



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 7, 2026 – 06:32 AM JST

PDB ID : 8GN2 / pdb_00008gn2
Title : Crystal structure of PPBQ-bound photosystem II complex
Authors : Kamada, S.; Nakajima, Y.; Shen, J.-R.
Deposited on : 2022-08-22
Resolution : 1.95 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>.

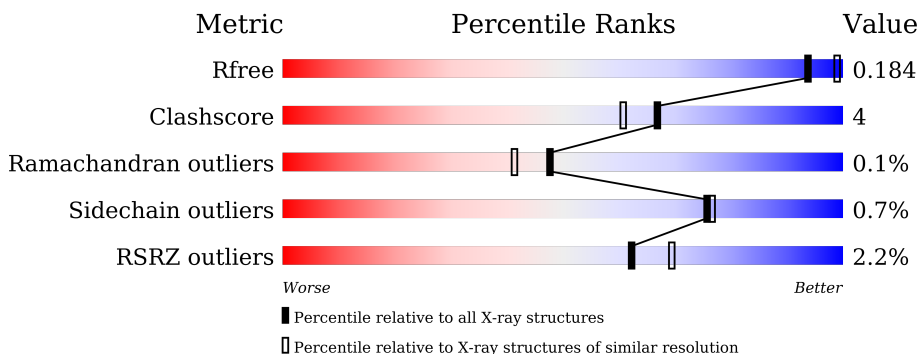
The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

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X-RAY DIFFRACTION

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.



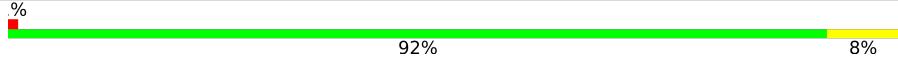
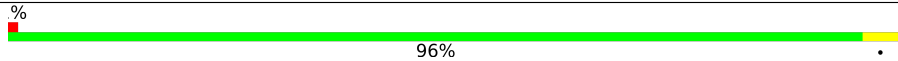
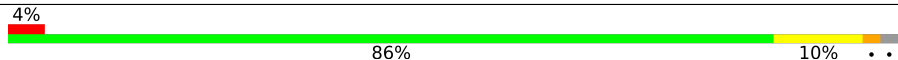
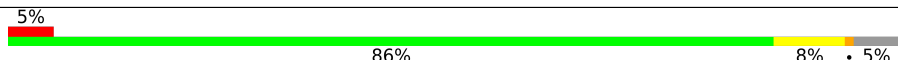
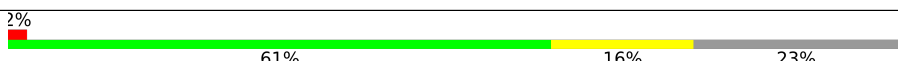
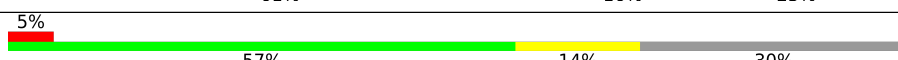
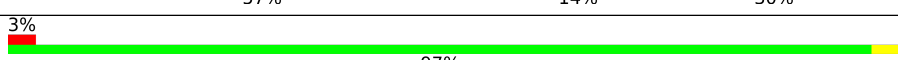
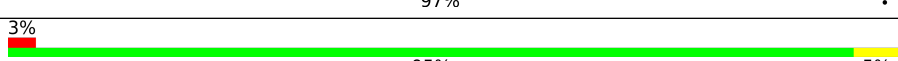
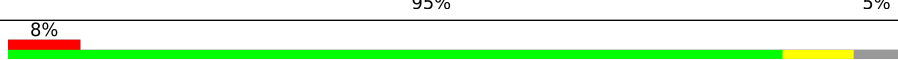
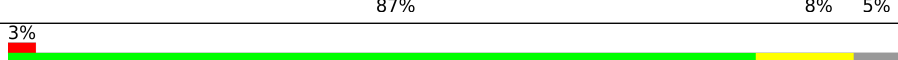
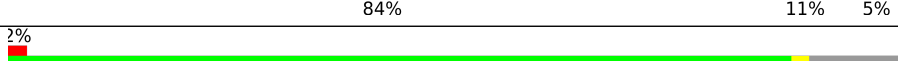
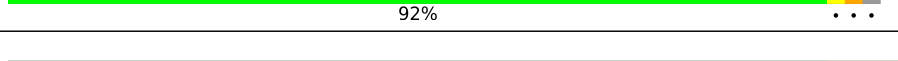
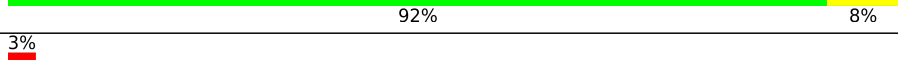
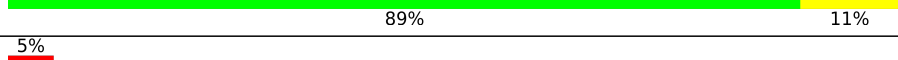
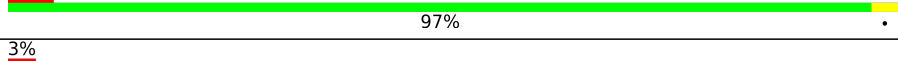
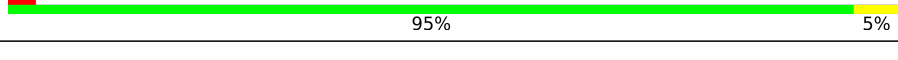
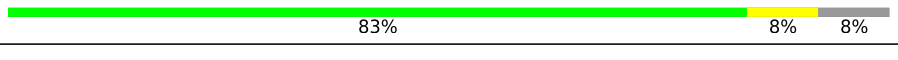
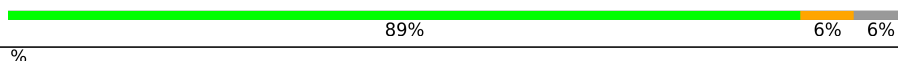
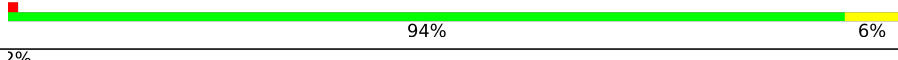
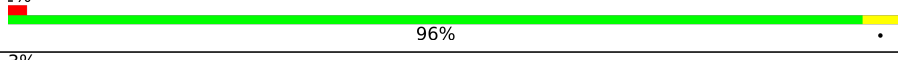
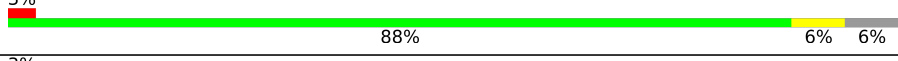
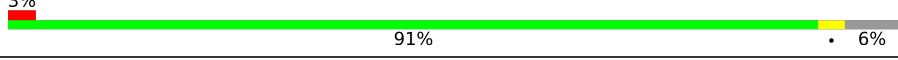
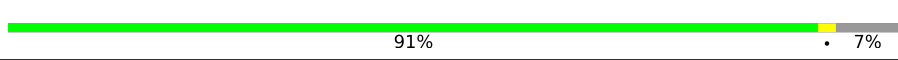
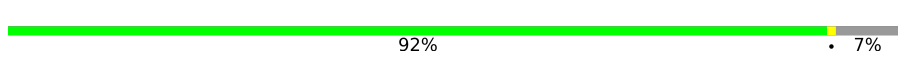
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	90% 7%
1	a	344	91% 6%
2	B	505	94% 6%
2	b	505	94% 6%
3	C	455	93% 6%
3	c	455	94% 6%

