



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 13, 2026 – 02:25 PM JST

PDB ID : 9LP8 / pdb_00009lp8
Title : Extrinsic-protein reconstituted PSII of Thermosynechococcus vulcanus NIES-2134
Authors : Nakajima, Y.; Kato, K.; Shen, J.R.; Nagao, R.
Deposited on : 2025-01-24
Resolution : 2.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

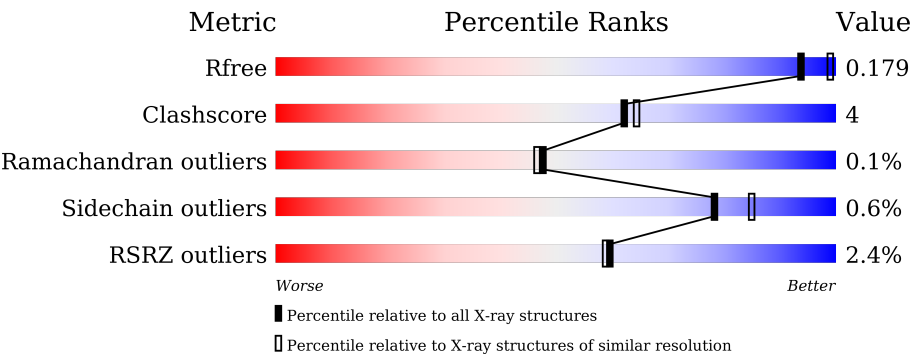
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

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



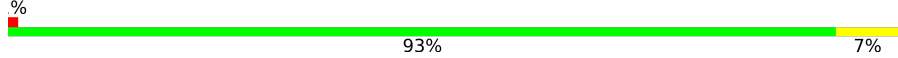
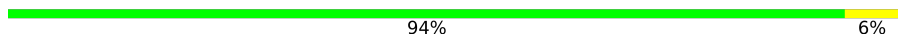
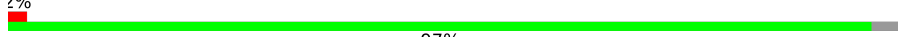
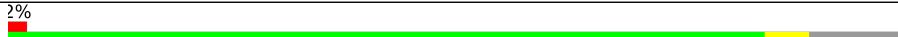
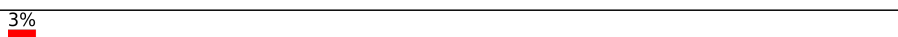
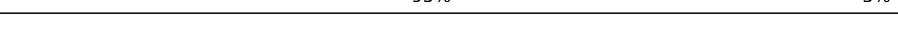
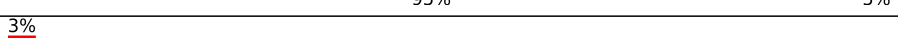
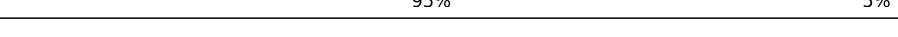
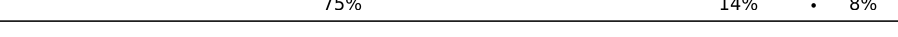
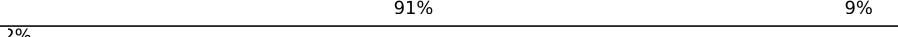
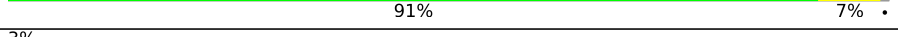
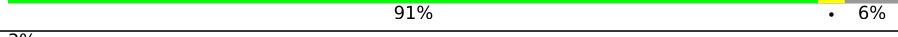
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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

Mol	Chain	Length	Quality of chain
1	A	360	2% 86% 6% 7%
1	a	360	3% 88% 5% 7%
2	B	505	2% 94% 5%
2	b	505	3% 94% 5%
3	C	473	% 88% 7% 5%
3	c	473	% 90% 7%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	D	342	
4	d	342	
5	E	84	
5	e	84	
6	F	45	
6	f	45	
7	H	65	
7	h	65	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	37	
10	k	37	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	244	
13	o	244	
14	T	32	
14	t	32	
15	U	104	
15	u	104	
16	V	163	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
16	v	163	
17	Y	30	
17	y	30	
18	X	40	
18	x	40	
19	Z	62	
19	z	62	
20	R	34	

2 Entry composition [i](#)

There are 42 unique types of molecules in this entry. The entry contains 54054 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	3	0
			2620	1719	429	457	15			
1	a	334	Total	C	N	O	S	0	3	0
			2615	1716	428	456	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	279	PRO	ARG	variant	UNP P51765
a	279	PRO	ARG	variant	UNP P51765

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	504	Total	C	N	O	S	0	8	0
			3991	2621	664	693	13			
2	b	501	Total	C	N	O	S	0	11	0
			3959	2603	656	687	13			

- Molecule 3 is a protein called Photosystem II 44 kDa reaction center protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	451	Total	C	N	O	S	0	2	0
			3488	2284	583	608	13			
3	c	455	Total	C	N	O	S	0	4	0
			3536	2315	593	615	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	341	Total	C	N	O	S	0	2	0
			2726	1809	443	462	12			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	d	341	Total	C	N	O	S	0	3	0
			2733	1812	446	463	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	81	Total	C	N	O		0	0	0
			657	429	106	122				
5	e	79	Total	C	N	O		0	0	0
			627	413	97	117				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	34	Total	C	N	O	S	0	0	0
			274	187	45	41	1			
6	f	32	Total	C	N	O	S	0	0	0
			255	173	43	38	1			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	36	Total	C	N	O	S	0	0	0
			291	198	45	47	1			
8	i	38	Total	C	N	O	S	0	0	0
			311	210	48	52	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	36	Total	C	N	O	S	0	0	0
			251	171	37	42	1			
9	j	39	Total	C	N	O	S	0	0	0
			267	180	40	46	1			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	K	37	Total	C	N	O	0	1	0
			287	201	42	44			
10	k	37	Total	C	N	O	0	0	0
			283	197	42	44			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	33	LEU	PHE	variant	UNP P19054
K	39	TRP	VAL	variant	UNP P19054
k	33	LEU	PHE	variant	UNP P19054
k	39	TRP	VAL	variant	UNP P19054

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	L	37	Total	C	N	O	0	1	0
			296	200	45	51			
11	l	37	Total	C	N	O	0	2	0
			300	204	45	51			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	33	Total	C	N	O	S	0	1	0
			261	176	37	47	1			
12	m	34	Total	C	N	O	S	0	2	0
			275	187	39	48	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	8	LEU	PHE	variant	UNP P12312
m	8	LEU	PHE	variant	UNP P12312

- Molecule 13 is a protein called Photosystem II extrinsic protein O.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	244	Total	C	N	O	S	0	5	0
			1865	1170	310	380	5			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	o	241	Total	C	N	O	S	0	5	0
			1837	1154	302	375	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	30	Total	C	N	O	S	0	0	0
			256	180	36	38	2			
14	t	30	Total	C	N	O	S	0	1	0
			265	185	37	41	2			

- Molecule 15 is a protein called Photosystem II extrinsic protein U.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	U	97	Total	C	N	O	S	0	0	0
			766	486	128	152				
15	u	97	Total	C	N	O	S	0	1	0
			769	489	129	151				

- Molecule 16 is a protein called Photosystem II extrinsic protein V.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total	C	N	O	S	0	1	0
			1057	672	178	203	4			
16	v	137	Total	C	N	O	S	0	1	0
			1050	667	176	203	4			

- Molecule 17 is a protein called Photosystem II reaction center protein Psb30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Y	27	Total	C	N	O	S	0	0	0
			193	127	32	31	3			
17	y	28	Total	C	N	O	S	0	0	0
			196	128	33	32	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	X	38	Total	C	N	O	S	0	1	0
			280	190	44	46				
18	x	38	Total	C	N	O	S	0	1	0
			280	190	44	46				

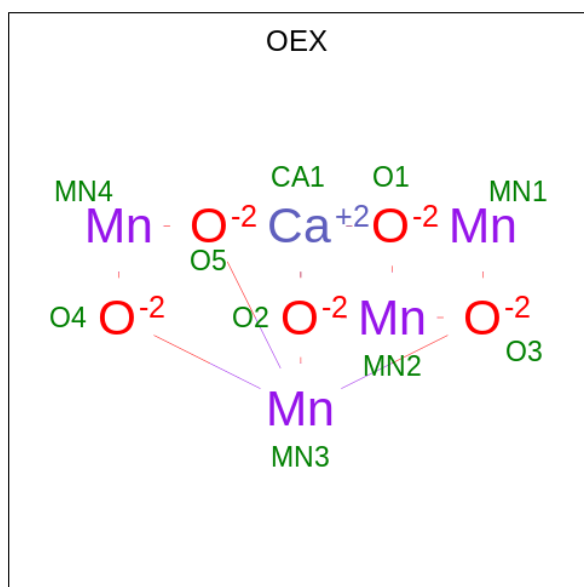
- Molecule 19 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Z	62	Total	C	N	O	S	0	0	0
			452	313	66	72	1			
19	z	60	Total	C	N	O	S	0	0	0
			432	301	64	66	1			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	R	30	Total	C	N	O	0	0	0
			162	99	33	30			

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



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

Continued on next page...

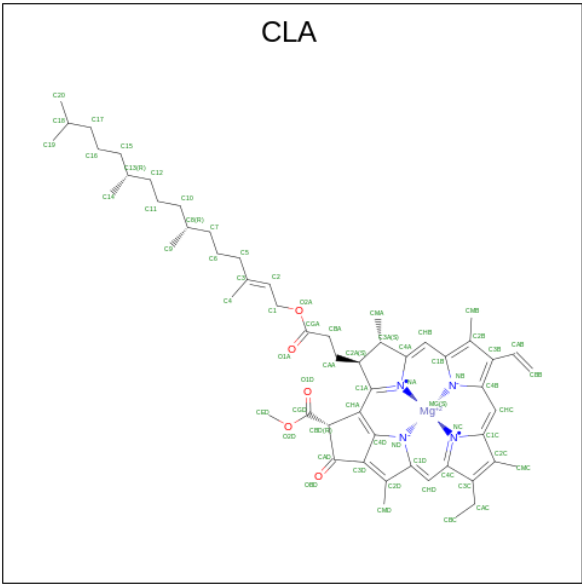
Continued from previous page...

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

- Molecule 23 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

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



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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

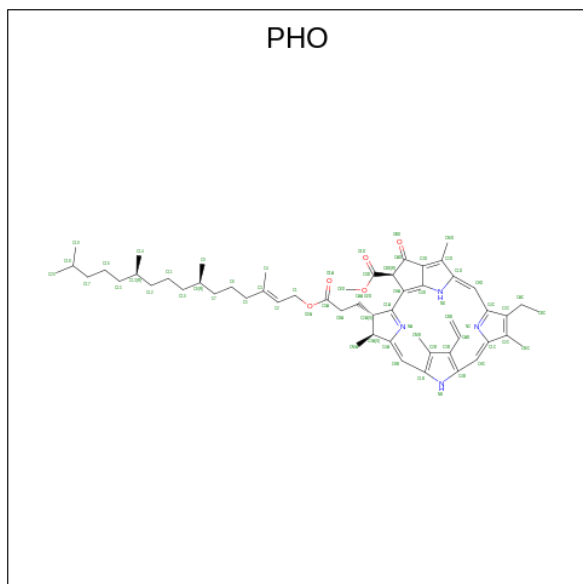
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N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

Continued on next page...

Continued from previous page...

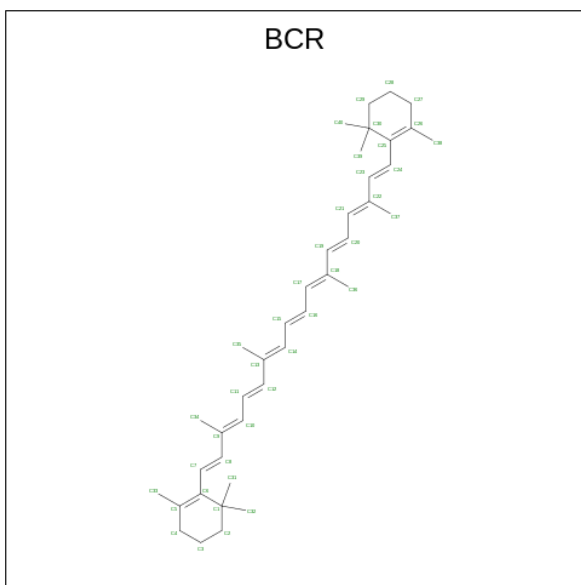
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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



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

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



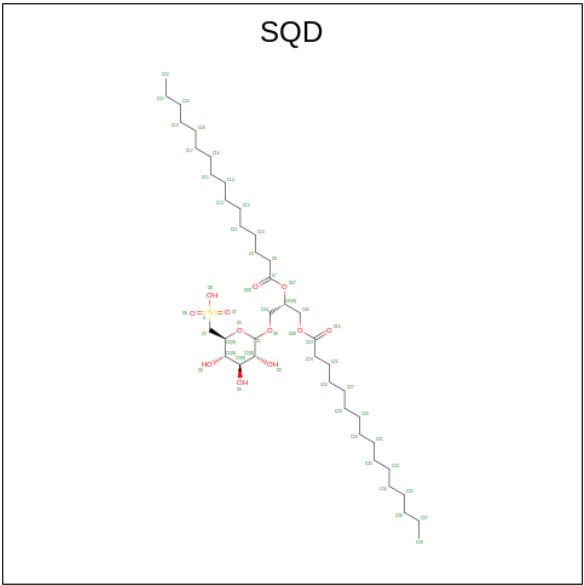
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	D	1	Total C 40 40	0	0
26	K	1	Total C 40 40	0	0
26	T	1	Total C 40 40	0	0
26	Y	1	Total C 40 40	0	0
26	a	1	Total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

Continued on next page...

Continued from previous page...

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

- Molecule 27 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



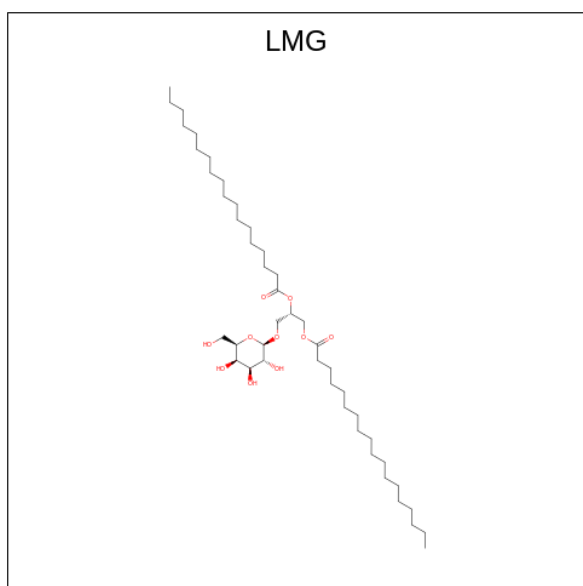
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	1	Total C O S 52 39 12 1	0	0
27	A	1	Total C O S 54 41 12 1	0	0
27	B	1	Total C O S 54 41 12 1	0	0
27	F	1	Total C O S 37 25 11 1	0	0
27	a	1	Total C O S 54 41 12 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	a	1	Total	C	O	S	0	0
			54	41	12	1		
27	b	1	Total	C	O	S	0	0
			54	41	12	1		
27	f	1	Total	C	O	S	0	0
			33	23	9	1		

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



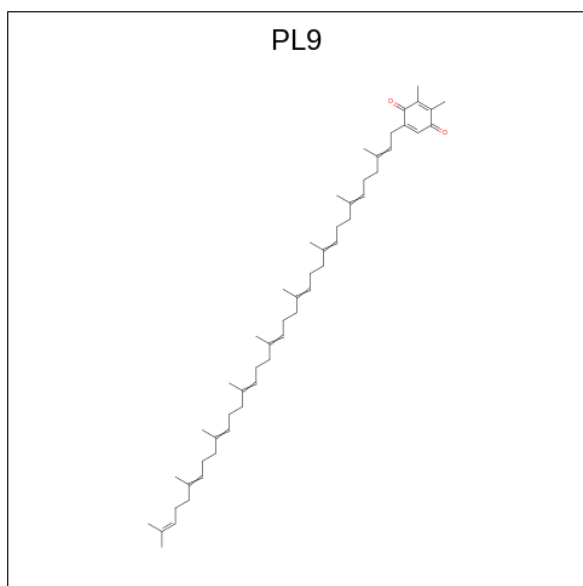
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	A	1	Total	C	O		0	0
			51	41	10			
28	B	1	Total	C	O		0	0
			51	41	10			
28	C	1	Total	C	O		0	0
			49	39	10			
28	C	1	Total	C	O		0	0
			51	41	10			
28	D	1	Total	C	O		0	0
			48	38	10			
28	a	1	Total	C	O		0	0
			51	41	10			
28	b	1	Total	C	O		0	0
			51	41	10			
28	c	1	Total	C	O		0	0
			51	41	10			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	c	1	Total	C	O	0	0
			51	41	10		
28	d	1	Total	C	O	0	0
			48	38	10		

- Molecule 29 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) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 30 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	A	3	Total	C	O	0	0
			54	49	5		
30	B	6	Total	C	O	0	0
			78	75	3		

Continued on next page...

Continued from previous page...

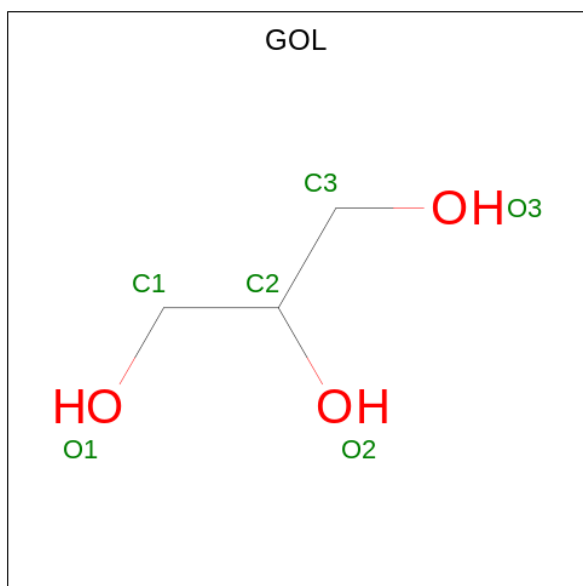
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	C	4	Total	C	O	0	0
			66	59	7		
30	D	2	Total	C	O	0	0
			53	48	5		
30	E	2	Total	C		0	0
			29	29			
30	H	1	Total	C		0	0
			7	7			
30	I	3	Total	C		0	0
			38	38			
30	J	2	Total	C		0	0
			29	29			
30	M	1	Total	C		0	0
			16	16			
30	T	1	Total	C		0	0
			15	15			
30	Y	1	Total	C		0	0
			10	10			
30	X	1	Total	C		0	0
			16	16			
30	a	3	Total	C	O	0	0
			56	51	5		
30	b	5	Total	C	O	0	0
			63	59	4		
30	c	5	Total	C	O	0	0
			74	65	9		
30	d	3	Total	C	O	0	0
			72	63	9		
30	e	1	Total	C		0	0
			15	15			
30	h	1	Total	C		0	0
			7	7			
30	i	4	Total	C	O	0	0
			55	53	2		
30	j	2	Total	C	O	0	0
			32	30	2		
30	m	1	Total	C		0	0
			13	13			
30	t	1	Total	C		0	0
			12	12			
30	v	1	Total	C		0	0
			7	7			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	y	1	Total C 10 10	0	0

- Molecule 31 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	A	1	Total C O 6 3 3	0	0
31	A	1	Total C O 6 3 3	0	0
31	A	1	Total C O 6 3 3	0	0
31	B	1	Total C O 6 3 3	0	0
31	B	1	Total C O 6 3 3	0	0
31	B	1	Total C O 6 3 3	0	0
31	B	1	Total C O 6 3 3	0	0
31	B	1	Total C O 6 3 3	0	0
31	B	1	Total C O 6 3 3	0	0
31	C	1	Total C O 6 3 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	C	1	Total 6	C 3	O 3	0	0
31	C	1	Total 6	C 3	O 3	0	0
31	C	1	Total 6	C 3	O 3	0	0
31	C	1	Total 6	C 3	O 3	0	0
31	C	1	Total 6	C 3	O 3	0	0
31	H	1	Total 6	C 3	O 3	0	0
31	L	1	Total 6	C 3	O 3	0	0
31	O	1	Total 6	C 3	O 3	0	0
31	O	1	Total 6	C 3	O 3	0	0
31	O	1	Total 6	C 3	O 3	0	0
31	V	1	Total 6	C 3	O 3	0	0
31	V	1	Total 6	C 3	O 3	0	0
31	V	1	Total 6	C 3	O 3	0	0
31	V	1	Total 6	C 3	O 3	0	0
31	Z	1	Total 6	C 3	O 3	0	0
31	a	1	Total 6	C 3	O 3	0	0
31	a	1	Total 6	C 3	O 3	0	0
31	a	1	Total 6	C 3	O 3	0	0
31	b	1	Total 6	C 3	O 3	0	0
31	b	1	Total 6	C 3	O 3	0	0
31	b	1	Total 6	C 3	O 3	0	0

Continued on next page...

Continued from previous page...

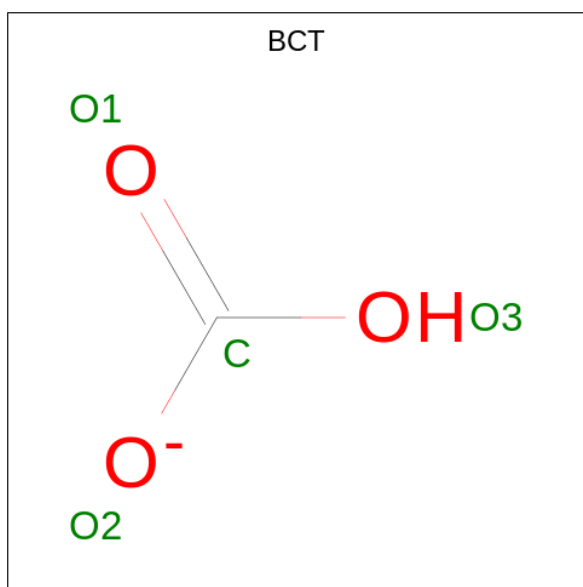
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	b	1	Total	C	O	0	0
			6	3	3		
31	b	1	Total	C	O	0	0
			6	3	3		
31	b	1	Total	C	O	0	0
			6	3	3		
31	b	1	Total	C	O	0	0
			6	3	3		
31	c	1	Total	C	O	0	0
			6	3	3		
31	c	1	Total	C	O	0	0
			6	3	3		
31	c	1	Total	C	O	0	0
			6	3	3		
31	c	1	Total	C	O	0	0
			6	3	3		
31	c	1	Total	C	O	0	0
			6	3	3		
31	c	1	Total	C	O	0	0
			6	3	3		
31	c	1	Total	C	O	0	0
			6	3	3		
31	c	1	Total	C	O	0	0
			6	3	3		
31	c	1	Total	C	O	0	0
			6	3	3		
31	f	1	Total	C	O	0	0
			6	3	3		
31	h	1	Total	C	O	0	0
			6	3	3		
31	o	1	Total	C	O	0	0
			6	3	3		
31	o	1	Total	C	O	0	0
			6	3	3		
31	t	1	Total	C	O	0	0
			6	3	3		
31	u	1	Total	C	O	0	0
			6	3	3		
31	u	1	Total	C	O	0	0
			6	3	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	v	1	Total	C	O	0	0
			6	3	3		
31	v	1	Total	C	O	0	0
			6	3	3		
31	v	1	Total	C	O	0	0
			6	3	3		

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



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

- Molecule 33 is CALCIUM ION (CCD ID: CA) (formula: Ca).

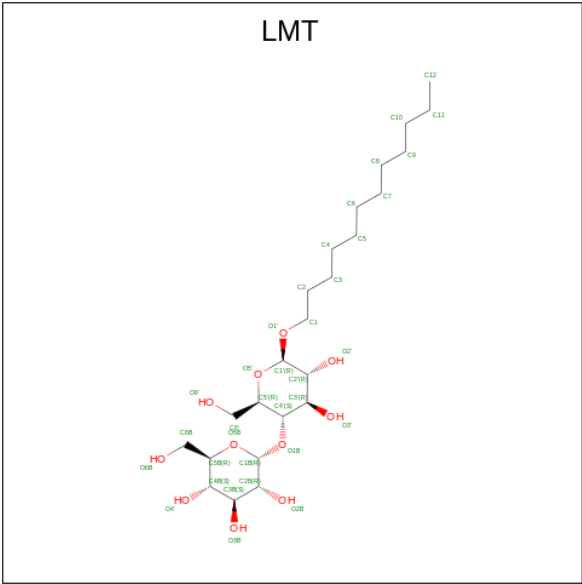
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	B	1	Total	Ca	0	0
			1	1		
33	F	1	Total	Ca	0	0
			1	1		
33	O	1	Total	Ca	0	0
			1	1		
33	b	1	Total	Ca	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	c	1	Total	Ca	0	0
			1	1		
33	f	1	Total	Ca	0	0
			1	1		
33	o	1	Total	Ca	0	0
			1	1		

- Molecule 34 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



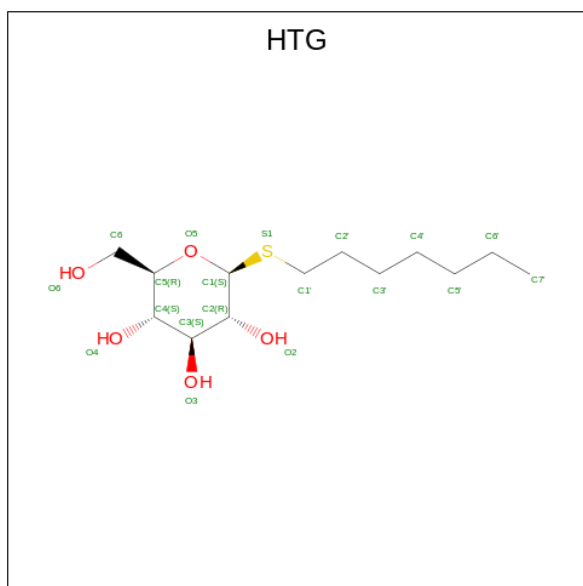
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	B	1	Total	C	O	0	0
			35	24	11		
34	C	1	Total	C	O	0	0
			35	24	11		
34	D	1	Total	C	O	0	0
			35	24	11		
34	F	1	Total	C	O	0	0
			26	15	11		
34	J	1	Total	C	O	0	0
			23	18	5		
34	M	1	Total	C	O	0	0
			35	24	11		
34	M	1	Total	C	O	0	0
			35	24	11		
34	T	1	Total	C	O	0	0
			24	18	6		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	Z	1	Total	C	O	0	0
			35	24	11		
34	a	1	Total	C	O	0	0
			35	24	11		
34	b	1	Total	C	O	0	0
			25	19	6		
34	c	1	Total	C	O	0	0
			35	24	11		
34	m	1	Total	C	O	0	0
			35	24	11		
34	m	1	Total	C	O	0	0
			35	24	11		
34	t	1	Total	C	O	0	0
			24	18	6		
34	z	1	Total	C	O	0	0
			32	21	11		

- Molecule 35 is heptyl 1-thio-beta-D-glucopyranoside (CCD ID: HTG) (formula: $C_{13}H_{26}O_5S$).



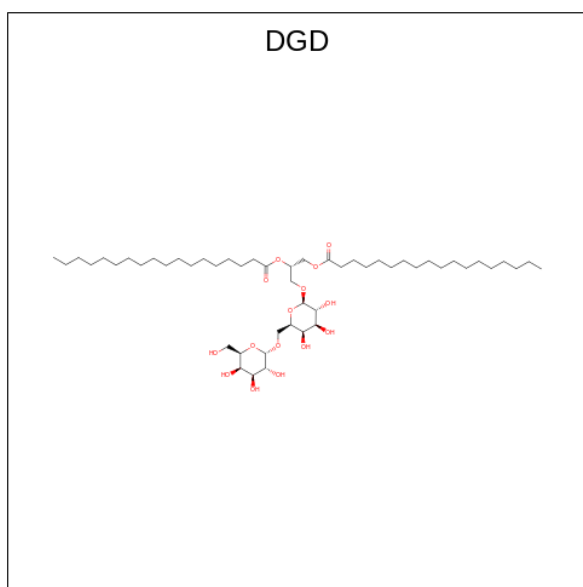
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		

Continued on next page...

Continued from previous page...

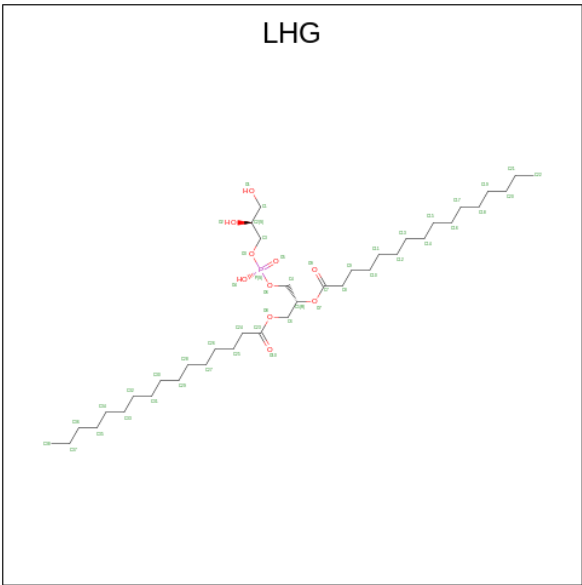
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	C	1	Total	C	O	S	0	0
			19	13	5	1		
35	C	1	Total	C	O	S	0	0
			19	13	5	1		
35	C	1	Total	C	O	S	0	0
			19	13	5	1		
35	H	1	Total	C	O	S	0	0
			16	13	2	1		
35	O	1	Total	C	O	S	0	0
			19	13	5	1		
35	U	1	Total	C	S		0	0
			9	8	1			
35	V	1	Total	C	O	S	0	0
			13	7	5	1		
35	X	1	Total	C	O	S	0	0
			12	7	4	1		
35	b	1	Total	C	O	S	0	0
			19	13	5	1		
35	b	1	Total	C	O	S	0	0
			19	13	5	1		
35	b	1	Total	C	O	S	0	0
			19	13	5	1		
35	b	1	Total	C	O	S	0	0
			19	13	5	1		
35	c	1	Total	C	O	S	0	0
			19	13	5	1		
35	c	1	Total	C	O	S	0	0
			19	13	5	1		
35	d	1	Total	C	O	S	0	0
			19	13	5	1		
35	o	1	Total	C	O	S	0	0
			19	13	5	1		
35	u	1	Total	C	O	S	0	0
			14	10	3	1		
35	v	1	Total	C	O	S	0	0
			13	7	5	1		

- Molecule 36 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



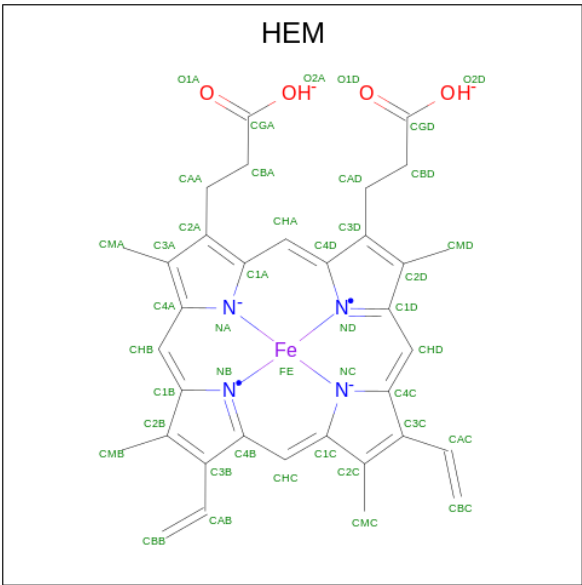
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
36	C	1	Total	C	O	0	0
			62	47	15		
36	C	1	Total	C	O	0	0
			56	41	15		
36	C	1	Total	C	O	0	0
			58	43	15		
36	D	1	Total	C	O	0	0
			53	42	11		
36	H	1	Total	C	O	0	0
			62	47	15		
36	c	1	Total	C	O	0	0
			62	47	15		
36	c	1	Total	C	O	0	0
			55	40	15		
36	c	1	Total	C	O	0	0
			60	45	15		
36	e	1	Total	C	O	0	0
			39	30	9		
36	h	1	Total	C	O	0	0
			62	47	15		

- Molecule 37 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



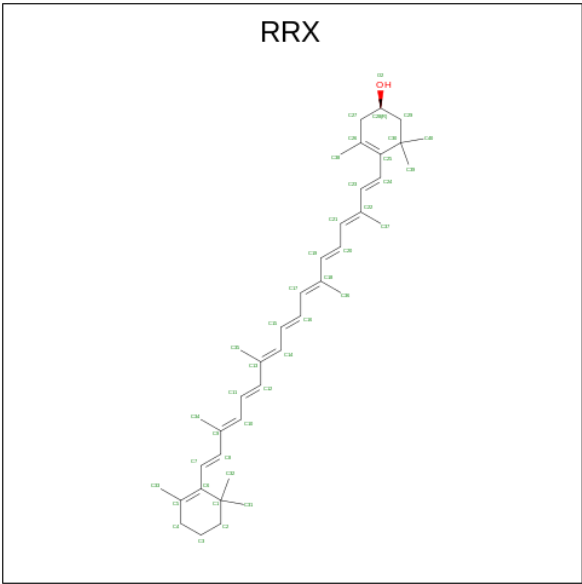
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
37	D	1	Total	C	O	P	0	0
			49	38	10	1		
37	D	1	Total	C	O	P	0	0
			49	38	10	1		
37	D	1	Total	C	O	P	0	0
			46	35	10	1		
37	E	1	Total	C	O	P	0	0
			49	38	10	1		
37	L	1	Total	C	O	P	0	0
			49	38	10	1		
37	b	1	Total	C	O	P	0	0
			49	38	10	1		
37	d	1	Total	C	O	P	0	0
			49	38	10	1		
37	d	1	Total	C	O	P	0	0
			49	38	10	1		
37	d	1	Total	C	O	P	0	0
			40	29	10	1		
37	e	1	Total	C	O	P	0	0
			27	17	9	1		

- Molecule 38 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 39 is (3R)-beta,beta-caroten-3-ol (CCD ID: RRX) (formula: C₄₀H₅₆O).

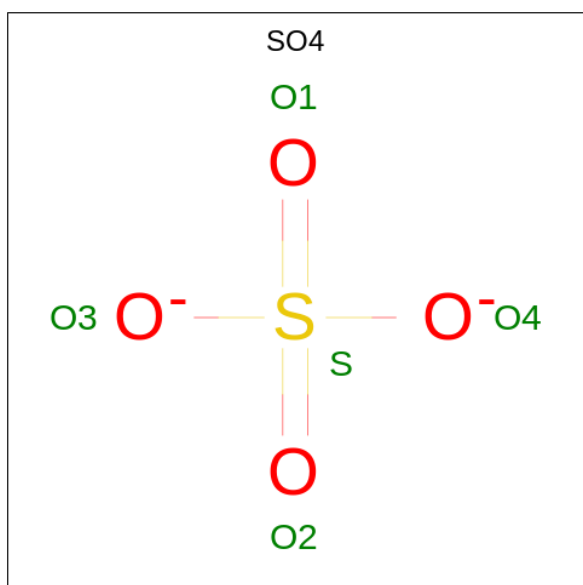


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
39	H	1	Total	C	O	0	0
			41	40	1		
39	h	1	Total	C	O	0	0
			41	40	1		

- Molecule 40 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	J	1	Total	Mg	0	0
			1	1		
40	j	1	Total	Mg	0	0
			1	1		

- Molecule 41 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
41	O	1	Total	O	S	0	0
			5	4	1		

- Molecule 42 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
42	A	151	Total	O	0	2
			153	153		
42	B	303	Total	O	0	7
			310	310		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
42	C	233	Total 237	O 237	0	4
42	D	151	Total 154	O 154	0	3
42	E	35	Total 36	O 36	0	1
42	F	17	Total 17	O 17	0	0
42	H	50	Total 51	O 51	0	1
42	I	11	Total 11	O 11	0	0
42	J	10	Total 10	O 10	0	0
42	K	7	Total 7	O 7	0	0
42	L	16	Total 16	O 16	0	0
42	M	17	Total 17	O 17	0	0
42	O	170	Total 176	O 176	0	6
42	T	16	Total 16	O 16	0	0
42	U	89	Total 90	O 90	0	1
42	V	134	Total 136	O 136	0	2
42	Y	7	Total 7	O 7	0	0
42	X	12	Total 12	O 12	0	0
42	a	156	Total 156	O 156	0	0
42	b	287	Total 291	O 291	0	4
42	c	225	Total 229	O 229	0	4
42	d	152	Total 157	O 157	0	5
42	e	24	Total 25	O 25	0	1

Continued on next page...

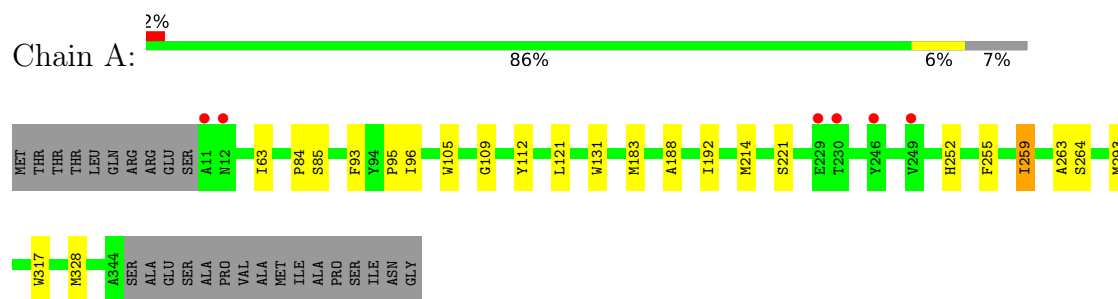
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
42	f	12	Total 12	O 12	0	0
42	h	37	Total 40	O 40	0	3
42	i	13	Total 13	O 13	0	0
42	j	8	Total 8	O 8	0	0
42	k	7	Total 7	O 7	0	0
42	l	13	Total 14	O 14	0	1
42	m	16	Total 16	O 16	0	0
42	o	152	Total 154	O 154	0	2
42	t	17	Total 19	O 19	0	2
42	u	94	Total 97	O 97	0	3
42	v	93	Total 97	O 97	0	4
42	y	4	Total 4	O 4	0	0
42	x	8	Total 8	O 8	0	0
42	z	3	Total 3	O 3	0	0

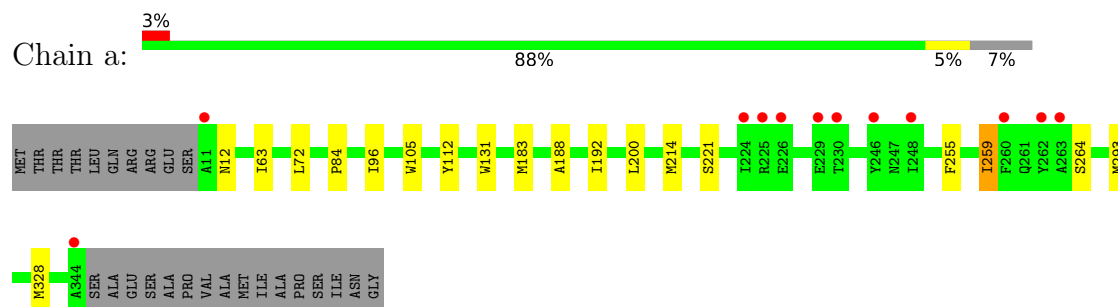
3 Residue-property plots [i](#)

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

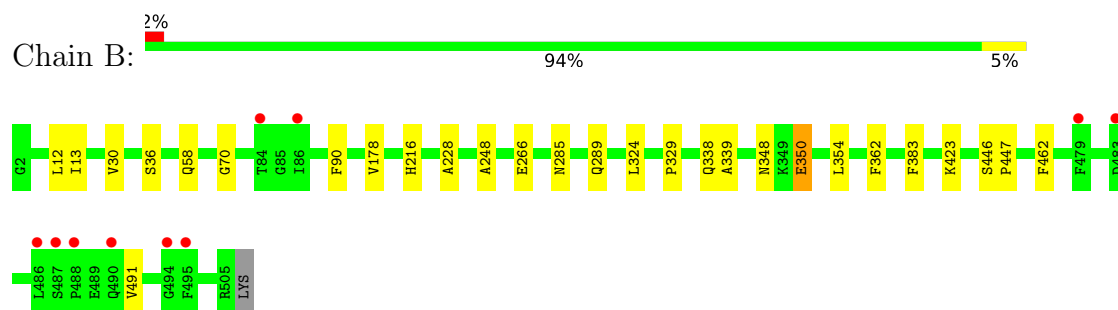
- Molecule 1: Photosystem II protein D1



- Molecule 1: Photosystem II protein D1

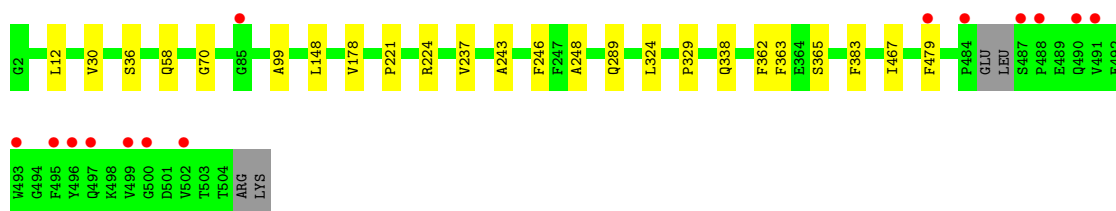


- Molecule 2: Photosystem II CP47 reaction center protein

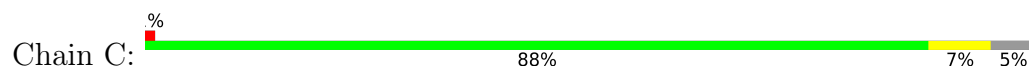


- Molecule 2: Photosystem II CP47 reaction center protein

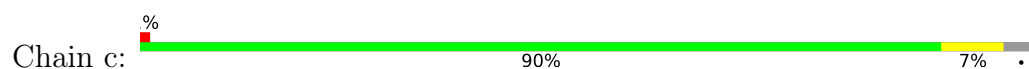




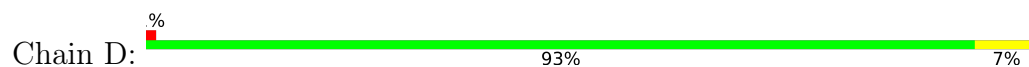
• Molecule 3: Photosystem II 44 kDa reaction center protein



• Molecule 3: Photosystem II 44 kDa reaction center protein



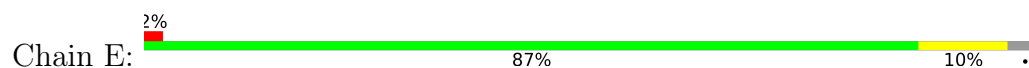
• Molecule 4: Photosystem II D2 protein



• Molecule 4: Photosystem II D2 protein

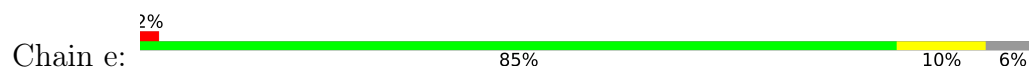


• Molecule 5: Cytochrome b559 subunit alpha





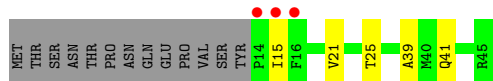
- Molecule 5: Cytochrome b559 subunit alpha



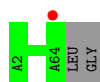
- Molecule 6: Cytochrome b559 subunit beta



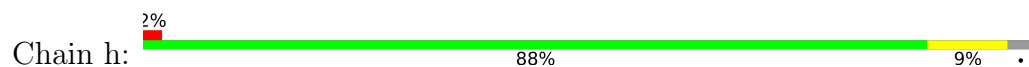
- Molecule 6: Cytochrome b559 subunit beta



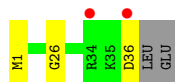
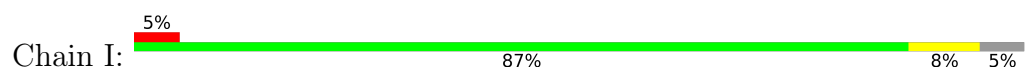
- Molecule 7: Photosystem II reaction center protein H



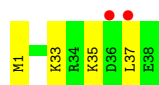
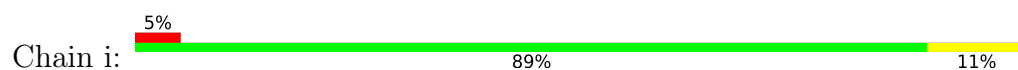
- Molecule 7: Photosystem II reaction center protein H



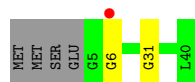
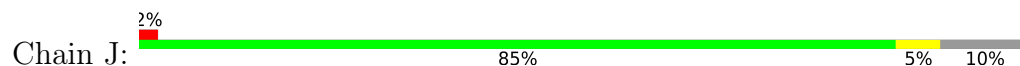
- Molecule 8: Photosystem II reaction center protein I



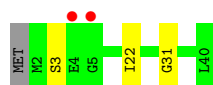
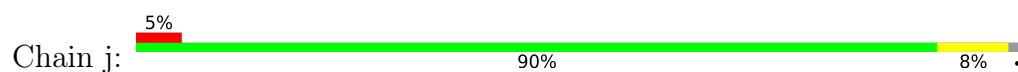
- Molecule 8: Photosystem II reaction center protein I



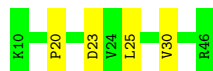
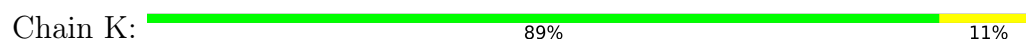
- Molecule 9: Photosystem II reaction center protein J



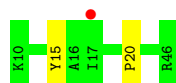
- Molecule 9: Photosystem II reaction center protein J



- Molecule 10: Photosystem II reaction center protein K



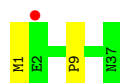
- Molecule 10: Photosystem II reaction center protein K



- Molecule 11: Photosystem II reaction center protein L



- Molecule 11: Photosystem II reaction center protein L



- Molecule 12: Photosystem II reaction center protein M

Chain M:  75% 14% • 8%



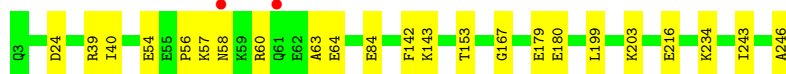
- Molecule 12: Photosystem II reaction center protein M

Chain m:  75% 17% • 6%



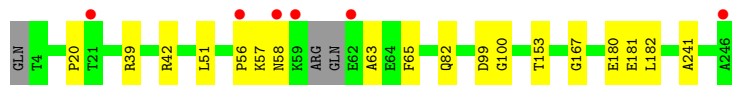
- Molecule 13: Photosystem II extrinsic protein O

Chain O:  91% 9%



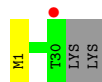
- Molecule 13: Photosystem II extrinsic protein O

Chain o:  91% 7% • 2%



- Molecule 14: Photosystem II reaction center protein T

Chain T:  91% 6% • 3%



- Molecule 14: Photosystem II reaction center protein T

Chain t:  81% 12% 6%



- Molecule 15: Photosystem II extrinsic protein U

Chain U:  89% 7%



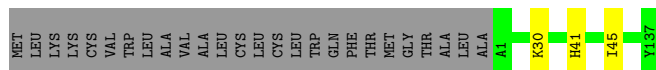
- Molecule 15: Photosystem II extrinsic protein U

Chain u:  88% 5% 7%



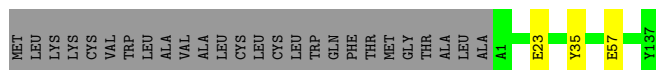
- Molecule 16: Photosystem II extrinsic protein V

Chain V:  82% 16%



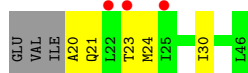
- Molecule 16: Photosystem II extrinsic protein V

Chain v:  82% 16%



- Molecule 17: Photosystem II reaction center protein Psb30

Chain Y:  10% 73% 17% 10%



- Molecule 17: Photosystem II reaction center protein Psb30

Chain y:  3% 77% 17% 7%

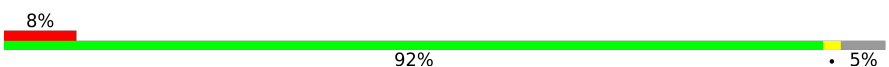


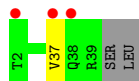
- Molecule 18: Photosystem II reaction center protein X

Chain X:  88% 8% 5%

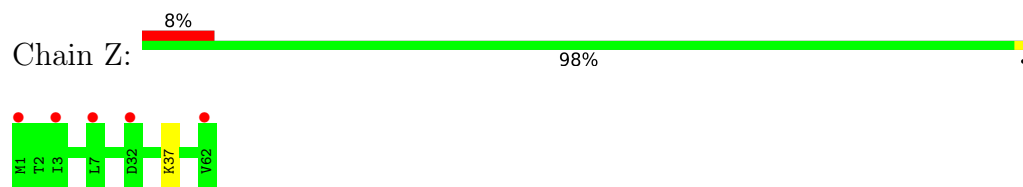


- Molecule 18: Photosystem II reaction center protein X

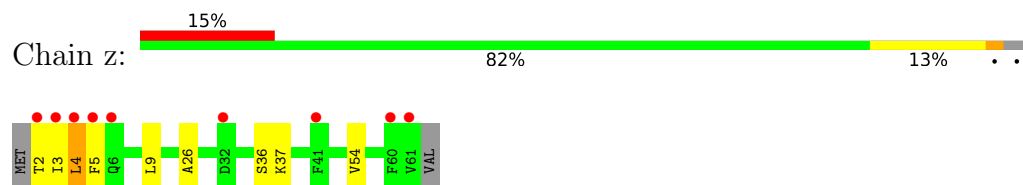
Chain x:  8% 92% 5%



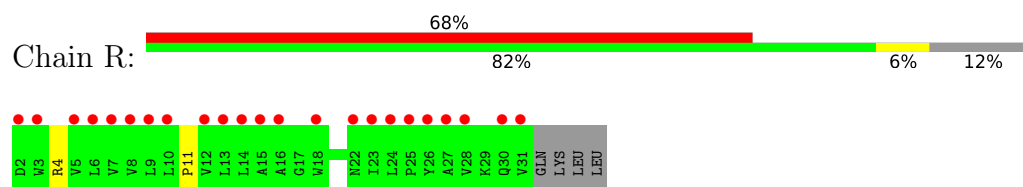
- Molecule 19: Photosystem II reaction center protein Z



- Molecule 19: Photosystem II reaction center protein Z



- Molecule 20: Photosystem II reaction center protein Y



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	123.34Å 228.88Å 286.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.10 – 2.00 49.10 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.10-2.00) 99.9 (49.10-2.00)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0103, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.152 , 0.178 0.154 , 0.179	Depositor DCC
R_{free} test set	27141 reflections (4.29%)	wwPDB-VP
Wilson B-factor (Å ²)	39.2	Xtriage
Anisotropy	0.513	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 62.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	54054	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.89% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, FME, PL9, BCR, FE2, LMG, CLA, HEM, MG, OEX, SQD, HTG, RRX, CA, PHO, LMT, CL, HSK, BCT, DGD, LHG, SO4, UNL

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	0.34	0/2714	0.50	0/3703
1	a	0.33	0/2708	0.50	0/3695
2	B	0.31	0/4152	0.47	0/5659
2	b	0.29	1/4129 (0.0%)	0.46	0/5627
3	C	0.27	0/3607	0.43	0/4911
3	c	0.25	0/3662	0.42	0/4986
4	D	0.34	0/2804	0.48	0/3820
4	d	0.31	0/2814	0.45	0/3833
5	E	0.25	0/676	0.41	0/924
5	e	0.22	0/646	0.40	0/885
6	F	0.26	0/283	0.41	0/386
6	f	0.32	0/262	0.39	0/356
7	H	0.25	0/511	0.41	0/697
7	h	0.23	0/511	0.42	0/697
8	I	0.20	0/288	0.33	0/390
8	i	0.23	0/308	0.37	0/415
9	J	0.22	0/257	0.37	0/349
9	j	0.21	0/273	0.34	0/371
10	K	0.24	0/300	0.38	0/414
10	k	0.22	0/293	0.36	0/404
11	L	0.36	0/306	0.44	0/418
11	l	0.33	0/313	0.41	0/428
12	M	0.35	0/257	0.52	0/352
12	m	0.30	0/274	0.48	0/374
13	O	0.29	0/1911	0.48	0/2595
13	o	0.26	0/1882	0.45	0/2555
14	T	0.32	0/255	0.42	0/346
14	t	0.32	0/264	0.41	0/359
15	U	0.28	0/777	0.47	0/1055
15	u	0.30	0/783	0.47	0/1063
16	V	0.31	0/1081	0.47	0/1469

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.25	0/1074	0.42	0/1462
17	Y	0.19	0/194	0.32	0/259
17	y	0.18	0/197	0.35	0/264
18	X	0.17	0/286	0.28	0/387
18	x	0.15	0/286	0.30	0/387
19	Z	0.17	0/463	0.36	0/636
19	z	0.17	0/443	0.36	0/609
20	R	0.18	0/162	0.30	0/224
All	All	0.29	1/42406 (0.0%)	0.45	0/57764

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	b	221	PRO	CA-C	5.85	1.55	1.51

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2620	0	2520	17	0
1	a	2615	0	2520	13	0
2	B	3991	0	3844	22	0
2	b	3959	0	3806	19	0
3	C	3488	0	3410	29	0
3	c	3536	0	3460	22	0
4	D	2726	0	2629	18	0
4	d	2733	0	2641	17	0
5	E	657	0	637	7	0
5	e	627	0	595	6	0
6	F	274	0	279	4	0
6	f	255	0	263	3	0
7	H	498	0	518	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	h	498	0	518	8	0
8	I	291	0	302	2	0
8	i	311	0	326	2	0
9	J	251	0	257	1	0
9	j	267	0	266	3	0
10	K	287	0	292	4	0
10	k	283	0	283	2	0
11	L	296	0	305	2	0
11	l	300	0	314	2	0
12	M	261	0	280	4	0
12	m	275	0	304	6	0
13	O	1865	0	1829	17	0
13	o	1837	0	1800	11	0
14	T	256	0	256	0	0
14	t	265	0	262	4	0
15	U	766	0	758	3	0
15	u	769	0	764	3	0
16	V	1057	0	1063	2	0
16	v	1050	0	1043	3	0
17	Y	193	0	210	4	0
17	y	196	0	208	3	0
18	X	280	0	312	3	0
18	x	280	0	312	2	0
19	Z	452	0	469	1	0
19	z	432	0	441	6	0
20	R	162	0	103	1	0
21	A	10	0	0	0	0
21	a	10	0	0	0	0
22	A	1	0	0	0	0
22	a	1	0	0	0	0
23	A	2	0	0	0	0
23	a	2	0	0	0	0
24	A	260	0	288	8	0
24	B	1040	0	1152	31	0
24	C	845	0	936	36	0
24	D	130	0	144	2	0
24	a	195	0	216	5	0
24	b	1040	0	1152	29	0
24	c	845	0	936	28	0
24	d	195	0	216	7	0
25	A	128	0	148	3	0
25	a	128	0	148	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	A	40	0	56	0	0
26	B	120	0	168	8	0
26	C	80	0	112	4	0
26	D	40	0	56	2	0
26	K	40	0	56	1	0
26	T	40	0	56	5	0
26	Y	40	0	56	1	0
26	a	40	0	56	2	0
26	b	120	0	168	7	0
26	c	80	0	112	5	0
26	d	40	0	56	1	0
26	k	40	0	56	2	0
26	t	40	0	56	6	0
26	y	40	0	56	2	0
27	A	106	0	149	3	0
27	B	54	0	78	1	0
27	F	37	0	46	1	0
27	a	108	0	156	7	0
27	b	54	0	78	1	0
27	f	33	0	39	1	0
28	A	51	0	72	2	0
28	B	51	0	72	4	0
28	C	100	0	140	2	0
28	D	48	0	66	3	0
28	a	51	0	72	2	0
28	b	51	0	72	1	0
28	c	102	0	144	1	0
28	d	48	0	66	0	0
29	A	55	0	80	5	0
29	D	55	0	80	0	0
29	a	55	0	80	5	0
29	d	55	0	80	0	0
30	A	54	0	0	0	0
30	B	78	0	0	0	0
30	C	66	0	0	0	0
30	D	53	0	0	0	0
30	E	29	0	0	0	0
30	H	7	0	0	0	0
30	I	38	0	0	0	0
30	J	29	0	0	0	0
30	M	16	0	0	0	0
30	T	15	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	X	16	0	0	0	0
30	Y	10	0	0	0	0
30	a	56	0	0	0	0
30	b	63	0	0	0	0
30	c	74	0	0	0	0
30	d	72	0	0	0	0
30	e	15	0	0	0	0
30	h	7	0	0	0	0
30	i	55	0	0	0	0
30	j	32	0	0	0	0
30	m	13	0	0	0	0
30	t	12	0	0	0	0
30	v	7	0	0	0	0
30	y	10	0	0	0	0
31	A	18	0	24	2	0
31	B	36	0	48	1	0
31	C	36	0	48	4	0
31	H	6	0	8	1	0
31	L	6	0	8	0	0
31	O	18	0	24	1	0
31	V	24	0	30	0	0
31	Z	6	0	8	0	0
31	a	18	0	24	1	0
31	b	42	0	56	0	0
31	c	60	0	80	9	0
31	f	6	0	7	0	0
31	h	6	0	8	1	0
31	o	12	0	16	0	0
31	t	6	0	8	0	0
31	u	12	0	15	0	0
31	v	18	0	24	0	0
32	A	4	0	0	0	0
32	a	4	0	0	0	0
33	B	1	0	0	0	0
33	F	1	0	0	0	0
33	O	1	0	0	0	0
33	b	1	0	0	0	0
33	c	1	0	0	0	0
33	f	1	0	0	0	0
33	o	1	0	0	0	0
34	B	35	0	46	1	0
34	C	35	0	46	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	D	35	0	46	0	0
34	F	26	0	25	0	0
34	J	23	0	32	0	0
34	M	70	0	92	2	0
34	T	24	0	35	0	0
34	Z	35	0	46	1	0
34	a	35	0	46	1	0
34	b	25	0	35	1	0
34	c	35	0	46	0	0
34	m	70	0	92	1	0
34	t	24	0	35	0	0
34	z	32	0	33	4	0
35	B	76	0	104	0	0
35	C	57	0	78	4	0
35	H	16	0	20	1	0
35	O	19	0	26	0	0
35	U	9	0	15	1	0
35	V	13	0	11	0	0
35	X	12	0	8	0	0
35	b	76	0	104	3	0
35	c	38	0	52	1	0
35	d	19	0	26	1	0
35	o	19	0	26	0	0
35	u	14	0	19	0	0
35	v	13	0	11	0	0
36	C	176	0	226	5	0
36	D	53	0	71	4	0
36	H	62	0	82	1	0
36	c	177	0	228	1	0
36	e	39	0	47	1	0
36	h	62	0	82	1	0
37	D	144	0	213	4	0
37	E	49	0	74	6	0
37	L	49	0	74	1	0
37	b	49	0	74	2	0
37	d	138	0	198	7	0
37	e	27	0	30	2	0
38	F	43	0	30	2	0
38	V	43	0	30	1	0
38	f	43	0	30	2	0
38	v	43	0	30	0	0
39	H	41	0	56	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	h	41	0	56	3	0
40	J	1	0	0	0	0
40	j	1	0	0	0	0
41	O	5	0	0	0	0
42	A	153	0	0	0	0
42	B	310	0	0	1	0
42	C	237	0	0	5	0
42	D	154	0	0	2	0
42	E	36	0	0	0	0
42	F	17	0	0	0	0
42	H	51	0	0	1	0
42	I	11	0	0	1	0
42	J	10	0	0	0	0
42	K	7	0	0	1	0
42	L	16	0	0	0	0
42	M	17	0	0	0	0
42	O	176	0	0	3	0
42	T	16	0	0	0	0
42	U	90	0	0	3	0
42	V	136	0	0	1	0
42	X	12	0	0	0	0
42	Y	7	0	0	1	0
42	a	156	0	0	0	0
42	b	291	0	0	0	0
42	c	229	0	0	4	0
42	d	157	0	0	0	0
42	e	25	0	0	0	0
42	f	12	0	0	0	0
42	h	40	0	0	0	0
42	i	13	0	0	1	0
42	j	8	0	0	0	0
42	k	7	0	0	0	0
42	l	14	0	0	1	0
42	m	16	0	0	1	0
42	o	154	0	0	0	0
42	t	19	0	0	1	0
42	u	97	0	0	1	0
42	v	97	0	0	1	0
42	x	8	0	0	0	0
42	y	4	0	0	0	0
42	z	3	0	0	0	0
All	All	54054	0	51647	422	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 422 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)
24:b:609:CLA:HHC	24:b:609:CLA:HBB1	1.58	0.85
36:D:406:DGD:HD4	5:E:45:ASP:HB3	1.59	0.83
3:c:320:ARG:HG3	31:c:927:GOL:H2	1.65	0.78
3:c:378:ASN:ND2	42:c:1001:HOH:O	2.18	0.77
24:B:611:CLA:HHC	24:B:611:CLA:HBB1	1.67	0.76

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	335/360 (93%)	331 (99%)	3 (1%)	1 (0%)	36	35
1	a	335/360 (93%)	330 (98%)	4 (1%)	1 (0%)	36	35
2	B	510/505 (101%)	505 (99%)	5 (1%)	0	100	100
2	b	508/505 (101%)	501 (99%)	7 (1%)	0	100	100
3	C	451/473 (95%)	443 (98%)	7 (2%)	1 (0%)	43	42
3	c	457/473 (97%)	446 (98%)	9 (2%)	2 (0%)	30	27
4	D	339/342 (99%)	333 (98%)	6 (2%)	0	100	100
4	d	340/342 (99%)	333 (98%)	7 (2%)	0	100	100
5	E	79/84 (94%)	79 (100%)	0	0	100	100
5	e	77/84 (92%)	77 (100%)	0	0	100	100
6	F	32/45 (71%)	32 (100%)	0	0	100	100
6	f	30/45 (67%)	30 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	H	61/65 (94%)	60 (98%)	1 (2%)	0	100	100
7	h	61/65 (94%)	59 (97%)	2 (3%)	0	100	100
8	I	34/38 (90%)	32 (94%)	2 (6%)	0	100	100
8	i	36/38 (95%)	31 (86%)	5 (14%)	0	100	100
9	J	34/40 (85%)	32 (94%)	1 (3%)	1 (3%)	3	1
9	j	37/40 (92%)	36 (97%)	1 (3%)	0	100	100
10	K	36/37 (97%)	36 (100%)	0	0	100	100
10	k	35/37 (95%)	35 (100%)	0	0	100	100
11	L	36/37 (97%)	36 (100%)	0	0	100	100
11	l	37/37 (100%)	37 (100%)	0	0	100	100
12	M	32/36 (89%)	32 (100%)	0	0	100	100
12	m	34/36 (94%)	34 (100%)	0	0	100	100
13	O	247/244 (101%)	241 (98%)	6 (2%)	0	100	100
13	o	242/244 (99%)	237 (98%)	5 (2%)	0	100	100
14	T	28/32 (88%)	28 (100%)	0	0	100	100
14	t	29/32 (91%)	29 (100%)	0	0	100	100
15	U	95/104 (91%)	92 (97%)	3 (3%)	0	100	100
15	u	96/104 (92%)	93 (97%)	3 (3%)	0	100	100
16	V	136/163 (83%)	134 (98%)	2 (2%)	0	100	100
16	v	136/163 (83%)	133 (98%)	3 (2%)	0	100	100
17	Y	25/30 (83%)	25 (100%)	0	0	100	100
17	y	26/30 (87%)	26 (100%)	0	0	100	100
18	X	37/40 (92%)	36 (97%)	1 (3%)	0	100	100
18	x	37/40 (92%)	36 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
19	z	58/62 (94%)	56 (97%)	1 (2%)	1 (2%)	7	3
20	R	28/34 (82%)	28 (100%)	0	0	100	100
All	All	5246/5508 (95%)	5153 (98%)	86 (2%)	7 (0%)	48	46

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	c	416[A]	SER
3	c	416[B]	SER
9	J	6	GLY
1	A	259	ILE

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	269/290 (93%)	269 (100%)	0	100	100
1	a	269/290 (93%)	268 (100%)	1 (0%)	84	89
2	B	403/403 (100%)	401 (100%)	2 (0%)	81	87
2	b	397/403 (98%)	395 (100%)	2 (0%)	81	87
3	C	353/374 (94%)	349 (99%)	4 (1%)	65	73
3	c	358/374 (96%)	353 (99%)	5 (1%)	59	66
4	D	275/276 (100%)	274 (100%)	1 (0%)	84	89
4	d	277/276 (100%)	275 (99%)	2 (1%)	76	82
5	E	71/73 (97%)	70 (99%)	1 (1%)	59	66
5	e	66/73 (90%)	65 (98%)	1 (2%)	57	64
6	F	27/39 (69%)	27 (100%)	0	100	100
6	f	25/39 (64%)	24 (96%)	1 (4%)	28	27
7	H	53/54 (98%)	53 (100%)	0	100	100
7	h	53/54 (98%)	53 (100%)	0	100	100
8	I	30/34 (88%)	30 (100%)	0	100	100
8	i	33/34 (97%)	33 (100%)	0	100	100
9	J	23/28 (82%)	23 (100%)	0	100	100
9	j	24/28 (86%)	24 (100%)	0	100	100
10	K	28/30 (93%)	28 (100%)	0	100	100
10	k	27/30 (90%)	27 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	L	33/35 (94%)	33 (100%)	0	100	100
11	l	34/35 (97%)	34 (100%)	0	100	100
12	M	29/32 (91%)	28 (97%)	1 (3%)	32	33
12	m	31/32 (97%)	31 (100%)	0	100	100
13	O	204/207 (99%)	204 (100%)	0	100	100
13	o	202/207 (98%)	200 (99%)	2 (1%)	68	75
14	T	25/28 (89%)	25 (100%)	0	100	100
14	t	26/28 (93%)	26 (100%)	0	100	100
15	U	82/89 (92%)	81 (99%)	1 (1%)	63	70
15	u	82/89 (92%)	82 (100%)	0	100	100
16	V	114/138 (83%)	114 (100%)	0	100	100
16	v	112/138 (81%)	111 (99%)	1 (1%)	70	78
17	Y	18/23 (78%)	17 (94%)	1 (6%)	19	16
17	y	18/23 (78%)	18 (100%)	0	100	100
18	X	30/33 (91%)	30 (100%)	0	100	100
18	x	30/33 (91%)	30 (100%)	0	100	100
19	Z	45/52 (86%)	45 (100%)	0	100	100
19	z	41/52 (79%)	40 (98%)	1 (2%)	43	47
20	R	4/29 (14%)	3 (75%)	1 (25%)	0	0
All	All	4221/4505 (94%)	4193 (99%)	28 (1%)	78	82

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	c	21	ILE
20	R	4	ARG
3	c	391[A]	ARG
13	o	182	LEU
3	c	315	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
4	d	301	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
15	u	81	HIS
15	u	78	ASN
1	a	165	GLN
4	d	186	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

10 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	$\# Z > 2$
14	FME	t	1	14	8,9,10	0.69	0	7,9,11	1.38	1 (14%)
12	FME	M	1	12	8,9,10	0.60	0	7,9,11	1.89	3 (42%)
8	FME	I	1	8	8,9,10	0.63	0	7,9,11	1.64	2 (28%)
12	FME	m	1	12	8,9,10	0.70	0	7,9,11	1.81	3 (42%)
4	HSK	D	336[A]	-	9,10,12	5.24	1 (11%)	6,12,16	1.74	2 (33%)
4	HSK	D	336[B]	-	9,11,12	1.92	2 (22%)	6,14,16	3.76	4 (66%)
8	FME	i	1	8	8,9,10	0.58	0	7,9,11	1.48	1 (14%)
4	HSK	d	336[A]	-	9,10,12	13.67	1 (11%)	6,12,16	1.60	2 (33%)
4	HSK	d	336[B]	-	9,11,12	1.69	2 (22%)	6,14,16	4.07	4 (66%)
14	FME	T	1	14	8,9,10	0.68	0	7,9,11	1.54	1 (14%)

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
14	FME	t	1	14	-	3/7/9/11	-
12	FME	M	1	12	-	3/7/9/11	-
8	FME	I	1	8	-	2/7/9/11	-
12	FME	m	1	12	-	3/7/9/11	-
4	HSK	D	336[A]	-	-	0/5/6/8	0/1/1/1
4	HSK	D	336[B]	-	-	0/5/6/8	0/1/1/1
8	FME	i	1	8	-	0/7/9/11	-
4	HSK	d	336[A]	-	-	0/5/6/8	0/1/1/1
4	HSK	d	336[B]	-	-	0/5/6/8	0/1/1/1
14	FME	T	1	14	-	1/7/9/11	-

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	d	336[A]	HSK	OM-ND1	40.87	1.92	1.38
4	D	336[A]	HSK	OM-ND1	-15.34	1.18	1.38
4	D	336[B]	HSK	OM-ND1	4.37	1.44	1.38
4	d	336[B]	HSK	OM-ND1	3.33	1.43	1.38
4	d	336[B]	HSK	CE1-ND1	-2.60	1.32	1.37

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	d	336[B]	HSK	ND1-CE1-NE2	-6.24	103.94	111.75
4	D	336[B]	HSK	ND1-CE1-NE2	-5.79	104.50	111.75
4	d	336[B]	HSK	CE1-ND1-CG	5.77	114.76	107.37
4	D	336[B]	HSK	CE1-ND1-CG	5.55	114.47	107.37
4	d	336[B]	HSK	CD2-NE2-CE1	3.78	109.83	105.22

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	I	1	FME	O1-CN-N-CA
12	M	1	FME	O1-CN-N-CA
12	M	1	FME	CB-CA-N-CN
14	T	1	FME	O1-CN-N-CA
12	m	1	FME	O1-CN-N-CA

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	M	1	FME	1	0
12	m	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 310 ligands modelled in this entry, 15 are monoatomic and 55 are unknown - leaving 240 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	$\# Z > 2$
34	LMT	b	625	-	25,25,36	0.53	1 (4%)	30,30,47	1.11	2 (6%)
31	GOL	f	104	33	5,5,5	0.99	0	5,5,5	0.93	0
24	CLA	c	903	3	69,73,73	2.39	24 (34%)	83,113,113	2.44	29 (34%)
31	GOL	Z	102	-	5,5,5	0.88	0	5,5,5	1.01	0
31	GOL	c	936	-	5,5,5	0.93	0	5,5,5	0.96	0
37	LHG	d	409	-	48,48,48	0.89	2 (4%)	51,54,54	1.02	5 (9%)
21	OEX	A	401	1,42,3	0,14,14	-	-	-	-	-
28	LMG	C	534	-	51,51,55	1.00	3 (5%)	59,59,63	1.31	6 (10%)
31	GOL	B	631	-	5,5,5	0.86	0	5,5,5	0.93	0
26	BCR	c	916	-	41,41,41	0.81	0	56,56,56	1.33	7 (12%)
24	CLA	B	603	2	69,73,73	2.42	23 (33%)	83,113,113	2.50	29 (34%)
24	CLA	b	619	2	69,73,73	2.35	22 (31%)	83,113,113	2.38	25 (30%)
31	GOL	c	934	-	5,5,5	0.82	0	5,5,5	1.12	0
37	LHG	d	408	-	48,48,48	0.90	2 (4%)	51,54,54	1.12	4 (7%)
24	CLA	B	608	42	69,73,73	2.30	22 (31%)	83,113,113	2.47	26 (31%)
26	BCR	T	702	-	41,41,41	0.73	0	56,56,56	1.55	11 (19%)
35	HTG	b	603	-	19,19,19	1.04	2 (10%)	23,24,24	1.08	1 (4%)
25	PHO	A	408	-	58,69,69	2.53	13 (22%)	56,99,99	2.81	14 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	HTG	H	105	-	14,16,19	1.05	1 (7%)	15,18,24	1.43	1 (6%)
31	GOL	O	304	-	5,5,5	0.88	0	5,5,5	1.00	0
31	GOL	V	206	-	5,5,5	0.84	0	5,5,5	1.01	0
24	CLA	B	606	2	69,73,73	2.32	21 (30%)	83,113,113	2.46	24 (28%)
35	HTG	c	923	-	19,19,19	1.04	2 (10%)	23,24,24	1.20	1 (4%)
38	HEM	V	202	16	50,50,50	1.90	8 (16%)	66,82,82	1.47	7 (10%)
31	GOL	c	929	-	5,5,5	0.92	0	5,5,5	1.01	0
24	CLA	d	405	4	69,73,73	2.38	25 (36%)	83,113,113	2.54	30 (36%)
34	LMT	J	102	-	23,23,36	0.61	1 (4%)	28,28,47	0.92	1 (3%)
35	HTG	X	902	-	11,12,19	0.63	0	14,17,24	0.93	1 (7%)
24	CLA	b	607	2	69,73,73	2.42	24 (34%)	83,113,113	2.42	29 (34%)
36	DGD	h	102	-	63,63,67	0.90	3 (4%)	77,77,81	1.00	4 (5%)
34	LMT	c	922	-	36,36,36	0.48	1 (2%)	47,47,47	0.82	2 (4%)
26	BCR	b	623	-	41,41,41	0.70	0	56,56,56	1.36	8 (14%)
31	GOL	b	631	-	5,5,5	0.73	0	5,5,5	1.03	0
24	CLA	D	403	4	69,73,73	2.45	24 (34%)	83,113,113	2.54	31 (37%)
34	LMT	C	520	-	36,36,36	0.47	0	47,47,47	1.23	4 (8%)
24	CLA	b	609	2	69,73,73	2.27	24 (34%)	83,113,113	2.59	28 (33%)
35	HTG	o	301	-	19,19,19	1.11	1 (5%)	23,24,24	1.09	1 (4%)
27	SQD	B	621	-	53,54,54	1.06	4 (7%)	62,65,65	1.53	10 (16%)
35	HTG	C	522	-	19,19,19	0.99	1 (5%)	23,24,24	1.74	4 (17%)
24	CLA	C	501	3	69,73,73	2.36	22 (31%)	83,113,113	2.49	25 (30%)
24	CLA	C	512	3	69,73,73	2.66	23 (33%)	83,113,113	2.54	28 (33%)
24	CLA	b	617	2	69,73,73	2.38	24 (34%)	83,113,113	2.56	28 (33%)
24	CLA	C	513	3	69,73,73	2.53	25 (36%)	83,113,113	2.38	25 (30%)
24	CLA	b	616	2	69,73,73	2.41	22 (31%)	83,113,113	2.50	24 (28%)
24	CLA	c	904	3	69,73,73	2.71	24 (34%)	83,113,113	2.29	26 (31%)
29	PL9	a	417	-	55,55,55	0.64	2 (3%)	68,69,69	1.92	20 (29%)
31	GOL	A	422	-	5,5,5	1.18	1 (20%)	5,5,5	0.94	0
37	LHG	e	101	-	26,26,48	0.95	1 (3%)	28,31,54	1.01	2 (7%)
24	CLA	B	615	2	69,73,73	2.27	21 (30%)	83,113,113	2.72	29 (34%)
31	GOL	C	525	-	5,5,5	1.16	0	5,5,5	0.80	0
31	GOL	a	421	-	5,5,5	1.11	0	5,5,5	0.95	0
27	SQD	A	412	-	51,52,54	0.99	3 (5%)	60,63,65	1.74	12 (20%)
26	BCR	b	621	-	41,41,41	0.82	1 (2%)	56,56,56	1.40	7 (12%)
35	HTG	U	201	-	8,8,19	0.37	0	7,7,24	1.17	1 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	SQD	a	415	-	53,54,54	0.96	3 (5%)	62,65,65	1.74	11 (17%)
24	CLA	C	510	3	69,73,73	2.52	25 (36%)	83,113,113	2.50	30 (36%)
27	SQD	f	102	-	31,32,54	1.97	4 (12%)	34,36,65	1.62	5 (14%)
26	BCR	B	619	-	41,41,41	0.88	0	56,56,56	1.21	9 (16%)
35	HTG	b	602	-	19,19,19	1.09	2 (10%)	23,24,24	1.54	3 (13%)
31	GOL	C	533	-	5,5,5	0.83	0	5,5,5	1.08	0
36	DGD	e	102	-	39,39,67	1.12	2 (5%)	47,47,81	1.70	9 (19%)
26	BCR	k	101	-	41,41,41	0.70	0	56,56,56	1.44	8 (14%)
24	CLA	b	606	2	69,73,73	2.44	23 (33%)	83,113,113	2.41	28 (33%)
24	CLA	b	613	2	69,73,73	2.64	24 (34%)	83,113,113	2.48	31 (37%)
27	SQD	b	601	-	53,54,54	1.05	3 (5%)	62,65,65	1.74	11 (17%)
26	BCR	C	514	-	41,41,41	0.73	0	56,56,56	1.44	8 (14%)
31	GOL	c	937	-	5,5,5	0.94	0	5,5,5	0.90	0
27	SQD	a	401	-	53,54,54	1.02	3 (5%)	62,65,65	1.24	4 (6%)
28	LMG	c	921	-	51,51,55	0.94	2 (3%)	59,59,63	1.25	7 (11%)
36	DGD	c	919	-	61,61,67	0.85	3 (4%)	75,75,81	0.99	4 (5%)
34	LMT	t	904	-	24,24,36	0.57	1 (4%)	29,29,47	0.89	1 (3%)
35	HTG	u	201	-	10,13,19	1.11	1 (10%)	13,14,24	1.60	1 (7%)
24	CLA	a	410	42	69,73,73	2.34	21 (30%)	83,113,113	2.62	30 (36%)
24	CLA	c	914	3	69,73,73	2.47	24 (34%)	83,113,113	2.35	24 (28%)
26	BCR	A	411	-	41,41,41	0.72	0	56,56,56	1.35	6 (10%)
26	BCR	K	101	-	41,41,41	0.74	0	56,56,56	1.44	7 (12%)
28	LMG	A	413	-	51,51,55	0.95	2 (3%)	59,59,63	1.12	5 (8%)
34	LMT	Z	101	-	36,36,36	0.43	0	47,47,47	0.87	0
24	CLA	C	507	42	69,73,73	2.55	25 (36%)	83,113,113	2.51	29 (34%)
35	HTG	C	521	-	19,19,19	0.96	2 (10%)	23,24,24	1.19	1 (4%)
24	CLA	B	604	2	69,73,73	2.38	23 (33%)	83,113,113	2.58	27 (32%)
35	HTG	V	203	-	12,13,19	0.53	0	16,18,24	2.40	4 (25%)
34	LMT	B	623	-	36,36,36	0.43	0	47,47,47	1.29	7 (14%)
24	CLA	c	912	3	69,73,73	2.46	20 (28%)	83,113,113	2.51	32 (38%)
24	CLA	c	908	42	69,73,73	2.48	24 (34%)	83,113,113	2.50	28 (33%)
24	CLA	B	614	2	69,73,73	2.33	22 (31%)	83,113,113	2.56	29 (34%)
24	CLA	D	402	4	69,73,73	2.11	23 (33%)	83,113,113	2.66	30 (36%)
31	GOL	b	640	-	5,5,5	0.90	0	5,5,5	1.07	0
31	GOL	C	530	-	5,5,5	1.00	0	5,5,5	1.05	0
31	GOL	c	938	-	5,5,5	0.96	0	5,5,5	1.05	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	c	905	42	69,73,73	2.34	25 (36%)	83,113,113	2.69	29 (34%)
24	CLA	c	907	3	69,73,73	2.66	25 (36%)	83,113,113	2.37	28 (33%)
26	BCR	b	622	-	41,41,41	0.79	0	56,56,56	1.17	7 (12%)
34	LMT	T	703	-	24,24,36	0.44	0	29,29,47	1.35	2 (6%)
24	CLA	C	503	3	69,73,73	2.55	24 (34%)	83,113,113	2.39	26 (31%)
31	GOL	c	926	-	5,5,5	1.03	0	5,5,5	0.83	0
31	GOL	V	201	33	5,5,5	0.78	0	5,5,5	1.04	0
34	LMT	a	402	-	36,36,36	0.50	1 (2%)	47,47,47	0.95	2 (4%)
26	BCR	B	620	-	41,41,41	0.74	0	56,56,56	1.25	3 (5%)
24	CLA	b	614	42	69,73,73	2.30	22 (31%)	83,113,113	2.49	27 (32%)
28	LMG	B	622	-	51,51,55	0.95	2 (3%)	59,59,63	1.14	4 (6%)
29	PL9	D	405	-	55,55,55	0.75	2 (3%)	68,69,69	1.53	15 (22%)
34	LMT	M	303	-	36,36,36	0.42	0	47,47,47	0.90	0
31	GOL	o	303	-	5,5,5	0.85	0	5,5,5	0.90	0
31	GOL	u	203	-	5,5,5	1.04	0	5,5,5	0.91	0
26	BCR	c	915	-	41,41,41	0.75	0	56,56,56	1.43	8 (14%)
31	GOL	L	102	-	5,5,5	1.12	0	5,5,5	1.01	0
24	CLA	C	502	3	69,73,73	2.58	24 (34%)	83,113,113	2.37	26 (31%)
35	HTG	B	627	-	19,19,19	0.99	1 (5%)	23,24,24	1.45	2 (8%)
37	LHG	d	410	-	39,39,48	1.04	2 (5%)	42,45,54	0.97	3 (7%)
25	PHO	A	409	-	58,69,69	2.66	13 (22%)	56,99,99	2.91	14 (25%)
24	CLA	C	504	42	69,73,73	2.42	24 (34%)	83,113,113	2.48	25 (30%)
31	GOL	O	305	-	5,5,5	0.84	0	5,5,5	1.04	0
37	LHG	L	101	-	48,48,48	0.91	3 (6%)	51,54,54	0.95	2 (3%)
24	CLA	b	611	42	69,73,73	2.39	24 (34%)	83,113,113	2.47	30 (36%)
24	CLA	b	620	2	69,73,73	2.39	22 (31%)	83,113,113	2.49	26 (31%)
24	CLA	B	613	2	69,73,73	2.22	22 (31%)	83,113,113	2.58	24 (28%)
24	CLA	B	607	2	69,73,73	2.40	22 (31%)	83,113,113	2.54	31 (37%)
24	CLA	B	616	2	69,73,73	2.50	22 (31%)	83,113,113	2.49	26 (31%)
35	HTG	b	627	-	19,19,19	1.03	1 (5%)	23,24,24	1.74	2 (8%)
36	DGD	H	103	-	63,63,67	0.90	3 (4%)	77,77,81	0.89	2 (2%)
31	GOL	o	304	-	5,5,5	0.90	0	5,5,5	1.00	0
31	GOL	t	902	-	5,5,5	1.06	0	5,5,5	1.07	0
34	LMT	D	401	-	36,36,36	0.43	0	47,47,47	0.95	0
28	LMG	D	410	40	48,48,55	0.84	2 (4%)	56,56,63	0.99	3 (5%)
28	LMG	a	416	-	51,51,55	0.90	2 (3%)	59,59,63	1.23	4 (6%)
35	HTG	B	625	-	19,19,19	0.98	1 (5%)	23,24,24	1.82	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	HTG	b	626	-	19,19,19	0.83	1 (5%)	23,24,24	1.42	1 (4%)
21	OEX	a	404	1,42,3	0,14,14	-	-	-		
31	GOL	B	633	-	5,5,5	1.42	1 (20%)	5,5,5	0.95	0
31	GOL	a	419	-	5,5,5	1.01	0	5,5,5	1.02	0
24	CLA	b	605	42	69,73,73	2.50	24 (34%)	83,113,113	2.37	25 (30%)
24	CLA	A	405	1	69,73,73	2.39	23 (33%)	83,113,113	2.46	27 (32%)
25	PHO	a	411	-	58,69,69	2.52	12 (20%)	56,99,99	2.77	14 (25%)
27	SQD	F	101	-	36,37,54	1.00	2 (5%)	44,47,65	1.46	6 (13%)
31	GOL	B	629	-	5,5,5	1.02	0	5,5,5	0.93	0
31	GOL	V	204	-	5,5,5	1.40	2 (40%)	5,5,5	0.92	0
34	LMT	F	103	-	27,27,36	0.54	1 (3%)	37,38,47	0.89	0
28	LMG	C	519	-	49,49,55	0.96	2 (4%)	57,57,63	1.17	6 (10%)
31	GOL	b	630	-	5,5,5	0.92	0	5,5,5	0.93	0
37	LHG	E	101	-	48,48,48	0.96	2 (4%)	51,54,54	1.00	2 (3%)
31	GOL	b	632	-	5,5,5	1.02	0	5,5,5	1.18	1 (20%)
31	GOL	B	632	-	5,5,5	0.49	0	5,5,5	1.13	0
26	BCR	y	101	-	41,41,41	0.74	1 (2%)	56,56,56	1.59	10 (17%)
32	BCT	A	421	22	2,3,3	0.65	0	2,3,3	0.66	0
24	CLA	c	909	3	69,73,73	2.52	25 (36%)	83,113,113	2.49	27 (32%)
36	DGD	C	518	-	59,59,67	0.90	2 (3%)	73,73,81	1.08	4 (5%)
24	CLA	b	612	2	69,73,73	2.60	24 (34%)	83,113,113	2.42	28 (33%)
28	LMG	d	411	40	48,48,55	0.95	2 (4%)	56,56,63	0.91	3 (5%)
31	GOL	O	306	-	5,5,5	0.90	0	5,5,5	0.98	0
31	GOL	c	939	-	5,5,5	0.90	0	5,5,5	1.19	1 (20%)
31	GOL	a	420	-	5,5,5	0.85	0	5,5,5	1.09	1 (20%)
31	GOL	b	629	-	5,5,5	0.91	0	5,5,5	0.98	0
34	LMT	m	1502	-	36,36,36	0.49	0	47,47,47	0.90	1 (2%)
31	GOL	b	638	-	5,5,5	0.83	0	5,5,5	1.07	0
36	DGD	C	517	-	57,57,67	0.88	2 (3%)	71,71,81	0.97	4 (5%)
26	BCR	t	903	-	41,41,41	0.73	0	56,56,56	1.62	15 (26%)
37	LHG	D	407	-	48,48,48	0.84	2 (4%)	51,54,54	1.16	3 (5%)
35	HTG	d	403	-	19,19,19	1.10	2 (10%)	23,24,24	1.39	2 (8%)
37	LHG	b	639	-	48,48,48	0.91	3 (6%)	51,54,54	0.90	3 (5%)
35	HTG	O	303	-	19,19,19	1.06	1 (5%)	23,24,24	1.03	2 (8%)
24	CLA	d	404	4	69,73,73	2.40	24 (34%)	83,113,113	2.54	28 (33%)
26	BCR	Y	101	-	41,41,41	0.79	0	56,56,56	1.57	8 (14%)
31	GOL	V	205	-	5,5,5	0.94	0	5,5,5	0.94	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	SQD	A	417	-	53,54,54	1.05	3 (5%)	62,65,65	1.24	8 (12%)
31	GOL	c	928	-	5,5,5	0.83	0	5,5,5	1.05	1 (20%)
26	BCR	C	515	-	41,41,41	0.71	0	56,56,56	1.38	5 (8%)
41	SO4	O	302	-	4,4,4	0.19	0	6,6,6	0.08	0
32	BCT	a	408	22	2,3,3	0.61	0	2,3,3	0.64	0
24	CLA	c	906	3	69,73,73	2.47	24 (34%)	83,113,113	2.45	26 (31%)
34	LMT	M	302	-	36,36,36	0.56	1 (2%)	47,47,47	0.93	2 (4%)
39	RRX	h	101	-	42,42,42	0.72	0	57,58,58	1.33	7 (12%)
31	GOL	A	420	-	5,5,5	1.09	0	5,5,5	0.94	0
37	LHG	D	408	-	48,48,48	0.88	2 (4%)	51,54,54	1.04	4 (7%)
31	GOL	b	628	-	5,5,5	0.72	0	5,5,5	1.17	1 (20%)
31	GOL	B	628	-	5,5,5	0.79	0	5,5,5	0.88	0
38	HEM	F	102	6,5	50,50,50	1.88	10 (20%)	66,82,82	1.53	10 (15%)
31	GOL	h	103	-	5,5,5	0.90	0	5,5,5	0.97	0
31	GOL	c	932	-	5,5,5	0.75	0	5,5,5	1.14	1 (20%)
28	LMG	b	624	-	51,51,55	0.90	2 (3%)	59,59,63	1.19	4 (6%)
24	CLA	a	413	1	69,73,73	2.27	22 (31%)	83,113,113	2.55	29 (34%)
36	DGD	c	918	-	56,56,67	0.93	2 (3%)	70,70,81	0.98	1 (1%)
24	CLA	d	401	42	69,73,73	2.28	23 (33%)	83,113,113	2.79	35 (42%)
24	CLA	a	409	1	69,73,73	2.32	23 (33%)	83,113,113	2.57	27 (32%)
39	RRX	H	102	-	42,42,42	0.72	0	57,58,58	1.35	6 (10%)
29	PL9	d	407	-	55,55,55	0.71	1 (1%)	68,69,69	1.47	13 (19%)
24	CLA	B	610	2	69,73,73	2.44	21 (30%)	83,113,113	2.44	29 (34%)
24	CLA	C	509	3	69,73,73	2.46	24 (34%)	83,113,113	2.42	27 (32%)
24	CLA	b	615	2	69,73,73	2.48	23 (33%)	83,113,113	2.53	30 (36%)
26	BCR	d	406	-	41,41,41	0.77	0	56,56,56	1.82	13 (23%)
24	CLA	A	406	42	69,73,73	2.26	22 (31%)	83,113,113	2.60	28 (33%)
25	PHO	a	412	-	58,69,69	2.65	12 (20%)	56,99,99	2.77	13 (23%)
35	HTG	B	624	-	19,19,19	0.81	1 (5%)	23,24,24	1.36	1 (4%)
31	GOL	H	101	-	5,5,5	0.98	0	5,5,5	1.08	0
24	CLA	C	508	3	69,73,73	2.47	24 (34%)	83,113,113	2.42	24 (28%)
35	HTG	B	626	-	19,19,19	1.05	2 (10%)	23,24,24	1.51	4 (17%)
36	DGD	c	917	-	63,63,67	0.79	2 (3%)	77,77,81	1.11	6 (7%)
24	CLA	c	913	3	69,73,73	2.55	24 (34%)	83,113,113	2.60	29 (34%)
28	LMG	c	920	-	51,51,55	0.95	2 (3%)	59,59,63	1.04	2 (3%)
24	CLA	B	605	2	69,73,73	2.63	23 (33%)	83,113,113	2.55	26 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	DGD	C	516	-	63,63,67	0.83	2 (3%)	77,77,81	1.05	6 (7%)
24	CLA	c	902	3	69,73,73	2.40	23 (33%)	83,113,113	2.62	27 (32%)
31	GOL	v	201	-	5,5,5	0.82	0	5,5,5	1.06	0
31	GOL	B	630	-	5,5,5	1.21	1 (20%)	5,5,5	0.45	0
38	HEM	v	202	16	50,50,50	1.84	9 (18%)	66,82,82	1.44	7 (10%)
31	GOL	v	203	-	5,5,5	1.19	0	5,5,5	0.79	0
24	CLA	B	612	2	69,73,73	2.28	22 (31%)	83,113,113	2.53	27 (32%)
31	GOL	C	531	-	5,5,5	0.89	0	5,5,5	1.19	0
24	CLA	B	617	2	69,73,73	2.30	23 (33%)	83,113,113	2.60	27 (32%)
31	GOL	C	524	-	5,5,5	0.89	0	5,5,5	1.03	0
34	LMT	m	1503	-	36,36,36	0.60	1 (2%)	47,47,47	1.09	4 (8%)
24	CLA	B	611	42	69,73,73	2.44	24 (34%)	83,113,113	2.51	30 (36%)
24	CLA	b	610	2	69,73,73	2.36	22 (31%)	83,113,113	2.44	25 (30%)
26	BCR	a	414	-	41,41,41	0.76	0	56,56,56	1.19	3 (5%)
38	HEM	f	101	6,5	50,50,50	1.89	9 (18%)	66,82,82	1.45	7 (10%)
31	GOL	c	927	-	5,5,5	1.12	0	5,5,5	1.11	1 (20%)
24	CLA	b	618	2	69,73,73	2.31	21 (30%)	83,113,113	2.67	31 (37%)
26	BCR	D	404	-	41,41,41	0.80	0	56,56,56	1.70	9 (16%)
31	GOL	A	419	-	5,5,5	0.83	0	5,5,5	1.26	1 (20%)
26	BCR	B	618	-	41,41,41	0.73	0	56,56,56	1.33	4 (7%)
31	GOL	u	202	-	5,5,5	0.92	0	5,5,5	0.89	0
24	CLA	c	911	3	69,73,73	2.39	23 (33%)	83,113,113	2.46	31 (37%)
31	GOL	v	204	-	5,5,5	0.77	0	5,5,5	1.07	0
29	PL9	A	414	-	55,55,55	0.62	2 (3%)	68,69,69	1.91	20 (29%)
24	CLA	B	609	2	69,73,73	2.38	24 (34%)	83,113,113	2.46	27 (32%)
35	HTG	C	528	-	19,19,19	1.11	2 (10%)	23,24,24	1.59	4 (17%)
35	HTG	c	924	-	19,19,19	0.99	2 (10%)	23,24,24	1.69	3 (13%)
37	LHG	D	409	-	45,45,48	0.93	2 (4%)	48,51,54	1.03	4 (8%)
24	CLA	A	407	42	69,73,73	2.20	22 (31%)	83,113,113	2.61	29 (34%)
24	CLA	A	410	1	69,73,73	2.24	24 (34%)	83,113,113	2.63	29 (34%)
24	CLA	b	608	2	69,73,73	2.69	24 (34%)	83,113,113	2.51	30 (36%)
24	CLA	C	511	3	69,73,73	2.48	23 (33%)	83,113,113	2.41	27 (32%)
24	CLA	C	505	3	69,73,73	2.61	25 (36%)	83,113,113	2.31	24 (28%)
24	CLA	C	506	3	69,73,73	2.54	25 (36%)	83,113,113	2.41	29 (34%)
24	CLA	B	602	42	69,73,73	2.61	26 (37%)	83,113,113	2.38	25 (30%)
35	HTG	v	205	-	12,13,19	0.75	0	16,18,24	1.64	5 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	DGD	D	406	-	53,53,67	0.98	2 (3%)	60,61,81	1.32	7 (11%)
24	CLA	c	910	3	69,73,73	2.58	26 (37%)	83,113,113	2.34	27 (32%)
34	LMT	z	101	-	32,32,36	0.49	0	42,42,47	0.92	1 (2%)
31	GOL	C	527	-	5,5,5	0.82	0	5,5,5	1.14	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
34	LMT	b	625	-	-	4/17/37/61	0/1/1/2
31	GOL	f	104	33	-	2/4/4/4	-
24	CLA	c	903	3	-	3/39/115/115	-
31	GOL	Z	102	-	-	0/4/4/4	-
31	GOL	c	936	-	-	2/4/4/4	-
37	LHG	d	409	-	-	11/53/53/53	-
28	LMG	C	534	-	-	9/46/66/70	0/1/1/1
31	GOL	B	631	-	-	2/4/4/4	-
26	BCR	c	916	-	-	2/29/63/63	0/2/2/2
24	CLA	B	603	2	-	5/39/115/115	-
24	CLA	b	619	2	-	9/39/115/115	-
31	GOL	c	934	-	-	4/4/4/4	-
37	LHG	d	408	-	-	6/53/53/53	-
24	CLA	B	608	42	-	1/39/115/115	-
26	BCR	T	702	-	-	1/29/63/63	0/2/2/2
35	HTG	b	603	-	-	1/10/30/30	0/1/1/1
25	PHO	A	408	-	-	4/37/103/103	0/5/6/6
35	HTG	H	105	-	-	3/10/20/30	0/1/1/1
31	GOL	O	304	-	-	0/4/4/4	-
31	GOL	V	206	-	-	0/4/4/4	-
24	CLA	B	606	2	-	4/39/115/115	-
35	HTG	c	923	-	-	1/10/30/30	0/1/1/1
38	HEM	V	202	16	-	4/14/54/54	-
31	GOL	c	929	-	-	2/4/4/4	-
24	CLA	d	405	4	-	8/39/115/115	-
34	LMT	J	102	-	-	3/13/33/61	0/1/1/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	HTG	X	902	-	-	2/2/22/30	0/1/1/1
24	CLA	b	607	2	-	5/39/115/115	-
36	DGD	h	102	-	-	5/51/91/95	0/2/2/2
34	LMT	c	922	-	-	2/21/61/61	0/2/2/2
26	BCR	b	623	-	-	2/29/63/63	0/2/2/2
31	GOL	b	631	-	-	2/4/4/4	-
24	CLA	D	403	4	-	8/39/115/115	-
34	LMT	C	520	-	-	8/21/61/61	0/2/2/2
24	CLA	b	609	2	-	3/39/115/115	-
35	HTG	o	301	-	-	1/10/30/30	0/1/1/1
27	SQD	B	621	-	-	25/49/69/69	0/1/1/1
35	HTG	C	522	-	-	2/10/30/30	0/1/1/1
24	CLA	C	501	3	-	4/39/115/115	-
24	CLA	C	512	3	-	8/39/115/115	-
24	CLA	b	617	2	-	3/39/115/115	-
24	CLA	C	513	3	-	5/39/115/115	-
24	CLA	b	616	2	-	3/39/115/115	-
24	CLA	c	904	3	-	5/39/115/115	-
29	PL9	a	417	-	-	10/53/73/73	0/1/1/1
31	GOL	A	422	-	-	2/4/4/4	-
37	LHG	e	101	-	-	3/30/30/53	-
24	CLA	B	615	2	-	5/39/115/115	-
31	GOL	C	525	-	-	0/4/4/4	-
31	GOL	a	421	-	-	4/4/4/4	-
27	SQD	A	412	-	-	10/47/67/69	0/1/1/1
26	BCR	b	621	-	-	2/29/63/63	0/2/2/2
35	HTG	U	201	-	-	1/6/6/30	-
27	SQD	a	415	-	-	10/49/69/69	0/1/1/1
24	CLA	C	510	3	-	6/39/115/115	-
27	SQD	f	102	-	-	11/33/33/69	-
26	BCR	B	619	-	-	0/29/63/63	0/2/2/2
35	HTG	b	602	-	-	2/10/30/30	0/1/1/1
31	GOL	C	533	-	-	2/4/4/4	-
36	DGD	e	102	-	-	4/33/53/95	0/1/1/2
26	BCR	k	101	-	-	1/29/63/63	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	b	606	2	-	3/39/115/115	-
24	CLA	b	613	2	-	4/39/115/115	-
27	SQD	b	601	-	-	28/49/69/69	0/1/1/1
26	BCR	C	514	-	-	3/29/63/63	0/2/2/2
31	GOL	c	937	-	-	2/4/4/4	-
27	SQD	a	401	-	-	14/49/69/69	0/1/1/1
28	LMG	c	921	-	-	4/46/66/70	0/1/1/1
36	DGD	c	919	-	-	6/49/89/95	0/2/2/2
34	LMT	t	904	-	-	9/15/35/61	0/1/1/2
35	HTG	u	201	-	-	6/12/14/30	-
24	CLA	a	410	42	-	6/39/115/115	-
24	CLA	c	914	3	-	3/39/115/115	-
26	BCR	A	411	-	-	0/29/63/63	0/2/2/2
26	BCR	K	101	-	-	1/29/63/63	0/2/2/2
28	LMG	A	413	-	-	17/46/66/70	0/1/1/1
34	LMT	Z	101	-	-	10/21/61/61	0/2/2/2
24	CLA	C	507	42	-	5/39/115/115	-
35	HTG	C	521	-	-	1/10/30/30	0/1/1/1
24	CLA	B	604	2	-	4/39/115/115	-
35	HTG	V	203	-	-	1/4/24/30	0/1/1/1
34	LMT	B	623	-	-	10/21/61/61	0/2/2/2
24	CLA	c	912	3	-	1/39/115/115	-
24	CLA	c	908	42	-	8/39/115/115	-
24	CLA	B	614	2	-	6/39/115/115	-
24	CLA	D	402	4	-	3/39/115/115	-
31	GOL	b	640	-	-	0/4/4/4	-
31	GOL	C	530	-	-	0/4/4/4	-
31	GOL	c	938	-	-	2/4/4/4	-
24	CLA	c	905	42	-	7/39/115/115	-
24	CLA	c	907	3	-	6/39/115/115	-
26	BCR	b	622	-	-	0/29/63/63	0/2/2/2
34	LMT	T	703	-	-	12/15/35/61	0/1/1/2
24	CLA	C	503	3	-	4/39/115/115	-
31	GOL	c	926	-	-	2/4/4/4	-
31	GOL	V	201	33	-	3/4/4/4	-
34	LMT	a	402	-	-	6/21/61/61	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	BCR	B	620	-	-	0/29/63/63	0/2/2/2
24	CLA	b	614	42	-	8/39/115/115	-
28	LMG	B	622	-	-	10/46/66/70	0/1/1/1
29	PL9	D	405	-	-	3/53/73/73	0/1/1/1
34	LMT	M	303	-	-	1/21/61/61	0/2/2/2
31	GOL	o	303	-	-	2/4/4/4	-
31	GOL	u	203	-	-	0/4/4/4	-
26	BCR	c	915	-	-	1/29/63/63	0/2/2/2
31	GOL	L	102	-	-	0/4/4/4	-
24	CLA	C	502	3	-	7/39/115/115	-
35	HTG	B	627	-	-	1/10/30/30	0/1/1/1
37	LHG	d	410	-	-	10/44/44/53	-
25	PHO	A	409	-	-	3/37/103/103	0/5/6/6
24	CLA	C	504	42	-	7/39/115/115	-
31	GOL	O	305	-	-	2/4/4/4	-
37	LHG	L	101	-	-	8/53/53/53	-
24	CLA	b	611	42	-	1/39/115/115	-
24	CLA	b	620	2	-	7/39/115/115	-
24	CLA	B	613	2	-	4/39/115/115	-
24	CLA	B	607	2	-	5/39/115/115	-
24	CLA	B	616	2	-	10/39/115/115	-
35	HTG	b	627	-	-	3/10/30/30	0/1/1/1
36	DGD	H	103	-	-	4/51/91/95	0/2/2/2
31	GOL	o	304	-	-	2/4/4/4	-
31	GOL	t	902	-	-	1/4/4/4	-
34	LMT	D	401	-	-	5/21/61/61	0/2/2/2
28	LMG	D	410	40	-	7/43/63/70	0/1/1/1
28	LMG	a	416	-	-	13/46/66/70	0/1/1/1
35	HTG	B	625	-	-	3/10/30/30	0/1/1/1
35	HTG	b	626	-	-	2/10/30/30	0/1/1/1
31	GOL	a	419	-	-	1/4/4/4	-
31	GOL	B	633	-	-	0/4/4/4	-
24	CLA	b	605	42	-	8/39/115/115	-
24	CLA	A	405	1	-	4/39/115/115	-
25	PHO	a	411	-	-	5/37/103/103	0/5/6/6
27	SQD	F	101	-	-	9/30/50/69	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	GOL	B	629	-	-	0/4/4/4	-
31	GOL	V	204	-	-	1/4/4/4	-
34	LMT	F	103	-	-	2/12/52/61	0/2/2/2
28	LMG	C	519	-	-	9/44/64/70	0/1/1/1
31	GOL	b	630	-	-	0/4/4/4	-
37	LHG	E	101	-	-	16/53/53/53	-
31	GOL	b	632	-	-	2/4/4/4	-
31	GOL	B	632	-	-	0/4/4/4	-
26	BCR	y	101	-	-	5/29/63/63	0/2/2/2
36	DGD	C	518	-	-	4/47/87/95	0/2/2/2
24	CLA	c	909	3	-	3/39/115/115	-
24	CLA	b	612	2	-	2/39/115/115	-
28	LMG	d	411	40	-	11/43/63/70	0/1/1/1
31	GOL	O	306	-	-	2/4/4/4	-
31	GOL	c	939	-	-	0/4/4/4	-
31	GOL	a	420	-	-	2/4/4/4	-
31	GOL	b	629	-	-	2/4/4/4	-
34	LMT	m	1502	-	-	1/21/61/61	0/2/2/2
31	GOL	b	638	-	-	2/4/4/4	-
36	DGD	C	517	-	-	13/45/85/95	0/2/2/2
26	BCR	t	903	-	-	1/29/63/63	0/2/2/2
37	LHG	D	407	-	-	6/53/53/53	-
35	HTG	d	403	-	-	2/10/30/30	0/1/1/1
37	LHG	b	639	-	-	9/53/53/53	-
35	HTG	O	303	-	-	1/10/30/30	0/1/1/1
24	CLA	d	404	4	-	3/39/115/115	-
26	BCR	Y	101	-	-	5/29/63/63	0/2/2/2
31	GOL	V	205	-	-	0/4/4/4	-
27	SQD	A	417	-	-	12/49/69/69	0/1/1/1
31	GOL	c	928	-	-	0/4/4/4	-
26	BCR	C	515	-	-	1/29/63/63	0/2/2/2
24	CLA	c	906	3	-	5/39/115/115	-
34	LMT	M	302	-	-	7/21/61/61	0/2/2/2
39	RRX	h	101	-	-	2/29/65/65	0/2/2/2
31	GOL	A	420	-	-	2/4/4/4	-
37	LHG	D	408	-	-	8/53/53/53	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	GOL	b	628	-	-	2/4/4/4	-
31	GOL	B	628	-	-	2/4/4/4	-
38	HEM	F	102	6,5	-	1/14/54/54	-
31	GOL	h	103	-	-	0/4/4/4	-
31	GOL	c	932	-	-	2/4/4/4	-
28	LMG	b	624	-	-	14/46/66/70	0/1/1/1
24	CLA	a	413	1	-	8/39/115/115	-
36	DGD	c	918	-	-	7/44/84/95	0/2/2/2
24	CLA	d	401	42	-	6/39/115/115	-
24	CLA	a	409	1	-	5/39/115/115	-
39	RRX	H	102	-	-	2/29/65/65	0/2/2/2
29	PL9	d	407	-	-	3/53/73/73	0/1/1/1
24	CLA	B	610	2	-	3/39/115/115	-
24	CLA	C	509	3	-	5/39/115/115	-
24	CLA	b	615	2	-	6/39/115/115	-
26	BCR	d	406	-	-	8/29/63/63	0/2/2/2
24	CLA	A	406	42	-	4/39/115/115	-
25	PHO	a	412	-	-	3/37/103/103	0/5/6/6
35	HTG	B	624	-	-	4/10/30/30	0/1/1/1
31	GOL	H	101	-	-	0/4/4/4	-
24	CLA	C	508	3	-	5/39/115/115	-
35	HTG	B	626	-	-	3/10/30/30	0/1/1/1
36	DGD	c	917	-	-	15/51/91/95	0/2/2/2
24	CLA	c	913	3	-	7/39/115/115	-
28	LMG	c	920	-	-	5/46/66/70	0/1/1/1
24	CLA	B	605	2	-	5/39/115/115	-
36	DGD	C	516	-	-	11/51/91/95	0/2/2/2
24	CLA	c	902	3	-	4/39/115/115	-
31	GOL	v	201	-	-	2/4/4/4	-
31	GOL	B	630	-	-	4/4/4/4	-
38	HEM	v	202	16	-	4/14/54/54	-
31	GOL	v	203	-	-	1/4/4/4	-
24	CLA	B	612	2	-	1/39/115/115	-
31	GOL	C	531	-	-	0/4/4/4	-
24	CLA	B	617	2	-	8/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	GOL	C	524	-	-	0/4/4/4	-
34	LMT	m	1503	-	-	2/21/61/61	0/2/2/2
24	CLA	B	611	42	-	2/39/115/115	-
24	CLA	b	610	2	-	6/39/115/115	-
26	BCR	a	414	-	-	1/29/63/63	0/2/2/2
38	HEM	f	101	6,5	-	1/14/54/54	-
31	GOL	c	927	-	-	0/4/4/4	-
24	CLA	b	618	2	-	11/39/115/115	-
26	BCR	D	404	-	-	8/29/63/63	0/2/2/2
31	GOL	A	419	-	-	1/4/4/4	-
26	BCR	B	618	-	-	2/29/63/63	0/2/2/2
31	GOL	u	202	-	-	3/4/4/4	-
24	CLA	c	911	3	-	4/39/115/115	-
31	GOL	v	204	-	-	0/4/4/4	-
29	PL9	A	414	-	-	9/53/73/73	0/1/1/1
24	CLA	B	609	2	-	1/39/115/115	-
35	HTG	C	528	-	-	0/10/30/30	0/1/1/1
35	HTG	c	924	-	-	3/10/30/30	0/1/1/1
37	LHG	D	409	-	-	8/50/50/53	-
24	CLA	A	407	42	-	2/39/115/115	-
24	CLA	A	410	1	-	4/39/115/115	-
24	CLA	b	608	2	-	2/39/115/115	-
24	CLA	C	511	3	-	1/39/115/115	-
24	CLA	C	505	3	-	3/39/115/115	-
24	CLA	C	506	3	-	9/39/115/115	-
24	CLA	B	602	42	-	14/39/115/115	-
35	HTG	v	205	-	-	1/4/24/30	0/1/1/1
36	DGD	D	406	-	-	14/47/68/95	0/1/1/2
24	CLA	c	910	3	-	8/39/115/115	-
34	LMT	z	101	-	-	5/15/55/61	0/2/2/2
31	GOL	C	527	-	-	2/4/4/4	-

The worst 5 of 1854 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	605	CLA	MG-ND	-10.48	1.85	2.05
24	C	503	CLA	MG-NA	9.73	2.29	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	507	CLA	MG-NA	9.35	2.28	2.06
25	a	412	PHO	C1D-C2D	9.32	1.49	1.39
24	c	904	CLA	MG-NA	9.27	2.28	2.06

The worst 5 of 2540 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	D	402	CLA	C1D-ND-C4D	-10.22	99.07	106.33
24	d	401	CLA	C1D-ND-C4D	-10.22	99.08	106.33
24	c	902	CLA	C1D-ND-C4D	-10.01	99.22	106.33
24	B	613	CLA	C1D-ND-C4D	-10.00	99.23	106.33
24	B	605	CLA	C1D-ND-C4D	-9.96	99.26	106.33

There are no chirality outliers.

