



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 13, 2026 – 06:55 PM JST

PDB ID : 8IRE / pdb_00008ire
Title : XFEL structure of cyanobacterial photosystem II following two flashes (2F)
with a 200-nanosecond delay
Authors : Li, H.; Suga, M.; Shen, J.R.
Deposited on : 2023-03-17
Resolution : 2.25 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

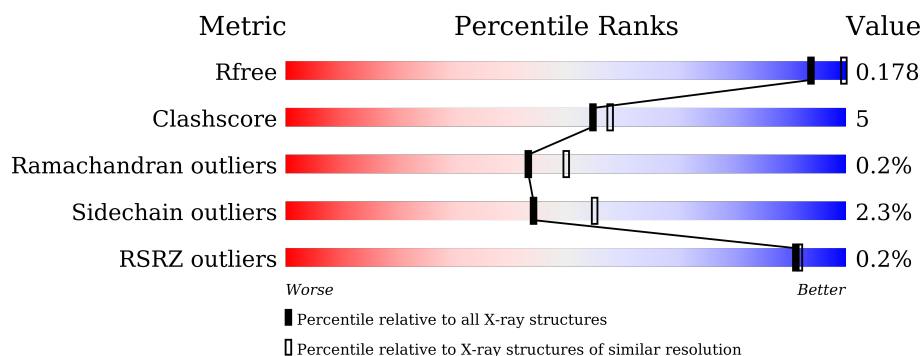
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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.



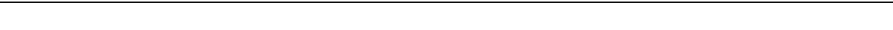
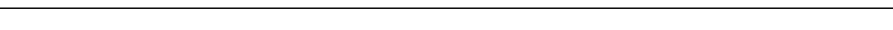
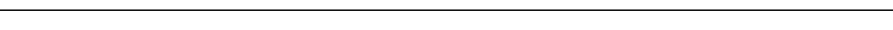
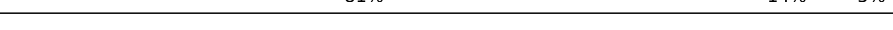
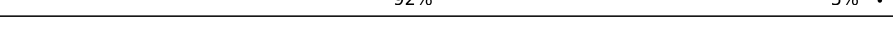
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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

Mol	Chain	Length	Quality of chain
1	A	344	91% 6% .
1	a	344	88% 9% .
2	B	505	93% 7%
2	b	505	91% 8% .
3	C	455	91% 8% .
3	c	455	92% 7% .

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Mol	Chain	Length	Quality of chain
4	D	342	 90% 10%
4	d	342	 90% 10%
5	E	84	 % 81% 15% .
5	e	84	 % 86% 8% 6%
6	F	44	 66% 11% 23%
6	f	44	 2% 64% 7% 30%
7	H	65	 2% 94% 5% .
7	h	65	 85% 14% .
8	I	38	 76% 21% .
8	i	38	 3% 89% 11%
9	J	39	 82% 13% . .
9	j	39	 87% 13%
10	K	37	 76% 19% 5%
10	k	37	 81% 14% 5%
11	L	37	 92% 5% .
11	l	37	 81% 16% .
12	M	36	 72% 14% 6% 8%
12	m	36	 75% 17% . 6%
13	O	244	 86% 14%
13	o	244	 91% 8%
14	T	32	 78% 16% 6%
14	t	32	 81% 12% 6%
15	U	104	 81% 12% 8%
15	u	104	 88% . . 7%
16	V	137	 96% .

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Mol	Chain	Length	Quality of chain
16	v	137	 92% 8%
17	X	40	 88% 8% 5%
17	x	40	 92% 5%
18	Y	30	 3% 87% 10% •
18	y	30	 57% 40% •
19	Z	62	 87% 11% •
19	z	62	 77% 21% •
20	R	34	 3% 71% 26% •

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
27	GOL	A	701	-	-	X	-
27	GOL	D	701	-	X	-	-
27	GOL	a	801	-	-	X	-
40	HEC	V	202	X	-	-	-
40	HEC	v	202	X	-	-	-

2 Entry composition

There are 41 unique types of molecules in this entry. The entry contains 62600 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	222	0
			4338	2836	717	760	25			
1	a	334	Total	C	N	O	S	0	221	0
			4330	2830	716	759	25			

There are 2 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	504	Total	C	N	O	S	0	20	0
			4146	2721	692	720	13			
2	b	504	Total	C	N	O	S	0	19	0
			4134	2718	687	716	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	451	Total	C	N	O	S	0	97	0
			4260	2788	713	741	18			
3	c	455	Total	C	N	O	S	0	100	0
			4308	2821	719	750	18			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	19	ASN	-	expression tag	UNP D0VWR7
C	20	SER	-	expression tag	UNP D0VWR7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	21	ILE	-	expression tag	UNP D0VWR7
C	22	PHE	-	expression tag	UNP D0VWR7
c	19	ASN	-	expression tag	UNP D0VWR7
c	20	SER	-	expression tag	UNP D0VWR7
c	21	ILE	-	expression tag	UNP D0VWR7
c	22	PHE	-	expression tag	UNP D0VWR7

- 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	114	0
			3620	2387	596	622	15			
4	d	341	Total	C	N	O	S	0	116	0
			3628	2391	599	623	15			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	81	Total	C	N	O	0	0	0
			662	432	107	123			
5	e	79	Total	C	N	O	0	2	0
			670	439	110	121			

- 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	31	Total	C	N	O	S	0	1	0
			261	179	43	38	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	64	Total	C	N	O	S	0	0	0
			506	339	81	84	2			
7	h	64	Total	C	N	O	S	0	1	0
			517	345	85	85	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	38	Total	C	N	O	S	0	0	0
			314	211	48	54	1			
8	i	38	Total	C	N	O	S	0	0	0
			314	211	48	54	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	38	Total	C	N	O	S	0	0	0
			272	182	42	47	1			
9	j	39	Total	C	N	O	S	0	0	0
			277	185	43	48	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			

There are 4 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	L	36	Total	C	N	O	0	2	0
			311	207	49	55			
11	l	36	Total	C	N	O	0	2	0
			311	207	49	55			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	33	Total	C	N	O	S	0	1	0
			268	179	39	49	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	m	34	Total	C	N	O	S	0	2	0
			286	190	43	52	1			

There are 2 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	243	Total	C	N	O	S	0	10	0
			1958	1221	335	398	4			
13	o	243	Total	C	N	O	S	0	8	0
			1933	1207	330	392	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	30	Total	C	N	O	S	0	6	0
			311	213	48	48	2			
14	t	30	Total	C	N	O	S	0	5	0
			302	208	47	45	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	U	96	Total	C	N	O		0	4	0
			800	508	133	159				
15	u	97	Total	C	N	O		0	4	0
			807	513	134	160				

- 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	6	0
			1120	711	185	220	4			
16	v	137	Total	C	N	O	S	0	6	0
			1117	712	185	216	4			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	X	38	Total	C	N	O	0	1	0
			289	194	46	49			
17	x	38	Total	C	N	O	0	0	0
			281	188	45	48			

- Molecule 18 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	Y	29	Total	C	N	O	S	0	0	0
			215	142	37	33	3			
18	y	29	Total	C	N	O	S	0	0	0
			215	142	37	33	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Z	62	Total	C	N	O	S	0	0	0
			479	328	72	77	2			
19	z	62	Total	C	N	O	S	0	0	0
			479	328	72	77	2			

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

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

- Molecule 21 is FE (II) ION (CCD ID: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	A	1	Total	Fe	0	1
			2	2		
21	a	1	Total	Fe	0	1
			2	2		

- Molecule 22 is CHLORIDE ION (CCD ID: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

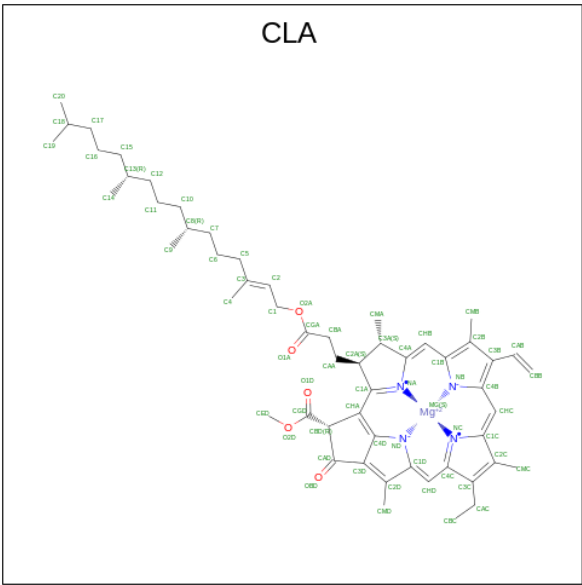
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	2	Total	Cl	0	2
			4	4		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	a	2	Total	Cl	0	2
			4	4		

- Molecule 23 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	A	1	Total	C	Mg	N	O	0	1
			130	110	2	8	10		
23	A	1	Total	C	Mg	N	O	0	1
			130	110	2	8	10		
23	A	1	Total	C	Mg	N	O	0	1
			130	110	2	8	10		
23	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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

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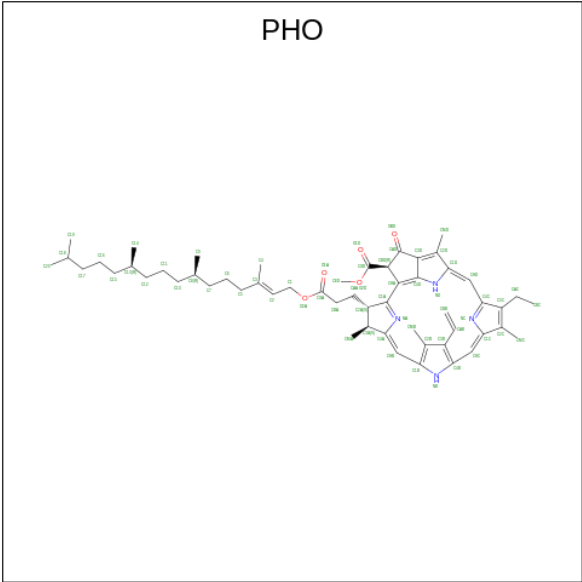
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	D	1	Total 130	C 110	Mg 2	N 8	O 10	0	1
23	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	a	1	Total 130	C 110	Mg 2	N 8	O 10	0	1
23	a	1	Total 130	C 110	Mg 2	N 8	O 10	0	1
23	a	1	Total 130	C 110	Mg 2	N 8	O 10	0	1
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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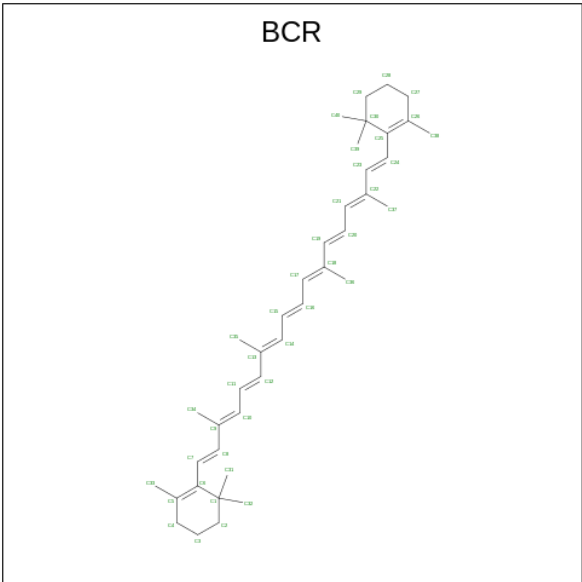
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	d	1	Total	C	Mg	N	O	0	1
			130	110	2	8	10		
23	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 24 is PHEOPHYTIN A (CCD ID: PHO) (formula: C₅₅H₇₄N₄O₅).



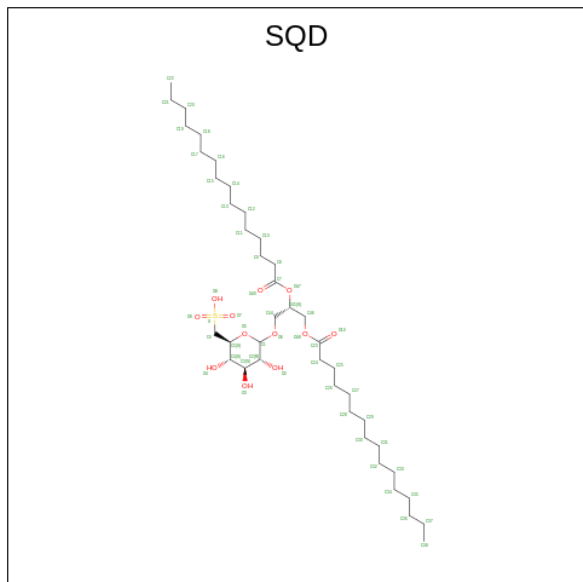
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	A	1	Total	C	N	O	0	1
			128	110	8	10		
24	A	1	Total	C	N	O	0	1
			128	110	8	10		
24	a	1	Total	C	N	O	0	1
			128	110	8	10		
24	a	1	Total	C	N	O	0	1
			128	110	8	10		

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



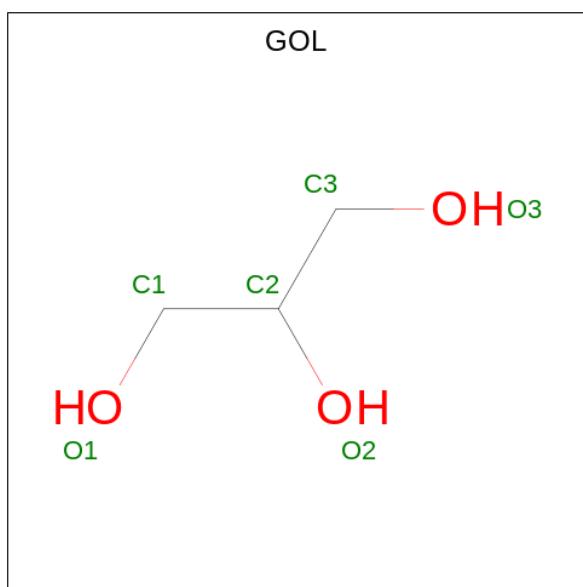
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	D	1	Total C 40 40	0	0
25	H	1	Total C 40 40	0	0
25	K	1	Total C 40 40	0	0
25	T	1	Total C 40 40	0	0
25	Y	1	Total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

- Molecule 26 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
26	A	1	Total	C	O	S	0	1
			108	82	24	2		
26	A	1	Total	C	O	S	0	0
			54	41	12	1		
26	B	1	Total	C	O	S	0	0
			54	41	12	1		
26	F	1	Total	C	O	S	0	0
			43	30	12	1		
26	a	1	Total	C	O	S	0	1
			108	82	24	2		
26	a	1	Total	C	O	S	0	0
			54	41	12	1		
26	b	1	Total	C	O	S	0	0
			54	41	12	1		
26	f	1	Total	C	O	S	0	0
			43	30	12	1		

- Molecule 27 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



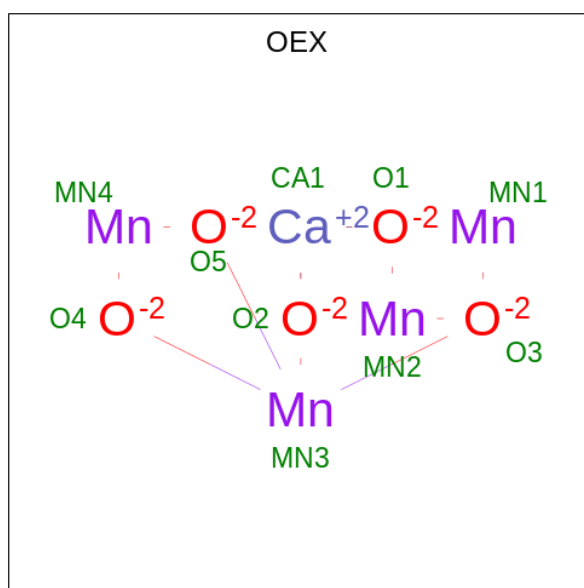
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	A	1	Total	C	O	0	0
			6	3	3		
27	A	1	Total	C	O	0	0
			6	3	3		
27	B	1	Total	C	O	0	0
			6	3	3		
27	B	1	Total	C	O	0	0
			6	3	3		
27	C	1	Total	C	O	0	1
			12	6	6		
27	D	1	Total	C	O	0	0
			6	3	3		
27	O	1	Total	C	O	0	0
			6	3	3		
27	O	1	Total	C	O	0	0
			6	3	3		
27	V	1	Total	C	O	0	1
			12	6	6		
27	a	1	Total	C	O	0	0
			6	3	3		
27	a	1	Total	C	O	0	0
			6	3	3		
27	a	1	Total	C	O	0	0
			6	3	3		
27	b	1	Total	C	O	0	0
			6	3	3		
27	b	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	c	1	Total	C	O	0	1
			12	6	6		
27	c	1	Total	C	O	0	0
			6	3	3		
27	d	1	Total	C	O	0	0
			6	3	3		
27	d	1	Total	C	O	0	1
			12	6	6		
27	o	1	Total	C	O	0	0
			6	3	3		
27	o	1	Total	C	O	0	0
			6	3	3		
27	v	1	Total	C	O	0	1
			12	6	6		

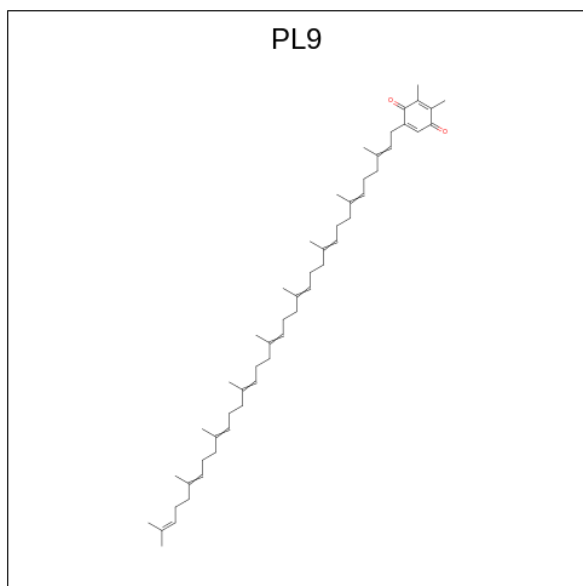
- Molecule 28 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 29 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: $\text{C}_{53}\text{H}_{80}\text{O}_2$)

(labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	A	1	Total	C	O	0	1
			110	106	4		
29	D	1	Total	C	O	0	1
			110	106	4		
29	a	1	Total	C	O	0	1
			110	106	4		
29	d	1	Total	C	O	0	1
			110	106	4		

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

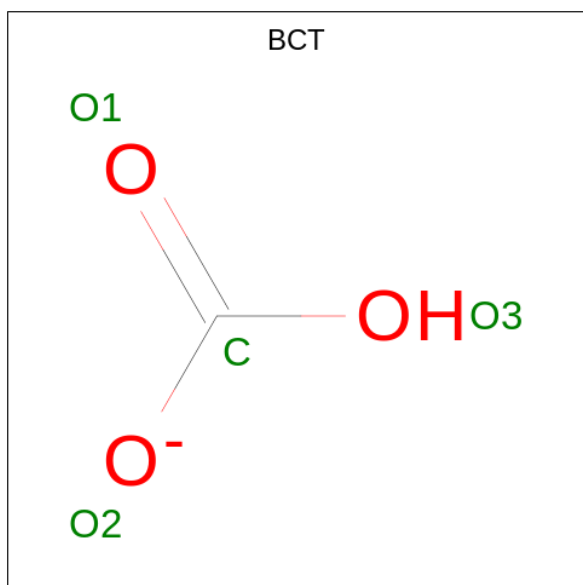
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	A	1	Total	C	O	0	0
			28	23	5		
30	B	1	Total	C	O	0	0
			33	28	5		
30	D	2	Total	C	O	0	0
			57	51	6		
30	I	1	Total	C	O	0	0
			40	35	5		
30	J	1	Total	C		0	0
			10	10			
30	K	1	Total	C	O	0	1
			68	58	10		
30	M	1	Total	C		0	0
			10	10			

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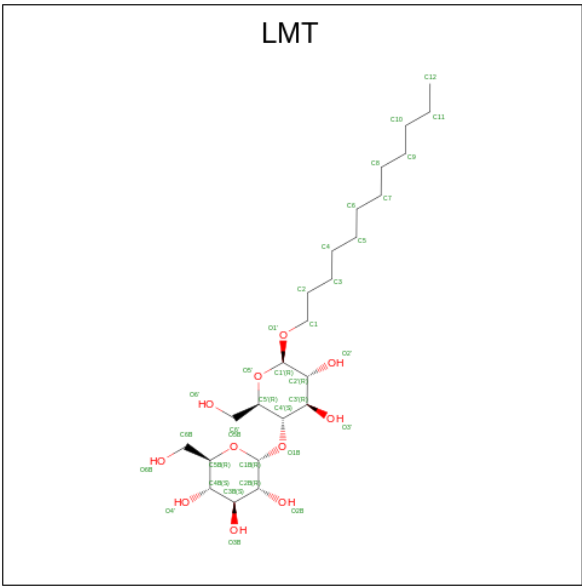
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	X	1	Total	C	O	0	0
			18	16	2		
30	a	1	Total	C	O	0	0
			30	25	5		
30	b	1	Total	C	O	0	0
			33	28	5		
30	c	1	Total	C	O	0	1
			64	54	10		
30	d	2	Total	C	O	0	0
			53	47	6		
30	i	1	Total	C	O	0	0
			40	35	5		
30	j	1	Total	C		0	0
			10	10			
30	m	1	Total	C		0	0
			10	10			
30	x	1	Total	C	O	0	0
			18	16	2		

- Molecule 31 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	A	1	Total	C	O	0	1
			8	2	6		
31	a	1	Total	C	O	0	1
			8	2	6		

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



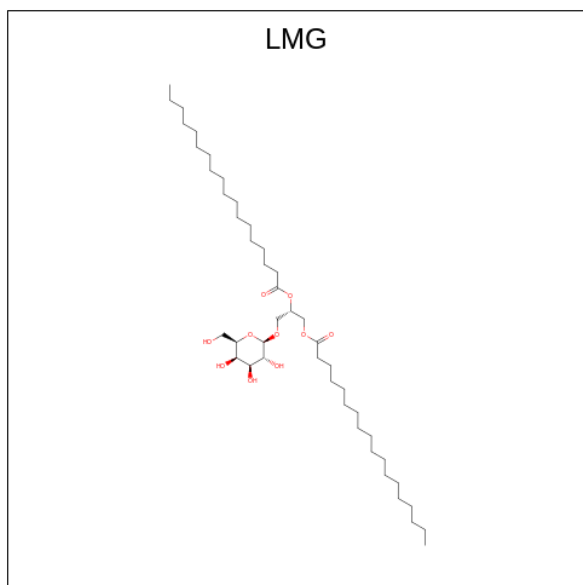
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	A	1	Total	C	O	0	0
			35	24	11		
32	D	1	Total	C	O	0	0
			35	24	11		
32	E	1	Total	C	O	0	0
			35	24	11		
32	I	1	Total	C	O	0	0
			35	24	11		
32	M	1	Total	C	O	0	0
			35	24	11		
32	M	1	Total	C	O	0	0
			35	24	11		
32	a	1	Total	C	O	0	0
			35	24	11		
32	a	1	Total	C	O	0	0
			35	24	11		
32	b	1	Total	C	O	0	0
			25	19	6		
32	b	1	Total	C	O	0	0
			25	19	6		
32	e	1	Total	C	O	0	0
			35	24	11		
32	m	1	Total	C	O	0	0
			35	24	11		
32	t	1	Total	C	O	0	0
			25	19	6		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	t	1	Total	C	O	0	0
			26	19	7		

- Molecule 33 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



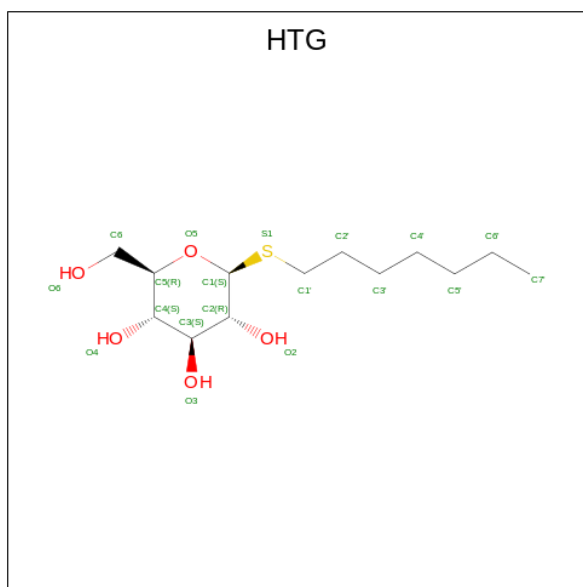
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	B	1	Total	C	O	0	0
			51	41	10		
33	C	1	Total	C	O	0	0
			51	41	10		
33	C	1	Total	C	O	0	0
			51	41	10		
33	C	1	Total	C	O	0	0
			51	41	10		
33	D	1	Total	C	O	0	0
			51	41	10		
33	a	1	Total	C	O	0	0
			51	41	10		
33	c	1	Total	C	O	0	0
			51	41	10		
33	c	1	Total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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	Z	1	Total	C	O	0	0
			37	27	10		
33	z	1	Total	C	O	0	0
			39	29	10		

- Molecule 34 is heptyl 1-thio-beta-D-glucopyranoside (CCD ID: HTG) (formula: C₁₃H₂₆O₅S).



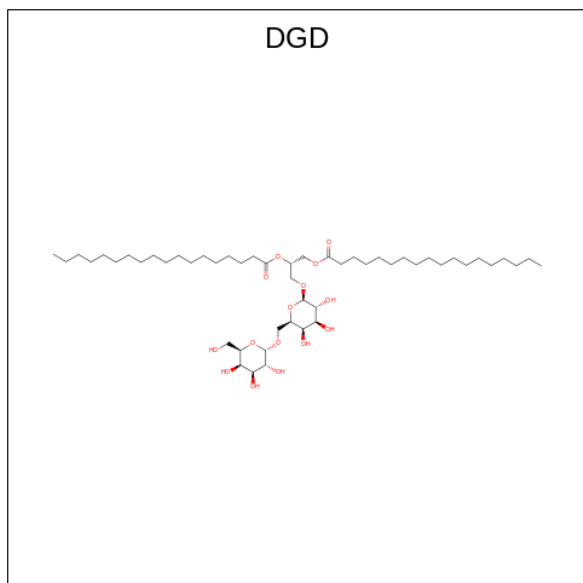
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	B	1	Total	C	O	S	0	0
			19	13	5	1		
34	B	1	Total	C	O	S	0	0
			19	13	5	1		
34	B	1	Total	C	O	S	0	0
			19	13	5	1		
34	C	1	Total	C	O	S	0	0
			19	13	5	1		
34	D	1	Total	C	O	S	0	0
			16	10	5	1		
34	V	1	Total	C	O		0	0
			11	6	5			
34	b	1	Total	C	O	S	0	0
			19	13	5	1		
34	b	1	Total	C	O	S	0	0
			19	13	5	1		
34	b	1	Total	C	O	S	0	0
			19	13	5	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	c	1	Total	C	O	S	0	0
			19	13	5	1		
34	d	1	Total	C	O	S	0	0
			16	10	5	1		

- Molecule 35 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).

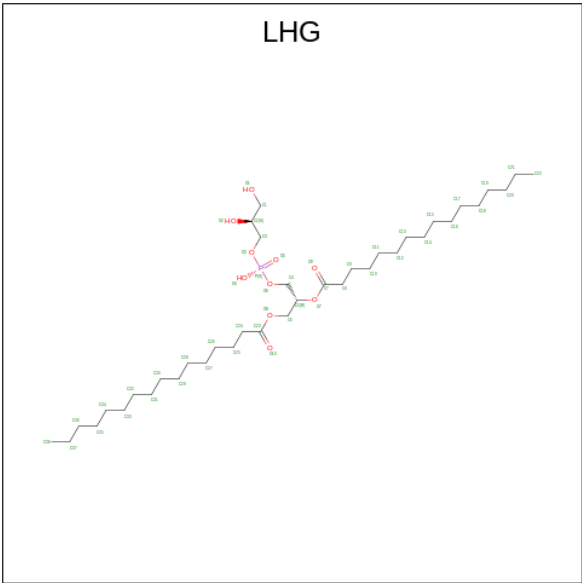


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
35	C	1	Total	C	O		0	1
			124	94	30			
35	C	1	Total	C	O		0	1
			124	94	30			
35	C	1	Total	C	O		0	0
			62	47	15			
35	H	1	Total	C	O		0	0
			62	47	15			
35	c	1	Total	C	O		0	1
			124	94	30			
35	c	1	Total	C	O		0	1
			124	94	30			
35	c	1	Total	C	O		0	0
			62	47	15			
35	h	1	Total	C	O		0	0
			62	47	15			

- Molecule 36 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	C	1	Total	Ca	0	0
			1	1		
36	F	1	Total	Ca	0	0
			1	1		
36	O	1	Total	Ca	0	0
			1	1		
36	c	2	Total	Ca	0	0
			2	2		
36	f	1	Total	Ca	0	0
			1	1		
36	o	1	Total	Ca	0	0
			1	1		

- Molecule 37 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
37	D	1	Total	C	O	P	0	1
			98	76	20	2		
37	D	1	Total	C	O	P	0	1
			98	76	20	2		
37	D	1	Total	C	O	P	0	1
			98	76	20	2		
37	E	1	Total	C	O	P	0	1
			84	62	20	2		
37	L	1	Total	C	O	P	0	1
			98	76	20	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
37	d	1	Total 98	C 76	O 20	P 2	0	1
37	d	1	Total 98	C 76	O 20	P 2	0	1
37	d	1	Total 98	C 76	O 20	P 2	0	1
37	e	1	Total 84	C 62	O 20	P 2	0	1
37	l	1	Total 98	C 76	O 20	P 2	0	1

-
- The diagram illustrates the chemical structure of the Heme (HEM) molecule. It features a central iron atom (Fe) coordinated by four nitrogen atoms (N) in a porphyrin-like ring. The ring is substituted with various side chains, including vinyl groups (C=C), methyl groups (CH₃), and a central heme group (CH₃CO). The structure is labeled with atom names and coordinates, such as O1A, O2A, O1D, O2D, CAA, CBA, CAD, CBD, CMA, C3A, C2A, C3D, C4D, C1D, C2D, C1A, C4A, C4B, C1B, C2B, C3B, C4B, C1C, C2C, C3C, C4C, C1D, C2D, C3D, C4D, C1E, C2E, C3E, C4E, C1F, C2F, C3F, C4F, C1G, C2G, C3G, C4G, C1H, C2H, C3H, C4H, C1I, C2I, C3I, C4I, C1J, C2J, C3J, C4J, C1K, C2K, C3K, C4K, C1L, C2L, C3L, C4L, C1M, C2M, C3M, C4M, C1N, C2N, C3N, C4N, C1O, C2O, C3O, C4O, C1P, C2P, C3P, C4P, C1Q, C2Q, C3Q, C4Q, C1R, C2R, C3R, C4R, C1S, C2S, C3S, C4S, C1T, C2T, C3T, C4T, C1U, C2U, C3U, C4U, C1V, C2V, C3V, C4V, C1W, C2W, C3W, C4W, C1X, C2X, C3X, C4X, C1Y, C2Y, C3Y, C4Y, C1Z, C2Z, C3Z, C4Z, C1AA, C2AA, C3AA, C4AA, C1AB, C2AB, C3AB, C4AB, C1AC, C2AC, C3AC, C4AC, C1AD, C2AD, C3AD, C4AD, C1AE, C2AE, C3AE, C4AE, C1AF, C2AF, C3AF, C4AF, C1AG, C2AG, C3AG, C4AG, C1AH, C2AH, C3AH, C4AH, C1AI, C2AI, C3AI, C4AI, C1AJ, C2AJ, C3AJ, C4AJ, C1AK, C2AK, C3AK, C4AK, C1AL, C2AL, C3AL, C4AL, C1AM, C2AM, C3AM, C4AM, C1AN, C2AN, C3AN, C4AN, C1AO, C2AO, C3AO, C4AO, C1AP, C2AP, C3AP, C4AP, C1AQ, C2AQ, C3AQ, C4AQ, C1AR, C2AR, C3AR, C4AR, C1AS, C2AS, C3AS, C4AS, C1AT, C2AT, C3AT, C4AT, C1AU, C2AU, C3AU, C4AU, C1AV, C2AV, C3AV, C4AV, C1AW, C2AW, C3AW, C4AW, C1AX, C2AX, C3AX, C4AX, C1AY, C2AY, C3AY, C4AY, C1AZ, C2AZ, C3AZ, C4AZ, C1BA, C2BA, C3BA, C4BA, C1BB, C2BB, C3BB, C4BB, C1BC, C2BC, C3BC, C4BC, C1BD, C2BD, C3BD, C4BD, C1BE, C2BE, C3BE, C4BE, C1BF, C2BF, C3BF, C4BF, C1BG, C2BG, C3BG, C4BG, C1BH, C2BH, C3BH, C4BH, C1BI, C2BI, C3BI, C4BI, C1BJ, C2BJ, C3BJ, C4BJ, C1BK, C2BK, C3BK, C4BK, C1BL, C2BL, C3BL, C4BL, C1BM, C2BM, C3BM, C4BM, C1BN, C2BN, C3BN, C4BN, C1BO, C2BO, C3BO, C4BO, C1BP, C2BP, C3BP, C4BP, C1BQ, C2BQ, C3BQ, C4BQ, C1BR, C2BR, C3BR, C4BR, C1BS, C2BS, C3BS, C4BS, C1BT, C2BT, C3BT, C4BT, C1BU, C2BU, C3BU, C4BU, C1BV, C2BV, C3BV, C4BV, C1BW, C2BW, C3BW, C4BW, C1BX, C2BX, C3BX, C4BX, C1BY, C2BY, C3BY, C4BY, C1BZ, C2BZ, C3BZ, C4BZ, C1CA, C2CA, C3CA, C4CA, C1CB, C2CB, C3CB, C4CB, C1CC, C2CC, C3CC, C4CC, C1CD, C2CD, C3CD, C4CD, C1CE, C2CE, C3CE, C4CE, C1CF, C2CF, C3CF, C4CF, C1CG, C2CG, C3CG, C4CG, C1CH, C2CH, C3CH, C4CH, C1CI, C2CI, C3CI, C4CI, C1CJ, C2CJ, C3CJ, C4CJ, C1CK, C2CK, C3CK, C4CK, C1CL, C2CL, C3CL, C4CL, C1CM, C2CM, C3CM, C4CM, C1CN, C2CN, C3CN, C4CN, C1CO, C2CO, C3CO, C4CO, C1CP, C2CP, C3CP, C4CP, C1CQ, C2CQ, C3CQ, C4CQ, C1CR, C2CR, C3CR, C4CR, C1CS, C2CS, C3CS, C4CS, C1CT, C2CT, C3CT, C4CT, C1CU, C2CU, C3CU, C4CU, C1CV, C2CV, C3CV, C4CV, C1CW, C2CW, C3CW, C4CW, C1CX, C2CX, C3CX, C4CX, C1CY, C2CY, C3CY, C4CY, C1CZ, C2CZ, C3CZ, C4CZ, C1DA, C2DA, C3DA, C4DA, C1DB, C2DB, C3DB, C4DB, C1DC, C2DC, C3DC, C4DC, C1DD, C2DD, C3DD, C4DD, C1DE, C2DE, C3DE, C4DE, C1DF, C2DF, C3DF, C4DF, C1DG, C2DG, C3DG, C4DG, C1DH, C2DH, C3DH, C4DH, C1DI, C2DI, C3DI, C4DI, C1DJ, C2DJ, C3DJ, C4DJ, C1DK, C2DK, C3DK, C4DK, C1DL, C2DL, C3DL, C4DL, C1DM, C2DM, C3DM, C4DM, C1DN, C2DN, C3DN, C4DN, C1DO, C2DO, C3DO, C4DO, C1DP, C2DP, C3DP, C4DP, C1DQ, C2DQ, C3DQ, C4DQ, C1DR, C2DR, C3DR, C4DR, C1DS, C2DS, C3DS, C4DS, C1DT, C2DT, C3DT, C4DT, C1DU, C2DU, C3DU, C4DU, C1DV, C2DV, C3DV, C4DV, C1DW, C2DW, C3DW, C4DW, C1DX, C2DX, C3DX, C4DX, C1DY, C2DY, C3DY, C4DY, C1DZ, C2DZ, C3DZ, C4DZ, C1EA, C2EA, C3EA, C4EA, C1EB, C2EB, C3EB, C4EB, C1EC, C2EC, C3EC, C4EC, C1ED, C2ED, C3ED, C4ED, C1EE, C2EE, C3EE, C4EE, C1EF, C2EF, C3EF, C4EF, C1EG, C2EG, C3EG, C4EG, C1EH, C2EH, C3EH, C4EH, C1EI, C2EI, C3EI, C4EI, C1EJ, C2EJ, C3EJ, C4EJ, C1EK, C2EK, C3EK, C4EK, C1EL, C2EL, C3EL, C4EL, C1EM, C2EM, C3EM, C4EM, C1EN, C2EN, C3EN, C4EN, C1EO, C2EO, C3EO, C4EO, C1EP, C2EP, C3EP, C4EP, C1EQ, C2EQ, C3EQ, C4EQ, C1ER, C2ER, C3ER, C4ER, C1ES, C2ES, C3ES, C4ES, C1ET, C2ET, C3ET, C4ET, C1EU, C2EU, C3EU, C4EU, C1EV, C2EV, C3EV, C4EV, C1EW, C2EW, C3EW, C4EW, C1EX, C2EX, C3EX, C4EX, C1EY, C2EY, C3EY, C4EY, C1EZ, C2EZ, C3EZ, C4EZ, C1FA, C2FA, C3FA, C4FA, C1FB, C2FB, C3FB, C4FB, C1FC, C2FC, C3FC, C4FC, C1FD, C2FD, C3FD, C4FD, C1FE, C2FE, C3FE, C4FE, C1FF, C2FF, C3FF, C4FF, C1FG, C2FG, C3FG, C4FG, C1FH, C2FH, C3FH, C4FH, C1FI, C2FI, C3FI, C4FI, C1FJ, C2FJ, C3FJ, C4FJ, C1FK, C2FK, C3FK, C4FK, C1FL, C2FL, C3FL, C4FL, C1FM, C2FM, C3FM, C4FM, C1FN, C2FN, C3FN, C4FN, C1FO, C2FO, C3FO, C4FO, C1FP, C2FP, C3FP, C4FP, C1FQ, C2FQ, C3FQ, C4FQ, C1FR, C2FR, C3FR, C4FR, C1FS, C2FS, C3FS, C4FS, C1FT, C2FT, C3FT, C4FT, C1FU, C2FU, C3FU, C4FU, C1FV, C2FV, C3FV, C4FV, C1FW, C2FW, C3FW, C4FW, C1FX, C2FX, C3FX, C4FX, C1FY, C2FY, C3FY, C4FY, C1FZ, C2FZ, C3FZ, C4FZ, C1GA, C2GA, C3GA, C4GA, C1GB, C2GB, C3GB, C4GB, C1GC, C2GC, C3GC, C4GC, C1GD, C2GD, C3GD, C4GD, C1GE, C2GE, C3GE, C4GE, C1GF, C2GF, C3GF, C4GF, C1GG, C2GG, C3GG, C4GG, C1GH, C2GH, C3GH, C4GH, C1GI, C2GI, C3GI, C4GI, C1GJ, C2GJ, C3GJ, C4GJ, C1GK, C2GK, C3GK, C4GK, C1GL, C2GL, C3GL, C4GL, C1GM, C2GM, C3GM, C4GM, C1GN, C2GN, C3GN, C4GN, C1GO, C2GO, C3GO, C4GO, C1GP, C2GP, C3GP, C4GP, C1GQ, C2GQ, C3GQ, C4GQ, C1GR, C2GR, C3GR, C4GR, C1GS, C2GS, C3GS, C4GS, C1GT, C2GT, C3GT, C4GT, C1GU, C2GU, C3GU, C4GU, C1GV, C2GV, C3GV, C4GV, C1GW, C2GW, C3GW, C4GW, C1GX, C2GX, C3GX, C4GX, C1GY, C2GY, C3GY, C4GY, C1GZ, C2GZ, C3GZ, C4GZ, C1HA, C2HA, C3HA, C4HA, C1HB, C2HB, C3HB, C4HB, C1HC, C2HC, C3HC, C4HC, C1HD, C2HD, C3HD, C4HD, C1HE, C2HE, C3HE, C4HE, C1HF, C2HF, C3HF, C4HF, C1HG, C2HG, C3HG, C4HG, C1HH, C2HH, C3HH, C4HH, C1HI, C2HI, C3HI, C4HI, C1HJ, C2HJ, C3HJ, C4HJ, C1HK, C2HK, C3HK, C4HK, C1HL, C2HL, C3HL, C4HL, C1HM, C2HM, C3HM, C4HM, C1HN, C2HN, C3HN, C4HN, C1HO, C2HO, C3HO, C4HO, C1HP, C2HP, C3HP, C4HP, C1HQ, C2HQ, C3HQ, C4HQ, C1HR, C2HR, C3HR, C4HR, C1HS, C2HS, C3HS, C4HS, C1HT, C2HT, C3HT, C4HT, C1HU, C2HU, C3HU, C4HU, C1HV, C2HV, C3HV, C4HV, C1HW, C2HW, C3HW, C4HW, C1HX, C2HX, C3HX, C4HX, C1HY, C2HY, C3HY, C4HY, C1HZ, C2HZ, C3HZ, C4HZ, C1IA, C2IA, C3IA, C4IA, C1IB, C2IB, C3IB, C4IB, C1IC, C2IC, C3IC, C4IC, C1ID, C2ID, C3ID, C4ID, C1IE, C2IE, C3IE, C4IE, C1IF

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

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

- # HEC
-
- The chemical structure of HEC (Hexaethylcobalamin) is shown. It features a central iron atom (Fe) coordinated by four nitrogen atoms (N) in a porphyrin-like ring. The side chains are labeled with green text: CBC, CMC, CAB, CBB, CAC, C2C, CHC, C3B, CMB, C3C, C4B, C2B, C1C, C1B, C4C, NC, CHB, CHD, ND, NA, C4A, C3A, C1D, C2D, C4D, C1A, C2A, C3D, C3A, C4A, CMA, CBA, CAA, CBD, CAD, CGD, CGA, O2D, O1D, O2A, O1A.

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

- | Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 41 | A | 126 | Total O
206 206 | 0 | 80 |
| 41 | B | 164 | Total O
166 166 | 0 | 2 |
| 41 | C | 141 | Total O
174 174 | 0 | 33 |
| 41 | D | 118 | Total O
150 150 | 0 | 32 |
| 41 | E | 14 | Total O
14 14 | 0 | 0 |
| 41 | F | 3 | Total O
3 3 | 0 | 0 |
| 41 | H | 17 | Total O
17 17 | 0 | 0 |
| 41 | I | 6 | Total O
6 6 | 0 | 0 |
| 41 | J | 5 | Total O
5 5 | 0 | 0 |



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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	K	5	Total 5	O 5	0	0
41	L	3	Total 3	O 3	0	0
41	M	5	Total 5	O 5	0	0
41	O	70	Total 73	O 73	0	3
41	T	8	Total 10	O 10	0	2
41	U	32	Total 32	O 32	0	0
41	V	65	Total 69	O 69	0	4
41	X	1	Total 1	O 1	0	0
41	a	128	Total 208	O 208	0	81
41	b	182	Total 184	O 184	0	2
41	c	133	Total 163	O 163	0	30
41	d	109	Total 140	O 140	0	31
41	e	8	Total 8	O 8	0	0
41	f	3	Total 3	O 3	0	0
41	h	15	Total 15	O 15	0	0
41	i	3	Total 3	O 3	0	0
41	j	2	Total 2	O 2	0	0
41	k	3	Total 3	O 3	0	0
41	l	4	Total 4	O 4	0	0
41	m	14	Total 14	O 14	0	0
41	o	76	Total 81	O 81	0	5

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	t	6	Total 7	O 7	0	1
41	u	47	Total 48	O 48	0	1
41	v	41	Total 41	O 41	0	0
41	x	2	Total 2	O 2	0	0
41	y	1	Total 1	O 1	0	0
41	G	263	Total 286	O 286	0	24

3 Residue-property plots

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

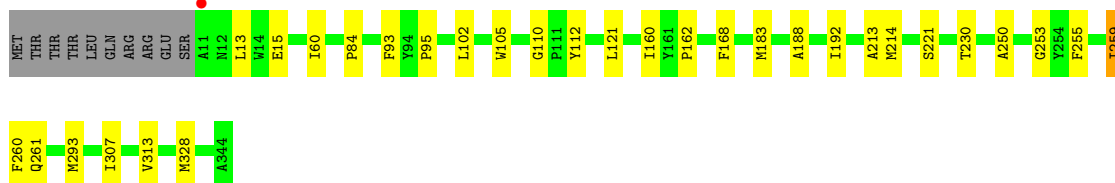
- Molecule 1: Photosystem II protein D1

Chain A: 

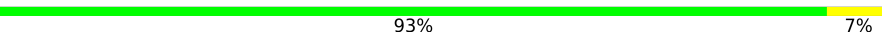


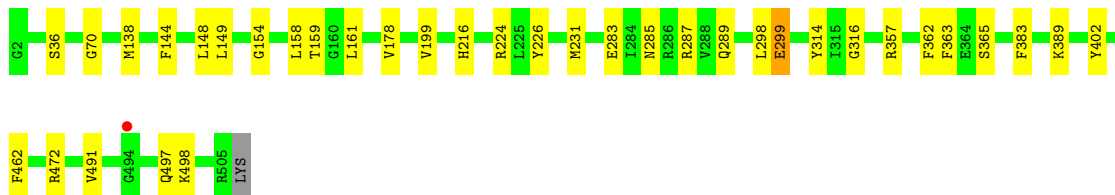
- Molecule 1: Photosystem II protein D1

Chain a: 



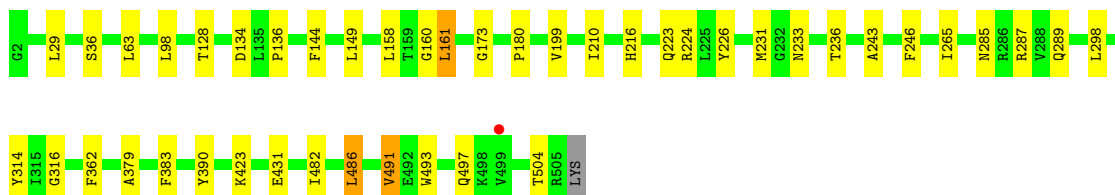
- Molecule 2: Photosystem II CP47 reaction center protein

Chain B: 

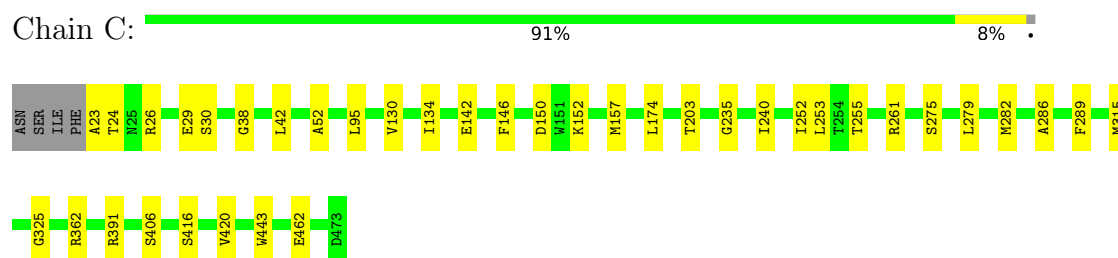


- Molecule 2: Photosystem II CP47 reaction center protein

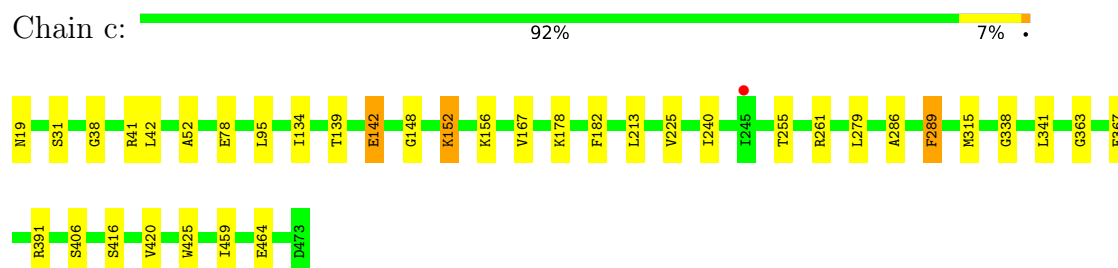
Chain b: 



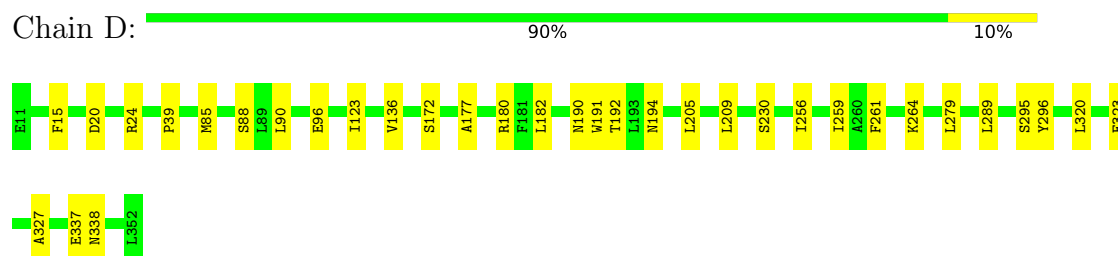
- Molecule 3: Photosystem II CP43 reaction center protein



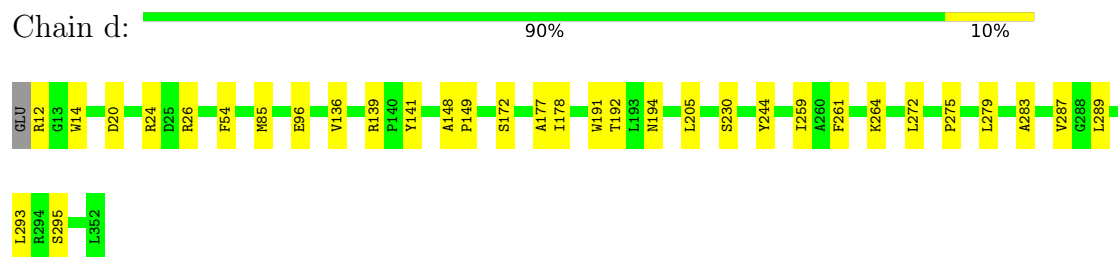
- Molecule 3: Photosystem II CP43 reaction center protein



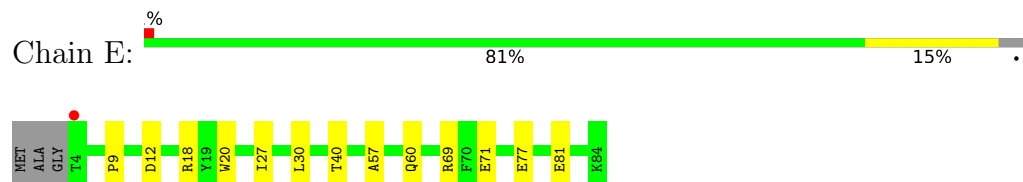
- Molecule 4: Photosystem II D2 protein



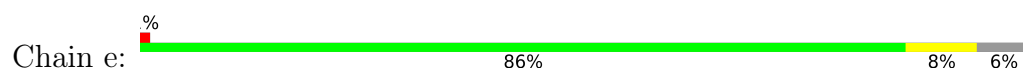
- Molecule 4: Photosystem II D2 protein



- Molecule 5: Cytochrome b559 subunit alpha



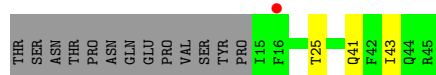
- Molecule 5: Cytochrome b559 subunit alpha



- Molecule 6: Cytochrome b559 subunit beta



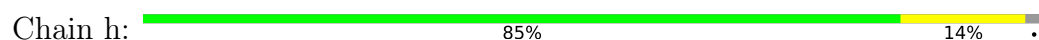
- Molecule 6: Cytochrome b559 subunit beta



- Molecule 7: Photosystem II reaction center protein H



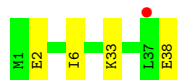
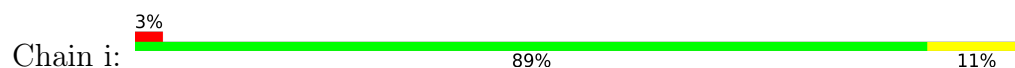
- Molecule 7: Photosystem II reaction center protein H



- Molecule 8: Photosystem II reaction center protein I



- Molecule 8: Photosystem II reaction center protein I



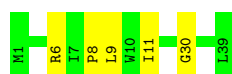
- Molecule 9: Photosystem II reaction center protein J

Chain J:  82% 13% . .



- Molecule 9: Photosystem II reaction center protein J

Chain j:  87% 13%



- Molecule 10: Photosystem II reaction center protein K

Chain K:  76% 19% 5%



- Molecule 10: Photosystem II reaction center protein K

Chain k:  81% 14% 5%



- Molecule 11: Photosystem II reaction center protein L

Chain L:  92% 5% .



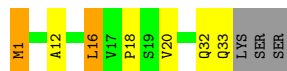
- Molecule 11: Photosystem II reaction center protein L

Chain l:  81% 16% .



- Molecule 12: Photosystem II reaction center protein M

Chain M:  72% 14% 6% 8%



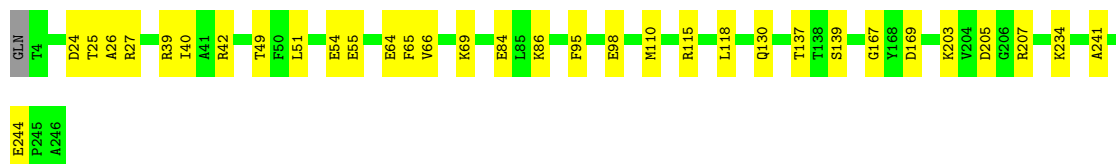
- Molecule 12: Photosystem II reaction center protein M

Chain m:  75% 17% 6%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:  86% 14%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:  91% 8%



- Molecule 14: Photosystem II reaction center protein T

Chain T:  78% 16% 6%



- Molecule 14: Photosystem II reaction center protein T

Chain t:  81% 12% 6%



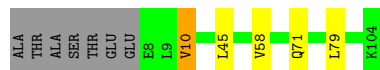
- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:  81% 12% 8%

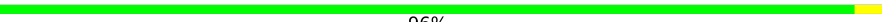


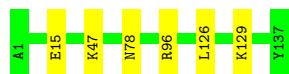
- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u:  88% 7%



- Molecule 16: Cytochrome c-550

Chain V:  96% .



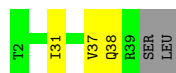
- Molecule 16: Cytochrome c-550

Chain v:  92% 8%



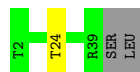
- Molecule 17: Photosystem II reaction center protein X

Chain X:  88% 8% 5%



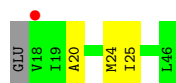
- Molecule 17: Photosystem II reaction center protein X

Chain x:  92% . 5%



- Molecule 18: Photosystem II reaction center protein Ycf12

Chain Y:  87% 10% 3%



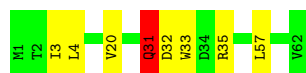
- Molecule 18: Photosystem II reaction center protein Ycf12

Chain y:  57% 40%



- Molecule 19: Photosystem II reaction center protein Z

Chain Z:  87% 11%



- Molecule 19: Photosystem II reaction center protein Z

Chain z:  77% 21% .



- Molecule 20: Photosystem II protein Y

Chain R:  3% 71% 26% .



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	125.77Å 231.76Å 288.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 2.25 19.99 – 2.25	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.99-2.25) 99.8 (19.99-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 2.26Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.139 , 0.177 0.140 , 0.178	Depositor DCC
R_{free} test set	19914 reflections (2.44%)	wwPDB-VP
Wilson B-factor (Å ²)	51.0	Xtriage
Anisotropy	0.483	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 72.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	62600	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.65% 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: HEM, DGD, GOL, CA, OEX, LMG, PHO, LHG, MG, LMT, CLA, HTG, BCR, CL, HEC, BCT, UNL, FME, SQD, FE2, PL9

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	0.27	0/4478	0.43	0/6098
1	a	0.24	0/4470	0.40	0/6087
2	B	0.37	0/4293	0.50	0/5851
2	b	0.34	0/4285	0.49	0/5841
3	C	0.28	0/4404	0.42	0/5997
3	c	0.28	0/4459	0.43	0/6071
4	D	0.34	0/3741	0.46	0/5095
4	d	0.31	0/3749	0.45	0/5106
5	E	0.32	0/681	0.51	0/928
5	e	0.31	0/690	0.49	0/939
6	F	0.42	0/284	0.45	0/387
6	f	0.29	0/269	0.44	0/365
7	H	0.33	0/519	0.51	0/708
7	h	0.29	0/530	0.48	0/722
8	I	0.30	0/311	0.46	0/419
8	i	0.34	0/311	0.51	0/419
9	J	0.30	0/278	0.39	0/376
9	j	0.32	0/283	0.41	0/383
10	K	0.32	0/303	0.47	0/416
10	k	0.33	0/303	0.48	0/416
11	L	0.37	0/318	0.48	0/433
11	l	0.40	0/318	0.45	0/433
12	M	0.43	0/261	0.48	0/357
12	m	0.34	0/279	0.47	0/380
13	O	0.34	0/1991	0.50	0/2698
13	o	0.34	0/1966	0.50	0/2665
14	T	0.34	0/310	0.44	0/419
14	t	0.34	0/301	0.42	0/406
15	U	0.38	0/811	0.53	0/1095
15	u	0.37	0/818	0.54	0/1105
16	V	0.36	0/1142	0.50	0/1545

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.30	0/1139	0.46	0/1542
17	X	0.24	0/292	0.37	0/395
17	x	0.24	0/284	0.37	0/384
18	Y	0.25	0/216	0.44	0/289
18	y	0.24	0/216	0.40	0/289
19	Z	0.22	0/490	0.36	0/669
19	z	0.21	0/490	0.35	0/669
20	R	0.25	0/279	0.36	0/383
All	All	0.31	0/50562	0.46	0/68780

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4338	0	4142	20	0
1	a	4330	0	4132	31	0
2	B	4146	0	3983	25	0
2	b	4134	0	3976	36	0
3	C	4260	0	4123	25	0
3	c	4308	0	4172	27	0
4	D	3620	0	3484	35	0
4	d	3628	0	3490	24	0
5	E	662	0	648	11	0
5	e	670	0	655	5	0
6	F	275	0	282	3	0
6	f	261	0	269	4	0
7	H	506	0	529	2	0
7	h	517	0	541	7	0
8	I	314	0	328	5	0
8	i	314	0	328	2	0
9	J	272	0	279	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	j	277	0	284	3	0
10	K	293	0	305	5	0
10	k	293	0	305	6	0
11	L	311	0	320	2	0
11	l	311	0	320	5	0
12	M	268	0	285	7	0
12	m	286	0	305	10	0
13	O	1958	0	1920	17	0
13	o	1933	0	1900	10	0
14	T	311	0	318	3	0
14	t	302	0	311	3	0
15	U	800	0	796	8	0
15	u	807	0	805	3	0
16	V	1120	0	1122	3	0
16	v	1117	0	1131	8	0
17	X	289	0	322	3	0
17	x	281	0	312	2	0
18	Y	215	0	246	2	0
18	y	215	0	246	8	0
19	Z	479	0	516	5	0
19	z	479	0	516	4	0
20	R	273	0	305	5	0
21	A	2	0	0	0	0
21	a	2	0	0	0	0
22	A	4	0	0	0	0
22	a	4	0	0	0	0
23	A	455	0	504	19	0
23	B	1040	0	1152	26	0
23	C	845	0	936	36	0
23	D	195	0	216	8	0
23	a	455	0	504	20	0
23	b	1040	0	1152	26	0
23	c	845	0	936	35	0
23	d	195	0	216	7	0
24	A	256	0	296	6	0
24	a	256	0	296	5	0
25	A	40	0	56	3	0
25	B	120	0	168	5	0
25	C	80	0	112	1	0
25	D	40	0	56	1	0
25	H	40	0	56	2	0
25	K	40	0	56	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	T	40	0	56	7	0
25	Y	40	0	56	1	0
25	a	40	0	56	1	0
25	b	120	0	168	7	0
25	c	80	0	112	4	0
25	d	40	0	56	2	0
25	h	40	0	56	5	0
25	k	40	0	56	2	0
25	t	40	0	56	5	0
25	y	40	0	56	2	0
26	A	162	0	234	3	0
26	B	54	0	78	1	0
26	F	43	0	53	2	0
26	a	162	0	232	7	0
26	b	54	0	78	4	0
26	f	43	0	53	0	0
27	A	12	0	15	7	0
27	B	12	0	16	2	0
27	C	12	0	16	1	0
27	D	6	0	7	3	0
27	O	12	0	16	2	0
27	V	12	0	16	0	0
27	a	18	0	24	6	0
27	b	12	0	16	1	0
27	c	18	0	24	1	0
27	d	18	0	23	1	0
27	o	12	0	16	0	0
27	v	12	0	16	3	0
28	A	20	0	0	0	0
28	a	20	0	0	0	0
29	A	110	0	160	20	0
29	D	110	0	160	1	0
29	a	110	0	160	10	0
29	d	110	0	160	0	0
30	A	28	0	0	0	0
30	B	33	0	0	0	0
30	D	57	0	0	0	0
30	I	40	0	0	0	0
30	J	10	0	0	0	0
30	K	68	0	0	0	0
30	M	10	0	0	0	0
30	X	18	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	a	30	0	0	0	0
30	b	33	0	0	0	0
30	c	64	0	0	0	0
30	d	53	0	0	0	0
30	i	40	0	0	0	0
30	j	10	0	0	0	0
30	m	10	0	0	0	0
30	x	18	0	0	0	0
31	A	8	0	0	0	0
31	a	8	0	0	0	0
32	A	35	0	46	0	0
32	D	35	0	46	0	0
32	E	35	0	46	0	0
32	I	35	0	46	1	0
32	M	70	0	92	2	0
32	a	70	0	91	2	0
32	b	50	0	70	1	0
32	e	35	0	46	1	0
32	m	35	0	46	1	0
32	t	51	0	70	2	0
33	B	51	0	72	0	0
33	C	153	0	216	2	0
33	D	51	0	72	0	0
33	Z	37	0	44	1	0
33	a	51	0	72	0	0
33	c	102	0	144	1	0
33	d	51	0	72	3	0
33	m	51	0	72	0	0
33	z	39	0	48	2	0
34	B	57	0	78	3	0
34	C	19	0	26	0	0
34	D	16	0	17	1	0
34	V	11	0	10	0	0
34	b	57	0	78	3	0
34	c	19	0	26	1	0
34	d	16	0	17	1	0
35	C	310	0	410	4	0
35	H	62	0	82	1	0
35	c	310	0	410	11	0
35	h	62	0	82	0	0
36	C	1	0	0	0	0
36	F	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	O	1	0	0	0	0
36	c	2	0	0	0	0
36	f	1	0	0	0	0
36	o	1	0	0	0	0
37	D	294	0	444	18	0
37	E	84	0	114	6	0
37	L	98	0	148	0	0
37	d	294	0	444	28	0
37	e	84	0	114	9	0
37	l	98	0	148	0	0
38	E	43	0	30	2	0
38	e	43	0	30	0	0
39	J	1	0	0	0	0
39	j	1	0	0	0	0
40	V	43	0	30	0	0
40	v	43	0	30	0	0
41	A	206	0	0	0	0
41	B	166	0	0	1	0
41	C	174	0	0	1	0
41	D	150	0	0	1	0
41	E	14	0	0	0	0
41	F	3	0	0	0	0
41	G	286	0	0	6	0
41	H	17	0	0	0	0
41	I	6	0	0	0	0
41	J	5	0	0	2	0
41	K	5	0	0	0	0
41	L	3	0	0	0	0
41	M	5	0	0	0	0
41	O	73	0	0	0	0
41	T	10	0	0	1	0
41	U	32	0	0	0	0
41	V	69	0	0	0	0
41	X	1	0	0	0	0
41	a	208	0	0	0	0
41	b	184	0	0	1	0
41	c	163	0	0	2	0
41	d	140	0	0	0	0
41	e	8	0	0	0	0
41	f	3	0	0	0	0
41	h	15	0	0	0	0
41	i	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	j	2	0	0	0	0
41	k	3	0	0	0	0
41	l	4	0	0	0	0
41	m	14	0	0	0	0
41	o	81	0	0	0	0
41	t	7	0	0	1	0
41	u	48	0	0	0	0
41	v	41	0	0	0	0
41	x	2	0	0	0	0
41	y	1	0	0	0	0
All	All	62600	0	61443	590	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 590 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)
1:a:250[A]:ALA:HA	2:b:491[A]:VAL:HG11	1.51	0.93
1:a:250[B]:ALA:HA	2:b:491[B]:VAL:HG11	1.51	0.93
23:B:604:CLA:H42	23:B:605:CLA:H2	1.53	0.91
27:A:701:GOL:H11	12:M:1:FME:HG2	1.55	0.87
23:B:601:CLA:H12	23:B:601:CLA:H71	1.62	0.81

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	553/344 (161%)	544 (98%)	7 (1%)	2 (0%)	30	31
1	a	552/344 (160%)	544 (99%)	6 (1%)	2 (0%)	30	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	522/505 (103%)	514 (98%)	8 (2%)	0	100	100
2	b	521/505 (103%)	509 (98%)	12 (2%)	0	100	100
3	C	546/455 (120%)	540 (99%)	5 (1%)	1 (0%)	43	50
3	c	553/455 (122%)	540 (98%)	12 (2%)	1 (0%)	43	50
4	D	453/342 (132%)	438 (97%)	15 (3%)	0	100	100
4	d	454/342 (133%)	443 (98%)	11 (2%)	0	100	100
5	E	79/84 (94%)	78 (99%)	1 (1%)	0	100	100
5	e	79/84 (94%)	79 (100%)	0	0	100	100
6	F	32/44 (73%)	32 (100%)	0	0	100	100
6	f	30/44 (68%)	30 (100%)	0	0	100	100
7	H	62/65 (95%)	62 (100%)	0	0	100	100
7	h	63/65 (97%)	59 (94%)	3 (5%)	1 (2%)	7	4
8	I	36/38 (95%)	34 (94%)	1 (3%)	1 (3%)	4	2
8	i	36/38 (95%)	32 (89%)	4 (11%)	0	100	100
9	J	36/39 (92%)	35 (97%)	1 (3%)	0	100	100
9	j	37/39 (95%)	37 (100%)	0	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100
10	k	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
11	L	36/37 (97%)	36 (100%)	0	0	100	100
11	l	36/37 (97%)	36 (100%)	0	0	100	100
12	M	32/36 (89%)	32 (100%)	0	0	100	100
12	m	34/36 (94%)	34 (100%)	0	0	100	100
13	O	251/244 (103%)	242 (96%)	8 (3%)	1 (0%)	30	31
13	o	249/244 (102%)	244 (98%)	5 (2%)	0	100	100
14	T	33/32 (103%)	33 (100%)	0	0	100	100
14	t	32/32 (100%)	32 (100%)	0	0	100	100
15	U	97/104 (93%)	93 (96%)	4 (4%)	0	100	100
15	u	98/104 (94%)	94 (96%)	4 (4%)	0	100	100
16	V	140/137 (102%)	136 (97%)	4 (3%)	0	100	100
16	v	140/137 (102%)	135 (96%)	5 (4%)	0	100	100
17	X	37/40 (92%)	36 (97%)	1 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	x	36/40 (90%)	36 (100%)	0	0	100	100
18	Y	27/30 (90%)	25 (93%)	2 (7%)	0	100	100
18	y	27/30 (90%)	27 (100%)	0	0	100	100
19	Z	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	7	3
19	z	60/62 (97%)	59 (98%)	0	1 (2%)	7	3
20	R	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
All	All	6171/5384 (115%)	6038 (98%)	122 (2%)	11 (0%)	43	50

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
8	I	36	ASP
3	c	416	SER
19	Z	31	GLN
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	444/279 (159%)	440 (99%)	4 (1%)	70	79
1	a	443/279 (159%)	441 (100%)	2 (0%)	81	87
2	B	421/403 (104%)	416 (99%)	5 (1%)	63	74
2	b	420/403 (104%)	409 (97%)	11 (3%)	40	50
3	C	430/356 (121%)	421 (98%)	9 (2%)	47	58
3	c	436/356 (122%)	428 (98%)	8 (2%)	51	63
4	D	368/277 (133%)	365 (99%)	3 (1%)	73	80
4	d	369/277 (133%)	361 (98%)	8 (2%)	45	56
5	E	72/73 (99%)	71 (99%)	1 (1%)	59	70
5	e	72/73 (99%)	71 (99%)	1 (1%)	59	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	28/38 (74%)	28 (100%)	0	100	100
6	f	26/38 (68%)	26 (100%)	0	100	100
7	H	54/54 (100%)	52 (96%)	2 (4%)	30	37
7	h	55/54 (102%)	55 (100%)	0	100	100
8	I	34/34 (100%)	32 (94%)	2 (6%)	18	18
8	i	34/34 (100%)	33 (97%)	1 (3%)	37	47
9	J	26/27 (96%)	24 (92%)	2 (8%)	12	10
9	j	26/27 (96%)	25 (96%)	1 (4%)	29	36
10	K	30/30 (100%)	26 (87%)	4 (13%)	4	2
10	k	30/30 (100%)	27 (90%)	3 (10%)	7	5
11	L	36/35 (103%)	36 (100%)	0	100	100
11	l	36/35 (103%)	35 (97%)	1 (3%)	38	48
12	M	30/32 (94%)	27 (90%)	3 (10%)	7	5
12	m	32/32 (100%)	30 (94%)	2 (6%)	16	16
13	O	216/207 (104%)	208 (96%)	8 (4%)	30	37
13	o	213/207 (103%)	206 (97%)	7 (3%)	33	42
14	T	32/28 (114%)	28 (88%)	4 (12%)	4	3
14	t	31/28 (111%)	31 (100%)	0	100	100
15	U	86/89 (97%)	84 (98%)	2 (2%)	44	55
15	u	87/89 (98%)	85 (98%)	2 (2%)	44	55
16	V	123/117 (105%)	122 (99%)	1 (1%)	73	80
16	v	123/117 (105%)	120 (98%)	3 (2%)	43	54
17	X	32/33 (97%)	32 (100%)	0	100	100
17	x	31/33 (94%)	31 (100%)	0	100	100
18	Y	22/23 (96%)	22 (100%)	0	100	100
18	y	22/23 (96%)	19 (86%)	3 (14%)	3	2
19	Z	52/52 (100%)	49 (94%)	3 (6%)	18	19
19	z	52/52 (100%)	45 (86%)	7 (14%)	4	2
20	R	29/29 (100%)	26 (90%)	3 (10%)	7	5
All	All	5103/4403 (116%)	4987 (98%)	116 (2%)	44	55

5 of 116 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	b	298	LEU
19	z	3	ILE
4	d	26	ARG
19	z	2	THR
16	v	85	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
2	b	331	ASN
3	c	415	ASN
19	Z	31	GLN
15	u	78	ASN
16	v	86	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
12	FME	m	1	12	8,9,10	0.56	0	7,9,11	1.53	2 (28%)
12	FME	M	1	12	8,9,10	0.60	0	7,9,11	1.15	1 (14%)
8	FME	I	1	8	8,9,10	0.59	0	7,9,11	1.19	1 (14%)
8	FME	i	1	8	8,9,10	0.71	0	7,9,11	1.23	0
14	FME	T	1	14	8,9,10	0.60	0	7,9,11	1.49	1 (14%)
14	FME	t	1	14	8,9,10	0.74	0	7,9,11	1.51	1 (14%)

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

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	FME	m	1	12	-	0/7/9/11	-
12	FME	M	1	12	-	1/7/9/11	-
8	FME	I	1	8	-	0/7/9/11	-
8	FME	i	1	8	-	0/7/9/11	-
14	FME	T	1	14	-	3/7/9/11	-
14	FME	t	1	14	-	1/7/9/11	-

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	m	1	FME	CA-N-CN	-2.59	118.84	122.82
14	T	1	FME	CG-CB-CA	2.48	119.83	112.95
14	t	1	FME	O-C-CA	-2.46	118.34	124.78
12	m	1	FME	O1-CN-N	-2.34	119.10	125.27
8	I	1	FME	O-C-CA	-2.16	119.11	124.78

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	M	1	FME	O1-CN-N-CA
14	T	1	FME	O1-CN-N-CA
14	t	1	FME	O1-CN-N-CA
14	T	1	FME	N-CA-CB-CG
14	T	1	FME	C-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	m	1	FME	4	0
12	M	1	FME	3	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 274 ligands modelled in this entry, 21 are monoatomic and 20 are unknown - leaving 233 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
23	CLA	d	403	4	69,73,73	2.01	18 (26%)	83,113,113	2.95	32 (38%)
25	BCR	b	619	-	41,41,41	1.04	1 (2%)	56,56,56	1.31	5 (8%)
25	BCR	c	516	-	41,41,41	1.02	1 (2%)	56,56,56	1.32	8 (14%)
37	LHG	l	101[A]	-	48,48,48	0.83	2 (4%)	51,54,54	1.04	4 (7%)
23	CLA	c	503	3	69,73,73	1.92	18 (26%)	83,113,113	2.76	27 (32%)
23	CLA	c	511	3	69,73,73	1.97	17 (24%)	83,113,113	2.83	33 (39%)
23	CLA	C	514	3	69,73,73	2.03	20 (28%)	83,113,113	2.85	31 (37%)
23	CLA	B	608	2	69,73,73	1.88	20 (28%)	83,113,113	2.88	34 (40%)
23	CLA	b	603	2	69,73,73	1.94	19 (27%)	83,113,113	2.91	31 (37%)
25	BCR	k	101	-	41,41,41	1.05	1 (2%)	56,56,56	1.37	7 (12%)
33	LMG	c	521	-	51,51,55	1.01	2 (3%)	59,59,63	1.33	6 (10%)
34	HTG	B	622	-	19,19,19	1.08	2 (10%)	23,24,24	1.56	5 (21%)
23	CLA	b	613	2	69,73,73	1.98	20 (28%)	83,113,113	2.81	31 (37%)
23	CLA	b	608	2	69,73,73	1.99	19 (27%)	83,113,113	2.82	35 (42%)
23	CLA	b	604	2	69,73,73	2.04	19 (27%)	83,113,113	2.77	27 (32%)
29	PL9	a	416[B]	-	55,55,55	0.63	2 (3%)	68,69,69	1.95	20 (29%)
27	GOL	A	701	-	5,5,5	1.48	2 (40%)	5,5,5	0.89	0
27	GOL	C	523[A]	-	5,5,5	1.11	0	5,5,5	0.88	0
34	HTG	C	522	-	19,19,19	0.84	1 (5%)	23,24,24	1.23	1 (4%)
32	LMT	b	627	-	25,25,36	0.86	0	30,30,47	1.11	3 (10%)
29	PL9	d	405[A]	-	55,55,55	0.70	1 (1%)	68,69,69	1.63	18 (26%)
33	LMG	a	419	-	51,51,55	0.91	2 (3%)	59,59,63	1.19	3 (5%)
23	CLA	c	512	3	69,73,73	2.06	21 (30%)	83,113,113	2.85	32 (38%)
34	HTG	b	623	-	19,19,19	1.01	1 (5%)	23,24,24	1.97	3 (13%)
25	BCR	C	515	-	41,41,41	1.02	1 (2%)	56,56,56	1.40	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	c	514	3	69,73,73	2.08	20 (28%)	83,113,113	2.87	30 (36%)
32	LMT	a	420	-	36,36,36	0.98	2 (5%)	47,47,47	1.04	2 (4%)
35	DGD	c	517[B]	-	63,63,67	0.88	2 (3%)	77,77,81	1.06	6 (7%)
26	SQD	B	620	-	53,54,54	1.08	4 (7%)	62,65,65	1.75	11 (17%)
35	DGD	C	517[B]	-	63,63,67	0.83	2 (3%)	77,77,81	1.05	7 (9%)
23	CLA	B	601	41	69,73,73	2.07	21 (30%)	83,113,113	2.85	27 (32%)
33	LMG	m	101	-	51,51,55	0.86	2 (3%)	59,59,63	1.32	7 (11%)
23	CLA	D	405[B]	4	69,73,73	1.98	20 (28%)	83,113,113	2.87	30 (36%)
27	GOL	b	624	-	5,5,5	1.12	1 (20%)	5,5,5	0.77	0
23	CLA	b	614	2	69,73,73	2.03	20 (28%)	83,113,113	2.99	30 (36%)
35	DGD	c	517[A]	-	63,63,67	0.85	2 (3%)	77,77,81	1.10	7 (9%)
38	HEM	E	103	5,6	50,50,50	1.55	8 (16%)	66,82,82	1.90	16 (24%)
35	DGD	C	517[A]	-	63,63,67	0.83	2 (3%)	77,77,81	1.20	8 (10%)
34	HTG	b	622	-	19,19,19	1.13	2 (10%)	23,24,24	2.01	7 (30%)
25	BCR	b	617	-	41,41,41	1.06	1 (2%)	56,56,56	1.34	3 (5%)
23	CLA	B	610	41	69,73,73	2.07	19 (27%)	83,113,113	2.85	30 (36%)
23	CLA	C	504	3	69,73,73	1.98	19 (27%)	83,113,113	2.83	29 (34%)
23	CLA	c	509	3	69,73,73	2.07	21 (30%)	83,113,113	2.79	29 (34%)
27	GOL	B	624	-	5,5,5	0.94	0	5,5,5	1.12	1 (20%)
26	SQD	A	410[B]	-	53,54,54	0.94	3 (5%)	62,65,65	1.72	11 (17%)
32	LMT	M	101	-	36,36,36	1.12	4 (11%)	47,47,47	1.22	4 (8%)
32	LMT	b	621	-	25,25,36	0.96	1 (4%)	30,30,47	1.21	3 (10%)
23	CLA	b	611	2	69,73,73	1.94	21 (30%)	83,113,113	2.88	27 (32%)
23	CLA	b	610	41	69,73,73	2.02	19 (27%)	83,113,113	2.88	31 (37%)
23	CLA	b	606	2	69,73,73	2.01	20 (28%)	83,113,113	2.93	31 (37%)
23	CLA	c	504	3	69,73,73	2.09	20 (28%)	83,113,113	2.83	28 (33%)
35	DGD	C	518[B]	-	63,63,67	0.86	2 (3%)	77,77,81	1.02	5 (6%)
23	CLA	C	511	3	69,73,73	2.01	20 (28%)	83,113,113	2.90	34 (40%)
23	CLA	B	603	2	69,73,73	1.98	20 (28%)	83,113,113	2.92	29 (34%)
23	CLA	D	406	4	69,73,73	2.07	18 (26%)	83,113,113	2.75	32 (38%)
23	CLA	a	406[B]	41	69,73,73	2.06	17 (24%)	83,113,113	2.84	32 (38%)
28	OEX	A	413[B]	1,3,41	0,14,14	-	-	-	-	-
31	BCT	A	348[B]	21	2,3,3	0.68	0	2,3,3	1.11	0
23	CLA	C	508	41	69,73,73	1.92	19 (27%)	83,113,113	2.78	32 (38%)
34	HTG	B	626	-	19,19,19	1.10	2 (10%)	23,24,24	1.34	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	GOL	d	701	-	5,5,5	1.26	1 (20%)	5,5,5	1.00	0
26	SQD	A	410[A]	-	53,54,54	0.93	3 (5%)	62,65,65	1.88	10 (16%)
32	LMT	e	102	-	36,36,36	1.01	2 (5%)	47,47,47	1.02	1 (2%)
29	PL9	A	414[B]	-	55,55,55	0.64	1 (1%)	68,69,69	1.99	23 (33%)
23	CLA	C	505	41	69,73,73	1.94	19 (27%)	83,113,113	2.86	29 (34%)
23	CLA	B	604	2	69,73,73	2.03	21 (30%)	83,113,113	2.70	32 (38%)
27	GOL	O	501	-	5,5,5	0.91	0	5,5,5	0.91	0
27	GOL	o	501	-	5,5,5	0.98	0	5,5,5	0.97	0
23	CLA	A	408	1	69,73,73	2.00	20 (28%)	83,113,113	3.02	33 (39%)
37	LHG	d	711[B]	-	48,48,48	0.90	2 (4%)	51,54,54	1.03	4 (7%)
29	PL9	D	408[B]	-	55,55,55	0.65	2 (3%)	68,69,69	1.63	17 (25%)
24	PHO	A	353[B]	-	58,69,69	2.78	16 (27%)	56,99,99	2.90	16 (28%)
23	CLA	a	406[A]	41	69,73,73	2.04	17 (24%)	83,113,113	2.86	32 (38%)
25	BCR	a	410	-	41,41,41	1.08	1 (2%)	56,56,56	1.37	9 (16%)
25	BCR	K	102	-	41,41,41	1.03	1 (2%)	56,56,56	1.50	13 (23%)
28	OEX	A	413[A]	1,3,41	0,14,14	-	-	-	-	-
31	BCT	A	348[A]	21	2,3,3	0.64	0	2,3,3	1.30	0
37	LHG	D	411[B]	-	48,48,48	0.92	2 (4%)	51,54,54	0.97	3 (5%)
23	CLA	b	612	2	69,73,73	2.01	19 (27%)	83,113,113	2.74	29 (34%)
23	CLA	B	609	2	69,73,73	1.99	18 (26%)	83,113,113	2.74	31 (37%)
26	SQD	b	620	-	53,54,54	1.06	3 (5%)	62,65,65	1.70	12 (19%)
27	GOL	d	801[B]	-	5,5,5	0.89	0	5,5,5	0.98	0
24	PHO	A	353[A]	-	58,69,69	2.79	15 (25%)	56,99,99	2.85	15 (26%)
29	PL9	a	416[A]	-	55,55,55	0.65	2 (3%)	68,69,69	2.01	22 (32%)
23	CLA	B	614	2	69,73,73	2.02	19 (27%)	83,113,113	3.02	31 (37%)
23	CLA	c	508	41	69,73,73	2.00	20 (28%)	83,113,113	2.87	29 (34%)
37	LHG	D	411[A]	-	48,48,48	0.93	2 (4%)	51,54,54	1.02	3 (5%)
27	GOL	a	412	-	5,5,5	0.88	0	5,5,5	1.00	0
35	DGD	c	518[B]	-	63,63,67	0.86	2 (3%)	77,77,81	0.94	5 (6%)
23	CLA	c	505	41	69,73,73	2.06	21 (30%)	83,113,113	2.84	29 (34%)
27	GOL	d	801[A]	-	5,5,5	0.93	0	5,5,5	0.98	0
27	GOL	D	701	-	5,5,5	1.52	2 (40%)	5,5,5	0.76	0
23	CLA	B	612	2	69,73,73	1.99	21 (30%)	83,113,113	2.69	29 (34%)
23	CLA	a	405[B]	1	69,73,73	2.05	20 (28%)	83,113,113	2.83	33 (39%)
35	DGD	h	102	-	63,63,67	0.87	3 (4%)	77,77,81	1.13	5 (6%)
23	CLA	C	503	3	69,73,73	2.02	19 (27%)	83,113,113	2.73	29 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	B	605	2	69,73,73	2.04	19 (27%)	83,113,113	2.99	31 (37%)
34	HTG	V	203	-	11,11,19	0.29	0	15,15,24	1.28	1 (6%)
23	CLA	D	405[A]	4	69,73,73	2.00	20 (28%)	83,113,113	2.86	32 (38%)
23	CLA	B	607	41	69,73,73	1.96	19 (27%)	83,113,113	2.82	29 (34%)
32	LMT	m	103	-	36,36,36	1.05	3 (8%)	47,47,47	1.19	4 (8%)
25	BCR	B	617	-	41,41,41	1.09	1 (2%)	56,56,56	1.27	8 (14%)
26	SQD	f	102	-	42,43,54	1.21	3 (7%)	51,54,65	1.48	12 (23%)
23	CLA	A	406[B]	41	69,73,73	2.08	19 (27%)	83,113,113	2.86	33 (39%)
32	LMT	M	103	-	36,36,36	1.05	3 (8%)	47,47,47	1.05	2 (4%)
23	CLA	a	405[A]	1	69,73,73	1.99	20 (28%)	83,113,113	2.87	33 (39%)
23	CLA	b	605	2	69,73,73	1.95	19 (27%)	83,113,113	2.97	30 (36%)
26	SQD	A	412	-	53,54,54	1.04	3 (5%)	62,65,65	1.30	7 (11%)
27	GOL	a	801	-	5,5,5	1.32	1 (20%)	5,5,5	1.09	1 (20%)
26	SQD	a	413	-	53,54,54	1.08	4 (7%)	62,65,65	1.18	8 (12%)
40	HEC	v	202	16	50,50,50	1.77	7 (14%)	68,82,82	1.43	12 (17%)
23	CLA	C	506	3	69,73,73	2.04	19 (27%)	83,113,113	2.82	30 (36%)
23	CLA	B	611	2	69,73,73	2.66	19 (27%)	83,113,113	4.21	28 (33%)
32	LMT	t	101	-	25,25,36	0.91	2 (8%)	30,30,47	1.16	3 (10%)
37	LHG	D	409[B]	-	48,48,48	0.88	2 (4%)	51,54,54	1.20	5 (9%)
33	LMG	C	520	-	51,51,55	0.95	2 (3%)	59,59,63	1.10	4 (6%)
34	HTG	D	414	-	16,16,19	0.98	1 (6%)	20,21,24	1.60	1 (5%)
23	CLA	A	406[A]	41	69,73,73	2.04	19 (27%)	83,113,113	2.85	32 (38%)
23	CLA	A	404[B]	1	69,73,73	2.08	19 (27%)	83,113,113	2.80	32 (38%)
25	BCR	D	407	-	41,41,41	1.12	1 (2%)	56,56,56	1.87	17 (30%)
23	CLA	C	512	3	69,73,73	2.04	21 (30%)	83,113,113	2.71	28 (33%)
23	CLA	c	510	3	69,73,73	2.04	19 (27%)	83,113,113	2.88	32 (38%)
23	CLA	B	616	2	69,73,73	2.03	20 (28%)	83,113,113	2.78	29 (34%)
24	PHO	A	407[B]	-	58,69,69	2.76	11 (18%)	56,99,99	2.70	16 (28%)
24	PHO	a	353[B]	-	58,69,69	2.80	14 (24%)	56,99,99	2.88	15 (26%)
24	PHO	a	408[B]	-	58,69,69	2.73	13 (22%)	56,99,99	2.73	14 (25%)
25	BCR	T	101	-	41,41,41	1.00	1 (2%)	56,56,56	1.53	13 (23%)
26	SQD	a	411[B]	-	53,54,54	0.97	3 (5%)	62,65,65	1.68	12 (19%)
32	LMT	D	404	-	36,36,36	1.18	4 (11%)	47,47,47	1.38	5 (10%)
23	CLA	d	402[B]	4	69,73,73	2.01	20 (28%)	83,113,113	2.84	30 (36%)
34	HTG	b	625	-	19,19,19	1.06	2 (10%)	23,24,24	1.53	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	GOL	a	701	-	5,5,5	1.07	0	5,5,5	1.02	0
23	CLA	B	602	2	69,73,73	2.05	21 (30%)	83,113,113	2.91	35 (42%)
27	GOL	V	401[B]	-	5,5,5	1.17	0	5,5,5	0.92	0
37	LHG	e	101[B]	-	41,41,48	1.04	2 (4%)	44,47,54	0.91	2 (4%)
33	LMG	C	501	-	51,51,55	0.91	2 (3%)	59,59,63	1.61	8 (13%)
34	HTG	d	411	-	16,16,19	0.92	1 (6%)	20,21,24	1.58	1 (5%)
23	CLA	A	405[B]	41	69,73,73	2.04	19 (27%)	83,113,113	2.85	33 (39%)
27	GOL	A	411	-	5,5,5	1.09	0	5,5,5	0.78	0
29	PL9	A	414[A]	-	55,55,55	0.69	2 (3%)	68,69,69	2.01	24 (35%)
23	CLA	a	407[B]	41	69,73,73	2.02	20 (28%)	83,113,113	2.90	31 (37%)
37	LHG	d	711[A]	-	48,48,48	0.89	2 (4%)	51,54,54	1.11	4 (7%)
25	BCR	Y	101	-	41,41,41	1.01	1 (2%)	56,56,56	1.80	16 (28%)
23	CLA	b	601	41	69,73,73	2.12	20 (28%)	83,113,113	2.81	27 (32%)
24	PHO	A	407[A]	-	58,69,69	2.66	12 (20%)	56,99,99	2.81	14 (25%)
24	PHO	a	353[A]	-	58,69,69	2.77	13 (22%)	56,99,99	2.94	17 (30%)
29	PL9	D	408[A]	-	55,55,55	0.63	1 (1%)	68,69,69	1.61	17 (25%)
24	PHO	a	408[A]	-	58,69,69	2.74	13 (22%)	56,99,99	2.81	14 (25%)
26	SQD	a	411[A]	-	53,54,54	0.96	3 (5%)	62,65,65	1.83	13 (20%)
32	LMT	A	359	-	36,36,36	0.91	0	47,47,47	1.10	1 (2%)
35	DGD	C	518[A]	-	63,63,67	0.90	3 (4%)	77,77,81	1.03	5 (6%)
27	GOL	V	401[A]	-	5,5,5	1.34	0	5,5,5	0.80	0
28	OEX	a	415[B]	1,3,41	0,14,14	-	-	-	-	-
34	HTG	B	623	-	19,19,19	0.76	1 (5%)	23,24,24	1.43	1 (4%)
27	GOL	v	401[B]	-	5,5,5	1.02	0	5,5,5	0.86	0
35	DGD	C	519	-	63,63,67	0.85	3 (4%)	77,77,81	1.01	4 (5%)
37	LHG	L	101[B]	-	48,48,48	0.93	3 (6%)	51,54,54	1.10	3 (5%)
23	CLA	A	405[A]	41	69,73,73	2.02	18 (26%)	83,113,113	2.85	33 (39%)
23	CLA	c	507	3	69,73,73	2.05	21 (30%)	83,113,113	2.82	30 (36%)
25	BCR	b	618	-	41,41,41	1.04	1 (2%)	56,56,56	1.30	9 (16%)
23	CLA	a	407[A]	41	69,73,73	1.98	19 (27%)	83,113,113	2.83	30 (36%)
25	BCR	H	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.43	8 (14%)
33	LMG	z	101	-	39,39,55	1.09	2 (5%)	47,47,63	1.10	5 (10%)
26	SQD	F	101	-	42,43,54	1.20	4 (9%)	51,54,65	2.18	14 (27%)
27	GOL	O	601	-	5,5,5	0.79	0	5,5,5	1.12	1 (20%)
34	HTG	c	522	-	19,19,19	0.89	1 (5%)	23,24,24	1.49	2 (8%)
25	BCR	h	101	-	41,41,41	1.04	1 (2%)	56,56,56	1.47	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	c	513	3	69,73,73	2.07	20 (28%)	83,113,113	2.84	31 (37%)
28	OEX	a	415[A]	1,3,41	0,14,14	-	-	-		
27	GOL	v	401[A]	-	5,5,5	1.20	0	5,5,5	0.82	0
25	BCR	B	618	-	41,41,41	0.98	1 (2%)	56,56,56	1.48	7 (12%)
35	DGD	c	518[A]	-	63,63,67	0.85	3 (4%)	77,77,81	0.97	3 (3%)
37	LHG	L	101[A]	-	48,48,48	0.88	2 (4%)	51,54,54	1.15	4 (7%)
27	GOL	B	901	-	5,5,5	1.13	0	5,5,5	1.00	0
33	LMG	d	412	39	51,51,55	0.89	2 (3%)	59,59,63	1.14	5 (8%)
27	GOL	C	523[B]	-	5,5,5	1.07	0	5,5,5	0.84	0
37	LHG	d	407[B]	-	48,48,48	0.89	2 (4%)	51,54,54	1.06	4 (7%)
23	CLA	b	616	2	69,73,73	2.01	20 (28%)	83,113,113	2.97	33 (39%)
27	GOL	o	601	-	5,5,5	1.15	1 (20%)	5,5,5	1.09	0
23	CLA	c	502	3	69,73,73	2.00	20 (28%)	83,113,113	2.86	31 (37%)
29	PL9	d	405[B]	-	55,55,55	0.65	1 (1%)	68,69,69	1.65	17 (25%)
33	LMG	D	415	39	51,51,55	0.81	2 (3%)	59,59,63	1.07	3 (5%)
37	LHG	d	408[B]	-	48,48,48	0.91	2 (4%)	51,54,54	1.07	3 (5%)
23	CLA	C	502	3	69,73,73	1.97	19 (27%)	83,113,113	2.87	32 (38%)
23	CLA	b	602	2	69,73,73	2.08	18 (26%)	83,113,113	2.96	34 (40%)
37	LHG	E	101[B]	-	41,41,48	1.06	2 (4%)	44,47,54	1.10	3 (6%)
23	CLA	a	409	1	69,73,73	1.97	17 (24%)	83,113,113	2.96	30 (36%)
31	BCT	a	404[B]	21	2,3,3	0.61	0	2,3,3	1.19	0
40	HEC	V	202	16	50,50,50	1.75	6 (12%)	68,82,82	1.49	10 (14%)
35	DGD	H	102	-	63,63,67	0.83	3 (4%)	77,77,81	1.07	7 (9%)
23	CLA	B	615	2	69,73,73	2.02	19 (27%)	83,113,113	2.87	29 (34%)
25	BCR	y	101	-	41,41,41	1.06	1 (2%)	56,56,56	1.56	8 (14%)
23	CLA	B	606	2	69,73,73	1.93	19 (27%)	83,113,113	2.98	33 (39%)
23	CLA	C	513	3	69,73,73	2.03	19 (27%)	83,113,113	2.86	34 (40%)
37	LHG	d	407[A]	-	48,48,48	0.87	2 (4%)	51,54,54	1.04	4 (7%)
27	GOL	c	742[B]	-	5,5,5	0.98	0	5,5,5	0.90	0
33	LMG	B	621	-	51,51,55	0.90	2 (3%)	59,59,63	1.29	4 (6%)
37	LHG	d	408[A]	-	48,48,48	0.92	2 (4%)	51,54,54	1.01	3 (5%)
23	CLA	c	506	3	69,73,73	2.03	19 (27%)	83,113,113	2.76	28 (33%)
37	LHG	D	410[B]	-	48,48,48	0.91	2 (4%)	51,54,54	0.99	4 (7%)
37	LHG	E	101[A]	-	41,41,48	1.08	2 (4%)	44,47,54	1.10	3 (6%)
23	CLA	b	615	2	69,73,73	2.03	19 (27%)	83,113,113	2.80	31 (37%)
33	LMG	c	520	-	51,51,55	0.90	2 (3%)	59,59,63	1.14	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	BCT	a	404[A]	21	2,3,3	0.59	0	2,3,3	1.49	0
35	DGD	c	519	-	63,63,67	0.87	4 (6%)	77,77,81	1.06	4 (5%)
33	LMG	C	521	-	51,51,55	1.08	3 (5%)	59,59,63	1.36	7 (11%)
25	BCR	C	516	-	41,41,41	1.05	1 (2%)	56,56,56	1.30	4 (7%)
37	LHG	D	409[A]	-	48,48,48	0.87	2 (4%)	51,54,54	1.27	6 (11%)
23	CLA	B	613	2	69,73,73	1.98	19 (27%)	83,113,113	2.78	30 (36%)
25	BCR	t	103	-	41,41,41	1.05	1 (2%)	56,56,56	1.63	11 (19%)
27	GOL	c	742[A]	-	5,5,5	1.00	0	5,5,5	0.98	0
23	CLA	A	404[A]	1	69,73,73	2.00	20 (28%)	83,113,113	2.87	30 (36%)
23	CLA	C	507	3	69,73,73	2.02	21 (30%)	83,113,113	2.84	31 (37%)
33	LMG	Z	101	-	37,37,55	1.02	2 (5%)	45,45,63	1.42	6 (13%)
37	LHG	D	410[A]	-	48,48,48	0.87	2 (4%)	51,54,54	1.01	3 (5%)
32	LMT	E	102	-	36,36,36	1.03	1 (2%)	47,47,47	1.01	2 (4%)
32	LMT	a	414	-	36,36,36	1.02	2 (5%)	47,47,47	1.17	5 (10%)
27	GOL	b	901	-	5,5,5	0.54	0	5,5,5	1.40	1 (20%)
37	LHG	e	101[A]	-	41,41,48	1.06	2 (4%)	44,47,54	0.92	2 (4%)
23	CLA	d	402[A]	4	69,73,73	1.95	20 (28%)	83,113,113	2.76	32 (38%)
25	BCR	d	404	-	41,41,41	1.10	1 (2%)	56,56,56	2.00	17 (30%)
25	BCR	c	515	-	41,41,41	0.99	1 (2%)	56,56,56	1.60	15 (26%)
25	BCR	A	409	-	41,41,41	0.97	1 (2%)	56,56,56	1.42	9 (16%)
23	CLA	C	509	3	69,73,73	2.00	20 (28%)	83,113,113	2.77	29 (34%)
23	CLA	b	607	41	69,73,73	1.96	19 (27%)	83,113,113	2.71	29 (34%)
37	LHG	l	101[B]	-	48,48,48	0.90	2 (4%)	51,54,54	1.00	2 (3%)
25	BCR	B	619	-	41,41,41	1.09	2 (4%)	56,56,56	1.38	8 (14%)
23	CLA	C	510	3	69,73,73	2.08	20 (28%)	83,113,113	2.83	30 (36%)
23	CLA	b	609	2	69,73,73	2.03	19 (27%)	83,113,113	2.79	30 (36%)
38	HEM	e	87	5,6	50,50,50	1.49	6 (12%)	66,82,82	1.77	13 (19%)
32	LMT	I	101	-	36,36,36	1.04	2 (5%)	47,47,47	1.19	4 (8%)
27	GOL	c	743	-	5,5,5	1.04	0	5,5,5	0.97	0
32	LMT	t	102	-	26,26,36	0.88	2 (7%)	31,31,47	1.33	3 (9%)

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
23	CLA	d	403	4	-	8/39/115/115	-
25	BCR	b	619	-	-	4/29/63/63	0/2/2/2
25	BCR	c	516	-	-	0/29/63/63	0/2/2/2
37	LHG	l	101[A]	-	-	14/53/53/53	-
23	CLA	c	503	3	-	7/39/115/115	-
23	CLA	c	511	3	-	11/39/115/115	-
23	CLA	C	514	3	-	6/39/115/115	-
23	CLA	B	608	2	-	3/39/115/115	-
23	CLA	b	603	2	-	8/39/115/115	-
25	BCR	k	101	-	-	0/29/63/63	0/2/2/2
33	LMG	c	521	-	-	11/46/66/70	0/1/1/1
34	HTG	B	622	-	-	4/10/30/30	0/1/1/1
23	CLA	b	613	2	-	6/39/115/115	-
23	CLA	b	608	2	-	6/39/115/115	-
23	CLA	b	604	2	-	13/39/115/115	-
29	PL9	a	416[B]	-	-	14/53/73/73	0/1/1/1
27	GOL	A	701	-	-	2/4/4/4	-
27	GOL	C	523[A]	-	-	0/4/4/4	-
34	HTG	C	522	-	-	0/10/30/30	0/1/1/1
32	LMT	b	627	-	-	11/17/37/61	0/1/1/2
29	PL9	d	405[A]	-	-	7/53/73/73	0/1/1/1
33	LMG	a	419	-	-	11/46/66/70	0/1/1/1
23	CLA	c	512	3	-	7/39/115/115	-
34	HTG	b	623	-	-	5/10/30/30	0/1/1/1
25	BCR	C	515	-	-	0/29/63/63	0/2/2/2
23	CLA	c	514	3	-	11/39/115/115	-
32	LMT	a	420	-	-	11/21/61/61	0/2/2/2
35	DGD	c	517[B]	-	-	20/51/91/95	0/2/2/2
26	SQD	B	620	-	-	11/49/69/69	0/1/1/1
35	DGD	C	517[B]	-	-	13/51/91/95	0/2/2/2
23	CLA	B	601	41	-	13/39/115/115	-
33	LMG	m	101	-	-	11/46/66/70	0/1/1/1
23	CLA	D	405[B]	4	-	5/39/115/115	-
27	GOL	b	624	-	-	2/4/4/4	-
23	CLA	b	614	2	-	14/39/115/115	-
35	DGD	c	517[A]	-	-	18/51/91/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	HEM	E	103	5,6	-	8/14/54/54	-
35	DGD	C	517[A]	-	-	14/51/91/95	0/2/2/2
34	HTG	b	622	-	-	5/10/30/30	0/1/1/1
25	BCR	b	617	-	-	2/29/63/63	0/2/2/2
23	CLA	B	610	41	-	9/39/115/115	-
23	CLA	C	504	3	-	3/39/115/115	-
23	CLA	c	509	3	-	5/39/115/115	-
27	GOL	B	624	-	-	4/4/4/4	-
26	SQD	A	410[B]	-	-	11/49/69/69	0/1/1/1
32	LMT	M	101	-	-	5/21/61/61	0/2/2/2
32	LMT	b	621	-	-	8/17/37/61	0/1/1/2
23	CLA	b	611	2	-	3/39/115/115	-
23	CLA	b	610	41	-	7/39/115/115	-
23	CLA	b	606	2	-	14/39/115/115	-
23	CLA	c	504	3	-	1/39/115/115	-
35	DGD	C	518[B]	-	-	13/51/91/95	0/2/2/2
23	CLA	C	511	3	-	14/39/115/115	-
23	CLA	B	603	2	-	5/39/115/115	-
23	CLA	D	406	4	-	14/39/115/115	-
23	CLA	a	406[B]	41	-	3/39/115/115	-
23	CLA	C	508	41	-	9/39/115/115	-
34	HTG	B	626	-	-	4/10/30/30	0/1/1/1
27	GOL	d	701	-	-	2/4/4/4	-
26	SQD	A	410[A]	-	-	12/49/69/69	0/1/1/1
32	LMT	e	102	-	-	14/21/61/61	0/2/2/2
29	PL9	A	414[B]	-	-	12/53/73/73	0/1/1/1
23	CLA	C	505	41	-	9/39/115/115	-
23	CLA	B	604	2	-	2/39/115/115	-
27	GOL	O	501	-	-	2/4/4/4	-
27	GOL	o	501	-	-	2/4/4/4	-
23	CLA	A	408	1	-	9/39/115/115	-
37	LHG	d	711[B]	-	-	10/53/53/53	-
29	PL9	D	408[B]	-	-	10/53/73/73	0/1/1/1
24	PHO	A	353[B]	-	-	0/37/103/103	0/5/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	a	406[A]	41	-	8/39/115/115	-
25	BCR	a	410	-	-	3/29/63/63	0/2/2/2
25	BCR	K	102	-	-	2/29/63/63	0/2/2/2
37	LHG	D	411[B]	-	-	14/53/53/53	-
23	CLA	b	612	2	-	5/39/115/115	-
23	CLA	B	609	2	-	1/39/115/115	-
26	SQD	b	620	-	-	18/49/69/69	0/1/1/1
27	GOL	d	801[B]	-	-	2/4/4/4	-
24	PHO	A	353[A]	-	-	1/37/103/103	0/5/6/6
29	PL9	a	416[A]	-	-	14/53/73/73	0/1/1/1
23	CLA	B	614	2	-	15/39/115/115	-
23	CLA	c	508	41	-	9/39/115/115	-
37	LHG	D	411[A]	-	-	14/53/53/53	-
27	GOL	a	412	-	-	4/4/4/4	-
35	DGD	c	518[B]	-	-	16/51/91/95	0/2/2/2
23	CLA	c	505	41	-	6/39/115/115	-
27	GOL	d	801[A]	-	-	1/4/4/4	-
27	GOL	D	701	-	-	4/4/4/4	-
23	CLA	B	612	2	-	5/39/115/115	-
23	CLA	a	405[B]	1	-	6/39/115/115	-
35	DGD	h	102	-	-	14/51/91/95	0/2/2/2
23	CLA	C	503	3	-	10/39/115/115	-
23	CLA	B	605	2	-	6/39/115/115	-
34	HTG	V	203	-	-	0/2/19/30	0/1/1/1
23	CLA	D	405[A]	4	-	2/39/115/115	-
23	CLA	B	607	41	-	3/39/115/115	-
32	LMT	m	103	-	-	6/21/61/61	0/2/2/2
25	BCR	B	617	-	-	1/29/63/63	0/2/2/2
26	SQD	f	102	-	-	12/38/58/69	0/1/1/1
23	CLA	A	406[B]	41	-	4/39/115/115	-
32	LMT	M	103	-	-	7/21/61/61	0/2/2/2
23	CLA	a	405[A]	1	-	4/39/115/115	-
23	CLA	b	605	2	-	7/39/115/115	-
26	SQD	A	412	-	-	13/49/69/69	0/1/1/1
27	GOL	a	801	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	SQD	a	413	-	-	14/49/69/69	0/1/1/1
40	HEC	v	202	16	1/1/3/7	6/14/54/54	-
23	CLA	C	506	3	-	7/39/115/115	-
23	CLA	B	611	2	-	2/39/115/115	-
32	LMT	t	101	-	-	9/17/37/61	0/1/1/2
37	LHG	D	409[B]	-	-	14/53/53/53	-
33	LMG	C	520	-	-	11/46/66/70	0/1/1/1
34	HTG	D	414	-	-	3/7/27/30	0/1/1/1
23	CLA	A	406[A]	41	-	5/39/115/115	-
23	CLA	A	404[B]	1	-	8/39/115/115	-
25	BCR	D	407	-	-	4/29/63/63	0/2/2/2
23	CLA	C	512	3	-	4/39/115/115	-
23	CLA	c	510	3	-	14/39/115/115	-
23	CLA	B	616	2	-	7/39/115/115	-
24	PHO	A	407[B]	-	-	3/37/103/103	0/5/6/6
24	PHO	a	353[B]	-	-	2/37/103/103	0/5/6/6
24	PHO	a	408[B]	-	-	5/37/103/103	0/5/6/6
25	BCR	T	101	-	-	1/29/63/63	0/2/2/2
26	SQD	a	411[B]	-	-	8/49/69/69	0/1/1/1
32	LMT	D	404	-	-	12/21/61/61	0/2/2/2
23	CLA	d	402[B]	4	-	5/39/115/115	-
34	HTG	b	625	-	-	3/10/30/30	0/1/1/1
27	GOL	a	701	-	-	2/4/4/4	-
23	CLA	B	602	2	-	9/39/115/115	-
27	GOL	V	401[B]	-	-	2/4/4/4	-
37	LHG	e	101[B]	-	-	16/46/46/53	-
33	LMG	C	501	-	-	13/46/66/70	0/1/1/1
34	HTG	d	411	-	-	1/7/27/30	0/1/1/1
23	CLA	A	405[B]	41	-	6/39/115/115	-
27	GOL	A	411	-	-	2/4/4/4	-
29	PL9	A	414[A]	-	-	15/53/73/73	0/1/1/1
23	CLA	a	407[B]	41	-	7/39/115/115	-
37	LHG	d	711[A]	-	-	17/53/53/53	-
25	BCR	Y	101	-	-	3/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	b	601	41	-	20/39/115/115	-
24	PHO	A	407[A]	-	-	3/37/103/103	0/5/6/6
24	PHO	a	353[A]	-	-	1/37/103/103	0/5/6/6
29	PL9	D	408[A]	-	-	6/53/73/73	0/1/1/1
24	PHO	a	408[A]	-	-	6/37/103/103	0/5/6/6
26	SQD	a	411[A]	-	-	9/49/69/69	0/1/1/1
32	LMT	A	359	-	-	8/21/61/61	0/2/2/2
35	DGD	C	518[A]	-	-	13/51/91/95	0/2/2/2
27	GOL	V	401[A]	-	-	2/4/4/4	-
34	HTG	B	623	-	-	2/10/30/30	0/1/1/1
27	GOL	v	401[B]	-	-	2/4/4/4	-
35	DGD	C	519	-	-	19/51/91/95	0/2/2/2
37	LHG	L	101[B]	-	-	20/53/53/53	-
23	CLA	A	405[A]	41	-	3/39/115/115	-
23	CLA	c	507	3	-	8/39/115/115	-
25	BCR	b	618	-	-	0/29/63/63	0/2/2/2
23	CLA	a	407[A]	41	-	8/39/115/115	-
25	BCR	H	101	-	-	2/29/63/63	0/2/2/2
33	LMG	z	101	-	-	9/34/54/70	0/1/1/1
26	SQD	F	101	-	-	15/38/58/69	0/1/1/1
27	GOL	O	601	-	-	2/4/4/4	-
34	HTG	c	522	-	-	2/10/30/30	0/1/1/1
25	BCR	h	101	-	-	2/29/63/63	0/2/2/2
23	CLA	c	513	3	-	12/39/115/115	-
27	GOL	v	401[A]	-	-	2/4/4/4	-
25	BCR	B	618	-	-	0/29/63/63	0/2/2/2
35	DGD	c	518[A]	-	-	16/51/91/95	0/2/2/2
37	LHG	L	101[A]	-	-	20/53/53/53	-
27	GOL	B	901	-	-	1/4/4/4	-
33	LMG	d	412	39	-	9/46/66/70	0/1/1/1
27	GOL	C	523[B]	-	-	0/4/4/4	-
37	LHG	d	407[B]	-	-	15/53/53/53	-
23	CLA	b	616	2	-	9/39/115/115	-
27	GOL	o	601	-	-	4/4/4/4	-
23	CLA	c	502	3	-	6/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PL9	d	405[B]	-	-	7/53/73/73	0/1/1/1
33	LMG	D	415	39	-	8/46/66/70	0/1/1/1
37	LHG	d	408[B]	-	-	16/53/53/53	-
23	CLA	C	502	3	-	5/39/115/115	-
23	CLA	b	602	2	-	3/39/115/115	-
37	LHG	E	101[B]	-	-	19/46/46/53	-
23	CLA	a	409	1	-	11/39/115/115	-
40	HEC	V	202	16	1/1/3/7	6/14/54/54	-
35	DGD	H	102	-	-	14/51/91/95	0/2/2/2
23	CLA	B	615	2	-	8/39/115/115	-
25	BCR	y	101	-	-	5/29/63/63	0/2/2/2
23	CLA	B	606	2	-	8/39/115/115	-
23	CLA	C	513	3	-	12/39/115/115	-
37	LHG	d	407[A]	-	-	13/53/53/53	-
27	GOL	c	742[B]	-	-	0/4/4/4	-
33	LMG	B	621	-	-	16/46/66/70	0/1/1/1
37	LHG	d	408[A]	-	-	13/53/53/53	-
23	CLA	c	506	3	-	7/39/115/115	-
37	LHG	D	410[B]	-	-	16/53/53/53	-
37	LHG	E	101[A]	-	-	22/46/46/53	-
23	CLA	b	615	2	-	8/39/115/115	-
33	LMG	c	520	-	-	11/46/66/70	0/1/1/1
35	DGD	c	519	-	-	10/51/91/95	0/2/2/2
33	LMG	C	521	-	-	15/46/66/70	0/1/1/1
25	BCR	C	516	-	-	0/29/63/63	0/2/2/2
37	LHG	D	409[A]	-	-	14/53/53/53	-
23	CLA	B	613	2	-	8/39/115/115	-
25	BCR	t	103	-	-	0/29/63/63	0/2/2/2
27	GOL	c	742[A]	-	-	0/4/4/4	-
23	CLA	A	404[A]	1	-	3/39/115/115	-
23	CLA	C	507	3	-	13/39/115/115	-
33	LMG	Z	101	-	-	11/31/51/70	0/1/1/1
37	LHG	D	410[A]	-	-	17/53/53/53	-
32	LMT	E	102	-	-	8/21/61/61	0/2/2/2
32	LMT	a	414	-	-	12/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	GOL	b	901	-	-	0/4/4/4	-
37	LHG	e	101[A]	-	-	16/46/46/53	-
23	CLA	d	402[A]	4	-	4/39/115/115	-
25	BCR	d	404	-	-	4/29/63/63	0/2/2/2
25	BCR	c	515	-	-	1/29/63/63	0/2/2/2
25	BCR	A	409	-	-	0/29/63/63	0/2/2/2
23	CLA	C	509	3	-	6/39/115/115	-
23	CLA	b	607	41	-	4/39/115/115	-
37	LHG	l	101[B]	-	-	17/53/53/53	-
25	BCR	B	619	-	-	0/29/63/63	0/2/2/2
23	CLA	C	510	3	-	6/39/115/115	-
23	CLA	b	609	2	-	1/39/115/115	-
38	HEM	e	87	5,6	-	8/14/54/54	-
32	LMT	I	101	-	-	15/21/61/61	0/2/2/2
27	GOL	c	743	-	-	4/4/4/4	-
32	LMT	t	102	-	-	9/17/38/61	0/1/1/2

The worst 5 of 1865 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	407[B]	PHO	C1D-C2D	9.36	1.50	1.39
24	a	408[A]	PHO	C1B-C2B	9.21	1.49	1.39
24	a	353[B]	PHO	C1D-C2D	9.12	1.49	1.39
24	A	407[B]	PHO	C1B-C2B	8.99	1.49	1.39
24	a	408[B]	PHO	C1B-C2B	8.96	1.49	1.39

The worst 5 of 3316 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	611	CLA	C2B-C1B-NB	17.87	122.21	110.23
23	B	611	CLA	C3B-C2B-C1B	-14.72	89.39	107.16
24	A	353[B]	PHO	C2D-C1D-ND	11.90	117.74	109.53
24	A	407[A]	PHO	C2D-C1D-ND	11.89	117.73	109.53
23	B	611	CLA	C1D-ND-C4D	-11.73	98.00	106.33

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
40	V	202	HEC	NA

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Mol	Chain	Res	Type	Atom
40	v	202	HEC	NA

5 of 1699 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	A	404[B]	CLA	C2B-C3B-CAB-CBB
23	A	404[B]	CLA	C4B-C3B-CAB-CBB
23	A	408	CLA	C2-C3-C5-C6
23	A	408	CLA	C4-C3-C5-C6
23	B	601	CLA	CHA-CBD-CGD-O1D

There are no ring outliers.