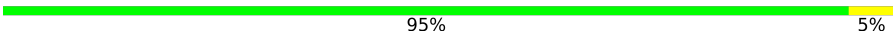
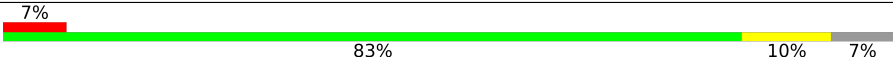
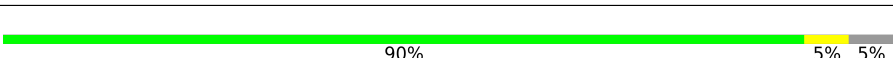
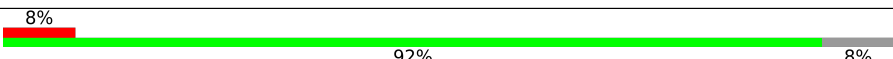
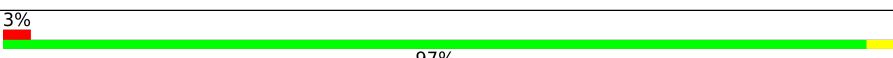
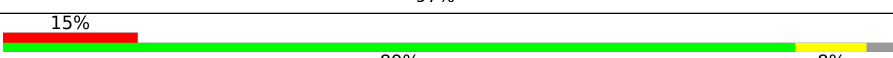
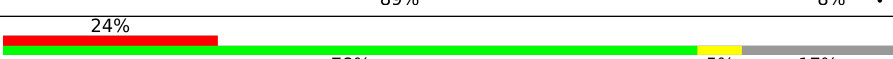
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Mol	Chain	Length	Quality of chain
4	D	342	
4	d	342	
5	E	83	
5	e	83	
6	F	44	
6	f	44	
7	H	63	
7	h	63	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	37	
10	k	37	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	244	
13	o	244	
14	T	32	
14	t	32	
15	U	104	
15	u	104	
16	V	137	

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Mol	Chain	Length	Quality of chain
16	v	137	
17	Y	30	
17	y	30	
18	X	40	
18	x	40	
19	Z	62	
19	z	62	
20	R	41	

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
43	HEC	V	202	X	-	-	-
43	HEC	v	1603	X	-	-	-

2 Entry composition

There are 44 unique types of molecules in this entry. The entry contains 55061 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	3	0
			2624	1720	431	458	15			
1	a	334	Total	C	N	O	S	0	3	0
			2620	1717	431	457	15			

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	505	Total	C	N	O	S	0	9	0
			4007	2631	670	693	13			
2	b	503	Total	C	N	O	S	0	10	0
			3989	2621	661	694	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	2	0
			3494	2286	585	610	13			
3	c	455	Total	C	N	O	S	0	2	0
			3516	2305	587	611	13			

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	2	0
			2731	1812	444	463	12			
4	d	342	Total	C	N	O	S	0	3	0
			2738	1815	447	464	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	81	Total	C	N	O		0	0	0
			657	429	106	122				
5	e	79	Total	C	N	O		0	0	0
			639	419	103	117				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	34	Total	C	N	O	S	0	0	0
			274	187	45	41	1			
6	f	31	Total	C	N	O	S	0	0	0
			250	170	42	37	1			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	36	Total	C	N	O	S	0	0	0
			285	195	42	47	1			
8	i	36	Total	C	N	O	S	0	0	0
			296	200	46	49	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	36	Total	C	N	O	S	0	0	0
			251	171	37	42	1			
9	j	39	Total	C	N	O	S	0	0	0
			271	182	40	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	1	0
			293	205	42	46			
10	k	37	Total	C	N	O	0	0	0
			286	198	42	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	37	Total	C	N	O	S	0	1	0
			305	205	48	51	1			
11	l	37	Total	C	N	O	S	0	2	0
			309	209	48	51	1			

