



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 5, 2026 – 07:52 AM EDT

PDB ID : 4IL6 / pdb_00004il6
Title : Structure of Sr-substituted photosystem II
Authors : Koua, F.H.M.; Umena, Y.; Kawakami, K.; Kamiya, N.; Shen, J.R.
Deposited on : 2012-12-29
Resolution : 2.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

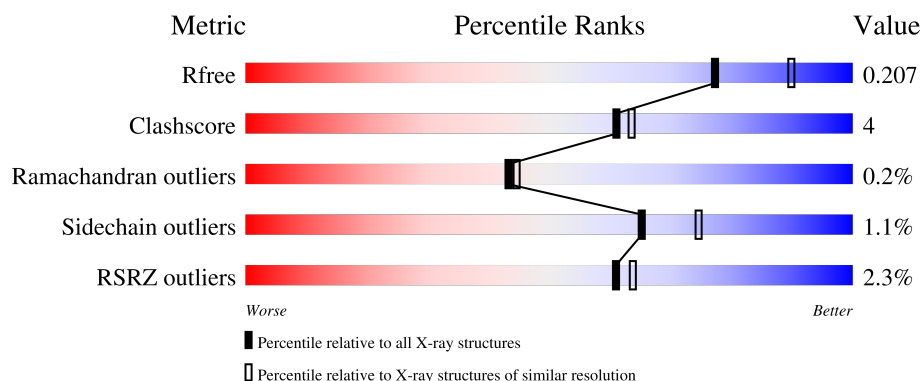
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

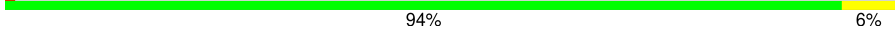
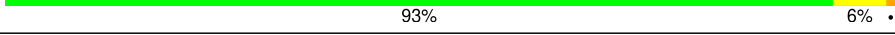
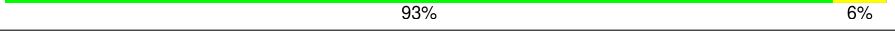
The reported resolution of this entry is 2.10 Å.

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.



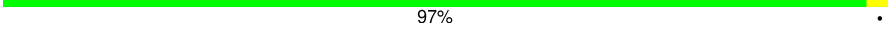
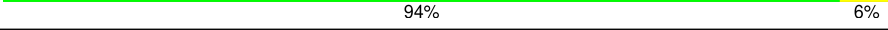
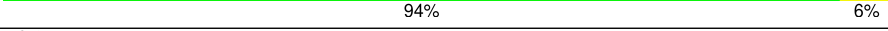
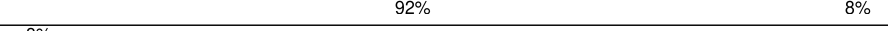
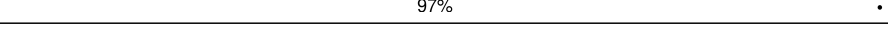
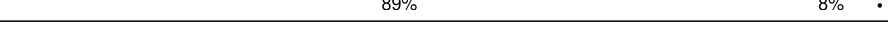
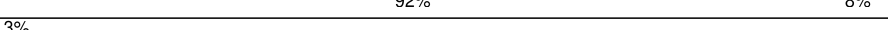
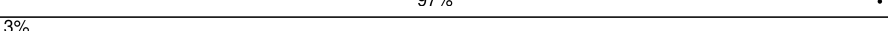
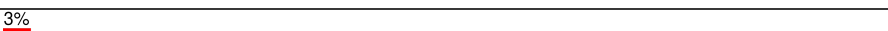
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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

Mol	Chain	Length	Quality of chain
1	A	334	 91% 9%
1	a	334	 92% 8%
2	B	505	 94% 6%
2	b	505	 93% 6% 3%
3	C	451	 93% 6%

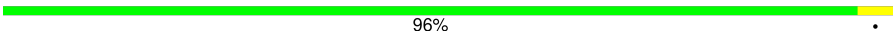
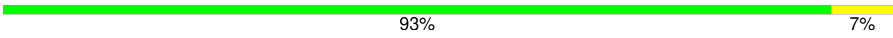
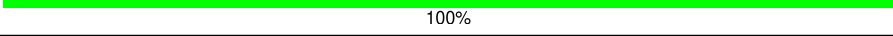
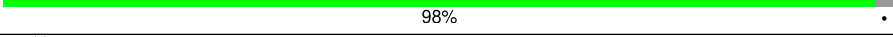
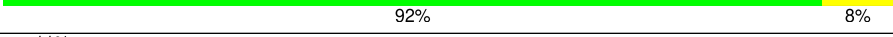
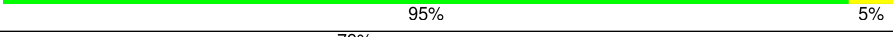
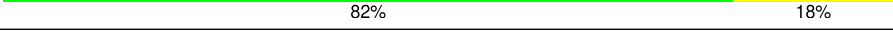
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Mol	Chain	Length	Quality of chain
3	c	451	 90% 9%
4	D	342	 90% 10%
4	d	342	 91% 9%
5	E	80	 84% 16% 8%
5	e	80	 85% 11% 2% ..
6	F	34	 97% .
6	f	34	 82% 12% 6% 6%
7	H	63	 92% 8% 2%
7	h	63	 94% 6% 2%
8	I	36	 94% 6% 3%
8	i	36	 86% 14% 6%
9	J	37	 92% 8% 8%
9	j	37	 97% . 8%
10	K	37	 89% 8% . 3%
10	k	37	 86% 11% . 3%
11	L	37	 92% 8% 3%
11	l	37	 97% . 3%
12	M	34	 79% 15% 6% 6%
12	m	34	 82% 18% 3%
13	O	244	 95% 5% 4%
13	o	244	 93% 6% 2%
14	T	31	 87% 6% 6% 6%
14	t	31	 90% 6% . 3%
15	U	97	 93% 7% 3%
15	u	97	 96% . 3%

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Mol	Chain	Length	Quality of chain
16	V	137	
16	v	137	
17	Y	30	
17	y	30	
18	X	40	
18	x	40	
19	Z	62	
19	z	62	
20	R	34	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	BCR	D	406	-	X	-	-
26	BCR	J	101	-	X	-	-
26	BCR	K	101	-	X	-	-
26	BCR	d	404	-	X	-	-
26	BCR	k	101	-	X	-	-
26	BCR	y	101	-	X	-	-

2 Entry composition [i](#)

There are 40 unique types of molecules in this entry. The entry contains 53568 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 Q(B) protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	5	0
			2643	1733	431	464	15			
1	a	334	Total	C	N	O	S	0	4	0
			2637	1729	431	462	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	279	PRO	ARG	SEE REMARK 999	UNP P51765
a	279	PRO	ARG	SEE REMARK 999	UNP P51765

- Molecule 2 is a protein called Photosystem II core light harvesting protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	505	Total	C	N	O	S	0	10	0
			4040	2652	674	701	13			
2	b	505	Total	C	N	O	S	0	9	0
			4033	2646	676	698	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	451	Total	C	N	O	S	0	3	0
			3500	2292	584	611	13			
3	c	450	Total	C	N	O	S	0	2	0
			3492	2287	583	609	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	342	Total	C	N	O	S	0	0	0
			2726	1805	445	464	12			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	d	342	Total	C	N	O	S	0	0	0
			2726	1805	445	464	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	80	Total	C	N	O		0	2	0
			660	431	105	124				
5	e	78	Total	C	N	O		0	0	0
			638	418	103	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
			275	187	45	42	1			
6	f	32	Total	C	N	O	S	0	0	0
			257	175	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	1	0
			506	338	83	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
			296	200	46	49	1			
8	i	36	Total	C	N	O	S	0	0	0
			296	200	46	49	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	37	Total	C	N	O	S	0	0	0
			266	179	41	45	1			
9	j	37	Total	C	N	O	S	0	0	0
			266	179	41	45	1			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	34	Total	C	N	O	S	0	1	0
			274	184	40	49	1			
12	m	34	Total	C	N	O	S	0	1	0
			274	184	40	49	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	244	Total	C	N	O	S	0	2	0
			1883	1176	317	386	4			
13	o	243	Total	C	N	O	S	0	1	0
			1868	1167	315	382	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	31	Total	C	N	O	S	0	0	0
			267	187	38	40	2			
14	t	30	Total	C	N	O	S	0	0	0
			258	181	36	39	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	U	97	Total	C	N	O	0	1	0
			780	495	129	156			
15	u	97	Total	C	N	O	0	1	0
			780	495	129	156			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total	C	N	O	S	0	3	0
			1081	687	179	211	4			
16	v	137	Total	C	N	O	S	0	2	0
			1076	683	177	212	4			

- Molecule 17 is a protein called Photosystem II reaction center protein ycf12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Y	30	Total	C	N	O	S	0	0	0
			224	147	38	36	3			
17	y	30	Total	C	N	O	S	0	0	0
			224	147	38	36	3			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	X	40	Total	C	N	O	0	0	0
			296	197	47	52			
18	x	39	Total	C	N	O	0	0	0
			287	191	46	50			

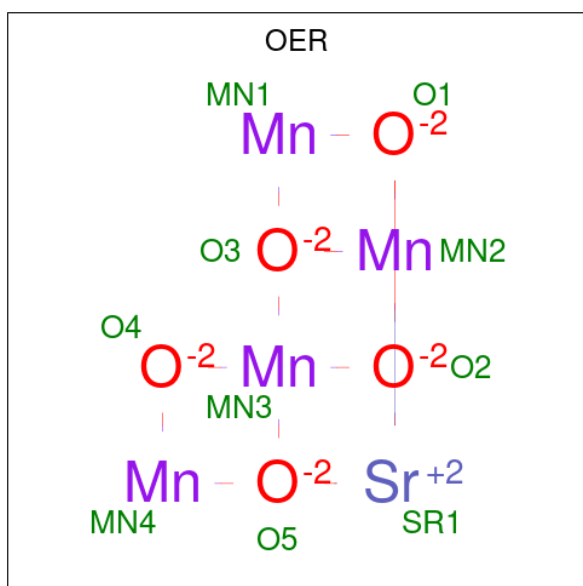
- Molecule 19 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Z	62	Total	C	N	O	S	0	0	0
			481	329	72	78	2			
19	z	62	Total	C	N	O	S	0	0	0
			481	329	72	78	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	R	34	Total	C	N	O	0	0	0
			273	186	47	40			

- Molecule 21 is SR-MN4-O5 CLUSTER (CCD ID: OER) (formula: $\text{Mn}_4\text{O}_5\text{Sr}$).



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

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

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

- Molecule 23 is 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: $\text{C}_{55}\text{H}_{72}\text{MgN}_4\text{O}_5$).



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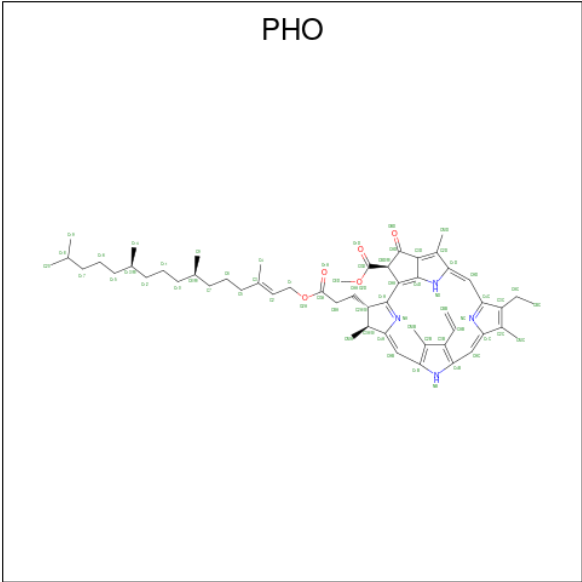
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N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

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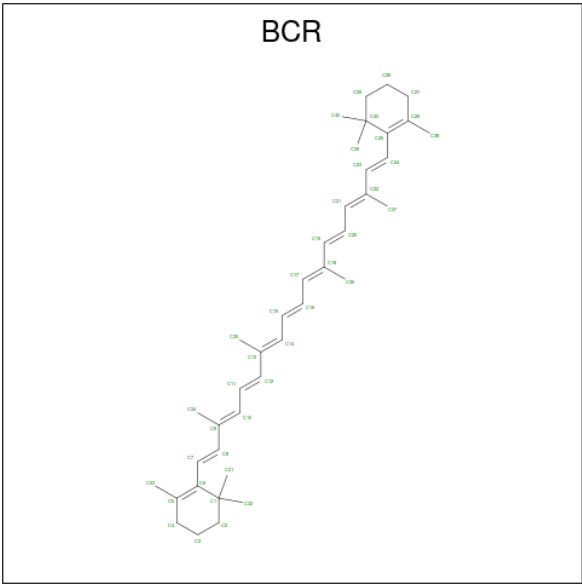
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total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

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



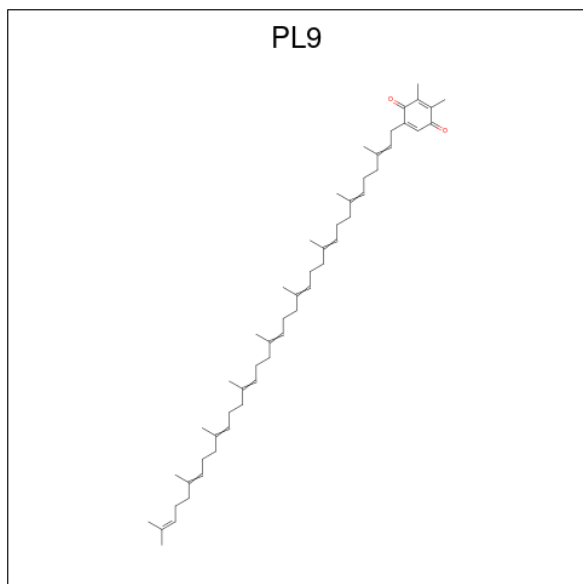
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	A	1	Total	C	N	O	0	0
			64	55	4	5		
25	D	1	Total	C	N	O	0	0
			64	55	4	5		
25	a	1	Total	C	N	O	0	0
			64	55	4	5		
25	a	1	Total	C	N	O	0	0
			64	55	4	5		

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



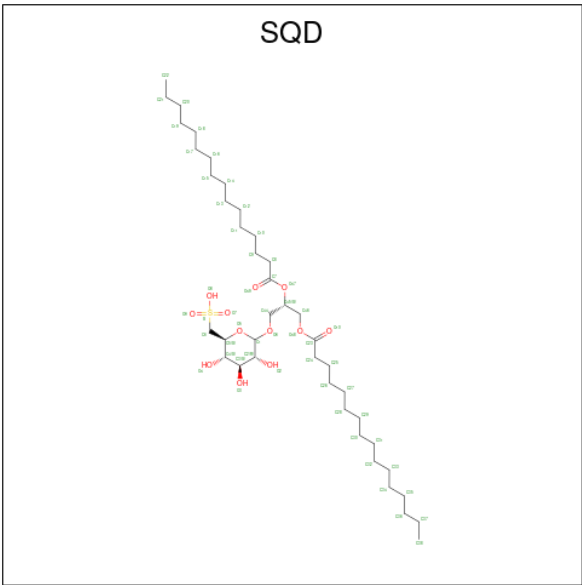
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	D	1	Total C 40 40	0	0
26	H	1	Total C 40 40	0	0
26	J	1	Total C 40 40	0	0
26	K	1	Total C 40 40	0	0
26	K	1	Total C 40 40	0	0
26	T	1	Total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

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



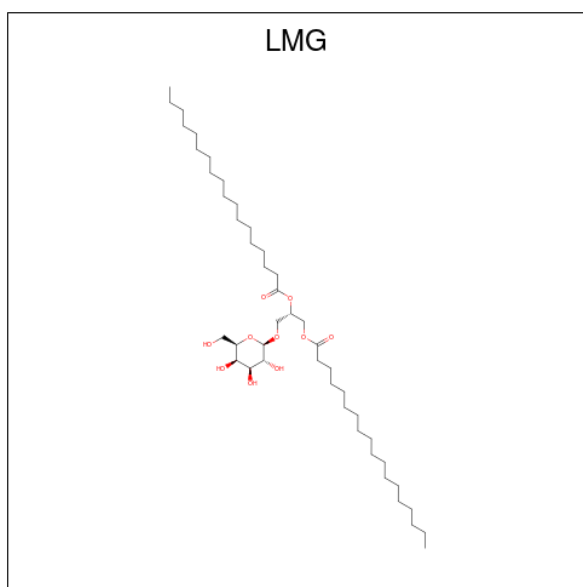
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	A	1	Total	C	O	0	0
			55	53	2		
27	D	1	Total	C	O	0	0
			55	53	2		
27	a	1	Total	C	O	0	0
			55	53	2		
27	d	1	Total	C	O	0	0
			55	53	2		

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



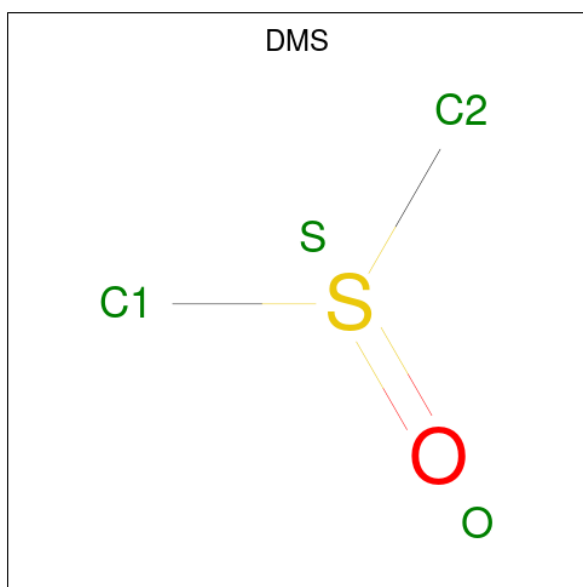
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	A	1	Total	C	O	S	0	0
			54	41	12	1		
28	A	1	Total	C	O	S	0	0
			54	41	12	1		
28	B	1	Total	C	O	S	0	1
			108	82	24	2		
28	D	1	Total	C	O	S	0	0
			43	30	12	1		
28	a	1	Total	C	O	S	0	0
			54	41	12	1		
28	b	1	Total	C	O	S	0	1
			108	82	24	2		
28	c	1	Total	C	O	S	0	0
			54	41	12	1		
28	f	1	Total	C	O	S	0	0
			43	30	12	1		

- Molecule 29 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	A	1	Total	C	O	0	0
			51	41	10		
29	B	1	Total	C	O	0	0
			51	41	10		
29	C	1	Total	C	O	0	0
			51	41	10		
29	C	1	Total	C	O	0	0
			51	41	10		
29	D	1	Total	C	O	0	0
			51	41	10		
29	Z	1	Total	C	O	0	0
			51	41	10		
29	a	1	Total	C	O	0	0
			51	41	10		
29	c	1	Total	C	O	0	0
			51	41	10		
29	c	1	Total	C	O	0	0
			51	41	10		
29	c	1	Total	C	O	0	0
			51	41	10		
29	d	1	Total	C	O	0	0
			51	41	10		
29	m	1	Total	C	O	0	0
			51	41	10		

- Molecule 30 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C₂H₆OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	A	1	Total	C	O	S	0	0
			4	2	1	1		
30	A	1	Total	C	O	S	0	0
			4	2	1	1		
30	B	1	Total	C	O	S	0	0
			4	2	1	1		
30	B	1	Total	C	O	S	0	0
			4	2	1	1		
30	B	1	Total	C	O	S	0	0
			4	2	1	1		
30	B	1	Total	C	O	S	0	0
			4	2	1	1		
30	C	1	Total	C	O	S	0	0
			4	2	1	1		
30	C	1	Total	C	O	S	0	0
			4	2	1	1		
30	C	1	Total	C	O	S	0	0
			4	2	1	1		
30	C	1	Total	C	O	S	0	0
			4	2	1	1		
30	D	1	Total	C	O	S	0	0
			4	2	1	1		
30	D	1	Total	C	O	S	0	0
			4	2	1	1		

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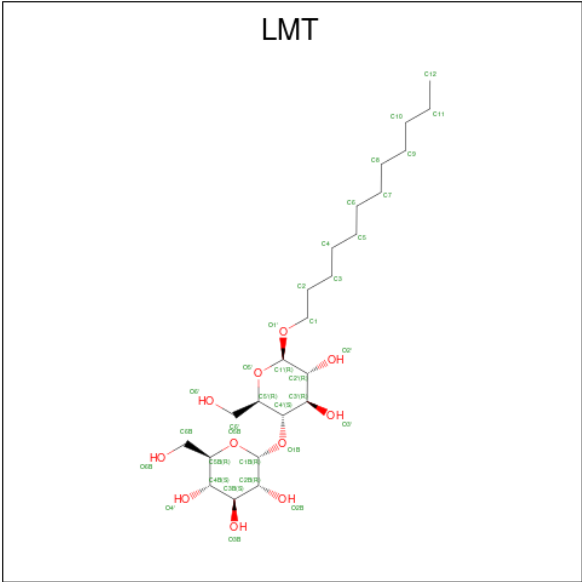
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	O	1	Total 4	C 2	O 1	S 1	0	0
30	O	1	Total 4	C 2	O 1	S 1	0	0
30	U	1	Total 4	C 2	O 1	S 1	0	0
30	V	1	Total 4	C 2	O 1	S 1	0	0
30	V	1	Total 4	C 2	O 1	S 1	0	0
30	a	1	Total 4	C 2	O 1	S 1	0	0
30	a	1	Total 4	C 2	O 1	S 1	0	0
30	b	1	Total 4	C 2	O 1	S 1	0	0
30	b	1	Total 4	C 2	O 1	S 1	0	0
30	b	1	Total 4	C 2	O 1	S 1	0	0
30	b	1	Total 4	C 2	O 1	S 1	0	0
30	b	1	Total 4	C 2	O 1	S 1	0	0
30	c	1	Total 4	C 2	O 1	S 1	0	0
30	c	1	Total 4	C 2	O 1	S 1	0	0
30	c	1	Total 4	C 2	O 1	S 1	0	0
30	c	1	Total 4	C 2	O 1	S 1	0	0
30	c	1	Total 4	C 2	O 1	S 1	0	0
30	d	1	Total 4	C 2	O 1	S 1	0	0
30	d	1	Total 4	C 2	O 1	S 1	0	0
30	u	1	Total 4	C 2	O 1	S 1	0	0
30	v	1	Total 4	C 2	O 1	S 1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	A	1	Total C O 28 23 5	0	0
31	B	2	Total C 32 32	0	0
31	D	2	Total C O 56 51 5	0	0
31	I	2	Total C 26 26	0	0
31	J	1	Total C 16 16	0	0
31	K	1	Total C O 34 29 5	0	0
31	L	1	Total C 16 16	0	0
31	Y	1	Total C 16 16	0	0
31	X	1	Total C 16 16	0	0
31	a	1	Total C O 30 25 5	0	0
31	b	2	Total C 32 32	0	0
31	c	1	Total C O 32 27 5	0	0
31	d	2	Total C O 52 47 5	0	0
31	i	1	Total C 16 16	0	0
31	j	1	Total C 16 16	0	0
31	l	1	Total C 16 16	0	0
31	t	1	Total C 16 16	0	0
31	y	1	Total C 16 16	0	0
31	x	1	Total C 16 16	0	0

- Molecule 32 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



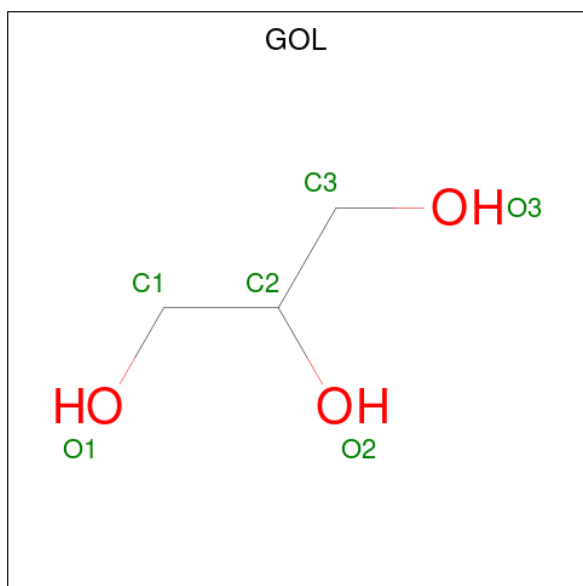
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	A	1	Total	C	O	0	0
			35	24	11		
32	A	1	Total	C	O	0	0
			35	24	11		
32	B	1	Total	C	O	0	0
			35	24	11		
32	C	1	Total	C	O	0	0
			35	24	11		
32	M	1	Total	C	O	0	0
			35	24	11		
32	M	1	Total	C	O	0	0
			35	24	11		
32	a	1	Total	C	O	0	0
			35	24	11		
32	a	1	Total	C	O	0	0
			35	24	11		
32	b	1	Total	C	O	0	0
			35	24	11		
32	b	1	Total	C	O	0	0
			35	24	11		
32	f	1	Total	C	O	0	0
			35	24	11		
32	i	1	Total	C	O	0	0
			35	24	11		
32	m	1	Total	C	O	0	0
			35	24	11		
32	m	1	Total	C	O	0	0
			35	24	11		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	t	1	Total	C	O	0	0
			35	24	11		

- Molecule 33 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



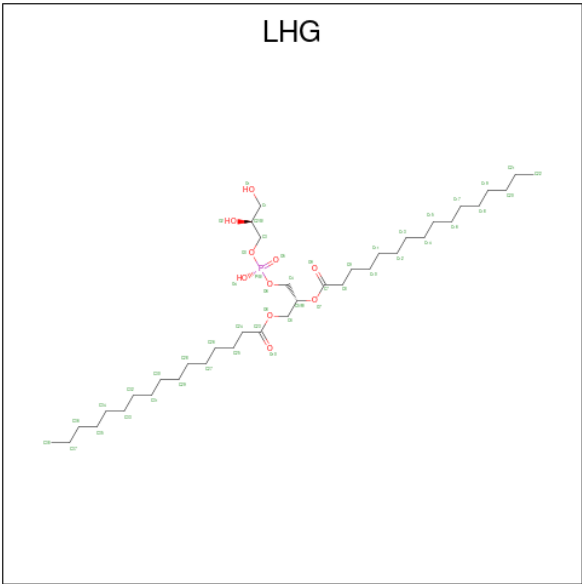
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	A	1	Total	C	O	0	0
			6	3	3		
33	B	1	Total	C	O	0	0
			6	3	3		
33	D	1	Total	C	O	0	0
			6	3	3		
33	V	1	Total	C	O	0	0
			6	3	3		
33	V	1	Total	C	O	0	0
			6	3	3		
33	V	1	Total	C	O	0	0
			6	3	3		
33	a	1	Total	C	O	0	0
			6	3	3		
33	b	1	Total	C	O	0	0
			6	3	3		
33	d	1	Total	C	O	0	0
			6	3	3		
33	d	1	Total	C	O	0	0
			6	3	3		

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

- Molecule 34 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



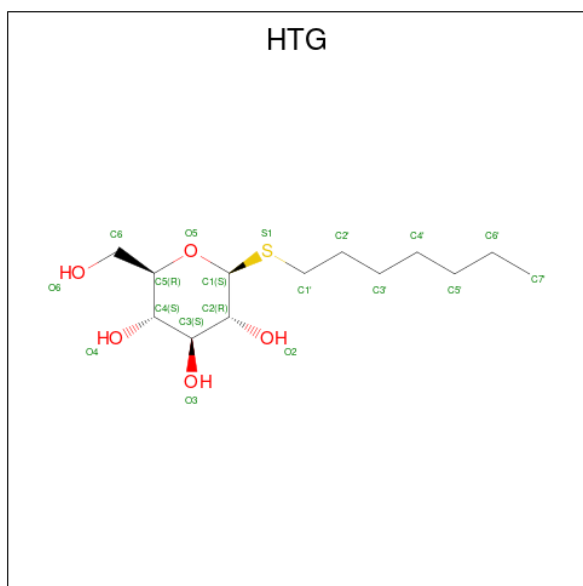
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	B	1	Total	C	O	P	0	0
			49	38	10	1		
34	D	1	Total	C	O	P	0	0
			49	38	10	1		
34	D	1	Total	C	O	P	0	0
			49	38	10	1		
34	D	1	Total	C	O	P	0	0
			49	38	10	1		
34	E	1	Total	C	O	P	0	0
			49	38	10	1		
34	b	1	Total	C	O	P	0	0
			49	38	10	1		
34	d	1	Total	C	O	P	0	0
			49	38	10	1		
34	d	1	Total	C	O	P	0	0
			49	38	10	1		
34	d	1	Total	C	O	P	0	0
			49	38	10	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	e	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 35 is heptyl 1-thio-beta-D-glucopyranoside (CCD ID: HTG) (formula: C₁₃H₂₆O₅S).



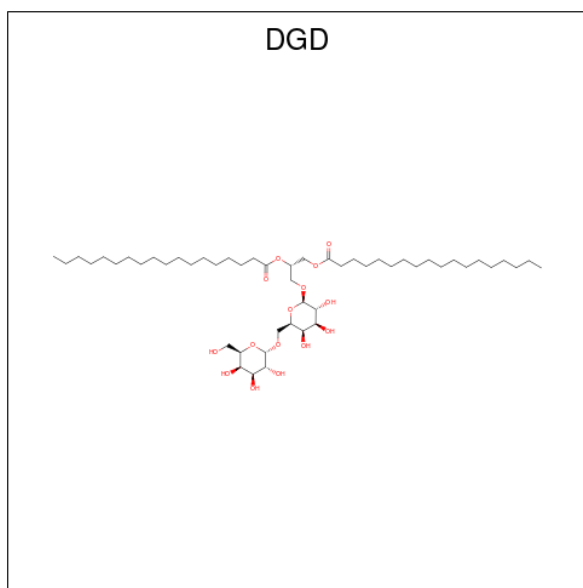
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	C	1	Total	C	O	S	0	0
			19	13	5	1		
35	C	1	Total	C	O	S	0	0
			19	13	5	1		
35	D	1	Total	C	O	S	0	0
			19	13	5	1		
35	D	1	Total	C	O	S	0	0
			19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

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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	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	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		

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



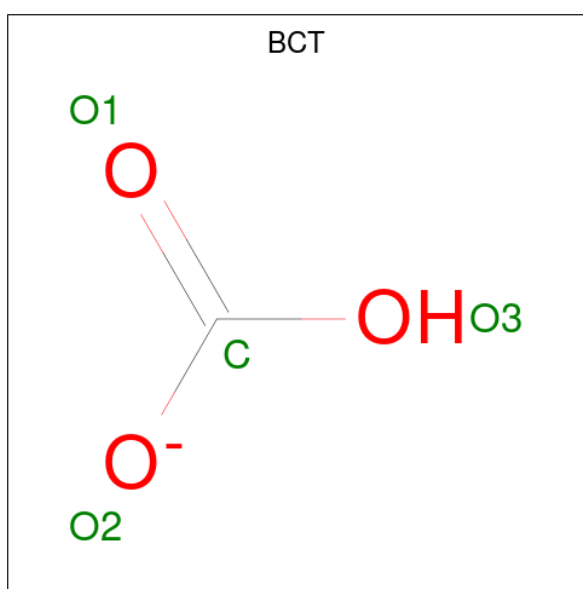
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
36	C	1	Total	C	O	0	0
			62	47	15		
36	C	1	Total	C	O	0	0
			62	47	15		
36	C	1	Total	C	O	0	0
			62	47	15		
36	H	1	Total	C	O	0	0
			62	47	15		

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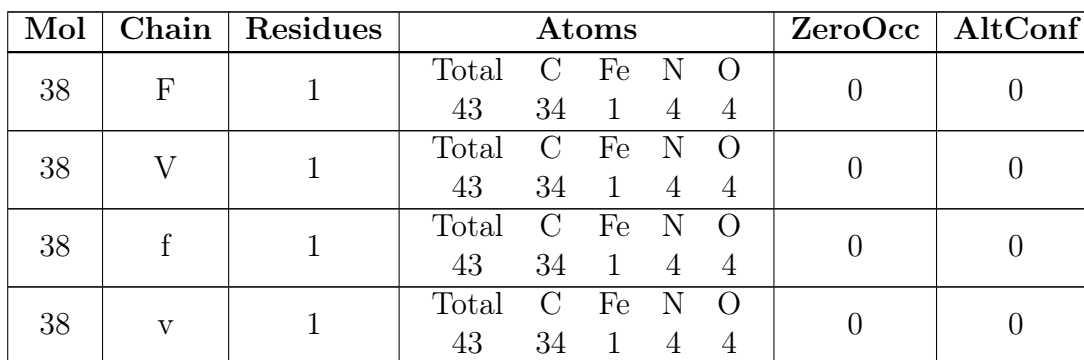
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
36	c	1	Total	C	O	0	0
			62	47	15		
36	c	1	Total	C	O	0	0
			62	47	15		
36	c	1	Total	C	O	0	0
			62	47	15		
36	h	1	Total	C	O	0	0
			62	47	15		

- Molecule 37 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
37	D	1	Total	C	O	0	0
			4	1	3		
37	d	1	Total	C	O	0	0
			4	1	3		

- Molecule 38 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4$).



- | Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 39 | J | 1 | Total Mg
1 1 | 0 | 0 |
| 39 | K | 1 | Total Mg
1 1 | 0 | 0 |
| 39 | j | 1 | Total Mg
1 1 | 0 | 0 |
| 39 | k | 1 | Total Mg
1 1 | 0 | 0 |

- | Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 40 | A | 134 | Total O
134 134 | 0 | 0 |



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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	B	252	Total 253	O 253	0	1
40	C	168	Total 168	O 168	0	0
40	D	132	Total 132	O 132	0	0
40	E	22	Total 22	O 22	0	0
40	F	6	Total 6	O 6	0	0
40	H	31	Total 31	O 31	0	0
40	I	4	Total 4	O 4	0	0
40	J	7	Total 7	O 7	0	0
40	K	7	Total 7	O 7	0	0
40	L	11	Total 11	O 11	0	0
40	M	6	Total 6	O 6	0	0
40	O	119	Total 119	O 119	0	0
40	T	10	Total 10	O 10	0	0
40	U	63	Total 63	O 63	0	0
40	V	96	Total 96	O 96	0	0
40	Y	1	Total 1	O 1	0	0
40	X	8	Total 8	O 8	0	0
40	Z	1	Total 1	O 1	0	0
40	R	1	Total 1	O 1	0	0
40	a	118	Total 118	O 118	0	0
40	b	209	Total 209	O 209	0	0

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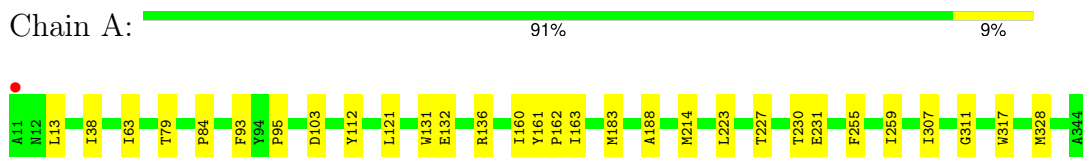
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	c	169	Total 169	O 169	0	0
40	d	121	Total 121	O 121	0	0
40	e	9	Total 9	O 9	0	0
40	f	5	Total 5	O 5	0	0
40	h	23	Total 23	O 23	0	0
40	i	4	Total 4	O 4	0	0
40	j	5	Total 5	O 5	0	0
40	k	3	Total 3	O 3	0	0
40	l	8	Total 8	O 8	0	0
40	m	10	Total 10	O 10	0	0
40	o	112	Total 112	O 112	0	0
40	t	13	Total 13	O 13	0	0
40	u	74	Total 74	O 74	0	0
40	v	65	Total 65	O 65	0	0
40	y	1	Total 1	O 1	0	0
40	x	9	Total 9	O 9	0	0

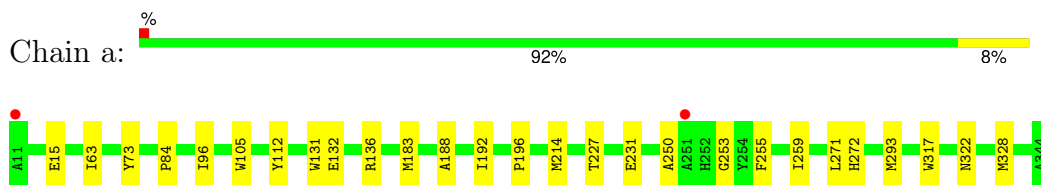
3 Residue-property plots

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

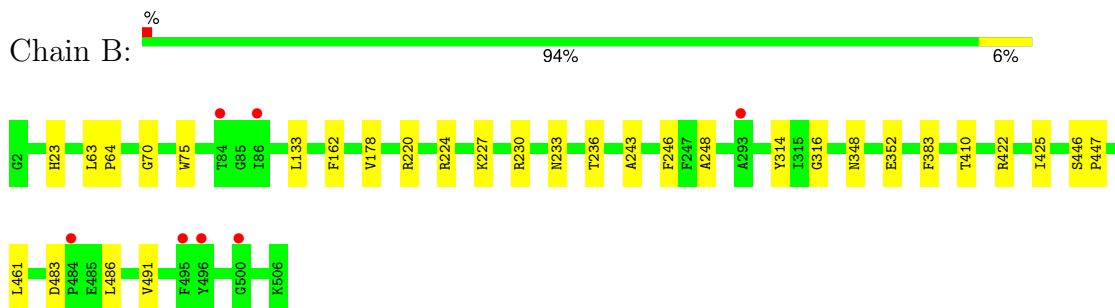
- Molecule 1: Photosystem Q(B) protein



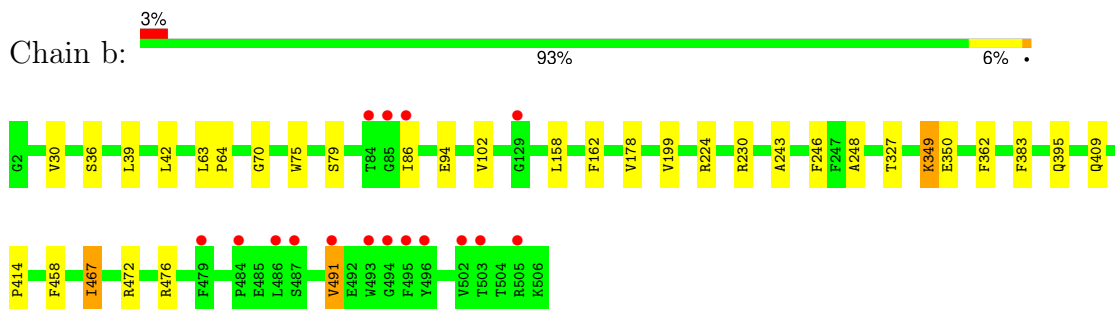
- Molecule 1: Photosystem Q(B) protein



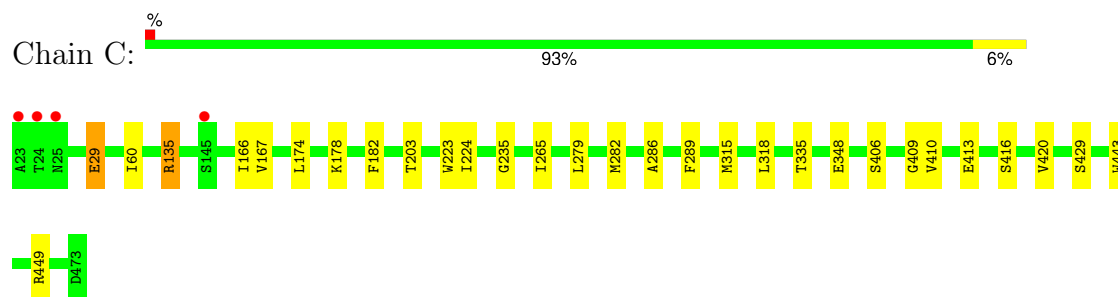
- Molecule 2: Photosystem II core light harvesting protein



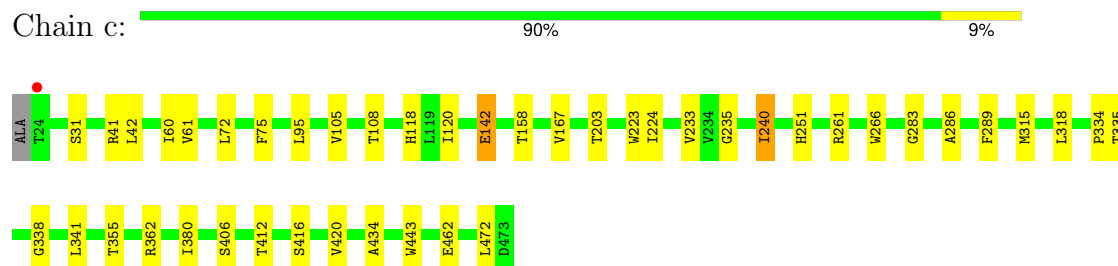
- Molecule 2: Photosystem II core light harvesting protein



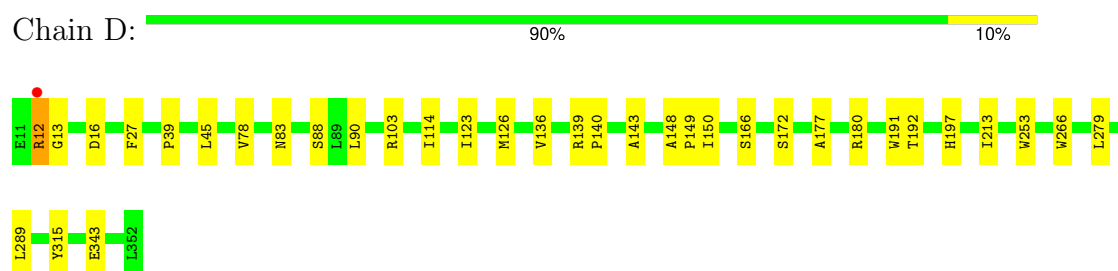
- Molecule 3: Photosystem II CP43 protein



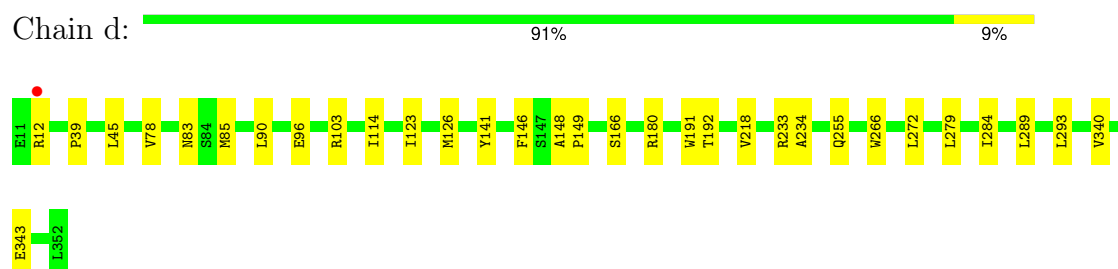
- Molecule 3: Photosystem II CP43 protein



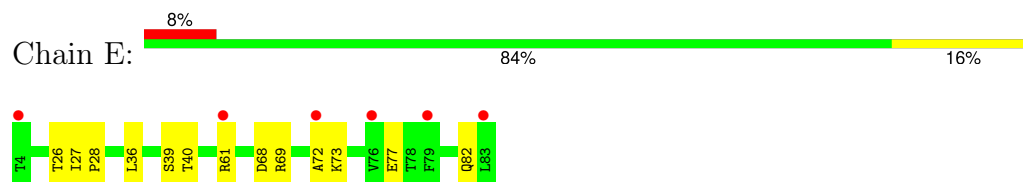
- Molecule 4: Photosystem II D2 protein



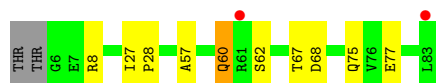
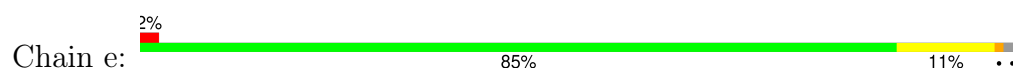
- Molecule 4: Photosystem II D2 protein



- Molecule 5: Cytochrome b559 subunit alpha



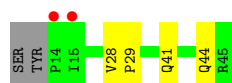
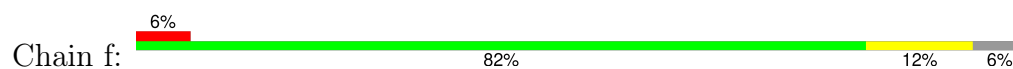
- Molecule 5: Cytochrome b559 subunit alpha



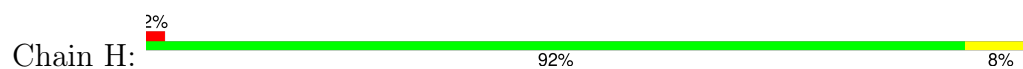
- Molecule 6: Cytochrome b559 subunit beta



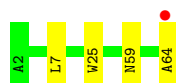
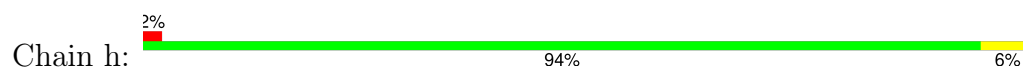
- Molecule 6: Cytochrome b559 subunit beta



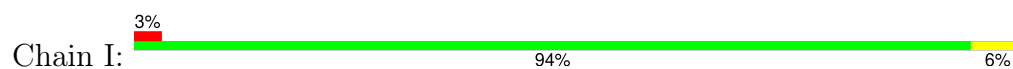
- Molecule 7: Photosystem II reaction center protein H



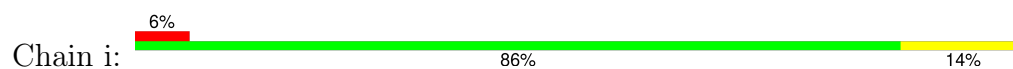
- Molecule 7: Photosystem II reaction center protein H



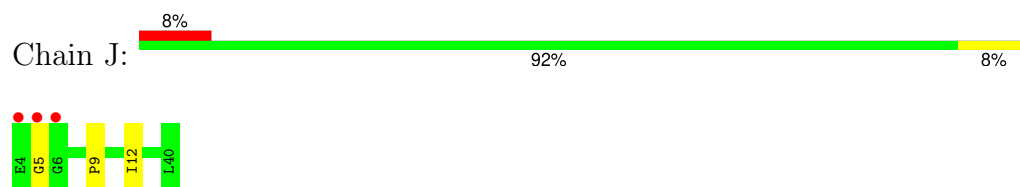
- Molecule 8: Photosystem II reaction center protein I



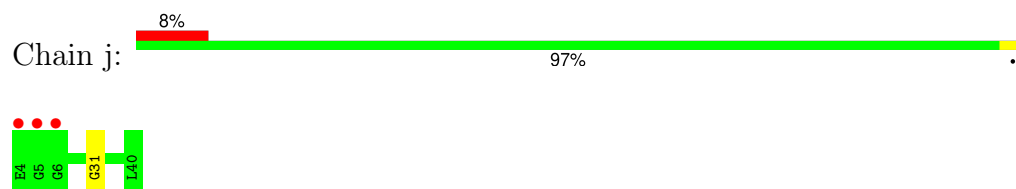
- Molecule 8: Photosystem II reaction center protein I



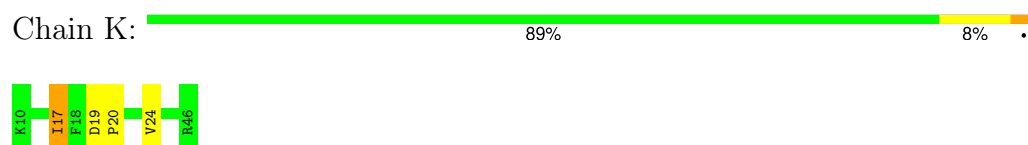
- Molecule 9: Photosystem II reaction center protein J



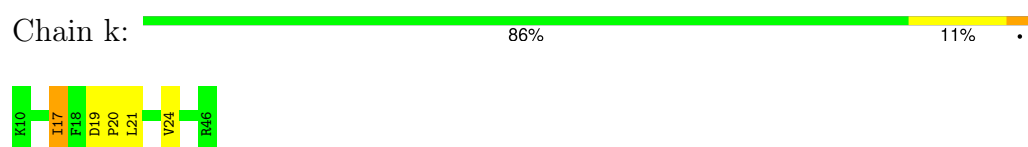
- Molecule 9: Photosystem II reaction center protein J



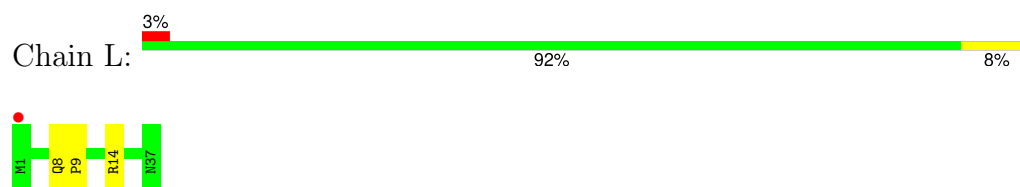
- Molecule 10: Photosystem II reaction center protein K



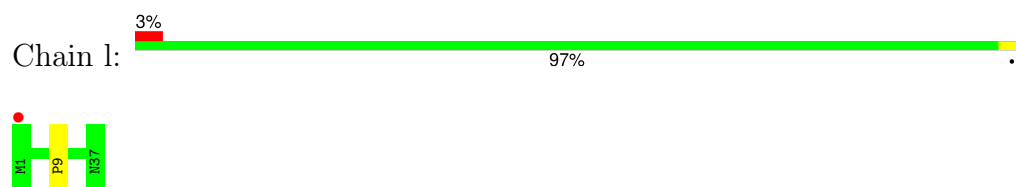
- Molecule 10: Photosystem II reaction center protein K



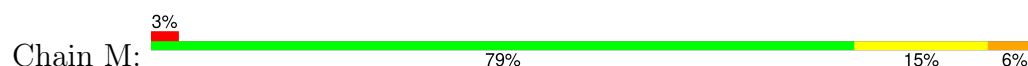
- Molecule 11: Photosystem II reaction center protein L



- Molecule 11: Photosystem II reaction center protein L



- Molecule 12: Photosystem II reaction center protein M





- Molecule 12: Photosystem II reaction center protein M

Chain m: 82% 18%



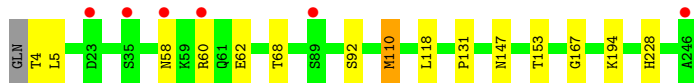
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O: 4% 95% 5%



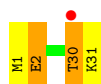
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o: 2% 93% 6%



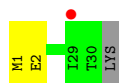
- Molecule 14: Photosystem II reaction center protein T

Chain T: 3% 87% 6% 6%



- Molecule 14: Photosystem II reaction center protein T

Chain t: 3% 90% 6% .

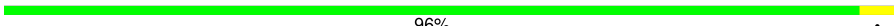


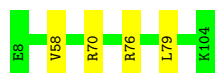
- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U: 93% 7%

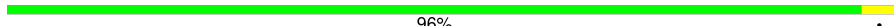


- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u:  96% .



- Molecule 16: Cytochrome c-550

Chain V:  96% .



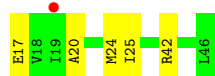
- Molecule 16: Cytochrome c-550

Chain v:  93% 7% .



- Molecule 17: Photosystem II reaction center protein ycf12

Chain Y:  3% 83% 17% .



- Molecule 17: Photosystem II reaction center protein ycf12

Chain y:  87% 7% 7% .

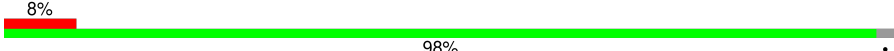


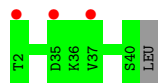
- Molecule 18: Photosystem II reaction center protein X

Chain X:  5% 100% .

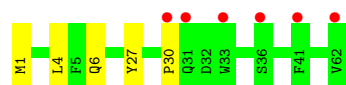
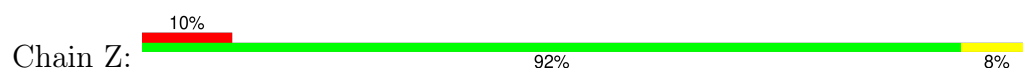


- Molecule 18: Photosystem II reaction center protein X

Chain x:  8% 98% .



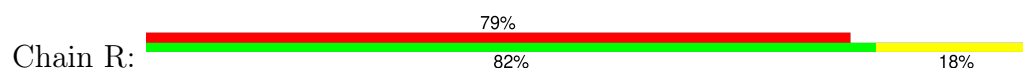
- Molecule 19: Photosystem II reaction center protein Z



• Molecule 19: Photosystem II reaction center protein Z



• Molecule 20: Photosystem II protein Y



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	121.86Å 228.79Å 285.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.96 – 2.10 19.96 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.96-2.10) 99.8 (19.96-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.14 (at 2.09Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.176 , 0.205 0.177 , 0.207	Depositor DCC
R_{free} test set	23034 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	31.9	Xtriage
Anisotropy	0.137	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 41.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	53568	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.77% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.69	0/2743	0.80	0/3740
1	a	0.68	0/2734	0.81	0/3728
2	B	0.67	0/4210	0.77	0/5731
2	b	0.67	0/4200	0.77	1/5719 (0.0%)
3	C	0.67	0/3622	0.79	0/4931
3	c	0.66	0/3611	0.79	0/4916
4	D	0.67	0/2821	0.79	0/3844
4	d	0.66	0/2821	0.79	0/3844
5	E	0.59	0/685	0.81	0/936
5	e	0.56	0/657	0.77	0/897
6	F	0.69	0/284	0.76	0/387
6	f	0.67	0/265	0.82	0/360
7	H	0.60	0/522	0.76	0/712
7	h	0.60	0/511	0.77	0/697
8	I	0.43	0/293	0.74	0/396
8	i	0.42	0/293	0.74	0/396
9	J	0.57	0/272	0.86	0/368
9	j	0.52	0/272	0.82	0/368
10	K	0.58	0/303	0.80	0/416
10	k	0.58	0/303	0.85	0/416
11	L	0.46	0/311	0.71	0/422
11	l	0.44	0/311	0.78	0/422
12	M	0.40	0/270	0.85	0/368
12	m	0.45	0/270	0.77	0/368
13	O	0.48	0/1920	0.71	0/2603
13	o	0.46	0/1902	0.70	0/2579
14	T	0.45	0/266	0.73	0/360
14	t	0.43	0/257	0.73	0/349
15	U	0.50	0/794	0.71	0/1076
15	u	0.48	0/794	0.74	0/1076
16	V	0.56	0/1111	0.74	0/1507

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.57	0/1103	0.79	1/1497 (0.1%)
17	Y	0.48	0/225	0.88	0/301
17	y	0.44	0/225	0.87	0/301
18	X	0.39	0/299	0.76	0/403
18	x	0.44	0/290	0.80	0/392
19	Z	0.51	0/482	0.86	0/659
19	z	0.51	0/482	0.88	0/659
20	R	0.66	0/279	0.87	0/383
All	All	0.62	0/43013	0.78	2/58527 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	414	PRO	N-CA-C	5.30	117.17	110.70
16	v	105	ARG	N-CA-C	5.29	117.04	111.28

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	2643	0	2550	23	0
1	a	2637	0	2544	22	0
2	B	4040	0	3928	25	0
2	b	4033	0	3921	30	0
3	C	3500	0	3429	23	0
3	c	3492	0	3419	26	0
4	D	2726	0	2627	27	0
4	d	2726	0	2627	27	0
5	E	660	0	644	9	0
5	e	638	0	621	6	0
6	F	275	0	282	1	0
6	f	257	0	269	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	H	506	0	531	3	0
7	h	498	0	518	3	0
8	I	296	0	311	2	0
8	i	296	0	311	4	0
9	J	266	0	274	1	0
9	j	266	0	274	1	0
10	K	293	0	305	4	0
10	k	293	0	305	4	0
11	L	304	0	316	4	0
11	l	304	0	316	1	0
12	M	274	0	299	6	0
12	m	274	0	299	6	0
13	O	1883	0	1857	8	0
13	o	1868	0	1843	8	0
14	T	267	0	274	2	0
14	t	258	0	261	1	0
15	U	780	0	779	3	0
15	u	780	0	779	2	0
16	V	1081	0	1100	9	0
16	v	1076	0	1087	11	0
17	Y	224	0	252	4	0
17	y	224	0	252	4	0
18	X	296	0	328	0	0
18	x	287	0	317	0	0
19	Z	481	0	515	1	0
19	z	481	0	515	0	0
20	R	273	0	305	4	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	195	0	216	9	0
24	B	1040	0	1152	17	0
24	C	845	0	936	28	0
24	D	195	0	216	6	0
24	a	260	0	288	8	0
24	b	1040	0	1152	22	0
24	c	845	0	936	21	0
24	d	130	0	144	3	0
25	A	64	0	74	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	D	64	0	74	5	0
25	a	128	0	148	3	0
26	A	40	0	48	0	0
26	B	120	0	140	2	0
26	C	40	0	46	2	0
26	D	40	0	46	1	0
26	H	40	0	46	0	0
26	J	40	0	48	1	0
26	K	80	0	95	0	0
26	T	40	0	47	0	0
26	a	40	0	46	0	0
26	b	120	0	141	4	0
26	c	40	0	47	3	0
26	d	40	0	47	1	0
26	h	40	0	48	0	0
26	k	80	0	94	2	0
26	t	40	0	47	0	0
26	y	40	0	46	1	0
27	A	55	0	80	5	0
27	D	55	0	80	0	0
27	a	55	0	80	5	0
27	d	55	0	80	0	0
28	A	108	0	156	3	0
28	B	108	0	156	21	0
28	D	43	0	53	1	0
28	a	54	0	78	0	0
28	b	108	0	156	19	0
28	c	54	0	78	0	0
28	f	43	0	53	1	0
29	A	51	0	72	0	0
29	B	51	0	72	2	0
29	C	102	0	144	0	0
29	D	51	0	72	1	0
29	Z	51	0	72	1	0
29	a	51	0	72	0	0
29	c	153	0	216	2	0
29	d	51	0	72	1	0
29	m	51	0	72	3	0
30	A	8	0	12	3	0
30	B	20	0	30	4	0
30	C	20	0	30	1	0
30	D	8	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	O	8	0	12	3	0
30	U	4	0	6	0	0
30	V	8	0	12	0	0
30	a	8	0	12	1	0
30	b	20	0	30	3	0
30	c	20	0	30	2	0
30	d	8	0	12	4	0
30	u	4	0	6	0	0
30	v	4	0	6	0	0
31	A	28	0	0	0	0
31	B	32	0	0	0	0
31	D	56	0	0	0	0
31	I	26	0	0	0	0
31	J	16	0	0	0	0
31	K	34	0	0	0	0
31	L	16	0	0	0	0
31	X	16	0	0	0	0
31	Y	16	0	0	0	0
31	a	30	0	0	0	0
31	b	32	0	0	0	0
31	c	32	0	0	0	0
31	d	52	0	0	0	0
31	i	16	0	0	0	0
31	j	16	0	0	0	0
31	l	16	0	0	0	0
31	t	16	0	0	0	0
31	x	16	0	0	0	0
31	y	16	0	0	0	0
32	A	70	0	92	4	0
32	B	35	0	46	0	0
32	C	35	0	46	0	0
32	M	70	0	92	2	0
32	a	70	0	92	3	0
32	b	70	0	92	1	0
32	f	35	0	46	0	0
32	i	35	0	46	1	0
32	m	70	0	92	2	0
32	t	35	0	46	0	0
33	A	6	0	8	0	0
33	B	6	0	8	1	0
33	D	6	0	8	0	0
33	V	18	0	24	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	a	6	0	8	0	0
33	b	6	0	8	1	0
33	d	12	0	16	0	0
33	v	12	0	16	2	0
34	B	49	0	74	1	0
34	D	147	0	222	13	0
34	E	49	0	74	3	0
34	b	49	0	74	3	0
34	d	147	0	222	11	0
34	e	49	0	74	0	0
35	B	57	0	78	1	0
35	C	38	0	52	0	0
35	D	38	0	52	1	0
35	V	19	0	26	0	0
35	b	76	0	104	2	0
35	c	38	0	52	0	0
35	d	38	0	52	0	0
35	o	19	0	26	1	0
36	C	186	0	246	4	0
36	H	62	0	82	1	0
36	c	186	0	246	2	0
36	h	62	0	82	2	0
37	D	4	0	0	0	0
37	d	4	0	0	0	0
38	F	43	0	30	2	0
38	V	43	0	30	7	0
38	f	43	0	30	2	0
38	v	43	0	30	6	0
39	J	1	0	0	0	0
39	K	1	0	0	0	0
39	j	1	0	0	0	0
39	k	1	0	0	0	0
40	A	134	0	0	1	0
40	B	253	0	0	0	0
40	C	168	0	0	2	0
40	D	132	0	0	0	0
40	E	22	0	0	1	0
40	F	6	0	0	0	0
40	H	31	0	0	0	0
40	I	4	0	0	0	0
40	J	7	0	0	0	0
40	K	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	L	11	0	0	0	0
40	M	6	0	0	0	0
40	O	119	0	0	1	0
40	R	1	0	0	0	0
40	T	10	0	0	0	0
40	U	63	0	0	0	0
40	V	96	0	0	0	0
40	X	8	0	0	0	0
40	Y	1	0	0	0	0
40	Z	1	0	0	0	0
40	a	118	0	0	0	0
40	b	209	0	0	0	0
40	c	169	0	0	1	0
40	d	121	0	0	1	0
40	e	9	0	0	0	0
40	f	5	0	0	0	0
40	h	23	0	0	0	0
40	i	4	0	0	0	0
40	j	5	0	0	0	0
40	k	3	0	0	0	0
40	l	8	0	0	0	0
40	m	10	0	0	0	0
40	o	112	0	0	1	0
40	t	13	0	0	0	0
40	u	74	0	0	0	0
40	v	65	0	0	0	0
40	x	9	0	0	0	0
40	y	1	0	0	0	0
All	All	53568	0	52620	436	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 436 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)
16:v:37:CYS:SG	38:v:201:HEM:HAB	1.48	1.53
28:b:623[B]:SQD:H192	28:b:623[B]:SQD:C38	1.46	1.44
28:B:620[B]:SQD:H141	28:B:620[B]:SQD:C38	1.48	1.42
16:V:37:CYS:SG	38:V:201:HEM:HAB	1.58	1.42
28:B:620[B]:SQD:H382	28:B:620[B]:SQD:C14	1.52	1.39

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	337/334 (101%)	333 (99%)	3 (1%)	1 (0%)	36	36
1	a	336/334 (101%)	331 (98%)	4 (1%)	1 (0%)	36	36
2	B	513/505 (102%)	505 (98%)	8 (2%)	0	100	100
2	b	512/505 (101%)	506 (99%)	6 (1%)	0	100	100
3	C	452/451 (100%)	442 (98%)	9 (2%)	1 (0%)	43	44
3	c	450/451 (100%)	441 (98%)	8 (2%)	1 (0%)	43	44
4	D	340/342 (99%)	331 (97%)	9 (3%)	0	100	100
4	d	340/342 (99%)	333 (98%)	6 (2%)	1 (0%)	36	36
5	E	80/80 (100%)	79 (99%)	1 (1%)	0	100	100
5	e	76/80 (95%)	74 (97%)	2 (3%)	0	100	100
6	F	32/34 (94%)	32 (100%)	0	0	100	100
6	f	30/34 (88%)	30 (100%)	0	0	100	100
7	H	62/63 (98%)	59 (95%)	3 (5%)	0	100	100
7	h	61/63 (97%)	58 (95%)	3 (5%)	0	100	100
8	I	34/36 (94%)	33 (97%)	1 (3%)	0	100	100
8	i	34/36 (94%)	31 (91%)	3 (9%)	0	100	100
9	J	35/37 (95%)	32 (91%)	2 (6%)	1 (3%)	3	1
9	j	35/37 (95%)	35 (100%)	0	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100
10	k	35/37 (95%)	35 (100%)	0	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	35/37 (95%)	35 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	M	33/34 (97%)	33 (100%)	0	0	100	100
12	m	33/34 (97%)	33 (100%)	0	0	100	100
13	O	244/244 (100%)	240 (98%)	4 (2%)	0	100	100
13	o	242/244 (99%)	234 (97%)	8 (3%)	0	100	100
14	T	29/31 (94%)	29 (100%)	0	0	100	100
14	t	28/31 (90%)	28 (100%)	0	0	100	100
15	U	96/97 (99%)	93 (97%)	3 (3%)	0	100	100
15	u	96/97 (99%)	94 (98%)	2 (2%)	0	100	100
16	V	138/137 (101%)	134 (97%)	4 (3%)	0	100	100
16	v	137/137 (100%)	134 (98%)	3 (2%)	0	100	100
17	Y	28/30 (93%)	28 (100%)	0	0	100	100
17	y	28/30 (93%)	26 (93%)	2 (7%)	0	100	100
18	X	38/40 (95%)	37 (97%)	1 (3%)	0	100	100
18	x	37/40 (92%)	37 (100%)	0	0	100	100
19	Z	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	7	3
19	z	60/62 (97%)	57 (95%)	2 (3%)	1 (2%)	7	3
20	R	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
All	All	5258/5296 (99%)	5151 (98%)	99 (2%)	8 (0%)	43	44

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
3	c	416	SER
9	J	5	GLY
4	d	234	ALA
19	z	30	PRO

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	274/269 (102%)	274 (100%)	0	100	100
1	a	273/269 (102%)	273 (100%)	0	100	100
2	B	413/403 (102%)	413 (100%)	0	100	100
2	b	412/403 (102%)	408 (99%)	4 (1%)	68	76
3	C	355/352 (101%)	351 (99%)	4 (1%)	65	74
3	c	354/352 (101%)	347 (98%)	7 (2%)	48	56
4	D	277/277 (100%)	274 (99%)	3 (1%)	65	74
4	d	277/277 (100%)	274 (99%)	3 (1%)	65	74
5	E	73/71 (103%)	72 (99%)	1 (1%)	59	67
5	e	69/71 (97%)	66 (96%)	3 (4%)	26	27
6	F	28/28 (100%)	28 (100%)	0	100	100
6	f	26/28 (93%)	25 (96%)	1 (4%)	29	32
7	H	54/53 (102%)	52 (96%)	2 (4%)	30	33
7	h	53/53 (100%)	53 (100%)	0	100	100
8	I	32/32 (100%)	32 (100%)	0	100	100
8	i	32/32 (100%)	32 (100%)	0	100	100
9	J	25/25 (100%)	25 (100%)	0	100	100
9	j	25/25 (100%)	25 (100%)	0	100	100
10	K	30/30 (100%)	29 (97%)	1 (3%)	33	37
10	k	30/30 (100%)	29 (97%)	1 (3%)	33	37
11	L	35/35 (100%)	35 (100%)	0	100	100
11	l	35/35 (100%)	35 (100%)	0	100	100
12	M	31/30 (103%)	28 (90%)	3 (10%)	8	5
12	m	31/30 (103%)	31 (100%)	0	100	100
13	O	209/207 (101%)	208 (100%)	1 (0%)	81	88
13	o	207/207 (100%)	204 (99%)	3 (1%)	59	67
14	T	27/27 (100%)	25 (93%)	2 (7%)	13	10
14	t	26/27 (96%)	26 (100%)	0	100	100
15	U	85/84 (101%)	84 (99%)	1 (1%)	63	72
15	u	85/84 (101%)	84 (99%)	1 (1%)	63	72
16	V	120/117 (103%)	119 (99%)	1 (1%)	73	81
16	v	119/117 (102%)	118 (99%)	1 (1%)	73	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	Y	23/23 (100%)	22 (96%)	1 (4%)	26	27
17	y	23/23 (100%)	21 (91%)	2 (9%)	9	7
18	X	33/33 (100%)	33 (100%)	0	100	100
18	x	32/33 (97%)	32 (100%)	0	100	100
19	Z	51/51 (100%)	49 (96%)	2 (4%)	28	31
19	z	51/51 (100%)	49 (96%)	2 (4%)	28	31
20	R	29/29 (100%)	29 (100%)	0	100	100
All	All	4364/4323 (101%)	4314 (99%)	50 (1%)	65	74

5 of 50 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	c	240	ILE
4	d	233	ARG
19	z	42	LEU
3	c	289	PHE
3	c	462	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 44 such sidechains are listed below:

Mol	Chain	Res	Type
3	c	28	GLN
5	e	75	GLN
3	c	415	ASN
4	d	186	GLN
13	o	124	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	FME	i	1	8	8,9,10	0.52	0	8,9,11	1.18	0
12	FME	M	1	12	8,9,10	0.50	0	8,9,11	1.28	1 (12%)
14	FME	t	1	14	8,9,10	0.51	0	8,9,11	1.37	1 (12%)
14	FME	T	1	14	8,9,10	0.55	0	8,9,11	1.54	2 (25%)
8	FME	I	1	8	8,9,10	0.53	0	8,9,11	1.11	0
19	FME	z	1	19	8,9,10	0.49	0	8,9,11	1.46	0
12	FME	m	1	12	8,9,10	0.51	0	8,9,11	1.35	1 (12%)
19	FME	Z	1	19	8,9,10	0.58	0	8,9,11	1.69	4 (50%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	FME	i	1	8	-	2/7/9/11	-
12	FME	M	1	12	-	1/7/9/11	-
14	FME	t	1	14	-	3/7/9/11	-
14	FME	T	1	14	-	2/7/9/11	-
8	FME	I	1	8	-	2/7/9/11	-
19	FME	z	1	19	-	4/7/9/11	-
12	FME	m	1	12	-	2/7/9/11	-
19	FME	Z	1	19	-	5/7/9/11	-

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	T	1	FME	C-CA-N	2.82	114.93	109.50
19	Z	1	FME	C-CA-N	2.71	114.73	109.50
14	T	1	FME	O-C-CA	-2.18	119.17	124.77
12	M	1	FME	O1-CN-N	-2.13	119.80	125.32
14	t	1	FME	O-C-CA	-2.13	119.28	124.77

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	i	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 261 ligands modelled in this entry, 10 are monoatomic and 24 are unknown - leaving 227 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
29	LMG	d	409	39	51,51,55	0.95	2 (3%)	59,59,63	0.87	2 (3%)
30	DMS	a	417	-	3,3,3	2.61	1 (33%)	3,3,3	0.40	0
26	BCR	h	101	-	41,41,41	3.68	14 (34%)	56,56,56	8.60	42 (75%)
34	LHG	D	410	-	48,48,48	0.88	3 (6%)	51,54,54	0.96	4 (7%)
38	HEM	F	101	5,6	50,50,50	2.00	9 (18%)	67,82,82	1.37	6 (8%)
34	LHG	d	408	-	48,48,48	0.95	2 (4%)	51,54,54	0.95	2 (3%)
30	DMS	b	628	-	3,3,3	2.57	1 (33%)	3,3,3	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	C	502	3	69,73,73	2.34	19 (27%)	82,113,113	2.50	24 (29%)
24	CLA	b	618	2	69,73,73	2.44	19 (27%)	82,113,113	2.52	24 (29%)
24	CLA	c	510	3	69,73,73	2.38	19 (27%)	82,113,113	2.45	26 (31%)
25	PHO	A	1007	-	58,69,69	2.63	11 (18%)	55,99,99	2.84	13 (23%)
30	DMS	C	525	-	3,3,3	2.73	1 (33%)	3,3,3	0.55	0
30	DMS	V	203	-	3,3,3	2.74	1 (33%)	3,3,3	0.53	0
34	LHG	E	101	-	48,48,48	0.97	2 (4%)	51,54,54	0.97	3 (5%)
28	SQD	B	620[B]	-	52,54,54	0.96	2 (3%)	62,65,65	1.15	5 (8%)
34	LHG	D	411	-	48,48,48	0.95	2 (4%)	51,54,54	0.95	2 (3%)
36	DGD	c	517	-	63,63,67	0.89	2 (3%)	77,77,81	0.82	3 (3%)
24	CLA	b	619	2	69,73,73	2.39	19 (27%)	82,113,113	2.48	27 (32%)
26	BCR	a	413	-	41,41,41	3.57	14 (34%)	56,56,56	8.62	41 (73%)
24	CLA	c	507	40	69,73,73	2.48	20 (28%)	82,113,113	2.63	26 (31%)
30	DMS	b	629	-	3,3,3	2.72	1 (33%)	3,3,3	0.46	0
28	SQD	B	620[A]	-	52,54,54	0.98	2 (3%)	62,65,65	1.07	5 (8%)
24	CLA	C	511	3	69,73,73	2.67	21 (30%)	82,113,113	2.53	23 (28%)
24	CLA	a	409	40	69,73,73	2.41	20 (28%)	82,113,113	2.40	25 (30%)
35	HTG	b	602	-	19,19,19	0.94	2 (10%)	23,24,24	1.19	1 (4%)
28	SQD	f	102	-	41,43,54	1.14	3 (7%)	51,54,65	1.34	6 (11%)
35	HTG	B	628	-	19,19,19	0.96	2 (10%)	23,24,24	1.10	1 (4%)
29	LMG	Z	101	-	51,51,55	0.98	2 (3%)	59,59,63	0.99	2 (3%)
24	CLA	C	503	3	69,73,73	2.52	19 (27%)	82,113,113	2.46	24 (29%)
24	CLA	D	402	4	69,73,73	2.19	20 (28%)	82,113,113	2.56	28 (34%)
24	CLA	B	605	2	69,73,73	2.35	20 (28%)	82,113,113	2.44	24 (29%)
35	HTG	c	525	-	19,19,19	0.97	2 (10%)	23,24,24	1.04	1 (4%)
38	HEM	f	101	5,6	50,50,50	1.97	10 (20%)	67,82,82	1.36	6 (8%)
24	CLA	b	611	2	69,73,73	2.35	18 (26%)	82,113,113	2.42	26 (31%)
24	CLA	B	604	2	69,73,73	2.40	18 (26%)	82,113,113	2.48	27 (32%)
32	LMT	M	101	-	36,36,36	0.48	0	47,47,47	0.90	0
24	CLA	B	608	2	69,73,73	2.44	19 (27%)	82,113,113	2.36	22 (26%)
24	CLA	d	403	4	69,73,73	2.49	21 (30%)	82,113,113	2.43	24 (29%)
30	DMS	C	524	-	3,3,3	2.65	1 (33%)	3,3,3	0.46	0
28	SQD	a	401	-	52,54,54	0.98	2 (3%)	62,65,65	1.13	4 (6%)
26	BCR	b	620	-	41,41,41	3.64	15 (36%)	56,56,56	8.20	41 (73%)
36	DGD	C	516	-	63,63,67	0.92	3 (4%)	77,77,81	0.94	4 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	DMS	C	526	-	3,3,3	2.72	1 (33%)	3,3,3	0.52	0
26	BCR	B	619	-	41,41,41	3.68	15 (36%)	56,56,56	8.12	38 (67%)
30	DMS	C	527	-	3,3,3	2.72	1 (33%)	3,3,3	0.57	0
33	GOL	V	206	-	5,5,5	0.28	0	5,5,5	0.26	0
33	GOL	d	415	-	5,5,5	0.28	0	5,5,5	0.36	0
36	DGD	h	102	-	63,63,67	0.92	3 (4%)	77,77,81	0.84	3 (3%)
24	CLA	b	613	40	69,73,73	2.35	18 (26%)	82,113,113	2.47	22 (26%)
35	HTG	V	202	-	19,19,19	0.90	2 (10%)	23,24,24	1.47	3 (13%)
35	HTG	o	301	-	19,19,19	0.96	1 (5%)	23,24,24	1.16	1 (4%)
24	CLA	b	616	2	69,73,73	2.52	18 (26%)	82,113,113	2.46	26 (31%)
24	CLA	c	502	3	69,73,73	2.41	19 (27%)	82,113,113	2.44	25 (30%)
32	LMT	C	520	-	36,36,36	0.52	1 (2%)	47,47,47	1.04	1 (2%)
32	LMT	m	103	-	36,36,36	0.53	1 (2%)	47,47,47	0.79	1 (2%)
33	GOL	b	632	-	5,5,5	0.22	0	5,5,5	0.32	0
24	CLA	a	407	1	69,73,73	2.33	20 (28%)	82,113,113	2.30	17 (20%)
32	LMT	A	1017	-	36,36,36	0.54	1 (2%)	47,47,47	0.87	2 (4%)
26	BCR	J	101	-	41,41,41	3.70	14 (34%)	56,56,56	8.87	40 (71%)
27	PL9	A	1010	-	55,55,55	0.70	2 (3%)	68,69,69	1.62	18 (26%)
30	DMS	O	302	-	3,3,3	2.73	1 (33%)	3,3,3	0.59	0
33	GOL	v	203	-	5,5,5	0.34	0	5,5,5	0.34	0
24	CLA	B	606	2	69,73,73	2.57	19 (27%)	82,113,113	2.57	27 (32%)
24	CLA	b	612	2	69,73,73	2.71	20 (28%)	82,113,113	2.44	25 (30%)
32	LMT	m	101	-	36,36,36	0.47	0	47,47,47	0.70	0
33	GOL	v	204	-	5,5,5	0.25	0	5,5,5	0.34	0
30	DMS	d	413	-	3,3,3	2.74	1 (33%)	3,3,3	0.62	0
38	HEM	V	201	16	50,50,50	1.85	10 (20%)	67,82,82	1.33	5 (7%)
29	LMG	D	412	39	51,51,55	0.91	2 (3%)	59,59,63	0.79	1 (1%)
24	CLA	b	617	2	69,73,73	2.70	20 (28%)	82,113,113	2.56	30 (36%)
24	CLA	B	616	2	69,73,73	2.25	17 (24%)	82,113,113	2.52	28 (34%)
26	BCR	B	618	-	41,41,41	3.63	15 (36%)	56,56,56	8.56	41 (73%)
30	DMS	A	1013	-	3,3,3	2.59	1 (33%)	3,3,3	0.59	0
34	LHG	B	621	-	48,48,48	0.93	2 (4%)	51,54,54	0.93	2 (3%)
30	DMS	a	418	-	3,3,3	2.75	1 (33%)	3,3,3	0.61	0
26	BCR	b	621	-	41,41,41	3.65	14 (34%)	56,56,56	8.57	43 (76%)
33	GOL	a	420	-	5,5,5	0.28	0	5,5,5	0.31	0
27	PL9	a	414	-	55,55,55	0.71	2 (3%)	68,69,69	1.49	16 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	HTG	b	626	-	19,19,19	0.92	1 (5%)	23,24,24	1.06	2 (8%)
24	CLA	A	1005	1	69,73,73	2.27	19 (27%)	82,113,113	2.38	22 (26%)
24	CLA	d	402	4	69,73,73	2.37	19 (27%)	82,113,113	2.45	23 (28%)
28	SQD	b	623[B]	-	52,54,54	0.97	2 (3%)	62,65,65	1.09	7 (11%)
29	LMG	m	102	-	51,51,55	0.99	2 (3%)	59,59,63	1.11	4 (6%)
30	DMS	B	634	-	3,3,3	2.74	1 (33%)	3,3,3	0.49	0
35	HTG	B	624	-	19,19,19	0.95	2 (10%)	23,24,24	1.34	1 (4%)
32	LMT	b	631	-	36,36,36	0.50	0	47,47,47	0.84	2 (4%)
24	CLA	b	609	2	69,73,73	2.68	21 (30%)	82,113,113	2.57	25 (30%)
30	DMS	O	301	-	3,3,3	2.74	1 (33%)	3,3,3	0.55	0
36	DGD	H	102	-	63,63,67	0.88	3 (4%)	77,77,81	0.83	3 (3%)
24	CLA	b	604	40	69,73,73	3.09	21 (30%)	82,113,113	2.48	27 (32%)
30	DMS	B	627	-	3,3,3	2.64	1 (33%)	3,3,3	0.47	0
24	CLA	c	506	3	69,73,73	2.70	19 (27%)	82,113,113	2.48	25 (30%)
35	HTG	D	413	-	19,19,19	0.96	2 (10%)	23,24,24	1.13	1 (4%)
24	CLA	B	611	2	69,73,73	2.44	19 (27%)	82,113,113	2.44	22 (26%)
30	DMS	V	205	-	3,3,3	2.73	1 (33%)	3,3,3	0.52	0
30	DMS	b	633	-	3,3,3	2.73	1 (33%)	3,3,3	0.67	0
30	DMS	d	414	-	3,3,3	2.72	1 (33%)	3,3,3	0.43	0
32	LMT	M	102	-	36,36,36	0.49	0	47,47,47	0.74	0
24	CLA	B	613	2	69,73,73	2.30	19 (27%)	82,113,113	2.48	25 (30%)
24	CLA	c	512	3	69,73,73	2.59	21 (30%)	82,113,113	2.51	25 (30%)
32	LMT	f	103	-	36,36,36	0.52	0	47,47,47	0.67	0
33	GOL	B	631	-	5,5,5	0.24	0	5,5,5	0.29	0
25	PHO	a	411	-	58,69,69	2.77	11 (18%)	55,99,99	2.82	15 (27%)
29	LMG	A	1012	-	51,51,55	0.95	2 (3%)	59,59,63	0.93	2 (3%)
33	GOL	V	207	-	5,5,5	0.24	0	5,5,5	0.39	0
26	BCR	T	101	-	41,41,41	3.71	15 (36%)	56,56,56	8.16	37 (66%)
30	DMS	D	416	-	3,3,3	2.77	1 (33%)	3,3,3	0.77	0
27	PL9	D	407	-	55,55,55	0.75	2 (3%)	68,69,69	1.41	14 (20%)
24	CLA	C	510	3	69,73,73	2.28	18 (26%)	82,113,113	2.53	26 (31%)
26	BCR	D	406	-	41,41,41	3.68	14 (34%)	56,56,56	8.26	45 (80%)
29	LMG	a	415	-	51,51,55	0.96	2 (3%)	59,59,63	0.97	2 (3%)
24	CLA	c	501	3	69,73,73	2.56	19 (27%)	82,113,113	2.54	25 (30%)
24	CLA	b	610	40	69,73,73	2.42	19 (27%)	82,113,113	2.46	26 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	B	612	2	69,73,73	2.42	20 (28%)	82,113,113	2.37	22 (26%)
24	CLA	c	509	3	69,73,73	2.45	20 (28%)	82,113,113	2.52	26 (31%)
34	LHG	e	101	-	48,48,48	0.97	2 (4%)	51,54,54	1.00	2 (3%)
24	CLA	c	504	40	69,73,73	2.49	18 (26%)	82,113,113	2.44	26 (31%)
35	HTG	B	629	-	19,19,19	0.94	1 (5%)	23,24,24	1.18	1 (4%)
26	BCR	d	404	-	41,41,41	3.72	15 (36%)	56,56,56	8.39	41 (73%)
26	BCR	b	622	-	41,41,41	3.71	15 (36%)	56,56,56	8.31	37 (66%)
24	CLA	b	614	2	69,73,73	2.34	19 (27%)	82,113,113	2.42	22 (26%)
24	CLA	c	508	3	69,73,73	2.85	22 (31%)	82,113,113	2.46	24 (29%)
26	BCR	C	514	-	41,41,41	3.74	15 (36%)	56,56,56	8.41	37 (66%)
24	CLA	B	603	2	69,73,73	2.41	20 (28%)	82,113,113	2.54	23 (28%)
28	SQD	D	408	-	41,43,54	1.11	2 (4%)	51,54,65	1.55	9 (17%)
24	CLA	B	610	40	69,73,73	2.23	19 (27%)	82,113,113	2.45	22 (26%)
32	LMT	b	625	-	36,36,36	0.51	0	47,47,47	1.22	5 (10%)
21	OER	a	403	3,1,40	0,14,14	-	-	-	-	-
24	CLA	B	609	2	69,73,73	2.51	19 (27%)	82,113,113	2.44	24 (29%)
26	BCR	A	1009	-	41,41,41	3.64	14 (34%)	56,56,56	8.32	40 (71%)
29	LMG	c	521	-	51,51,55	1.00	3 (5%)	59,59,63	1.07	3 (5%)
26	BCR	t	101	-	41,41,41	3.70	15 (36%)	56,56,56	8.22	41 (73%)
36	DGD	C	517	-	63,63,67	0.86	2 (3%)	77,77,81	0.88	2 (2%)
24	CLA	C	512	3	69,73,73	3.06	21 (30%)	82,113,113	2.42	25 (30%)
24	CLA	C	507	40	69,73,73	2.65	19 (27%)	82,113,113	2.63	26 (31%)
24	CLA	c	511	3	69,73,73	2.70	19 (27%)	82,113,113	2.47	24 (29%)
30	DMS	b	635	-	3,3,3	2.73	1 (33%)	3,3,3	0.46	0
30	DMS	D	417	-	3,3,3	2.74	1 (33%)	3,3,3	0.46	0
24	CLA	C	509	3	69,73,73	2.31	20 (28%)	82,113,113	2.54	26 (31%)
26	BCR	c	514	-	41,41,41	3.72	15 (36%)	56,56,56	8.86	41 (73%)
28	SQD	b	623[A]	-	52,54,54	0.96	2 (3%)	62,65,65	1.11	5 (8%)
24	CLA	b	607	2	69,73,73	2.42	18 (26%)	82,113,113	2.55	23 (28%)
34	LHG	b	624	-	48,48,48	0.91	2 (4%)	51,54,54	0.96	2 (3%)
28	SQD	A	1016	-	52,54,54	0.97	2 (3%)	62,65,65	1.13	4 (6%)
25	PHO	D	404	-	58,69,69	2.75	11 (18%)	55,99,99	2.76	14 (25%)
35	HTG	d	416	-	19,19,19	0.93	1 (5%)	23,24,24	1.39	1 (4%)
37	BCT	D	401	22	3,3,3	0.59	0	2,3,3	0.37	0
24	CLA	C	513	3	69,73,73	2.60	22 (31%)	82,113,113	2.42	27 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	DMS	b	634	-	3,3,3	2.78	1 (33%)	3,3,3	0.65	0
24	CLA	A	1008	1	69,73,73	2.39	19 (27%)	82,113,113	2.46	24 (29%)
30	DMS	c	528	-	3,3,3	2.72	1 (33%)	3,3,3	0.55	0
30	DMS	B	633	-	3,3,3	2.75	1 (33%)	3,3,3	0.59	0
21	OER	A	1001	3,1,40	0,14,14	-	-	-	-	-
30	DMS	u	201	-	3,3,3	2.69	1 (33%)	3,3,3	0.52	0
32	LMT	i	102	-	36,36,36	0.51	0	47,47,47	1.04	2 (4%)
26	BCR	K	102	-	41,41,41	3.74	15 (36%)	56,56,56	8.62	39 (69%)
35	HTG	D	419	-	19,19,19	0.93	1 (5%)	23,24,24	1.33	1 (4%)
24	CLA	B	601	40	69,73,73	2.44	20 (28%)	82,113,113	2.54	27 (32%)
26	BCR	k	101	-	41,41,41	3.69	15 (36%)	56,56,56	8.76	40 (71%)
30	DMS	B	632	-	3,3,3	2.72	1 (33%)	3,3,3	0.50	0
35	HTG	d	410	-	19,19,19	0.96	1 (5%)	23,24,24	1.11	1 (4%)
27	PL9	d	405	-	55,55,55	0.75	2 (3%)	68,69,69	1.37	9 (13%)
34	LHG	d	406	-	48,48,48	0.95	2 (4%)	51,54,54	0.93	3 (5%)
36	DGD	c	516	-	63,63,67	0.92	3 (4%)	77,77,81	0.91	3 (3%)
38	HEM	v	201	16	50,50,50	1.84	10 (20%)	67,82,82	1.27	6 (8%)
29	LMG	C	519	-	51,51,55	0.99	3 (5%)	59,59,63	1.07	4 (6%)
24	CLA	B	607	40	69,73,73	2.46	19 (27%)	82,113,113	2.45	26 (31%)
24	CLA	C	504	40	69,73,73	2.50	20 (28%)	82,113,113	2.48	25 (30%)
24	CLA	C	501	3	69,73,73	2.37	18 (26%)	82,113,113	2.51	25 (30%)
34	LHG	d	407	-	48,48,48	0.88	2 (4%)	51,54,54	0.93	3 (5%)
24	CLA	a	412	1	69,73,73	2.21	19 (27%)	82,113,113	2.47	24 (29%)
26	BCR	y	101	-	41,41,41	3.72	15 (36%)	56,56,56	8.97	44 (78%)
24	CLA	a	408	40	69,73,73	2.29	19 (27%)	82,113,113	2.43	24 (29%)
24	CLA	C	506	3	69,73,73	2.41	19 (27%)	82,113,113	2.46	24 (29%)
26	BCR	B	617	-	41,41,41	3.63	15 (36%)	56,56,56	8.26	39 (69%)
32	LMT	t	103	-	36,36,36	0.45	0	47,47,47	1.03	2 (4%)
32	LMT	a	402	-	36,36,36	0.58	1 (2%)	47,47,47	0.87	3 (6%)
37	BCT	d	401	22	3,3,3	0.53	0	2,3,3	0.26	0
35	HTG	C	522	-	19,19,19	0.94	1 (5%)	23,24,24	1.81	5 (21%)
35	HTG	c	522	-	19,19,19	0.92	2 (10%)	23,24,24	1.03	1 (4%)
26	BCR	k	102	-	41,41,41	3.61	15 (36%)	56,56,56	8.51	37 (66%)
35	HTG	b	630	-	19,19,19	0.99	2 (10%)	23,24,24	1.53	2 (8%)
24	CLA	c	513	3	69,73,73	2.60	22 (31%)	82,113,113	2.39	26 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	DGD	c	515	-	63,63,67	0.89	3 (4%)	77,77,81	0.90	2 (2%)
28	SQD	c	518	-	52,54,54	0.98	2 (3%)	62,65,65	1.26	6 (9%)
24	CLA	c	503	3	69,73,73	2.74	22 (31%)	82,113,113	2.47	28 (34%)
29	LMG	B	622	-	51,51,55	0.98	2 (3%)	59,59,63	0.91	2 (3%)
30	DMS	c	524	-	3,3,3	2.64	1 (33%)	3,3,3	0.36	0
30	DMS	U	201	-	3,3,3	2.70	1 (33%)	3,3,3	0.50	0
33	GOL	V	204	-	5,5,5	0.29	0	5,5,5	0.24	0
24	CLA	b	608	2	69,73,73	2.34	21 (30%)	82,113,113	2.47	23 (28%)
29	LMG	C	518	-	51,51,55	0.98	2 (3%)	59,59,63	0.88	3 (5%)
30	DMS	c	527	-	3,3,3	2.75	1 (33%)	3,3,3	0.61	0
32	LMT	B	623	-	36,36,36	0.48	0	47,47,47	1.01	2 (4%)
24	CLA	c	505	3	69,73,73	2.38	20 (28%)	82,113,113	2.44	25 (30%)
24	CLA	B	614	2	69,73,73	2.49	18 (26%)	82,113,113	2.60	29 (35%)
33	GOL	A	1019	-	5,5,5	0.26	0	5,5,5	0.34	0
25	PHO	a	410	-	58,69,69	2.69	11 (18%)	55,99,99	2.72	14 (25%)
35	HTG	C	521	-	19,19,19	0.96	2 (10%)	23,24,24	1.07	1 (4%)
24	CLA	C	508	3	69,73,73	2.55	21 (30%)	82,113,113	2.43	24 (29%)
26	BCR	H	101	-	41,41,41	3.65	15 (36%)	56,56,56	8.50	42 (75%)
26	BCR	K	101	-	41,41,41	3.67	15 (36%)	56,56,56	8.14	42 (75%)
30	DMS	B	626	-	3,3,3	2.60	1 (33%)	3,3,3	0.36	0
33	GOL	d	417	-	5,5,5	0.33	0	5,5,5	0.19	0
32	LMT	A	1018	-	36,36,36	0.53	0	47,47,47	1.01	5 (10%)
24	CLA	A	1006	40	69,73,73	2.14	18 (26%)	82,113,113	2.41	24 (29%)
30	DMS	C	523	-	3,3,3	2.60	1 (33%)	3,3,3	0.39	0
24	CLA	b	606	2	69,73,73	2.34	18 (26%)	82,113,113	2.47	25 (30%)
36	DGD	C	515	-	63,63,67	0.87	2 (3%)	77,77,81	0.88	3 (3%)
24	CLA	B	615	2	69,73,73	2.59	22 (31%)	82,113,113	2.54	25 (30%)
34	LHG	D	409	-	48,48,48	0.91	2 (4%)	51,54,54	0.97	4 (7%)
24	CLA	C	505	3	69,73,73	2.55	18 (26%)	82,113,113	2.44	22 (26%)
30	DMS	v	202	-	3,3,3	2.69	1 (33%)	3,3,3	0.52	0
24	CLA	b	615	2	69,73,73	2.34	18 (26%)	82,113,113	2.44	24 (29%)
30	DMS	c	529	-	3,3,3	2.66	1 (33%)	3,3,3	0.49	0
24	CLA	D	403	40	69,73,73	2.10	20 (28%)	82,113,113	2.51	23 (28%)
32	LMT	a	416	-	36,36,36	0.50	0	47,47,47	0.76	1 (2%)
24	CLA	D	405	4	69,73,73	2.50	19 (27%)	82,113,113	2.42	26 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	b	605	2	69,73,73	2.46	20 (28%)	82,113,113	2.40	25 (30%)
33	GOL	D	418	-	5,5,5	0.29	0	5,5,5	0.35	0
35	HTG	b	601	-	19,19,19	0.92	1 (5%)	23,24,24	1.21	1 (4%)
30	DMS	c	526	-	3,3,3	2.71	1 (33%)	3,3,3	0.47	0
30	DMS	A	1014	-	3,3,3	2.74	1 (33%)	3,3,3	0.56	0
24	CLA	B	602	2	69,73,73	2.31	18 (26%)	82,113,113	2.39	23 (28%)
28	SQD	A	1011	-	52,54,54	0.96	2 (3%)	62,65,65	1.29	8 (12%)
29	LMG	c	520	-	51,51,55	1.00	3 (5%)	59,59,63	1.03	3 (5%)
29	LMG	c	519	-	51,51,55	0.98	2 (3%)	59,59,63	0.89	3 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	LMG	d	409	39	-	17/46/66/70	0/1/1/1
26	BCR	h	101	-	-	7/29/63/63	0/2/2/2
34	LHG	D	410	-	-	15/53/53/53	-
38	HEM	F	101	5,6	-	3/14/54/54	-
34	LHG	d	408	-	-	12/53/53/53	-
24	CLA	C	502	3	-	7/39/115/115	-
24	CLA	b	618	2	-	7/39/115/115	-
24	CLA	c	510	3	-	8/39/115/115	-
25	PHO	A	1007	-	-	2/37/103/103	0/5/6/6
34	LHG	E	101	-	-	32/53/53/53	-
28	SQD	B	620[B]	-	-	24/49/69/69	0/1/1/1
34	LHG	D	411	-	-	15/53/53/53	-
36	DGD	c	517	-	-	19/51/91/95	0/2/2/2
24	CLA	b	619	2	-	10/39/115/115	-
26	BCR	a	413	-	-	5/29/63/63	0/2/2/2
24	CLA	c	507	40	-	9/39/115/115	-
28	SQD	B	620[A]	-	-	30/49/69/69	0/1/1/1
24	CLA	C	511	3	-	6/39/115/115	-
24	CLA	a	409	40	-	10/39/115/115	-
35	HTG	b	602	-	-	2/10/30/30	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	SQD	f	102	-	-	24/38/58/69	0/1/1/1
35	HTG	B	628	-	-	3/10/30/30	0/1/1/1
29	LMG	Z	101	-	-	29/46/66/70	0/1/1/1
24	CLA	C	503	3	-	4/39/115/115	-
24	CLA	D	402	4	-	5/39/115/115	-
24	CLA	B	605	2	-	4/39/115/115	-
35	HTG	c	525	-	-	4/10/30/30	0/1/1/1
38	HEM	f	101	5,6	-	6/14/54/54	-
24	CLA	b	611	2	-	1/39/115/115	-
24	CLA	B	604	2	-	11/39/115/115	-
32	LMT	M	101	-	-	9/21/61/61	0/2/2/2
24	CLA	B	608	2	-	1/39/115/115	-
24	CLA	d	403	4	-	12/39/115/115	-
28	SQD	a	401	-	-	24/49/69/69	0/1/1/1
26	BCR	b	620	-	-	5/29/63/63	0/2/2/2
36	DGD	C	516	-	-	22/51/91/95	0/2/2/2
26	BCR	B	619	-	-	2/29/63/63	0/2/2/2
33	GOL	V	206	-	-	3/4/4/4	-
33	GOL	d	415	-	-	2/4/4/4	-
36	DGD	h	102	-	-	18/51/91/95	0/2/2/2
24	CLA	b	613	40	-	5/39/115/115	-
35	HTG	V	202	-	-	6/10/30/30	0/1/1/1
35	HTG	o	301	-	-	4/10/30/30	0/1/1/1
24	CLA	b	616	2	-	8/39/115/115	-
24	CLA	c	502	3	-	6/39/115/115	-
32	LMT	C	520	-	-	10/21/61/61	0/2/2/2
32	LMT	m	103	-	-	7/21/61/61	0/2/2/2
33	GOL	b	632	-	-	2/4/4/4	-
24	CLA	a	407	1	-	0/39/115/115	-
32	LMT	A	1017	-	-	10/21/61/61	0/2/2/2
26	BCR	J	101	-	-	12/29/63/63	0/2/2/2
27	PL9	A	1010	-	-	6/53/73/73	0/1/1/1
33	GOL	v	203	-	-	1/4/4/4	-
24	CLA	B	606	2	-	8/39/115/115	-
24	CLA	b	612	2	-	3/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	LMT	m	101	-	-	0/21/61/61	0/2/2/2
33	GOL	v	204	-	-	3/4/4/4	-
38	HEM	V	201	16	-	6/14/54/54	-
29	LMG	D	412	39	-	14/46/66/70	0/1/1/1
24	CLA	b	617	2	-	17/39/115/115	-
24	CLA	B	616	2	-	14/39/115/115	-
26	BCR	B	618	-	-	5/29/63/63	0/2/2/2
34	LHG	B	621	-	-	20/53/53/53	-
26	BCR	b	621	-	-	5/29/63/63	0/2/2/2
33	GOL	a	420	-	-	2/4/4/4	-
27	PL9	a	414	-	-	5/53/73/73	0/1/1/1
35	HTG	b	626	-	-	5/10/30/30	0/1/1/1
24	CLA	A	1005	1	-	0/39/115/115	-
24	CLA	d	402	4	-	5/39/115/115	-
28	SQD	b	623[B]	-	-	29/49/69/69	0/1/1/1
29	LMG	m	102	-	-	21/46/66/70	0/1/1/1
35	HTG	B	624	-	-	7/10/30/30	0/1/1/1
32	LMT	b	631	-	-	10/21/61/61	0/2/2/2
24	CLA	b	609	2	-	7/39/115/115	-
36	DGD	H	102	-	-	16/51/91/95	0/2/2/2
24	CLA	b	604	40	-	19/39/115/115	-
24	CLA	c	506	3	-	12/39/115/115	-
35	HTG	D	413	-	-	5/10/30/30	0/1/1/1
24	CLA	B	611	2	-	5/39/115/115	-
32	LMT	M	102	-	-	6/21/61/61	0/2/2/2
24	CLA	B	613	2	-	5/39/115/115	-
24	CLA	c	512	3	-	15/39/115/115	-
32	LMT	f	103	-	-	15/21/61/61	0/2/2/2
33	GOL	B	631	-	-	0/4/4/4	-
25	PHO	a	411	-	-	4/37/103/103	0/5/6/6
29	LMG	A	1012	-	-	27/46/66/70	0/1/1/1
33	GOL	V	207	-	-	2/4/4/4	-
26	BCR	T	101	-	-	6/29/63/63	0/2/2/2
27	PL9	D	407	-	-	1/53/73/73	0/1/1/1
24	CLA	C	510	3	-	6/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	BCR	D	406	-	-	6/29/63/63	0/2/2/2
29	LMG	a	415	-	-	24/46/66/70	0/1/1/1
24	CLA	c	501	3	-	3/39/115/115	-
24	CLA	b	610	40	-	6/39/115/115	-
24	CLA	B	612	2	-	4/39/115/115	-
24	CLA	c	509	3	-	10/39/115/115	-
34	LHG	e	101	-	-	28/53/53/53	-
24	CLA	c	504	40	-	13/39/115/115	-
35	HTG	B	629	-	-	2/10/30/30	0/1/1/1
26	BCR	d	404	-	-	10/29/63/63	0/2/2/2
26	BCR	b	622	-	-	6/29/63/63	0/2/2/2
24	CLA	b	614	2	-	3/39/115/115	-
24	CLA	c	508	3	-	12/39/115/115	-
26	BCR	C	514	-	-	5/29/63/63	0/2/2/2
24	CLA	B	603	2	-	5/39/115/115	-
28	SQD	D	408	-	-	22/38/58/69	0/1/1/1
24	CLA	B	610	40	-	8/39/115/115	-
32	LMT	b	625	-	-	10/21/61/61	0/2/2/2
24	CLA	B	609	2	-	2/39/115/115	-
26	BCR	A	1009	-	-	6/29/63/63	0/2/2/2
29	LMG	c	521	-	-	25/46/66/70	0/1/1/1
26	BCR	t	101	-	-	5/29/63/63	0/2/2/2
36	DGD	C	517	-	-	10/51/91/95	0/2/2/2
24	CLA	C	512	3	-	15/39/115/115	-
24	CLA	C	507	40	-	17/39/115/115	-
24	CLA	c	511	3	-	2/39/115/115	-
24	CLA	C	509	3	-	6/39/115/115	-
26	BCR	c	514	-	-	6/29/63/63	0/2/2/2
28	SQD	b	623[A]	-	-	22/49/69/69	0/1/1/1
24	CLA	b	607	2	-	3/39/115/115	-
34	LHG	b	624	-	-	20/53/53/53	-
28	SQD	A	1016	-	-	22/49/69/69	0/1/1/1
25	PHO	D	404	-	-	4/37/103/103	0/5/6/6
35	HTG	d	416	-	-	4/10/30/30	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	C	513	3	-	10/39/115/115	-
24	CLA	A	1008	1	-	7/39/115/115	-
32	LMT	i	102	-	-	12/21/61/61	0/2/2/2
35	HTG	d	410	-	-	4/10/30/30	0/1/1/1
26	BCR	K	102	-	-	8/29/63/63	0/2/2/2
35	HTG	D	419	-	-	7/10/30/30	0/1/1/1
24	CLA	B	601	40	-	14/39/115/115	-
26	BCR	k	101	-	-	14/29/63/63	0/2/2/2
36	DGD	c	516	-	-	27/51/91/95	0/2/2/2
38	HEM	v	201	16	-	6/14/54/54	-
27	PL9	d	405	-	-	1/53/73/73	0/1/1/1
34	LHG	d	406	-	-	16/53/53/53	-
29	LMG	C	519	-	-	22/46/66/70	0/1/1/1
24	CLA	B	607	40	-	2/39/115/115	-
24	CLA	C	504	40	-	9/39/115/115	-
24	CLA	C	501	3	-	4/39/115/115	-
34	LHG	d	407	-	-	14/53/53/53	-
24	CLA	a	412	1	-	14/39/115/115	-
26	BCR	y	101	-	-	11/29/63/63	0/2/2/2
24	CLA	a	408	40	-	1/39/115/115	-
24	CLA	C	506	3	-	13/39/115/115	-
26	BCR	B	617	-	-	4/29/63/63	0/2/2/2
32	LMT	t	103	-	-	16/21/61/61	0/2/2/2
32	LMT	a	402	-	-	7/21/61/61	0/2/2/2
35	HTG	C	522	-	-	5/10/30/30	0/1/1/1
35	HTG	c	522	-	-	5/10/30/30	0/1/1/1
26	BCR	k	102	-	-	9/29/63/63	0/2/2/2
35	HTG	b	630	-	-	7/10/30/30	0/1/1/1
24	CLA	c	513	3	-	20/39/115/115	-
36	DGD	c	515	-	-	23/51/91/95	0/2/2/2
28	SQD	c	518	-	-	19/49/69/69	0/1/1/1
24	CLA	c	503	3	-	3/39/115/115	-
29	LMG	B	622	-	-	22/46/66/70	0/1/1/1
33	GOL	V	204	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	b	608	2	-	9/39/115/115	-
29	LMG	C	518	-	-	20/46/66/70	0/1/1/1
32	LMT	B	623	-	-	14/21/61/61	0/2/2/2
24	CLA	c	505	3	-	7/39/115/115	-
24	CLA	B	614	2	-	9/39/115/115	-
33	GOL	A	1019	-	-	1/4/4/4	-
25	PHO	a	410	-	-	3/37/103/103	0/5/6/6
35	HTG	C	521	-	-	5/10/30/30	0/1/1/1
24	CLA	C	508	3	-	9/39/115/115	-
26	BCR	H	101	-	-	7/29/63/63	0/2/2/2
26	BCR	K	101	-	-	8/29/63/63	0/2/2/2
33	GOL	d	417	-	-	2/4/4/4	-
32	LMT	A	1018	-	-	12/21/61/61	0/2/2/2
24	CLA	A	1006	40	-	9/39/115/115	-
24	CLA	b	606	2	-	8/39/115/115	-
36	DGD	C	515	-	-	26/51/91/95	0/2/2/2
24	CLA	B	615	2	-	7/39/115/115	-
34	LHG	D	409	-	-	16/53/53/53	-
24	CLA	C	505	3	-	9/39/115/115	-
24	CLA	b	615	2	-	8/39/115/115	-
24	CLA	D	403	40	-	2/39/115/115	-
32	LMT	a	416	-	-	8/21/61/61	0/2/2/2
24	CLA	D	405	4	-	13/39/115/115	-
24	CLA	b	605	2	-	3/39/115/115	-
33	GOL	D	418	-	-	4/4/4/4	-
35	HTG	b	601	-	-	3/10/30/30	0/1/1/1
24	CLA	B	602	2	-	4/39/115/115	-
28	SQD	A	1011	-	-	22/49/69/69	0/1/1/1
29	LMG	c	520	-	-	17/46/66/70	0/1/1/1
29	LMG	c	519	-	-	25/46/66/70	0/1/1/1

The worst 5 of 1931 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	512	CLA	MG-NA	17.54	2.47	2.06
24	b	604	CLA	MG-NC	13.70	2.38	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	617	CLA	MG-NA	13.60	2.38	2.06
24	C	505	CLA	MG-NA	13.03	2.37	2.06
24	C	507	CLA	MG-NA	12.84	2.36	2.06

The worst 5 of 2947 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	1009	BCR	C20-C21-C22	28.60	167.39	127.28
26	J	101	BCR	C16-C17-C18	28.55	167.31	127.28
26	y	101	BCR	C20-C21-C22	27.70	166.12	127.28
26	c	514	BCR	C16-C17-C18	27.49	165.84	127.28
26	b	621	BCR	C20-C21-C22	27.46	165.78	127.28

There are no chirality outliers.