170 monomers are involved in 360 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	d	403	CLA	2	0
25	b	619	BCR	4	0
25	c	516	BCR	1	0
23	c	503	CLA	2	0
23	c	511	CLA	1	0
23	C	514	CLA	2	0
25	k	101	BCR	2	0
33	c	521	LMG	1	0
34	B	622	HTG	1	0
23	b	613	CLA	1	0
23	b	604	CLA	2	0
29	a	416[B]	PL9	5	0
27	A	701	GOL	6	0
23	c	512	CLA	6	0
25	C	515	BCR	1	0
23	c	514	CLA	2	0
32	a	420	LMT	1	0
35	c	517[B]	DGD	2	0
26	B	620	SQD	1	0
35	C	517[B]	DGD	1	0
23	B	601	CLA	3	0
23	D	405[B]	CLA	5	0
23	b	614	CLA	2	0
35	c	517[A]	DGD	1	0
38	E	103	HEM	2	0
35	C	517[A]	DGD	1	0
34	b	622	HTG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	b	617	BCR	1	0
23	C	504	CLA	4	0
23	c	509	CLA	3	0
27	B	624	GOL	2	0
26	A	410[B]	SQD	2	0
32	M	101	LMT	2	0
32	b	621	LMT	1	0
23	b	611	CLA	1	0
23	b	610	CLA	1	0
23	b	606	CLA	2	0
23	c	504	CLA	3	0
23	C	511	CLA	5	0
23	a	406[B]	CLA	1	0
23	C	508	CLA	2	0
34	B	626	HTG	1	0
26	A	410[A]	SQD	1	0
32	e	102	LMT	1	0
29	A	414[B]	PL9	9	0
23	C	505	CLA	1	0
23	B	604	CLA	2	0
27	O	501	GOL	1	0
23	A	408	CLA	3	0
37	d	711[B]	LHG	2	0
24	A	353[B]	PHO	3	0
23	a	406[A]	CLA	3	0
25	a	410	BCR	1	0
25	K	102	BCR	2	0
37	D	411[B]	LHG	5	0
23	b	612	CLA	1	0
23	B	609	CLA	2	0
26	b	620	SQD	4	0
24	A	353[A]	PHO	1	0
29	a	416[A]	PL9	5	0
23	B	614	CLA	2	0
23	c	508	CLA	3	0
37	D	411[A]	LHG	4	0
35	c	518[B]	DGD	2	0
23	c	505	CLA	2	0
27	d	801[A]	GOL	1	0
27	D	701	GOL	3	0
23	B	612	CLA	2	0
23	a	405[B]	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	C	503	CLA	4	0
23	B	605	CLA	3	0
23	D	405[A]	CLA	3	0
32	m	103	LMT	1	0
23	A	406[B]	CLA	2	0
23	a	405[A]	CLA	2	0
23	b	605	CLA	3	0
27	a	801	GOL	4	0
26	a	413	SQD	1	0
23	C	506	CLA	5	0
32	t	101	LMT	1	0
37	D	409[B]	LHG	2	0
34	D	414	HTG	1	0
23	A	406[A]	CLA	1	0
23	A	404[B]	CLA	7	0
25	D	407	BCR	1	0
23	C	512	CLA	3	0
23	c	510	CLA	4	0
23	B	616	CLA	4	0
24	A	407[B]	PHO	1	0
24	a	353[B]	PHO	1	0
24	a	408[B]	PHO	3	0
25	T	101	BCR	7	0
26	a	411[B]	SQD	3	0
23	d	402[B]	CLA	4	0
34	b	625	HTG	1	0
27	a	701	GOL	2	0
23	B	602	CLA	1	0
37	e	101[B]	LHG	4	0
34	d	411	HTG	1	0
23	A	405[B]	CLA	5	0
27	A	411	GOL	1	0
29	A	414[A]	PL9	11	0
23	a	407[B]	CLA	3	0
25	Y	101	BCR	1	0
23	b	601	CLA	2	0
24	A	407[A]	PHO	1	0
24	a	353[A]	PHO	1	0
29	D	408[A]	PL9	1	0
26	a	411[A]	SQD	3	0
35	C	518[A]	DGD	1	0
34	B	623	HTG	1	0

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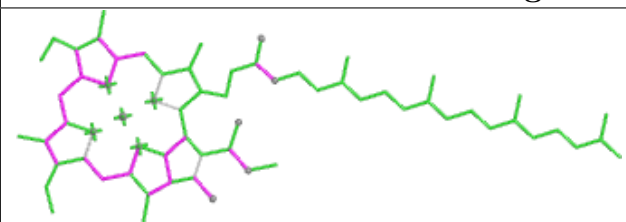
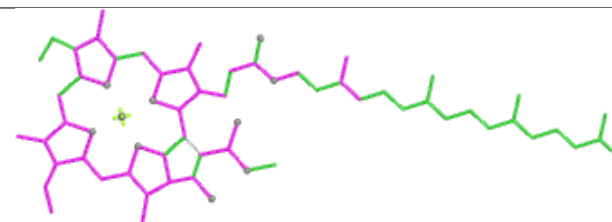
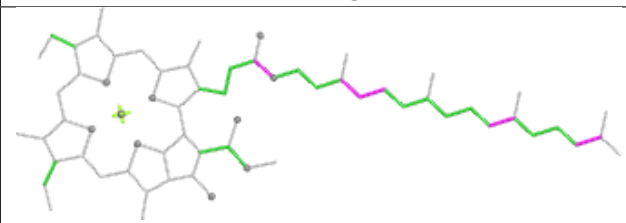
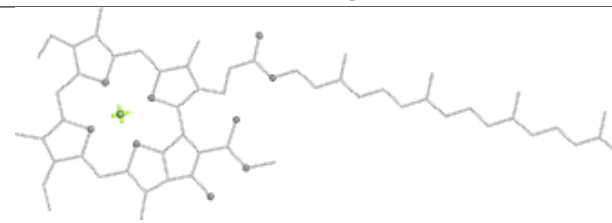
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27	v	401[B]	GOL	2	0
35	C	519	DGD	1	0
23	A	405[A]	CLA	1	0
23	c	507	CLA	3	0
25	b	618	BCR	2	0
23	a	407[A]	CLA	2	0
25	H	101	BCR	2	0
33	z	101	LMG	2	0
26	F	101	SQD	2	0
27	O	601	GOL	1	0
34	c	522	HTG	1	0
25	h	101	BCR	5	0
23	c	513	CLA	7	0
27	v	401[A]	GOL	1	0
25	B	618	BCR	5	0
35	c	518[A]	DGD	3	0
33	d	412	LMG	3	0
27	C	523[B]	GOL	1	0
37	d	407[B]	LHG	3	0
23	b	616	CLA	3	0
23	c	502	CLA	3	0
37	d	408[B]	LHG	10	0
23	C	502	CLA	4	0
37	E	101[B]	LHG	3	0
23	a	409	CLA	5	0
35	H	102	DGD	1	0
23	B	615	CLA	4	0
25	y	101	BCR	2	0
23	B	606	CLA	2	0
23	C	513	CLA	3	0
37	d	407[A]	LHG	2	0
27	c	742[B]	GOL	1	0
37	d	408[A]	LHG	11	0
23	c	506	CLA	4	0
37	D	410[B]	LHG	3	0
37	E	101[A]	LHG	3	0
23	b	615	CLA	4	0
35	c	519	DGD	4	0
33	C	521	LMG	2	0
37	D	409[A]	LHG	2	0
23	B	613	CLA	6	0
25	t	103	BCR	5	0

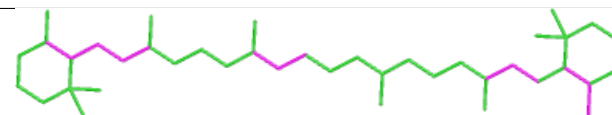
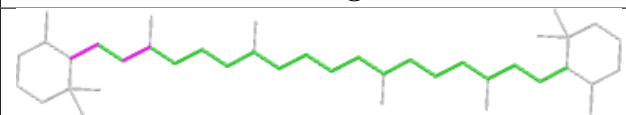
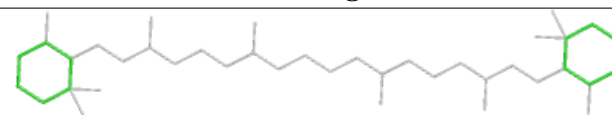
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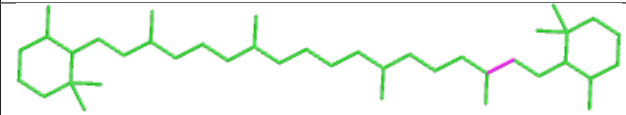
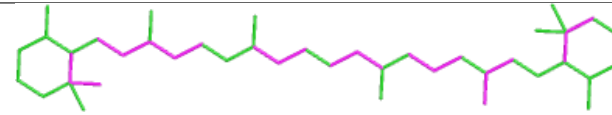
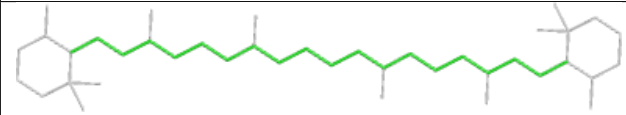
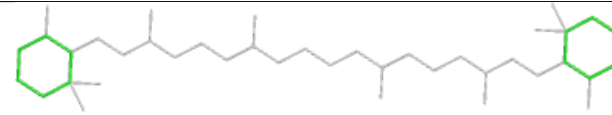
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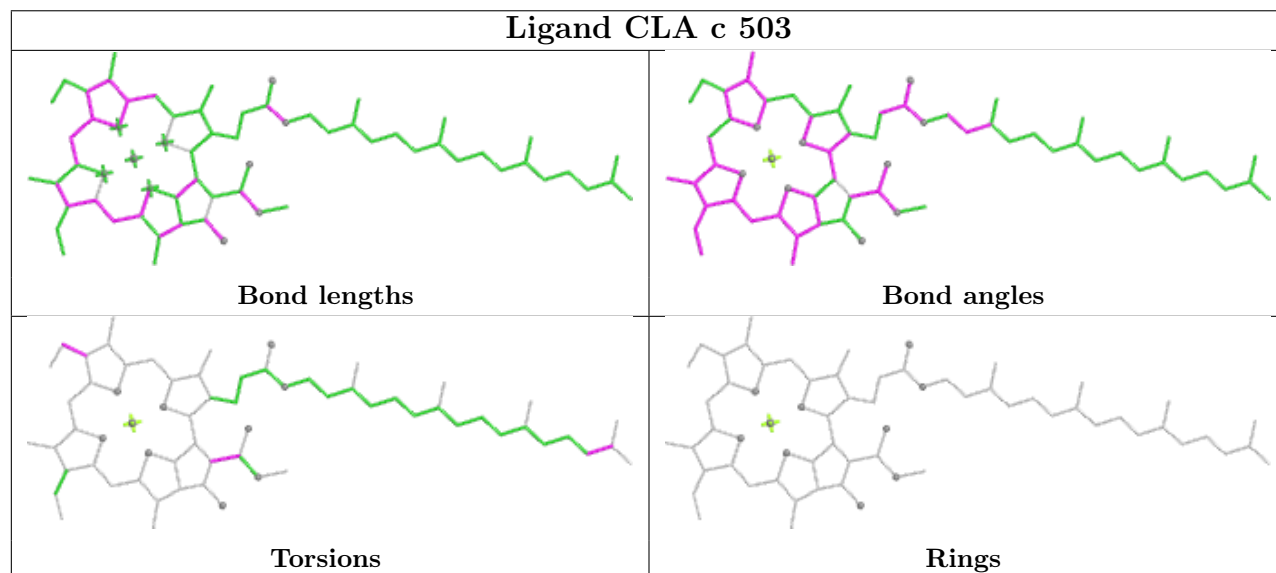
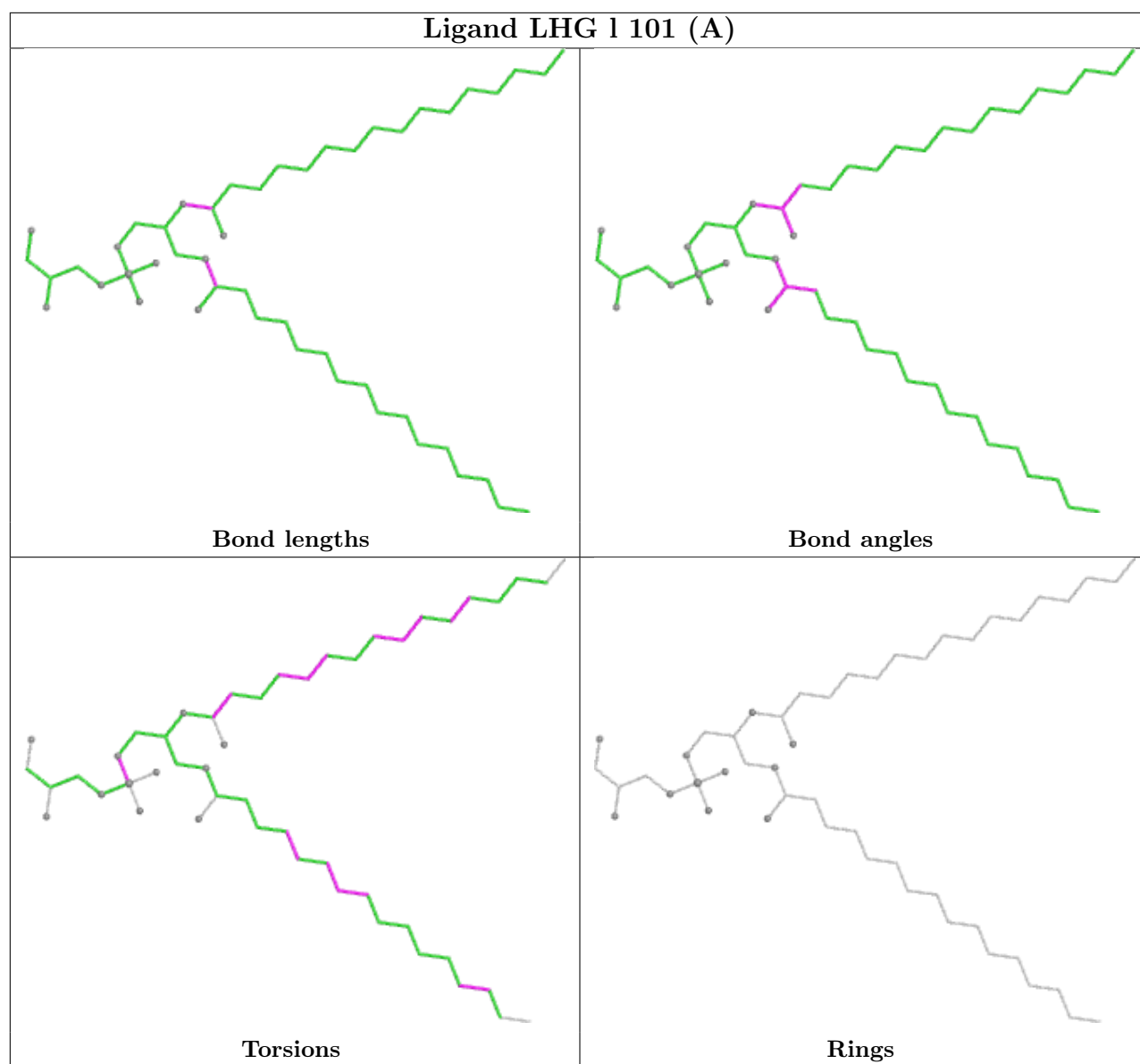
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	A	404[A]	CLA	2	0
23	C	507	CLA	4	0
33	Z	101	LMG	1	0
37	D	410[A]	LHG	2	0
32	a	414	LMT	1	0
27	b	901	GOL	1	0
37	e	101[A]	LHG	5	0
23	d	402[A]	CLA	1	0
25	d	404	BCR	2	0
25	c	515	BCR	3	0
25	A	409	BCR	3	0
23	C	509	CLA	3	0
23	b	607	CLA	1	0
23	C	510	CLA	4	0
23	b	609	CLA	6	0
32	I	101	LMT	1	0
32	t	102	LMT	2	0

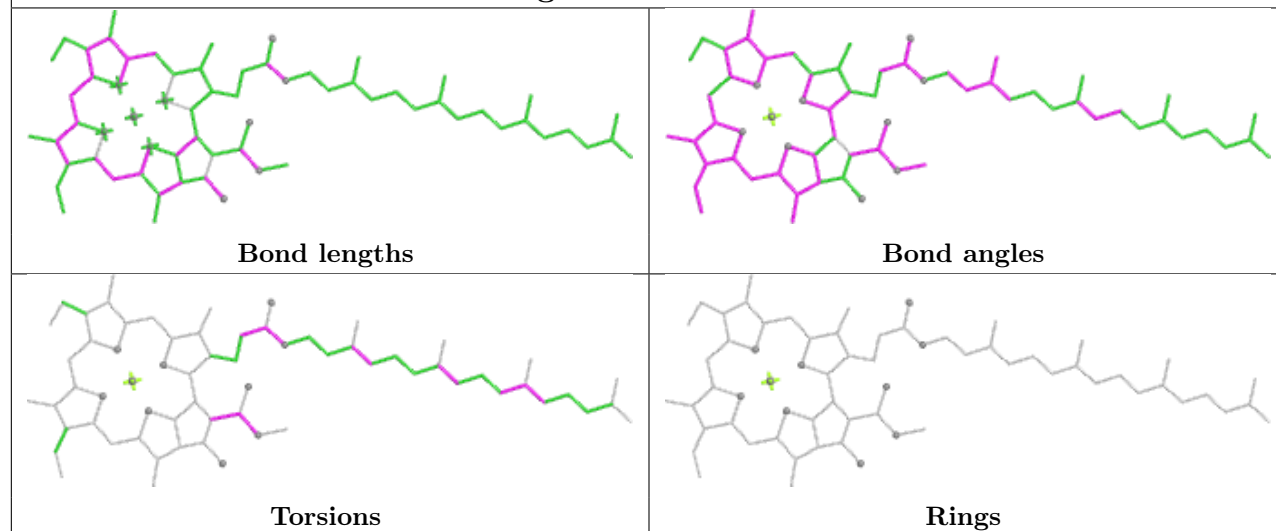
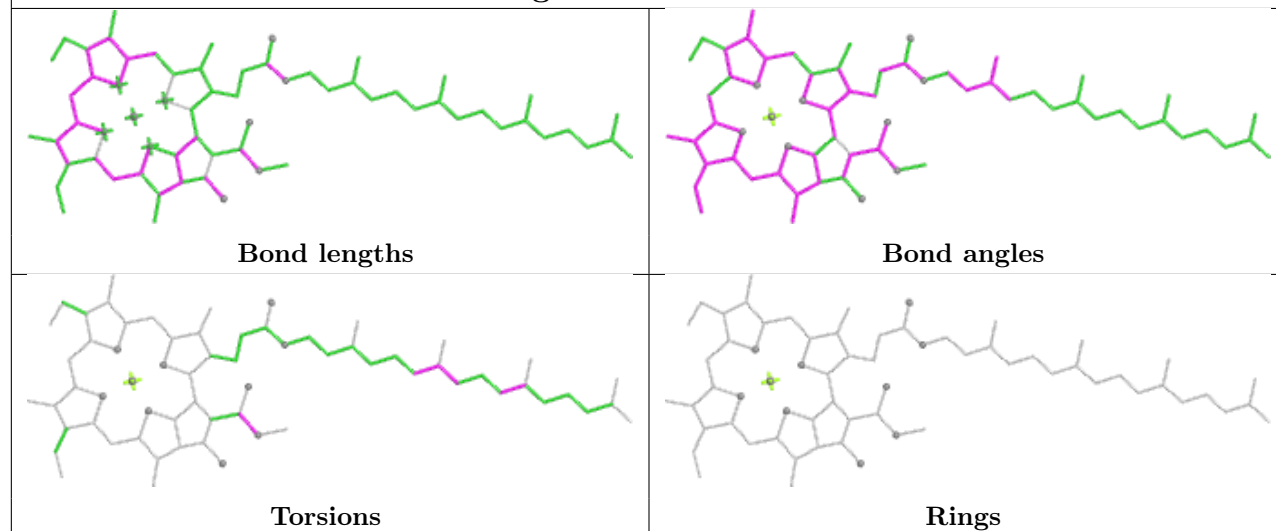
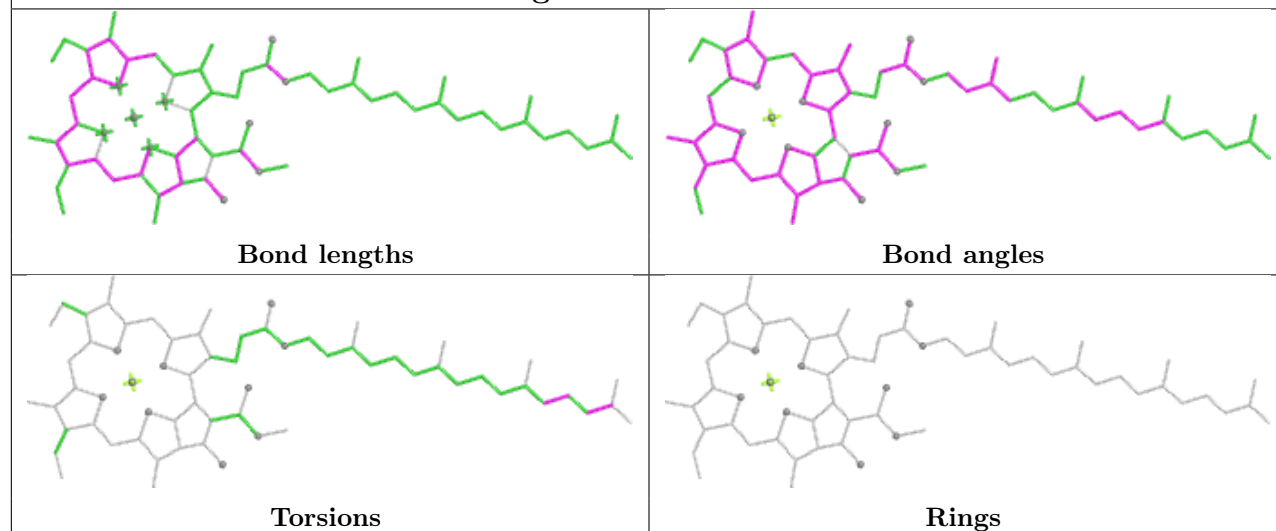
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

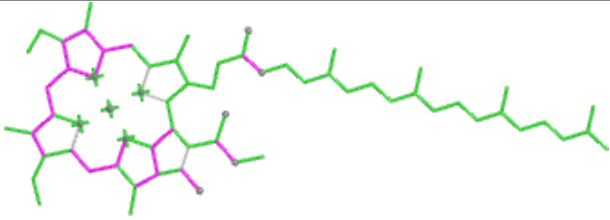
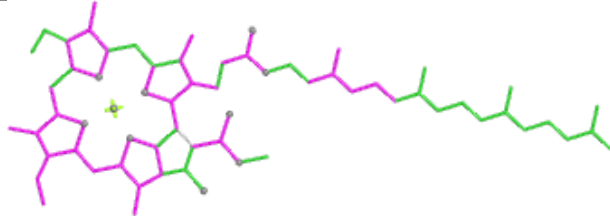
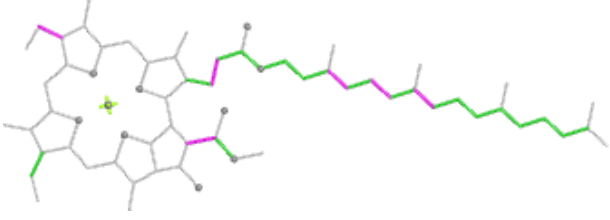
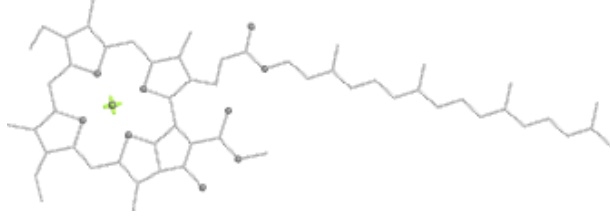
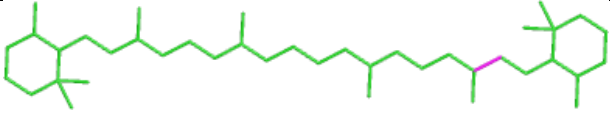
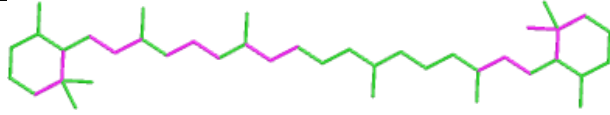
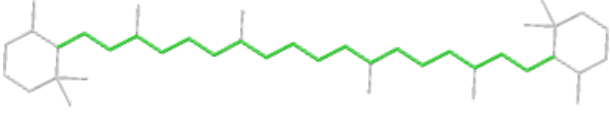
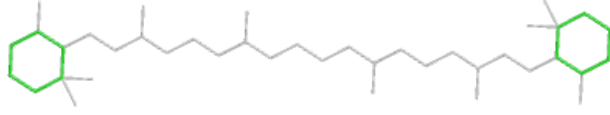
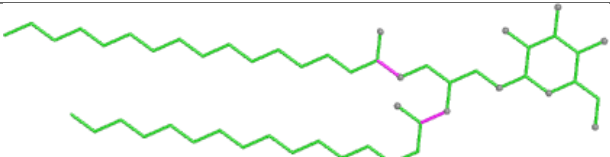
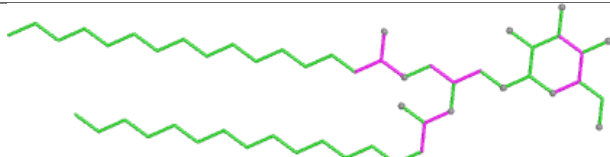
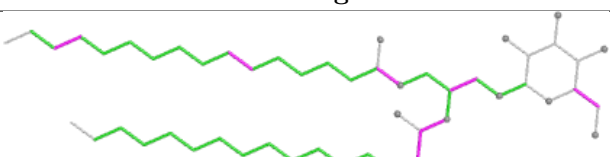
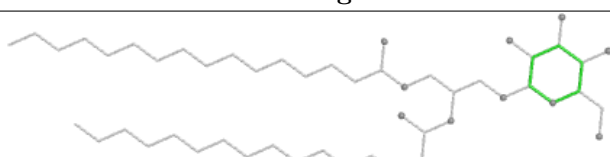
Ligand CLA d 403	
	
Bond lengths	Bond angles
	
Torsions	Rings

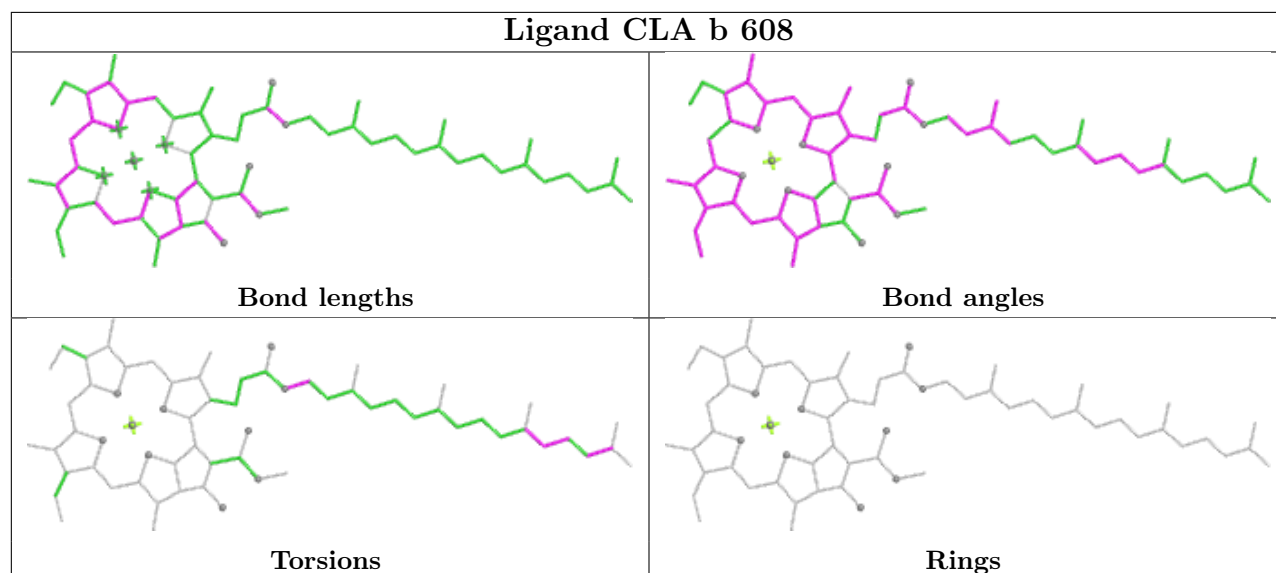
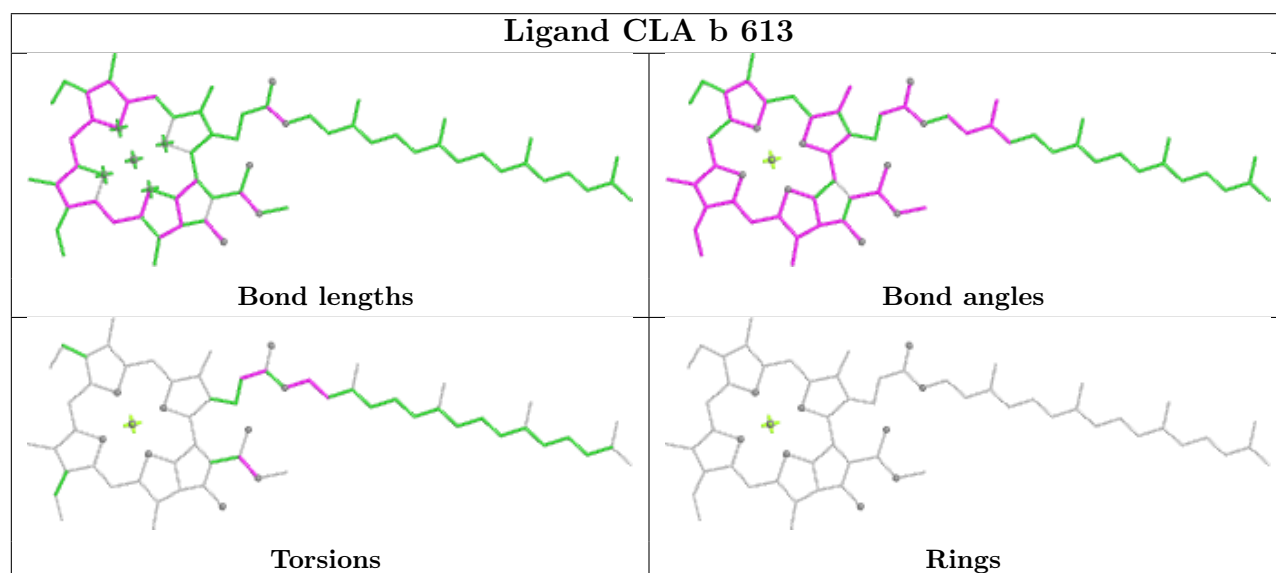
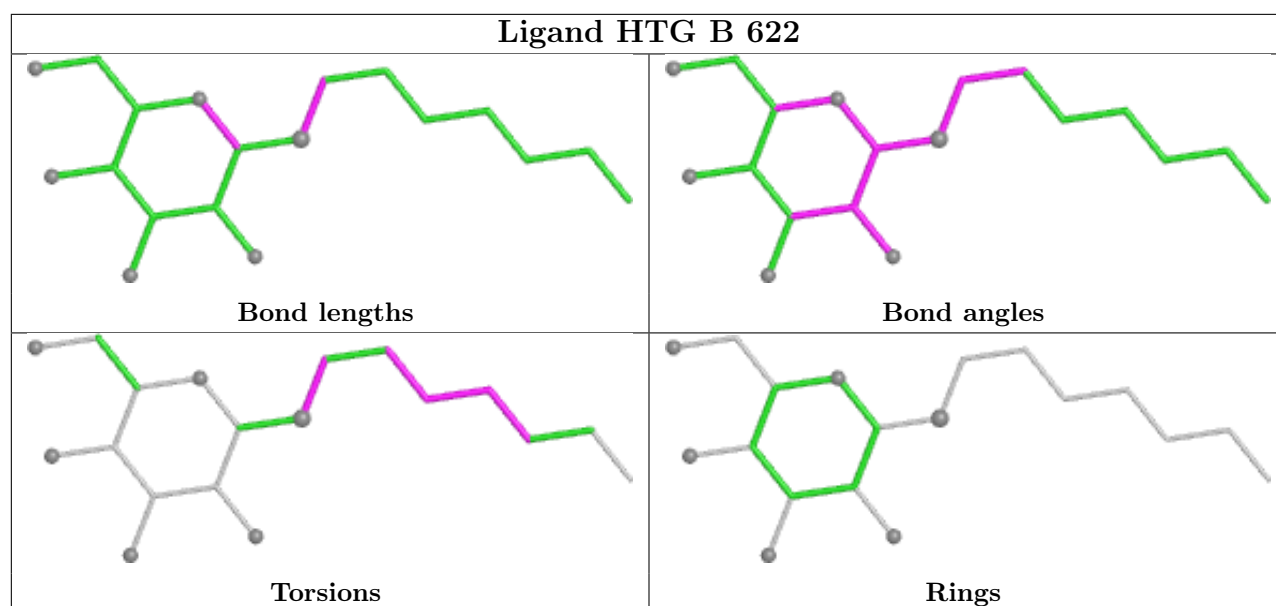
Ligand BCR b 619	
	
Bond lengths	Bond angles
	
Torsions	Rings

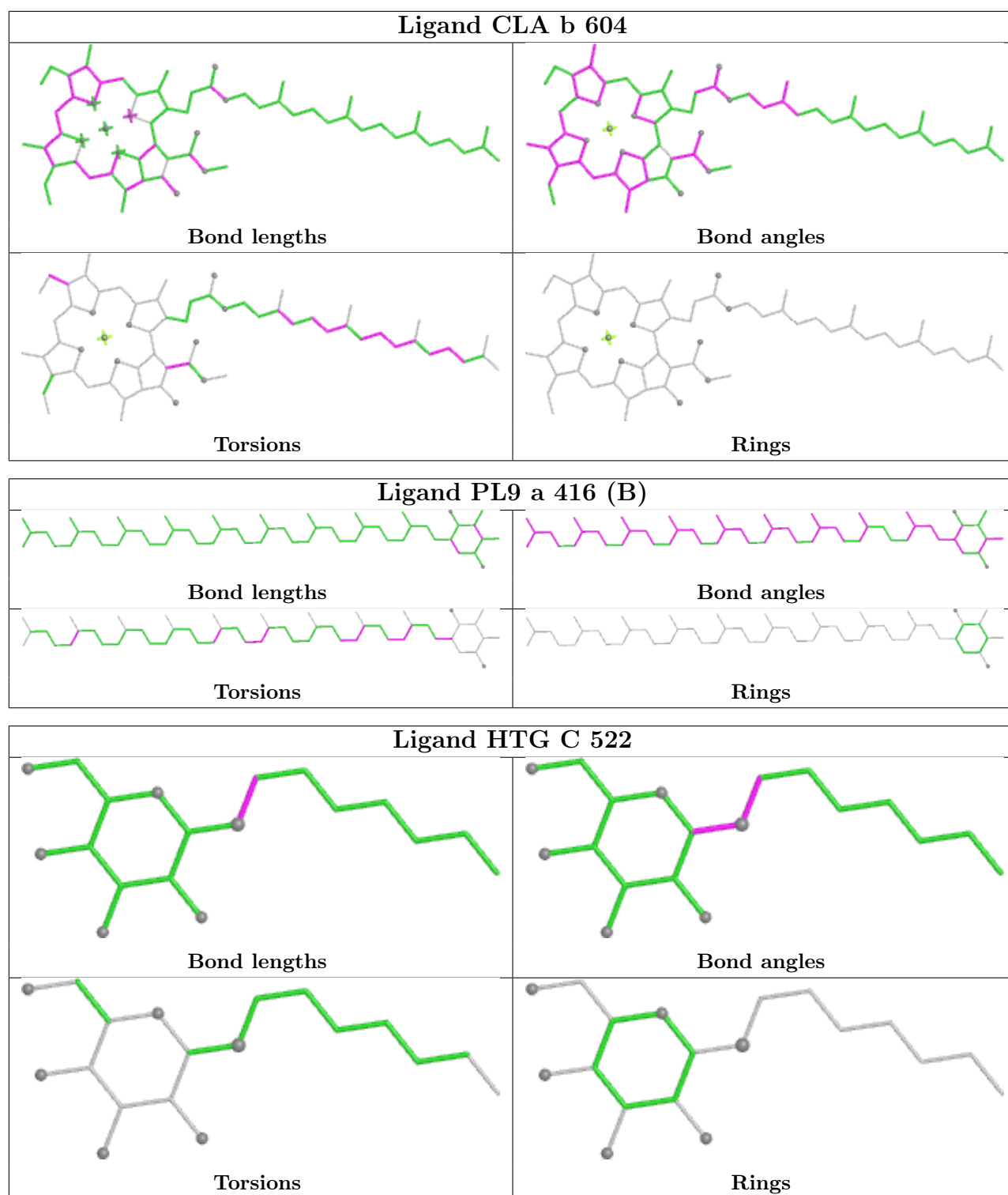
Ligand BCR c 516	
	
Bond lengths	Bond angles
	
Torsions	Rings

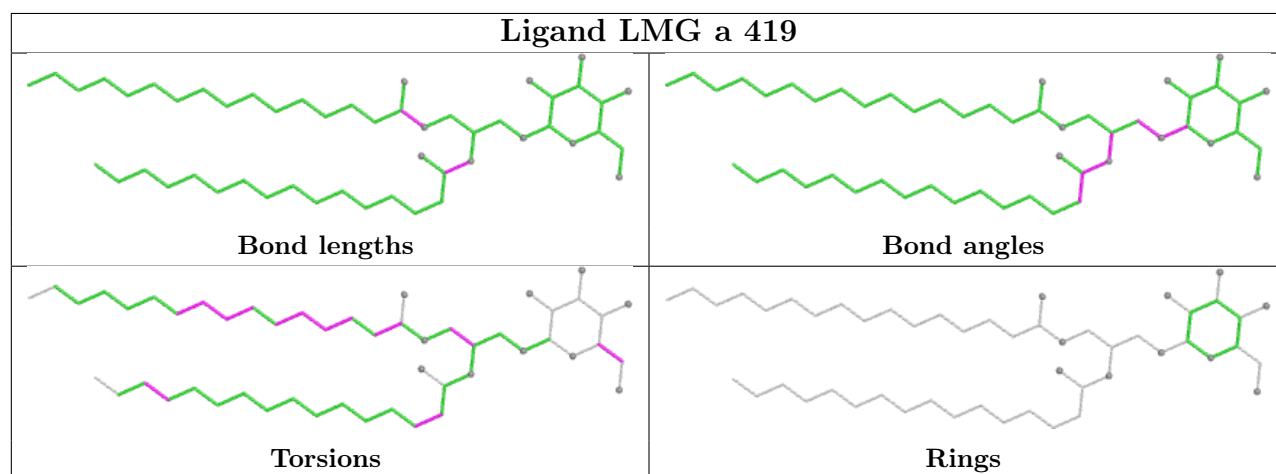
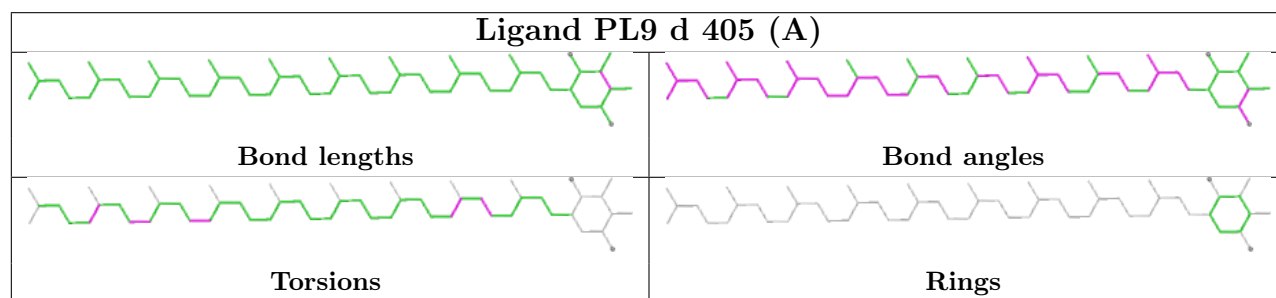
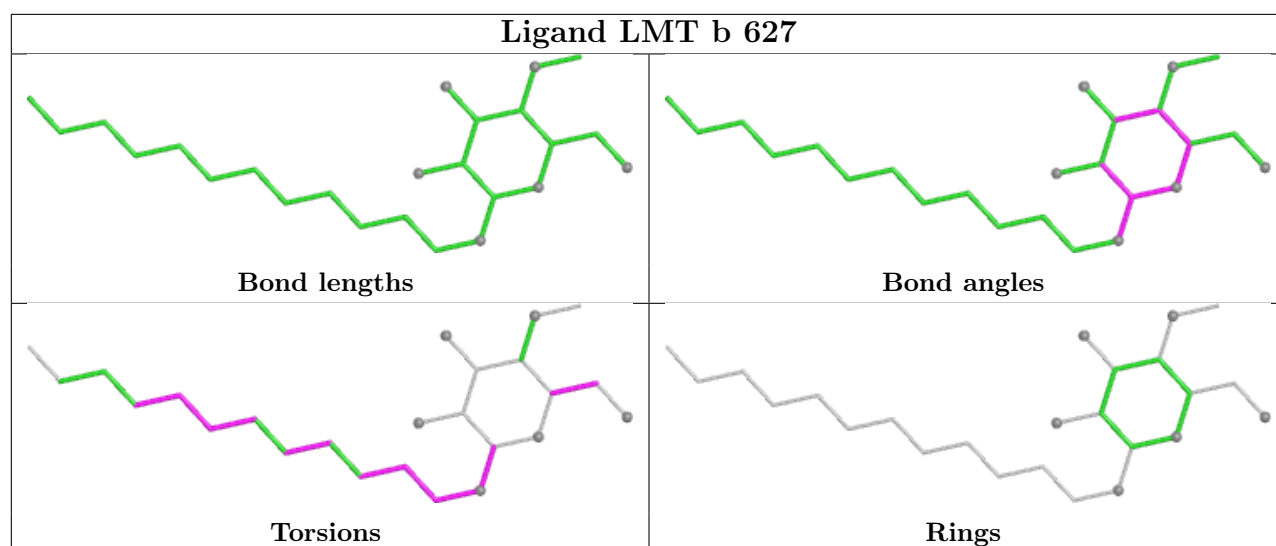


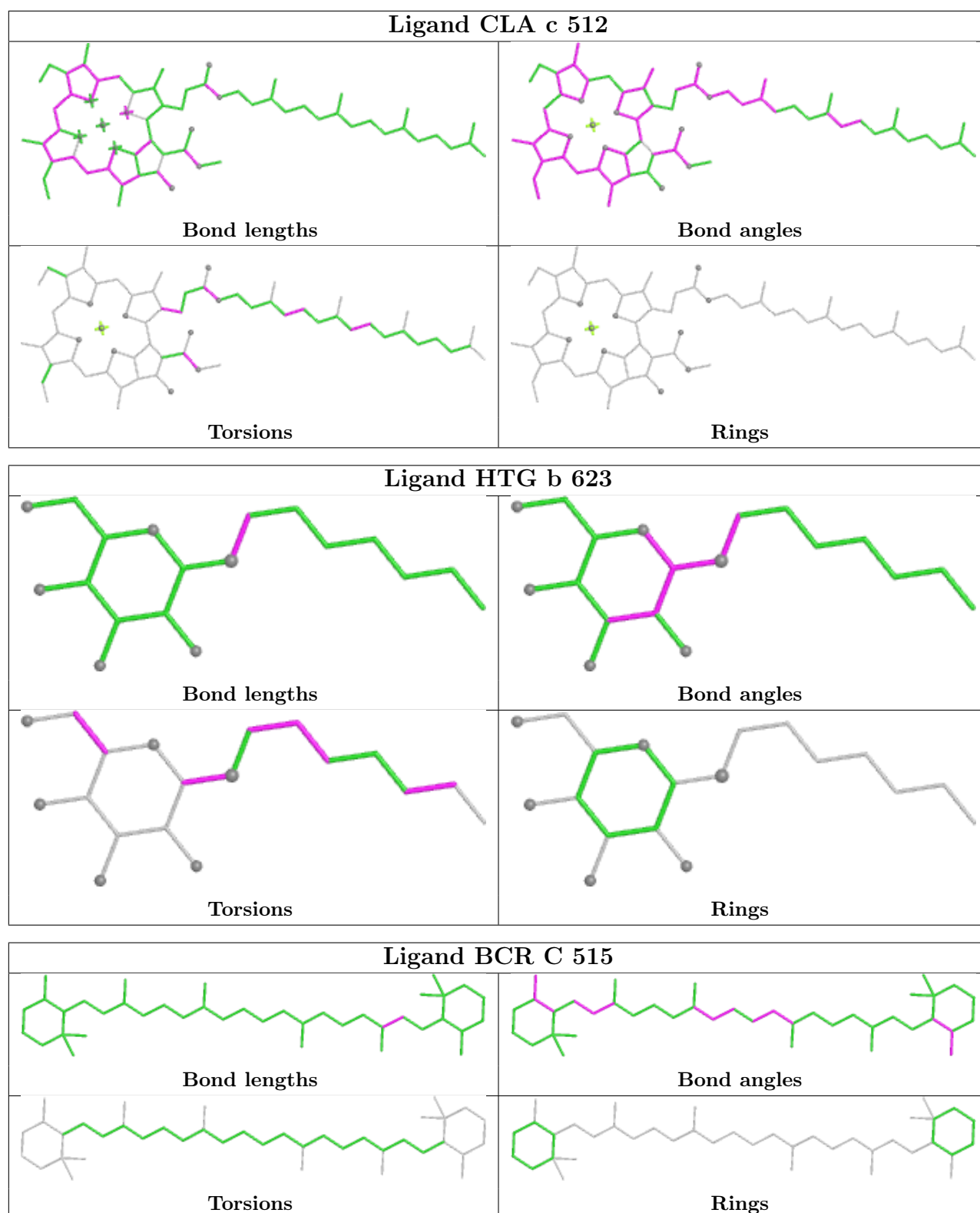
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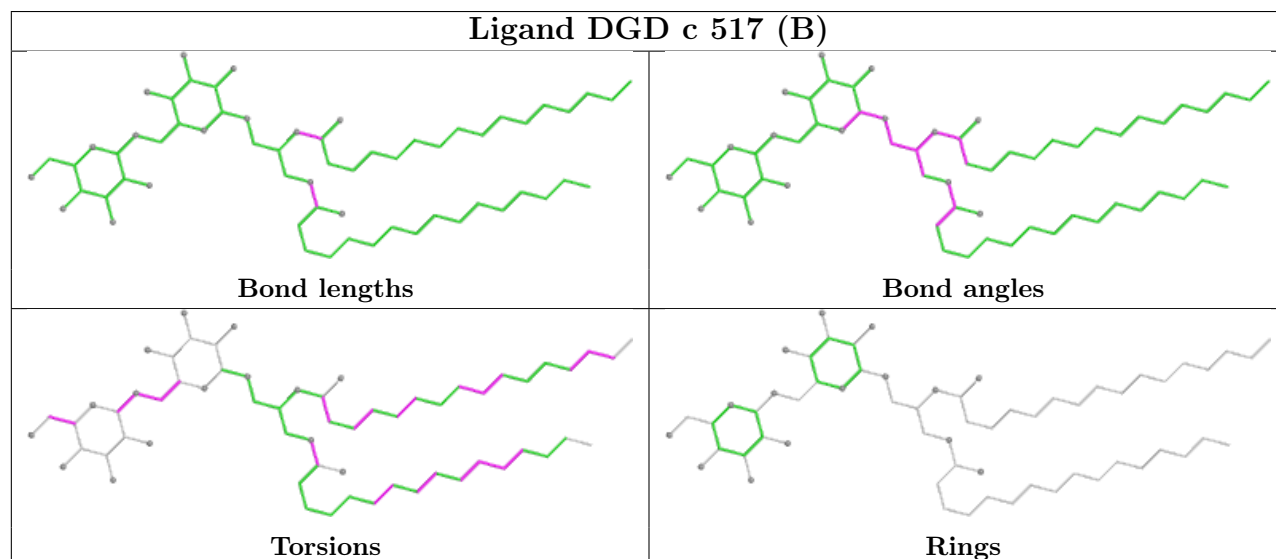
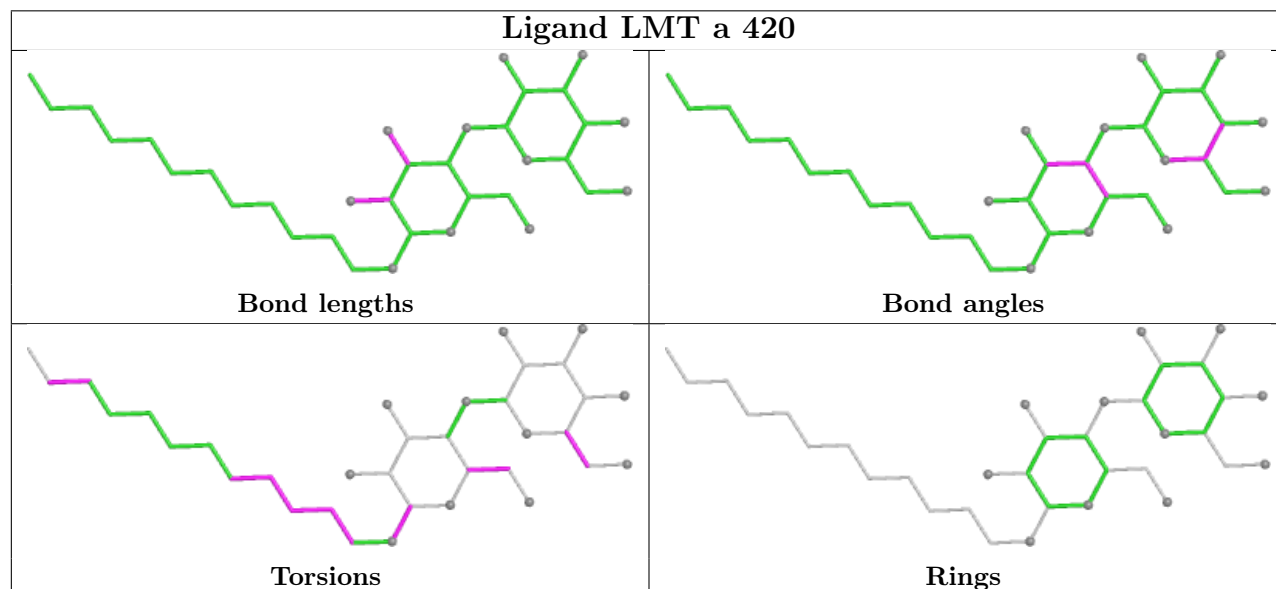
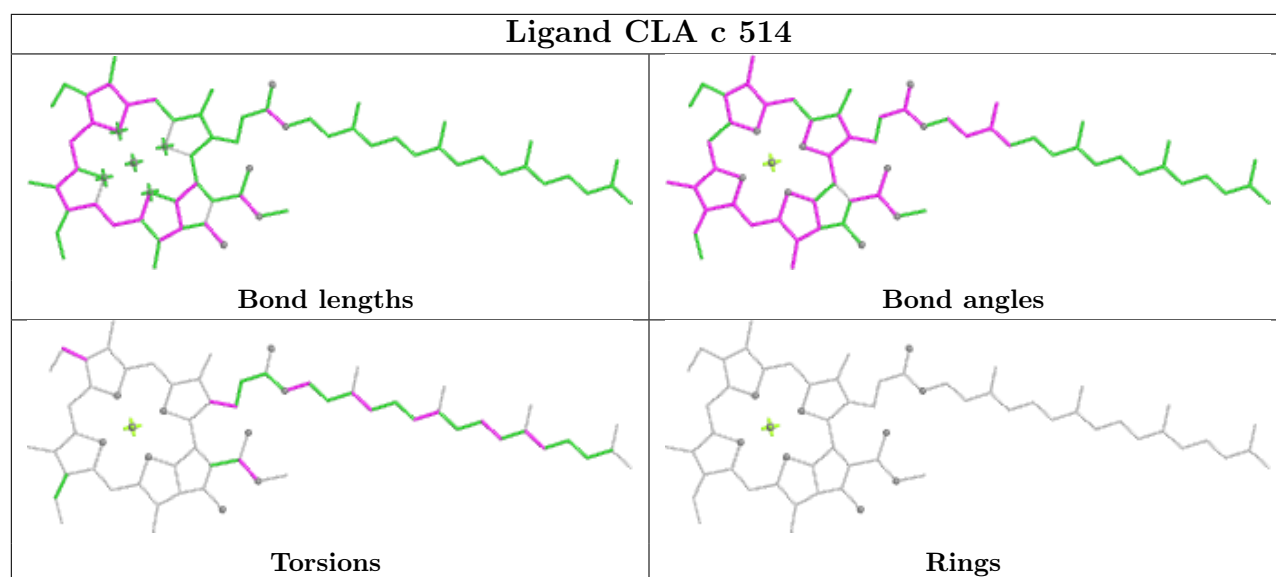
Ligand CLA b 603	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR k 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG c 521	
 Bond lengths	 Bond angles
 Torsions	 Rings

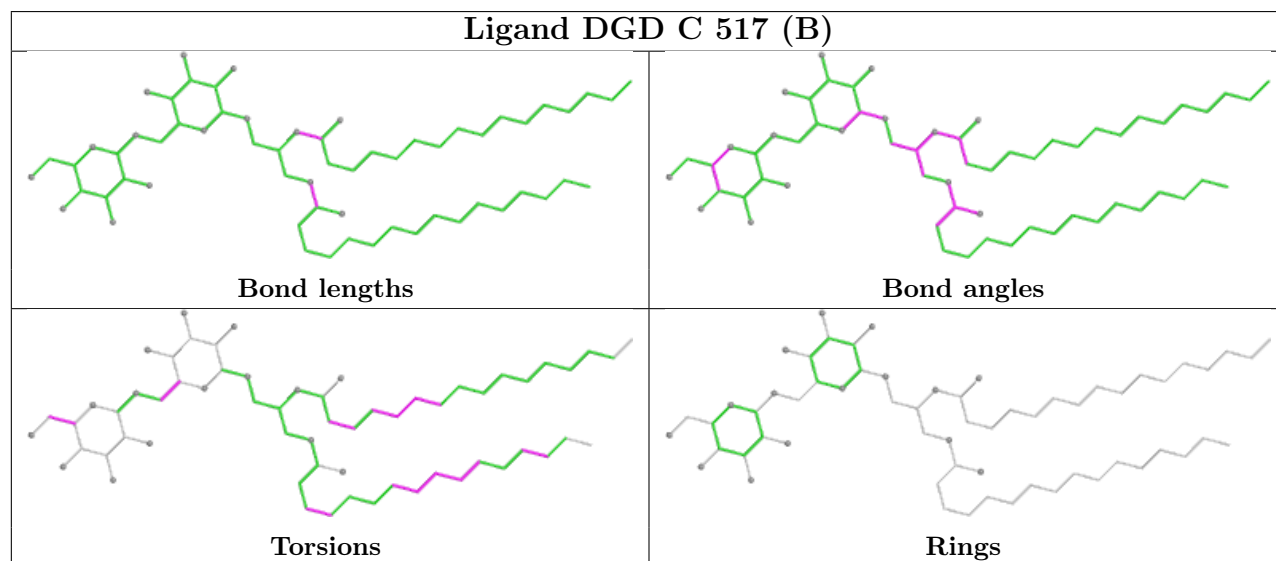
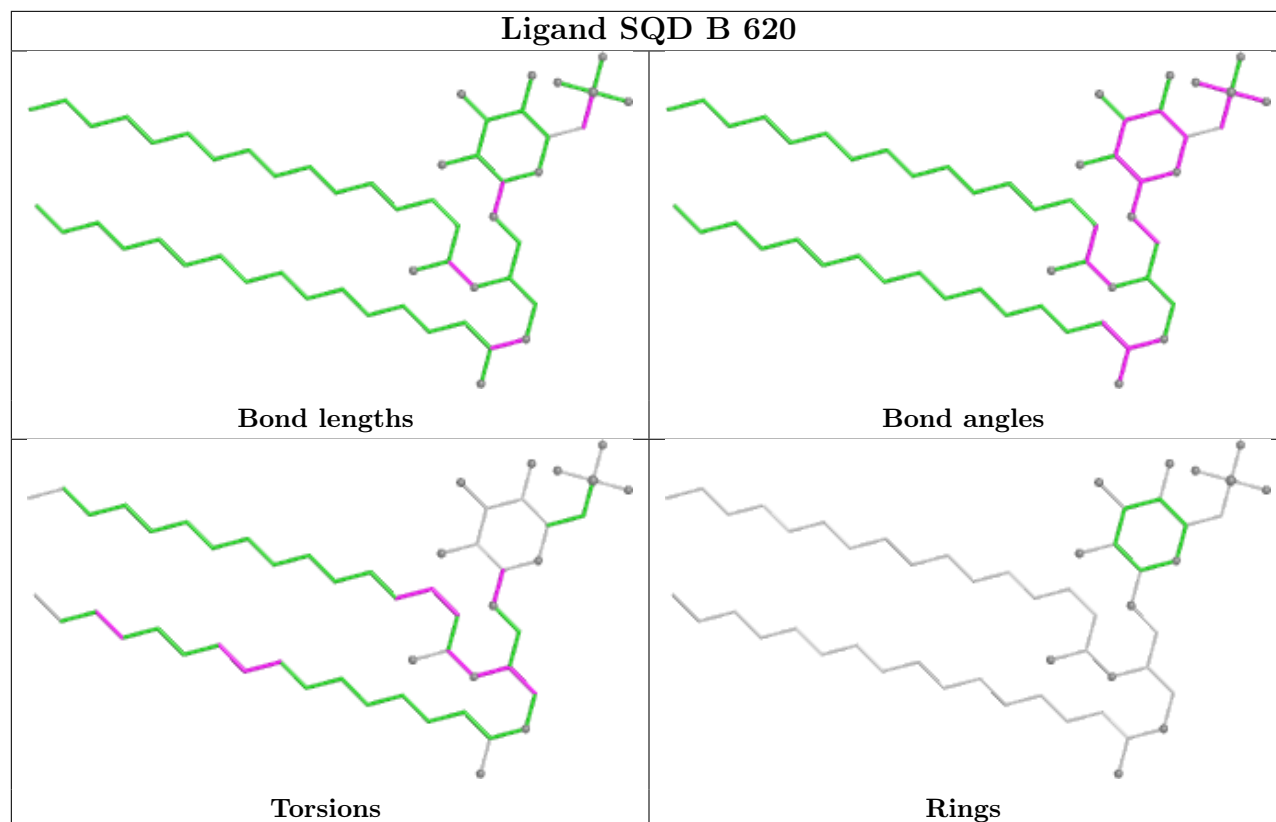


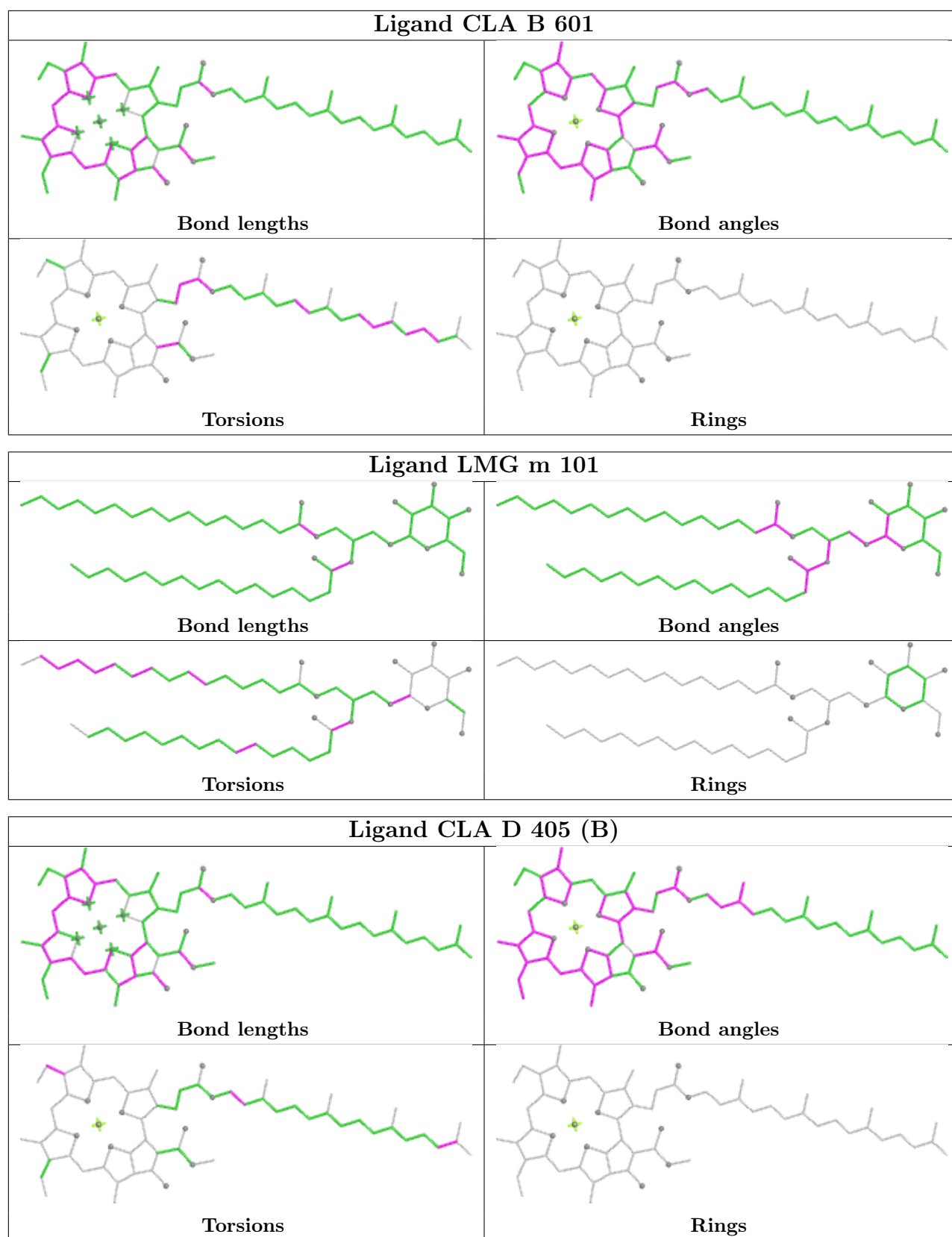




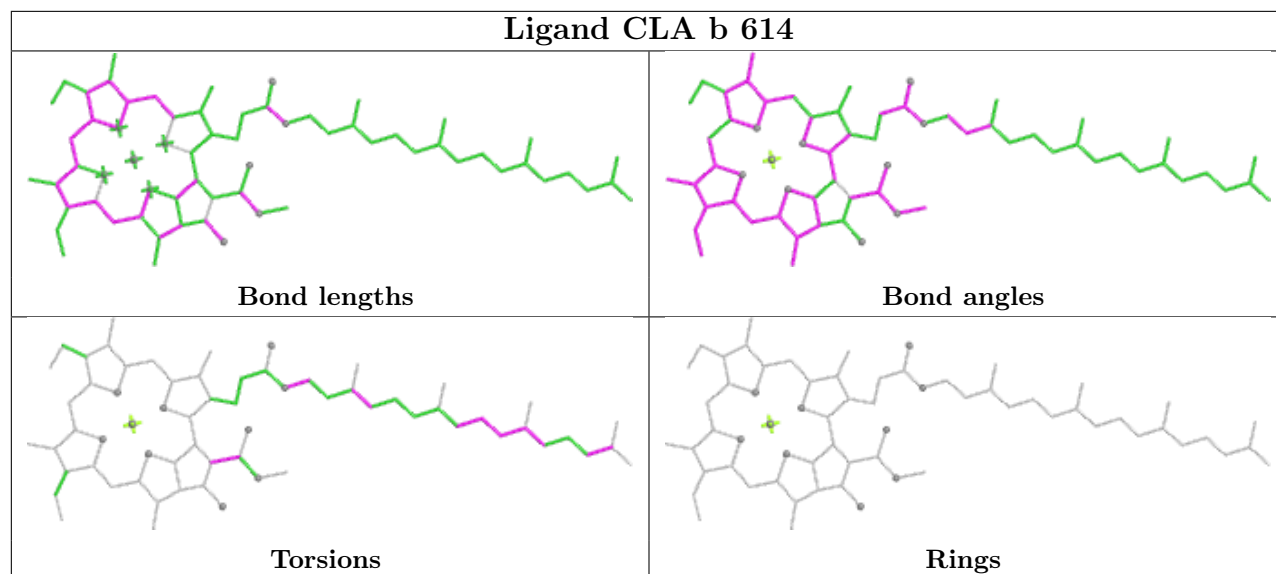




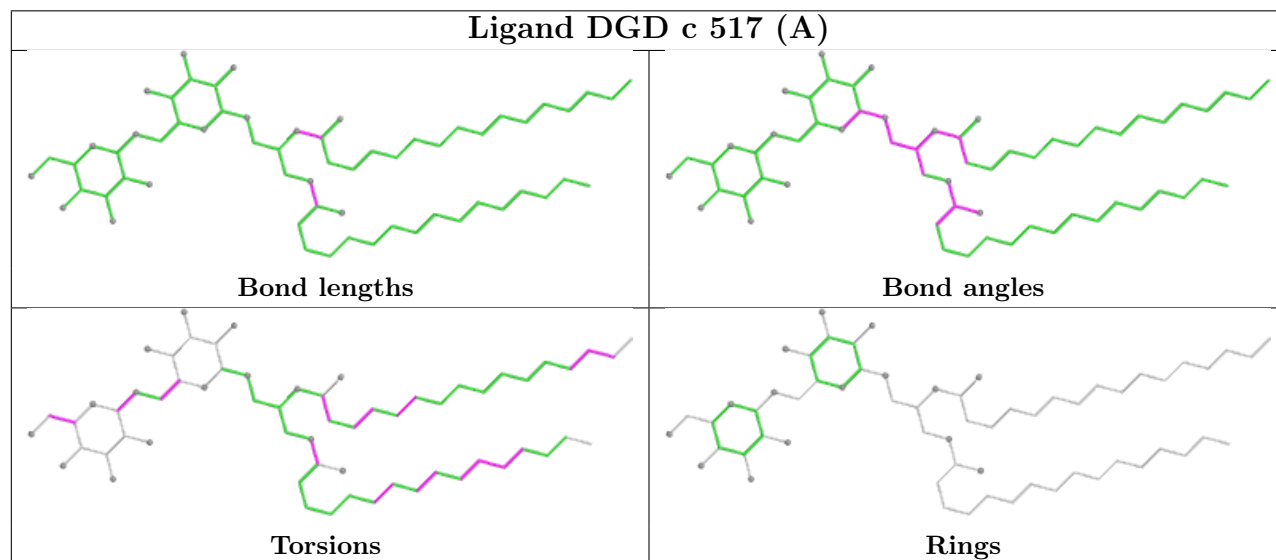


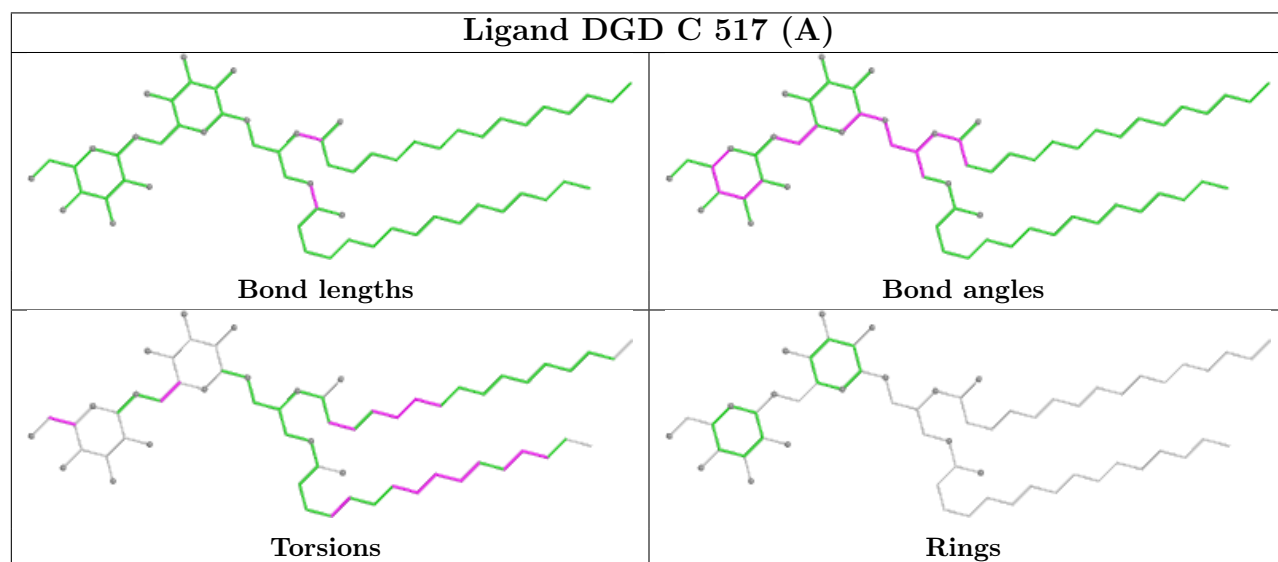
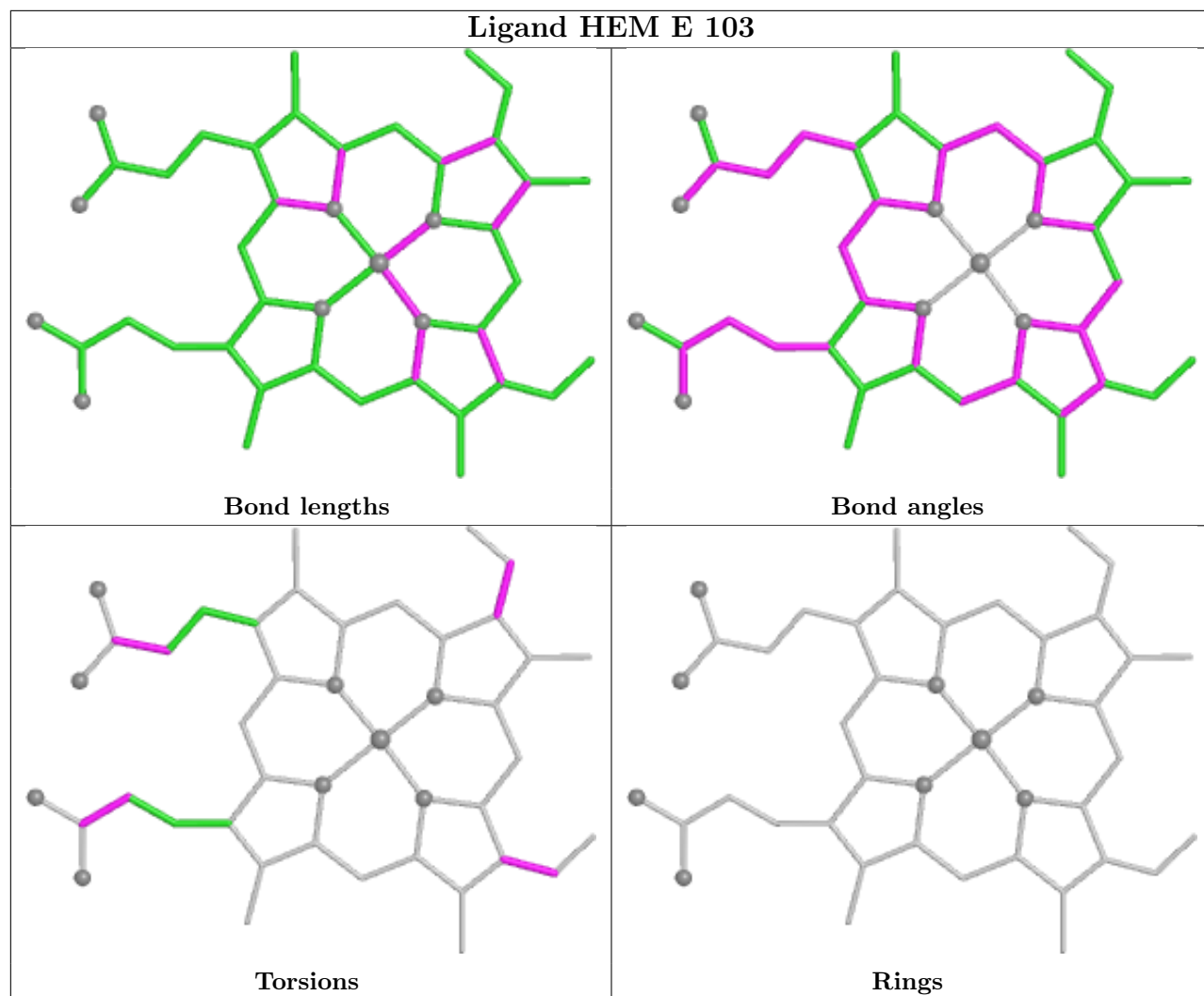


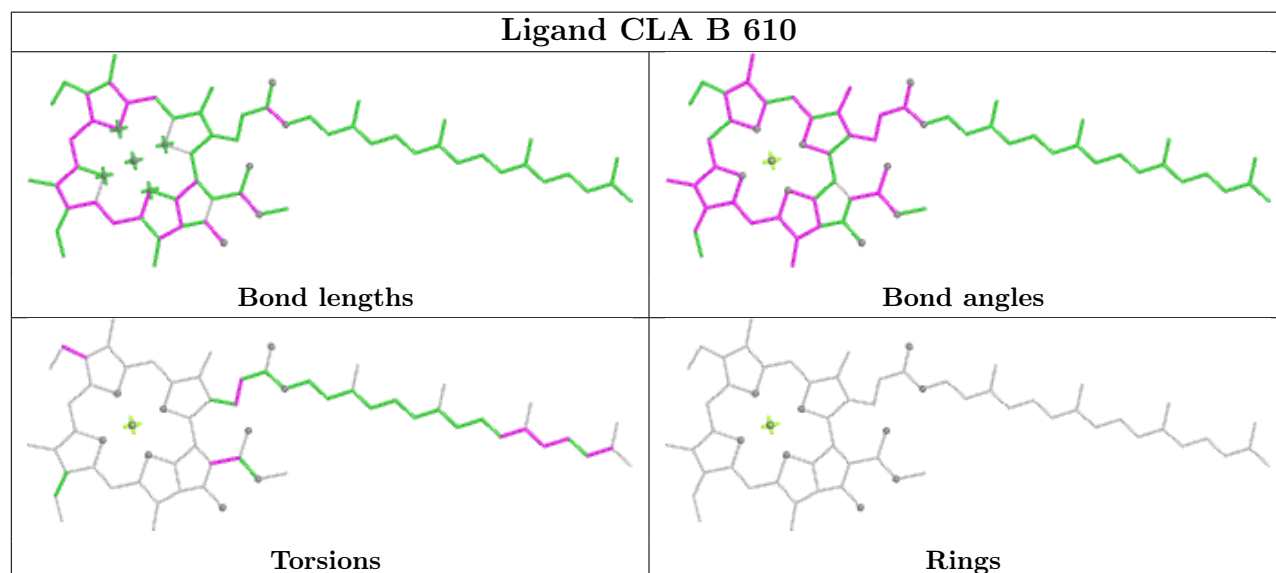
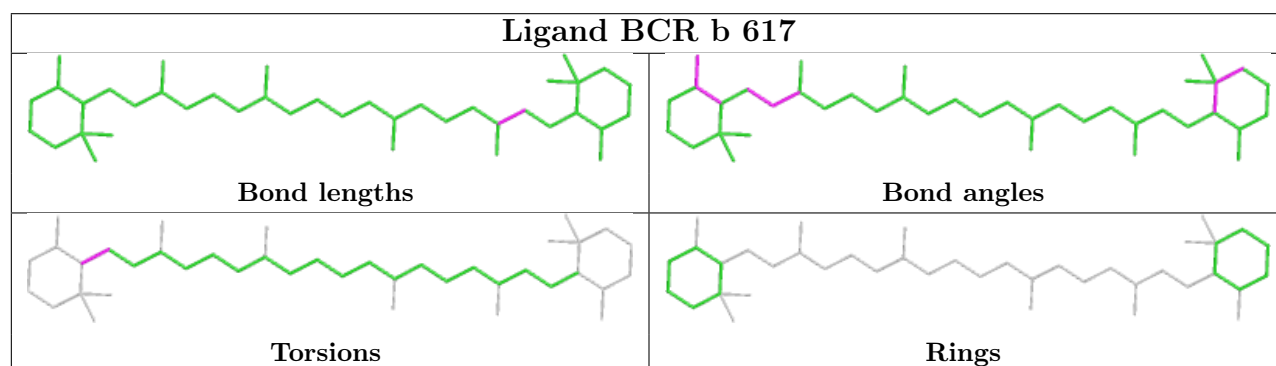
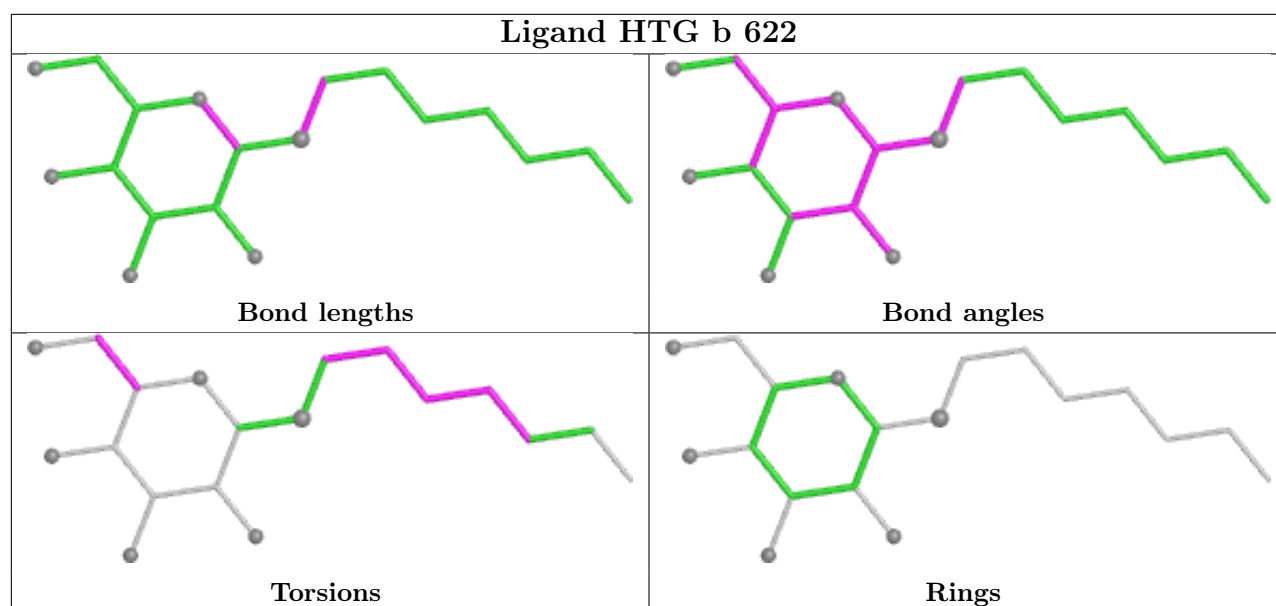
Ligand CLA b 614

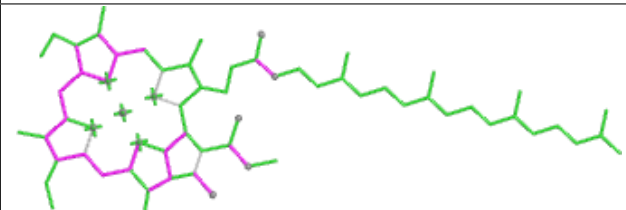
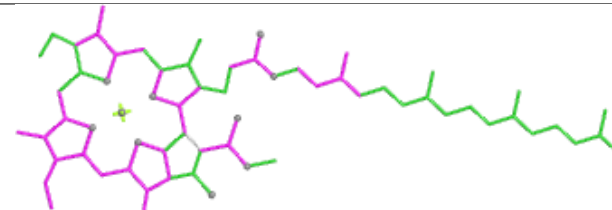
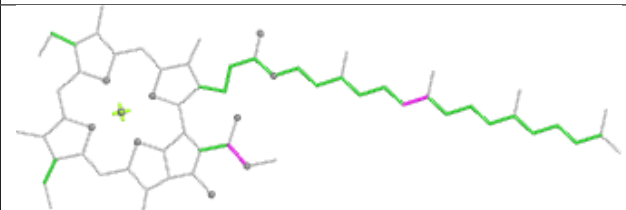
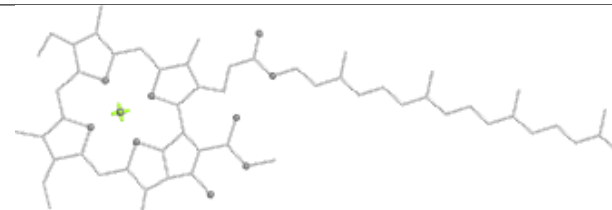
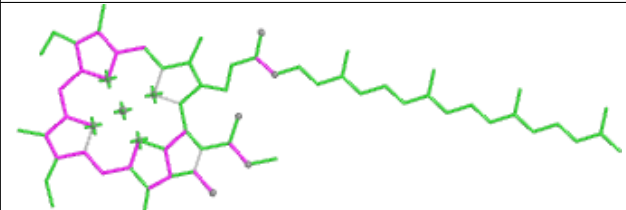
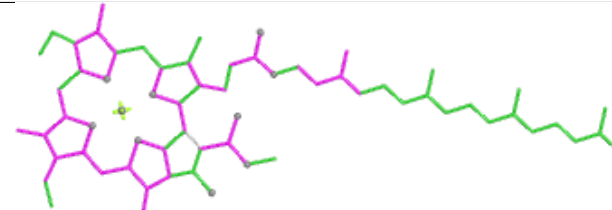
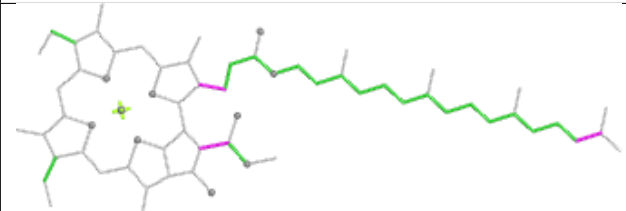
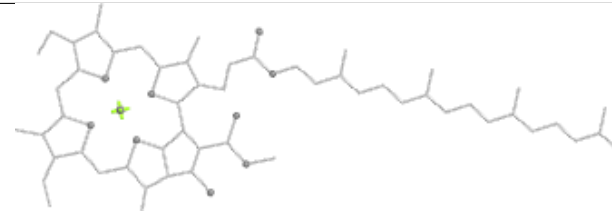


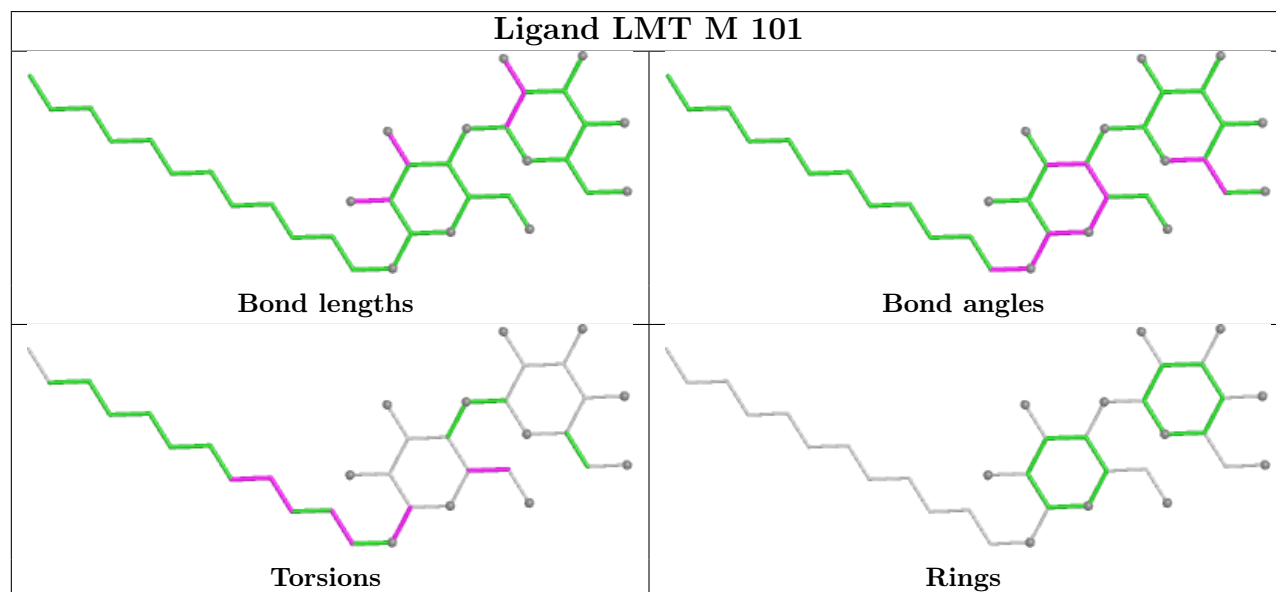
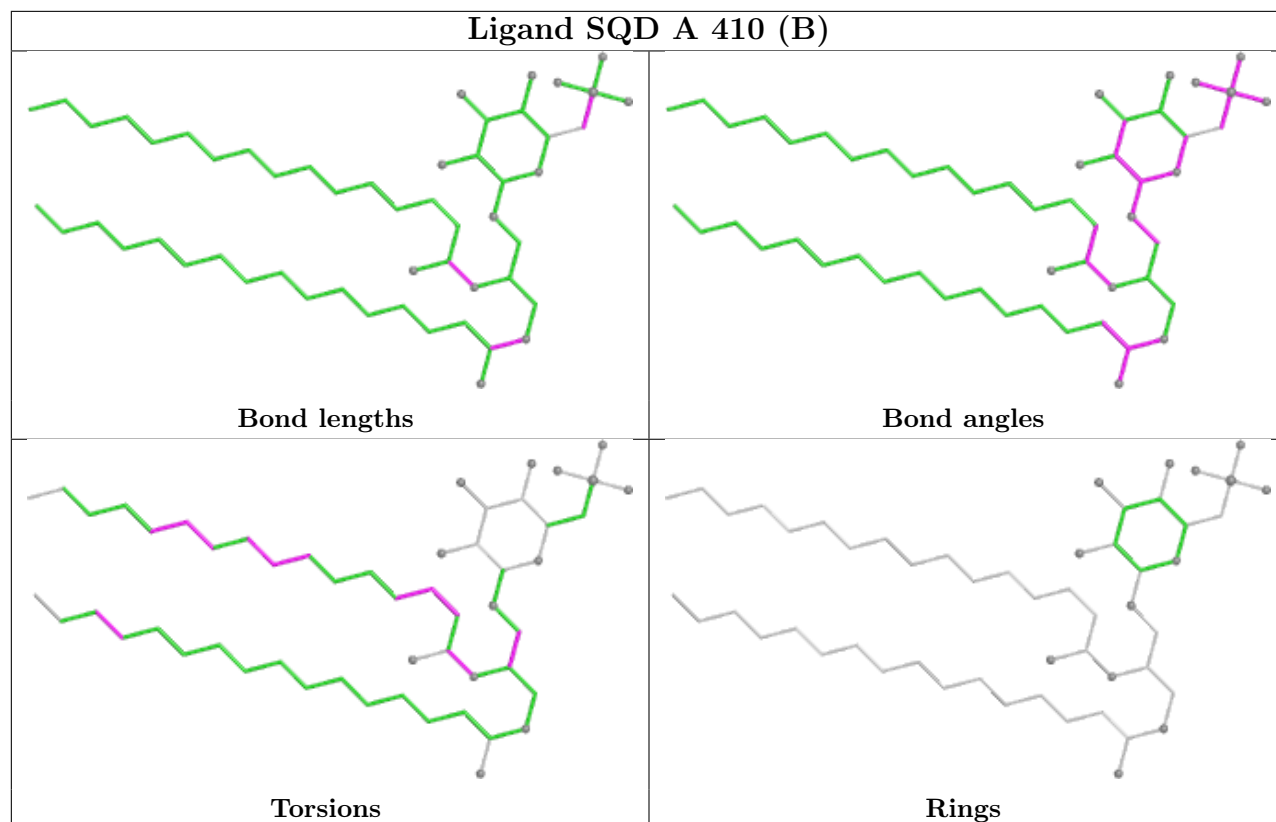
Ligand DGD c 517 (A)

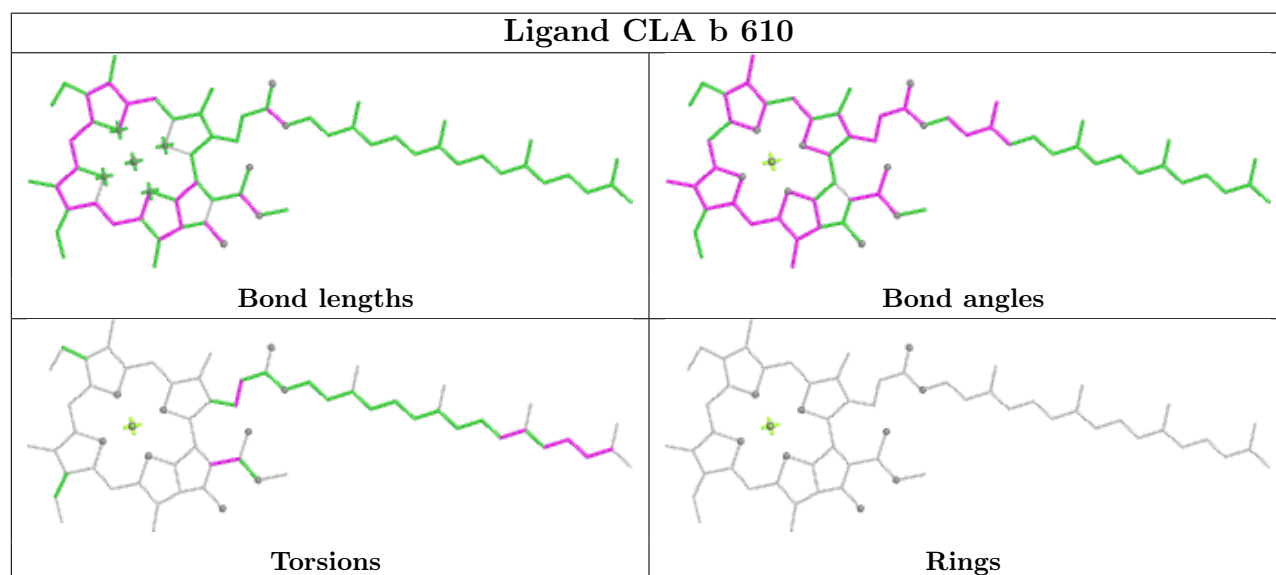
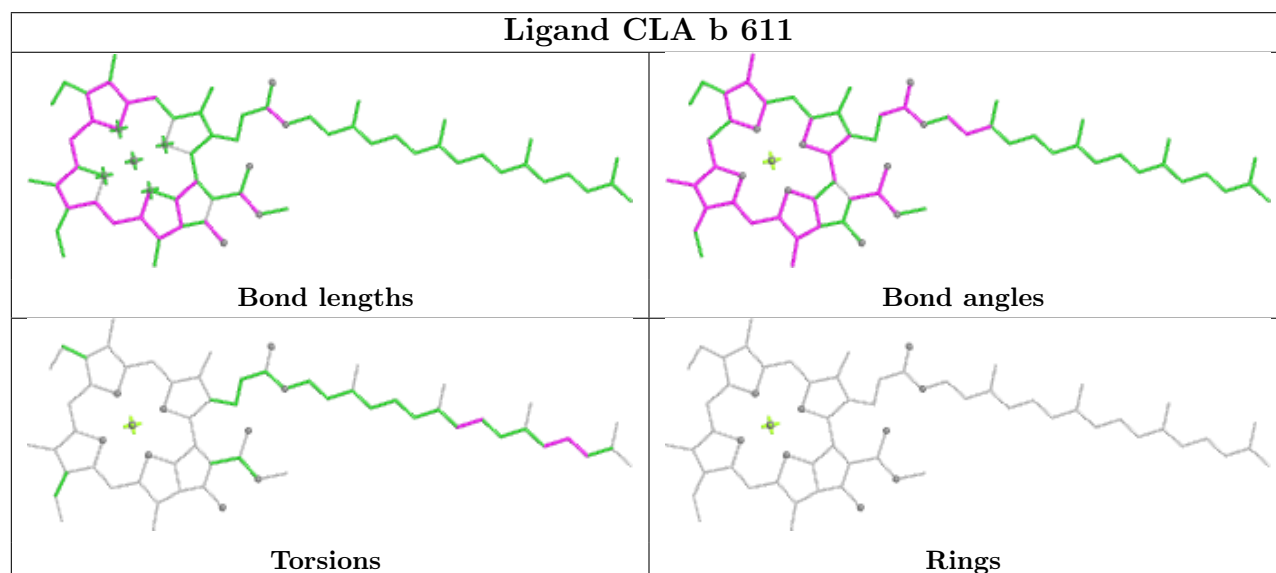
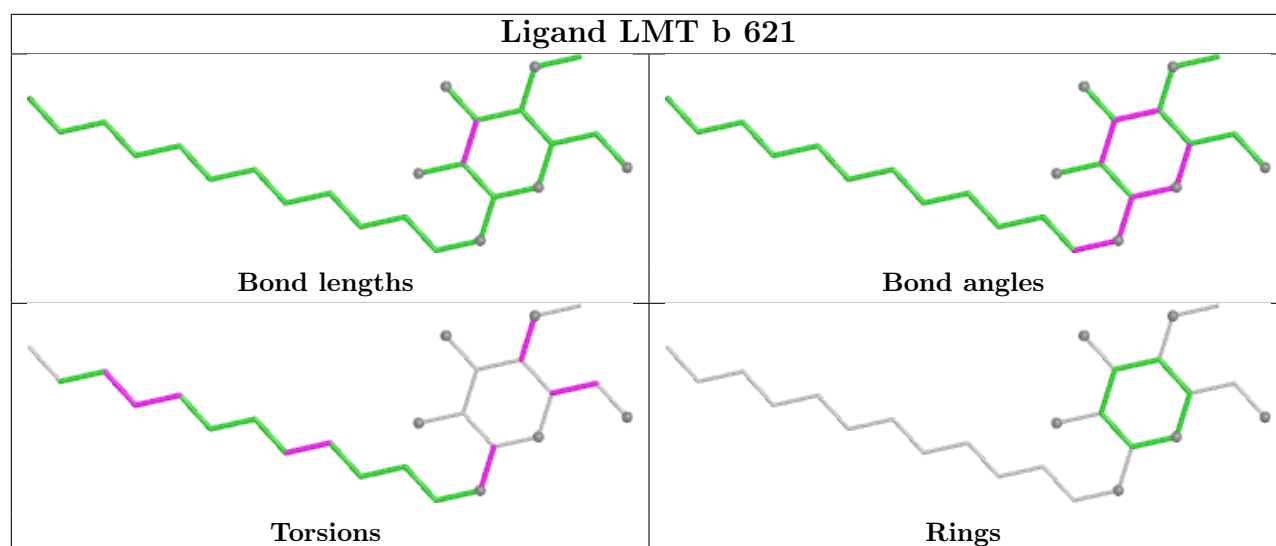


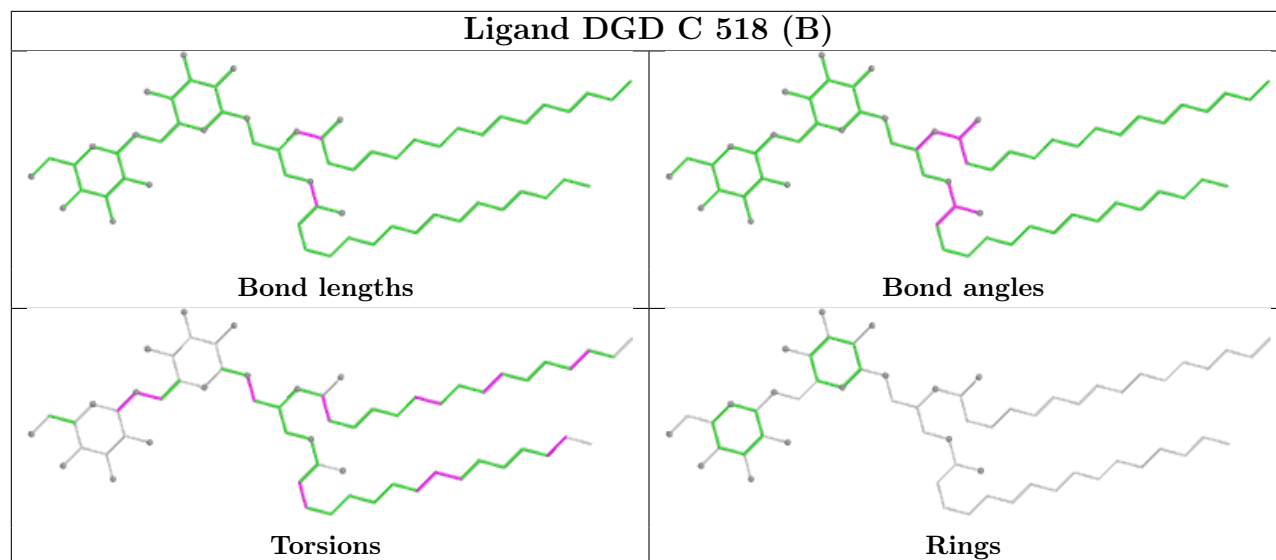
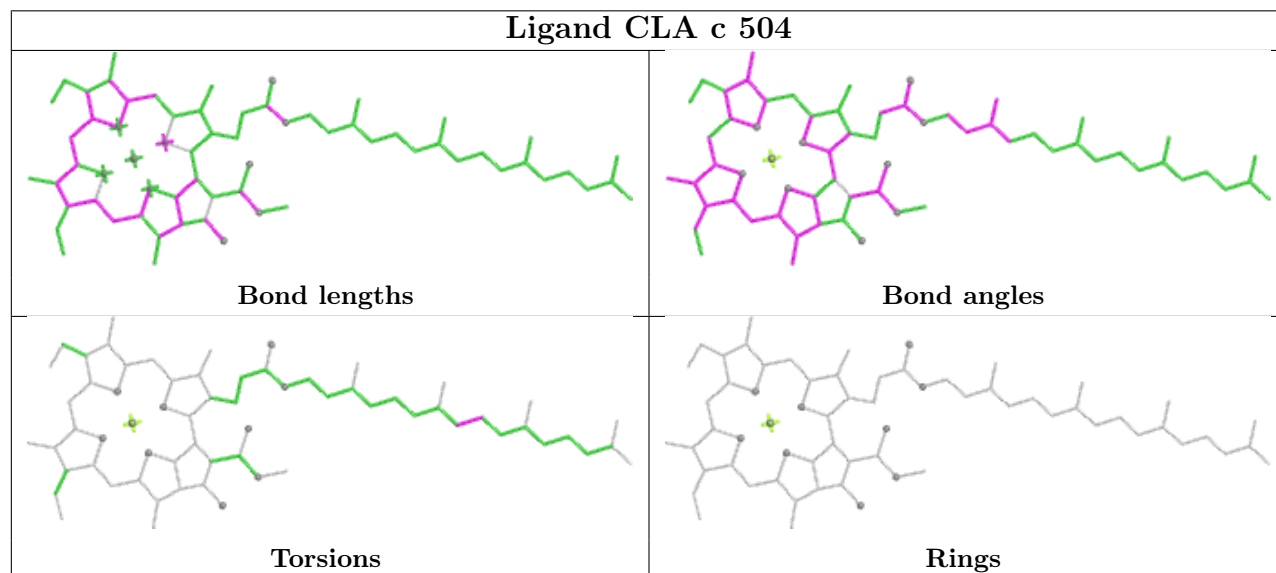
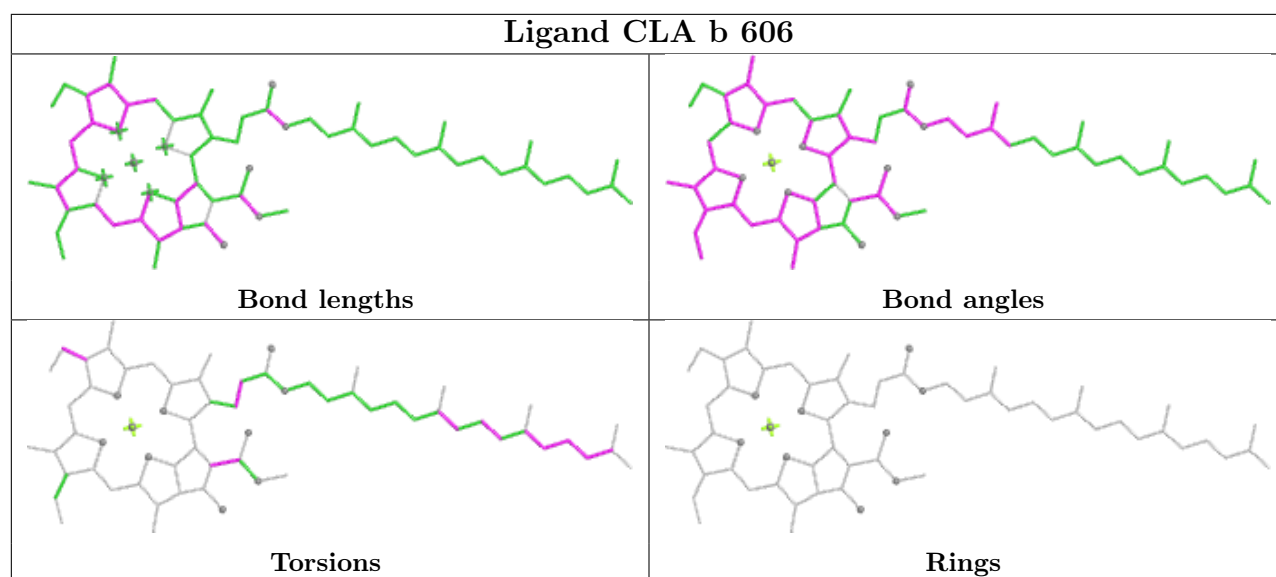


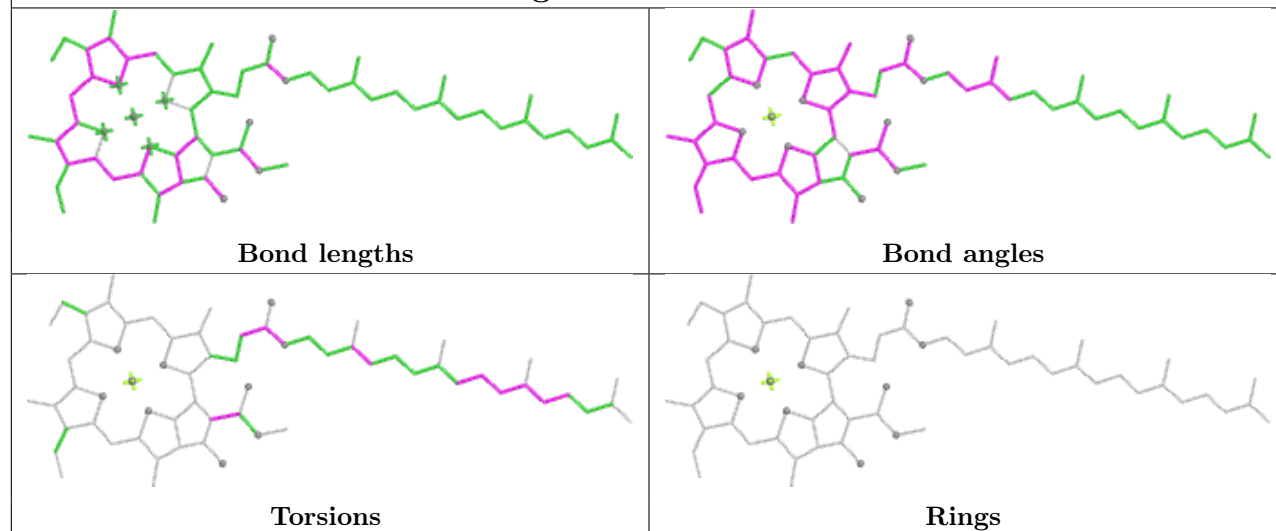
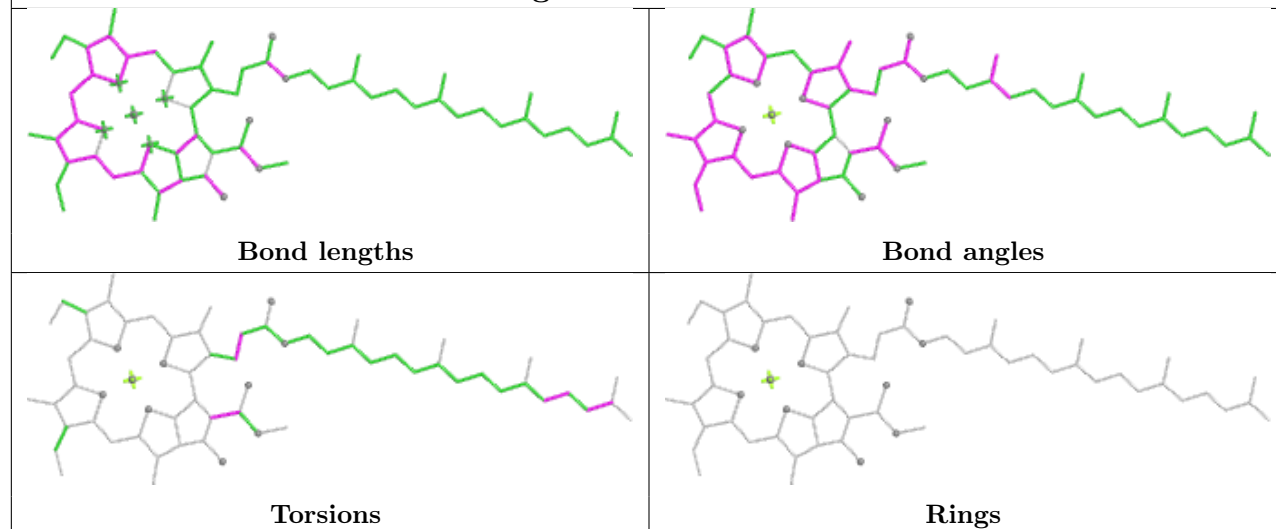
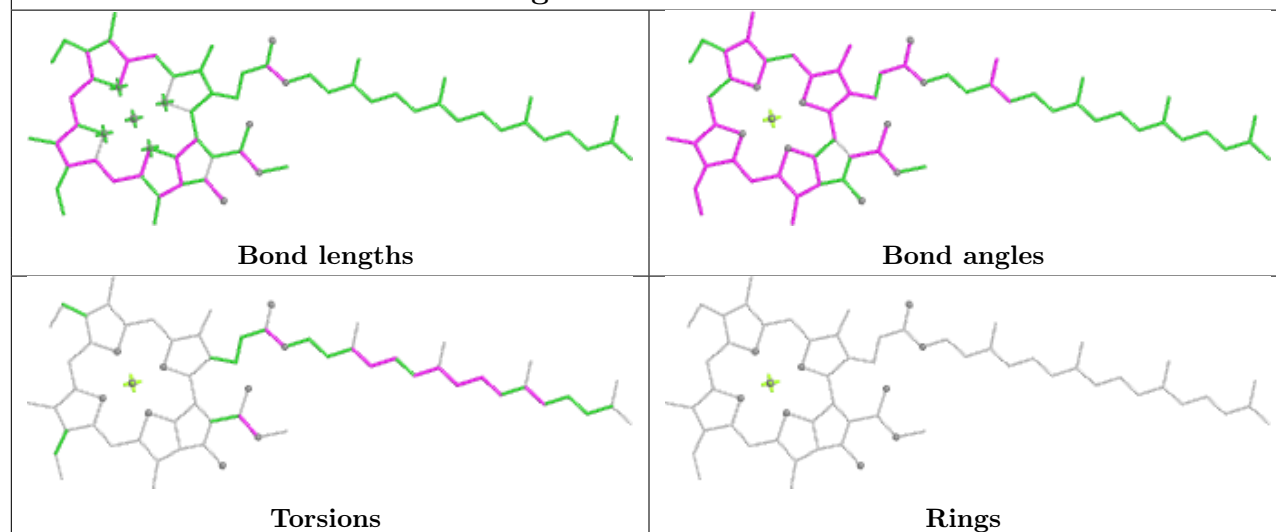


Ligand CLA C 504	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand CLA c 509	
	
Bond lengths	Bond angles
	
Torsions	Rings

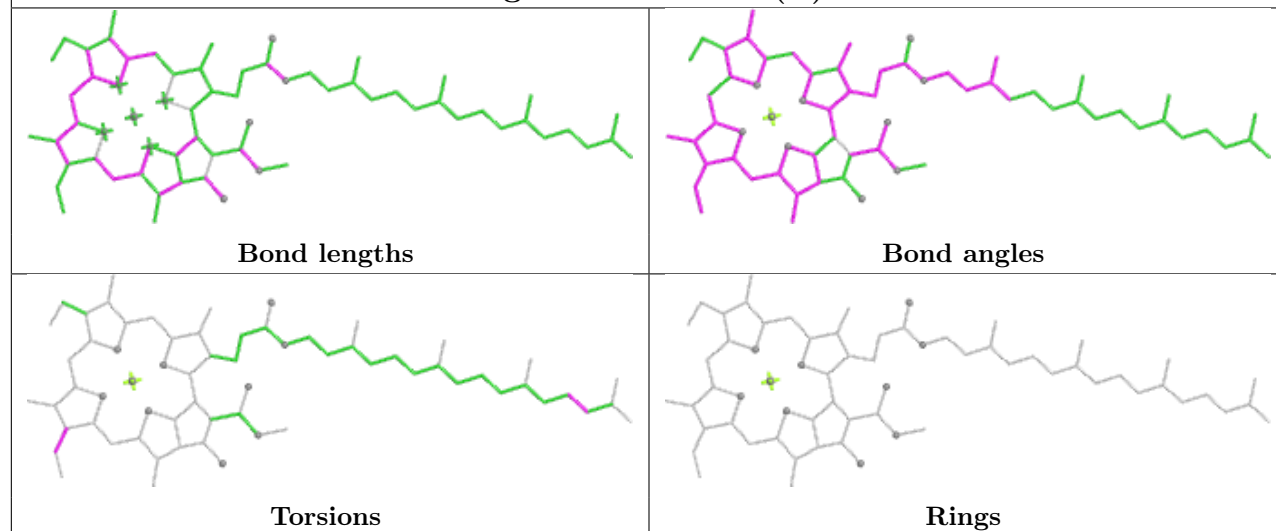




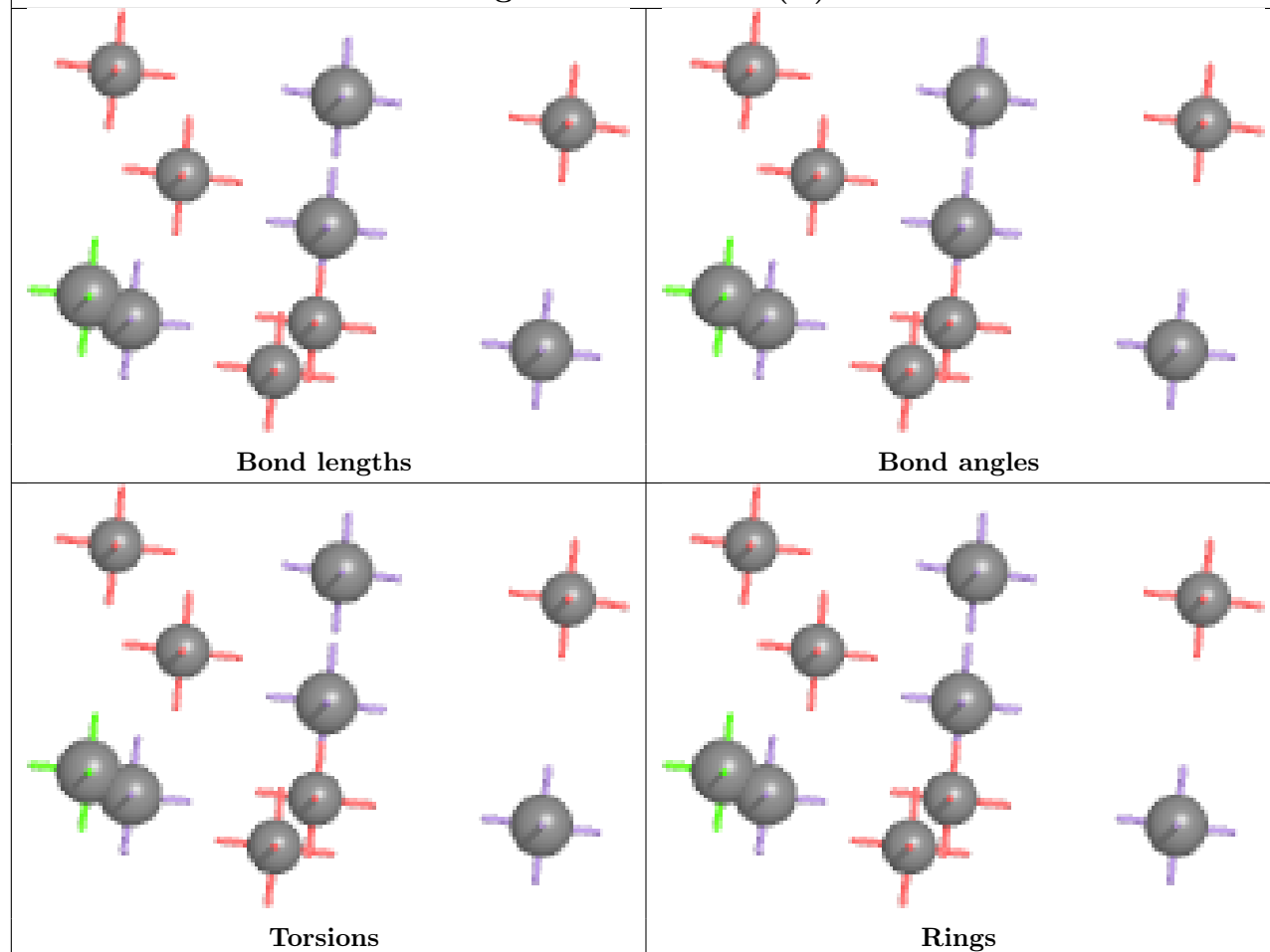


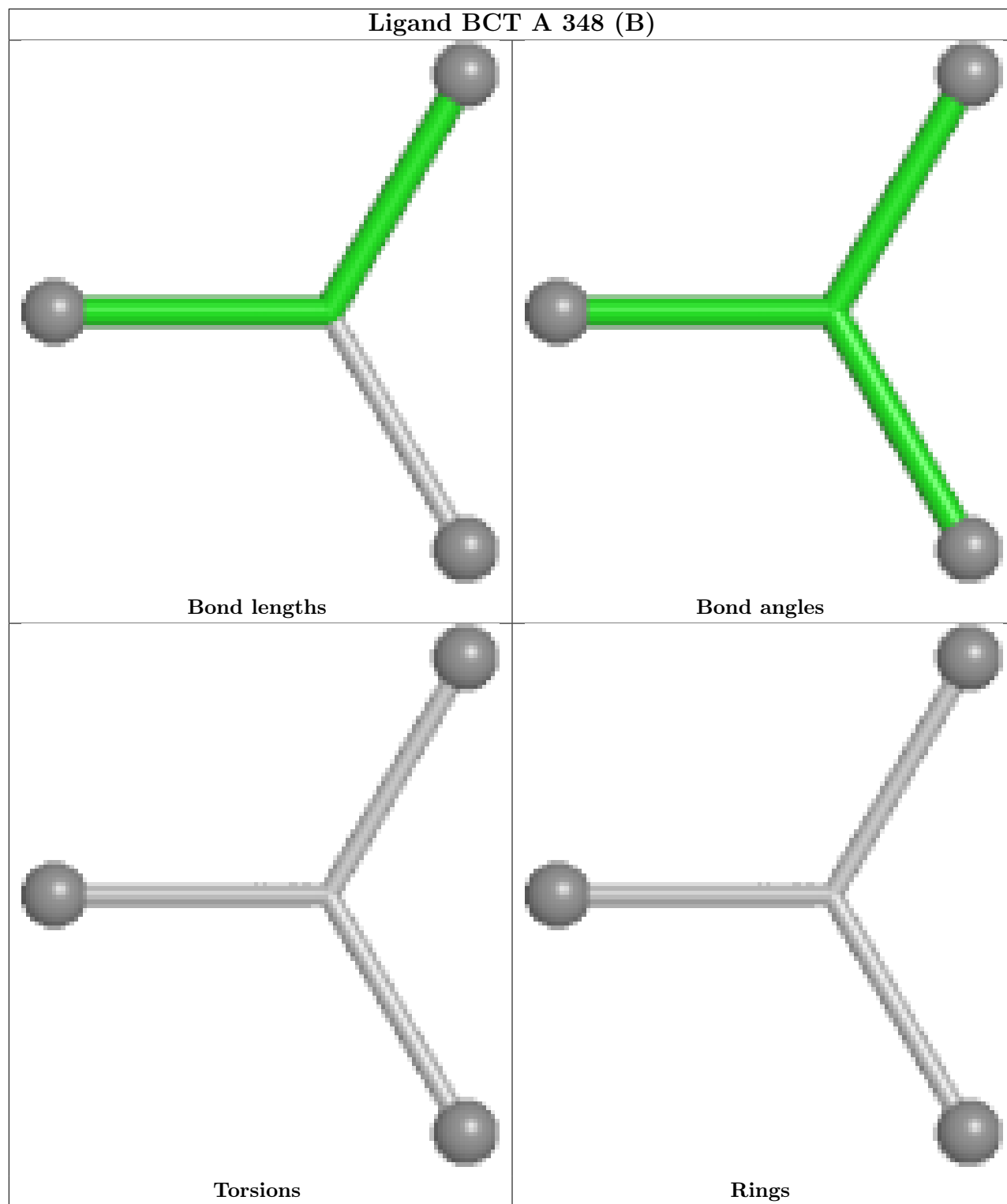
Ligand CLA C 511**Ligand CLA B 603****Ligand CLA D 406**

Ligand CLA a 406 (B)

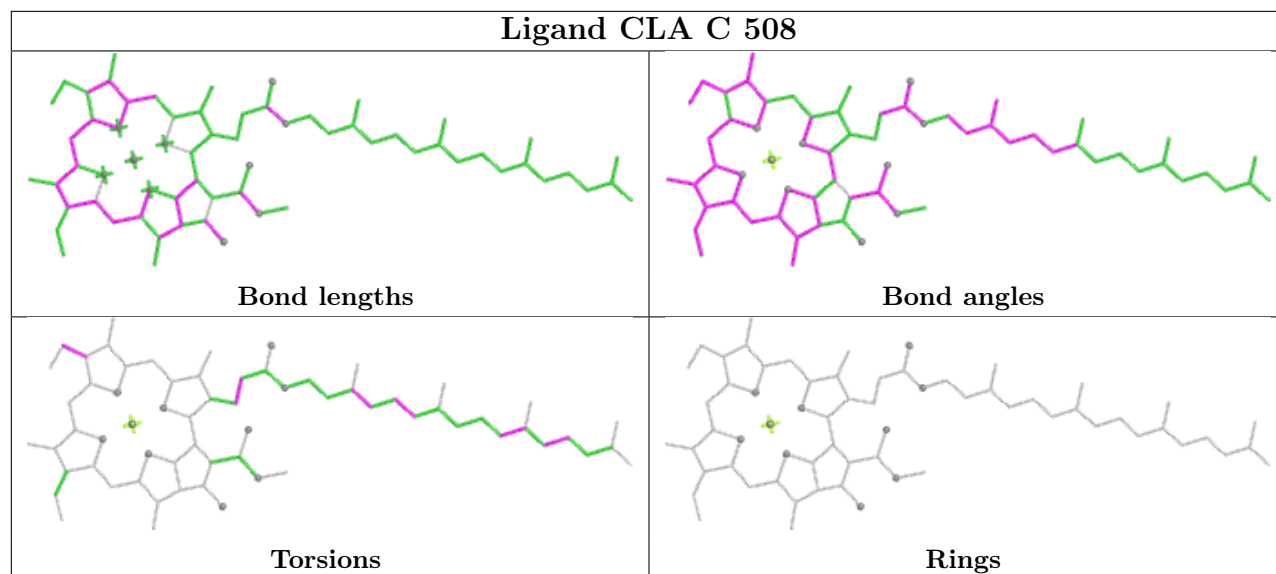


Ligand OEX A 413 (B)

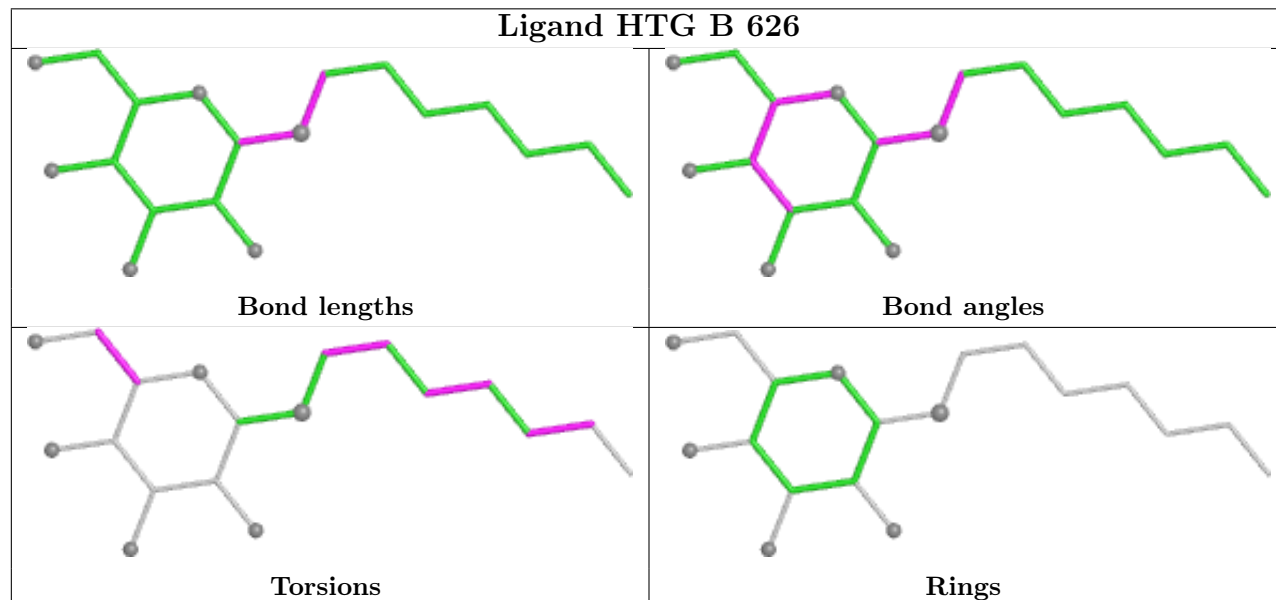


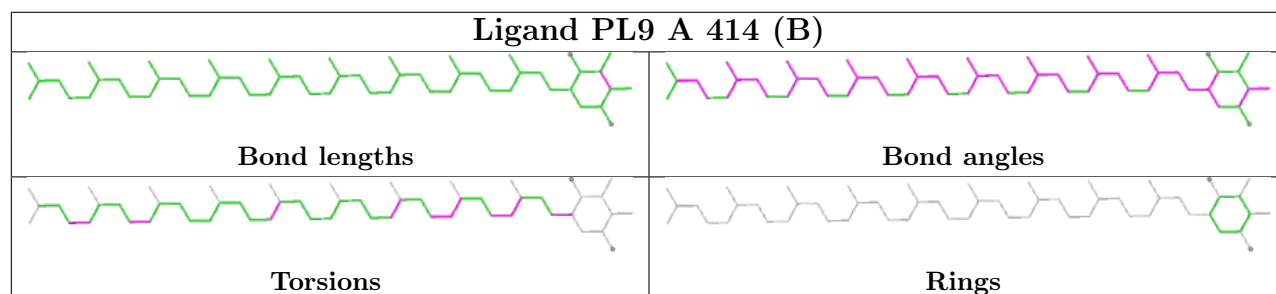
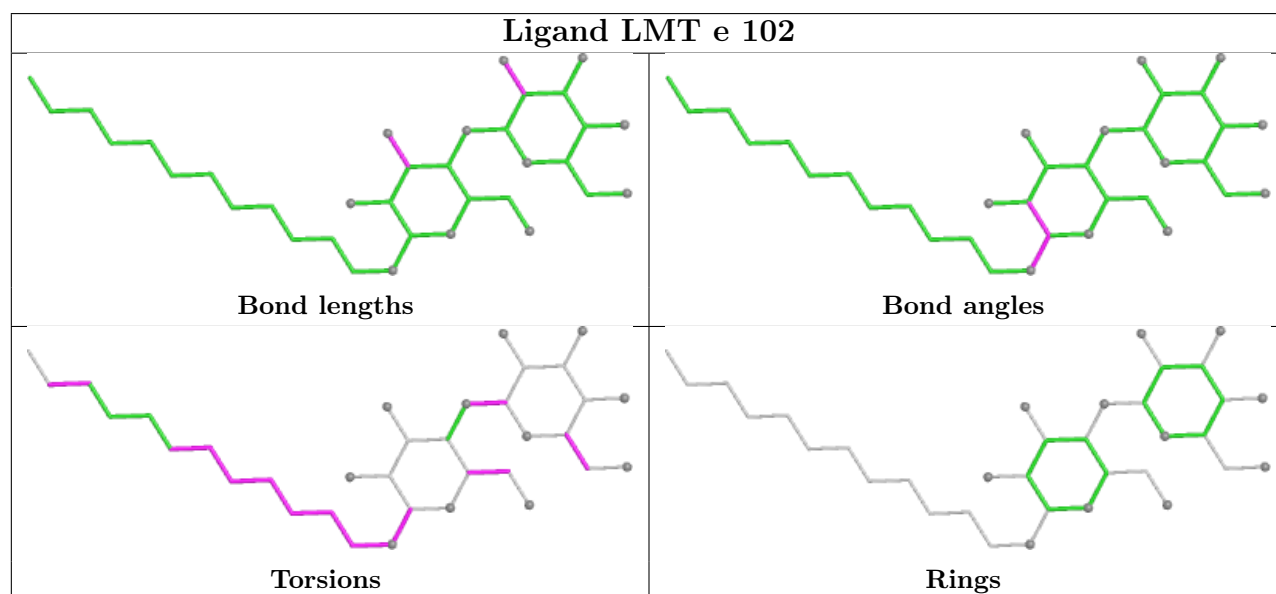
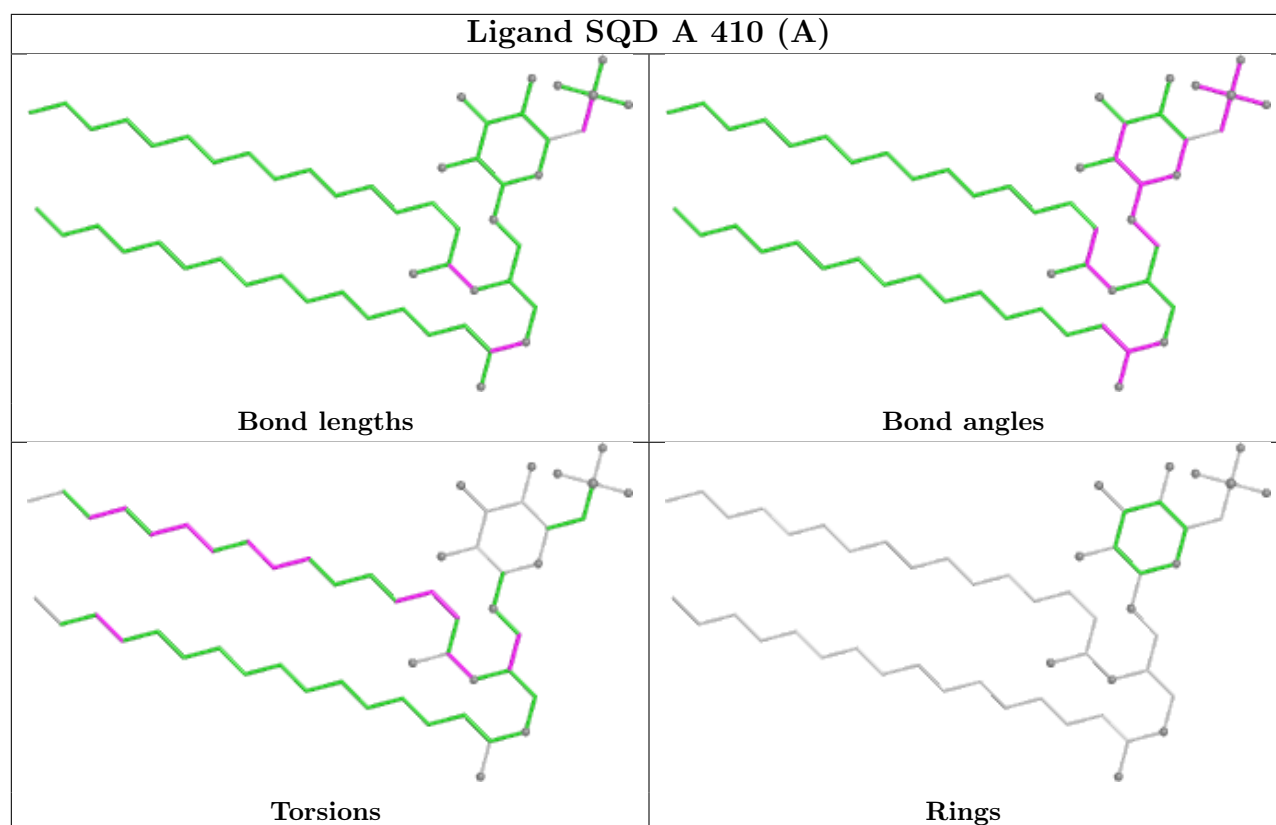