- 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
			265	178	38	48	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	m	34	Total	C	N	O	S	0	3	0
			281	191	39	50	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	244	Total	C	N	O	S	0	6	0
			1884	1180	313	386	5			
13	o	243	Total	C	N	O	S	0	5	0
			1871	1172	311	382	6			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	U	97	Total	C	N	O		0	1	0
			776	493	130	153				
15	u	97	Total	C	N	O		0	1	0
			780	495	130	155				

- 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	2	0
			1063	676	178	205	4			
16	v	137	Total	C	N	O	S	0	1	0
			1060	671	177	208	4			

- Molecule 17 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Y	28	Total	C	N	O	S	0	0	0
			198	130	33	32	3			
17	y	28	Total	C	N	O	S	0	0	0
			196	128	33	32	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	X	38	Total	C	N	O	S	0	0	0
			279	187	45	47				
18	x	37	Total	C	N	O	S	0	1	0
			273	185	43	45				

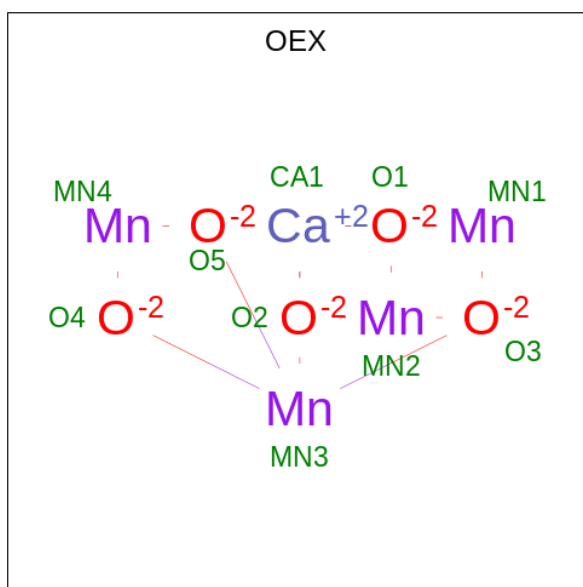
- Molecule 19 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Z	62	Total	C	N	O	S	0	0	0
			461	319	67	73	2			
19	z	60	Total	C	N	O	S	0	0	0
			446	306	69	70	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	R	34	Total	C	N	O	S	0	0	0
			240	159	42	39				

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



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

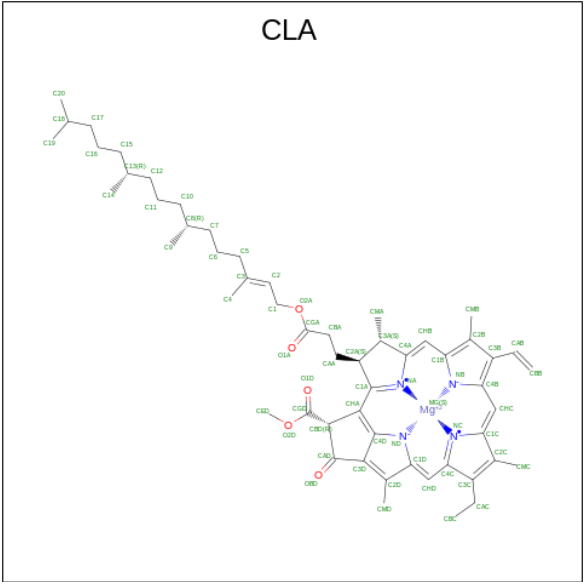
- Molecule 22 is FE (II) ION (CCD ID: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

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

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

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

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



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

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

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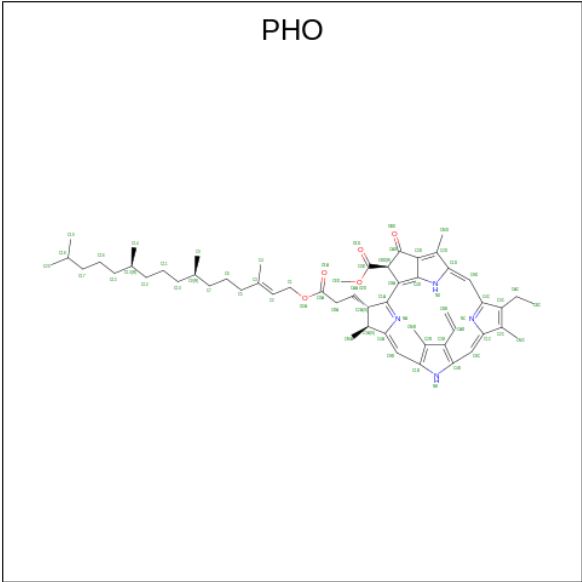
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N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

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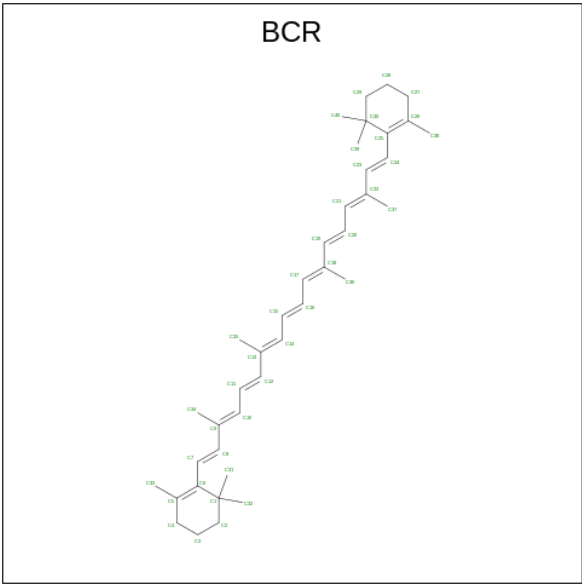
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N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

- Molecule 25 is PHEOPHYTIN A (CCD ID: PHO) (formula: C₅₅H₇₄N₄O₅).



