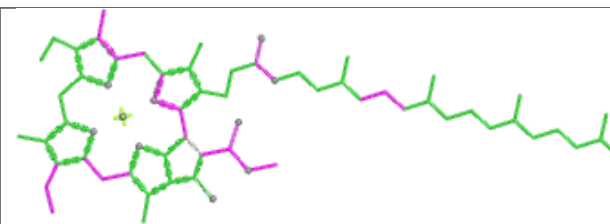
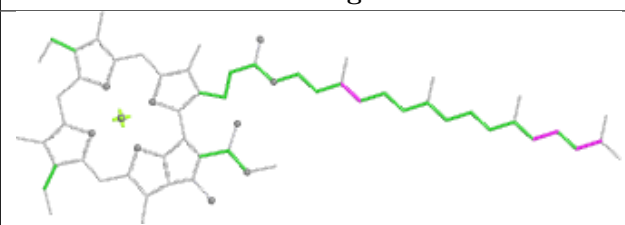
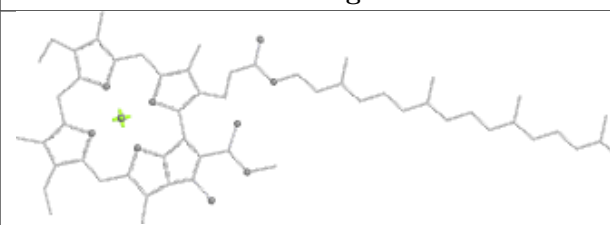


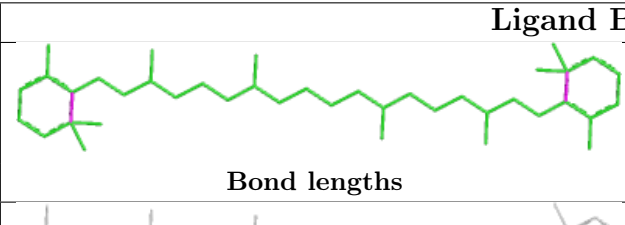
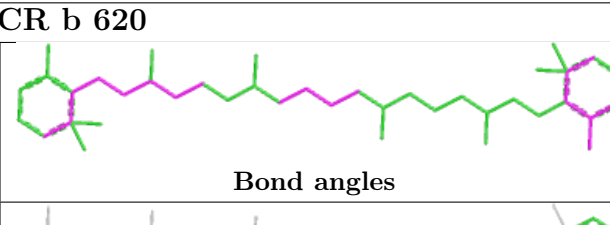
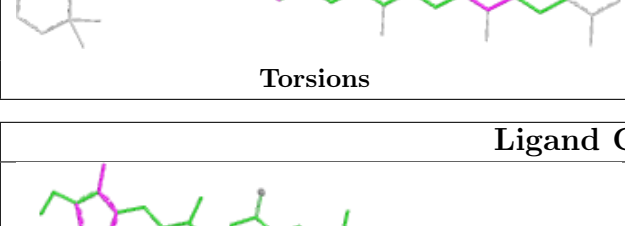
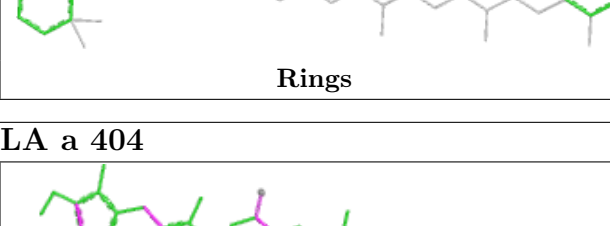


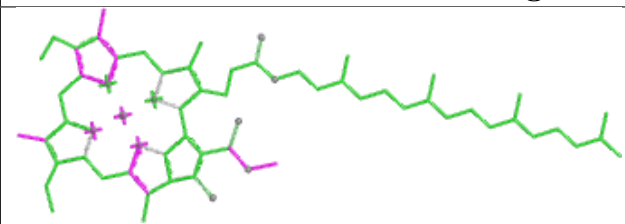
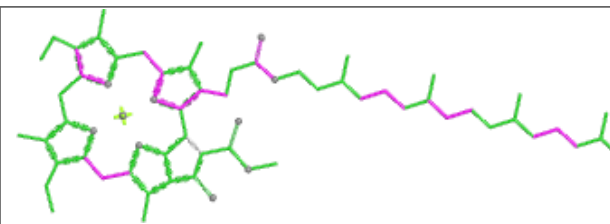
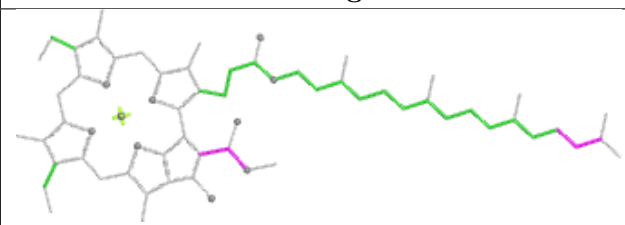
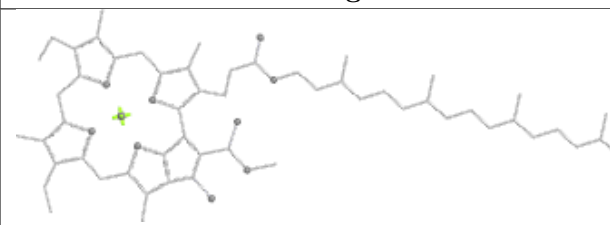


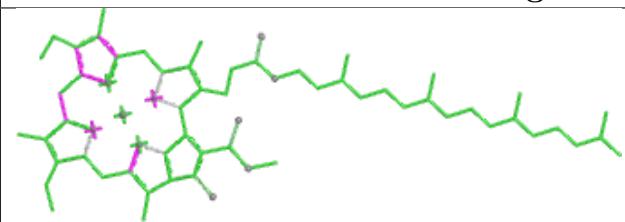
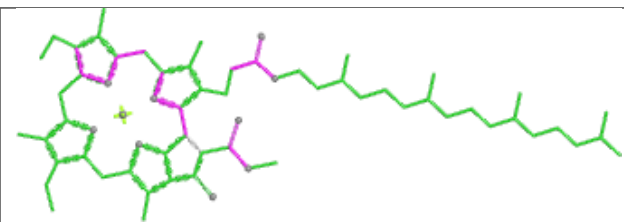
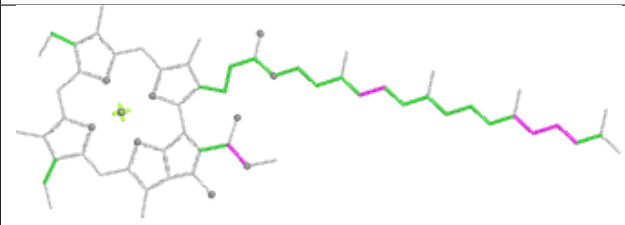
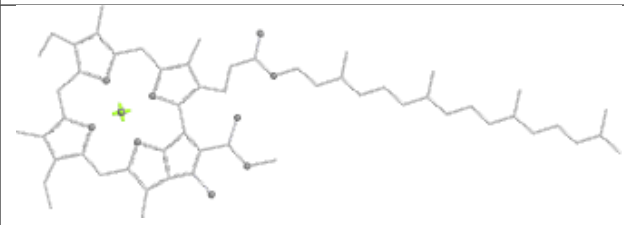


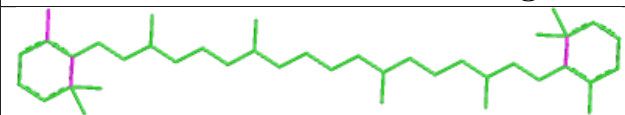
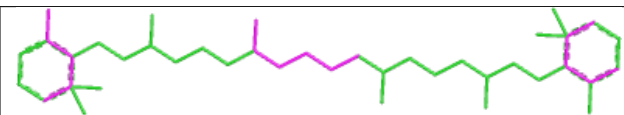
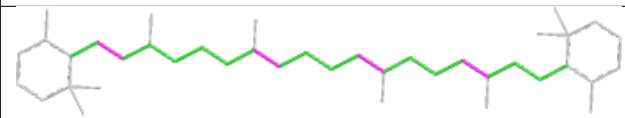
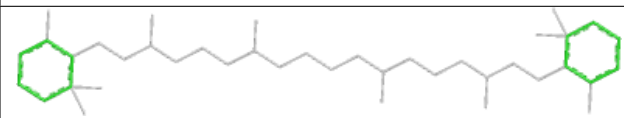


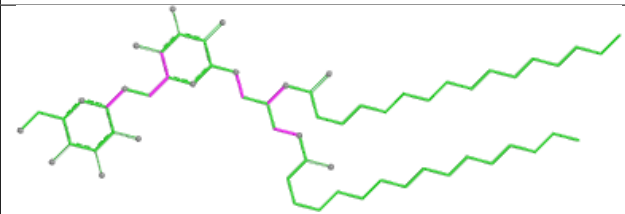
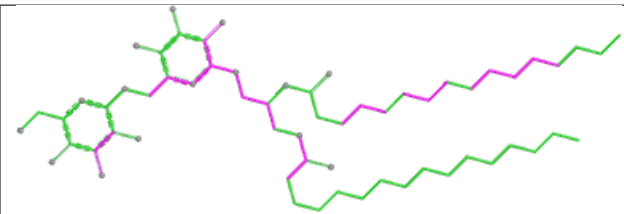
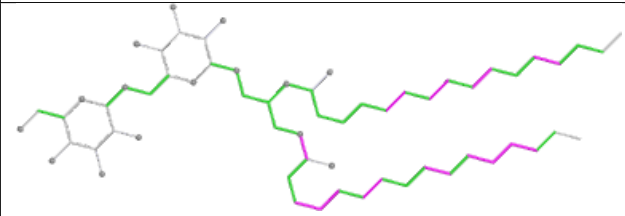
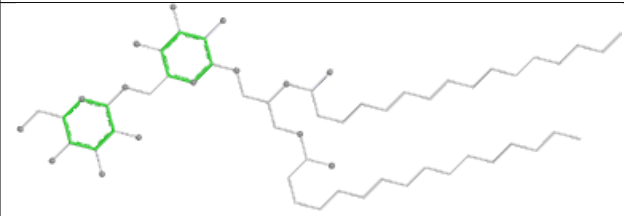
Ligand CLA B 609	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR b 620	
	
Bond lengths	Bond angles
	
Torsions	Rings

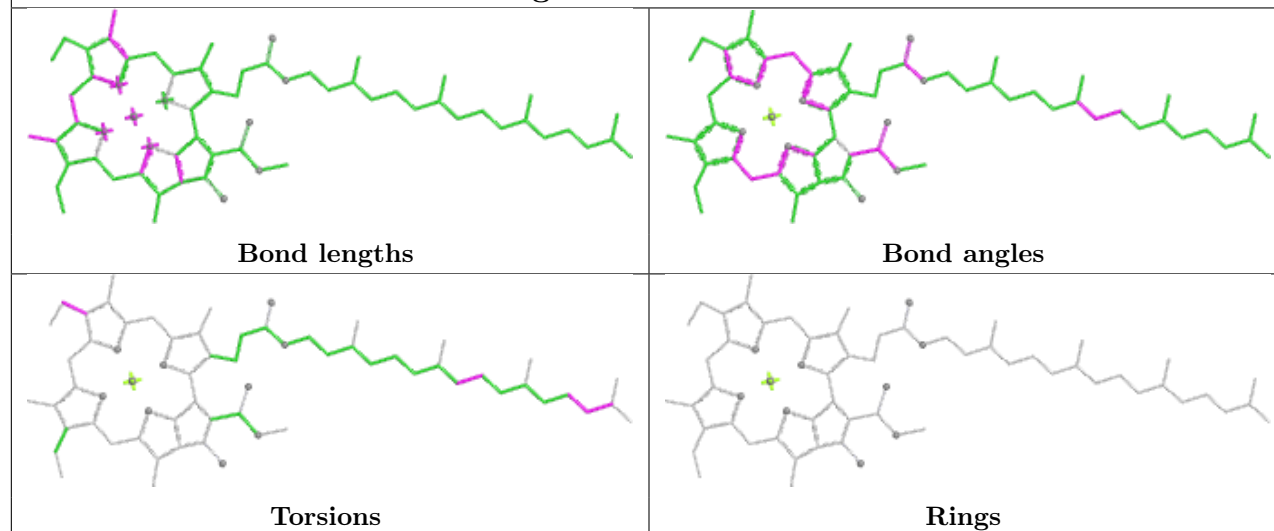
Ligand CLA a 404	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA c 511	
	
Bond lengths	Bond angles
	
Torsions	Rings

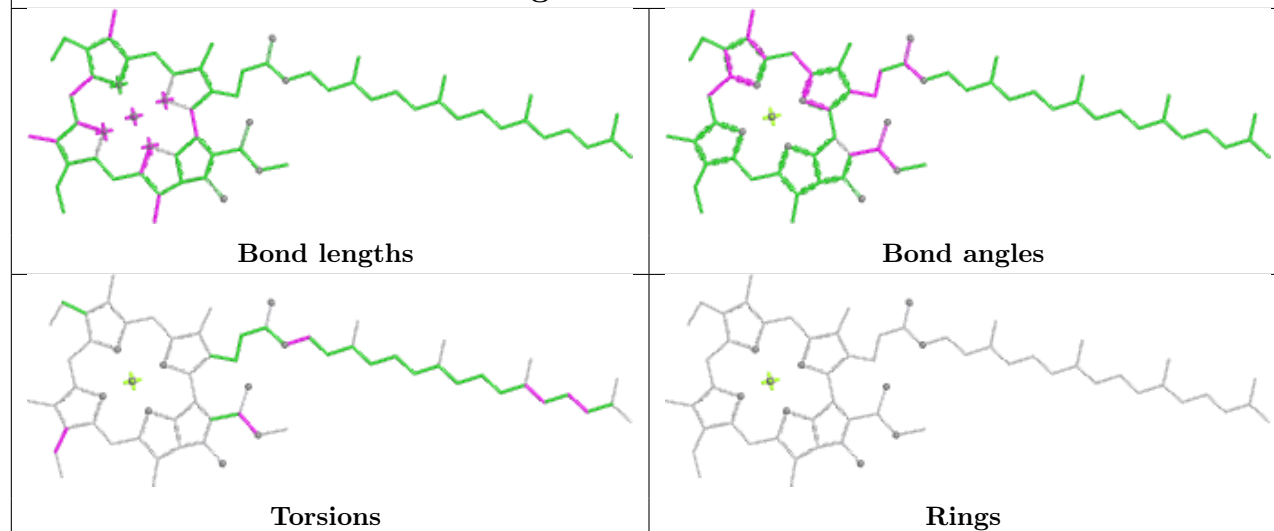
Ligand BCR B 617	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand DGD C 518	
	
Bond lengths	Bond angles
	
Torsions	Rings

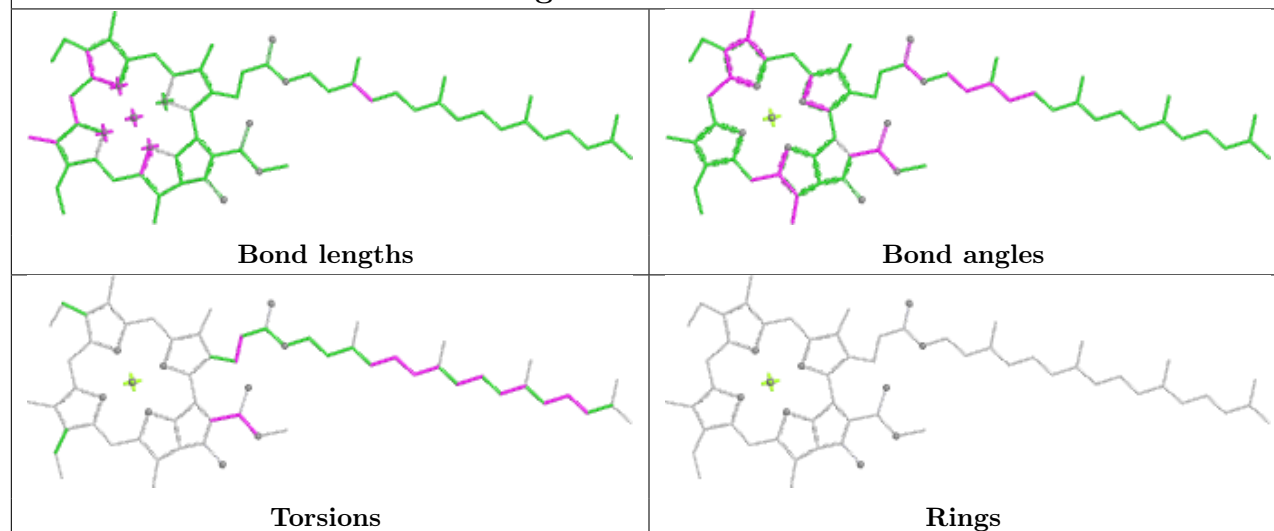
Ligand CLA B 610

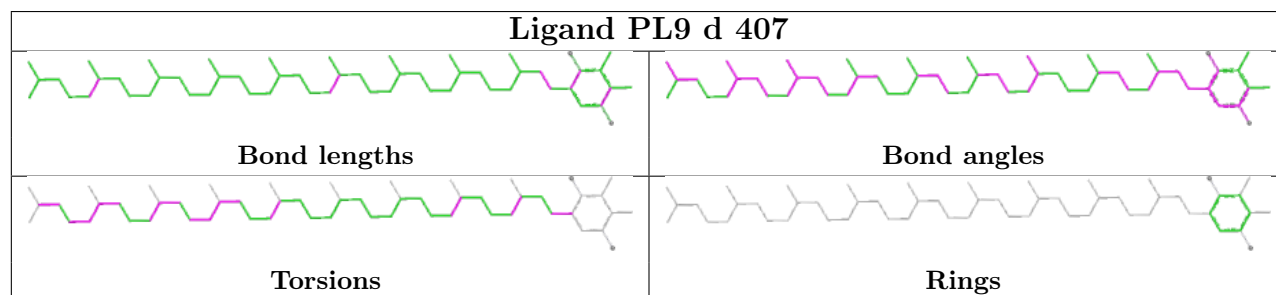
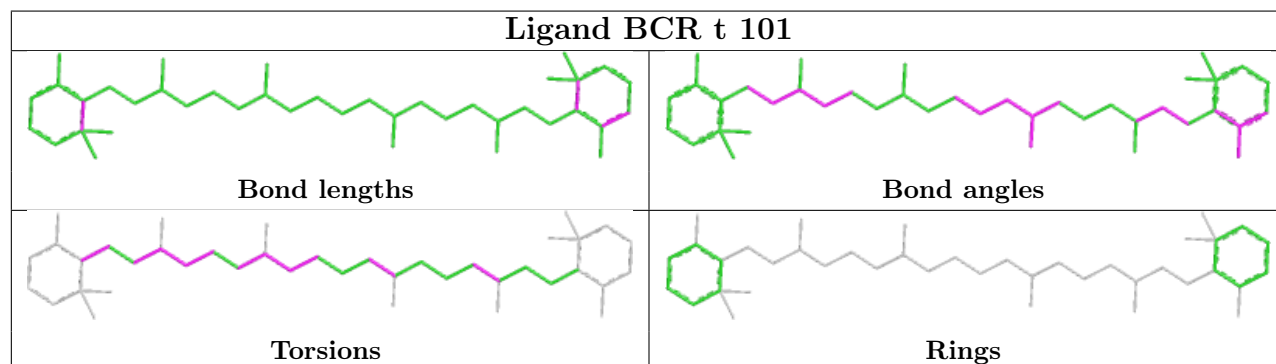
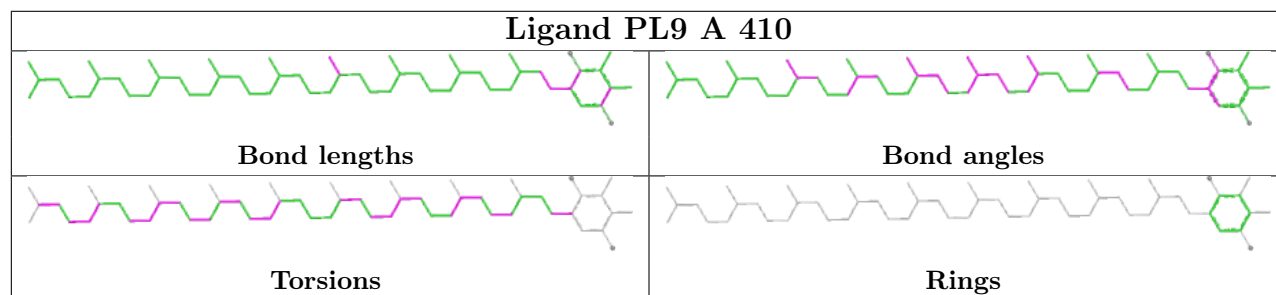
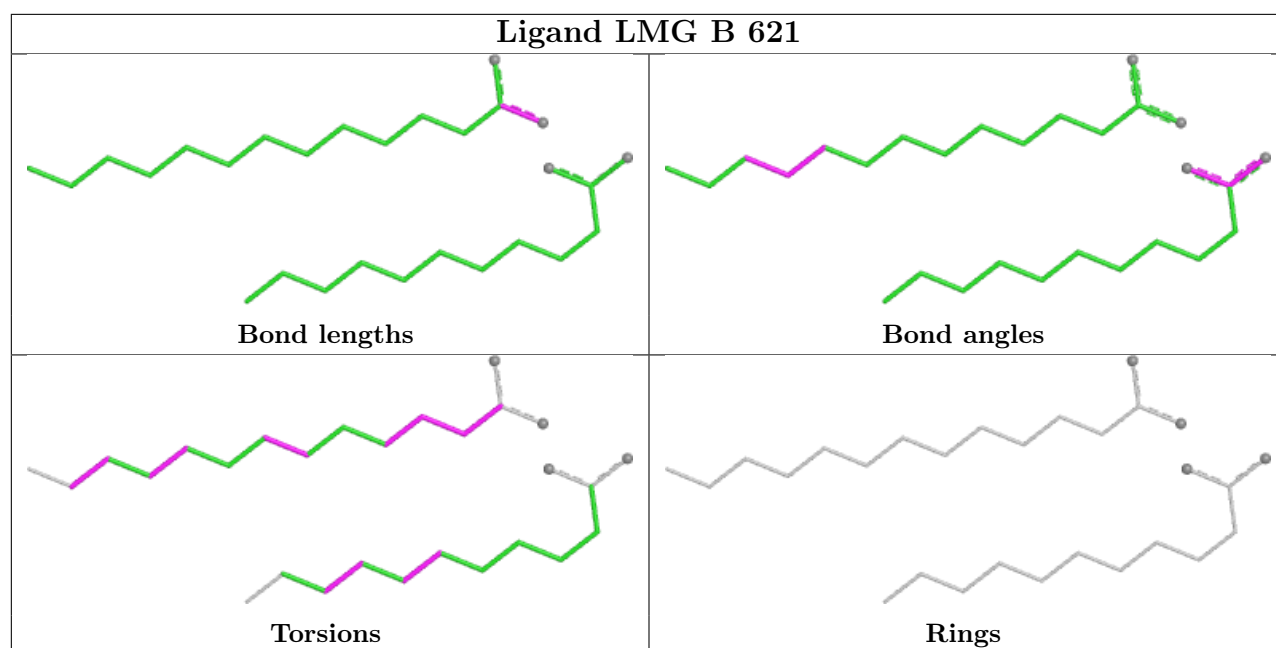


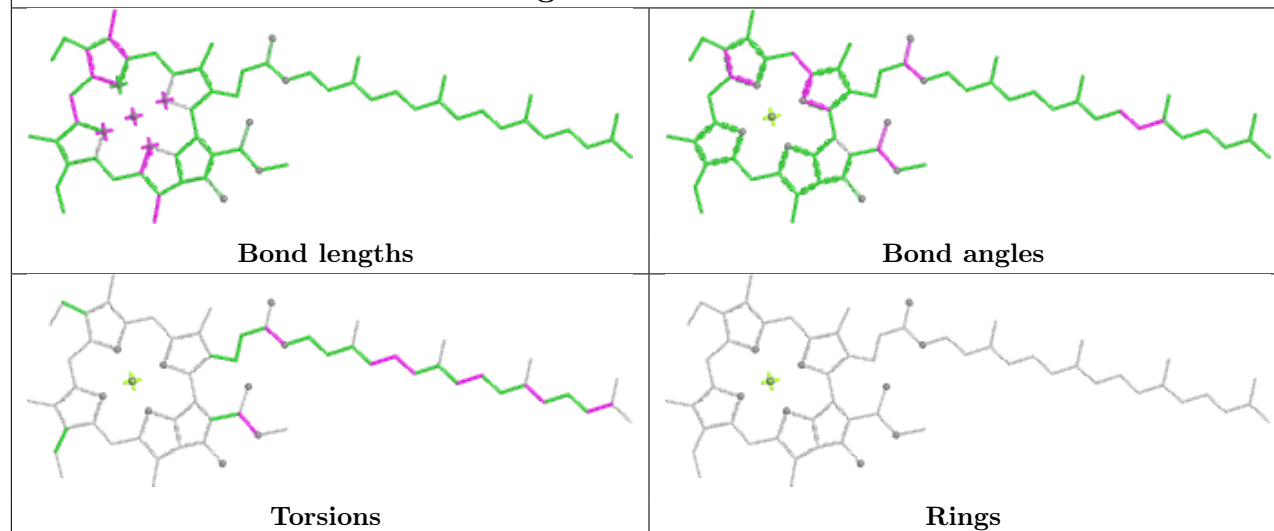
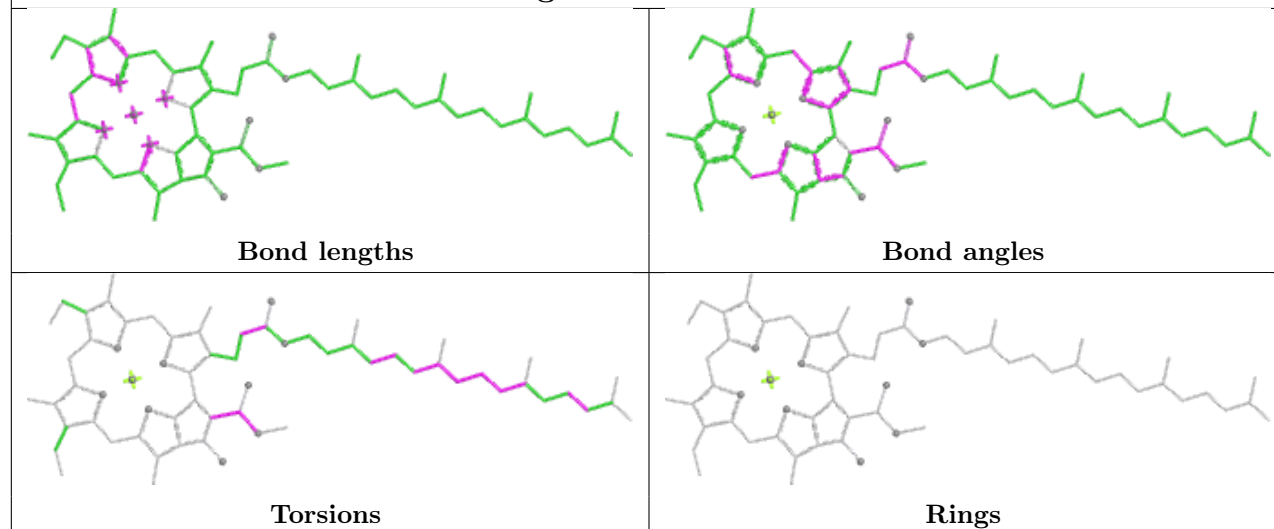
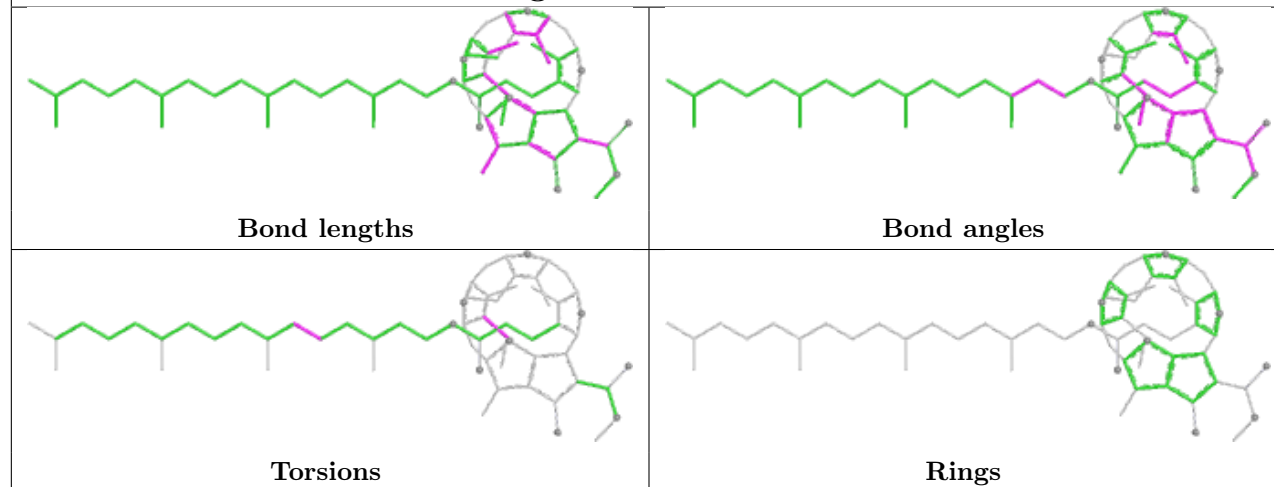
Ligand CLA D 403

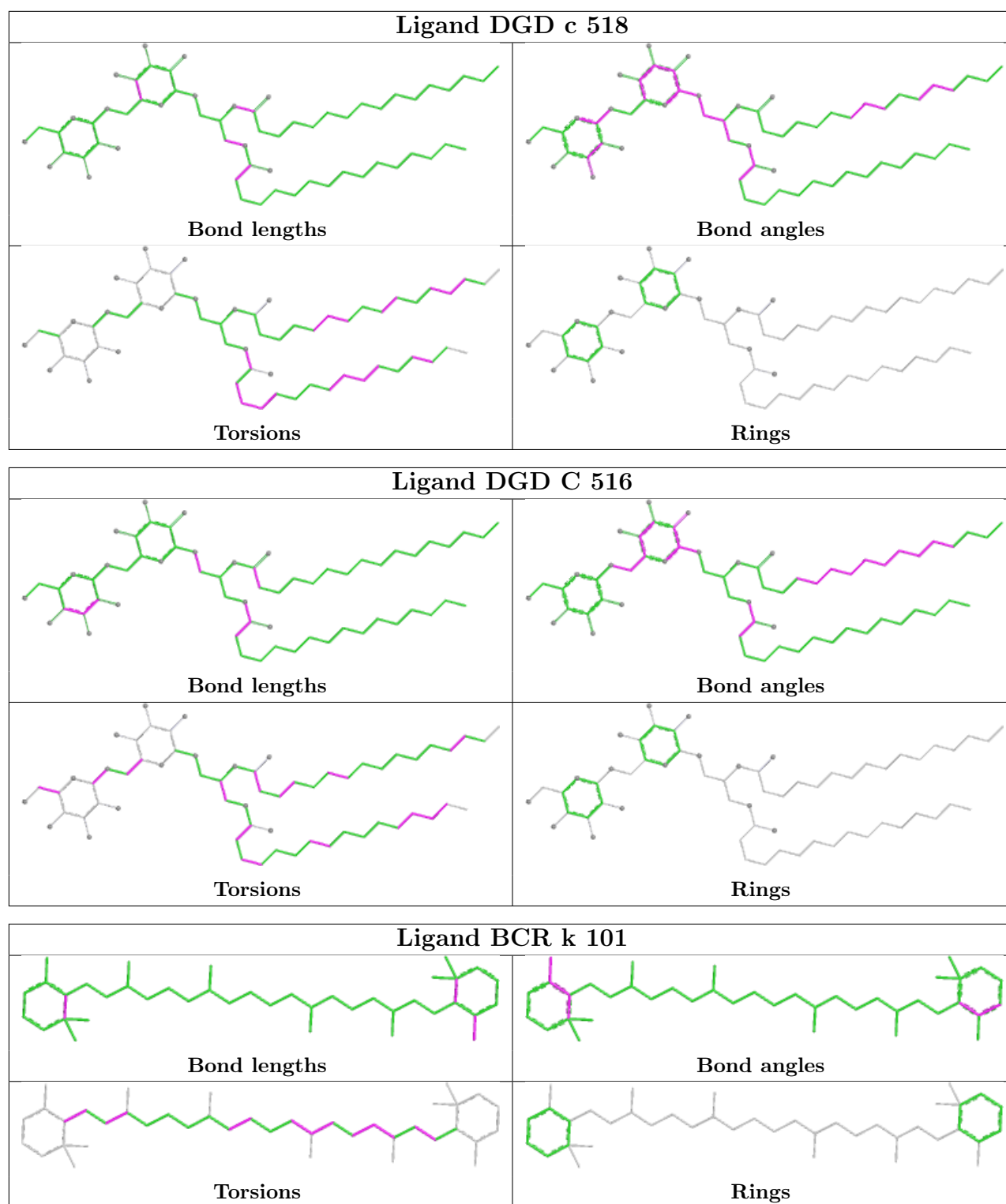


Ligand CLA b 615





Ligand CLA c 513**Ligand CLA c 509****Ligand PHO D 401**



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	468:SER	C	469:MET	N	1.17

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	334/334 (100%)	-0.65	1 (0%) 90 91	22, 31, 52, 84	0
1	a	334/334 (100%)	-0.54	1 (0%) 90 91	23, 33, 65, 89	0
2	B	505/505 (100%)	-0.51	0 100 100	18, 35, 66, 98	4 (0%)
2	b	505/505 (100%)	-0.38	2 (0%) 88 90	26, 39, 76, 117	0
3	C	442/451 (98%)	-0.45	0 100 100	24, 39, 59, 85	1 (0%)
3	c	451/451 (100%)	-0.38	1 (0%) 91 92	22, 43, 67, 115	2 (0%)
4	D	341/341 (100%)	-0.64	0 100 100	22, 33, 51, 84	0
4	d	341/341 (100%)	-0.48	0 100 100	21, 37, 65, 94	1 (0%)
5	E	81/82 (98%)	0.10	0 100 100	32, 55, 76, 84	1 (1%)
5	e	82/82 (100%)	0.19	0 100 100	42, 66, 87, 98	0
6	F	34/34 (100%)	-0.23	1 (2%) 53 56	38, 47, 71, 88	0
6	f	34/34 (100%)	0.18	0 100 100	44, 54, 82, 101	0
7	H	65/65 (100%)	-0.27	1 (1%) 72 74	36, 45, 65, 81	0
7	h	63/65 (96%)	-0.08	0 100 100	42, 54, 69, 75	0
8	I	35/36 (97%)	-0.41	0 100 100	34, 40, 73, 84	0
8	i	35/36 (97%)	-0.29	0 100 100	33, 44, 75, 83	0
9	J	36/36 (100%)	-0.14	0 100 100	38, 52, 81, 105	0
9	j	36/36 (100%)	0.10	1 (2%) 55 57	44, 56, 90, 92	0
10	K	37/37 (100%)	0.06	1 (2%) 56 58	34, 56, 76, 78	1 (2%)
10	k	37/37 (100%)	0.23	1 (2%) 56 58	49, 63, 81, 90	0
11	L	37/37 (100%)	-0.76	0 100 100	23, 32, 65, 72	0
11	l	36/37 (97%)	-0.58	0 100 100	26, 33, 75, 86	0
12	M	32/33 (96%)	-0.55	0 100 100	28, 36, 65, 82	0
12	m	31/33 (93%)	-0.52	0 100 100	28, 37, 50, 74	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/244 (100%)	-0.32	0 100 100	26, 44, 88, 146	1 (0%)
13	o	244/244 (100%)	-0.32	1 (0%) 88 90	24, 44, 84, 138	0
14	T	29/30 (96%)	-0.60	0 100 100	27, 35, 66, 74	0
14	t	29/30 (96%)	-0.42	1 (3%) 48 50	26, 34, 84, 102	0
15	U	97/97 (100%)	-0.31	0 100 100	33, 46, 74, 98	0
15	u	97/97 (100%)	-0.32	1 (1%) 79 82	32, 44, 60, 93	0
16	V	137/137 (100%)	-0.45	0 100 100	26, 44, 59, 88	0
16	v	137/137 (100%)	-0.19	0 100 100	34, 51, 75, 91	0
17	Y	27/30 (90%)	0.95	2 (7%) 20 22	57, 83, 119, 133	0
17	y	30/30 (100%)	0.65	0 100 100	66, 78, 108, 114	0
18	X	38/38 (100%)	-0.04	1 (2%) 57 60	40, 54, 83, 95	0
18	x	38/38 (100%)	0.16	0 100 100	52, 66, 95, 114	0
19	Z	62/62 (100%)	0.55	2 (3%) 50 52	56, 72, 119, 136	0
19	z	62/62 (100%)	0.74	2 (3%) 50 52	59, 79, 121, 134	0
20	R	34/34 (100%)	0.57	1 (2%) 53 56	64, 75, 96, 102	0
20	r	31/34 (91%)	1.17	3 (9%) 13 14	73, 95, 107, 116	0
All	All	5300/5326 (99%)	-0.35	24 (0%) 87 89	18, 41, 80, 146	11 (0%)