5 of 1830 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	B	601	CLA	CAD-CBD-CGD-O1D
24	B	601	CLA	CAD-CBD-CGD-O2D
24	B	607	CLA	CAD-CBD-CGD-O2D
24	B	614	CLA	CAD-CBD-CGD-O1D
24	B	614	CLA	CAD-CBD-CGD-O2D

There are no ring outliers.

137 monomers are involved in 269 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	d	409	LMG	1	0
34	D	410	LHG	1	0
38	F	101	HEM	2	0
34	d	408	LHG	6	0
24	C	502	CLA	3	0
24	b	618	CLA	3	0
24	c	510	CLA	3	0
34	E	101	LHG	3	0
28	B	620[B]	SQD	12	0
34	D	411	LHG	8	0
36	c	517	DGD	2	0
24	b	619	CLA	2	0
24	c	507	CLA	1	0
28	B	620[A]	SQD	9	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	a	409	CLA	3	0
28	f	102	SQD	1	0
29	Z	101	LMG	1	0
24	C	503	CLA	2	0
24	D	402	CLA	2	0
24	B	605	CLA	4	0
38	f	101	HEM	2	0
24	b	611	CLA	1	0
24	B	604	CLA	2	0
32	M	101	LMT	1	0
24	d	403	CLA	1	0
26	b	620	BCR	1	0
36	C	516	DGD	1	0
30	C	526	DMS	1	0
36	h	102	DGD	2	0
24	b	613	CLA	2	0
35	o	301	HTG	1	0
24	b	616	CLA	2	0
24	c	502	CLA	2	0
32	m	103	LMT	1	0
33	b	632	GOL	1	0
24	a	407	CLA	4	0
32	A	1017	LMT	3	0
26	J	101	BCR	1	0
27	A	1010	PL9	5	0
30	O	302	DMS	1	0
33	v	203	GOL	2	0
24	B	606	CLA	2	0
32	m	101	LMT	1	0
30	d	413	DMS	3	0
38	V	201	HEM	7	0
29	D	412	LMG	1	0
24	b	617	CLA	2	0
24	B	616	CLA	1	0
26	B	618	BCR	1	0
34	B	621	LHG	1	0
30	a	418	DMS	1	0
26	b	621	BCR	3	0
27	a	414	PL9	5	0
35	b	626	HTG	2	0
24	A	1005	CLA	6	0
24	d	402	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	b	623[B]	SQD	17	0
29	m	102	LMG	3	0
30	B	634	DMS	3	0
24	b	609	CLA	1	0
30	O	301	DMS	2	0
36	H	102	DGD	1	0
24	b	604	CLA	1	0
24	c	506	CLA	2	0
35	D	413	HTG	1	0
24	B	611	CLA	1	0
30	d	414	DMS	1	0
32	M	102	LMT	1	0
24	B	613	CLA	2	0
24	c	512	CLA	3	0
33	B	631	GOL	1	0
25	a	411	PHO	3	0
24	C	510	CLA	7	0
26	D	406	BCR	1	0
24	c	501	CLA	2	0
24	B	612	CLA	1	0
24	c	509	CLA	1	0
35	B	629	HTG	1	0
26	d	404	BCR	1	0
24	c	508	CLA	1	0
26	C	514	BCR	2	0
24	B	603	CLA	2	0
28	D	408	SQD	1	0
24	B	610	CLA	4	0
32	b	625	LMT	1	0
29	c	521	LMG	1	0
24	C	512	CLA	2	0
24	C	507	CLA	3	0
24	c	511	CLA	1	0
30	b	635	DMS	3	0
30	D	417	DMS	1	0
24	C	509	CLA	2	0
26	c	514	BCR	3	0
28	b	623[A]	SQD	2	0
24	b	607	CLA	5	0
34	b	624	LHG	3	0
28	A	1016	SQD	1	0
25	D	404	PHO	5	0

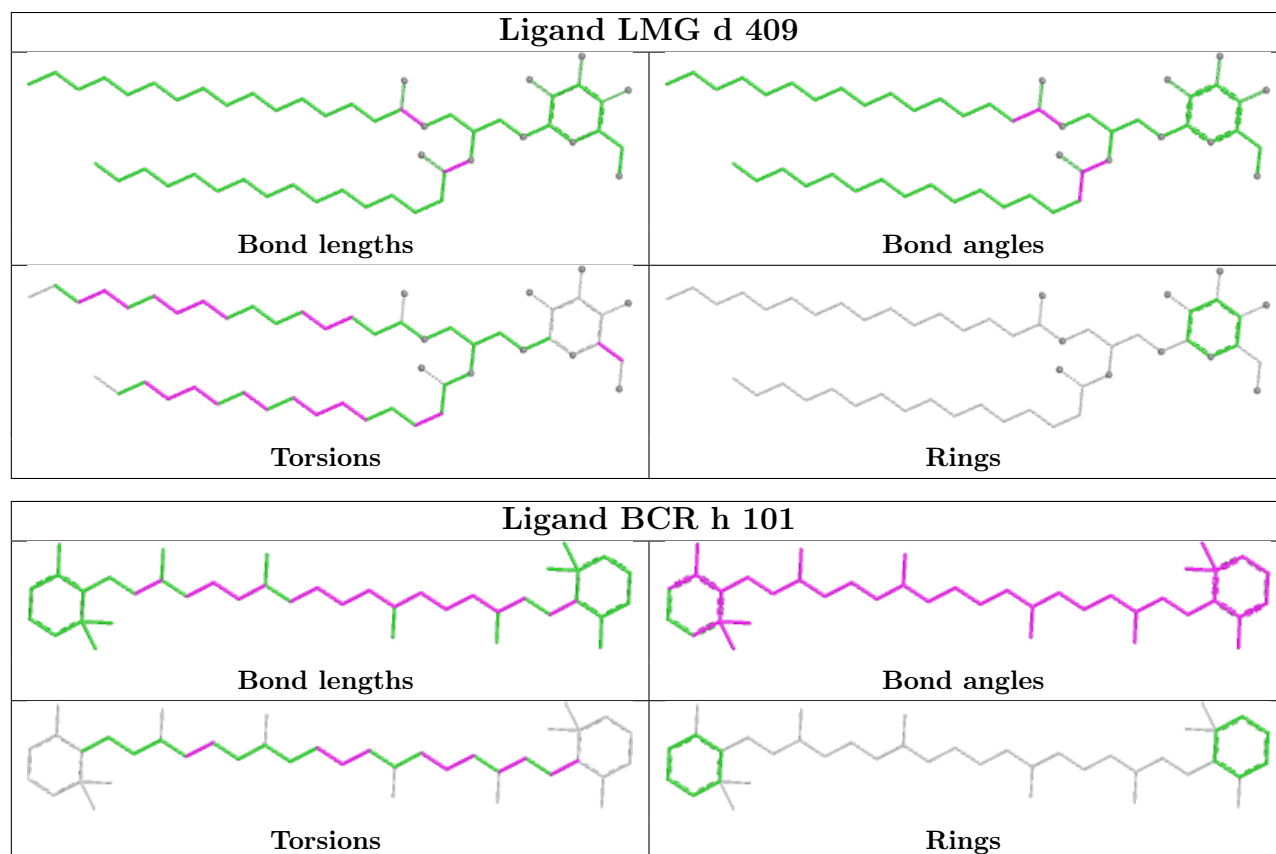
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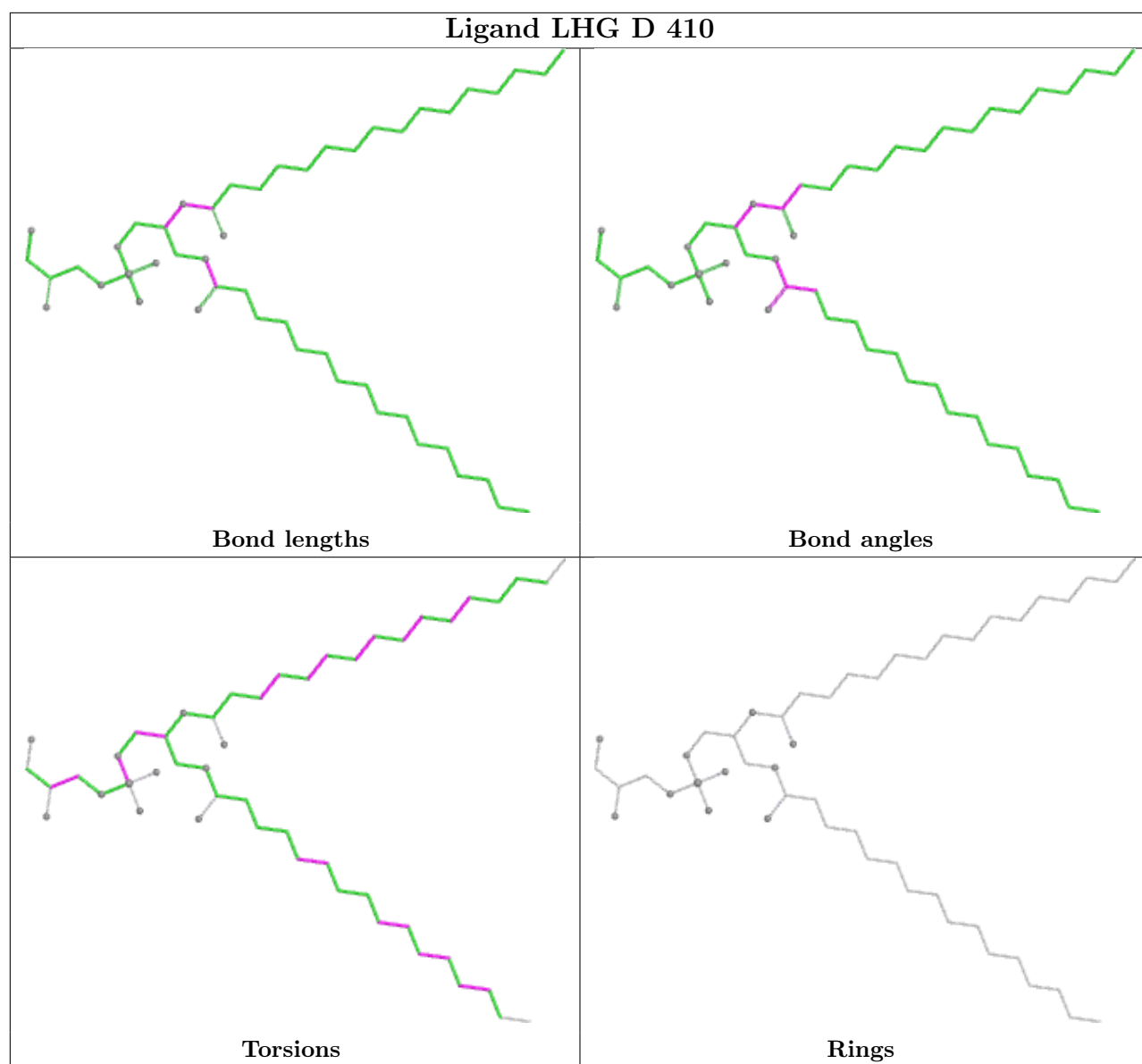
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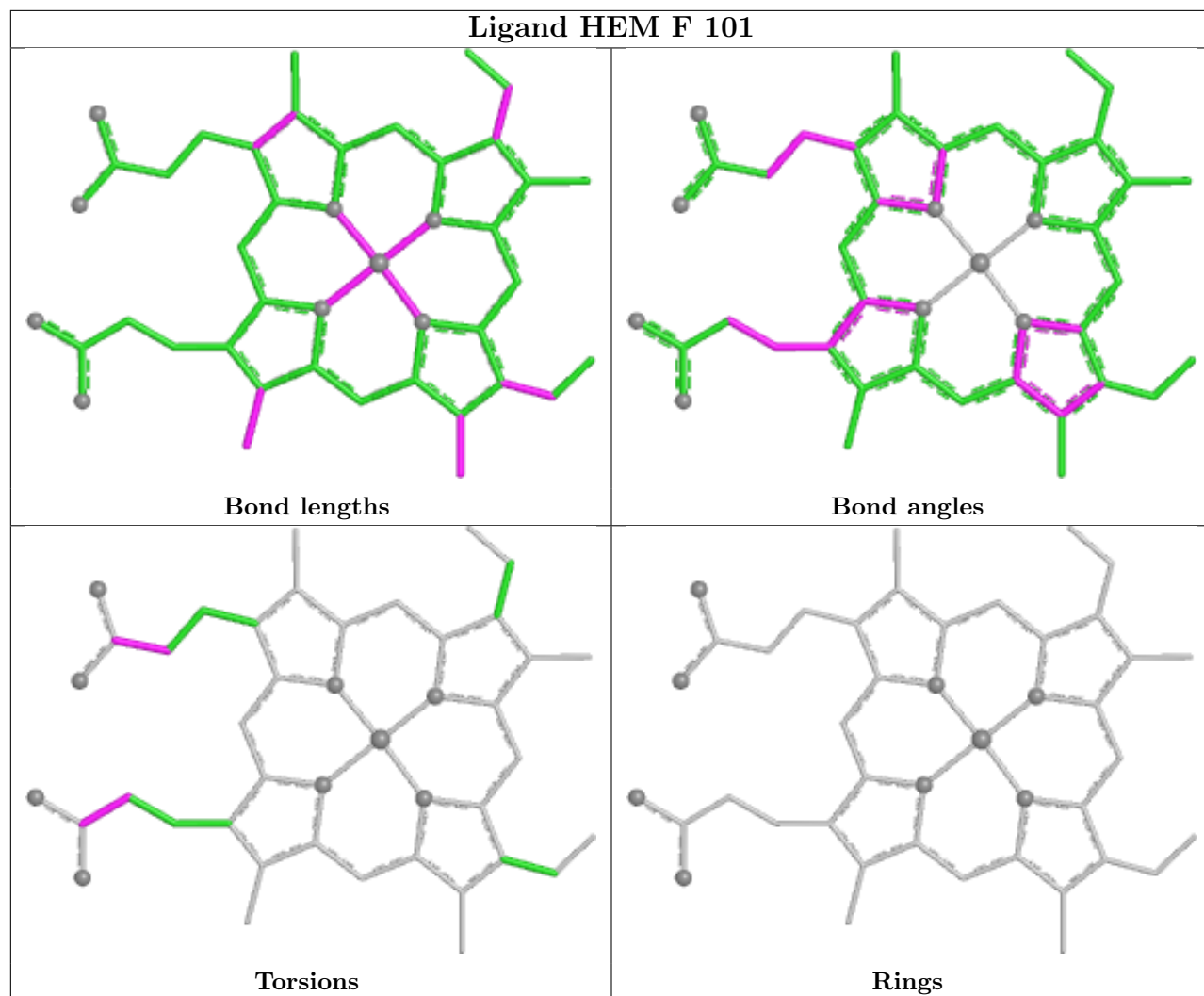
Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	C	513	CLA	1	0
24	A	1008	CLA	2	0
32	i	102	LMT	1	0
24	B	601	CLA	1	0
30	B	632	DMS	1	0
34	d	406	LHG	4	0
38	v	201	HEM	6	0
24	B	607	CLA	1	0
24	C	504	CLA	3	0
24	C	501	CLA	1	0
34	d	407	LHG	1	0
26	y	101	BCR	1	0
24	a	408	CLA	4	0
24	C	506	CLA	2	0
26	B	617	BCR	1	0
32	a	402	LMT	2	0
26	k	102	BCR	2	0
24	c	513	CLA	2	0
24	c	503	CLA	3	0
29	B	622	LMG	2	0
24	b	608	CLA	3	0
24	c	505	CLA	4	0
24	B	614	CLA	2	0
24	C	508	CLA	3	0
32	A	1018	LMT	1	0
24	A	1006	CLA	1	0
24	b	606	CLA	3	0
36	C	515	DGD	3	0
24	B	615	CLA	1	0
34	D	409	LHG	4	0
24	C	505	CLA	4	0
24	b	615	CLA	4	0
30	c	529	DMS	2	0
24	D	403	CLA	4	0
32	a	416	LMT	1	0
24	b	605	CLA	1	0
30	A	1014	DMS	3	0
28	A	1011	SQD	2	0
29	c	519	LMG	1	0

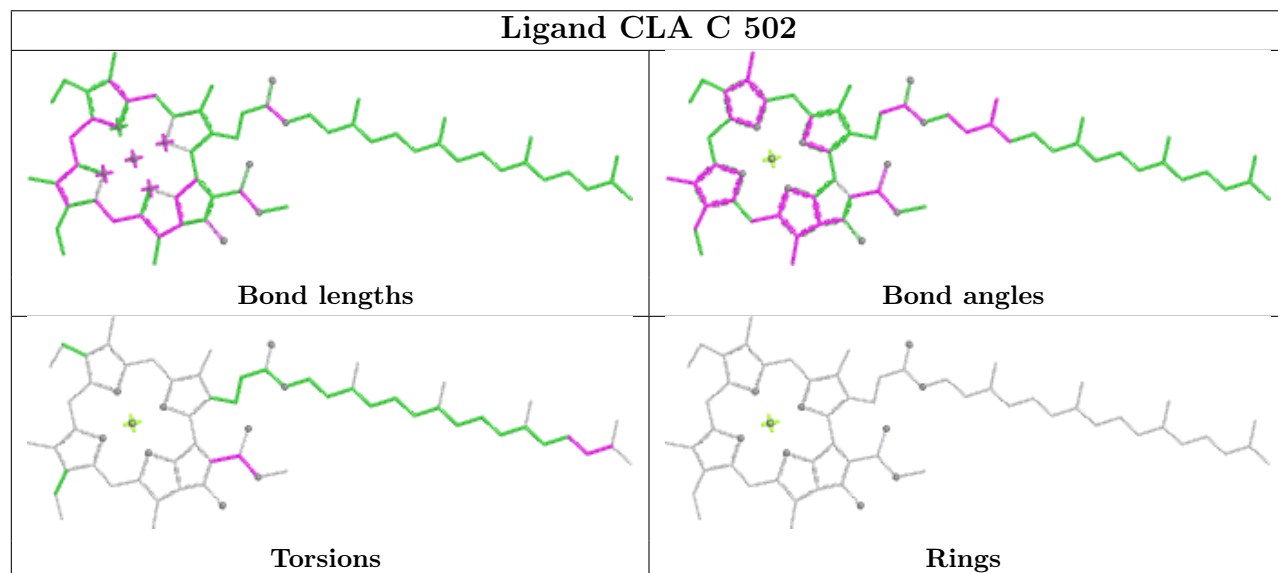
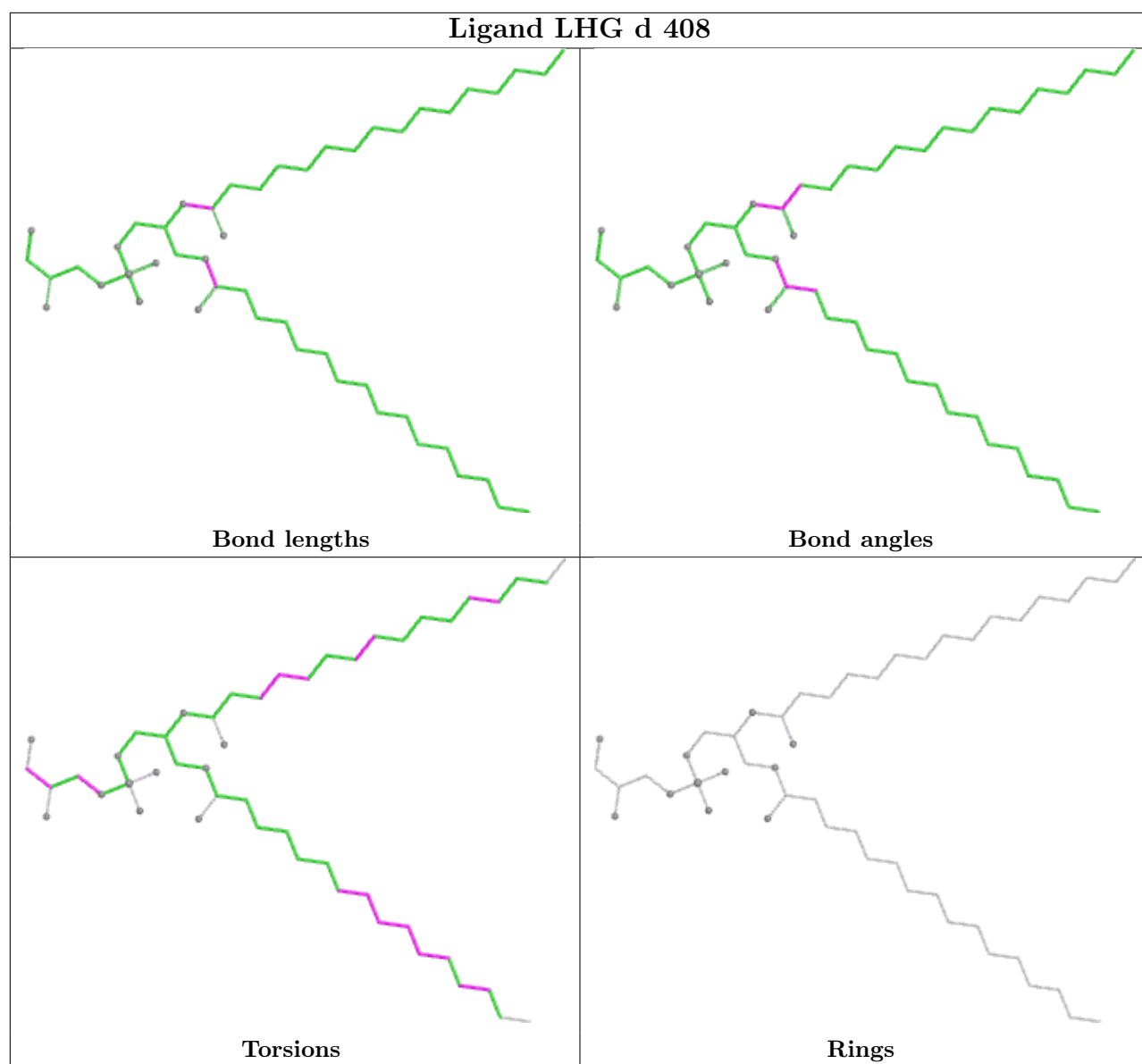
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

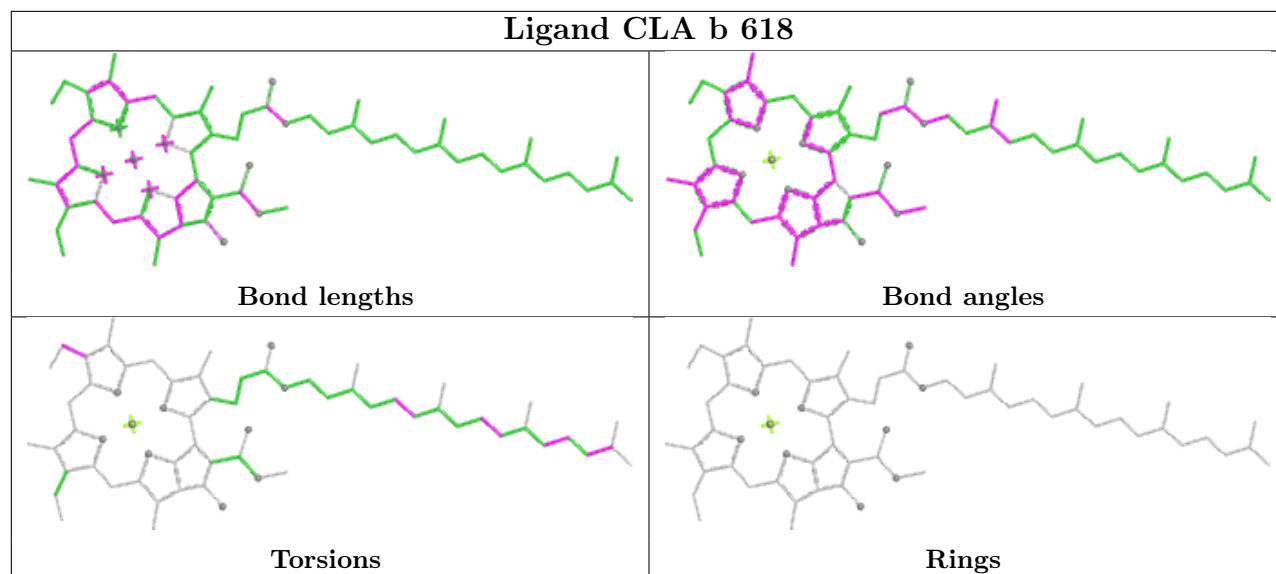




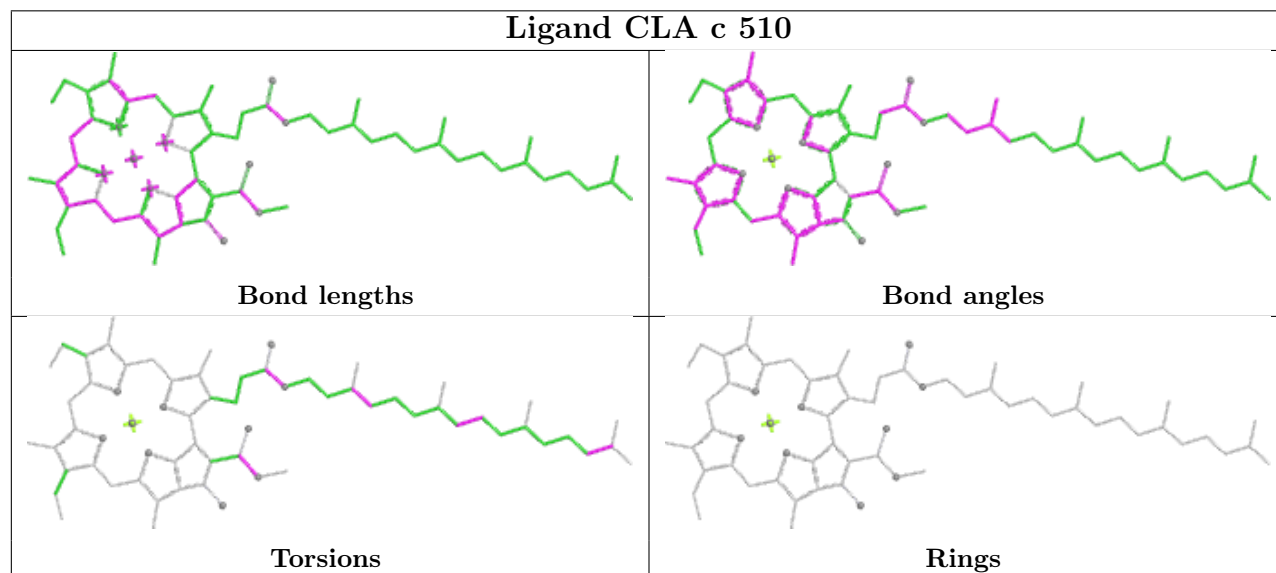




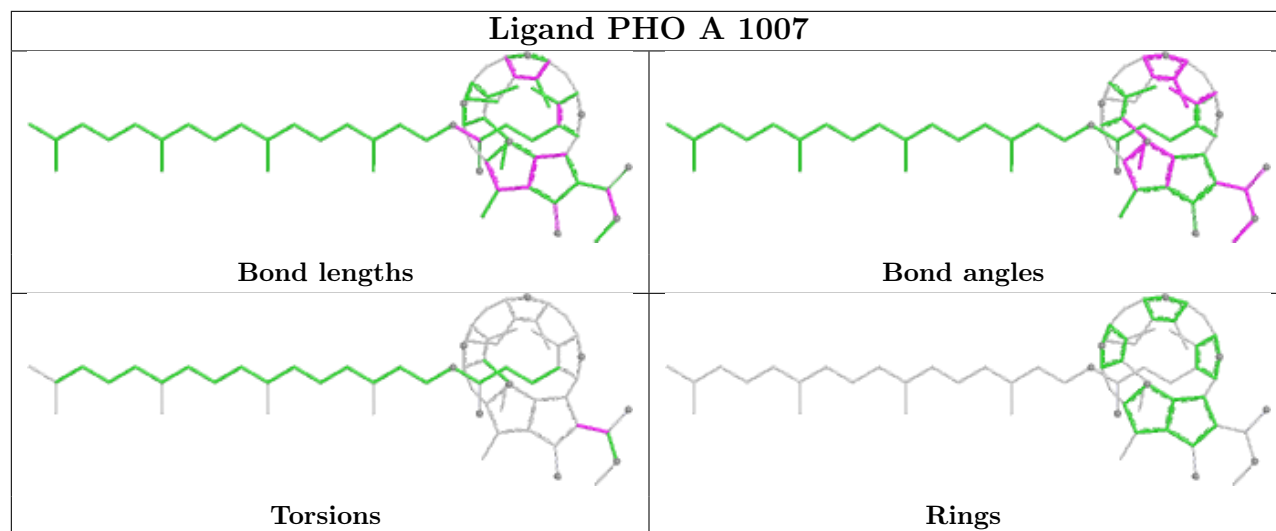
Ligand CLA b 618

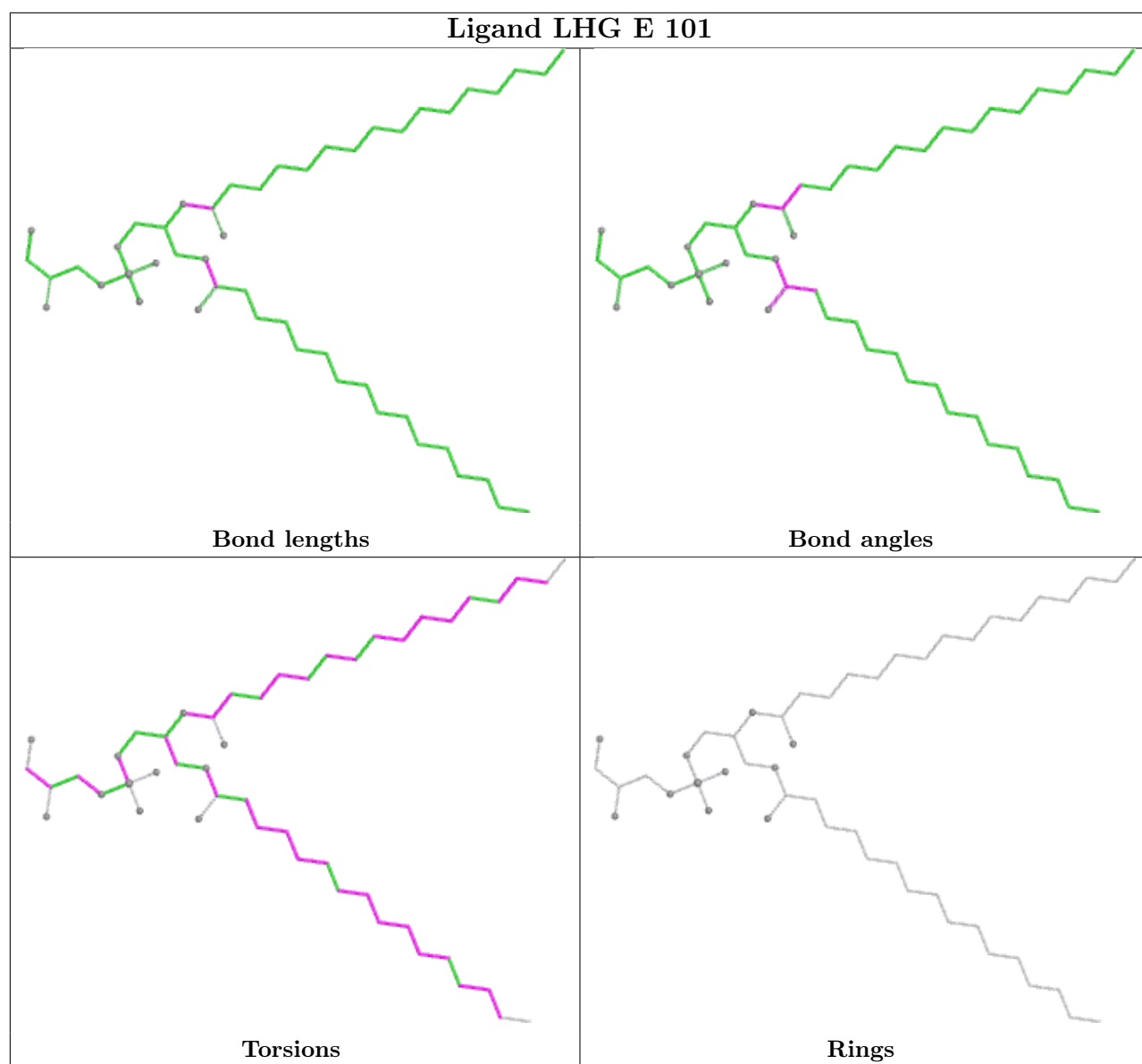


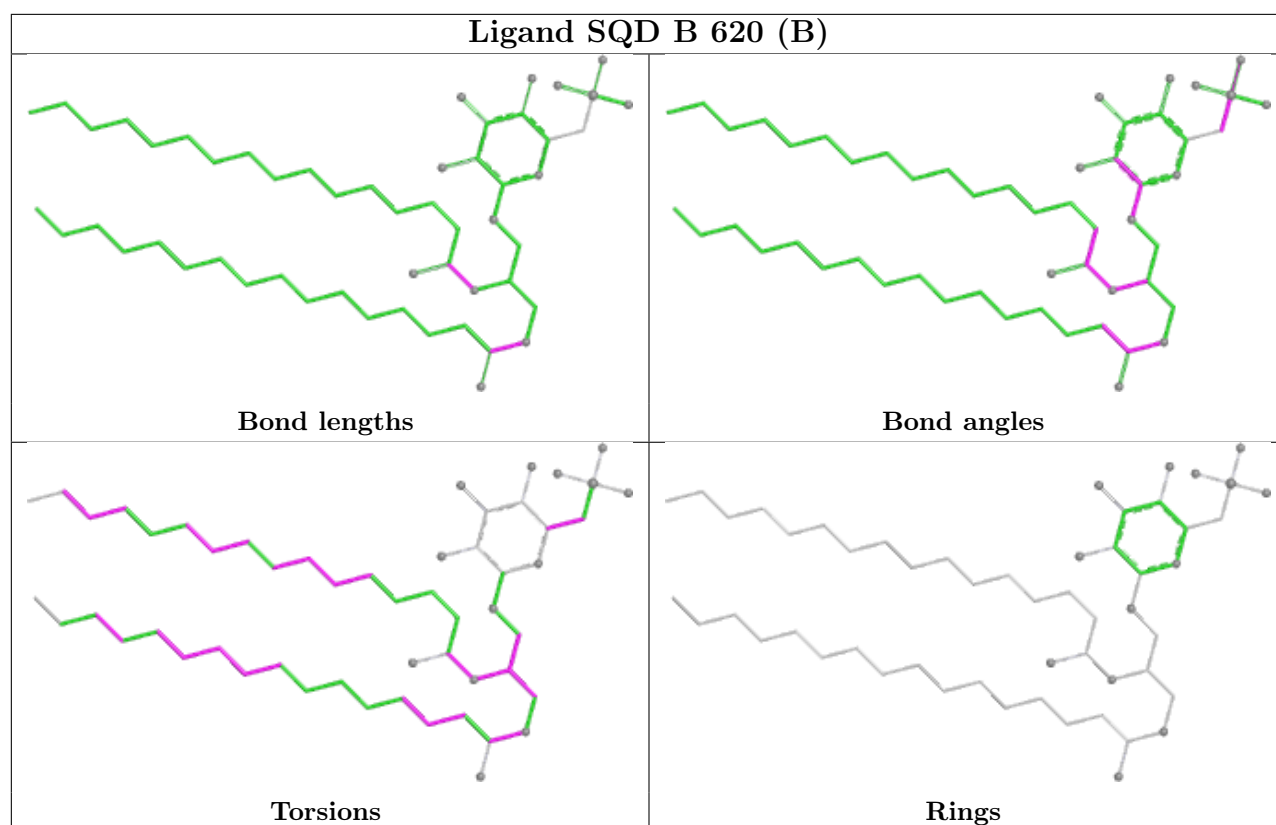
Ligand CLA c 510

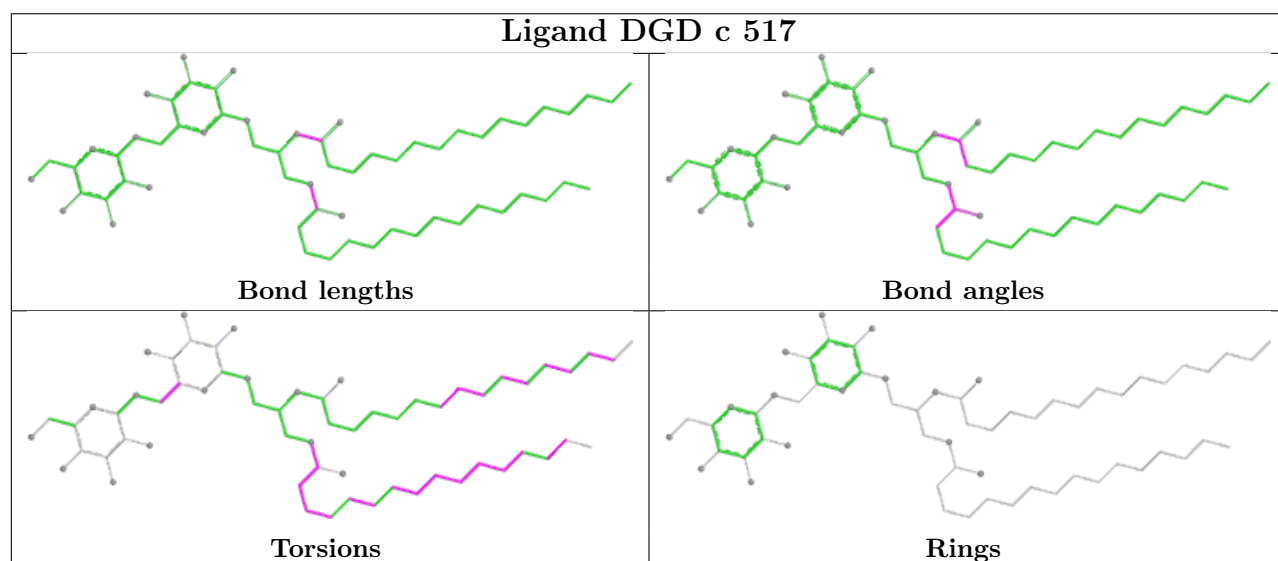
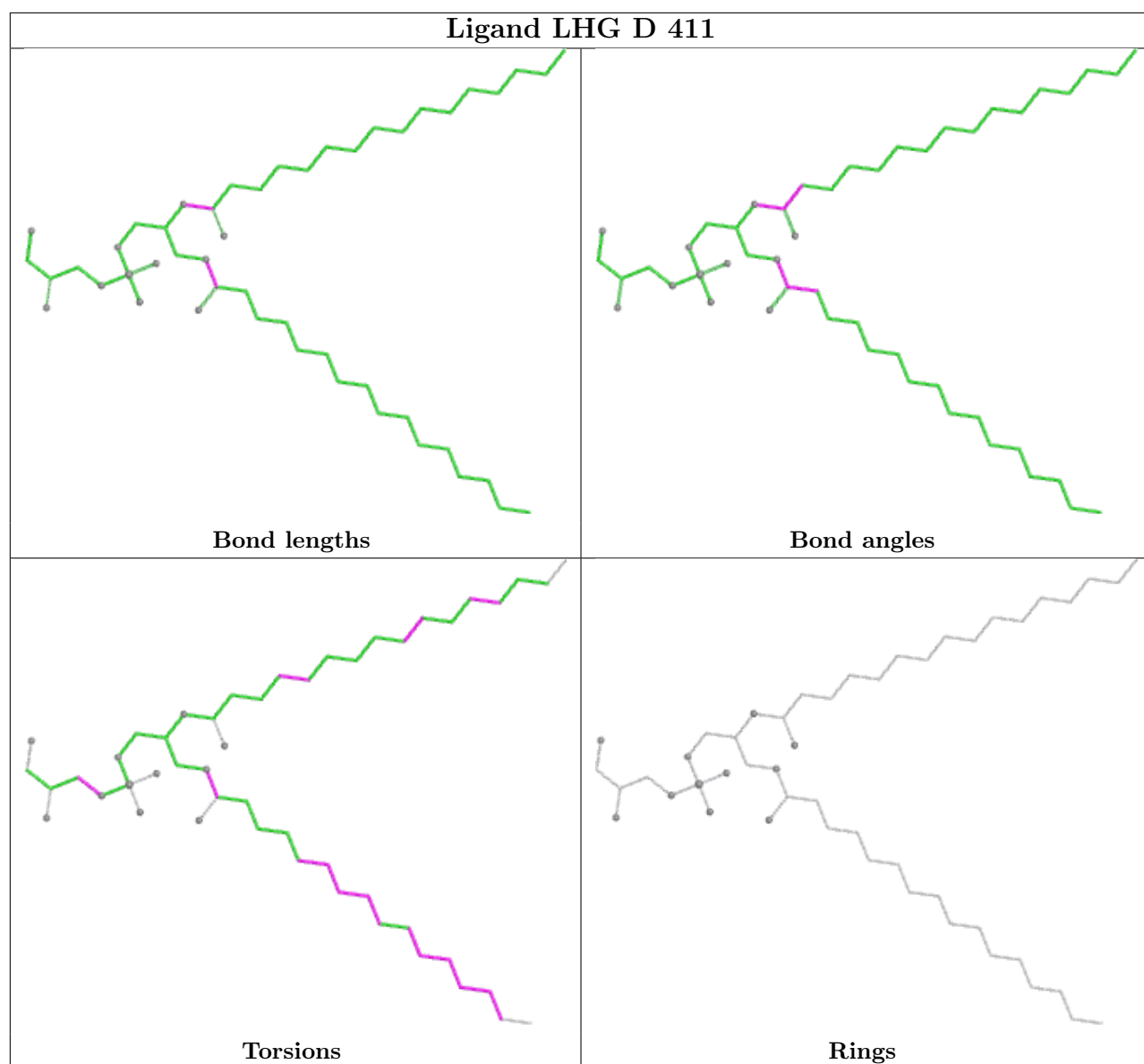


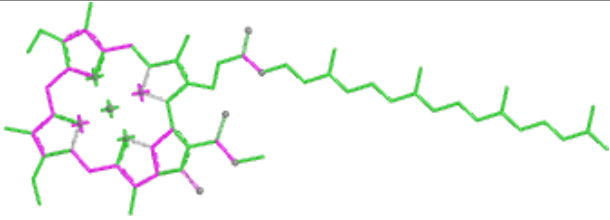
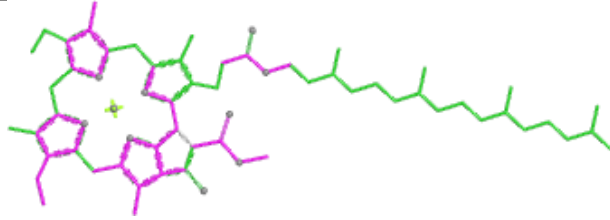
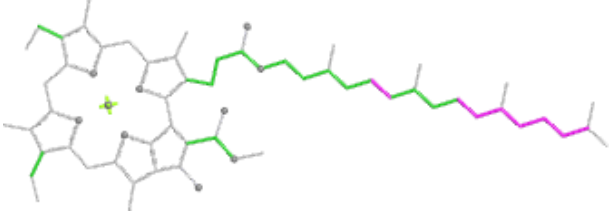
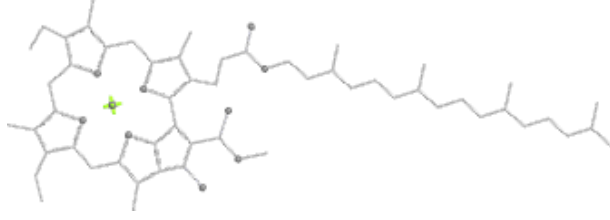
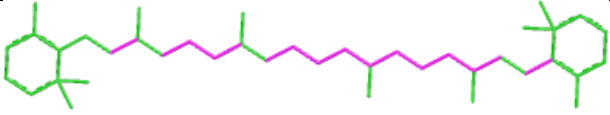
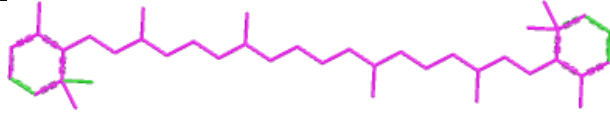
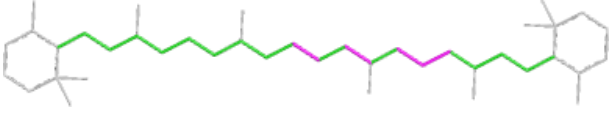
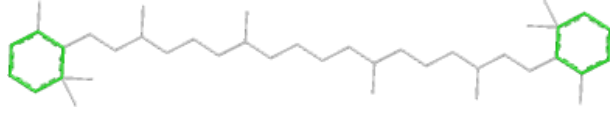
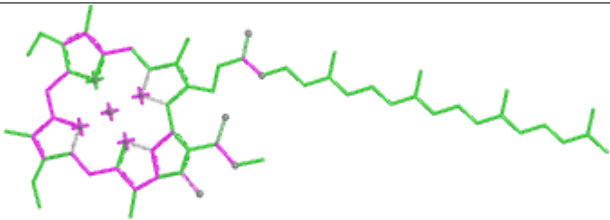
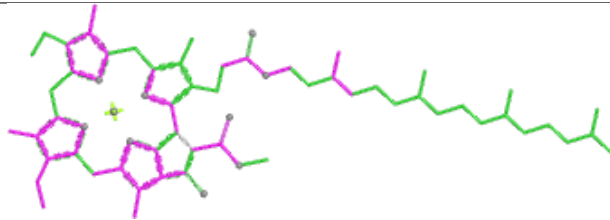
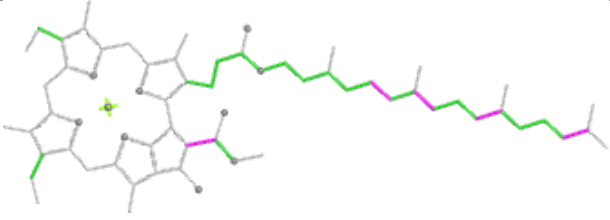
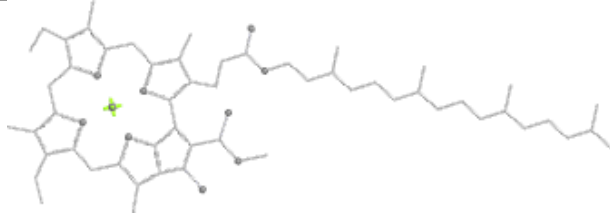
Ligand PHO A 1007

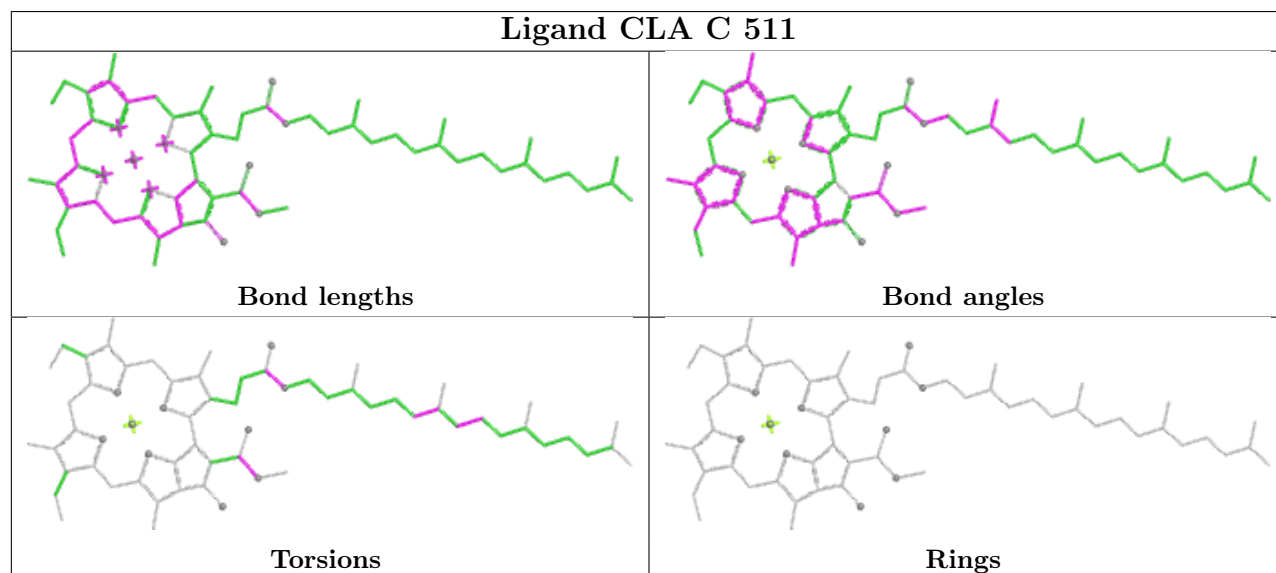
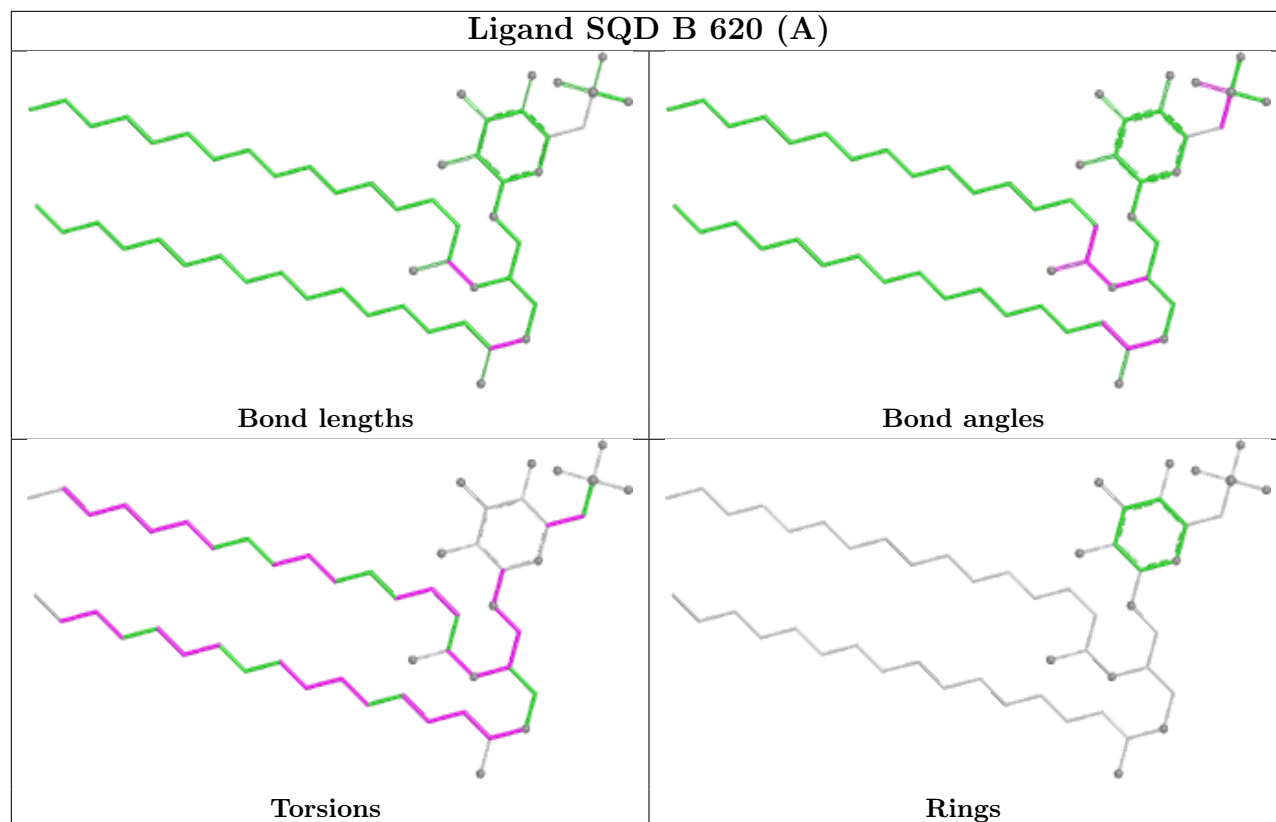




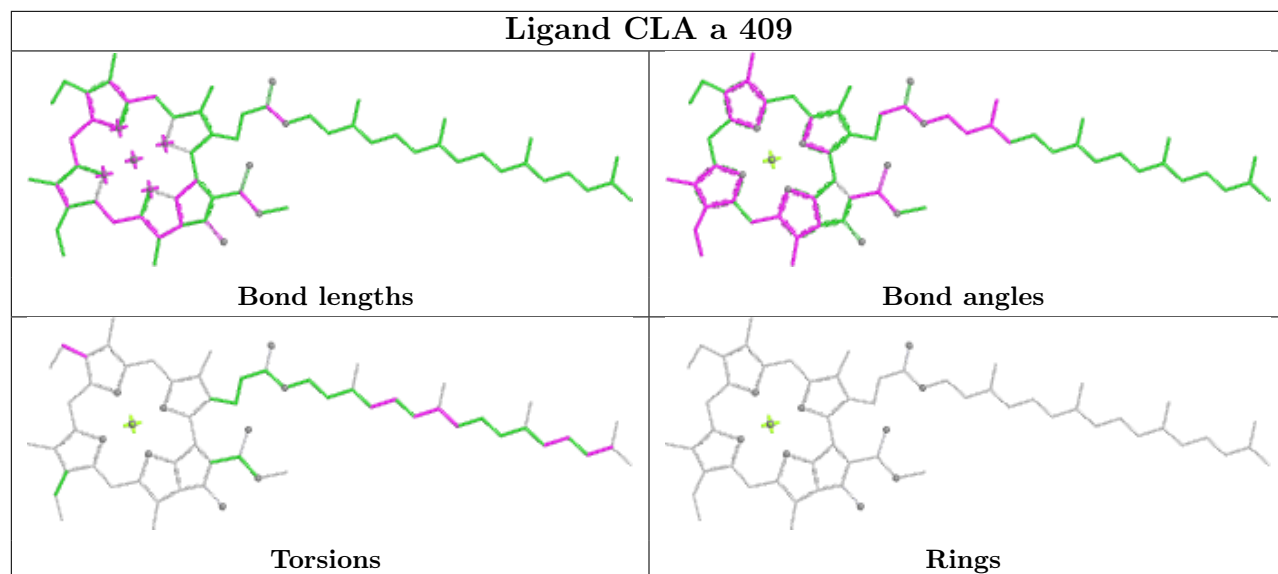




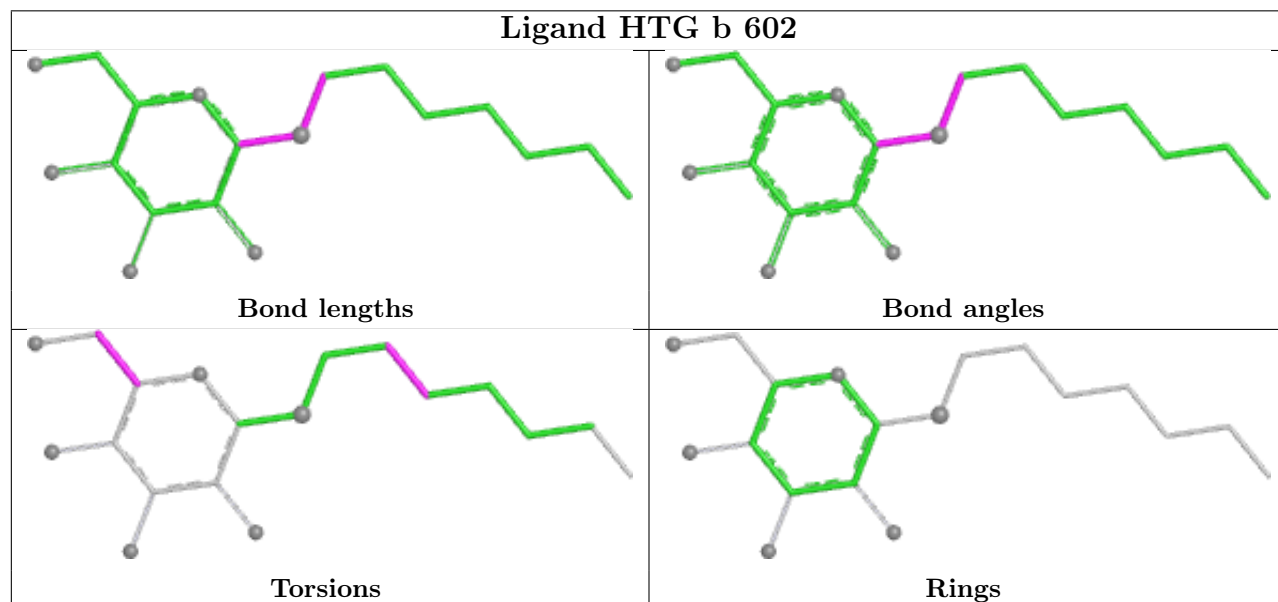
Ligand CLA b 619	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR a 413	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA c 507	
 Bond lengths	 Bond angles
 Torsions	 Rings

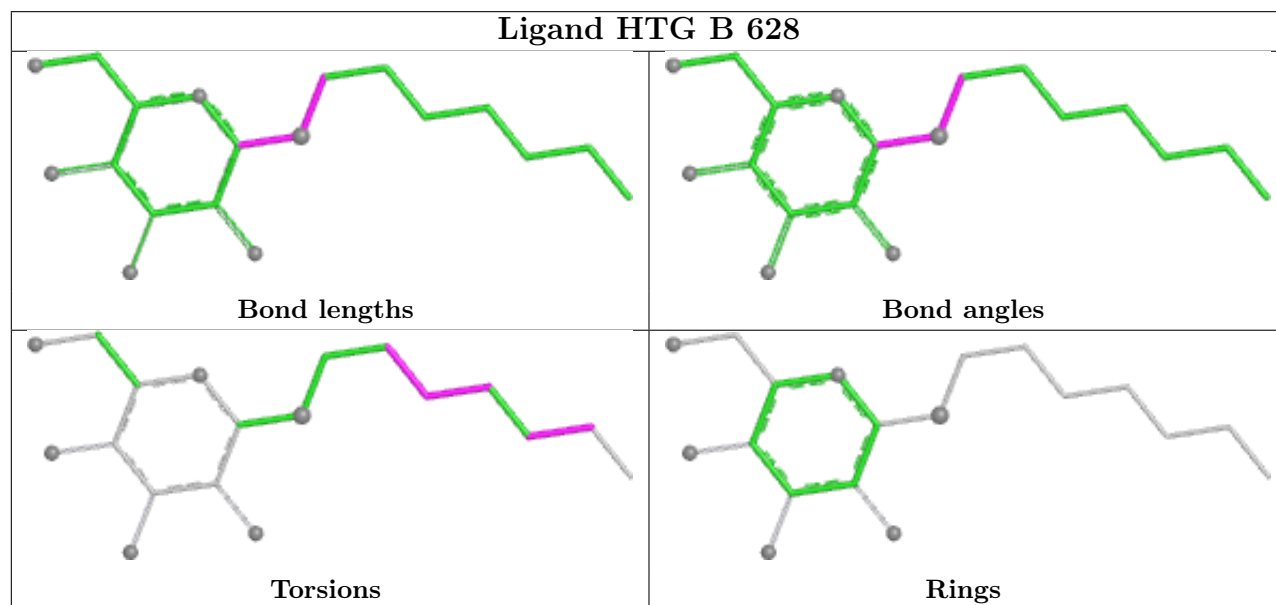
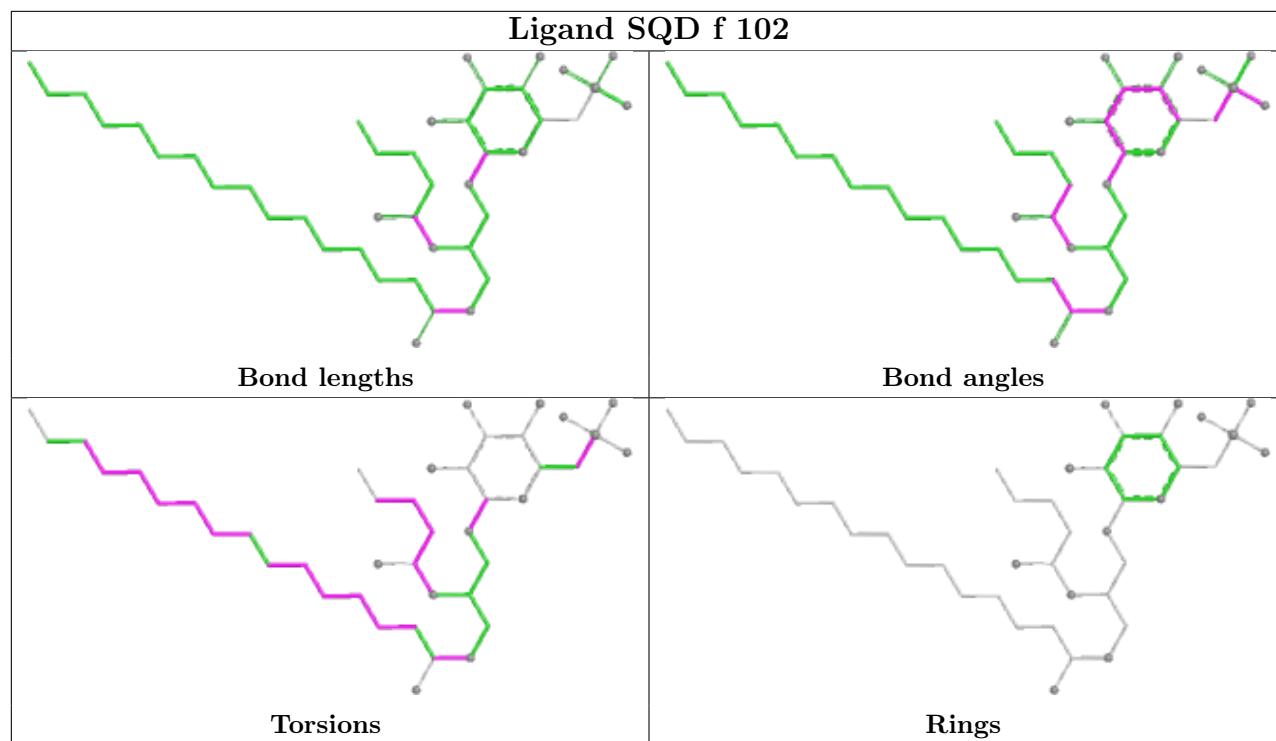


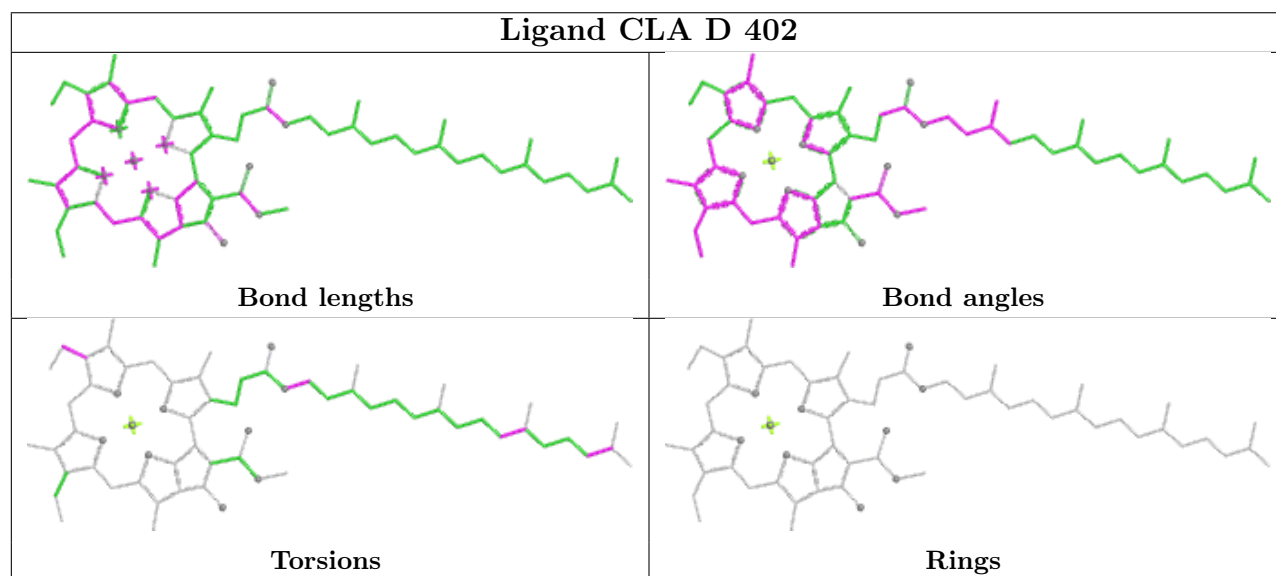
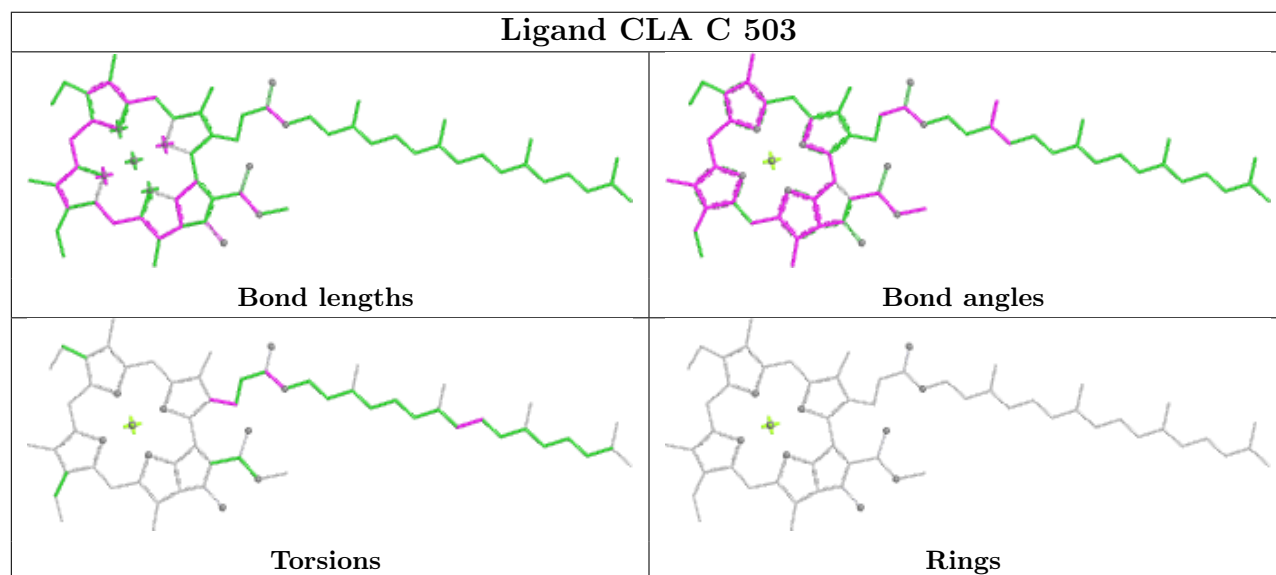
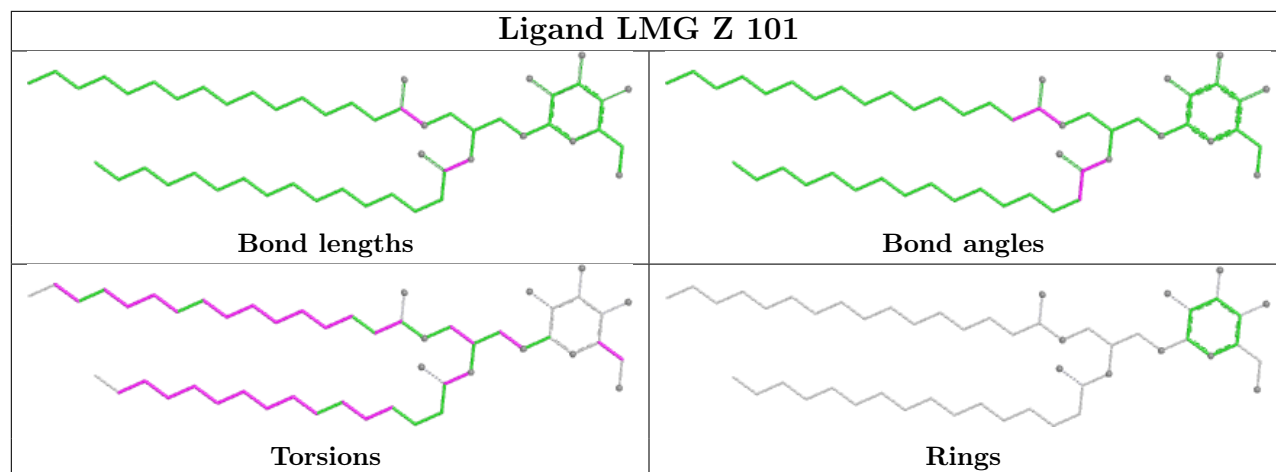
Ligand CLA a 409

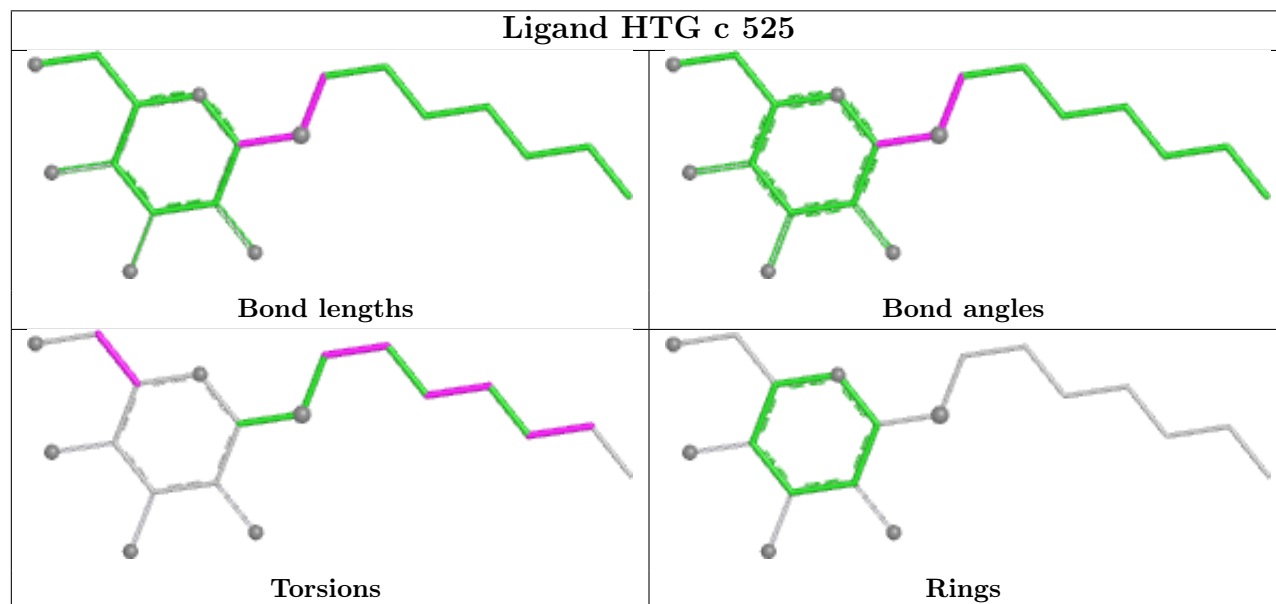
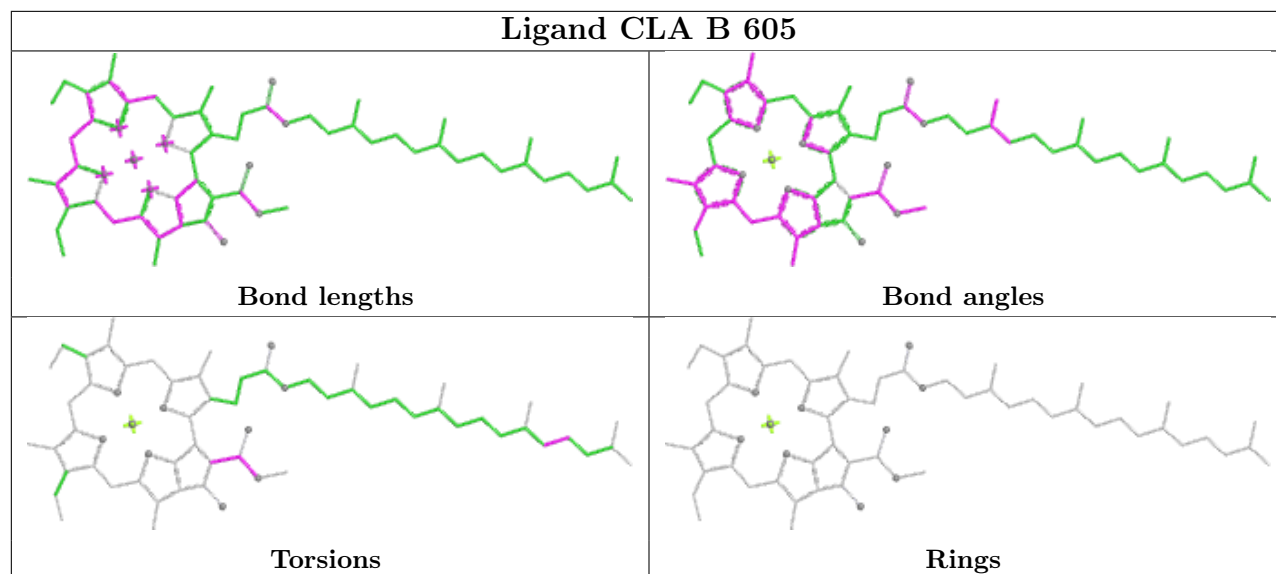