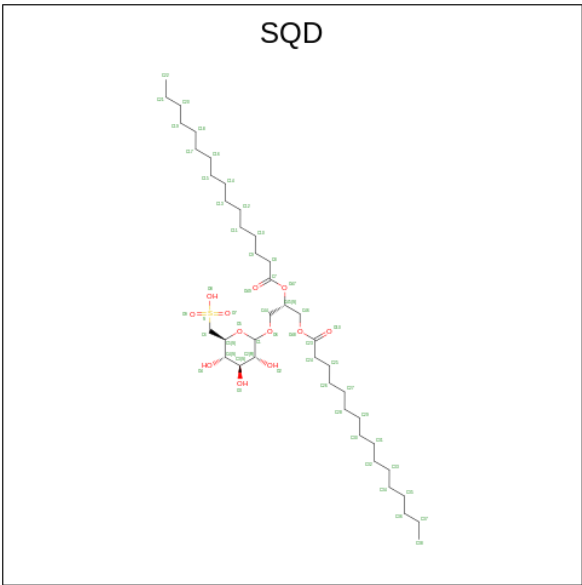
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	A	1	Total	C	N	O	0	0
			64	55	4	5		
25	D	1	Total	C	N	O	0	0
			64	55	4	5		
25	a	1	Total	C	N	O	0	0
			64	55	4	5		
25	d	1	Total	C	N	O	0	0
			64	55	4	5		

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



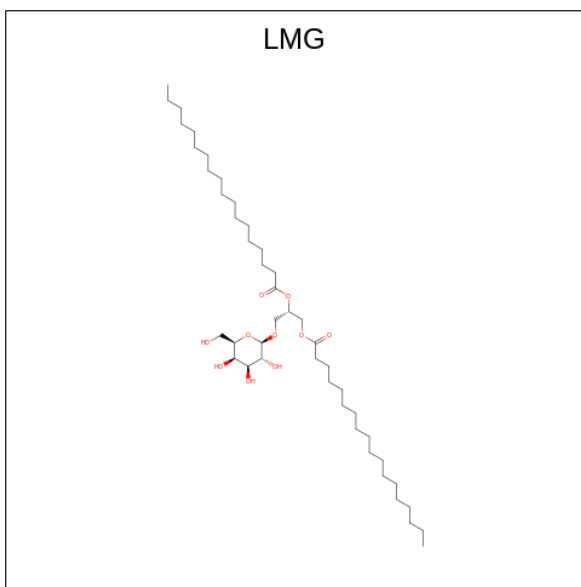
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	D	1	Total C 40 40	0	0
26	K	1	Total C 40 40	0	0
26	T	1	Total C 40 40	0	0
26	Y	1	Total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

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



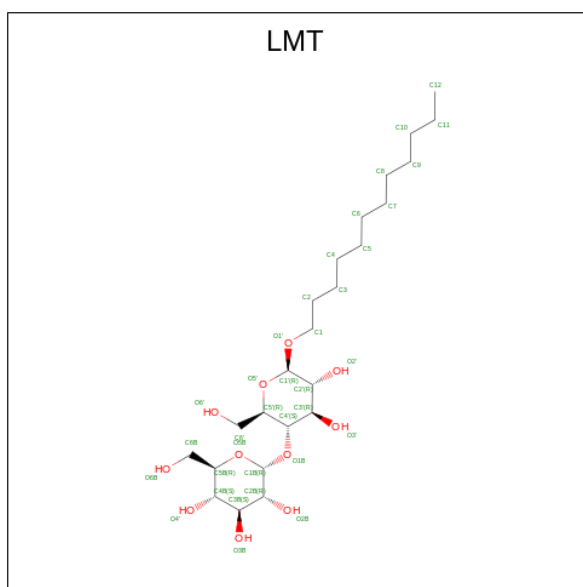
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	A	1	Total	C	O	S	0	0
			54	41	12	1		
27	A	1	Total	C	O	S	0	0
			54	41	12	1		
27	D	1	Total	C	O	S	0	0
			45	32	12	1		
27	L	1	Total	C	O	S	0	0
			54	41	12	1		
27	L	1	Total	C	O	S	0	0
			54	41	12	1		
27	a	1	Total	C	O	S	0	0
			54	41	12	1		
27	a	1	Total	C	O	S	0	0
			54	41	12	1		
27	f	1	Total	C	O	S	0	0
			33	23	9	1		