The worst 5 of 24 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
14	t	30	THR	3.7
19	z	33	TRP	3.4
20	r	32	GLN	3.1
2	b	495	PHE	3.0
20	R	35	LEU	2.9

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	FME	I	1	10/11	0.95	0.07	33,53,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
14	FME	T	1	10/11	0.95	0.08	30,49,70,70	0
14	FME	t	1	10/11	0.95	0.07	26,38,64,65	0
8	FME	i	1	10/11	0.96	0.07	38,52,64,68	0
12	FME	m	1	10/11	0.96	0.08	29,50,66,80	0
12	FME	M	1	10/11	0.96	0.08	33,47,76,79	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
31	UNL	b	626	26/-	0.78	0.15	39,52,61,63	0
31	UNL	H	103	53/-	0.80	0.14	51,73,94,97	0
31	UNL	c	523	28/-	0.80	0.12	49,72,88,89	0
32	LMG	c	522	48/55	0.82	0.14	42,80,114,117	0
33	LHG	E	101	49/49	0.82	0.13	48,83,108,119	0
33	LHG	e	101	42/49	0.82	0.13	58,87,114,129	0
32	LMG	b	623	55/55	0.83	0.14	44,76,98,109	0
31	UNL	B	625	28/-	0.84	0.16	52,73,90,103	0
32	LMG	h	102	23/55	0.84	0.17	41,77,102,105	0
31	UNL	B	626	47/-	0.84	0.15	48,66,91,94	0
29	DGD	a	412	44/66	0.84	0.12	32,57,76,84	0
31	UNL	a	413	28/-	0.85	0.11	31,63,70,81	0
31	UNL	b	624	40/-	0.85	0.13	52,69,88,88	0
31	UNL	b	625	55/-	0.85	0.12	40,60,80,81	0
31	UNL	T	101	47/-	0.85	0.13	38,49,65,71	0
31	UNL	T	102	44/-	0.85	0.14	41,57,76,77	0
29	DGD	A	413	66/66	0.86	0.11	36,68,84,102	0
27	PL9	A	410	55/55	0.86	0.13	31,58,79,91	0
27	PL9	a	409	55/55	0.86	0.13	36,66,86,99	0
31	UNL	c	520	55/-	0.86	0.11	34,61,83,90	0
28	SQD	a	411	36/54	0.86	0.12	38,65,87,97	0
31	UNL	t	103	26/-	0.87	0.12	38,64,77,81	0
32	LMG	K	102	48/55	0.87	0.11	48,71,92,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	CLA	h	101	65/65	0.87	0.11	45,67,92,104	0
32	LMG	c	519	37/55	0.87	0.11	41,70,83,88	0
31	UNL	I	101	41/-	0.87	0.13	40,51,76,78	0
31	UNL	b	622	55/-	0.87	0.12	39,60,84,89	0
31	UNL	C	522	47/-	0.87	0.12	44,56,66,67	0
31	UNL	d	412	43/-	0.87	0.13	43,58,70,77	0
31	UNL	x	101	55/-	0.88	0.11	39,58,75,78	0
32	LMG	D	410	33/55	0.88	0.11	35,54,89,98	0
28	SQD	b	601	49/54	0.88	0.10	39,58,97,111	0
28	SQD	f	101	41/54	0.89	0.13	55,90,116,124	0
31	UNL	B	620	43/-	0.89	0.09	35,49,60,70	0
31	UNL	X	101	55/-	0.89	0.11	33,54,76,78	0
31	UNL	E	102	28/-	0.89	0.11	53,74,84,86	0
32	LMG	c	524	49/55	0.89	0.10	37,54,88,107	0
31	UNL	B	623	28/-	0.89	0.10	35,51,67,77	0
28	SQD	A	412	39/54	0.89	0.12	41,68,96,103	0
31	UNL	J	101	28/-	0.89	0.11	50,63,71,81	0
31	UNL	m	101	28/-	0.90	0.12	38,53,74,82	0
26	BCR	h	103	40/40	0.90	0.10	31,54,78,88	0
31	UNL	C	521	28/-	0.90	0.10	44,54,60,67	0
32	LMG	B	621	28/55	0.90	0.11	33,50,62,66	0
32	LMG	C	501	48/55	0.90	0.09	34,57,72,109	0
28	SQD	B	622	54/54	0.90	0.09	33,60,88,102	0
31	UNL	j	101	28/-	0.90	0.10	44,56,67,68	0
26	BCR	k	101	40/40	0.91	0.10	41,64,77,79	0
31	UNL	B	624	46/-	0.91	0.09	39,54,66,72	0
24	CLA	B	601	65/65	0.91	0.10	32,65,102,107	0
31	UNL	M	103	26/-	0.91	0.11	39,51,59,64	0
31	UNL	M	104	53/-	0.91	0.12	36,48,88,90	0
26	BCR	K	101	40/40	0.91	0.10	33,56,69,76	0
31	UNL	C	520	28/-	0.91	0.09	33,46,50,62	0
26	BCR	c	514	40/40	0.91	0.09	35,60,72,74	0
31	UNL	t	102	34/-	0.91	0.09	38,51,64,77	0
24	CLA	C	514	65/65	0.91	0.10	45,65,91,105	0
28	SQD	a	410	54/54	0.91	0.10	41,68,93,95	0
32	LMG	M	101	51/55	0.92	0.08	25,47,71,81	0
32	LMG	b	621	51/55	0.92	0.09	32,51,76,91	0
26	BCR	d	406	40/40	0.92	0.09	32,56,100,106	0
26	BCR	D	405	40/40	0.92	0.09	29,46,90,104	0
24	CLA	c	513	65/65	0.92	0.10	40,74,109,115	0
26	BCR	Y	101	40/40	0.92	0.08	37,54,73,75	0
24	CLA	c	512	65/65	0.92	0.10	42,60,99,125	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
26	BCR	c	521	40/40	0.92	0.10	40,56,70,75	0
29	DGD	C	517	62/66	0.92	0.09	32,56,96,109	0
24	CLA	c	511	65/65	0.93	0.10	43,56,76,80	0
31	UNL	M	102	37/-	0.93	0.08	33,47,65,67	0
24	CLA	C	513	65/65	0.93	0.09	33,56,93,103	0
28	SQD	A	411	52/54	0.93	0.09	33,59,89,94	0
26	BCR	C	519	40/40	0.93	0.10	29,56,68,74	0
26	BCR	b	619	40/40	0.93	0.07	27,41,54,56	0
29	DGD	H	102	62/66	0.93	0.08	27,48,63,78	0
28	SQD	F	101	36/54	0.93	0.10	41,74,93,99	0
29	DGD	c	517	62/66	0.93	0.08	31,55,92,107	0
29	DGD	h	104	62/66	0.93	0.08	30,51,68,76	0
26	BCR	b	620	40/40	0.93	0.07	29,50,62,66	0
26	BCR	B	619	40/40	0.94	0.07	21,40,62,72	0
26	BCR	t	101	40/40	0.94	0.07	25,40,56,60	0
26	BCR	C	515	40/40	0.94	0.08	28,39,49,64	0
29	DGD	c	518	62/66	0.94	0.08	26,53,78,88	0
26	BCR	c	515	40/40	0.94	0.09	25,45,64,78	0
26	BCR	b	602	40/40	0.94	0.07	23,41,66,72	0
32	LMG	d	411	44/55	0.94	0.09	31,55,91,97	0
32	LMG	D	407	51/55	0.94	0.10	24,58,93,98	0
26	BCR	b	618	40/40	0.94	0.07	25,43,56,61	0
33	LHG	d	408	49/49	0.94	0.09	31,51,85,94	0
26	BCR	H	101	40/40	0.94	0.07	30,47,67,71	0
24	CLA	B	606	65/65	0.95	0.07	24,38,76,83	0
29	DGD	C	516	62/66	0.95	0.08	21,40,79,95	0
24	CLA	b	613	65/65	0.95	0.07	20,35,45,61	0
29	DGD	C	518	62/66	0.95	0.07	26,48,79,89	0
24	CLA	b	616	65/65	0.95	0.07	26,41,60,72	0
26	BCR	a	408	40/40	0.95	0.06	17,32,48,53	0
24	CLA	b	617	60/65	0.95	0.08	24,44,89,98	0
24	CLA	c	503	65/65	0.95	0.07	24,44,55,60	0
24	CLA	c	504	60/65	0.95	0.08	26,46,87,91	0
24	CLA	c	505	65/65	0.95	0.07	24,42,66,70	0
24	CLA	c	506	65/65	0.95	0.09	25,53,110,118	0
24	CLA	c	508	64/65	0.95	0.08	29,48,80,108	0
24	CLA	c	509	65/65	0.95	0.08	29,48,64,68	0
24	CLA	c	510	65/65	0.95	0.07	32,49,73,84	0
24	CLA	B	609	65/65	0.95	0.07	22,40,57,64	0
24	CLA	C	503	65/65	0.95	0.07	27,42,60,69	0
24	CLA	C	504	65/65	0.95	0.07	22,42,54,57	0
24	CLA	d	405	65/65	0.95	0.08	25,49,107,114	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	CLA	C	507	65/65	0.95	0.08	25,42,99,113	0
27	PL9	d	407	55/55	0.95	0.06	19,35,43,50	0
25	PHO	d	402	64/64	0.95	0.07	25,39,53,62	0
26	BCR	A	409	40/40	0.95	0.06	21,34,44,48	0
26	BCR	B	617	40/40	0.95	0.07	24,42,54,55	0
26	BCR	B	618	40/40	0.95	0.06	22,39,51,56	0
24	CLA	C	509	65/65	0.95	0.08	24,42,96,114	0
33	LHG	D	409	47/49	0.95	0.09	20,45,83,99	0
33	LHG	D	411	49/49	0.95	0.08	26,44,69,81	0
24	CLA	C	511	65/65	0.95	0.07	28,47,67,72	0
24	CLA	C	512	65/65	0.95	0.08	34,53,69,75	0
33	LHG	d	410	39/49	0.95	0.08	32,48,71,76	0
23	BCT	d	401	4/4	0.95	0.08	29,29,38,46	0
33	LHG	l	101	49/49	0.95	0.07	28,46,61,67	0
24	CLA	C	505	59/65	0.96	0.07	26,46,75,87	0
24	CLA	c	501	65/65	0.96	0.06	28,39,53,55	0
24	CLA	c	502	65/65	0.96	0.07	27,42,63,71	0
24	CLA	C	506	65/65	0.96	0.08	23,39,65,76	0
24	CLA	A	405	65/65	0.96	0.06	15,28,41,49	0
29	DGD	c	516	62/66	0.96	0.08	22,41,77,90	0
24	CLA	C	508	65/65	0.96	0.06	23,40,61,67	0
24	CLA	B	602	65/65	0.96	0.06	22,36,63,74	0
24	CLA	c	507	65/65	0.96	0.07	28,45,64,65	0
24	CLA	C	510	65/65	0.96	0.07	22,46,61,72	0
24	CLA	B	612	65/65	0.96	0.06	17,32,49,59	0
24	CLA	B	614	65/65	0.96	0.08	16,37,88,97	0
24	CLA	B	615	65/65	0.96	0.07	20,38,64,87	0
24	CLA	B	616	60/65	0.96	0.08	23,42,93,98	0
24	CLA	a	404	65/65	0.96	0.06	16,29,44,59	0
24	CLA	d	403	65/65	0.96	0.06	16,30,44,47	0
24	CLA	d	404	65/65	0.96	0.07	19,33,63,70	0
24	CLA	a	405	65/65	0.96	0.08	22,40,97,115	0
27	PL9	D	406	55/55	0.96	0.06	18,34,46,50	0
24	CLA	a	407	65/65	0.96	0.08	17,36,89,116	0
25	PHO	A	407	64/64	0.96	0.05	16,28,39,44	0
25	PHO	D	401	64/64	0.96	0.05	21,33,48,50	0
25	PHO	a	406	64/64	0.96	0.06	22,32,41,45	0
33	LHG	D	408	49/49	0.96	0.07	19,42,59,63	0
24	CLA	b	603	65/65	0.96	0.08	24,44,69,80	0
24	CLA	b	607	65/65	0.96	0.07	22,41,77,84	0
24	CLA	b	609	65/65	0.96	0.07	25,42,58,69	0
24	CLA	b	610	65/65	0.96	0.08	26,46,64,79	0

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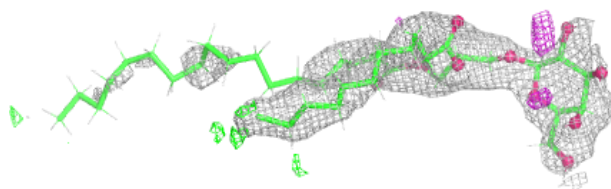
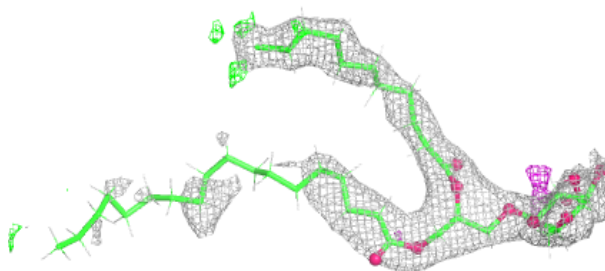
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
33	LHG	d	409	49/49	0.96	0.07	22,39,62,67	0
24	CLA	B	604	65/65	0.96	0.07	18,33,77,84	0
24	CLA	b	615	65/65	0.96	0.07	24,42,81,97	0
24	CLA	B	605	65/65	0.96	0.06	15,30,44,61	0
24	CLA	A	406	65/65	0.97	0.08	21,37,99,112	0
24	CLA	b	611	65/65	0.97	0.07	19,38,53,61	0
24	CLA	b	612	65/65	0.97	0.05	19,32,48,58	0
24	CLA	B	613	65/65	0.97	0.06	17,30,65,73	0
24	CLA	b	614	65/65	0.97	0.06	15,33,74,88	0
24	CLA	D	402	65/65	0.97	0.05	17,28,50,57	0
24	CLA	D	403	65/65	0.97	0.06	16,29,61,74	0
24	CLA	D	404	65/65	0.97	0.07	21,42,123,126	0
24	CLA	B	607	65/65	0.97	0.06	15,34,62,70	0
24	CLA	B	608	65/65	0.97	0.05	17,34,59,63	0
24	CLA	B	603	65/65	0.97	0.06	17,34,66,68	0
24	CLA	C	502	65/65	0.97	0.06	22,36,50,60	0
24	CLA	b	604	65/65	0.97	0.06	21,35,67,77	0
33	LHG	L	101	49/49	0.97	0.06	25,41,56,66	0
24	CLA	b	605	65/65	0.97	0.06	18,33,82,98	0
24	CLA	b	606	65/65	0.97	0.06	20,35,50,52	0
24	CLA	B	610	65/65	0.97	0.06	18,32,43,48	0
24	CLA	b	608	65/65	0.97	0.07	16,36,69,79	0
24	CLA	B	611	65/65	0.97	0.05	18,32,46,54	0
34	HEM	F	102	43/43	0.97	0.08	35,49,65,69	0
34	HEM	e	102	43/43	0.97	0.08	43,55,79,79	0
23	BCT	A	404	4/4	0.98	0.04	28,28,30,36	0
22	CL	a	402	1/1	0.98	0.04	28,28,28,28	0
24	CLA	A	408	54/65	0.98	0.06	16,32,62,73	0
35	HEC	v	201	43/43	0.98	0.06	27,36,47,54	0
21	FE2	A	401	1/1	0.99	0.01	28,28,28,28	0
22	CL	a	403	1/1	0.99	0.08	25,25,25,25	0
30	OEX	A	414	10/10	0.99	0.03	19,29,33,33	0
22	CL	A	402	1/1	0.99	0.02	25,25,25,25	0
35	HEC	V	201	43/43	0.99	0.05	22,33,42,48	0
22	CL	A	403	1/1	0.99	0.02	29,29,29,29	0
21	FE2	a	401	1/1	1.00	0.02	33,33,33,33	0
30	OEX	a	414	10/10	1.00	0.02	23,29,33,34	1

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.

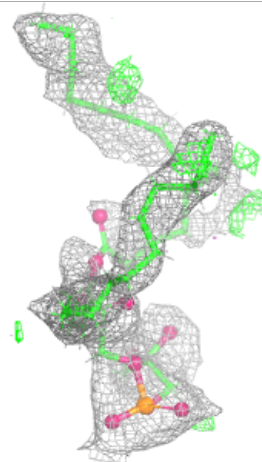
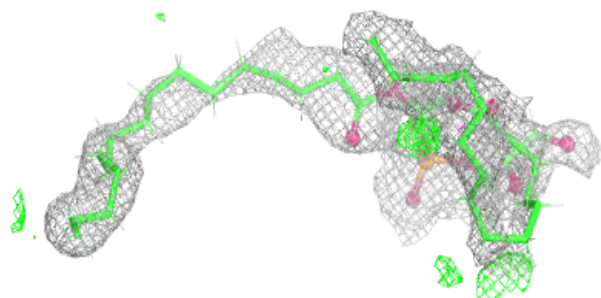
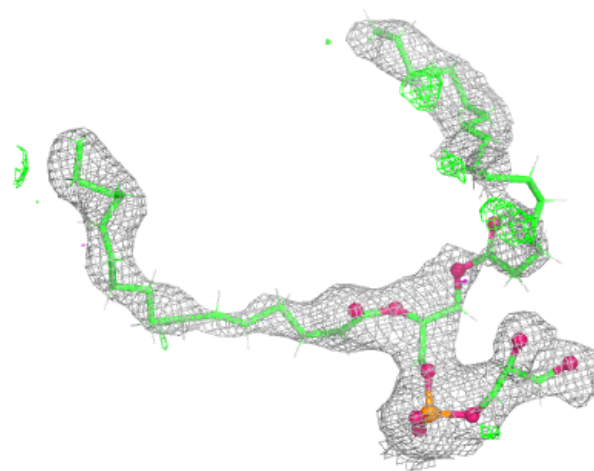
Electron density around LMG c 522:

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



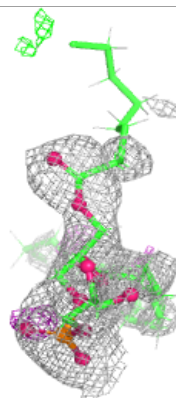
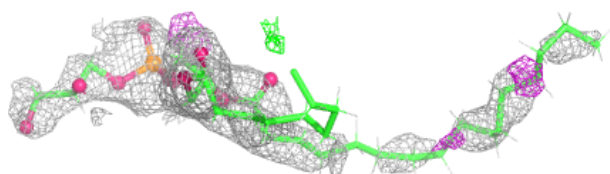
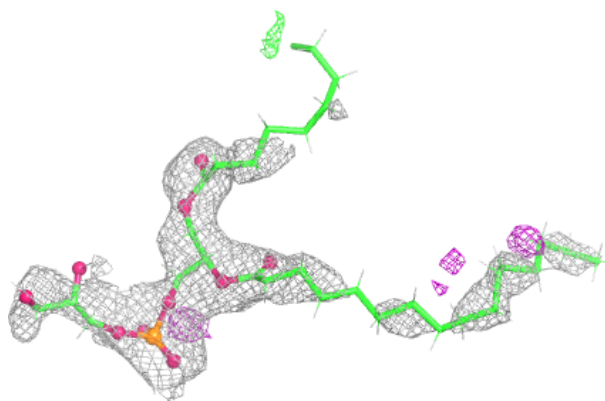
Electron density around LHG E 101:

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

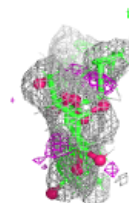
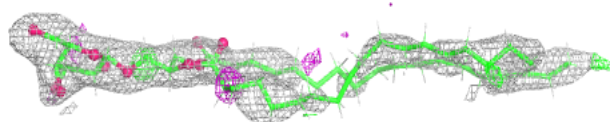
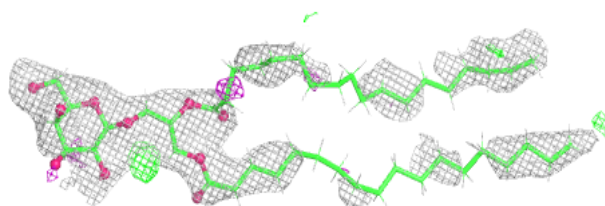


Electron density around LHG e 101:

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

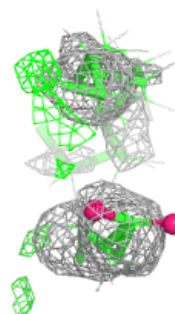
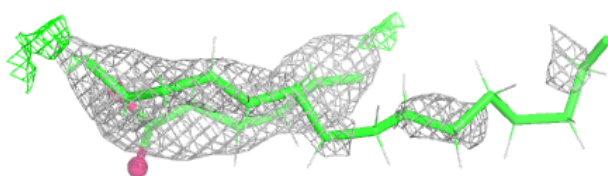
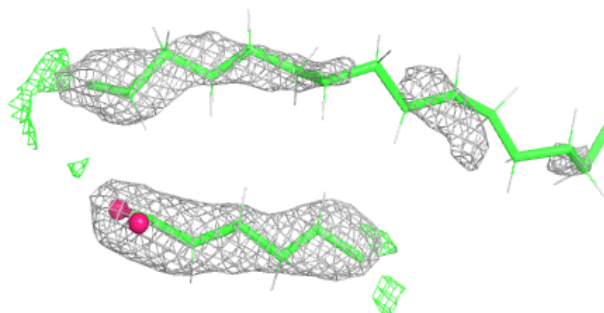
**Electron density around LMG b 623:**

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

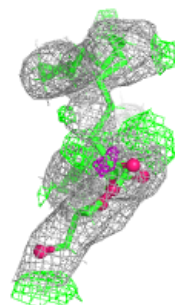
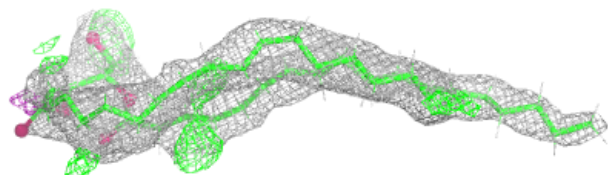
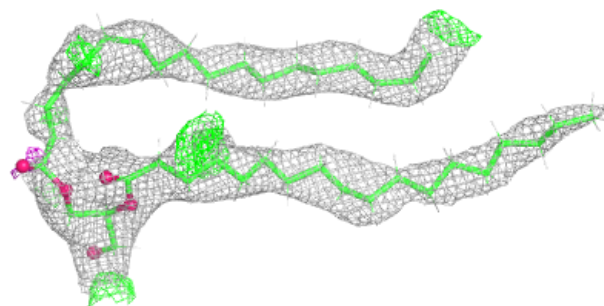


Electron density around LMG h 102:

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

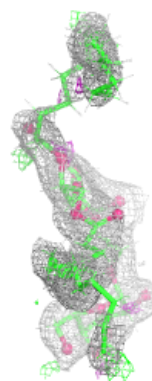
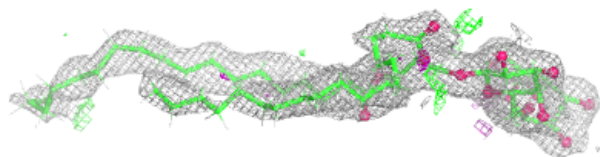
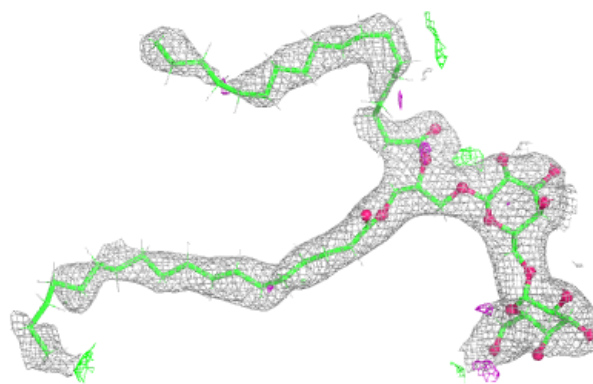
**Electron density around DGD a 412:**

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

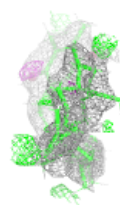
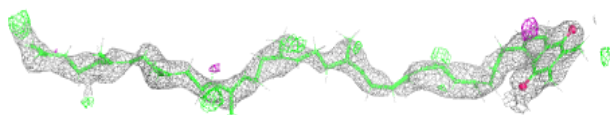
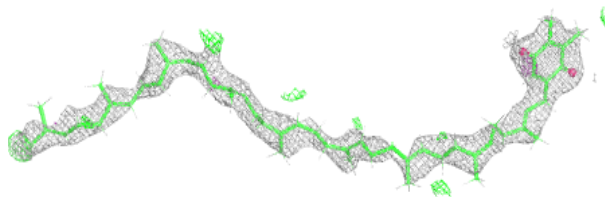


Electron density around DGD A 413:

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

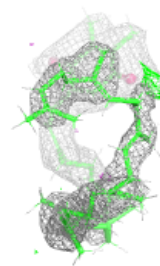
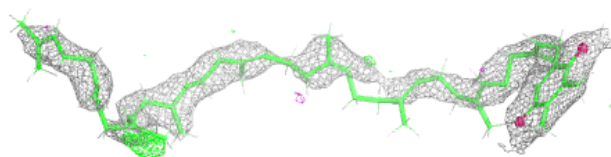
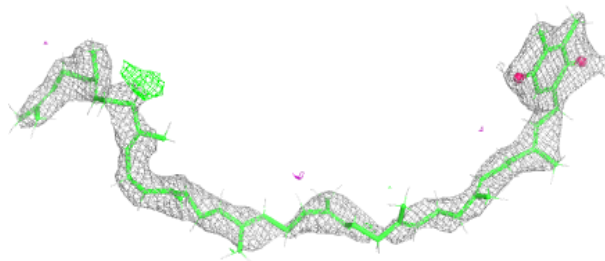
**Electron density around PL9 A 410:**

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



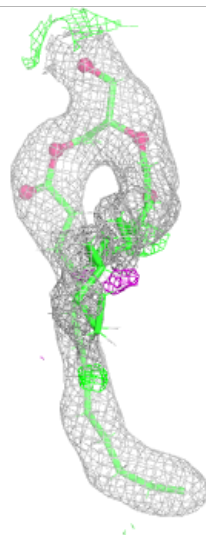
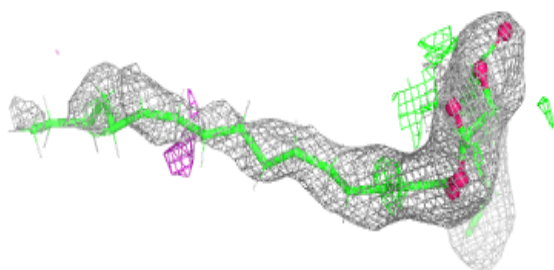
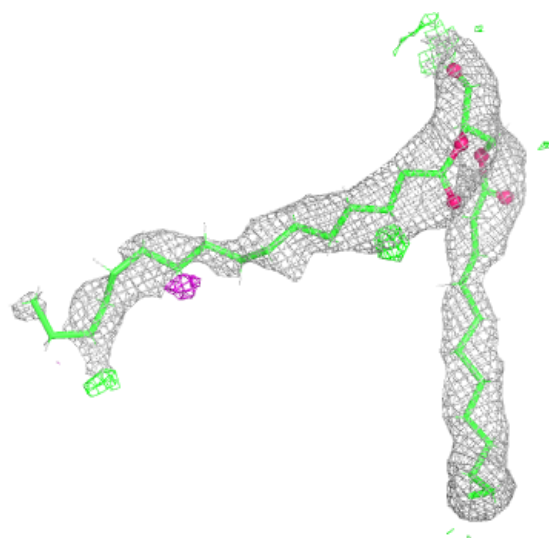
Electron density around PL9 a 409:

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and green (positive)



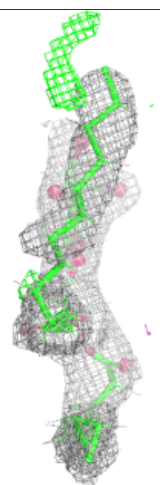
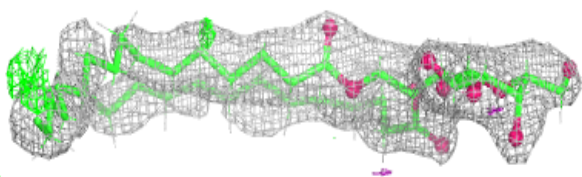
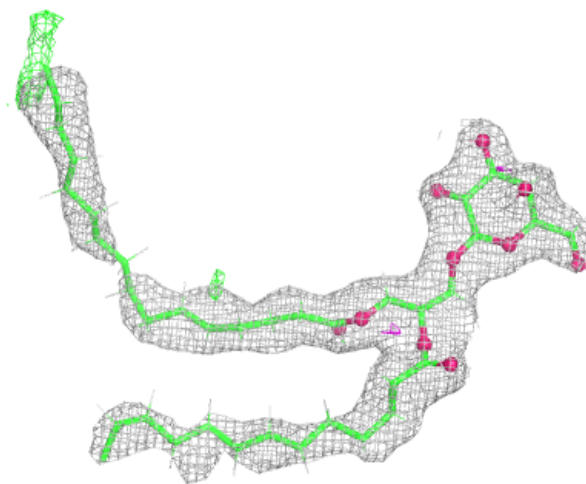
Electron density around SQD a 411:

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



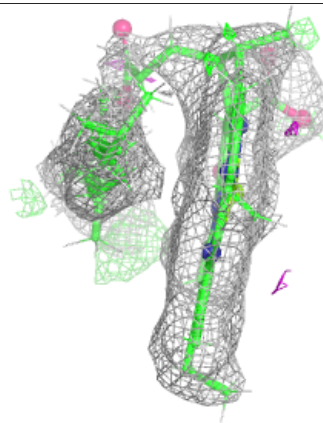
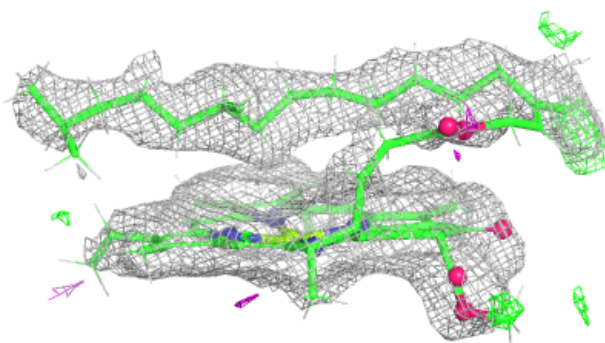
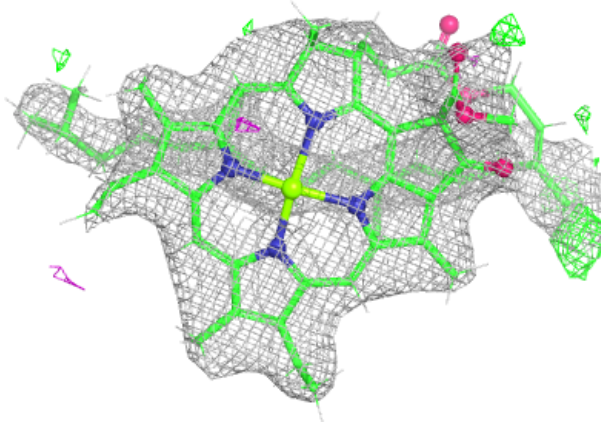
Electron density around LMG K 102:

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

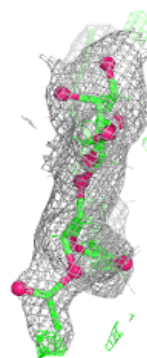
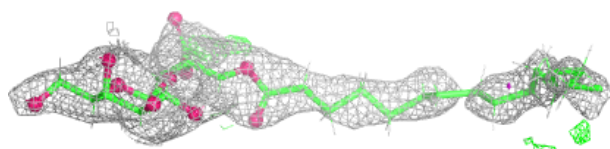
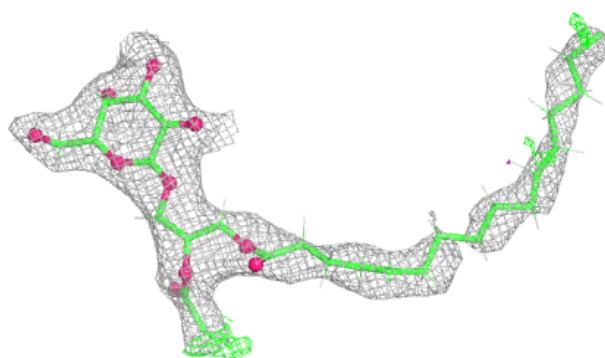


Electron density around CLA h 101:

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

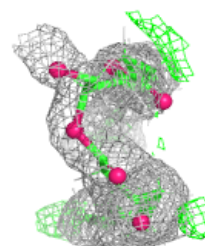
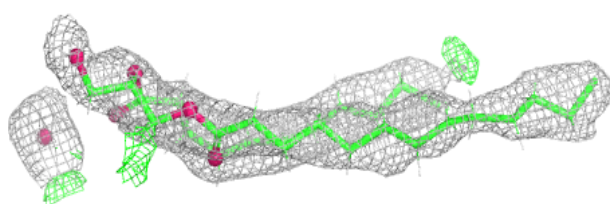
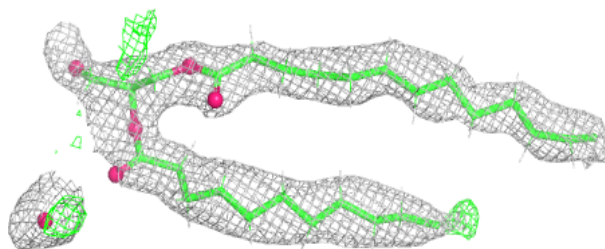
**Electron density around LMG c 519:**

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

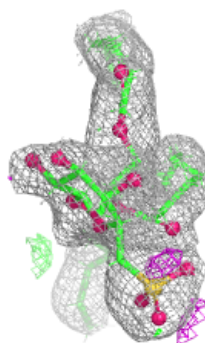
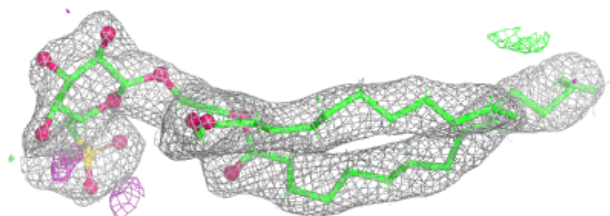
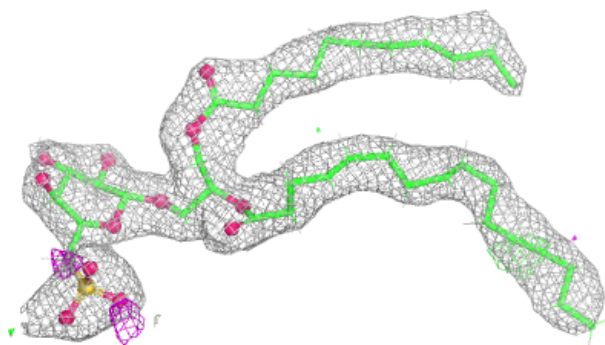


Electron density around LMG D 410:

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

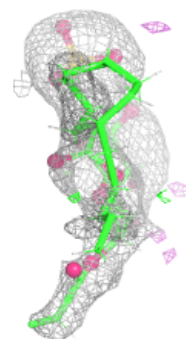
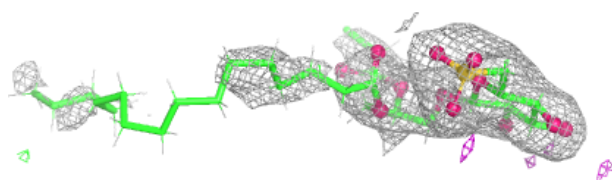
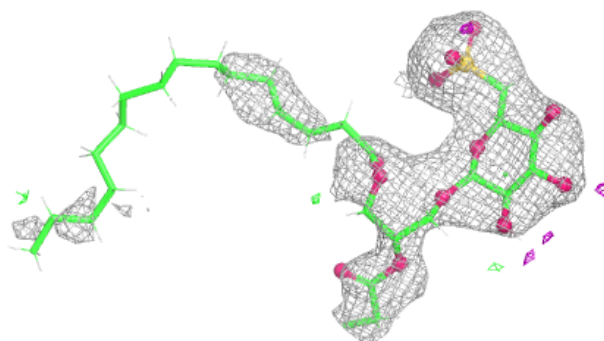
**Electron density around SQD b 601:**

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

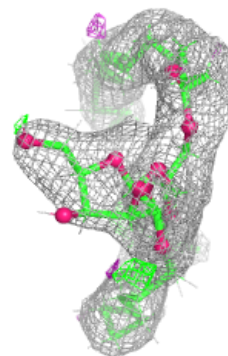
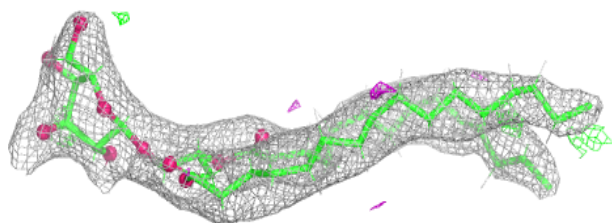
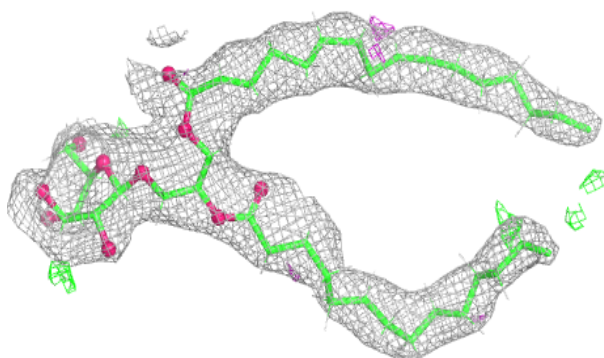


Electron density around SQD f 101:

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

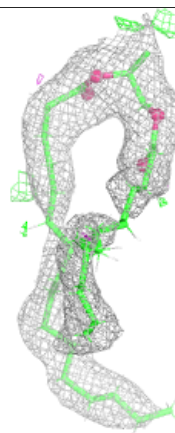
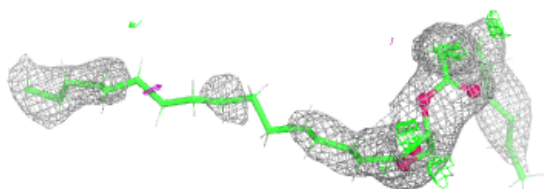
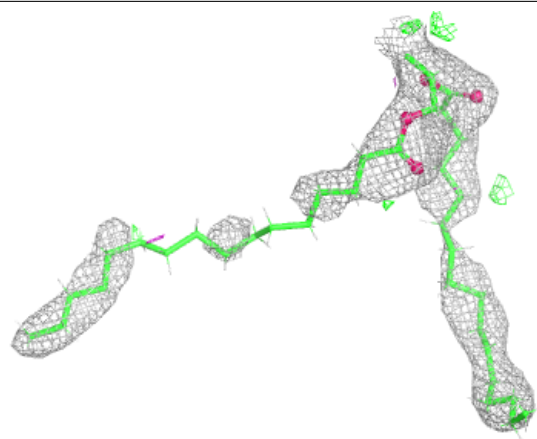
**Electron density around LMG c 524:**

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

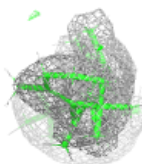
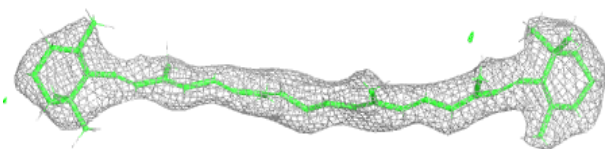
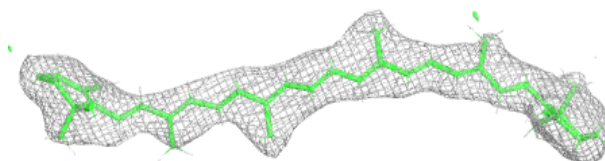


Electron density around SQD A 412:

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

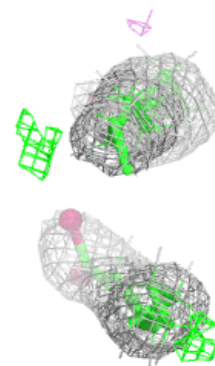
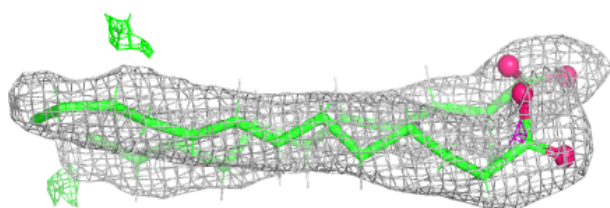
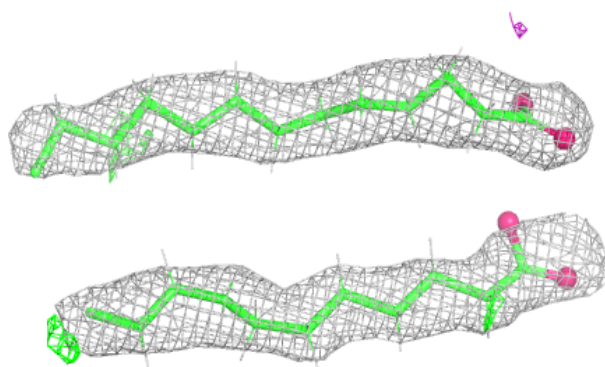
**Electron density around BCR h 103:**

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

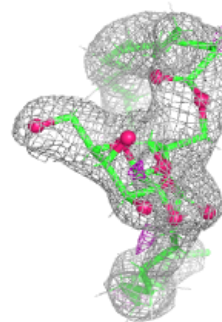
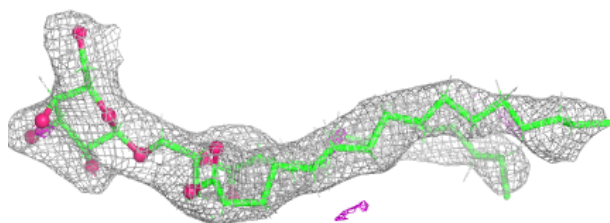
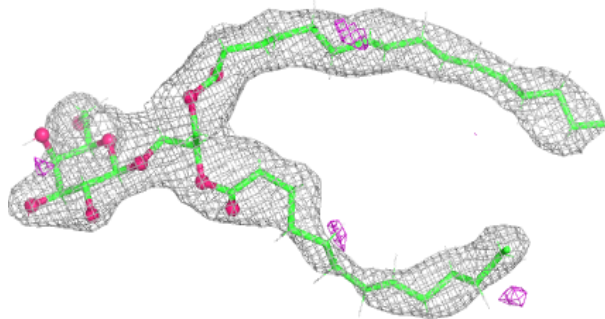


Electron density around LMG B 621:

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

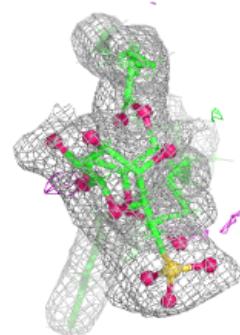
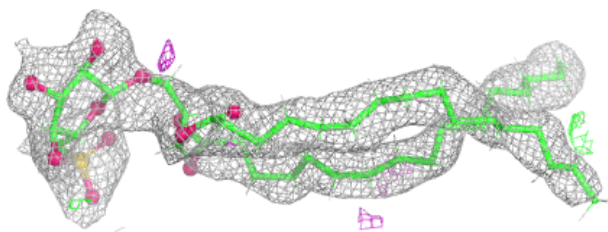
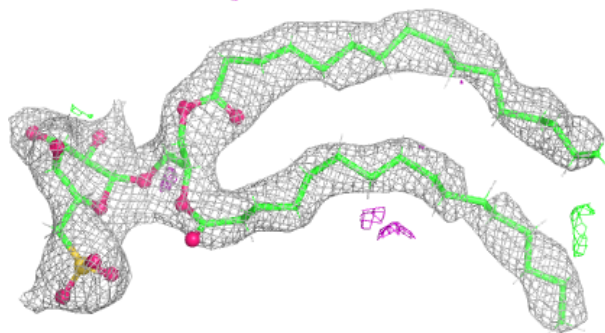
**Electron density around LMG C 501:**

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

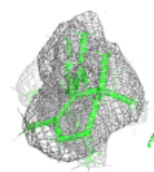
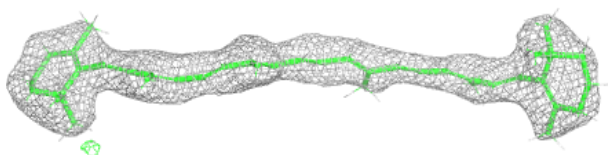
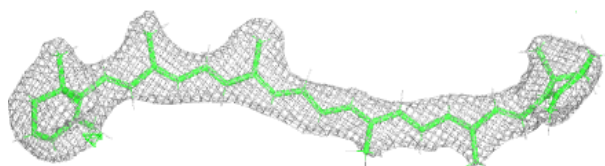


Electron density around SQD B 622:

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

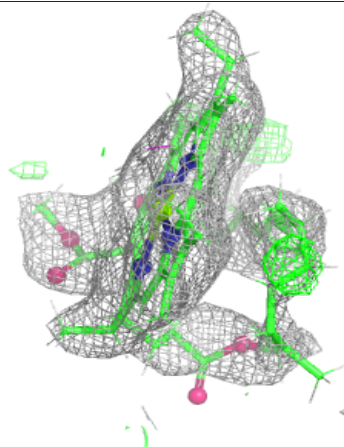
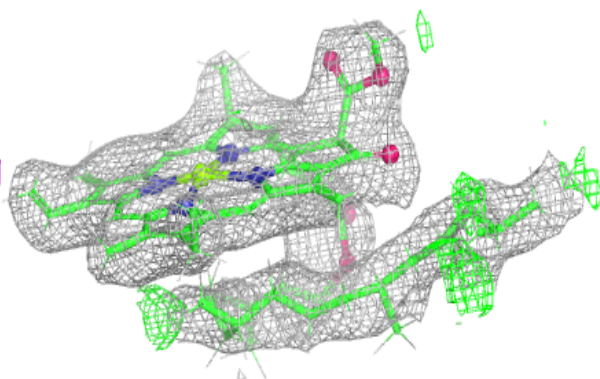
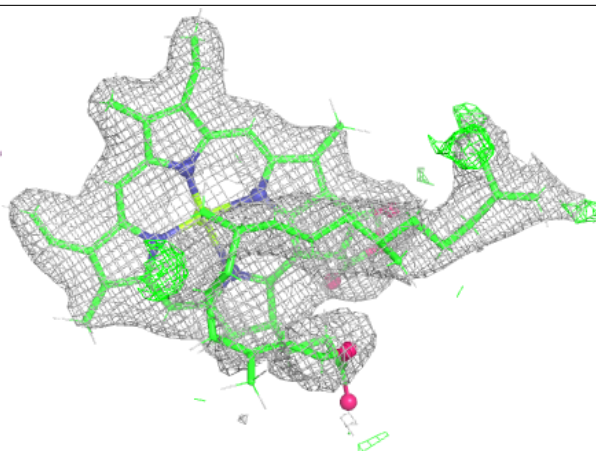
**Electron density around BCR k 101:**

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

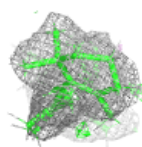
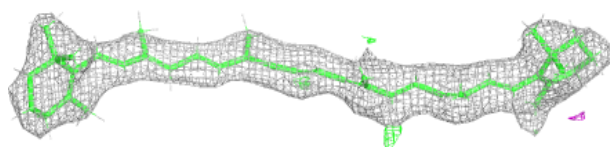


Electron density around CLA B 601:

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

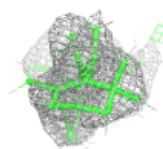
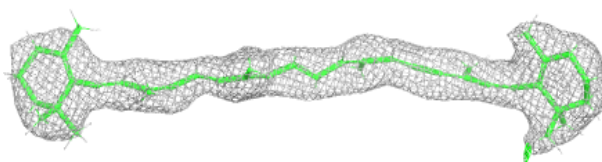
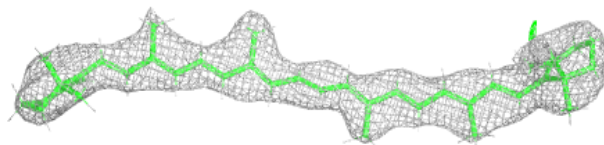
**Electron density around BCR K 101:**

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

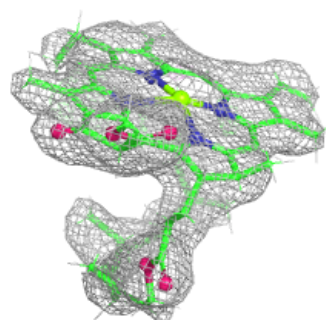
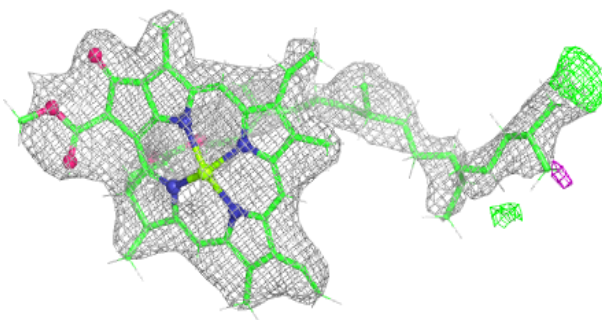
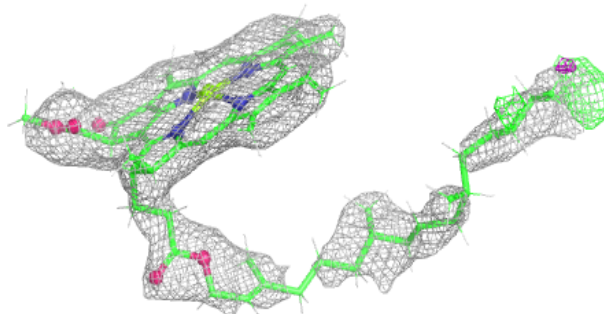


Electron density around BCR c 514:

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

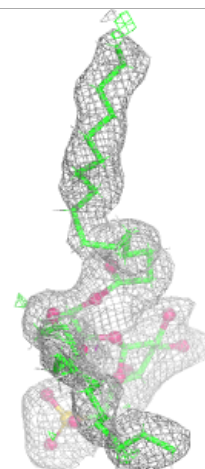
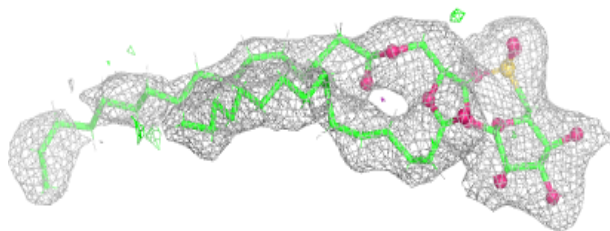
**Electron density around CLA C 514:**

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



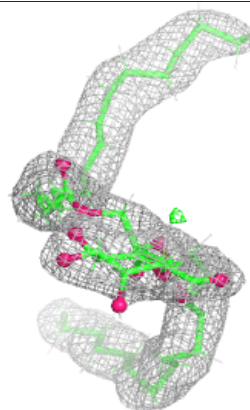
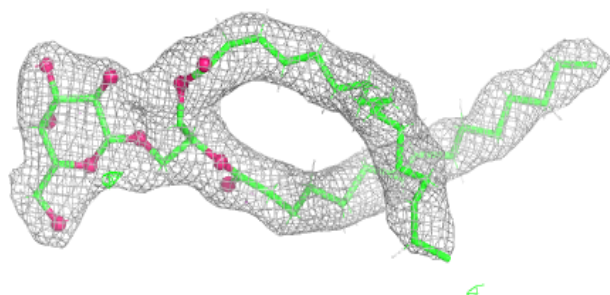
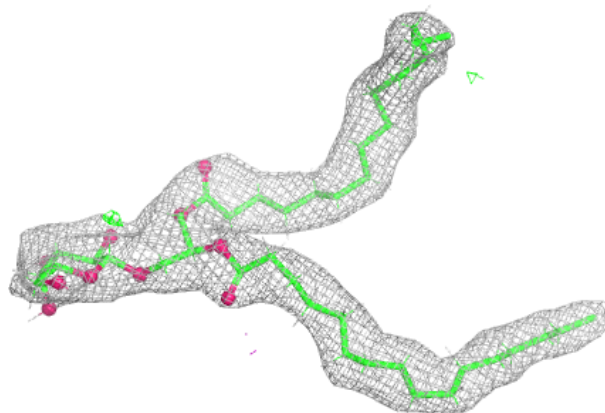
Electron density around SQD a 410:

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

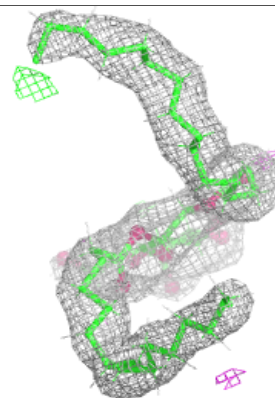
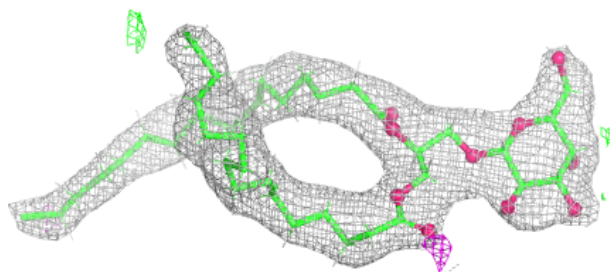
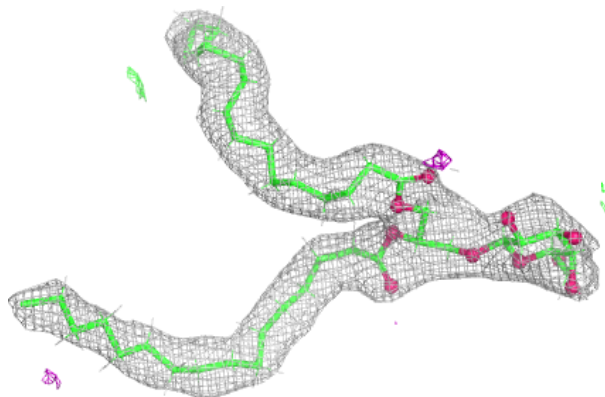


Electron density around LMG M 101:

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

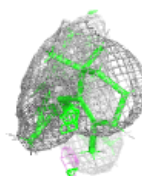
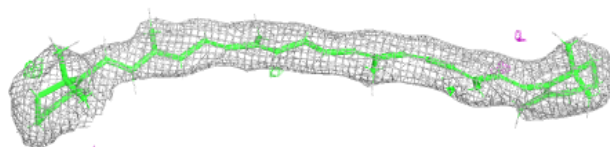
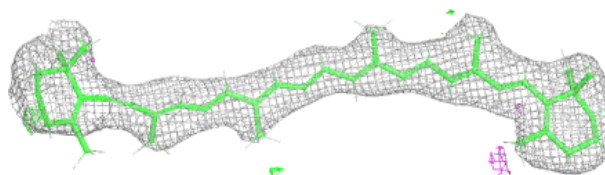
**Electron density around LMG b 621:**

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

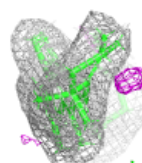
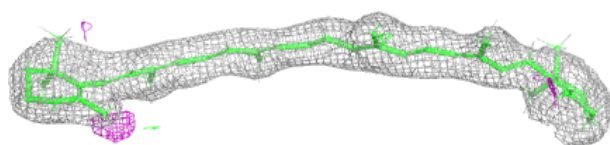
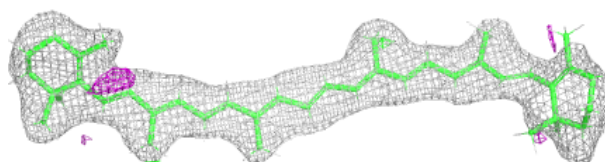


Electron density around BCR d 406:

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

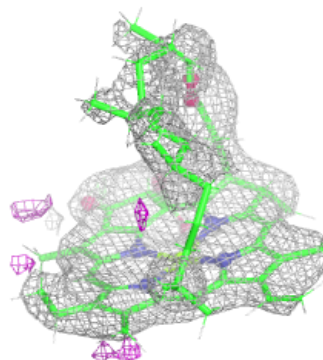
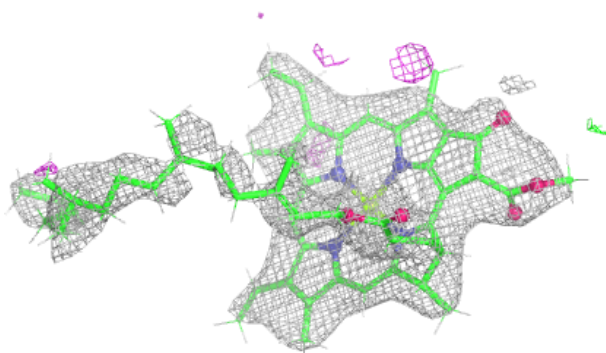
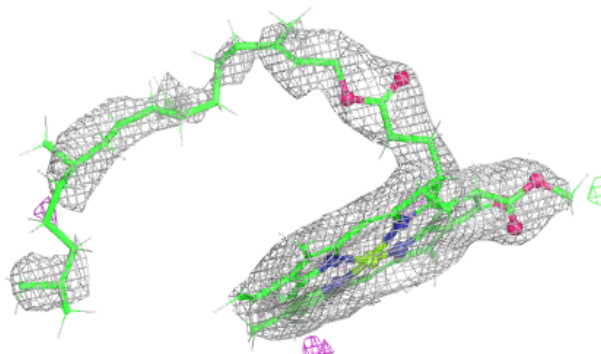
**Electron density around BCR D 405:**

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

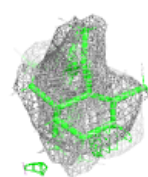
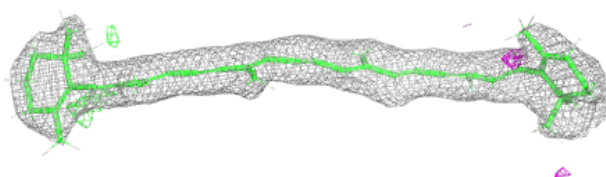
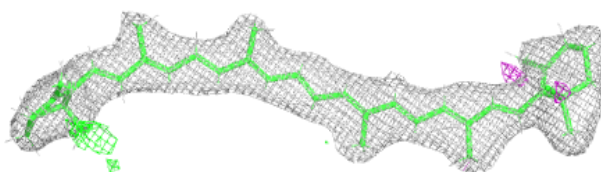


Electron density around CLA c 513:

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

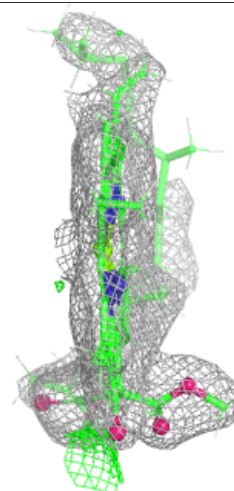
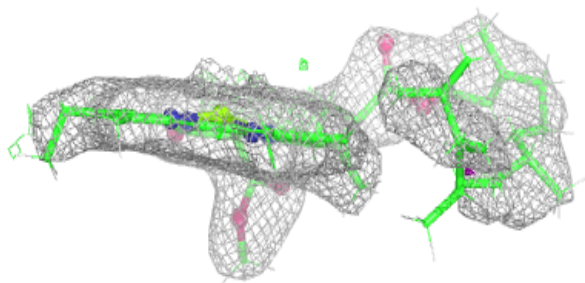
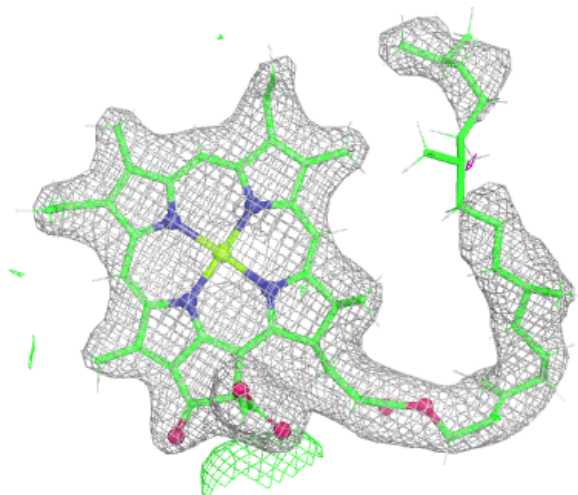
**Electron density around BCR Y 101:**

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



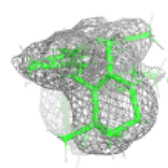
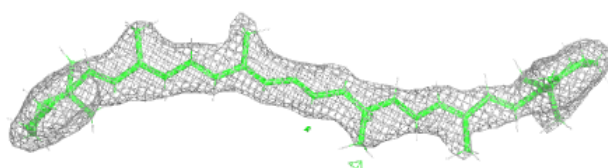
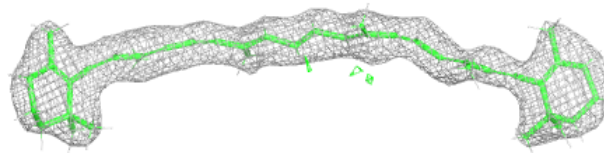
Electron density around CLA c 512:

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

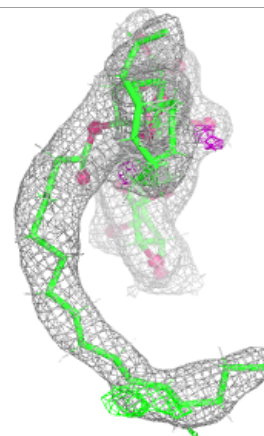
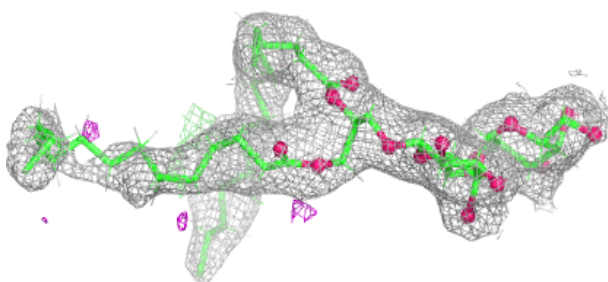
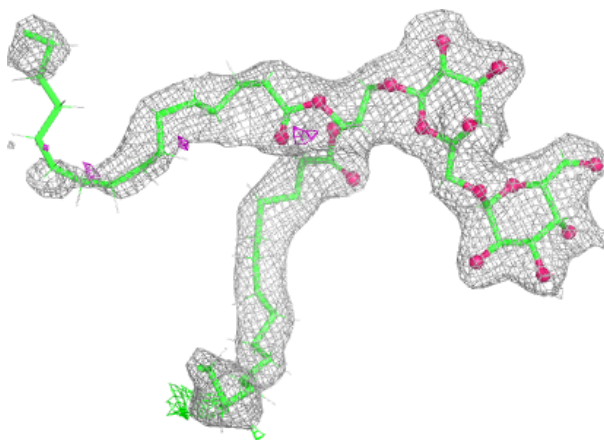


Electron density around BCR c 521:

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

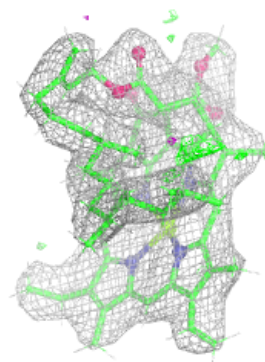
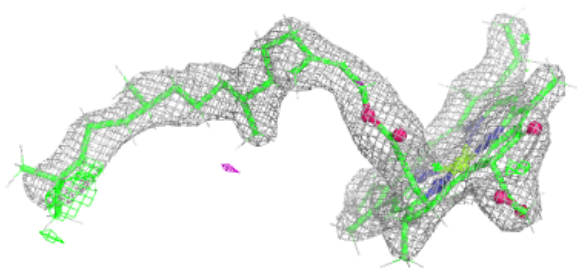
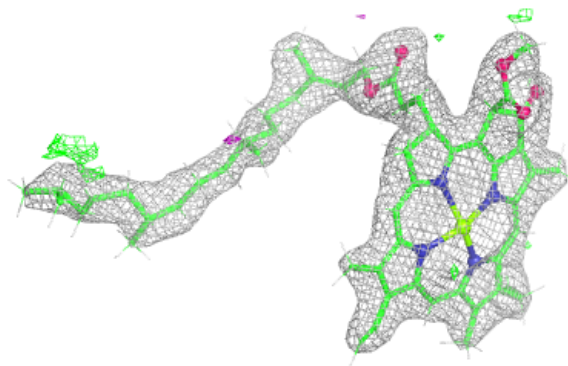
**Electron density around DGD C 517:**