5 of 1039 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	A	406	CLA	CHA-CBD-CGD-O1D
24	B	602	CLA	C11-C10-C8-C9
24	B	606	CLA	C2-C3-C5-C6
24	B	606	CLA	C4-C3-C5-C6
24	B	607	CLA	CHA-CBD-CGD-O1D

There are no ring outliers.

158 monomers are involved in 284 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	b	625	LMT	1	0
24	c	903	CLA	1	0
31	c	936	GOL	1	0
37	d	409	LHG	2	0
28	C	534	LMG	1	0
26	c	916	BCR	2	0
24	b	619	CLA	4	0
37	d	408	LHG	1	0
24	B	608	CLA	1	0
26	T	702	BCR	5	0
35	b	603	HTG	1	0
25	A	408	PHO	1	0
35	H	105	HTG	1	0
24	B	606	CLA	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	V	202	HEM	1	0
31	c	929	GOL	1	0
24	d	405	CLA	2	0
24	b	607	CLA	2	0
36	h	102	DGD	1	0
26	b	623	BCR	2	0
24	D	403	CLA	1	0
34	C	520	LMT	4	0
24	b	609	CLA	4	0
27	B	621	SQD	1	0
24	C	501	CLA	5	0
24	C	512	CLA	6	0
24	b	617	CLA	3	0
24	C	513	CLA	7	0
24	b	616	CLA	1	0
24	c	904	CLA	4	0
29	a	417	PL9	5	0
31	A	422	GOL	1	0
37	e	101	LHG	2	0
24	B	615	CLA	8	0
27	A	412	SQD	2	0
26	b	621	BCR	2	0
35	U	201	HTG	1	0
27	a	415	SQD	6	0
24	C	510	CLA	2	0
27	f	102	SQD	1	0
26	B	619	BCR	5	0
36	e	102	DGD	1	0
26	k	101	BCR	2	0
24	b	606	CLA	1	0
24	b	613	CLA	2	0
27	b	601	SQD	1	0
26	C	514	BCR	2	0
31	c	937	GOL	1	0
27	a	401	SQD	1	0
28	c	921	LMG	1	0
36	c	919	DGD	1	0
24	c	914	CLA	5	0
26	K	101	BCR	1	0
28	A	413	LMG	2	0
34	Z	101	LMT	1	0
24	C	507	CLA	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	C	521	HTG	3	0
24	B	604	CLA	2	0
34	B	623	LMT	1	0
24	c	912	CLA	3	0
24	c	908	CLA	3	0
24	B	614	CLA	3	0
24	D	402	CLA	1	0
31	C	530	GOL	1	0
24	c	905	CLA	1	0
24	c	907	CLA	3	0
26	b	622	BCR	3	0
24	C	503	CLA	3	0
31	c	926	GOL	2	0
34	a	402	LMT	1	0
26	B	620	BCR	1	0
24	b	614	CLA	3	0
28	B	622	LMG	4	0
34	M	303	LMT	1	0
26	c	915	BCR	3	0
24	C	502	CLA	4	0
37	d	410	LHG	4	0
25	A	409	PHO	2	0
24	C	504	CLA	1	0
37	L	101	LHG	1	0
24	b	620	CLA	3	0
24	B	613	CLA	2	0
24	B	607	CLA	2	0
24	B	616	CLA	4	0
35	b	627	HTG	1	0
36	H	103	DGD	1	0
28	D	410	LMG	3	0
28	a	416	LMG	2	0
35	b	626	HTG	1	0
24	b	605	CLA	3	0
24	A	405	CLA	3	0
27	F	101	SQD	1	0
28	C	519	LMG	1	0
37	E	101	LHG	6	0
26	y	101	BCR	2	0
24	c	909	CLA	3	0
36	C	518	DGD	1	0
31	O	306	GOL	1	0

Continued on next page...

Continued from previous page...

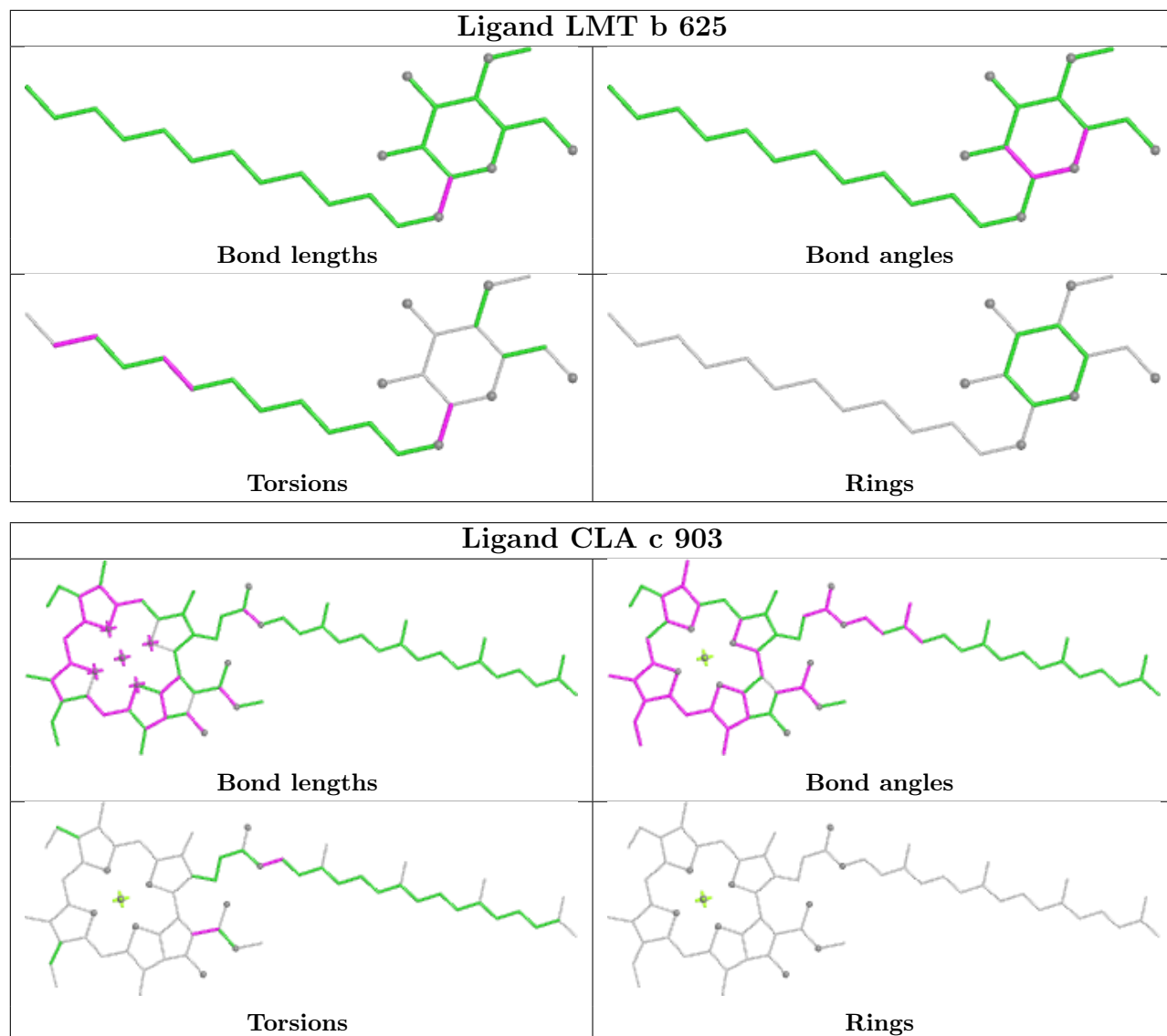
Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	a	420	GOL	1	0
34	m	1502	LMT	1	0
36	C	517	DGD	3	0
26	t	903	BCR	6	0
35	d	403	HTG	1	0
37	b	639	LHG	2	0
24	d	404	CLA	1	0
26	Y	101	BCR	1	0
27	A	417	SQD	1	0
26	C	515	BCR	2	0
24	c	906	CLA	5	0
34	M	302	LMT	1	0
39	h	101	RRX	3	0
31	A	420	GOL	1	0
38	F	102	HEM	2	0
31	h	103	GOL	1	0
31	c	932	GOL	1	0
28	b	624	LMG	1	0
24	a	413	CLA	1	0
24	d	401	CLA	4	0
24	a	409	CLA	4	0
39	H	102	RRX	2	0
24	B	610	CLA	1	0
24	C	509	CLA	3	0
24	b	615	CLA	1	0
26	d	406	BCR	1	0
24	A	406	CLA	2	0
25	a	412	PHO	1	0
31	H	101	GOL	1	0
24	C	508	CLA	4	0
24	c	913	CLA	3	0
24	B	605	CLA	1	0
36	C	516	DGD	1	0
24	c	902	CLA	3	0
31	B	630	GOL	1	0
24	B	612	CLA	1	0
31	C	531	GOL	3	0
24	B	617	CLA	3	0
24	B	611	CLA	4	0
24	b	610	CLA	3	0
26	a	414	BCR	2	0
38	f	101	HEM	2	0

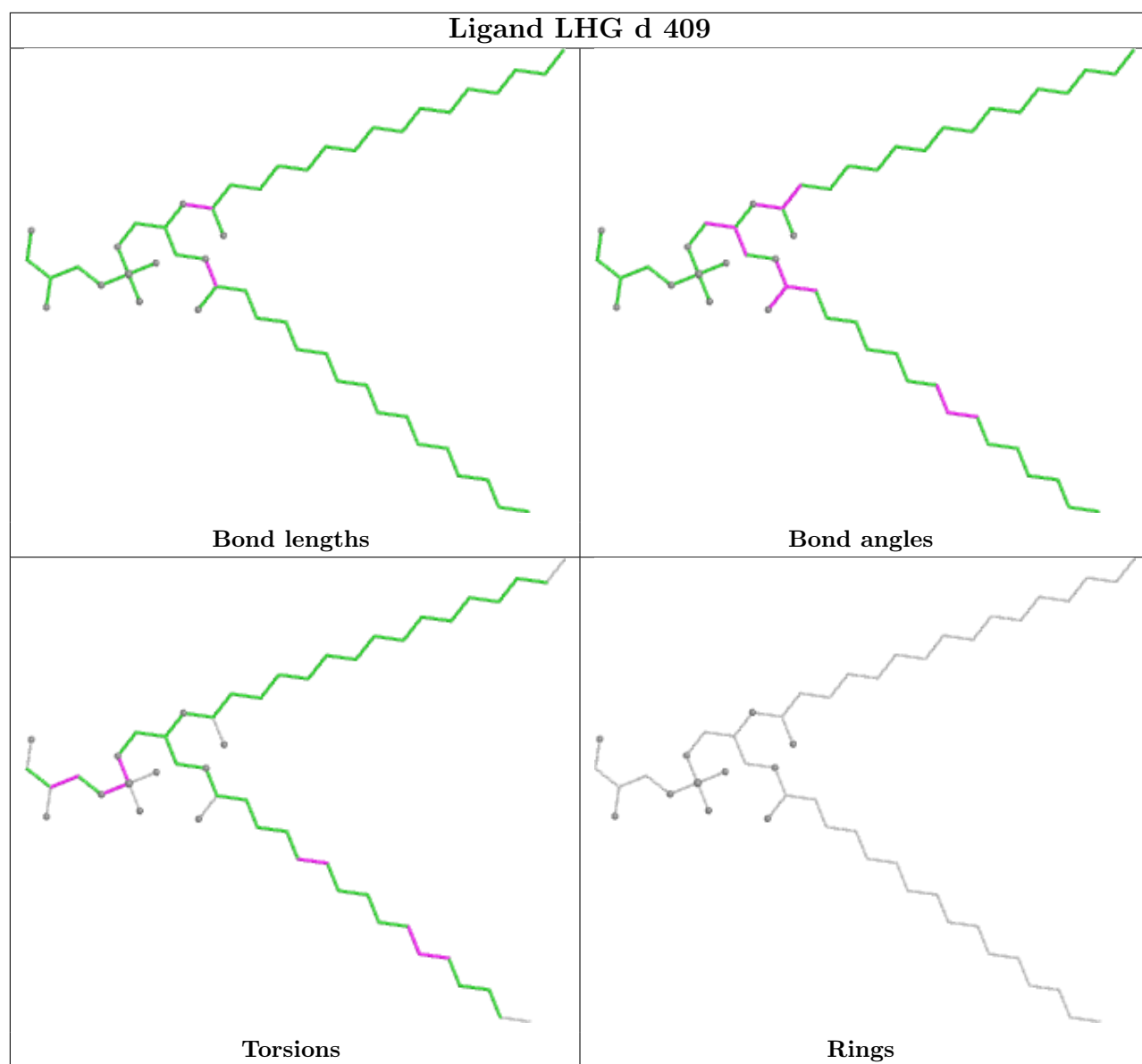
Continued on next page...

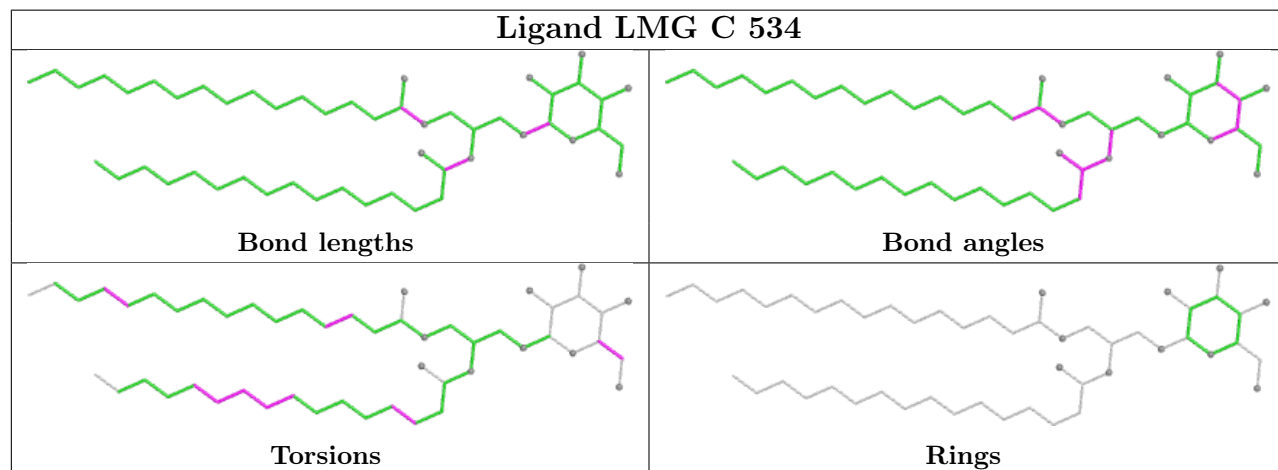
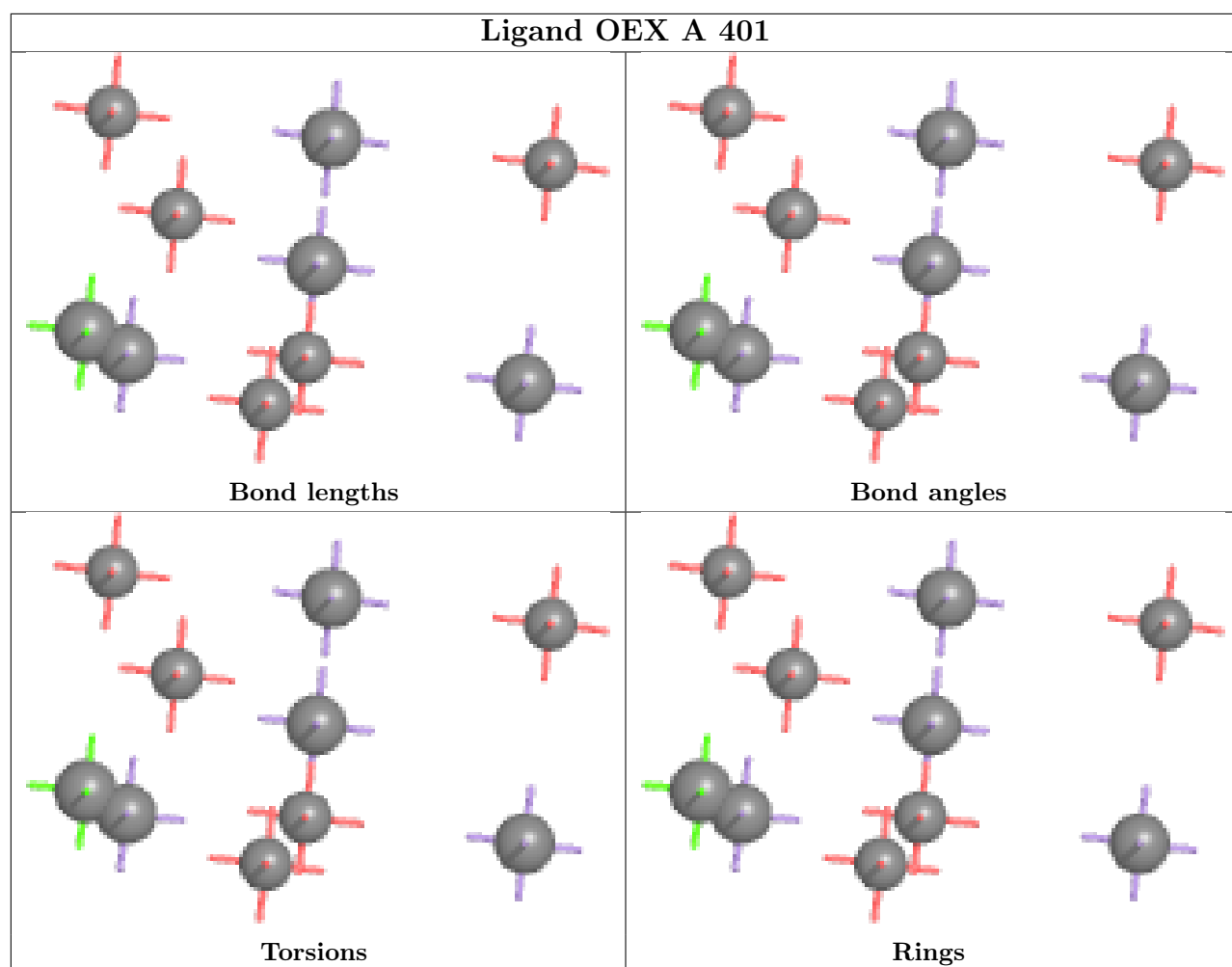
Continued from previous page...

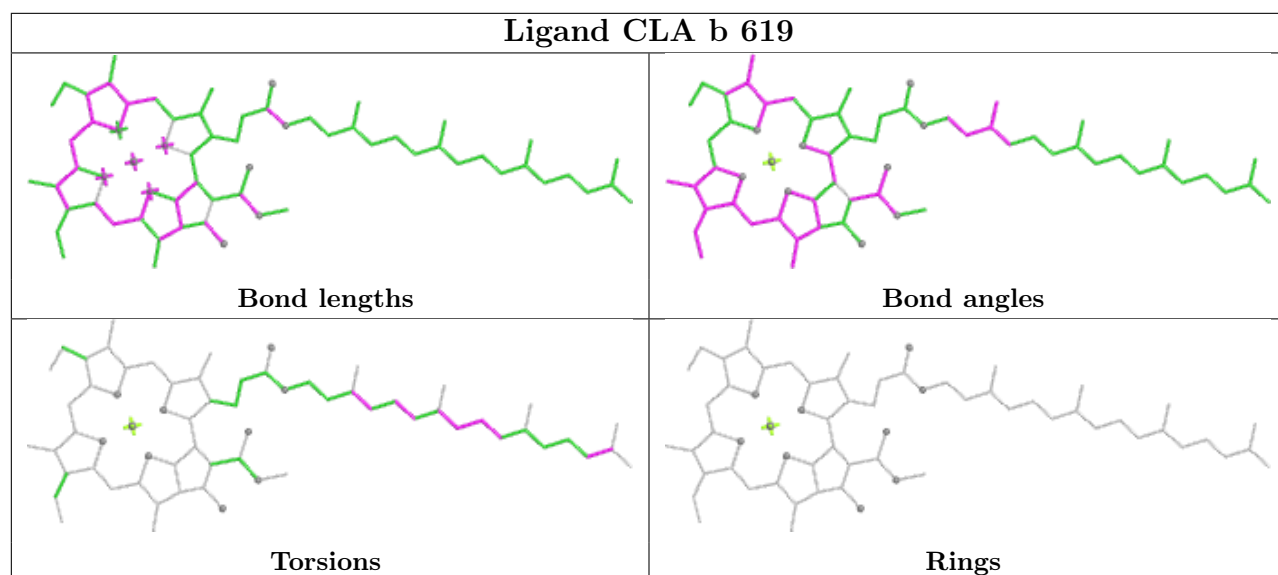
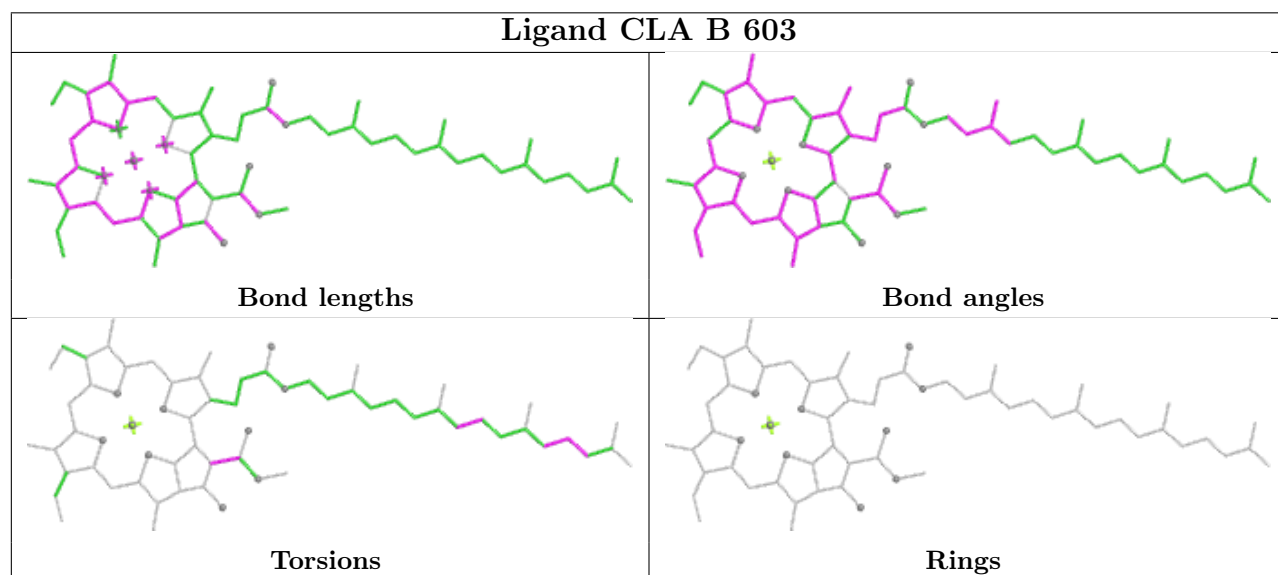
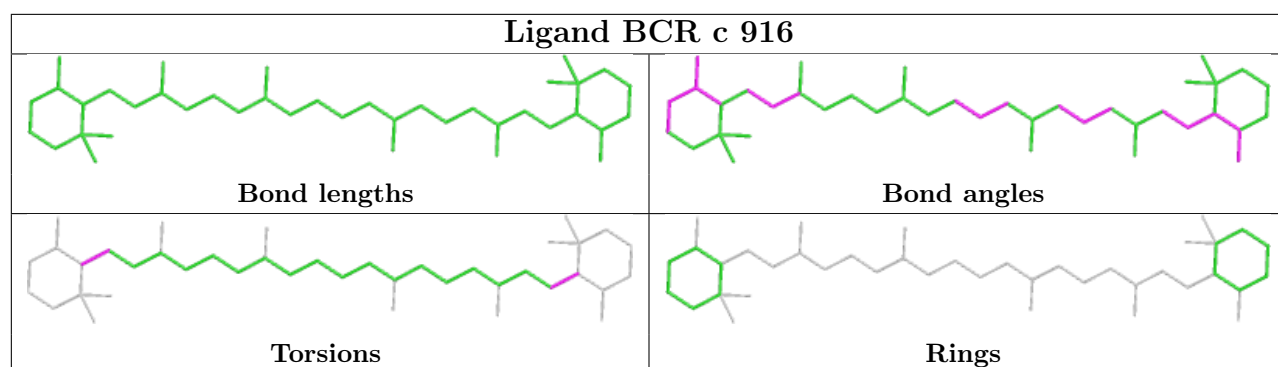
Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	c	927	GOL	3	0
24	b	618	CLA	1	0
26	D	404	BCR	2	0
26	B	618	BCR	2	0
29	A	414	PL9	5	0
35	C	528	HTG	1	0
35	c	924	HTG	1	0
37	D	409	LHG	4	0
24	A	407	CLA	2	0
24	A	410	CLA	2	0
24	b	608	CLA	2	0
24	C	511	CLA	3	0
24	C	505	CLA	2	0
24	C	506	CLA	3	0
24	B	602	CLA	1	0
36	D	406	DGD	4	0
24	c	910	CLA	2	0
34	z	101	LMT	4	0

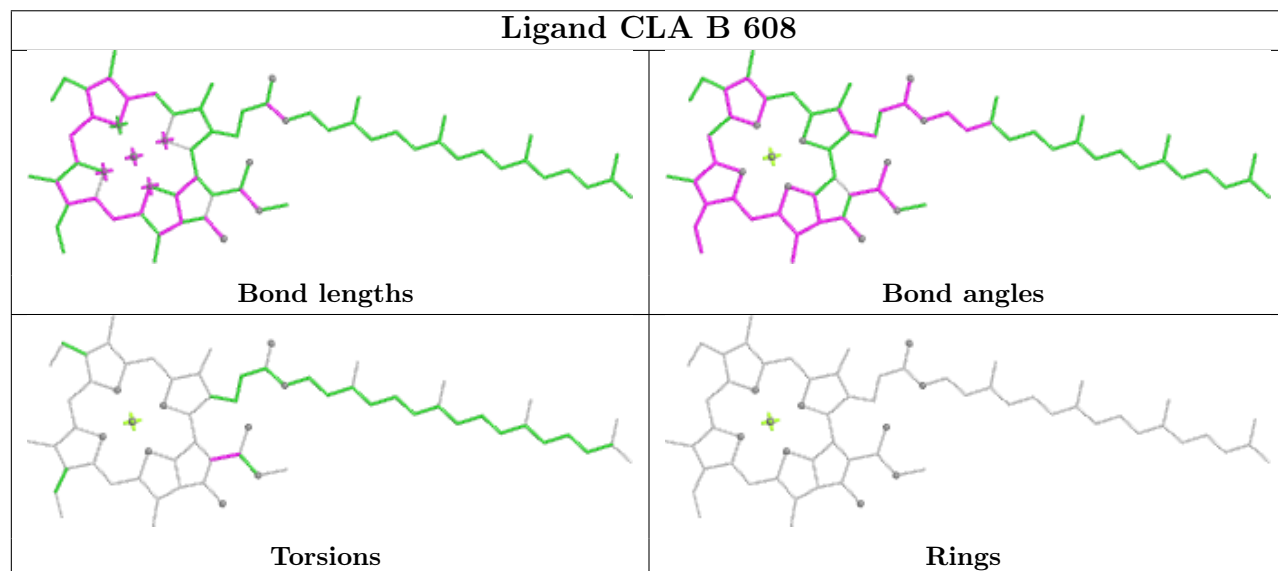
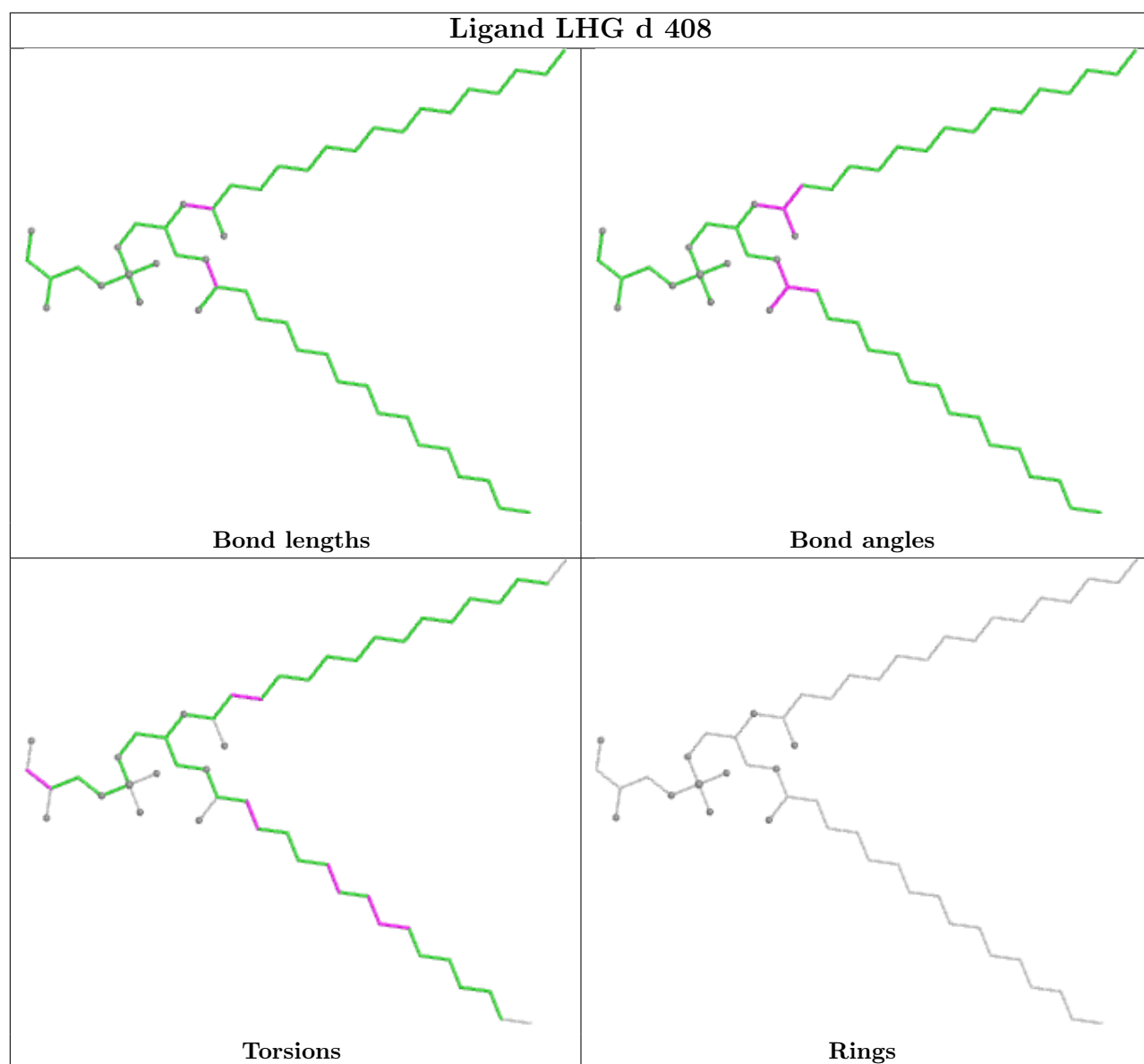
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

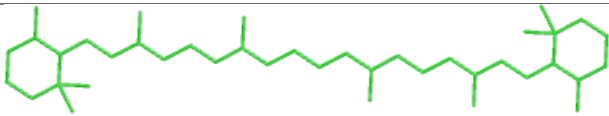
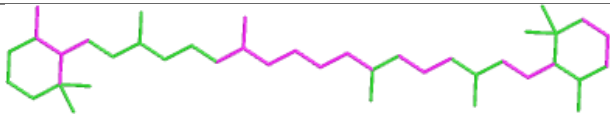
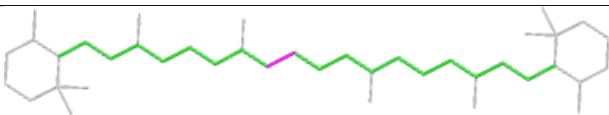
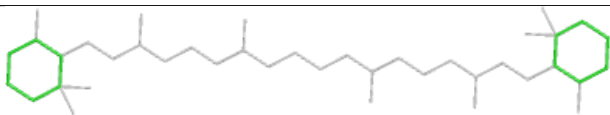


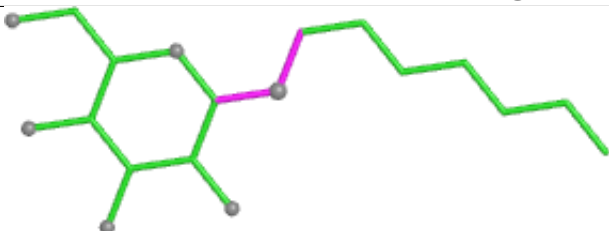
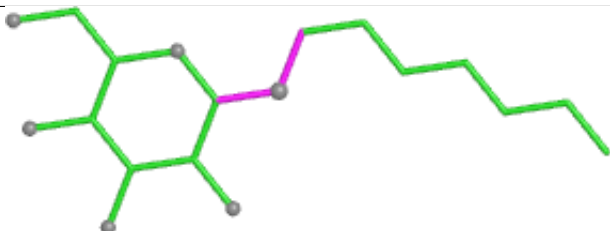
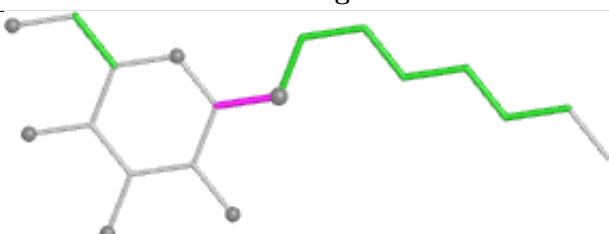
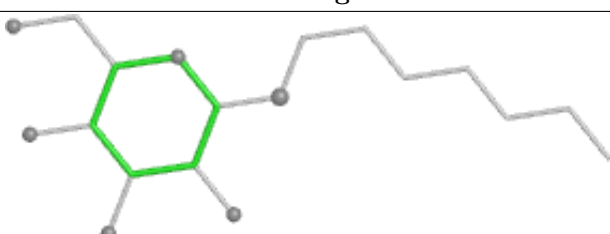


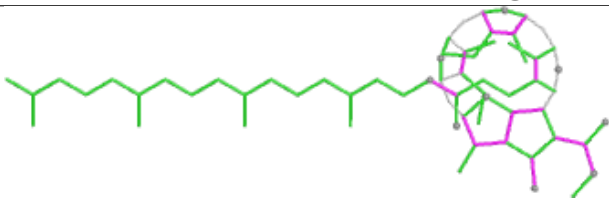
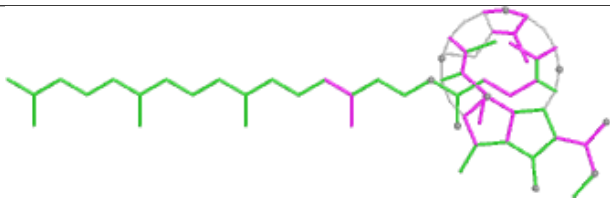
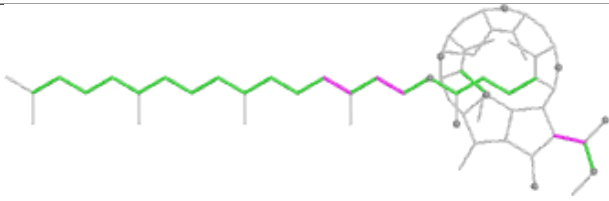
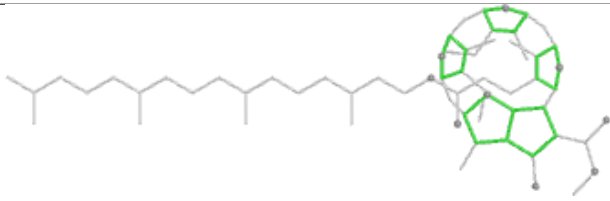


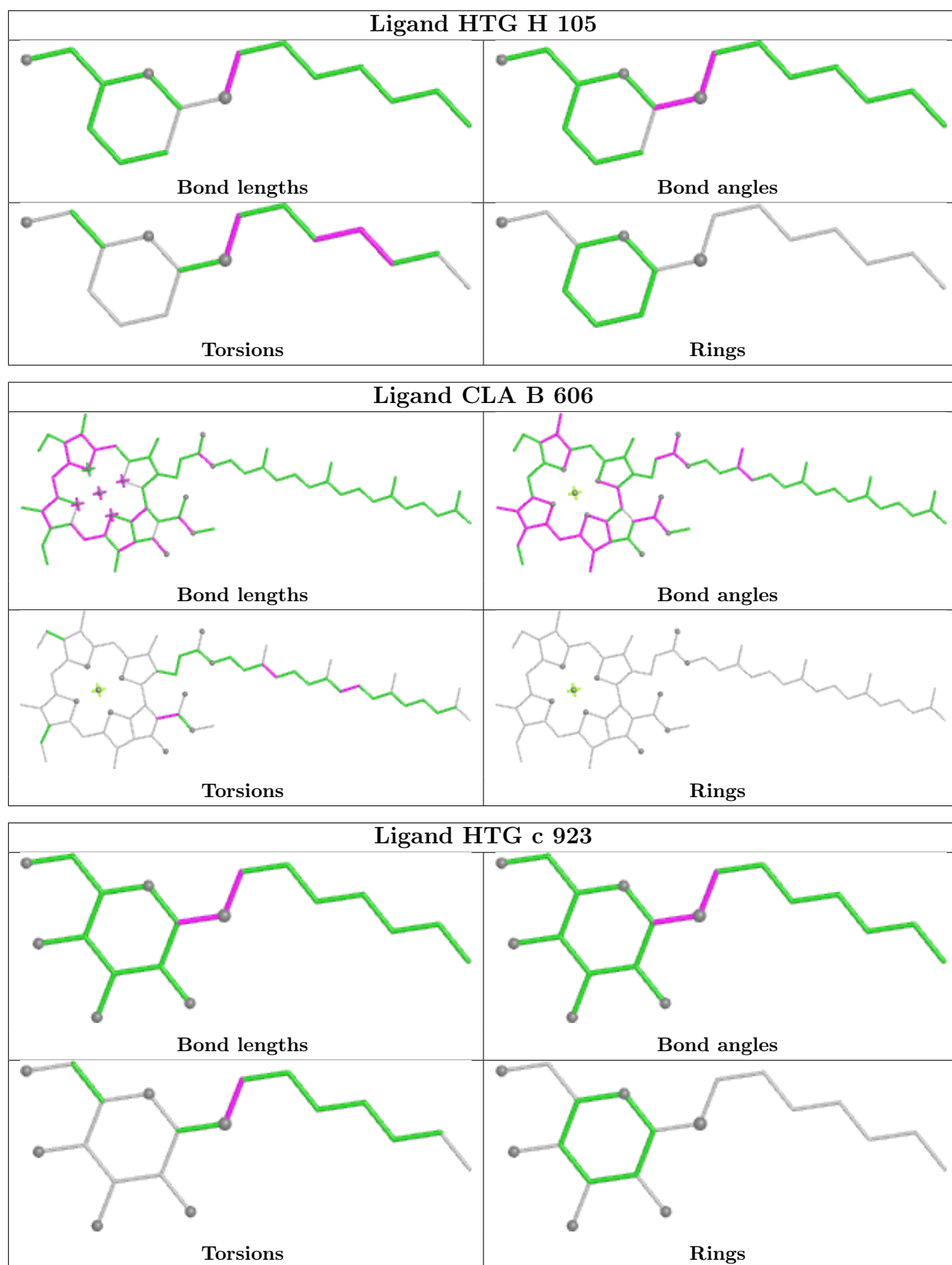


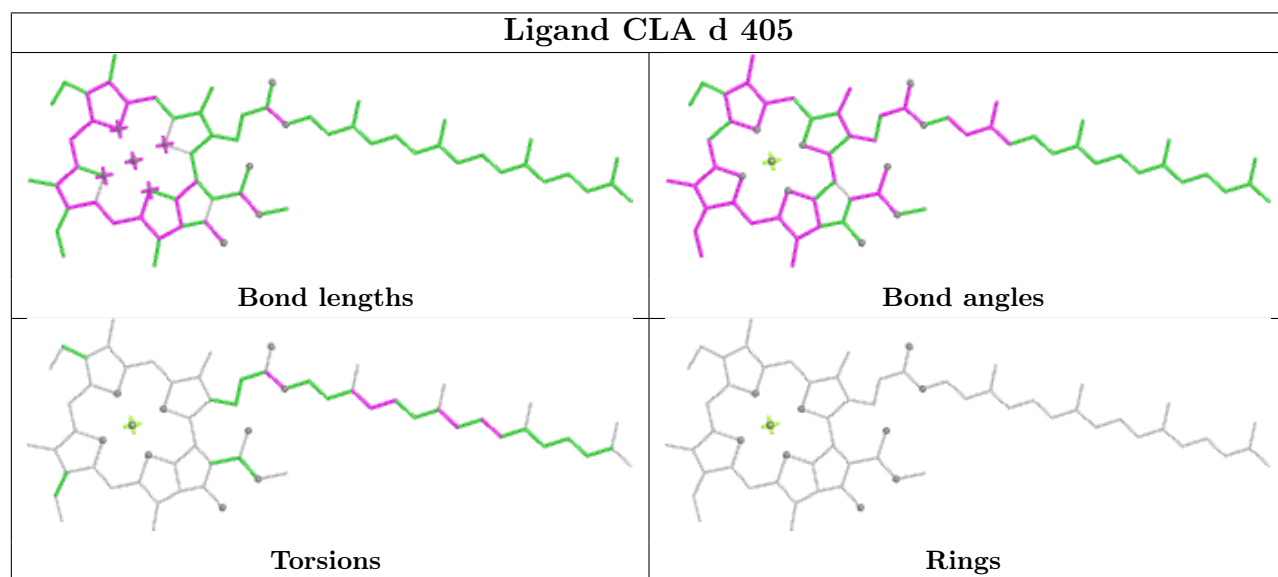
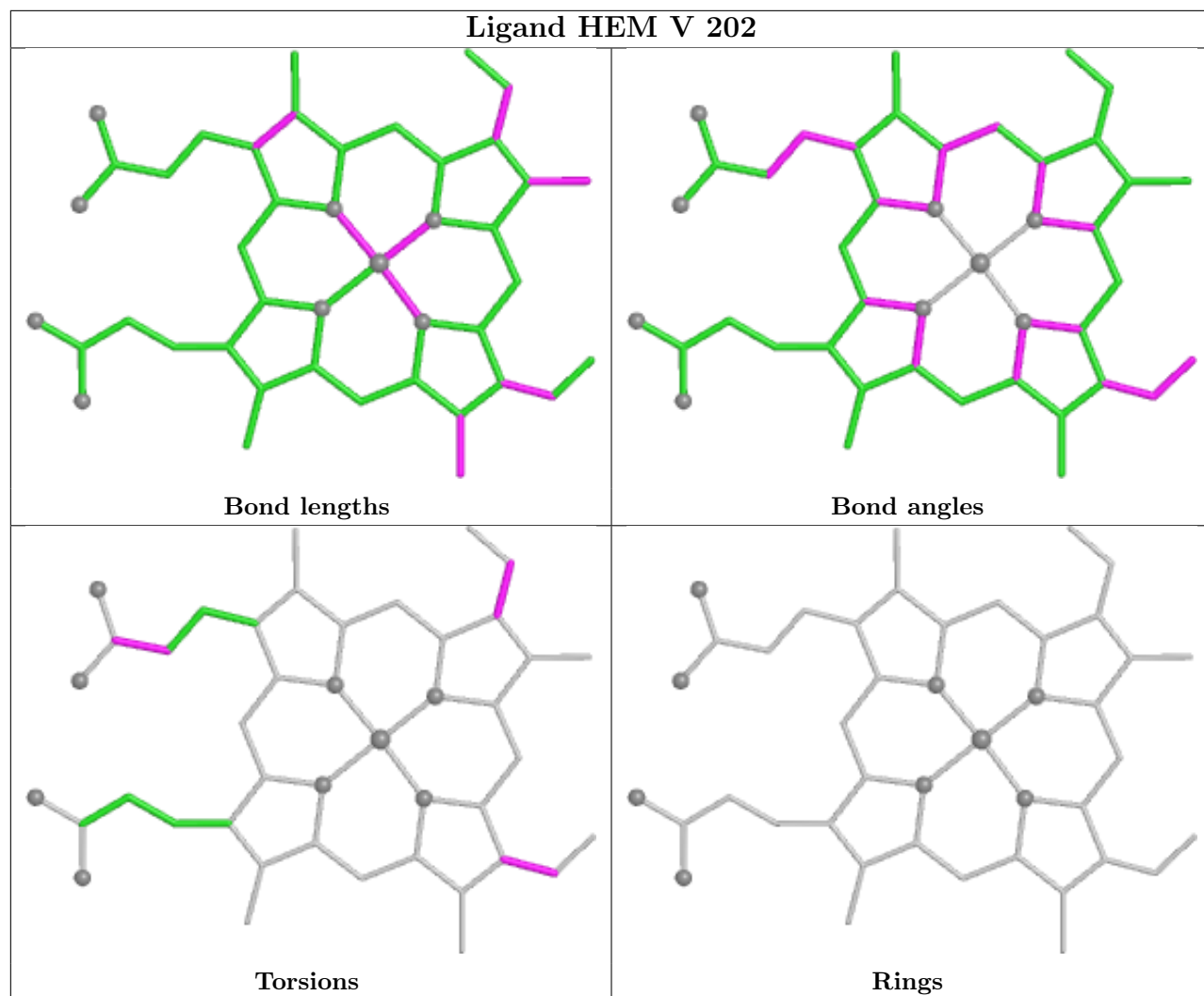


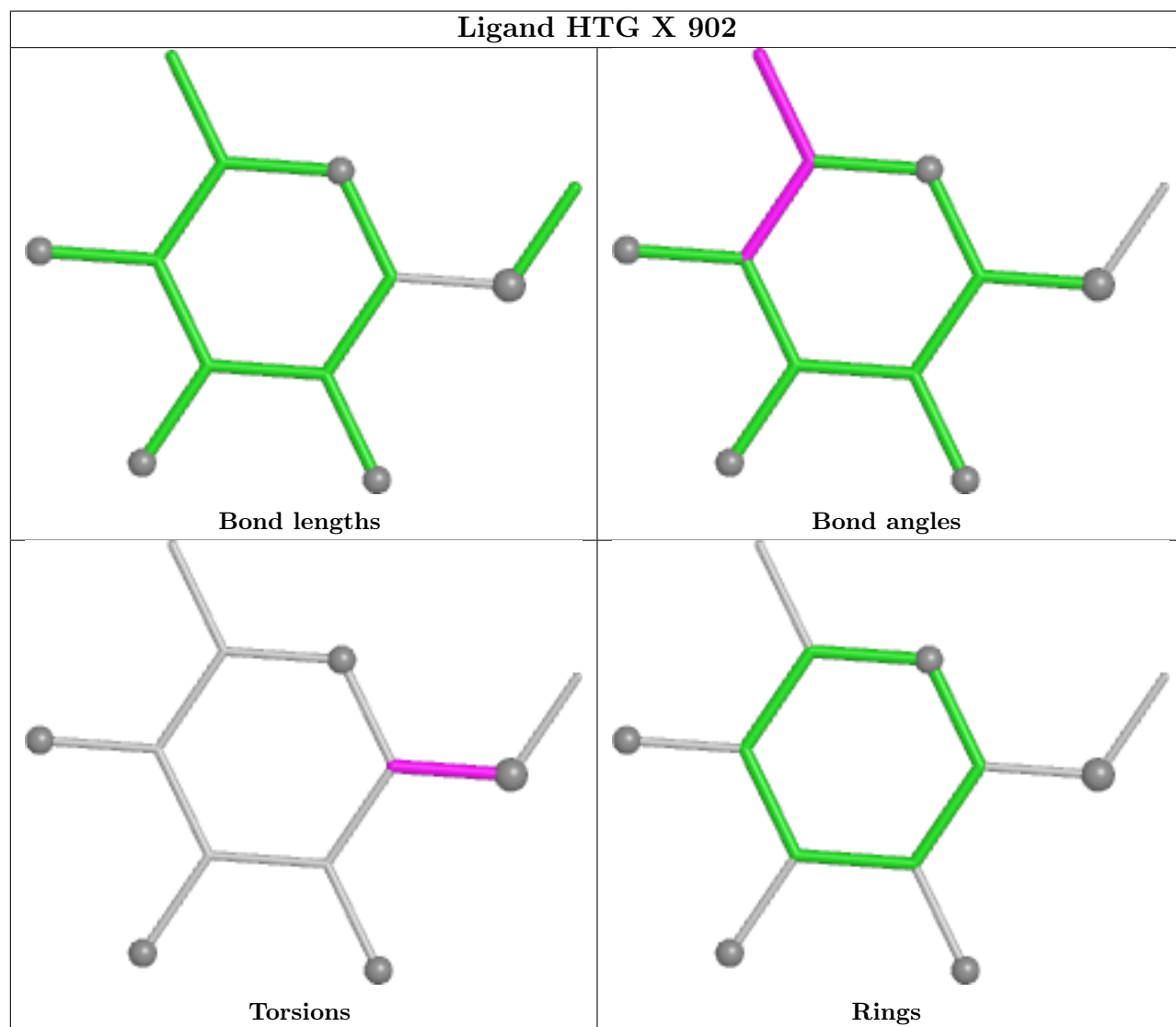
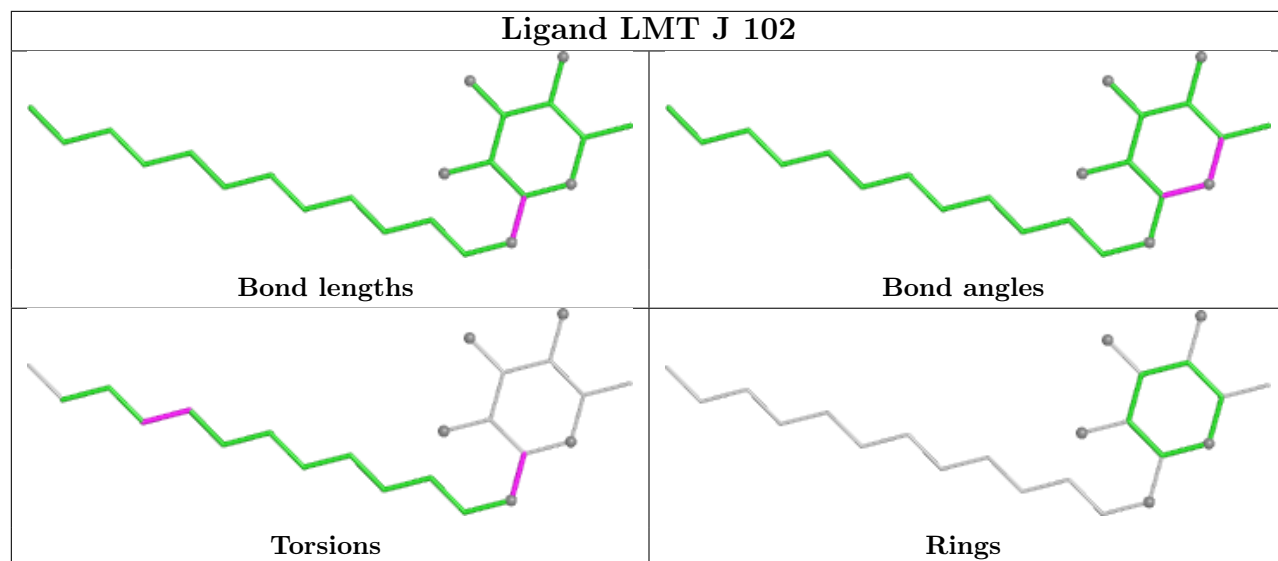
Ligand BCR T 702	
	
Bond lengths	Bond angles
	
Torsions	Rings

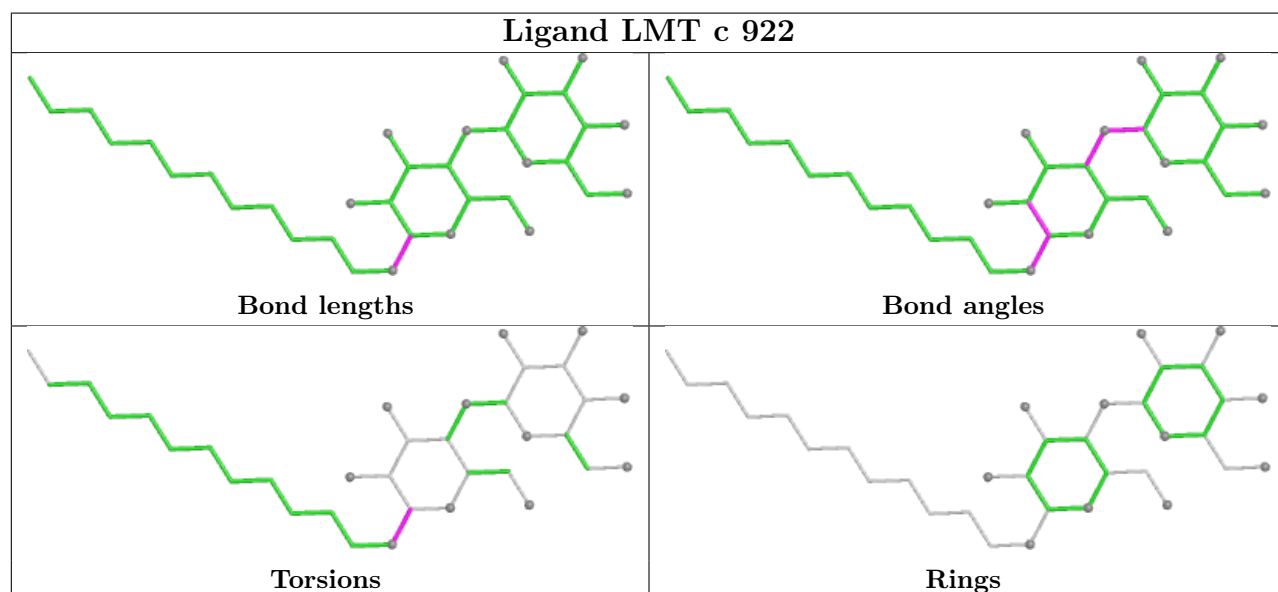
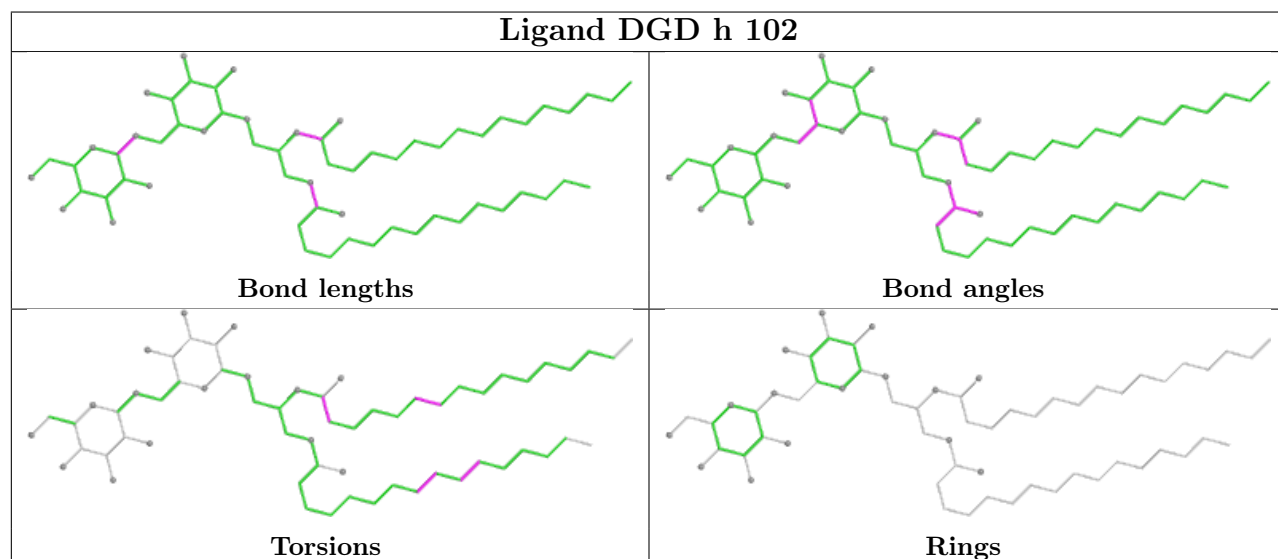
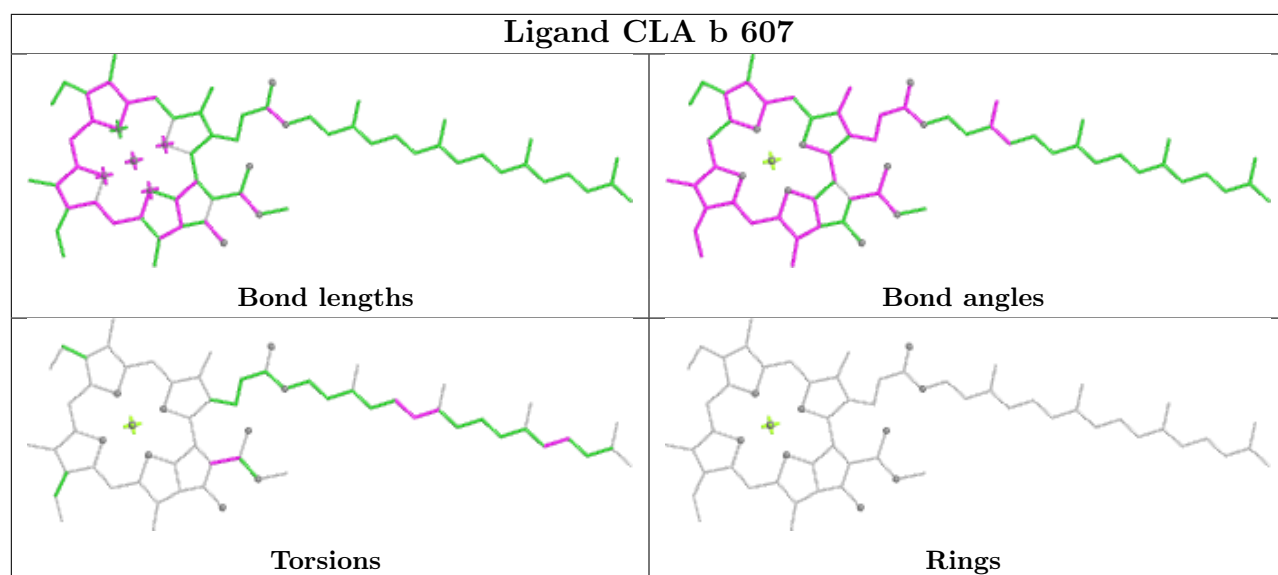
Ligand HTG b 603	
	
Bond lengths	Bond angles
	
Torsions	Rings

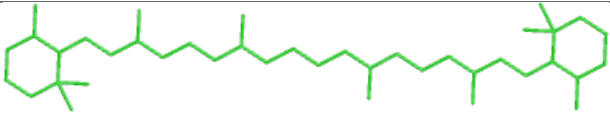
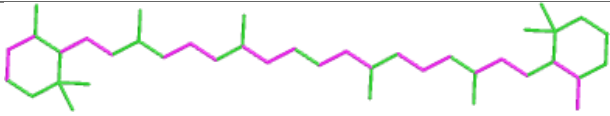
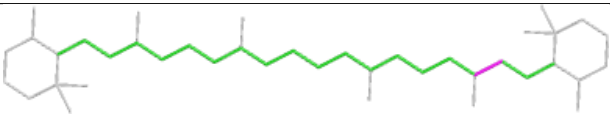
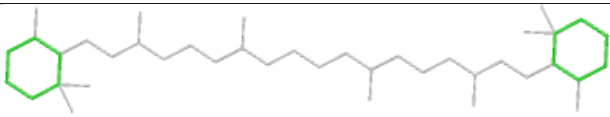
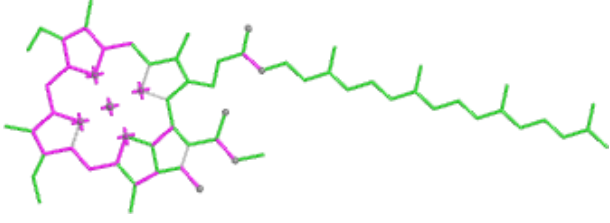
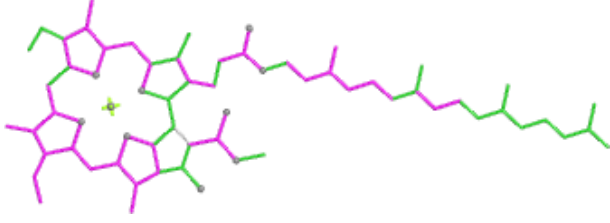
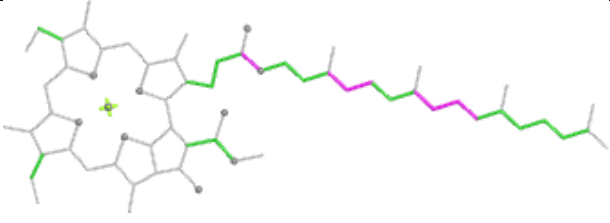
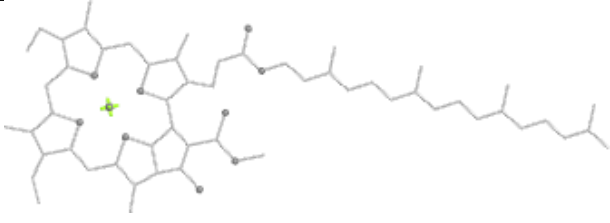
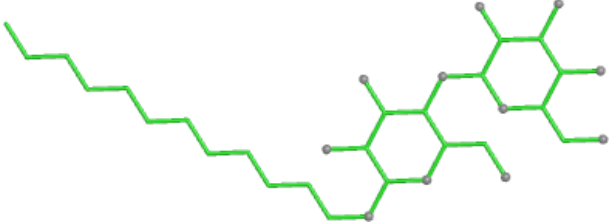
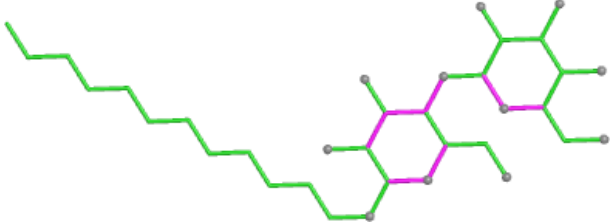
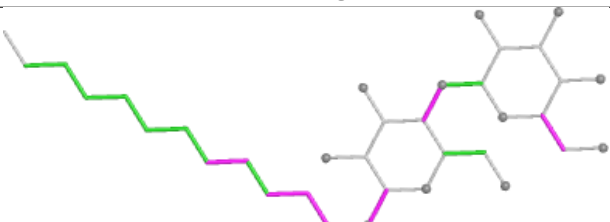
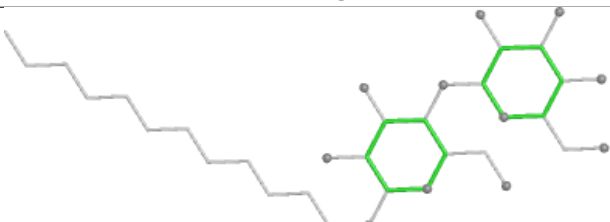
Ligand PHO A 408	
	
Bond lengths	Bond angles
	
Torsions	Rings



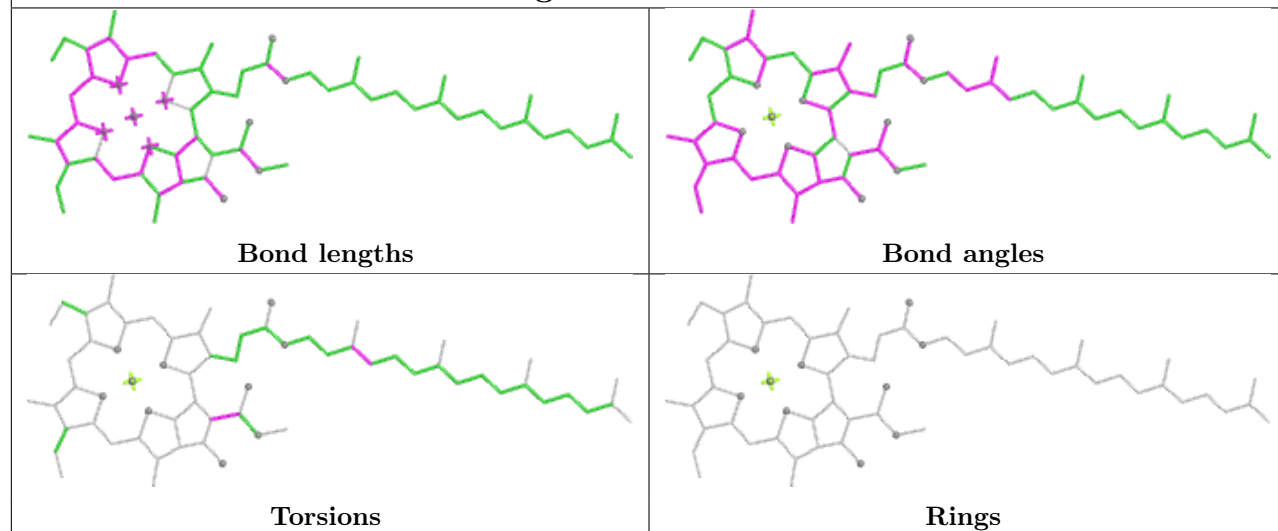




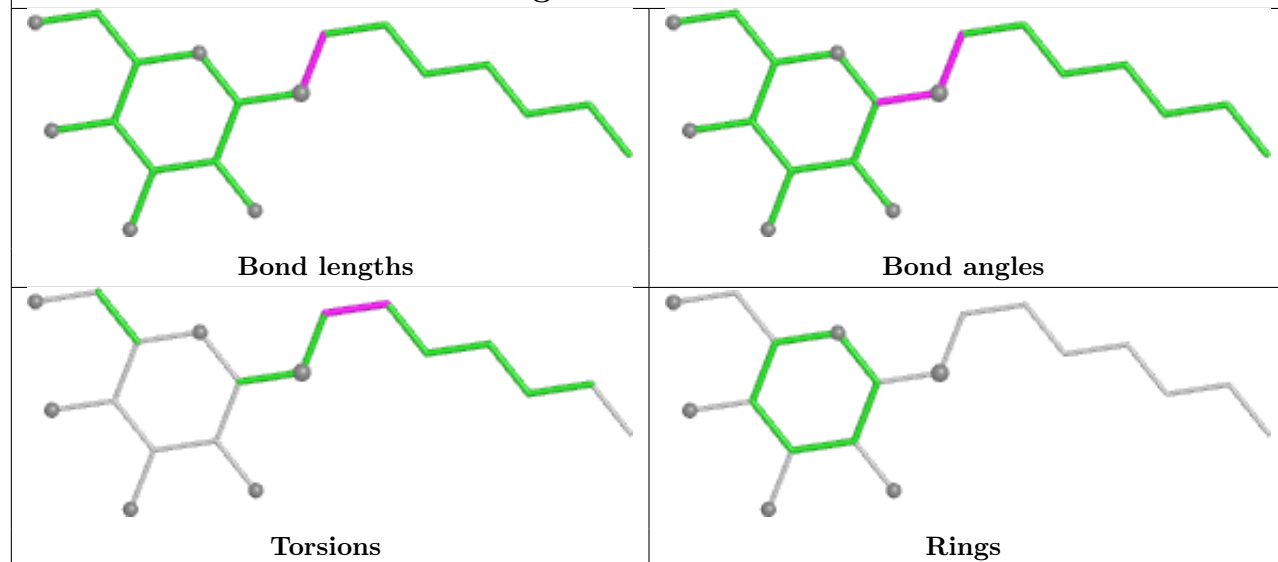


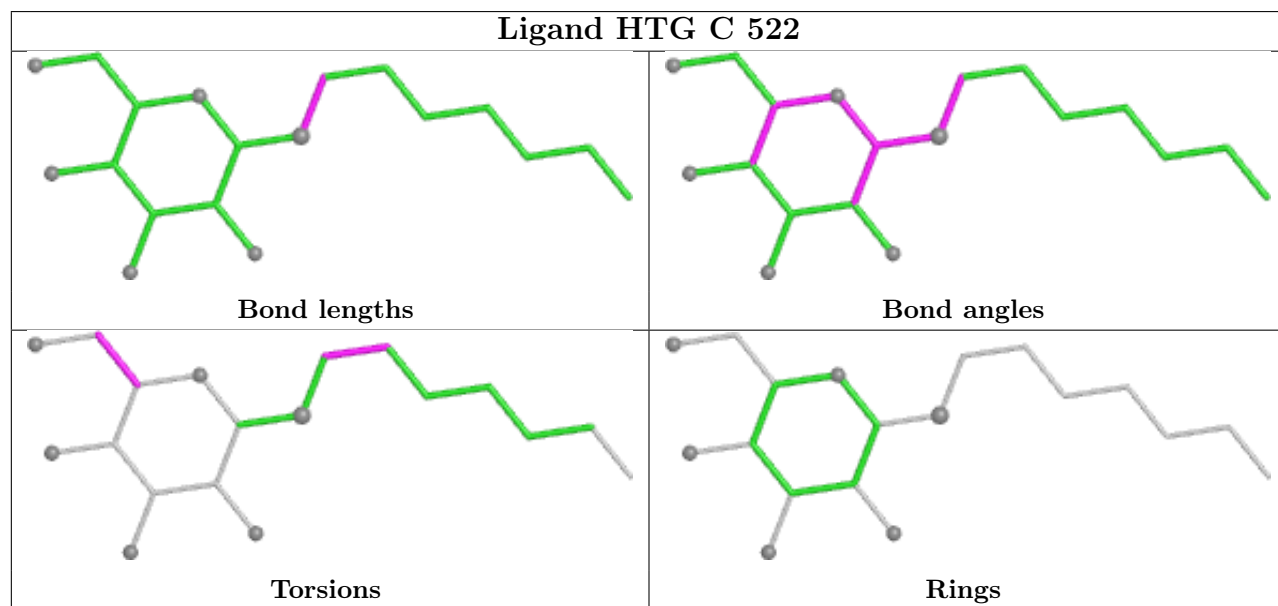
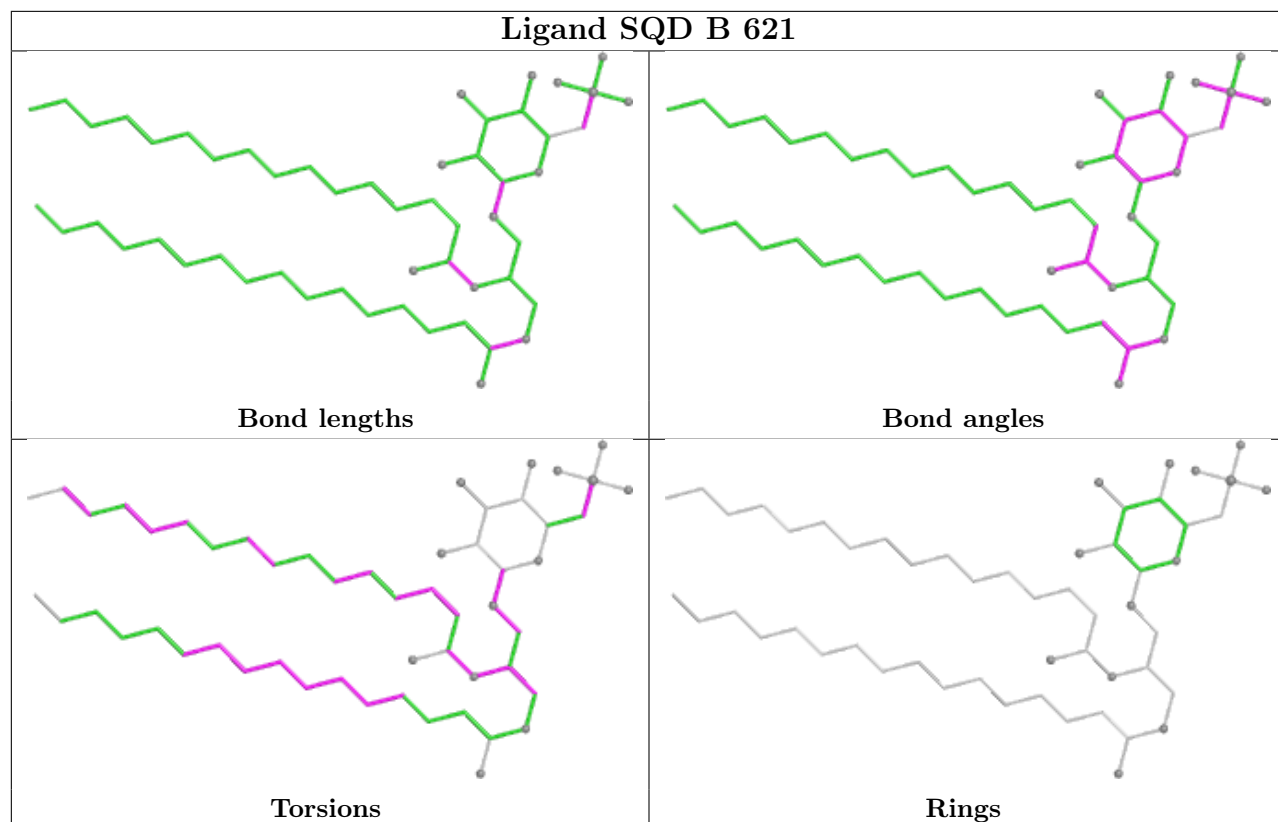
Ligand BCR b 623	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA D 403	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMT C 520	
 Bond lengths	 Bond angles
 Torsions	 Rings

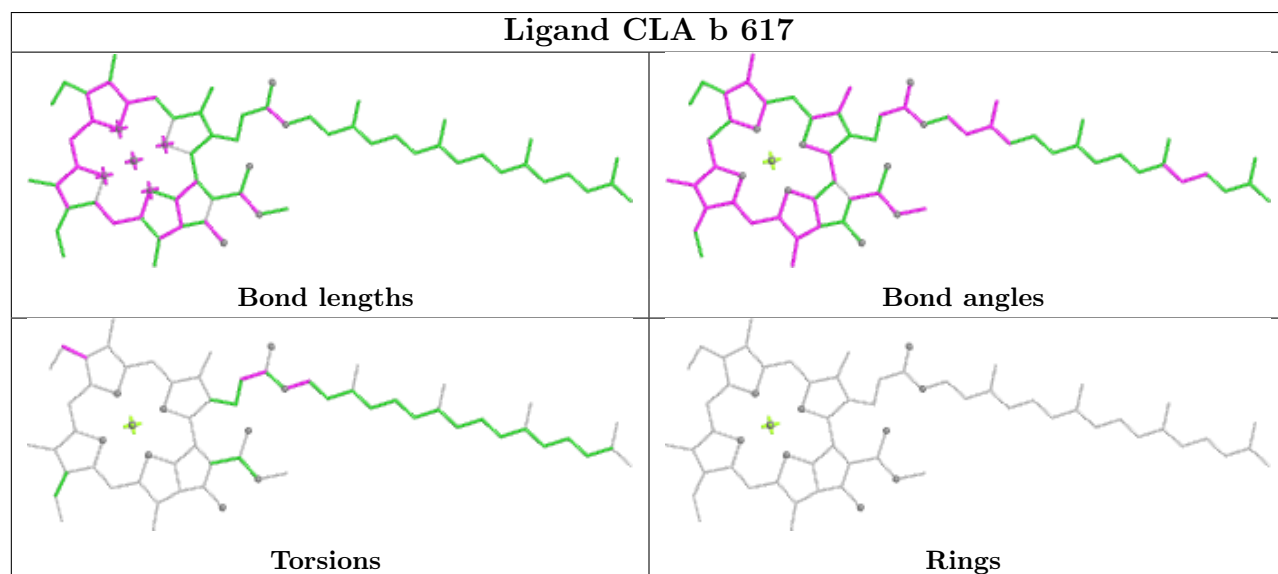
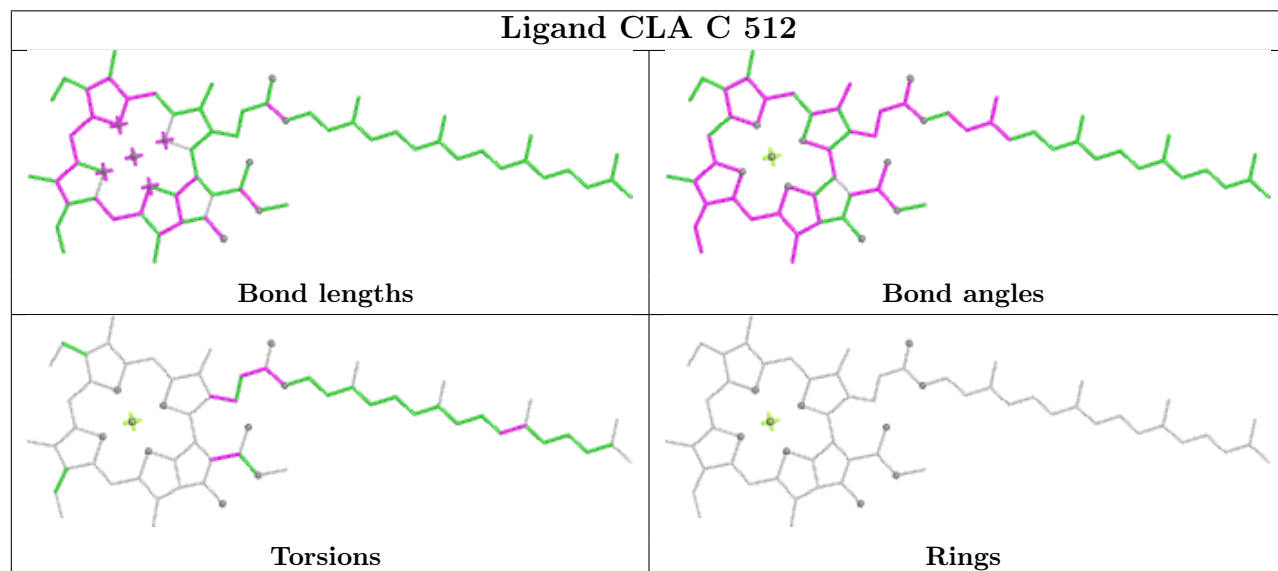
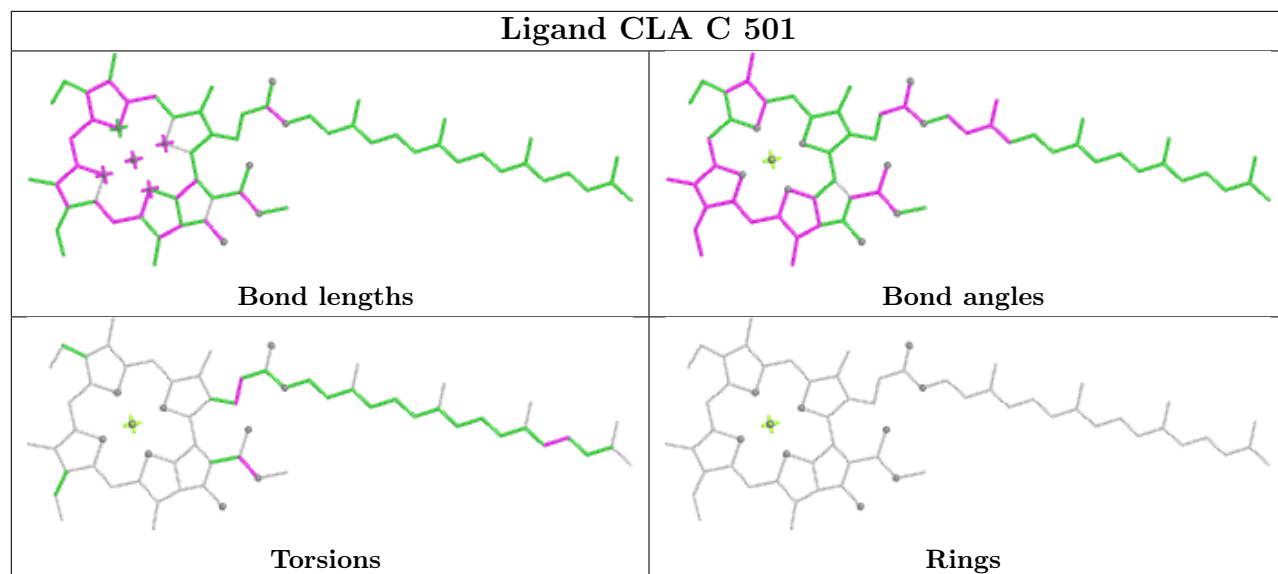
Ligand CLA b 609

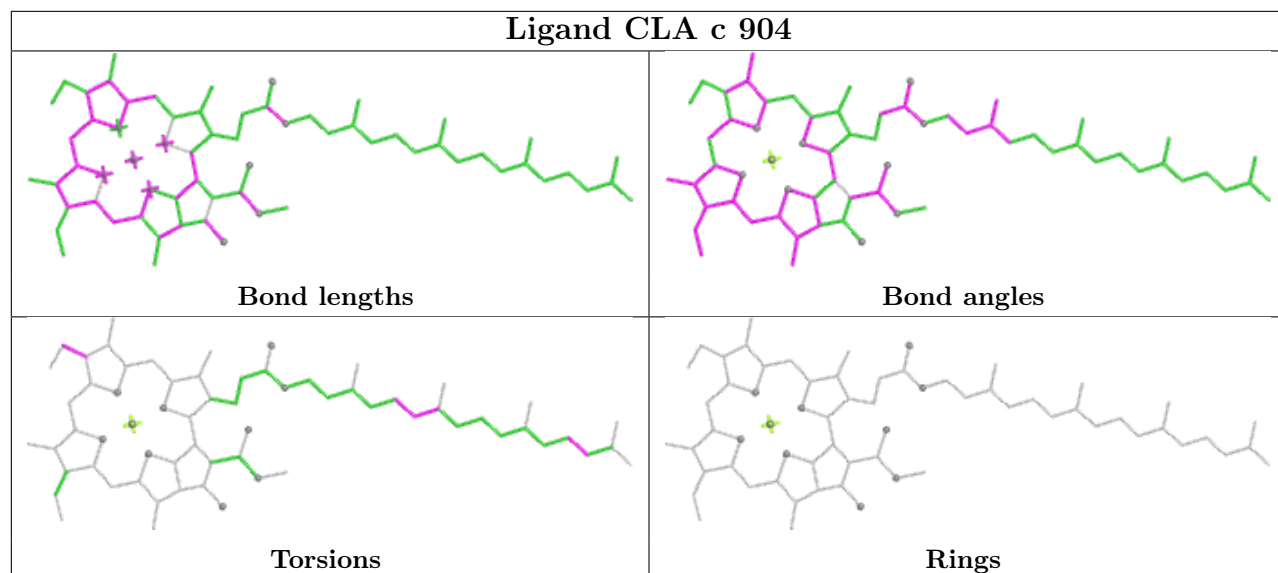
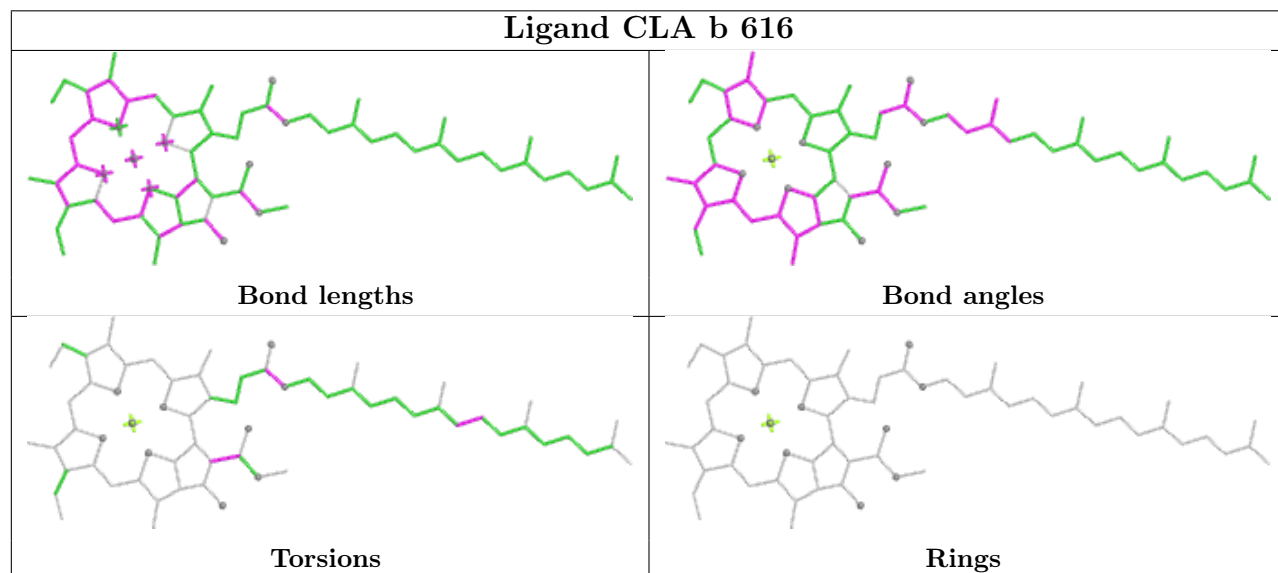
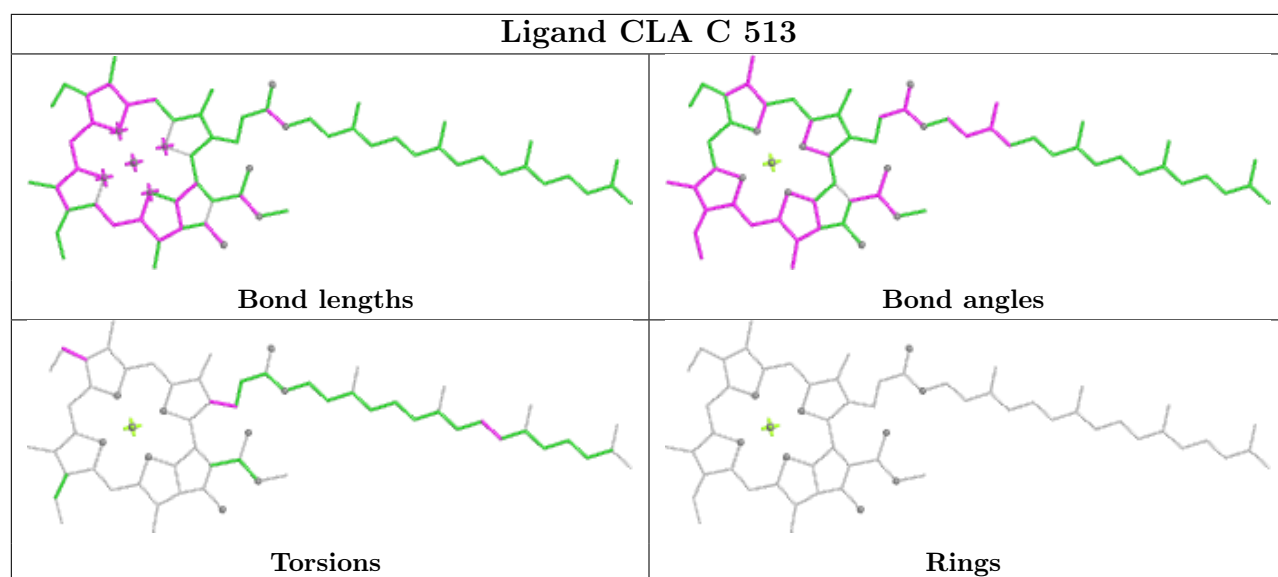


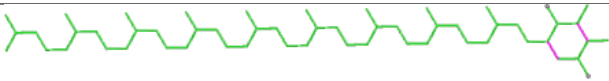
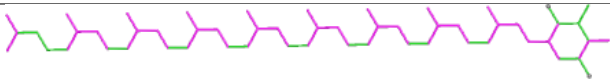
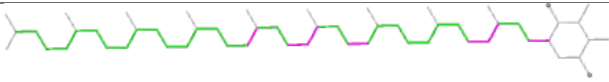
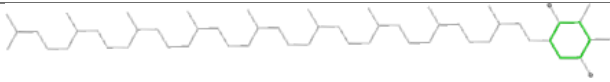
Ligand HTG o 301

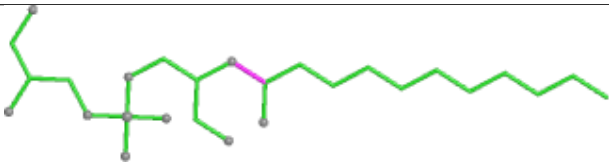
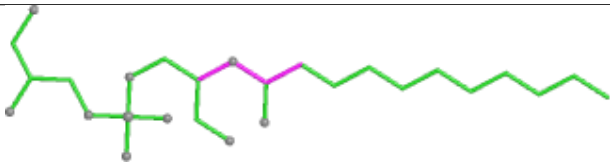
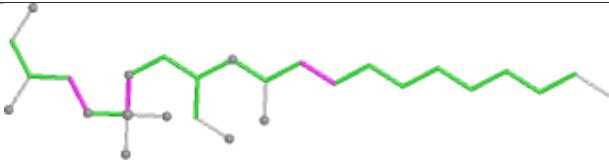
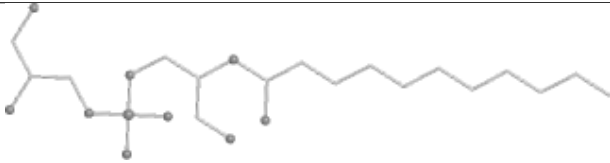