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



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

- Molecule 29 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



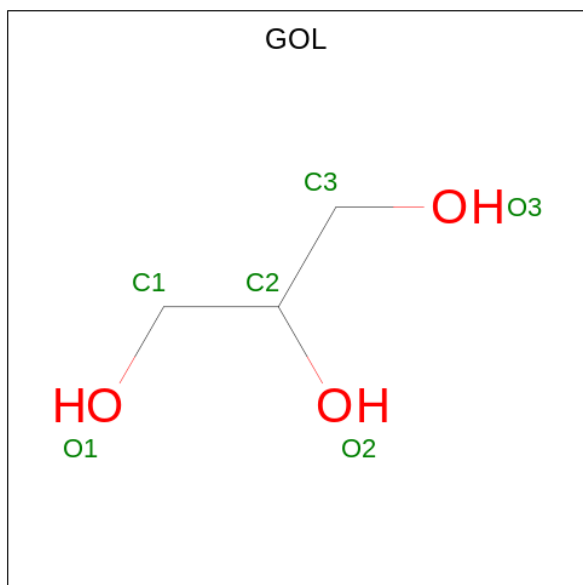
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	A	1	Total 35	C 24	O 11	0	0
29	B	1	Total 35	C 24	O 11	0	0
29	B	1	Total 24	C 18	O 6	0	0
29	C	1	Total 35	C 24	O 11	0	0
29	E	1	Total 24	C 18	O 6	0	0
29	J	1	Total 24	C 18	O 6	0	0
29	M	1	Total 35	C 24	O 11	0	0
29	T	1	Total 24	C 18	O 6	0	0
29	Z	1	Total 35	C 24	O 11	0	0
29	a	1	Total 35	C 24	O 11	0	0
29	b	1	Total 25	C 19	O 6	0	0
29	c	1	Total 35	C 24	O 11	0	0
29	f	1	Total 35	C 24	O 11	0	0
29	m	1	Total 35	C 24	O 11	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	m	1	Total	C	O	0	0
			35	24	11		
29	m	1	Total	C	O	0	0
			35	24	11		
29	z	1	Total	C	O	0	0
			32	21	11		

- Molecule 30 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	C	1	Total 6	C 3	O 3	0	0
30	C	1	Total 6	C 3	O 3	0	0
30	C	1	Total 6	C 3	O 3	0	0
30	C	1	Total 6	C 3	O 3	0	0
30	C	1	Total 6	C 3	O 3	0	0
30	E	1	Total 6	C 3	O 3	0	0
30	L	1	Total 6	C 3	O 3	0	0
30	M	1	Total 6	C 3	O 3	0	0
30	O	1	Total 6	C 3	O 3	0	0
30	T	1	Total 6	C 3	O 3	0	0
30	T	1	Total 6	C 3	O 3	0	0
30	V	1	Total 6	C 3	O 3	0	0
30	V	1	Total 6	C 3	O 3	0	0
30	V	1	Total 6	C 3	O 3	0	0
30	V	1	Total 6	C 3	O 3	0	0
30	a	1	Total 6	C 3	O 3	0	0
30	a	1	Total 6	C 3	O 3	0	0
30	a	1	Total 6	C 3	O 3	0	0
30	a	1	Total 6	C 3	O 3	0	0
30	b	1	Total 6	C 3	O 3	0	0
30	b	1	Total 6	C 3	O 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	b	1	Total	C	O	0	0
			6	3	3		
30	b	1	Total	C	O	0	0
			6	3	3		
30	c	1	Total	C	O	0	0
			6	3	3		
30	c	1	Total	C	O	0	0
			6	3	3		
30	c	1	Total	C	O	0	0
			6	3	3		
30	c	1	Total	C	O	0	0
			6	3	3		
30	d	1	Total	C	O	0	0
			6	3	3		
30	d	1	Total	C	O	0	0
			6	3	3		
30	h	1	Total	C	O	0	0
			6	3	3		
30	k	1	Total	C	O	0	0
			6	3	3		
30	o	1	Total	C	O	0	0
			6	3	3		
30	o	1	Total	C	O	0	0
			6	3	3		
30	u	1	Total	C	O	0	0
			6	3	3		
30	v	1	Total	C	O	0	0
			6	3	3		
30	v	1	Total	C	O	0	0
			6	3	3		
30	v	1	Total	C	O	0	0
			6	3	3		
30	v	1	Total	C	O	0	0
			6	3	3		
30	v	1	Total	C	O	0	0
			6	3	3		

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

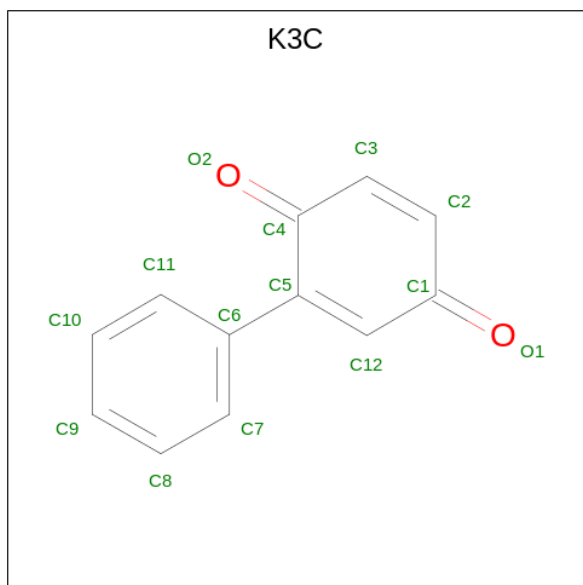
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	A	4	Total C O 74 69 5	0	0
31	B	7	Total C O 99 95 4	0	0
31	C	3	Total C O 73 66 7	0	0
31	D	3	Total C O 68 63 5	0	0
31	E	2	Total C 30 30	0	0
31	H	1	Total C 8 8	0	0
31	I	3	Total C 47 47	0	0
31	J	2	Total C 31 31	0	0
31	T	1	Total C 9 9	0	0
31	Y	1	Total C 12 12	0	0
31	X	1	Total C 16 16	0	0
31	a	4	Total C O 73 68 5	0	0
31	b	5	Total C 70 70	0	0
31	c	4	Total C O 74 67 7	0	0
31	d	2	Total C O 56 51 5	0	0
31	e	1	Total C 15 15	0	0
31	h	3	Total C 39 39	0	0
31	i	3	Total C O 71 66 5	0	0
31	j	2	Total C O 34 32 2	0	0
31	k	1	Total C 16 16	0	0
31	l	1	Total C O 16 14 2	0	0
31	t	1	Total C 8 8	0	0

