



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 09:45 PM UTC

PDB ID : 6DHP / pdb_00006dhp
Title : RT XFEL structure of the three-flash state of Photosystem II (3F, S0-rich) at 2.04 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 : 2.04 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

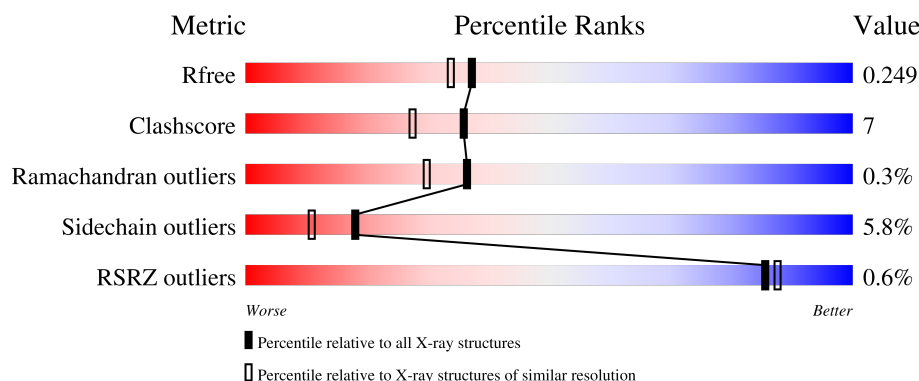
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.04 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	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

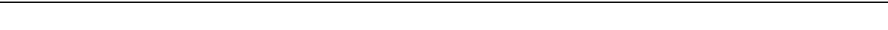
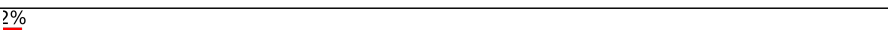
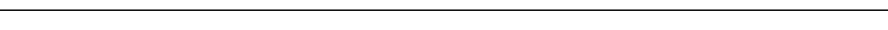
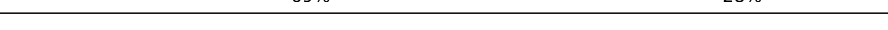
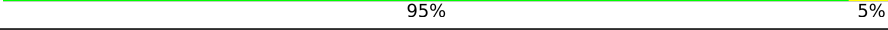
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	 84% 14% .
2	B	505	 83% 16% .
2	b	505	 87% 12% .
3	C	451	 84% 13% ..
3	c	451	 84% 14% .
4	D	341	 88% 11% .
4	d	341	 85% 14% .
5	E	82	 63% 33% ..
5	e	82	 68% 30% .
6	F	34	 85% 12% .
6	f	34	 59% 35% 6% .
7	H	65	 75% 22% .
7	h	65	 68% 26% . .
8	I	36	 69% 28% .
8	i	36	 78% 19% .
9	J	36	 78% 22% .
9	j	36	 72% 22% 6% .
10	K	37	 65% 30% 5% .
10	k	37	 46% 46% 8% .
11	L	37	 95% 5% .
11	l	37	 70% 24% . .
12	M	33	 82% 15% .
12	m	33	 82% 15% .
13	O	244	 78% 20% .
13	o	244	 80% 18% .

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	A	603	X	-	-	-
23	CLA	A	607	X	-	-	-
23	CLA	B	601	X	-	-	-
23	CLA	B	602	X	-	-	-
23	CLA	B	603	X	-	-	-
23	CLA	B	604	X	-	-	-
23	CLA	B	606	X	-	-	-
23	CLA	B	607	X	-	-	-
23	CLA	B	610	X	-	-	-
23	CLA	B	612	X	-	-	-
23	CLA	B	613	X	-	-	-
23	CLA	B	614	X	-	-	-
23	CLA	B	615	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	B	616	X	-	-	-
23	CLA	C	501	X	-	-	-
23	CLA	C	502	X	-	-	-
23	CLA	C	503	X	-	-	-
23	CLA	C	504	X	-	-	-
23	CLA	C	505	X	-	-	-
23	CLA	C	507	X	-	-	-
23	CLA	C	509	X	-	-	-
23	CLA	C	510	X	-	-	-
23	CLA	C	511	X	-	-	-
23	CLA	C	512	X	-	-	-
23	CLA	C	513	X	-	-	-
23	CLA	D	403	X	-	-	-
23	CLA	a	603	X	-	-	-
23	CLA	a	606	X	-	-	-
23	CLA	a	612	X	-	-	-
23	CLA	b	602	X	-	-	-
23	CLA	b	603	X	-	-	-
23	CLA	b	604	X	-	-	-
23	CLA	b	605	X	-	-	-
23	CLA	b	606	X	-	-	-
23	CLA	b	607	X	-	-	-
23	CLA	b	609	X	-	-	-
23	CLA	b	610	X	-	-	-
23	CLA	b	611	X	-	-	-
23	CLA	b	612	X	-	-	-
23	CLA	b	613	X	-	-	-
23	CLA	b	614	X	-	-	-
23	CLA	b	615	X	-	-	-
23	CLA	b	616	X	-	-	-
23	CLA	c	501	X	-	-	-
23	CLA	c	503	X	-	-	-
23	CLA	c	504	X	-	-	-
23	CLA	c	505	X	-	-	-
23	CLA	c	506	X	-	-	-
23	CLA	c	507	X	-	-	-
23	CLA	c	508	X	-	-	-
23	CLA	c	509	X	-	-	-
23	CLA	c	510	X	-	-	-
23	CLA	c	511	X	-	-	-
23	CLA	c	512	X	-	-	-
23	CLA	c	513	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	d	402	X	-	-	-
23	CLA	h	101	X	-	-	-

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 105751 atoms, of which 52470 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	59	0
			6018	2010	2937	507	545	19			
1	a	334	Total	C	H	N	O	S	0	59	0
			6006	2007	2928	507	545	19			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	505	Total	C	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	7	0
			6868	2282	3392	579	601	14			
3	c	451	Total	C	H	N	O	S	0	8	0
			7017	2324	3464	596	619	14			

- 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	1	0
			5350	1806	2624	445	463	12			
4	d	341	Total	C	H	N	O	S	0	2	0
			5362	1810	2630	445	465	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 protein Y.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	R	34	Total	C	H	N	O	0	0	0
			569	184	298	47	40			
14	r	31	Total	C	H	N	O	0	0	0
			461	154	234	40	33			

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

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

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

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

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
17	V	137	Total	C	H	N	O	S	0	0	0
			2134	675	1070	177	208	4			
17	v	137	Total	C	H	N	O	S	0	0	0
			2134	675	1070	177	208	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	X	38	Total	C	H	N	O	0	0	0
			593	188	312	45	48			
18	x	38	Total	C	H	N	O	0	0	0
			593	188	312	45	48			

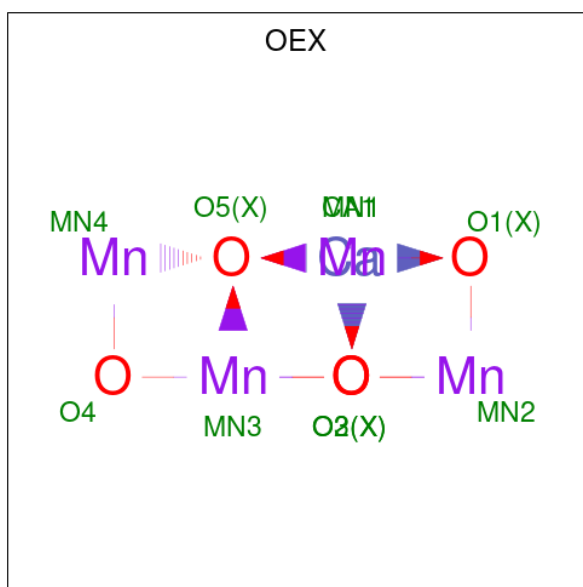
- Molecule 19 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
19	Y	27	Total 404	C 128	H 208	N 35	O 30	S 3	0	0	0
19	y	30	Total 459	C 144	H 241	N 35	O 36	S 3	0	0	0

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
20	Z	62	Total 988	C 328	H 509	N 72	O 77	S 2	0	0	0
20	z	62	Total 986	C 326	H 509	N 72	O 77	S 2	0	0	0

- Molecule 21 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5).

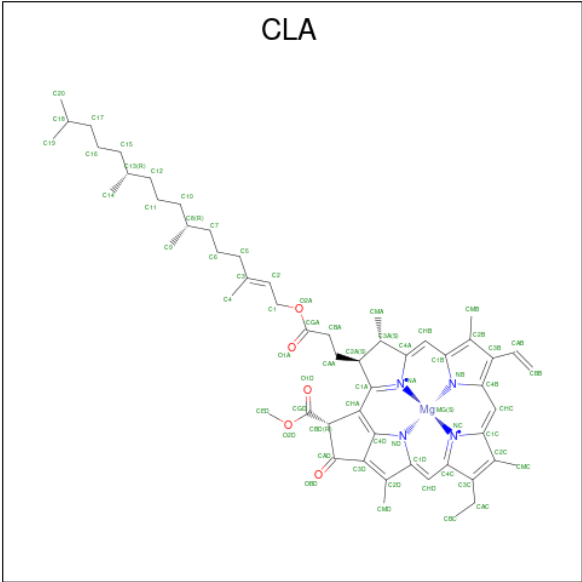


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
21	A	1	Total	Ca	Mn	O	0	1
			10	1	4	5		
21	a	1	Total	Ca	Mn	O	0	1
			10	1	4	5		

- Molecule 22 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

- Molecule 23 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
23	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	A	1	Total	C	H	Mg	N	O	0	0
			102	44	48	1	4	5		
23	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	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
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			119	50	59	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			117	49	58	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	D	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	D	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

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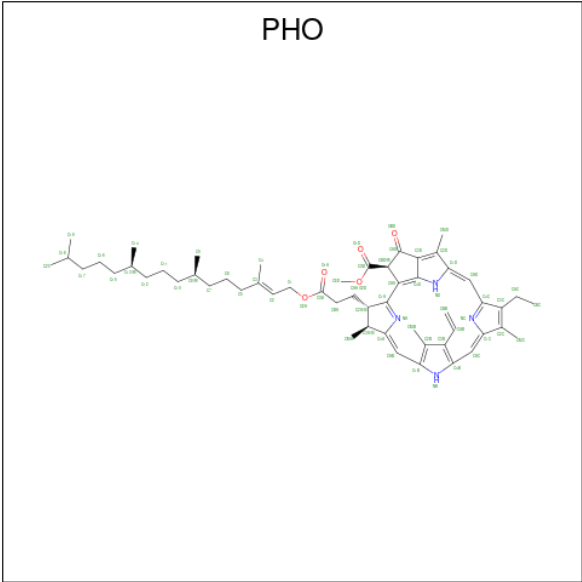
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23	a	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	a	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	a	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	a	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	c	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	c	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0

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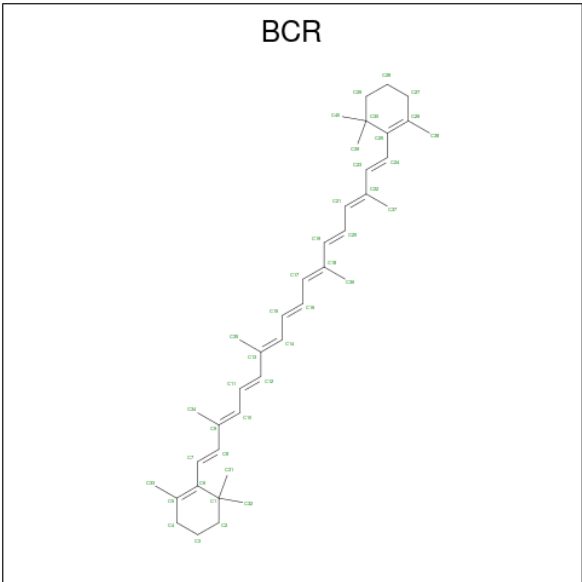
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
23	c	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	c	1	Total 119	C 50	H 59	Mg 1	N 4	O 5	0	0
23	c	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	c	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	c	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	c	1	Total 132	C 54	H 68	Mg 1	N 4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

- Molecule 24 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



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

- Molecule 25 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).

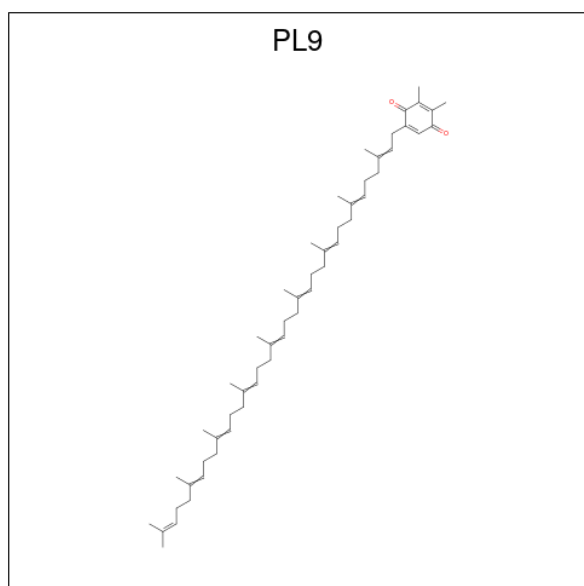


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	A	1	Total	C	H	0	0
			96	40	56		
25	B	1	Total	C	H	0	0
			96	40	56		
25	B	1	Total	C	H	0	0
			96	40	56		
25	B	1	Total	C	H	0	0
			96	40	56		
25	C	1	Total	C	H	0	0
			96	40	56		
25	C	1	Total	C	H	0	0
			96	40	56		
25	C	1	Total	C	H	0	0
			96	40	56		
25	D	1	Total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

- Molecule 26 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

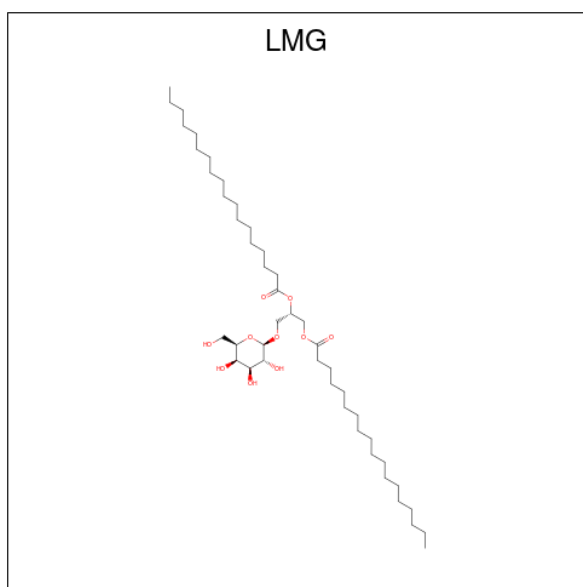
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
26	A	2	Total	Cl	0	0
			2	2		
26	a	2	Total	Cl	0	0
			2	2		

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	A	1	Total	C	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		

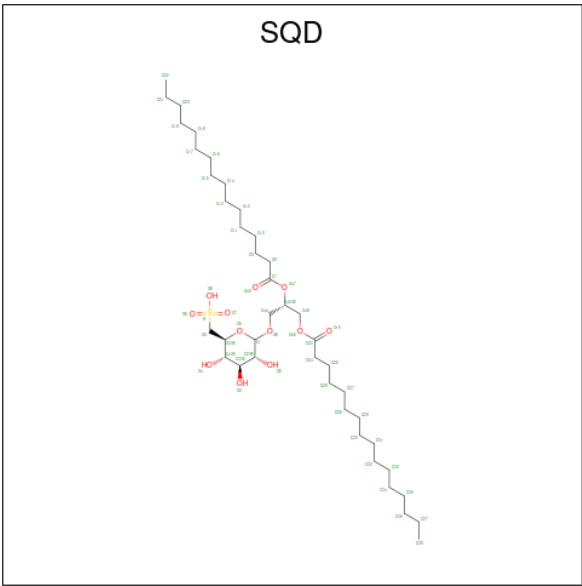
- Molecule 28 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	A	1	Total	C	H	O	0	0
			114	38	66	10		
28	B	1	Total	C	H	O	0	0
			123	41	72	10		
28	B	1	Total	C	H	O	0	0
			68	24	40	4		
28	C	1	Total	C	H	O	0	0
			114	38	66	10		
28	D	1	Total	C	H	O	0	0
			123	41	72	10		
28	D	1	Total	C	H	O	0	0
			78	27	45	6		
28	b	1	Total	C	H	O	0	0
			141	45	86	10		
28	c	1	Total	C	H	O	0	0
			81	27	44	10		
28	c	1	Total	C	H	O	0	0
			117	38	69	10		
28	c	1	Total	C	H	O	0	0
			117	39	68	10		
28	d	1	Total	C	H	O	0	0
			102	34	58	10		
28	d	1	Total	C	H	O	0	0
			57	21	34	2		
28	m	1	Total	C	H	O	0	0
			123	41	72	10		

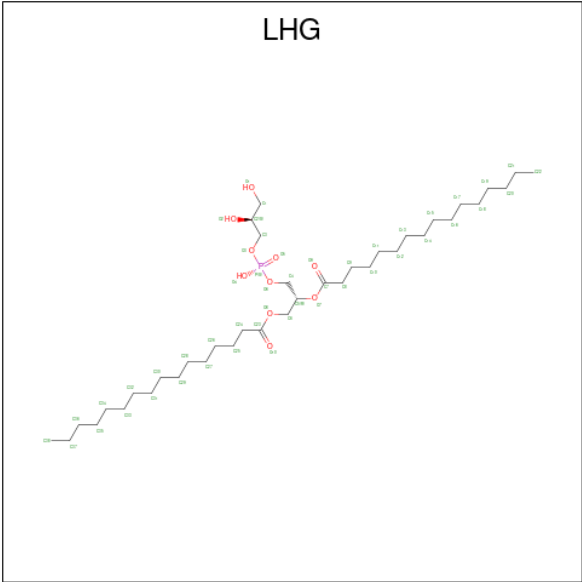
- Molecule 29 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSY

L]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



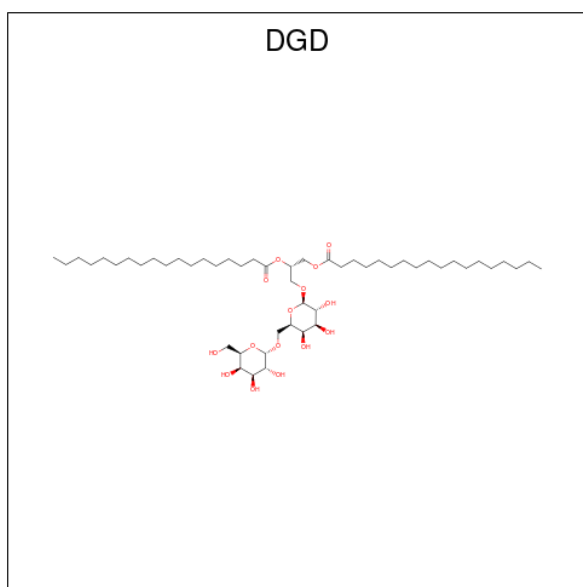
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
29	A	1	Total	C	H	O	S	0	0
			122	39	70	12	1		
29	A	1	Total	C	H	O		0	0
			104	35	65	4			
29	B	1	Total	C	H	O	S	0	0
			132	41	78	12	1		
29	F	1	Total	C	H	O	S	0	0
			81	25	45	10	1		
29	a	1	Total	C	H	O	S	0	0
			132	41	78	12	1		
29	a	1	Total	C	H	O		0	0
			92	31	56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

- Molecule 30 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



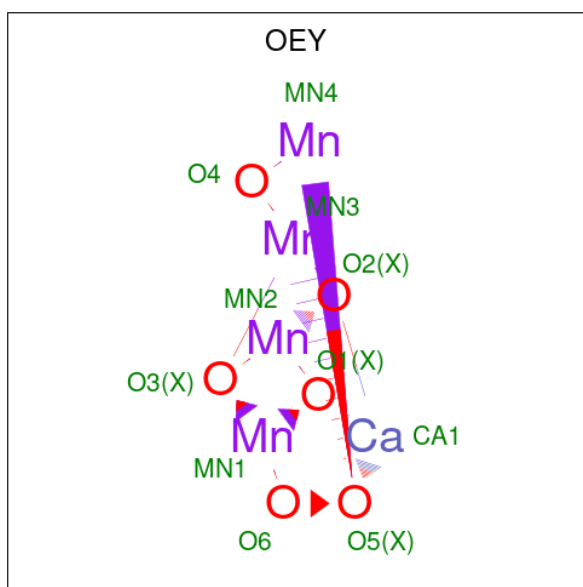
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
30	A	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
30	B	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
30	D	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
30	D	1	Total	C	H	O	P	0	0
			114	36	67	10	1		
30	L	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
30	a	1	Total	C	H	O	P	0	0
			99	31	57	10	1		
30	d	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
30	d	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
30	d	1	Total	C	H	O	P	0	0
			90	28	51	10	1		
30	l	1	Total	C	H	O	P	0	0
			123	38	74	10	1		

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



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

- Molecule 32 is CA-MN4-O6 CLUSTER (CCD ID: OEY) (formula: CaMn_4O_6).



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

- Molecule 33 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

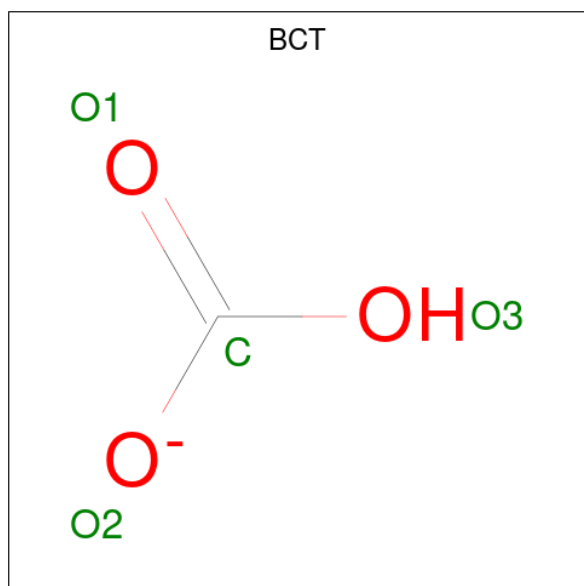
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	B	5	Total	C	H	O	0	0
			192	67	117	8		
33	C	3	Total	C	H	O	0	0
			103	36	63	4		
33	E	1	Total	C	H	O	0	0
			28	10	16	2		
33	H	1	Total	C	H		0	0
			53	18	35			
33	I	1	Total	C	H		0	0
			41	15	26			
33	J	1	Total	C	H	O	0	0
			28	10	16	2		
33	M	2	Total	C	H	O	0	0
			63	23	38	2		
33	T	2	Total	C	H		0	0
			91	31	60			
33	X	1	Total	C	H	O	0	0
			55	18	35	2		
33	a	1	Total	C	H	O	0	0
			28	10	16	2		

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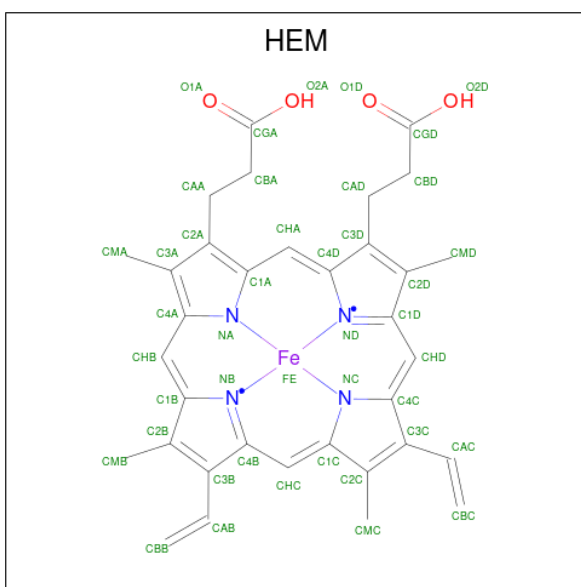
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	b	4	Total	C	H	O	0	0
			176	60	110	6		
33	c	2	Total	C	H	O	0	0
			83	28	51	4		
33	d	1	Total	C	H	O	0	0
			43	15	26	2		
33	j	1	Total	C	H	O	0	0
			28	10	16	2		
33	l	1	Total	C	H		0	0
			53	18	35			
33	m	1	Total	C	H	O	0	0
			28	10	16	2		
33	t	2	Total	C	H	O	0	0
			60	22	36	2		
33	x	1	Total	C	H	O	0	0
			55	18	35	2		

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



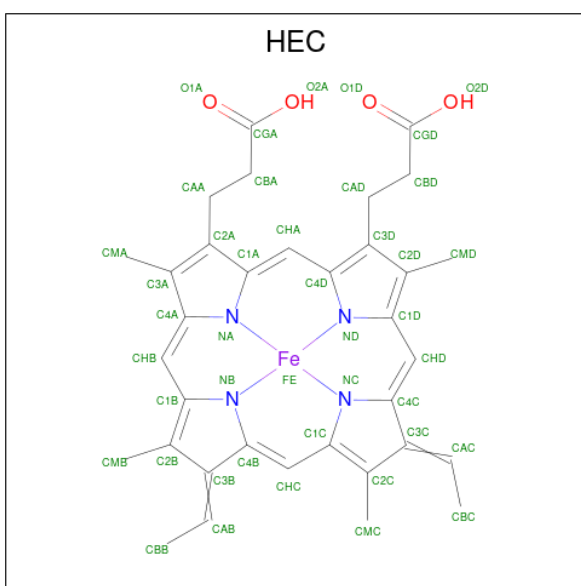
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	D	1	Total	C	H	O	0	0
			5	1	1	3		
34	a	1	Total	C	H	O	0	0
			5	1	1	3		

- Molecule 35 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4$).



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

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



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

- Molecule 37 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	A	147	Total O 147 147	0	8
37	B	218	Total O 218 218	0	0
37	C	190	Total O 190 190	0	0
37	D	129	Total O 129 129	0	0
37	E	30	Total O 30 30	0	0
37	F	13	Total O 13 13	0	0
37	H	28	Total O 28 28	0	0
37	I	12	Total O 12 12	0	0
37	J	12	Total O 12 12	0	0
37	K	2	Total O 2 2	0	0
37	L	9	Total O 9 9	0	0
37	M	6	Total O 6 6	0	0
37	O	129	Total O 129 129	0	0
37	R	4	Total O 4 4	0	0
37	T	13	Total O 13 13	0	0
37	U	47	Total O 47 47	0	0
37	V	78	Total O 78 78	0	0
37	X	8	Total O 8 8	0	0
37	Y	5	Total O 5 5	0	0
37	Z	5	Total O 5 5	0	0
37	a	132	Total O 132 132	0	8

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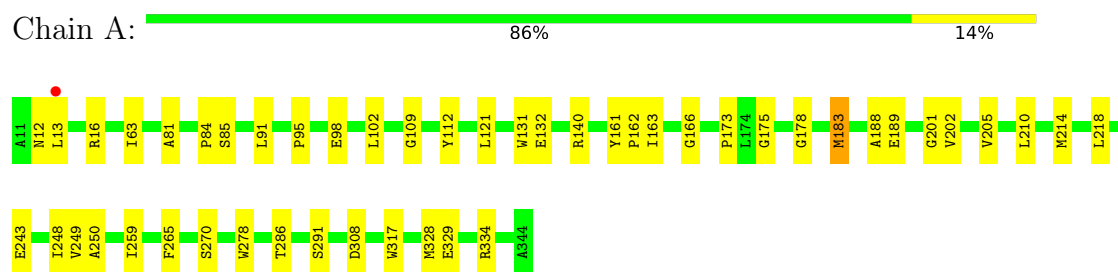
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	b	188	Total 188	O 188	0	0
37	c	155	Total 155	O 155	0	0
37	d	118	Total 118	O 118	0	0
37	e	19	Total 19	O 19	0	0
37	f	8	Total 8	O 8	0	0
37	h	19	Total 19	O 19	0	0
37	i	10	Total 10	O 10	0	0
37	j	10	Total 10	O 10	0	0
37	k	6	Total 6	O 6	0	0
37	l	13	Total 13	O 13	0	0
37	m	7	Total 7	O 7	0	0
37	o	109	Total 109	O 109	0	0
37	r	5	Total 5	O 5	0	0
37	t	14	Total 14	O 14	0	0
37	u	54	Total 54	O 54	0	0
37	v	59	Total 59	O 59	0	0
37	x	10	Total 10	O 10	0	0
37	y	4	Total 4	O 4	0	0
37	z	1	Total 1	O 1	0	0

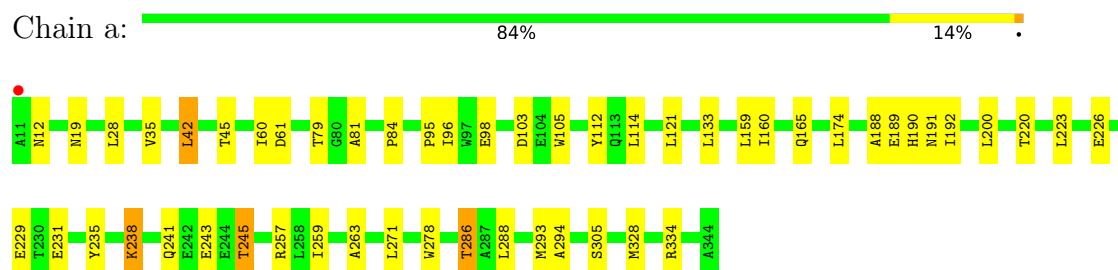
3 Residue-property plots

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

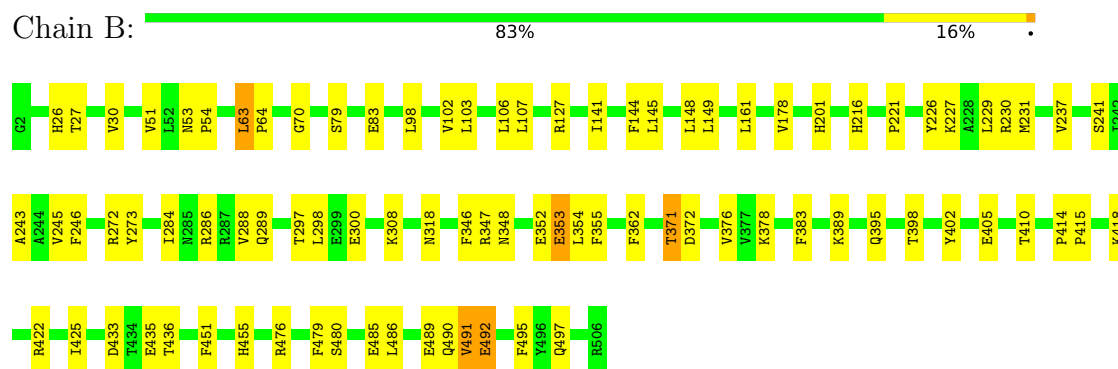
• Molecule 1: Photosystem II protein D1 1



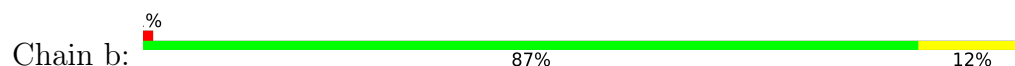
• Molecule 1: Photosystem II protein D1 1

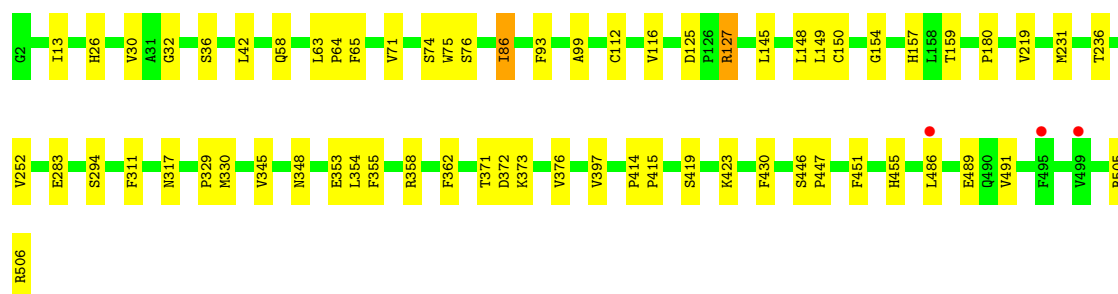


• Molecule 2: Photosystem II CP47 reaction center protein



• Molecule 2: Photosystem II CP47 reaction center protein





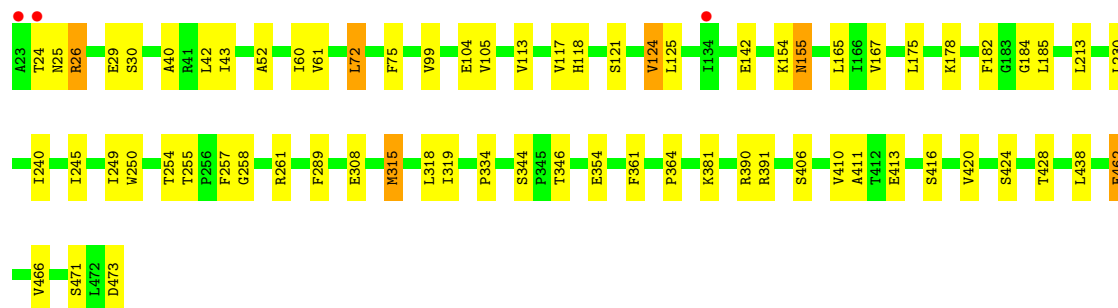
- Molecule 3: Photosystem II CP43 reaction center protein

Chain C: 84% 13% ..



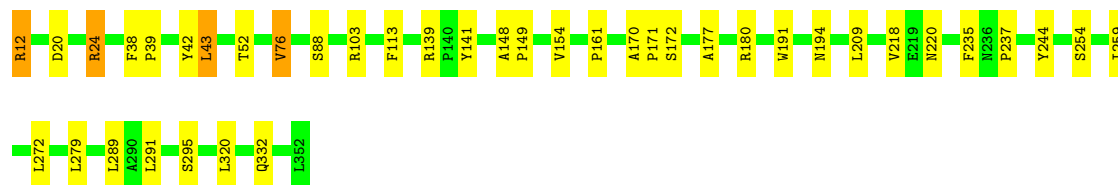
- Molecule 3: Photosystem II CP43 reaction center protein

Chain c: 84% 14% .



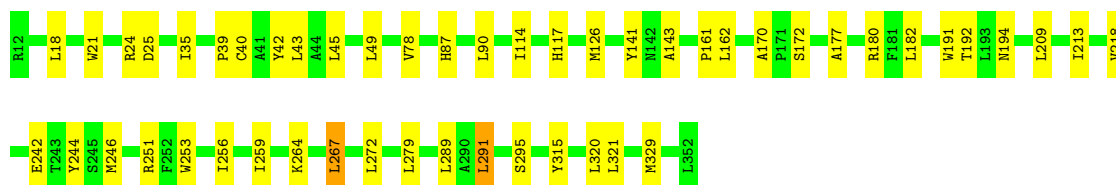
- Molecule 4: Photosystem II D2 protein

Chain D: 88% 11% .



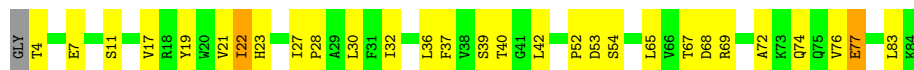
- Molecule 4: Photosystem II D2 protein

Chain d: 85% 14% .



• Molecule 5: Cytochrome b559 subunit alpha

Chain E: 63% 33% ..



• Molecule 5: Cytochrome b559 subunit alpha

Chain e: 68% 30% .



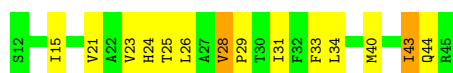
• Molecule 6: Cytochrome b559 subunit beta

Chain F: 85% 12% .



• Molecule 6: Cytochrome b559 subunit beta

Chain f: 59% 35% 6%



• Molecule 7: Photosystem II reaction center protein H

Chain H: 75% 22% .



• Molecule 7: Photosystem II reaction center protein H

Chain h: 2% 68% 26% ..



• Molecule 8: Photosystem II reaction center protein I

Chain I:  69% 28% .



- Molecule 8: Photosystem II reaction center protein I

Chain i:  78% 19% .



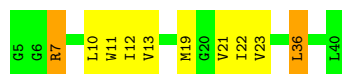
- Molecule 9: Photosystem II reaction center protein J

Chain J:  78% 22%



- Molecule 9: Photosystem II reaction center protein J

Chain j:  72% 22% 6%



- Molecule 10: Photosystem II reaction center protein K

Chain K:  3% 65% 30% 5%

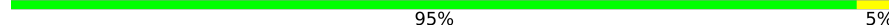


- Molecule 10: Photosystem II reaction center protein K

Chain k:  46% 46% 8%



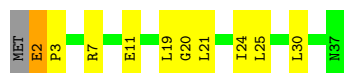
- Molecule 11: Photosystem II reaction center protein L

Chain L:  95% 5%



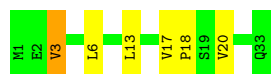
- Molecule 11: Photosystem II reaction center protein L

Chain l:  70% 24% . .



- Molecule 12: Photosystem II reaction center protein M

Chain M:  82% 15% .



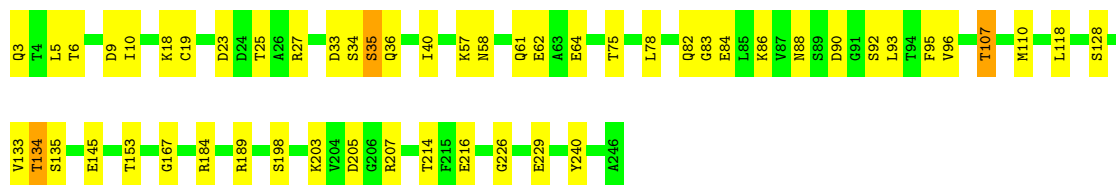
- Molecule 12: Photosystem II reaction center protein M

Chain m:  82% 15% .



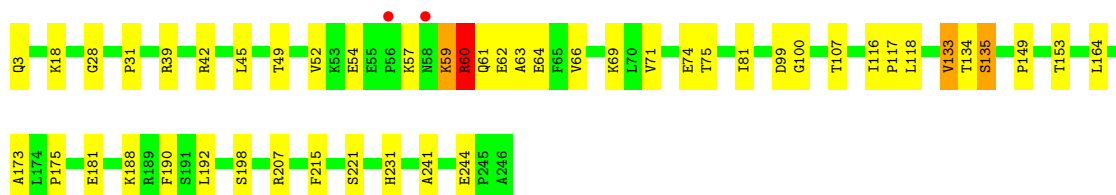
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:  78% 20% .



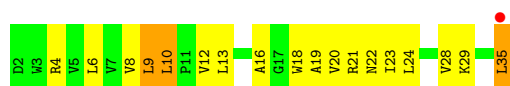
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:  80% 18% .



- Molecule 14: Photosystem II protein Y

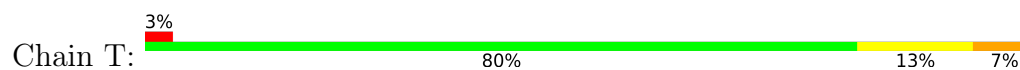
Chain R:  3% 47% 44% 9% .



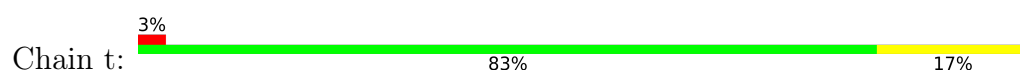
- Molecule 14: Photosystem II protein Y



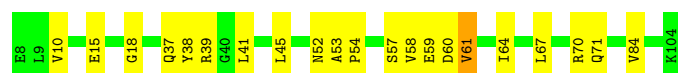
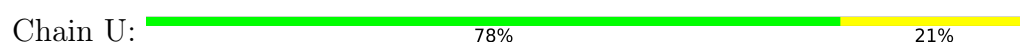
• Molecule 15: Photosystem II reaction center protein T



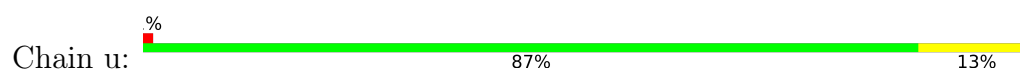
• Molecule 15: Photosystem II reaction center protein T



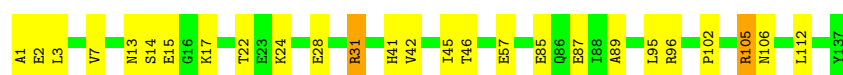
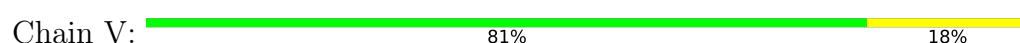
• Molecule 16: Photosystem II 12 kDa extrinsic protein



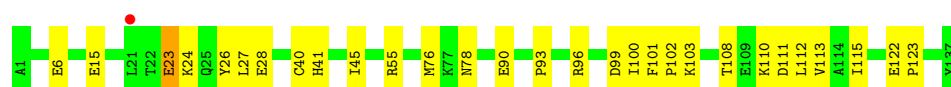
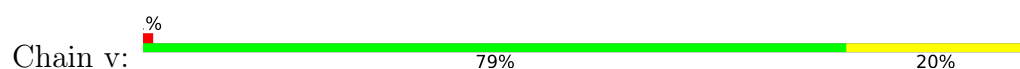
• Molecule 16: Photosystem II 12 kDa extrinsic protein



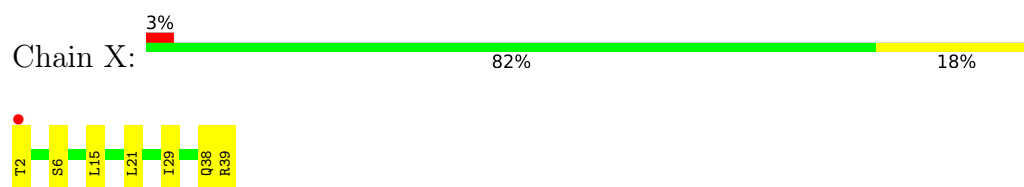
• Molecule 17: Cytochrome c-550



• Molecule 17: Cytochrome c-550



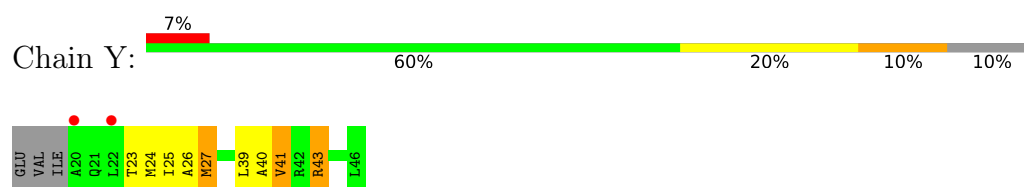
• Molecule 18: Photosystem II reaction center X protein



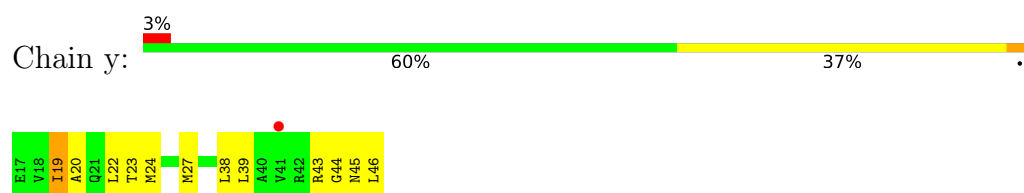
- Molecule 18: Photosystem II reaction center X protein



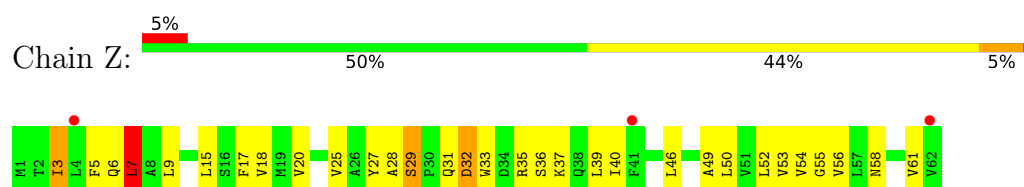
- Molecule 19: Photosystem II reaction center protein Ycf12



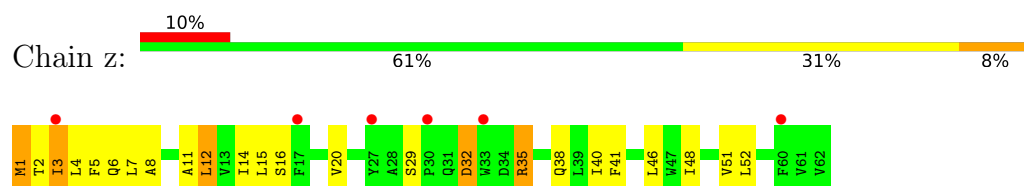
- Molecule 19: Photosystem II reaction center protein Ycf12



- Molecule 20: Photosystem II reaction center protein Z



- Molecule 20: Photosystem II reaction center protein Z



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	116.86Å 221.19Å 307.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.00 – 2.04 31.00 – 2.04	Depositor EDS
% Data completeness (in resolution range)	99.8 (31.00-2.04) 88.5 (31.00-2.04)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.59 (at 2.05Å)	Xtriage
Refinement program	PHENIX dev_svn	Depositor
R, R_{free}	0.186 , 0.248 0.187 , 0.249	Depositor DCC
R_{free} test set	4461 reflections (0.76%)	wwPDB-VP
Wilson B-factor (Å ²)	27.1	Xtriage
Anisotropy	0.337	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 60.3	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	0.96	EDS
Total number of atoms	105751	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.60	0/3179	0.69	0/4331
1	a	0.56	0/3176	0.68	0/4327
2	B	0.65	0/4160	0.73	0/5668
2	b	0.62	0/4118	0.71	0/5611
3	C	0.61	0/3593	0.69	1/4891 (0.0%)
3	c	0.56	0/3673	0.69	0/4998
4	D	0.68	0/2820	0.75	0/3840
4	d	0.63	0/2829	0.70	0/3852
5	E	0.51	0/684	0.67	0/935
5	e	0.44	0/683	0.60	0/932
6	F	0.53	0/284	0.66	0/387
6	f	0.44	0/284	0.68	0/387
7	H	0.64	0/520	0.72	0/709
7	h	0.53	0/511	0.69	0/697
8	I	0.65	0/293	0.68	0/396
8	i	0.67	0/293	0.78	0/396
9	J	0.50	0/263	0.65	0/356
9	j	0.47	0/261	0.60	0/353
10	K	0.43	0/314	0.60	0/427
10	k	0.42	0/303	0.54	0/416
11	L	0.68	0/311	0.75	0/422
11	l	0.67	0/303	0.74	0/412
12	M	0.61	0/249	0.71	0/341
12	m	0.63	0/244	0.73	0/334
13	O	0.57	0/1914	0.70	0/2596
13	o	0.58	0/1905	0.70	0/2583
14	R	0.39	0/277	0.57	0/380
14	r	0.31	0/233	0.48	0/323
15	T	0.70	0/257	0.78	0/349
15	t	0.67	0/255	0.73	0/346
16	U	0.56	0/785	0.64	0/1064

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	u	0.59	0/785	0.76	0/1064
17	V	0.59	0/1085	0.67	0/1473
17	v	0.53	0/1085	0.70	0/1473
18	X	0.50	0/284	0.63	0/384
18	x	0.39	0/284	0.47	0/384
19	Y	0.42	0/197	0.68	0/264
19	y	0.32	0/219	0.53	0/294
20	Z	0.44	0/490	0.59	0/669
20	z	0.37	0/488	0.57	0/666
All	All	0.59	0/43891	0.69	1/59730 (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
16	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(°)
3	C	396	MET	CG-SD-CE	-6.00	87.69	100.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	u	52	ASN	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3081	2937	2950	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a	3078	2928	2941	32	0
2	B	4004	3845	3864	54	0
2	b	3978	3811	3836	39	0
3	C	3476	3392	3405	43	0
3	c	3553	3464	3477	44	0
4	D	2726	2624	2632	35	0
4	d	2732	2630	2638	38	0
5	E	662	647	648	19	0
5	e	664	647	648	22	0
6	F	275	281	282	8	0
6	f	275	281	282	9	0
7	H	507	523	523	12	0
7	h	498	518	518	10	0
8	I	296	311	311	4	0
8	i	296	311	311	7	0
9	J	257	268	268	6	0
9	j	255	261	261	11	0
10	K	302	318	318	14	0
10	k	293	305	305	14	0
11	L	304	316	316	2	0
11	l	296	304	304	6	0
12	M	256	269	269	7	0
12	m	251	267	267	4	0
13	O	1880	1850	1852	33	0
13	o	1874	1844	1846	24	0
14	R	271	298	298	10	0
14	r	227	234	224	11	0
15	T	258	261	261	4	0
15	t	256	256	256	4	0
16	U	774	772	773	12	0
16	u	774	772	773	10	0
17	V	1064	1070	1073	16	0
17	v	1064	1070	1073	17	0
18	X	281	312	312	4	0
18	x	281	312	312	13	0
19	Y	196	208	217	6	0
19	y	218	241	241	6	0
20	Z	479	509	516	17	0
20	z	477	509	509	21	0
21	A	10	0	0	0	0
21	a	10	0	0	0	0
22	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	a	1	0	0	0	0
23	A	249	264	264	8	0
23	B	1035	1139	1139	24	0
23	C	839	922	922	14	0
23	D	130	144	144	2	0
23	a	260	288	288	12	0
23	b	970	1067	1067	27	0
23	c	839	919	919	15	0
23	d	130	144	144	2	0
23	h	65	72	72	3	0
24	A	128	148	148	3	0
24	a	64	74	74	2	0
24	d	64	74	74	4	0
25	A	40	56	56	1	0
25	B	120	168	168	7	0
25	C	120	168	168	4	0
25	D	40	56	56	4	0
25	H	40	56	56	4	0
25	T	40	56	56	5	0
25	Y	40	56	56	3	0
25	a	40	56	56	1	0
25	b	120	168	168	9	0
25	c	80	112	112	3	0
25	d	40	56	56	3	0
25	h	40	56	56	2	0
25	k	80	112	112	4	0
25	t	40	56	56	7	0
26	A	2	0	0	0	0
26	a	2	0	0	0	0
27	A	55	80	80	6	0
27	D	55	80	80	1	0
27	a	55	80	80	9	0
27	d	55	80	80	0	0
28	A	48	66	66	0	0
28	B	79	112	112	2	0
28	C	48	66	66	0	0
28	D	84	117	117	1	0
28	b	55	86	86	1	0
28	c	134	181	181	3	0
28	d	67	92	92	1	0
28	m	51	72	72	1	0
29	A	91	135	134	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	B	54	78	78	0	0
29	F	36	45	45	0	0
29	a	90	134	134	6	0
29	b	49	65	64	2	0
29	f	41	49	49	3	0
30	A	49	74	74	1	0
30	B	49	74	74	4	0
30	D	96	141	141	3	0
30	L	49	74	74	0	0
30	a	42	57	57	3	0
30	d	137	199	199	7	0
30	l	49	74	74	0	0
31	A	66	96	96	2	0
31	C	186	246	245	3	0
31	H	62	82	81	1	0
31	a	44	75	75	4	0
31	c	186	246	242	1	0
31	h	62	82	81	2	0
32	A	11	0	0	2	0
32	a	11	0	0	2	0
33	B	75	117	0	0	0
33	C	40	63	0	0	0
33	E	12	16	0	0	0
33	H	18	35	0	0	0
33	I	15	26	0	0	0
33	J	12	16	0	0	0
33	M	25	38	0	0	0
33	T	31	60	0	0	0
33	X	20	35	0	1	0
33	a	12	16	0	0	0
33	b	66	110	0	0	0
33	c	32	51	0	0	0
33	d	17	26	0	0	0
33	j	12	16	0	0	0
33	l	18	35	0	0	0
33	m	12	16	0	0	0
33	t	24	36	0	0	0
33	x	20	35	0	1	0
34	D	4	1	1	0	0
34	a	4	1	1	0	0
35	F	43	30	30	3	0
35	f	43	30	30	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	V	43	30	30	1	0
36	v	43	30	30	1	0
37	A	147	0	0	6	0
37	B	218	0	0	6	0
37	C	190	0	0	4	1
37	D	129	0	0	3	0
37	E	30	0	0	1	0
37	F	13	0	0	2	0
37	H	28	0	0	2	1
37	I	12	0	0	1	0
37	J	12	0	0	2	0
37	K	2	0	0	0	0
37	L	9	0	0	0	0
37	M	6	0	0	0	0
37	O	129	0	0	10	0
37	R	4	0	0	0	0
37	T	13	0	0	1	0
37	U	47	0	0	2	0
37	V	78	0	0	5	0
37	X	8	0	0	0	0
37	Y	5	0	0	0	0
37	Z	5	0	0	0	0
37	a	132	0	0	3	0
37	b	188	0	0	6	0
37	c	155	0	0	6	0
37	d	118	0	0	2	0
37	e	19	0	0	0	0
37	f	8	0	0	0	0
37	h	19	0	0	2	0
37	i	10	0	0	0	0
37	j	10	0	0	1	0
37	k	6	0	0	1	0
37	l	13	0	0	1	0
37	m	7	0	0	1	0
37	o	109	0	0	2	0
37	r	5	0	0	1	0
37	t	14	0	0	0	0
37	u	54	0	0	3	0
37	v	59	0	0	2	0
37	x	10	0	0	3	0
37	y	4	0	0	0	0
37	z	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	53281	52470	51848	751	1

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 751 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	37:B:701:HOH:O	1.79	1.00
13:O:216:GLU:OE2	37:O:301:HOH:O	1.83	0.97
4:D:332:GLN:NE2	37:D:501:HOH:O	1.98	0.96
18:x:39:ARG:O	37:x:201:HOH:O	1.86	0.94
9:J:15:THR:HG22	9:J:19:MET:HE3	1.51	0.93

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:C:607:HOH:O	37:H:214:HOH:O[4_557]	2.14	0.06

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	390/334 (117%)	380 (97%)	9 (2%)	1 (0%)	36	30
1	a	390/334 (117%)	383 (98%)	7 (2%)	0	100	100
2	B	508/505 (101%)	497 (98%)	11 (2%)	0	100	100
2	b	503/505 (100%)	491 (98%)	11 (2%)	1 (0%)	43	37
3	C	447/451 (99%)	435 (97%)	10 (2%)	2 (0%)	30	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	c	457/451 (101%)	439 (96%)	17 (4%)	1 (0%)	43	37
4	D	339/341 (99%)	329 (97%)	10 (3%)	0	100	100
4	d	340/341 (100%)	329 (97%)	11 (3%)	0	100	100
5	E	80/82 (98%)	78 (98%)	2 (2%)	0	100	100
5	e	80/82 (98%)	79 (99%)	1 (1%)	0	100	100
6	F	32/34 (94%)	32 (100%)	0	0	100	100
6	f	32/34 (94%)	32 (100%)	0	0	100	100
7	H	63/65 (97%)	58 (92%)	5 (8%)	0	100	100
7	h	61/65 (94%)	57 (93%)	4 (7%)	0	100	100
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%)	32 (94%)	1 (3%)	1 (3%)	3	0
9	j	34/36 (94%)	32 (94%)	2 (6%)	0	100	100
10	K	35/37 (95%)	33 (94%)	1 (3%)	1 (3%)	3	0
10	k	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	34/37 (92%)	34 (100%)	0	0	100	100
12	M	31/33 (94%)	30 (97%)	1 (3%)	0	100	100
12	m	30/33 (91%)	30 (100%)	0	0	100	100
13	O	243/244 (100%)	226 (93%)	16 (7%)	1 (0%)	30	22
13	o	242/244 (99%)	232 (96%)	8 (3%)	2 (1%)	16	9
14	R	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
14	r	29/34 (85%)	23 (79%)	5 (17%)	1 (3%)	3	0
15	T	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
15	t	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
16	U	95/97 (98%)	92 (97%)	3 (3%)	0	100	100
16	u	95/97 (98%)	91 (96%)	4 (4%)	0	100	100
17	V	135/137 (98%)	131 (97%)	4 (3%)	0	100	100
17	v	135/137 (98%)	127 (94%)	8 (6%)	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	Y	25/30 (83%)	17 (68%)	6 (24%)	2 (8%)	1	0
19	y	28/30 (93%)	25 (89%)	2 (7%)	1 (4%)	2	0
20	Z	60/62 (97%)	55 (92%)	3 (5%)	2 (3%)	3	0
20	z	60/62 (97%)	50 (83%)	9 (15%)	1 (2%)	7	2
All	All	5365/5326 (101%)	5165 (96%)	183 (3%)	17 (0%)	36	30

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
10	K	16	ALA
13	O	62	GLU
19	Y	41	VAL
19	Y	43	ARG

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	319/270 (118%)	309 (97%)	10 (3%)	35	30
1	a	318/270 (118%)	304 (96%)	14 (4%)	25	19
2	B	407/403 (101%)	382 (94%)	25 (6%)	17	10
2	b	402/403 (100%)	390 (97%)	12 (3%)	36	32
3	C	351/352 (100%)	342 (97%)	9 (3%)	40	37
3	c	360/352 (102%)	338 (94%)	22 (6%)	17	10
4	D	277/276 (100%)	271 (98%)	6 (2%)	45	44
4	d	278/276 (101%)	270 (97%)	8 (3%)	37	33
5	E	72/72 (100%)	61 (85%)	11 (15%)	3	0
5	e	71/72 (99%)	63 (89%)	8 (11%)	5	1
6	F	28/28 (100%)	27 (96%)	1 (4%)	31	26
6	f	28/28 (100%)	23 (82%)	5 (18%)	2	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	H	53/54 (98%)	50 (94%)	3 (6%)	18	11
7	h	53/54 (98%)	48 (91%)	5 (9%)	8	3
8	I	32/32 (100%)	27 (84%)	5 (16%)	2	0
8	i	32/32 (100%)	31 (97%)	1 (3%)	35	30
9	J	24/24 (100%)	23 (96%)	1 (4%)	26	20
9	j	23/24 (96%)	20 (87%)	3 (13%)	4	1
10	K	31/30 (103%)	29 (94%)	2 (6%)	15	9
10	k	30/30 (100%)	22 (73%)	8 (27%)	0	0
11	L	35/35 (100%)	35 (100%)	0	100	100
11	l	34/35 (97%)	30 (88%)	4 (12%)	5	1
12	M	28/29 (97%)	26 (93%)	2 (7%)	13	7
12	m	28/29 (97%)	27 (96%)	1 (4%)	31	26
13	O	208/207 (100%)	195 (94%)	13 (6%)	16	9
13	o	207/207 (100%)	196 (95%)	11 (5%)	20	13
14	R	28/29 (97%)	21 (75%)	7 (25%)	0	0
14	r	19/29 (66%)	14 (74%)	5 (26%)	0	0
15	T	26/26 (100%)	22 (85%)	4 (15%)	2	0
15	t	25/26 (96%)	25 (100%)	0	100	100
16	U	84/84 (100%)	79 (94%)	5 (6%)	17	10
16	u	84/84 (100%)	84 (100%)	0	100	100
17	V	117/117 (100%)	109 (93%)	8 (7%)	14	8
17	v	117/117 (100%)	112 (96%)	5 (4%)	26	20
18	X	31/31 (100%)	29 (94%)	2 (6%)	15	9
18	x	31/31 (100%)	29 (94%)	2 (6%)	15	9
19	Y	19/23 (83%)	16 (84%)	3 (16%)	2	0
19	y	22/23 (96%)	17 (77%)	5 (23%)	1	0
20	Z	52/52 (100%)	41 (79%)	11 (21%)	1	0
20	z	51/52 (98%)	41 (80%)	10 (20%)	1	0
All	All	4435/4348 (102%)	4178 (94%)	257 (6%)	18	11

5 of 257 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
14	r	6	LEU
17	v	24	LYS
15	T	25	GLU
14	R	35	LEU
19	y	22	LEU

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

Mol	Chain	Res	Type
18	X	38	GLN
4	d	250	ASN
20	Z	6	GLN
13	o	58	ASN
3	c	322	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	FME	I	1	8	8,9,10	0.90	0	8,9,11	1.51	2 (25%)
15	FME	t	1	15	8,9,10	1.16	1 (12%)	8,9,11	1.07	0
15	FME	T	1	15	8,9,10	1.21	1 (12%)	8,9,11	1.87	3 (37%)
12	FME	m	1	12	8,9,10	0.90	0	8,9,11	0.96	1 (12%)
8	FME	i	1	8	8,9,10	1.07	0	8,9,11	1.52	2 (25%)
12	FME	M	1	12	8,9,10	1.00	0	8,9,11	0.73	0

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

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	FME	I	1	8	-	2/7/9/11	-
15	FME	t	1	15	-	1/7/9/11	-
15	FME	T	1	15	-	1/7/9/11	-
12	FME	m	1	12	-	0/7/9/11	-
8	FME	i	1	8	-	1/7/9/11	-
12	FME	M	1	12	-	1/7/9/11	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	t	1	FME	CA-N	-2.75	1.42	1.46
15	T	1	FME	CA-N	-2.10	1.43	1.46

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	i	1	FME	C-CA-N	2.83	114.96	109.50
15	T	1	FME	CA-N-CN	-2.81	118.50	122.82
15	T	1	FME	C-CA-N	2.71	114.72	109.50
8	I	1	FME	C-CA-N	2.59	114.50	109.50
15	T	1	FME	O1-CN-N	-2.25	119.50	125.32

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	T	1	FME	CB-CG-SD-CE
15	t	1	FME	CB-CG-SD-CE
8	I	1	FME	C-CA-CB-CG
12	M	1	FME	CA-CB-CG-SD
8	I	1	FME	CA-CB-CG-SD

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 188 ligands modelled in this entry, 6 are monoatomic and 31 are unknown - leaving 151 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	SQD	f	101	-	39,41,54	1.16	4 (10%)	49,52,65	1.56	9 (18%)
23	CLA	C	504	37	63,67,73	1.38	9 (14%)	74,105,113	1.32	10 (13%)
25	BCR	D	404	-	41,41,41	1.19	2 (4%)	56,56,56	1.19	6 (10%)
31	DGD	C	516	-	63,63,67	1.30	10 (15%)	77,77,81	1.32	8 (10%)
23	CLA	c	513	-	69,73,73	1.41	10 (14%)	82,113,113	1.03	5 (6%)
23	CLA	c	511	3	69,73,73	1.48	9 (13%)	82,113,113	1.31	9 (10%)
23	CLA	B	602	-	69,73,73	1.20	8 (11%)	82,113,113	1.24	10 (12%)
23	CLA	b	608	-	69,73,73	1.23	6 (8%)	82,113,113	1.35	12 (14%)
31	DGD	h	103	-	63,63,67	1.02	2 (3%)	77,77,81	1.42	9 (11%)
28	LMG	D	409	-	31,31,55	1.47	5 (16%)	33,33,63	1.12	4 (12%)
23	CLA	b	612	-	69,73,73	1.18	8 (11%)	82,113,113	1.46	14 (17%)
30	LHG	D	408	-	46,46,48	1.08	3 (6%)	49,52,54	1.38	5 (10%)
36	HEC	v	201	17	46,50,50	1.87	5 (10%)	58,82,82	1.53	6 (10%)
30	LHG	d	407	-	48,48,48	0.96	2 (4%)	51,54,54	1.17	3 (5%)
23	CLA	b	615	-	69,73,73	1.73	10 (14%)	82,113,113	1.49	13 (15%)
28	LMG	D	405	-	51,51,55	1.11	3 (5%)	59,59,63	1.18	5 (8%)
29	SQD	A	614	-	50,52,54	1.09	4 (8%)	60,63,65	2.36	14 (23%)
23	CLA	b	602	-	69,73,73	1.19	8 (11%)	82,113,113	1.52	10 (12%)
25	BCR	A	608	-	41,41,41	1.20	2 (4%)	56,56,56	1.48	11 (19%)
25	BCR	C	514	-	41,41,41	1.23	2 (4%)	56,56,56	1.41	9 (16%)
25	BCR	C	520	-	41,41,41	1.11	4 (9%)	56,56,56	1.22	4 (7%)
31	DGD	H	102	-	63,63,67	1.54	10 (15%)	77,77,81	1.55	13 (16%)
23	CLA	B	616	-	64,68,73	1.53	9 (14%)	76,107,113	1.43	10 (13%)
23	CLA	d	403	-	69,73,73	1.15	6 (8%)	82,113,113	1.25	10 (12%)
21	OEX	a	601[A]	37,1,3	0,15,15	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	B	610	37	69,73,73	1.28	9 (13%)	82,113,113	1.54	11 (13%)
23	CLA	C	507	37	69,73,73	1.12	6 (8%)	82,113,113	1.50	11 (13%)
23	CLA	C	512	-	69,73,73	1.64	11 (15%)	82,113,113	1.36	9 (10%)
35	HEM	F	102	5,6	50,50,50	1.40	8 (16%)	67,82,82	1.17	6 (8%)
23	CLA	A	613	37	69,73,73	1.42	10 (14%)	82,113,113	1.36	8 (9%)
25	BCR	B	617	-	41,41,41	1.20	3 (7%)	56,56,56	1.29	5 (8%)
31	DGD	c	517	-	63,63,67	1.31	11 (17%)	77,77,81	1.45	12 (15%)
31	DGD	C	518	-	63,63,67	0.92	3 (4%)	77,77,81	1.38	9 (11%)
23	CLA	A	607	-	58,62,73	1.62	9 (15%)	68,99,113	1.64	11 (16%)
25	BCR	d	404	-	41,41,41	1.32	3 (7%)	56,56,56	1.27	6 (10%)
23	CLA	C	505	-	69,73,73	1.12	5 (7%)	82,113,113	1.28	10 (12%)
23	CLA	d	402	-	69,73,73	1.41	9 (13%)	82,113,113	1.31	6 (7%)
30	LHG	A	615	-	48,48,48	0.97	3 (6%)	51,54,54	1.17	3 (5%)
25	BCR	c	515	-	41,41,41	1.38	4 (9%)	56,56,56	1.54	14 (25%)
25	BCR	a	607	-	41,41,41	1.22	4 (9%)	56,56,56	1.41	8 (14%)
23	CLA	b	616	-	64,68,73	1.19	8 (12%)	76,107,113	1.47	10 (13%)
30	LHG	a	614	-	41,41,48	0.81	0	44,47,54	1.31	4 (9%)
29	SQD	a	613	-	52,54,54	0.94	3 (5%)	62,65,65	1.89	12 (19%)
27	PL9	A	611	-	55,55,55	0.98	2 (3%)	68,69,69	1.60	13 (19%)
28	LMG	B	622	-	26,26,55	0.91	2 (7%)	26,26,63	1.11	2 (7%)
23	CLA	B	615	-	69,73,73	1.39	12 (17%)	82,113,113	1.37	12 (14%)
23	CLA	c	512	-	69,73,73	1.30	9 (13%)	82,113,113	1.39	9 (10%)
25	BCR	k	102	-	41,41,41	1.01	2 (4%)	56,56,56	1.30	7 (12%)
28	LMG	m	101	-	51,51,55	0.85	2 (3%)	59,59,63	1.57	12 (20%)
23	CLA	a	612	37	69,73,73	1.48	10 (14%)	82,113,113	1.47	9 (10%)
23	CLA	B	609	-	69,73,73	1.42	9 (13%)	82,113,113	1.40	6 (7%)
28	LMG	b	621	-	55,55,55	0.90	2 (3%)	63,63,63	1.39	8 (12%)
23	CLA	a	604	37	69,73,73	1.40	10 (14%)	82,113,113	1.39	12 (14%)
23	CLA	C	511	3	69,73,73	1.64	7 (10%)	82,113,113	1.42	6 (7%)
28	LMG	B	620	-	51,51,55	1.11	4 (7%)	59,59,63	1.49	11 (18%)
29	SQD	b	601	-	47,49,54	0.97	4 (8%)	57,60,65	2.07	14 (24%)
23	CLA	b	604	-	69,73,73	1.20	9 (13%)	82,113,113	1.52	11 (13%)
31	DGD	a	616	-	43,43,67	1.34	4 (9%)	45,45,81	1.43	5 (11%)
23	CLA	D	402	-	69,73,73	1.31	8 (11%)	82,113,113	1.23	8 (9%)
23	CLA	B	601	37	69,73,73	1.71	9 (13%)	82,113,113	1.71	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	LMG	C	519	-	48,48,55	1.20	5 (10%)	56,56,63	1.29	4 (7%)
23	CLA	C	506	-	69,73,73	1.66	8 (11%)	82,113,113	1.16	8 (9%)
23	CLA	B	607	37	69,73,73	1.68	11 (15%)	82,113,113	1.17	6 (7%)
30	LHG	L	101	-	48,48,48	0.91	1 (2%)	51,54,54	1.13	3 (5%)
25	BCR	B	619	-	41,41,41	1.29	3 (7%)	56,56,56	1.49	9 (16%)
24	PHO	A	606	-	58,69,69	1.96	11 (18%)	55,99,99	1.28	5 (9%)
27	PL9	D	407	-	55,55,55	1.76	12 (21%)	68,69,69	1.52	12 (17%)
31	DGD	c	518	-	63,63,67	1.11	7 (11%)	77,77,81	1.44	13 (16%)
25	BCR	c	514	-	41,41,41	1.18	3 (7%)	56,56,56	1.37	10 (17%)
27	PL9	d	408	-	55,55,55	1.57	9 (16%)	68,69,69	1.75	15 (22%)
32	OEY	a	618[B]	37,1,3	0,16,16	-	-	-	-	-
31	DGD	A	617	-	67,67,67	1.46	10 (14%)	81,81,81	1.44	12 (14%)
23	CLA	C	508	-	69,73,73	1.15	7 (10%)	82,113,113	1.33	9 (10%)
23	CLA	B	614	-	69,73,73	1.43	7 (10%)	82,113,113	1.44	11 (13%)
29	SQD	a	615	-	35,35,54	1.14	2 (5%)	37,37,65	1.46	7 (18%)
23	CLA	b	607	37	69,73,73	1.15	6 (8%)	82,113,113	1.34	10 (12%)
25	BCR	T	101	-	41,41,41	1.22	5 (12%)	56,56,56	1.41	8 (14%)
23	CLA	h	101	37	69,73,73	1.42	10 (14%)	82,113,113	1.47	13 (15%)
23	CLA	C	502	-	69,73,73	1.33	6 (8%)	82,113,113	1.26	6 (7%)
30	LHG	D	406	-	48,48,48	0.88	1 (2%)	51,54,54	1.30	8 (15%)
23	CLA	B	604	-	69,73,73	1.41	7 (10%)	82,113,113	1.69	8 (9%)
23	CLA	b	610	37	69,73,73	1.26	11 (15%)	82,113,113	1.25	7 (8%)
36	HEC	V	201	17	46,50,50	1.94	10 (21%)	58,82,82	1.35	3 (5%)
23	CLA	b	611	-	69,73,73	1.23	9 (13%)	82,113,113	1.55	19 (23%)
25	BCR	b	617	-	41,41,41	1.17	3 (7%)	56,56,56	1.43	7 (12%)
30	LHG	d	405	-	48,48,48	0.69	0	51,54,54	1.29	4 (7%)
32	OEY	A	618[B]	37,1,3	0,16,16	-	-	-	-	-
23	CLA	b	614	-	69,73,73	1.18	9 (13%)	82,113,113	1.42	12 (14%)
25	BCR	b	619	-	41,41,41	1.20	3 (7%)	56,56,56	1.28	6 (10%)
23	CLA	B	606	-	69,73,73	1.55	10 (14%)	82,113,113	1.55	13 (15%)
29	SQD	A	616	-	38,38,54	1.04	3 (7%)	40,40,65	1.54	3 (7%)
31	DGD	c	516	-	63,63,67	1.17	7 (11%)	77,77,81	1.35	11 (14%)
30	LHG	B	623	-	48,48,48	0.89	1 (2%)	51,54,54	1.46	9 (17%)
28	LMG	A	612	-	48,48,55	1.02	3 (6%)	56,56,63	1.43	11 (19%)
23	CLA	c	505	-	69,73,73	1.17	9 (13%)	82,113,113	1.43	13 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	BCR	B	618	-	41,41,41	1.26	3 (7%)	56,56,56	1.24	6 (10%)
23	CLA	c	510	-	69,73,73	1.23	10 (14%)	82,113,113	1.39	10 (12%)
23	CLA	A	604	37	69,73,73	1.19	5 (7%)	82,113,113	1.32	10 (12%)
24	PHO	d	401	-	58,69,69	2.14	10 (17%)	55,99,99	1.74	13 (23%)
23	CLA	B	603	-	69,73,73	1.33	9 (13%)	82,113,113	1.44	11 (13%)
23	CLA	b	609	-	69,73,73	1.32	8 (11%)	82,113,113	1.32	10 (12%)
23	CLA	C	503	-	69,73,73	1.47	10 (14%)	82,113,113	1.55	13 (15%)
24	PHO	A	605	-	58,69,69	2.00	10 (17%)	55,99,99	1.96	8 (14%)
23	CLA	B	605	-	69,73,73	1.34	7 (10%)	82,113,113	1.58	16 (19%)
23	CLA	B	611	-	69,73,73	1.36	10 (14%)	82,113,113	1.40	11 (13%)
23	CLA	c	503	-	69,73,73	1.33	10 (14%)	82,113,113	1.42	12 (14%)
30	LHG	l	101	-	48,48,48	0.77	2 (4%)	51,54,54	1.33	8 (15%)
23	CLA	b	613	-	69,73,73	1.39	8 (11%)	82,113,113	1.53	14 (17%)
27	PL9	a	611	-	55,55,55	1.13	5 (9%)	68,69,69	1.58	13 (19%)
28	LMG	d	406	-	44,44,55	1.27	4 (9%)	52,52,63	1.34	6 (11%)
23	CLA	b	603	-	69,73,73	1.32	8 (11%)	82,113,113	1.42	12 (14%)
25	BCR	h	102	-	41,41,41	1.19	2 (4%)	56,56,56	1.48	11 (19%)
23	CLA	C	501	-	69,73,73	1.46	11 (15%)	82,113,113	1.54	12 (14%)
28	LMG	d	410	-	21,21,55	0.75	0	20,20,63	1.03	0
23	CLA	c	509	-	69,73,73	1.14	5 (7%)	82,113,113	1.45	12 (14%)
23	CLA	C	509	-	69,73,73	1.45	8 (11%)	82,113,113	1.18	6 (7%)
29	SQD	B	624	-	52,54,54	0.92	3 (5%)	62,65,65	1.72	13 (20%)
23	CLA	b	605	-	69,73,73	1.24	8 (11%)	82,113,113	1.67	16 (19%)
34	BCT	a	610	22	3,3,3	1.31	0	2,3,3	2.62	1 (50%)
23	CLA	c	508	-	68,72,73	1.32	10 (14%)	80,111,113	1.18	10 (12%)
25	BCR	k	101	-	41,41,41	1.07	3 (7%)	56,56,56	1.10	4 (7%)
35	HEM	f	102	5,6	50,50,50	1.40	6 (12%)	67,82,82	1.14	4 (5%)
23	CLA	c	504	37	64,68,73	1.33	6 (9%)	76,107,113	1.30	8 (10%)
23	CLA	A	603	-	69,73,73	1.37	14 (20%)	82,113,113	1.21	9 (10%)
25	BCR	H	101	-	41,41,41	1.15	2 (4%)	56,56,56	1.50	9 (16%)
25	BCR	Y	101	-	41,41,41	1.15	2 (4%)	56,56,56	1.29	8 (14%)
34	BCT	D	401	22	3,3,3	1.04	0	2,3,3	3.28	2 (100%)
28	LMG	c	522	-	49,49,55	1.04	2 (4%)	57,57,63	1.32	4 (7%)
25	BCR	t	101	-	41,41,41	1.17	4 (9%)	56,56,56	1.60	13 (23%)
23	CLA	a	606	-	69,73,73	1.44	13 (18%)	82,113,113	1.50	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	C	513	-	69,73,73	1.29	9 (13%)	82,113,113	1.32	7 (8%)
29	SQD	F	101	-	34,36,54	1.07	3 (8%)	42,45,65	1.86	10 (23%)
31	DGD	C	517	-	63,63,67	1.24	6 (9%)	77,77,81	1.58	12 (15%)
23	CLA	c	502	-	69,73,73	1.08	6 (8%)	82,113,113	1.64	12 (14%)
23	CLA	B	608	-	69,73,73	1.03	3 (4%)	82,113,113	1.43	8 (9%)
23	CLA	b	606	-	69,73,73	1.47	8 (11%)	82,113,113	1.44	7 (8%)
23	CLA	a	603	-	69,73,73	1.44	8 (11%)	82,113,113	1.60	11 (13%)
28	LMG	c	521	-	48,48,55	1.18	5 (10%)	56,56,63	1.34	6 (10%)
23	CLA	c	501	-	69,73,73	1.36	10 (14%)	82,113,113	1.69	17 (20%)
23	CLA	B	613	-	69,73,73	1.27	8 (11%)	82,113,113	1.34	9 (10%)
25	BCR	b	618	-	41,41,41	1.39	4 (9%)	56,56,56	1.31	10 (17%)
23	CLA	c	507	37	69,73,73	1.29	10 (14%)	82,113,113	1.60	12 (14%)
21	OEX	A	601[A]	37,1,3	0,15,15	-	-	-	-	-
25	BCR	C	515	-	41,41,41	1.30	4 (9%)	56,56,56	1.20	6 (10%)
24	PHO	a	605	-	58,69,69	2.04	12 (20%)	55,99,99	1.56	6 (10%)
23	CLA	D	403	-	69,73,73	1.65	9 (13%)	82,113,113	1.15	11 (13%)
23	CLA	C	510	-	69,73,73	1.26	13 (18%)	82,113,113	1.41	9 (10%)
30	LHG	d	409	-	38,38,48	0.98	1 (2%)	41,44,54	1.27	4 (9%)
28	LMG	c	519	-	37,37,55	1.21	3 (8%)	45,45,63	1.22	4 (8%)
23	CLA	B	612	-	69,73,73	1.15	5 (7%)	82,113,113	1.38	8 (9%)
23	CLA	c	506	-	69,73,73	1.83	9 (13%)	82,113,113	1.38	11 (13%)

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	SQD	f	101	-	-	18/36/56/69	0/1/1/1
23	CLA	C	504	37	1/1/18/20	8/32/108/115	-
25	BCR	D	404	-	-	7/29/63/63	0/2/2/2
31	DGD	C	516	-	-	18/51/91/95	0/2/2/2
23	CLA	c	513	-	1/1/20/20	4/39/115/115	-
23	CLA	c	511	3	1/1/20/20	10/39/115/115	-
23	CLA	B	602	-	1/1/20/20	4/39/115/115	-
23	CLA	b	608	-	-	8/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	DGD	h	103	-	-	18/51/91/95	0/2/2/2
28	LMG	D	409	-	-	17/33/33/70	-
23	CLA	b	612	-	1/1/20/20	6/39/115/115	-
30	LHG	D	408	-	-	20/51/51/53	-
36	HEC	v	201	17	-	6/14/54/54	-
30	LHG	d	407	-	-	19/53/53/53	-
23	CLA	b	615	-	1/1/20/20	8/39/115/115	-
28	LMG	D	405	-	-	17/46/66/70	0/1/1/1
29	SQD	A	614	-	-	23/47/67/69	0/1/1/1
23	CLA	b	602	-	1/1/20/20	6/39/115/115	-
25	BCR	A	608	-	-	6/29/63/63	0/2/2/2
25	BCR	C	514	-	-	7/29/63/63	0/2/2/2
25	BCR	C	520	-	-	7/29/63/63	0/2/2/2
31	DGD	H	102	-	-	15/51/91/95	0/2/2/2
23	CLA	B	616	-	1/1/19/20	9/33/109/115	-
23	CLA	d	403	-	-	6/39/115/115	-
23	CLA	B	610	37	1/1/20/20	5/39/115/115	-
23	CLA	C	507	37	1/1/20/20	10/39/115/115	-
23	CLA	C	512	-	1/1/20/20	14/39/115/115	-
35	HEM	F	102	5,6	-	2/14/54/54	-
23	CLA	A	613	37	-	2/39/115/115	-
25	BCR	B	617	-	-	5/29/63/63	0/2/2/2
31	DGD	c	517	-	-	20/51/91/95	0/2/2/2
31	DGD	C	518	-	-	17/51/91/95	0/2/2/2
23	CLA	A	607	-	1/1/17/20	3/26/102/115	-
25	BCR	d	404	-	-	8/29/63/63	0/2/2/2
23	CLA	C	505	-	1/1/20/20	11/39/115/115	-
23	CLA	d	402	-	1/1/20/20	11/39/115/115	-
30	LHG	A	615	-	-	27/53/53/53	-
25	BCR	c	515	-	-	4/29/63/63	0/2/2/2
25	BCR	a	607	-	-	3/29/63/63	0/2/2/2
23	CLA	b	616	-	1/1/19/20	6/33/109/115	-
30	LHG	a	614	-	-	28/46/46/53	-
29	SQD	a	613	-	-	25/49/69/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	PL9	A	611	-	-	28/53/73/73	0/1/1/1
28	LMG	B	622	-	-	11/22/22/70	-
23	CLA	B	615	-	1/1/20/20	11/39/115/115	-
23	CLA	c	512	-	1/1/20/20	15/39/115/115	-
25	BCR	k	102	-	-	3/29/63/63	0/2/2/2
28	LMG	m	101	-	-	20/46/66/70	0/1/1/1
23	CLA	a	612	37	1/1/20/20	1/39/115/115	-
23	CLA	B	609	-	-	5/39/115/115	-
28	LMG	b	621	-	-	16/50/70/70	0/1/1/1
23	CLA	a	604	37	-	10/39/115/115	-
23	CLA	C	511	3	1/1/20/20	7/39/115/115	-
28	LMG	B	620	-	-	22/46/66/70	0/1/1/1
29	SQD	b	601	-	-	18/44/64/69	0/1/1/1
23	CLA	b	604	-	1/1/20/20	10/39/115/115	-
31	DGD	a	616	-	-	26/45/45/95	-
23	CLA	D	402	-	-	6/39/115/115	-
23	CLA	B	601	37	1/1/20/20	16/39/115/115	-
28	LMG	C	519	-	-	15/43/63/70	0/1/1/1
23	CLA	C	506	-	-	11/39/115/115	-
23	CLA	B	607	37	1/1/20/20	11/39/115/115	-
30	LHG	L	101	-	-	18/53/53/53	-
25	BCR	B	619	-	-	8/29/63/63	0/2/2/2
24	PHO	A	606	-	-	4/37/103/103	0/5/6/6
27	PL9	D	407	-	-	11/53/73/73	0/1/1/1
31	DGD	c	518	-	-	17/51/91/95	0/2/2/2
25	BCR	c	514	-	-	16/29/63/63	0/2/2/2
27	PL9	d	408	-	-	20/53/73/73	0/1/1/1
31	DGD	A	617	-	-	24/55/95/95	0/2/2/2
23	CLA	C	508	-	-	9/39/115/115	-
23	CLA	B	614	-	1/1/20/20	14/39/115/115	-
29	SQD	a	615	-	-	18/37/37/69	-
23	CLA	b	607	37	1/1/20/20	12/39/115/115	-
25	BCR	T	101	-	-	10/29/63/63	0/2/2/2
23	CLA	h	101	37	1/1/20/20	19/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	C	502	-	1/1/20/20	7/39/115/115	-
30	LHG	D	406	-	-	20/53/53/53	-
23	CLA	B	604	-	1/1/20/20	7/39/115/115	-
23	CLA	b	610	37	1/1/20/20	8/39/115/115	-
36	HEC	V	201	17	-	6/14/54/54	-
23	CLA	b	611	-	1/1/20/20	6/39/115/115	-
25	BCR	b	617	-	-	0/29/63/63	0/2/2/2
30	LHG	d	405	-	-	24/53/53/53	-
23	CLA	b	614	-	1/1/20/20	16/39/115/115	-
25	BCR	b	619	-	-	4/29/63/63	0/2/2/2
23	CLA	B	606	-	1/1/20/20	7/39/115/115	-
29	SQD	A	616	-	-	17/39/39/69	-
31	DGD	c	516	-	-	26/51/91/95	0/2/2/2
30	LHG	B	623	-	-	15/53/53/53	-
28	LMG	A	612	-	-	21/43/63/70	0/1/1/1
23	CLA	c	505	-	1/1/20/20	8/39/115/115	-
25	BCR	B	618	-	-	5/29/63/63	0/2/2/2
23	CLA	c	510	-	1/1/20/20	12/39/115/115	-
23	CLA	A	604	37	-	6/39/115/115	-
24	PHO	d	401	-	-	7/37/103/103	0/5/6/6
23	CLA	B	603	-	1/1/20/20	14/39/115/115	-
23	CLA	b	609	-	1/1/20/20	13/39/115/115	-
23	CLA	C	503	-	1/1/20/20	3/39/115/115	-
24	PHO	A	605	-	-	5/37/103/103	0/5/6/6
23	CLA	B	605	-	-	10/39/115/115	-
23	CLA	B	611	-	-	8/39/115/115	-
23	CLA	c	503	-	1/1/20/20	7/39/115/115	-
30	LHG	l	101	-	-	19/53/53/53	-
23	CLA	b	613	-	1/1/20/20	8/39/115/115	-
27	PL9	a	611	-	-	25/53/73/73	0/1/1/1
28	LMG	d	406	-	-	13/39/59/70	0/1/1/1
23	CLA	b	603	-	1/1/20/20	8/39/115/115	-
25	BCR	h	102	-	-	11/29/63/63	0/2/2/2
23	CLA	C	501	-	1/1/20/20	4/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	LMG	d	410	-	-	10/17/17/70	-
23	CLA	c	509	-	1/1/20/20	12/39/115/115	-
23	CLA	C	509	-	1/1/20/20	14/39/115/115	-
29	SQD	B	624	-	-	23/49/69/69	0/1/1/1
23	CLA	b	605	-	1/1/20/20	5/39/115/115	-
23	CLA	c	508	-	1/1/19/20	9/38/114/115	-
25	BCR	k	101	-	-	9/29/63/63	0/2/2/2
35	HEM	f	102	5,6	-	3/14/54/54	-
23	CLA	c	504	37	1/1/19/20	8/33/109/115	-
23	CLA	A	603	-	1/1/20/20	2/39/115/115	-
25	BCR	H	101	-	-	6/29/63/63	0/2/2/2
25	BCR	Y	101	-	-	12/29/63/63	0/2/2/2
28	LMG	c	522	-	-	25/44/64/70	0/1/1/1
25	BCR	t	101	-	-	9/29/63/63	0/2/2/2
23	CLA	a	606	-	1/1/20/20	10/39/115/115	-
23	CLA	C	513	-	1/1/20/20	7/39/115/115	-
29	SQD	F	101	-	-	16/28/48/69	0/1/1/1
31	DGD	C	517	-	-	21/51/91/95	0/2/2/2
23	CLA	c	502	-	-	3/39/115/115	-
23	CLA	b	606	-	1/1/20/20	11/39/115/115	-
23	CLA	B	608	-	-	1/39/115/115	-
23	CLA	a	603	-	1/1/20/20	1/39/115/115	-
28	LMG	c	521	-	-	20/43/63/70	0/1/1/1
23	CLA	c	501	-	1/1/20/20	5/39/115/115	-
23	CLA	B	613	-	1/1/20/20	7/39/115/115	-
25	BCR	b	618	-	-	6/29/63/63	0/2/2/2
23	CLA	c	507	37	1/1/20/20	10/39/115/115	-
25	BCR	C	515	-	-	6/29/63/63	0/2/2/2
24	PHO	a	605	-	-	8/37/103/103	0/5/6/6
23	CLA	D	403	-	1/1/20/20	17/39/115/115	-
23	CLA	C	510	-	1/1/20/20	5/39/115/115	-
30	LHG	d	409	-	-	13/43/43/53	-
28	LMG	c	519	-	-	10/31/51/70	0/1/1/1
23	CLA	B	612	-	1/1/20/20	11/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	c	506	-	1/1/20/20	18/39/115/115	-

The worst 5 of 918 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	506	CLA	MG-ND	-10.99	1.84	2.05
23	b	615	CLA	MG-NA	9.73	2.29	2.06
24	d	401	PHO	C1B-C2B	9.70	1.50	1.39
23	C	511	CLA	MG-NA	9.42	2.28	2.06
24	a	605	PHO	C1B-C2B	9.27	1.49	1.39

The worst 5 of 1314 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	604	CLA	C4A-NA-C1A	10.98	111.69	106.68
29	A	614	SQD	O6-C1-C2	10.25	123.84	108.27
23	B	601	CLA	C4A-NA-C1A	10.00	111.24	106.68
29	b	601	SQD	O6-C1-C2	9.81	123.17	108.27
24	A	605	PHO	C4D-CHA-CBD	-9.67	103.82	108.45

5 of 57 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	A	603	CLA	ND
23	A	607	CLA	ND
23	B	601	CLA	ND
23	B	602	CLA	ND
23	B	603	CLA	ND

5 of 1653 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	B	601	CLA	CAD-CBD-CGD-O1D
23	B	601	CLA	CAD-CBD-CGD-O2D
23	B	614	CLA	C11-C12-C13-C14
23	B	615	CLA	C2B-C3B-CAB-CBB
23	B	615	CLA	C4B-C3B-CAB-CBB

There are no ring outliers.