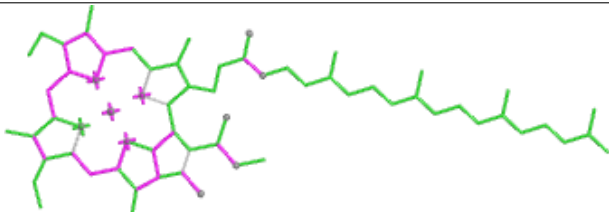
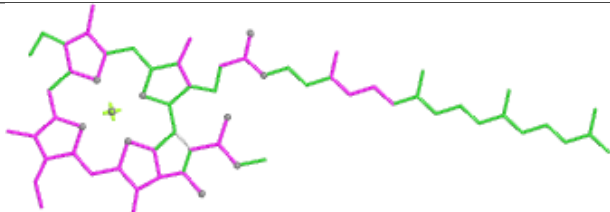
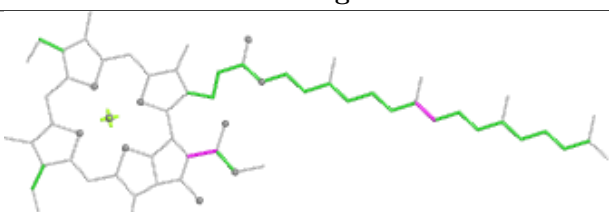
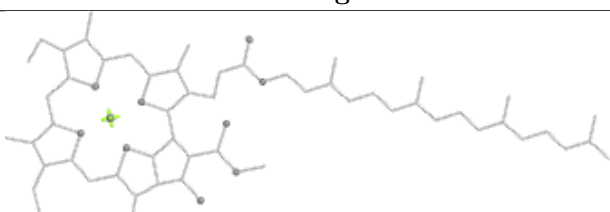


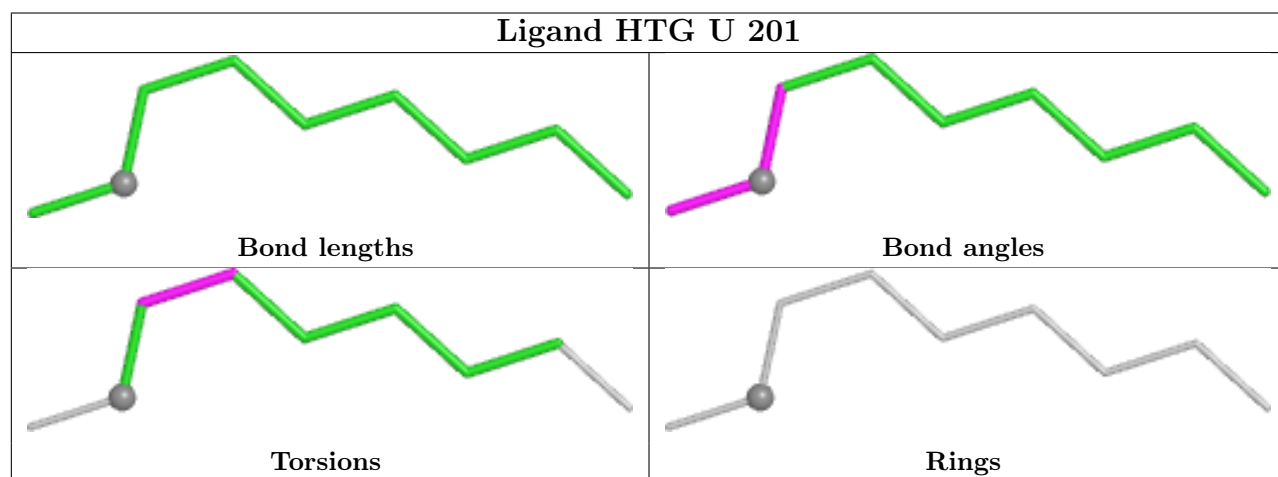
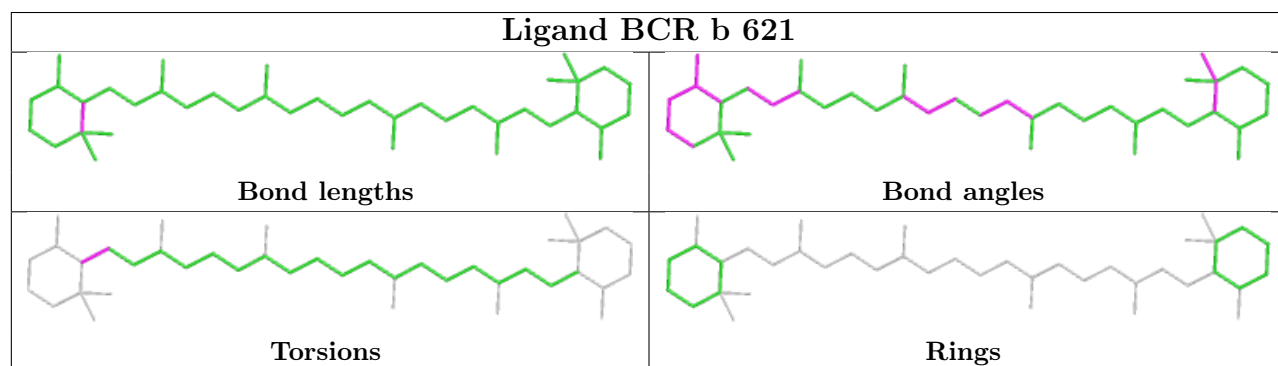
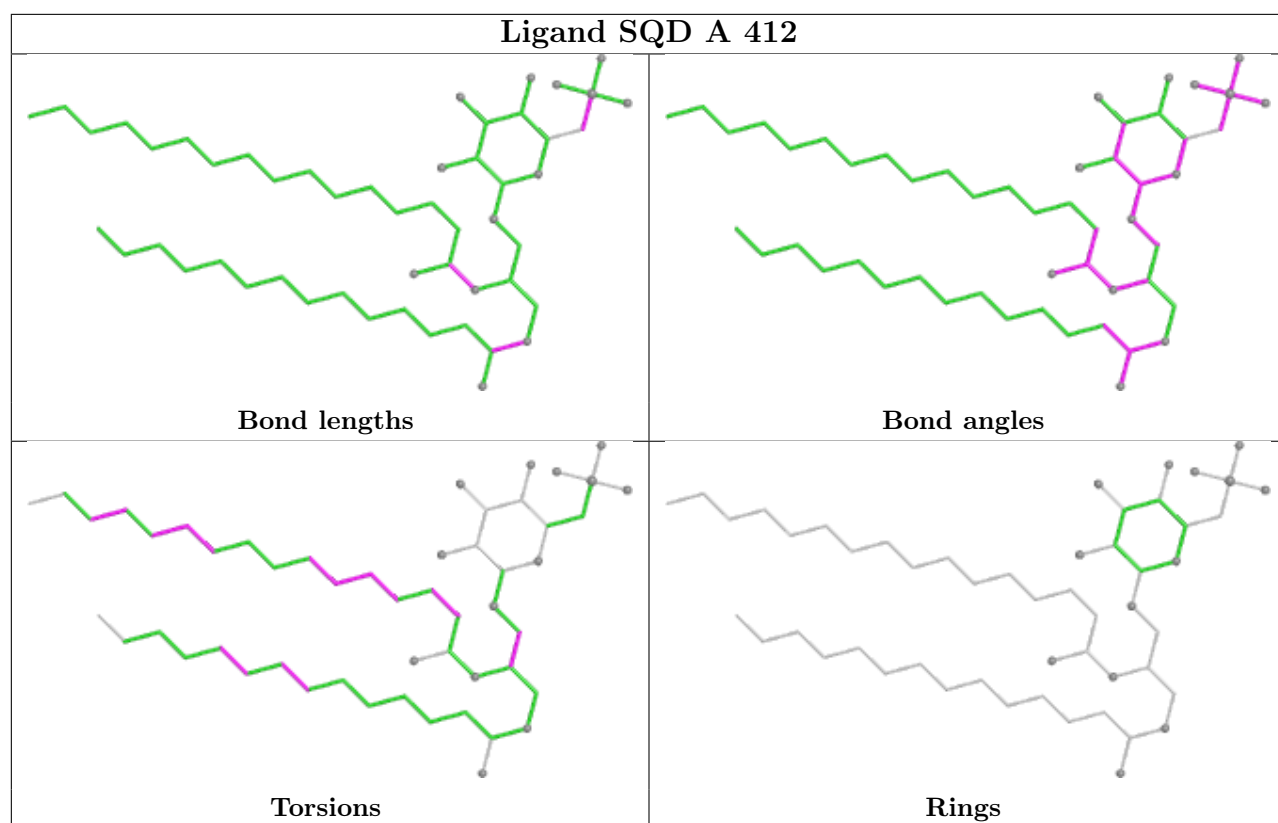


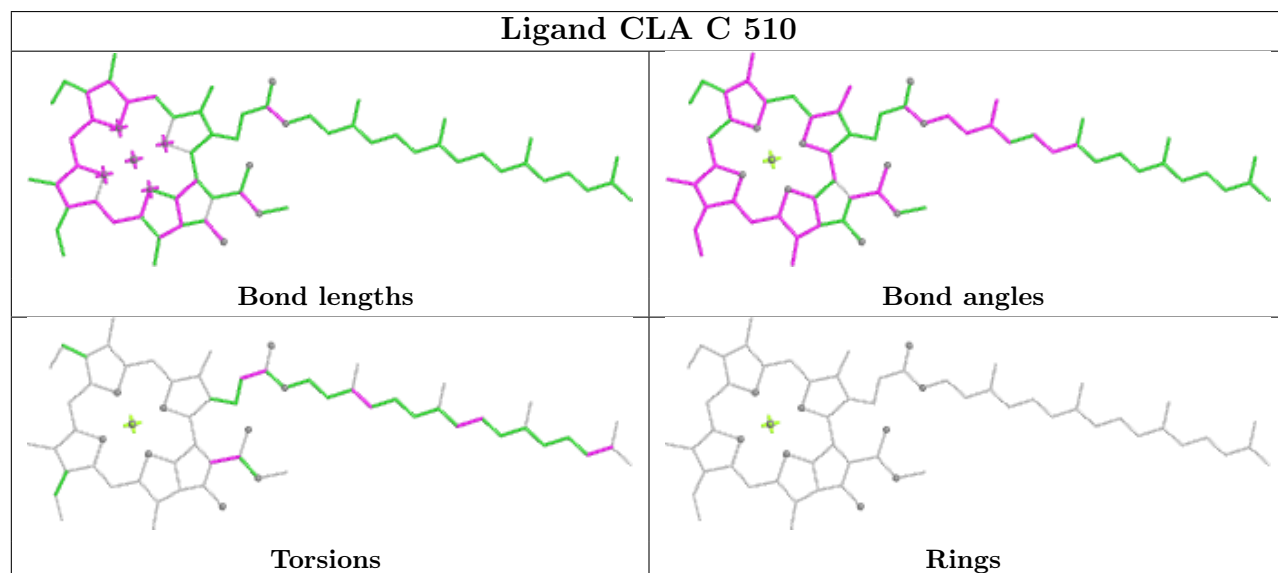
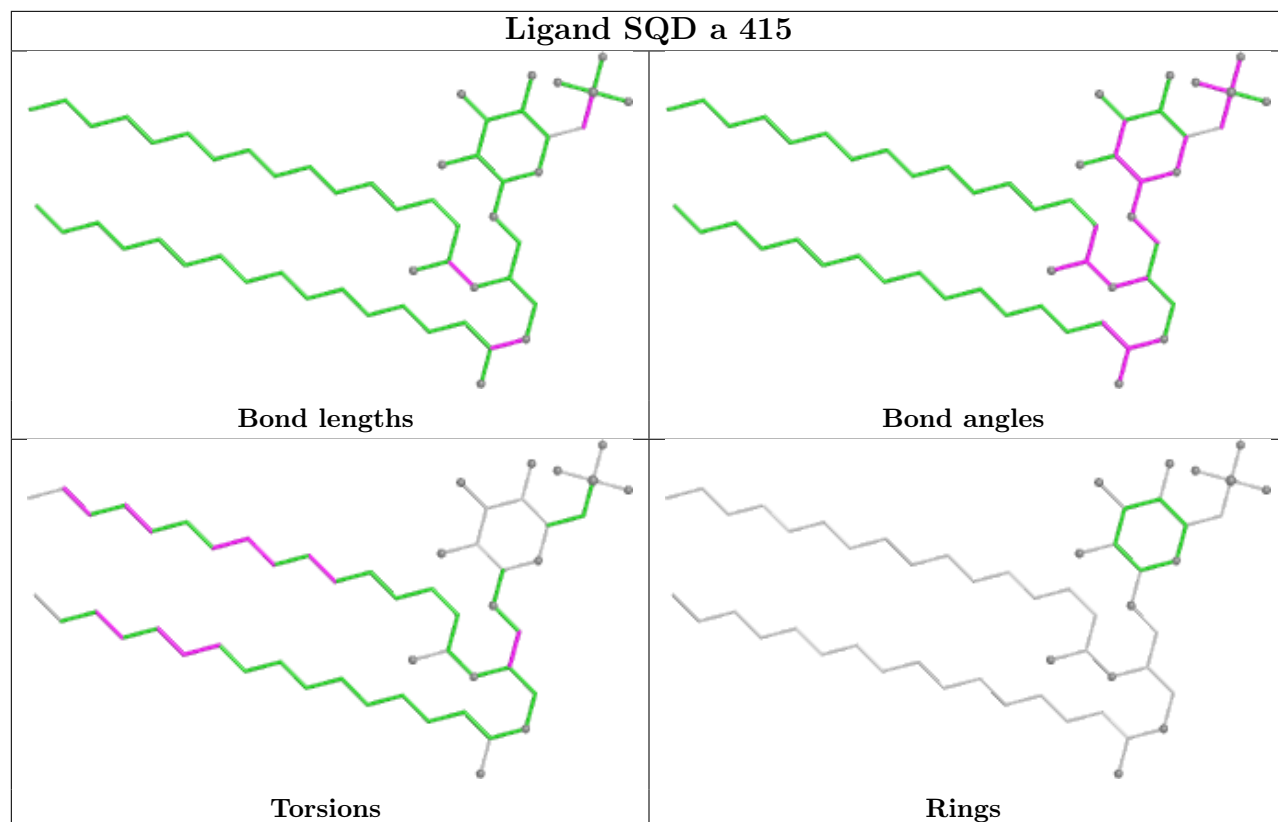


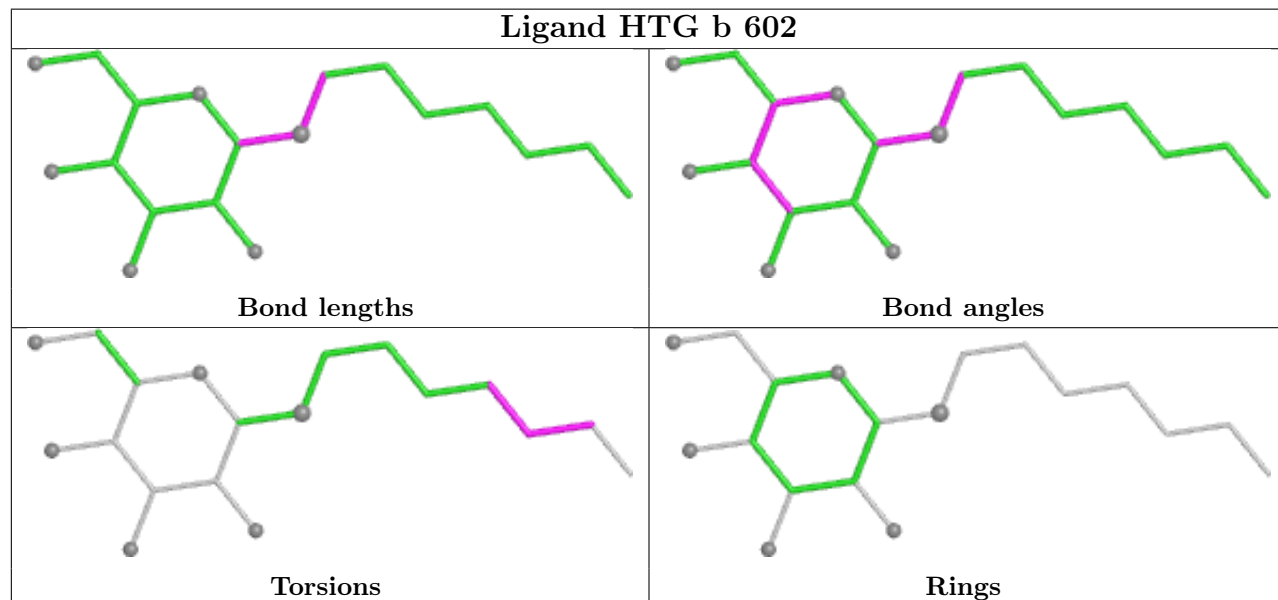
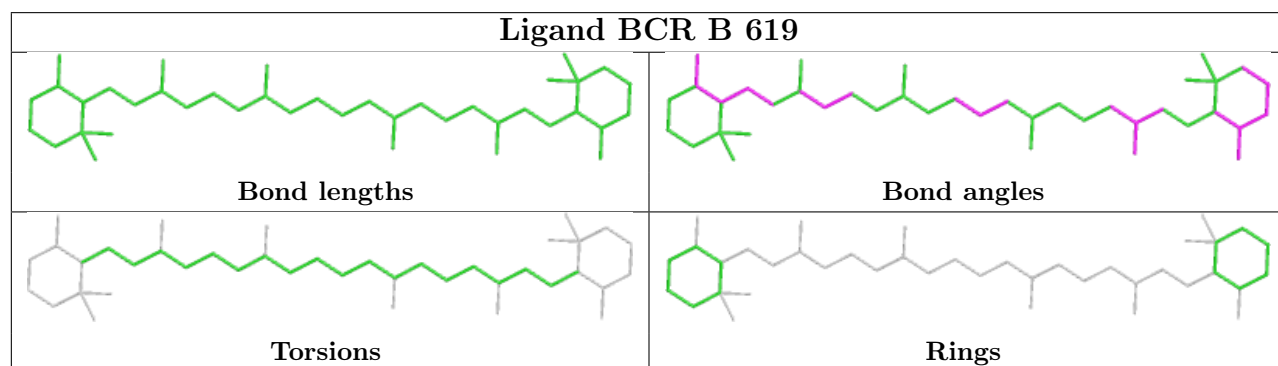
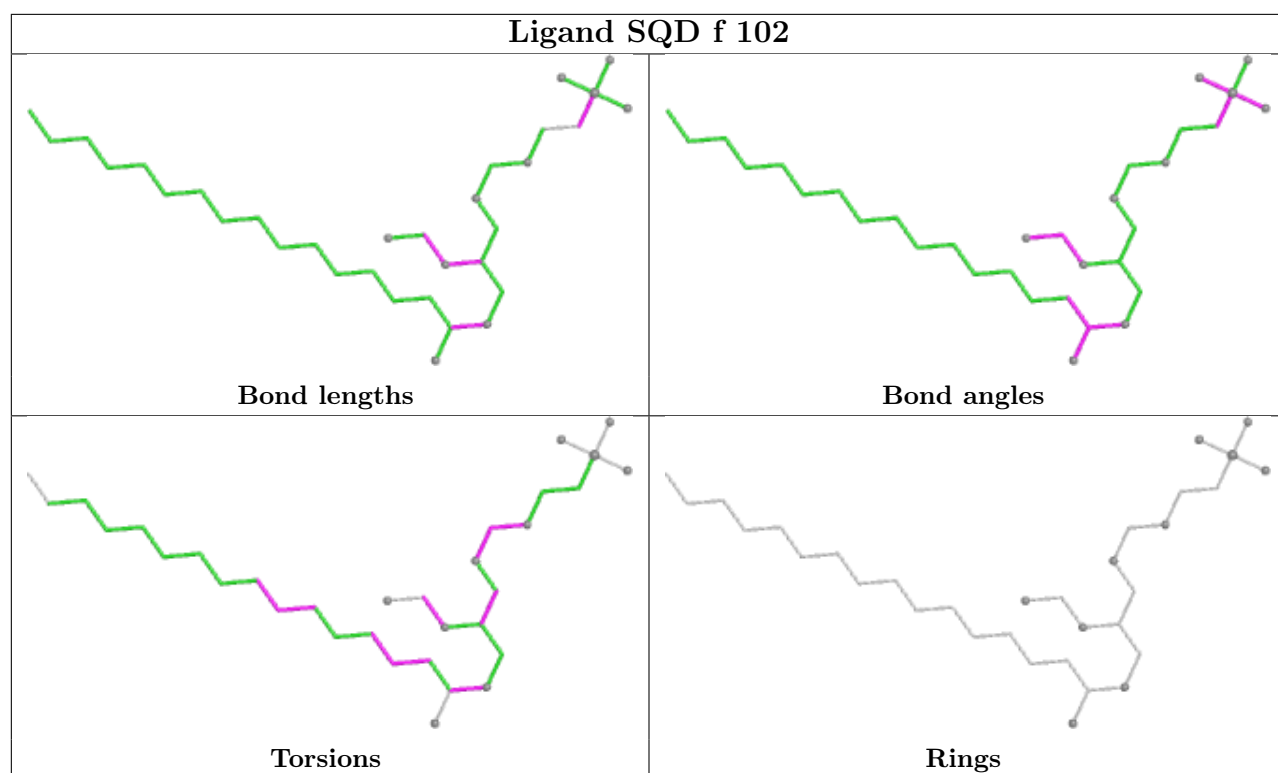
Ligand PL9 a 417	
 Bond lengths	 Bond angles
 Torsions	 Rings

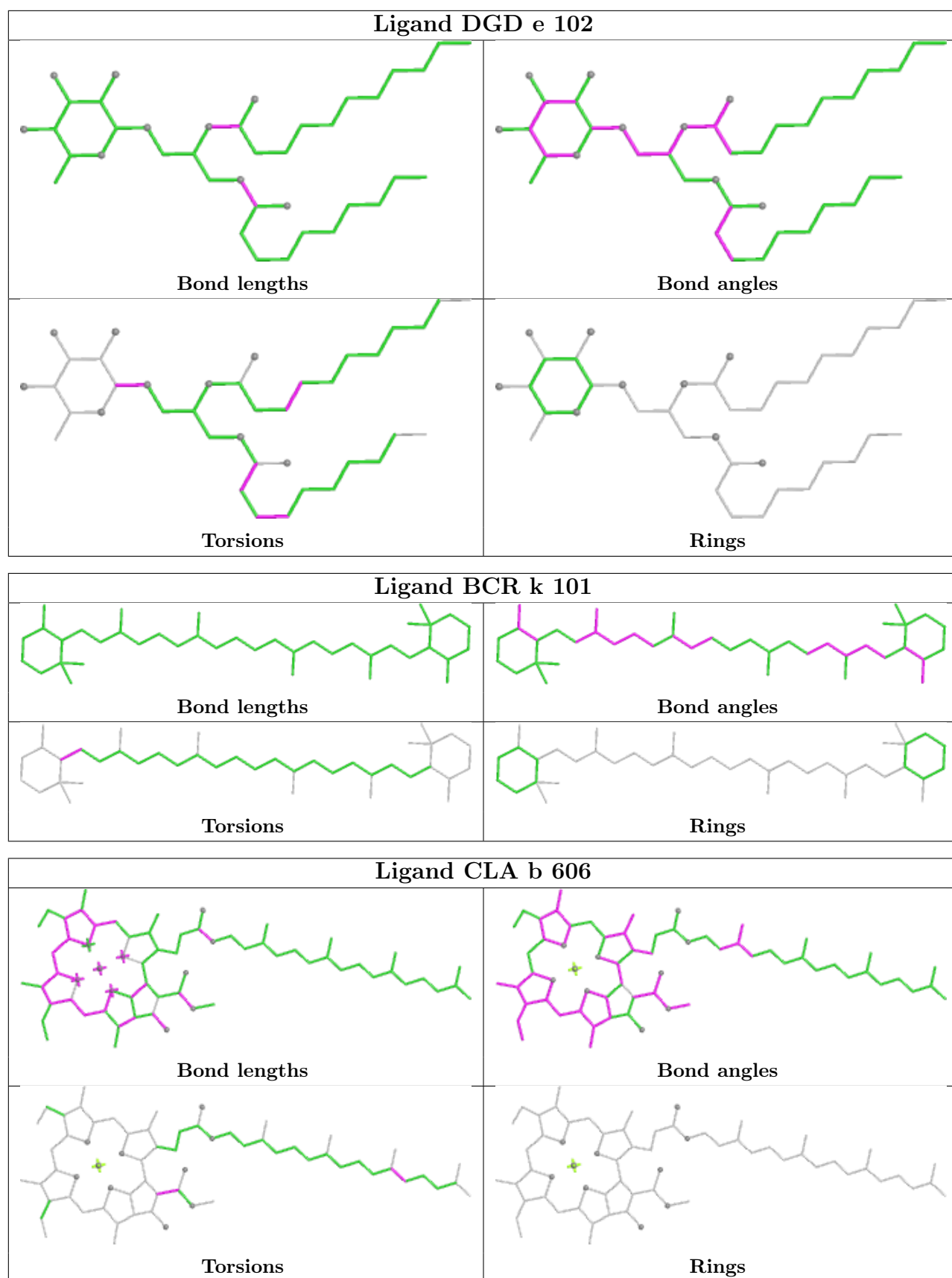
Ligand LHG e 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 615	
 Bond lengths	 Bond angles
 Torsions	 Rings

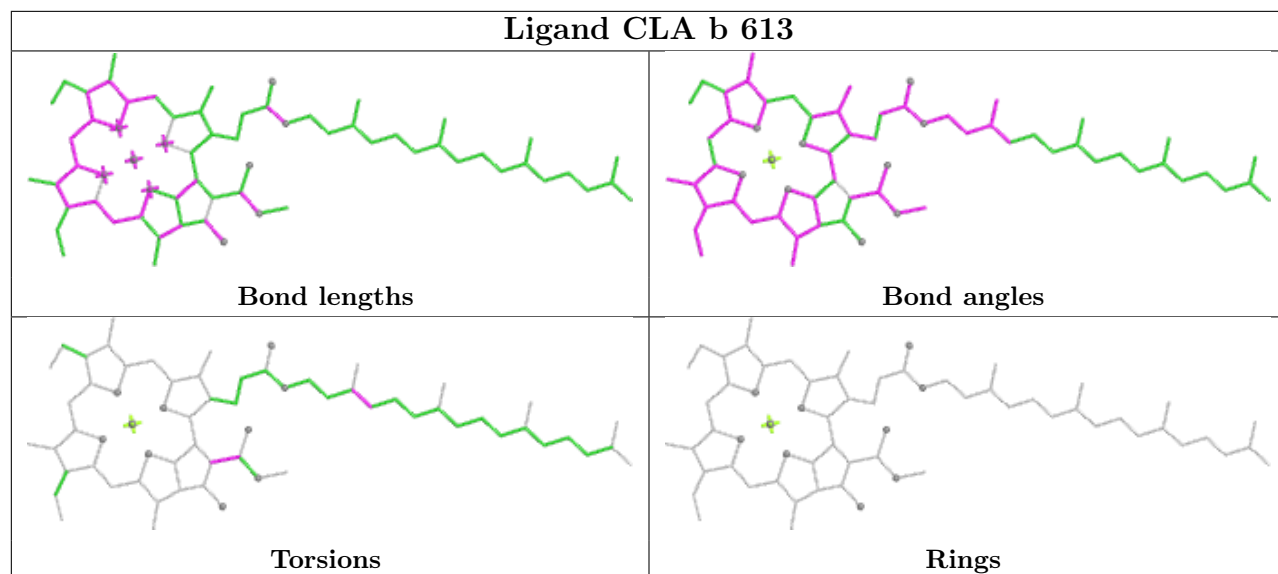




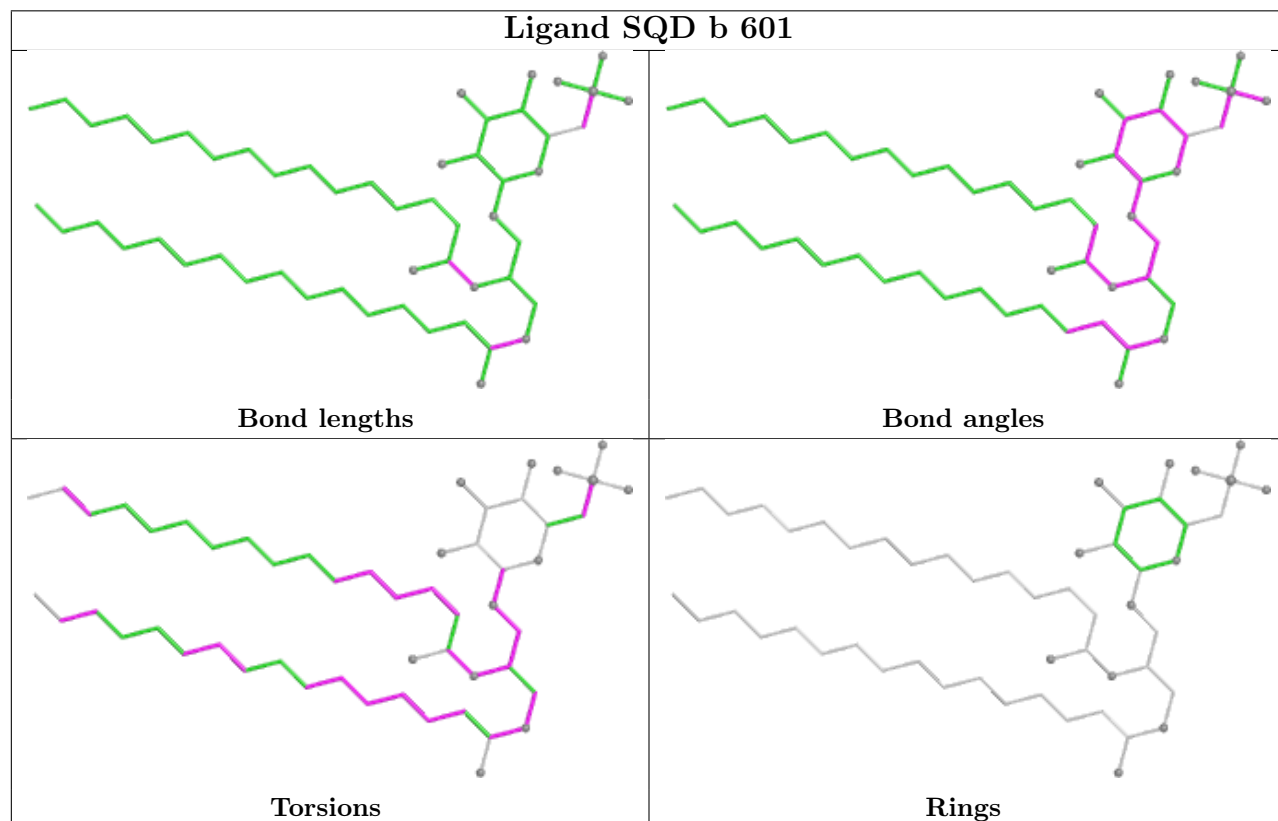




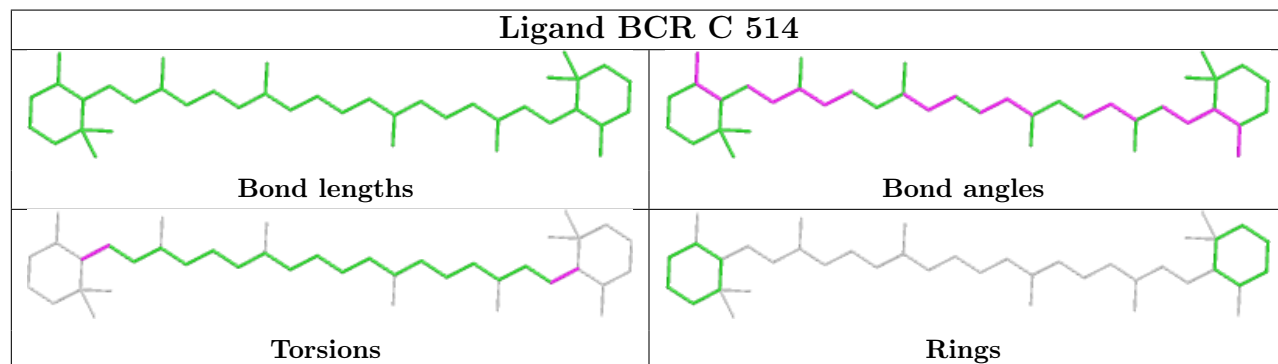
Ligand CLA b 613

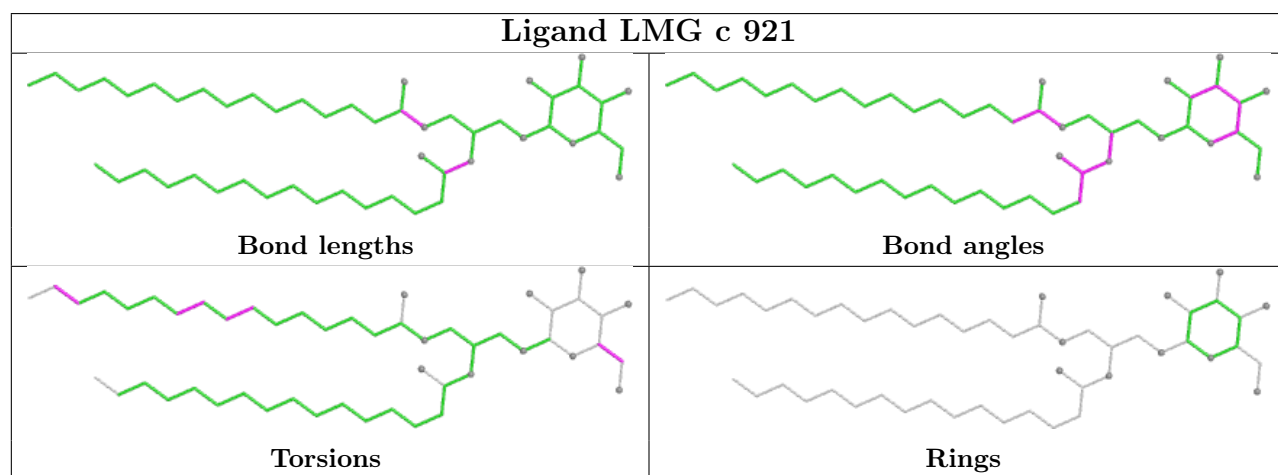
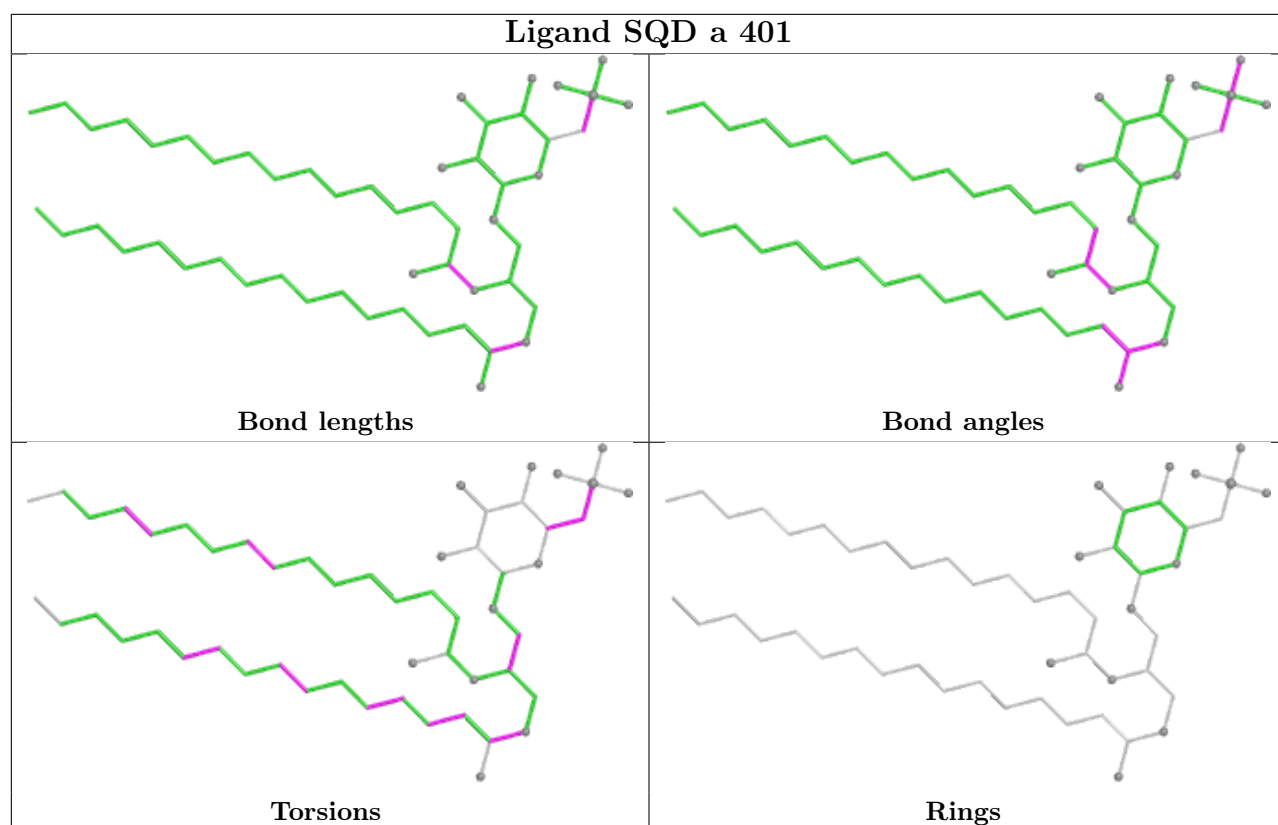


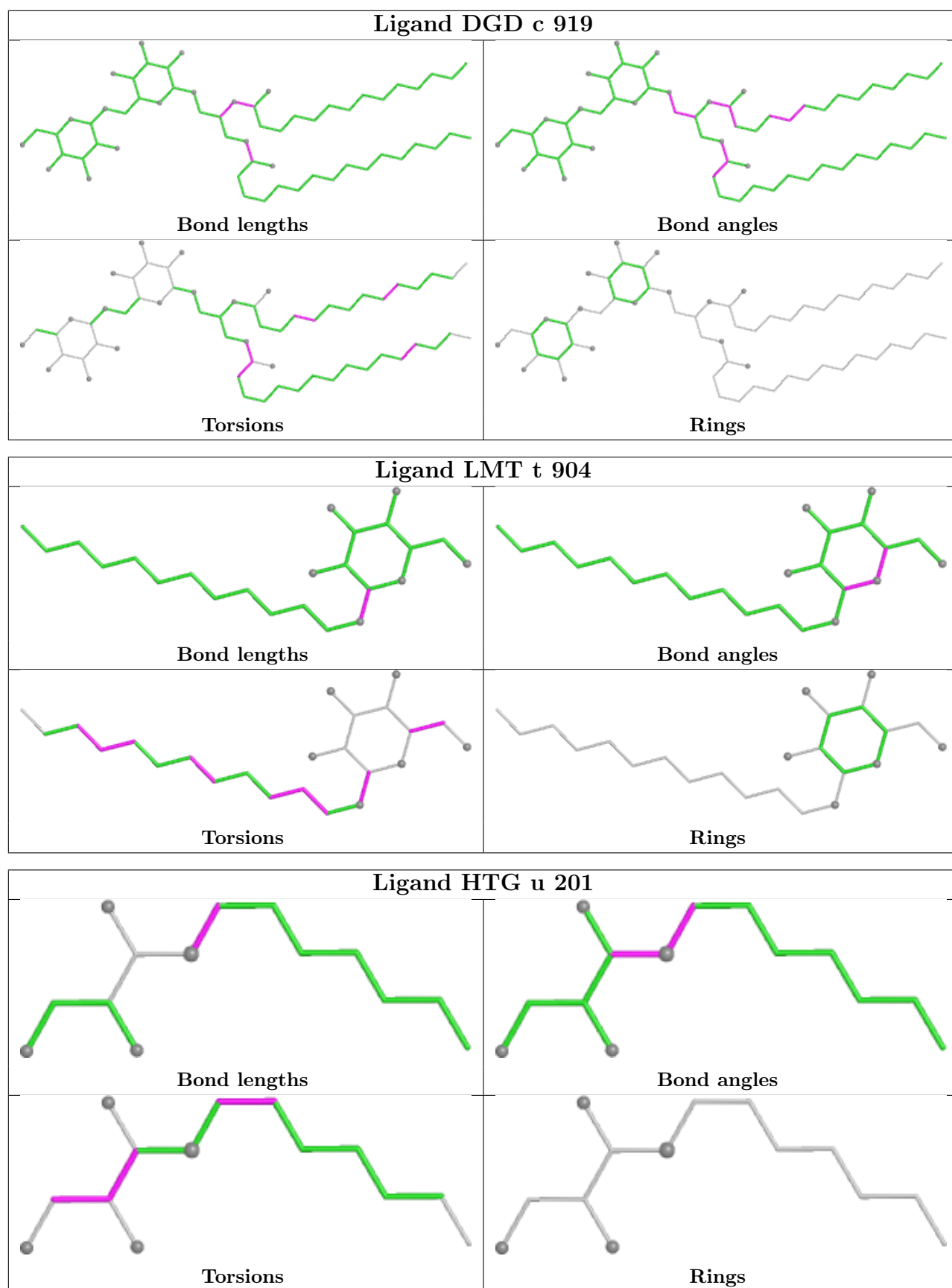
Ligand SQD b 601

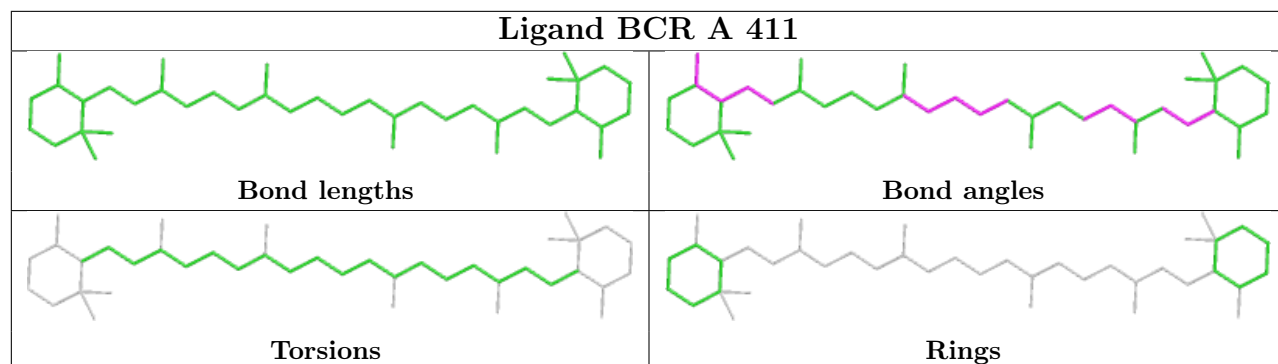
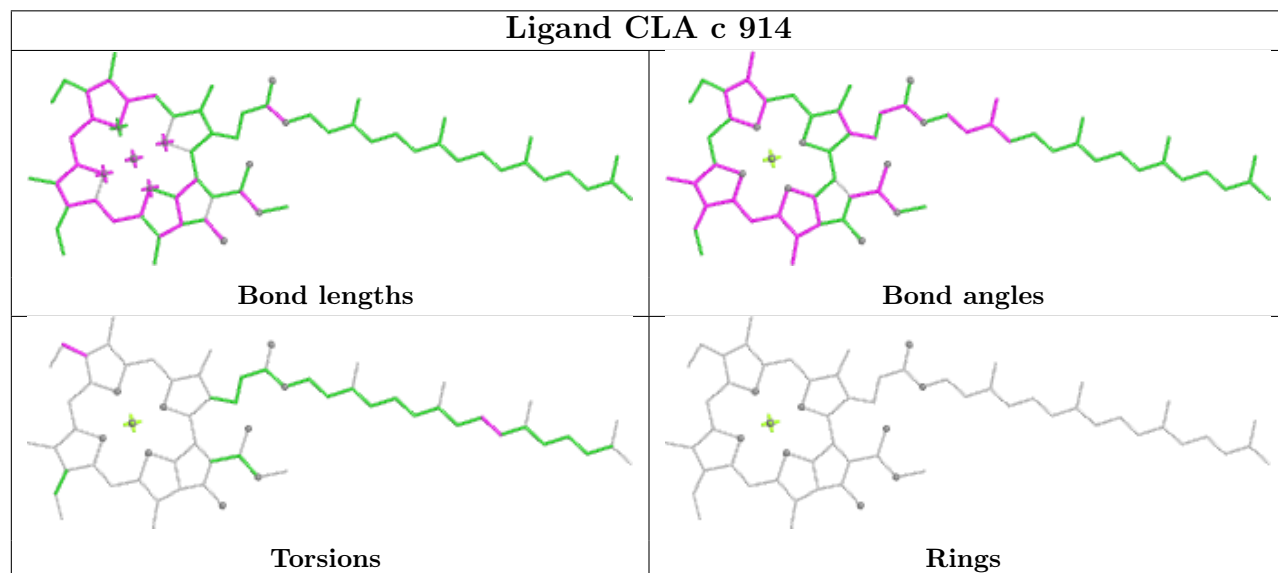
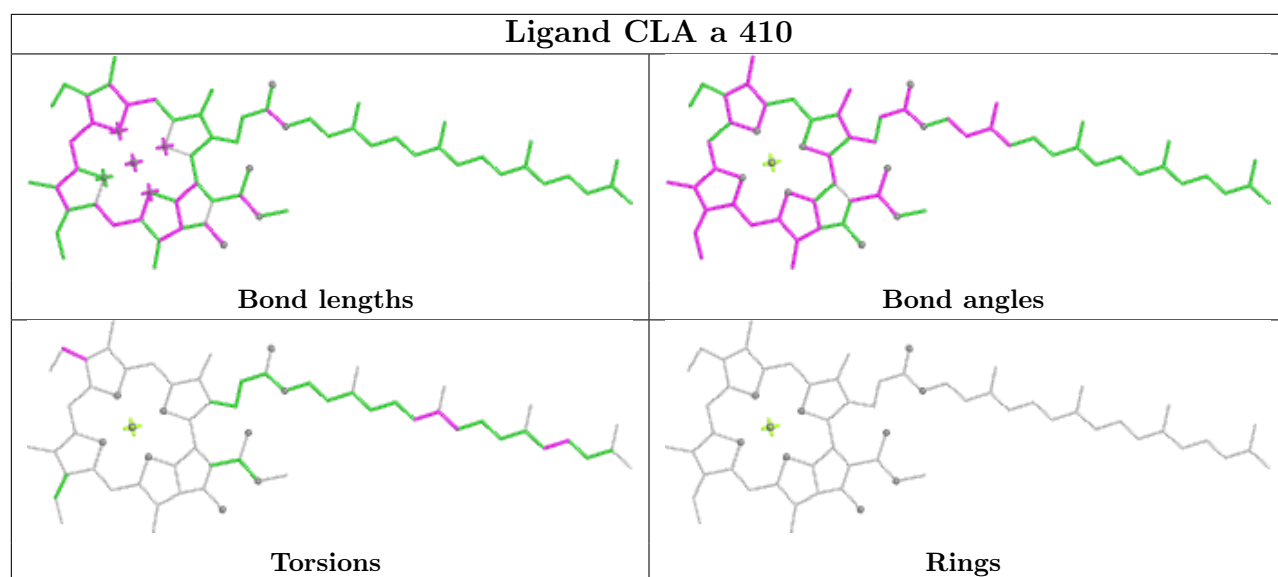


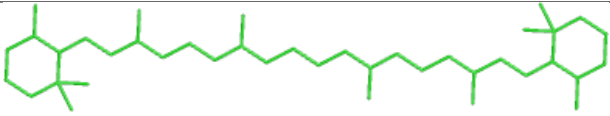
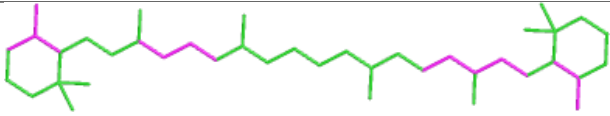
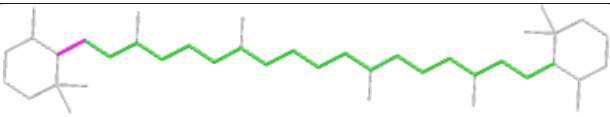
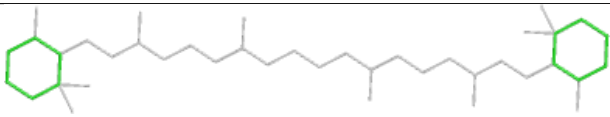
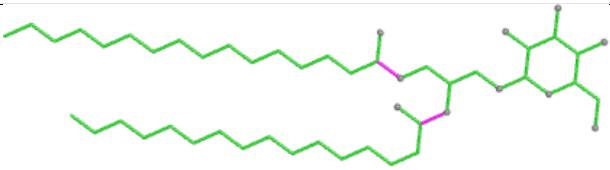
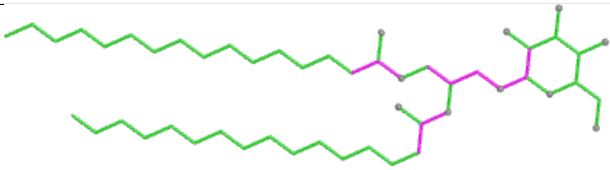
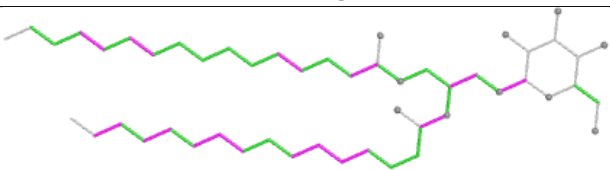
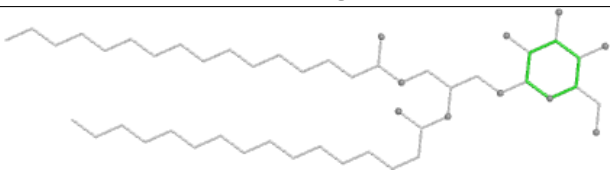
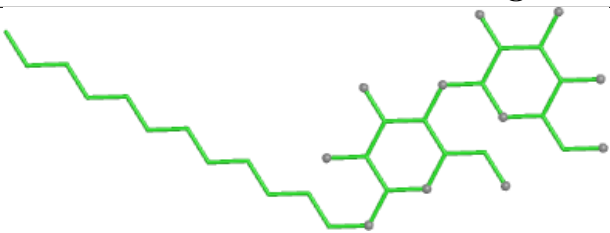
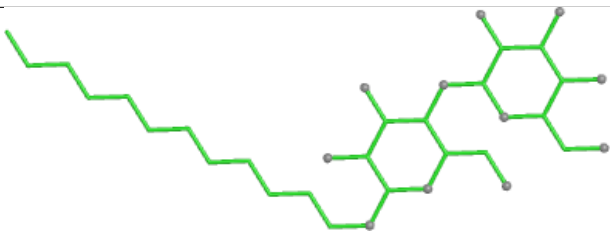
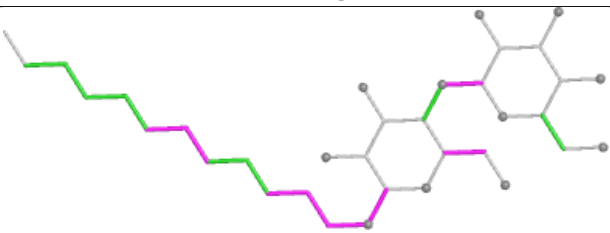
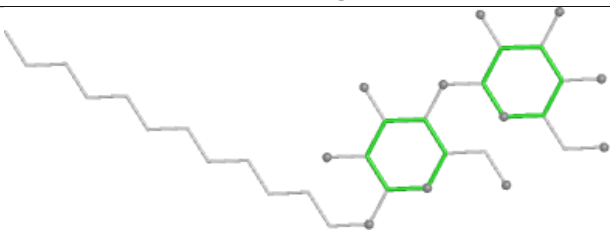
Ligand BCR C 514



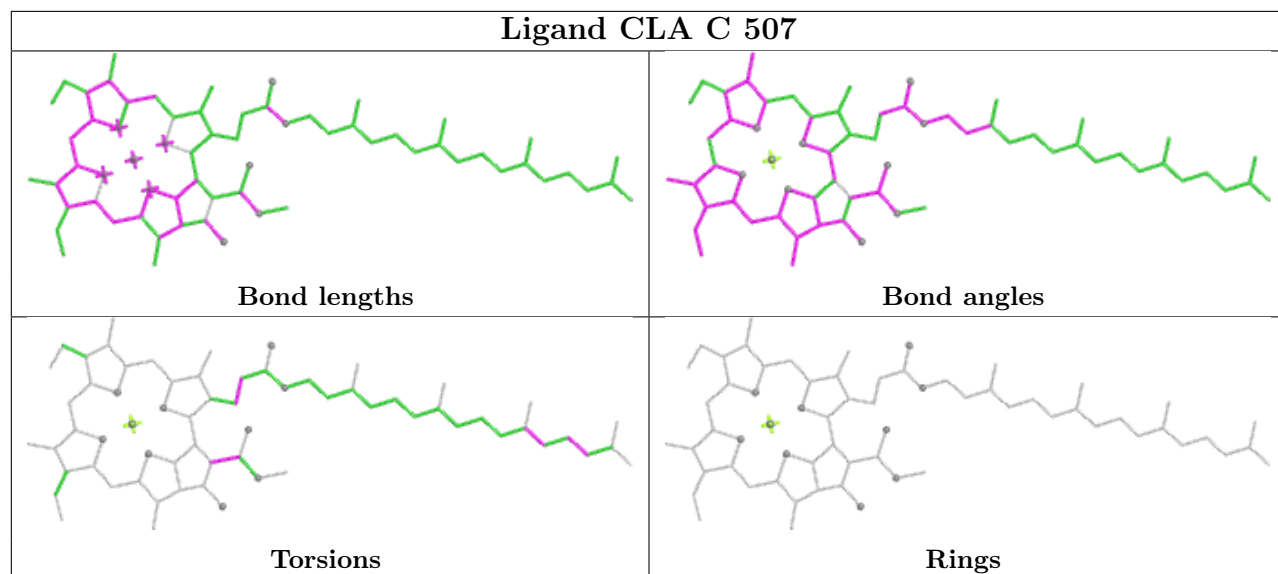




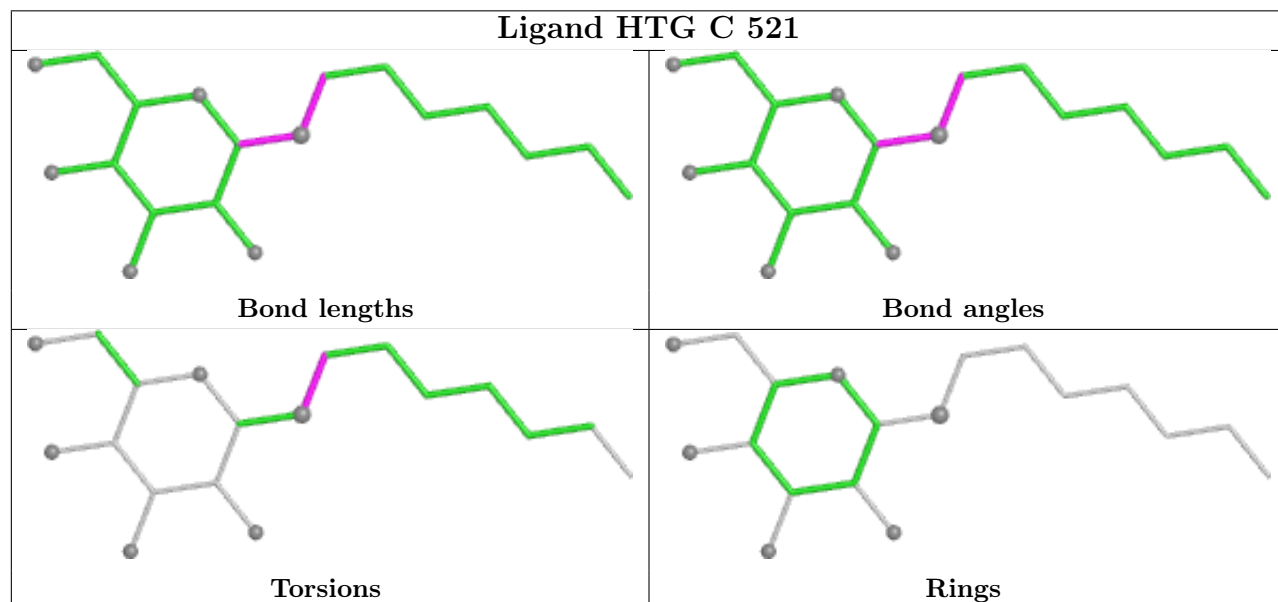


Ligand BCR K 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG A 413	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMT Z 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

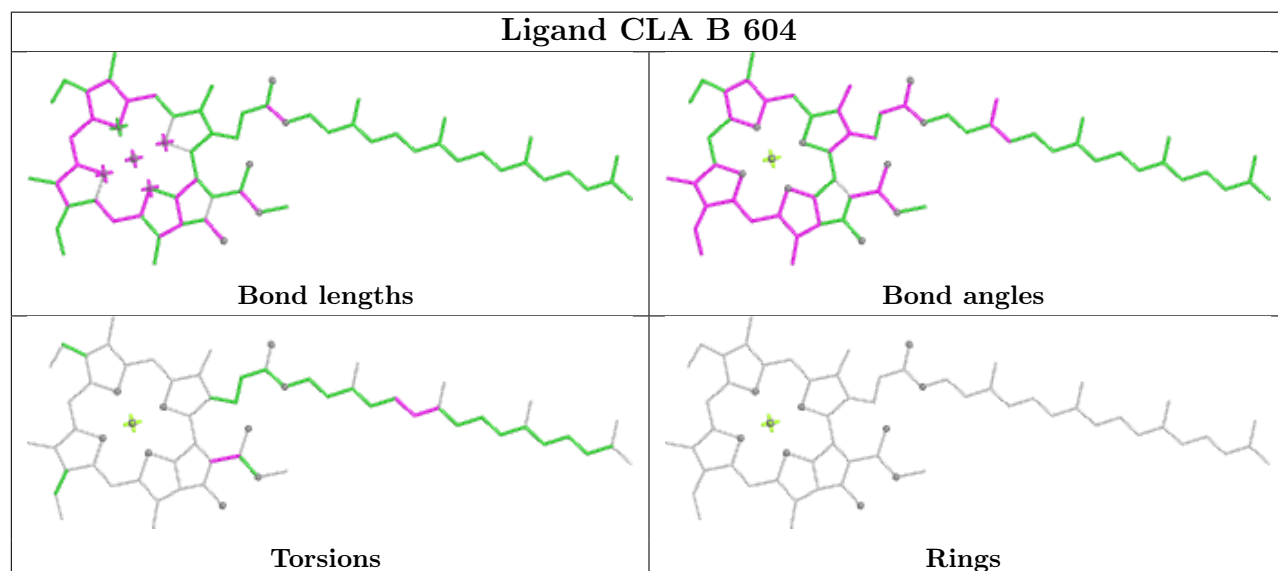
Ligand CLA C 507

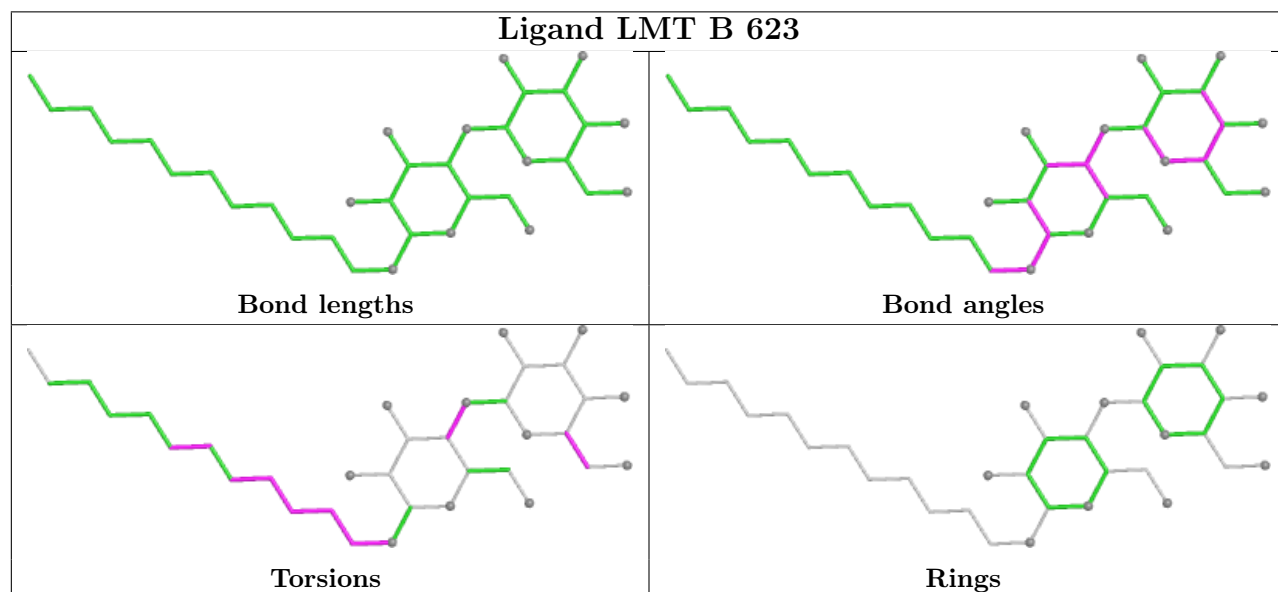
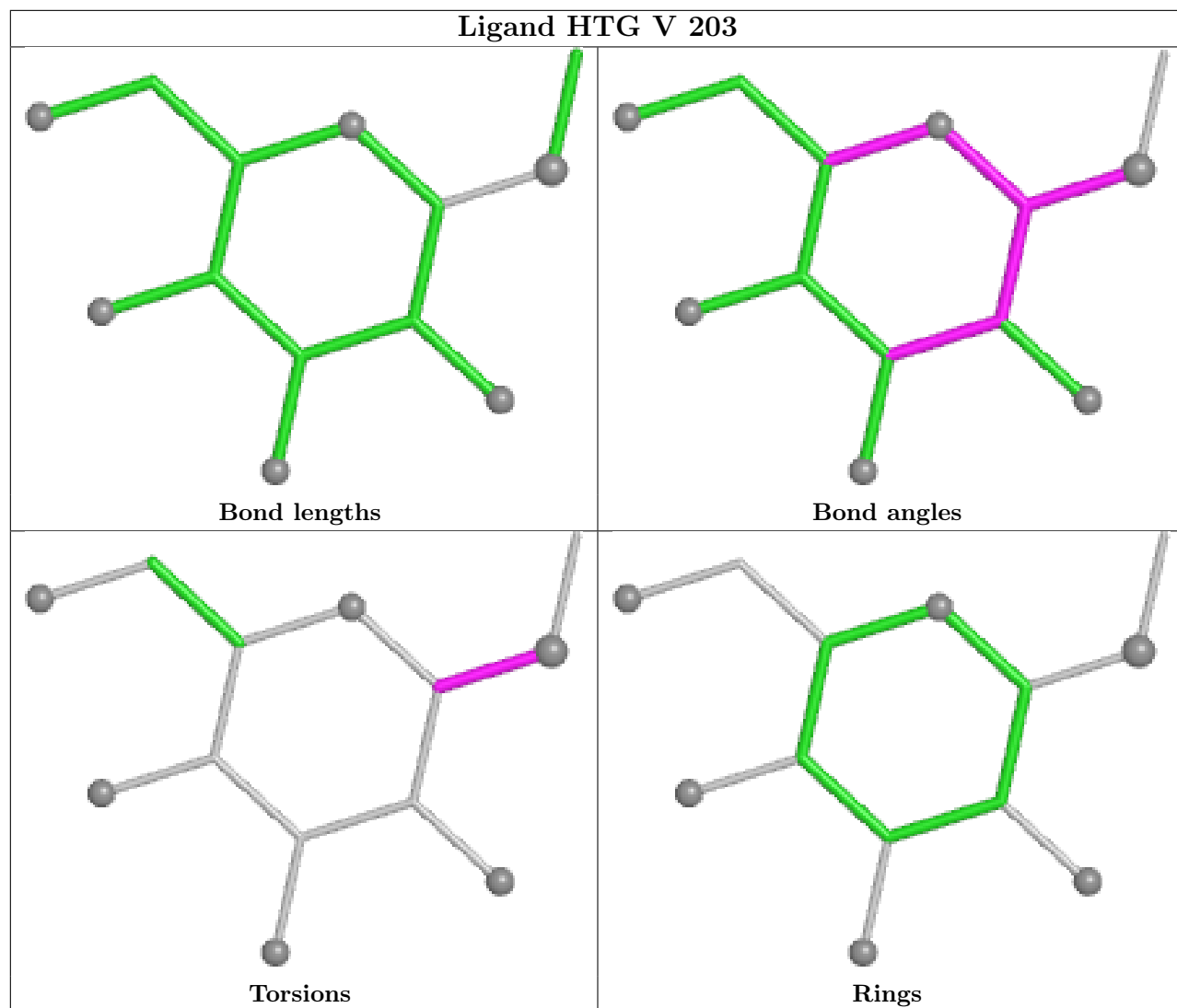


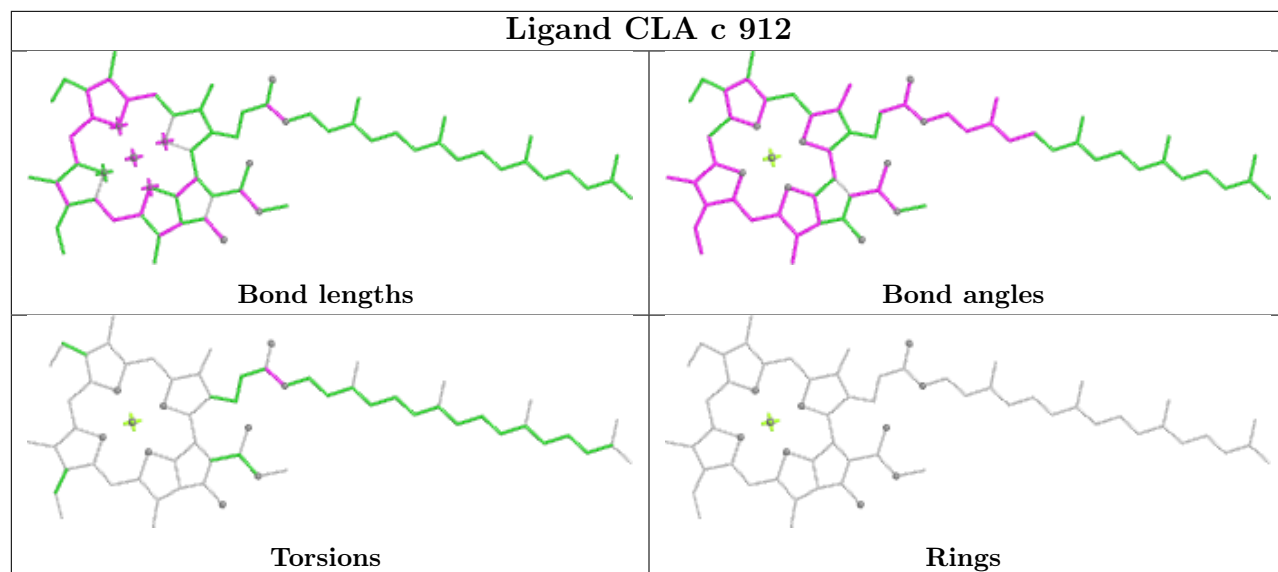
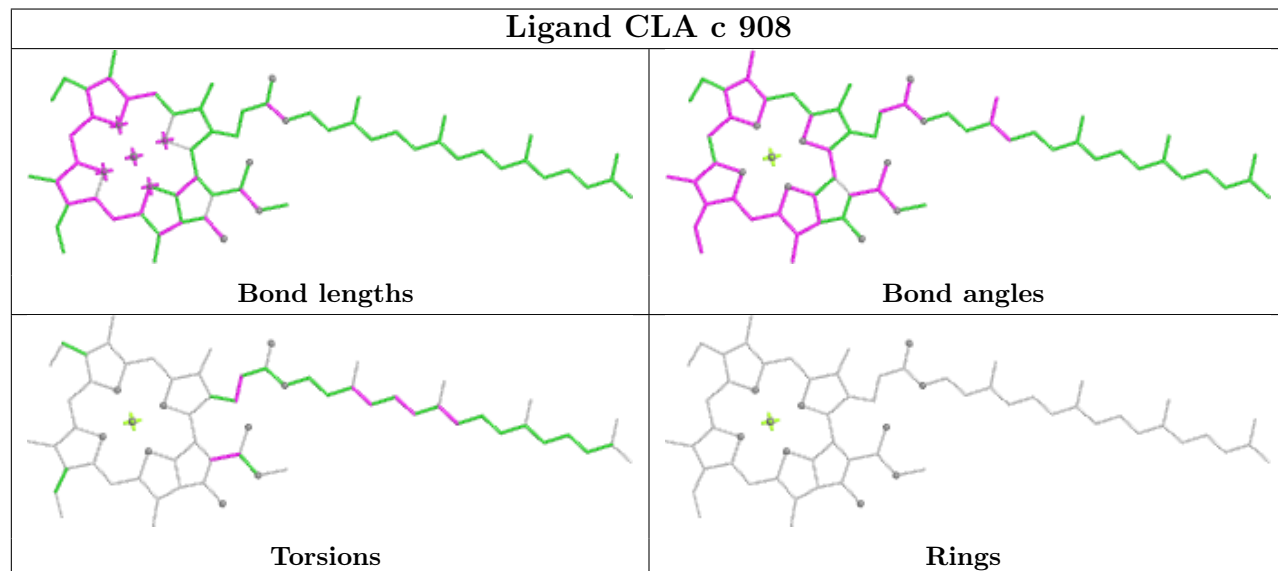
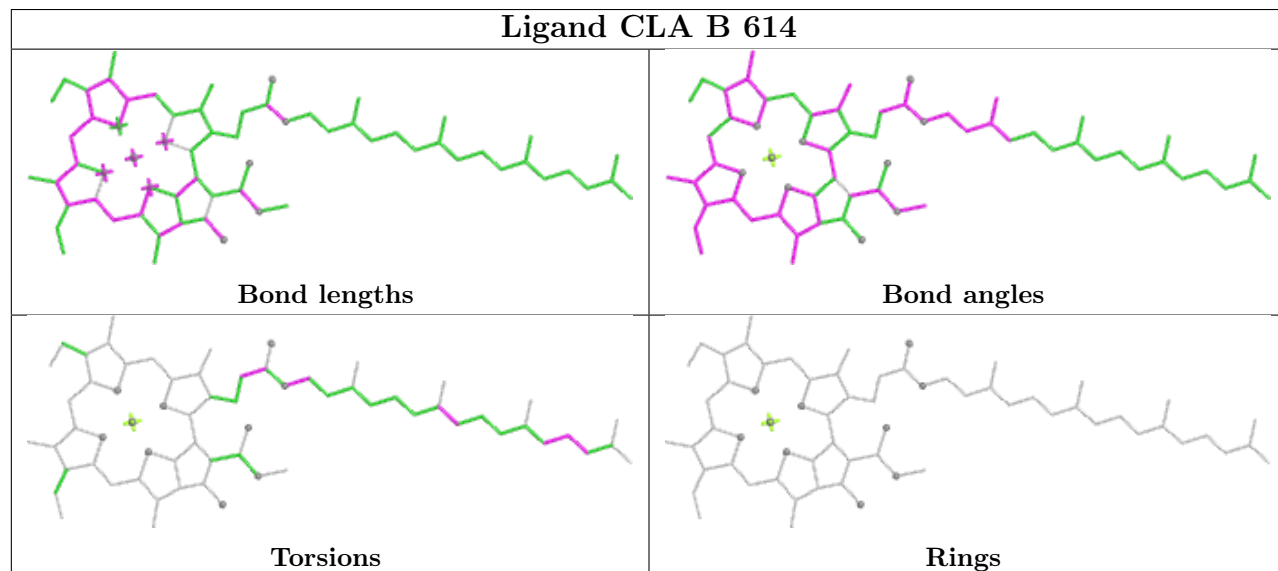
Ligand HTG C 521



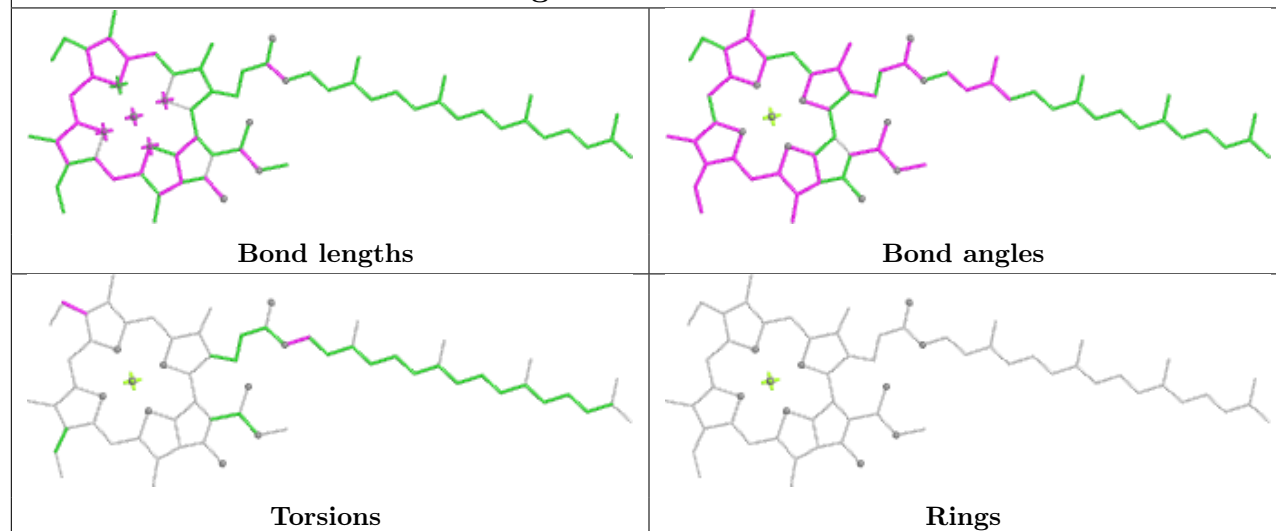
Ligand CLA B 604



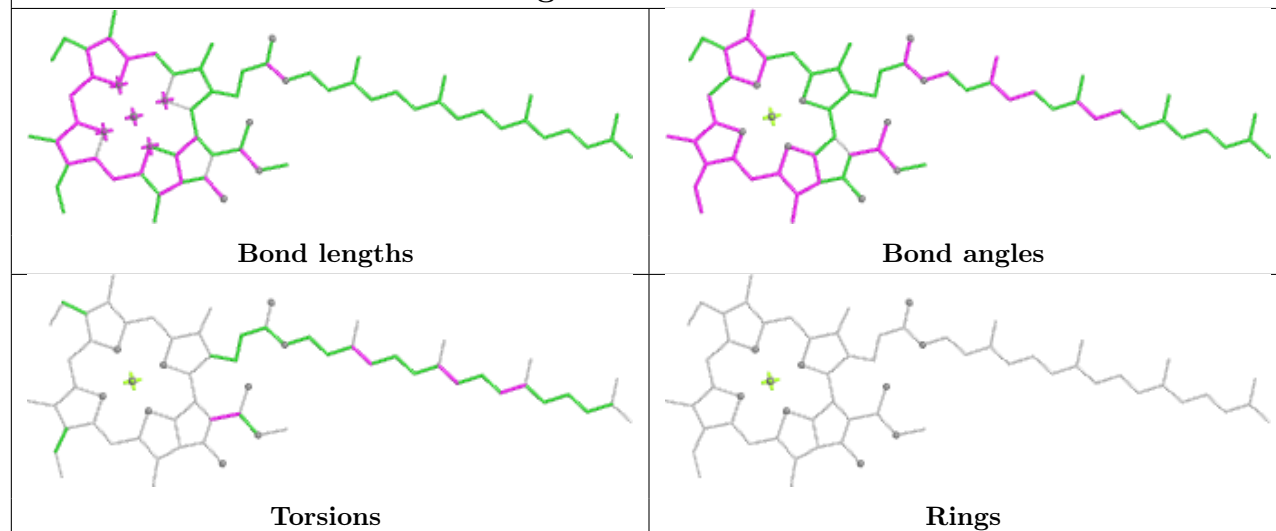


Ligand CLA c 912**Ligand CLA c 908****Ligand CLA B 614**

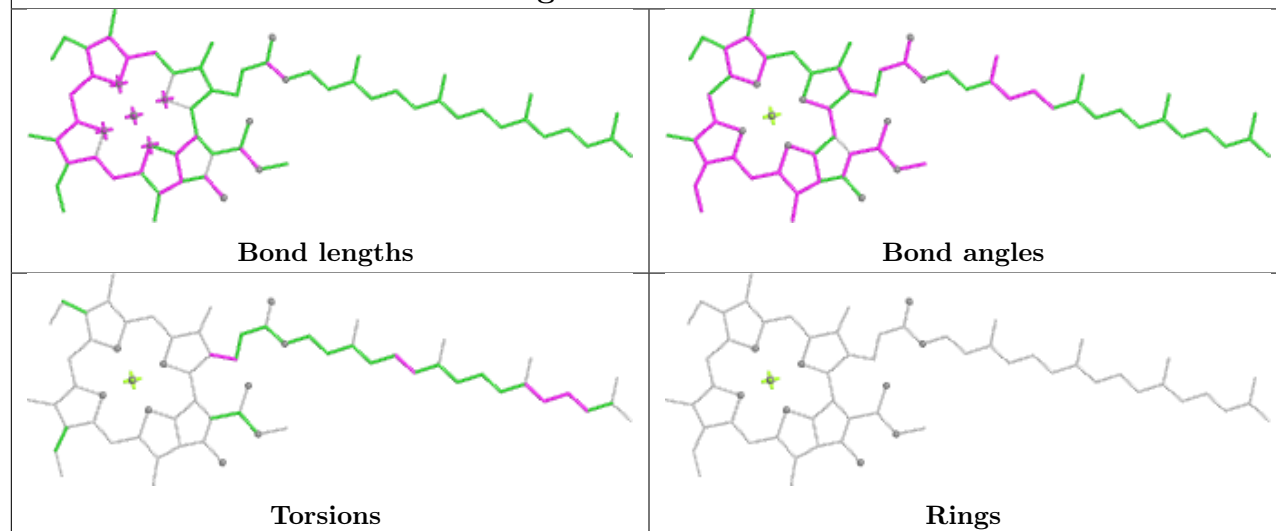
Ligand CLA D 402

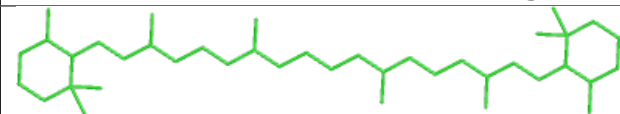
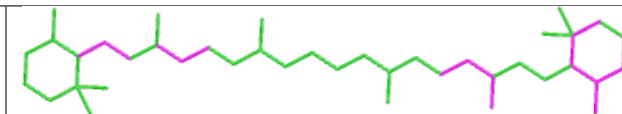
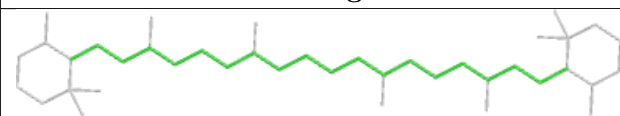
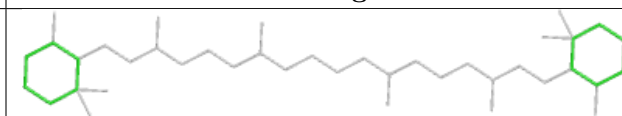


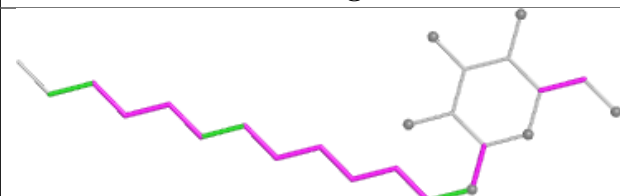
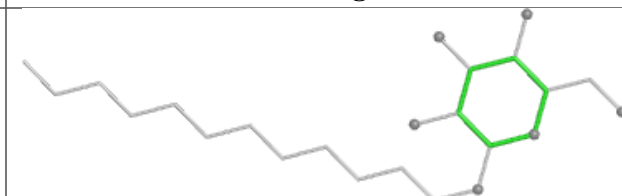
Ligand CLA c 905

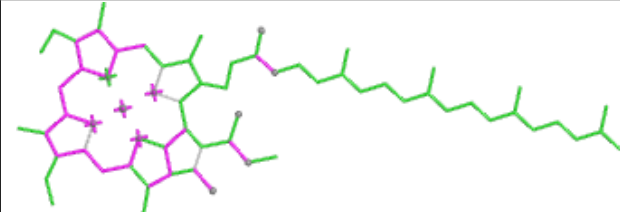
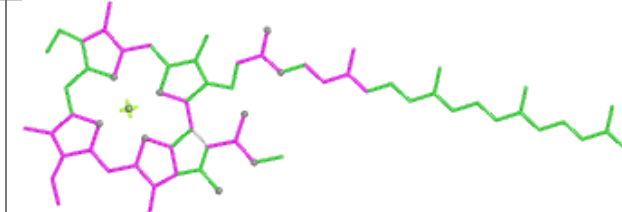
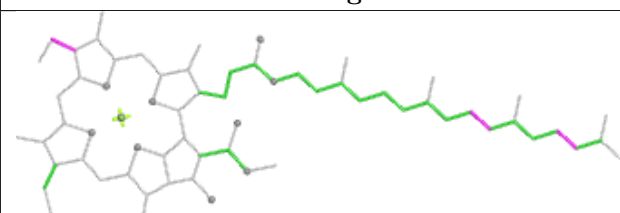
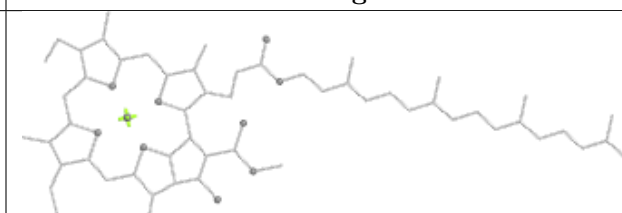


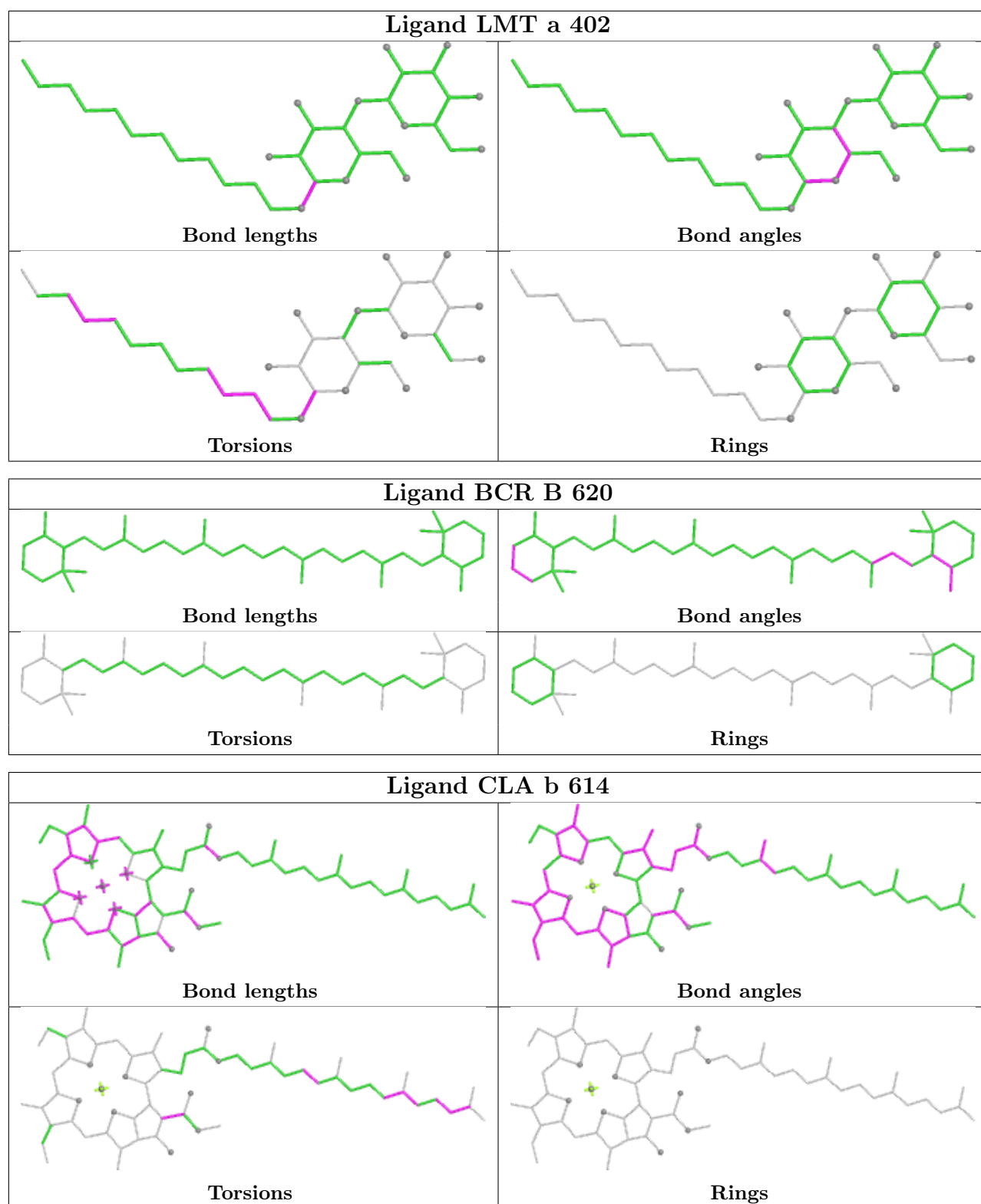
Ligand CLA c 907

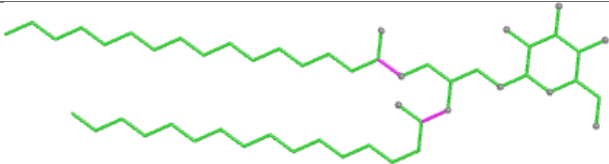
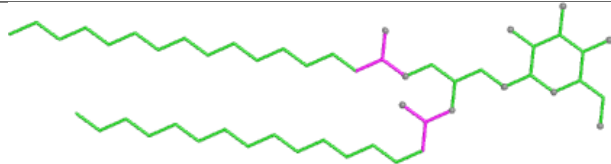
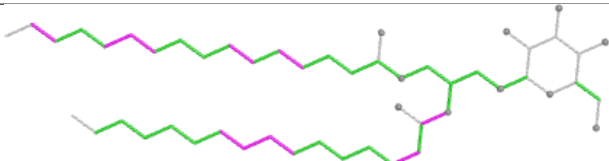
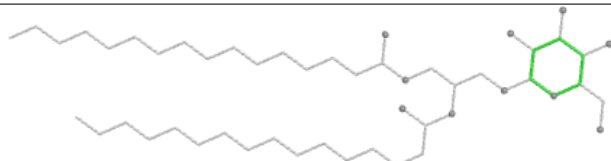
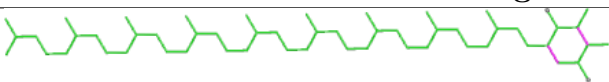
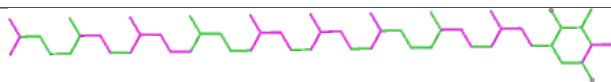
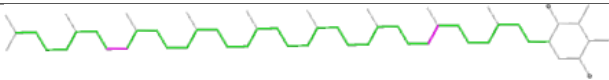
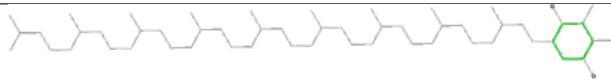
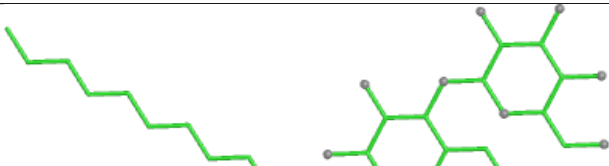
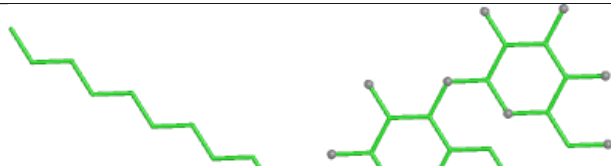
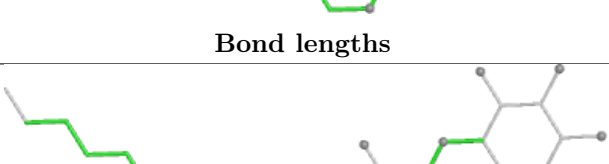
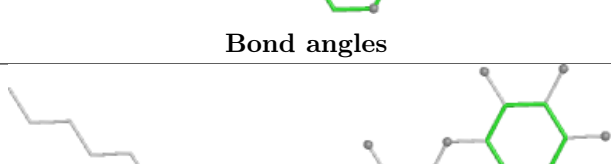
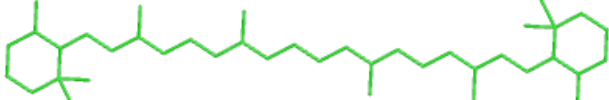
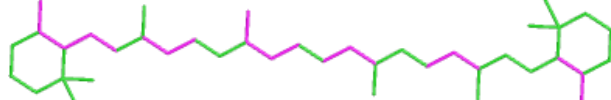
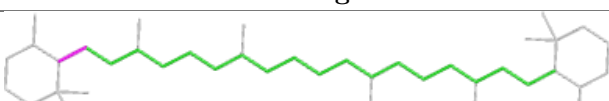
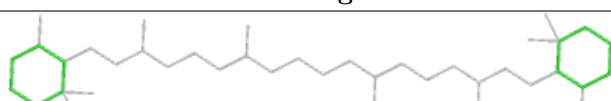


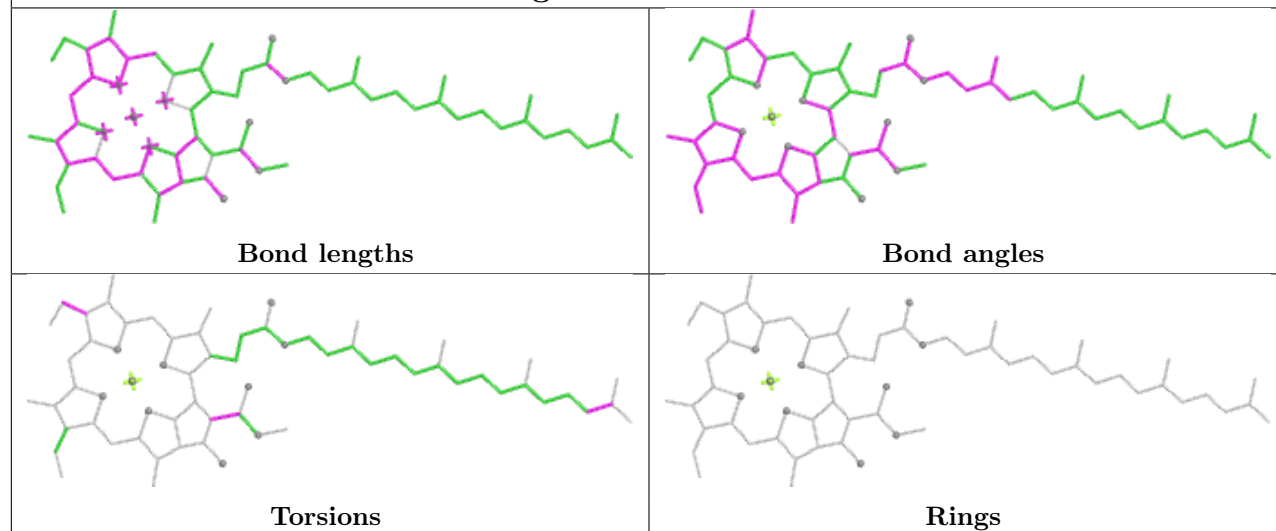
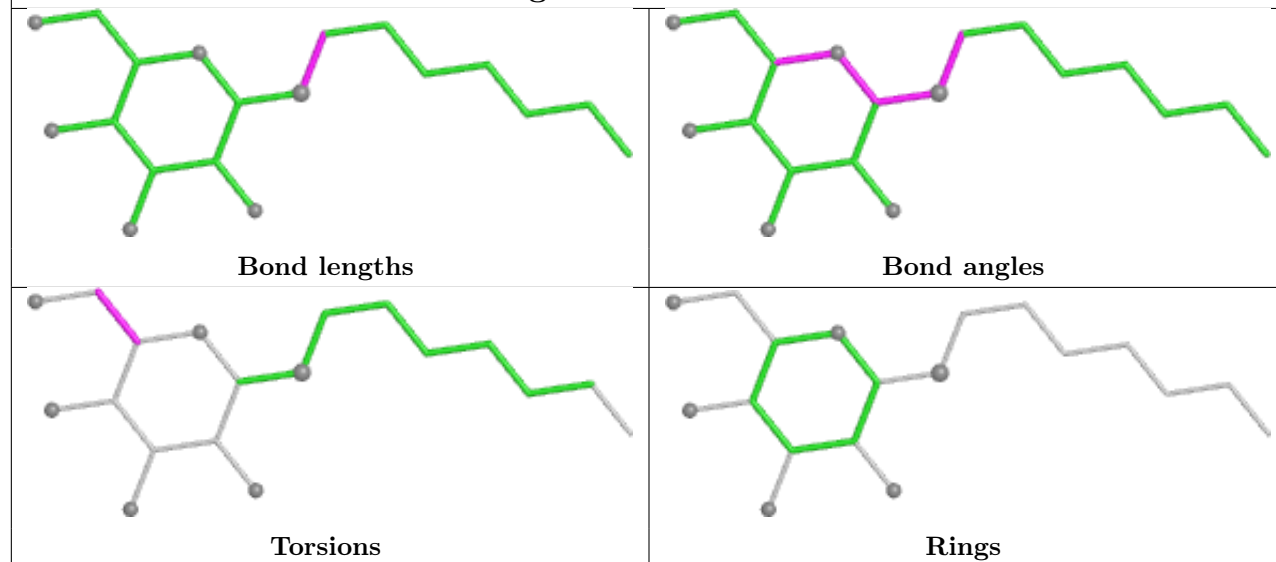
Ligand BCR b 622	
	
Bond lengths	Bond angles
	
Torsions	Rings

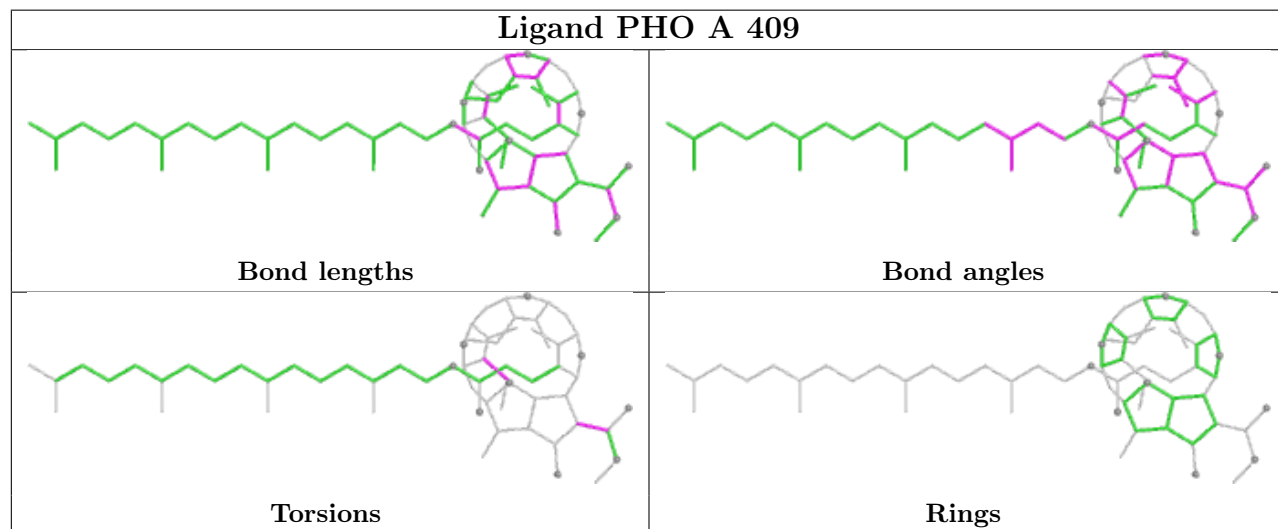
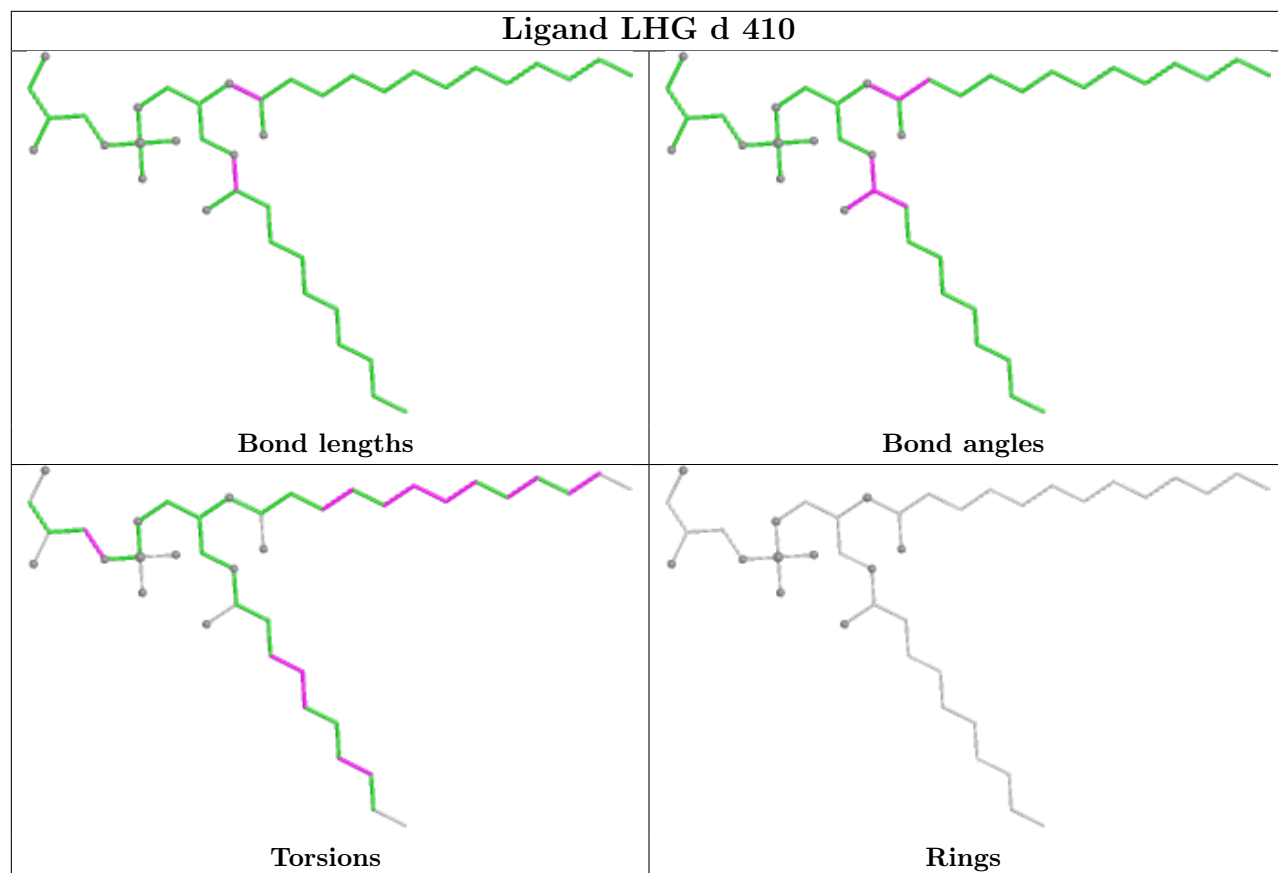
Ligand LMT T 703	
	