Ligand HTG b 602

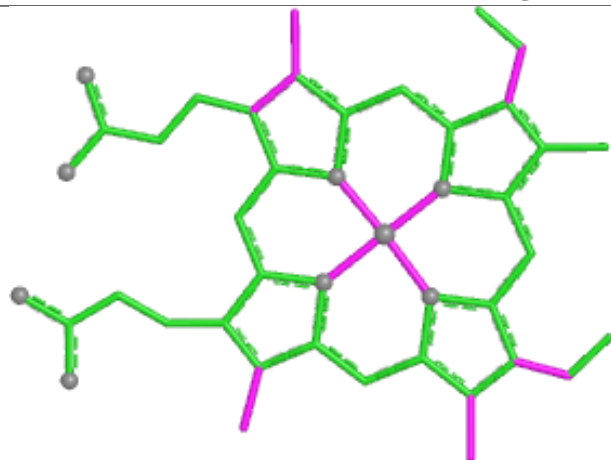




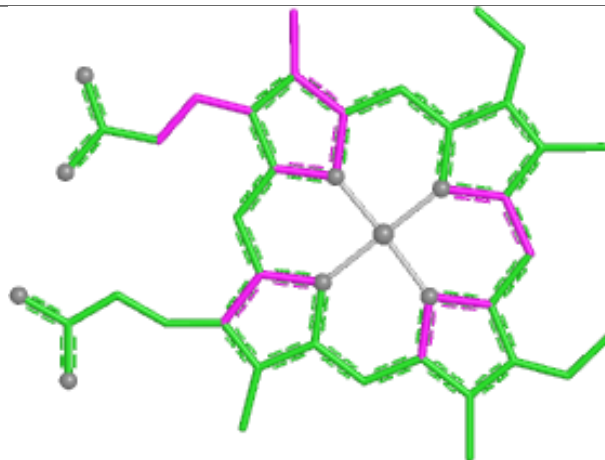




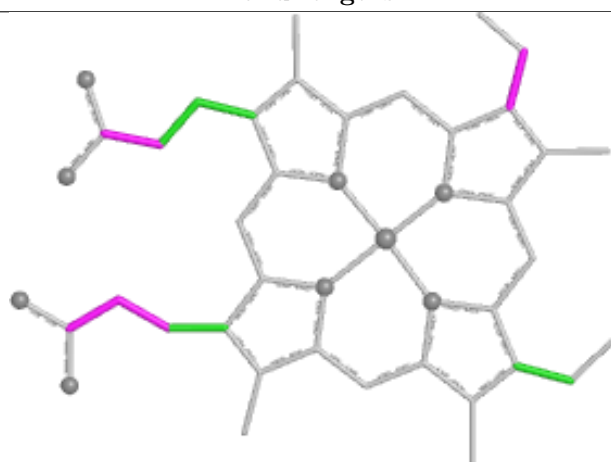
Ligand HEM f 101



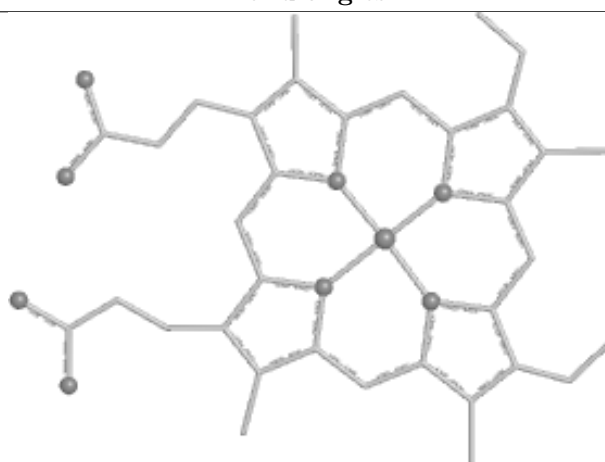
Bond lengths



Bond angles

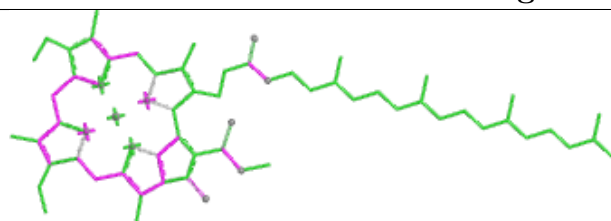


Torsions

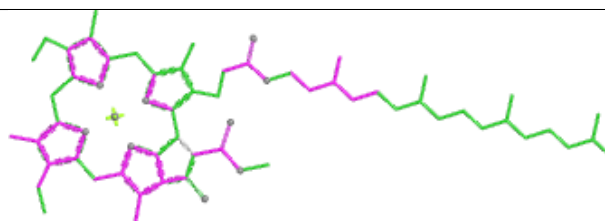


Rings

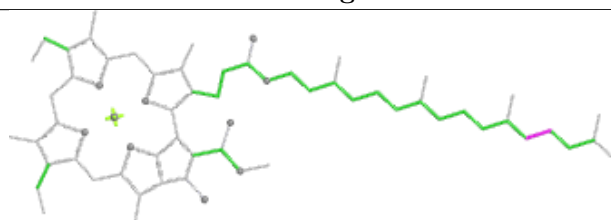
Ligand CLA b 611



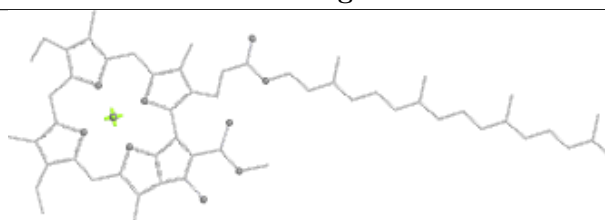
Bond lengths



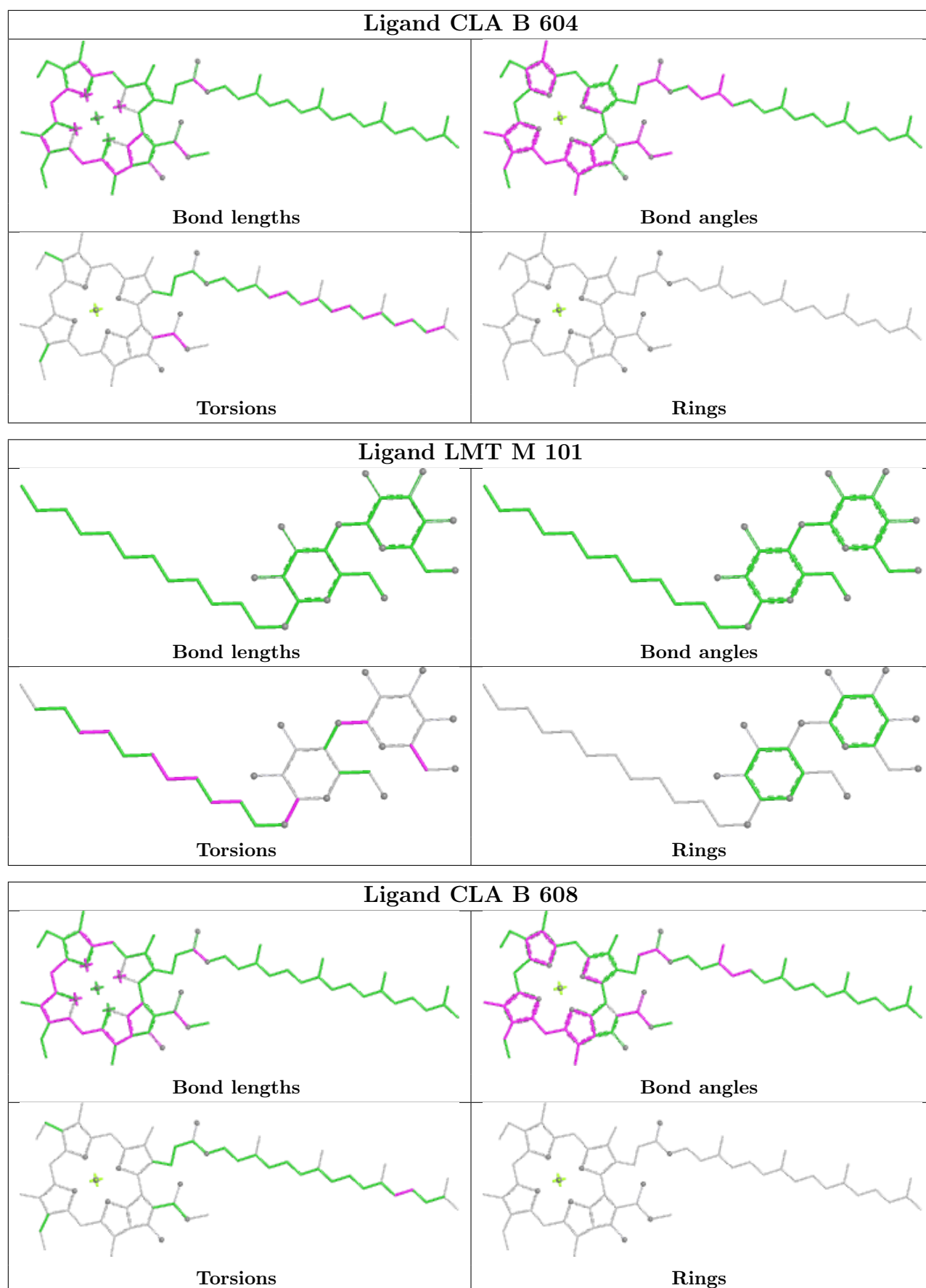
Bond angles



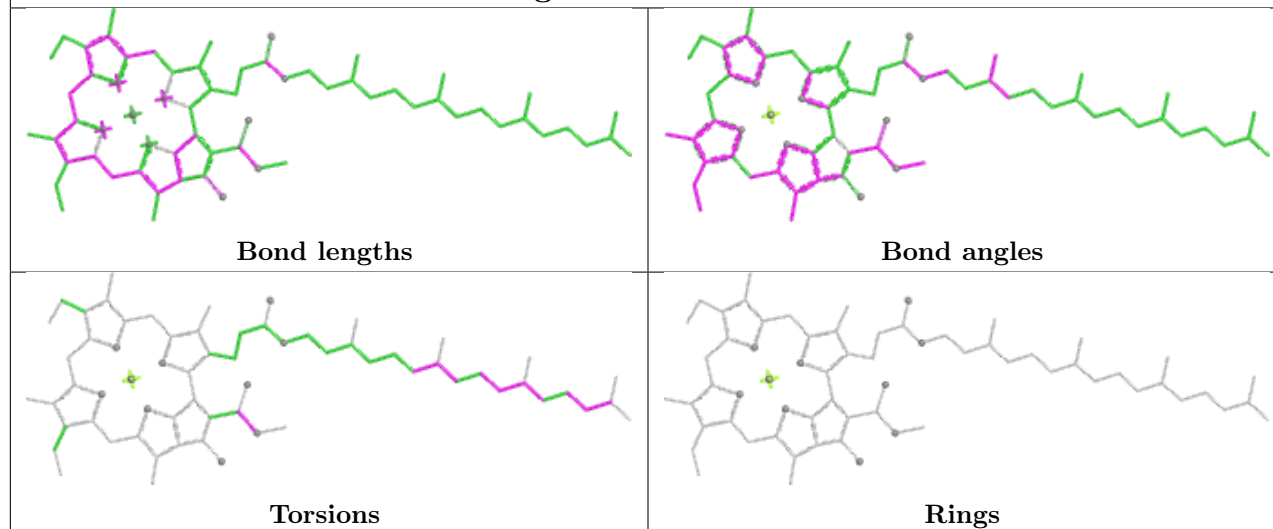
Torsions



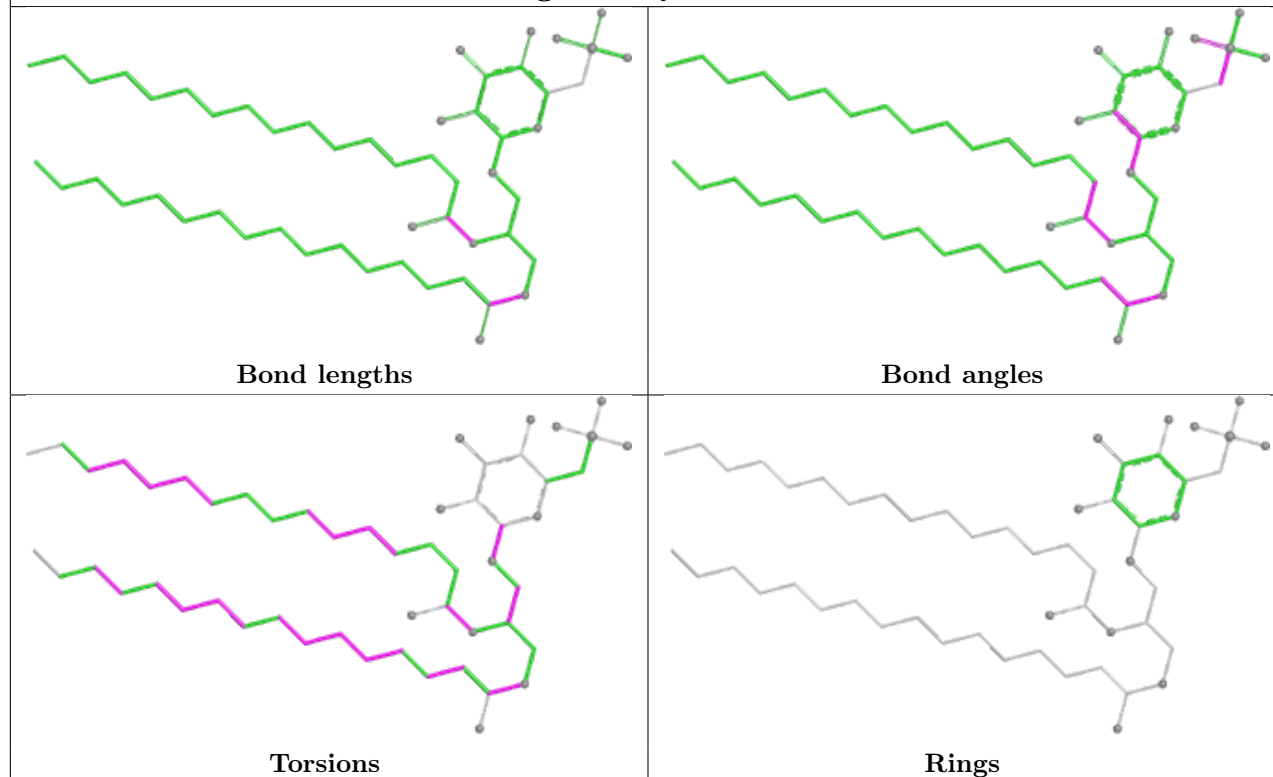
Rings



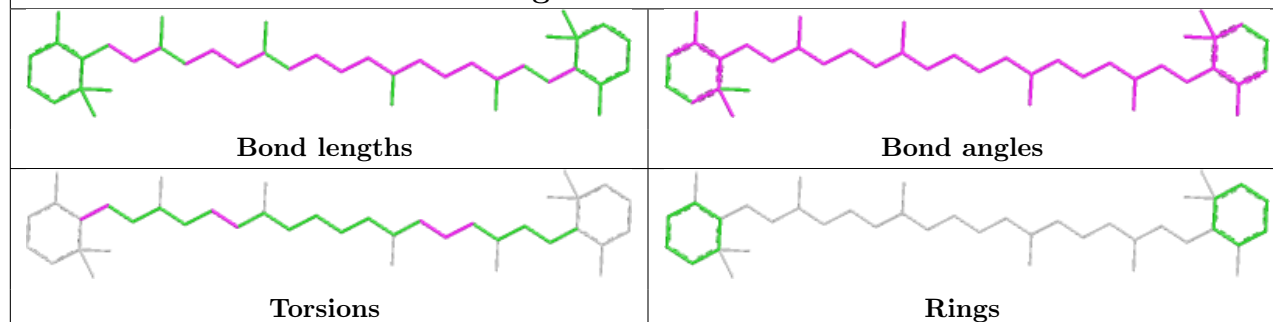
Ligand CLA d 403

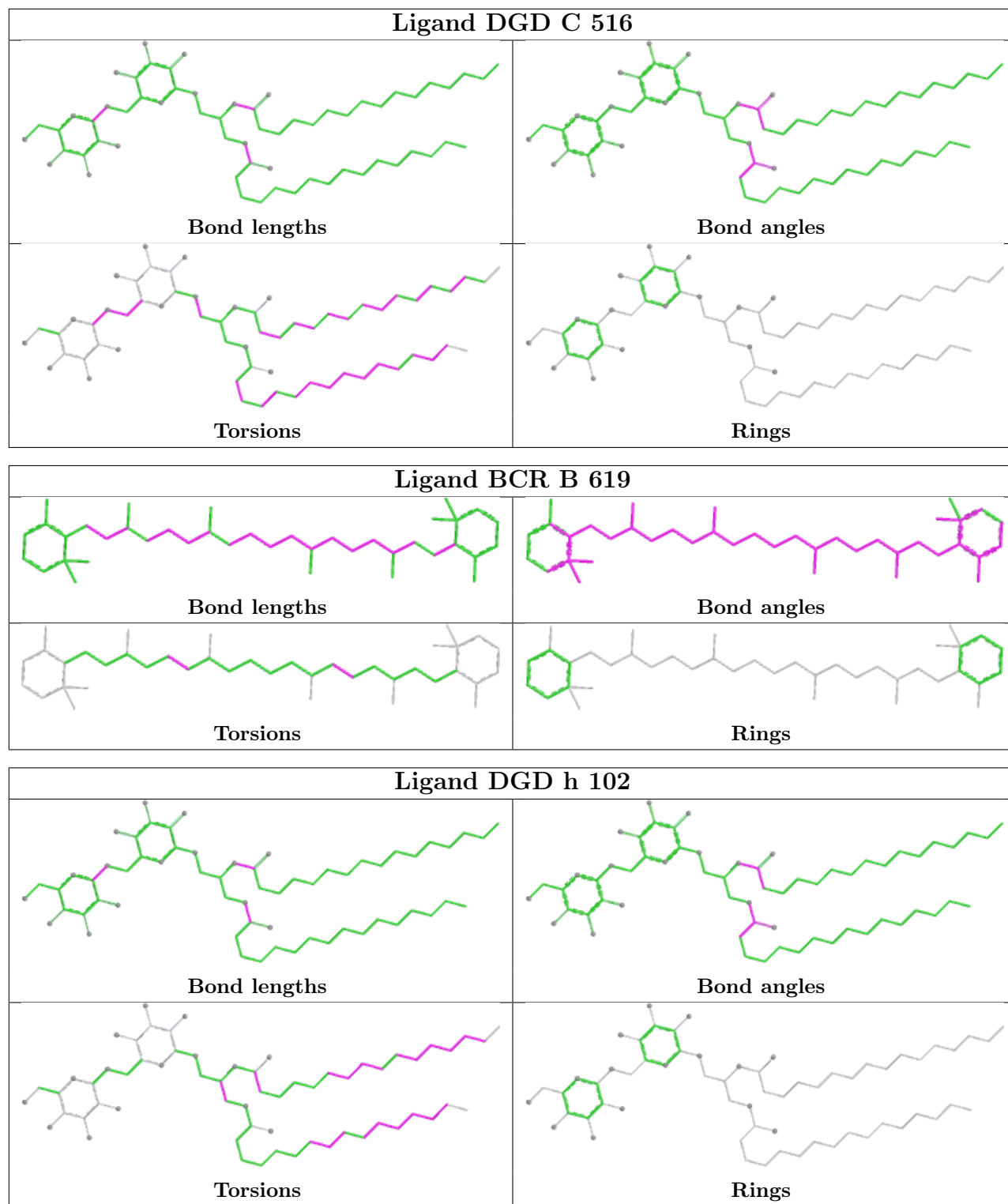


Ligand SQD a 401

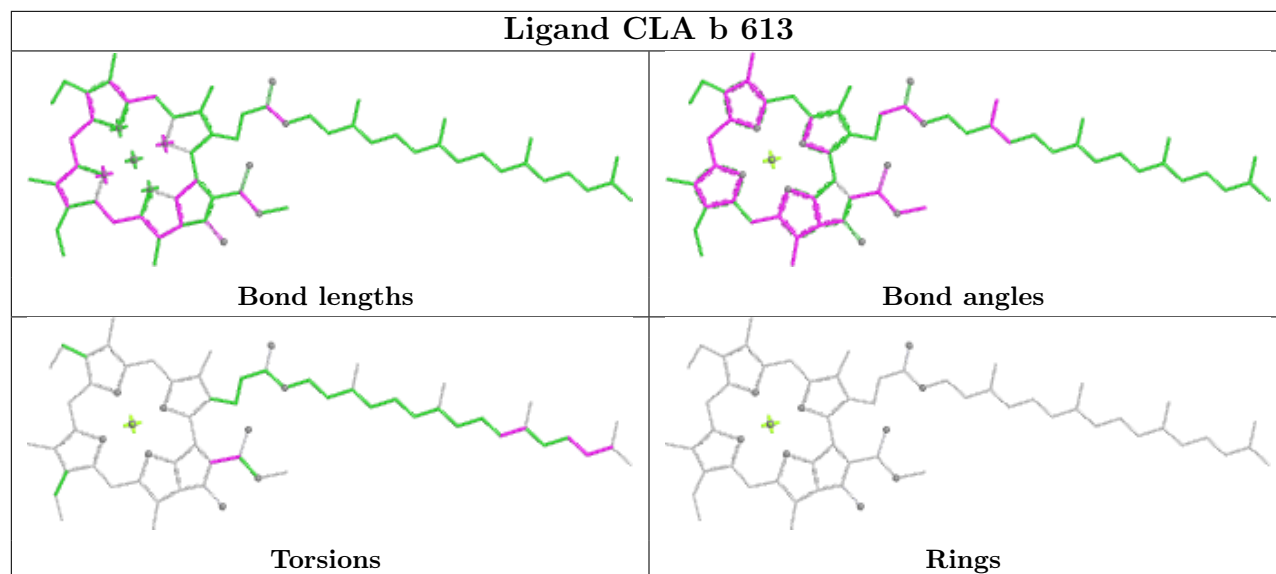


Ligand BCR b 620

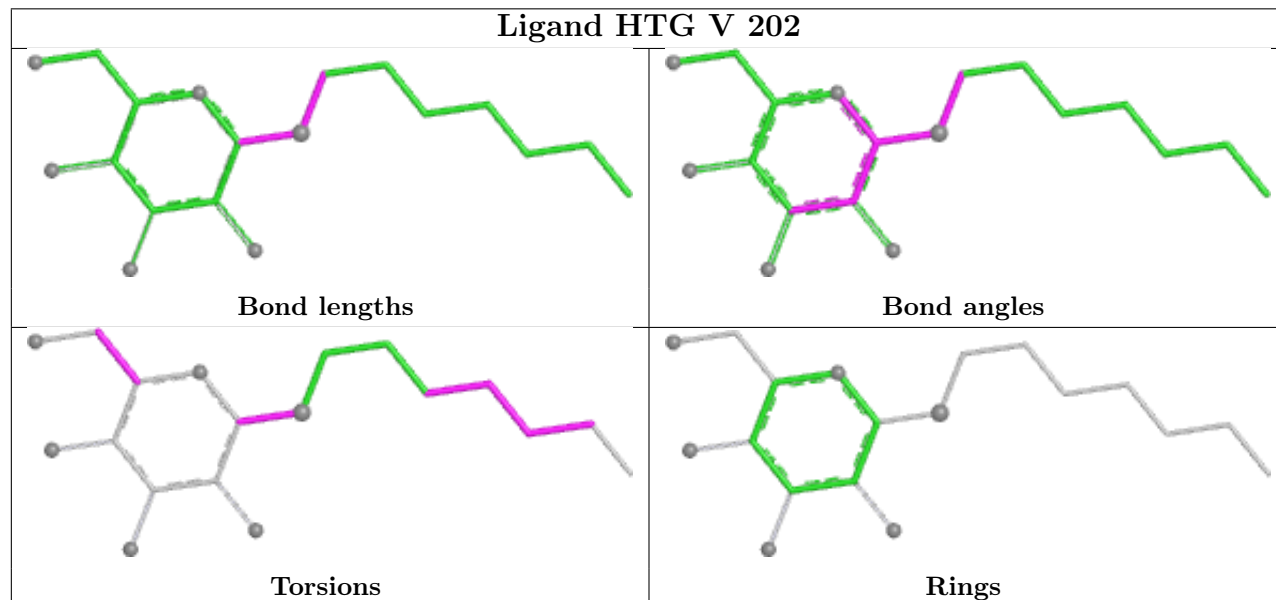




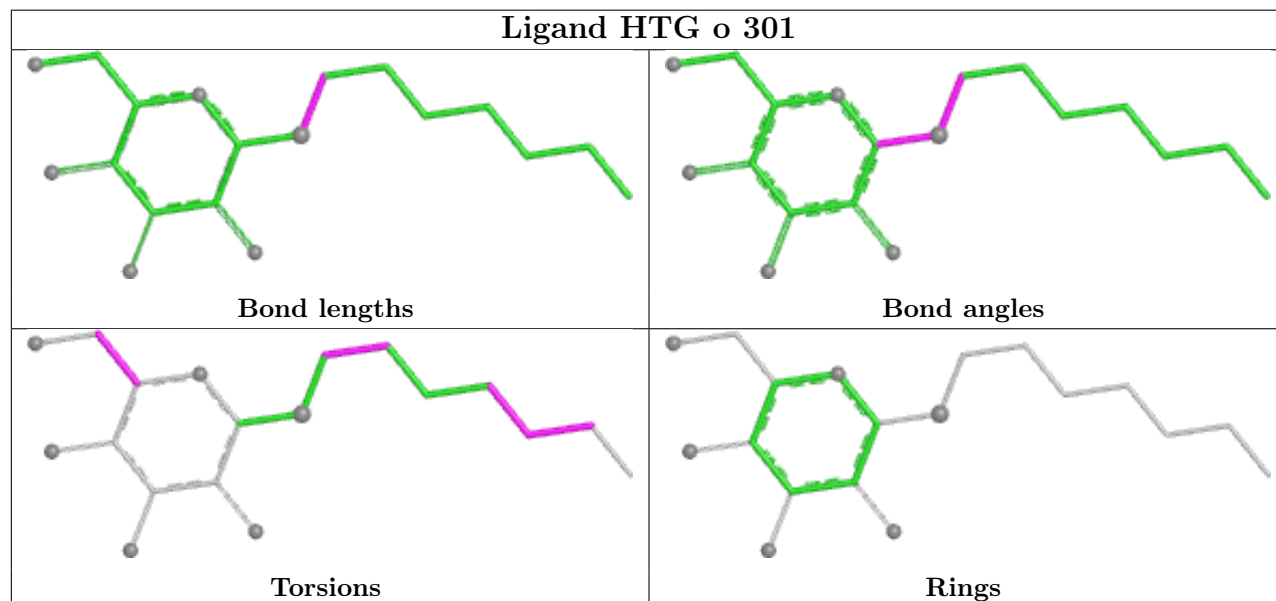
Ligand CLA b 613

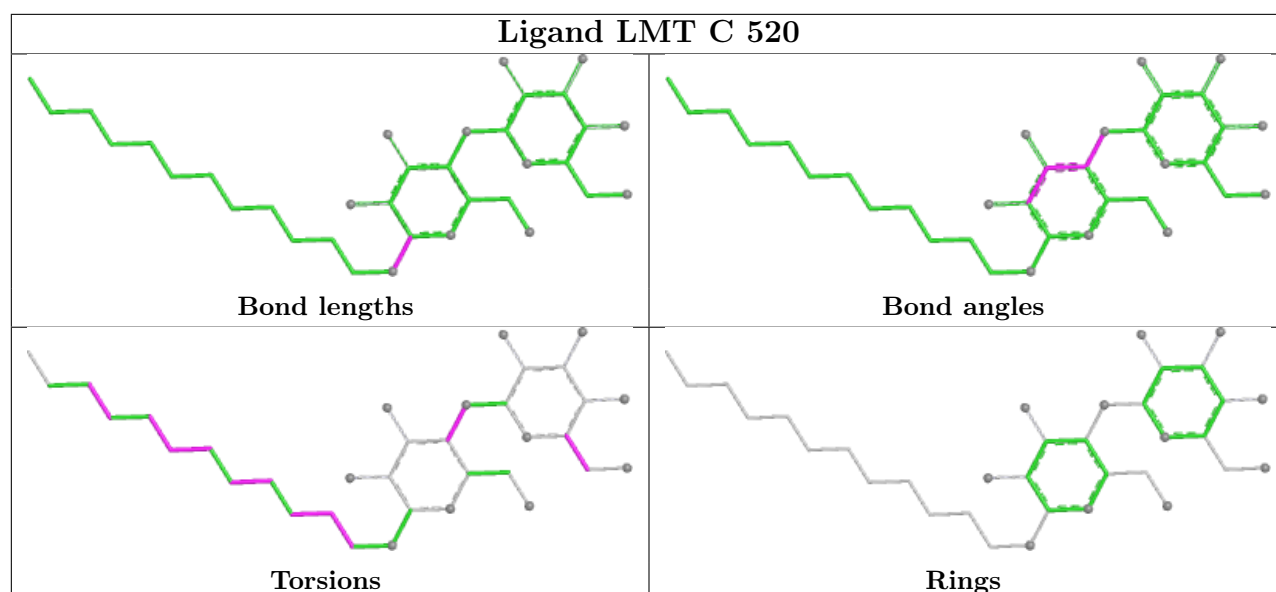
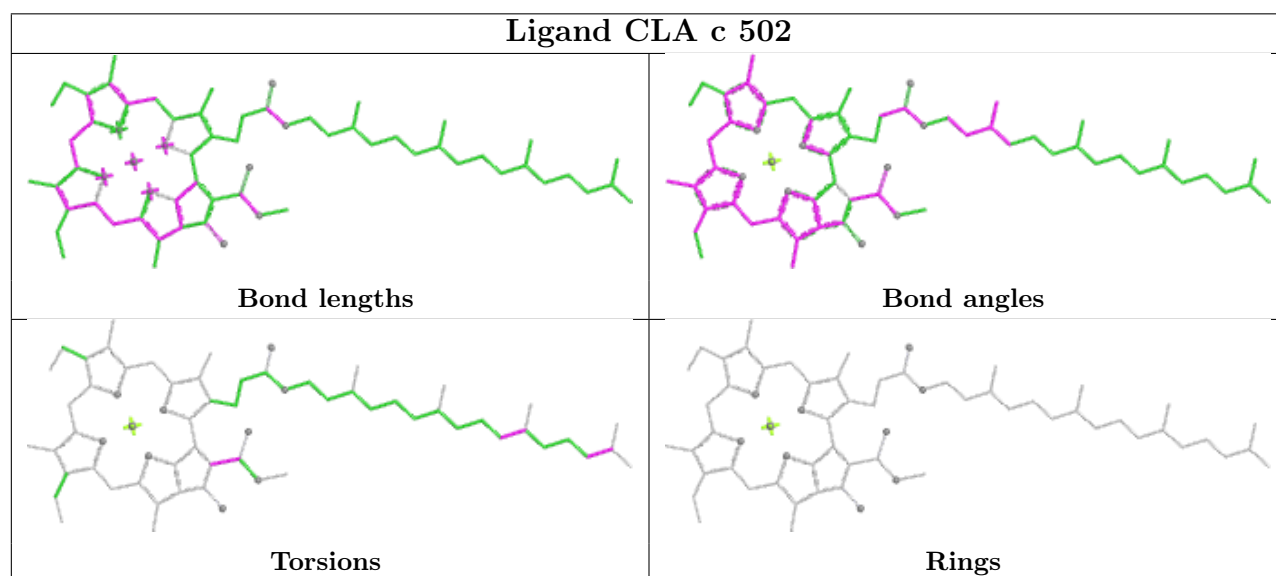
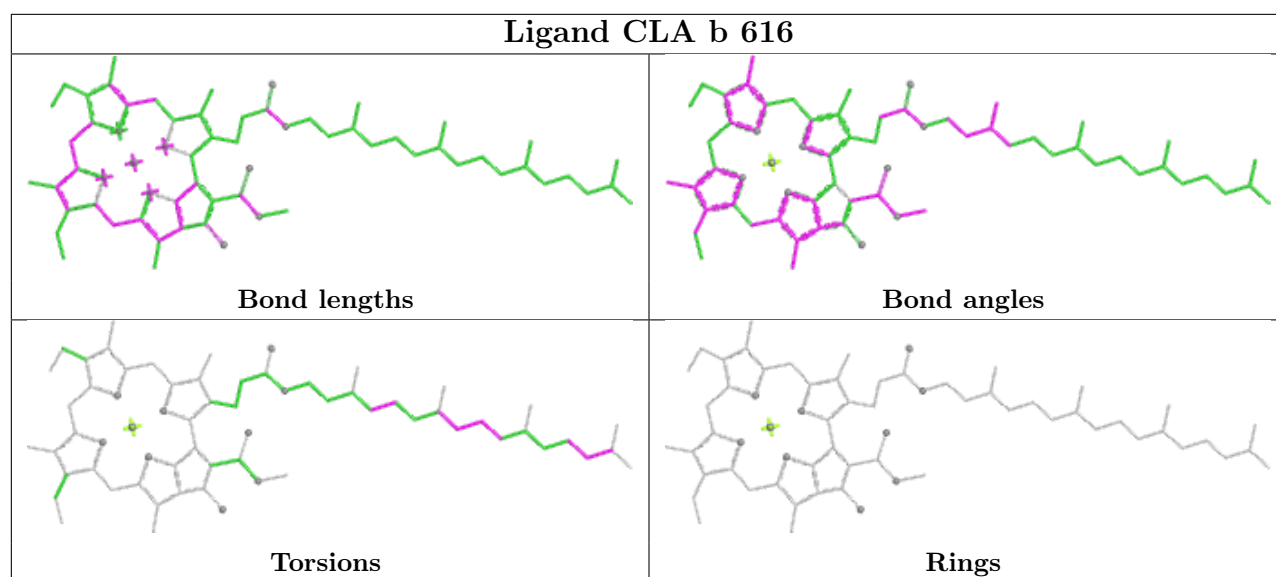


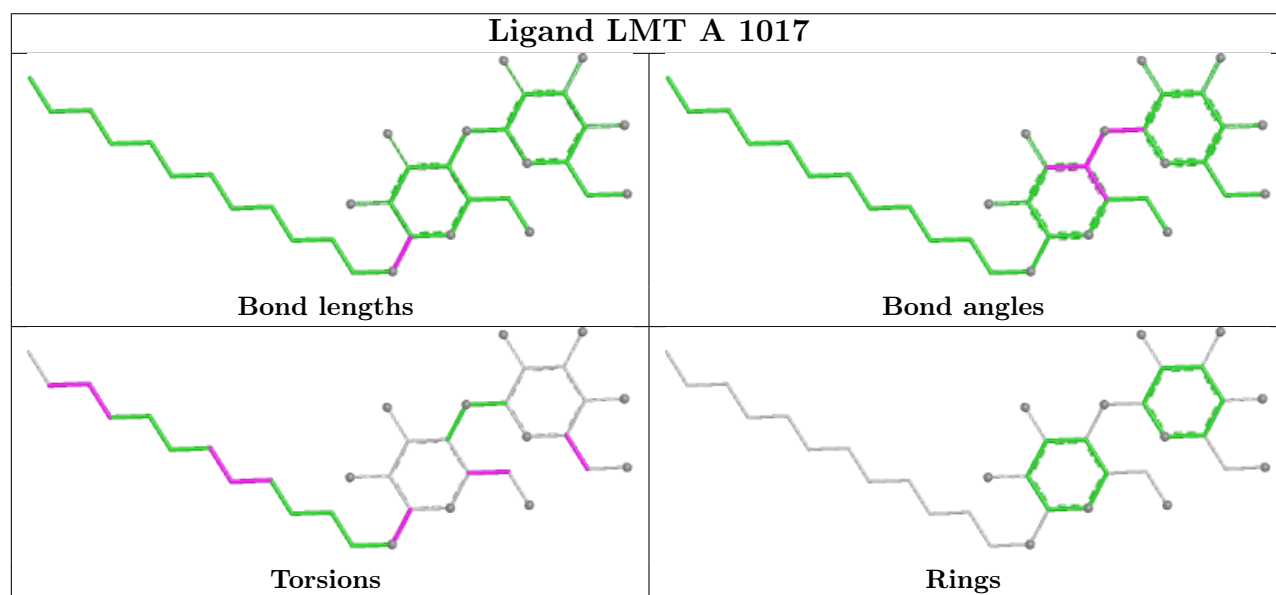
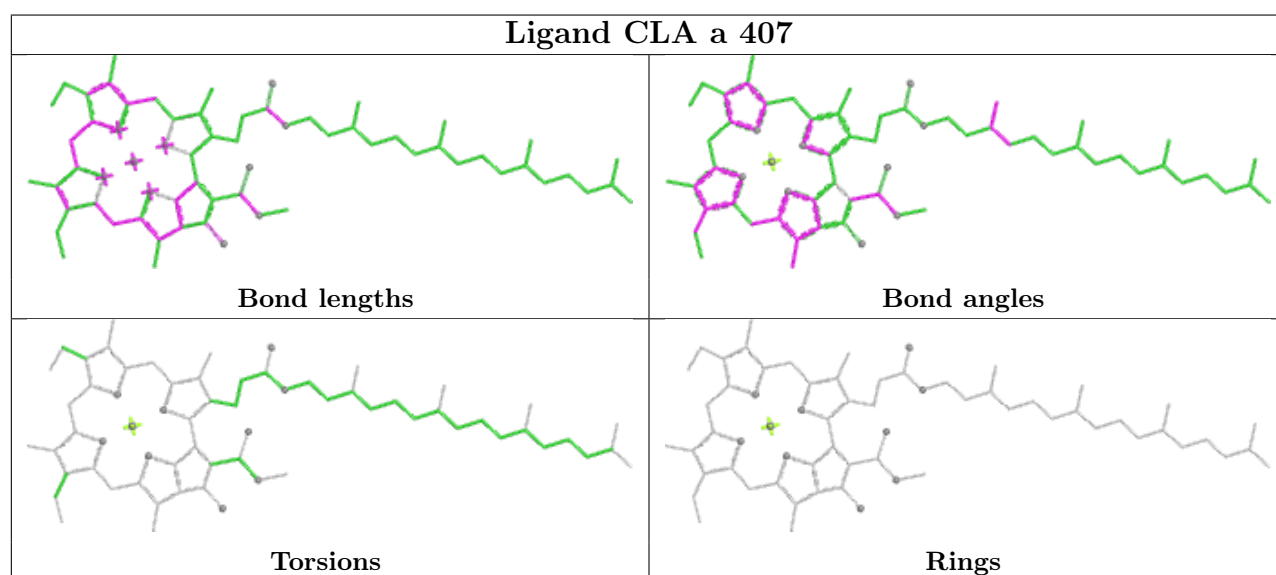
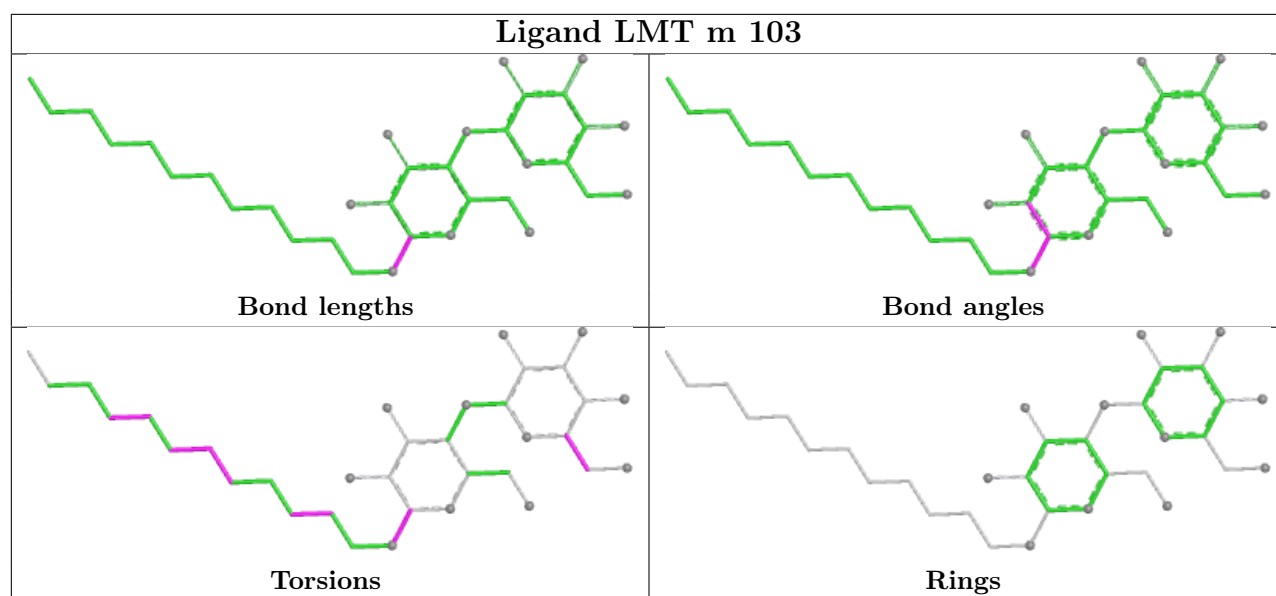
Ligand HTG V 202

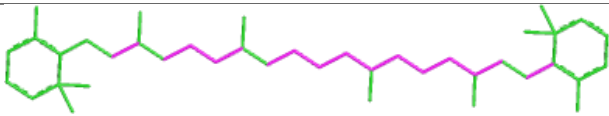
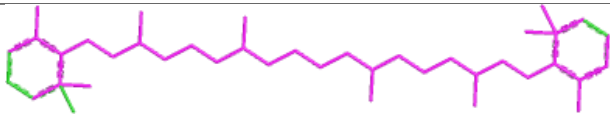
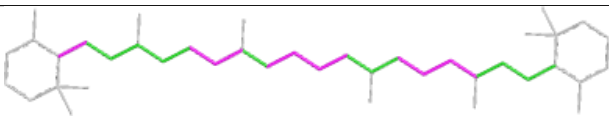
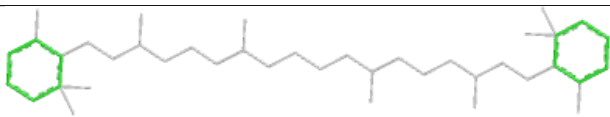


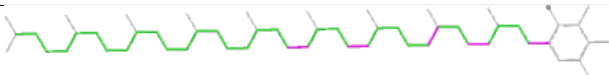
Ligand HTG o 301

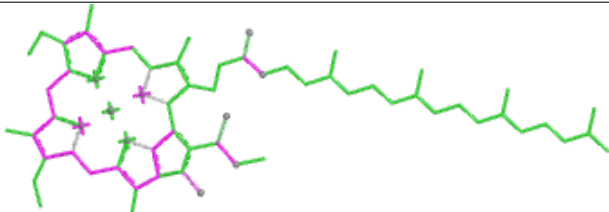
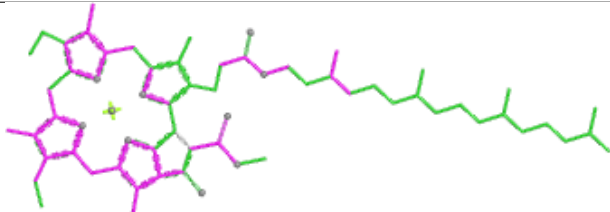
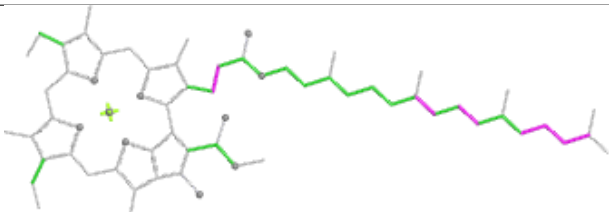
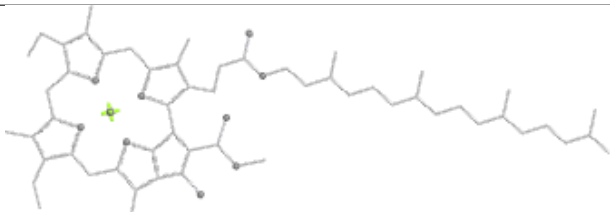




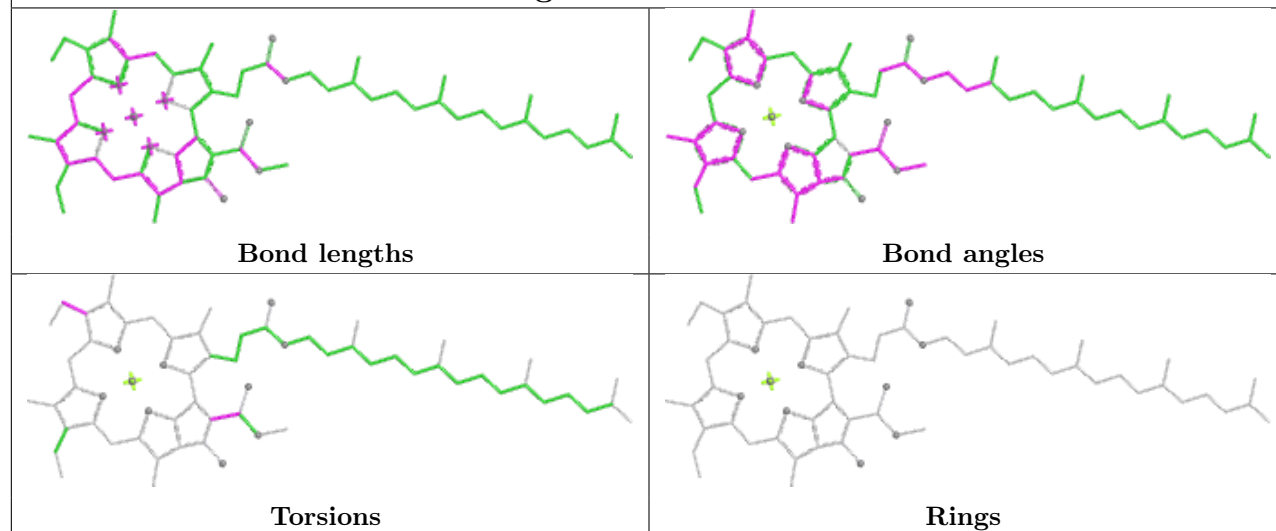


Ligand BCR J 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

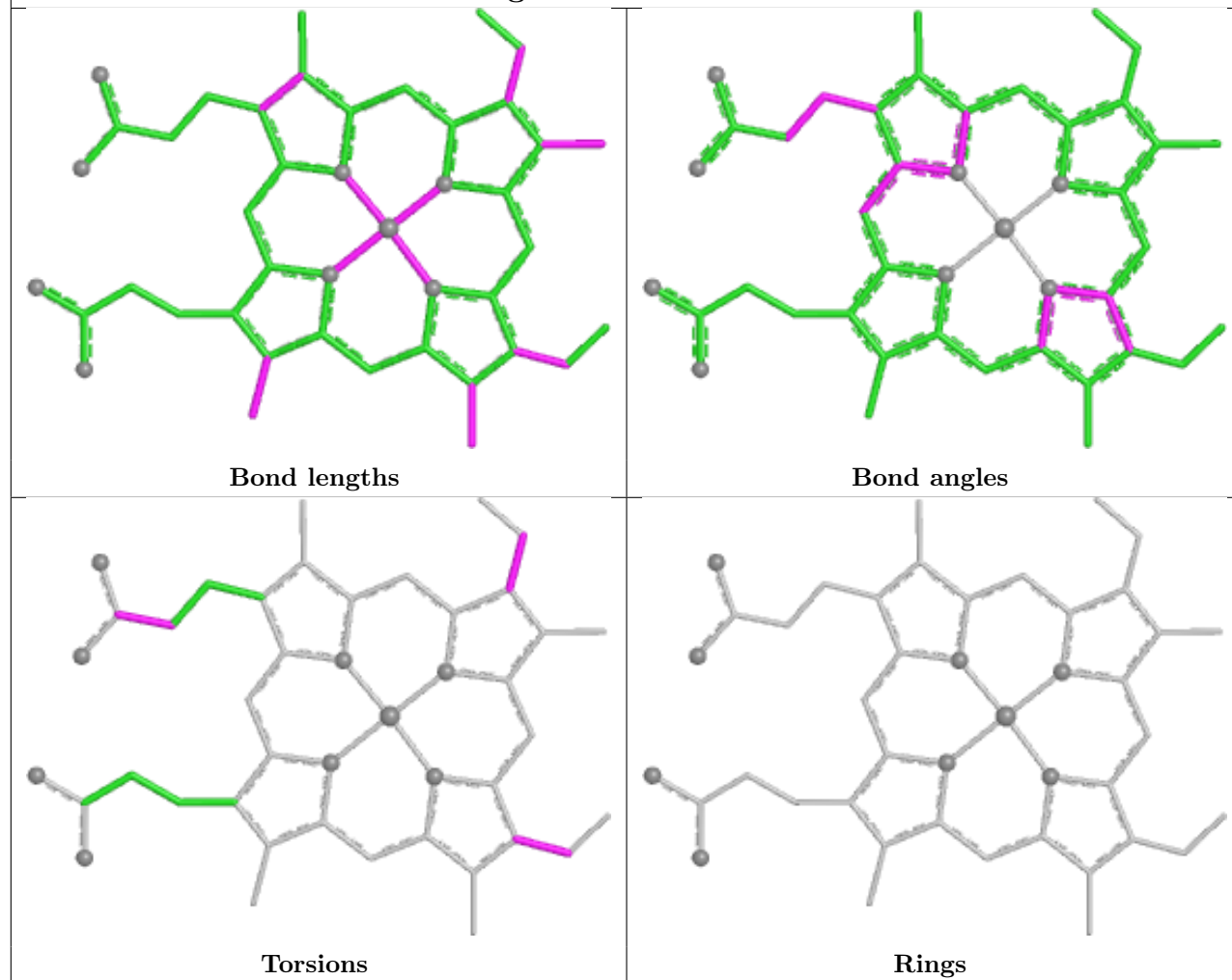
Ligand PL9 A 1010	
	
Bond lengths	Bond angles
	
Torsions	Rings

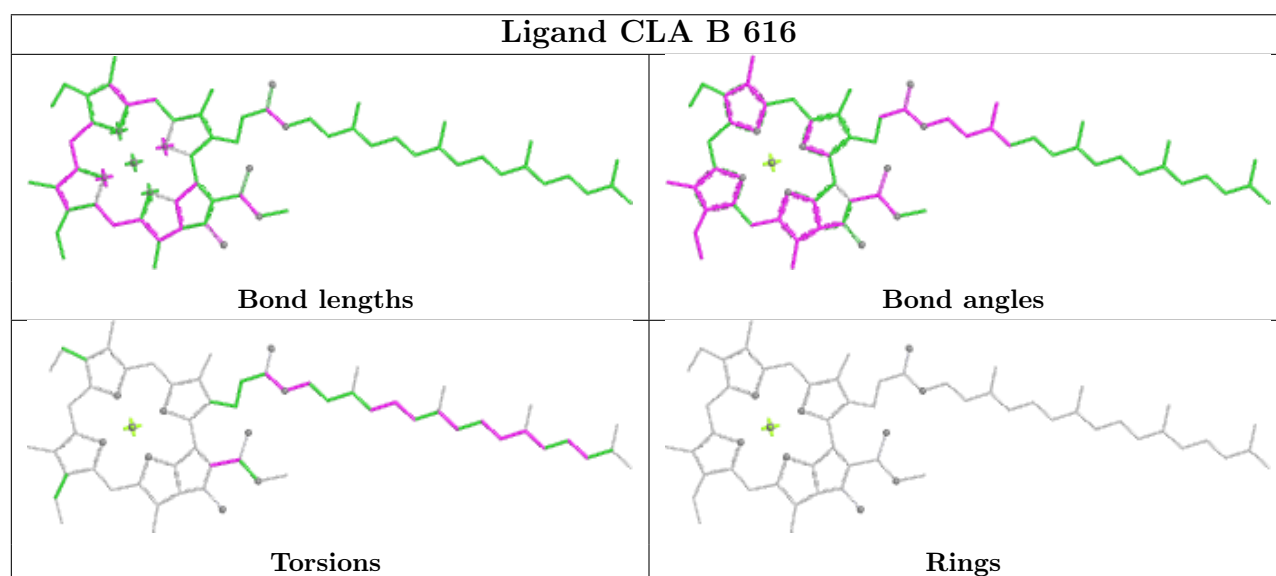
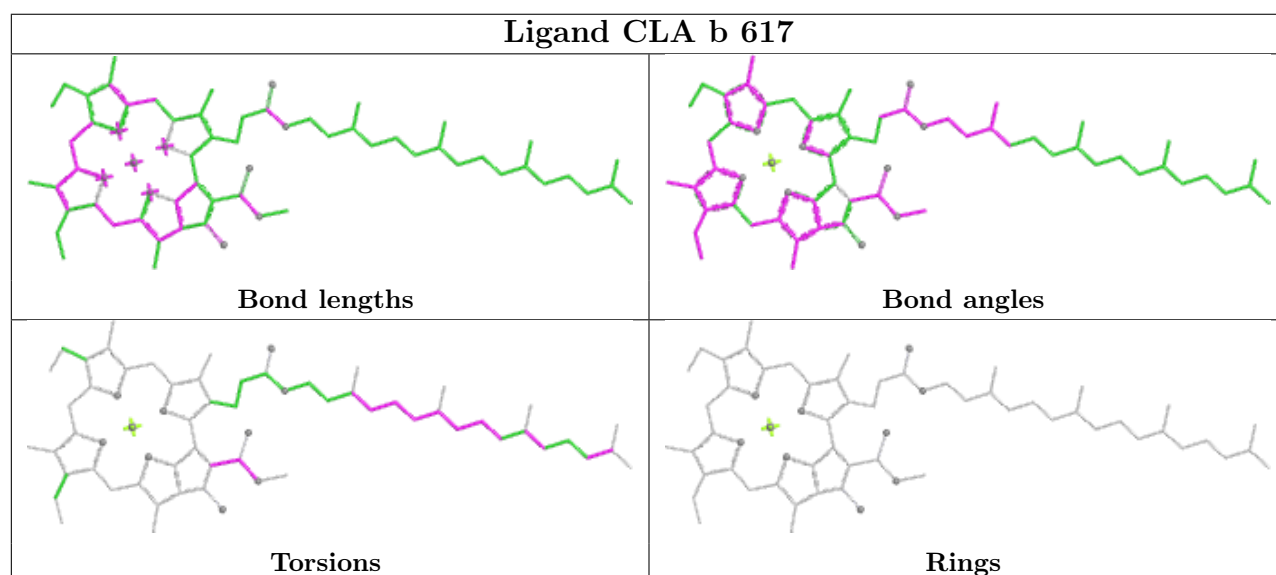
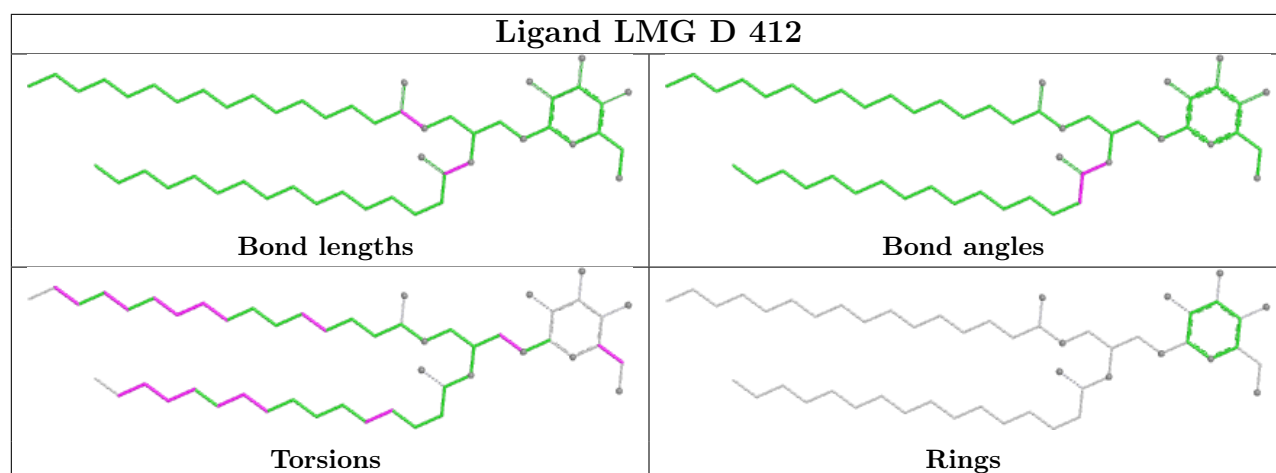
Ligand CLA B 606	
	
Bond lengths	Bond angles
	
Torsions	Rings

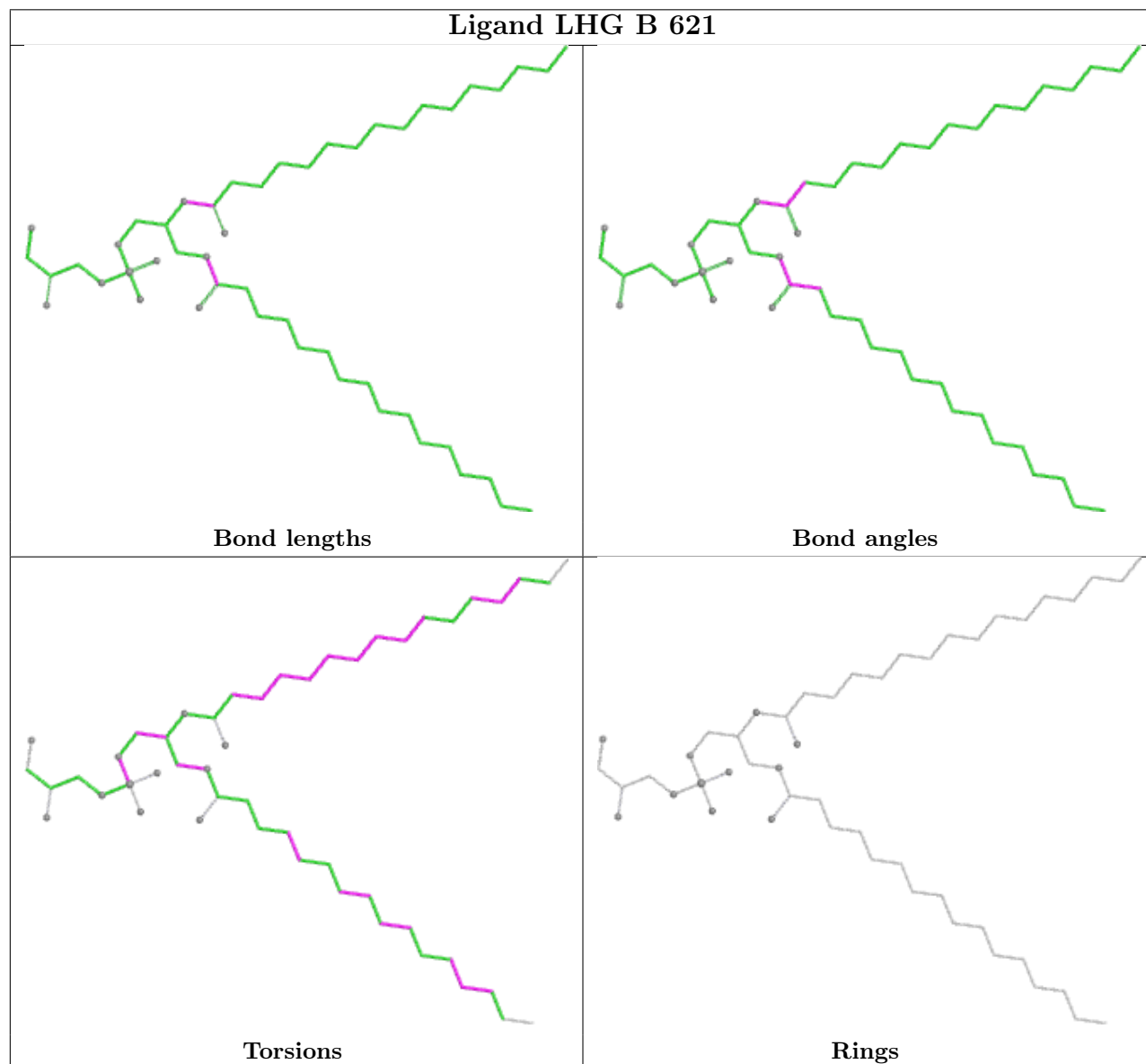
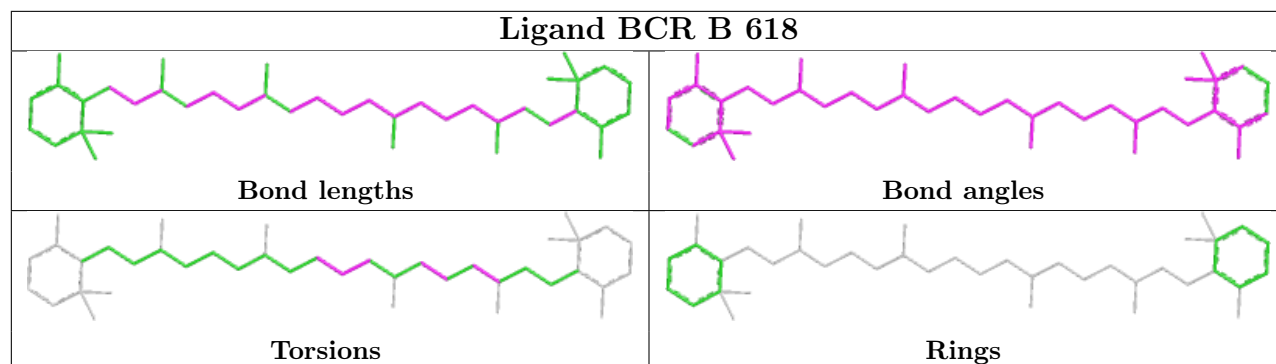
Ligand CLA b 612

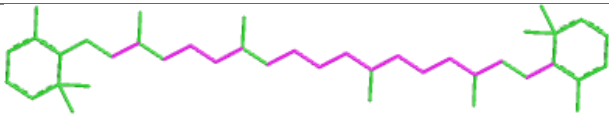
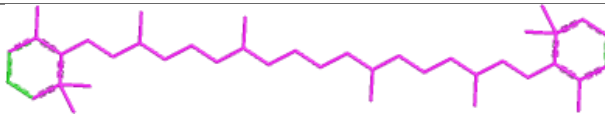
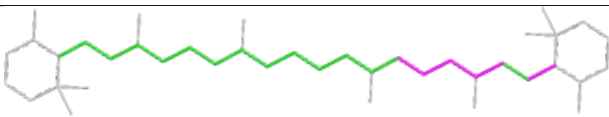
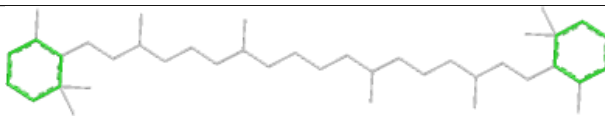


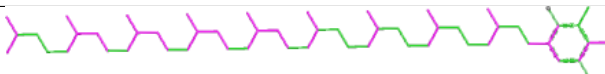
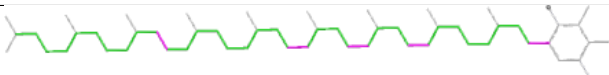
Ligand HEM V 201

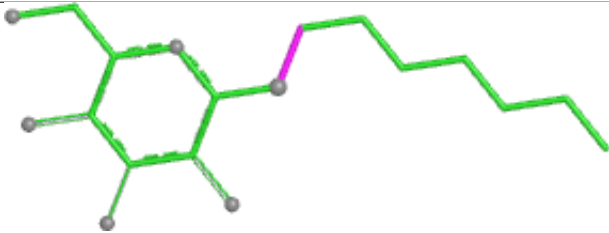
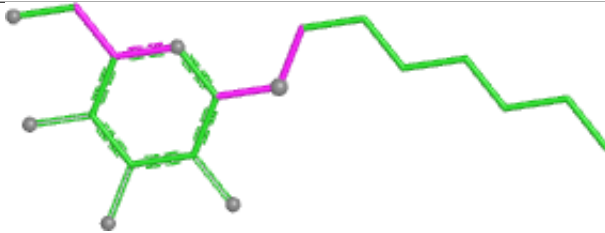
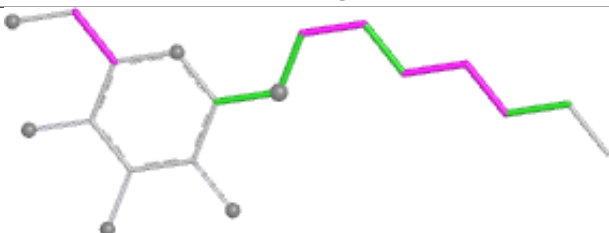
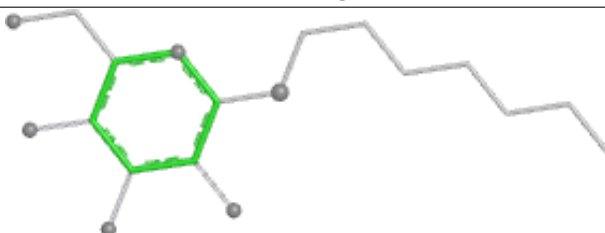


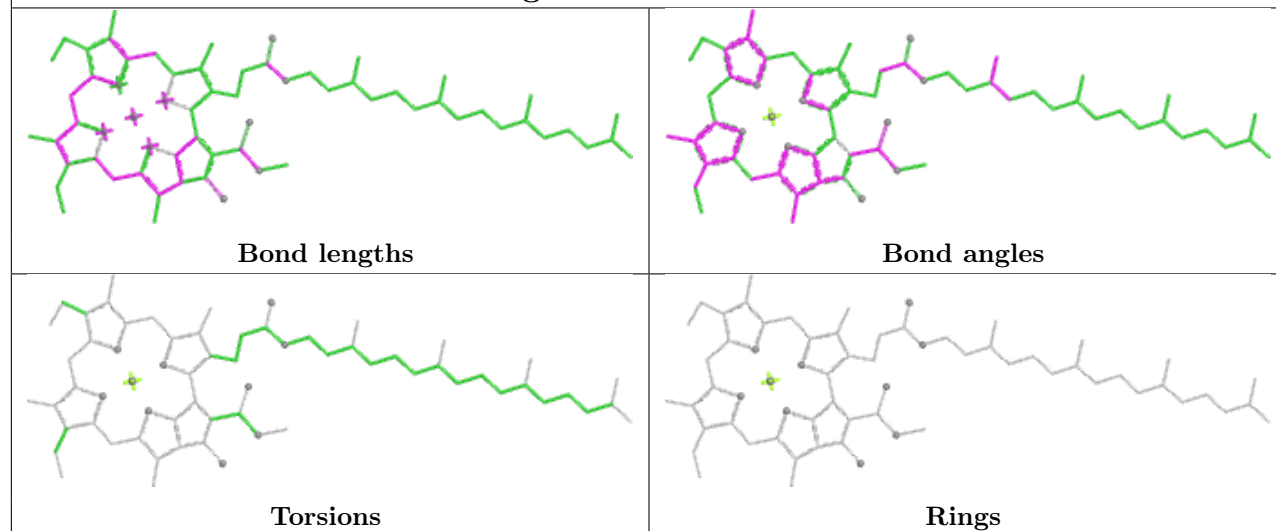
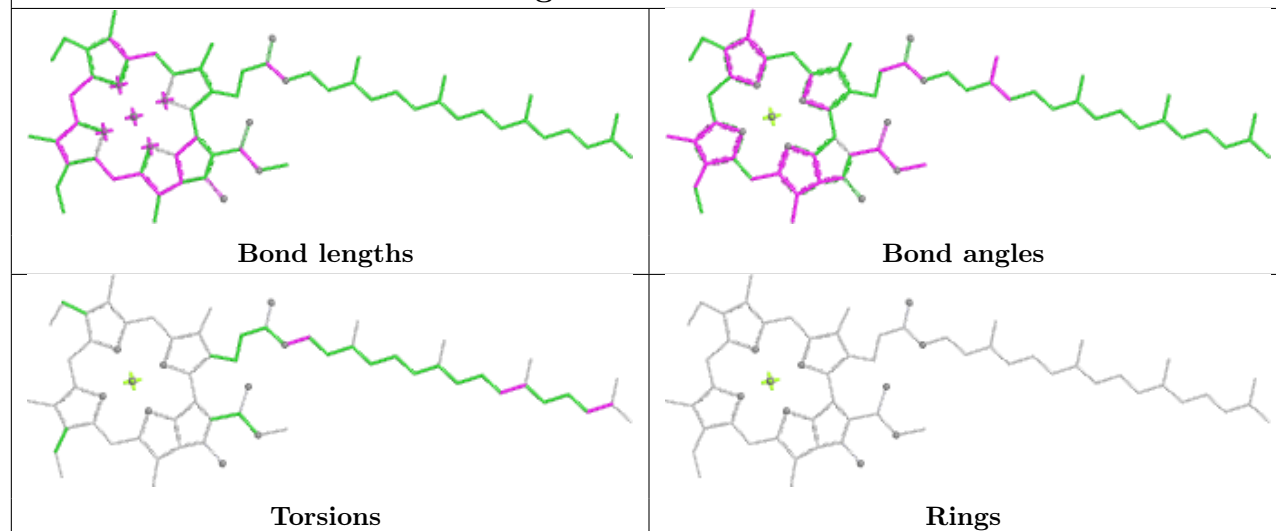


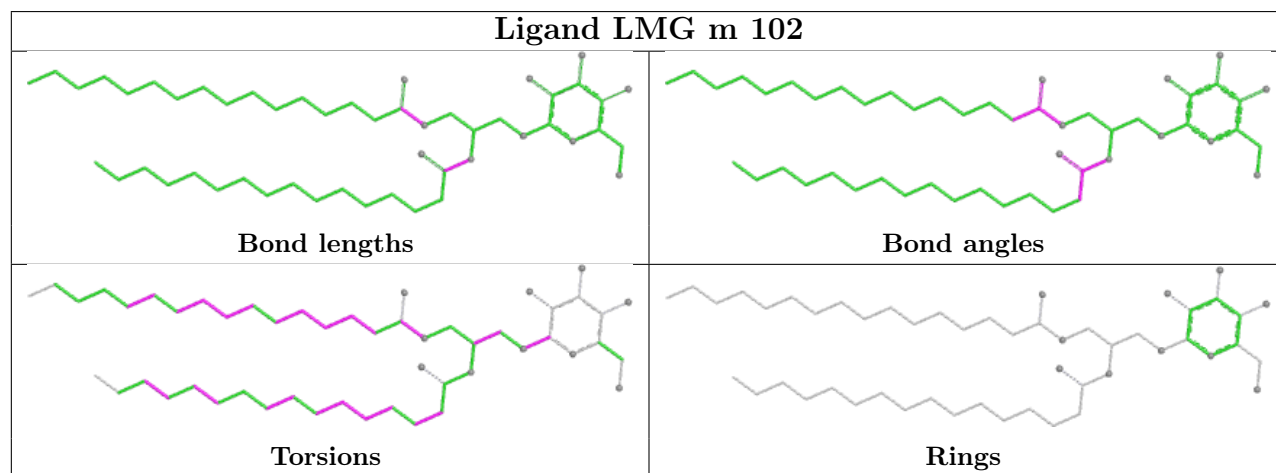
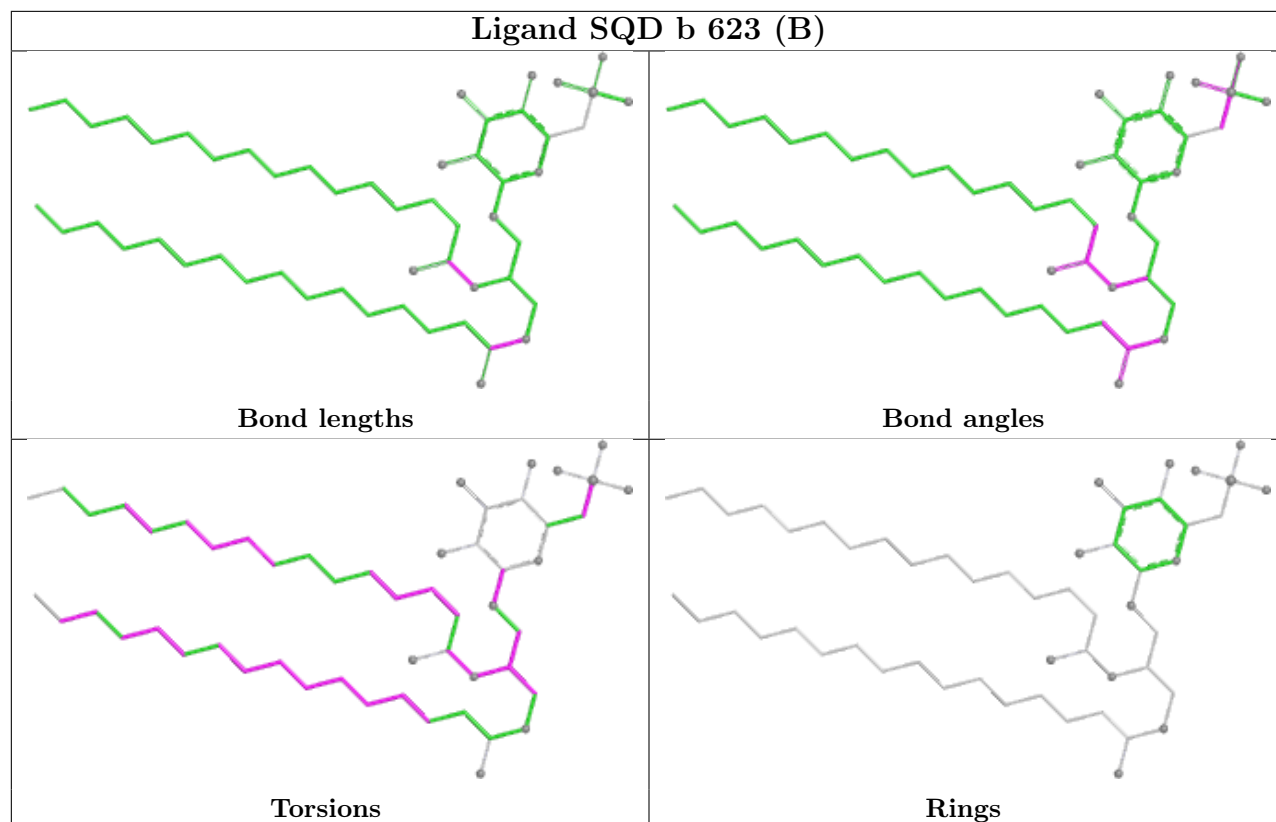


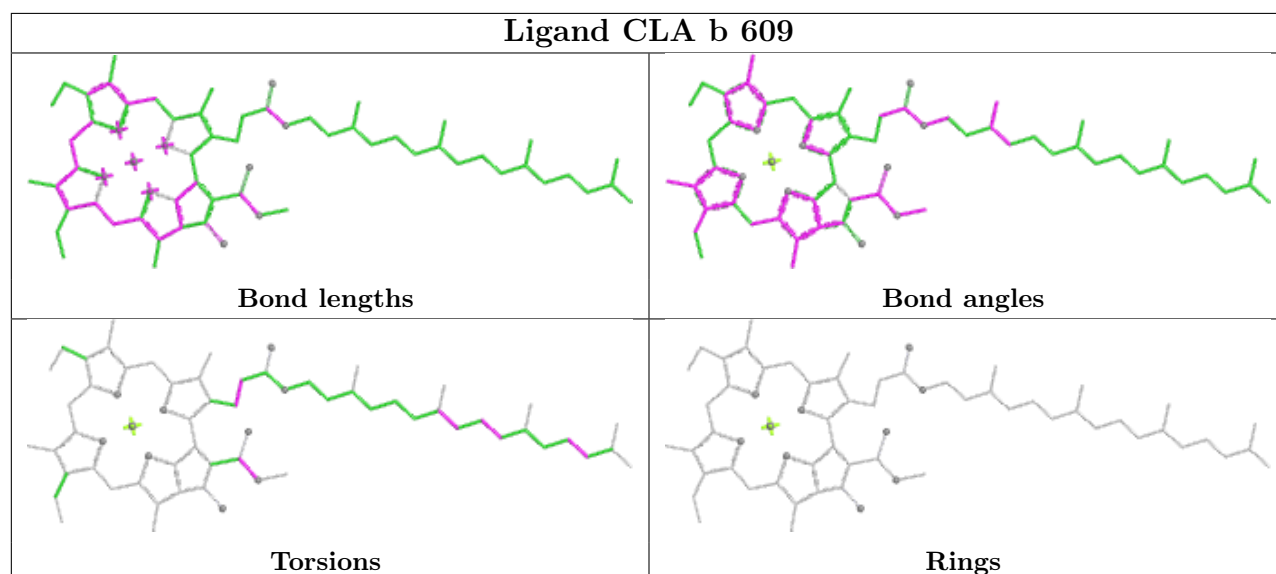
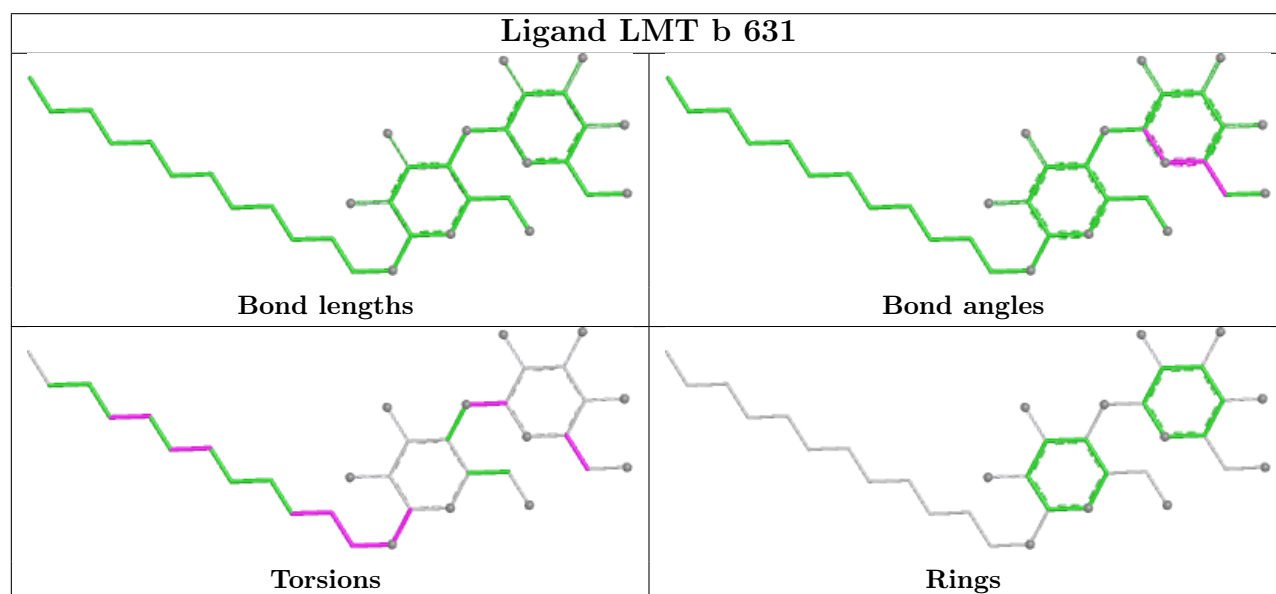
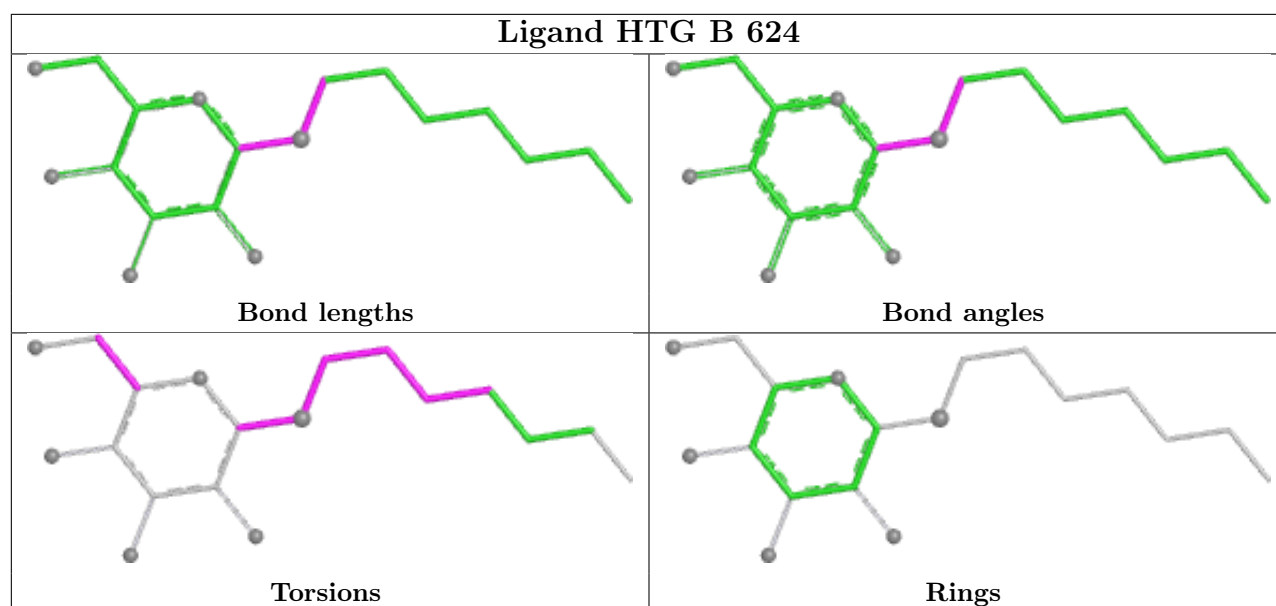
Ligand BCR b 621	
	
Bond lengths	Bond angles
	
Torsions	Rings

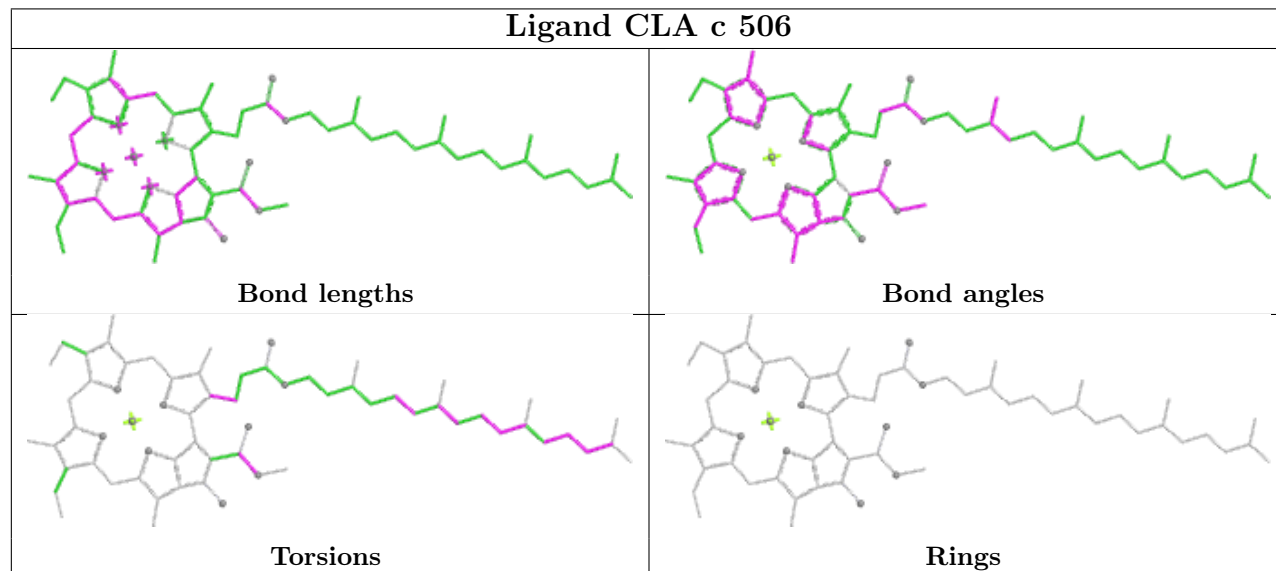
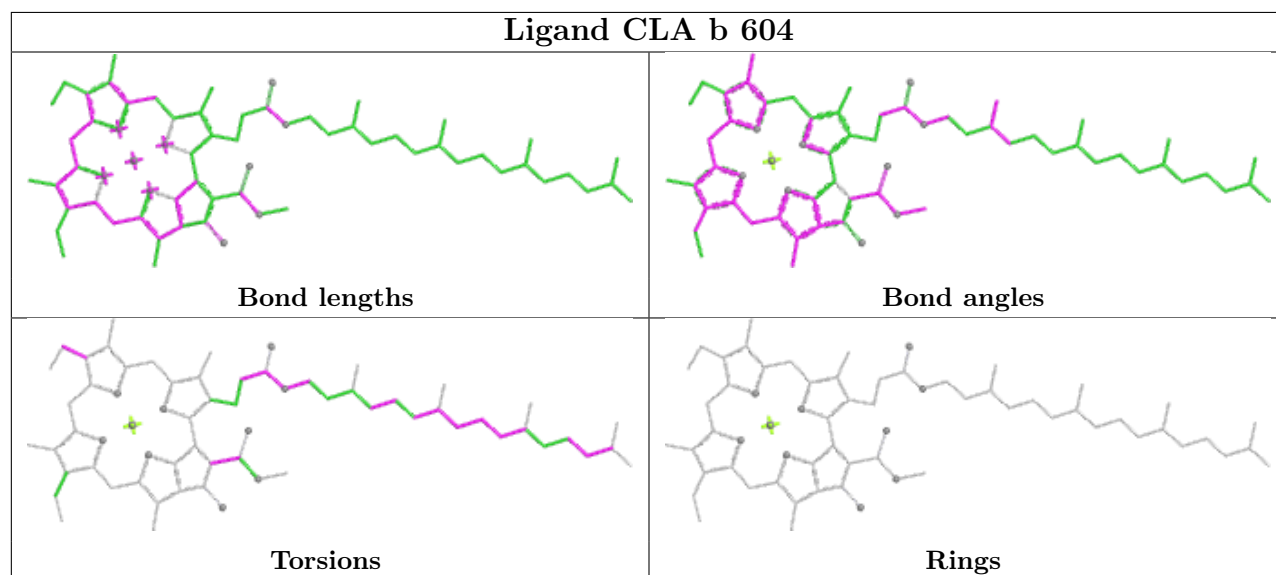
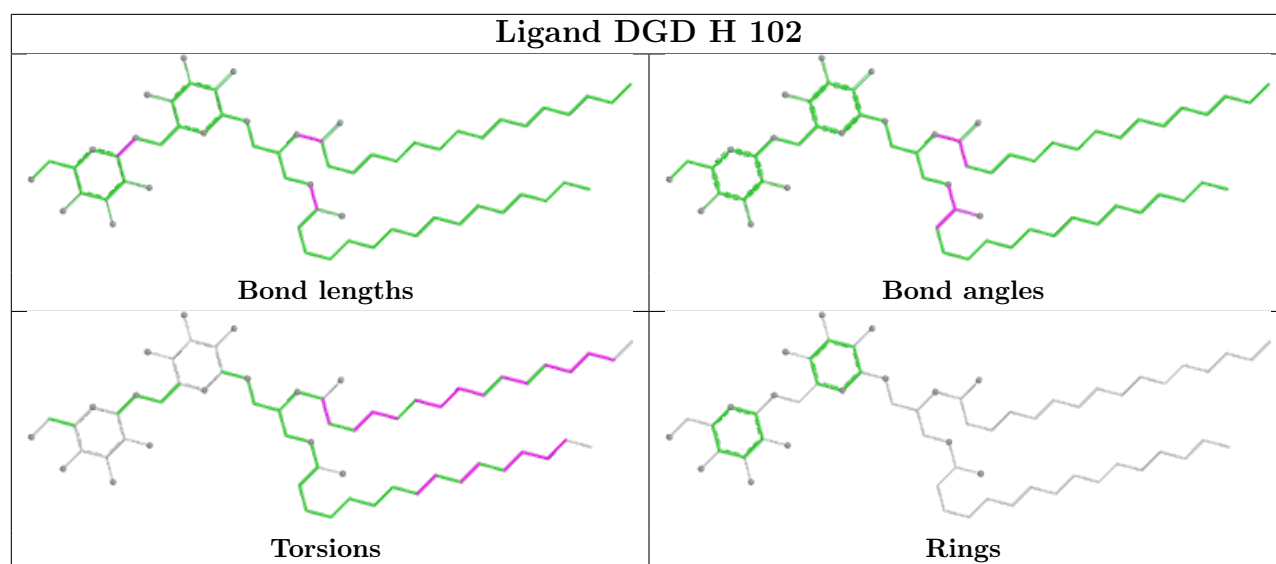
Ligand PL9 a 414	
	
Bond lengths	Bond angles
	
Torsions	Rings

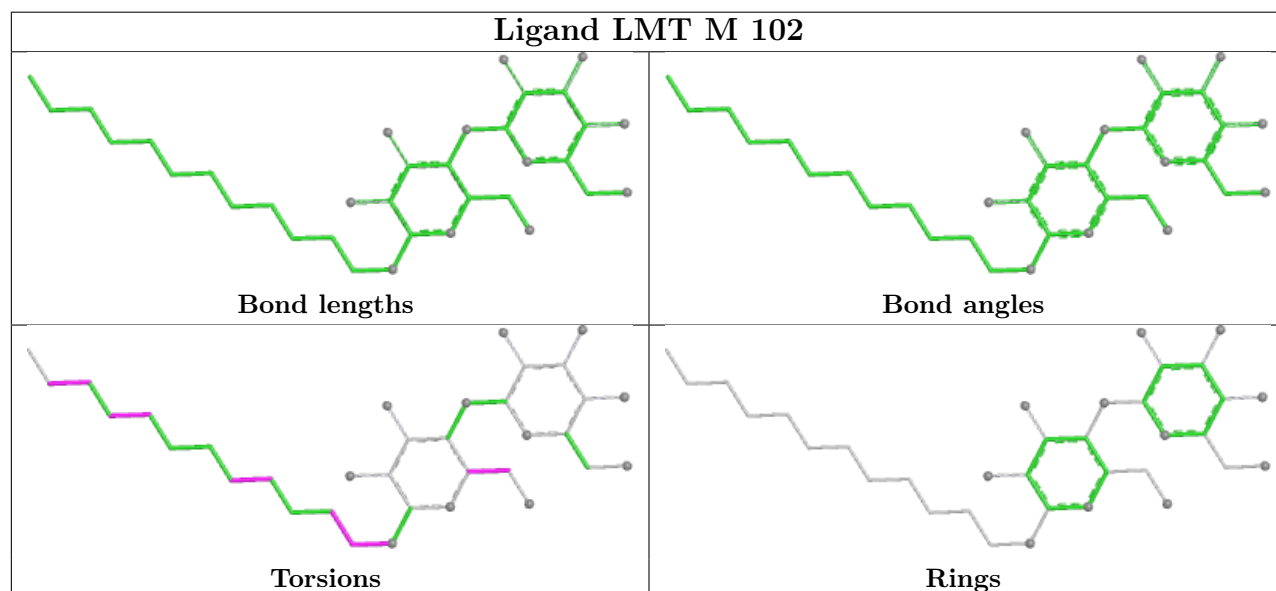
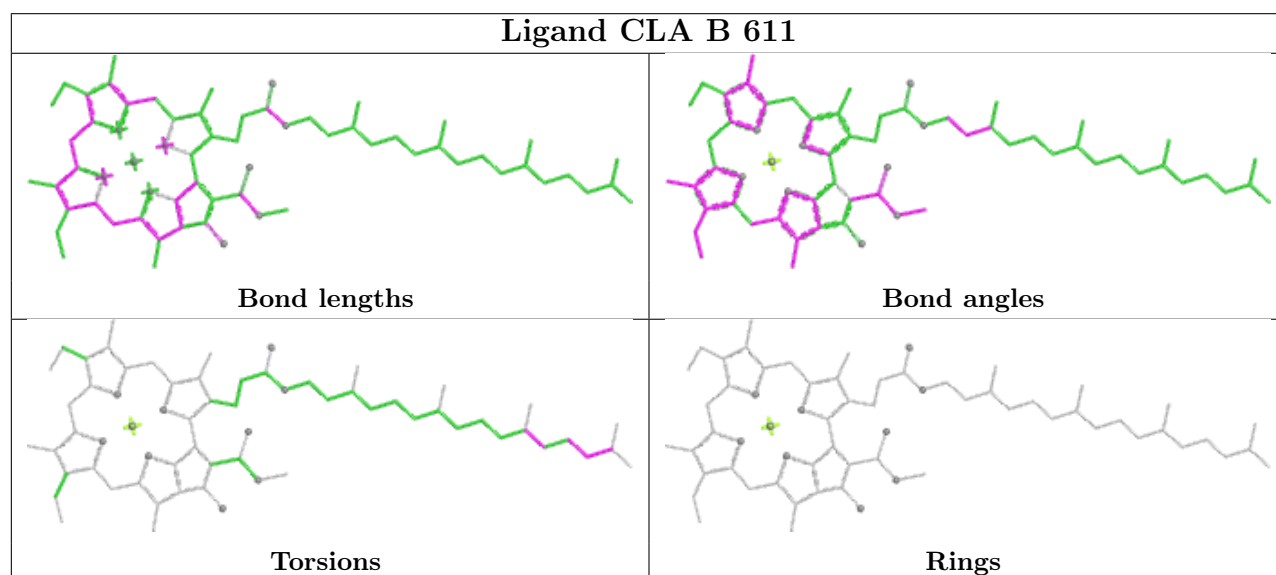
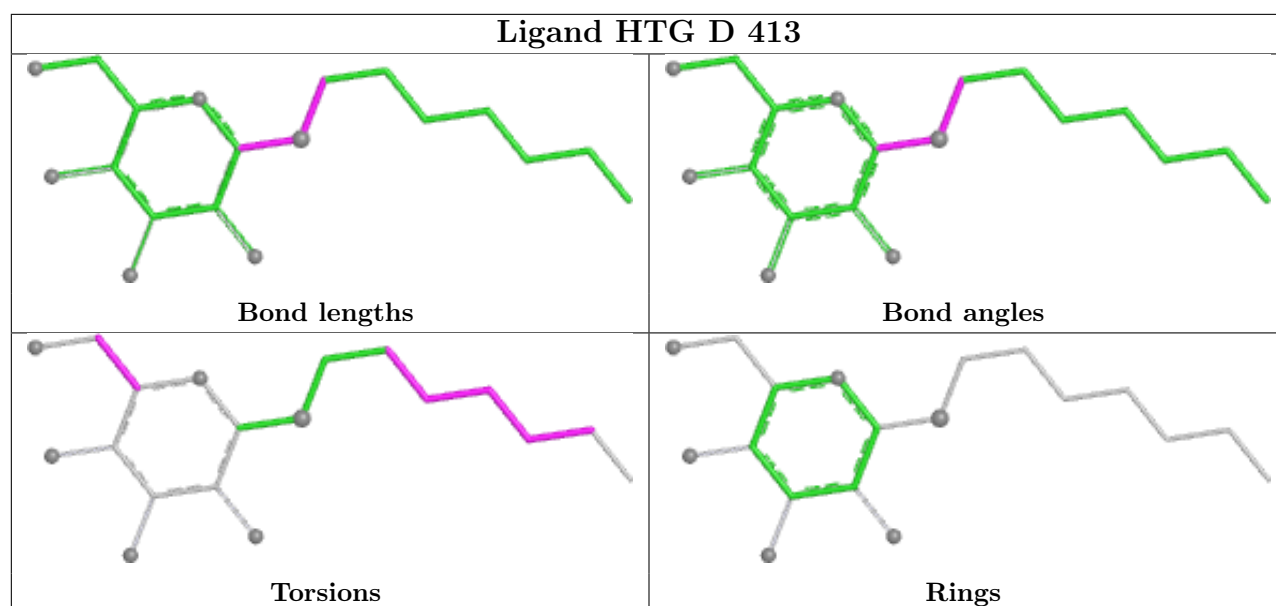
Ligand HTG b 626	
	
Bond lengths	Bond angles
	
Torsions	Rings

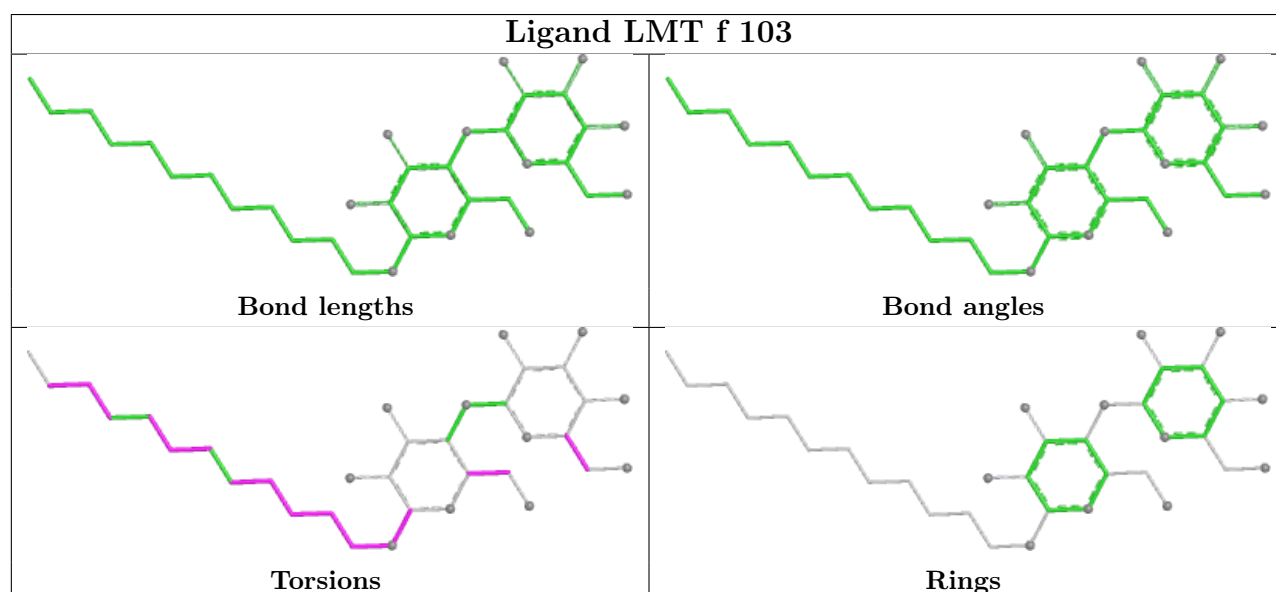
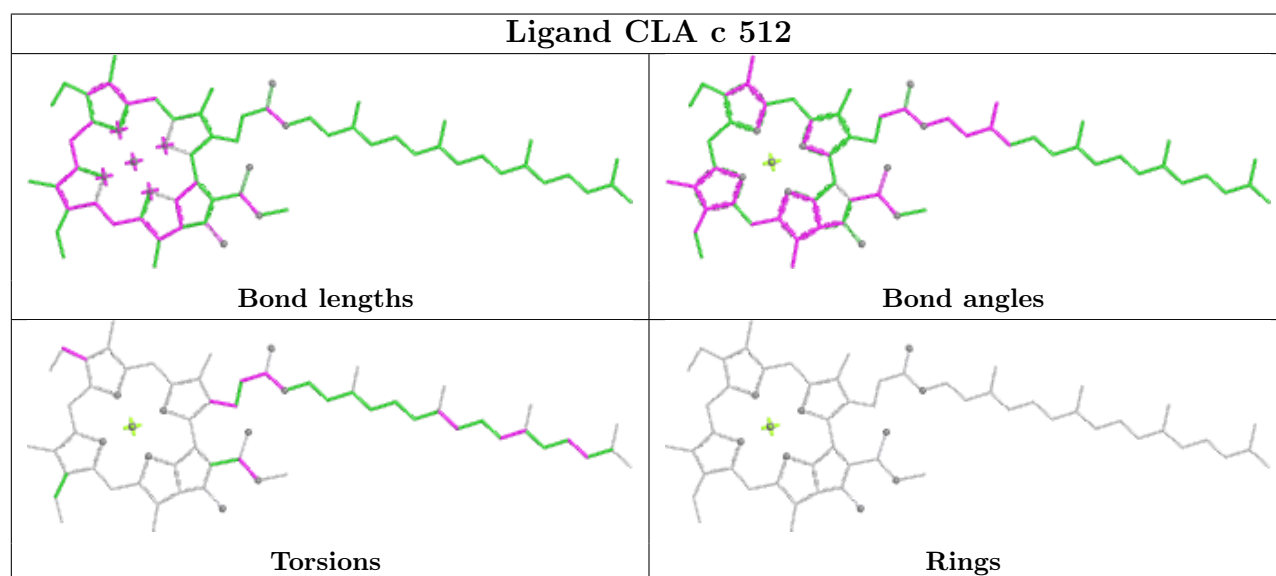
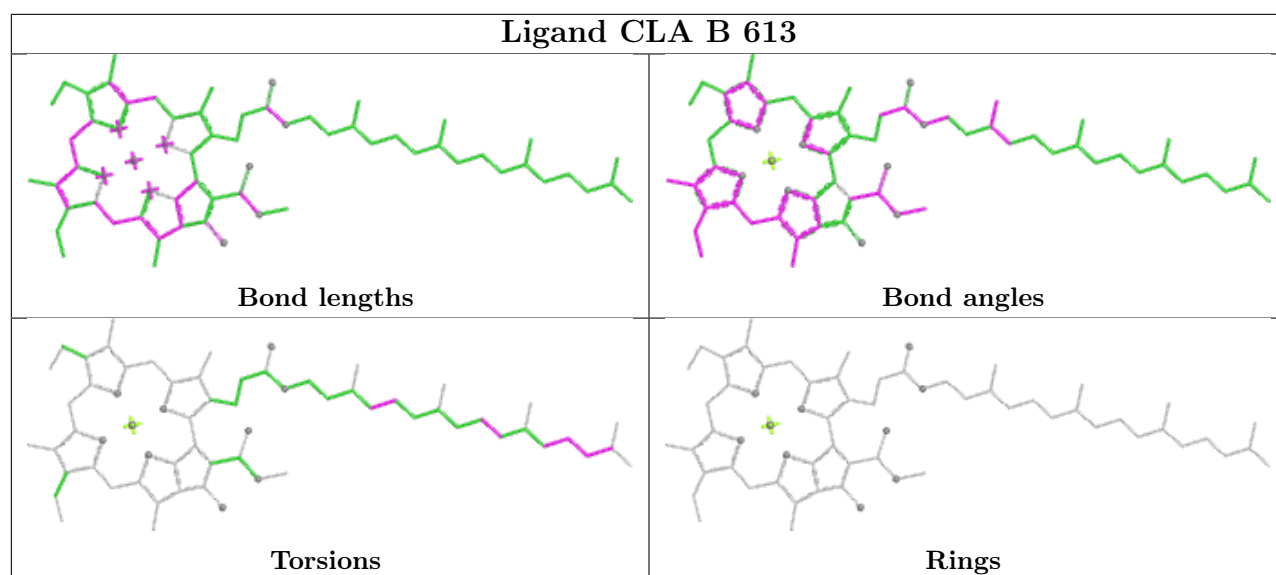
Ligand CLA A 1005**Ligand CLA d 402**

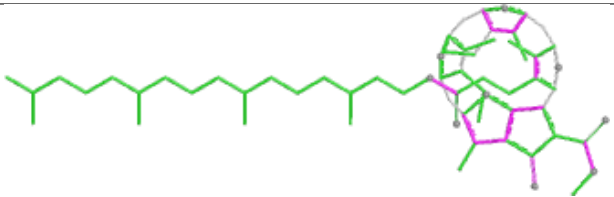
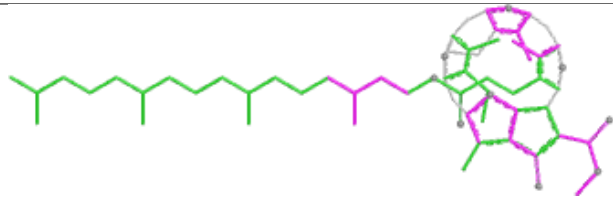
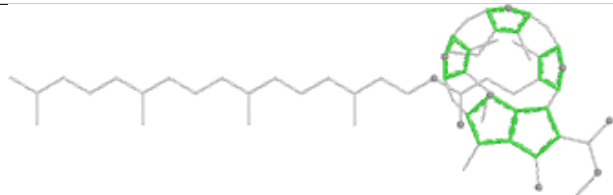


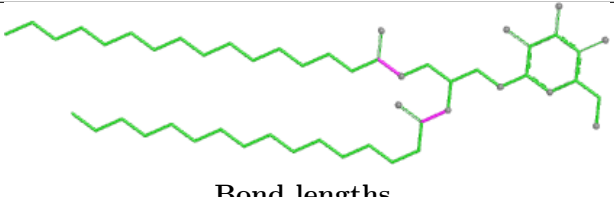
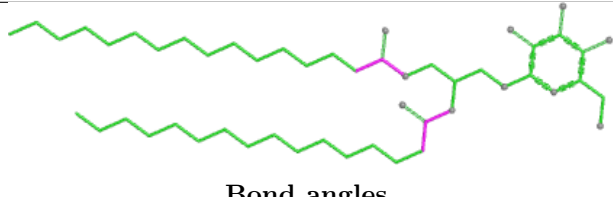
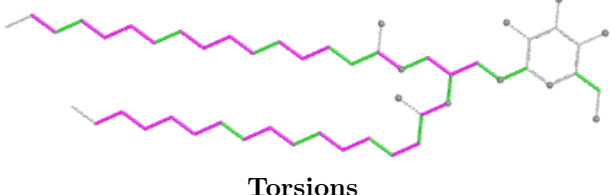
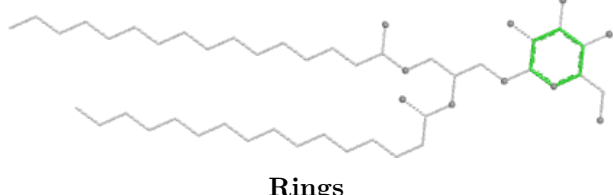


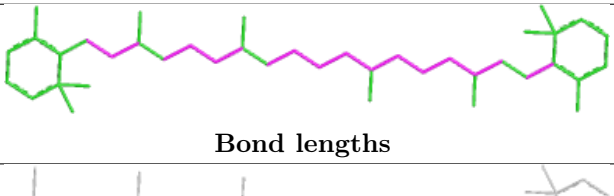
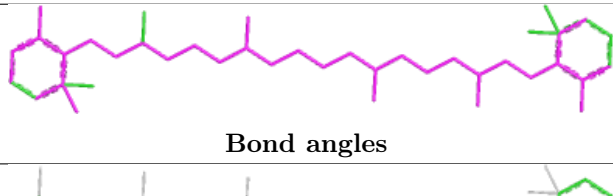
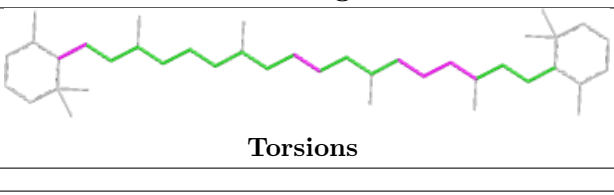
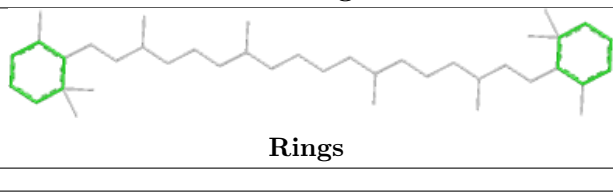