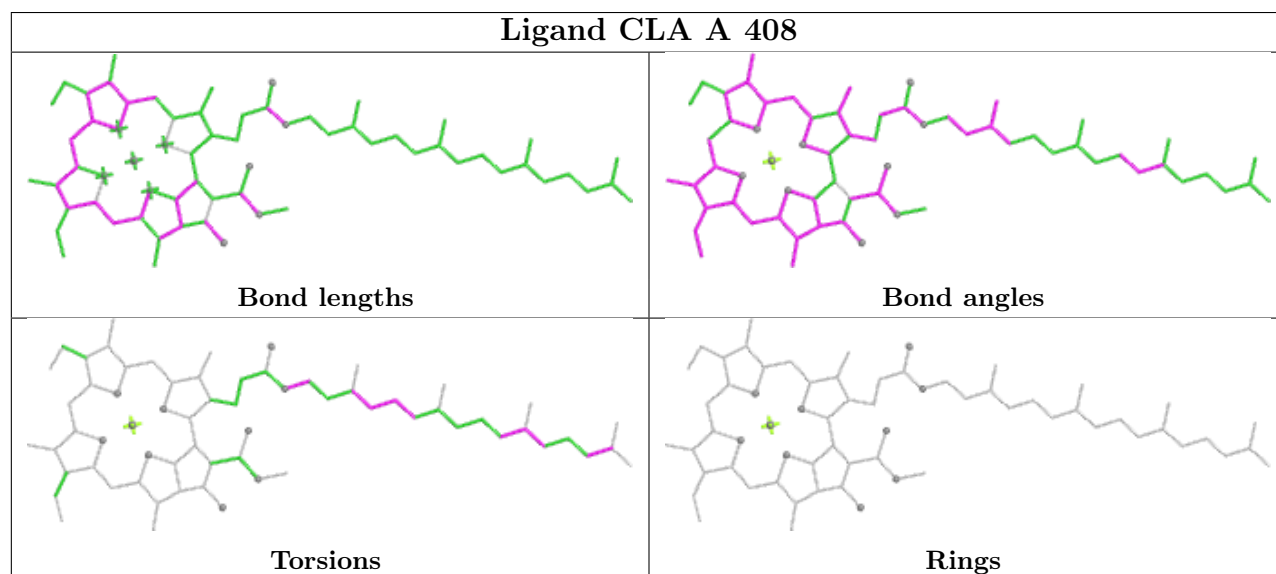
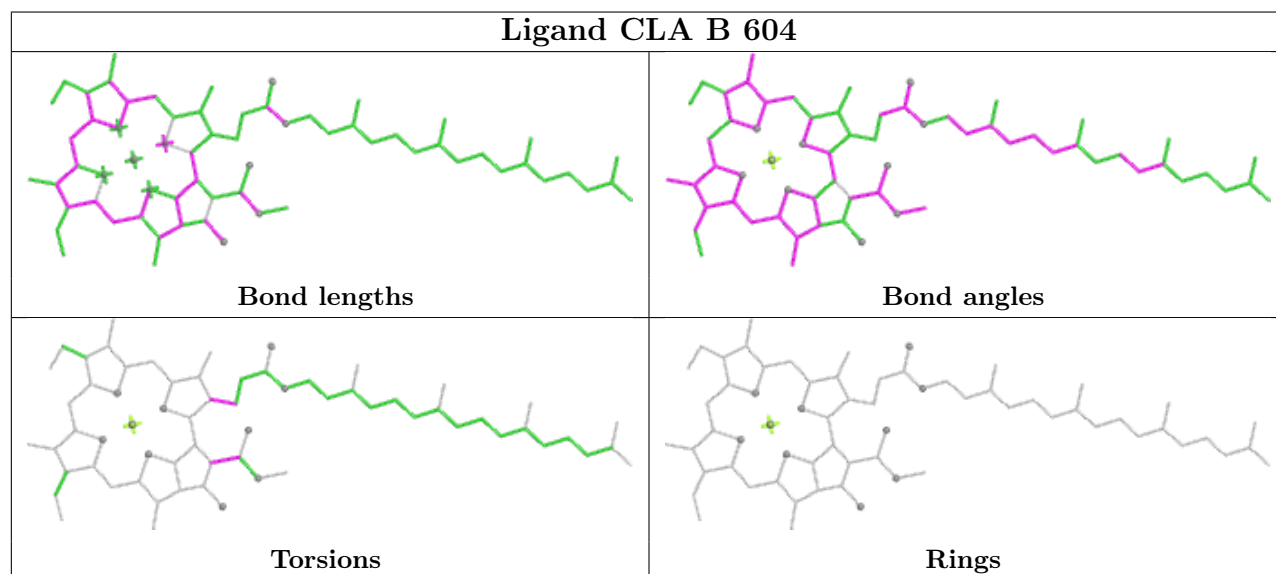
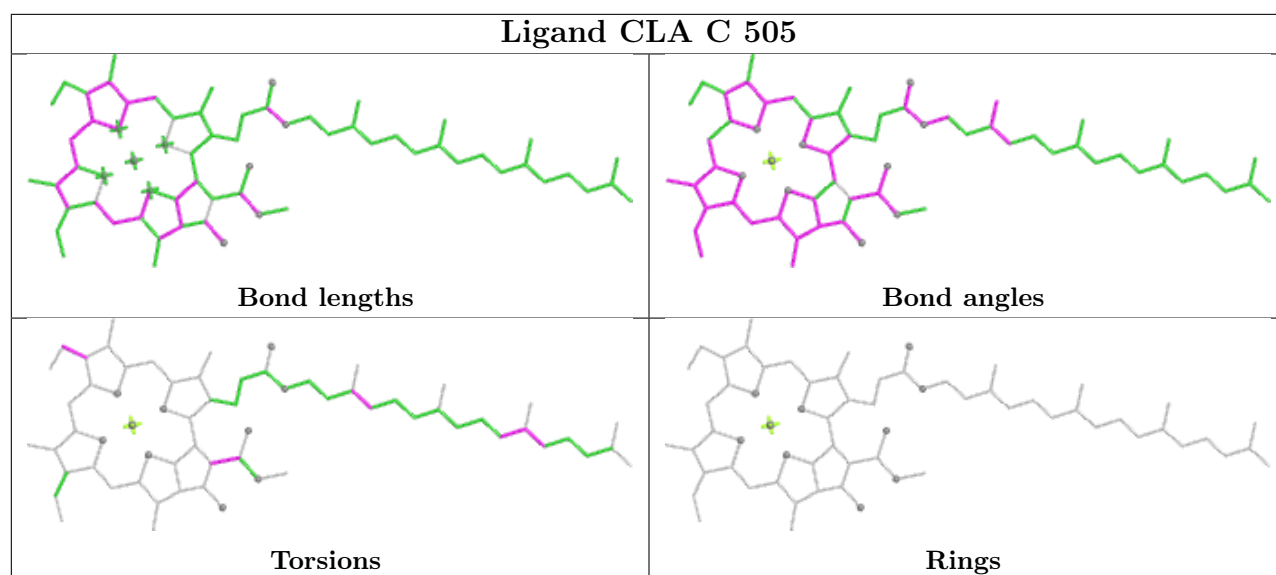
Ligand CLA C 508

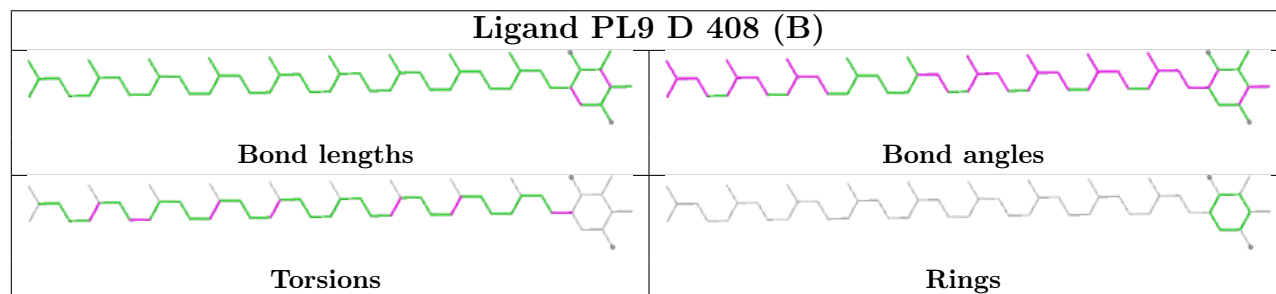
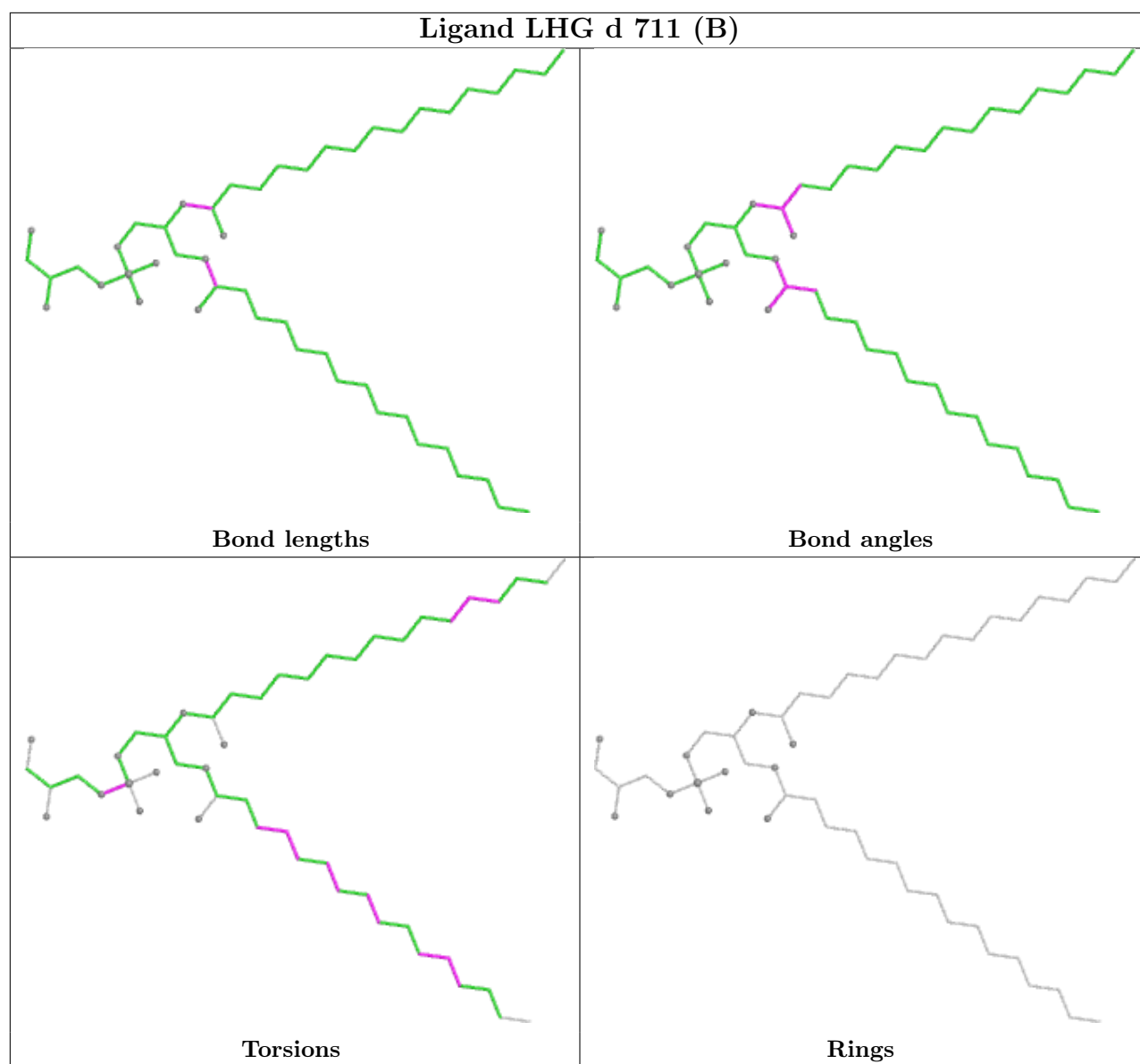


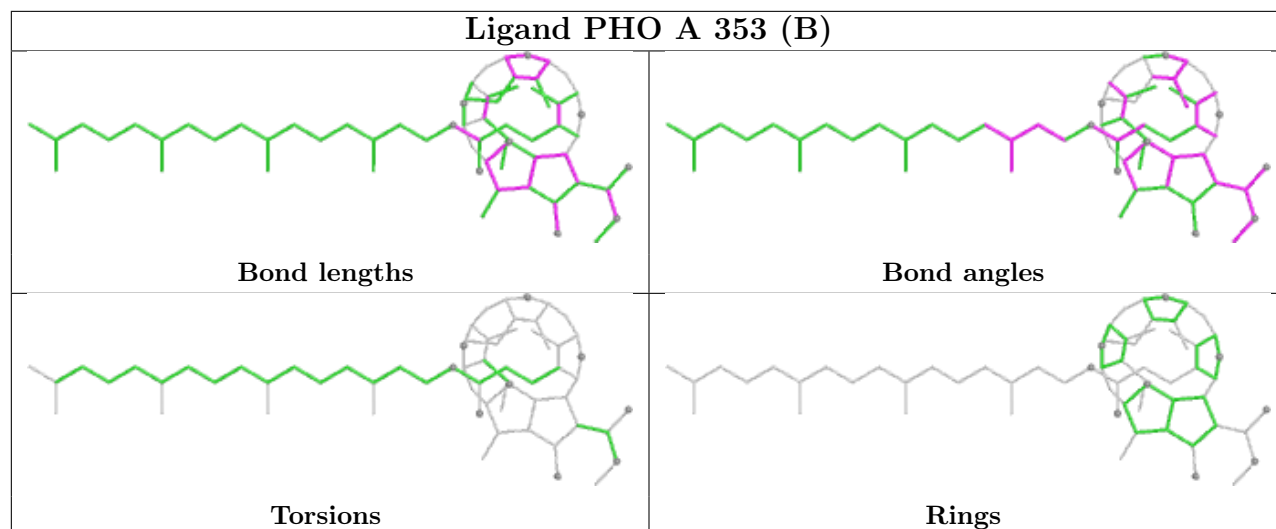
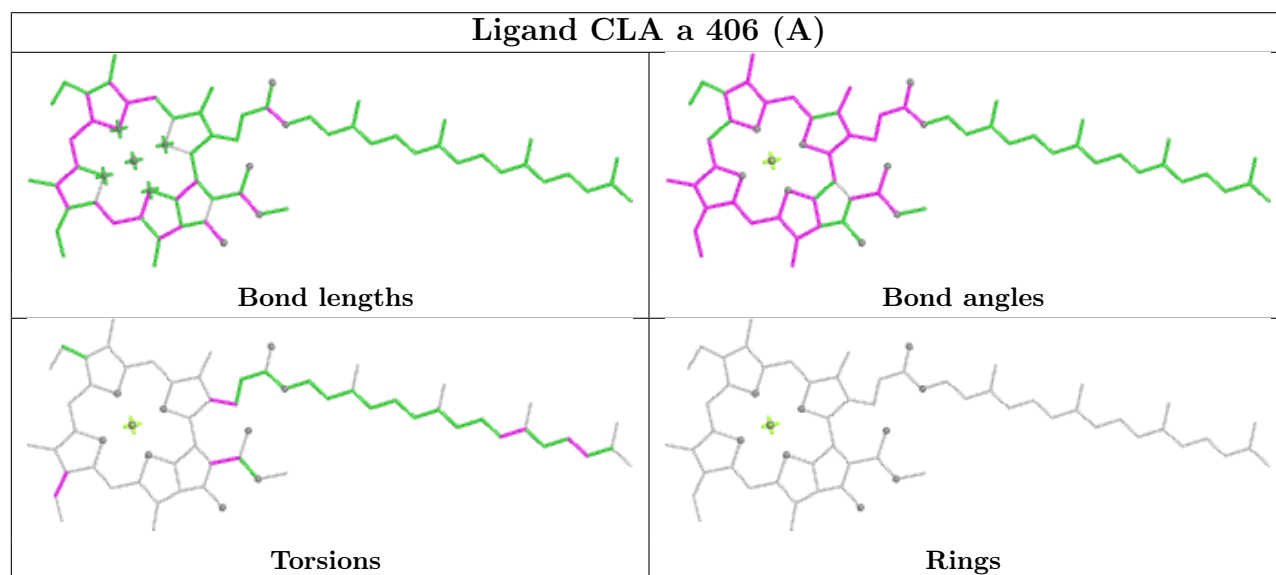
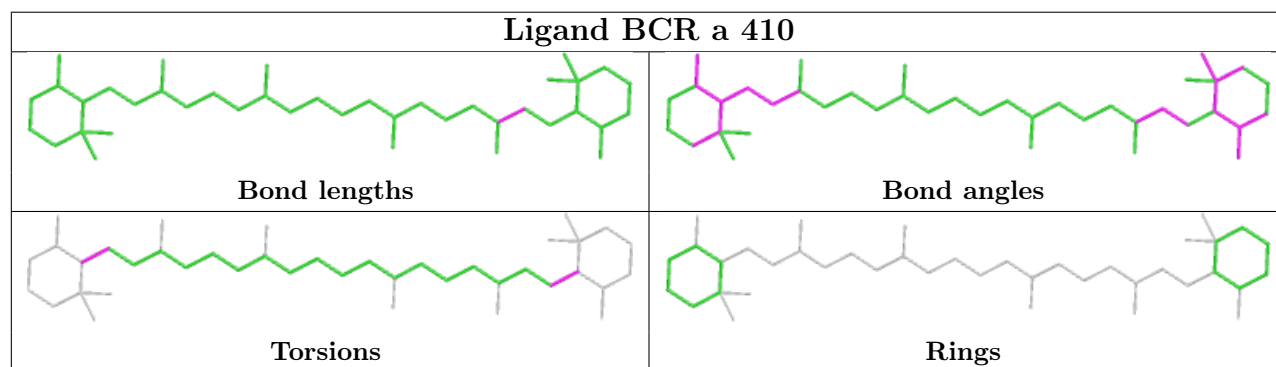
Ligand HTG B 626

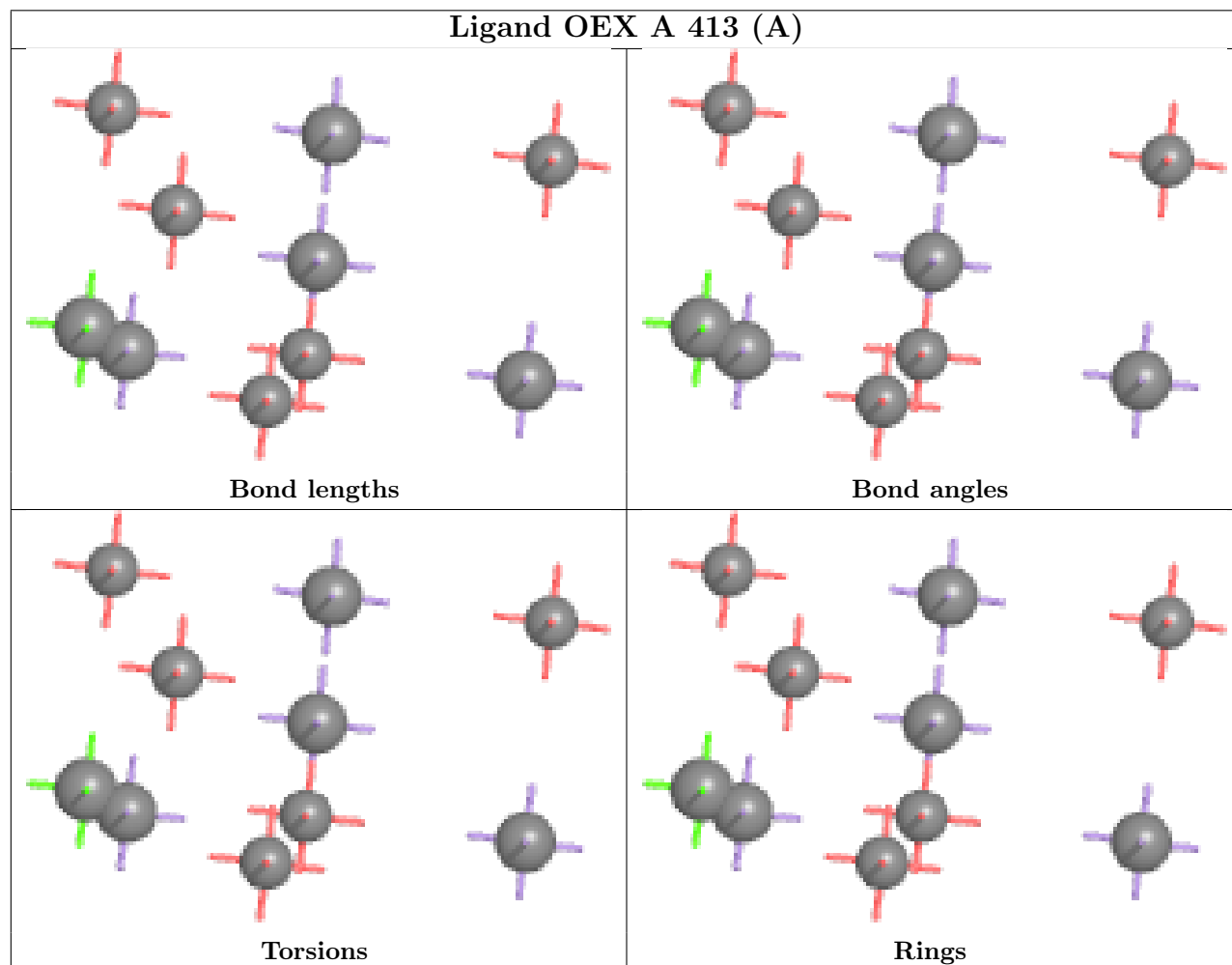
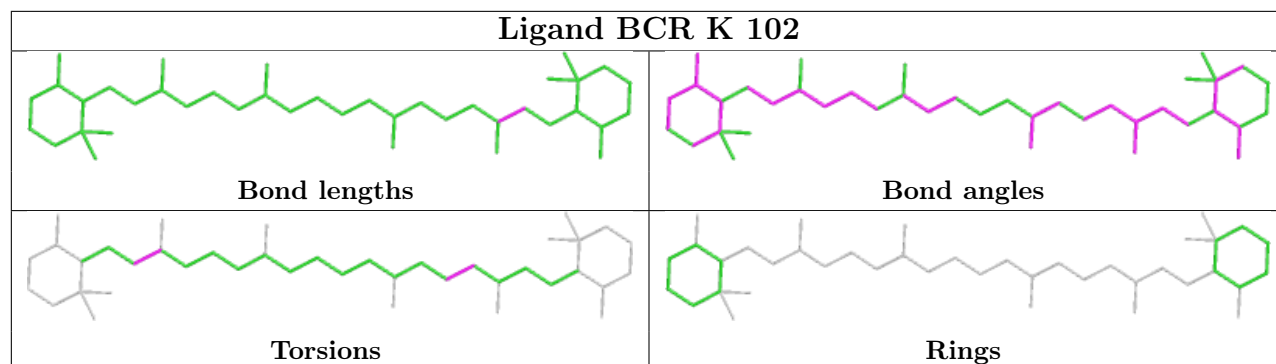


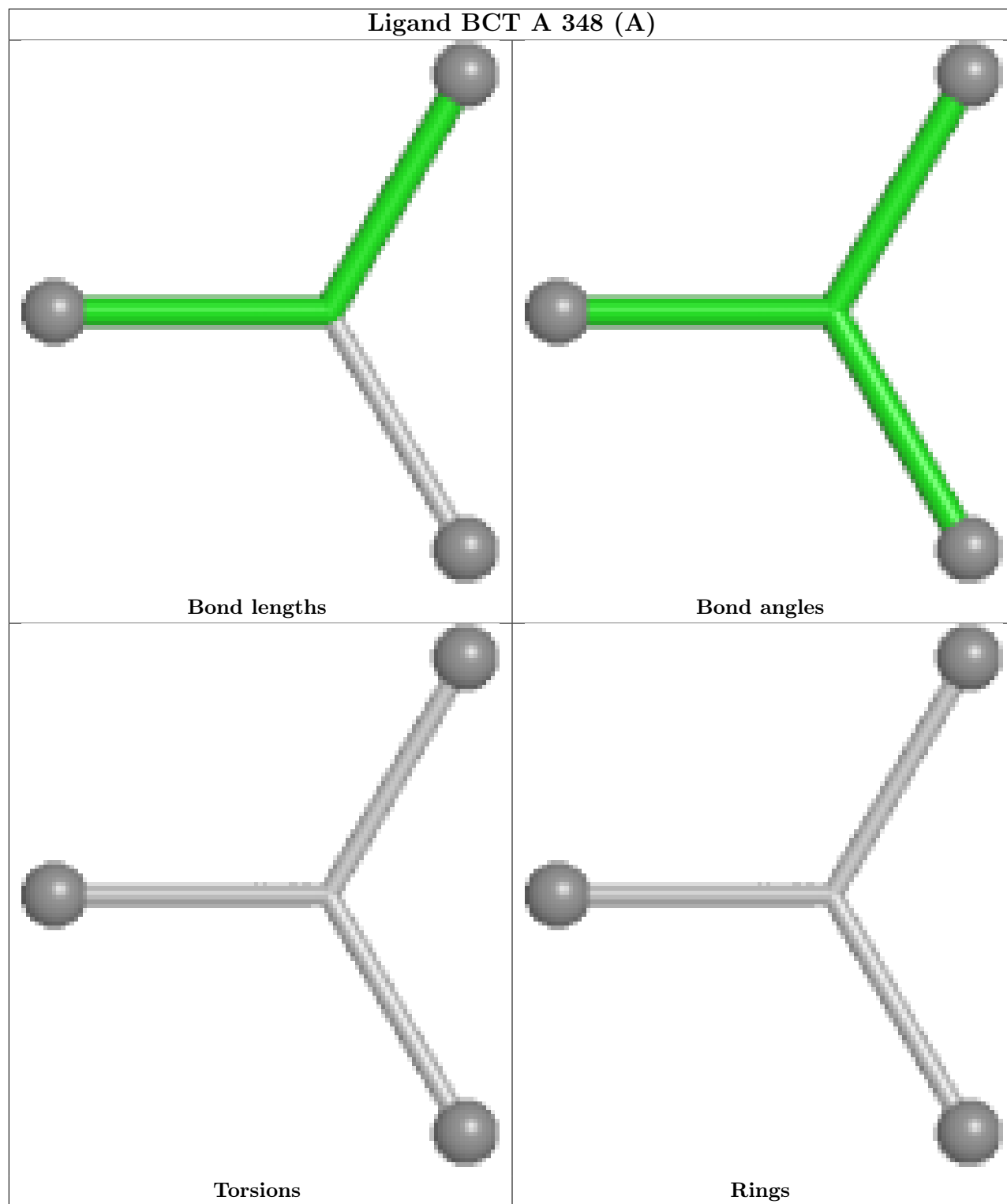


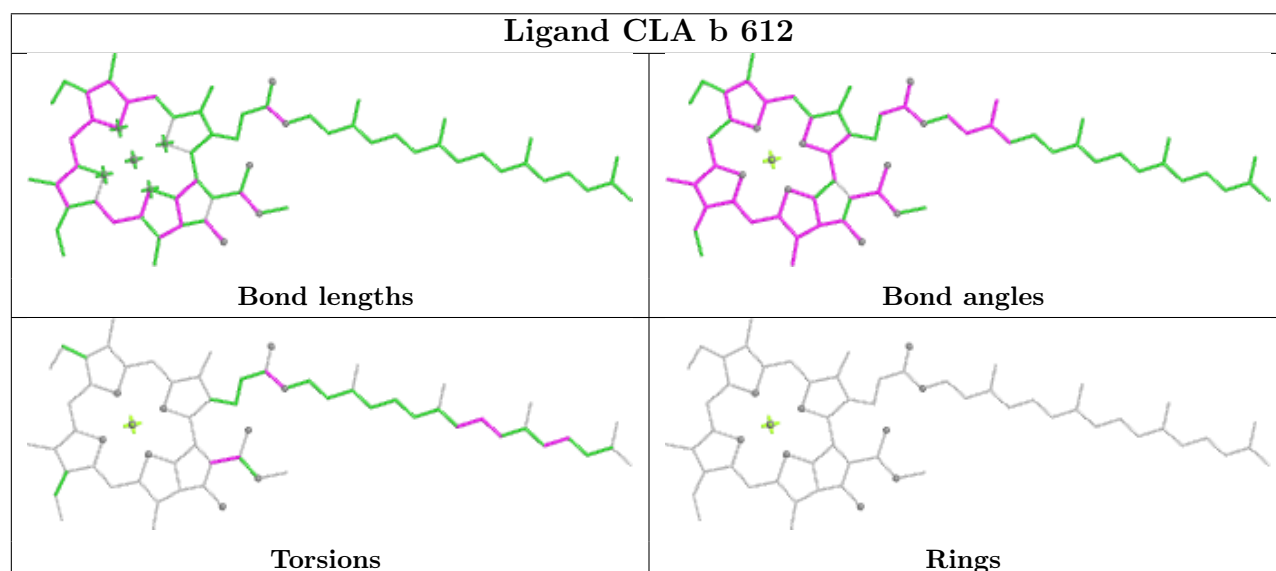
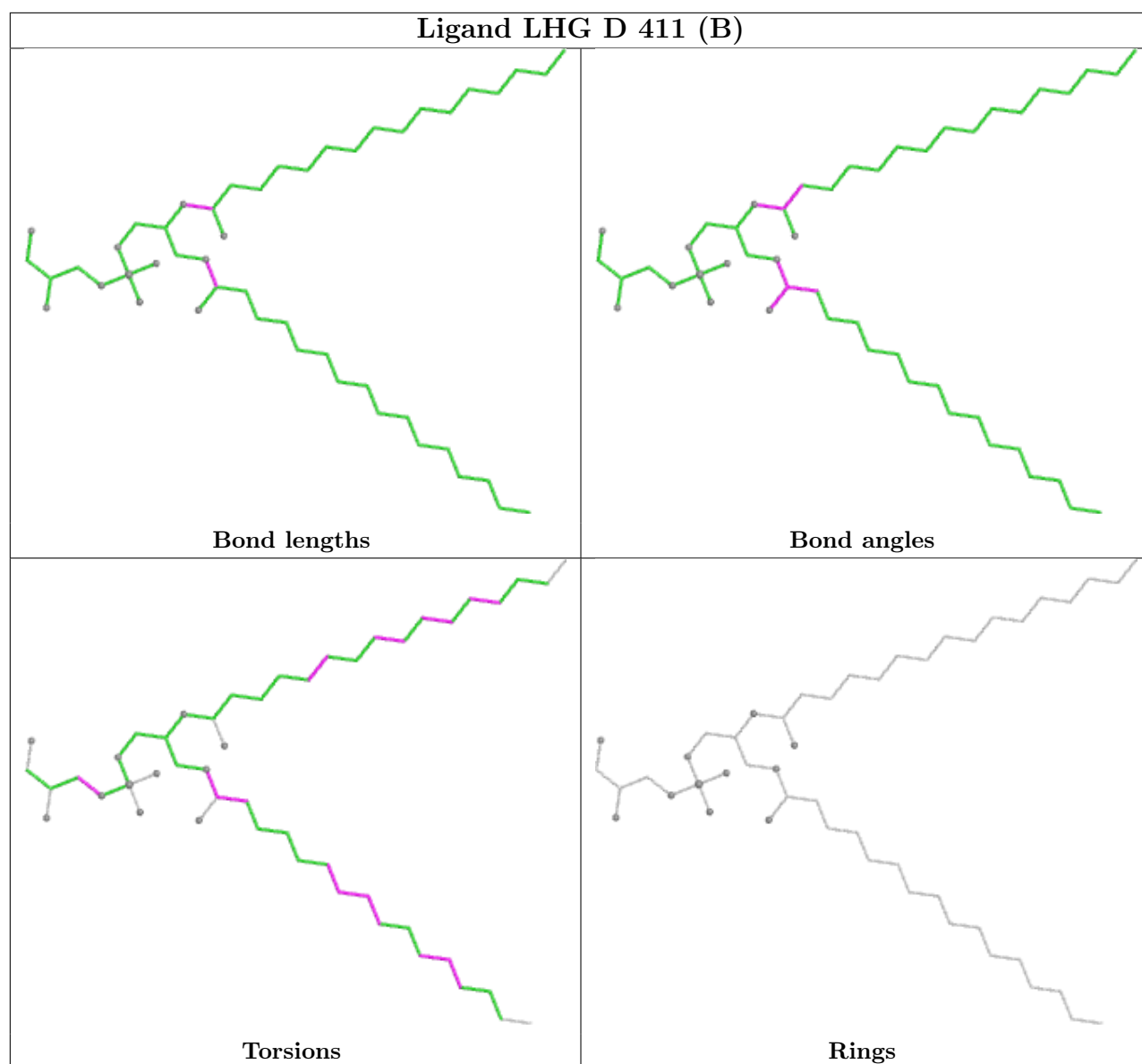


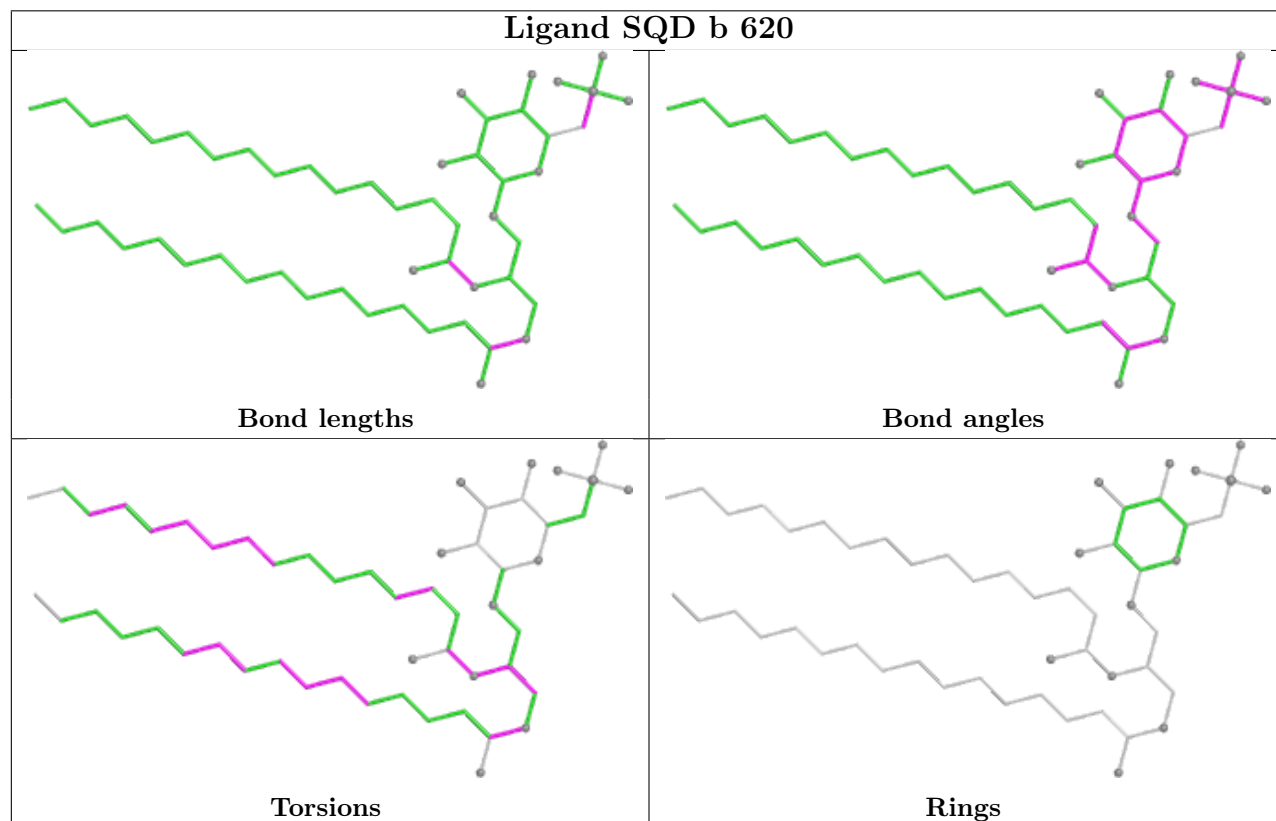
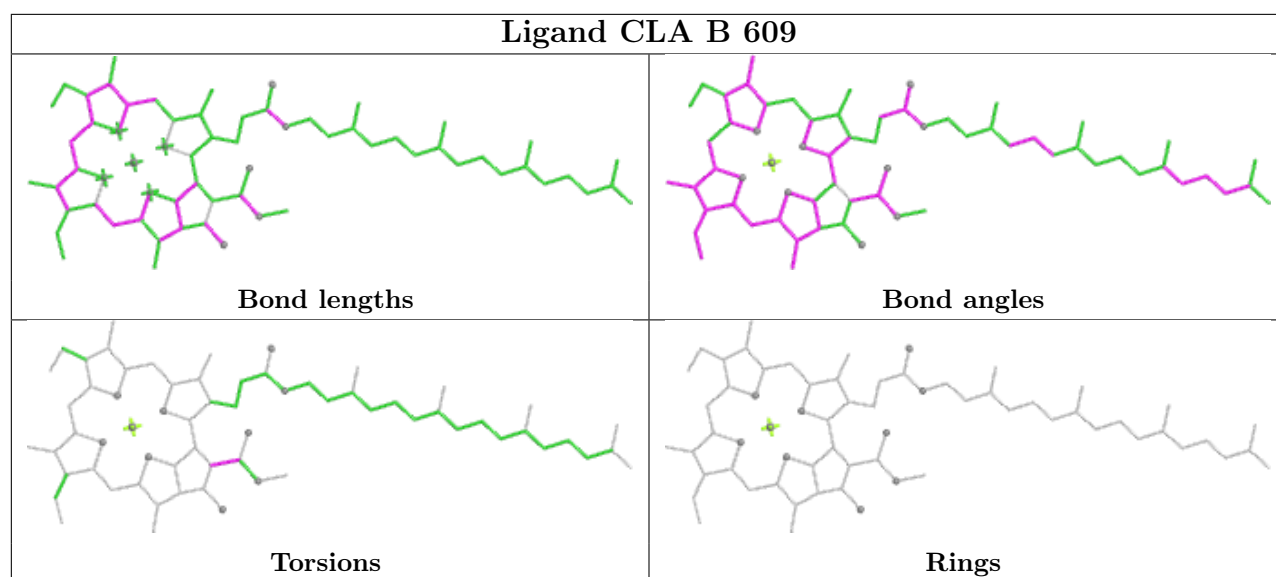


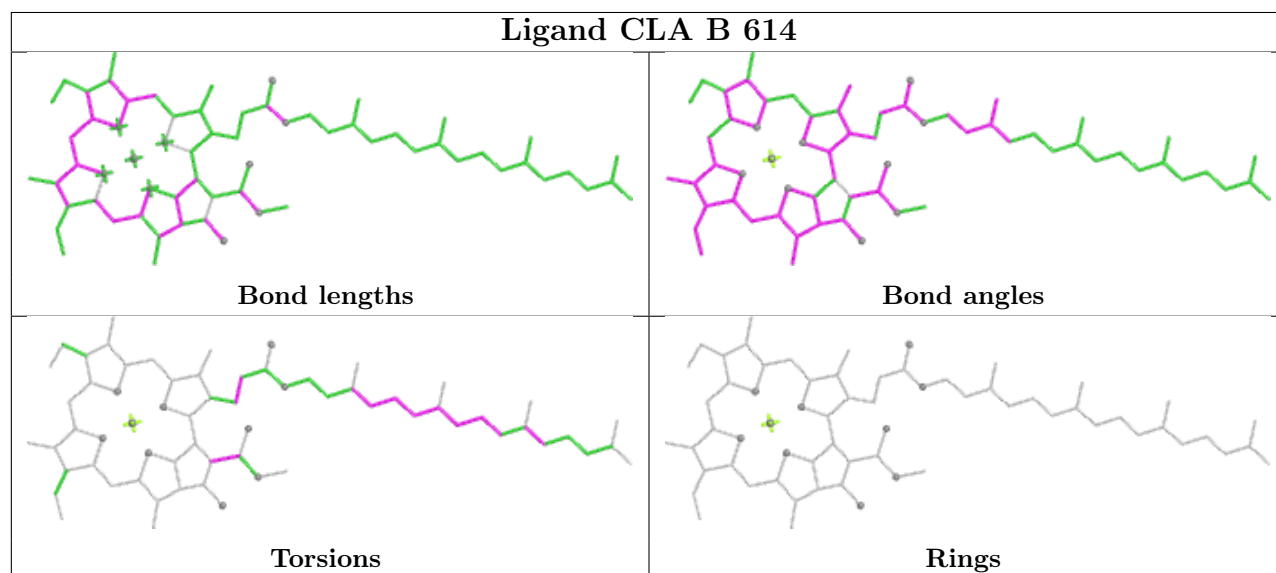
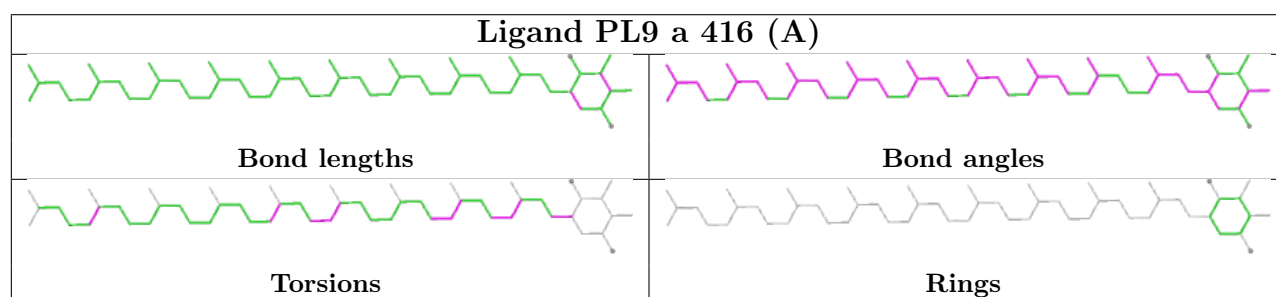
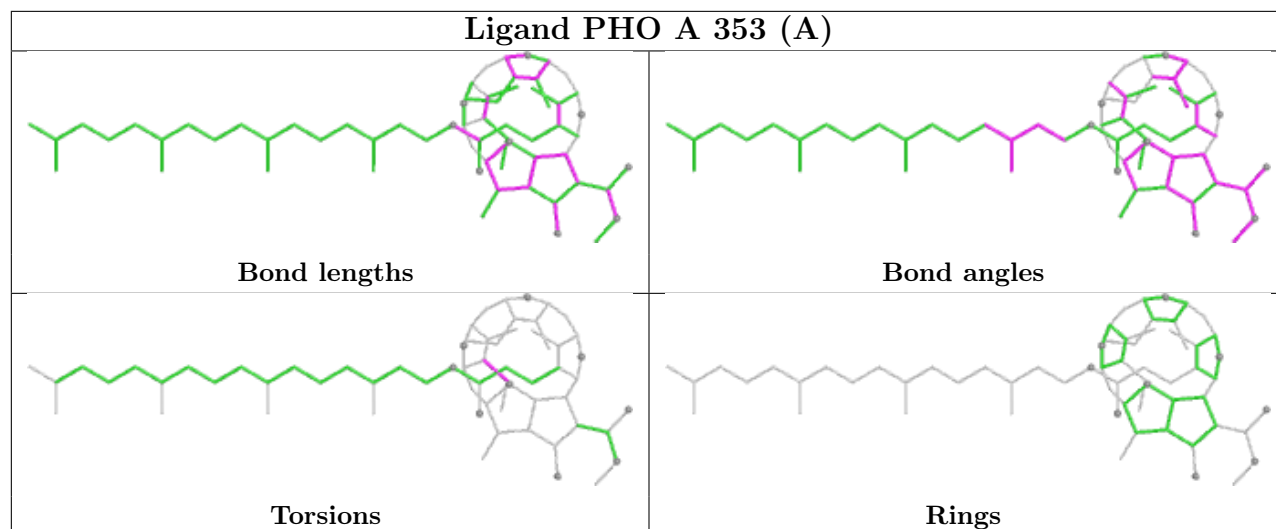
Ligand PHO A 353 (B)**Ligand CLA a 406 (A)****Ligand BCR a 410**

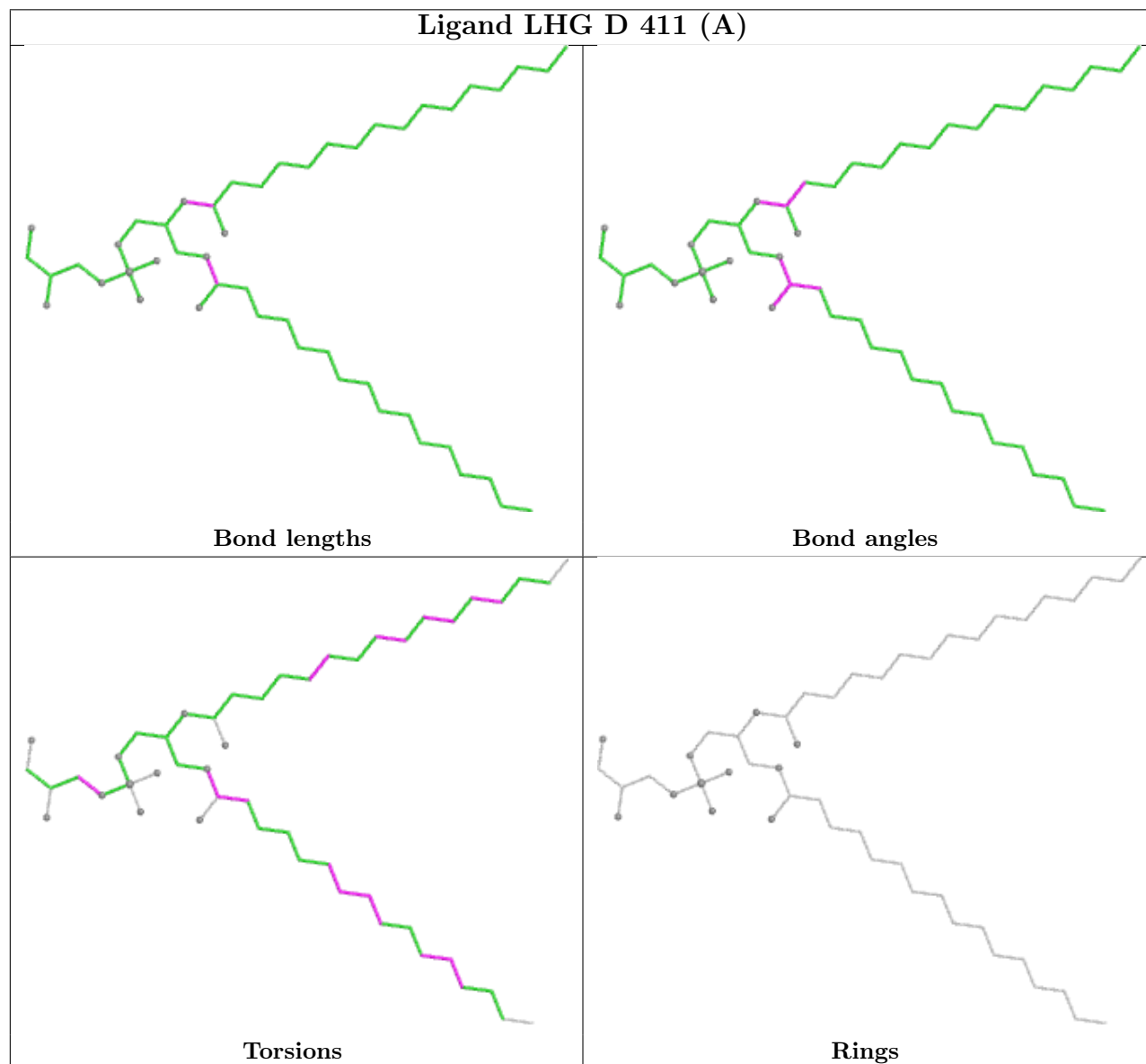
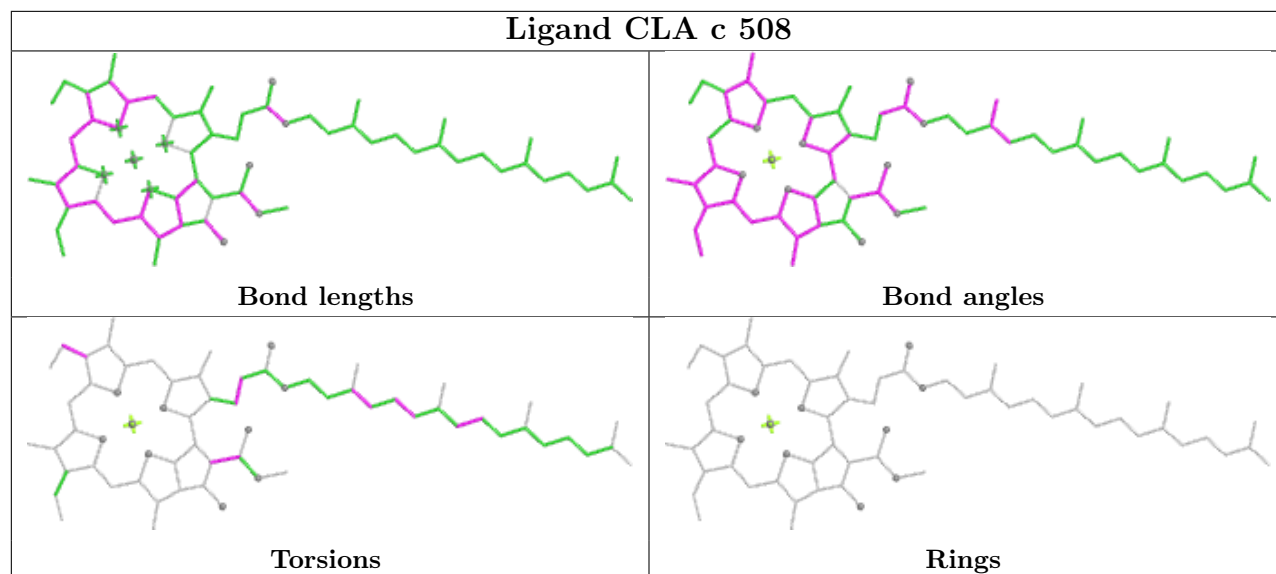


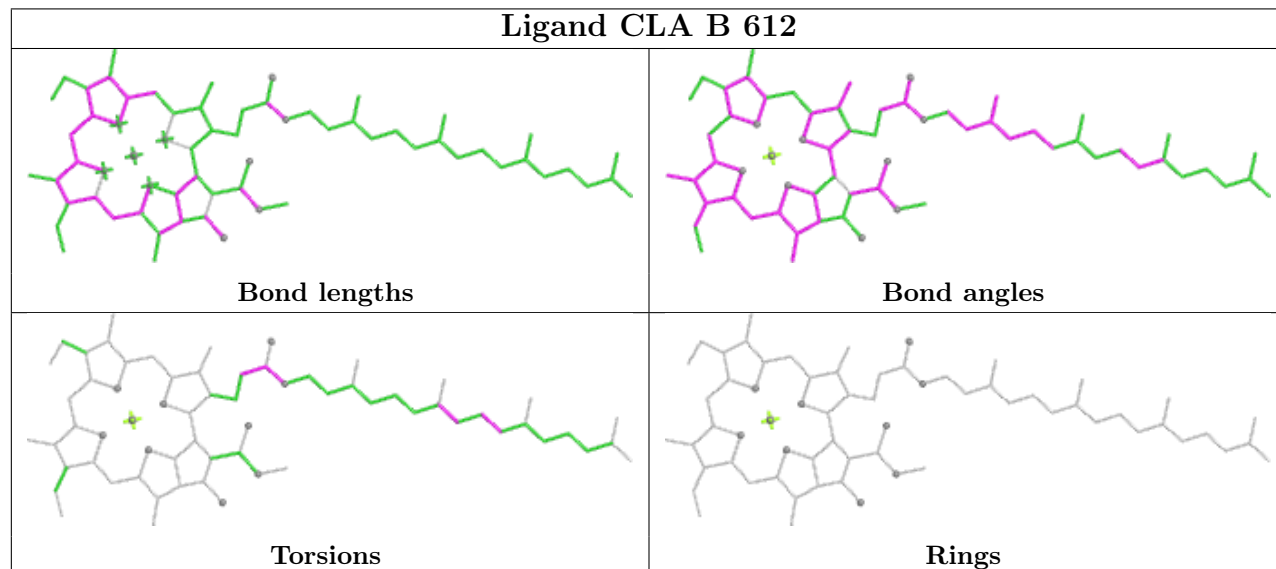
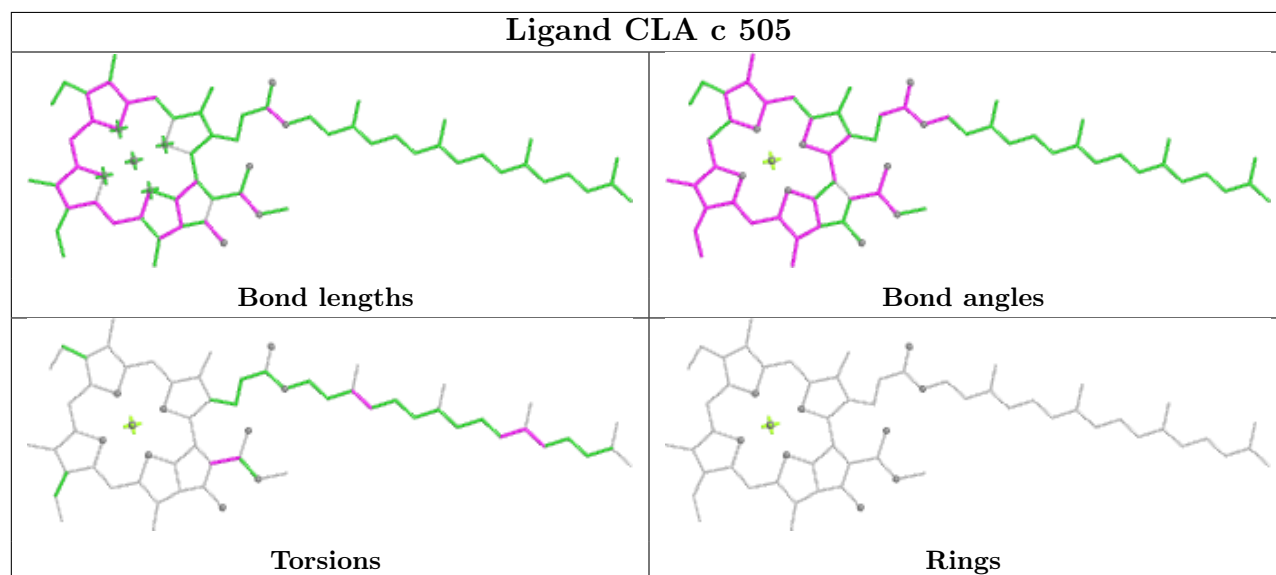
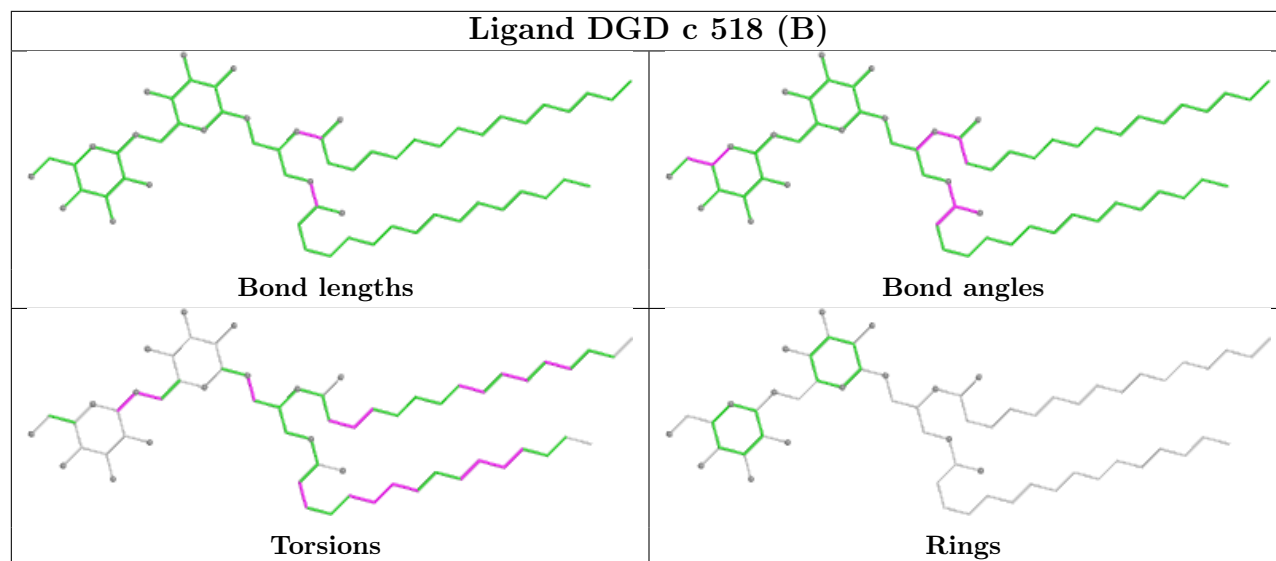


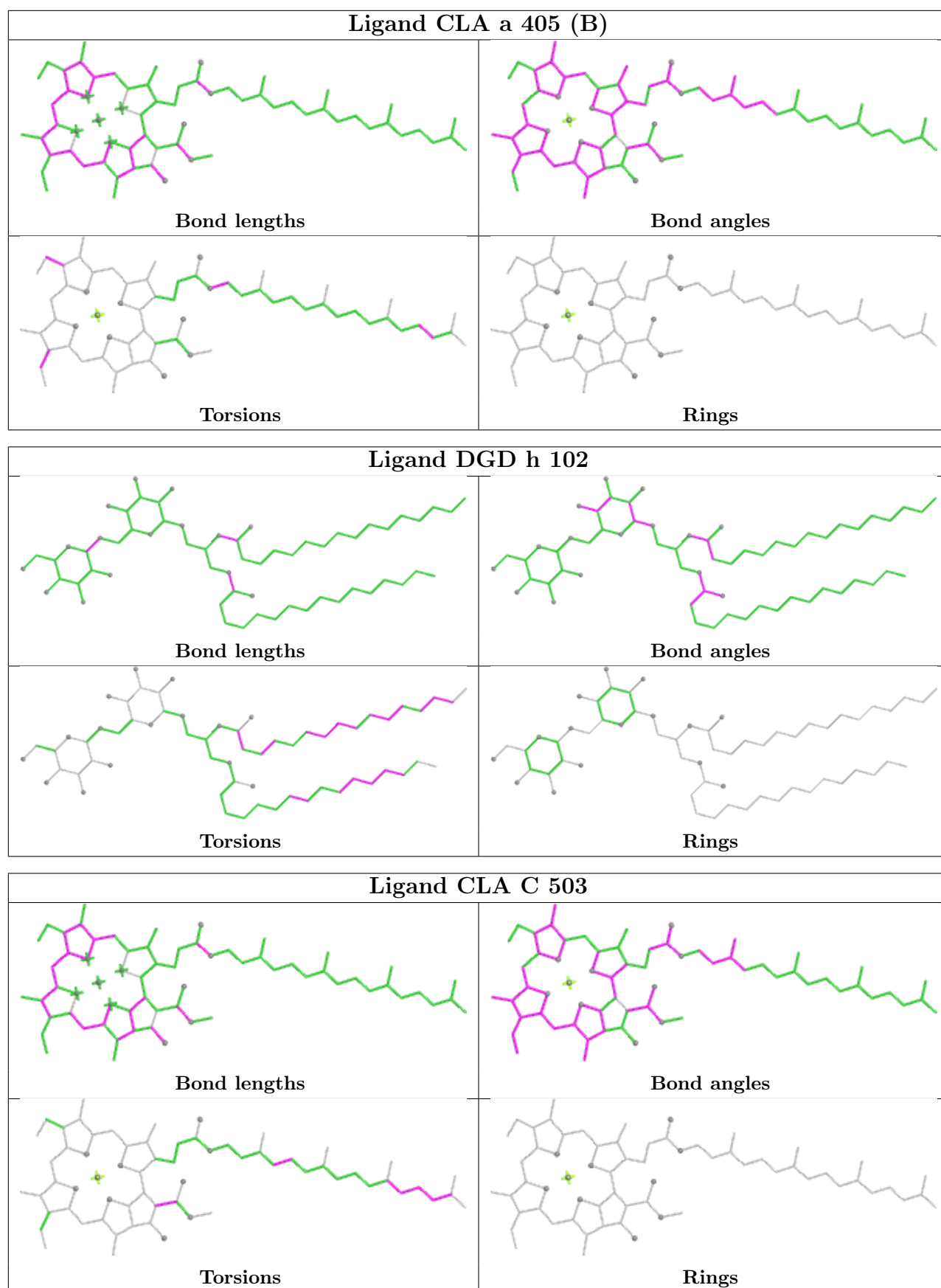




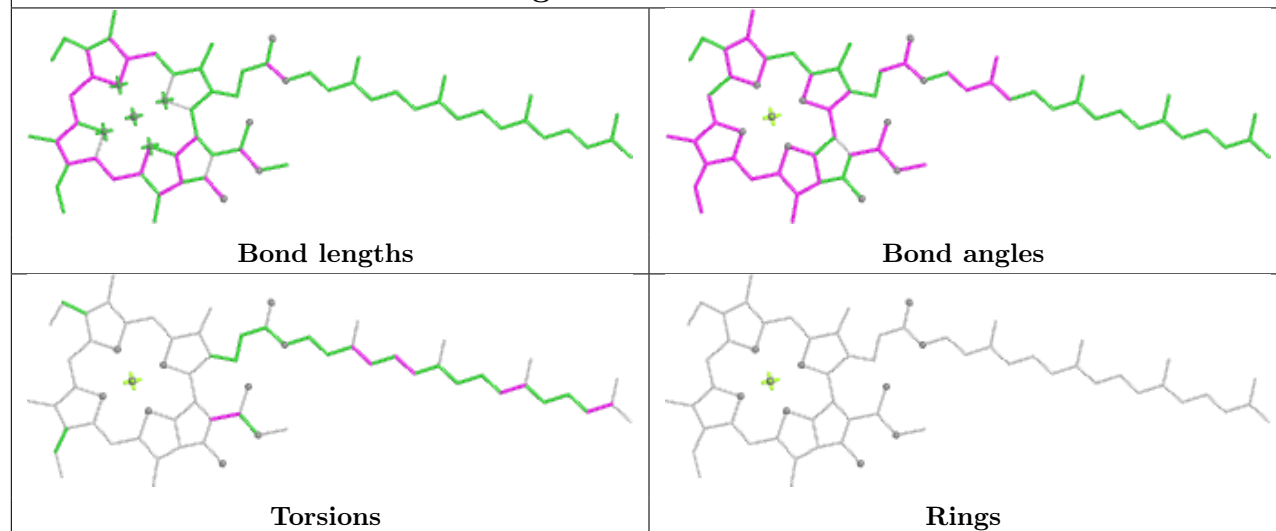




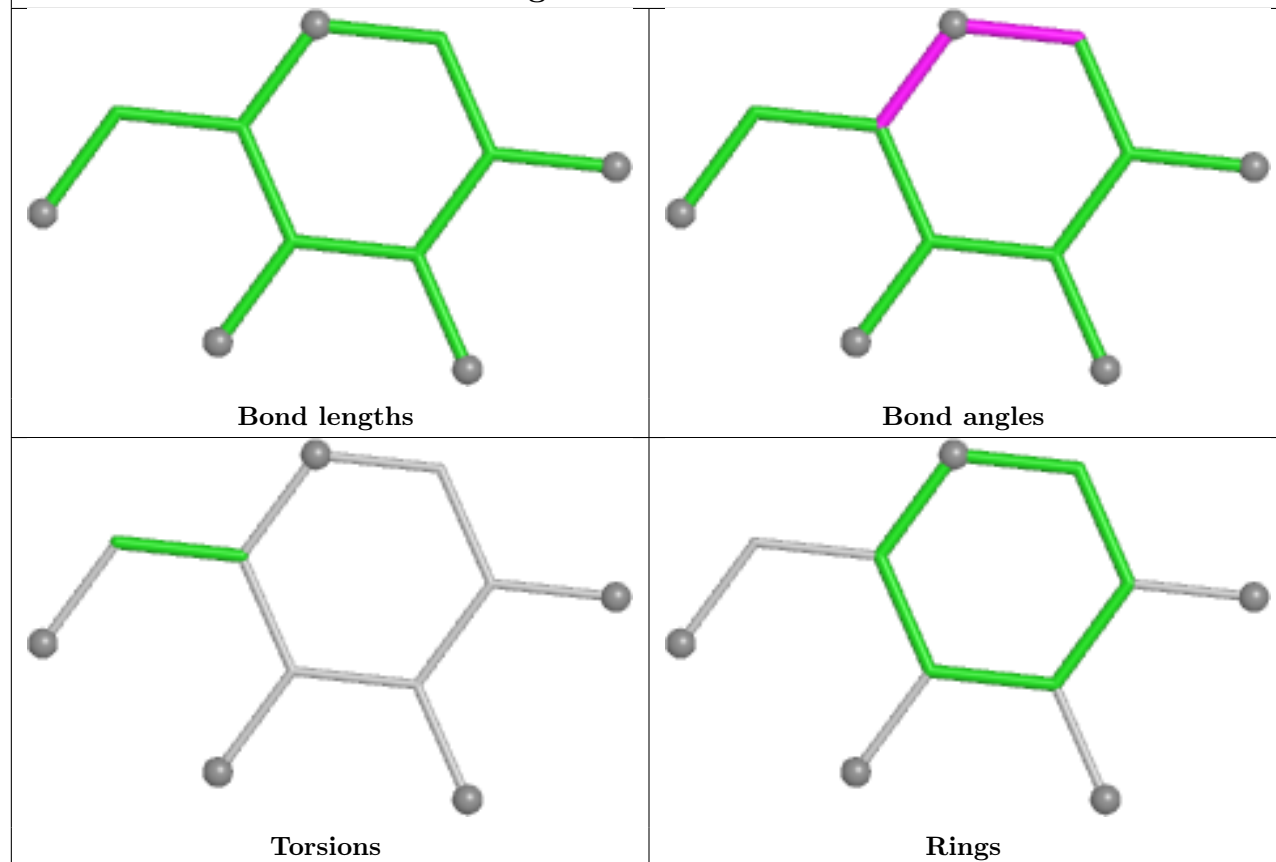


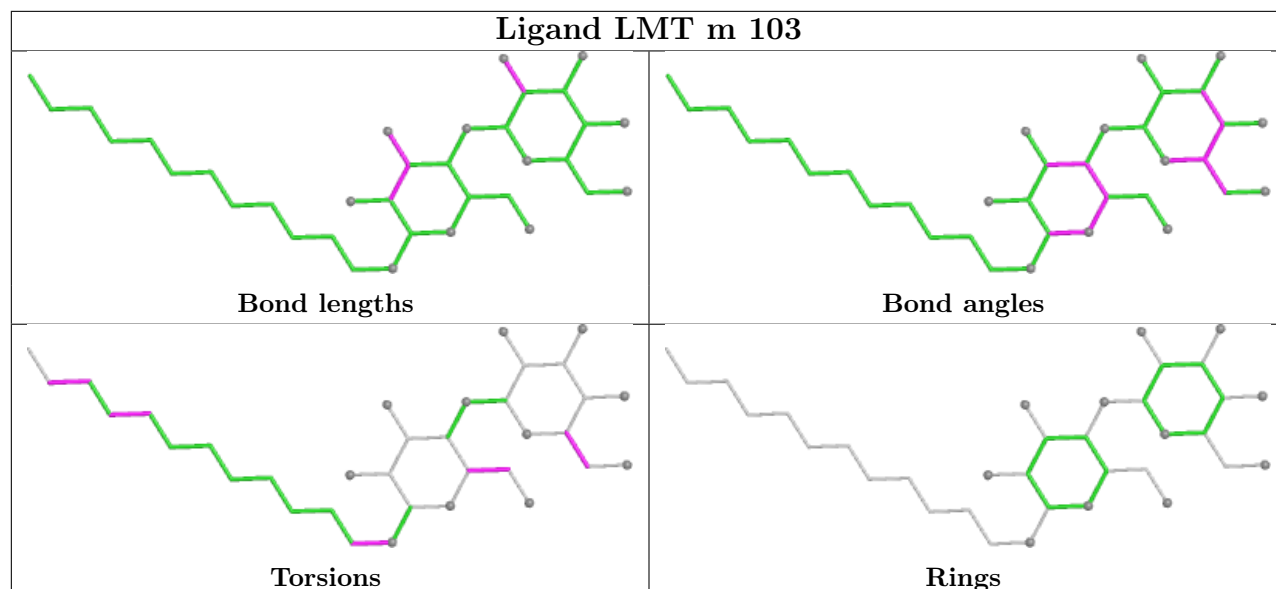
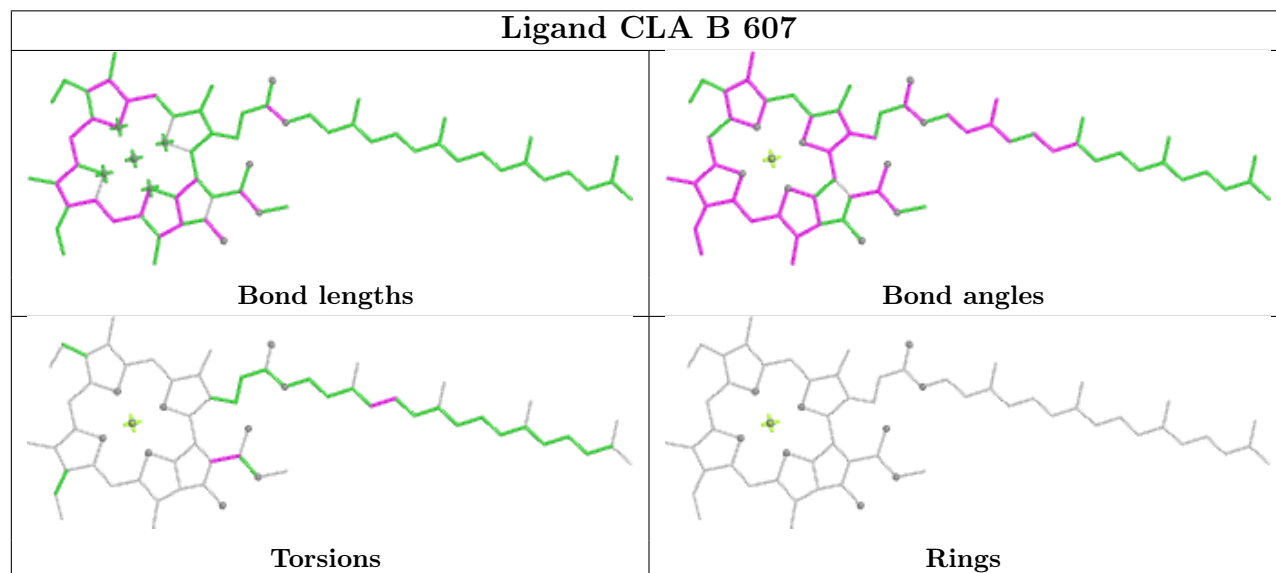
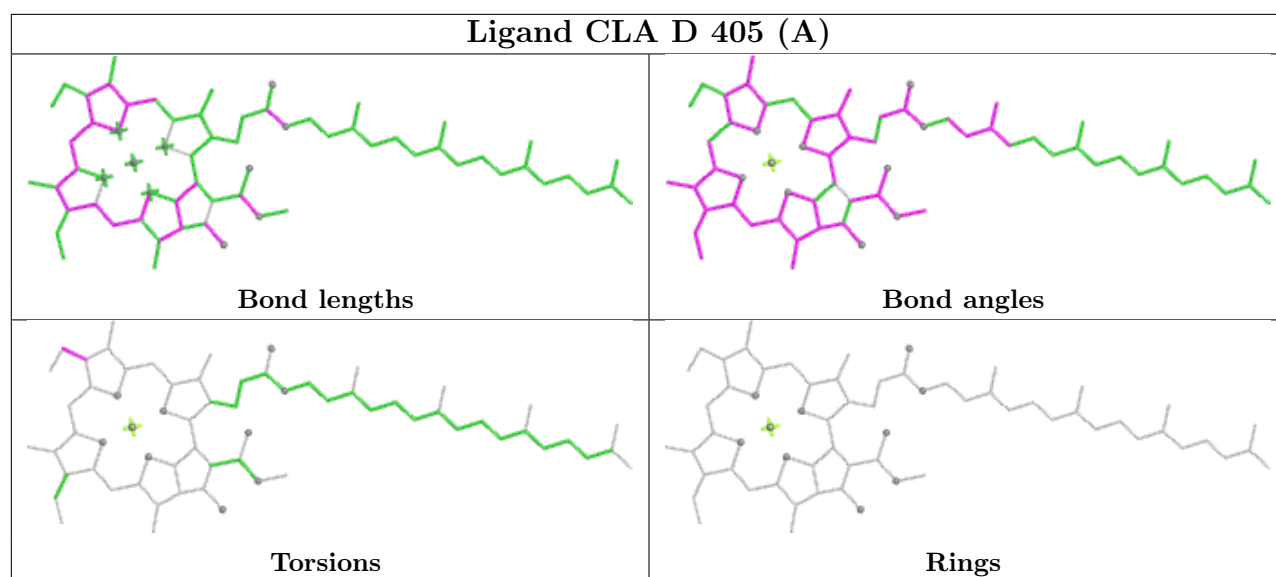


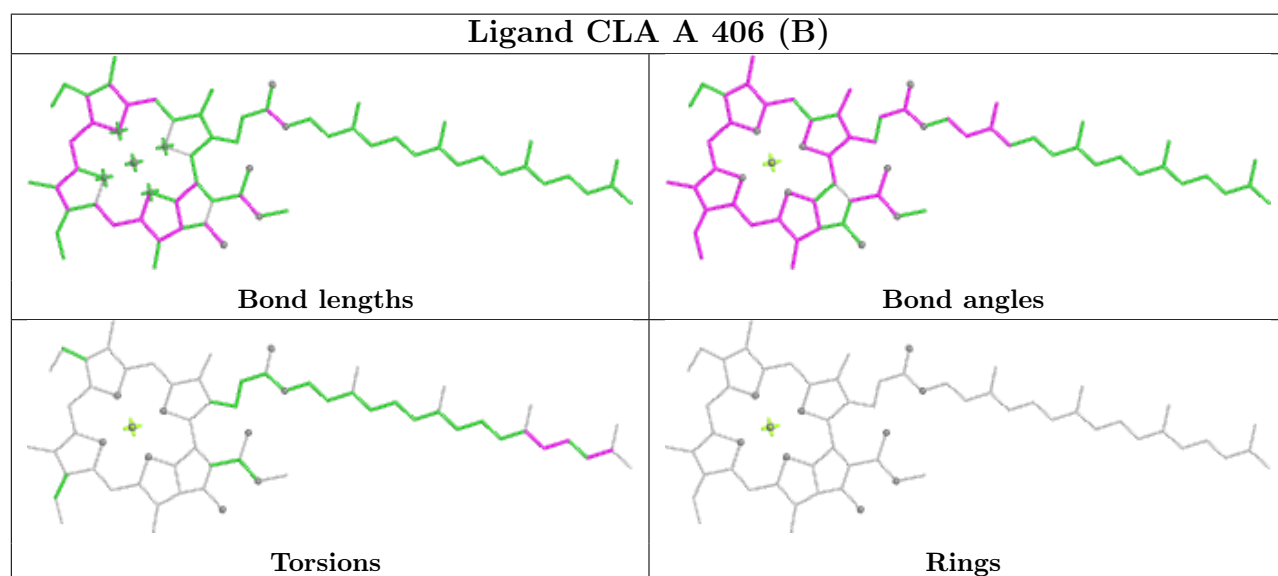
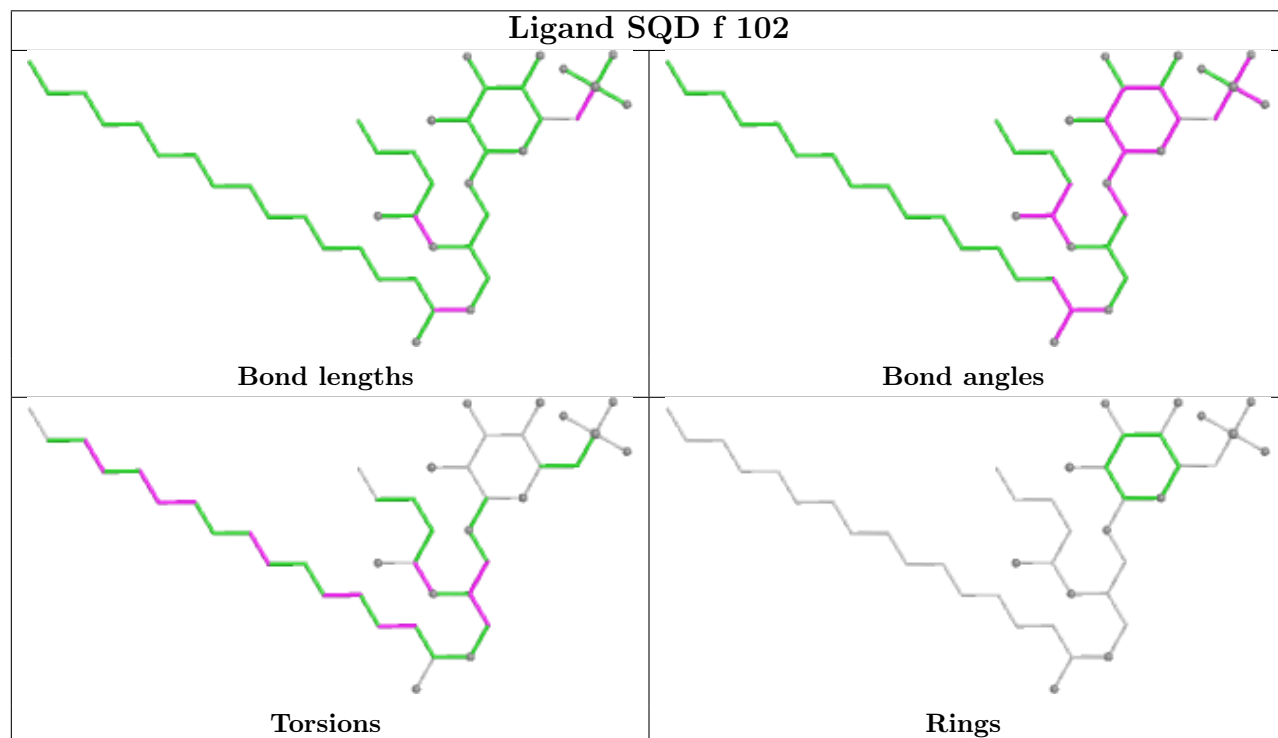
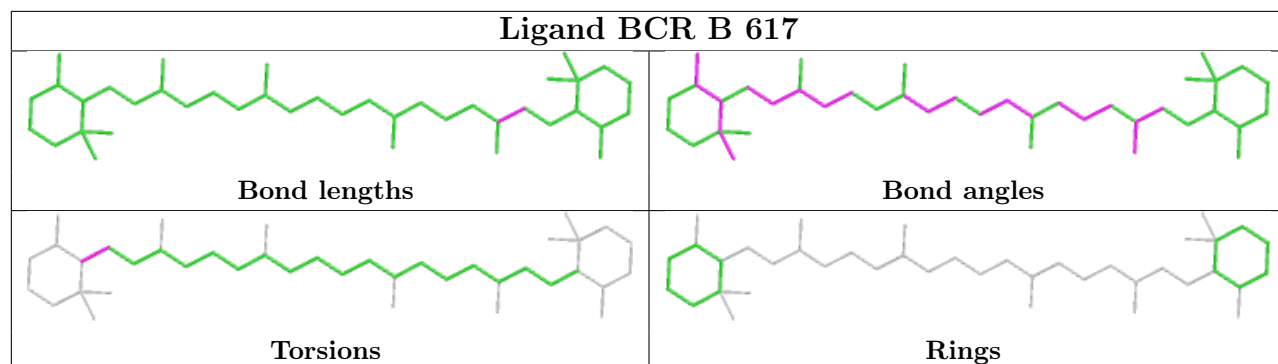
Ligand CLA B 605

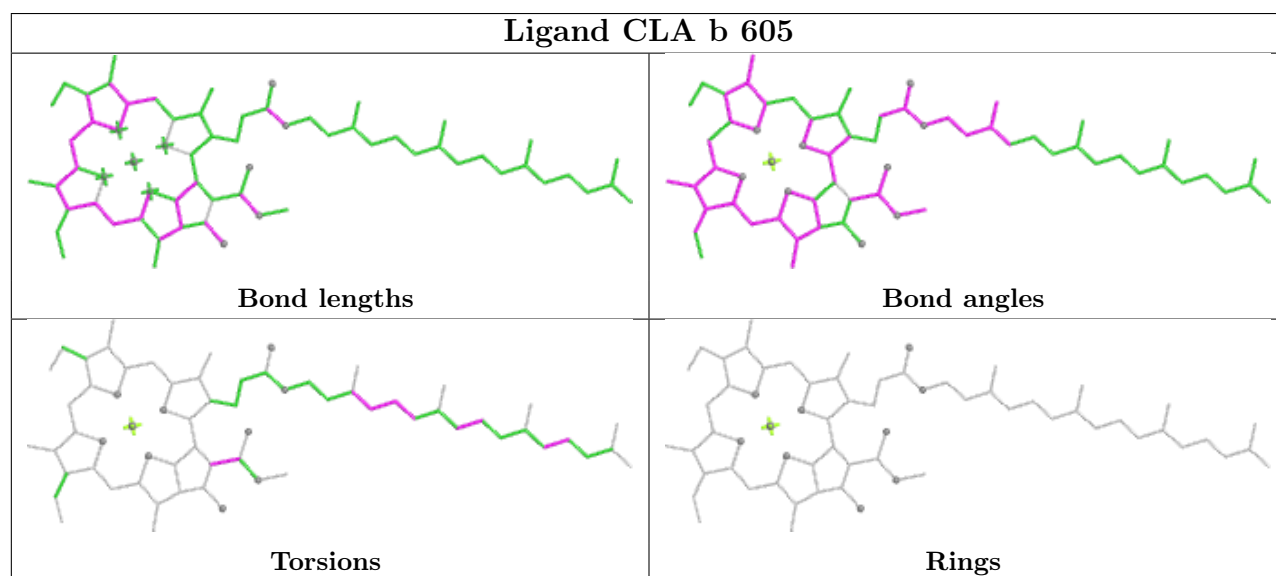
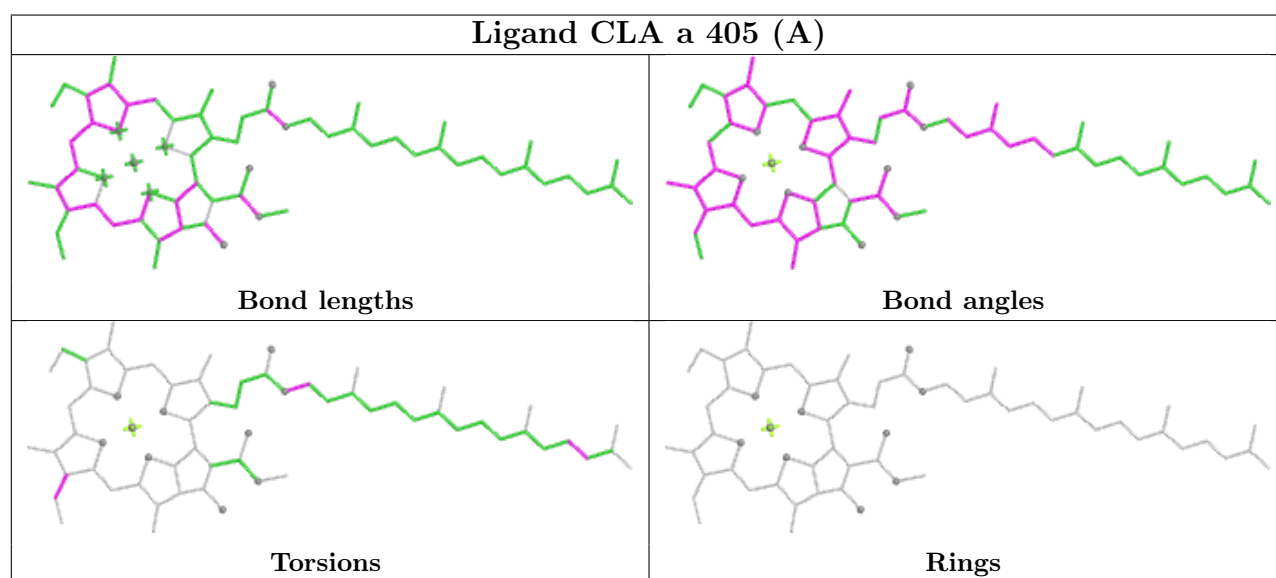
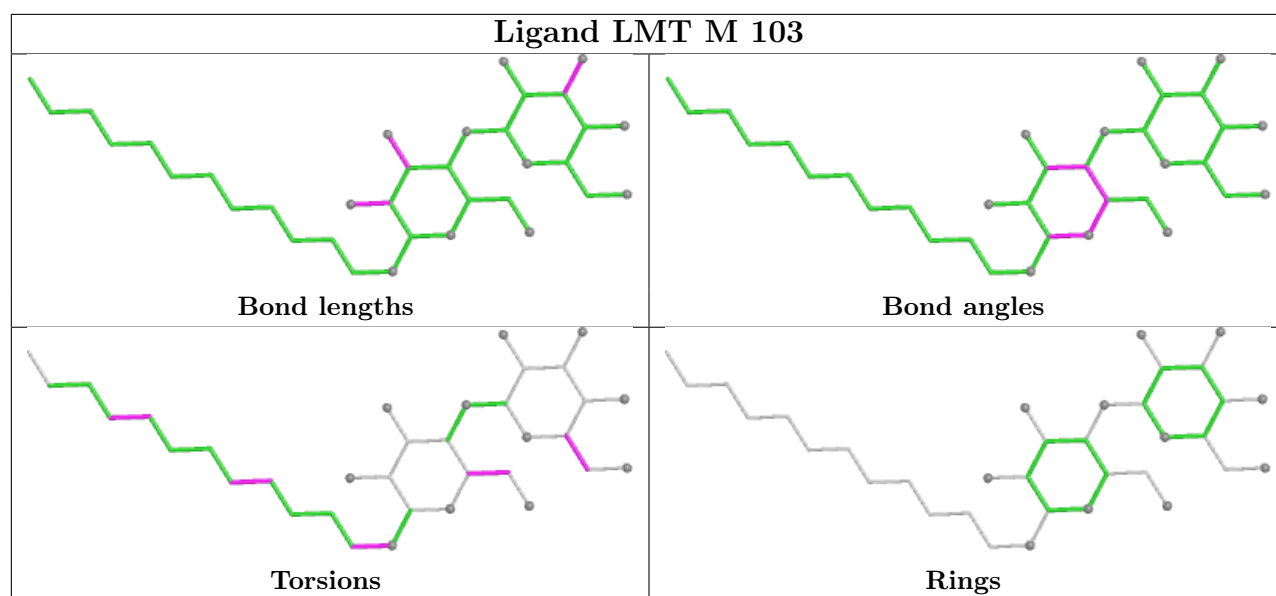


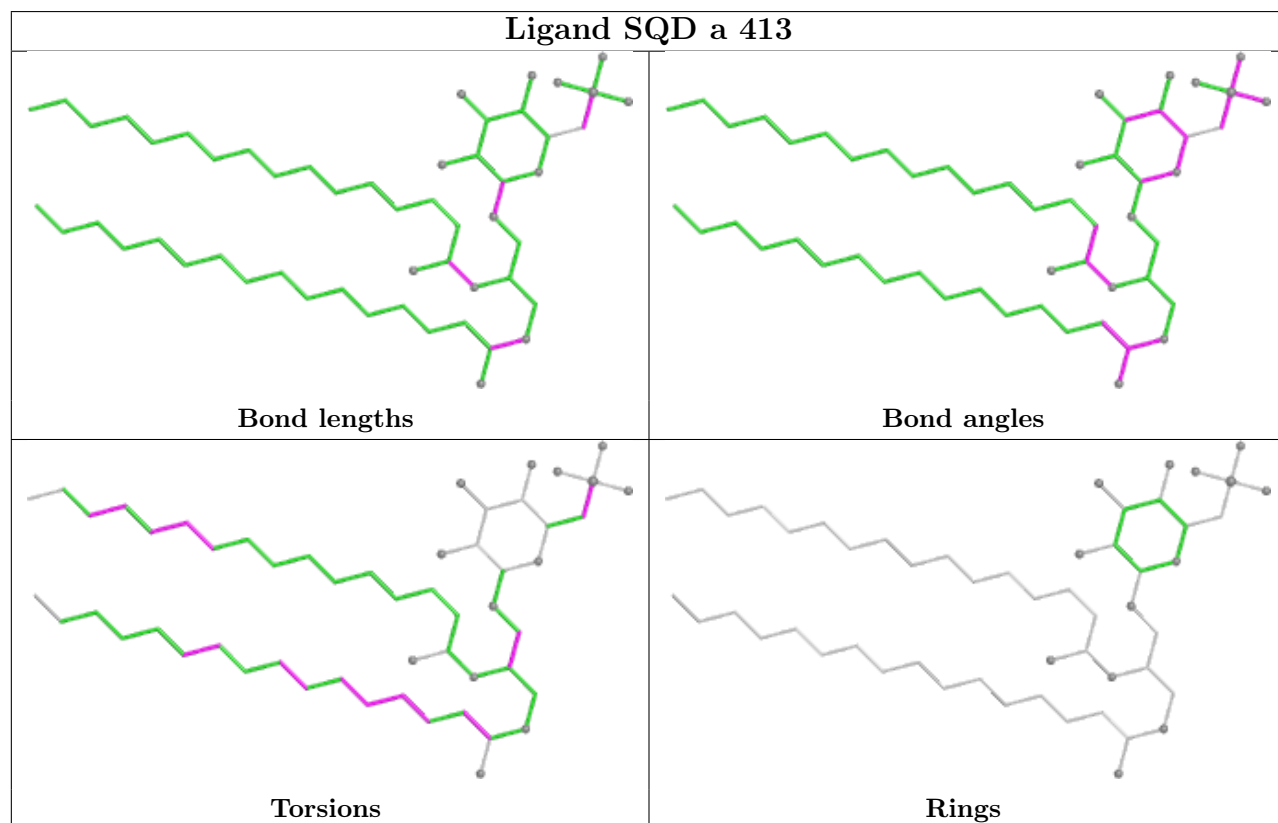
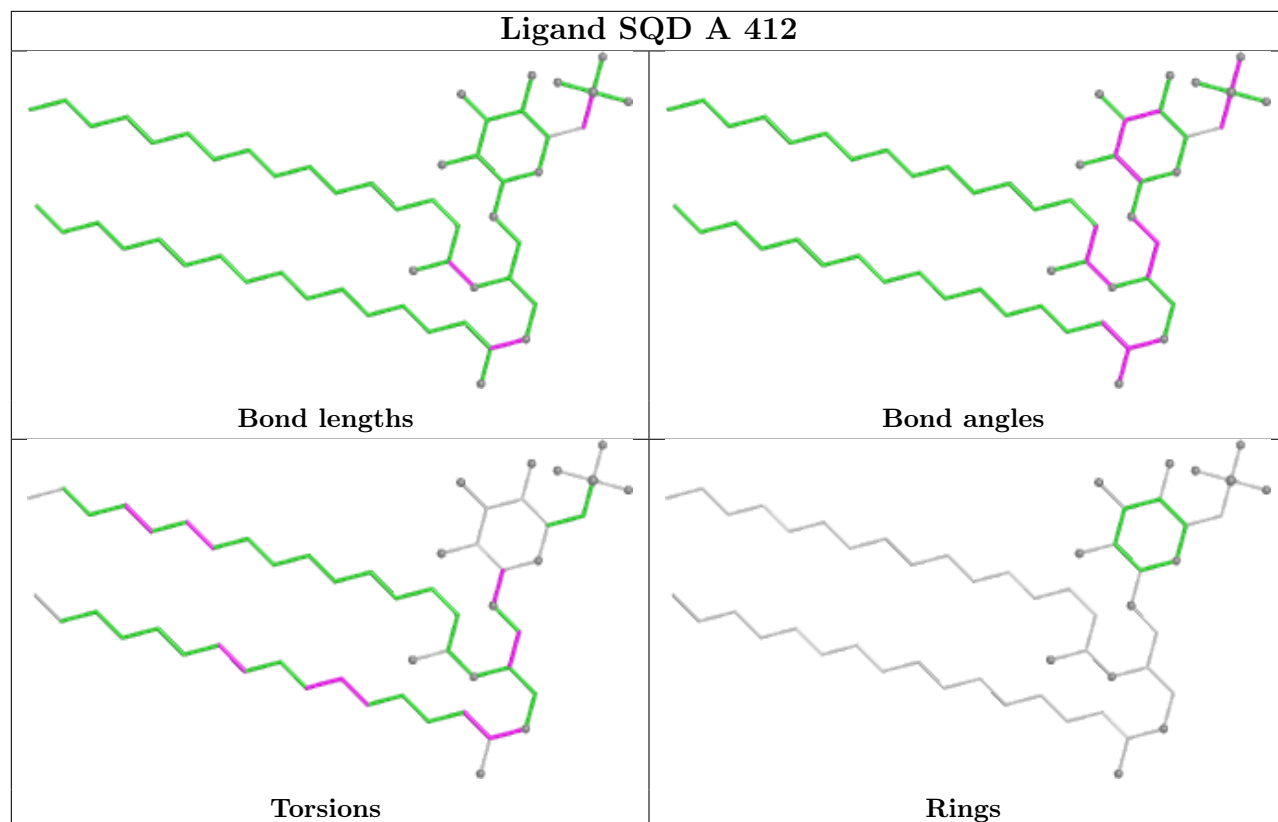
Ligand HTG V 203



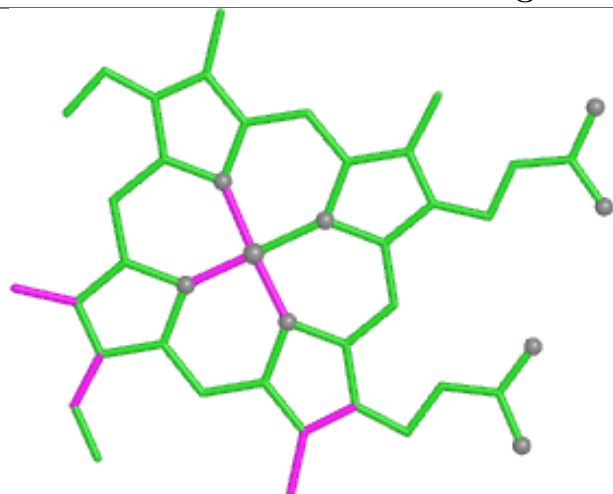




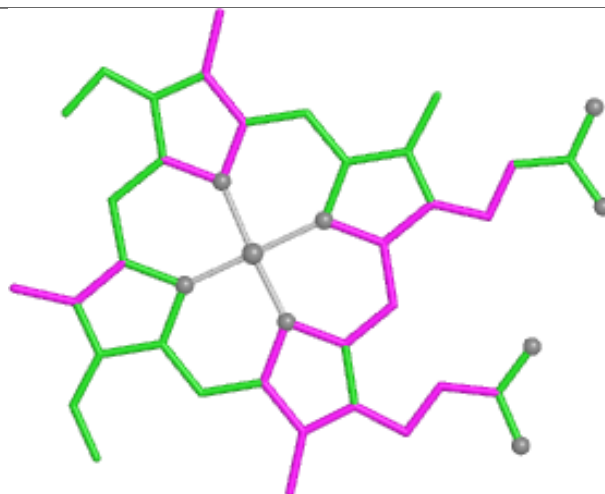




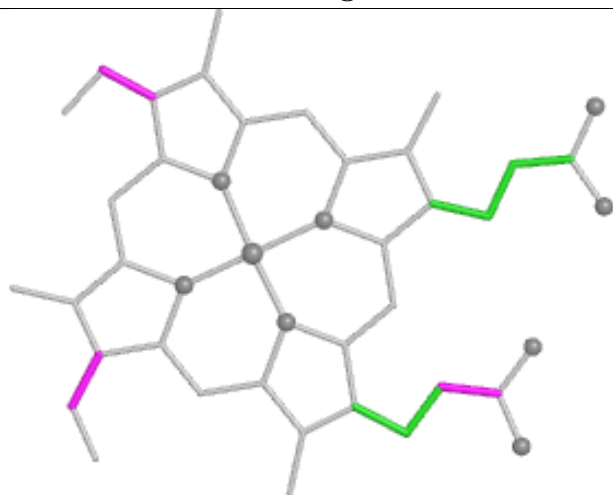
Ligand HEC v 202



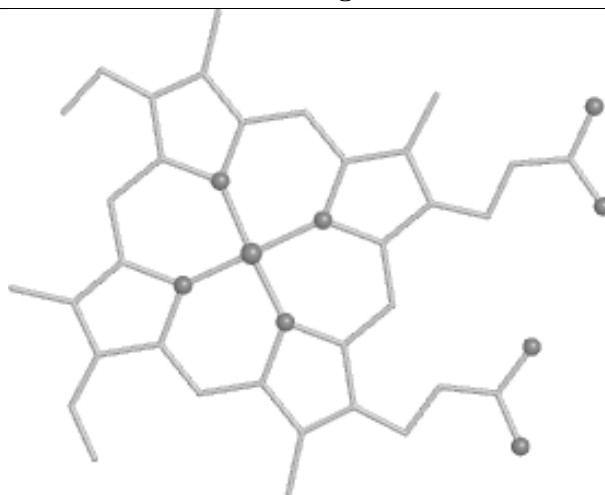
Bond lengths



Bond angles

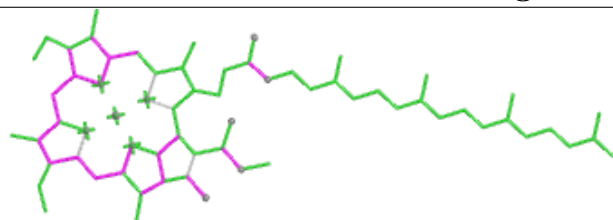


Torsions

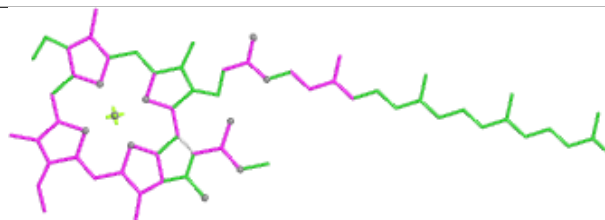


Rings

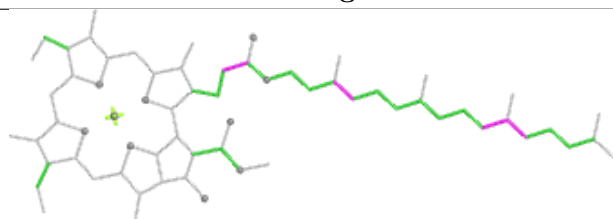
Ligand CLA C 506



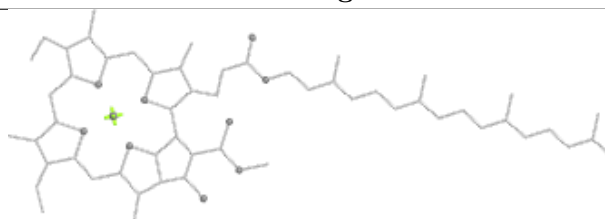
Bond lengths



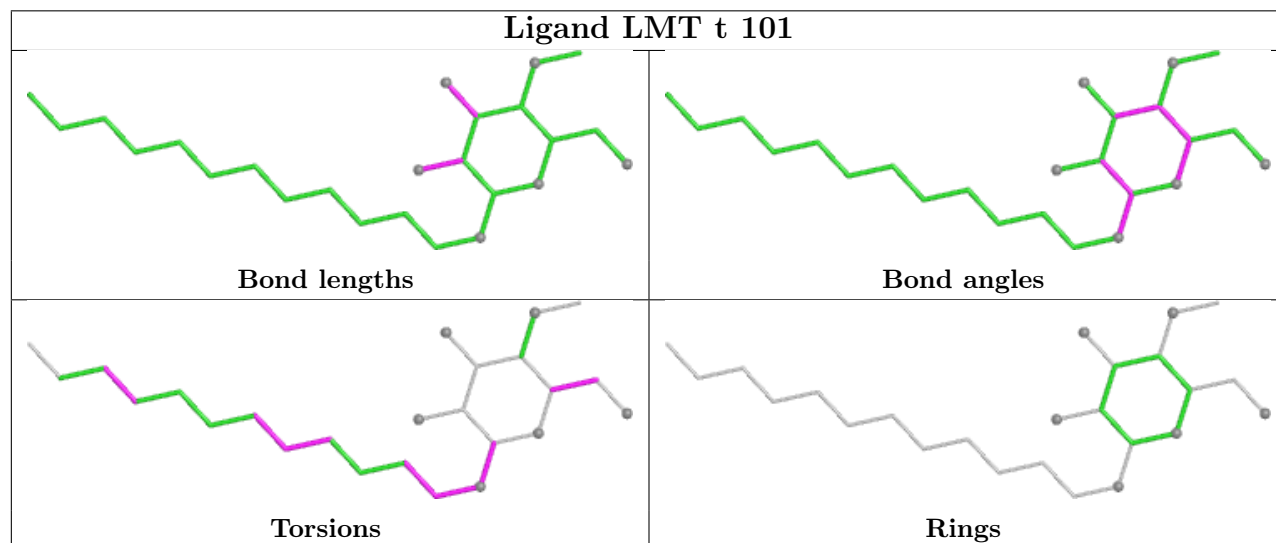
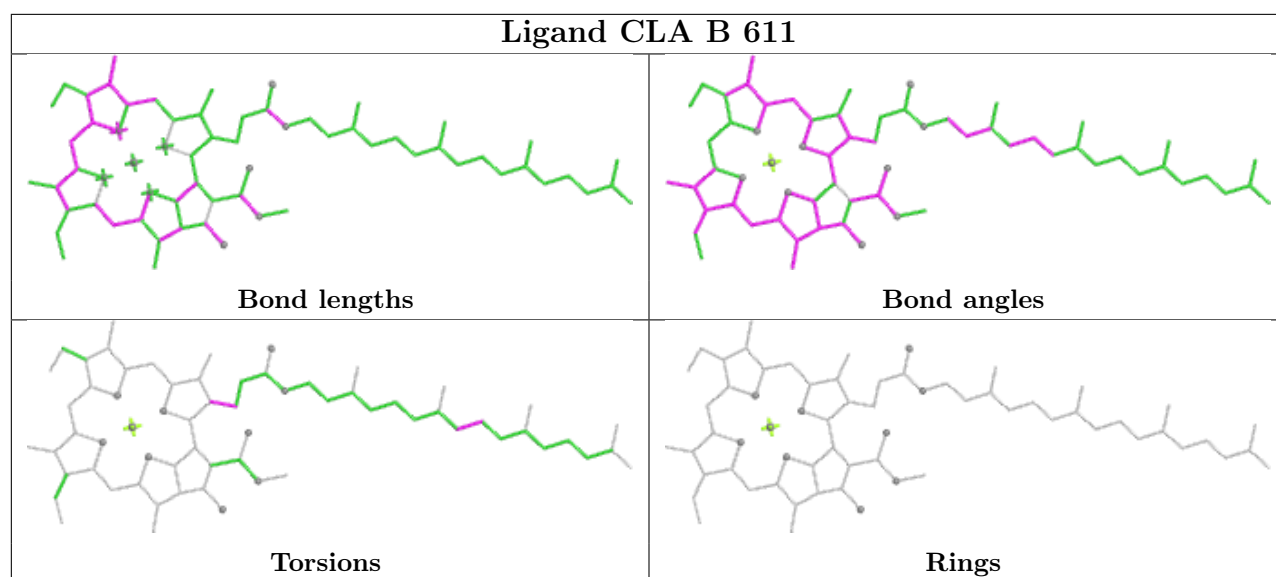
Bond angles

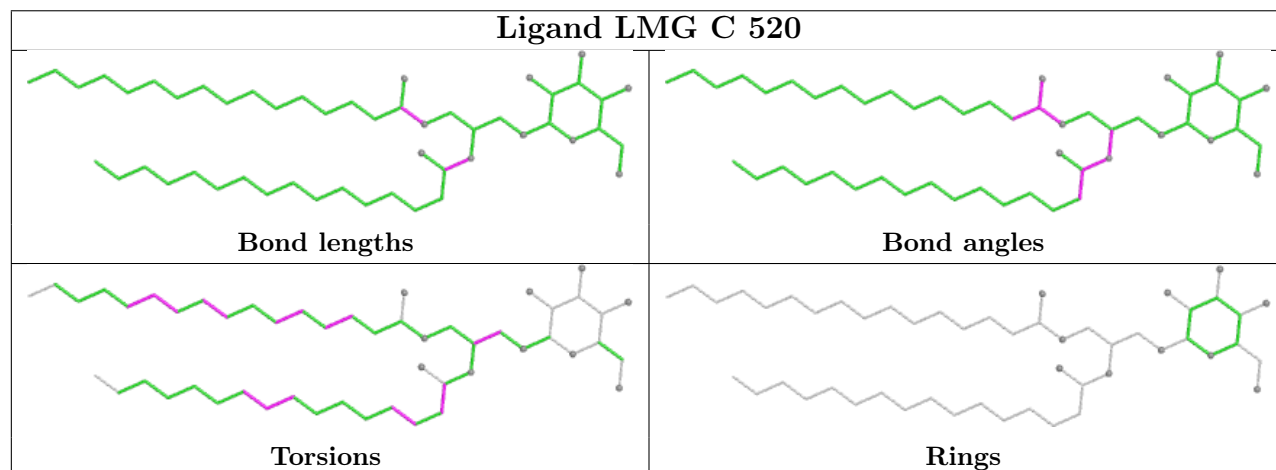
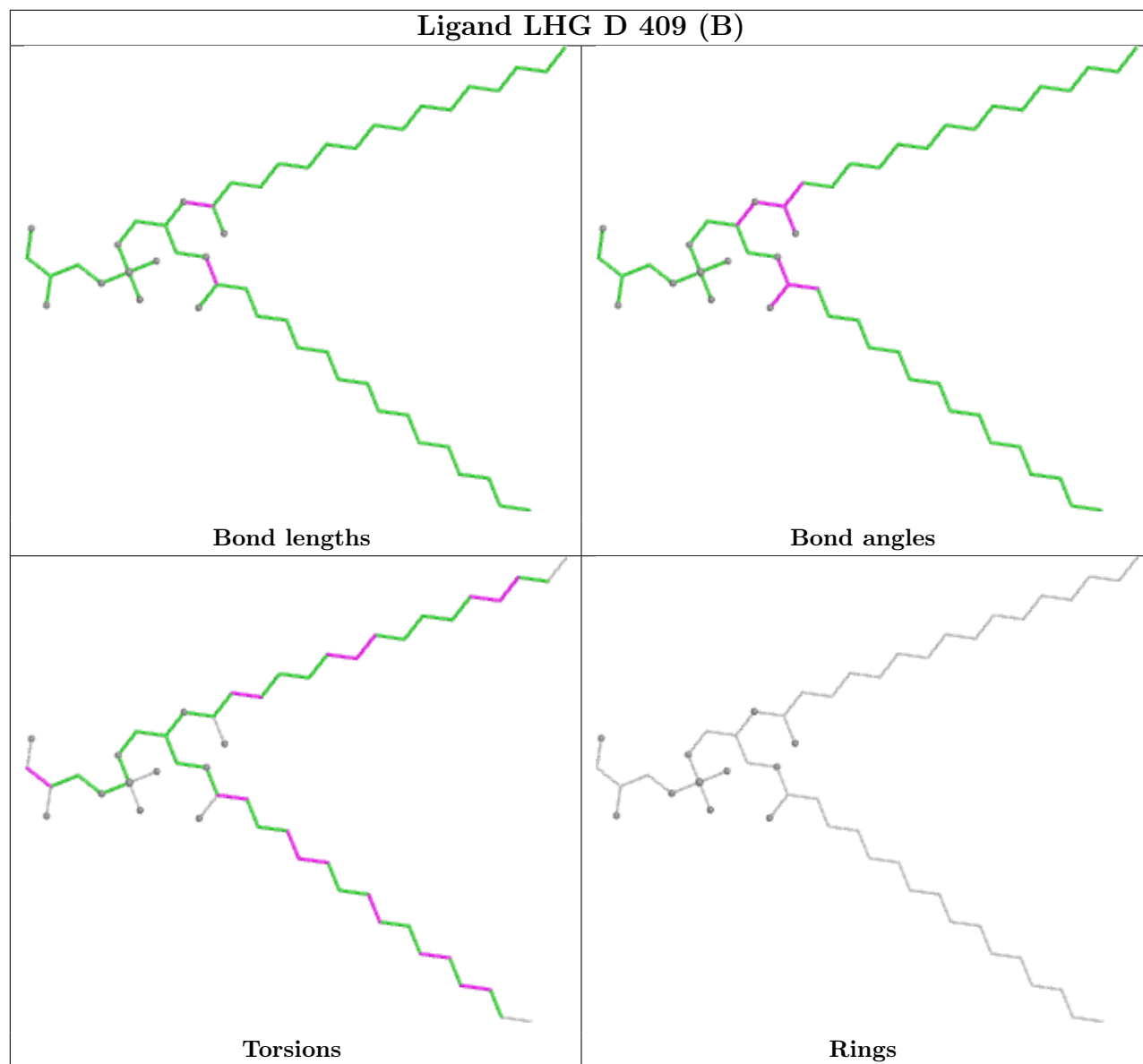


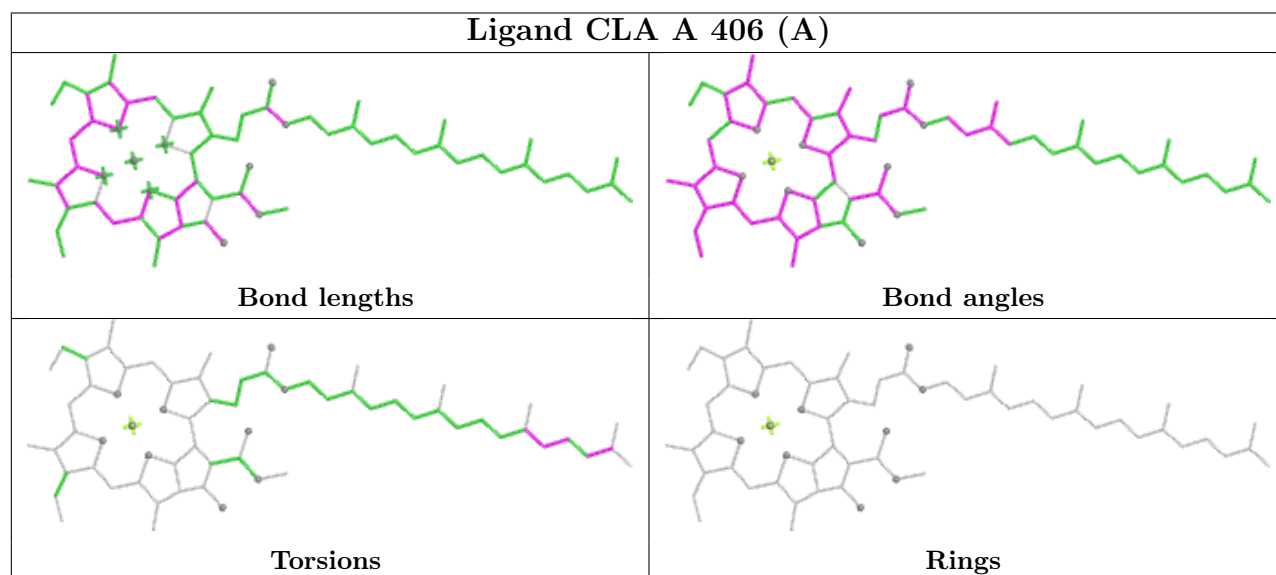
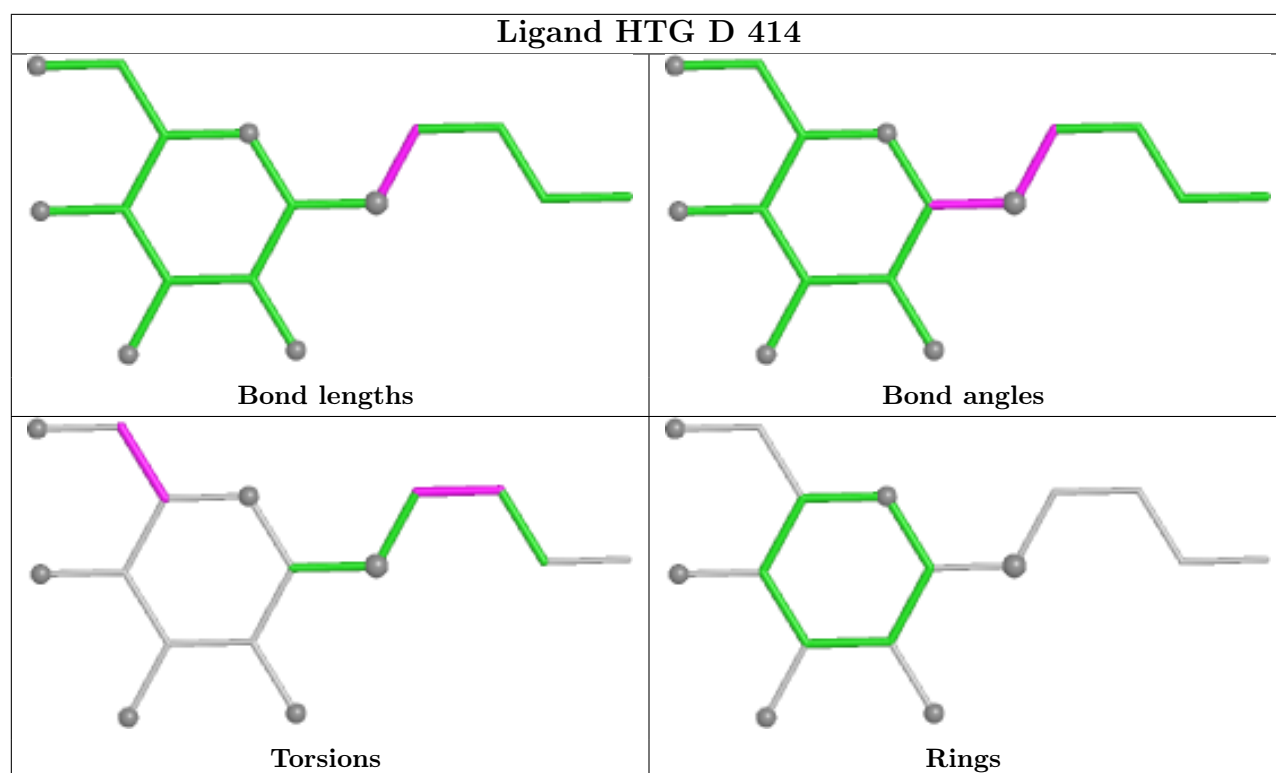
Torsions



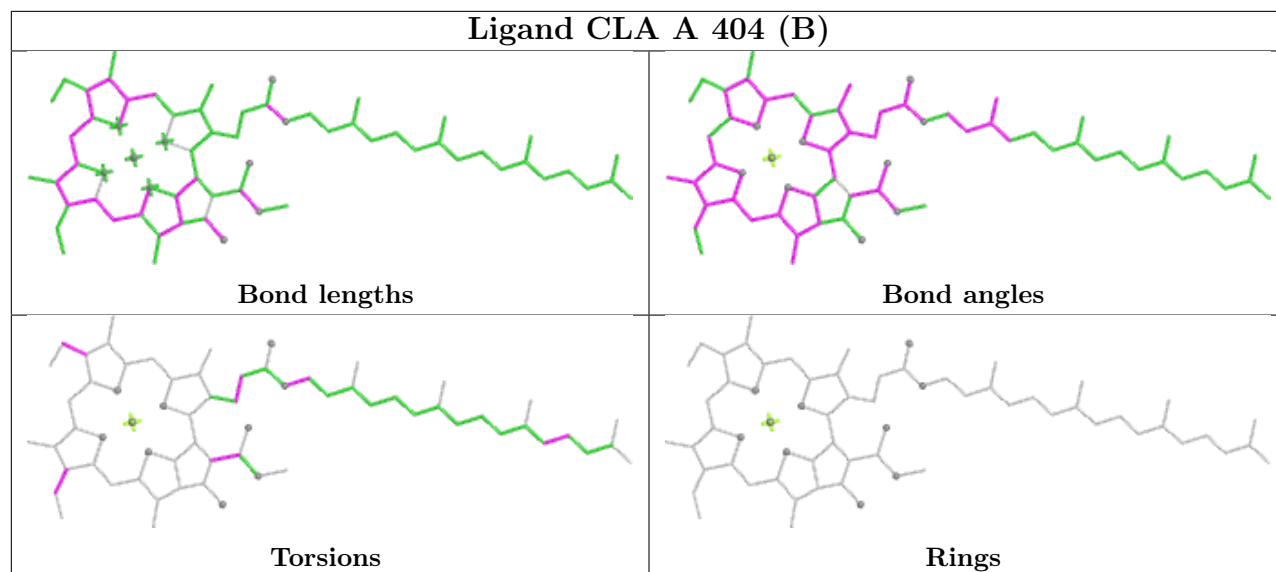
Rings



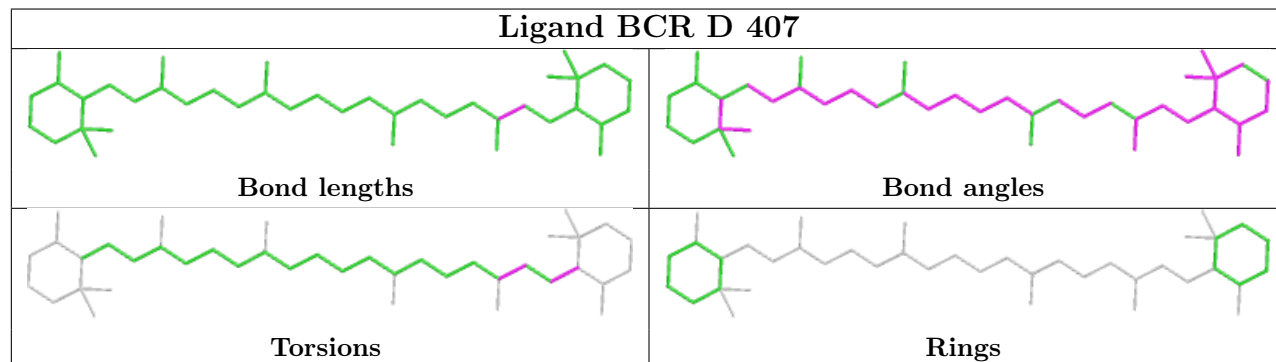




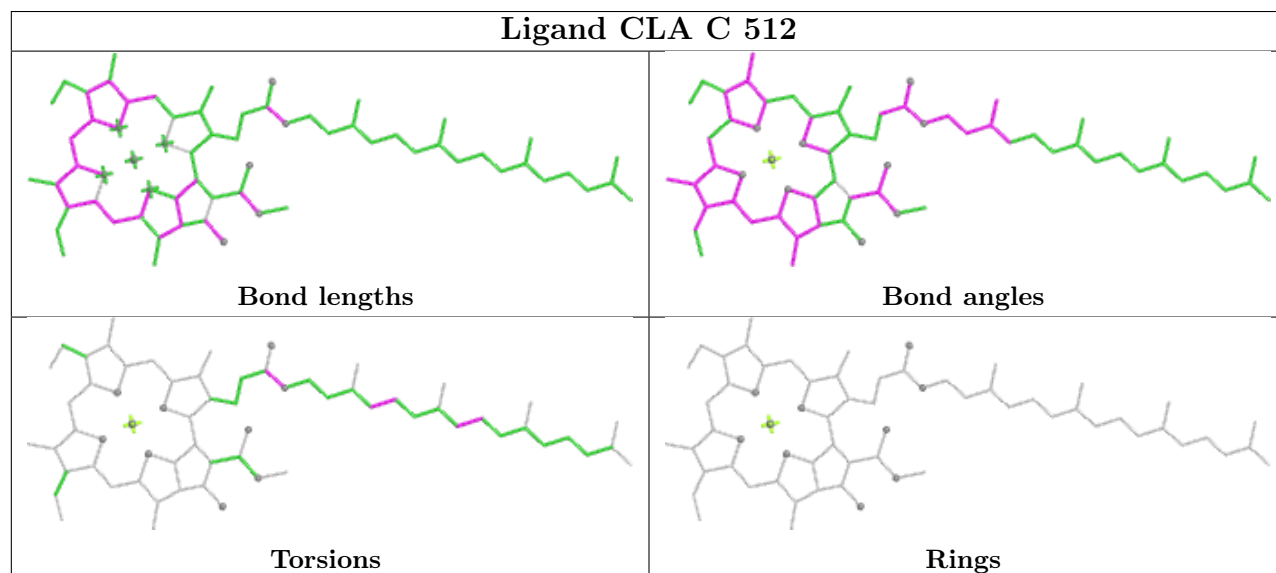
Ligand CLA A 404 (B)