Bond lengths	Bond angles
	
Torsions	Rings

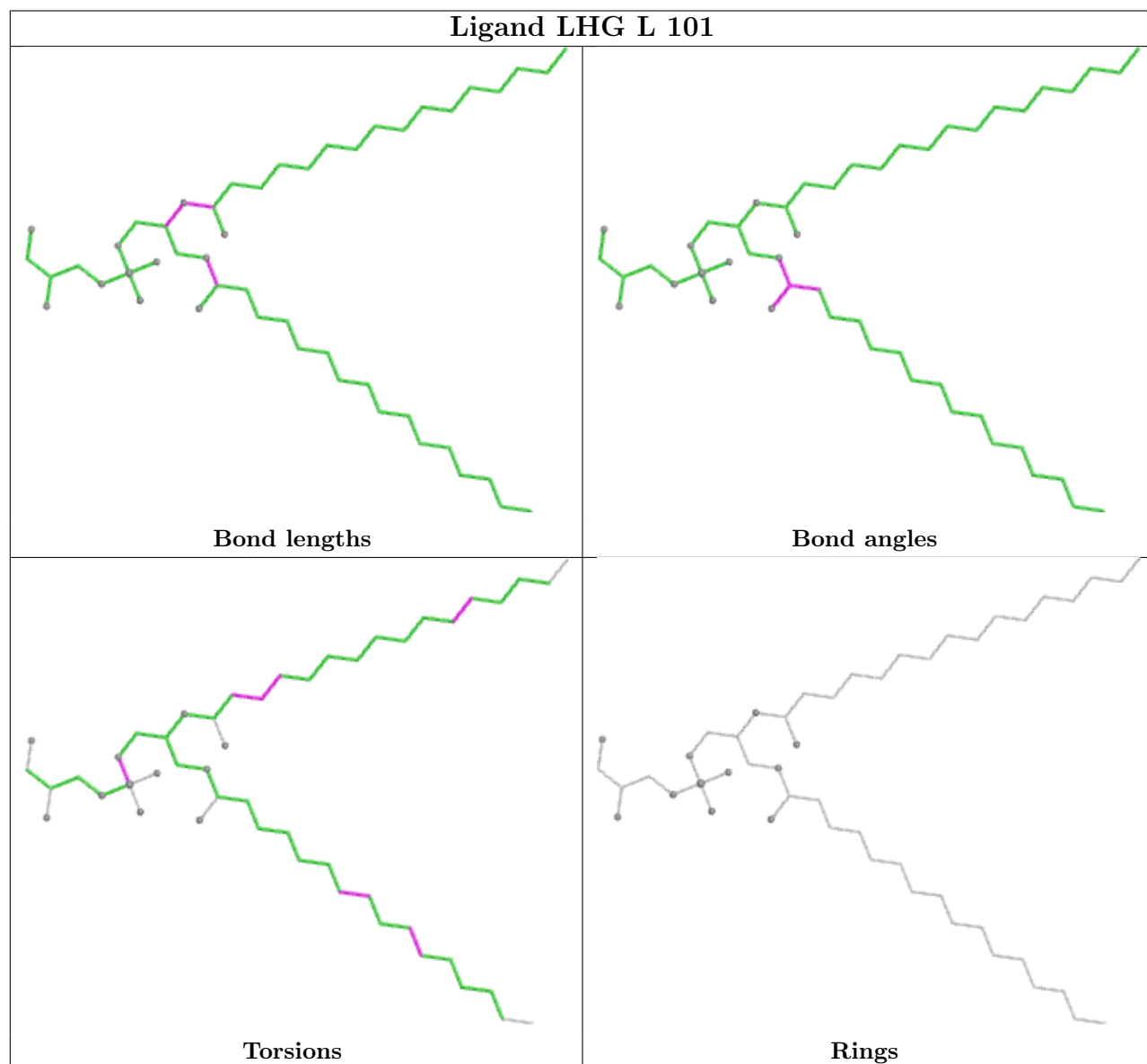
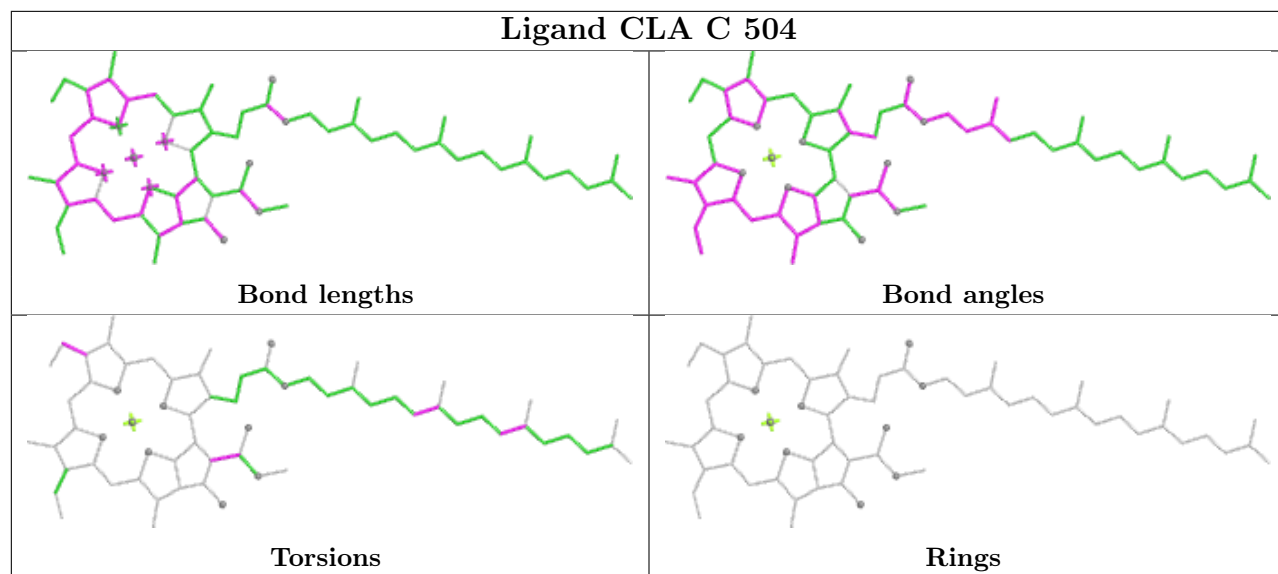
Ligand CLA C 503	
	
Bond lengths	Bond angles
	
Torsions	Rings

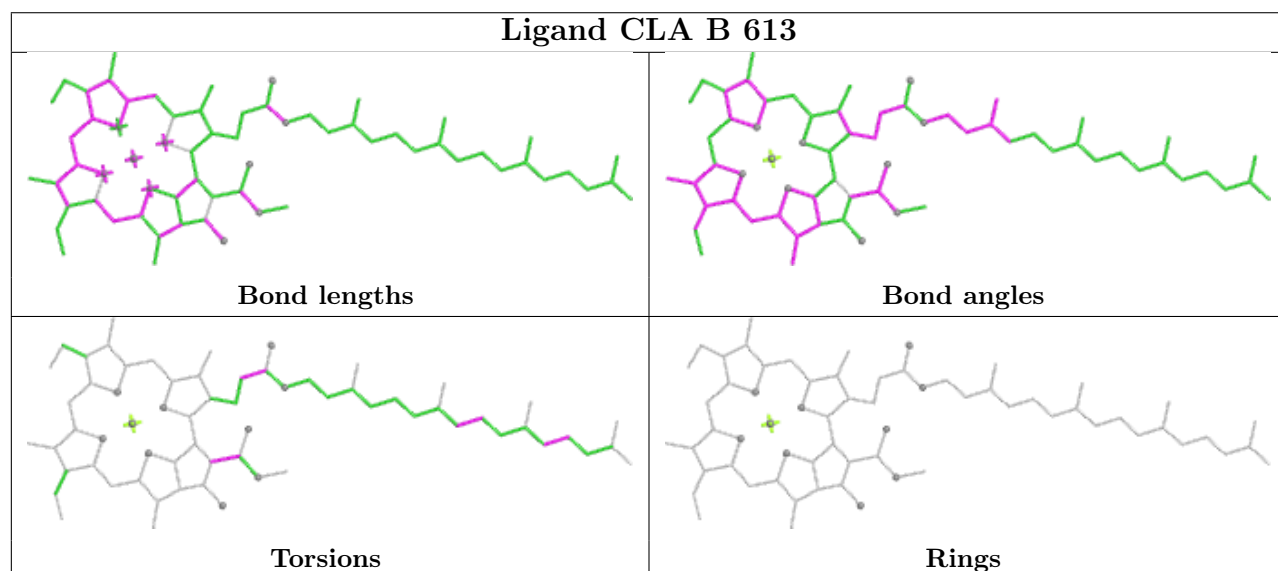
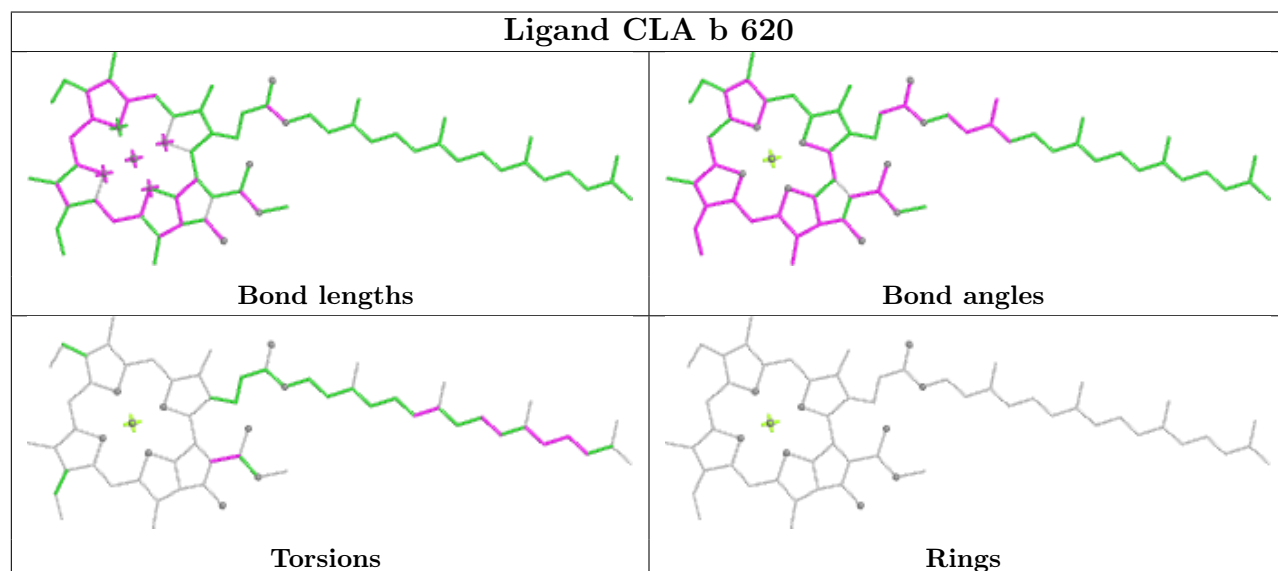
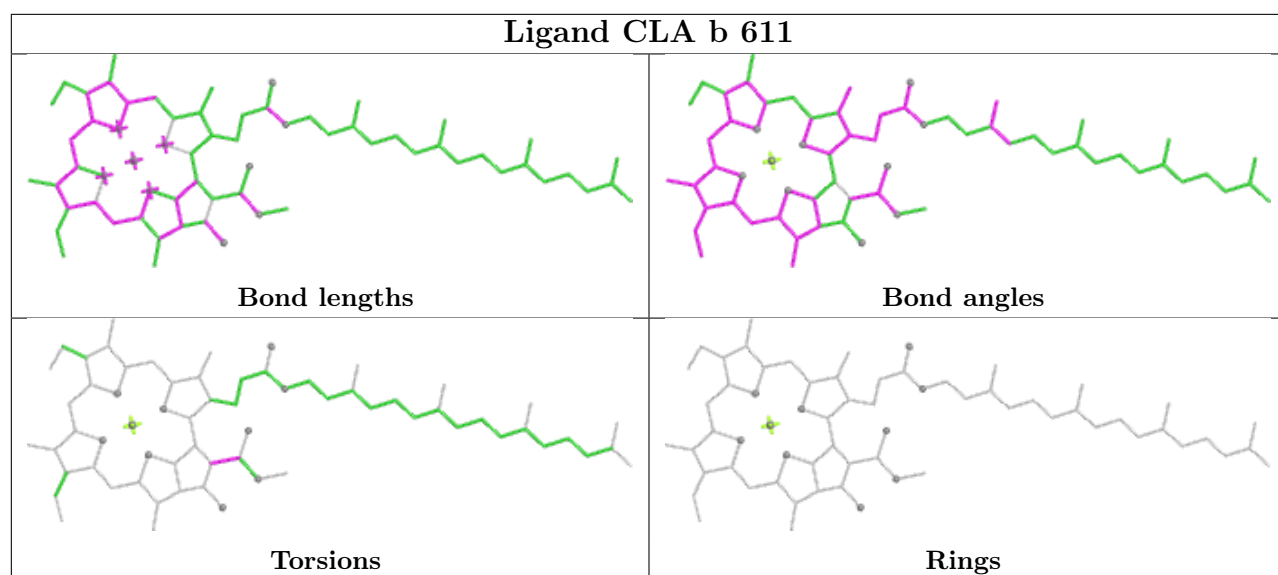


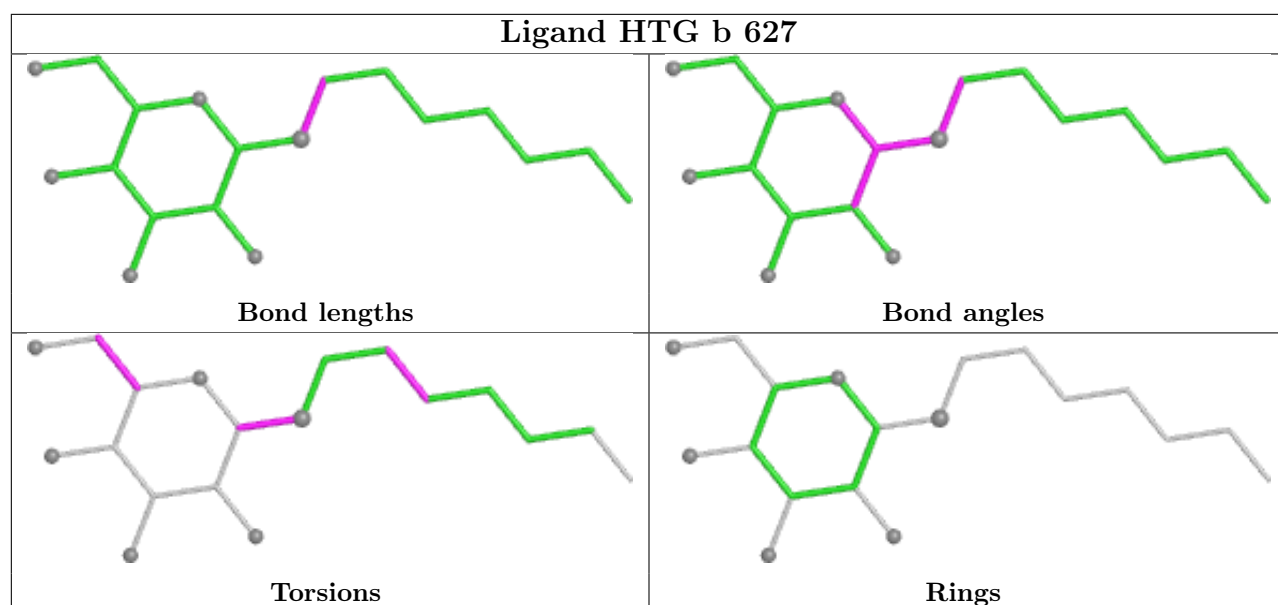
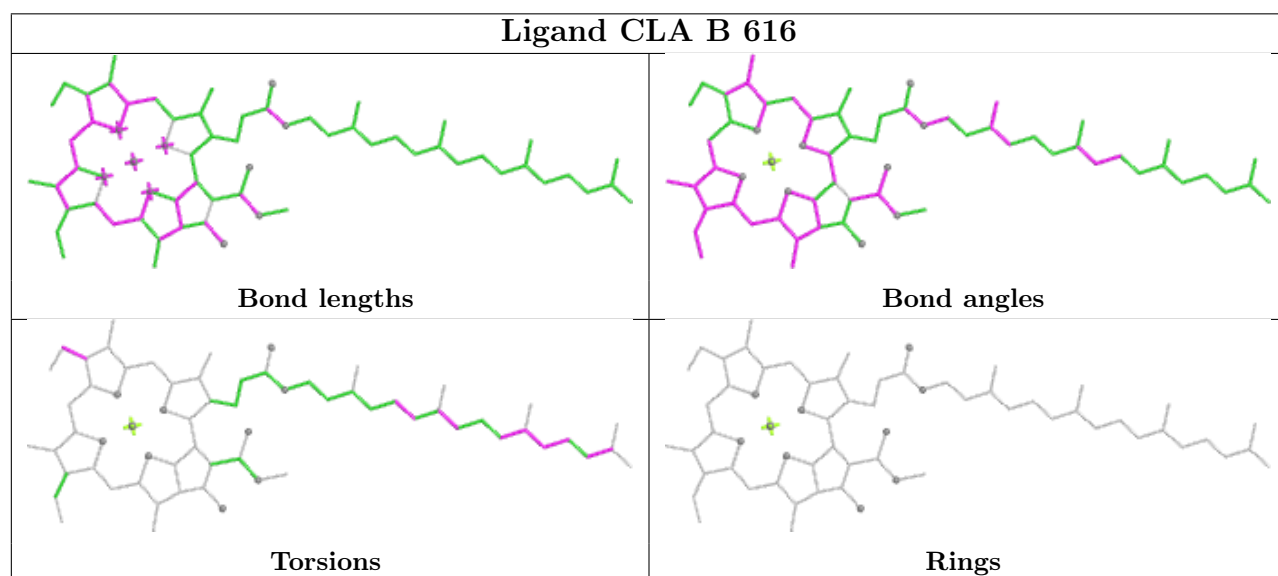
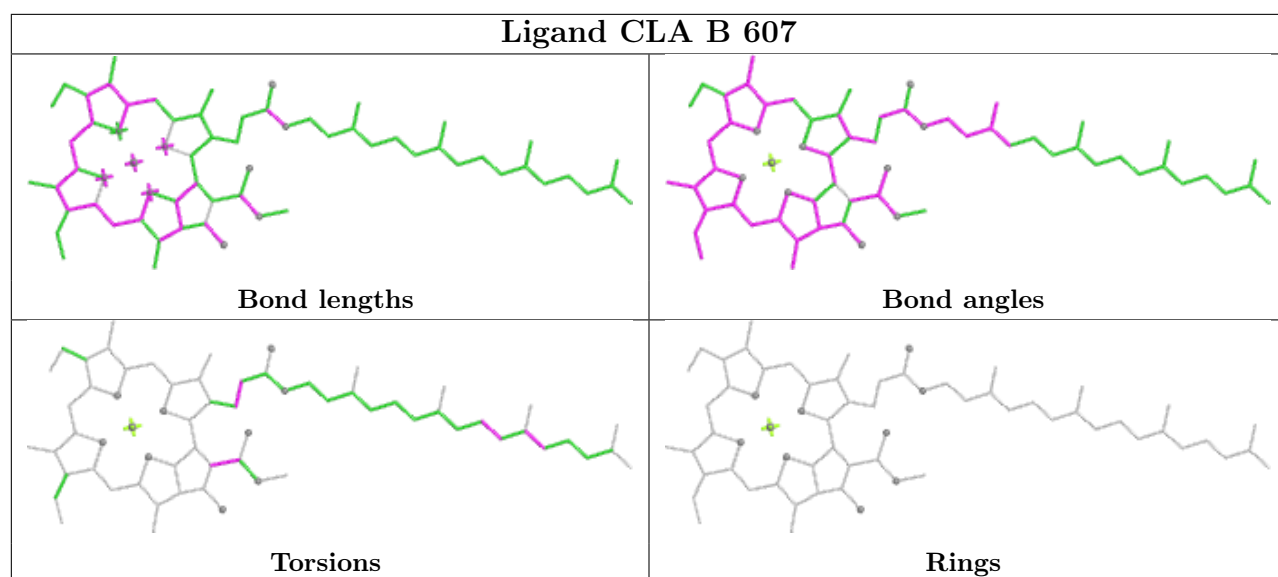
Ligand LMG B 622			
			
Bond lengths		Bond angles	
			
Torsions		Rings	
Ligand PL9 D 405			
			
Bond lengths		Bond angles	
			
Torsions		Rings	
Ligand LMT M 303			
			
Bond lengths		Bond angles	
			
Torsions		Rings	
Ligand BCR c 915			
			
Bond lengths		Bond angles	
			
Torsions		Rings	

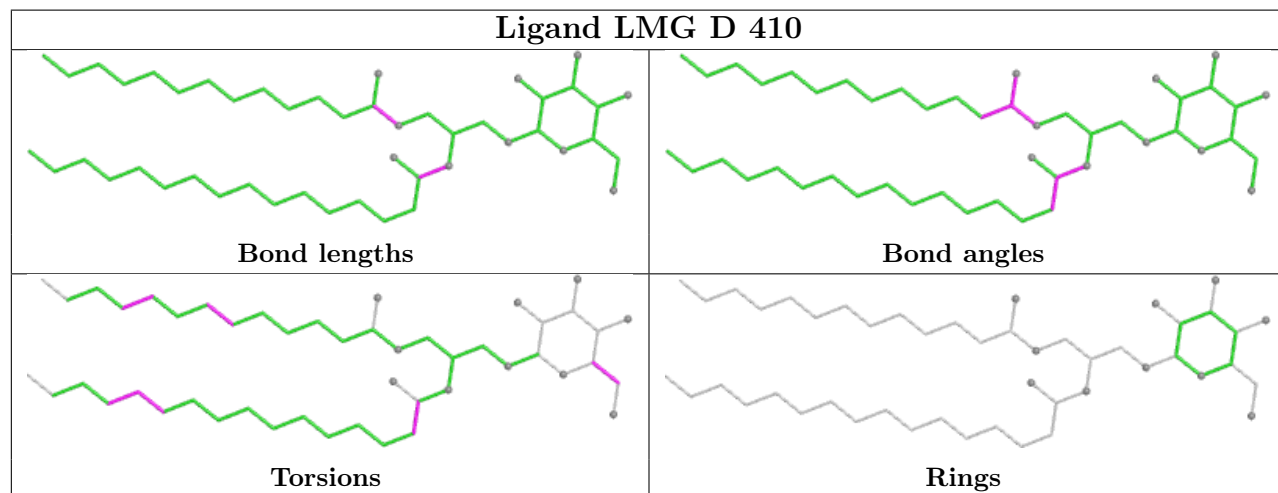
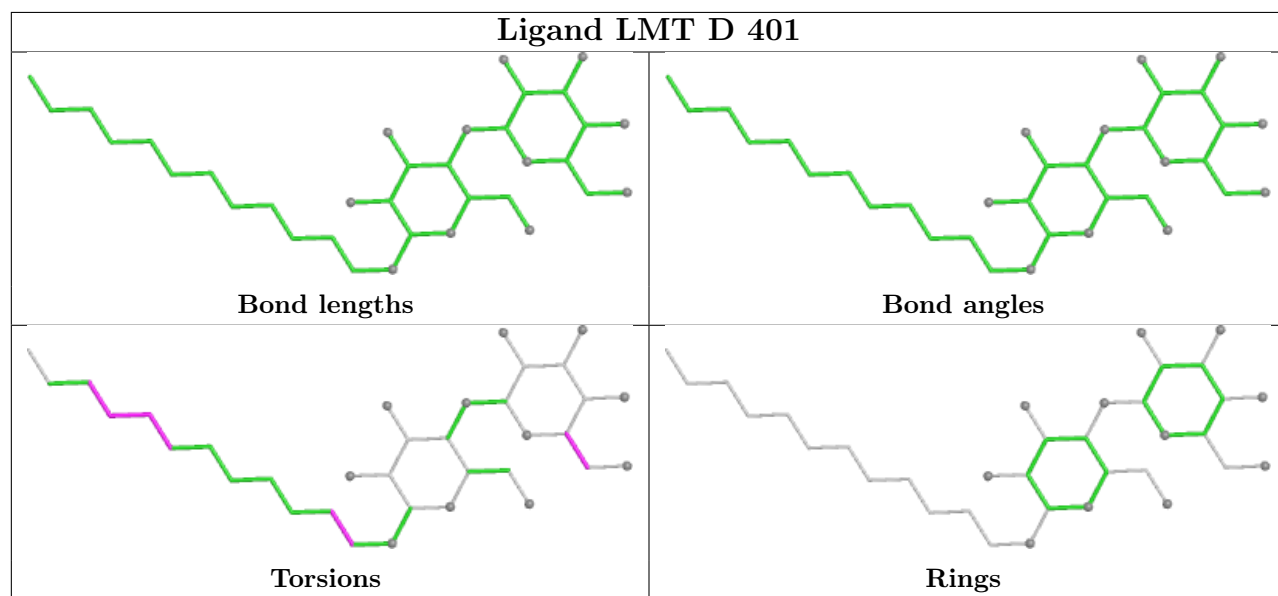
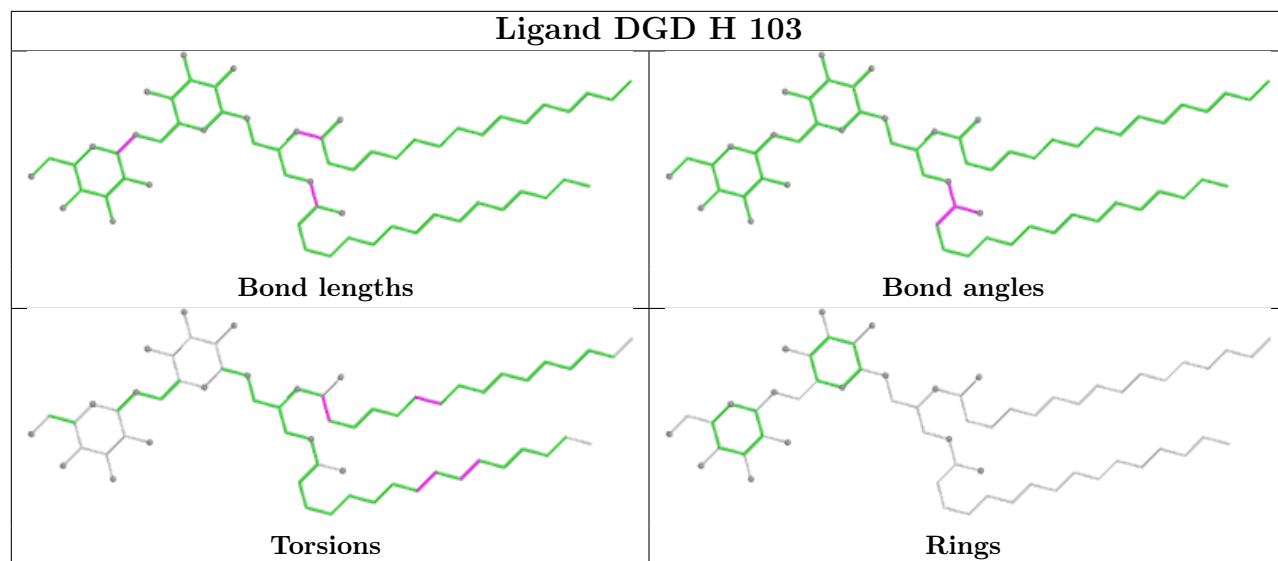
Ligand CLA C 502**Ligand HTG B 627**

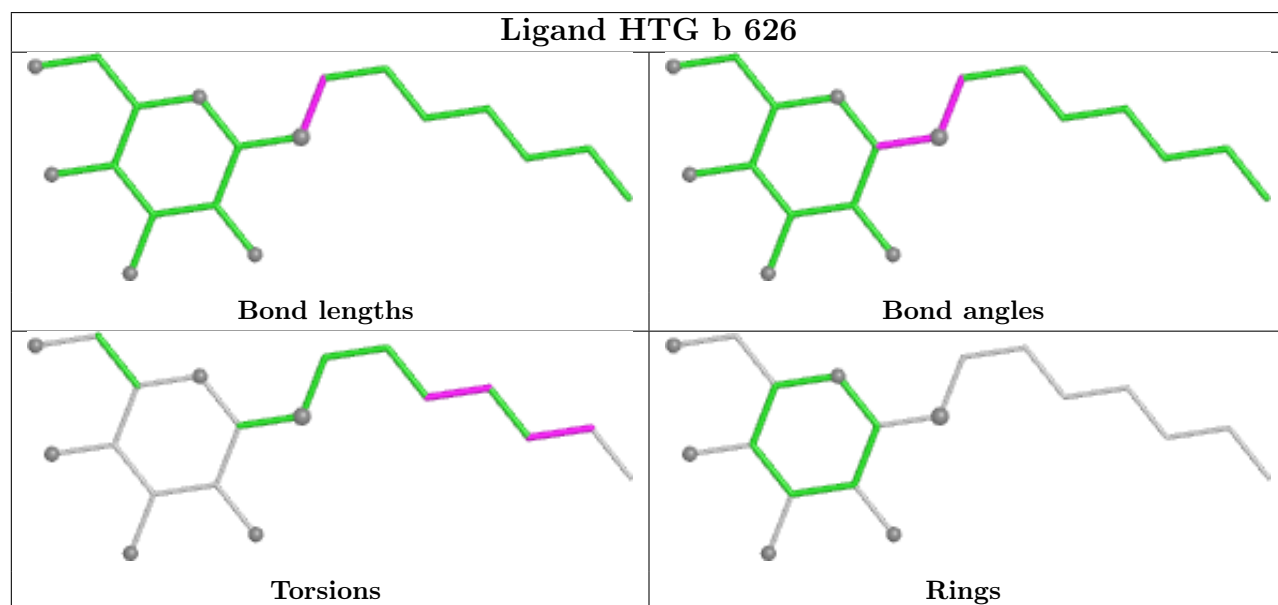
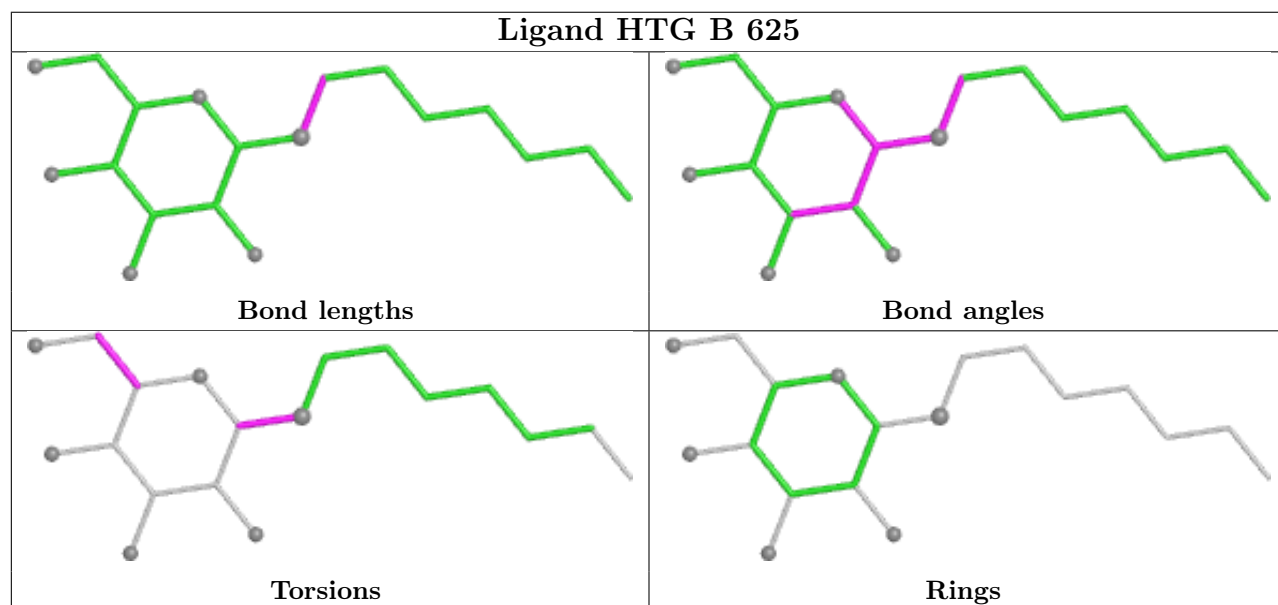
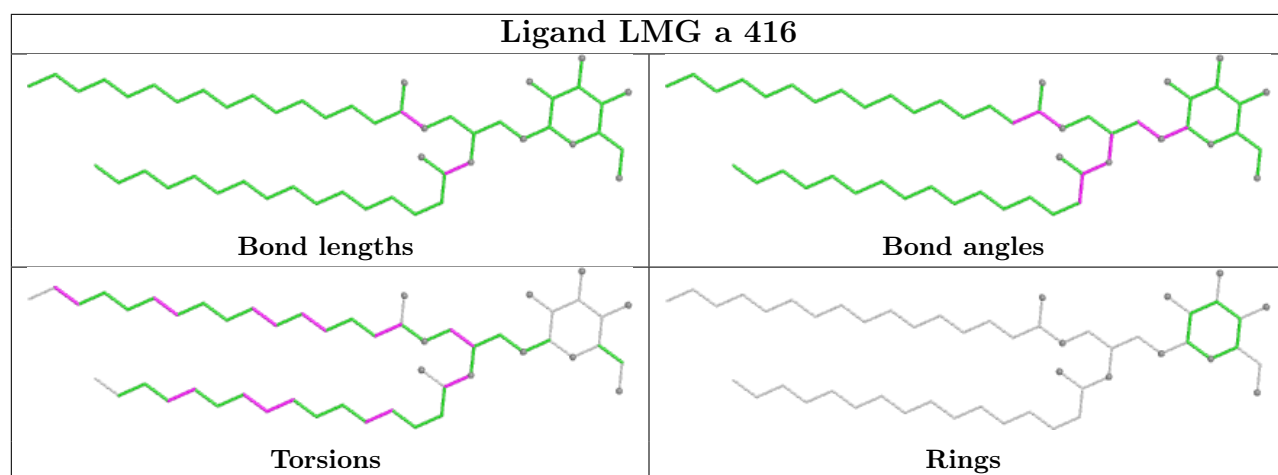


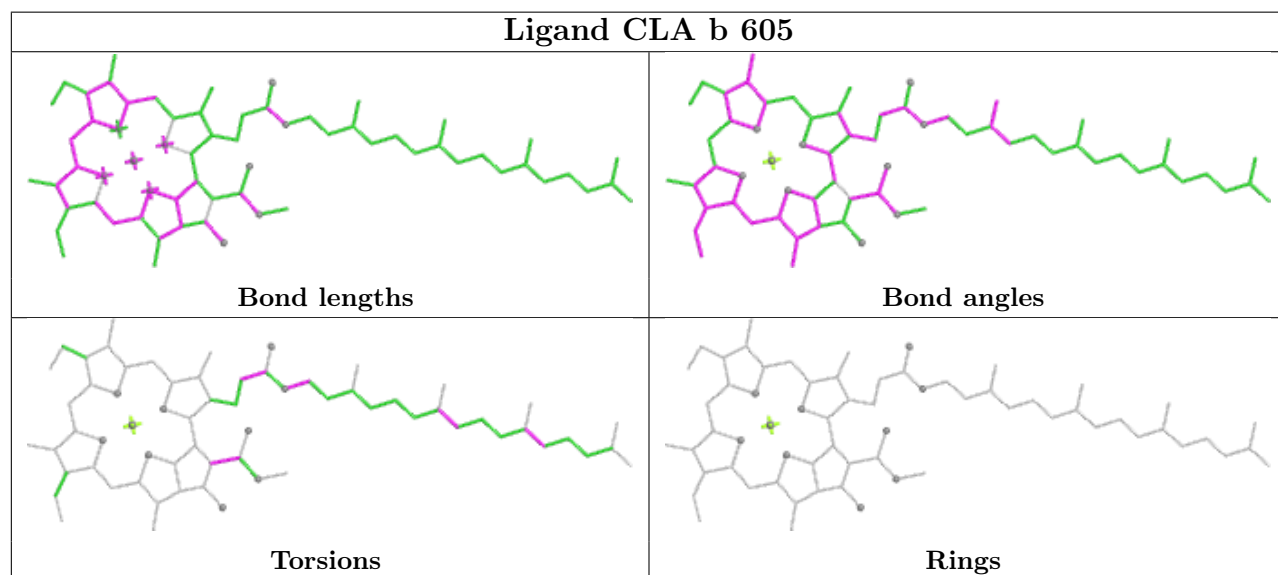
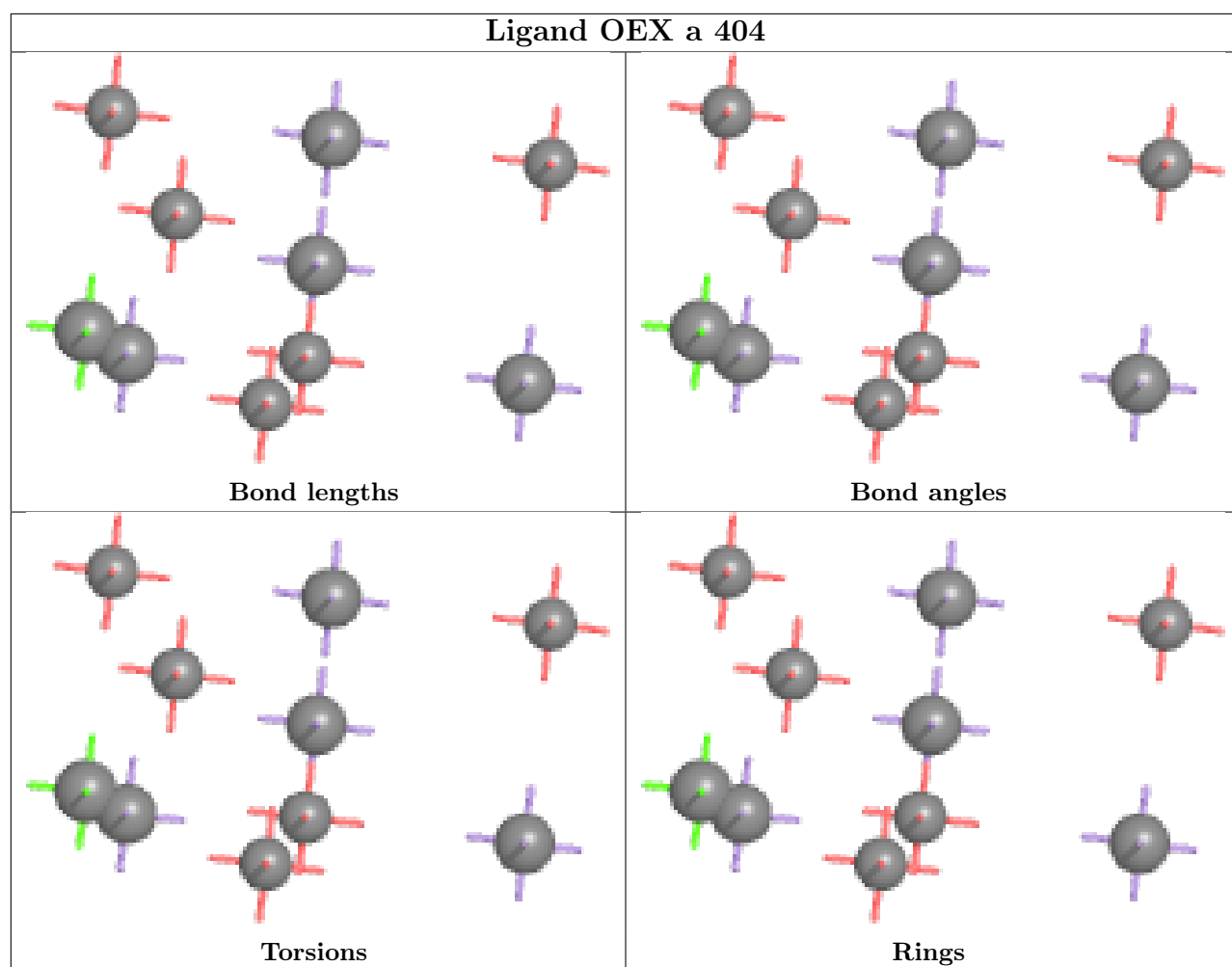


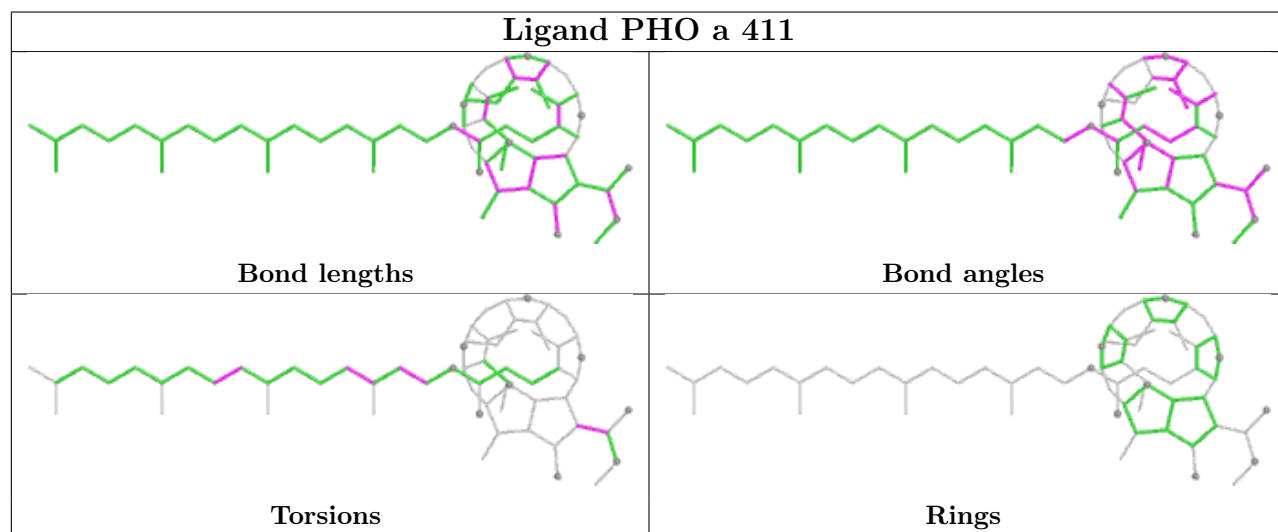
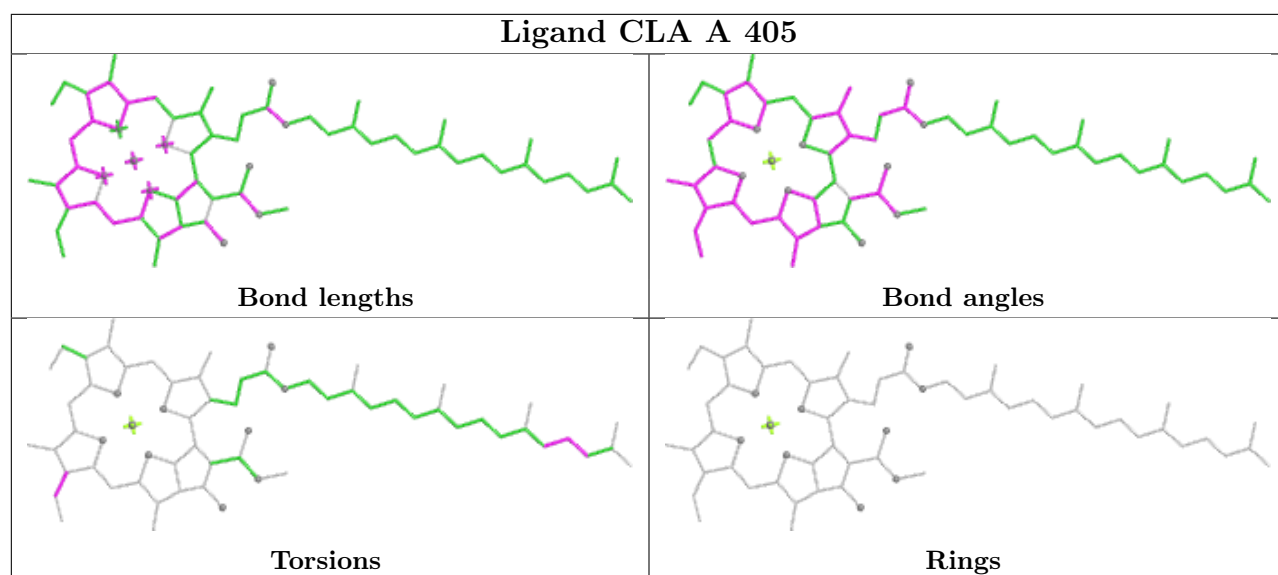


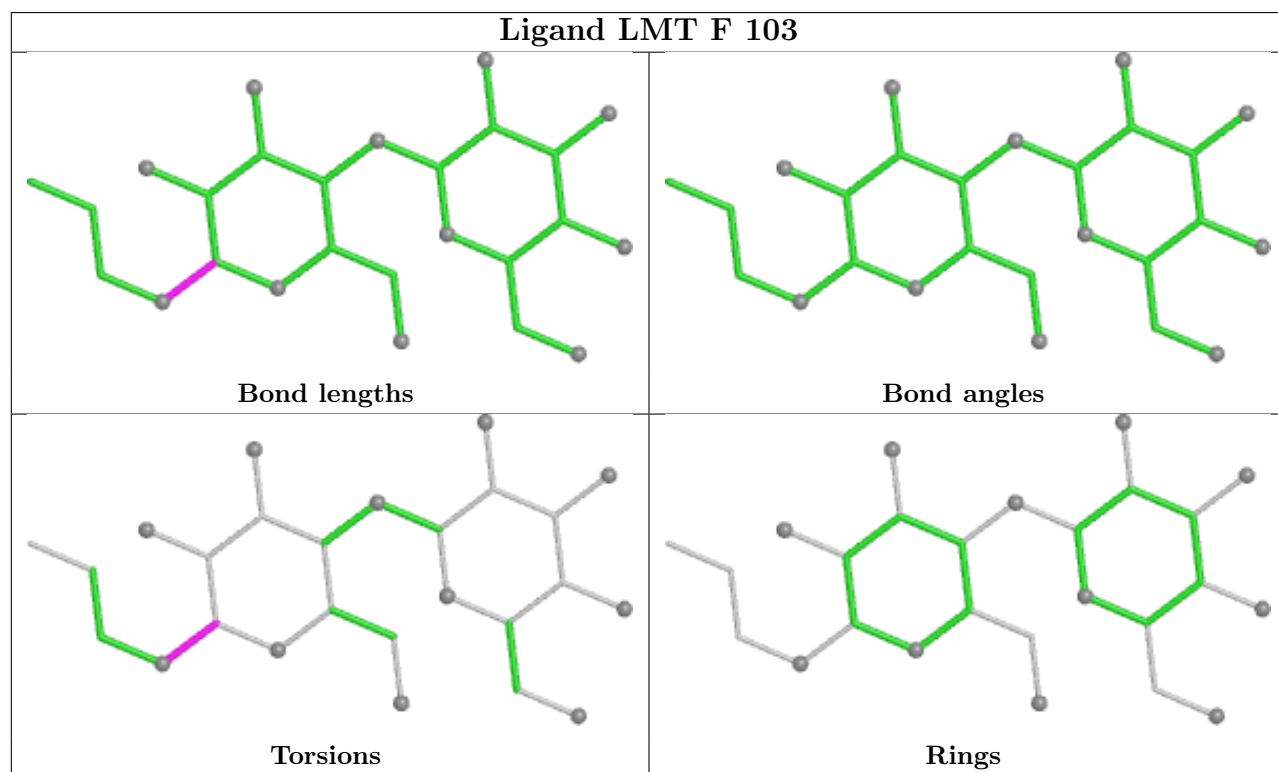
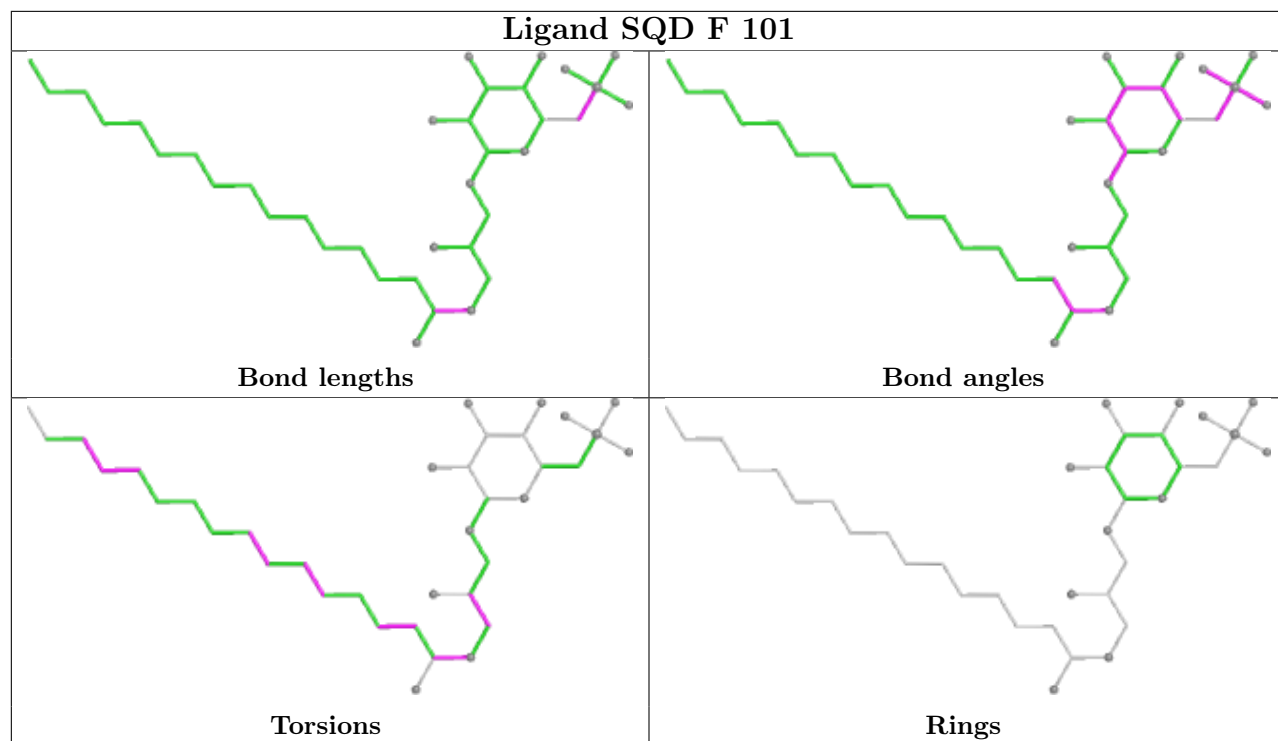


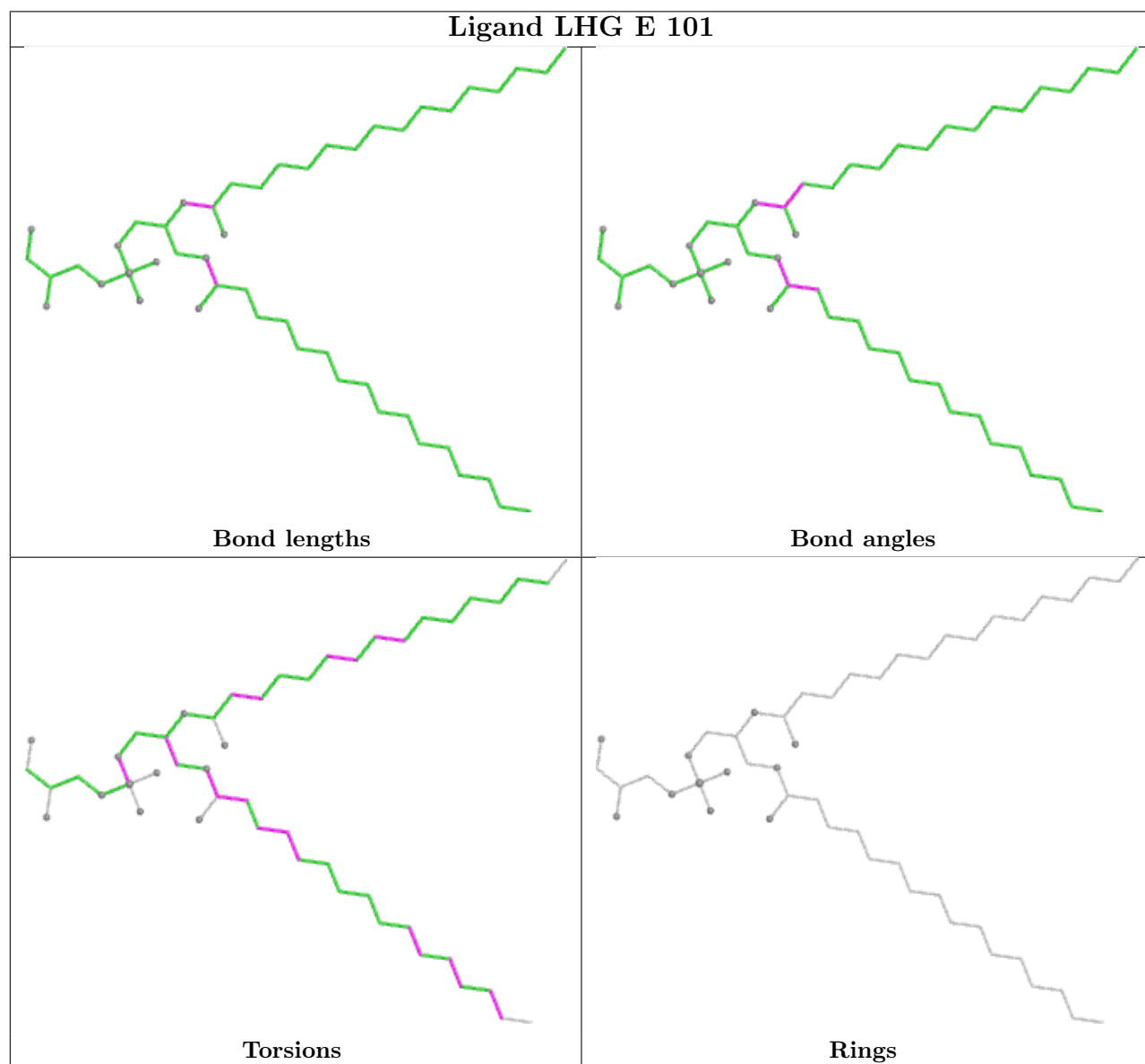
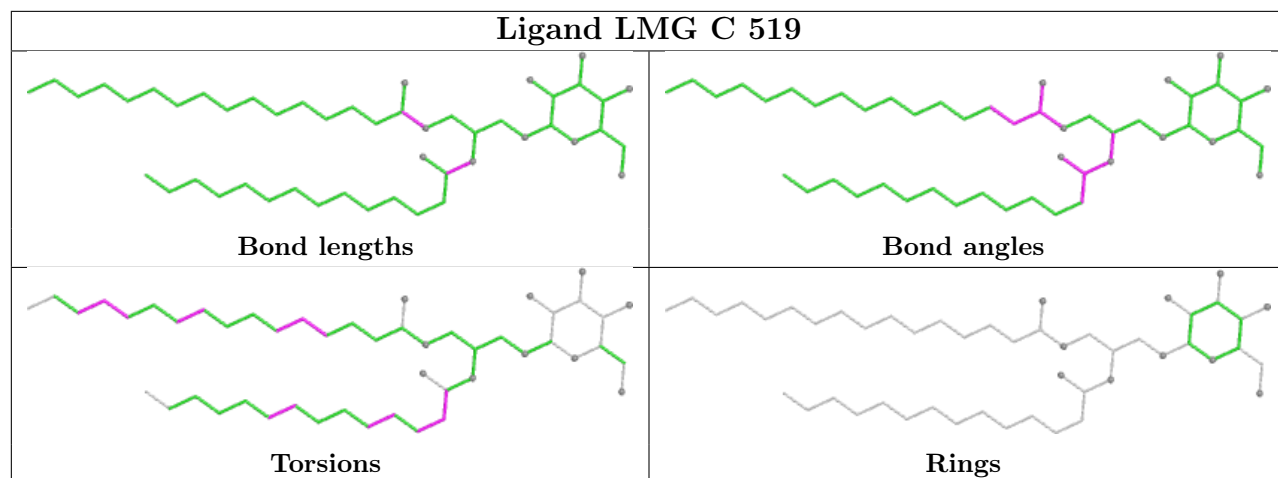


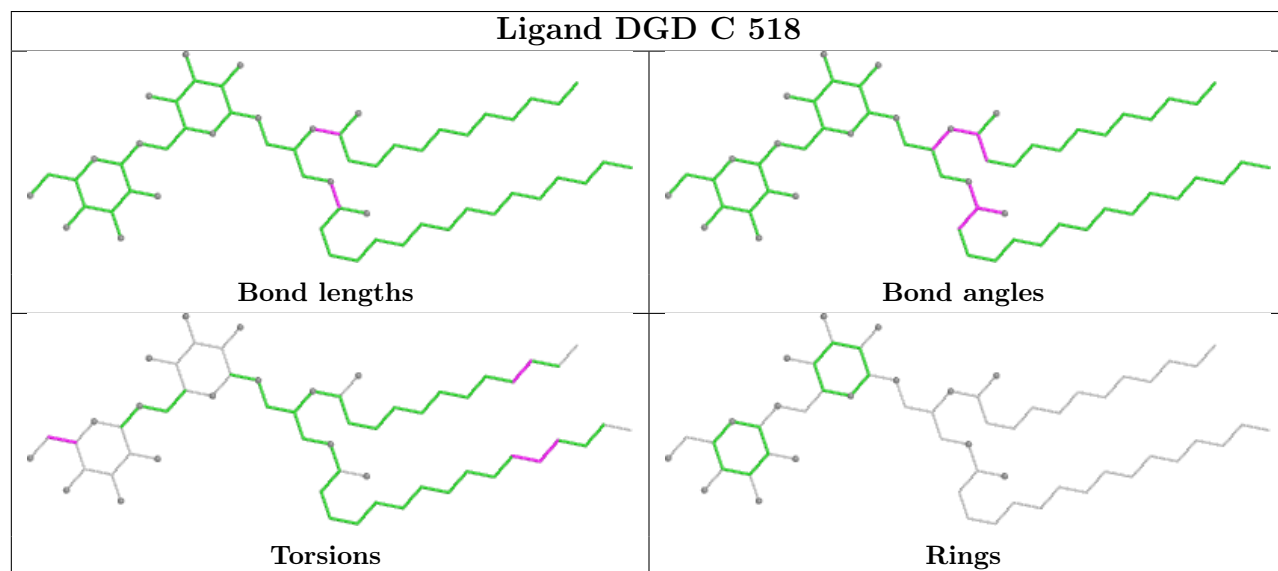
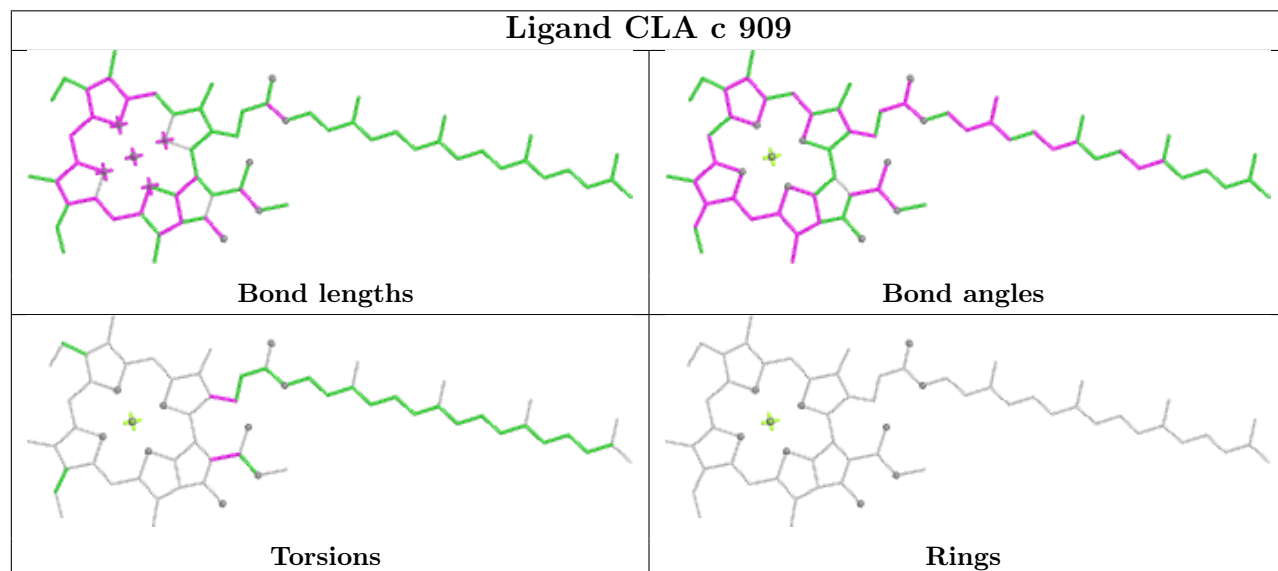
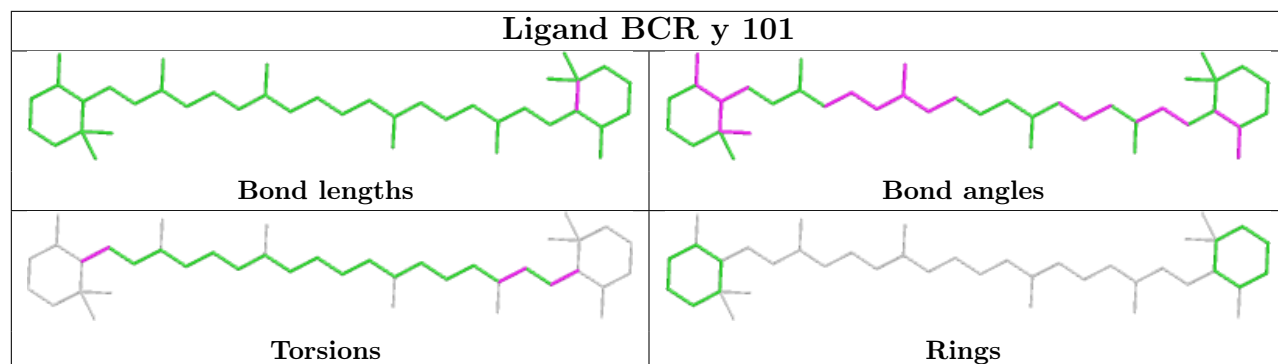


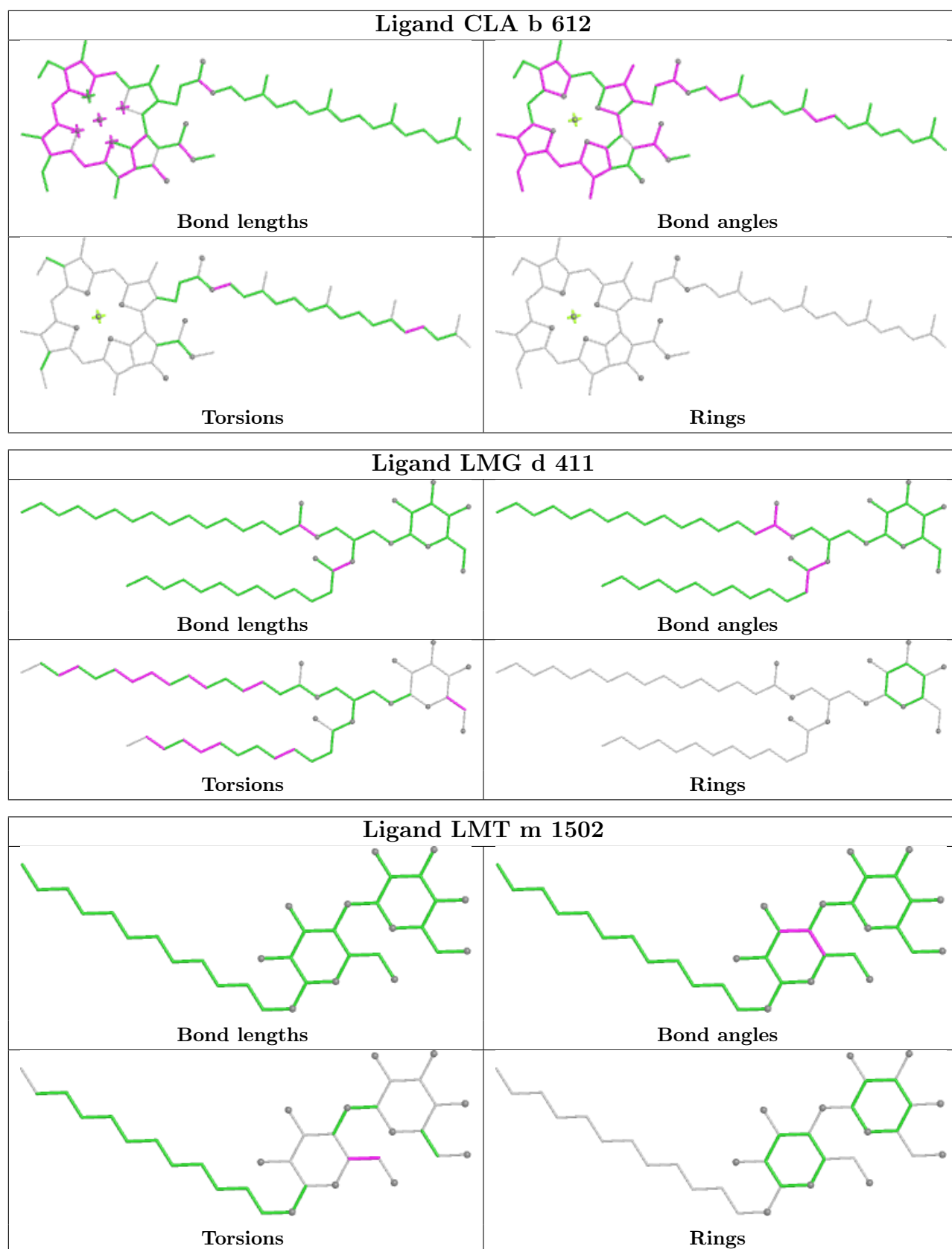


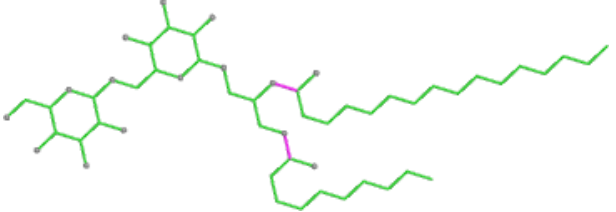
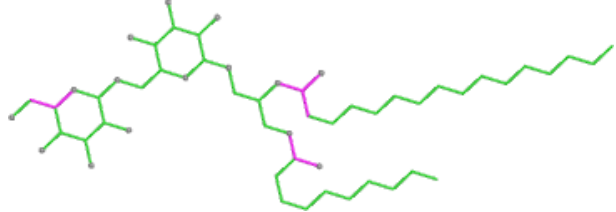
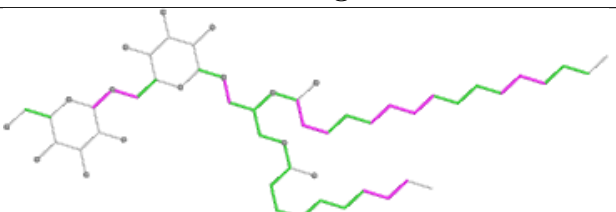
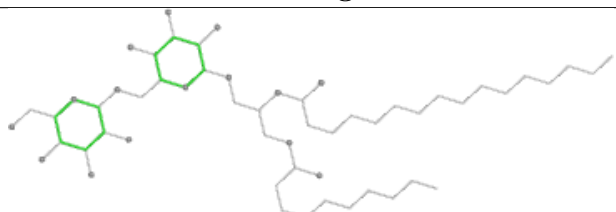


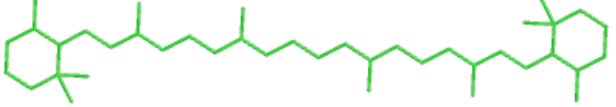
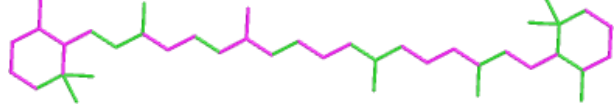
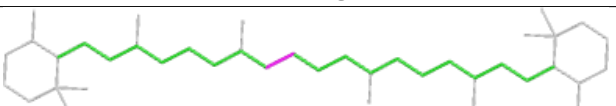
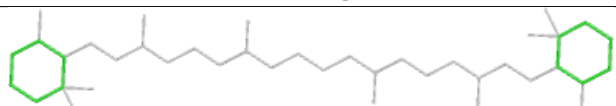


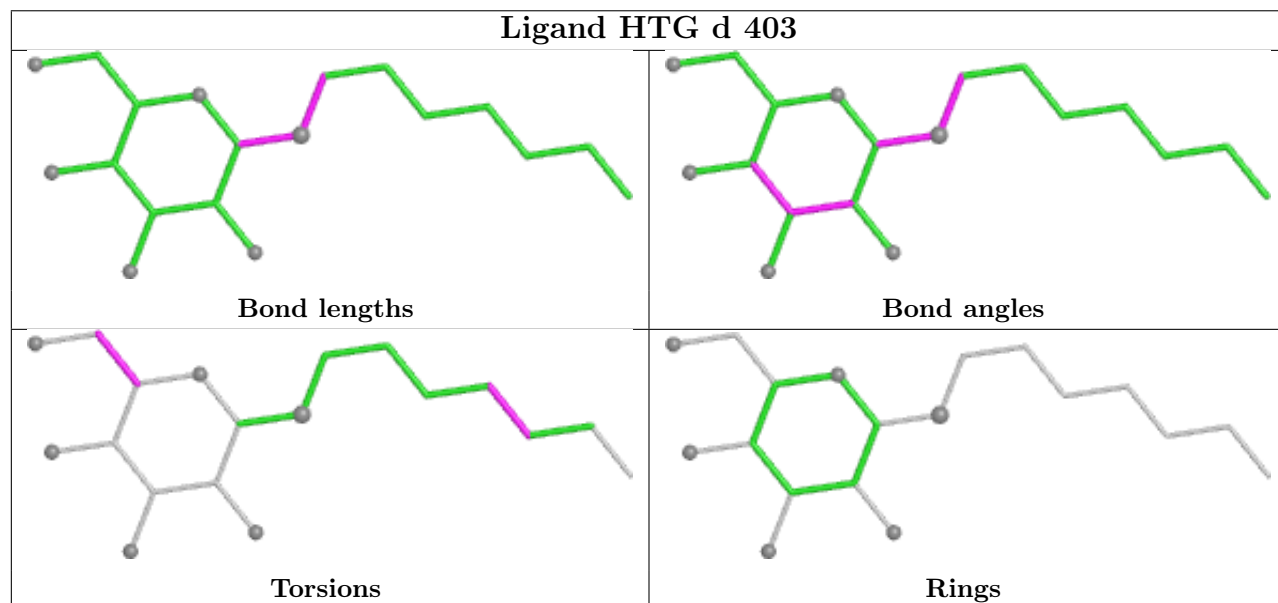
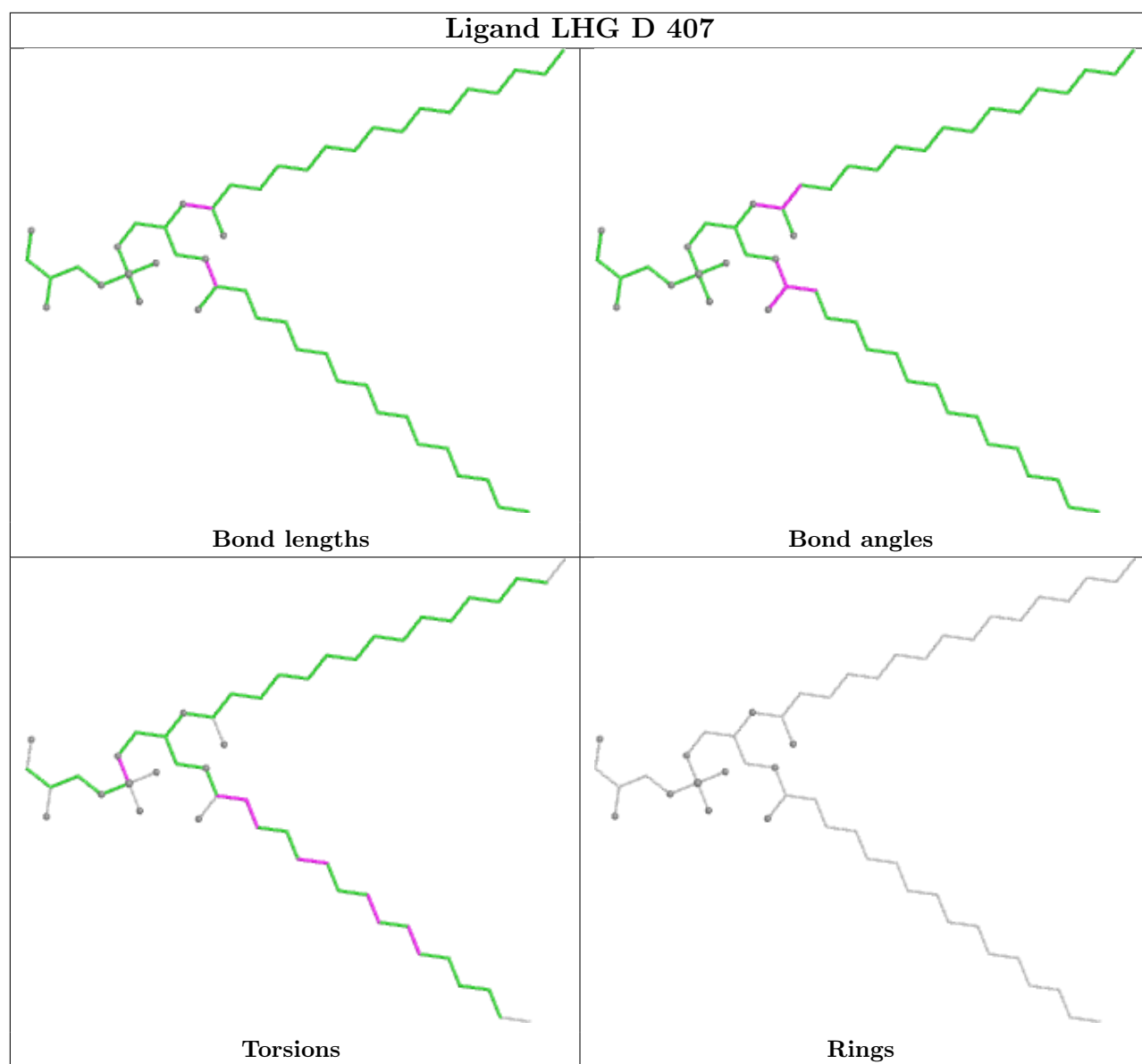


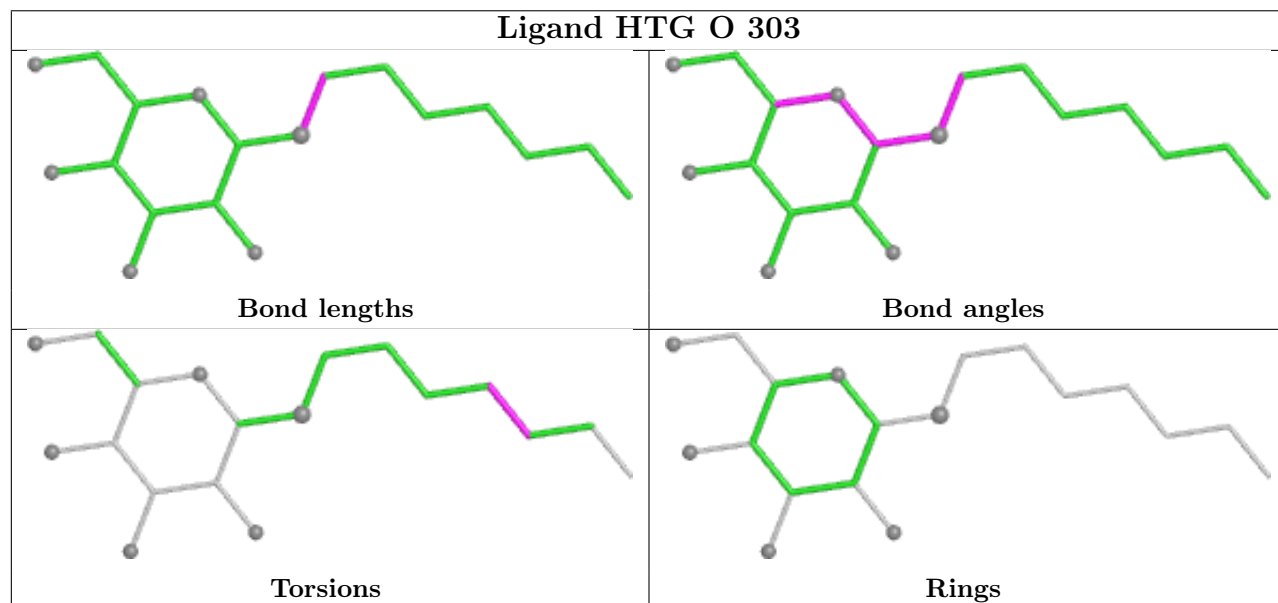
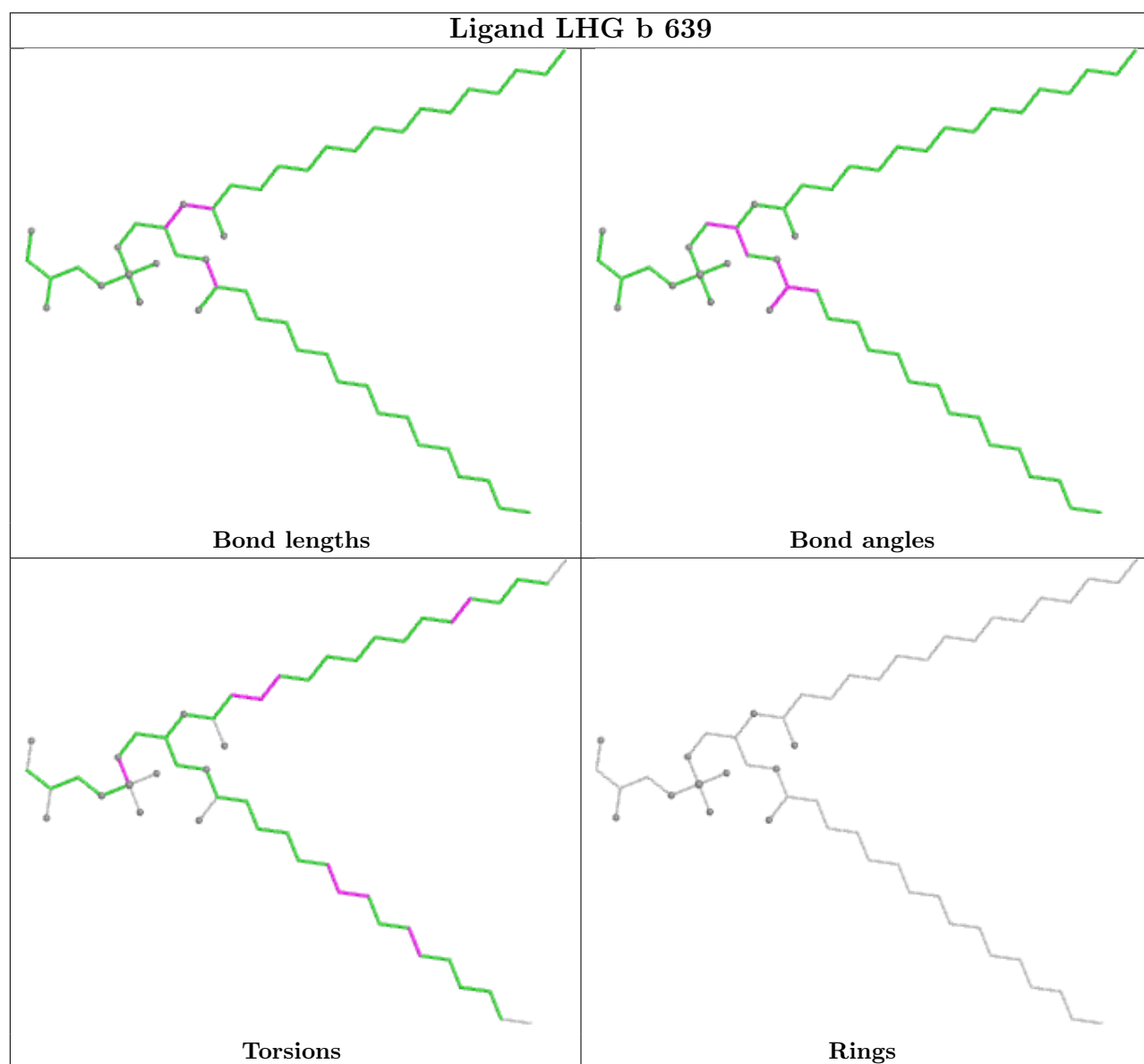


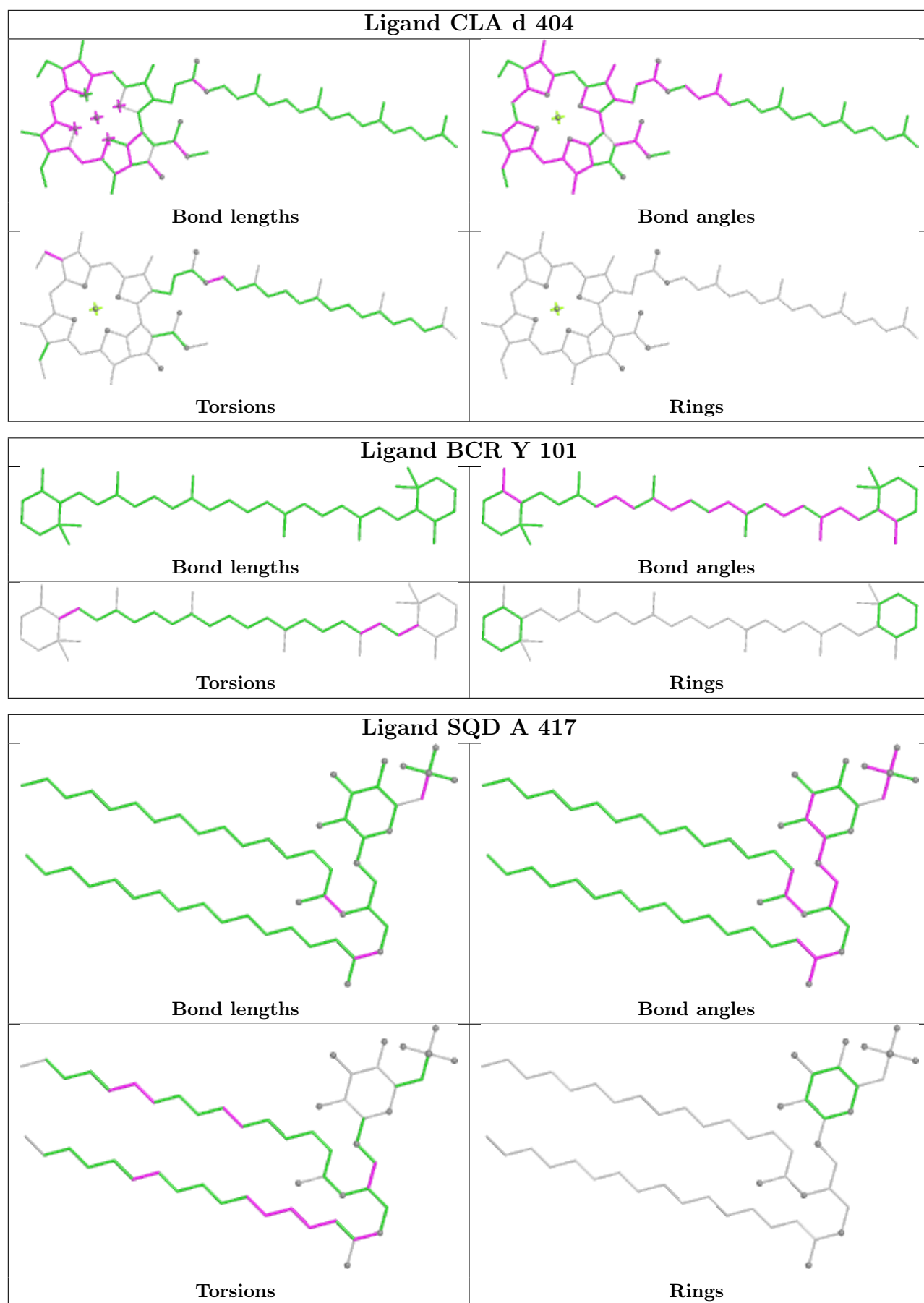


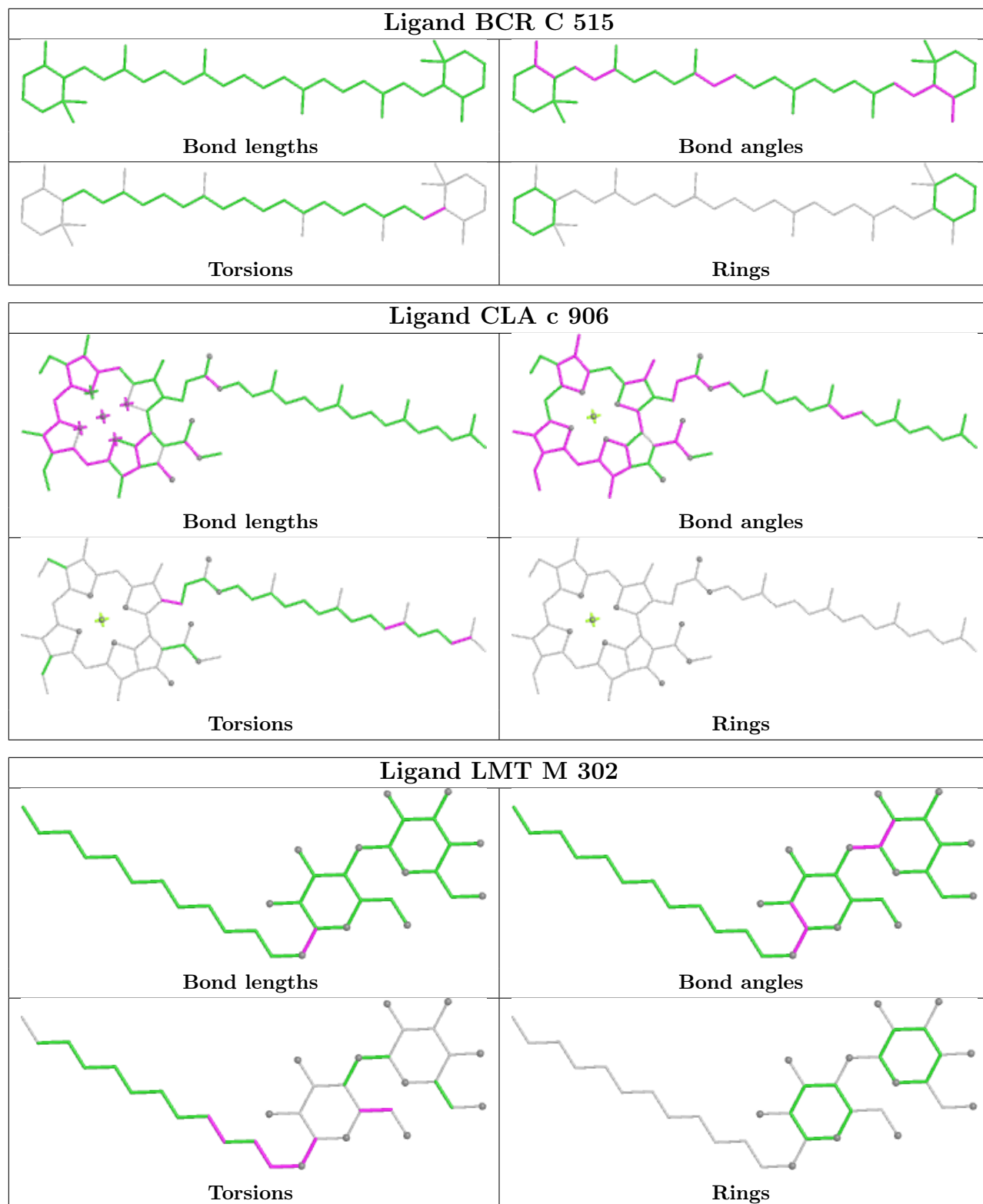
Ligand DGD C 517			
			
Bond lengths	Bond angles		
			
Torsions	Rings		

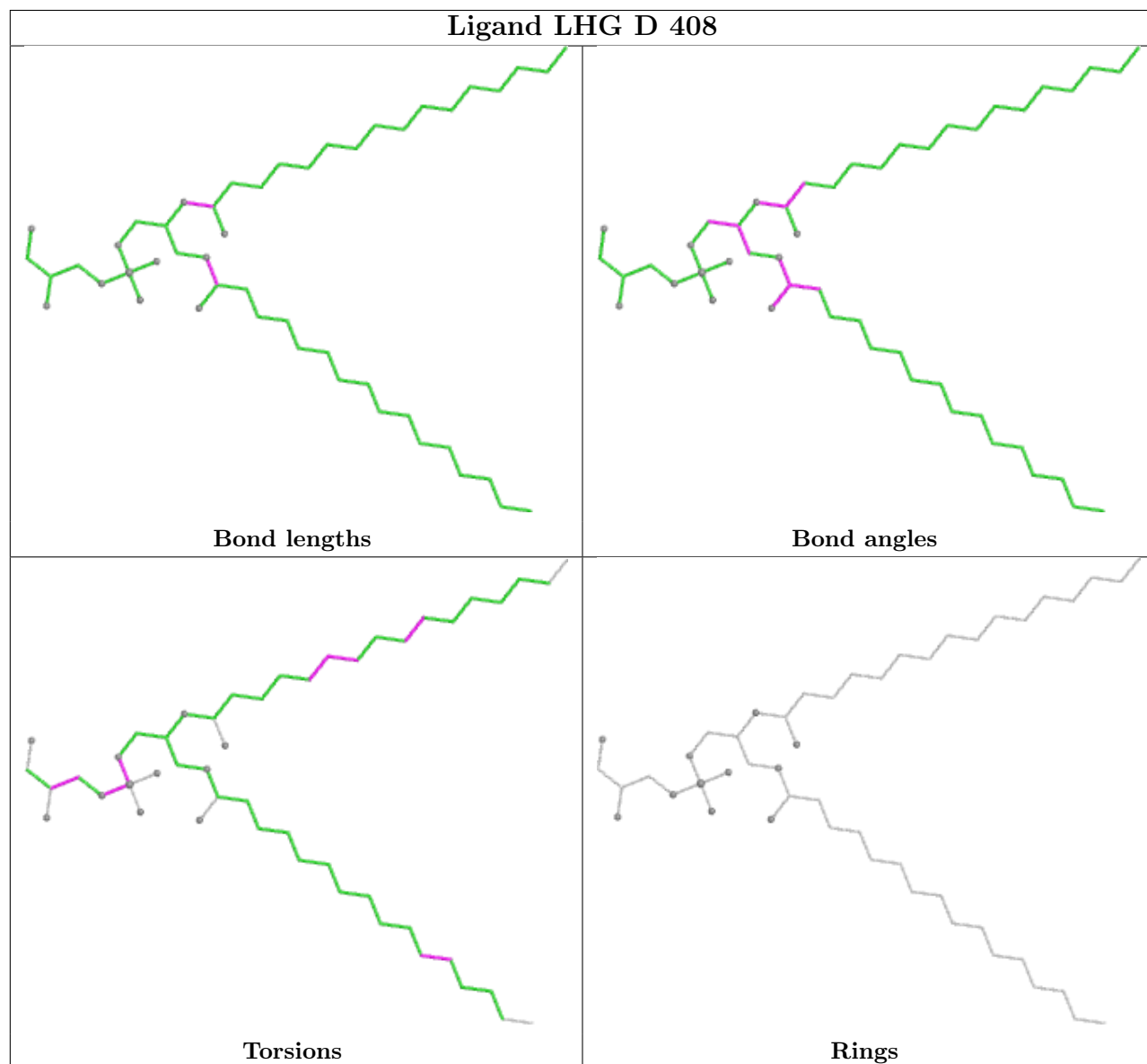
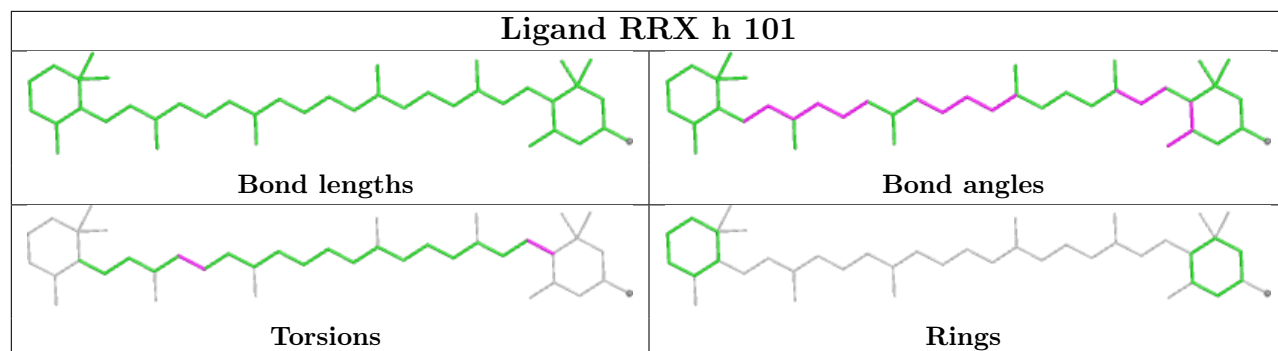
Ligand BCR t 903			
			
Bond lengths	Bond angles		
			
Torsions	Rings		

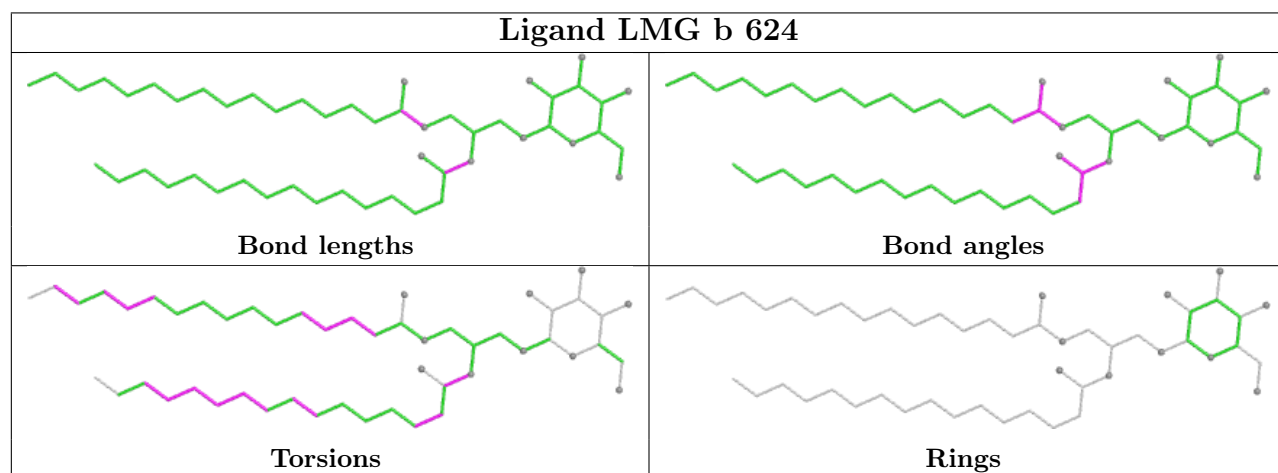
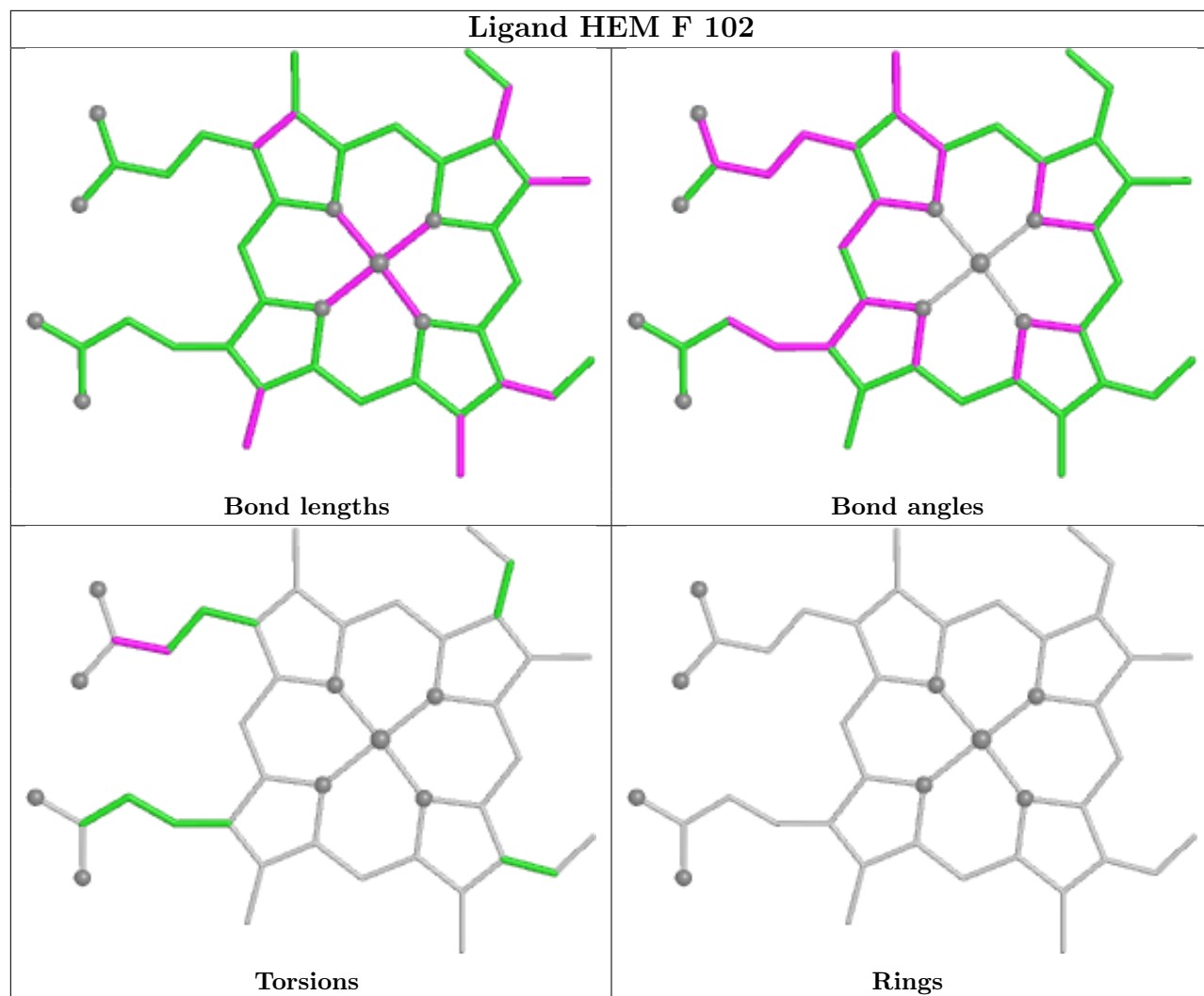