116 monomers are involved in 229 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	f	101	SQD	3	0
23	C	504	CLA	1	0
25	D	404	BCR	4	0
23	c	513	CLA	1	0
23	c	511	CLA	2	0
23	B	602	CLA	3	0
31	h	103	DGD	2	0
23	b	612	CLA	2	0
30	D	408	LHG	1	0
36	v	201	HEC	1	0
30	d	407	LHG	2	0
23	b	615	CLA	4	0
28	D	405	LMG	1	0
23	b	602	CLA	1	0
25	A	608	BCR	1	0
25	C	514	BCR	2	0
31	H	102	DGD	1	0
23	B	616	CLA	2	0
23	d	403	CLA	1	0
23	B	610	CLA	2	0
23	C	512	CLA	1	0
35	F	102	HEM	3	0
23	A	613	CLA	2	0
25	B	617	BCR	2	0
31	C	518	DGD	1	0
25	d	404	BCR	3	0
23	C	505	CLA	2	0
23	d	402	CLA	1	0
30	A	615	LHG	1	0
25	c	515	BCR	3	0
25	a	607	BCR	1	0
23	b	616	CLA	4	0
30	a	614	LHG	3	0
29	a	613	SQD	3	0
27	A	611	PL9	6	0
23	B	615	CLA	3	0
23	c	512	CLA	1	0
25	k	102	BCR	1	0
28	m	101	LMG	1	0
23	a	612	CLA	2	0
23	B	609	CLA	4	0
28	b	621	LMG	1	0
23	C	511	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	B	620	LMG	2	0
29	b	601	SQD	2	0
23	b	604	CLA	1	0
31	a	616	DGD	4	0
23	D	402	CLA	1	0
23	C	506	CLA	1	0
23	B	607	CLA	1	0
25	B	619	BCR	2	0
24	A	606	PHO	2	0
27	D	407	PL9	1	0
31	c	518	DGD	1	0
32	a	618[B]	OEY	2	0
31	A	617	DGD	2	0
23	C	508	CLA	1	0
29	a	615	SQD	3	0
23	b	607	CLA	1	0
25	T	101	BCR	5	0
23	h	101	CLA	3	0
23	C	502	CLA	1	0
30	D	406	LHG	2	0
23	B	604	CLA	3	0
23	b	610	CLA	2	0
36	V	201	HEC	1	0
25	b	617	BCR	3	0
30	d	405	LHG	4	0
32	A	618[B]	OEY	2	0
23	b	614	CLA	2	0
25	b	619	BCR	1	0
23	B	606	CLA	5	0
30	B	623	LHG	4	0
23	c	505	CLA	1	0
25	B	618	BCR	3	0
23	A	604	CLA	3	0
24	d	401	PHO	4	0
23	B	603	CLA	1	0
23	b	609	CLA	1	0
24	A	605	PHO	1	0
23	B	605	CLA	2	0
23	c	503	CLA	2	0
23	b	613	CLA	4	0
27	a	611	PL9	9	0
28	d	406	LMG	1	0

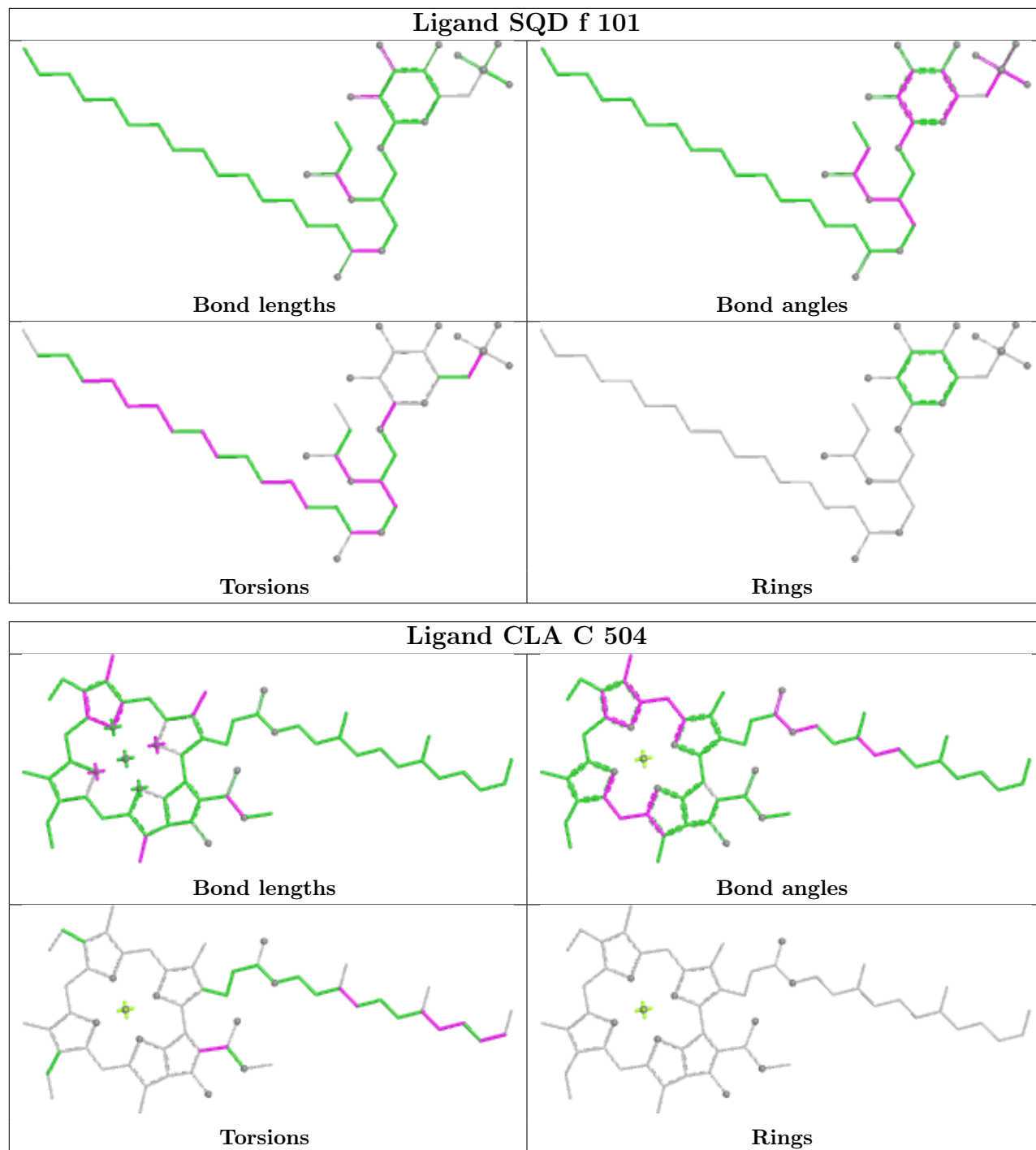
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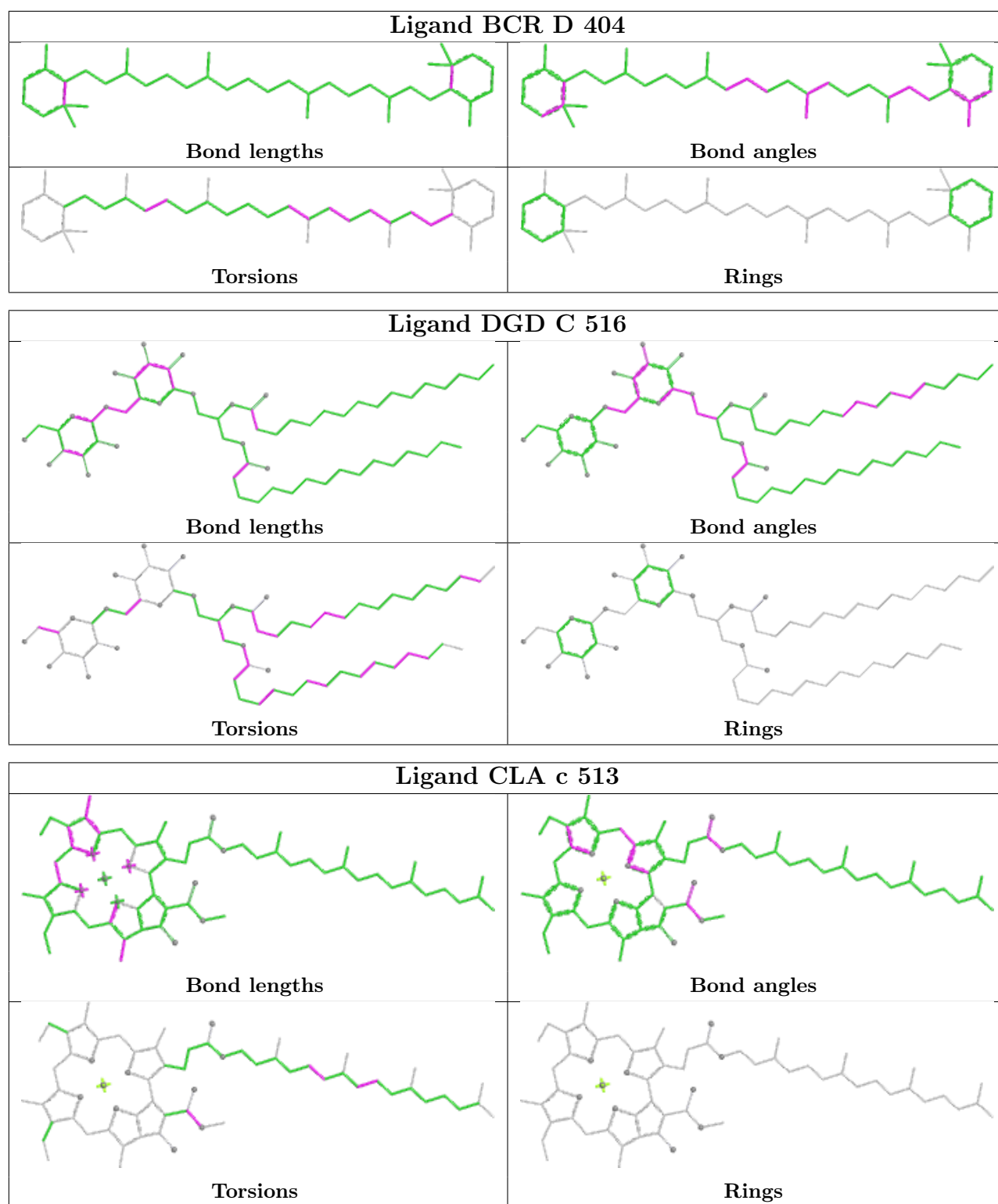
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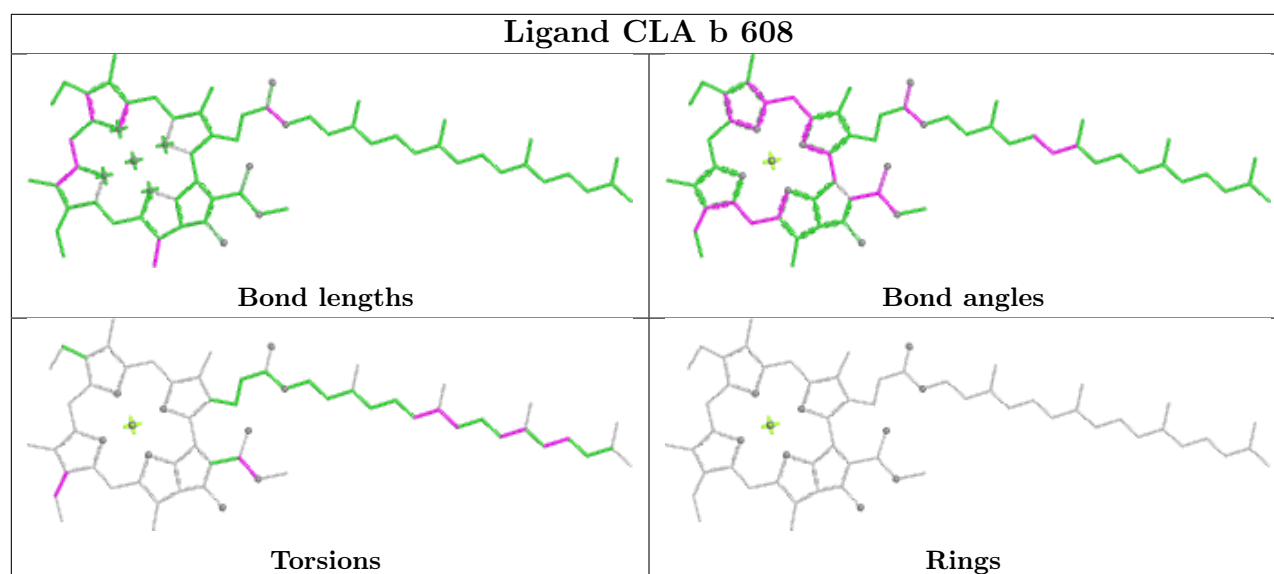
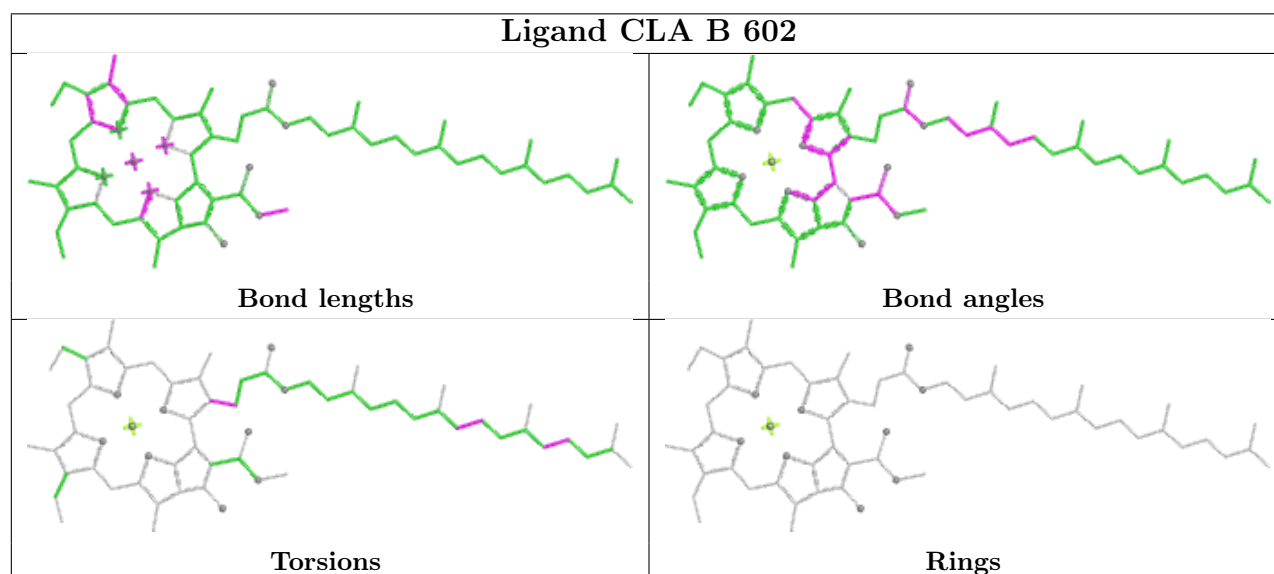
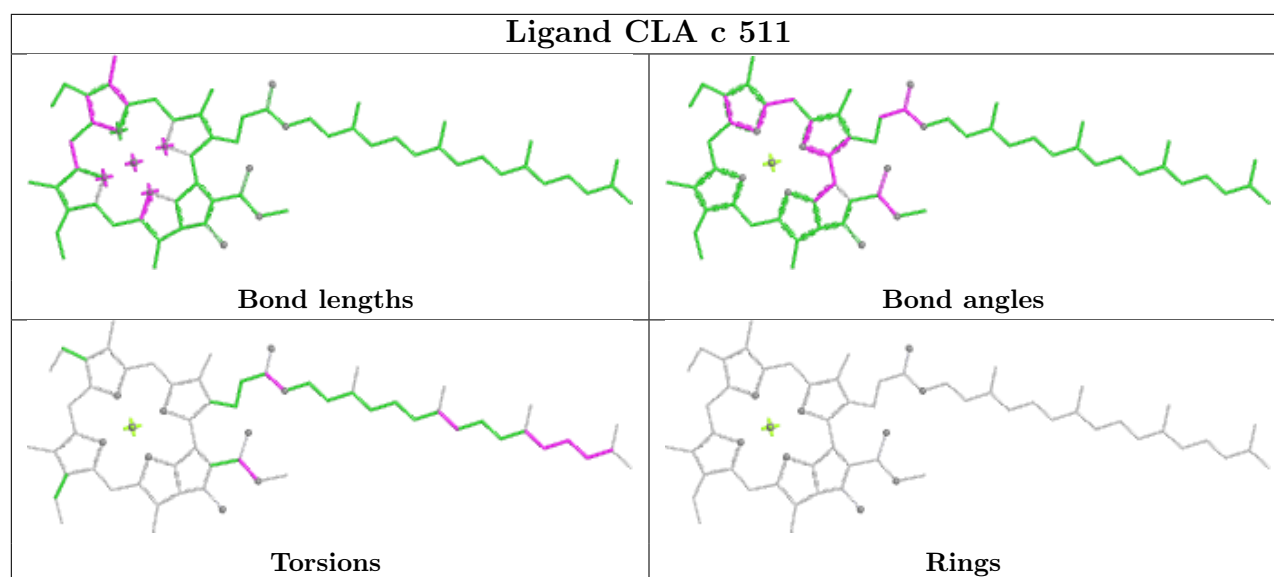
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	b	603	CLA	2	0
25	h	102	BCR	2	0
23	C	501	CLA	2	0
23	c	509	CLA	1	0
23	b	605	CLA	3	0
23	c	508	CLA	2	0
25	k	101	BCR	3	0
35	f	102	HEM	7	0
23	c	504	CLA	2	0
23	A	603	CLA	3	0
25	H	101	BCR	4	0
25	Y	101	BCR	3	0
28	c	522	LMG	2	0
25	t	101	BCR	7	0
23	a	606	CLA	6	0
23	C	513	CLA	1	0
31	C	517	DGD	2	0
23	B	608	CLA	2	0
23	b	606	CLA	4	0
23	a	603	CLA	4	0
28	c	521	LMG	1	0
23	c	501	CLA	3	0
23	B	613	CLA	2	0
25	b	618	BCR	5	0
23	c	507	CLA	1	0
25	C	515	BCR	2	0
24	a	605	PHO	2	0
23	D	403	CLA	1	0
23	C	510	CLA	1	0
30	d	409	LHG	1	0
23	c	506	CLA	2	0

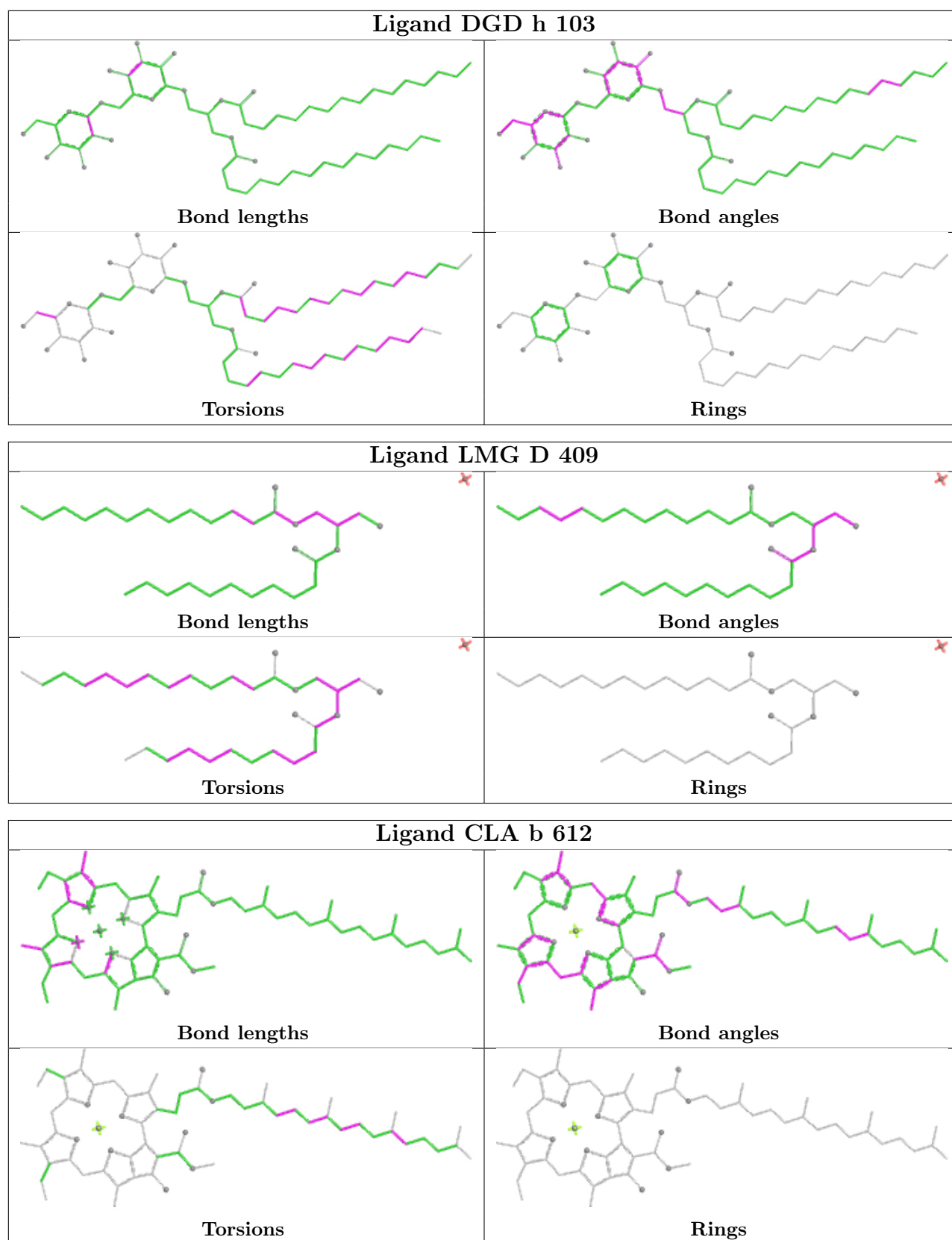
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

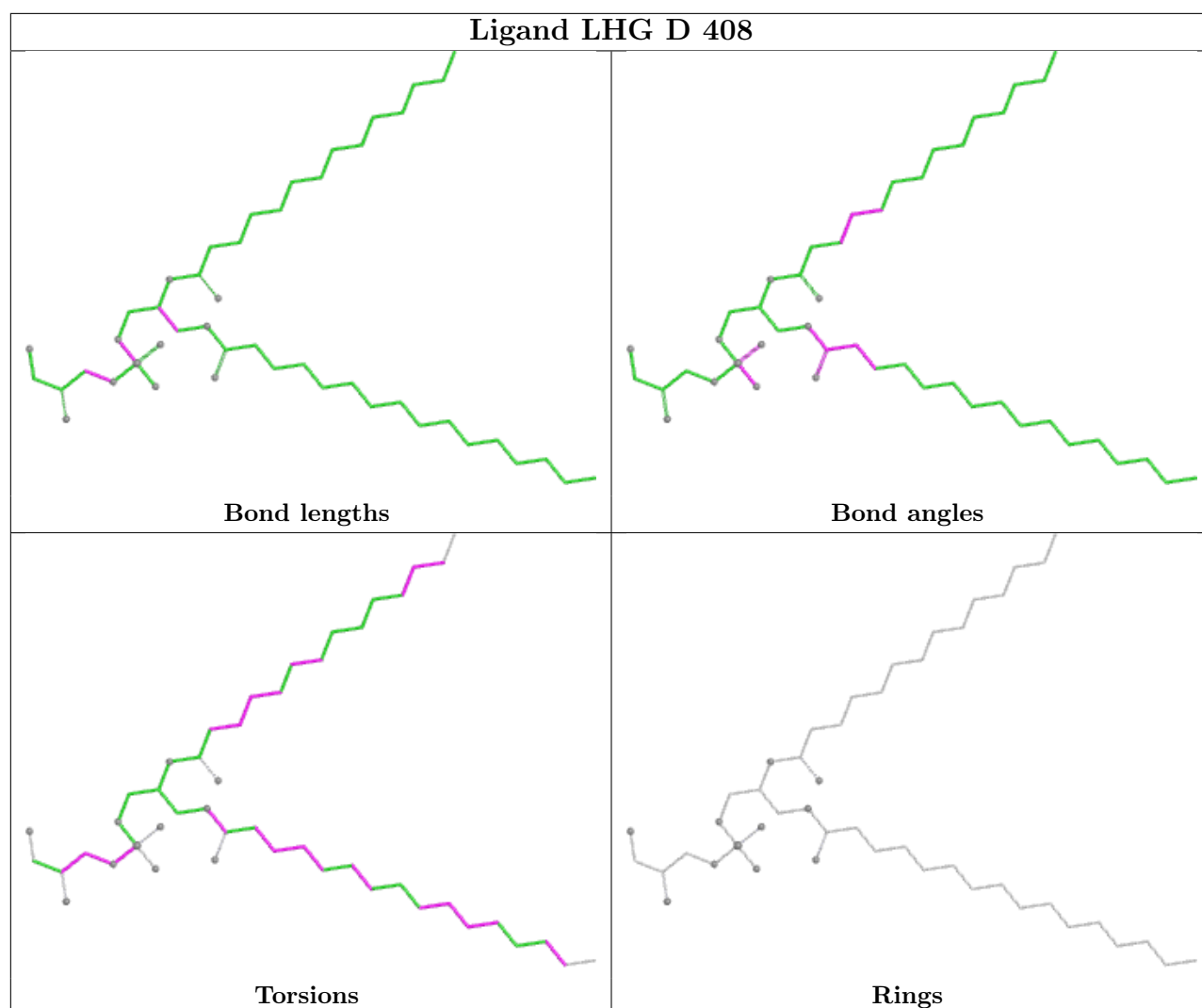
equivalents in the CSD to analyse the geometry.



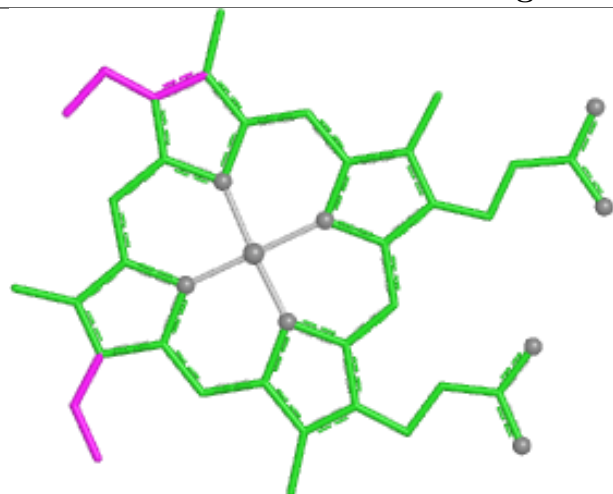




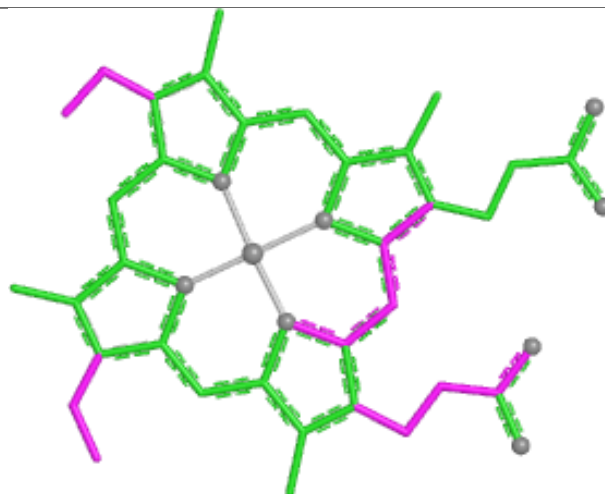




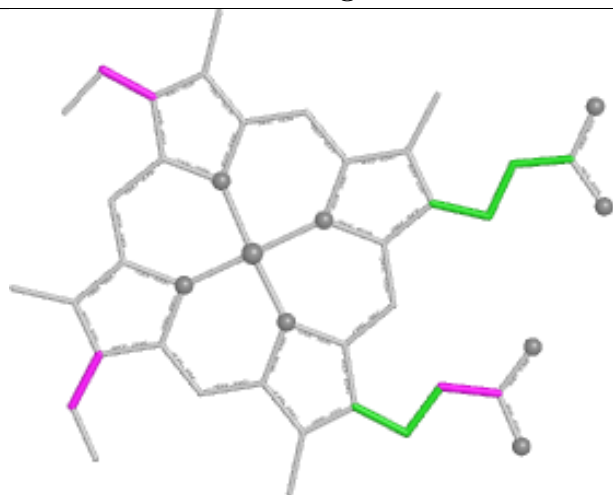
Ligand HEC v 201



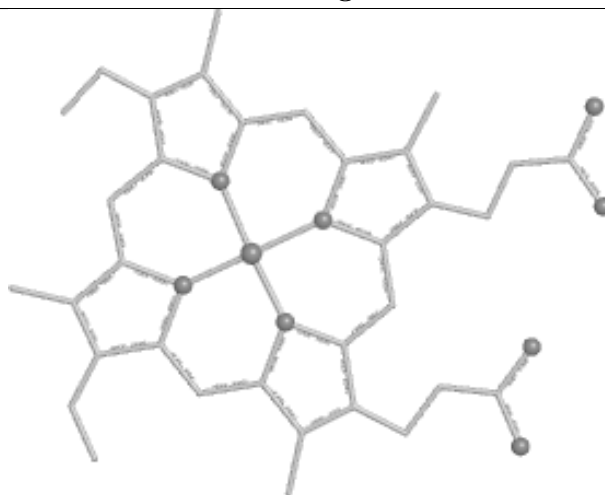
Bond lengths



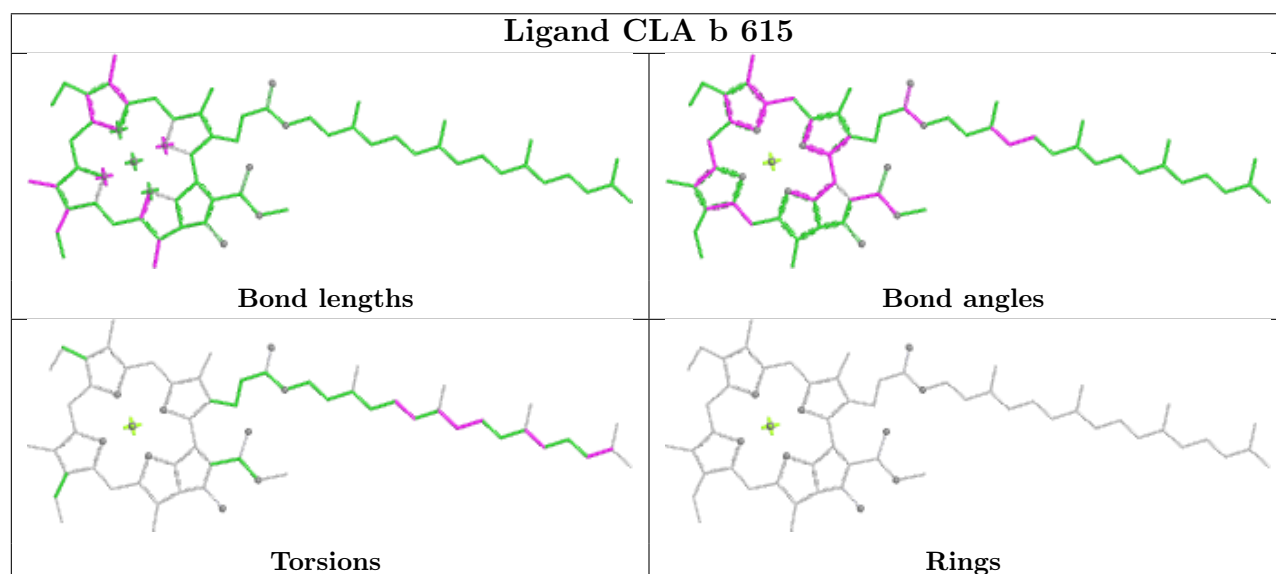
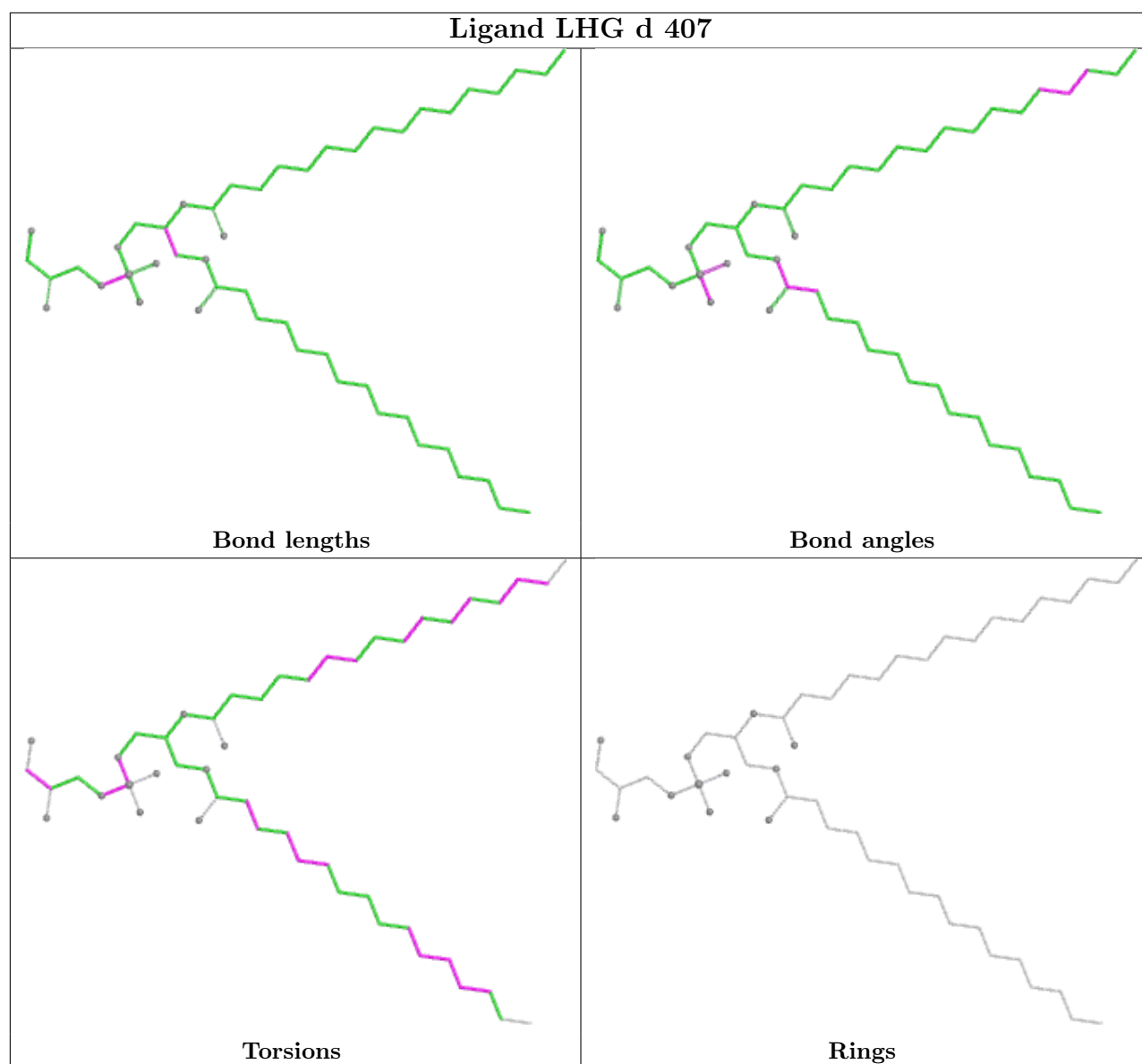
Bond angles

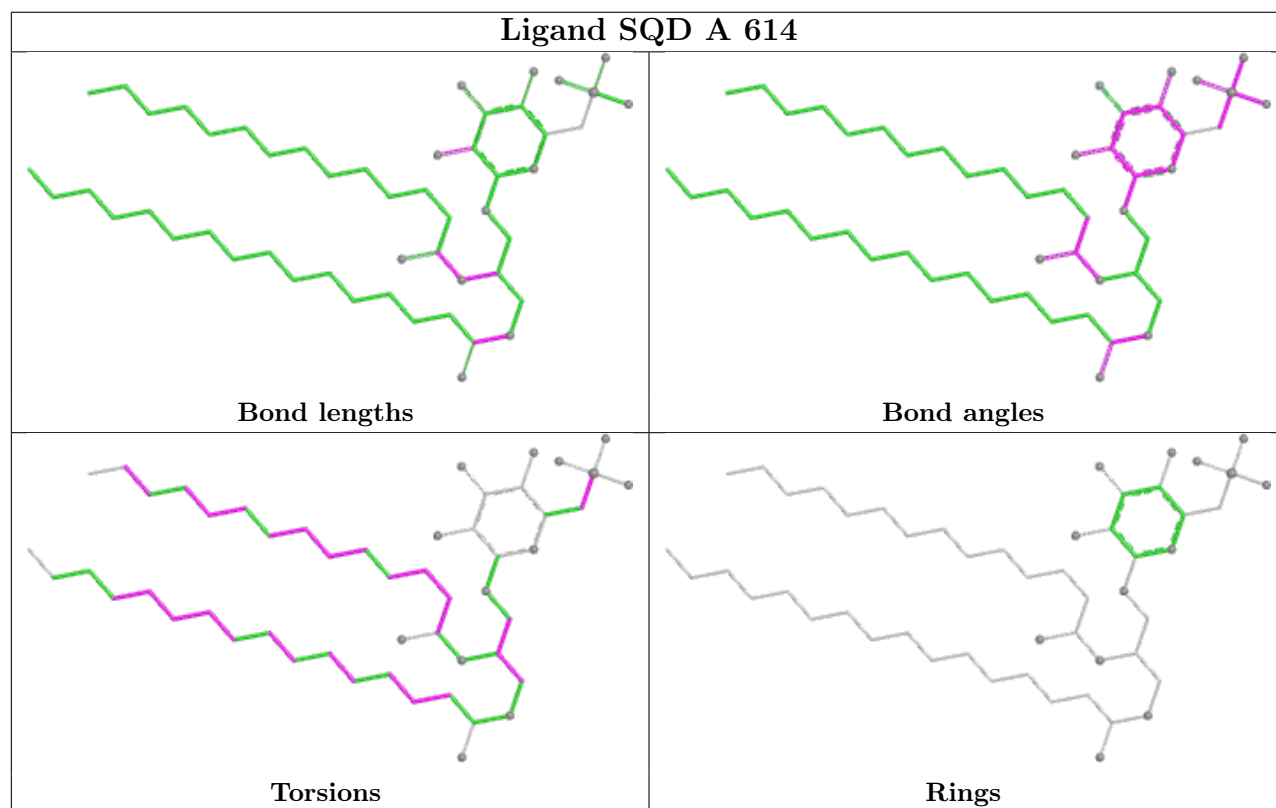
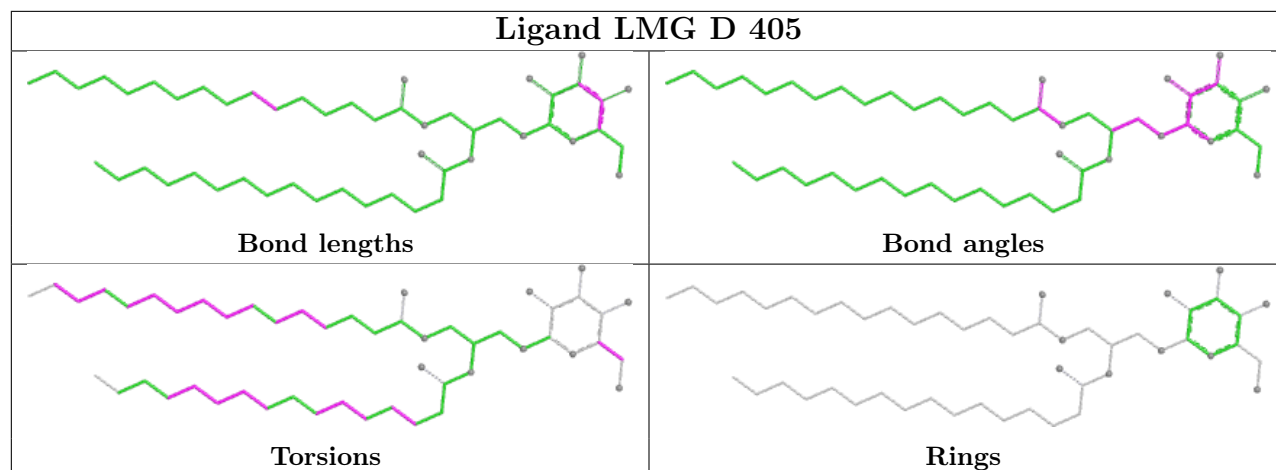


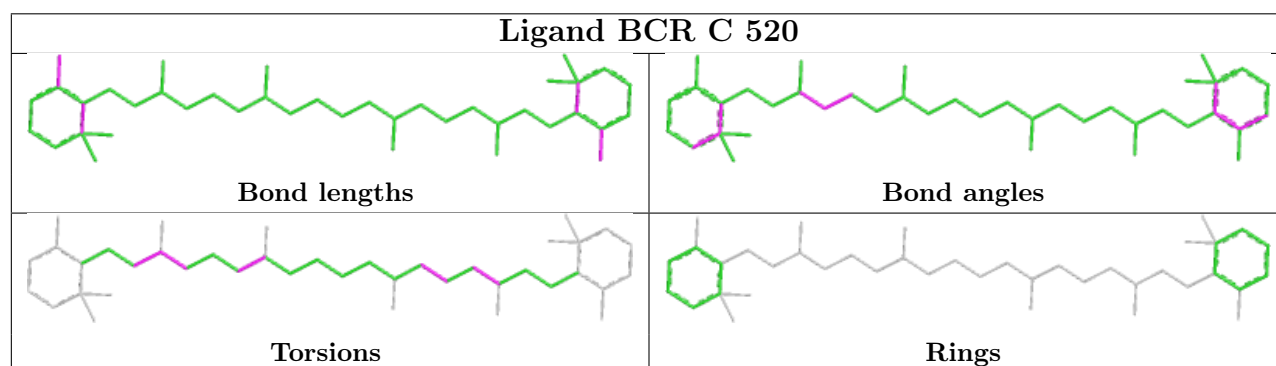
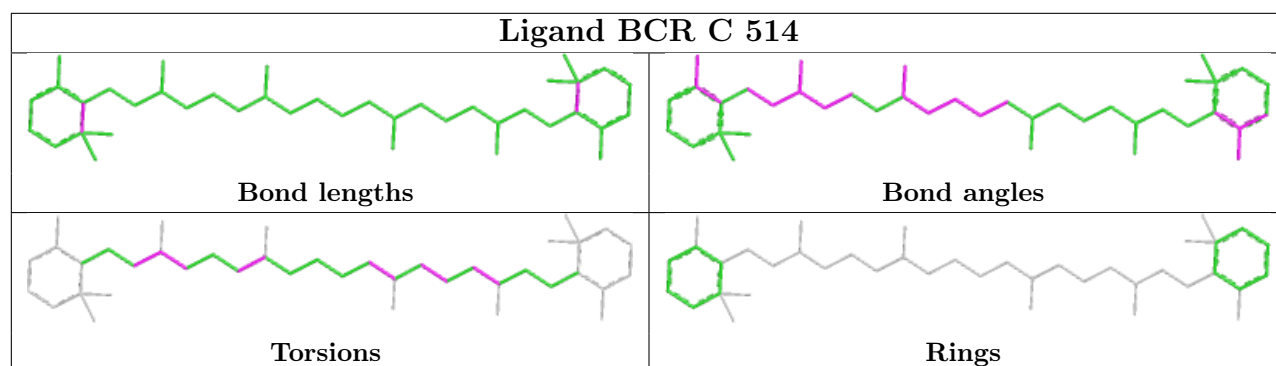
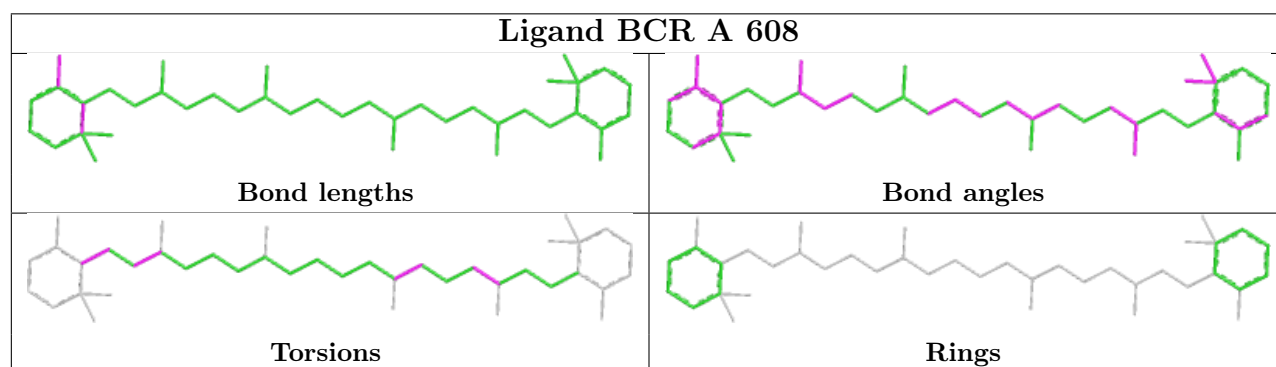
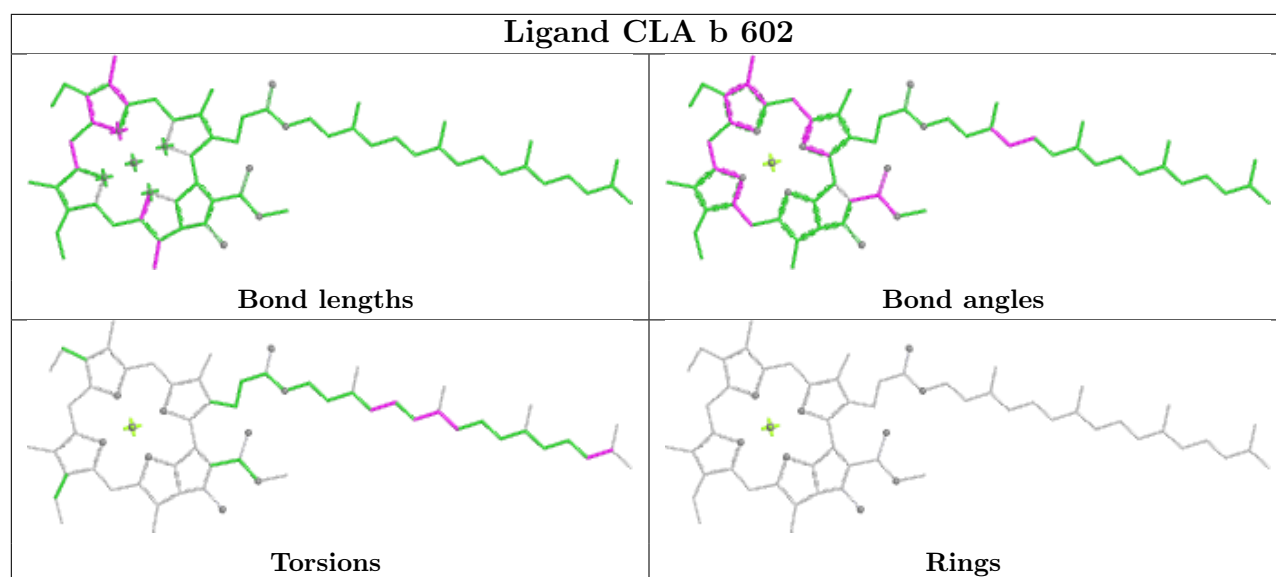
Torsions

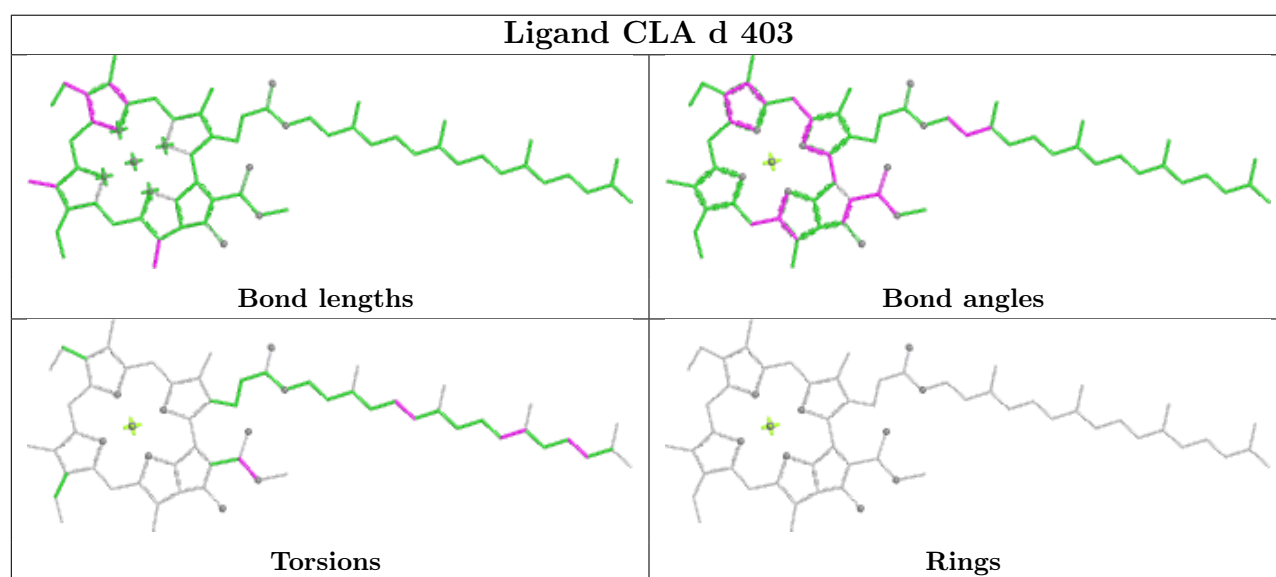
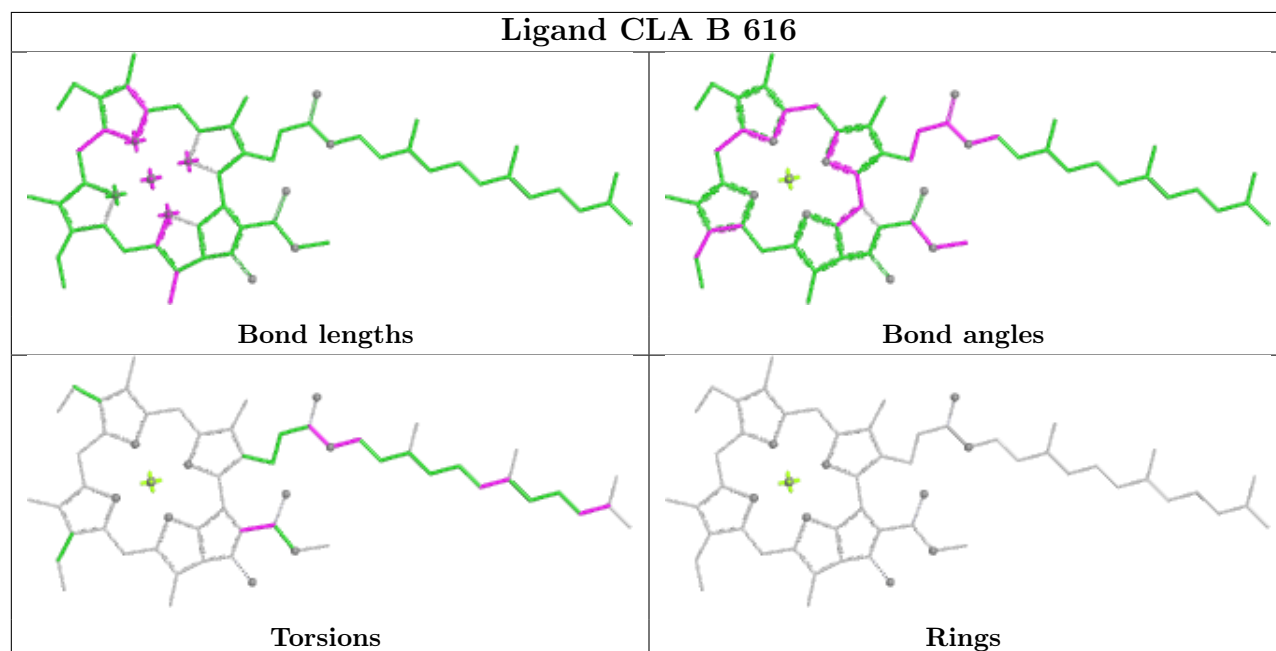
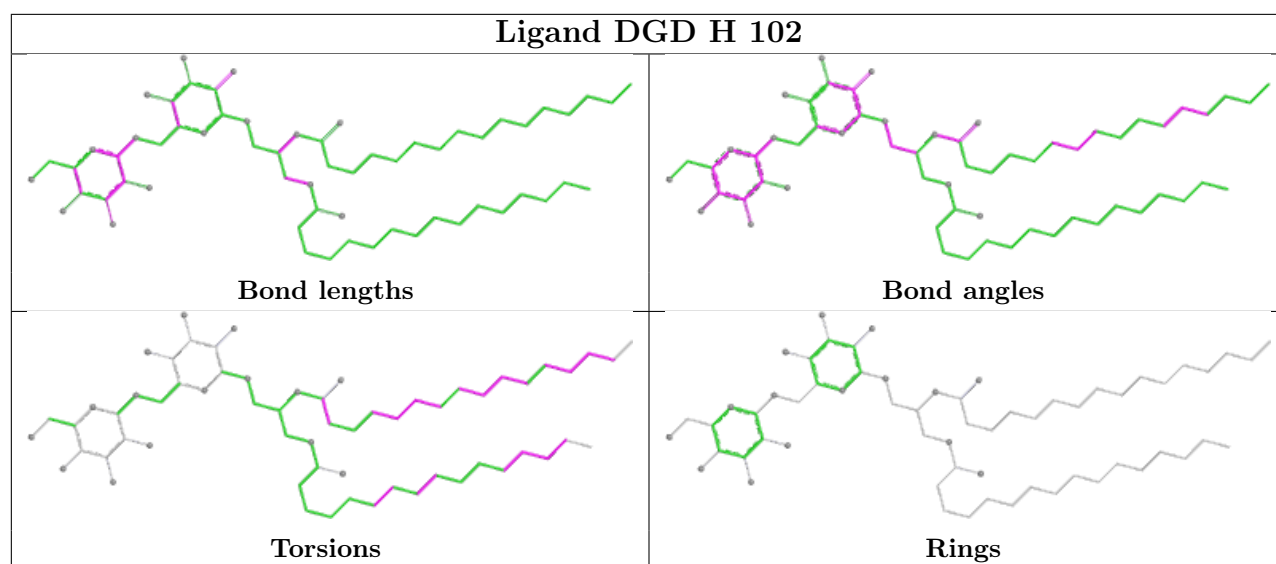


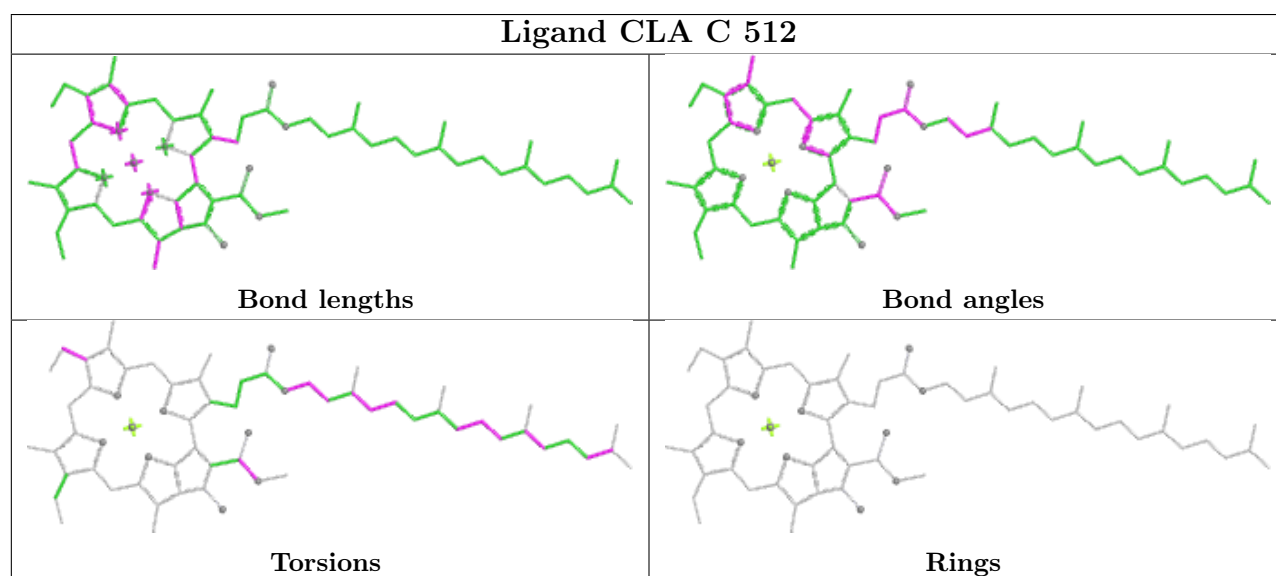
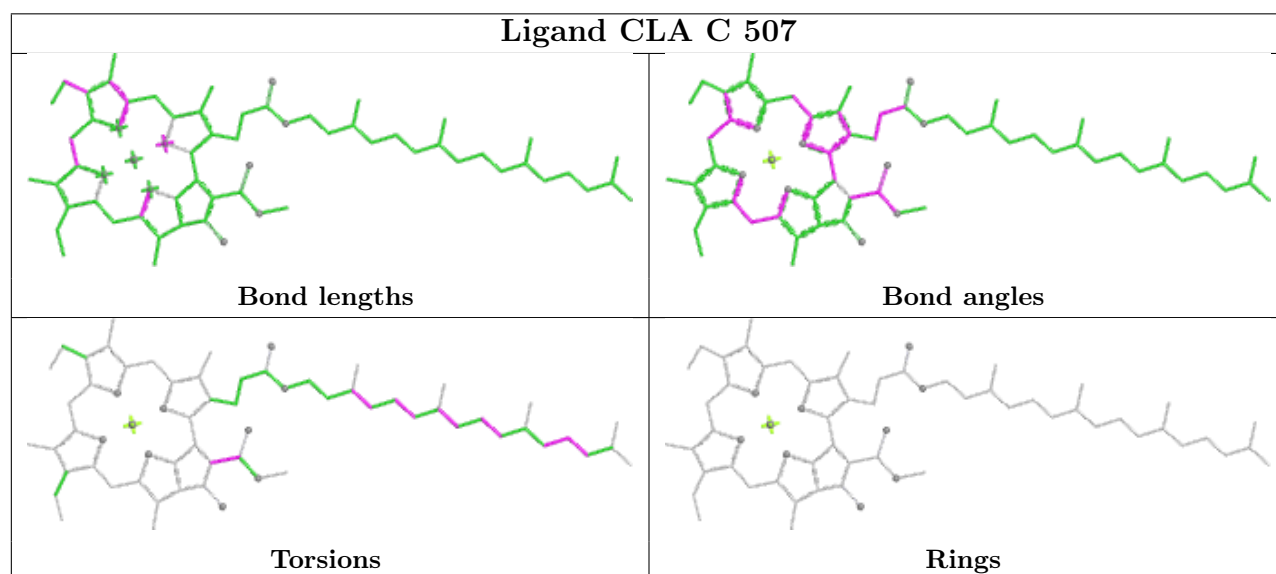
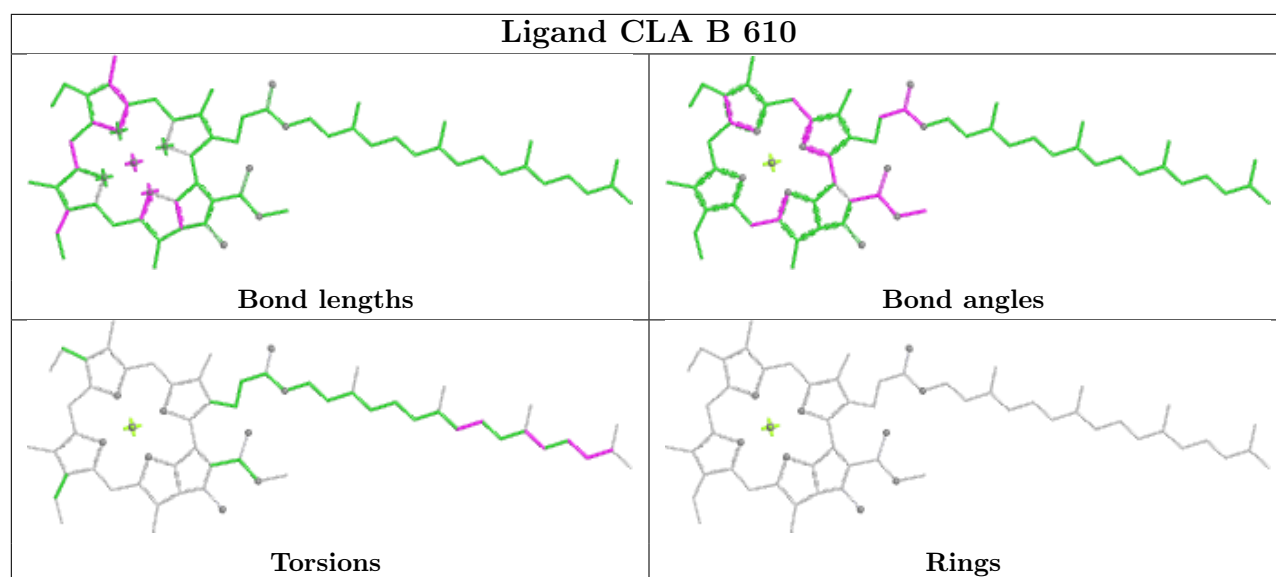
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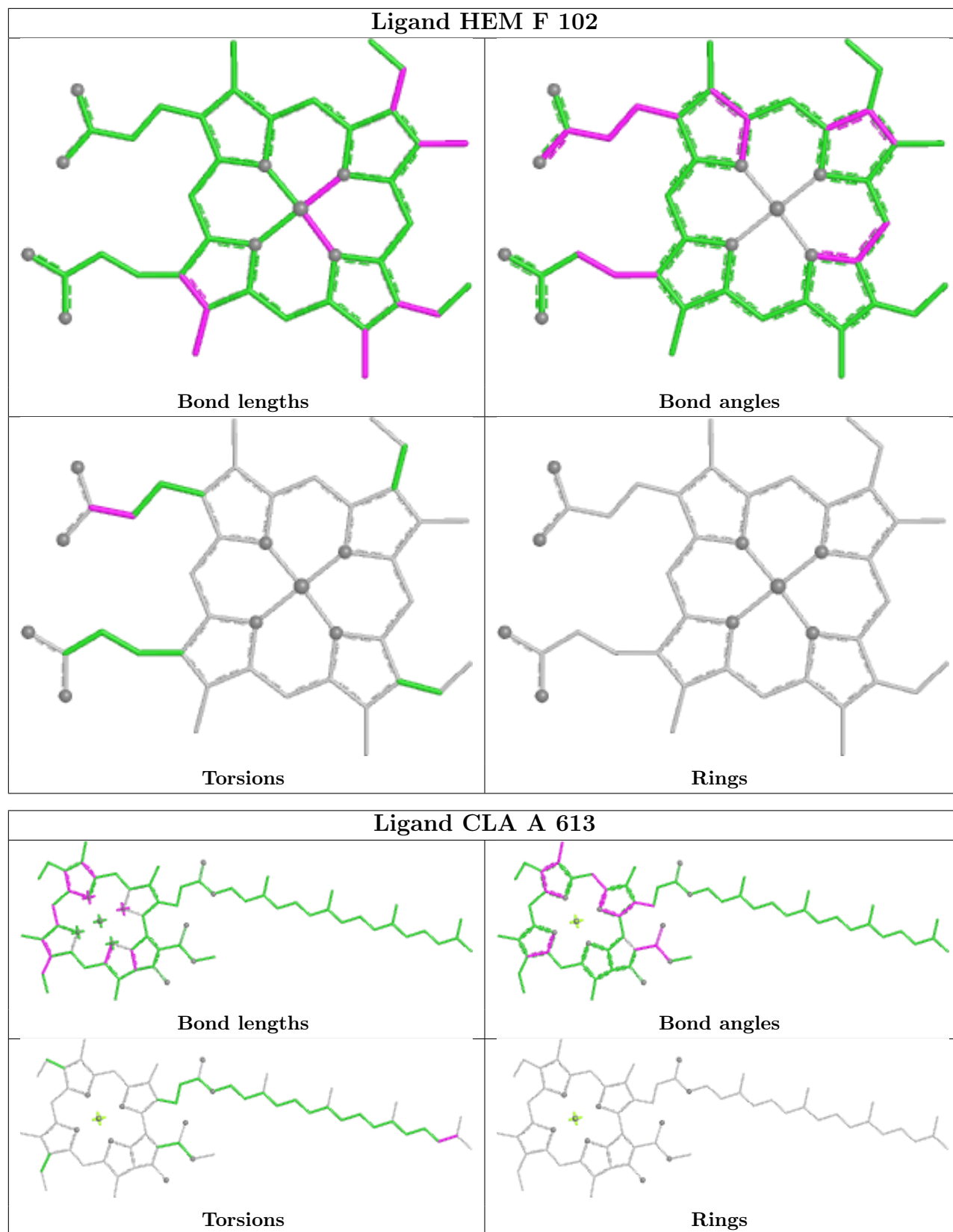


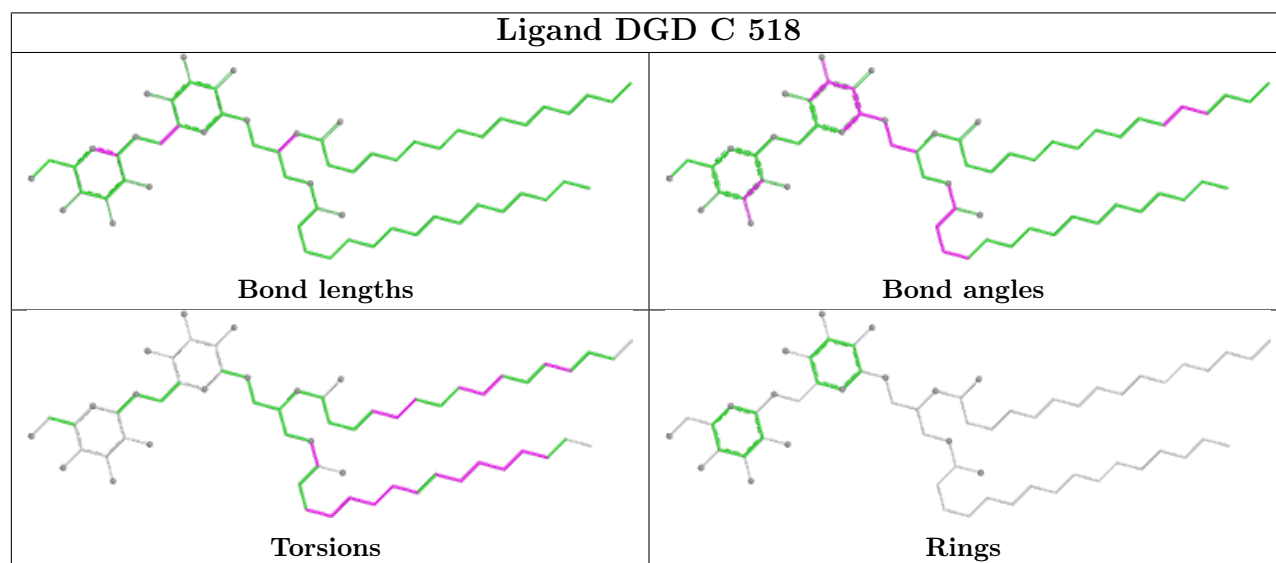
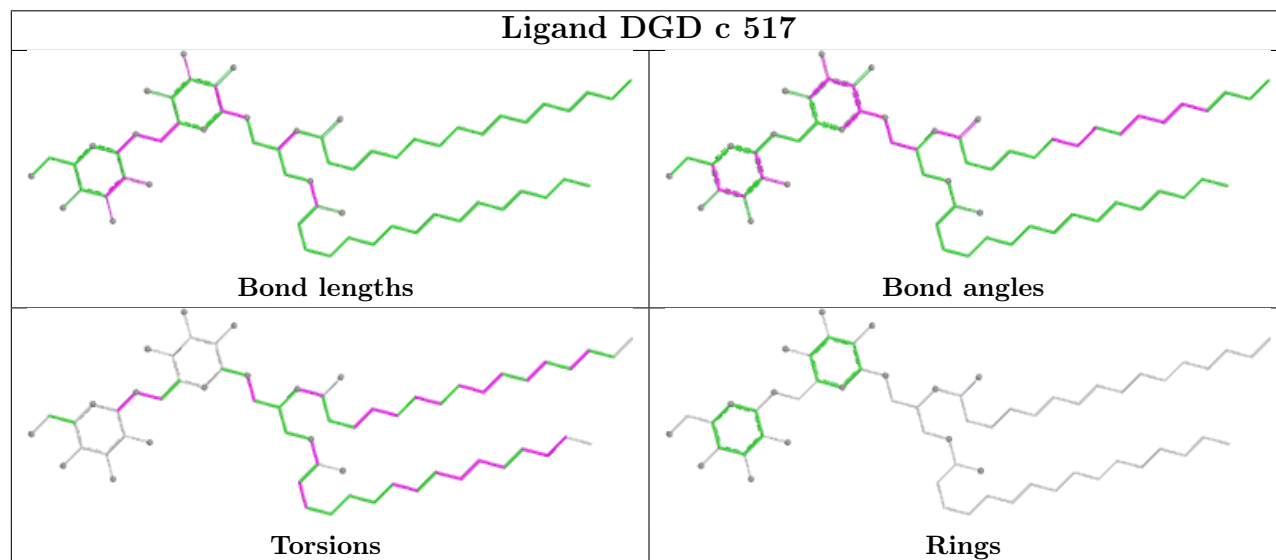
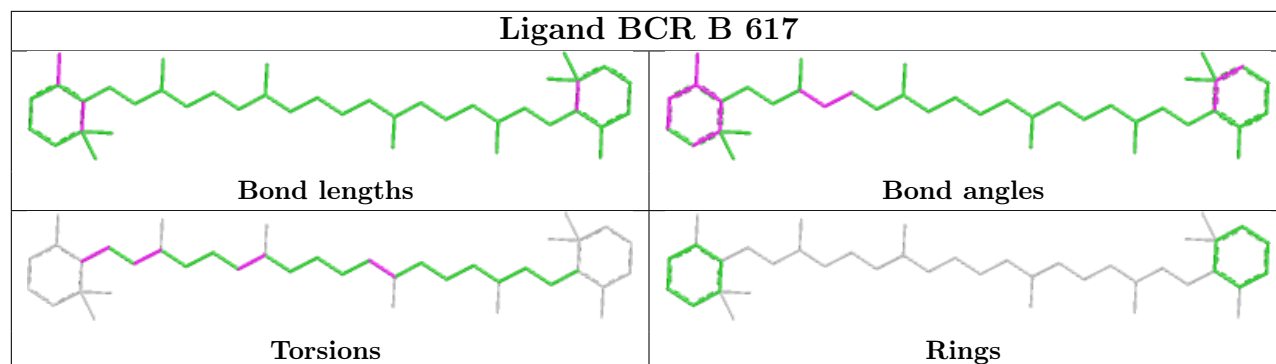