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



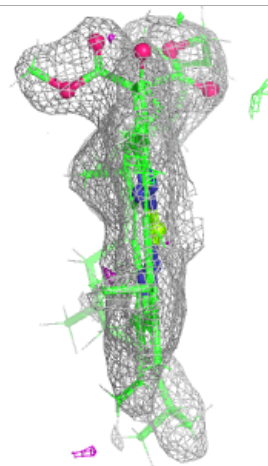
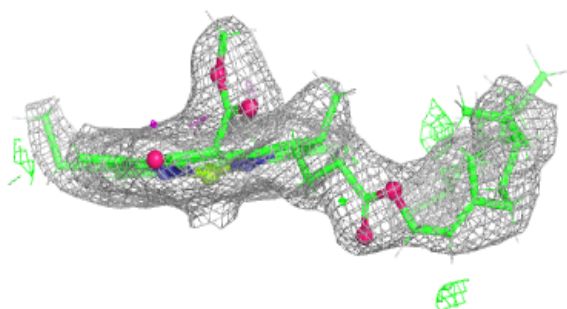
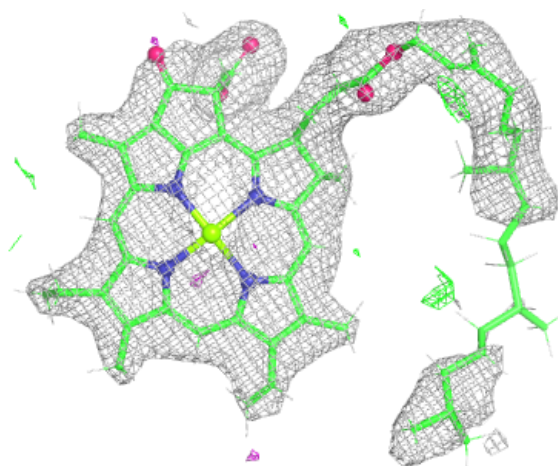
Electron density around CLA c 511:

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



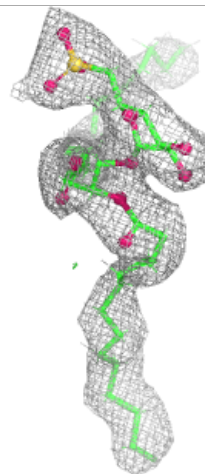
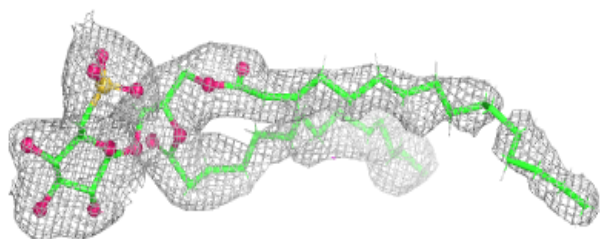
Electron density around CLA C 513:

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



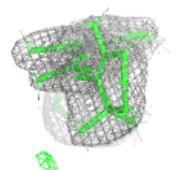
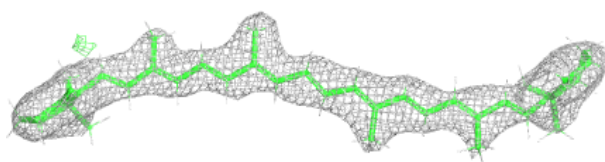
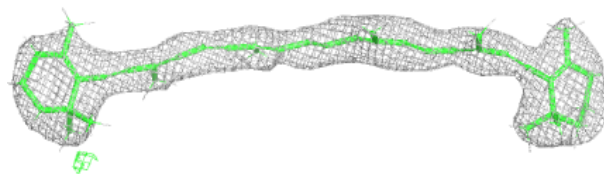
Electron density around SQD A 411:

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

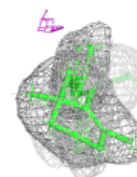
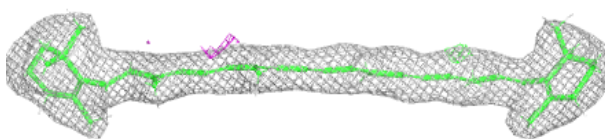
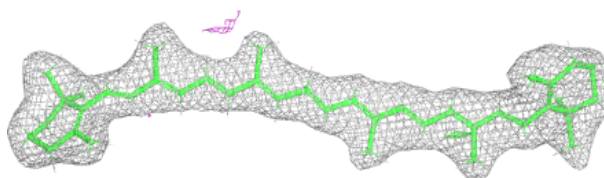


Electron density around BCR C 519:

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

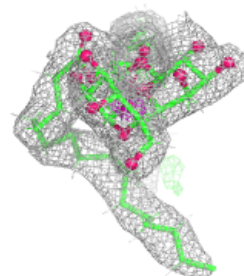
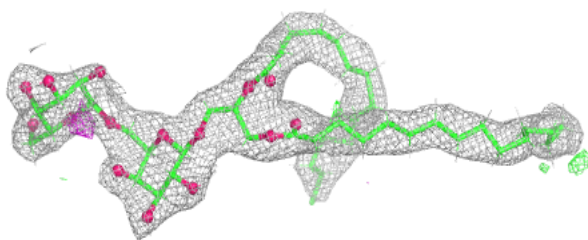
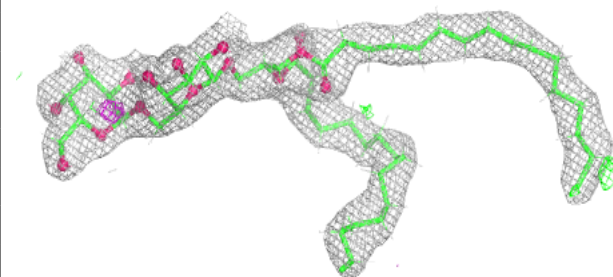
**Electron density around BCR b 619:**

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

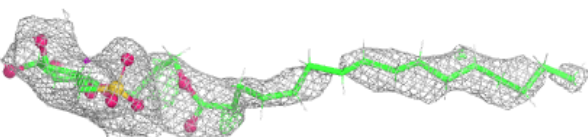
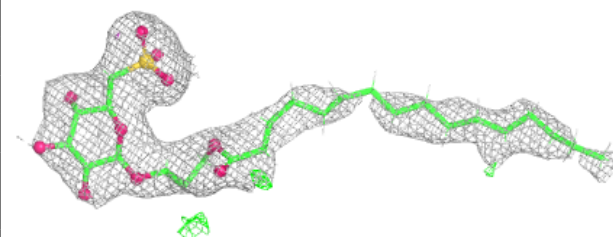


Electron density around DGD H 102:

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

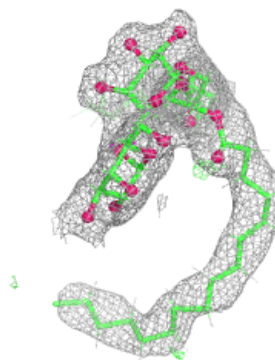
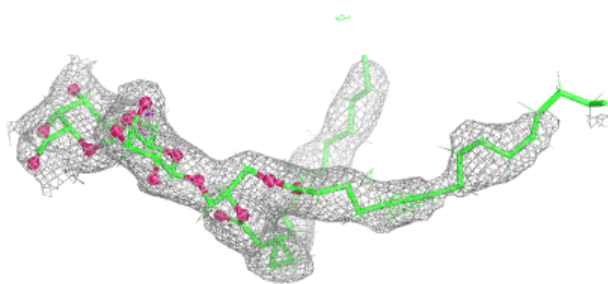
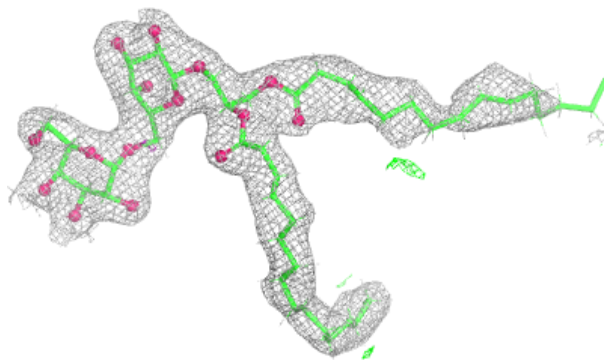
**Electron density around SQD F 101:**

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

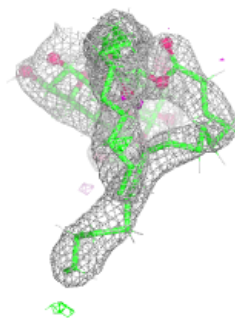
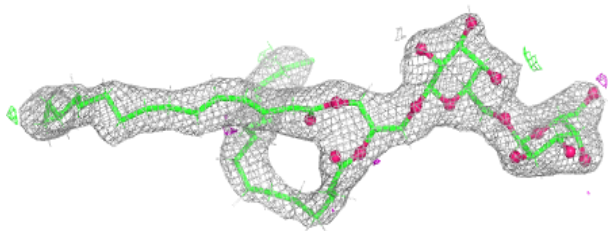
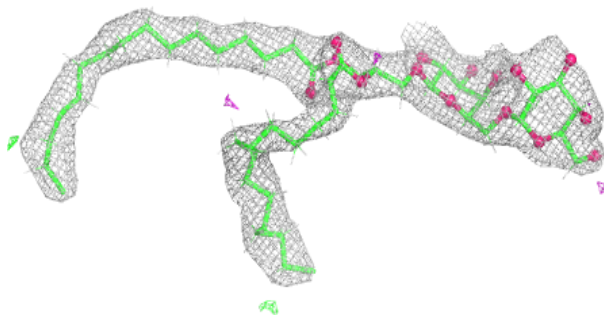


Electron density around DGD c 517:

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

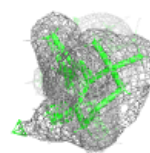
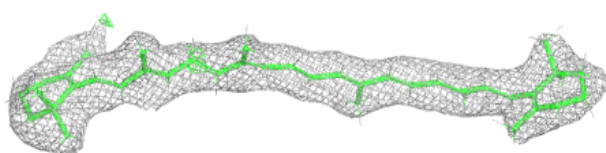
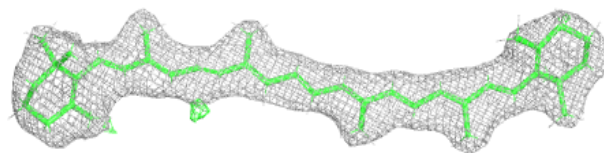
**Electron density around DGD h 104:**

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

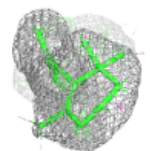
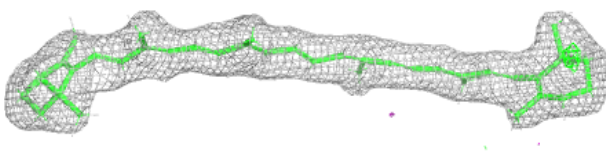
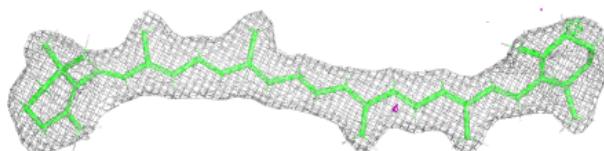


Electron density around BCR b 620:

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

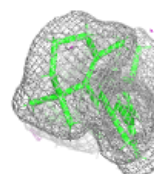
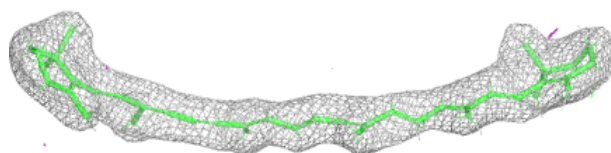
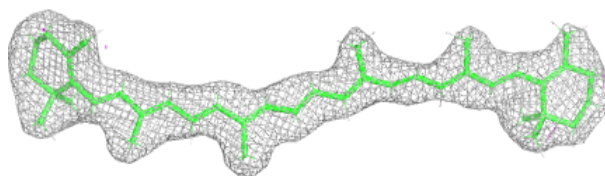
**Electron density around BCR B 619:**

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

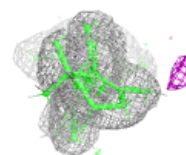
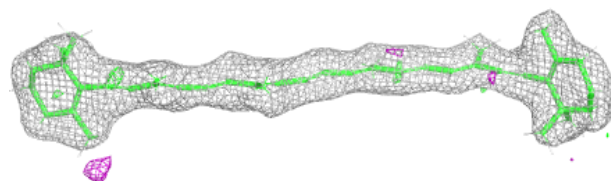
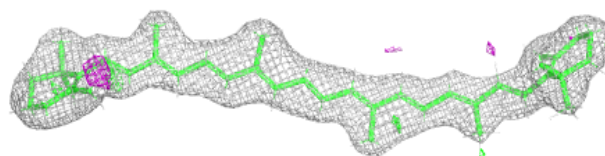


Electron density around BCR t 101:

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

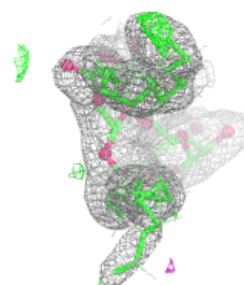
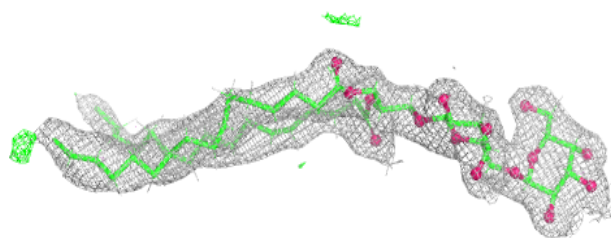
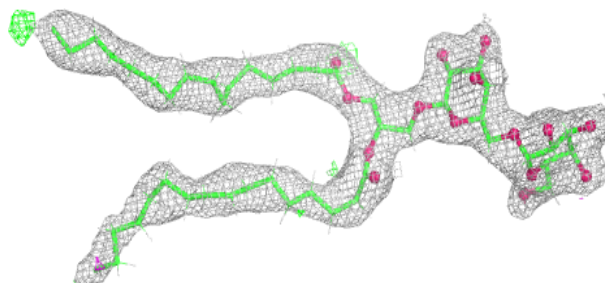
**Electron density around BCR C 515:**

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

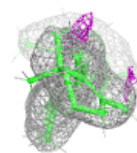
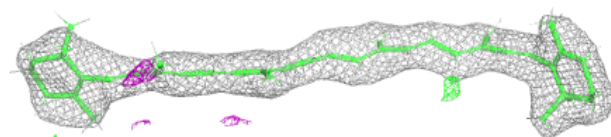
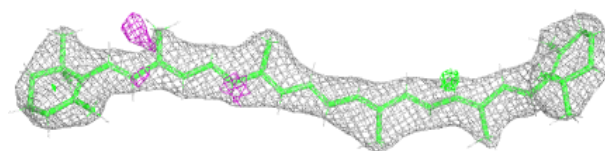


Electron density around DGD c 518:

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

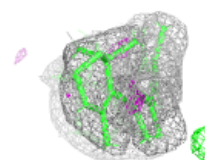
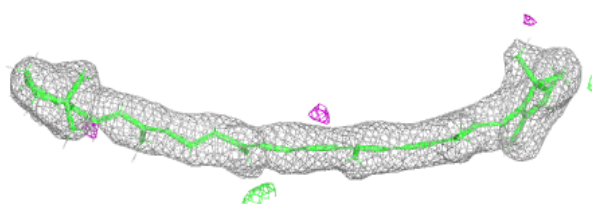
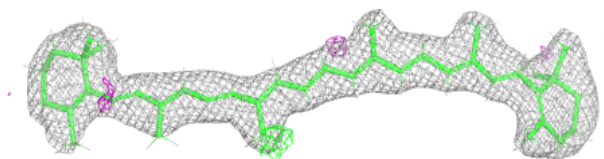
**Electron density around BCR c 515:**

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

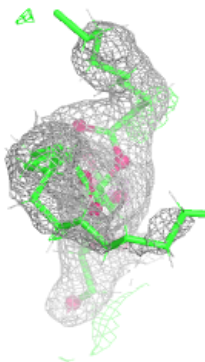
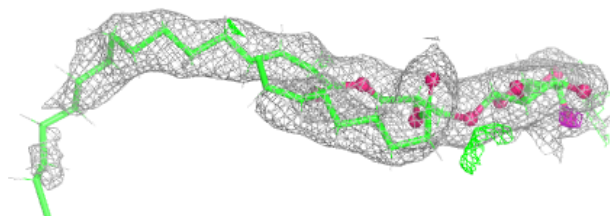
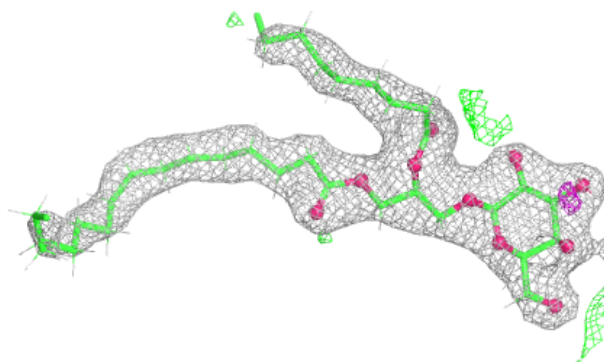


Electron density around BCR b 602:

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

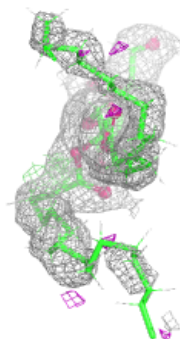
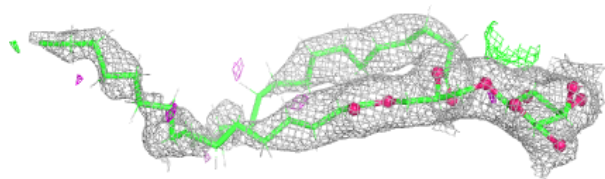
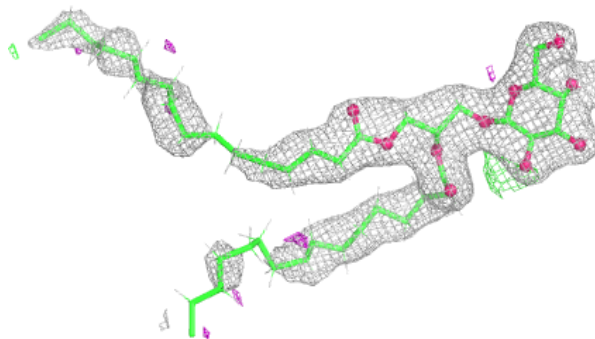
**Electron density around LMG d 411:**

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

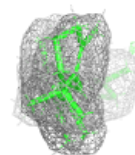
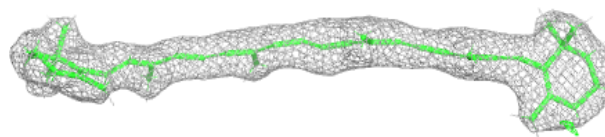
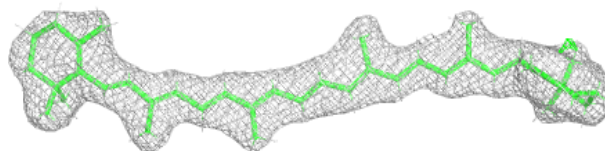


Electron density around LMG D 407:

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

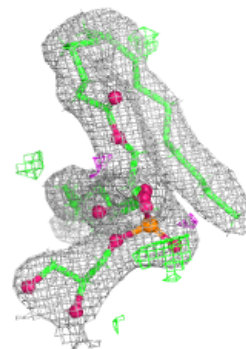
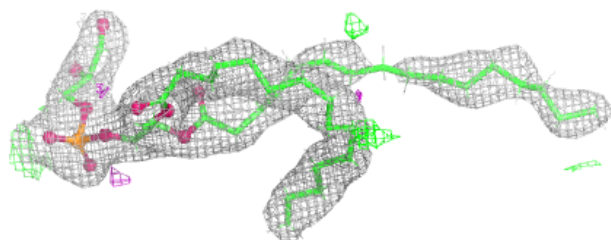
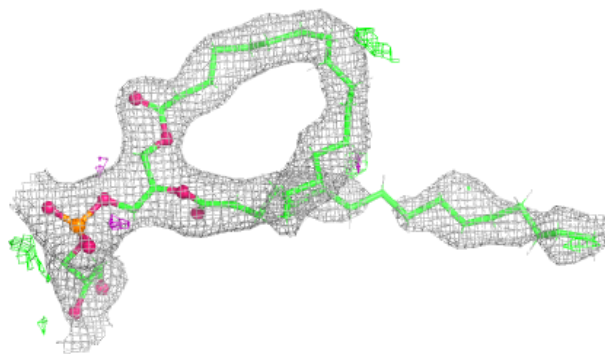
**Electron density around BCR b 618:**

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

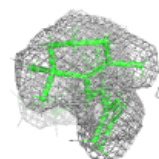
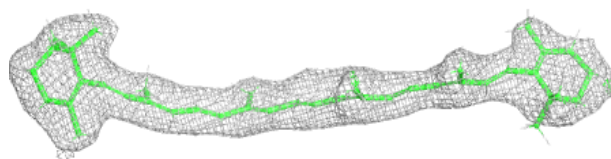
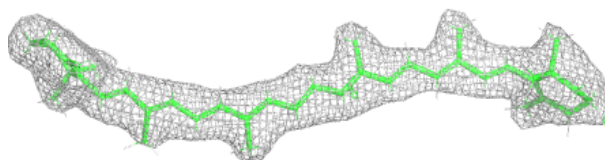


Electron density around LHG d 408:

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

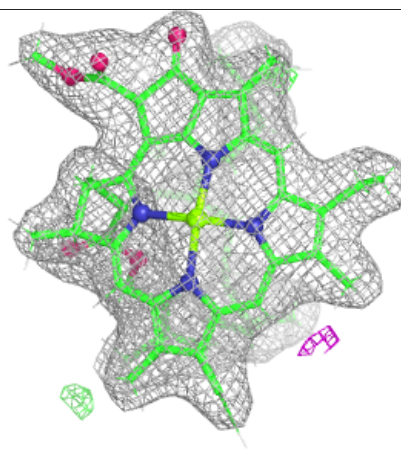
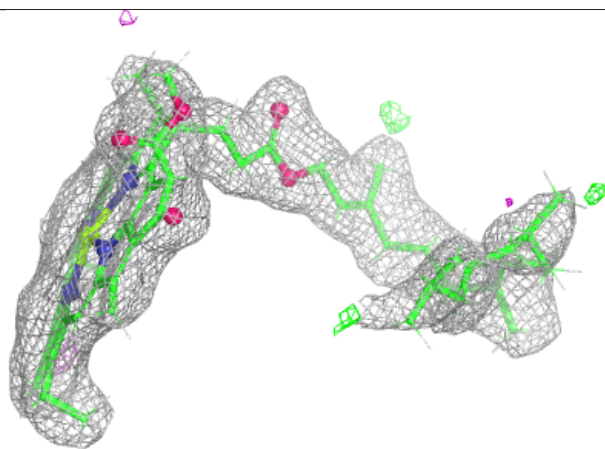
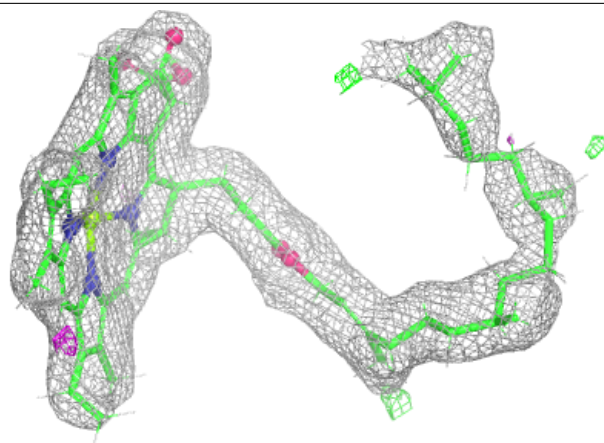
**Electron density around BCR H 101:**

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

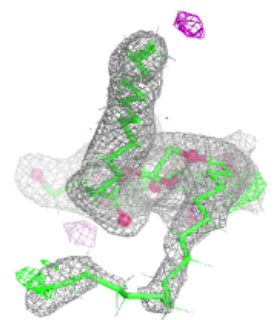
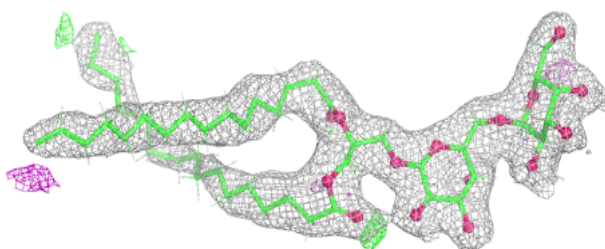
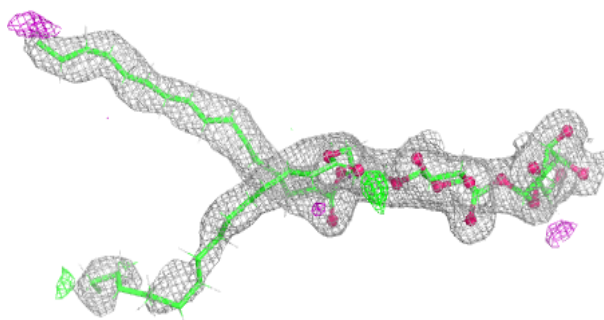


Electron density around CLA B 606:

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

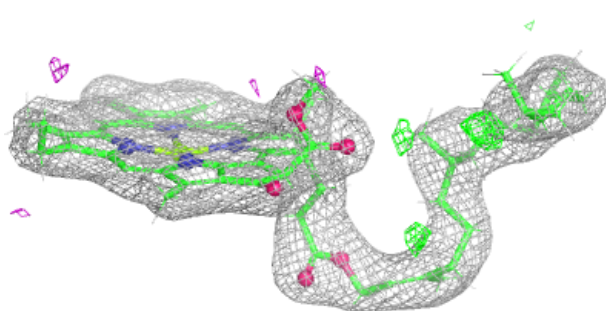
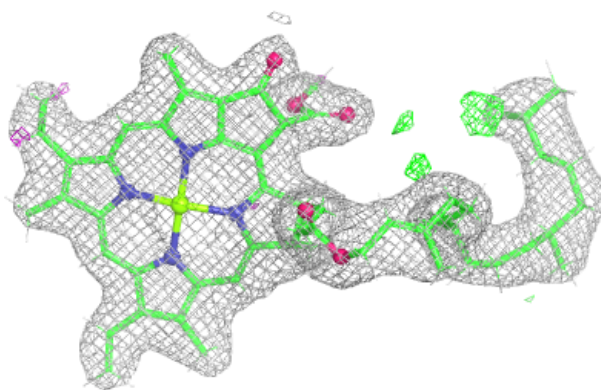
**Electron density around DGD C 516:**

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

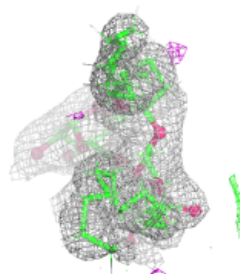
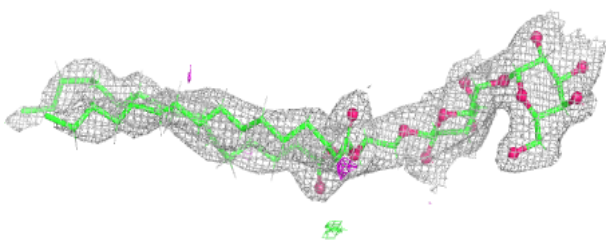
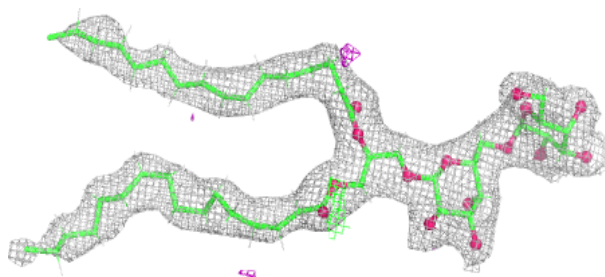


Electron density around CLA b 613:

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

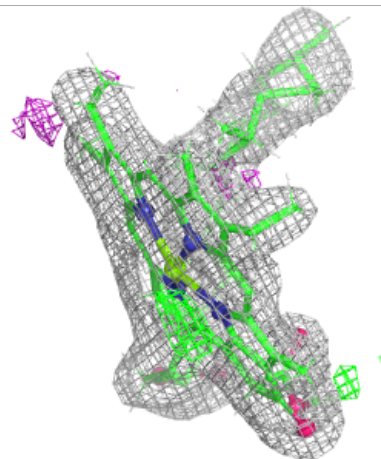
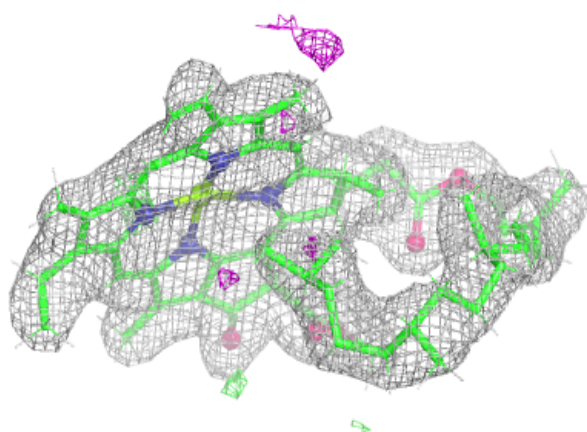
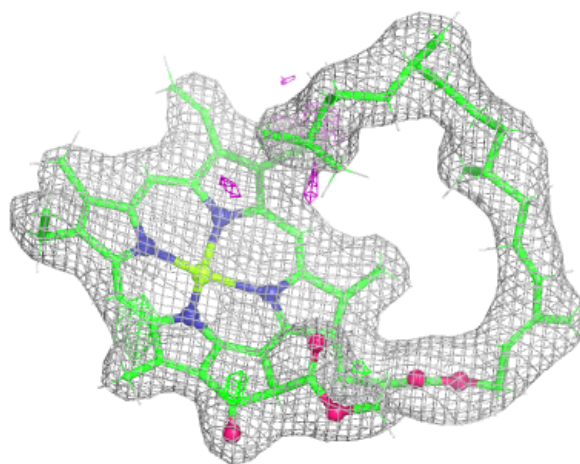
**Electron density around DGD C 518:**

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



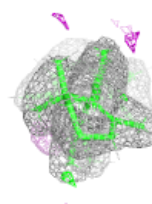
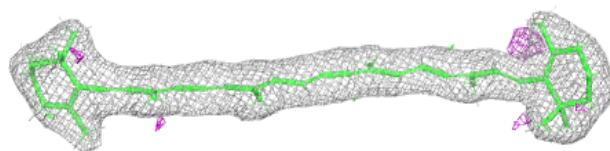
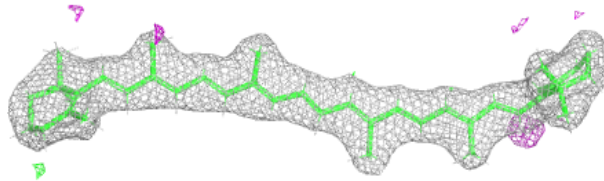
Electron density around CLA b 616:

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



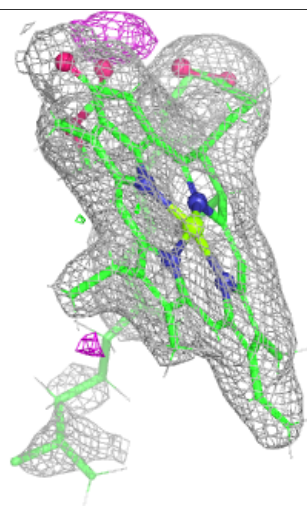
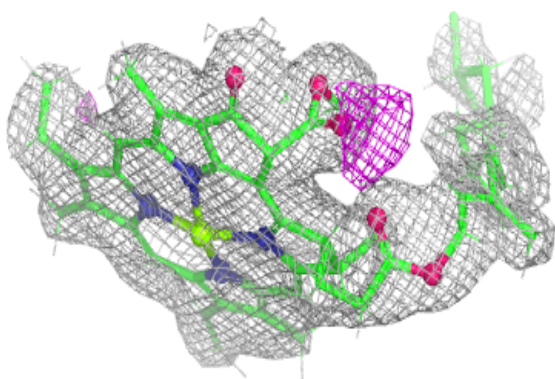
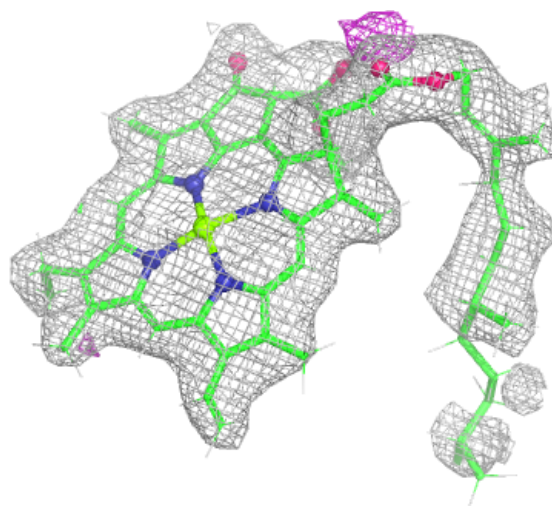
Electron density around BCR a 408:

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



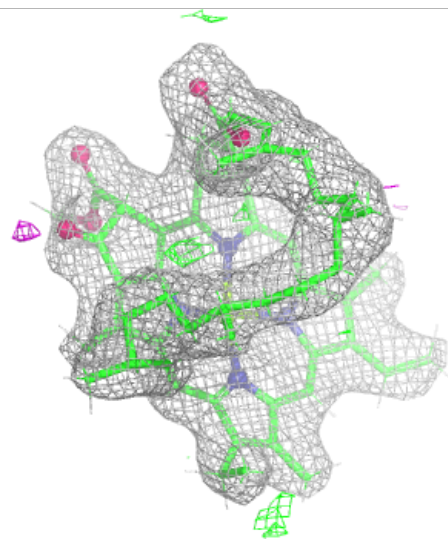
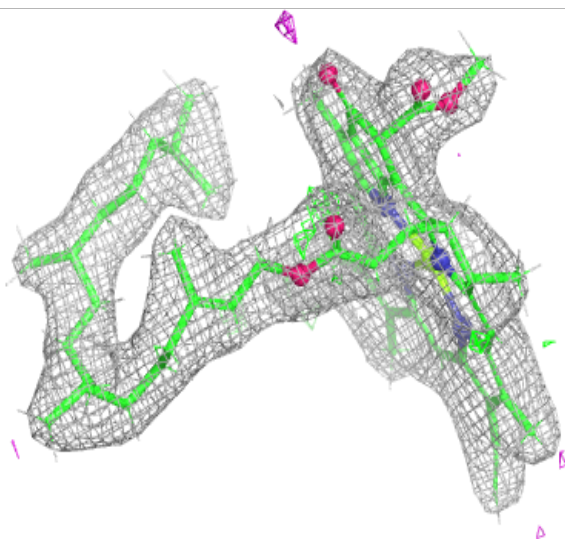
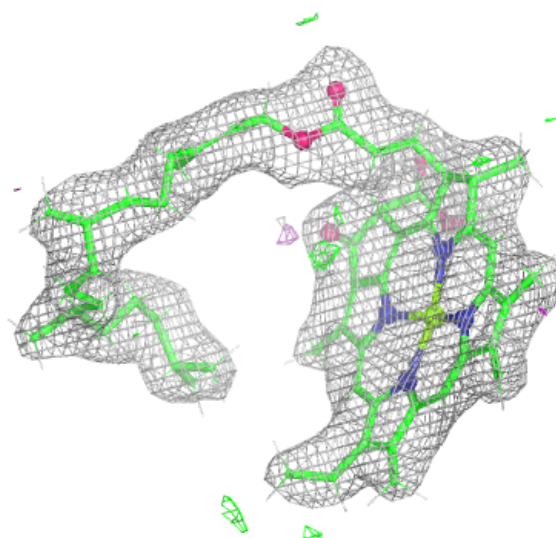
Electron density around CLA b 617:

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



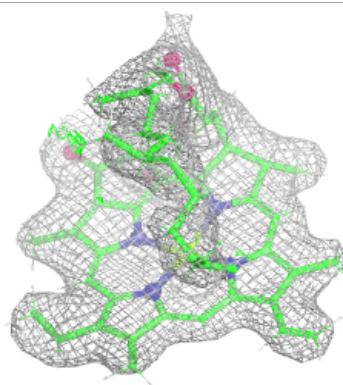
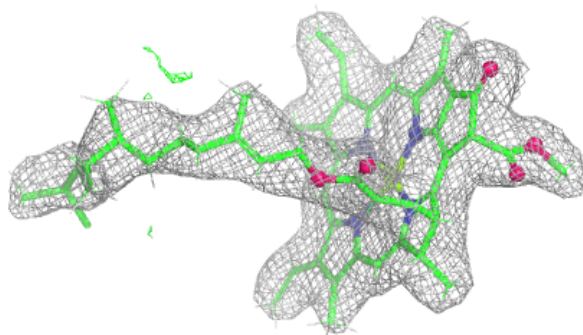
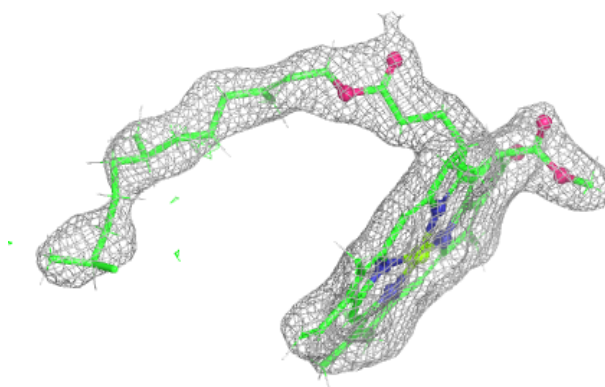
Electron density around CLA c 503:

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

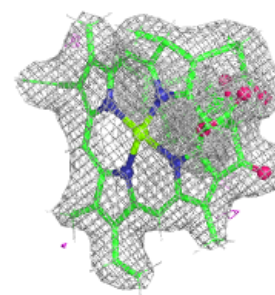
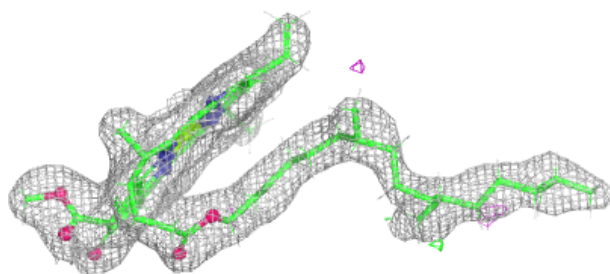
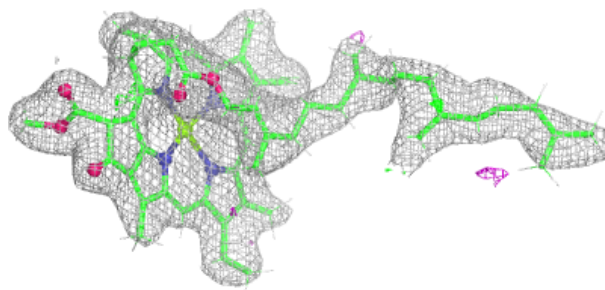


Electron density around CLA c 504:

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

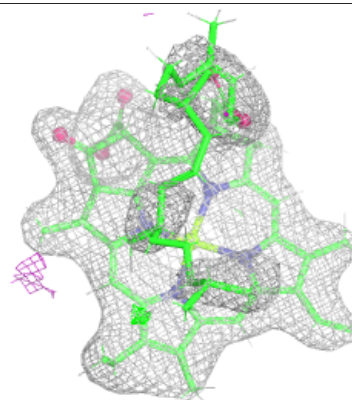
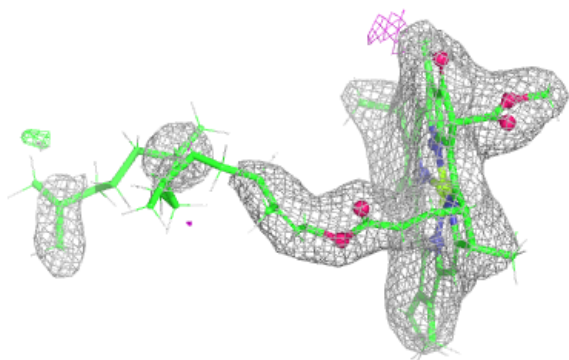
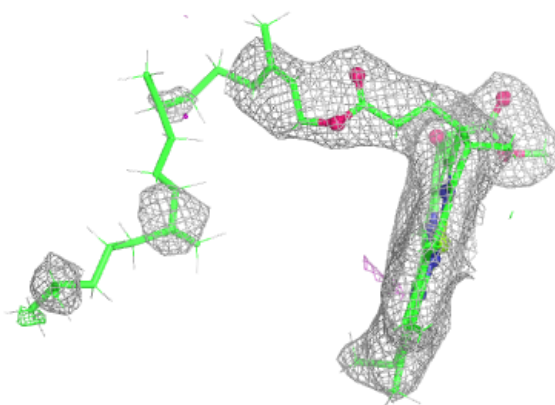
**Electron density around CLA c 505:**

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

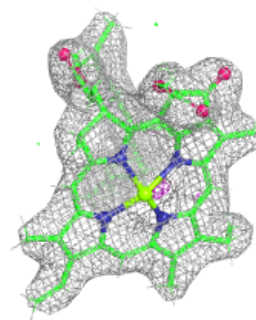
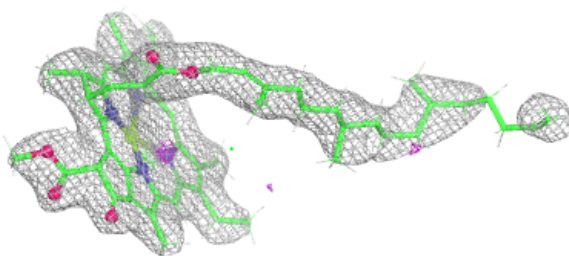
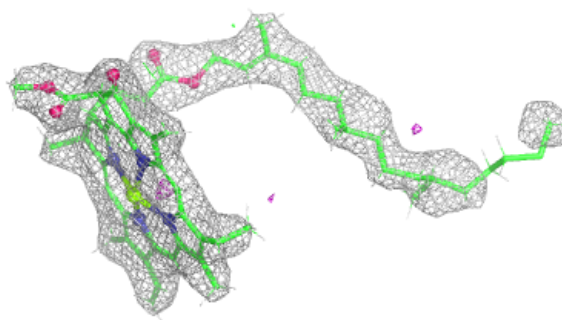


Electron density around CLA c 506:

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

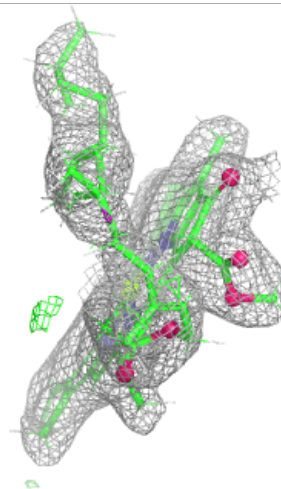
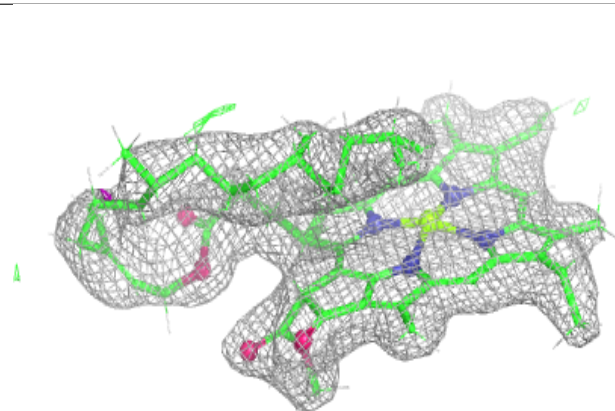
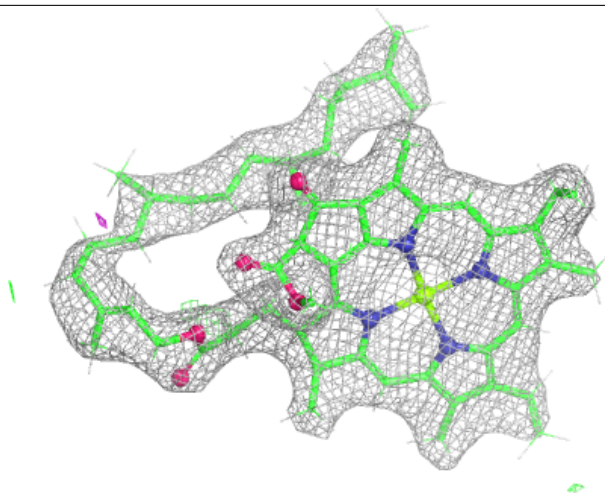
**Electron density around CLA c 508:**

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



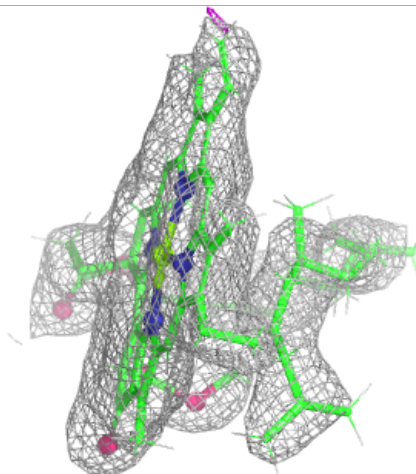
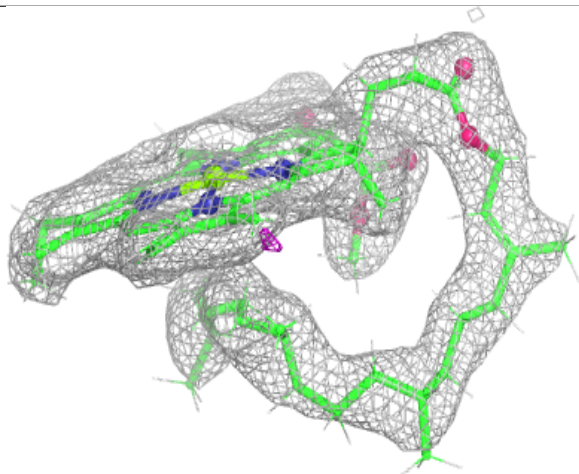
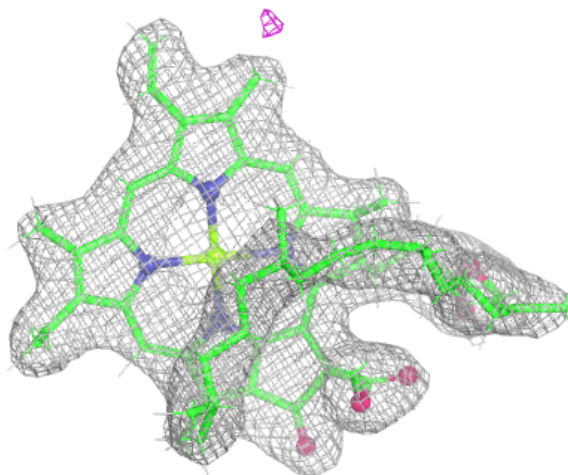
Electron density around CLA c 509:

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



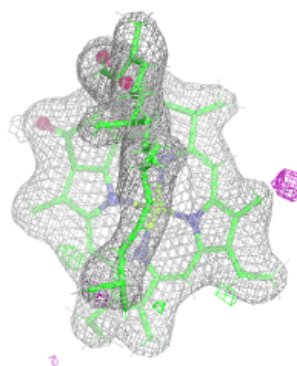
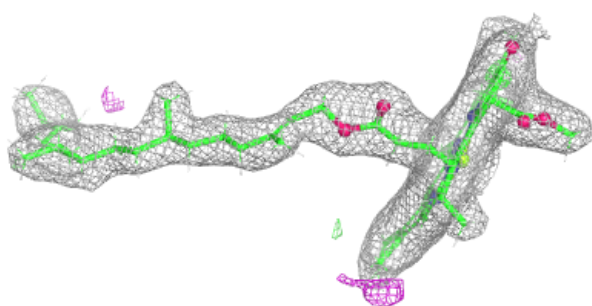
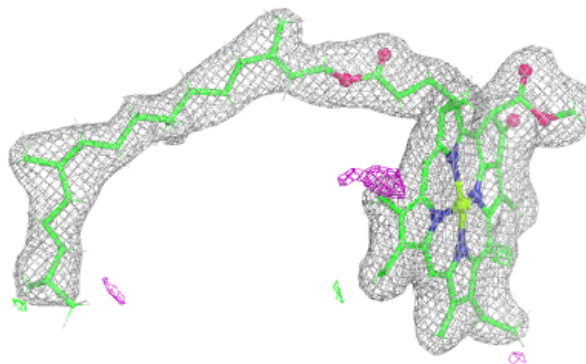
Electron density around CLA c 510:

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

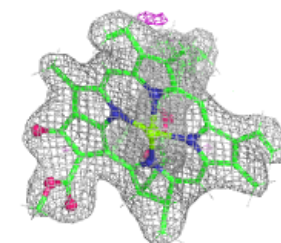
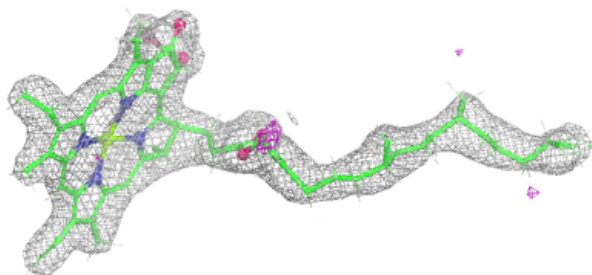
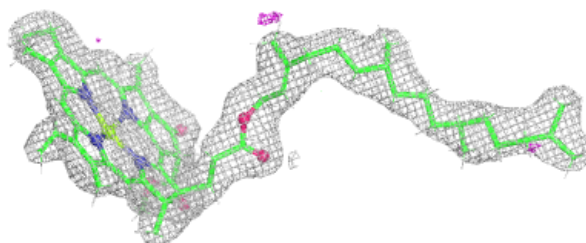


Electron density around CLA B 609:

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

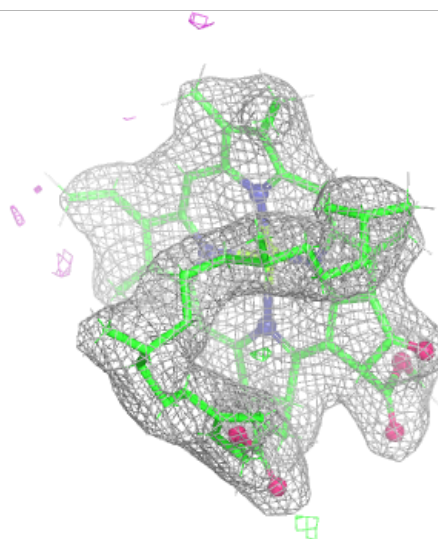
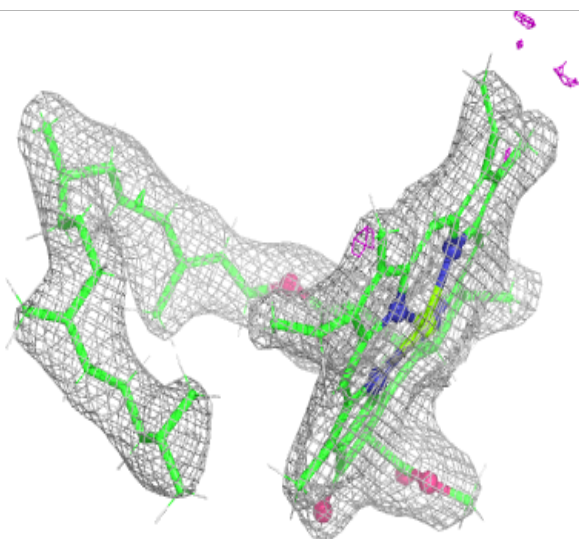
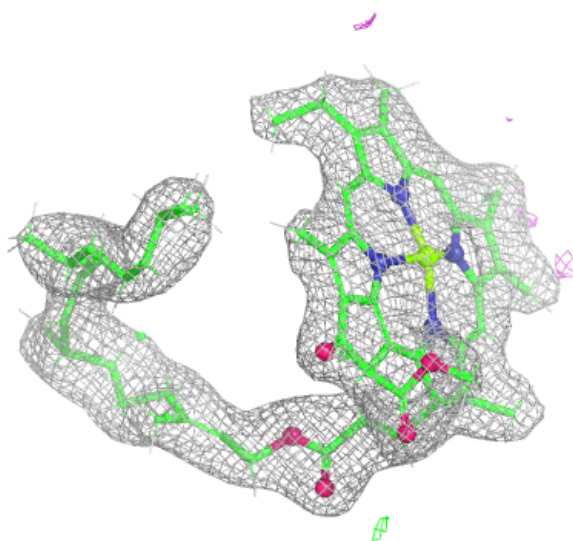
**Electron density around CLA C 503:**

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



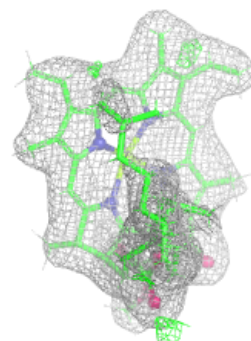
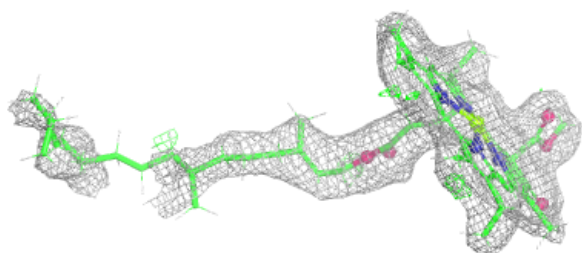
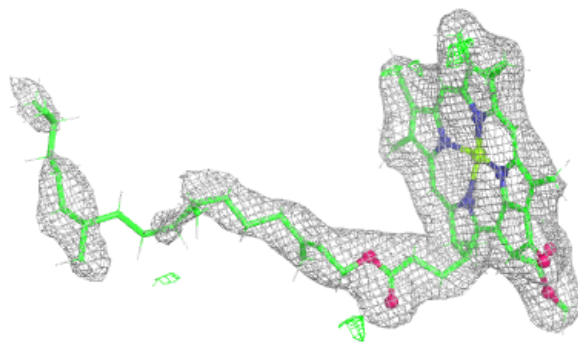
Electron density around CLA C 504:

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

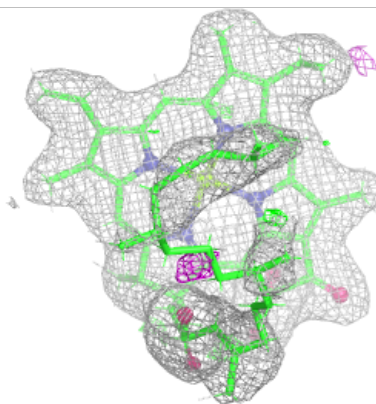
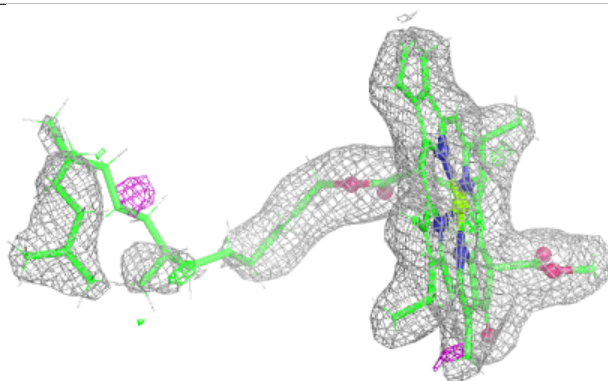
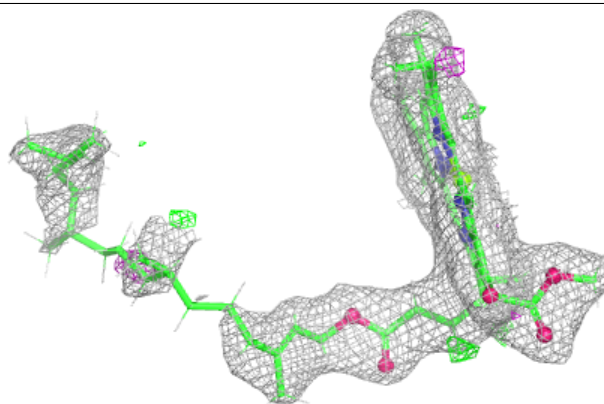


Electron density around CLA d 405:

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

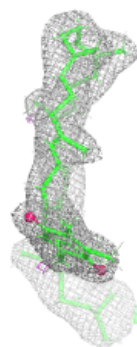
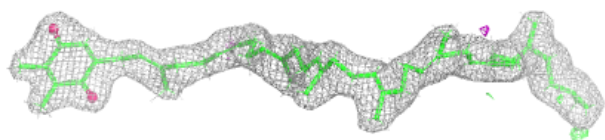
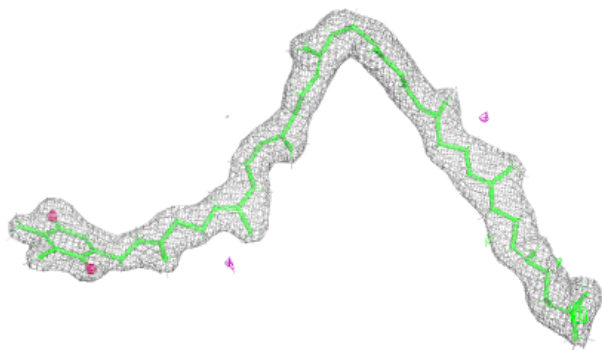
**Electron density around CLA C 507:**

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

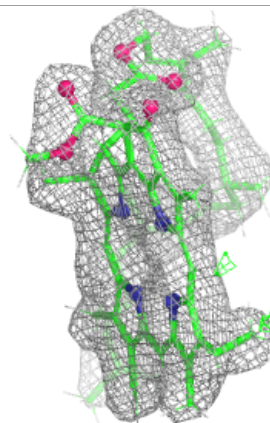
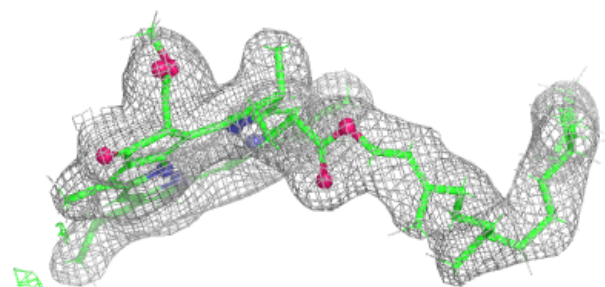
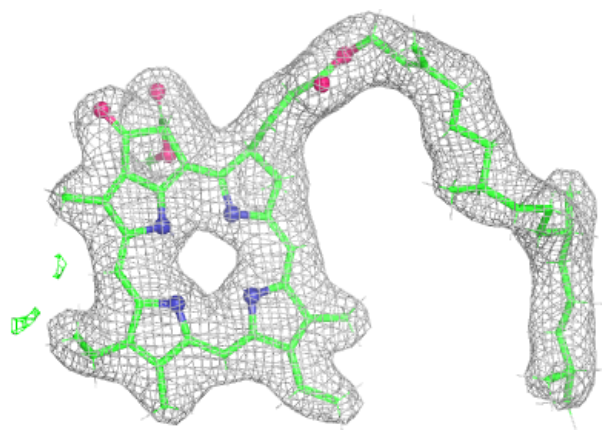


Electron density around PL9 d 407:

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

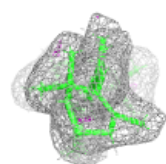
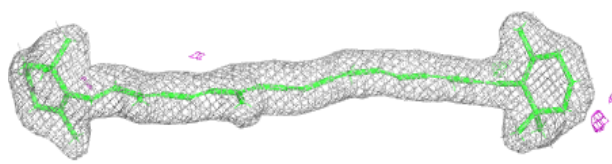
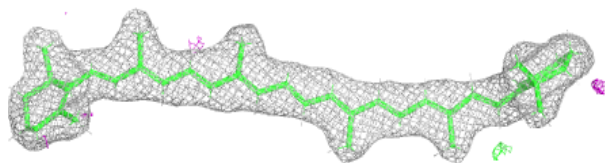
**Electron density around PHO d 402:**

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

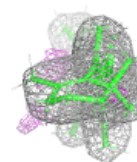
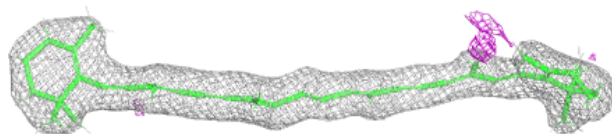
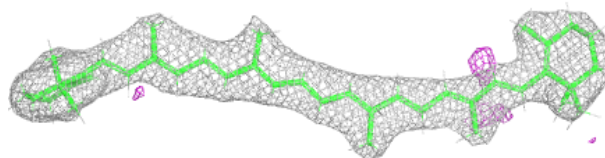


Electron density around BCR A 409:

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

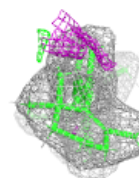
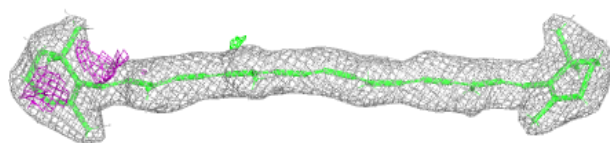
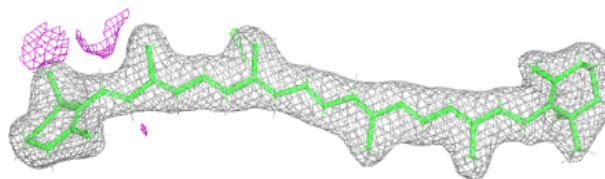
**Electron density around BCR B 617:**

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

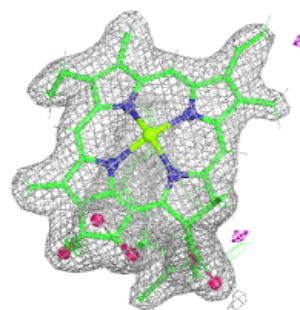
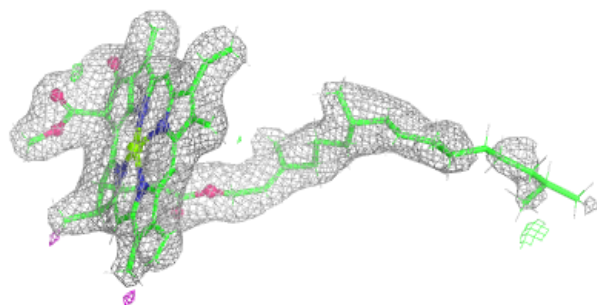
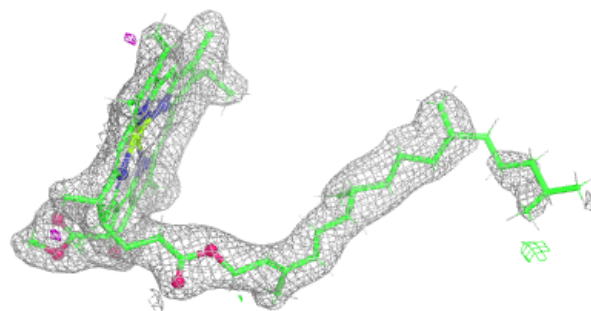


Electron density around BCR B 618:

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

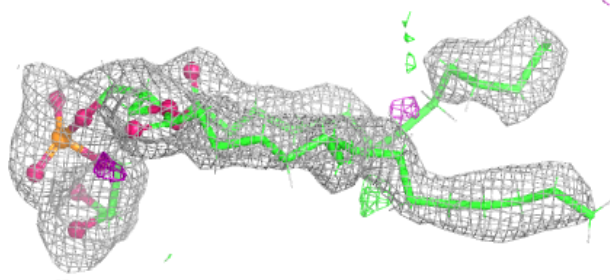
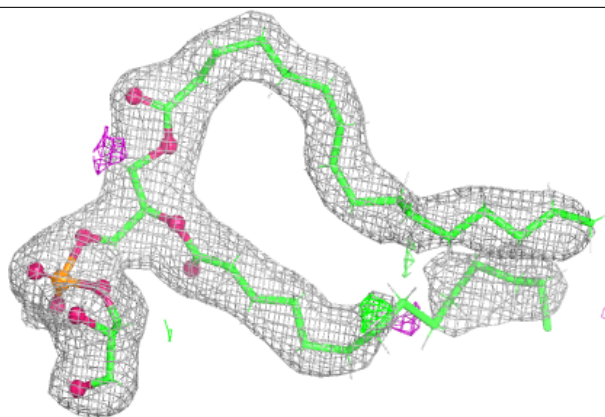
**Electron density around CLA C 509:**

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

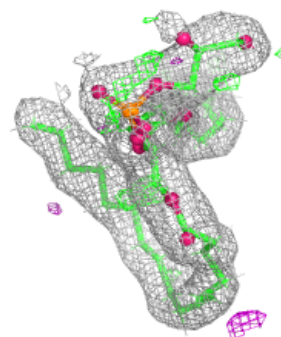
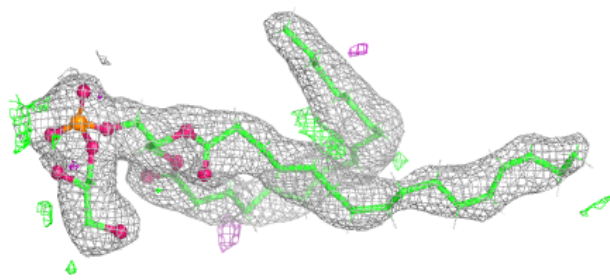
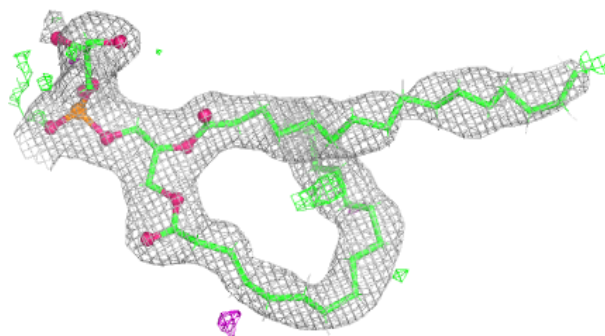


Electron density around LHG D 409:

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

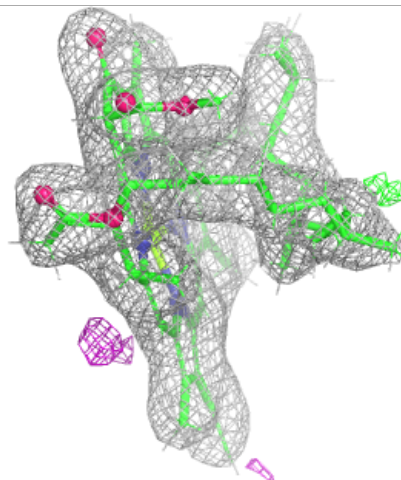
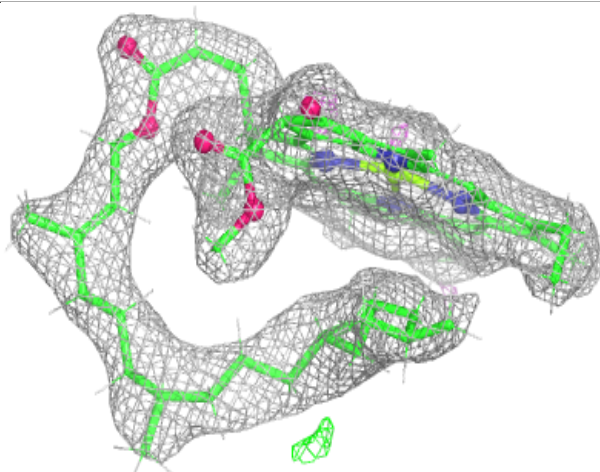
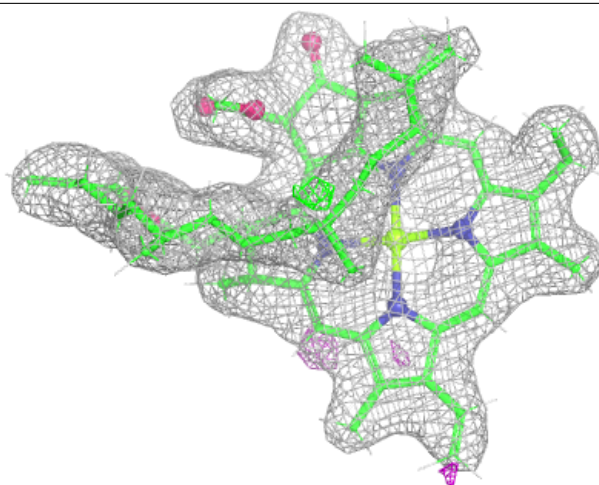
**Electron density around LHG D 411:**