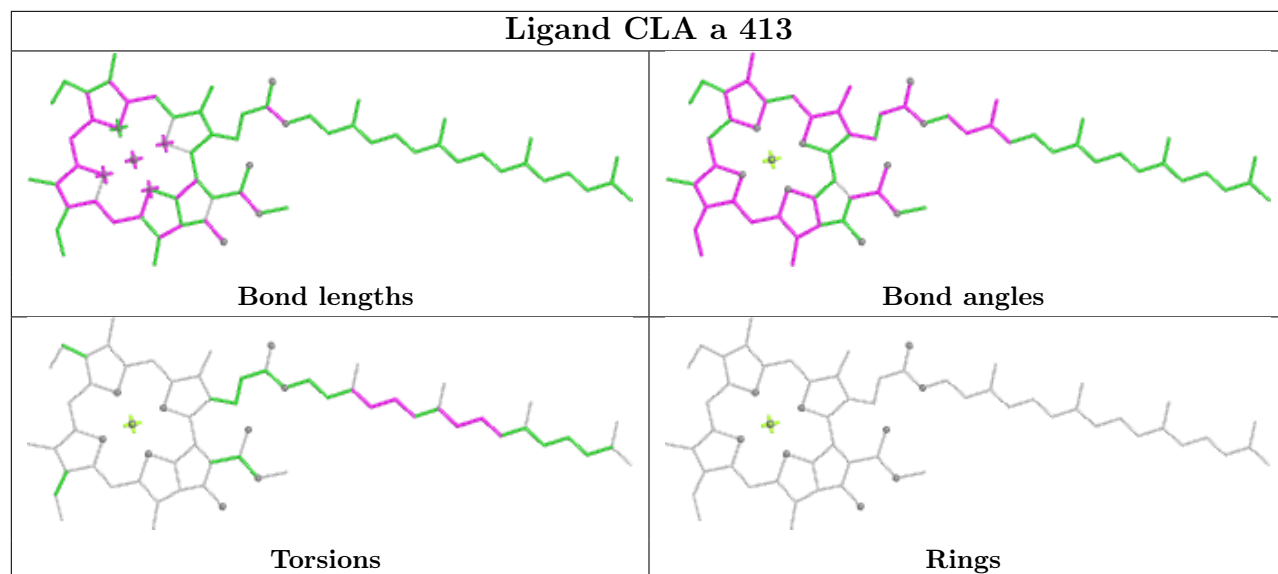




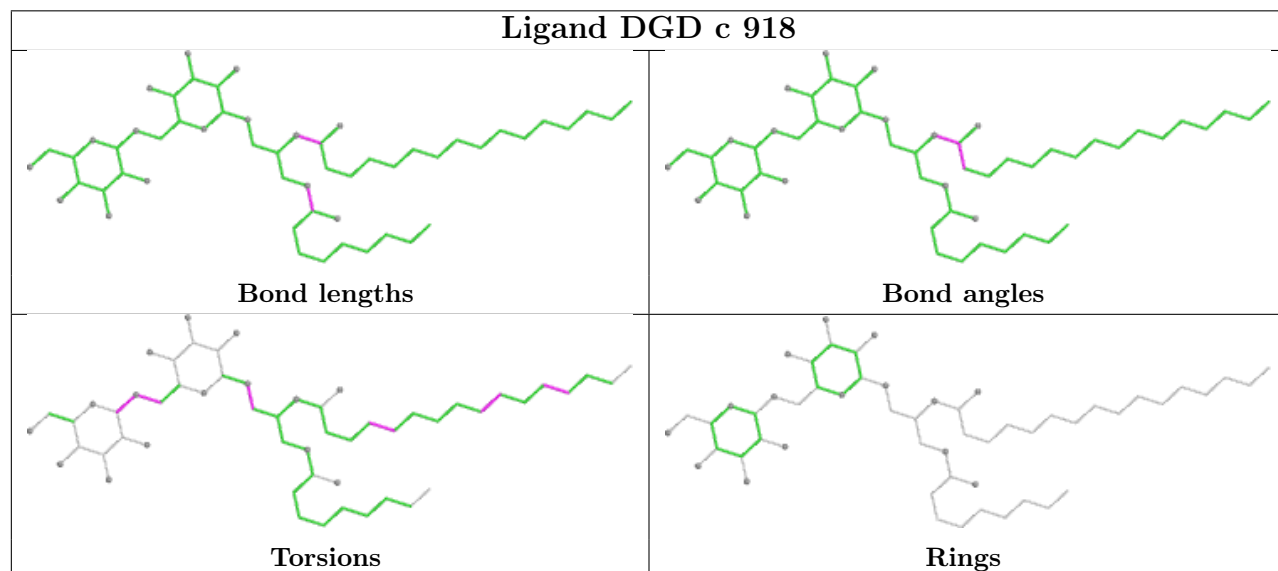




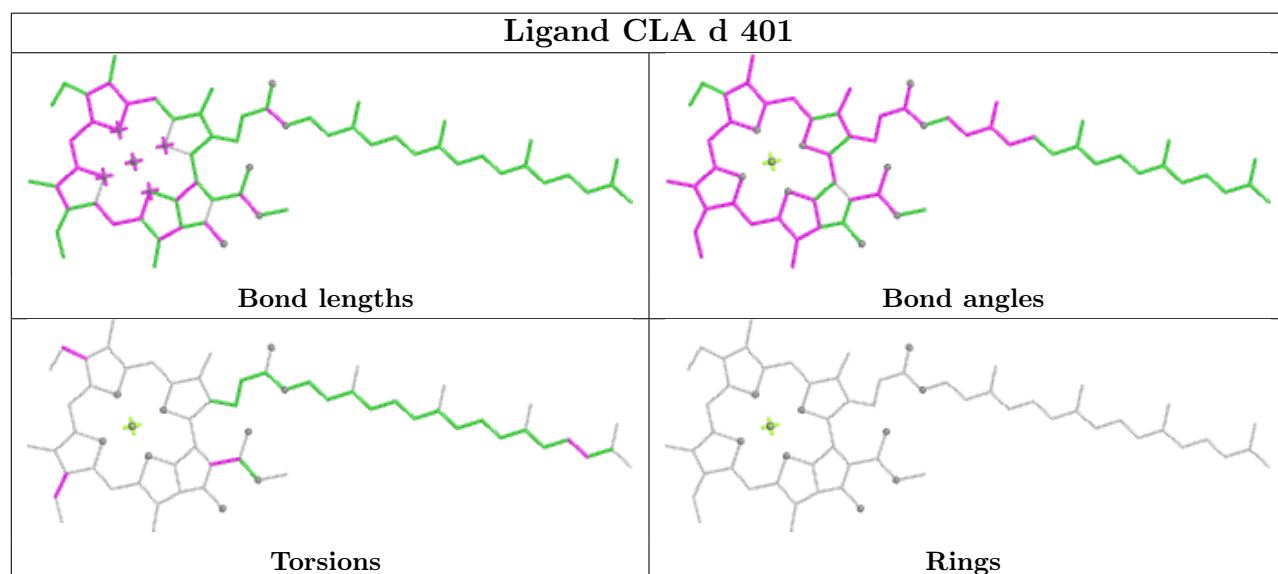
Ligand CLA a 413

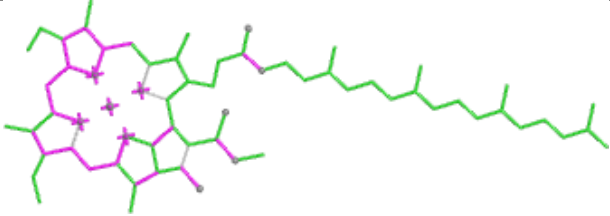
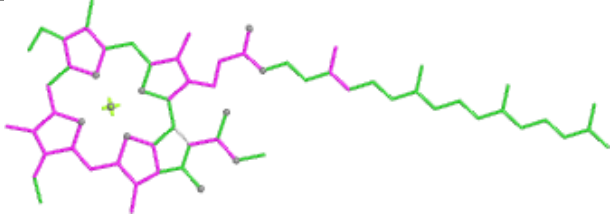
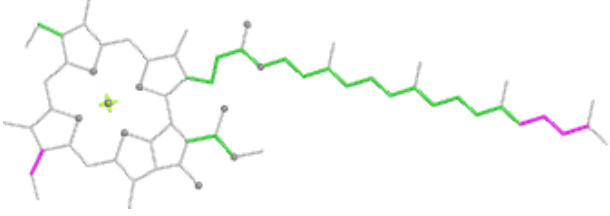
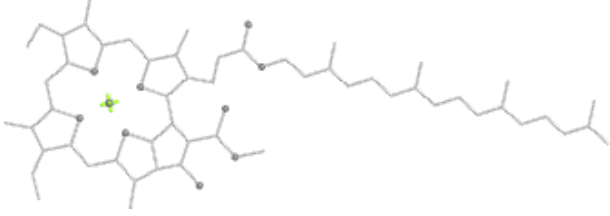
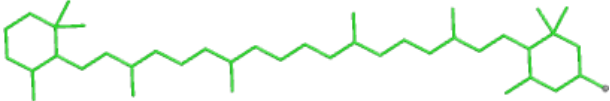
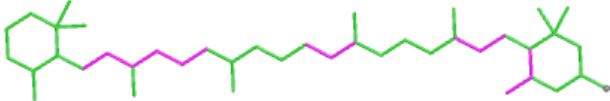
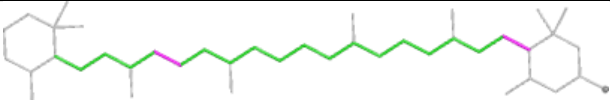
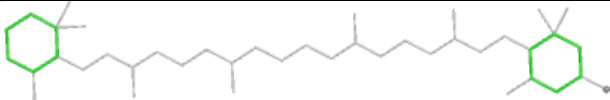
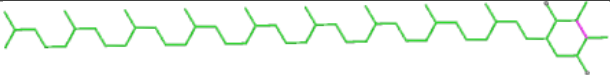
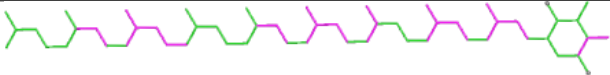
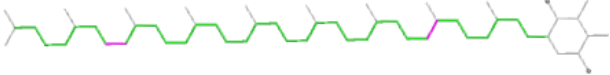
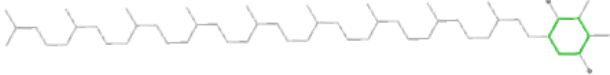


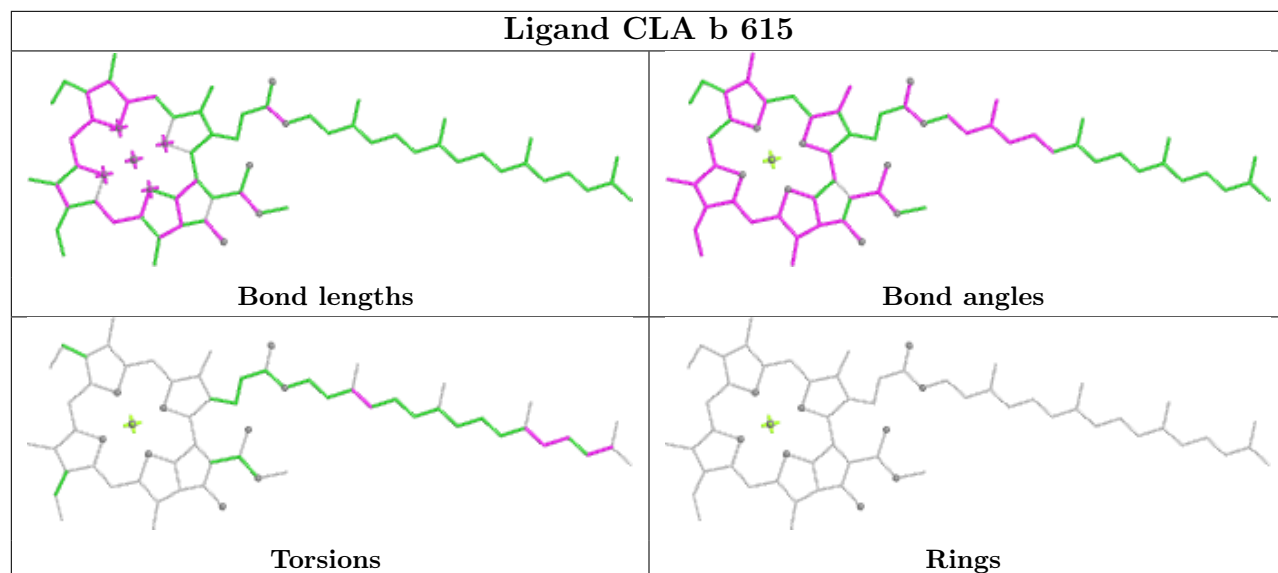
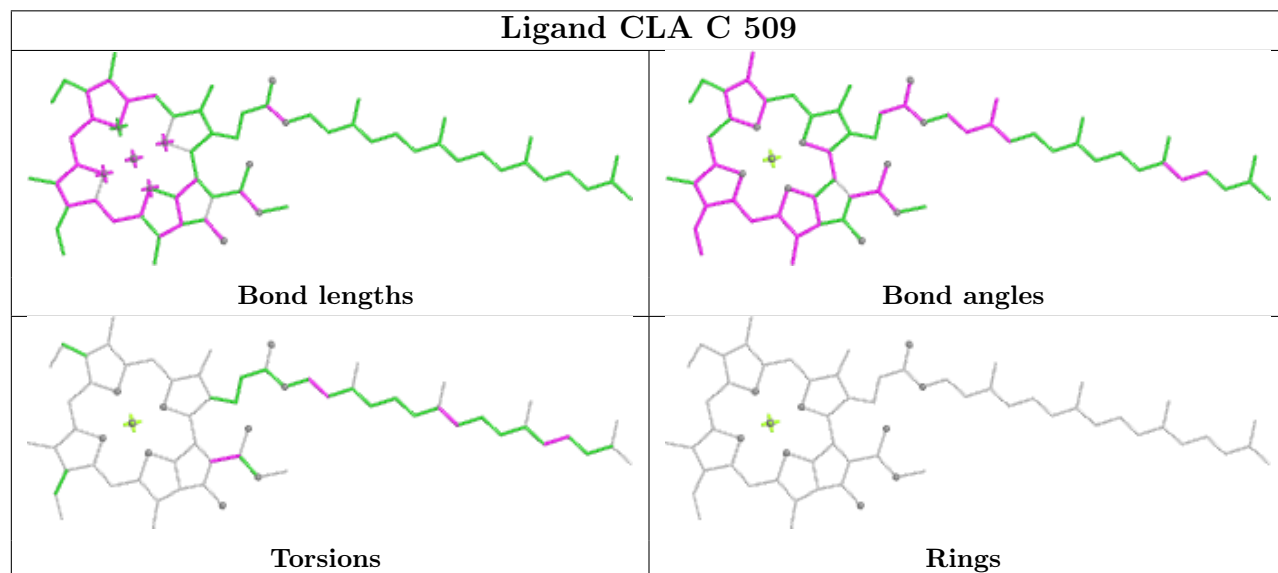
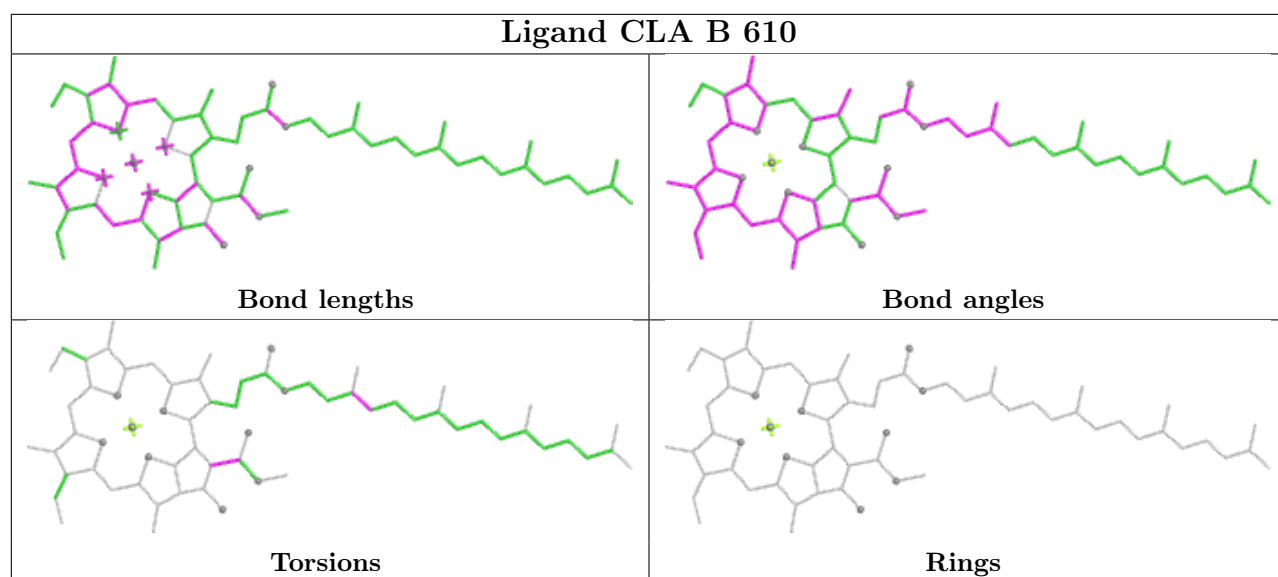
Ligand DGD c 918

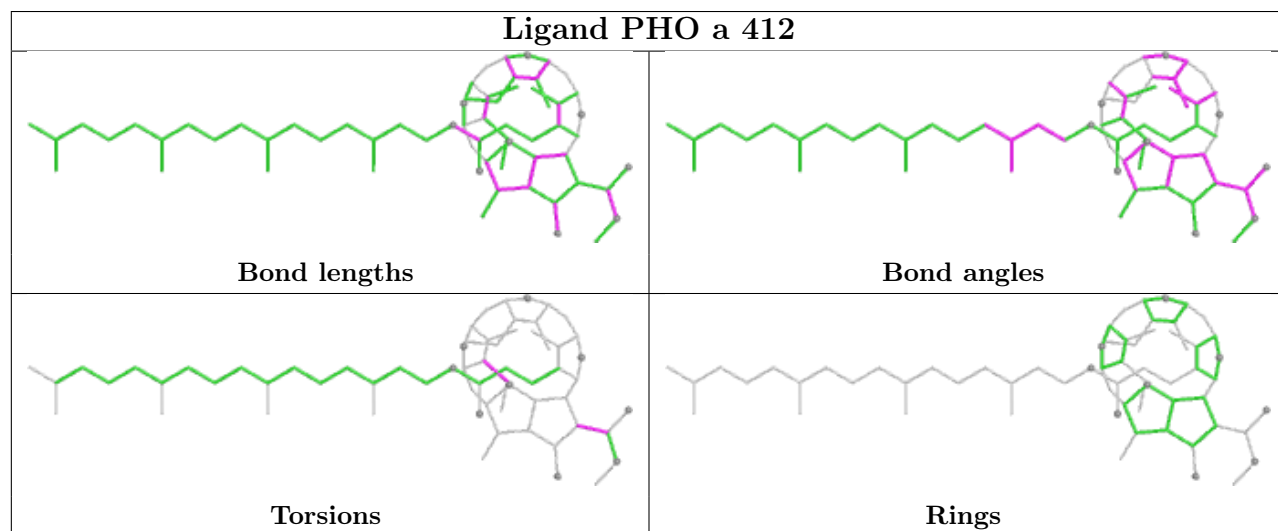
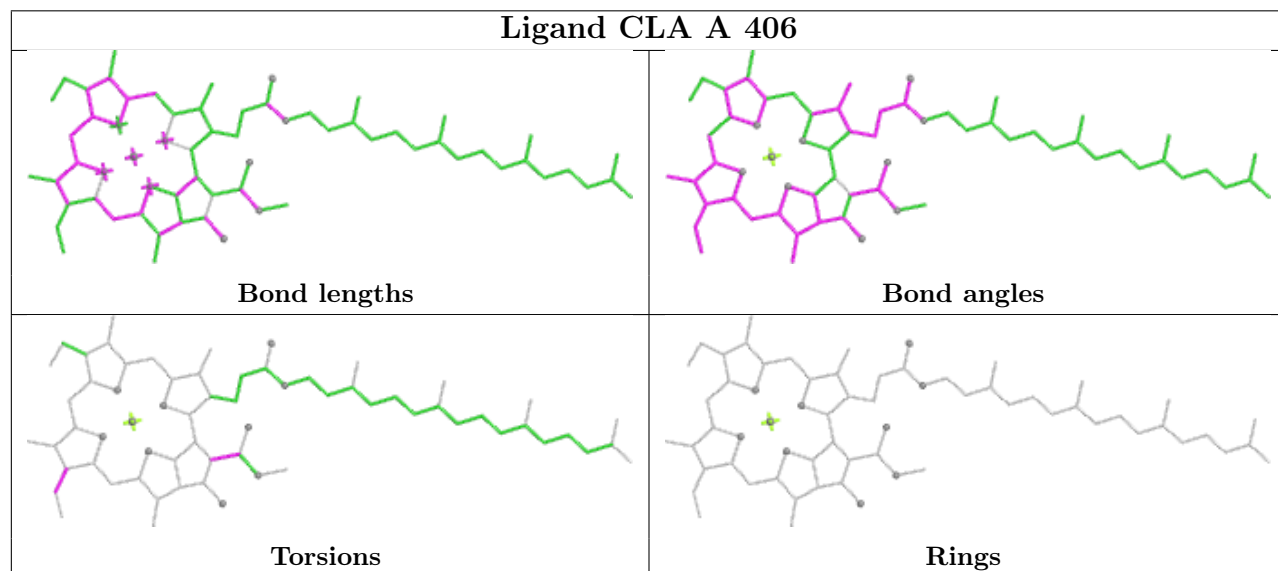
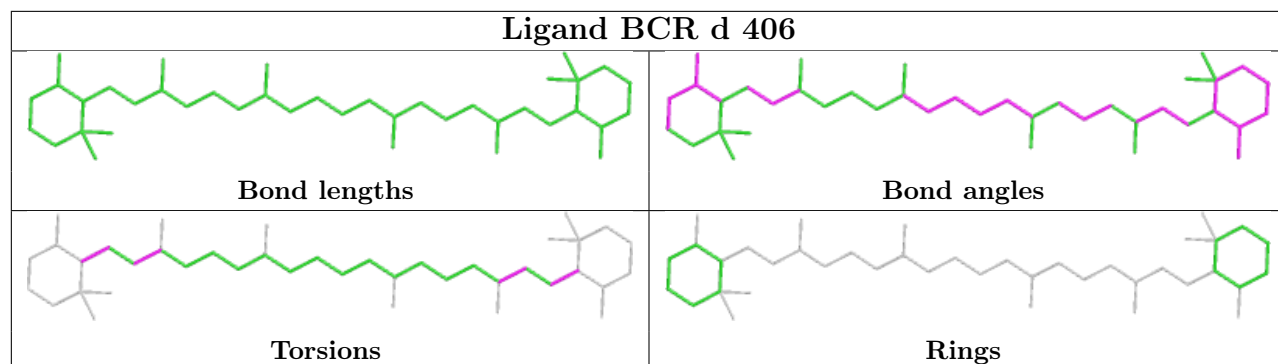


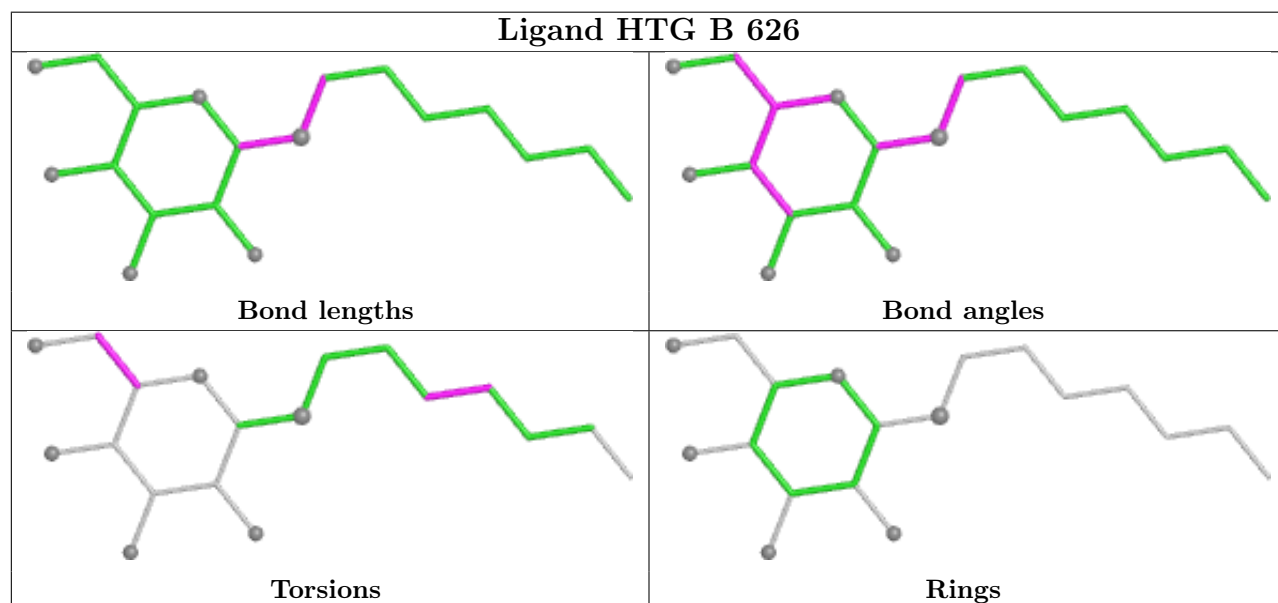
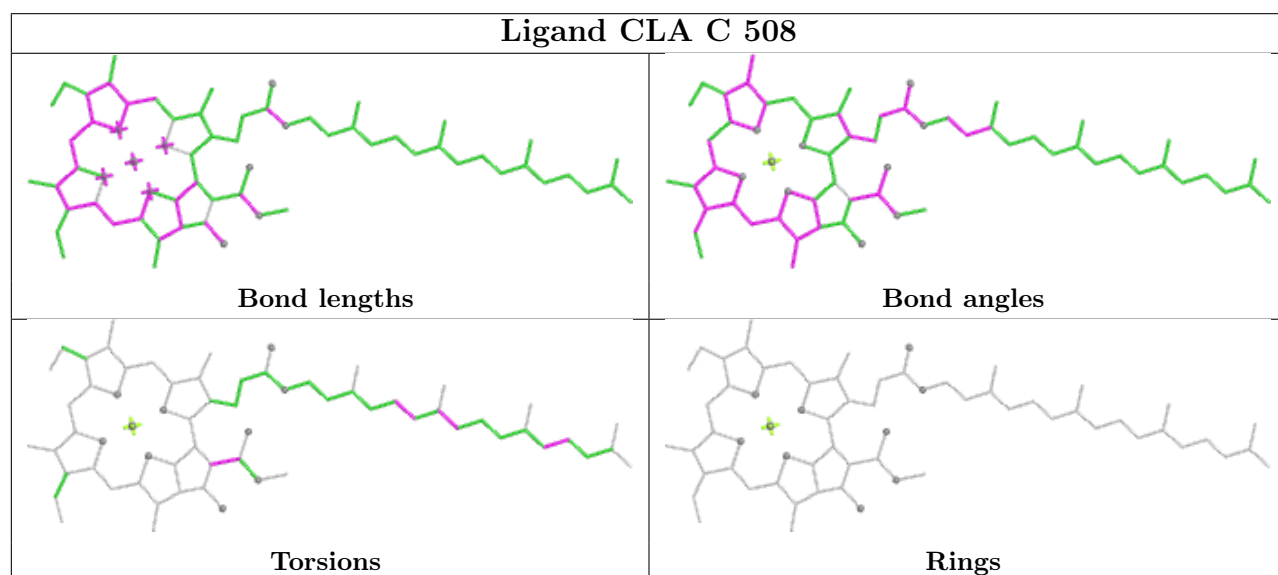
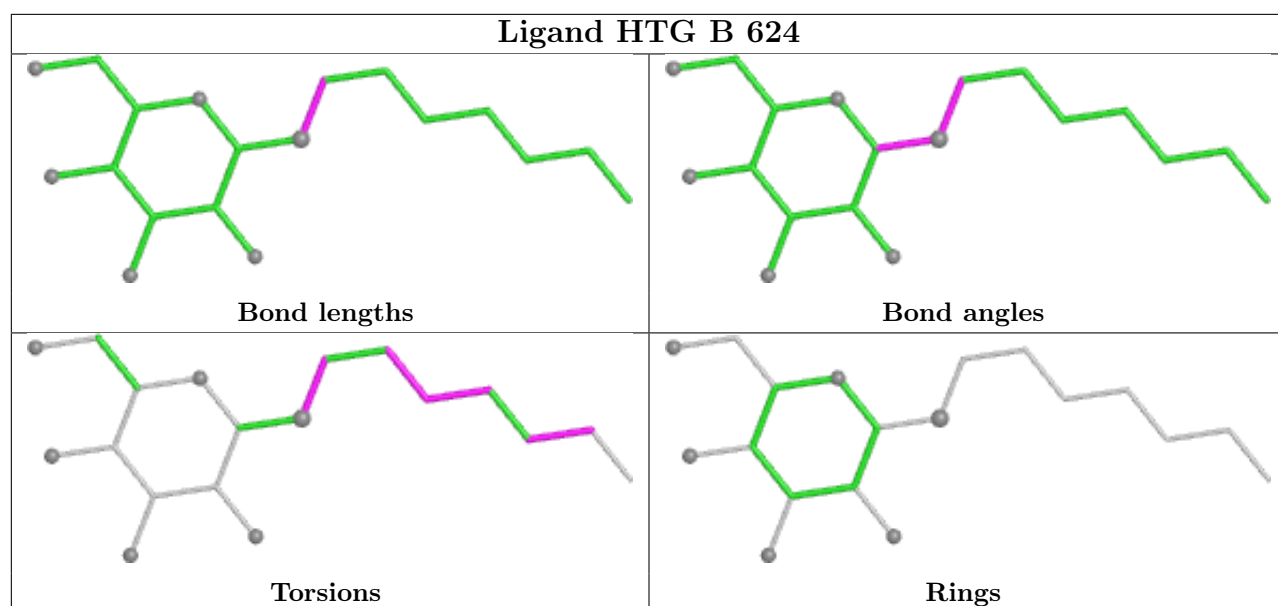
Ligand CLA d 401

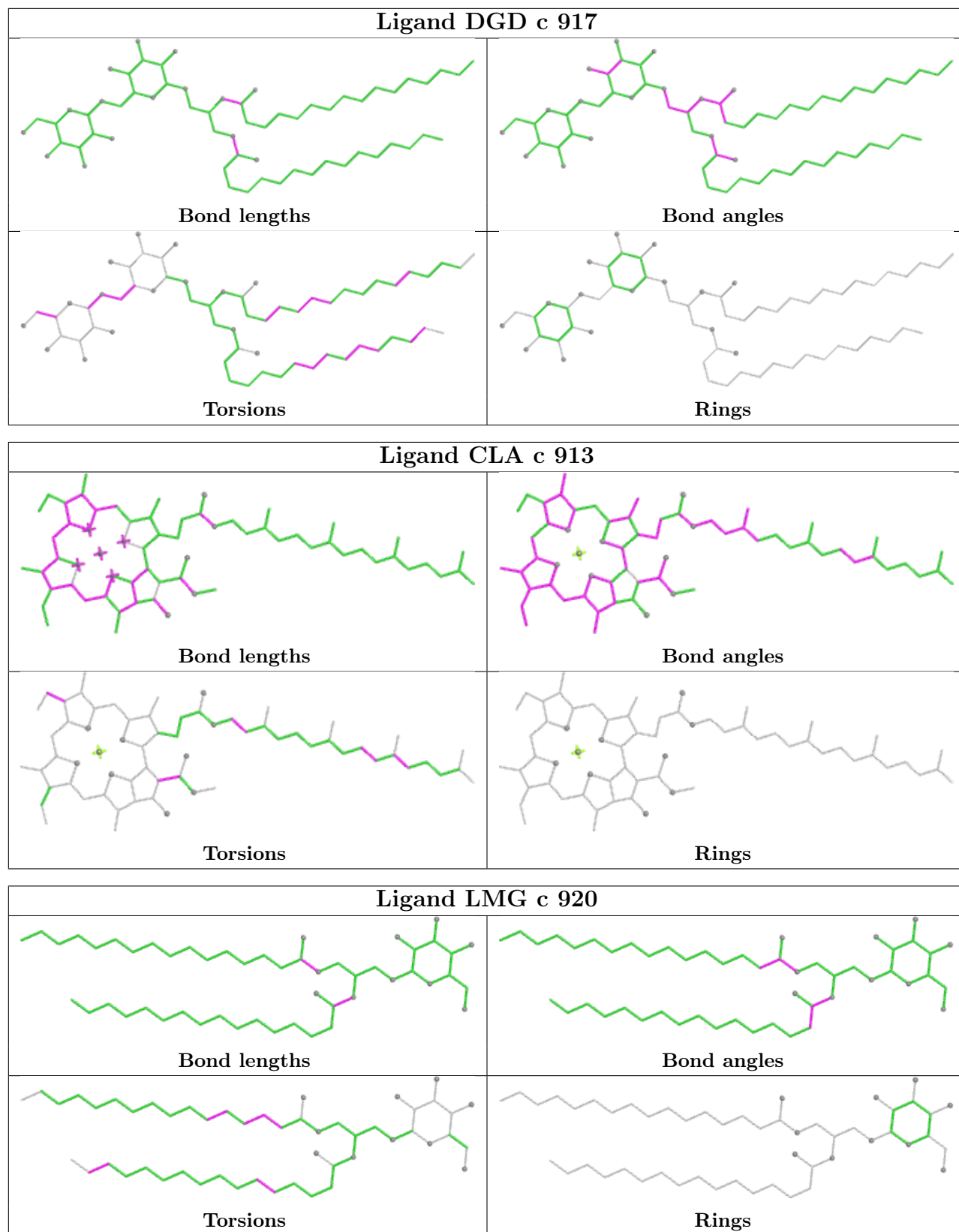


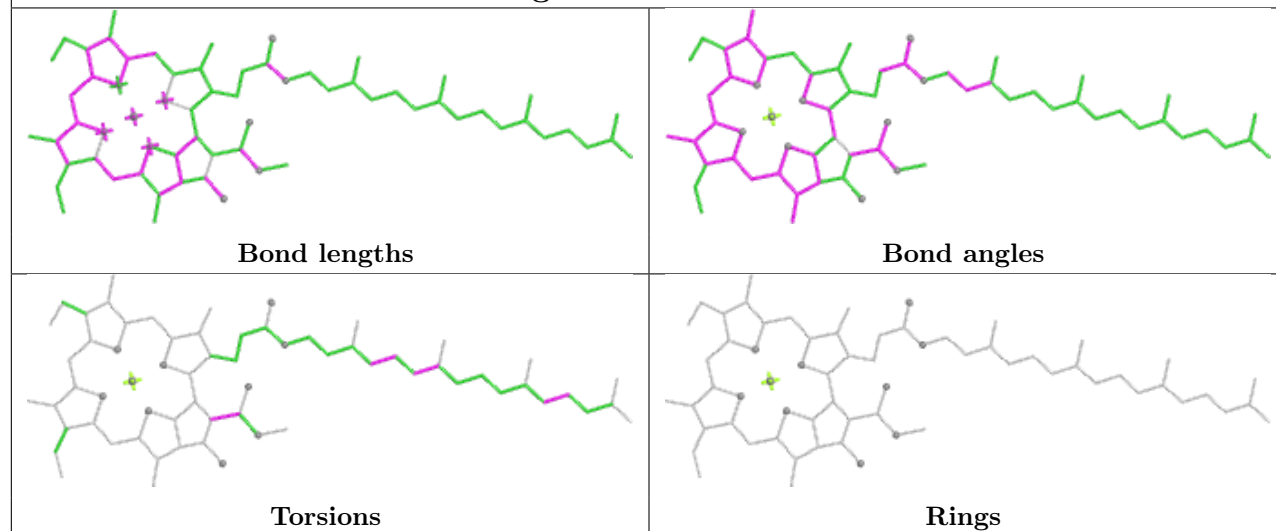
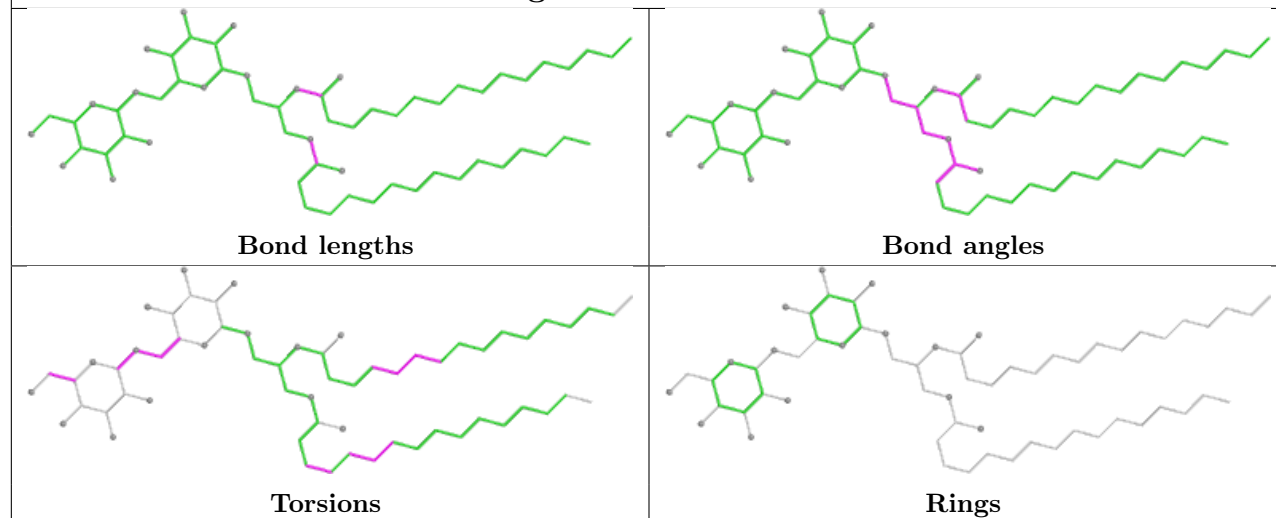
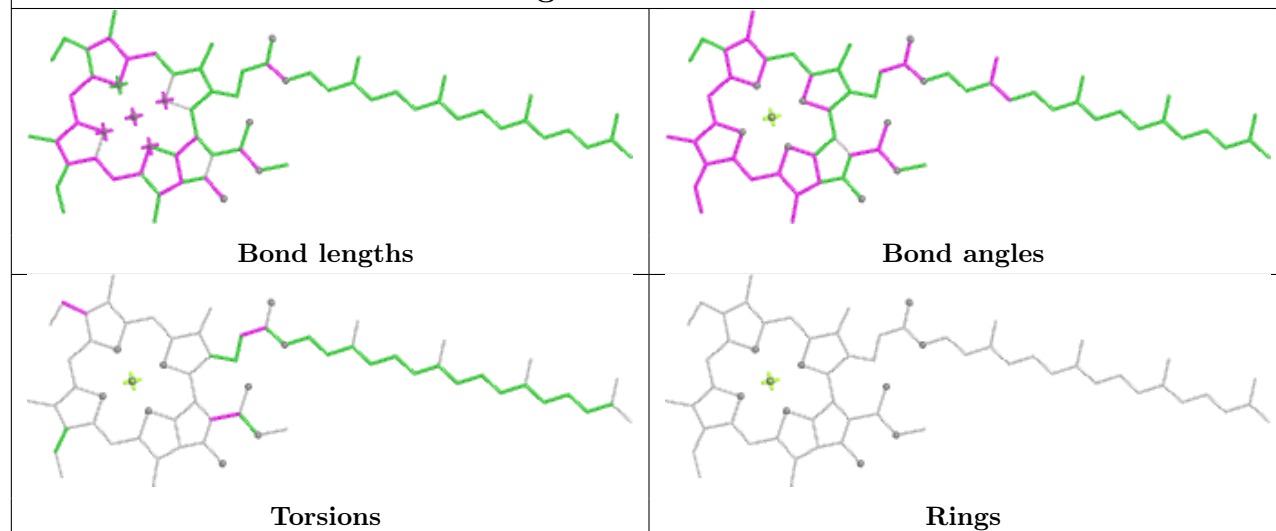
Ligand CLA a 409	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand RRX H 102	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PL9 d 407	
 Bond lengths	 Bond angles
 Torsions	 Rings



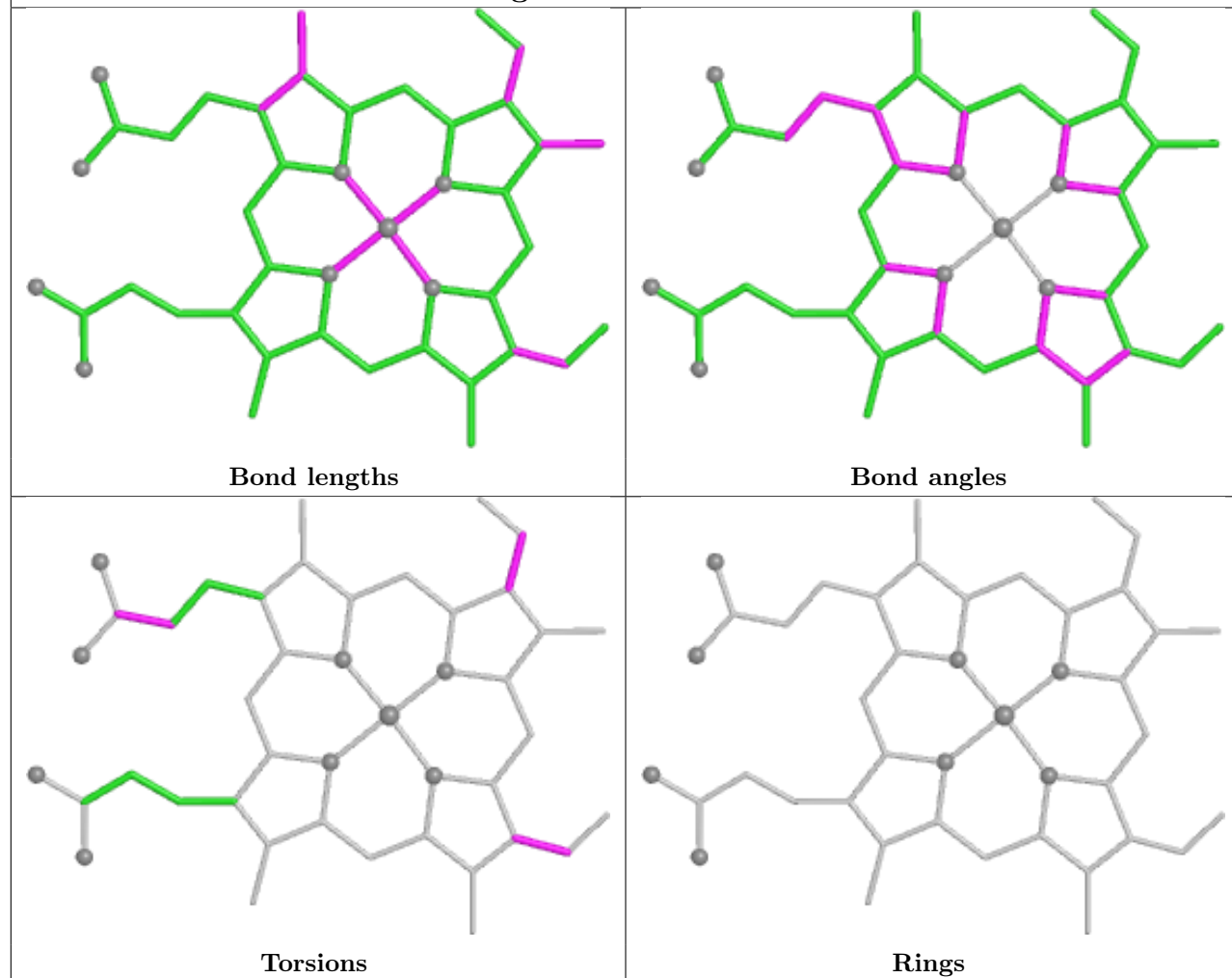




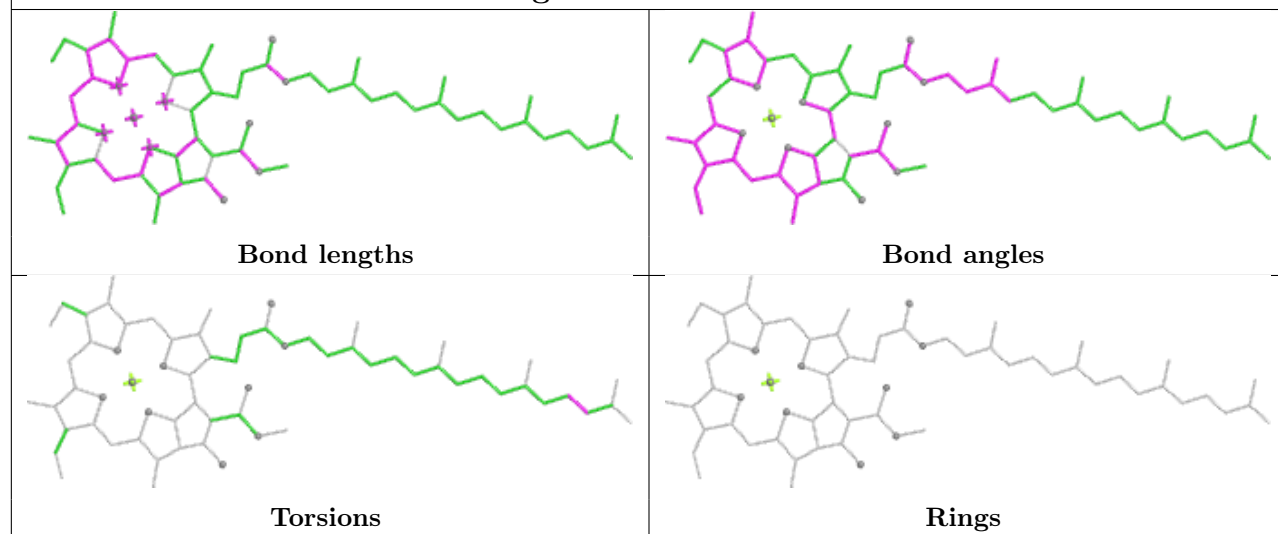


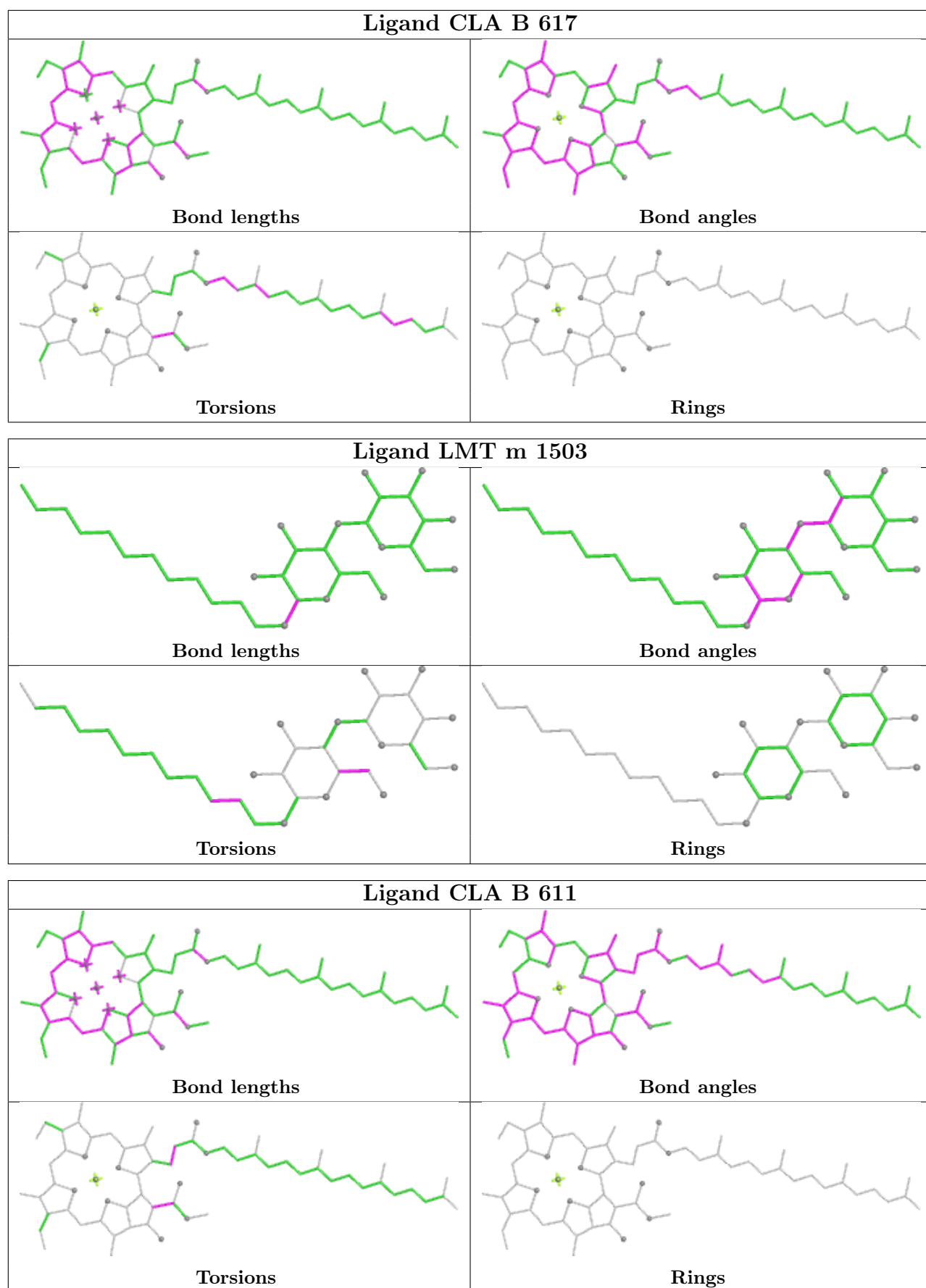
Ligand CLA B 605**Ligand DGD C 516****Ligand CLA c 902**

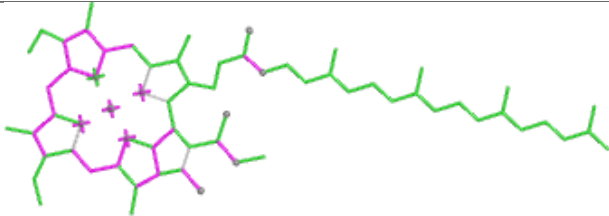
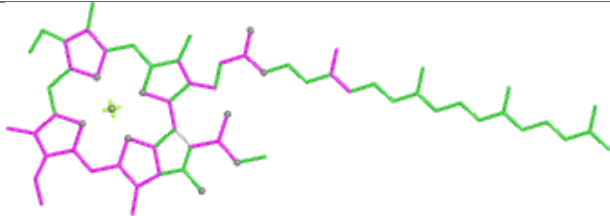
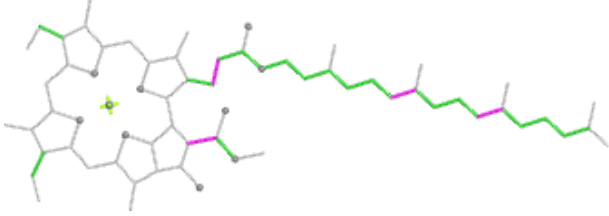
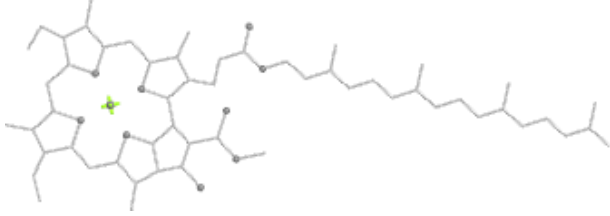
Ligand HEM v 202

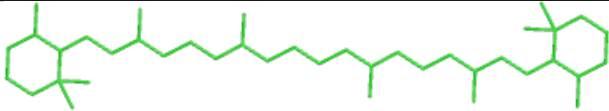
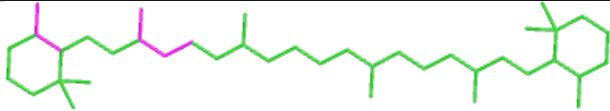
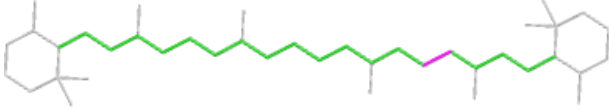
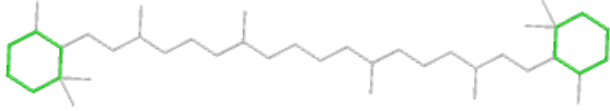


Ligand CLA B 612

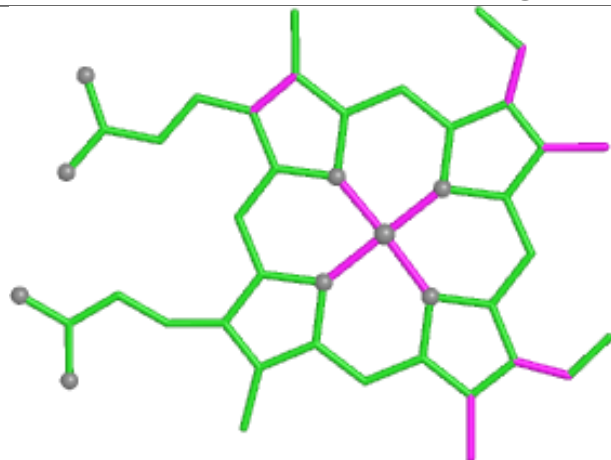




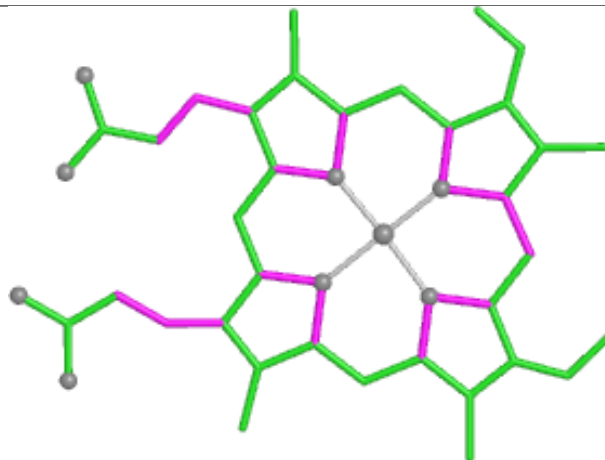
Ligand CLA b 610	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR a 414	
	
Bond lengths	Bond angles
	
Torsions	Rings

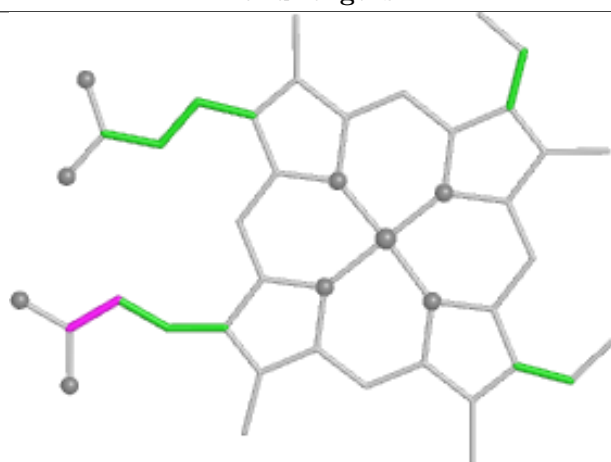
Ligand HEM f 101



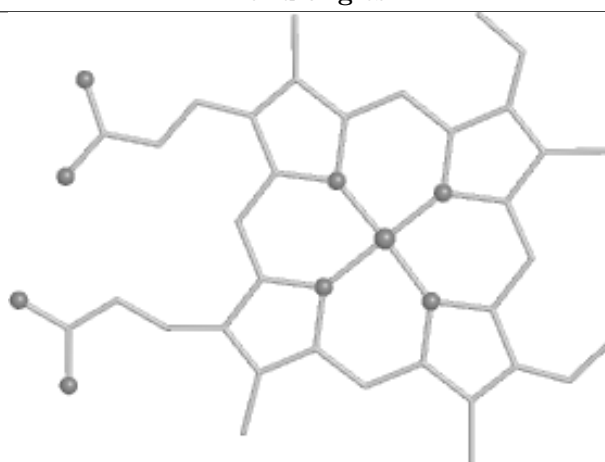
Bond lengths



Bond angles

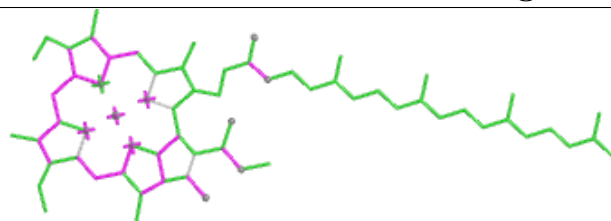


Torsions

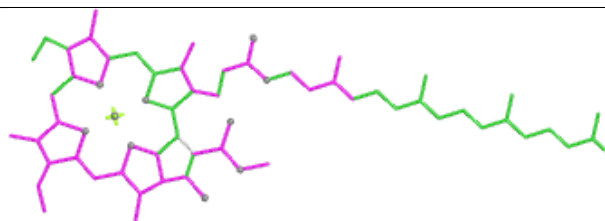


Rings

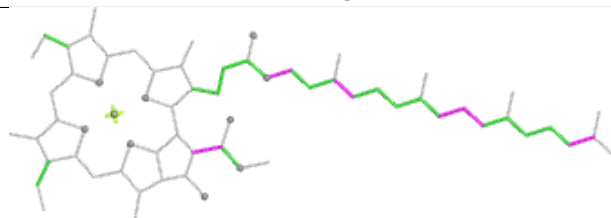
Ligand CLA b 618



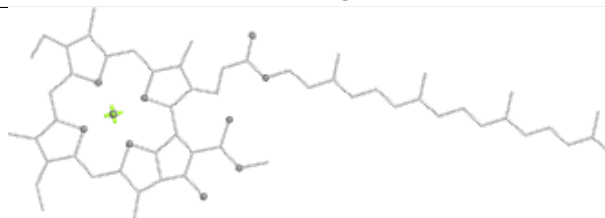
Bond lengths



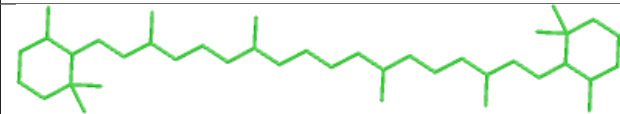
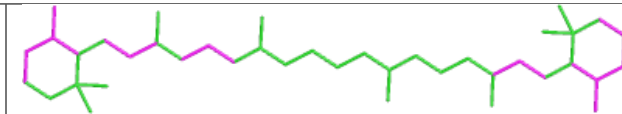
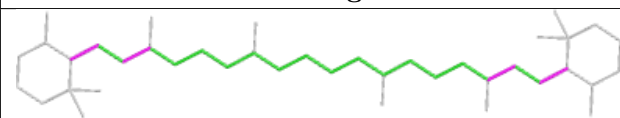
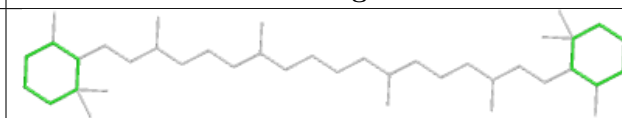
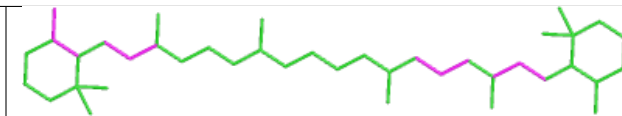
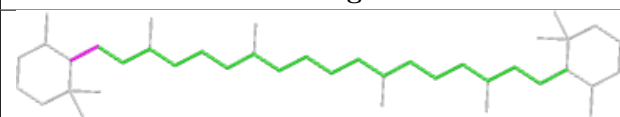
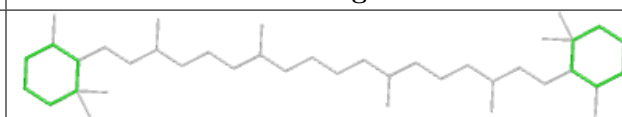
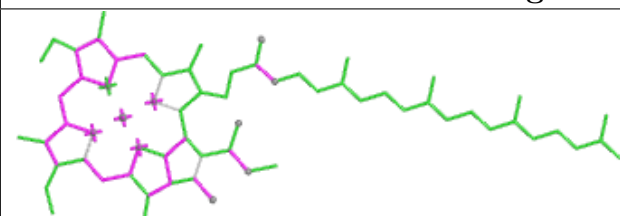
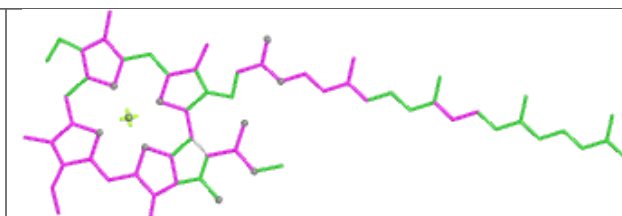
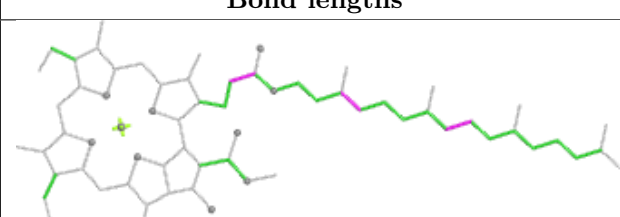
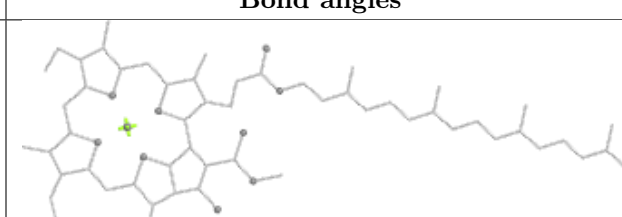
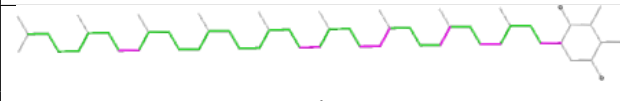
Bond angles

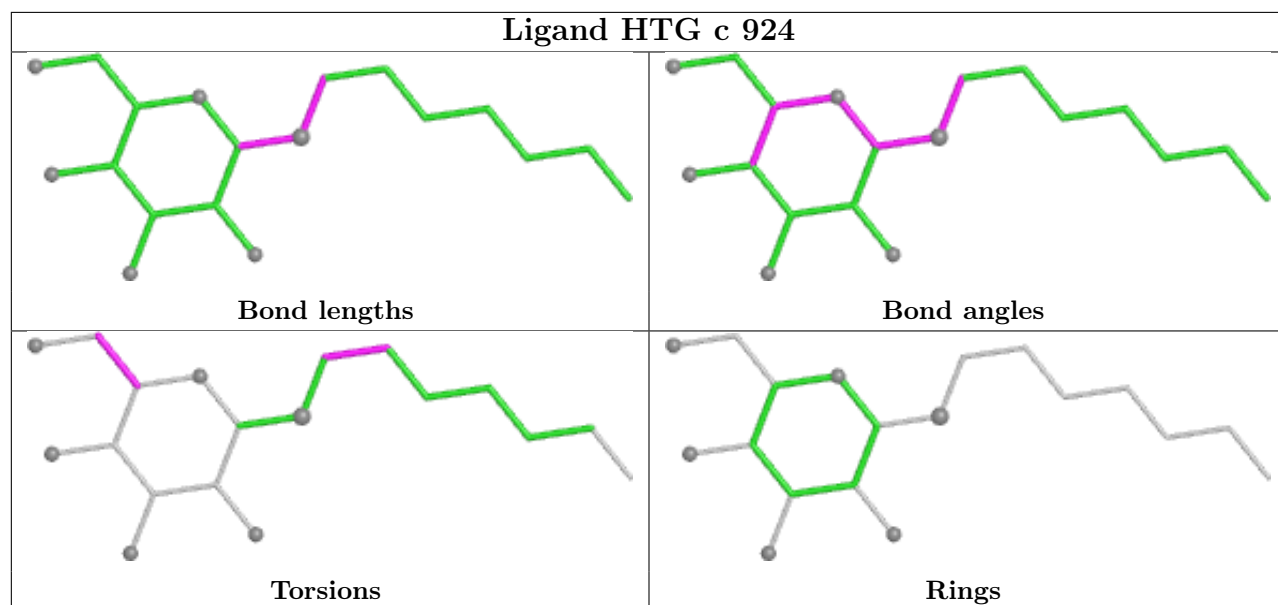
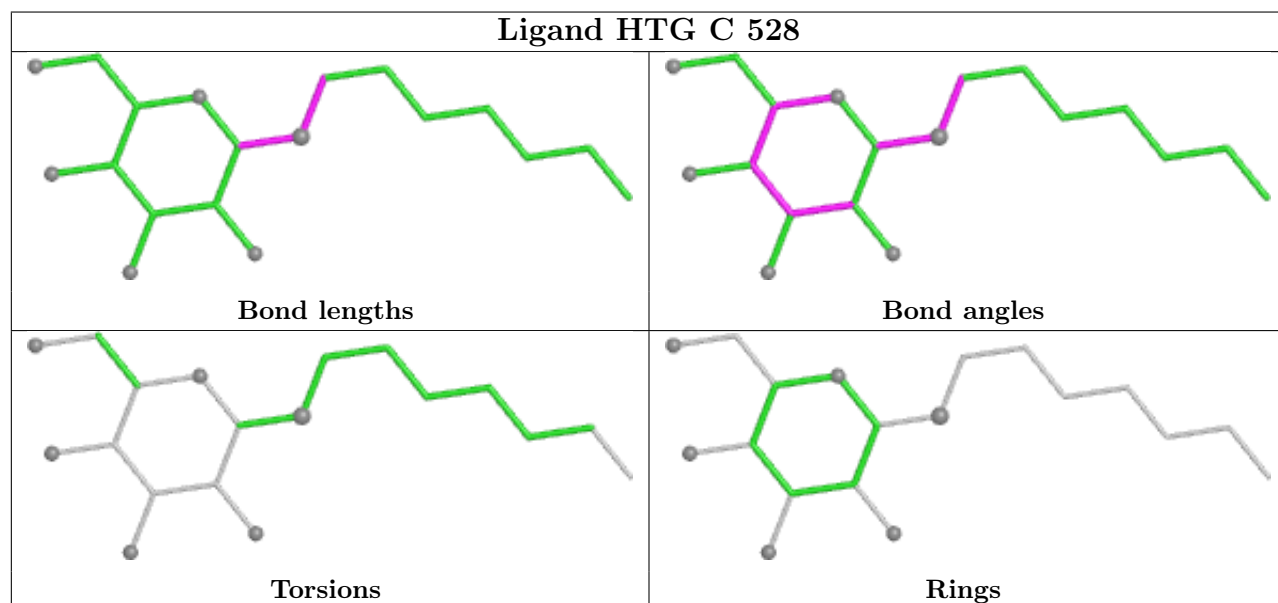
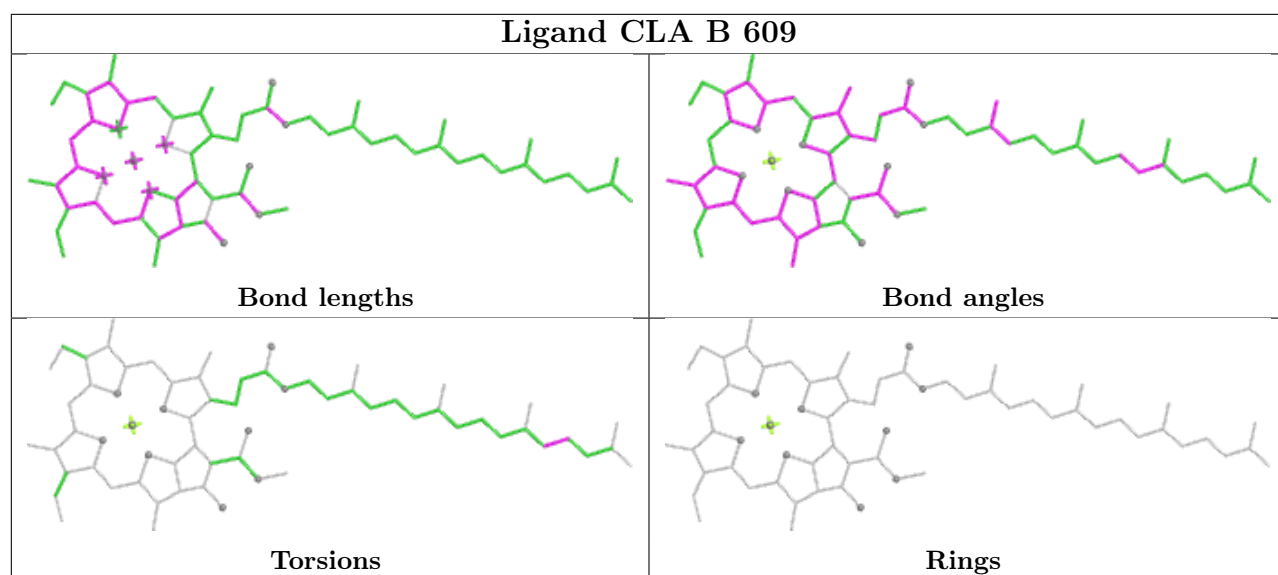


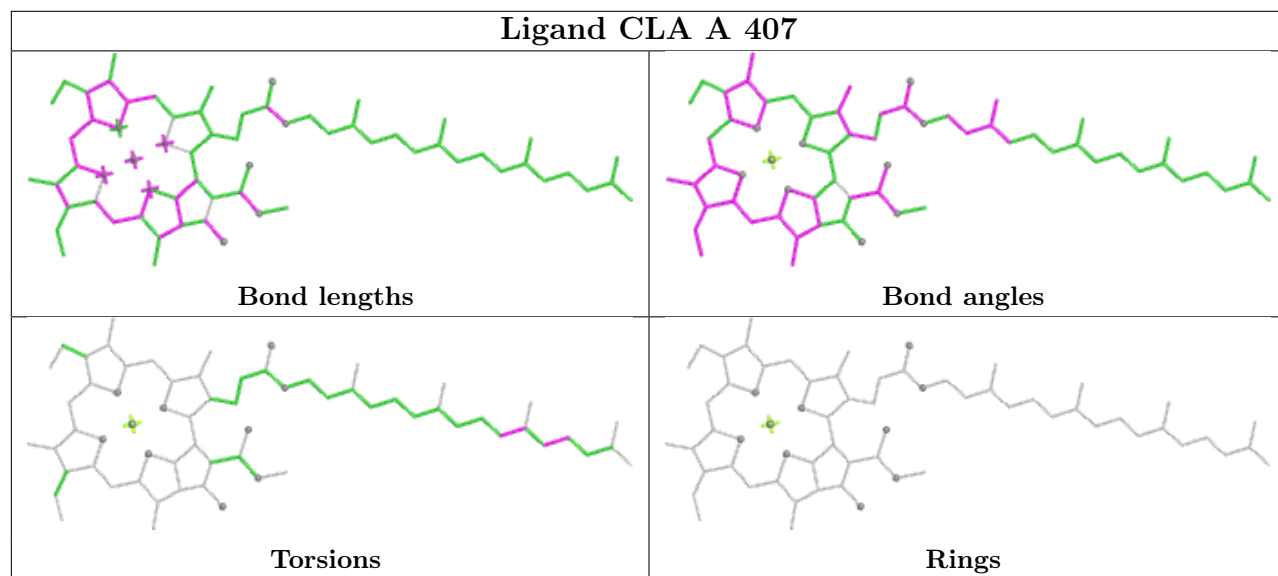
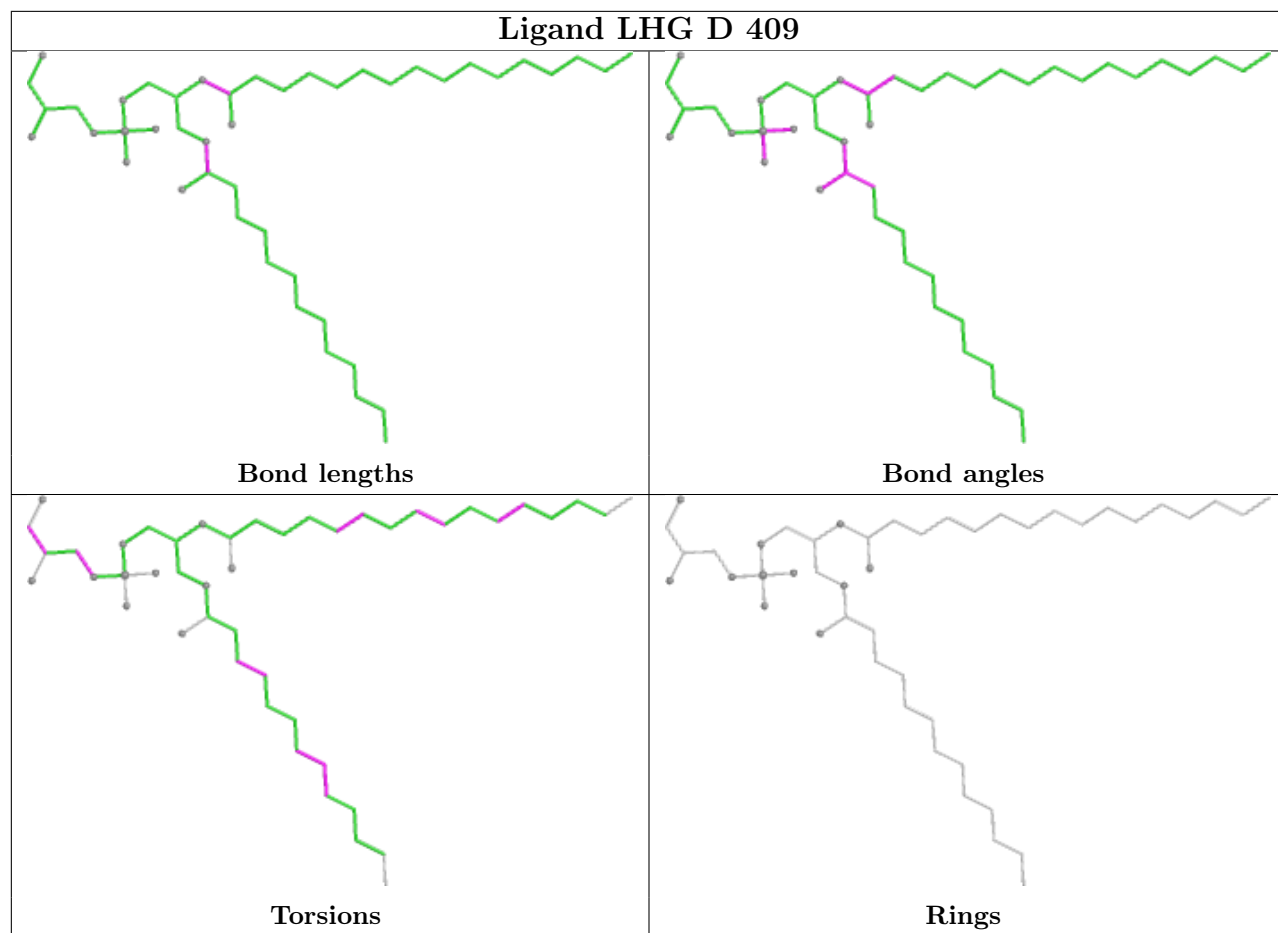
Torsions

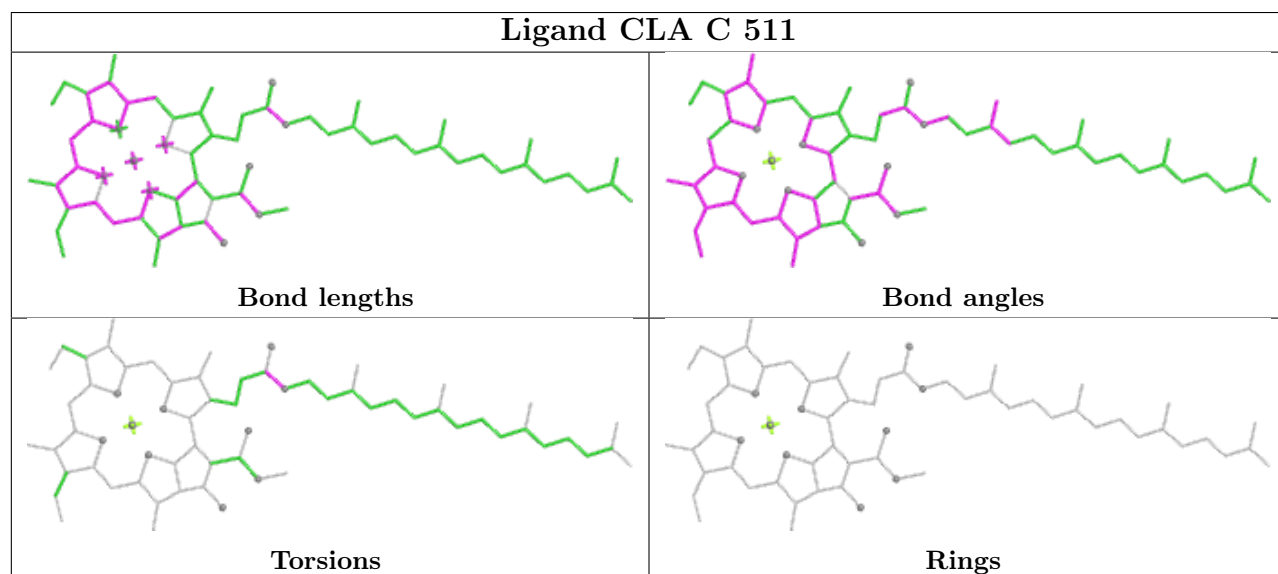
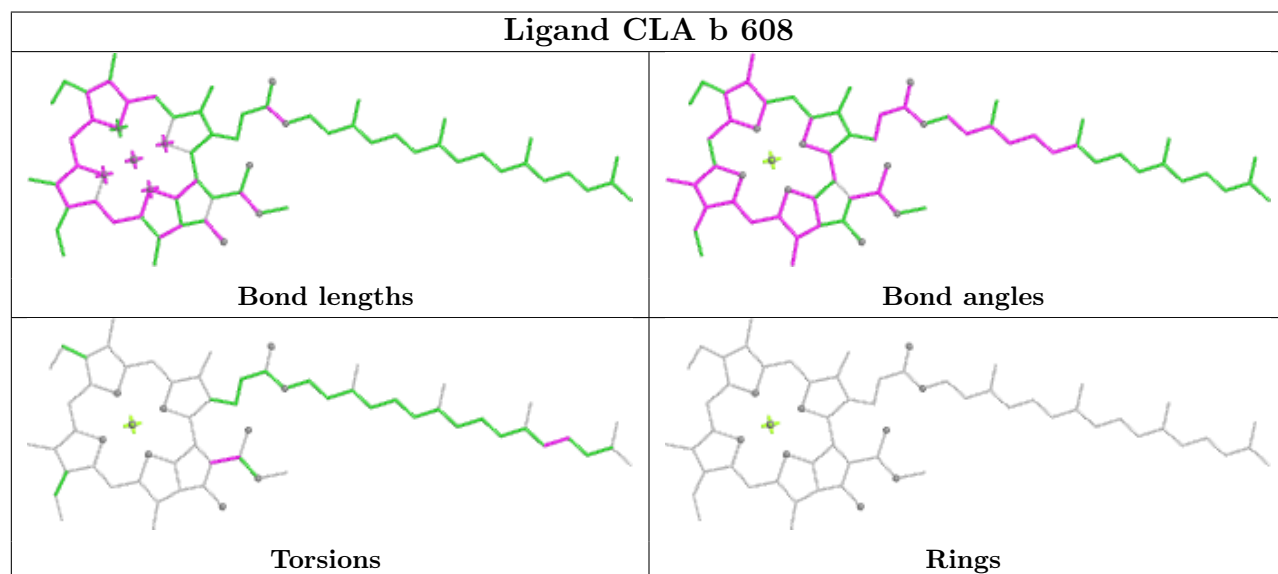
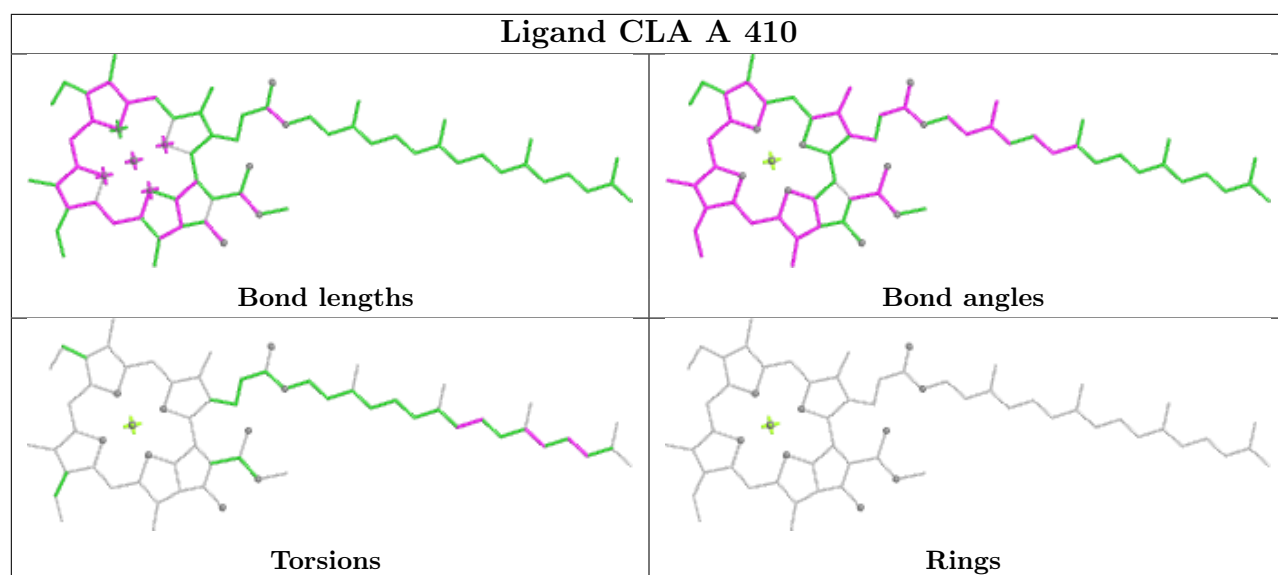


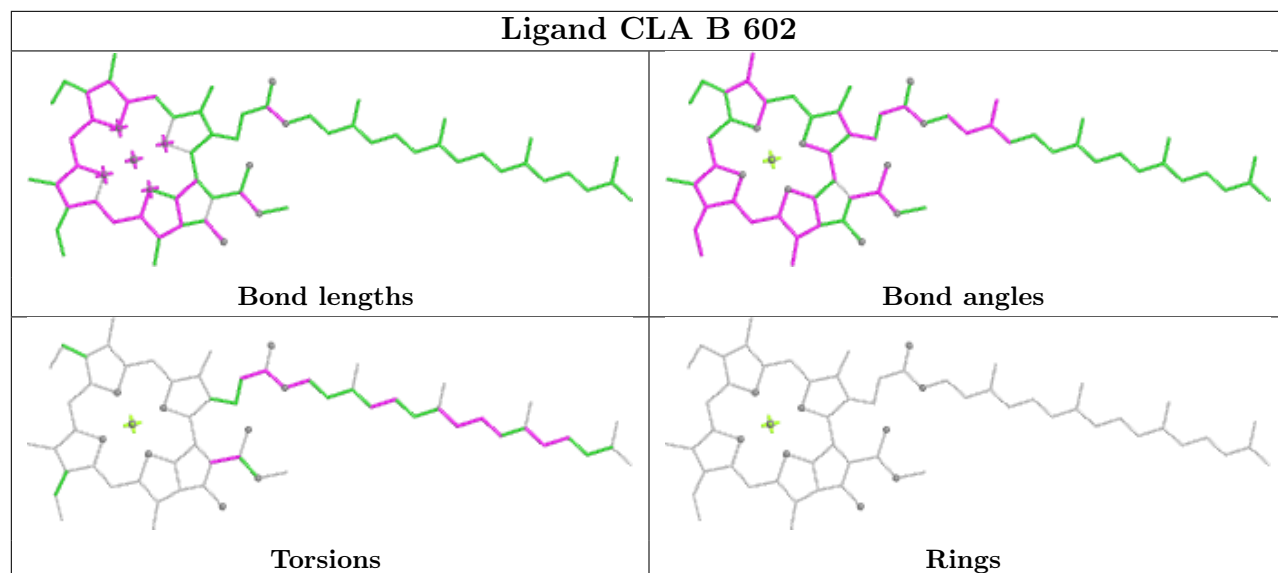
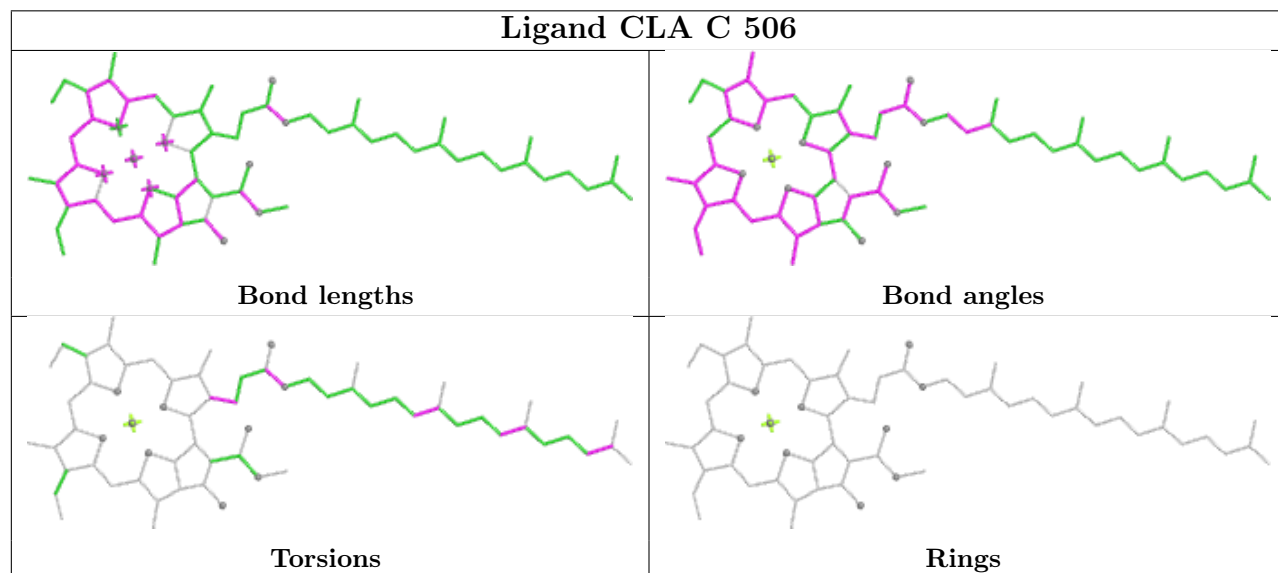
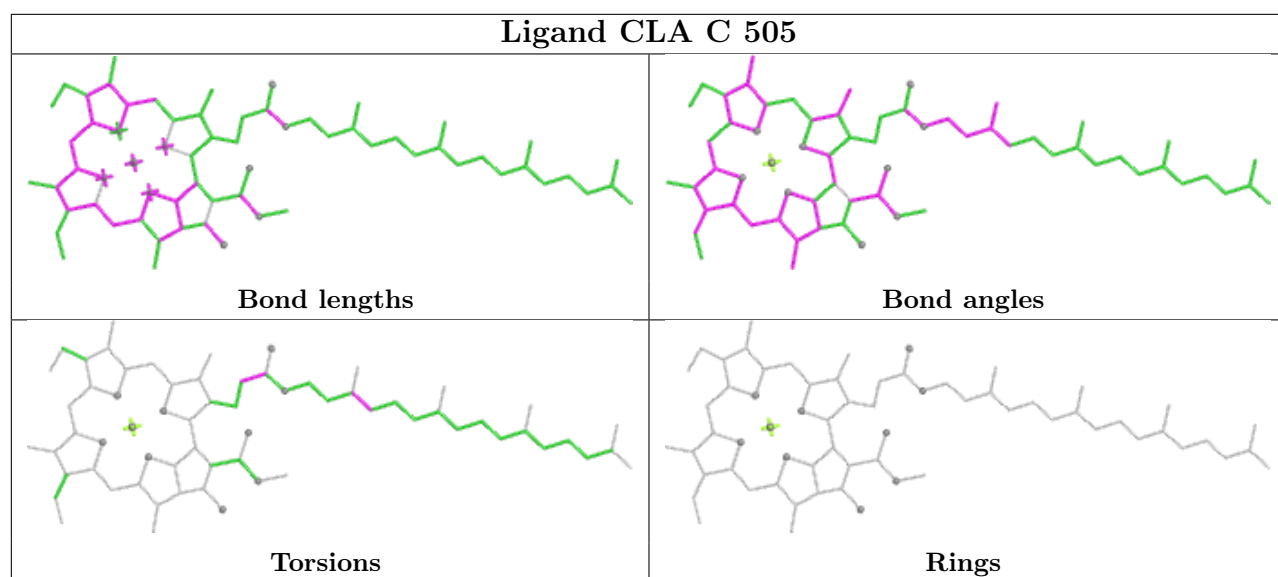
Rings

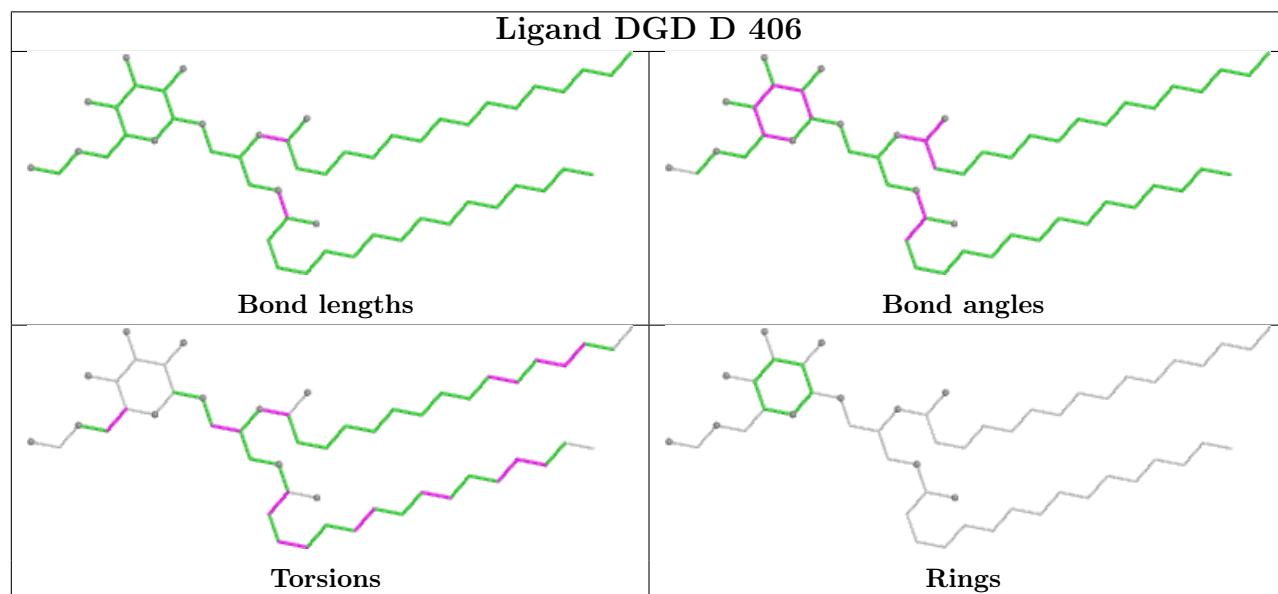
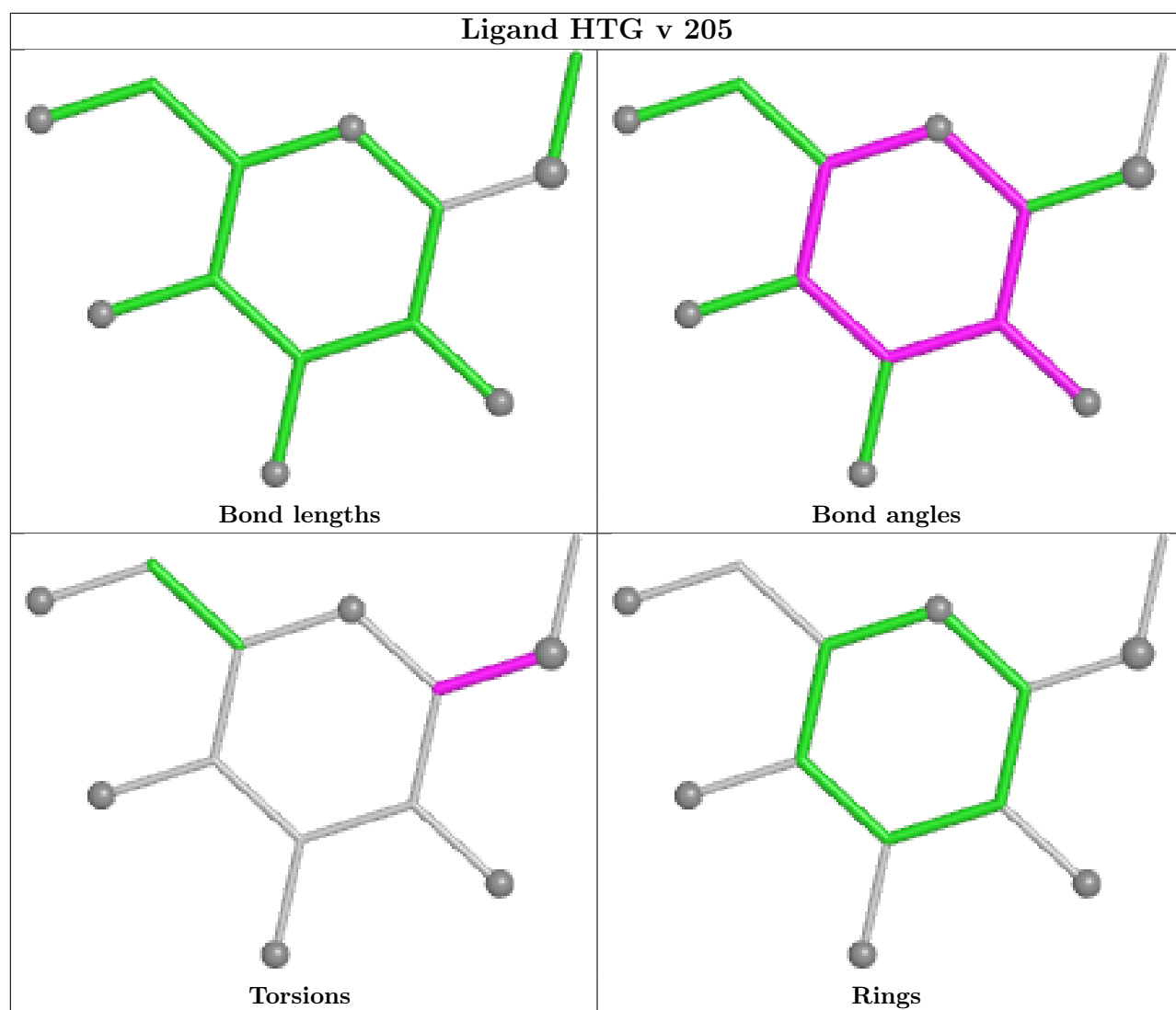
Ligand BCR D 404	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand BCR B 618	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand CLA c 911	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand PL9 A 414	
	
Bond lengths	Bond angles
	
Torsions	Rings

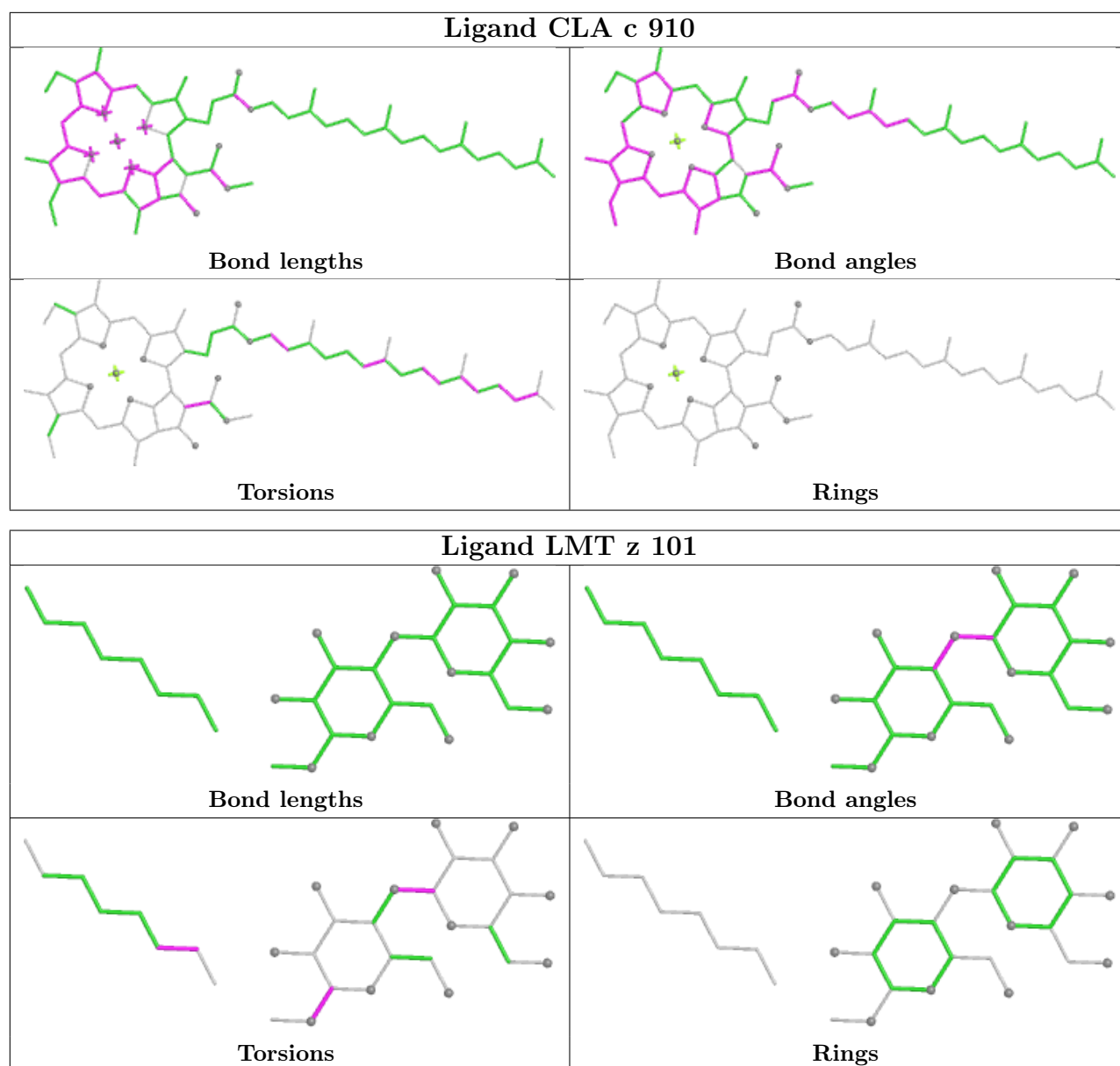












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	334/360 (92%)	-0.43	6 (1%) 67 67	24, 36, 63, 91	3 (0%)
1	a	334/360 (92%)	-0.32	12 (3%) 46 45	25, 39, 68, 104	5 (1%)
2	B	504/505 (99%)	-0.34	10 (1%) 65 64	23, 42, 67, 94	11 (2%)
2	b	501/505 (99%)	-0.24	14 (2%) 55 54	27, 45, 71, 110	12 (2%)
3	C	451/473 (95%)	-0.27	5 (1%) 78 77	33, 47, 64, 117	2 (0%)
3	c	455/473 (96%)	-0.15	4 (0%) 81 80	32, 52, 66, 101	5 (1%)
4	D	340/342 (99%)	-0.53	3 (0%) 81 80	20, 37, 57, 101	1 (0%)
4	d	340/342 (99%)	-0.43	1 (0%) 90 89	22, 42, 63, 95	2 (0%)
5	E	81/84 (96%)	0.20	2 (2%) 58 58	41, 58, 77, 105	0
5	e	79/84 (94%)	0.27	2 (2%) 58 58	49, 62, 87, 105	1 (1%)
6	F	34/45 (75%)	-0.11	0 100 100	43, 49, 76, 87	1 (2%)
6	f	32/45 (71%)	0.14	3 (9%) 14 13	47, 56, 104, 120	0
7	H	63/65 (96%)	-0.16	1 (1%) 70 70	39, 49, 58, 80	0
7	h	63/65 (96%)	0.17	1 (1%) 70 70	44, 55, 65, 104	0
8	I	35/38 (92%)	0.17	2 (5%) 29 28	44, 51, 79, 106	0
8	i	37/38 (97%)	-0.04	2 (5%) 31 30	43, 50, 85, 93	0
9	J	36/40 (90%)	-0.04	1 (2%) 55 54	40, 55, 84, 97	0
9	j	39/40 (97%)	0.38	2 (5%) 33 32	48, 60, 84, 89	0
10	K	37/37 (100%)	-0.17	0 100 100	36, 54, 64, 66	1 (2%)
10	k	37/37 (100%)	0.24	1 (2%) 56 55	53, 61, 73, 75	0
11	L	37/37 (100%)	-0.55	0 100 100	20, 34, 67, 97	1 (2%)
11	l	37/37 (100%)	-0.44	1 (2%) 56 55	21, 36, 80, 110	2 (5%)
12	M	32/36 (88%)	-0.46	0 100 100	21, 36, 48, 70	2 (6%)
12	m	33/36 (91%)	-0.36	0 100 100	21, 36, 57, 84	3 (9%)