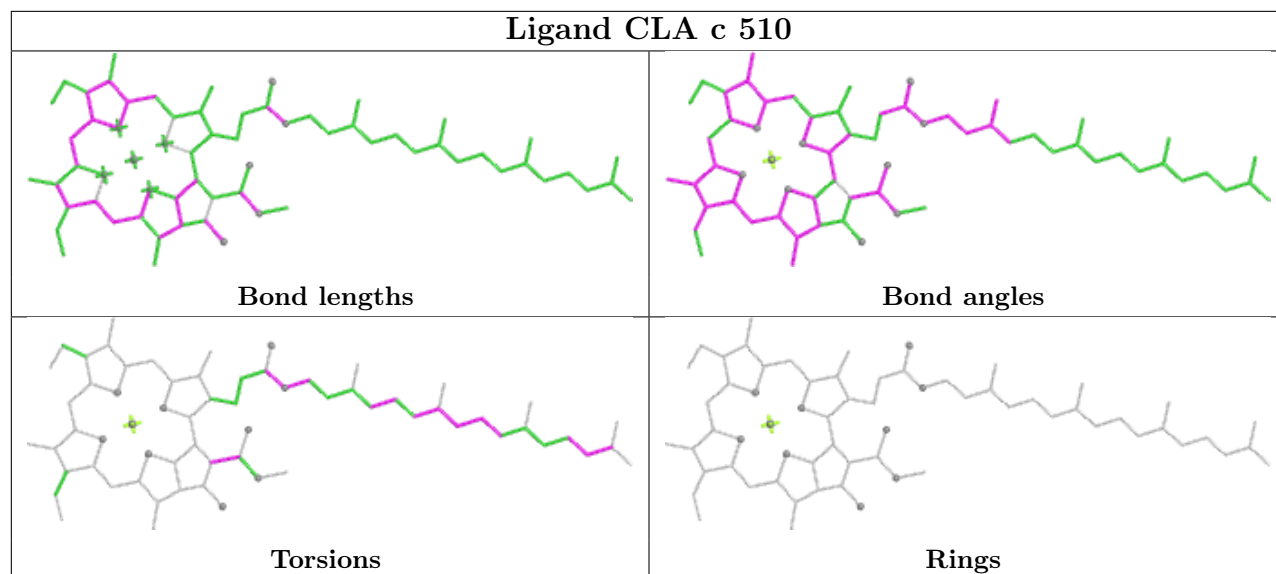
Ligand BCR D 407



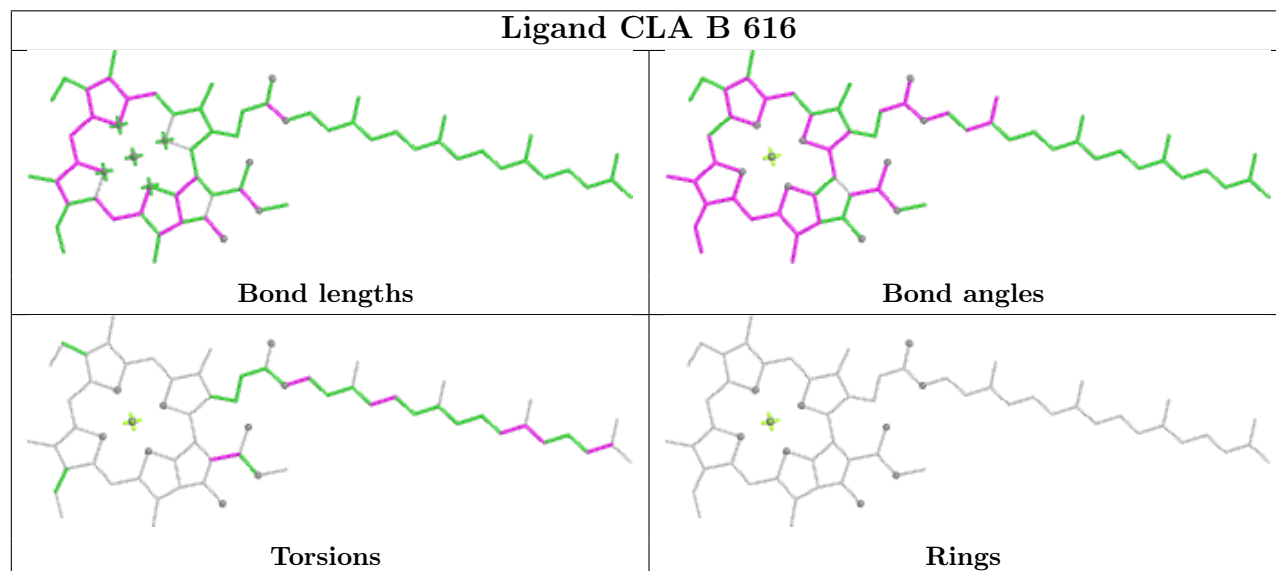
Ligand CLA C 512



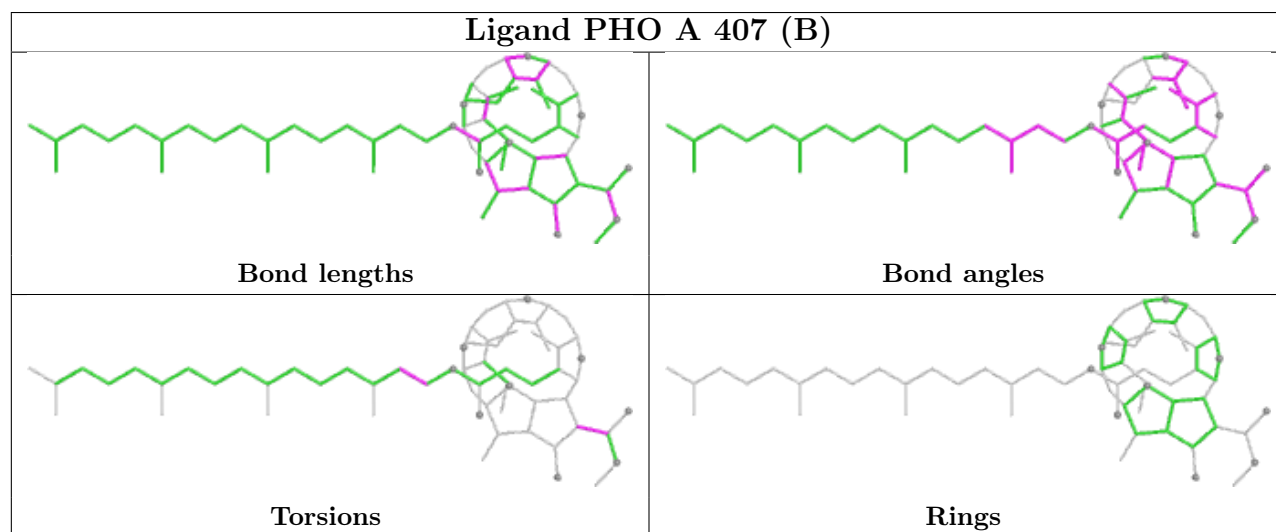
Ligand CLA c 510

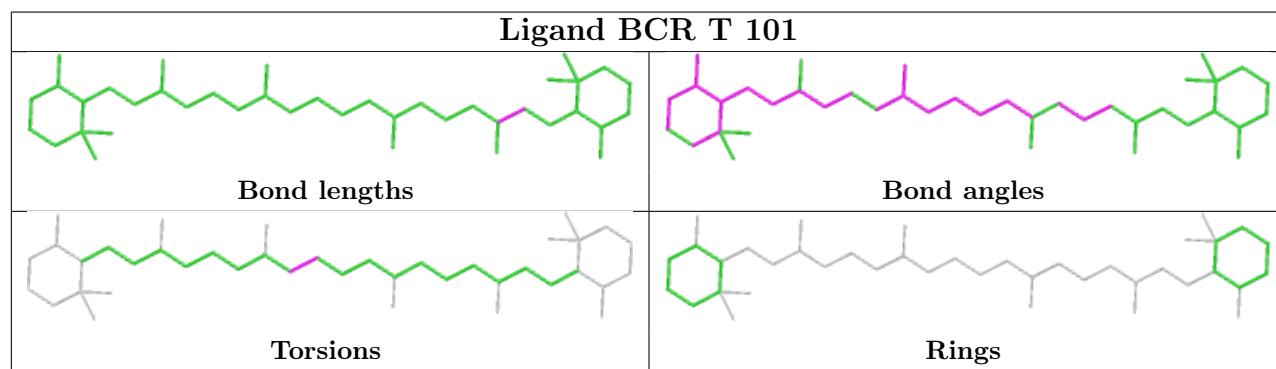
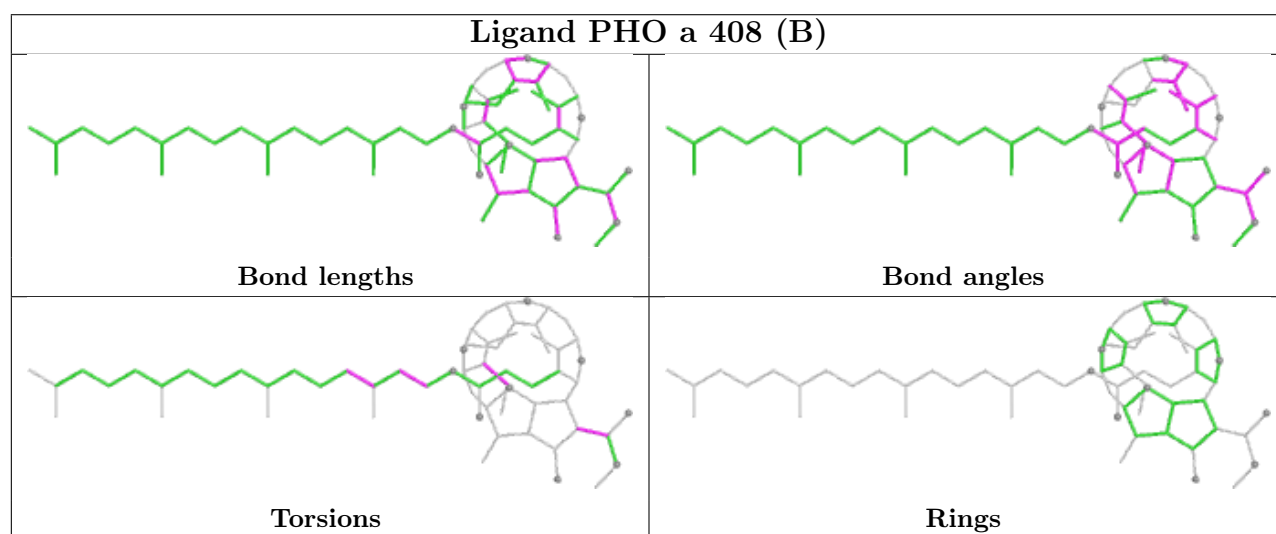
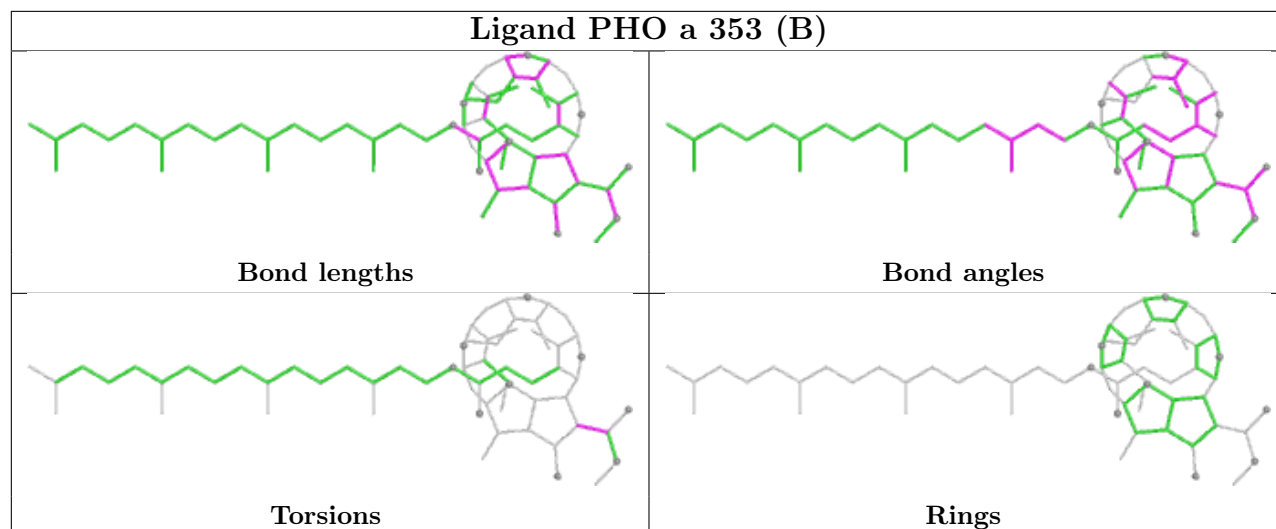


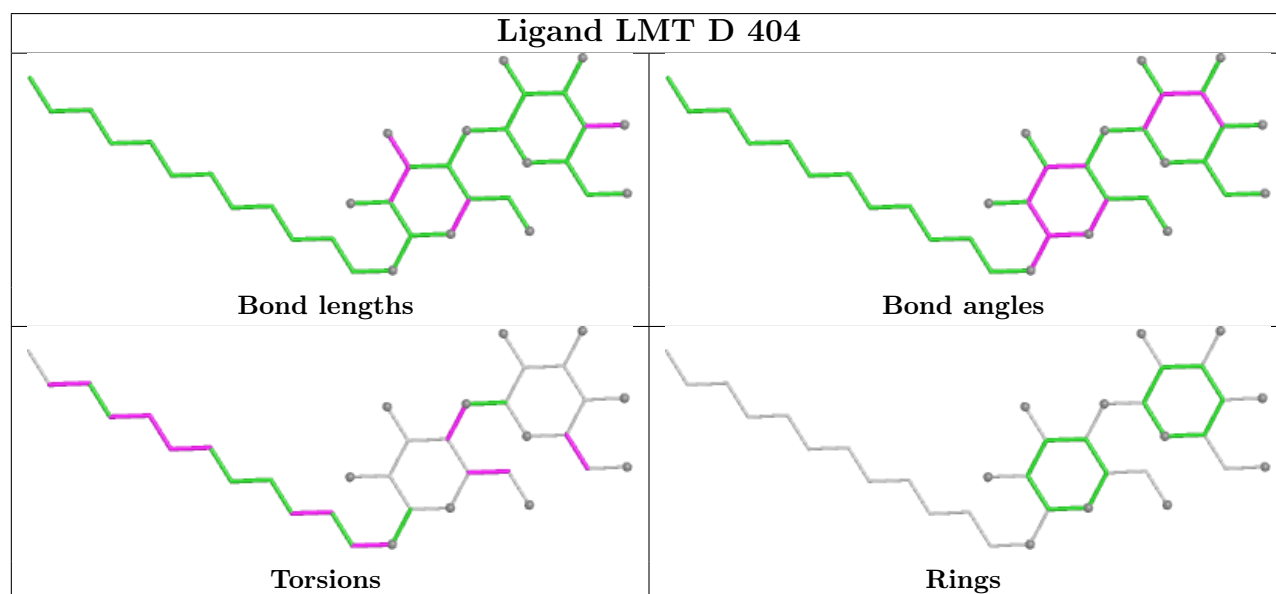
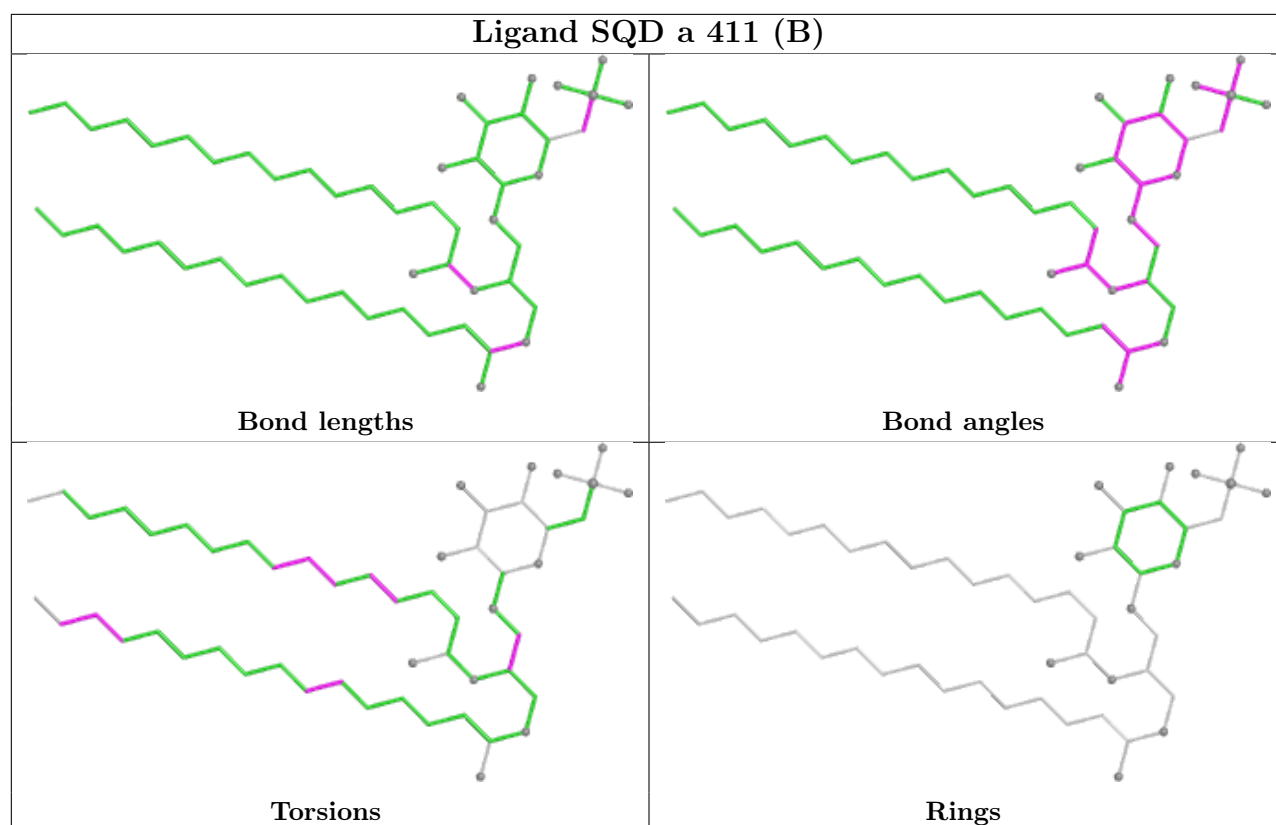
Ligand CLA B 616



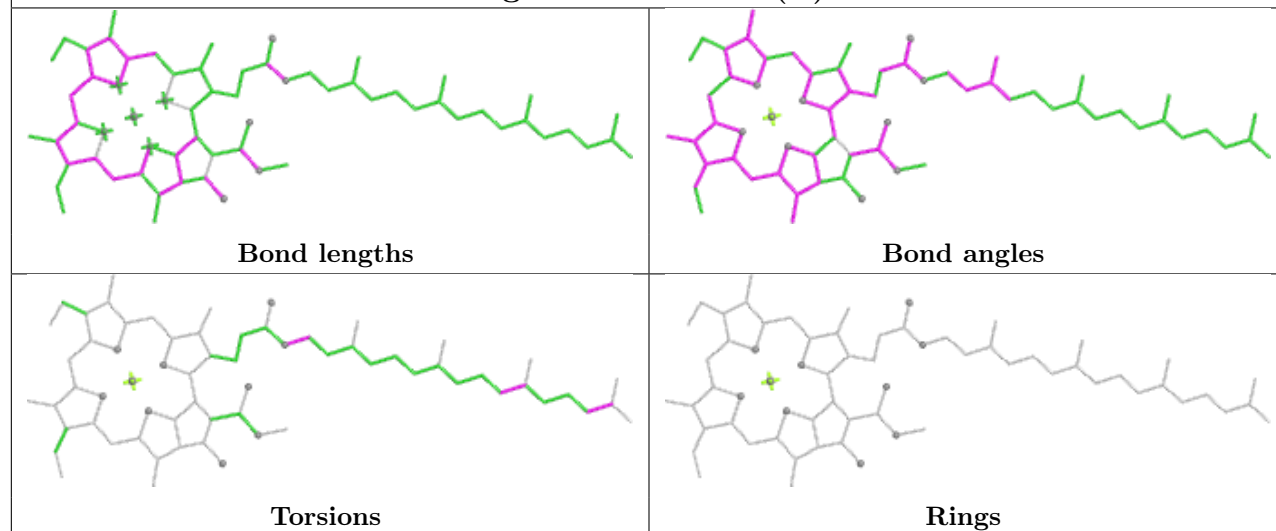
Ligand PHO A 407 (B)



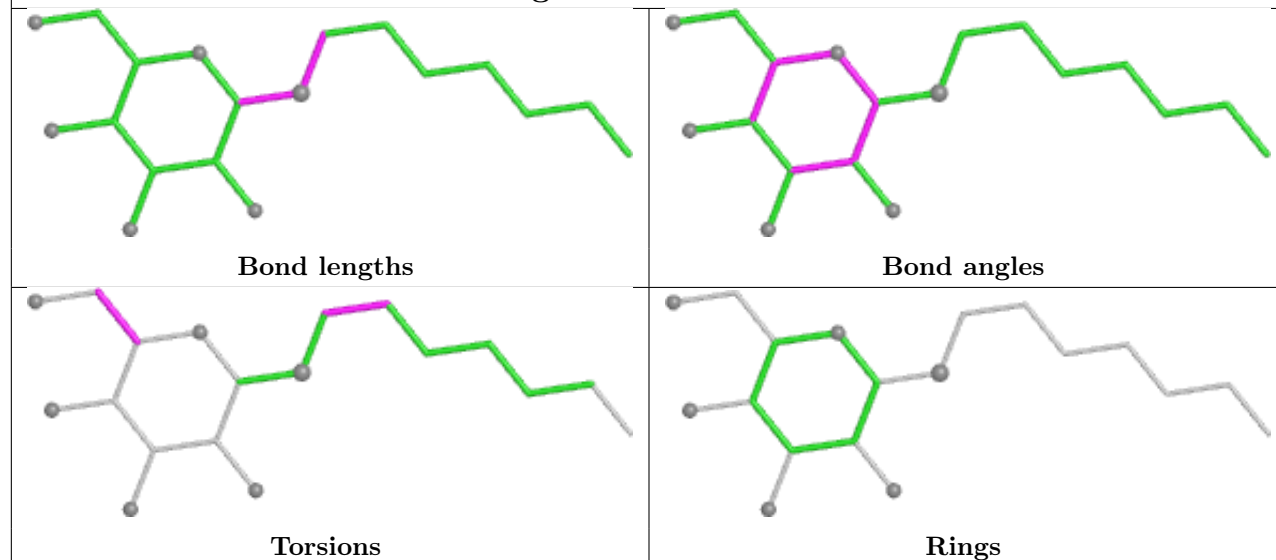




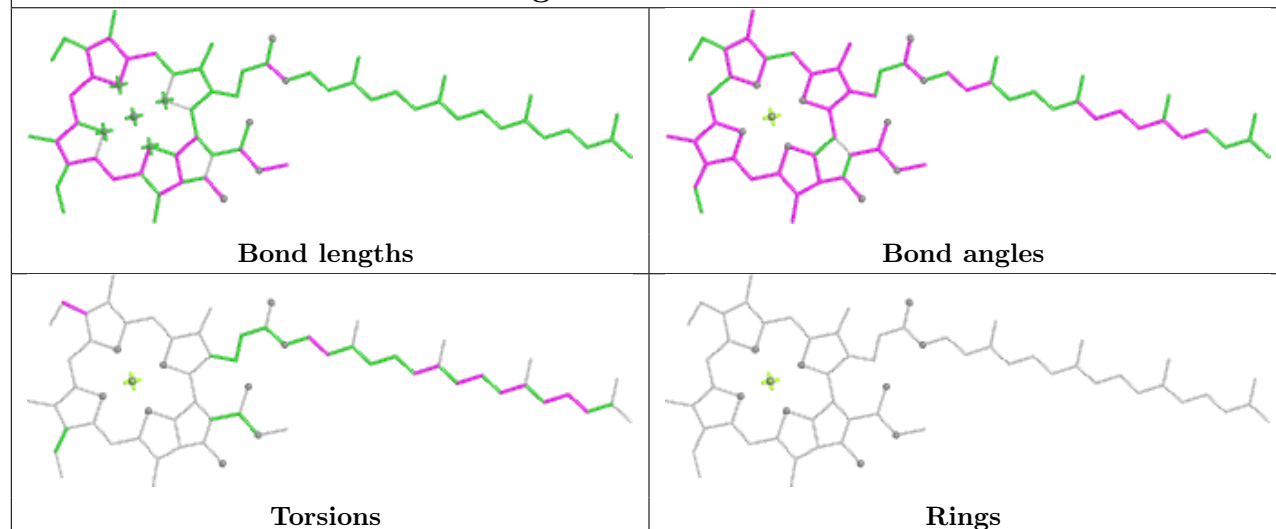
Ligand CLA d 402 (B)



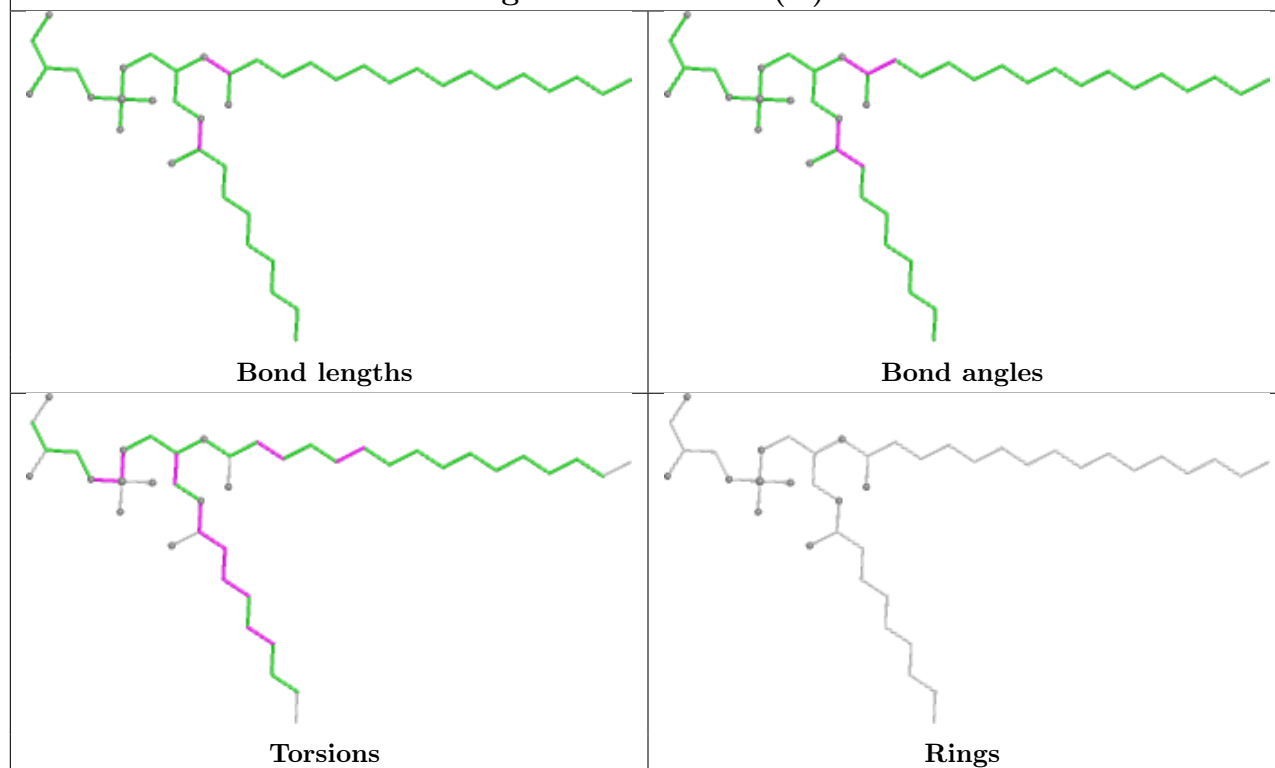
Ligand HTG b 625



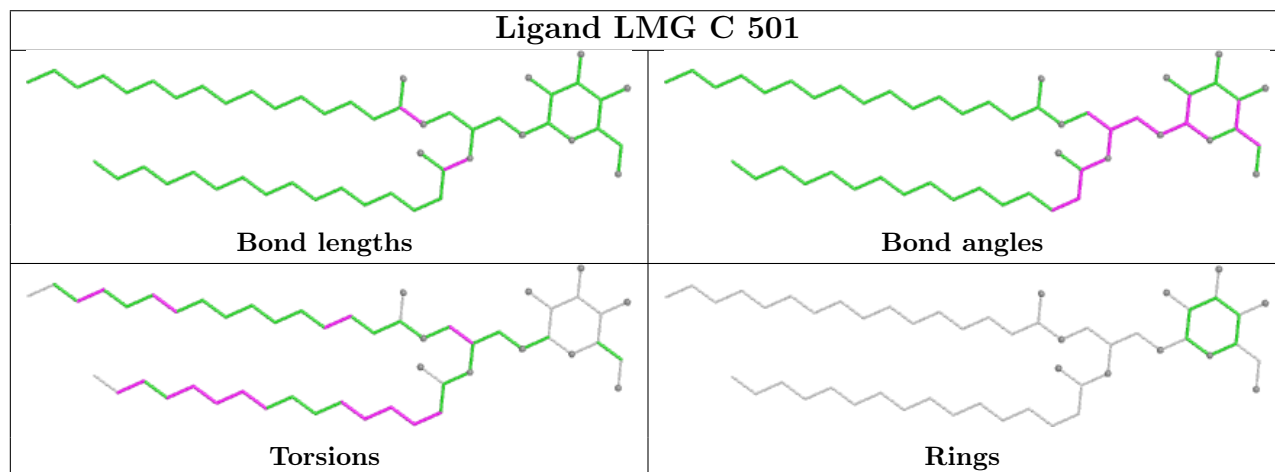
Ligand CLA B 602

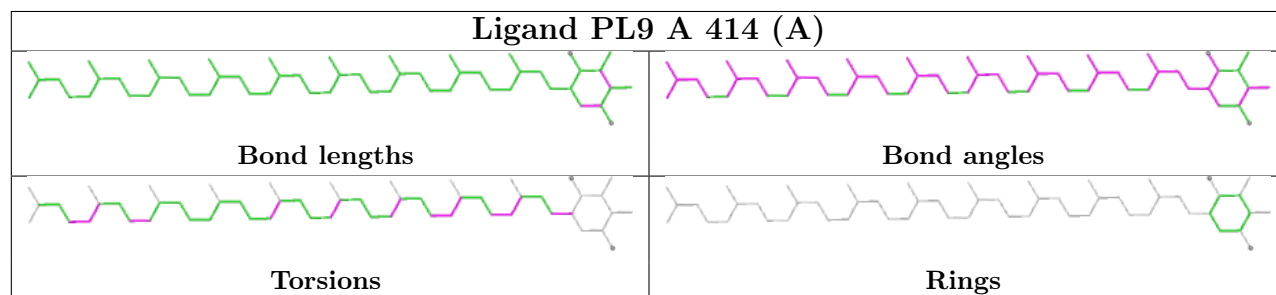
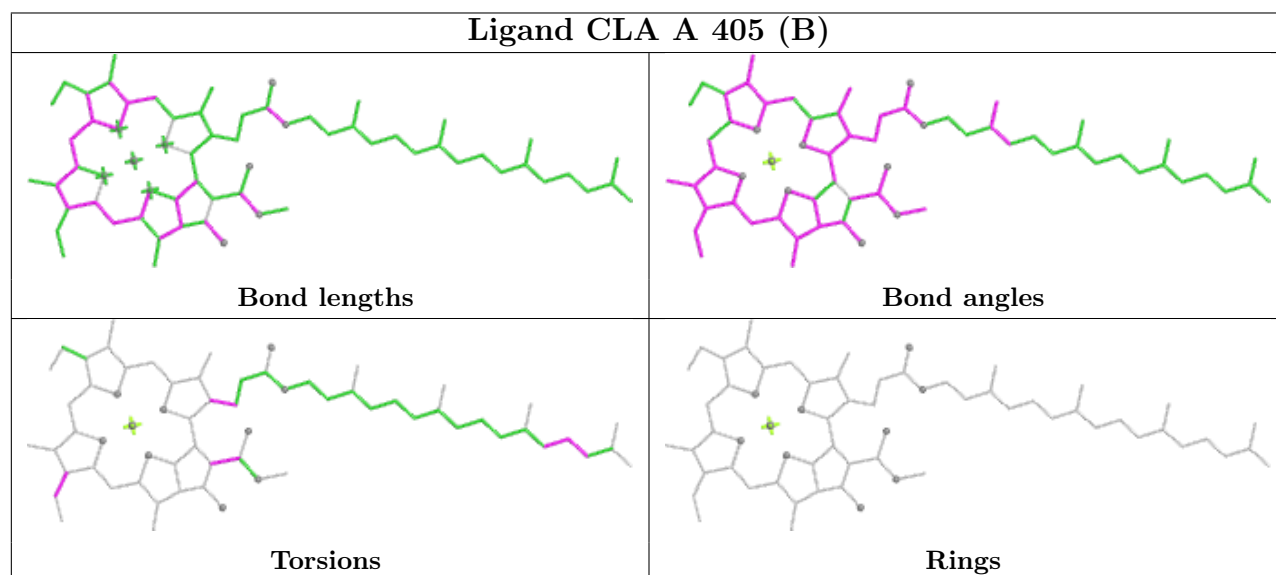
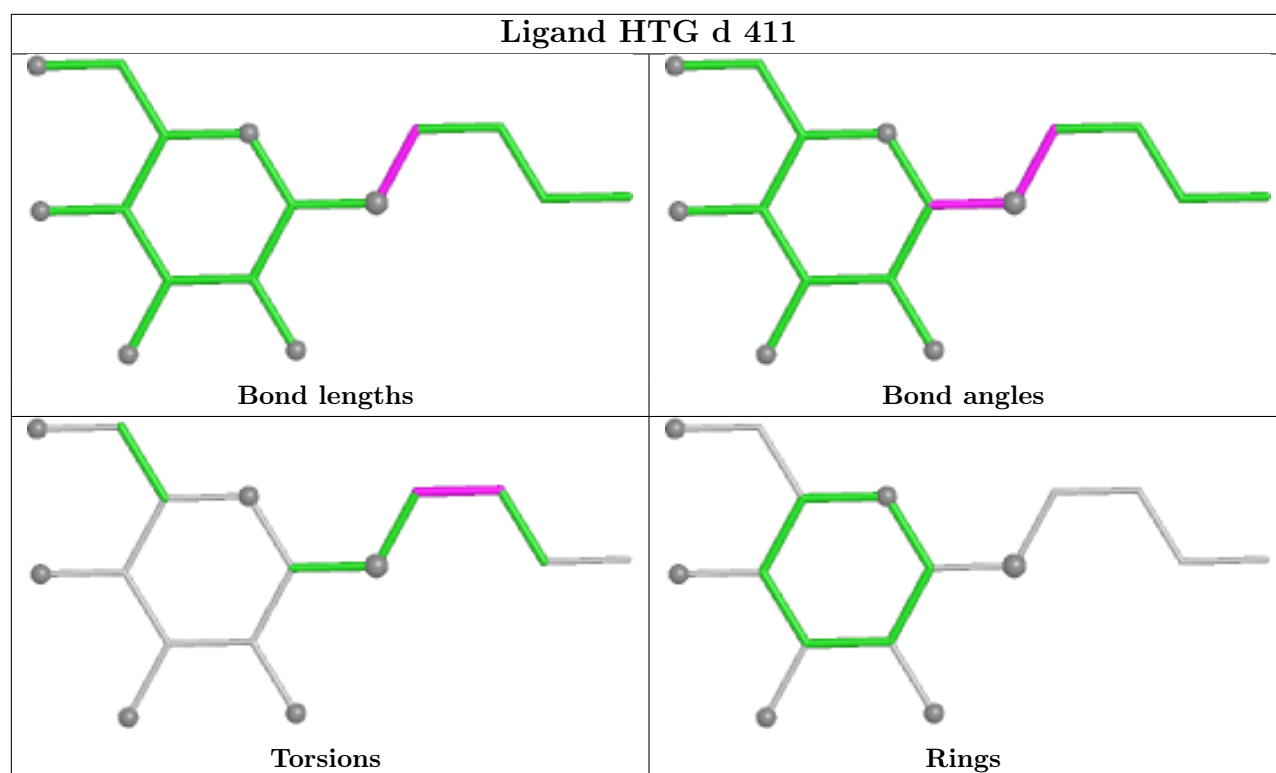


Ligand LHG e 101 (B)

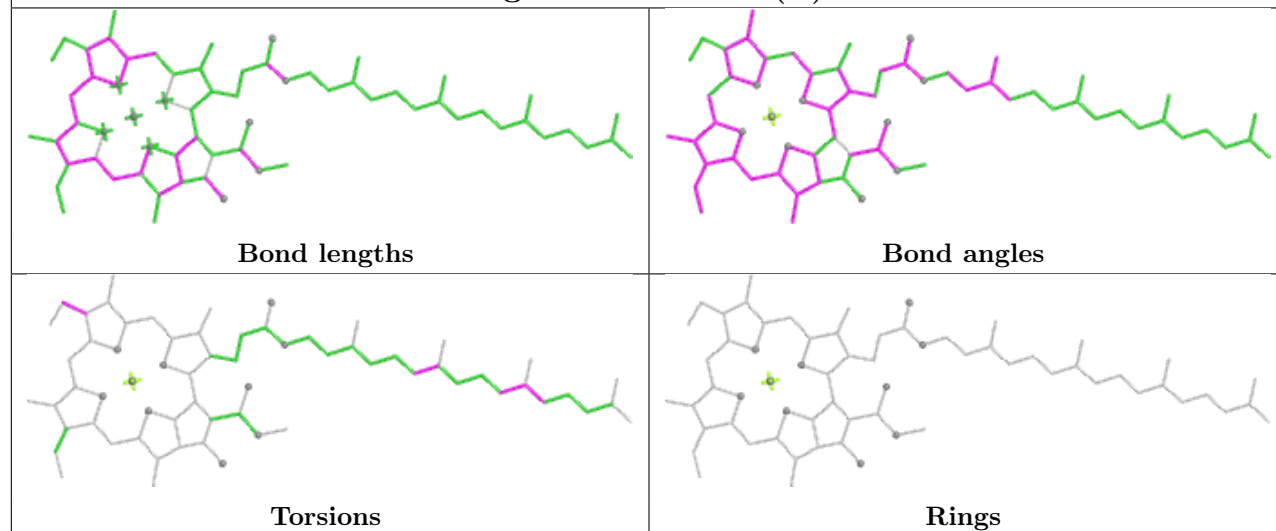


Ligand LMG C 501

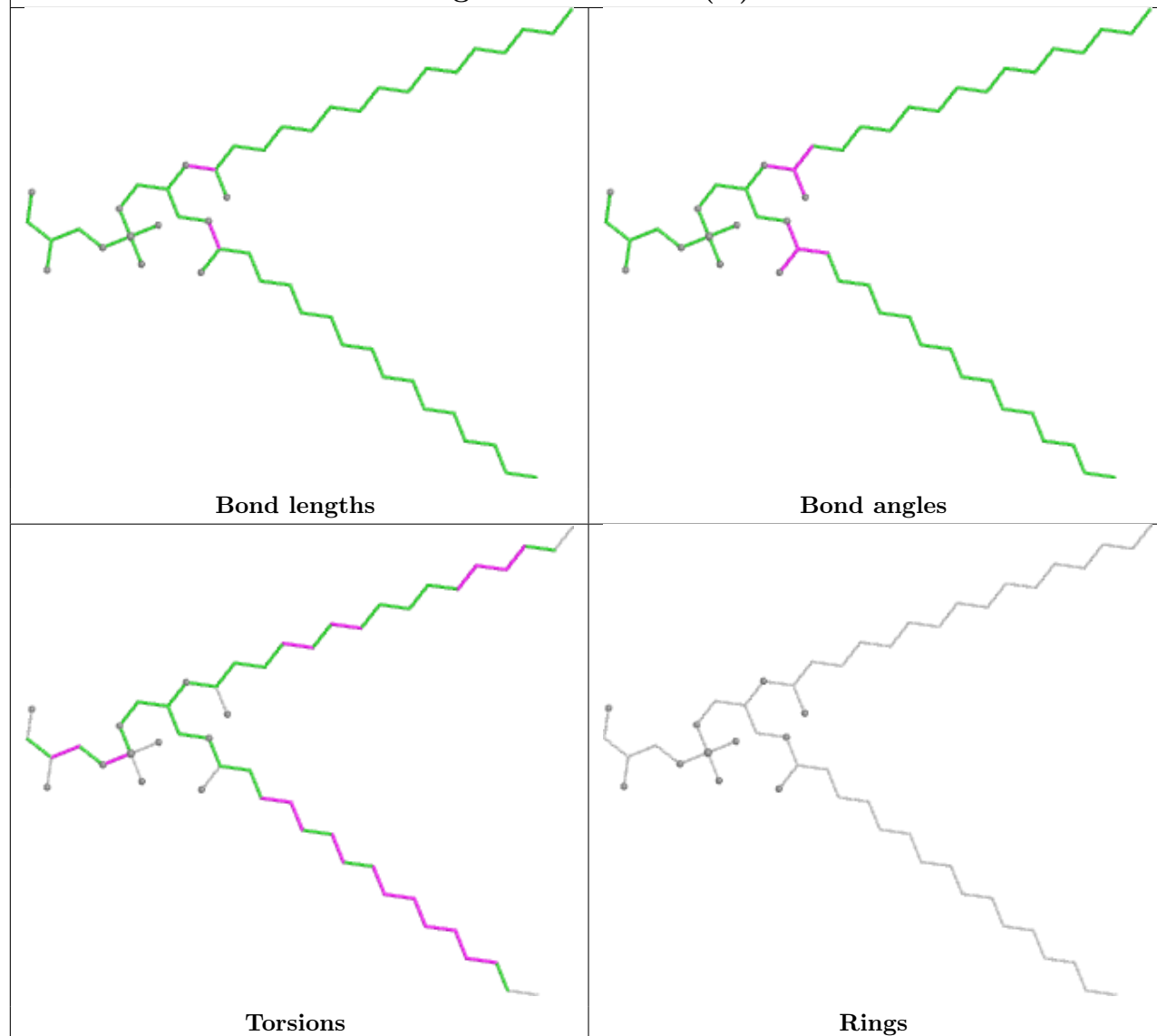


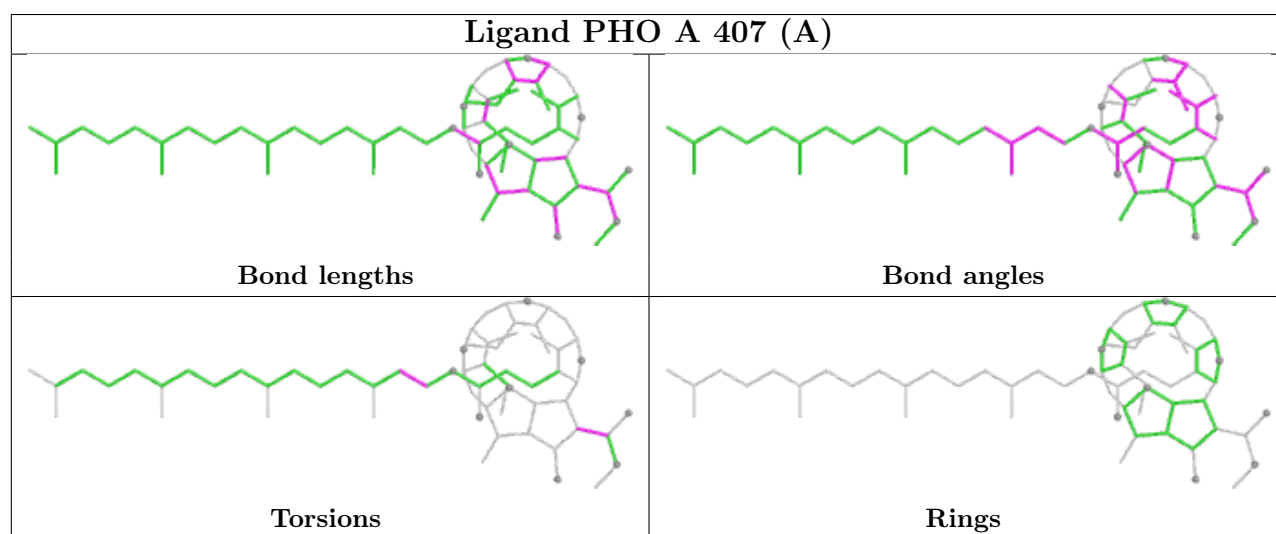
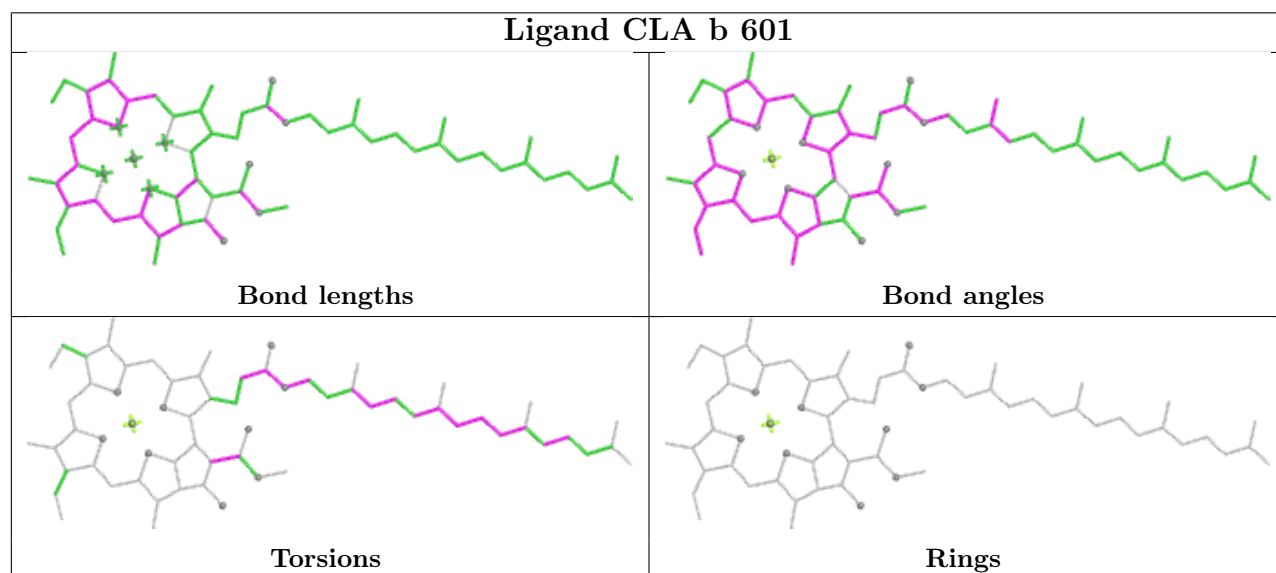
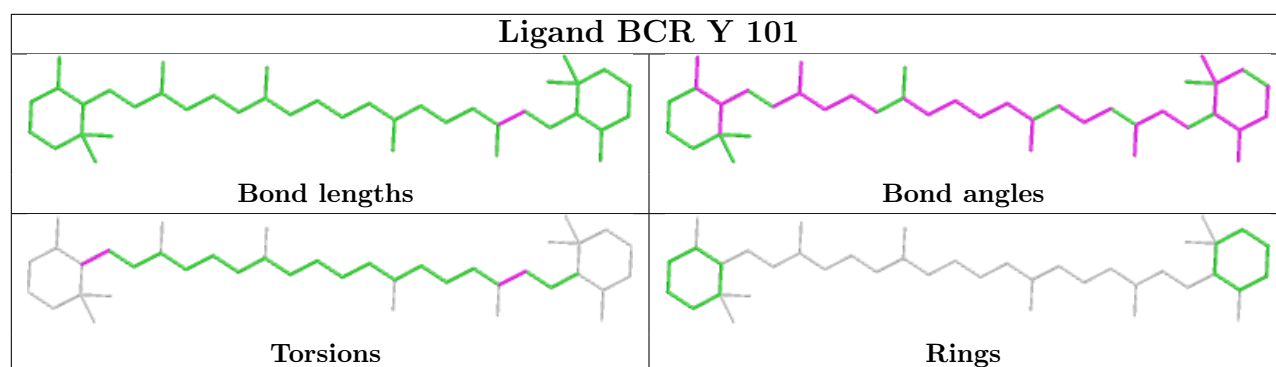


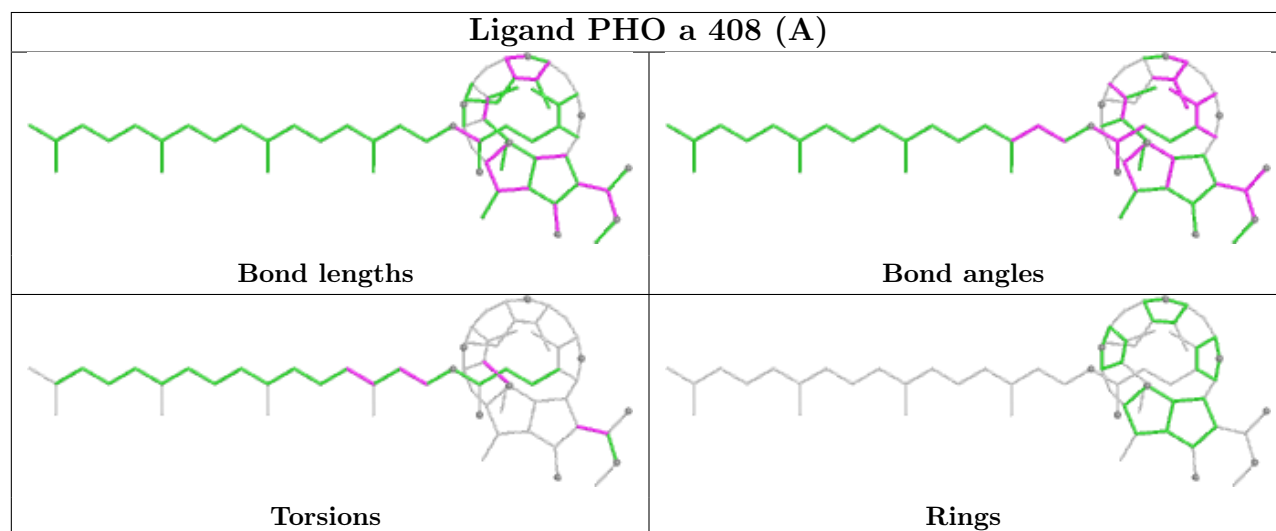
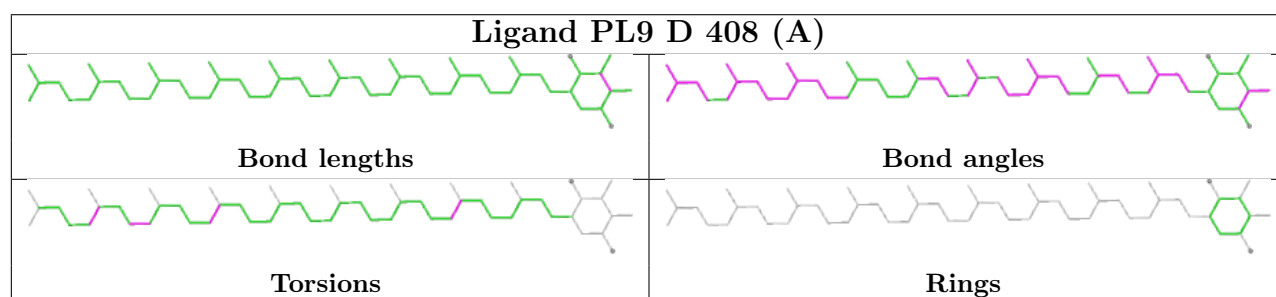
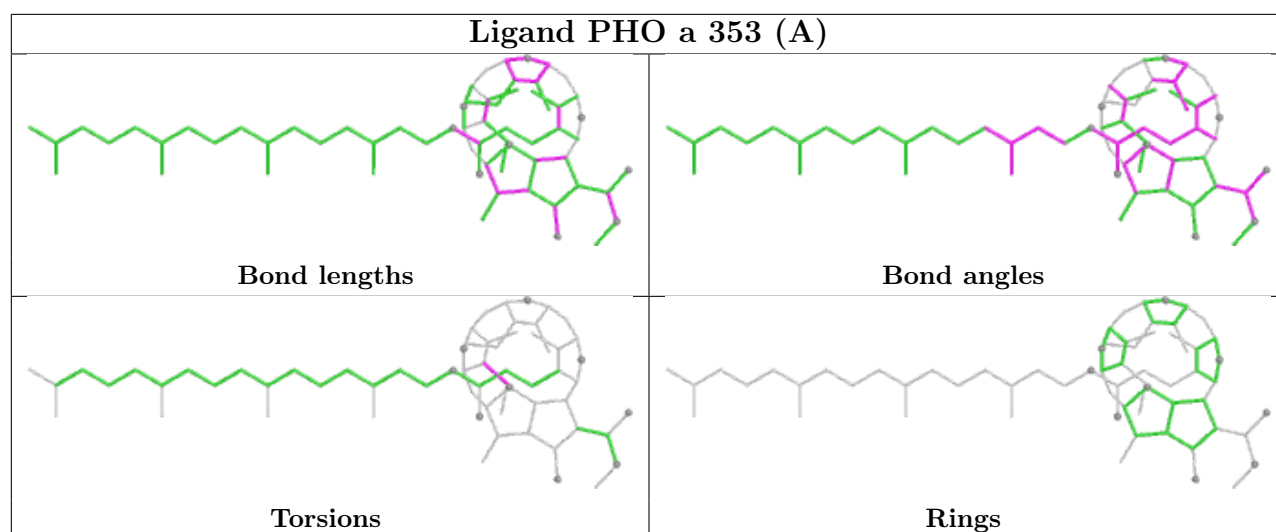
Ligand CLA a 407 (B)

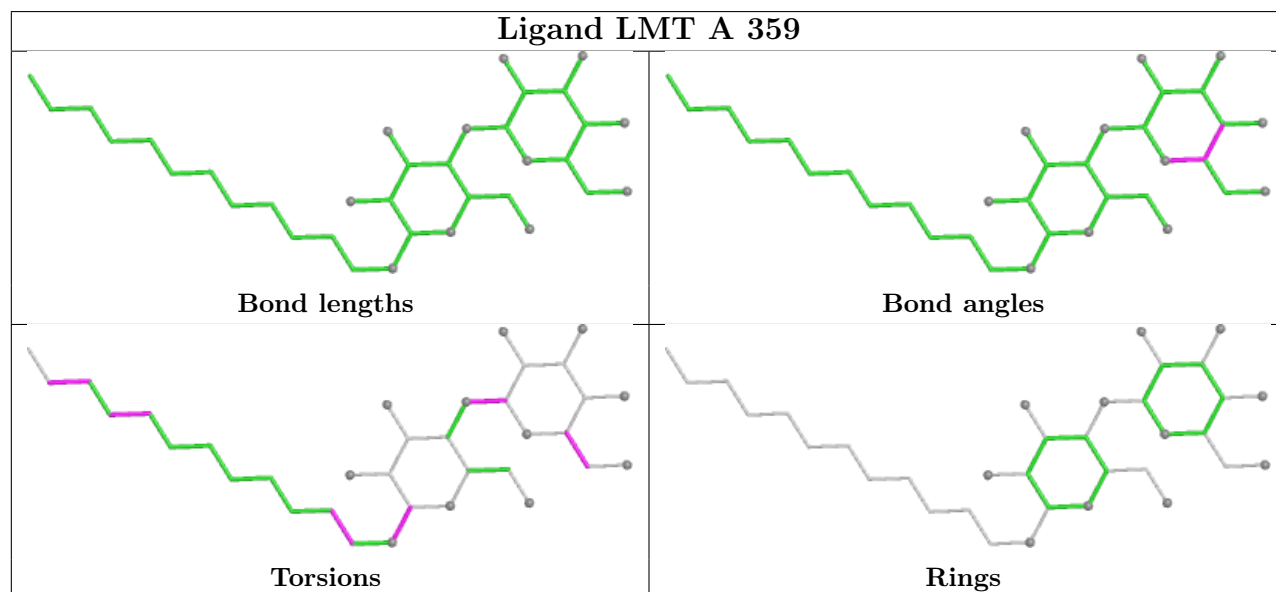
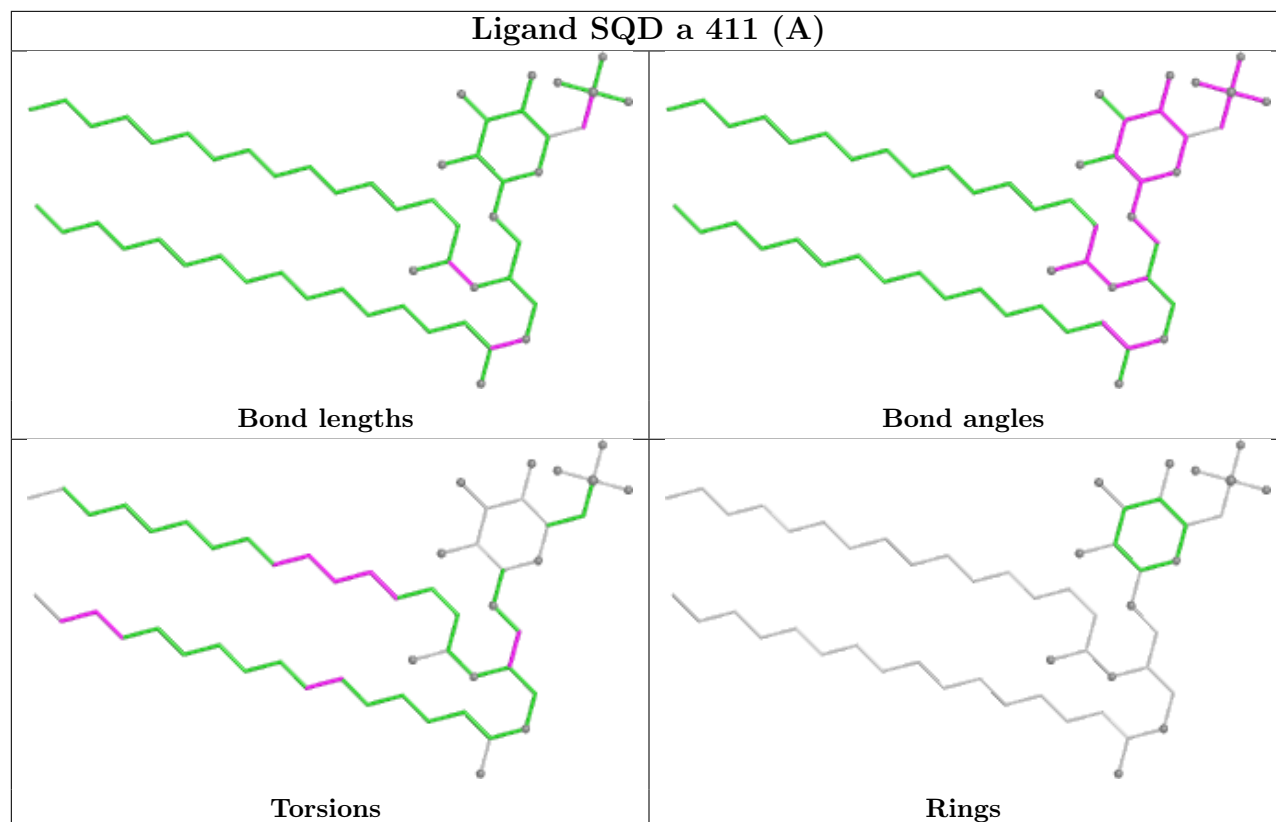


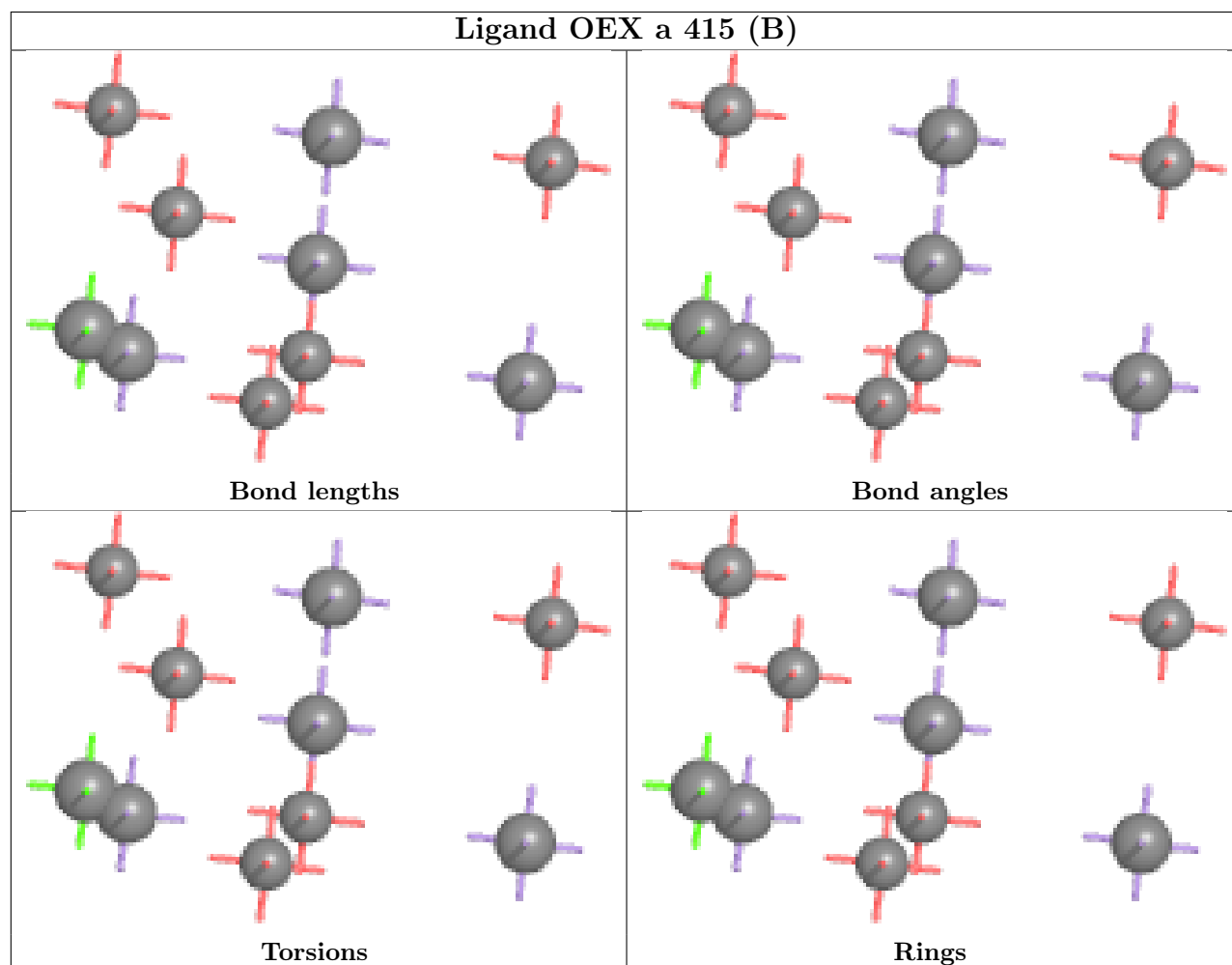
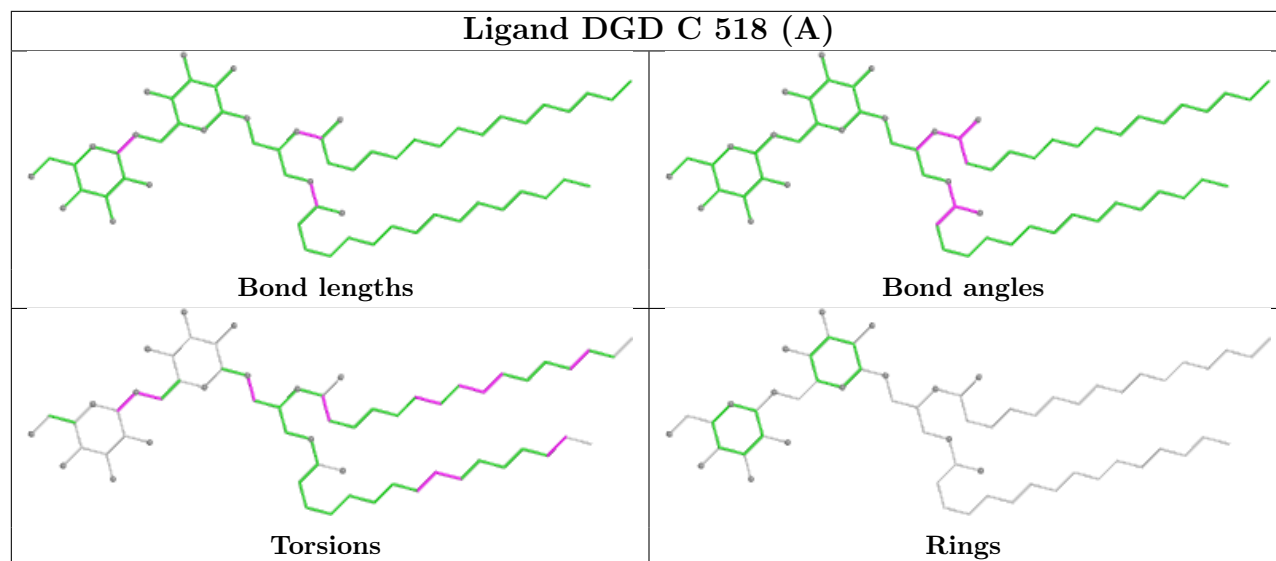
Ligand LHG d 711 (A)

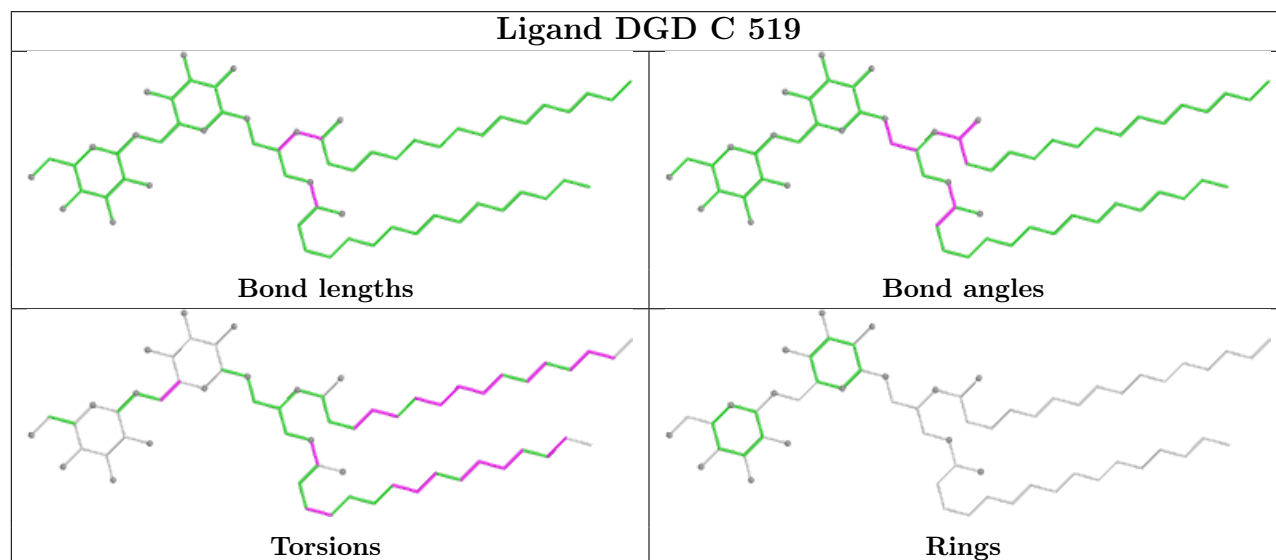
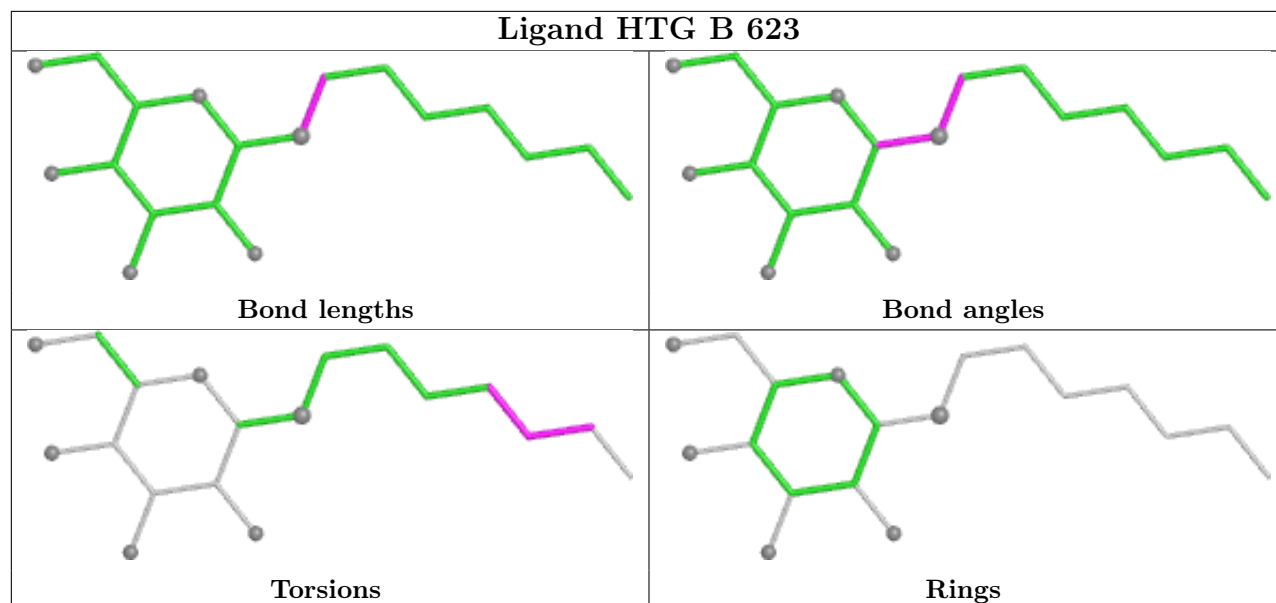




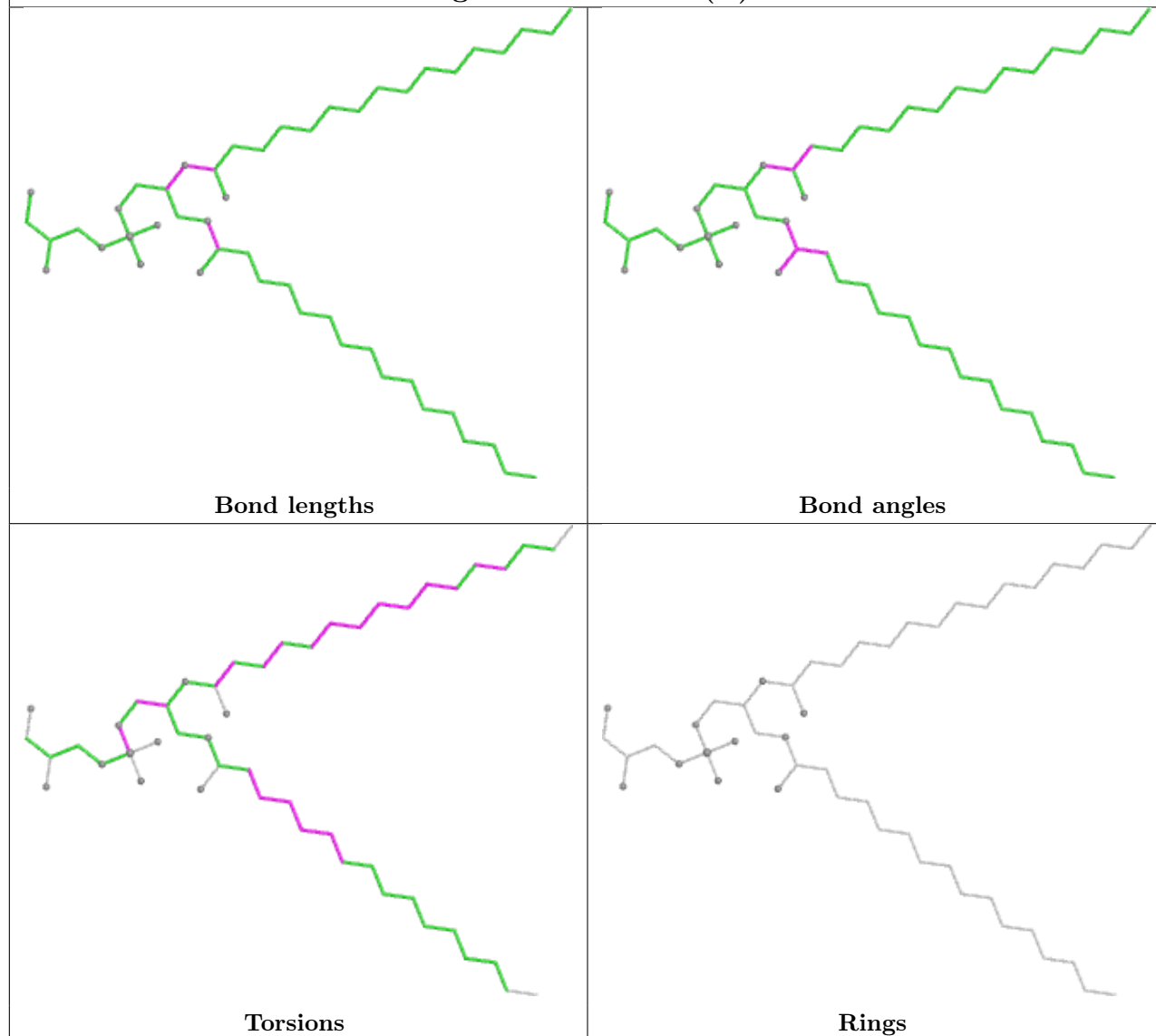




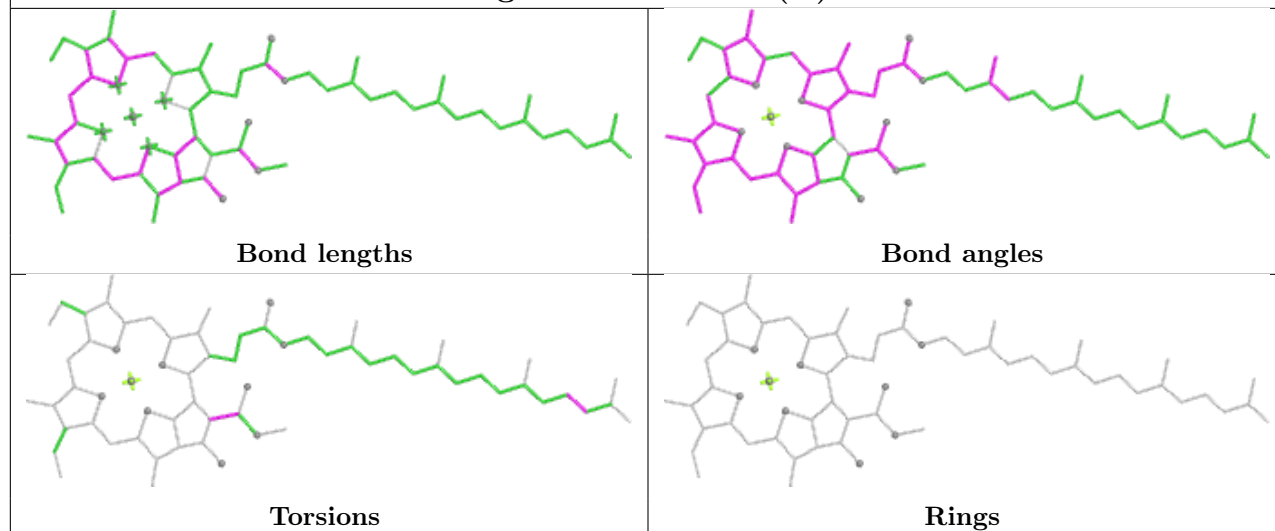


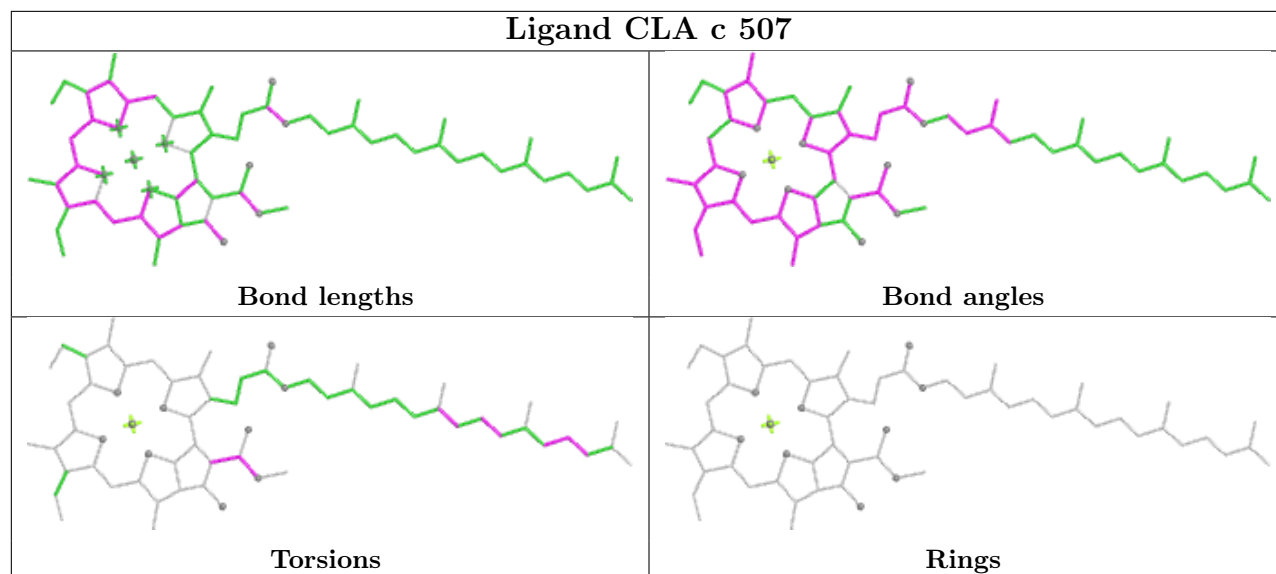
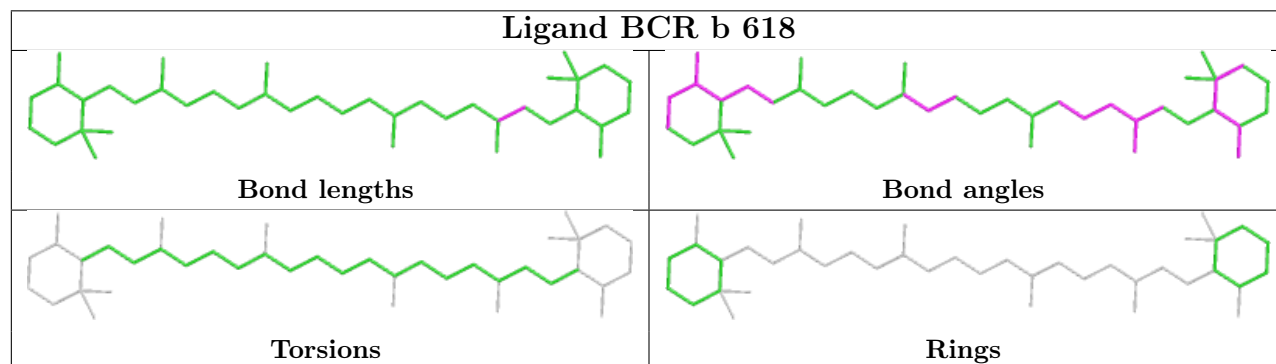
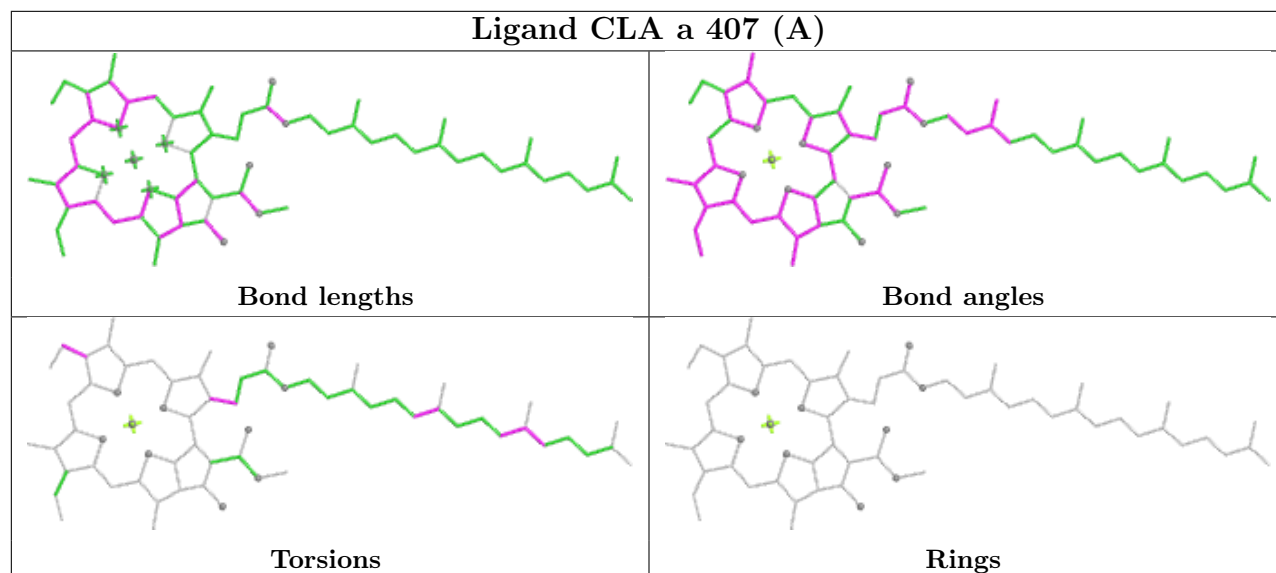


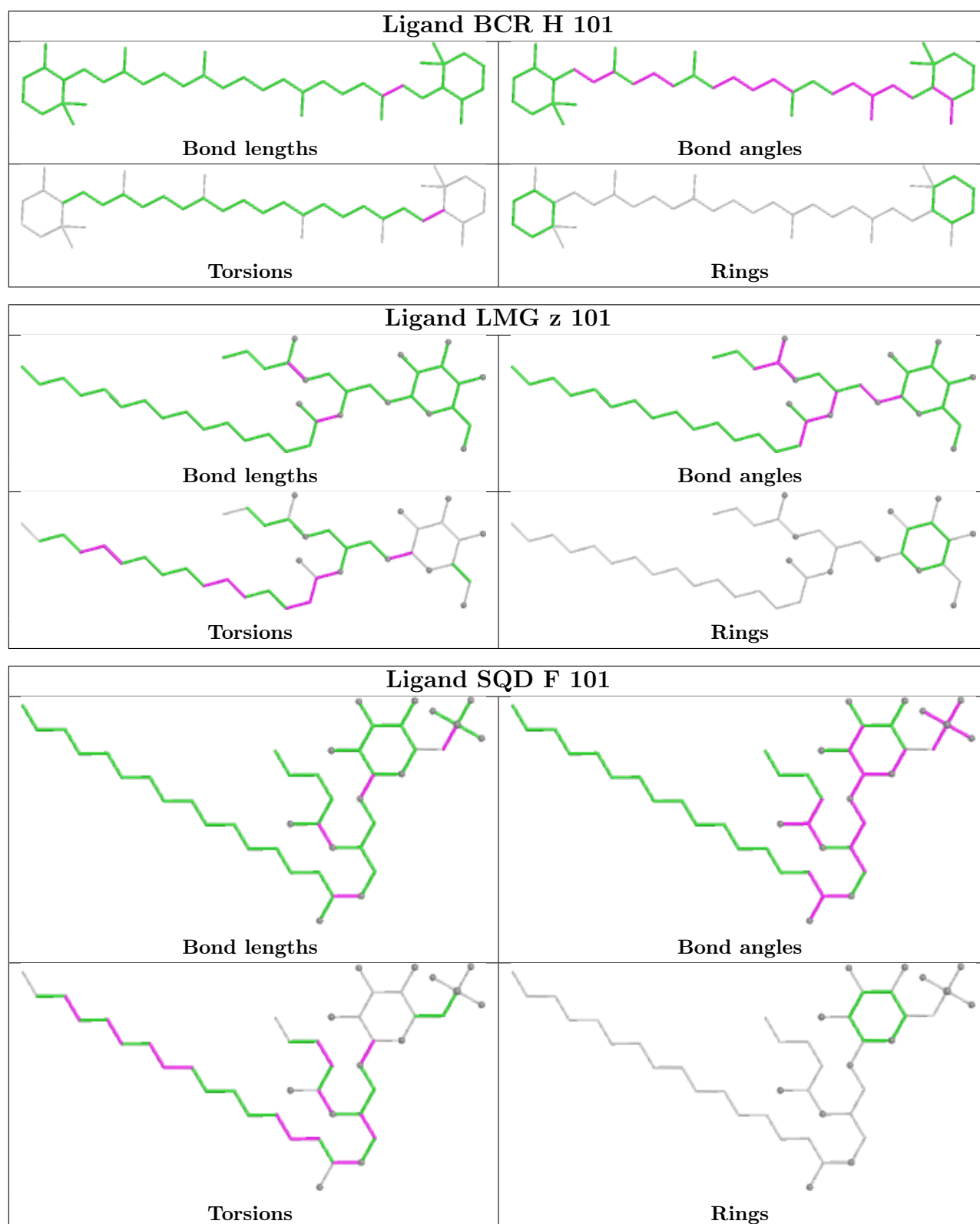
Ligand LHG L 101 (B)

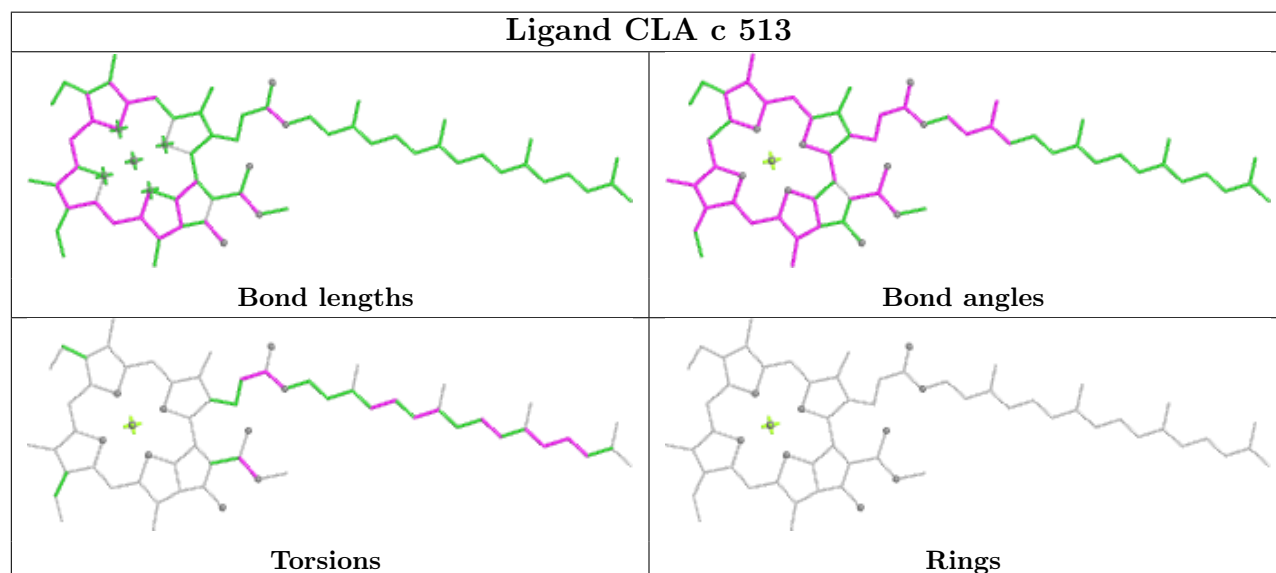
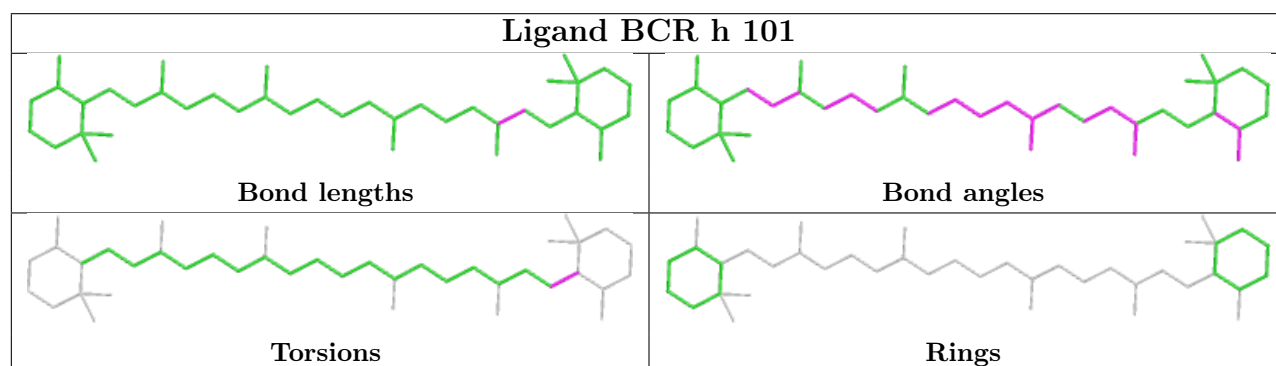
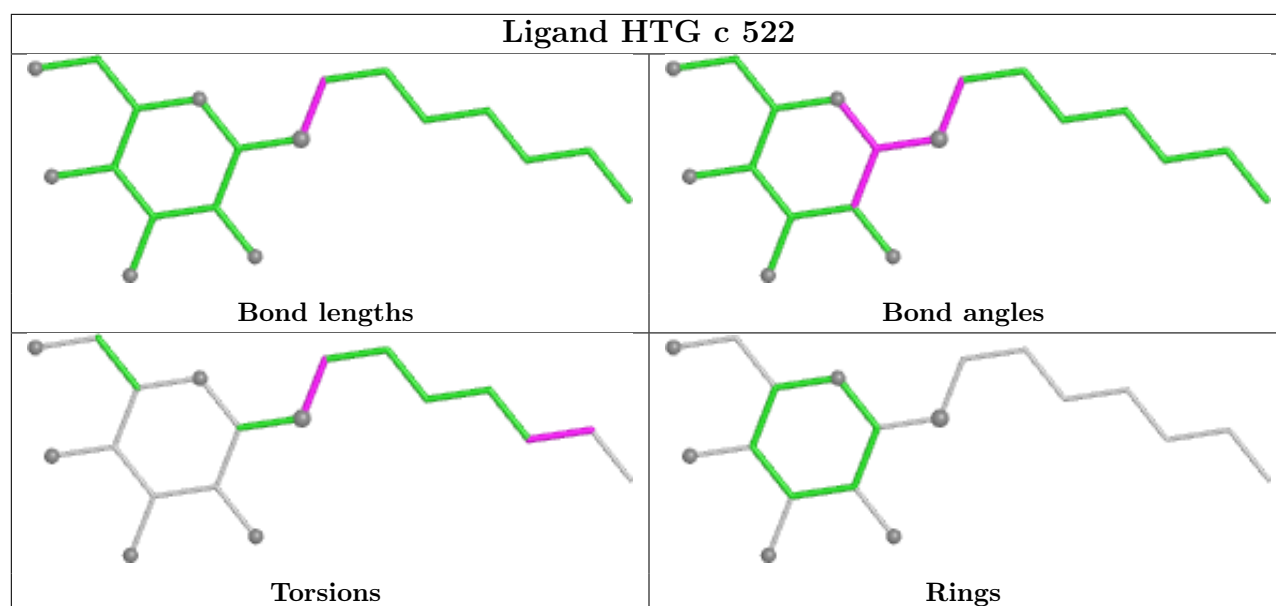


Ligand CLA A 405 (A)

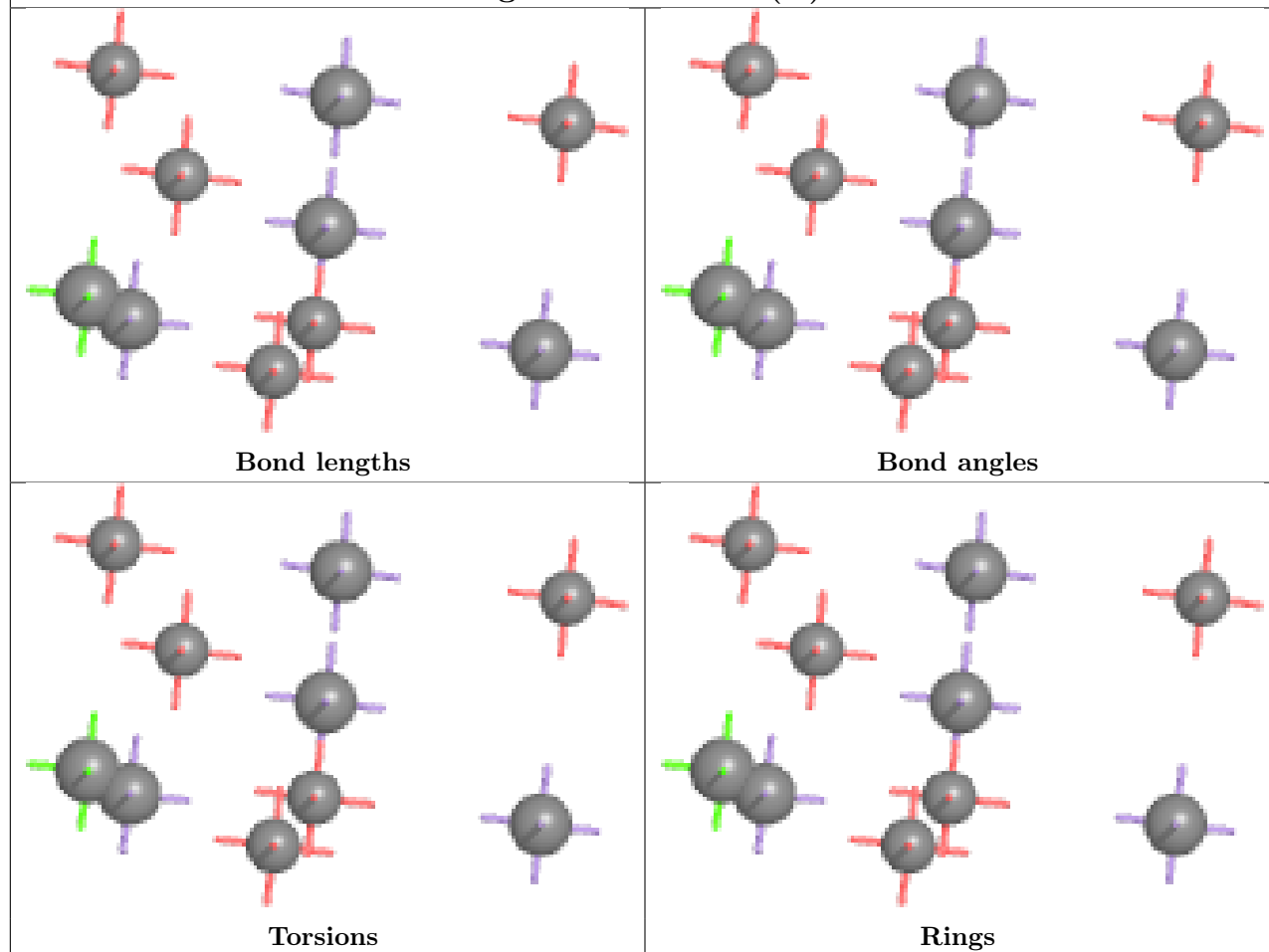


Ligand CLA c 507**Ligand BCR b 618****Ligand CLA a 407 (A)**

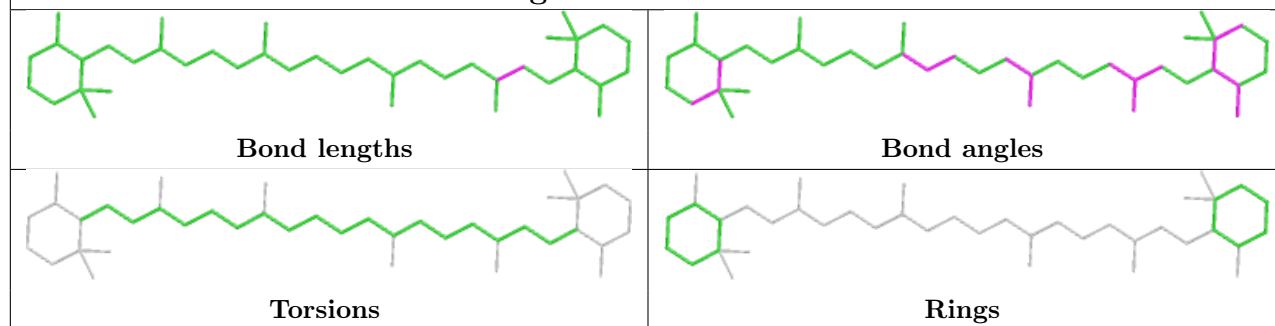


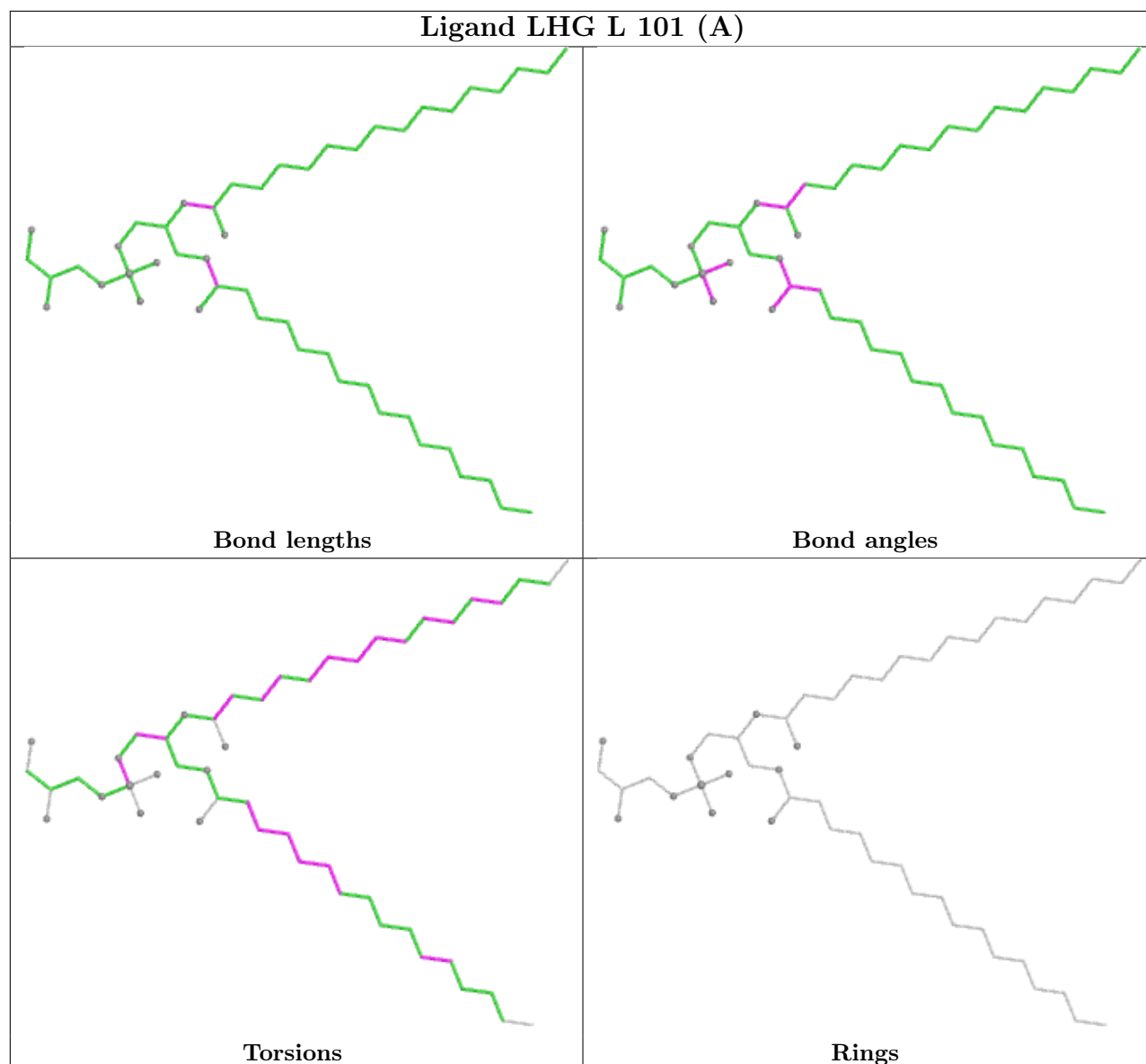
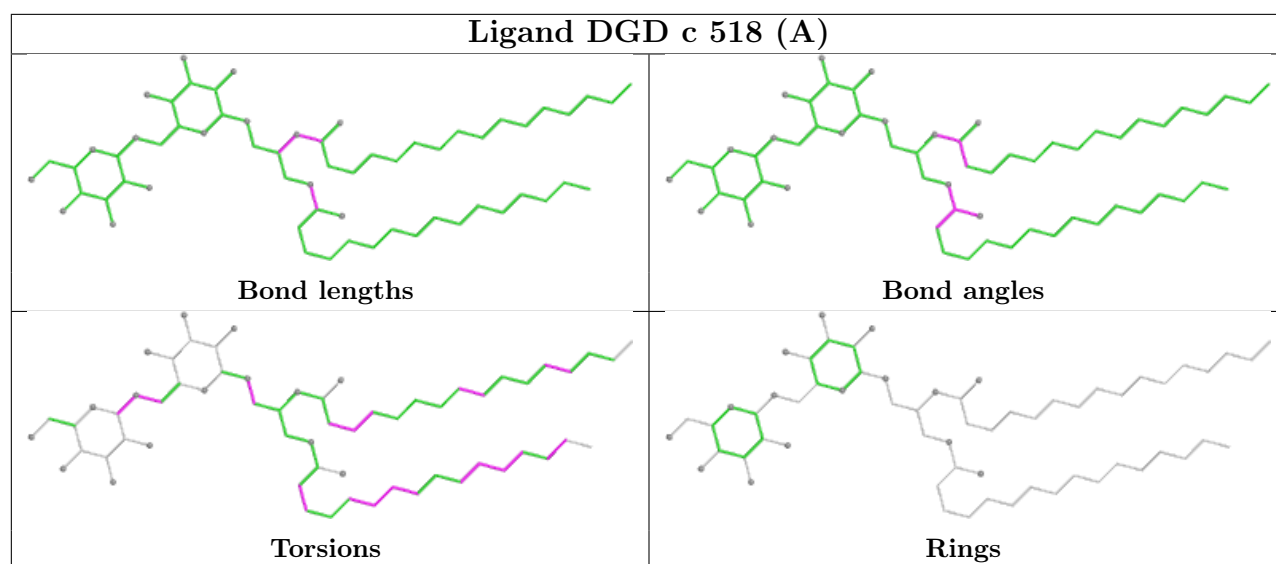


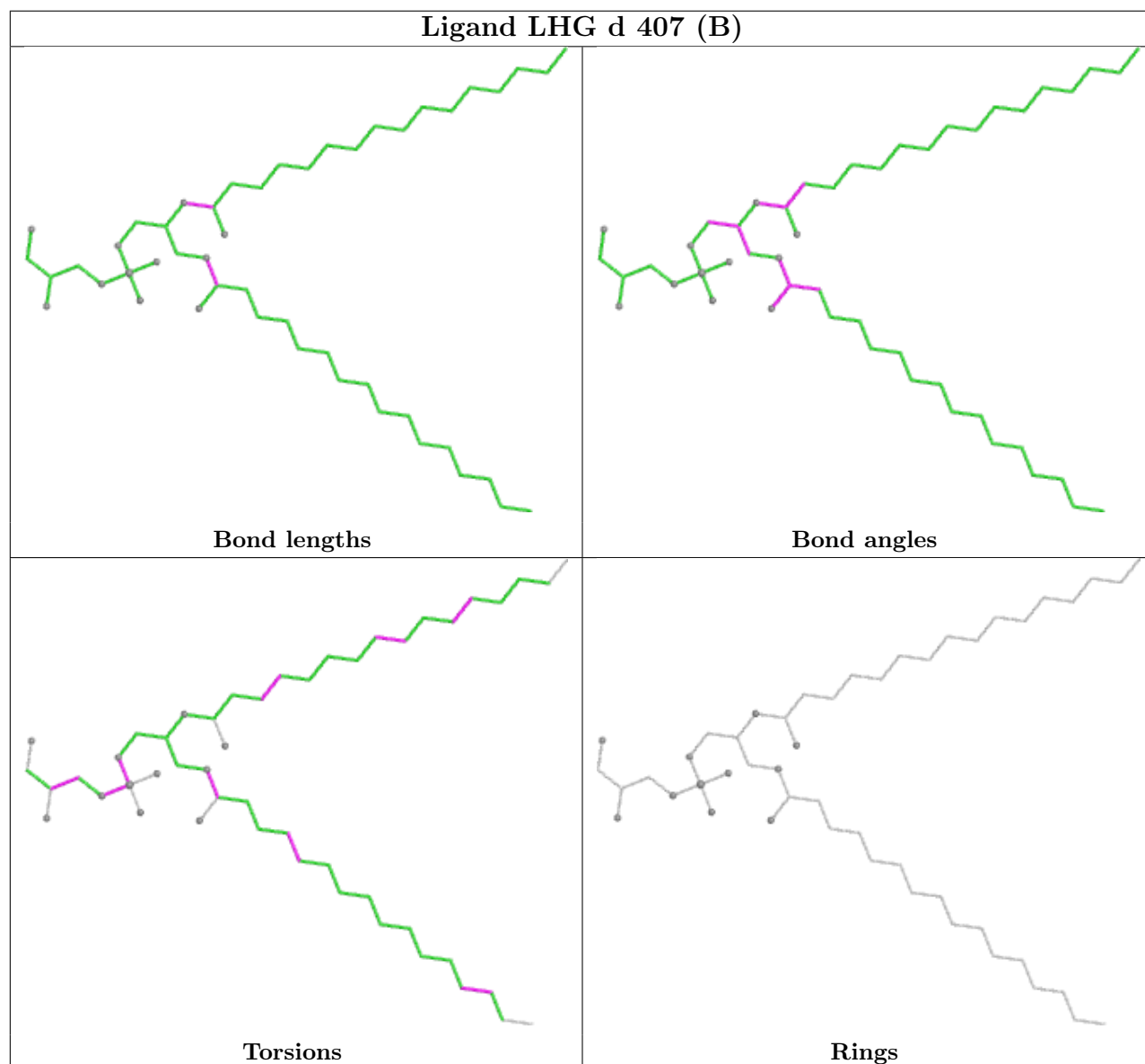
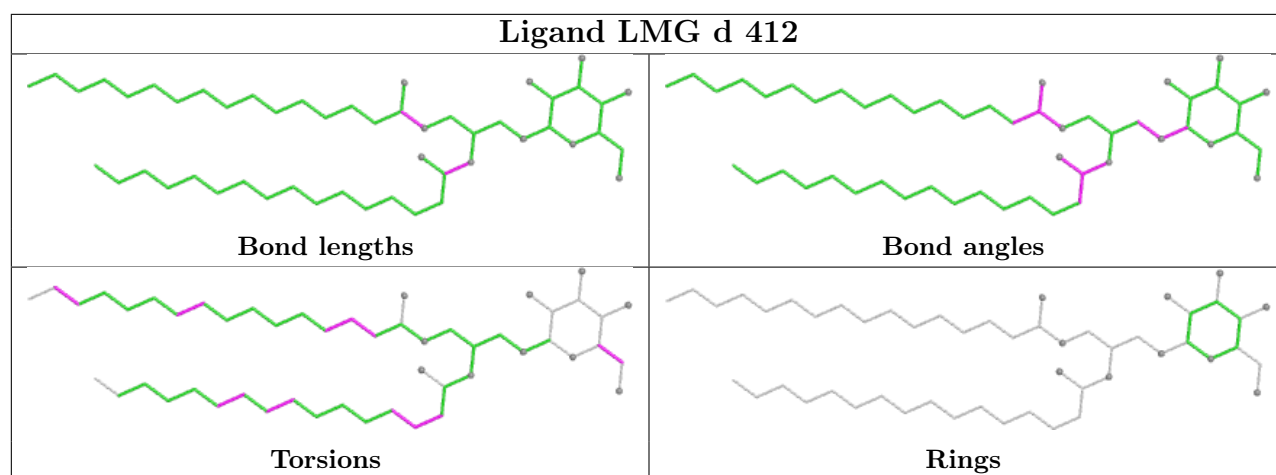
Ligand OEX a 415 (A)

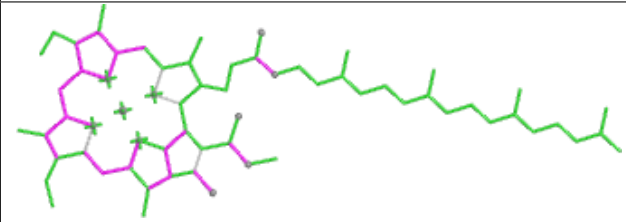
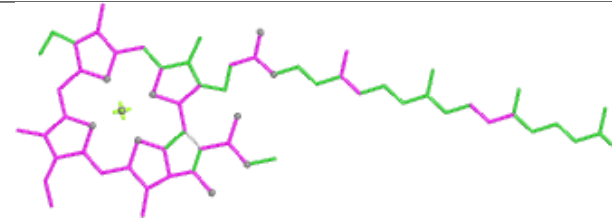
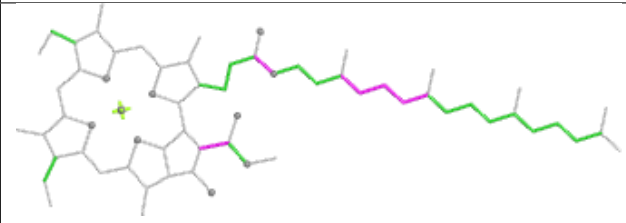
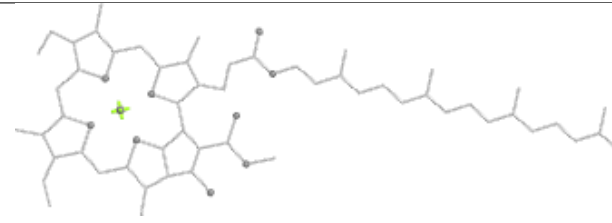


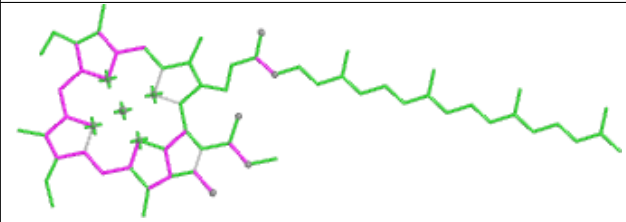
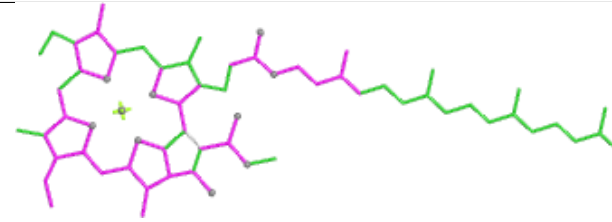
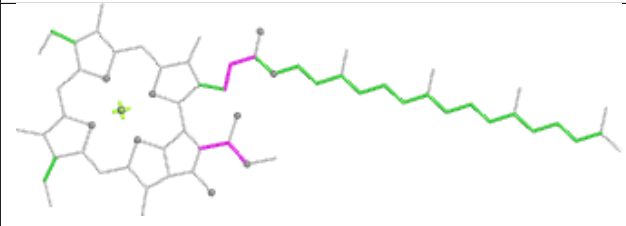
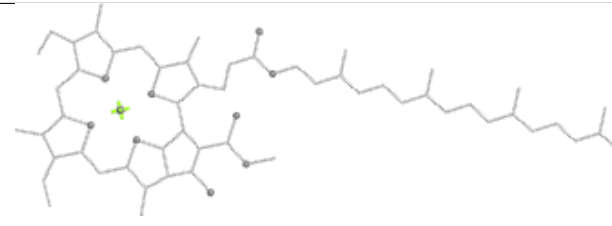
Ligand BCR B 618

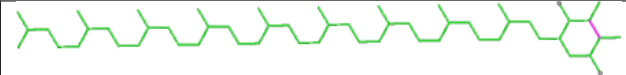
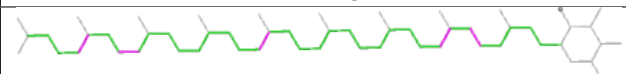
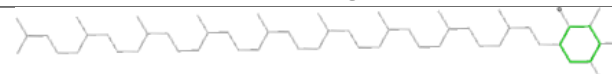


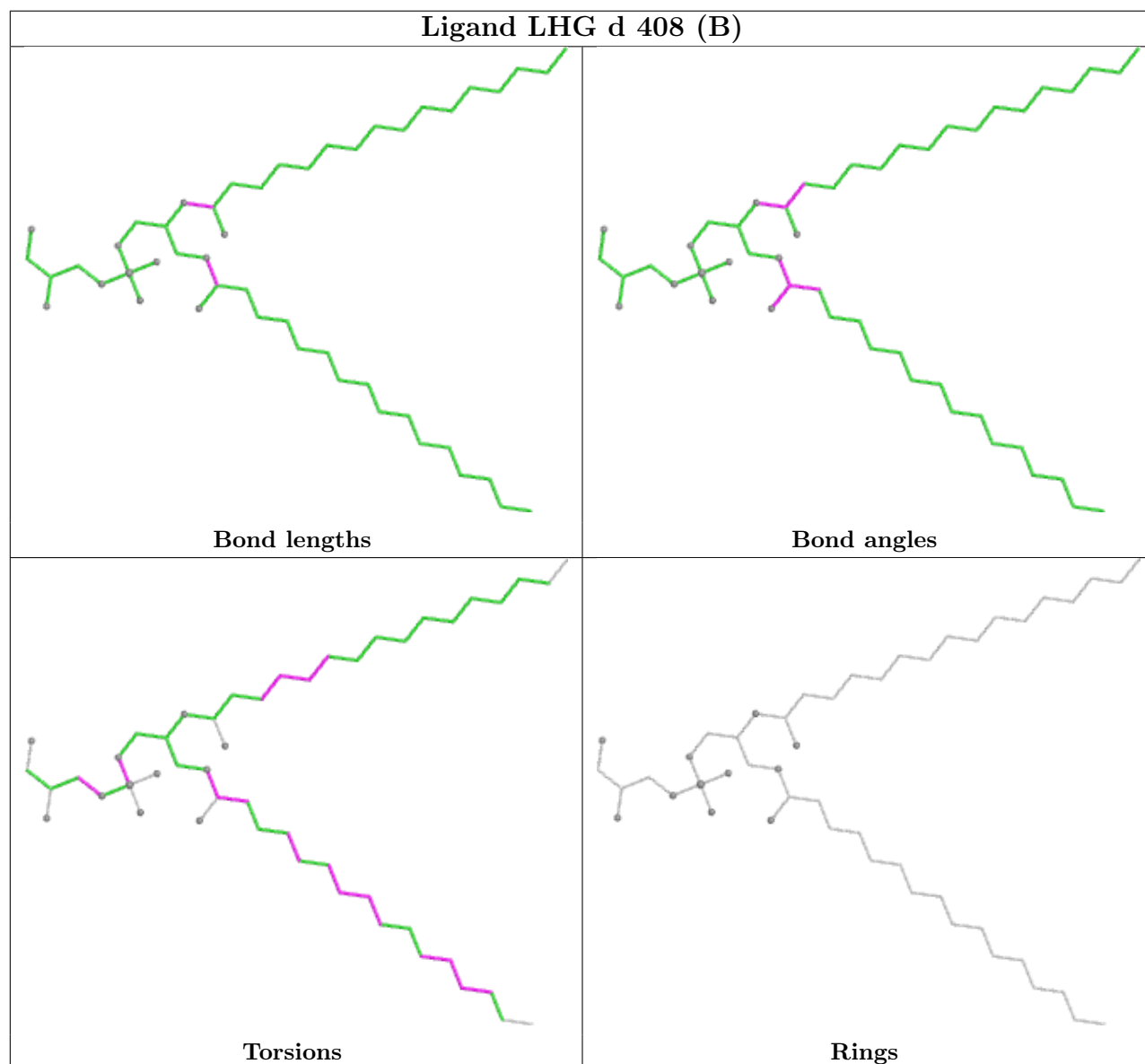
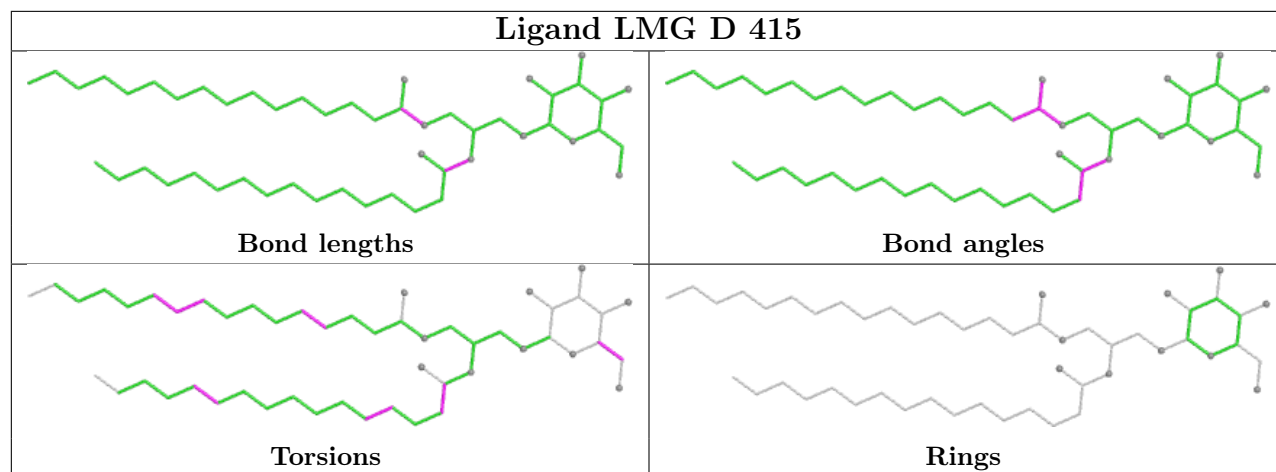


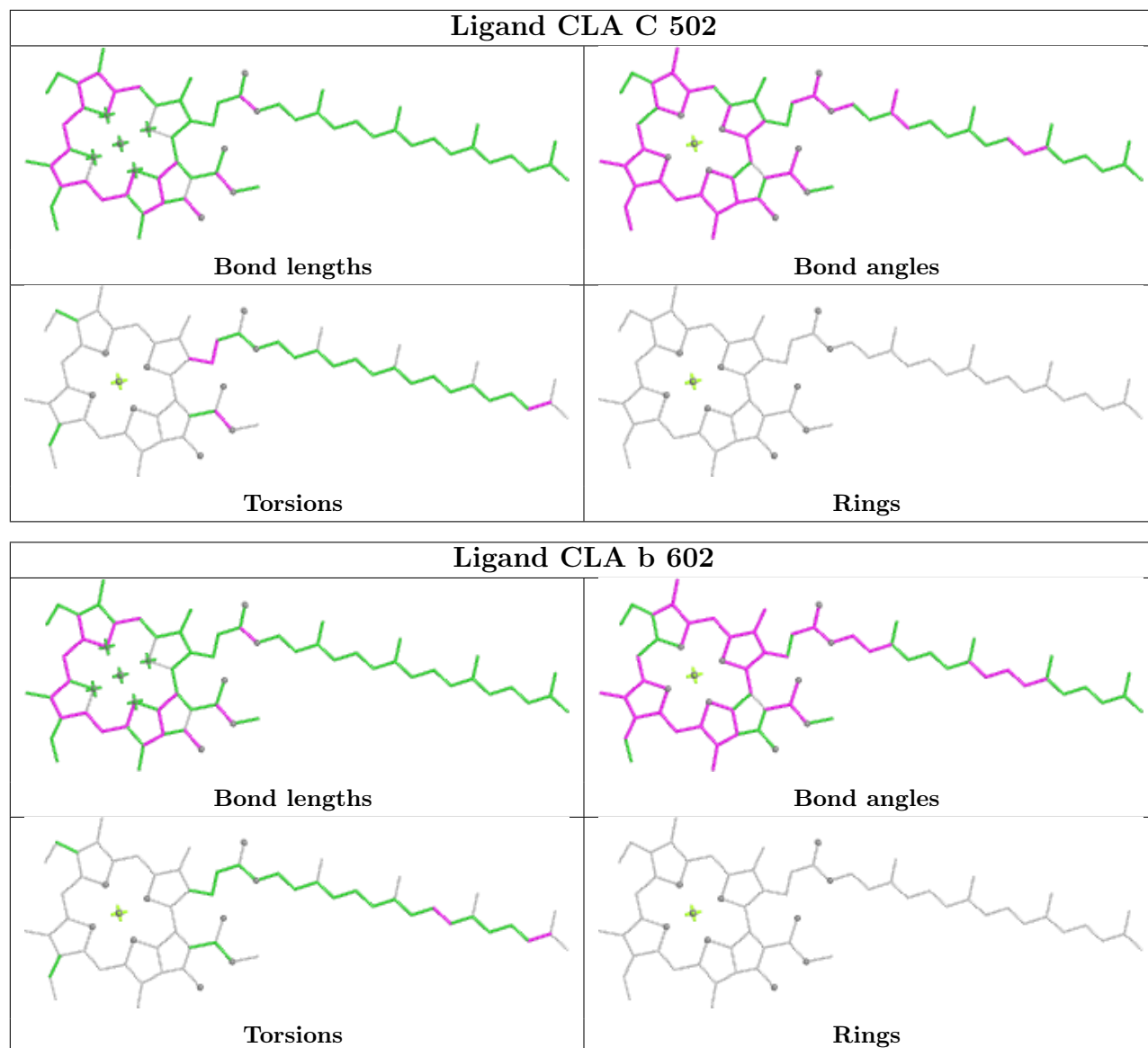


Ligand CLA b 616	
	
Bond lengths	Bond angles
	
Torsions	Rings

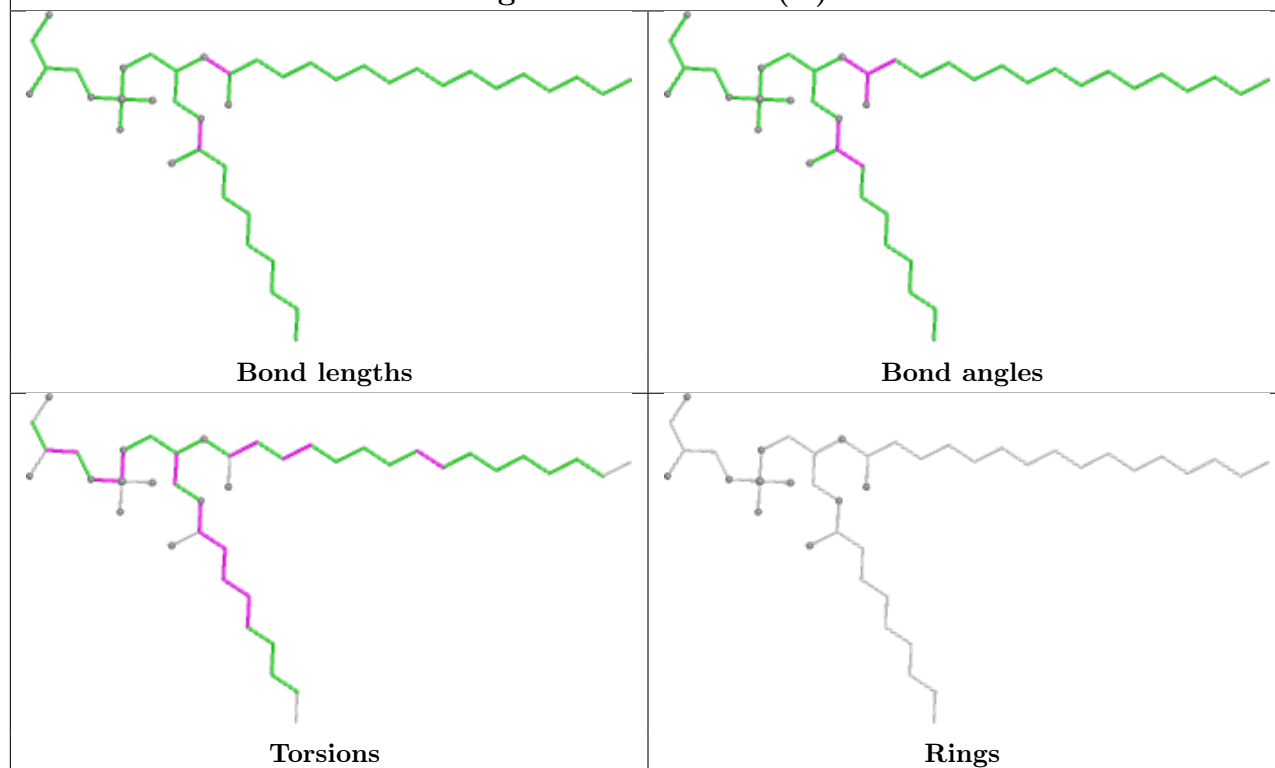
Ligand CLA c 502	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PL9 d 405 (B)	
	