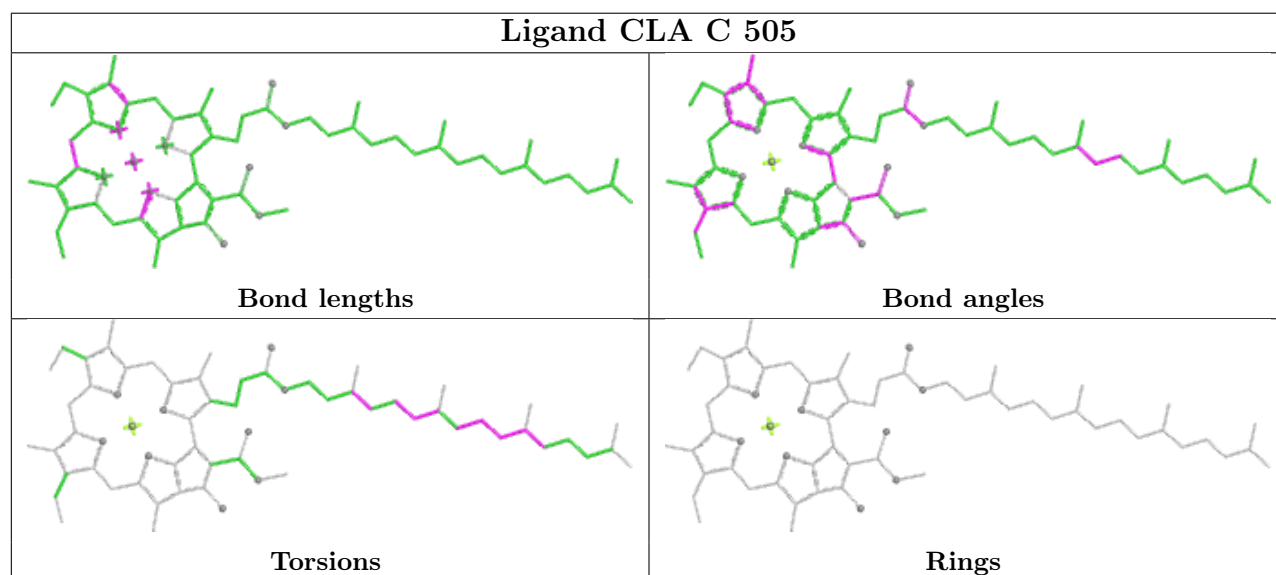
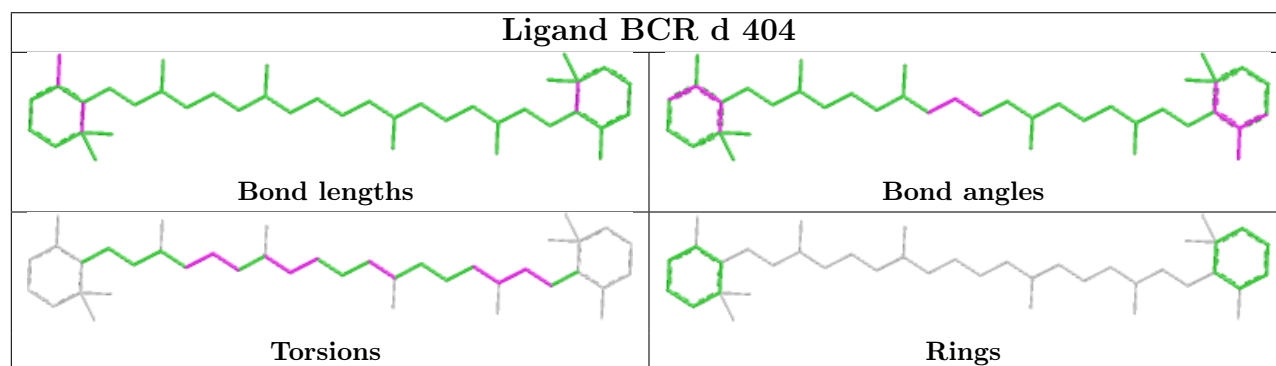
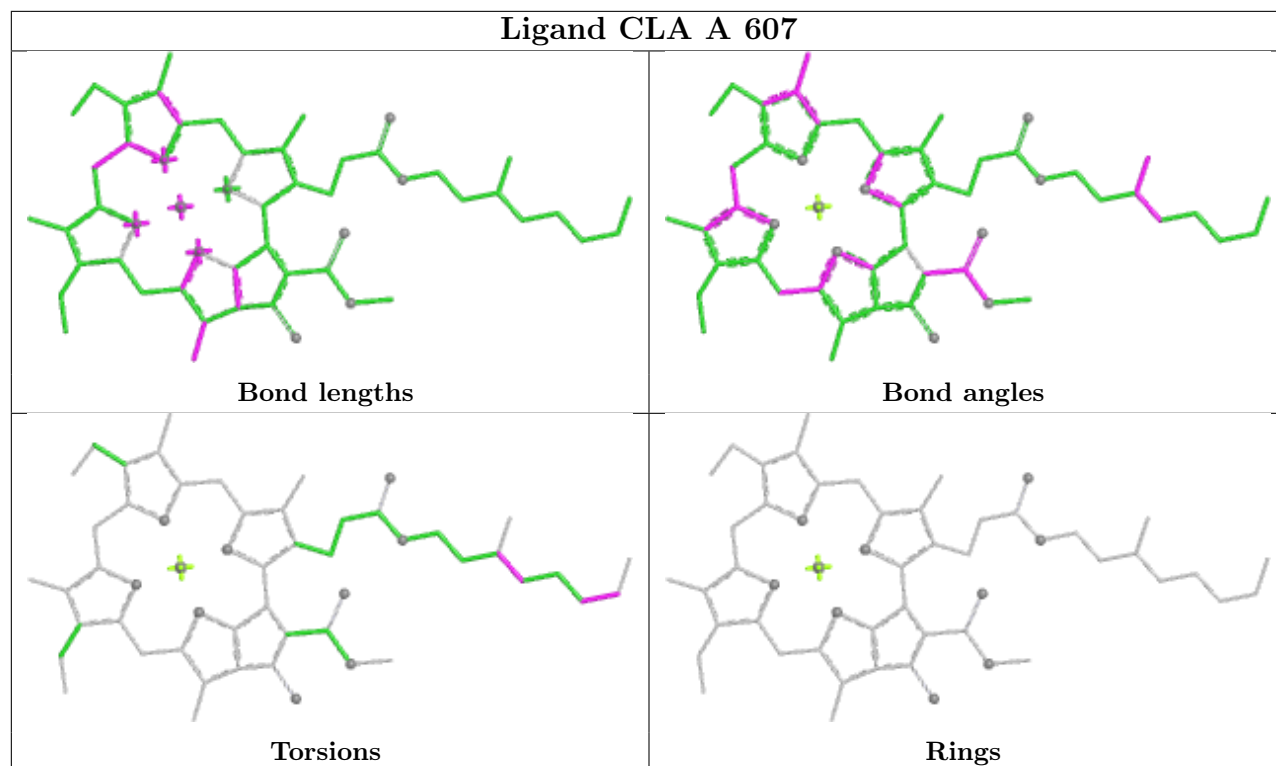


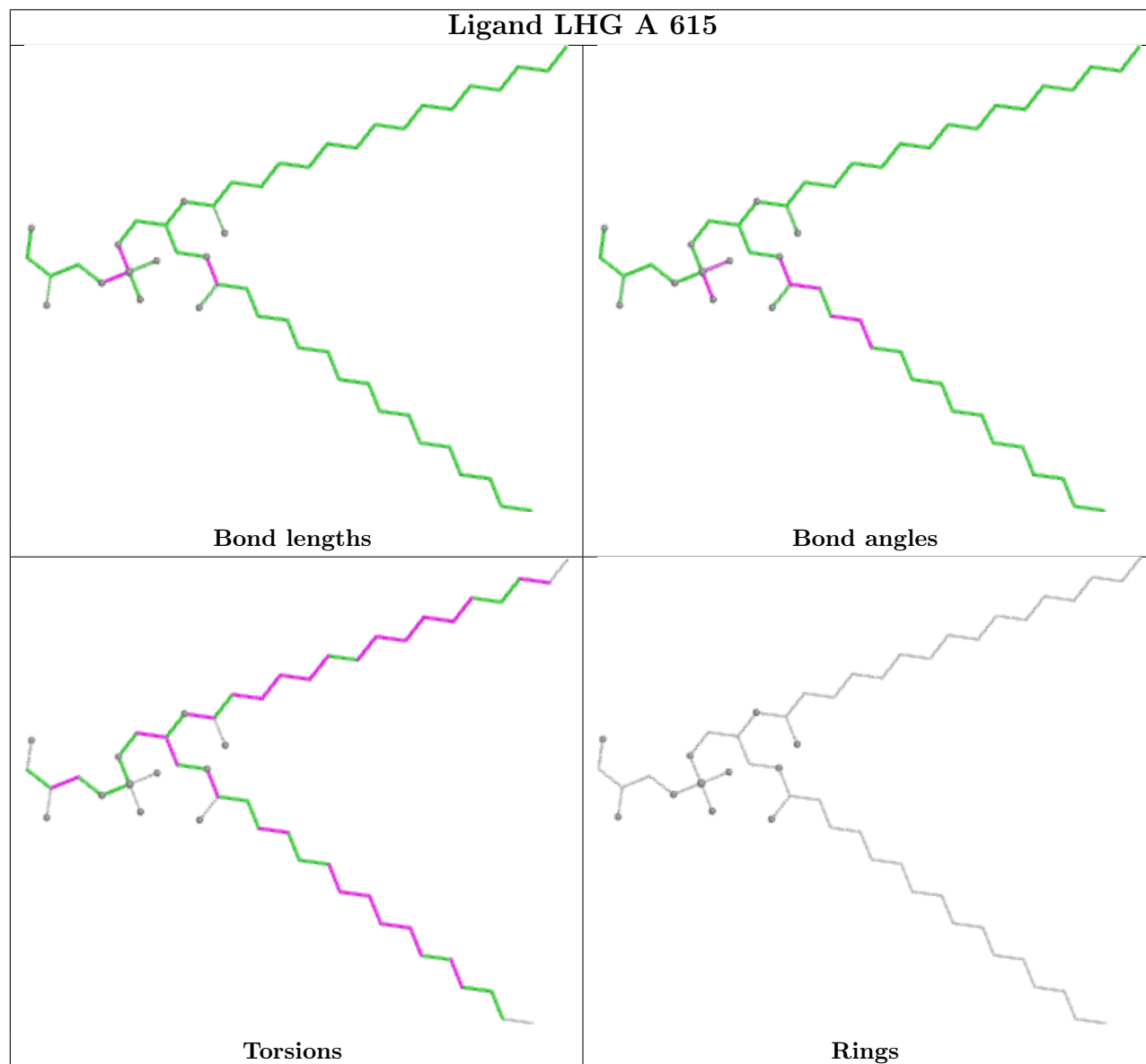
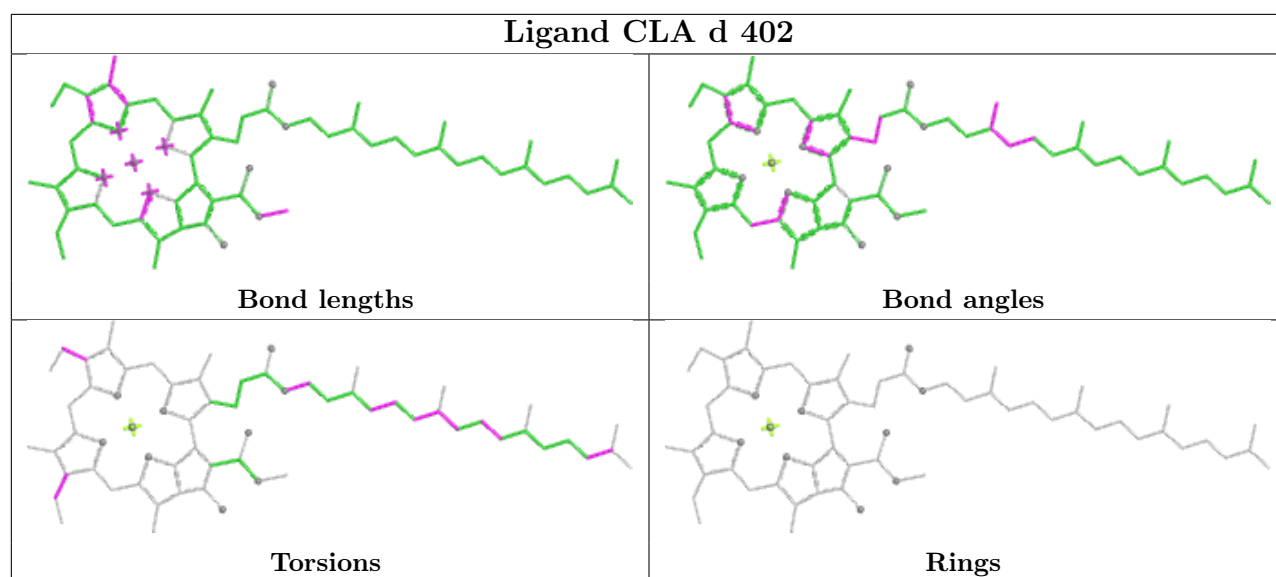


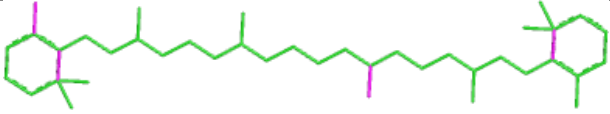
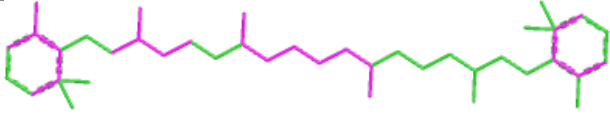
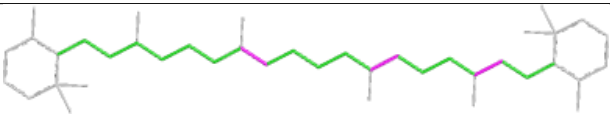
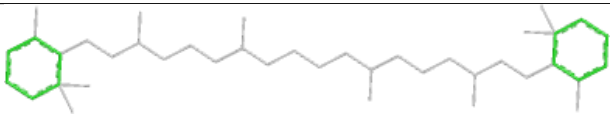
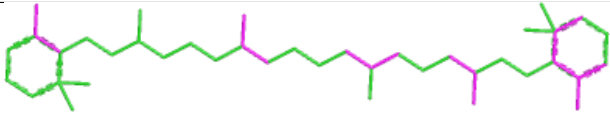
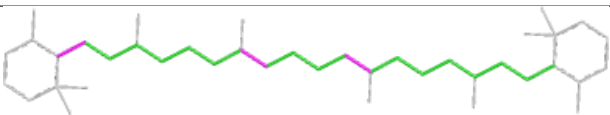
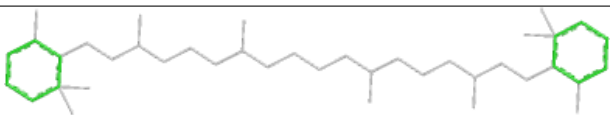
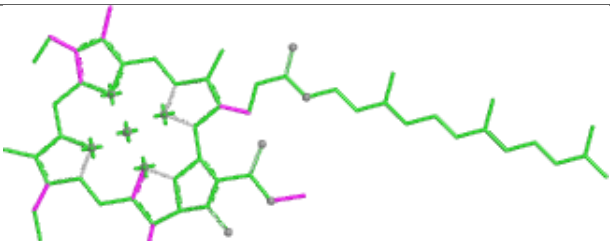
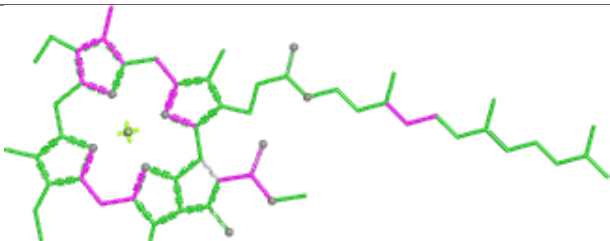
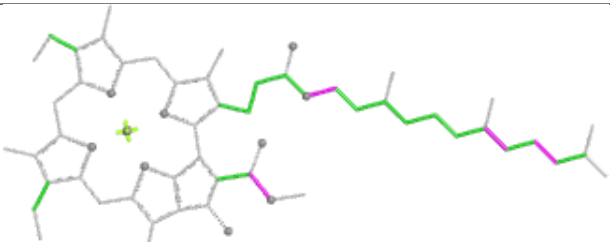
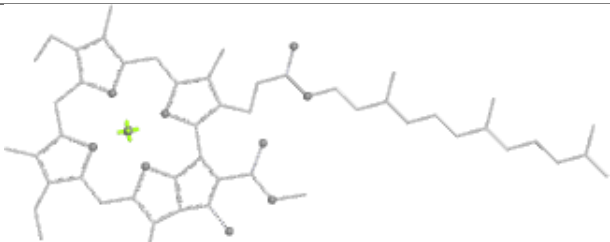


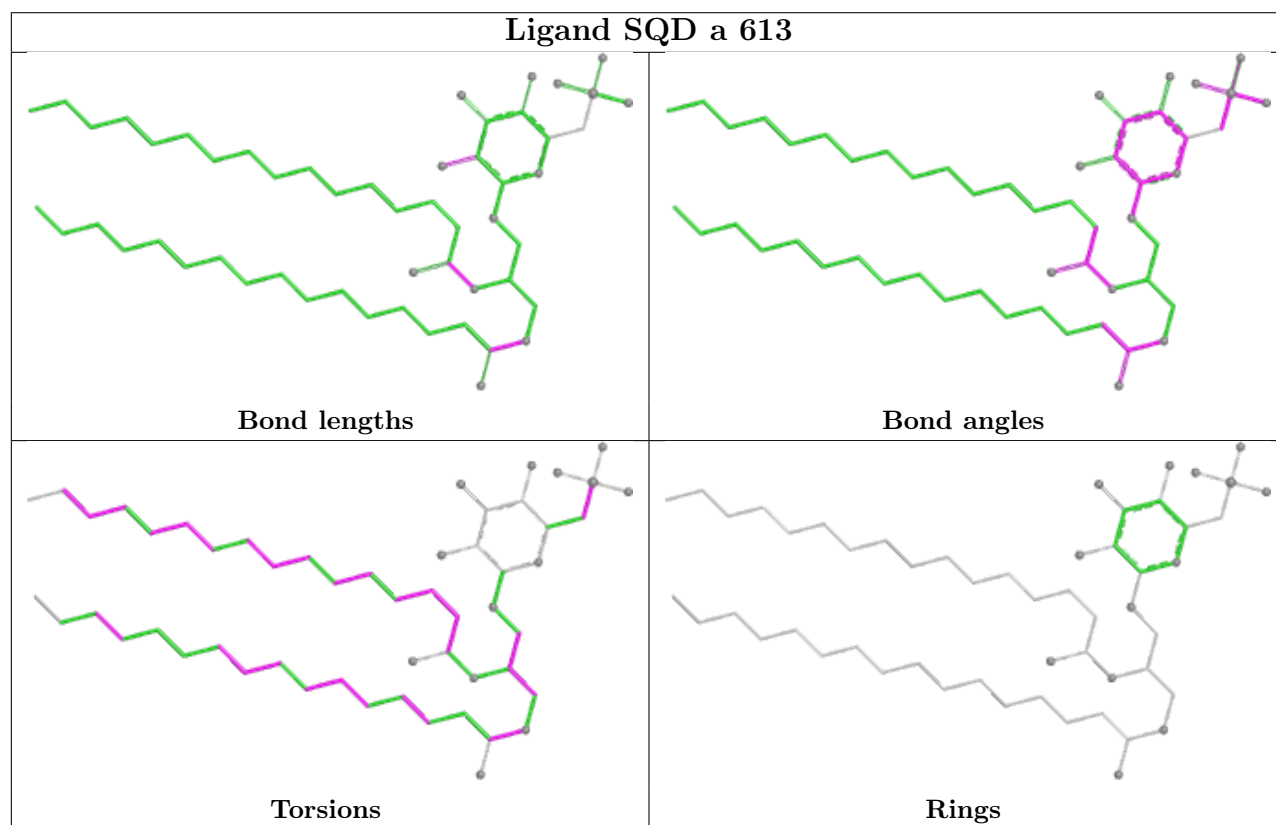
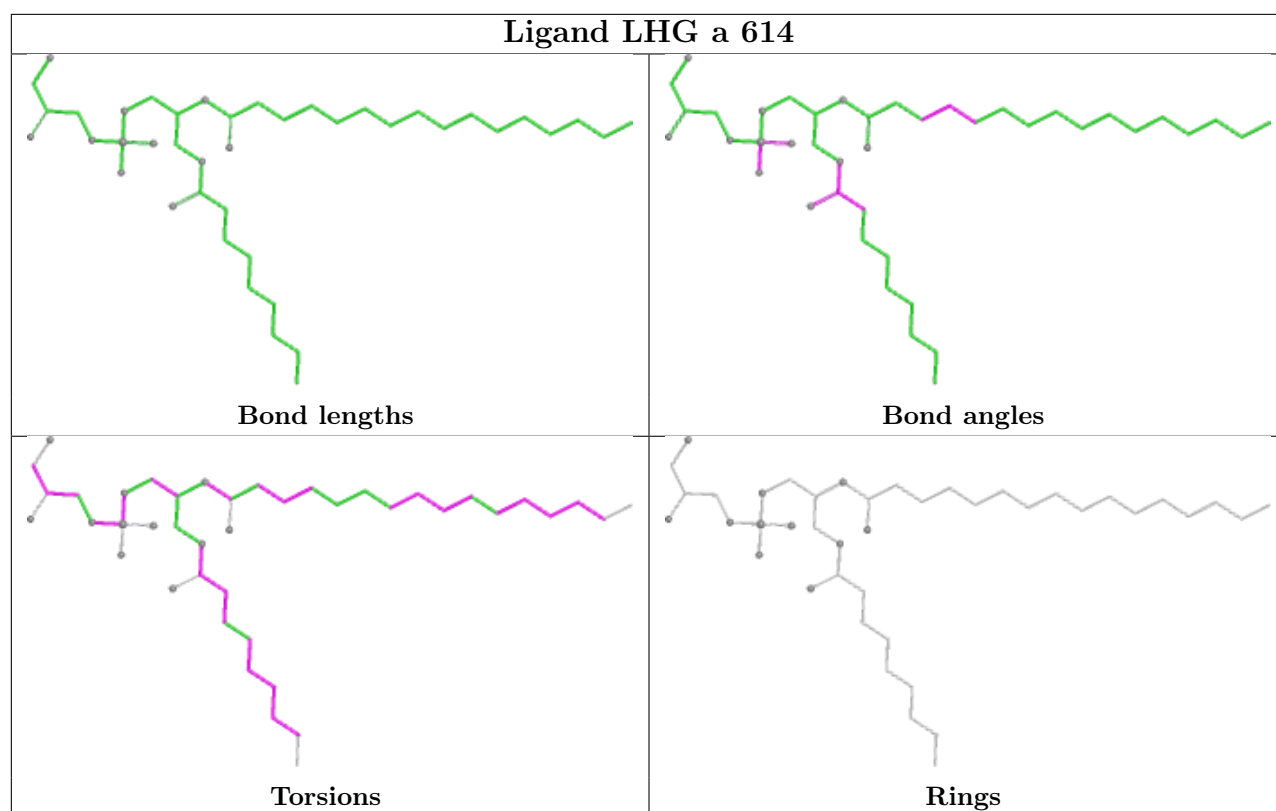


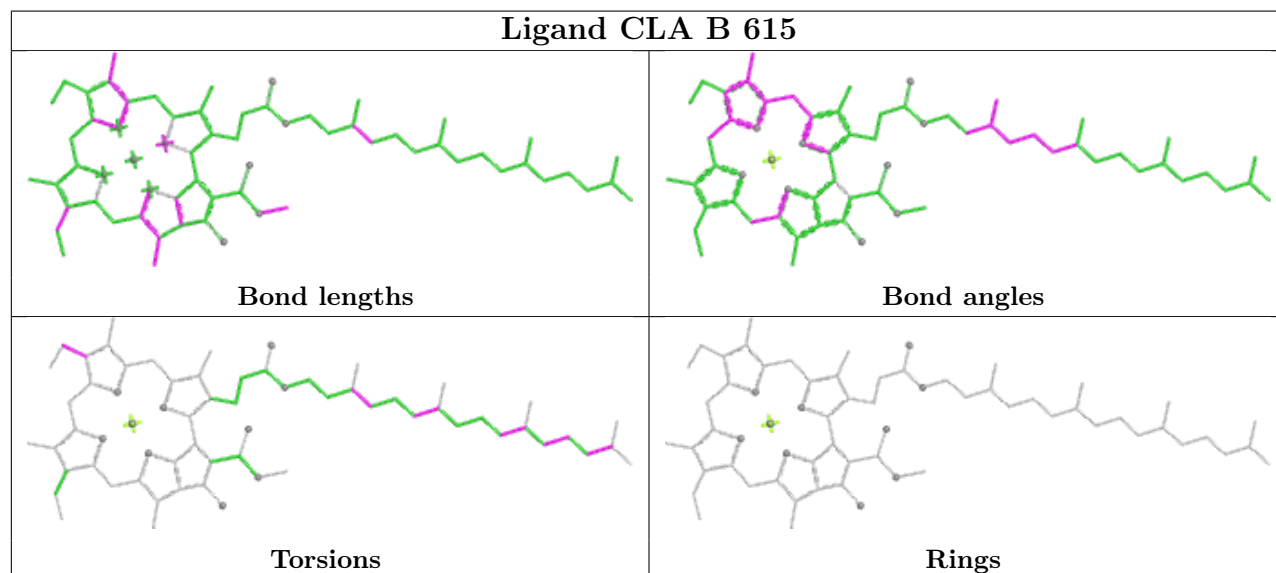
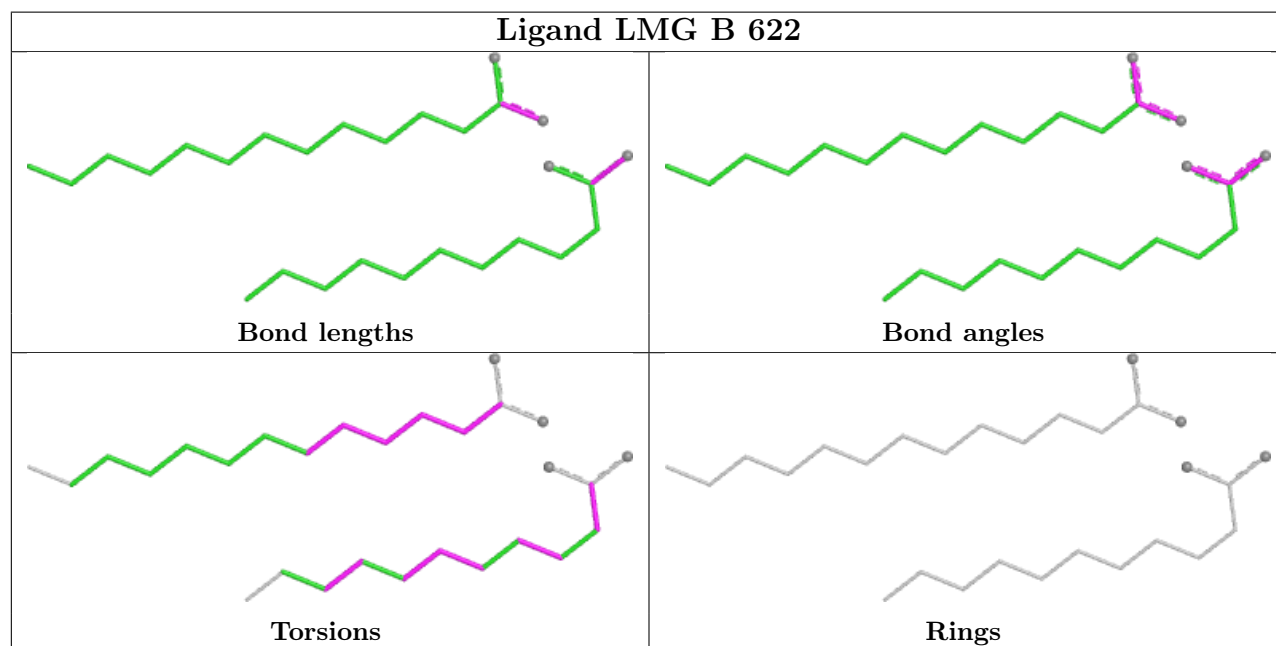
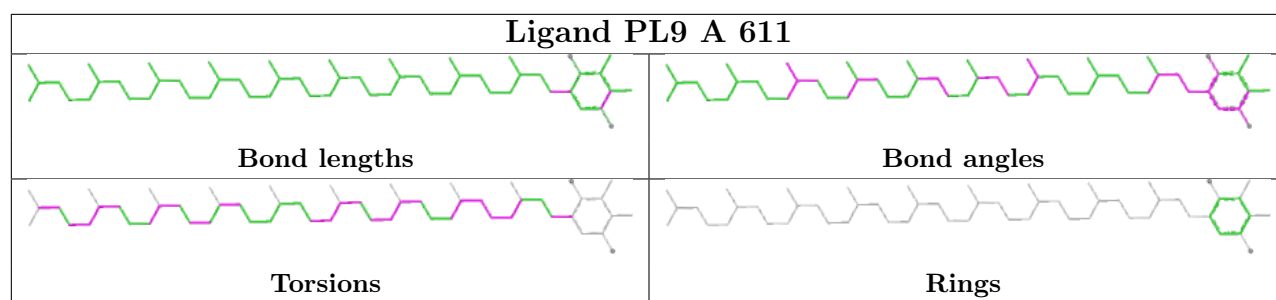


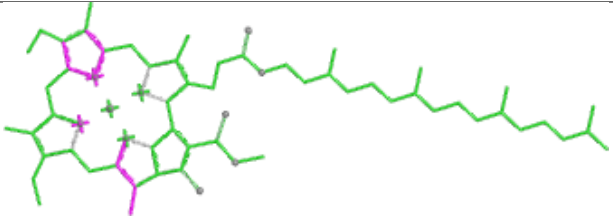
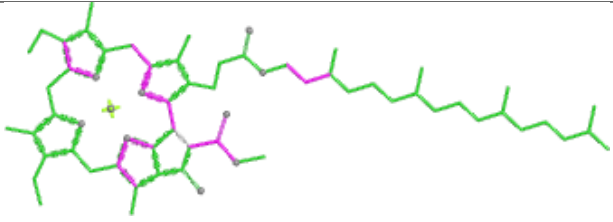
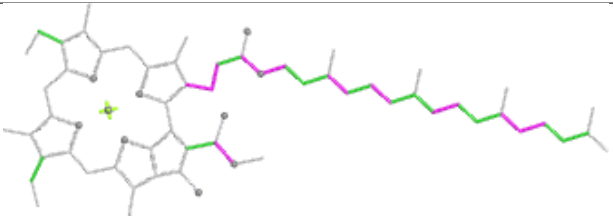
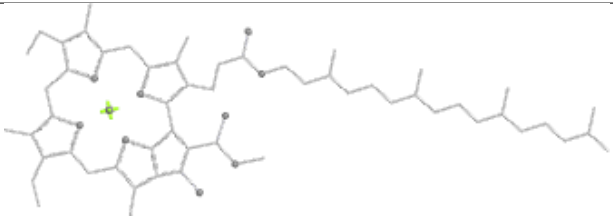
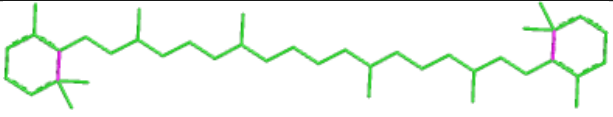
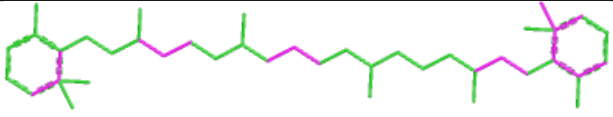
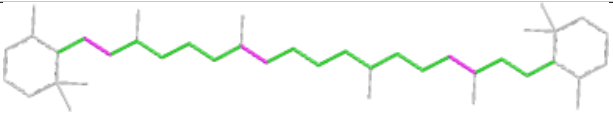
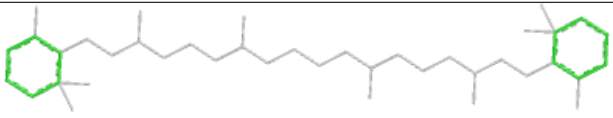
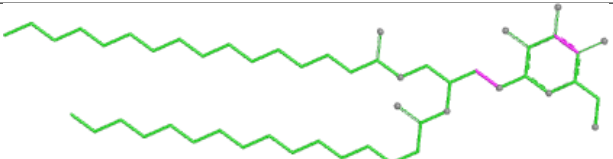
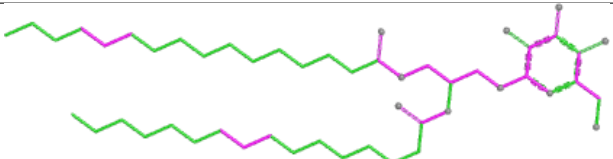
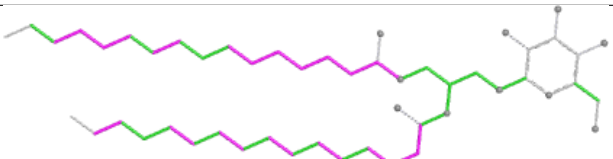
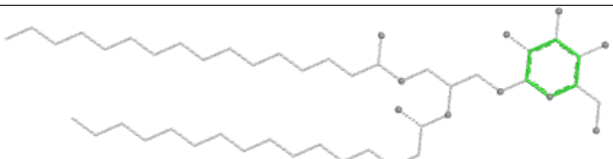


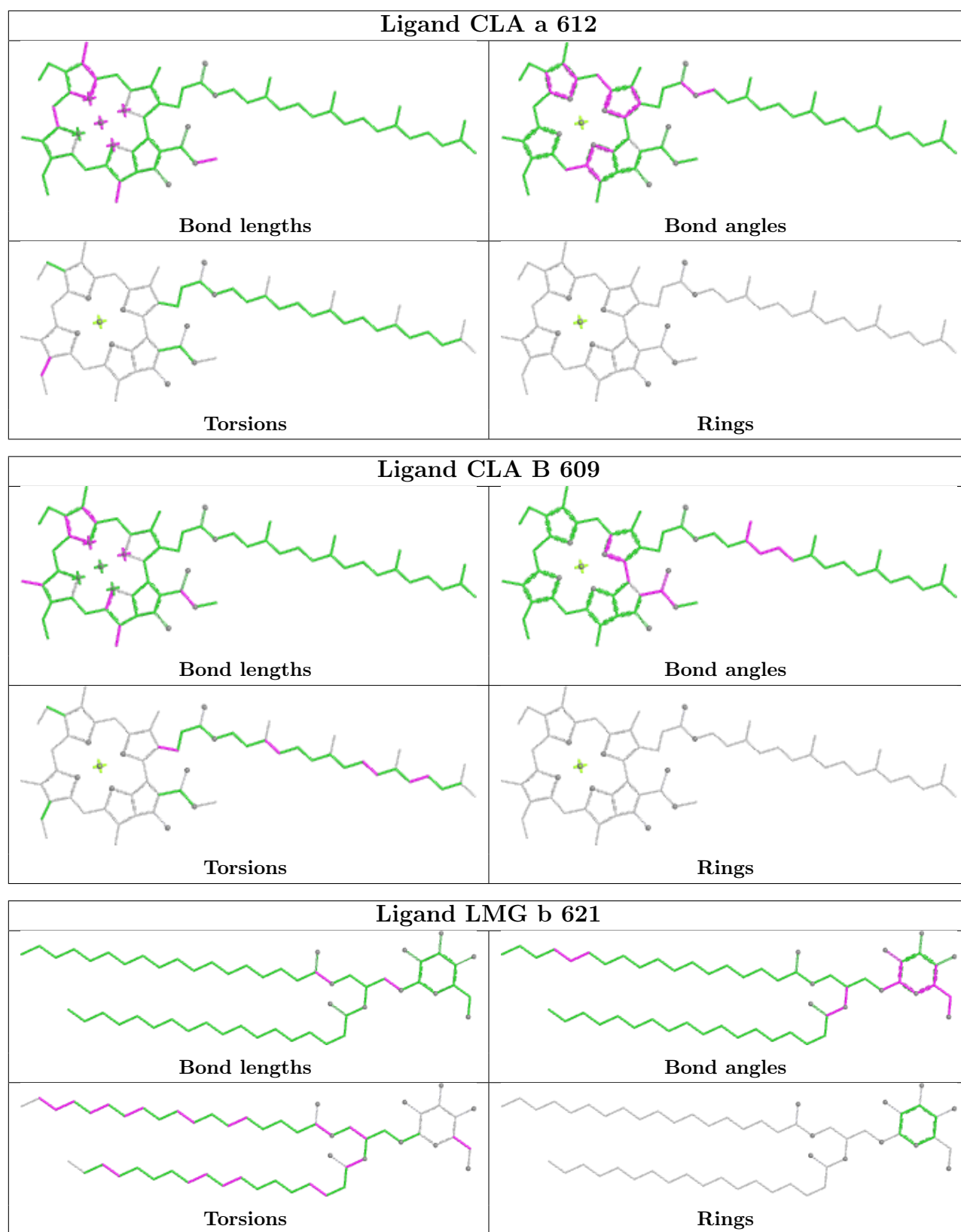


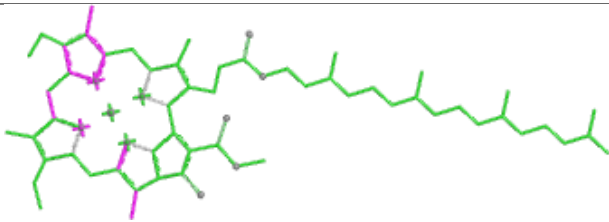
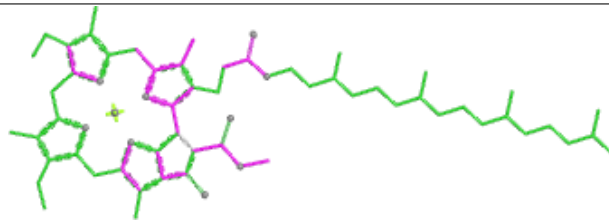
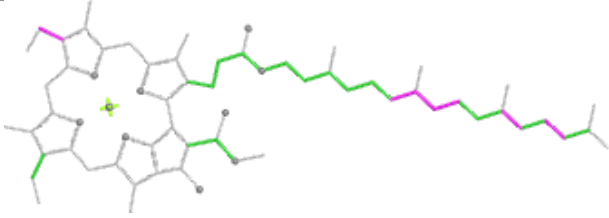
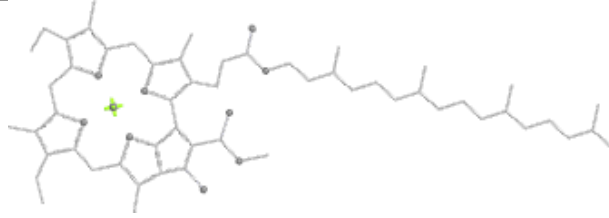
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 Bond lengths	 Bond angles
 Torsions	 Rings
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 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA b 616	
 Bond lengths	 Bond angles
 Torsions	 Rings

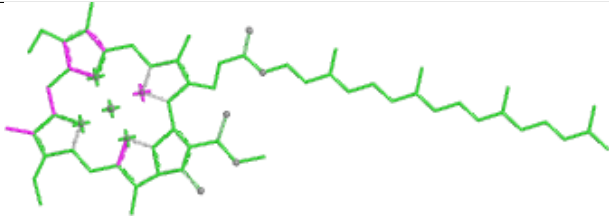
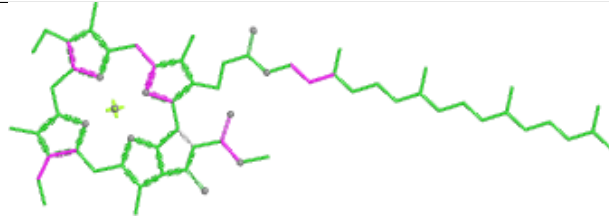
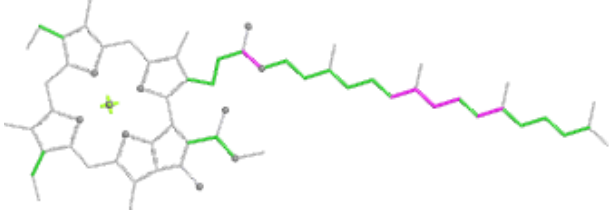
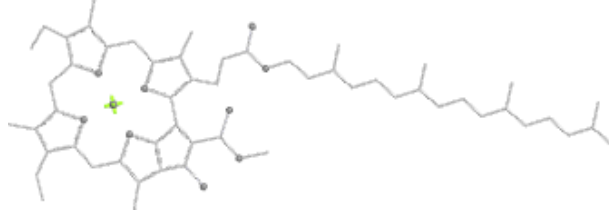


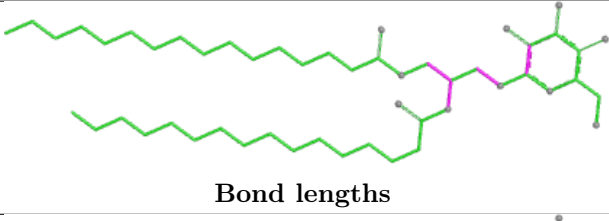
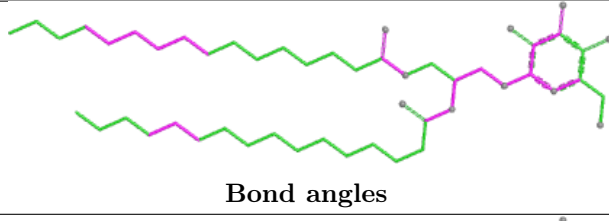
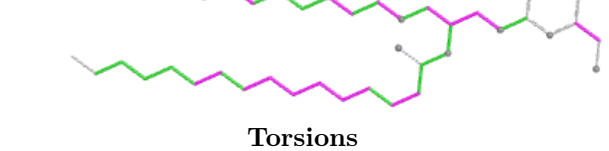


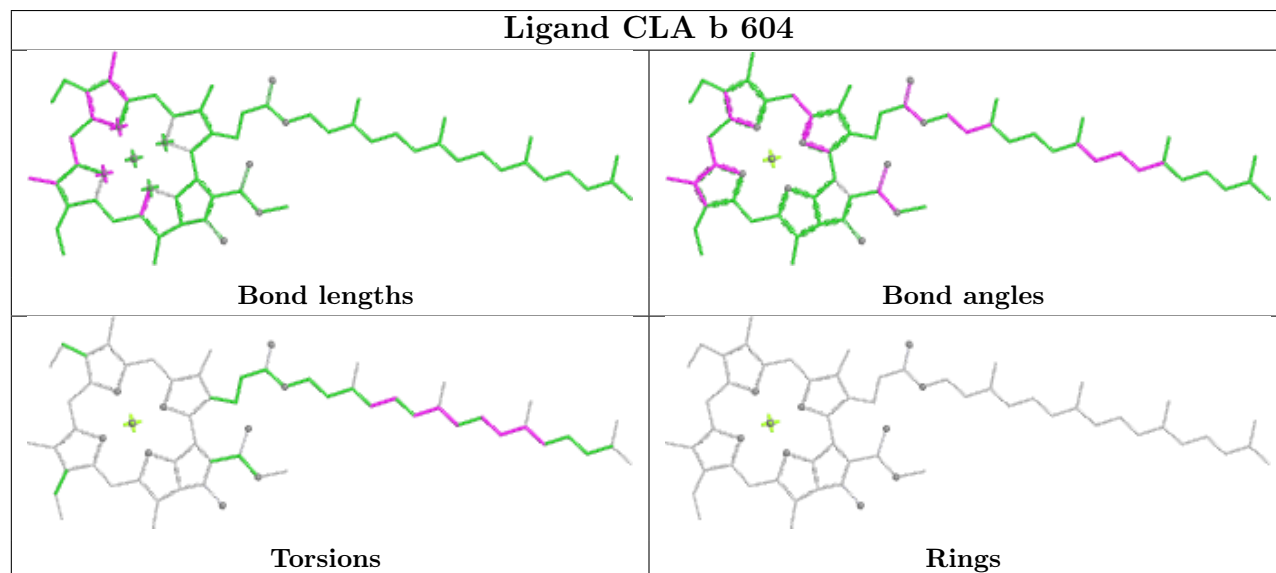
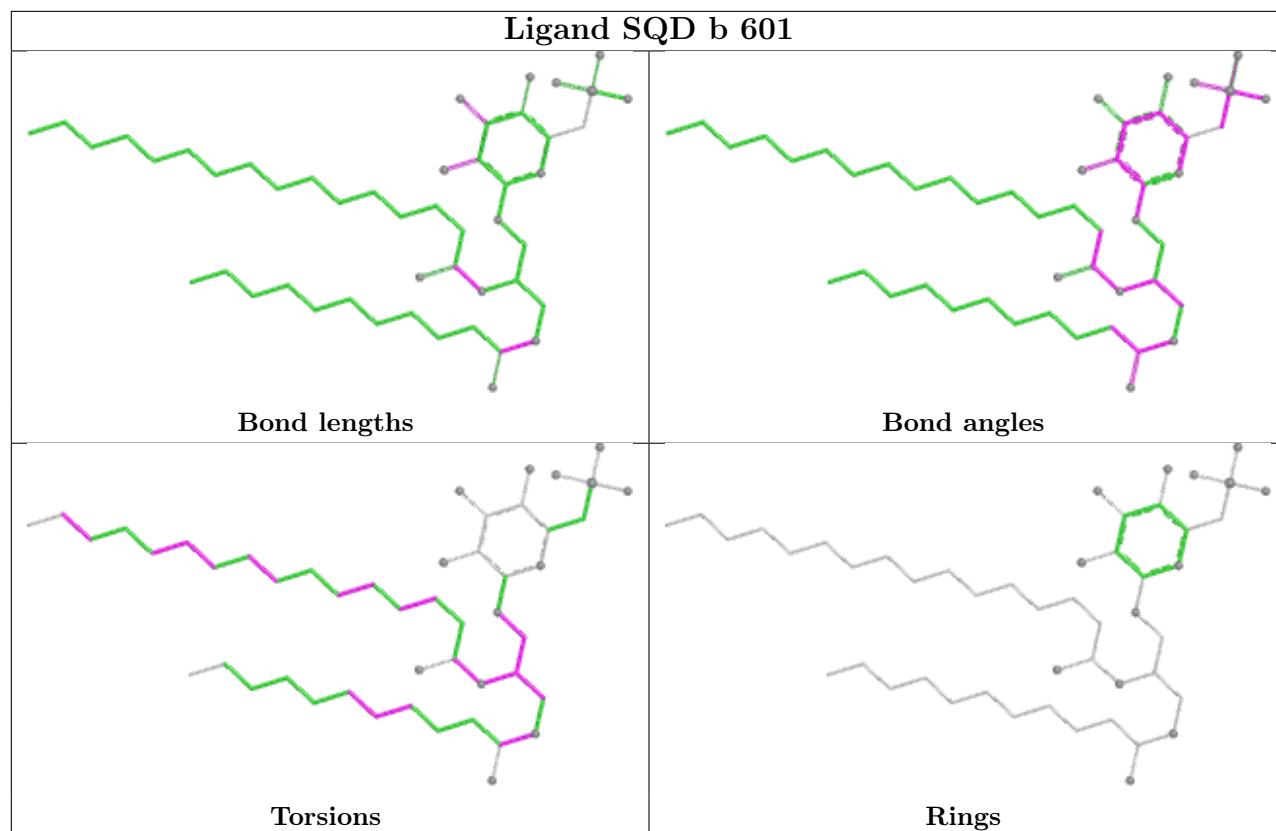
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 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR k 102	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG m 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

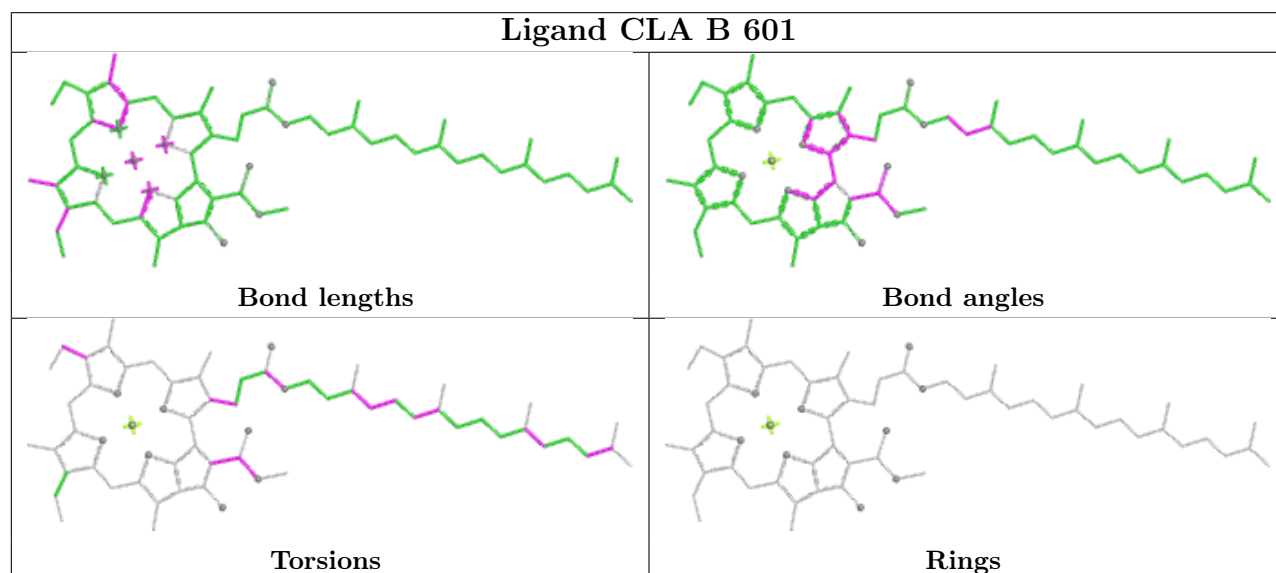
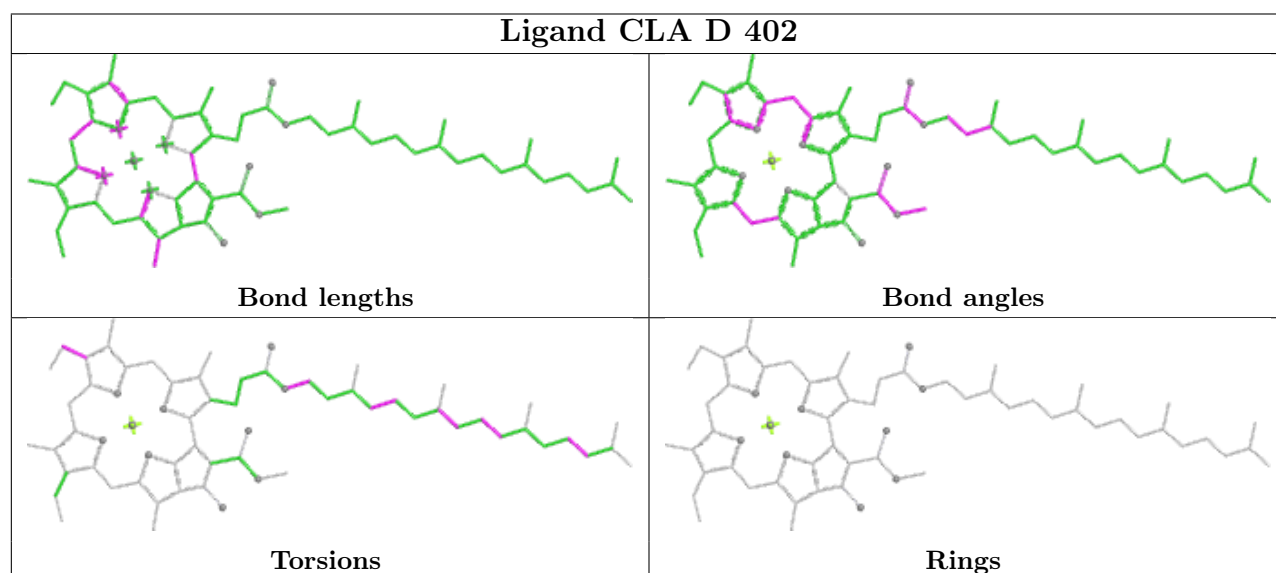
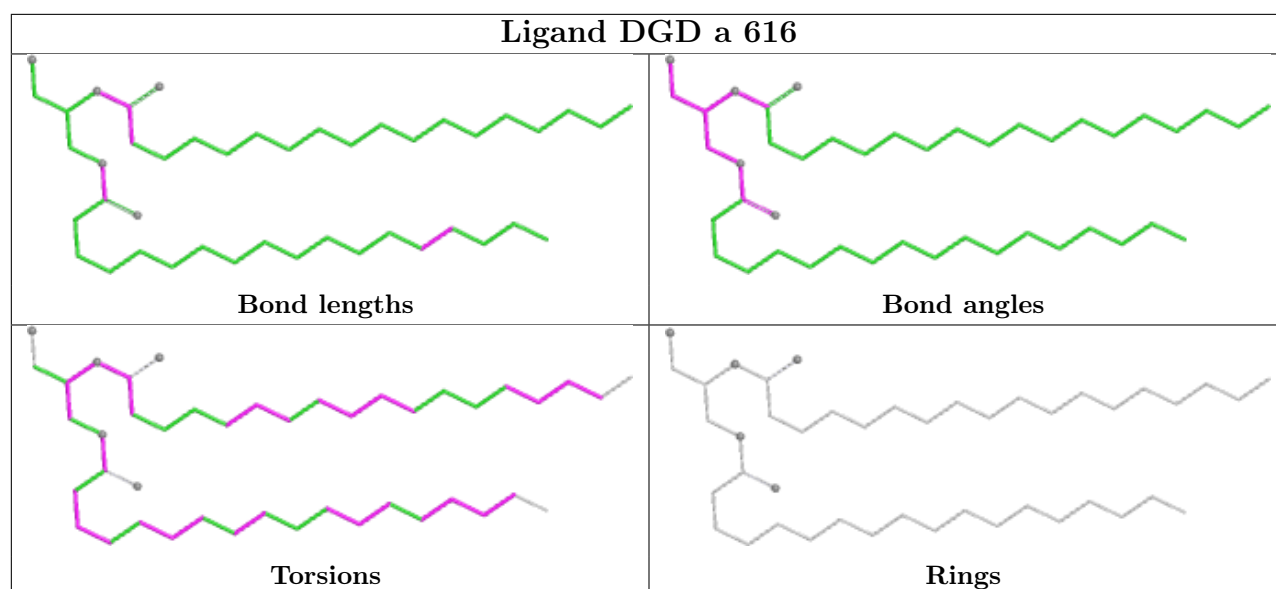


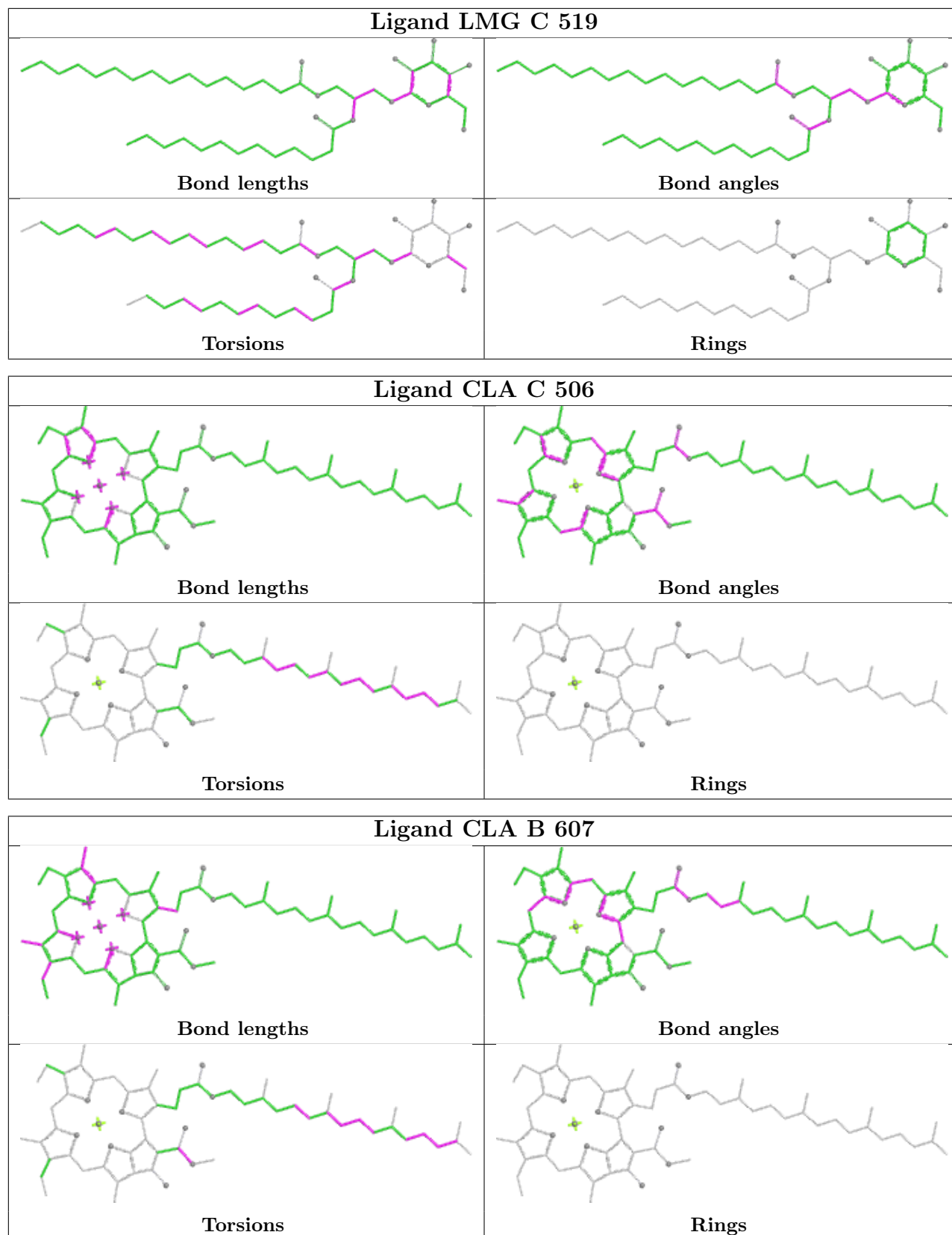
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Bond lengths	Bond angles
	
Torsions	Rings

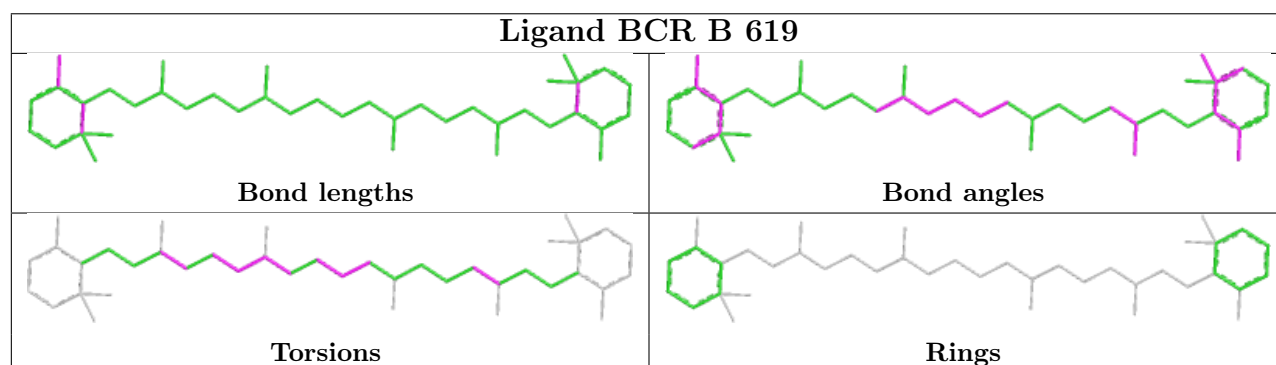
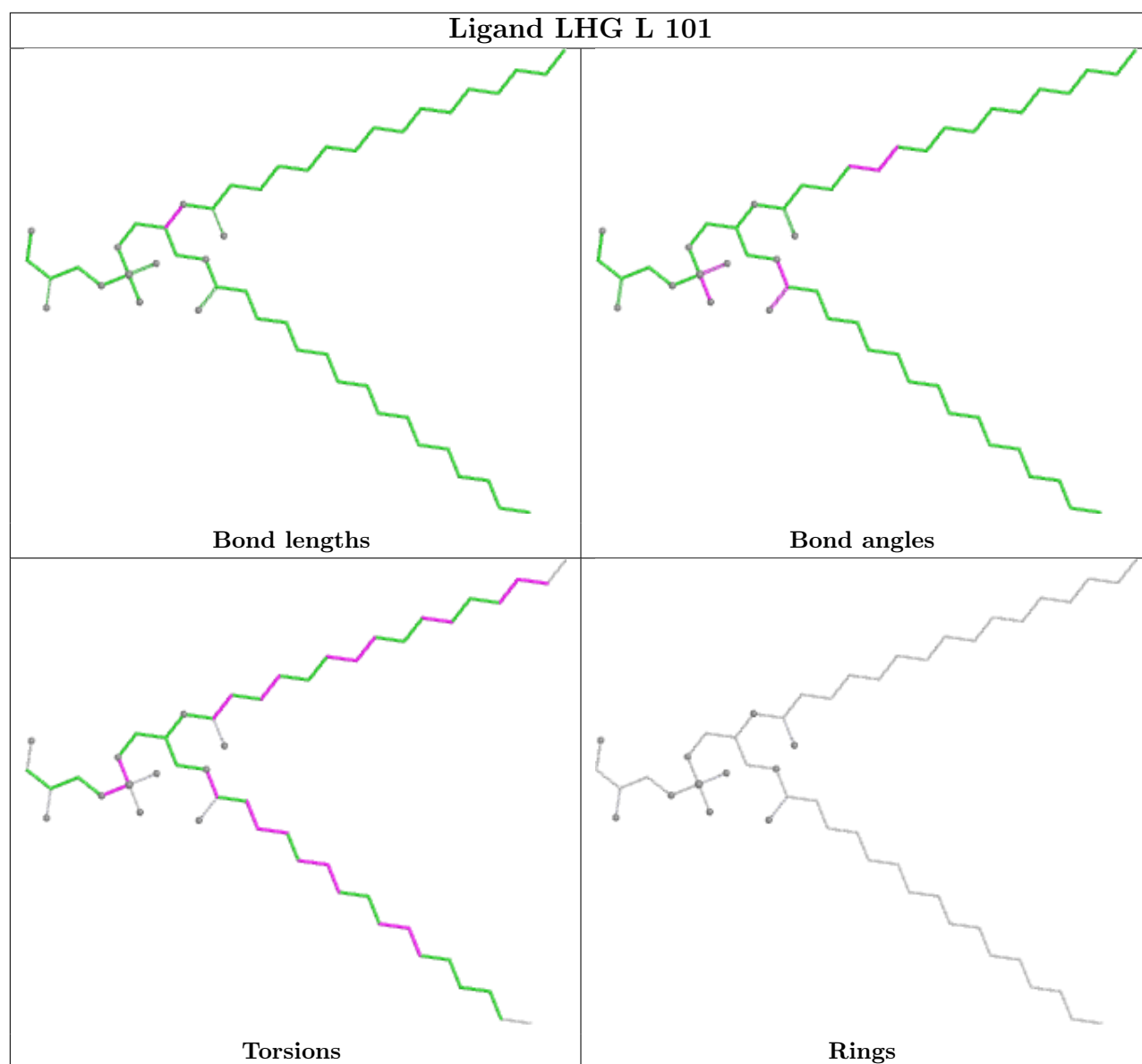
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Bond lengths	Bond angles
	
Torsions	Rings

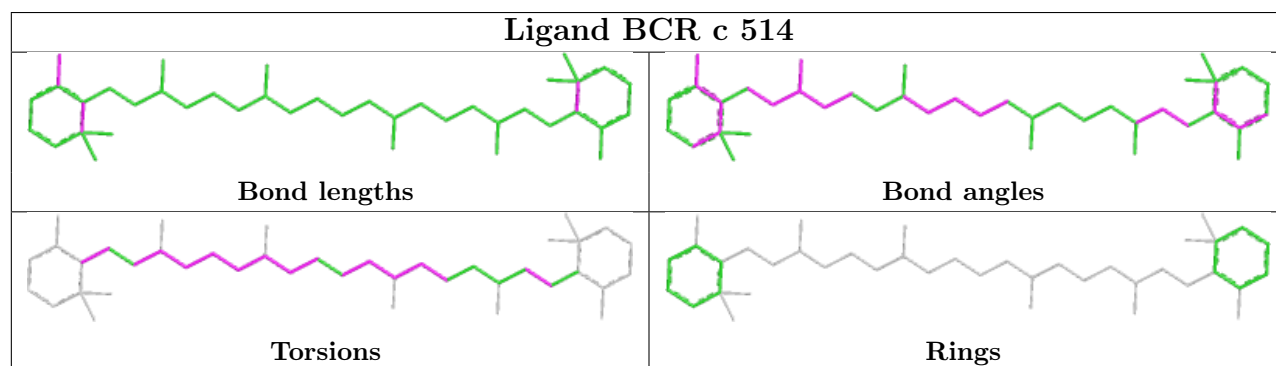
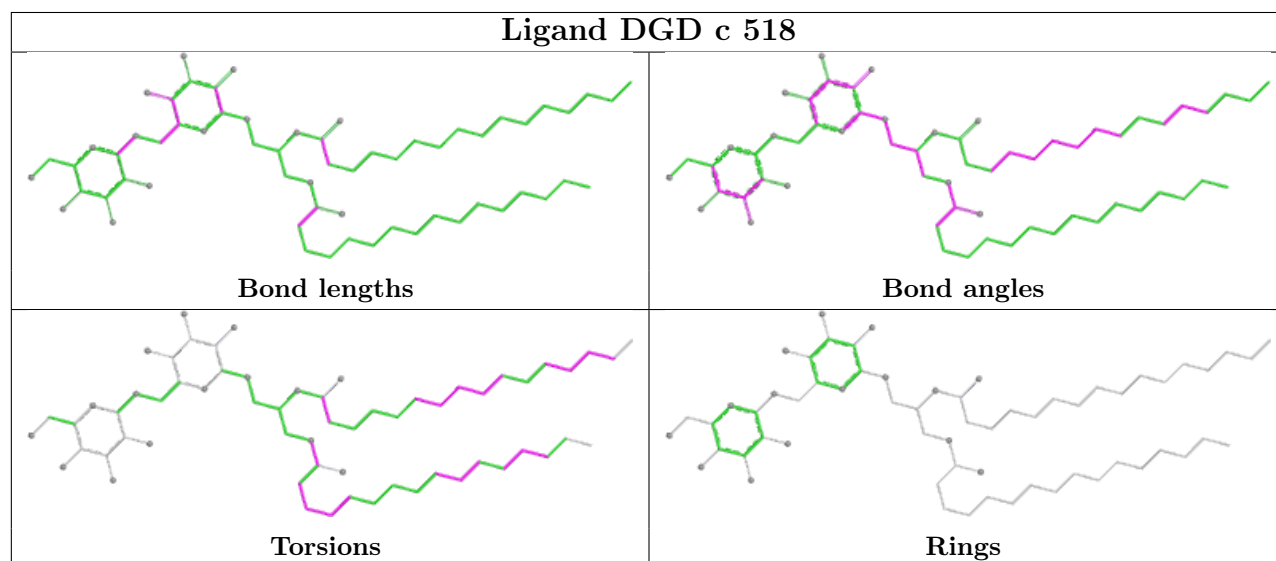
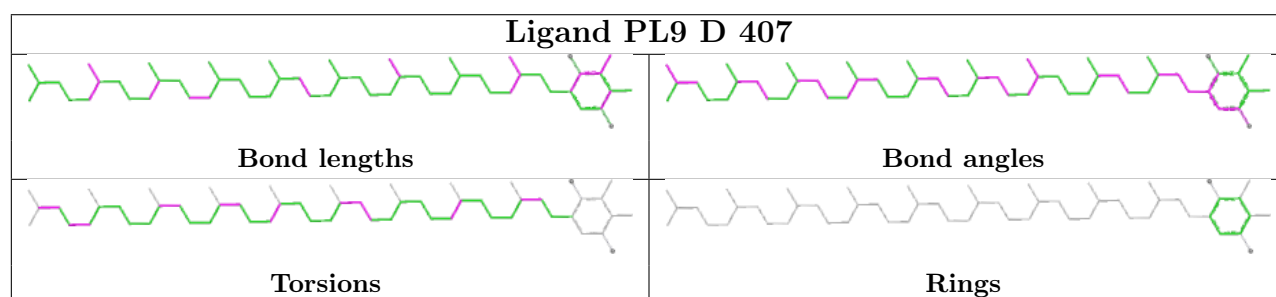
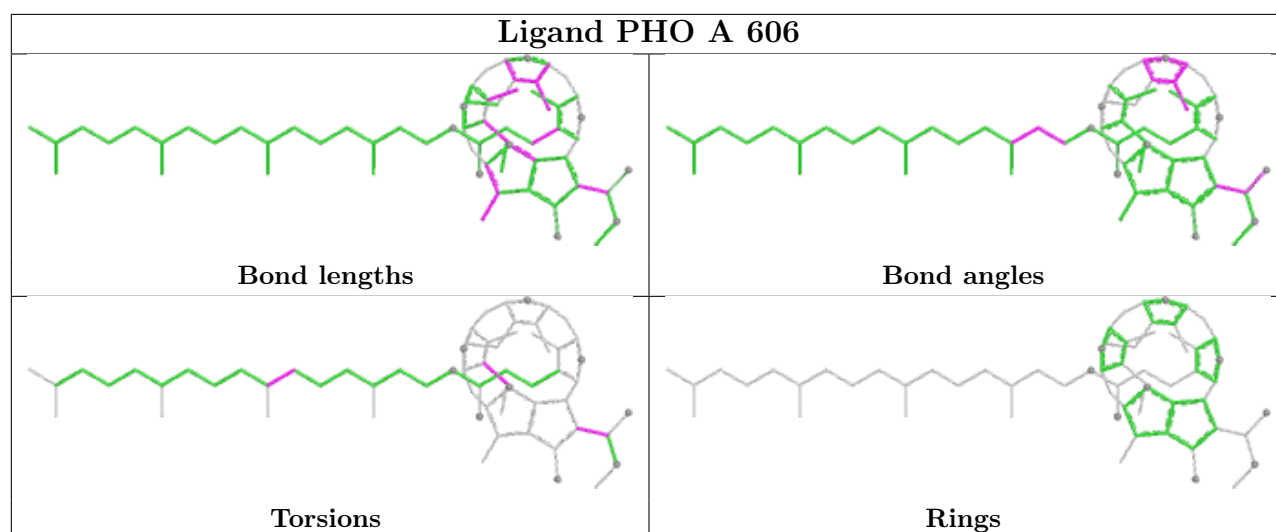
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Bond lengths	Bond angles
	
Torsions	Rings

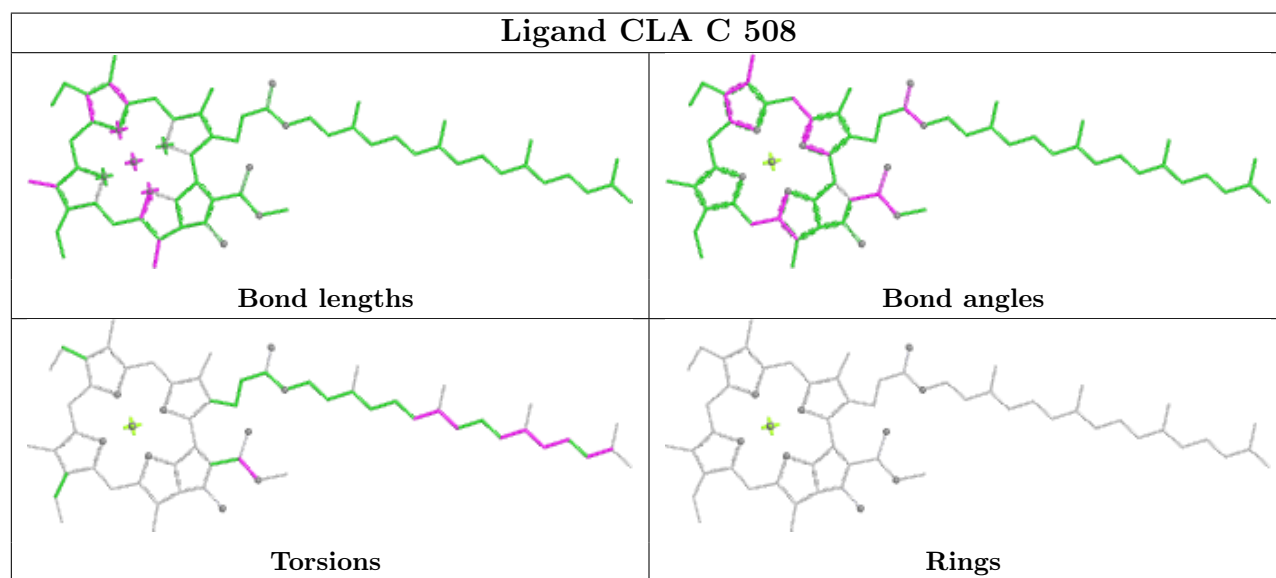
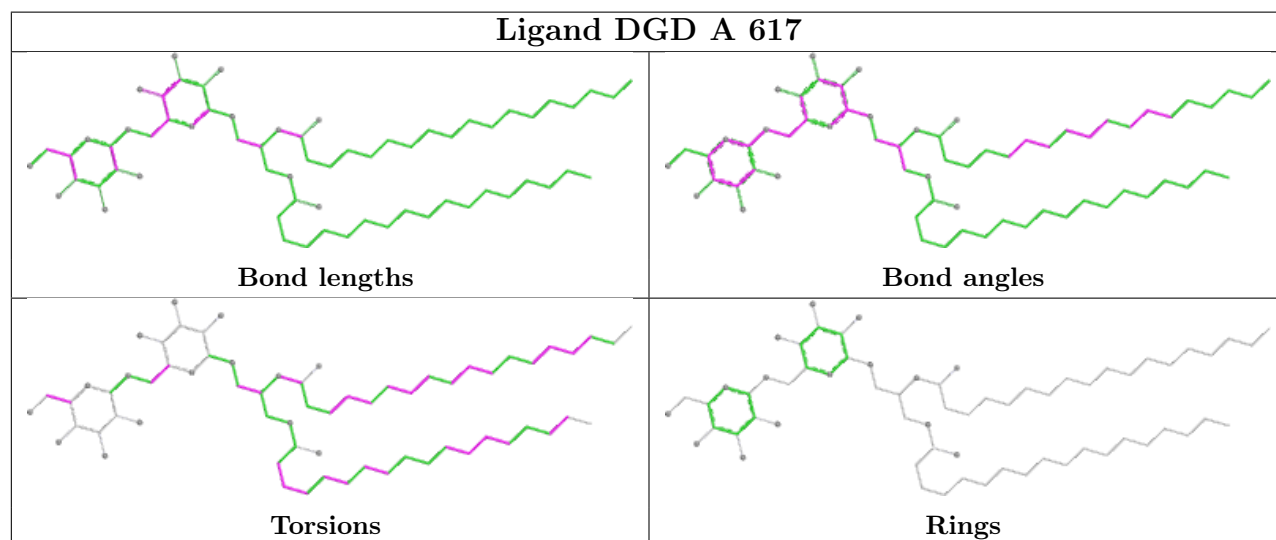
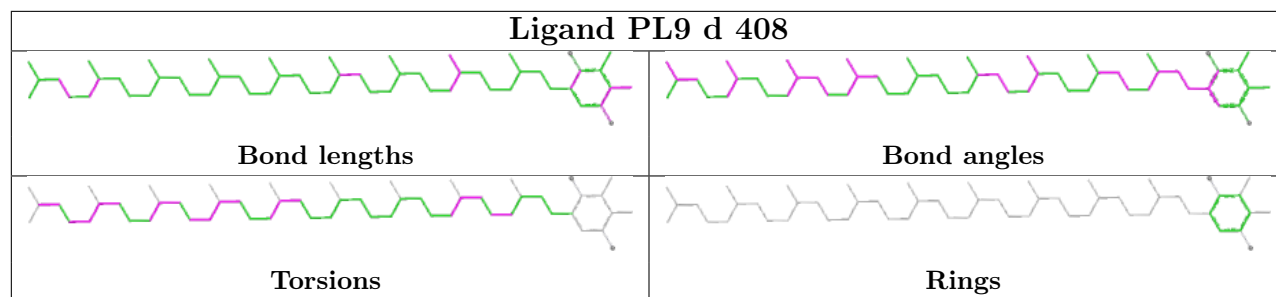