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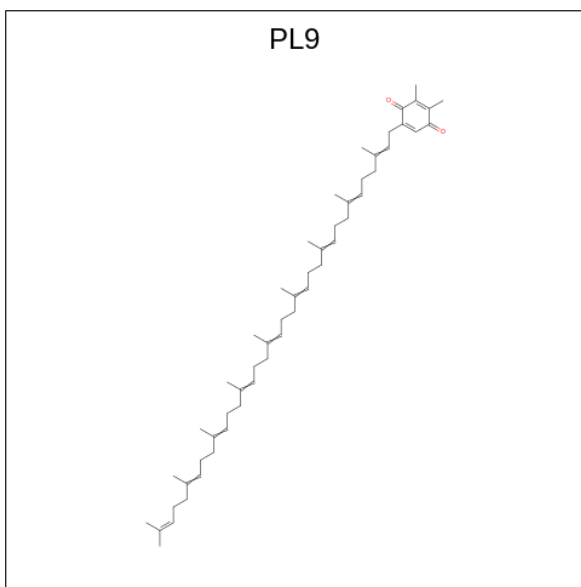
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	x	2	Total	C	O	0	0
			30	28	2		

- Molecule 32 is 2-phenylcyclohexa-2,5-diene-1,4-dione (CCD ID: K3C) (formula: $C_{12}H_8O_2$) (labeled as "Ligand of Interest" by depositor).



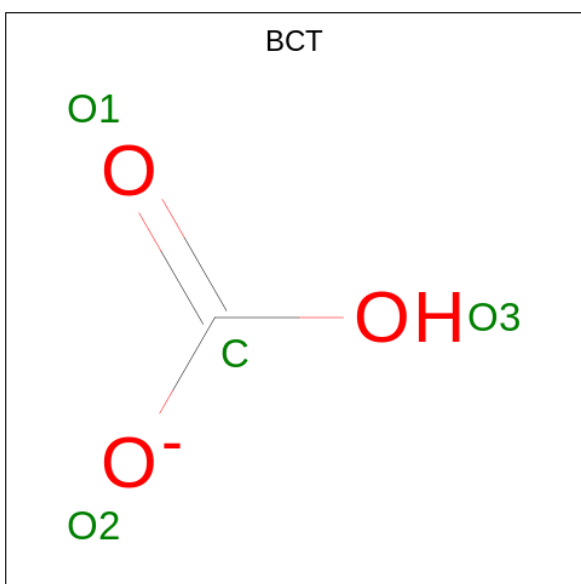
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	A	1	Total	C	O	0	1
			14	12	2		
32	a	1	Total	C	O	0	1
			14	12	2		

- Molecule 33 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: $C_{53}H_{80}O_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 34 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3) (labeled as "Ligand of Interest" by depositor).

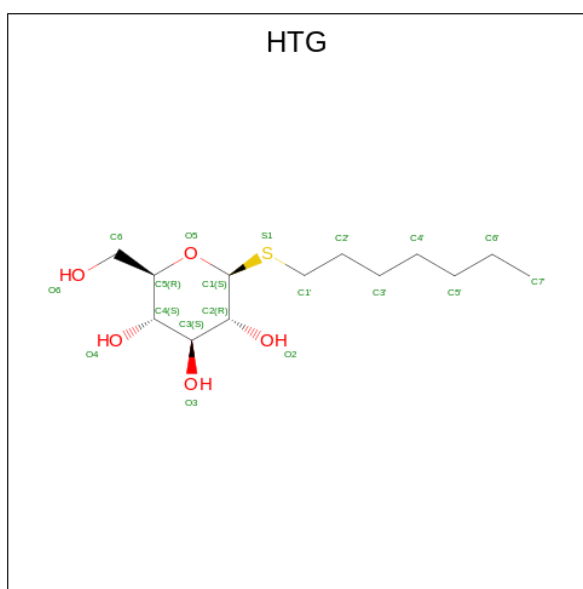


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	A	1	Total	C	O	0	0
			4	1	3		
34	a	1	Total	C	O	0	0
			4	1	3		

- Molecule 35 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	B	1	Total	Ca	0	0
			1	1		
35	F	1	Total	Ca	0	0
			1	1		
35	O	1	Total	Ca	0	0
			1	1		
35	b	1	Total	Ca	0	0
			1	1		
35	c	1	Total	Ca	0	0
			1	1		
35	f	1	Total	Ca	0	0
			1	1		
35	o	1	Total	Ca	0	0
			1	1		

- Molecule 36 is heptyl 1-thio-beta-D-glucopyranoside (CCD ID: HTG) (formula: C₁₃H₂₆O₅S).