Bond lengths	Bond angles
	
Torsions	Rings

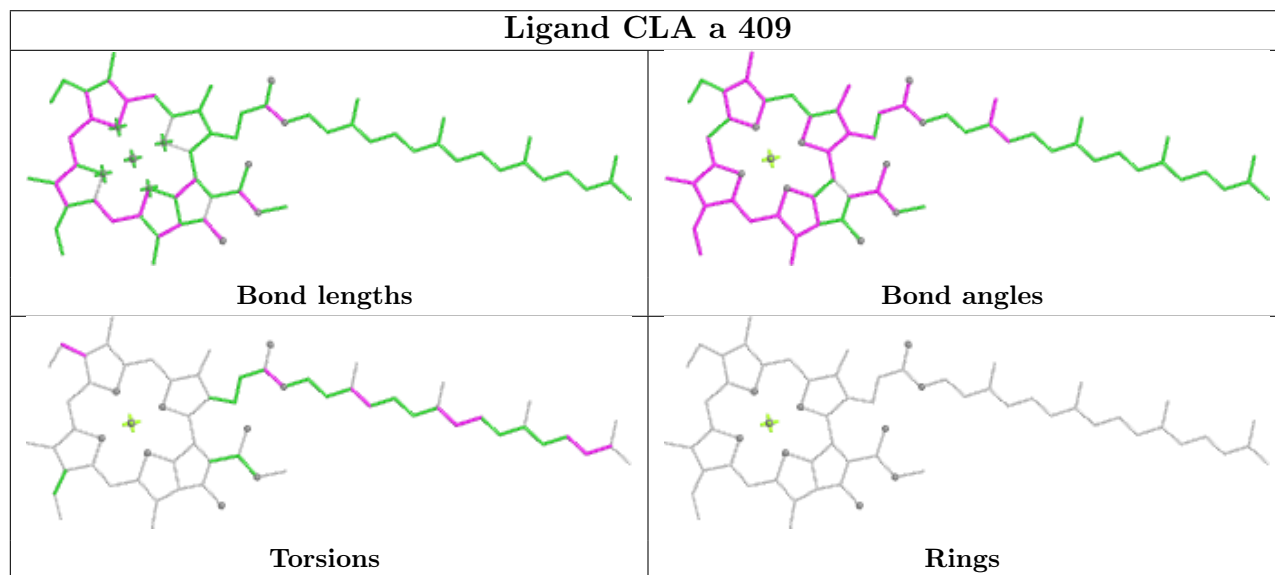


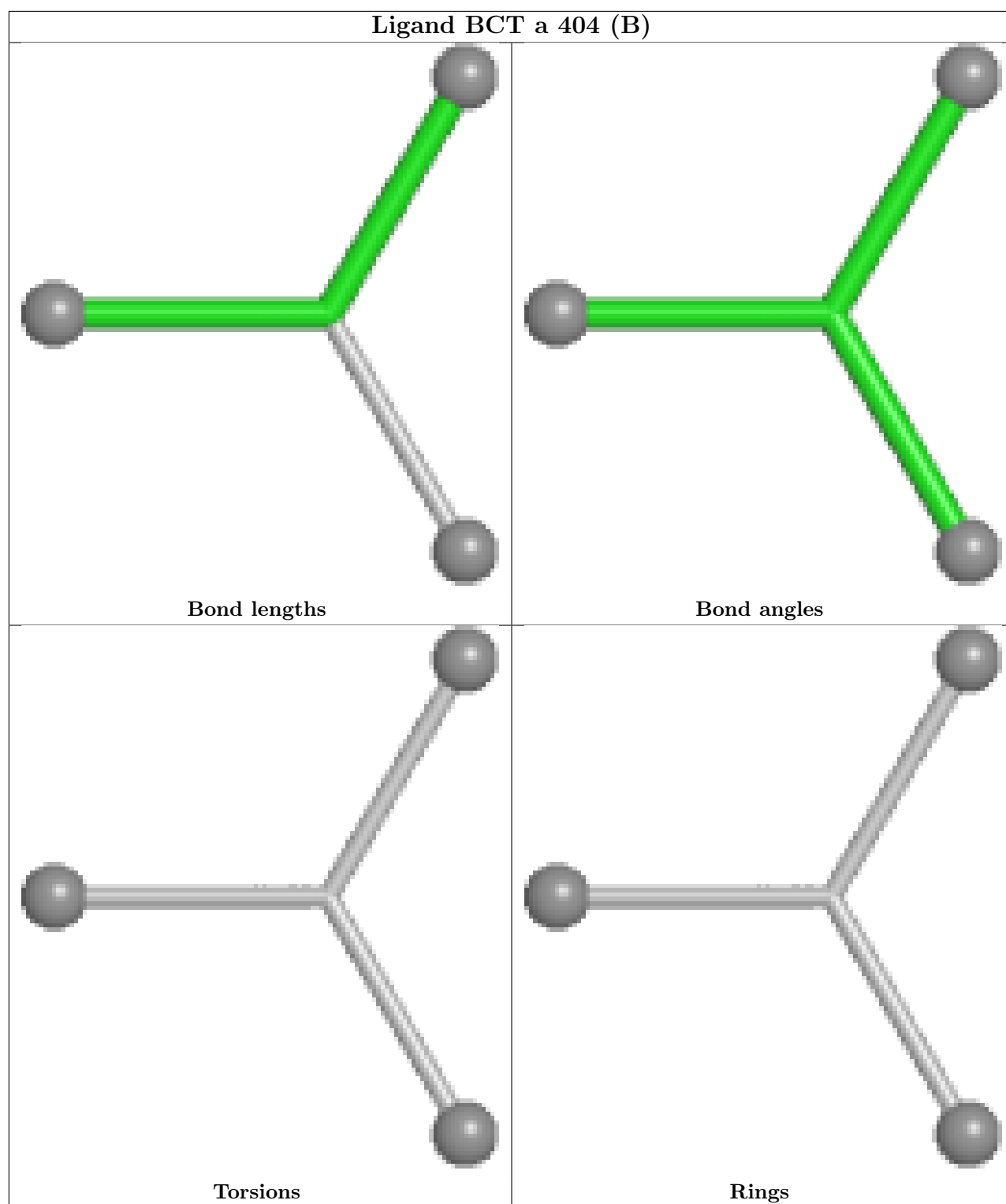


Ligand LHG E 101 (B)

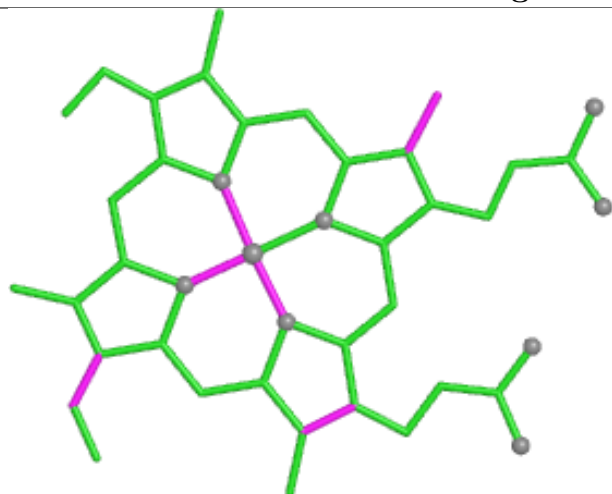


Ligand CLA a 409

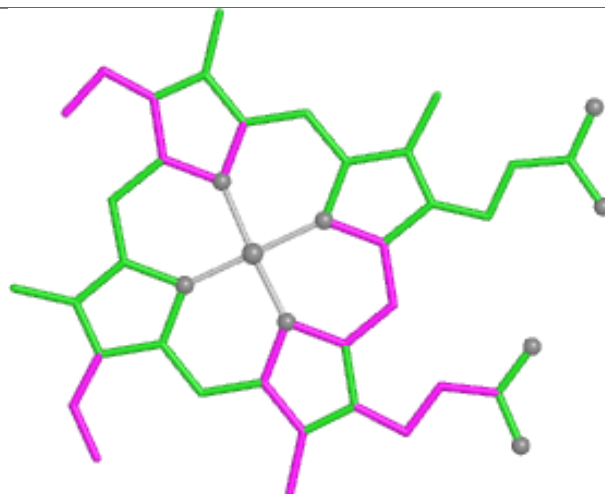




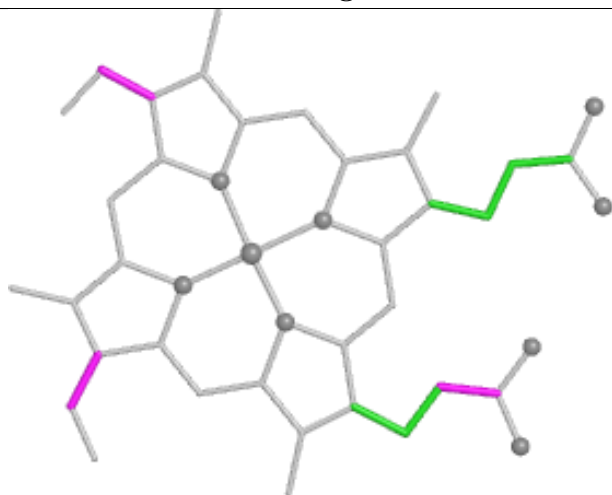
Ligand HEC V 202



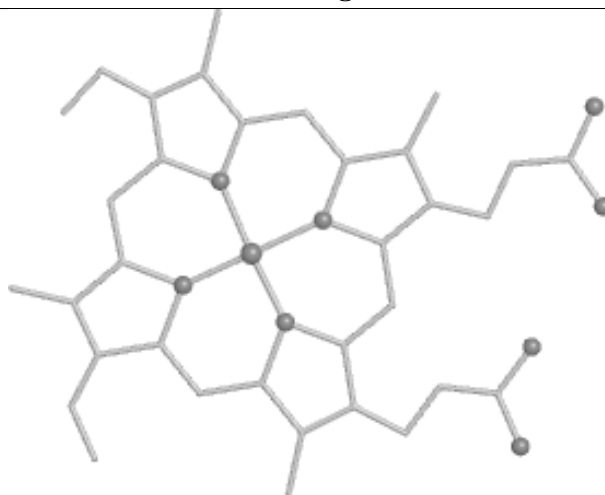
Bond lengths



Bond angles

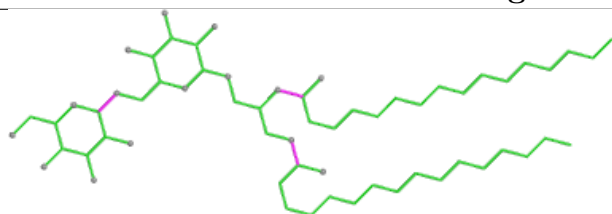


Torsions

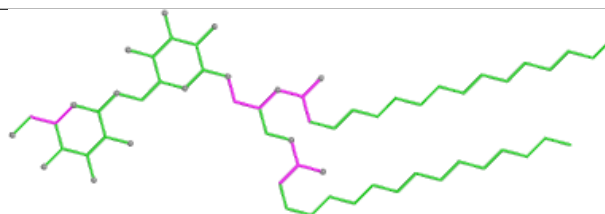


Rings

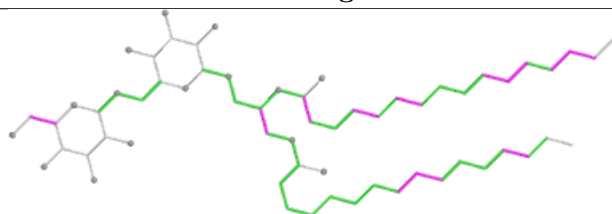
Ligand DGD H 102



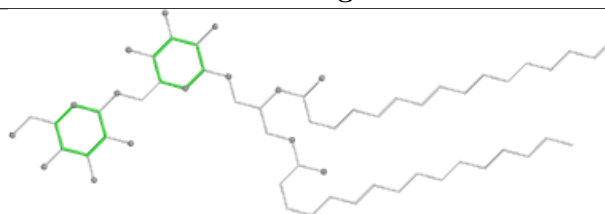
Bond lengths



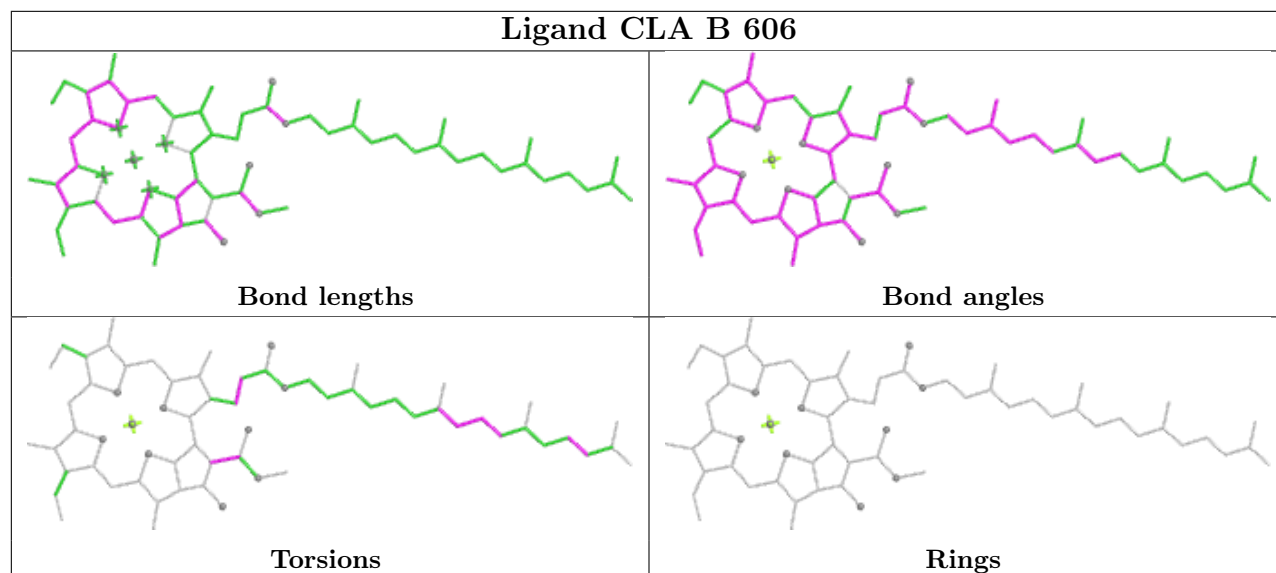
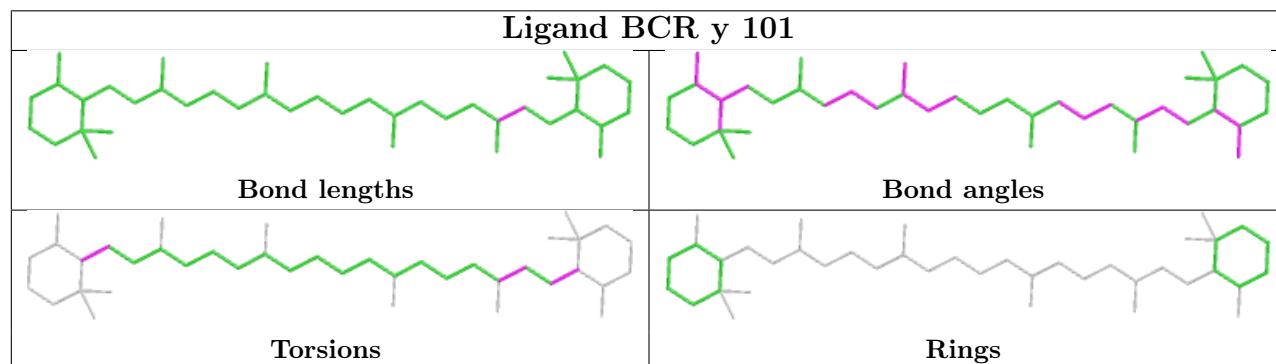
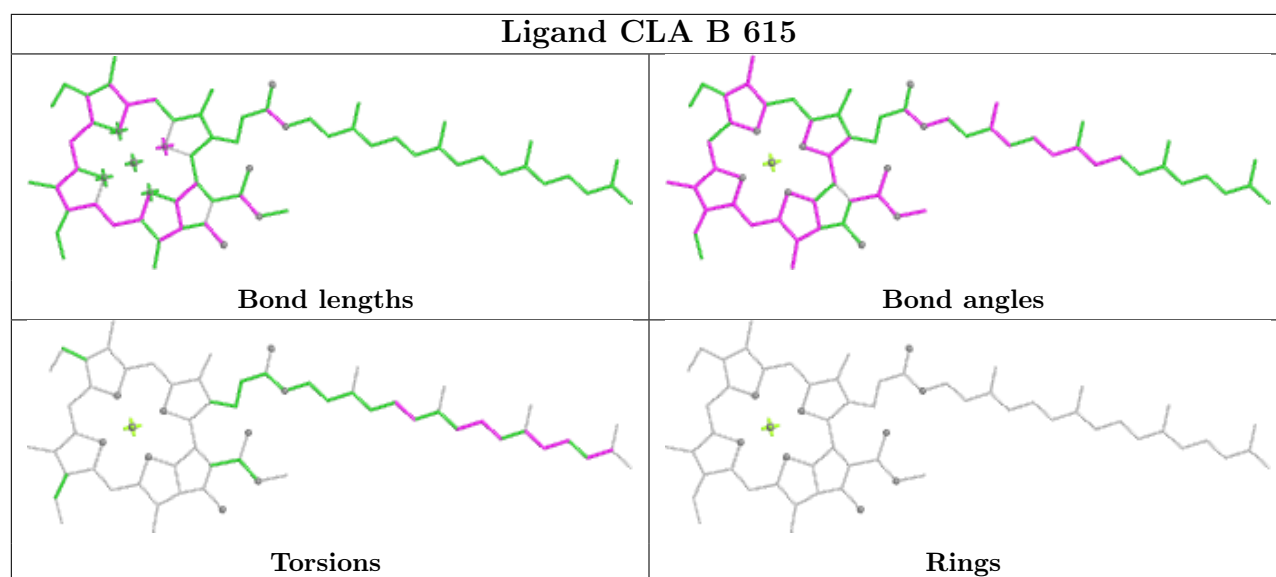
Bond angles

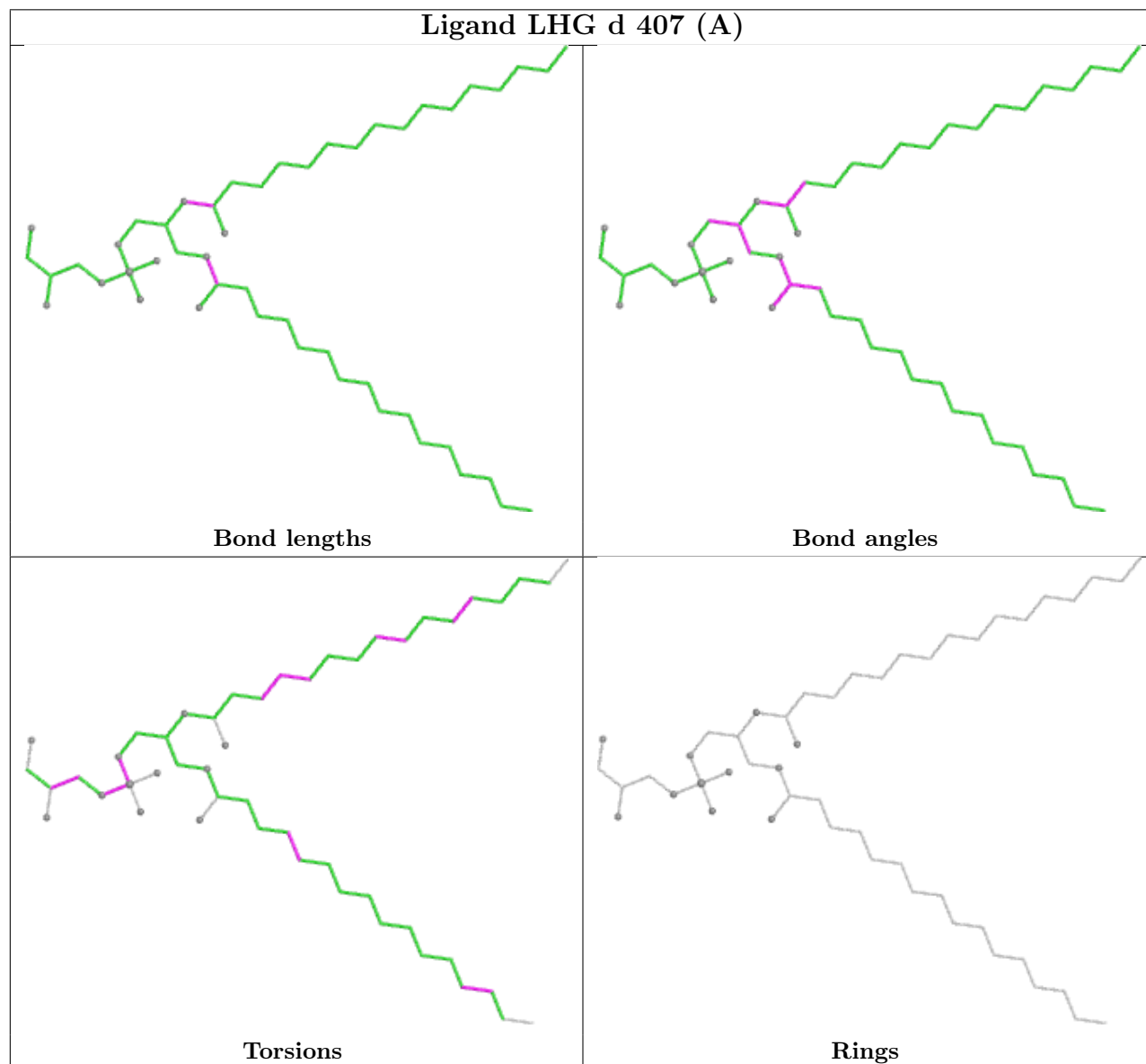
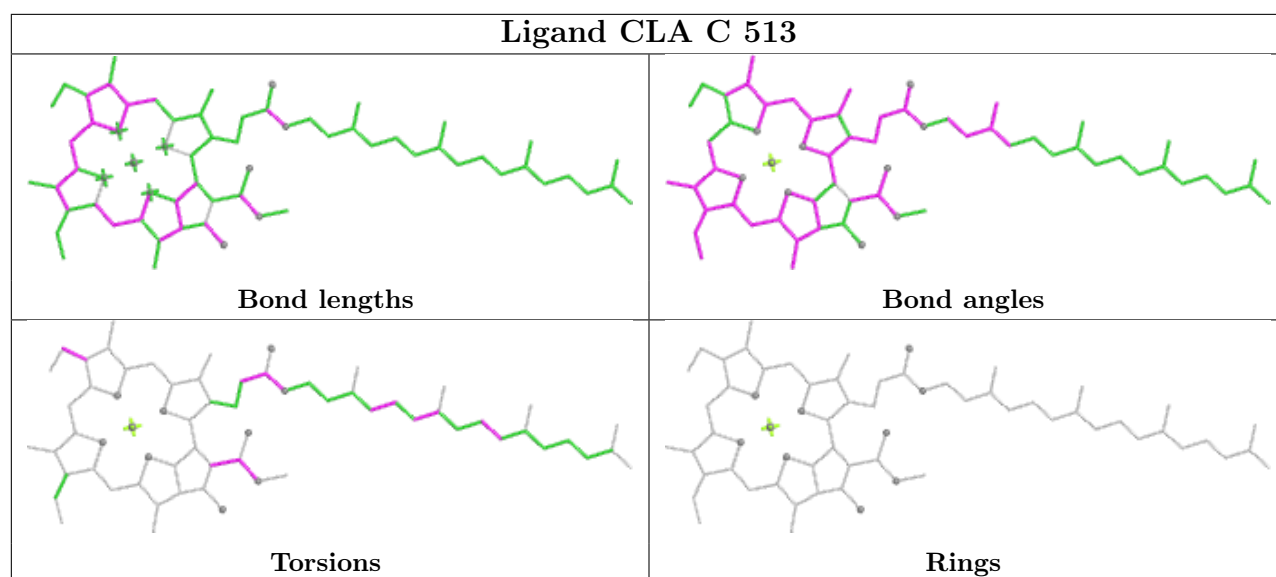


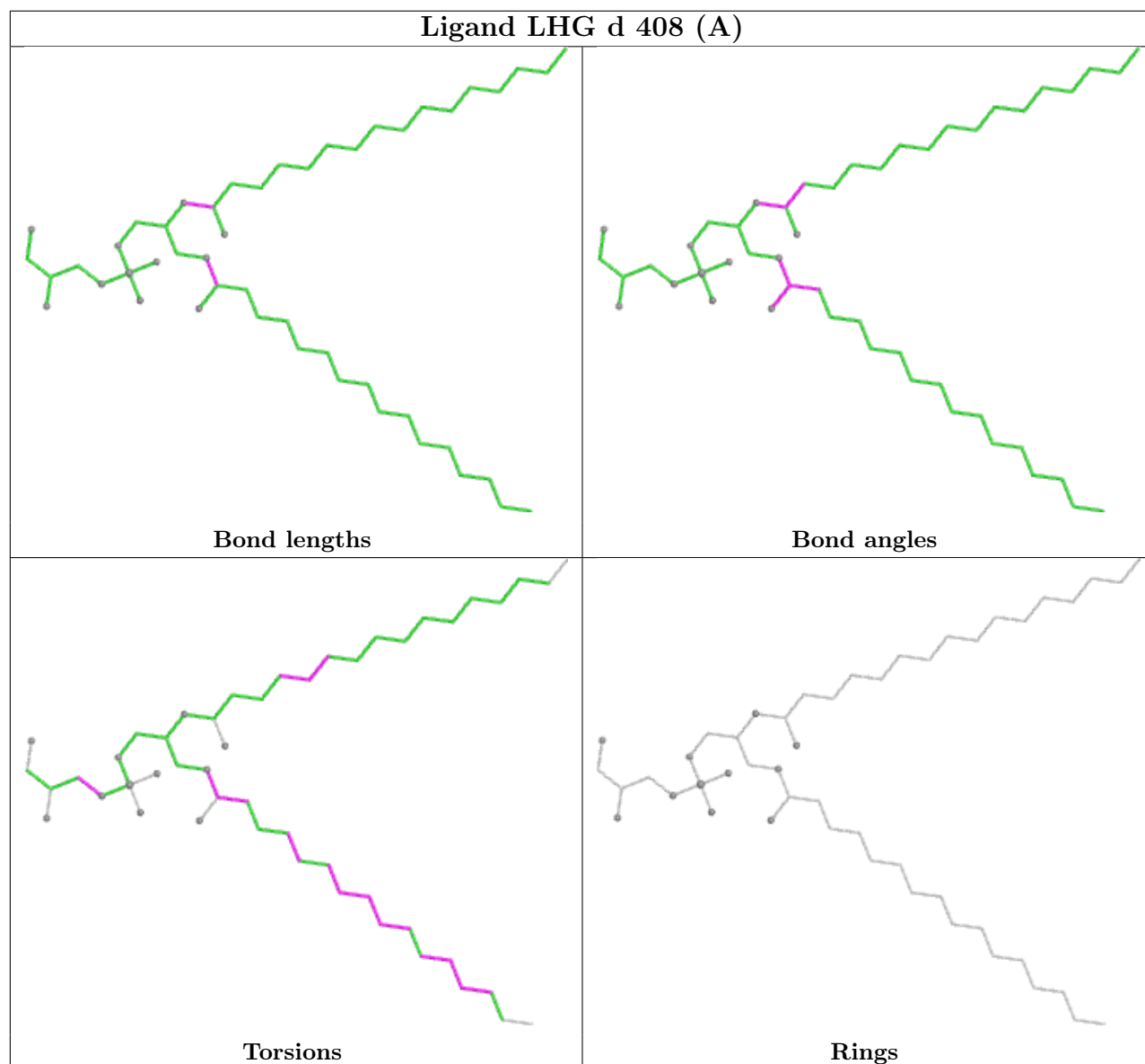
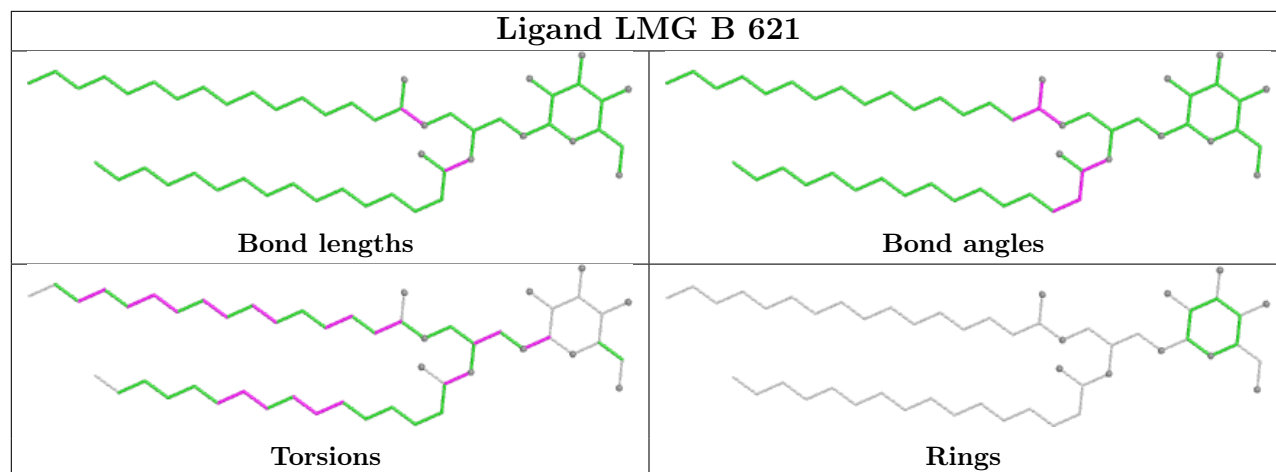
Torsions

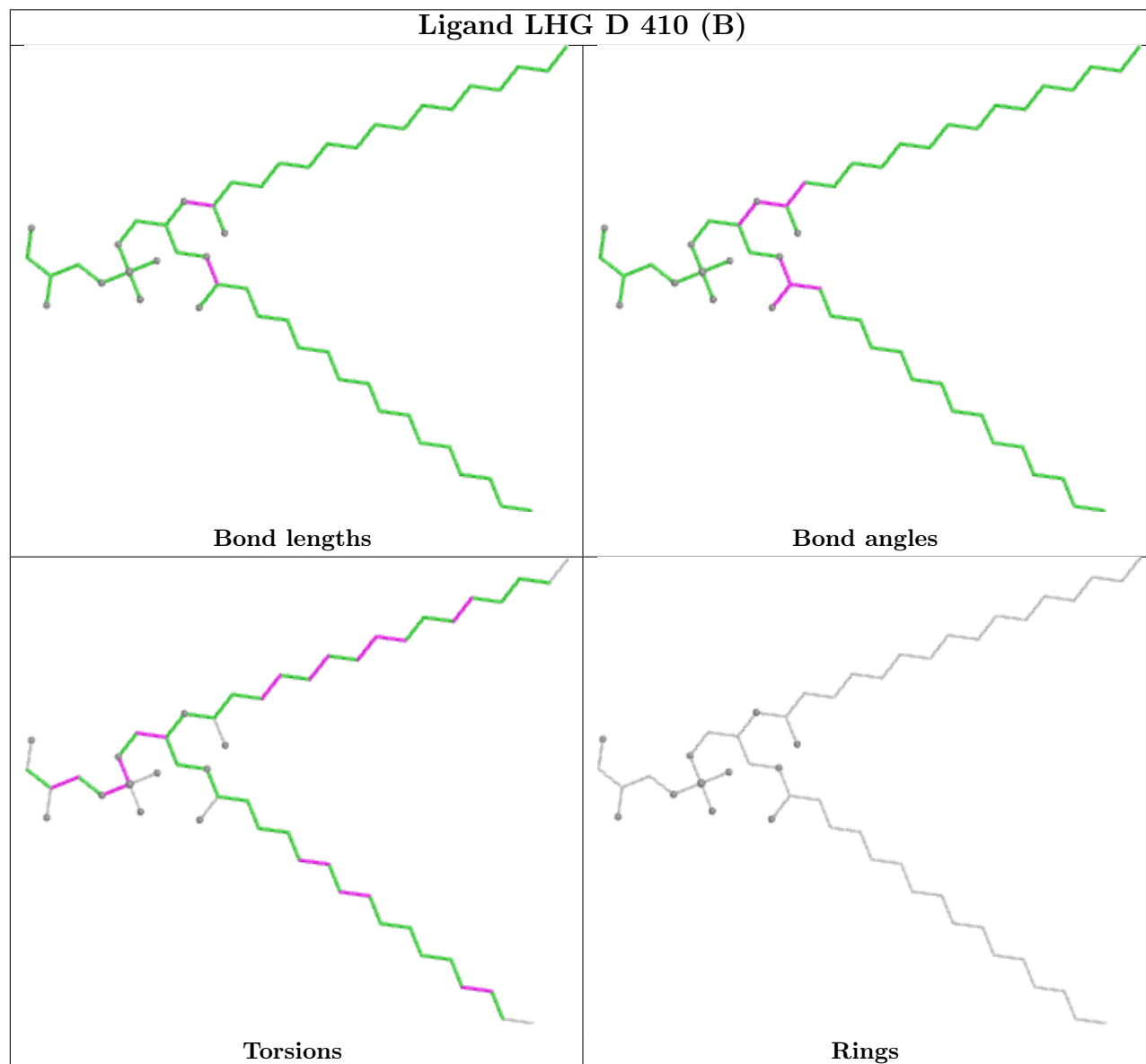
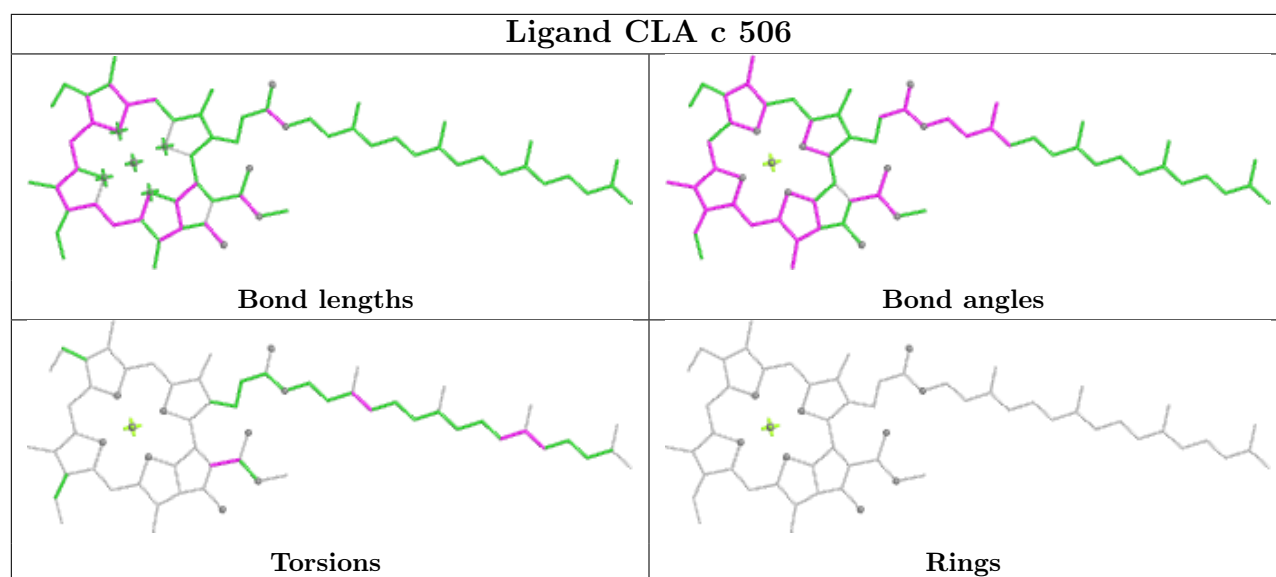


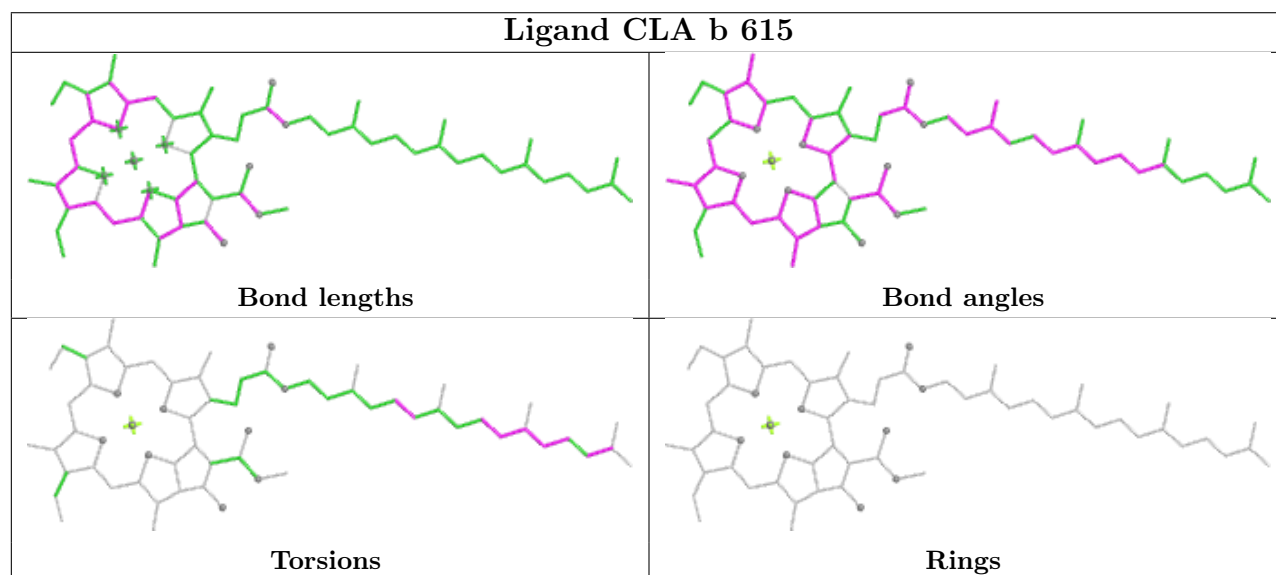
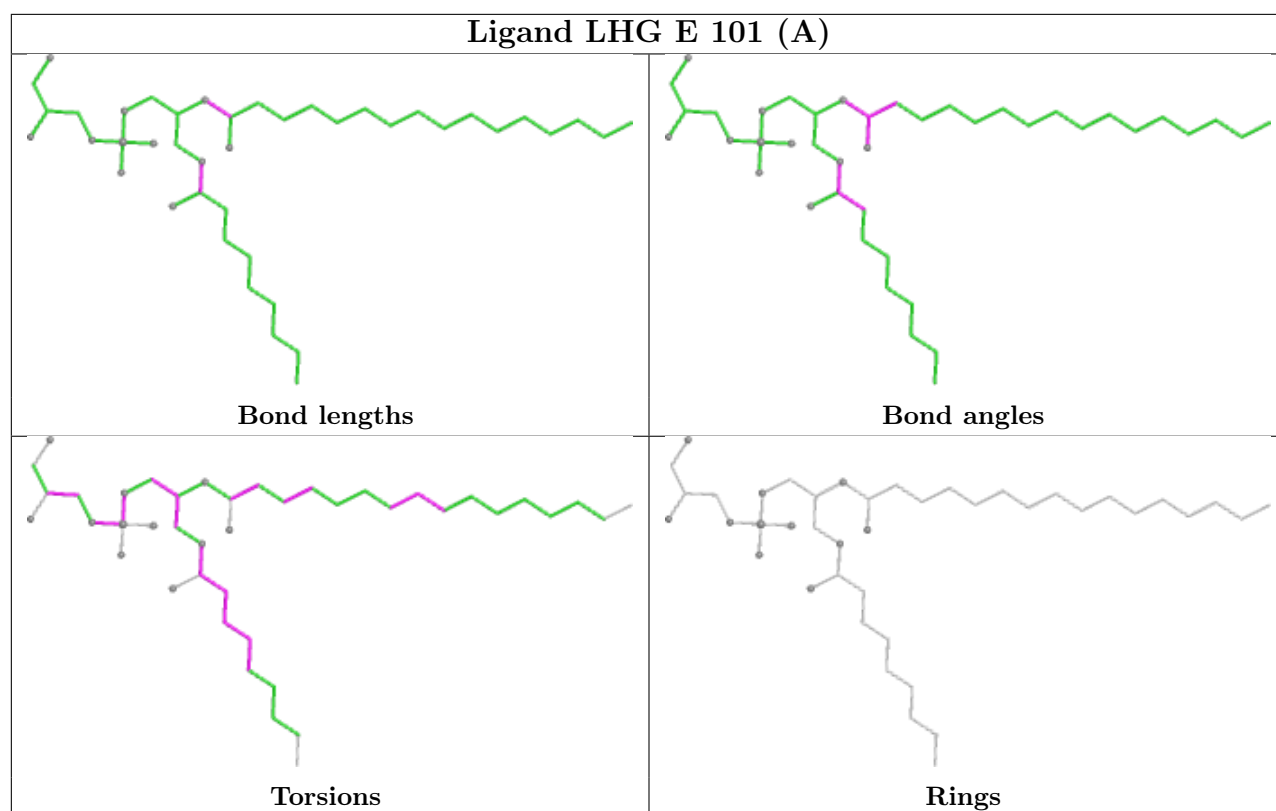
Rings

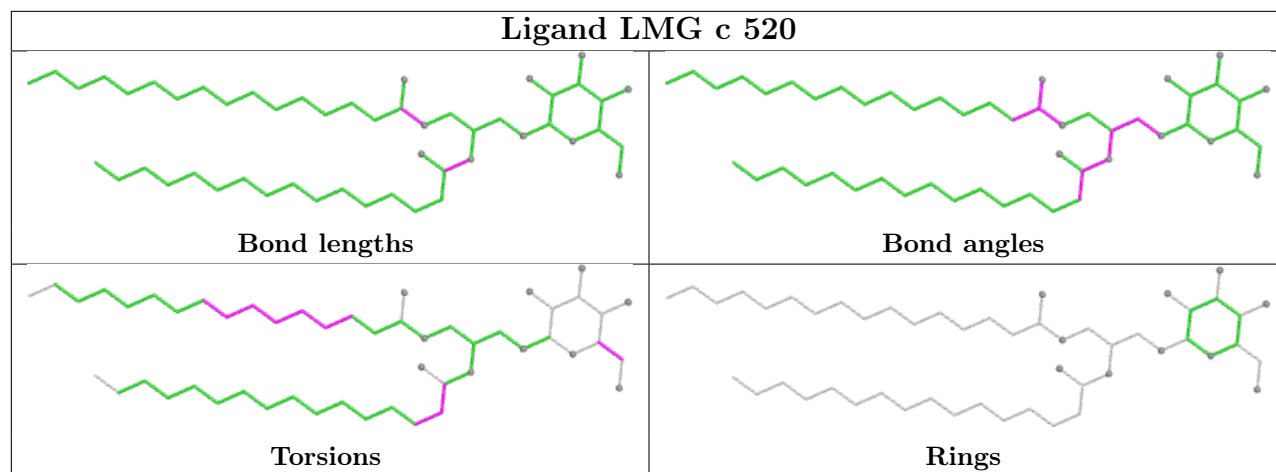


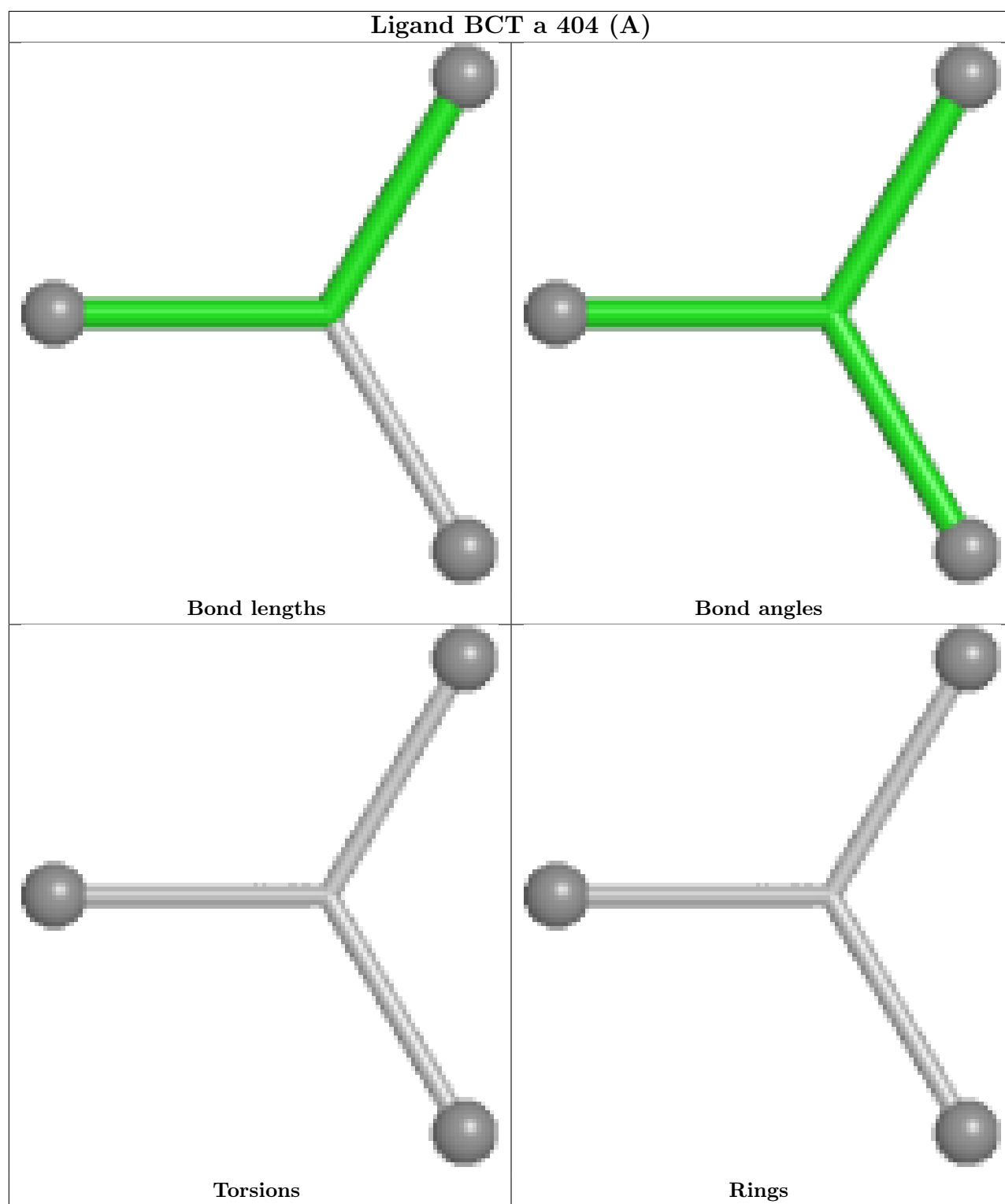


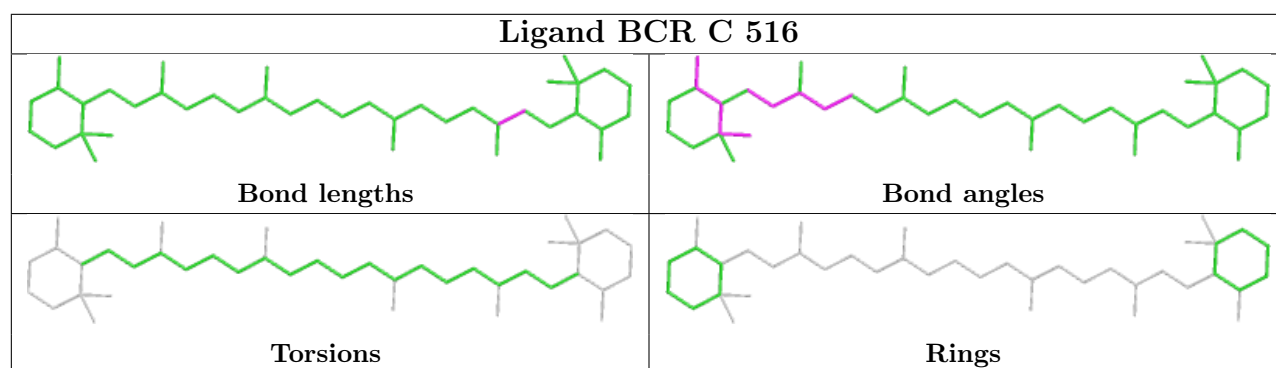
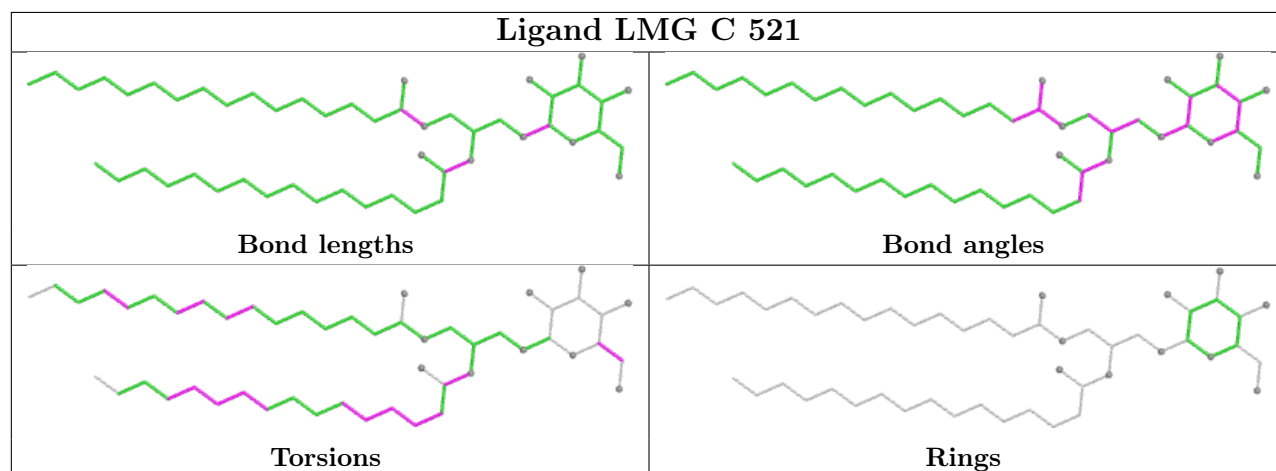
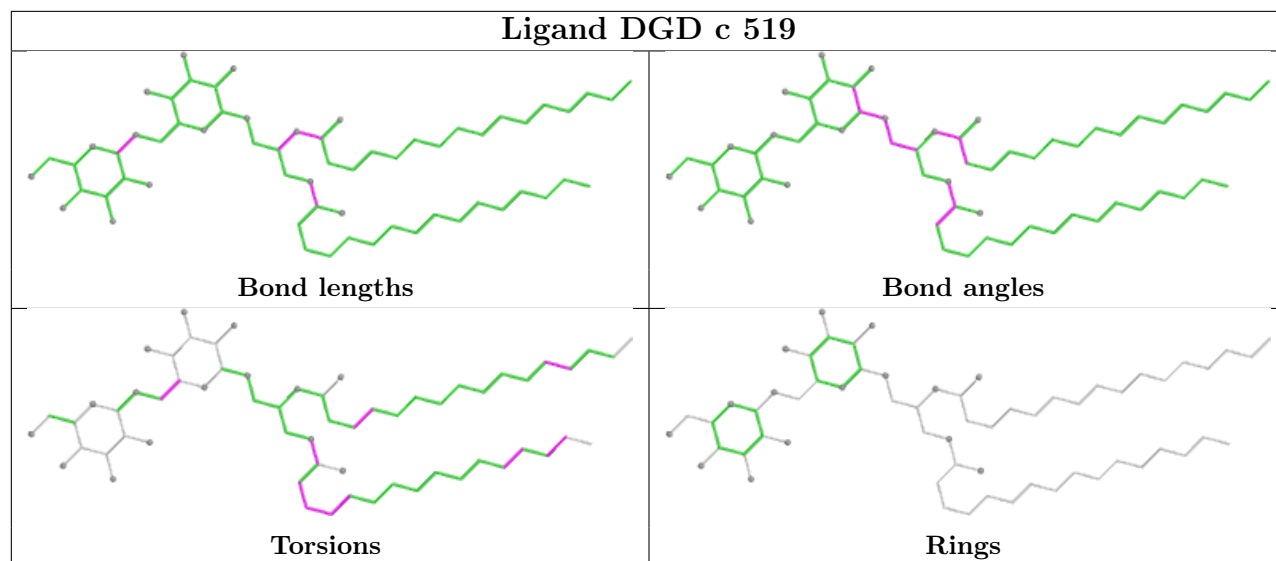




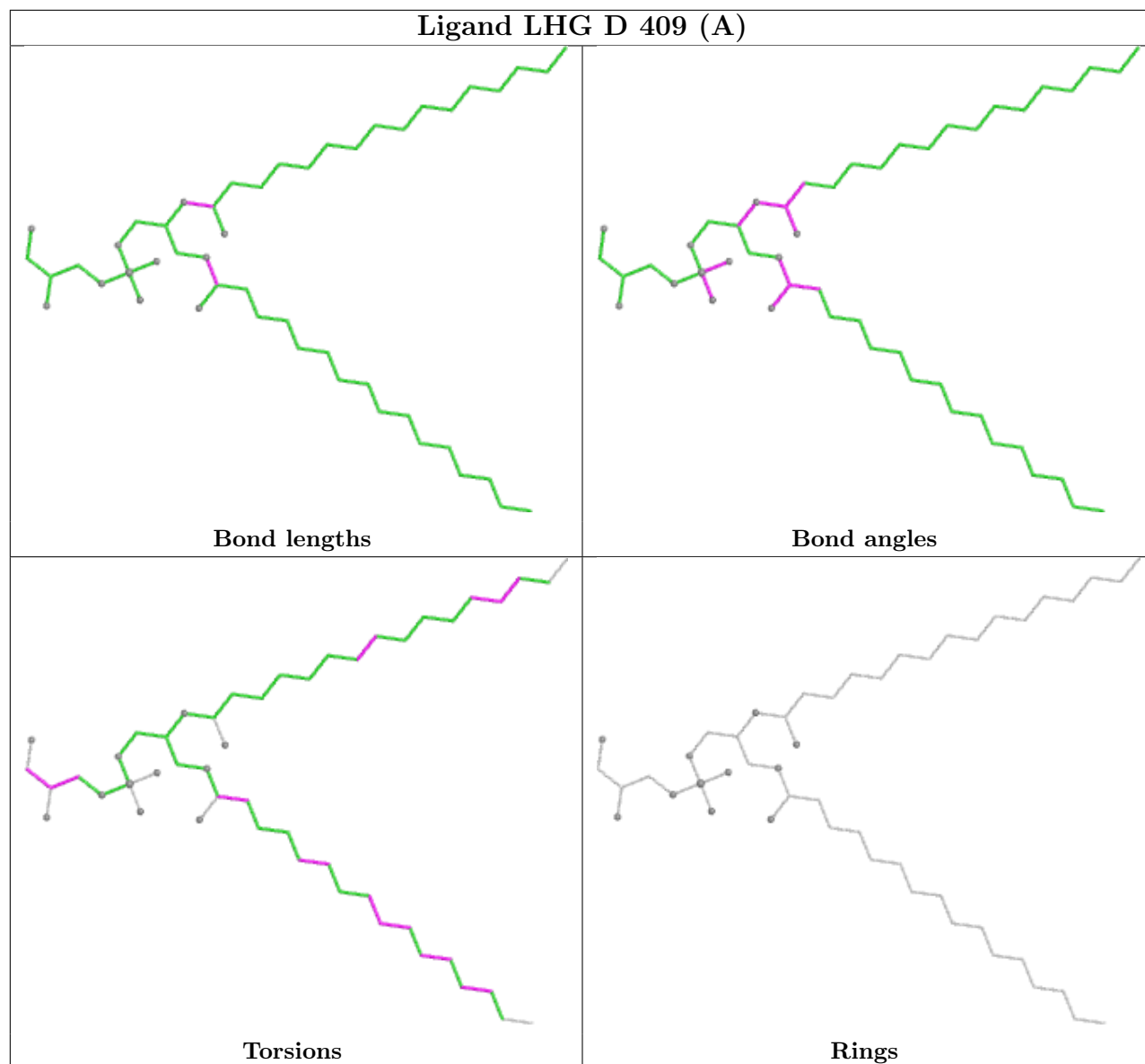




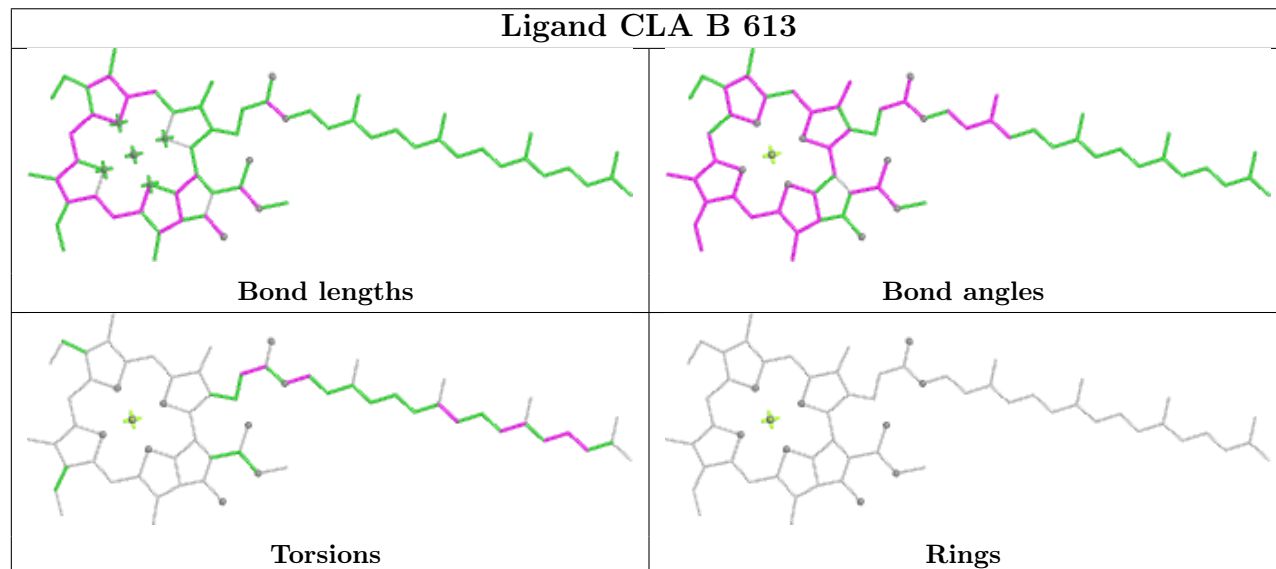


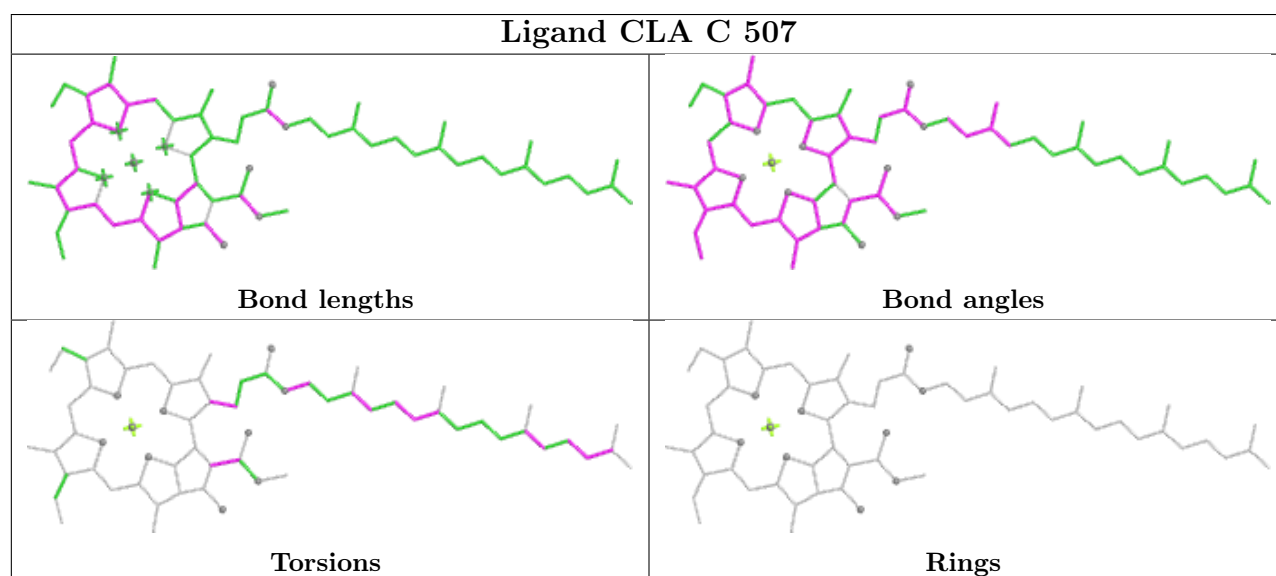
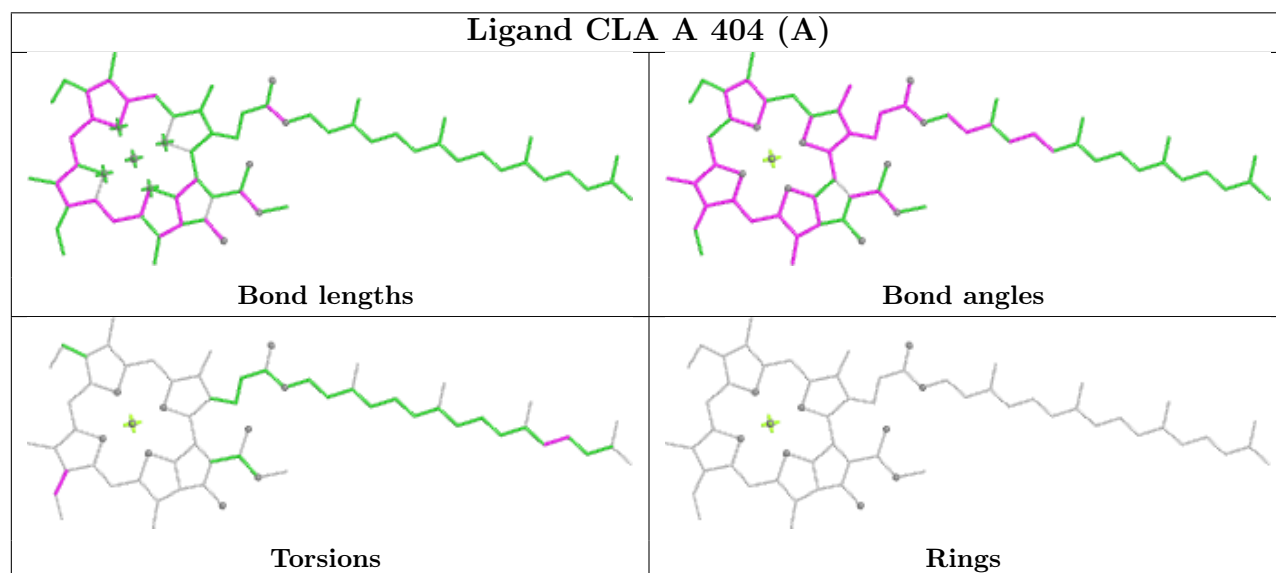
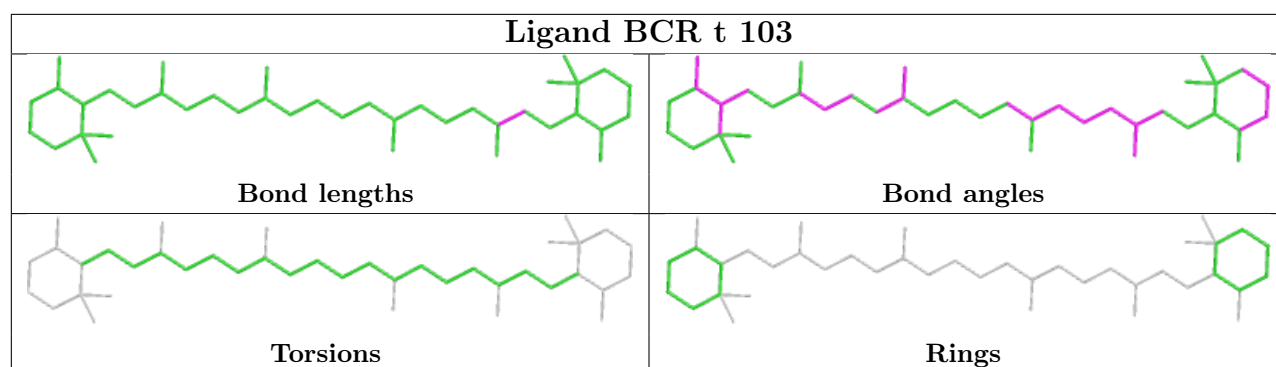


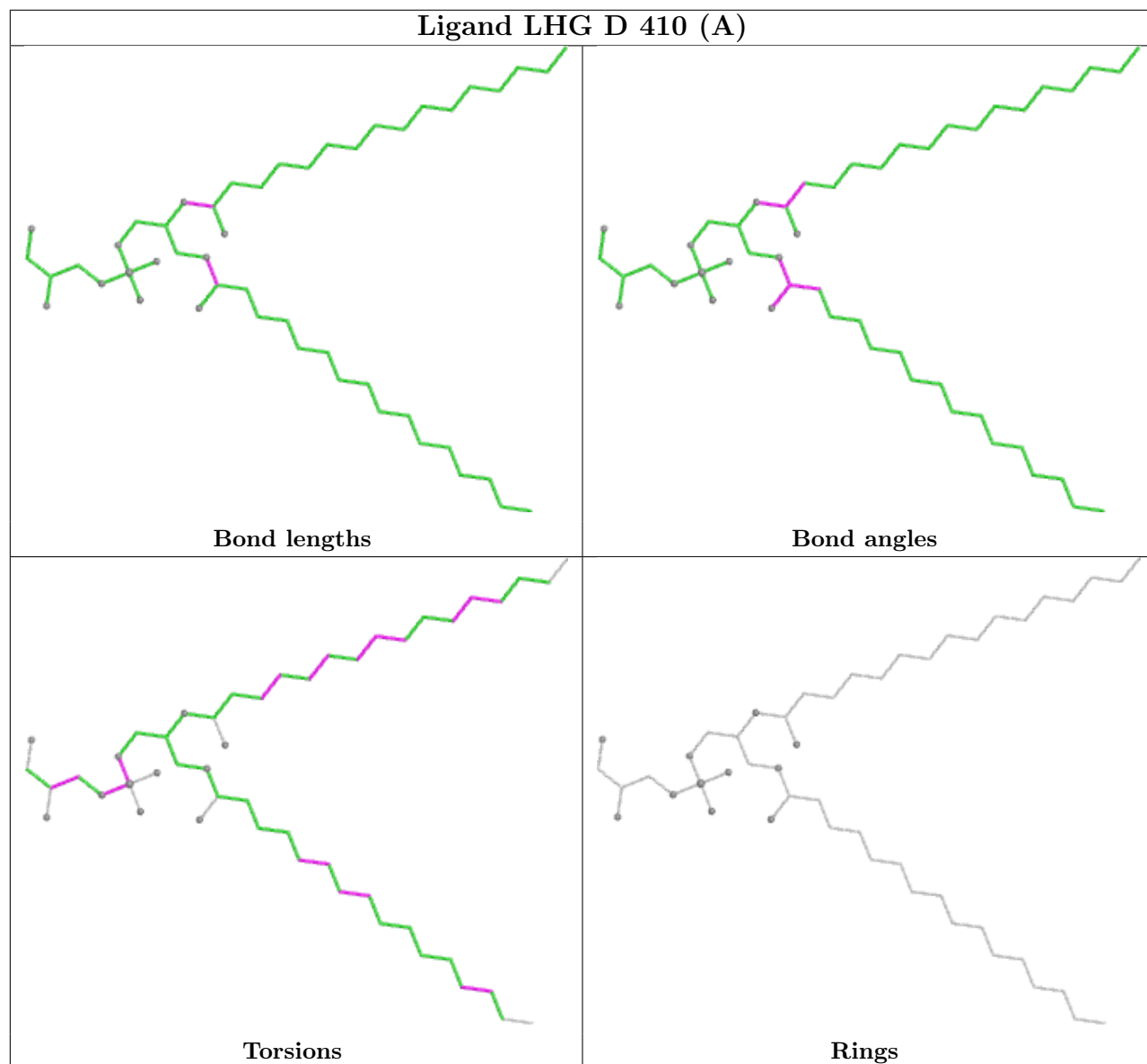
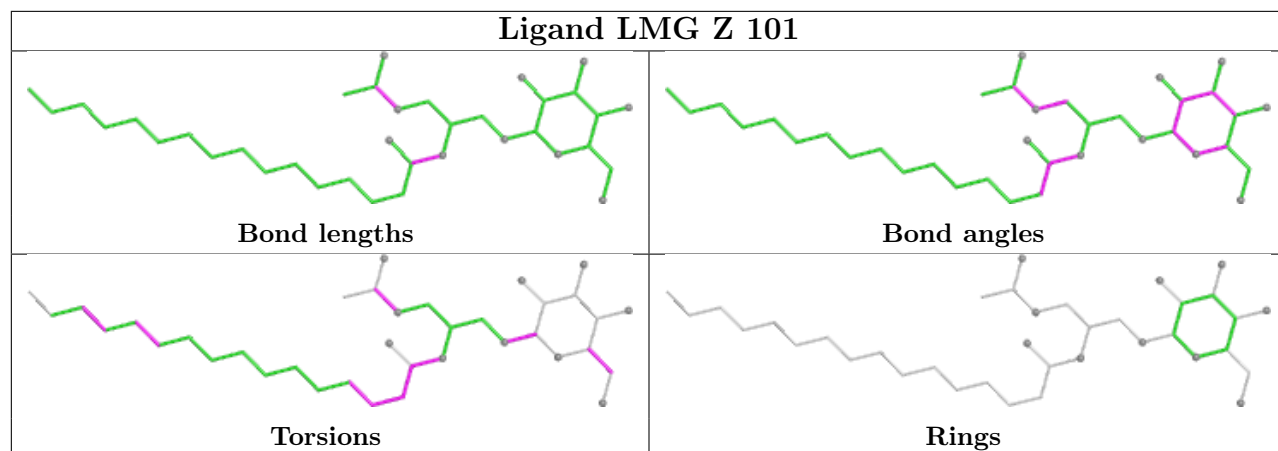
Ligand LHG D 409 (A)

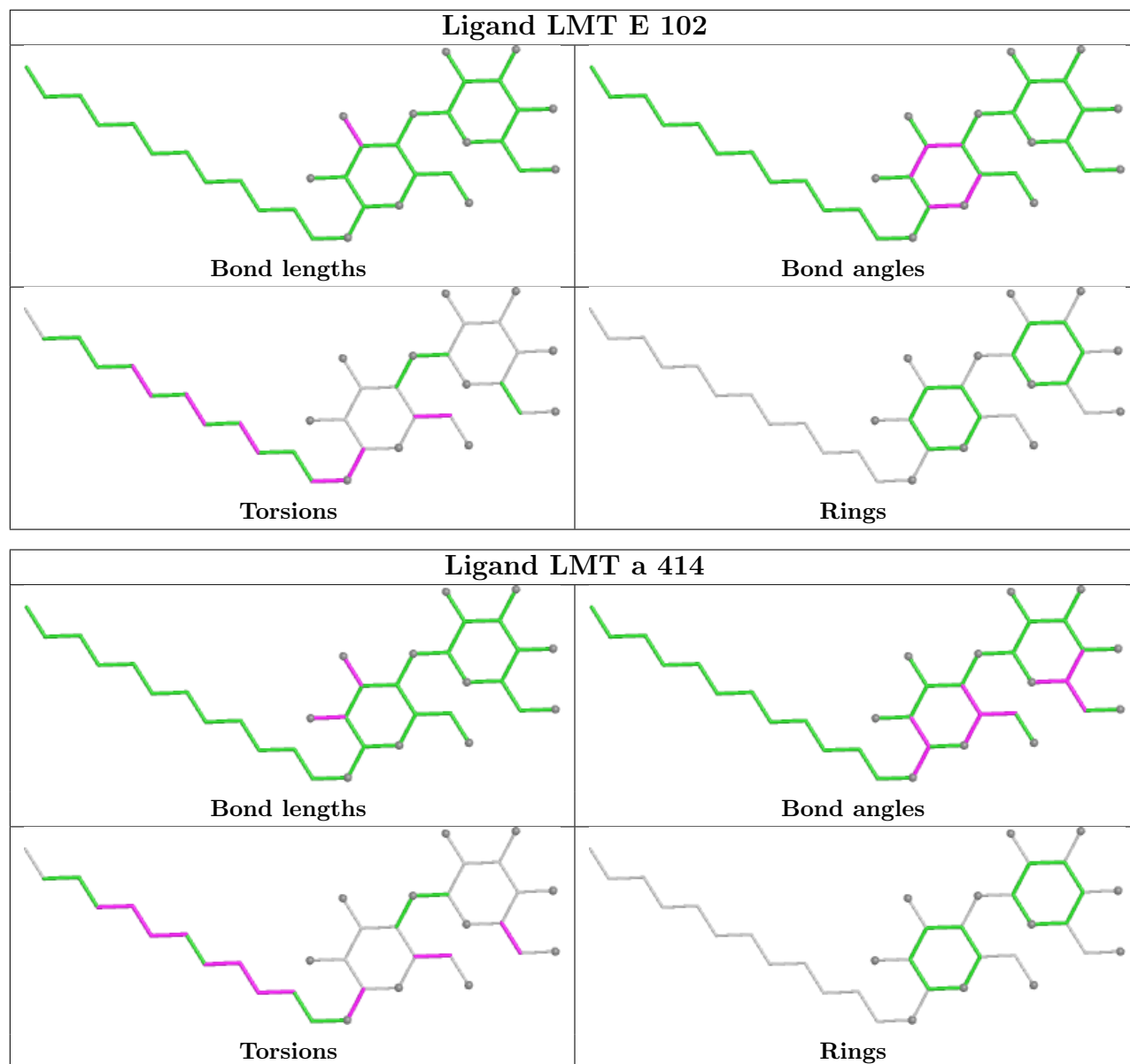


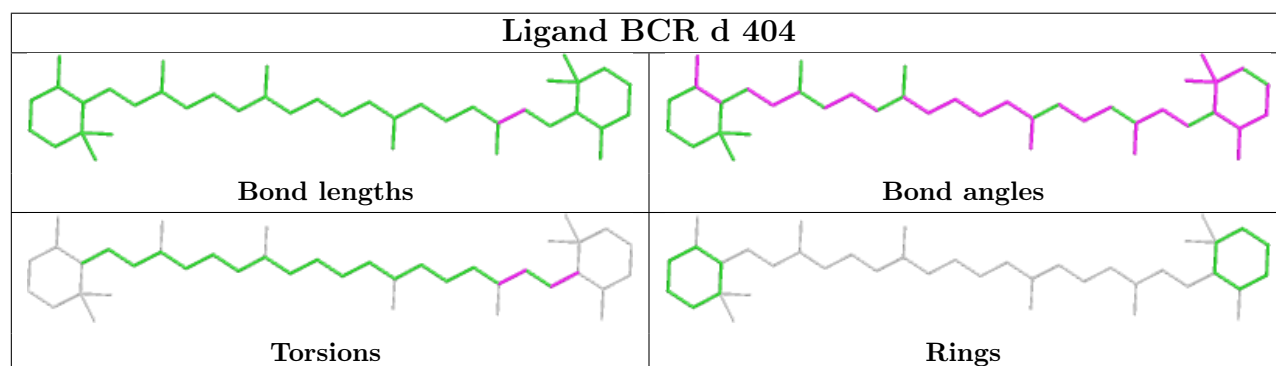
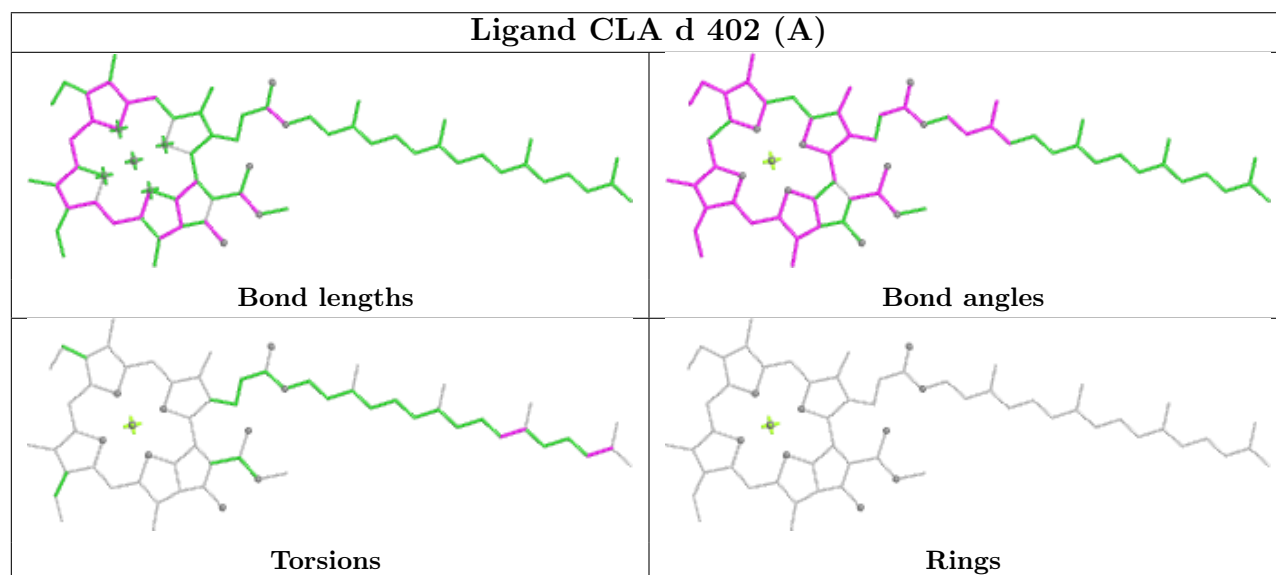
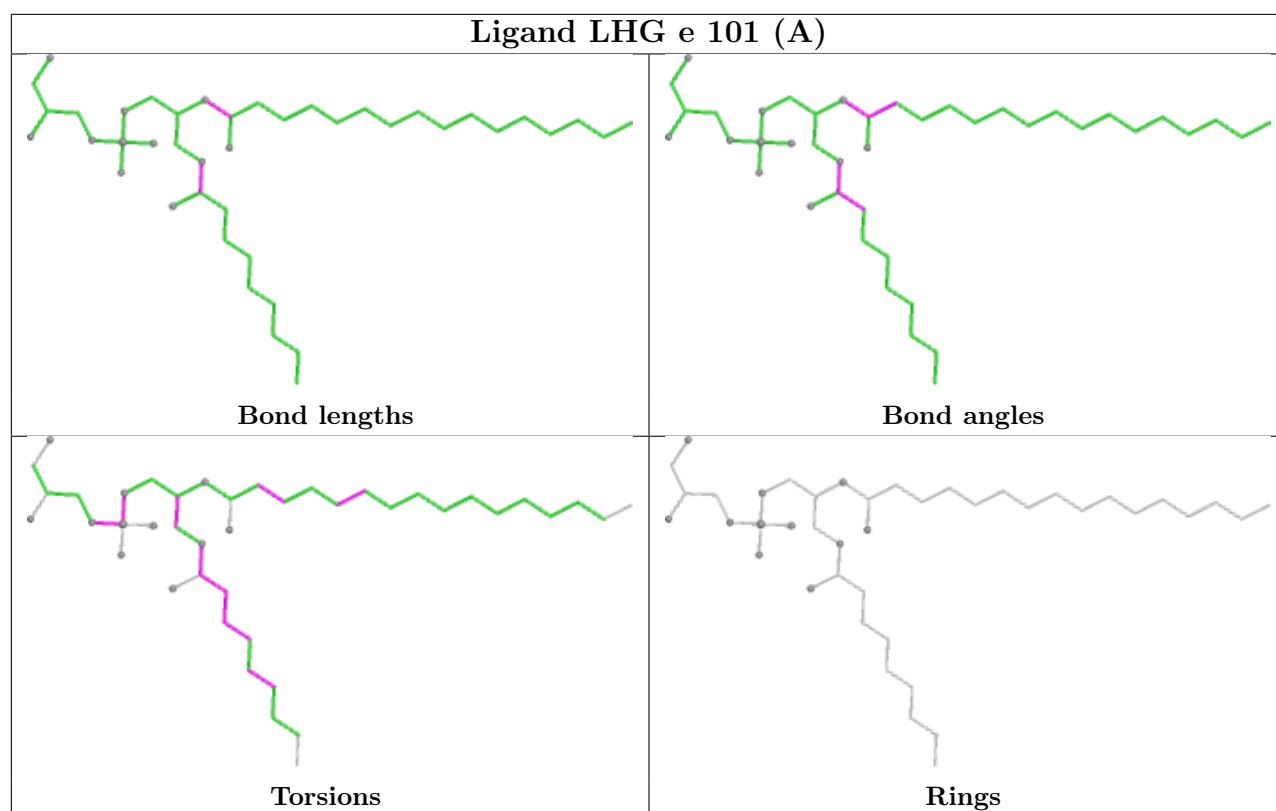
Ligand CLA B 613

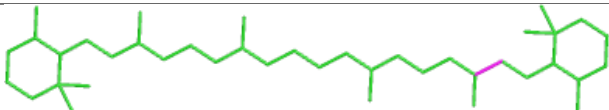
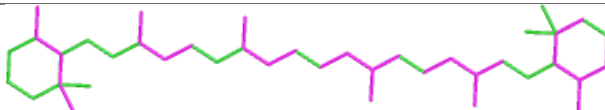
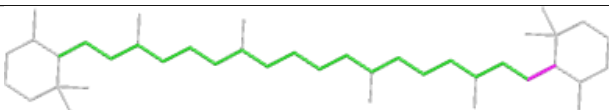
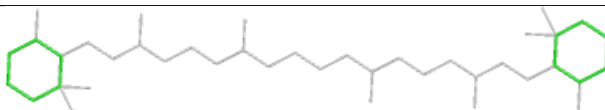


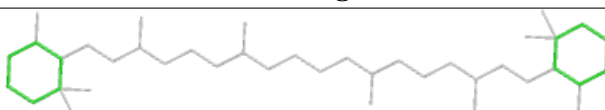


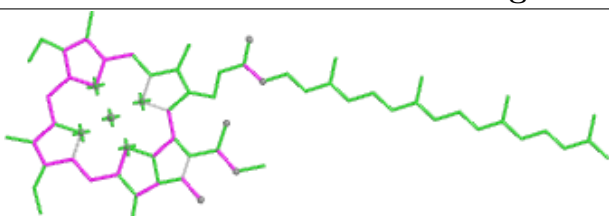
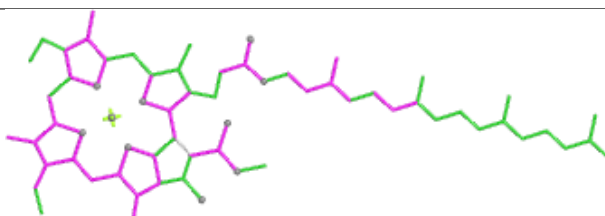
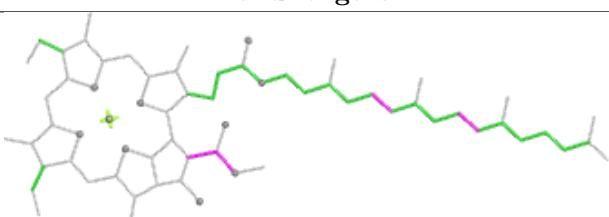
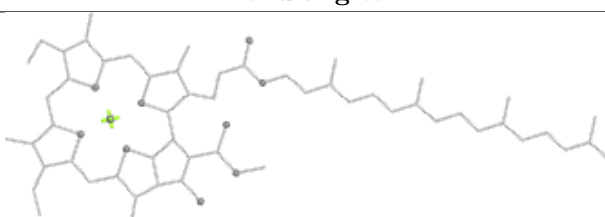


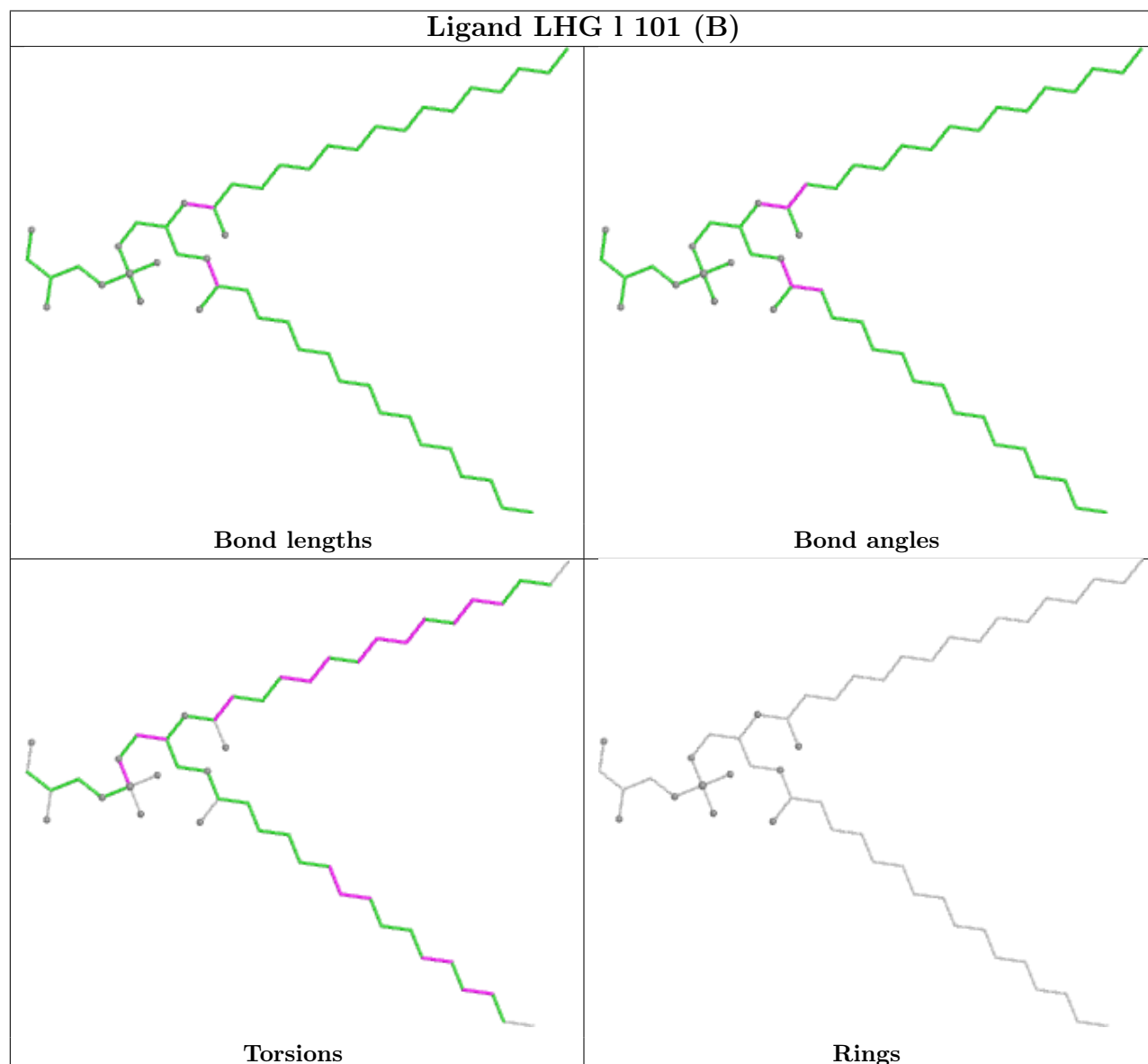
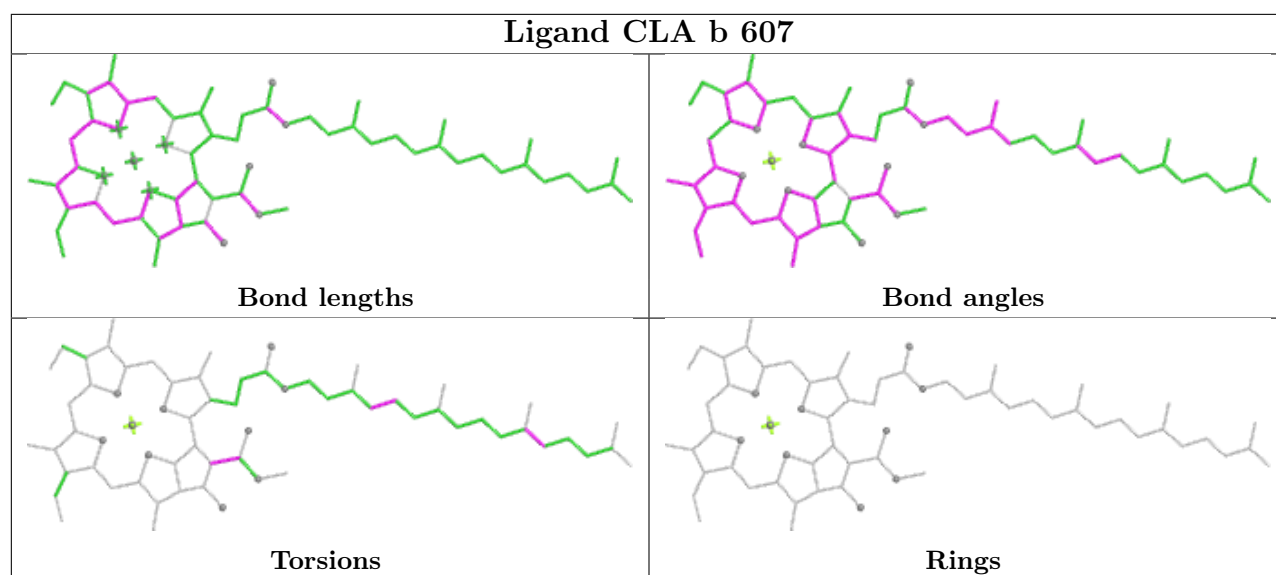


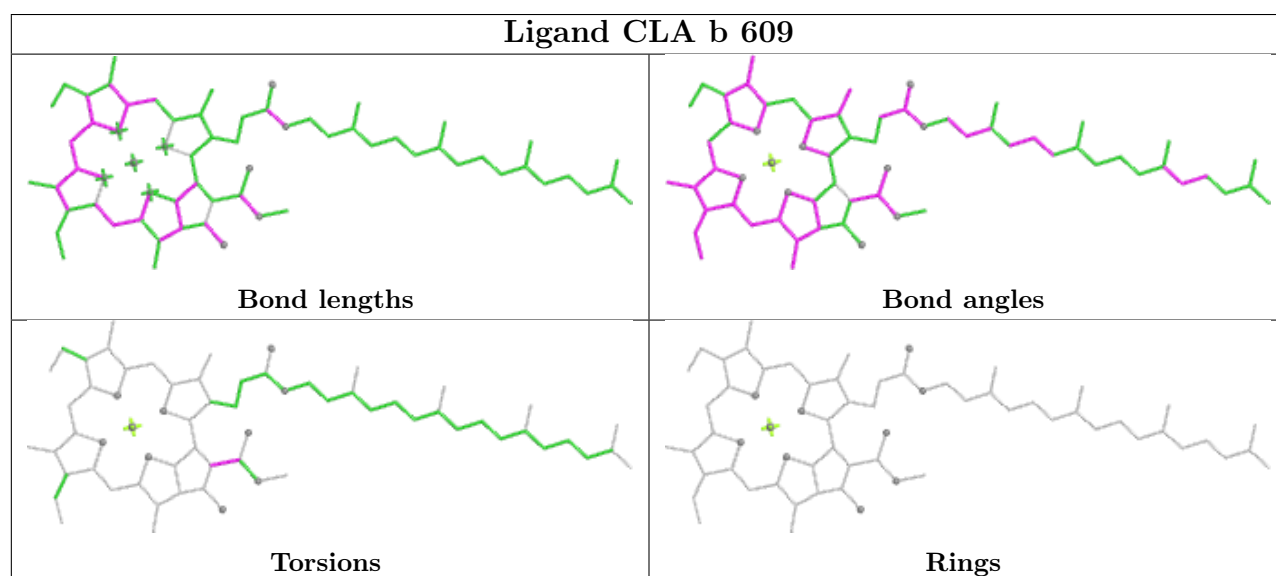
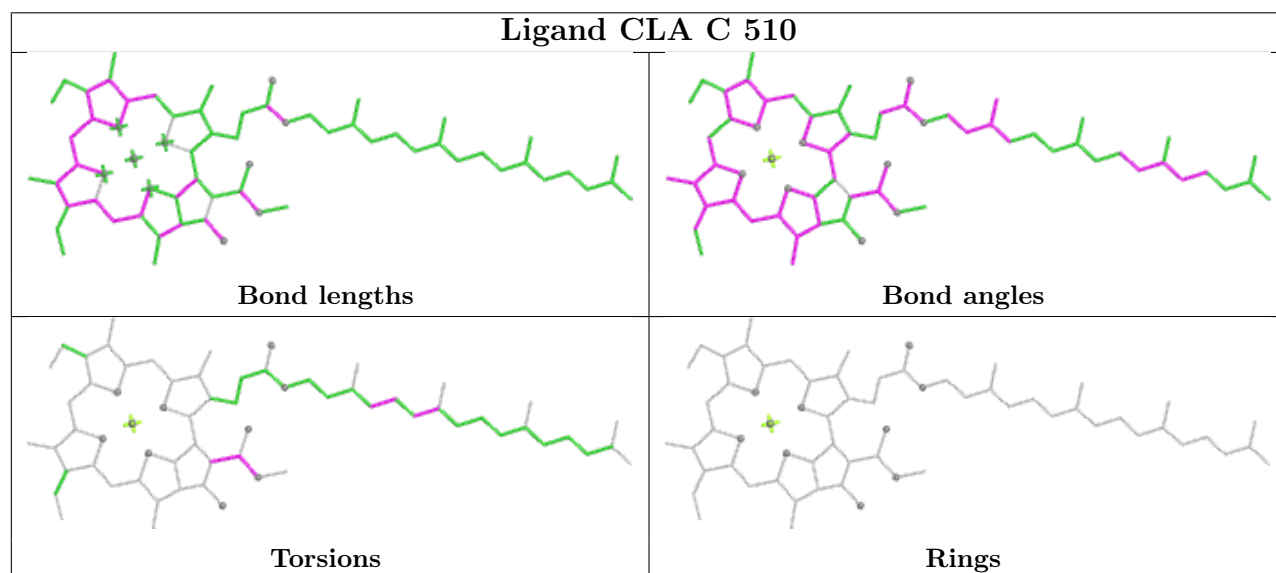
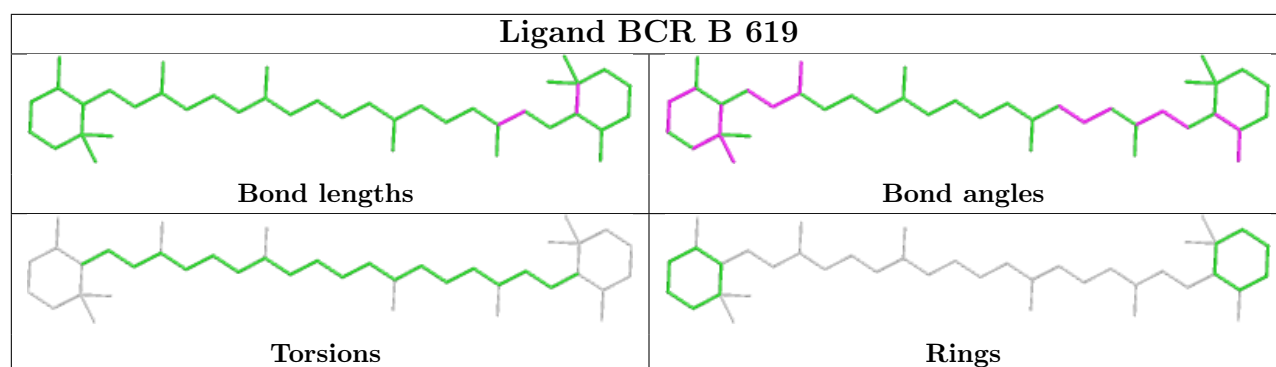


Ligand BCR c 515	
	
Bond lengths	Bond angles
	
Torsions	Rings

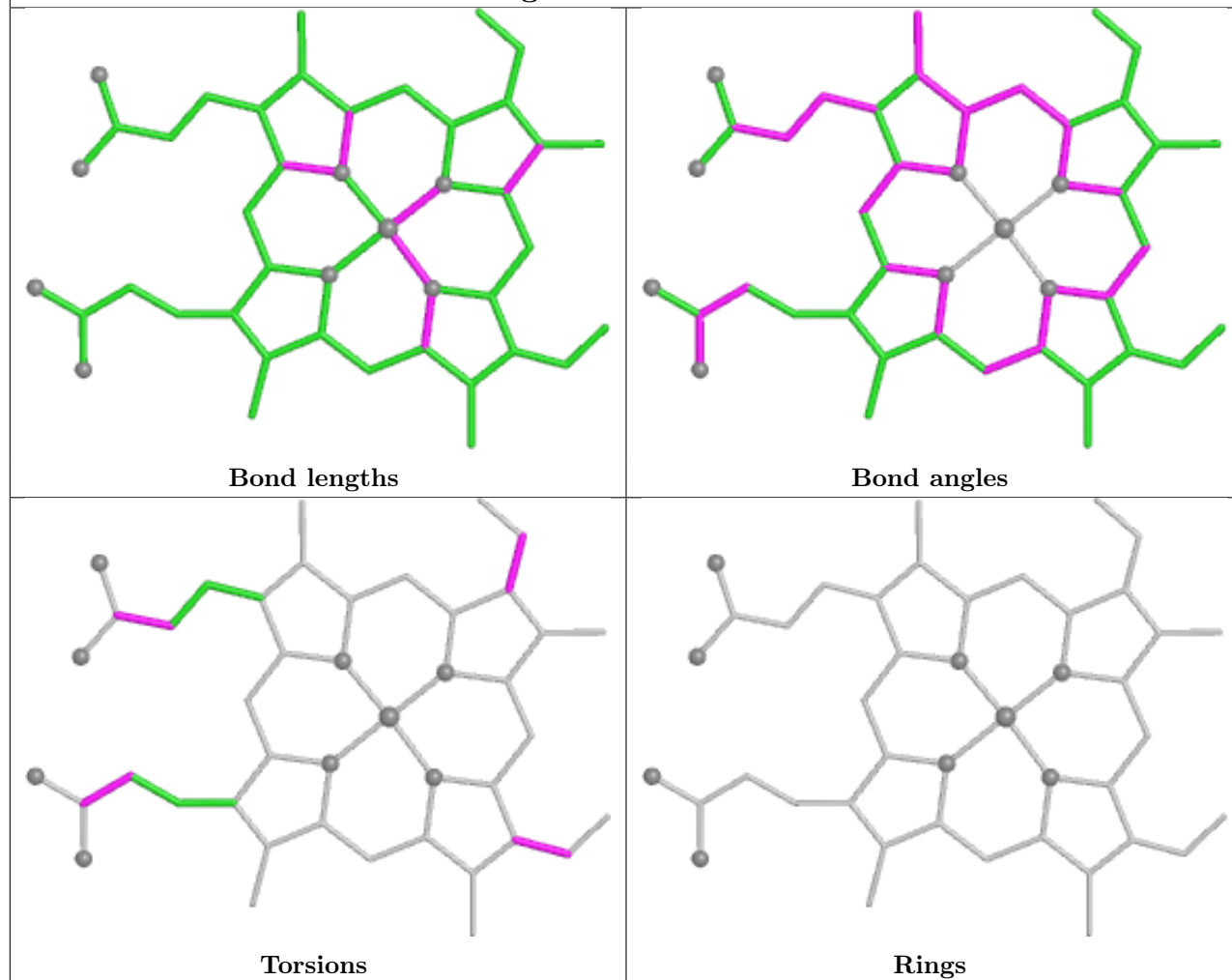
Ligand BCR A 409	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA C 509	
	
Bond lengths	Bond angles
	
Torsions	Rings

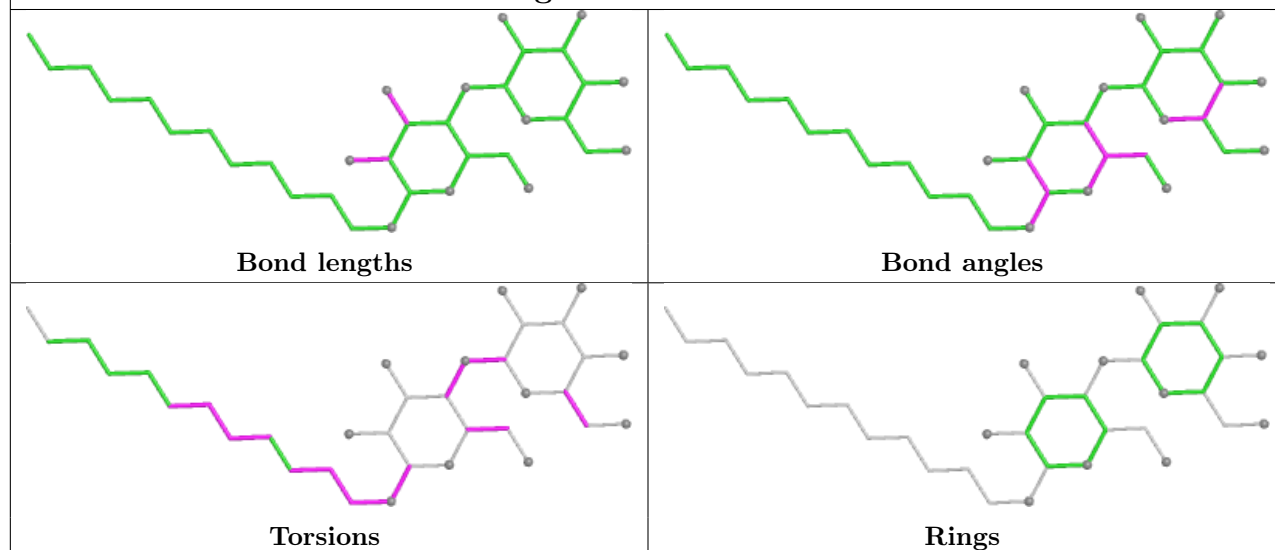


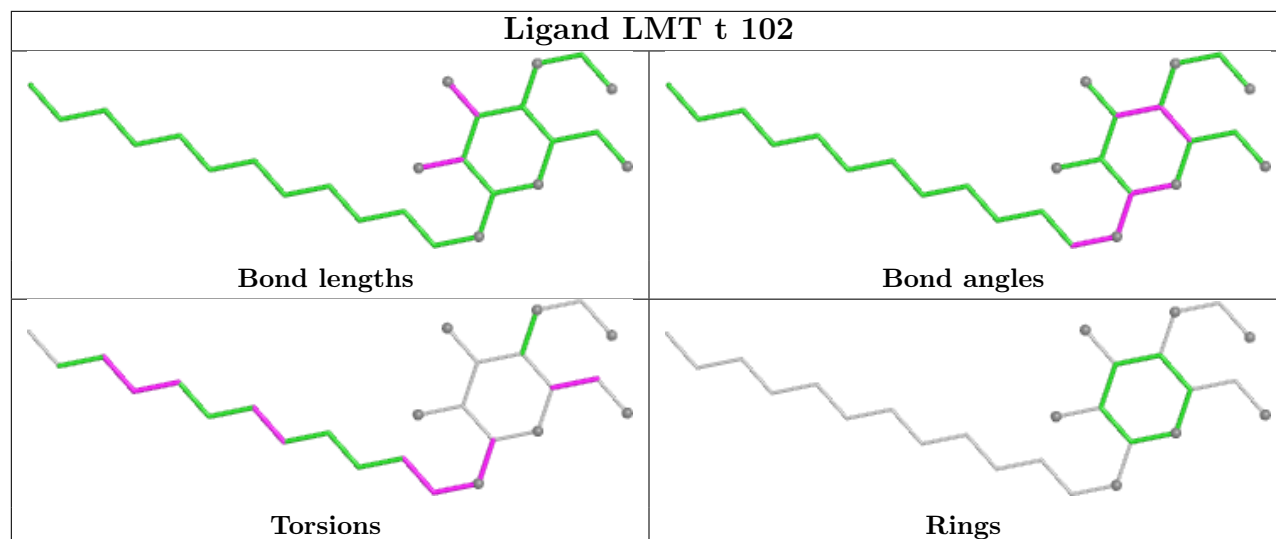


Ligand HEM e 87



Ligand LMT I 101





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	334/344 (97%)	-0.68	0 100 100	19, 25, 60, 122	222 (66%)
1	a	334/344 (97%)	-0.65	1 (0%) 90 90	20, 28, 63, 128	221 (66%)
2	B	504/505 (99%)	-0.58	1 (0%) 91 92	22, 52, 83, 114	20 (3%)
2	b	504/505 (99%)	-0.48	1 (0%) 91 92	24, 57, 100, 152	19 (3%)
3	C	451/455 (99%)	-0.58	0 100 100	21, 59, 82, 133	97 (21%)
3	c	455/455 (100%)	-0.53	1 (0%) 91 92	24, 65, 88, 127	100 (21%)
4	D	342/342 (100%)	-0.70	0 100 100	18, 44, 64, 129	114 (33%)
4	d	341/342 (99%)	-0.70	0 100 100	21, 49, 75, 127	116 (34%)
5	E	81/84 (96%)	-0.41	1 (1%) 76 77	52, 69, 97, 148	0
5	e	79/84 (94%)	-0.40	1 (1%) 75 76	33, 77, 120, 141	2 (2%)
6	F	34/44 (77%)	-0.63	0 100 100	54, 61, 91, 116	0
6	f	31/44 (70%)	-0.40	1 (3%) 50 50	54, 67, 96, 137	1 (3%)
7	H	64/65 (98%)	-0.31	1 (1%) 70 71	52, 63, 88, 112	0
7	h	64/65 (98%)	-0.37	0 100 100	40, 73, 95, 105	1 (1%)
8	I	37/38 (97%)	-0.21	0 100 100	56, 65, 121, 145	0
8	i	37/38 (97%)	-0.32	1 (2%) 56 57	55, 64, 116, 133	0
9	J	38/39 (97%)	-0.42	0 100 100	49, 67, 117, 155	0
9	j	39/39 (100%)	-0.37	0 100 100	57, 76, 132, 157	0
10	K	37/37 (100%)	-0.68	0 100 100	56, 67, 86, 103	0
10	k	37/37 (100%)	-0.53	0 100 100	64, 75, 99, 111	0
11	L	36/37 (97%)	-0.66	0 100 100	22, 44, 109, 130	2 (5%)
11	l	36/37 (97%)	-0.66	0 100 100	23, 46, 108, 119	2 (5%)
12	M	32/36 (88%)	-0.62	0 100 100	26, 47, 78, 123	1 (3%)
12	m	33/36 (91%)	-0.60	0 100 100	24, 47, 70, 137	2 (6%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/244 (99%)	-0.54	0 100 100	21, 65, 118, 161	10 (4%)
13	o	243/244 (99%)	-0.51	0 100 100	22, 69, 122, 155	8 (3%)
14	T	29/32 (90%)	-0.65	0 100 100	26, 46, 55, 67	6 (20%)
14	t	29/32 (90%)	-0.63	0 100 100	27, 47, 60, 71	5 (17%)
15	U	96/104 (92%)	-0.64	0 100 100	25, 57, 88, 100	4 (4%)
15	u	97/104 (93%)	-0.70	0 100 100	28, 61, 80, 124	4 (4%)
16	V	137/137 (100%)	-0.69	0 100 100	23, 56, 83, 107	6 (4%)
16	v	137/137 (100%)	-0.60	0 100 100	26, 71, 101, 132	6 (4%)
17	X	38/40 (95%)	-0.29	0 100 100	34, 73, 93, 114	1 (2%)
17	x	38/40 (95%)	-0.10	0 100 100	67, 80, 123, 152	0
18	Y	29/30 (96%)	-0.14	1 (3%) 48 48	68, 83, 122, 124	0
18	y	29/30 (96%)	-0.23	0 100 100	74, 91, 113, 115	0
19	Z	62/62 (100%)	-0.32	0 100 100	67, 80, 132, 148	0
19	z	62/62 (100%)	0.08	0 100 100	81, 95, 140, 165	0
20	R	34/34 (100%)	0.46	1 (2%) 53 54	87, 114, 135, 147	0
All	All	5283/5384 (98%)	-0.55	11 (0%) 91 92	18, 57, 101, 165	970 (18%)

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	H	65	LEU	4.1
5	e	79[A]	PHE	3.6
6	f	16[A]	PHE	2.9
1	a	11	ALA	2.7
3	c	245[A]	ILE	2.6

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
14	FME	T	1	10/11	0.95	0.08	42,50,63,69	0
8	FME	I	1	10/11	0.96	0.07	61,69,83,84	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	0.96	0.07	42,47,56,74	0
8	FME	i	1	10/11	0.97	0.07	59,70,80,86	0
12	FME	M	1	10/11	0.97	0.07	46,58,100,100	0
12	FME	m	1	10/11	0.98	0.07	52,61,91,116	0

6.3 Carbohydrates [\(i\)](#)

There are no oligosaccharides in this entry.