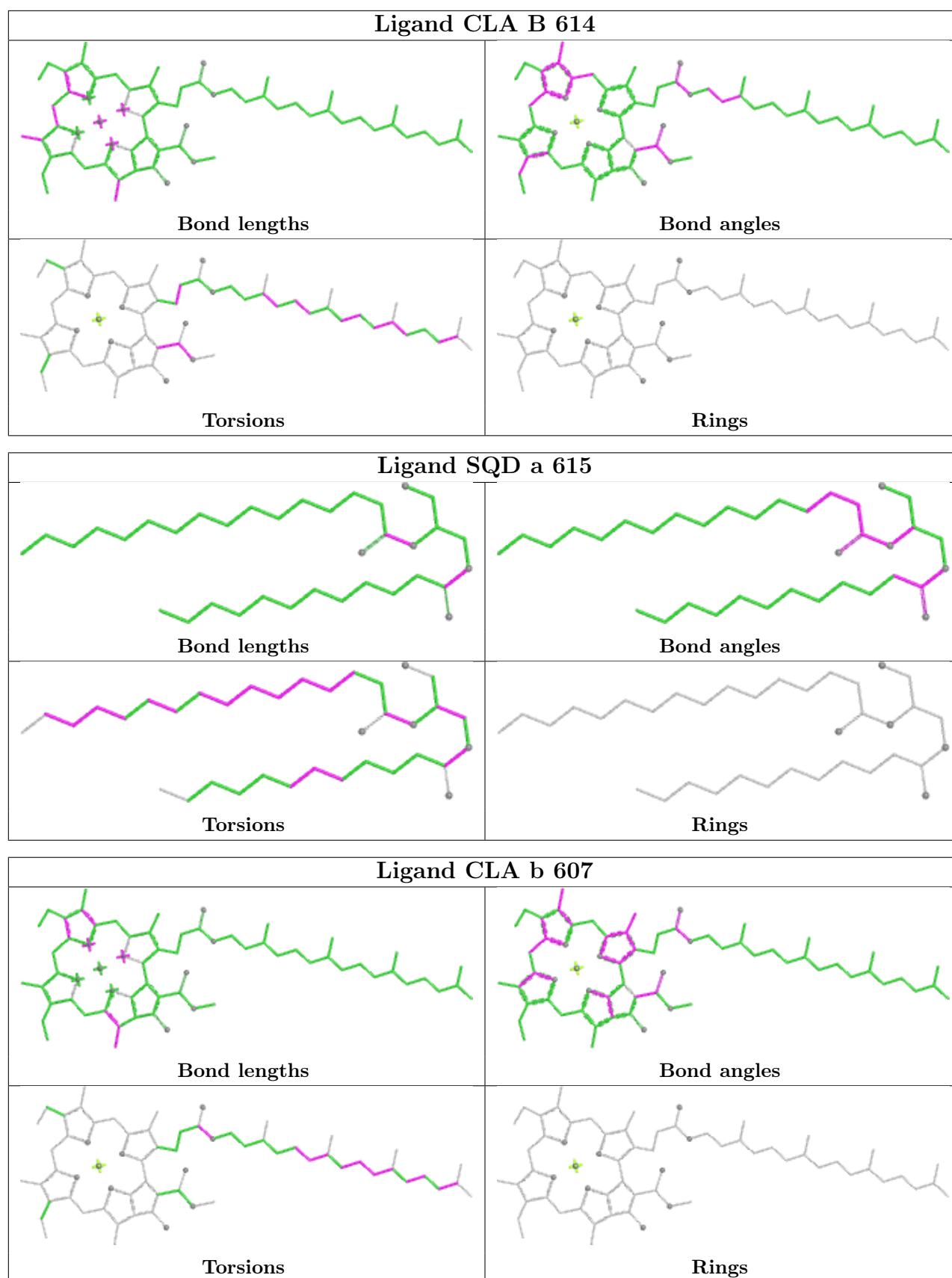


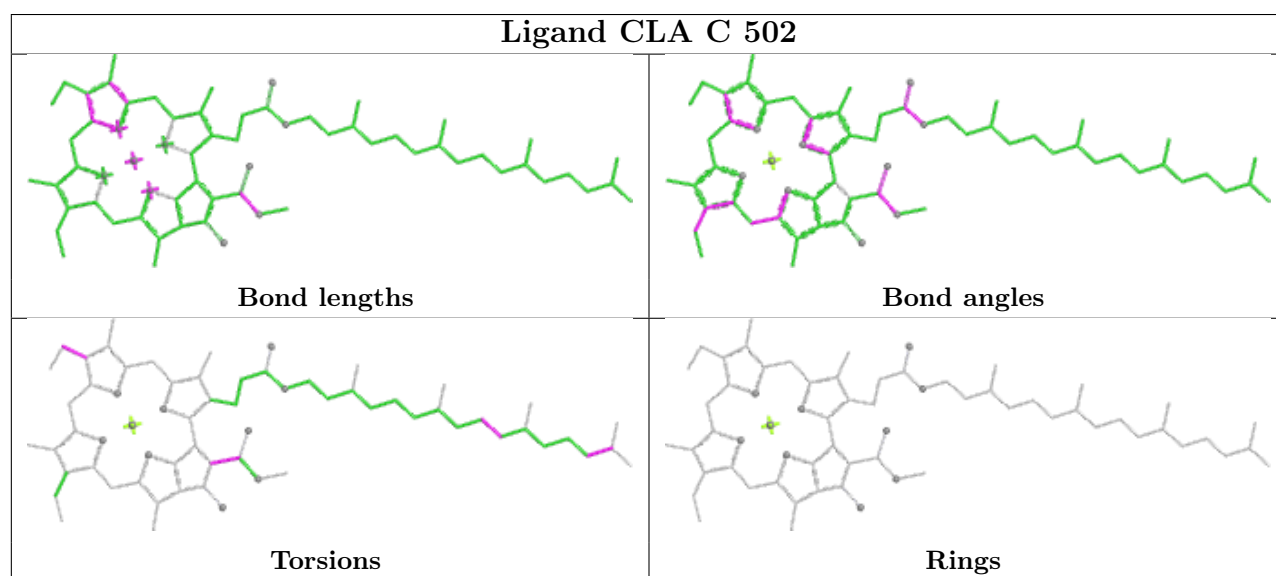
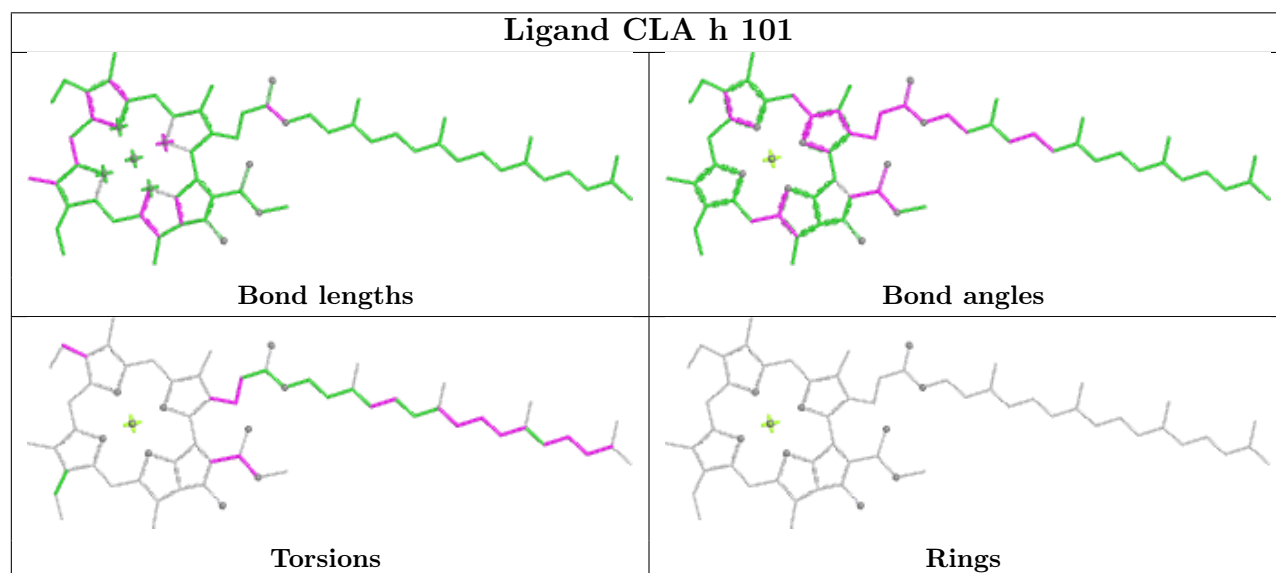
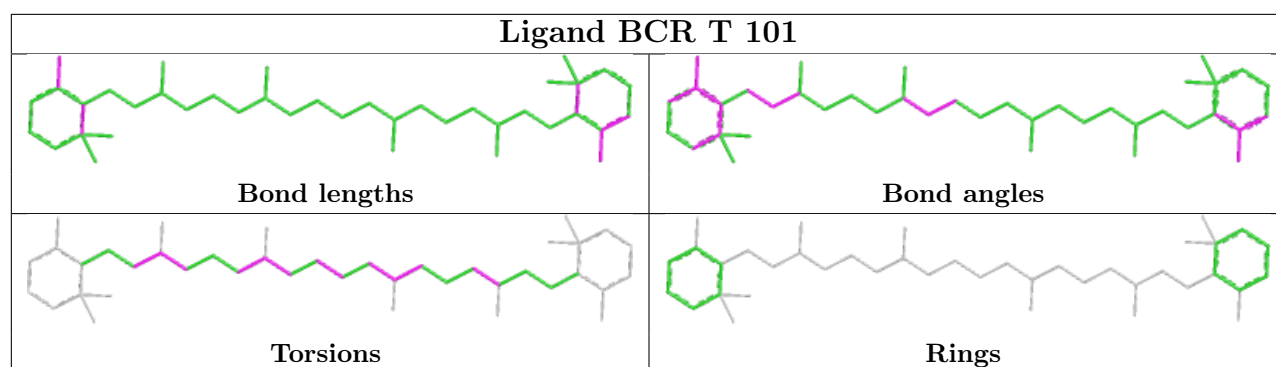


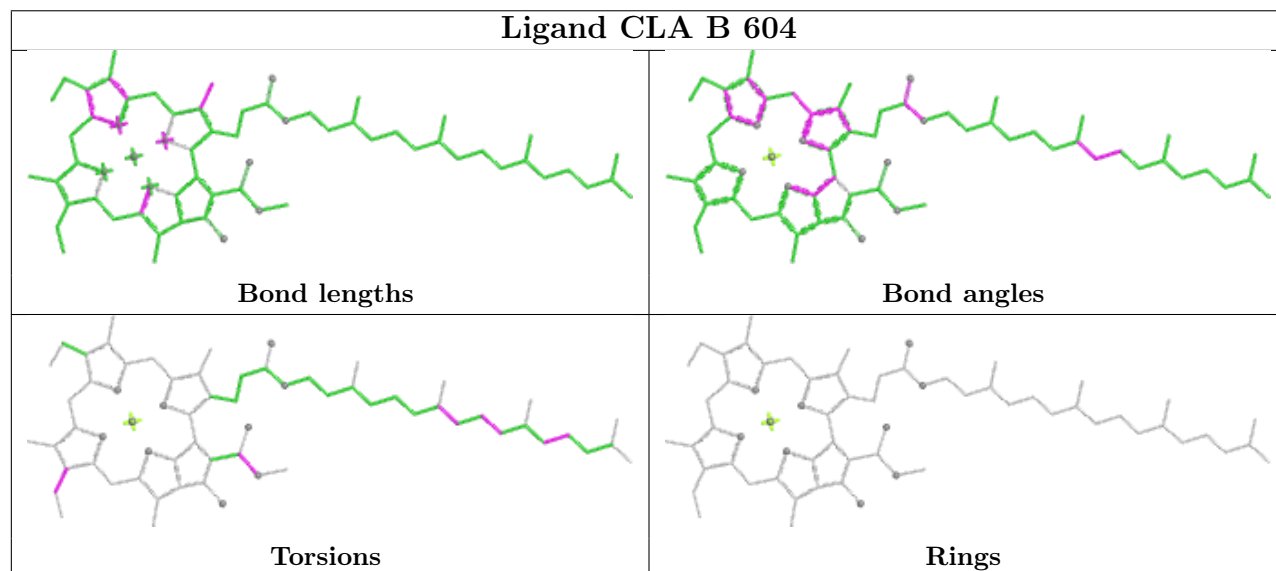
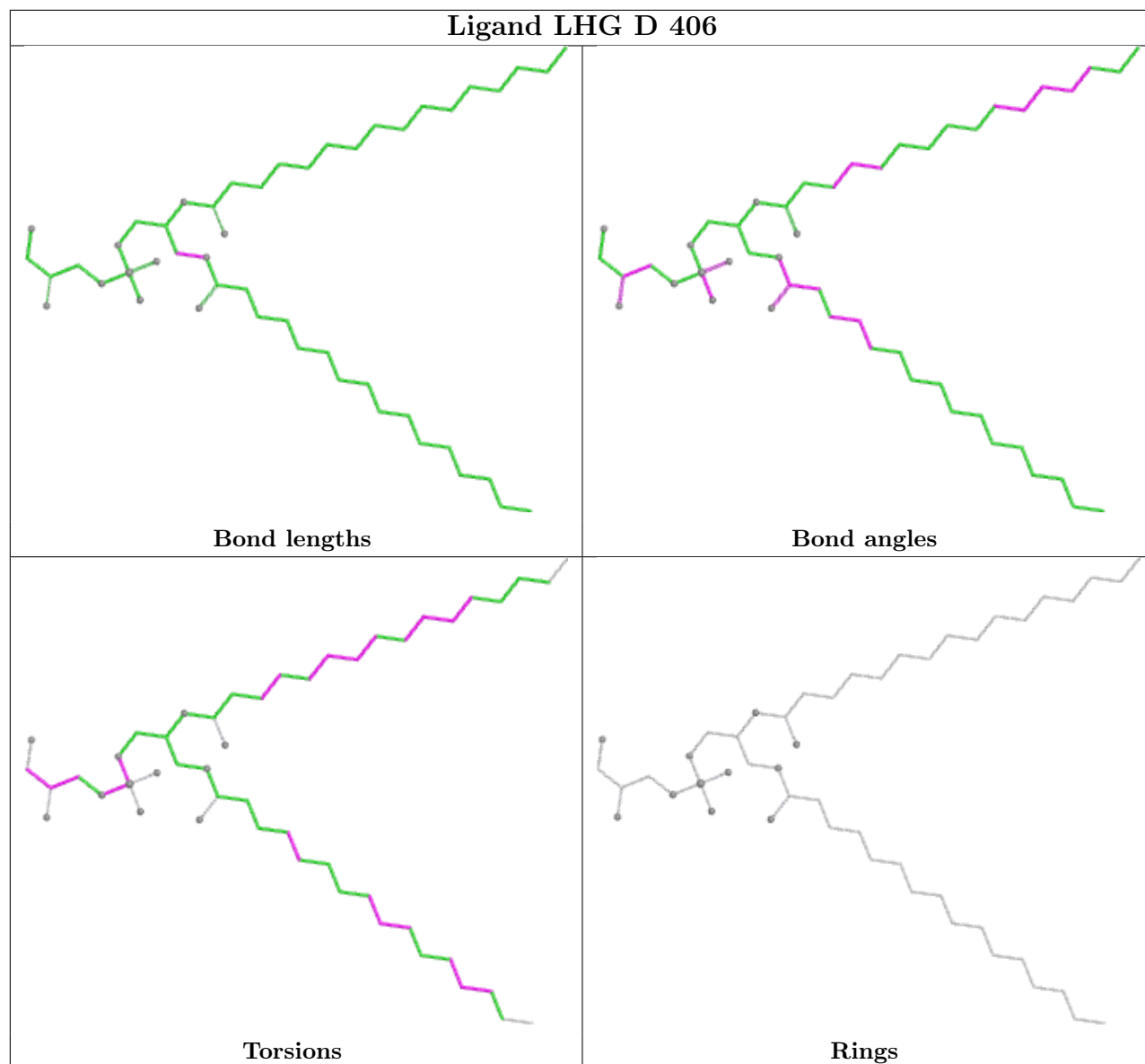




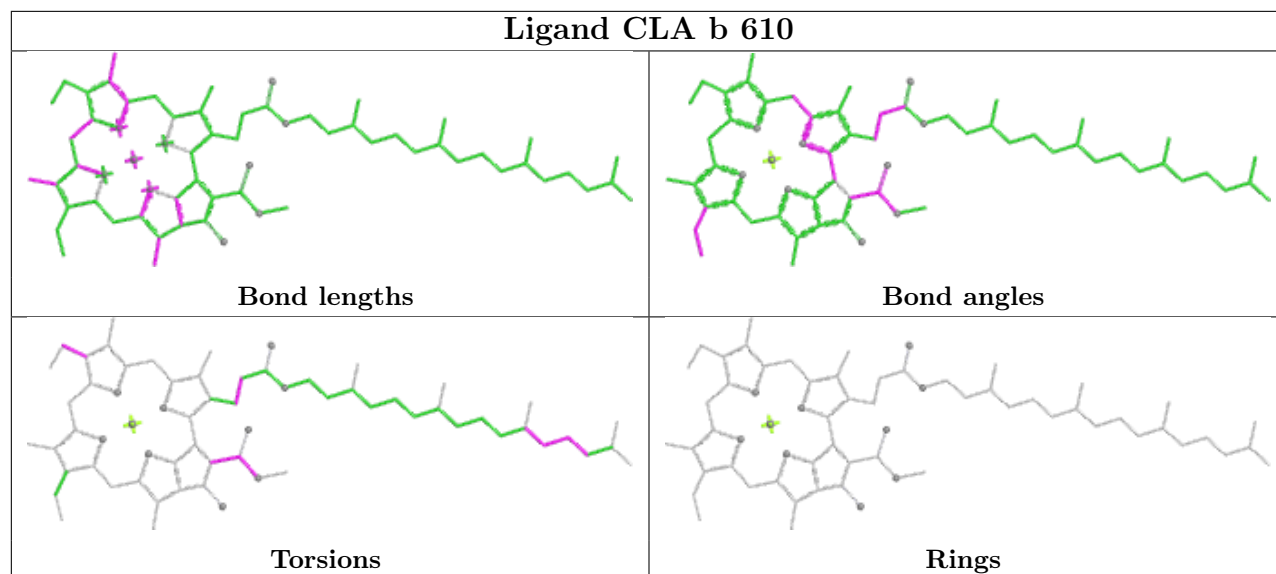




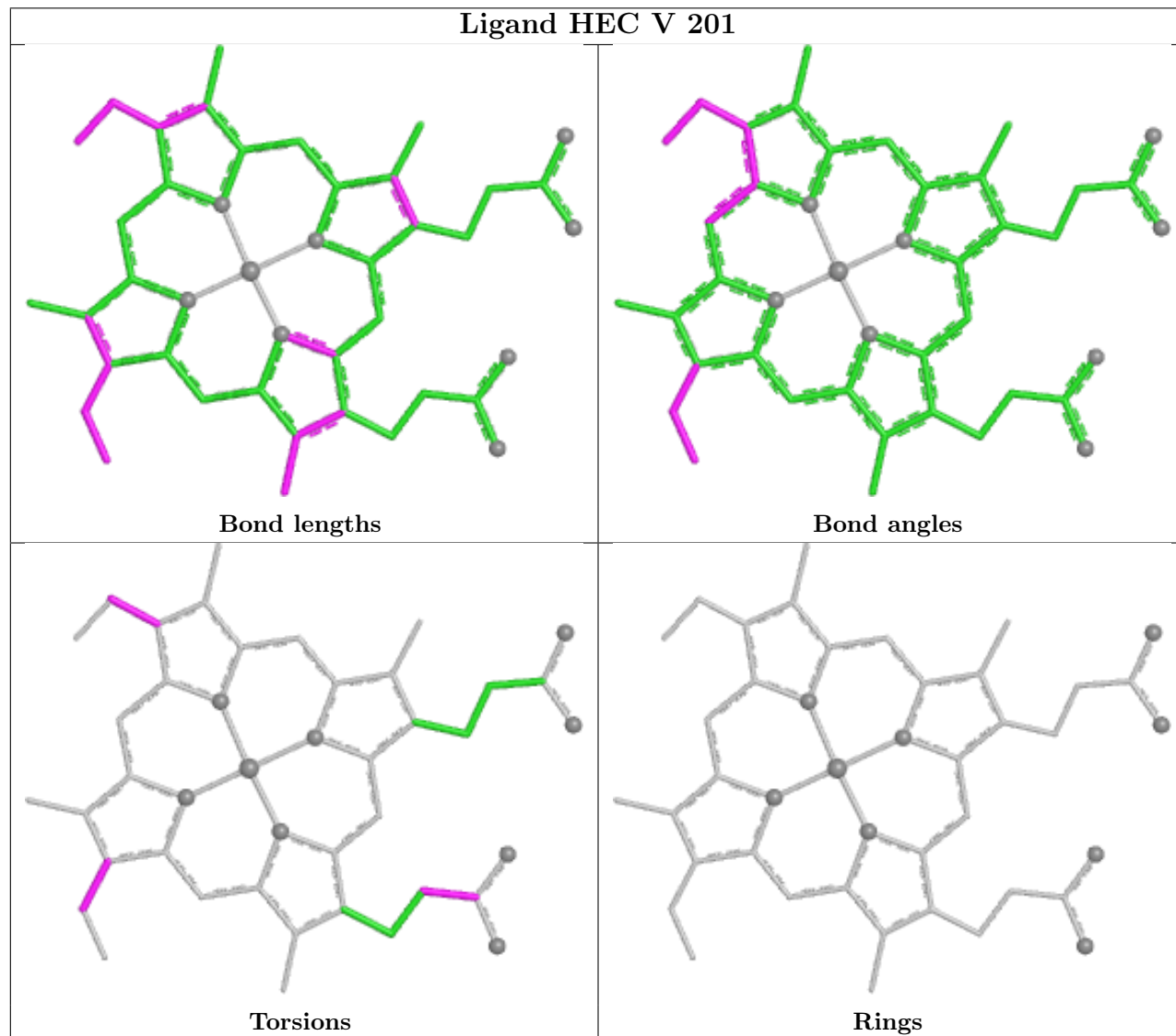


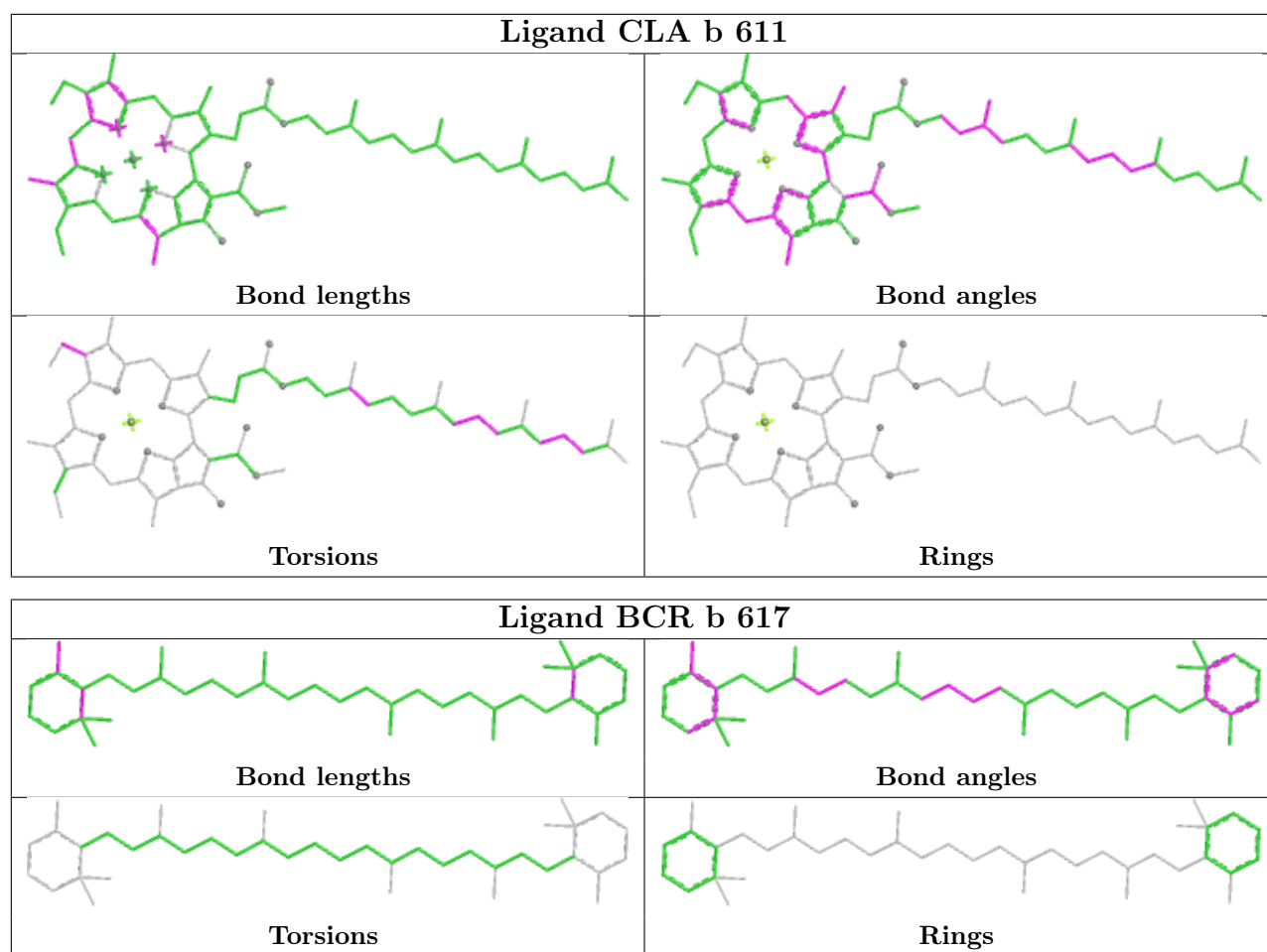


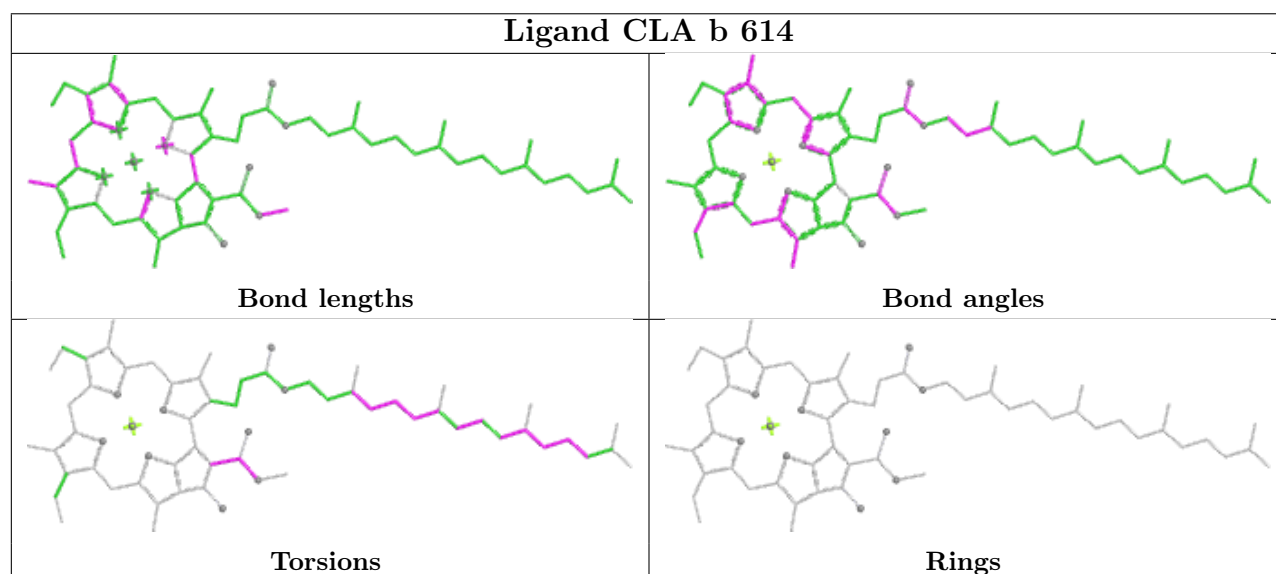
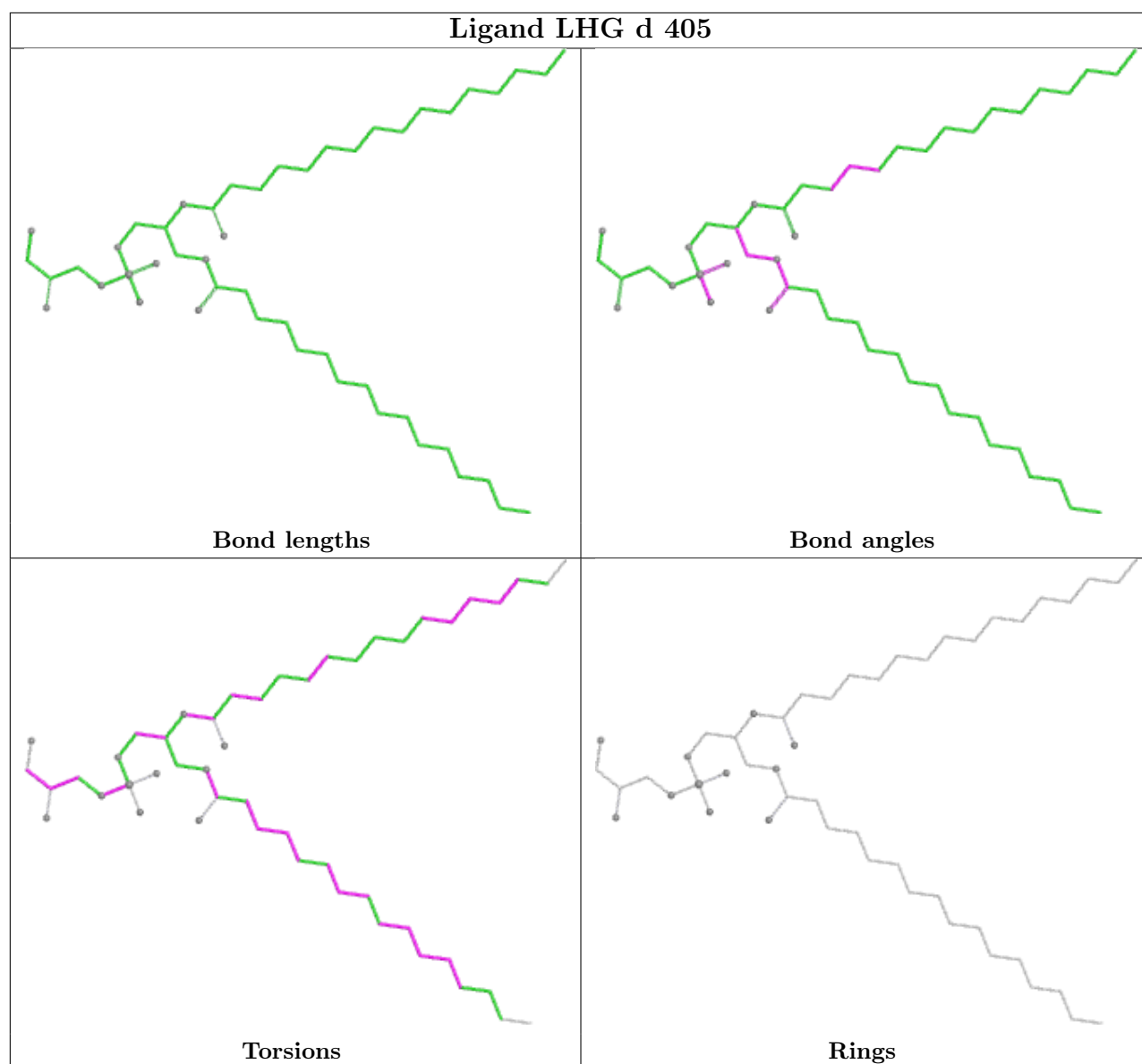
Ligand CLA b 610

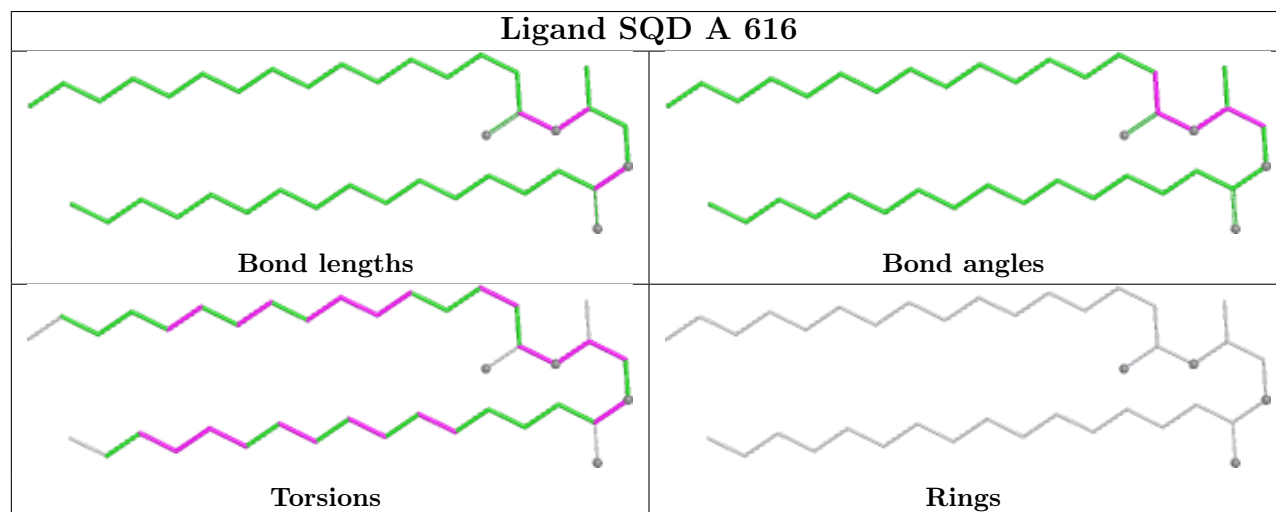
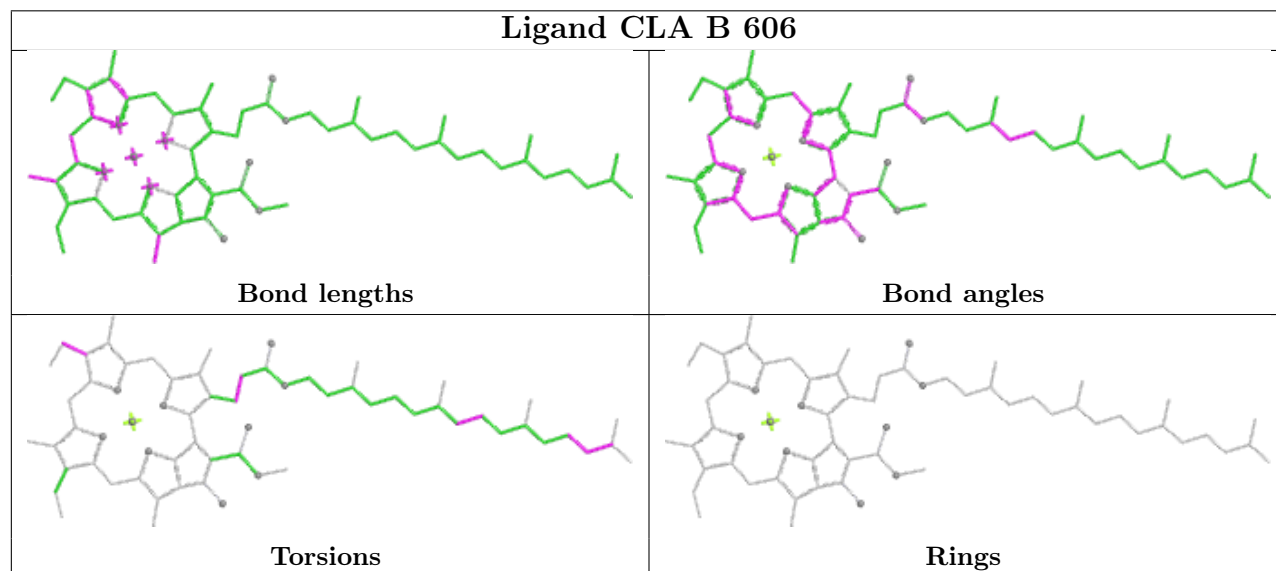
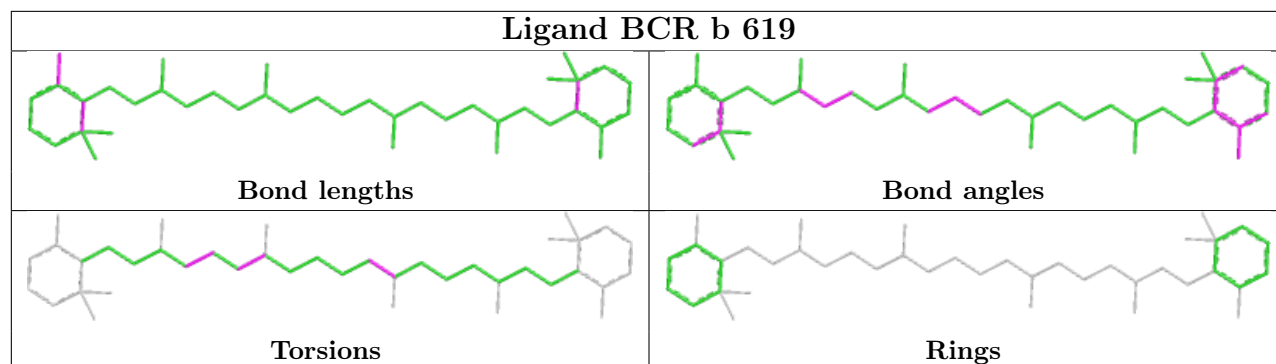


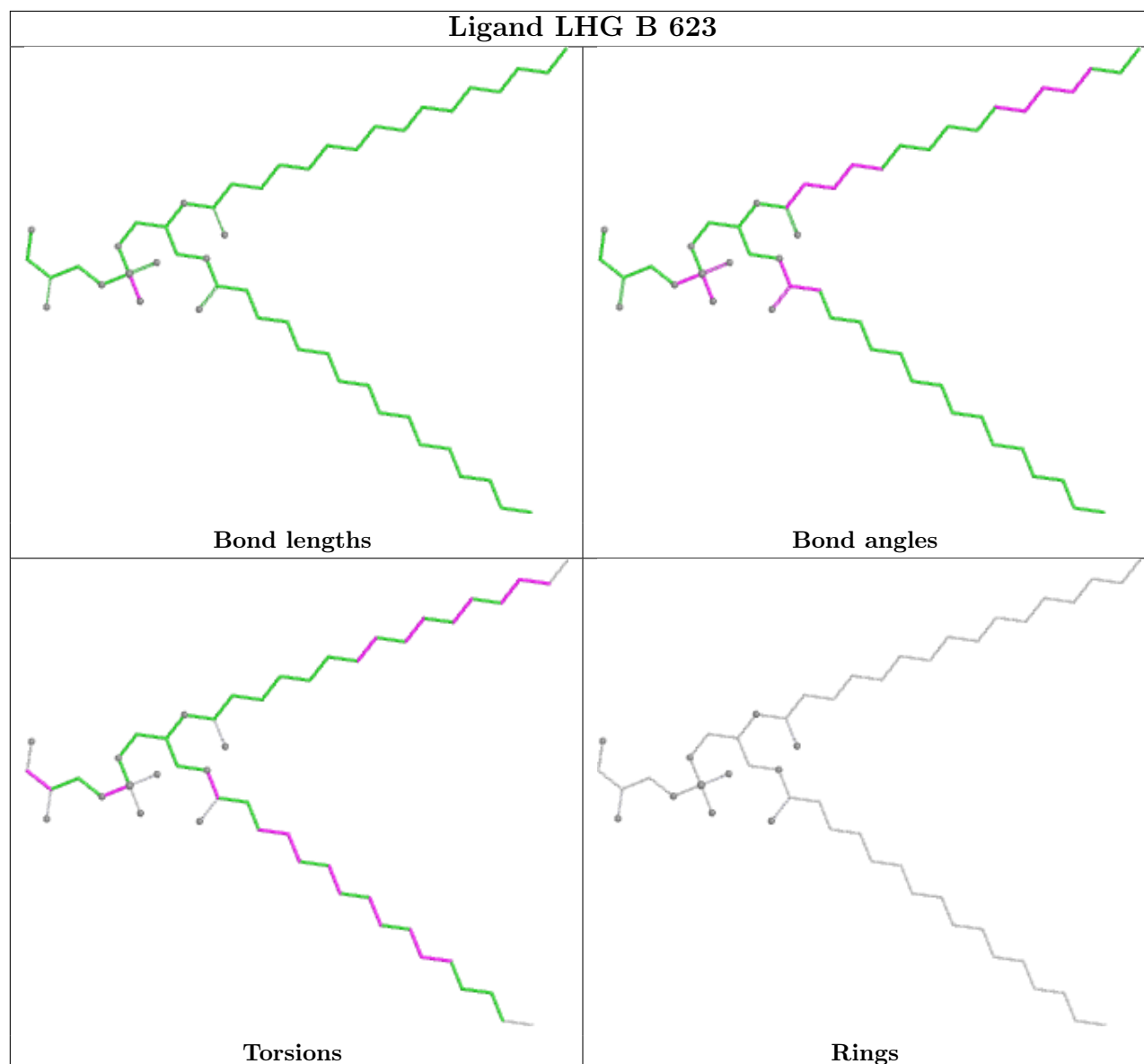
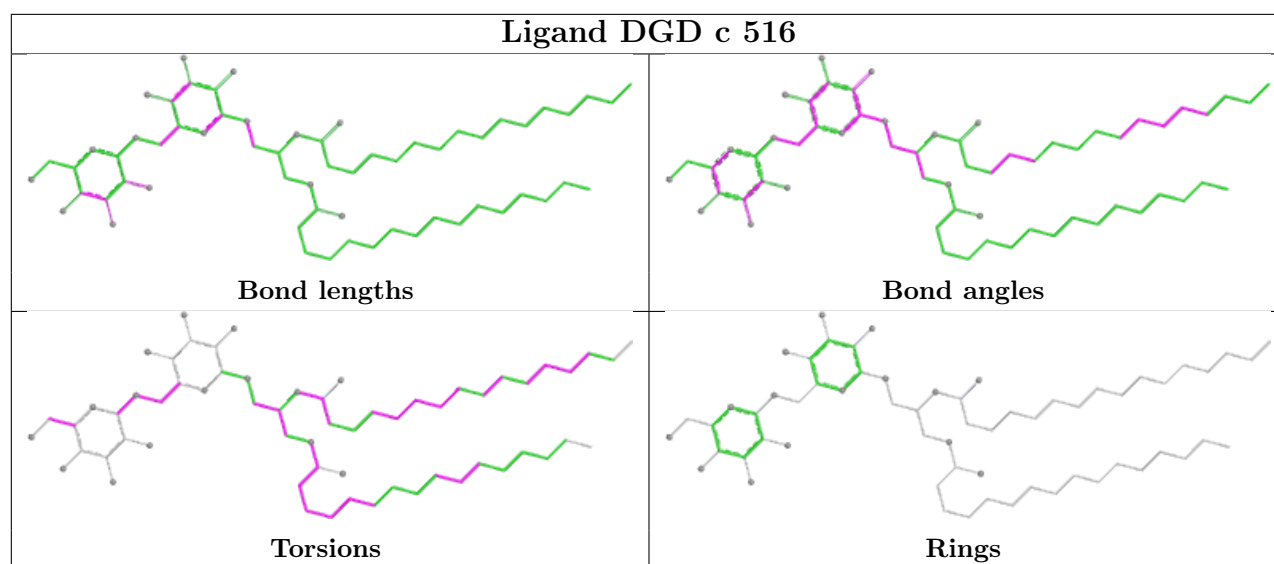
Ligand HEC V 201

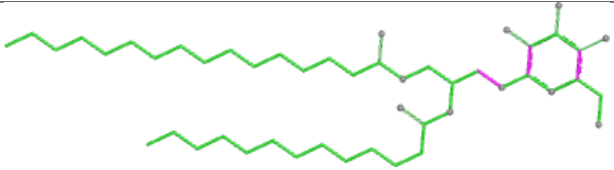
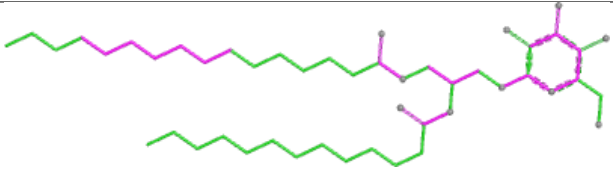
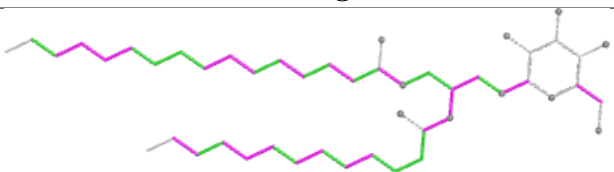
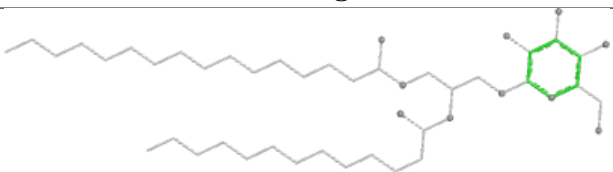


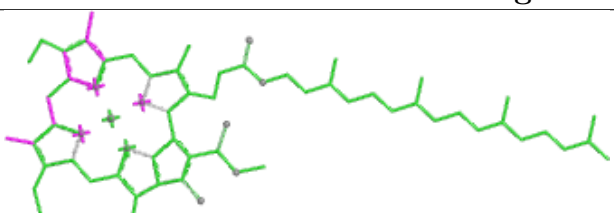
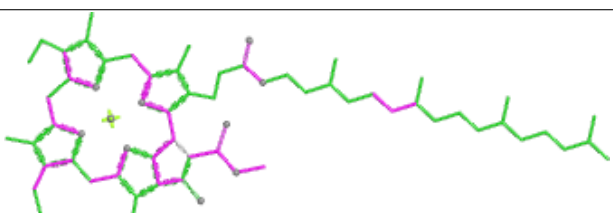
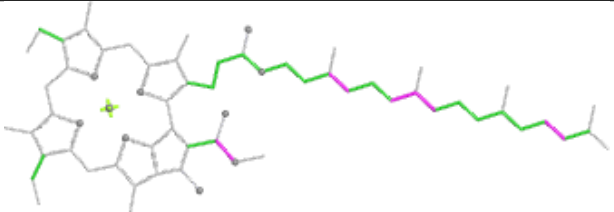
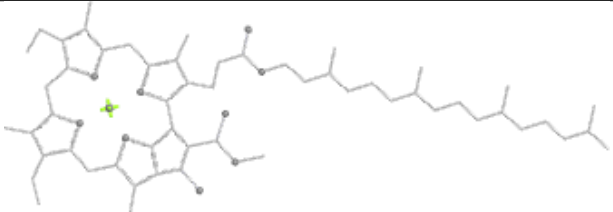


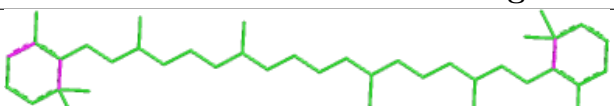
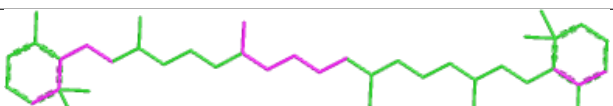
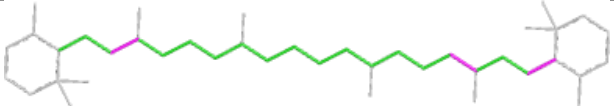
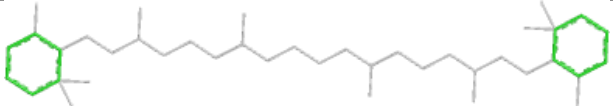




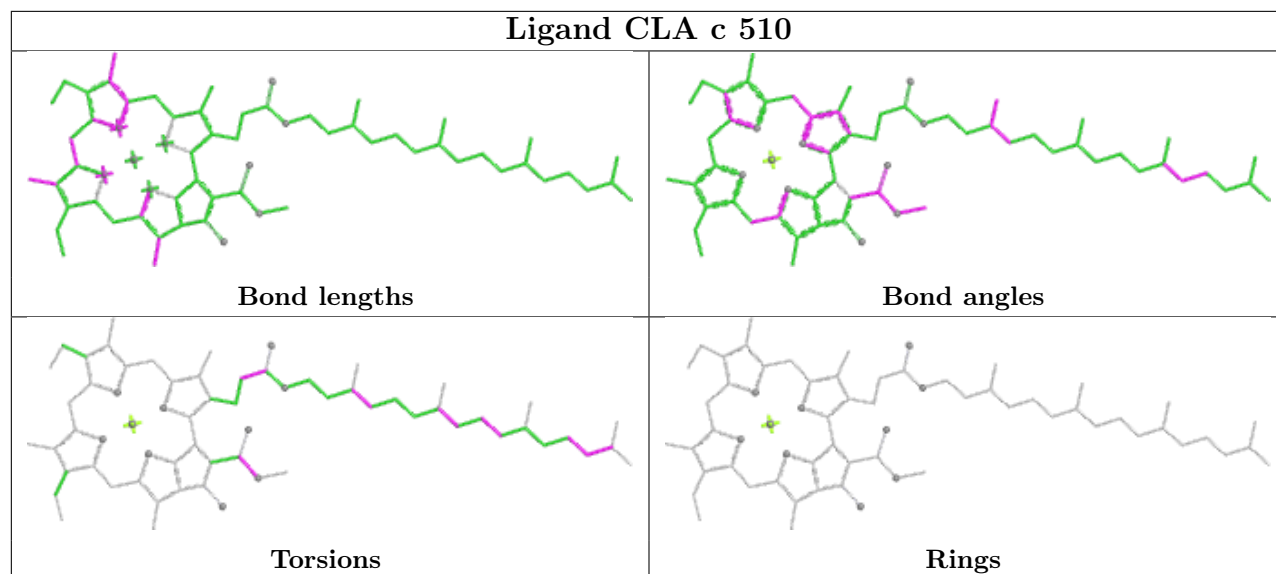


Ligand LMG A 612	
	
Bond lengths	Bond angles
	
Torsions	Rings

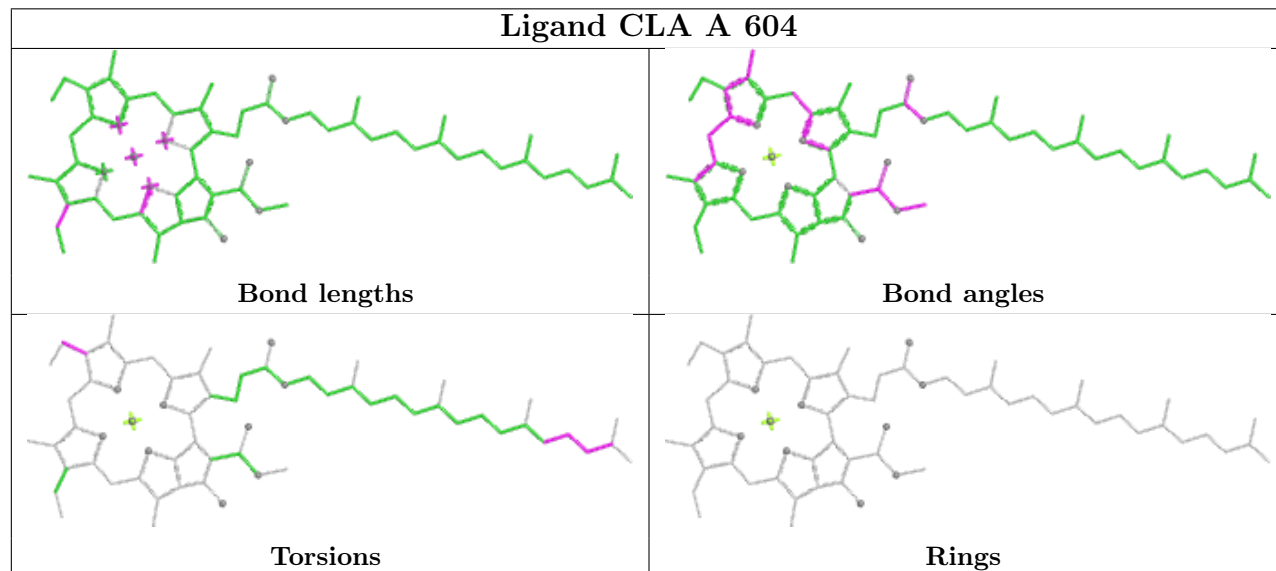
Ligand CLA c 505	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR B 618	
	
Bond lengths	Bond angles
	
Torsions	Rings

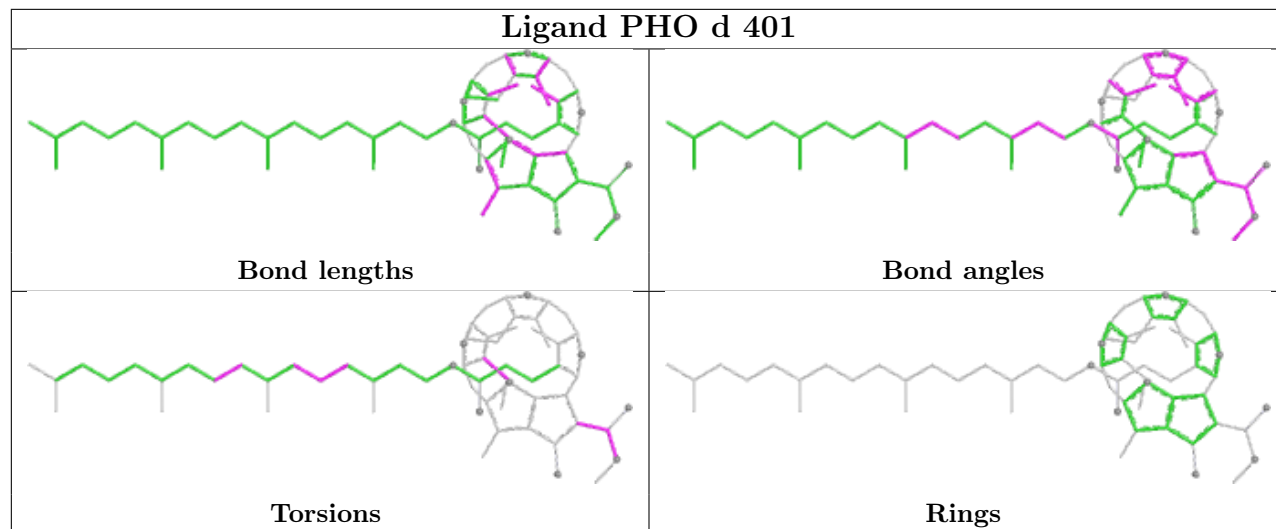
Ligand CLA c 510

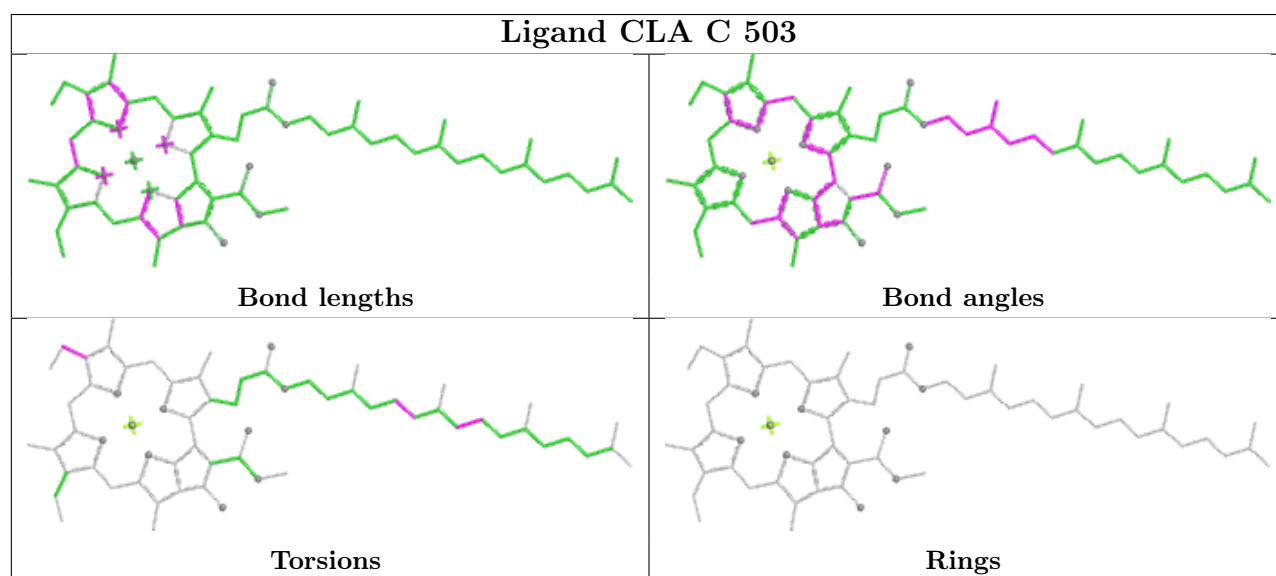
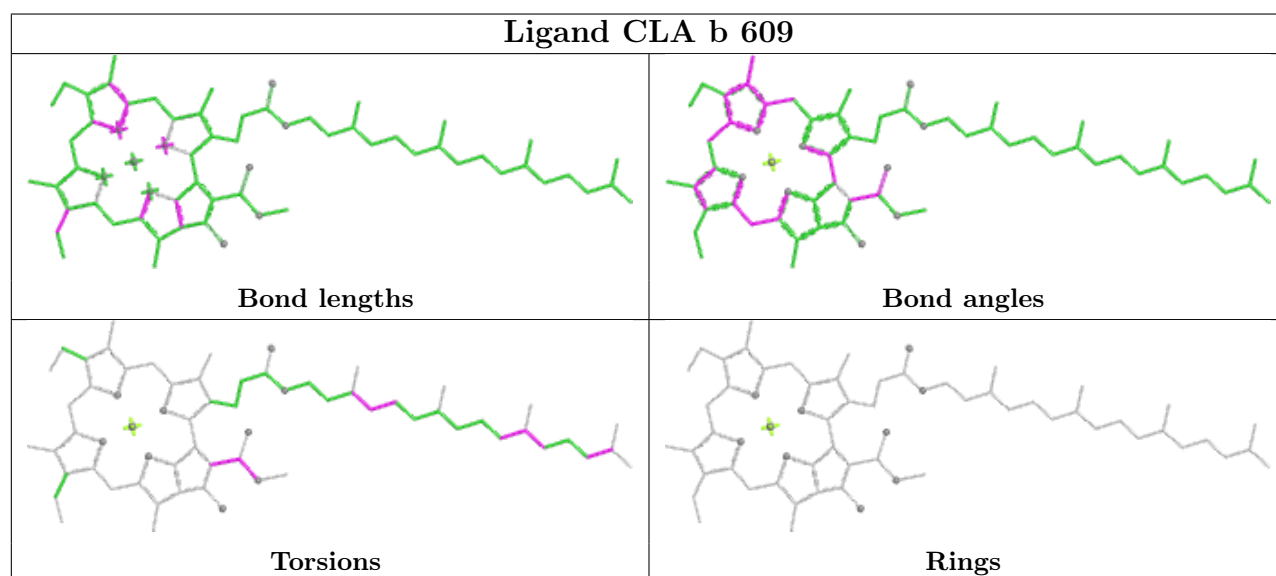
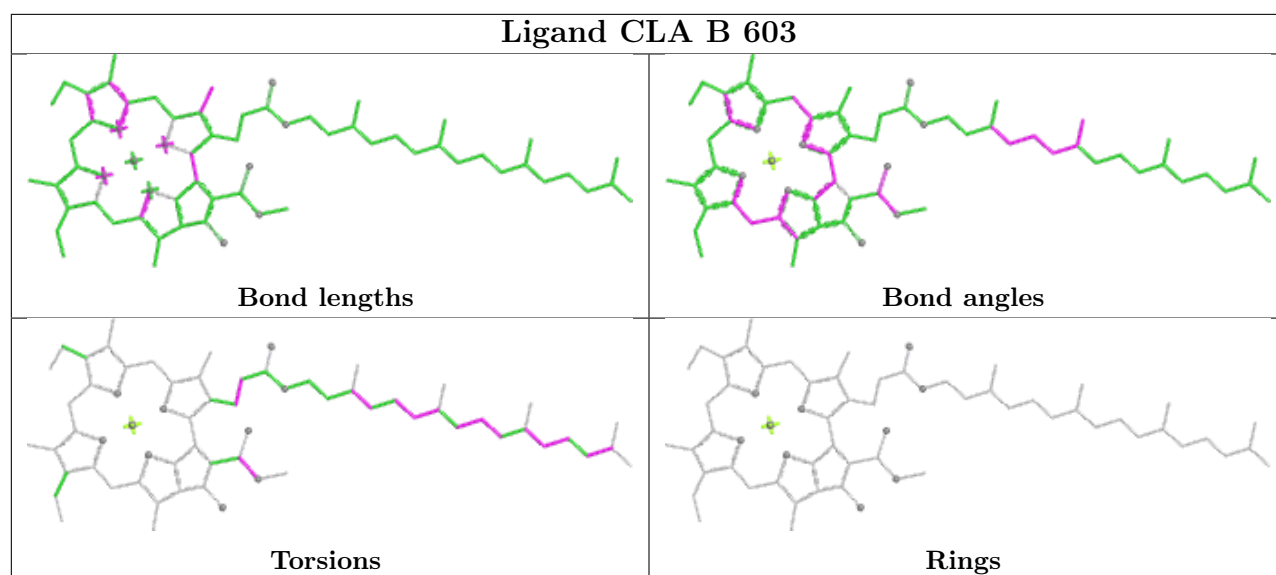


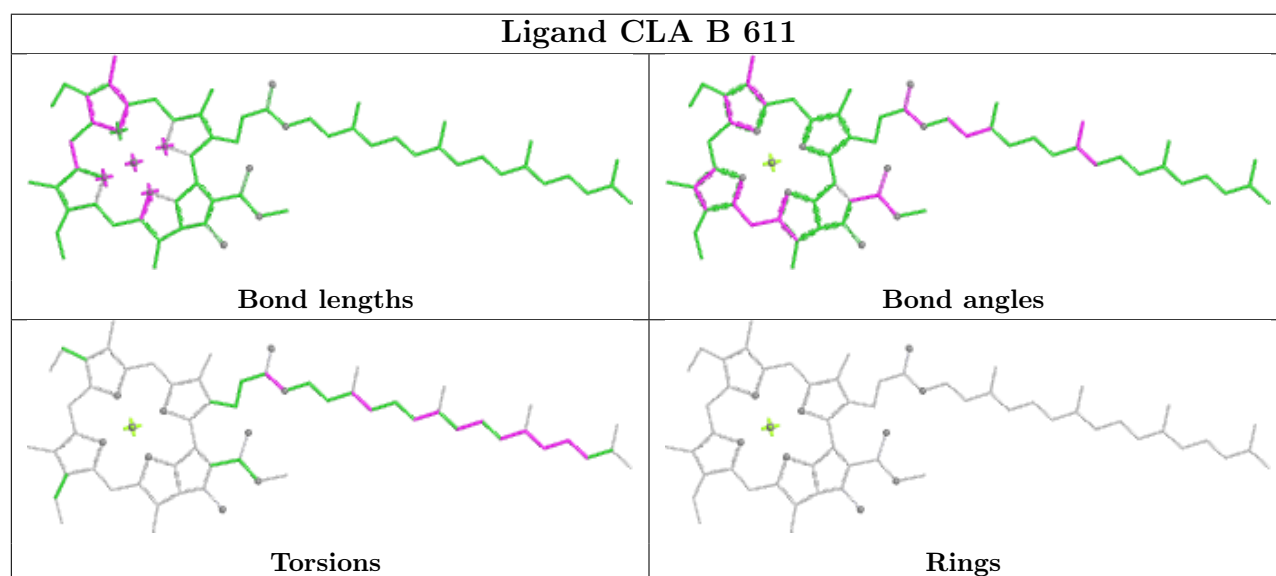
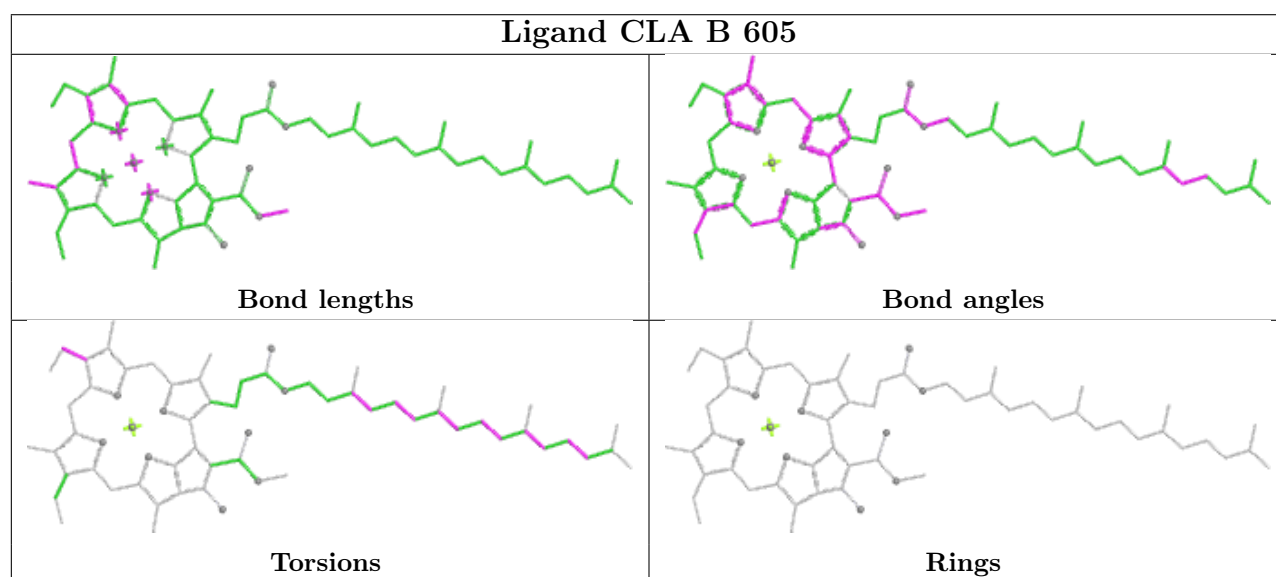
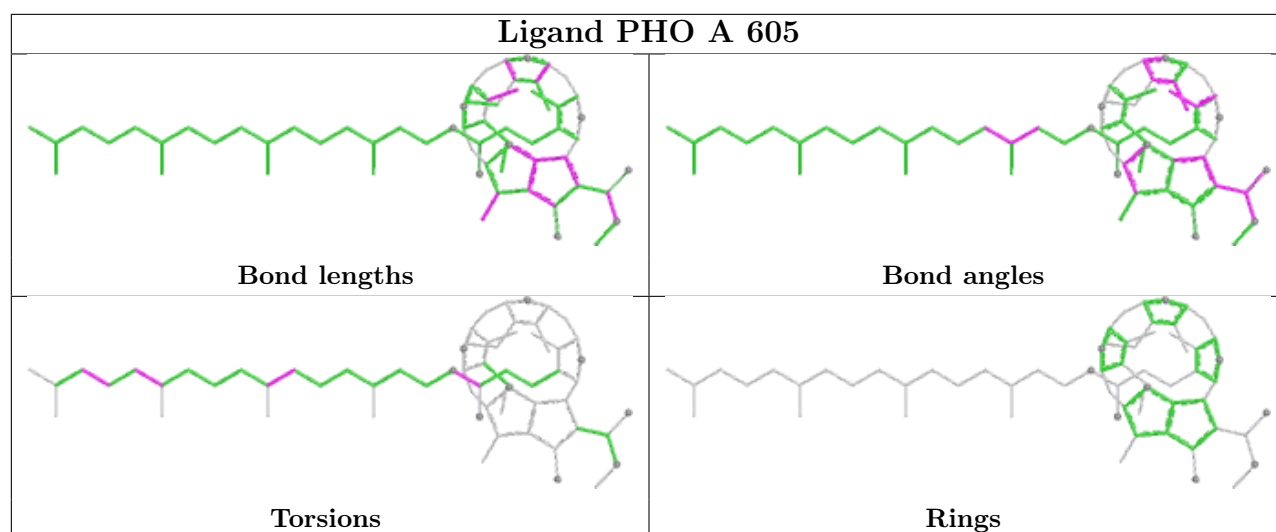
Ligand CLA A 604

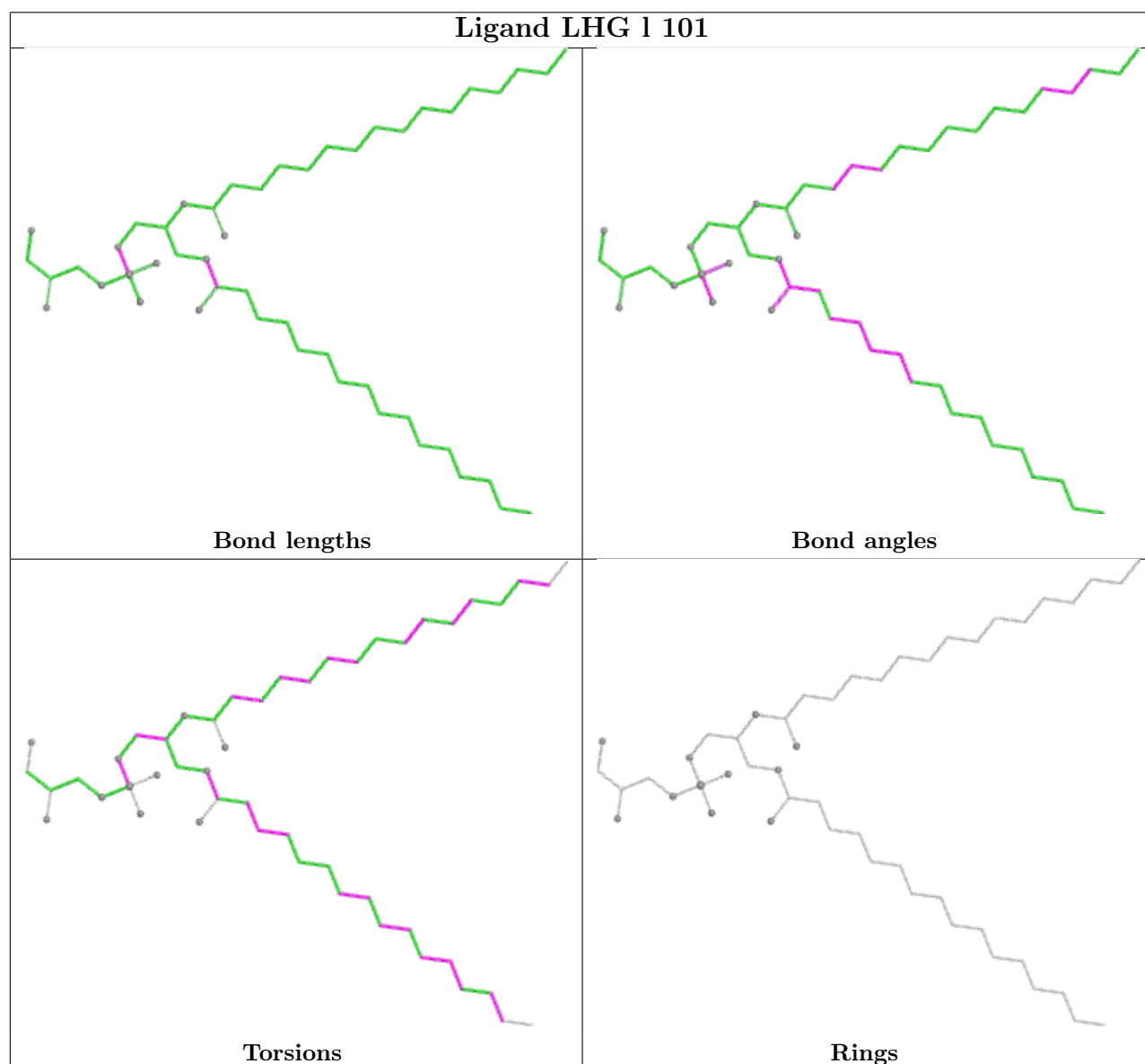
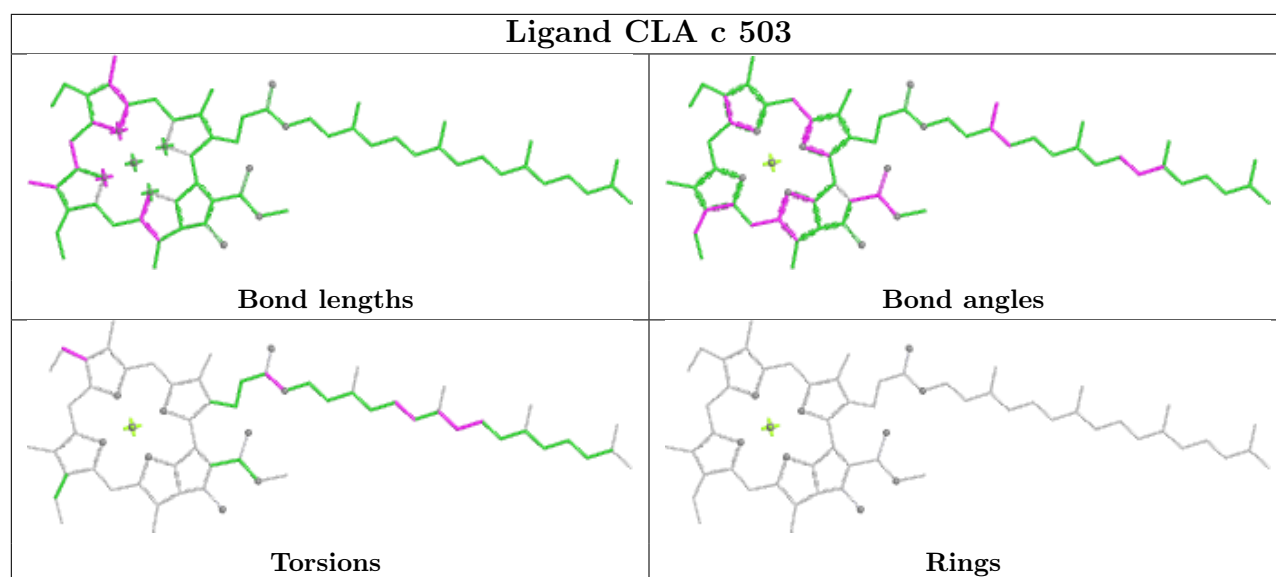


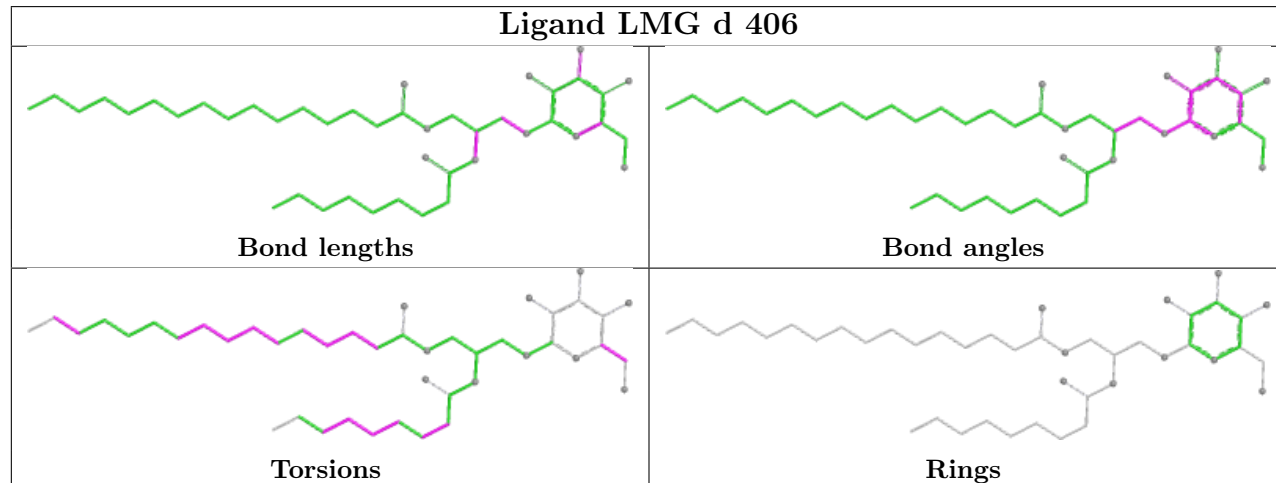
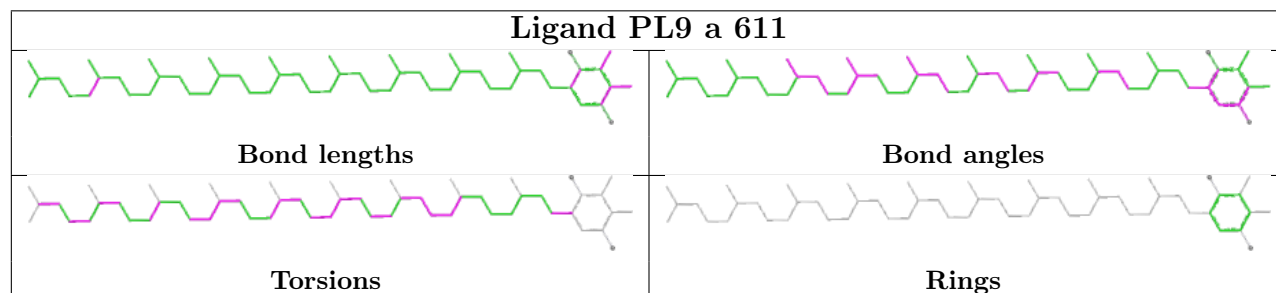
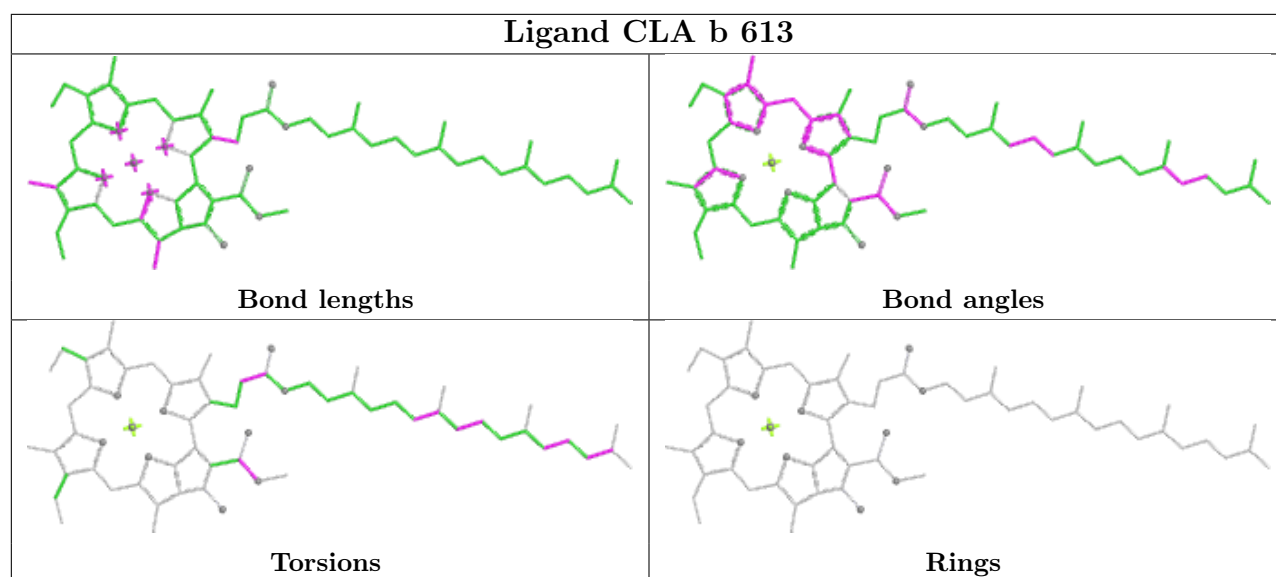
Ligand PHO d 401