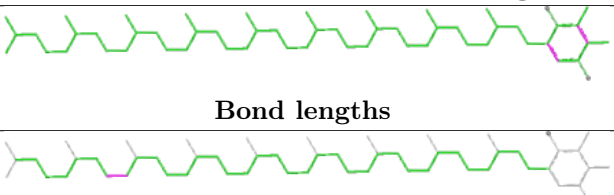
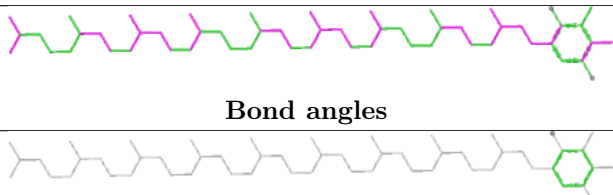
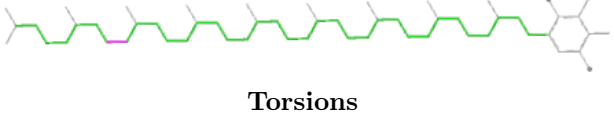
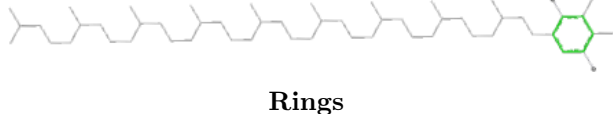


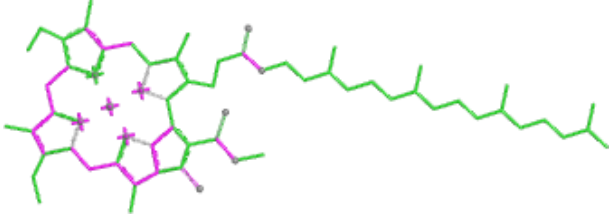
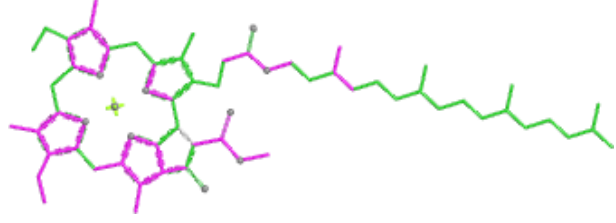
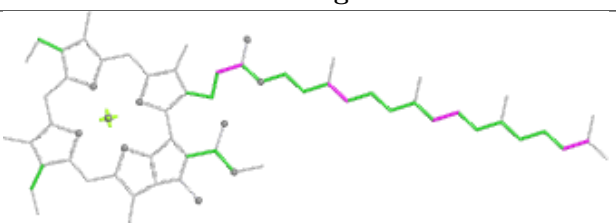
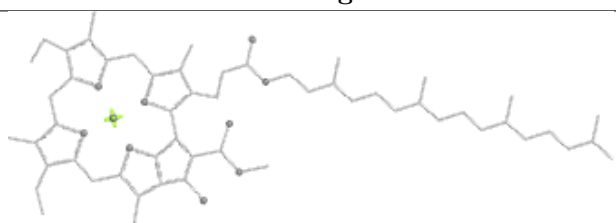
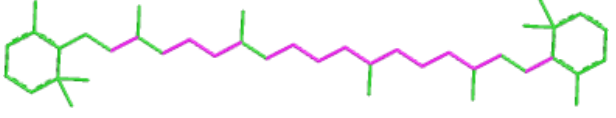
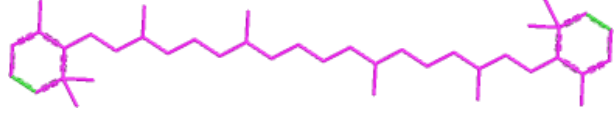
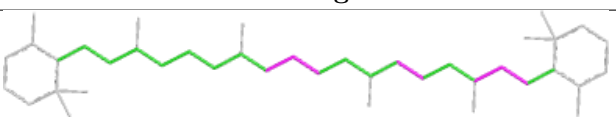
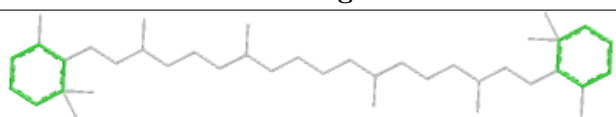
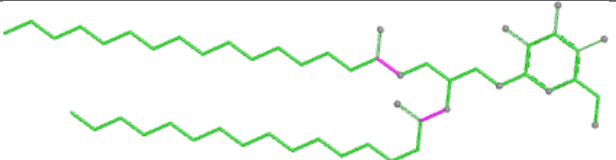
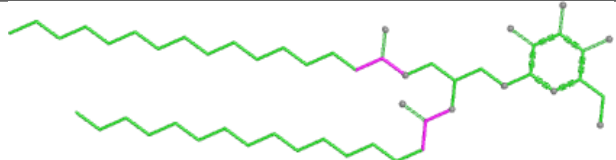
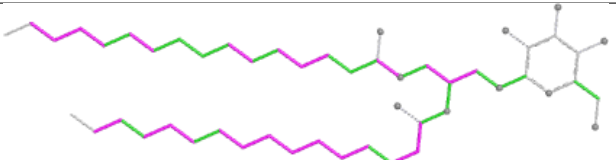
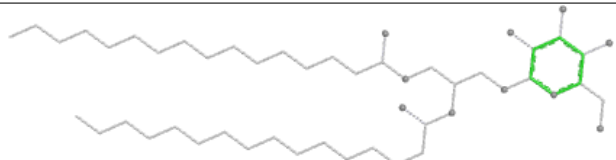


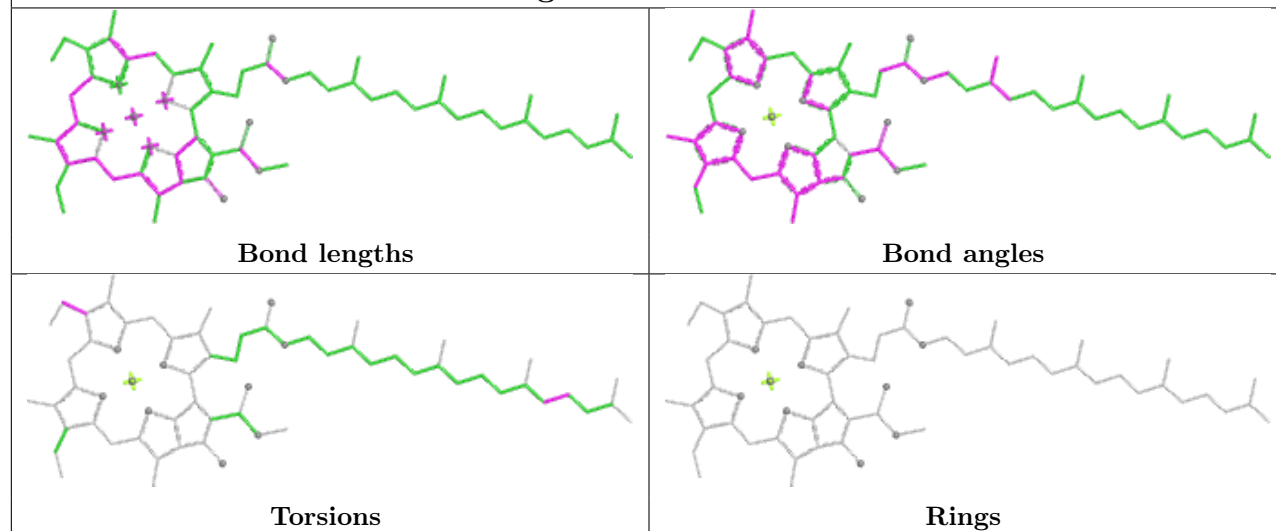
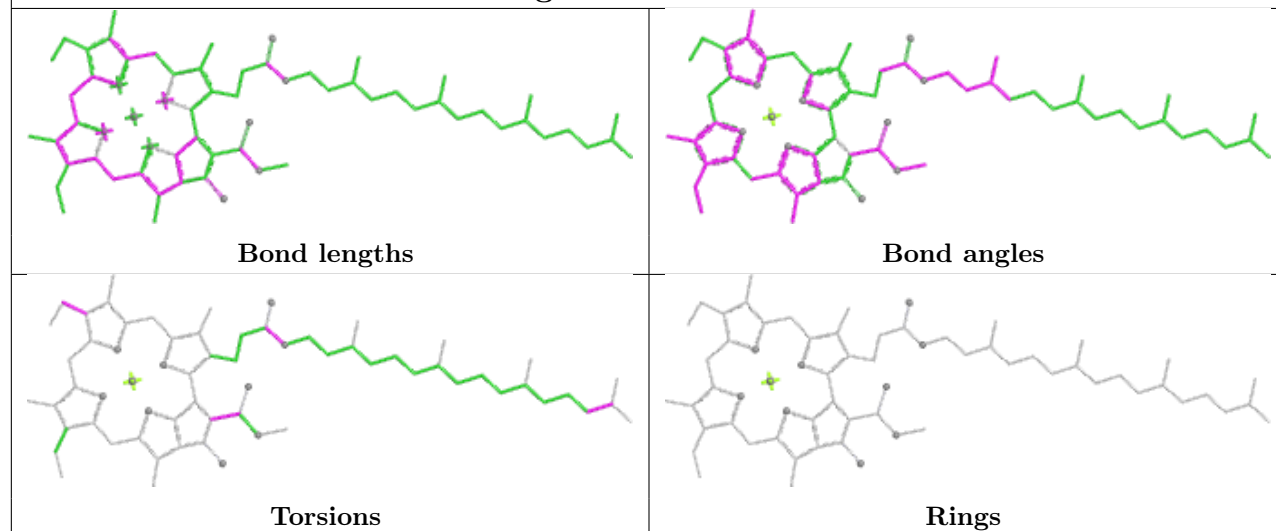
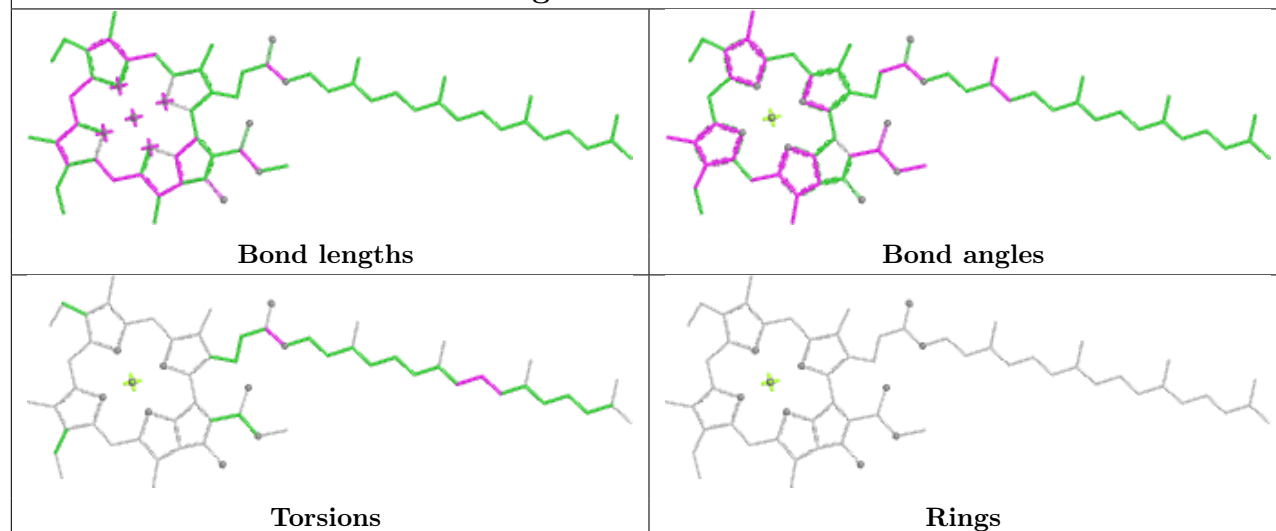
Ligand PHO a 411	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LMG A 1012	
	
Bond lengths	Bond angles
	
Torsions	Rings

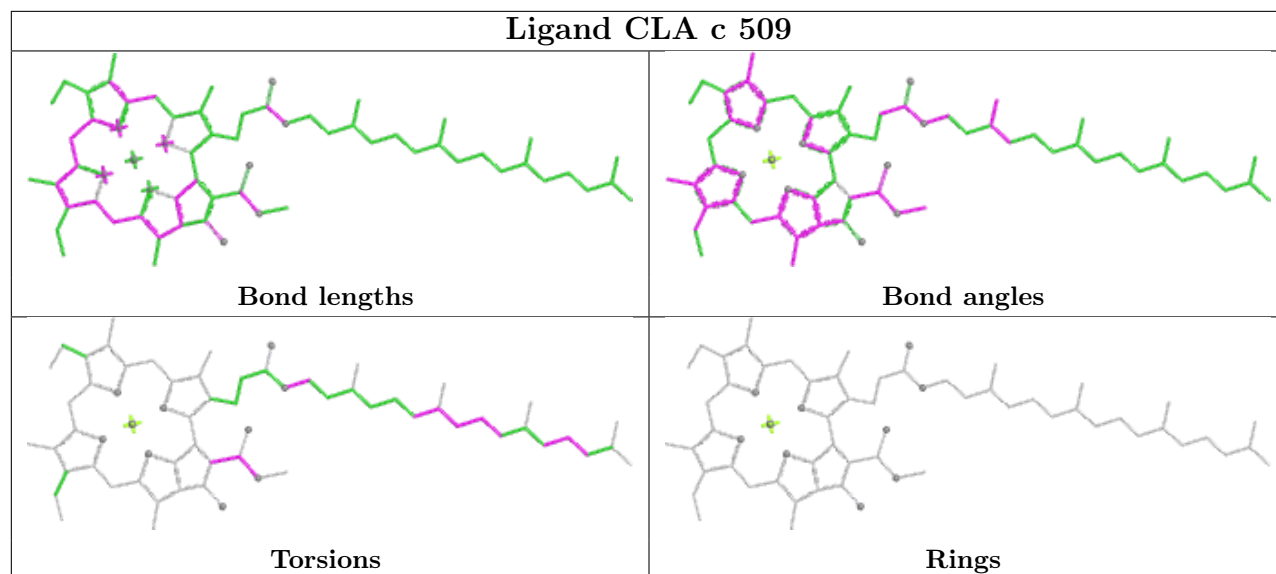
Ligand BCR T 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PL9 D 407	
	
Bond lengths	Bond angles
	
Torsions	Rings

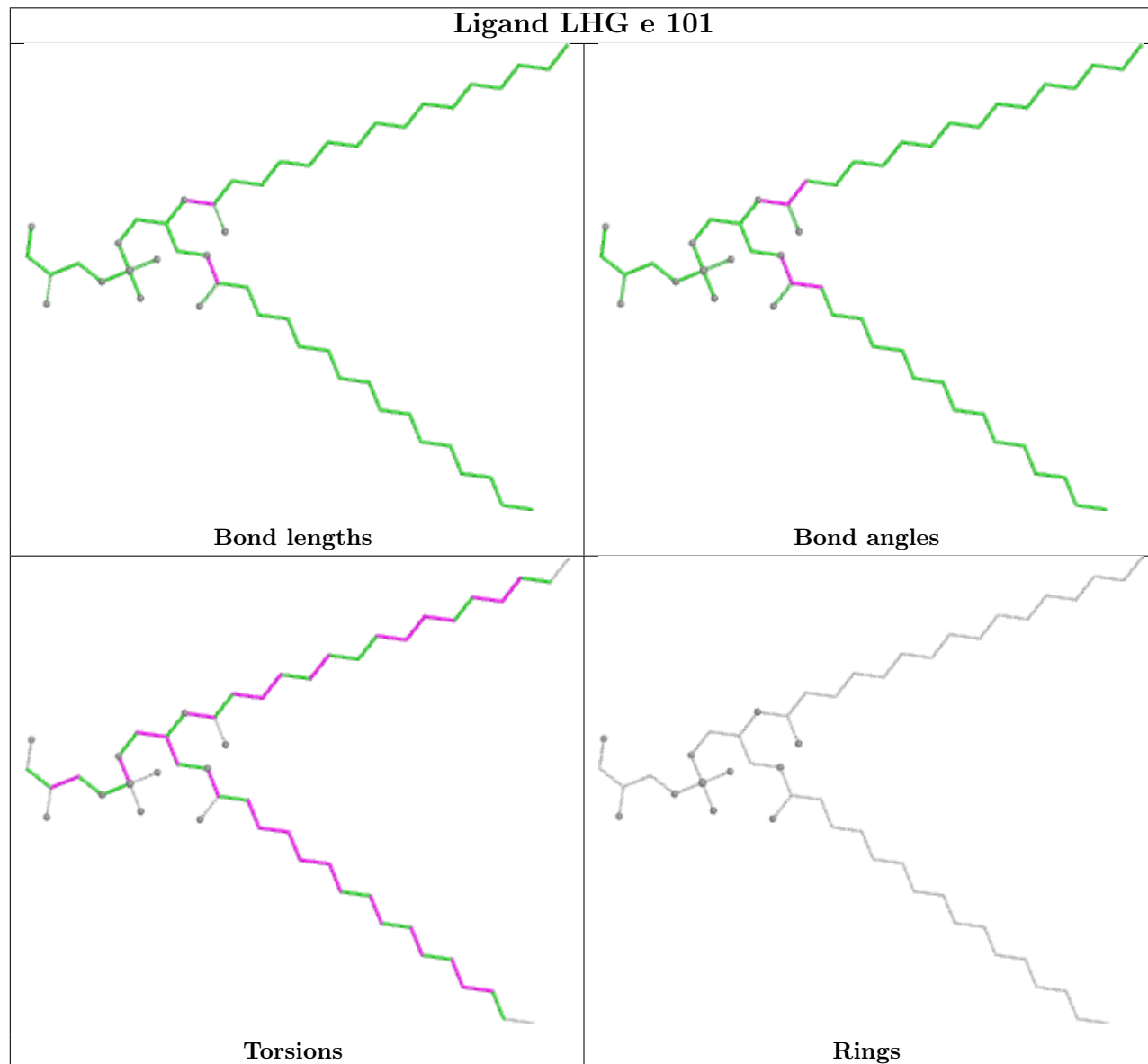
Ligand CLA C 510	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR D 406	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG a 415	
 Bond lengths	 Bond angles
 Torsions	 Rings

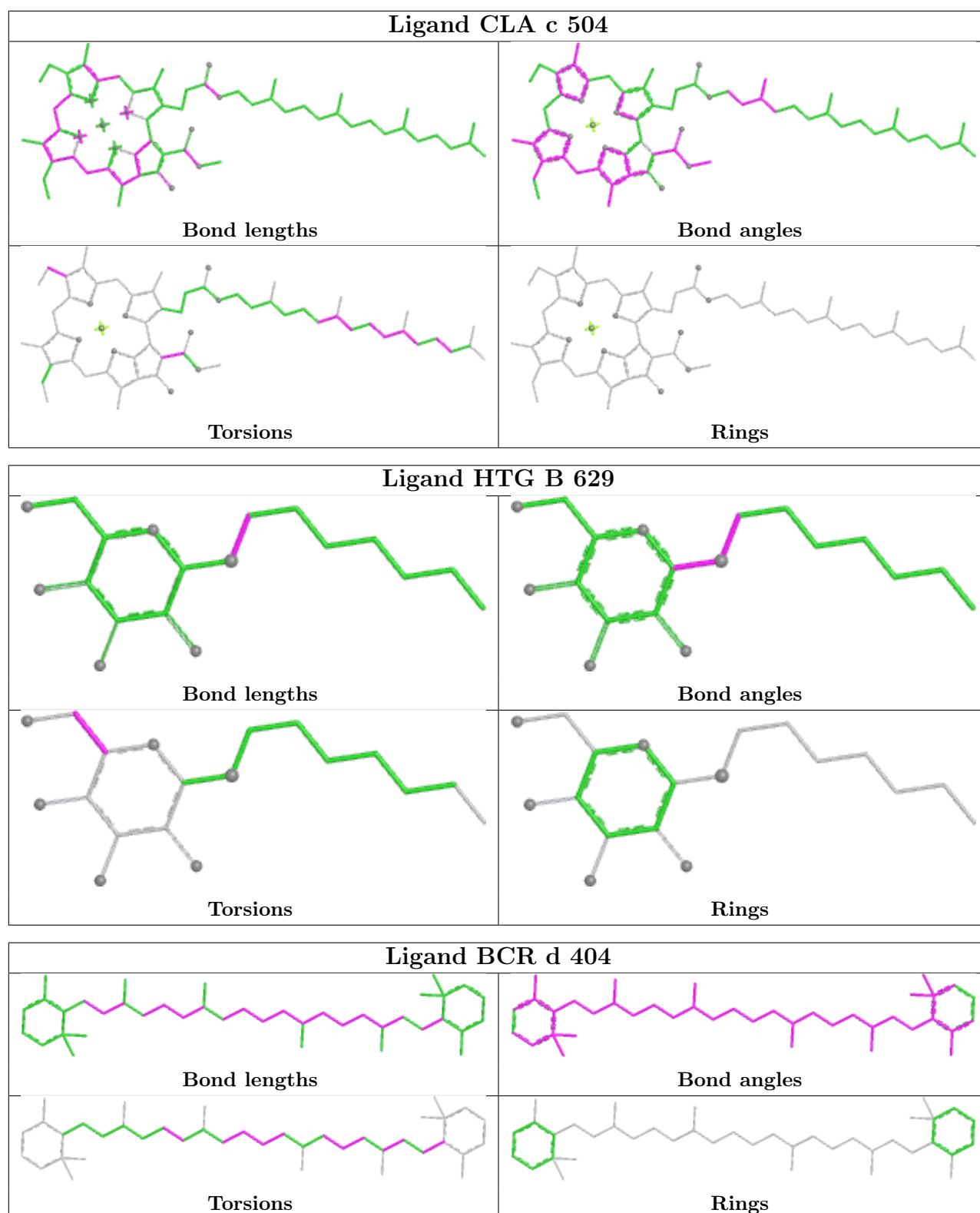
Ligand CLA c 501**Ligand CLA b 610****Ligand CLA B 612**

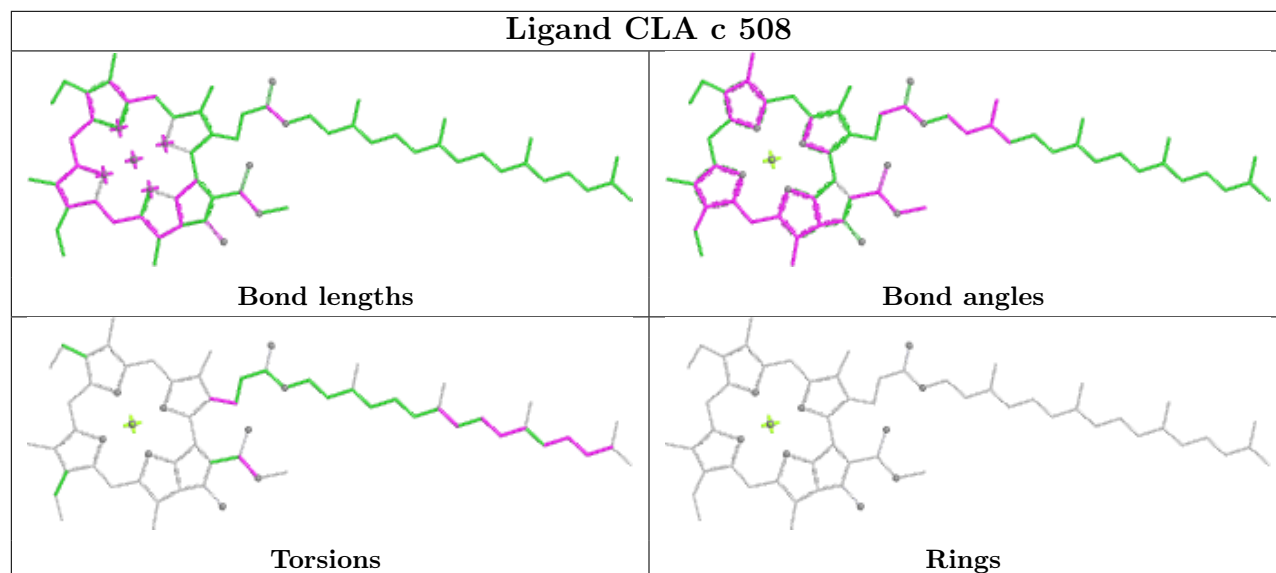
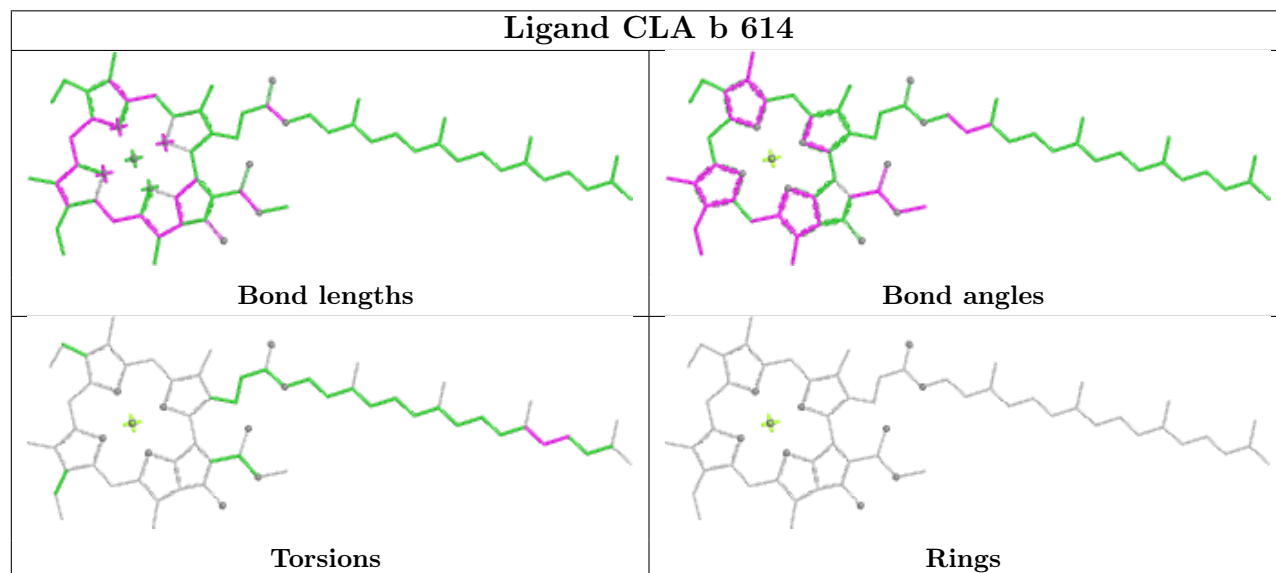
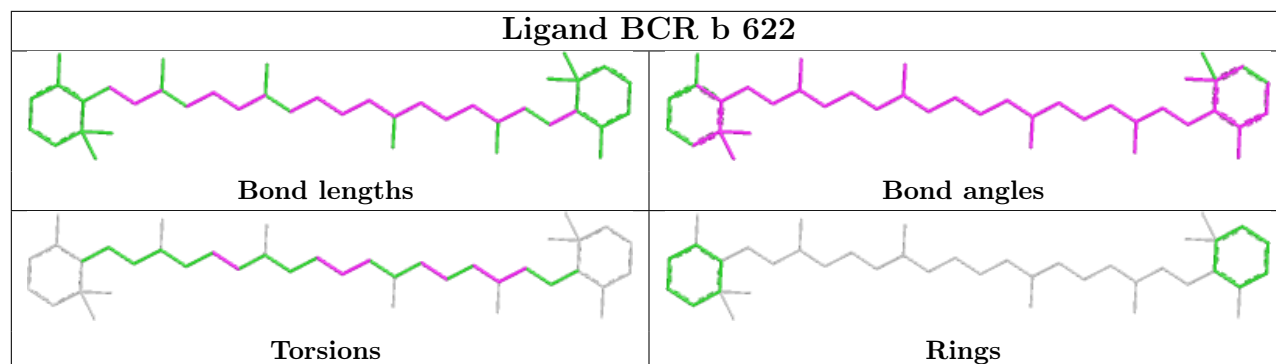
Ligand CLA c 509

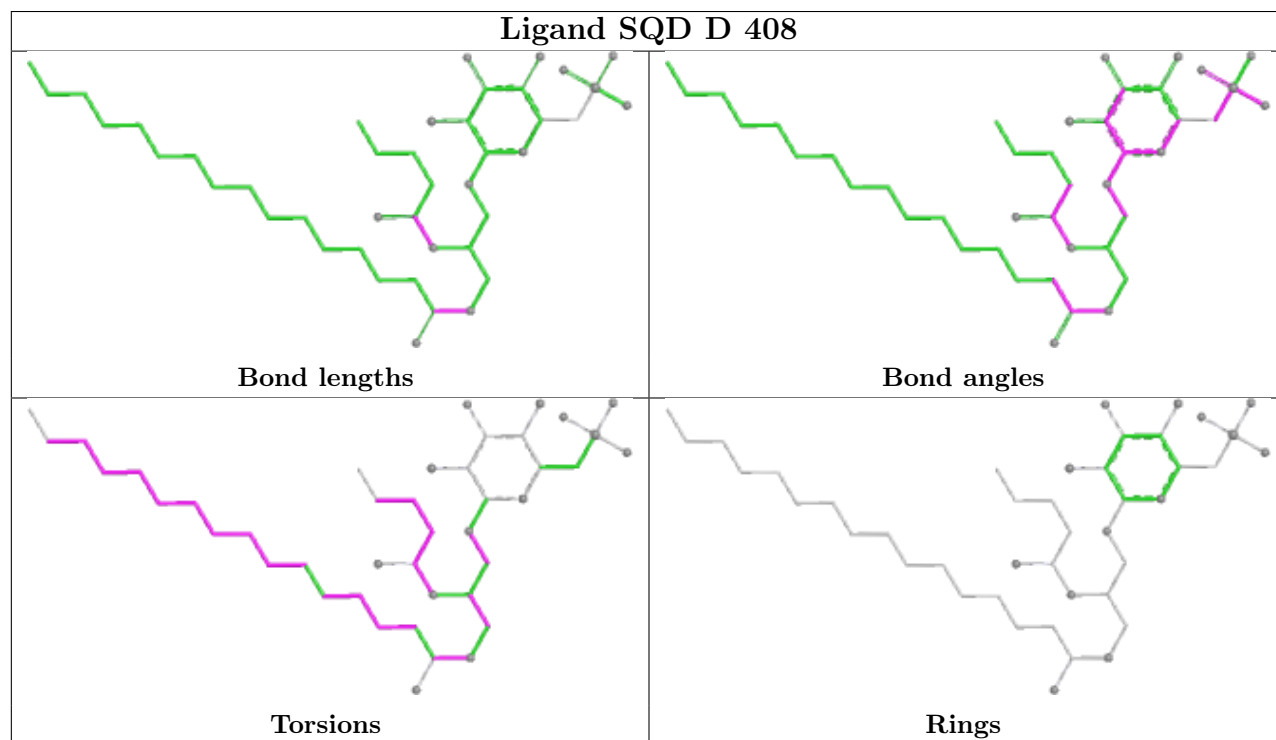
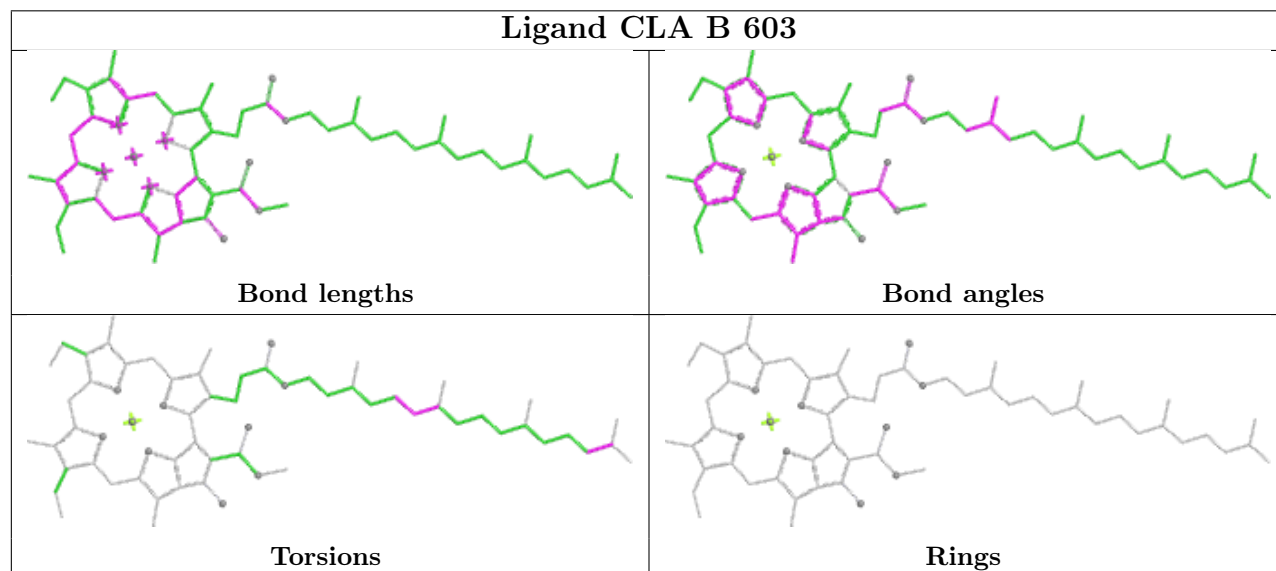
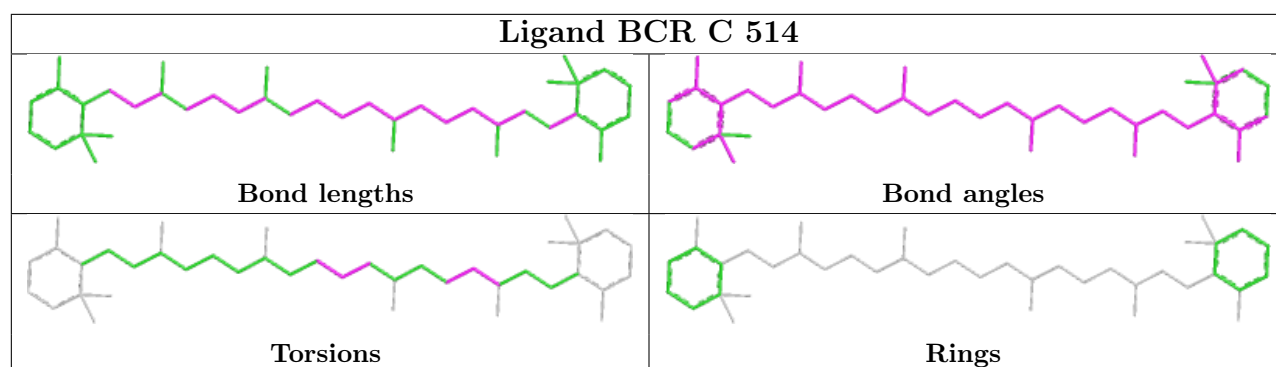


Ligand LHG e 101

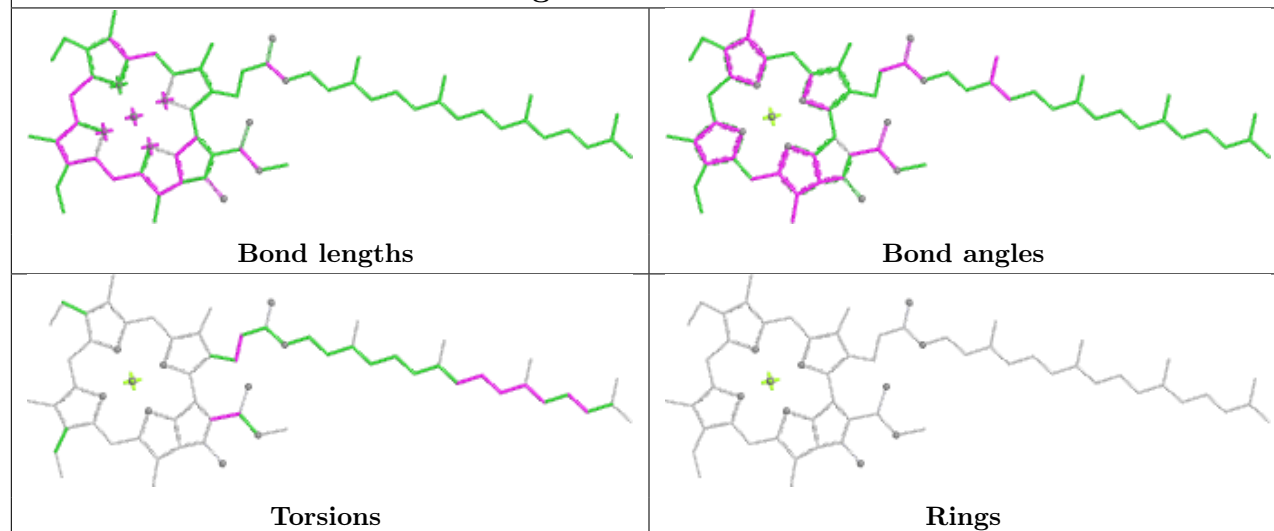




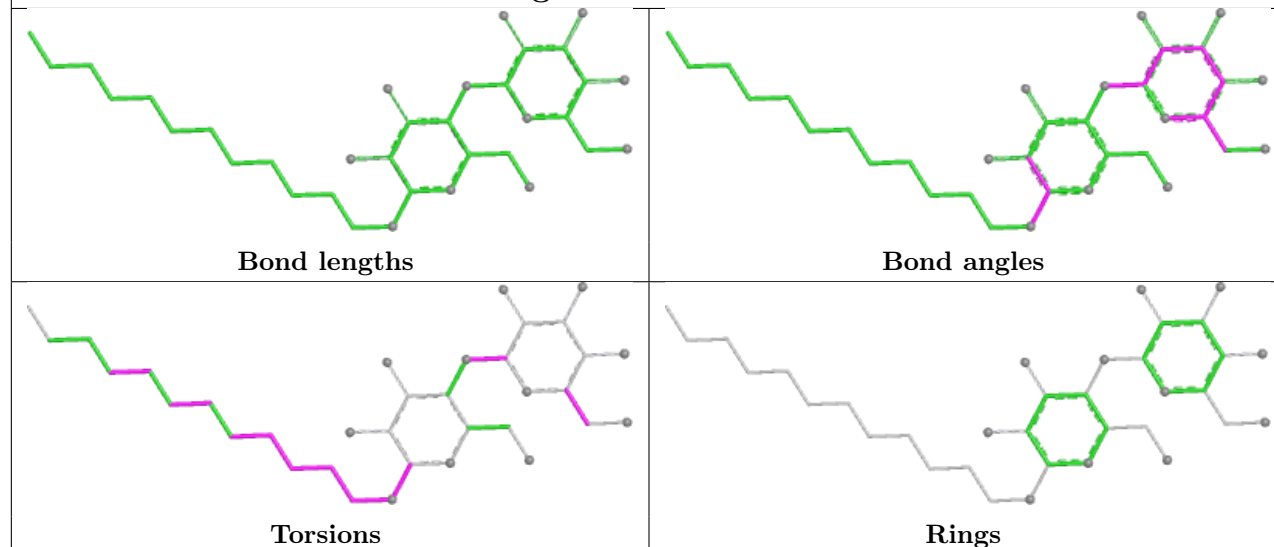




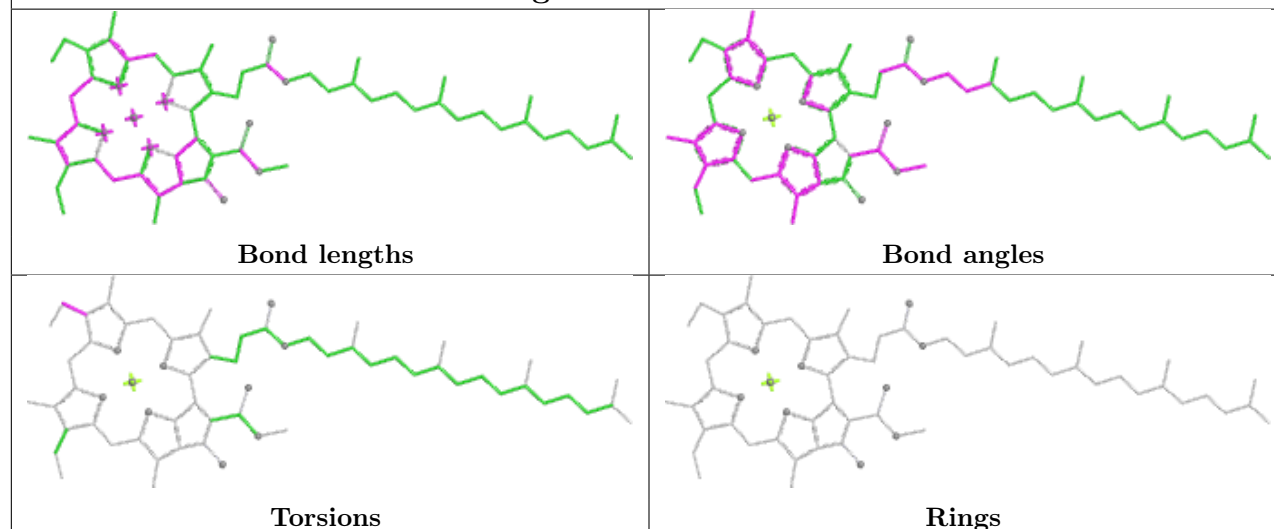
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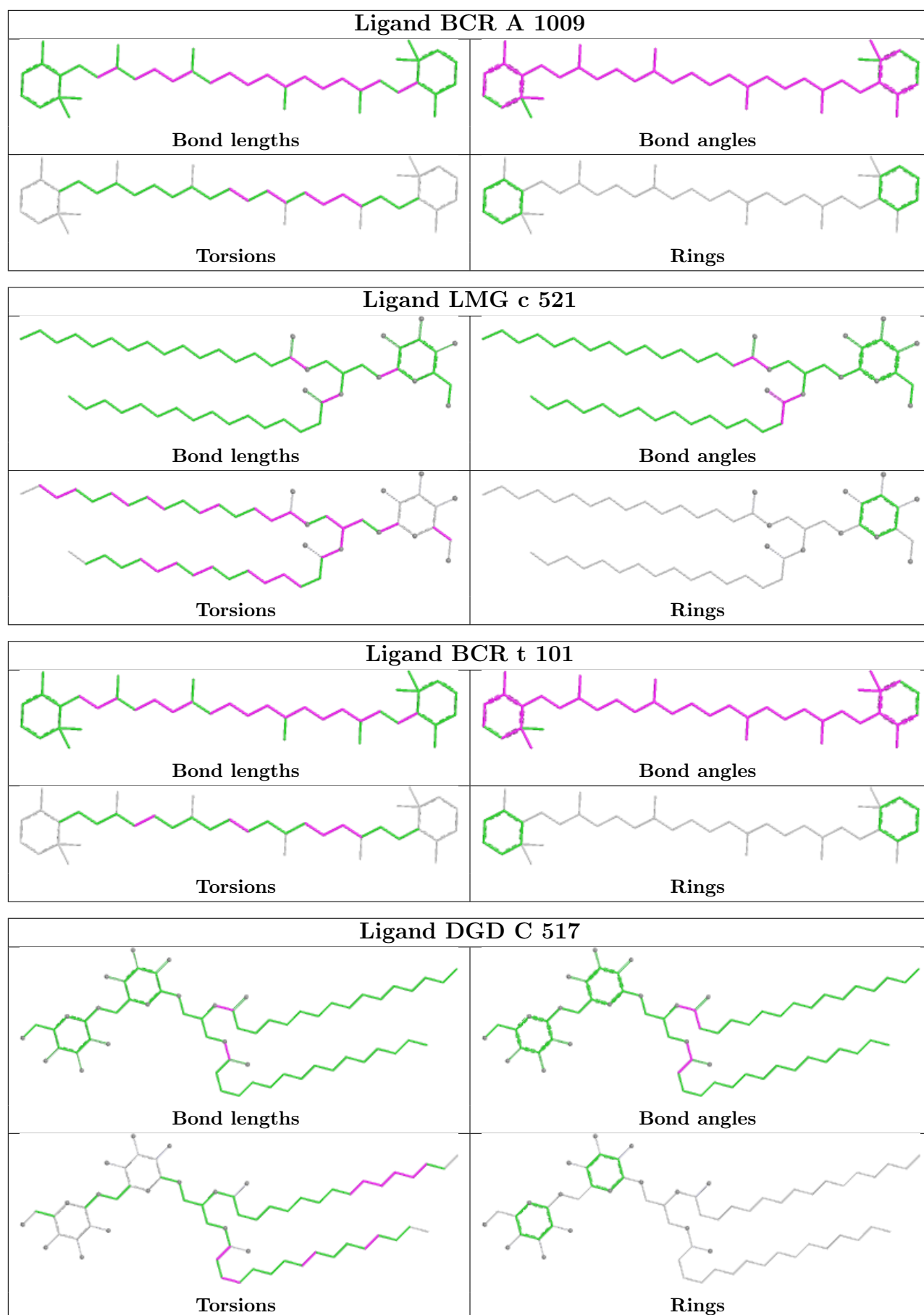


Ligand LMT b 625

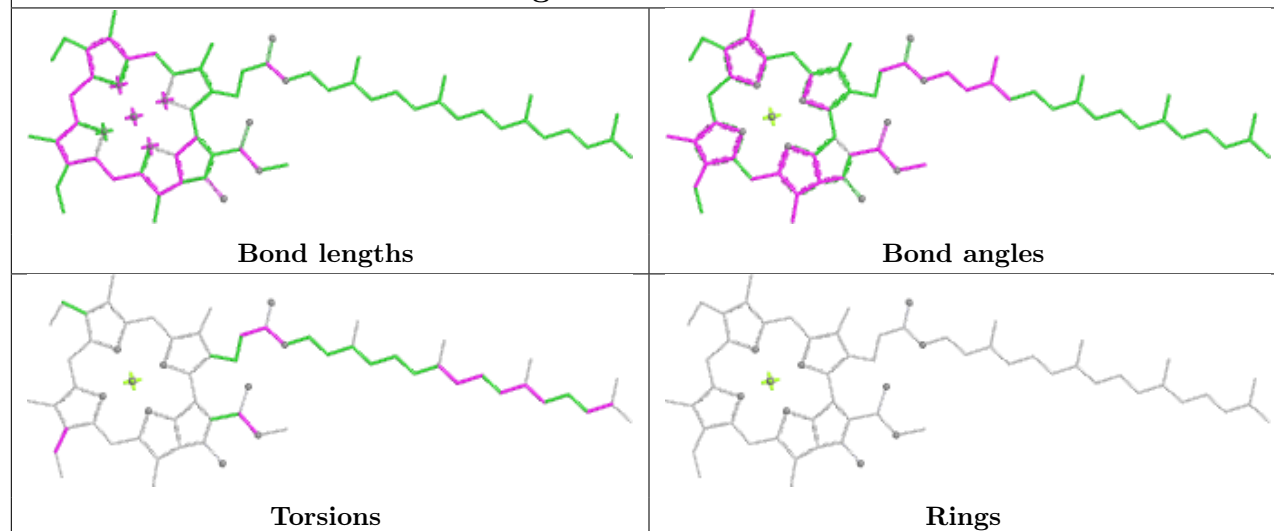


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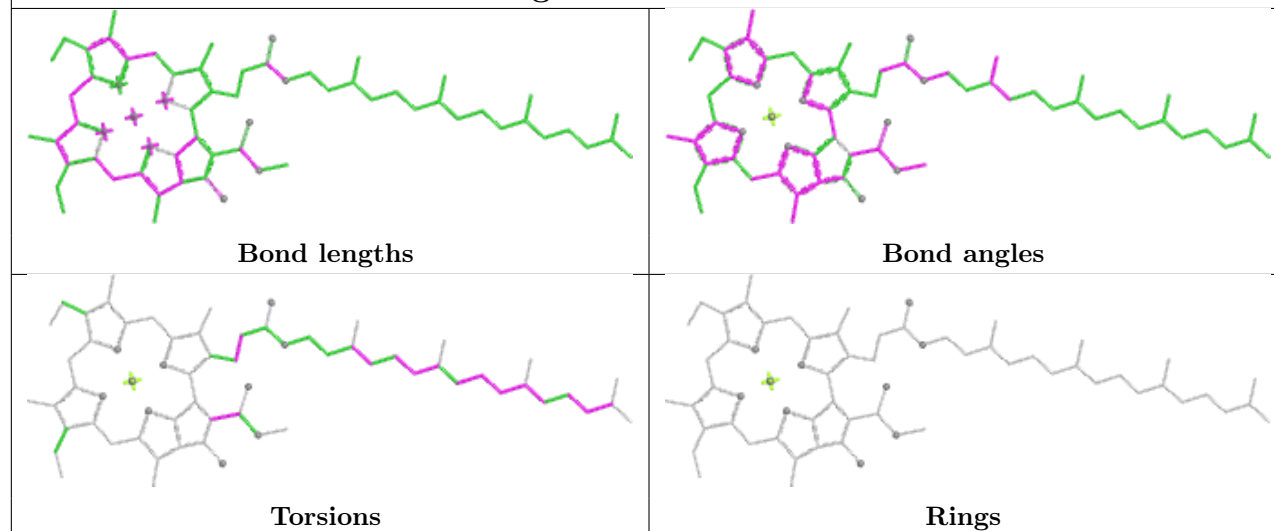




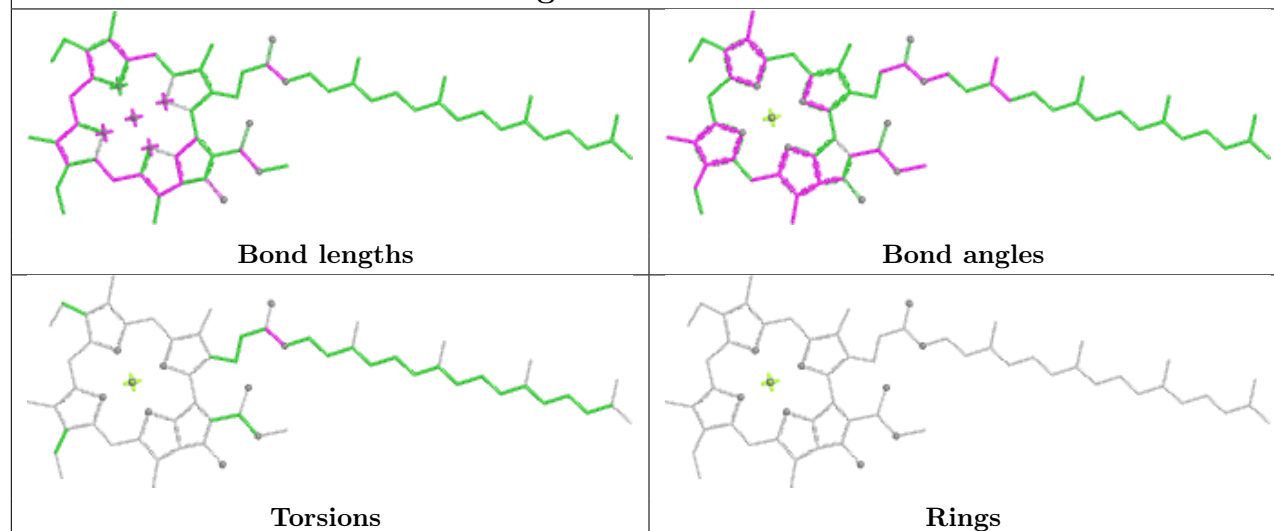
Ligand CLA C 512

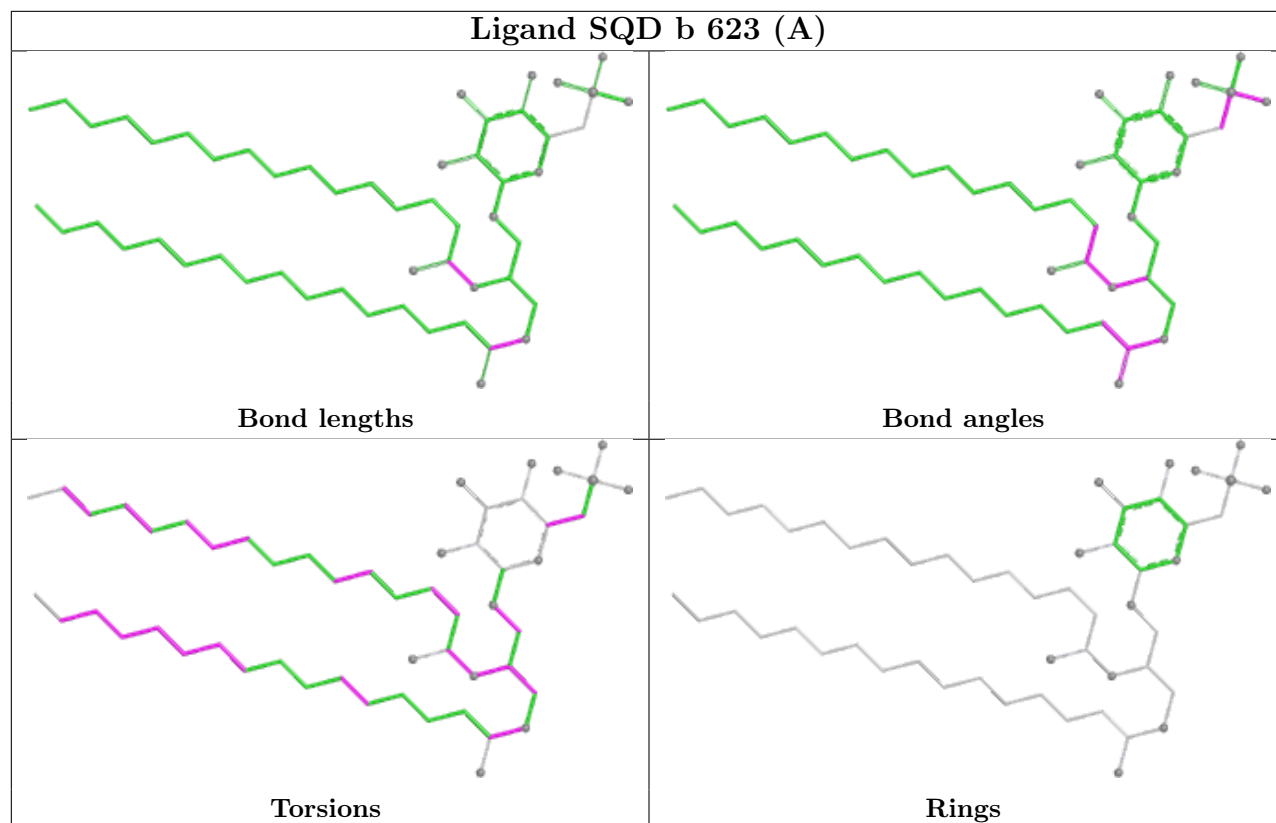
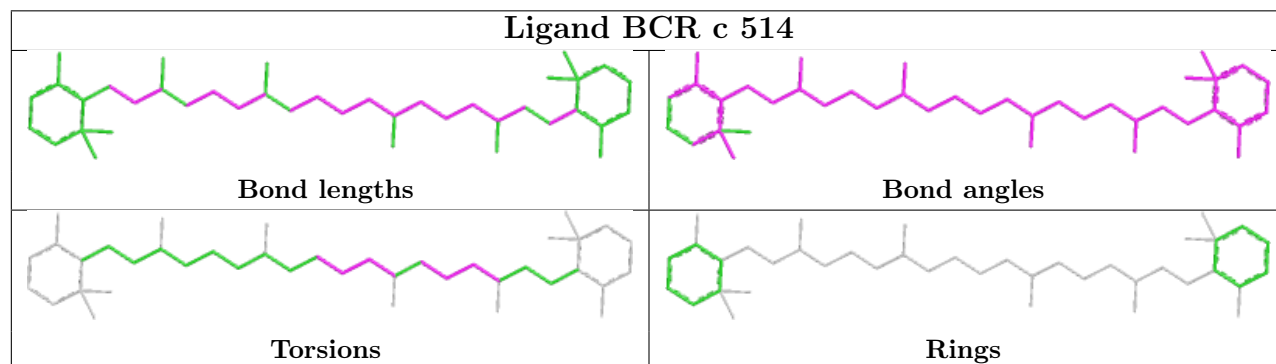
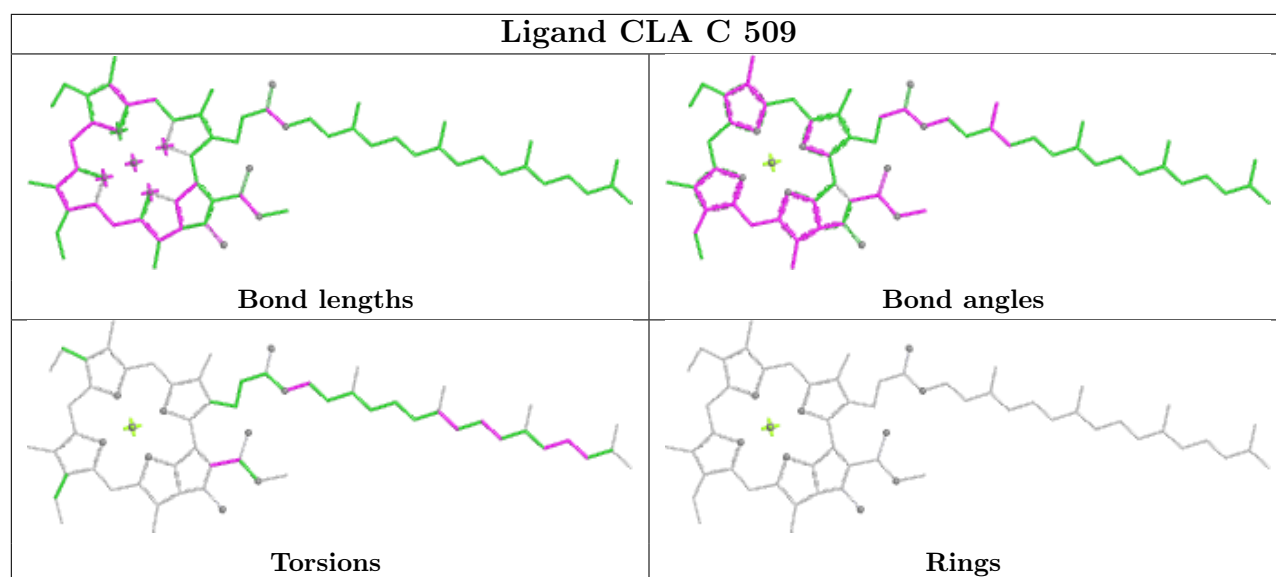


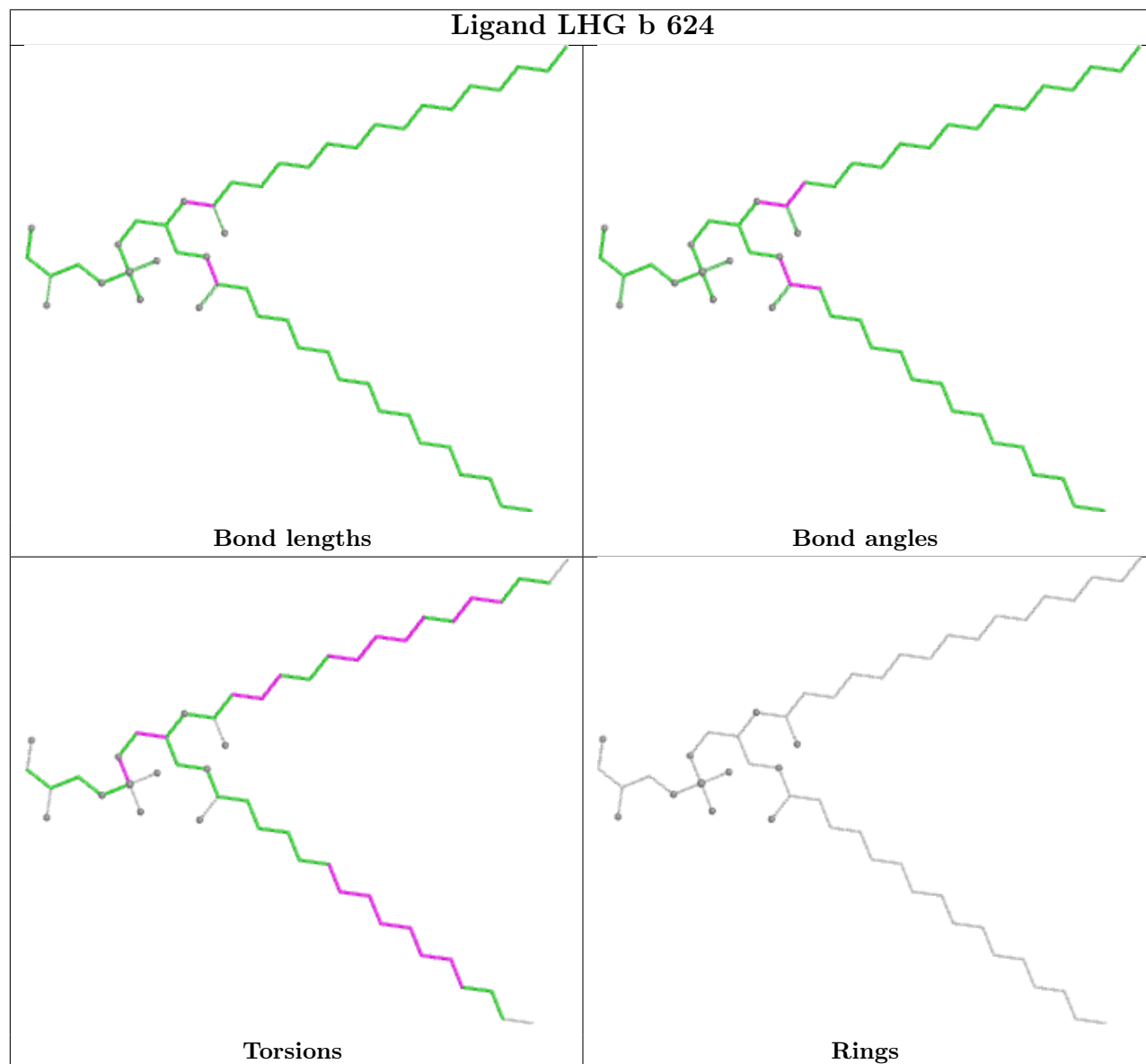
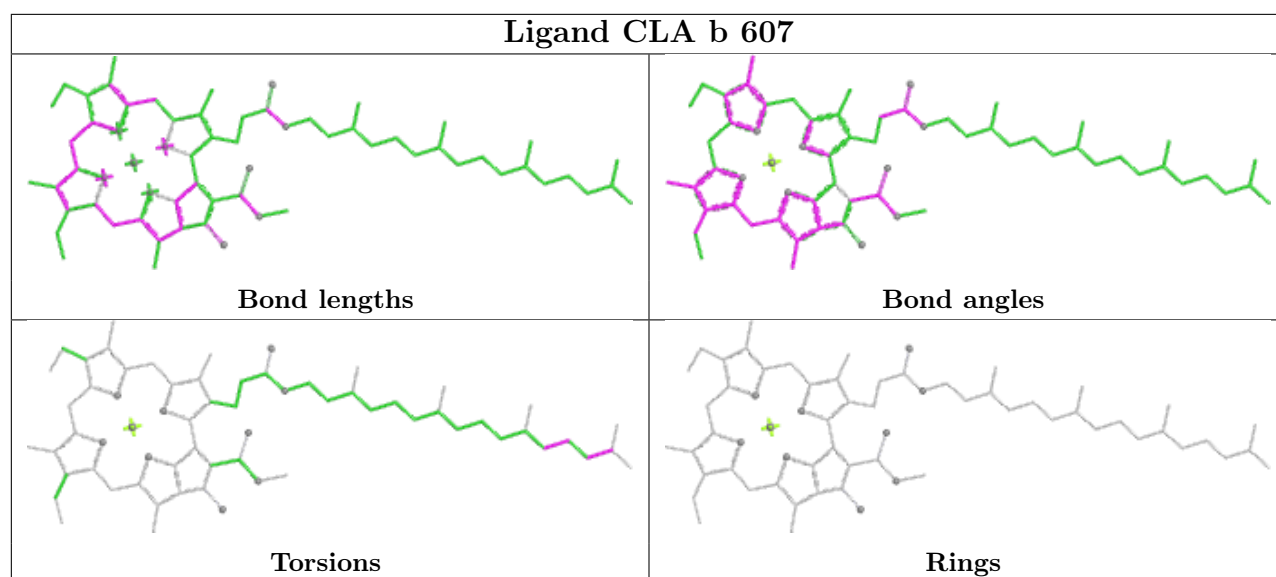
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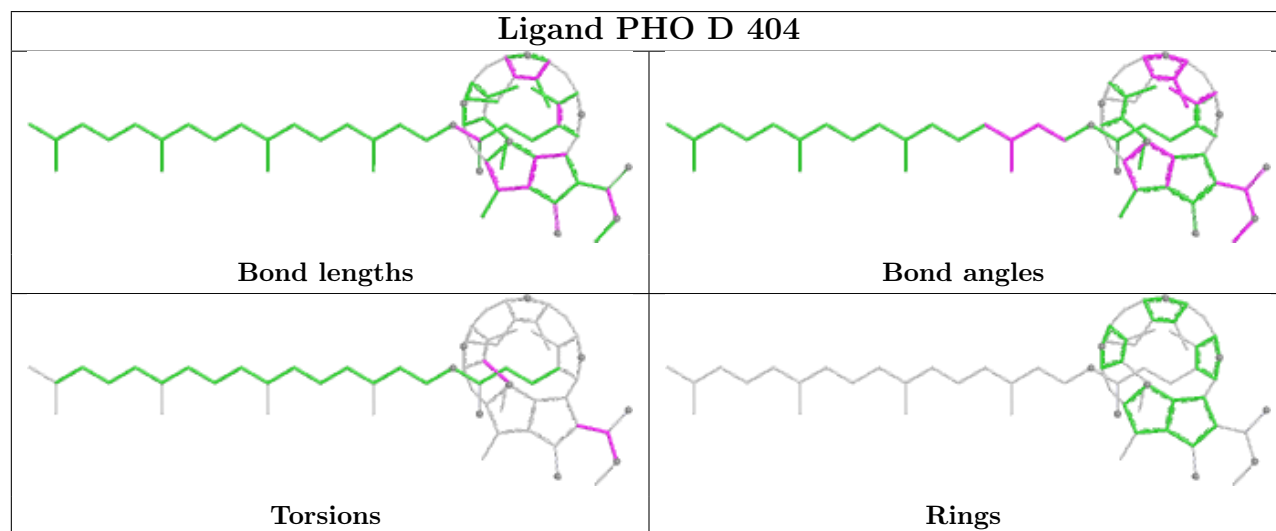
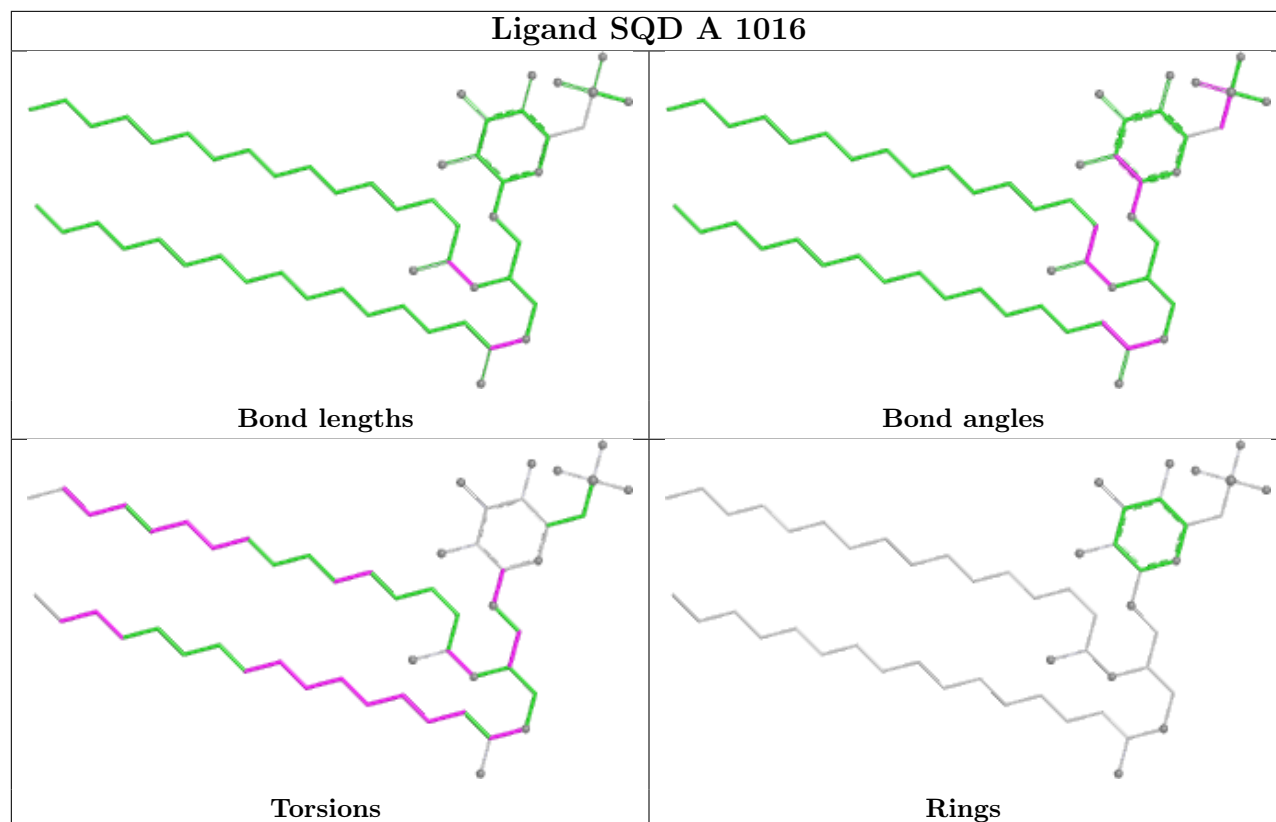


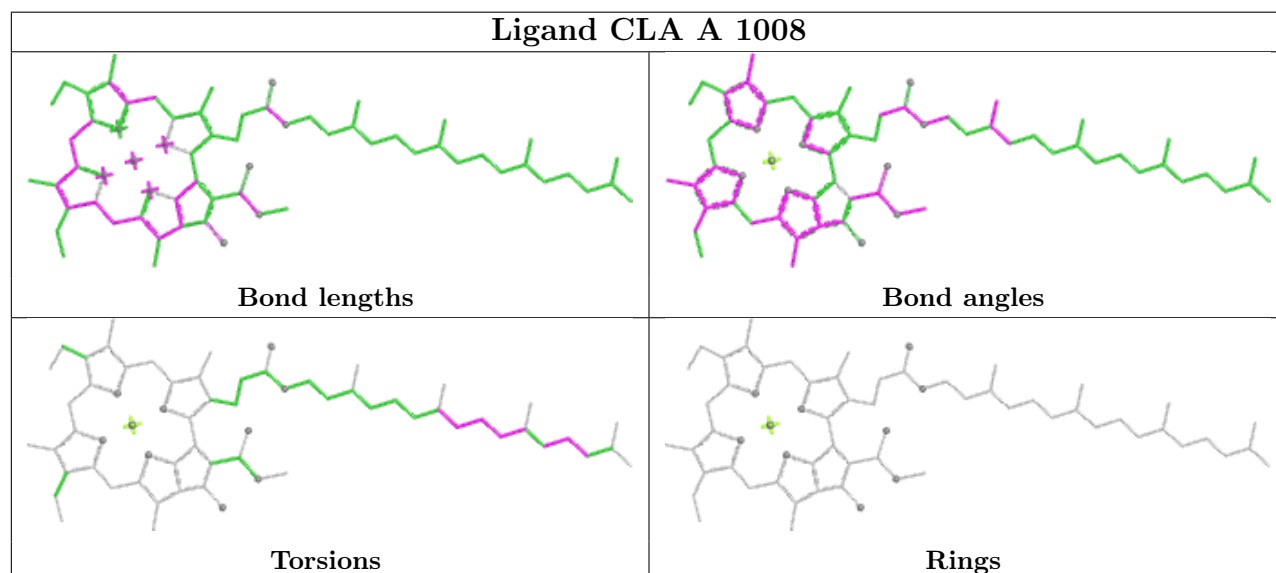
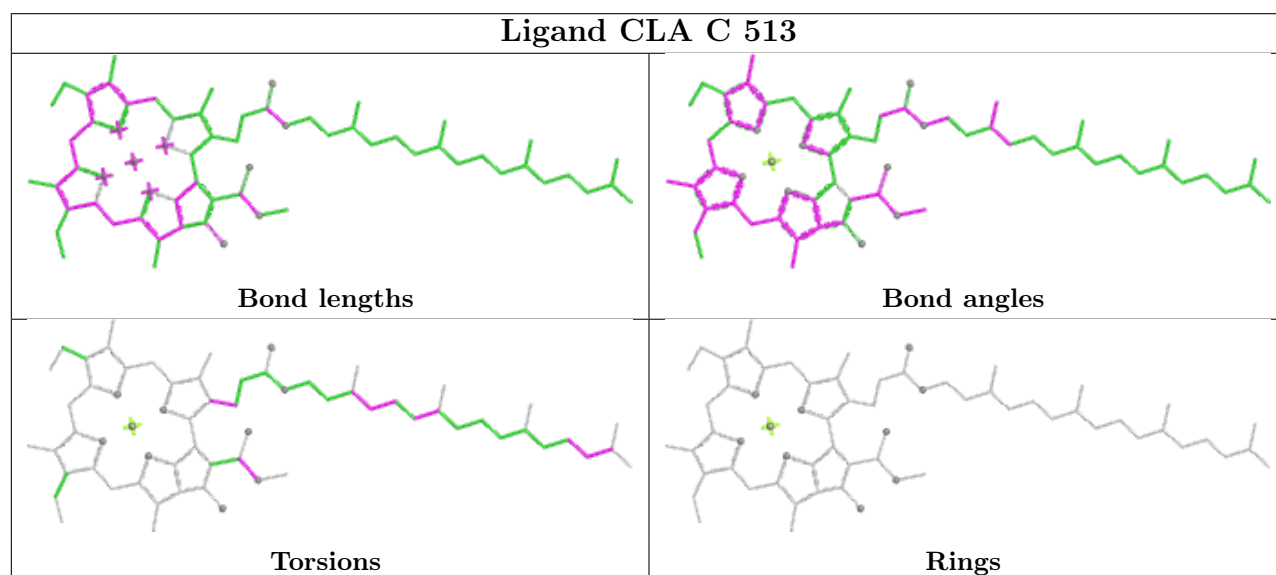
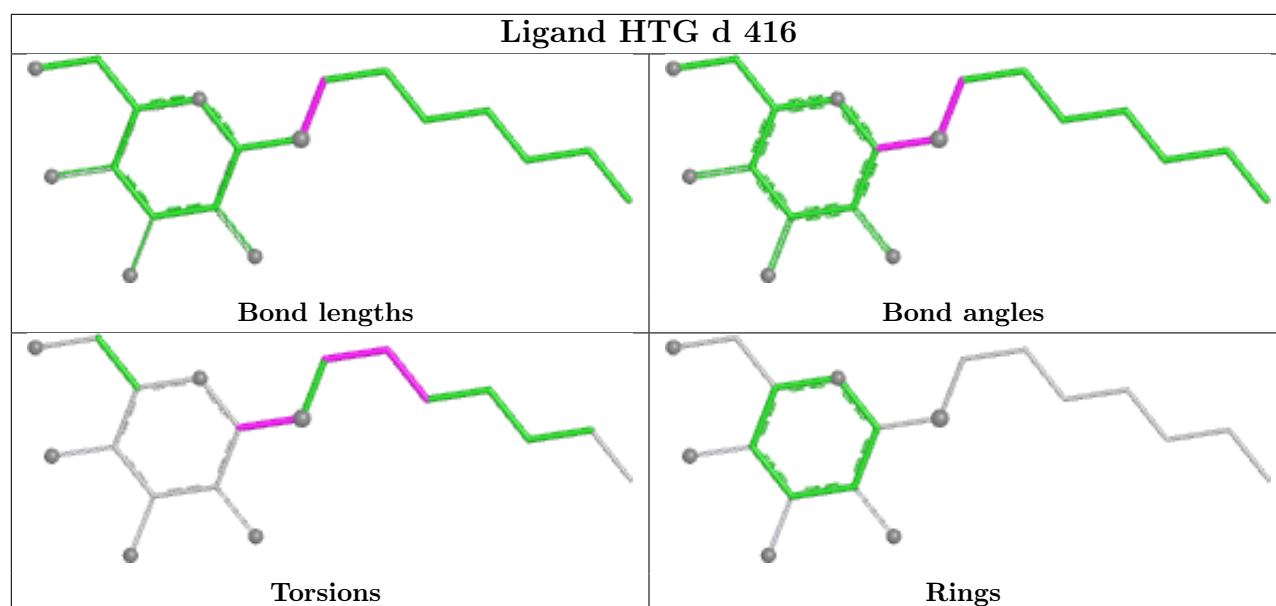
Ligand CLA c 511

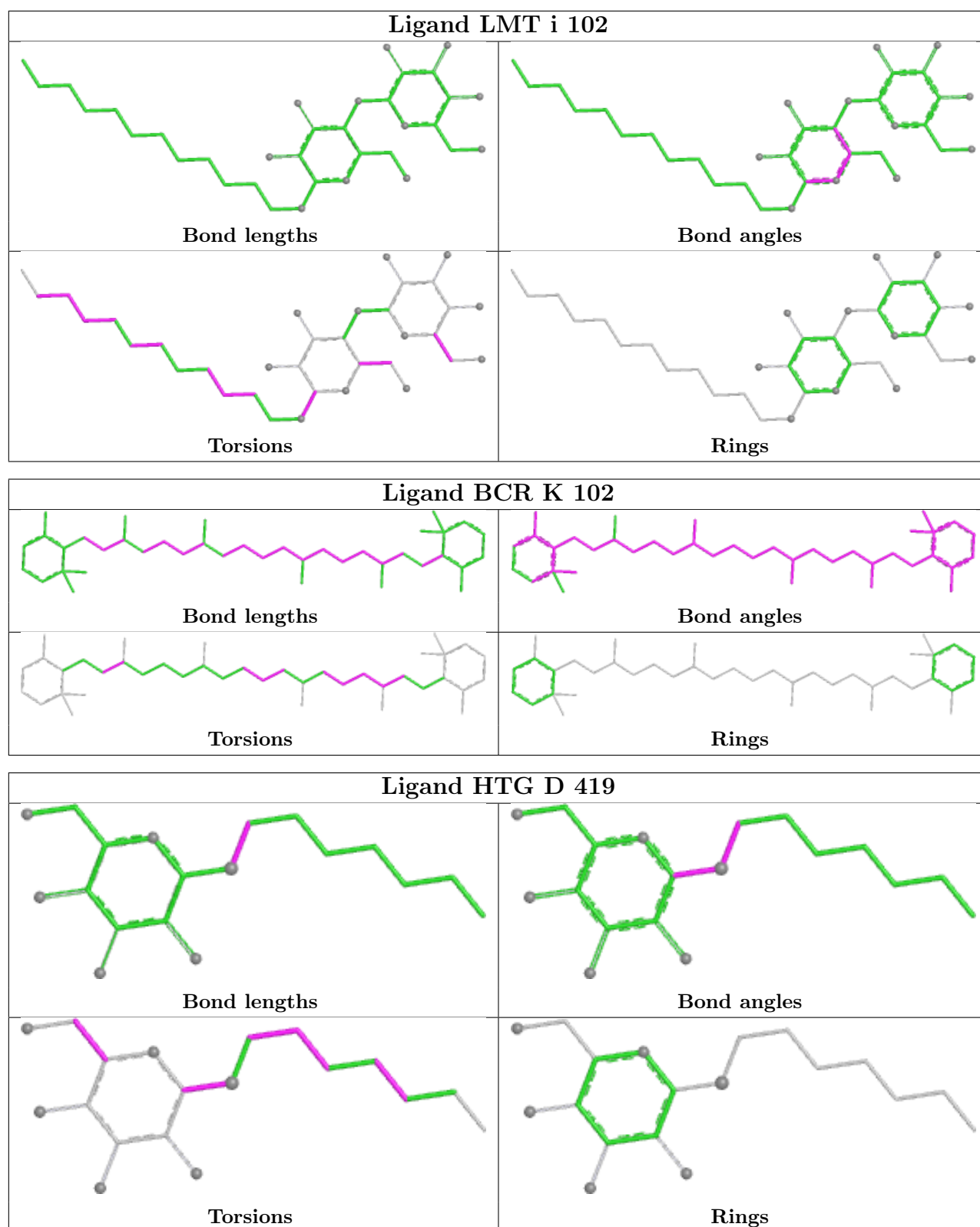


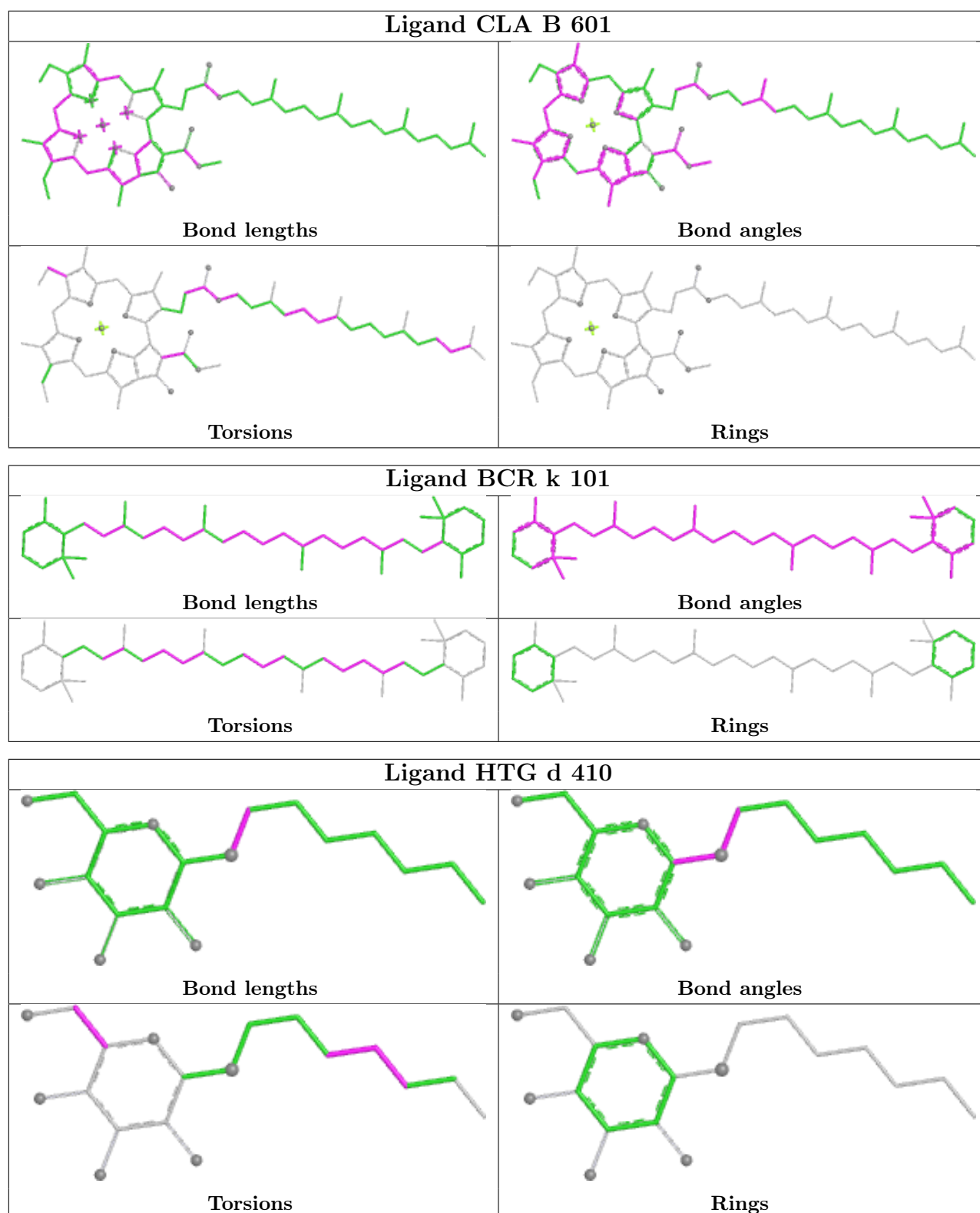


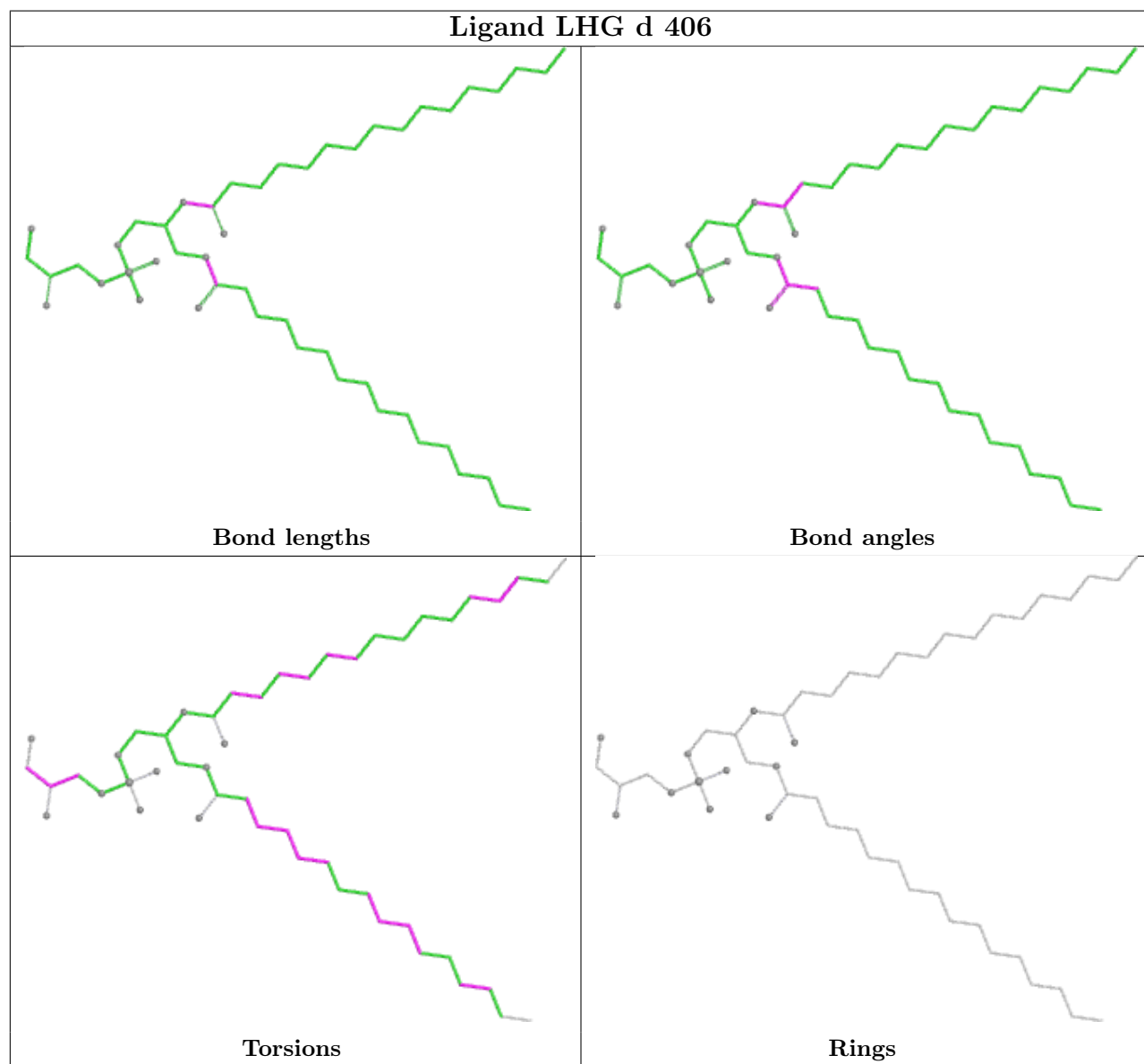
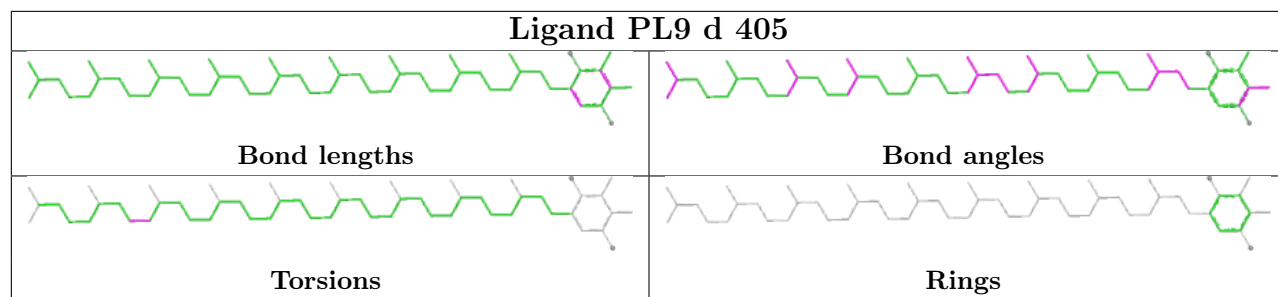




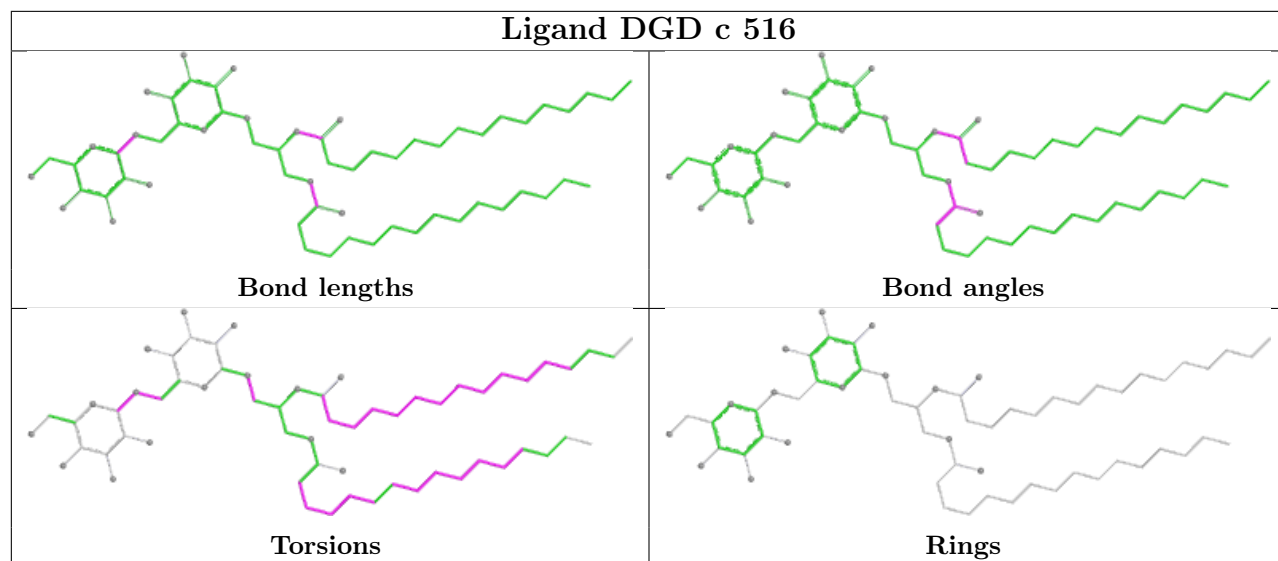




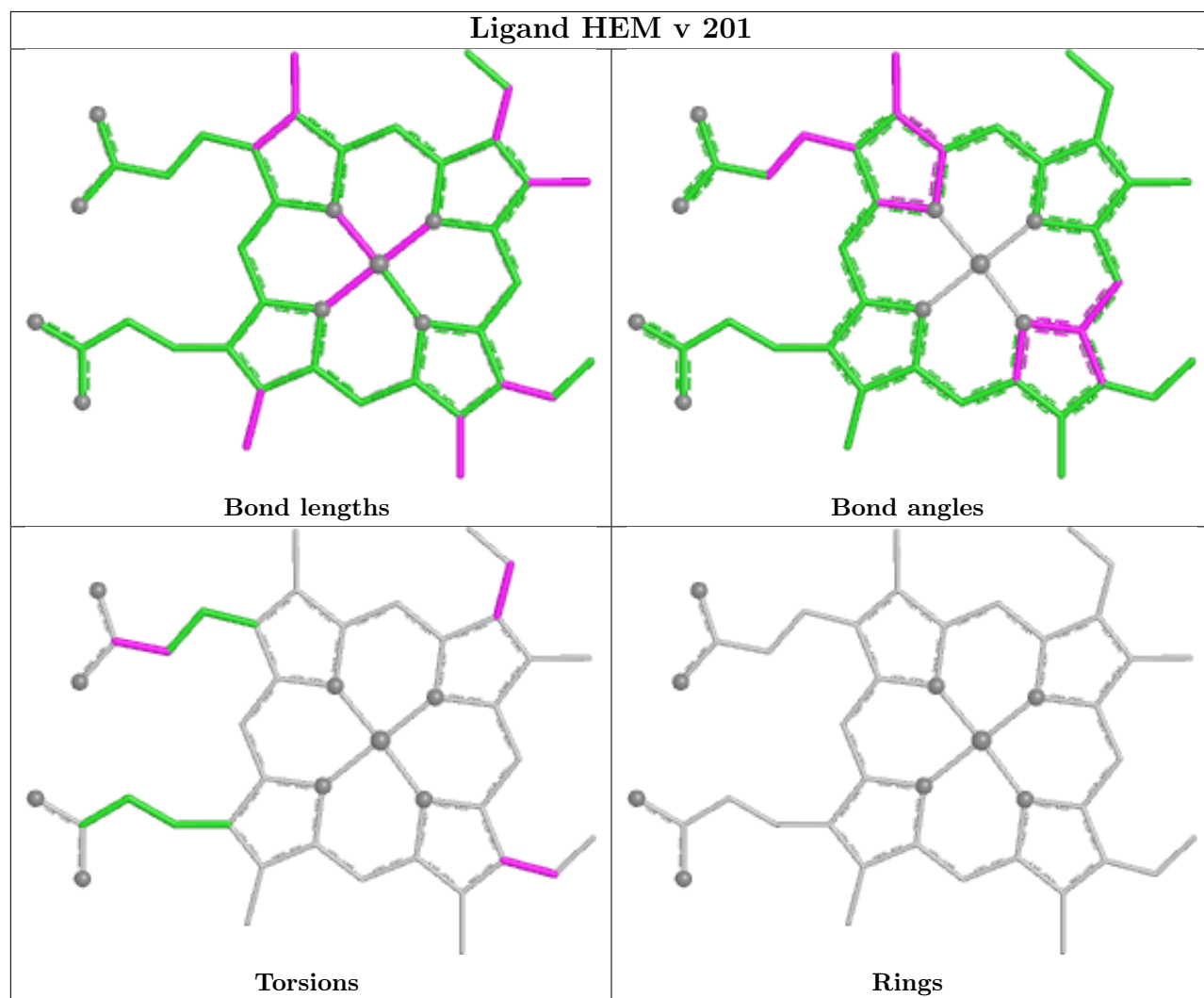


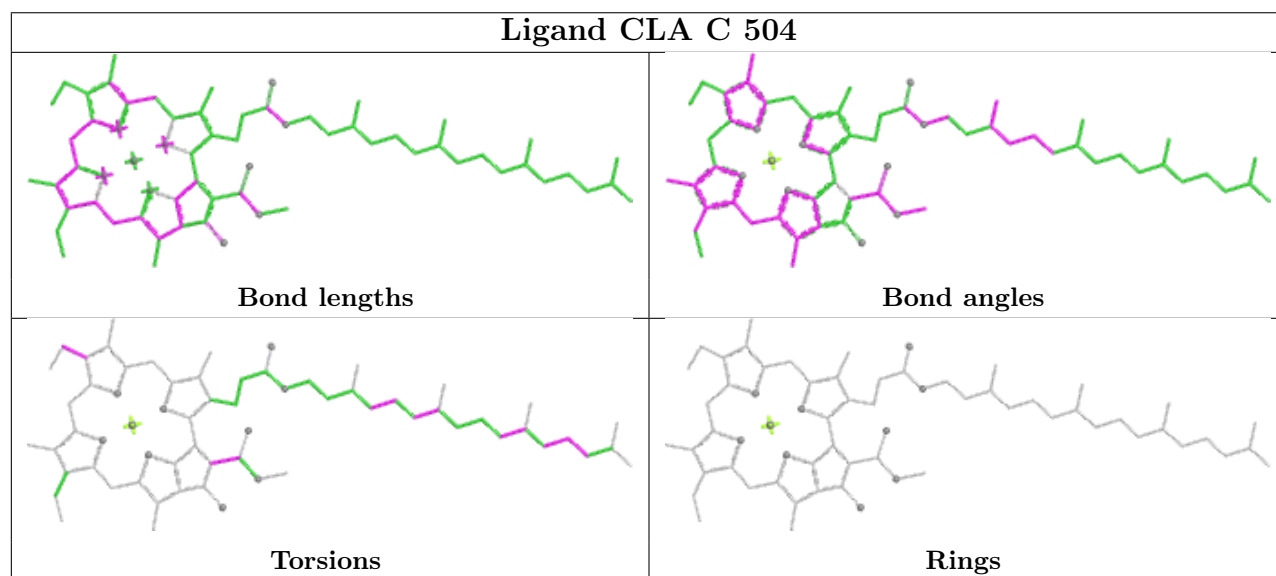
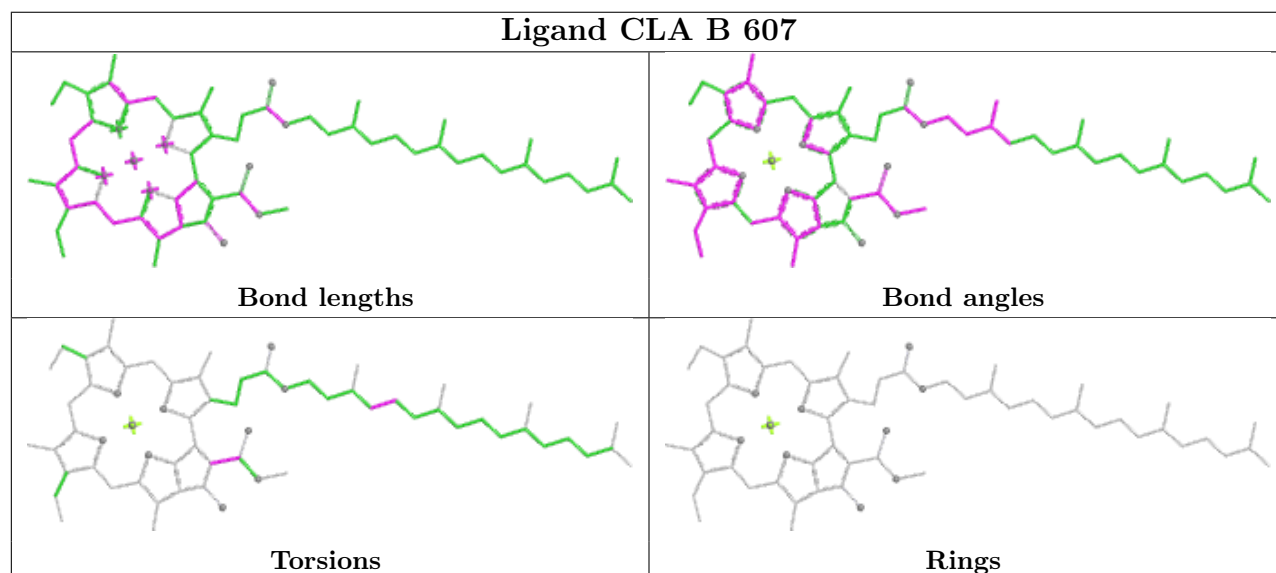
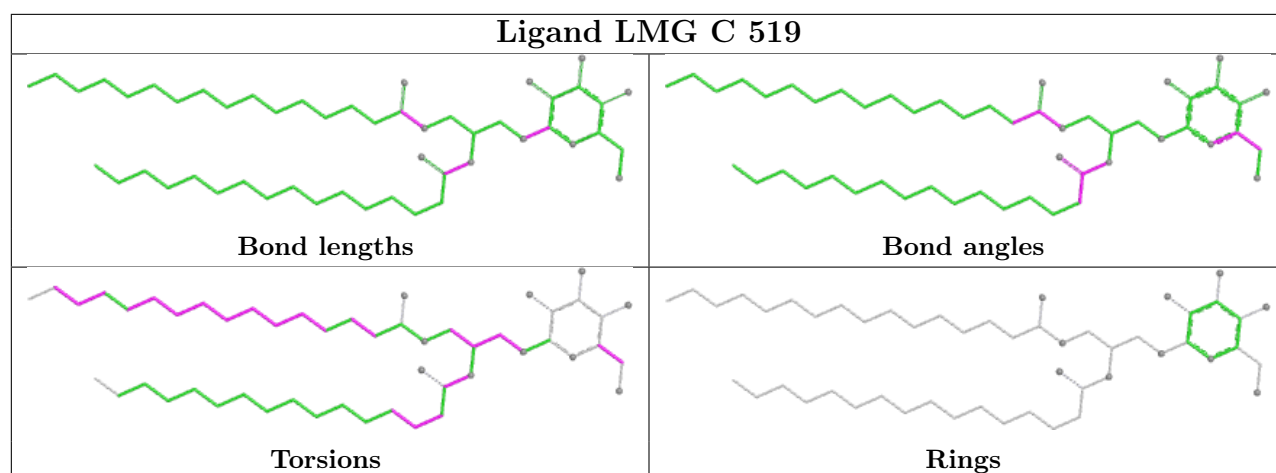