6.4 Ligands [\(i\)](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	LMT	E	102	35/35	0.65	0.15	91,128,168,171	0
30	UNL	A	415	28/-	0.70	0.13	80,104,125,143	0
30	UNL	a	417	30/-	0.70	0.12	85,108,137,149	0
27	GOL	a	701	6/6	0.70	0.16	76,98,100,110	0
30	UNL	m	102	10/-	0.71	0.19	68,73,88,96	0
30	UNL	j	101	10/-	0.71	0.17	75,87,105,106	0
30	UNL	K	101[A]	34/-	0.72	0.14	77,99,112,119	34
30	UNL	K	101[B]	34/-	0.72	0.14	77,99,112,119	34
30	UNL	J	101	10/-	0.72	0.24	70,81,89,93	0
32	LMT	I	101	35/35	0.72	0.12	89,124,145,158	0
32	LMT	a	420	35/35	0.72	0.13	102,128,153,158	0
32	LMT	e	102	35/35	0.72	0.14	105,142,178,187	0
30	UNL	I	102	40/-	0.73	0.15	75,100,151,158	0
32	LMT	a	414	35/35	0.73	0.14	63,118,143,159	0
37	LHG	e	101[A]	42/49	0.74	0.12	87,125,143,156	42
37	LHG	e	101[B]	42/49	0.74	0.12	87,125,143,157	42
26	SQD	f	102	43/54	0.75	0.12	96,127,172,187	0
34	HTG	C	522	19/19	0.75	0.12	98,125,139,139	0
30	UNL	M	102	10/-	0.76	0.16	65,74,86,91	0
27	GOL	o	501	6/6	0.77	0.18	87,100,112,126	0
32	LMT	A	359	35/35	0.77	0.12	58,115,139,142	0
30	UNL	i	101	40/-	0.78	0.13	74,103,146,164	0
27	GOL	O	601	6/6	0.78	0.15	74,91,94,104	0
30	UNL	c	525[A]	32/-	0.78	0.14	86,103,117,128	32

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	UNL	c	525[B]	32/-	0.78	0.14	86,103,117,128	32
30	UNL	b	626	33/-	0.79	0.12	67,95,148,162	0
34	HTG	D	414	16/19	0.79	0.12	89,105,139,149	0
33	LMG	C	521	51/55	0.79	0.11	59,112,155,180	0
34	HTG	B	623	19/19	0.79	0.15	64,98,120,127	0
27	GOL	o	601	6/6	0.80	0.14	79,90,95,95	0
32	LMT	b	621	25/35	0.80	0.12	80,106,154,170	0
27	GOL	d	701	6/6	0.80	0.22	49,68,78,91	0
30	UNL	D	413	40/-	0.81	0.12	64,84,131,145	0
34	HTG	b	623	19/19	0.82	0.11	85,131,161,163	0
27	GOL	B	901	6/6	0.82	0.14	63,92,105,111	0
32	LMT	M	103	35/35	0.82	0.10	64,121,173,173	0
29	PL9	a	416[A]	55/55	0.83	0.14	76,95,109,113	55
30	UNL	d	410	36/-	0.83	0.11	65,96,126,137	0
29	PL9	a	416[B]	55/55	0.83	0.14	76,95,109,113	55
34	HTG	c	522	19/19	0.83	0.09	101,122,142,144	0
36	CA	F	102	1/1	0.83	0.21	124,124,124,124	0
27	GOL	d	801[A]	6/6	0.83	0.18	63,95,101,101	6
27	GOL	d	801[B]	6/6	0.83	0.18	62,95,101,101	6
40	HEC	V	202	43/43	0.83	0.10	36,52,73,160	0
29	PL9	A	414[A]	55/55	0.84	0.13	62,86,100,105	55
34	HTG	V	203	11/19	0.84	0.10	80,115,125,142	0
29	PL9	A	414[B]	55/55	0.84	0.13	62,86,100,105	55
27	GOL	A	411	6/6	0.84	0.12	63,80,84,85	0
32	LMT	D	404	35/35	0.85	0.11	66,111,146,151	0
26	SQD	a	413	54/54	0.85	0.09	66,92,138,151	0
32	LMT	t	102	26/35	0.85	0.11	68,101,136,149	0
34	HTG	d	411	16/19	0.85	0.10	88,119,142,147	0
27	GOL	v	401[A]	6/6	0.85	0.13	64,80,82,84	6
27	GOL	v	401[B]	6/6	0.85	0.13	64,80,82,84	6
27	GOL	O	501	6/6	0.85	0.09	77,92,105,105	0
30	UNL	B	627	33/-	0.85	0.13	53,105,143,149	0
26	SQD	A	412	54/54	0.86	0.10	61,86,126,153	0
27	GOL	b	624	6/6	0.86	0.14	87,95,105,108	0
33	LMG	c	521	51/55	0.86	0.10	77,128,157,190	0
32	LMT	b	627	25/35	0.86	0.12	54,96,143,150	0
27	GOL	c	743	6/6	0.86	0.16	99,103,109,114	0
32	LMT	m	103	35/35	0.86	0.11	61,93,108,119	0
32	LMT	t	101	25/35	0.86	0.12	58,84,141,151	0
33	LMG	z	101	39/55	0.87	0.11	74,123,146,161	0
33	LMG	Z	101	37/55	0.87	0.12	68,117,149,168	0
27	GOL	a	801	6/6	0.88	0.26	52,76,81,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
34	HTG	b	622	19/19	0.88	0.11	59,85,118,122	0
32	LMT	M	101	35/35	0.88	0.10	58,103,129,138	0
37	LHG	E	101[A]	42/49	0.89	0.10	71,98,113,121	42
37	LHG	E	101[B]	42/49	0.89	0.10	71,98,113,121	42
26	SQD	F	101	43/54	0.89	0.11	69,103,128,137	0
26	SQD	B	620	54/54	0.89	0.09	60,89,130,150	0
26	SQD	b	620	54/54	0.89	0.09	59,92,120,132	0
23	CLA	b	601	65/65	0.90	0.09	64,87,123,160	0
34	HTG	B	622	19/19	0.90	0.11	63,81,124,126	0
30	UNL	D	412	17/-	0.90	0.10	58,77,99,114	0
27	GOL	a	412	6/6	0.90	0.11	75,77,87,92	0
36	CA	o	301	1/1	0.91	0.07	116,116,116,116	0
23	CLA	B	601	65/65	0.91	0.09	55,79,111,156	0
27	GOL	A	701	6/6	0.91	0.25	49,73,80,83	0
33	LMG	C	501	51/55	0.91	0.09	64,89,115,129	0
34	HTG	B	626	19/19	0.91	0.07	67,81,97,106	0
36	CA	f	103	1/1	0.91	0.12	124,124,124,124	0
33	LMG	a	419	51/55	0.92	0.08	67,94,110,121	0
33	LMG	c	520	51/55	0.92	0.09	59,90,130,156	0
27	GOL	V	401[B]	6/6	0.92	0.12	59,67,73,77	6
33	LMG	m	101	51/55	0.92	0.08	47,73,96,109	0
23	CLA	c	514	65/65	0.92	0.09	69,95,119,147	0
33	LMG	B	621	51/55	0.92	0.08	47,68,91,111	0
27	GOL	V	401[A]	6/6	0.92	0.12	59,67,73,76	6
30	UNL	d	409	17/-	0.92	0.09	64,79,116,123	0
33	LMG	C	520	51/55	0.93	0.09	54,84,115,125	0
35	DGD	C	518[A]	62/66	0.93	0.08	48,63,108,112	62
35	DGD	C	518[B]	62/66	0.93	0.08	48,63,108,112	62
27	GOL	C	523[B]	6/6	0.93	0.09	57,62,65,66	6
33	LMG	D	415	51/55	0.93	0.09	49,66,117,139	0
27	GOL	D	701	6/6	0.93	0.15	45,60,70,92	0
23	CLA	C	514	65/65	0.93	0.08	62,88,111,123	0
25	BCR	T	101	40/40	0.93	0.07	43,58,69,69	0
27	GOL	B	624	6/6	0.93	0.08	65,73,81,84	0
25	BCR	d	404	40/40	0.93	0.08	48,65,105,108	0
27	GOL	C	523[A]	6/6	0.93	0.09	58,61,64,67	6
23	CLA	C	507	65/65	0.94	0.08	54,70,121,141	0
25	BCR	C	515	40/40	0.94	0.08	53,77,89,90	0
25	BCR	D	407	40/40	0.94	0.08	43,58,100,103	0
26	SQD	a	411[A]	54/54	0.94	0.09	56,80,112,121	54
34	HTG	b	625	19/19	0.94	0.07	62,76,93,109	0
26	SQD	a	411[B]	54/54	0.94	0.09	56,80,112,121	54

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	CLA	b	616	65/65	0.94	0.08	48,63,124,134	0
30	UNL	X	101	18/-	0.94	0.10	56,71,105,107	0
25	BCR	Y	101	40/40	0.94	0.08	52,64,83,87	0
35	DGD	c	518[A]	62/66	0.94	0.07	54,67,113,129	62
35	DGD	c	518[B]	62/66	0.94	0.07	54,67,113,129	62
33	LMG	d	412	51/55	0.94	0.08	53,73,117,144	0
25	BCR	c	515	40/40	0.94	0.08	69,84,96,97	0
23	CLA	c	513	65/65	0.94	0.09	59,82,121,133	0
37	LHG	D	409[A]	49/49	0.94	0.08	46,61,83,87	49
37	LHG	D	409[B]	49/49	0.94	0.08	46,61,83,87	49
37	LHG	D	411[A]	49/49	0.94	0.09	47,61,105,108	49
37	LHG	D	411[B]	49/49	0.94	0.09	47,60,105,108	49
25	BCR	t	103	40/40	0.94	0.06	43,58,77,81	0
26	SQD	A	410[A]	54/54	0.94	0.08	57,78,112,116	54
27	GOL	c	742[A]	6/6	0.94	0.07	64,66,75,76	6
27	GOL	c	742[B]	6/6	0.94	0.07	65,66,75,76	6
26	SQD	A	410[B]	54/54	0.94	0.08	57,78,112,116	54
23	CLA	c	508	65/65	0.95	0.08	56,69,85,90	0
23	CLA	C	505	65/65	0.95	0.07	40,55,102,129	0
23	CLA	A	408	65/65	0.95	0.08	38,52,127,140	0
23	CLA	d	403	65/65	0.95	0.08	50,68,116,148	0
25	BCR	A	409	40/40	0.95	0.07	37,50,63,66	0
25	BCR	B	618	40/40	0.95	0.05	40,52,67,75	0
25	BCR	B	619	40/40	0.95	0.07	48,58,88,99	0
23	CLA	C	509	65/65	0.95	0.07	47,56,116,149	0
29	PL9	D	408[A]	55/55	0.95	0.06	37,47,59,70	55
29	PL9	D	408[B]	55/55	0.95	0.06	37,47,59,71	55
23	CLA	C	513	65/65	0.95	0.08	59,78,111,125	0
25	BCR	H	101	40/40	0.95	0.08	52,66,86,89	0
25	BCR	K	102	40/40	0.95	0.08	57,66,83,86	0
23	CLA	B	606	65/65	0.95	0.07	41,55,101,128	0
35	DGD	C	519	62/66	0.95	0.07	42,58,93,111	0
35	DGD	H	102	62/66	0.95	0.08	42,61,79,101	0
35	DGD	c	517[A]	62/66	0.95	0.07	50,65,99,106	62
35	DGD	c	517[B]	62/66	0.95	0.07	50,65,99,106	62
23	CLA	a	407[A]	65/65	0.95	0.07	38,51,119,128	65
25	BCR	a	410	40/40	0.95	0.07	44,54,61,69	0
35	DGD	c	519	62/66	0.95	0.07	49,64,99,125	0
25	BCR	b	619	40/40	0.95	0.07	51,62,88,91	0
23	CLA	a	407[B]	65/65	0.95	0.07	38,51,119,128	65
23	CLA	a	409	65/65	0.95	0.09	44,57,138,156	0
25	BCR	h	101	40/40	0.95	0.09	59,73,94,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	BCR	k	101	40/40	0.95	0.09	60,73,90,92	0
23	CLA	B	614	65/65	0.95	0.07	36,48,103,127	0
25	BCR	y	101	40/40	0.95	0.07	58,70,85,97	0
27	GOL	b	901	6/6	0.95	0.07	78,79,83,88	0
23	CLA	b	614	65/65	0.95	0.07	40,51,102,120	0
37	LHG	d	408[A]	49/49	0.95	0.08	50,62,109,125	49
37	LHG	d	408[B]	49/49	0.95	0.08	50,62,109,125	49
37	LHG	d	711[A]	49/49	0.95	0.08	46,67,80,89	49
37	LHG	d	711[B]	49/49	0.95	0.08	45,67,80,89	49
23	CLA	B	616	65/65	0.95	0.08	41,58,131,139	0
23	CLA	c	505	65/65	0.95	0.07	50,63,108,146	0
37	LHG	l	101[A]	49/49	0.95	0.08	48,58,72,93	49
37	LHG	l	101[B]	49/49	0.95	0.08	48,57,72,93	49
23	CLA	c	507	65/65	0.95	0.08	51,68,125,135	0
23	CLA	A	406[B]	65/65	0.96	0.06	38,47,110,122	65
25	BCR	B	617	40/40	0.96	0.06	40,49,62,66	0
23	CLA	A	404[A]	65/65	0.96	0.06	35,41,58,68	65
23	CLA	C	502	65/65	0.96	0.07	47,61,74,84	0
35	DGD	C	517[A]	62/66	0.96	0.06	44,58,99,101	62
35	DGD	C	517[B]	62/66	0.96	0.06	44,58,99,101	62
23	CLA	b	602	65/65	0.96	0.07	50,60,82,92	0
23	CLA	b	604	65/65	0.96	0.07	41,52,96,119	0
23	CLA	b	606	65/65	0.96	0.07	44,61,120,133	0
29	PL9	d	405[A]	55/55	0.96	0.06	37,49,61,72	55
29	PL9	d	405[B]	55/55	0.96	0.06	36,49,61,72	55
23	CLA	b	607	65/65	0.96	0.06	37,46,79,94	0
23	CLA	b	611	65/65	0.96	0.06	37,48,71,81	0
23	CLA	b	612	65/65	0.96	0.07	44,53,68,81	0
23	CLA	A	404[B]	65/65	0.96	0.06	35,42,60,68	65
35	DGD	h	102	62/66	0.96	0.07	51,66,81,95	0
25	BCR	b	617	40/40	0.96	0.05	45,52,61,70	0
36	CA	O	301	1/1	0.96	0.05	105,105,105,105	0
25	BCR	b	618	40/40	0.96	0.06	44,58,75,87	0
23	CLA	B	602	65/65	0.96	0.07	46,58,75,94	0
23	CLA	c	502	65/65	0.96	0.07	56,67,80,86	0
25	BCR	c	516	40/40	0.96	0.06	57,67,80,96	0
37	LHG	D	410[A]	49/49	0.96	0.07	43,54,67,76	49
37	LHG	D	410[B]	49/49	0.96	0.07	43,54,66,76	49
23	CLA	c	504	65/65	0.96	0.07	48,70,86,92	0
23	CLA	C	508	65/65	0.96	0.08	50,63,82,93	0
23	CLA	c	506	65/65	0.96	0.07	50,64,92,101	0
23	CLA	B	603	65/65	0.96	0.07	40,53,74,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
37	LHG	d	407[A]	49/49	0.96	0.07	45,55,67,79	49
37	LHG	d	407[B]	49/49	0.96	0.07	45,56,68,79	49
23	CLA	A	406[A]	65/65	0.96	0.06	38,47,110,122	65
23	CLA	c	509	65/65	0.96	0.07	46,63,125,155	0
23	CLA	c	512	65/65	0.96	0.07	56,70,89,101	0
23	CLA	B	609	65/65	0.96	0.07	50,59,72,83	0
23	CLA	D	406	65/65	0.96	0.07	46,59,123,146	0
23	CLA	B	611	65/65	0.96	0.07	34,44,64,73	0
30	UNL	x	101	18/-	0.96	0.10	70,76,127,129	0
24	PHO	a	353[A]	64/64	0.96	0.06	43,54,61,66	64
24	PHO	a	353[B]	64/64	0.96	0.06	43,54,61,66	64
24	PHO	A	353[A]	64/64	0.97	0.05	38,48,54,62	64
24	PHO	A	353[B]	64/64	0.97	0.05	38,48,54,61	64
24	PHO	a	408[A]	64/64	0.97	0.05	38,47,55,57	64
24	PHO	a	408[B]	64/64	0.97	0.05	38,47,55,57	64
23	CLA	A	405[A]	65/65	0.97	0.05	32,42,54,71	65
23	CLA	B	607	65/65	0.97	0.06	36,45,72,86	0
23	CLA	C	503	65/65	0.97	0.06	44,54,80,92	0
23	CLA	C	504	65/65	0.97	0.06	48,61,73,79	0
23	CLA	b	603	65/65	0.97	0.06	43,56,81,93	0
23	CLA	B	608	65/65	0.97	0.05	37,48,69,74	0
23	CLA	b	605	65/65	0.97	0.06	38,50,77,79	0
25	BCR	C	516	40/40	0.97	0.06	52,66,77,90	0
31	BCT	A	348[A]	4/4	0.97	0.06	51,52,58,68	4
31	BCT	A	348[B]	4/4	0.97	0.06	51,52,58,69	4
31	BCT	a	404[A]	4/4	0.97	0.06	55,58,67,76	4
31	BCT	a	404[B]	4/4	0.97	0.06	55,58,67,76	4
23	CLA	C	506	65/65	0.97	0.06	45,61,88,104	0
23	CLA	A	405[B]	65/65	0.97	0.05	33,42,54,71	65
23	CLA	b	609	65/65	0.97	0.06	52,66,84,94	0
23	CLA	b	610	65/65	0.97	0.07	47,58,69,74	0
23	CLA	B	610	65/65	0.97	0.07	39,54,66,83	0
36	CA	C	524	1/1	0.97	0.05	77,77,77,77	0
23	CLA	B	604	65/65	0.97	0.06	36,47,112,136	0
23	CLA	b	613	65/65	0.97	0.05	39,50,88,105	0
36	CA	c	523	1/1	0.97	0.08	78,78,78,78	0
23	CLA	C	510	65/65	0.97	0.07	45,58,82,88	0
23	CLA	b	615	65/65	0.97	0.06	52,62,83,88	0
23	CLA	C	511	65/65	0.97	0.06	48,57,79,89	0
23	CLA	C	512	65/65	0.97	0.07	51,62,81,87	0
23	CLA	c	503	65/65	0.97	0.06	44,59,90,102	0
23	CLA	B	612	65/65	0.97	0.06	34,49,60,66	0

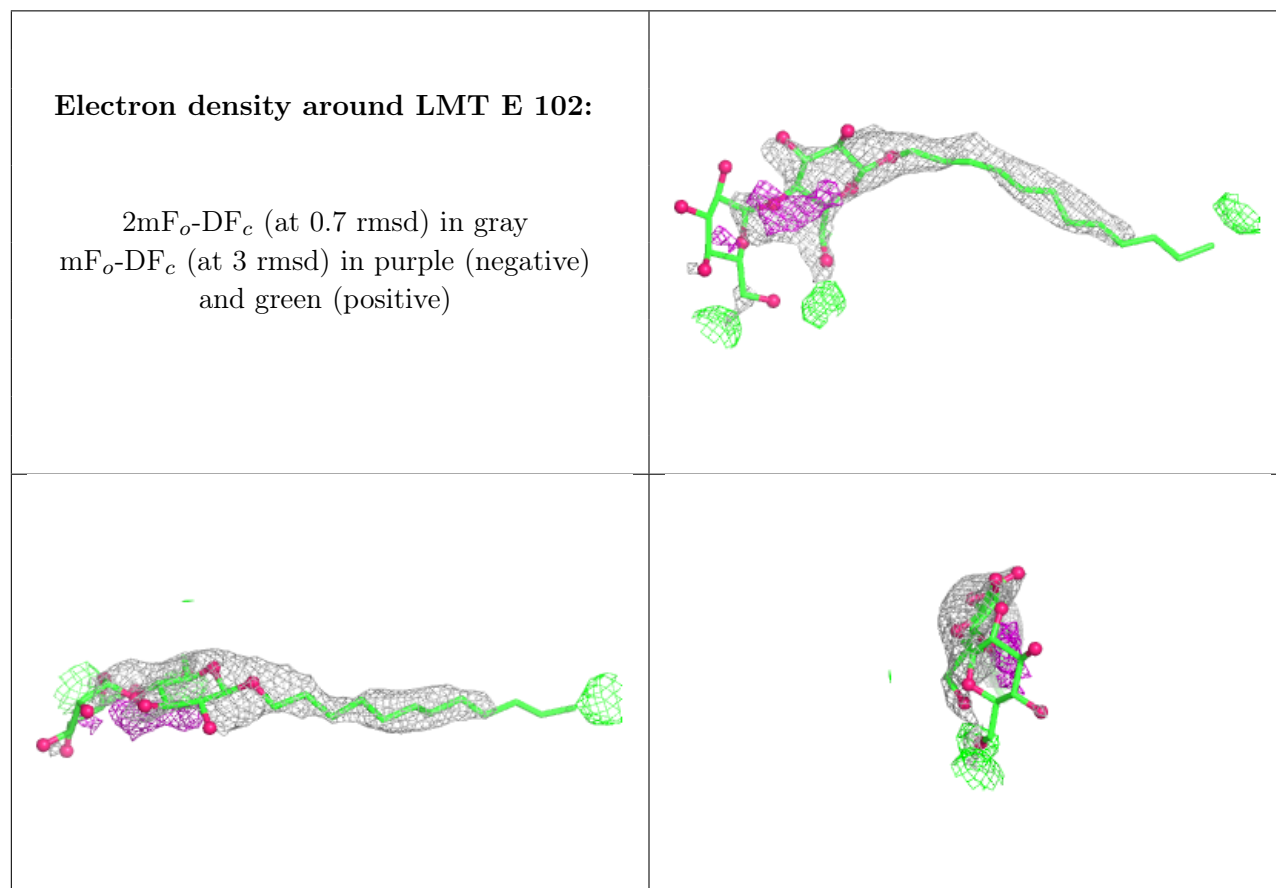
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	CLA	B	613	65/65	0.97	0.06	36,45,98,113	0
23	CLA	D	405[A]	65/65	0.97	0.06	32,43,68,76	65
23	CLA	D	405[B]	65/65	0.97	0.06	32,43,68,76	65
23	CLA	B	605	65/65	0.97	0.06	39,48,67,83	0
37	LHG	L	101[A]	49/49	0.97	0.06	45,55,66,88	49
37	LHG	L	101[B]	49/49	0.97	0.06	45,55,66,88	49
23	CLA	a	405[A]	65/65	0.97	0.06	33,44,60,74	65
23	CLA	c	510	65/65	0.97	0.07	46,61,90,95	0
23	CLA	c	511	65/65	0.97	0.06	47,63,79,93	0
23	CLA	a	405[B]	65/65	0.97	0.06	38,44,62,74	65
23	CLA	a	406[A]	65/65	0.97	0.05	36,43,59,68	65
23	CLA	a	406[B]	65/65	0.97	0.05	36,43,59,68	65
23	CLA	d	402[A]	65/65	0.97	0.06	36,45,72,89	65
23	CLA	d	402[B]	65/65	0.97	0.06	36,45,72,89	65
23	CLA	B	615	65/65	0.97	0.06	42,54,79,90	0
24	PHO	A	407[A]	64/64	0.97	0.04	35,45,50,56	64
24	PHO	A	407[B]	64/64	0.97	0.04	35,45,50,56	64
22	CL	A	403[B]	1/1	0.98	0.04	45,45,45,45	1
22	CL	A	403[A]	1/1	0.98	0.04	46,46,46,46	1
38	HEM	E	103	43/43	0.98	0.06	52,70,83,95	0
38	HEM	e	87	43/43	0.98	0.08	63,85,118,137	0
23	CLA	b	608	65/65	0.98	0.05	42,54,78,91	0
40	HEC	v	202	43/43	0.98	0.07	51,63,70,77	0
36	CA	c	524	1/1	0.99	0.05	78,78,78,78	0
22	CL	a	403[B]	1/1	0.99	0.07	53,53,53,53	1
28	OEX	A	413[A]	10/10	0.99	0.03	37,45,50,50	10
28	OEX	A	413[B]	10/10	0.99	0.03	37,45,49,50	10
22	CL	A	402[A]	1/1	0.99	0.07	41,41,41,41	1
22	CL	A	402[B]	1/1	0.99	0.07	41,41,41,41	1
22	CL	a	402[A]	1/1	0.99	0.06	48,48,48,48	1
39	MG	J	102	1/1	0.99	0.03	57,57,57,57	0
39	MG	j	102	1/1	0.99	0.03	65,65,65,65	0
22	CL	a	402[B]	1/1	0.99	0.06	48,48,48,48	1
22	CL	a	403[A]	1/1	0.99	0.07	53,53,53,53	1
21	FE2	a	401[A]	1/1	1.00	0.01	52,52,52,52	1
21	FE2	a	401[B]	1/1	1.00	0.01	52,52,52,52	1
21	FE2	A	401[A]	1/1	1.00	0.01	50,50,50,50	1
21	FE2	A	401[B]	1/1	1.00	0.01	50,50,50,50	1
28	OEX	a	415[A]	10/10	1.00	0.03	47,49,55,56	10
28	OEX	a	415[B]	10/10	1.00	0.03	47,49,55,56	10

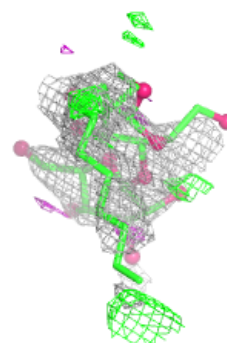
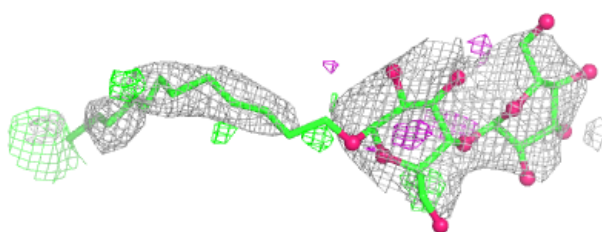
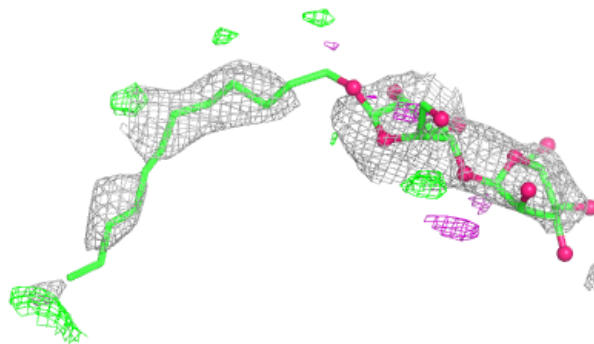
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

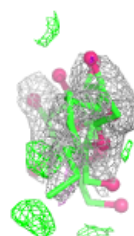
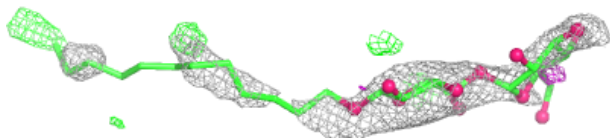
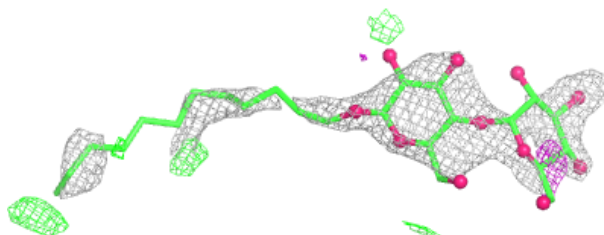


Electron density around LMT I 101:

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

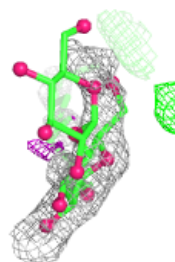
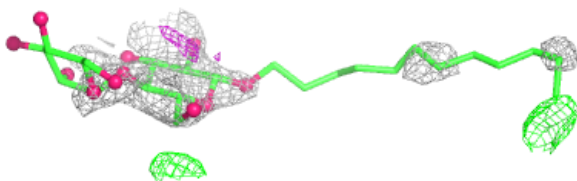
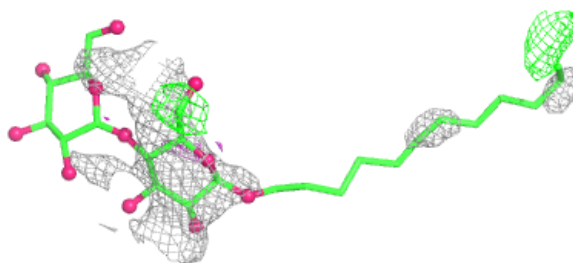
**Electron density around LMT a 420:**

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

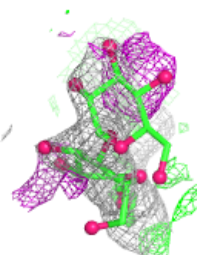
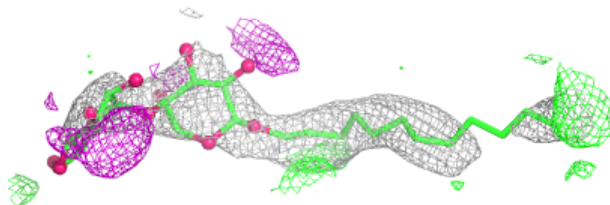
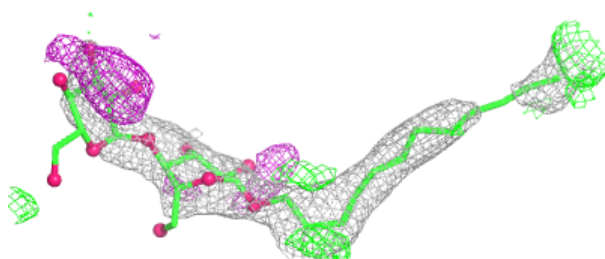


Electron density around LMT e 102:

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

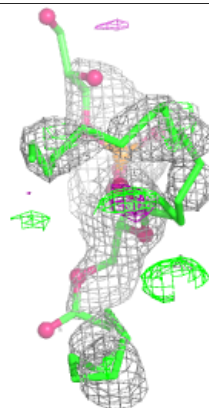
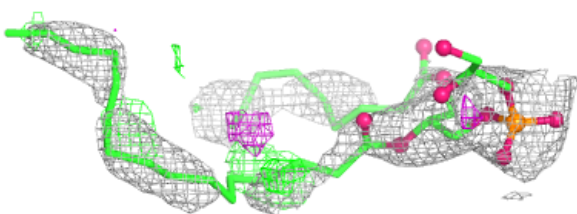
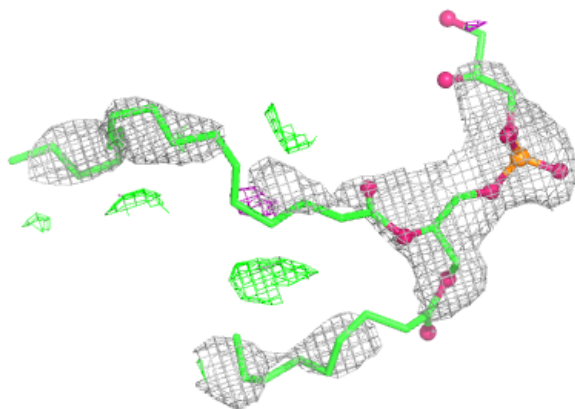
**Electron density around LMT a 414:**

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

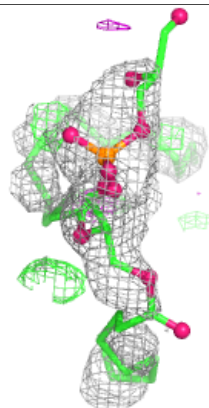
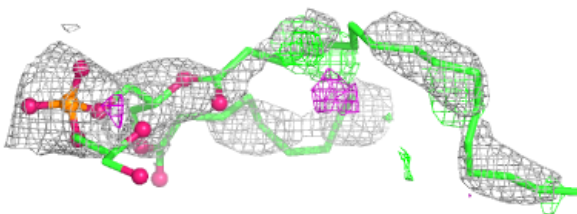
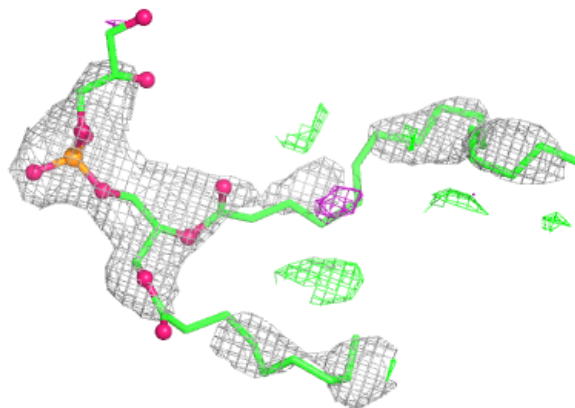


Electron density around LHG e 101 (A):

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

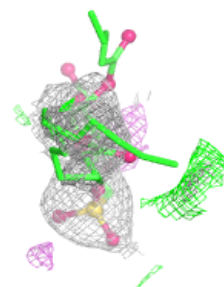
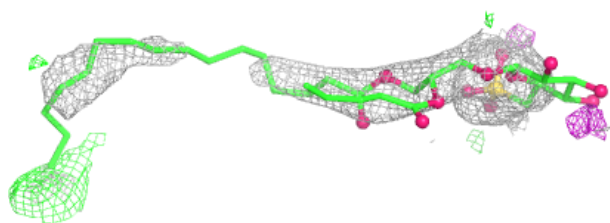
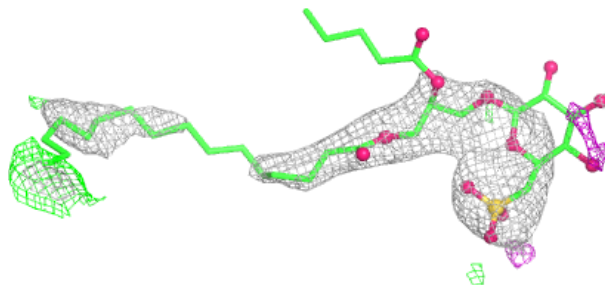
**Electron density around LHG e 101 (B):**

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

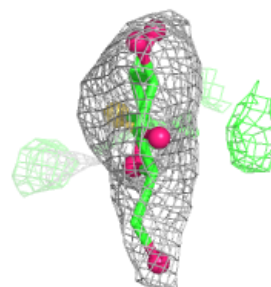
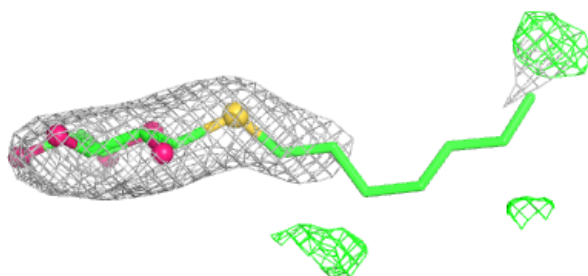
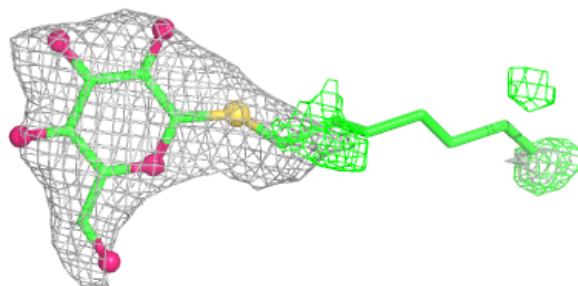


Electron density around SQD f 102:

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

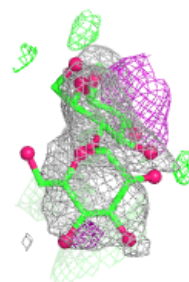
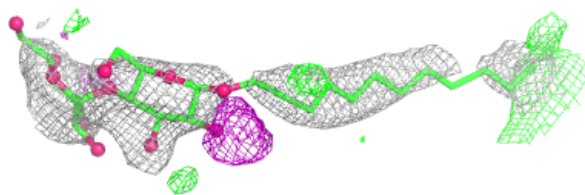
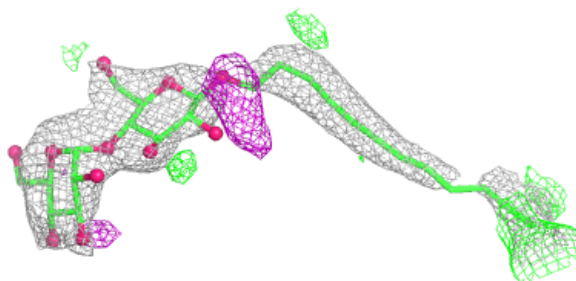
**Electron density around HTG C 522:**

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

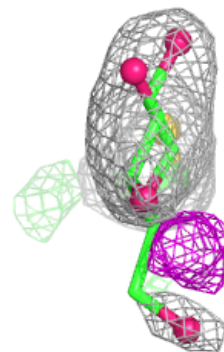
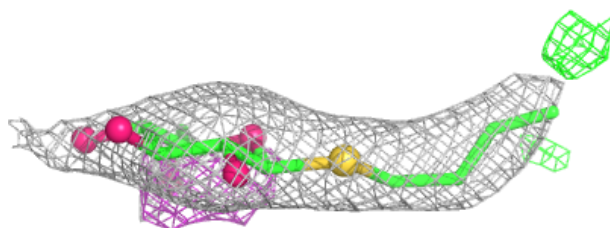
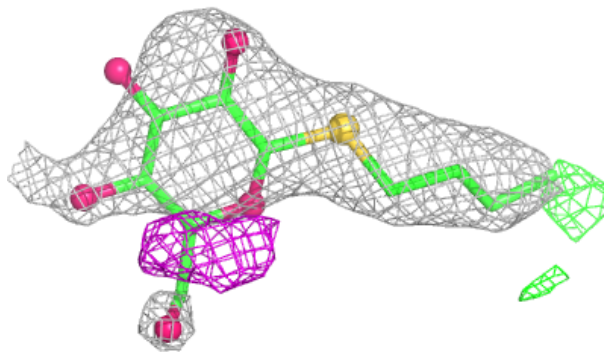


Electron density around LMT A 359:

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

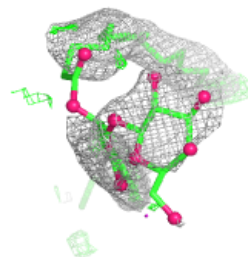
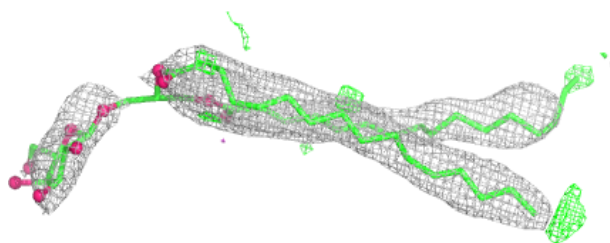
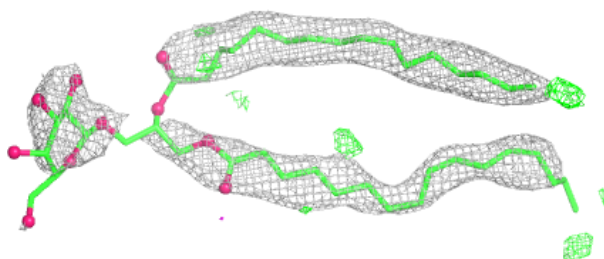
**Electron density around HTG D 414:**

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

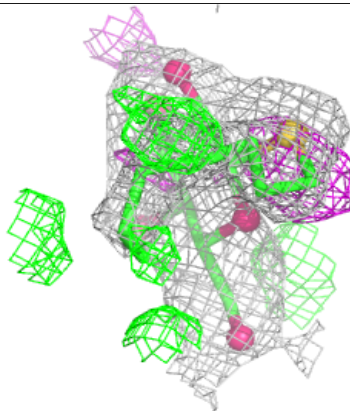
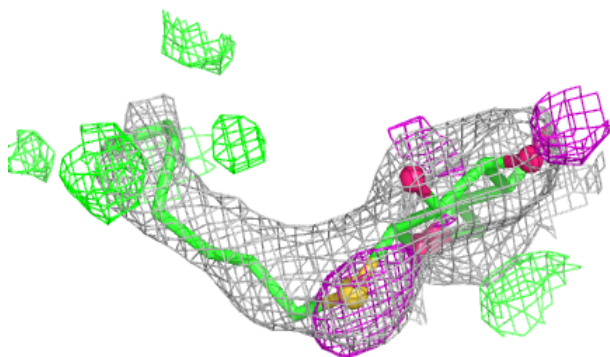
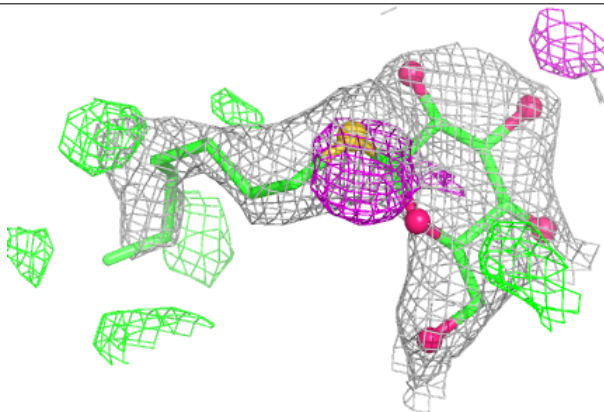


Electron density around LMG C 521:

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

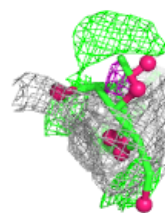
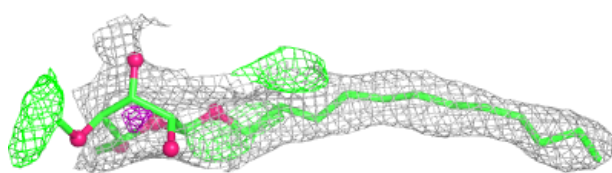
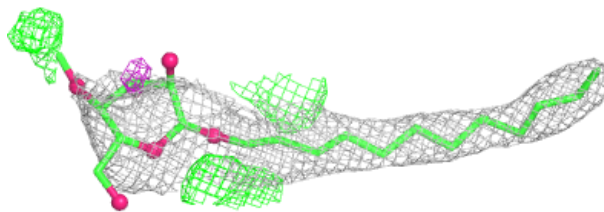
**Electron density around HTG B 623:**

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

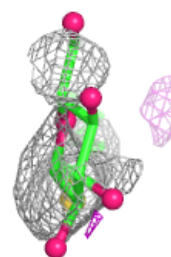
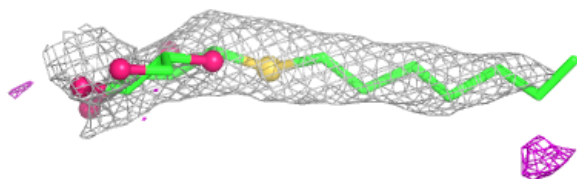
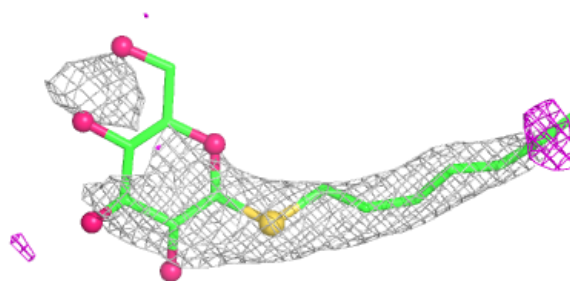


Electron density around LMT b 621:

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

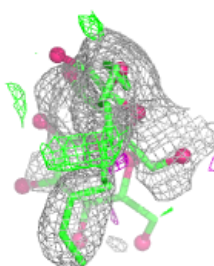
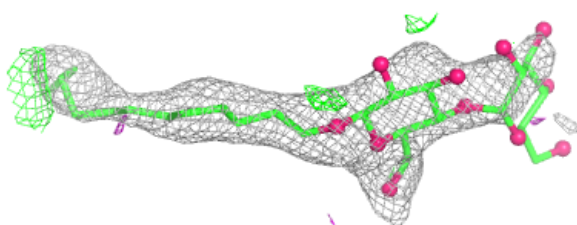
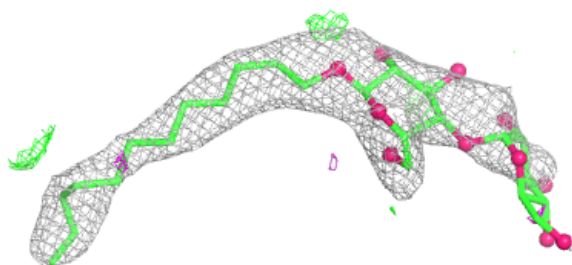
**Electron density around HTG b 623:**

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

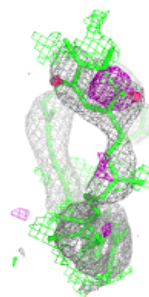
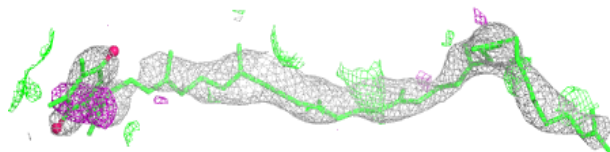
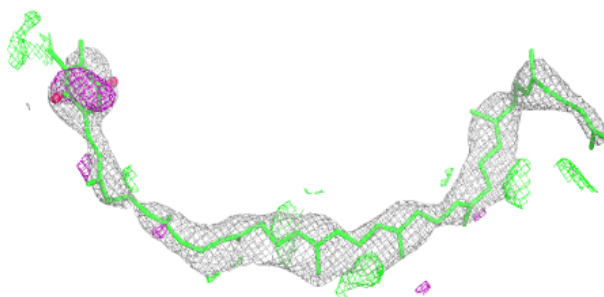


Electron density around LMT M 103:

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

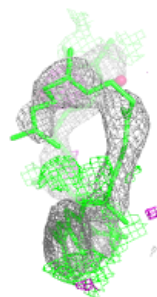
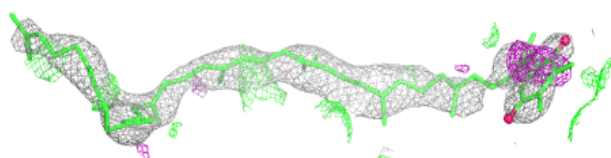
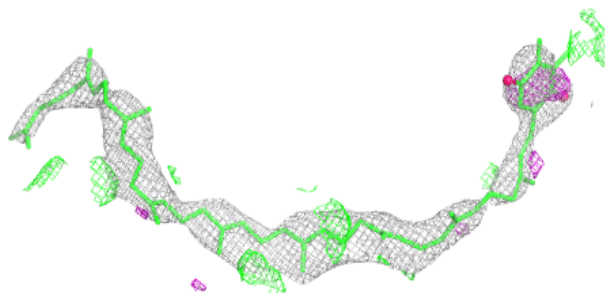
**Electron density around PL9 a 416 (A):**

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

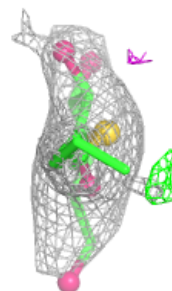
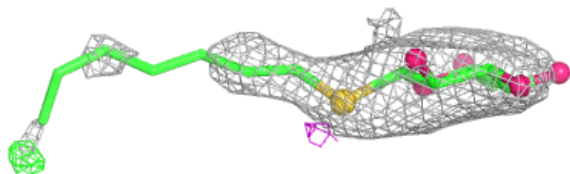
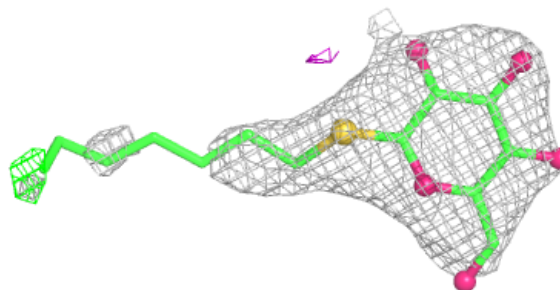


Electron density around PL9 a 416 (B):

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

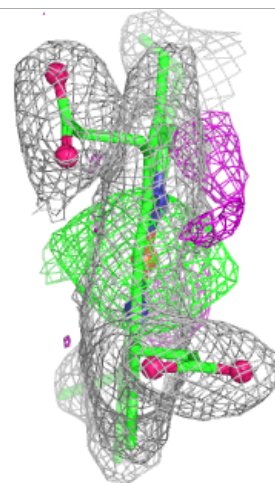
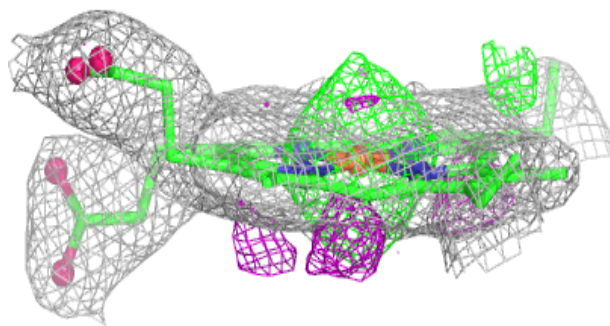
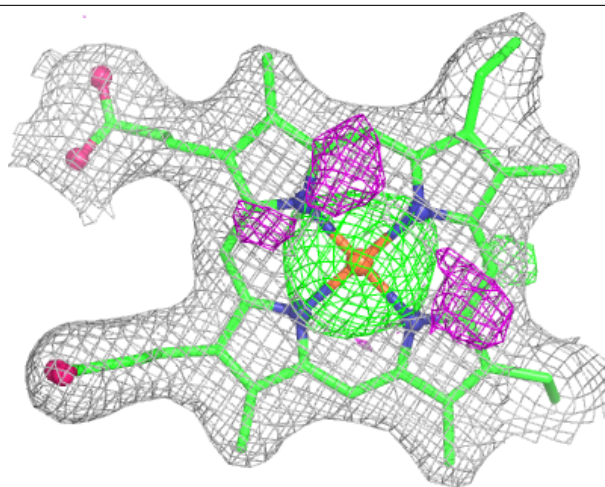
**Electron density around HTG c 522:**

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



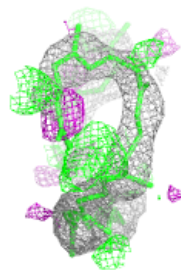
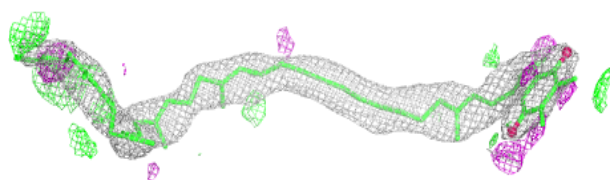
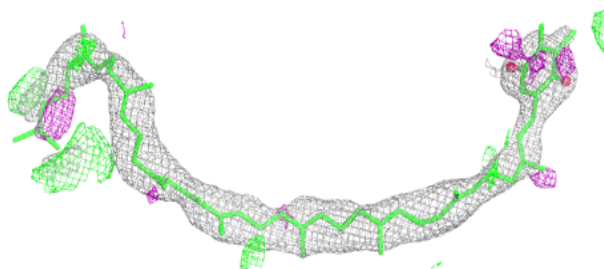
Electron density around HEC V 202:

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



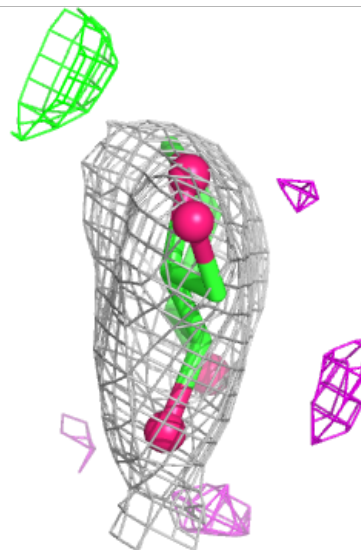
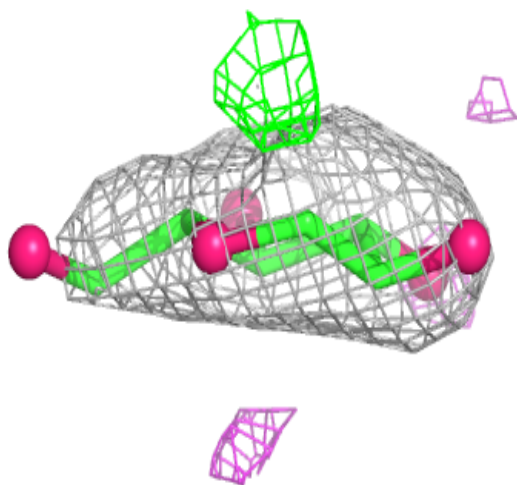
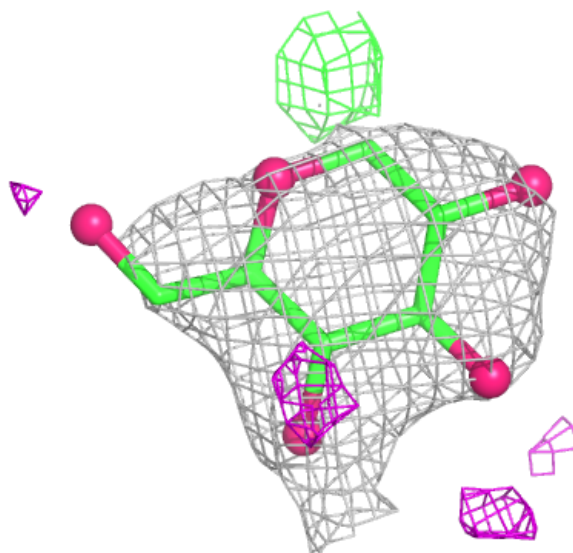
Electron density around PL9 A 414 (A):

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



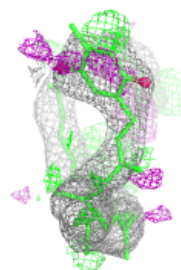
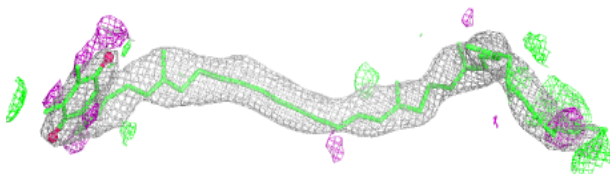
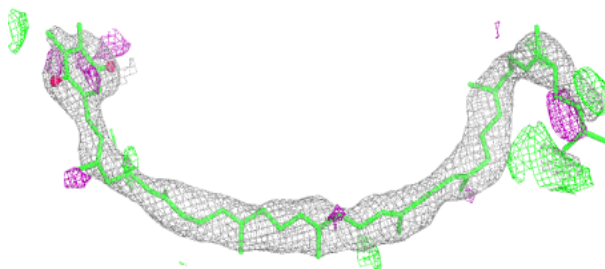
Electron density around HTG V 203:

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

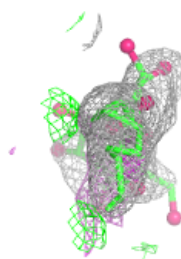
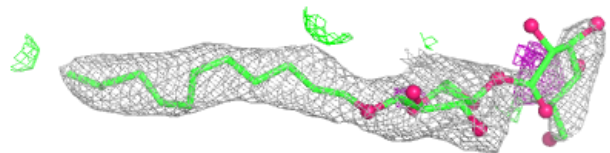
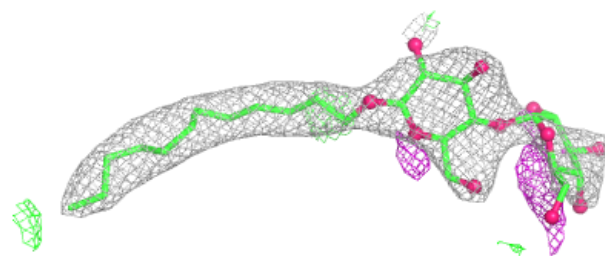


Electron density around PL9 A 414 (B):

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

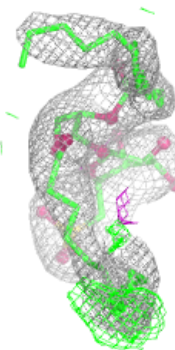
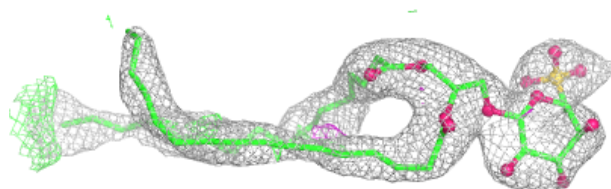
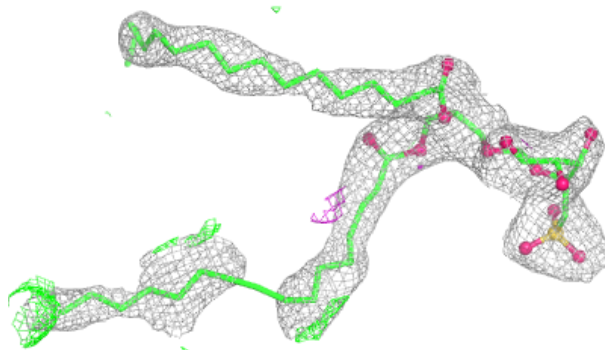
**Electron density around LMT D 404:**

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

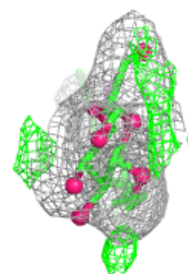
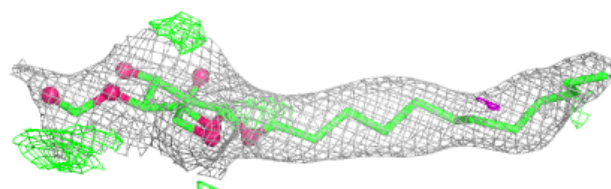
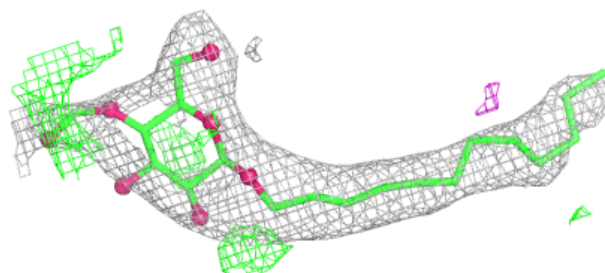


Electron density around SQD a 413:

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

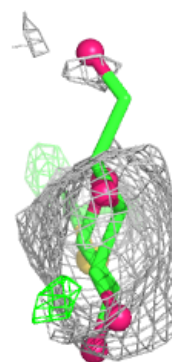
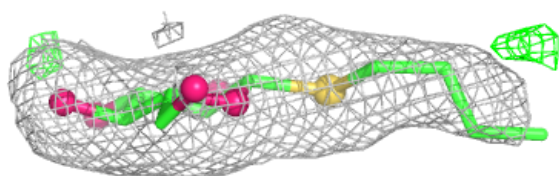
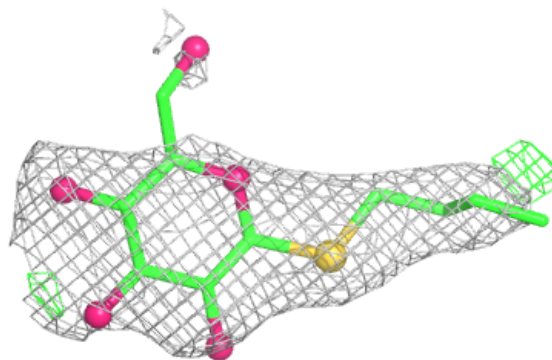
**Electron density around LMT t 102:**

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

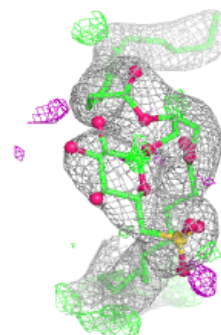
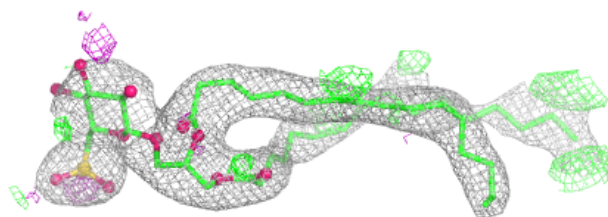
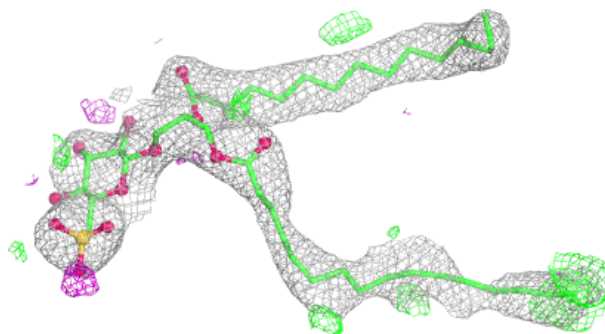


Electron density around HTG d 411:

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

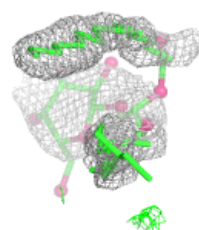
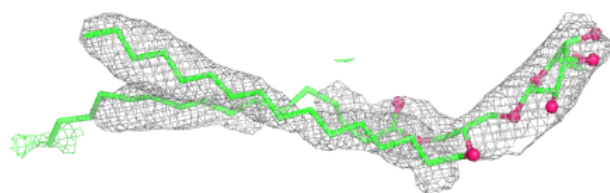
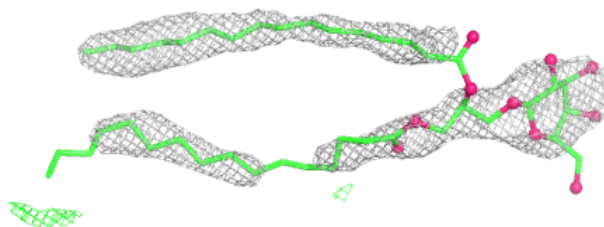
**Electron density around SQD A 412:**

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

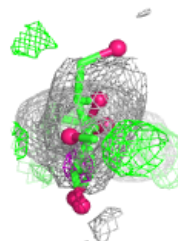
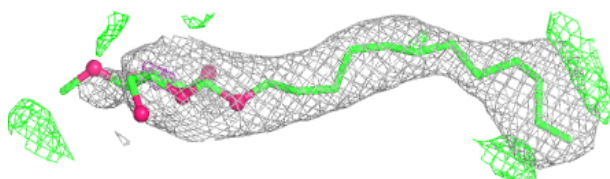
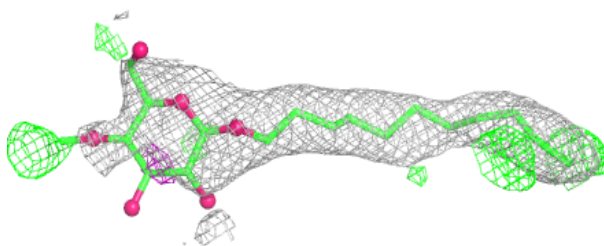


Electron density around LMG c 521:

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

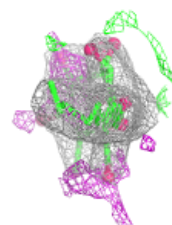
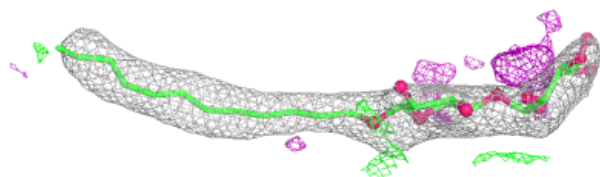
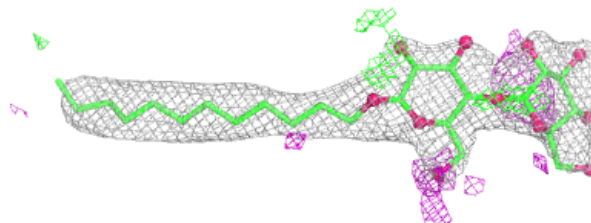
**Electron density around LMT b 627:**

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

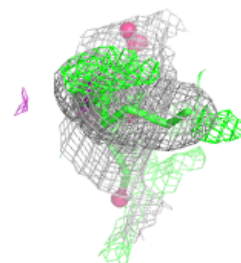
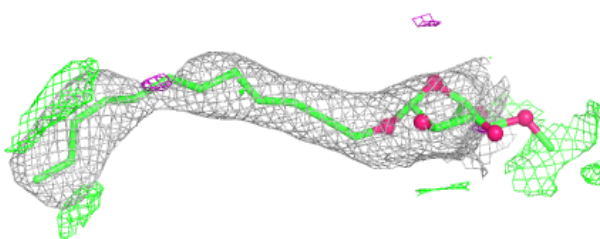
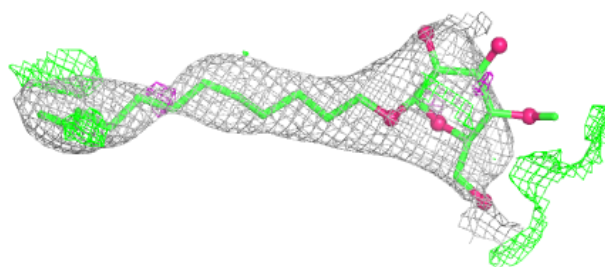


Electron density around LMT m 103:

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

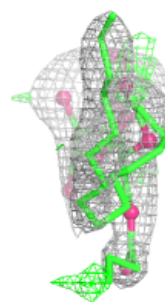
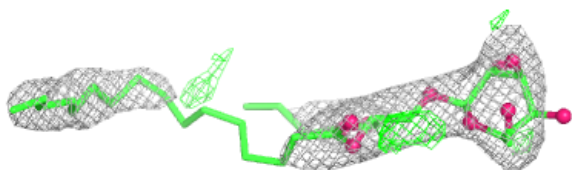
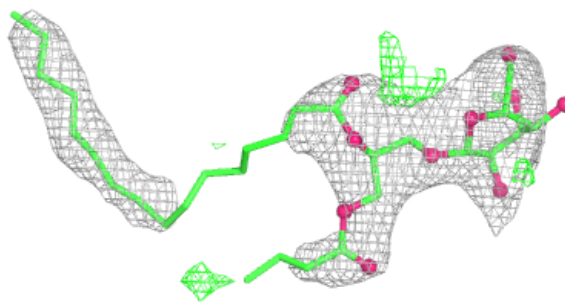
**Electron density around LMT t 101:**

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

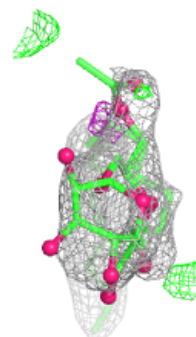
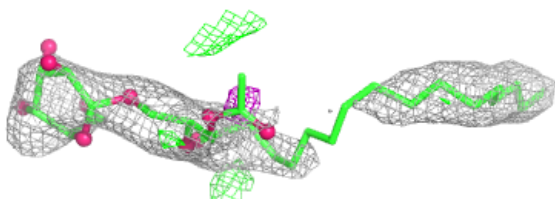
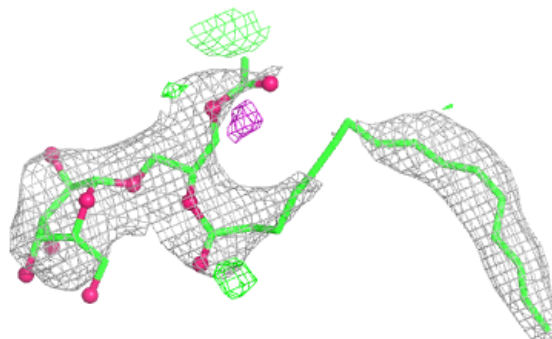


Electron density around LMG z 101:

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

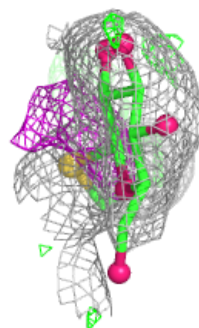
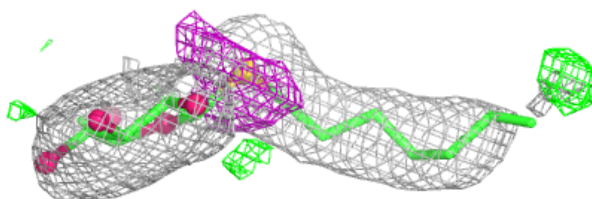
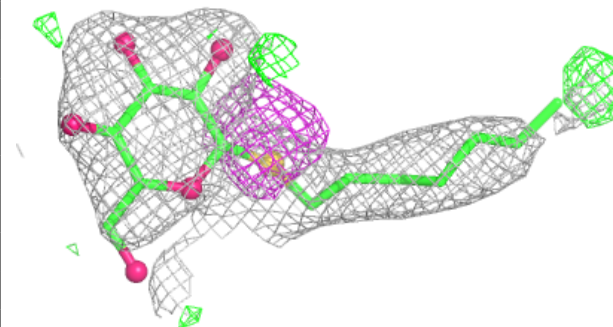
**Electron density around LMG Z 101:**

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

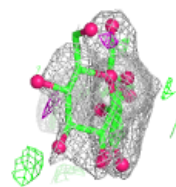
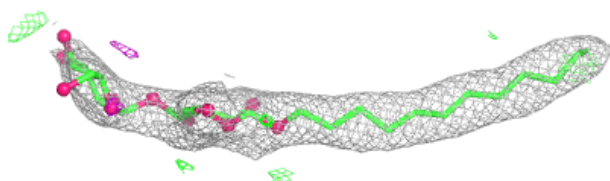
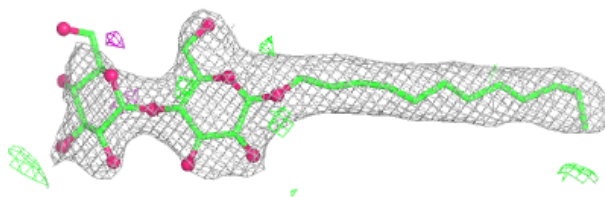


Electron density around HTG b 622:

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

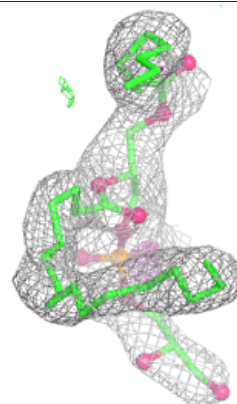
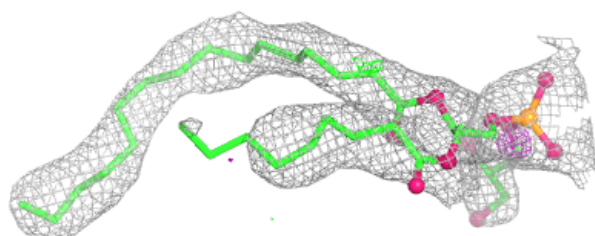
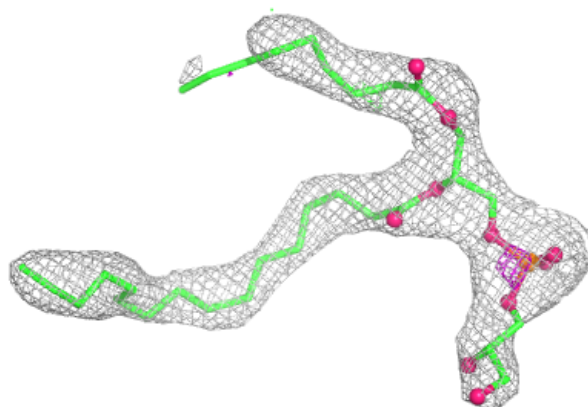
**Electron density around LMT M 101:**

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

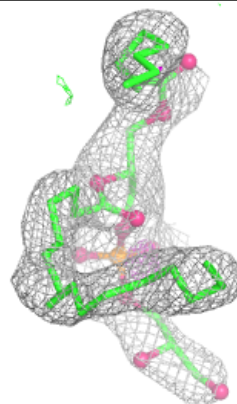
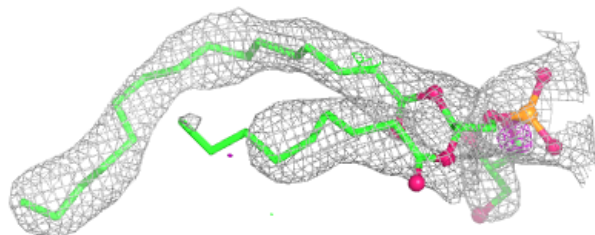
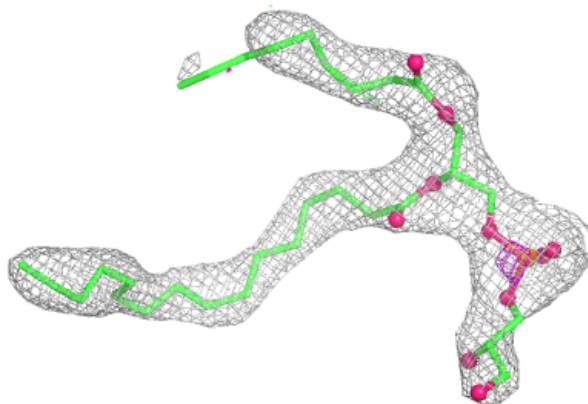


Electron density around LHG E 101 (A):

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

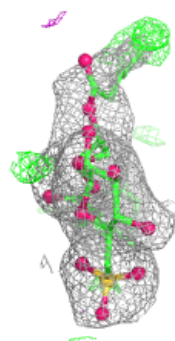
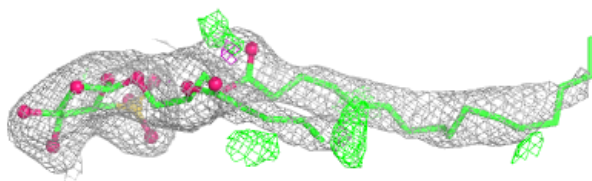
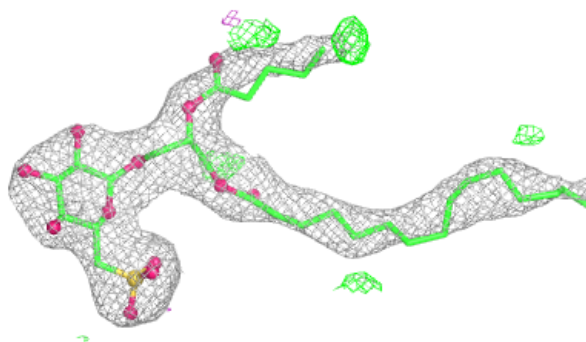
**Electron density around LHG E 101 (B):**

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

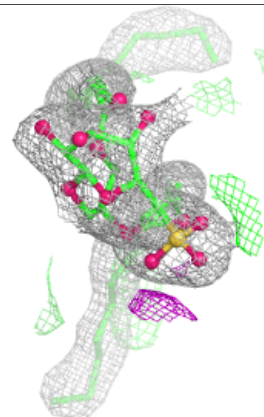
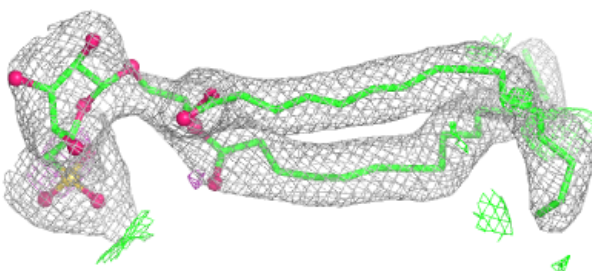
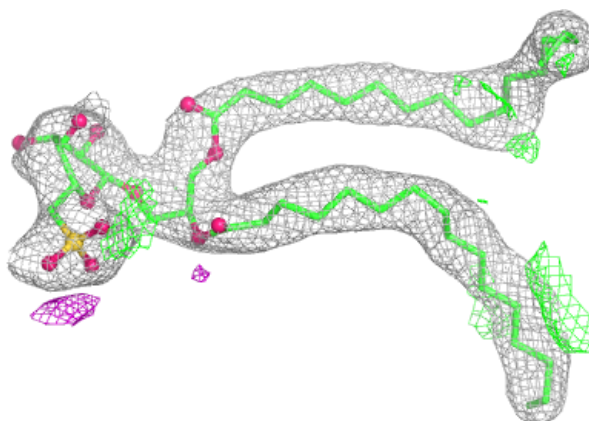


Electron density around SQD F 101:

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

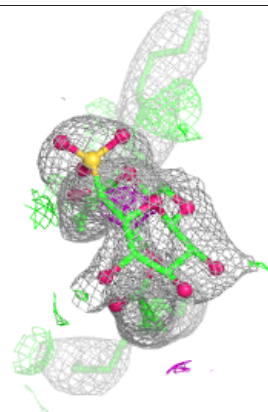
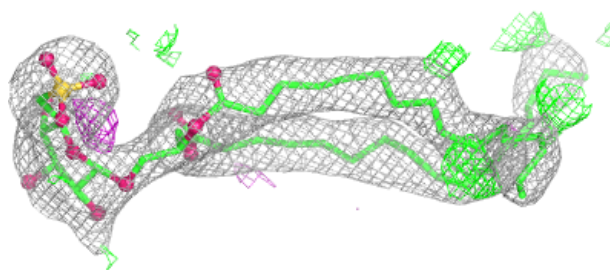
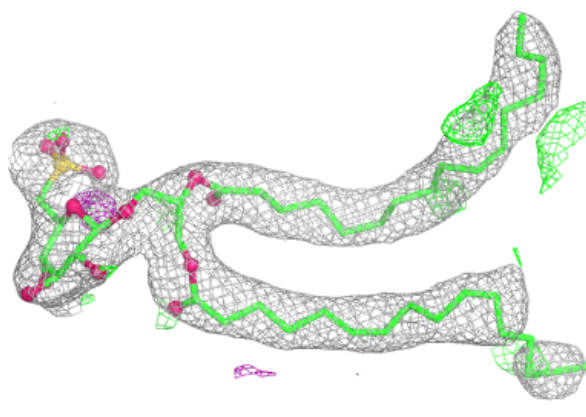
**Electron density around SQD B 620:**

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



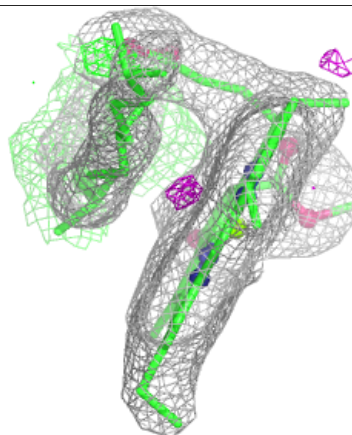
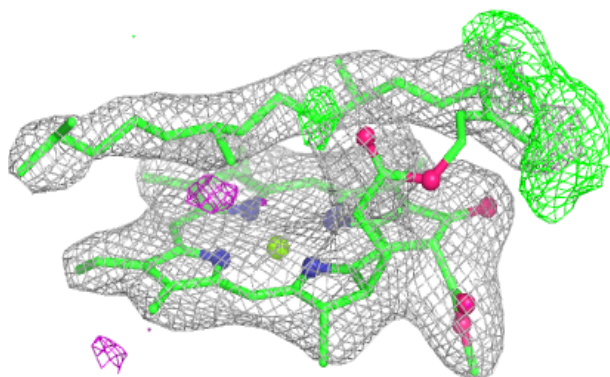
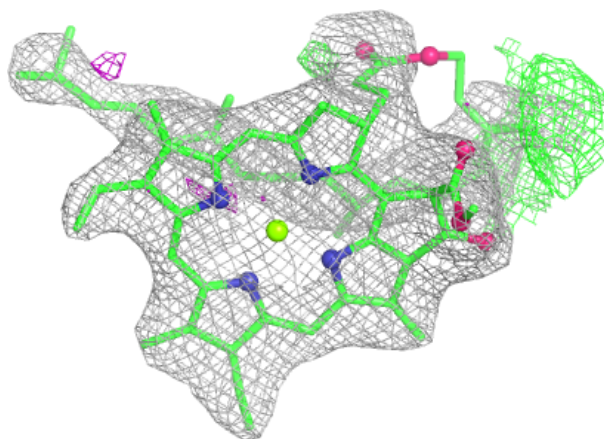
Electron density around SQD b 620:

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



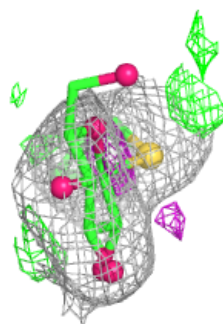
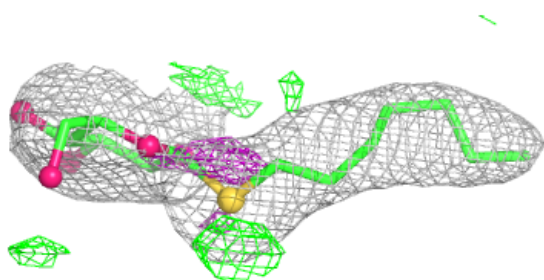
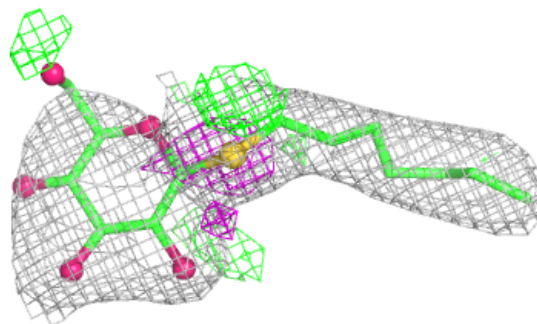
Electron density around CLA b 601:

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

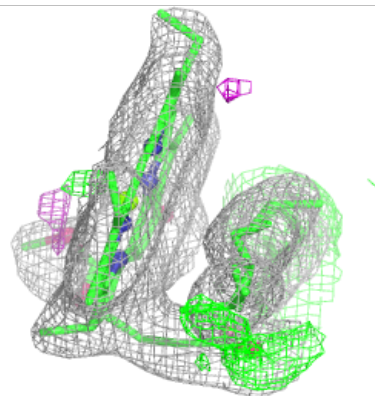
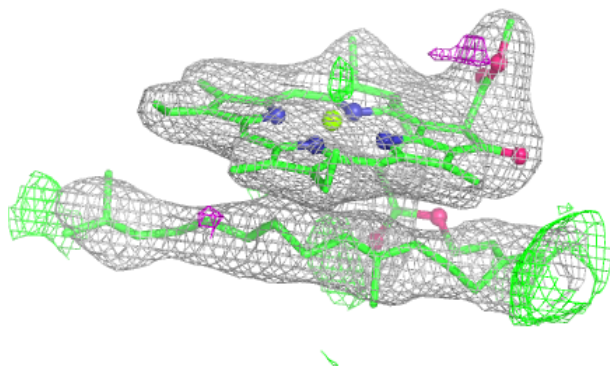
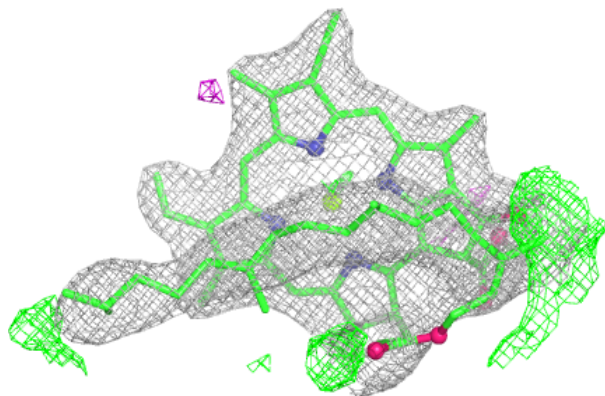


Electron density around HTG B 622:

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

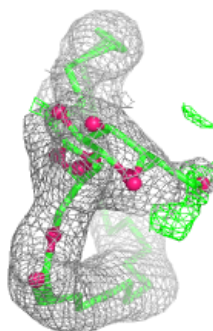
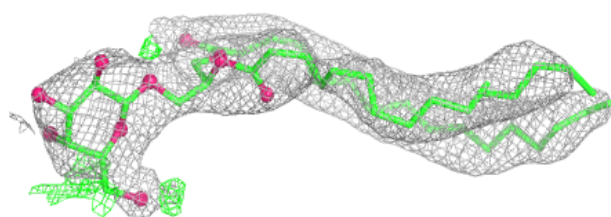
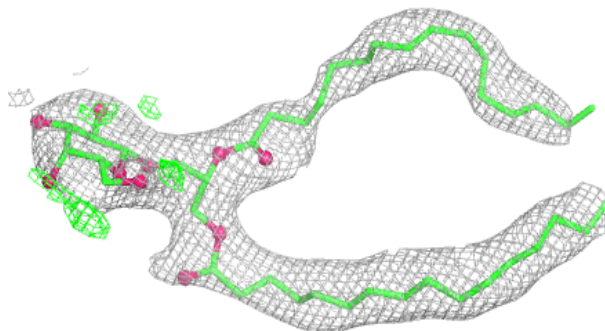
**Electron density around CLA B 601:**

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

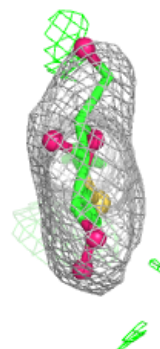
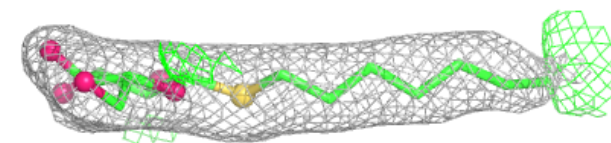
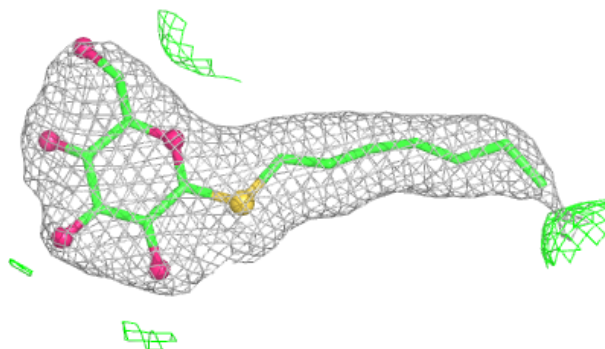


Electron density around LMG C 501:

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

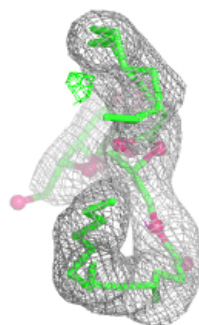
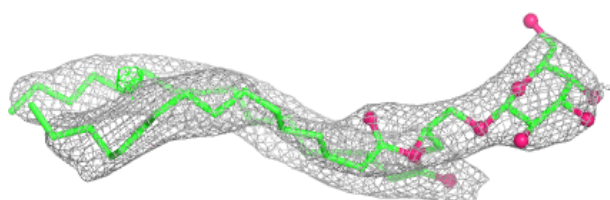
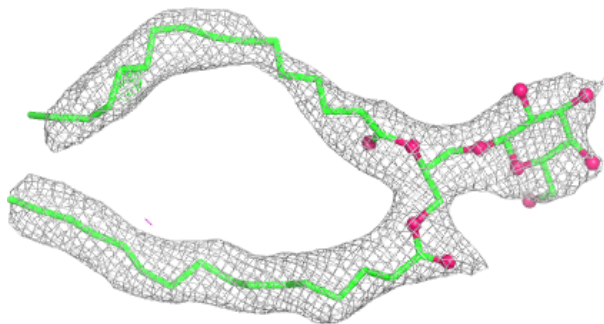
**Electron density around HTG B 626:**

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

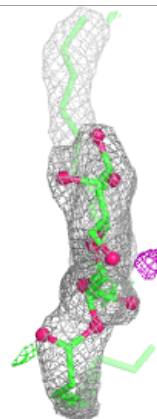
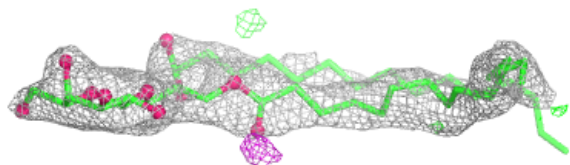
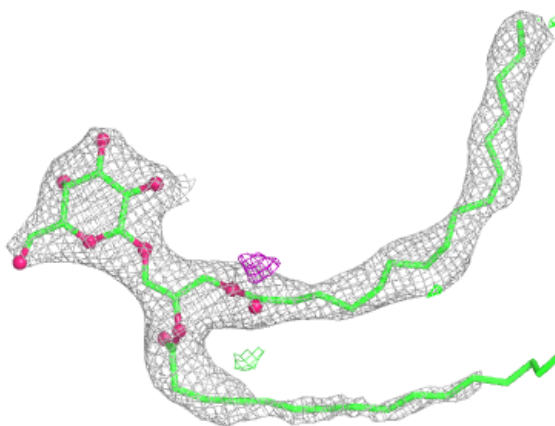


Electron density around LMG a 419:

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

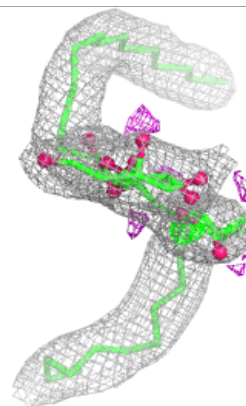
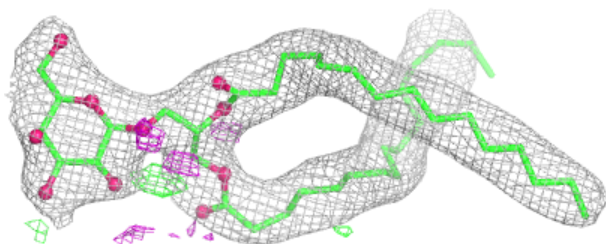
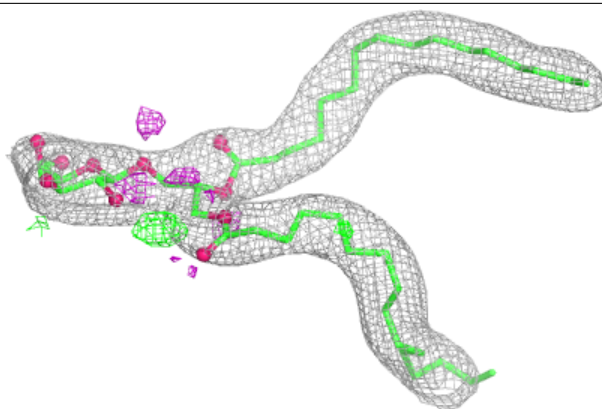
**Electron density around LMG c 520:**

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

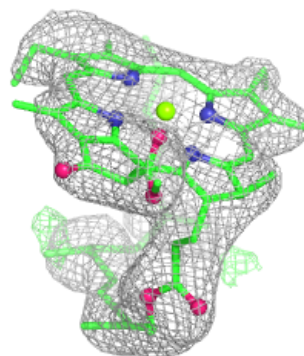
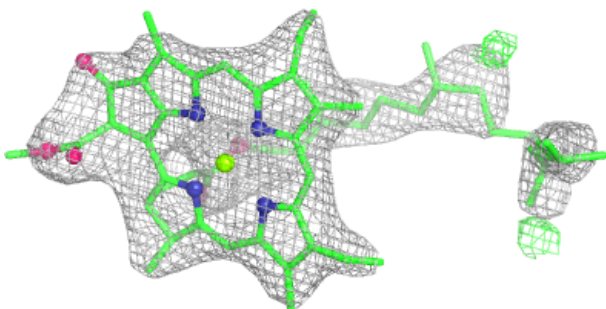
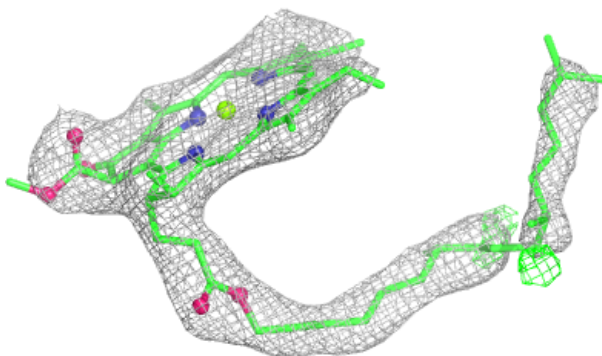


Electron density around LMG m 101:

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

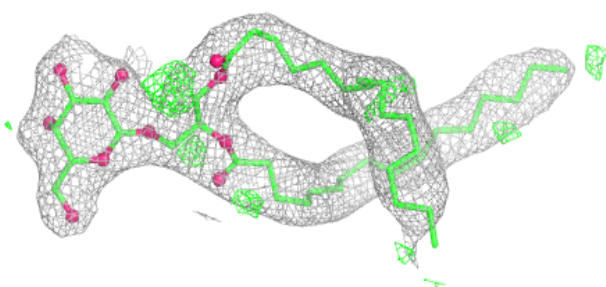
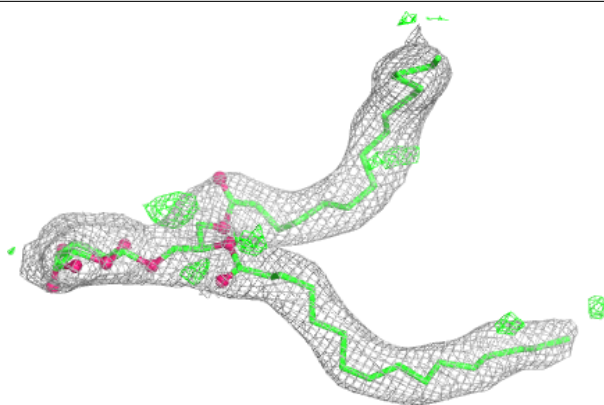
**Electron density around CLA c 514:**

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

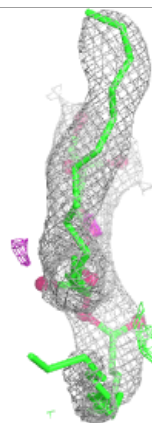
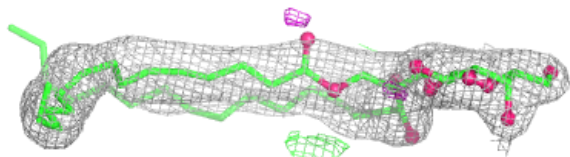
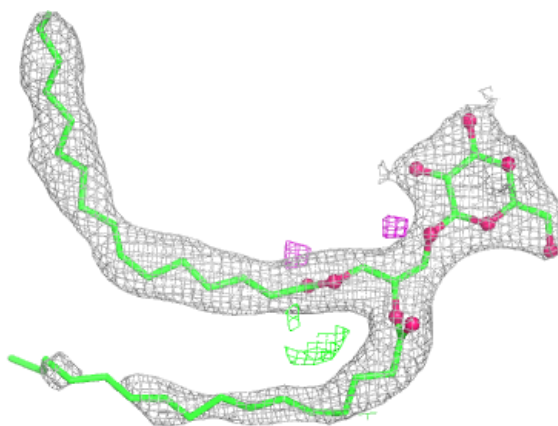


Electron density around LMG B 621:

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

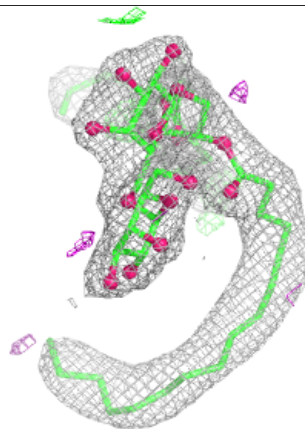
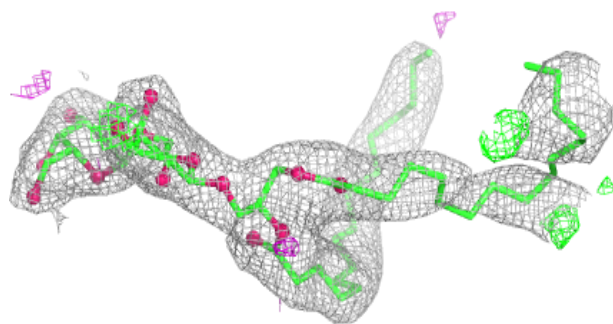
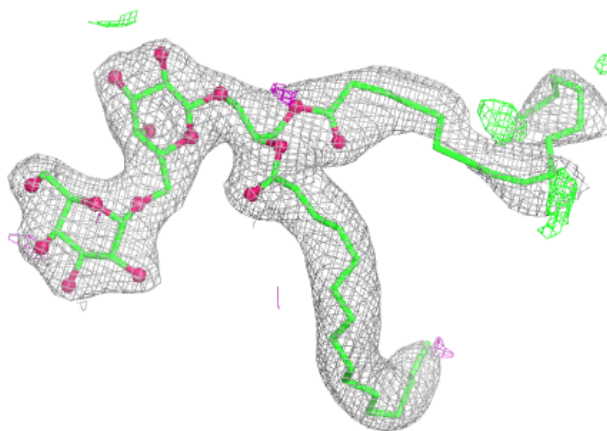
**Electron density around LMG C 520:**

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



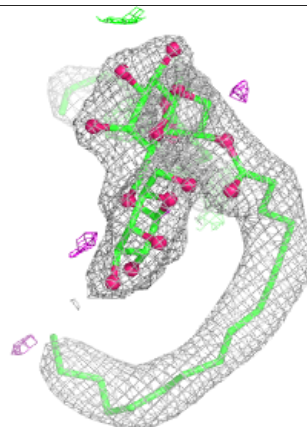
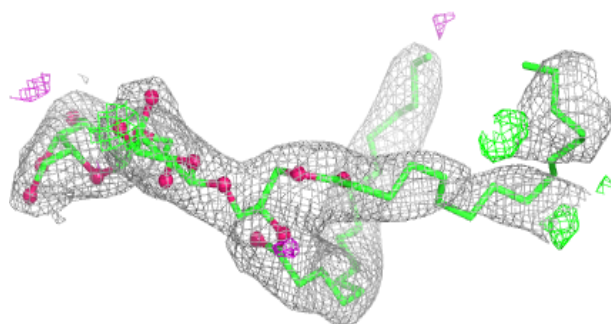
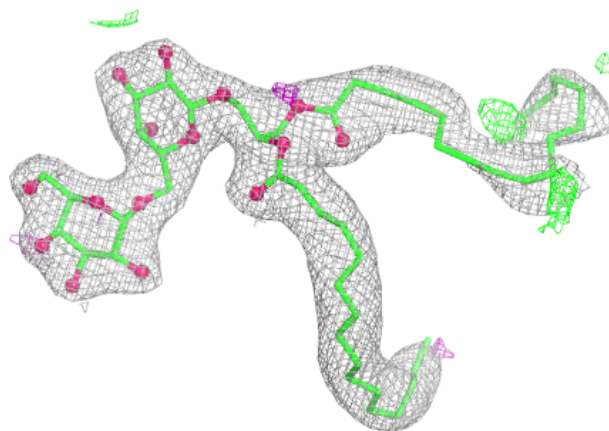
Electron density around DGD C 518 (A):

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

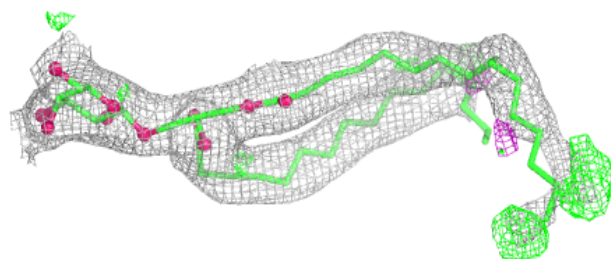
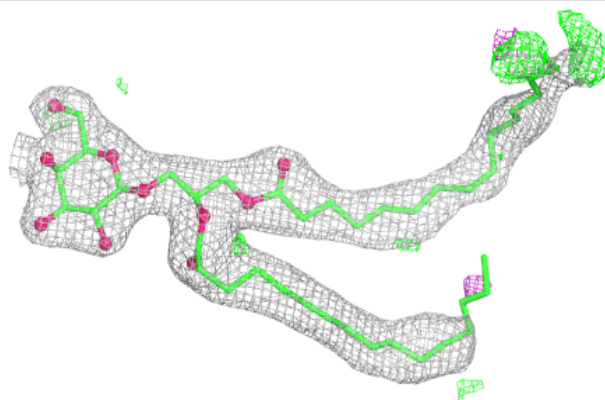


Electron density around DGD C 518 (B):

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

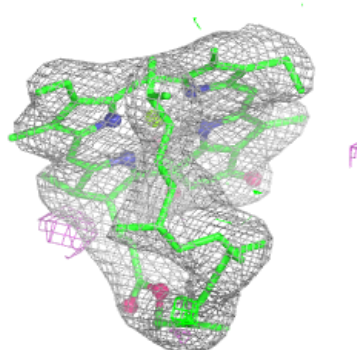
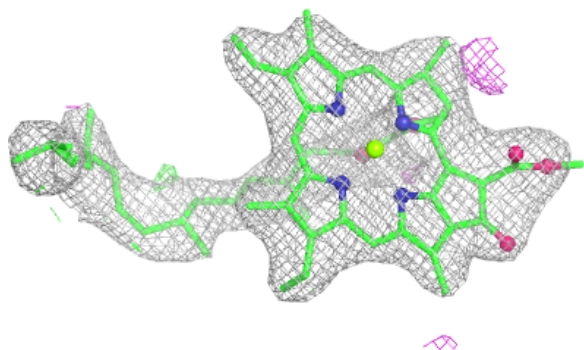
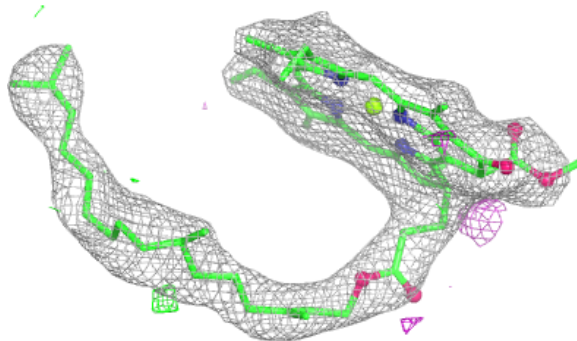
**Electron density around LMG D 415:**

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

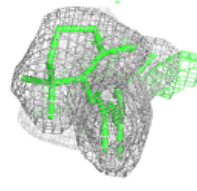
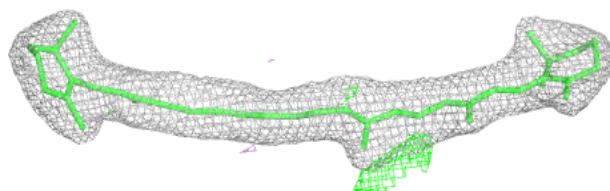
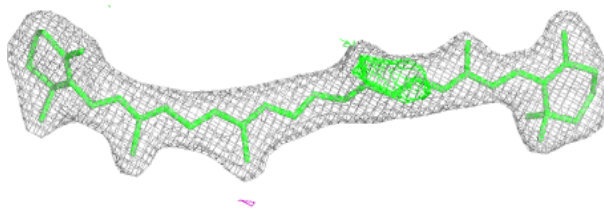


Electron density around CLA C 514:

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

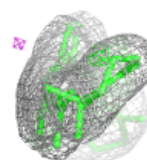
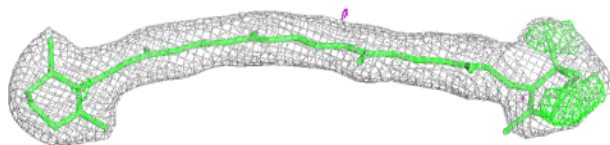
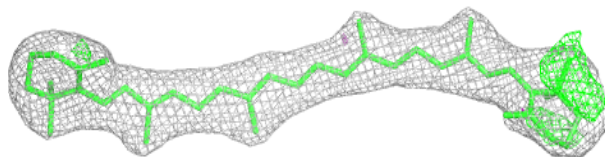
**Electron density around BCR T 101:**

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

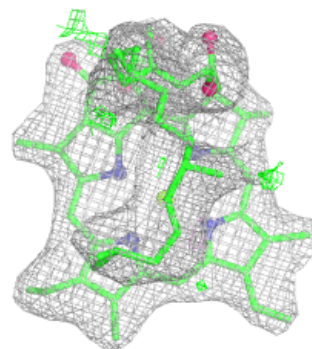
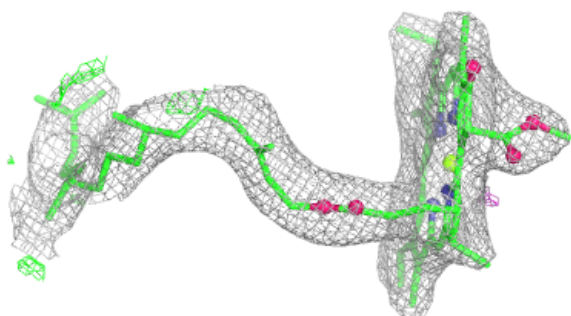
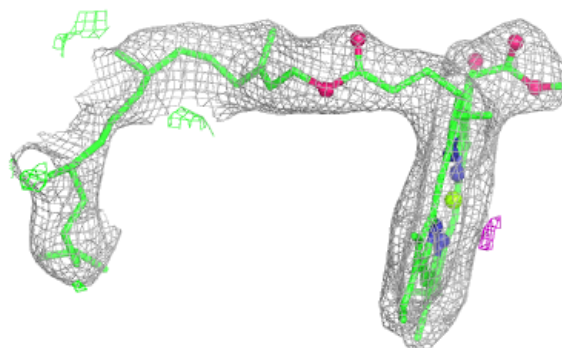


Electron density around BCR d 404:

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

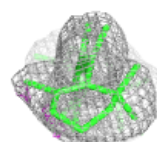
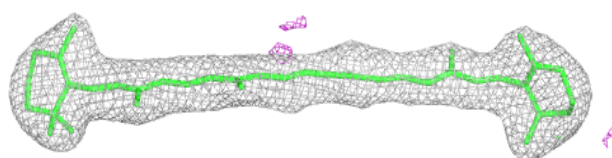
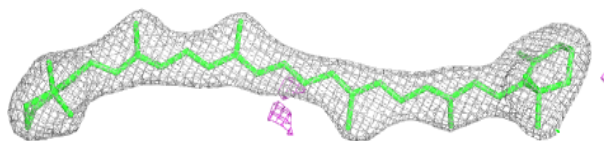
**Electron density around CLA C 507:**

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

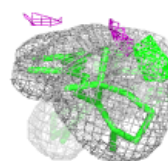
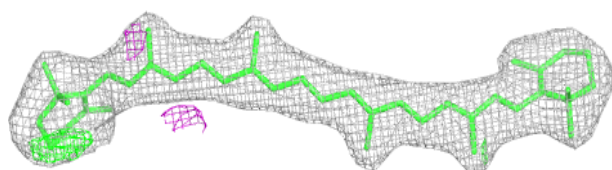
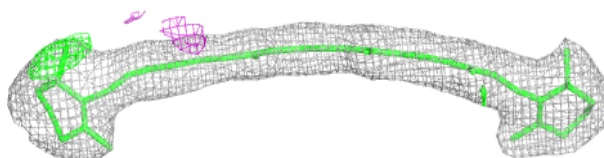


Electron density around BCR C 515:

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

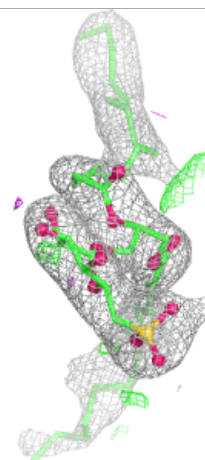
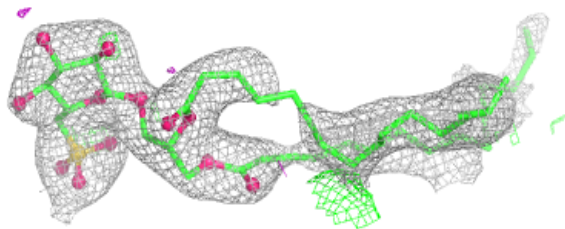
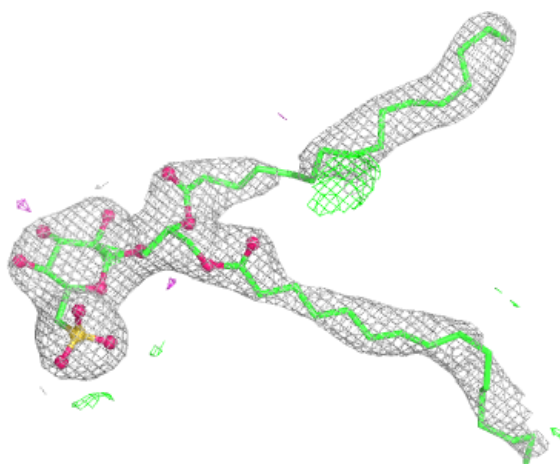
**Electron density around BCR D 407:**

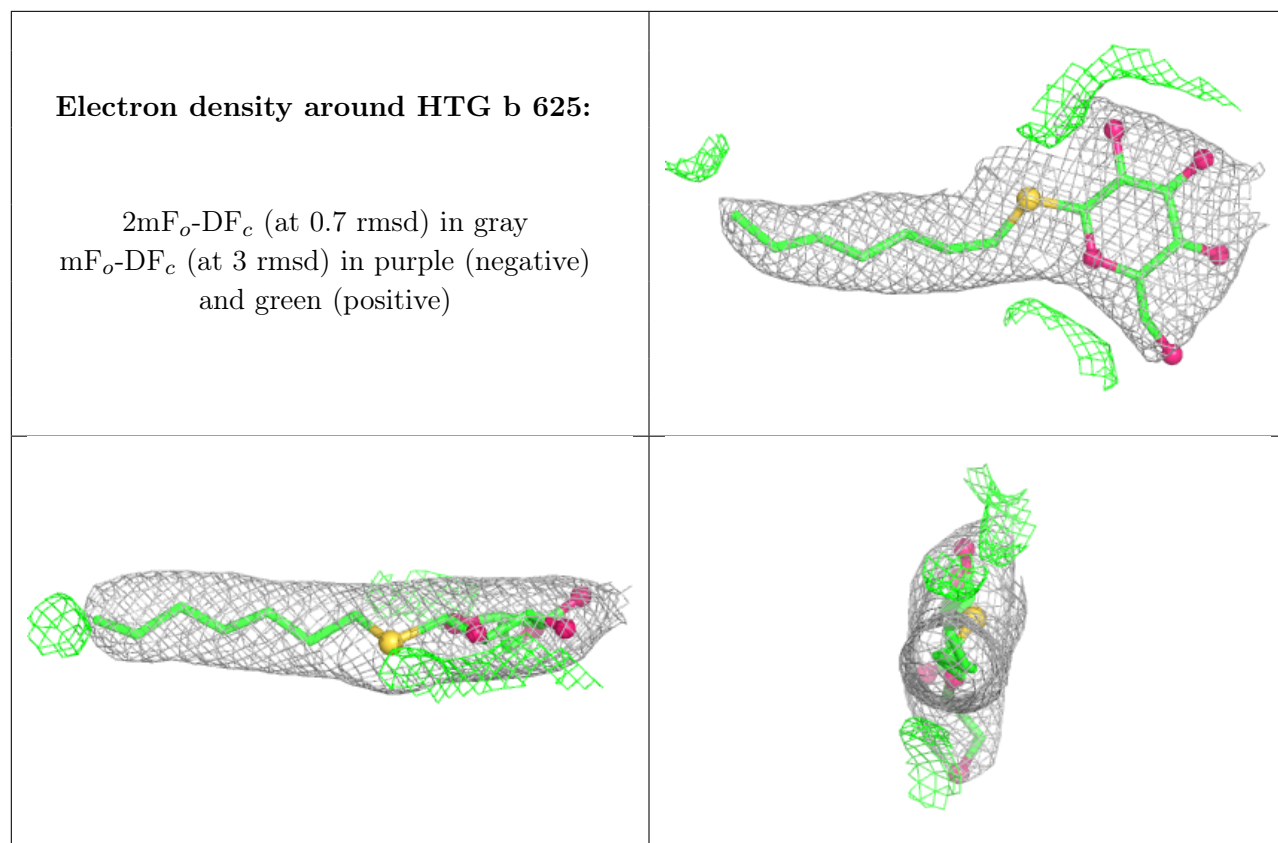
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around SQD a 411 (A):

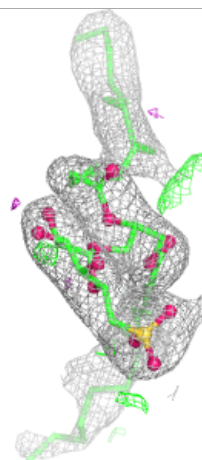
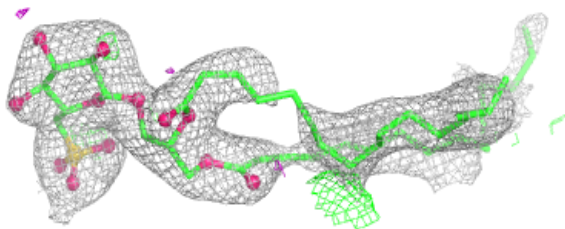
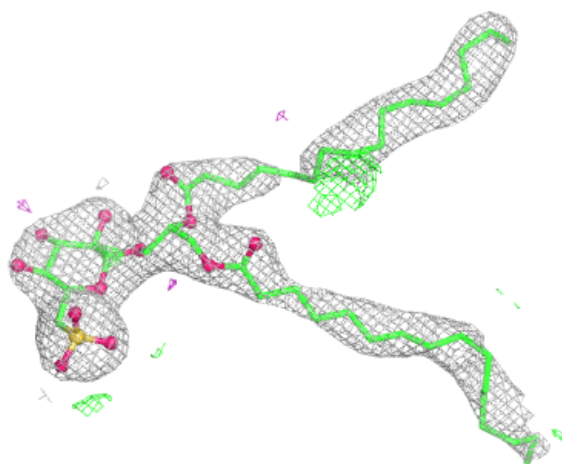
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





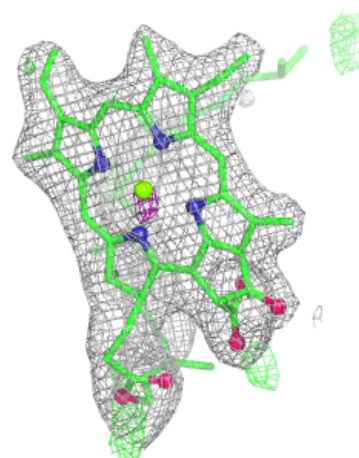
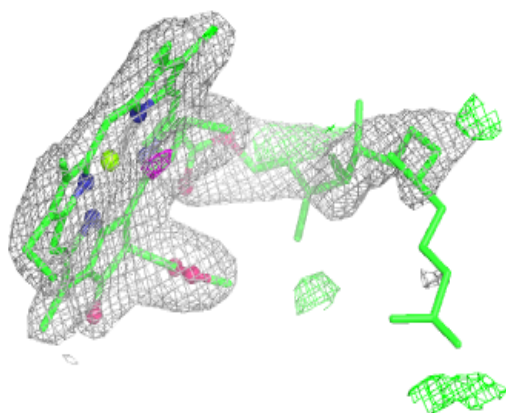
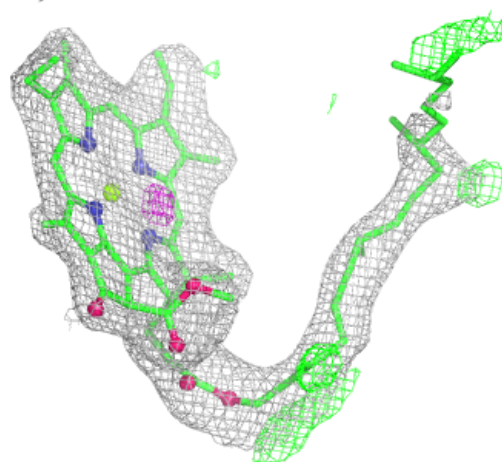
Electron density around SQD a 411 (B):

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



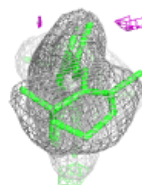
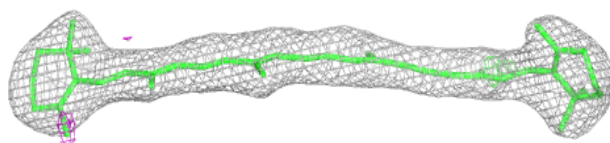
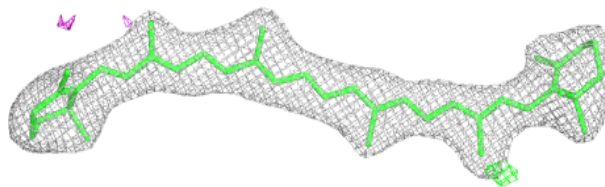
Electron density around CLA b 616:

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

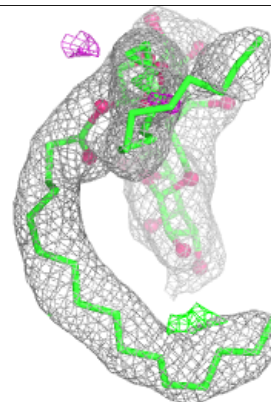
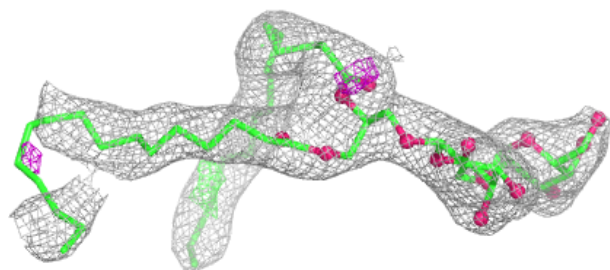
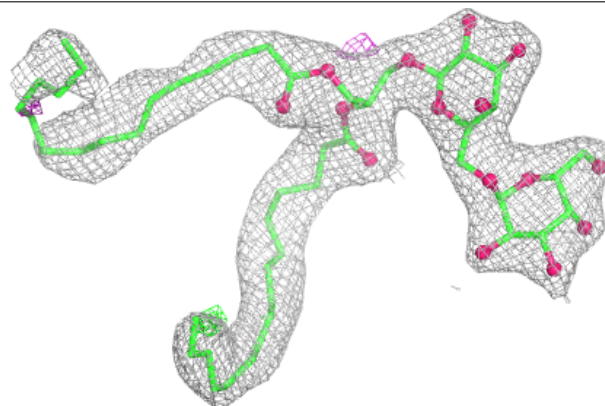


Electron density around BCR Y 101:

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

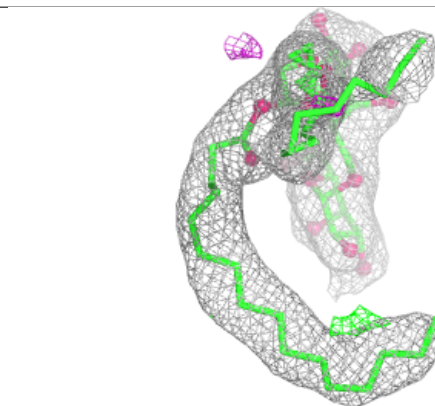
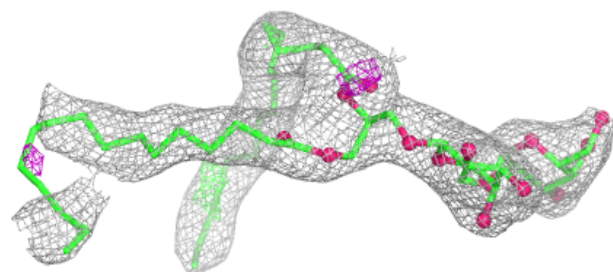
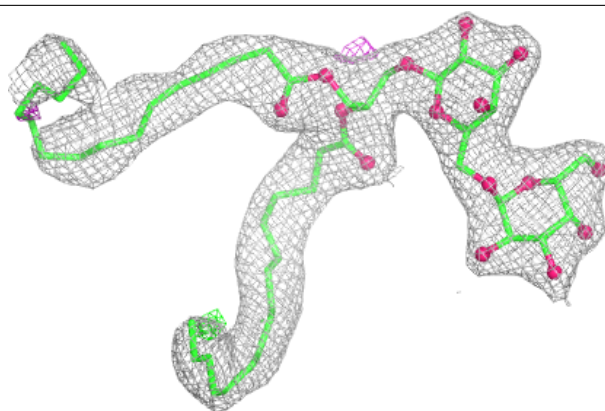
**Electron density around DGD c 518 (A):**

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

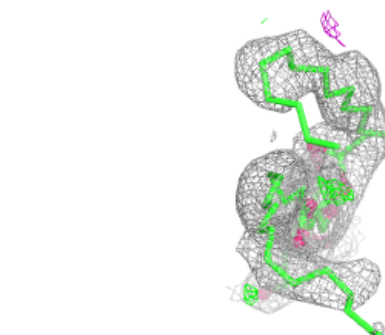
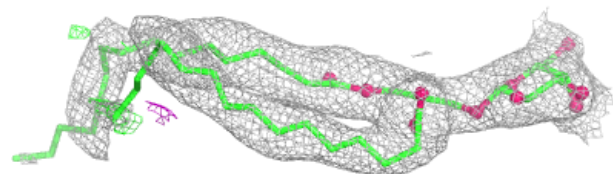
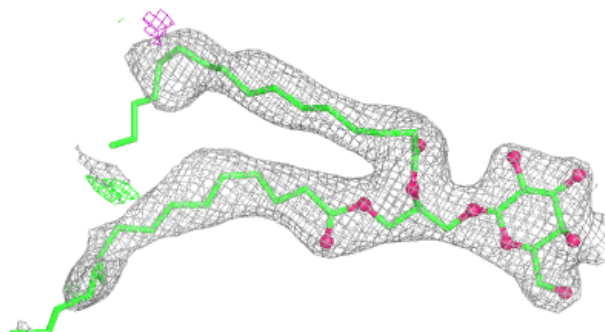


Electron density around DGD c 518 (B):

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

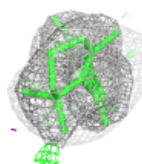
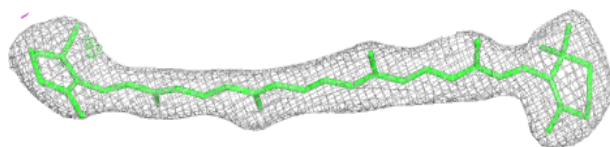
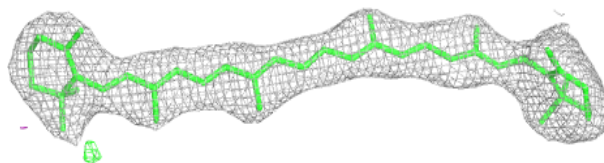
**Electron density around LMG d 412:**

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



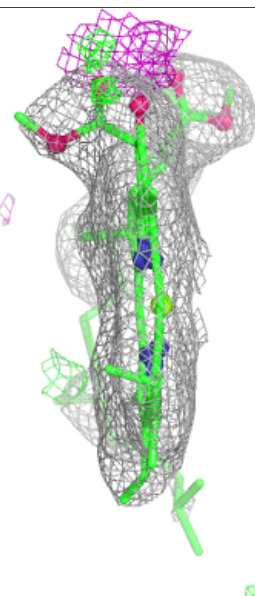
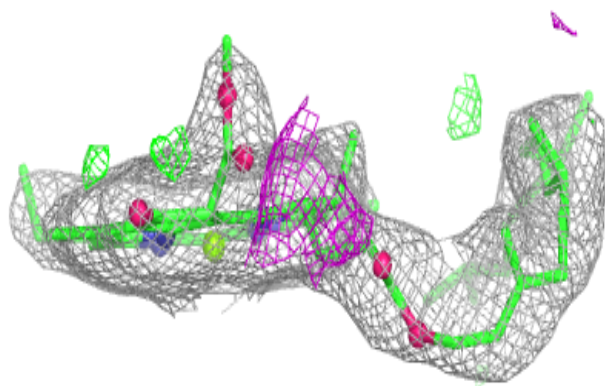
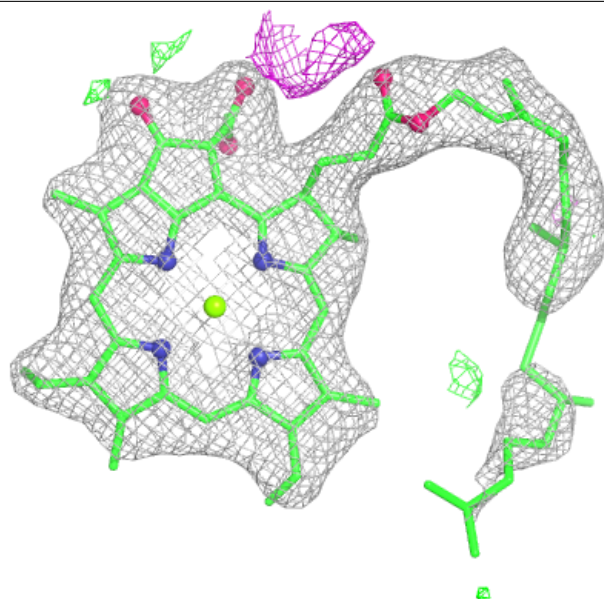
Electron density around BCR c 515:

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



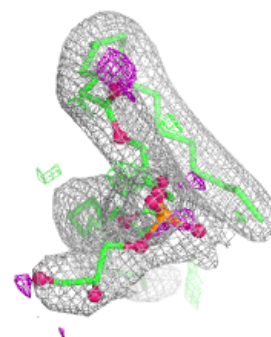
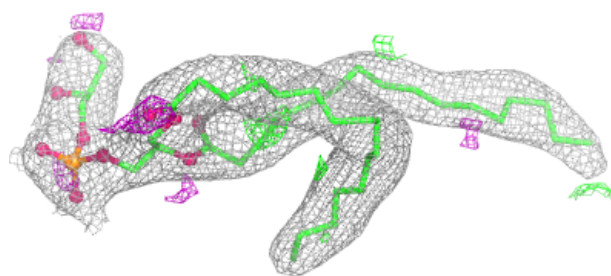
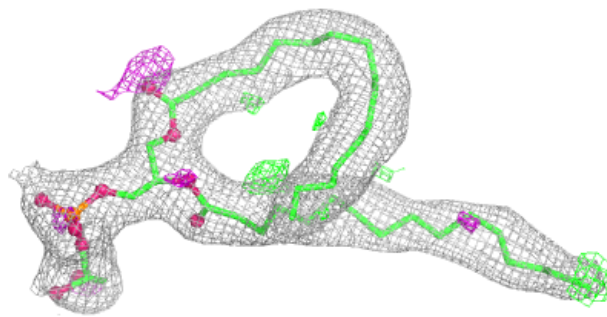
Electron density around CLA c 513:

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

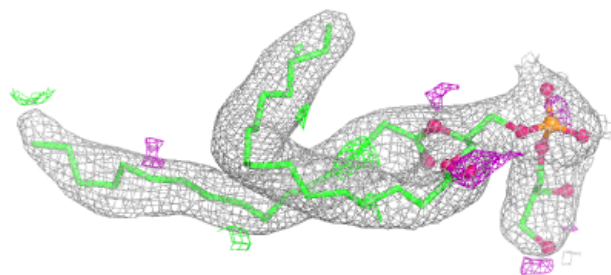
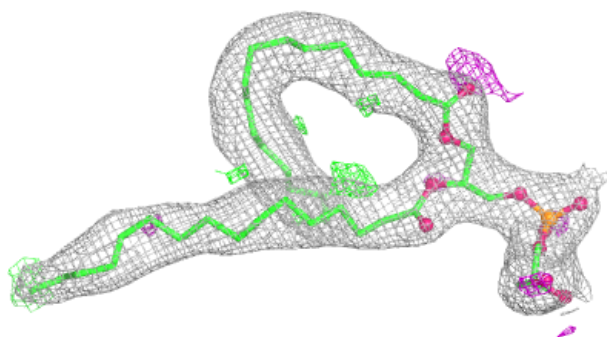


Electron density around LHG D 409 (A):

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

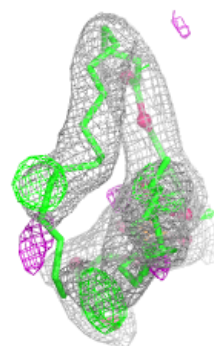
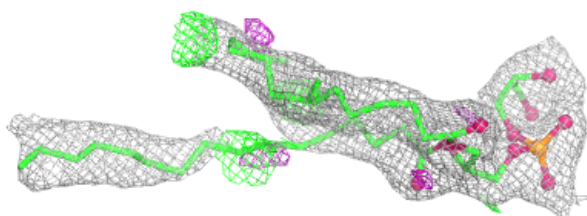
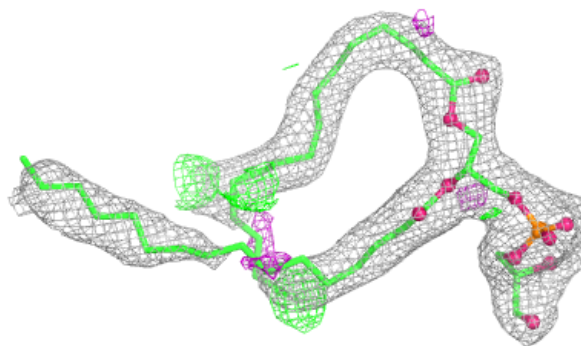
**Electron density around LHG D 409 (B):**

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

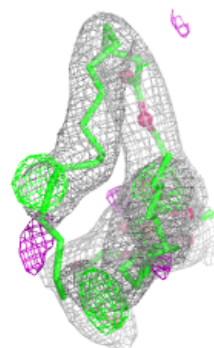
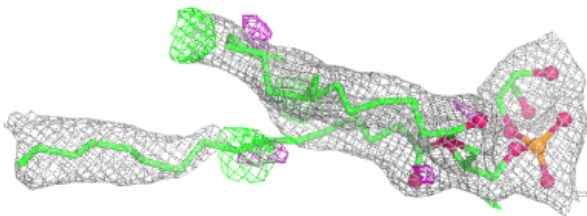
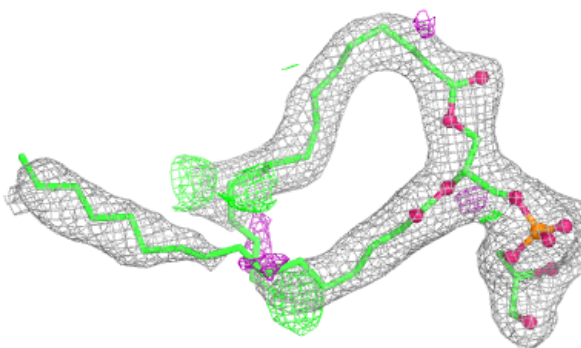


Electron density around LHG D 411 (A):

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

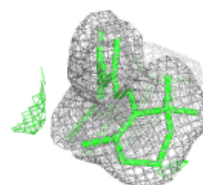
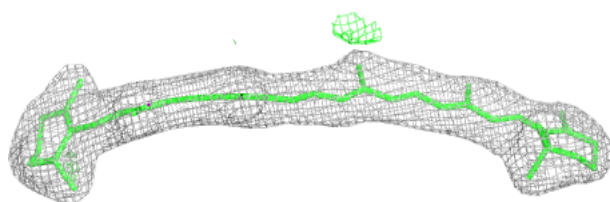
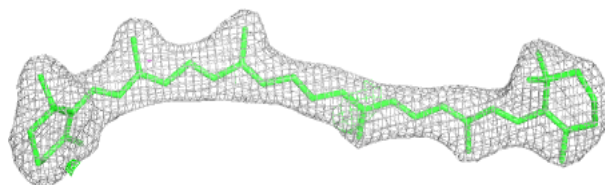
**Electron density around LHG D 411 (B):**

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



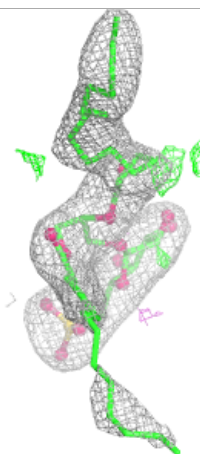
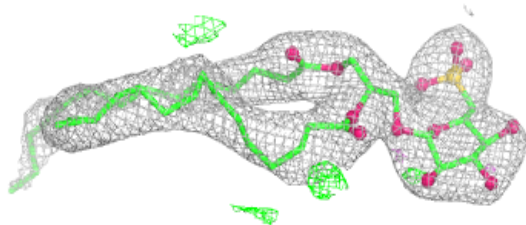
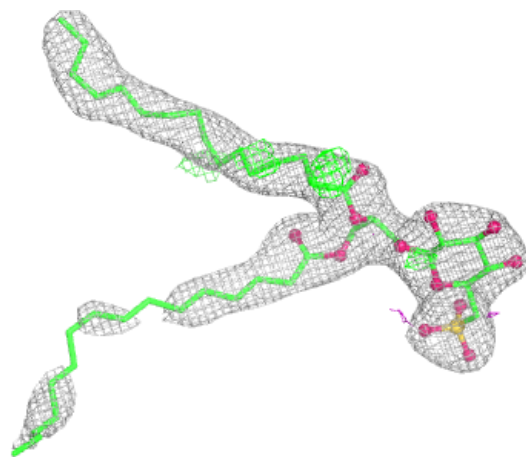
Electron density around BCR t 103:

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



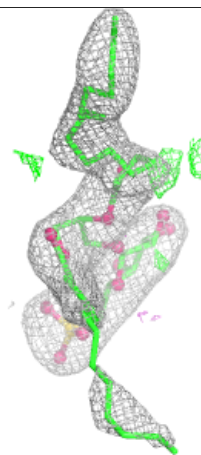
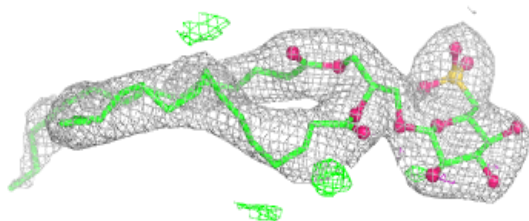
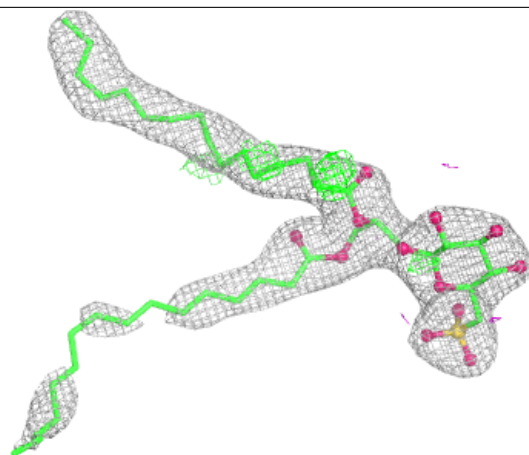
Electron density around SQD A 410 (A):

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



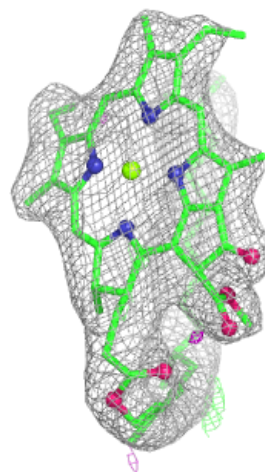
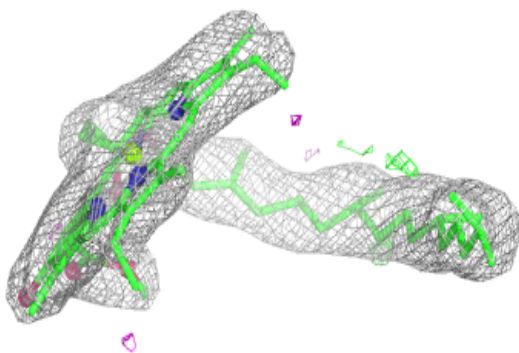
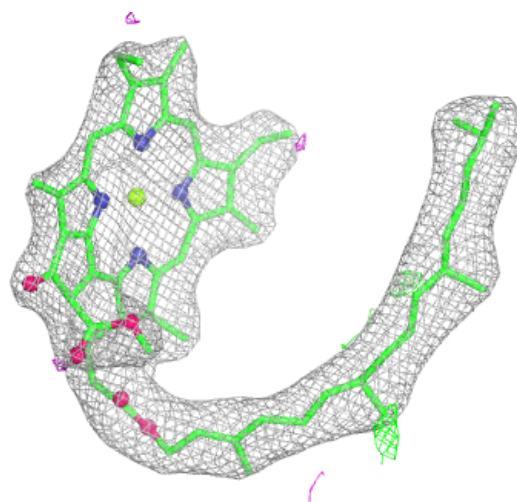
Electron density around SQD A 410 (B):

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



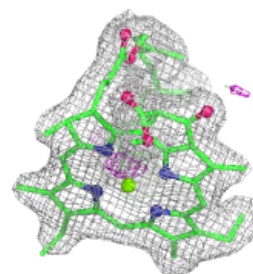
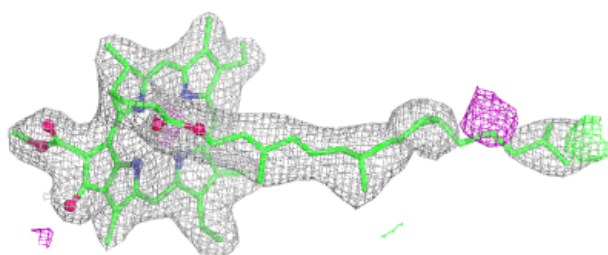
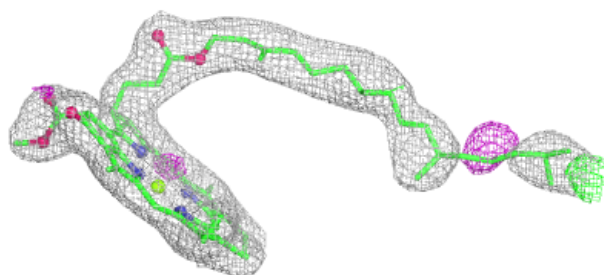
Electron density around CLA c 508:

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

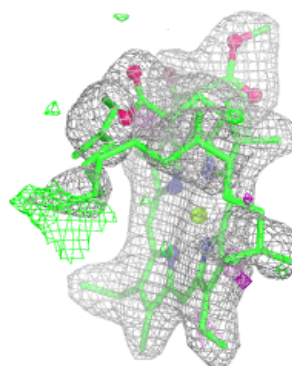
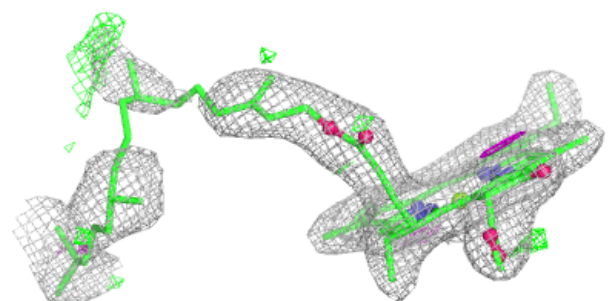
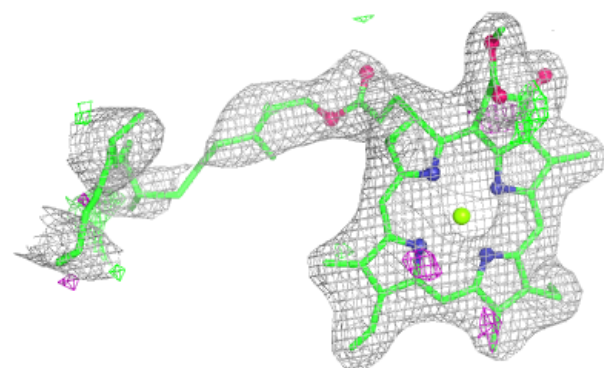


Electron density around CLA C 505:

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

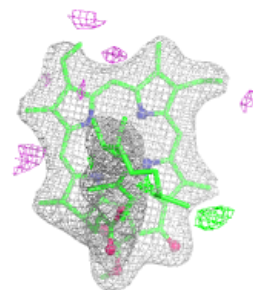
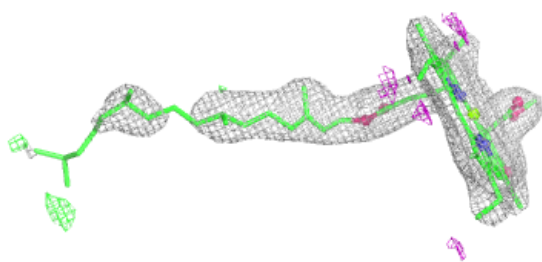
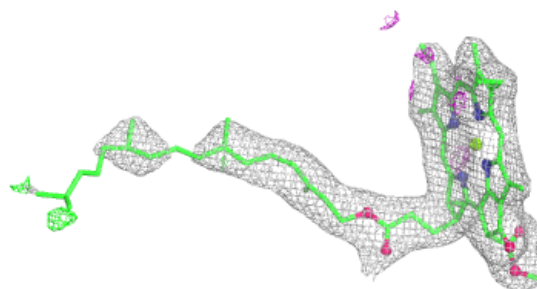
**Electron density around CLA A 408:**

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

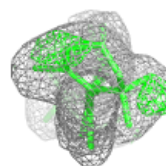
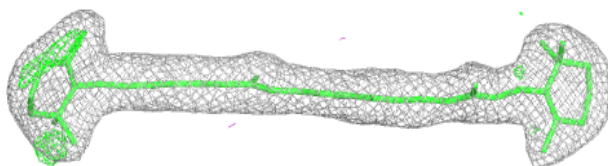
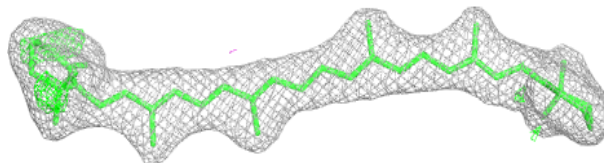


Electron density around CLA d 403:

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

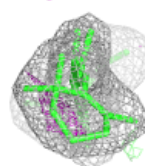
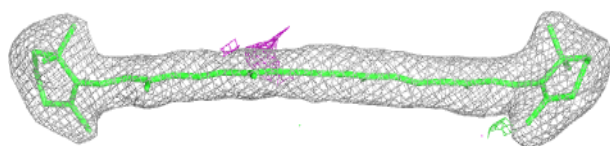
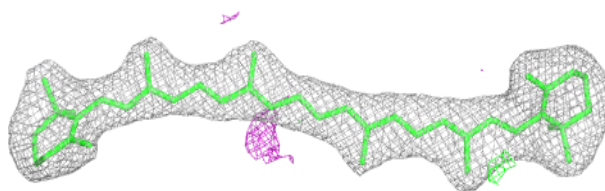
**Electron density around BCR A 409:**

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

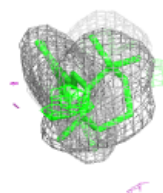
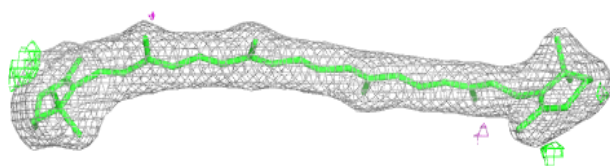
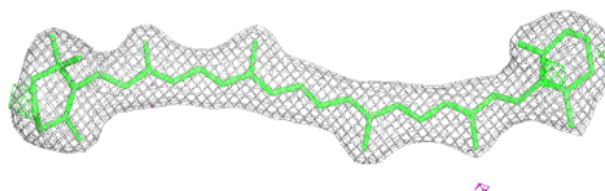


Electron density around BCR B 618:

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

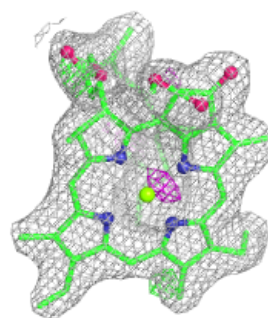
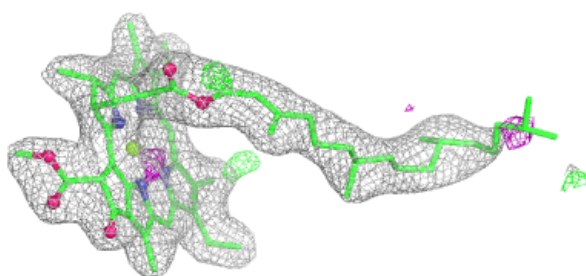
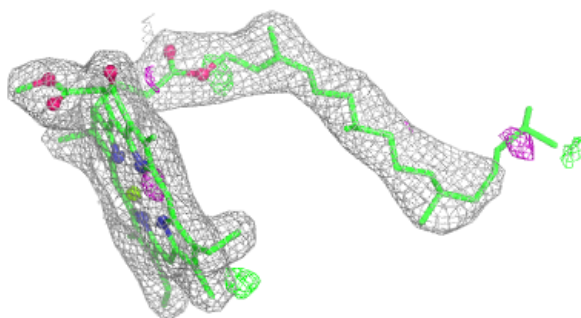
**Electron density around BCR B 619:**

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

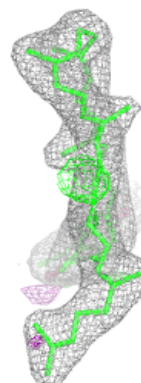
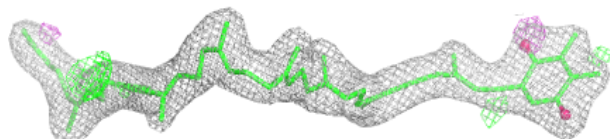
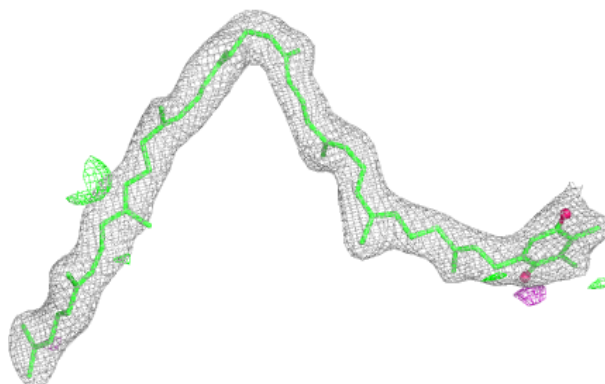


Electron density around CLA C 509:

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

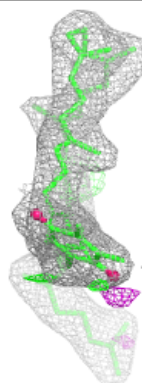
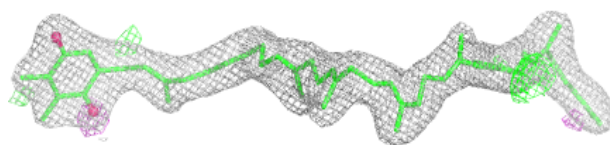
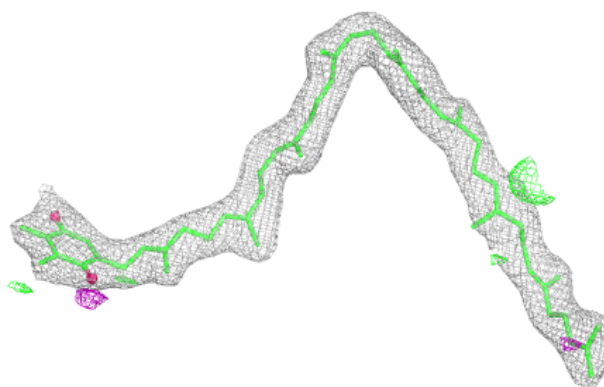
**Electron density around PL9 D 408 (A):**

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



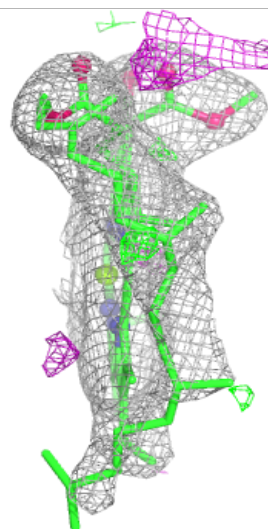
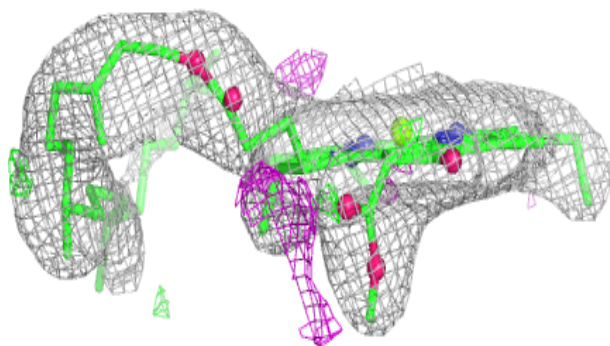
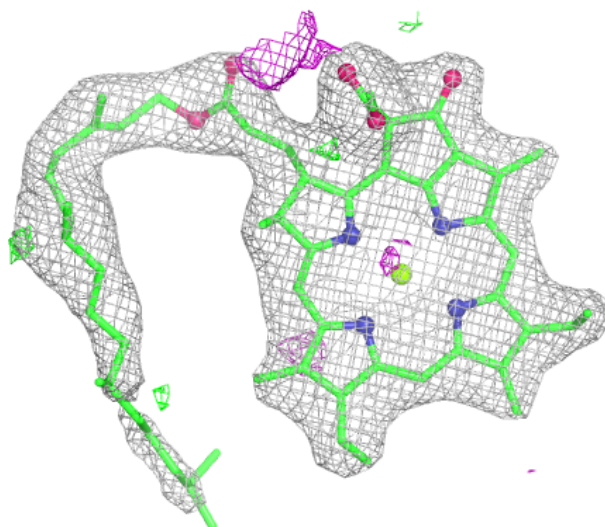
Electron density around PL9 D 408 (B):

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



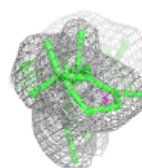
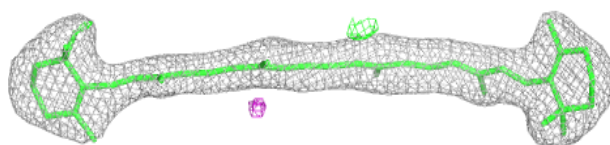
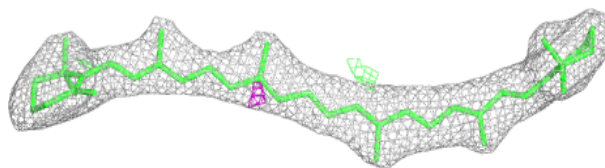
Electron density around CLA C 513:

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

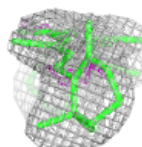
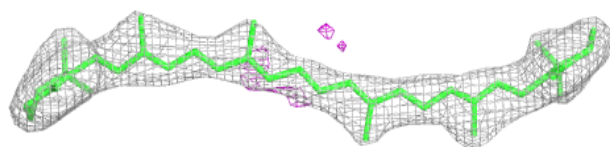
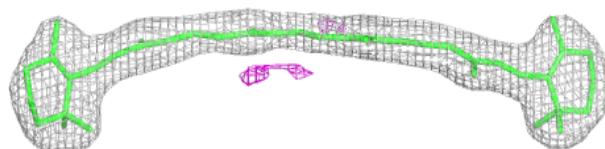


Electron density around BCR H 101:

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

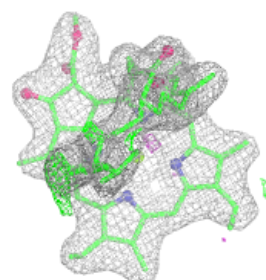
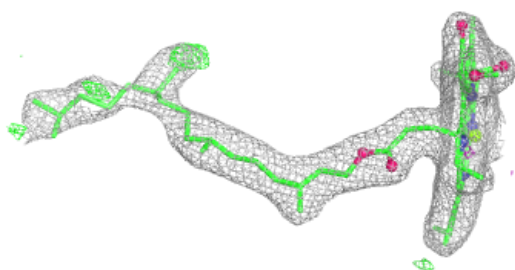
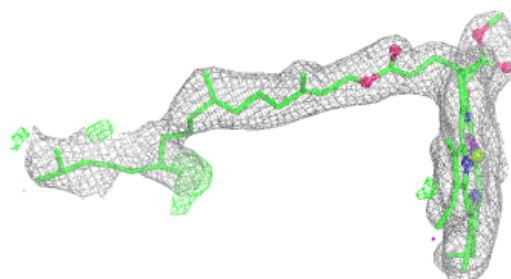
**Electron density around BCR K 102:**

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

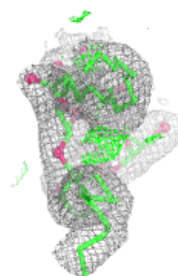
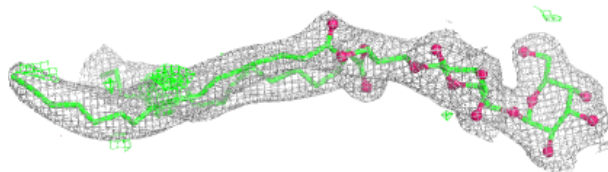
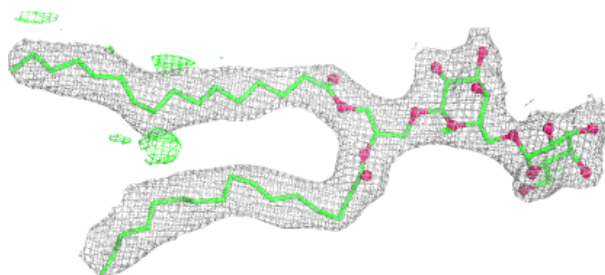


Electron density around CLA B 606:

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

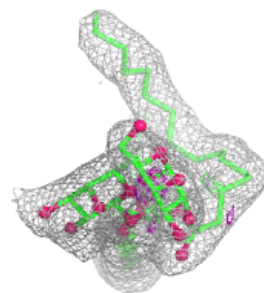
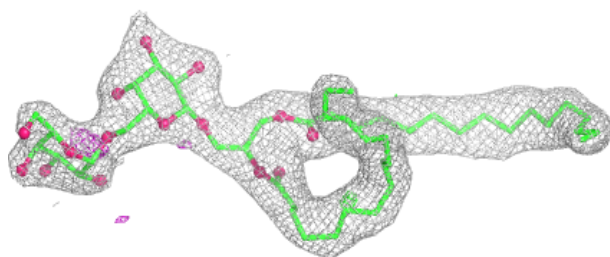
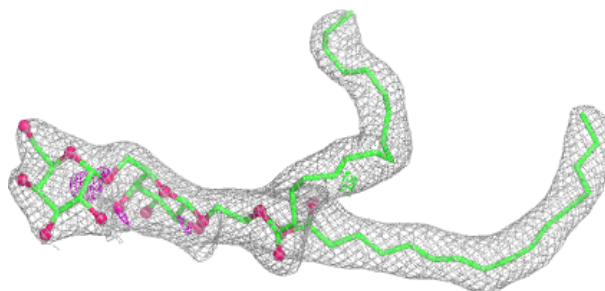
**Electron density around DGD C 519:**

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

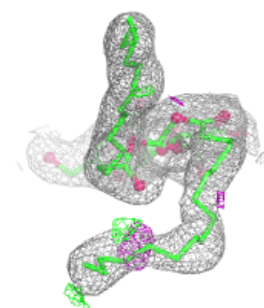
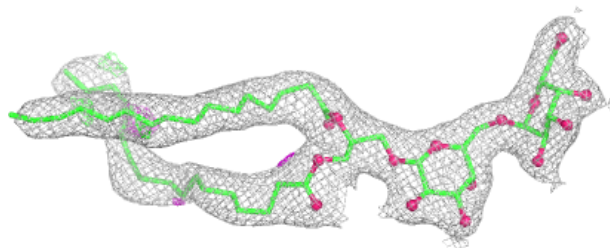
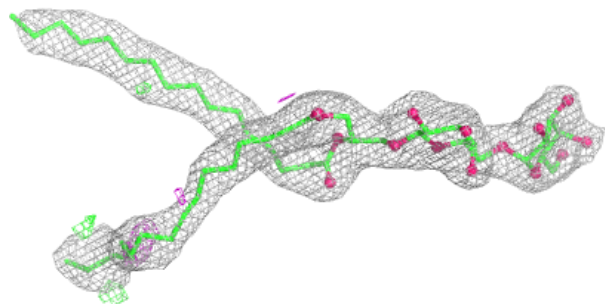


Electron density around DGD H 102:

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

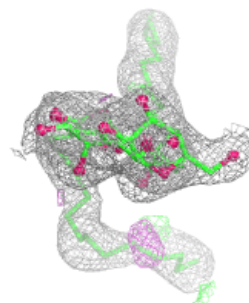
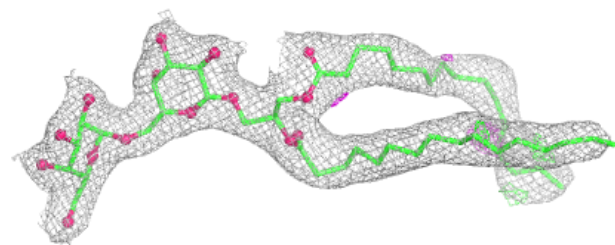
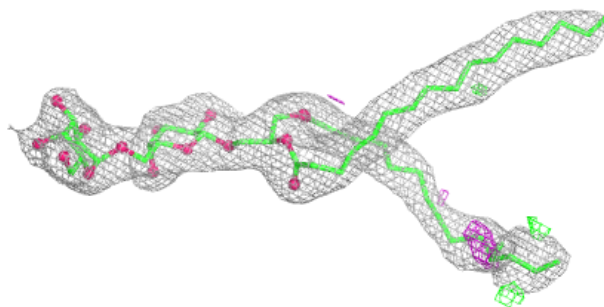
**Electron density around DGD c 517 (A):**

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

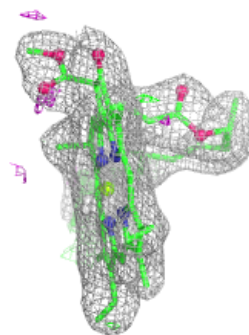
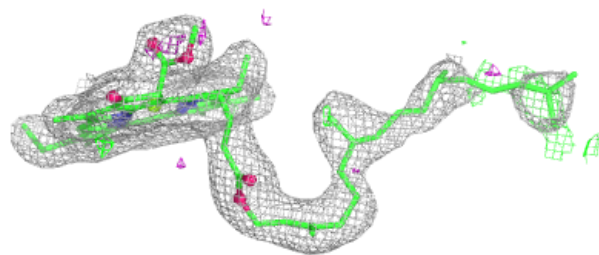
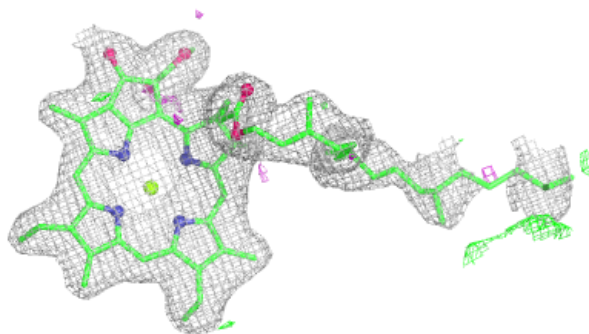


Electron density around DGD c 517 (B):

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

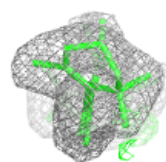
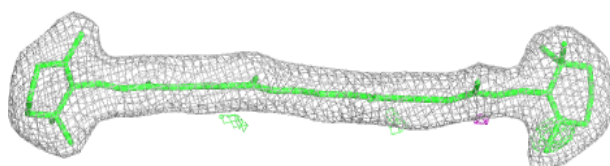
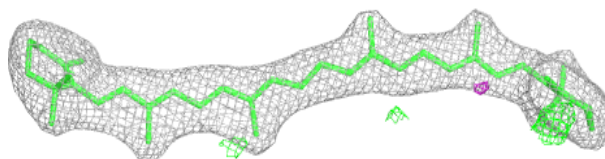
**Electron density around CLA a 407 (A):**

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

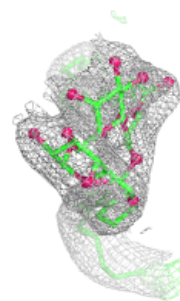
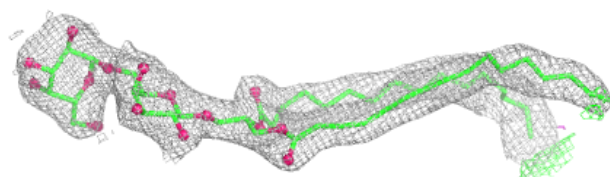
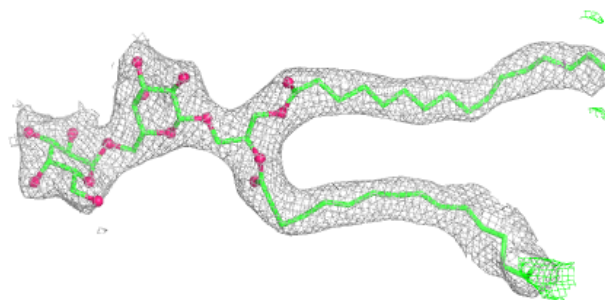


Electron density around BCR a 410:

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

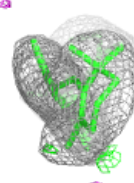
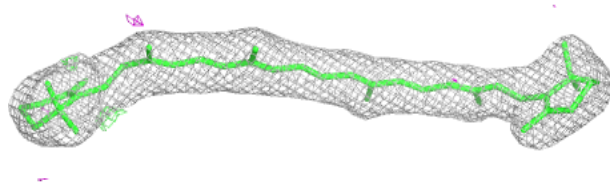
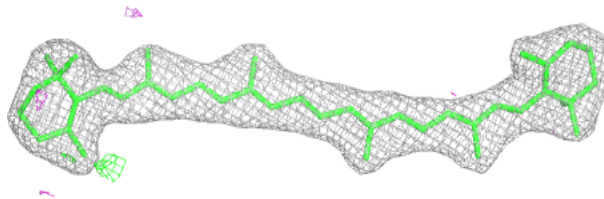
**Electron density around DGD c 519:**

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

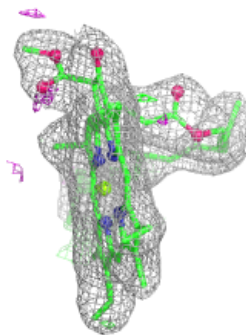
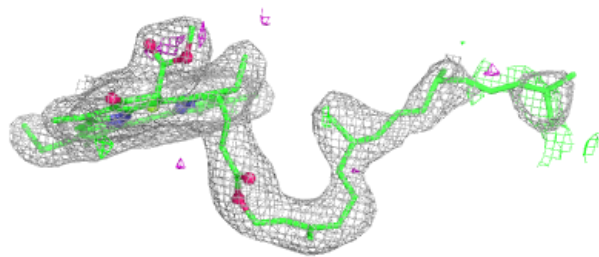
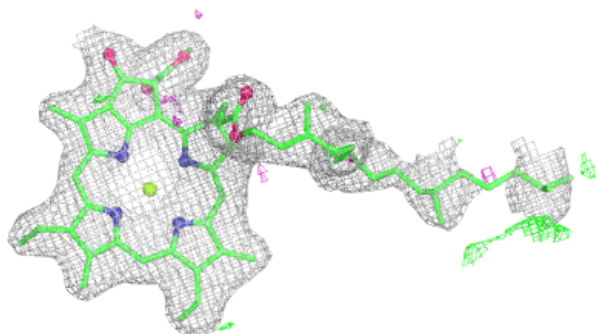


Electron density around BCR b 619:

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

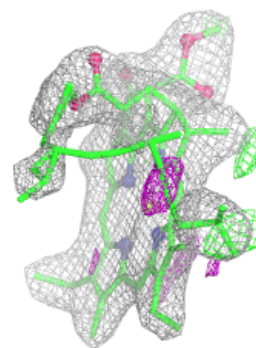
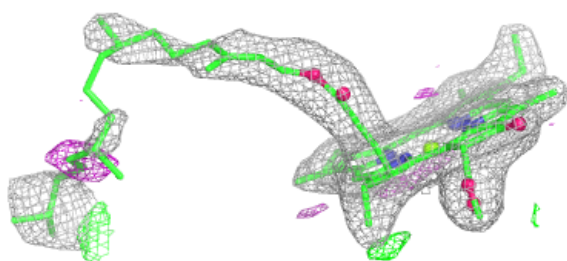
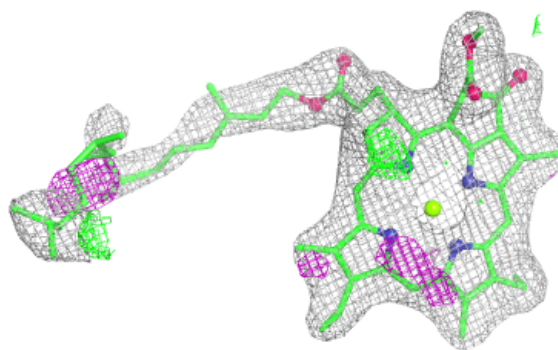
**Electron density around CLA a 407 (B):**

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

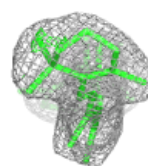
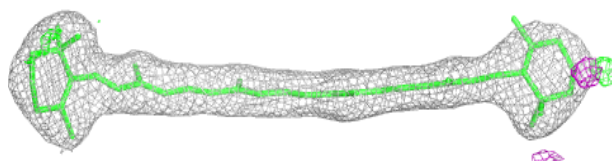
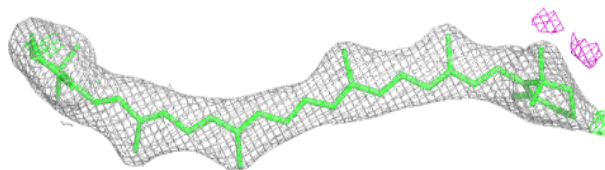


Electron density around CLA a 409:

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

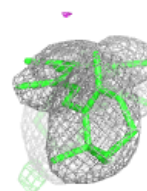
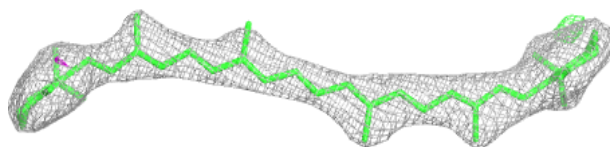
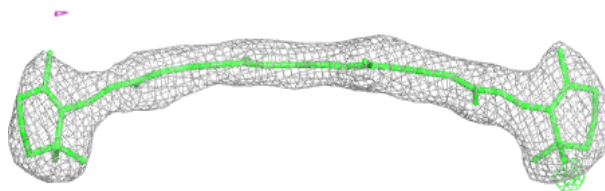
**Electron density around BCR h 101:**

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

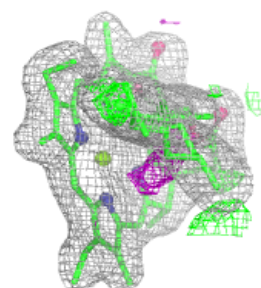
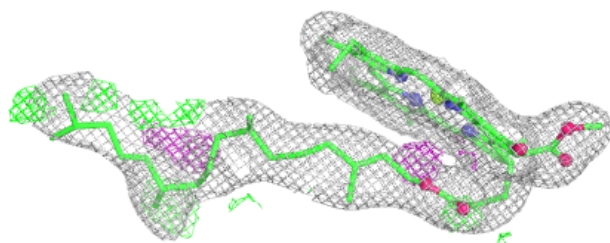
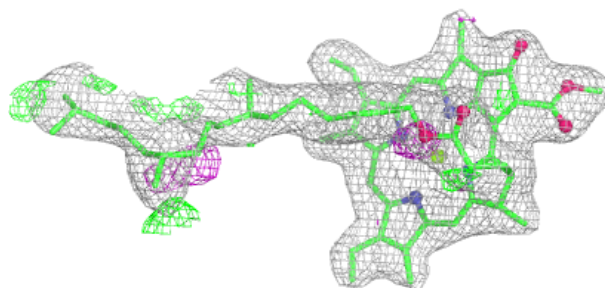


Electron density around BCR k 101:

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

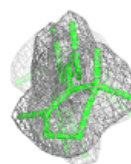
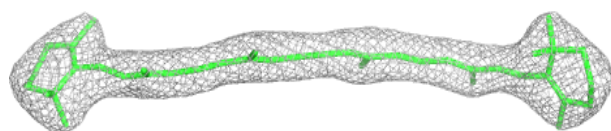
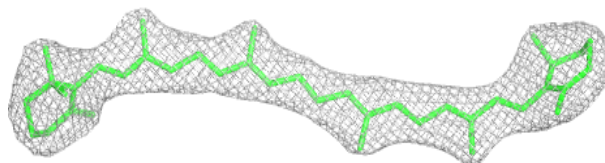
**Electron density around CLA B 614:**

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

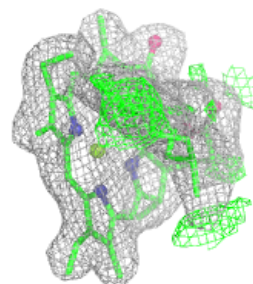
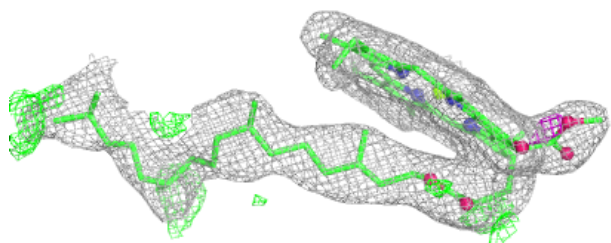
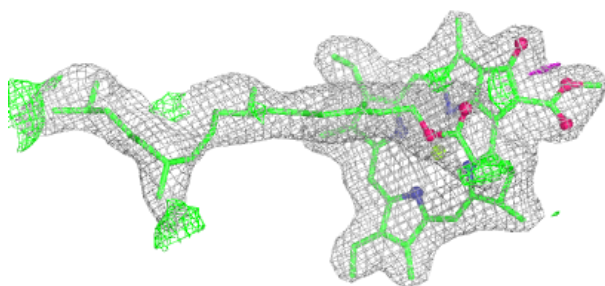


Electron density around BCR y 101:

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

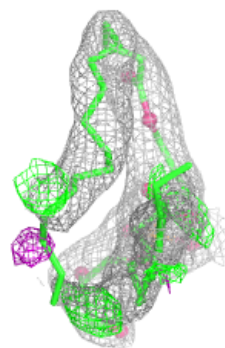
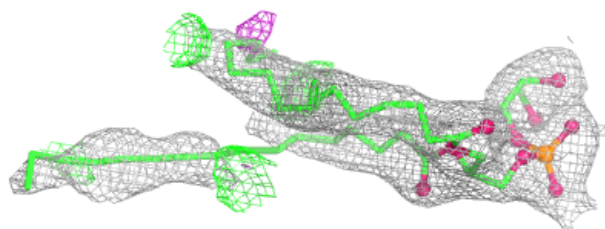
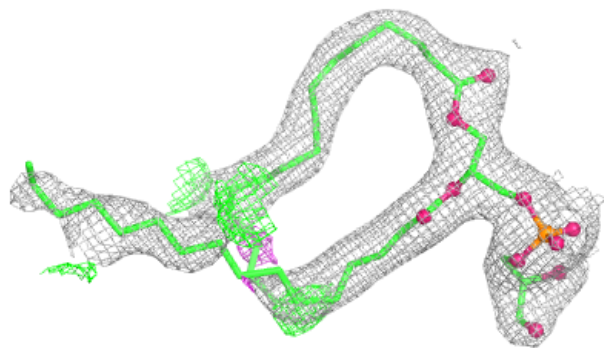
**Electron density around CLA b 614:**

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

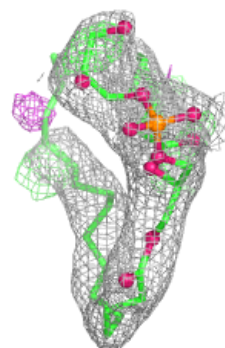
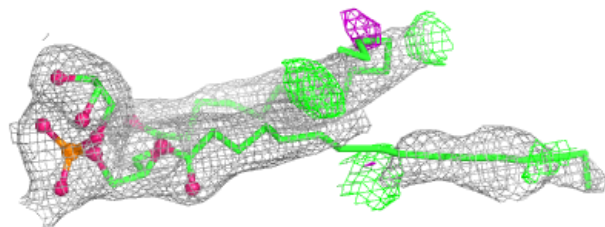
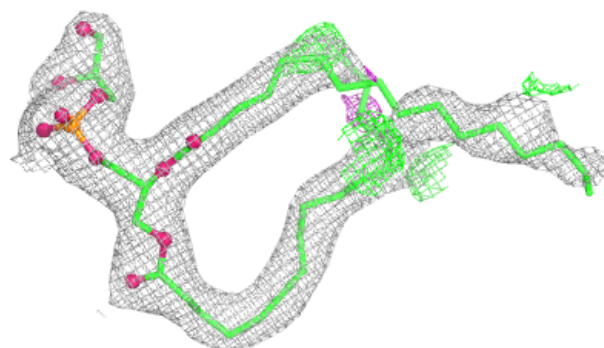


Electron density around LHG d 408 (A):

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

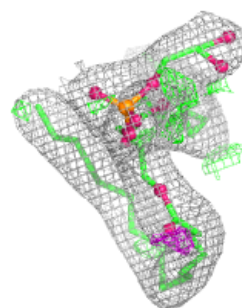
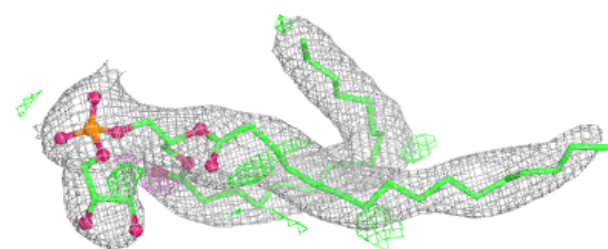
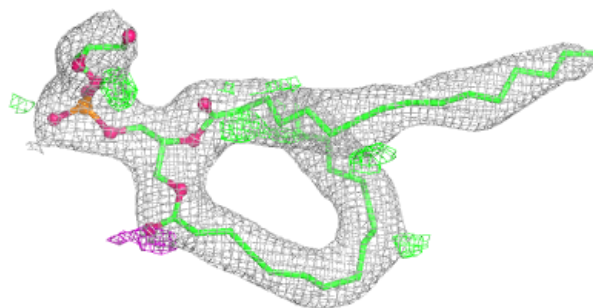
**Electron density around LHG d 408 (B):**

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

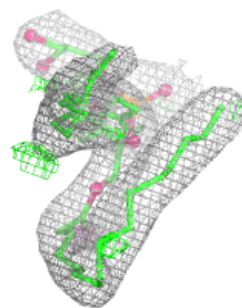
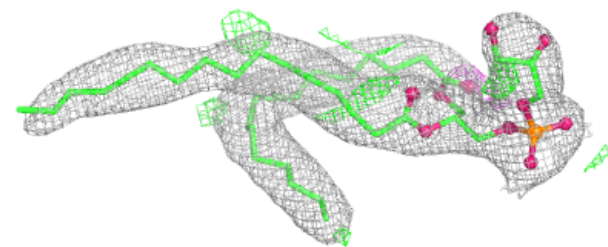
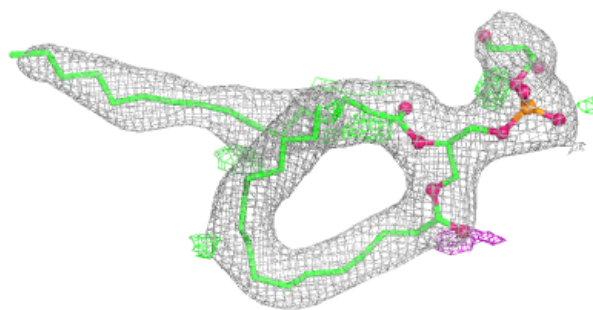


Electron density around LHG d 711 (A):

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

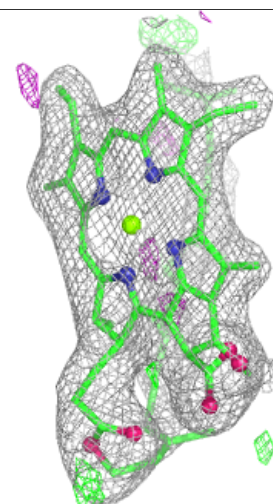
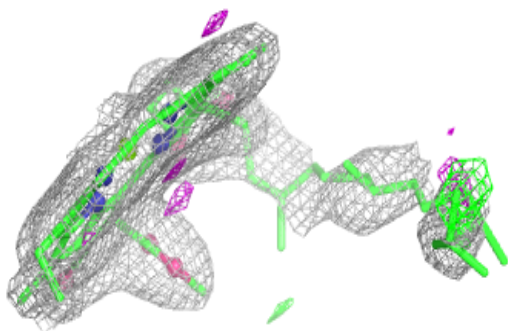
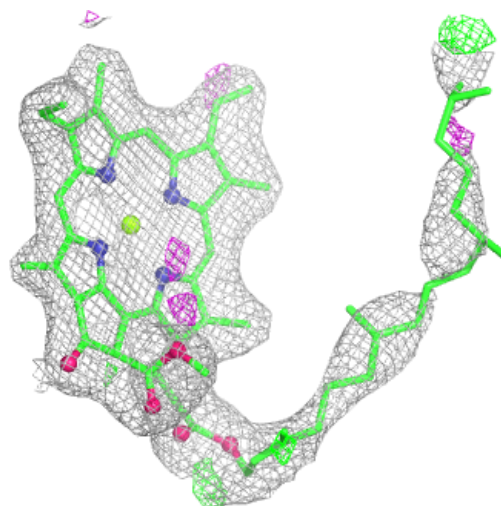
**Electron density around LHG d 711 (B):**

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



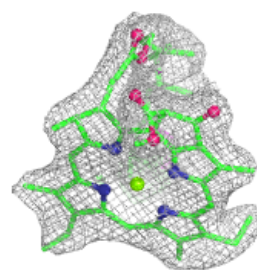
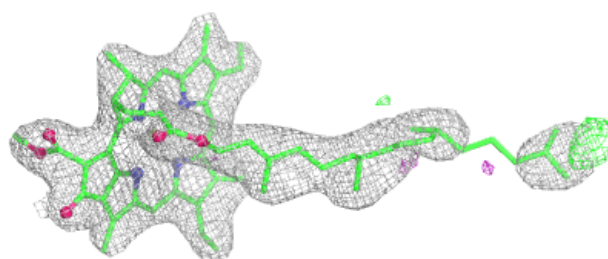
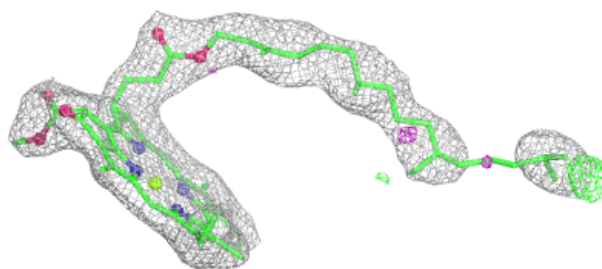
Electron density around CLA B 616:

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



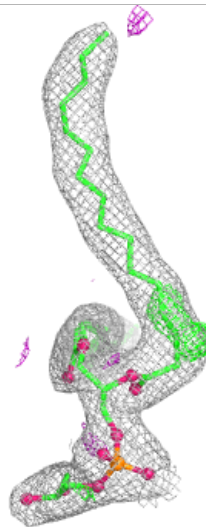
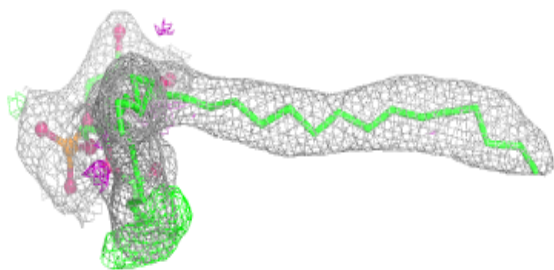
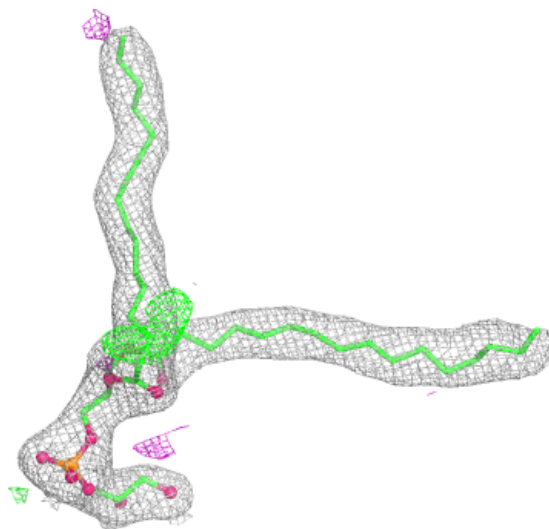
Electron density around CLA c 505:

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



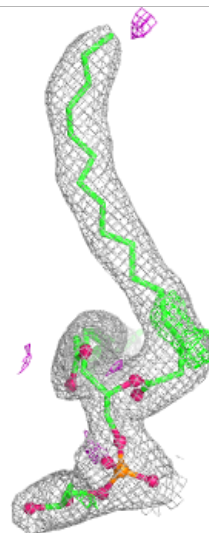
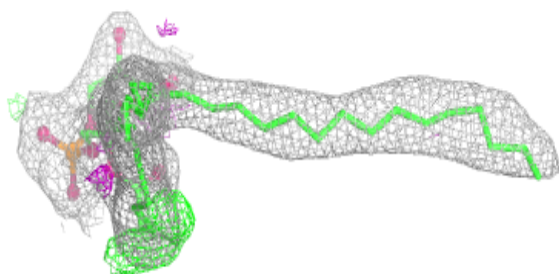
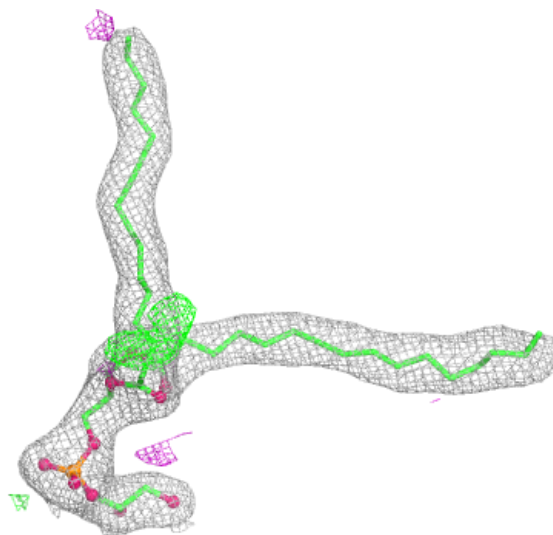
Electron density around LHG 1 101 (A):

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



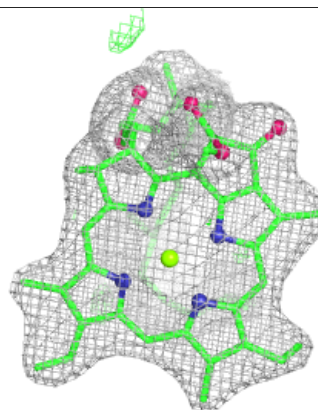
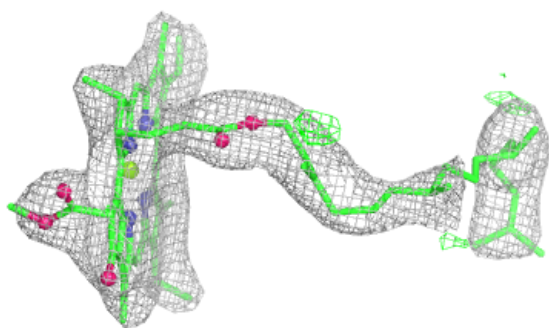
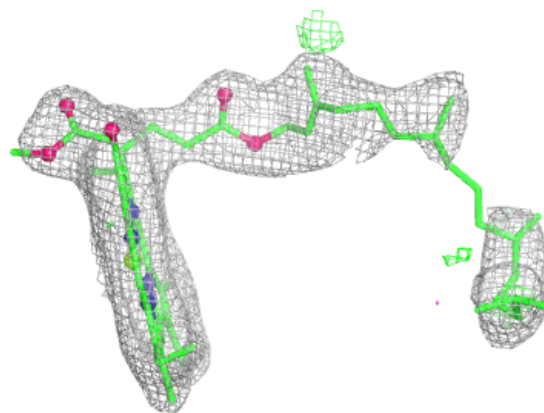
Electron density around LHG 1 101 (B):

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

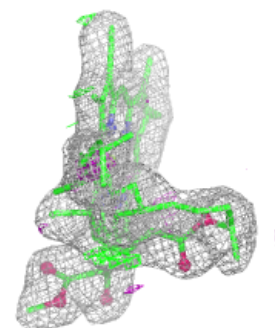
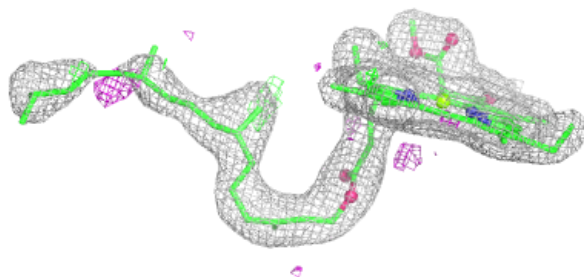
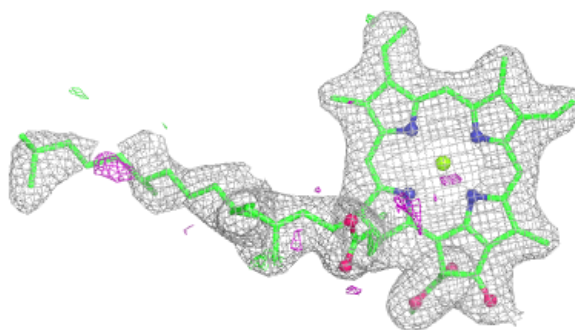


Electron density around CLA c 507:

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

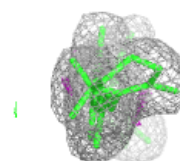
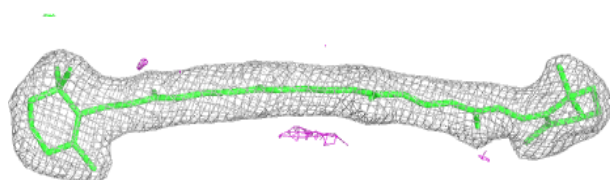
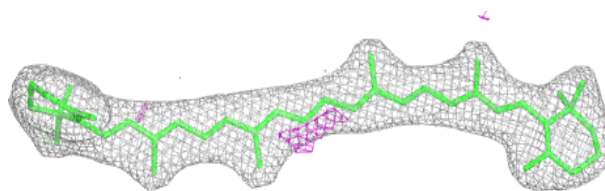
**Electron density around CLA A 406 (B):**

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

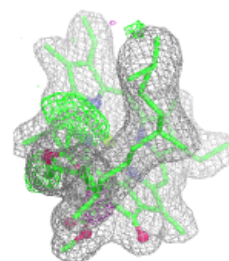
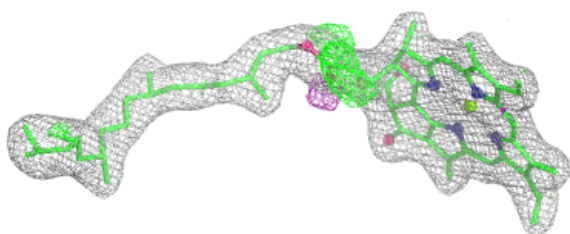
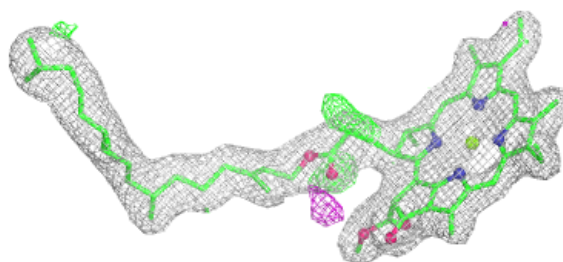


Electron density around BCR B 617:

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

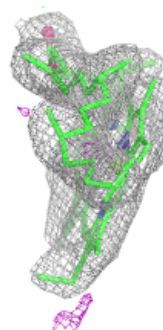
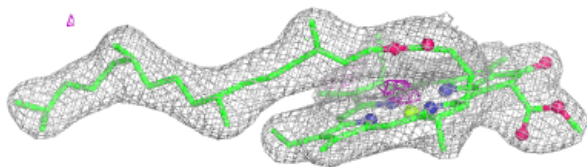
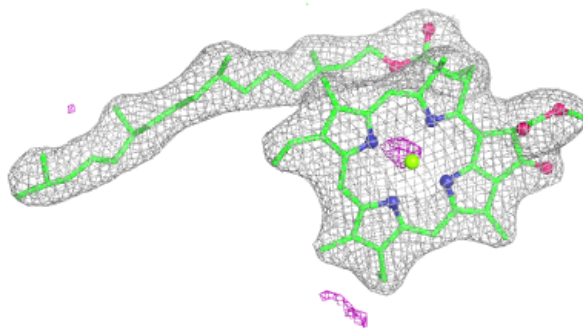
**Electron density around CLA A 404 (A):**

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

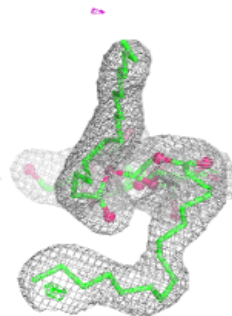
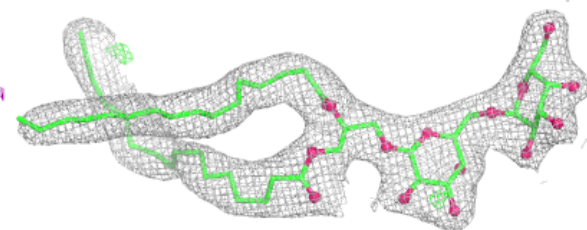
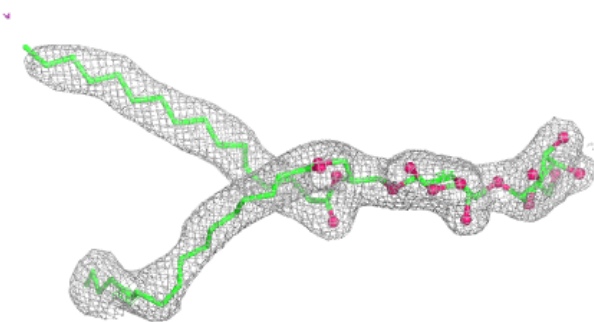


Electron density around CLA C 502:

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

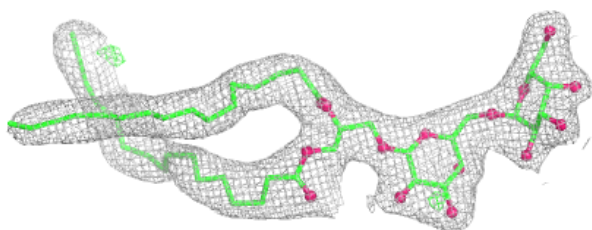
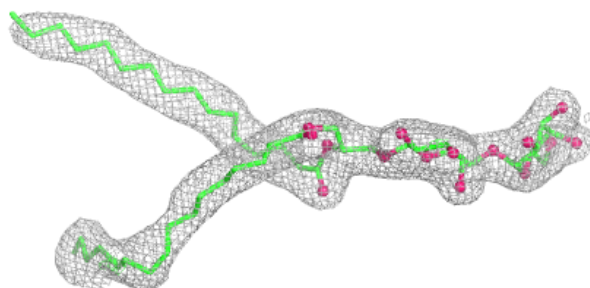
**Electron density around DGD C 517 (A):**

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

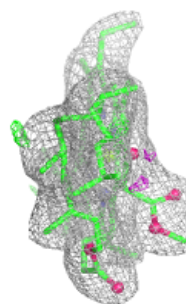
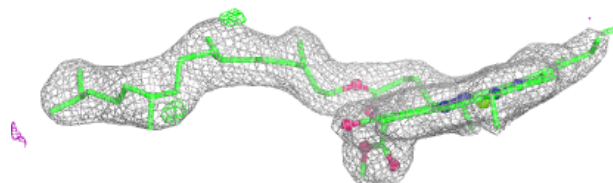
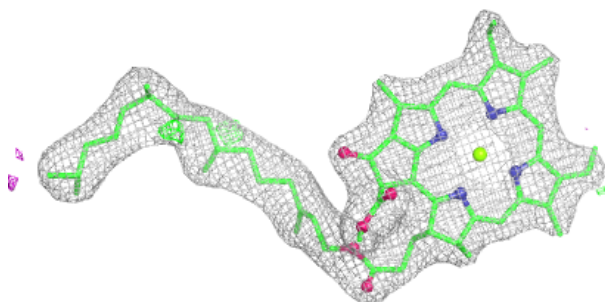


Electron density around DGD C 517 (B):

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

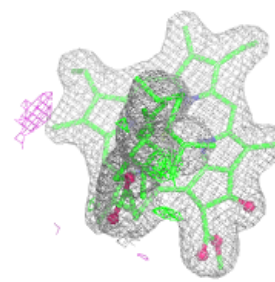
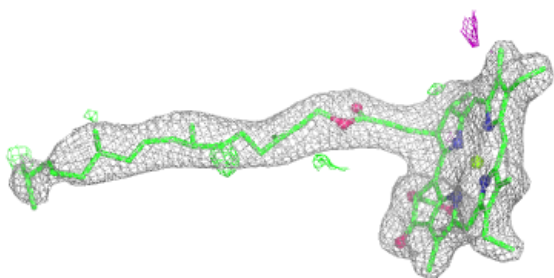
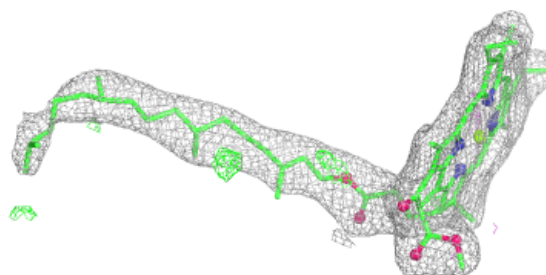
**Electron density around CLA b 602:**

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

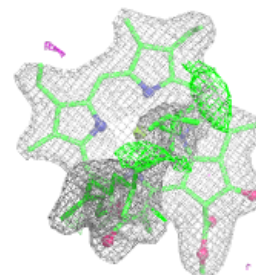
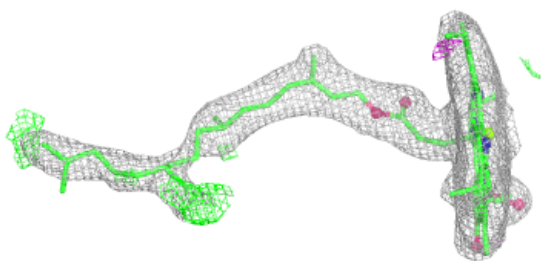
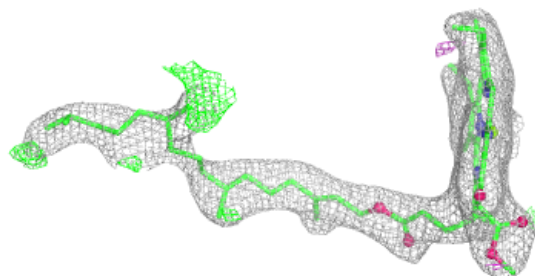


Electron density around CLA b 604:

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

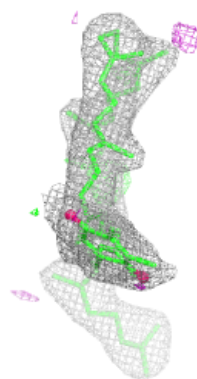
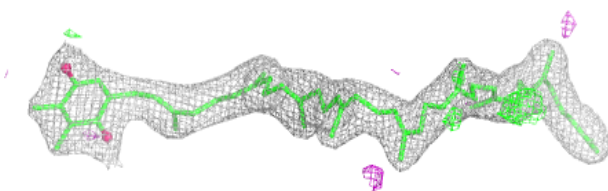
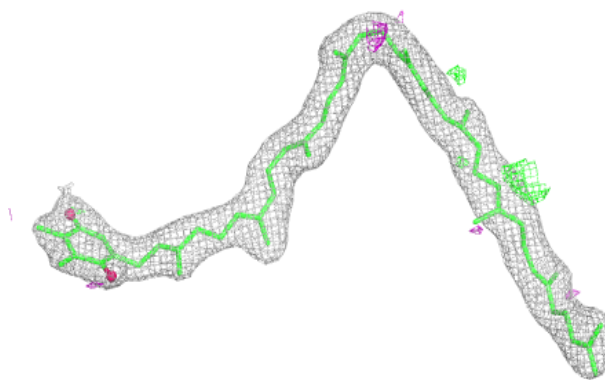
**Electron density around CLA b 606:**

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

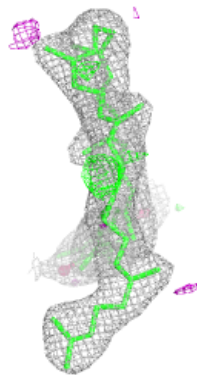
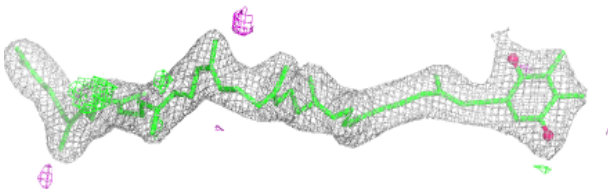
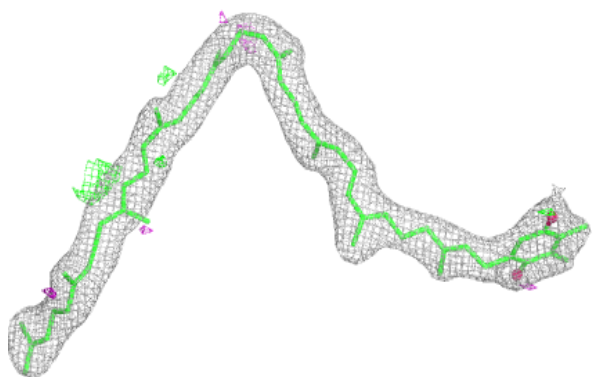


Electron density around PL9 d 405 (A):

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

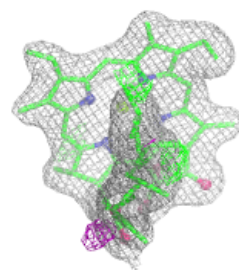
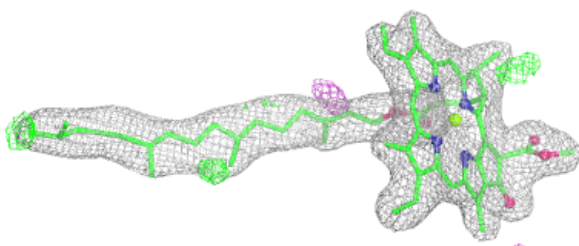
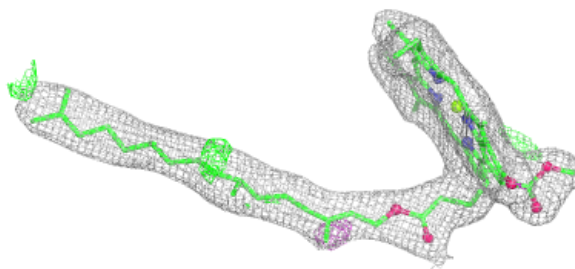
**Electron density around PL9 d 405 (B):**

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



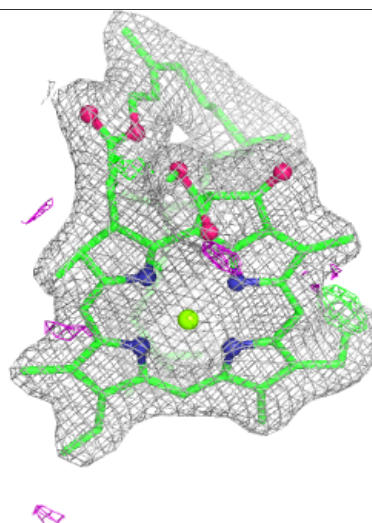
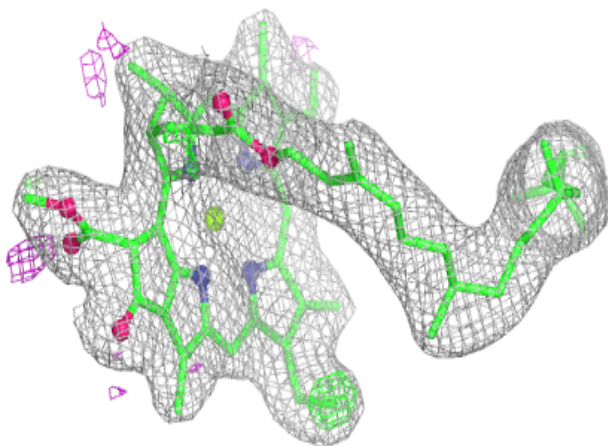
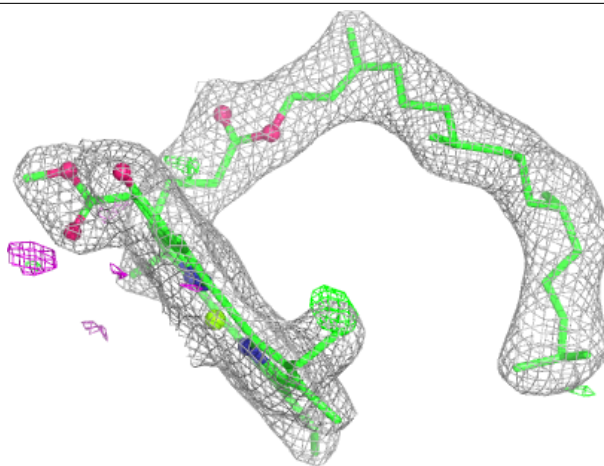
Electron density around CLA b 607:

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



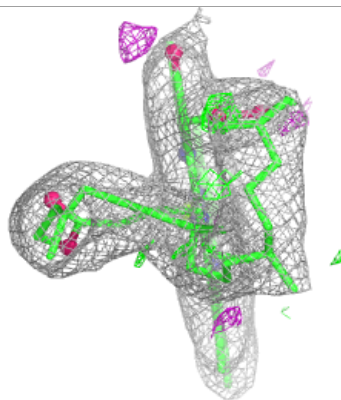
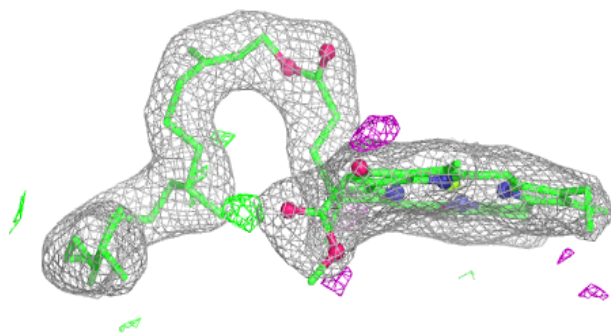
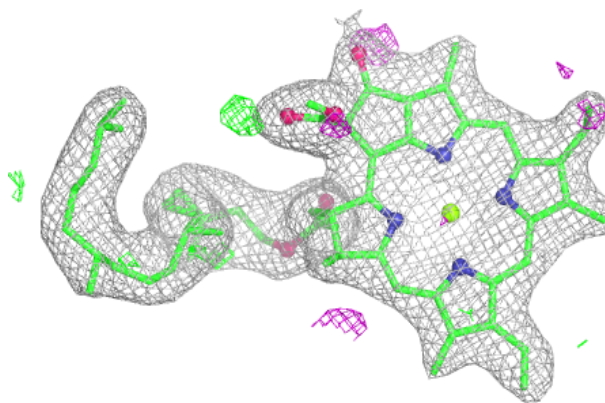
Electron density around CLA b 611:

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

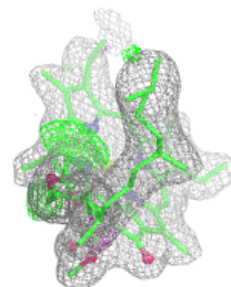
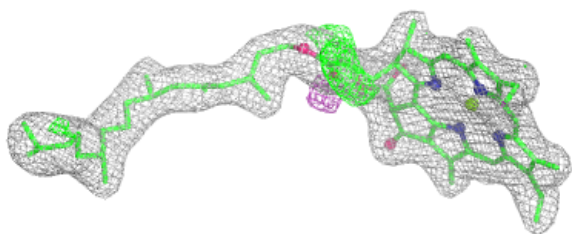
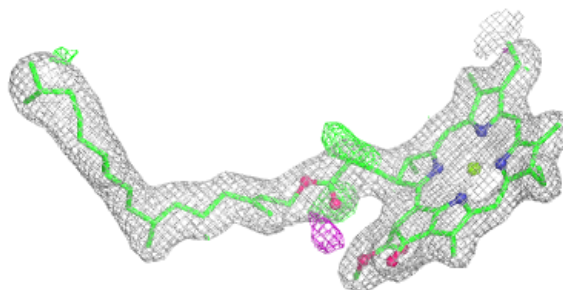


Electron density around CLA b 612:

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

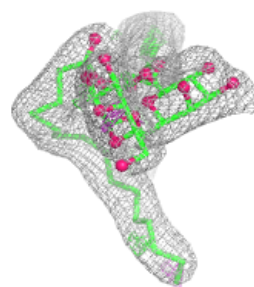
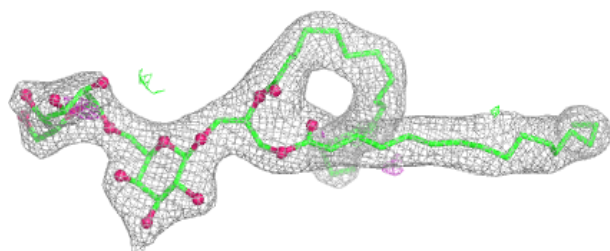
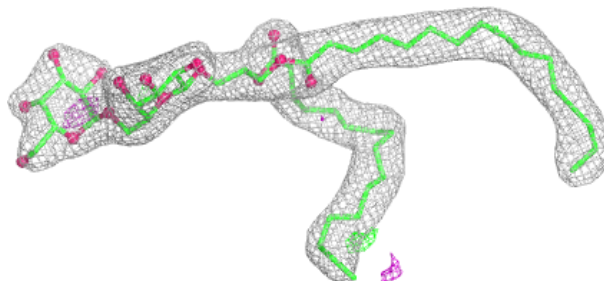
**Electron density around CLA A 404 (B):**

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

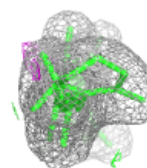
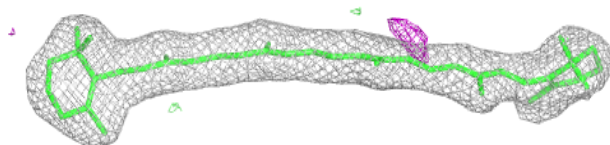
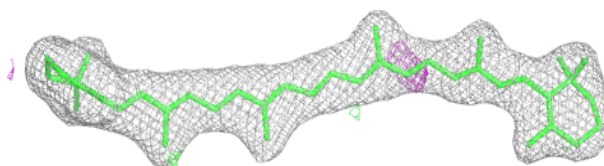


Electron density around DGD h 102:

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

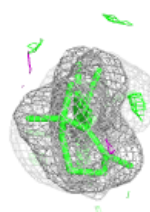
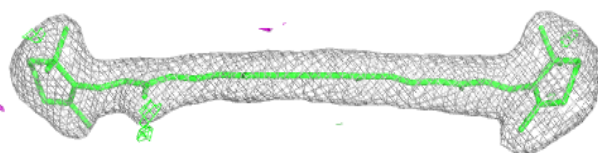
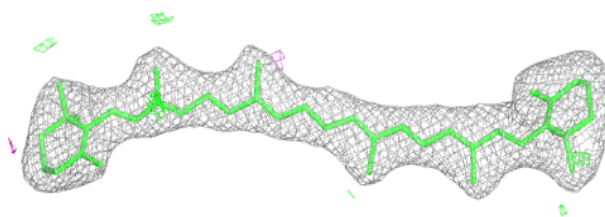
**Electron density around BCR b 617:**

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

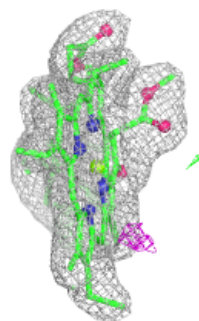
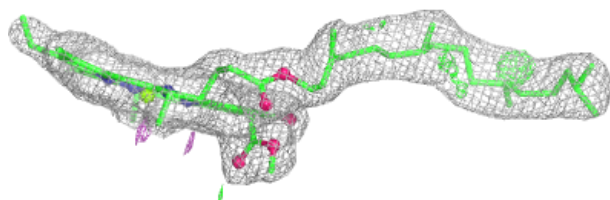
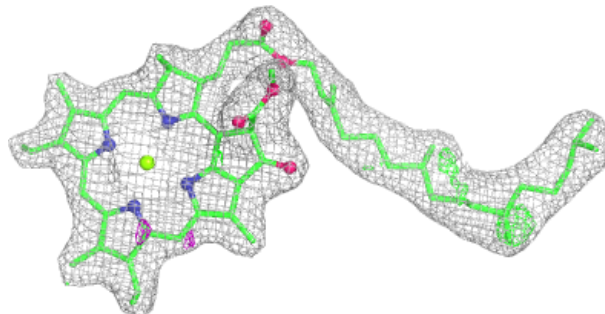


Electron density around BCR b 618:

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

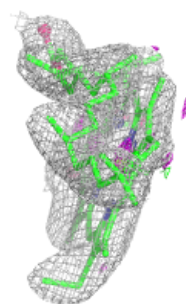
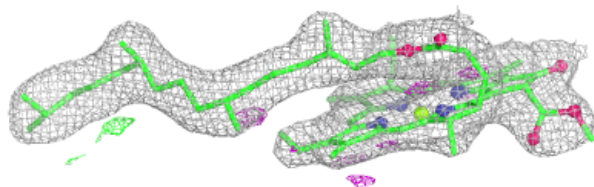
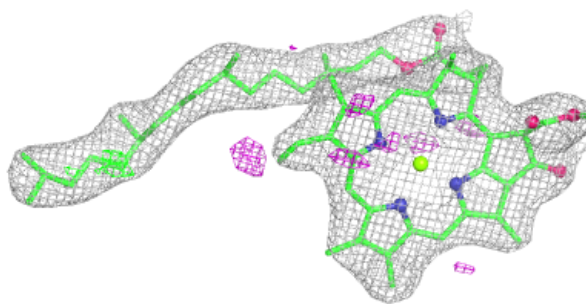
**Electron density around CLA B 602:**

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

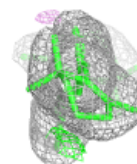
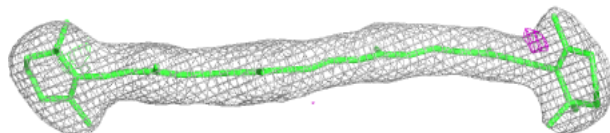
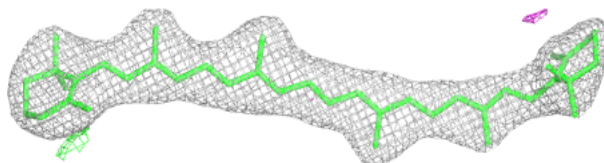


Electron density around CLA c 502:

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

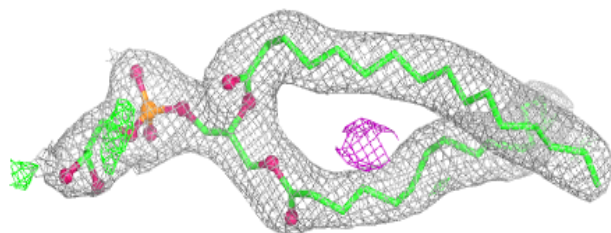
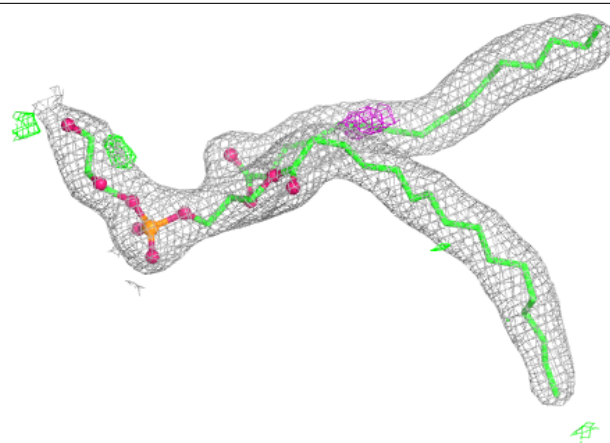
**Electron density around BCR c 516:**

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



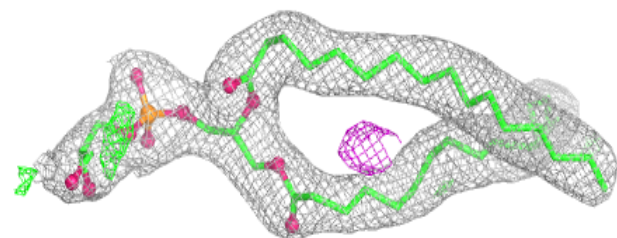
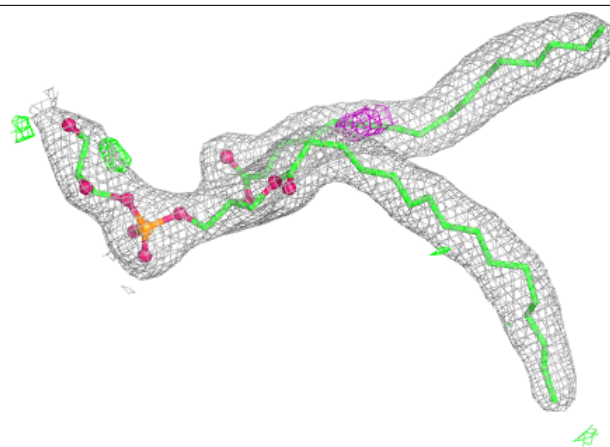
Electron density around LHG D 410 (A):

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



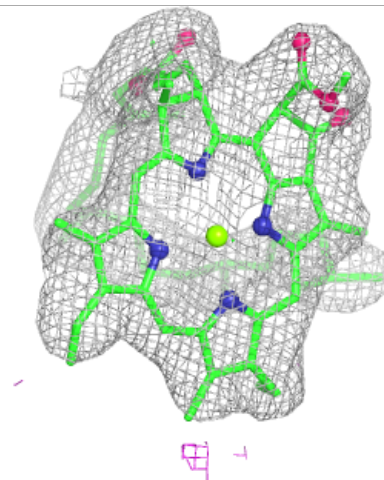
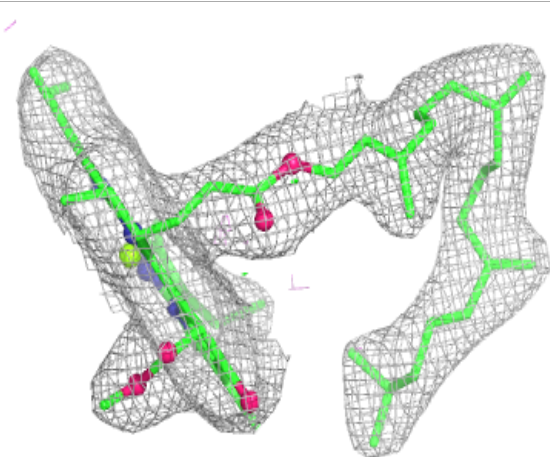
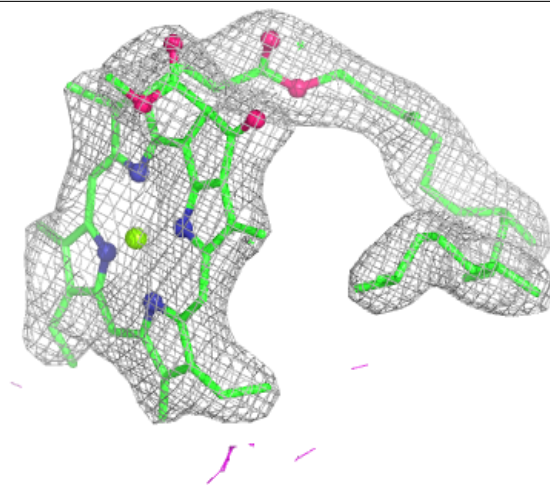
Electron density around LHG D 410 (B):

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



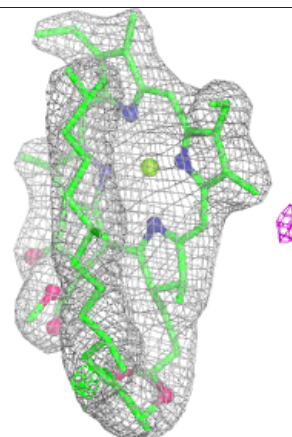
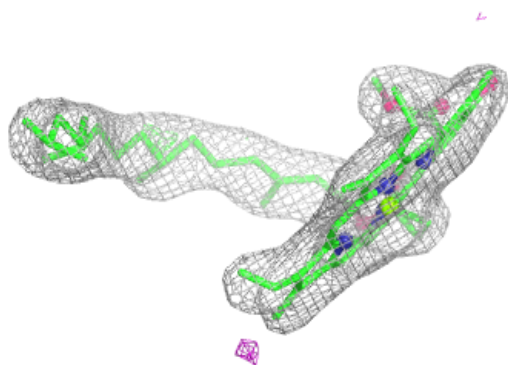
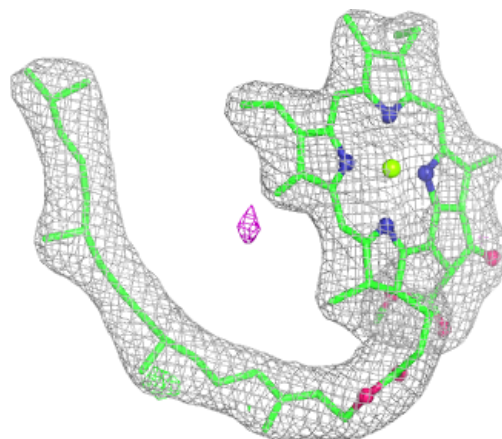
Electron density around CLA c 504:

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



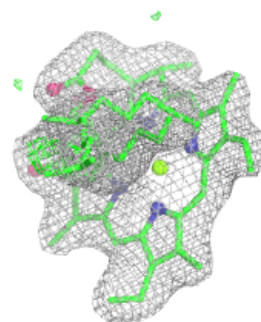
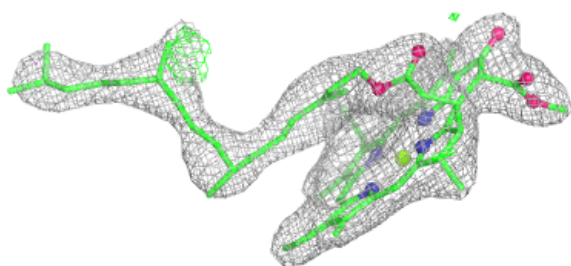
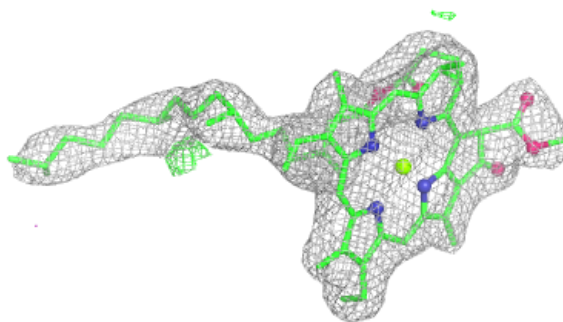
Electron density around CLA C 508:

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

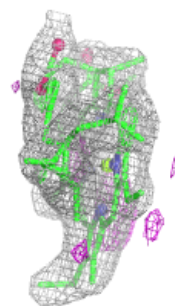
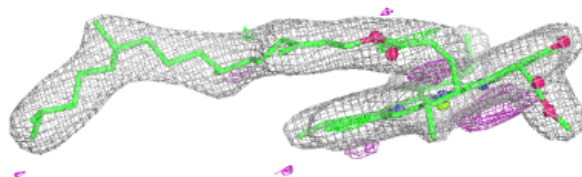
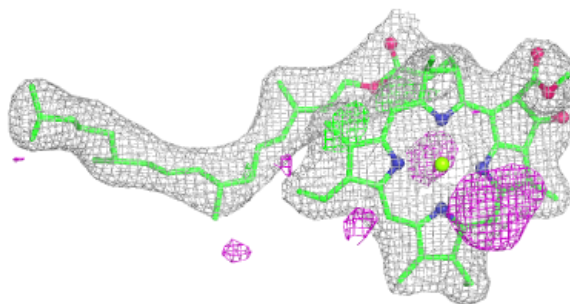


Electron density around CLA c 506:

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

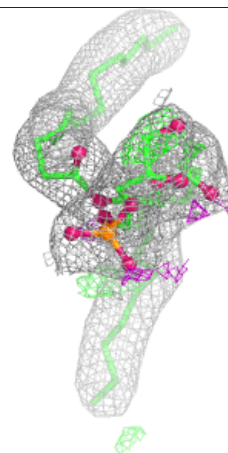
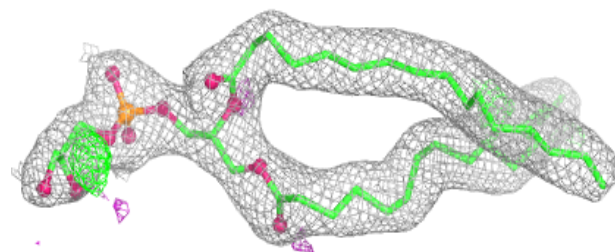
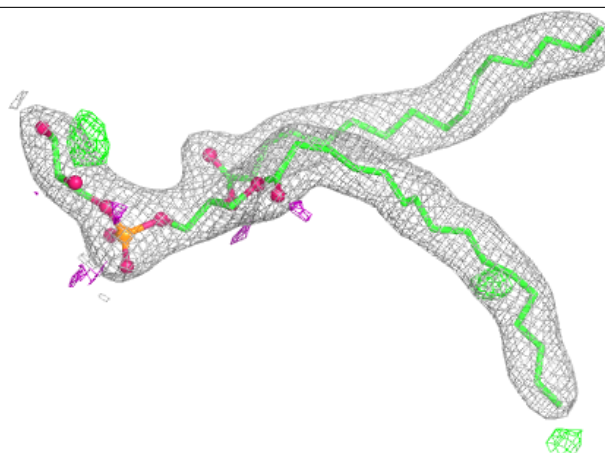
**Electron density around CLA B 603:**

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



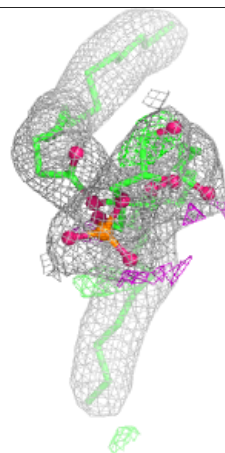
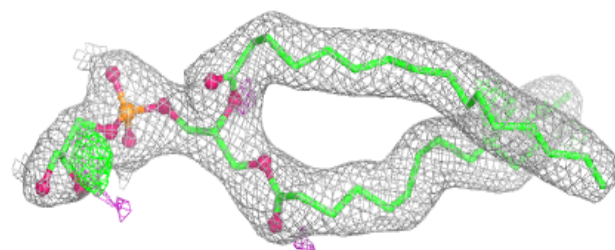
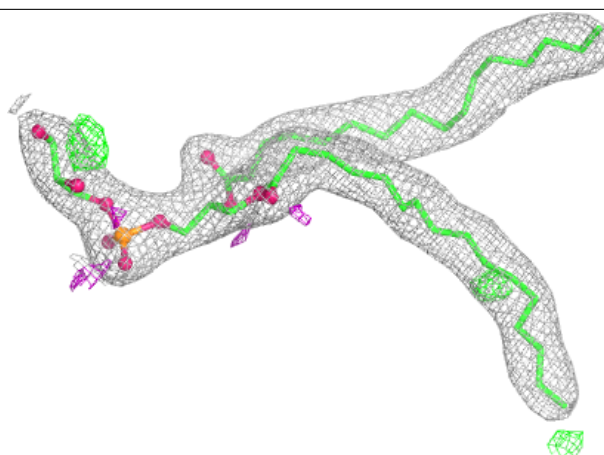
Electron density around LHG d 407 (A):

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



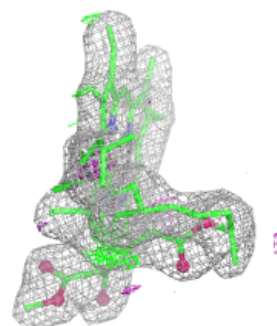
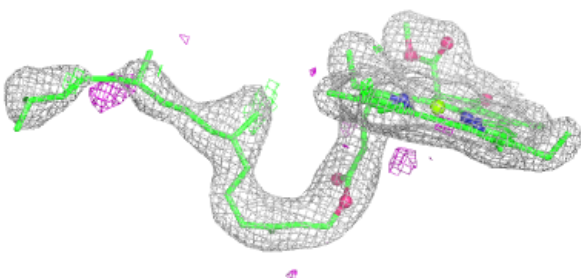
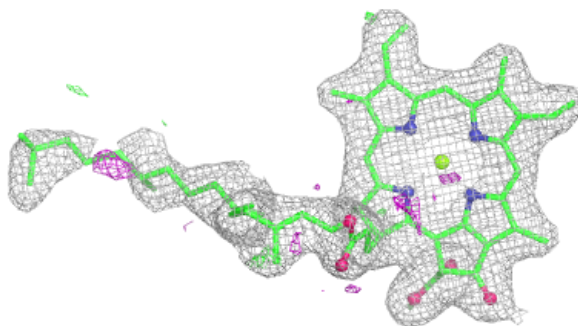
Electron density around LHG d 407 (B):

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

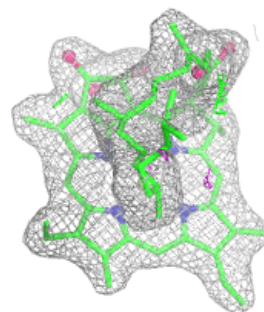
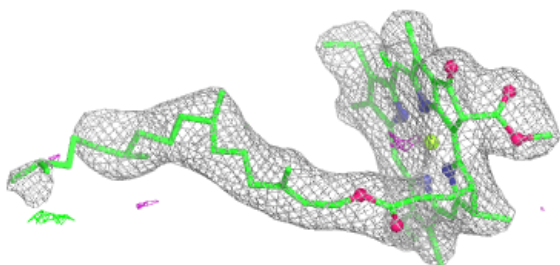
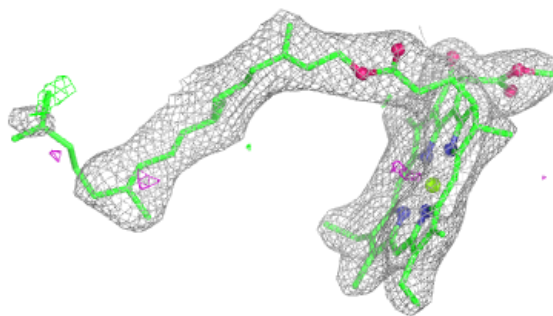


Electron density around CLA A 406 (A):

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

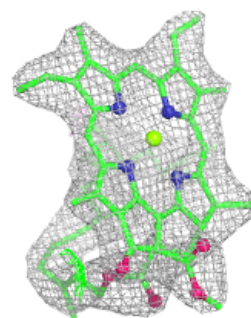
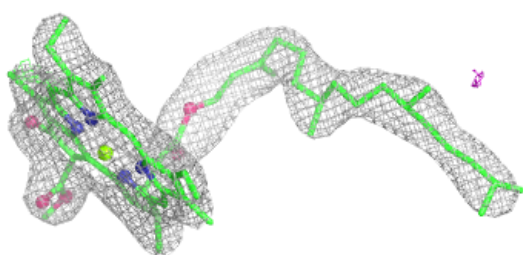
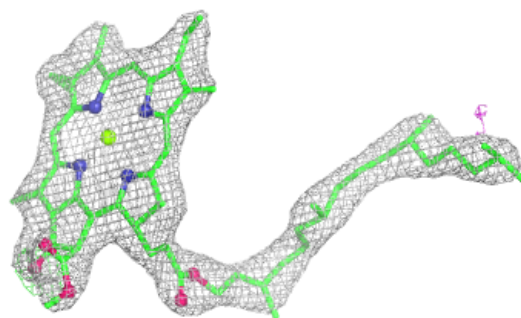
**Electron density around CLA c 509:**

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

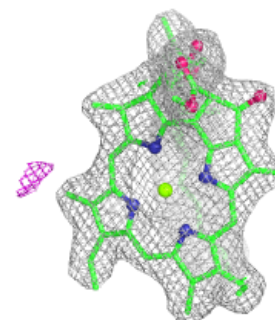
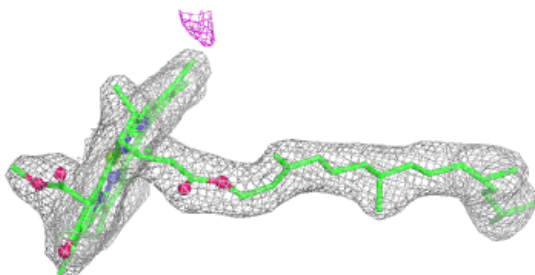
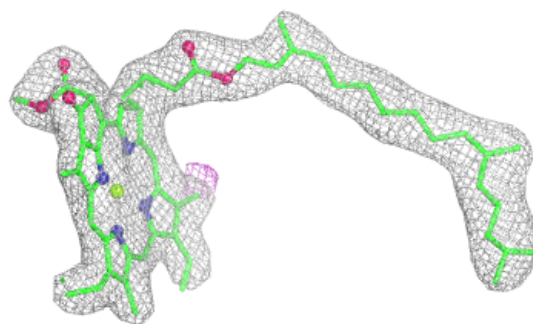


Electron density around CLA c 512:

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

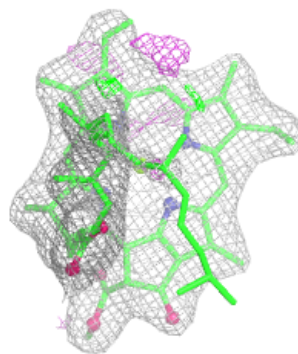
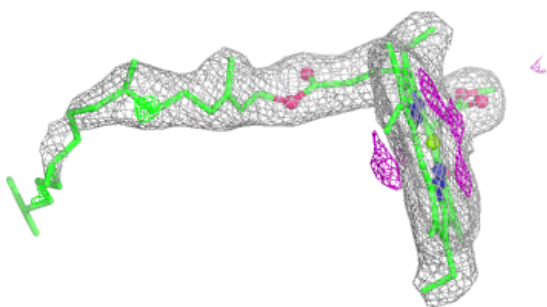
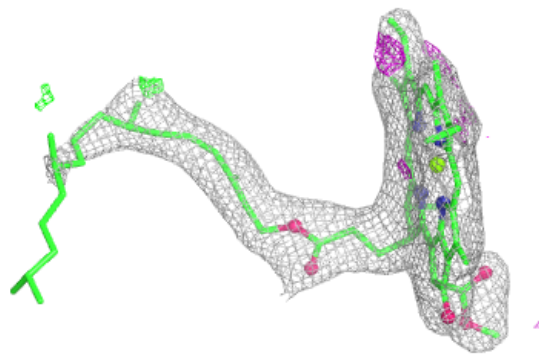
**Electron density around CLA B 609:**

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



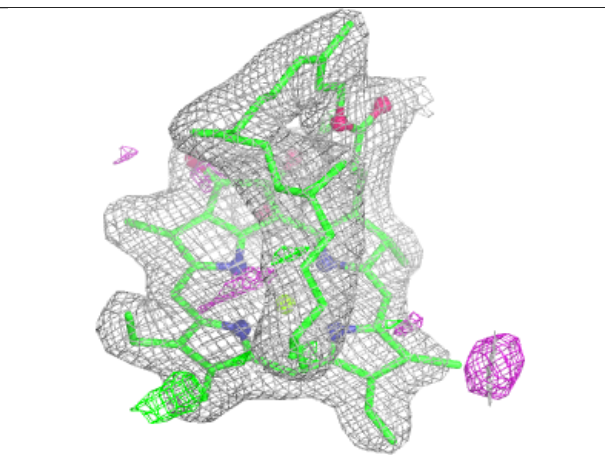
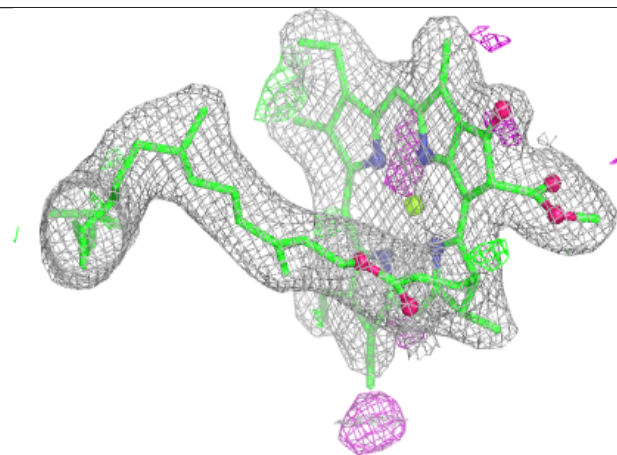
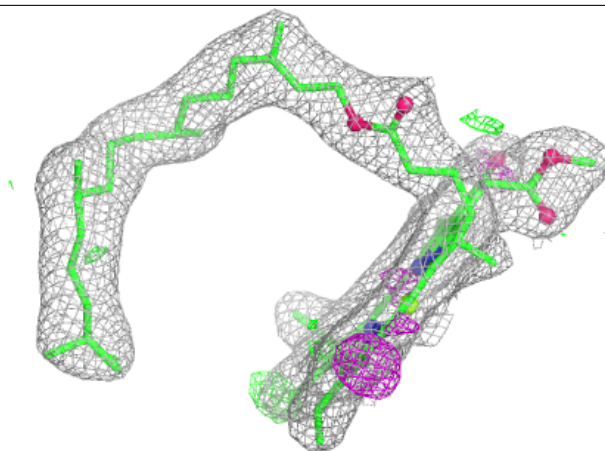
Electron density around CLA D 406:

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



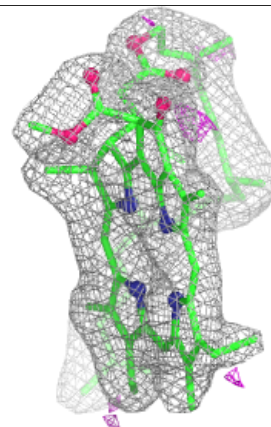
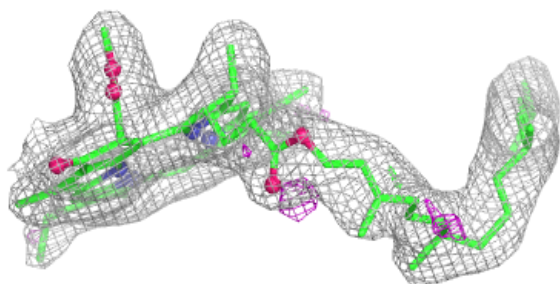
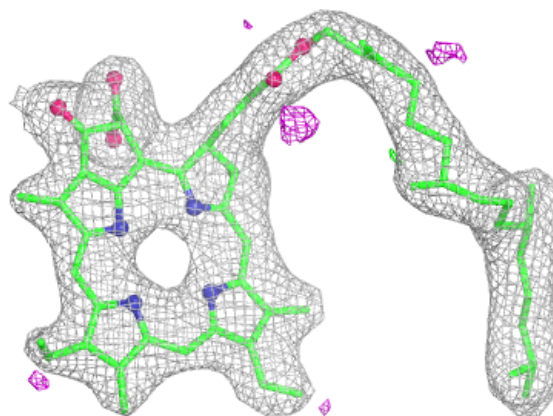
Electron density around CLA B 611:

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



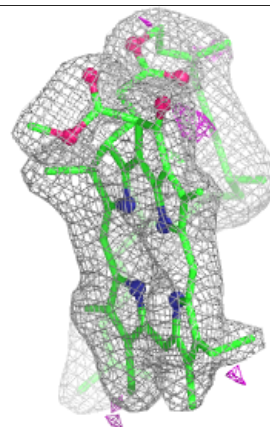
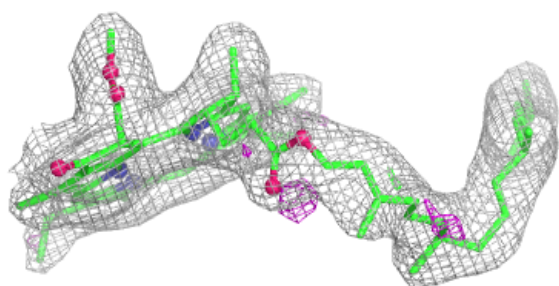
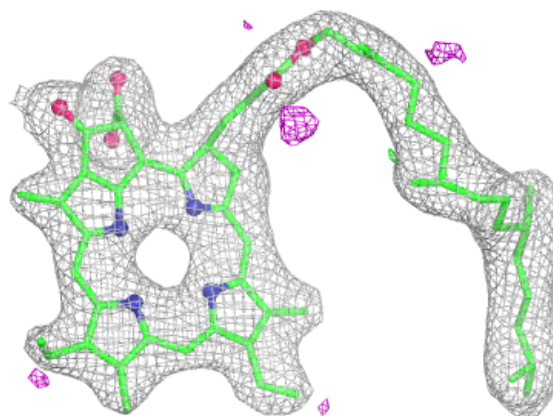
Electron density around PHO a 353 (A):

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



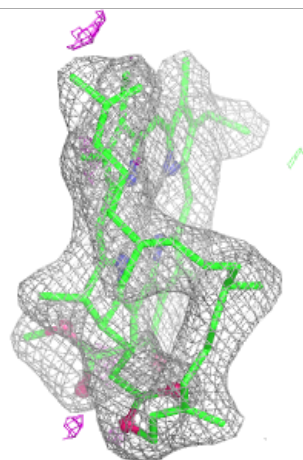
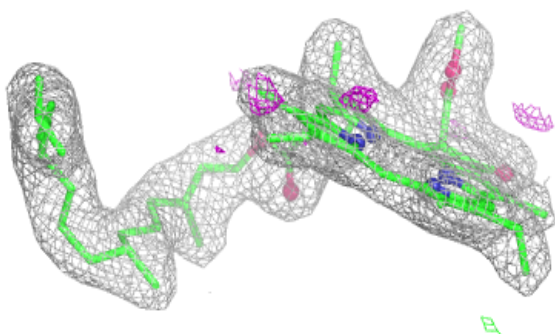
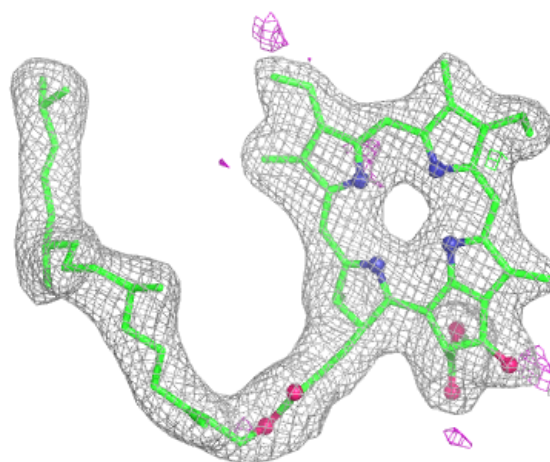
Electron density around PHO a 353 (B):

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



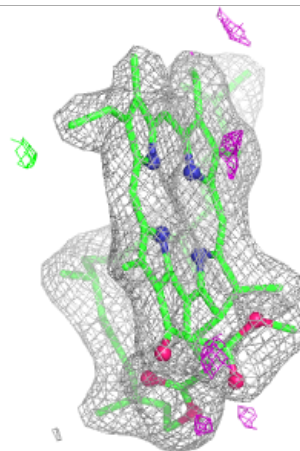
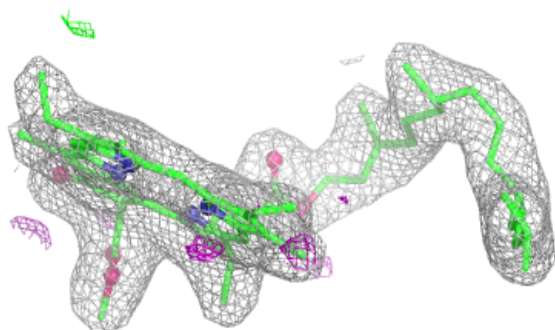
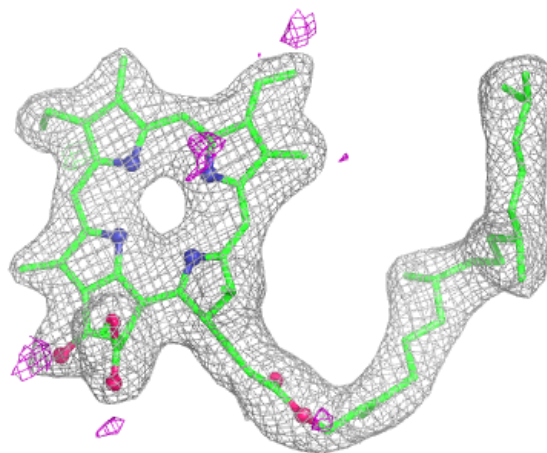
Electron density around PHO A 353 (A):

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



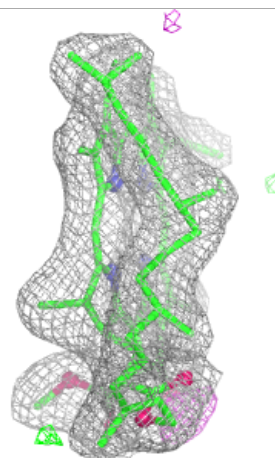
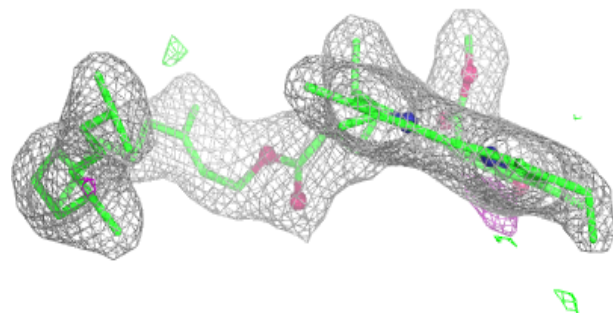
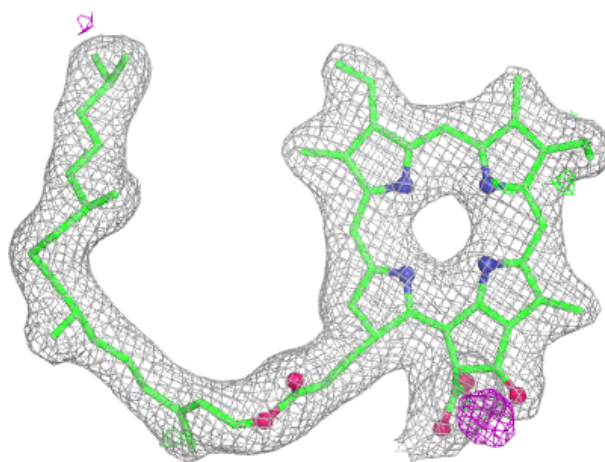
Electron density around PHO A 353 (B):

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



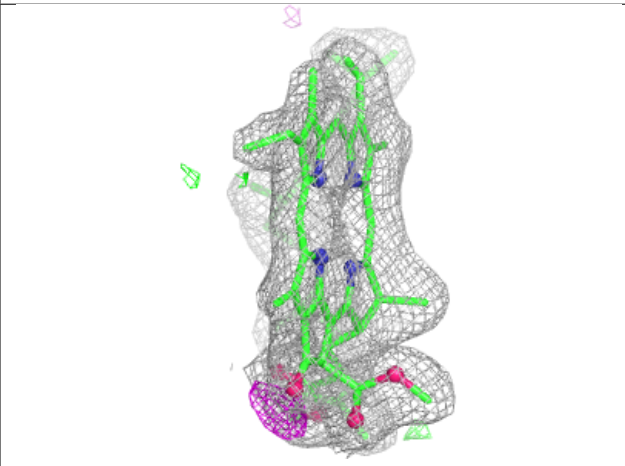
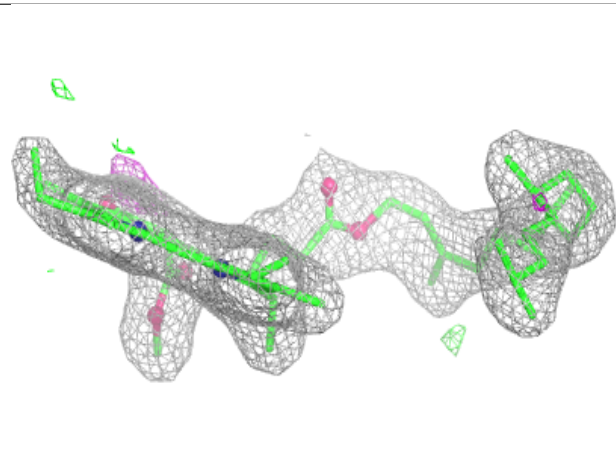
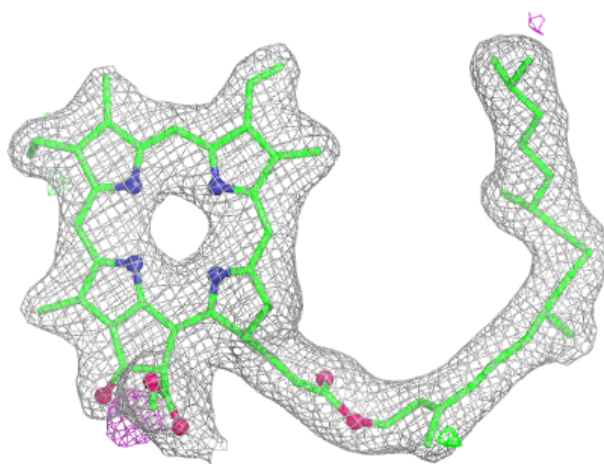
Electron density around PHO a 408 (A):

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



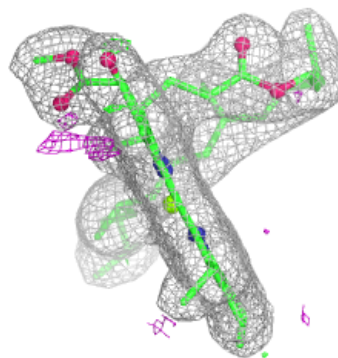
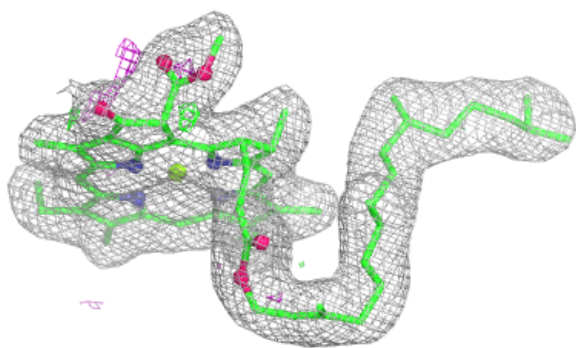
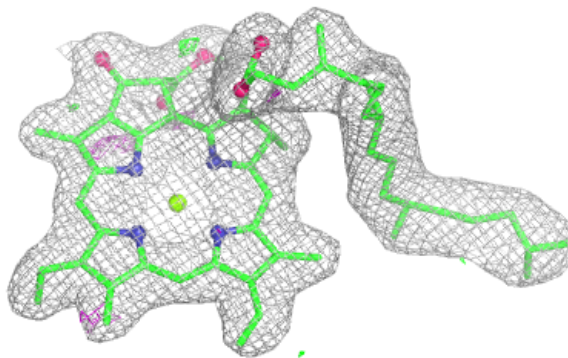
Electron density around PHO a 408 (B):

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

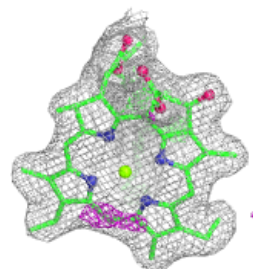
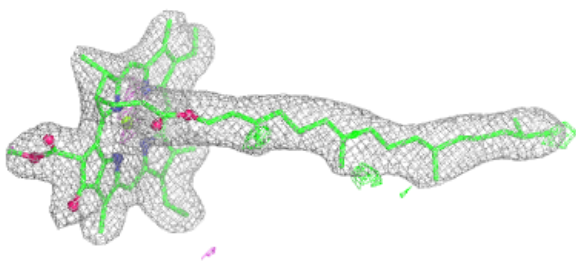
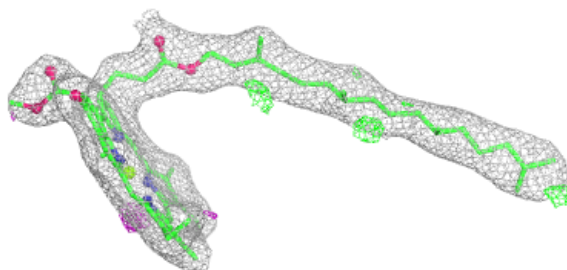


Electron density around CLA A 405 (A):

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

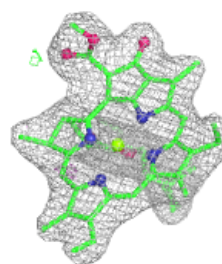
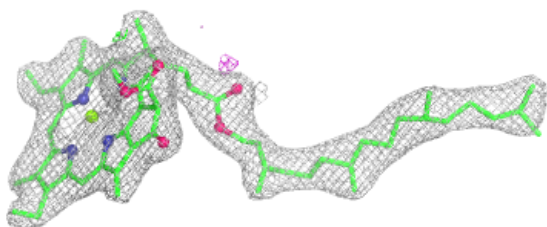
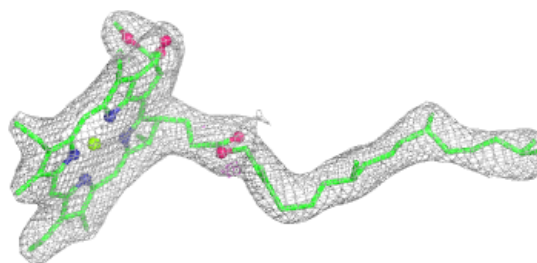
**Electron density around CLA B 607:**

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



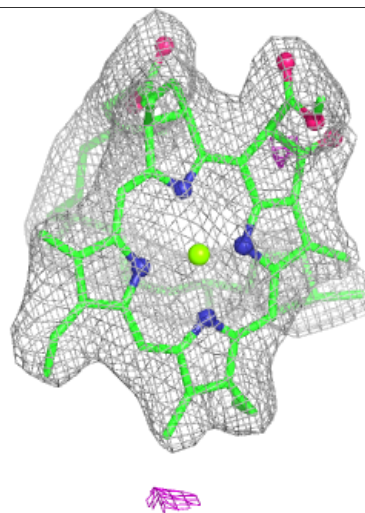
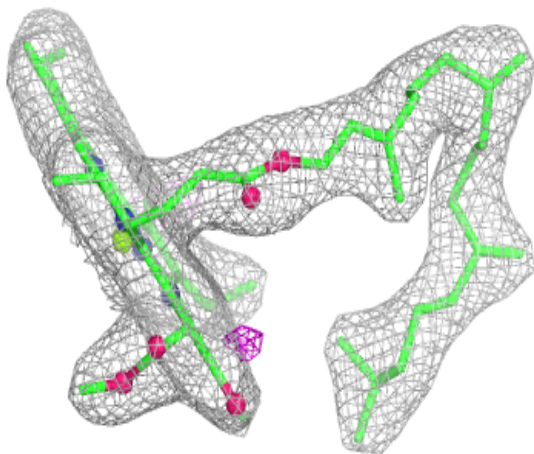
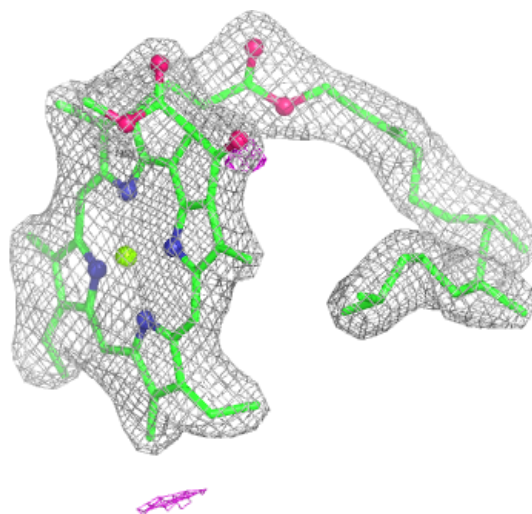
Electron density around CLA C 503:

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



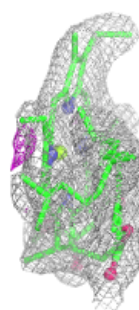
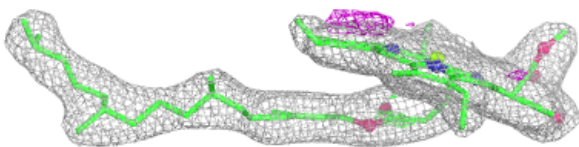
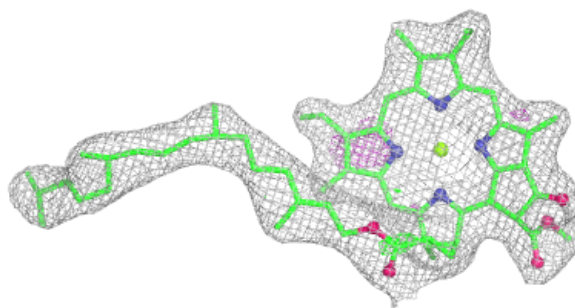
Electron density around CLA C 504:

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

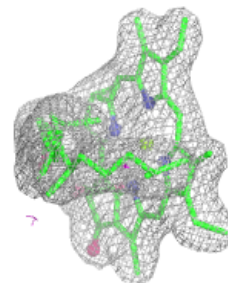
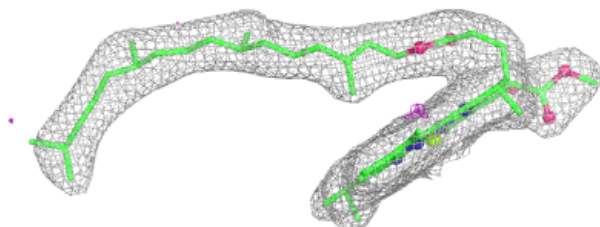
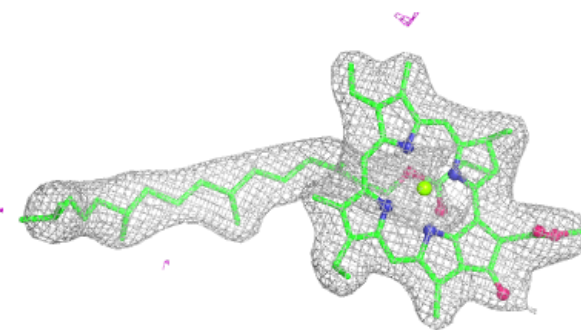


Electron density around CLA b 603:

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

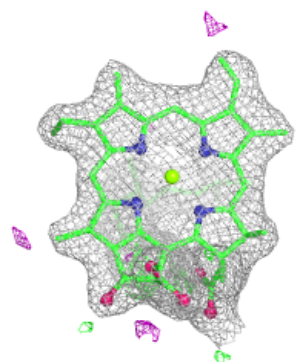
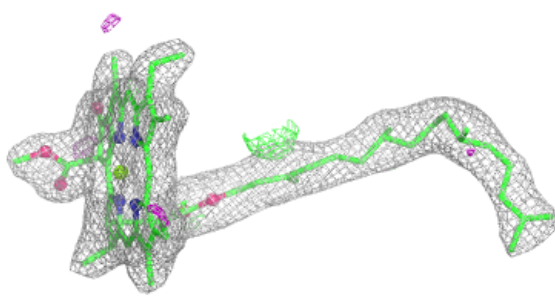
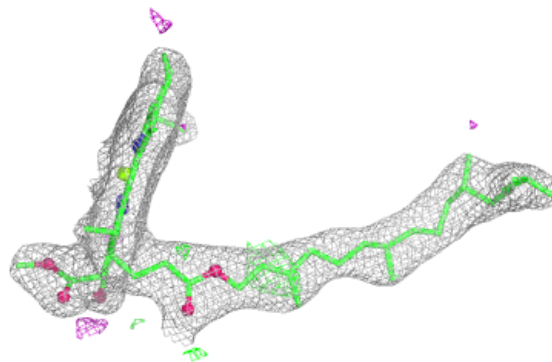
**Electron density around CLA B 608:**

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

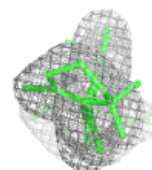
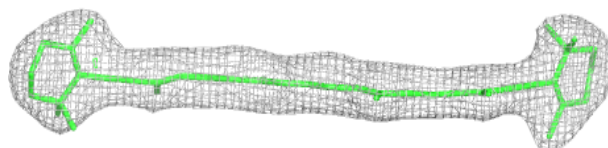
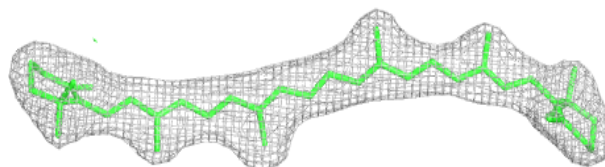


Electron density around CLA b 605:

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

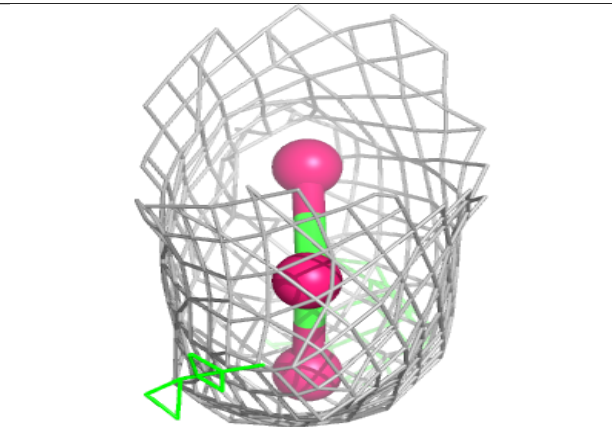
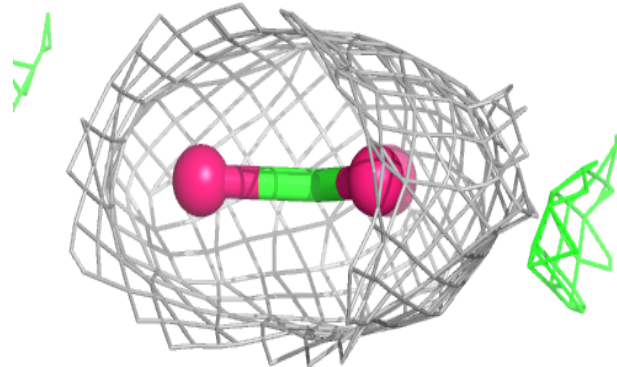
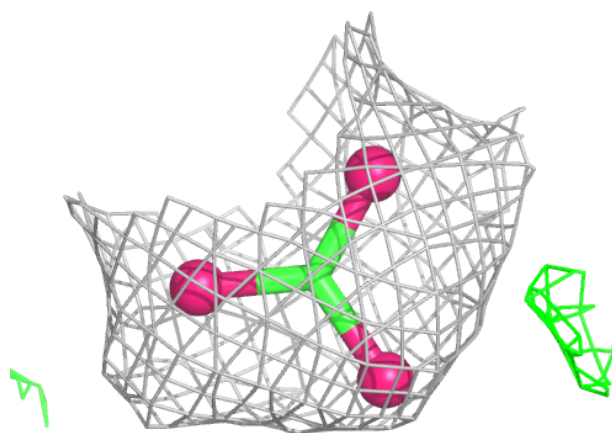
**Electron density around BCR C 516:**