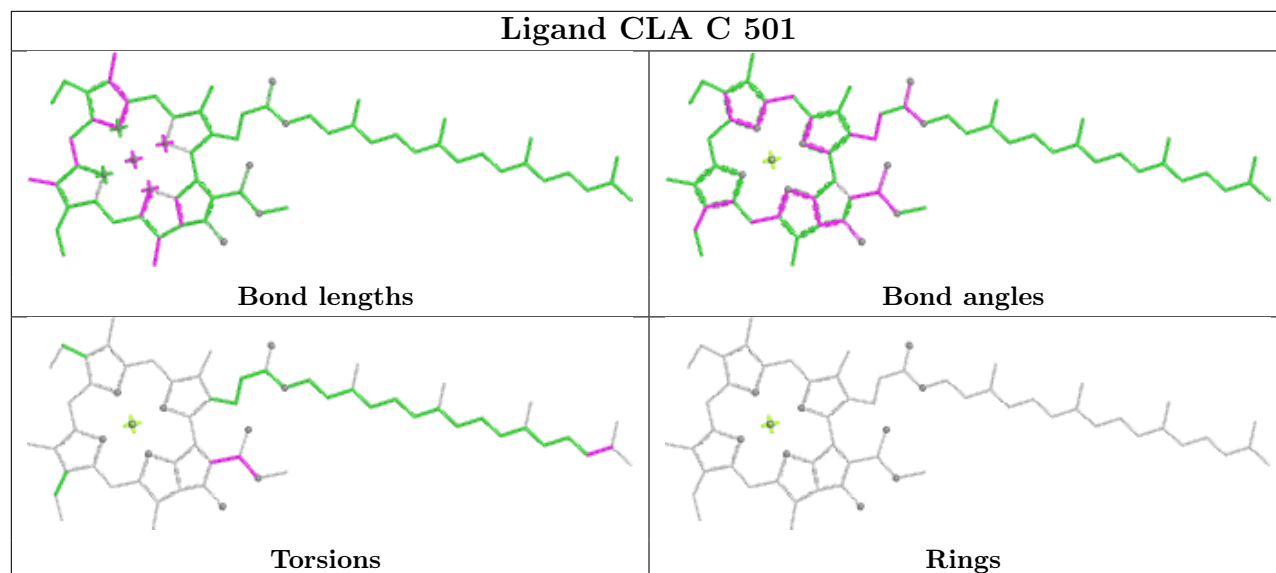
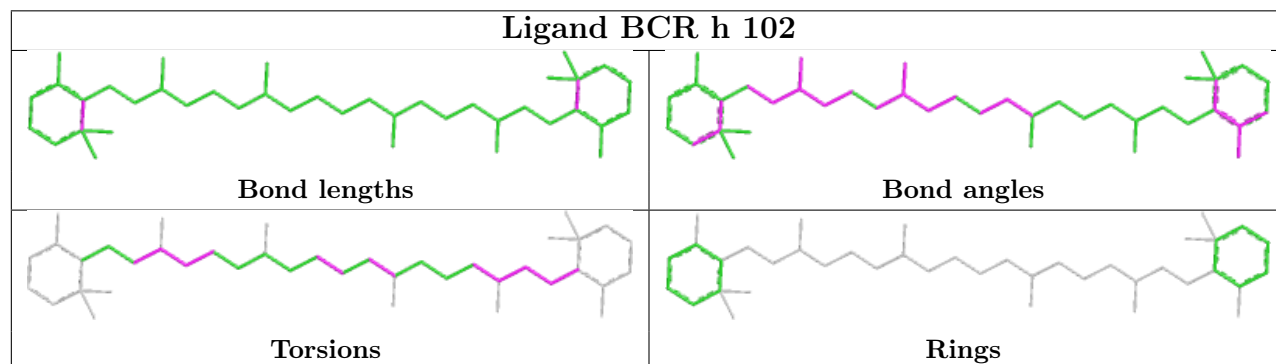
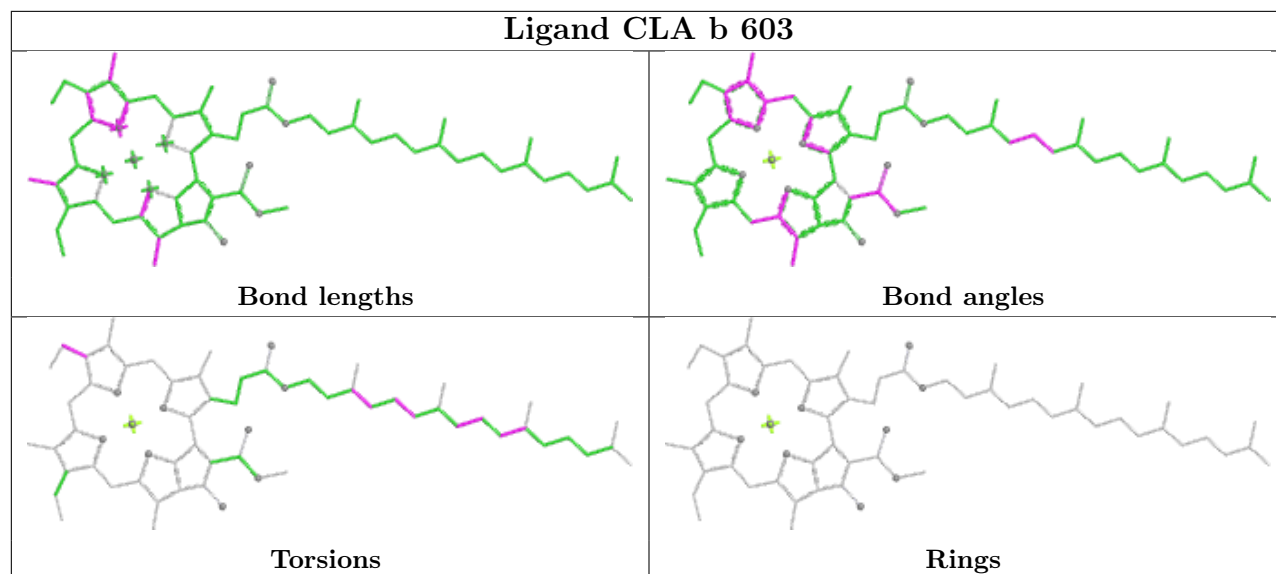


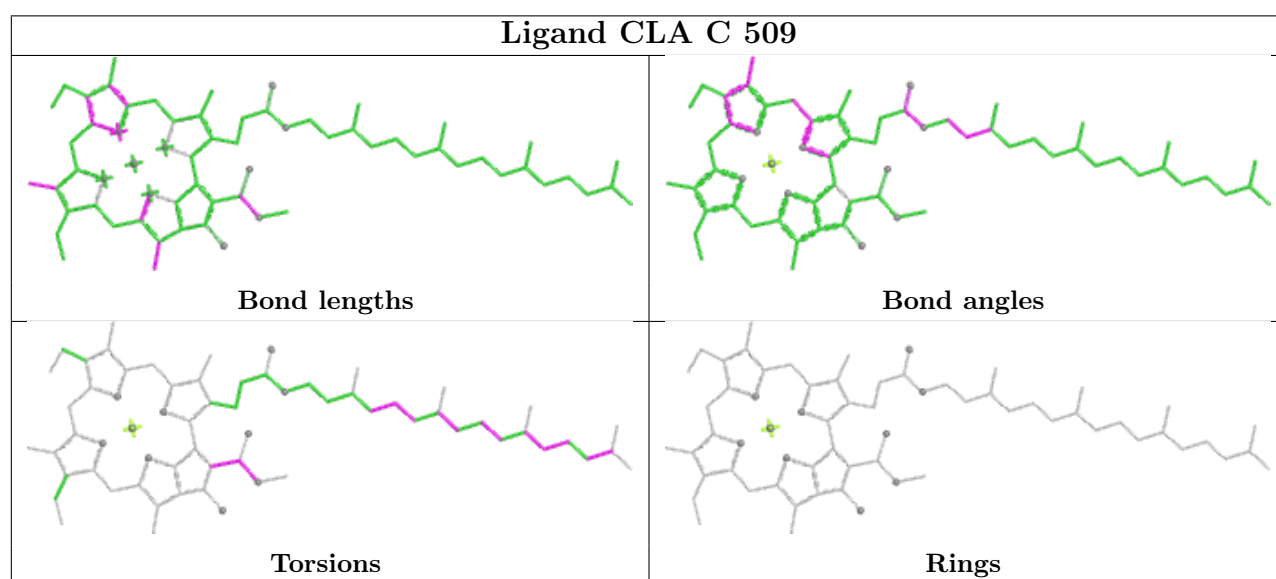
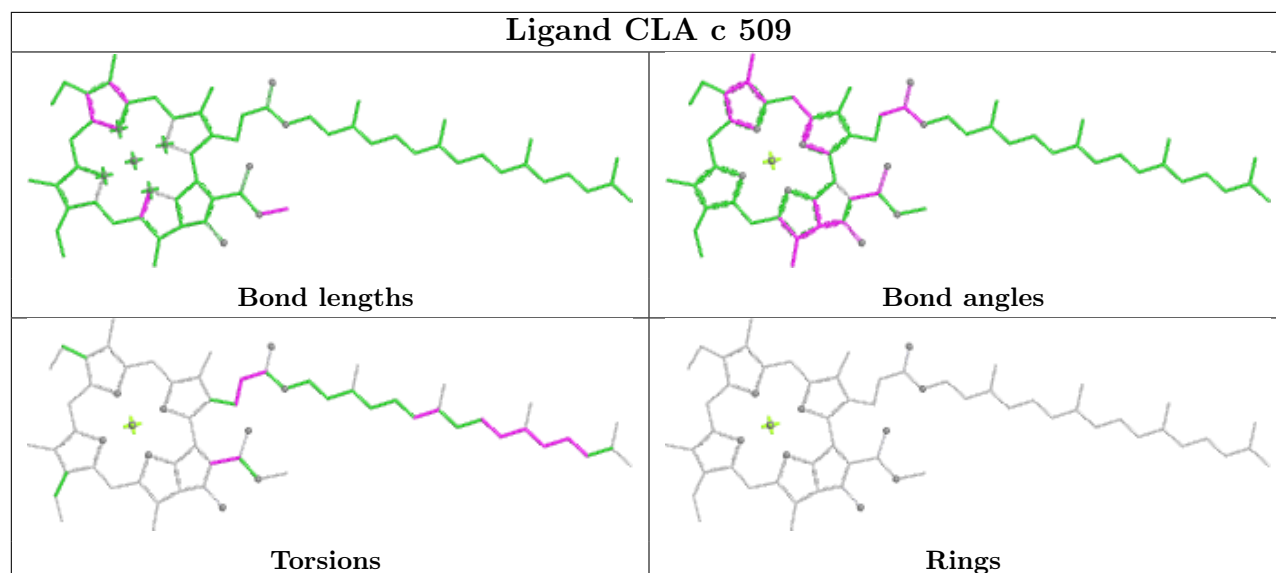
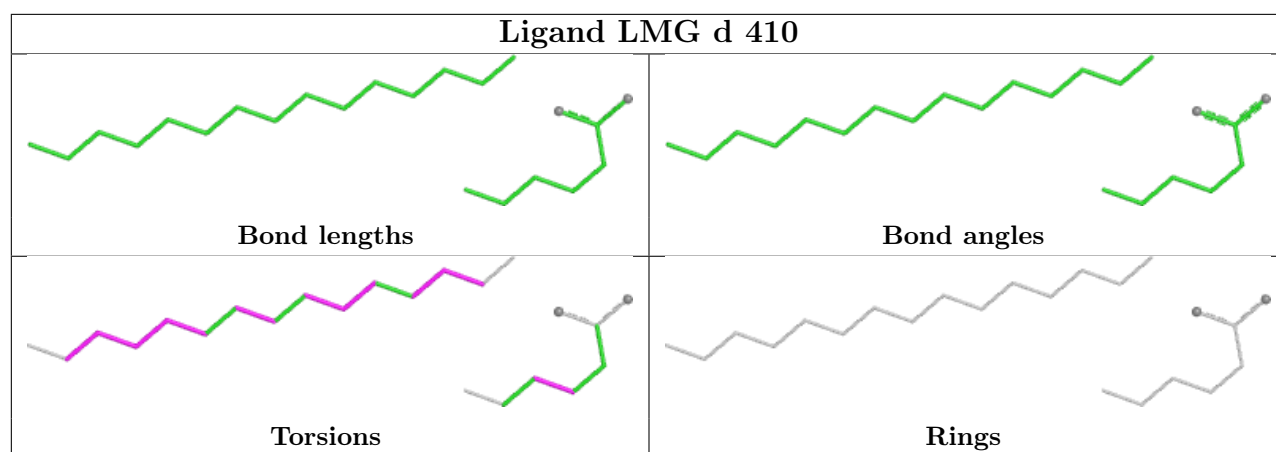


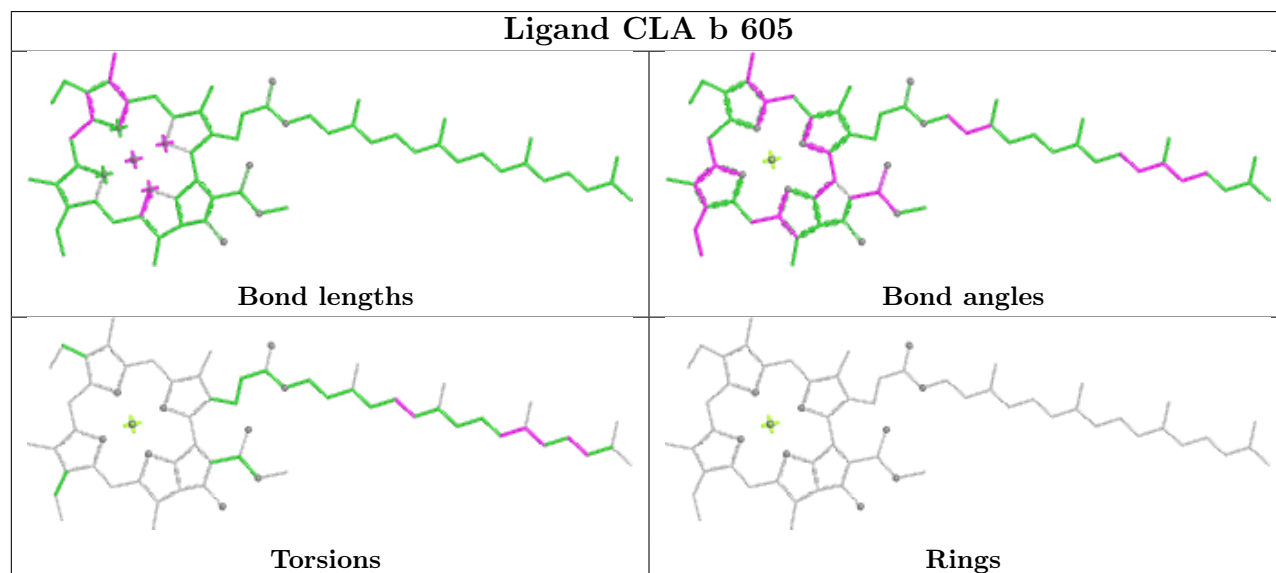
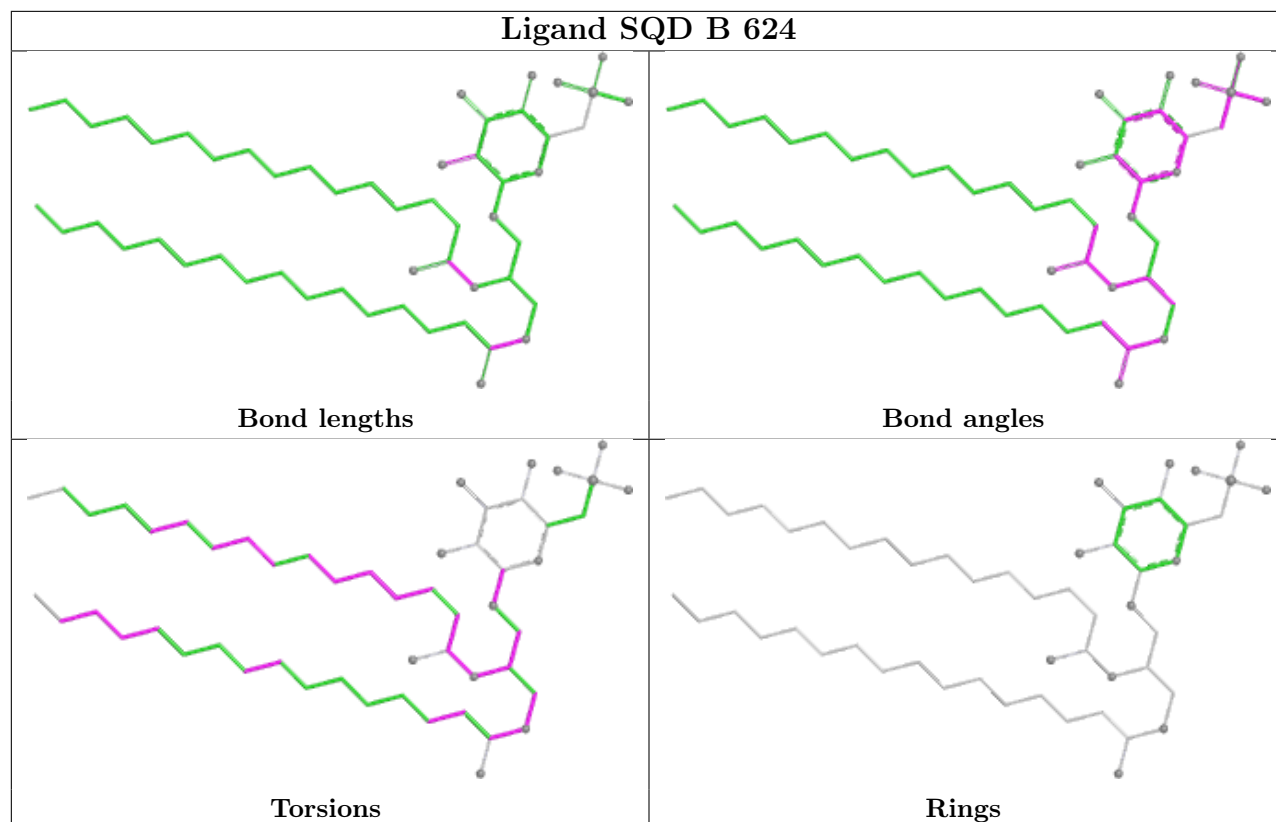


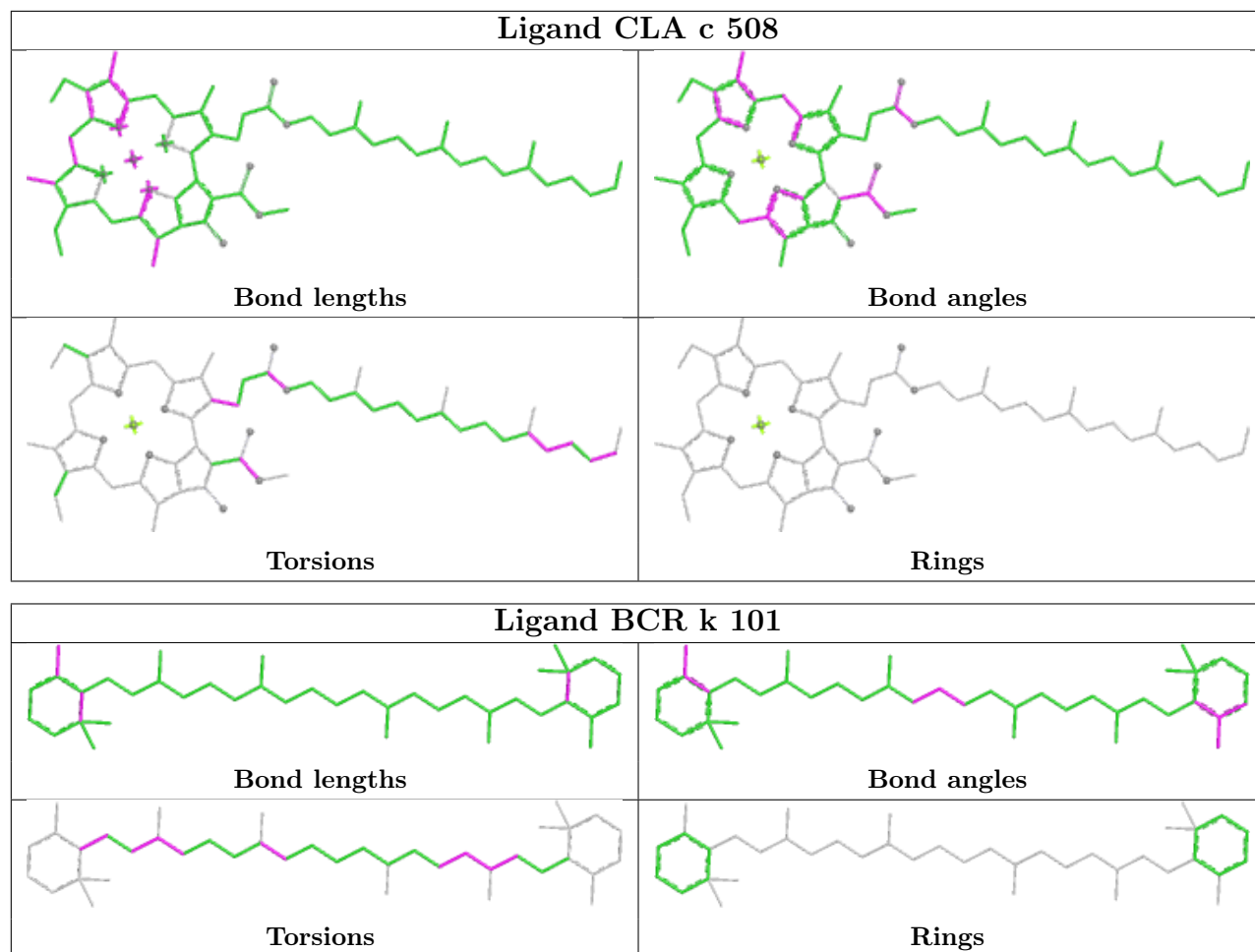




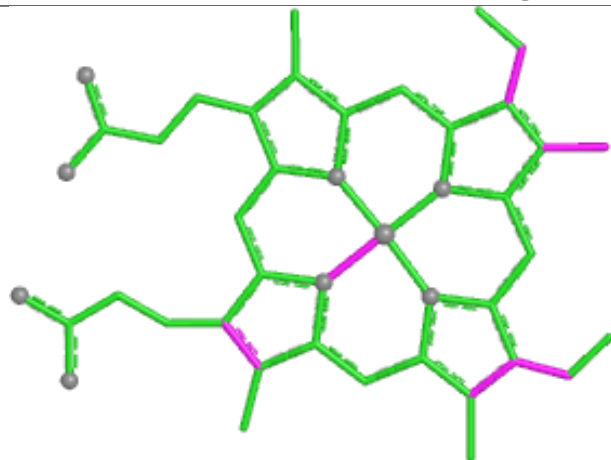




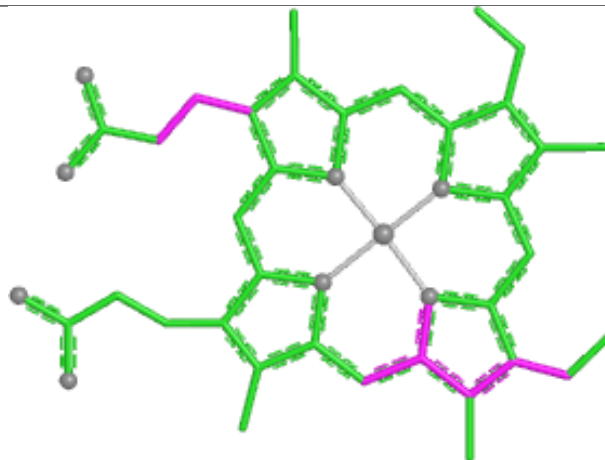




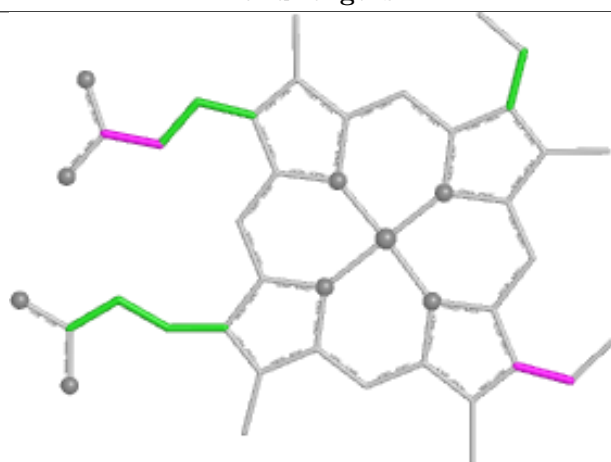
Ligand HEM f 102



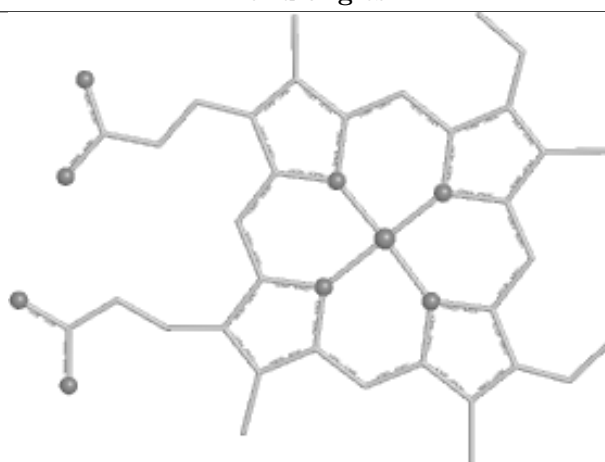
Bond lengths



Bond angles

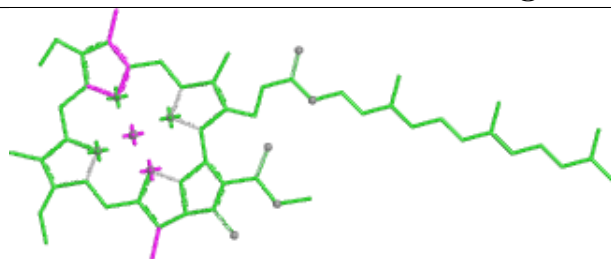


Torsions

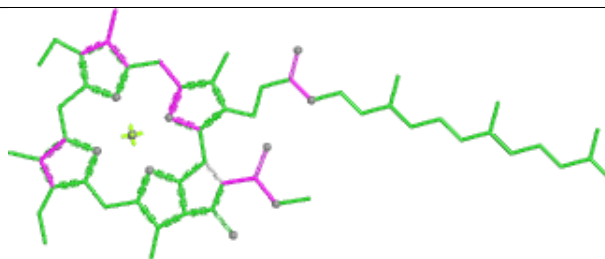


Rings

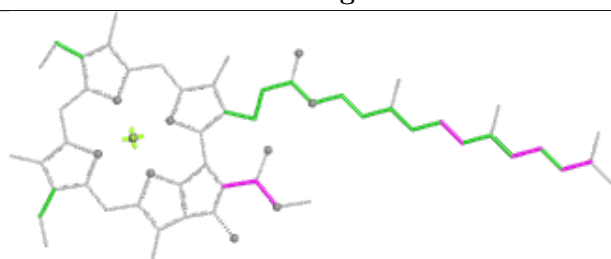
Ligand CLA c 504



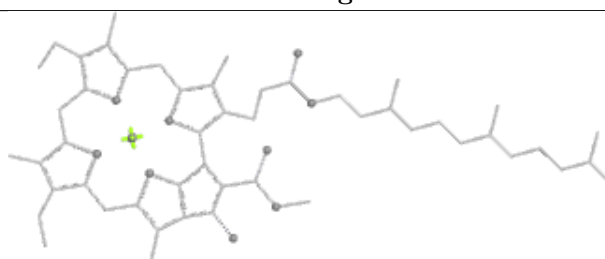
Bond lengths



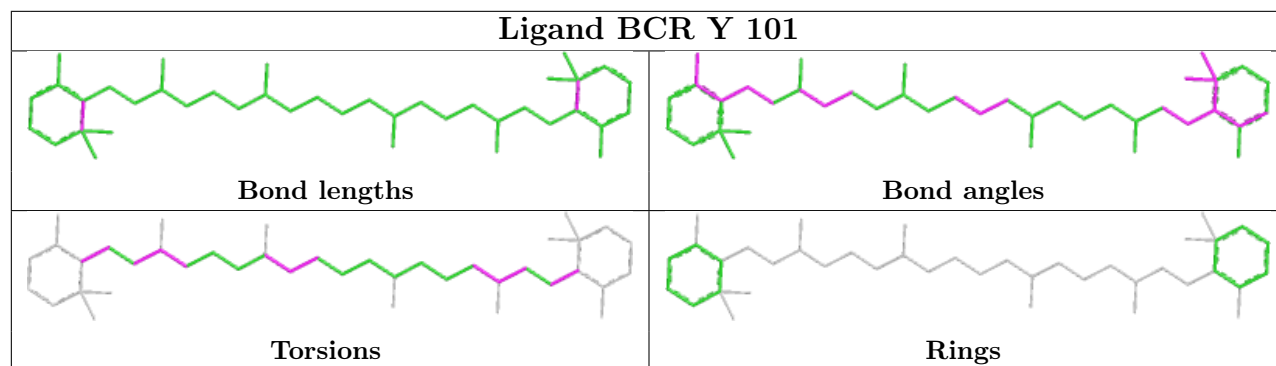
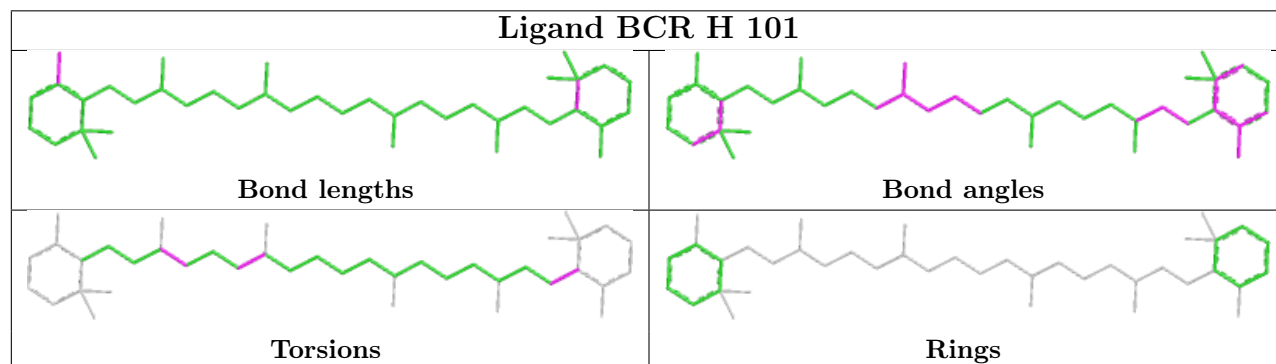
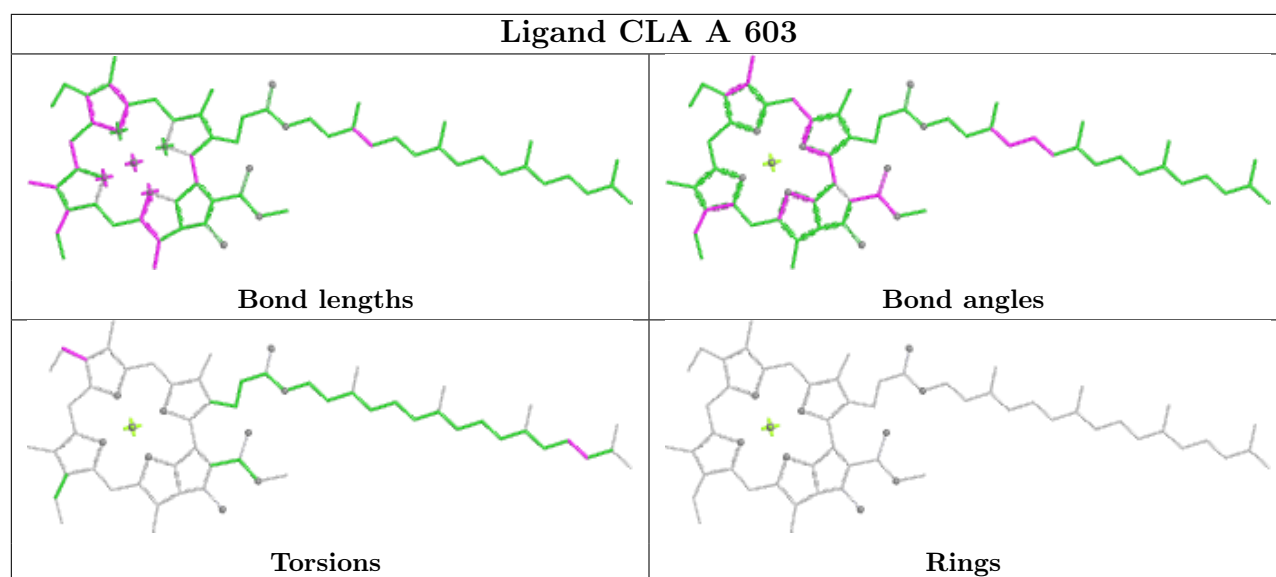
Bond angles

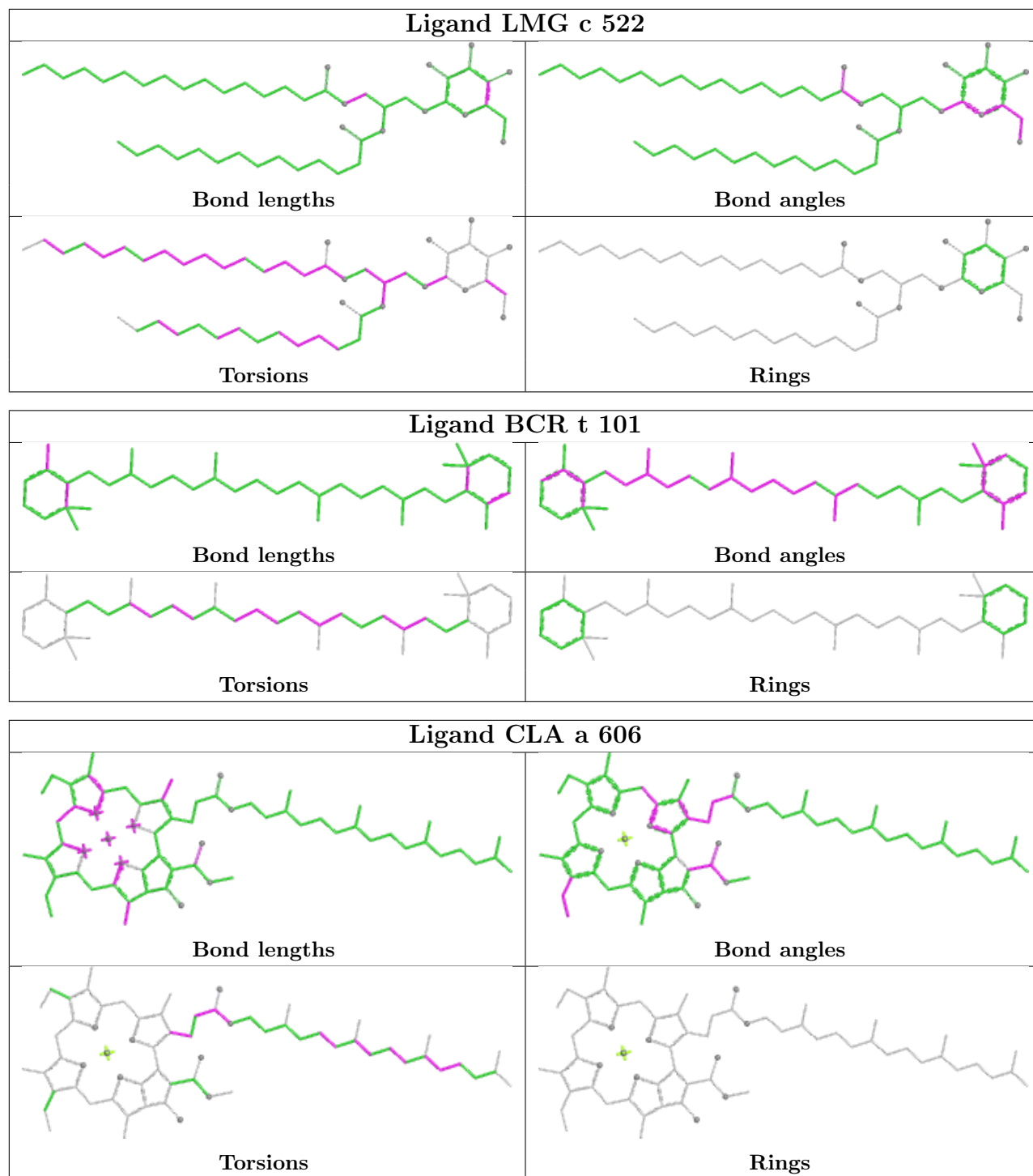


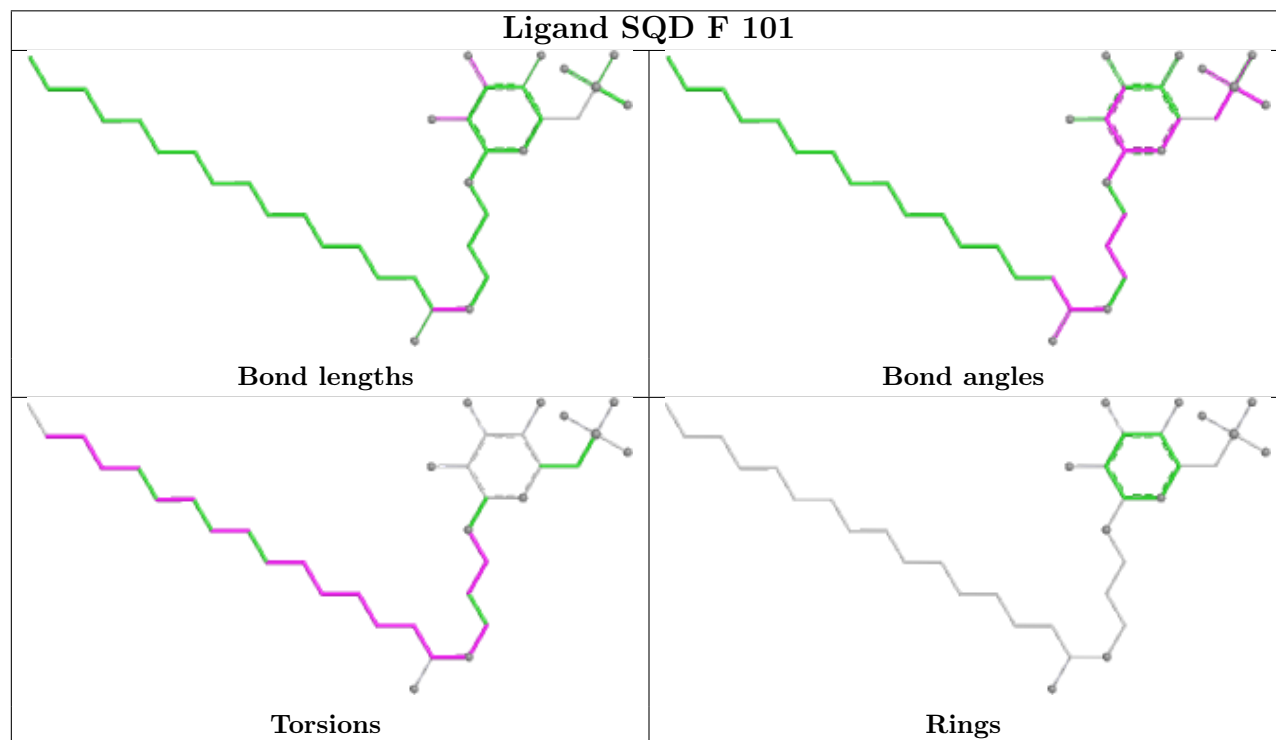
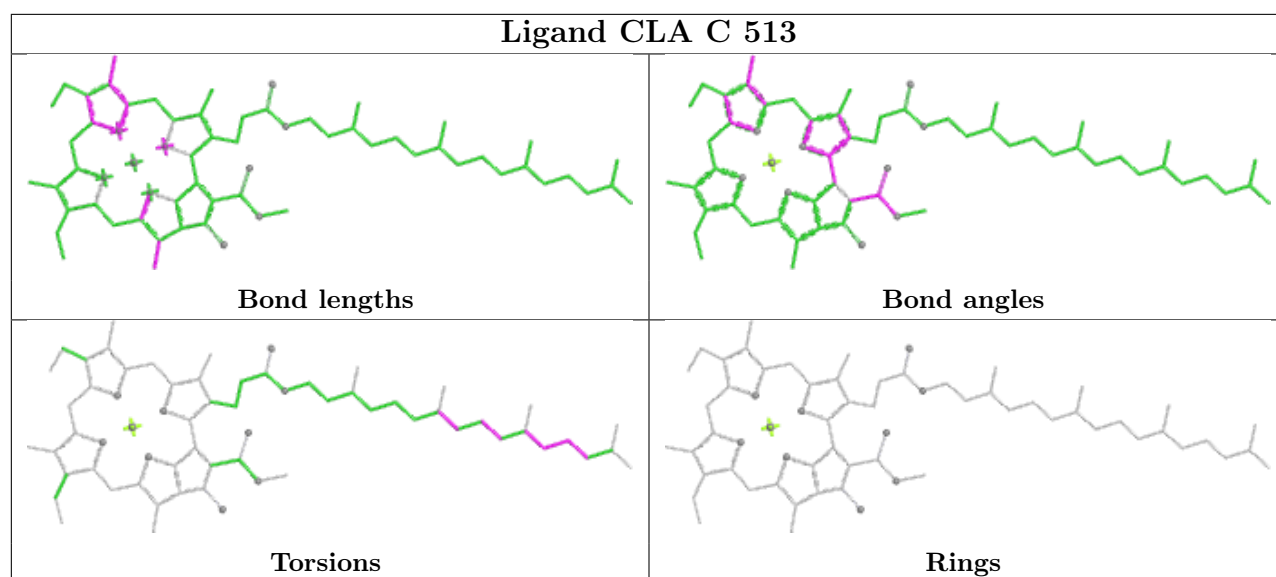
Torsions

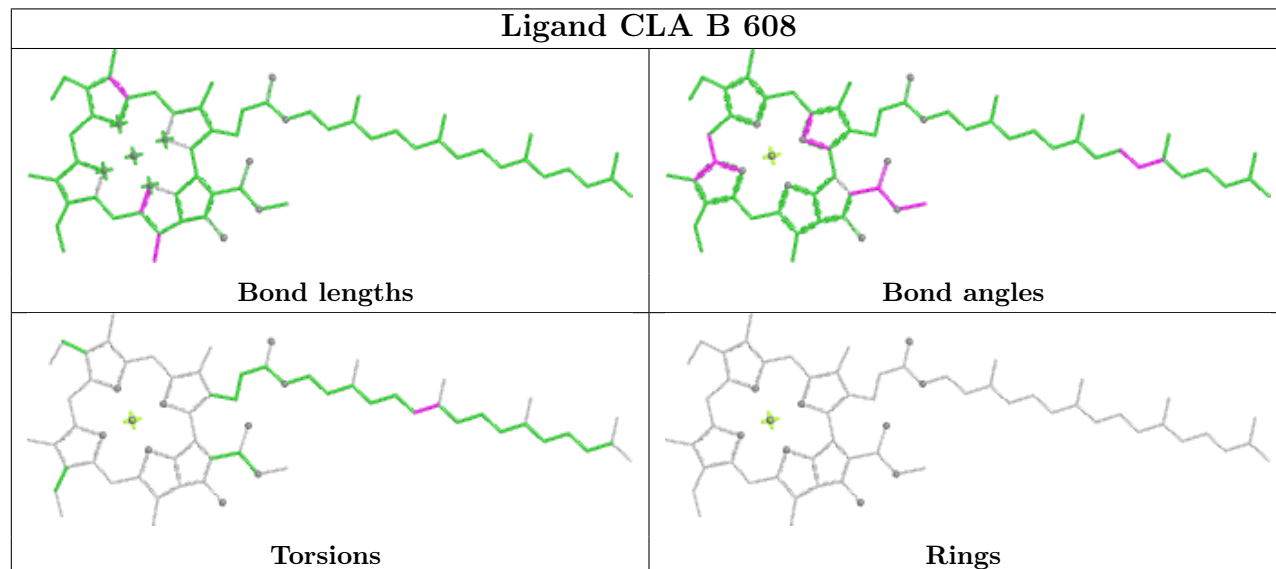
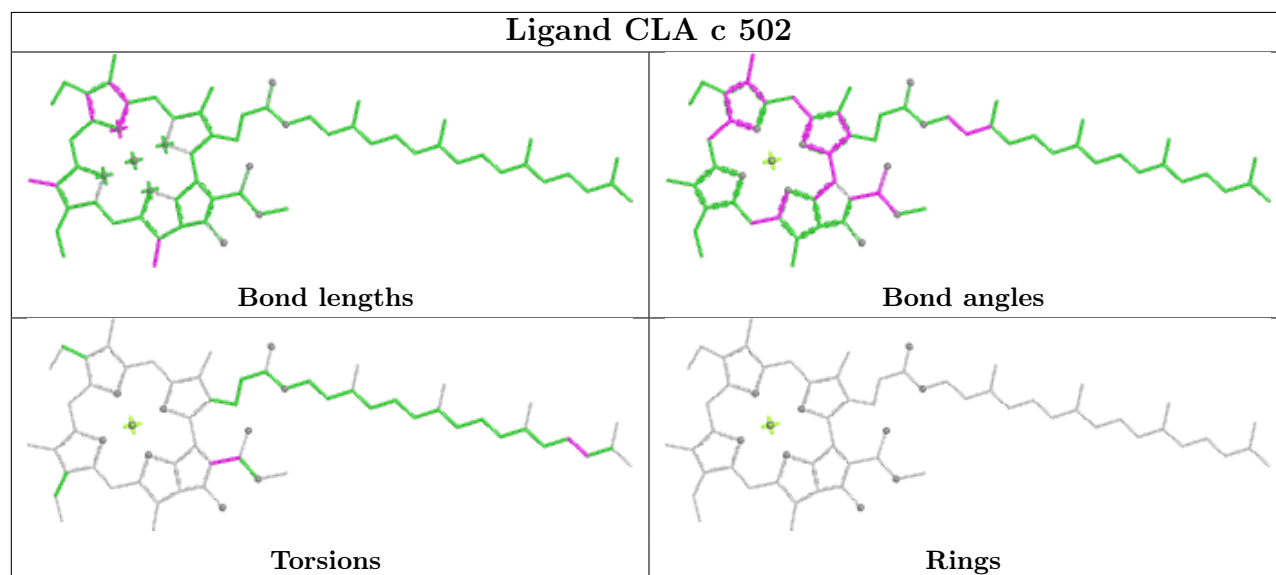
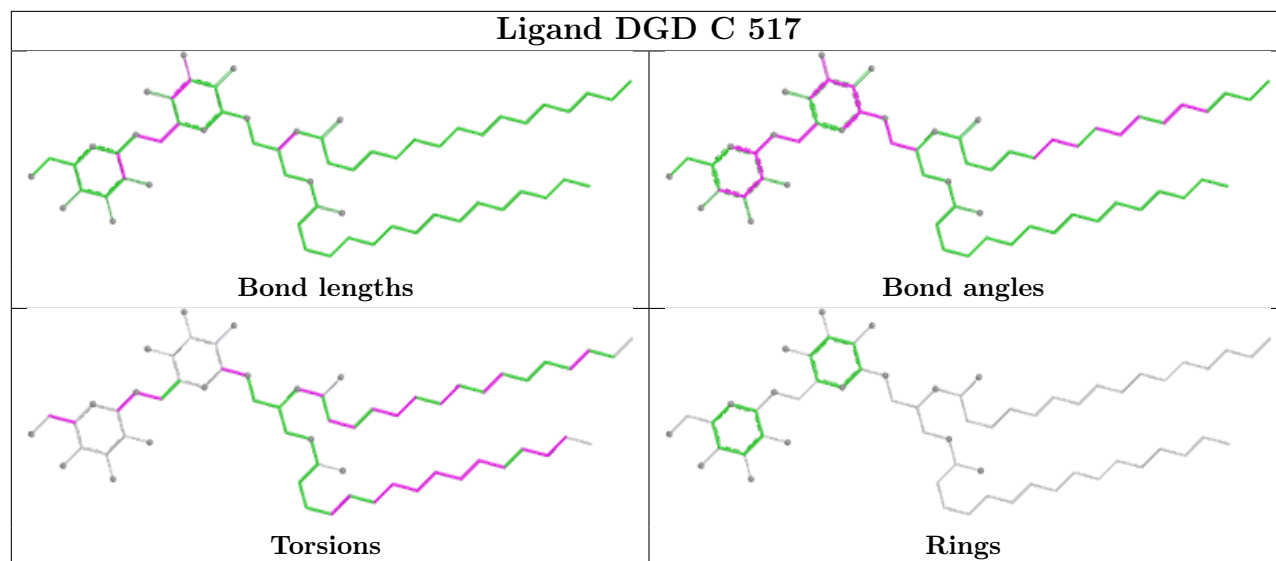


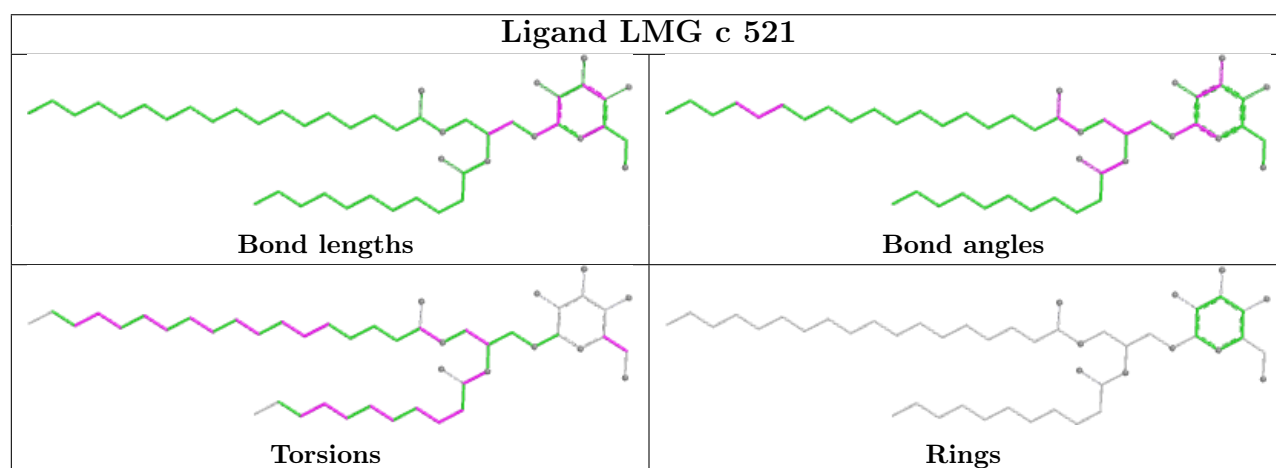
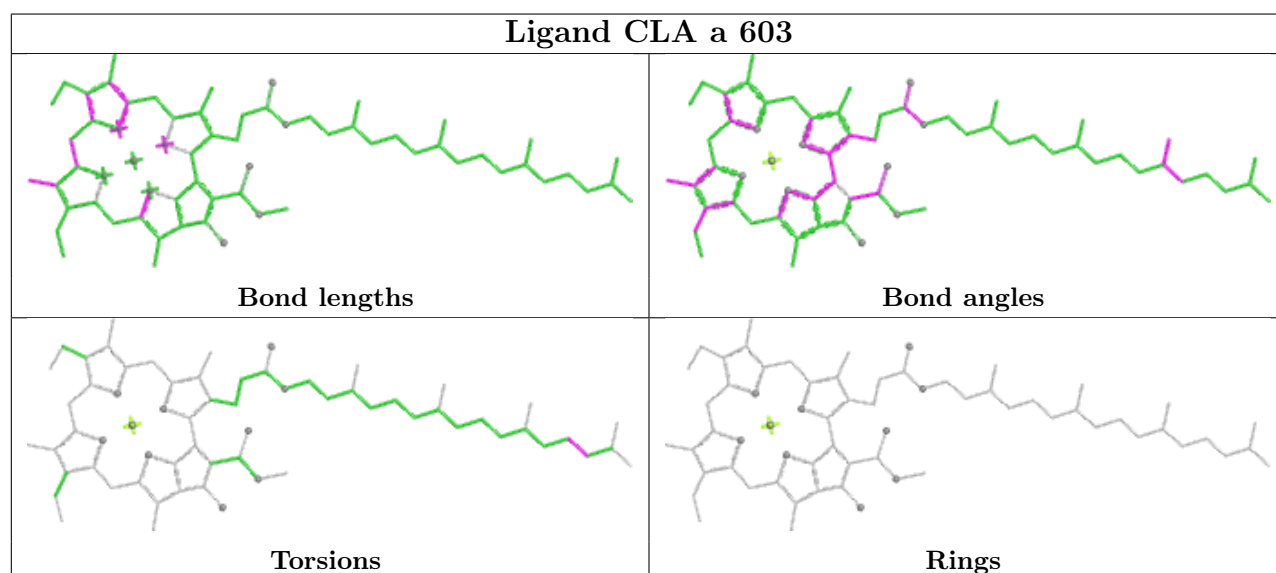
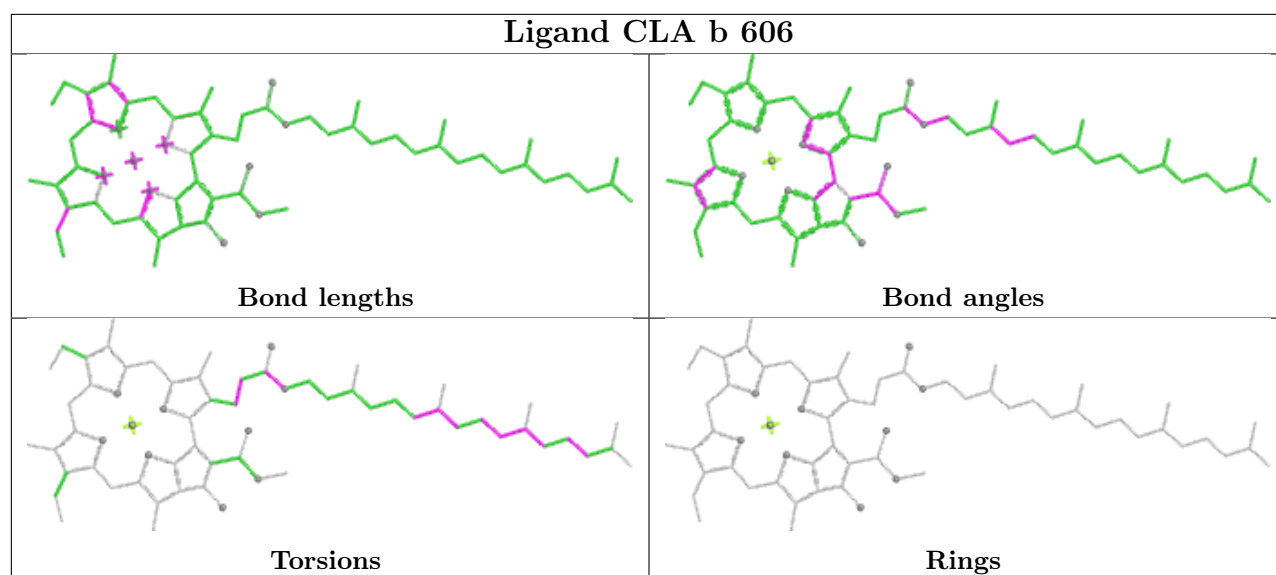
Rings

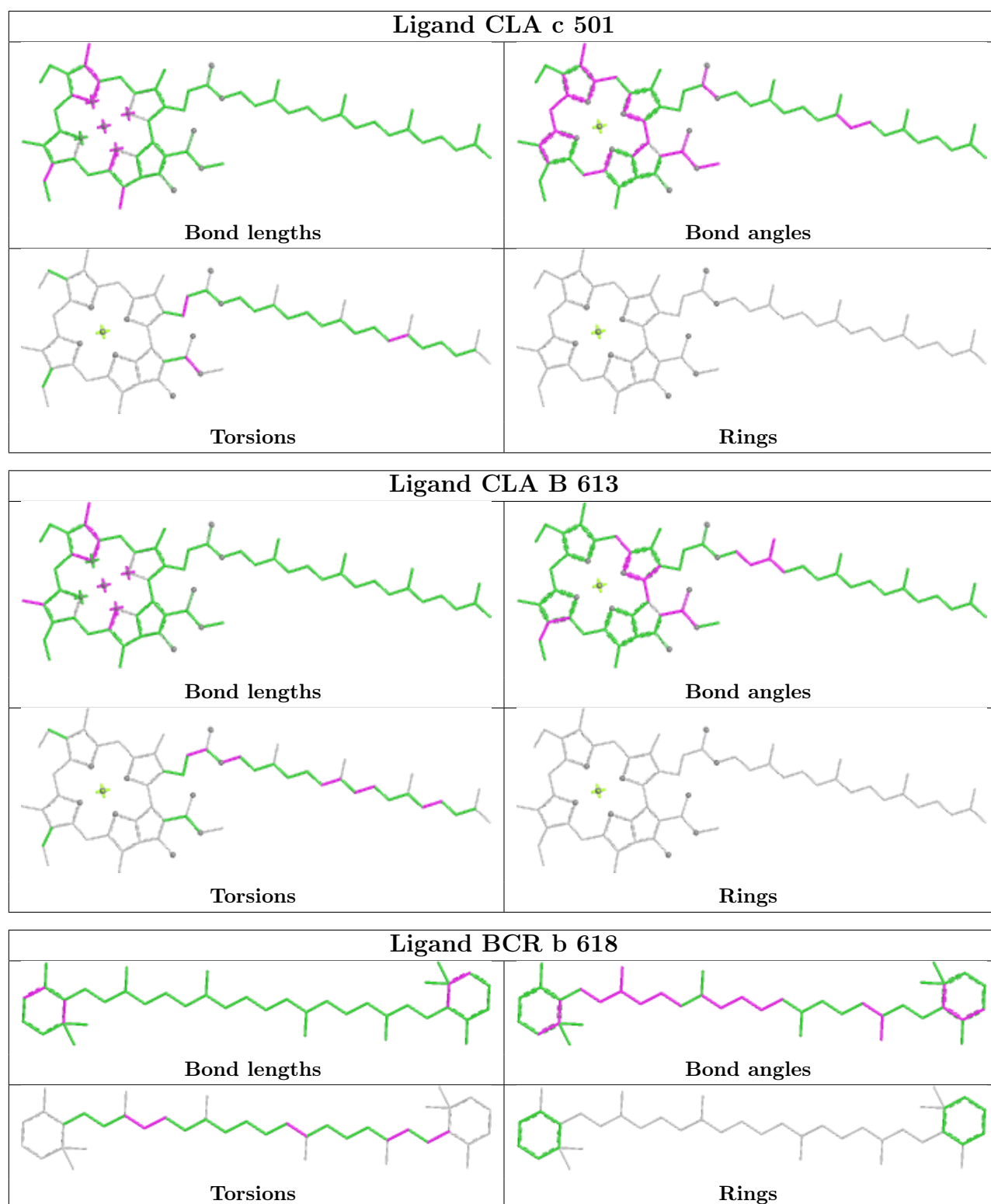




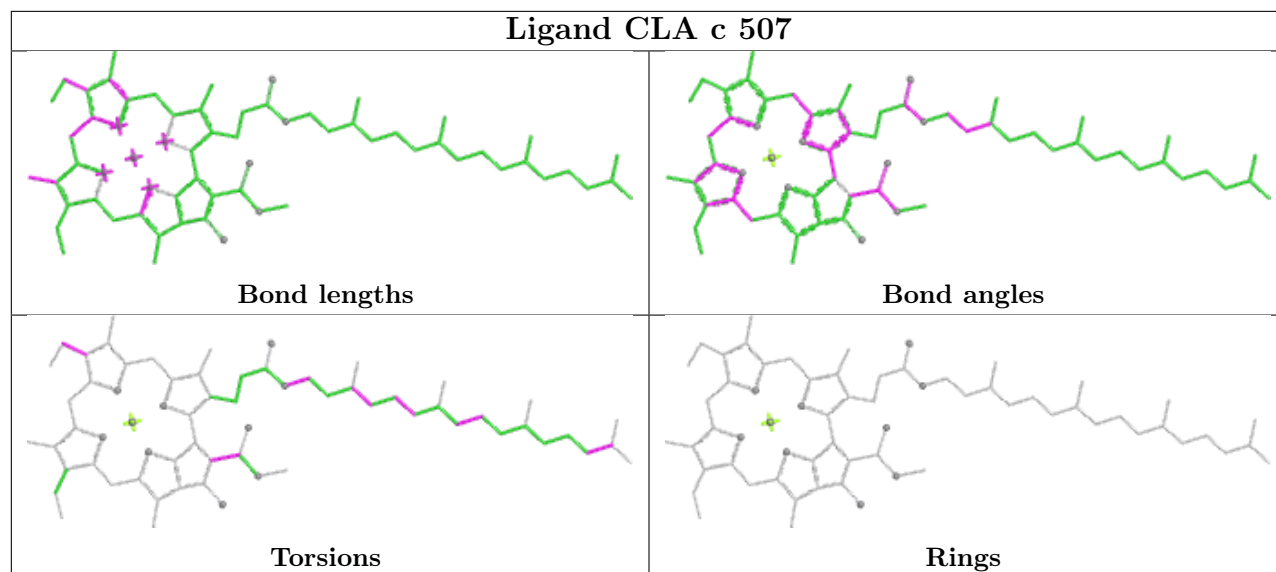




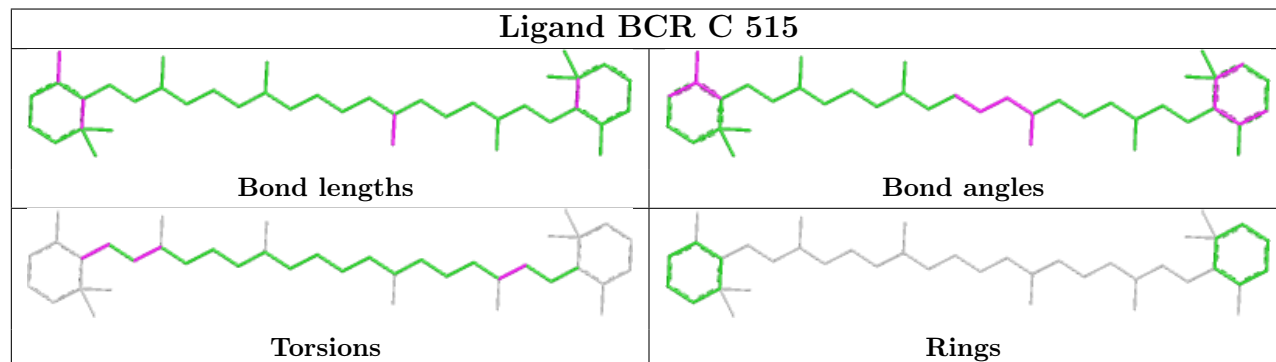




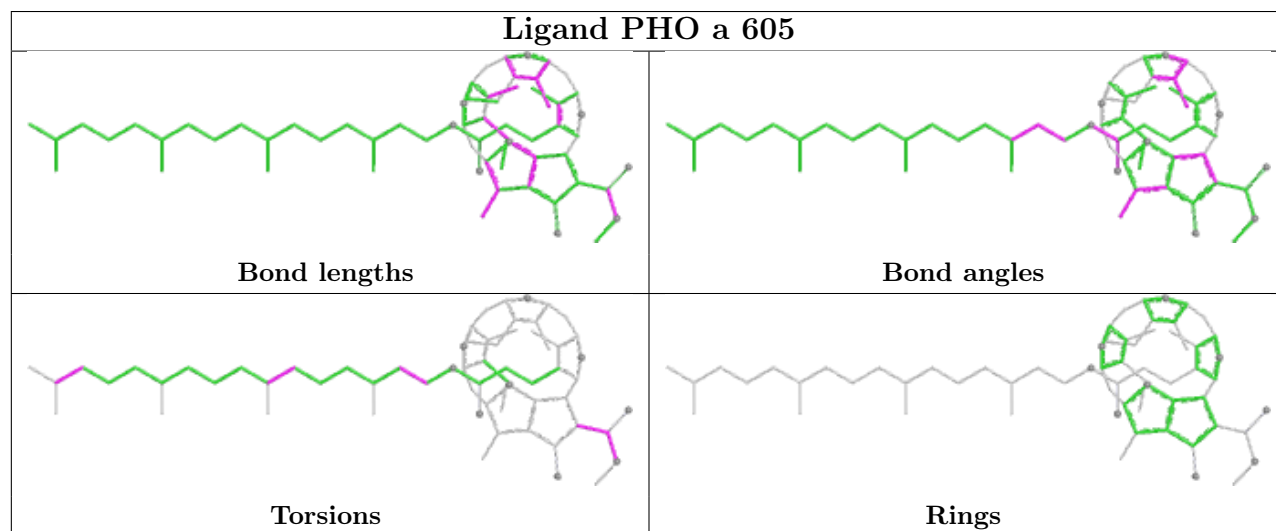
Ligand CLA c 507

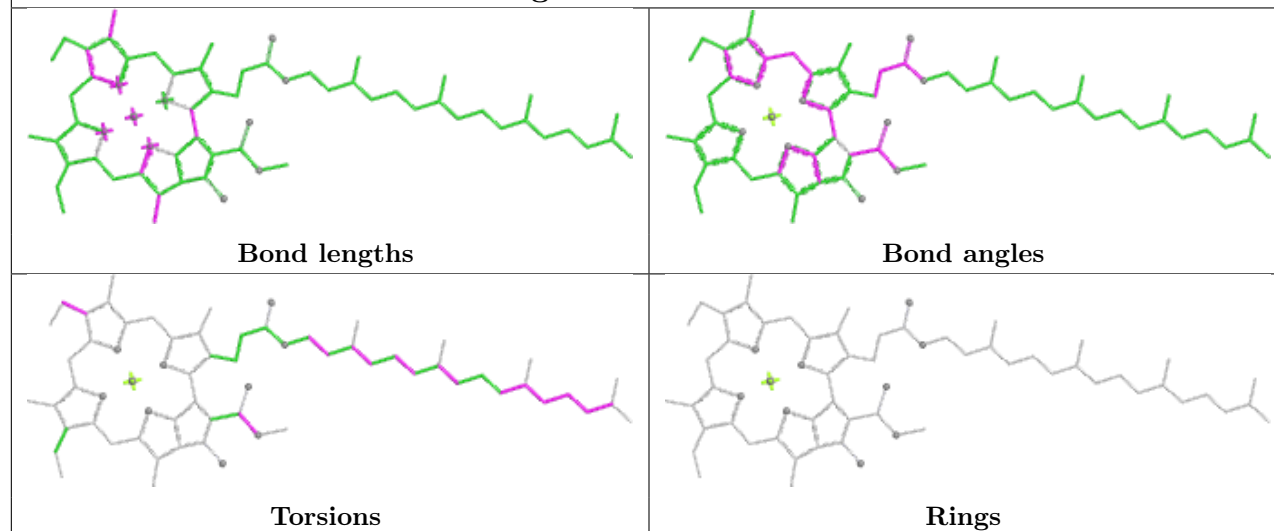
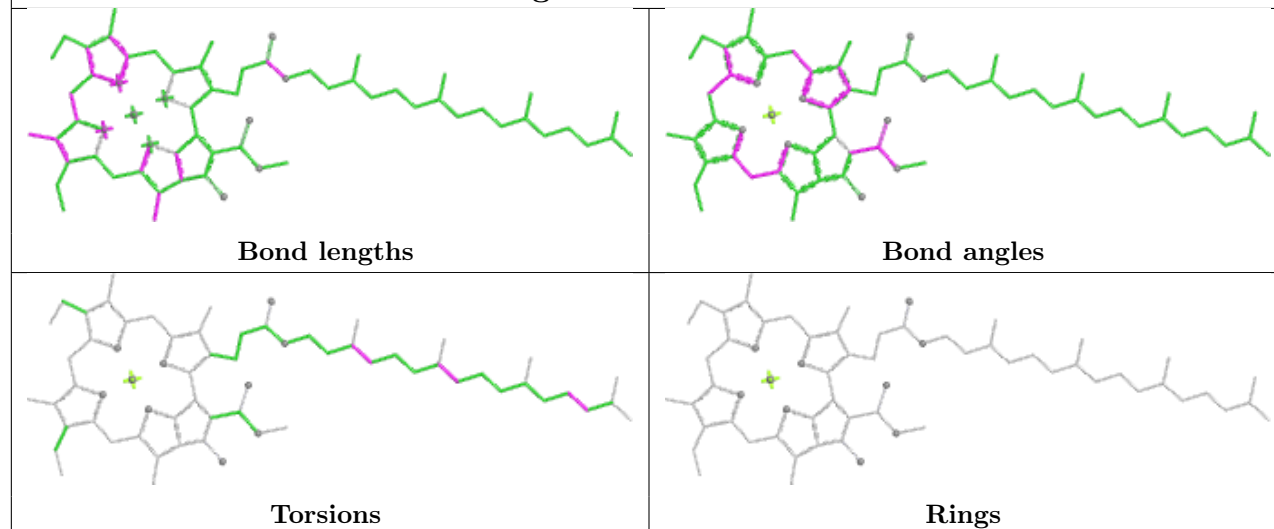


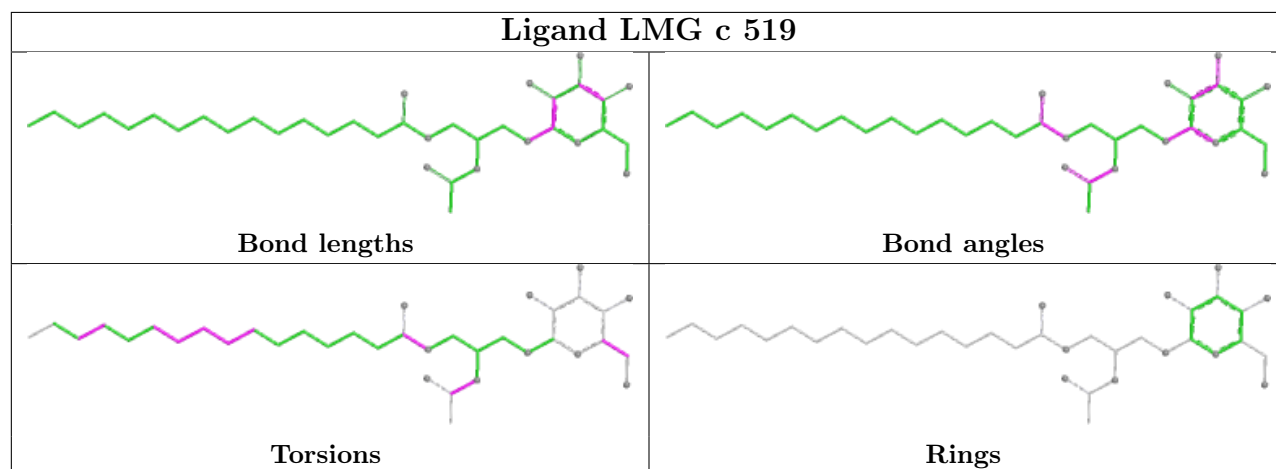
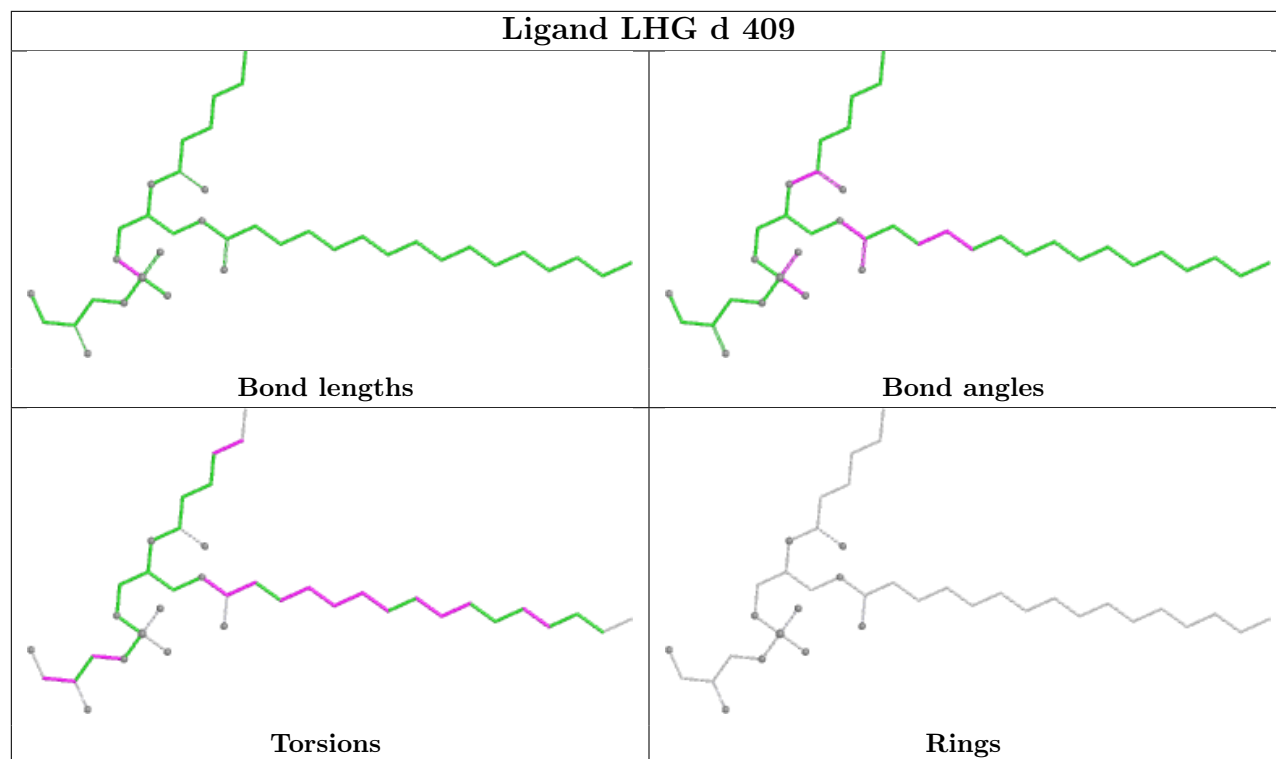
Ligand BCR C 515

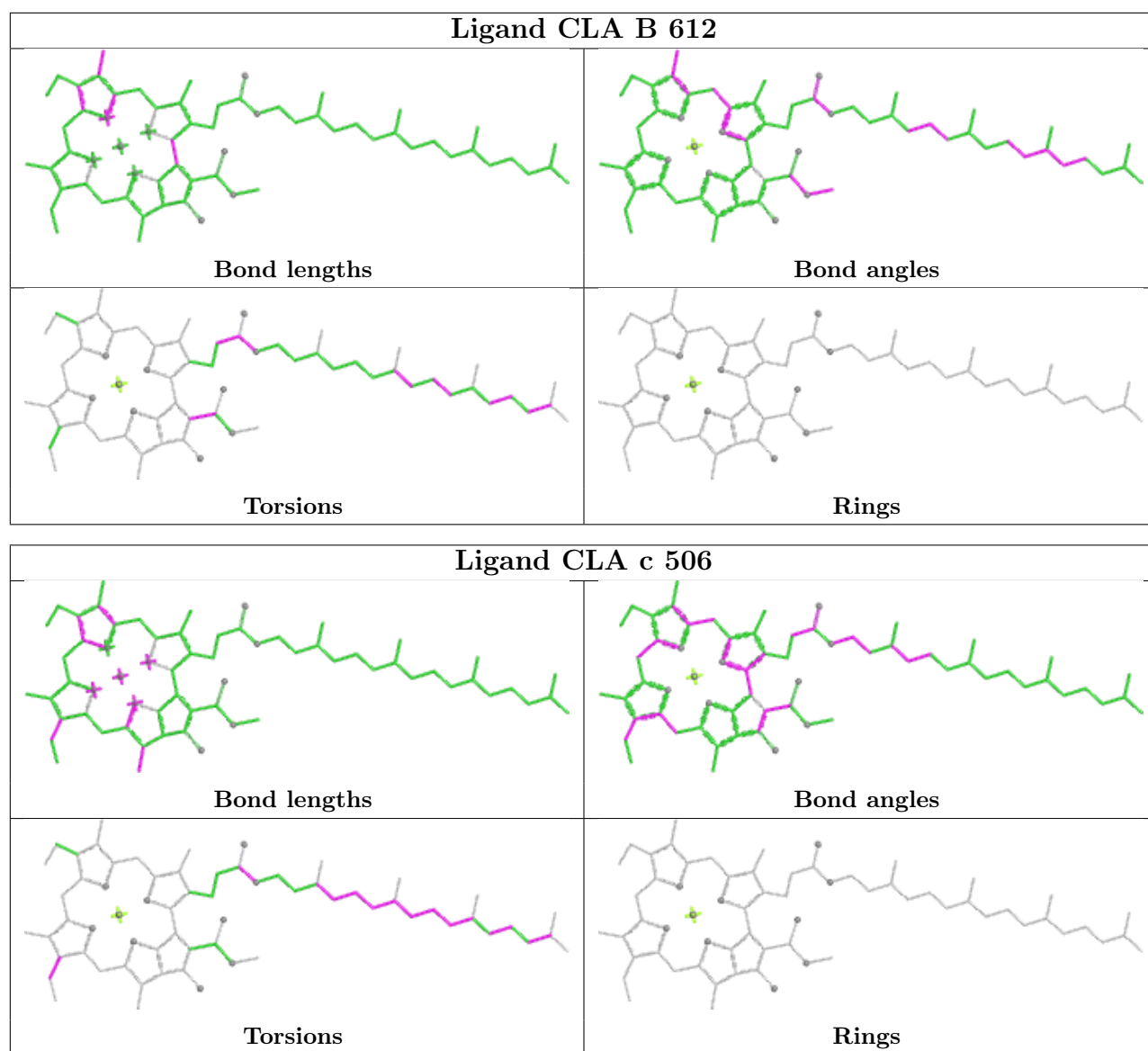


Ligand PHO a 605



Ligand CLA D 403**Ligand CLA C 510**





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	334/334 (100%)	-0.69	1 (0%) 90 92	12, 28, 50, 81	59 (17%)
1	a	334/334 (100%)	-0.59	1 (0%) 90 92	12, 31, 62, 85	59 (17%)
2	B	505/505 (100%)	-0.55	0 100 100	15, 34, 65, 106	4 (0%)
2	b	505/505 (100%)	-0.42	3 (0%) 85 87	24, 38, 77, 118	0
3	C	442/451 (98%)	-0.49	1 (0%) 91 93	13, 37, 57, 81	7 (1%)
3	c	451/451 (100%)	-0.39	3 (0%) 84 85	14, 42, 66, 107	8 (1%)
4	D	341/341 (100%)	-0.69	0 100 100	15, 31, 50, 95	1 (0%)
4	d	341/341 (100%)	-0.53	0 100 100	16, 35, 62, 86	2 (0%)
5	E	81/82 (98%)	0.03	0 100 100	29, 54, 75, 95	1 (1%)
5	e	82/82 (100%)	0.21	0 100 100	40, 62, 90, 98	0
6	F	34/34 (100%)	-0.22	0 100 100	35, 45, 64, 83	0
6	f	34/34 (100%)	0.16	0 100 100	45, 54, 87, 94	0
7	H	65/65 (100%)	-0.33	0 100 100	33, 41, 64, 80	0
7	h	63/65 (96%)	-0.03	1 (1%) 70 72	40, 53, 63, 76	0
8	I	35/36 (97%)	-0.39	0 100 100	30, 39, 71, 82	0
8	i	35/36 (97%)	-0.26	0 100 100	33, 43, 75, 80	0
9	J	36/36 (100%)	-0.18	0 100 100	35, 51, 82, 102	0
9	j	36/36 (100%)	0.08	0 100 100	39, 54, 91, 99	0
10	K	37/37 (100%)	0.03	1 (2%) 56 58	32, 54, 73, 76	1 (2%)
10	k	37/37 (100%)	0.21	0 100 100	48, 61, 77, 86	0
11	L	37/37 (100%)	-0.75	0 100 100	24, 30, 71, 74	0
11	l	36/37 (97%)	-0.66	0 100 100	24, 32, 74, 86	0
12	M	32/33 (96%)	-0.53	0 100 100	27, 35, 66, 77	0
12	m	31/33 (93%)	-0.52	0 100 100	28, 37, 52, 72	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/244 (100%)	-0.33	0 100 100	22, 44, 88, 150	1 (0%)
13	o	244/244 (100%)	-0.34	2 (0%) 82 84	24, 42, 83, 145	0
14	R	34/34 (100%)	0.66	1 (2%) 53 55	62, 76, 92, 100	0
14	r	31/34 (91%)	1.14	3 (9%) 13 13	70, 95, 107, 116	0
15	T	29/30 (96%)	-0.67	1 (3%) 48 48	26, 33, 63, 78	0
15	t	29/30 (96%)	-0.50	1 (3%) 48 48	25, 32, 83, 97	0
16	U	97/97 (100%)	-0.30	0 100 100	32, 44, 72, 102	0
16	u	97/97 (100%)	-0.34	1 (1%) 79 81	30, 42, 59, 94	0
17	V	137/137 (100%)	-0.45	0 100 100	27, 42, 59, 85	0
17	v	137/137 (100%)	-0.20	1 (0%) 84 85	34, 49, 76, 87	0
18	X	38/38 (100%)	-0.02	1 (2%) 57 59	39, 54, 81, 95	0
18	x	38/38 (100%)	0.12	0 100 100	49, 65, 91, 106	0
19	Y	27/30 (90%)	0.93	2 (7%) 20 21	56, 81, 125, 130	0
19	y	30/30 (100%)	0.59	1 (3%) 49 49	63, 80, 108, 113	0
20	Z	62/62 (100%)	0.58	3 (4%) 35 36	53, 70, 123, 142	0
20	z	62/62 (100%)	0.78	6 (9%) 13 13	57, 76, 123, 135	0
All	All	5300/5326 (99%)	-0.38	34 (0%) 85 87	12, 39, 79, 150	143 (2%)