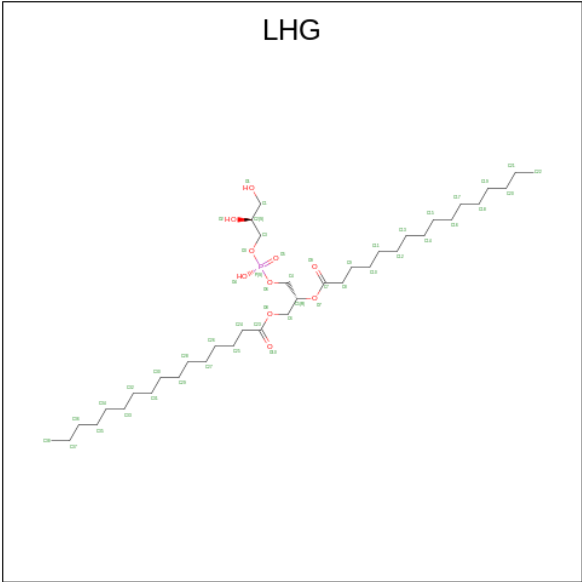
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
36	B	1	Total	C	O	S	0	1
			38	26	10	2		

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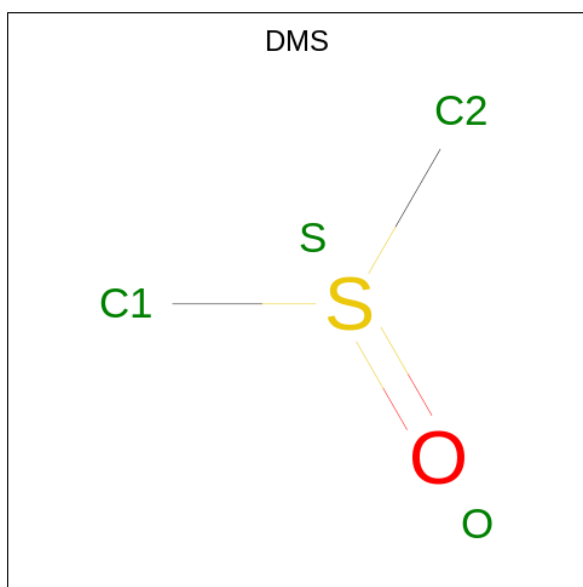
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
36	B	1	Total	C	O	S	0	0
			19	13	5	1		
36	B	1	Total	C	O	S	0	0
			19	13	5	1		
36	B	1	Total	C	O	S	0	0
			19	13	5	1		
36	C	1	Total	C	O	S	0	0
			19	13	5	1		
36	C	1	Total	C	O	S	0	0
			19	13	5	1		
36	D	1	Total	C	O	S	0	0
			19	13	5	1		
36	I	1	Total	C	O	S	0	0
			19	13	5	1		
36	O	1	Total	C	O	S	0	0
			19	13	5	1		
36	U	1	Total	C	S		0	0
			9	8	1			
36	V	1	Total	C	O	S	0	0
			13	7	5	1		
36	b	1	Total	C	O	S	0	0
			19	13	5	1		
36	b	1	Total	C	O	S	0	0
			19	13	5	1		
36	b	1	Total	C	O	S	0	0
			19	13	5	1		
36	b	1	Total	C	O	S	0	0
			19	13	5	1		
36	c	1	Total	C	O	S	0	0
			19	13	5	1		
36	c	1	Total	C	O	S	0	0
			19	13	5	1		
36	d	1	Total	C	O	S	0	0
			19	13	5	1		
36	h	1	Total	C	O	S	0	0
			19	13	5	1		
36	o	1	Total	C	O	S	0	0
			19	13	5	1		
36	u	1	Total	C	O	S	0	0
			14	10	3	1		

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
37	B	1	Total	C	O	P	0	0
			49	38	10	1		
37	D	1	Total	C	O	P	0	0
			49	38	10	1		
37	D	1	Total	C	O	P	0	0
			49	38	10	1		
37	D	1	Total	C	O	P	0	0
			46	35	10	1		
37	E	1	Total	C	O	P	0	0
			49	38	10	1		
37	d	1	Total	C	O	P	0	0
			49	38	10	1		
37	d	1	Total	C	O	P	0	0
			49	38	10	1		
37	d	1	Total	C	O	P	0	0
			39	28	10	1		
37	e	1	Total	C	O	P	0	0
			40	29	10	1		
37	l	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 38 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C₂H₆OS).



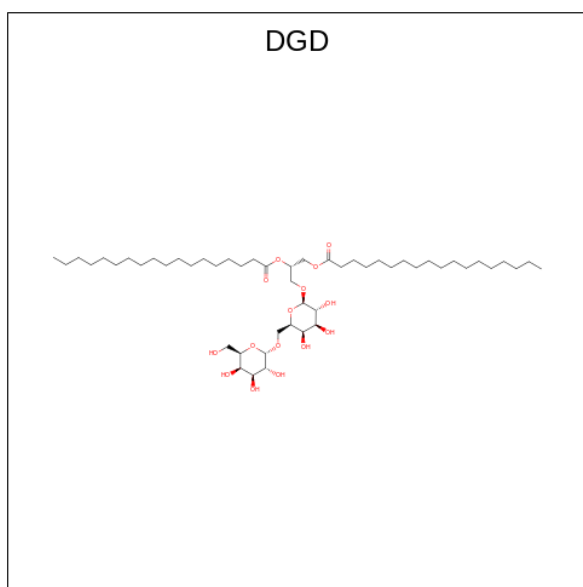
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
38	B	1	Total	C	O	S	0	0
			4	2	1	1		
38	B	1	Total	C	O	S	0	0
			4	2	1	1		
38	B	1	Total	C	O	S	0	0
			4	2	1	1		
38	B	1	Total	C	O	S	0	0
			4	2	1	1		
38	B	1	Total	C	O	S	0	0
			4	2	1	1		
38	C	1	Total	C	O	S	0	0
			4	2	1	1		
38	C	1	Total	C	O	S	0	0
			4	2	1	1		
38	D	1	Total	C	O	S	0	0
			4	2	1	1		
38	E	1	Total	C	O	S	0	0
			4	2	1	1		
38	O	1	Total	C	O	S	0	0
			4	2	1	1		
38	V	1	Total	C	O	S	0	0
			4	2	1	1		
38	Y	1	Total	C	O	S	0	0
			4	2	1	1		
38	a	1	Total	C	O	S	0	0
			4	2	1	1		
38	b	1	Total	C	O	S	0	0
			4	2	1	1		