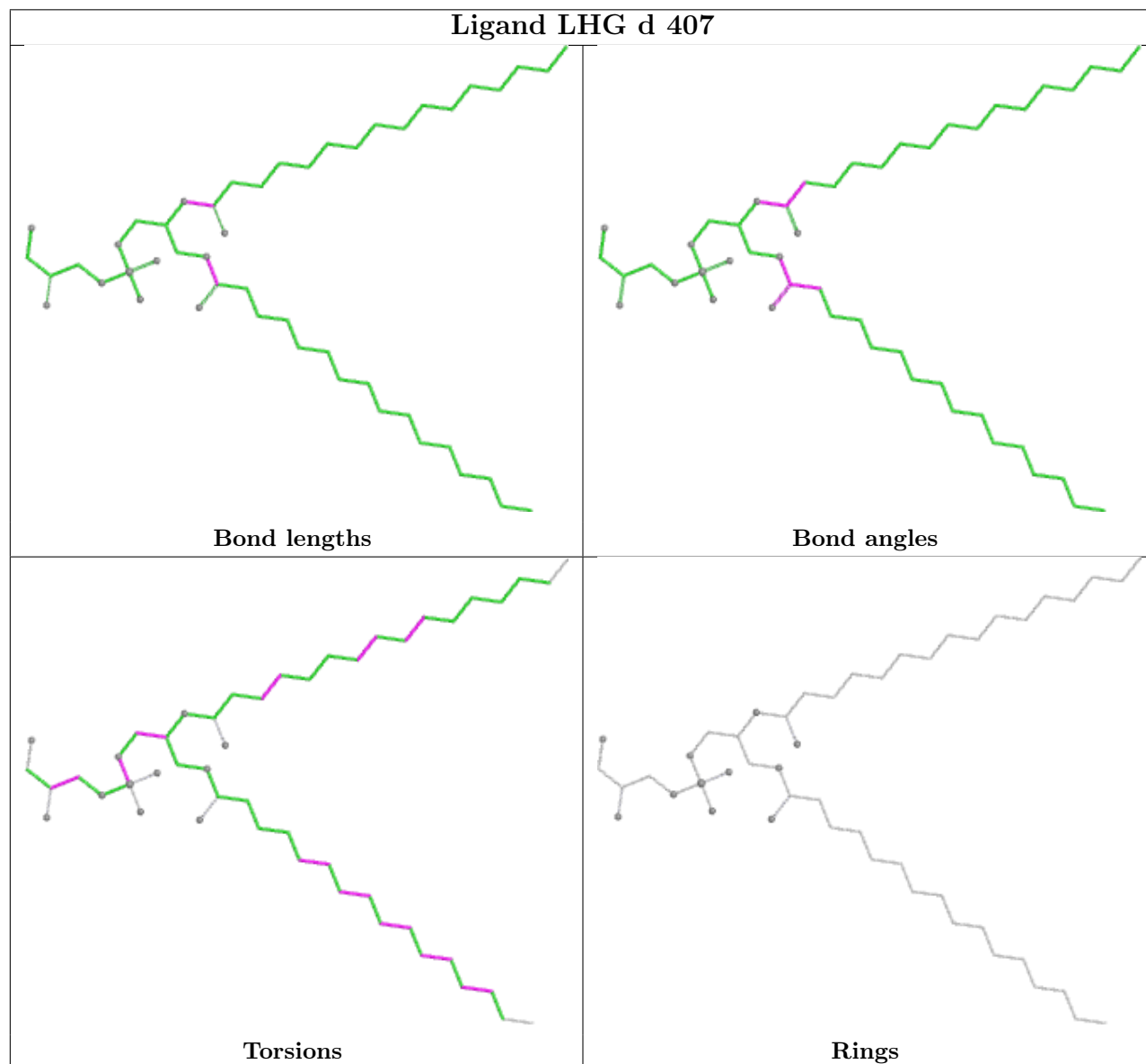
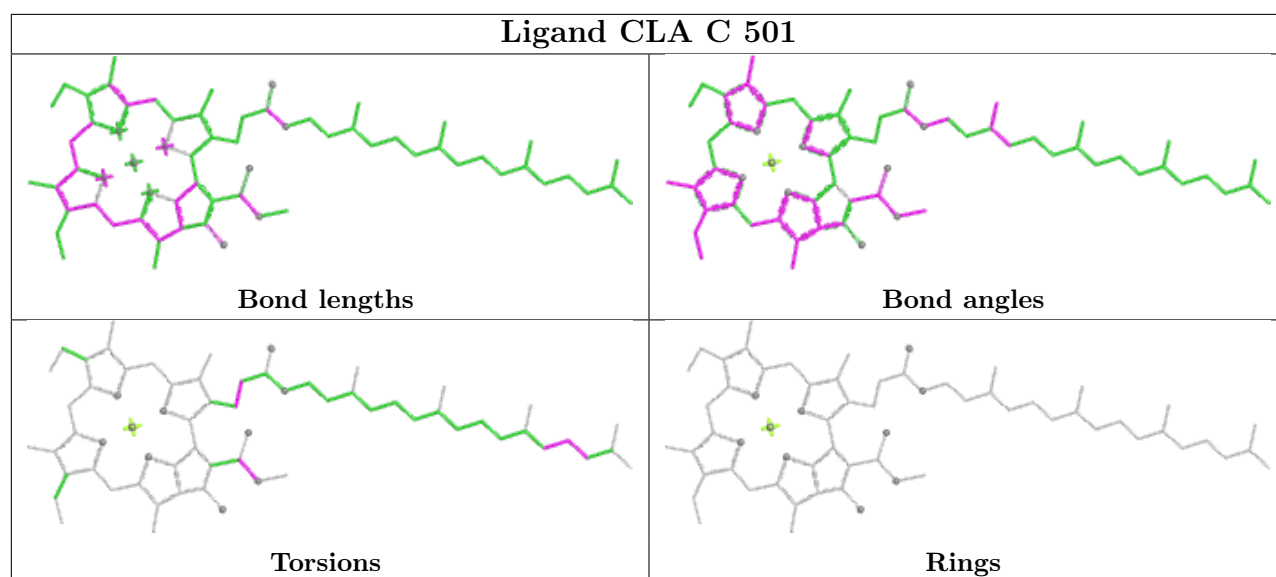
Ligand DGD c 516



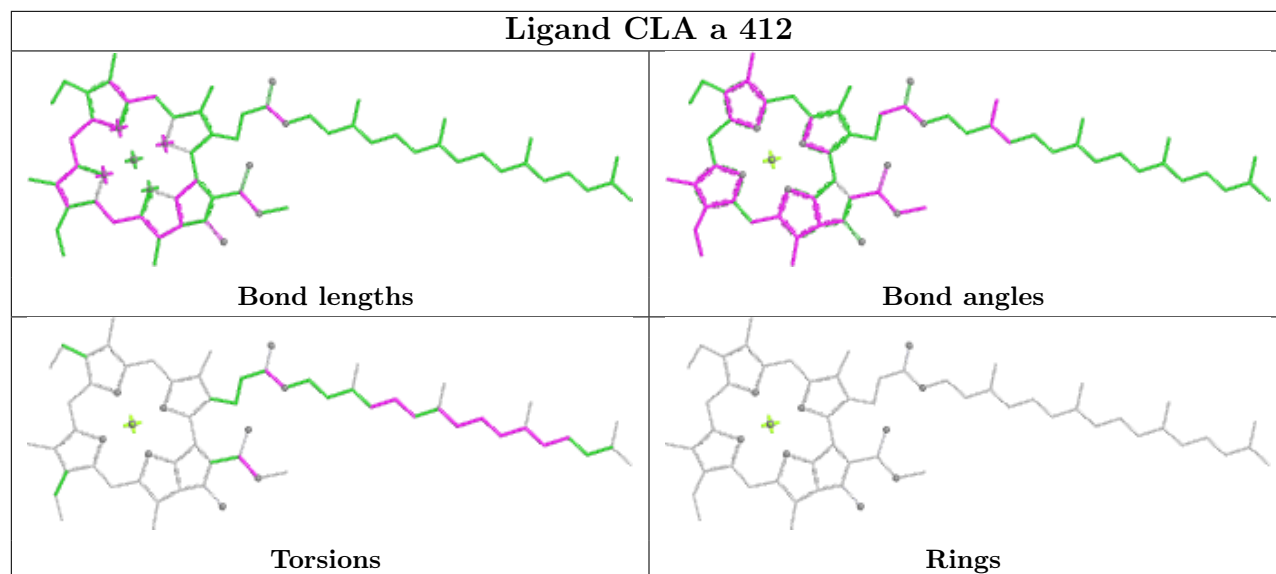
Ligand HEM v 201



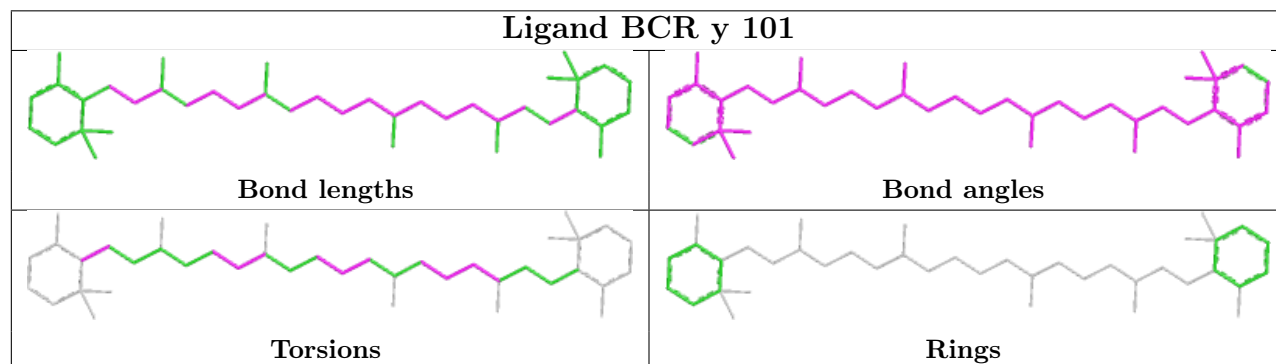




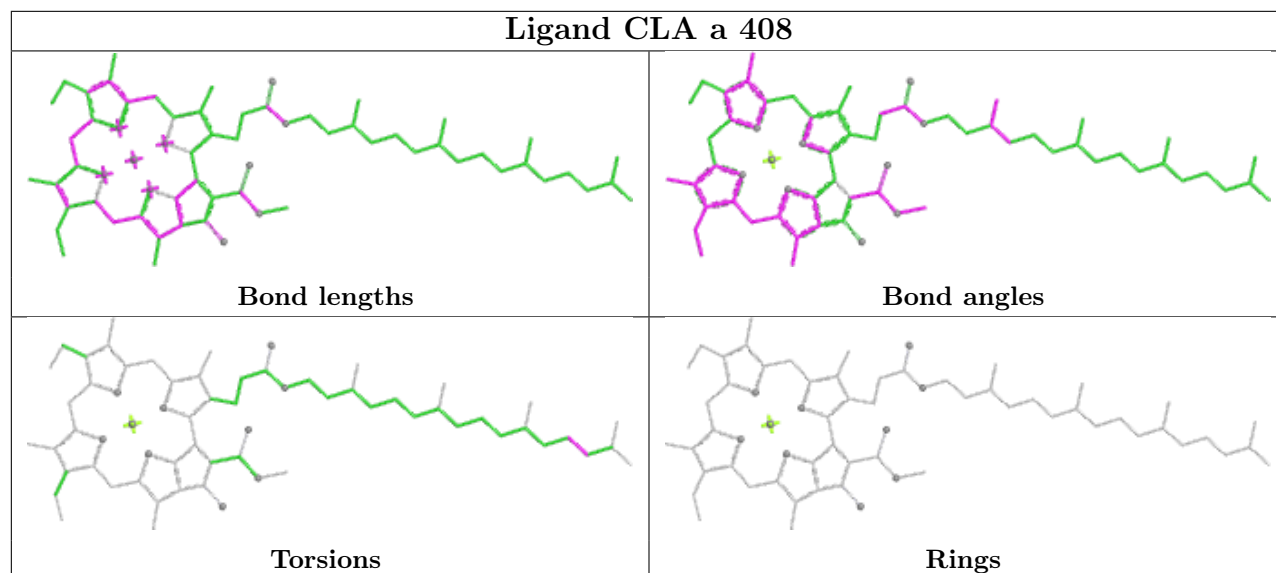
Ligand CLA a 412

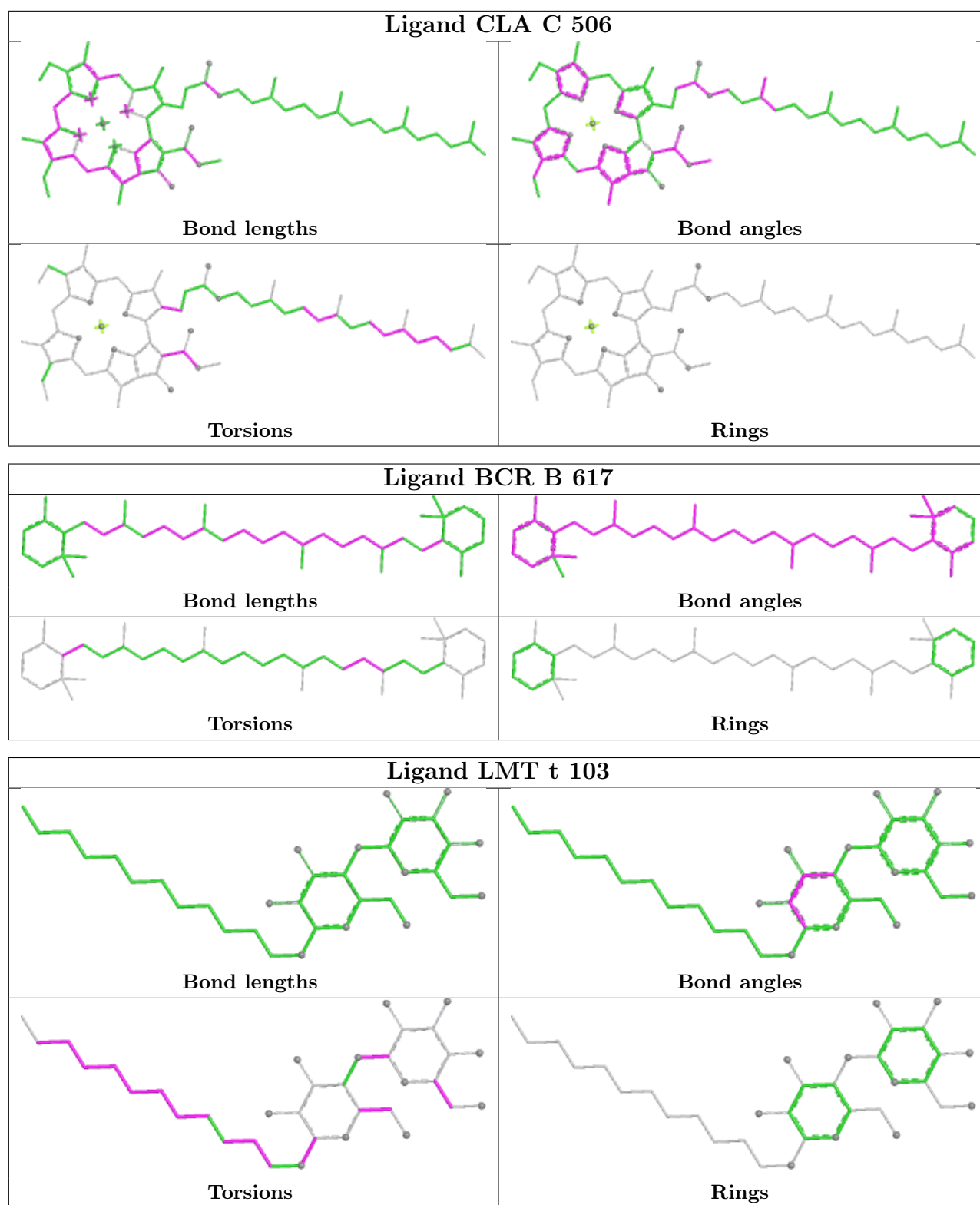


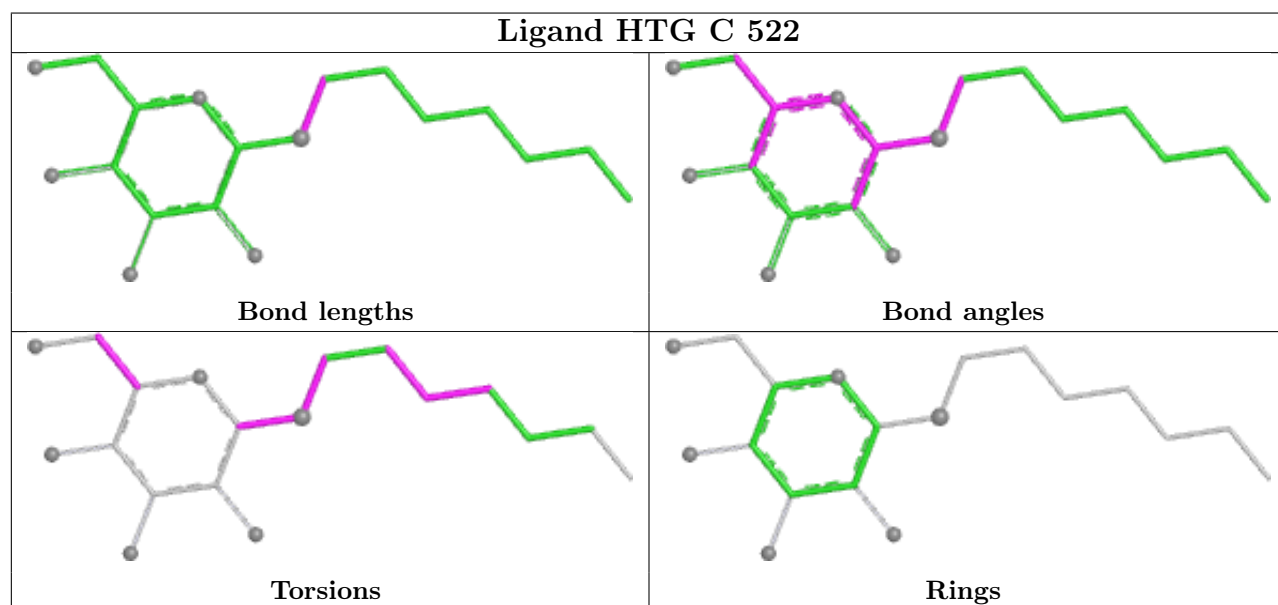
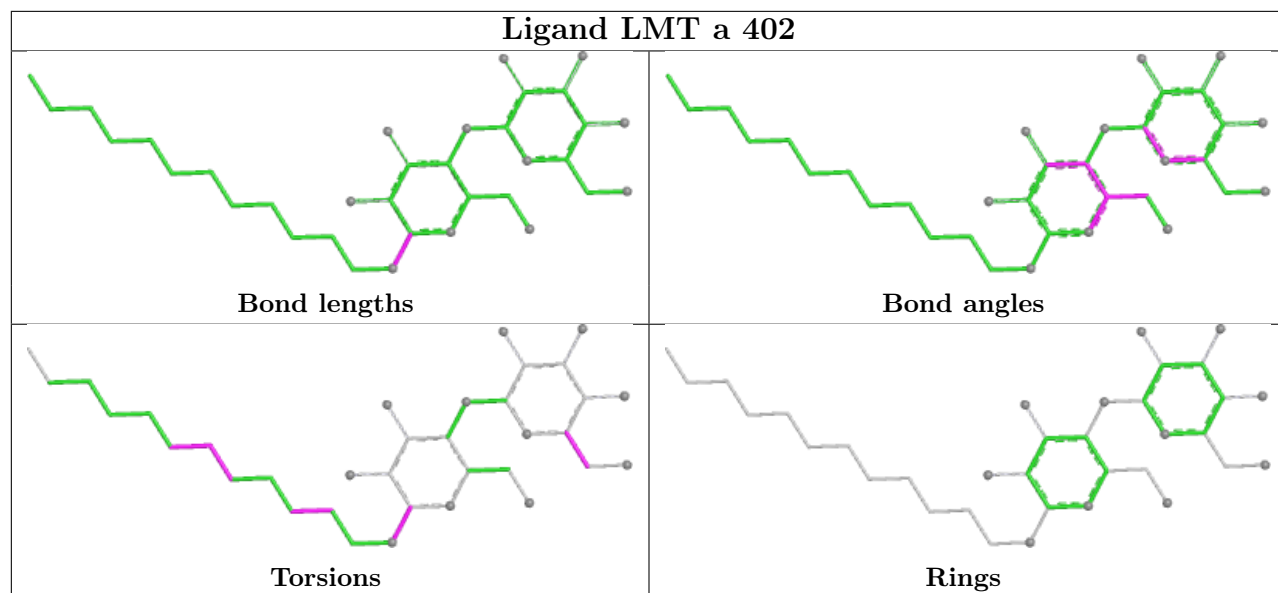
Ligand BCR y 101

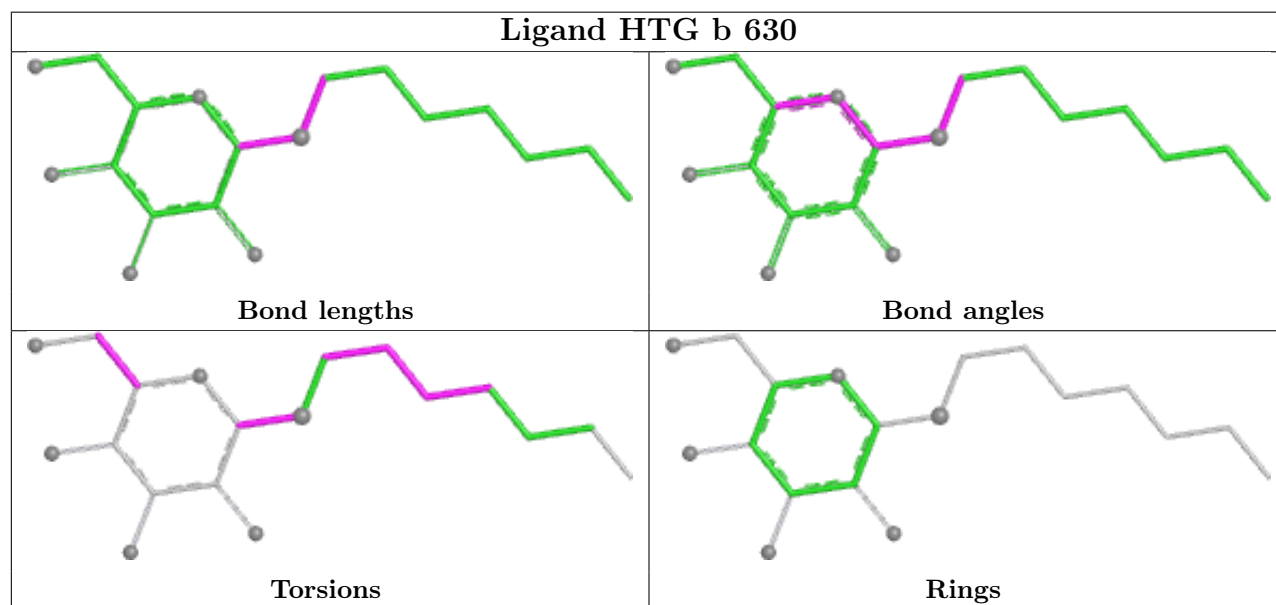
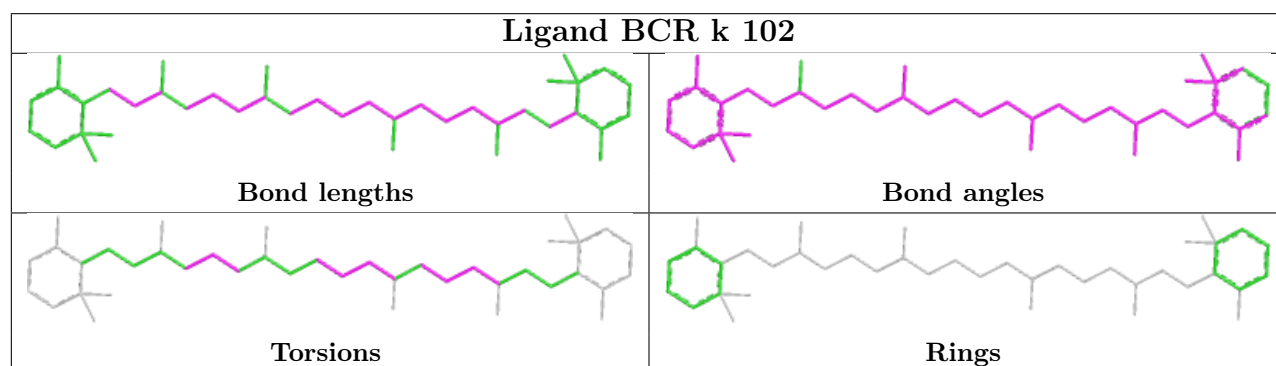
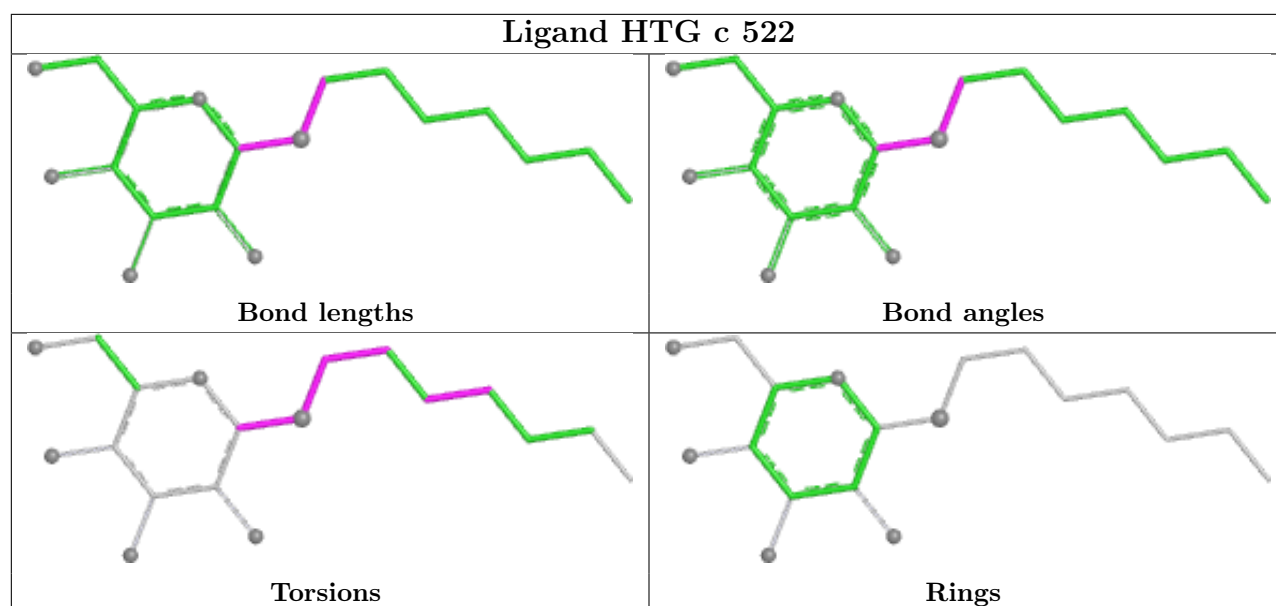


Ligand CLA a 408

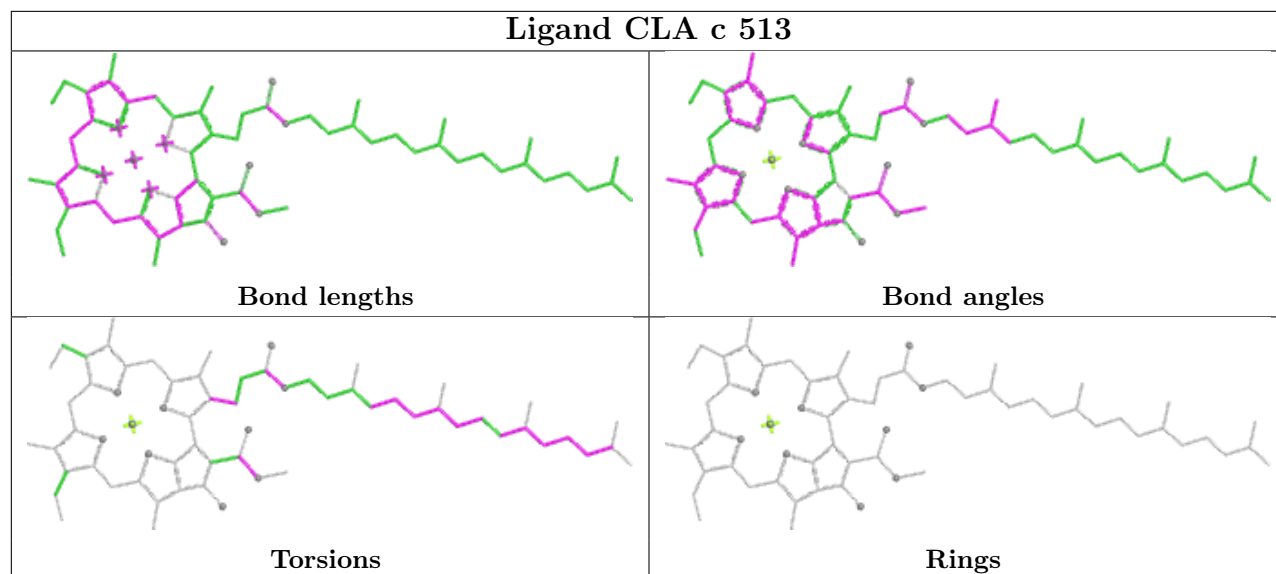




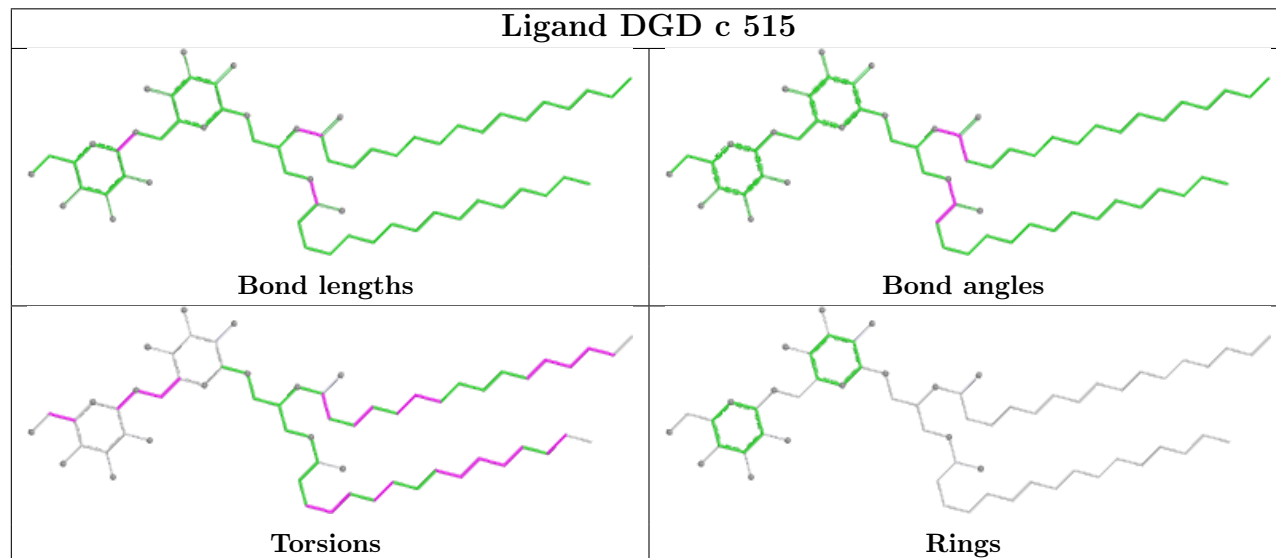


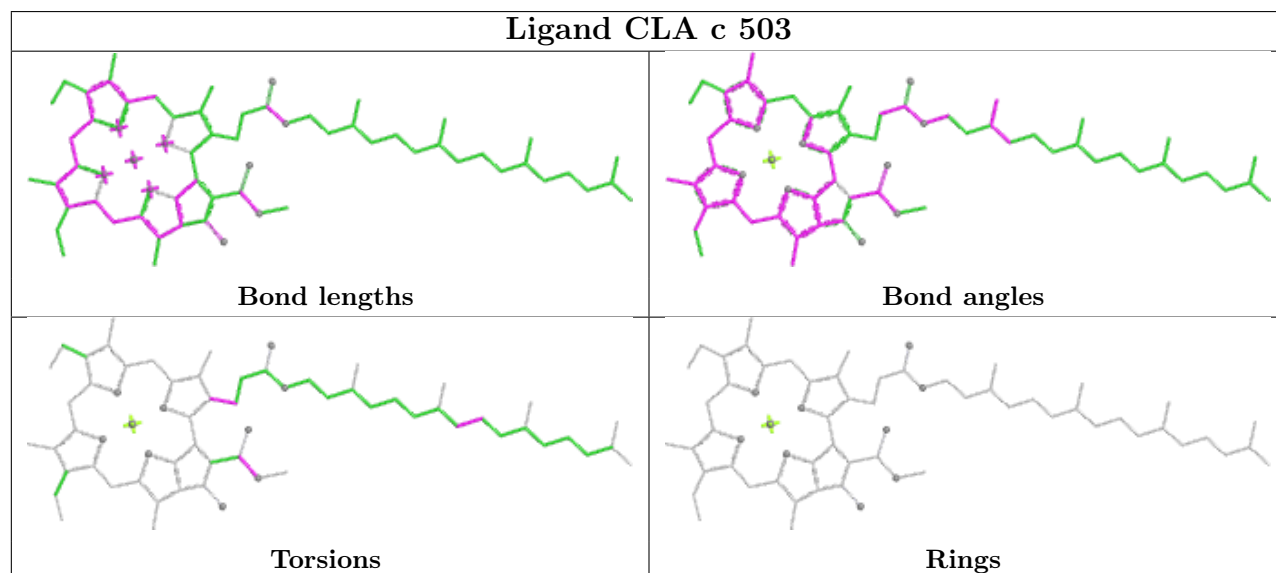
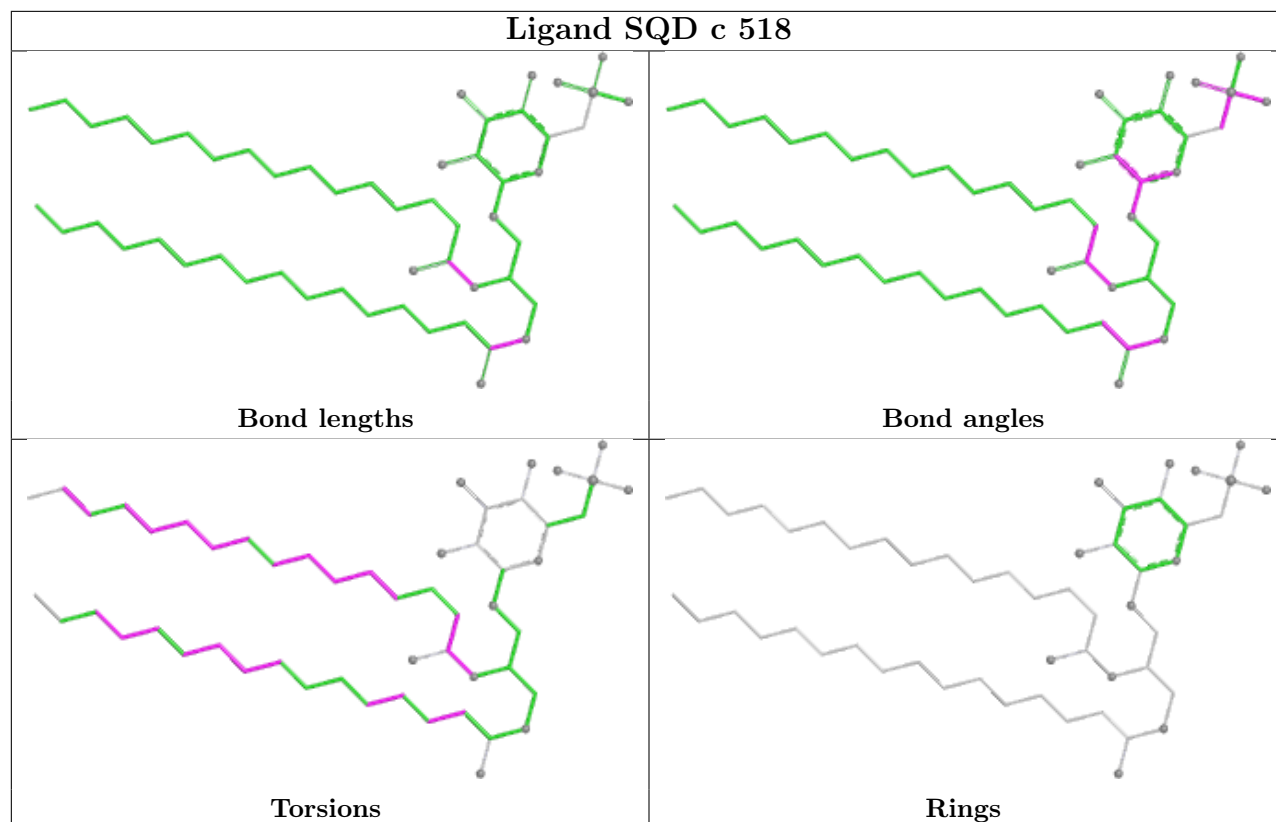


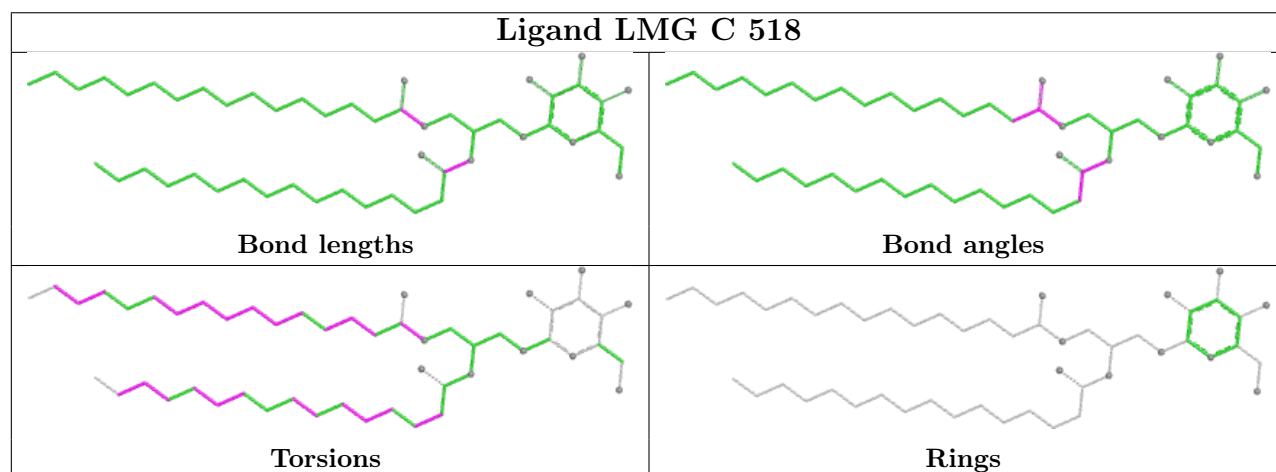
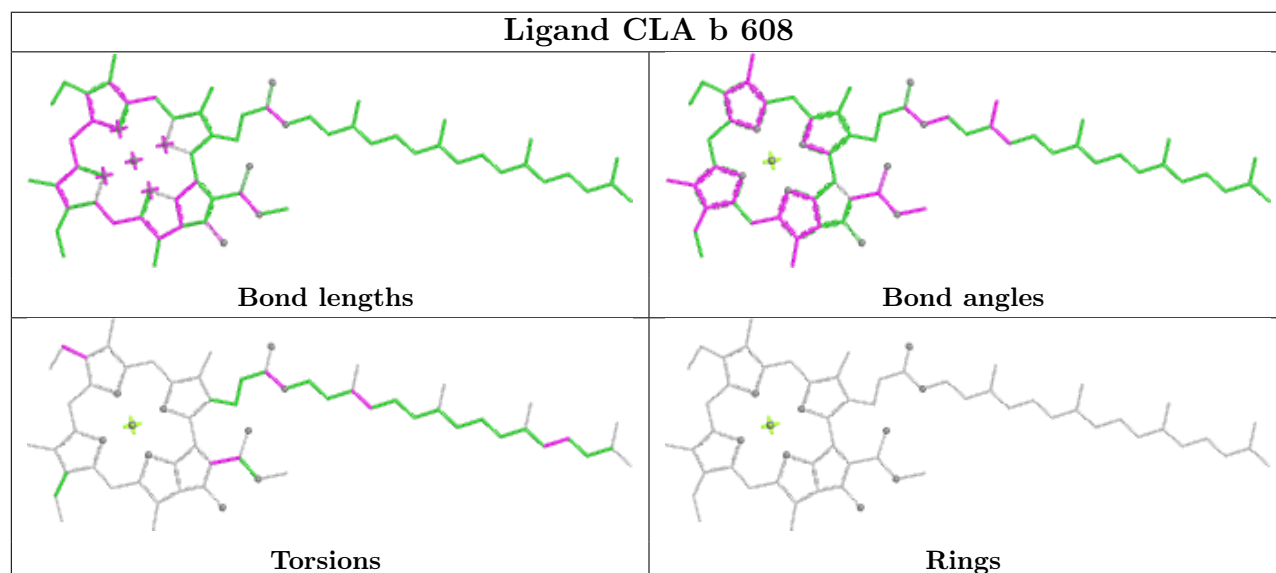
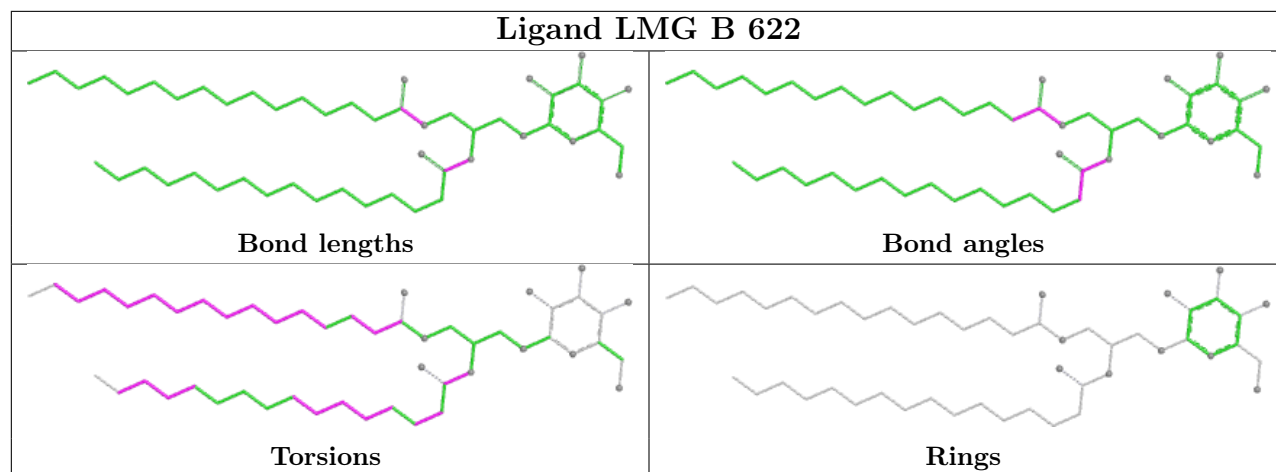
Ligand CLA c 513

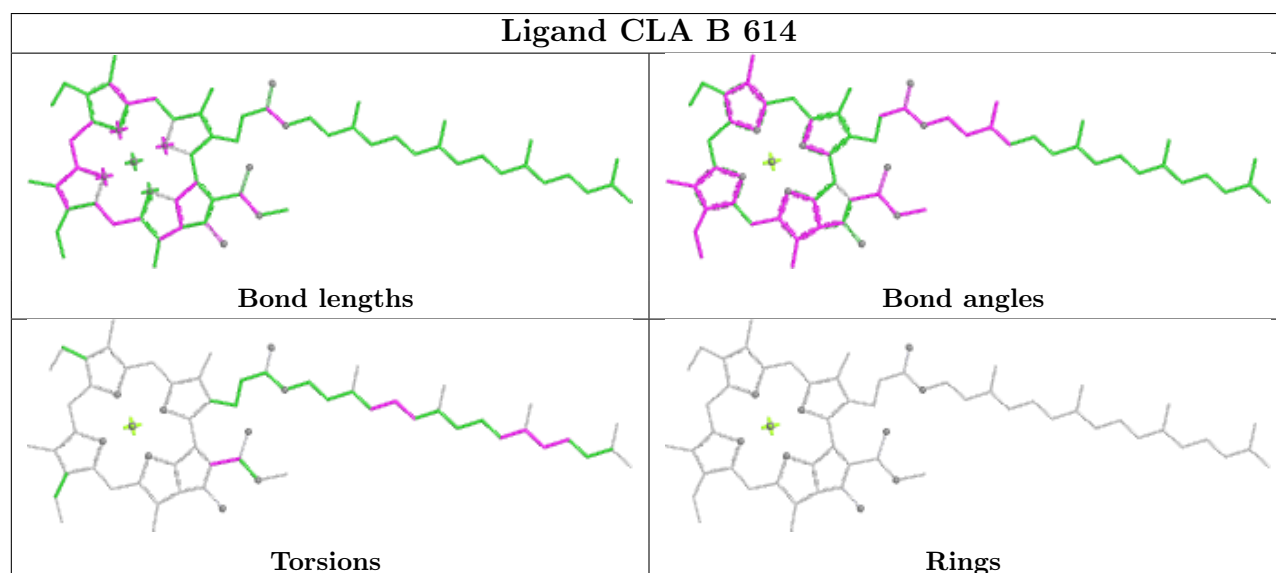
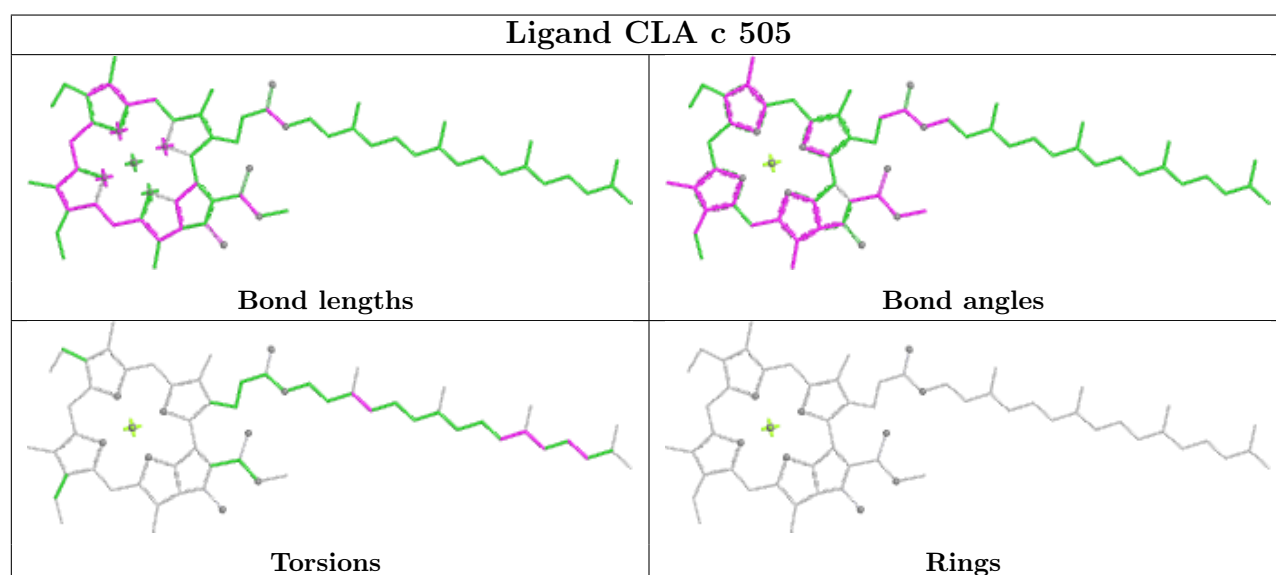
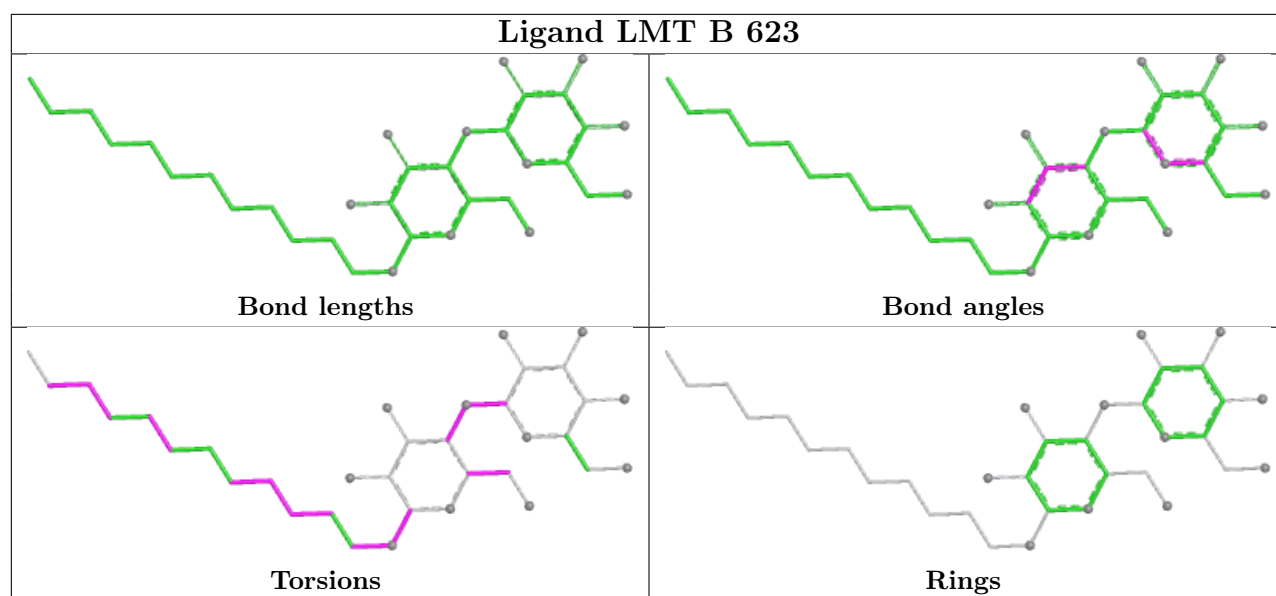


Ligand DGD c 515

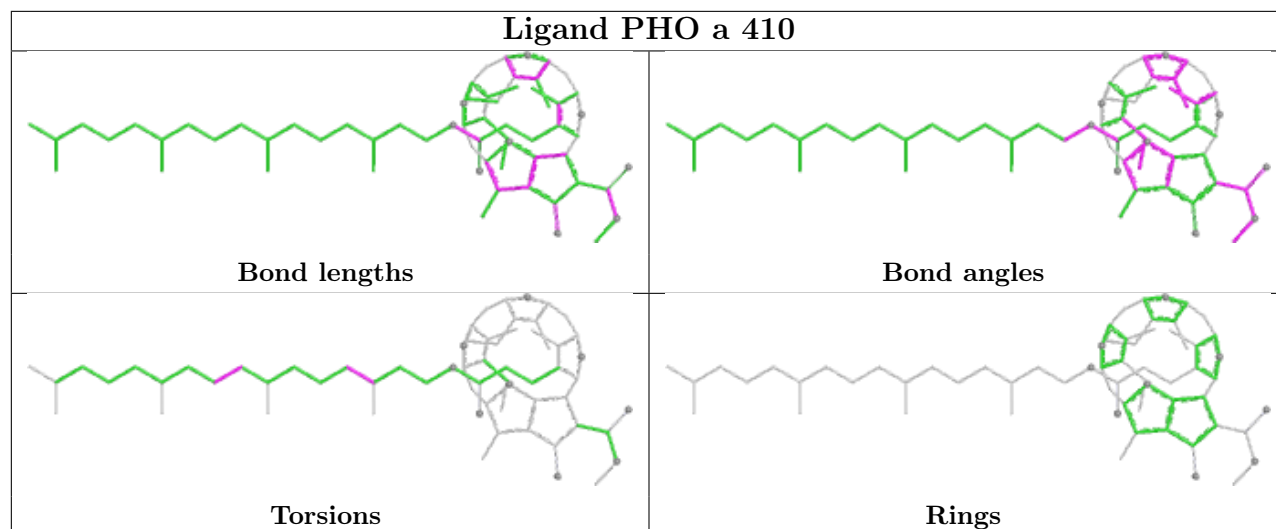




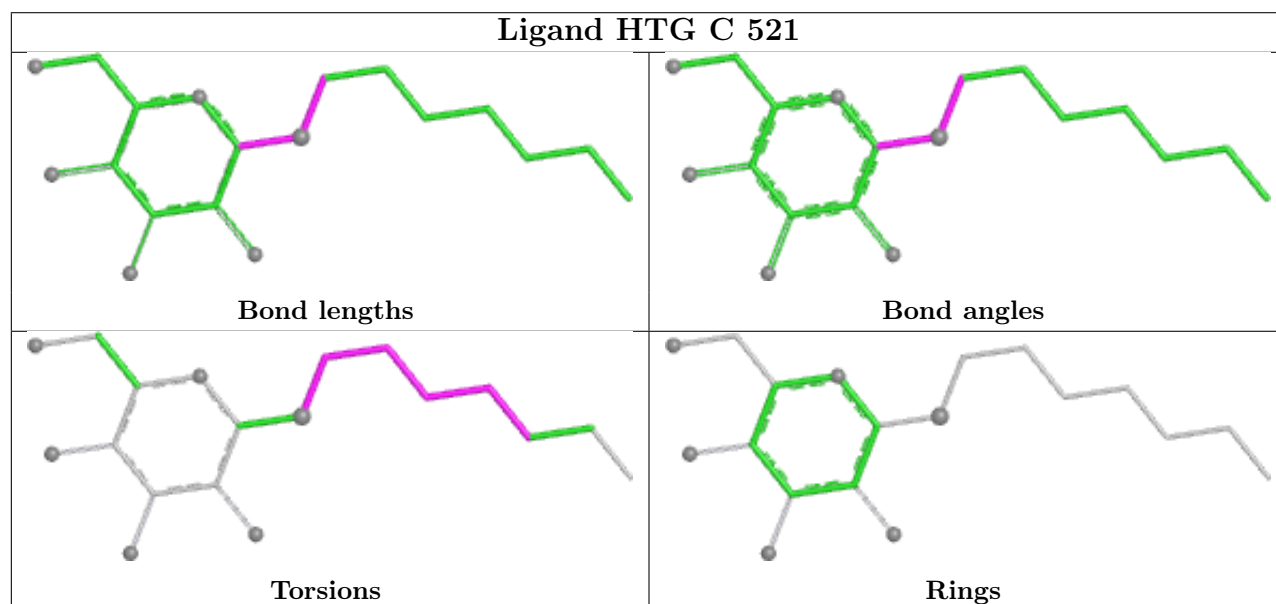




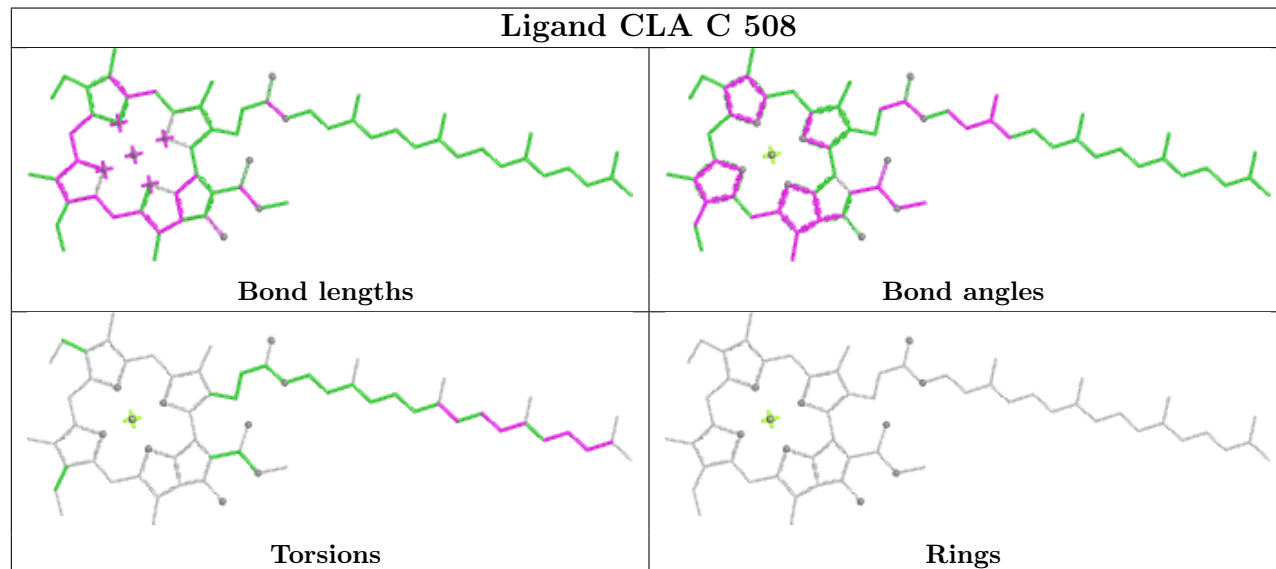
Ligand PHO a 410

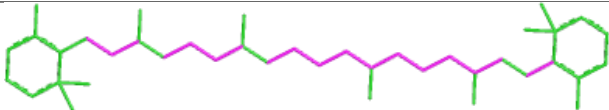
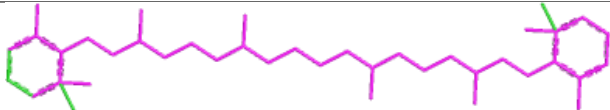
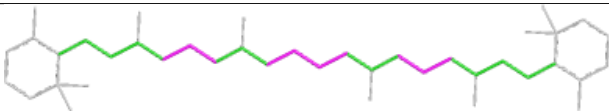
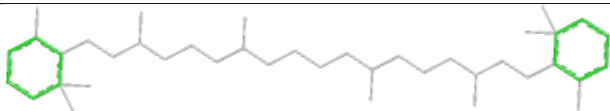


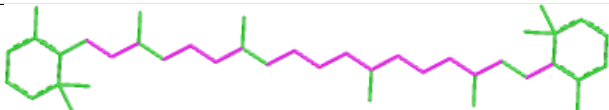
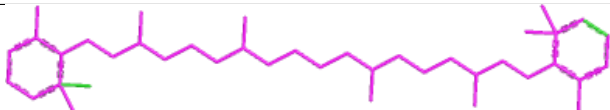
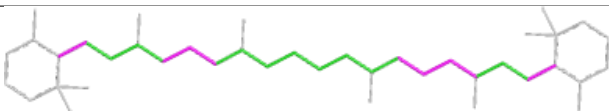
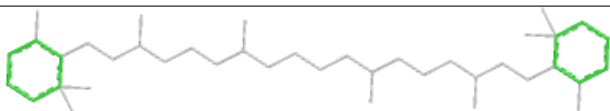
Ligand HTG C 521

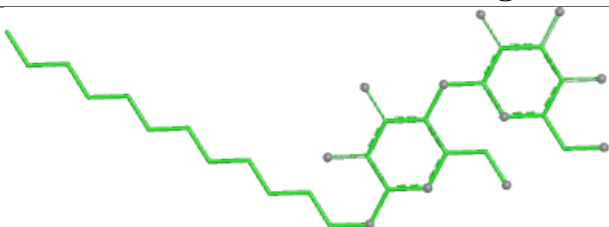
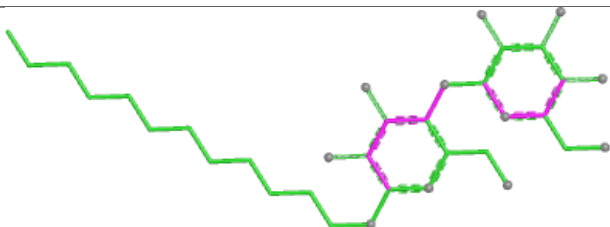
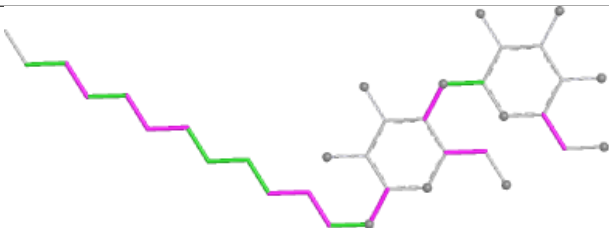
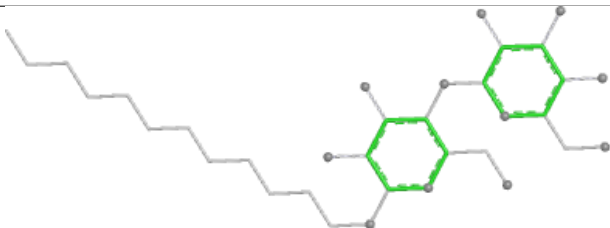


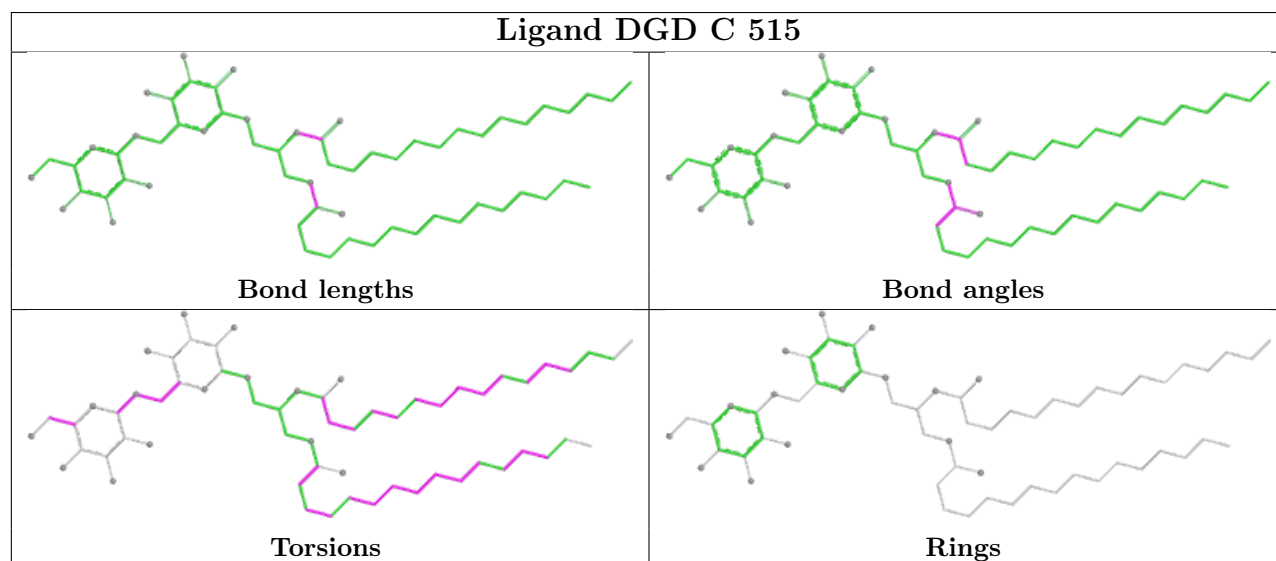
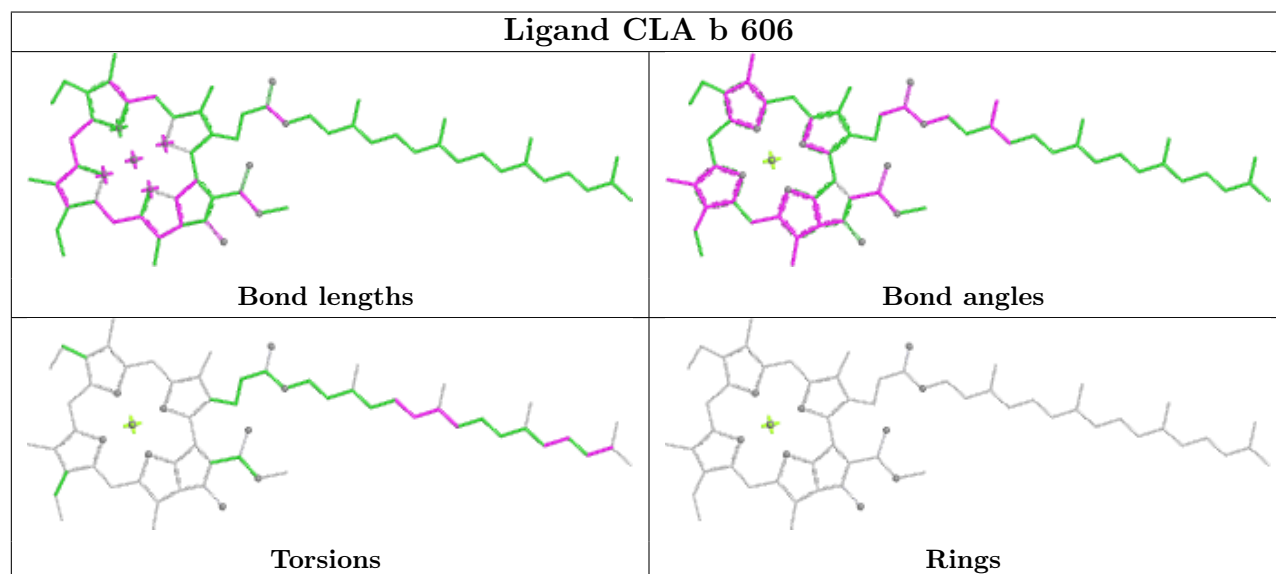
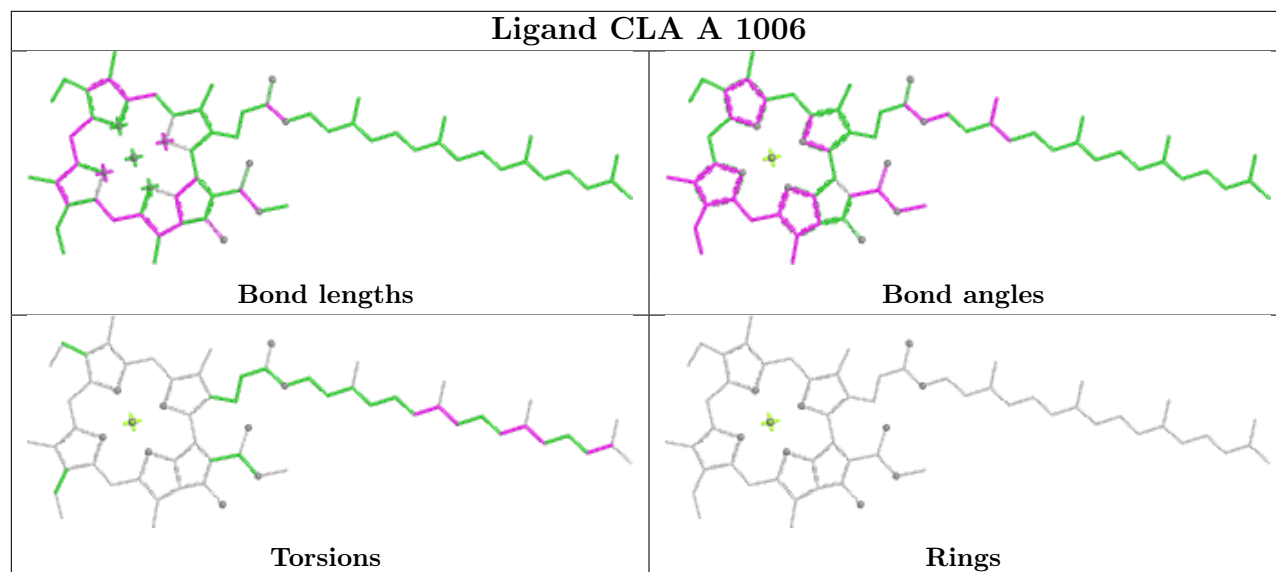
Ligand CLA C 508



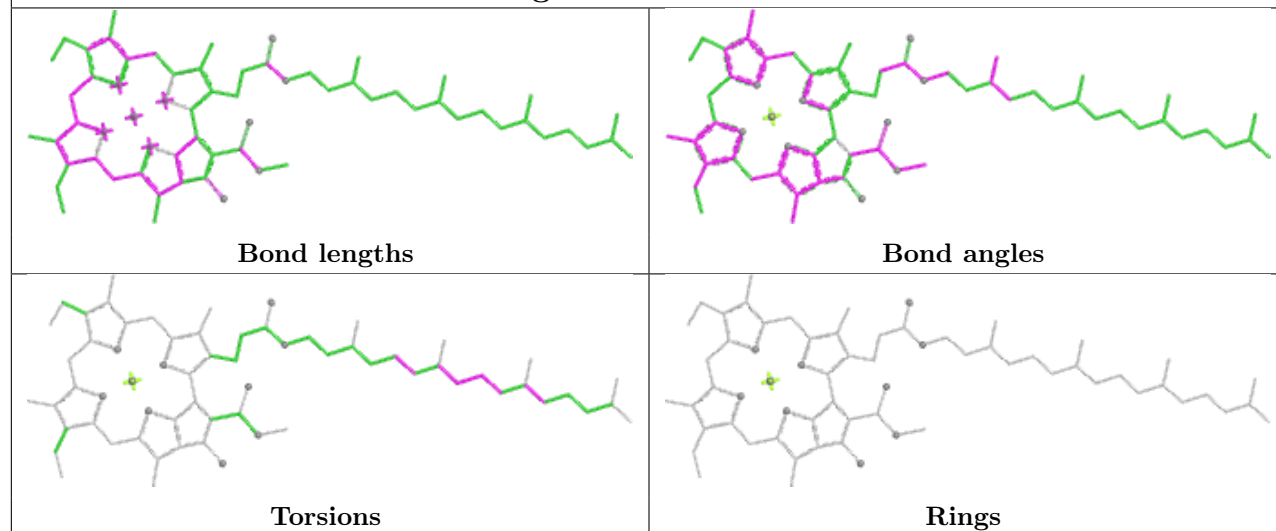
Ligand BCR H 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR K 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

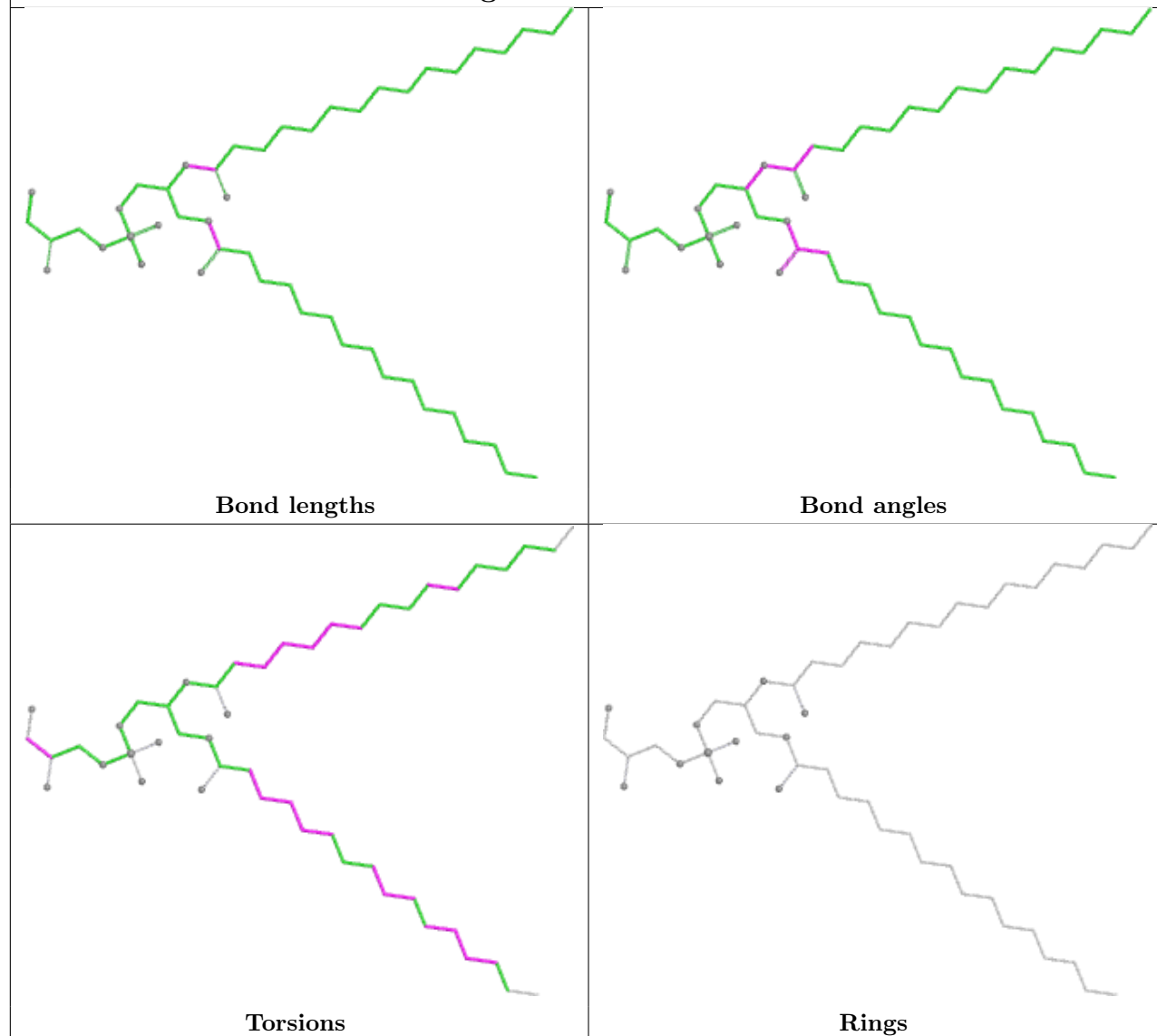
Ligand LMT A 1018	
	
Bond lengths	Bond angles
	
Torsions	Rings



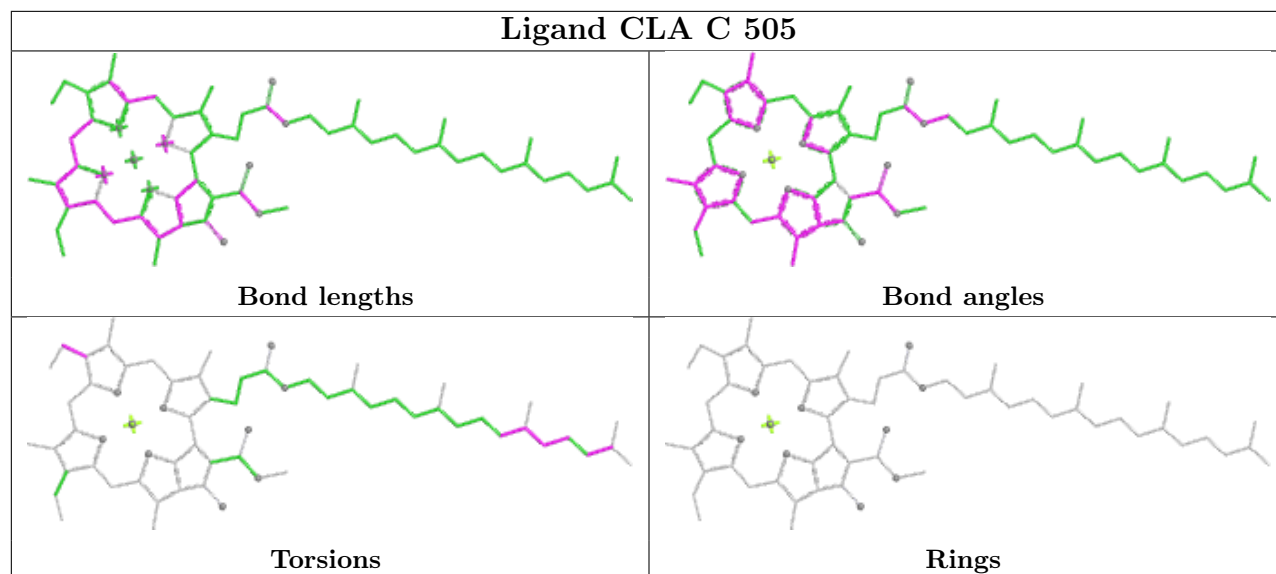
Ligand CLA B 615



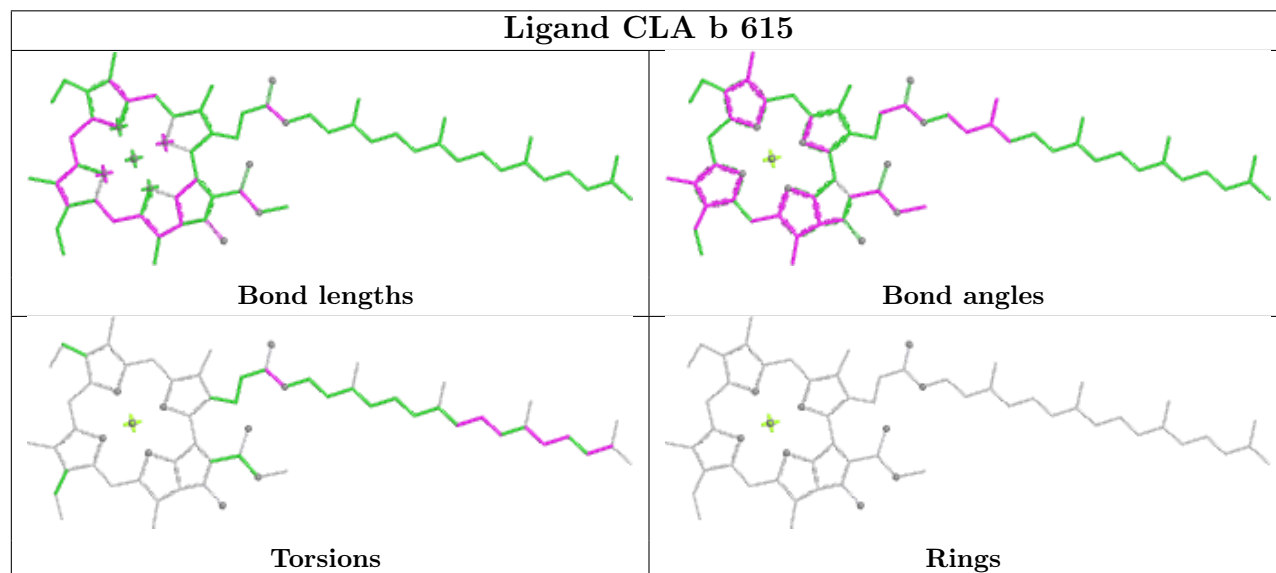
Ligand LHG D 409



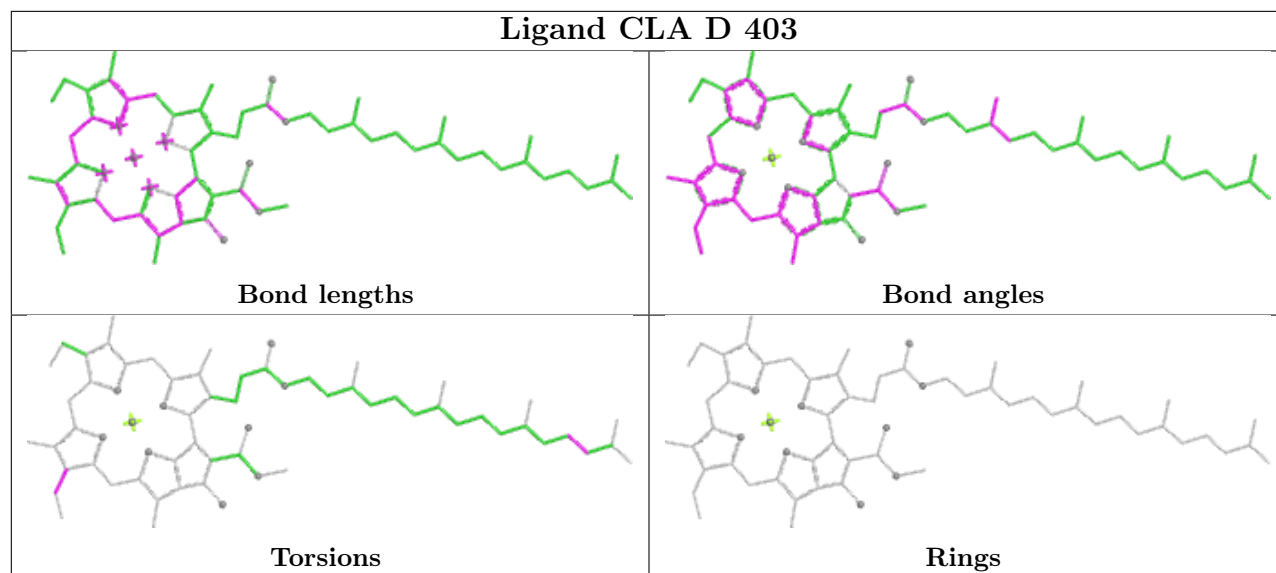
Ligand CLA C 505

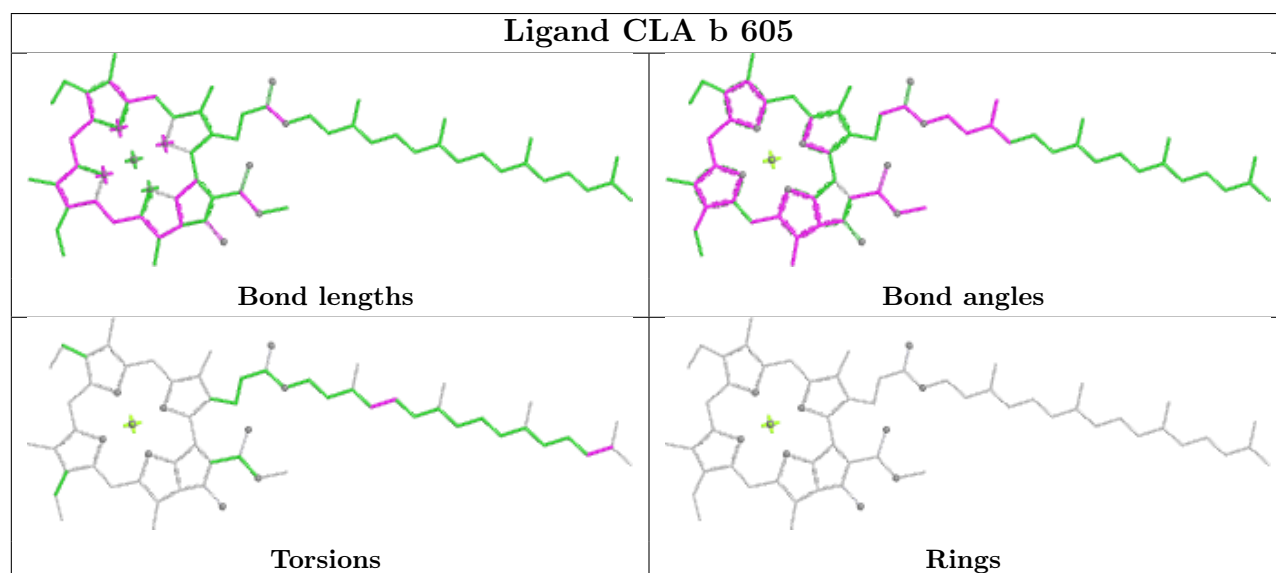
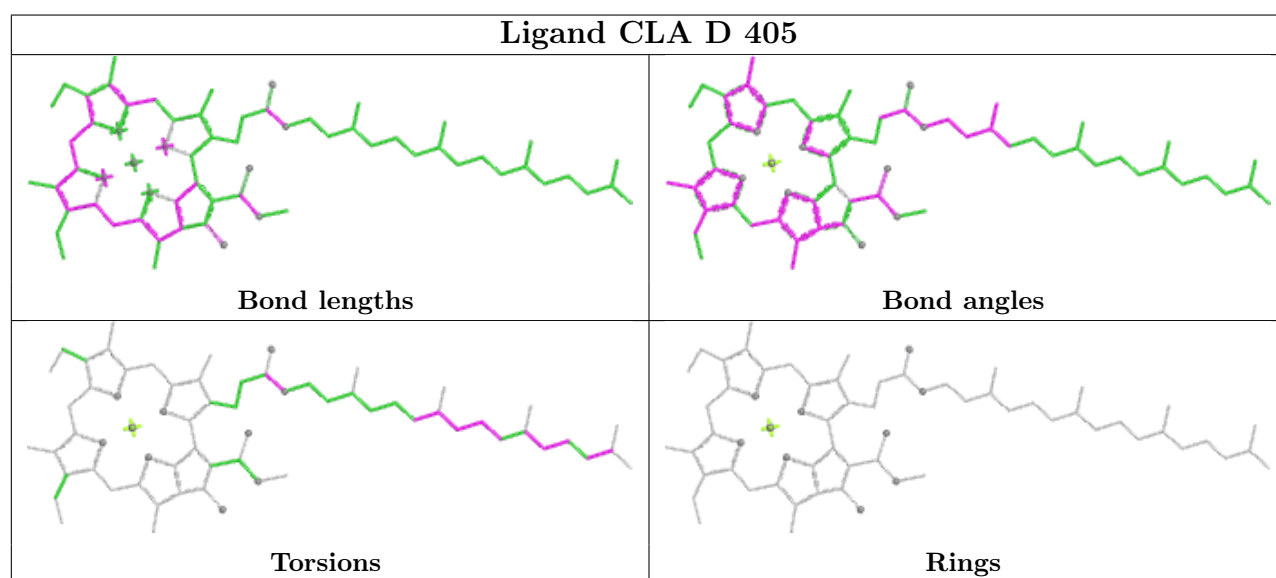
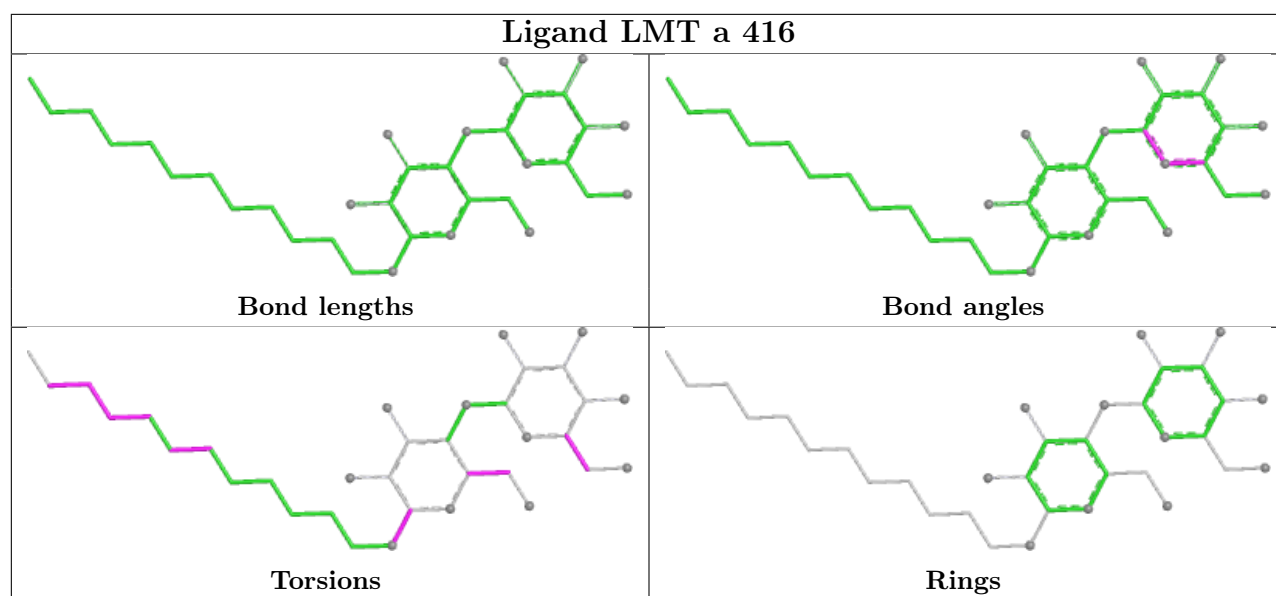