The worst 5 of 34 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
20	z	33	TRP	3.3
14	R	35	LEU	3.2
16	u	53	ALA	2.7
1	A	13	LEU	2.7
18	X	2	THR	2.7

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
12	FME	M	1	10/11	0.95	0.08	36,45,71,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
15	FME	T	1	10/11	0.95	0.10	27,45,71,71	0
8	FME	i	1	10/11	0.95	0.07	35,43,56,58	0
8	FME	I	1	10/11	0.96	0.06	34,47,61,64	0
15	FME	t	1	10/11	0.96	0.07	19,33,65,69	0
12	FME	m	1	10/11	0.97	0.08	26,49,72,73	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
33	UNL	b	624	26/-	0.77	0.16	39,54,65,72	0
33	UNL	H	103	53/-	0.79	0.14	45,74,95,103	0
30	LHG	A	615	49/49	0.82	0.13	48,80,108,117	0
33	UNL	c	523	28/-	0.82	0.11	45,67,86,88	0
28	LMG	c	521	48/55	0.83	0.14	39,81,114,121	0
33	UNL	b	623	55/-	0.83	0.12	42,64,85,85	0
28	LMG	D	409	33/55	0.84	0.12	34,53,93,95	0
33	UNL	J	101	28/-	0.84	0.12	48,62,68,70	0
33	UNL	a	617	28/-	0.84	0.11	42,65,78,78	0
28	LMG	b	621	55/55	0.84	0.14	40,76,103,112	0
31	DGD	A	617	66/66	0.84	0.12	42,64,85,111	0
33	UNL	E	101	28/-	0.84	0.12	45,71,88,95	0
30	LHG	a	614	42/49	0.85	0.12	58,86,109,122	0
33	UNL	T	103	44/-	0.85	0.14	38,57,79,84	0
33	UNL	B	627	47/-	0.85	0.14	44,63,79,79	0
33	UNL	d	411	43/-	0.85	0.13	39,55,66,70	0
33	UNL	t	103	26/-	0.85	0.12	35,59,76,83	0
33	UNL	x	101	55/-	0.85	0.11	39,58,75,75	0
28	LMG	d	410	23/55	0.86	0.15	31,71,94,98	0
33	UNL	B	628	28/-	0.86	0.17	52,70,102,107	0
27	PL9	A	611	55/55	0.86	0.14	35,58,81,84	135
27	PL9	a	611	55/55	0.86	0.14	38,69,88,94	0
28	LMG	B	622	28/55	0.86	0.12	31,48,58,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
33	UNL	j	101	28/-	0.86	0.12	46,61,70,74	0
33	UNL	T	102	47/-	0.86	0.13	35,51,66,74	0
31	DGD	a	616	44/66	0.86	0.12	33,56,77,89	0
33	UNL	B	621	43/-	0.87	0.11	31,50,71,76	0
29	SQD	A	616	39/54	0.87	0.12	41,65,88,92	0
33	UNL	I	101	41/-	0.87	0.13	36,53,72,79	0
33	UNL	b	620	55/-	0.87	0.11	37,60,83,90	0
33	UNL	b	622	40/-	0.87	0.11	43,59,81,83	0
29	SQD	a	615	36/54	0.87	0.12	30,66,85,87	0
33	UNL	B	626	46/-	0.88	0.11	39,59,72,77	0
28	LMG	c	519	37/55	0.88	0.12	38,69,88,92	0
28	LMG	C	519	48/55	0.88	0.11	46,73,95,106	0
33	UNL	C	522	28/-	0.88	0.10	43,54,64,66	0
29	SQD	f	101	41/54	0.89	0.12	45,84,111,119	0
23	CLA	h	101	65/65	0.89	0.10	41,62,91,97	0
33	UNL	c	520	55/-	0.89	0.11	34,54,93,94	0
28	LMG	A	612	48/55	0.89	0.10	31,56,74,91	0
29	SQD	B	624	54/54	0.89	0.10	37,59,97,109	0
33	UNL	C	523	47/-	0.89	0.10	37,53,71,75	0
33	UNL	t	102	34/-	0.89	0.10	35,50,56,63	0
28	LMG	c	522	49/55	0.89	0.10	32,56,91,110	0
29	SQD	b	601	49/54	0.89	0.10	39,58,99,111	0
33	UNL	X	101	55/-	0.90	0.10	33,52,73,79	0
25	BCR	h	102	40/40	0.90	0.10	35,54,74,82	0
33	UNL	m	102	28/-	0.90	0.12	42,63,77,78	0
29	SQD	a	613	54/54	0.91	0.09	39,67,93,101	0
23	CLA	C	513	65/65	0.91	0.10	43,62,88,97	0
28	LMG	m	101	51/55	0.91	0.09	33,51,81,98	0
33	UNL	M	101	37/-	0.91	0.10	31,43,63,70	0
33	UNL	M	102	26/-	0.91	0.11	30,50,60,62	0
25	BCR	k	101	40/40	0.91	0.10	44,63,75,80	0
23	CLA	B	601	65/65	0.91	0.10	25,60,104,130	0
28	LMG	B	620	51/55	0.92	0.08	25,49,73,87	0
23	CLA	c	513	65/65	0.92	0.09	44,69,104,112	0
23	CLA	c	512	65/65	0.92	0.10	38,55,94,108	0
33	UNL	B	625	28/-	0.92	0.09	26,48,64,71	0
33	UNL	l	102	53/-	0.92	0.12	25,48,87,99	0
25	BCR	Y	101	40/40	0.92	0.09	33,53,73,76	0
25	BCR	c	514	40/40	0.92	0.09	39,60,71,72	0
25	BCR	d	404	40/40	0.92	0.08	32,51,90,97	0
33	UNL	C	521	28/-	0.92	0.09	28,40,53,66	0
25	BCR	C	514	40/40	0.93	0.09	35,54,66,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	BCR	D	404	40/40	0.93	0.09	28,43,98,109	0
25	BCR	H	101	40/40	0.93	0.07	29,45,59,68	0
29	SQD	A	614	52/54	0.93	0.09	31,58,84,89	0
30	LHG	d	409	39/49	0.93	0.09	27,47,66,70	0
25	BCR	k	102	40/40	0.93	0.10	36,51,72,74	0
31	DGD	C	517	62/66	0.93	0.09	32,51,107,118	0
31	DGD	H	102	62/66	0.93	0.09	30,48,61,73	0
23	CLA	c	511	65/65	0.93	0.10	36,54,72,75	0
31	DGD	c	517	62/66	0.93	0.08	29,50,83,96	0
31	DGD	h	103	62/66	0.93	0.08	31,48,61,74	0
29	SQD	F	101	36/54	0.93	0.10	45,67,87,92	0
25	BCR	b	618	40/40	0.93	0.07	25,37,53,60	0
23	CLA	C	512	65/65	0.93	0.09	31,53,103,112	0
31	DGD	c	518	62/66	0.94	0.08	27,50,77,91	0
25	BCR	B	619	40/40	0.94	0.07	20,39,59,66	0
25	BCR	b	619	40/40	0.94	0.07	25,47,58,64	0
28	LMG	D	405	51/55	0.94	0.09	26,54,98,102	0
30	LHG	d	405	49/49	0.94	0.09	35,50,72,88	0
25	BCR	t	101	40/40	0.94	0.07	24,36,57,63	0
25	BCR	B	618	40/40	0.94	0.06	21,37,56,56	0
25	BCR	c	515	40/40	0.94	0.08	28,41,52,71	0
25	BCR	C	520	40/40	0.94	0.09	36,51,66,69	0
25	BCR	b	617	40/40	0.94	0.07	24,42,54,58	0
28	LMG	d	406	44/55	0.94	0.08	31,54,94,113	0
30	LHG	D	408	47/49	0.95	0.08	23,46,81,103	0
23	CLA	c	509	65/65	0.95	0.08	28,46,64,68	0
23	CLA	C	511	65/65	0.95	0.08	28,50,68,68	0
23	CLA	C	503	65/65	0.95	0.07	24,39,51,63	0
30	LHG	l	101	49/49	0.95	0.07	29,43,59,64	0
23	CLA	C	510	65/65	0.95	0.07	28,45,67,73	0
23	CLA	a	604	65/65	0.95	0.08	26,40,89,107	0
24	PHO	d	401	64/64	0.95	0.06	25,38,46,65	0
25	BCR	B	617	40/40	0.95	0.07	25,39,53,56	0
31	DGD	c	516	62/66	0.95	0.08	19,41,75,84	0
23	CLA	b	609	65/65	0.95	0.08	27,45,69,79	0
23	CLA	b	616	60/65	0.95	0.08	25,42,90,95	0
23	CLA	c	503	65/65	0.95	0.07	32,44,57,62	0
25	BCR	C	515	40/40	0.95	0.07	21,35,50,54	0
27	PL9	D	407	55/55	0.95	0.06	20,31,40,48	0
23	CLA	c	504	60/65	0.95	0.08	31,45,79,90	0
27	PL9	d	408	55/55	0.95	0.06	21,33,43,47	0
23	CLA	c	505	65/65	0.95	0.08	22,41,66,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	CLA	c	506	65/65	0.95	0.09	31,52,107,111	0
25	BCR	T	101	40/40	0.95	0.06	25,42,61,68	0
23	CLA	c	508	64/65	0.95	0.08	28,44,83,104	0
30	LHG	B	623	49/49	0.95	0.08	25,42,70,73	0
23	CLA	B	616	60/65	0.96	0.08	21,39,94,99	0
23	CLA	C	502	65/65	0.96	0.06	26,40,54,61	0
23	CLA	c	510	65/65	0.96	0.07	33,49,67,74	0
23	CLA	B	606	65/65	0.96	0.07	17,32,74,80	0
23	CLA	a	606	65/65	0.96	0.08	17,34,86,104	0
23	CLA	a	612	65/65	0.96	0.06	18,28,38,44	0
23	CLA	d	403	65/65	0.96	0.07	31,48,100,105	0
23	CLA	b	602	65/65	0.96	0.07	23,41,65,75	0
24	PHO	a	605	64/64	0.96	0.05	18,29,38,43	0
30	LHG	D	406	49/49	0.96	0.07	22,38,54,65	0
23	CLA	b	606	65/65	0.96	0.07	20,38,69,74	0
25	BCR	A	608	40/40	0.96	0.06	20,32,40,46	0
23	CLA	b	608	65/65	0.96	0.06	24,39,61,64	0
23	CLA	C	505	65/65	0.96	0.07	20,39,71,83	0
23	CLA	b	610	65/65	0.96	0.07	22,36,53,55	0
23	CLA	b	612	65/65	0.96	0.07	16,33,47,56	0
31	DGD	C	516	62/66	0.96	0.08	21,41,76,90	0
23	CLA	b	615	65/65	0.96	0.06	25,40,55,65	0
31	DGD	C	518	62/66	0.96	0.07	25,44,75,84	0
23	CLA	C	506	65/65	0.96	0.08	25,40,101,113	0
23	CLA	c	501	65/65	0.96	0.06	27,38,49,55	0
23	CLA	c	502	65/65	0.96	0.07	28,41,65,67	0
23	CLA	C	508	65/65	0.96	0.07	23,40,100,118	0
23	CLA	C	509	65/65	0.96	0.07	22,41,63,64	0
25	BCR	a	607	40/40	0.96	0.06	15,31,41,49	0
23	CLA	B	609	65/65	0.96	0.06	23,35,58,66	0
23	CLA	B	615	65/65	0.96	0.07	22,37,67,83	0
23	CLA	c	507	65/65	0.96	0.07	23,42,57,66	0
34	BCT	a	610	4/4	0.96	0.07	26,32,41,50	0
23	CLA	B	605	65/65	0.97	0.06	17,29,47,49	0
23	CLA	b	613	65/65	0.97	0.06	18,32,65,75	0
23	CLA	b	614	65/65	0.97	0.07	22,36,77,87	0
23	CLA	A	604	65/65	0.97	0.08	14,33,101,121	0
23	CLA	C	507	65/65	0.97	0.06	20,38,60,68	0
23	CLA	B	607	65/65	0.97	0.06	15,31,59,67	0
23	CLA	B	608	65/65	0.97	0.05	20,33,52,64	0
23	CLA	A	613	65/65	0.97	0.05	14,26,48,58	0
23	CLA	B	610	65/65	0.97	0.06	18,30,43,47	0

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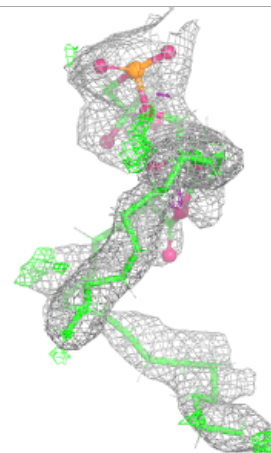
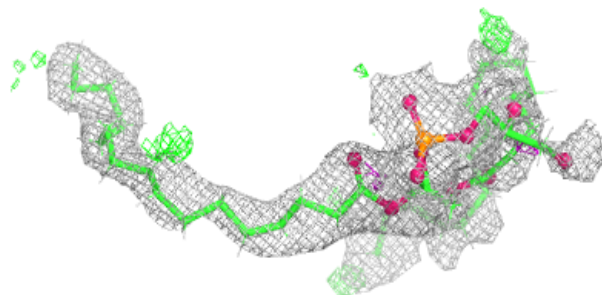
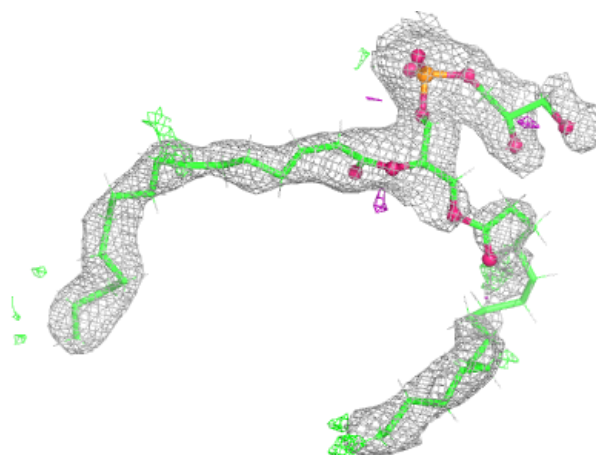
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	CLA	B	611	65/65	0.97	0.05	18,30,47,53	0
23	CLA	B	612	65/65	0.97	0.06	19,30,44,44	0
23	CLA	D	402	65/65	0.97	0.06	16,30,56,64	0
23	CLA	D	403	65/65	0.97	0.07	19,39,104,113	0
23	CLA	a	603	65/65	0.97	0.05	16,29,43,51	0
23	CLA	B	613	65/65	0.97	0.06	17,30,68,73	0
23	CLA	B	614	65/65	0.97	0.07	20,34,82,95	0
30	LHG	L	101	49/49	0.97	0.07	24,39,54,65	0
23	CLA	A	603	65/65	0.97	0.05	13,25,44,57	0
23	CLA	B	602	65/65	0.97	0.06	22,34,59,63	0
30	LHG	d	407	49/49	0.97	0.06	25,42,60,64	0
23	CLA	d	402	65/65	0.97	0.06	20,34,64,70	0
23	CLA	b	603	65/65	0.97	0.06	21,36,69,76	0
23	CLA	b	604	65/65	0.97	0.07	20,34,80,90	0
24	PHO	A	605	64/64	0.97	0.05	12,27,36,40	0
24	PHO	A	606	64/64	0.97	0.05	19,30,44,50	0
23	CLA	b	605	65/65	0.97	0.06	19,33,47,56	0
23	CLA	C	501	65/65	0.97	0.06	23,35,49,60	0
23	CLA	b	607	65/65	0.97	0.07	19,36,61,68	0
23	CLA	B	603	65/65	0.97	0.06	14,31,62,69	0
23	CLA	B	604	65/65	0.97	0.07	18,31,82,93	0
23	CLA	C	504	59/65	0.97	0.07	24,42,80,85	0
34	BCT	D	401	4/4	0.97	0.05	26,27,32,37	0
23	CLA	b	611	65/65	0.97	0.06	20,34,51,55	0
35	HEM	F	102	43/43	0.97	0.08	34,48,68,69	0
35	HEM	f	102	43/43	0.97	0.09	41,55,76,78	0
23	CLA	A	607	54/65	0.98	0.06	15,28,62,69	0
36	HEC	v	201	43/43	0.98	0.06	27,36,49,53	0
21	OEX	a	601[A]	10/10	0.99	0.03	19,22,28,28	10
26	CL	A	609	1/1	0.99	0.03	27,27,27,27	0
26	CL	A	610	1/1	0.99	0.03	24,24,24,24	0
26	CL	a	608	1/1	0.99	0.03	25,25,25,25	0
32	OEY	A	618[B]	11/11	0.99	0.03	23,27,30,31	11
32	OEY	a	618[B]	11/11	0.99	0.03	22,28,30,31	11
36	HEC	V	201	43/43	0.99	0.05	21,31,42,46	0
21	OEX	A	601[A]	10/10	0.99	0.03	21,25,28,32	10
22	FE2	a	602	1/1	1.00	0.02	30,30,30,30	0
22	FE2	A	602	1/1	1.00	0.01	25,25,25,25	0
26	CL	a	609	1/1	1.00	0.10	25,25,25,25	0

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

orientation to approximate a three-dimensional view.

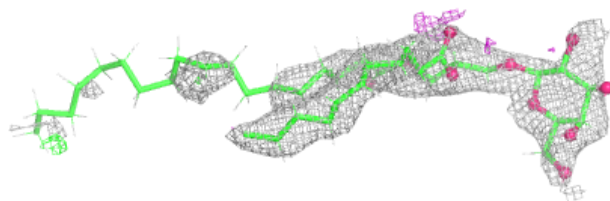
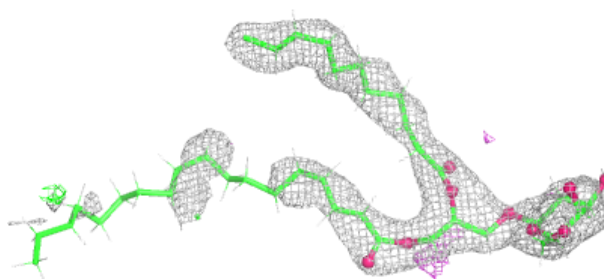
Electron density around LHG A 615:

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

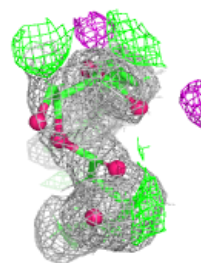
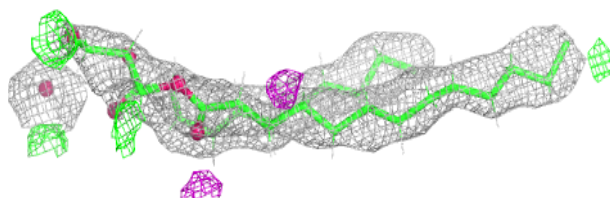
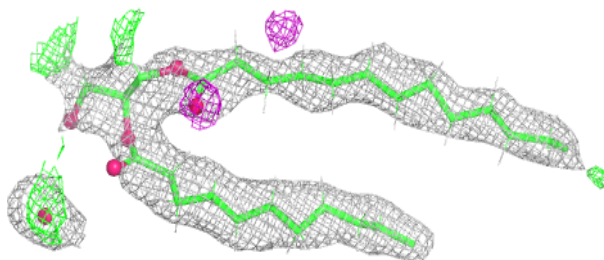


Electron density around LMG c 521:

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

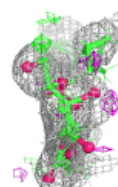
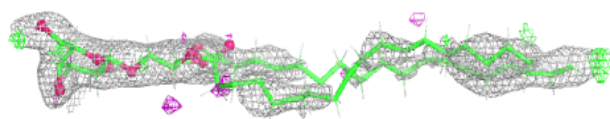
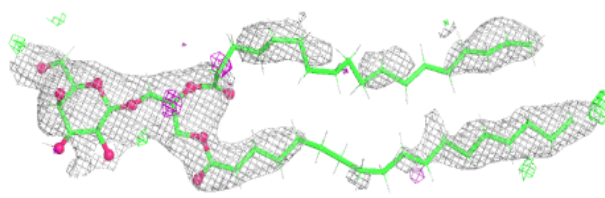
**Electron density around LMG D 409:**

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

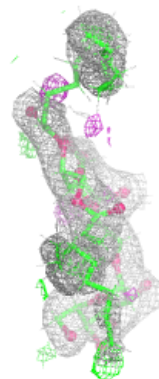
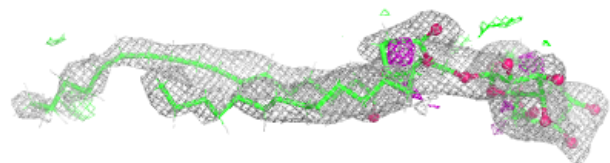
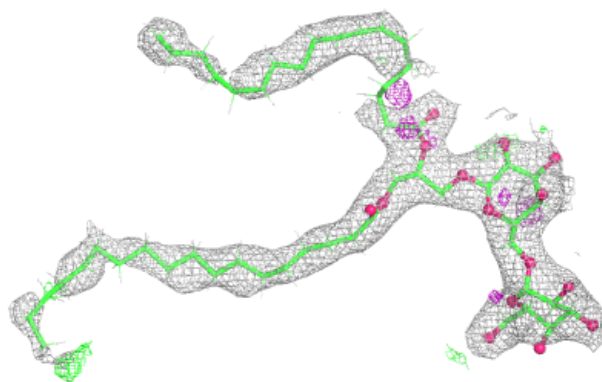


Electron density around LMG b 621:

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

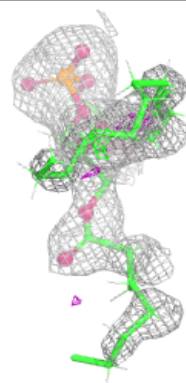
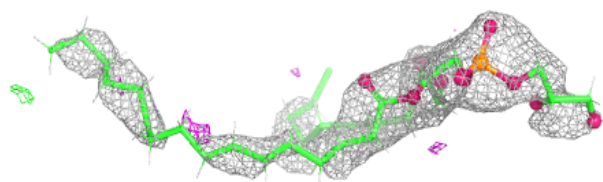
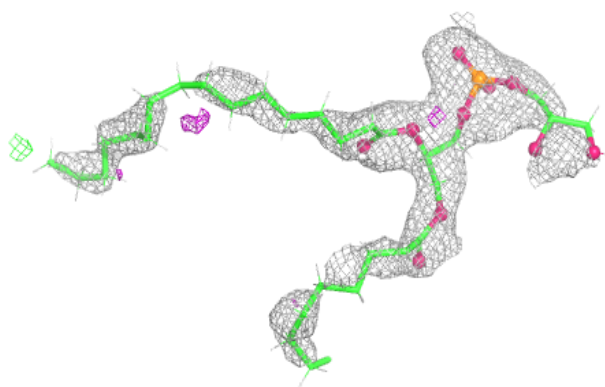
**Electron density around DGD A 617:**

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

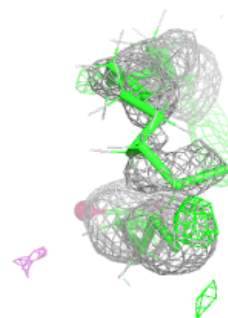
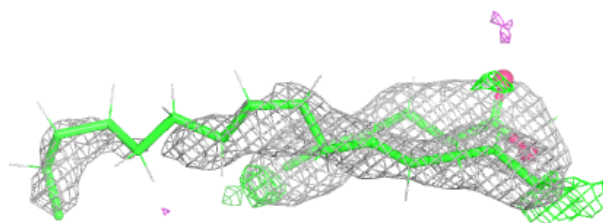
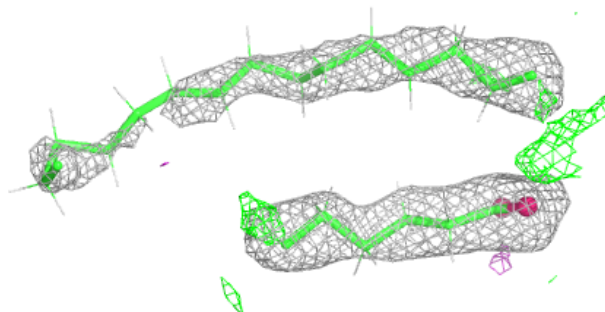


Electron density around LHG a 614:

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

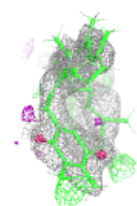
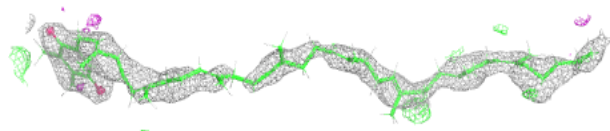
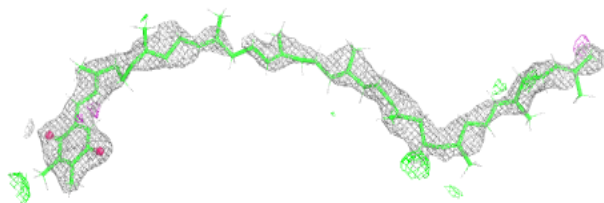
**Electron density around LMG d 410:**

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

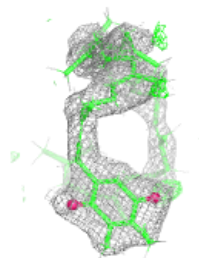
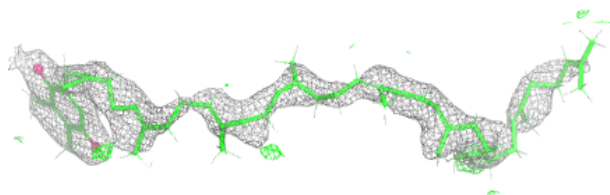
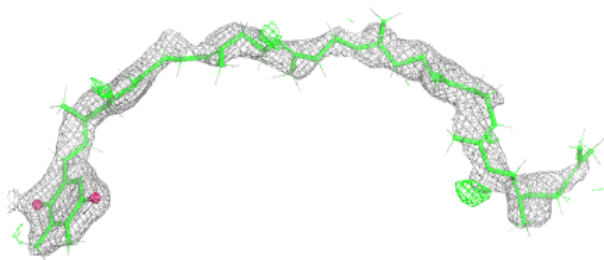


Electron density around PL9 A 611:

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

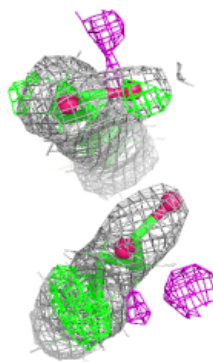
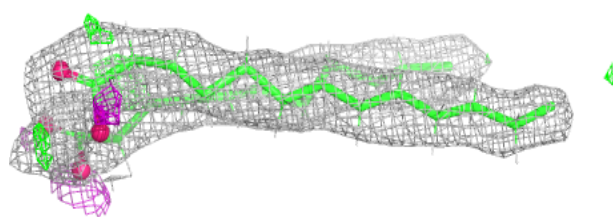
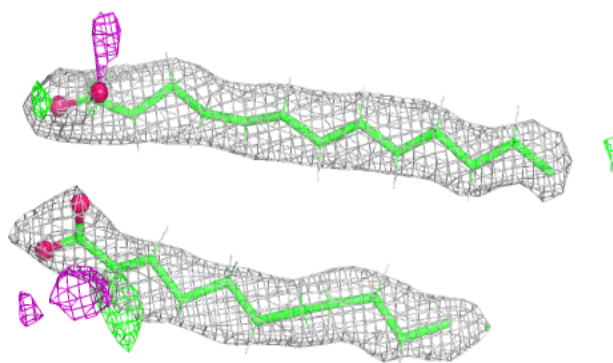
**Electron density around PL9 a 611:**

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

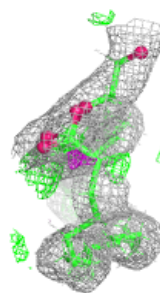
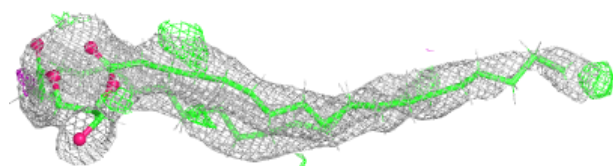
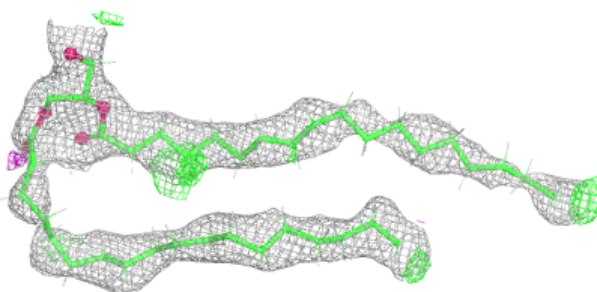


Electron density around LMG B 622:

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

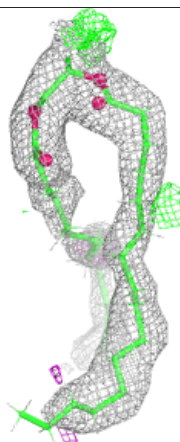
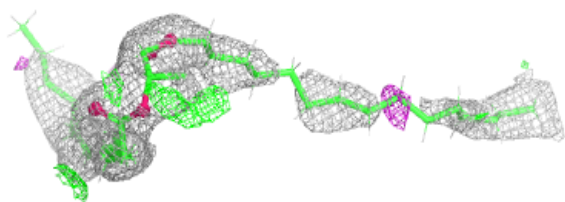
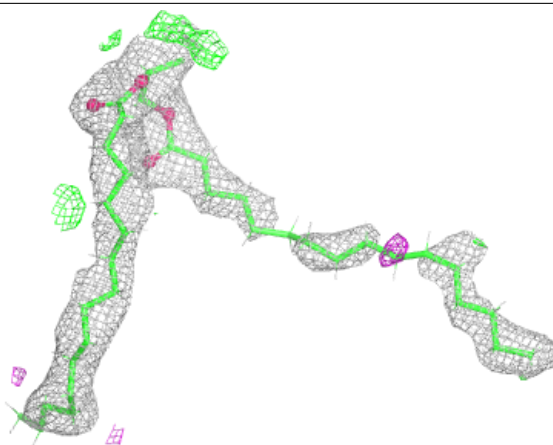
**Electron density around DGD a 616:**

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



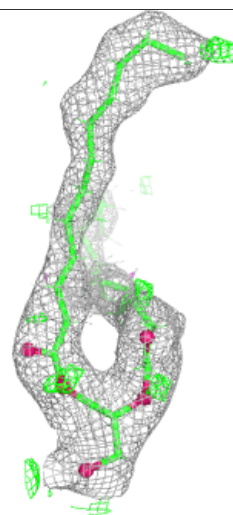
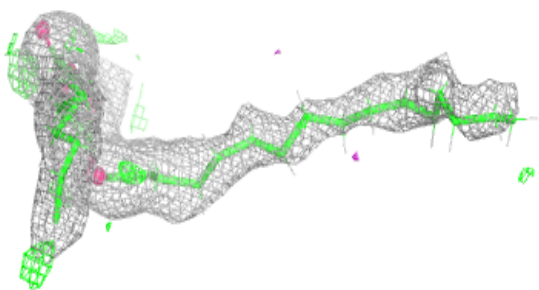
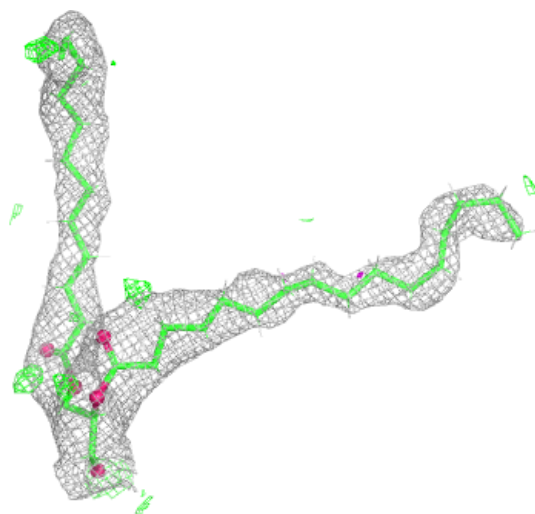
Electron density around SQD A 616:

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



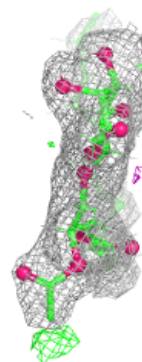
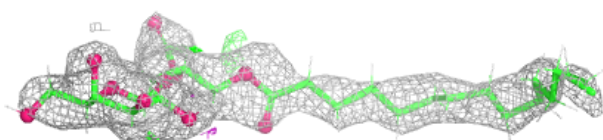
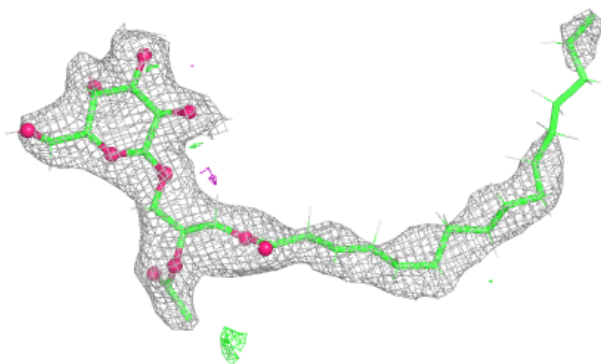
Electron density around SQD a 615:

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



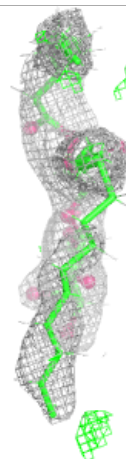
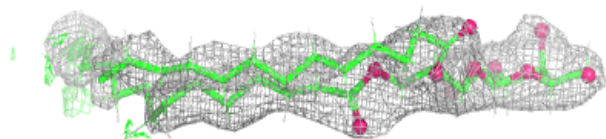
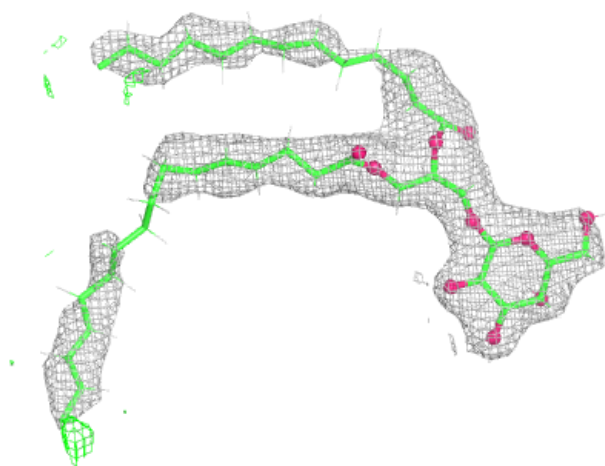
Electron density around LMG c 519:

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



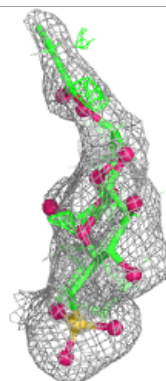
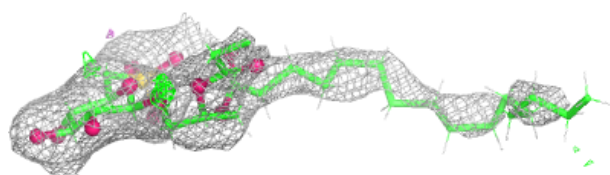
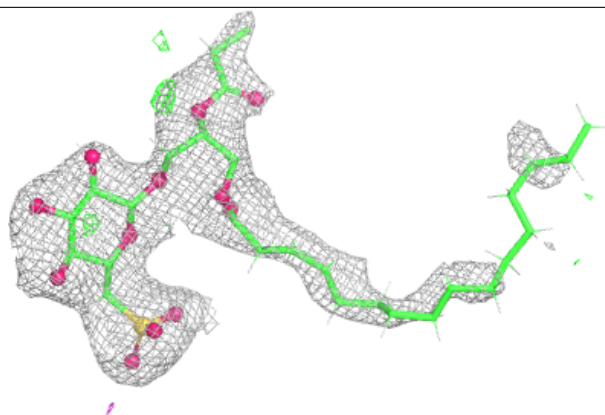
Electron density around LMG C 519:

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

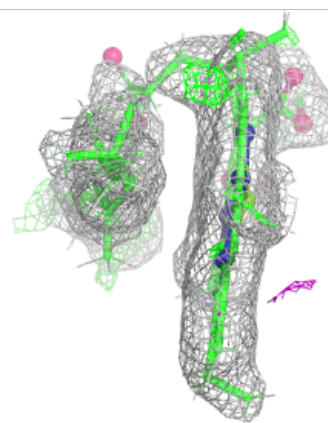
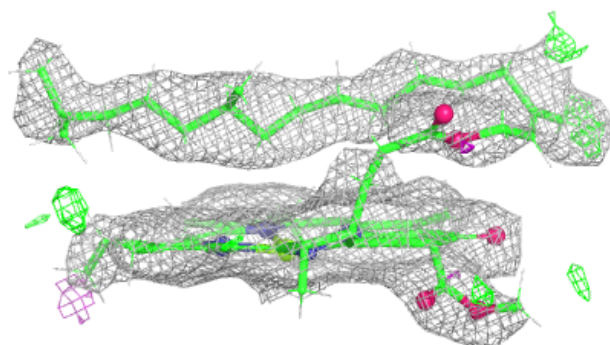
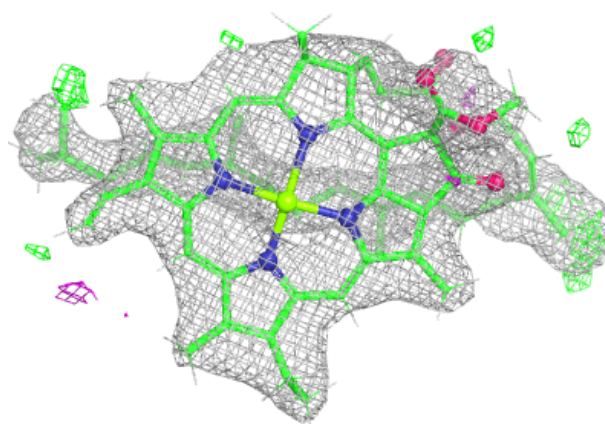


Electron density around SQD f 101:

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

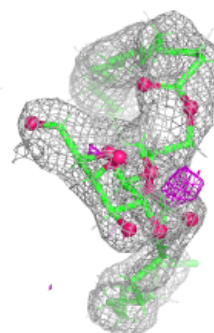
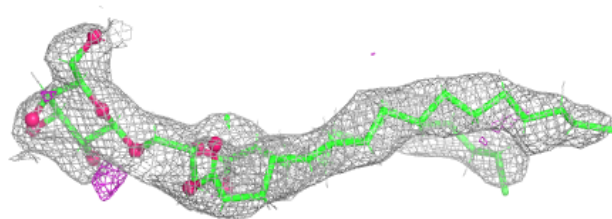
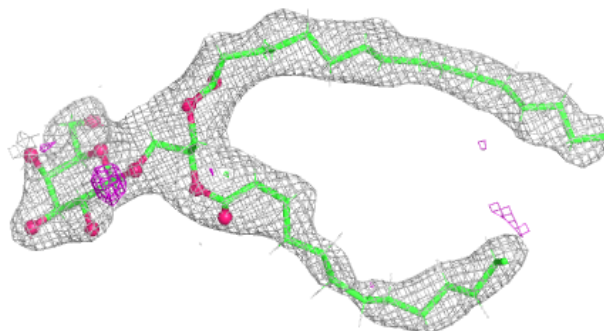
**Electron density around CLA h 101:**

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

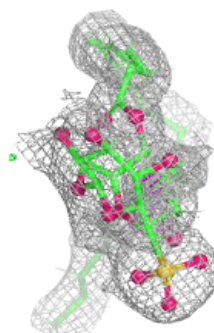
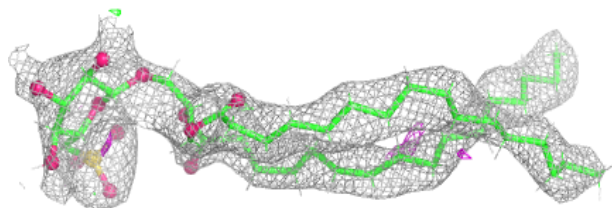
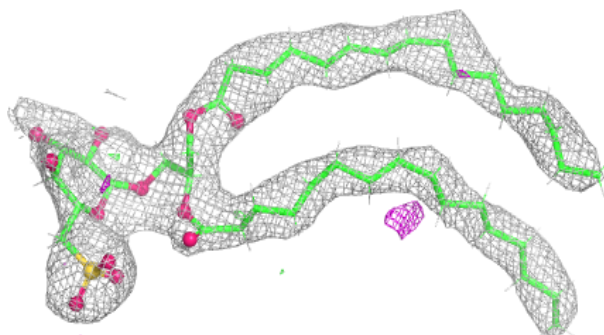


Electron density around LMG A 612:

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

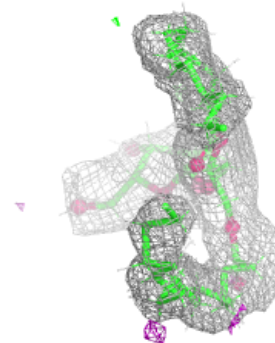
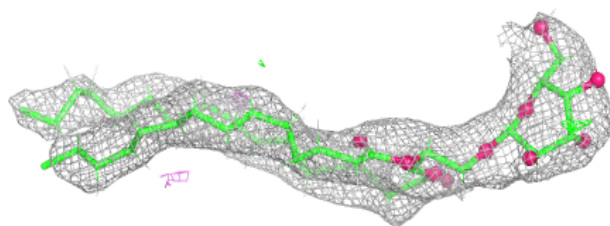
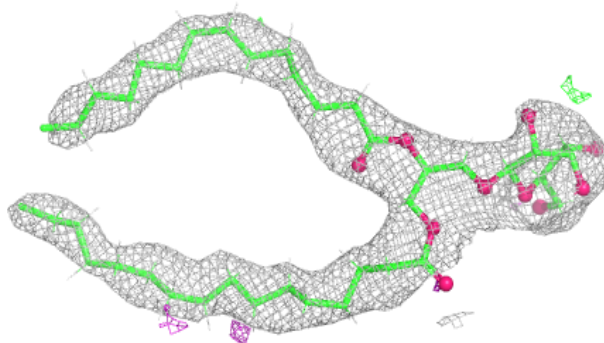
**Electron density around SQD B 624:**

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

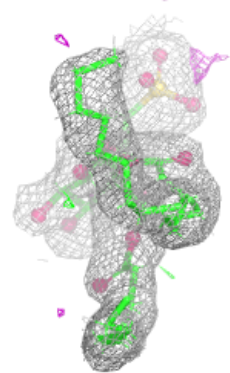
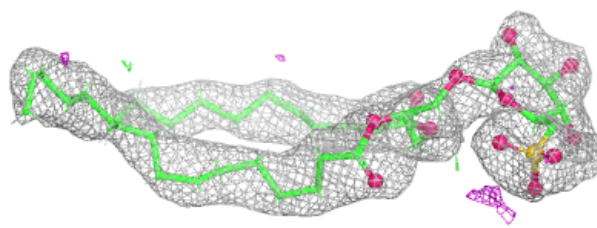
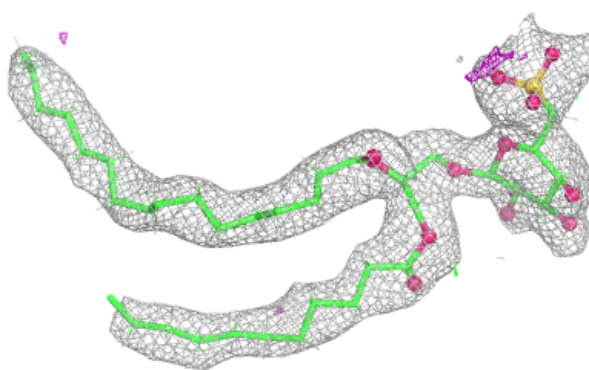


Electron density around LMG c 522:

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

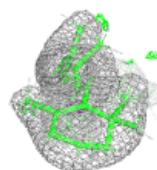
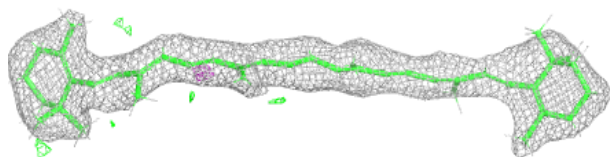
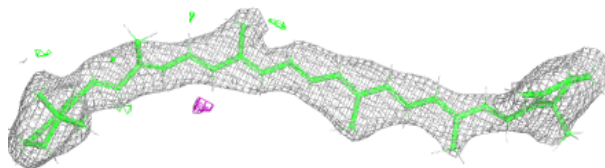
**Electron density around SQD b 601:**

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



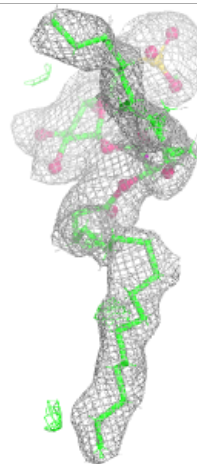
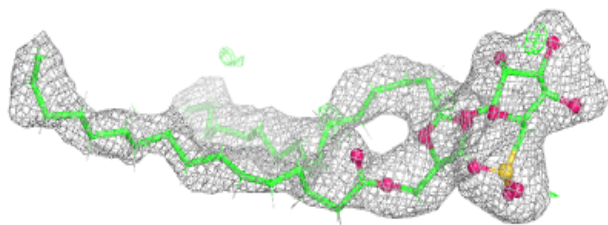
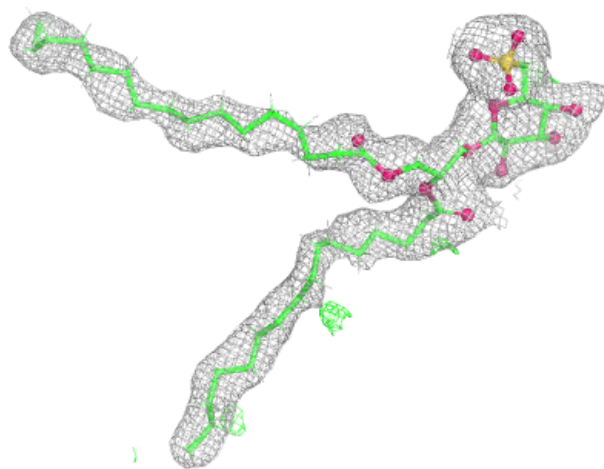
Electron density around BCR h 102:

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



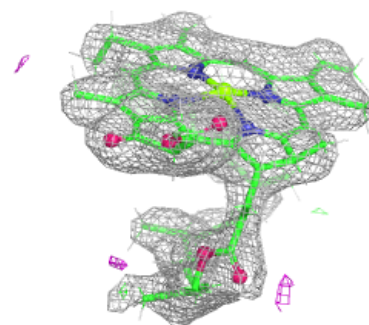
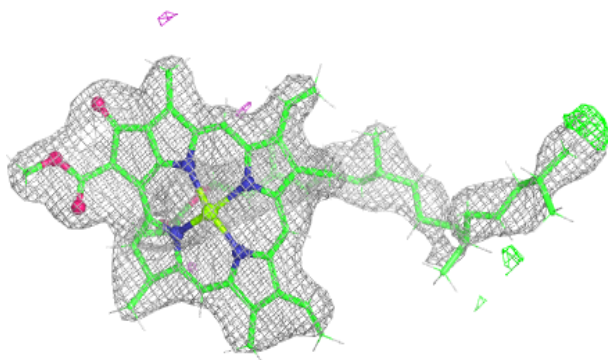
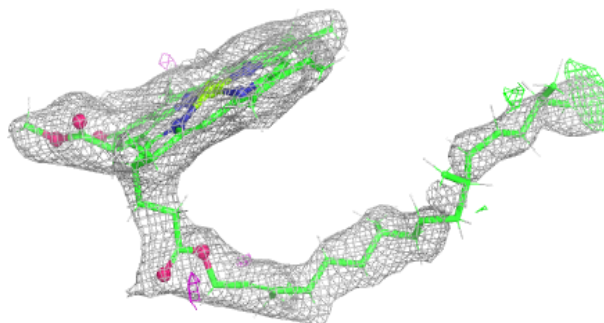
Electron density around SQD a 613:

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

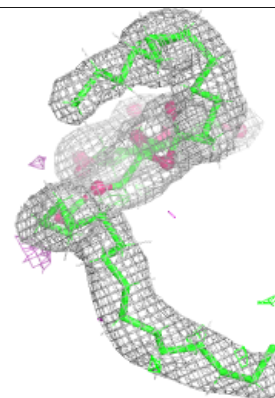
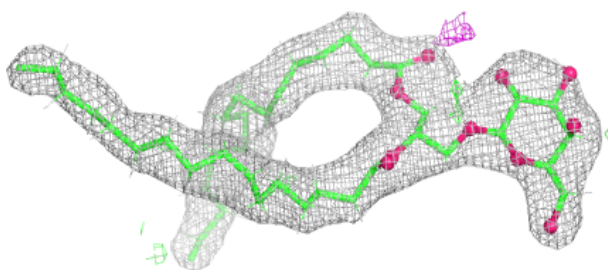
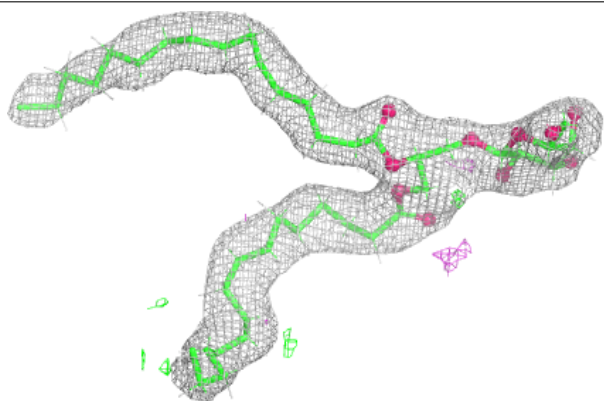


Electron density around CLA C 513:

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

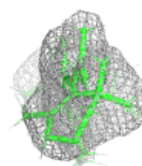
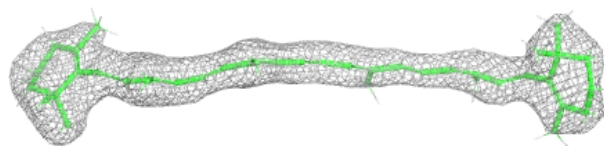
**Electron density around LMG m 101:**

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

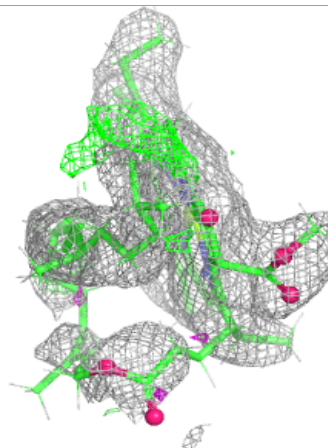
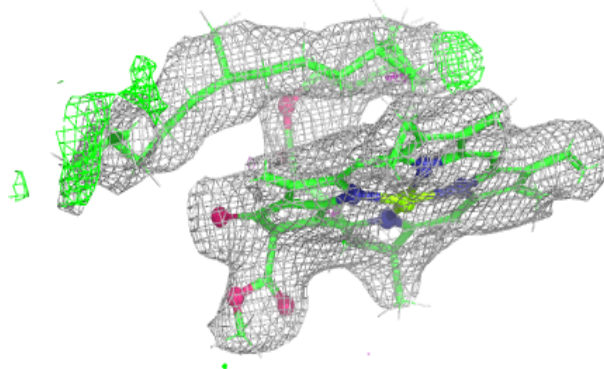
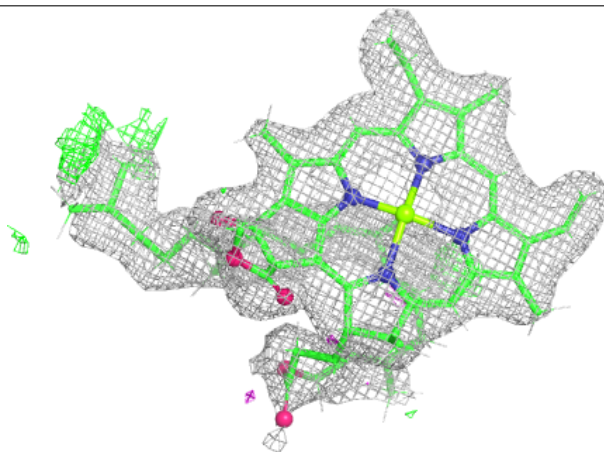


Electron density around BCR k 101:

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

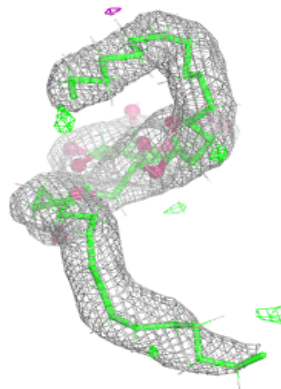
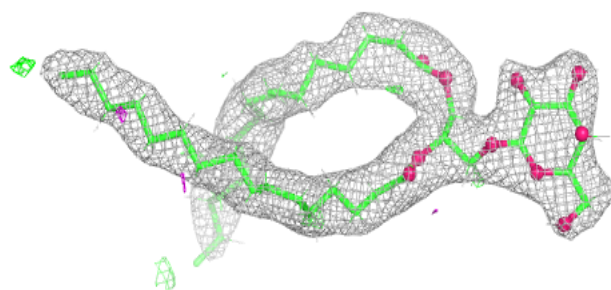
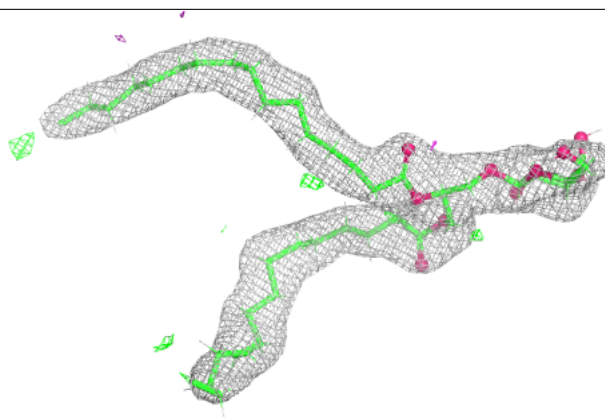
**Electron density around CLA B 601:**

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

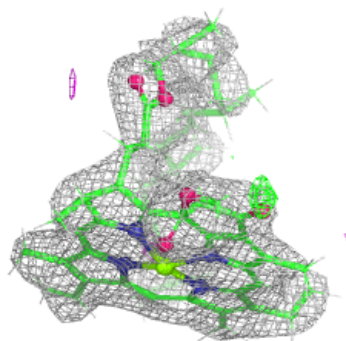
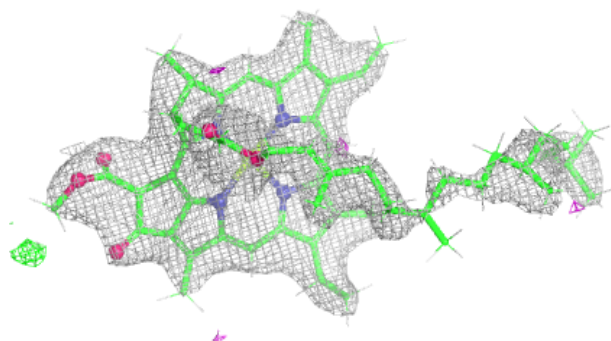
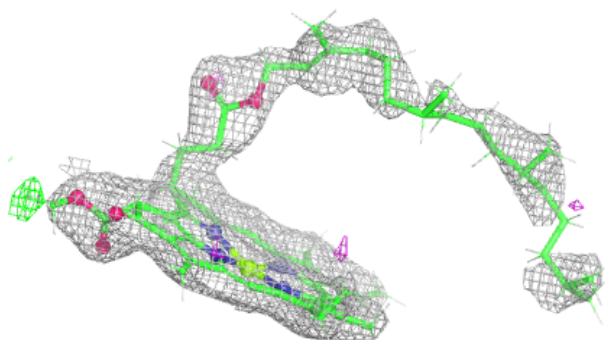


Electron density around LMG B 620:

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

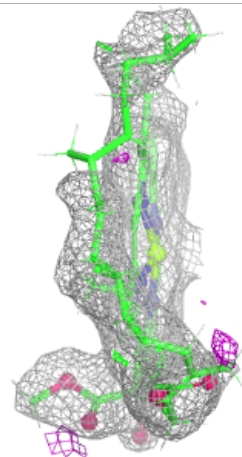
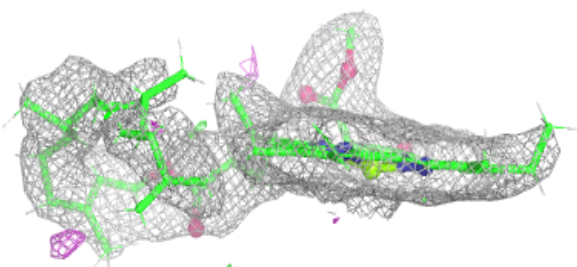
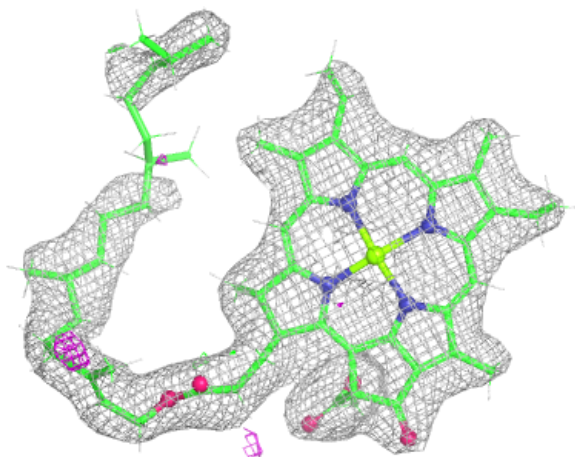
**Electron density around CLA c 513:**

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



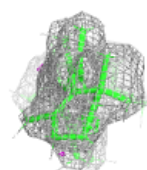
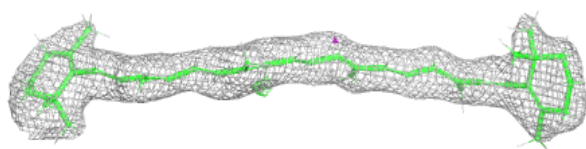
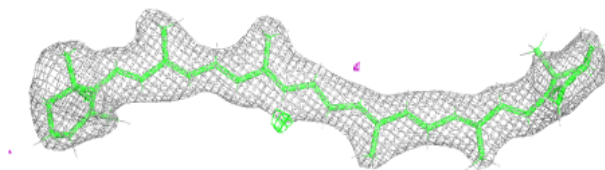
Electron density around CLA c 512:

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

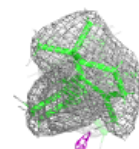
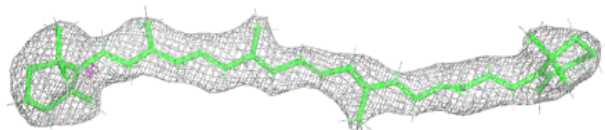
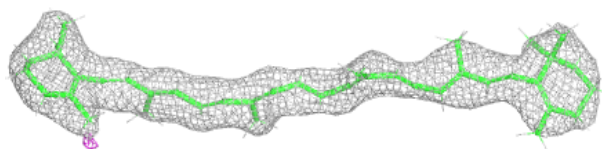


Electron density around BCR Y 101:

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

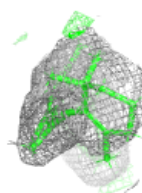
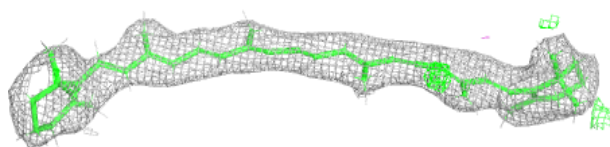
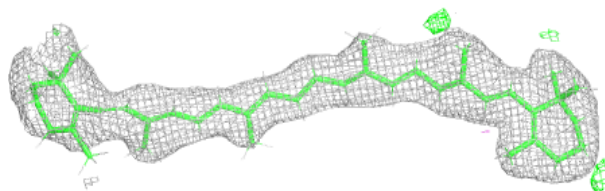
**Electron density around BCR c 514:**

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

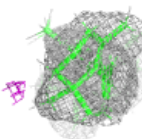
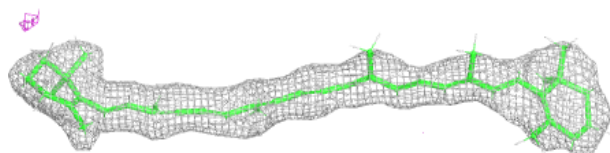
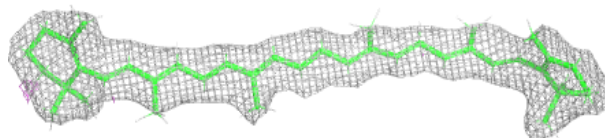


Electron density around BCR d 404:

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

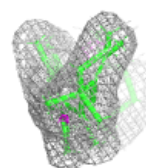
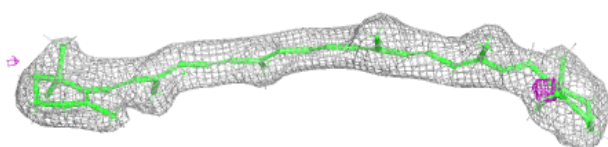
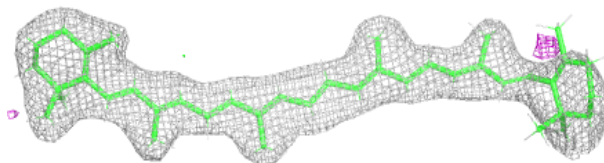
**Electron density around BCR C 514:**

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

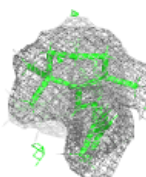
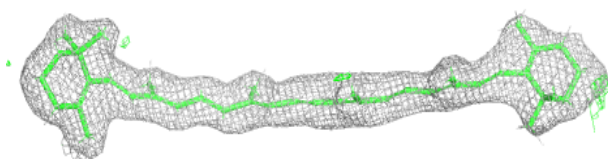
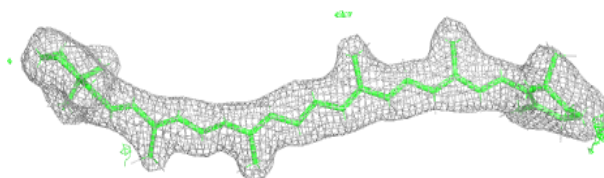


Electron density around BCR D 404:

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

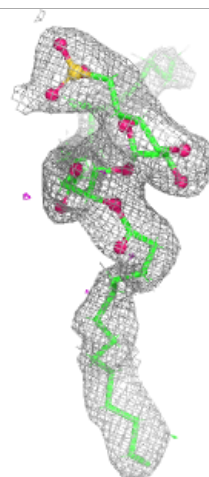
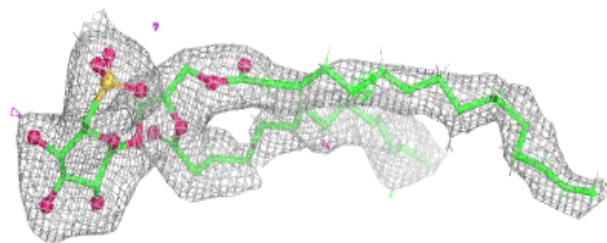
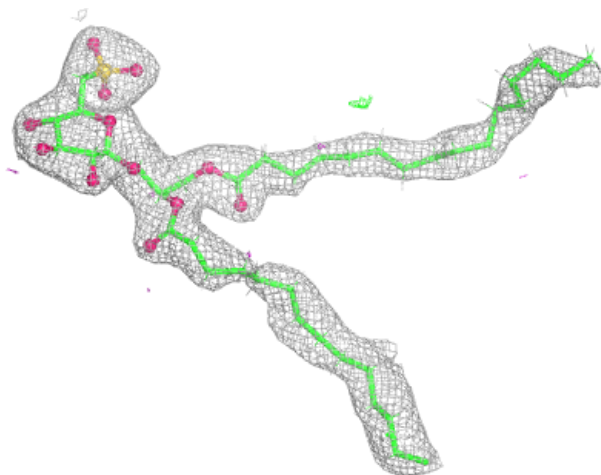
**Electron density around BCR H 101:**

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



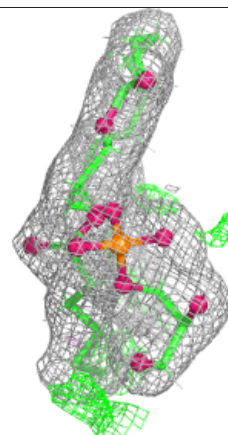
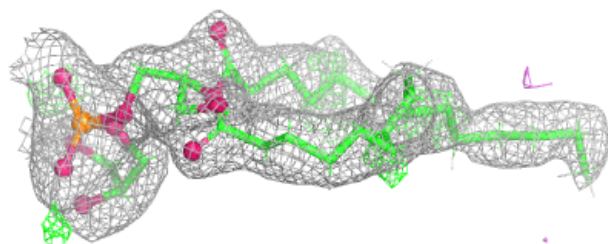
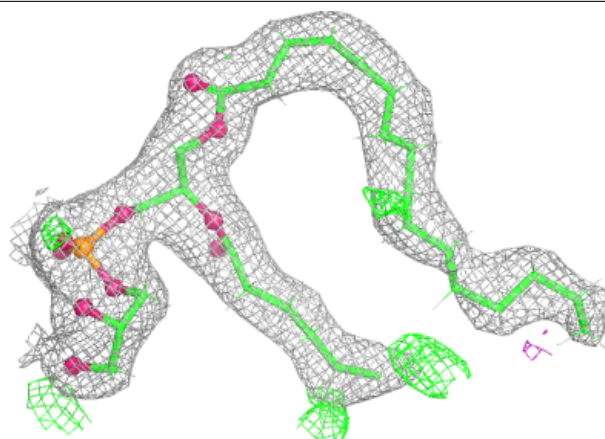
Electron density around SQD A 614:

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

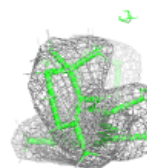
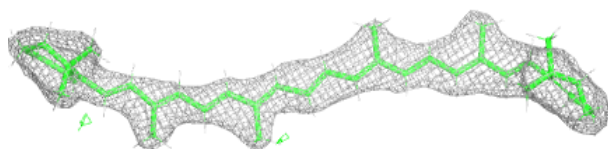
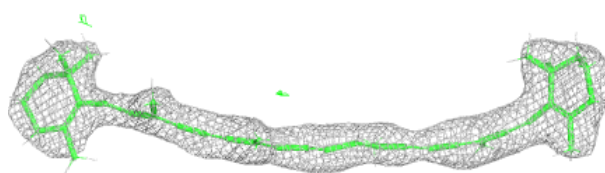


Electron density around LHG d 409:

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

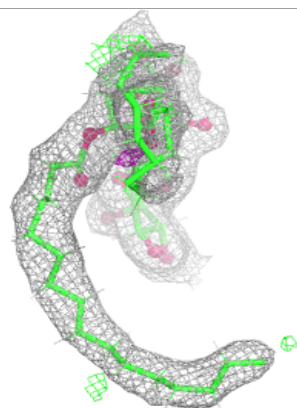
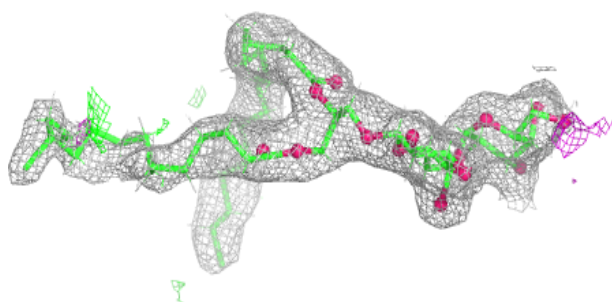
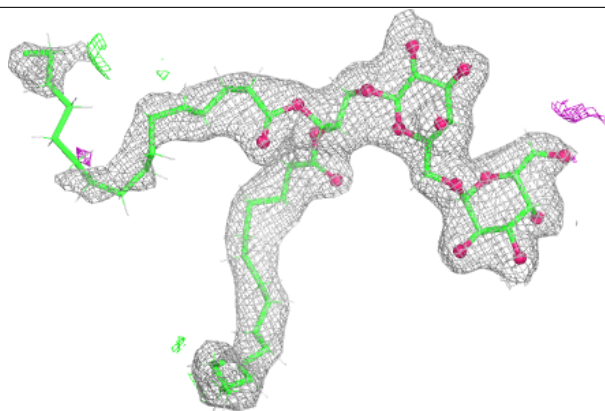
**Electron density around BCR k 102:**

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

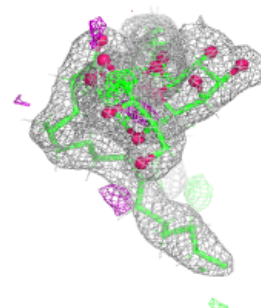
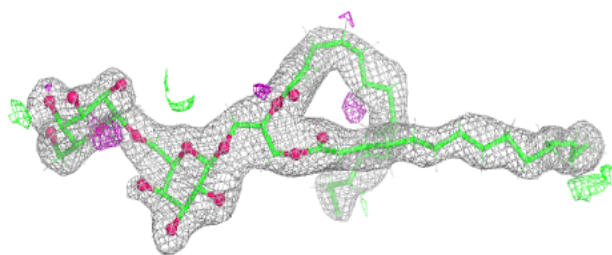
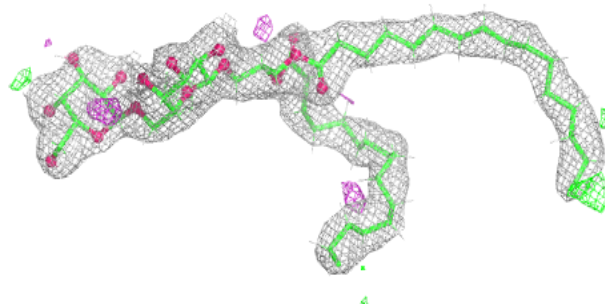


Electron density around DGD C 517:

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

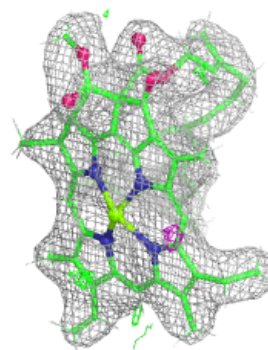
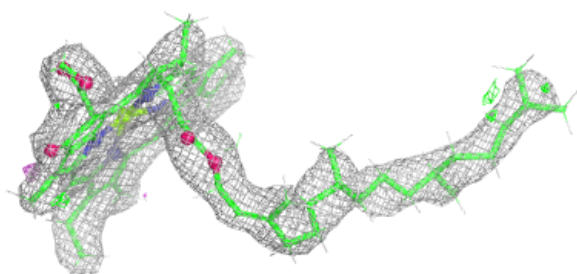
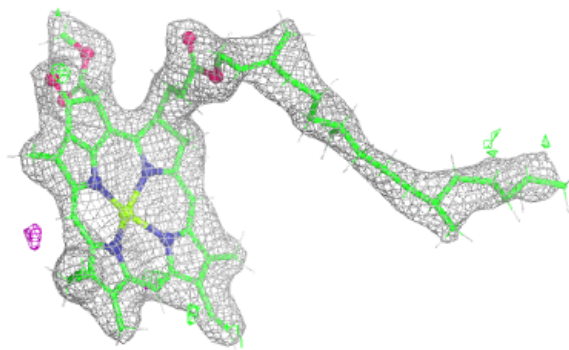
**Electron density around DGD H 102:**

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

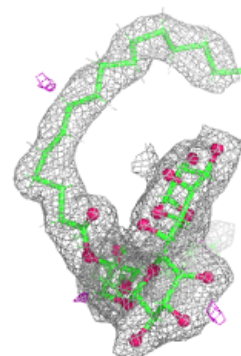
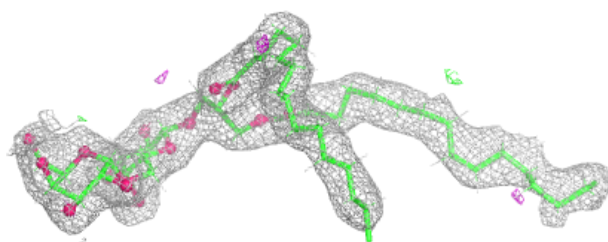
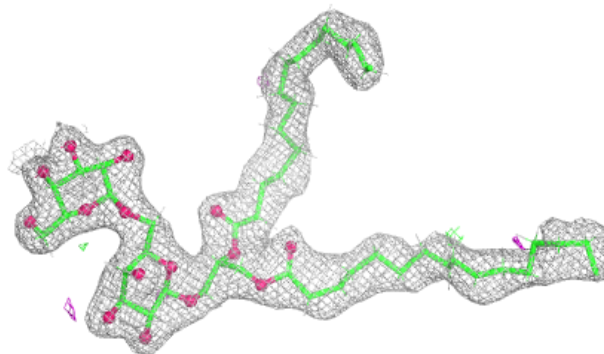


Electron density around CLA c 511:

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

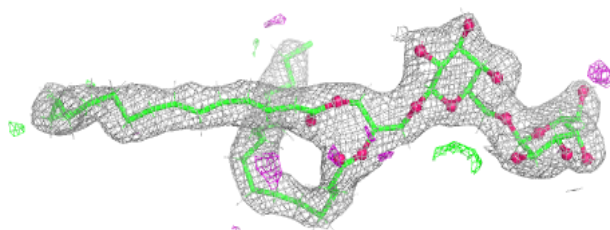
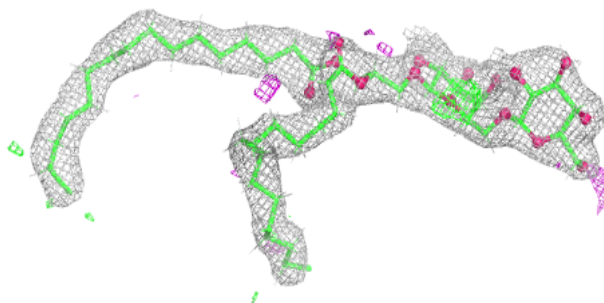
**Electron density around DGD c 517:**

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

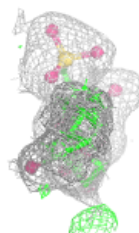
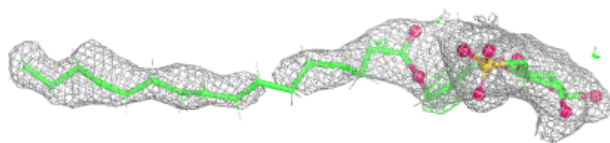
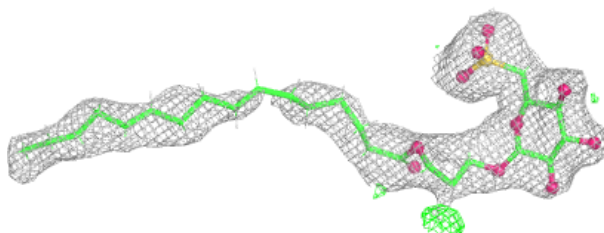


Electron density around DGD h 103:

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

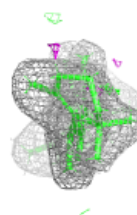
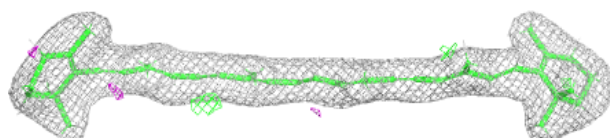
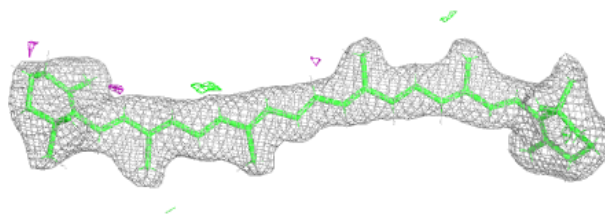
**Electron density around SQD F 101:**