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



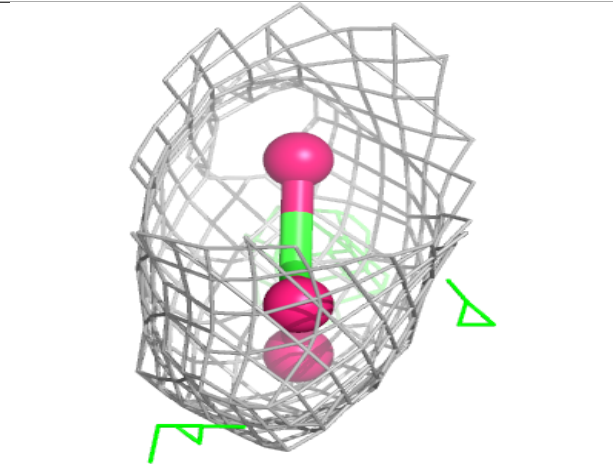
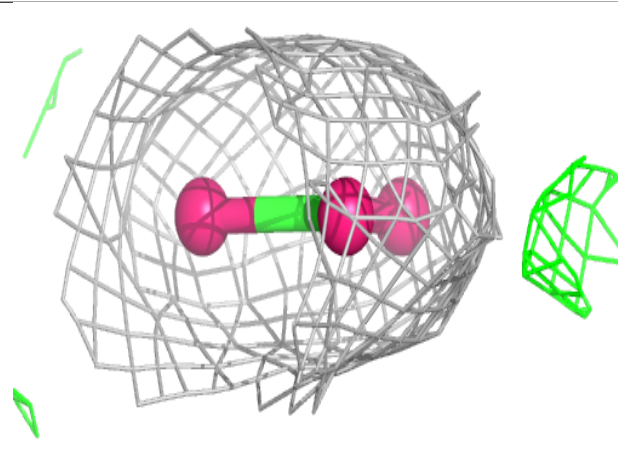
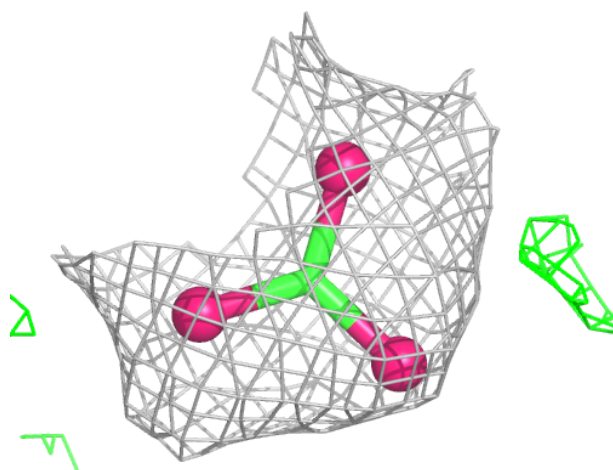
Electron density around BCT A 348 (A):

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



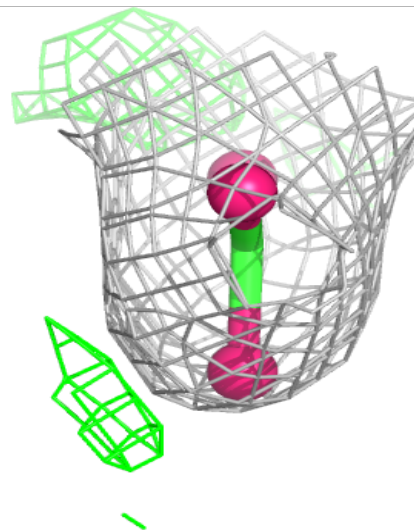
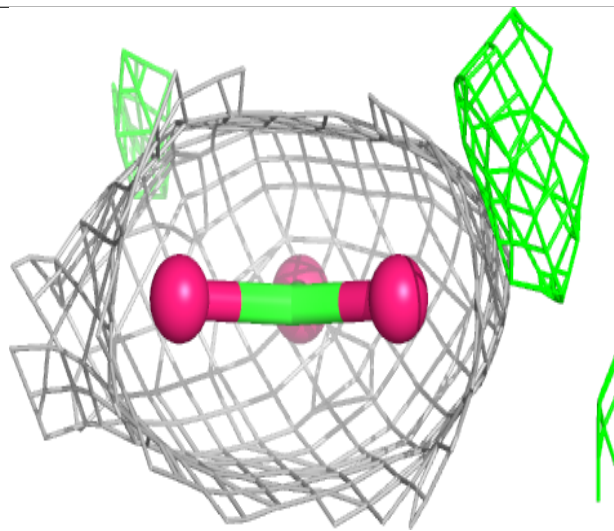
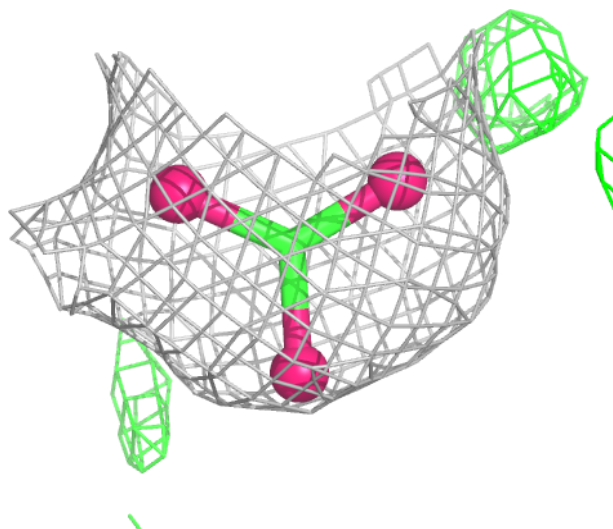
Electron density around BCT A 348 (B):

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



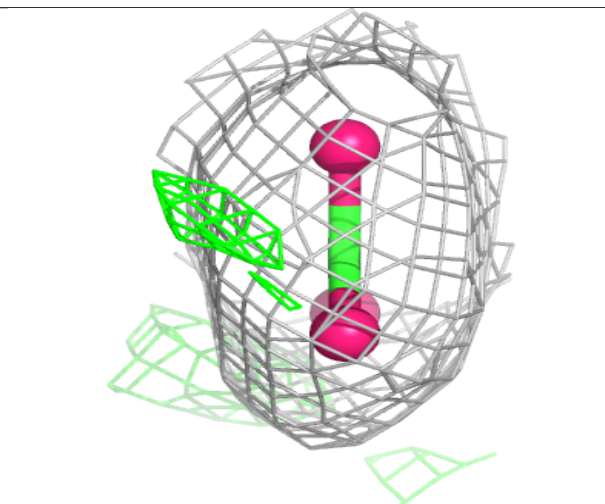
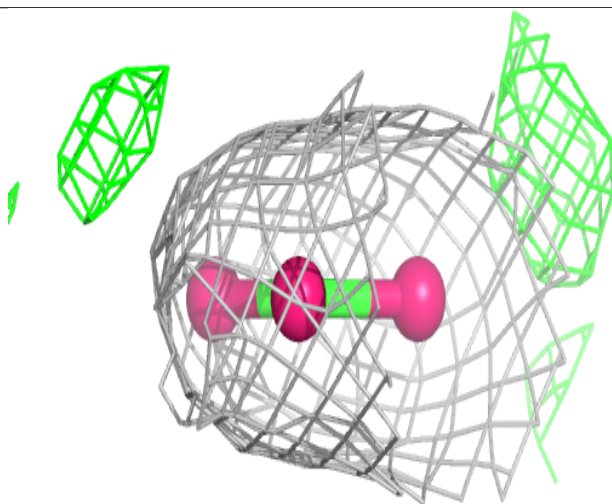
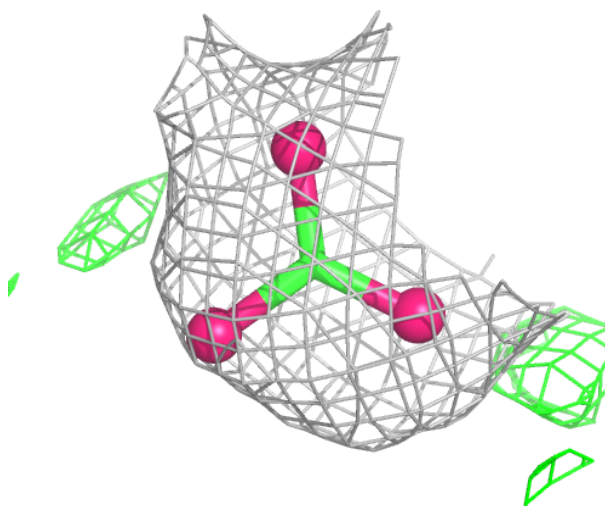
Electron density around BCT a 404 (A):

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



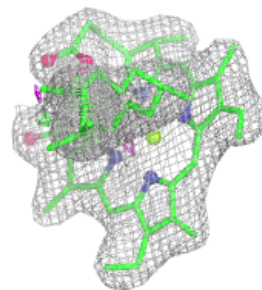
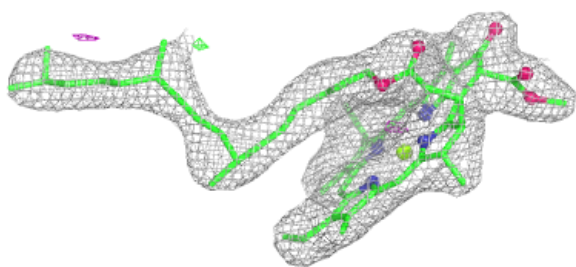
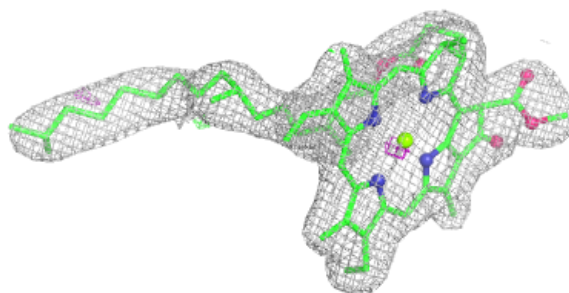
Electron density around BCT a 404 (B):

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

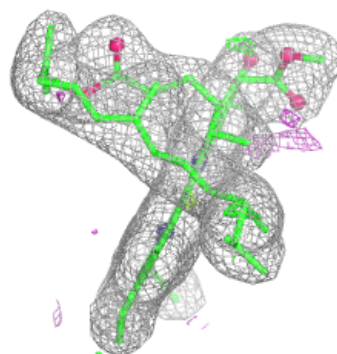
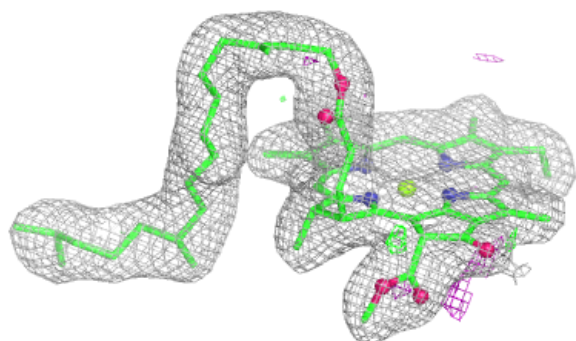
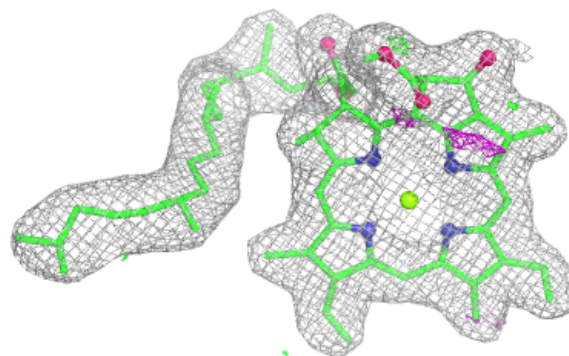


Electron density around CLA C 506:

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

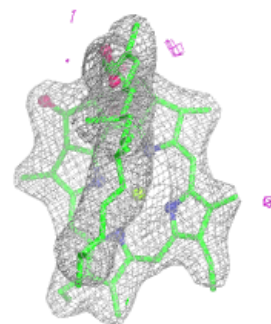
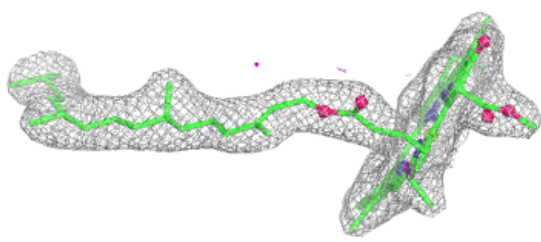
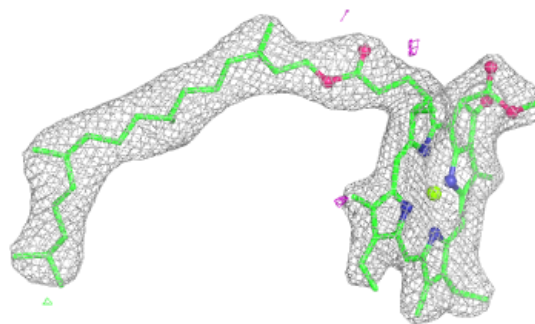
**Electron density around CLA A 405 (B):**

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

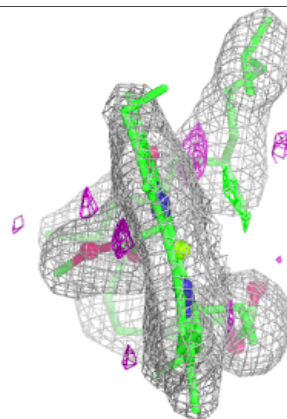
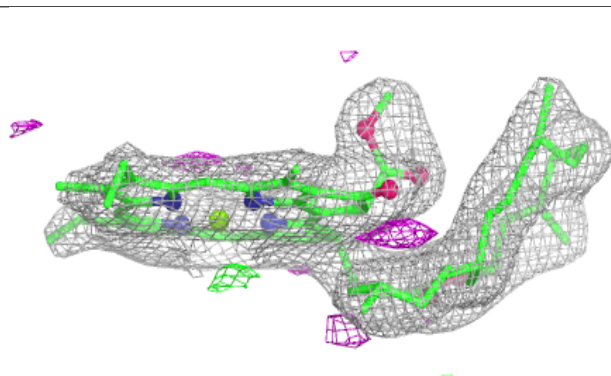
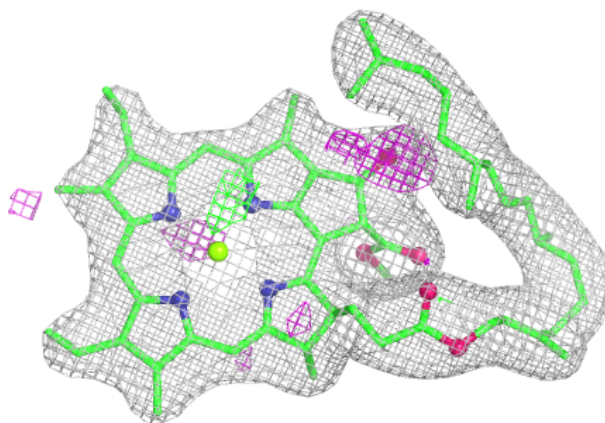


Electron density around CLA b 609:

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

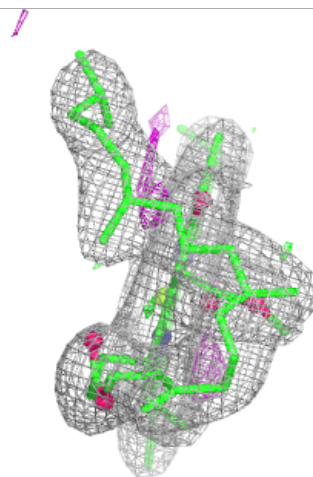
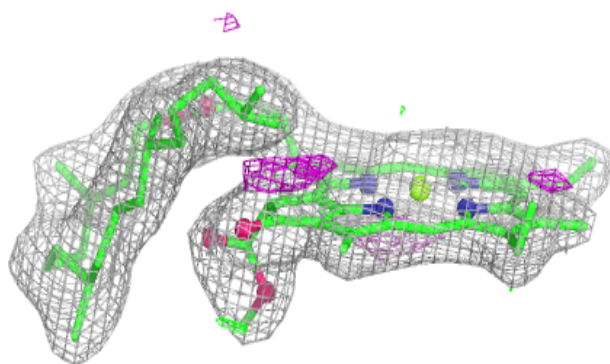
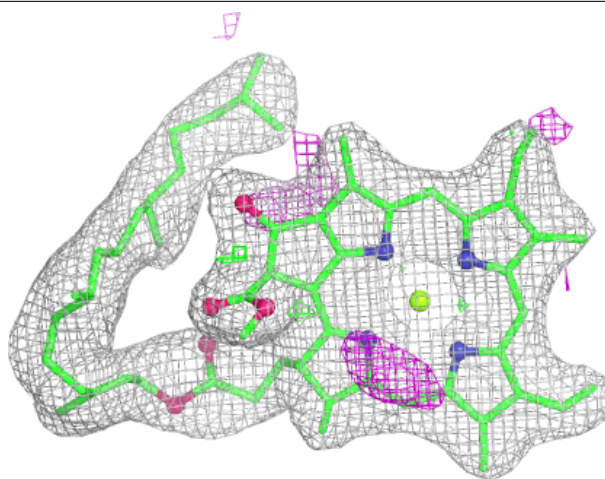
**Electron density around CLA b 610:**

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



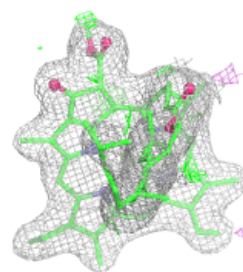
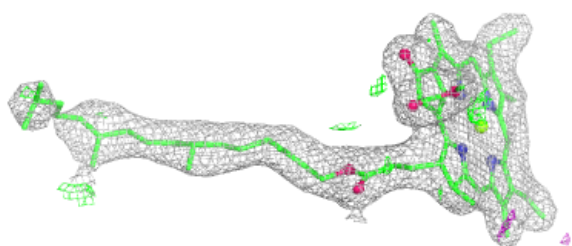
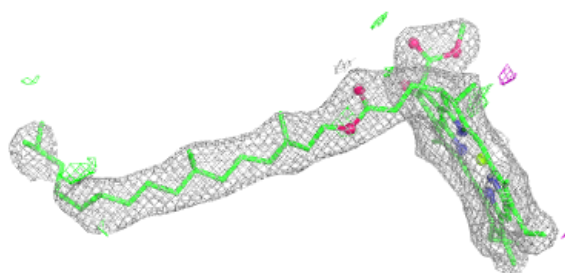
Electron density around CLA B 610:

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



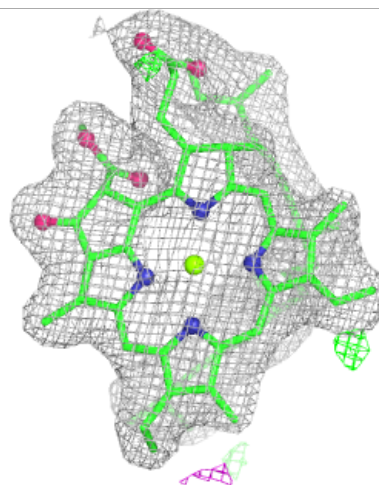
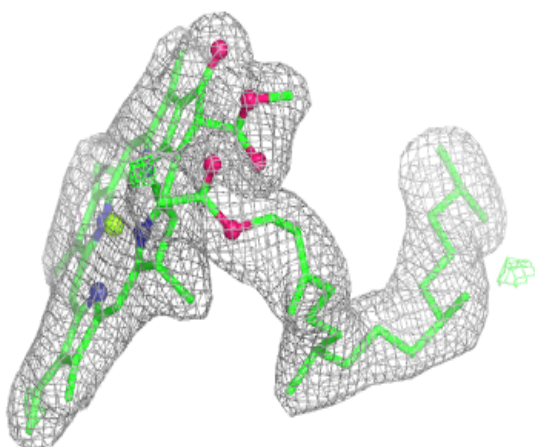
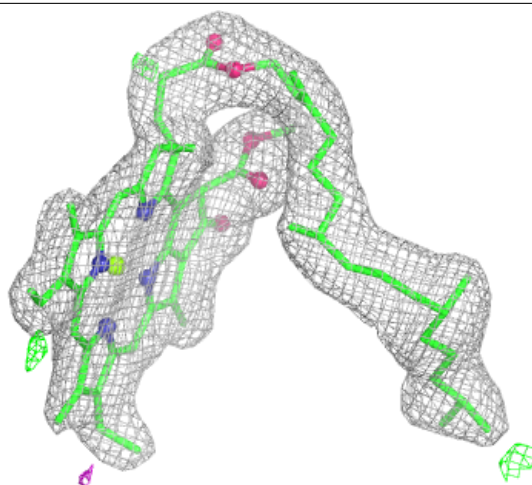
Electron density around CLA B 604:

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



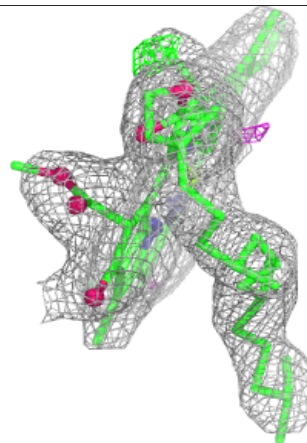
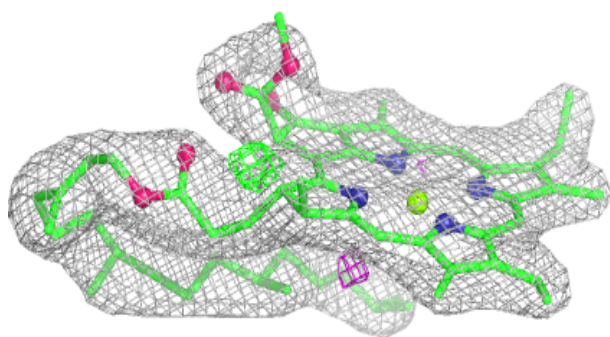
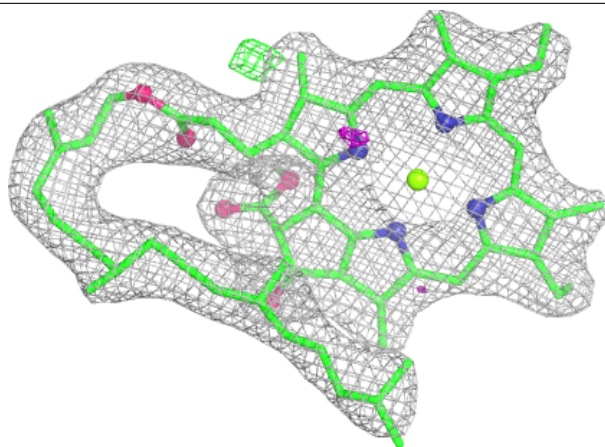
Electron density around CLA b 613:

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



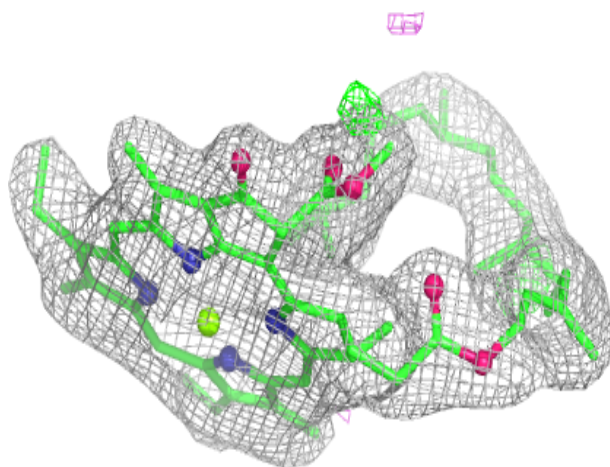
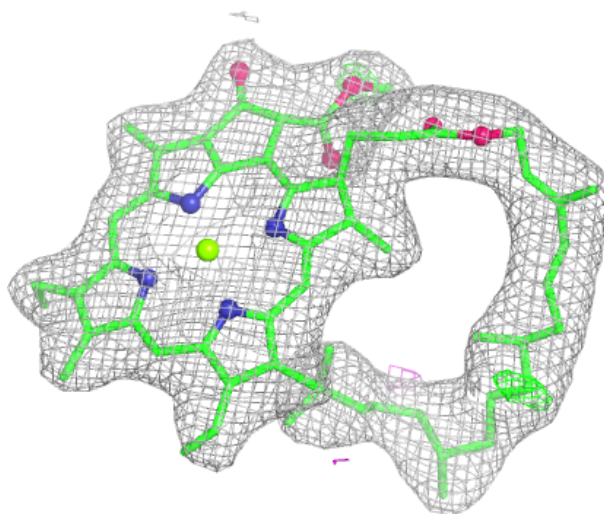
Electron density around CLA C 510:

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



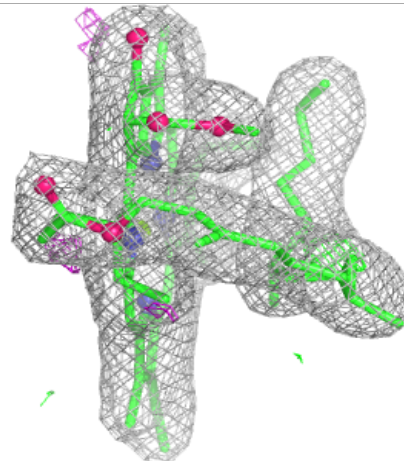
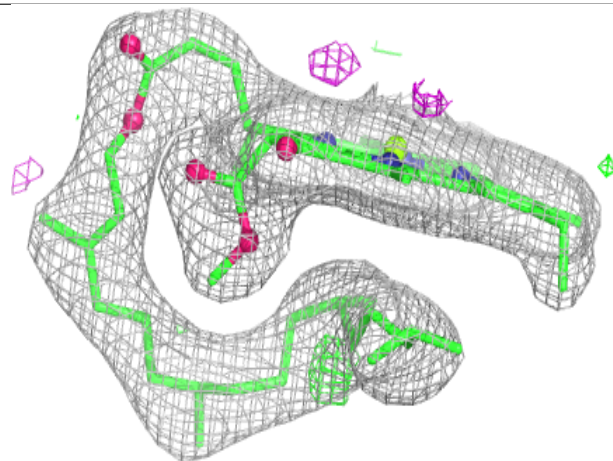
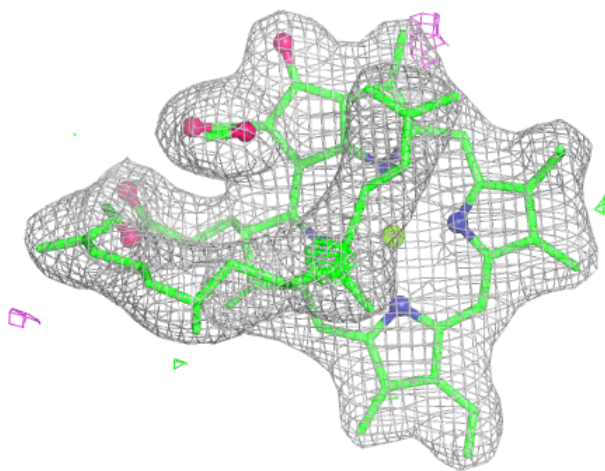
Electron density around CLA b 615:

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



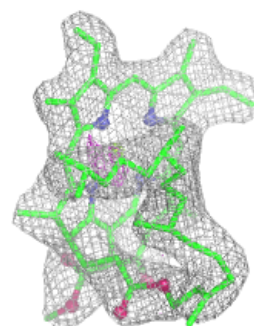
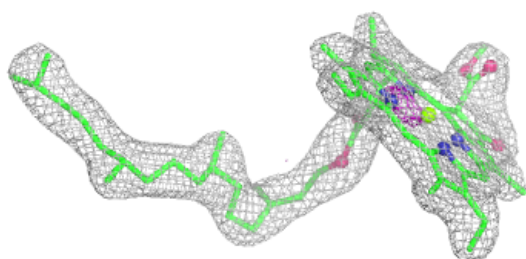
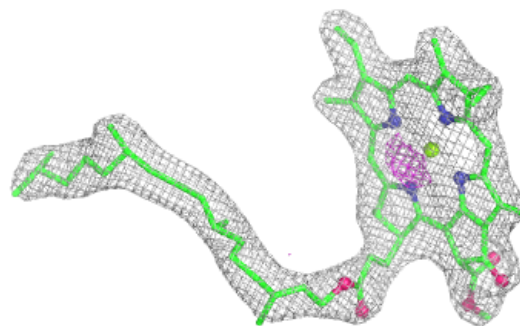
Electron density around CLA C 511:

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

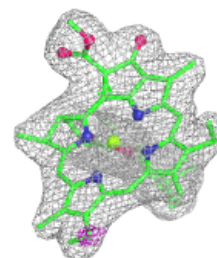
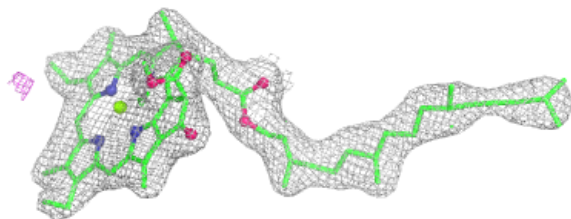
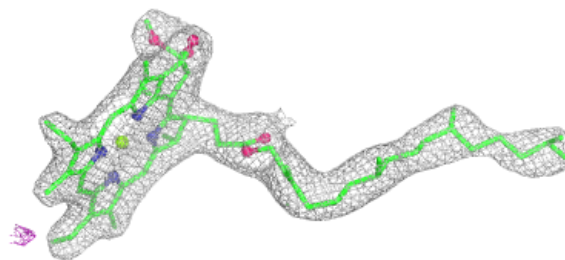


Electron density around CLA C 512:

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

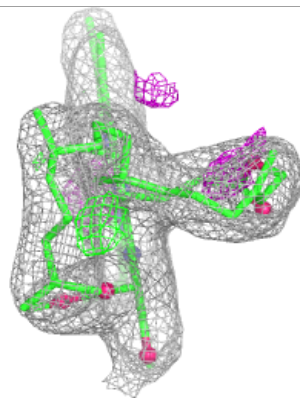
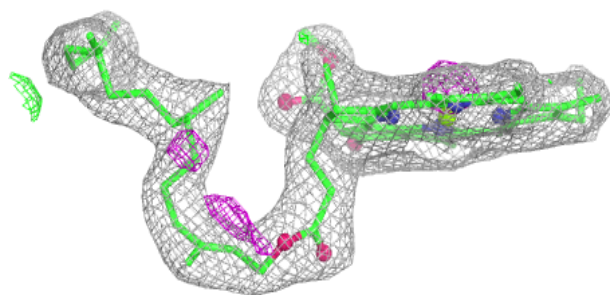
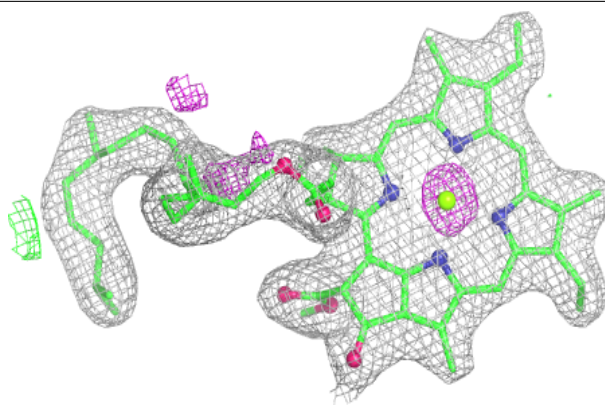
**Electron density around CLA c 503:**

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



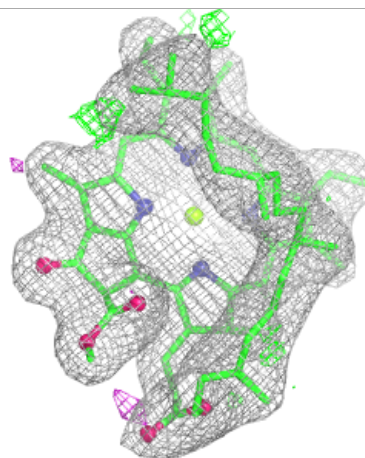
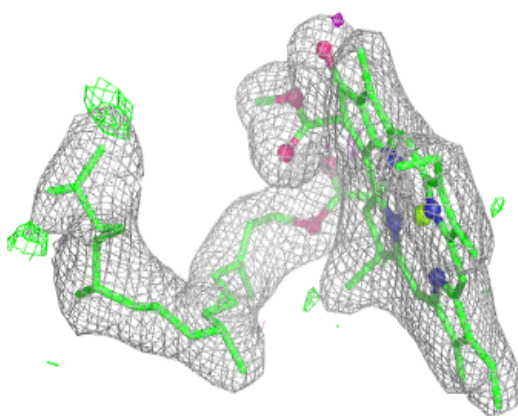
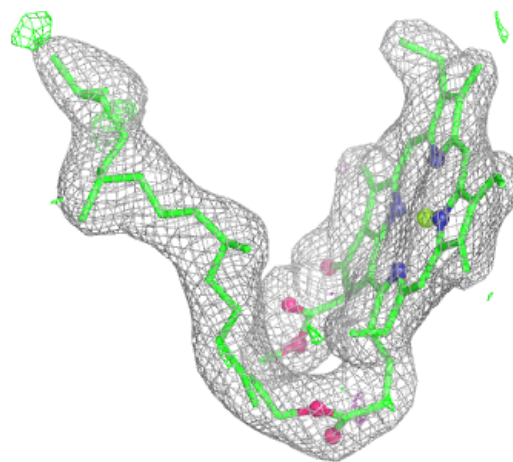
Electron density around CLA B 612:

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



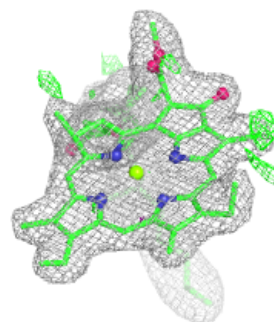
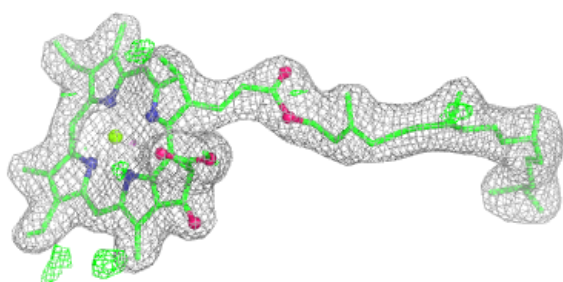
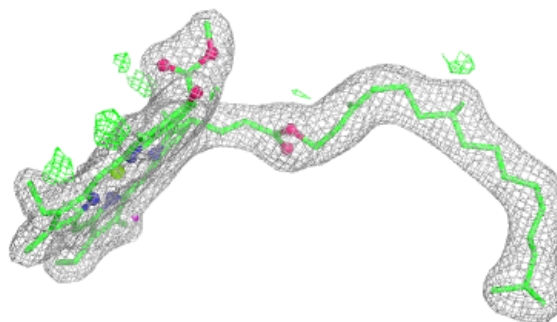
Electron density around CLA B 613:

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

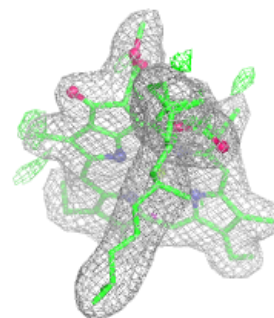
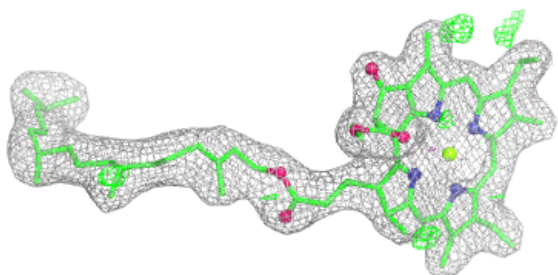
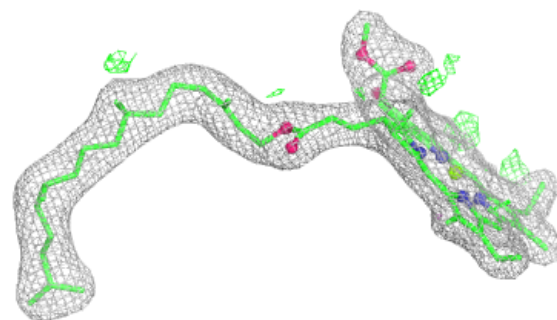


Electron density around CLA D 405 (A):

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

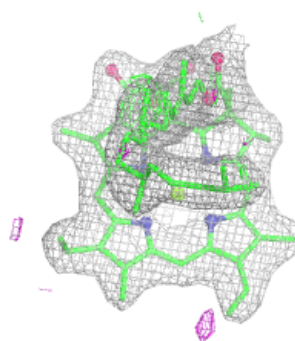
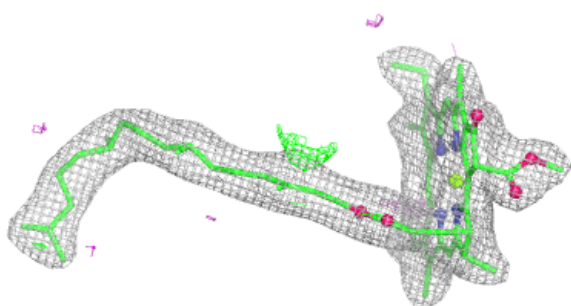
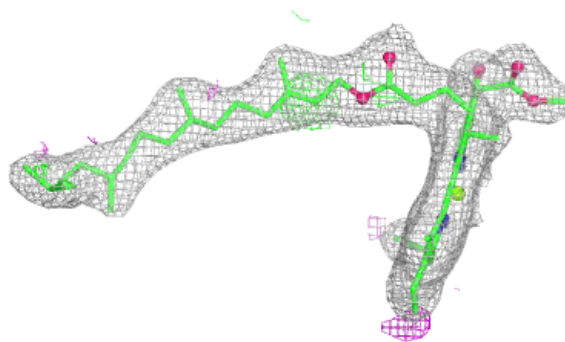
**Electron density around CLA D 405 (B):**

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



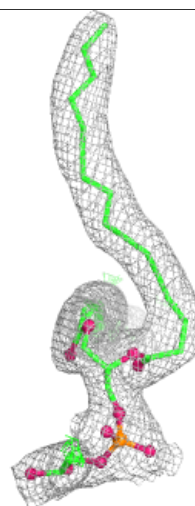
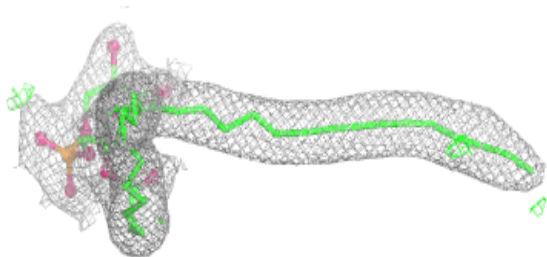
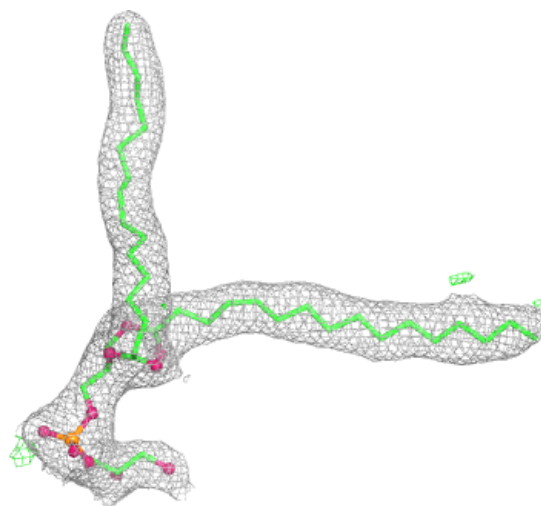
Electron density around CLA B 605:

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



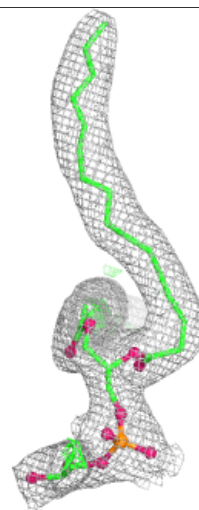
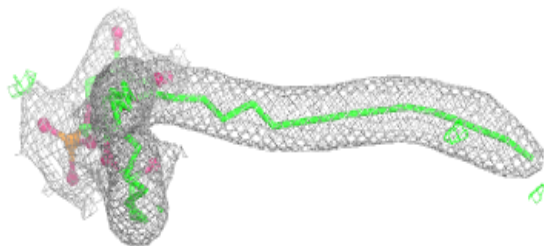
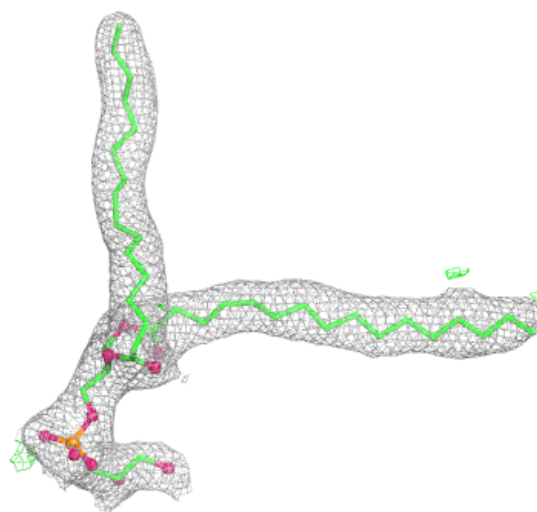
Electron density around LHG L 101 (A):

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



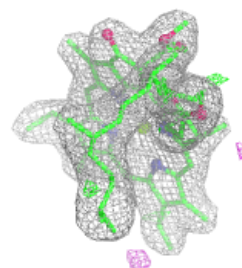
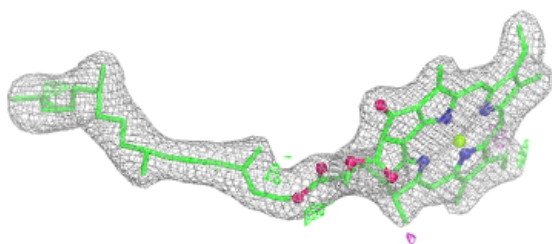
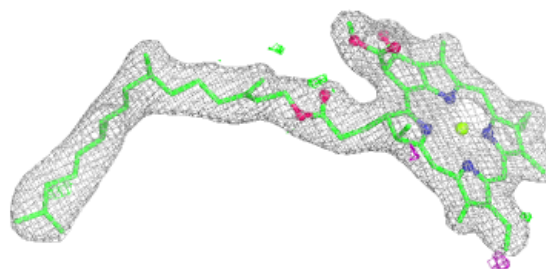
Electron density around LHG L 101 (B):

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



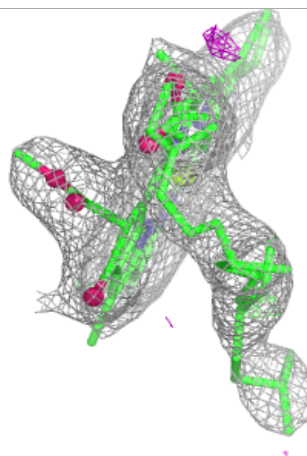
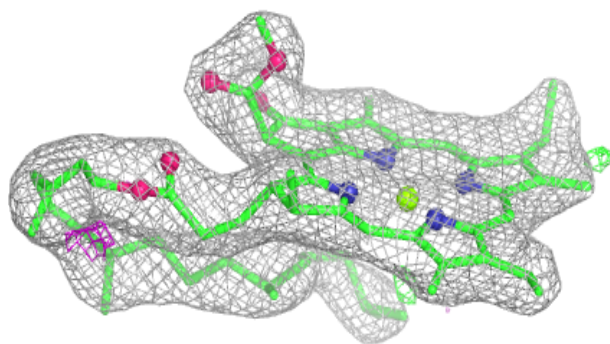
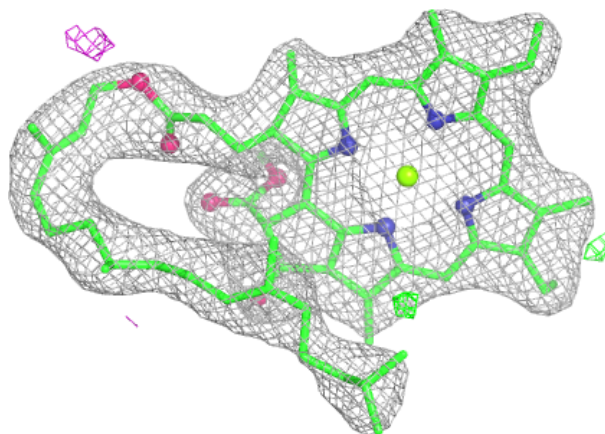
Electron density around CLA a 405 (A):

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



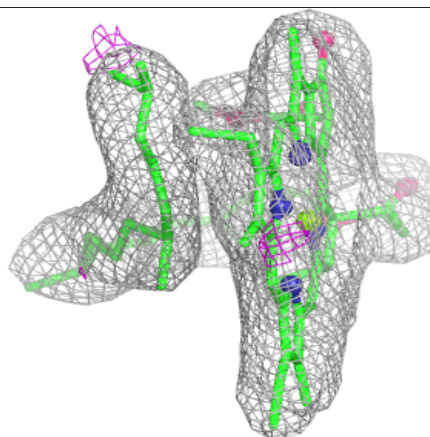
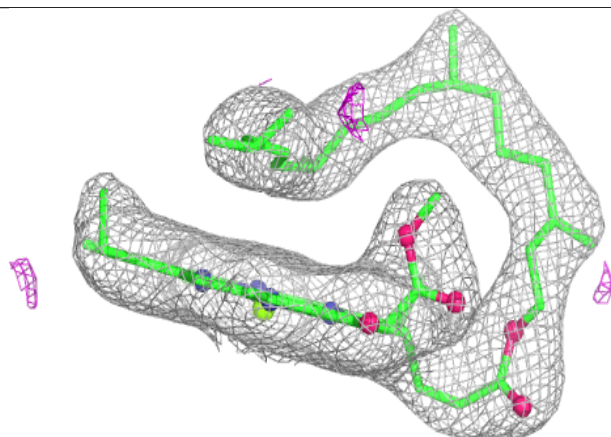
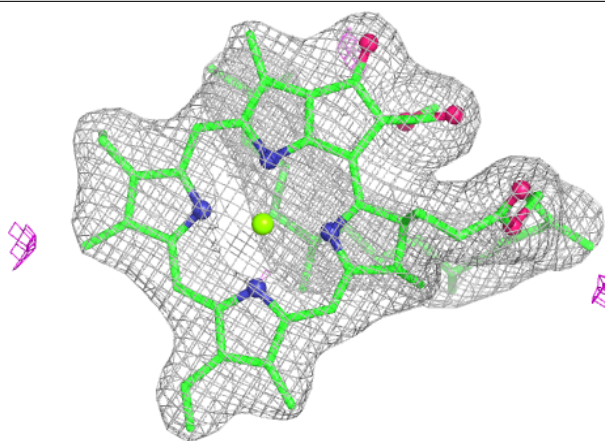
Electron density around CLA c 510:

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



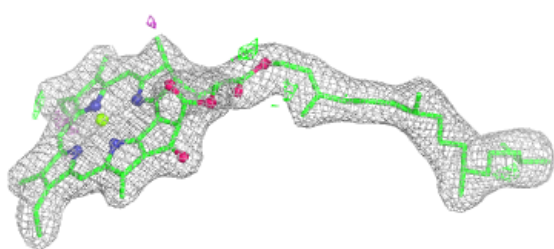
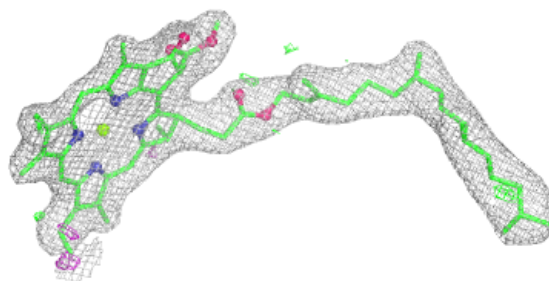
Electron density around CLA c 511:

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

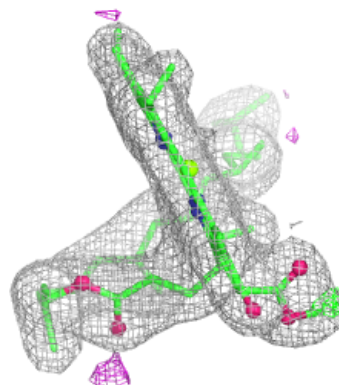
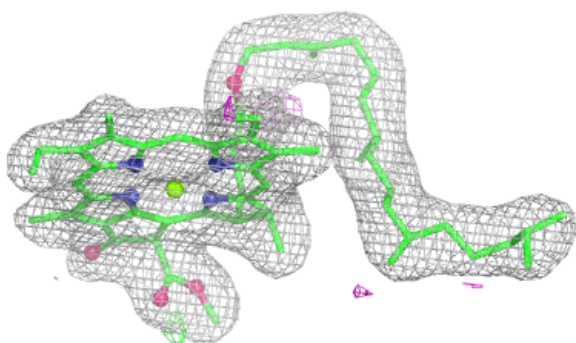
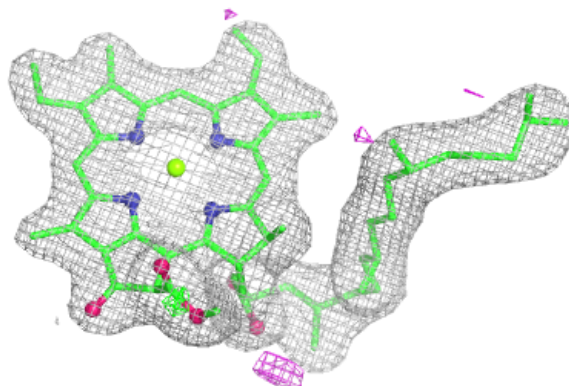


Electron density around CLA a 405 (B):

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

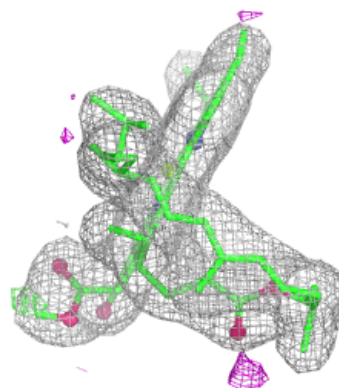
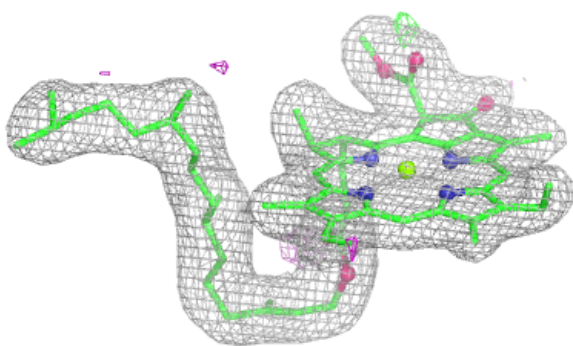
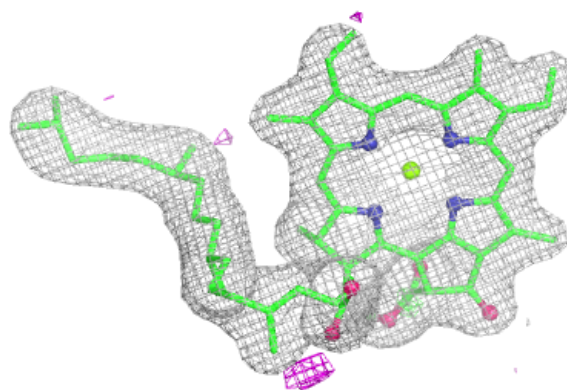
**Electron density around CLA a 406 (A):**

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

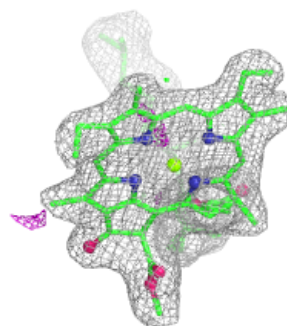
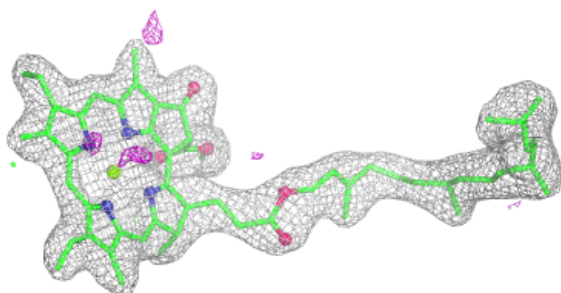
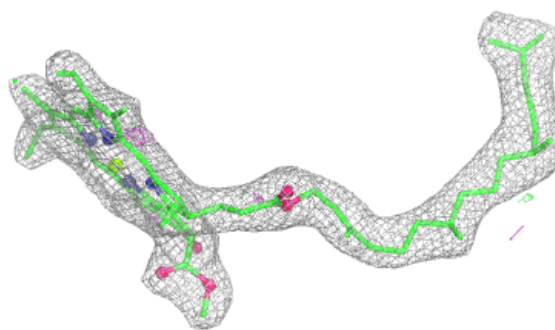


Electron density around CLA a 406 (B):

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

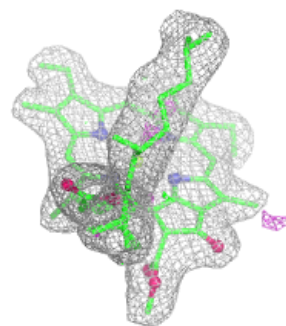
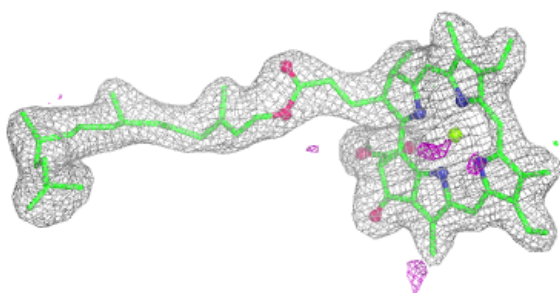
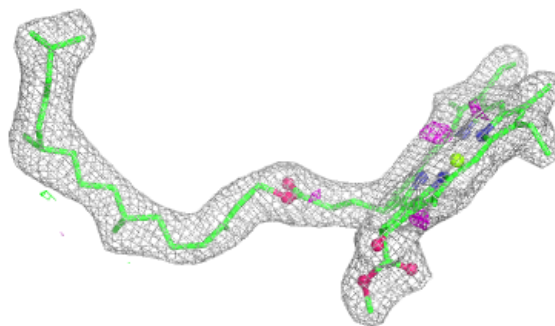
**Electron density around CLA d 402 (A):**

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



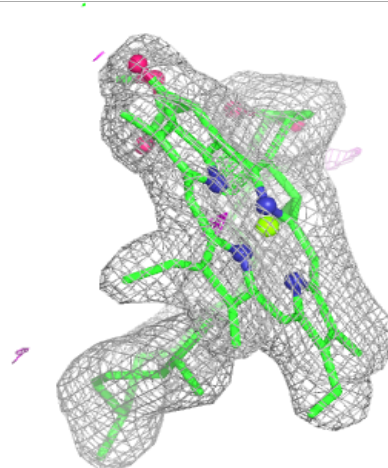
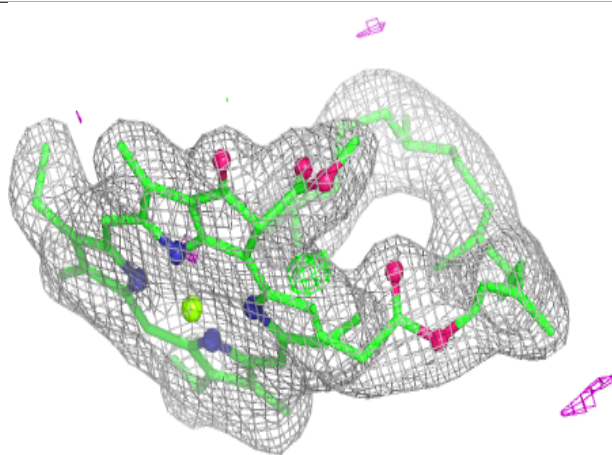
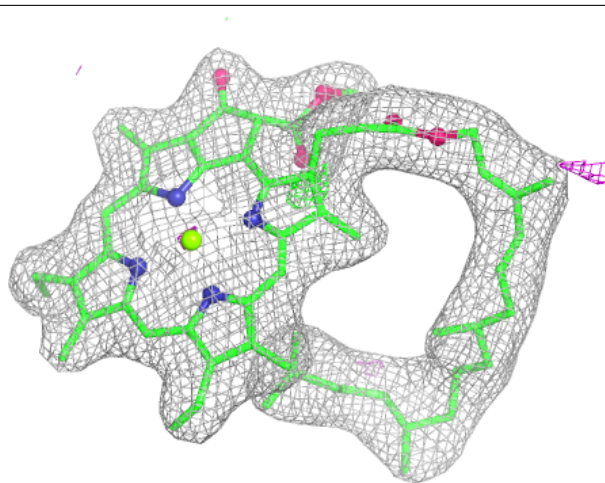
Electron density around CLA d 402 (B):

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



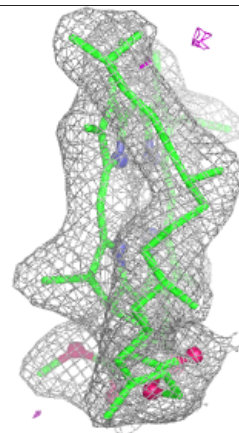
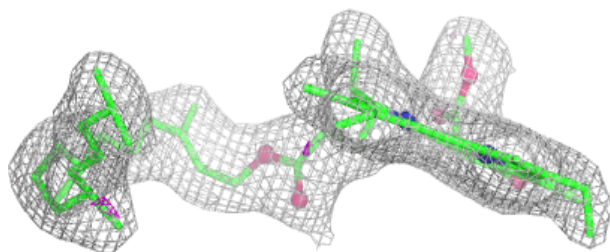
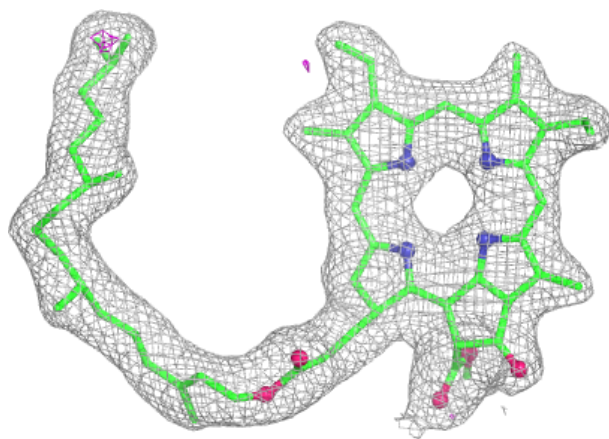
Electron density around CLA B 615:

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



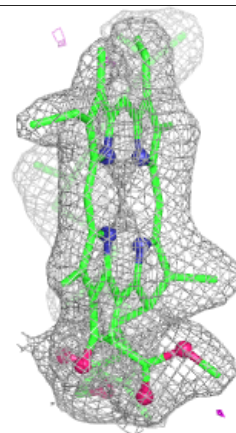
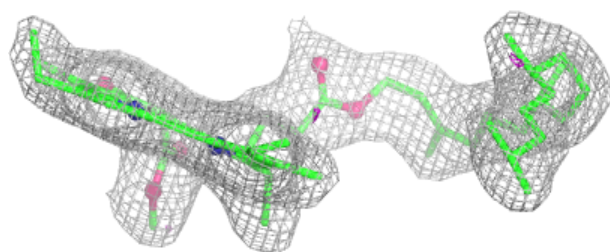
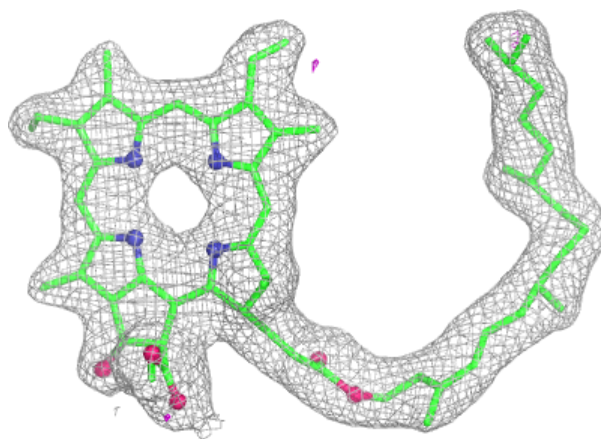
Electron density around PHO A 407 (A):

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



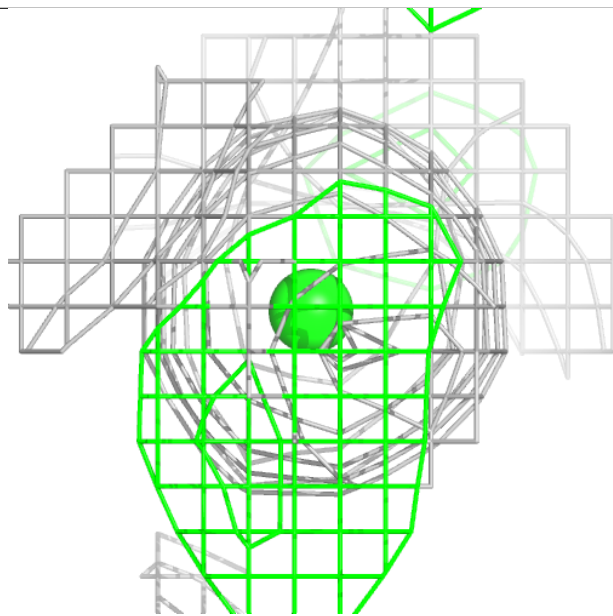
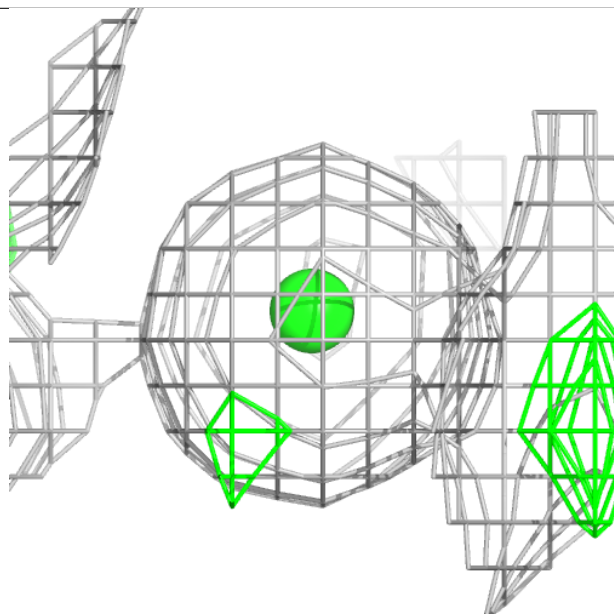
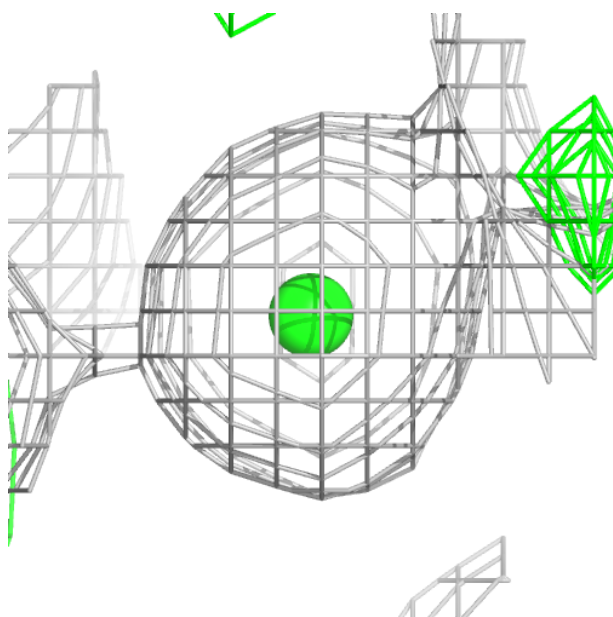
Electron density around PHO A 407 (B):

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



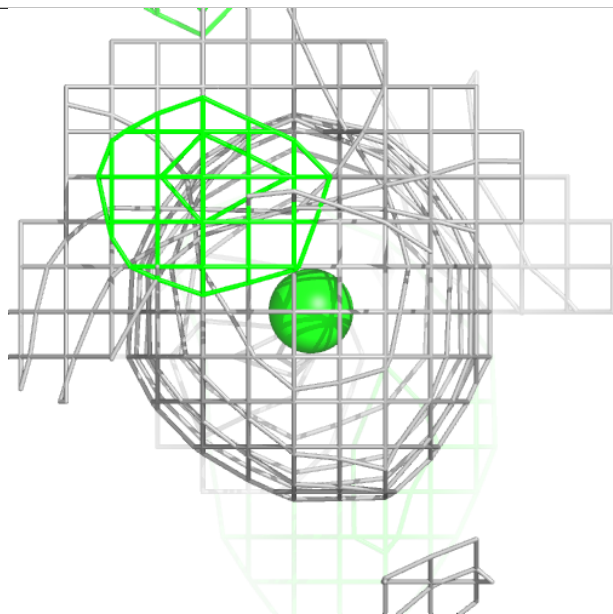
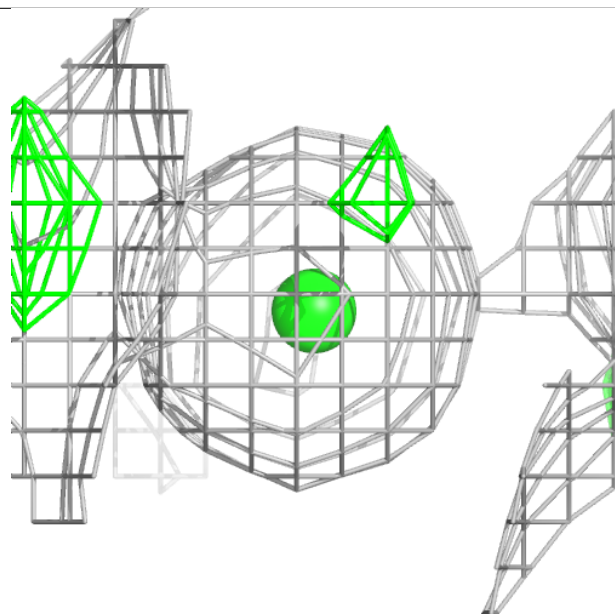
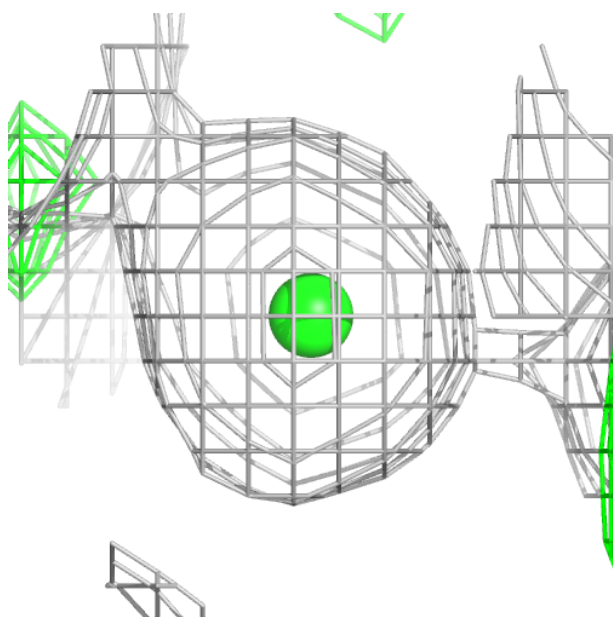
Electron density around CL A 403 (B):

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



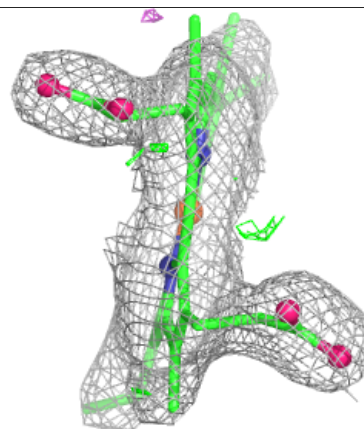
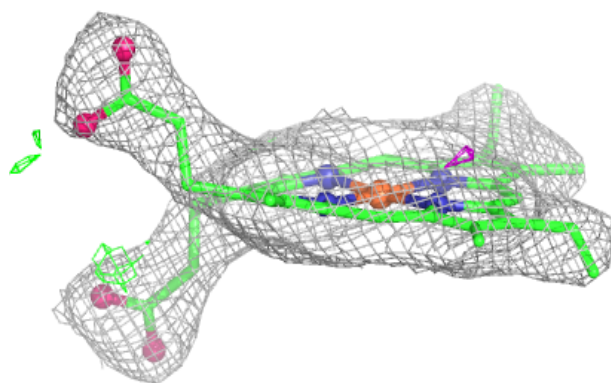
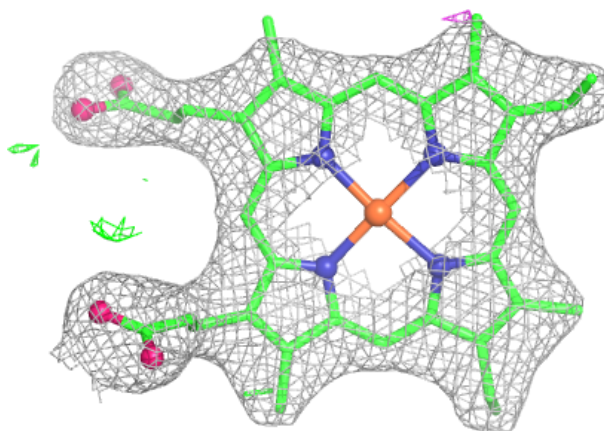
Electron density around CL A 403 (A):

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



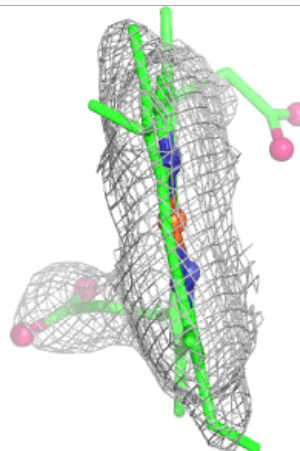
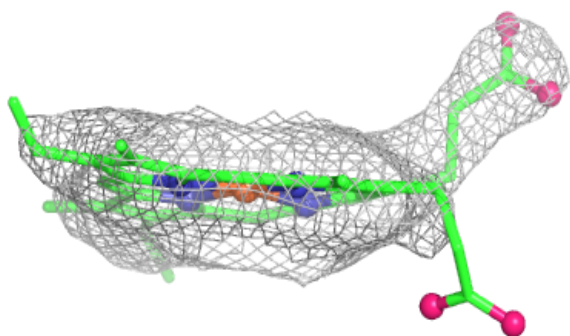
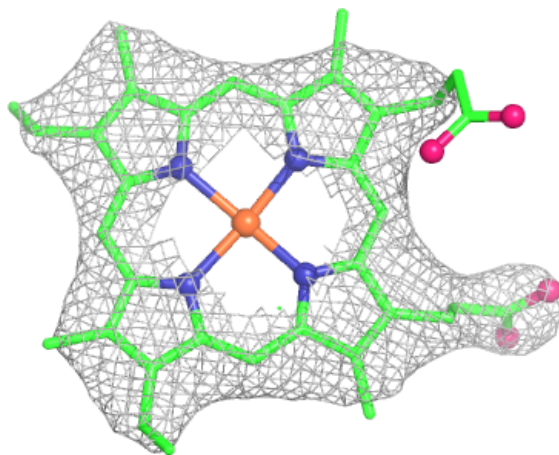
Electron density around HEM E 103:

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



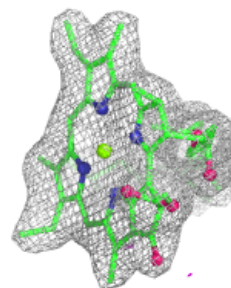
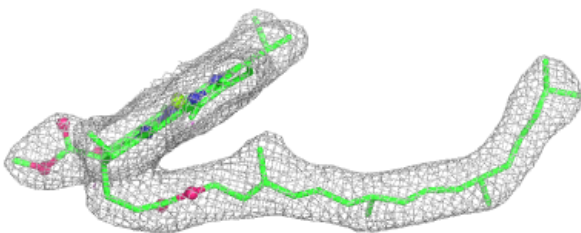
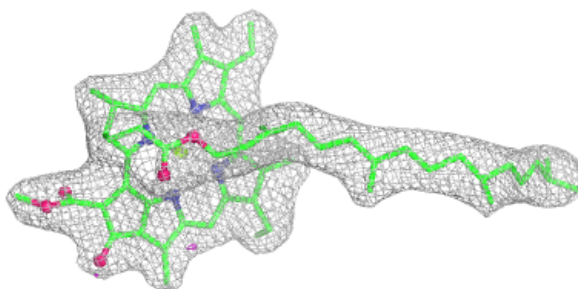
Electron density around HEM e 87:

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



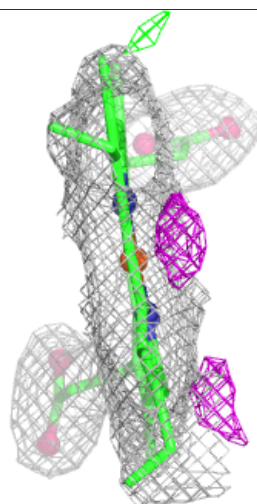
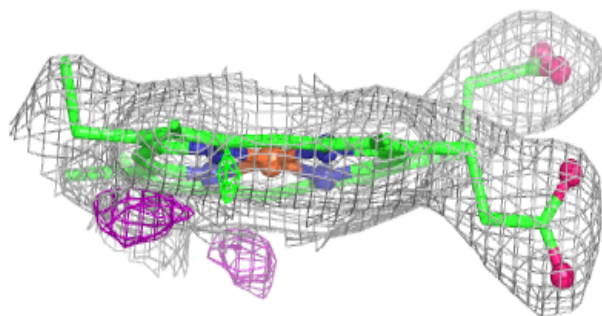
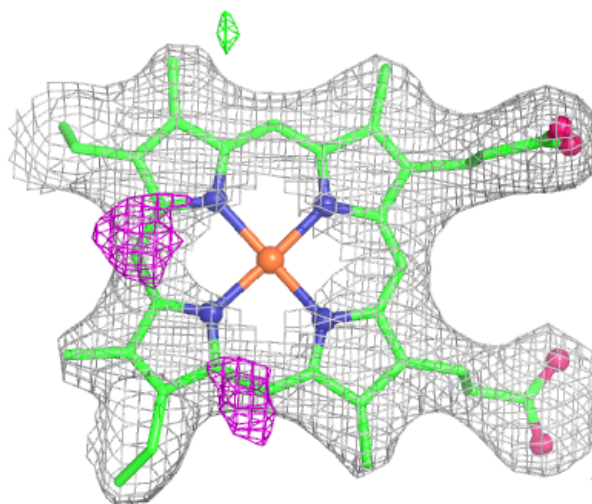
Electron density around CLA b 608:

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



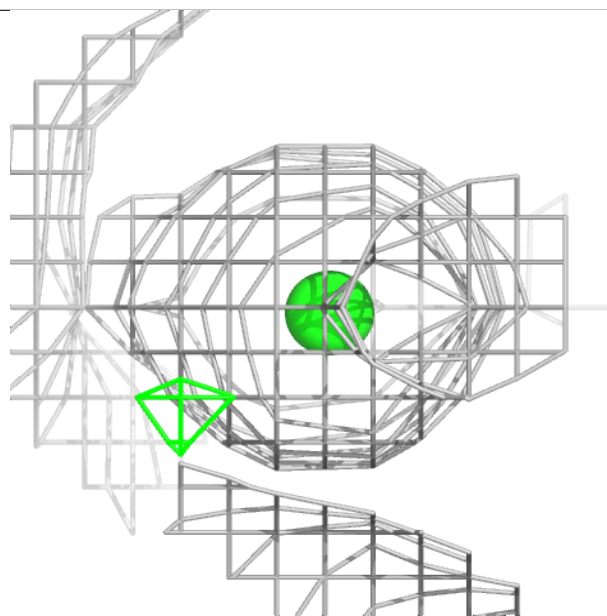
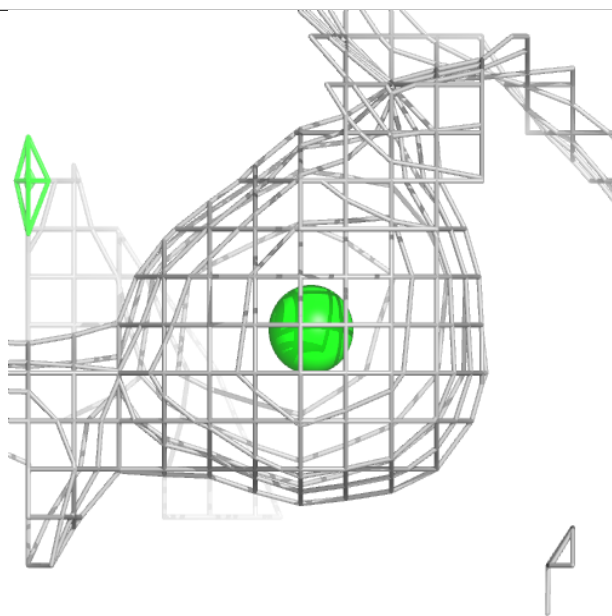
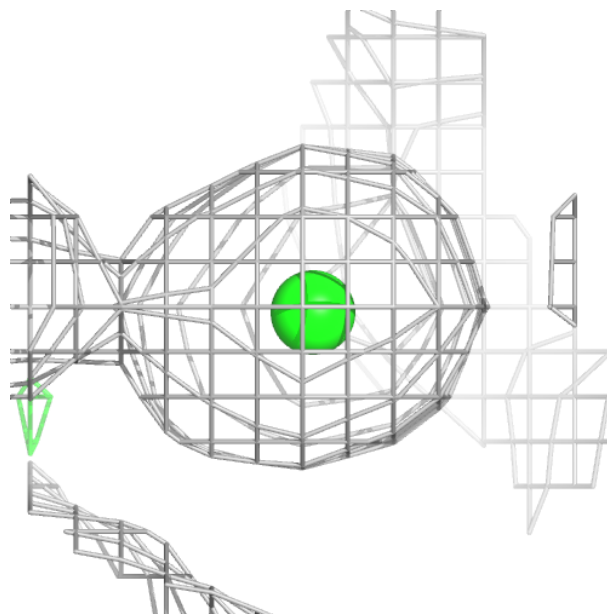
Electron density around HEC v 202:

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



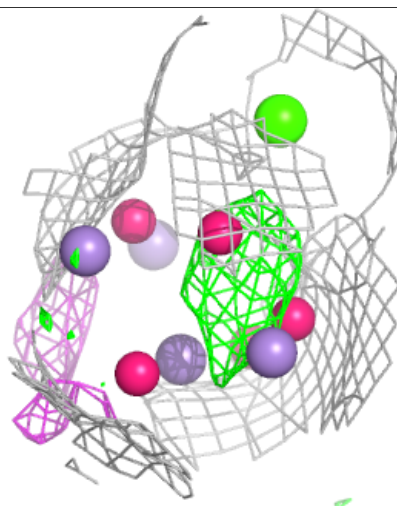
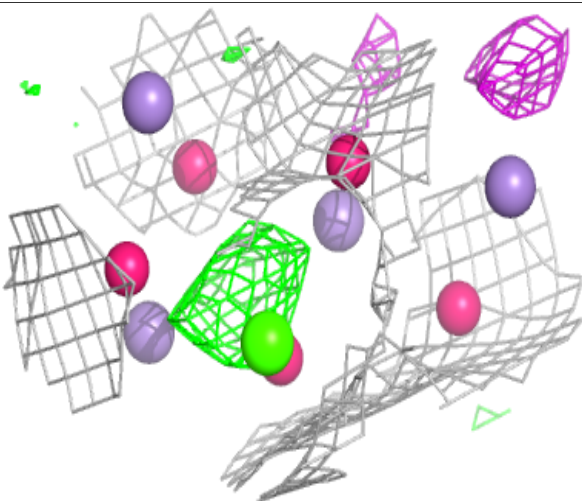
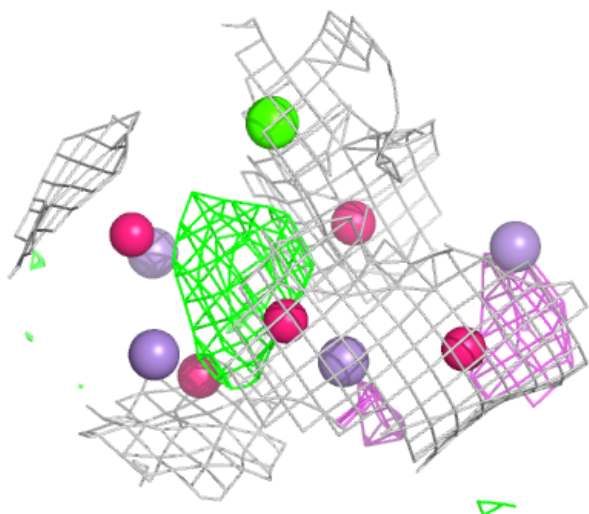
Electron density around CL a 403 (B):

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



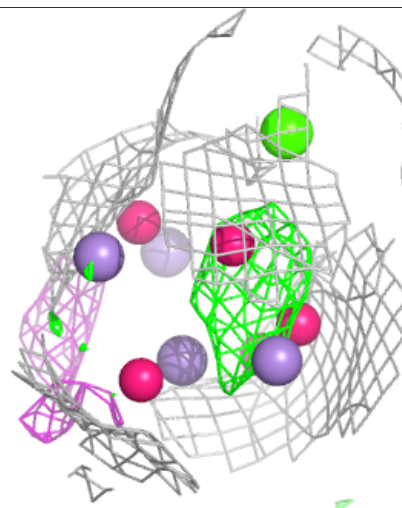
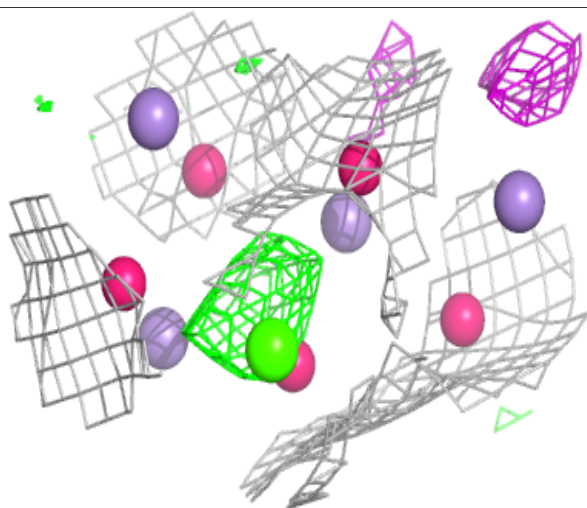
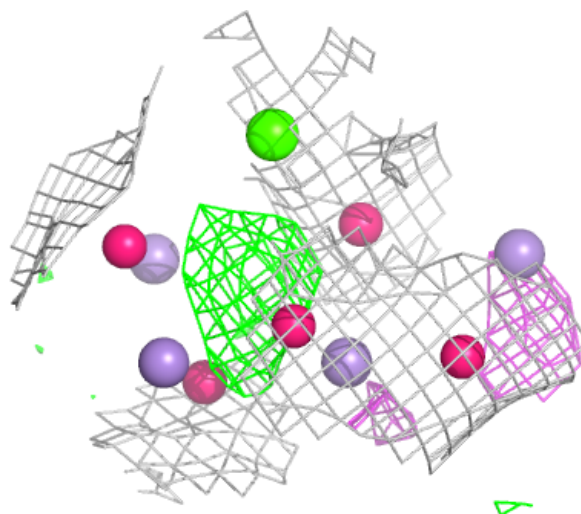
Electron density around OEX A 413 (A):

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



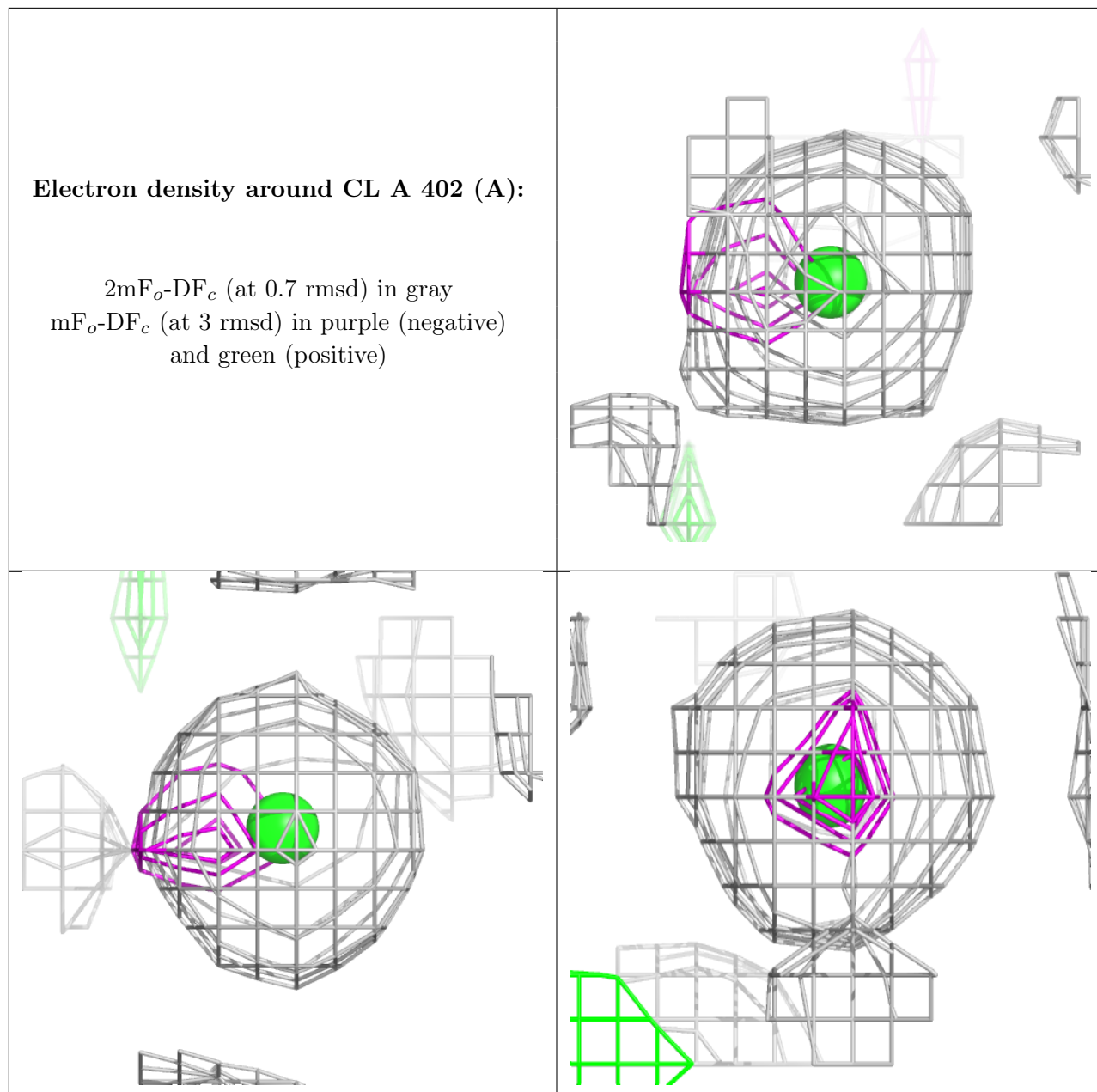
Electron density around OEX A 413 (B):

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



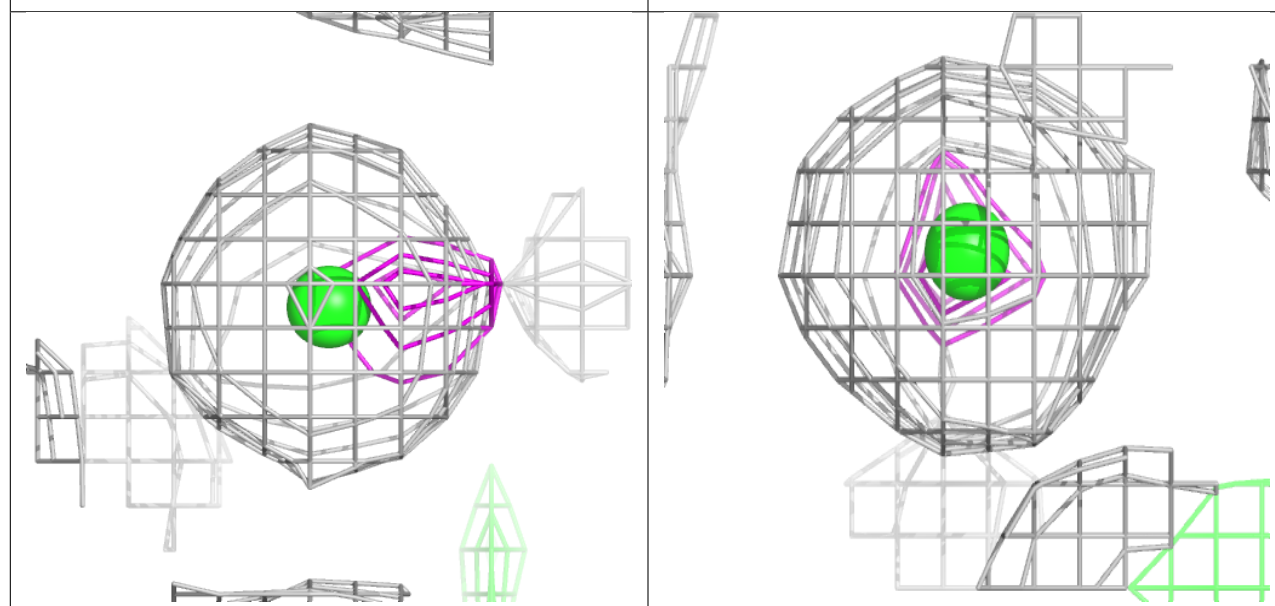
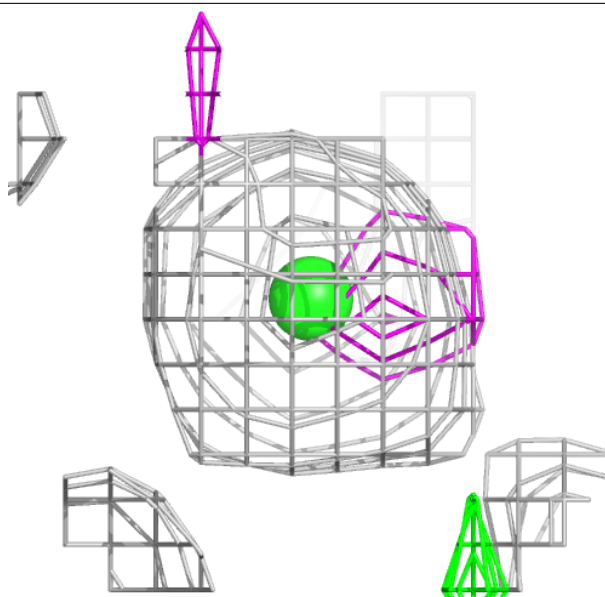
Electron density around CL A 402 (A):

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



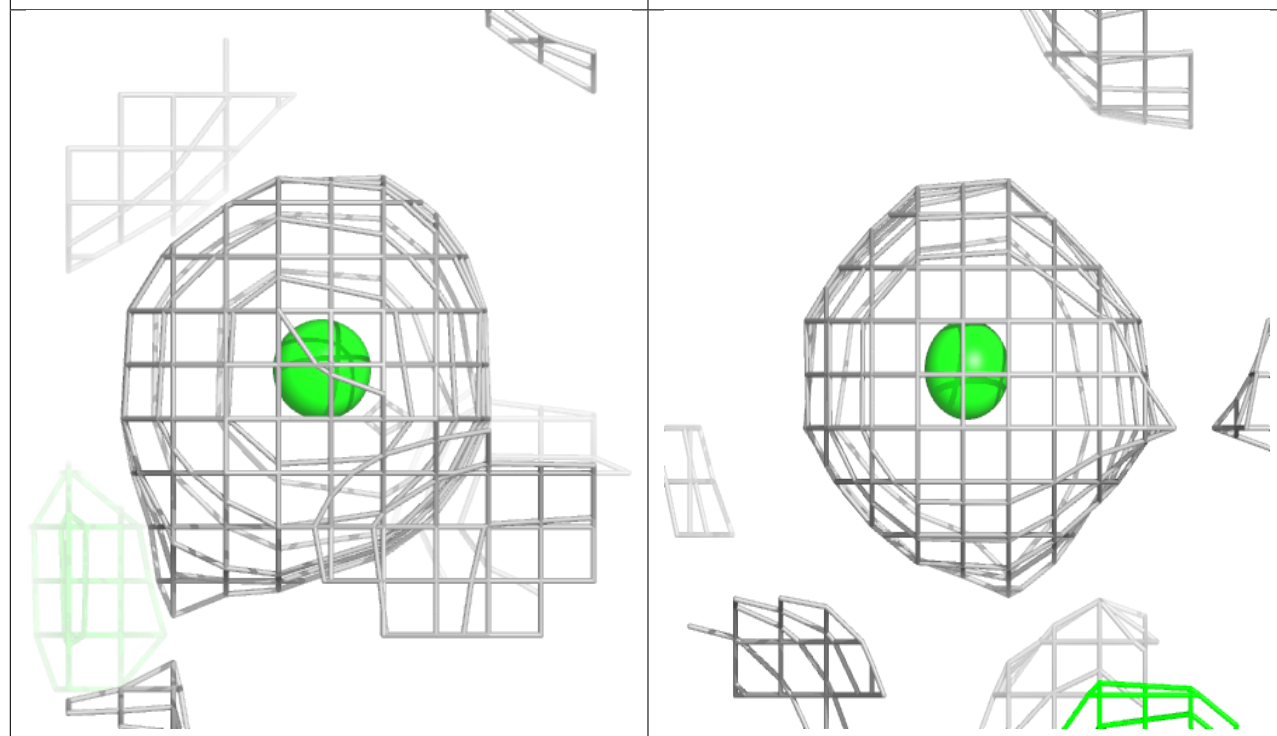
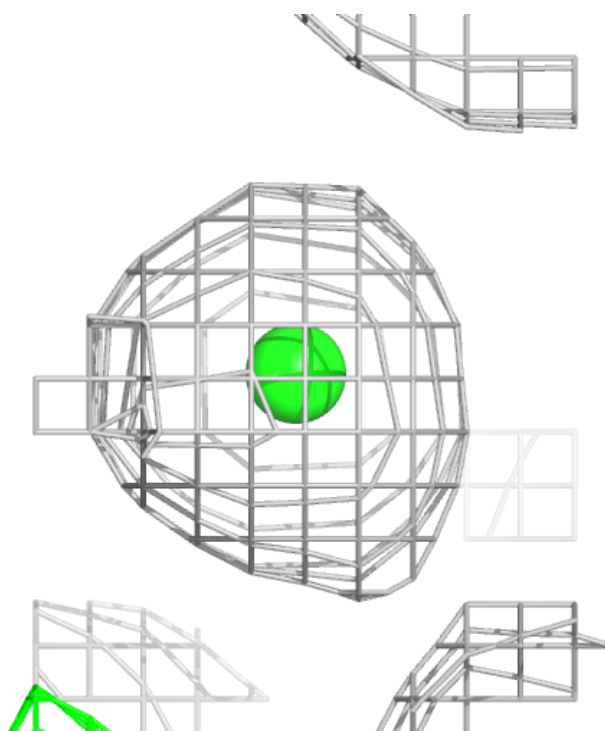
Electron density around CL A 402 (B):

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



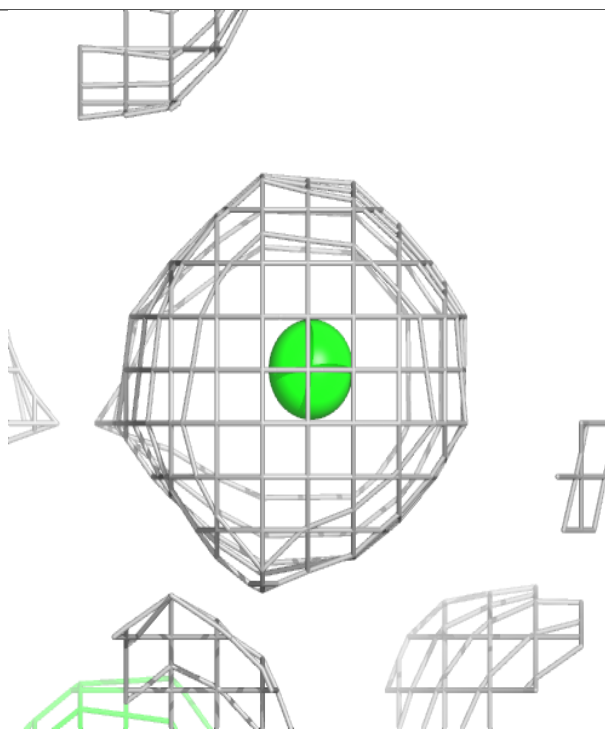
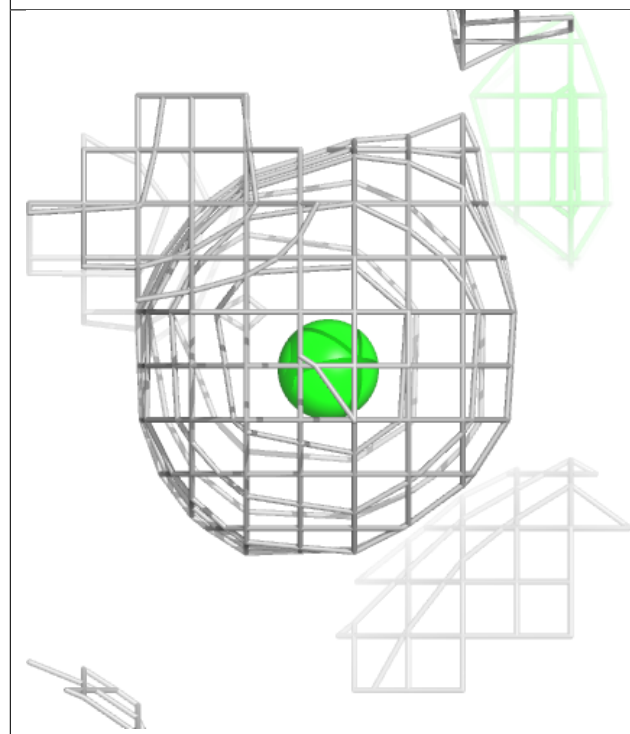
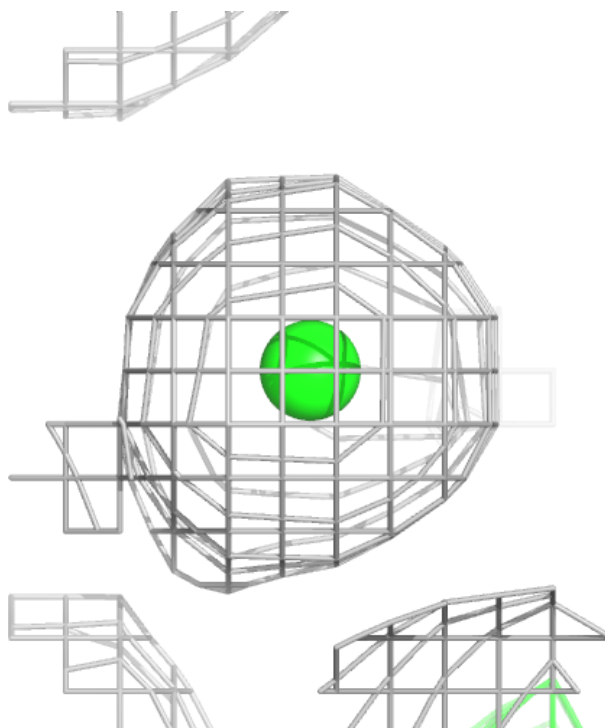
Electron density around CL a 402 (A):

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



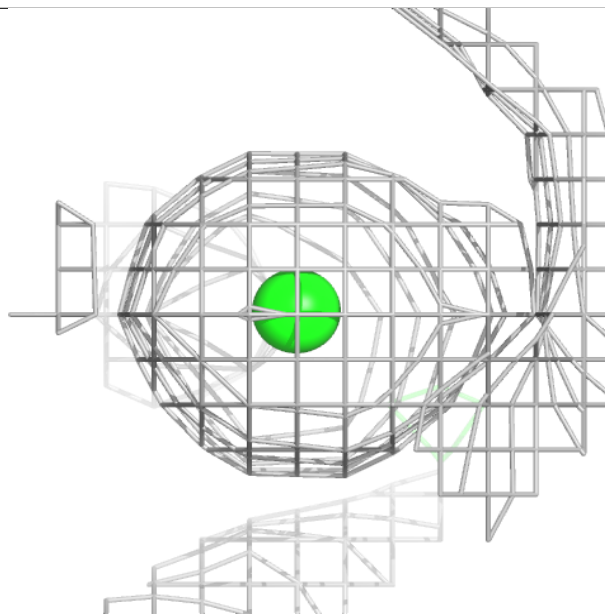
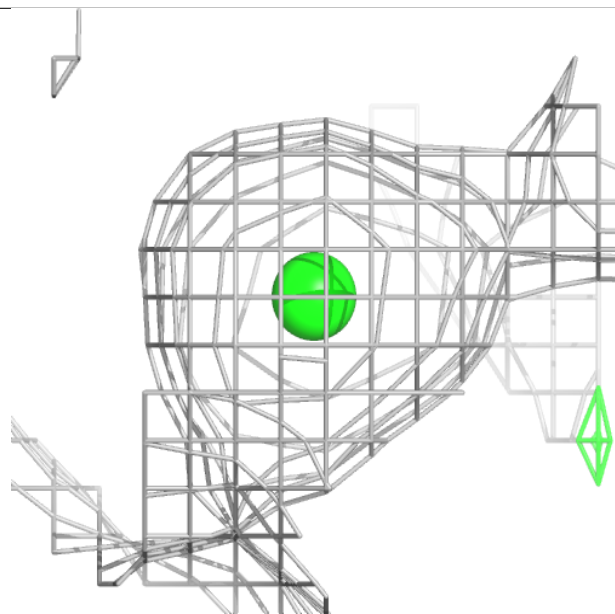
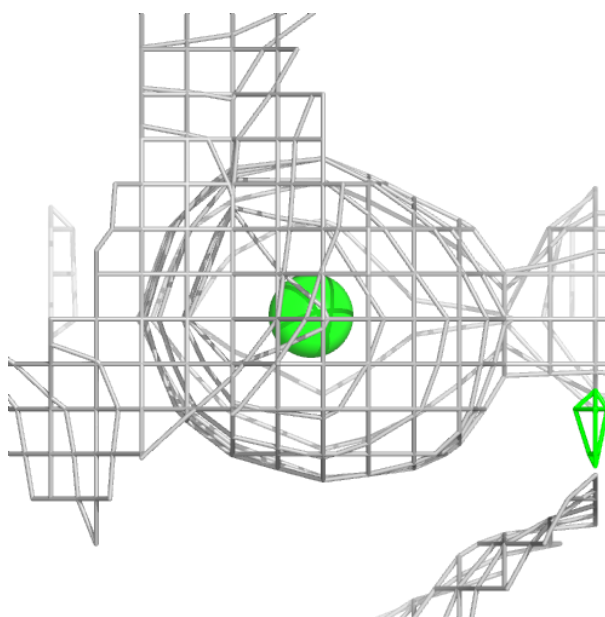
Electron density around CL a 402 (B):

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



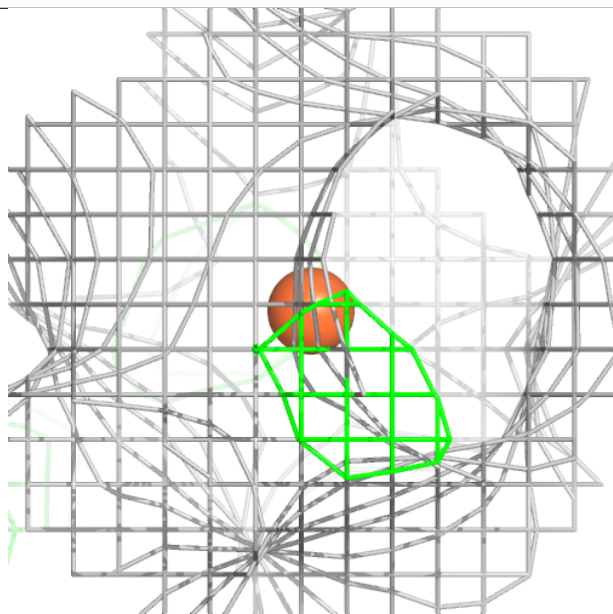
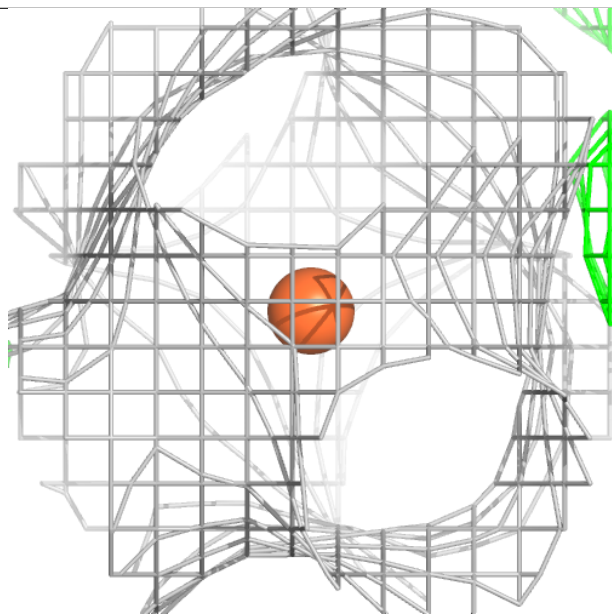
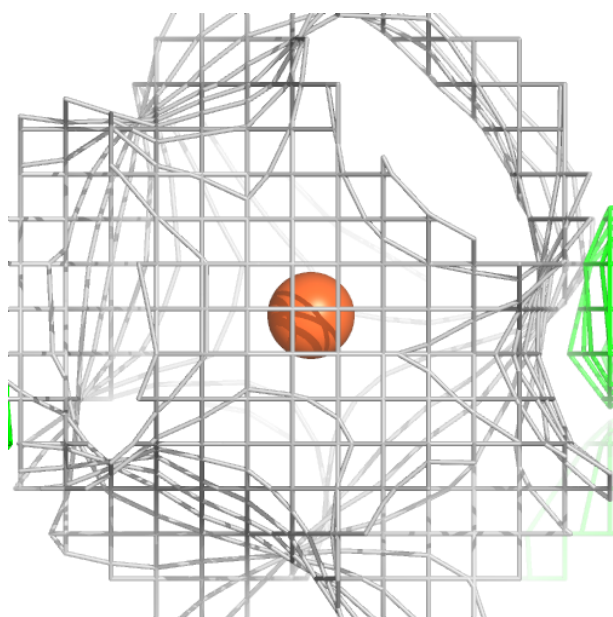
Electron density around CL a 403 (A):

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



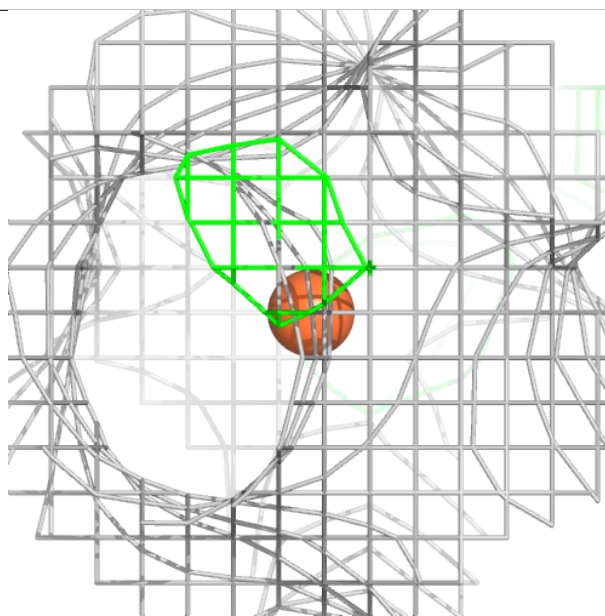
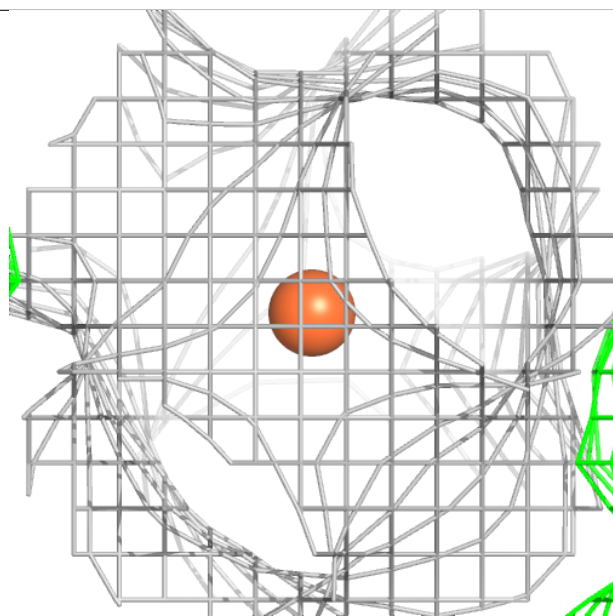
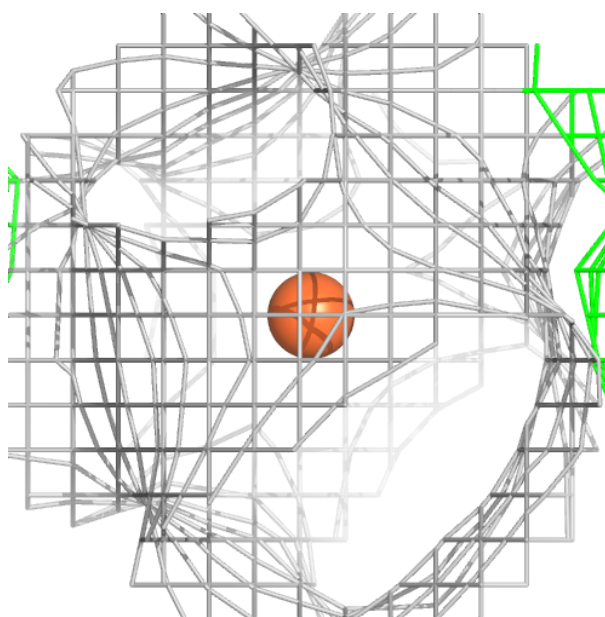
Electron density around FE2 a 401 (A):

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



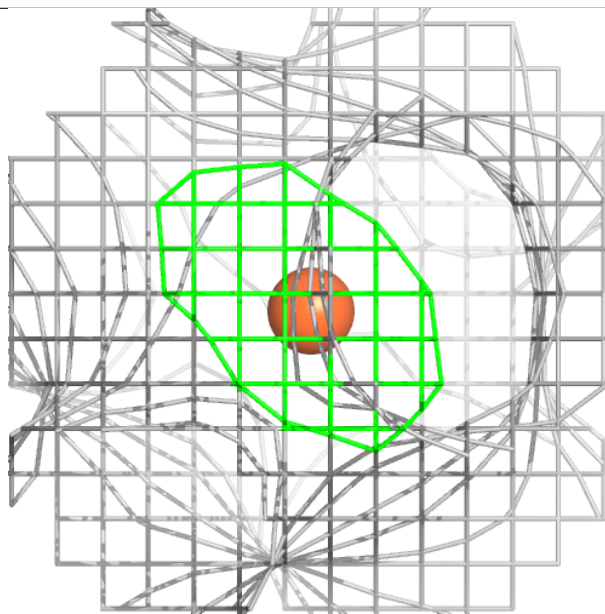
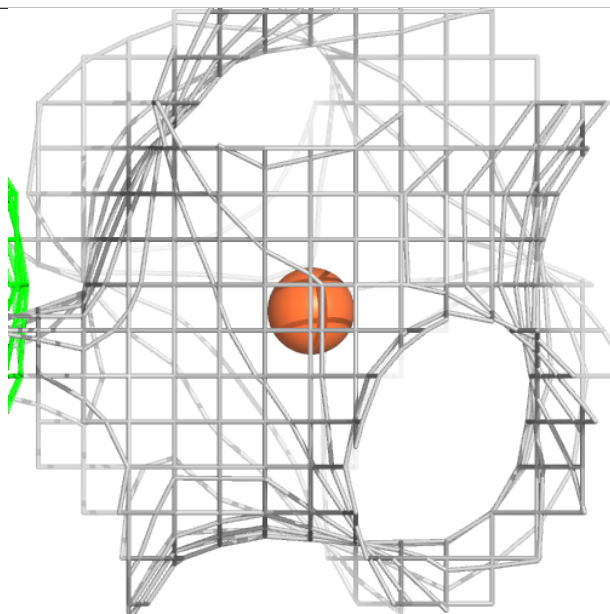
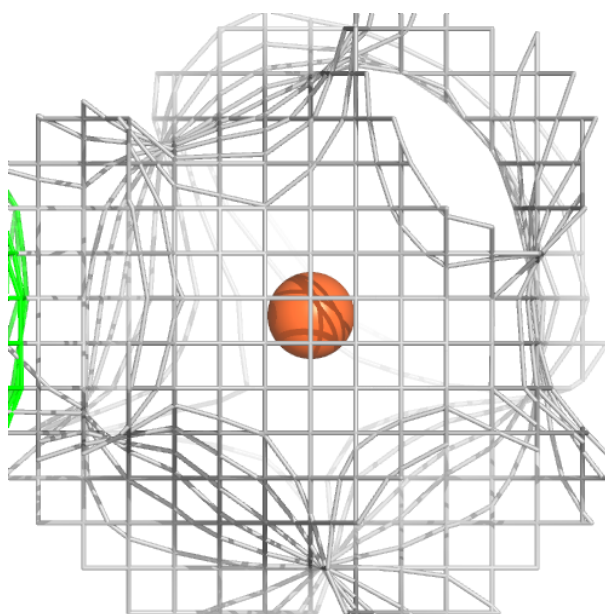
Electron density around FE2 a 401 (B):

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



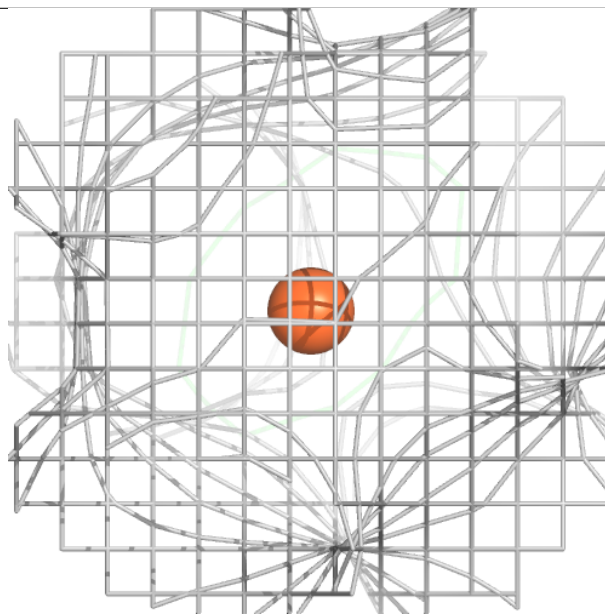
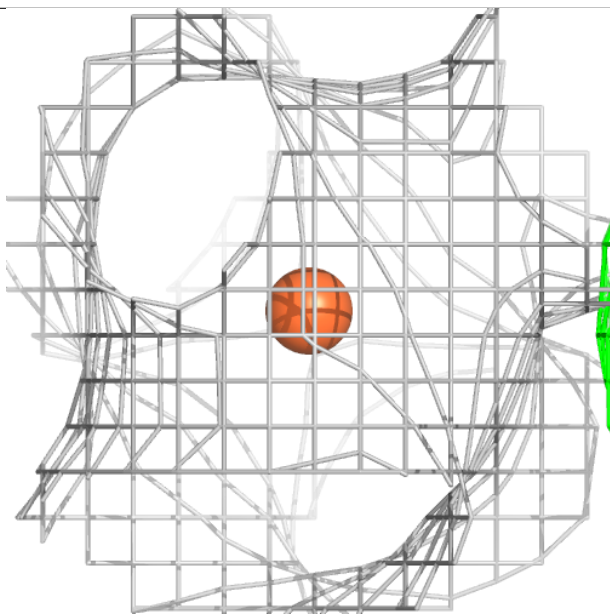
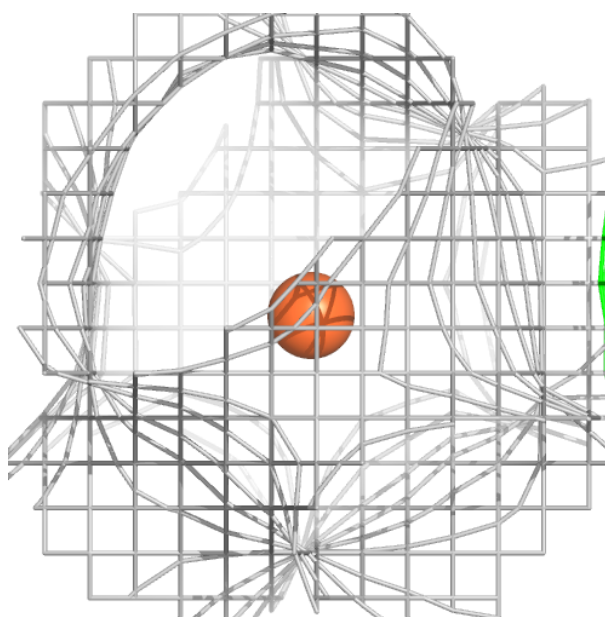
Electron density around FE2 A 401 (A):

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



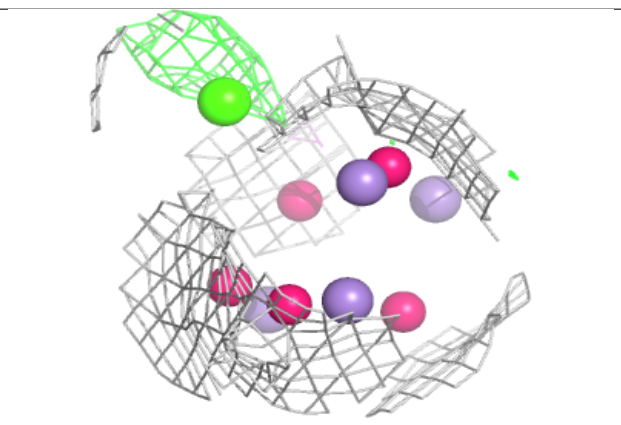
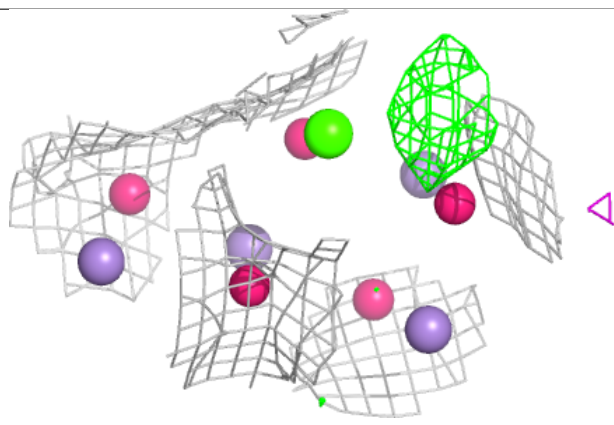
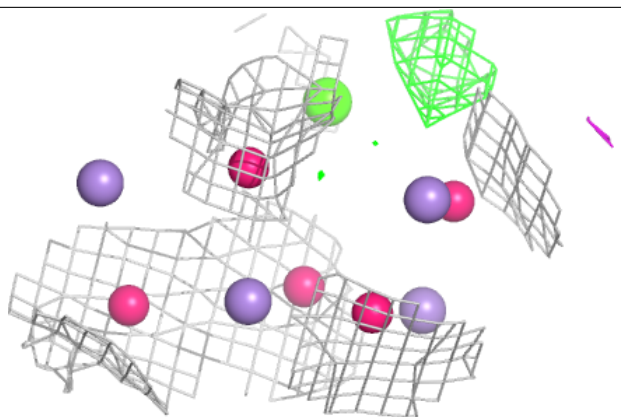
Electron density around FE2 A 401 (B):

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

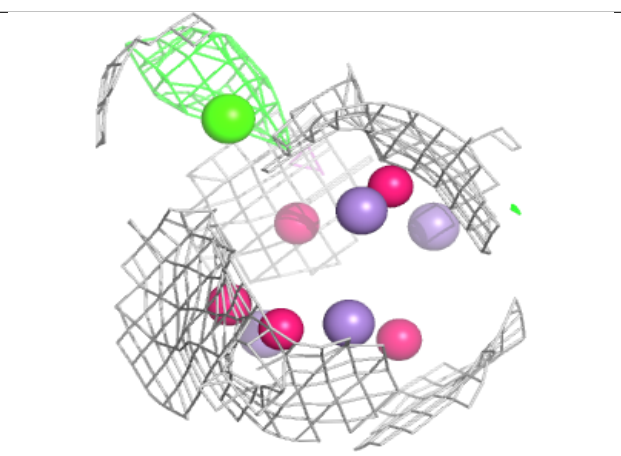
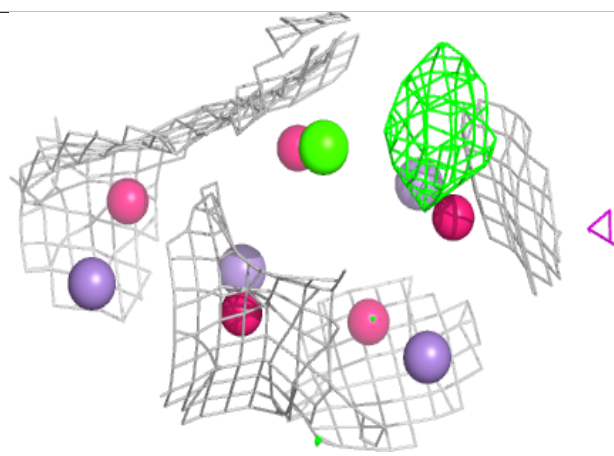
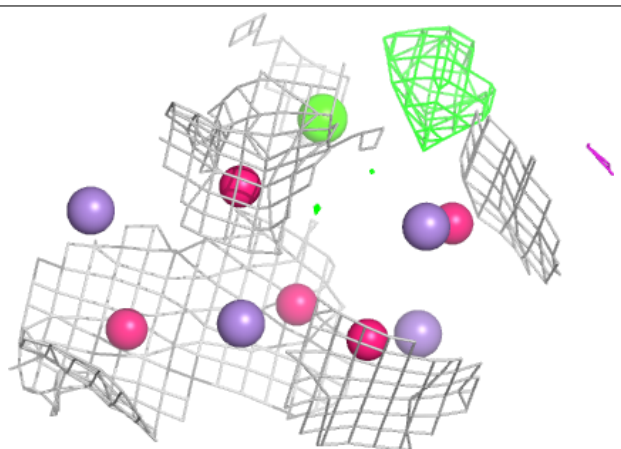


Electron density around OEX a 415 (A):

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

**Electron density around OEX a 415 (B):**

$2mF_o-DF_c$ (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.