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



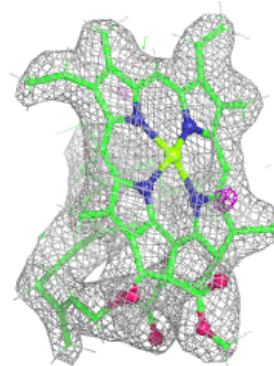
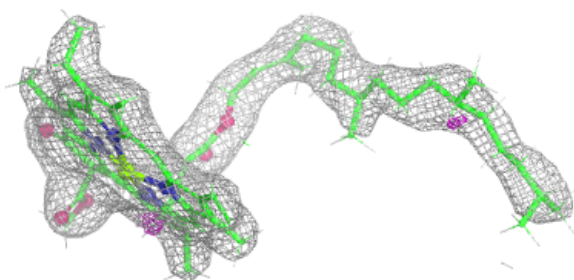
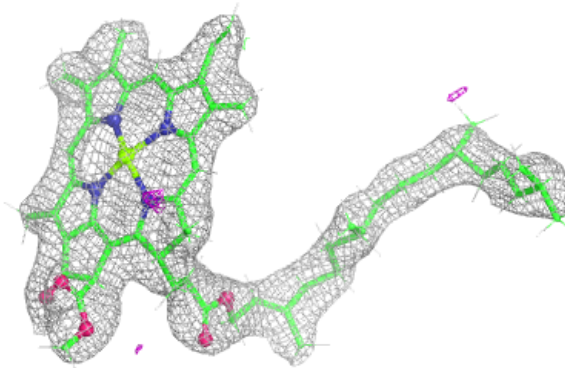
Electron density around CLA C 511:

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

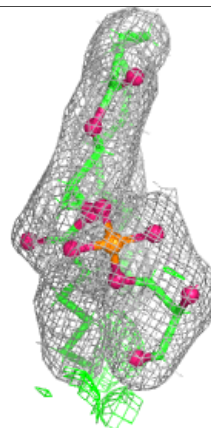
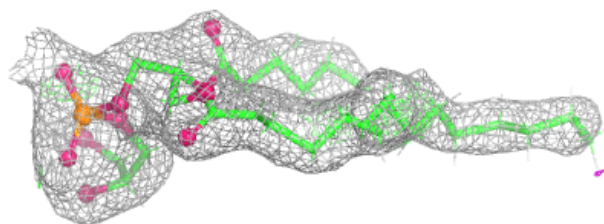
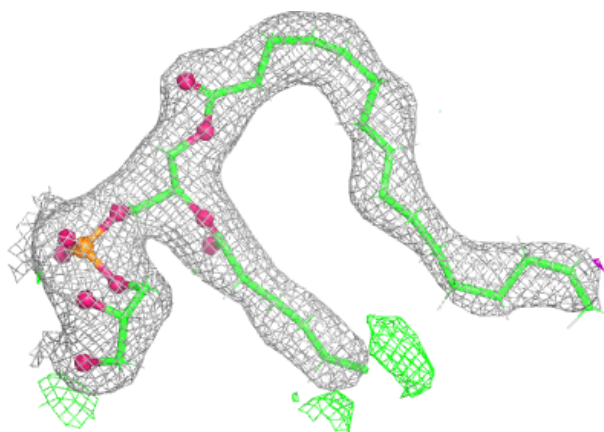


Electron density around CLA C 512:

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

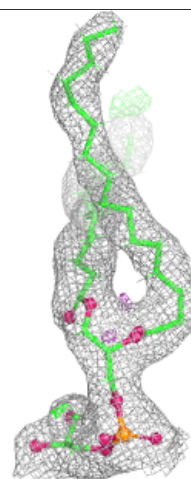
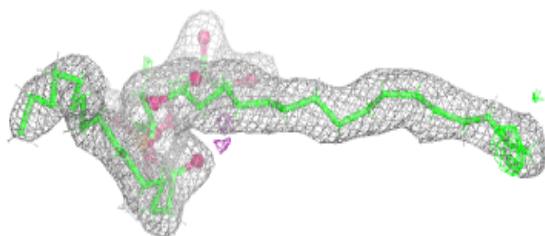
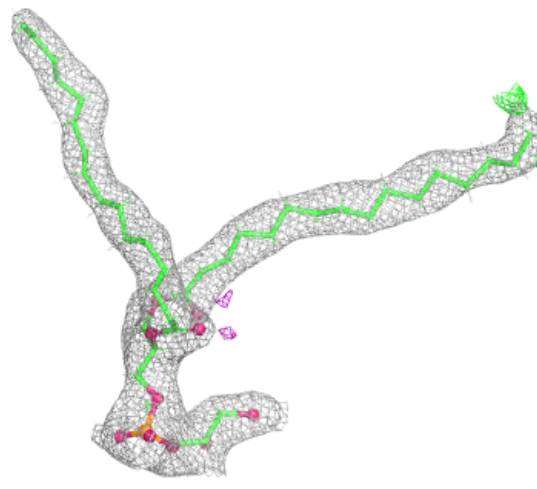
**Electron density around LHG d 410:**

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



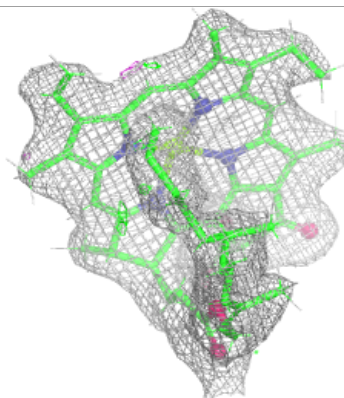
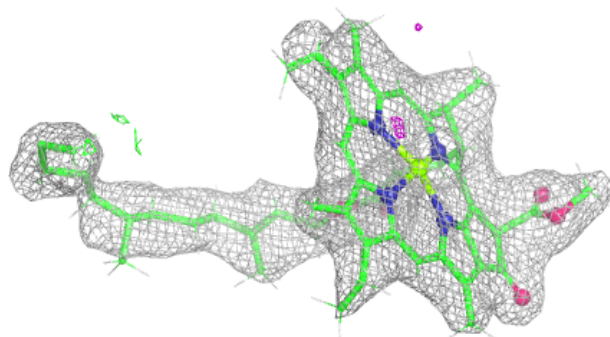
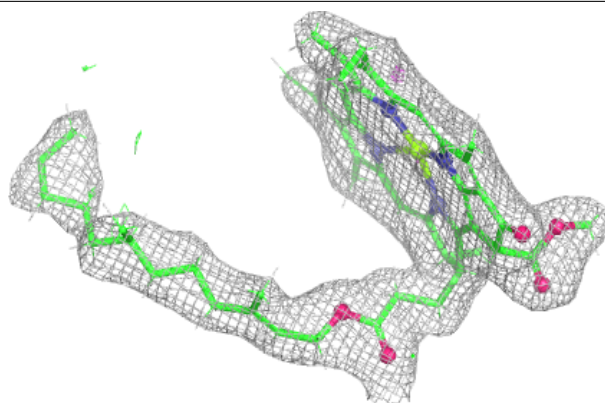
Electron density around LHG 1 101:

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

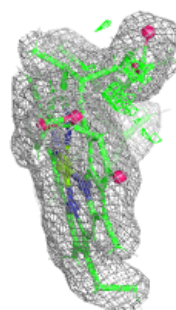
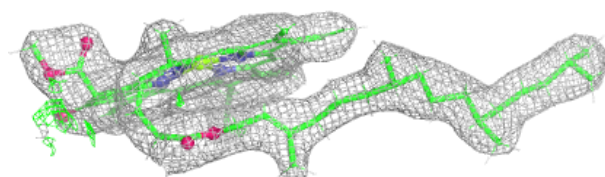
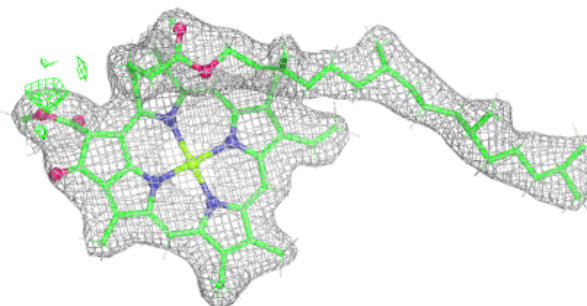


Electron density around CLA C 505:

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

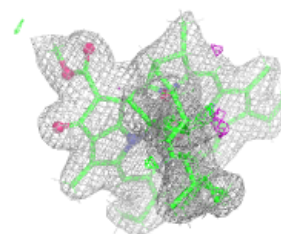
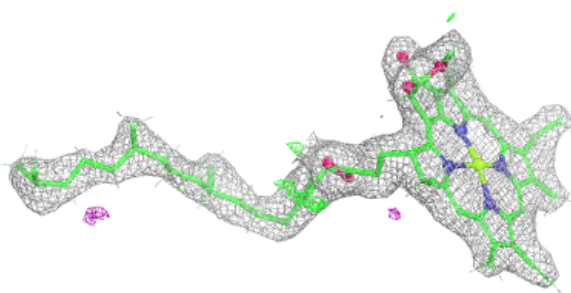
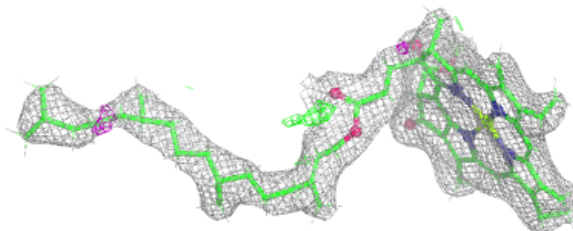
**Electron density around CLA c 501:**

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

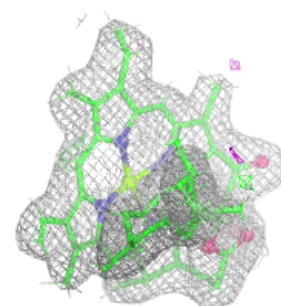
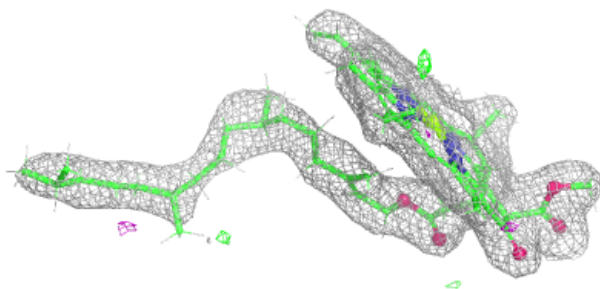
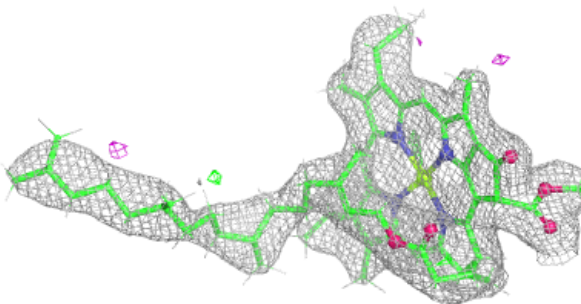


Electron density around CLA c 502:

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

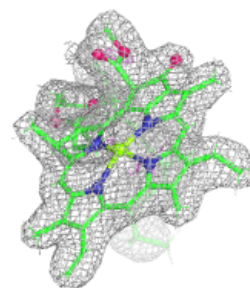
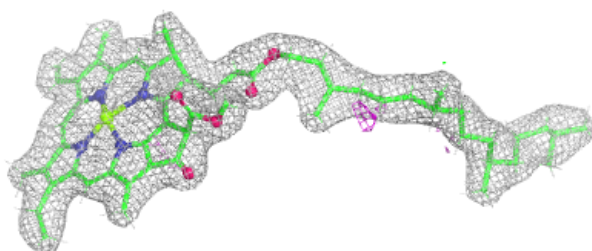
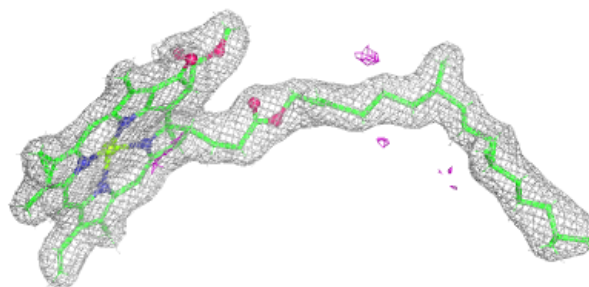
**Electron density around CLA C 506:**

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

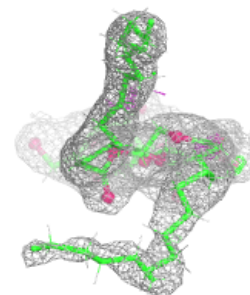
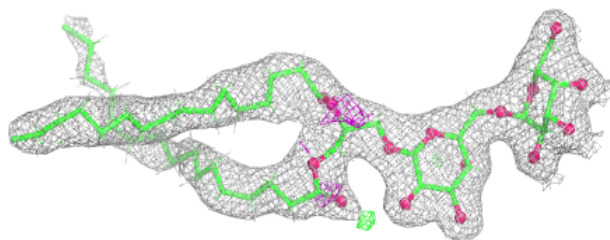
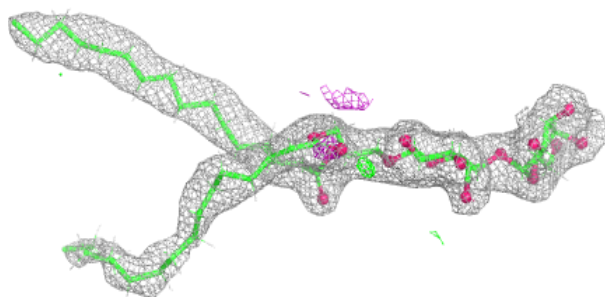


Electron density around CLA A 405:

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

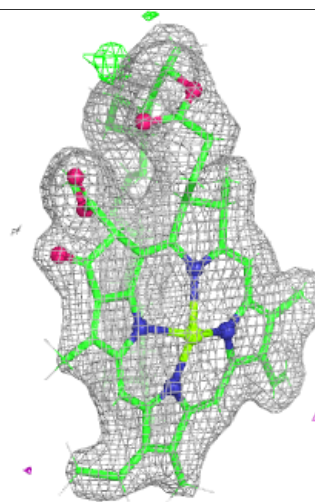
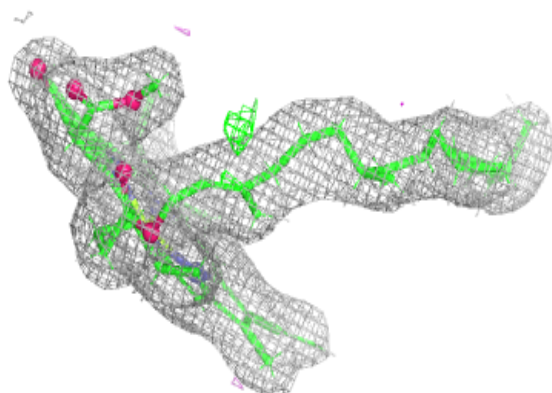
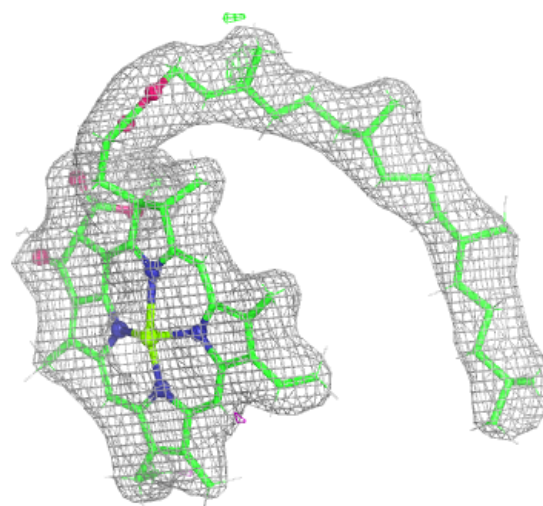
**Electron density around DGD c 516:**

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



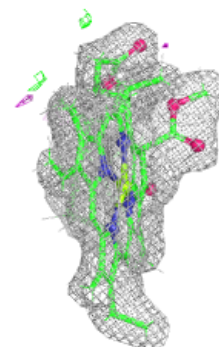
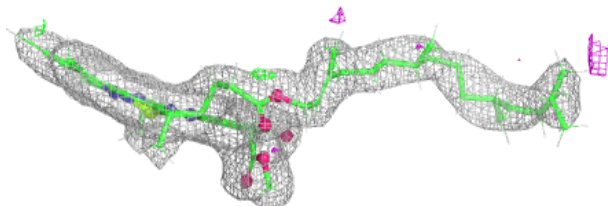
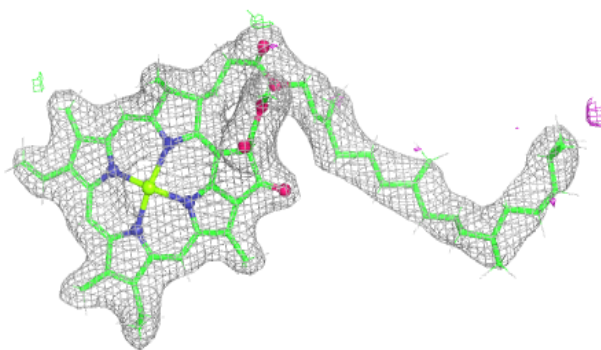
Electron density around CLA C 508:

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



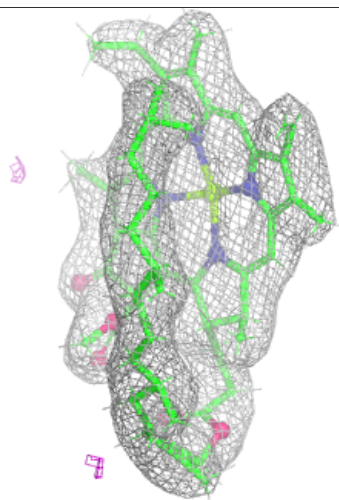
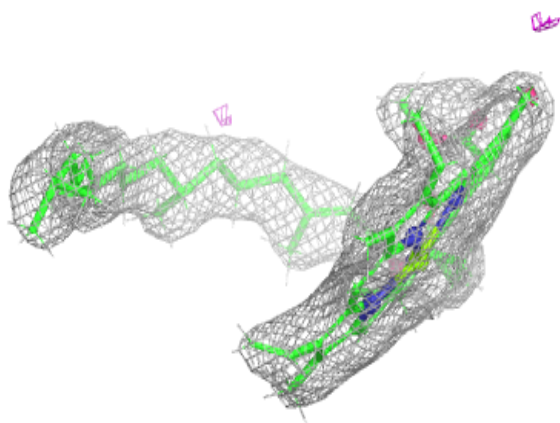
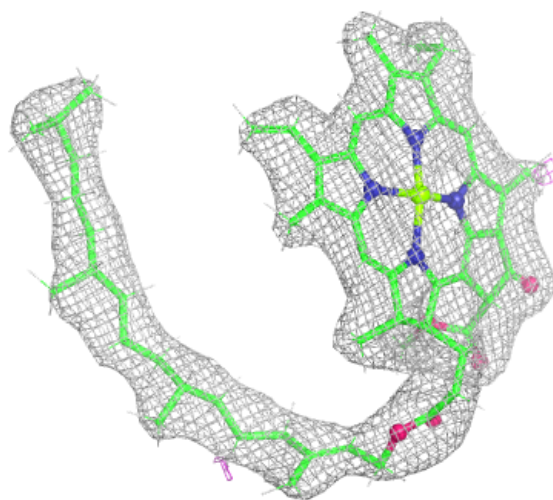
Electron density around CLA B 602:

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



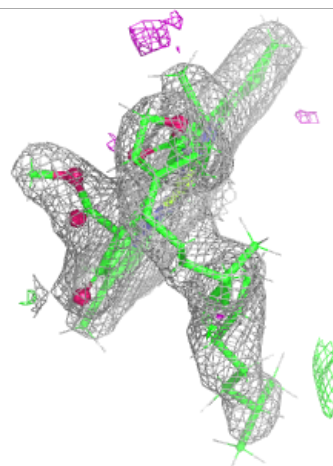
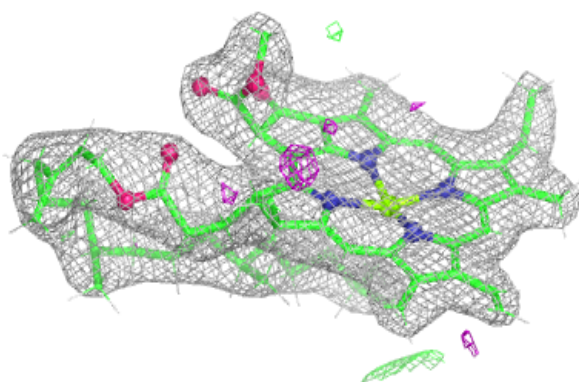
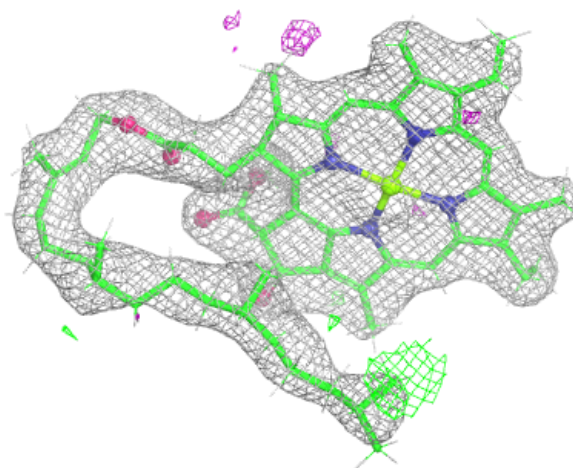
Electron density around CLA c 507:

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



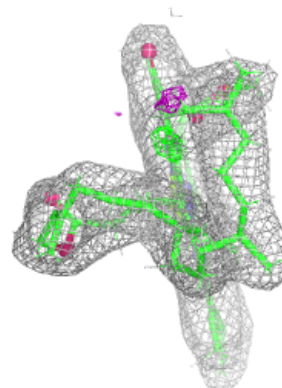
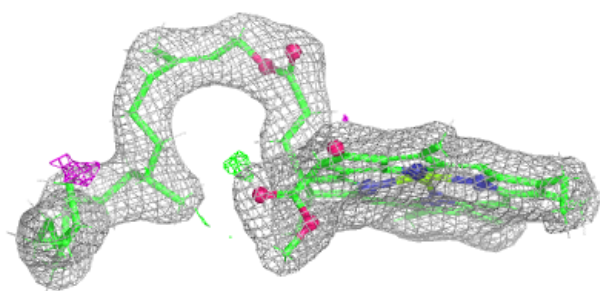
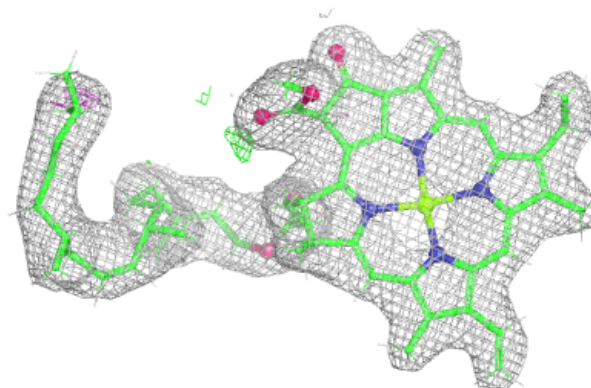
Electron density around CLA C 510:

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

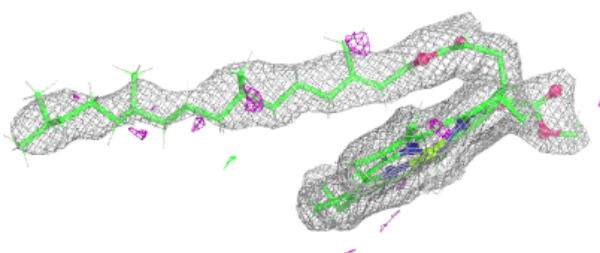
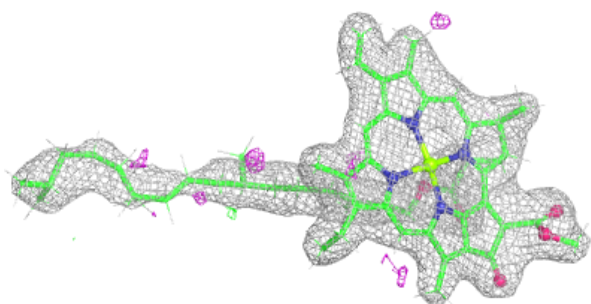


Electron density around CLA B 612:

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

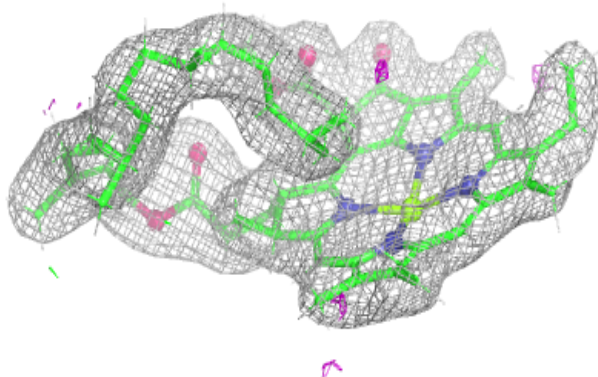
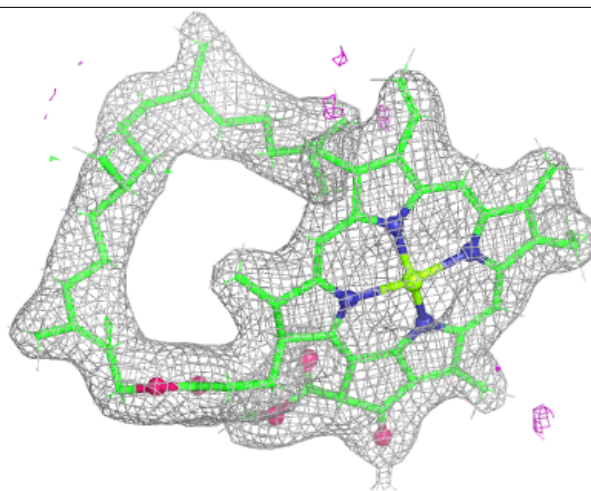
**Electron density around CLA B 614:**

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



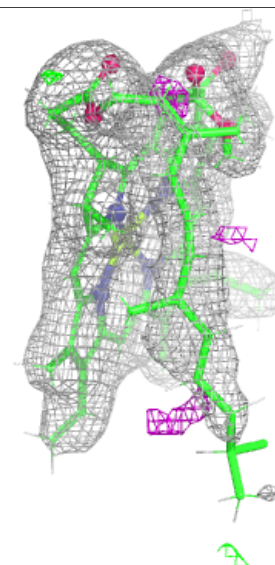
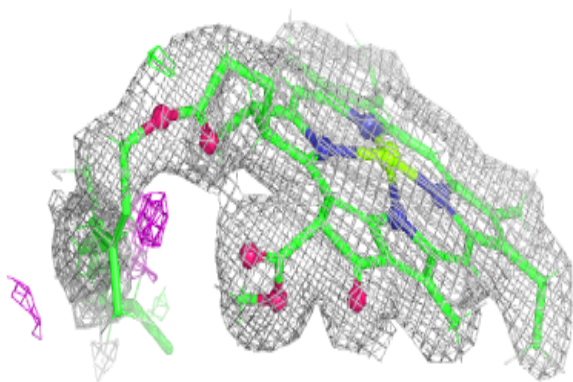
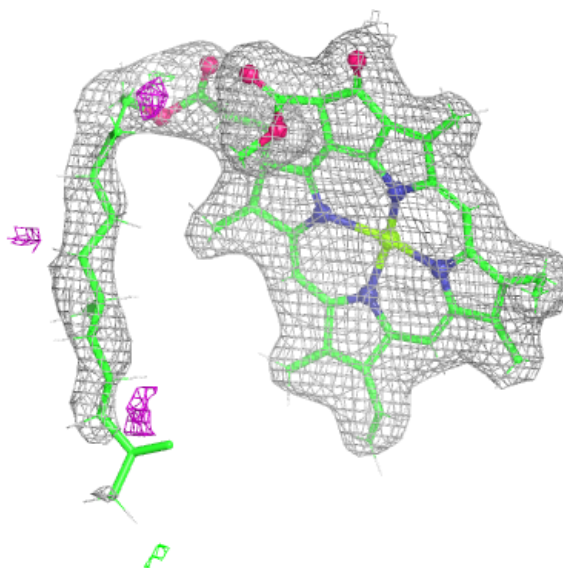
Electron density around CLA B 615:

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



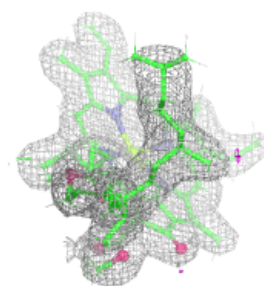
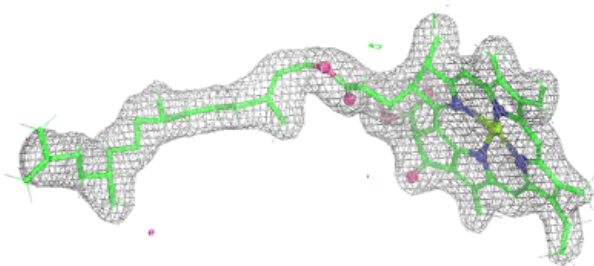
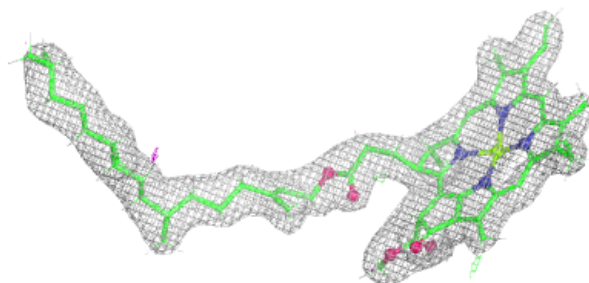
Electron density around CLA B 616:

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

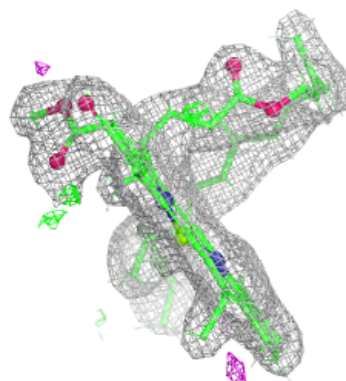
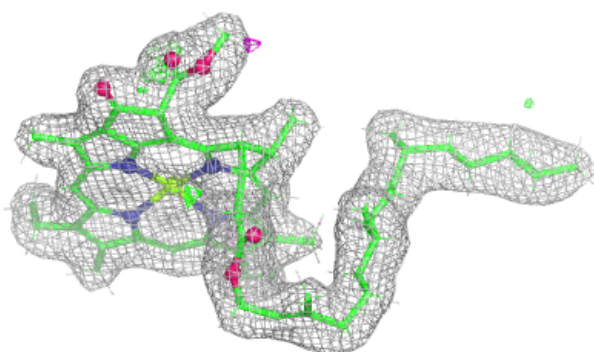
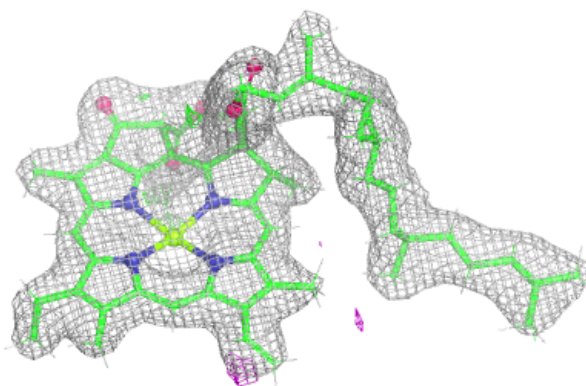


Electron density around CLA a 404:

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

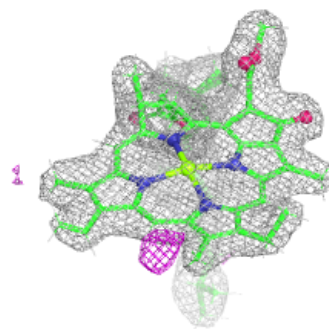
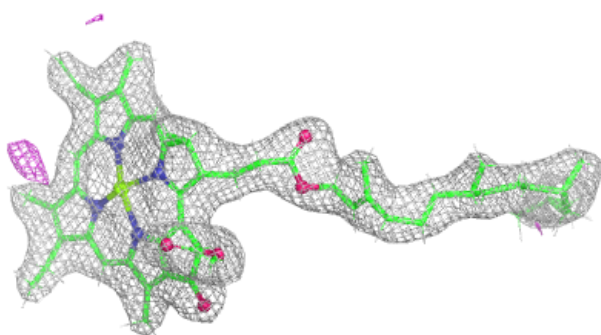
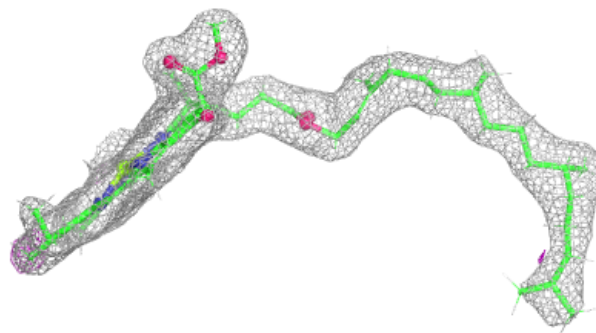
**Electron density around CLA d 403:**

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

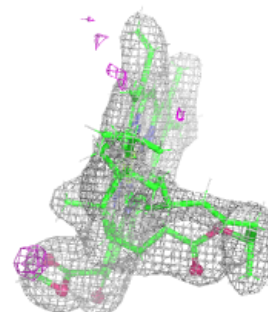
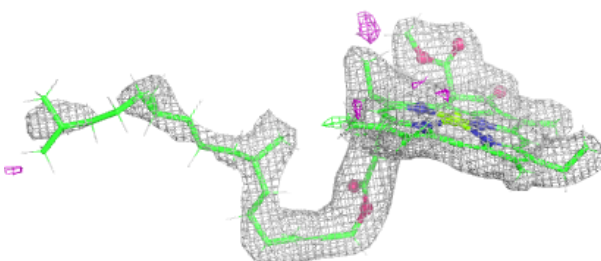
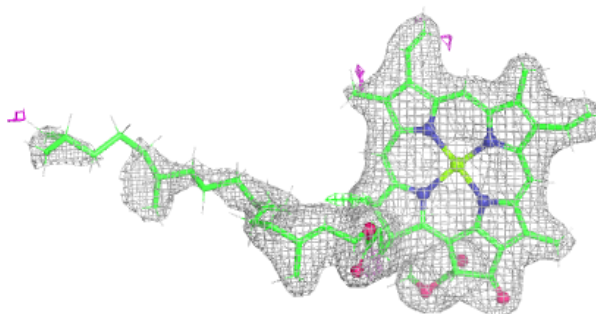