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



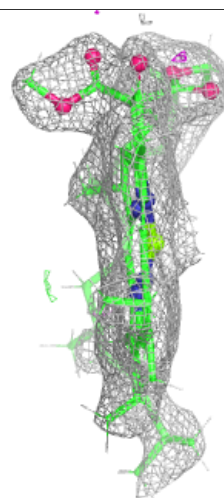
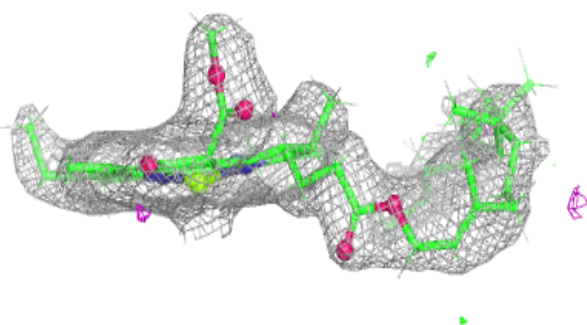
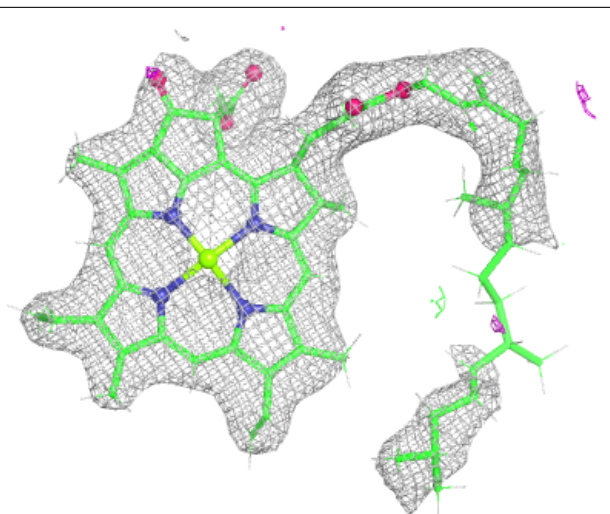
Electron density around BCR b 618:

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



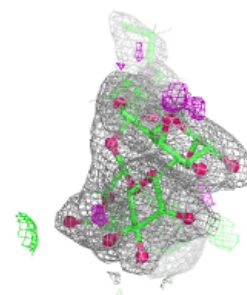
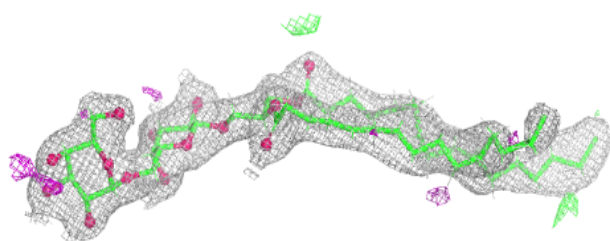
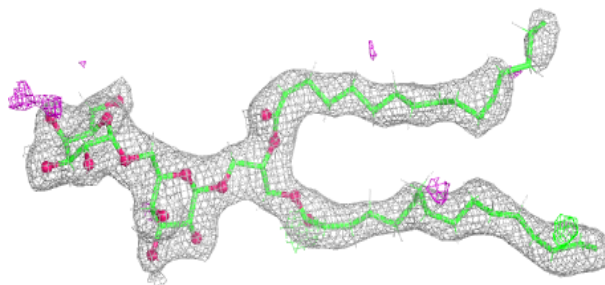
Electron density around CLA C 512:

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

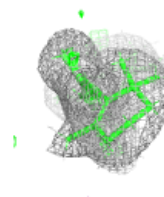
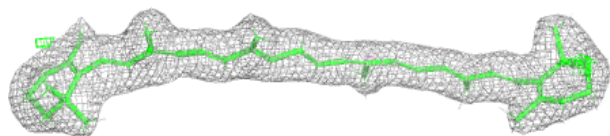
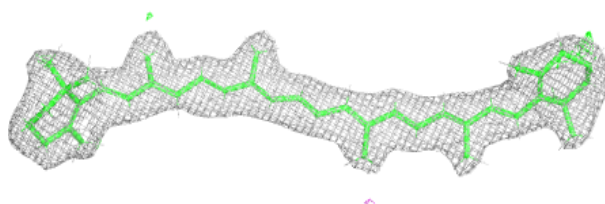


Electron density around DGD c 518:

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

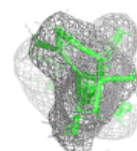
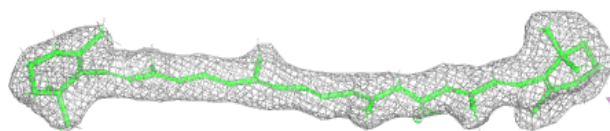
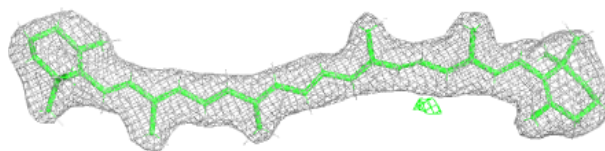
**Electron density around BCR B 619:**

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

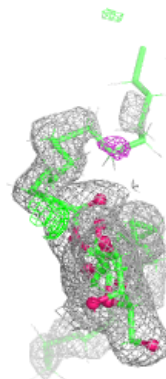
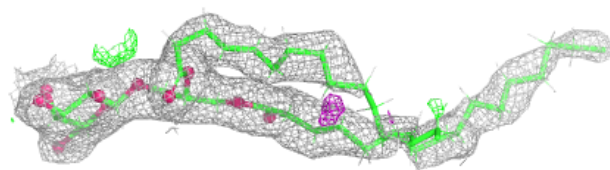
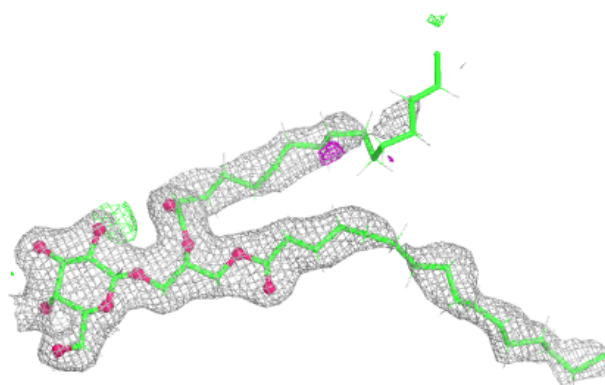


Electron density around BCR b 619:

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

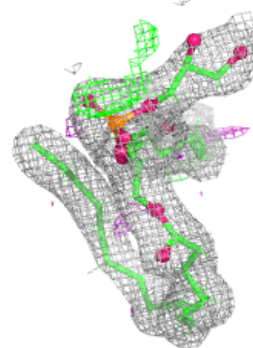
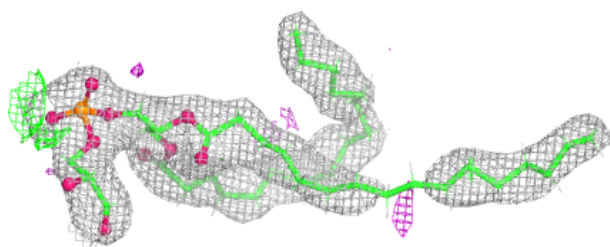
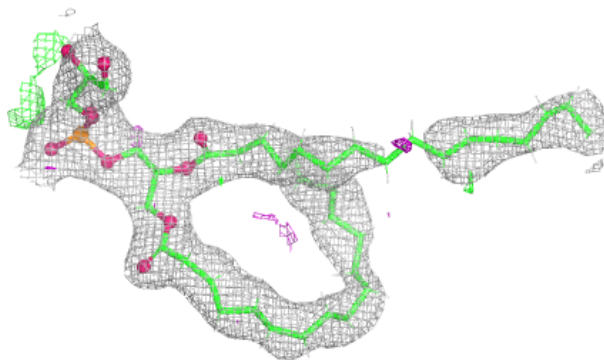
**Electron density around LMG D 405:**

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

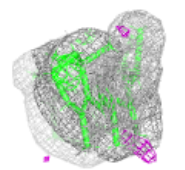
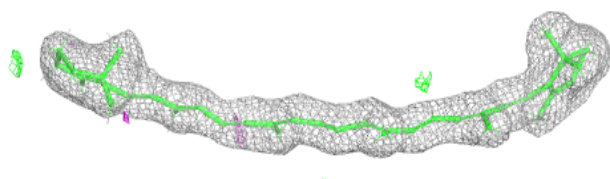
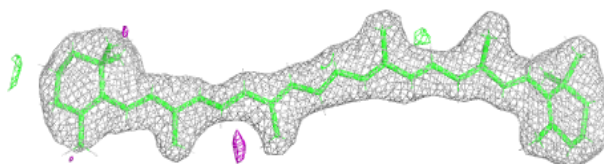


Electron density around LHG d 405:

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

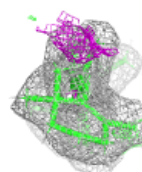
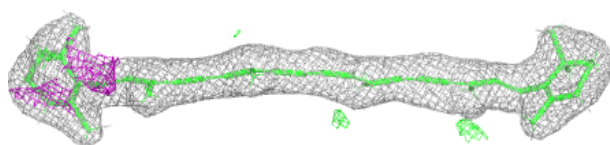
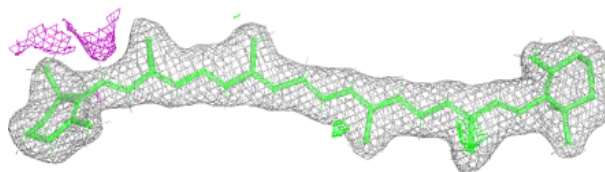
**Electron density around BCR t 101:**

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

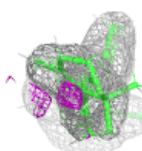
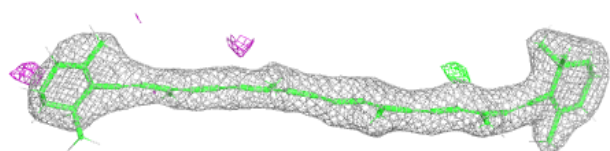
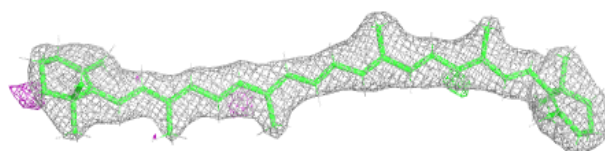


Electron density around BCR B 618:

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

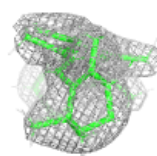
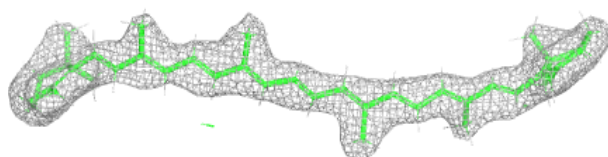
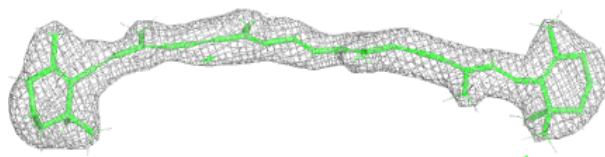
**Electron density around BCR c 515:**

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

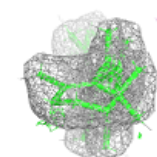
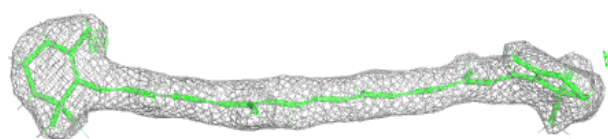


Electron density around BCR C 520:

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

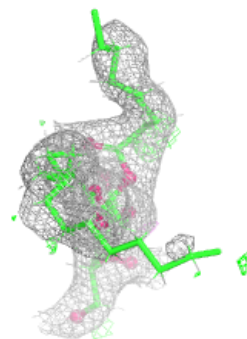
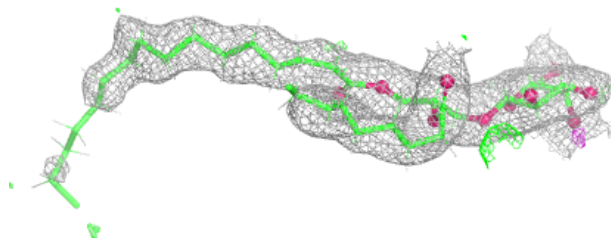
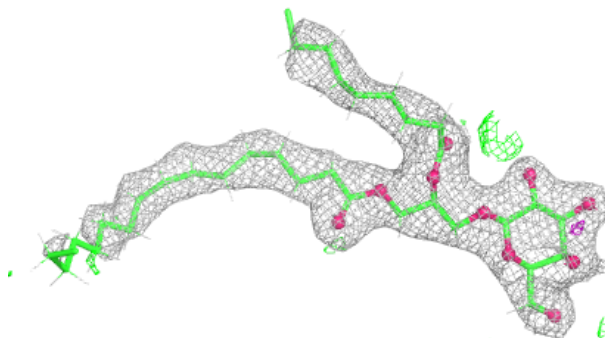
**Electron density around BCR b 617:**

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

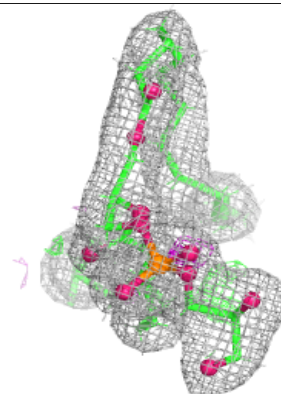
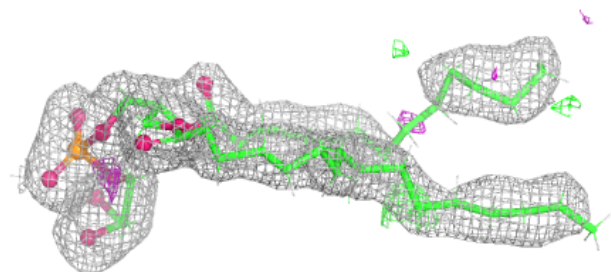
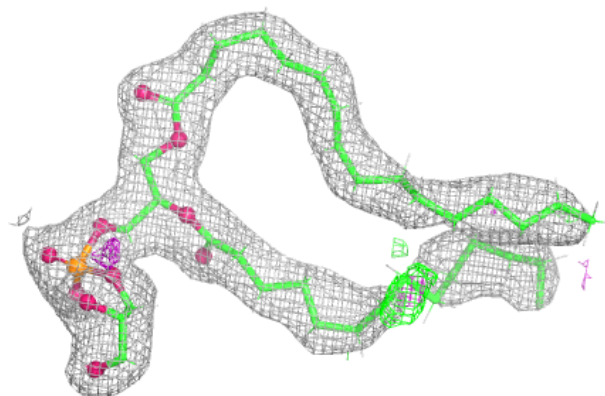


Electron density around LMG d 406:

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

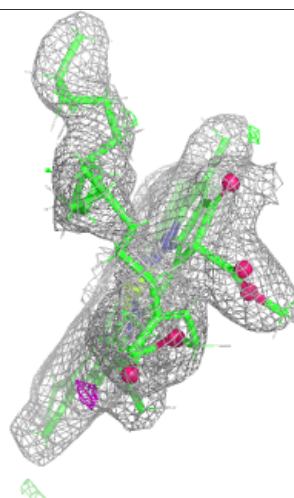
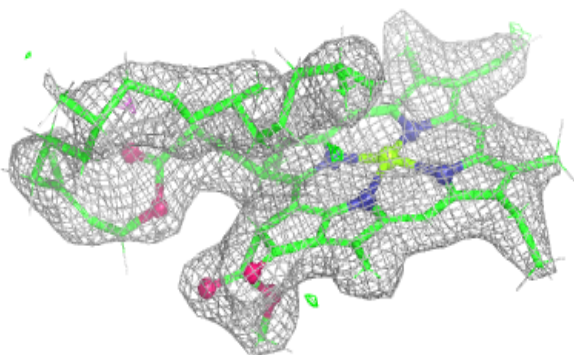
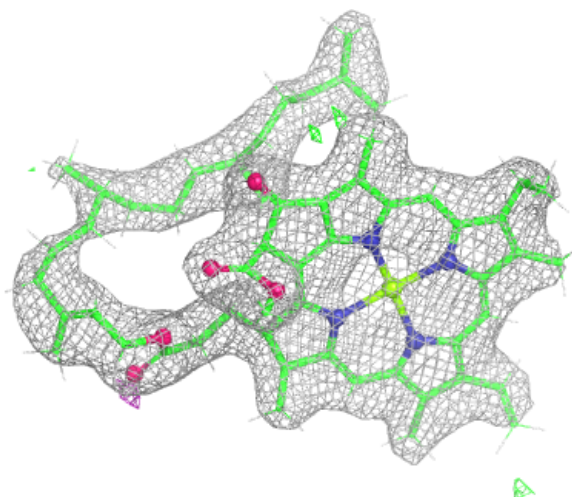
**Electron density around LHG D 408:**

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



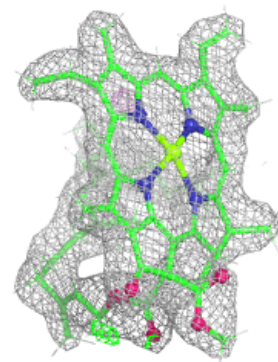
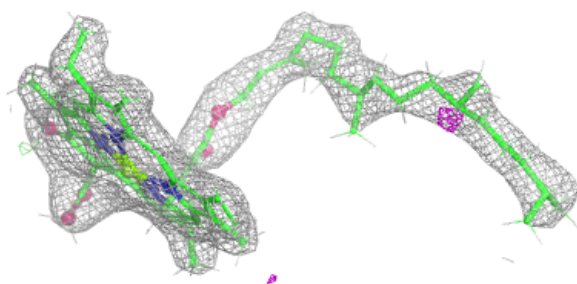
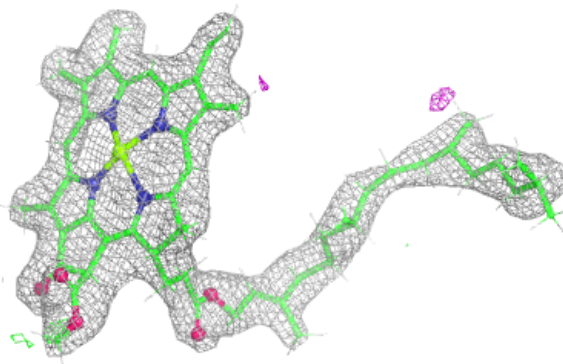
Electron density around CLA c 509:

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



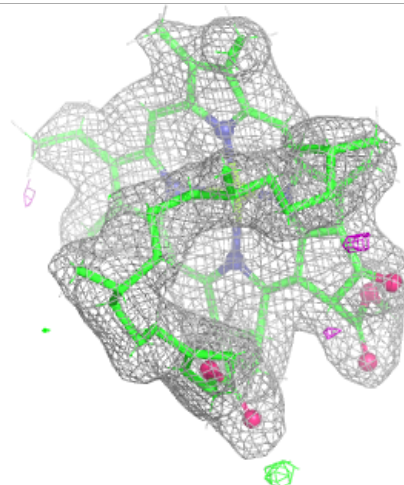
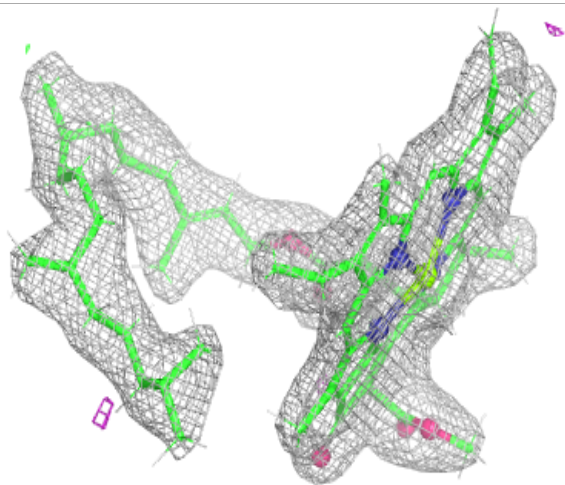
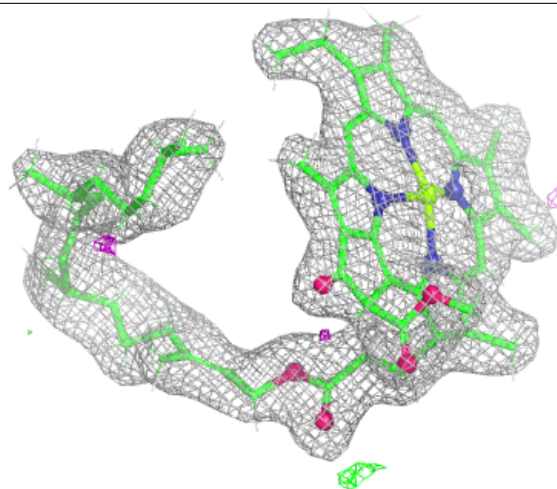
Electron density around CLA C 511:

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



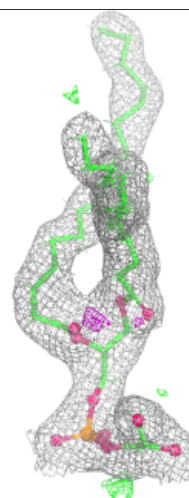
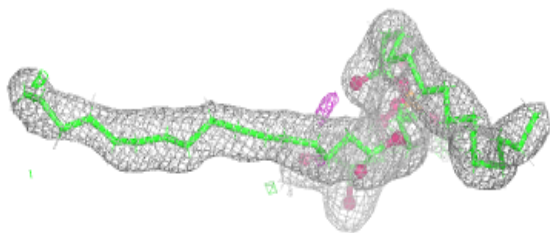
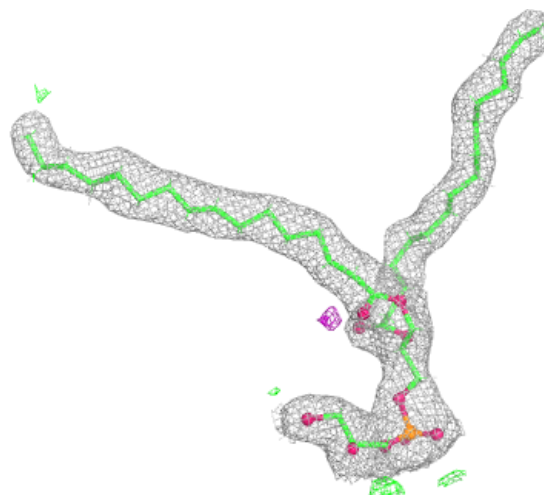
Electron density around CLA C 503:

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



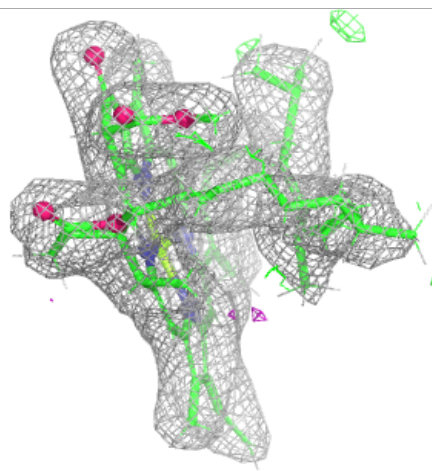
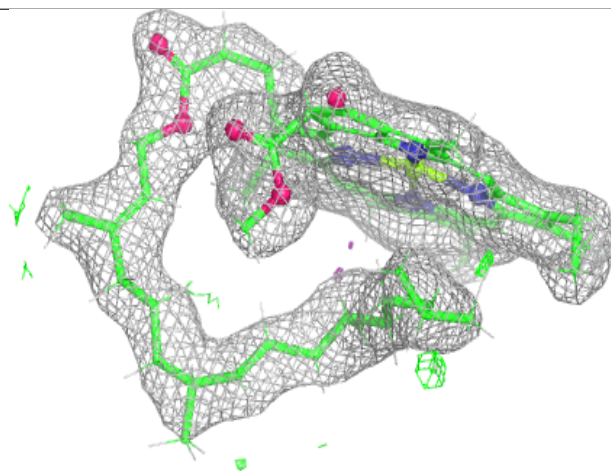
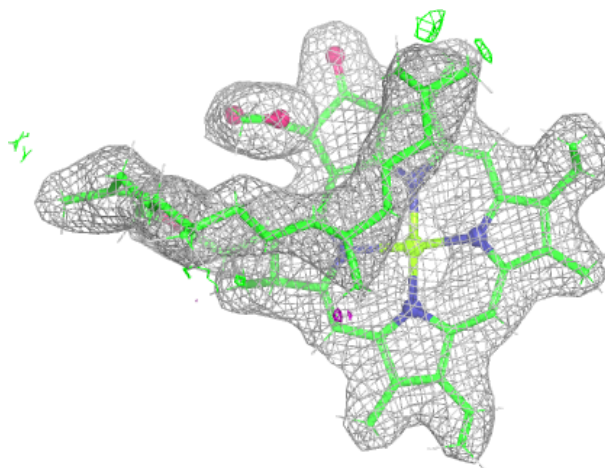
Electron density around LHG 1 101:

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



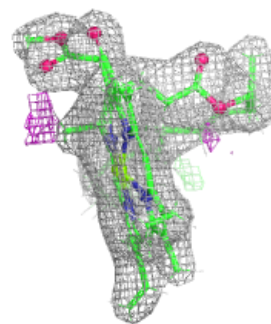
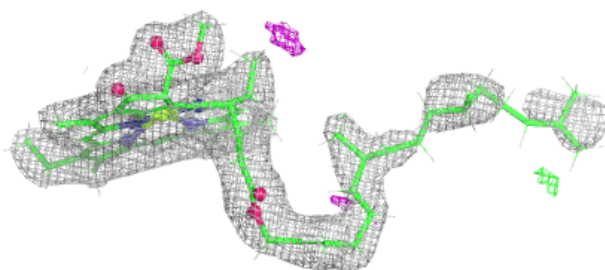
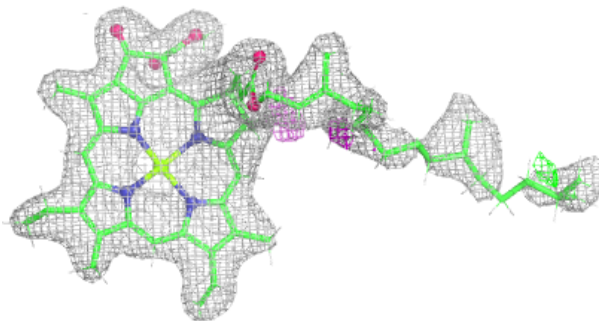
Electron density around CLA C 510:

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

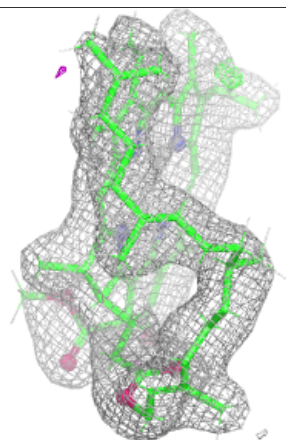
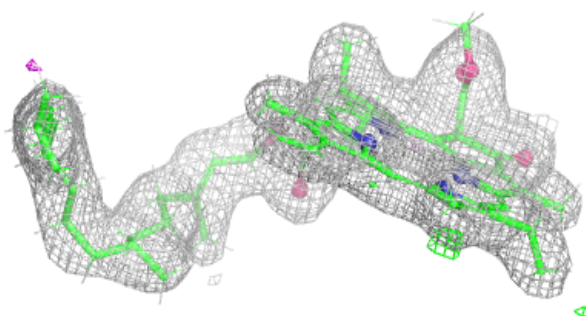
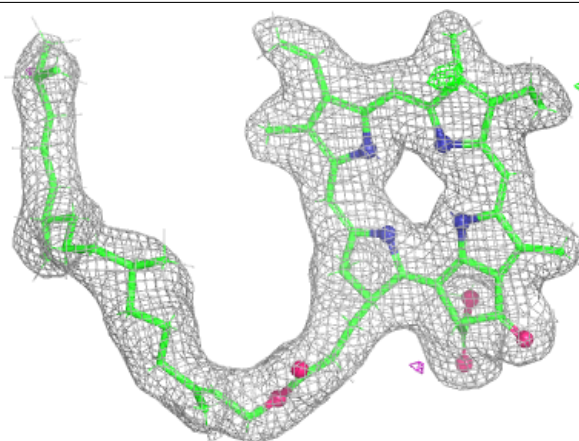


Electron density around CLA a 604:

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

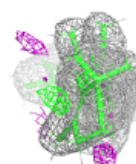
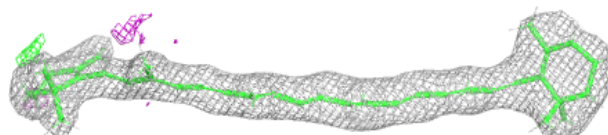
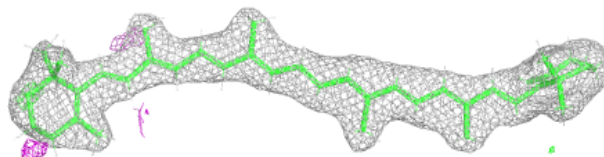
**Electron density around PHO d 401:**

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

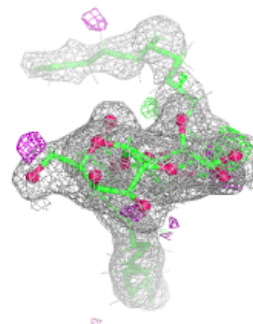
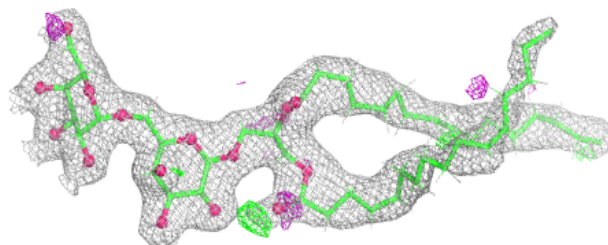
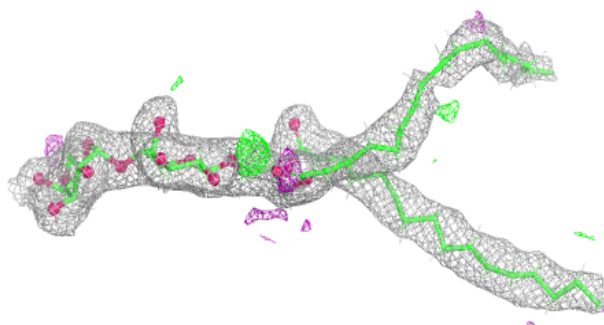


Electron density around BCR B 617:

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

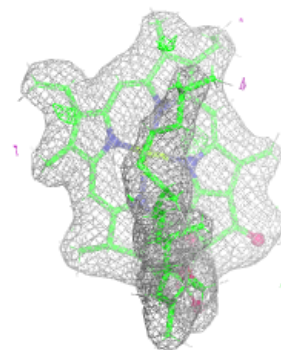
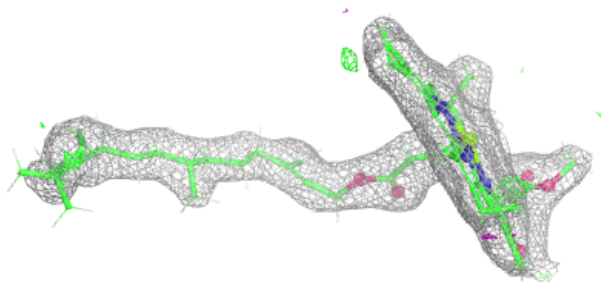
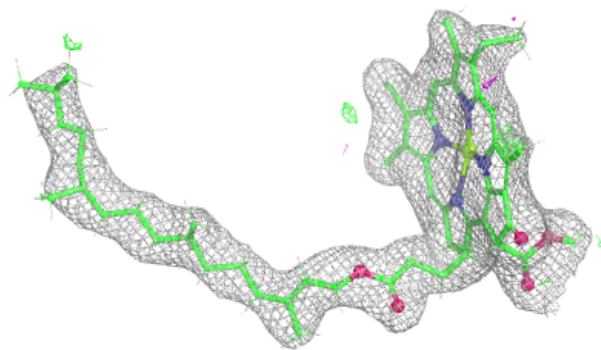
**Electron density around DGD c 516:**

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



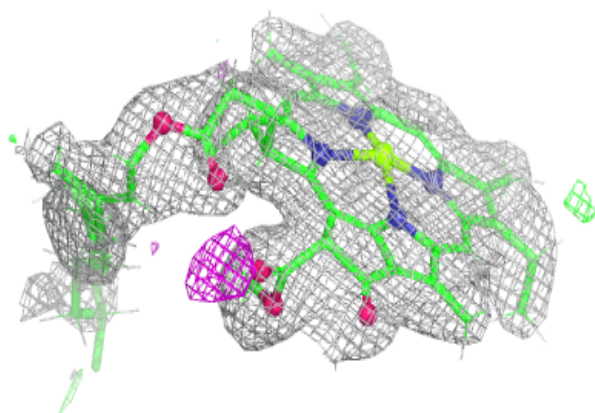
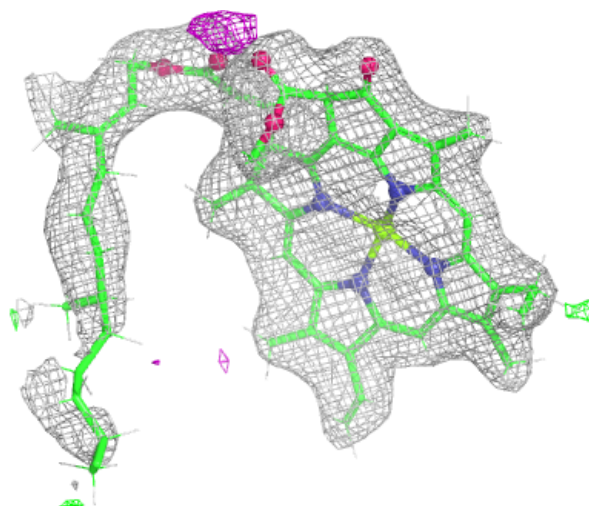
Electron density around CLA b 609:

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



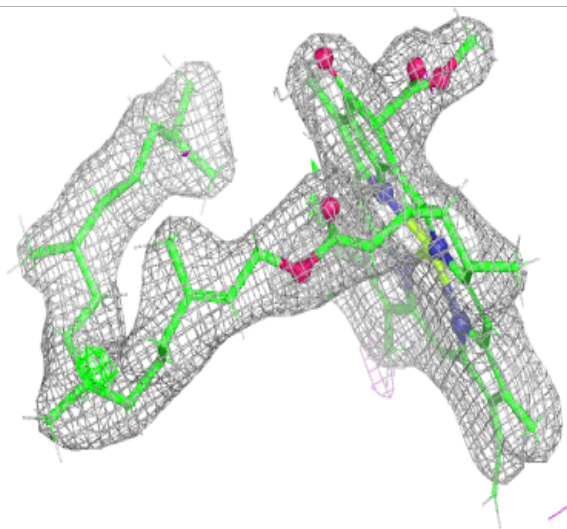
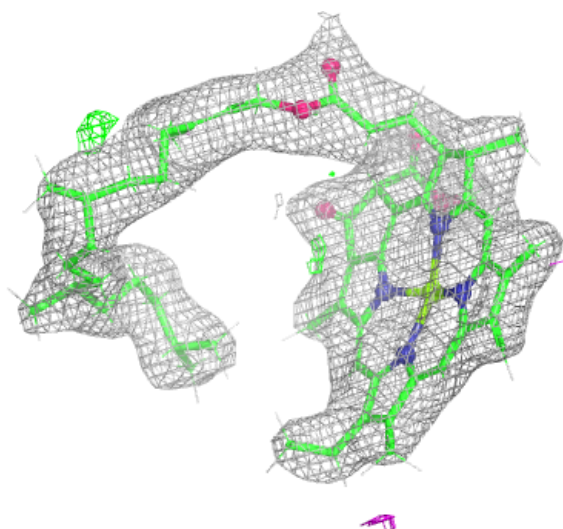
Electron density around CLA b 616:

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



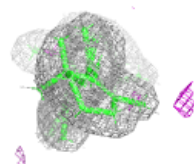
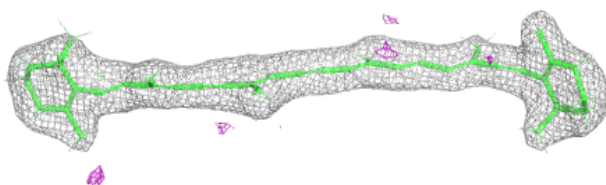
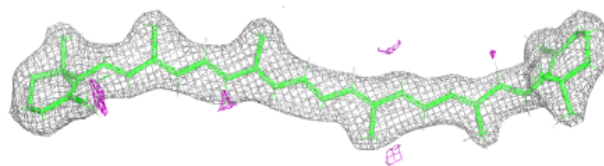
Electron density around CLA c 503:

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

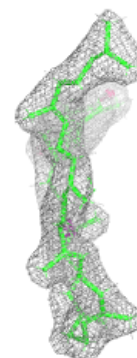
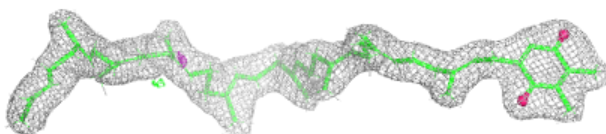
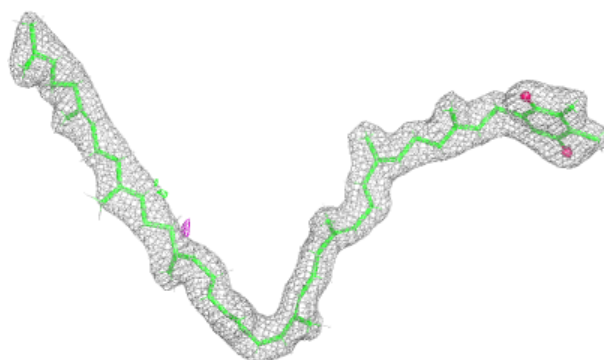


Electron density around BCR C 515:

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

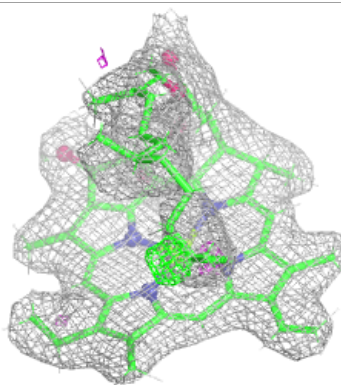
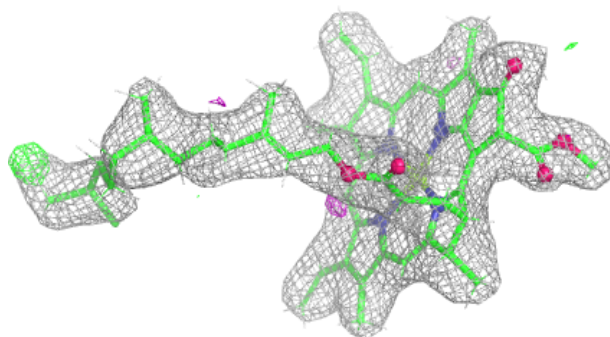
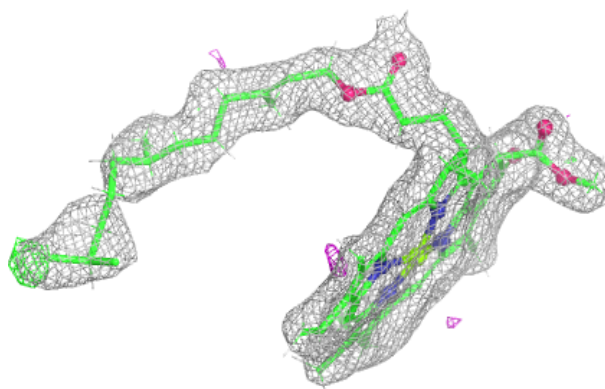
**Electron density around PL9 D 407:**

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

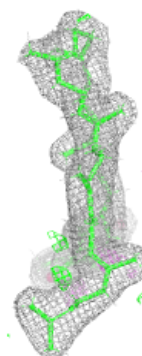
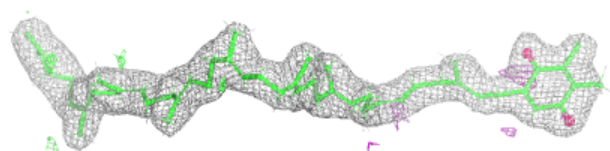
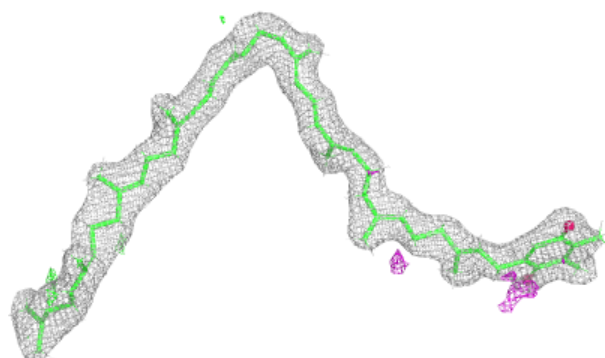


Electron density around CLA c 504:

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

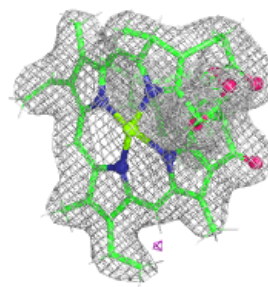
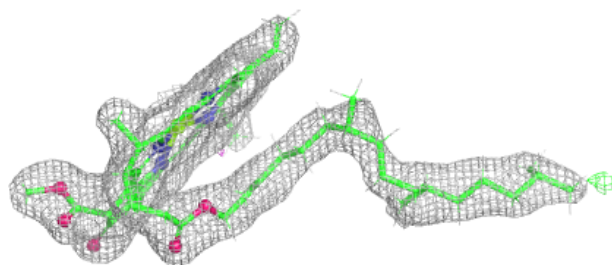
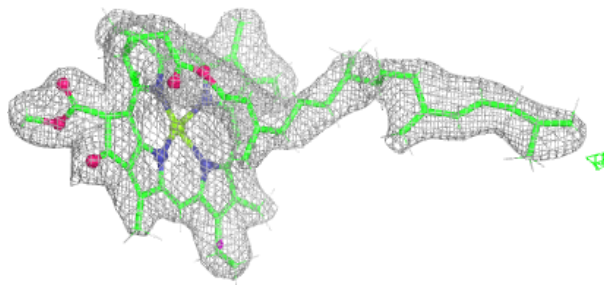
**Electron density around PL9 d 408:**

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

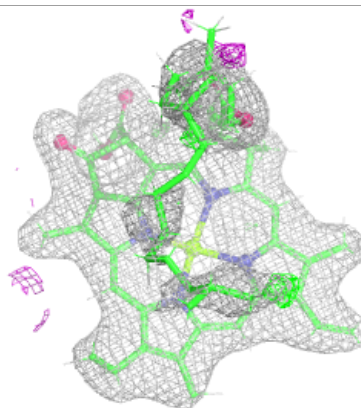
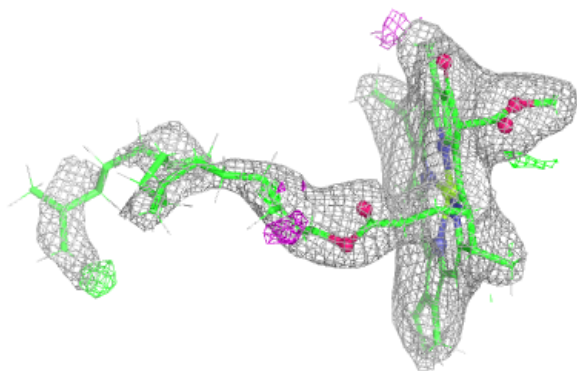
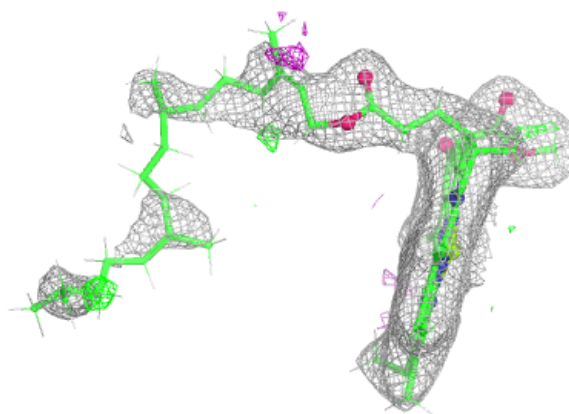


Electron density around CLA c 505:

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

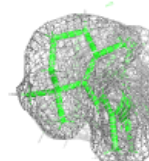
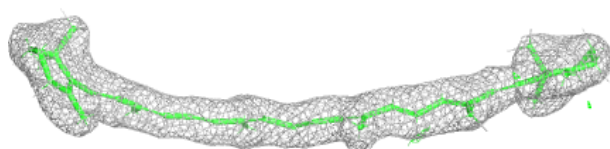
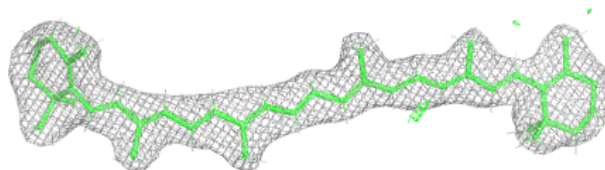
**Electron density around CLA c 506:**

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

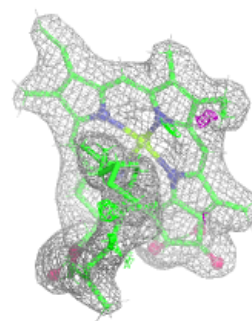
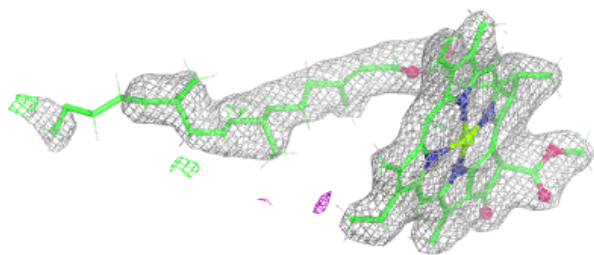
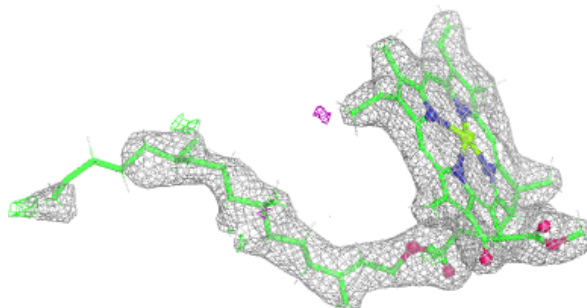


Electron density around BCR T 101:

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

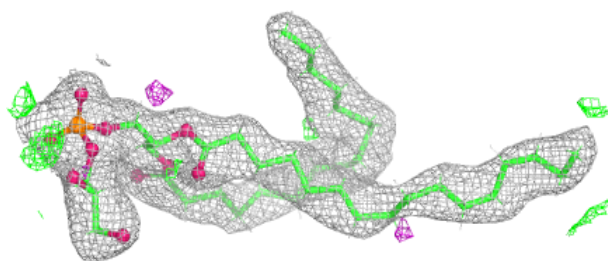
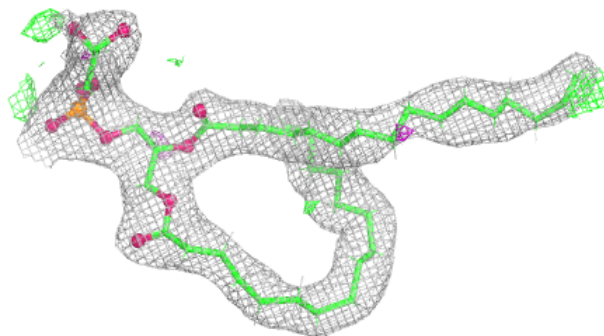
**Electron density around CLA c 508:**

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



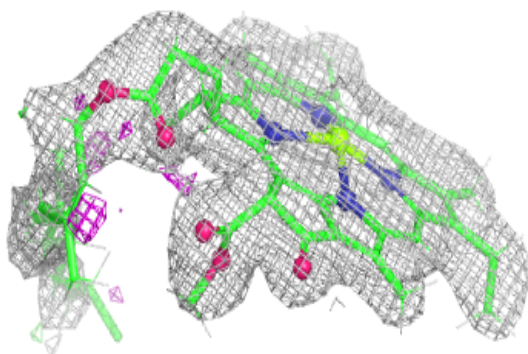
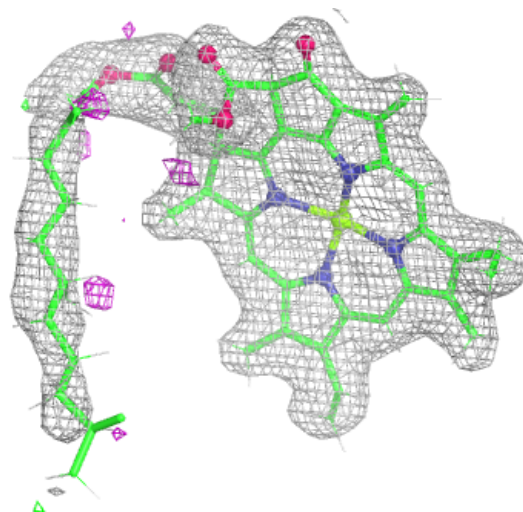
Electron density around LHG B 623:

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



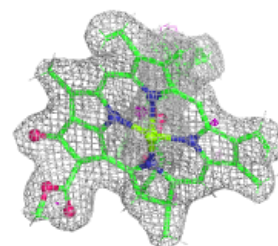
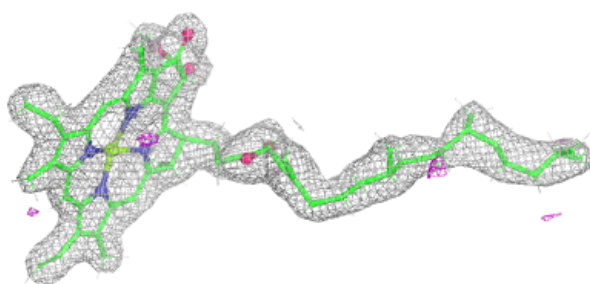
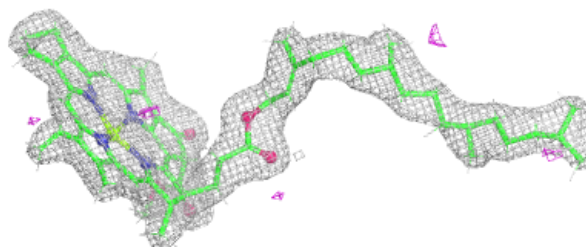
Electron density around CLA B 616:

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



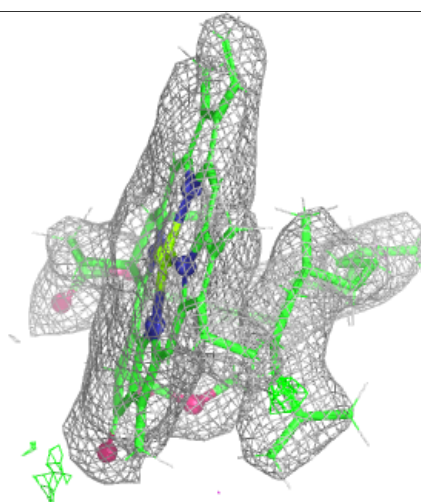
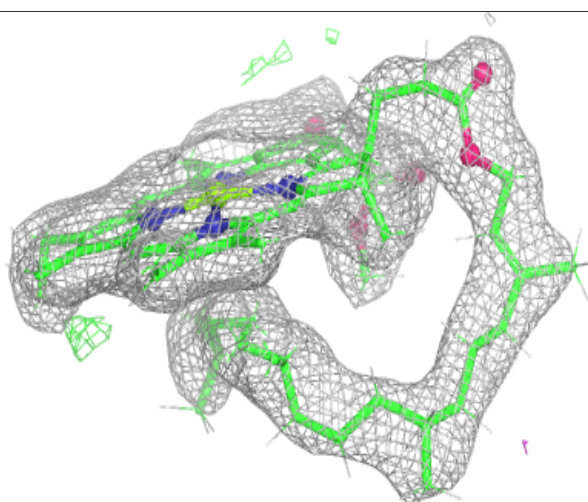
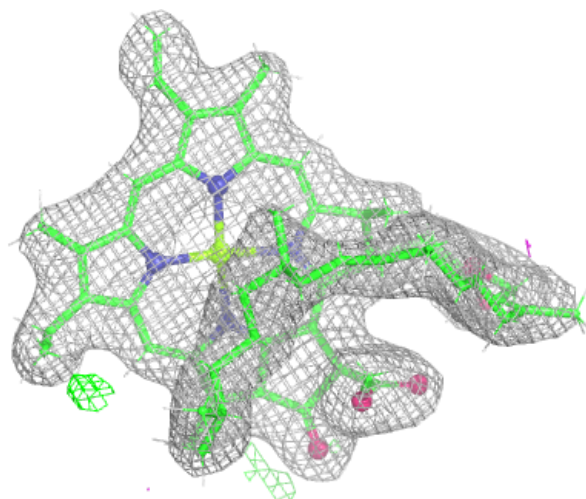
Electron density around CLA C 502:

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



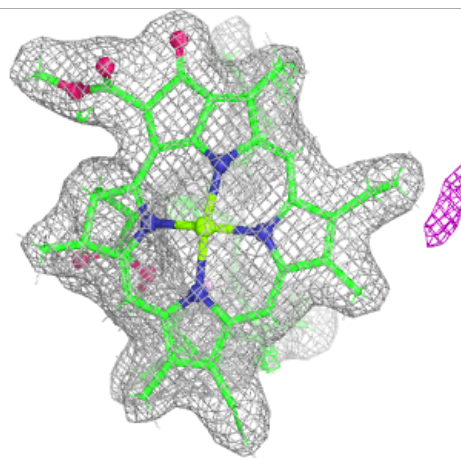
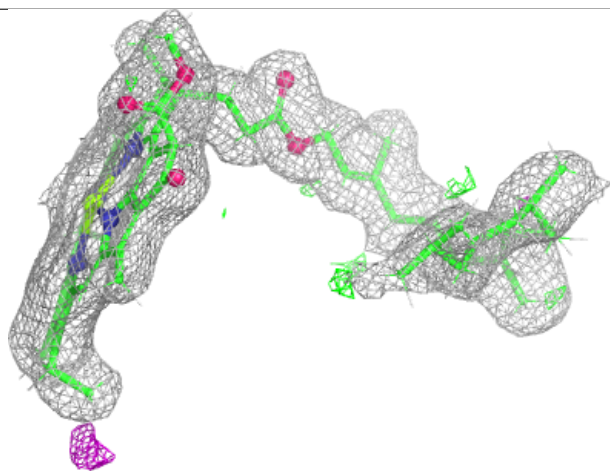
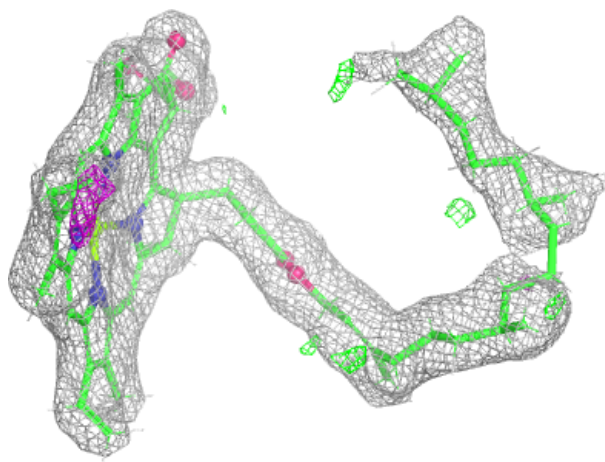
Electron density around CLA c 510:

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



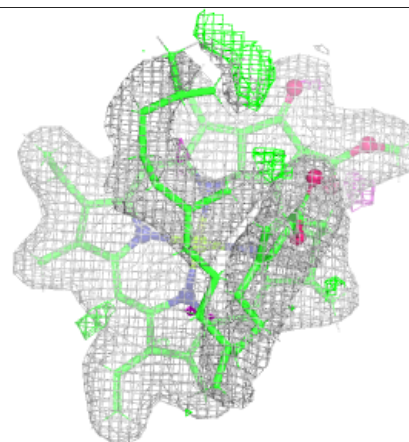
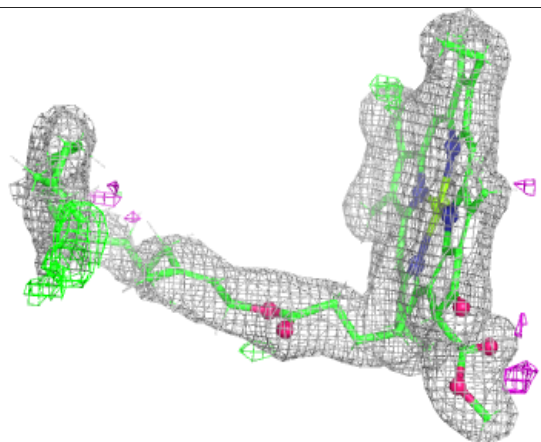
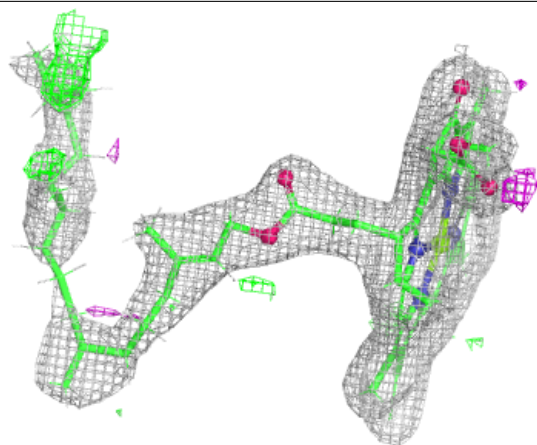
Electron density around CLA B 606:

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

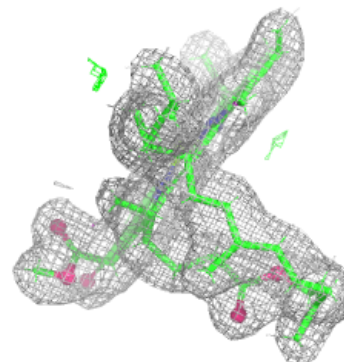
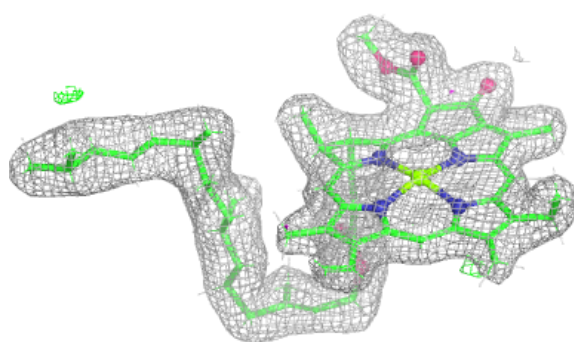
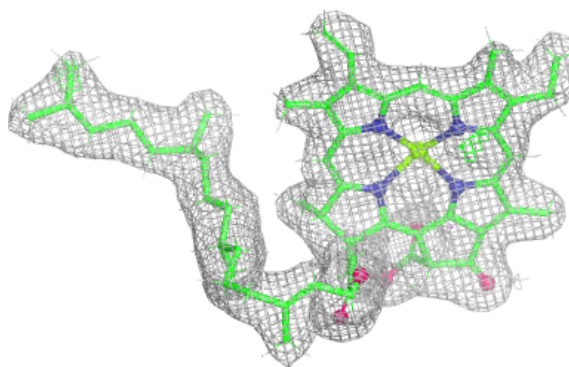


Electron density around CLA a 606:

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

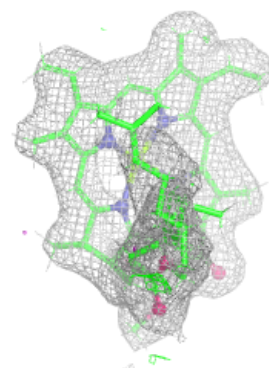
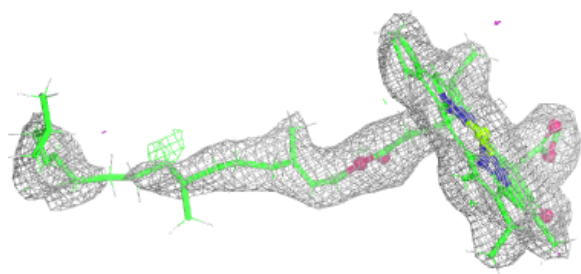
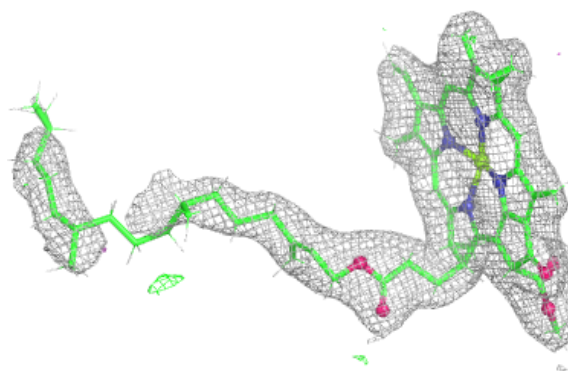
**Electron density around CLA a 612:**

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

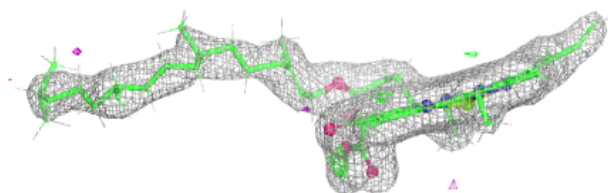
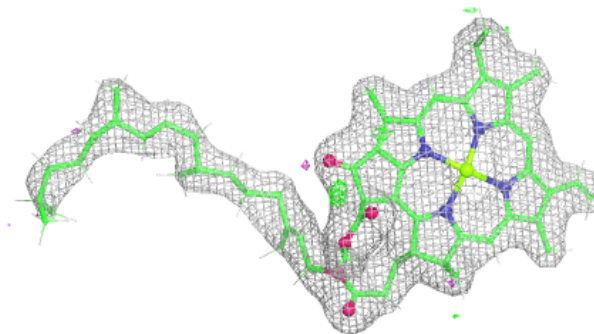


Electron density around CLA d 403:

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

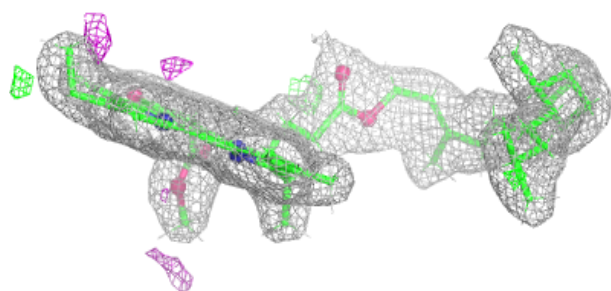
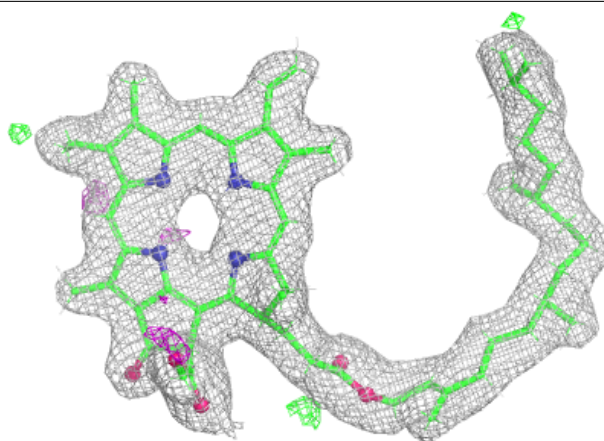
**Electron density around CLA b 602:**

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



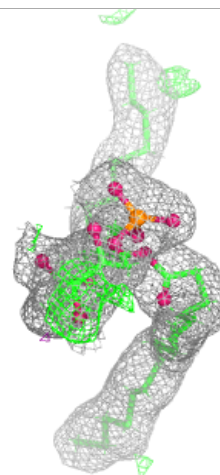
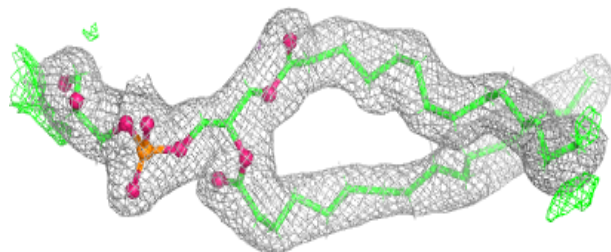
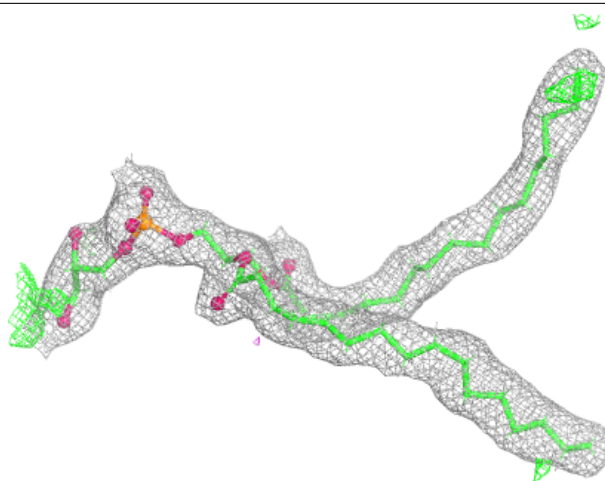
Electron density around PHO a 605:

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



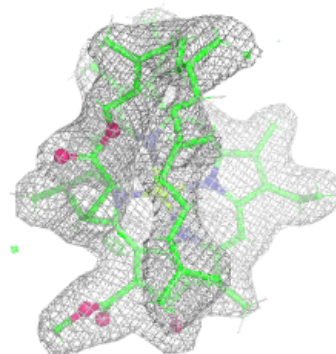
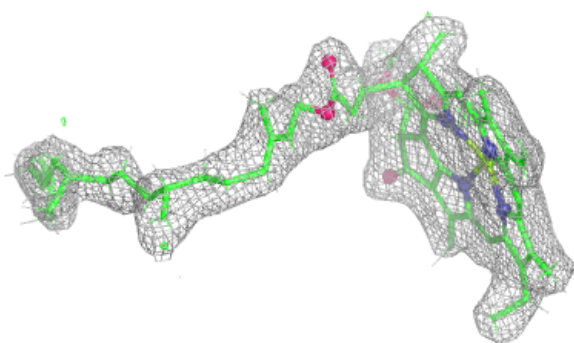
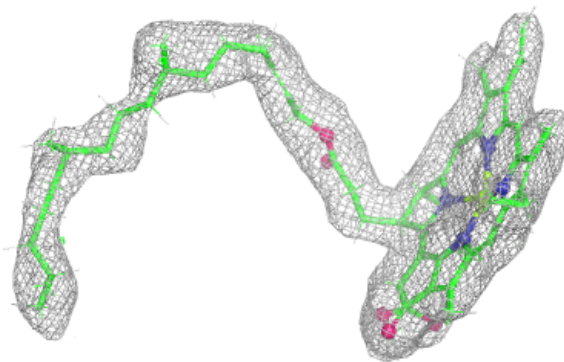
Electron density around LHG D 406:

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

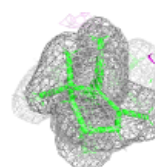
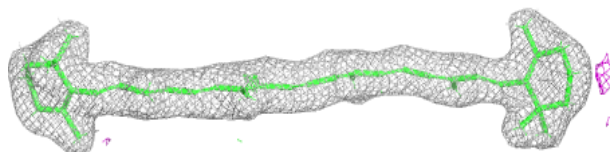
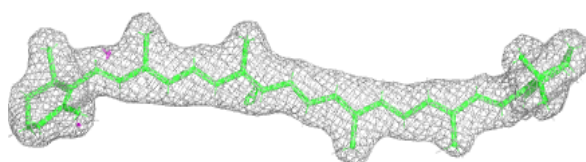


Electron density around CLA b 606:

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

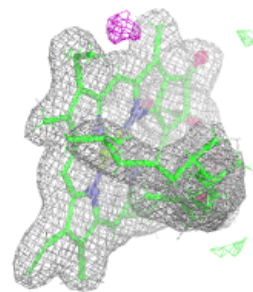
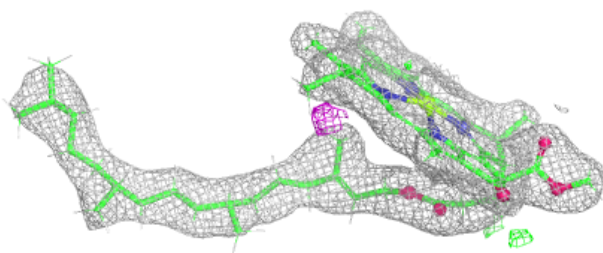
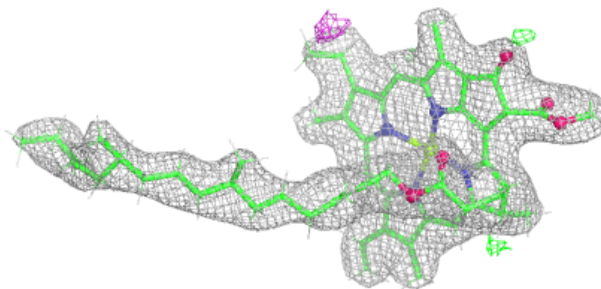
**Electron density around BCR A 608:**

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

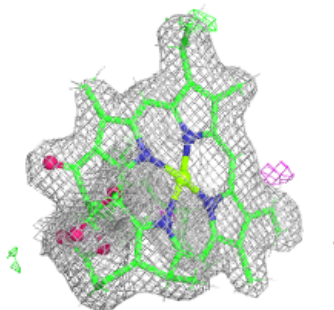
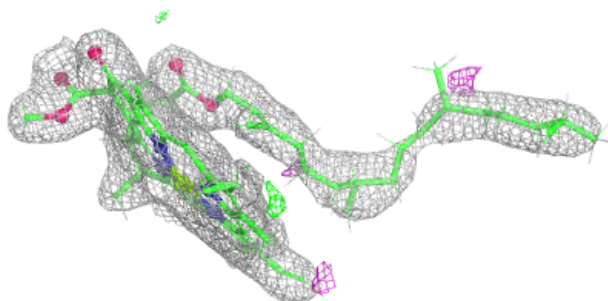
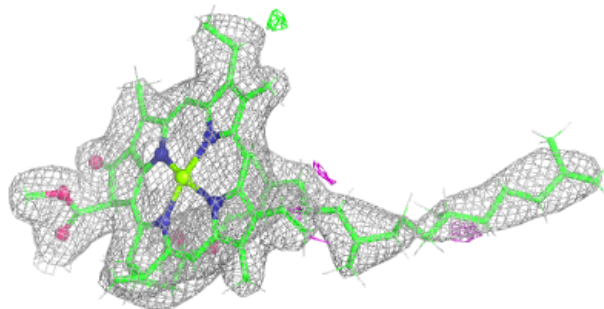


Electron density around CLA b 608:

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

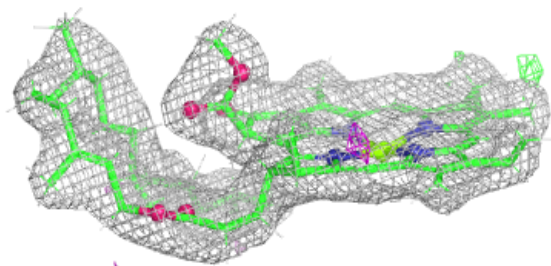
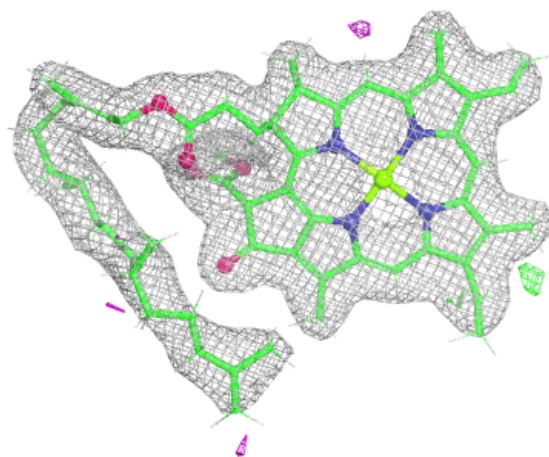
**Electron density around CLA C 505:**

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



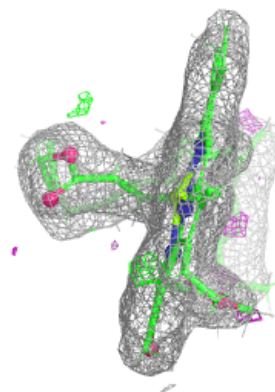
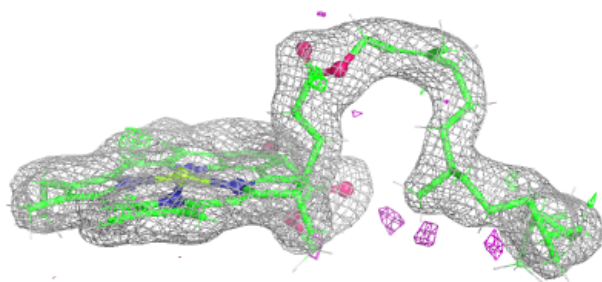
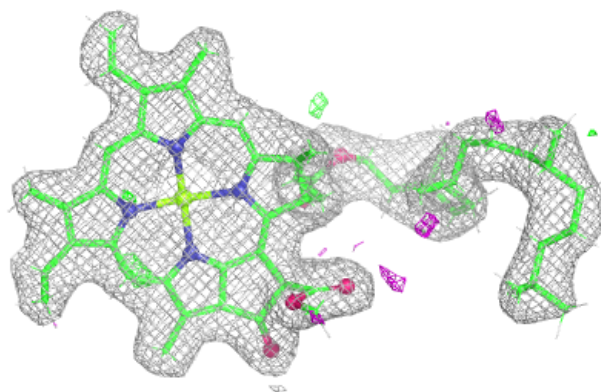
Electron density around CLA b 610:

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

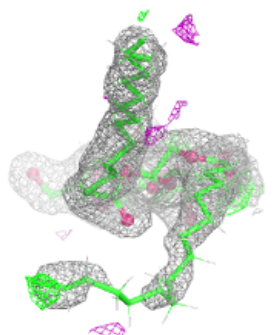
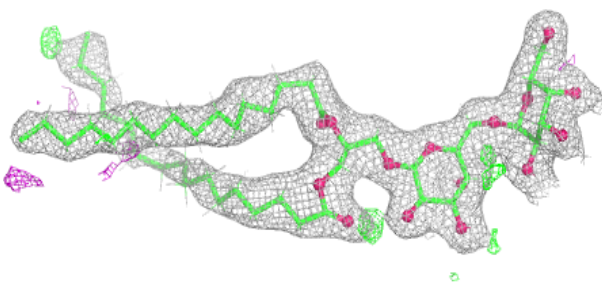
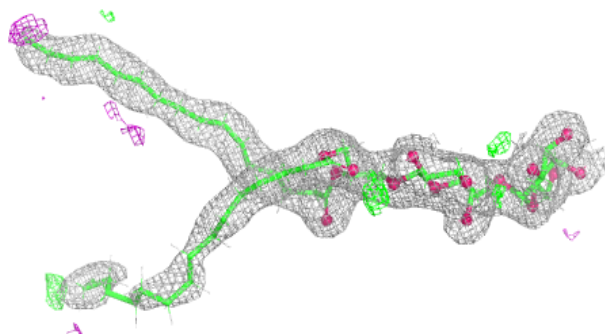


Electron density around CLA b 612:

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

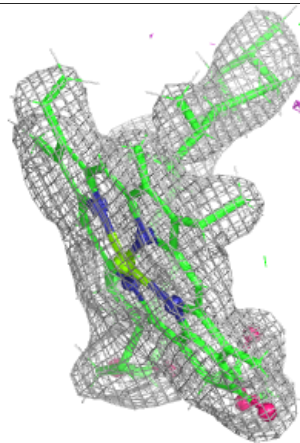
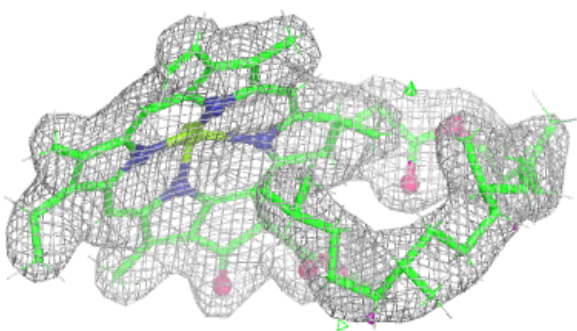
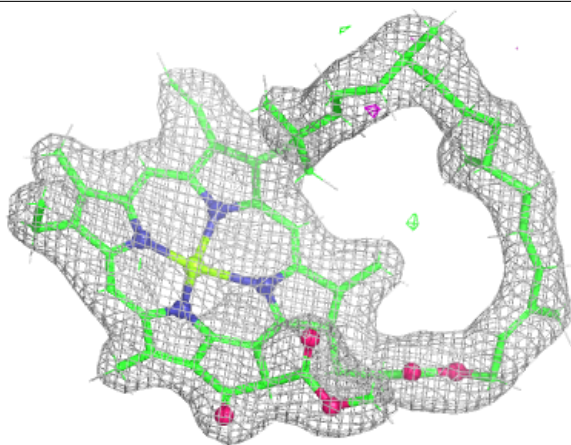
**Electron density around DGD C 516:**

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

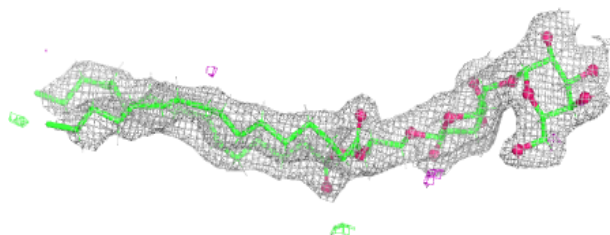
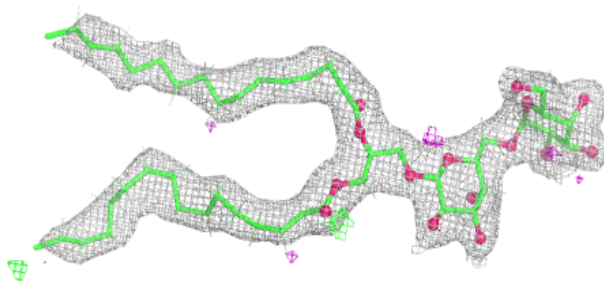


Electron density around CLA b 615:

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

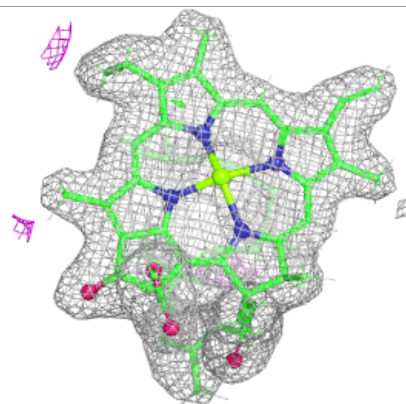
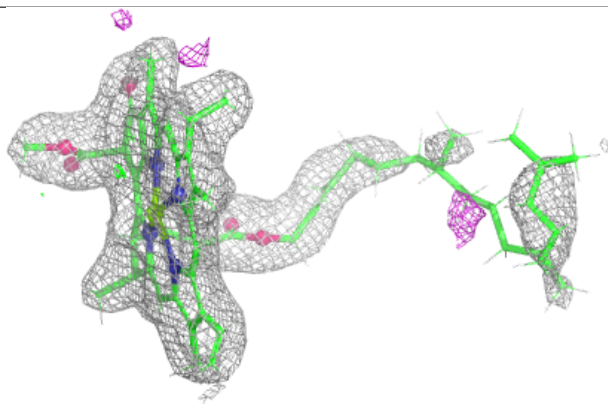
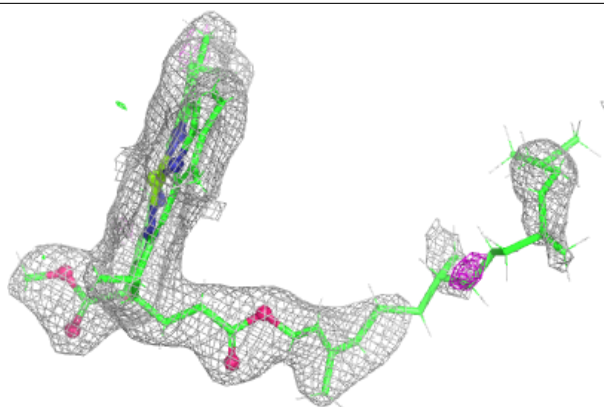
**Electron density around DGD C 518:**