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/244 (100%)	-0.19	2 (0%) 82 82	26, 49, 83, 125	7 (2%)
13	o	241/244 (98%)	0.02	6 (2%) 58 58	26, 50, 84, 120	7 (2%)
14	T	29/32 (90%)	-0.39	1 (3%) 48 47	31, 37, 62, 93	0
14	t	29/32 (90%)	-0.28	1 (3%) 48 47	25, 37, 62, 99	1 (3%)
15	U	97/104 (93%)	-0.27	0 100 100	38, 47, 68, 78	4 (4%)
15	u	97/104 (93%)	-0.26	0 100 100	34, 50, 62, 95	1 (1%)
16	V	137/163 (84%)	-0.44	0 100 100	25, 45, 57, 74	2 (1%)
16	v	137/163 (84%)	-0.22	0 100 100	30, 57, 71, 94	1 (0%)
17	Y	27/30 (90%)	0.56	3 (11%) 10 9	59, 66, 95, 101	0
17	y	28/30 (93%)	0.90	1 (3%) 46 45	66, 75, 99, 112	0
18	X	38/40 (95%)	0.14	0 100 100	33, 57, 75, 81	1 (2%)
18	x	38/40 (95%)	0.38	3 (7%) 18 17	35, 63, 94, 108	1 (2%)
19	Z	62/62 (100%)	0.45	5 (8%) 18 17	58, 68, 99, 104	0
19	z	60/62 (96%)	0.94	9 (15%) 5 5	68, 76, 105, 123	0
20	R	30/34 (88%)	2.45	23 (76%) 0 0	85, 107, 118, 123	0
All	All	5265/5508 (95%)	-0.20	127 (2%) 59 59	20, 46, 77, 125	77 (1%)

The worst 5 of 127 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	h	64	ALA	6.0
13	O	58	ASN	4.9
19	z	3	ILE	4.8
2	b	495	PHE	4.7
14	T	30	THR	4.6

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
14	FME	t	1	10/11	0.92	0.10	35,39,52,64	0
12	FME	m	1	10/11	0.93	0.13	40,47,63,69	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	HSK	d	336[A]	10/12	0.94	0.09	44,46,47,47	7
4	HSK	d	336[B]	11/12	0.94	0.09	44,46,46,47	8
12	FME	M	1	10/11	0.95	0.11	39,47,68,68	0
14	FME	T	1	10/11	0.95	0.08	37,42,55,60	0
4	HSK	D	336[A]	10/12	0.97	0.07	40,41,42,43	7
4	HSK	D	336[B]	11/12	0.97	0.07	40,41,42,42	8
8	FME	I	1	10/11	0.98	0.06	42,49,55,57	0
8	FME	i	1	10/11	0.98	0.07	44,51,57,58	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
35	HTG	X	902	12/19	0.46	0.16	107,121,127,127	0
34	LMT	M	302	35/35	0.70	0.18	53,76,89,91	0
31	GOL	h	103	6/6	0.73	0.13	83,88,89,91	0
30	UNL	j	1401	18/-	0.73	0.23	65,78,86,91	0
31	GOL	Z	102	6/6	0.73	0.15	108,110,112,118	0
30	UNL	E	103	13/-	0.74	0.25	81,89,92,92	0
31	GOL	O	305	6/6	0.74	0.15	98,101,103,104	0
30	UNL	M	301	16/-	0.75	0.24	59,67,81,82	0
36	DGD	D	406	53/66	0.75	0.19	82,93,104,108	0
35	HTG	u	201	14/19	0.76	0.19	73,87,103,108	0
30	UNL	y	102	10/-	0.76	0.28	93,99,101,103	0
36	DGD	e	102	39/66	0.76	0.18	83,100,111,113	0
30	UNL	a	418	40/-	0.77	0.19	76,86,97,103	0
31	GOL	C	533	6/6	0.77	0.17	86,88,90,96	0
35	HTG	V	203	13/19	0.78	0.13	60,67,81,99	0
30	UNL	B	635	10/-	0.78	0.24	68,77,86,91	0
31	GOL	o	303	6/6	0.78	0.14	69,76,83,88	0
34	LMT	F	103	26/35	0.78	0.19	59,71,79,82	26
30	UNL	E	102	16/-	0.78	0.25	76,80,88,88	0
41	SO4	O	302	5/5	0.78	0.12	93,106,108,126	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	UNL	c	933	9/-	0.79	0.23	74,83,93,97	0
31	GOL	c	934	6/6	0.79	0.17	67,77,78,80	0
34	LMT	m	1503	35/35	0.79	0.15	52,76,88,88	0
35	HTG	B	625	19/19	0.79	0.13	66,96,101,101	0
34	LMT	C	520	35/35	0.79	0.16	82,89,94,97	0
30	UNL	c	931	18/-	0.80	0.20	87,93,101,104	0
30	UNL	C	523	34/-	0.80	0.18	79,87,96,101	0
30	UNL	e	103	15/-	0.80	0.19	66,75,83,83	0
30	UNL	C	526	19/-	0.80	0.17	70,82,93,94	0
30	UNL	m	1501	13/-	0.80	0.23	63,67,77,81	0
30	UNL	A	415	36/-	0.80	0.18	68,78,90,91	0
35	HTG	B	627	19/19	0.80	0.17	75,92,105,106	0
28	LMG	C	534	51/55	0.80	0.16	67,87,95,105	0
30	UNL	J	104	13/-	0.80	0.23	78,84,93,94	0
35	HTG	c	924	19/19	0.80	0.13	75,96,105,109	0
30	UNL	B	636	15/-	0.80	0.24	69,82,91,92	0
30	UNL	B	638	22/-	0.80	0.14	71,79,97,100	0
31	GOL	c	937	6/6	0.80	0.15	99,99,99,100	0
30	UNL	a	422	10/-	0.80	0.21	69,72,84,90	0
30	UNL	i	804	9/-	0.81	0.18	80,82,84,84	0
34	LMT	t	904	24/35	0.81	0.17	56,65,87,95	0
31	GOL	a	421	6/6	0.81	0.16	69,77,77,80	0
30	UNL	A	418	4/-	0.81	0.24	78,79,82,84	0
30	UNL	j	1403	14/-	0.81	0.19	70,76,79,87	0
31	GOL	c	939	6/6	0.81	0.16	78,79,83,84	0
30	UNL	Y	102	10/-	0.81	0.23	82,87,93,98	0
30	UNL	c	935	6/-	0.81	0.19	75,82,87,87	0
31	GOL	C	531	6/6	0.81	0.15	52,55,58,59	0
30	UNL	b	636	8/-	0.81	0.18	61,68,73,78	0
30	UNL	i	803	16/-	0.81	0.18	71,79,88,91	0
30	UNL	t	901	12/-	0.82	0.18	70,77,83,85	0
35	HTG	d	403	19/19	0.82	0.14	83,97,112,112	0
30	UNL	b	633	18/-	0.82	0.19	59,64,79,79	0
30	UNL	b	635	9/-	0.82	0.23	71,78,82,83	0
34	LMT	T	703	24/35	0.82	0.17	53,67,81,92	0
34	LMT	B	623	35/35	0.82	0.14	63,79,93,96	0
30	UNL	i	801	18/-	0.83	0.19	53,64,80,89	0
35	HTG	b	627	19/19	0.83	0.14	89,109,113,114	0
34	LMT	c	922	35/35	0.83	0.14	77,85,101,103	0
31	GOL	t	902	6/6	0.83	0.15	54,59,60,60	0
30	UNL	A	416	14/-	0.83	0.18	66,76,88,89	0
31	GOL	O	304	6/6	0.83	0.10	69,76,77,85	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
27	SQD	B	621	54/54	0.83	0.15	62,75,100,111	0
37	LHG	E	101	49/49	0.83	0.18	72,94,100,105	0
27	SQD	b	601	54/54	0.83	0.15	55,71,92,98	0
35	HTG	C	522	19/19	0.84	0.12	76,93,101,104	0
34	LMT	J	102	23/35	0.84	0.17	65,77,93,97	0
30	UNL	B	637	11/-	0.84	0.20	72,78,85,91	0
35	HTG	b	603	19/19	0.84	0.14	78,91,101,106	0
30	UNL	h	104	7/-	0.84	0.17	65,68,75,77	0
34	LMT	Z	101	35/35	0.84	0.15	71,96,106,112	0
34	LMT	b	625	25/35	0.84	0.15	72,87,99,101	0
31	GOL	v	201	6/6	0.84	0.17	102,103,103,105	0
33	CA	B	601	1/1	0.84	0.11	86,86,86,86	0
27	SQD	a	401	54/54	0.84	0.14	53,70,88,95	0
30	UNL	T	701	15/-	0.84	0.20	73,80,88,89	0
27	SQD	f	102	33/54	0.84	0.15	83,92,110,112	0
30	UNL	c	925	30/-	0.85	0.17	83,94,106,108	0
31	GOL	u	202	6/6	0.85	0.11	76,80,89,95	0
30	UNL	B	634	15/-	0.85	0.18	54,60,76,81	0
31	GOL	L	102	6/6	0.85	0.14	55,56,59,60	0
35	HTG	v	205	13/19	0.85	0.12	69,80,89,92	0
35	HTG	U	201	9/19	0.85	0.20	79,83,102,116	0
30	UNL	B	639	5/-	0.85	0.16	72,72,75,76	0
30	UNL	H	104	7/-	0.85	0.18	61,66,76,79	0
30	UNL	d	402	36/-	0.85	0.18	63,74,89,92	0
27	SQD	A	417	54/54	0.86	0.13	52,68,83,87	0
29	PL9	a	417	55/55	0.86	0.18	68,79,90,94	0
30	UNL	b	634	18/-	0.86	0.20	83,94,109,115	0
30	UNL	I	102	12/-	0.86	0.17	63,68,74,74	0
30	UNL	I	103	12/-	0.86	0.16	67,71,84,88	0
30	UNL	X	901	16/-	0.86	0.15	50,53,69,72	0
31	GOL	b	631	6/6	0.86	0.16	60,64,65,72	0
34	LMT	z	101	32/35	0.86	0.14	66,98,106,107	0
31	GOL	c	927	6/6	0.86	0.13	58,61,62,64	0
31	GOL	c	932	6/6	0.86	0.14	67,68,74,75	0
31	GOL	C	530	6/6	0.86	0.21	84,85,85,87	0
37	LHG	e	101	27/49	0.86	0.13	102,117,131,137	0
30	UNL	J	103	16/-	0.86	0.21	82,88,104,107	0
35	HTG	H	105	16/19	0.87	0.16	82,95,106,108	0
31	GOL	u	203	6/6	0.87	0.12	71,72,77,78	0
31	GOL	b	632	6/6	0.87	0.16	57,60,65,66	0
30	UNL	C	532	4/-	0.87	0.20	76,78,80,80	0
29	PL9	A	414	55/55	0.87	0.18	65,74,87,90	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	GOL	B	630	6/6	0.87	0.14	47,51,55,57	0
35	HTG	c	923	19/19	0.87	0.11	88,93,99,102	0
30	UNL	I	101	14/-	0.87	0.17	54,59,72,77	0
30	UNL	c	930	11/-	0.88	0.13	82,91,105,109	0
28	LMG	c	921	51/55	0.88	0.13	60,87,94,96	0
31	GOL	c	938	6/6	0.88	0.12	60,64,70,77	0
30	UNL	i	802	12/-	0.88	0.19	66,71,81,81	0
30	UNL	D	411	37/-	0.88	0.16	54,67,82,84	0
31	GOL	B	632	6/6	0.88	0.14	52,55,61,71	0
34	LMT	M	303	35/35	0.88	0.11	46,58,66,66	0
30	UNL	a	403	6/-	0.88	0.17	73,79,79,80	0
27	SQD	F	101	37/54	0.88	0.12	60,74,80,84	0
30	UNL	C	529	9/-	0.88	0.16	80,81,83,84	0
31	GOL	H	101	6/6	0.88	0.15	95,95,98,100	0
34	LMT	a	402	35/35	0.89	0.11	47,60,70,77	0
30	UNL	v	206	7/-	0.89	0.17	69,72,76,78	0
30	UNL	b	637	10/-	0.89	0.16	63,83,91,91	0
34	LMT	m	1502	35/35	0.89	0.10	44,56,63,66	0
35	HTG	C	528	19/19	0.89	0.12	89,101,108,114	0
31	GOL	C	525	6/6	0.89	0.13	48,51,56,60	0
33	CA	b	604	1/1	0.89	0.08	107,107,107,107	0
30	UNL	d	412	18/-	0.90	0.14	54,66,76,78	0
30	UNL	D	412	16/-	0.90	0.15	45,54,68,70	0
31	GOL	o	304	6/6	0.90	0.13	87,89,89,89	0
28	LMG	b	624	51/55	0.90	0.12	42,54,60,64	0
31	GOL	b	638	6/6	0.90	0.18	91,91,92,95	0
34	LMT	D	401	35/35	0.90	0.11	50,61,74,75	0
35	HTG	b	602	19/19	0.90	0.11	52,62,69,76	0
28	LMG	a	416	51/55	0.90	0.12	56,69,76,79	0
35	HTG	b	626	19/19	0.90	0.14	47,54,76,79	0
35	HTG	C	521	19/19	0.90	0.11	77,83,92,94	0
28	LMG	C	519	49/55	0.91	0.13	43,67,78,81	0
35	HTG	B	626	19/19	0.91	0.11	50,64,70,73	0
31	GOL	B	631	6/6	0.91	0.11	43,51,54,61	0
31	GOL	c	936	6/6	0.91	0.16	87,87,87,87	0
31	GOL	v	204	6/6	0.91	0.10	65,71,77,79	0
31	GOL	b	630	6/6	0.91	0.11	44,49,55,56	0
28	LMG	B	622	51/55	0.91	0.11	39,50,59,63	0
28	LMG	c	920	51/55	0.91	0.13	47,71,83,85	0
31	GOL	C	527	6/6	0.91	0.17	74,75,75,76	0
31	GOL	c	926	6/6	0.91	0.11	56,63,69,74	0
31	GOL	B	628	6/6	0.91	0.11	47,52,55,58	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	GOL	c	929	6/6	0.91	0.11	62,63,72,72	0
31	GOL	A	422	6/6	0.92	0.10	41,43,45,47	0
26	BCR	t	903	40/40	0.92	0.09	34,47,56,59	0
28	LMG	A	413	51/55	0.92	0.11	54,66,75,79	0
31	GOL	V	204	6/6	0.92	0.12	38,47,48,49	0
27	SQD	A	412	52/54	0.92	0.12	41,66,75,79	0
35	HTG	B	624	19/19	0.92	0.14	43,51,69,69	0
31	GOL	a	419	6/6	0.92	0.11	40,45,50,52	0
24	CLA	B	602	65/65	0.92	0.10	44,58,78,81	0
31	GOL	b	628	6/6	0.92	0.11	56,60,64,66	0
24	CLA	C	506	65/65	0.92	0.11	48,59,75,78	0
30	UNL	d	413	18/-	0.92	0.14	58,65,82,84	0
24	CLA	b	605	65/65	0.92	0.10	49,65,82,88	0
37	LHG	D	407	49/49	0.92	0.10	37,44,52,56	0
24	CLA	c	914	65/65	0.92	0.10	55,68,83,86	0
26	BCR	T	702	40/40	0.92	0.09	36,48,57,58	0
31	GOL	A	420	6/6	0.92	0.11	47,53,60,60	0
31	GOL	b	629	6/6	0.93	0.11	52,57,57,61	0
24	CLA	C	513	65/65	0.93	0.10	55,66,80,81	0
27	SQD	a	415	54/54	0.93	0.12	42,71,82,83	0
26	BCR	d	406	40/40	0.93	0.10	45,52,67,71	0
31	GOL	B	633	6/6	0.93	0.10	47,50,52,54	0
31	GOL	O	306	6/6	0.93	0.09	73,77,81,86	0
24	CLA	B	617	65/65	0.93	0.10	37,44,71,73	0
24	CLA	b	618	65/65	0.93	0.10	33,40,65,71	0
24	CLA	b	620	65/65	0.93	0.10	40,47,77,79	0
24	CLA	c	907	65/65	0.93	0.12	49,58,71,75	0
39	RRX	h	101	41/41	0.93	0.10	44,54,63,71	0
24	CLA	B	615	65/65	0.93	0.10	32,38,63,67	0
24	CLA	b	610	65/65	0.94	0.09	37,46,58,64	0
26	BCR	C	514	40/40	0.94	0.09	52,62,67,70	0
26	BCR	D	404	40/40	0.94	0.10	41,47,68,69	0
26	BCR	K	101	40/40	0.94	0.09	47,51,56,58	0
32	BCT	a	408	4/4	0.94	0.09	45,46,52,59	0
31	GOL	A	419	6/6	0.94	0.08	41,45,46,50	0
37	LHG	D	409	46/49	0.94	0.10	37,45,76,78	0
24	CLA	C	512	65/65	0.94	0.09	52,58,73,76	0
37	LHG	d	408	49/49	0.94	0.09	40,47,54,58	0
26	BCR	c	915	40/40	0.94	0.10	61,69,75,75	0
28	LMG	D	410	48/55	0.94	0.10	39,45,69,75	0
24	CLA	c	913	65/65	0.94	0.09	53,60,74,78	0
24	CLA	C	508	65/65	0.95	0.08	38,44,70,73	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	GOL	V	205	6/6	0.95	0.07	59,66,69,75	0
24	CLA	d	405	65/65	0.95	0.09	43,51,79,82	0
26	BCR	B	618	40/40	0.95	0.07	37,42,47,49	0
31	GOL	a	420	6/6	0.95	0.07	42,44,45,49	0
28	LMG	d	411	48/55	0.95	0.09	44,50,70,74	0
26	BCR	B	619	40/40	0.95	0.07	34,43,54,59	0
24	CLA	B	607	65/65	0.95	0.08	34,42,60,65	0
29	PL9	d	407	55/55	0.95	0.07	31,37,42,45	0
24	CLA	C	504	65/65	0.95	0.08	37,43,63,69	0
31	GOL	v	203	6/6	0.95	0.09	43,51,53,54	0
24	CLA	c	905	65/65	0.95	0.08	42,48,65,68	0
36	DGD	H	103	62/66	0.95	0.09	37,43,51,54	0
36	DGD	c	917	62/66	0.95	0.09	38,47,74,79	0
24	CLA	a	413	65/65	0.95	0.09	35,40,77,79	0
36	DGD	h	102	62/66	0.95	0.08	42,48,55,59	0
31	GOL	b	640	6/6	0.95	0.08	44,52,54,54	0
26	BCR	Y	101	40/40	0.95	0.08	49,54,61,62	0
26	BCR	b	623	40/40	0.95	0.08	43,48,59,60	0
37	LHG	b	639	49/49	0.95	0.09	36,45,54,65	0
24	CLA	c	908	65/65	0.95	0.09	43,50,64,67	0
24	CLA	c	909	65/65	0.95	0.09	40,46,77,81	0
24	CLA	A	410	65/65	0.95	0.10	35,39,77,82	0
26	BCR	y	101	40/40	0.95	0.09	51,60,66,67	0
24	CLA	a	410	65/65	0.96	0.09	35,39,75,85	0
24	CLA	c	911	65/65	0.96	0.07	42,49,54,64	0
31	GOL	V	206	6/6	0.96	0.06	50,53,55,58	0
24	CLA	C	507	65/65	0.96	0.08	44,49,64,66	0
24	CLA	C	503	65/65	0.96	0.07	42,47,55,63	0
32	BCT	A	421	4/4	0.96	0.07	41,42,49,57	0
24	CLA	b	606	65/65	0.96	0.07	40,44,50,55	0
24	CLA	C	509	65/65	0.96	0.07	43,47,59,62	0
24	CLA	b	613	65/65	0.96	0.07	44,48,53,56	0
26	BCR	B	620	40/40	0.96	0.07	40,46,59,60	0
24	CLA	b	614	65/65	0.96	0.07	38,44,47,49	0
26	BCR	C	515	40/40	0.96	0.08	44,52,56,58	0
31	GOL	B	629	6/6	0.96	0.08	42,44,46,47	0
24	CLA	C	510	65/65	0.96	0.07	40,45,53,59	0
35	HTG	o	301	19/19	0.96	0.08	41,45,54,54	0
24	CLA	b	619	65/65	0.96	0.07	38,46,59,63	0
24	CLA	C	511	65/65	0.96	0.07	42,52,58,59	0
36	DGD	C	516	62/66	0.96	0.09	35,43,72,77	0
36	DGD	C	517	56/66	0.96	0.07	38,46,67,71	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
36	DGD	C	518	58/66	0.96	0.08	36,43,61,69	0
24	CLA	c	902	65/65	0.96	0.08	42,51,58,61	0
26	BCR	a	414	40/40	0.96	0.07	33,40,47,48	0
26	BCR	b	621	40/40	0.96	0.07	38,44,48,52	0
36	DGD	c	918	55/66	0.96	0.08	41,52,65,68	0
36	DGD	c	919	60/66	0.96	0.08	42,48,60,68	0
26	BCR	b	622	40/40	0.96	0.07	36,44,56,59	0
24	CLA	c	904	65/65	0.96	0.07	44,52,58,70	0
24	CLA	B	611	65/65	0.96	0.07	37,40,44,47	0
37	LHG	D	408	49/49	0.96	0.08	32,40,52,57	0
26	BCR	c	916	40/40	0.96	0.08	48,53,58,59	0
29	PL9	D	405	55/55	0.96	0.06	30,35,39,42	0
31	GOL	f	104	6/6	0.96	0.07	61,63,66,68	0
24	CLA	C	501	65/65	0.96	0.08	40,47,55,60	0
37	LHG	d	409	49/49	0.96	0.08	35,41,52,57	0
37	LHG	d	410	40/49	0.96	0.09	42,48,76,78	0
26	BCR	k	101	40/40	0.96	0.08	51,58,66,67	0
39	RRX	H	102	41/41	0.96	0.07	41,48,58,70	0
24	CLA	D	403	65/65	0.96	0.07	38,44,72,74	0
31	GOL	V	201	6/6	0.96	0.07	53,58,62,62	0
24	CLA	B	608	65/65	0.97	0.06	30,35,46,49	0
24	CLA	b	607	65/65	0.97	0.06	38,42,49,54	0
24	CLA	b	608	65/65	0.97	0.06	33,37,63,68	0
25	PHO	A	408	64/64	0.97	0.05	28,33,38,40	0
25	PHO	A	409	64/64	0.97	0.06	31,37,45,51	0
25	PHO	a	411	64/64	0.97	0.06	31,35,39,44	0
25	PHO	a	412	64/64	0.97	0.06	34,41,48,57	0
26	BCR	A	411	40/40	0.97	0.07	34,40,47,48	0
24	CLA	b	609	65/65	0.97	0.06	34,38,49,51	0
24	CLA	C	505	65/65	0.97	0.07	38,44,57,60	0
24	CLA	b	611	65/65	0.97	0.06	32,37,47,48	0
24	CLA	b	612	65/65	0.97	0.06	39,44,52,56	0
24	CLA	B	609	65/65	0.97	0.06	34,39,47,50	0
24	CLA	B	610	65/65	0.97	0.06	39,42,47,54	0
24	CLA	b	615	65/65	0.97	0.06	33,38,48,52	0
24	CLA	b	616	65/65	0.97	0.06	33,39,44,48	0
31	GOL	c	928	6/6	0.97	0.07	42,44,45,46	0
24	CLA	b	617	65/65	0.97	0.06	32,37,58,63	0
24	CLA	B	603	65/65	0.97	0.07	36,40,47,48	0
24	CLA	B	612	65/65	0.97	0.06	30,35,45,48	0
24	CLA	B	613	65/65	0.97	0.06	30,36,42,44	0
24	CLA	B	614	65/65	0.97	0.06	30,35,56,60	0

Continued on next page...

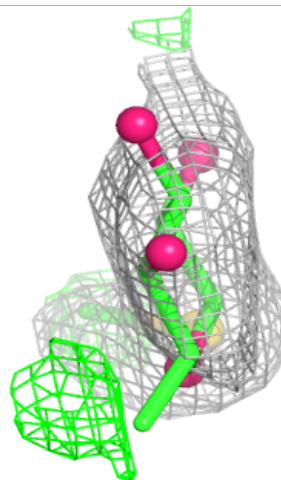
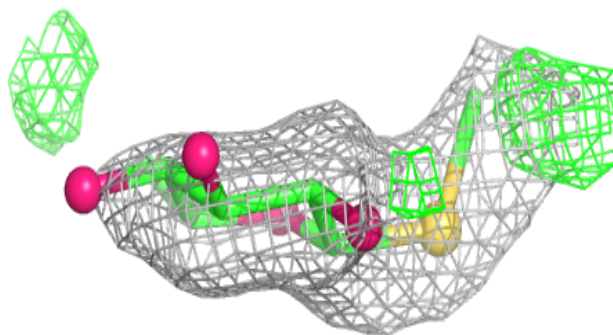
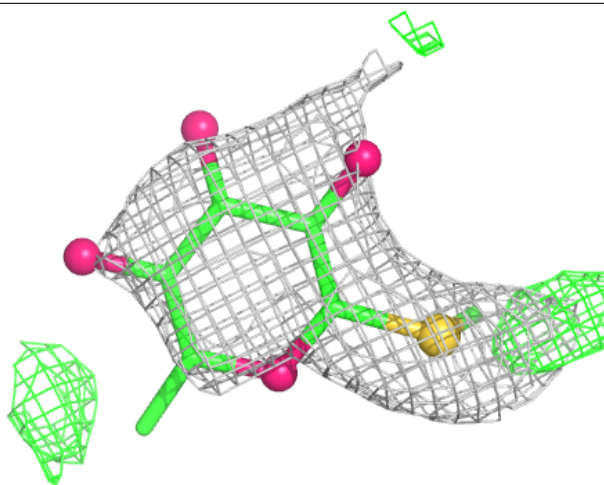
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	CLA	c	903	65/65	0.97	0.07	40,47,60,71	0
24	CLA	B	604	65/65	0.97	0.06	34,38,46,48	0
24	CLA	B	616	65/65	0.97	0.07	37,41,56,59	0
37	LHG	L	101	49/49	0.97	0.07	35,43,53,61	0
24	CLA	c	906	65/65	0.97	0.06	41,45,56,64	0
24	CLA	B	605	65/65	0.97	0.07	30,34,57,68	0
24	CLA	B	606	65/65	0.97	0.06	32,35,45,49	0
24	CLA	C	502	65/65	0.97	0.06	39,42,54,60	0
24	CLA	c	910	65/65	0.97	0.07	44,50,61,66	0
38	HEM	F	102	43/43	0.97	0.08	53,58,70,74	0
38	HEM	f	101	43/43	0.97	0.08	59,65,75,91	0
35	HTG	O	303	19/19	0.97	0.08	41,45,57,58	0
24	CLA	A	407	65/65	0.97	0.07	29,34,73,77	0
40	MG	j	1402	1/1	0.97	0.14	51,51,51,51	0
24	CLA	c	912	65/65	0.97	0.07	45,54,63,65	0
24	CLA	A	406	65/65	0.98	0.05	27,31,40,43	0
24	CLA	d	401	65/65	0.98	0.05	30,33,41,48	0
24	CLA	d	404	65/65	0.98	0.06	30,35,55,59	0
24	CLA	a	409	65/65	0.98	0.05	31,35,40,51	0
38	HEM	v	202	43/43	0.98	0.06	44,49,51,54	0
24	CLA	A	405	65/65	0.98	0.05	27,31,38,49	0
24	CLA	D	402	65/65	0.98	0.05	25,31,49,54	0
31	GOL	C	524	6/6	0.98	0.06	37,38,40,40	0
33	CA	f	103	1/1	0.98	0.08	70,70,70,70	0
33	CA	O	301	1/1	0.99	0.06	68,68,68,68	0
38	HEM	V	202	43/43	0.99	0.06	37,40,43,45	0
21	OEX	a	404	10/10	0.99	0.03	38,39,41,44	0
33	CA	c	901	1/1	0.99	0.05	61,61,61,61	0
23	CL	A	403	1/1	0.99	0.06	36,36,36,36	0
33	CA	o	302	1/1	0.99	0.04	69,69,69,69	0
40	MG	J	101	1/1	0.99	0.08	43,43,43,43	0
21	OEX	A	401	10/10	0.99	0.04	34,37,40,41	0
33	CA	F	104	1/1	0.99	0.06	63,63,63,63	0
23	CL	A	404	1/1	1.00	0.03	35,35,35,35	0
23	CL	a	406	1/1	1.00	0.07	43,43,43,43	0
23	CL	a	407	1/1	1.00	0.02	41,41,41,41	0
22	FE2	a	405	1/1	1.00	0.02	41,41,41,41	0
22	FE2	A	402	1/1	1.00	0.01	37,37,37,37	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.

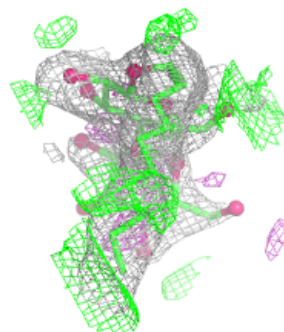
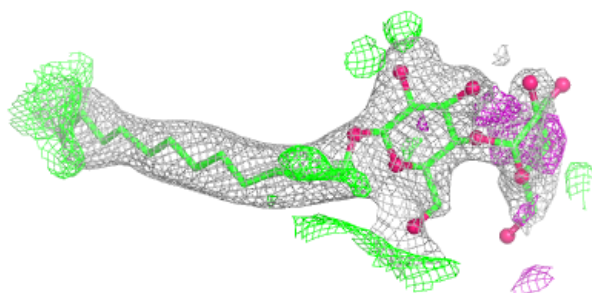
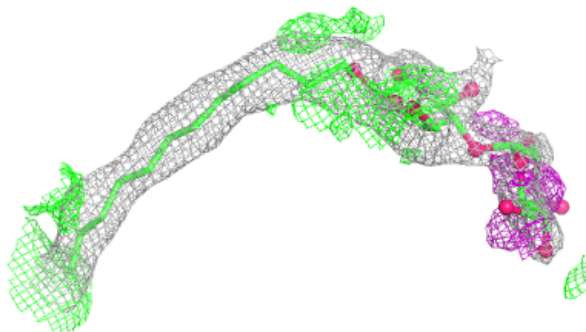
Electron density around HTG X 902:

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

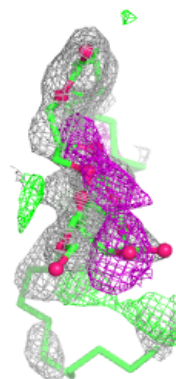
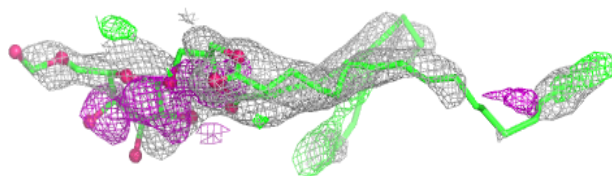
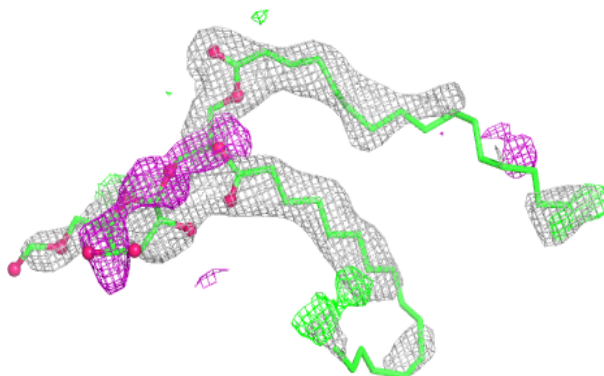


Electron density around LMT M 302:

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

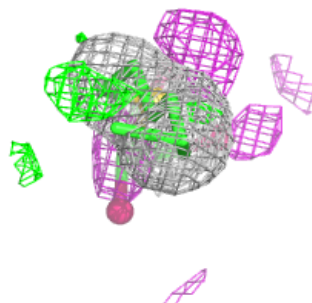
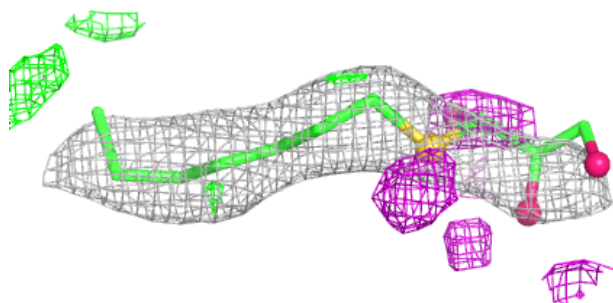
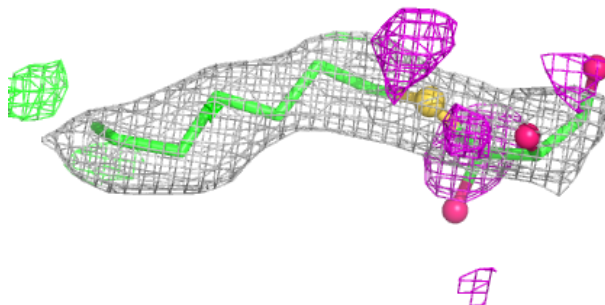
**Electron density around DGD D 406:**

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

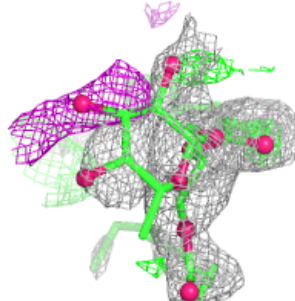
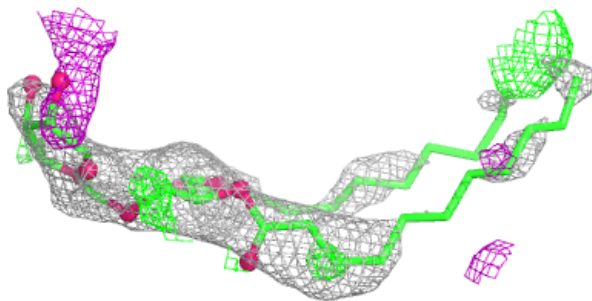
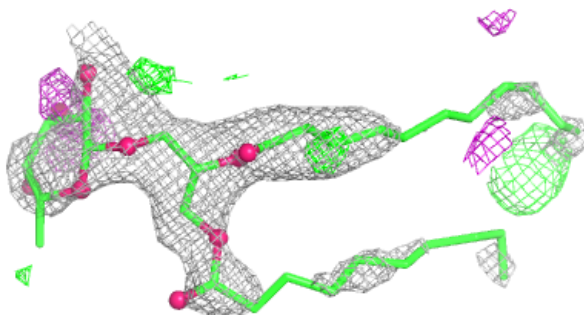


Electron density around HTG u 201:

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

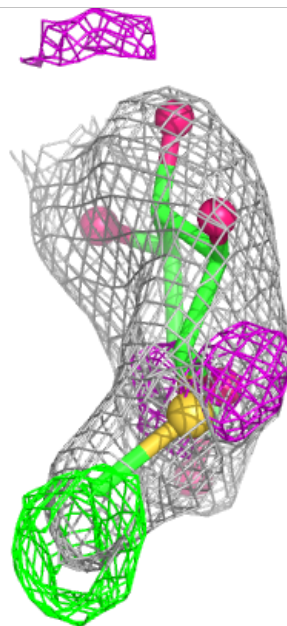
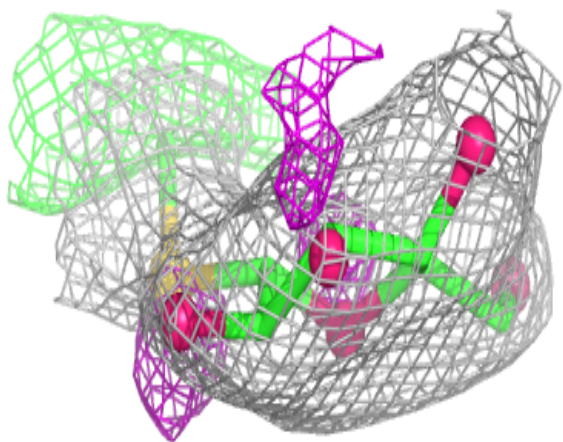
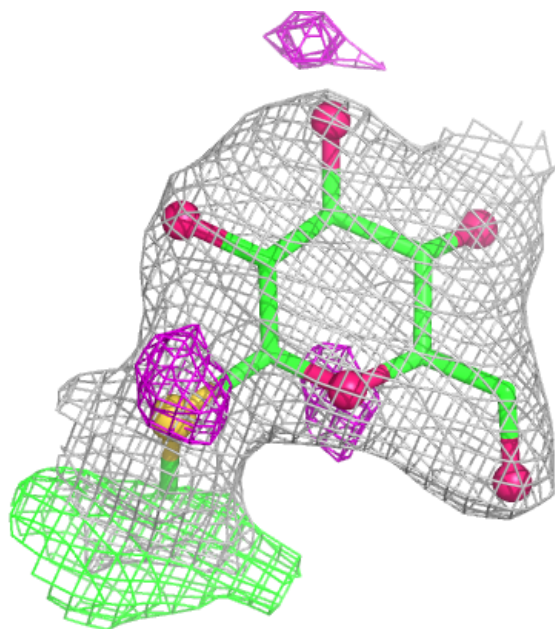
**Electron density around DGD e 102:**

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



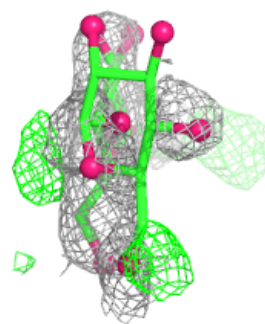
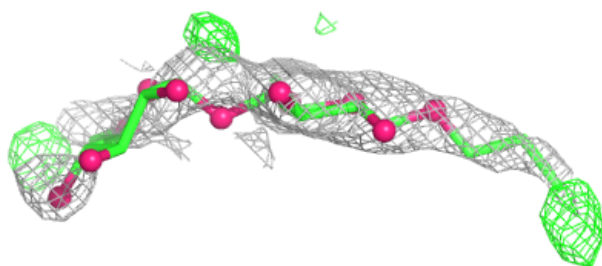
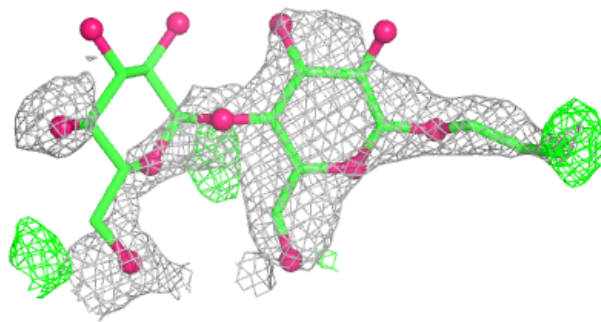
Electron density around HTG V 203:

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

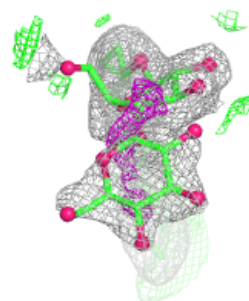
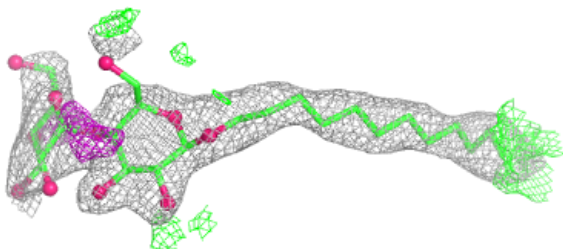
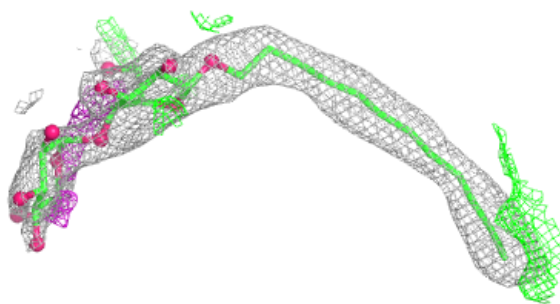


Electron density around LMT F 103:

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

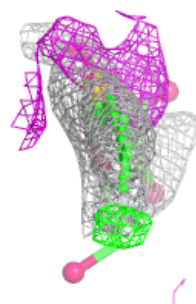
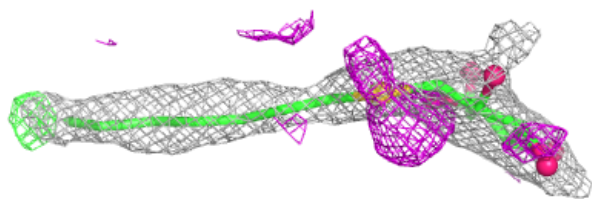
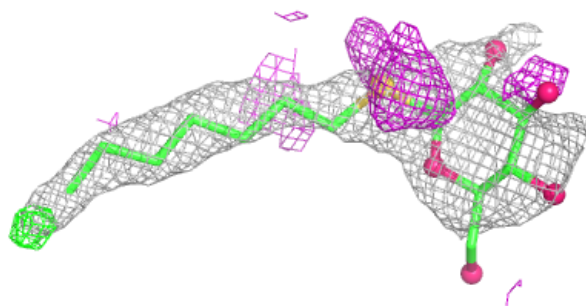
**Electron density around LMT m 1503:**

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

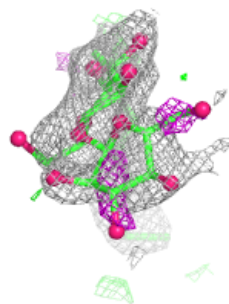
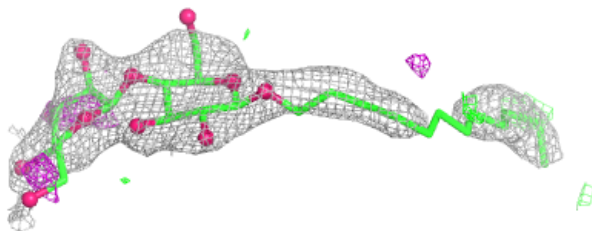
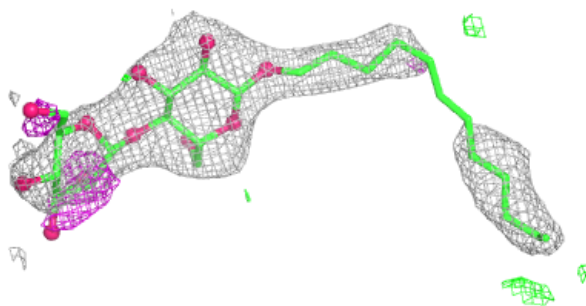


Electron density around HTG B 625:

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

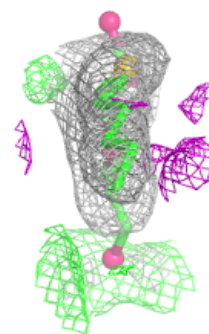
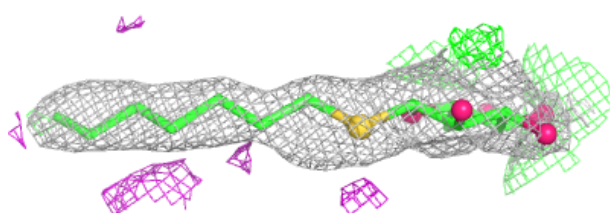
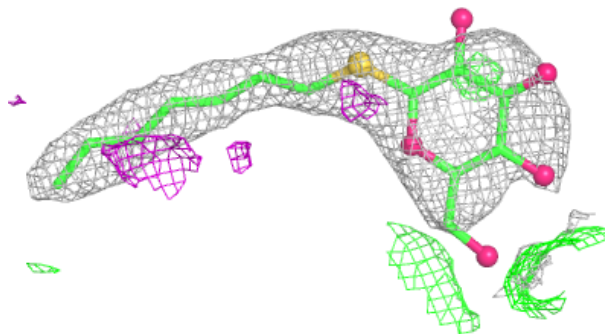
**Electron density around LMT C 520:**

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

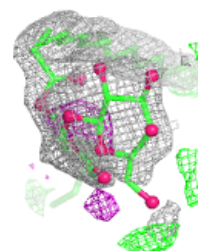
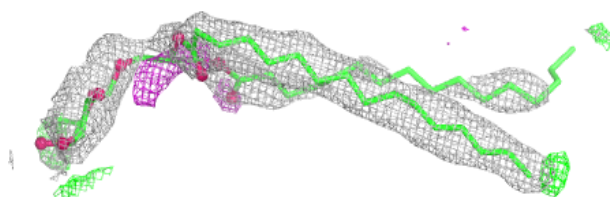
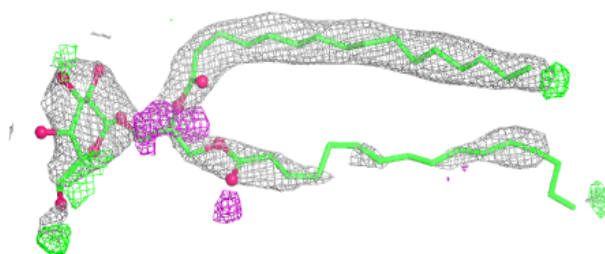


Electron density around HTG B 627:

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

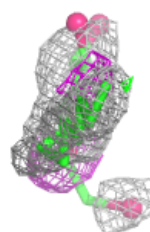
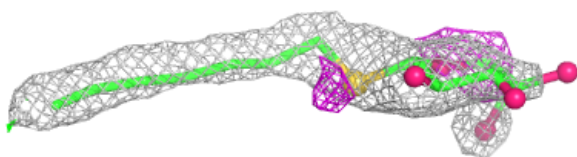
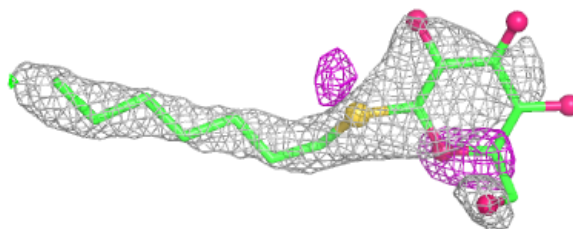
**Electron density around LMG C 534:**

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

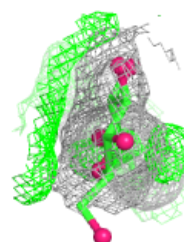
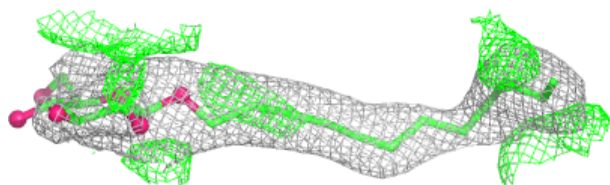
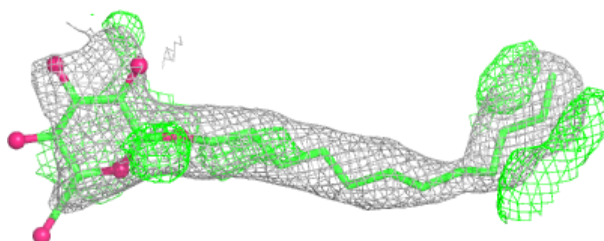


Electron density around HTG c 924:

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

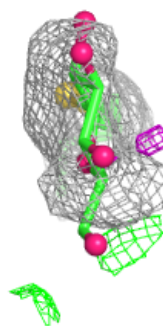
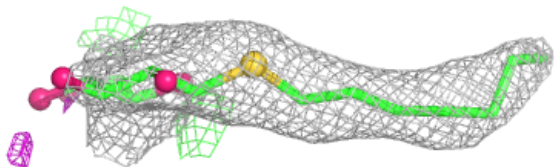
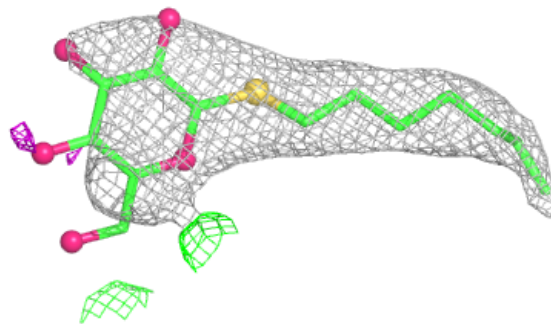
**Electron density around LMT t 904:**

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

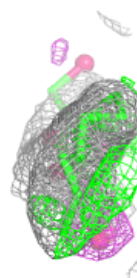
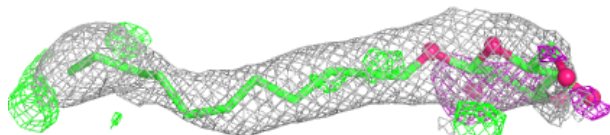
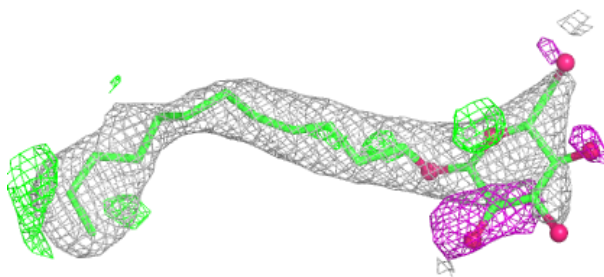


Electron density around HTG d 403:

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

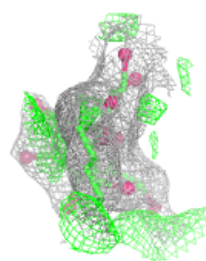
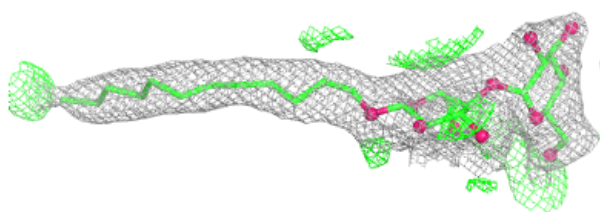
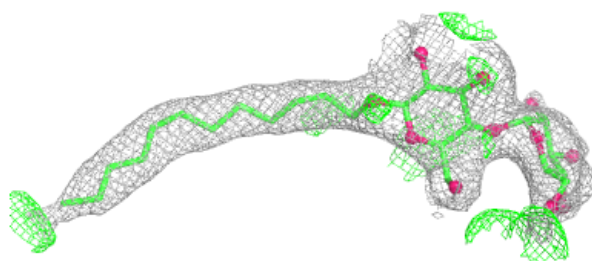
**Electron density around LMT T 703:**

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

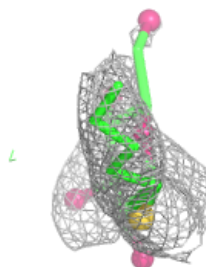
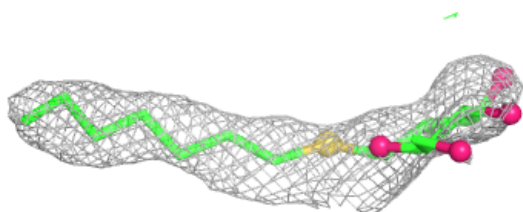
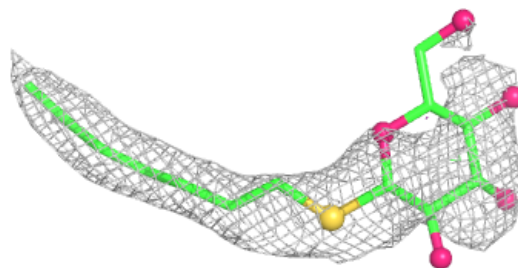


Electron density around LMT B 623:

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

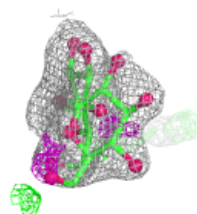
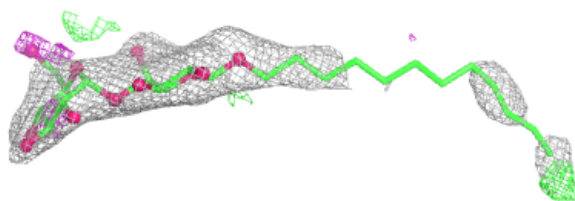
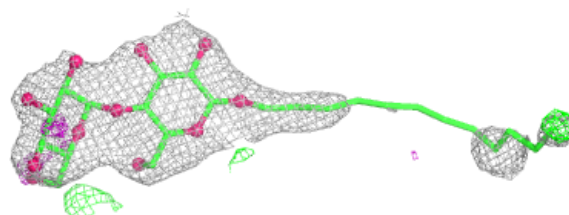
**Electron density around HTG b 627:**

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

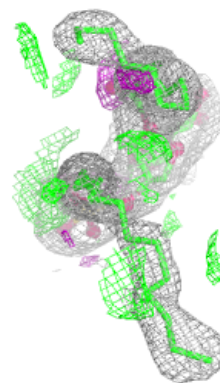
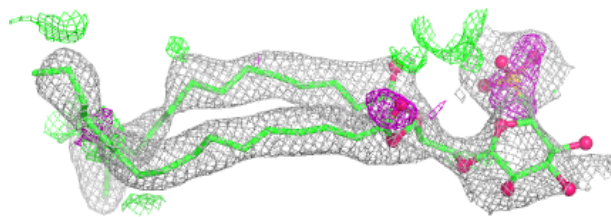
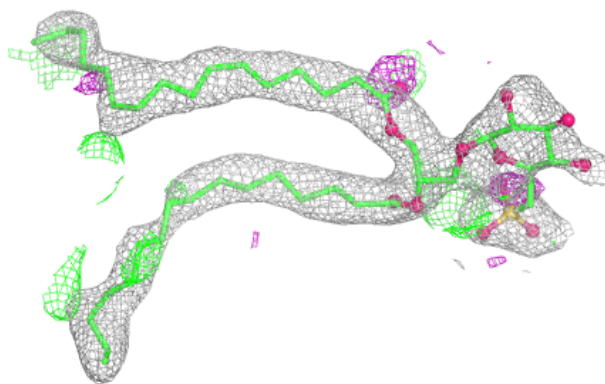


Electron density around LMT c 922:

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

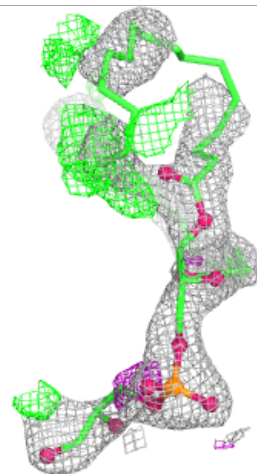
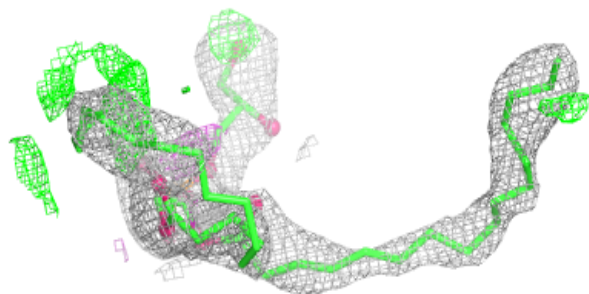
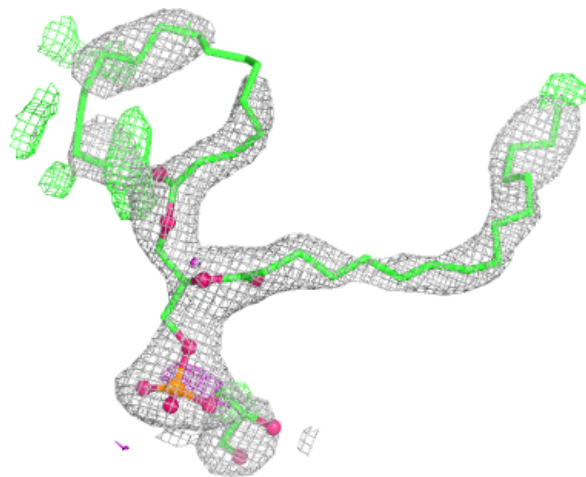
**Electron density around SQD B 621:**

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



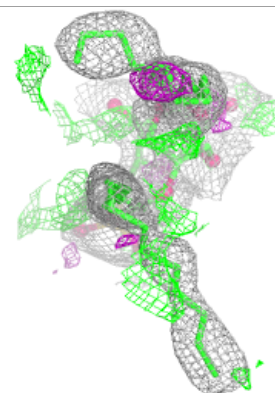
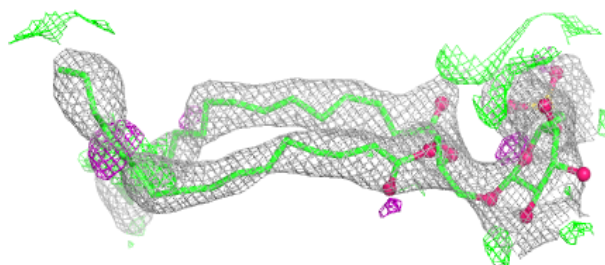
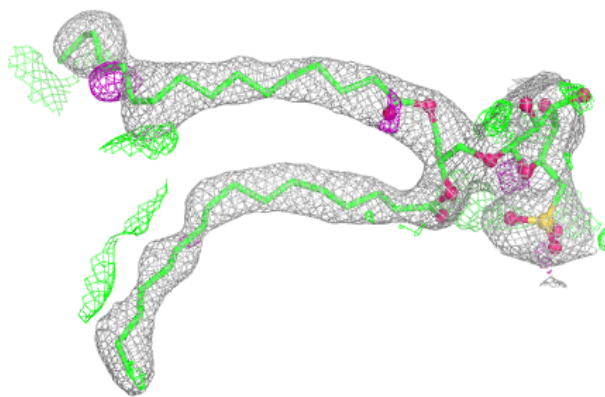
Electron density around LHG E 101:

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

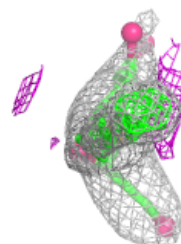
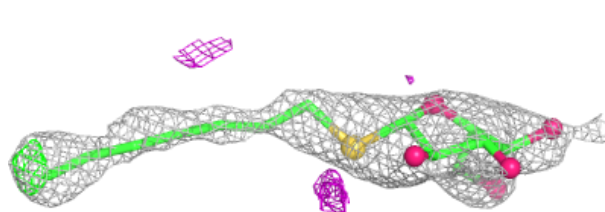
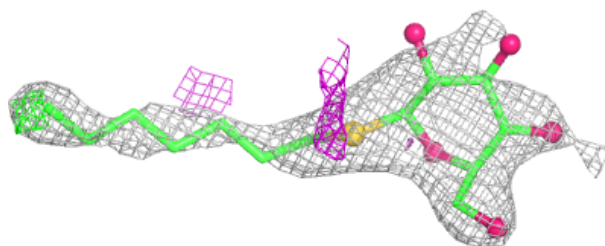


Electron density around SQD b 601:

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

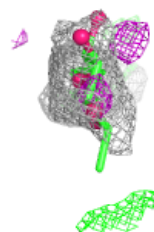
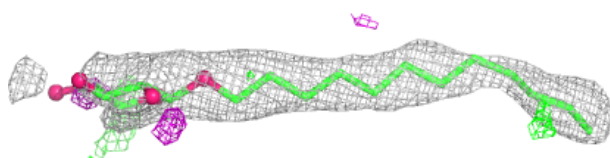
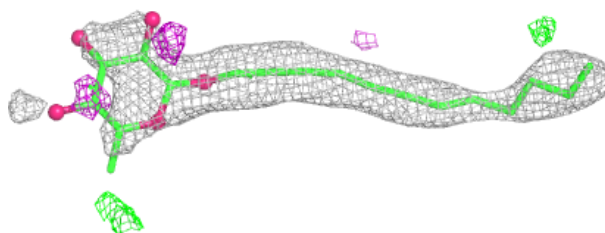
**Electron density around HTG C 522:**

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

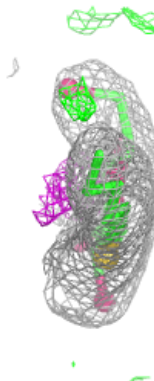
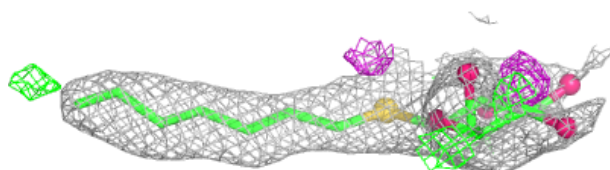
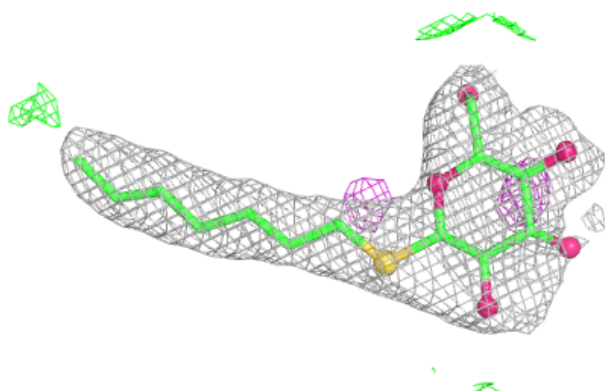


Electron density around LMT J 102:

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

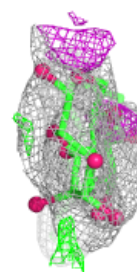
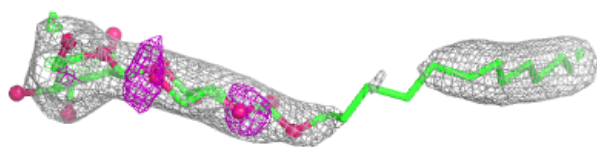
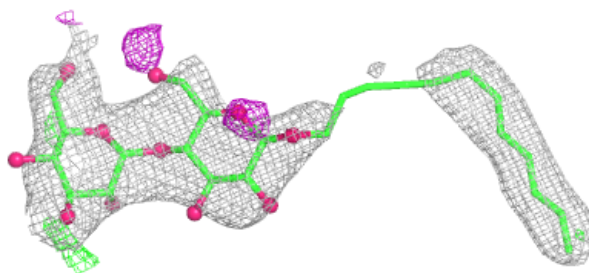
**Electron density around HTG b 603:**

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

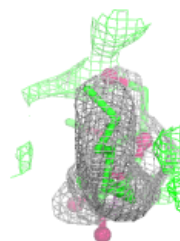
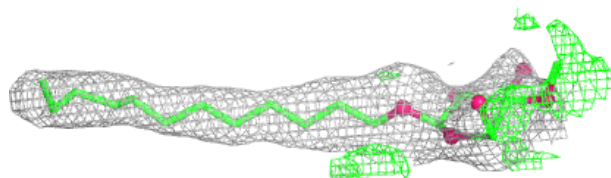
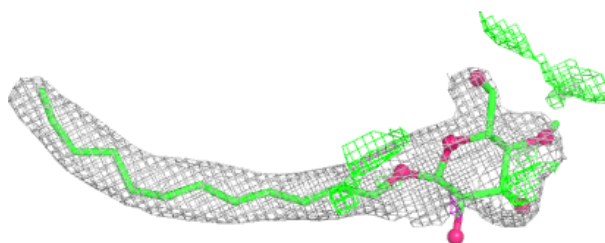


Electron density around LMT Z 101:

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

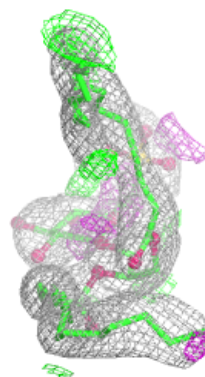
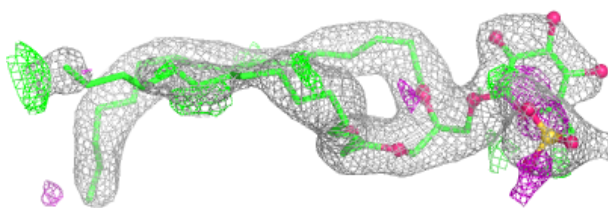
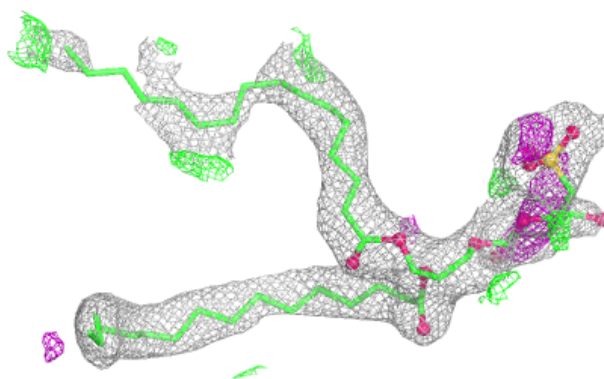
**Electron density around LMT b 625:**

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

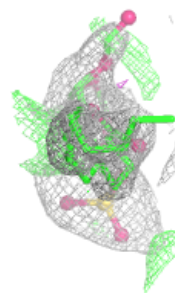
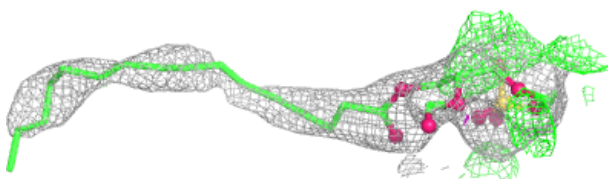
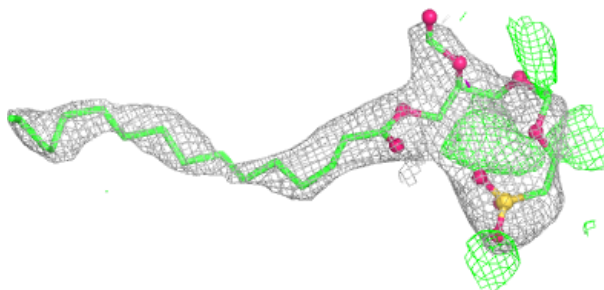


Electron density around SQD a 401:

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

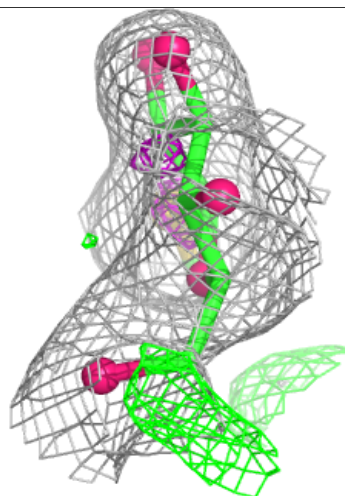
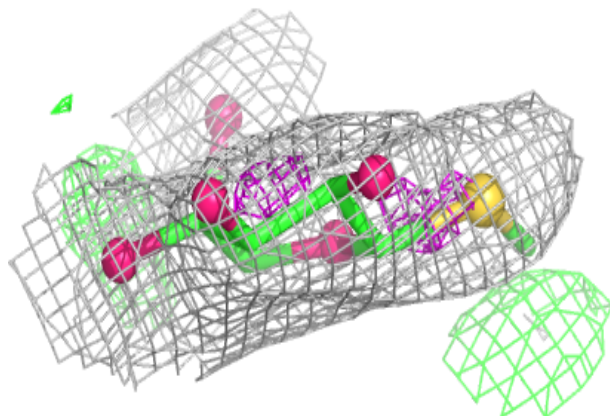
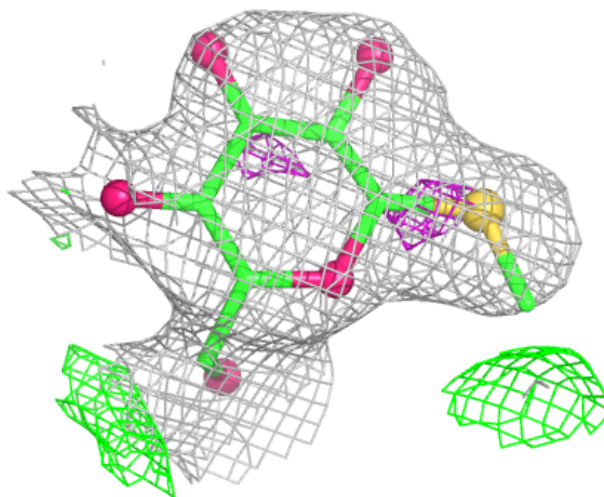
**Electron density around SQD f 102:**

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



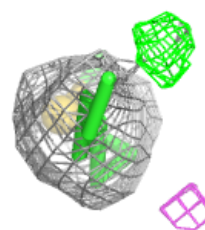
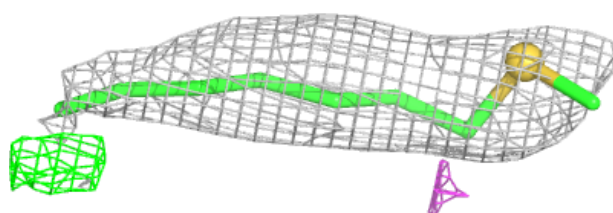
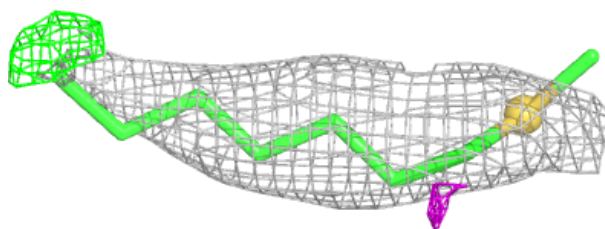
Electron density around HTG v 205:

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

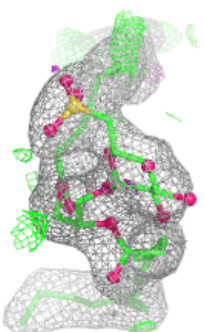
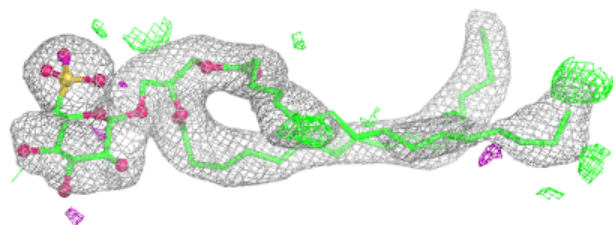
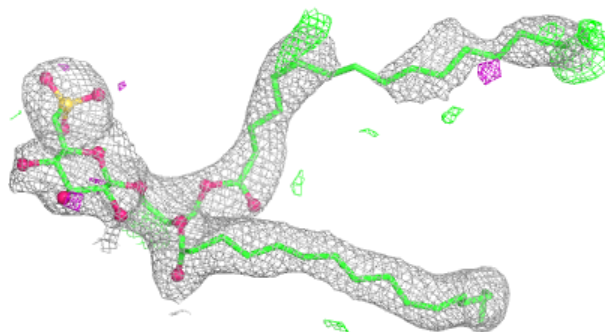


Electron density around HTG U 201:

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

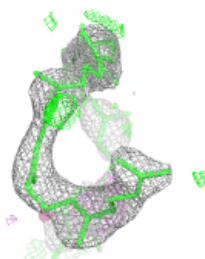
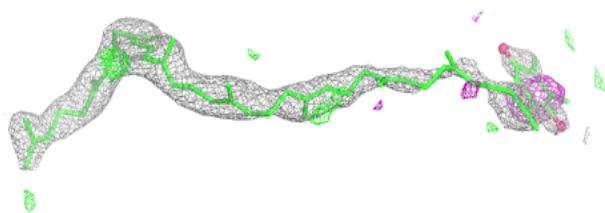
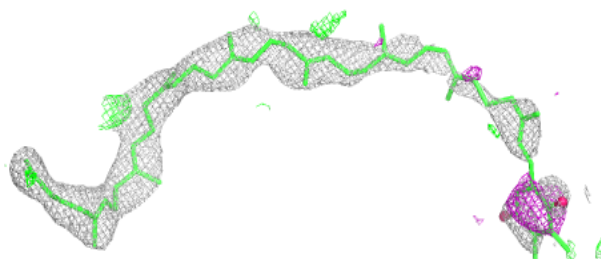
**Electron density around SQD A 417:**

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

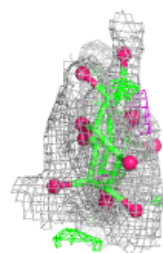
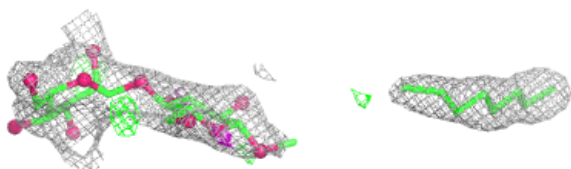
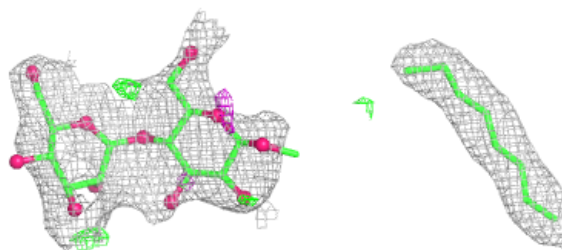


Electron density around PL9 a 417:

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

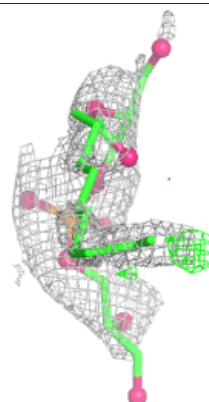
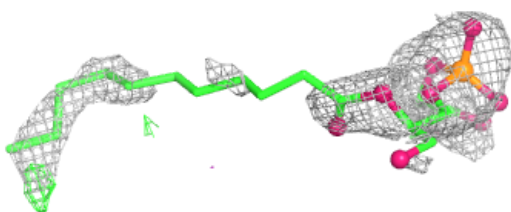
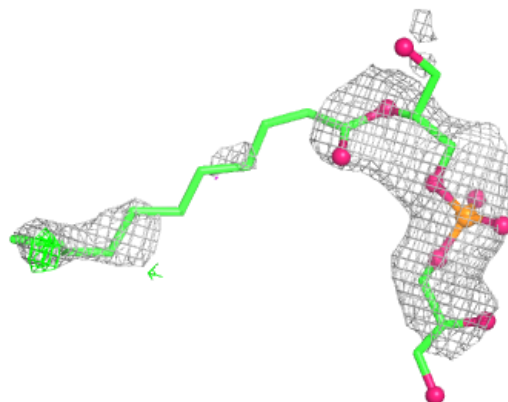
**Electron density around LMT z 101:**

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

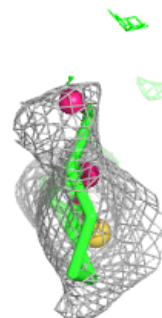
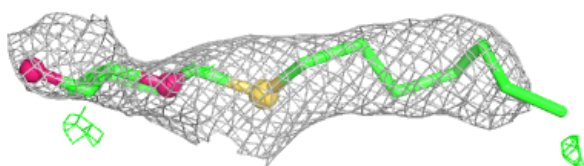
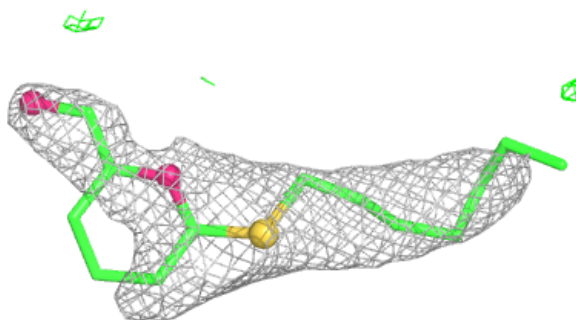


Electron density around LHG e 101:

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

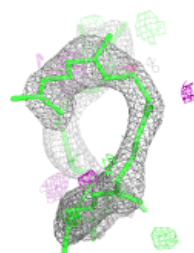
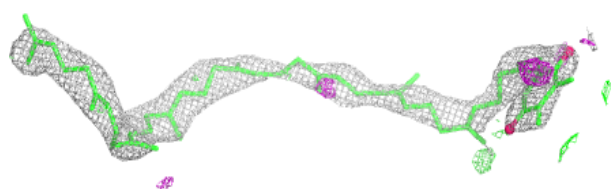
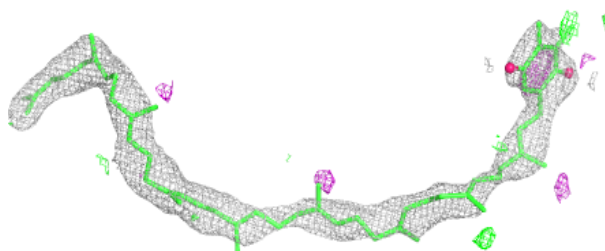
**Electron density around HTG H 105:**

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

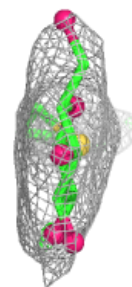
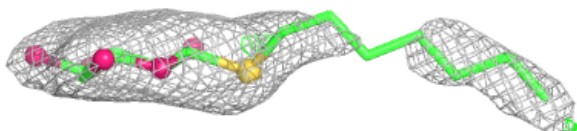
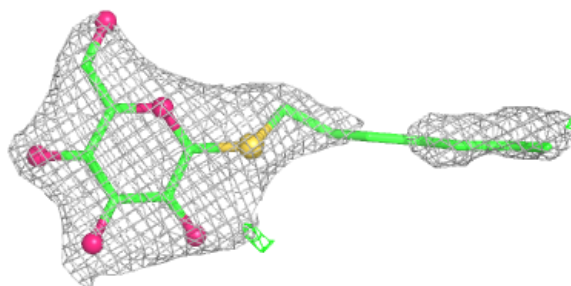


Electron density around PL9 A 414:

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

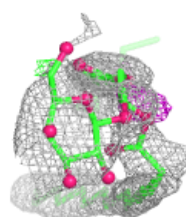
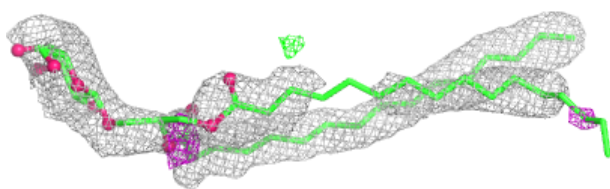
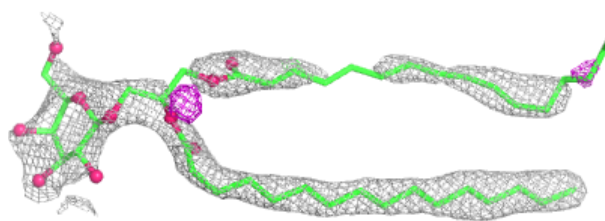
**Electron density around HTG c 923:**

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

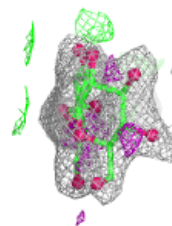
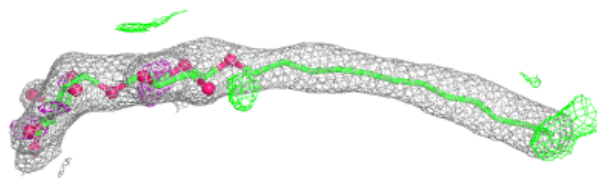
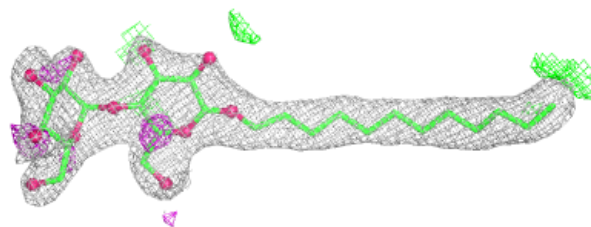


Electron density around LMG c 921:

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

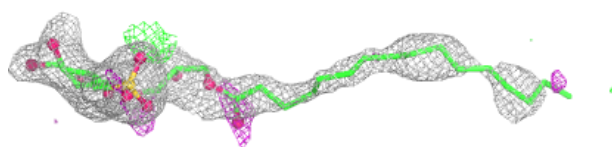
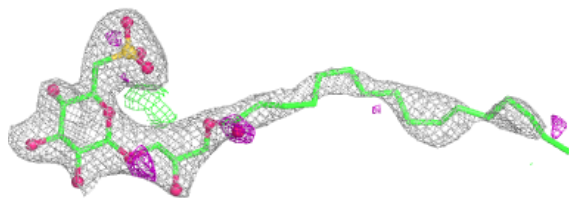
**Electron density around LMT M 303:**

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

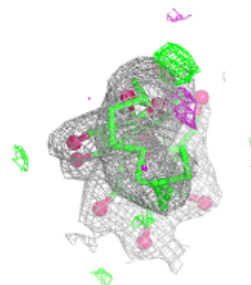
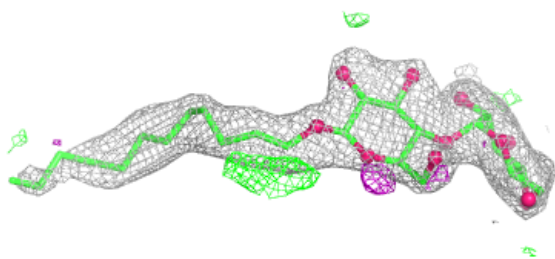
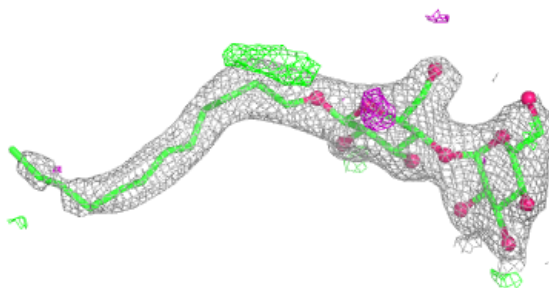


Electron density around SQD F 101:

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

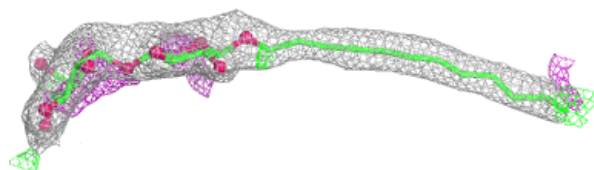
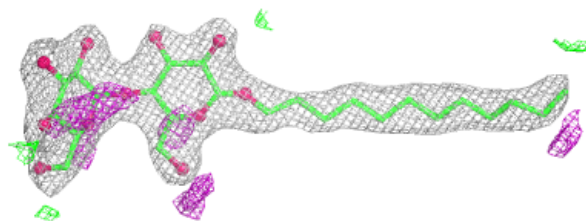
**Electron density around LMT a 402:**

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

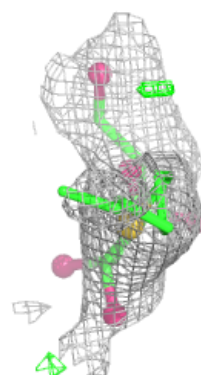
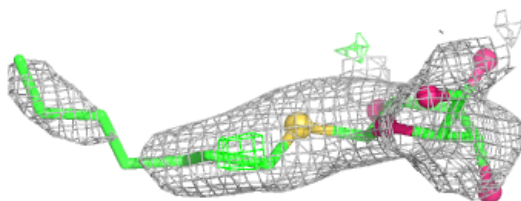


Electron density around LMT m 1502:

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

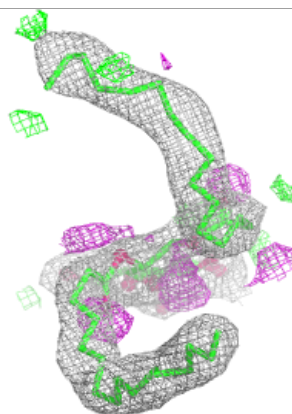
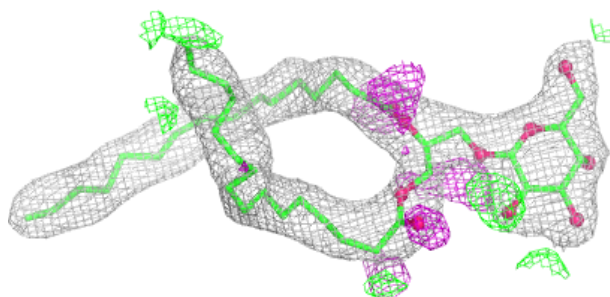
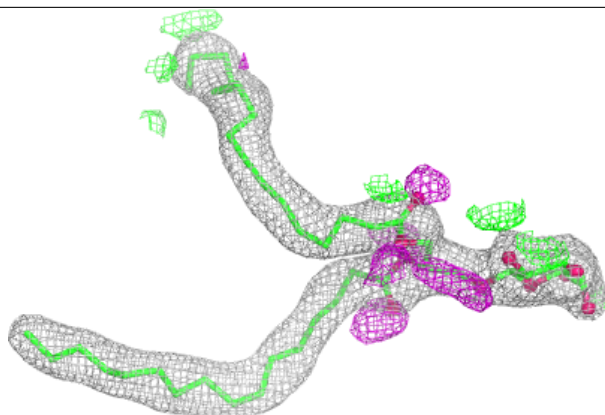
**Electron density around HTG C 528:**

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

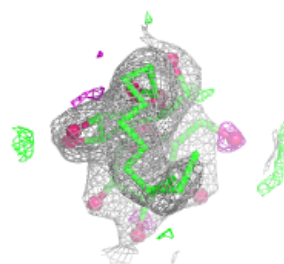
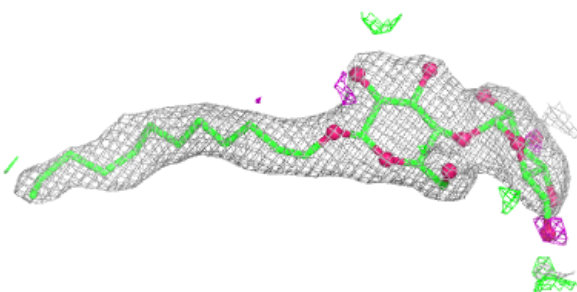
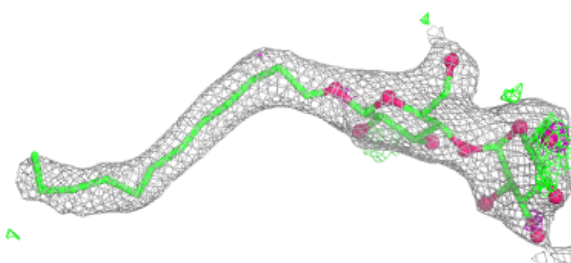


Electron density around LMG b 624:

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

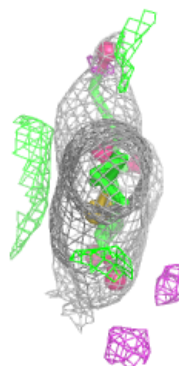
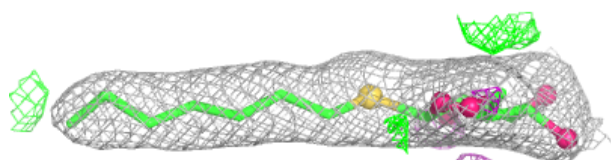
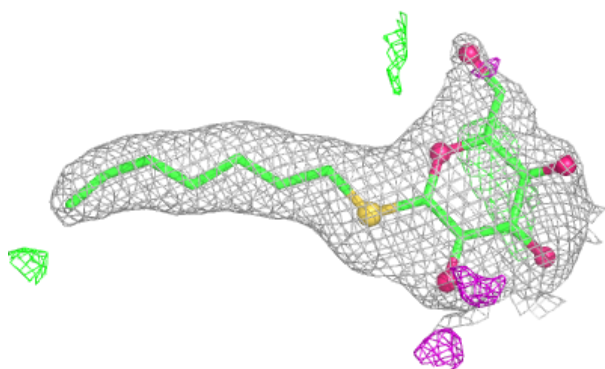
**Electron density around LMT D 401:**

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

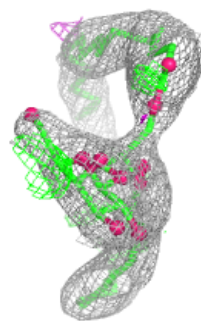
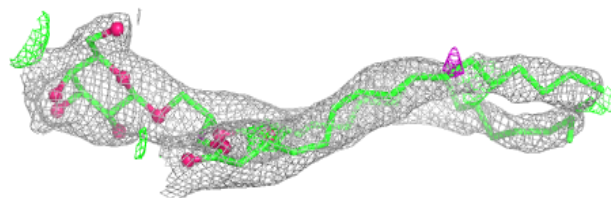
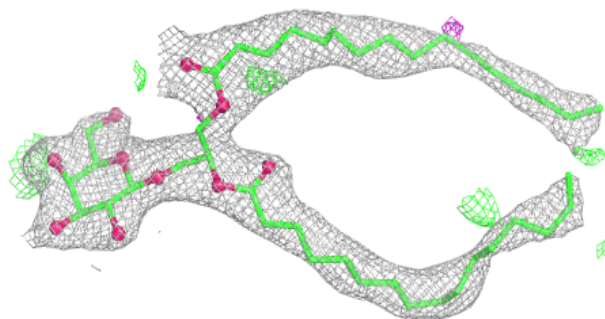


Electron density around HTG b 602:

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

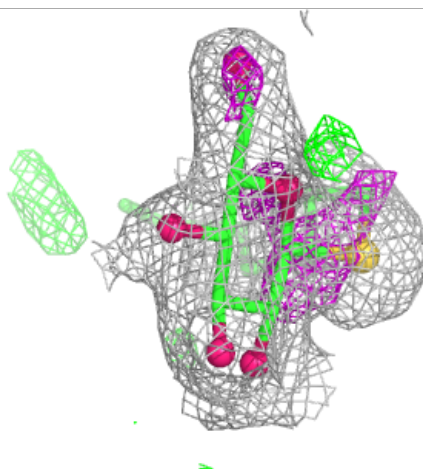
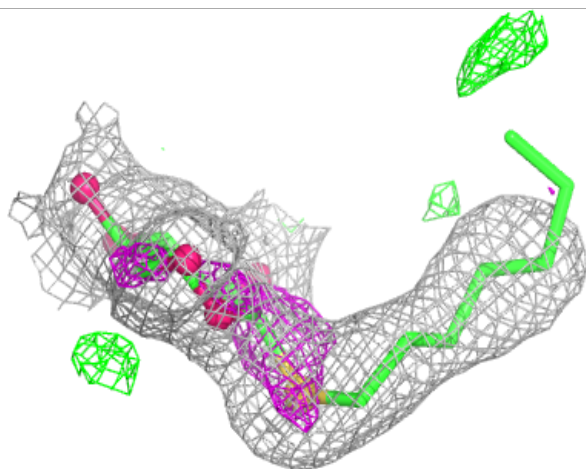
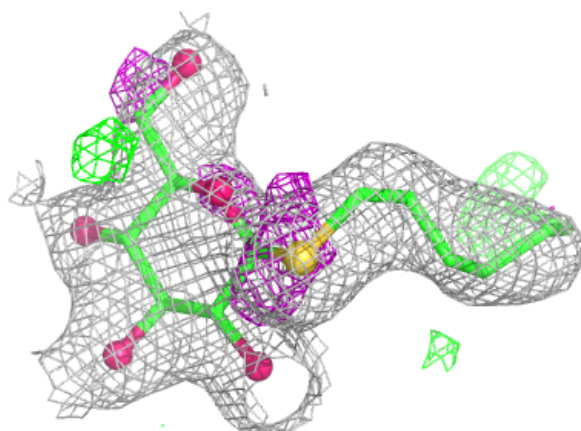
**Electron density around LMG a 416:**

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



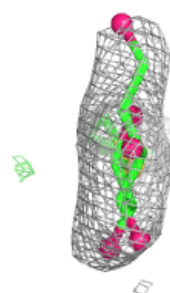
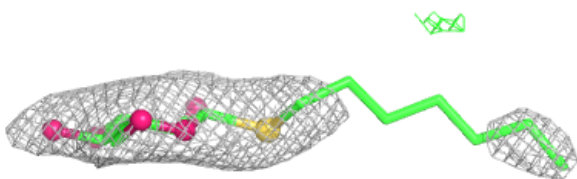
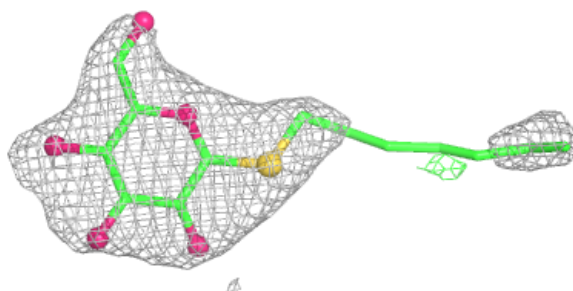
Electron density around HTG b 626:

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



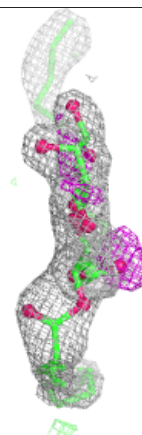
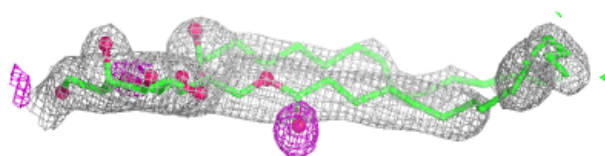
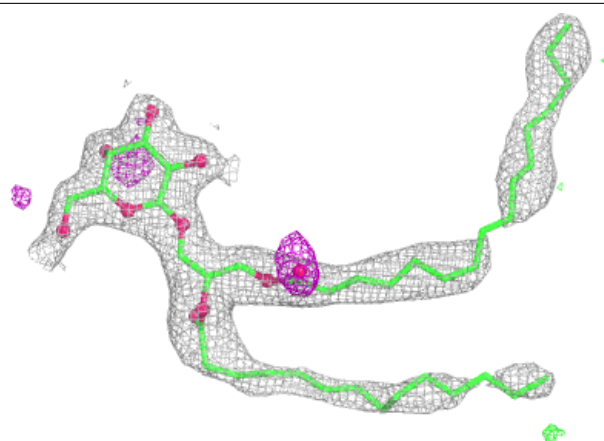
Electron density around HTG C 521:

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

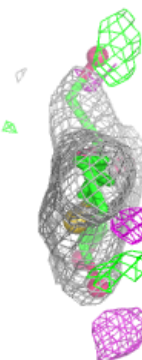
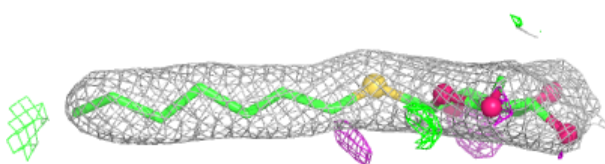
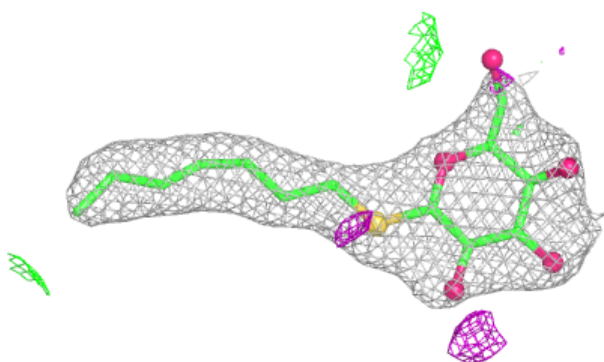


Electron density around LMG C 519:

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

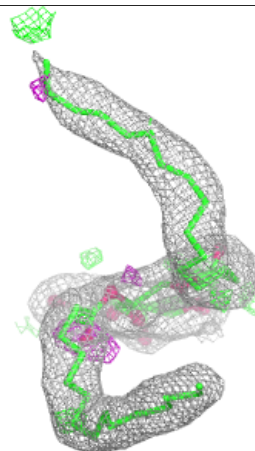
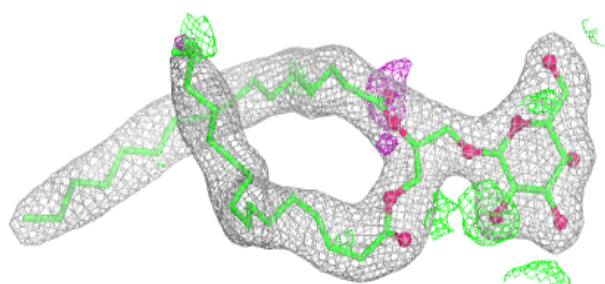
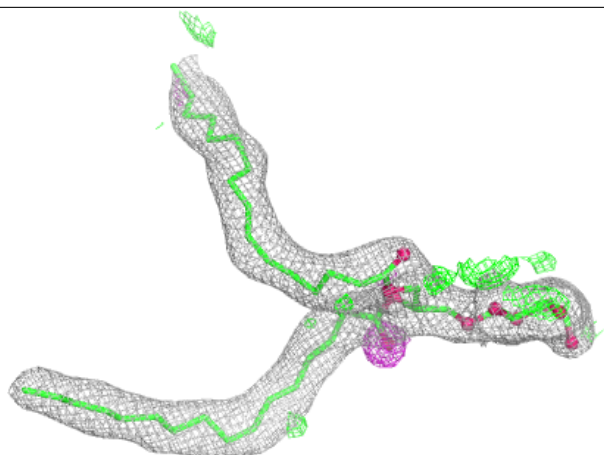
**Electron density around HTG B 626:**

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



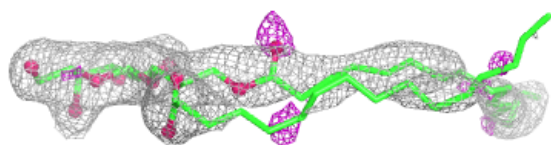
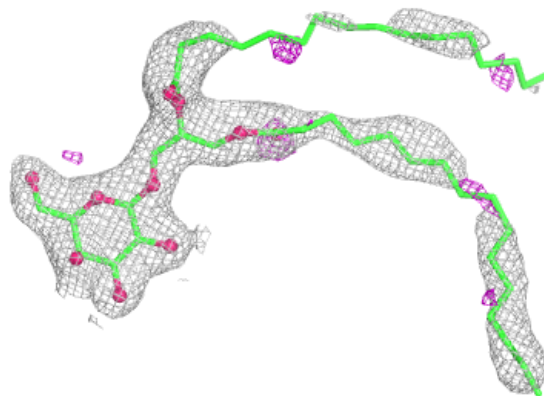
Electron density around LMG B 622:

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

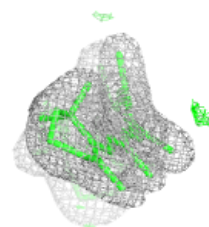
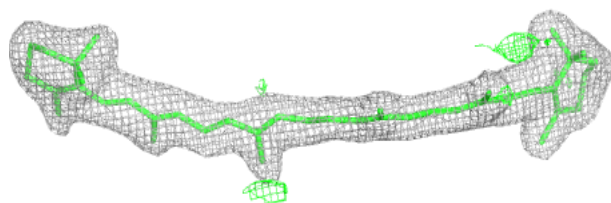
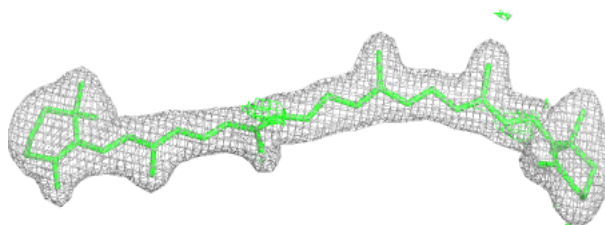


Electron density around LMG c 920:

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

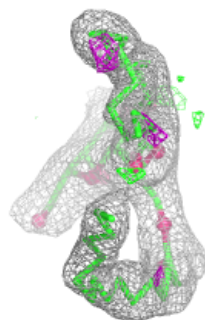
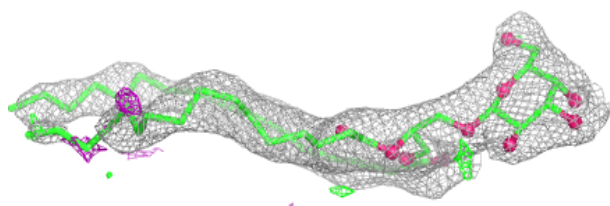
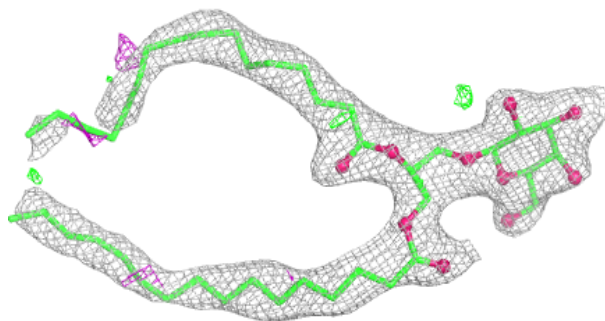
**Electron density around BCR t 903:**

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



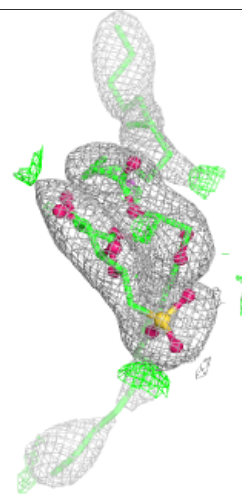
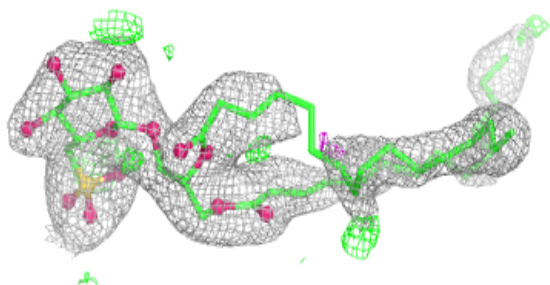
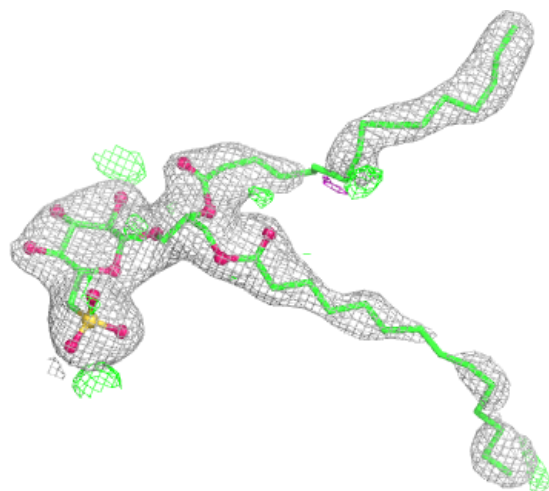
Electron density around LMG A 413:

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



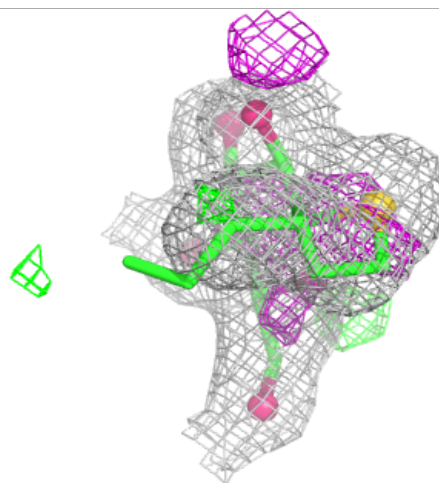
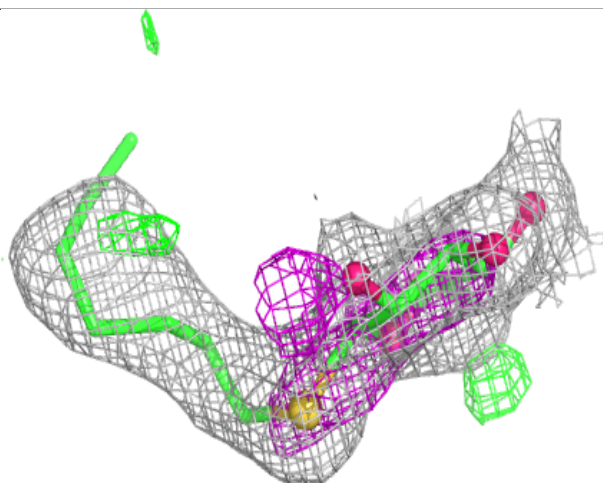
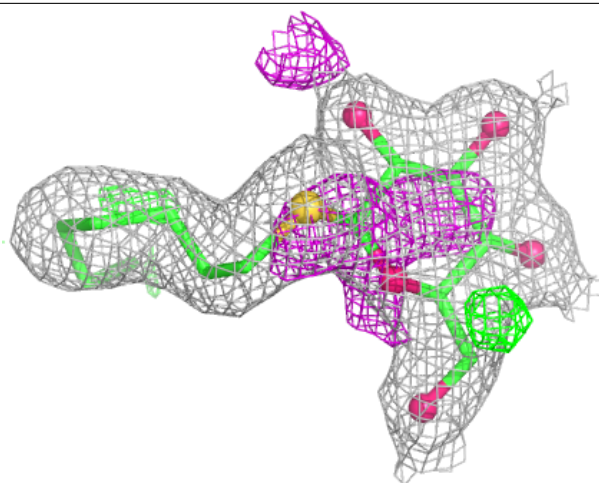
Electron density around SQD A 412:

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



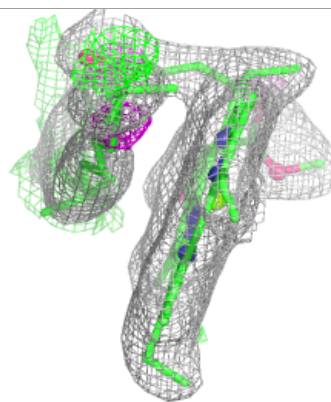
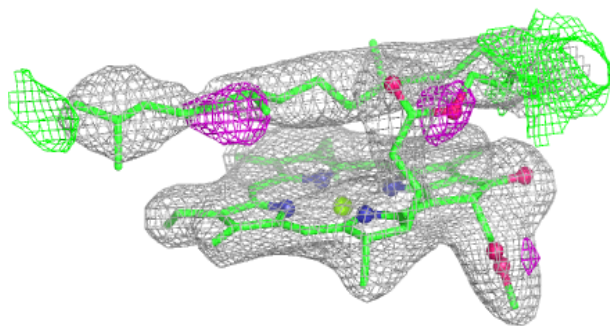
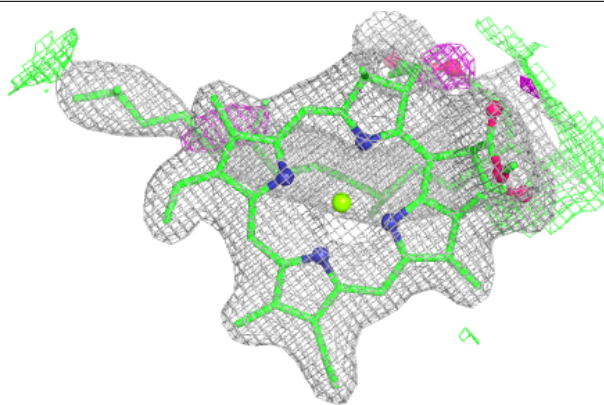
Electron density around HTG B 624:

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

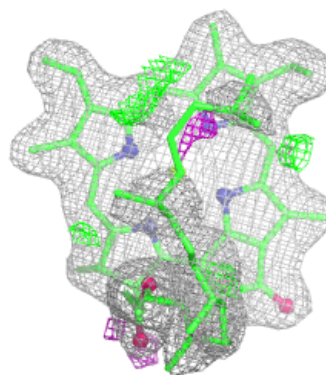
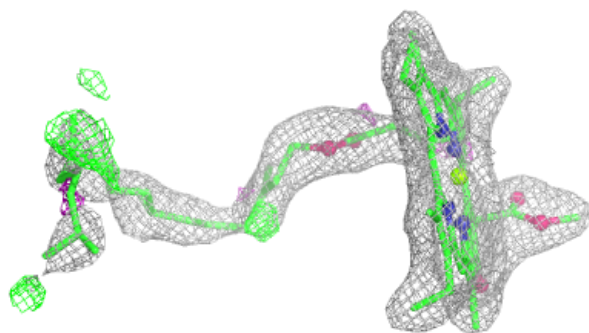
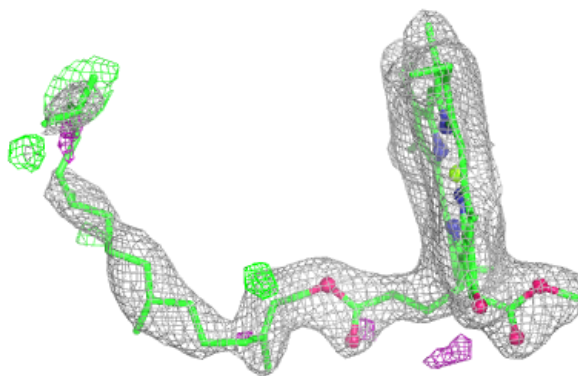


Electron density around CLA B 602:

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

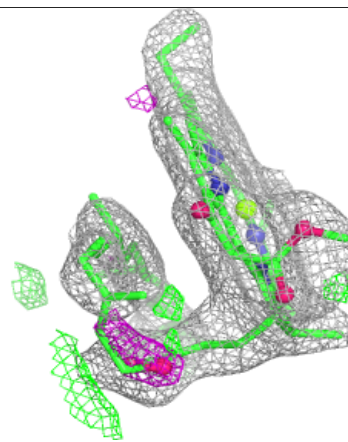
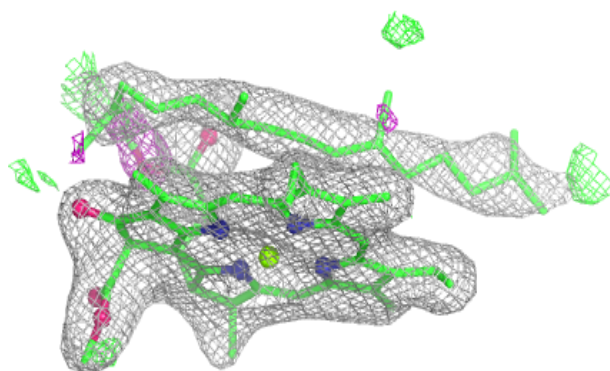
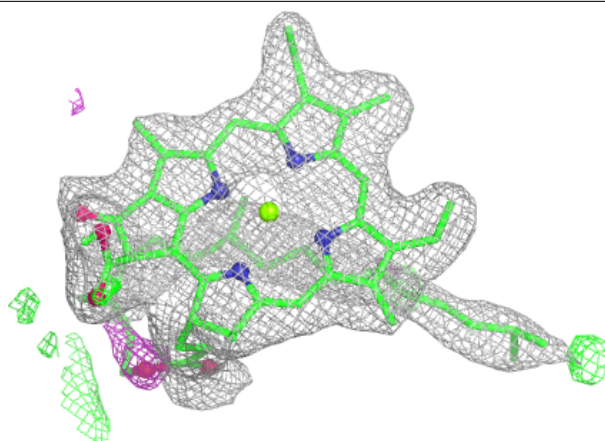
**Electron density around CLA C 506:**

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

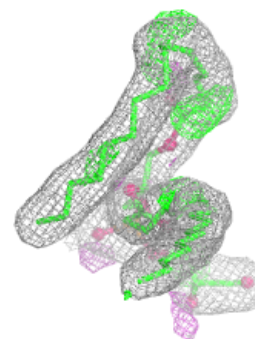
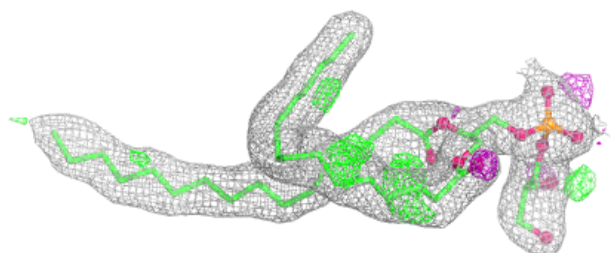
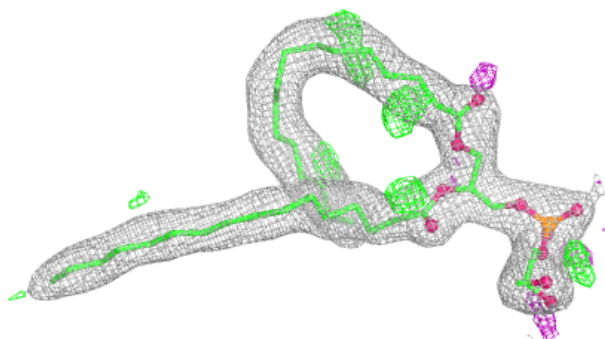


Electron density around CLA b 605:

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

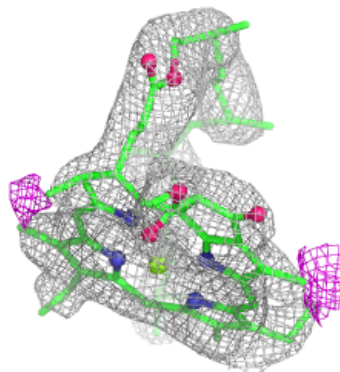
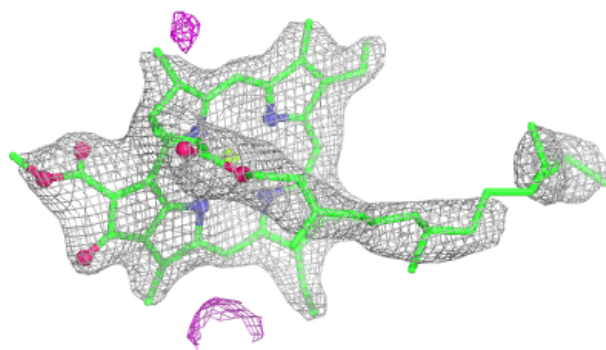
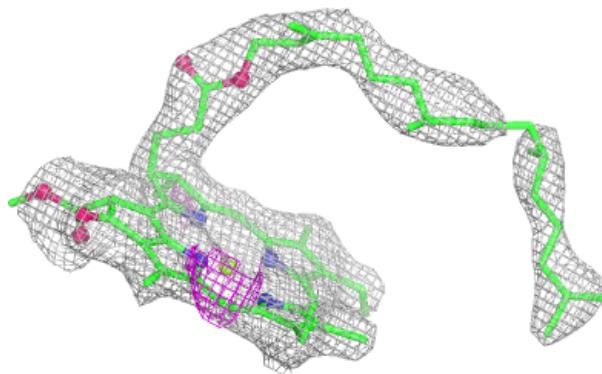
**Electron density around LHG D 407:**

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

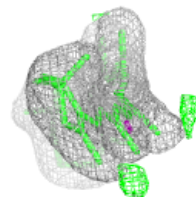
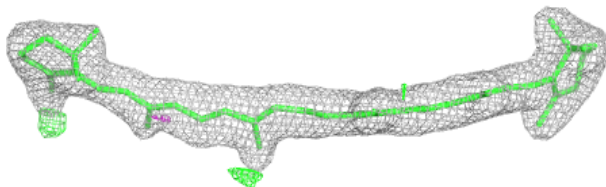
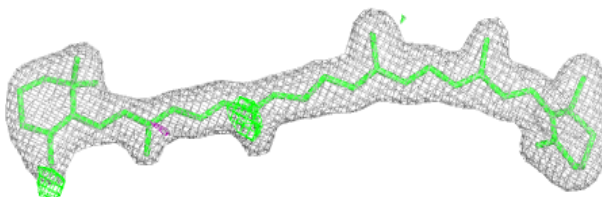


Electron density around CLA c 914:

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

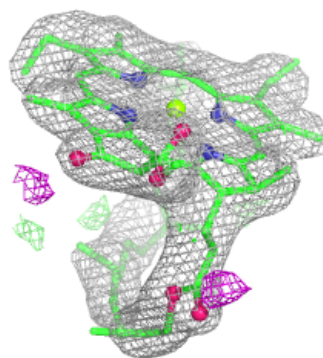
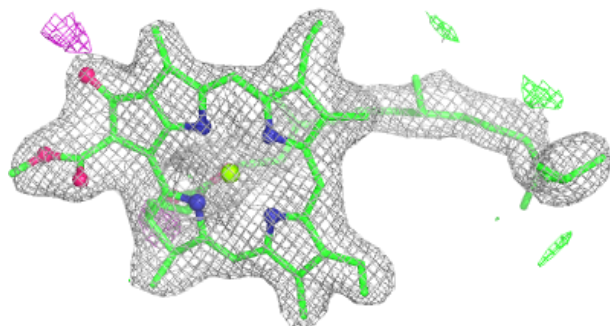
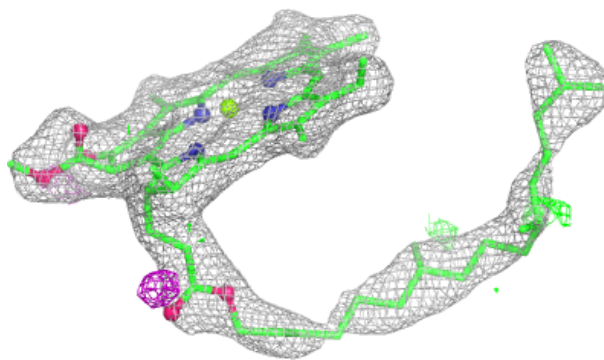
**Electron density around BCR T 702:**

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



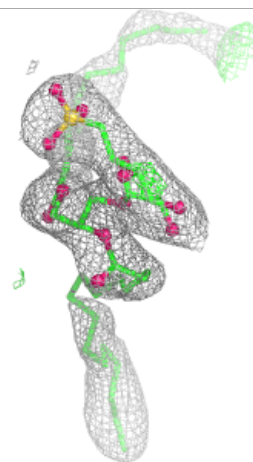
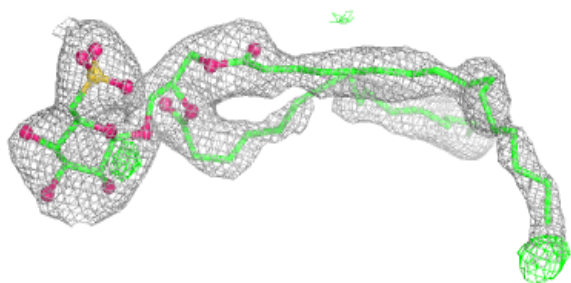
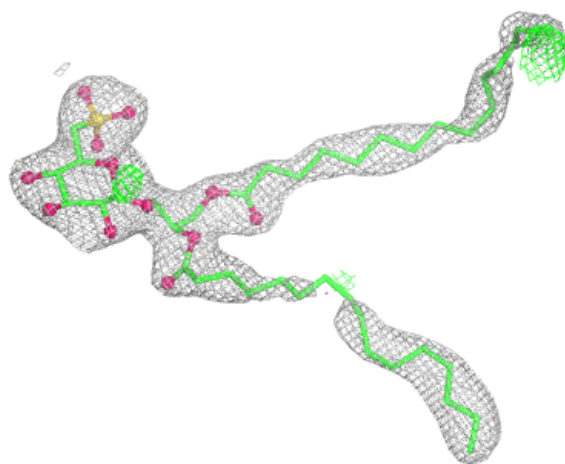
Electron density around CLA C 513:

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



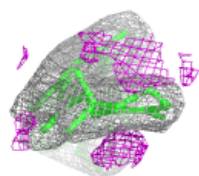
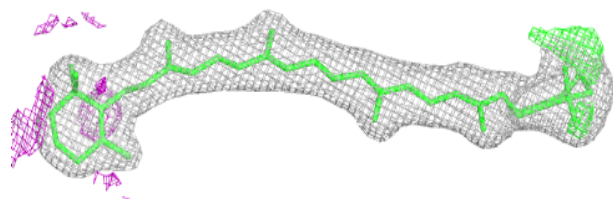
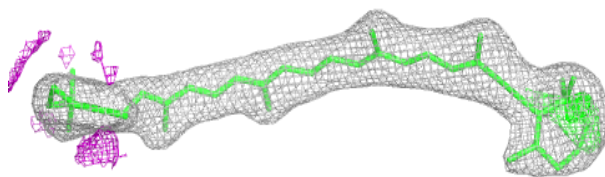
Electron density around SQD a 415:

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



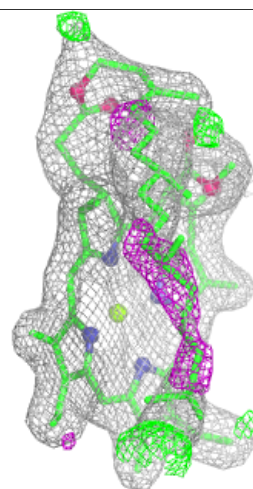
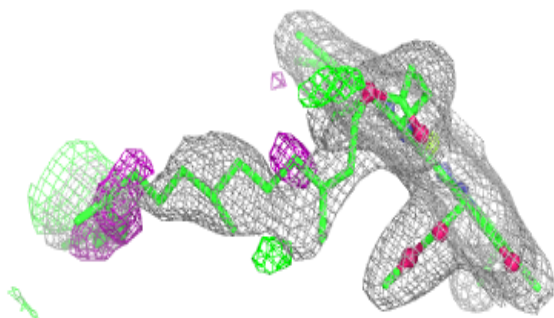
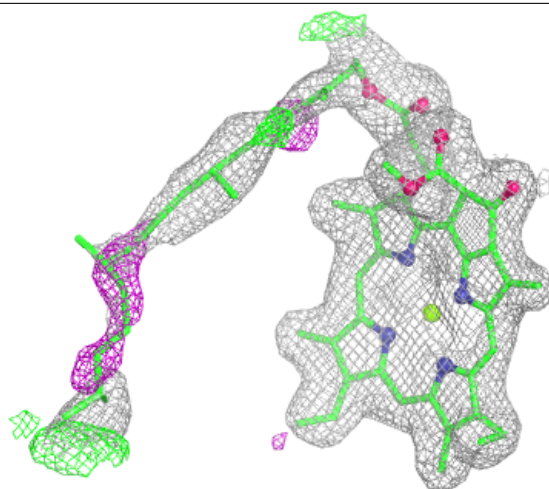
Electron density around BCR d 406:

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



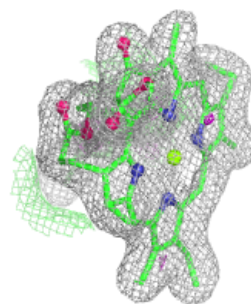
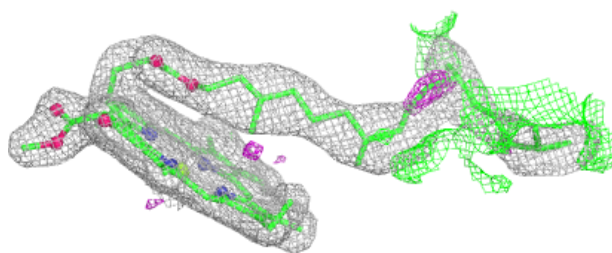
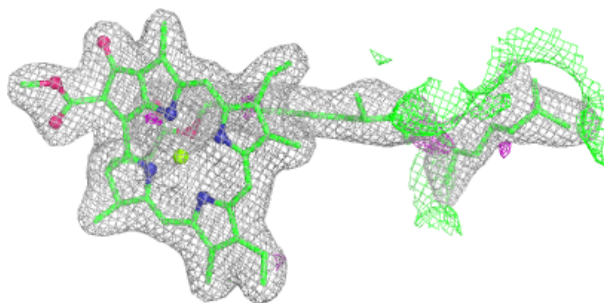
Electron density around CLA B 617:

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



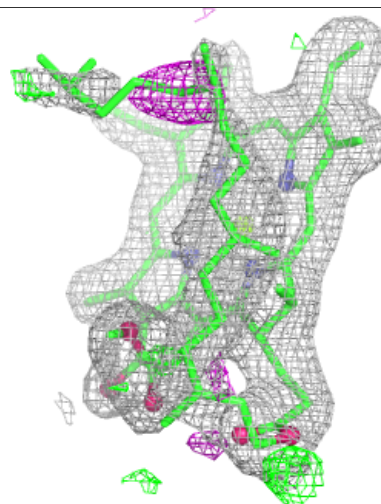
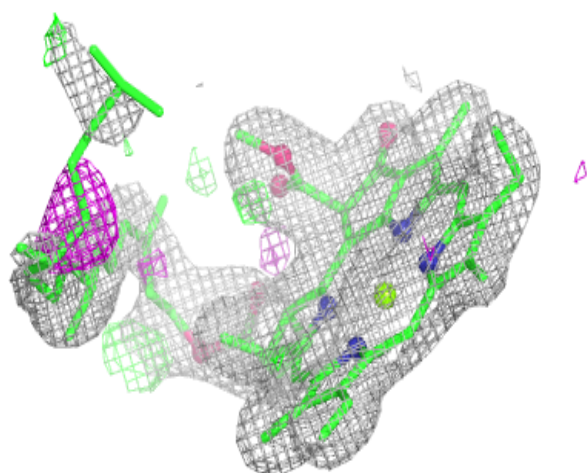
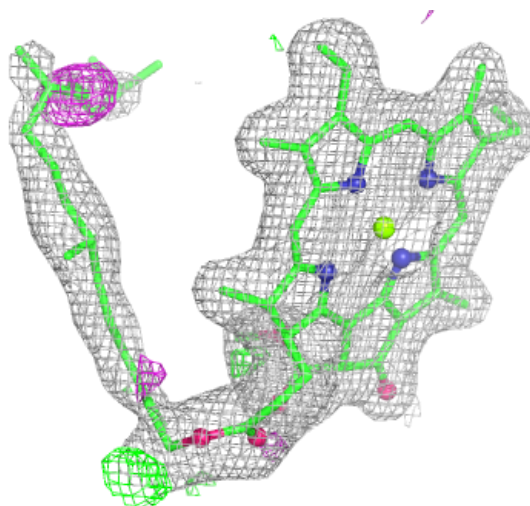
Electron density around CLA b 618:

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



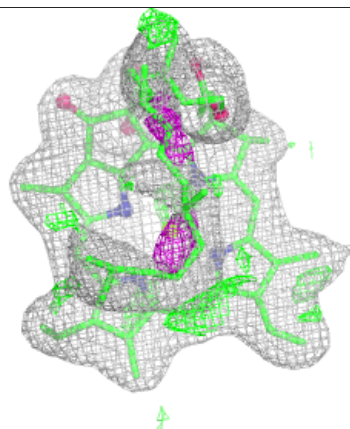
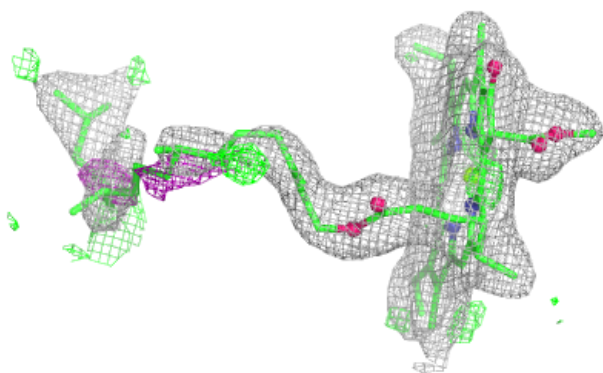
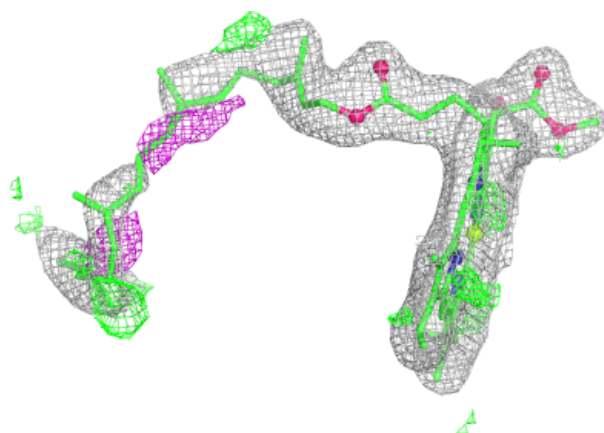
Electron density around CLA b 620:

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

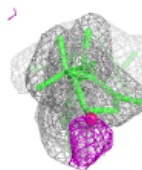
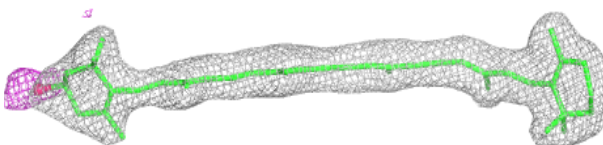
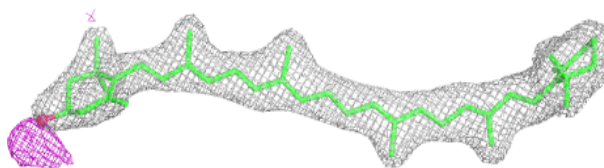


Electron density around CLA c 907:

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

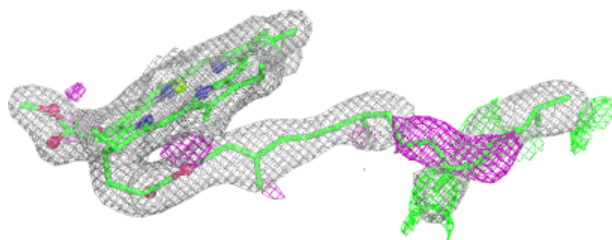
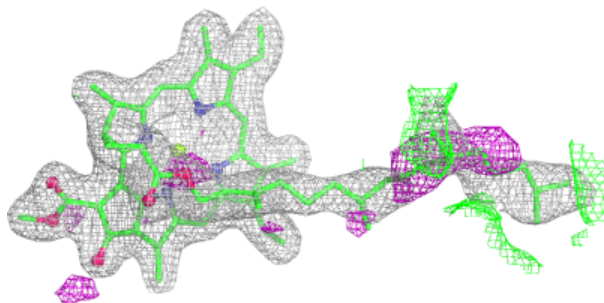
**Electron density around RRX h 101:**

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



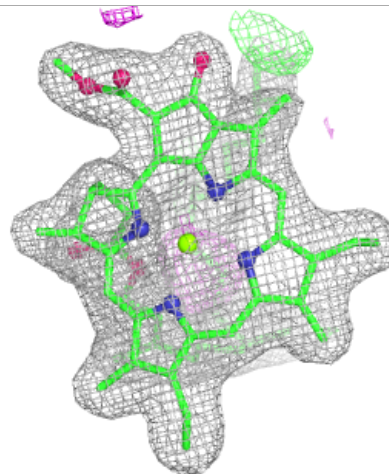
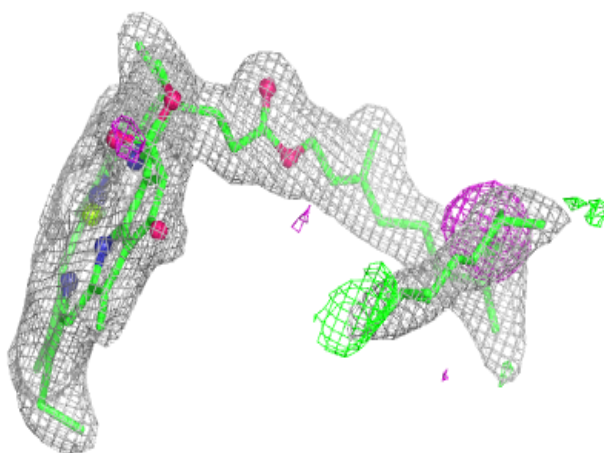
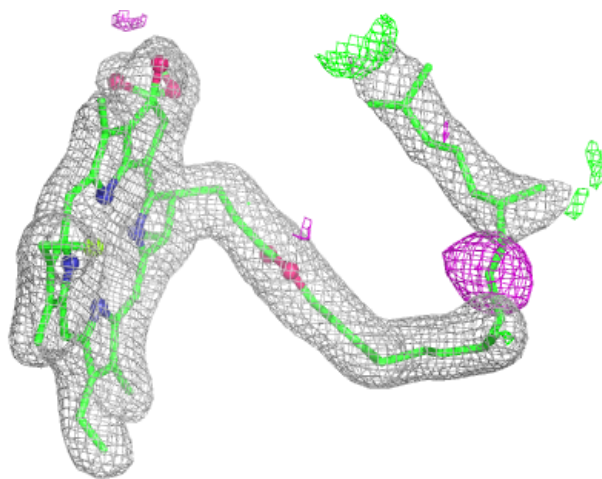
Electron density around CLA B 615:

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



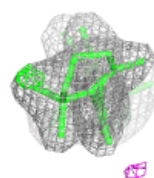
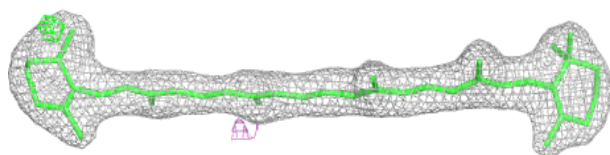
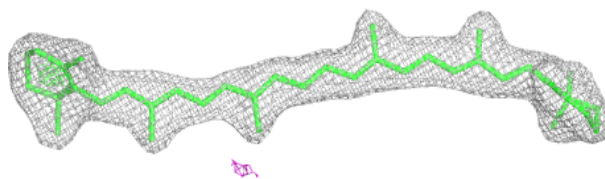
Electron density around CLA b 610:

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

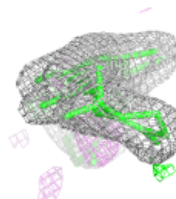
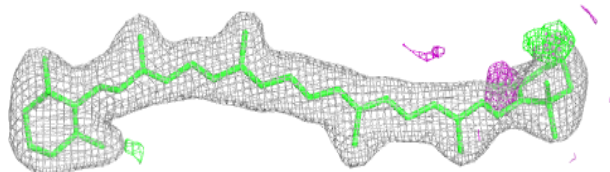
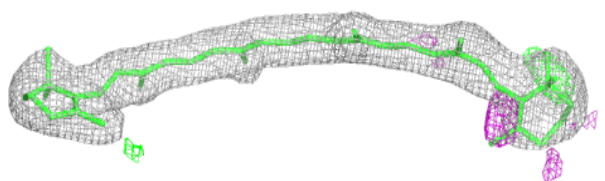


Electron density around BCR C 514:

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

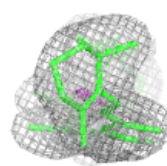
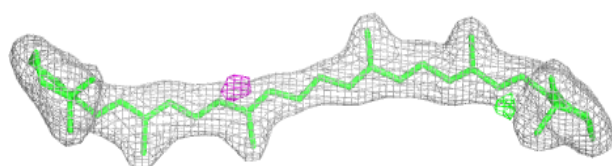
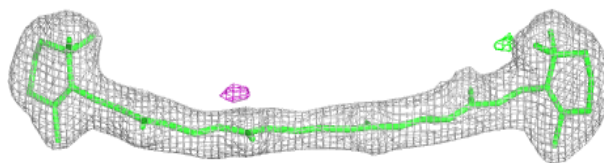
**Electron density around BCR D 404:**

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

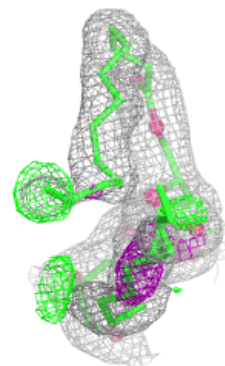
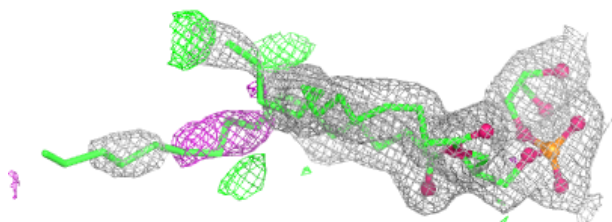
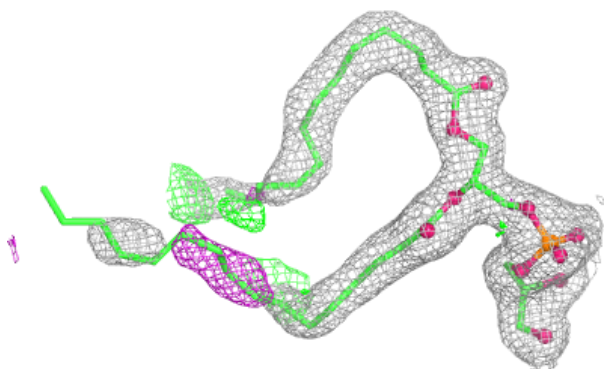


Electron density around BCR K 101:

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

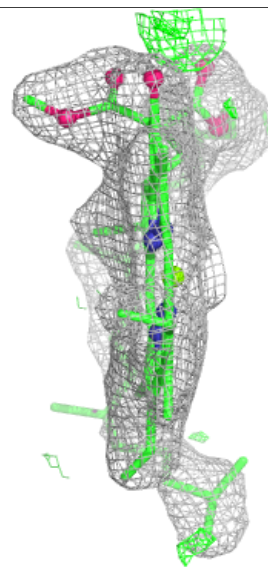
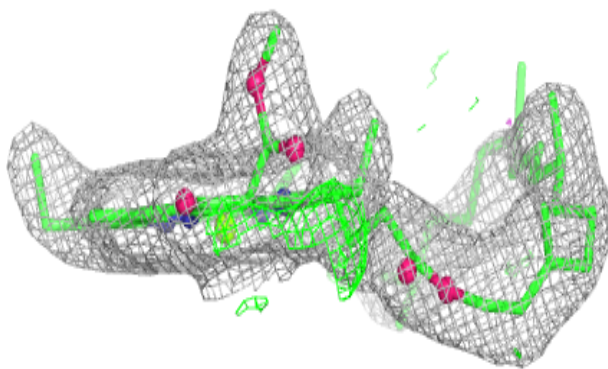
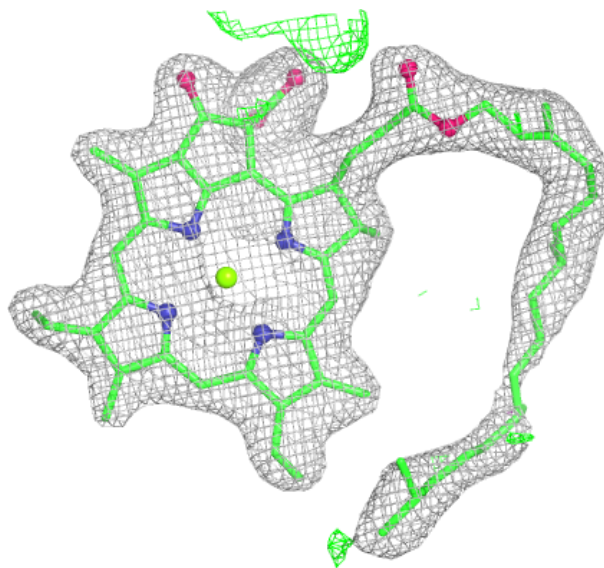
**Electron density around LHG D 409:**

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



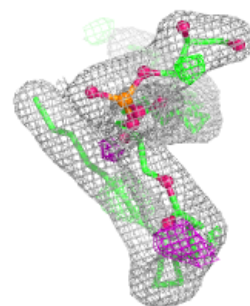
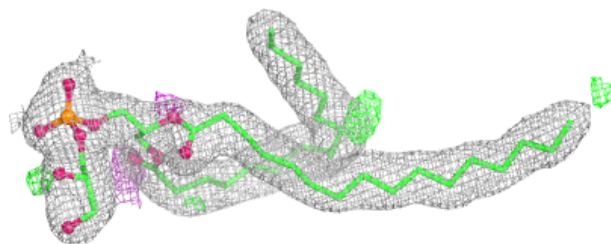
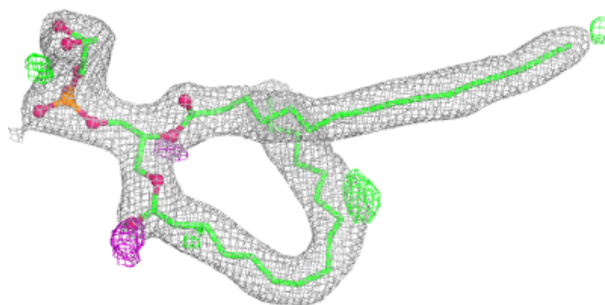
Electron density around CLA C 512:

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

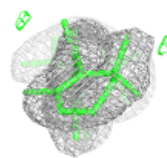
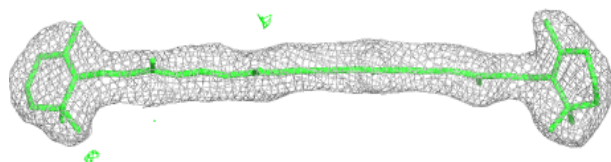
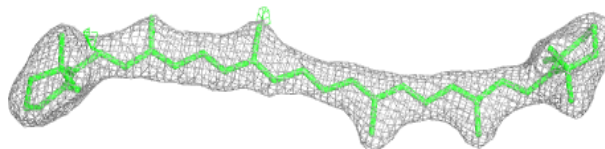


Electron density around LHG d 408:

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

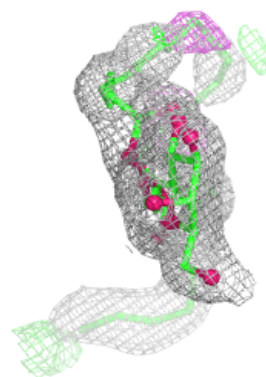
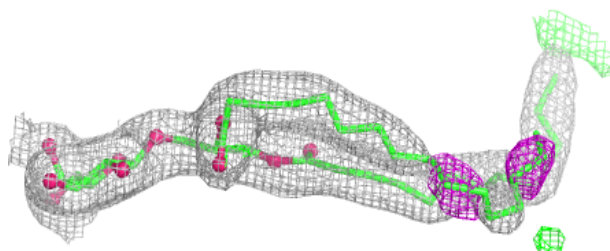
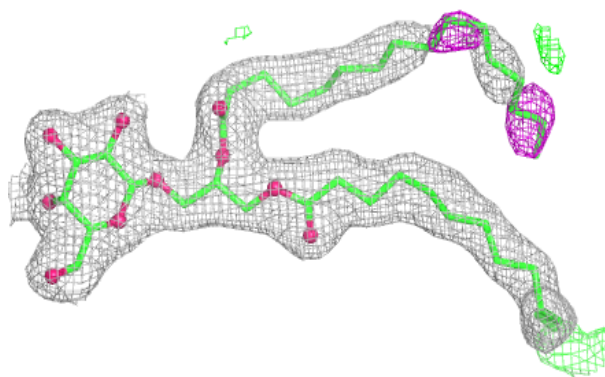
**Electron density around BCR c 915:**

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



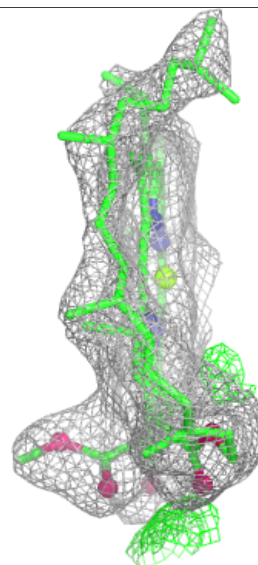
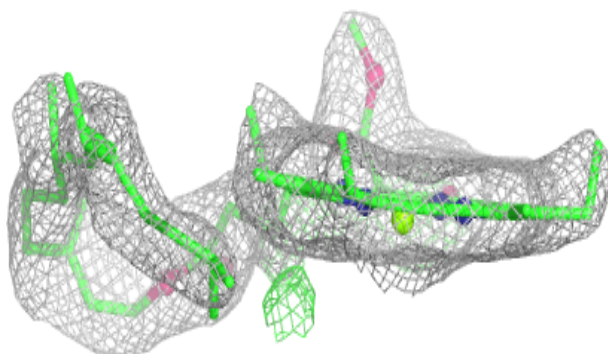
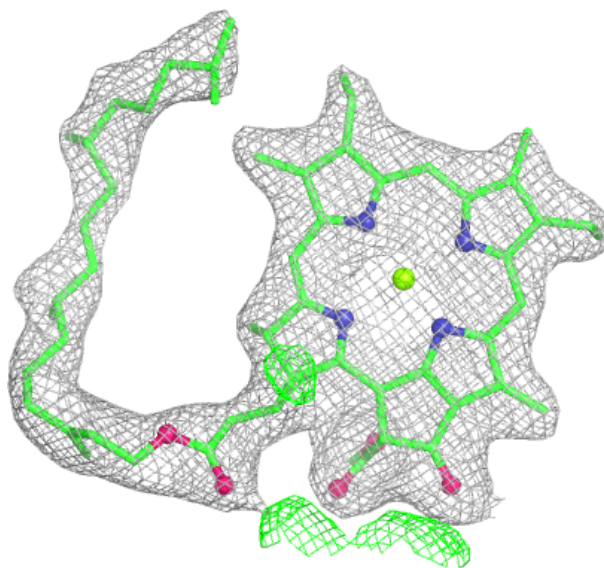
Electron density around LMG D 410:

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



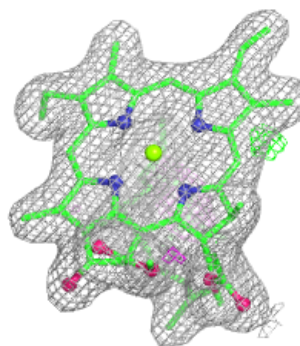
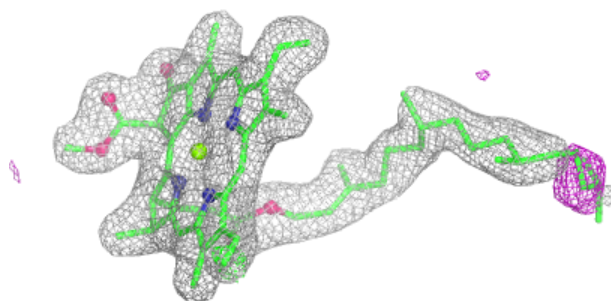
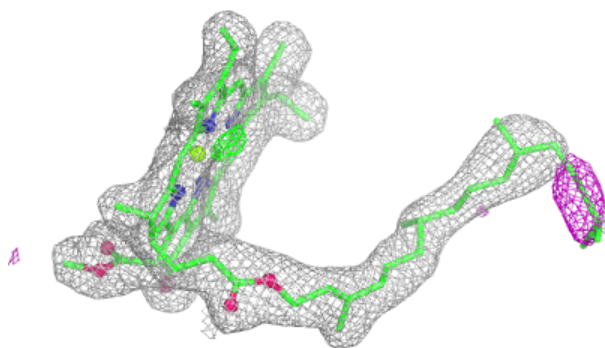
Electron density around CLA c 913:

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

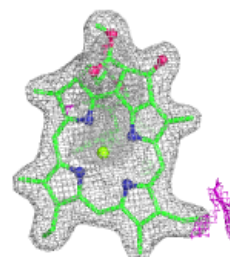
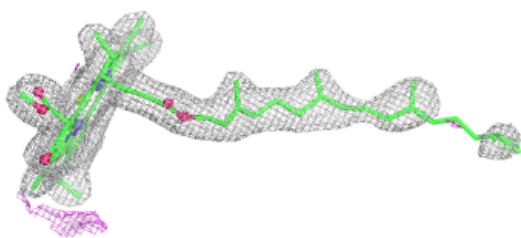
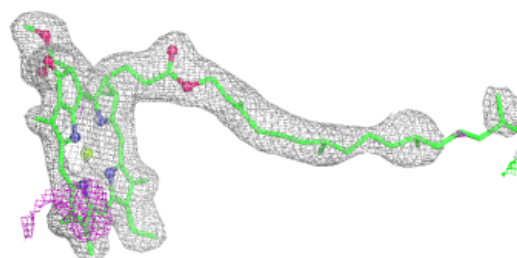


Electron density around CLA C 508:

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

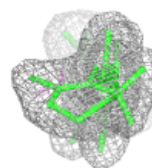
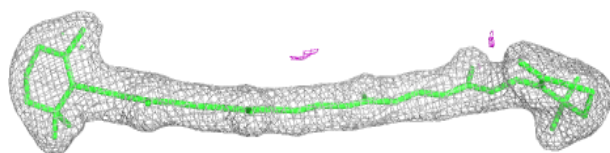
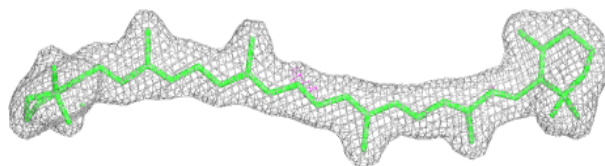
**Electron density around CLA d 405:**

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

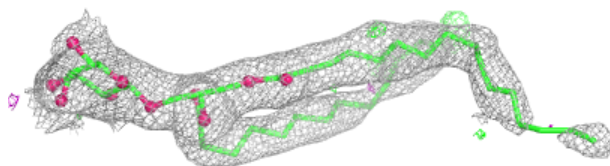
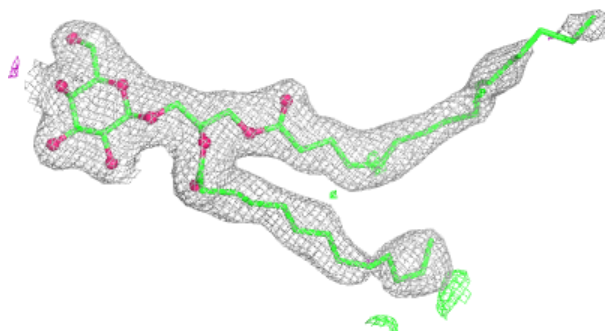


Electron density around BCR B 618:

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

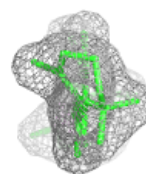
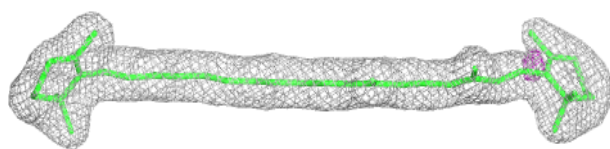
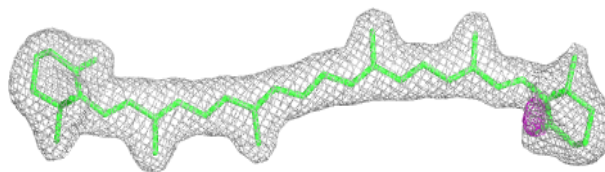
**Electron density around LMG d 411:**

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



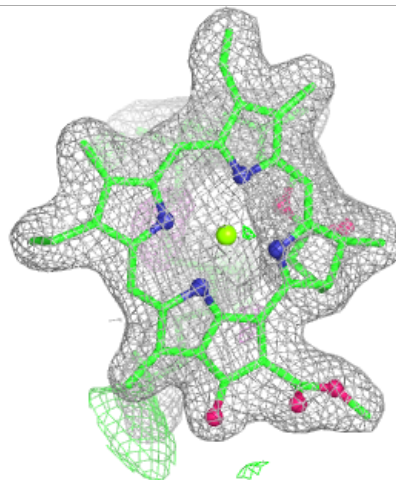
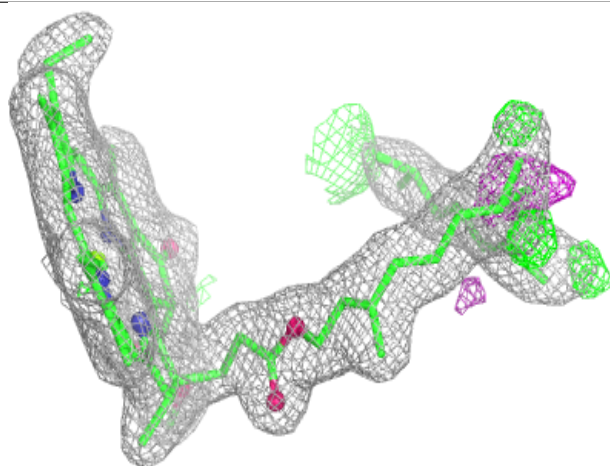
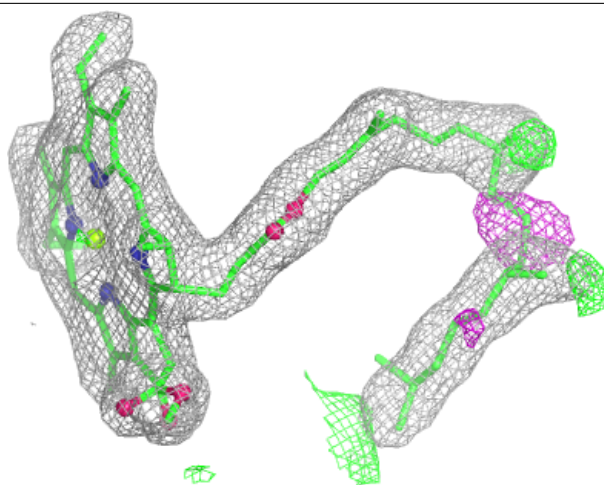
Electron density around BCR B 619:

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



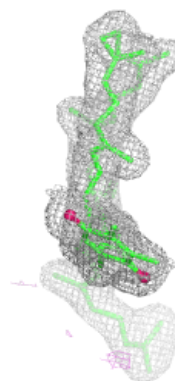
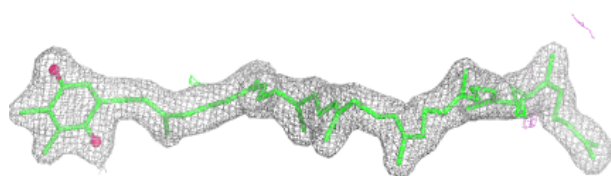
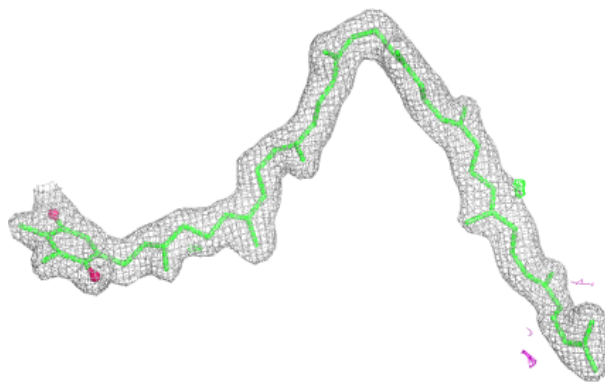
Electron density around CLA B 607:

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

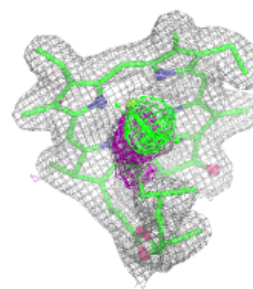
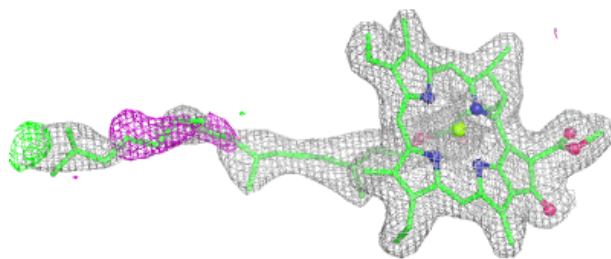
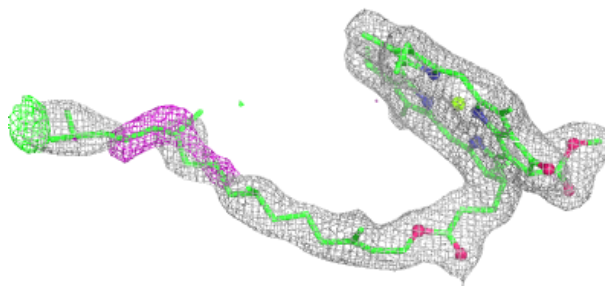


Electron density around PL9 d 407:

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

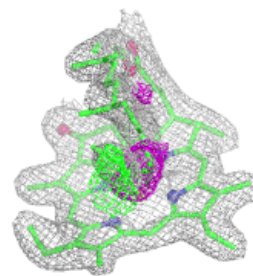
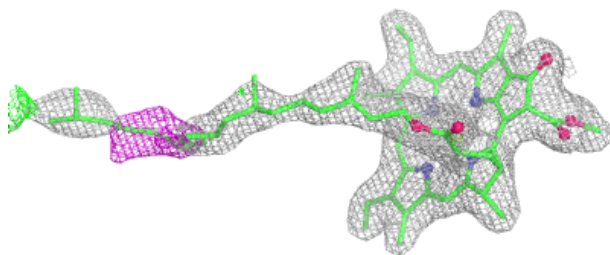
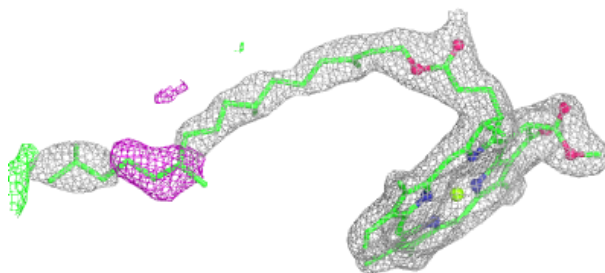
**Electron density around CLA C 504:**

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

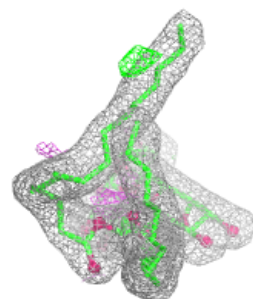
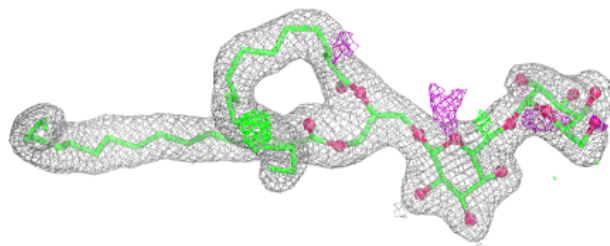
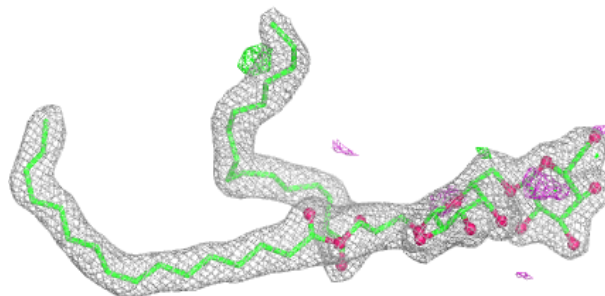


Electron density around CLA c 905:

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

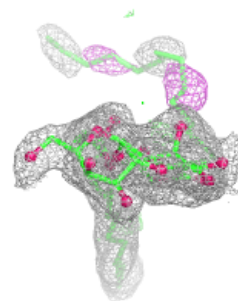
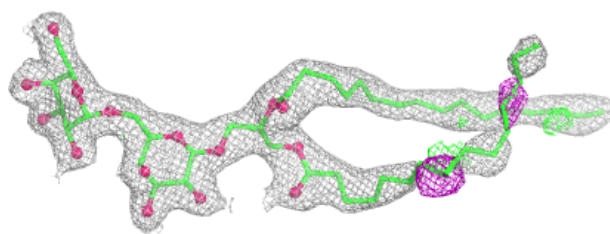
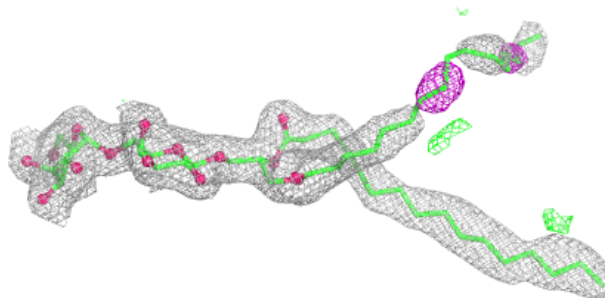
**Electron density around DGD H 103:**

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

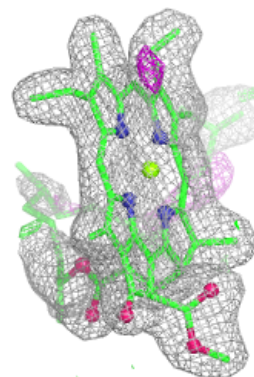
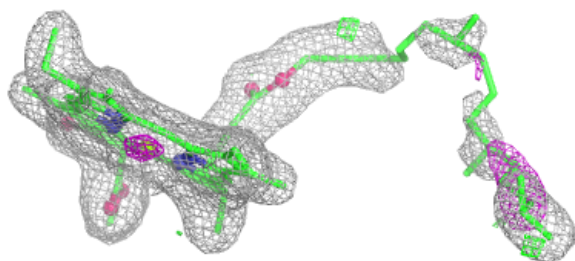
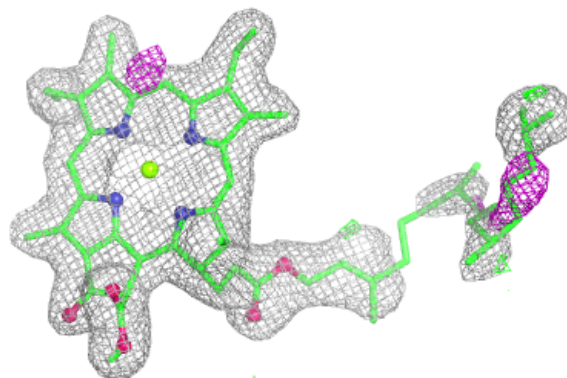


Electron density around DGD c 917:

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

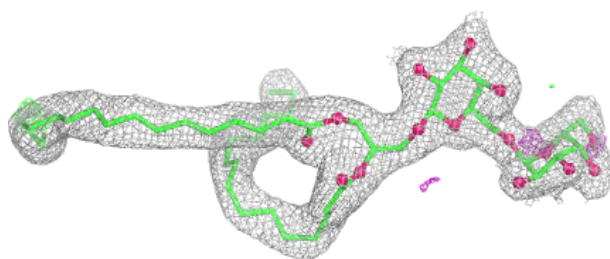
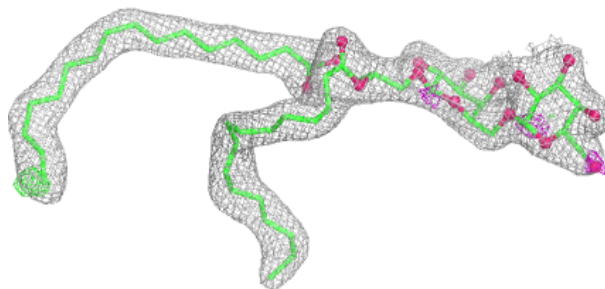
**Electron density around CLA a 413:**

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

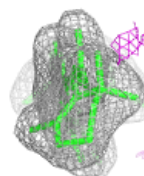
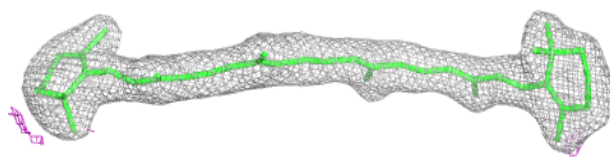
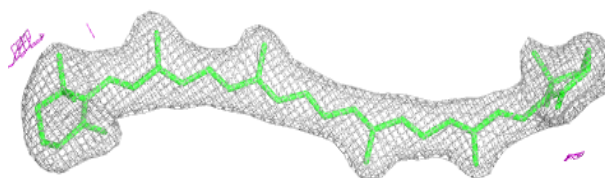


Electron density around DGD h 102:

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

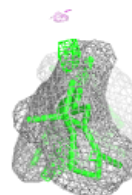
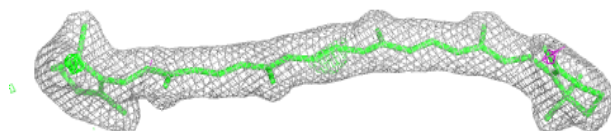
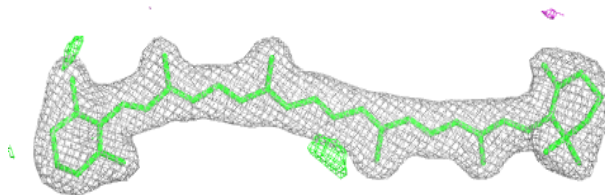
**Electron density around BCR Y 101:**

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



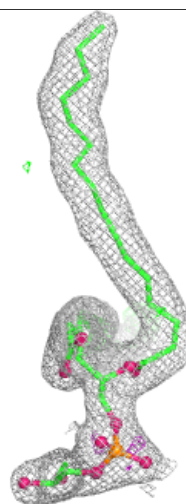
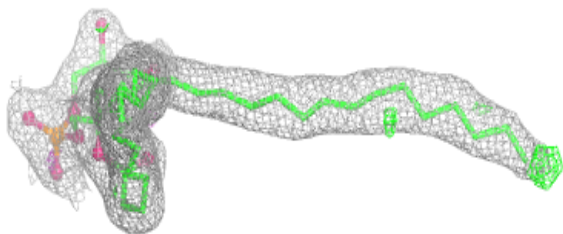
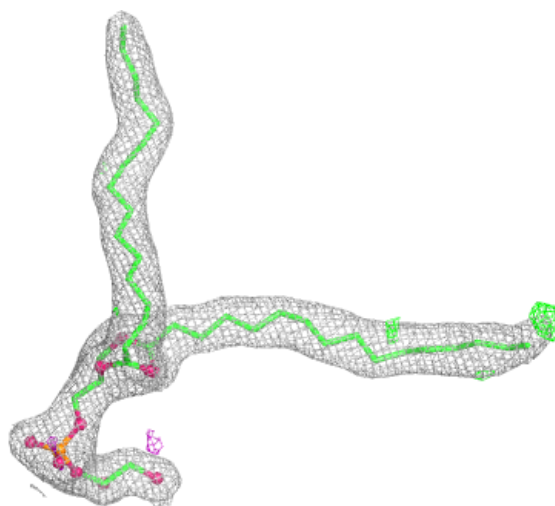
Electron density around BCR b 623:

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



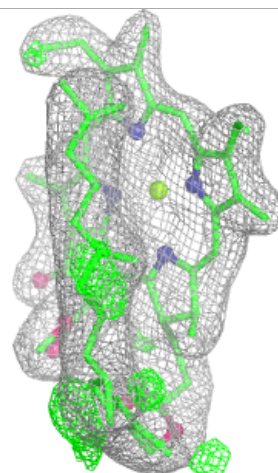
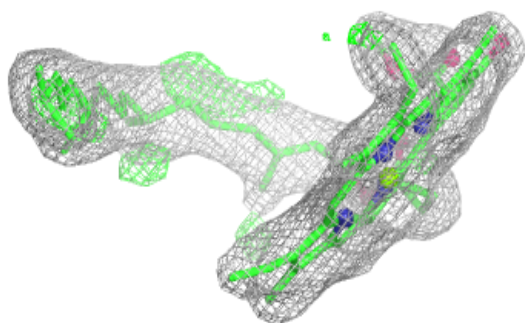
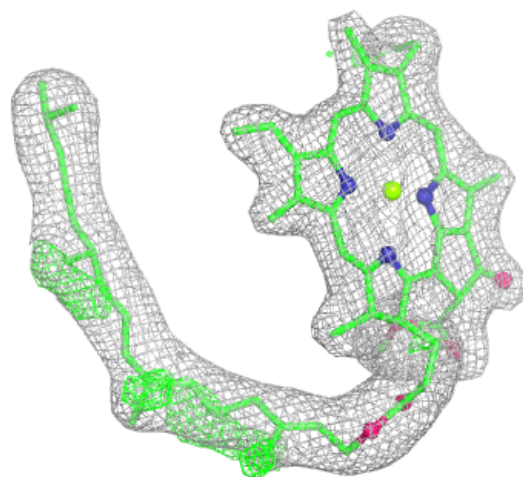
Electron density around LHG b 639:

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



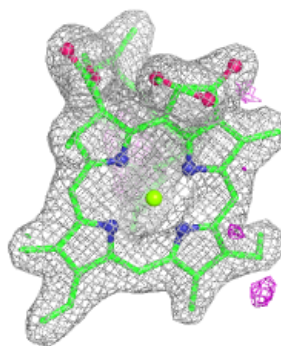
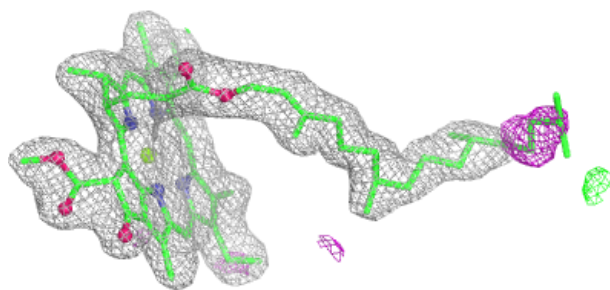
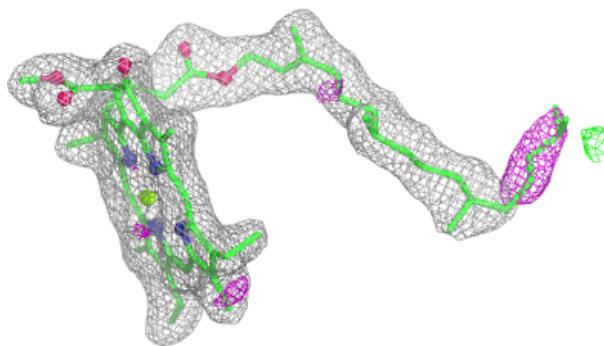
Electron density around CLA c 908:

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

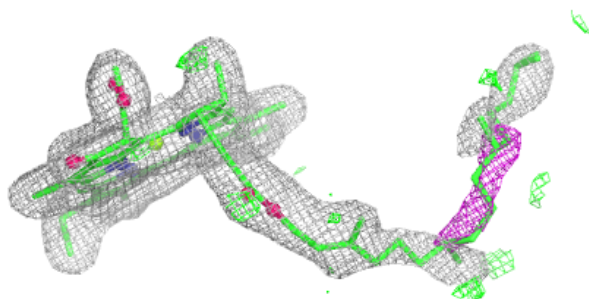
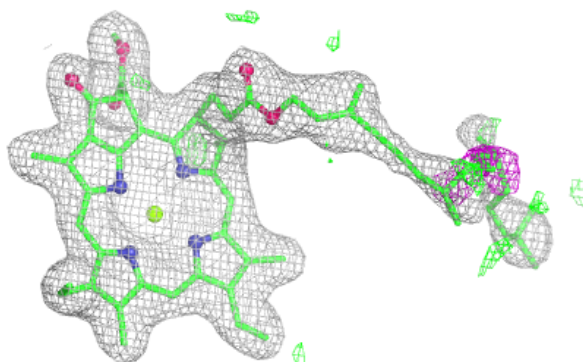


Electron density around CLA c 909:

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

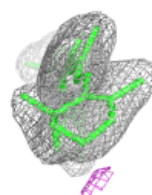
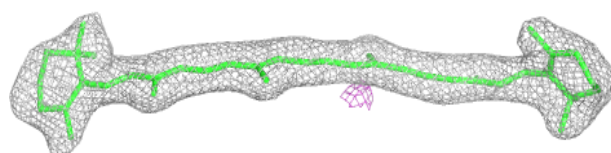
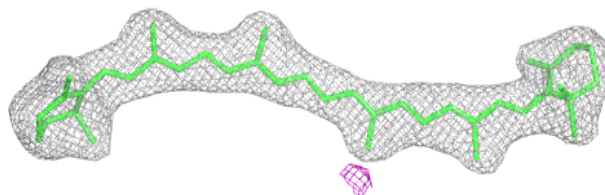
**Electron density around CLA A 410:**

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

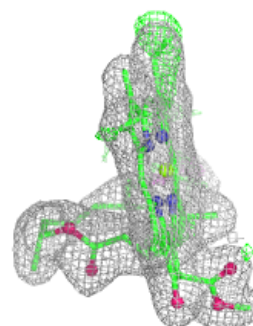
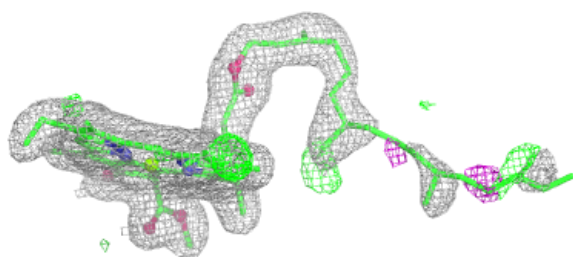
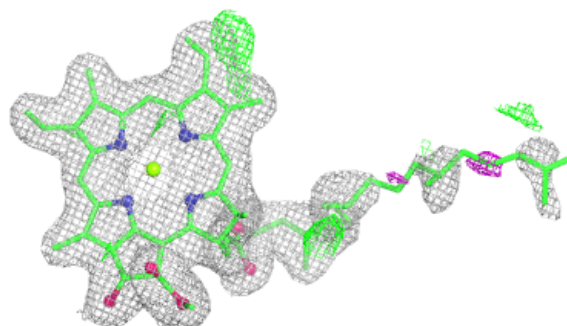


Electron density around BCR y 101:

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

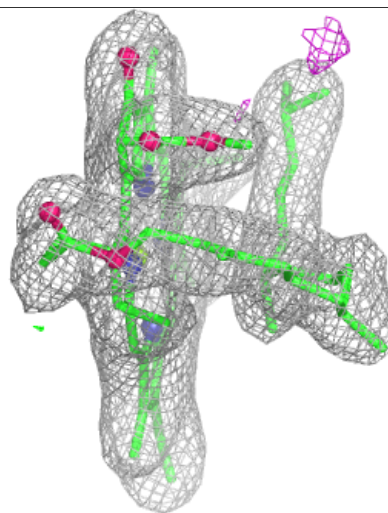
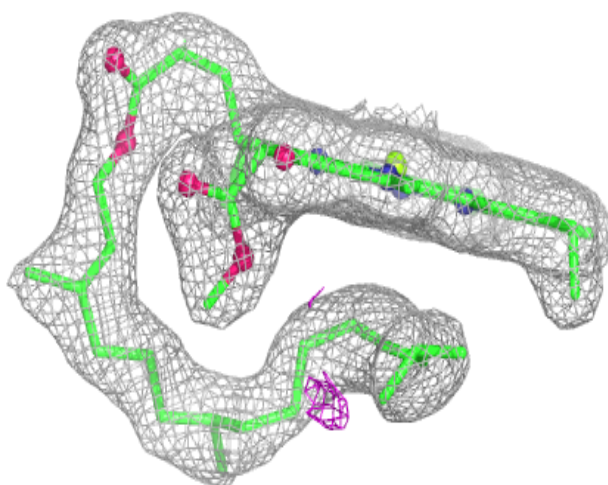
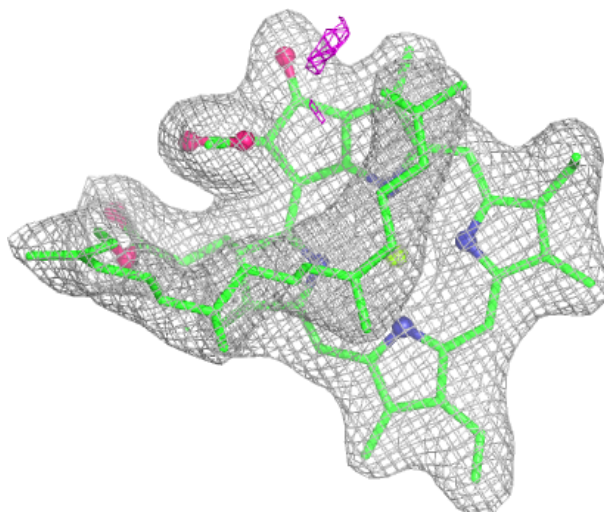
**Electron density around CLA a 410:**

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



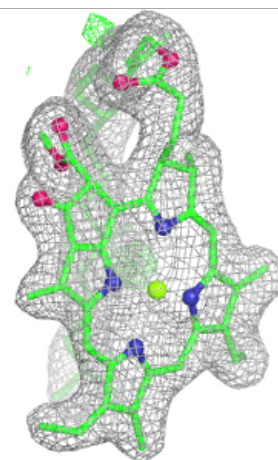
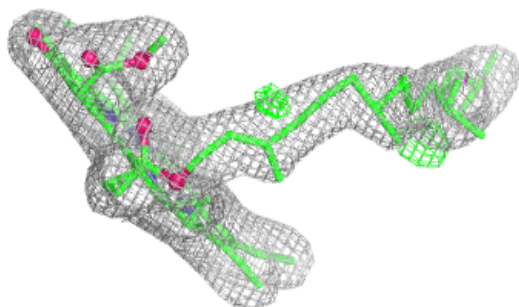
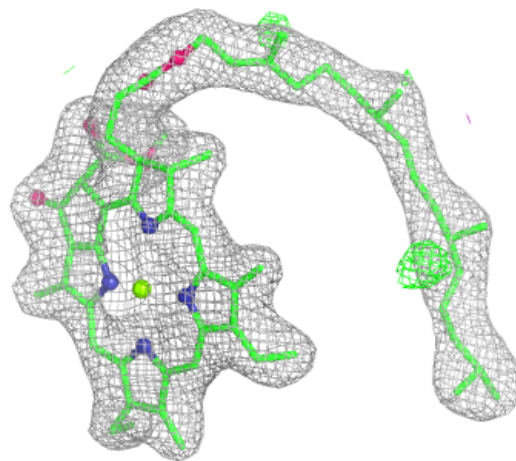
Electron density around CLA c 911:

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



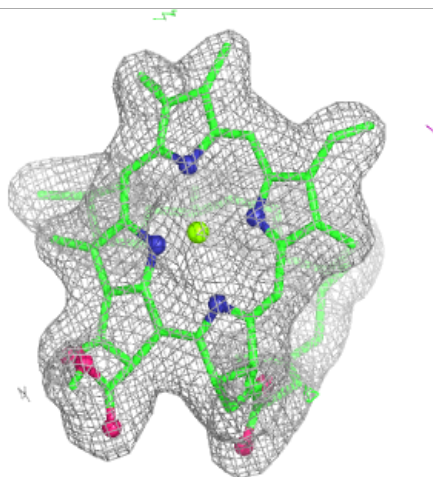
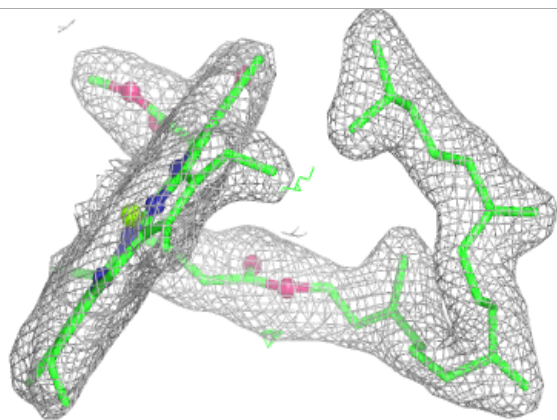
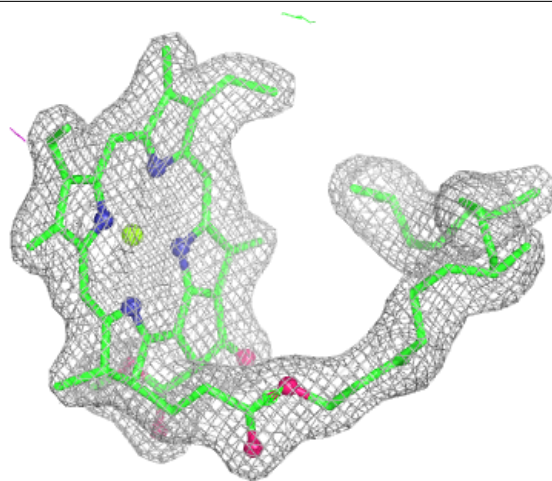
Electron density around CLA C 507:

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



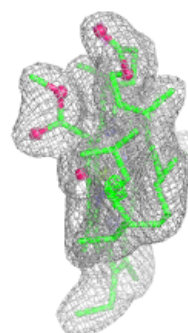
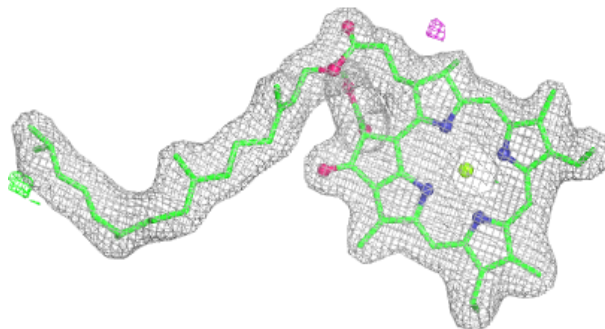
Electron density around CLA C 503:

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



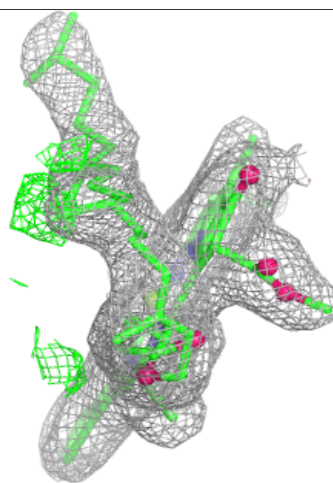
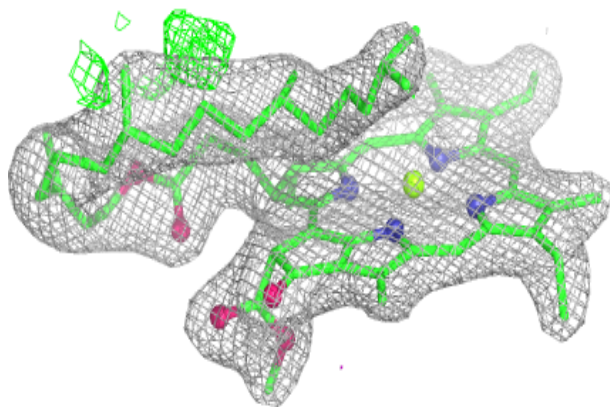
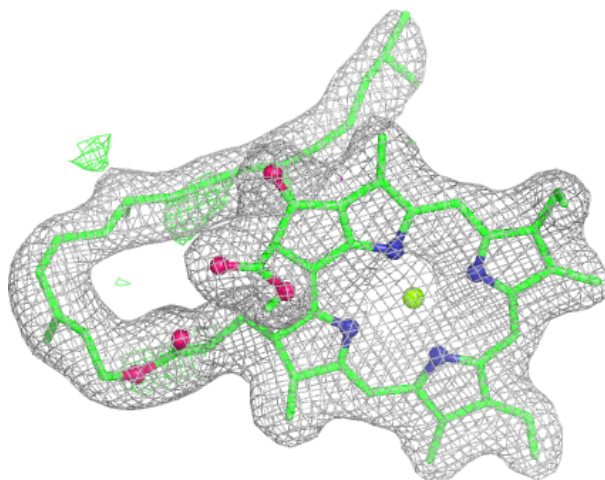
Electron density around CLA b 606:

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



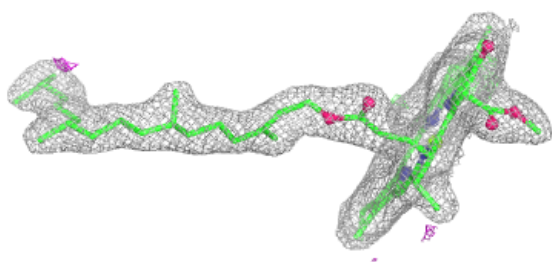
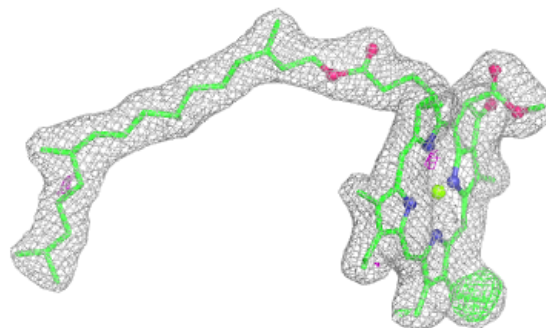
Electron density around CLA C 509:

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

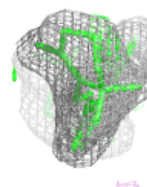
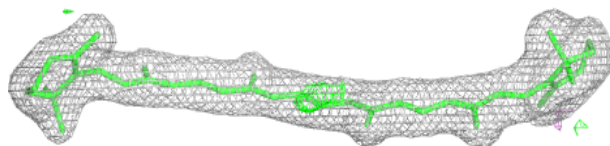
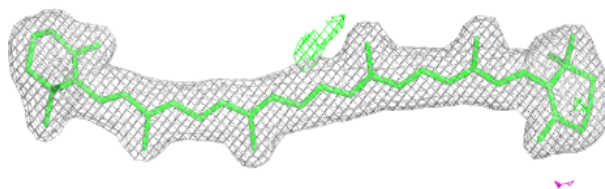


Electron density around CLA b 613:

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

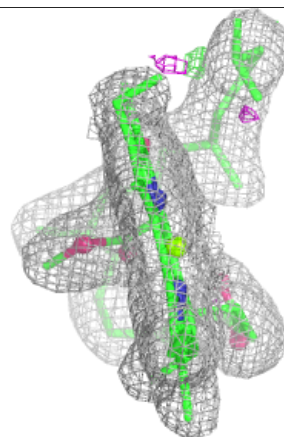
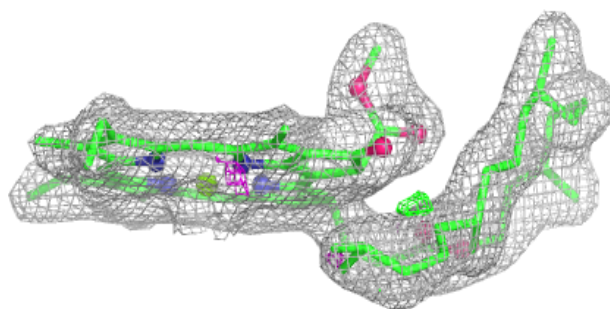
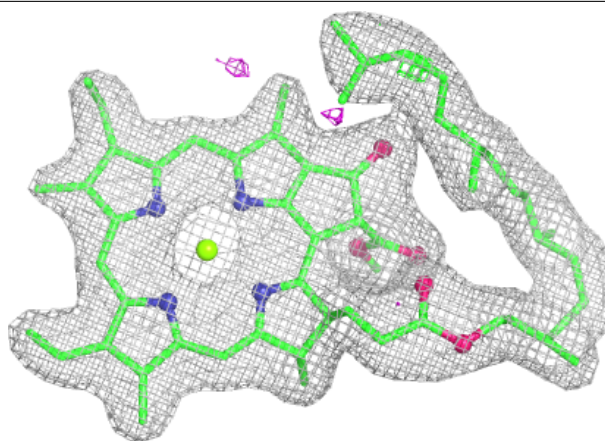
**Electron density around BCR B 620:**

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

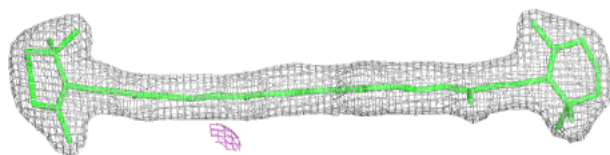
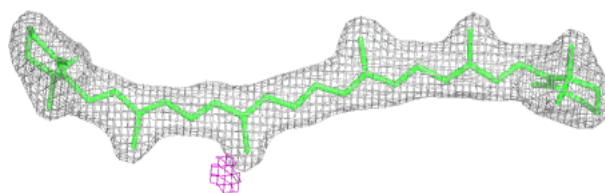


Electron density around CLA b 614:

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

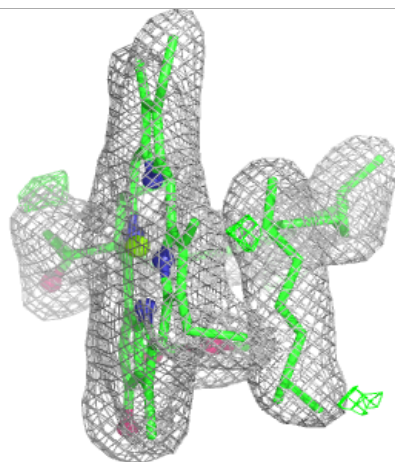
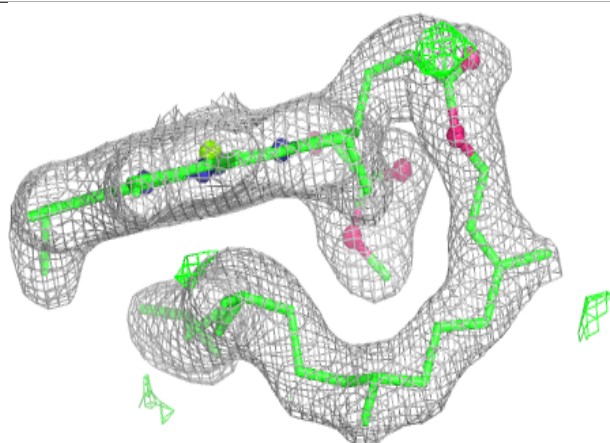
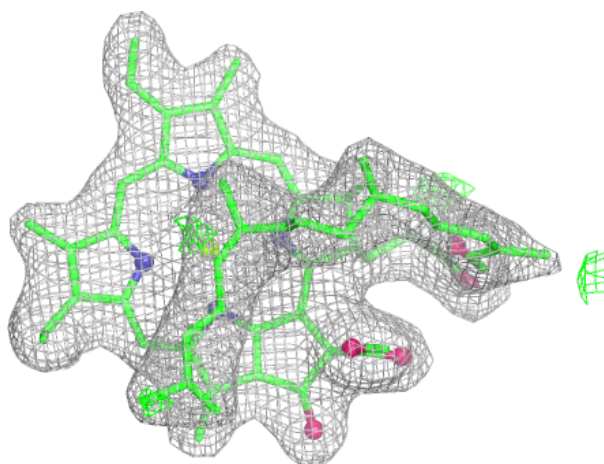
**Electron density around BCR C 515:**

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



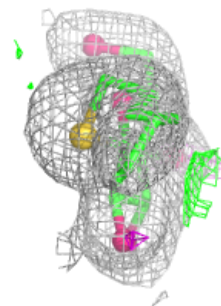
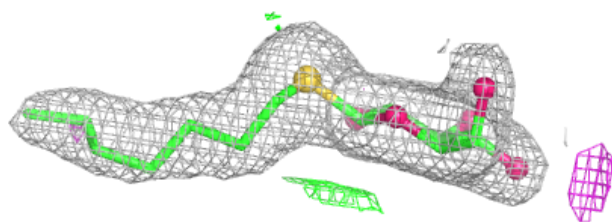
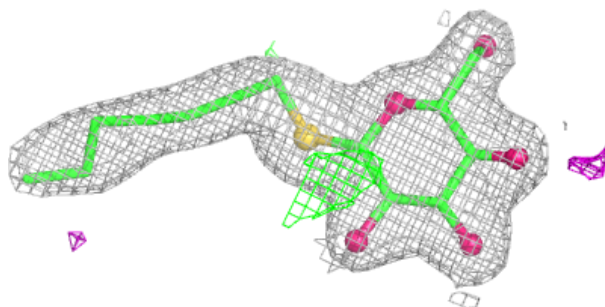
Electron density around CLA C 510:

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



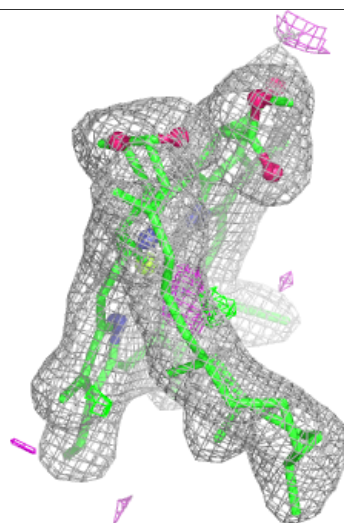
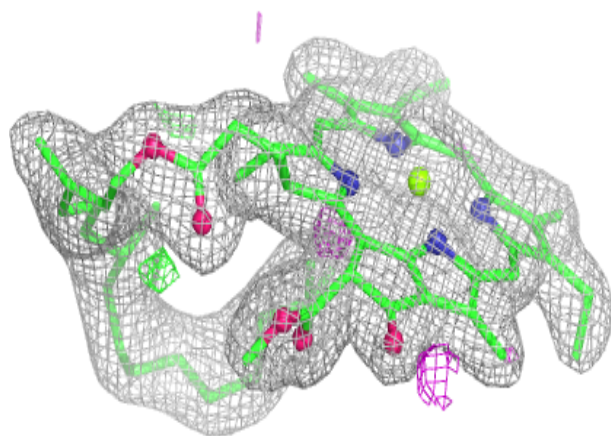
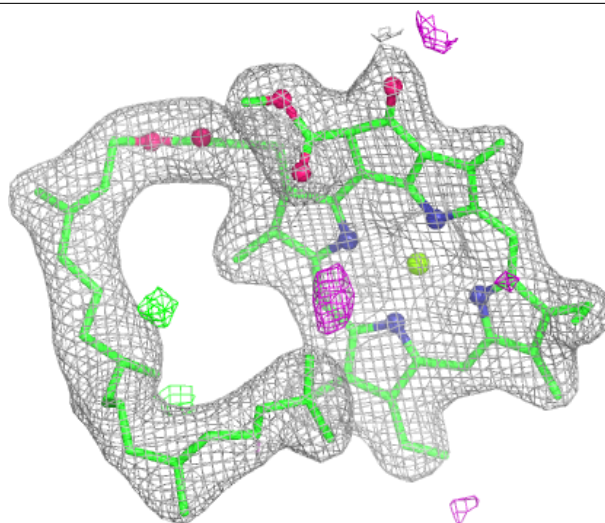
Electron density around HTG o 301:

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



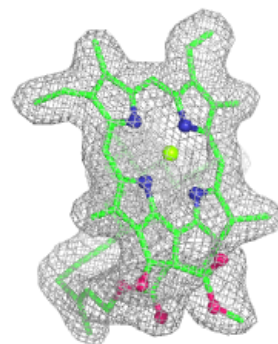
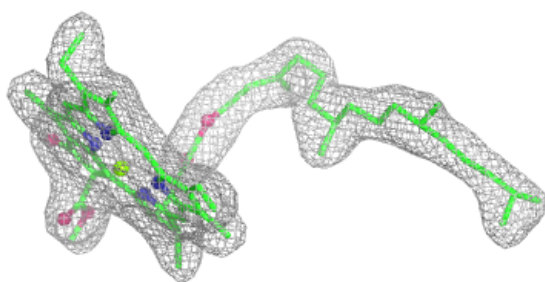
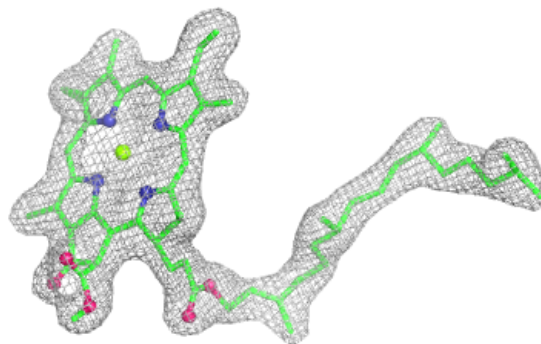
Electron density around CLA b 619:

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

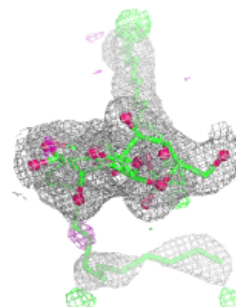
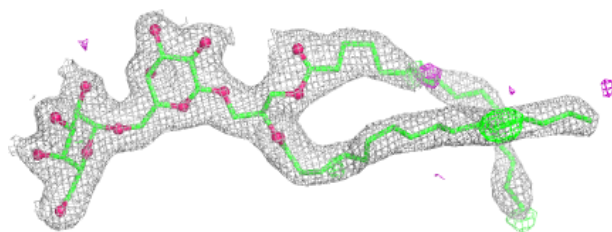
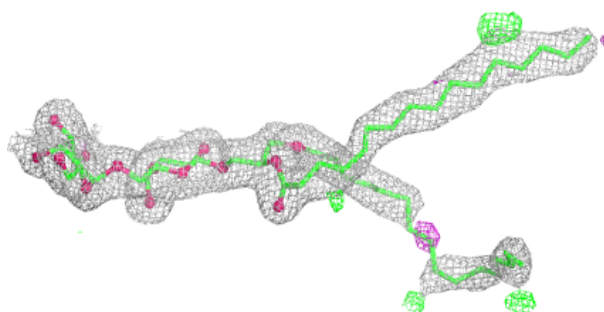


Electron density around CLA C 511:

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

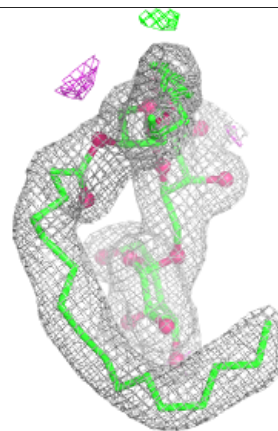
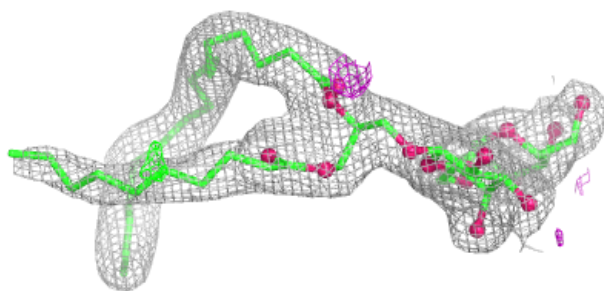
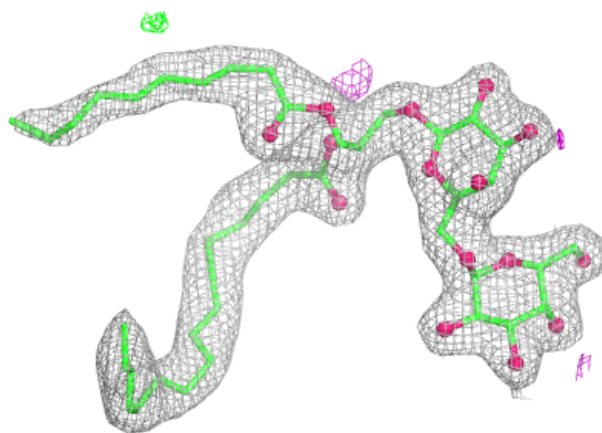
**Electron density around DGD C 516:**