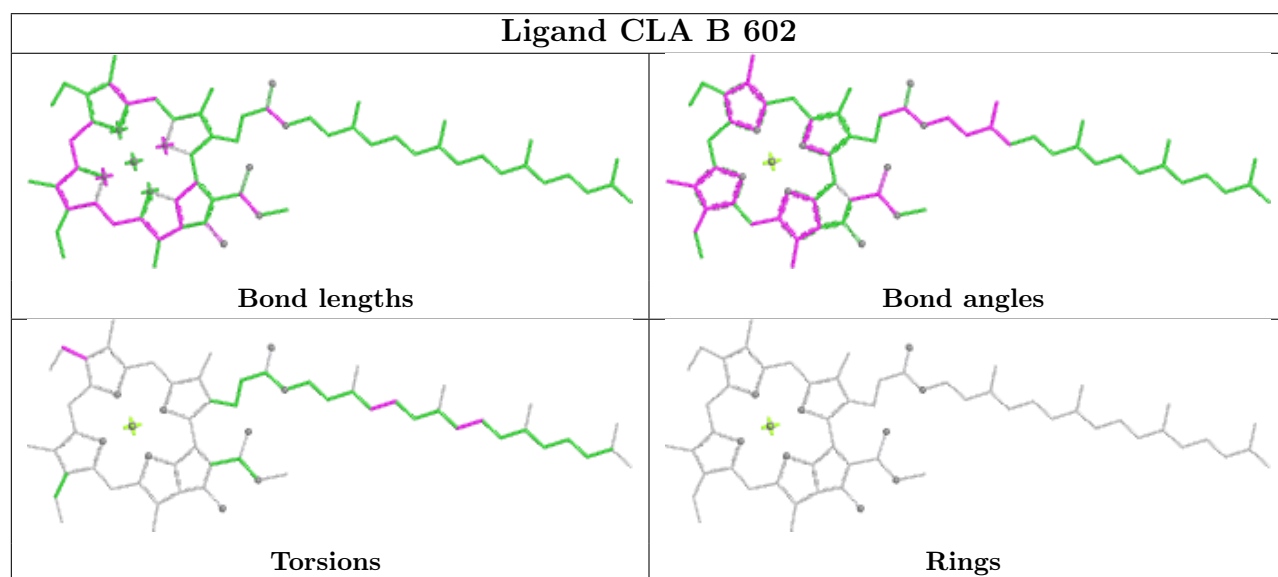
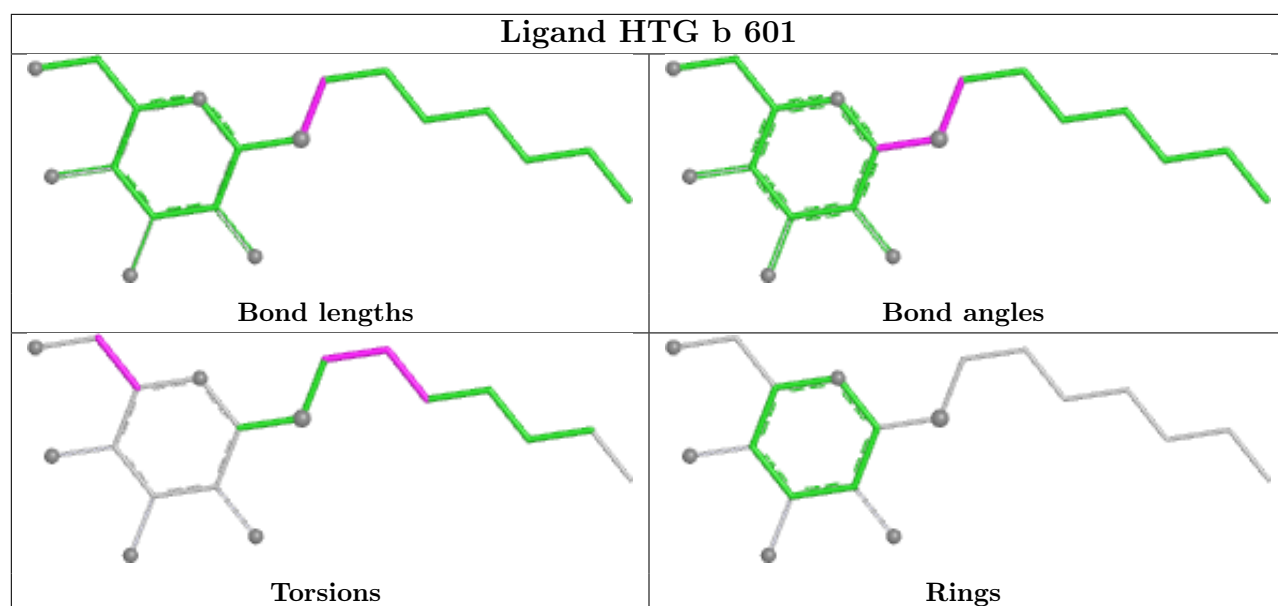
Ligand CLA b 615

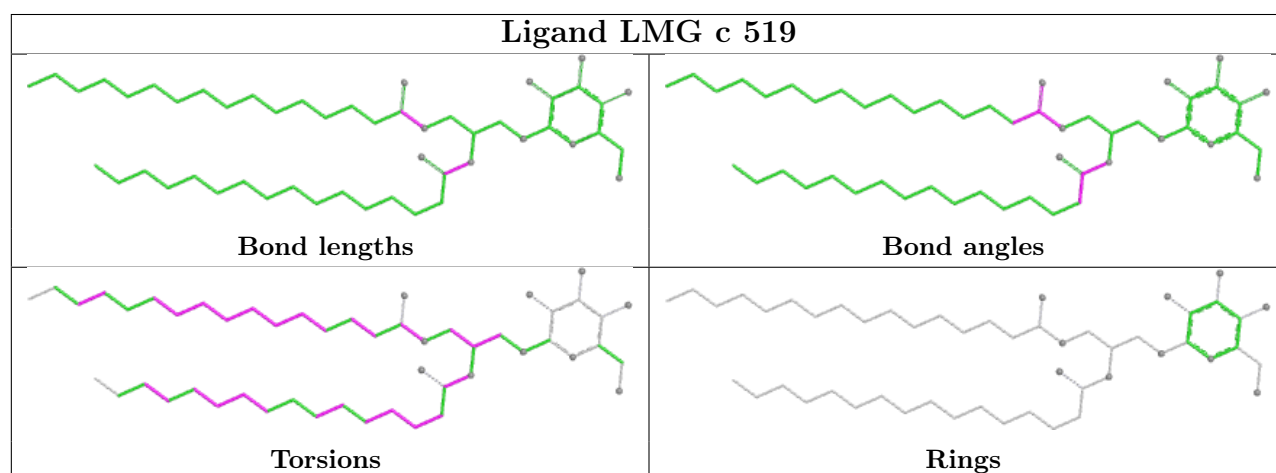
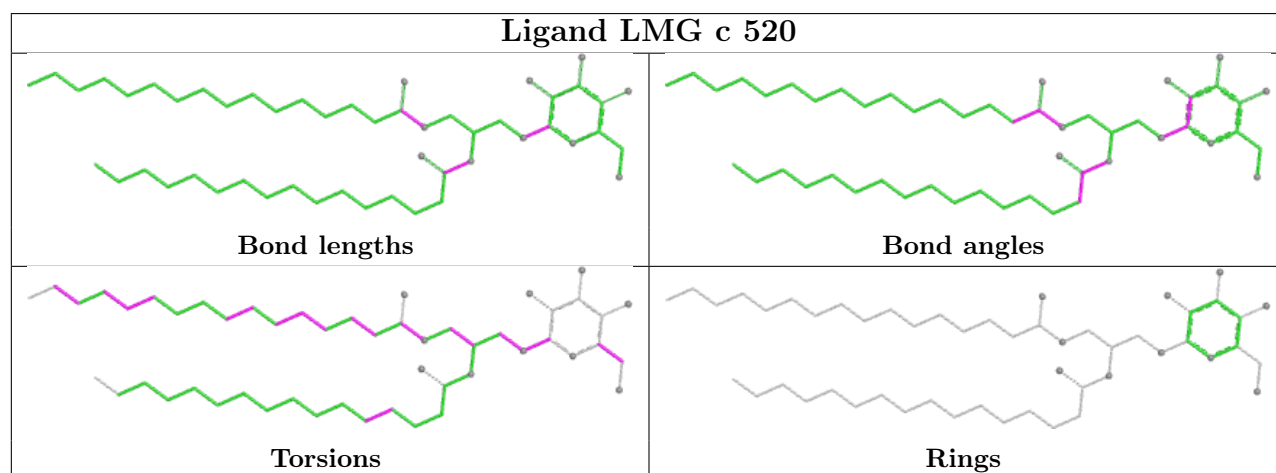
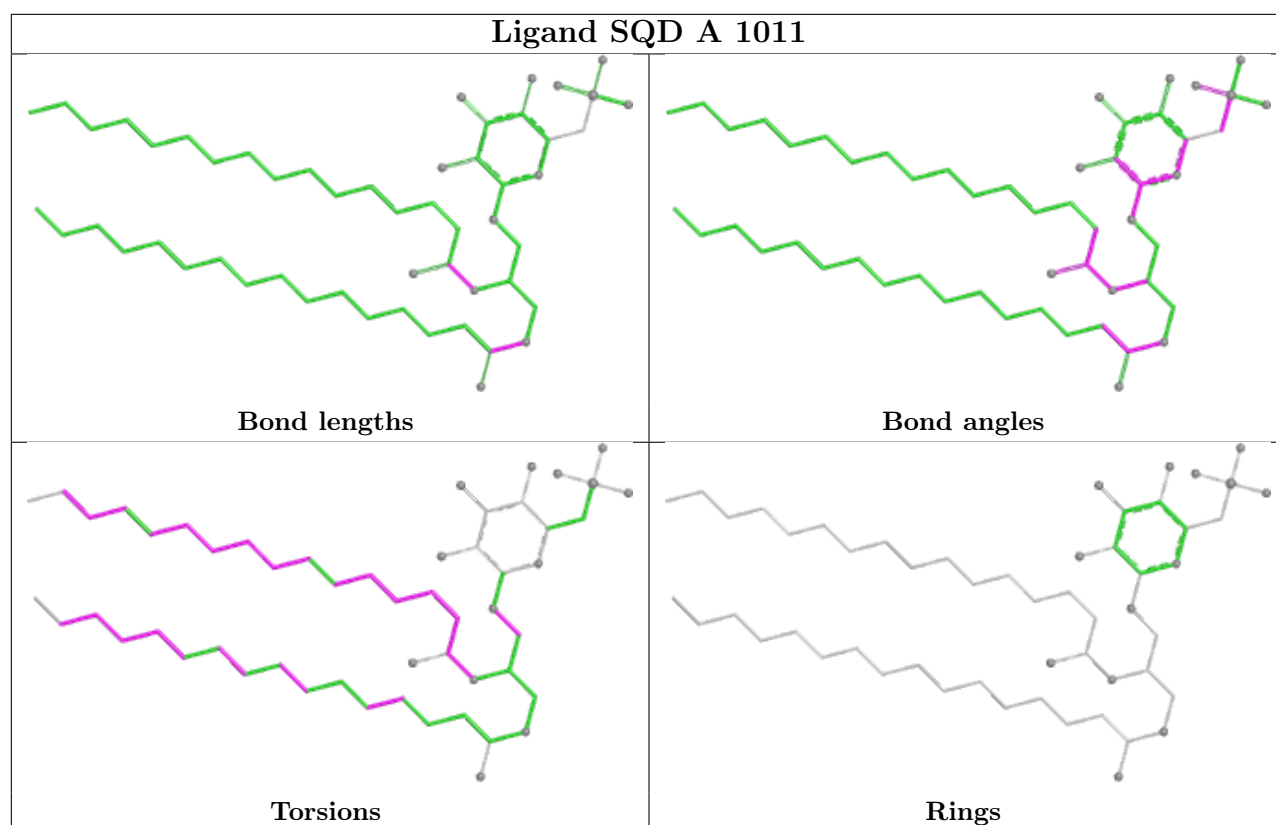


Ligand CLA D 403









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	334/334 (100%)	-0.56	1 (0%) 90 91	16, 25, 41, 64	5 (1%)
1	a	334/334 (100%)	-0.40	2 (0%) 85 87	17, 27, 51, 72	4 (1%)
2	B	505/505 (100%)	-0.41	7 (1%) 73 75	17, 29, 49, 69	10 (1%)
2	b	505/505 (100%)	-0.25	16 (3%) 50 53	17, 31, 59, 88	9 (1%)
3	C	451/451 (100%)	-0.36	4 (0%) 81 83	15, 33, 47, 72	3 (0%)
3	c	450/451 (99%)	-0.11	1 (0%) 91 92	18, 37, 51, 68	2 (0%)
4	D	342/342 (100%)	-0.58	1 (0%) 90 91	18, 26, 39, 88	0
4	d	342/342 (100%)	-0.47	1 (0%) 90 91	21, 29, 46, 80	0
5	E	80/80 (100%)	0.37	6 (7%) 20 21	21, 43, 65, 74	2 (2%)
5	e	78/80 (97%)	0.51	2 (2%) 57 60	35, 47, 68, 75	0
6	F	34/34 (100%)	-0.08	0 100 100	29, 34, 55, 67	0
6	f	32/34 (94%)	0.14	2 (6%) 26 27	33, 40, 69, 78	0
7	H	63/63 (100%)	-0.07	1 (1%) 70 73	21, 36, 45, 54	1 (1%)
7	h	63/63 (100%)	0.12	1 (1%) 70 73	30, 39, 49, 56	0
8	I	35/36 (97%)	0.09	1 (2%) 53 56	32, 37, 71, 87	0
8	i	35/36 (97%)	0.15	2 (5%) 29 31	32, 37, 71, 92	0
9	J	37/37 (100%)	0.16	3 (8%) 18 19	28, 37, 84, 92	0
9	j	37/37 (100%)	0.32	3 (8%) 18 19	33, 44, 68, 75	0
10	K	37/37 (100%)	-0.19	0 100 100	33, 38, 50, 52	0
10	k	37/37 (100%)	0.24	0 100 100	38, 44, 61, 71	0
11	L	37/37 (100%)	-0.43	1 (2%) 56 59	21, 24, 57, 73	0
11	l	37/37 (100%)	-0.43	1 (2%) 56 59	22, 25, 63, 88	0
12	M	33/34 (97%)	-0.40	1 (3%) 52 55	16, 27, 51, 76	1 (3%)
12	m	33/34 (97%)	-0.36	0 100 100	16, 29, 52, 65	1 (3%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/244 (100%)	0.10	9 (3%) 45 47	20, 37, 68, 88	2 (0%)
13	o	243/244 (99%)	0.02	6 (2%) 58 61	24, 38, 68, 78	1 (0%)
14	T	30/31 (96%)	-0.42	1 (3%) 49 51	22, 27, 56, 84	0
14	t	29/31 (93%)	-0.39	1 (3%) 48 50	23, 27, 53, 66	0
15	U	97/97 (100%)	-0.28	0 100 100	24, 31, 48, 66	1 (1%)
15	u	97/97 (100%)	-0.33	0 100 100	24, 32, 42, 71	1 (1%)
16	V	137/137 (100%)	-0.45	0 100 100	21, 30, 43, 62	3 (2%)
16	v	137/137 (100%)	0.02	0 100 100	22, 40, 57, 66	2 (1%)
17	Y	30/30 (100%)	0.29	1 (3%) 49 51	40, 47, 58, 63	0
17	y	30/30 (100%)	0.56	0 100 100	45, 56, 69, 75	0
18	X	40/40 (100%)	0.39	2 (5%) 34 36	33, 40, 65, 80	0
18	x	39/40 (97%)	0.53	3 (7%) 19 21	38, 47, 76, 83	0
19	Z	61/62 (98%)	0.63	6 (9%) 13 13	37, 45, 77, 86	0
19	z	61/62 (98%)	1.15	7 (11%) 9 10	49, 59, 90, 96	0
20	R	34/34 (100%)	2.48	27 (79%) 0 0	71, 86, 100, 101	0
All	All	5280/5296 (99%)	-0.20	120 (2%) 61 64	15, 32, 60, 101	48 (0%)

The worst 5 of 120 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
19	z	62	VAL	5.7
7	h	64	ALA	5.2
2	b	486	LEU	4.3
2	b	85	GLY	4.3
20	R	20	VAL	4.2

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
19	FME	Z	1	10/11	0.81	0.16	69,71,74,78	0
19	FME	z	1	10/11	0.81	0.14	87,91,94,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
14	FME	t	1	10/11	0.93	0.09	28,30,46,49	0
12	FME	M	1	10/11	0.94	0.08	33,36,43,49	0
14	FME	T	1	10/11	0.95	0.08	27,29,44,46	0
12	FME	m	1	10/11	0.95	0.09	35,38,49,54	0
8	FME	i	1	10/11	0.96	0.07	36,38,40,40	0
8	FME	I	1	10/11	0.97	0.07	34,39,40,40	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
30	DMS	b	635	4/4	0.59	0.21	66,70,72,74	0
35	HTG	d	416	19/19	0.60	0.17	70,92,94,96	0
32	LMT	a	402	35/35	0.62	0.18	52,65,69,70	0
31	UNL	A	1015	28/-	0.64	0.18	62,73,78,78	0
31	UNL	a	419	30/-	0.64	0.19	62,74,87,89	0
28	SQD	B	620[B]	54/54	0.64	0.18	40,54,66,66	54
28	SQD	B	620[A]	54/54	0.64	0.18	42,56,75,76	54
32	LMT	A	1017	35/35	0.66	0.18	54,72,75,80	0
31	UNL	t	102	16/-	0.66	0.15	68,72,74,74	0
32	LMT	f	103	35/35	0.66	0.17	71,92,104,104	0
31	UNL	y	102	16/-	0.66	0.19	63,65,67,67	0
35	HTG	D	419	19/19	0.67	0.16	59,79,83,84	0
35	HTG	b	630	19/19	0.67	0.20	66,83,88,90	0
34	LHG	e	101	49/49	0.67	0.16	66,97,101,102	0
32	LMT	m	103	35/35	0.68	0.17	55,90,100,101	0
35	HTG	b	602	19/19	0.69	0.16	60,89,94,94	0
33	GOL	d	417	6/6	0.70	0.16	58,61,62,62	0
35	HTG	B	624	19/19	0.70	0.16	58,86,92,92	0
33	GOL	v	204	6/6	0.70	0.15	74,75,76,76	0
32	LMT	A	1018	35/35	0.71	0.16	51,93,113,116	0
32	LMT	C	520	35/35	0.71	0.15	68,75,79,79	0
35	HTG	d	410	19/19	0.71	0.16	74,84,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	LMT	i	102	35/35	0.71	0.16	52,88,111,111	0
31	UNL	K	103	34/-	0.72	0.16	57,76,82,83	0
31	UNL	b	603	16/-	0.72	0.18	64,67,71,71	0
31	UNL	Y	101	16/-	0.72	0.18	66,68,70,70	0
35	HTG	B	629	19/19	0.72	0.14	52,86,90,90	0
35	HTG	D	413	19/19	0.72	0.16	69,80,85,86	0
30	DMS	O	301	4/4	0.73	0.23	72,73,75,76	0
28	SQD	b	623[A]	54/54	0.73	0.17	41,53,70,71	54
33	GOL	b	632	6/6	0.73	0.14	51,56,61,63	0
28	SQD	b	623[B]	54/54	0.73	0.17	49,57,77,80	54
31	UNL	D	414	40/-	0.73	0.16	48,58,72,73	0
35	HTG	c	522	19/19	0.73	0.16	82,85,89,90	0
31	UNL	j	101	16/-	0.73	0.17	58,60,62,63	0
31	UNL	J	102	16/-	0.73	0.16	50,52,58,59	0
31	UNL	d	411	36/-	0.74	0.15	46,56,78,79	0
34	LHG	E	101	49/49	0.74	0.15	51,77,83,85	0
32	LMT	M	101	35/35	0.74	0.14	52,85,95,97	0
33	GOL	V	207	6/6	0.74	0.14	60,63,64,64	0
29	LMG	c	521	51/55	0.74	0.17	53,81,93,97	0
31	UNL	b	627	16/-	0.74	0.15	47,48,50,50	0
35	HTG	c	525	19/19	0.75	0.14	76,90,95,96	0
35	HTG	C	522	19/19	0.75	0.16	65,75,80,80	0
29	LMG	Z	101	51/55	0.75	0.17	47,77,104,110	0
33	GOL	D	418	6/6	0.76	0.12	70,72,73,74	0
32	LMT	a	416	35/35	0.76	0.13	73,75,79,79	0
28	SQD	f	102	43/54	0.76	0.17	61,80,89,91	0
32	LMT	b	625	35/35	0.77	0.14	52,82,103,104	0
31	UNL	c	523	32/-	0.77	0.14	63,75,84,87	0
35	HTG	V	202	19/19	0.77	0.16	56,63,77,77	0
29	LMG	c	520	51/55	0.78	0.14	42,74,84,89	0
30	DMS	b	634	4/4	0.78	0.21	61,63,65,68	0
31	UNL	l	101	16/-	0.78	0.16	49,58,68,69	0
32	LMT	t	103	35/35	0.78	0.15	46,75,96,99	0
27	PL9	a	414	55/55	0.78	0.16	53,63,77,78	0
33	GOL	V	204	6/6	0.78	0.15	57,58,59,60	0
29	LMG	C	519	51/55	0.79	0.14	38,74,84,85	0
31	UNL	I	101	13/-	0.79	0.14	54,56,56,57	0
27	PL9	A	1010	55/55	0.79	0.14	43,55,72,72	0
32	LMT	b	631	35/35	0.80	0.15	40,74,94,96	0
35	HTG	C	521	19/19	0.80	0.13	69,71,74,75	0
32	LMT	B	623	35/35	0.80	0.13	48,65,71,72	0
31	UNL	i	101	16/-	0.81	0.15	55,57,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	DMS	V	205	4/4	0.81	0.17	61,62,64,65	0
33	GOL	d	415	6/6	0.81	0.10	63,66,66,67	0
31	UNL	B	625	16/-	0.81	0.13	44,46,52,54	0
30	DMS	a	418	4/4	0.81	0.20	62,63,66,69	0
32	LMT	m	101	35/35	0.82	0.12	38,51,56,57	0
30	DMS	C	525	4/4	0.82	0.19	71,73,73,74	0
30	DMS	B	633	4/4	0.82	0.18	67,69,70,75	0
30	DMS	B	634	4/4	0.82	0.20	54,57,59,59	0
30	DMS	c	528	4/4	0.82	0.24	83,85,86,88	0
31	UNL	B	630	16/-	0.83	0.13	53,56,60,60	0
28	SQD	A	1016	54/54	0.83	0.12	46,60,72,73	0
33	GOL	B	631	6/6	0.84	0.13	56,57,60,62	0
30	DMS	d	413	4/4	0.84	0.17	57,62,62,63	0
29	LMG	A	1012	51/55	0.84	0.12	49,56,67,71	0
30	DMS	C	527	4/4	0.84	0.19	75,75,77,80	0
33	GOL	a	420	6/6	0.84	0.12	53,56,57,59	0
31	UNL	X	101	16/-	0.84	0.12	39,43,51,51	0
30	DMS	A	1014	4/4	0.85	0.17	54,54,55,61	0
28	SQD	a	401	54/54	0.85	0.11	42,60,74,76	0
29	LMG	B	622	51/55	0.85	0.11	38,47,58,64	0
32	LMT	M	102	35/35	0.85	0.11	39,58,64,66	0
35	HTG	b	626	19/19	0.85	0.13	43,48,51,51	0
35	HTG	B	628	19/19	0.86	0.13	45,68,72,74	0
31	UNL	L	101	16/-	0.86	0.15	53,56,63,63	0
29	LMG	C	518	51/55	0.86	0.12	36,62,70,70	0
29	LMG	a	415	51/55	0.86	0.10	50,60,70,71	0
31	UNL	d	412	16/-	0.86	0.13	48,53,62,63	0
29	LMG	c	519	51/55	0.86	0.11	45,62,77,80	0
28	SQD	c	518	54/54	0.86	0.13	41,59,74,76	0
35	HTG	o	301	19/19	0.86	0.12	47,49,53,53	0
28	SQD	D	408	43/54	0.87	0.14	41,67,74,76	0
31	UNL	x	101	16/-	0.87	0.11	41,45,59,60	0
30	DMS	b	633	4/4	0.87	0.15	55,55,56,62	0
31	UNL	I	102	13/-	0.87	0.12	55,57,60,60	0
33	GOL	v	203	6/6	0.87	0.11	48,52,53,53	0
30	DMS	O	302	4/4	0.87	0.18	58,59,62,62	0
24	CLA	b	604	65/65	0.87	0.11	40,48,69,70	0
30	DMS	c	527	4/4	0.87	0.15	65,65,66,66	0
33	GOL	A	1019	6/6	0.88	0.14	60,61,62,62	0
26	BCR	d	404	40/40	0.88	0.09	31,36,59,59	0
31	UNL	D	415	16/-	0.88	0.10	39,42,48,49	0
29	LMG	m	102	51/55	0.88	0.10	35,49,57,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
33	GOL	V	206	6/6	0.88	0.10	53,56,57,58	0
35	HTG	b	601	19/19	0.89	0.10	44,60,67,67	0
26	BCR	D	406	40/40	0.89	0.10	28,32,50,51	0
30	DMS	C	526	4/4	0.89	0.18	71,71,72,72	0
30	DMS	d	414	4/4	0.89	0.17	58,59,59,60	0
26	BCR	J	101	40/40	0.89	0.08	35,37,41,41	0
30	DMS	D	416	4/4	0.89	0.16	55,55,56,59	0
26	BCR	K	102	40/40	0.89	0.09	39,49,52,52	0
30	DMS	c	526	4/4	0.89	0.18	73,74,74,75	0
24	CLA	c	513	65/65	0.89	0.11	45,54,69,70	0
24	CLA	C	513	65/65	0.90	0.10	41,48,66,68	0
28	SQD	A	1011	54/54	0.90	0.12	43,57,69,69	0
24	CLA	C	506	65/65	0.90	0.09	36,43,73,76	0
26	BCR	h	101	40/40	0.90	0.09	32,39,47,48	0
30	DMS	D	417	4/4	0.90	0.16	57,58,62,64	0
26	BCR	k	102	40/40	0.90	0.09	48,54,64,66	0
24	CLA	c	506	65/65	0.90	0.10	38,40,78,81	0
30	DMS	U	201	4/4	0.90	0.14	56,56,58,58	0
29	LMG	D	412	51/55	0.91	0.10	27,38,77,78	0
26	BCR	t	101	40/40	0.91	0.07	26,39,46,47	0
26	BCR	y	101	40/40	0.91	0.08	40,44,46,47	0
24	CLA	B	601	65/65	0.91	0.10	34,42,66,69	0
26	BCR	K	101	40/40	0.91	0.08	32,35,37,38	0
26	BCR	B	618	40/40	0.91	0.07	27,32,41,41	0
29	LMG	d	409	51/55	0.91	0.10	33,42,72,76	0
26	BCR	B	619	40/40	0.91	0.08	31,34,42,43	0
24	CLA	c	512	65/65	0.91	0.10	42,46,65,67	0
26	BCR	k	101	40/40	0.91	0.09	36,45,47,48	0
26	BCR	H	101	40/40	0.91	0.08	27,36,42,42	0
26	BCR	c	514	40/40	0.92	0.08	34,41,43,44	0
24	CLA	c	507	65/65	0.92	0.09	33,34,50,51	0
30	DMS	u	201	4/4	0.92	0.12	56,57,57,59	0
30	DMS	v	202	4/4	0.92	0.14	55,56,58,58	0
26	BCR	T	101	40/40	0.92	0.07	27,37,42,43	0
26	BCR	a	413	40/40	0.92	0.07	24,30,34,34	0
26	BCR	b	622	40/40	0.92	0.08	33,36,40,41	0
34	LHG	d	406	49/49	0.92	0.09	38,41,46,46	0
34	LHG	d	408	49/49	0.92	0.11	32,41,72,74	0
36	DGD	c	516	62/66	0.92	0.09	36,42,75,79	0
36	DGD	h	102	62/66	0.92	0.09	32,38,46,48	0
24	CLA	B	606	65/65	0.93	0.08	27,30,51,53	0
24	CLA	C	512	65/65	0.93	0.08	39,42,71,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	DMS	B	632	4/4	0.93	0.15	57,58,60,61	0
24	CLA	c	508	65/65	0.93	0.08	32,35,65,72	0
24	CLA	B	616	65/65	0.93	0.10	27,31,79,80	0
30	DMS	C	524	4/4	0.93	0.18	40,41,41,42	0
24	CLA	C	504	65/65	0.93	0.08	27,30,55,57	0
34	LHG	D	409	49/49	0.93	0.09	35,38,43,45	0
34	LHG	D	411	49/49	0.93	0.10	29,38,73,76	0
26	BCR	A	1009	40/40	0.93	0.07	25,29,32,32	0
26	BCR	B	617	40/40	0.93	0.06	28,30,33,33	0
24	CLA	b	612	65/65	0.93	0.08	30,34,37,38	0
24	CLA	b	619	65/65	0.93	0.09	31,35,80,81	0
26	BCR	C	514	40/40	0.93	0.07	31,38,41,41	0
36	DGD	C	515	62/66	0.93	0.08	27,36,63,64	0
36	DGD	H	102	62/66	0.93	0.08	27,34,38,39	0
36	DGD	c	515	62/66	0.93	0.09	28,38,69,71	0
24	CLA	c	501	65/65	0.93	0.08	35,36,43,44	0
24	CLA	c	504	65/65	0.93	0.07	32,35,57,59	0
39	MG	k	103	1/1	0.93	0.06	45,45,45,45	0
24	CLA	C	507	65/65	0.94	0.08	34,37,51,53	0
24	CLA	b	605	65/65	0.94	0.07	29,32,37,37	0
24	CLA	b	609	65/65	0.94	0.07	29,32,65,68	0
24	CLA	C	508	65/65	0.94	0.07	28,31,65,70	0
24	CLA	d	403	65/65	0.94	0.08	31,34,76,77	0
30	DMS	c	529	4/4	0.94	0.17	51,51,53,54	0
25	PHO	a	411	64/64	0.94	0.07	24,30,35,36	0
26	BCR	b	620	40/40	0.94	0.06	28,34,35,35	0
26	BCR	b	621	40/40	0.94	0.06	28,31,41,42	0
24	CLA	C	511	65/65	0.94	0.07	29,35,40,42	0
36	DGD	C	516	62/66	0.94	0.08	28,36,70,72	0
24	CLA	C	505	65/65	0.94	0.07	32,35,44,48	0
24	CLA	c	503	65/65	0.94	0.07	33,39,42,44	0
24	CLA	B	614	65/65	0.94	0.08	24,27,67,68	0
36	DGD	c	517	62/66	0.94	0.08	29,38,64,73	0
24	CLA	c	505	65/65	0.94	0.07	34,36,48,48	0
37	BCT	D	401	4/4	0.94	0.10	37,38,38,41	0
24	CLA	D	405	65/65	0.94	0.08	28,30,70,71	0
24	CLA	c	509	65/65	0.95	0.08	33,35,50,51	0
24	CLA	c	510	65/65	0.95	0.07	33,35,41,43	0
30	DMS	V	203	4/4	0.95	0.11	50,51,51,52	0
24	CLA	c	511	65/65	0.95	0.07	36,39,43,46	0
24	CLA	B	615	65/65	0.95	0.07	27,28,44,46	0
24	CLA	b	608	65/65	0.95	0.07	24,26,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	CLA	A	1008	65/65	0.95	0.08	25,27,79,81	0
25	PHO	D	404	64/64	0.95	0.06	22,25,29,30	0
24	CLA	C	509	65/65	0.95	0.08	28,31,52,53	0
24	CLA	b	613	65/65	0.95	0.07	28,31,38,40	0
24	CLA	b	614	65/65	0.95	0.07	24,26,40,41	0
27	PL9	D	407	55/55	0.95	0.06	21,25,32,33	0
24	CLA	b	615	65/65	0.95	0.07	25,28,32,35	0
27	PL9	d	405	55/55	0.95	0.06	21,27,32,33	0
24	CLA	b	617	65/65	0.95	0.08	24,28,67,68	0
24	CLA	C	510	65/65	0.95	0.06	27,31,38,39	0
24	CLA	C	501	65/65	0.95	0.06	31,35,41,42	0
24	CLA	c	502	65/65	0.95	0.07	28,31,50,51	0
24	CLA	C	503	65/65	0.95	0.06	28,33,36,38	0
24	CLA	B	609	65/65	0.95	0.06	28,31,33,35	0
36	DGD	C	517	62/66	0.95	0.08	24,33,62,69	0
34	LHG	D	410	49/49	0.95	0.07	26,30,38,41	0
24	CLA	B	610	65/65	0.95	0.07	24,26,34,36	0
24	CLA	a	409	65/65	0.95	0.08	24,26,85,90	0
34	LHG	b	624	49/49	0.95	0.07	27,32,48,53	0
24	CLA	a	412	65/65	0.95	0.10	26,28,90,92	0
34	LHG	d	407	49/49	0.95	0.07	26,31,40,45	0
24	CLA	B	602	65/65	0.95	0.06	25,27,34,35	0
24	CLA	b	610	65/65	0.96	0.06	23,25,34,35	0
24	CLA	b	611	65/65	0.96	0.06	26,28,38,39	0
24	CLA	B	607	65/65	0.96	0.06	20,22,36,37	0
24	CLA	C	502	65/65	0.96	0.06	26,28,42,44	0
24	CLA	B	608	65/65	0.96	0.06	25,27,31,31	0
25	PHO	A	1007	64/64	0.96	0.05	21,24,26,28	0
24	CLA	D	402	65/65	0.96	0.06	17,20,35,37	0
24	CLA	b	616	65/65	0.96	0.06	25,25,50,52	0
24	CLA	D	403	65/65	0.96	0.05	18,20,29,33	0
34	LHG	B	621	49/49	0.96	0.06	26,32,45,49	0
24	CLA	b	618	65/65	0.96	0.06	30,32,44,46	0
24	CLA	A	1005	65/65	0.96	0.06	17,20,29,33	0
24	CLA	a	407	65/65	0.96	0.06	21,23,30,35	0
30	DMS	b	629	4/4	0.96	0.10	48,49,52,53	0
24	CLA	B	603	65/65	0.96	0.06	25,26,32,34	0
24	CLA	B	611	65/65	0.96	0.06	22,24,36,37	0
24	CLA	B	612	65/65	0.96	0.06	24,26,30,31	0
24	CLA	B	604	65/65	0.96	0.07	22,24,53,55	0
24	CLA	b	606	65/65	0.96	0.06	26,29,35,39	0
30	DMS	B	627	4/4	0.96	0.10	41,41,42,44	0

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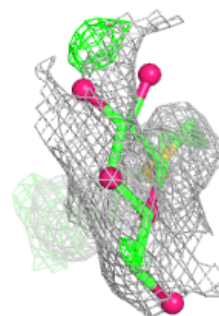
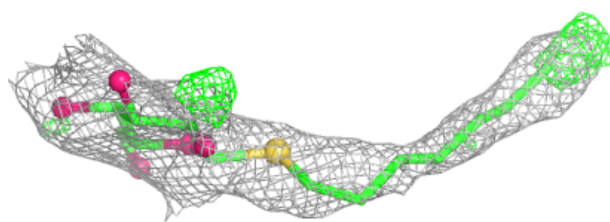
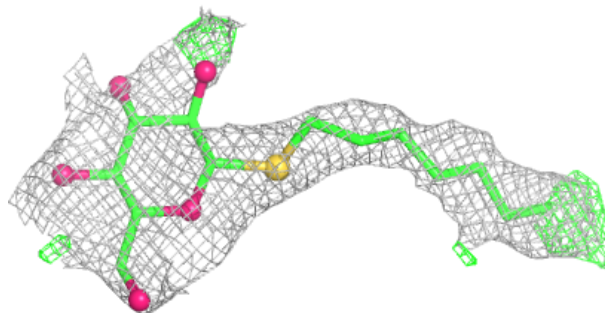
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	CLA	b	607	65/65	0.96	0.07	24,26,50,51	0
24	CLA	B	605	65/65	0.96	0.06	23,26,31,32	0
37	BCT	d	401	4/4	0.96	0.06	40,40,41,42	0
38	HEM	f	101	43/43	0.96	0.09	42,44,57,63	0
24	CLA	A	1006	65/65	0.96	0.06	22,23,66,69	0
24	CLA	d	402	65/65	0.97	0.06	21,23,39,43	0
30	DMS	b	628	4/4	0.97	0.08	30,31,31,32	0
25	PHO	a	410	64/64	0.97	0.05	22,24,29,31	0
24	CLA	a	408	65/65	0.97	0.05	20,23,31,34	0
24	CLA	B	613	65/65	0.97	0.06	23,25,49,53	0
38	HEM	F	101	43/43	0.97	0.08	39,41,44,46	0
30	DMS	B	626	4/4	0.97	0.07	25,26,26,27	0
38	HEM	v	201	43/43	0.97	0.07	31,32,36,37	0
39	MG	K	104	1/1	0.97	0.03	48,48,48,48	0
39	MG	j	102	1/1	0.97	0.09	37,37,37,37	0
30	DMS	c	524	4/4	0.97	0.12	43,43,43,43	0
39	MG	J	103	1/1	0.98	0.03	32,32,32,32	0
38	HEM	V	201	43/43	0.98	0.06	25,26,28,29	0
30	DMS	C	523	4/4	0.98	0.07	36,37,38,38	0
30	DMS	a	417	4/4	0.98	0.07	31,32,33,33	0
21	OER	a	403	10/10	0.99	0.03	27,28,29,31	1
30	DMS	A	1013	4/4	0.99	0.06	29,29,30,31	0
23	CL	a	406	1/1	0.99	0.02	27,27,27,27	0
21	OER	A	1001	10/10	0.99	0.04	24,25,28,28	1
23	CL	a	405	1/1	1.00	0.05	26,26,26,26	0
22	FE2	A	1002	1/1	1.00	0.02	29,29,29,29	0
22	FE2	a	404	1/1	1.00	0.01	29,29,29,29	0
23	CL	A	1003	1/1	1.00	0.05	25,25,25,25	0
23	CL	A	1004	1/1	1.00	0.03	22,22,22,22	0

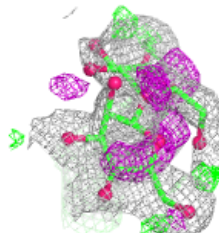
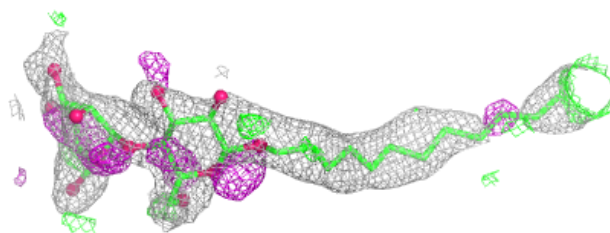
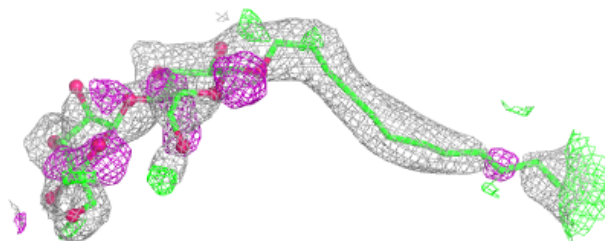
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HTG d 416:

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

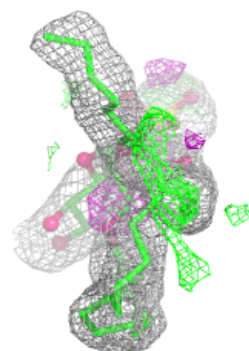
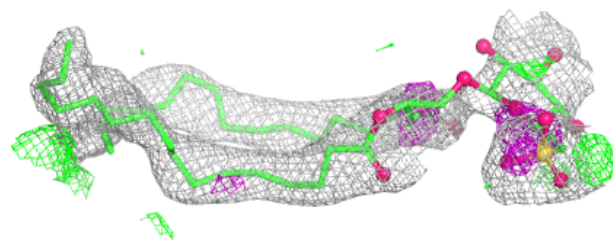
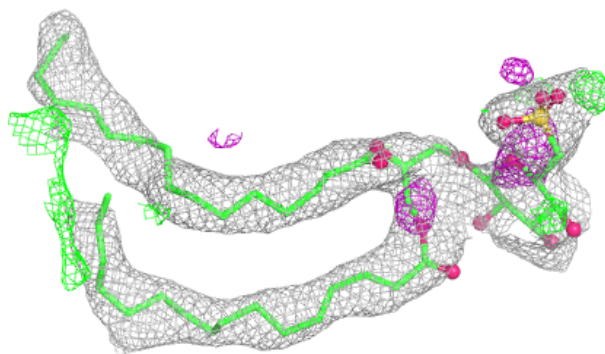
**Electron density around LMT a 402:**

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

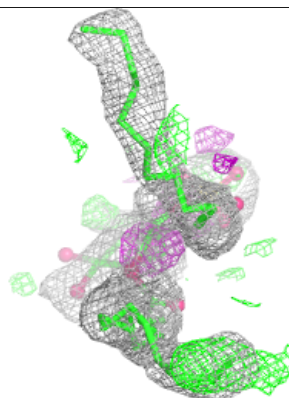
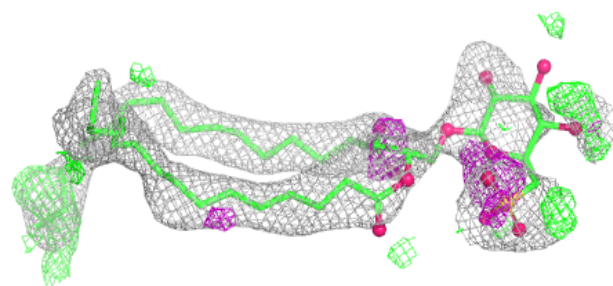
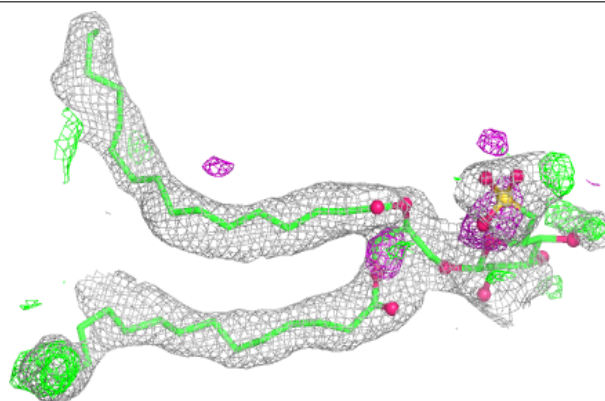


Electron density around SQD B 620 (B):

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

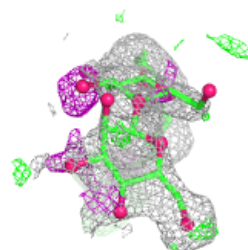
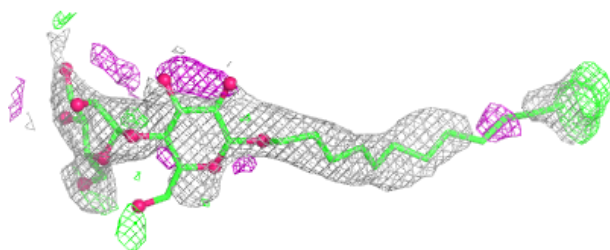
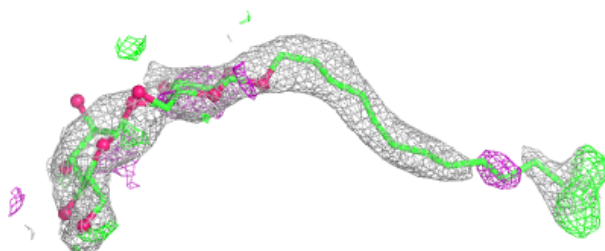
**Electron density around SQD B 620 (A):**

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

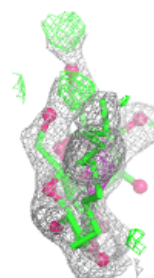
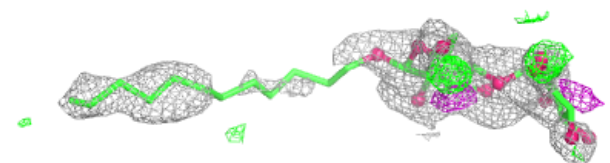
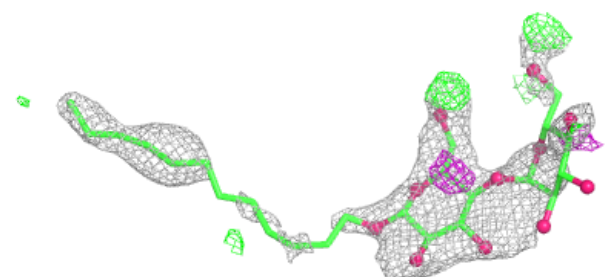


Electron density around LMT A 1017:

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

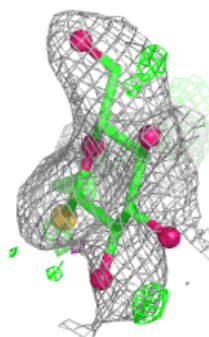
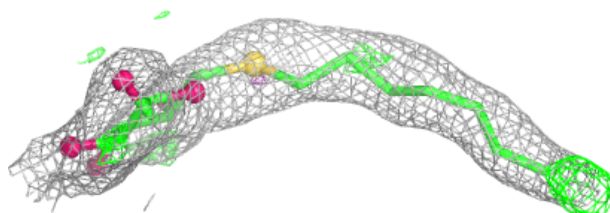
**Electron density around LMT f 103:**

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

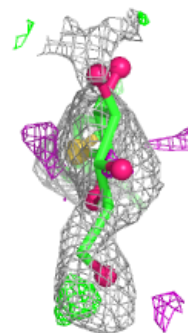
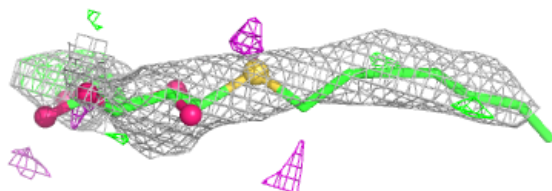
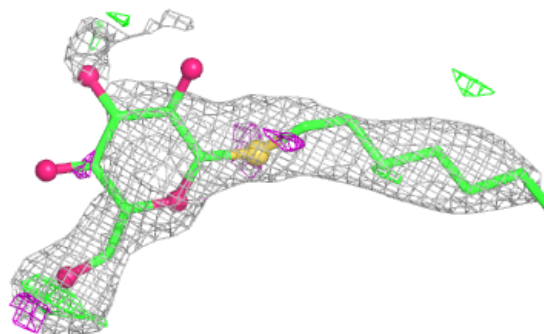


Electron density around HTG D 419:

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

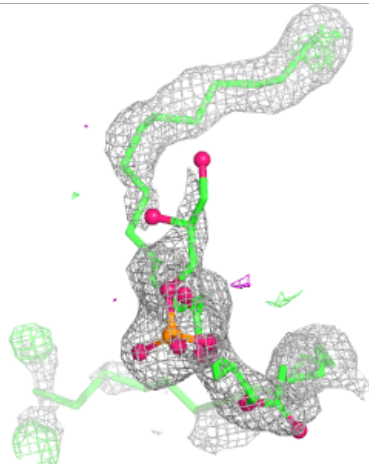
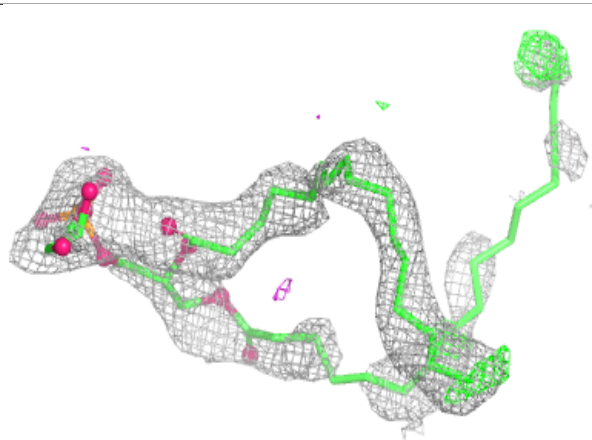
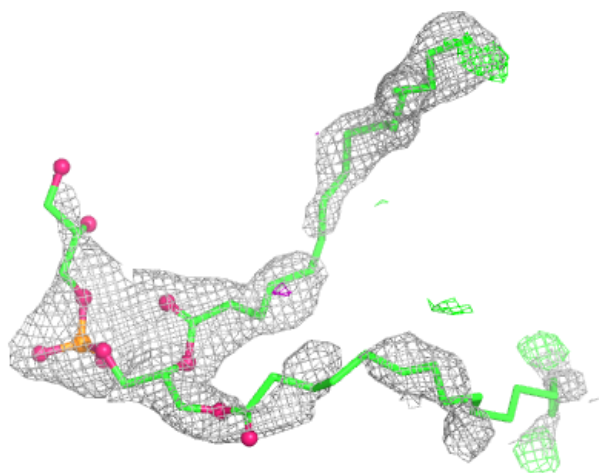
**Electron density around HTG b 630:**

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



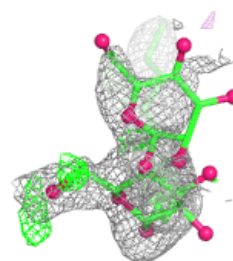
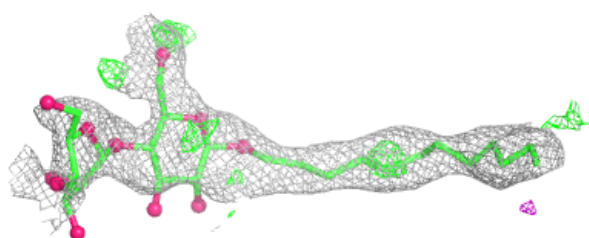
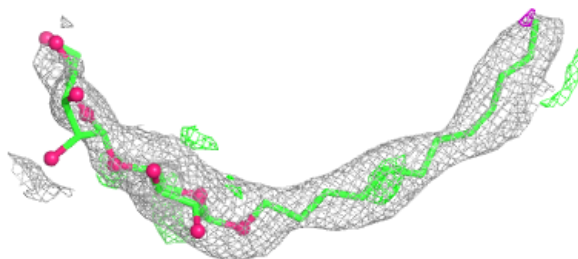
Electron density around LHG e 101:

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

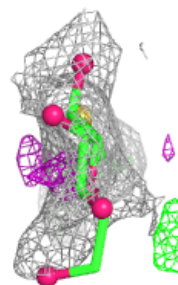
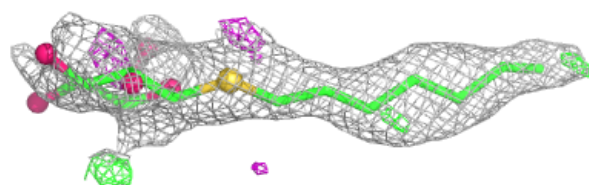
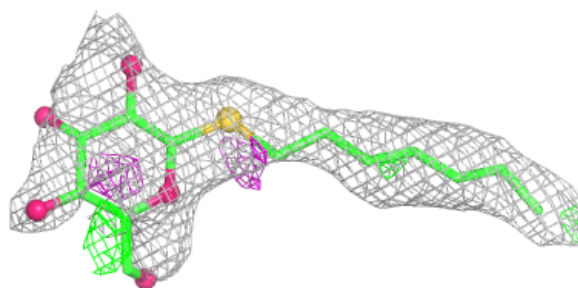


Electron density around LMT m 103:

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

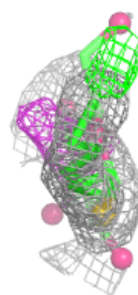
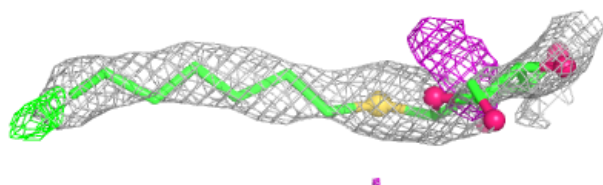
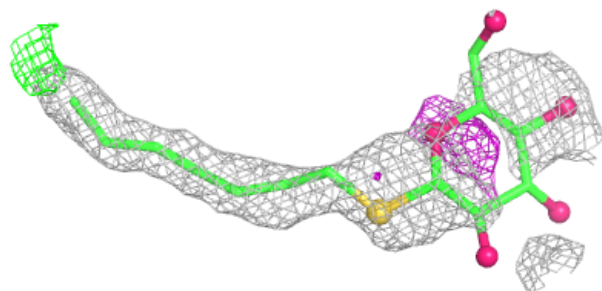
**Electron density around HTG b 602:**

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

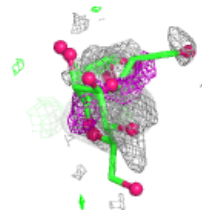
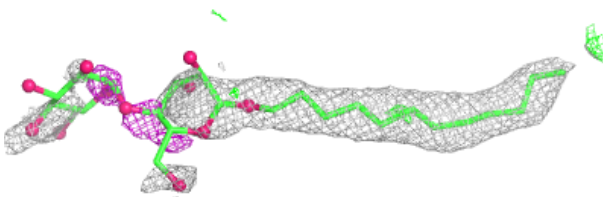
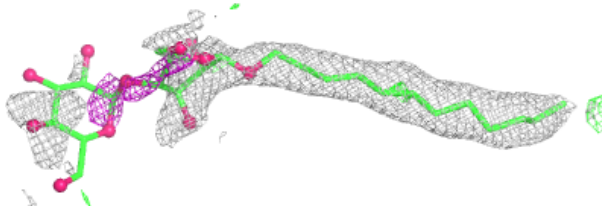


Electron density around HTG B 624:

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

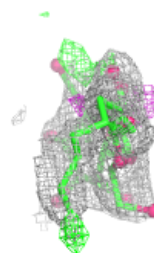
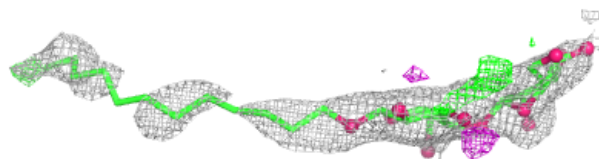
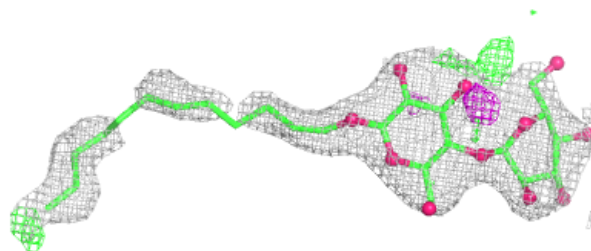
**Electron density around LMT A 1018:**

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

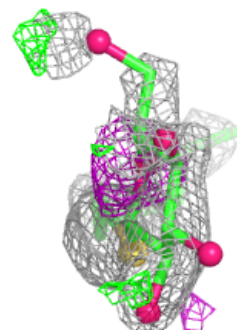
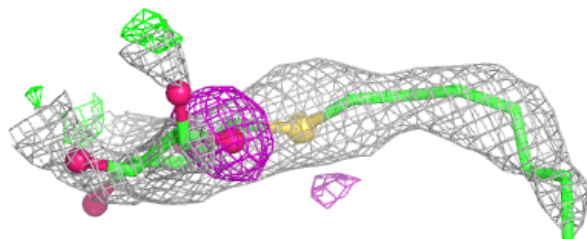
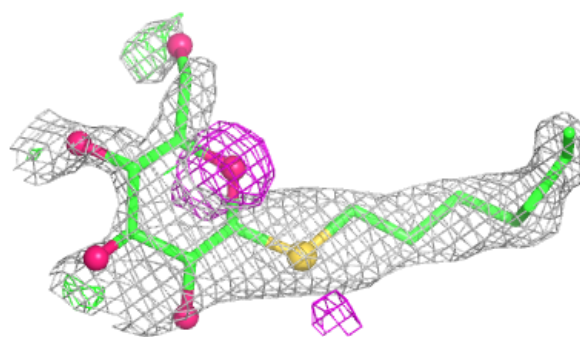


Electron density around LMT C 520:

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

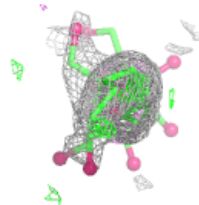
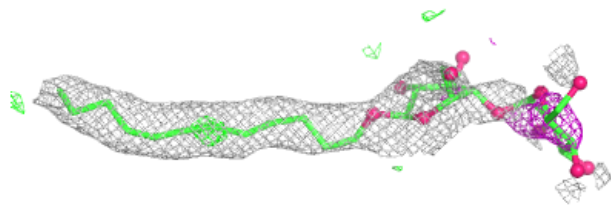
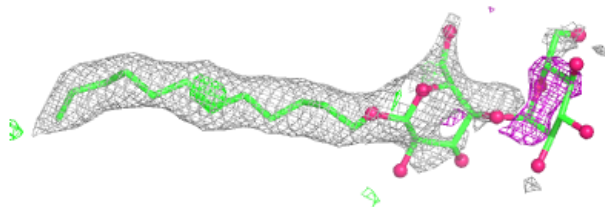
**Electron density around HTG d 410:**

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

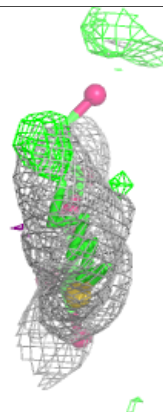
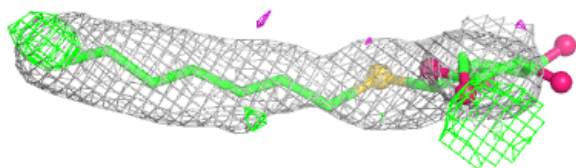
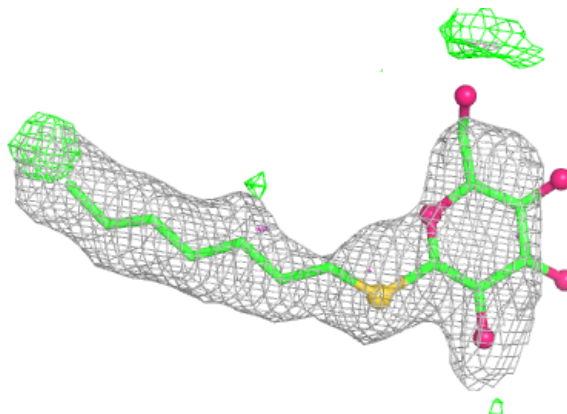


Electron density around LMT i 102:

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

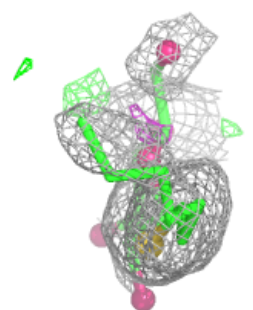
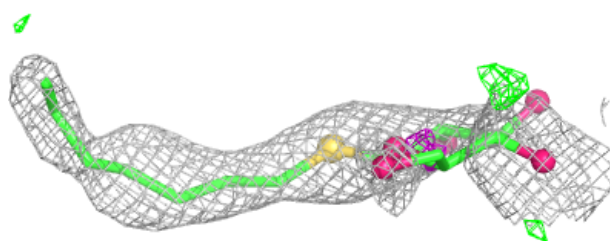
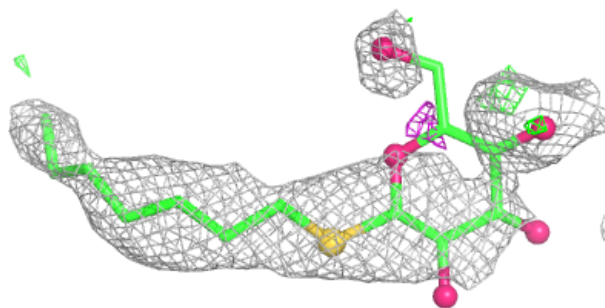
**Electron density around HTG B 629:**

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

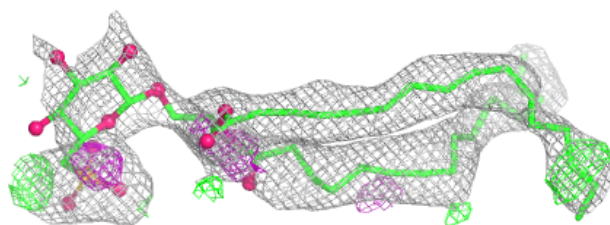
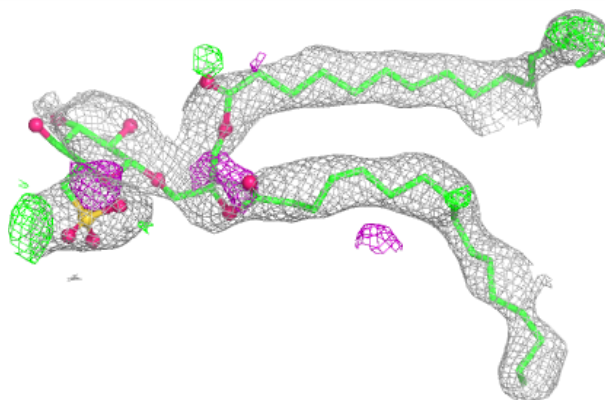


Electron density around HTG D 413:

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

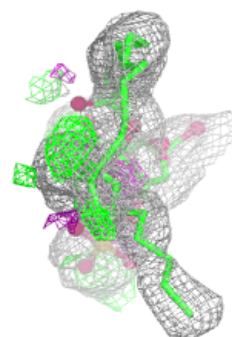
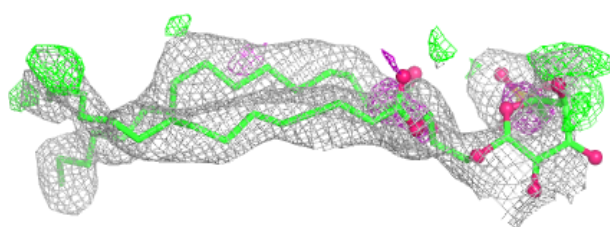
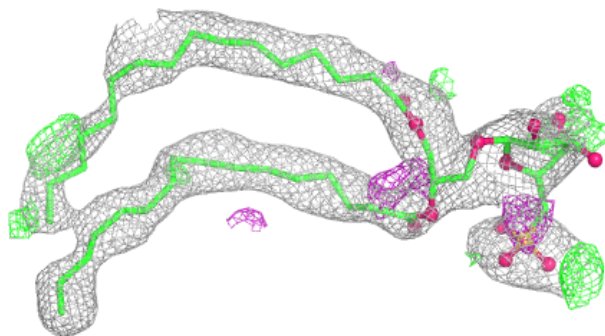
**Electron density around SQD b 623 (A):**

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

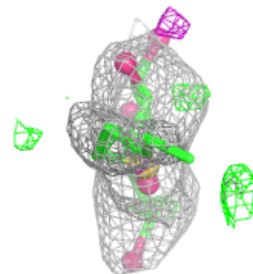
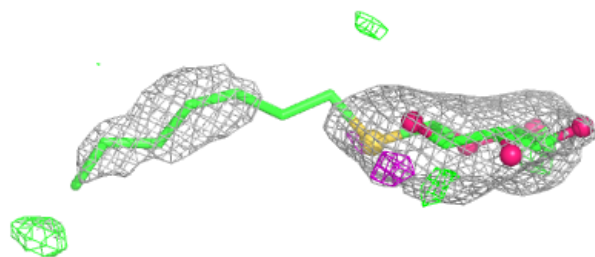
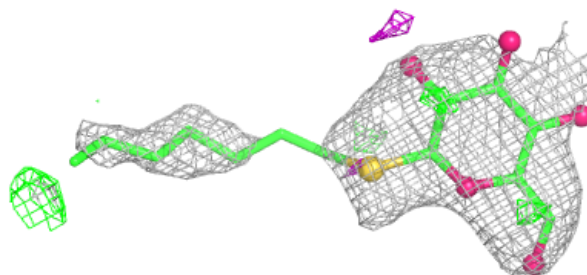


Electron density around SQD b 623 (B):

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

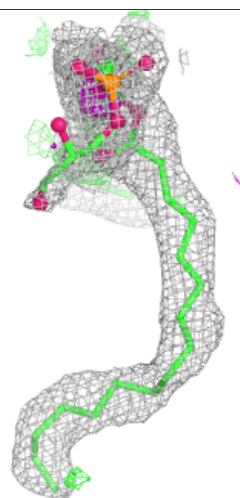
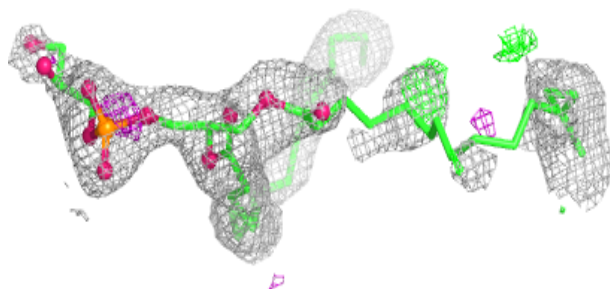
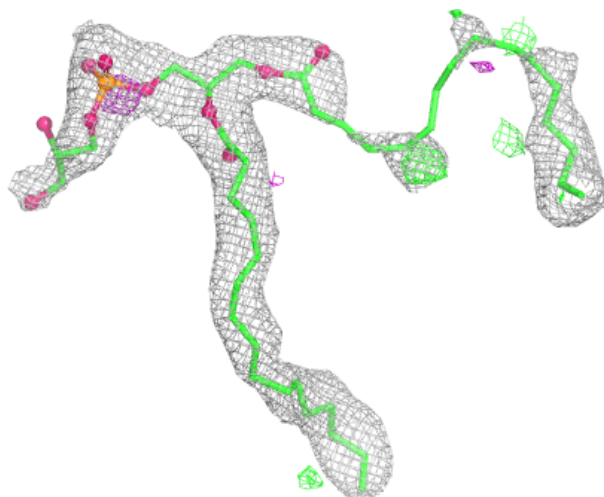
**Electron density around HTG c 522:**

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



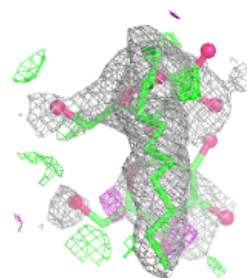
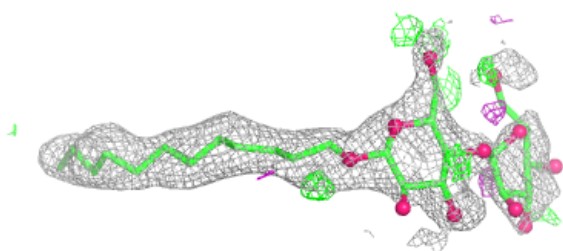
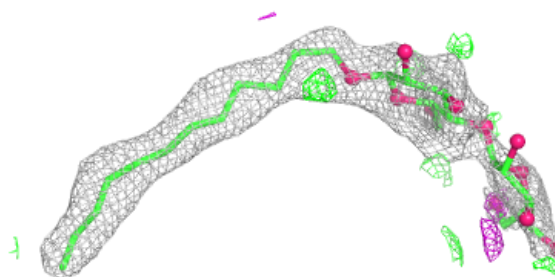
Electron density around LHG E 101:

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

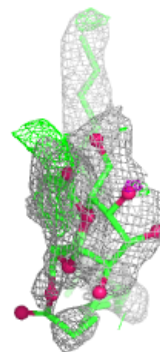
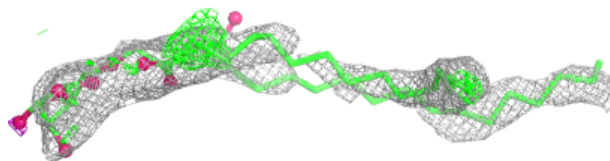
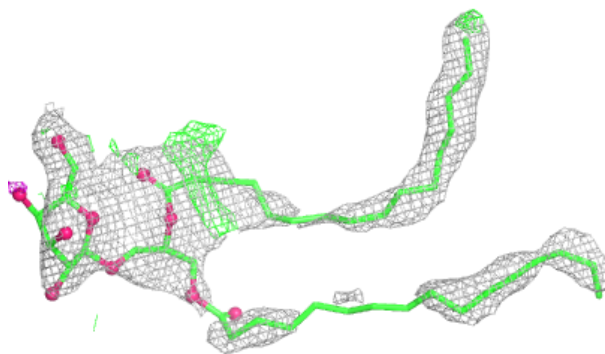


Electron density around LMT M 101:

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

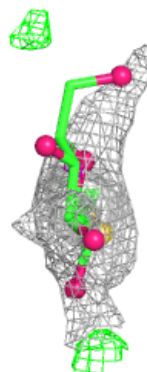
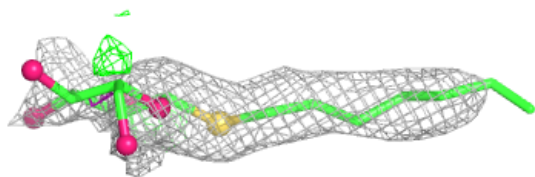
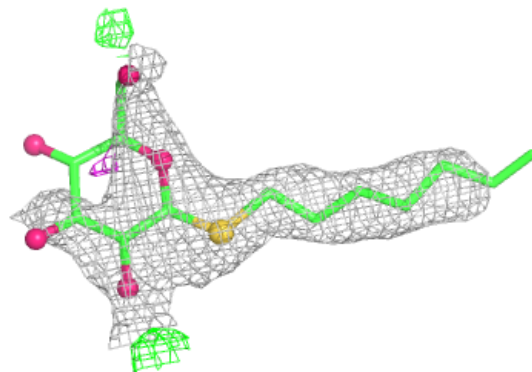
**Electron density around LMG c 521:**

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

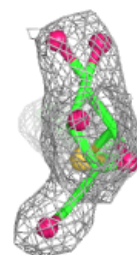
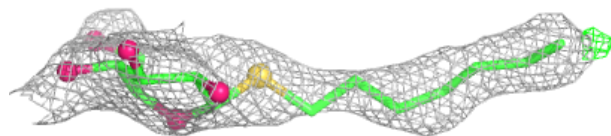
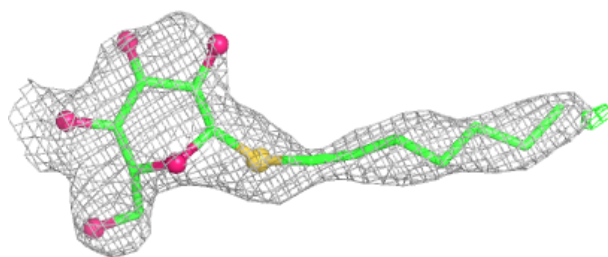


Electron density around HTG c 525:

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

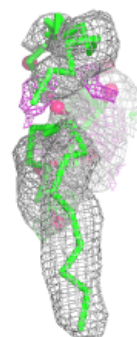
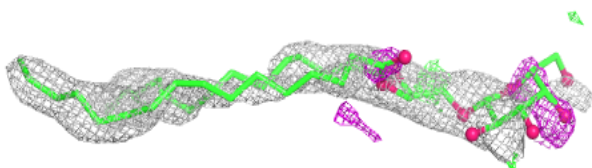
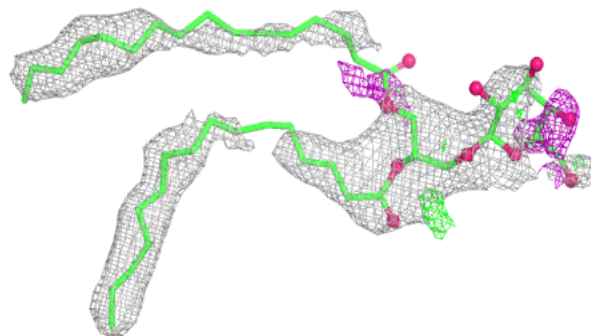
**Electron density around HTG C 522:**

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

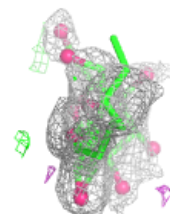
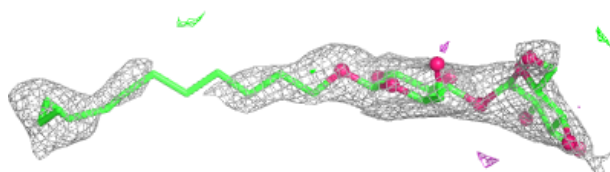
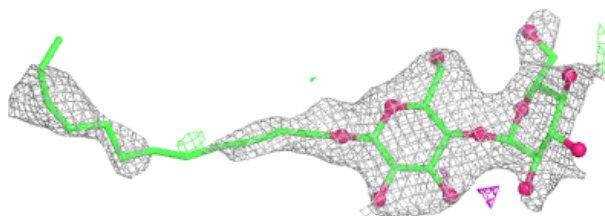


Electron density around LMG Z 101:

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

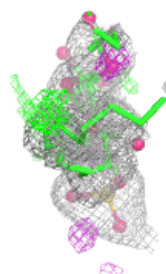
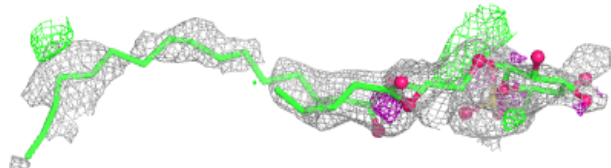
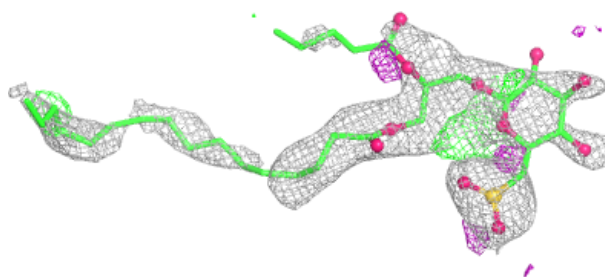
**Electron density around LMT a 416:**

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

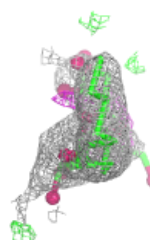
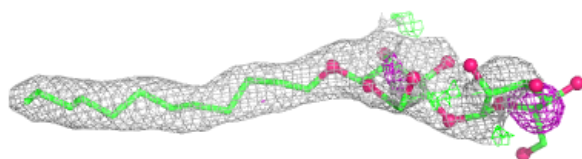
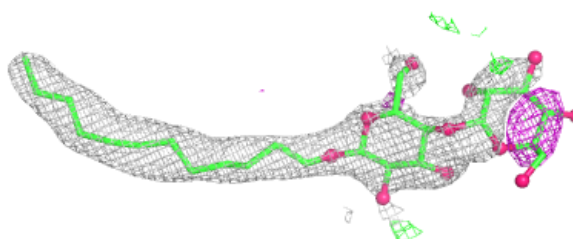


Electron density around SQD f 102:

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

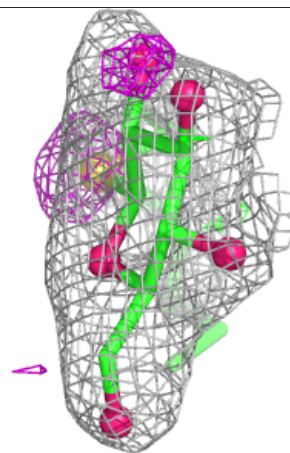
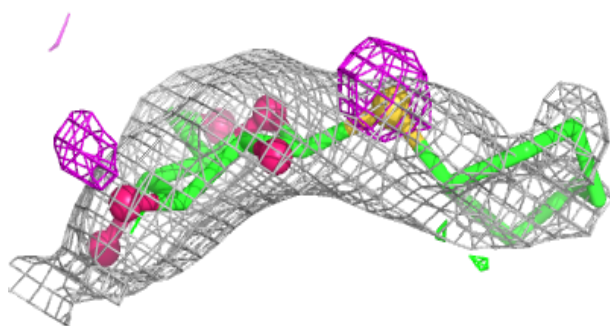
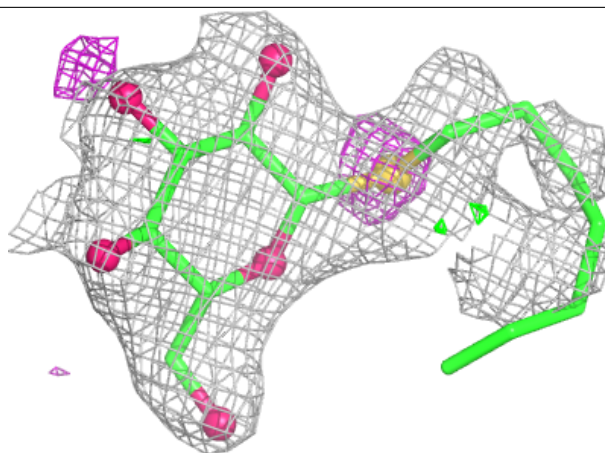
**Electron density around LMT b 625:**

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

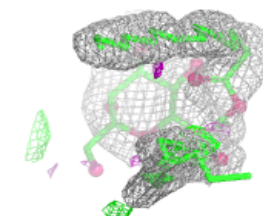
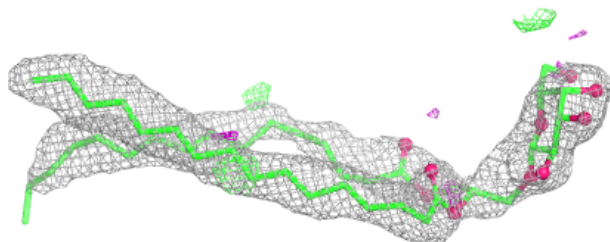
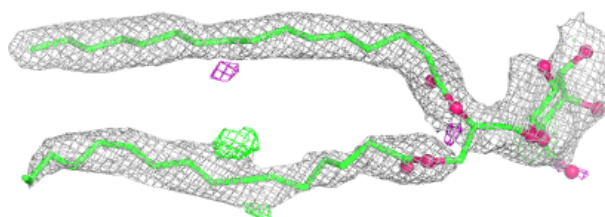


Electron density around HTG V 202:

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

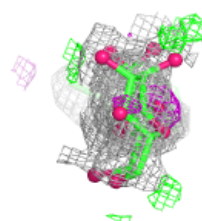
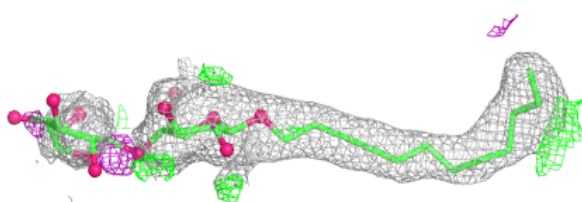
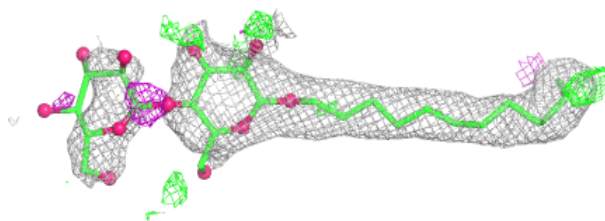
**Electron density around LMG c 520:**

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

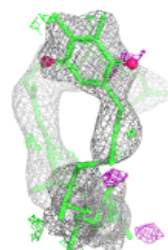
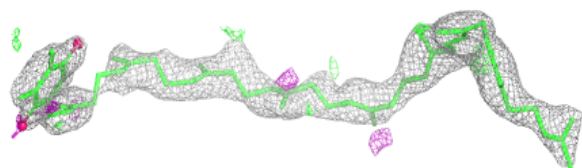
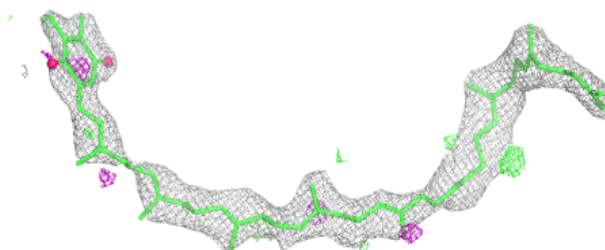


Electron density around LMT t 103:

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

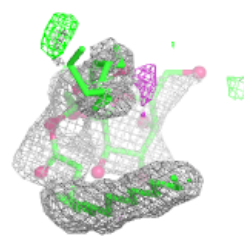
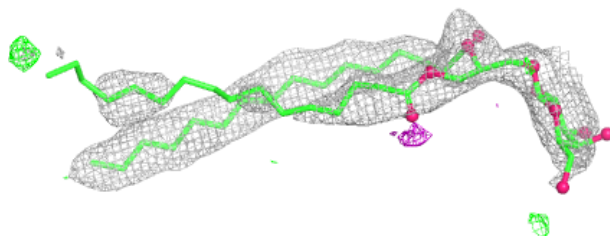
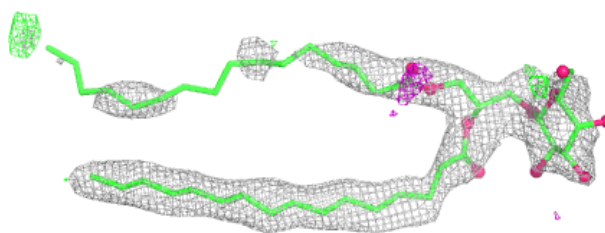
**Electron density around PL9 a 414:**

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

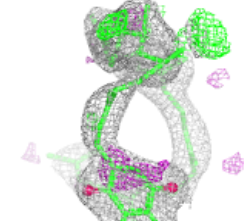
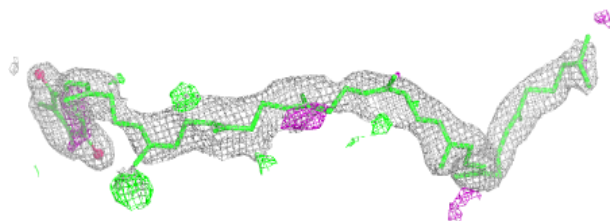
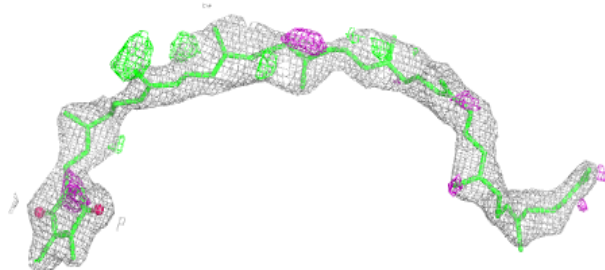


Electron density around LMG C 519:

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

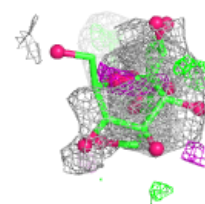
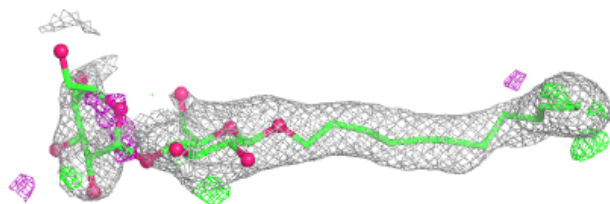
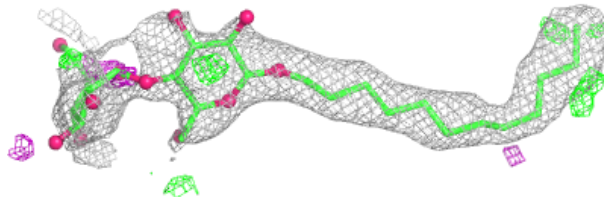
**Electron density around PL9 A 1010:**

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

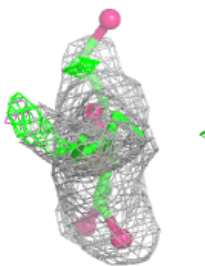
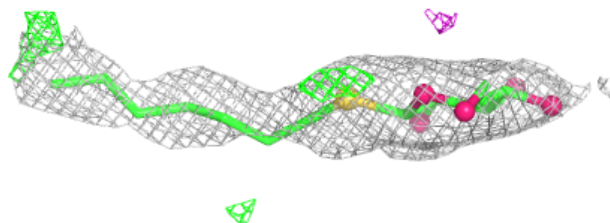
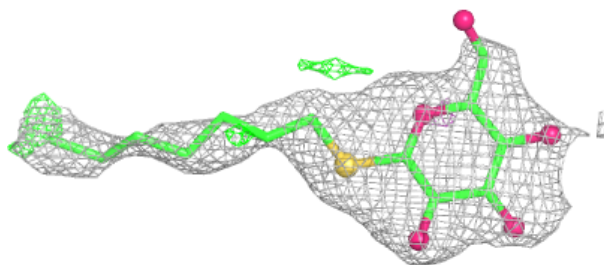


Electron density around LMT b 631:

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

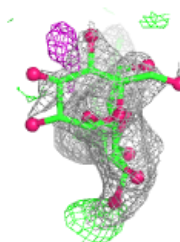
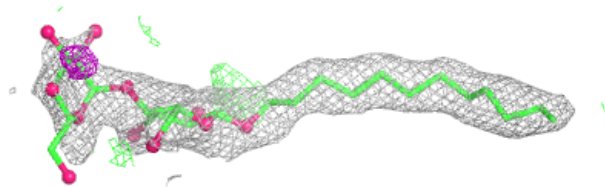
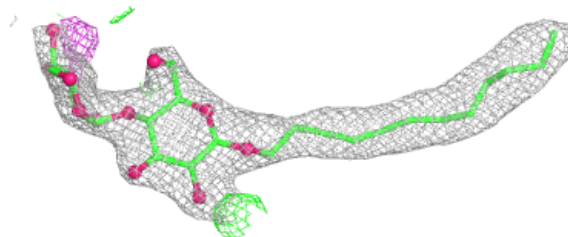
**Electron density around HTG C 521:**

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

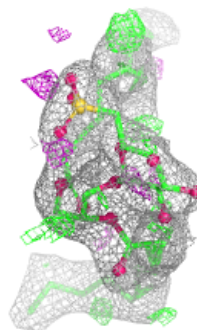
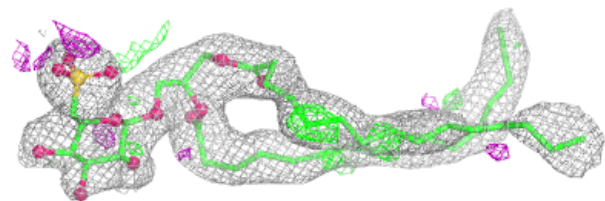
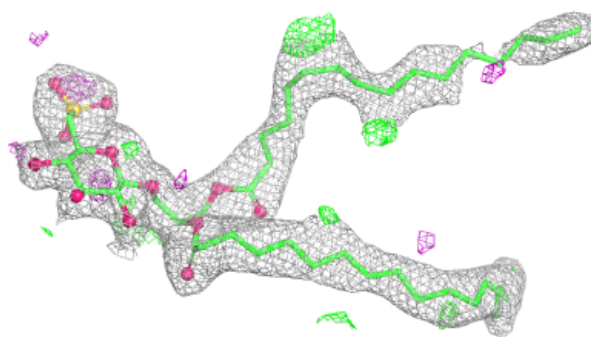


Electron density around LMT B 623:

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

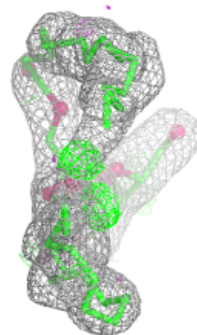
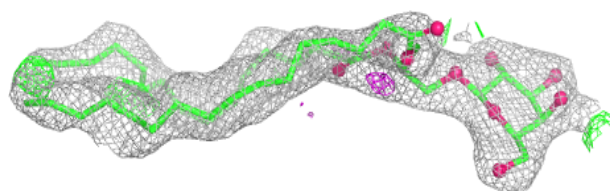
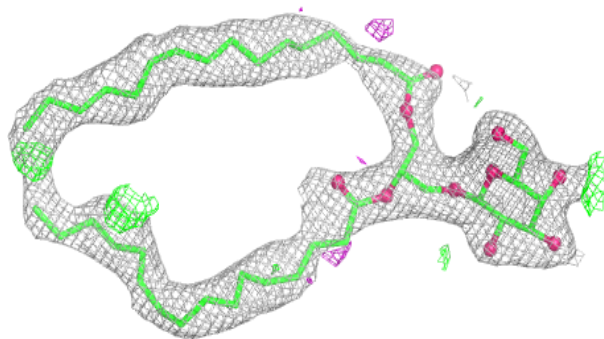
**Electron density around SQD A 1016:**

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

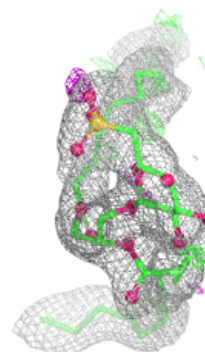
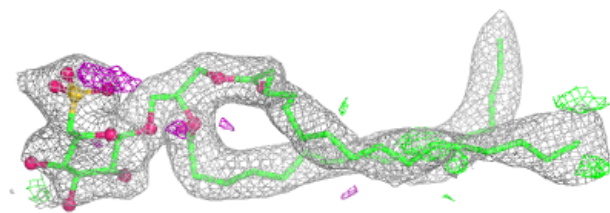
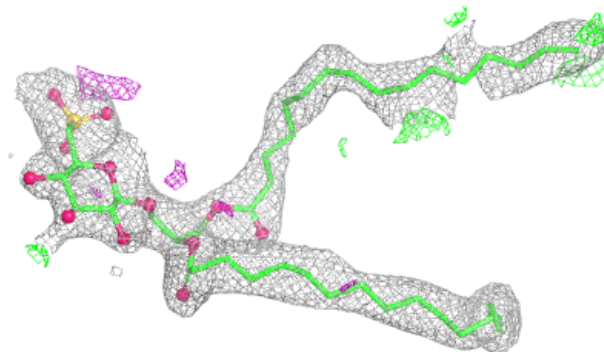


Electron density around LMG A 1012:

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

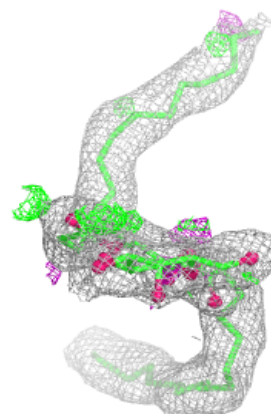
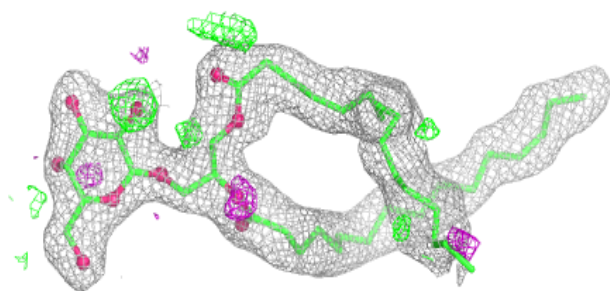
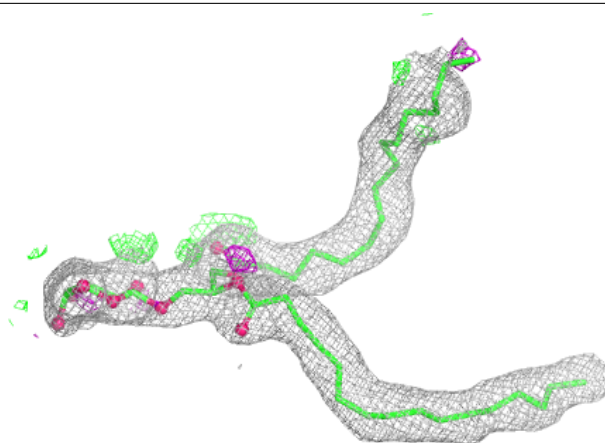
**Electron density around SQD a 401:**

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



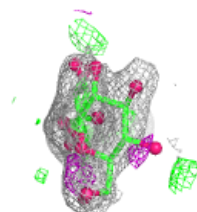
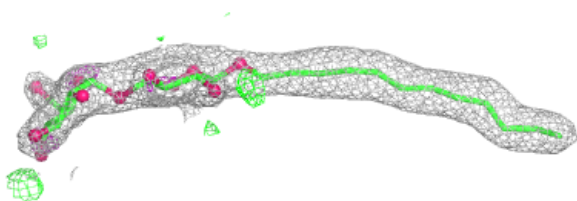
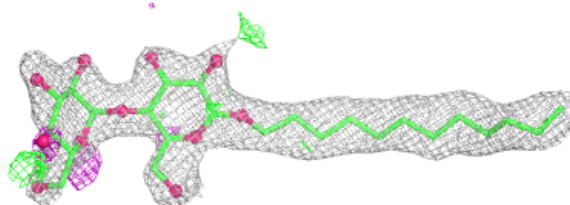
Electron density around LMG B 622:

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

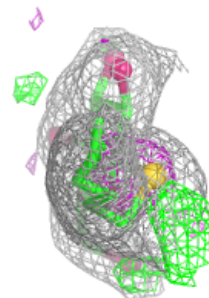
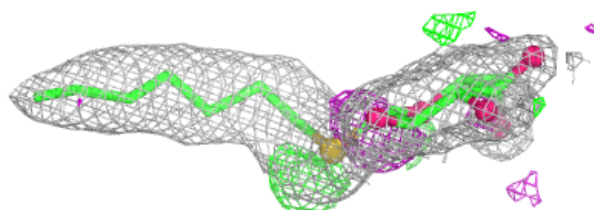
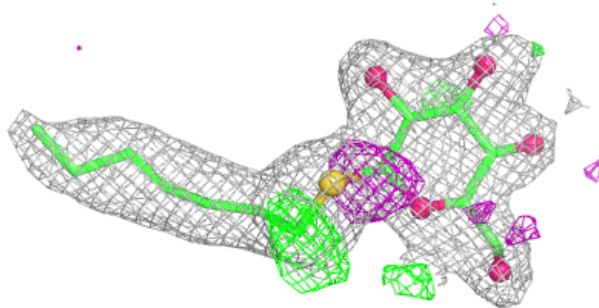


Electron density around LMT M 102:

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

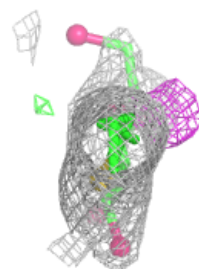
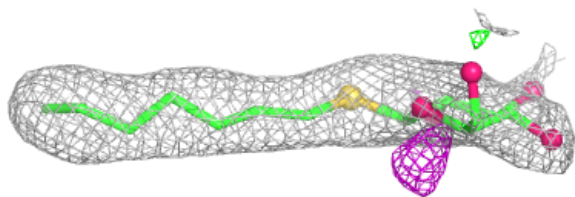
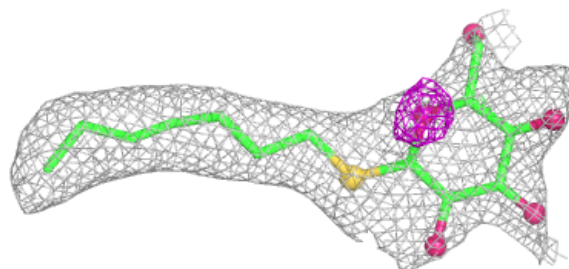
**Electron density around HTG b 626:**

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



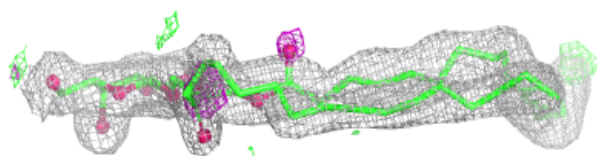
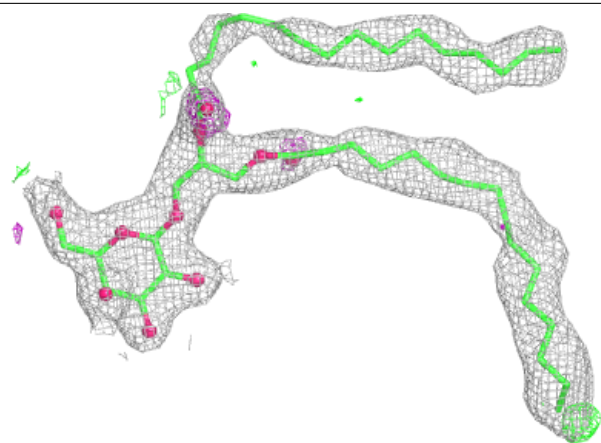
Electron density around HTG B 628:

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

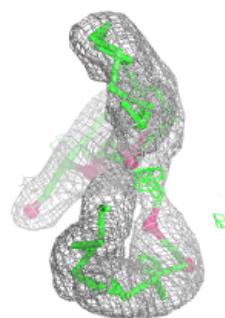
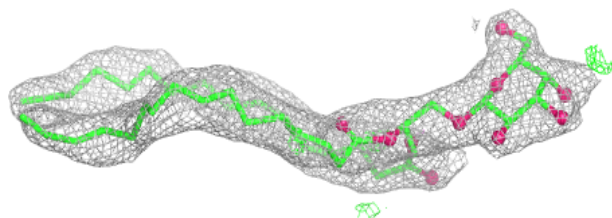
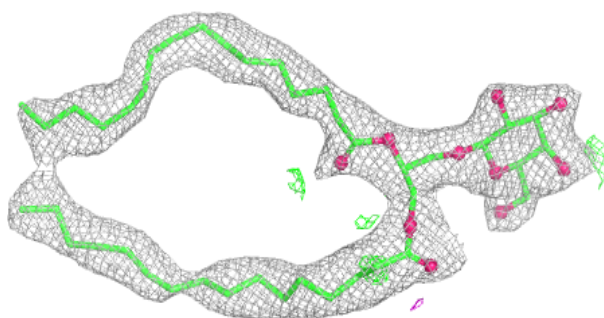


Electron density around LMG C 518:

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

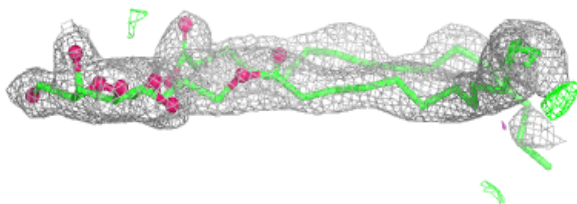
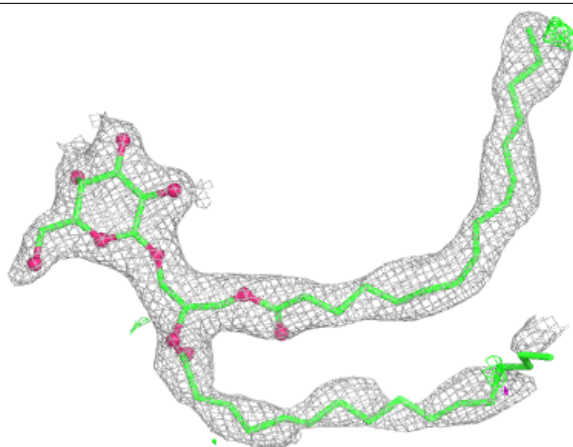
**Electron density around LMG a 415:**

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



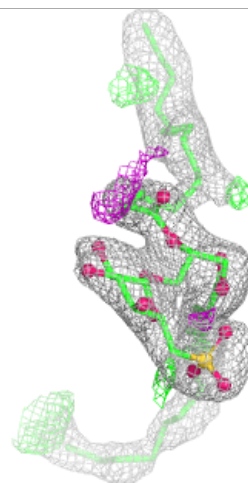
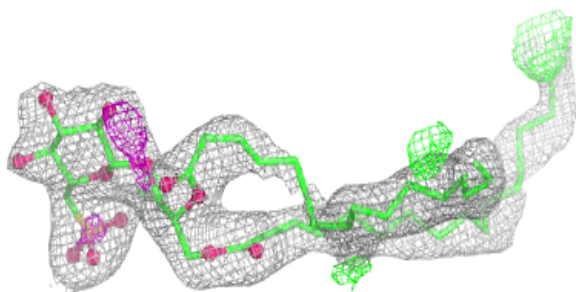
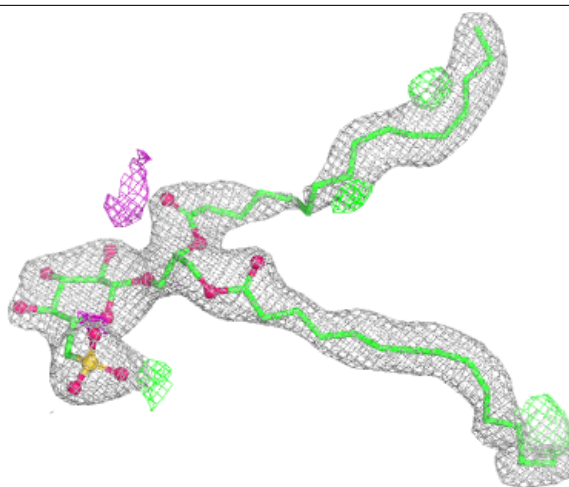
Electron density around LMG c 519:

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



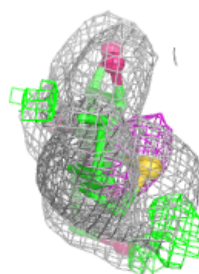
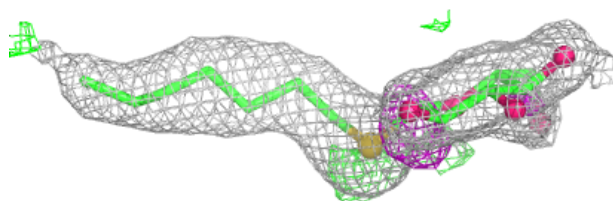
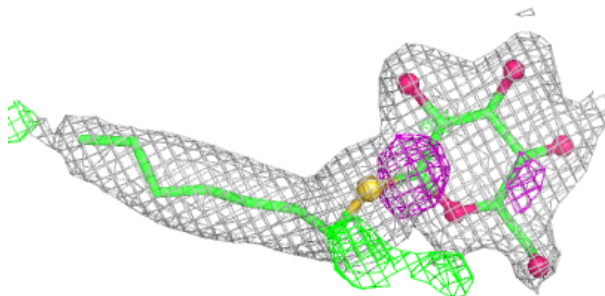
Electron density around SQD c 518:

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

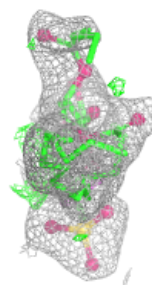
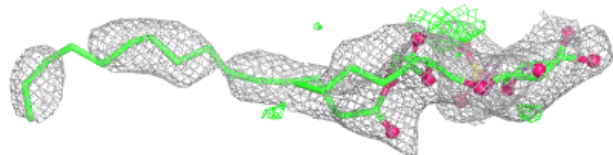
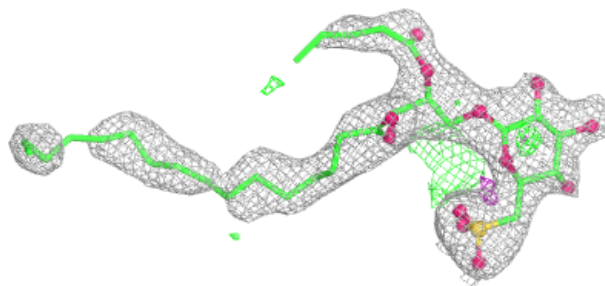


Electron density around HTG o 301:

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

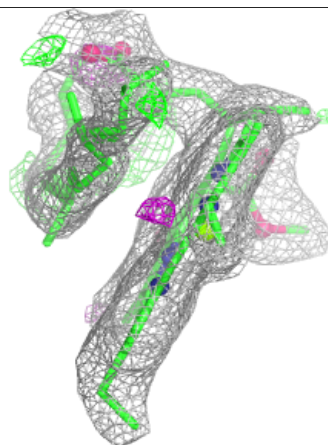
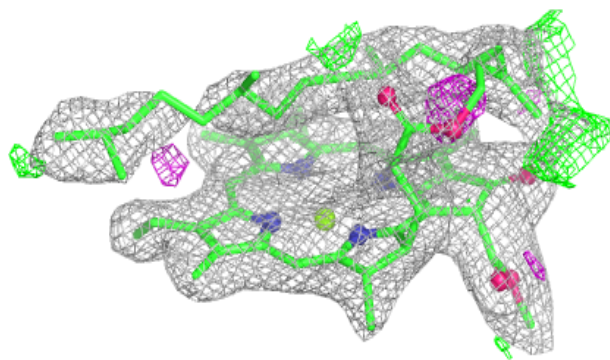
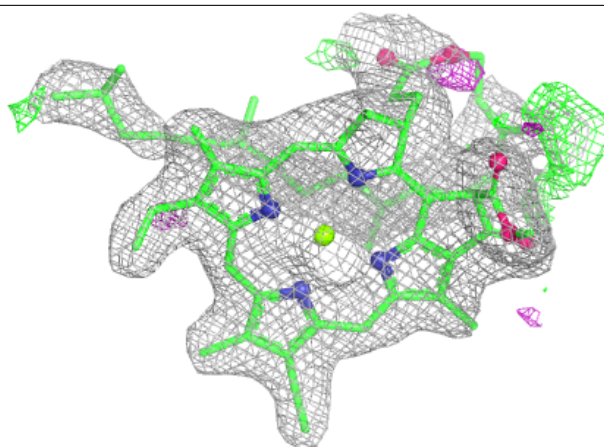
**Electron density around SQD D 408:**

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

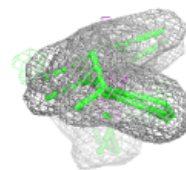
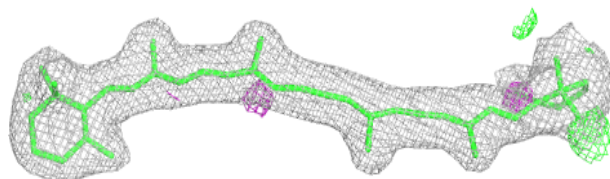
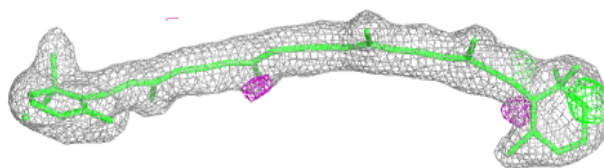


Electron density around CLA b 604:

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

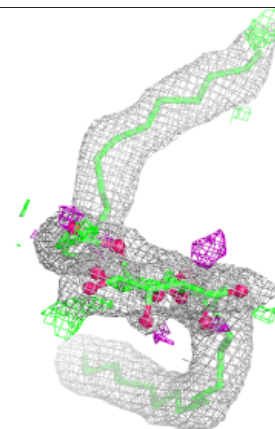
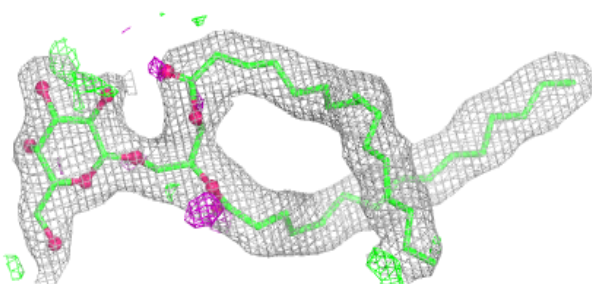
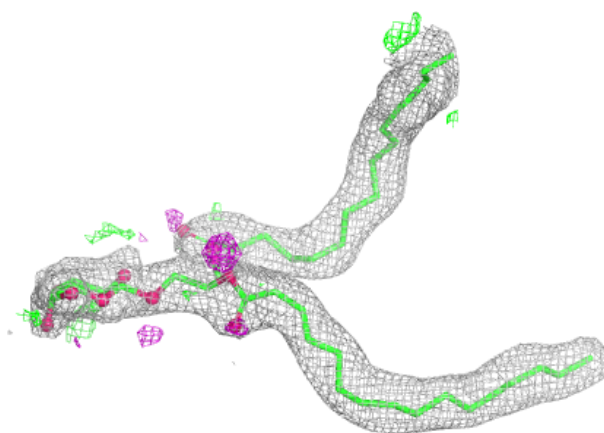
**Electron density around BCR d 404:**

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

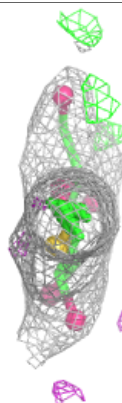
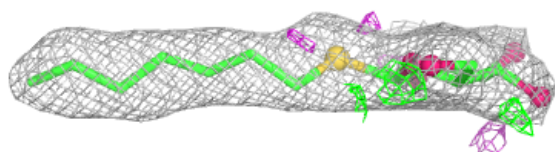
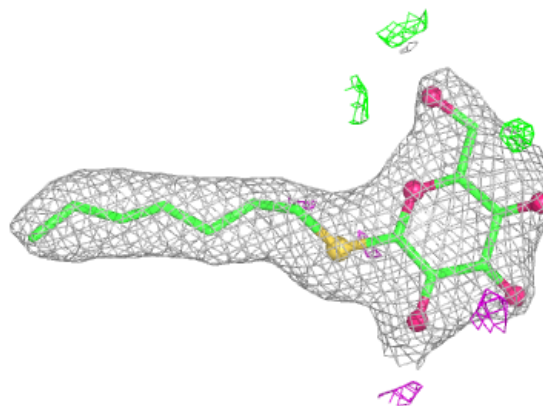


Electron density around LMG m 102:

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

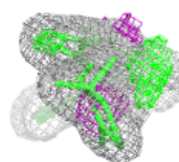
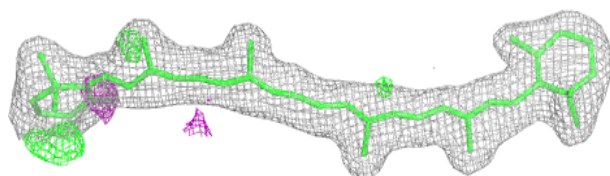
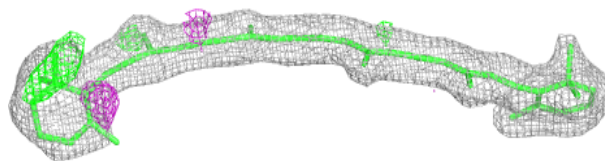
**Electron density around HTG b 601:**

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

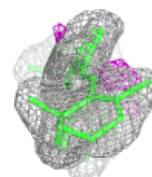
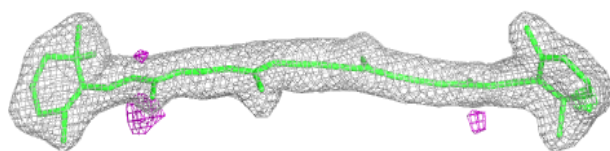
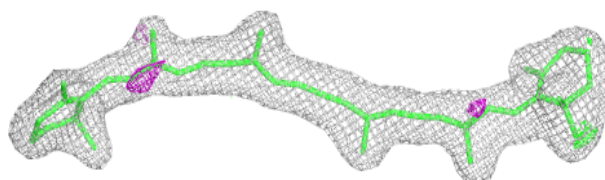


Electron density around BCR D 406:

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

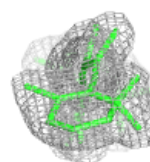
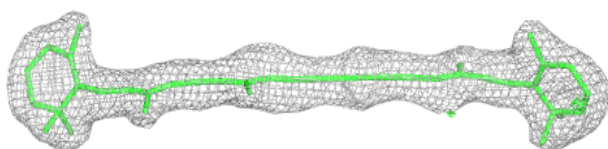
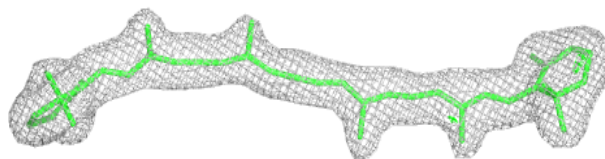
**Electron density around BCR J 101:**

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

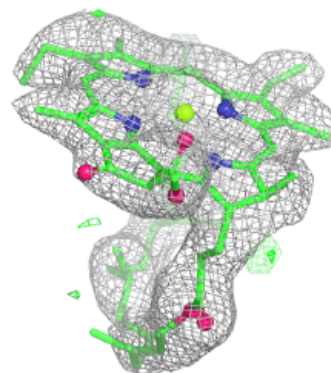
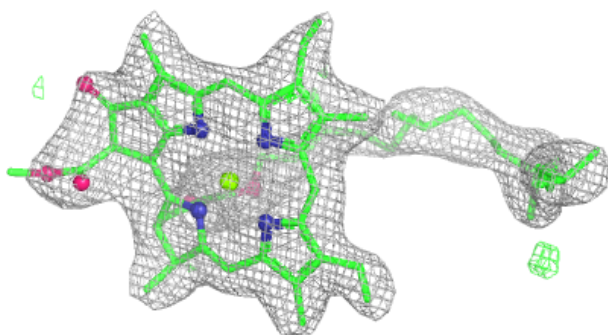
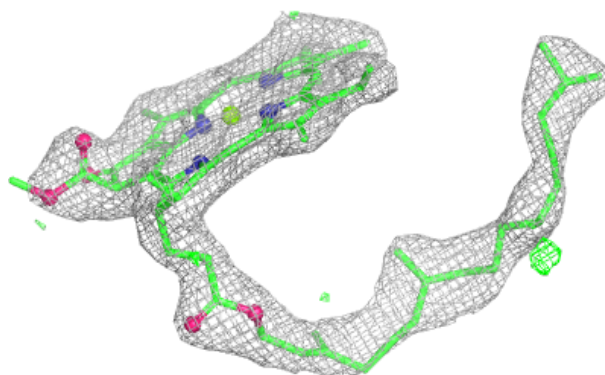


Electron density around BCR K 102:

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

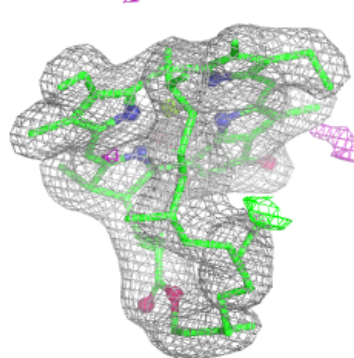
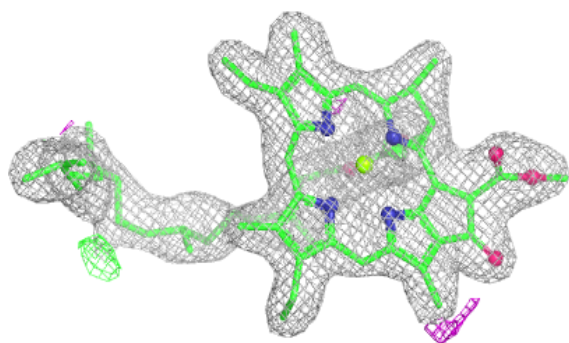
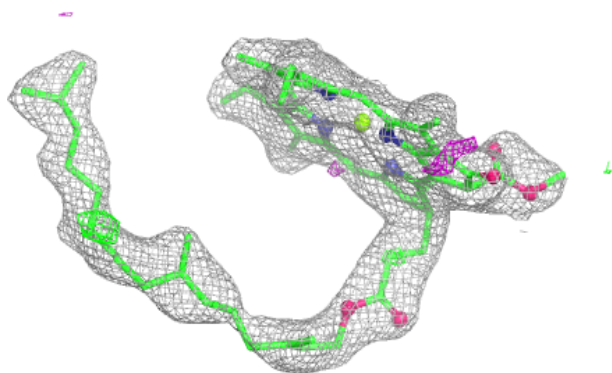
**Electron density around CLA c 513:**

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



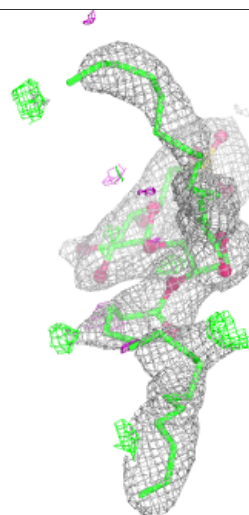
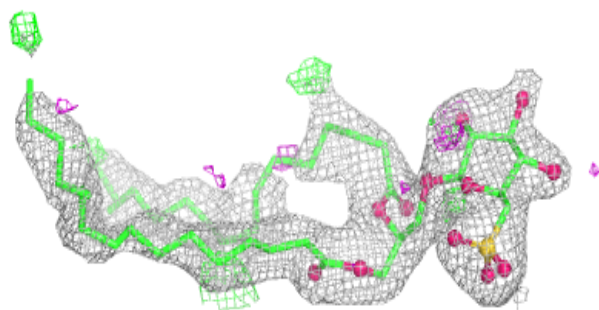
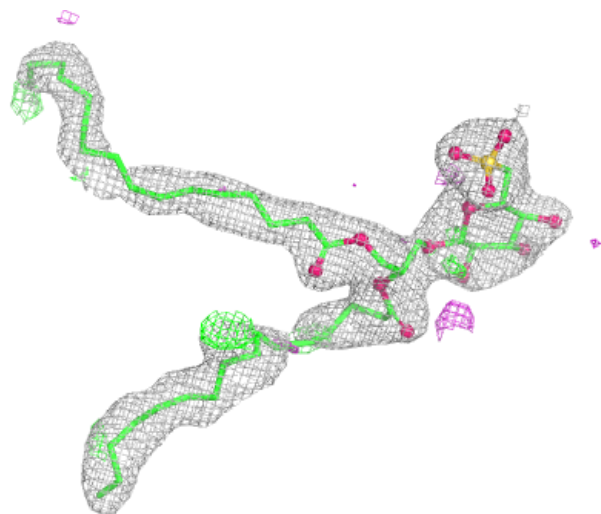
Electron density around CLA C 513:

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



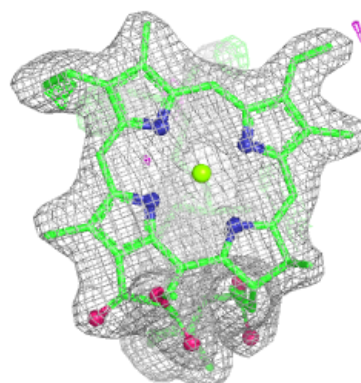
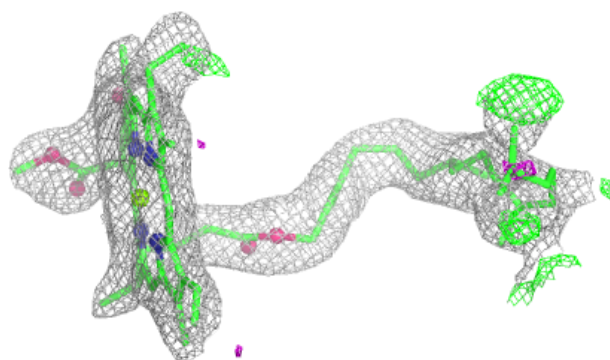
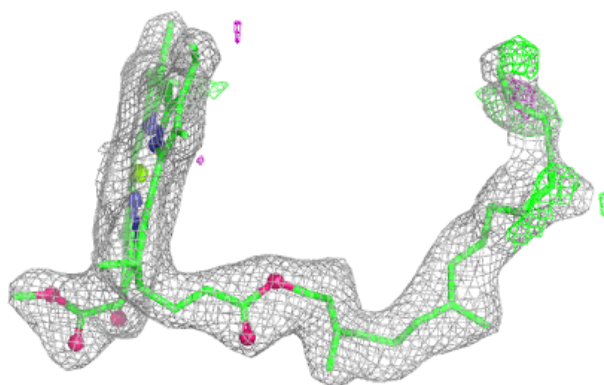
Electron density around SQD A 1011:

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

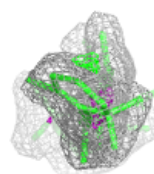
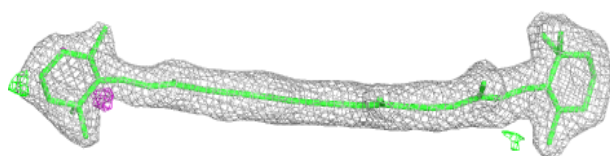


Electron density around CLA C 506:

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

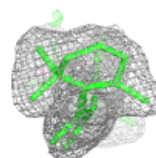
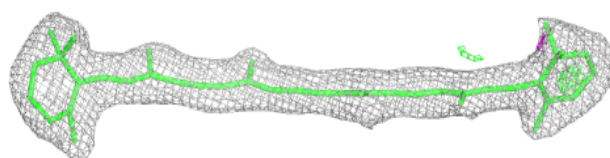
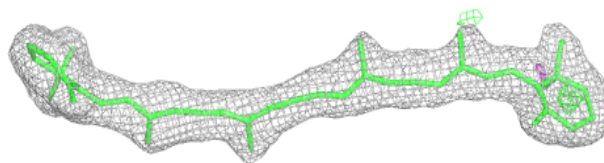
**Electron density around BCR h 101:**

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

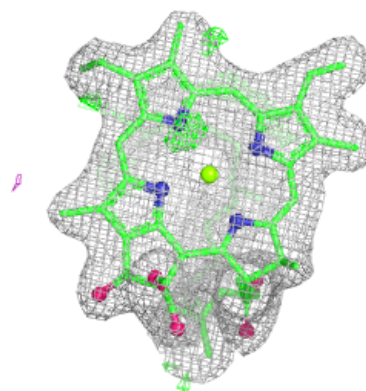
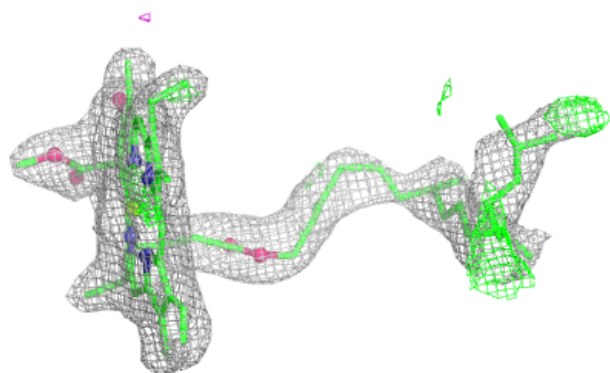
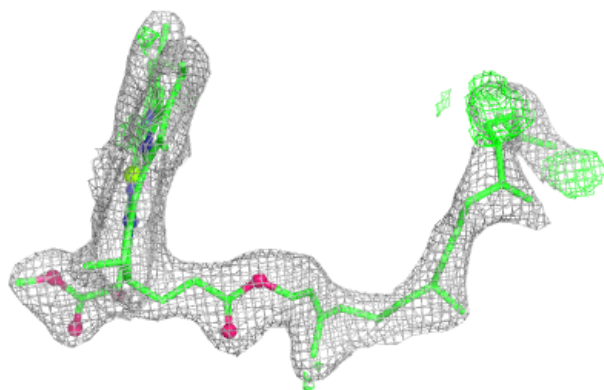


Electron density around BCR k 102:

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

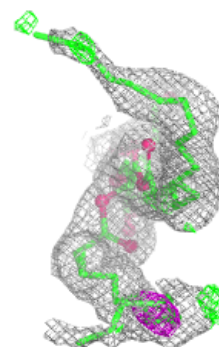
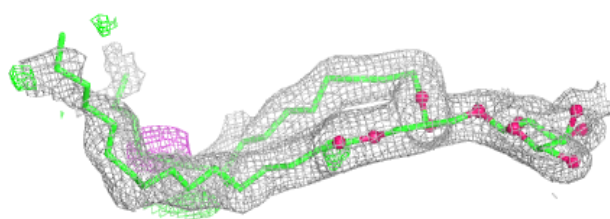
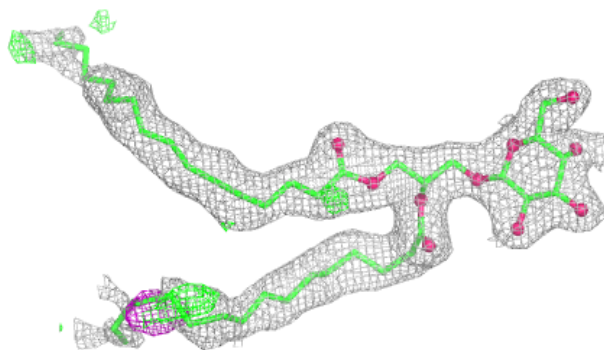
**Electron density around CLA c 506:**

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

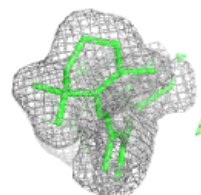
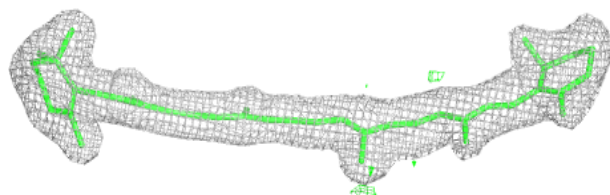
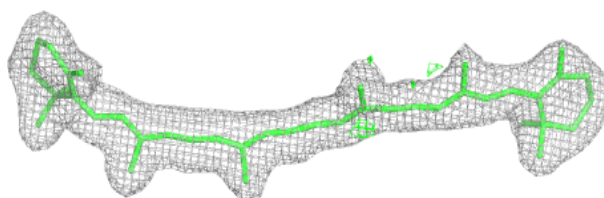


Electron density around LMG D 412:

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

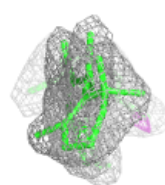
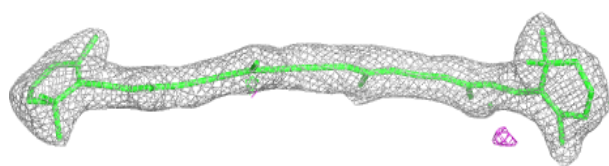
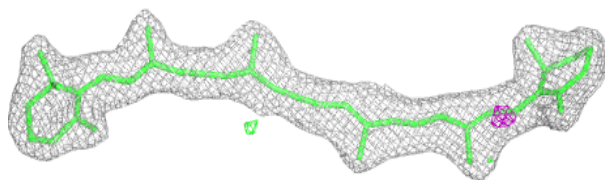
**Electron density around BCR t 101:**

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

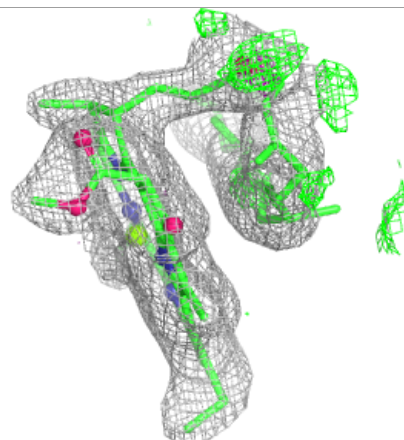
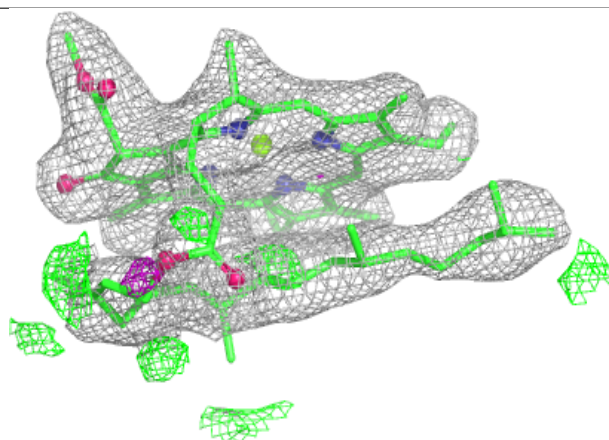
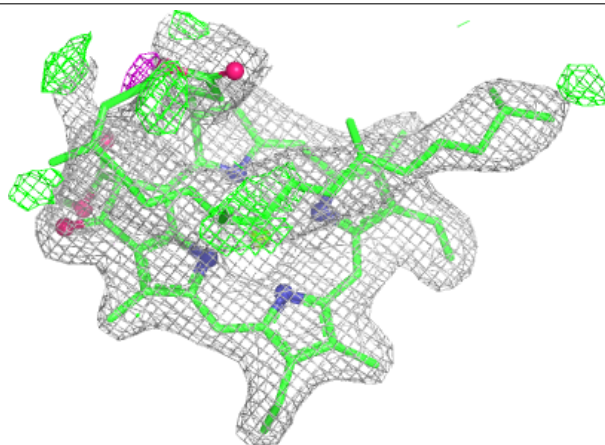


Electron density around BCR y 101:

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

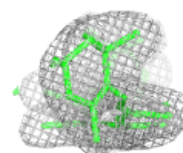
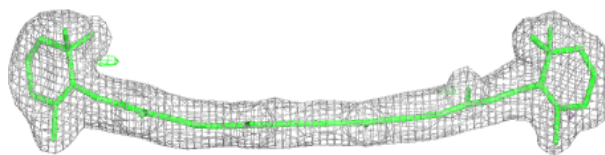
**Electron density around CLA B 601:**

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

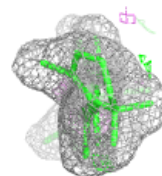
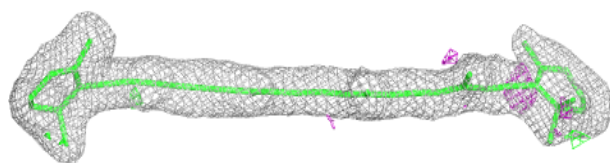
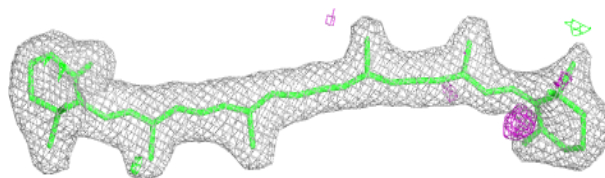


Electron density around BCR K 101:

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

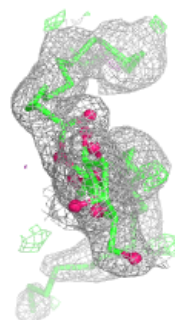
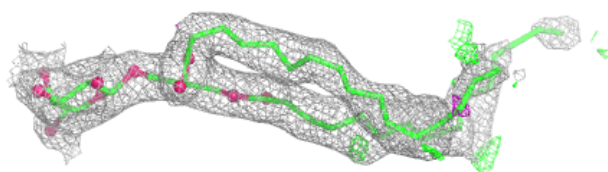
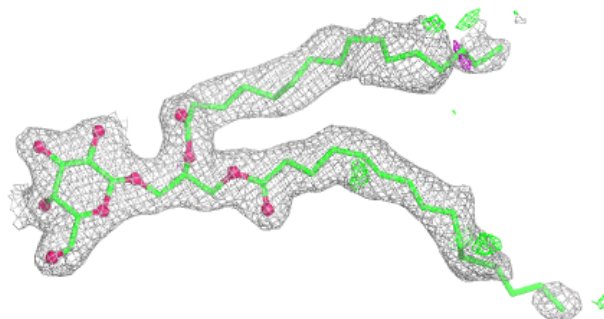
**Electron density around BCR B 618:**

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

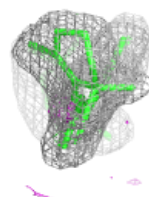
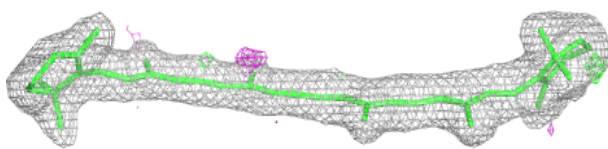
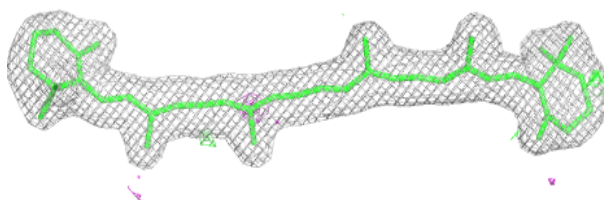


Electron density around LMG d 409:

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

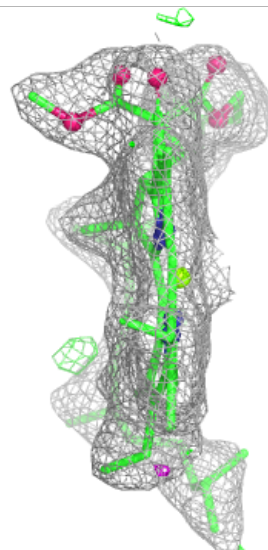
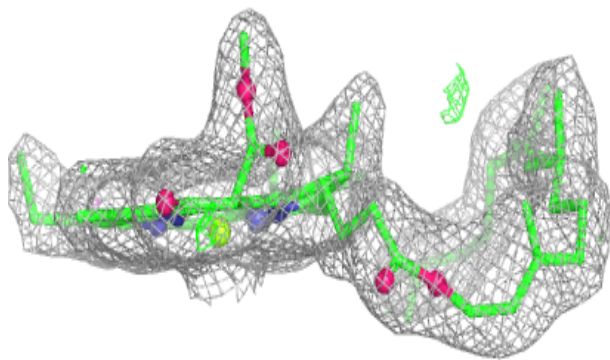
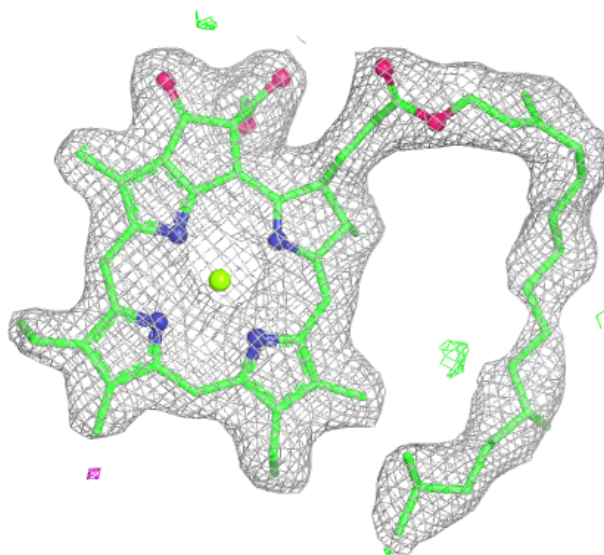
**Electron density around BCR B 619:**

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



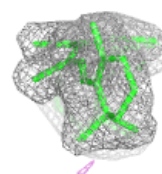
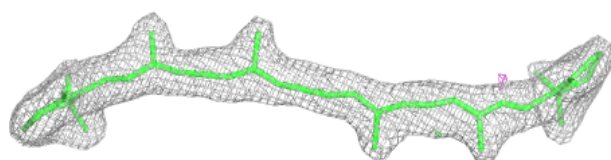
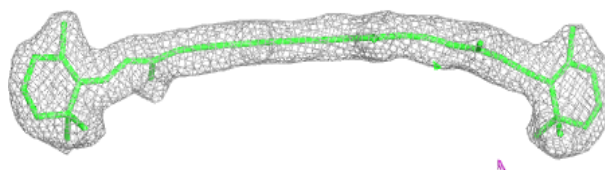
Electron density around CLA c 512:

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

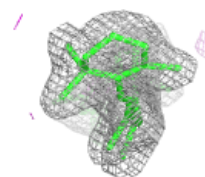
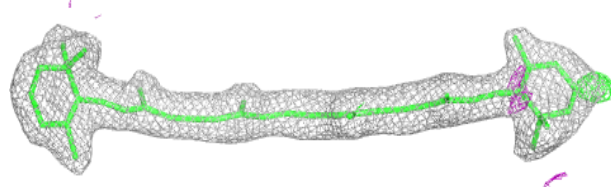
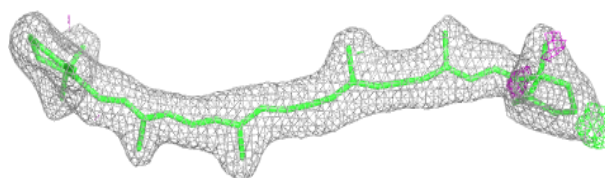


Electron density around BCR k 101:

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

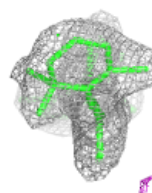
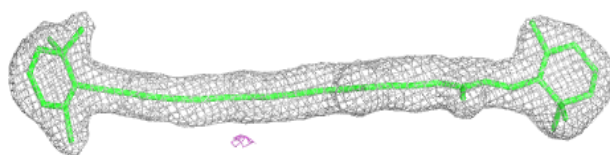
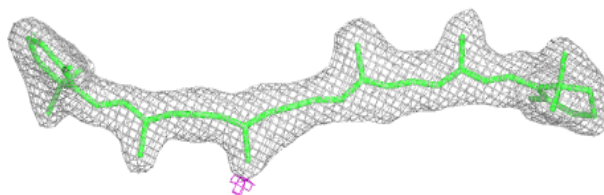
**Electron density around BCR H 101:**

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



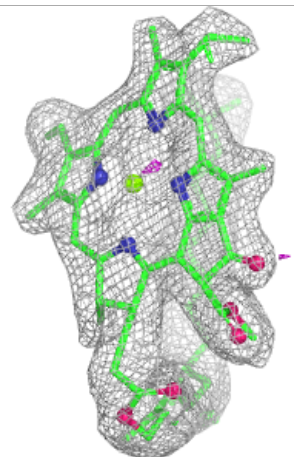
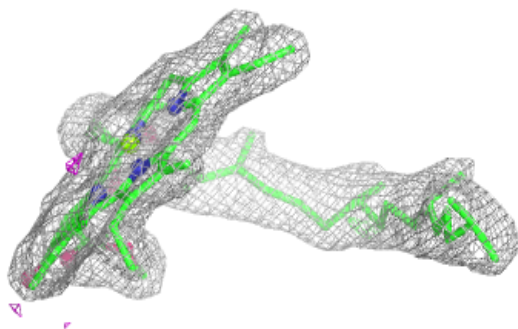
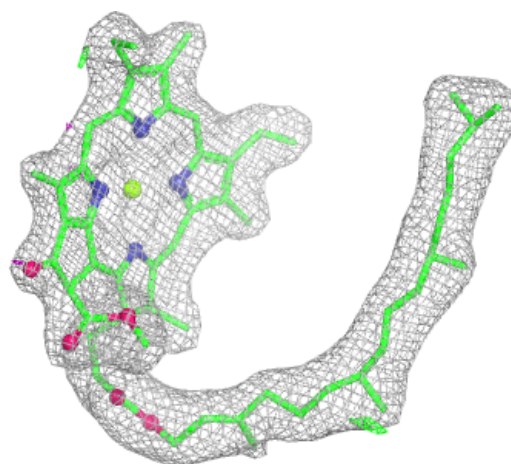
Electron density around BCR c 514:

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



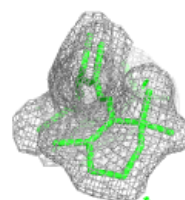
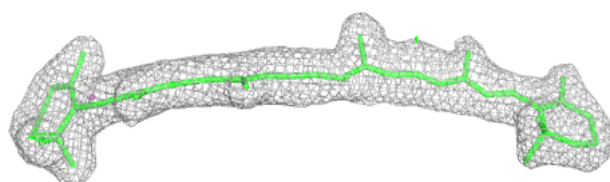
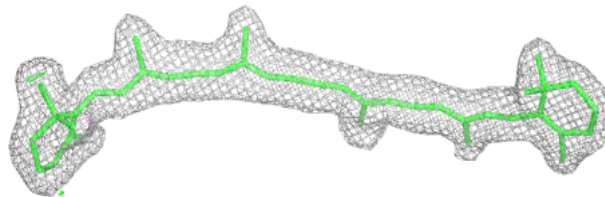
Electron density around CLA c 507:

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

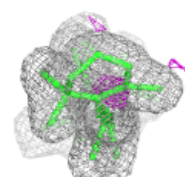
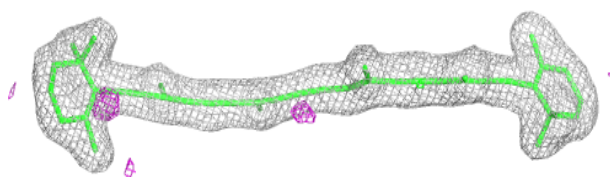
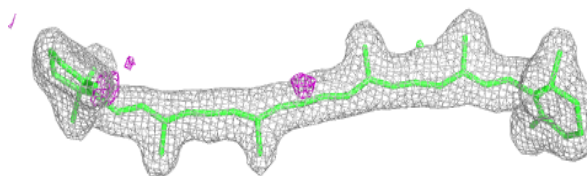


Electron density around BCR T 101:

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

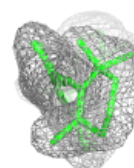
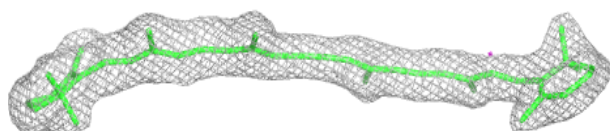
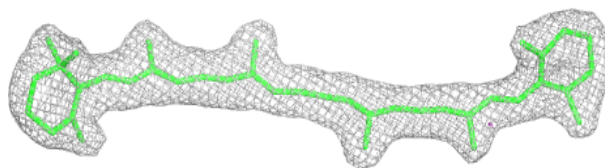
**Electron density around BCR a 413:**

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

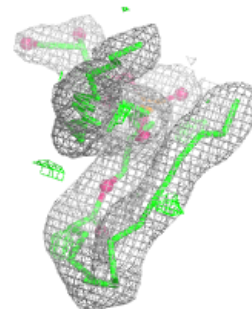
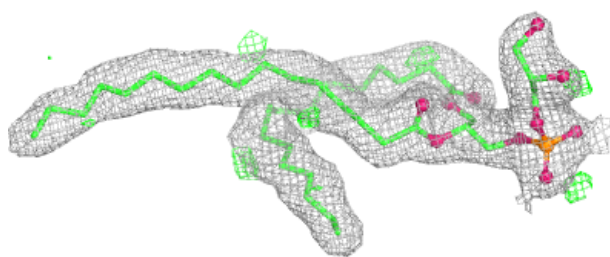
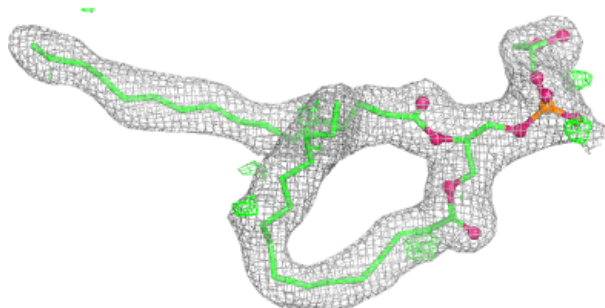


Electron density around BCR b 622:

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

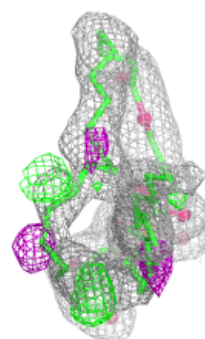
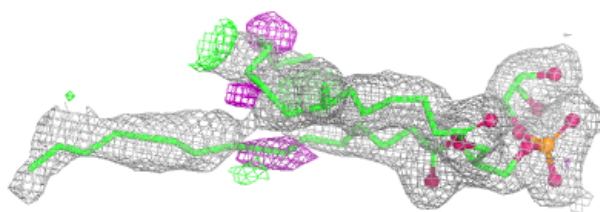
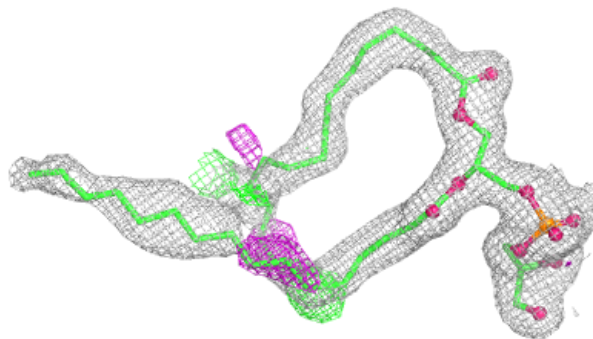
**Electron density around LHG d 406:**

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

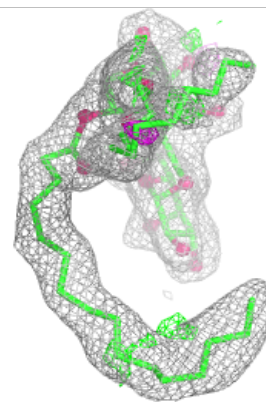
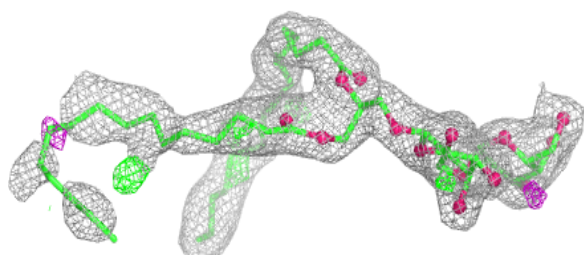
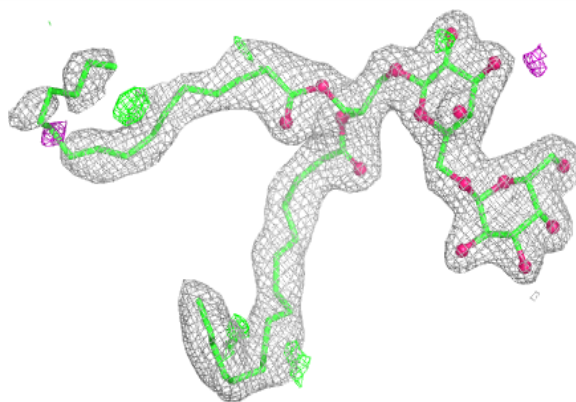


Electron density around LHG d 408:

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

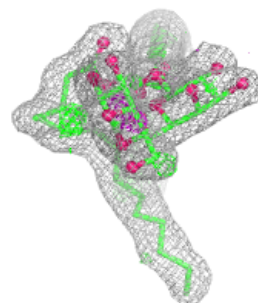
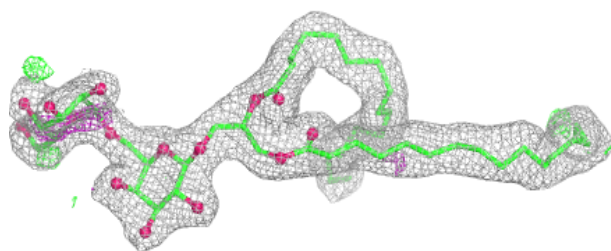
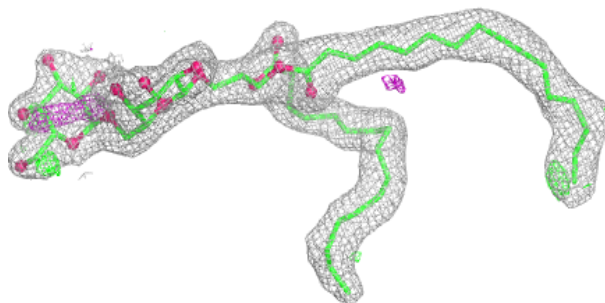
**Electron density around DGD c 516:**

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

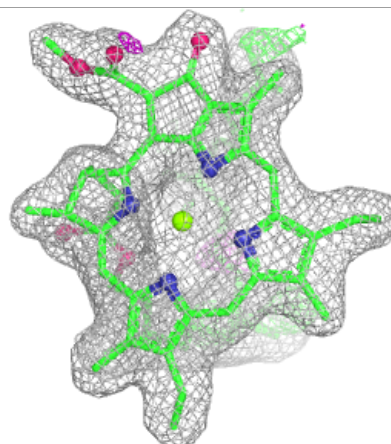
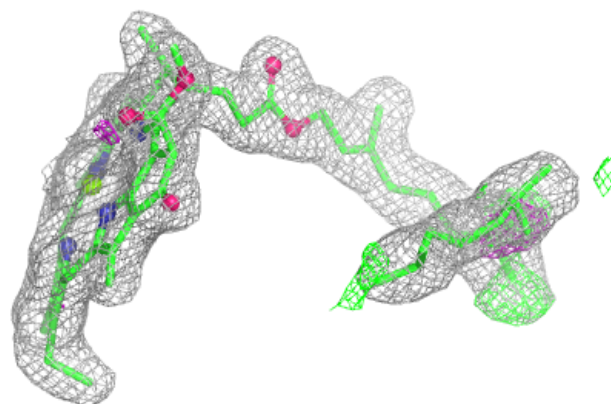
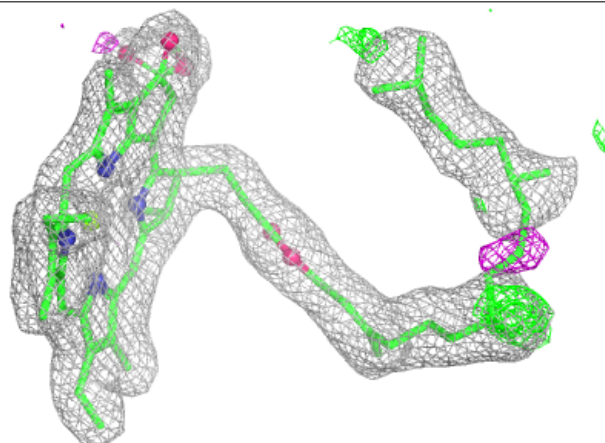


Electron density around DGD h 102:

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

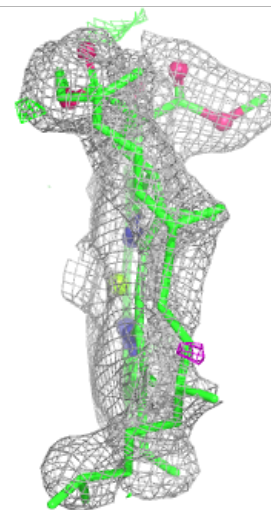
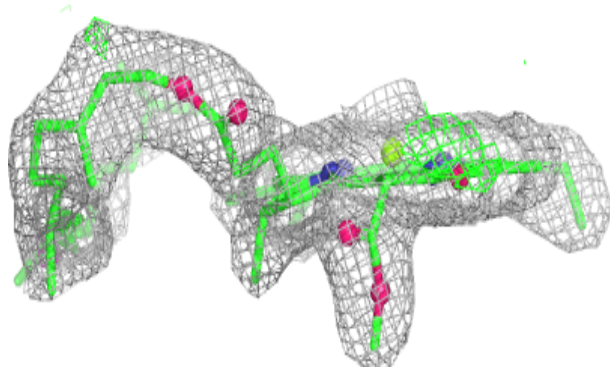
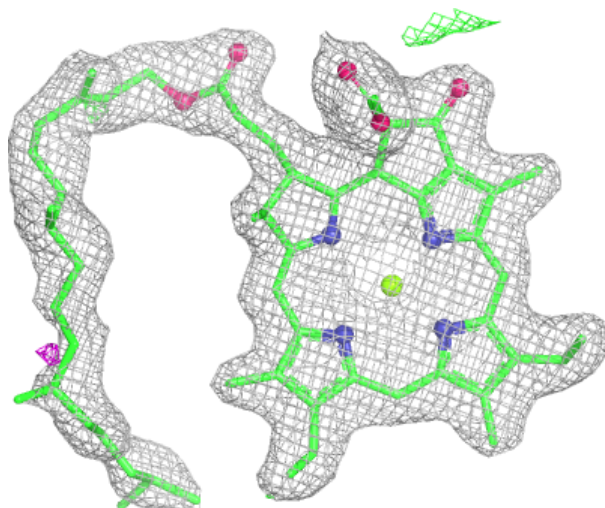
**Electron density around CLA B 606:**

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



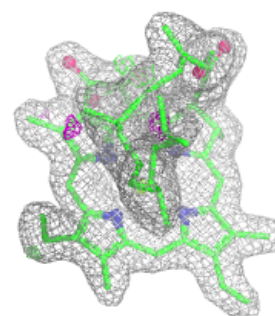
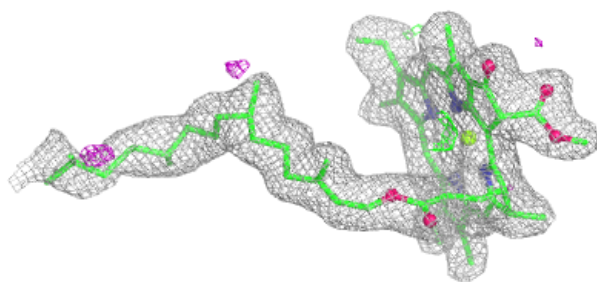
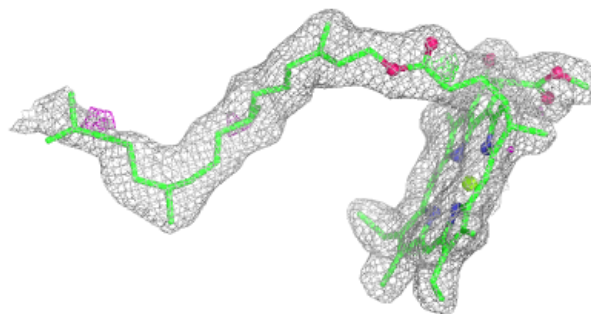
Electron density around CLA C 512:

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



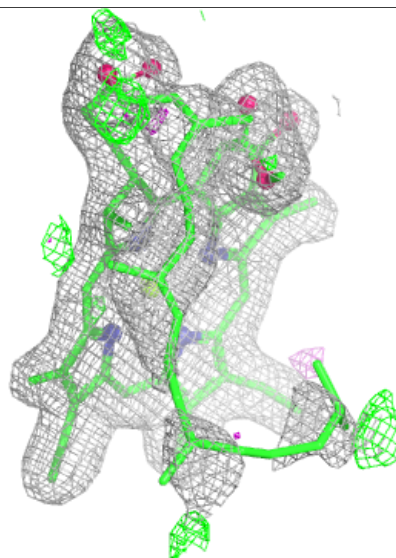
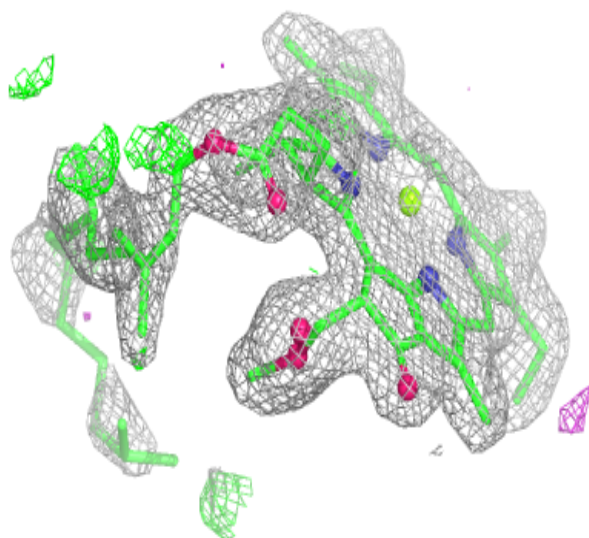
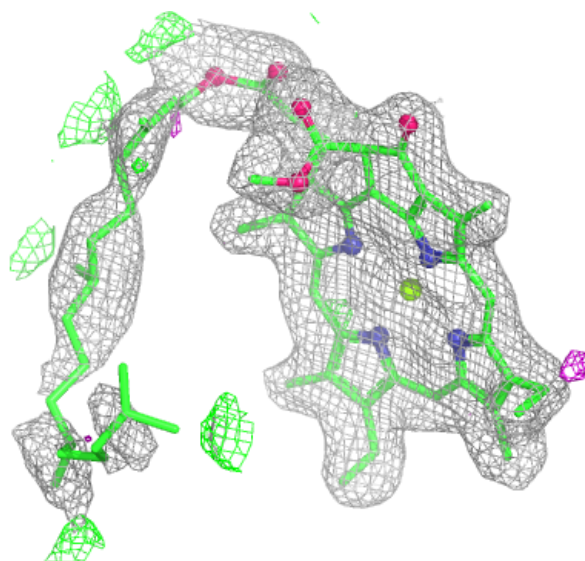
Electron density around CLA c 508:

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



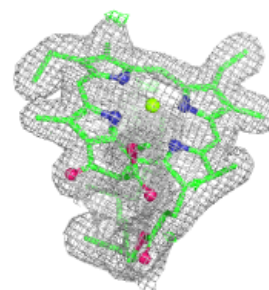
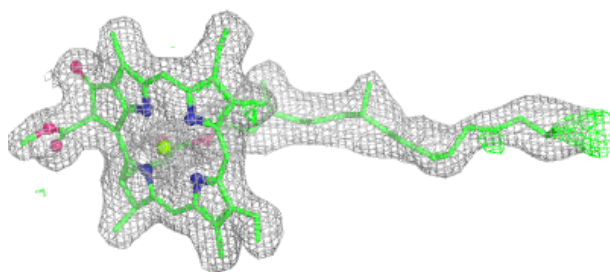
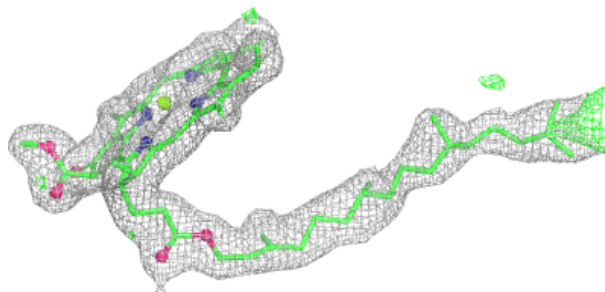
Electron density around CLA B 616:

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

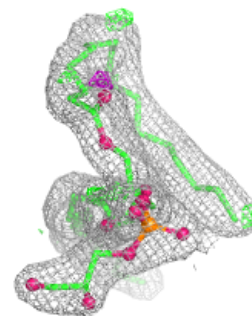
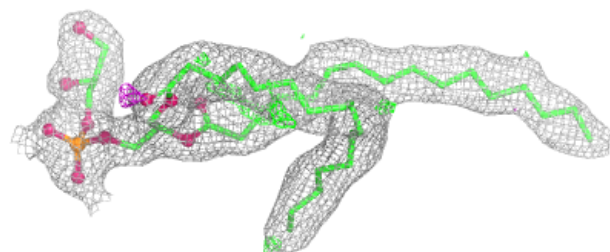
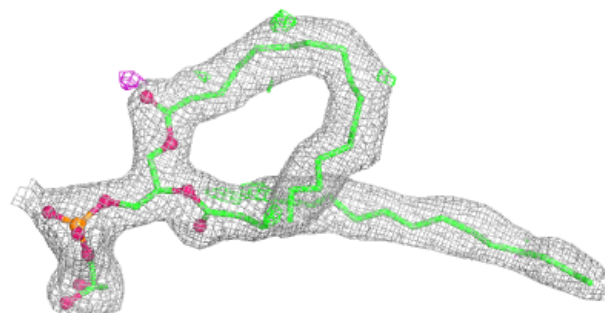


Electron density around CLA C 504:

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

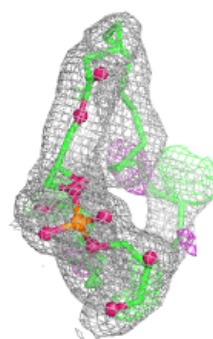
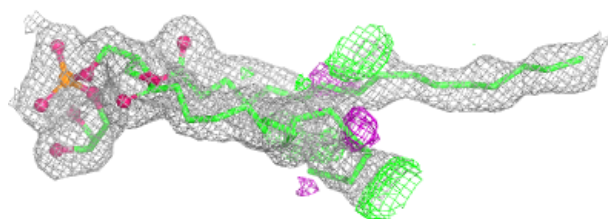
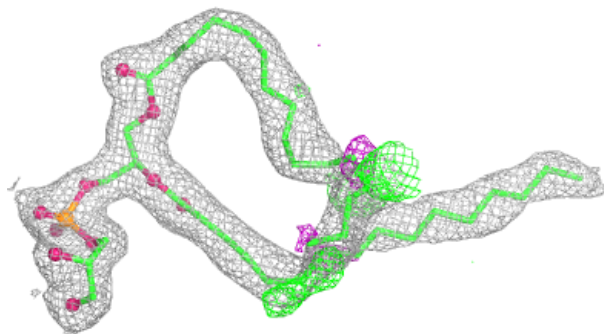
**Electron density around LHG D 409:**

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

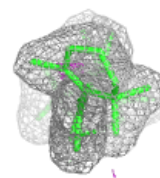
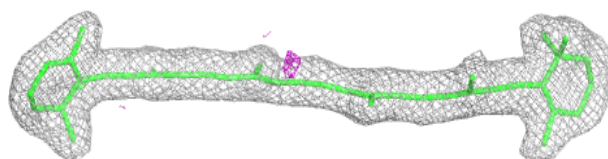
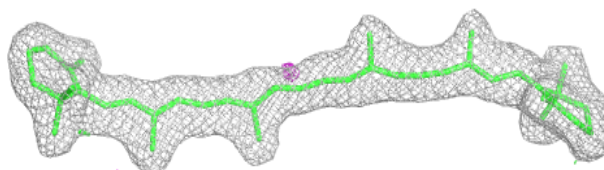


Electron density around LHG D 411:

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

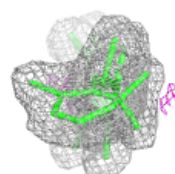
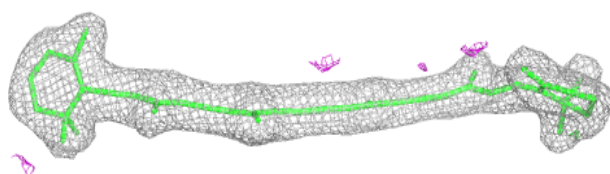
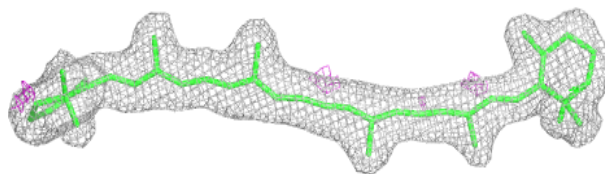
**Electron density around BCR A 1009:**

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

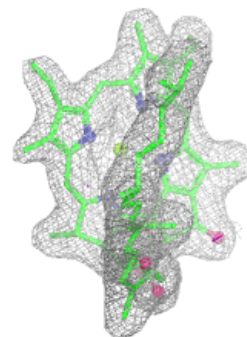
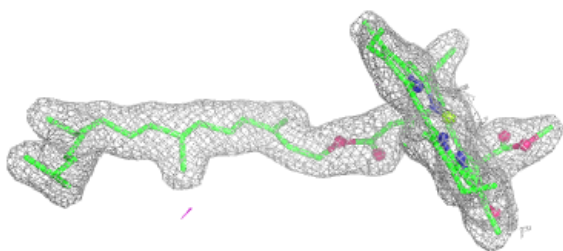
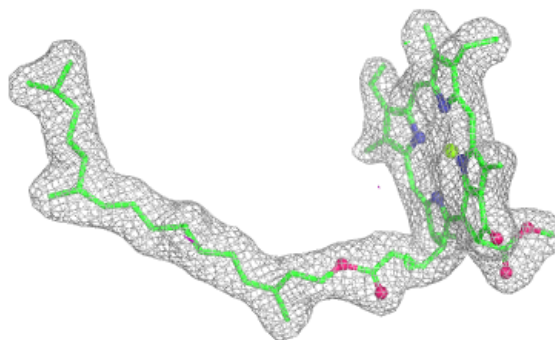


Electron density around BCR B 617:

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

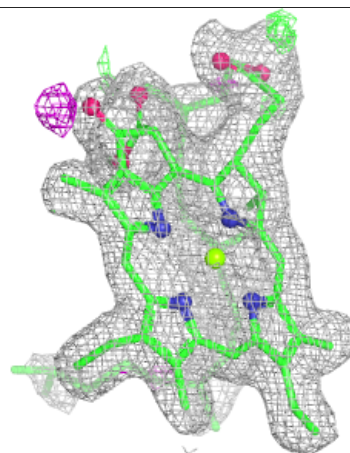
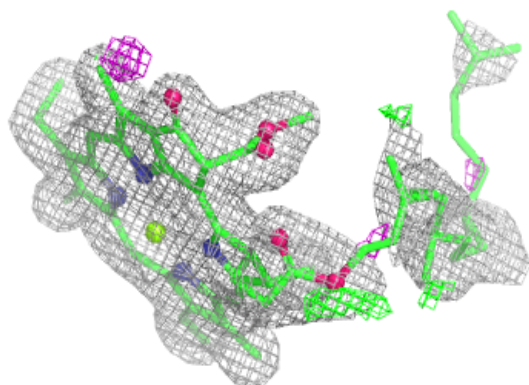
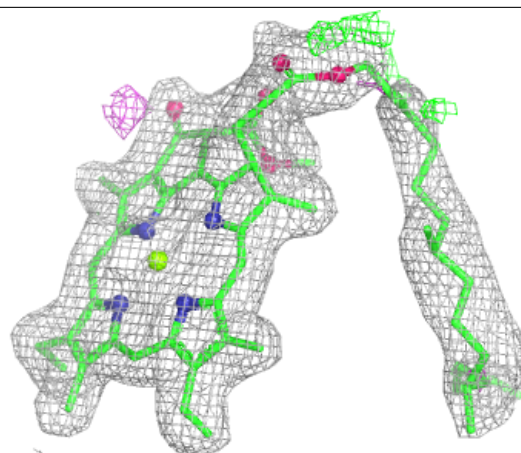
**Electron density around CLA b 612:**

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

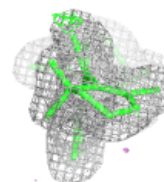
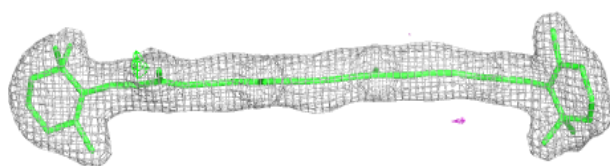
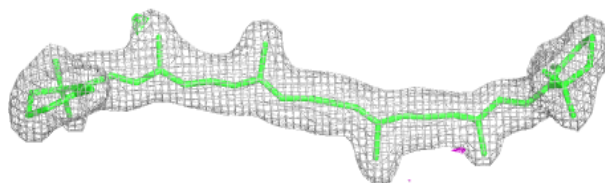


Electron density around CLA b 619:

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

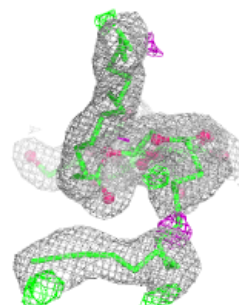
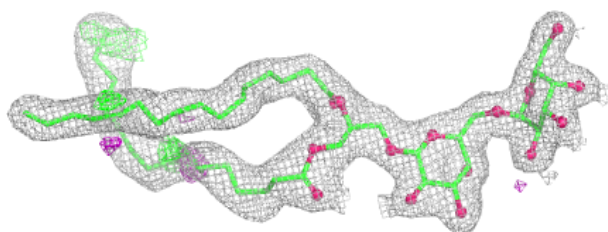
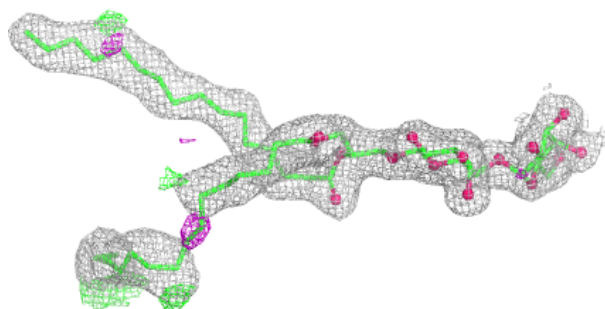
**Electron density around BCR C 514:**

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

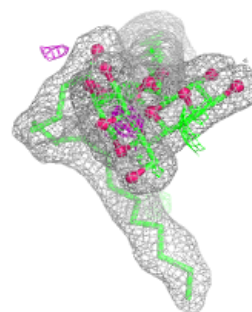
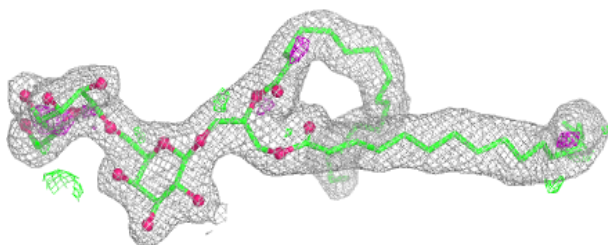
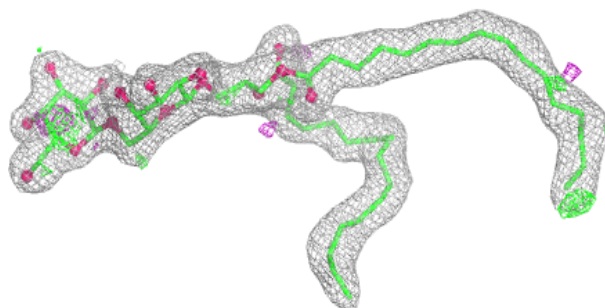


Electron density around DGD C 515:

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

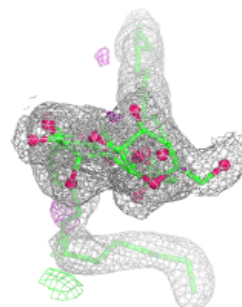
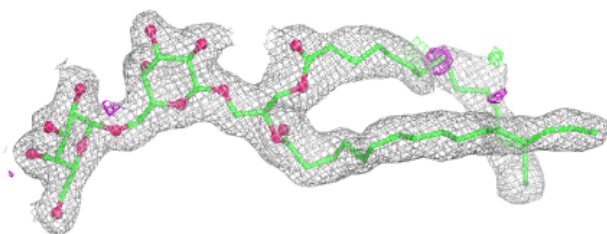
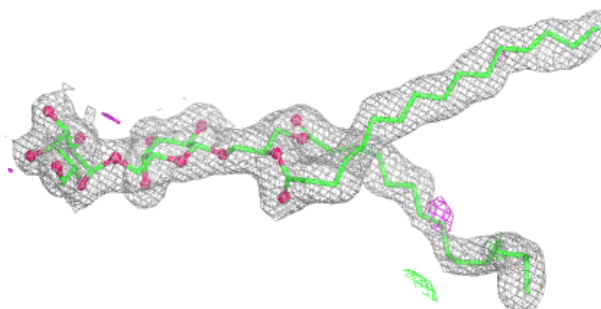
**Electron density around DGD H 102:**

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

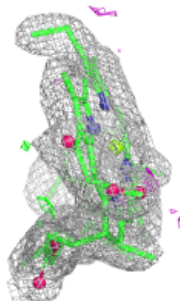
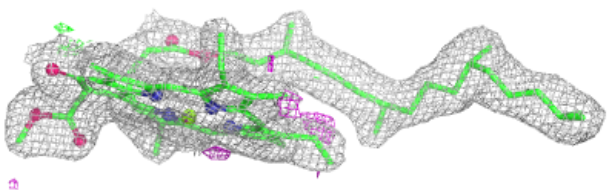
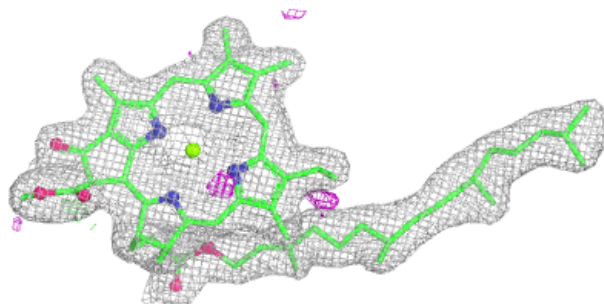


Electron density around DGD c 515:

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

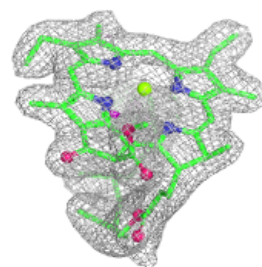
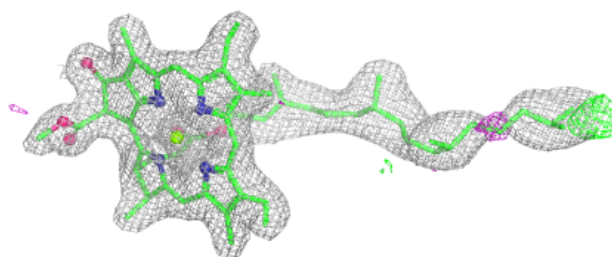
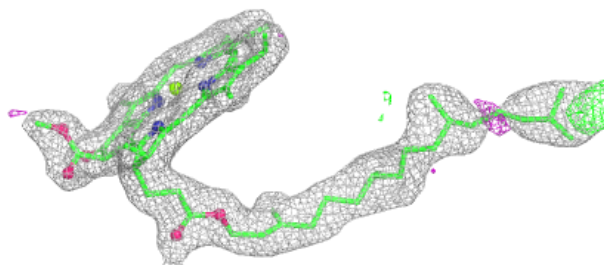
**Electron density around CLA c 501:**

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



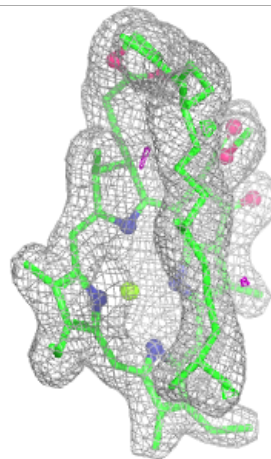
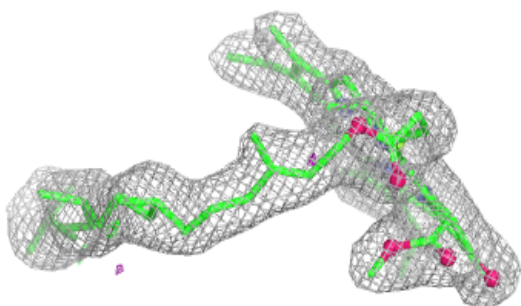
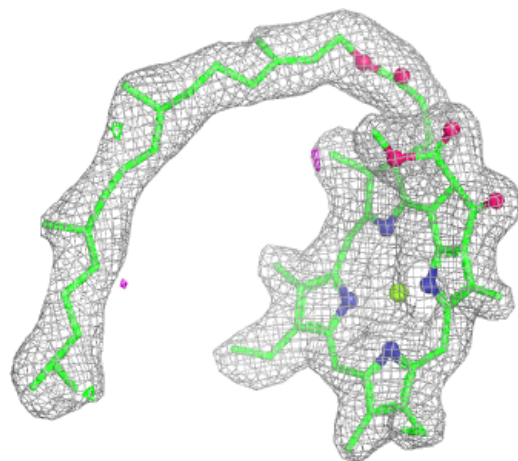
Electron density around CLA c 504:

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



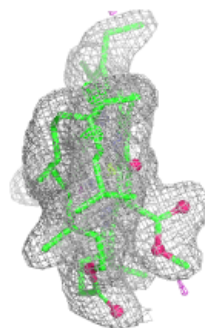
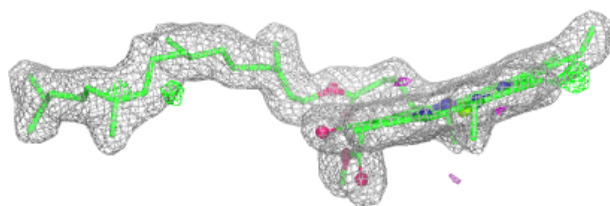
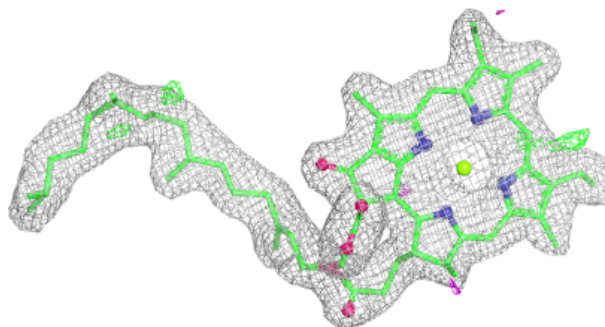
Electron density around CLA C 507:

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

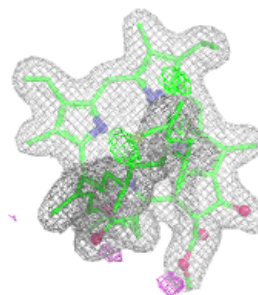
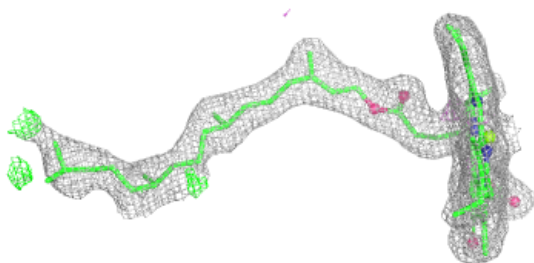
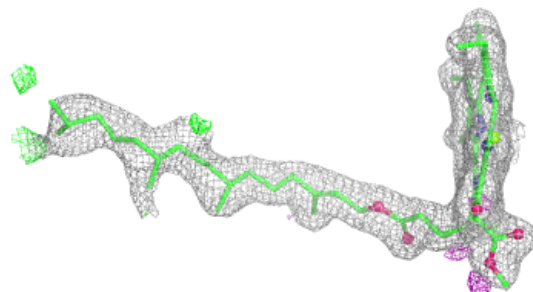


Electron density around CLA b 605:

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

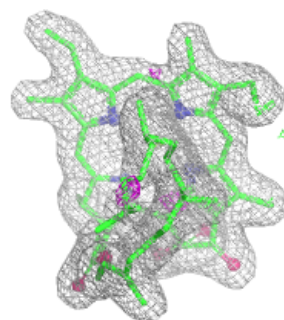
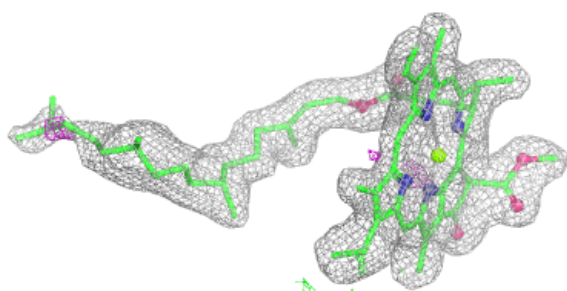
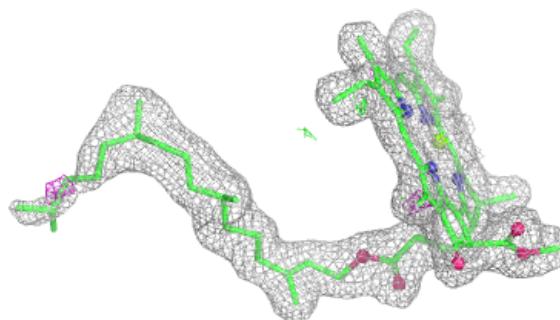
**Electron density around CLA b 609:**

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

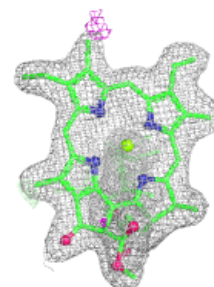
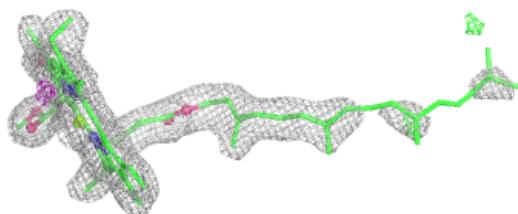
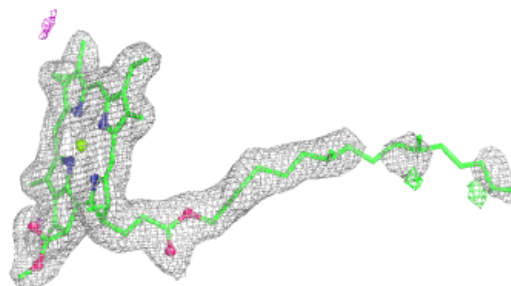


Electron density around CLA C 508:

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

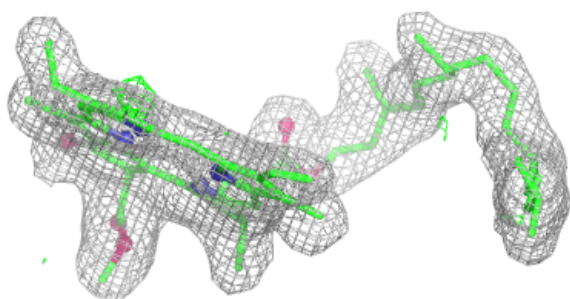
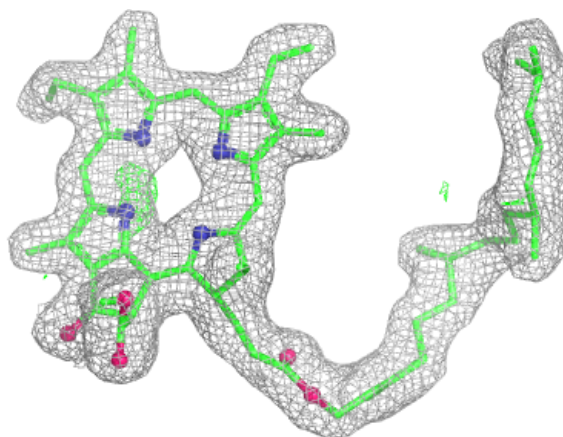
**Electron density around CLA d 403:**

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

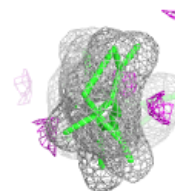
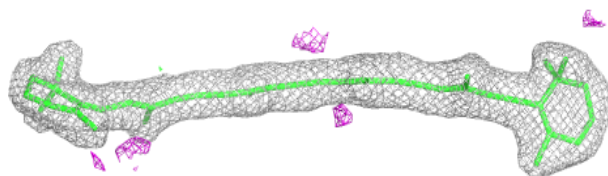
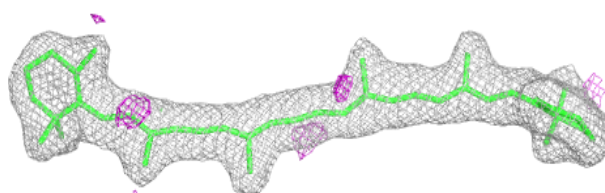


Electron density around PHO a 411:

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

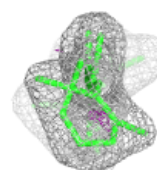
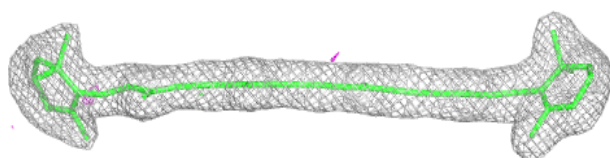
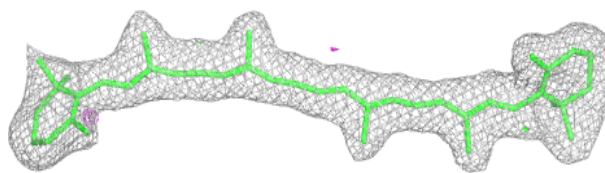
**Electron density around BCR b 620:**

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

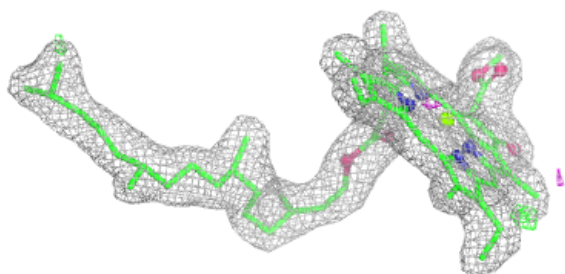
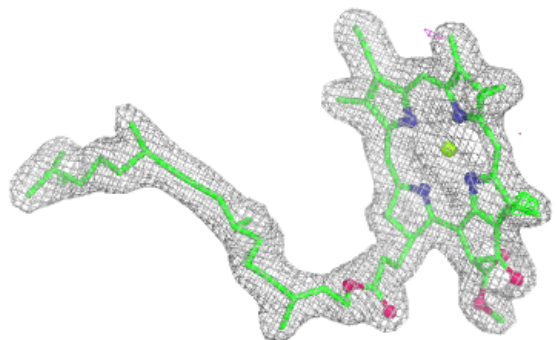


Electron density around BCR b 621:

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

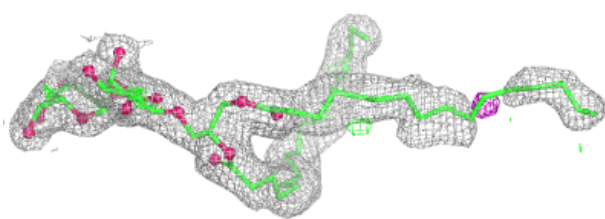
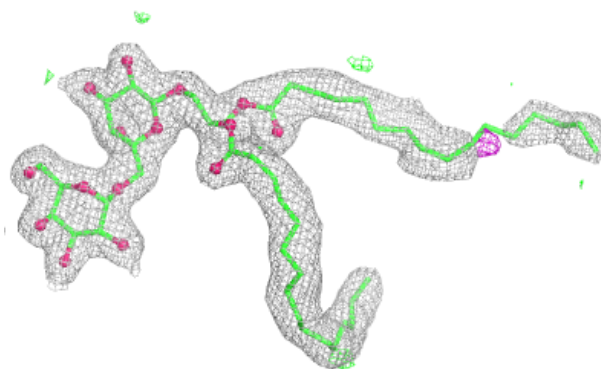
**Electron density around CLA C 511:**

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

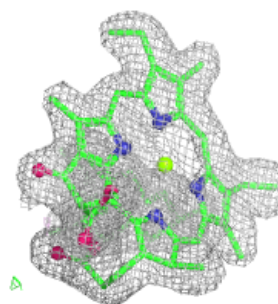
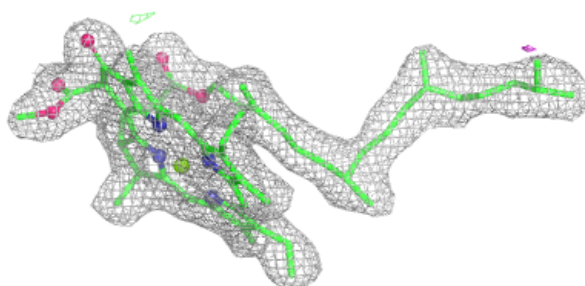
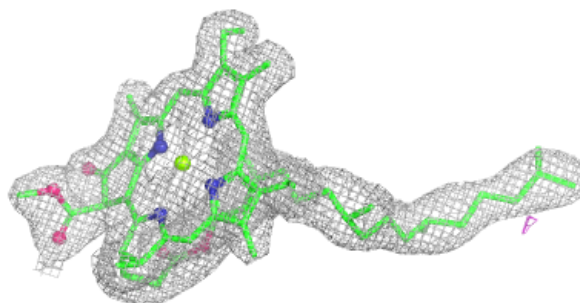


Electron density around DGD C 516:

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

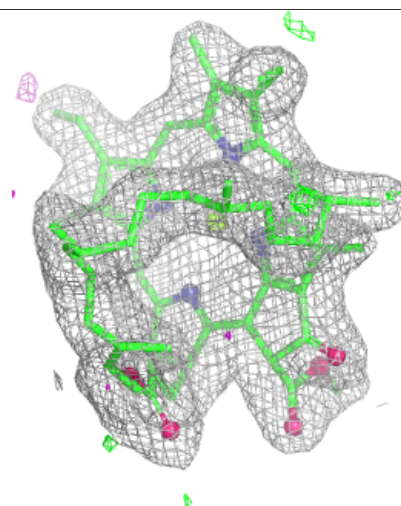
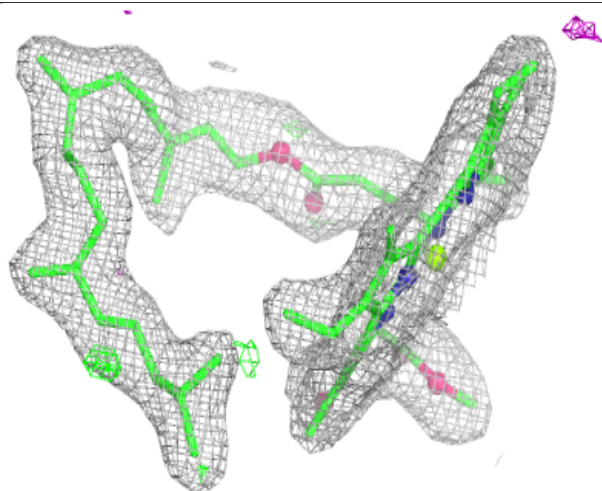
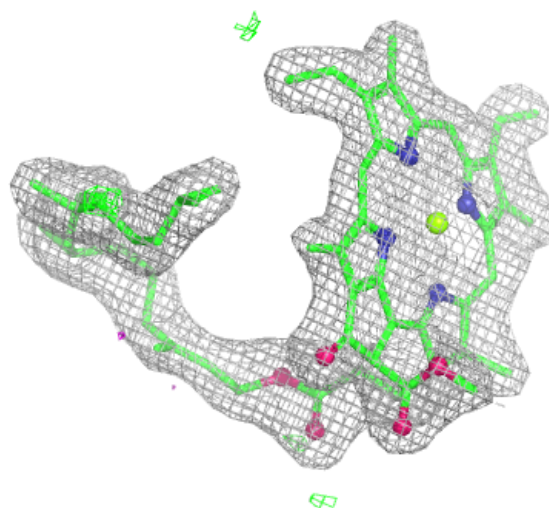
**Electron density around CLA C 505:**

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



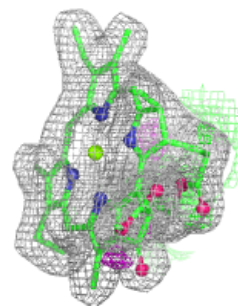
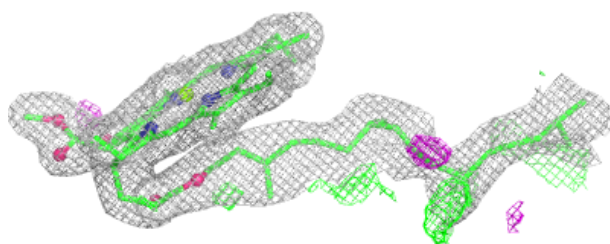
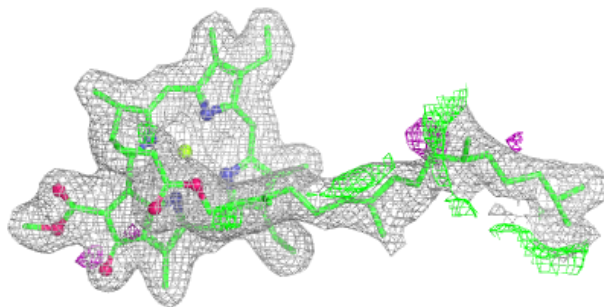
Electron density around CLA c 503:

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

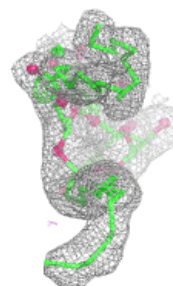
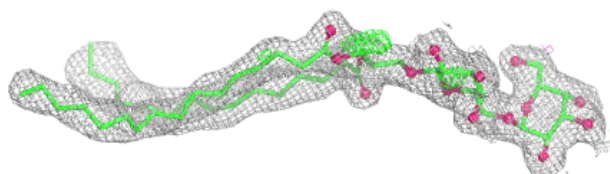
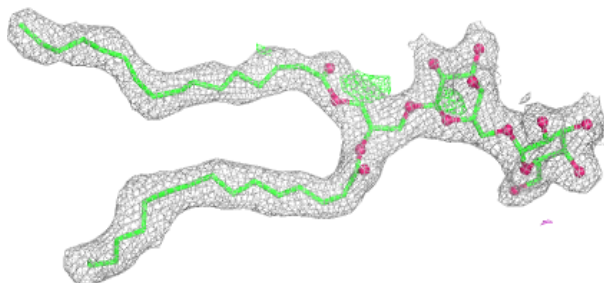


Electron density around CLA B 614:

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

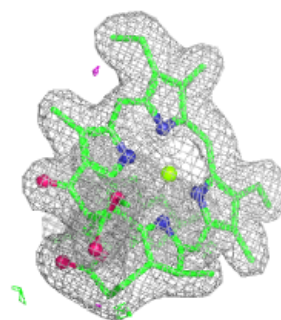
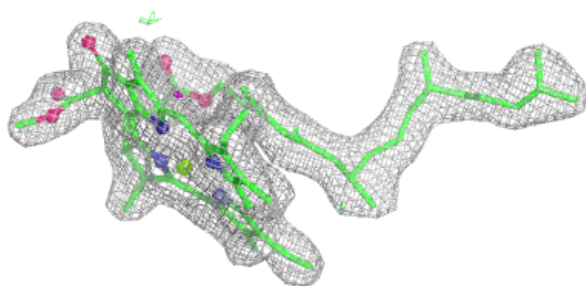
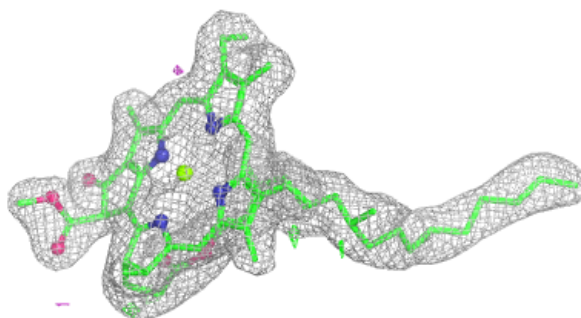
**Electron density around DGD c 517:**