Electron density around CLA d 404:

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

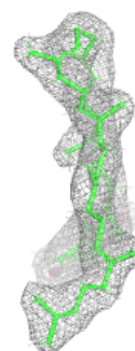
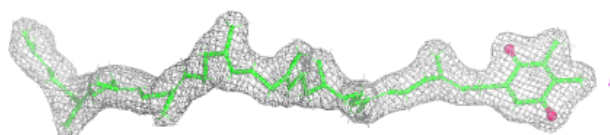
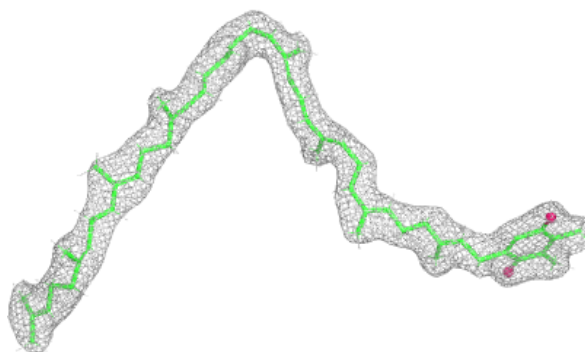
**Electron density around CLA a 405:**

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

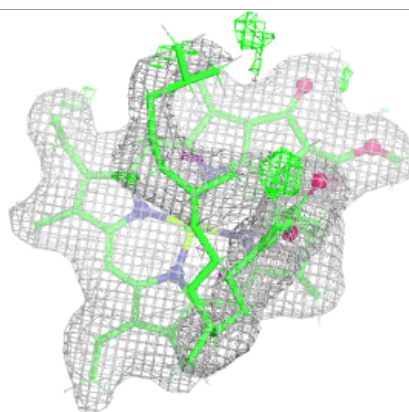
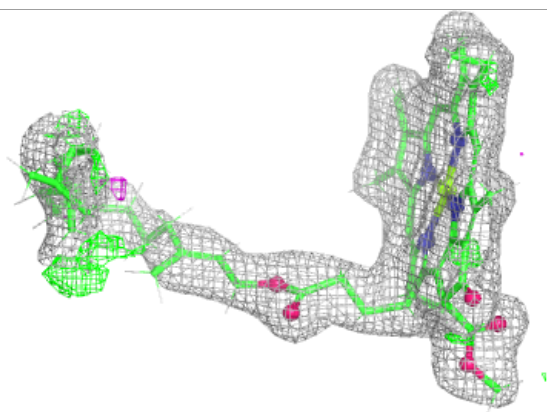
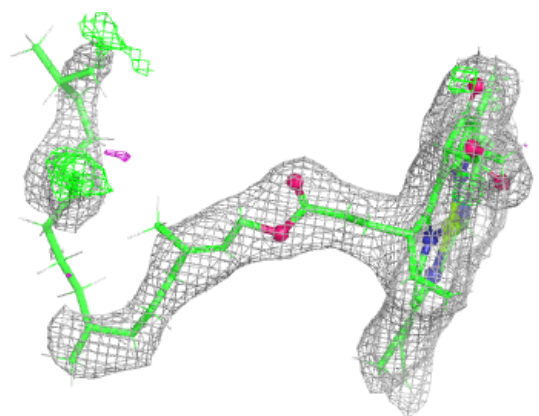


Electron density around PL9 D 406:

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

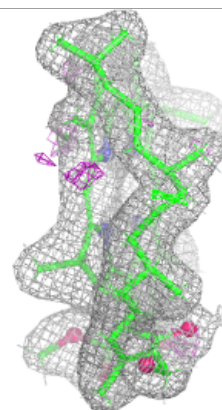
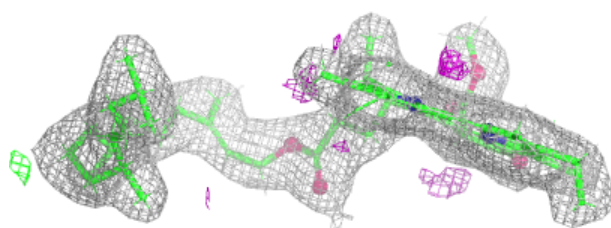
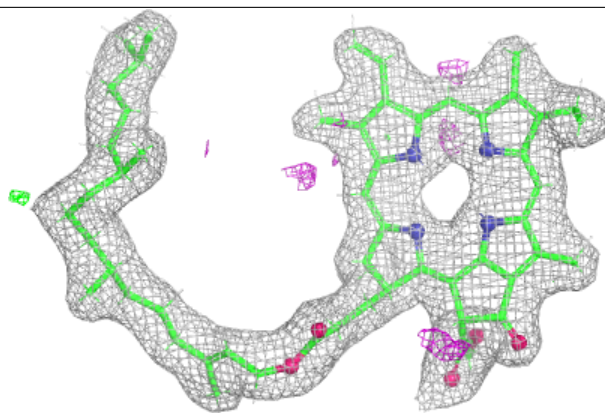
**Electron density around CLA a 407:**

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

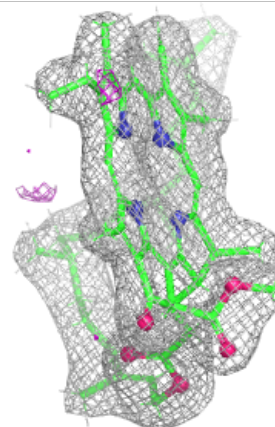
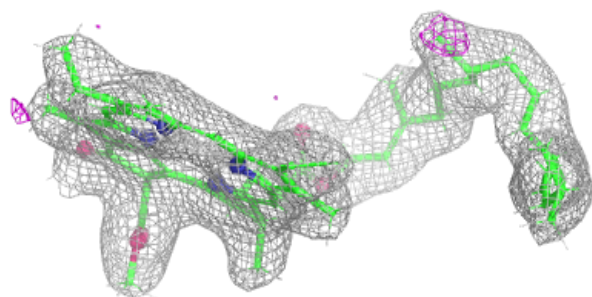
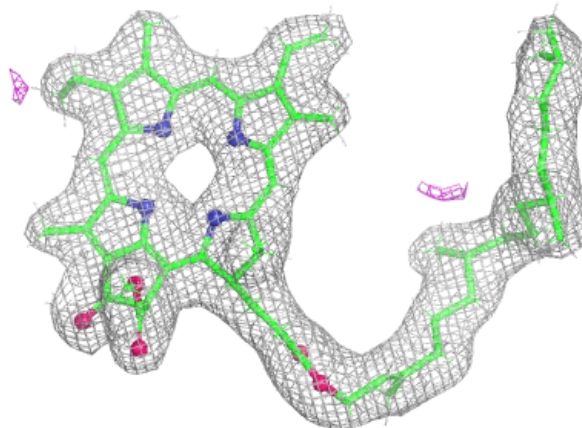


Electron density around PHO A 407:

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

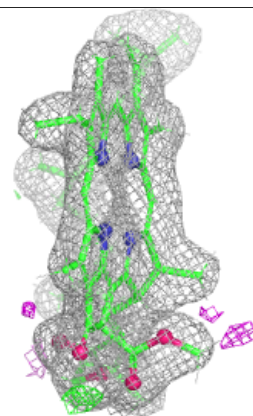
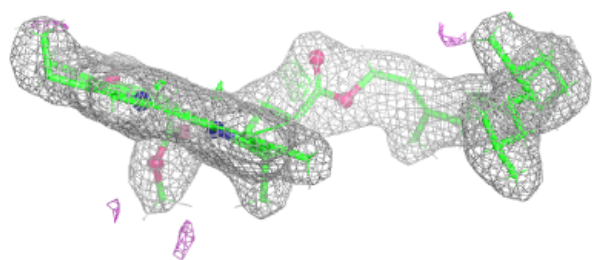
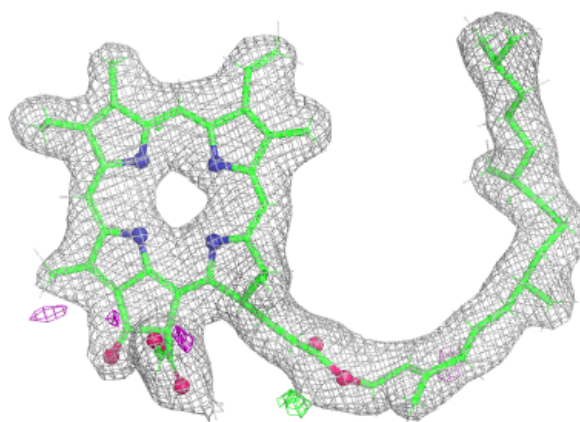
**Electron density around PHO D 401:**

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



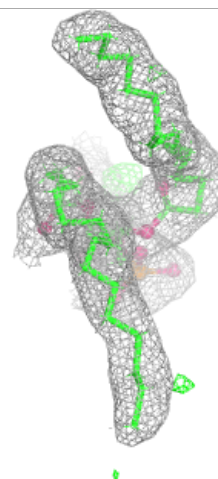
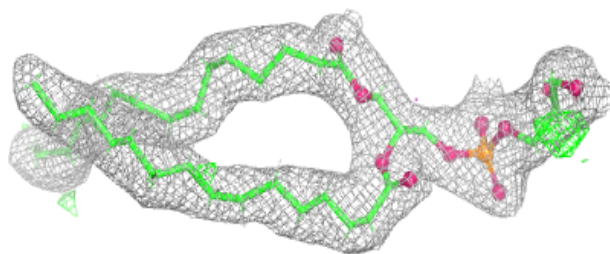
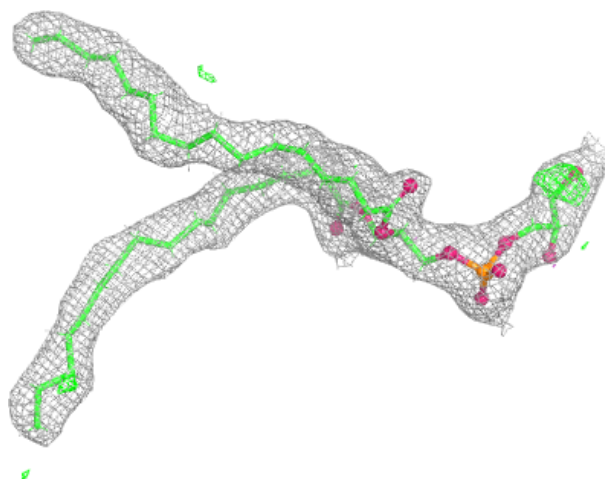
Electron density around PHO a 406:

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



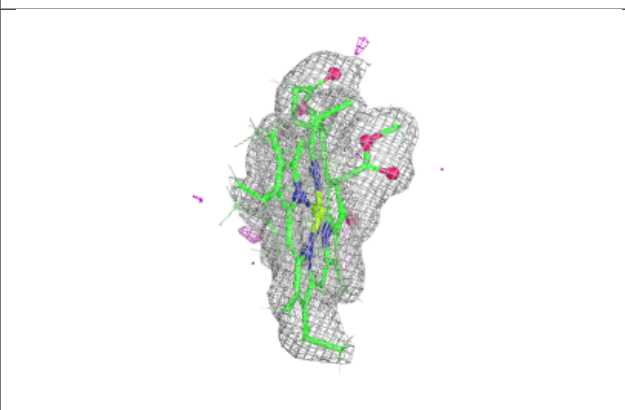
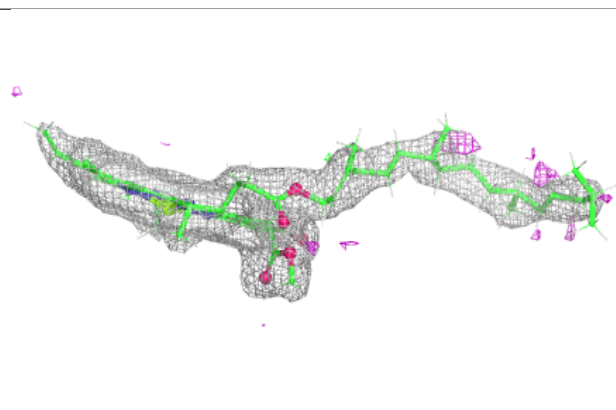
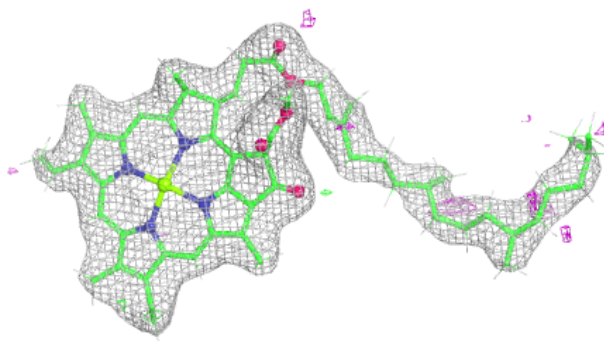
Electron density around LHG D 408:

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

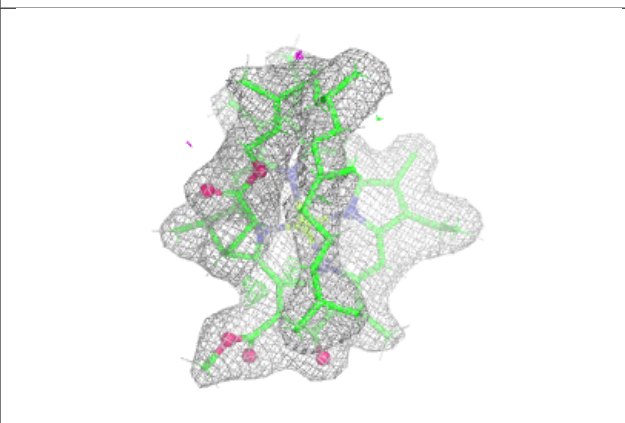
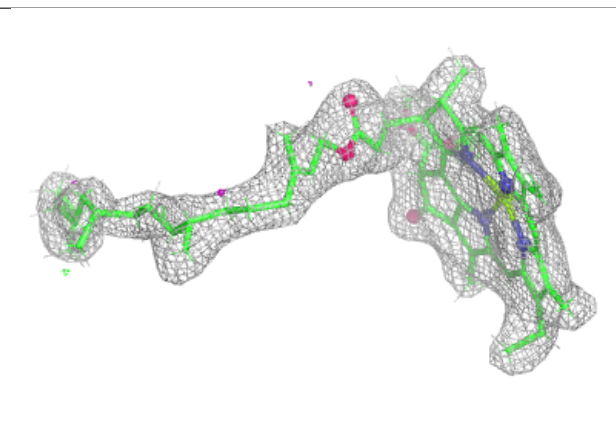
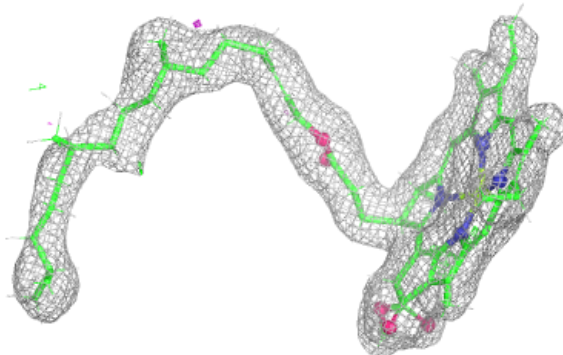


Electron density around CLA b 603:

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

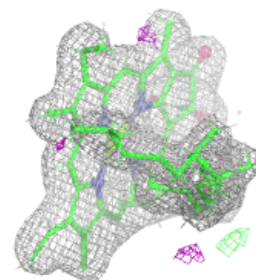
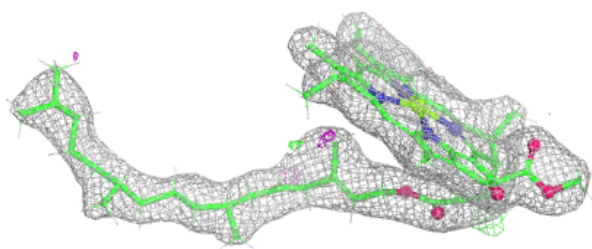
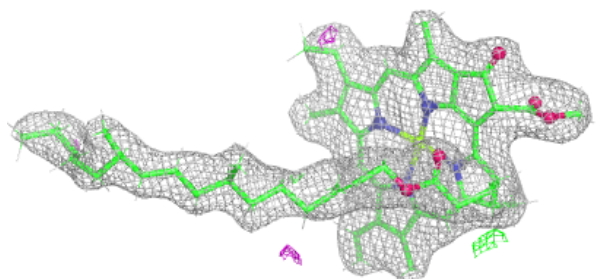
**Electron density around CLA b 607:**

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

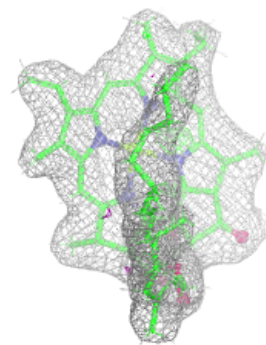
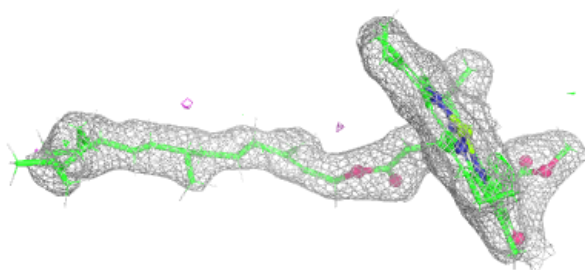
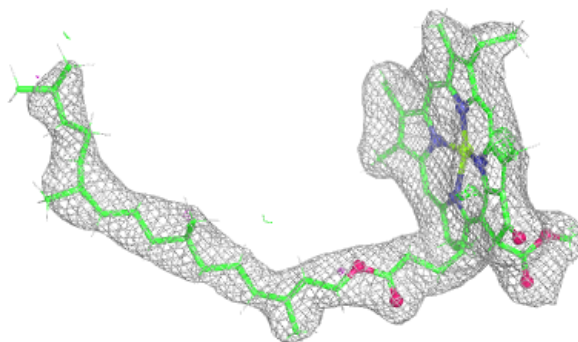


Electron density around CLA b 609:

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

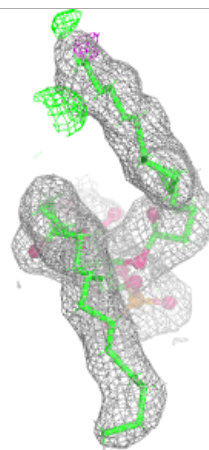
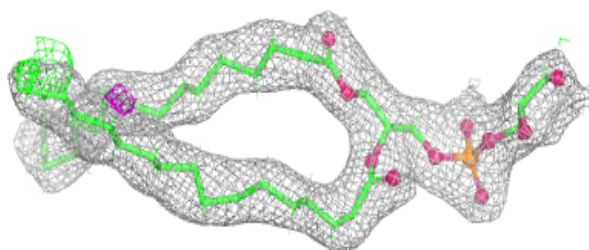
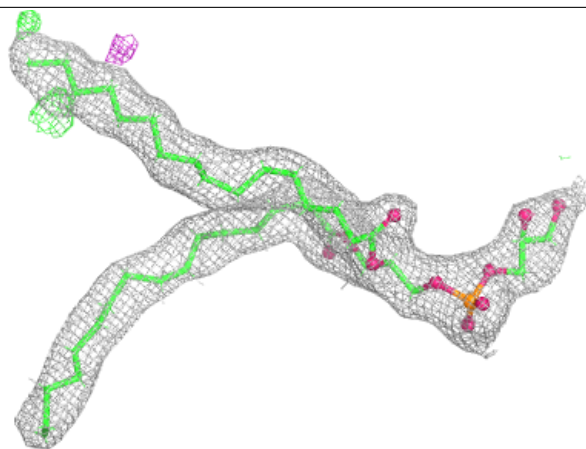
**Electron density around CLA b 610:**

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



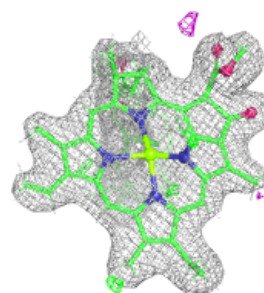
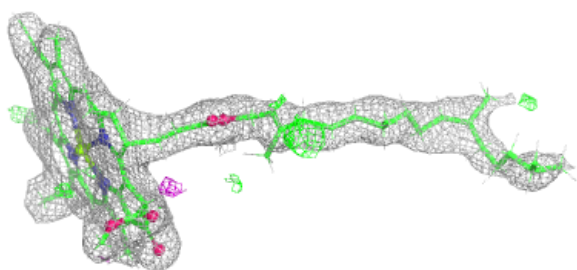
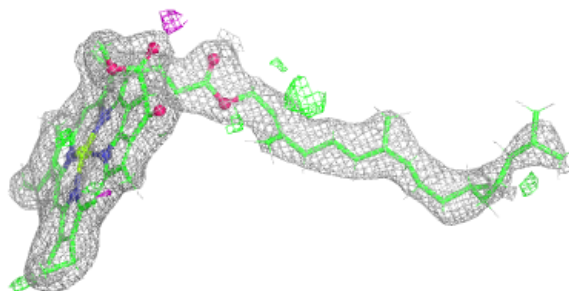
Electron density around LHG d 409:

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

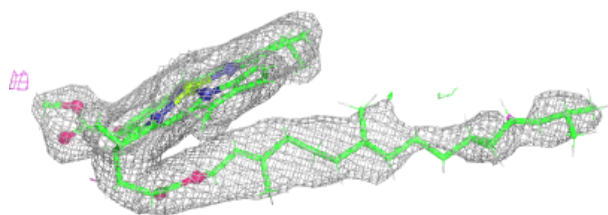
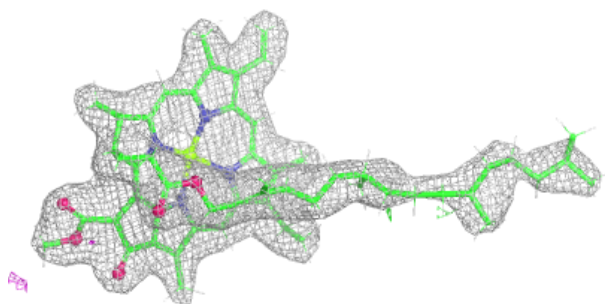


Electron density around CLA B 604:

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

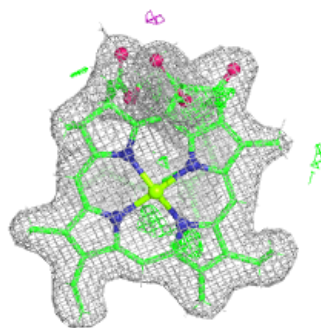
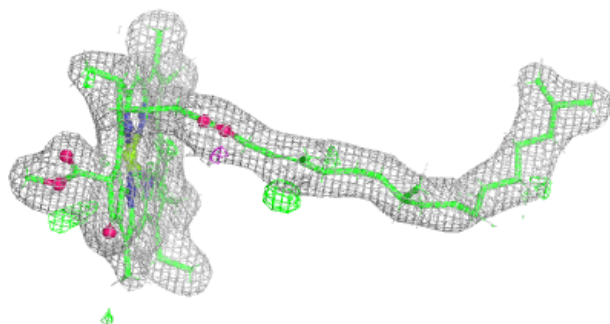
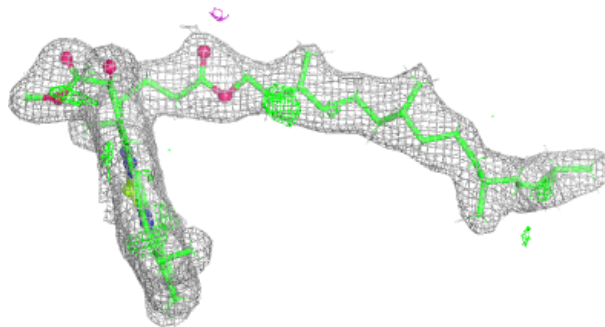
**Electron density around CLA b 615:**

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

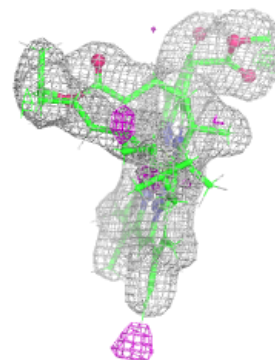
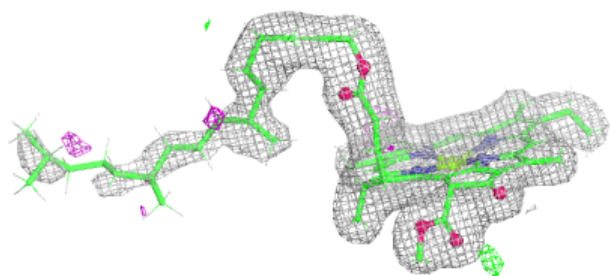
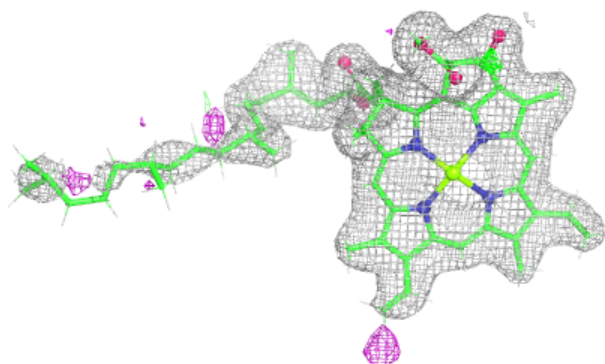


Electron density around CLA B 605:

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

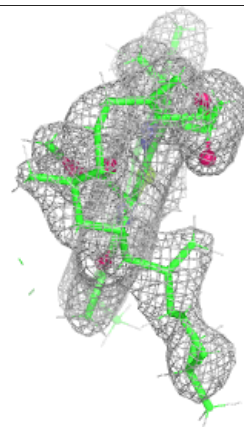
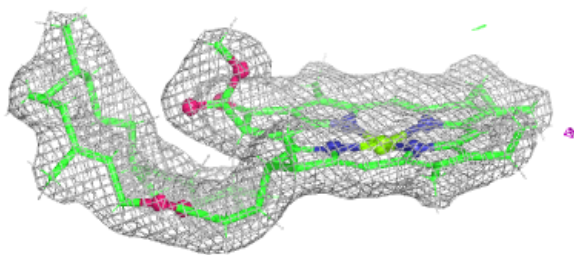
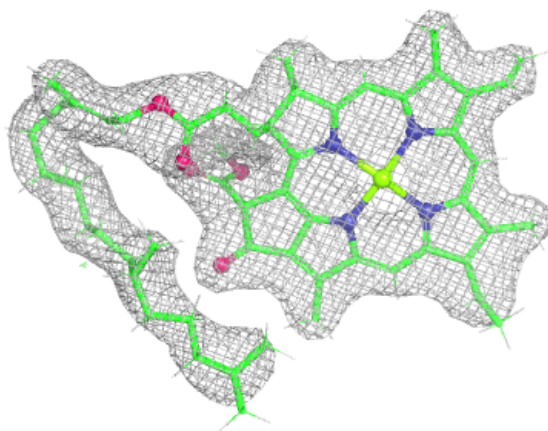
**Electron density around CLA A 406:**

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



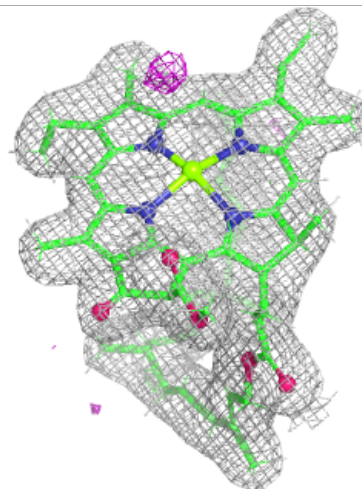
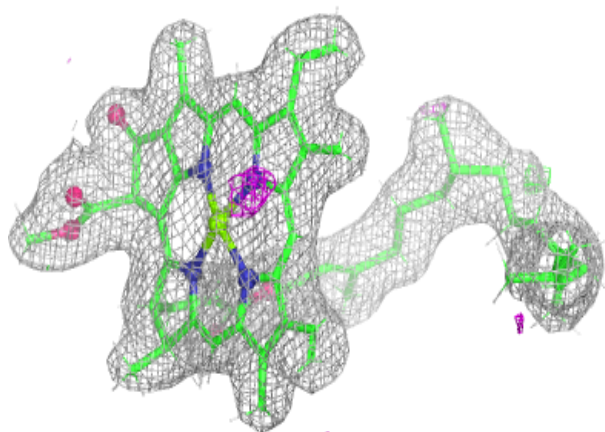
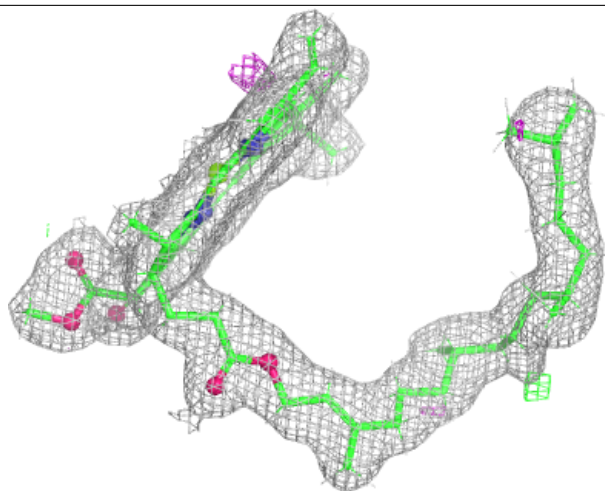
Electron density around CLA b 611:

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



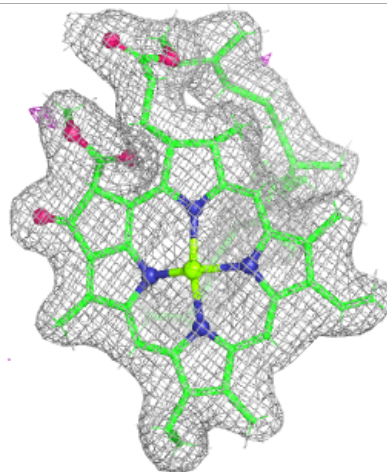
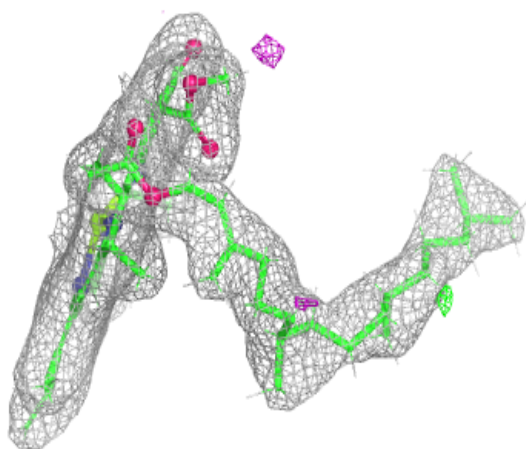
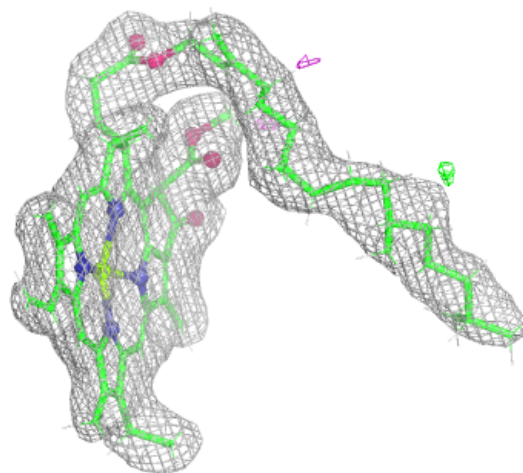
Electron density around CLA b 612:

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



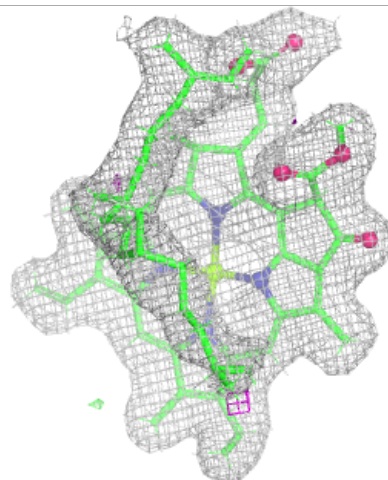
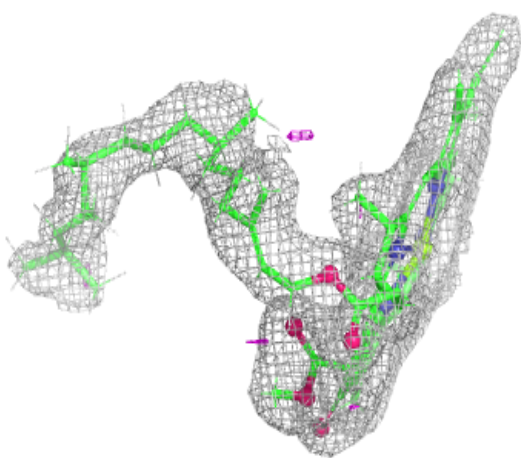
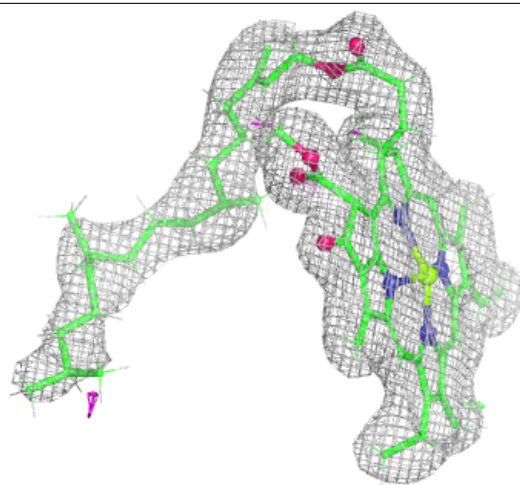
Electron density around CLA B 613:

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



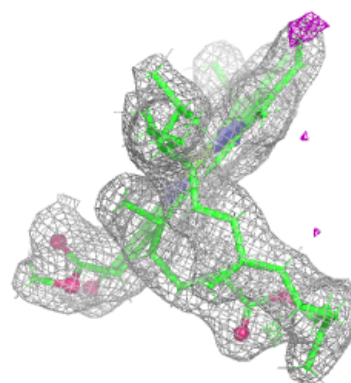
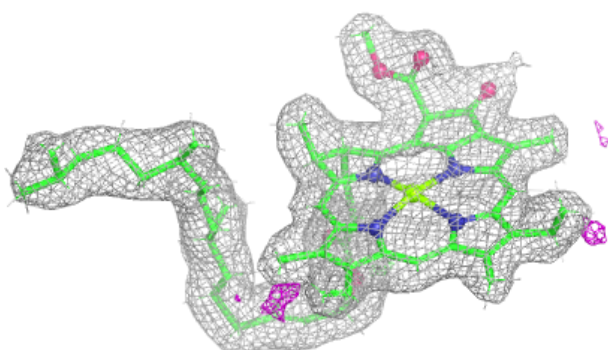
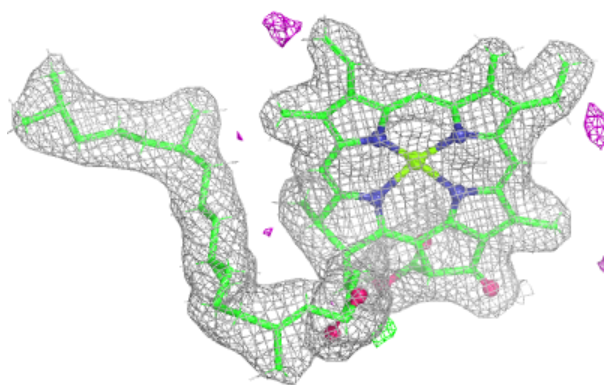
Electron density around CLA b 614:

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

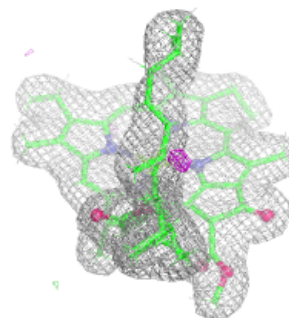
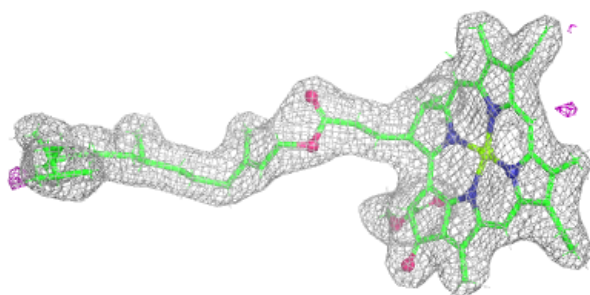
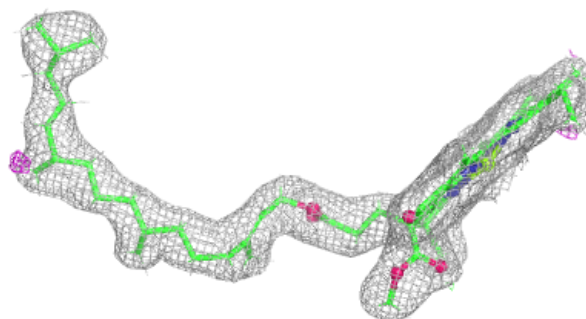


Electron density around CLA D 402:

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

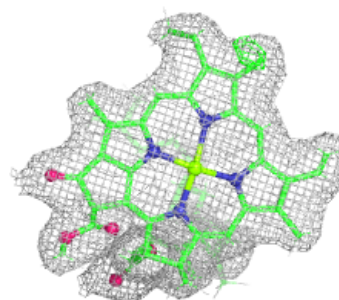
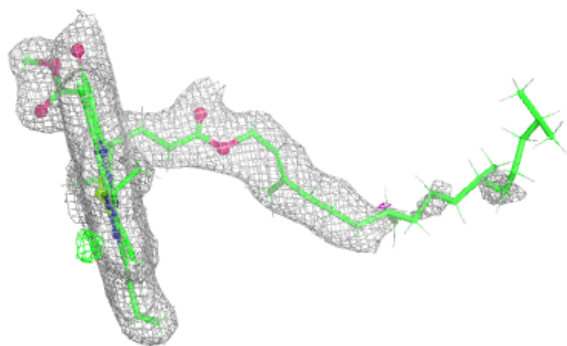
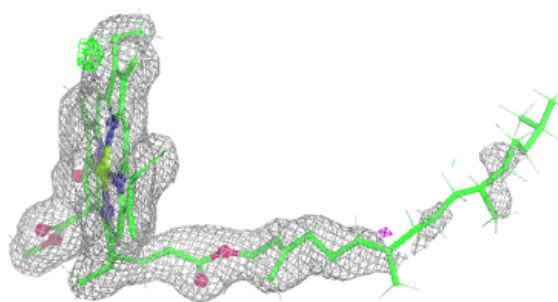
**Electron density around CLA D 403:**

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

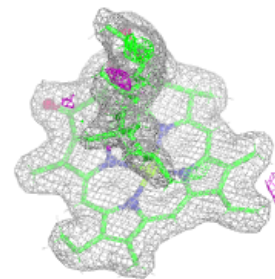
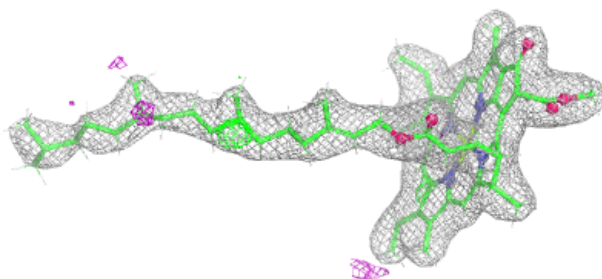
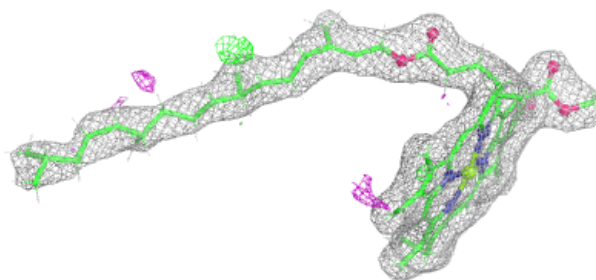


Electron density around CLA D 404:

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

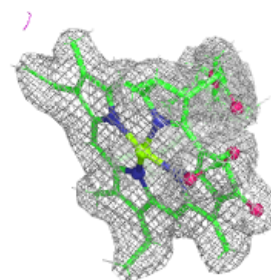
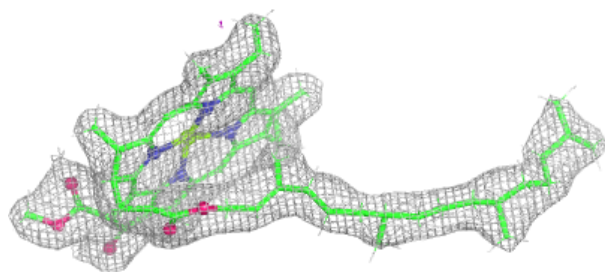
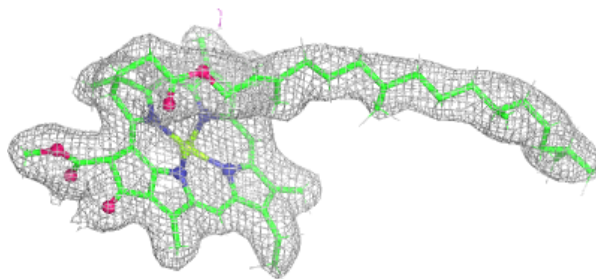
**Electron density around CLA B 607:**

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

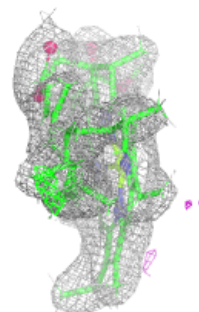
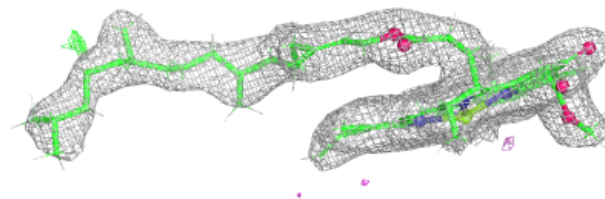
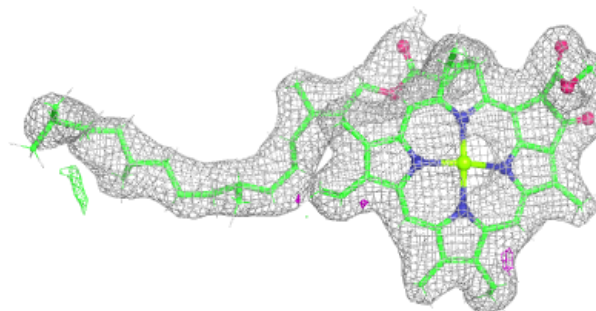


Electron density around CLA B 608:

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

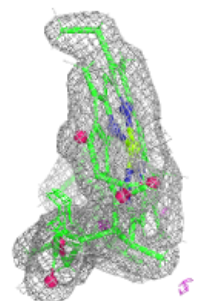
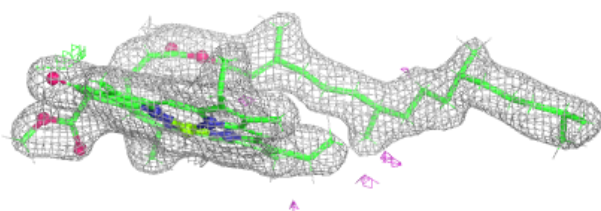
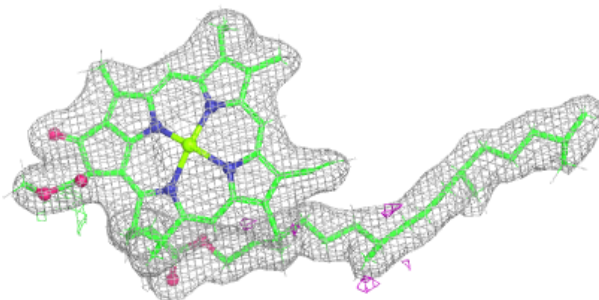
**Electron density around CLA B 603:**

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

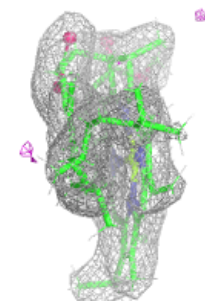
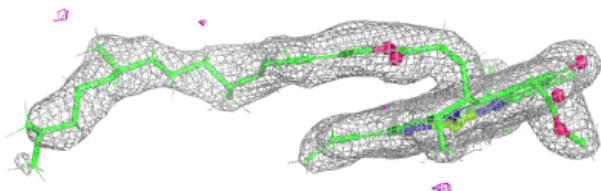
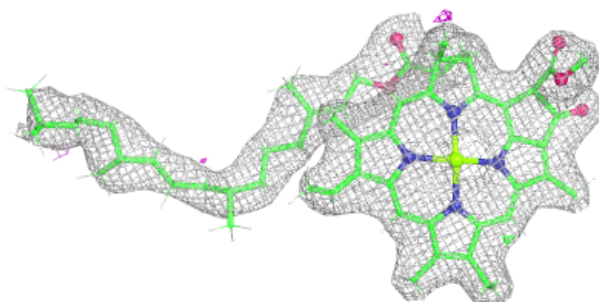


Electron density around CLA C 502:

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

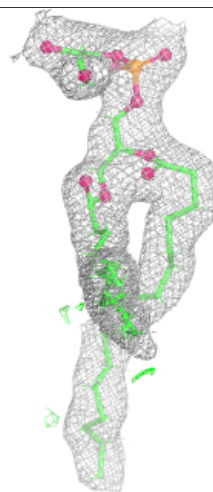
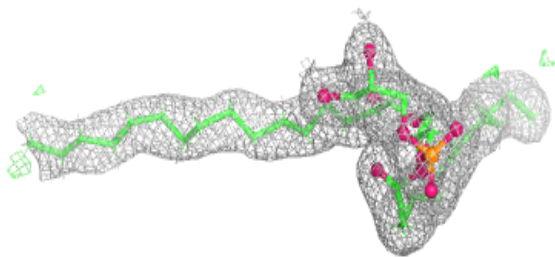
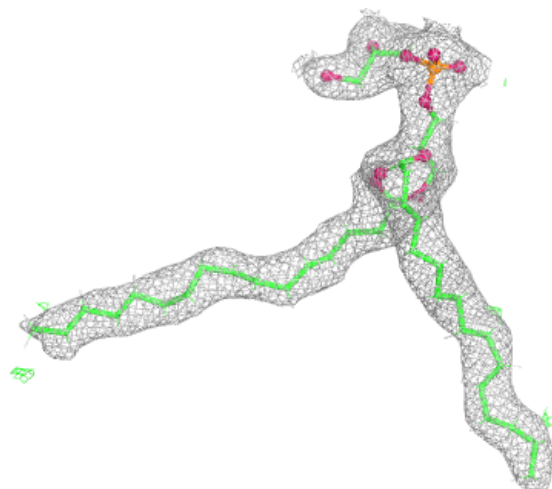
**Electron density around CLA b 604:**

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



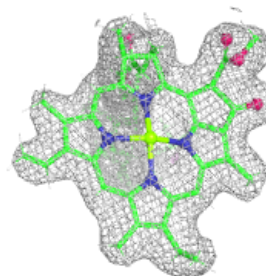
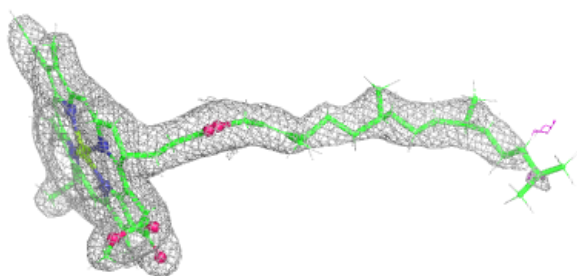
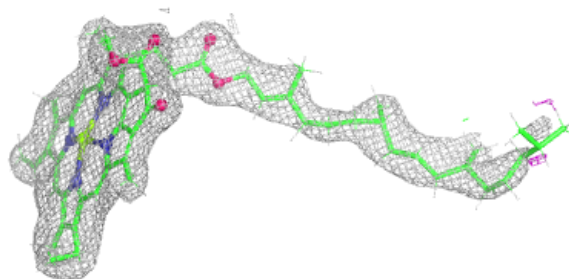
Electron density around LHG L 101:

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

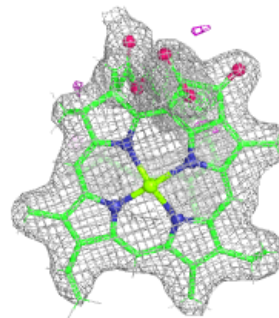
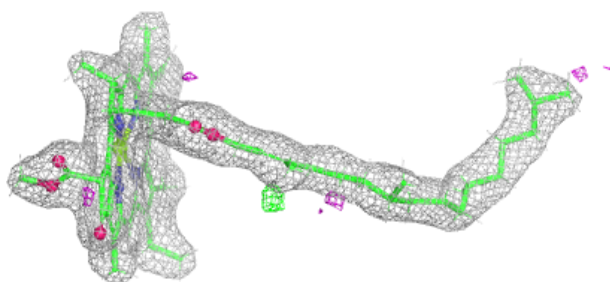
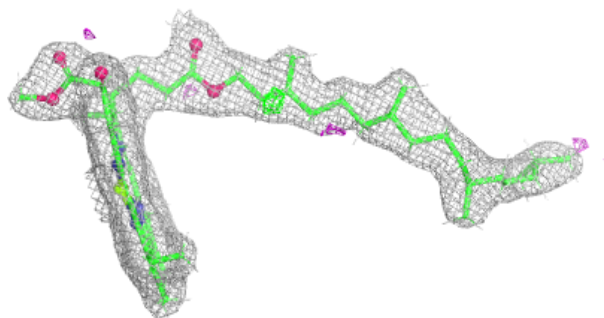


Electron density around CLA b 605:

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

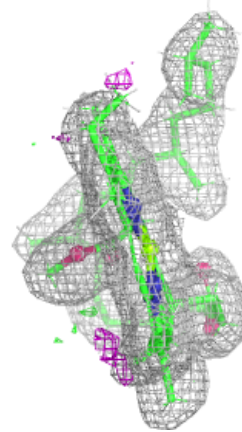
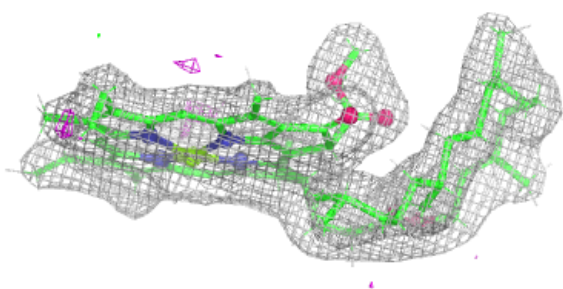
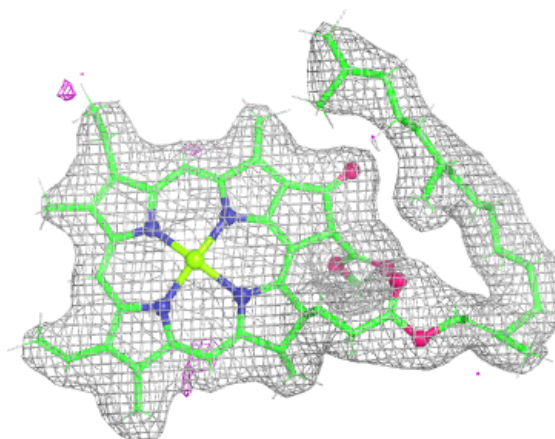
**Electron density around CLA b 606:**

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



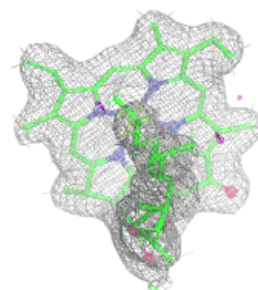
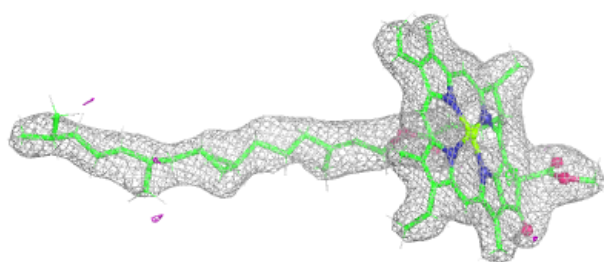
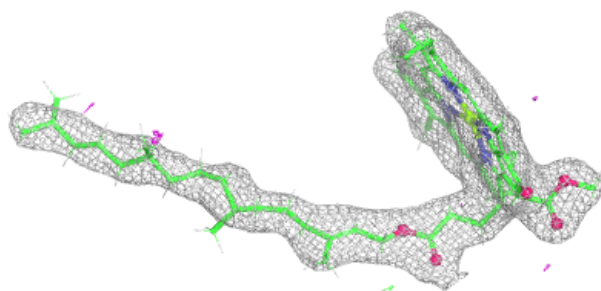
Electron density around CLA B 610:

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



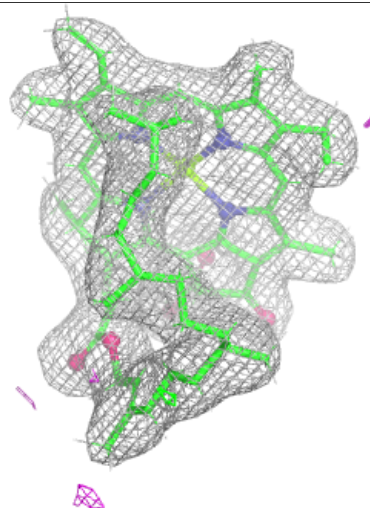
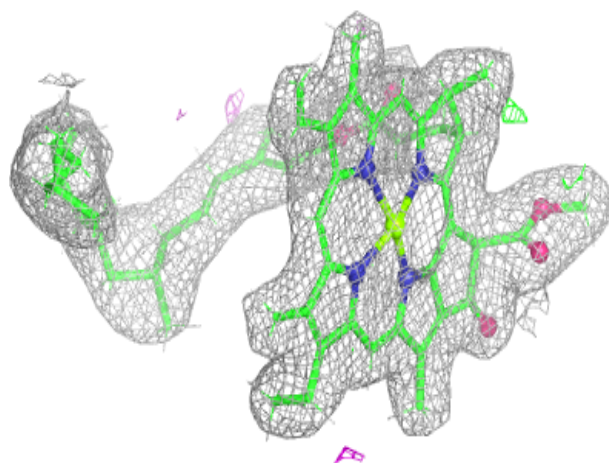
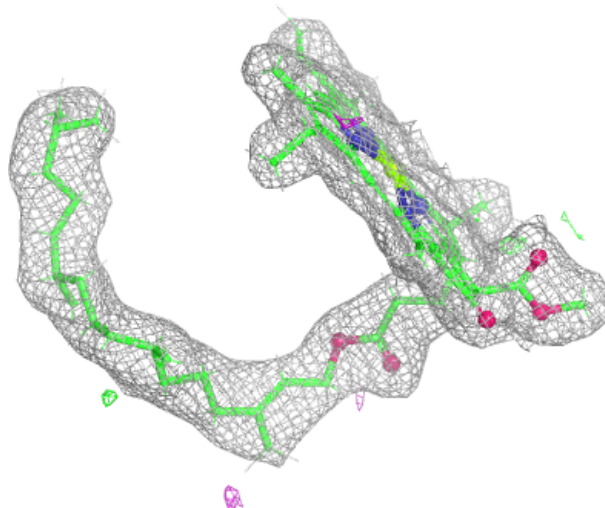
Electron density around CLA b 608:

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



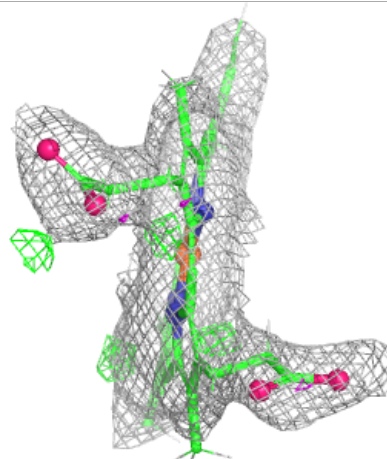
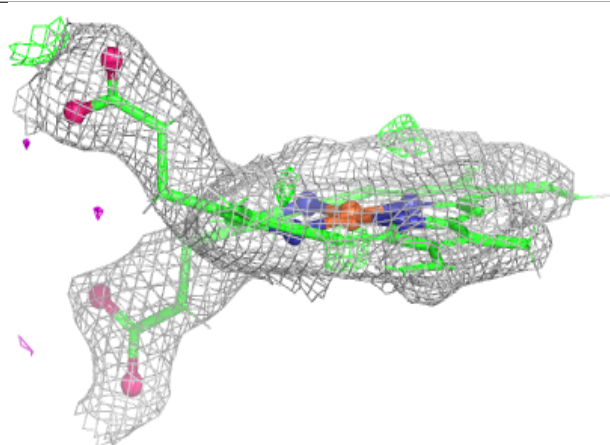
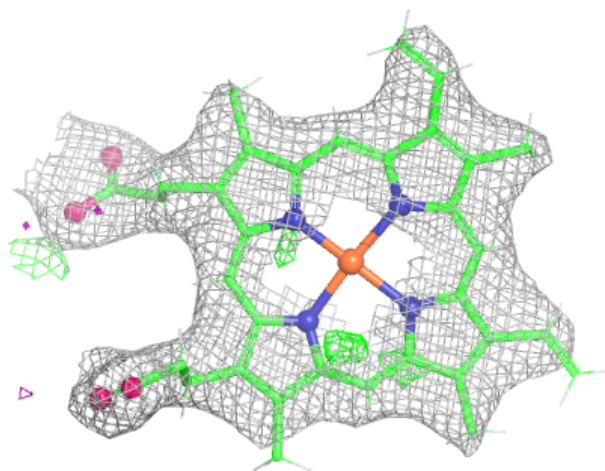
Electron density around CLA B 611:

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



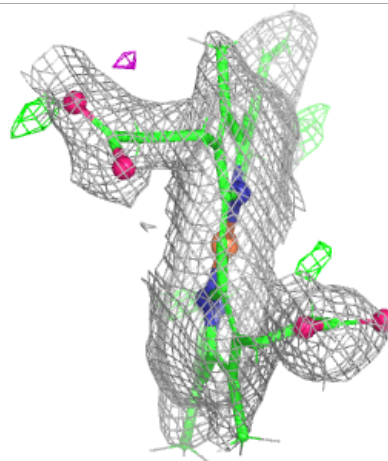
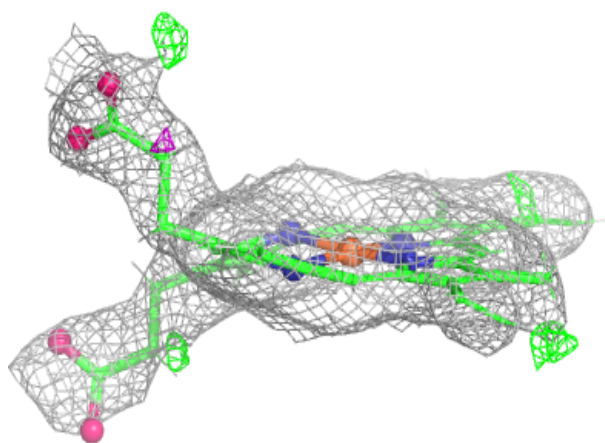
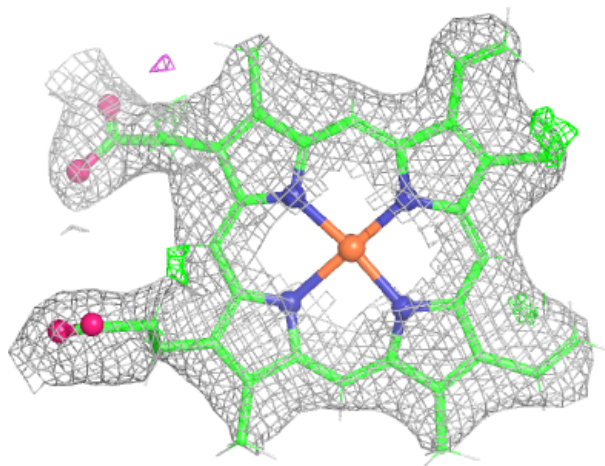
Electron density around HEM F 102:

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



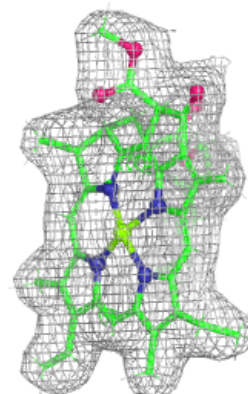
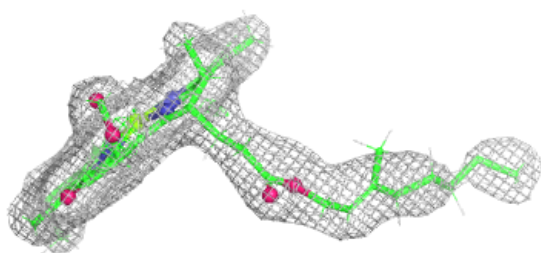
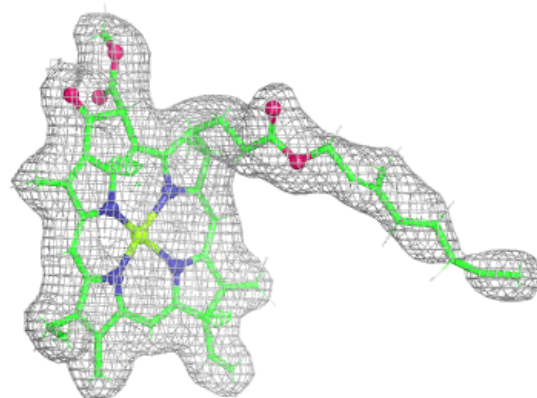
Electron density around HEM e 102:

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



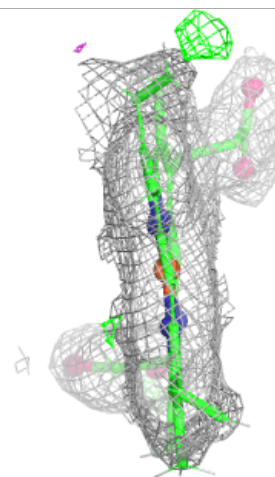
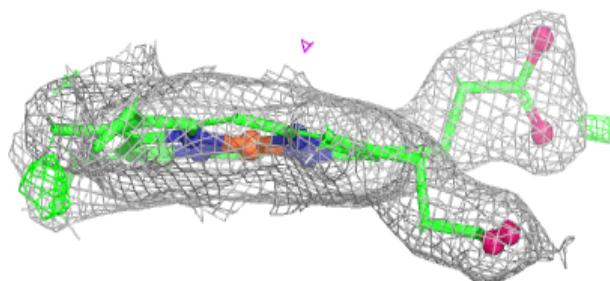
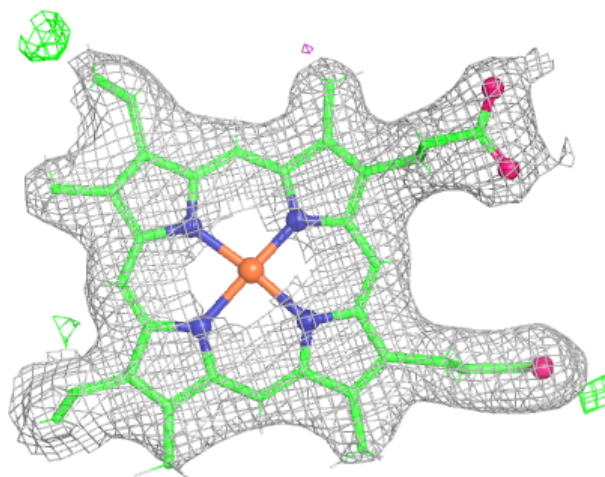
Electron density around CLA A 408:

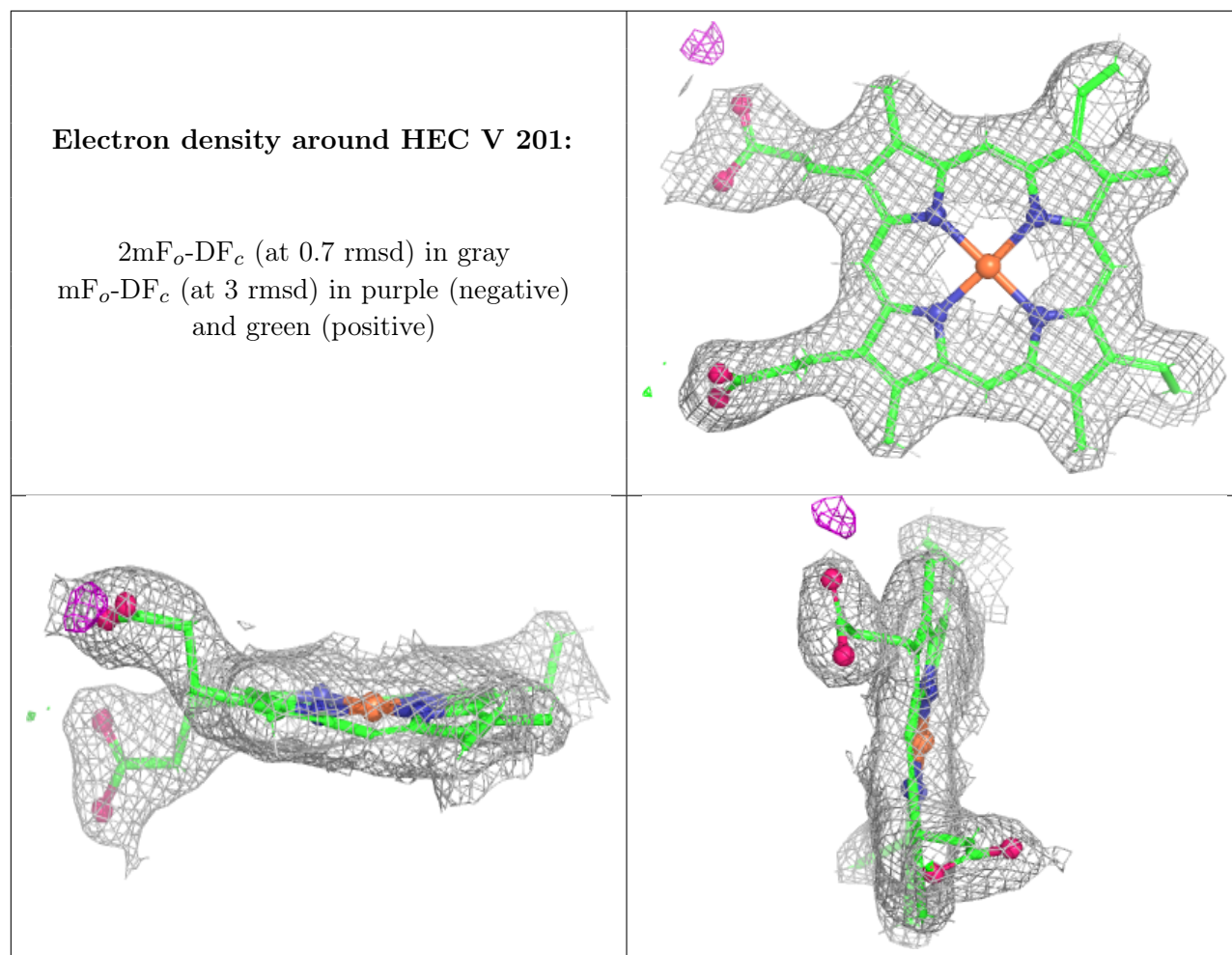
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEC v 201:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.