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

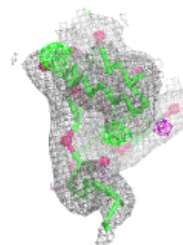
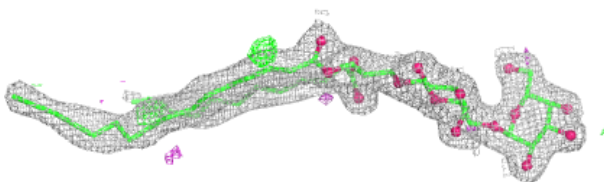
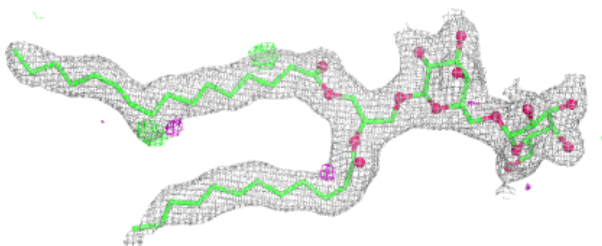


Electron density around DGD C 517:

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

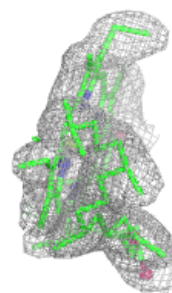
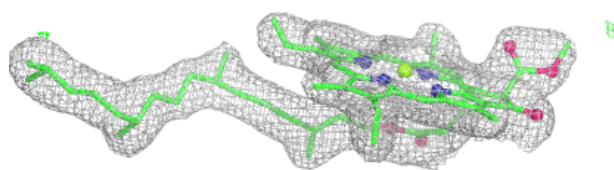
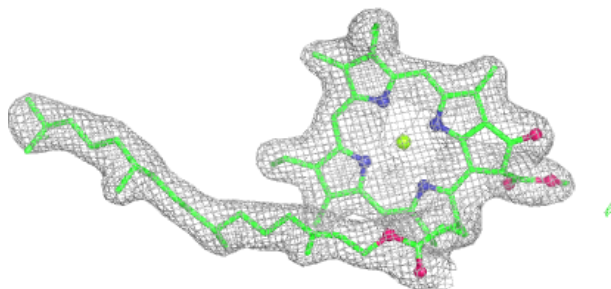
**Electron density around DGD C 518:**

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

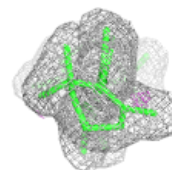
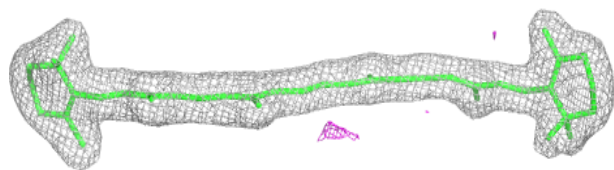
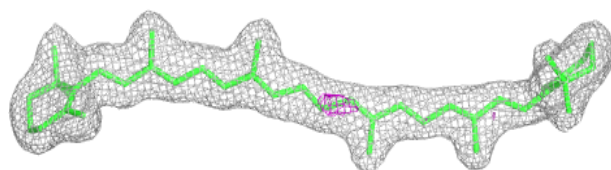


Electron density around CLA c 902:

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

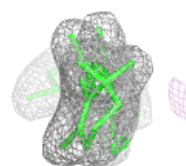
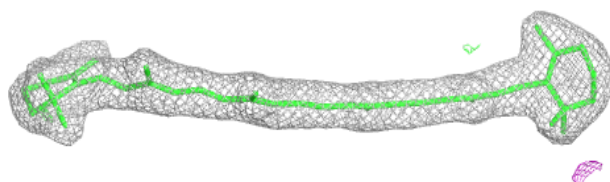
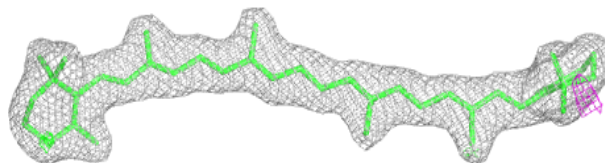
**Electron density around BCR a 414:**

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

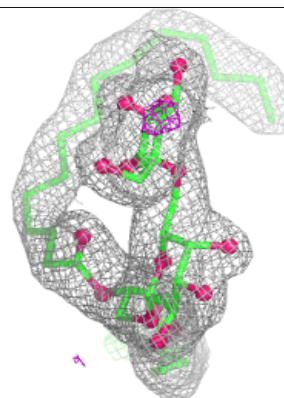
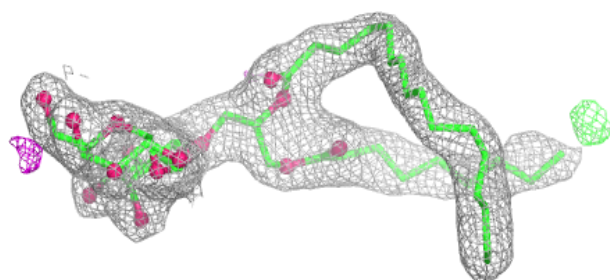
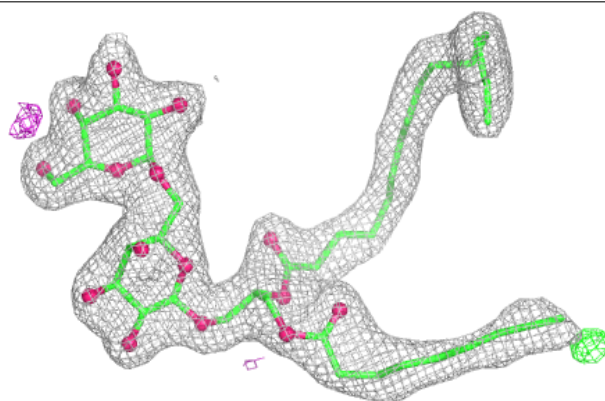


Electron density around BCR b 621:

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

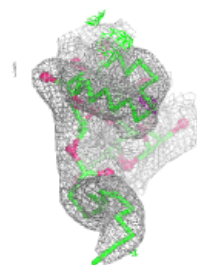
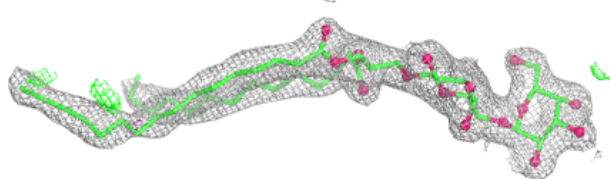
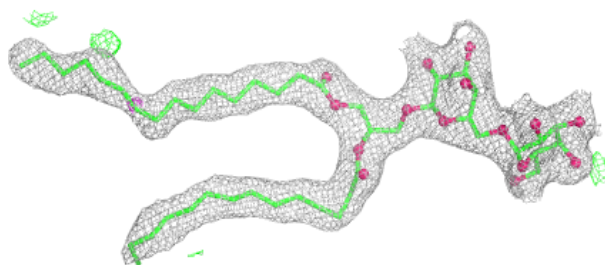
**Electron density around DGD c 918:**

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

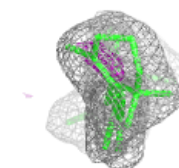
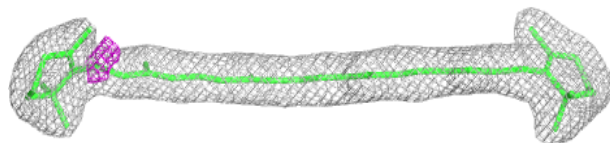
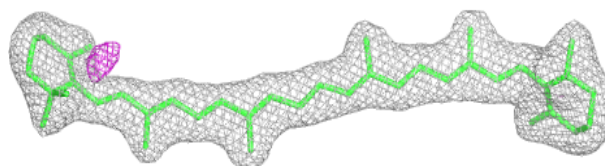


Electron density around DGD c 919:

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

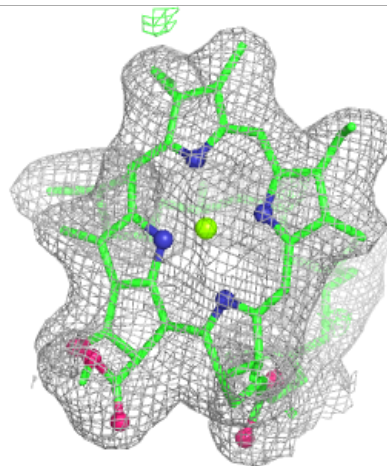
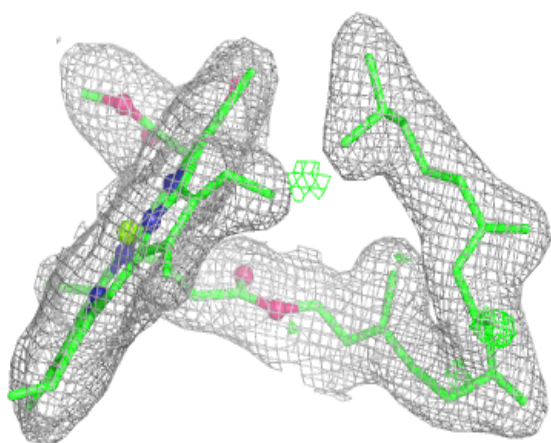
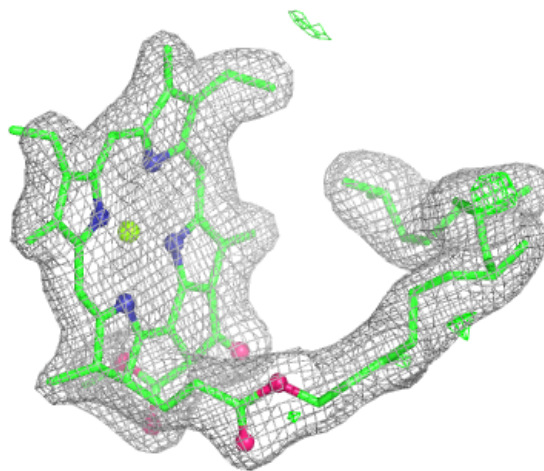
**Electron density around BCR b 622:**

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



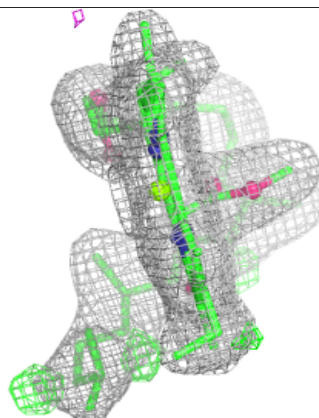
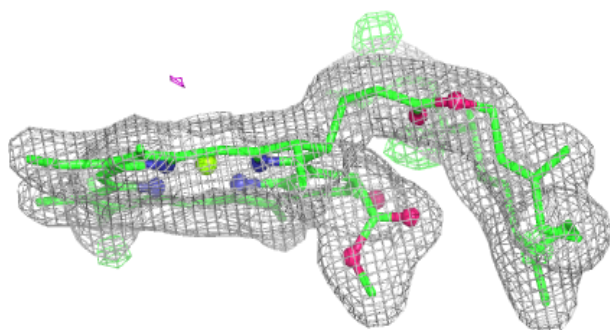
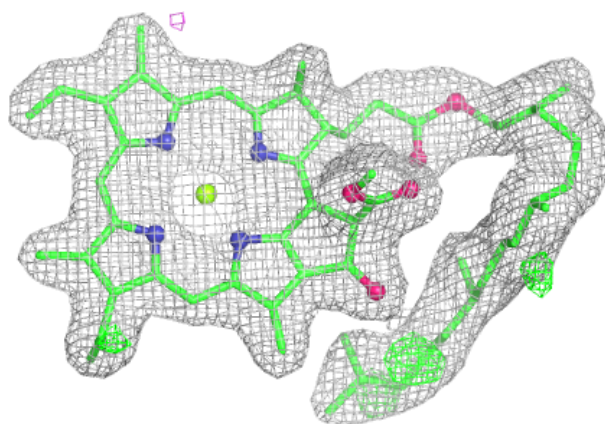
Electron density around CLA c 904:

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



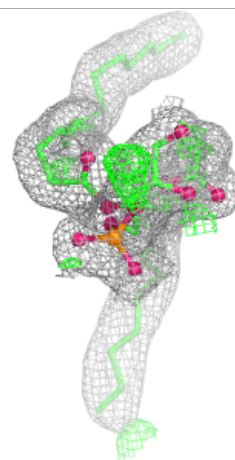
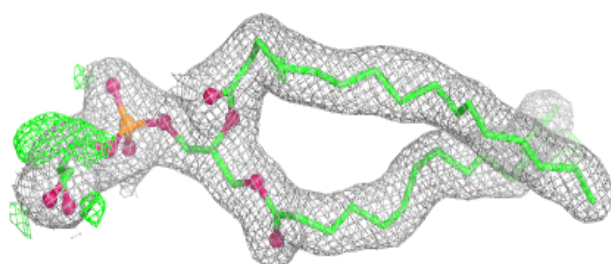
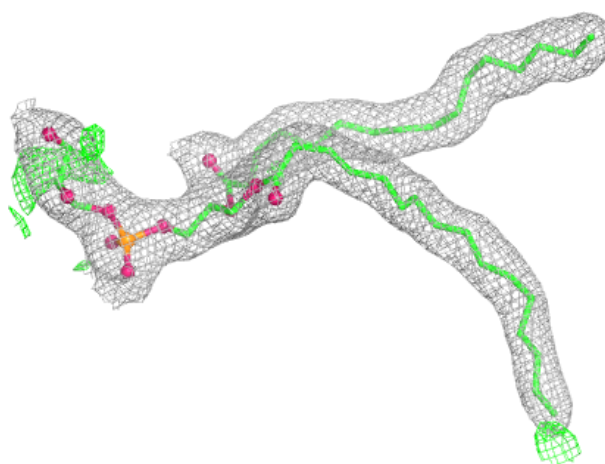
Electron density around CLA B 611:

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



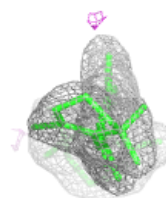
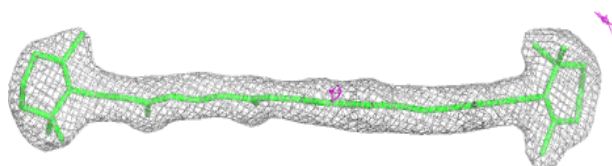
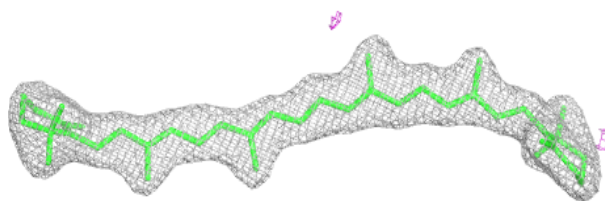
Electron density around LHG D 408:

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

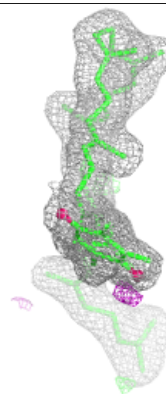
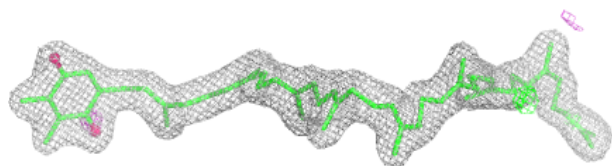
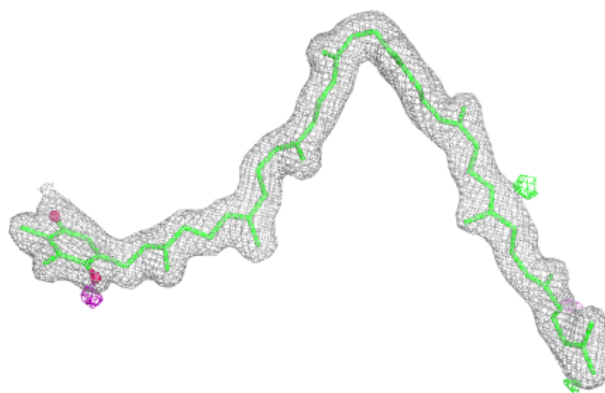


Electron density around BCR c 916:

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

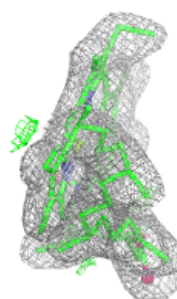
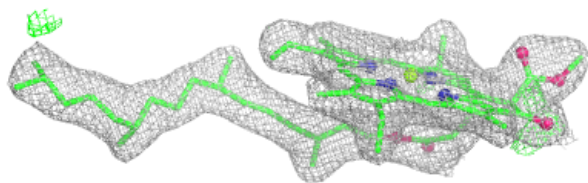
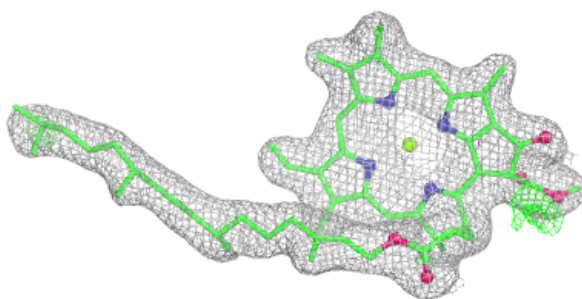
**Electron density around PL9 D 405:**

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



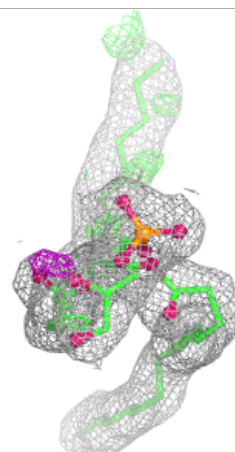
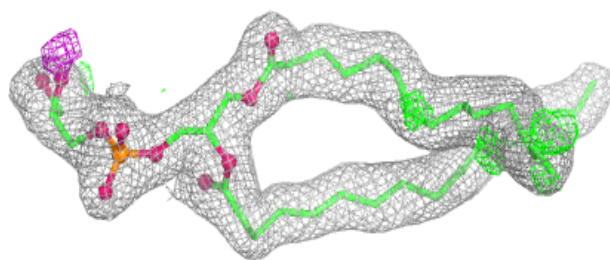
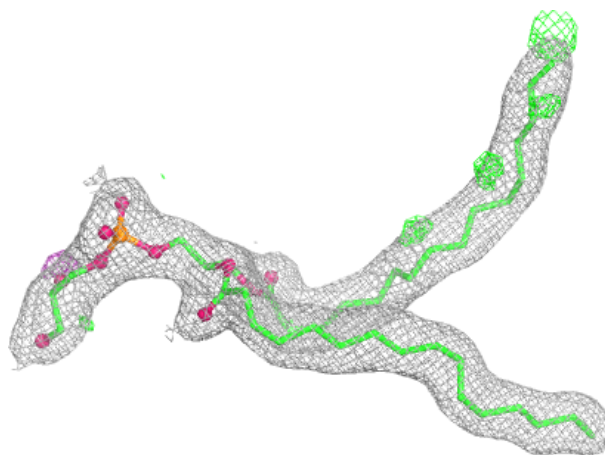
Electron density around CLA C 501:

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



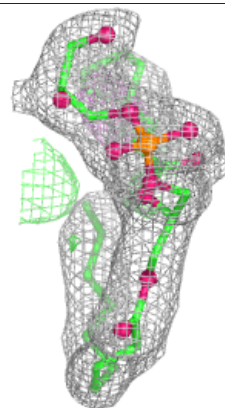
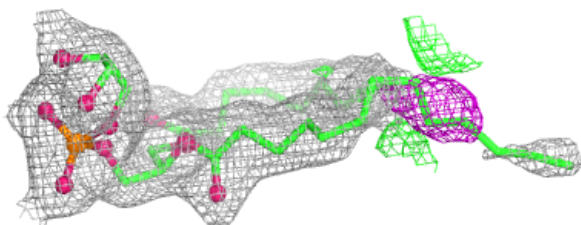
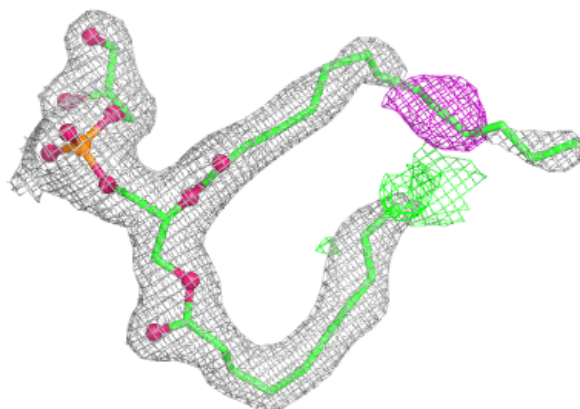
Electron density around LHG d 409:

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

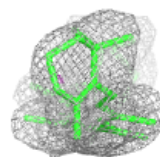
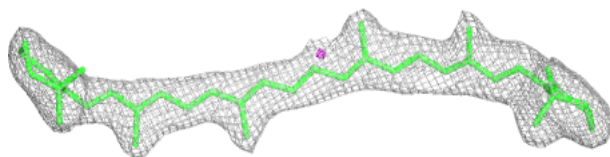
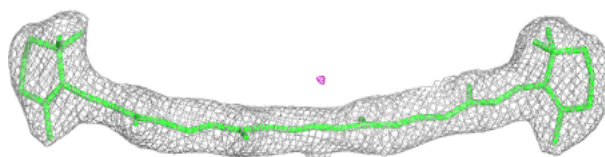


Electron density around LHG d 410:

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

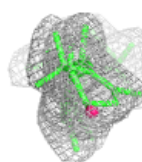
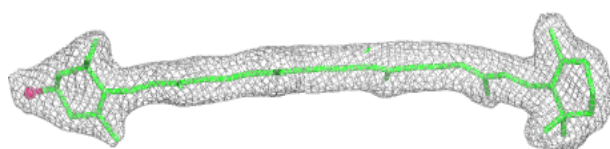
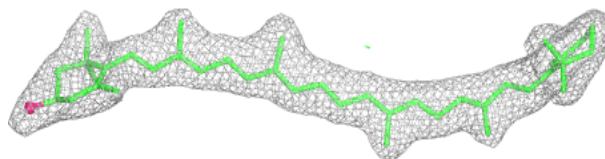
**Electron density around BCR k 101:**

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

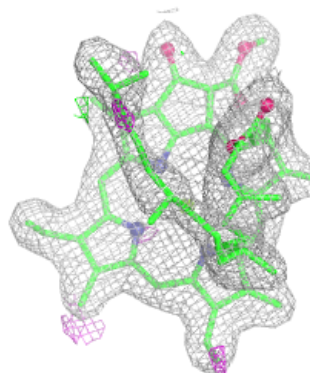
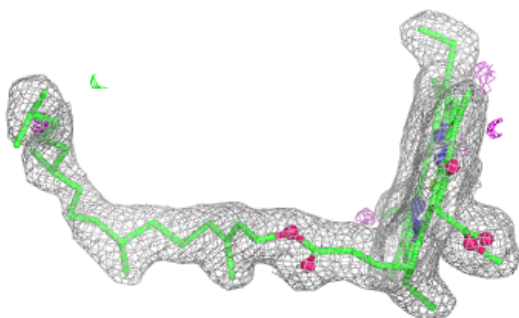
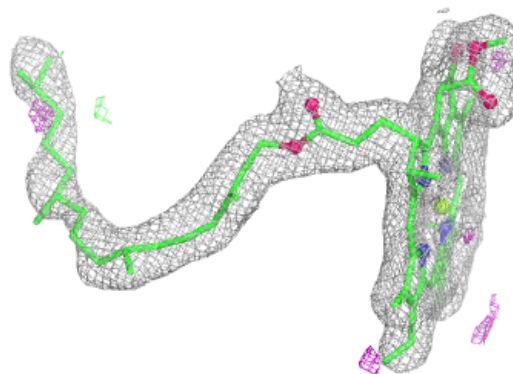


Electron density around RRX H 102:

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

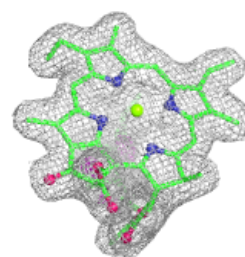
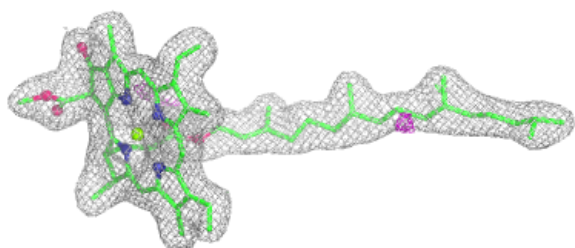
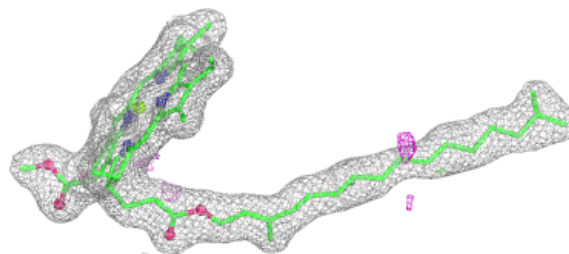
**Electron density around CLA D 403:**

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

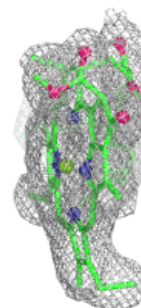
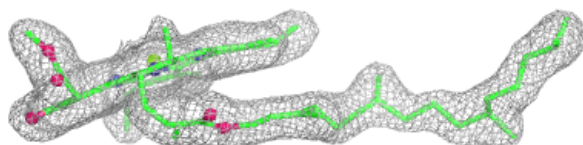
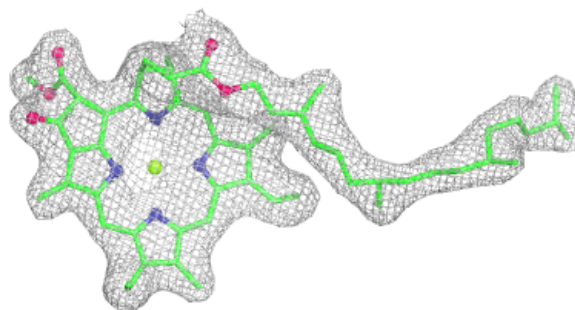


Electron density around CLA B 608:

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

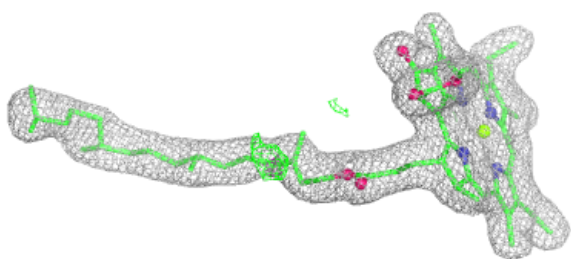
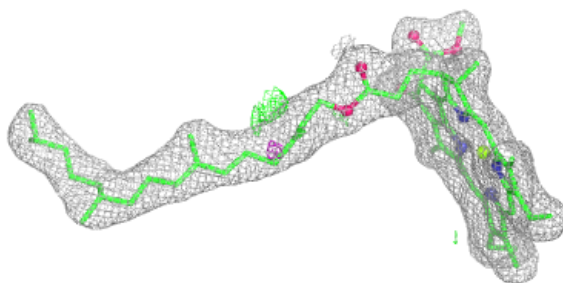
**Electron density around CLA b 607:**

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



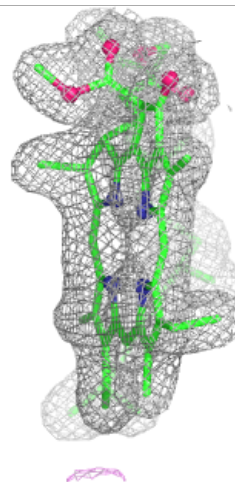
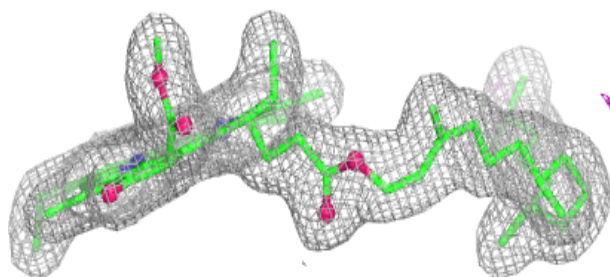
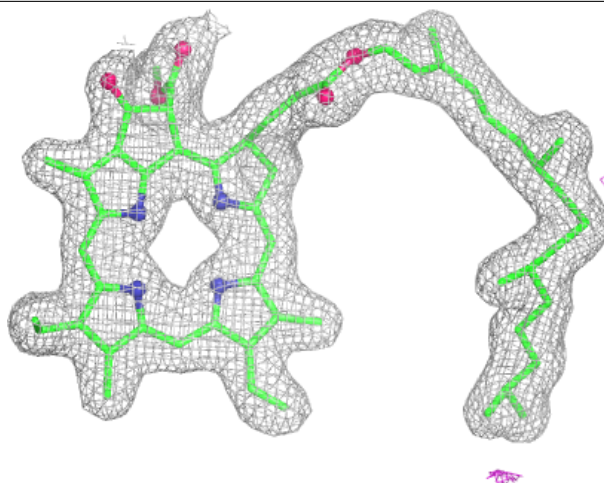
Electron density around CLA b 608:

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



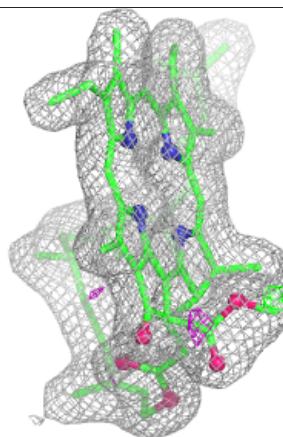
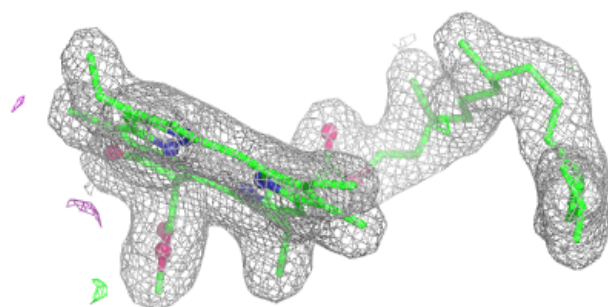
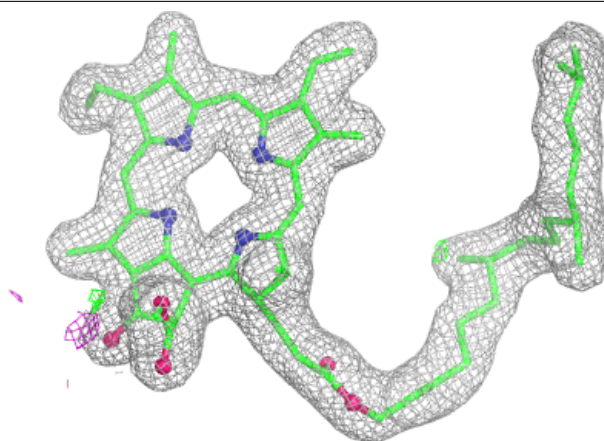
Electron density around PHO A 408:

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



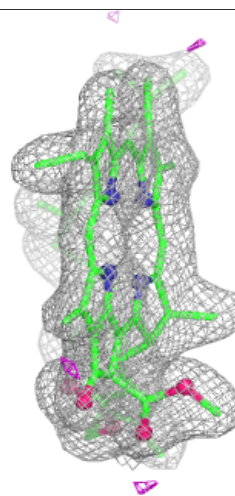
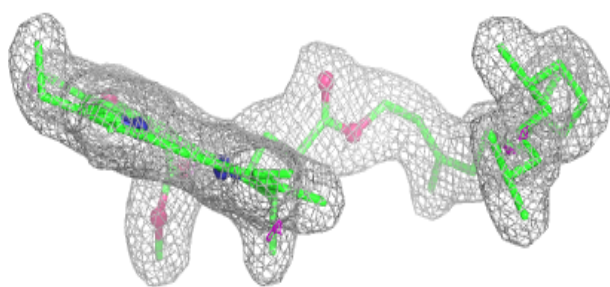
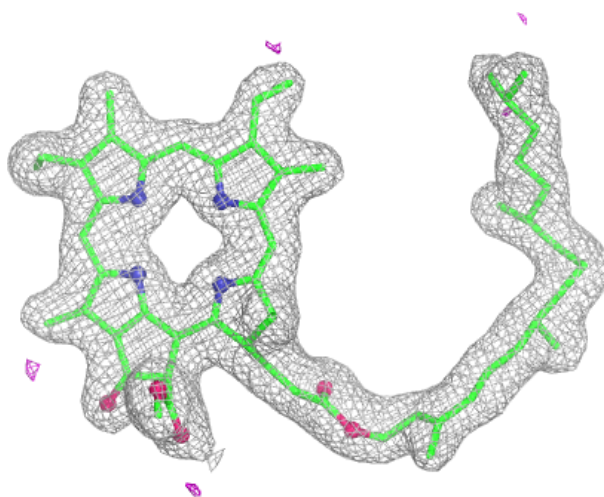
Electron density around PHO A 409:

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



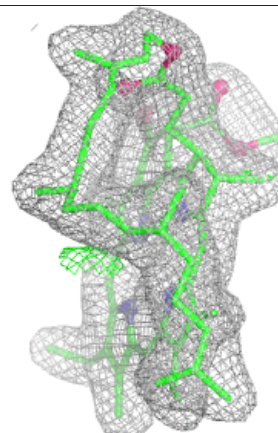
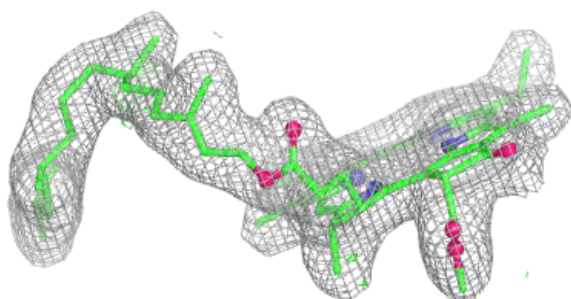
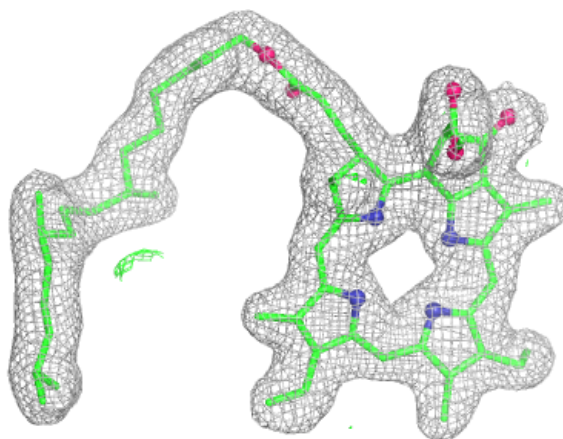
Electron density around PHO a 411:

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

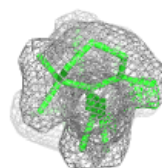
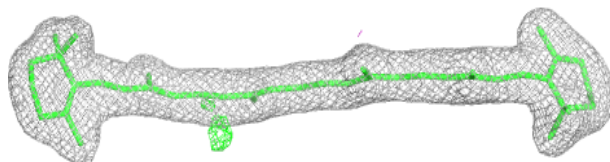
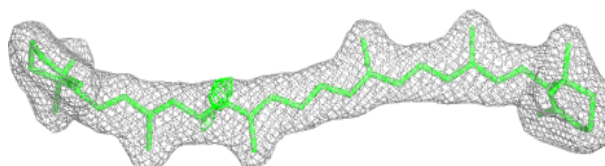


Electron density around PHO a 412:

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

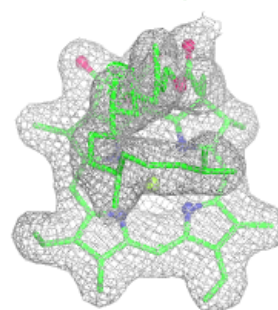
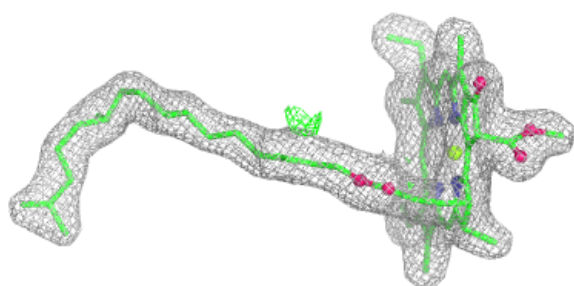
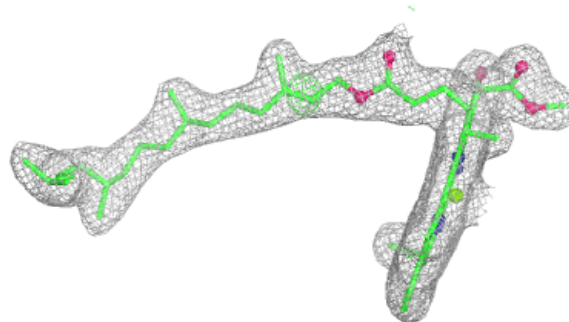
**Electron density around BCR A 411:**

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

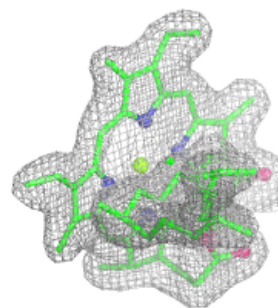
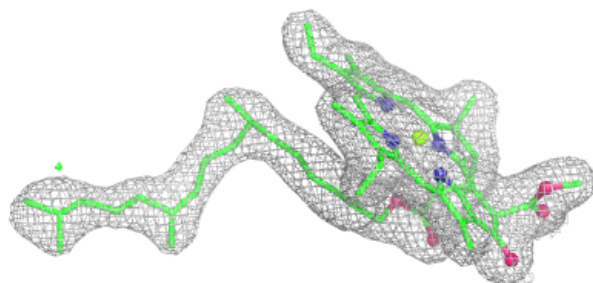
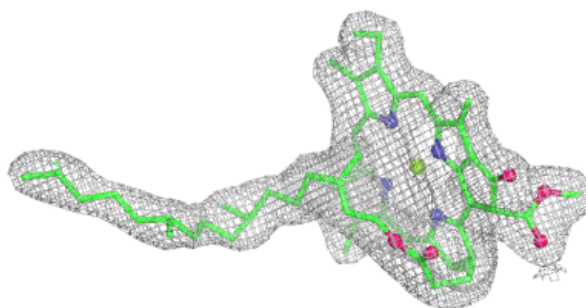


Electron density around CLA b 609:

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

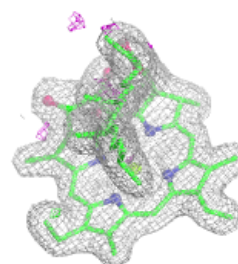
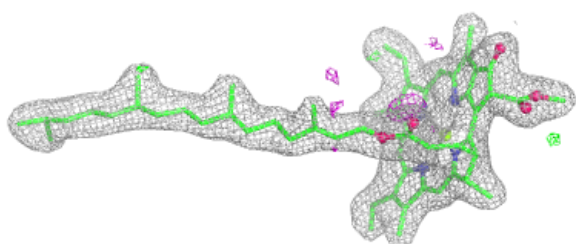
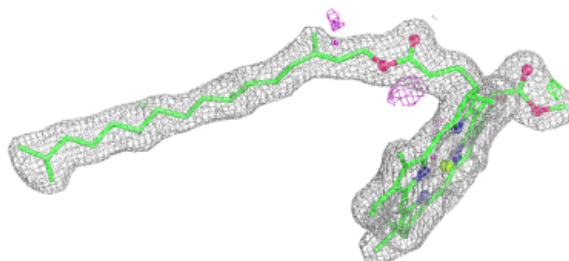
**Electron density around CLA C 505:**

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

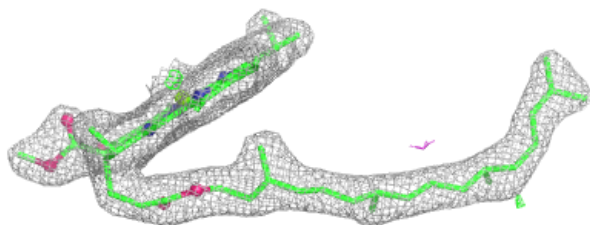
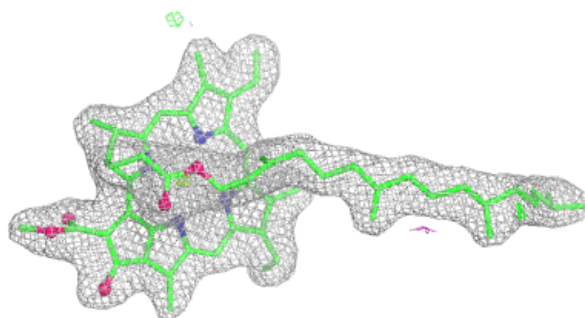


Electron density around CLA b 611:

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

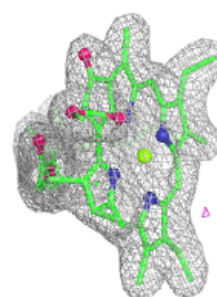
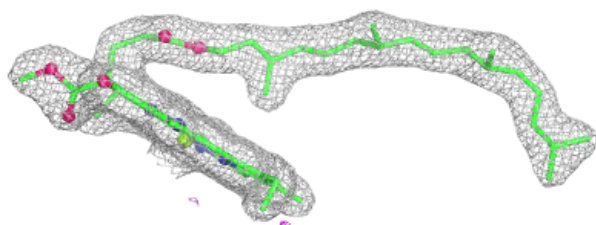
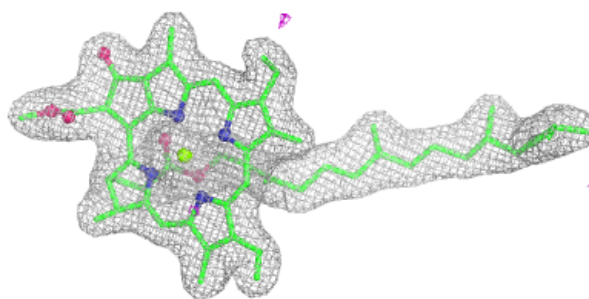
**Electron density around CLA b 612:**

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

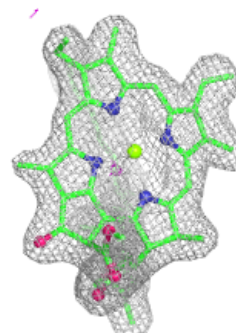
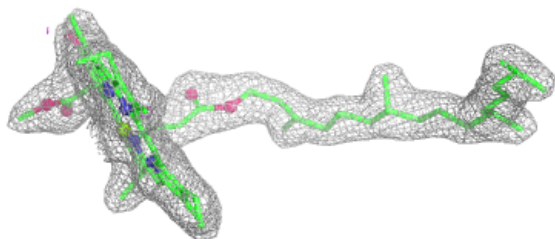
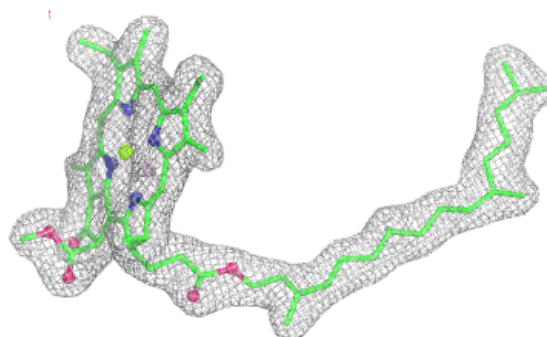


Electron density around CLA B 609:

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

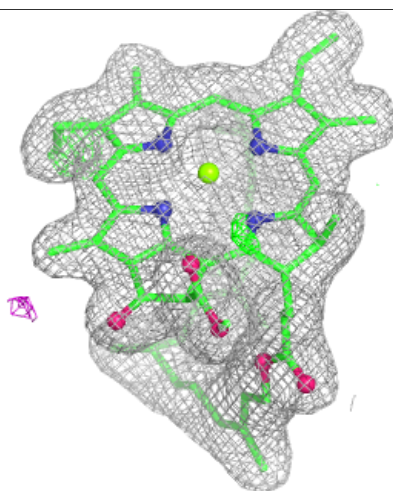
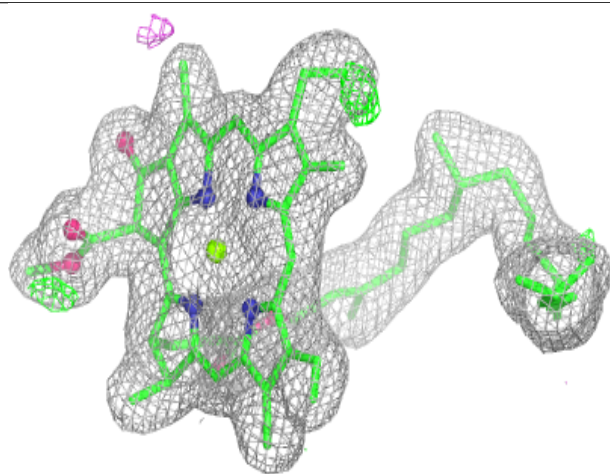
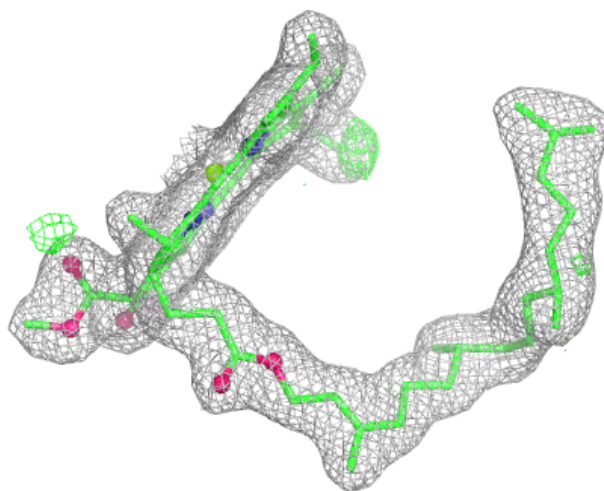
**Electron density around CLA B 610:**

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



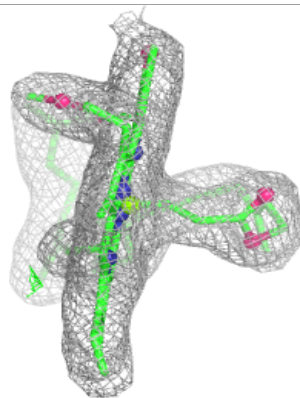
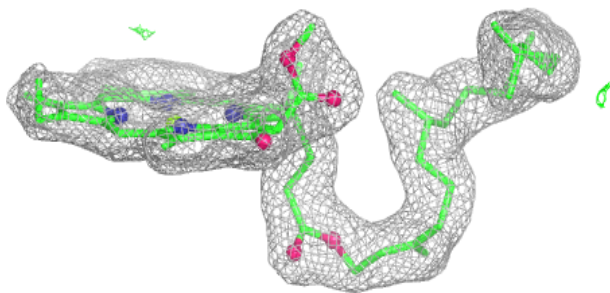
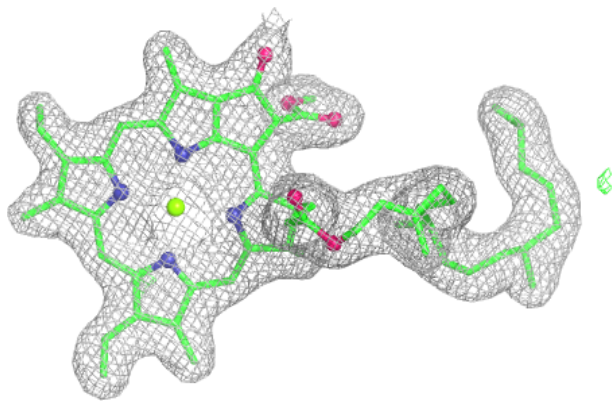
Electron density around CLA b 615:

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



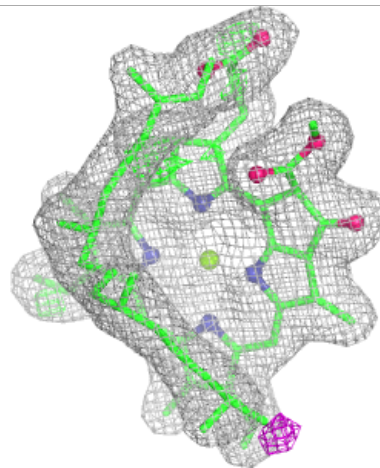
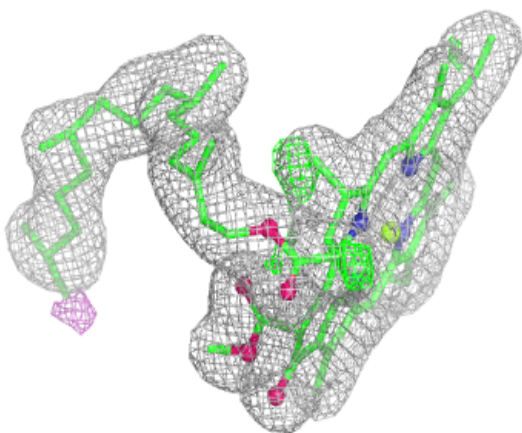
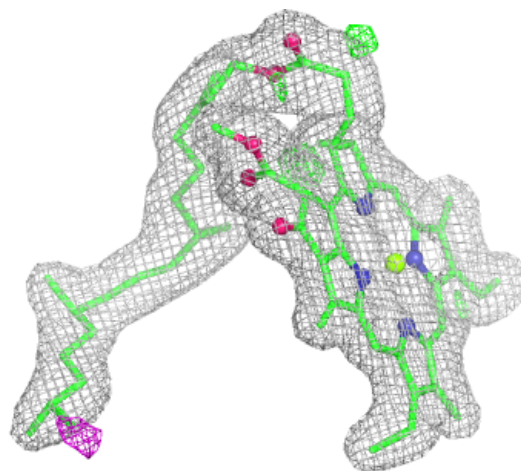
Electron density around CLA b 616:

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



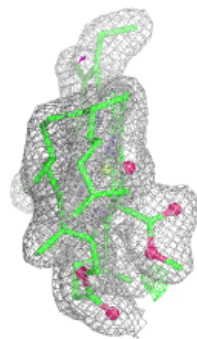
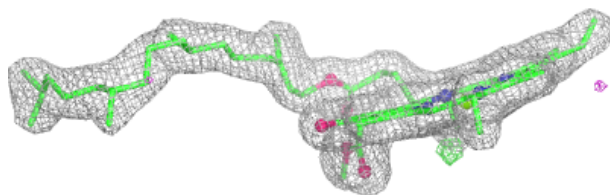
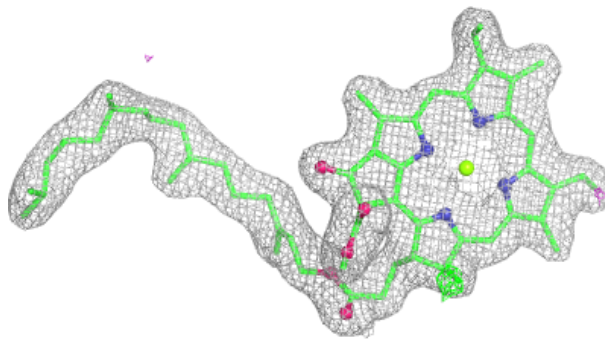
Electron density around CLA b 617:

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



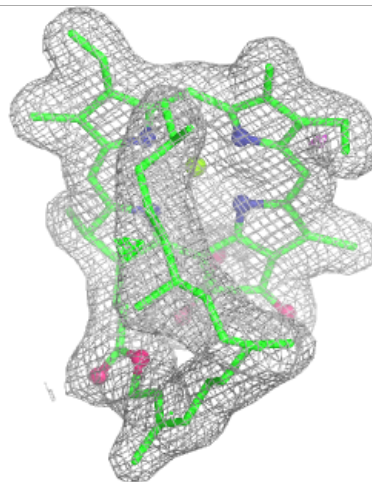
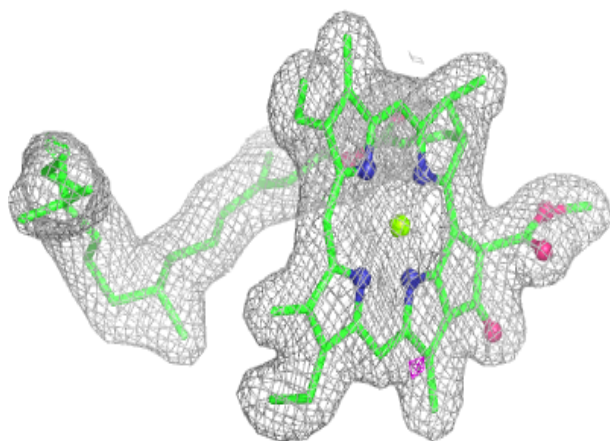
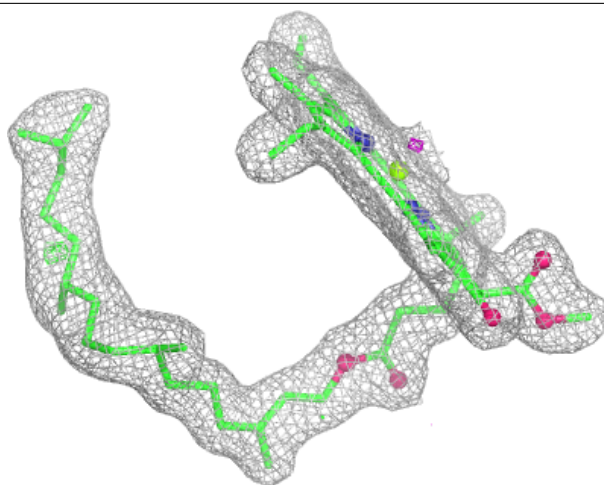
Electron density around CLA B 603:

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



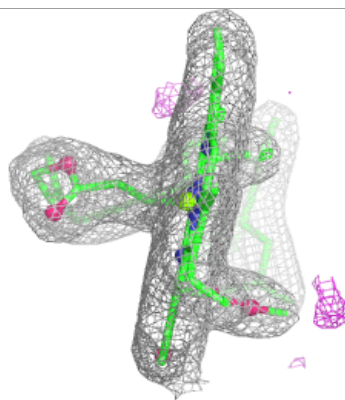
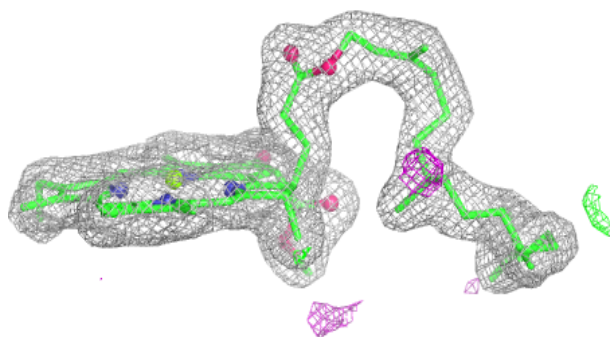
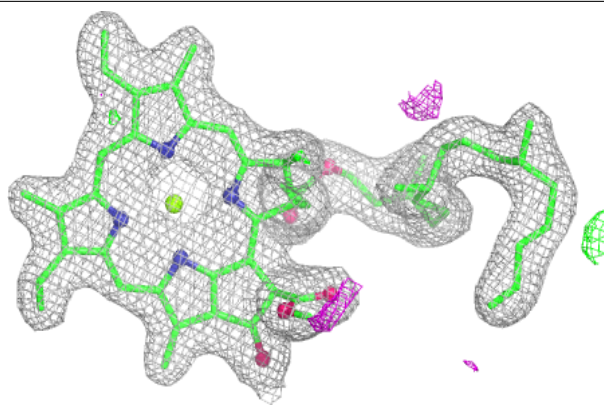
Electron density around CLA B 612:

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



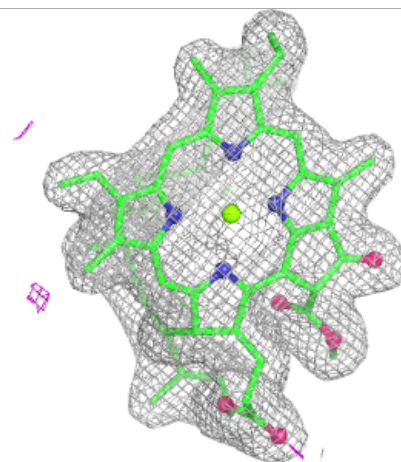
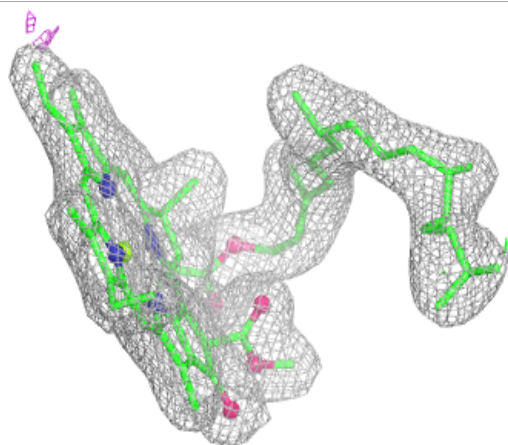
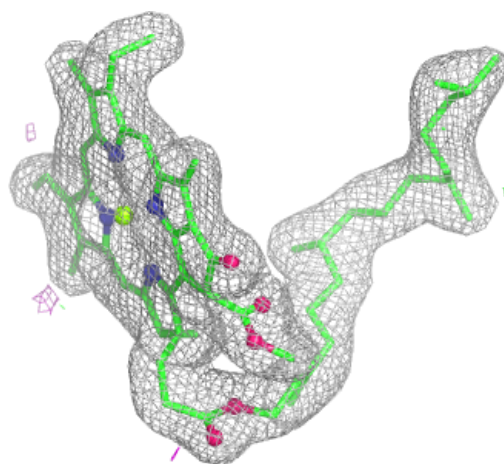
Electron density around CLA B 613:

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



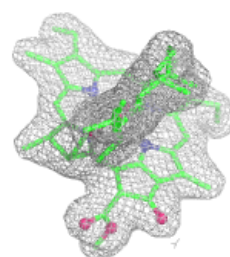
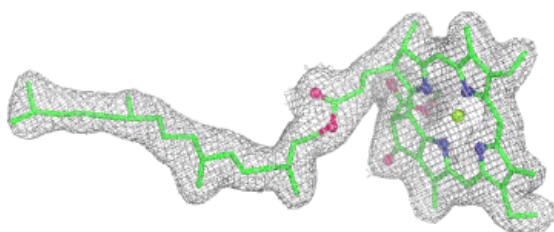
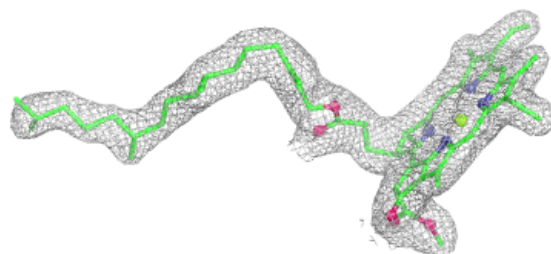
Electron density around CLA B 614:

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

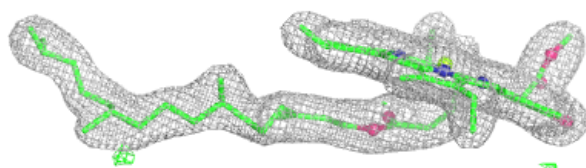
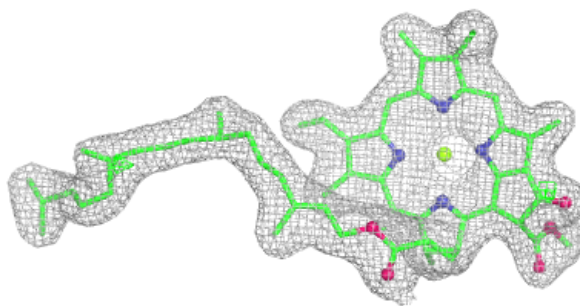


Electron density around CLA c 903:

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

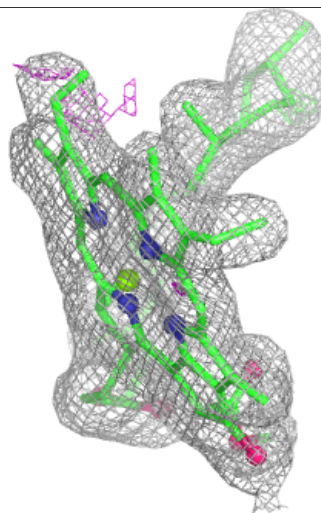
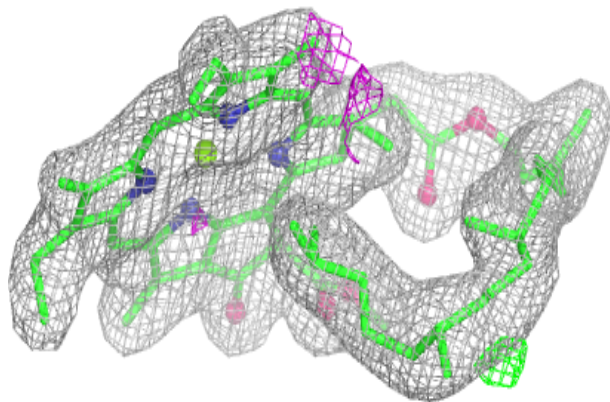
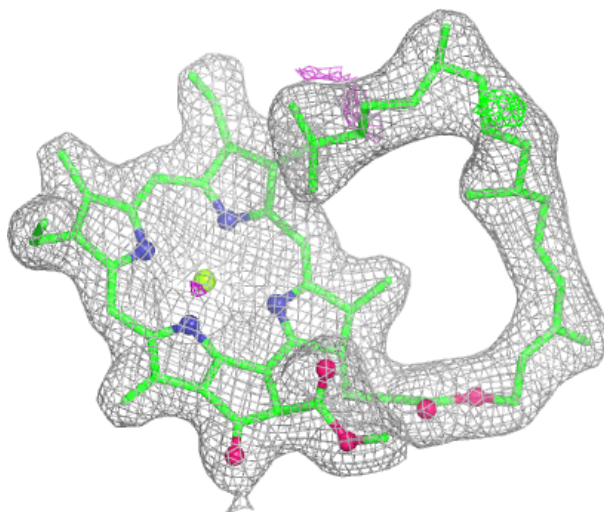
**Electron density around CLA B 604:**

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



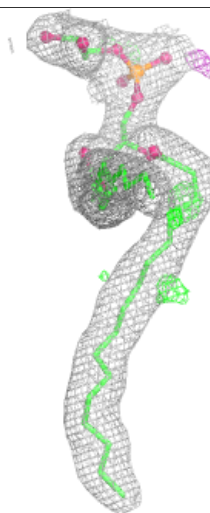
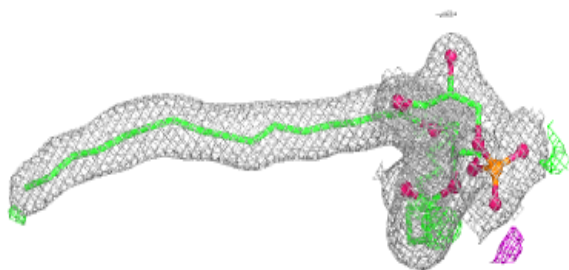
Electron density around CLA B 616:

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



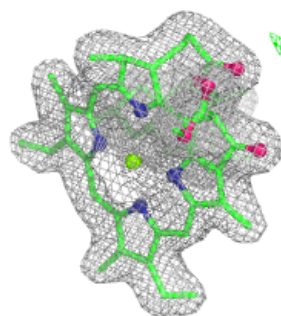
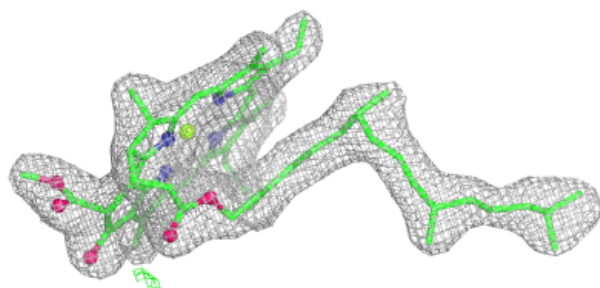
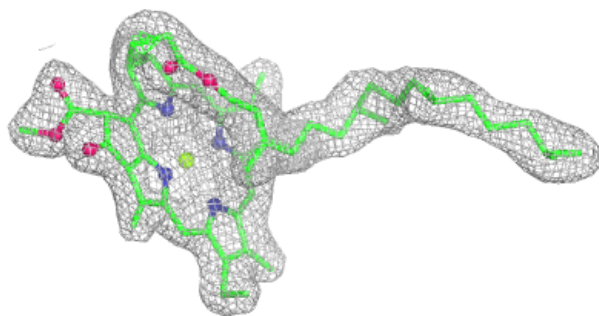
Electron density around LHG L 101:

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

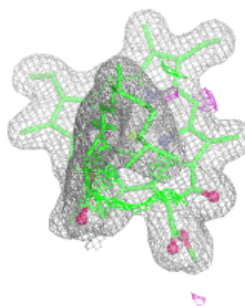
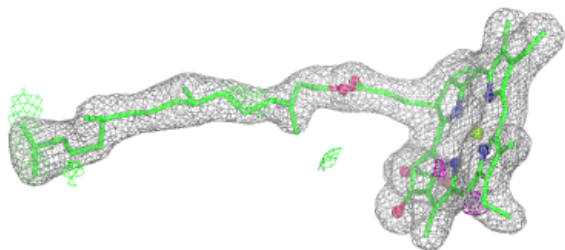
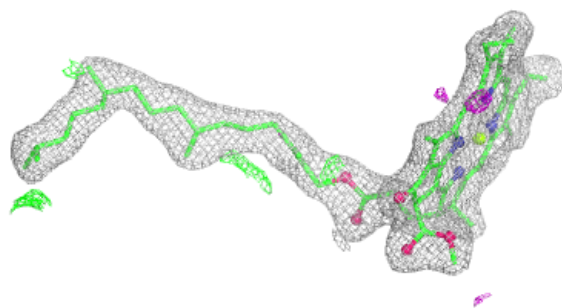


Electron density around CLA c 906:

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

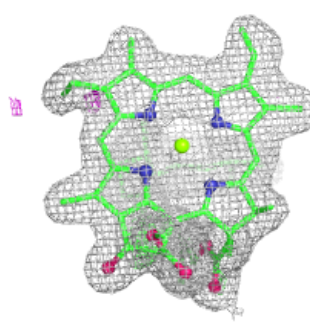
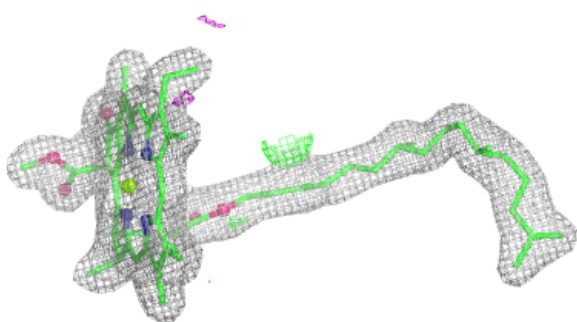
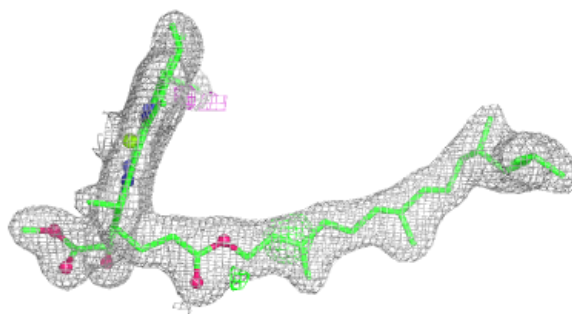
**Electron density around CLA B 605:**

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

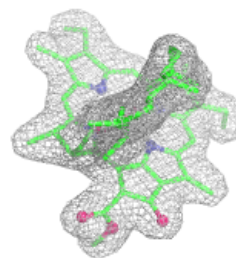
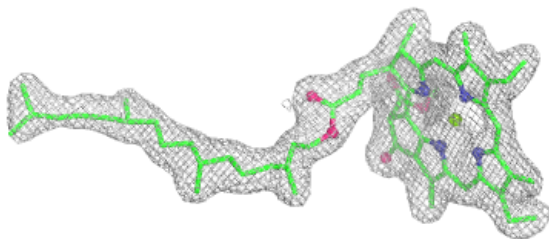
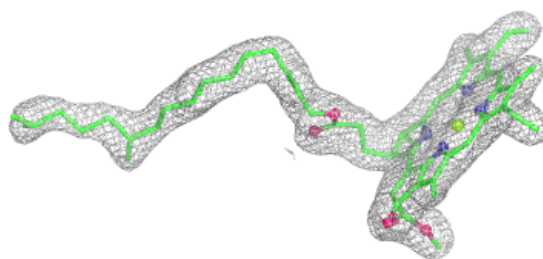


Electron density around CLA B 606:

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

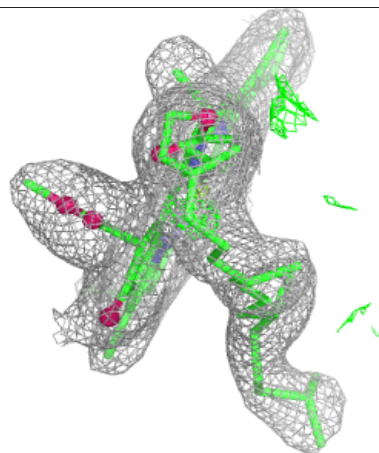
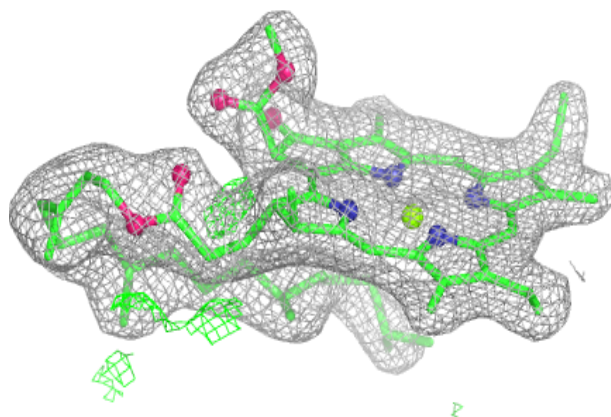
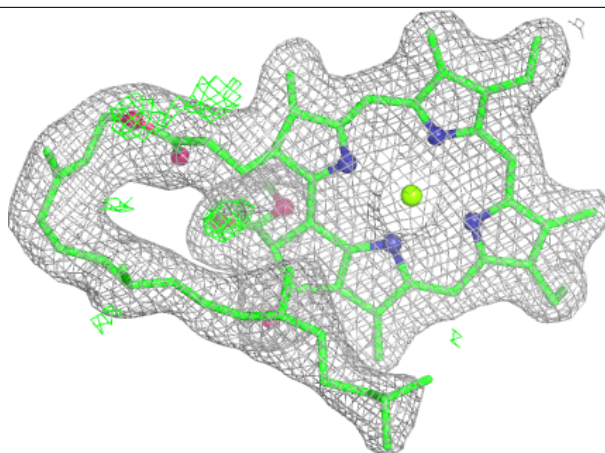
**Electron density around CLA C 502:**

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



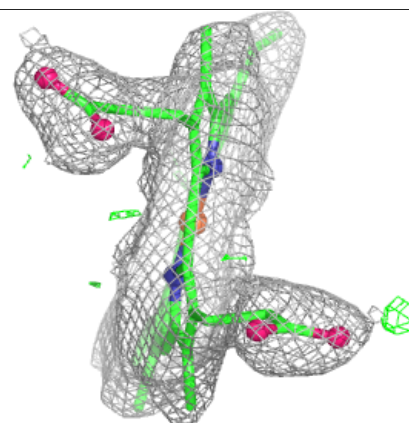
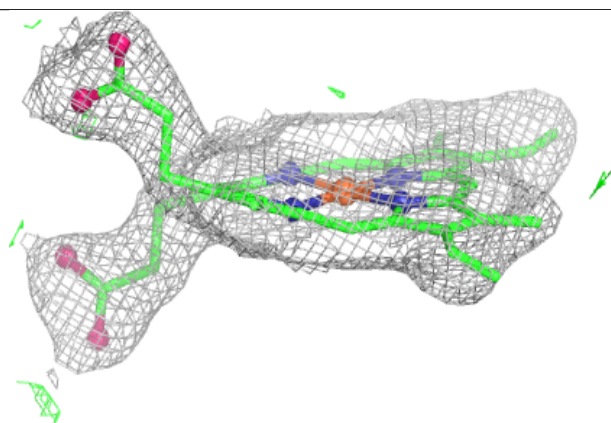
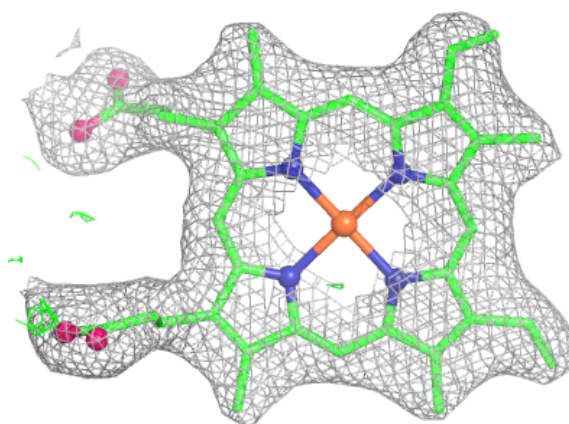
Electron density around CLA c 910:

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



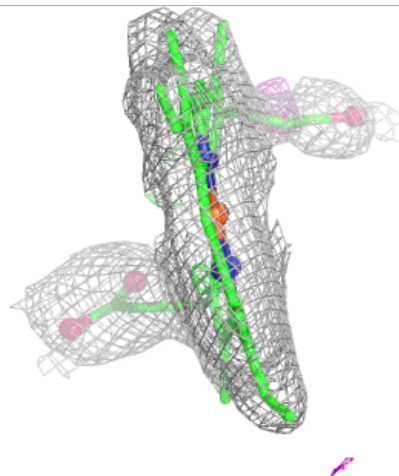
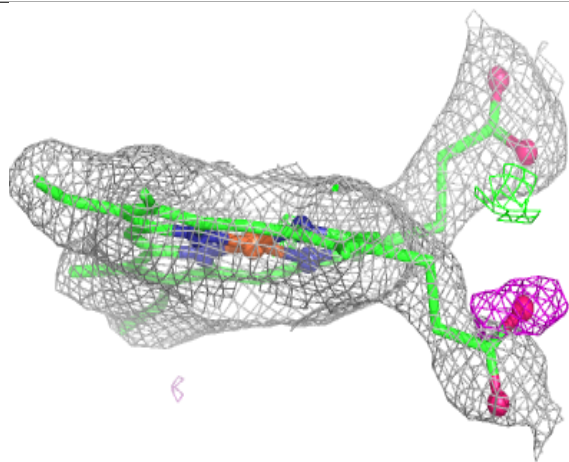
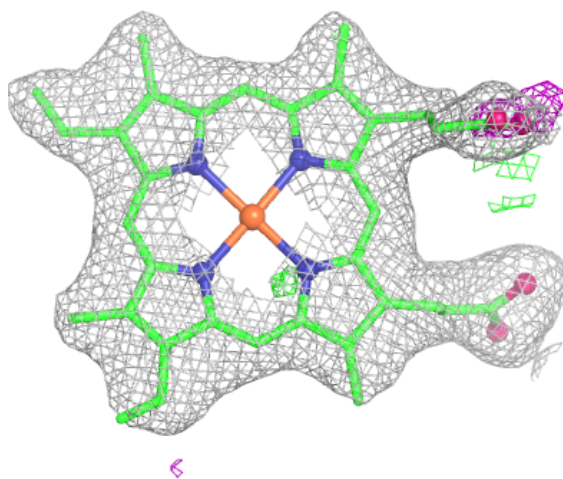
Electron density around HEM F 102:

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



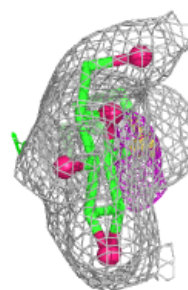
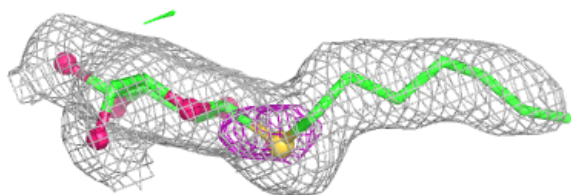
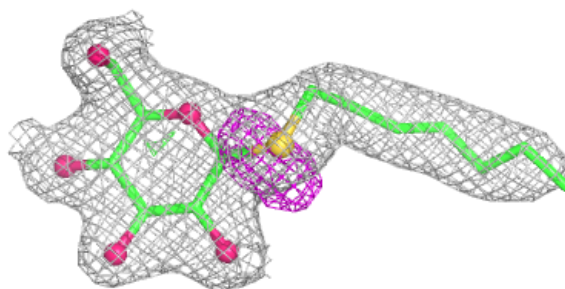
Electron density around HEM f 101:

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

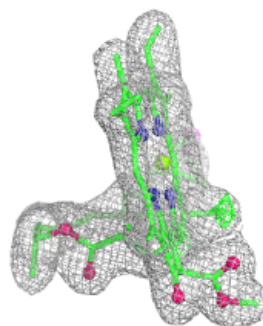
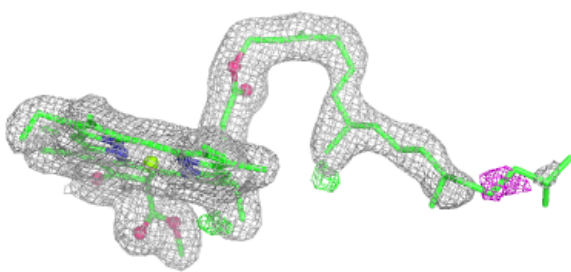
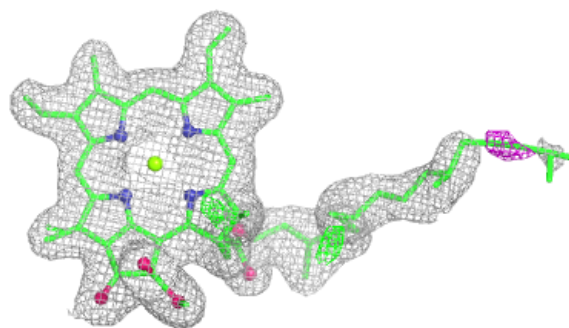


Electron density around HTG O 303:

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

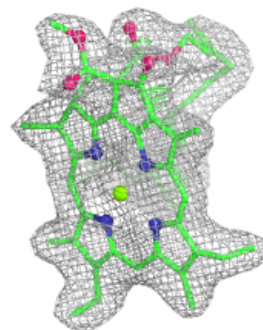
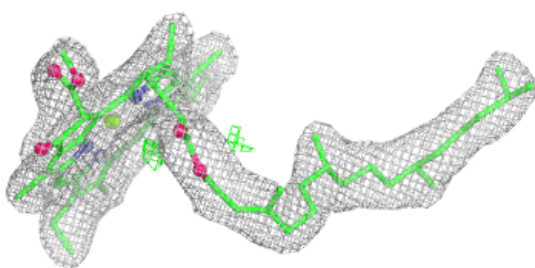
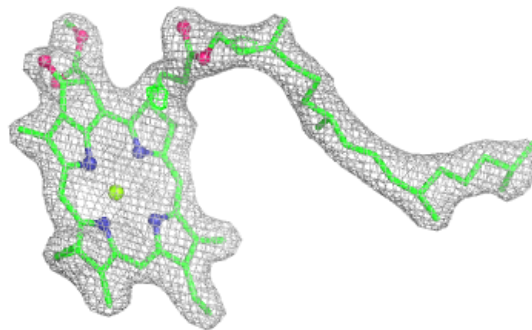
**Electron density around CLA A 407:**

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

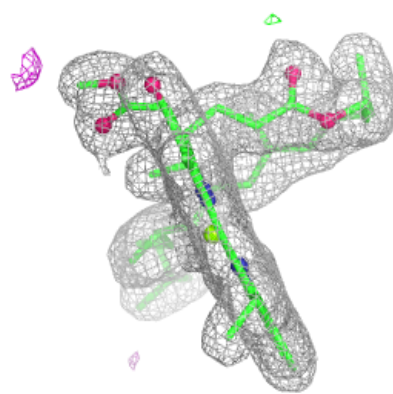
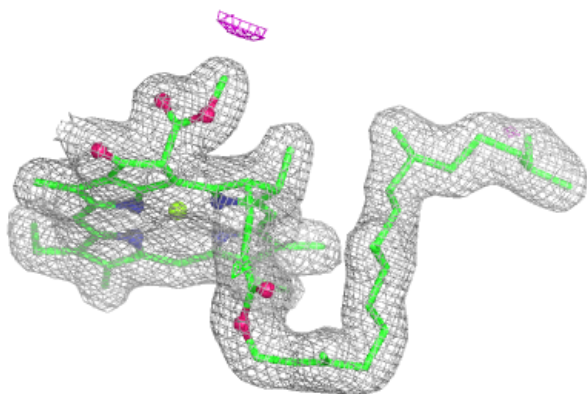
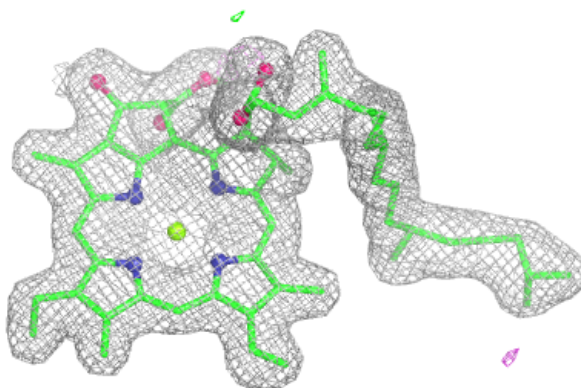


Electron density around CLA c 912:

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

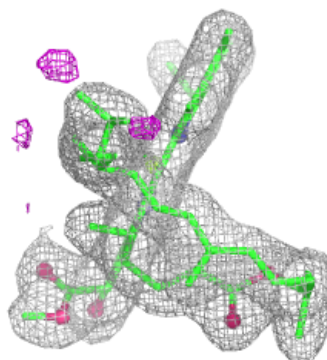
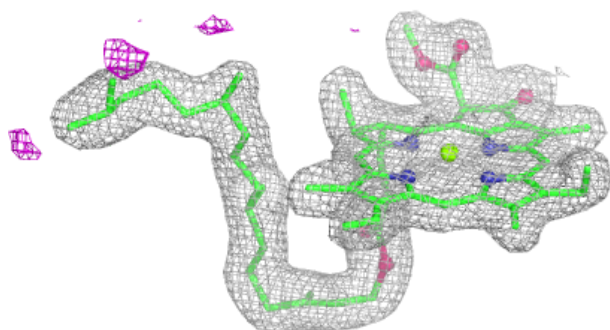
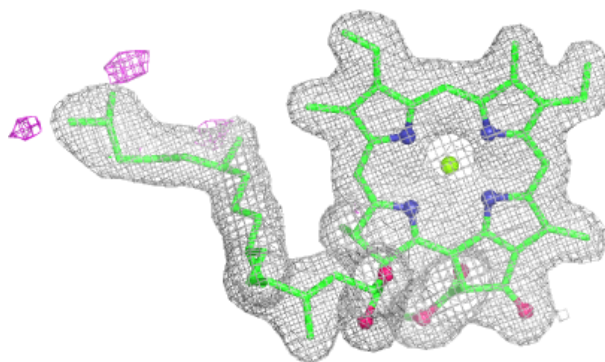
**Electron density around CLA A 406:**

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

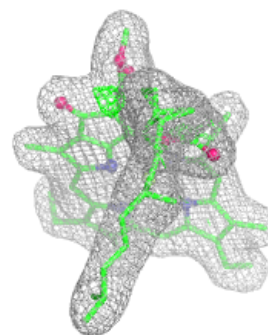
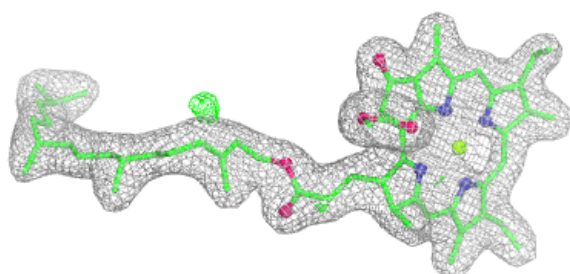
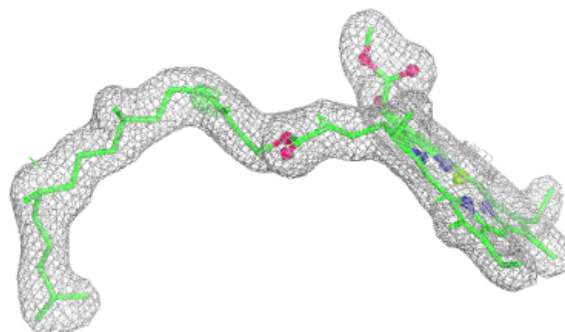


Electron density around CLA d 401:

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

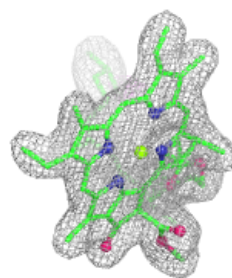
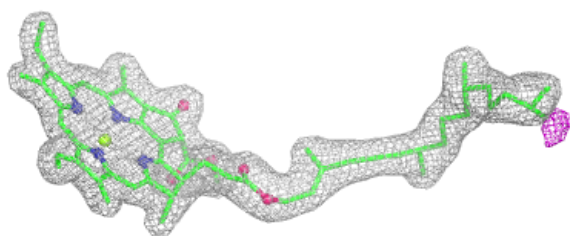
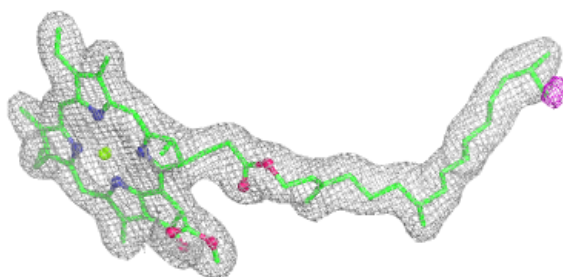
**Electron density around CLA d 404:**

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



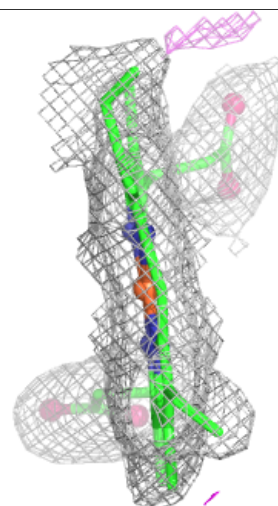
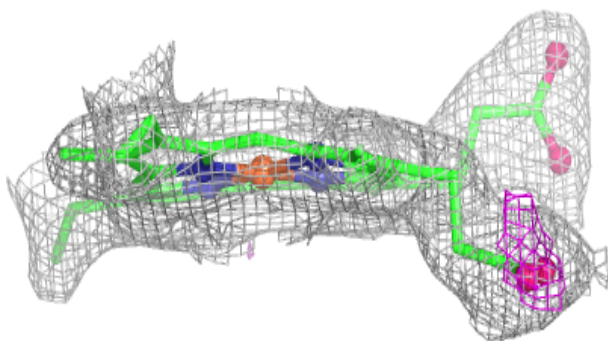
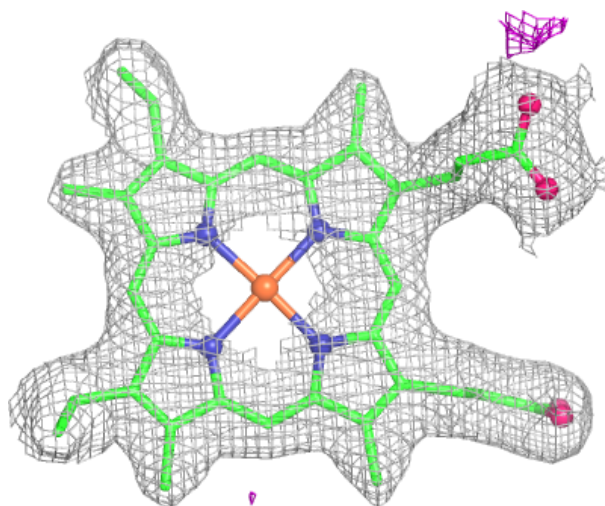
Electron density around CLA a 409:

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



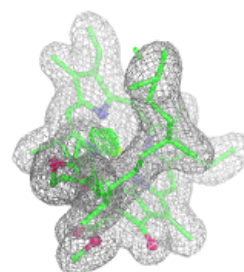
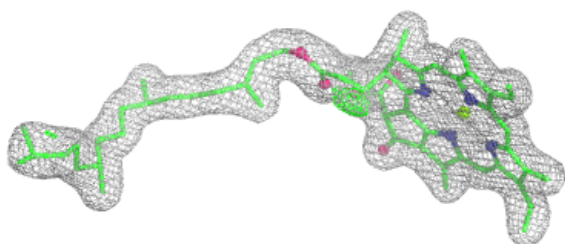
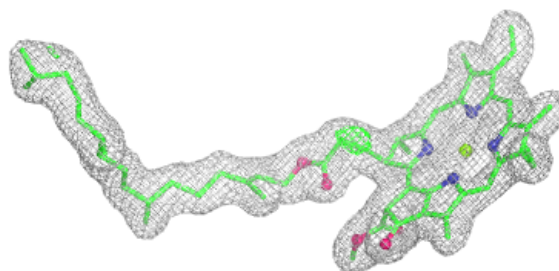
Electron density around HEM v 202:

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

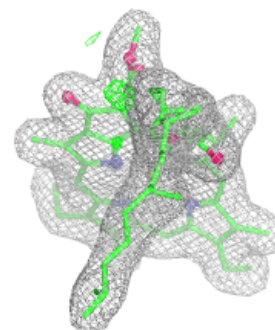
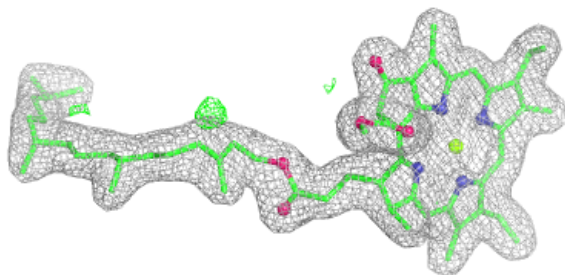
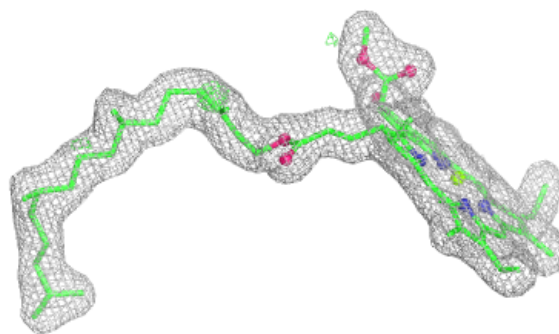


Electron density around CLA A 405:

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

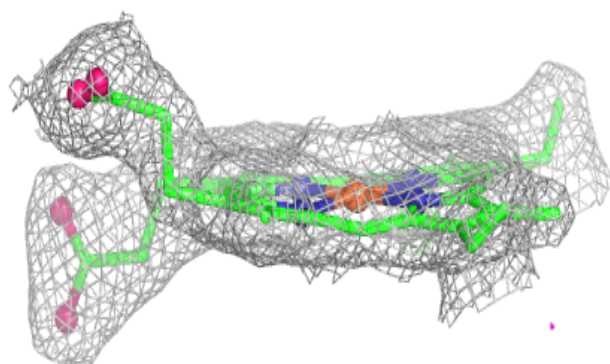
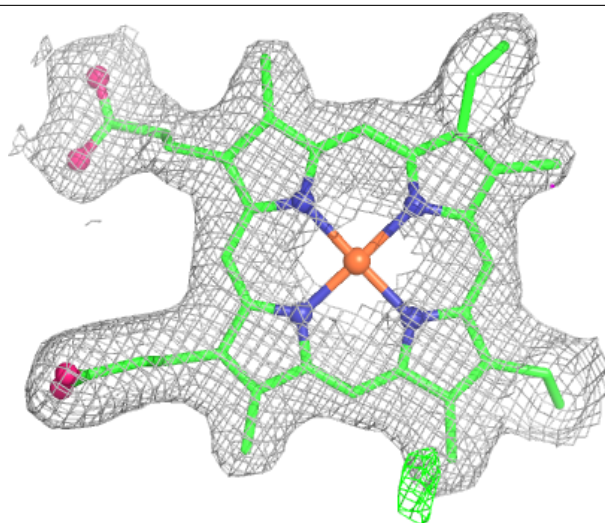
**Electron density around CLA D 402:**

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



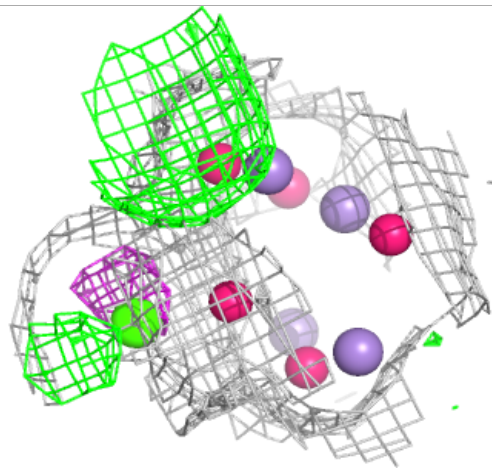
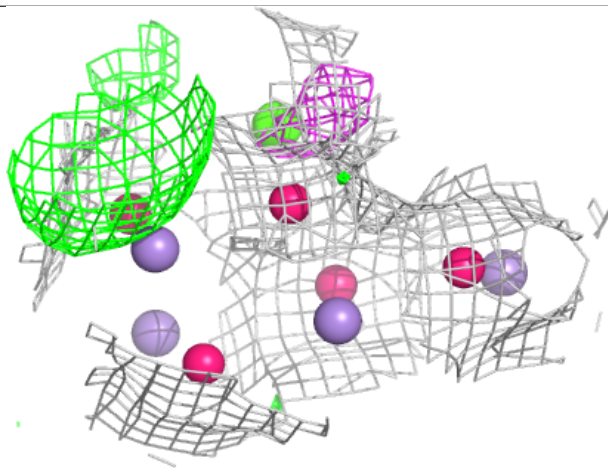
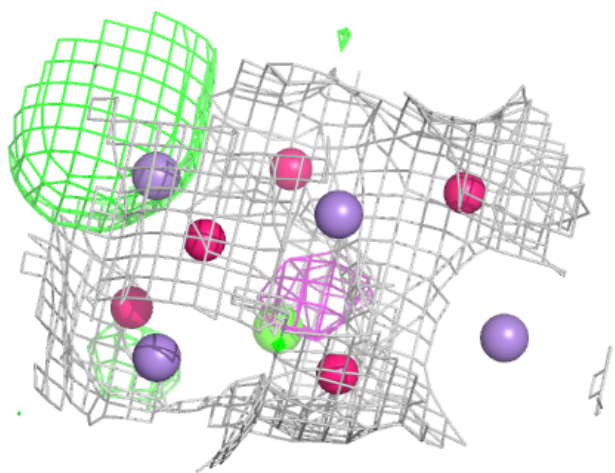
Electron density around HEM V 202:

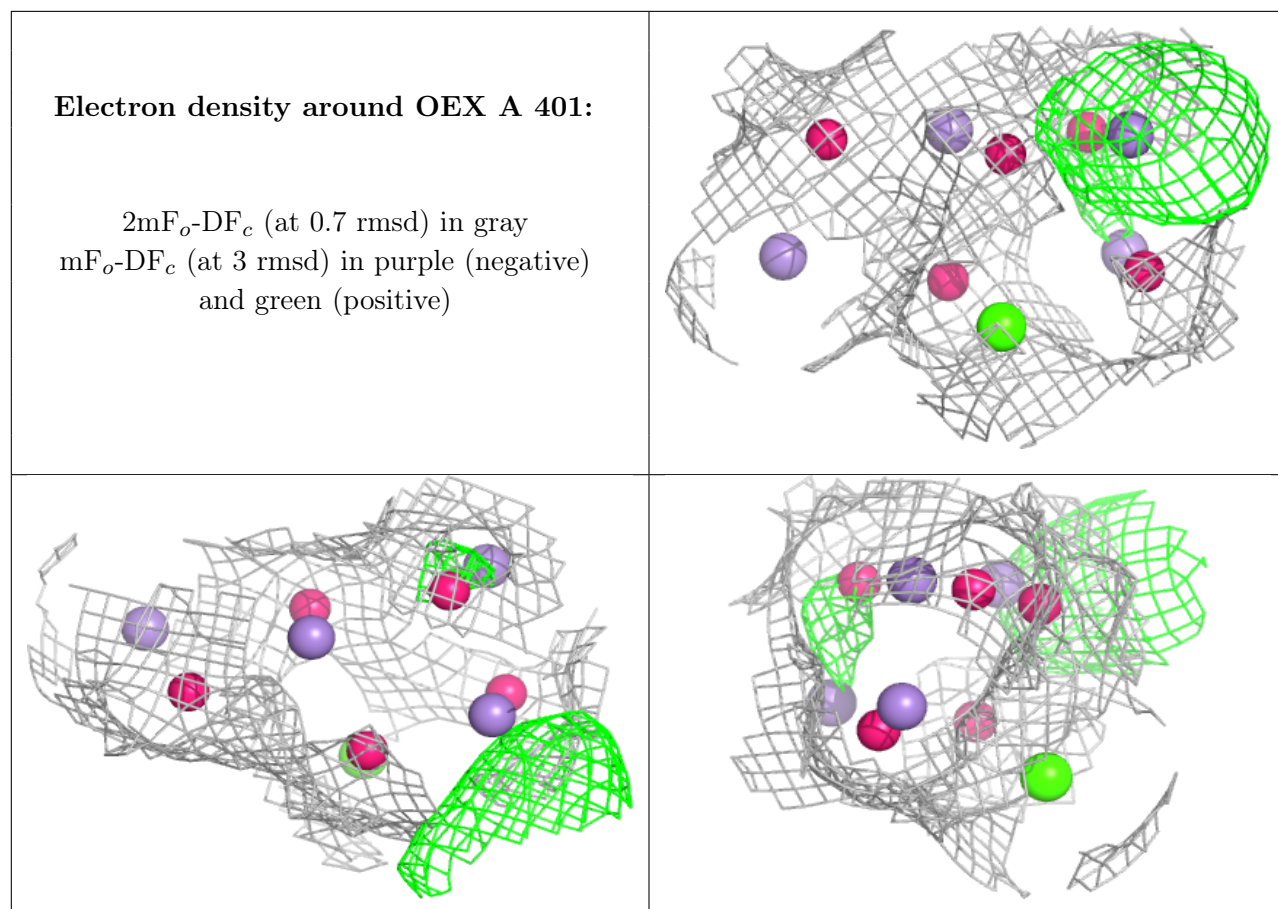
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around OEX a 404:

$2mF_o-DF_c$ (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.