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

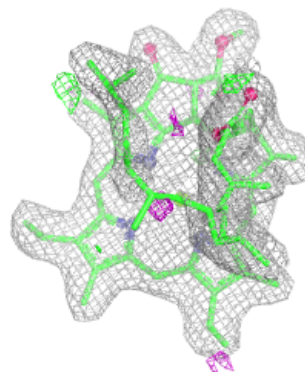
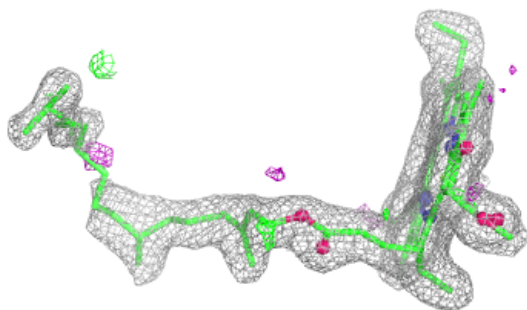
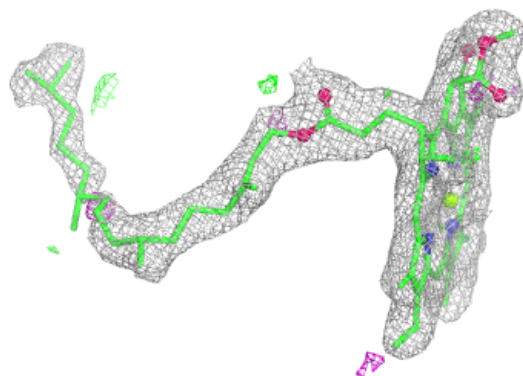


Electron density around CLA c 505:

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

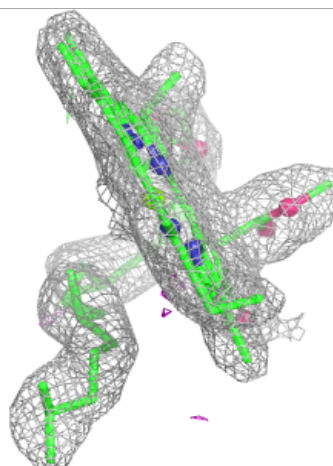
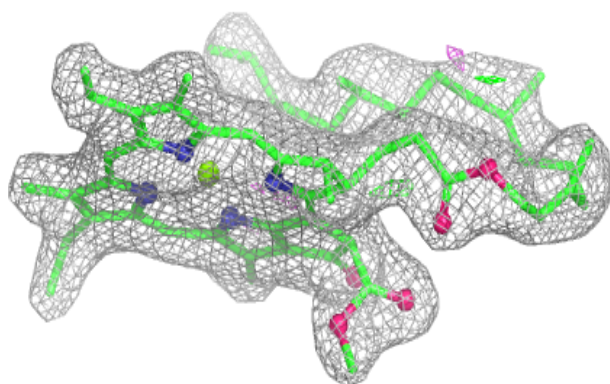
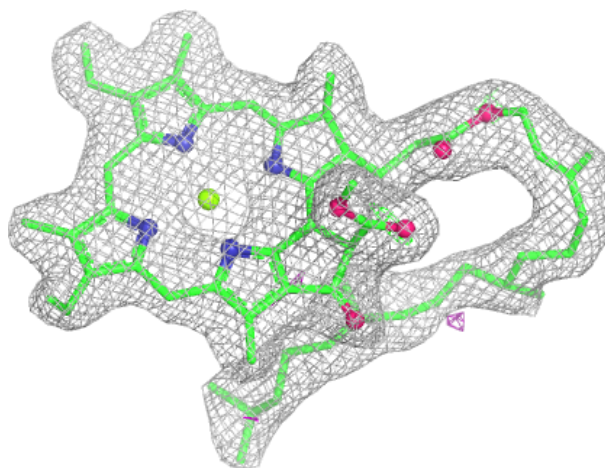
**Electron density around CLA D 405:**

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



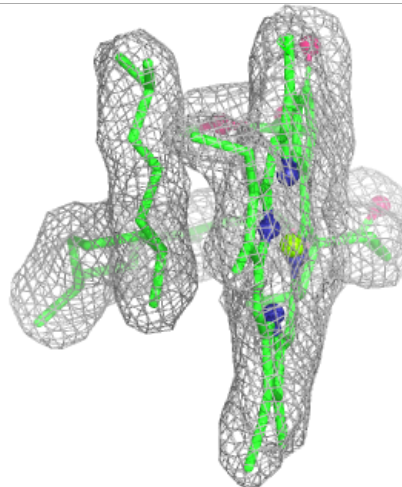
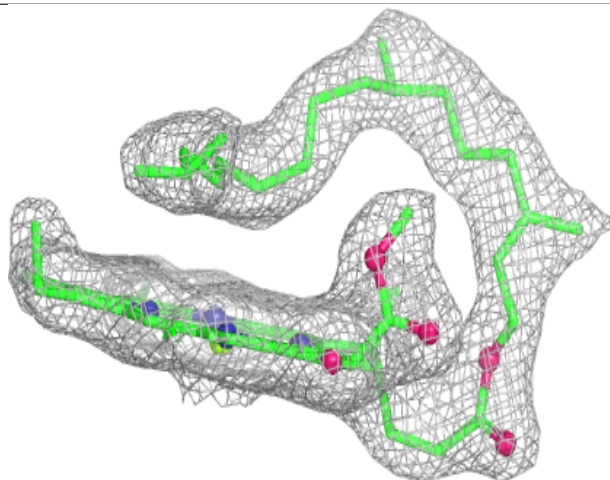
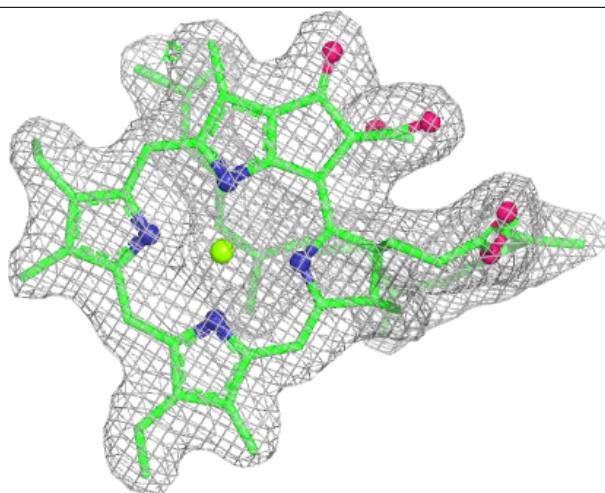
Electron density around CLA c 509:

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



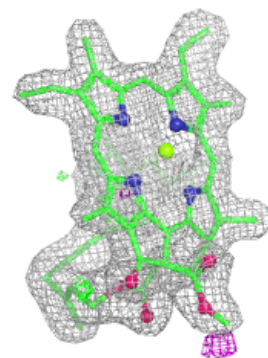
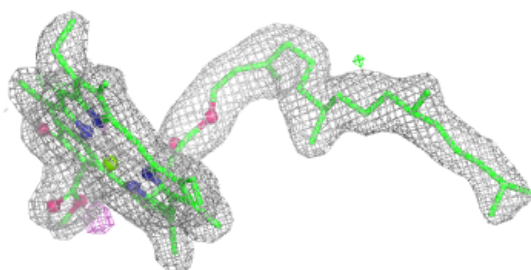
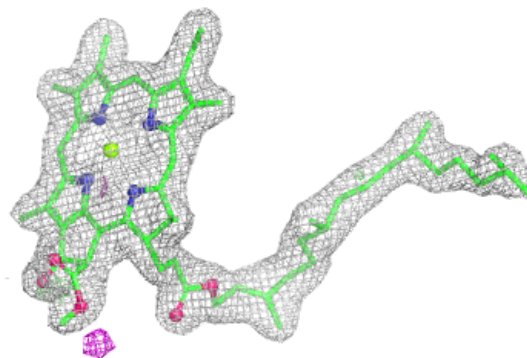
Electron density around CLA c 510:

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



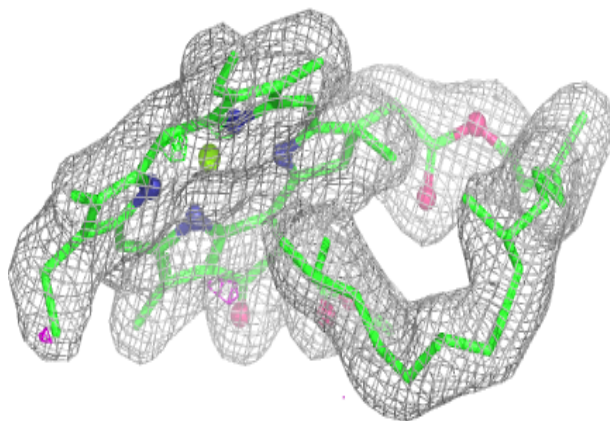
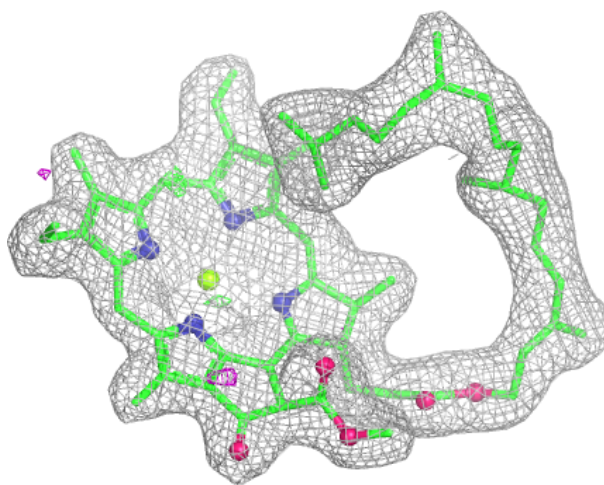
Electron density around CLA c 511:

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



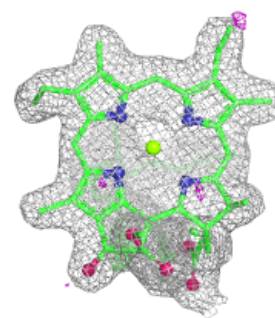
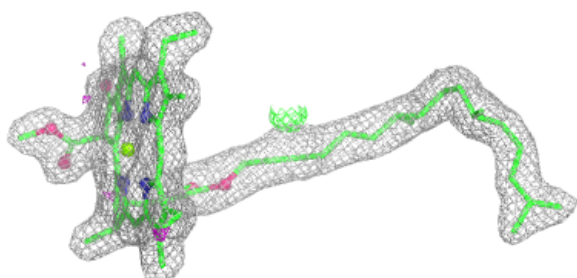
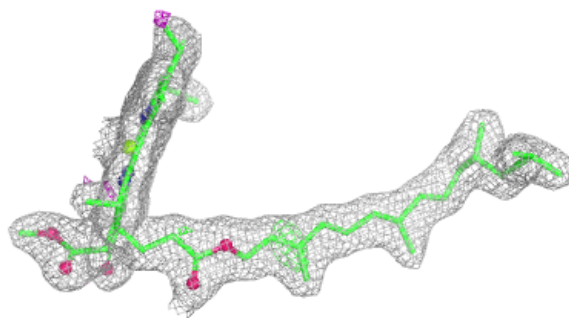
Electron density around CLA B 615:

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

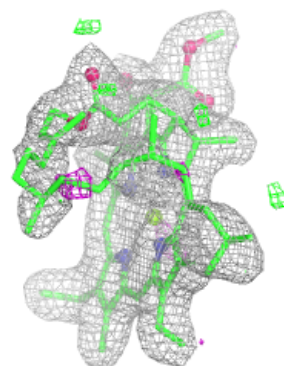
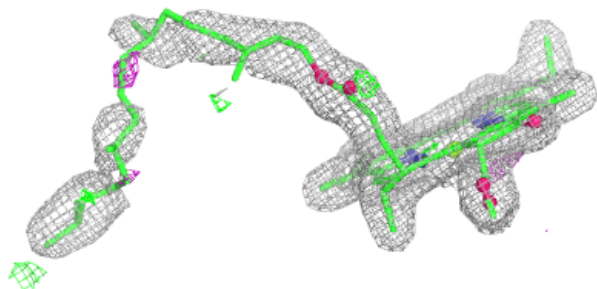
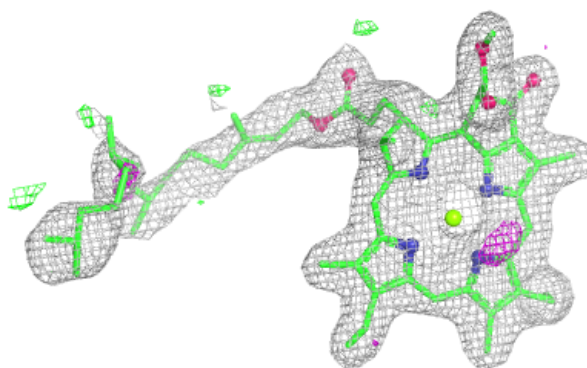


Electron density around CLA b 608:

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

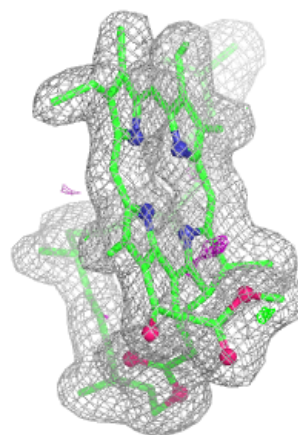
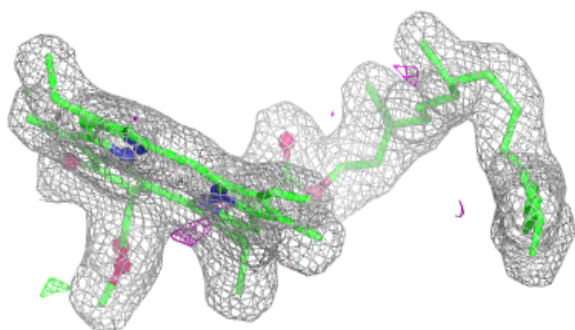
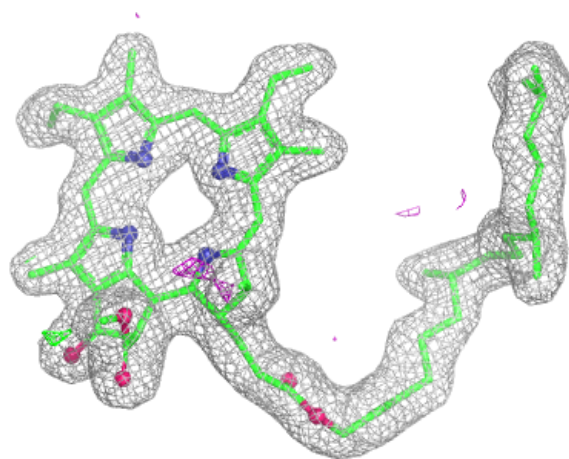
**Electron density around CLA A 1008:**

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



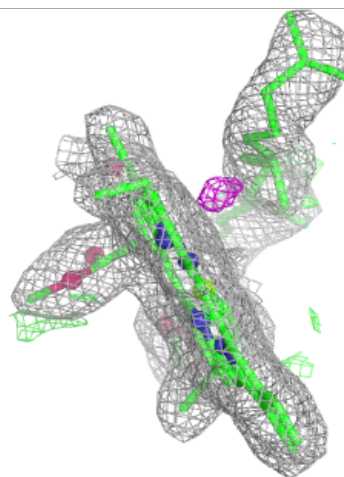
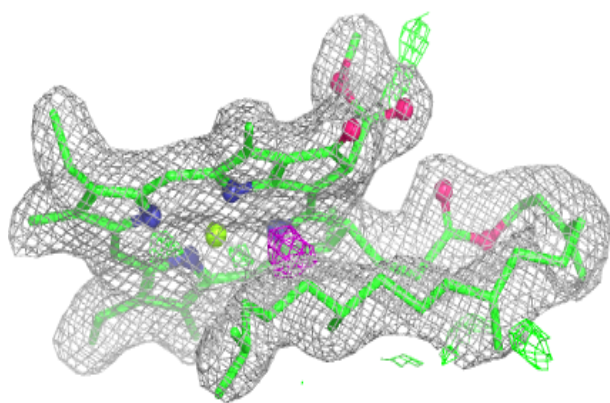
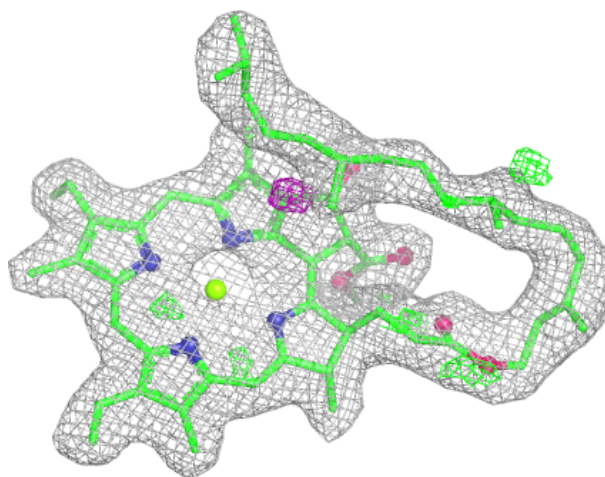
Electron density around PHO D 404:

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



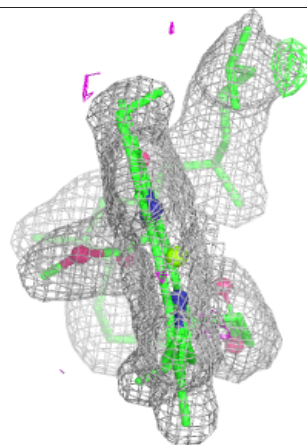
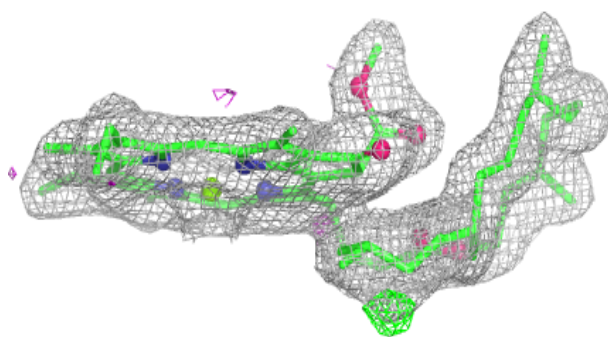
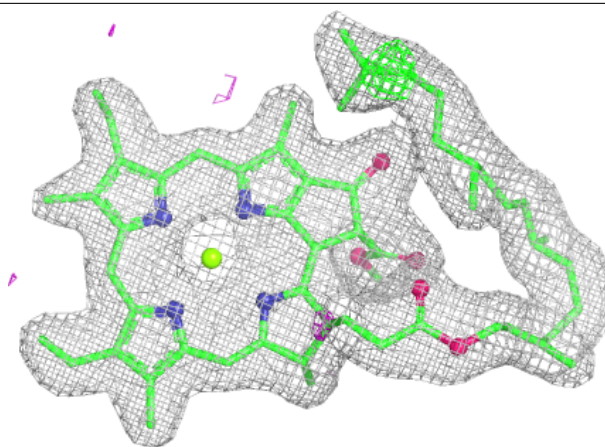
Electron density around CLA C 509:

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



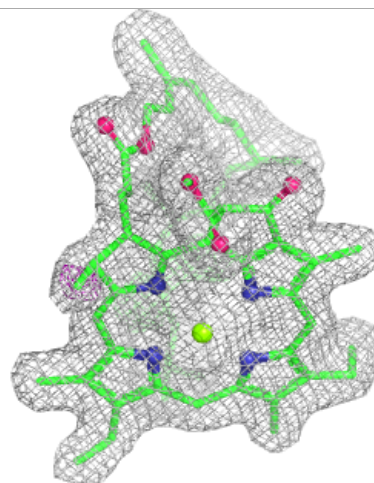
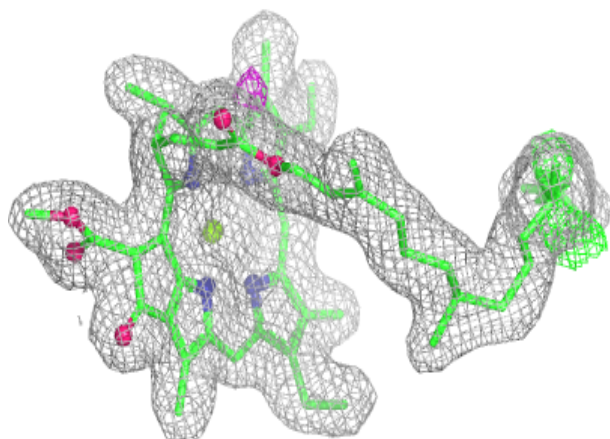
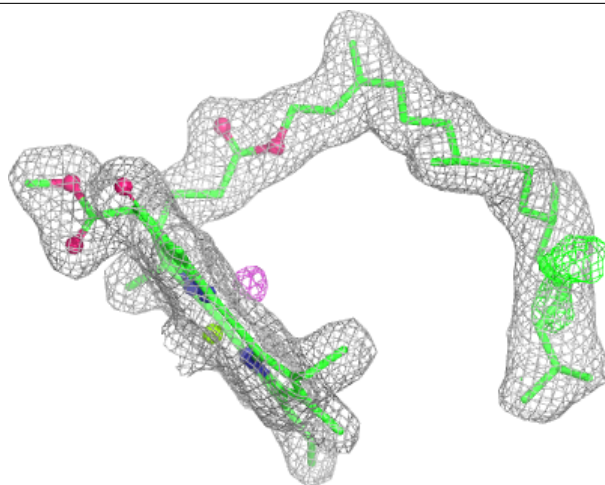
Electron density around CLA b 613:

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



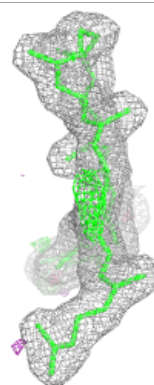
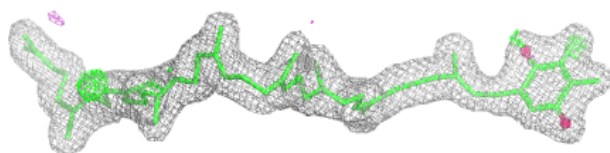
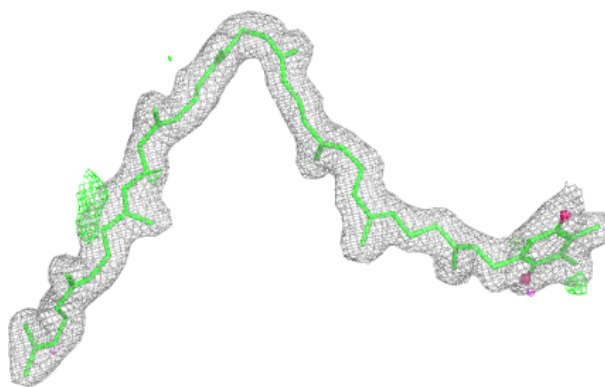
Electron density around CLA b 614:

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

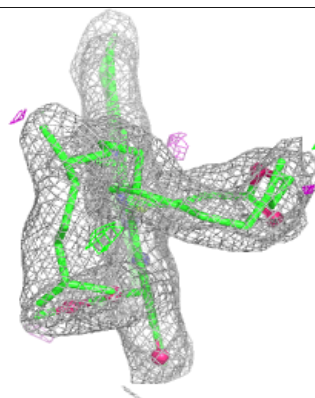
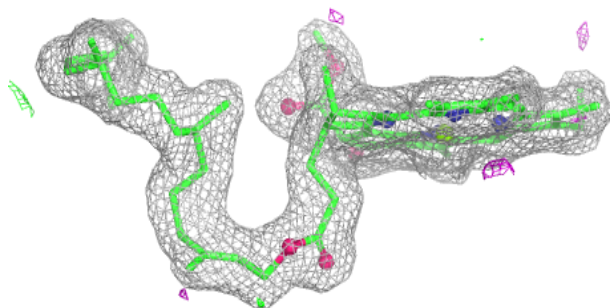
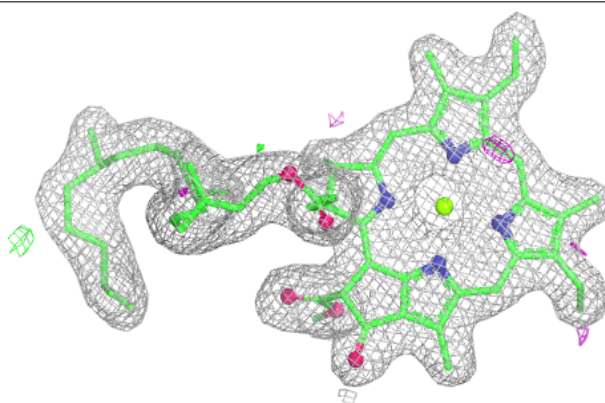


Electron density around PL9 D 407:

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

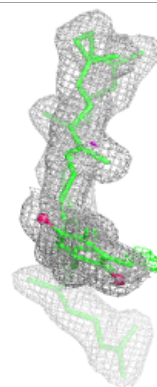
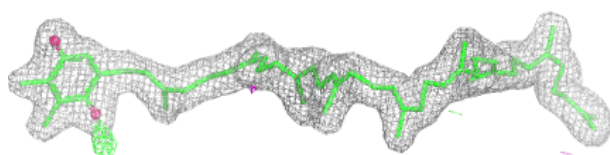
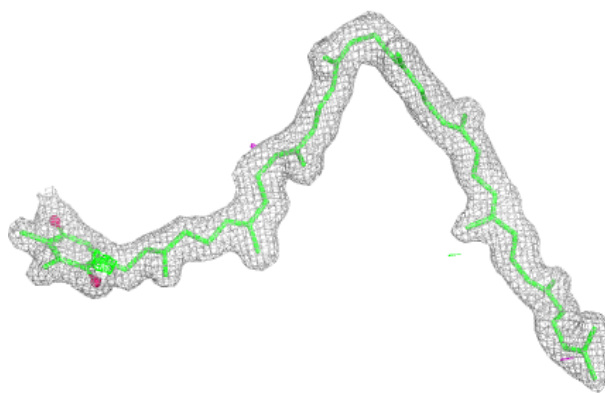
**Electron density around CLA b 615:**

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

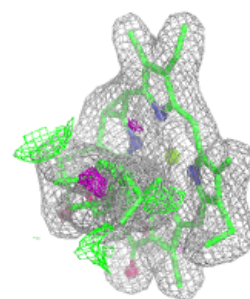
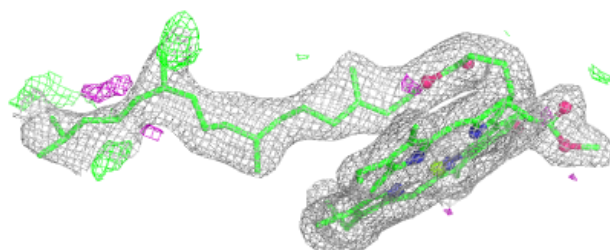
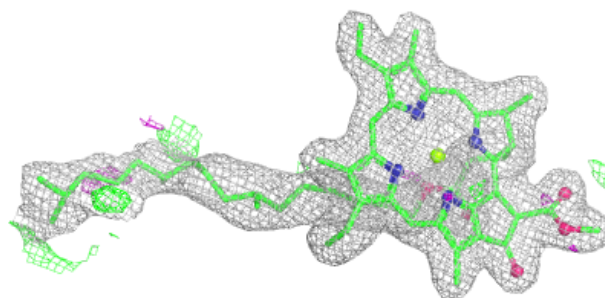


Electron density around PL9 d 405:

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

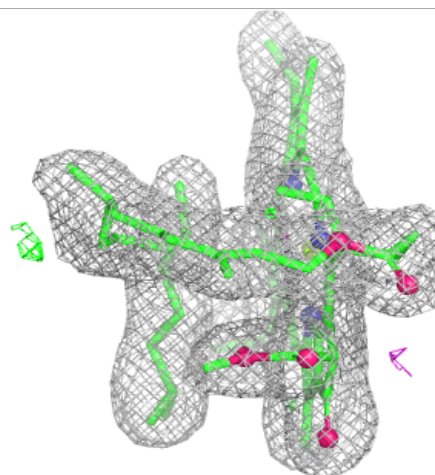
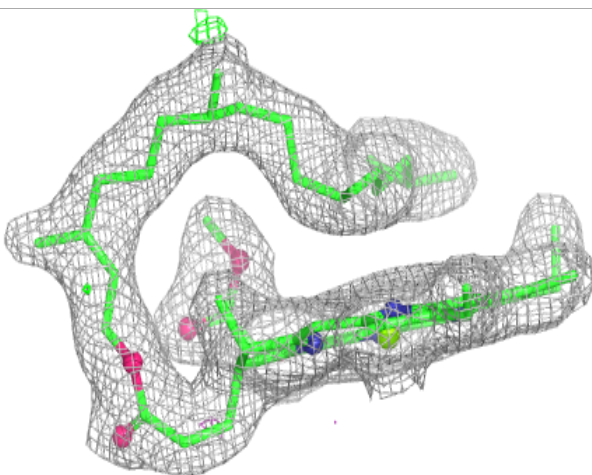
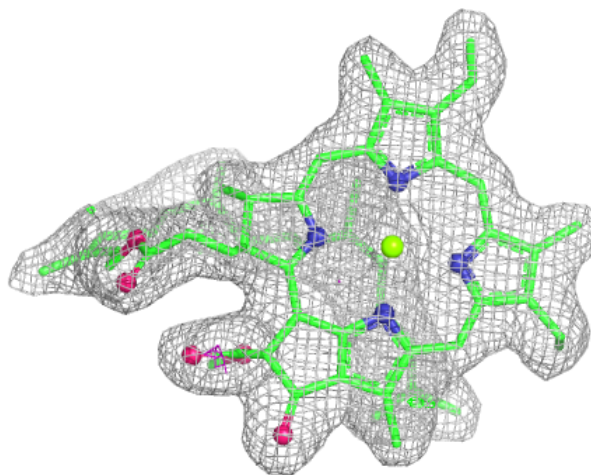
**Electron density around CLA b 617:**

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



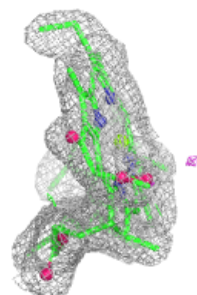
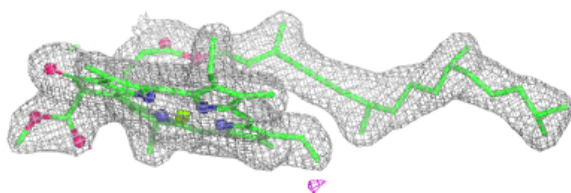
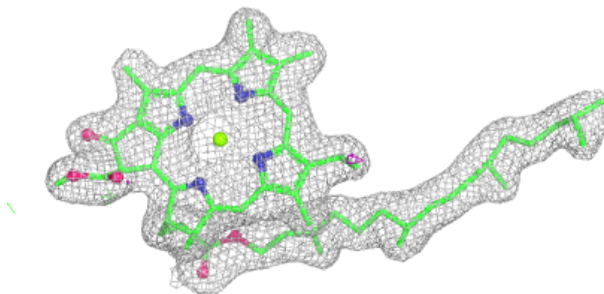
Electron density around CLA C 510:

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

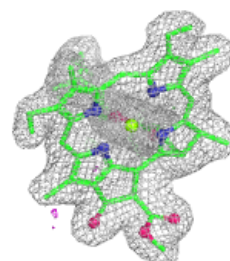
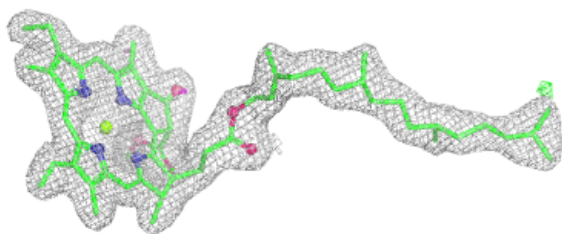
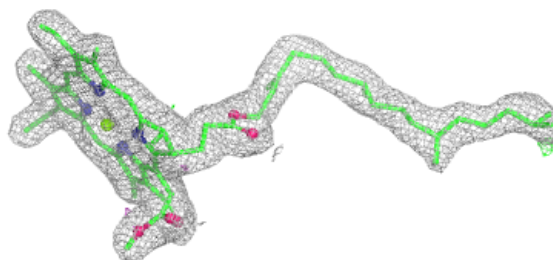


Electron density around CLA C 501:

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

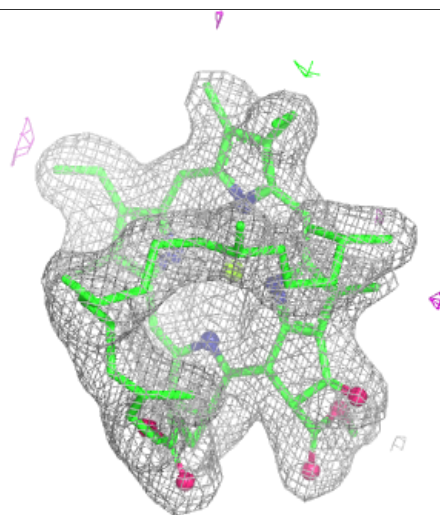
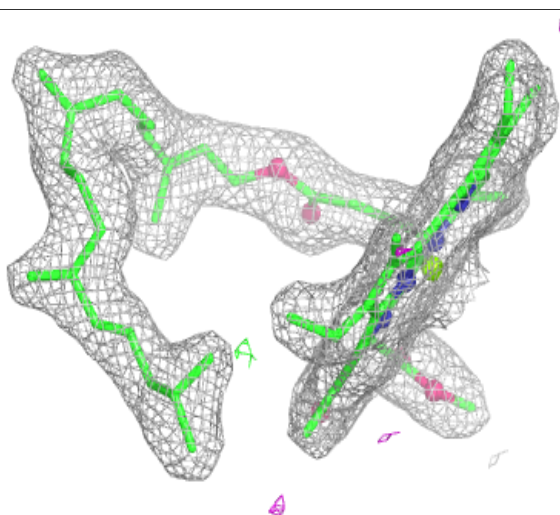
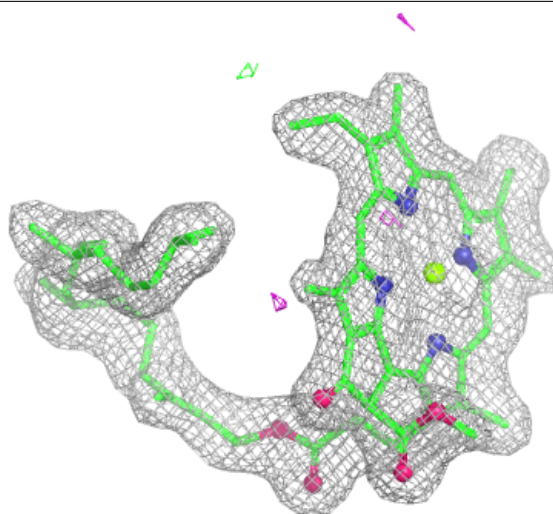
**Electron density around CLA c 502:**

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



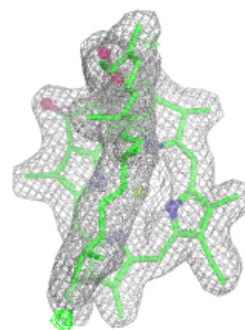
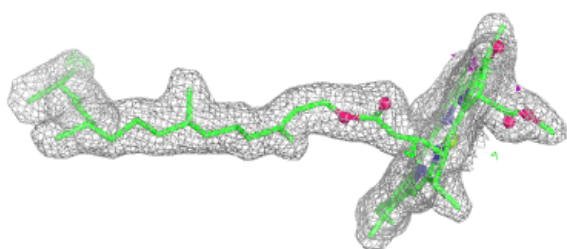
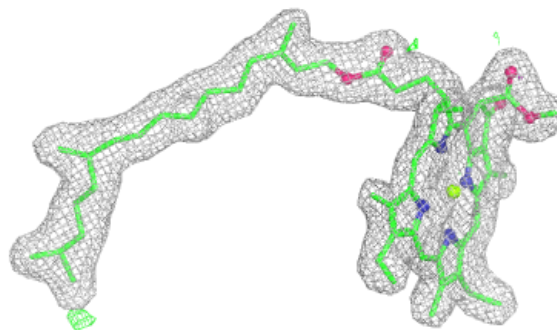
Electron density around CLA C 503:

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

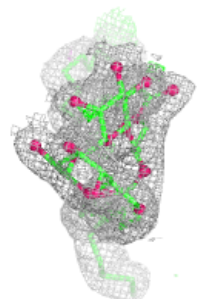
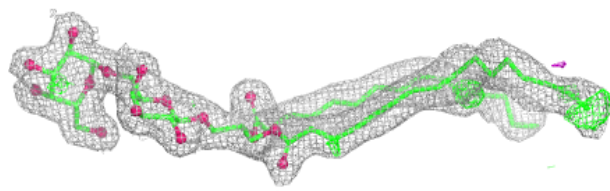
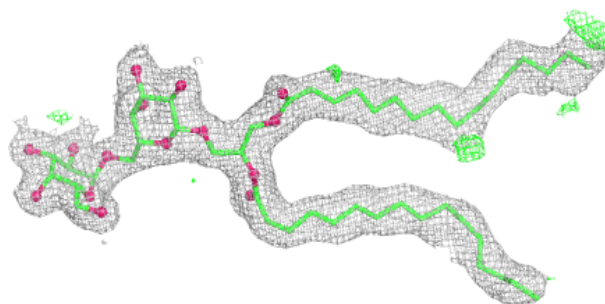


Electron density around CLA B 609:

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

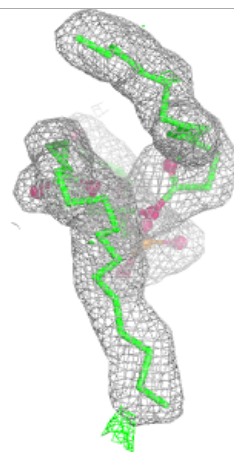
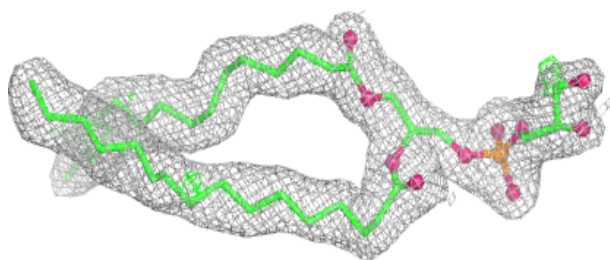
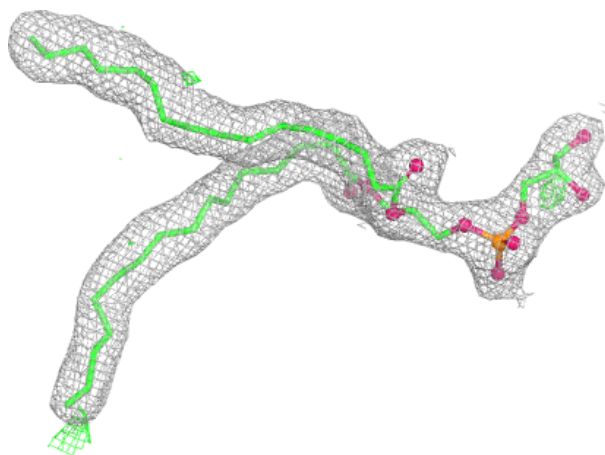
**Electron density around DGD C 517:**

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



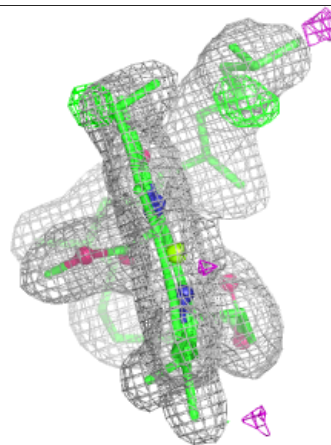
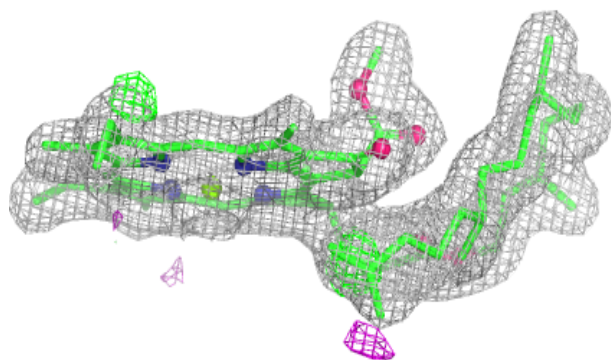
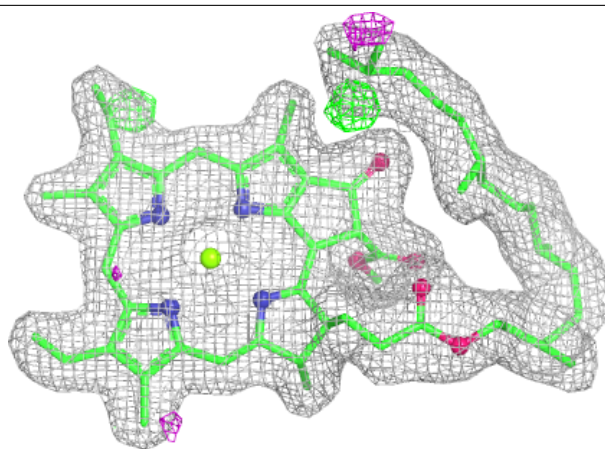
Electron density around LHG D 410:

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



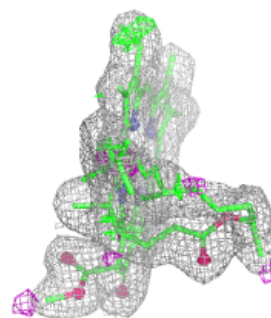
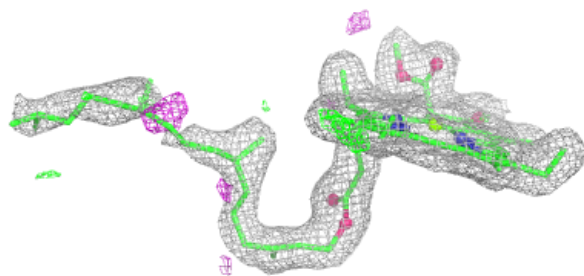
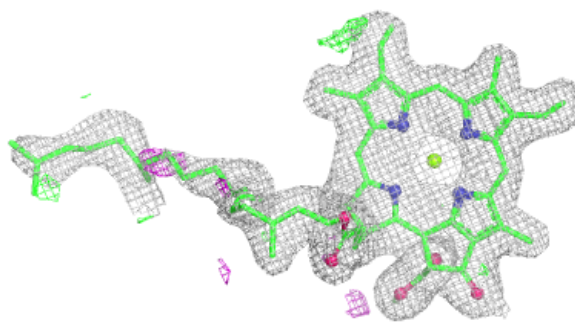
Electron density around CLA B 610:

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



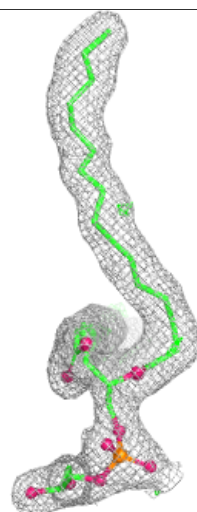
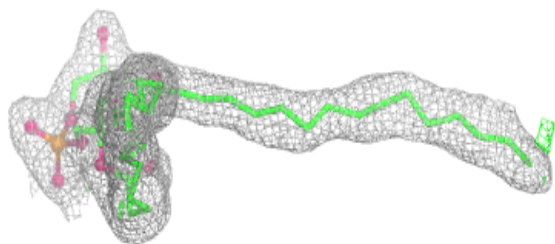
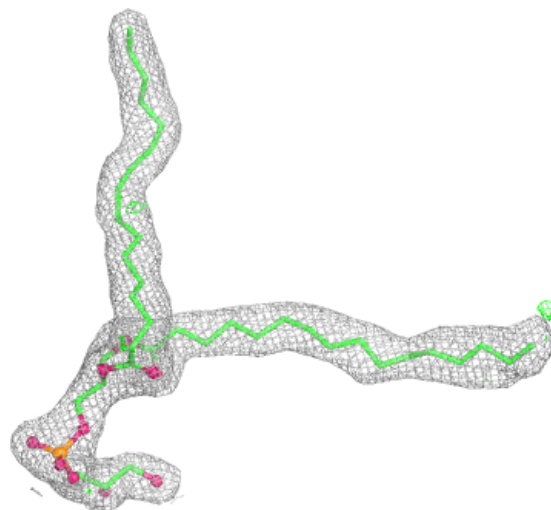
Electron density around CLA a 409:

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



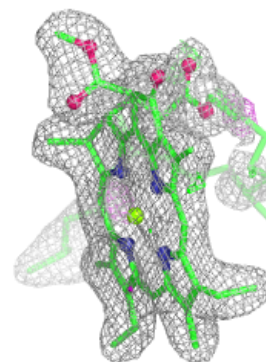
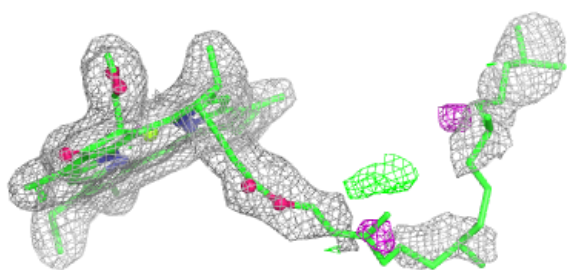
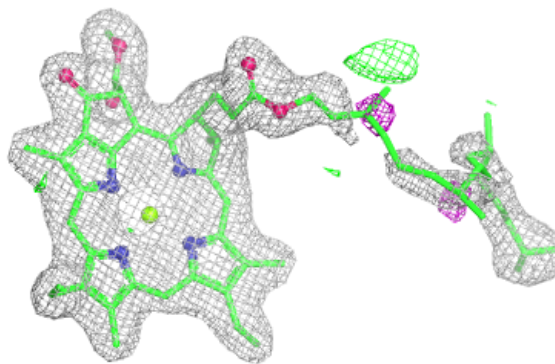
Electron density around LHG b 624:

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

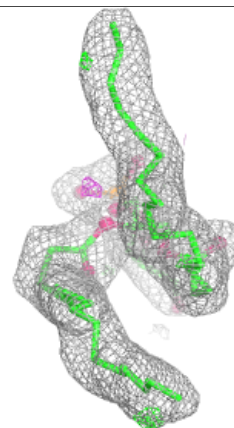
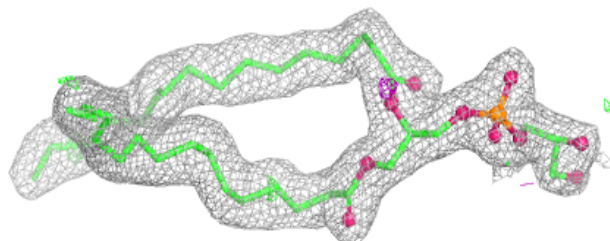
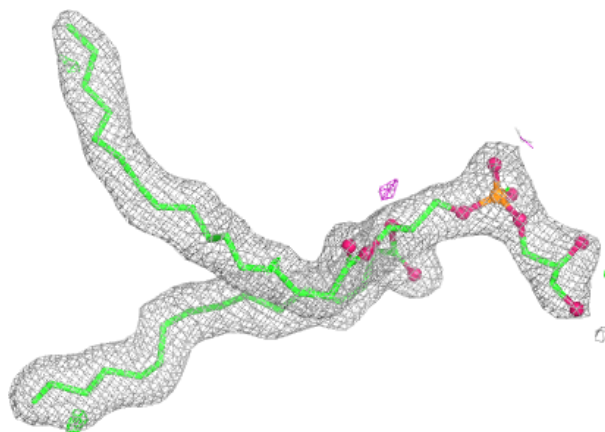


Electron density around CLA a 412:

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

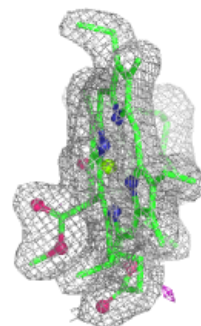
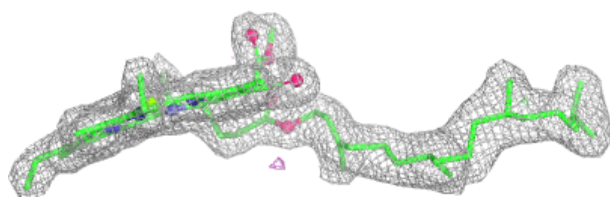
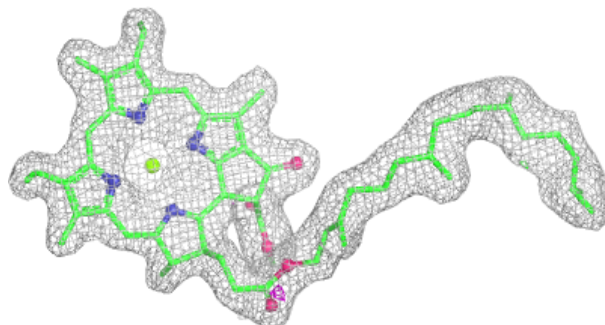
**Electron density around LHG d 407:**

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

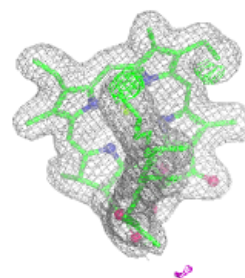
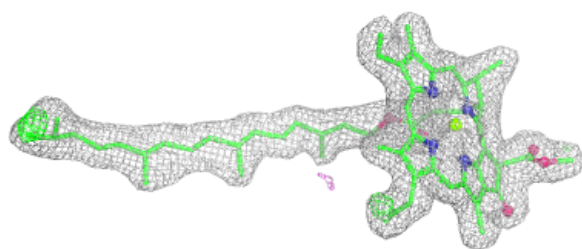
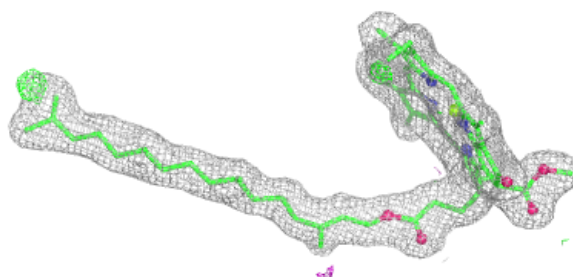


Electron density around CLA B 602:

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

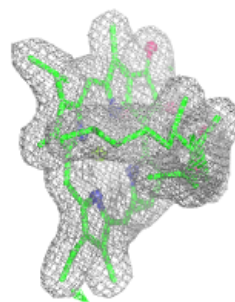
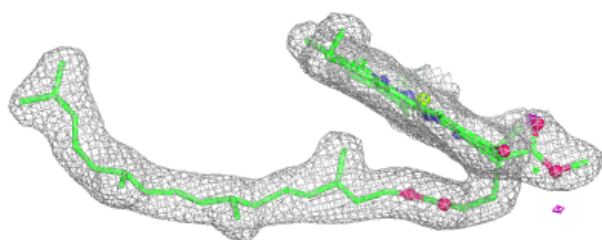
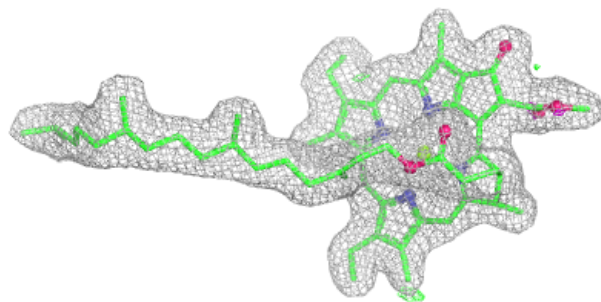
**Electron density around CLA b 610:**

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

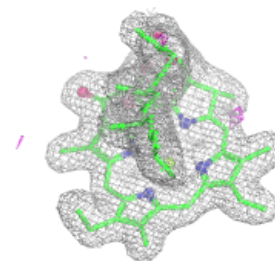
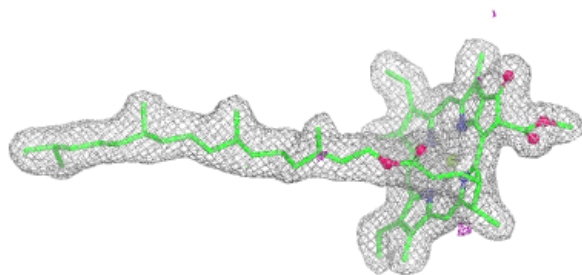
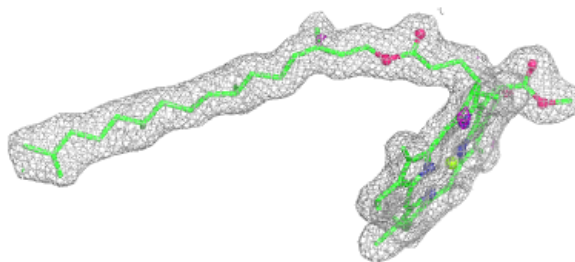


Electron density around CLA b 611:

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

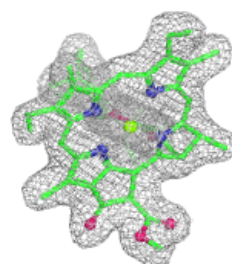
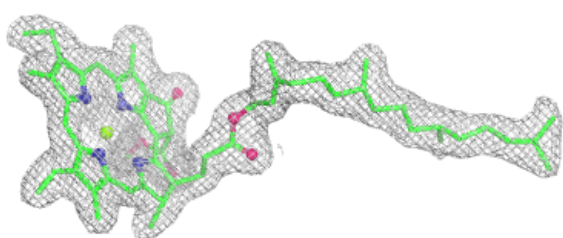
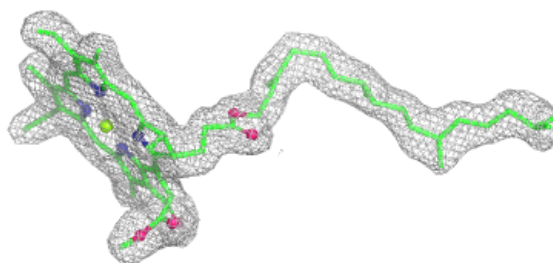
**Electron density around CLA B 607:**

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

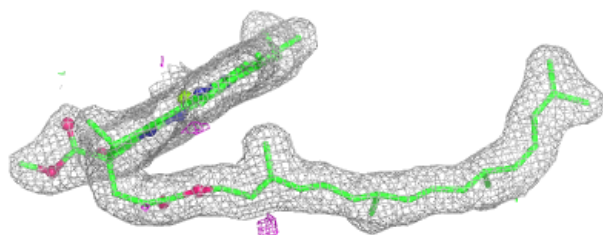
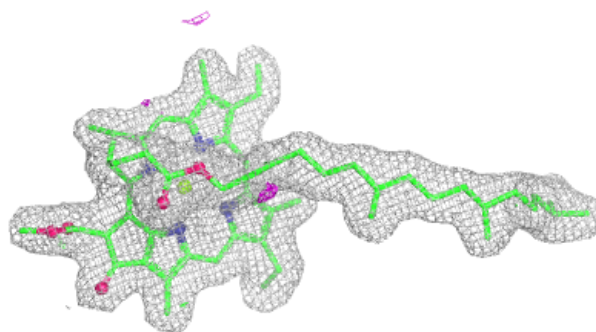


Electron density around CLA C 502:

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

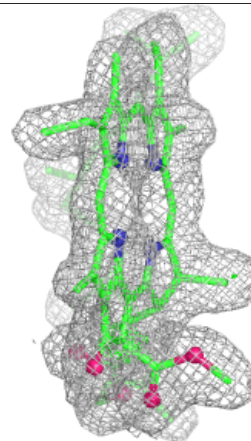
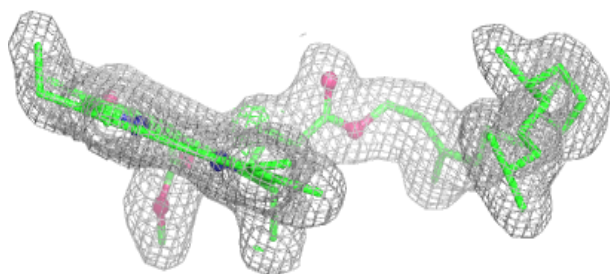
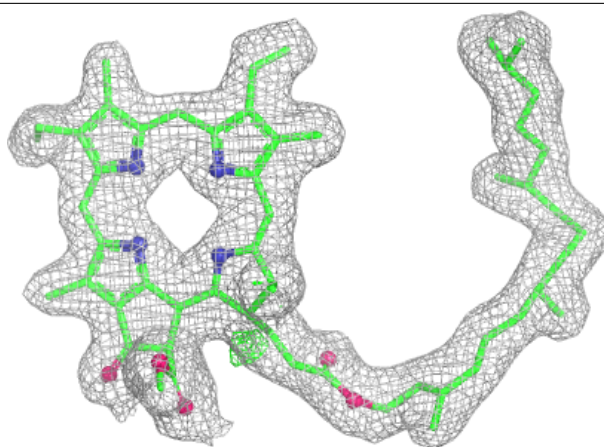
**Electron density around CLA B 608:**

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



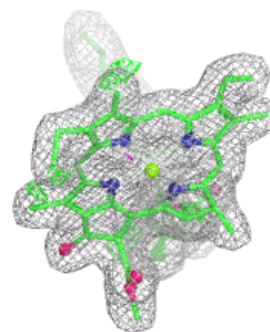
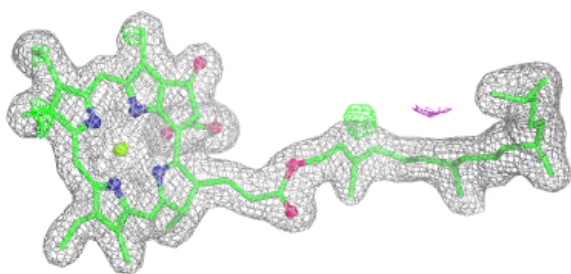
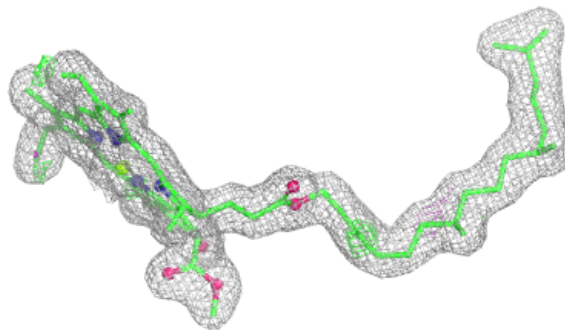
Electron density around PHO A 1007:

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



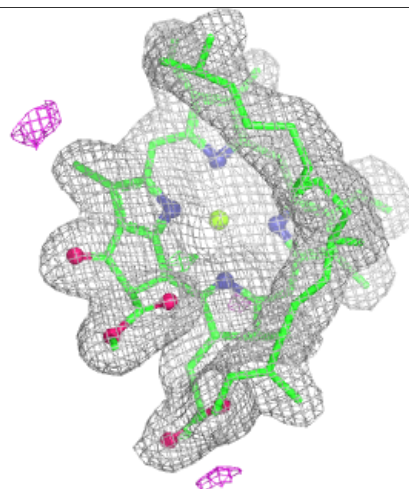
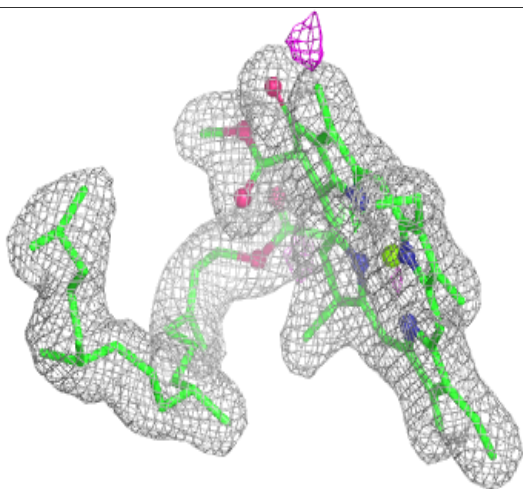
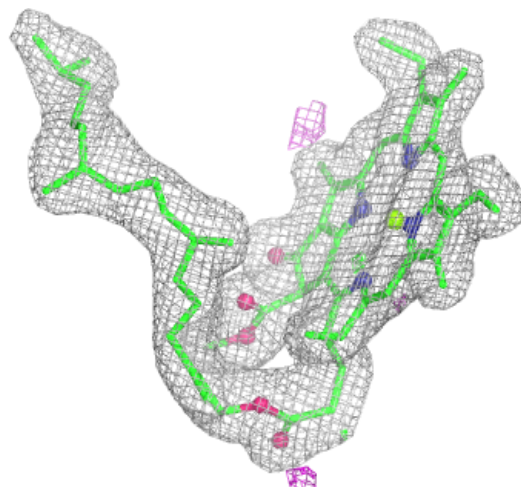
Electron density around CLA D 402:

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



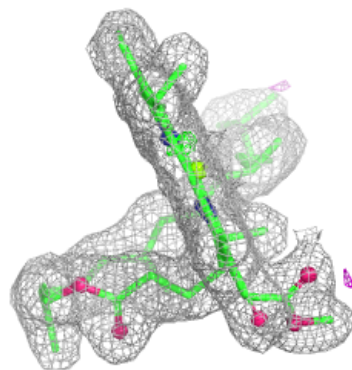
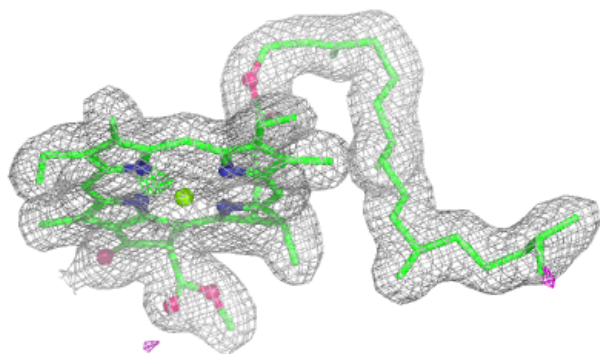
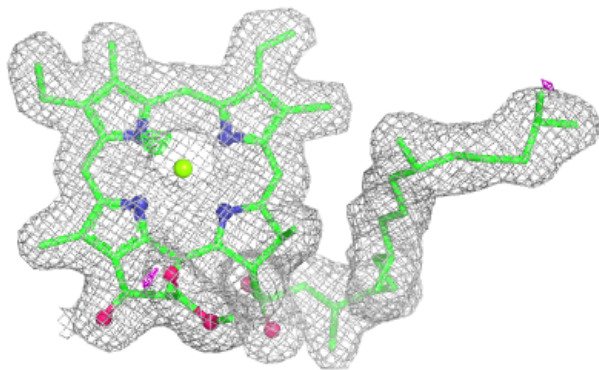
Electron density around CLA b 616:

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



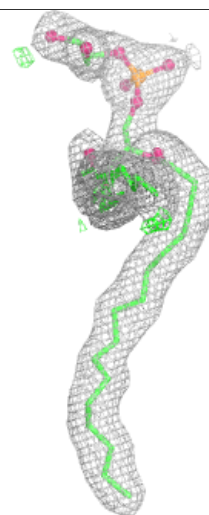
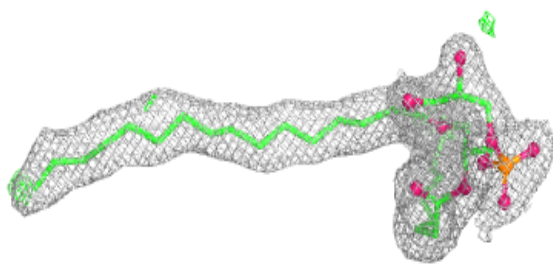
Electron density around CLA D 403:

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



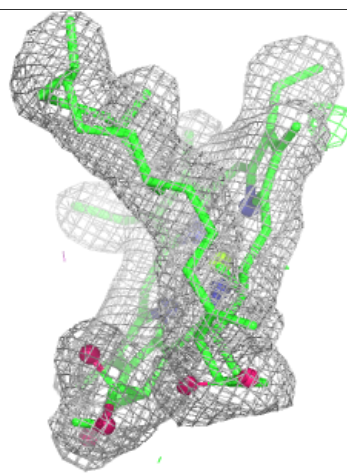
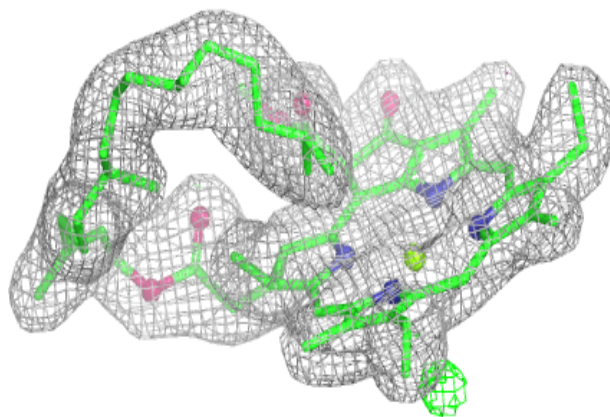
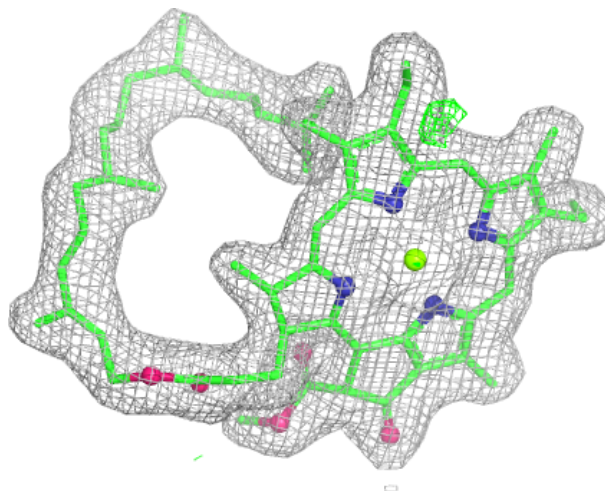
Electron density around LHG B 621:

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



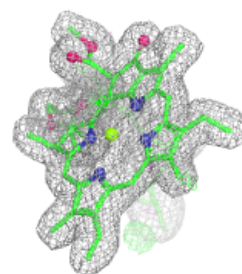
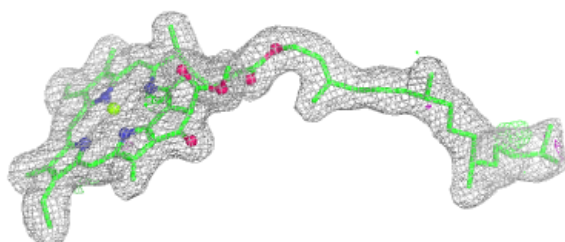
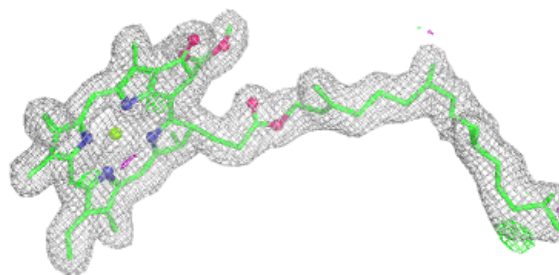
Electron density around CLA b 618:

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

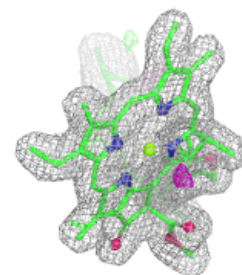
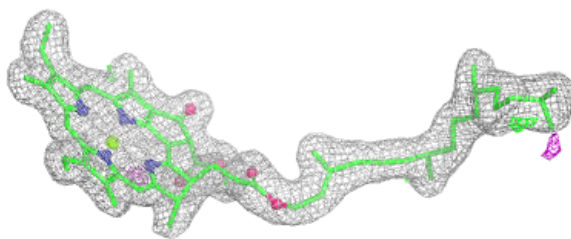
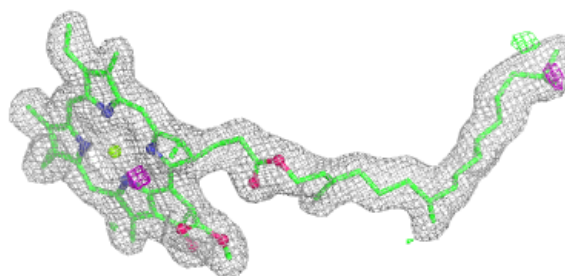


Electron density around CLA A 1005:

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

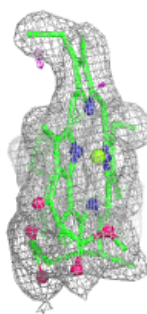
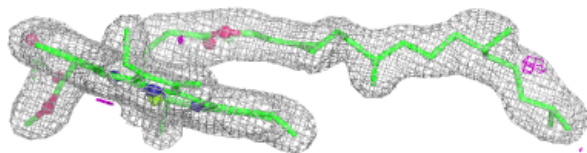
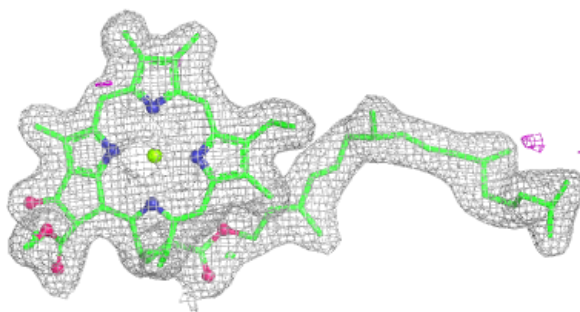
**Electron density around CLA a 407:**

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



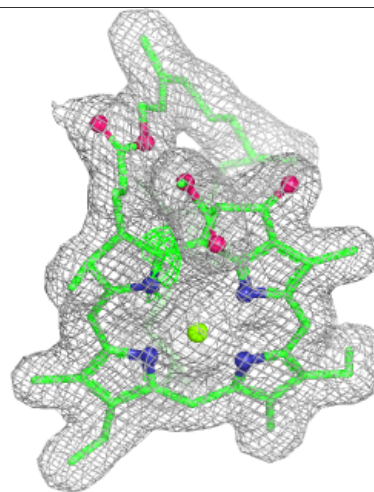
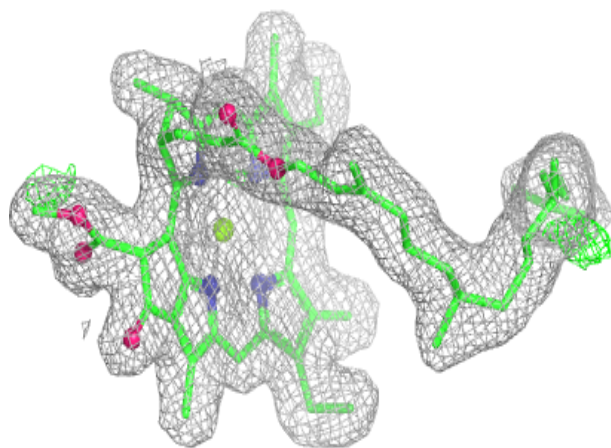
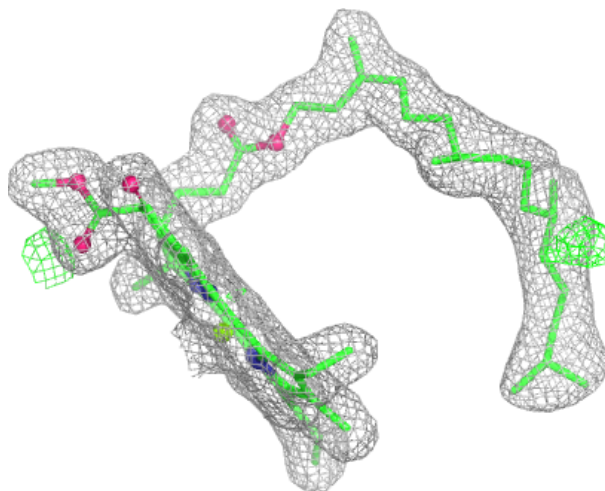
Electron density around CLA B 603:

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



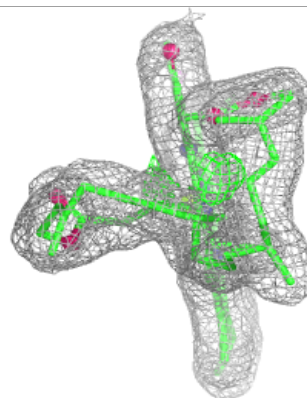
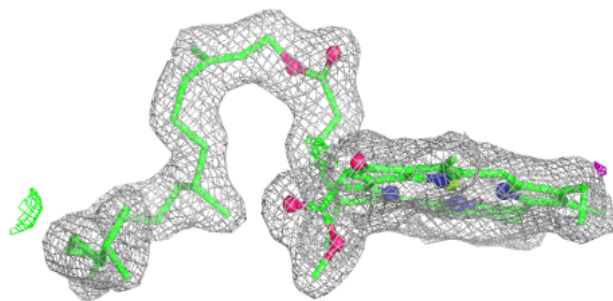
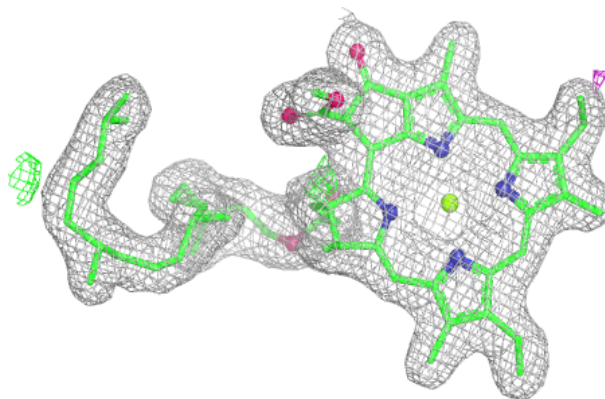
Electron density around CLA B 611:

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

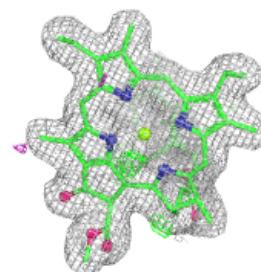
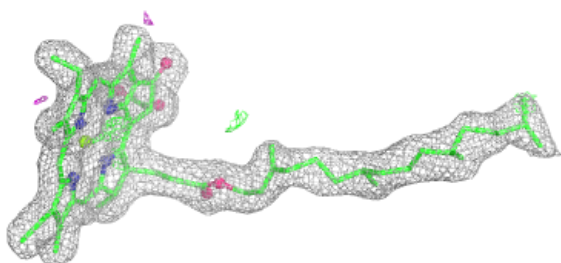
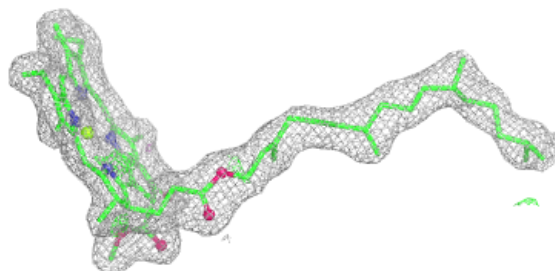


Electron density around CLA B 612:

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

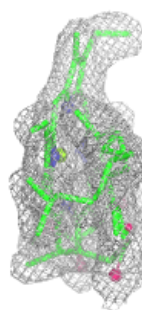
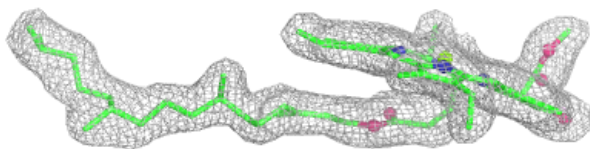
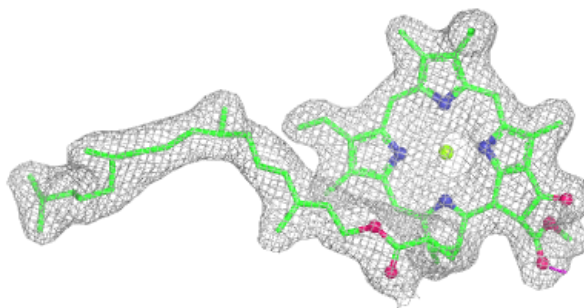
**Electron density around CLA B 604:**

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

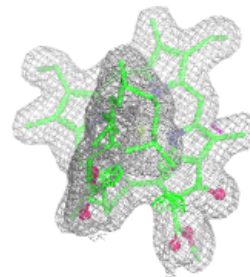
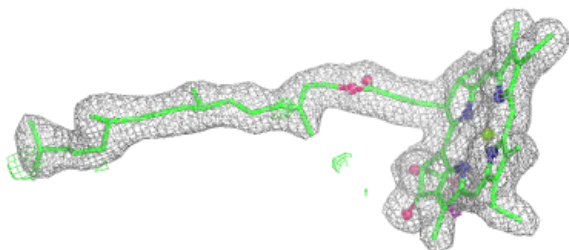
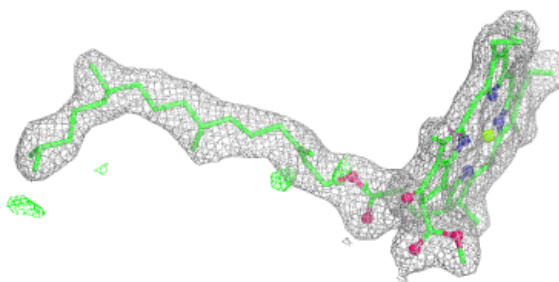


Electron density around CLA b 606:

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

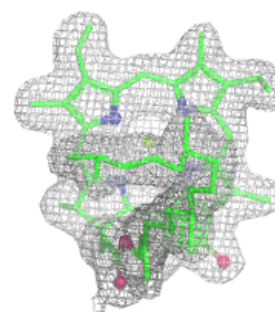
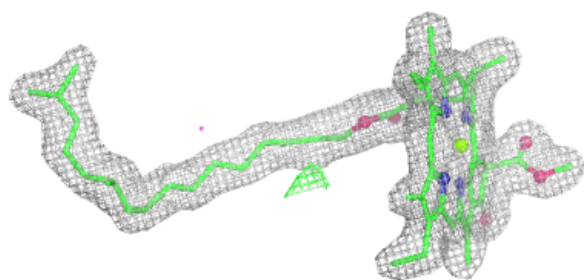
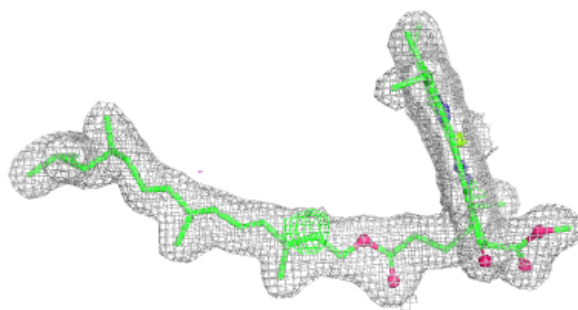
**Electron density around CLA b 607:**

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



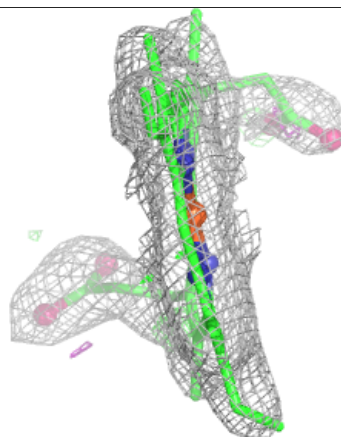
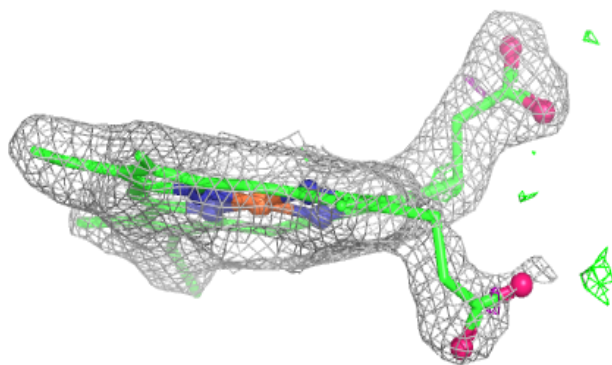
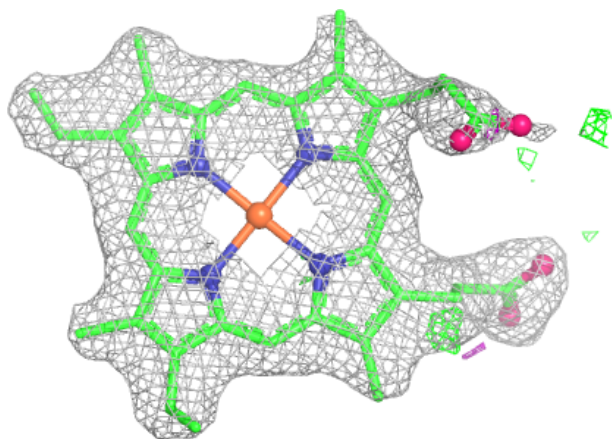
Electron density around CLA B 605:

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



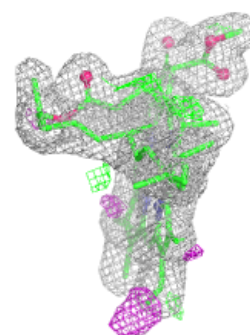
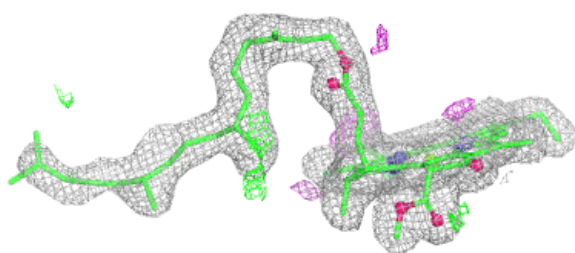
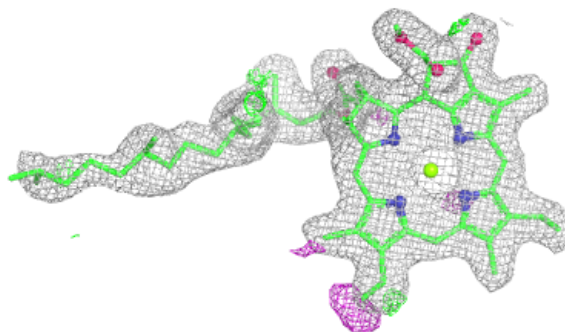
Electron density around HEM f 101:

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

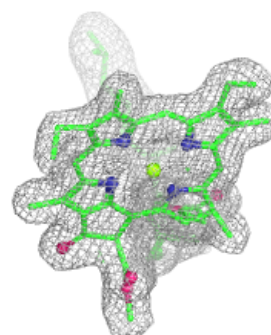
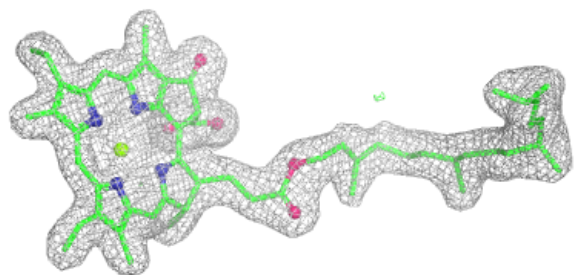
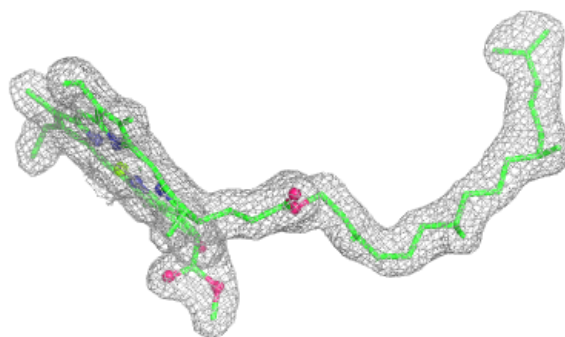


Electron density around CLA A 1006:

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

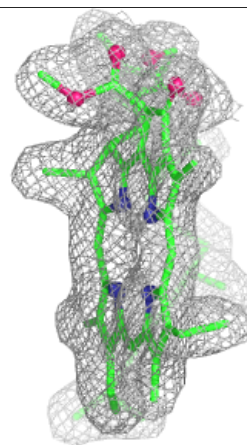
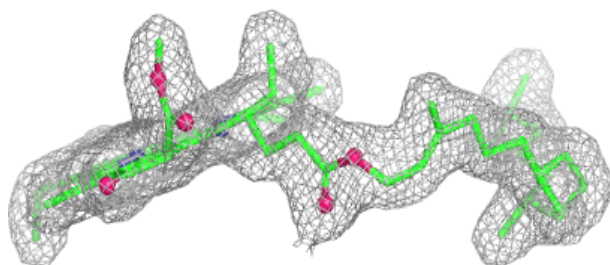
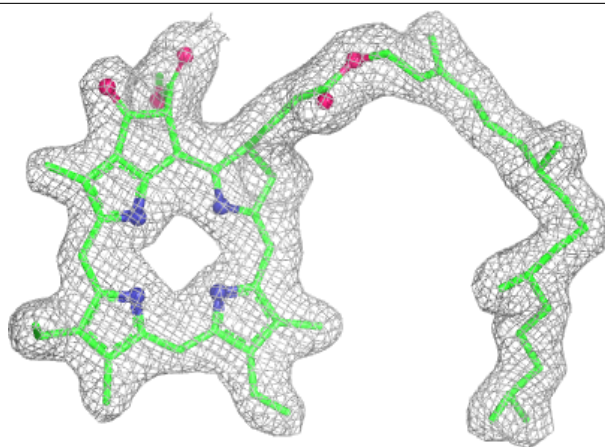
**Electron density around CLA d 402:**

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



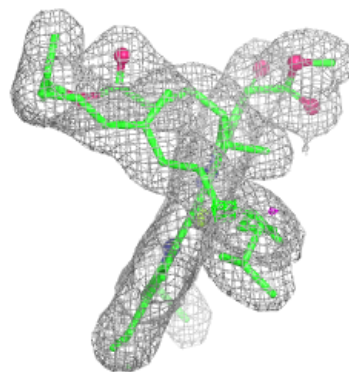
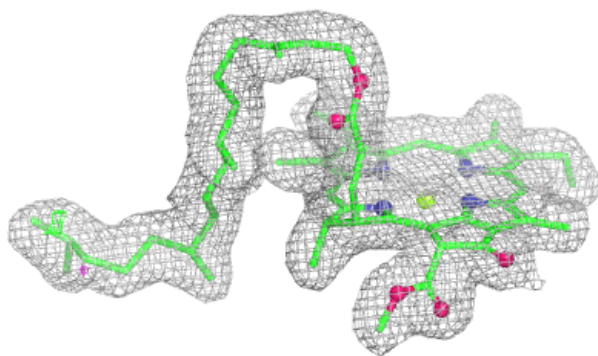
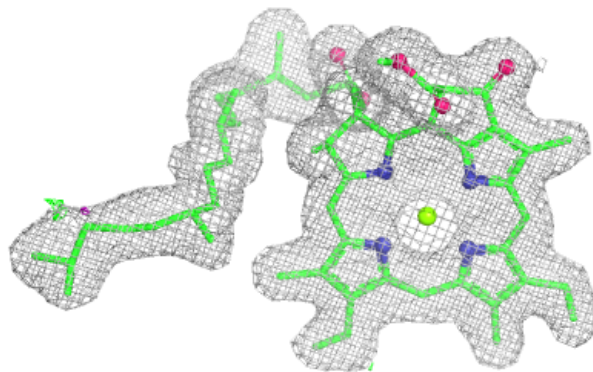
Electron density around PHO a 410:

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



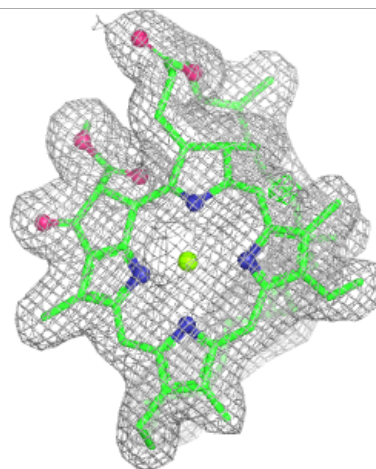
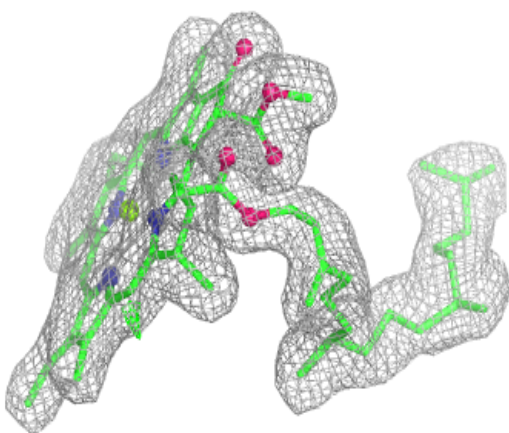
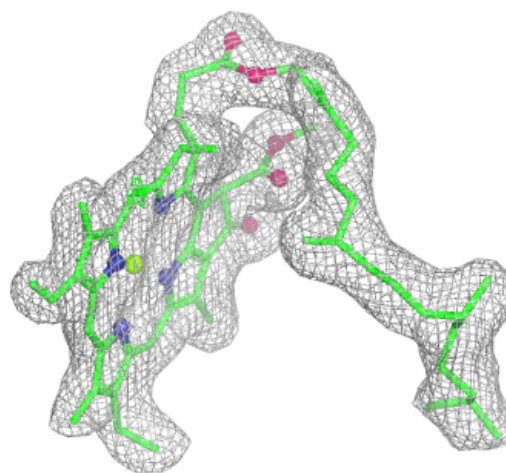
Electron density around CLA a 408:

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



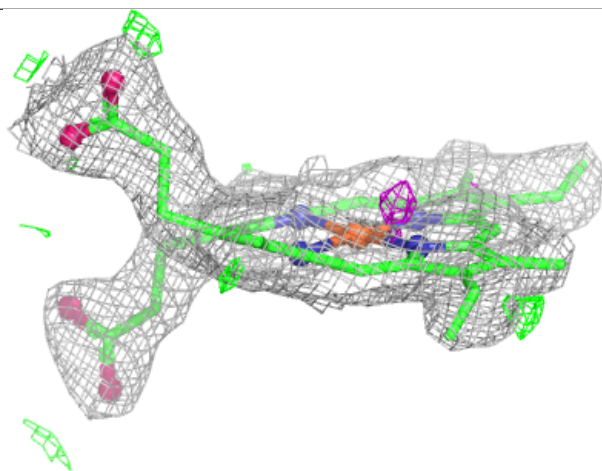
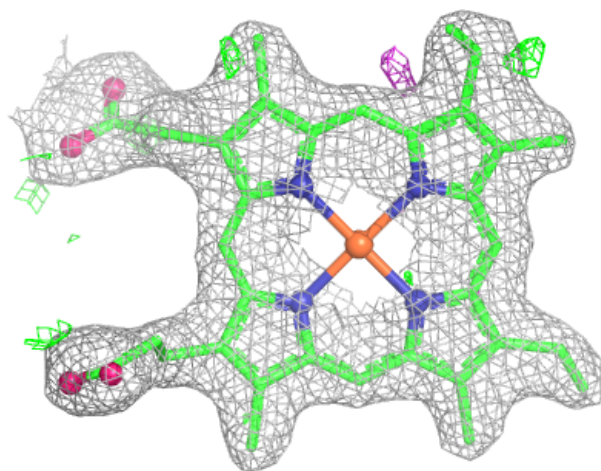
Electron density around CLA B 613:

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



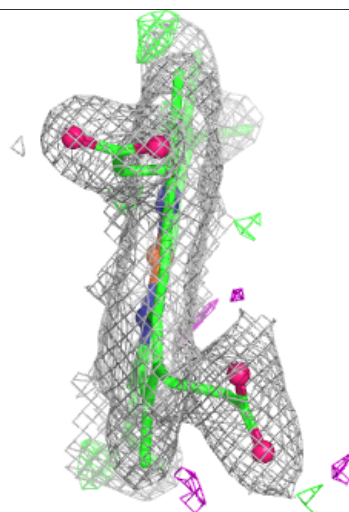
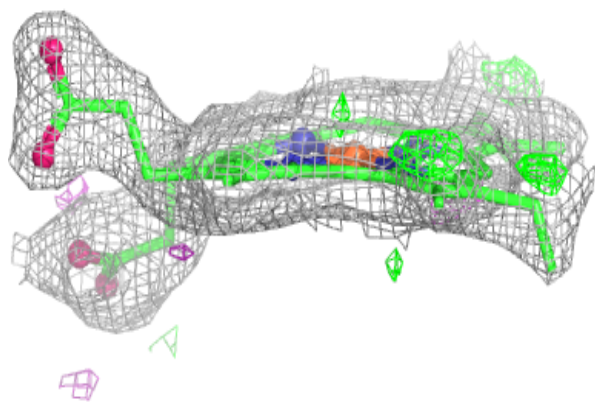
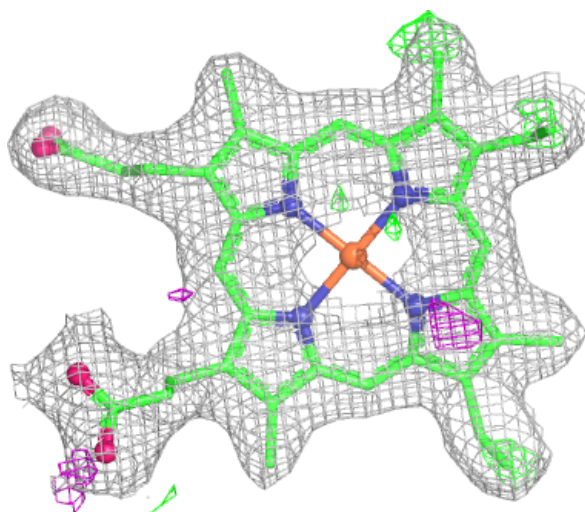
Electron density around HEM F 101:

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



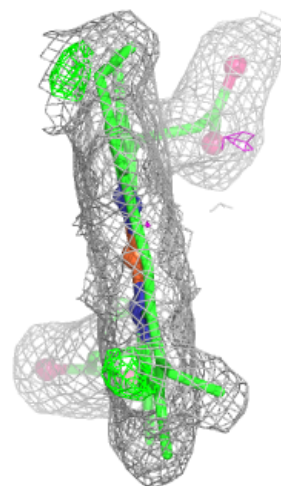
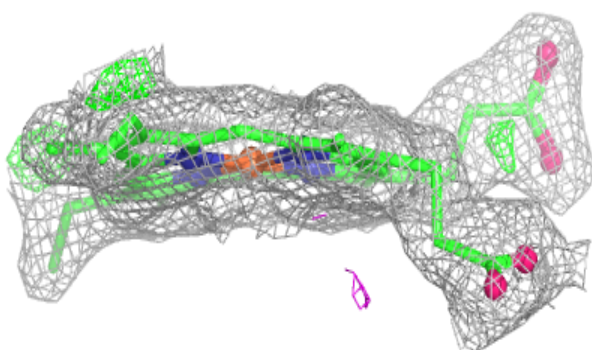
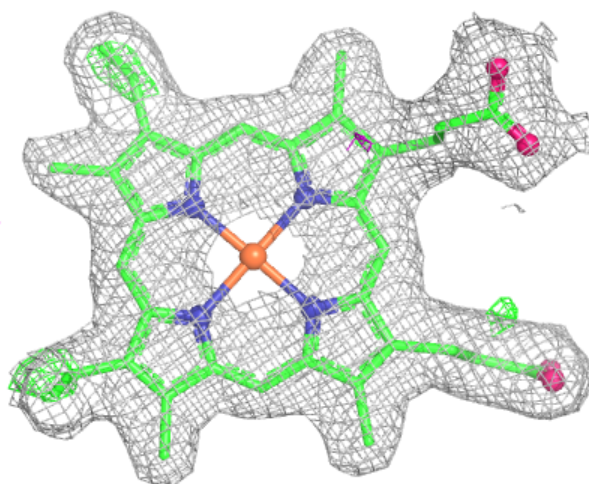
Electron density around HEM v 201:

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



Electron density around HEM V 201:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.