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

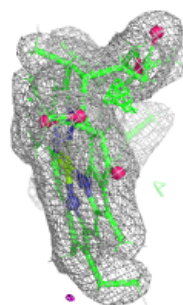
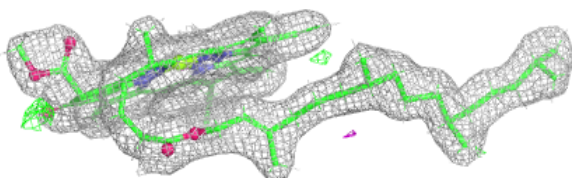
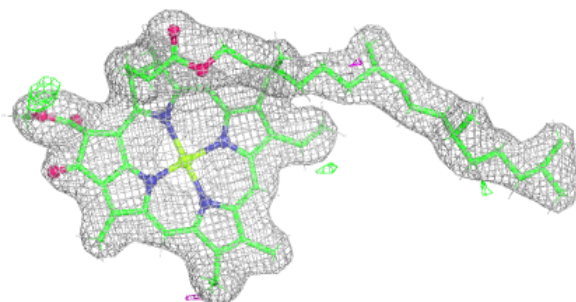


Electron density around CLA C 506:

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

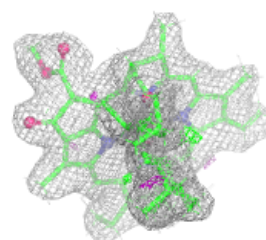
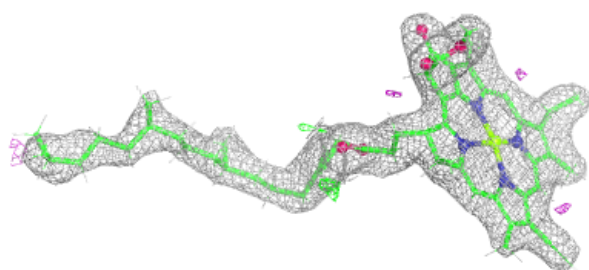
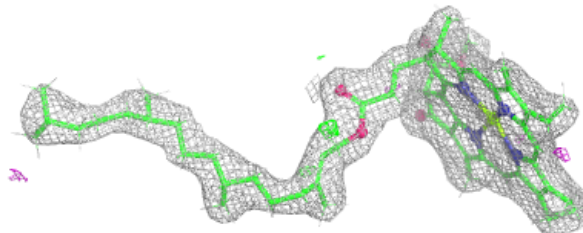
**Electron density around CLA c 501:**

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

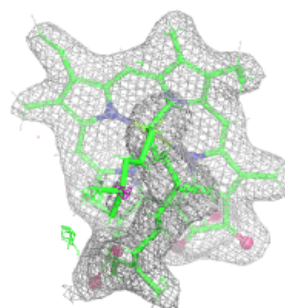
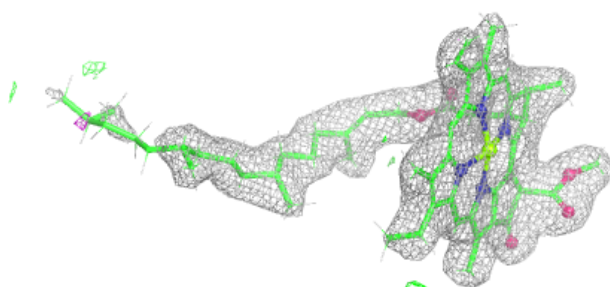
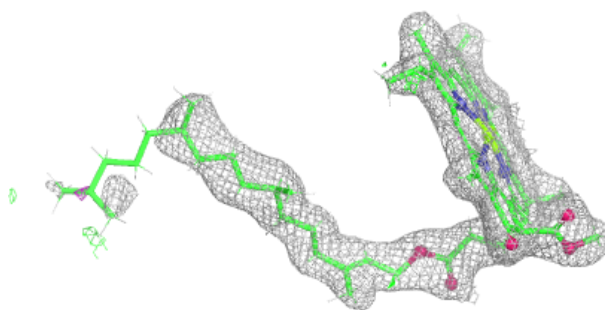


Electron density around CLA c 502:

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

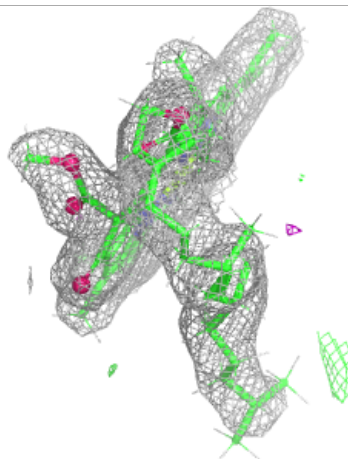
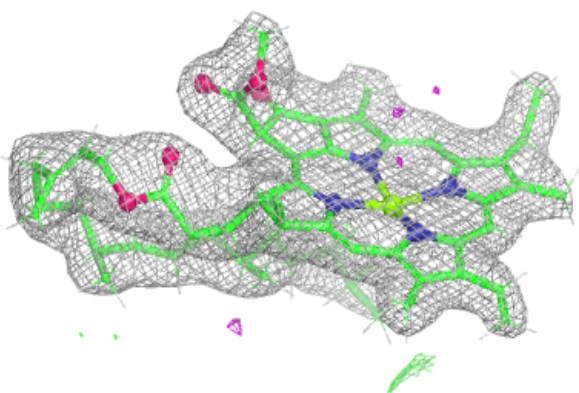
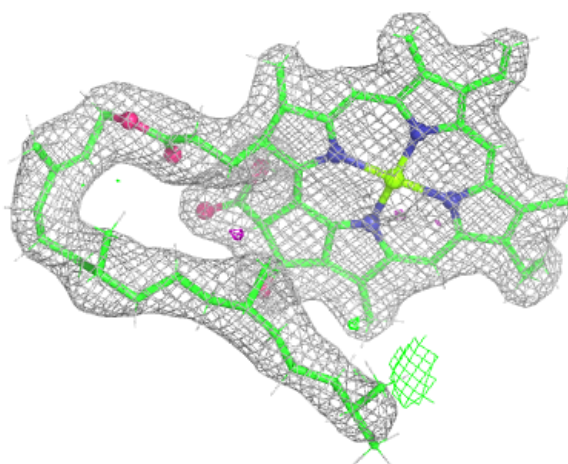
**Electron density around CLA C 508:**

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



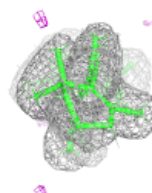
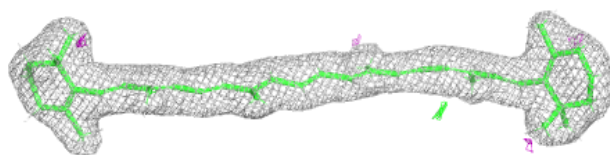
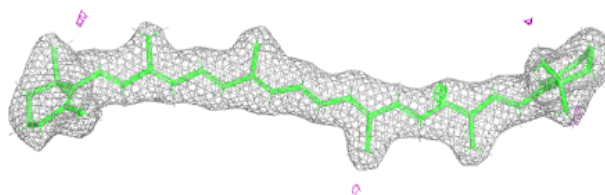
Electron density around CLA C 509:

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

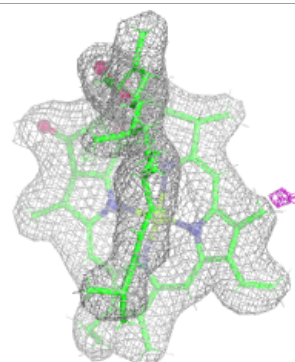
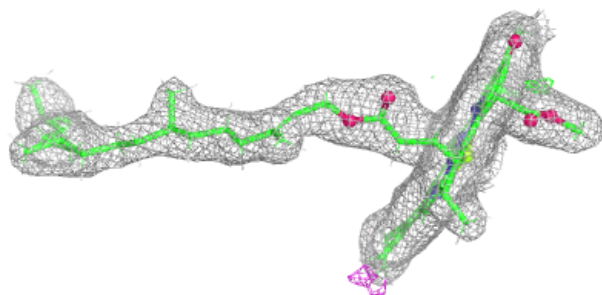
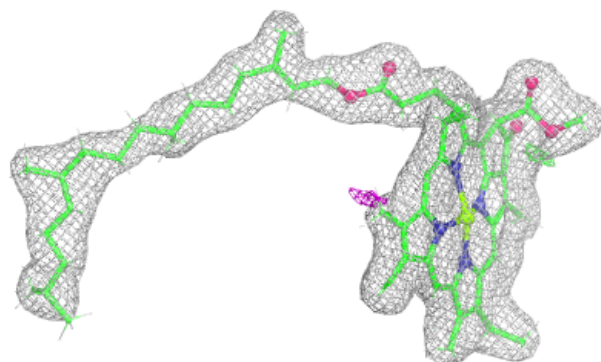


Electron density around BCR a 607:

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

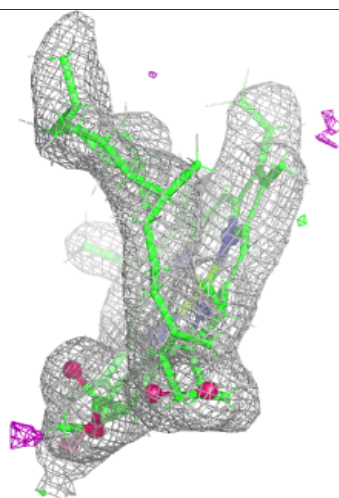
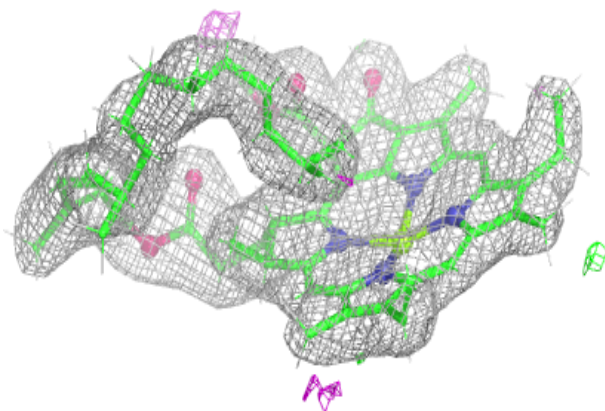
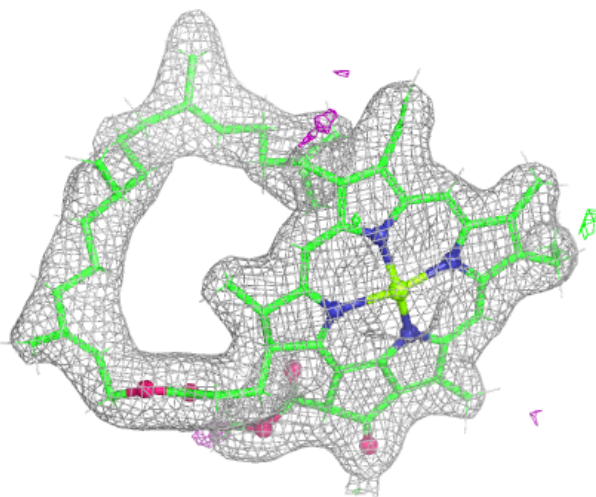
**Electron density around CLA B 609:**

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



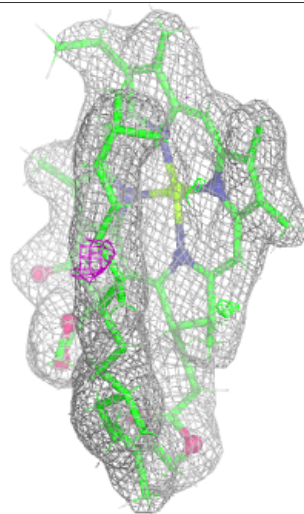
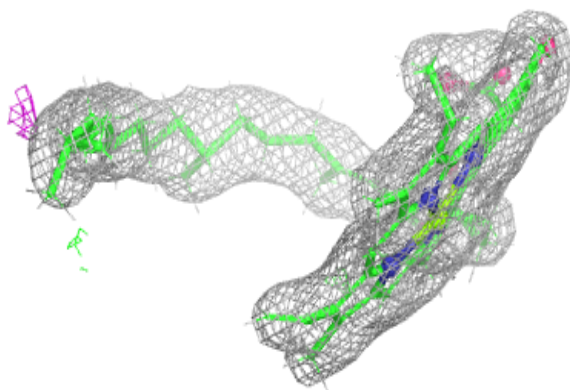
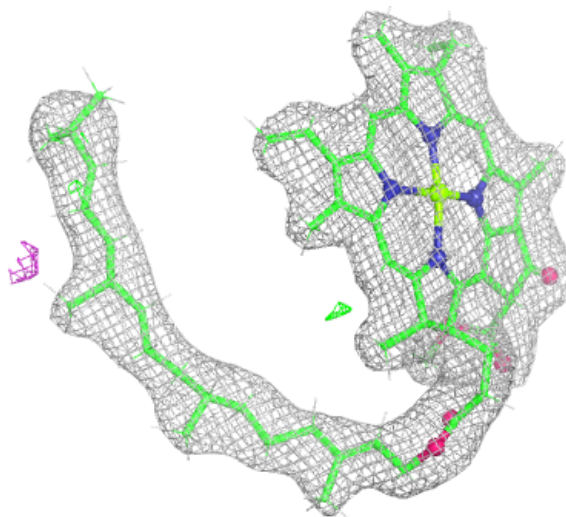
Electron density around CLA B 615:

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



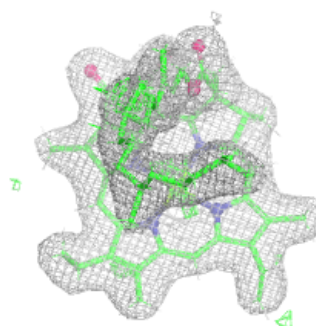
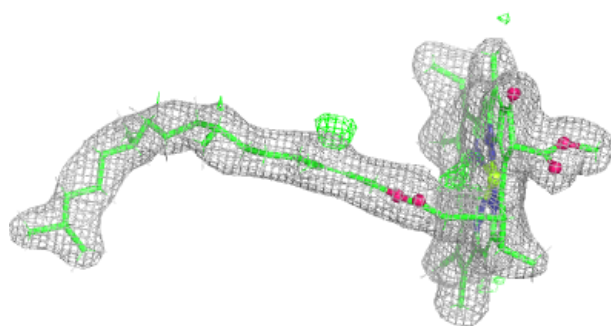
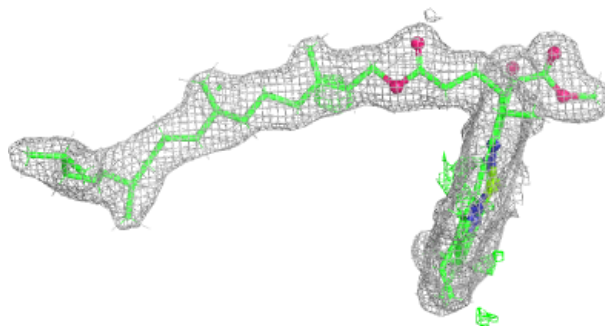
Electron density around CLA c 507:

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



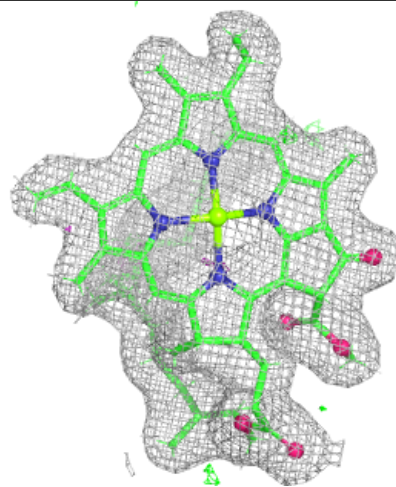
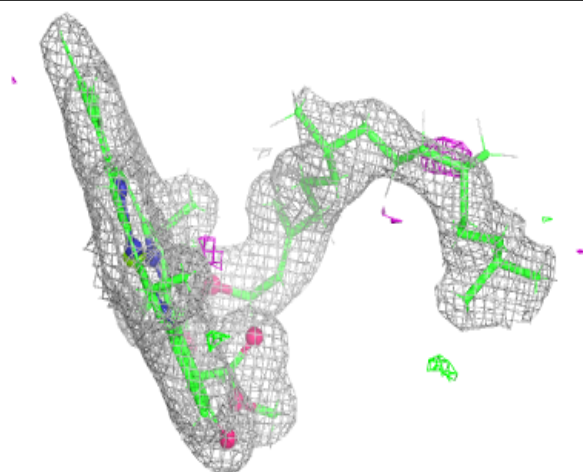
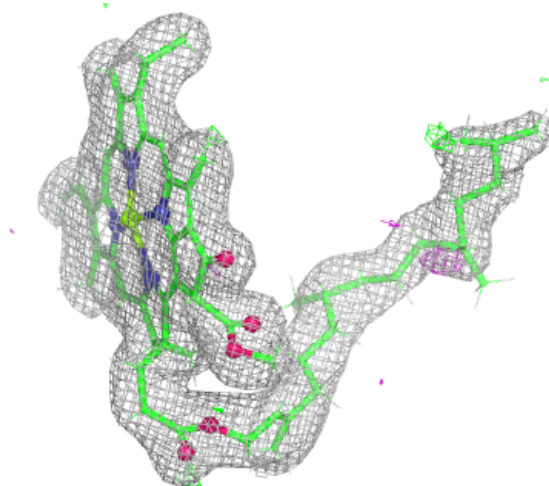
Electron density around CLA B 605:

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



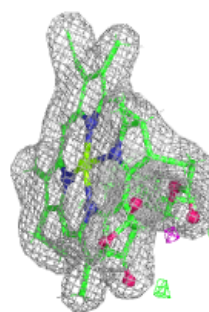
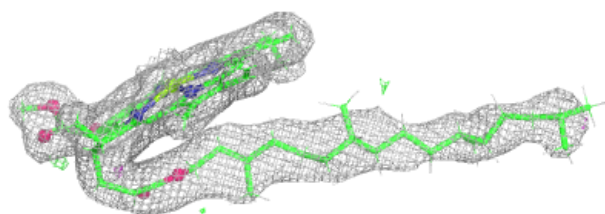
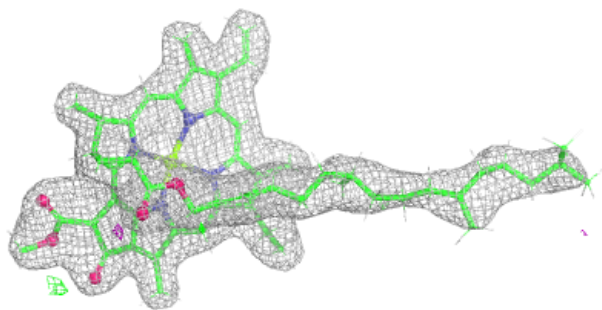
Electron density around CLA b 613:

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

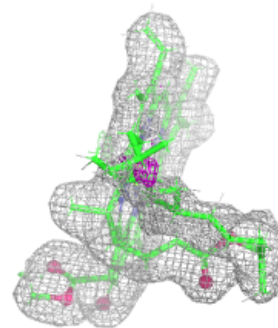
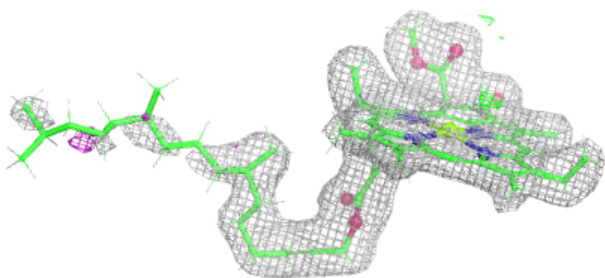
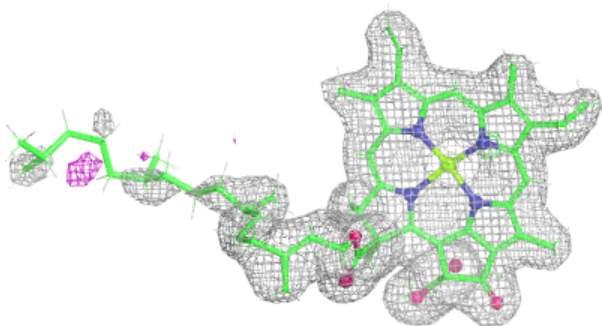


Electron density around CLA b 614:

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

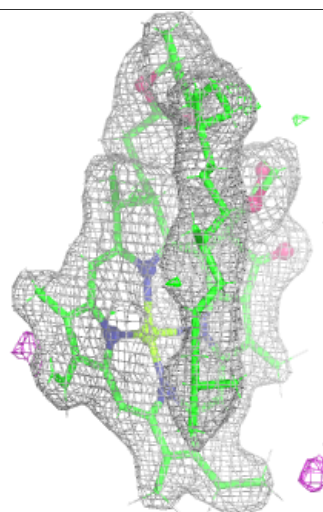
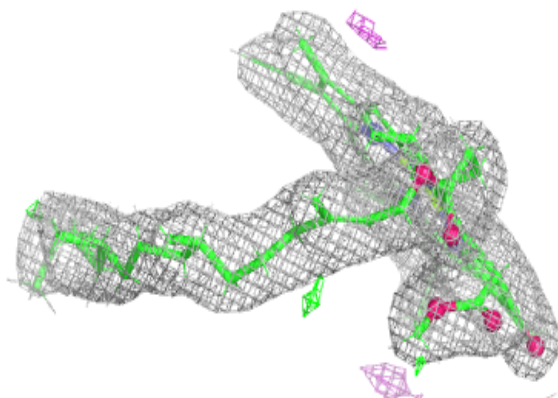
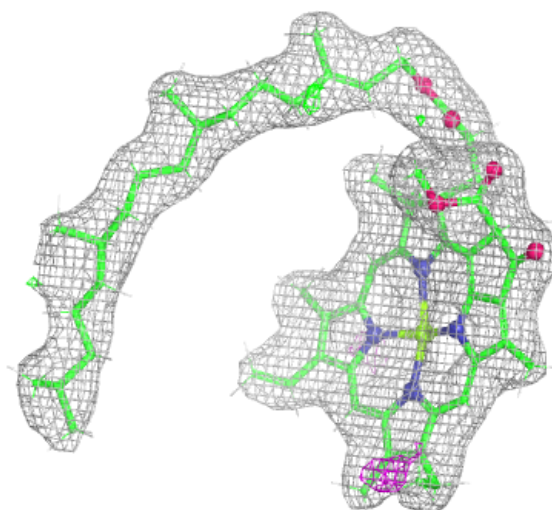
**Electron density around CLA A 604:**

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



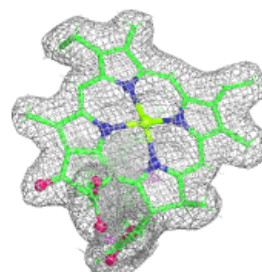
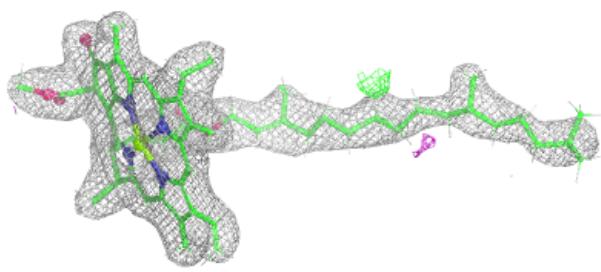
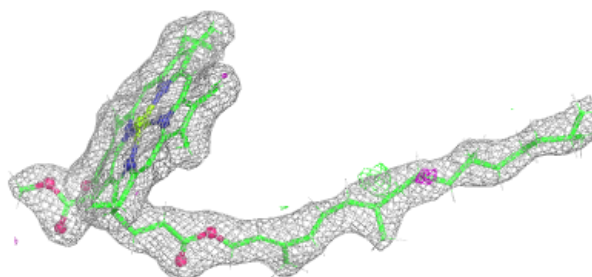
Electron density around CLA C 507:

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

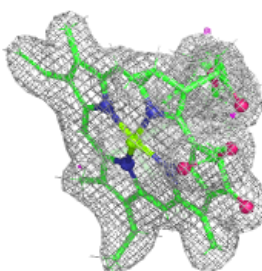
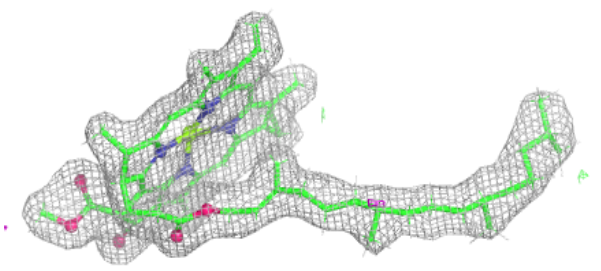
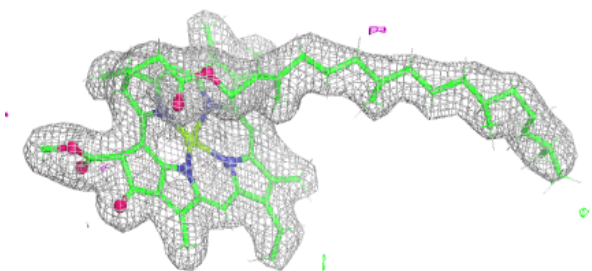


Electron density around CLA B 607:

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

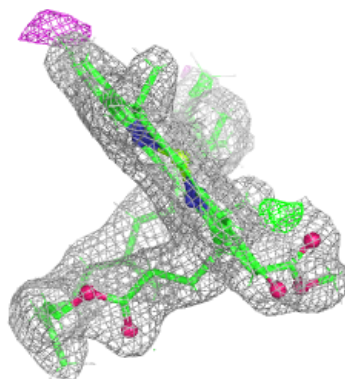
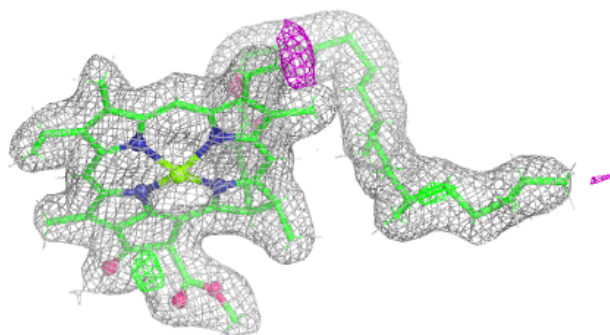
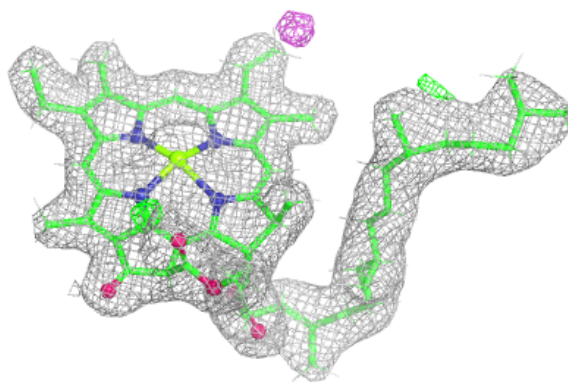
**Electron density around CLA B 608:**

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

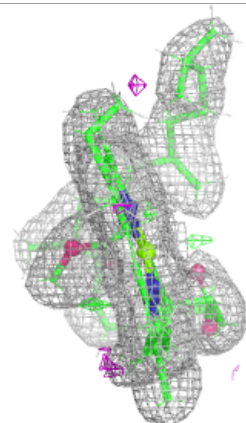
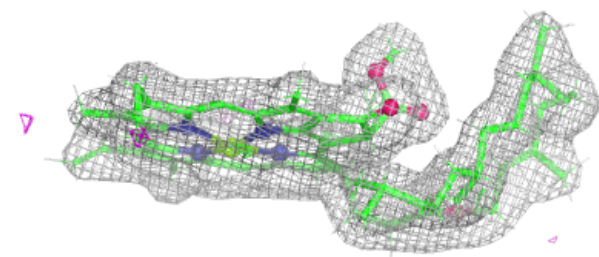
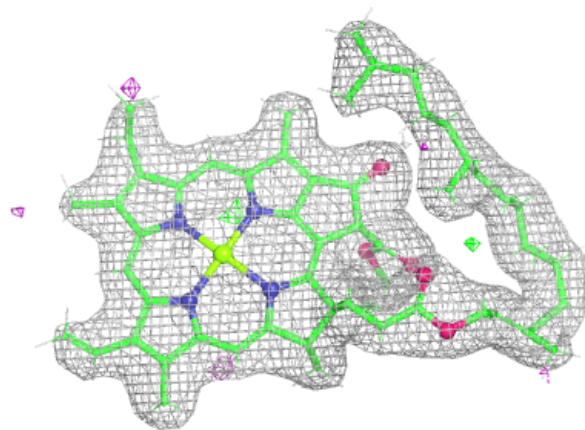


Electron density around CLA A 613:

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

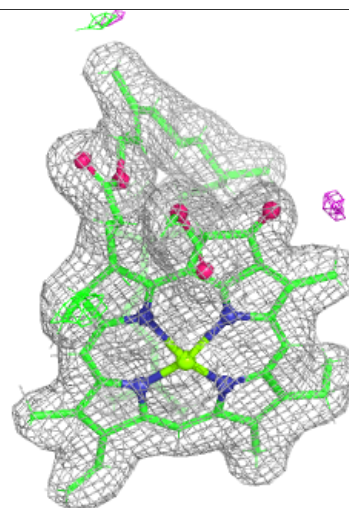
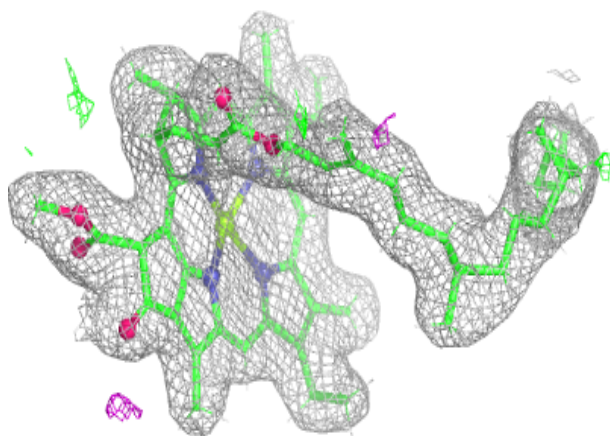
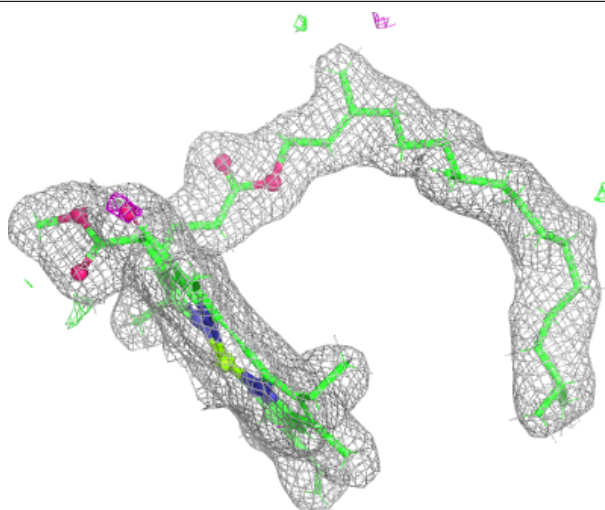
**Electron density around CLA B 610:**

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



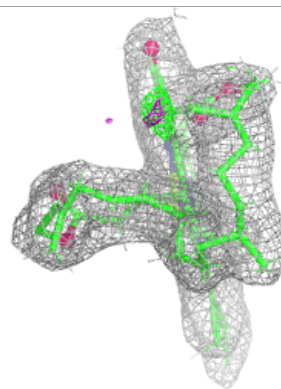
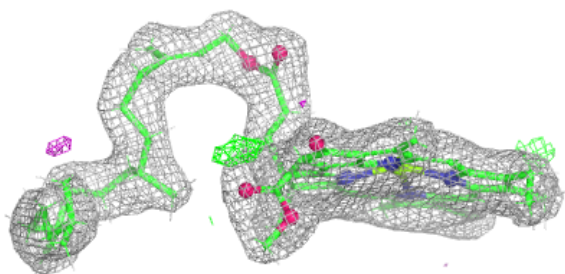
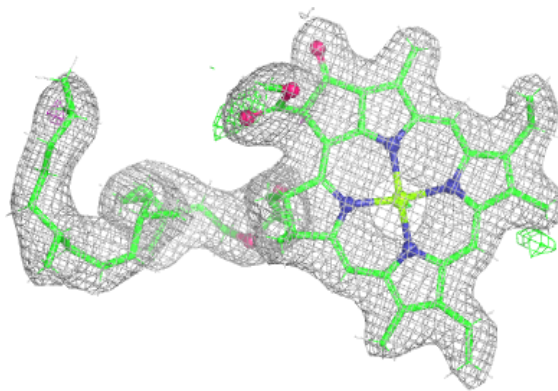
Electron density around CLA B 611:

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

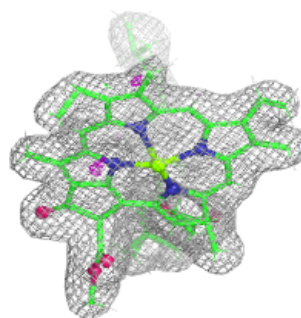
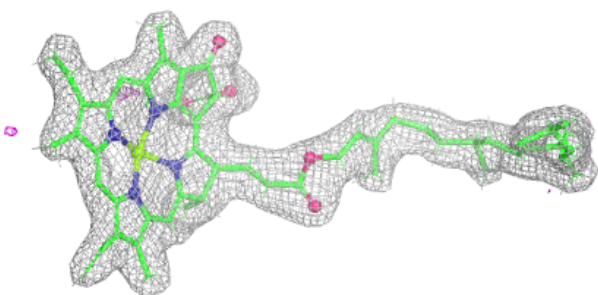
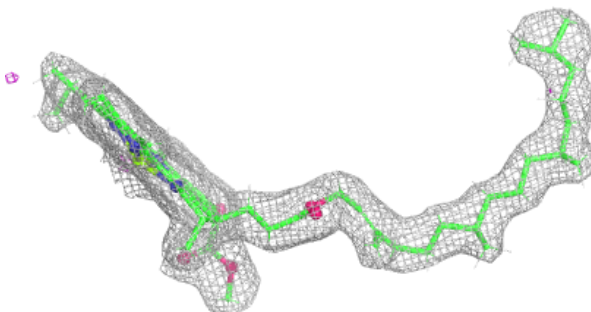


Electron density around CLA B 612:

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

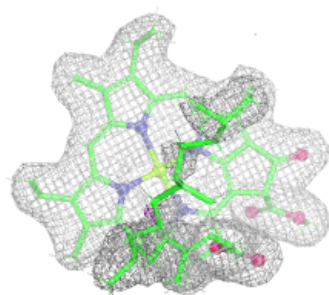
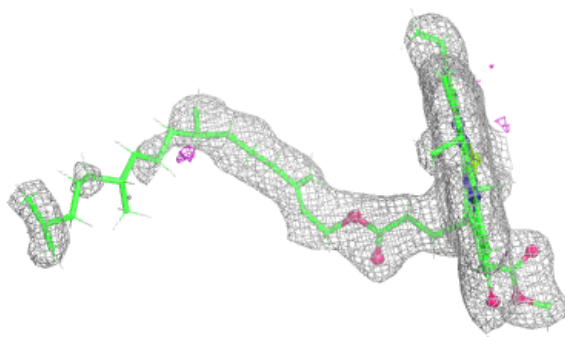
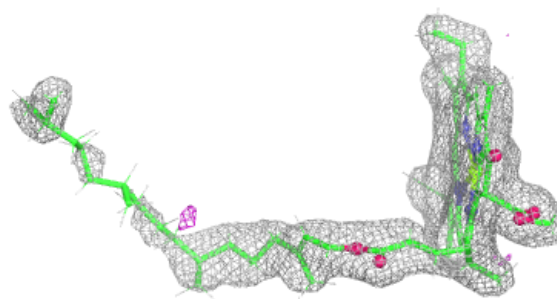
**Electron density around CLA D 402:**

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

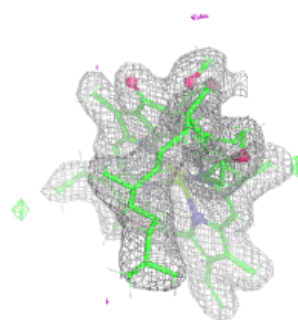
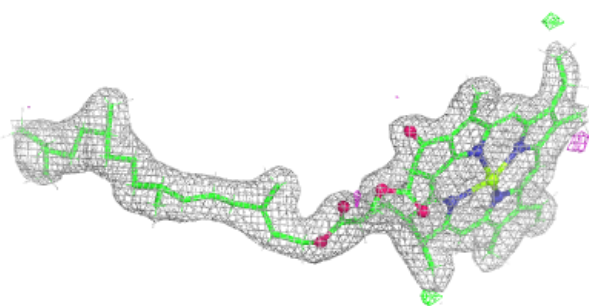
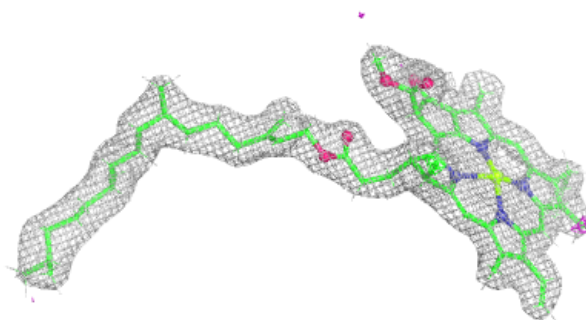


Electron density around CLA D 403:

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

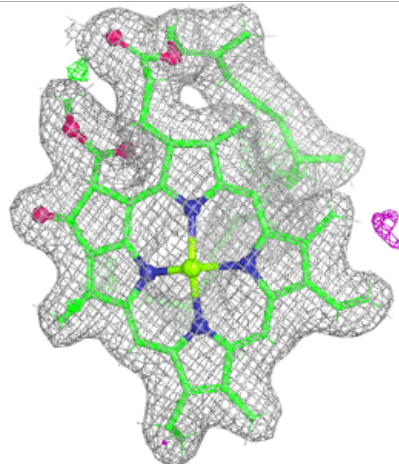
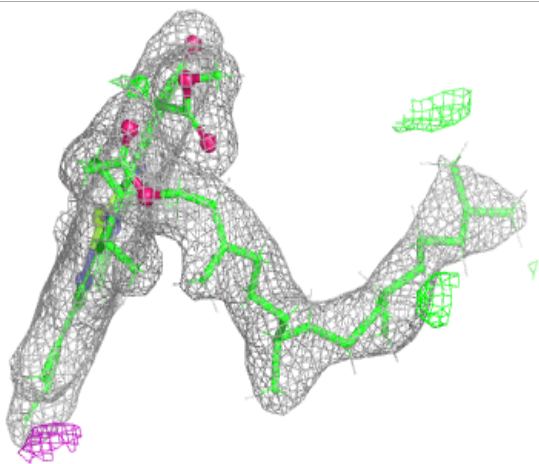
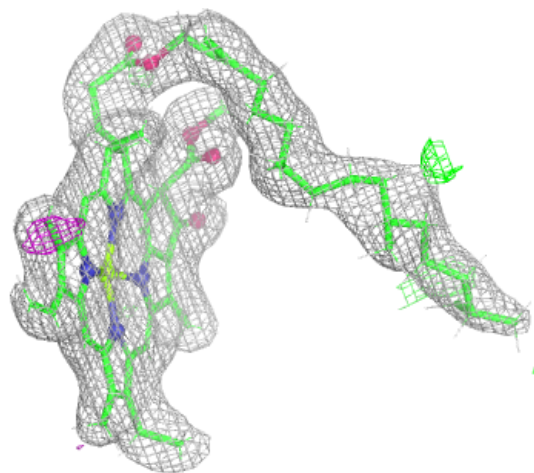
**Electron density around CLA a 603:**

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



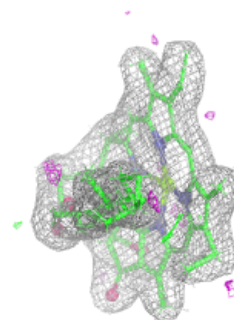
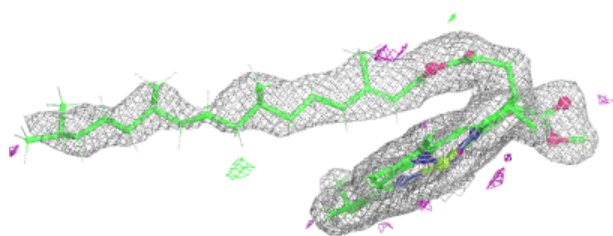
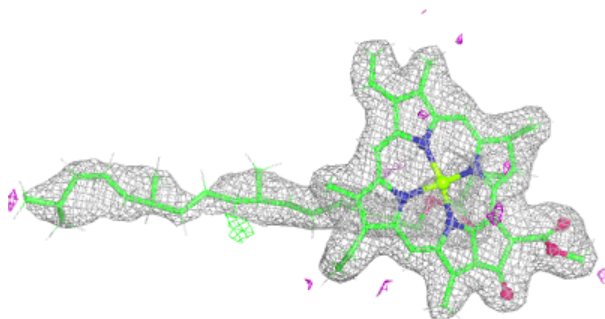
Electron density around CLA B 613:

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



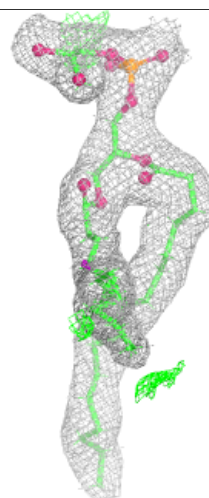
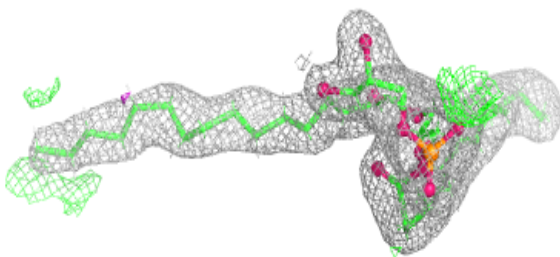
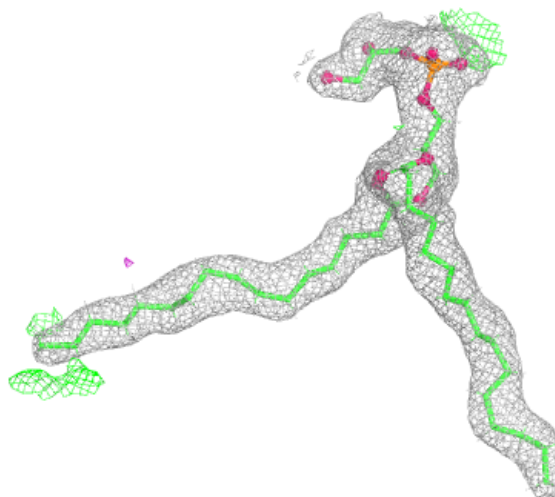
Electron density around CLA B 614:

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



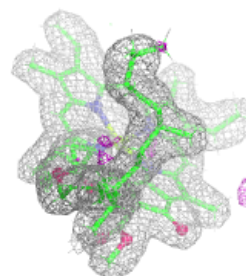
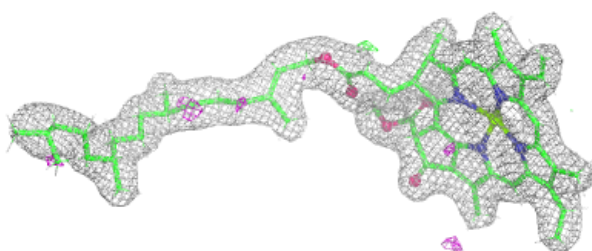
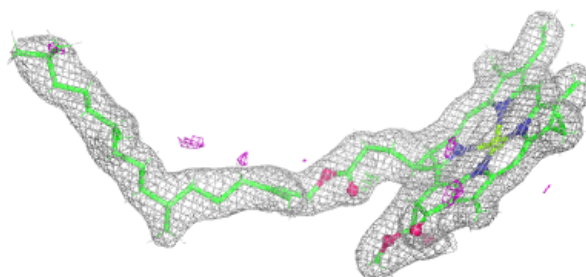
Electron density around LHG L 101:

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

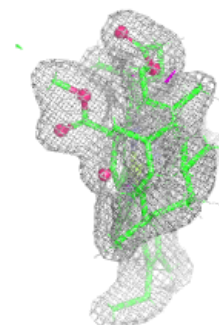
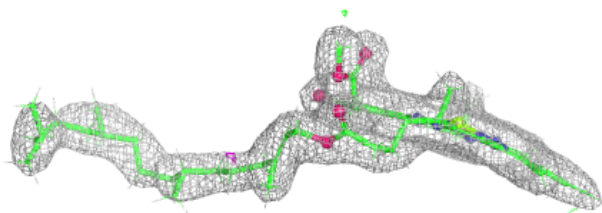
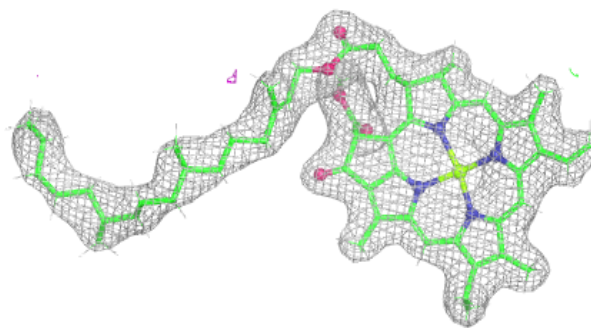


Electron density around CLA A 603:

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

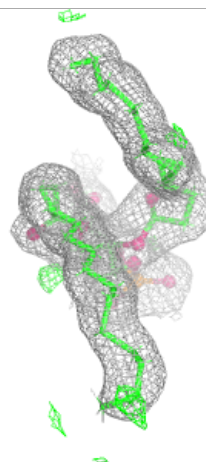
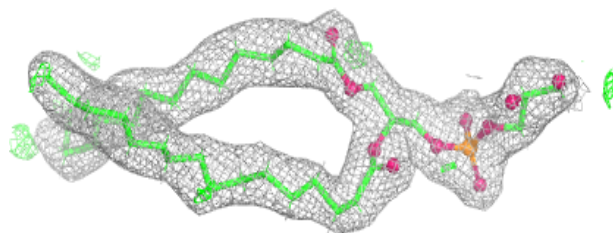
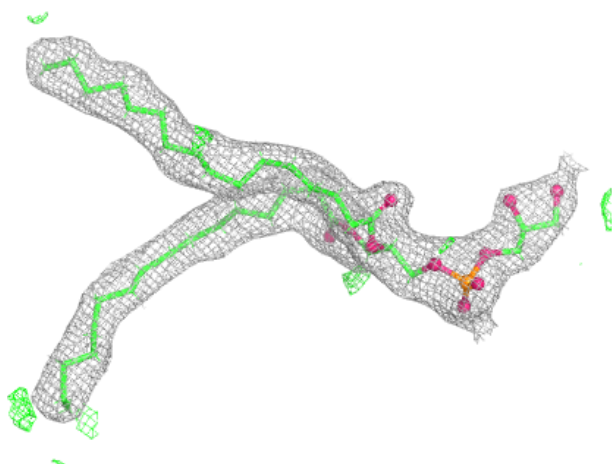
**Electron density around CLA B 602:**

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



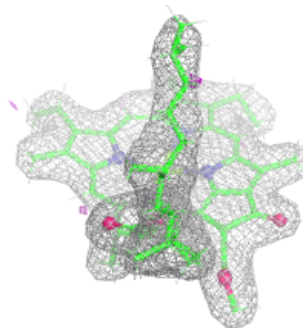
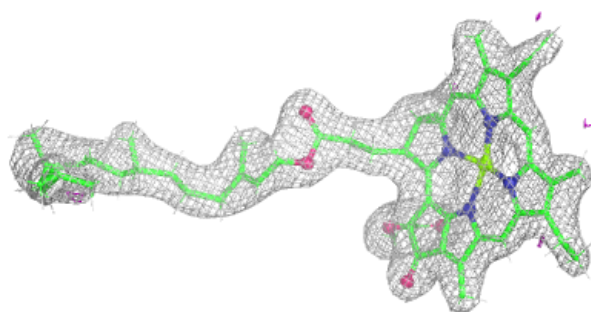
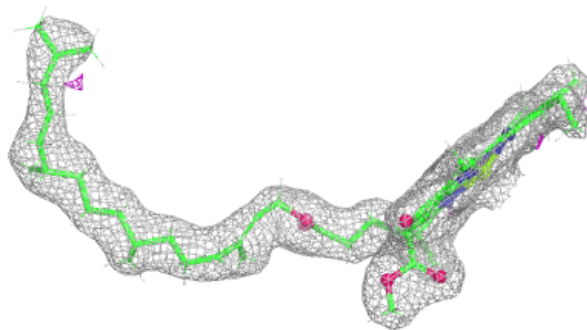
Electron density around LHG d 407:

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

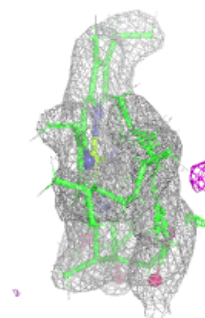
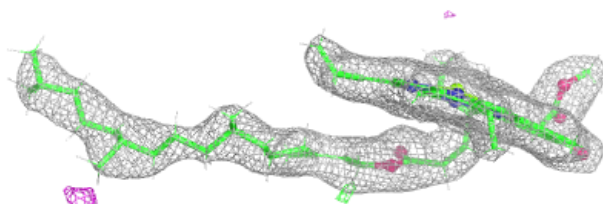
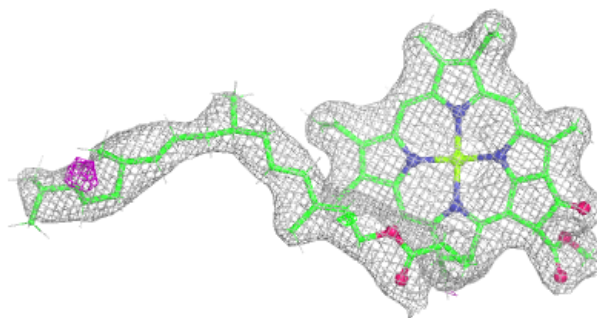


Electron density around CLA d 402:

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

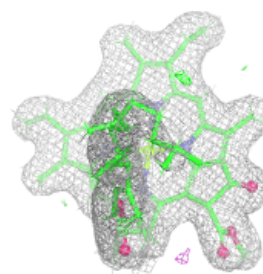
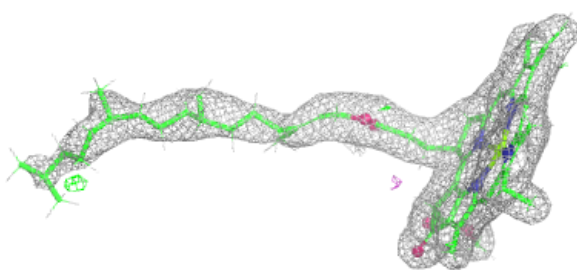
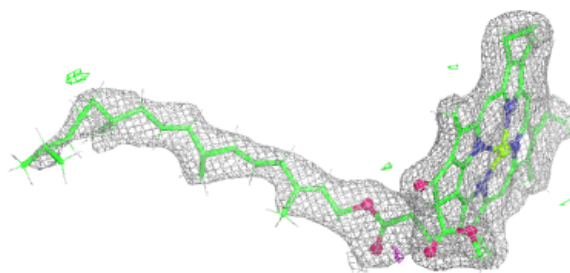
**Electron density around CLA b 603:**

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

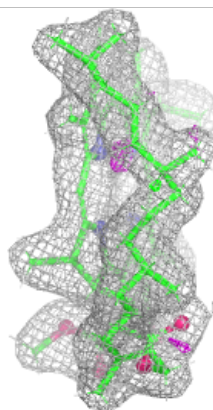
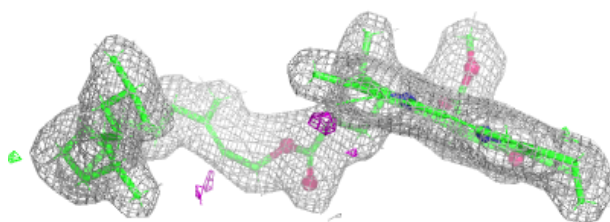
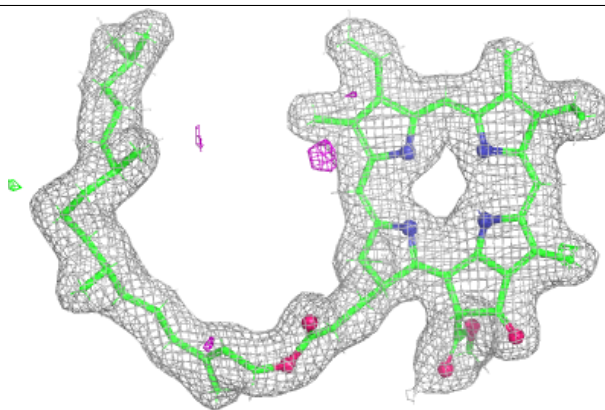


Electron density around CLA b 604:

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

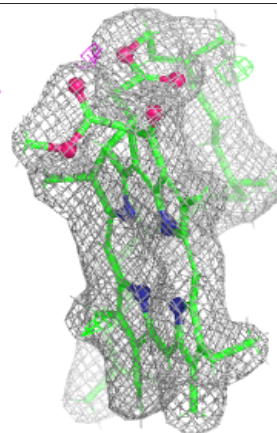
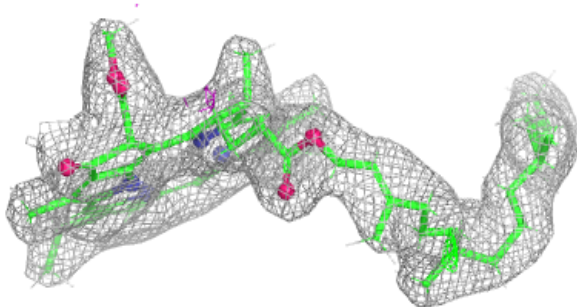
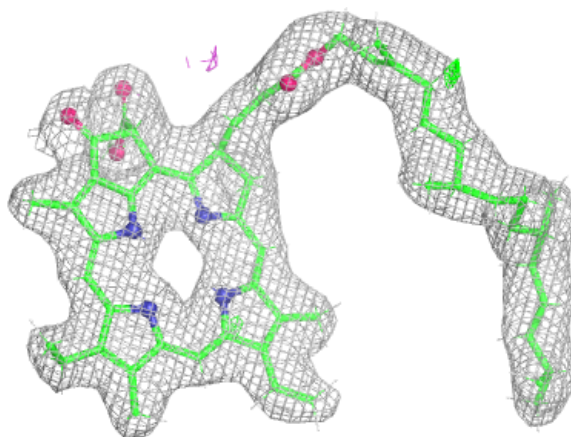
**Electron density around PHO A 605:**

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



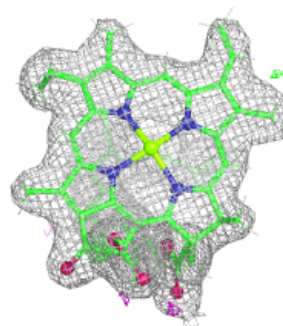
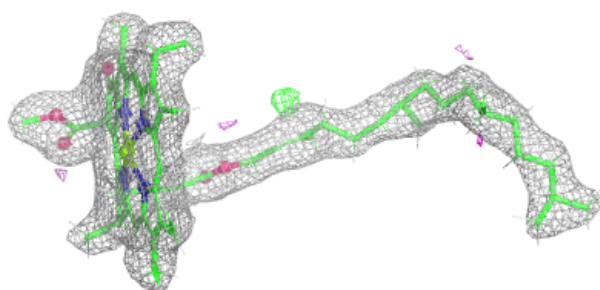
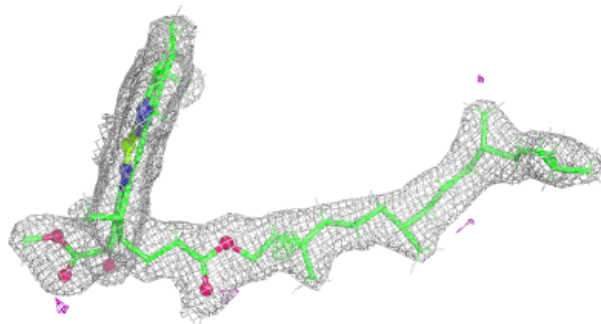
Electron density around PHO A 606:

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

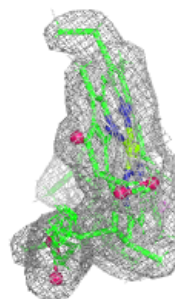
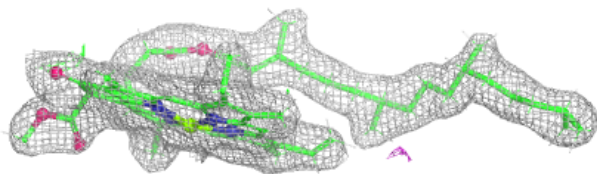
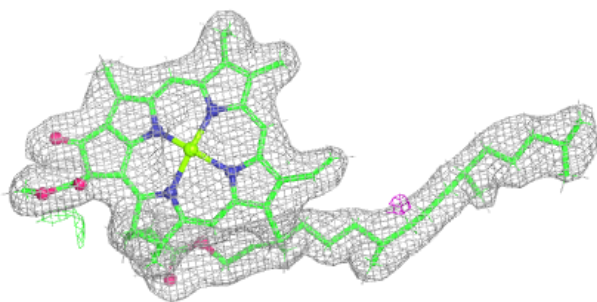


Electron density around CLA b 605:

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

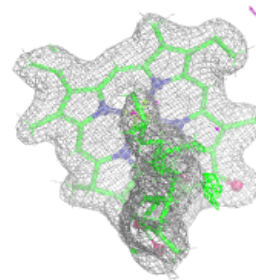
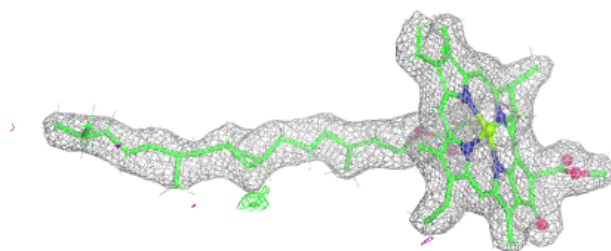
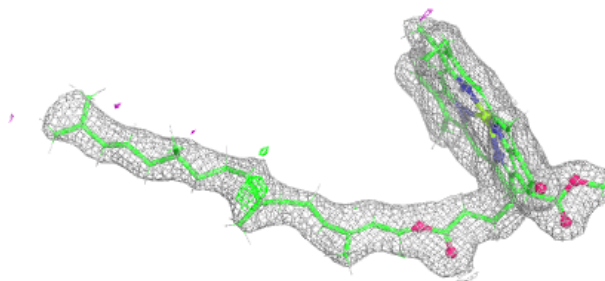
**Electron density around CLA C 501:**

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

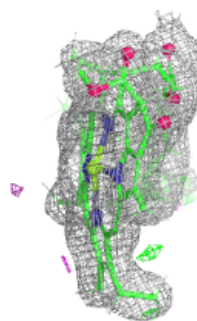
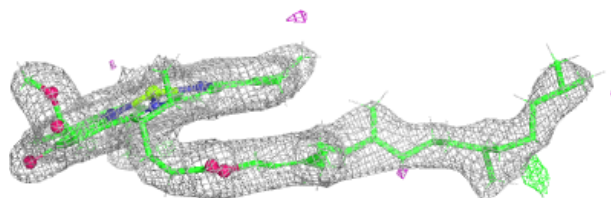
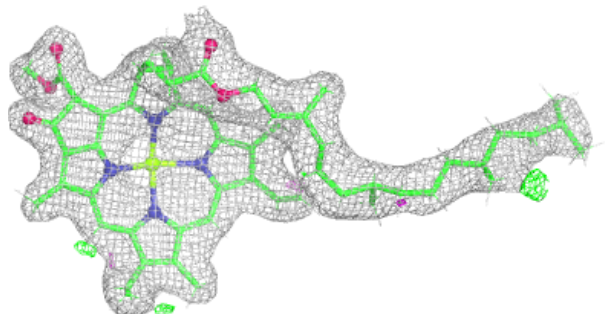


Electron density around CLA b 607:

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

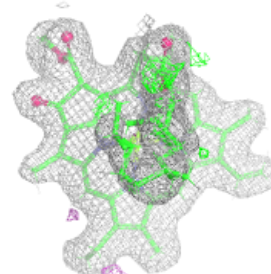
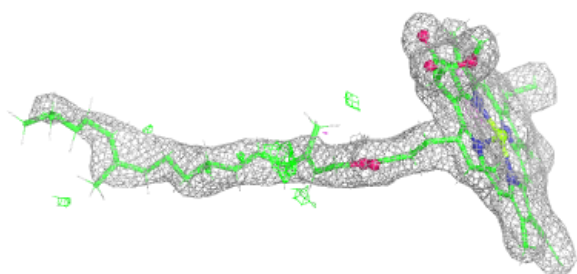
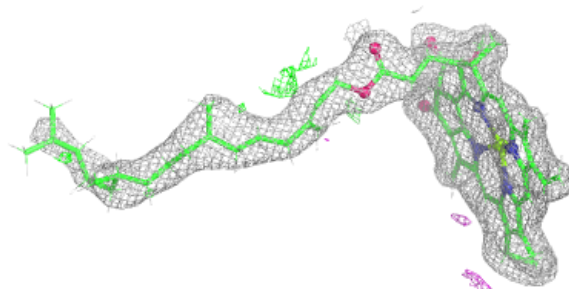
**Electron density around CLA B 603:**

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

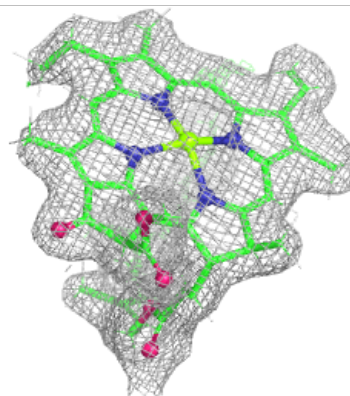
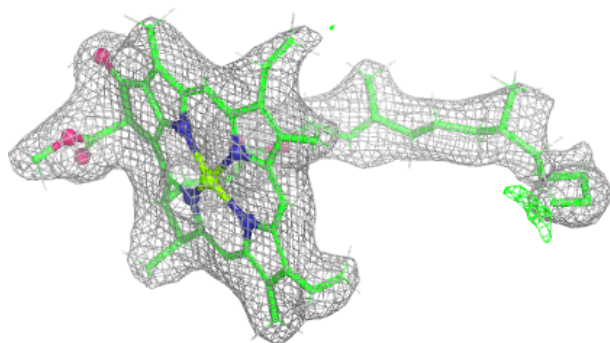
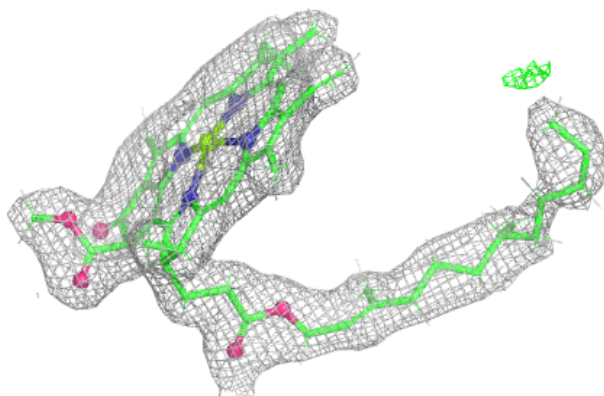


Electron density around CLA B 604:

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

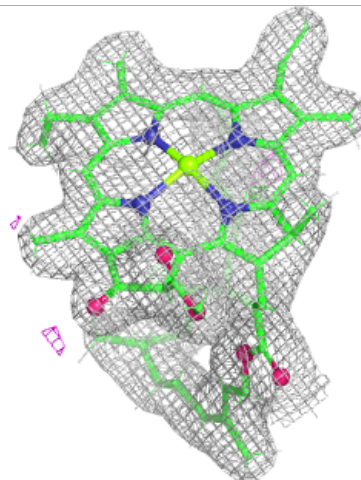
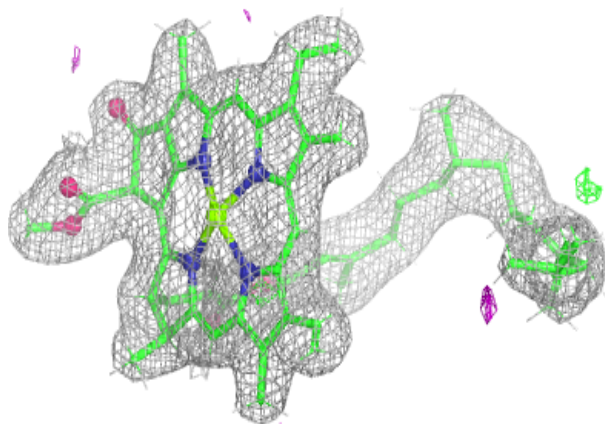
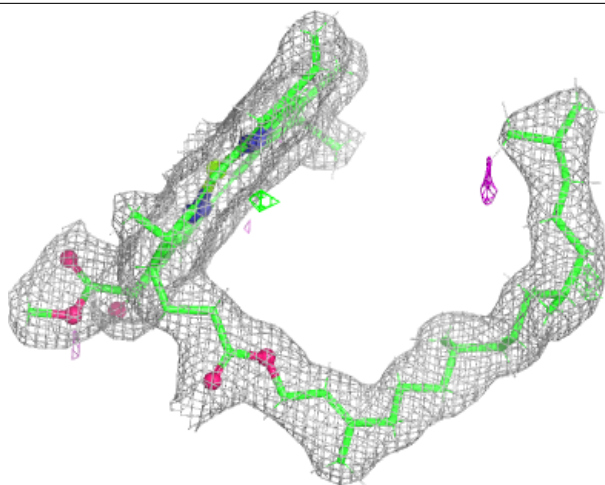
**Electron density around CLA C 504:**

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



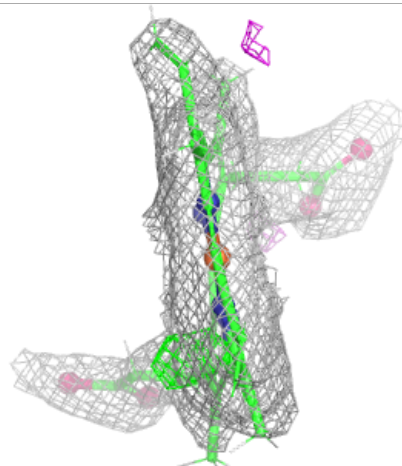
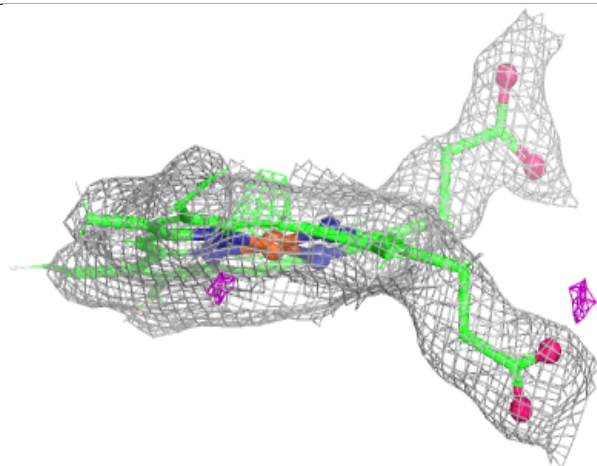
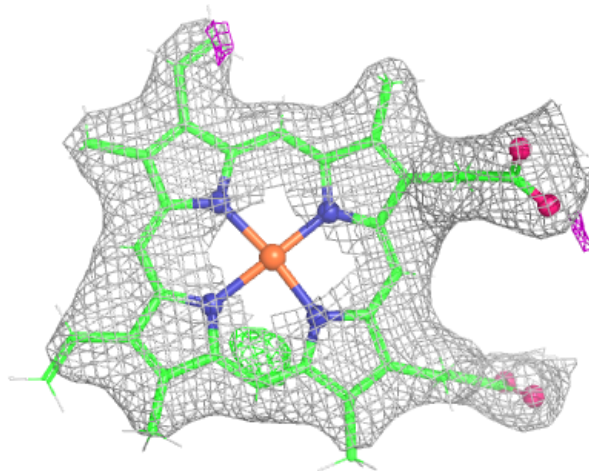
Electron density around CLA b 611:

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



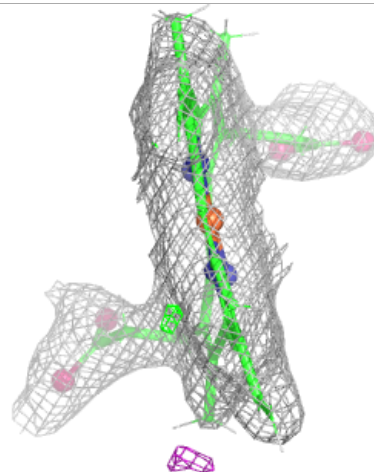
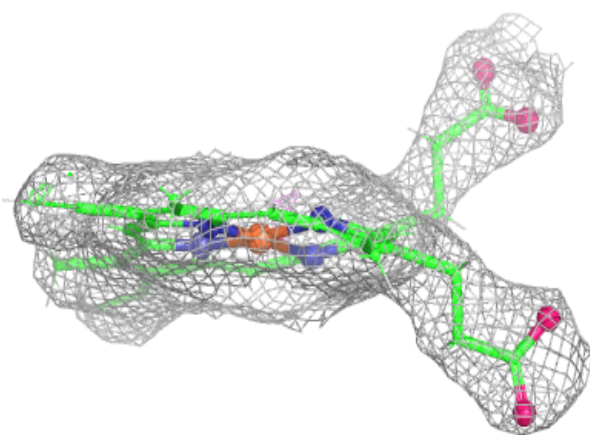
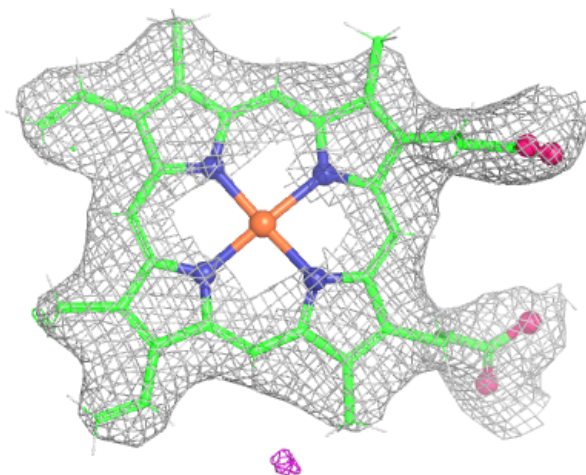
Electron density around HEM F 102:

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



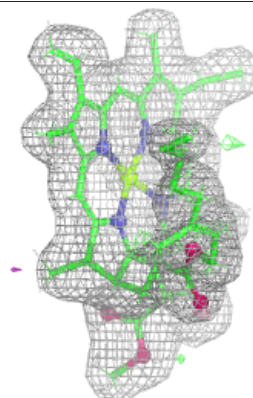
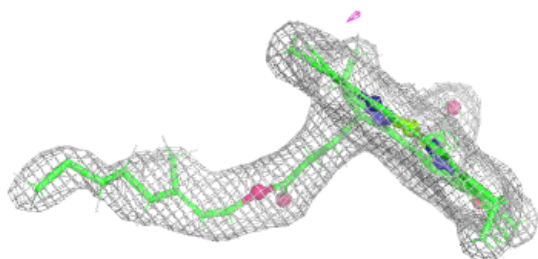
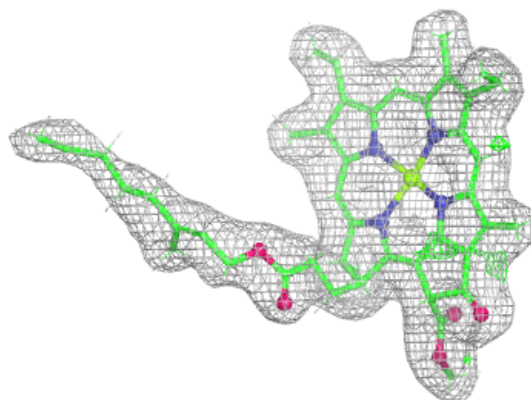
Electron density around HEM f 102:

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



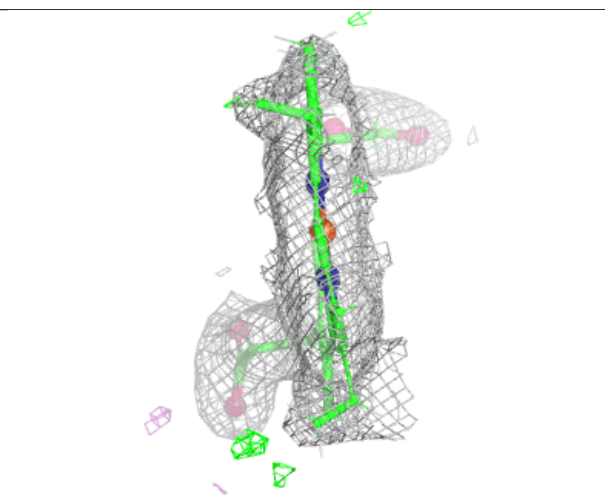
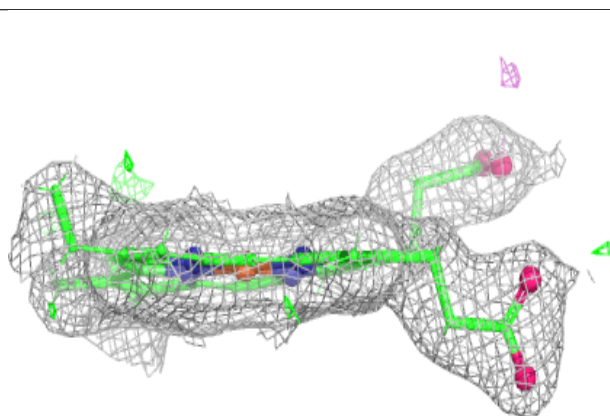
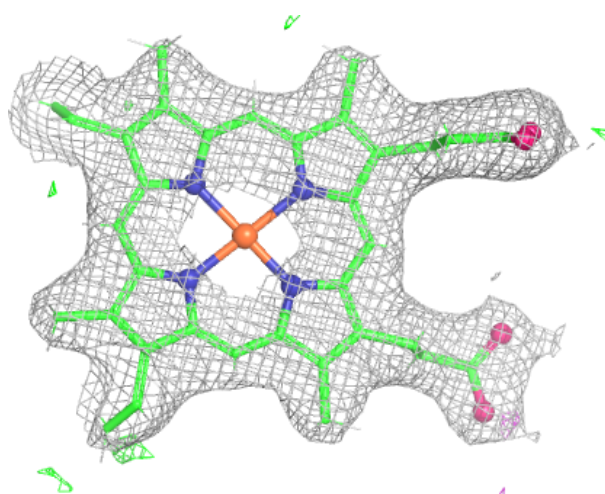
Electron density around CLA A 607:

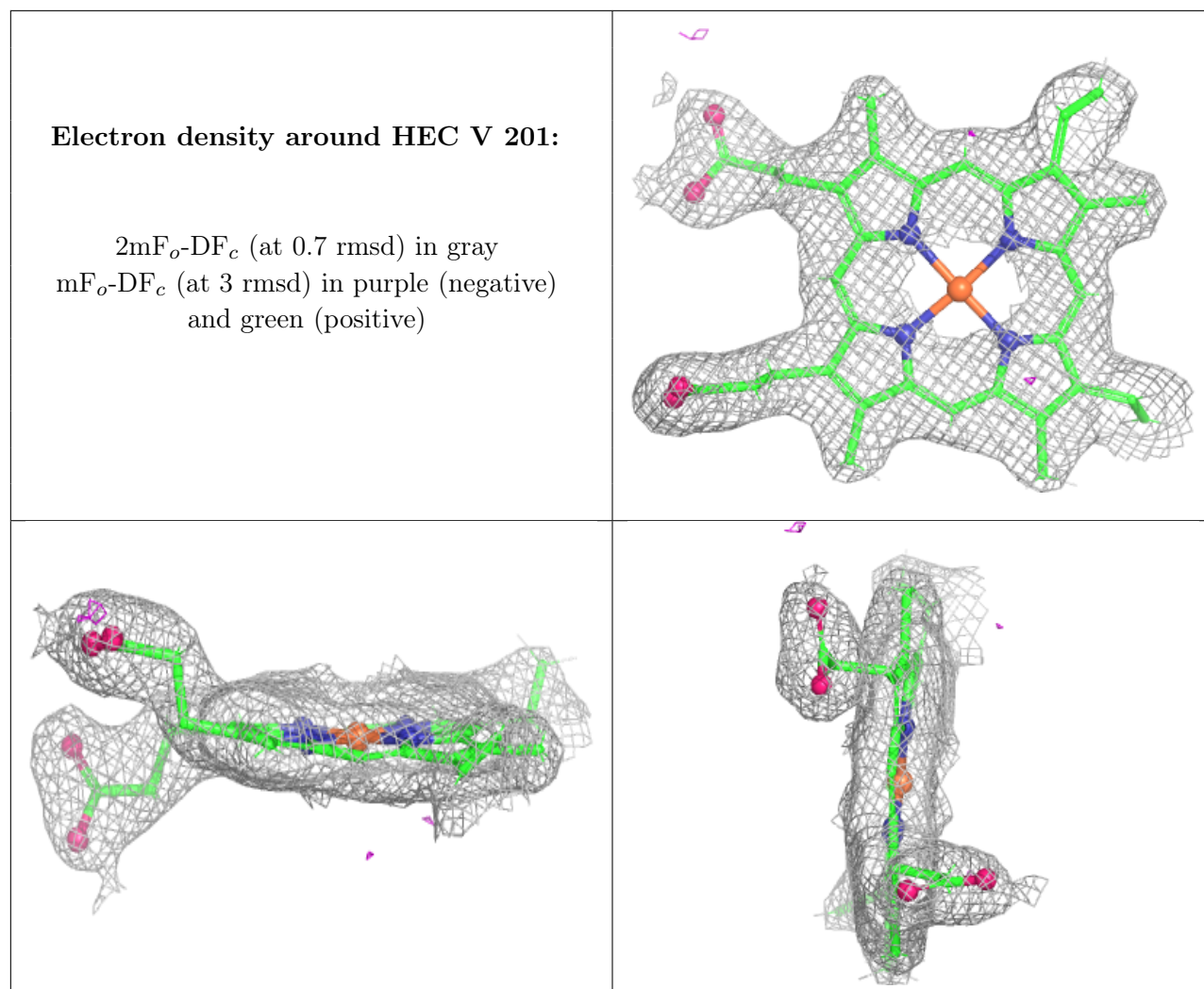
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 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.