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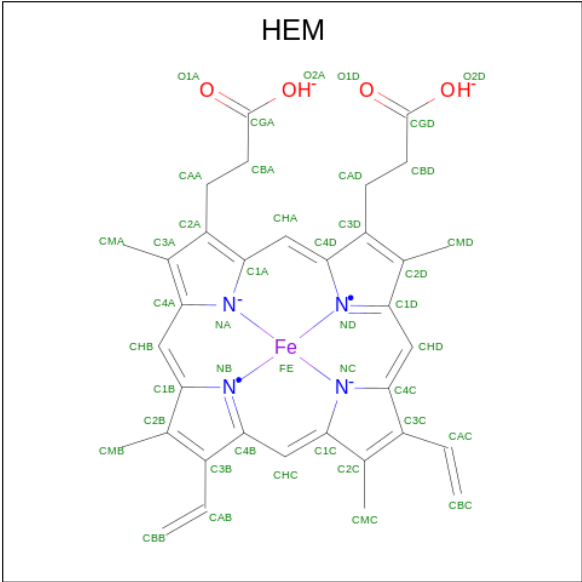
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
38	b	1	Total 4	C 2	O 1	S 1	0	0
38	b	1	Total 4	C 2	O 1	S 1	0	0
38	c	1	Total 4	C 2	O 1	S 1	0	0
38	c	1	Total 4	C 2	O 1	S 1	0	0
38	c	1	Total 4	C 2	O 1	S 1	0	0
38	c	1	Total 4	C 2	O 1	S 1	0	0
38	c	1	Total 4	C 2	O 1	S 1	0	0
38	d	1	Total 4	C 2	O 1	S 1	0	0
38	d	1	Total 4	C 2	O 1	S 1	0	0
38	i	1	Total 4	C 2	O 1	S 1	0	0
38	o	1	Total 4	C 2	O 1	S 1	0	0
38	o	1	Total 4	C 2	O 1	S 1	0	0
38	o	1	Total 4	C 2	O 1	S 1	0	0
38	o	1	Total 4	C 2	O 1	S 1	0	0
38	o	1	Total 4	C 2	O 1	S 1	0	0
38	v	1	Total 4	C 2	O 1	S 1	0	0
38	z	1	Total 4	C 2	O 1	S 1	0	0

- Molecule 39 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



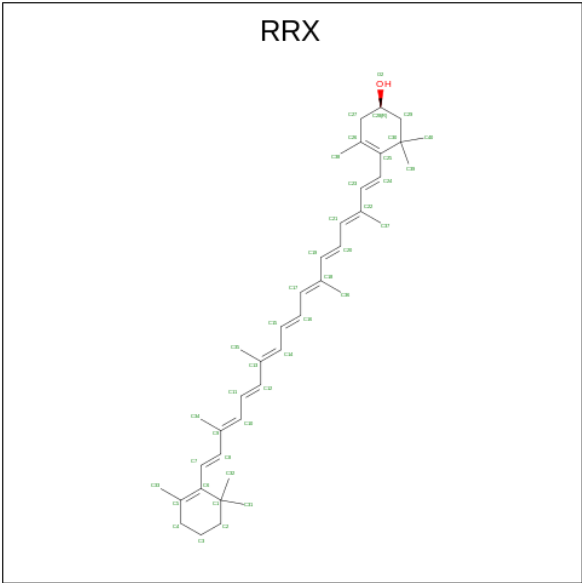
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
39	C	1	Total	C	O	0	0
			62	47	15		
39	C	1	Total	C	O	0	0
			62	47	15		
39	C	1	Total	C	O	0	0
			62	47	15		
39	D	1	Total	C	O	0	0
			53	42	11		
39	H	1	Total	C	O	0	0
			62	47	15		
39	c	1	Total	C	O	0	0
			62	47	15		
39	c	1	Total	C	O	0	0
			62	47	15		
39	c	1	Total	C	O	0	0
			62	47	15		
39	h	1	Total	C	O	0	0
			62	47	15		

- Molecule 40 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 41 is (3R)-beta,beta-caroten-3-ol (CCD ID: RRX) (formula: C₄₀H₅₆O).

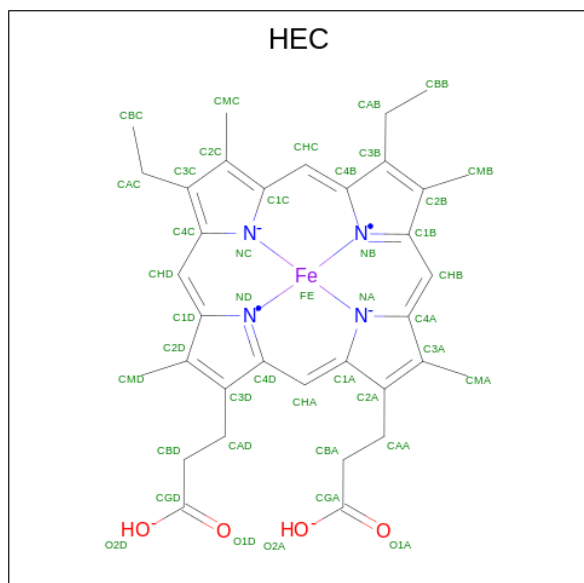


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
41	H	1	Total	C	O	0	0
			41	40	1		
41	h	1	Total	C	O	0	0
			41	40	1		

- Molecule 42 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 43 is HEME C (CCD ID: HEC) (formula: $\text{C}_{34}\text{H}_{36}\text{FeN}_4\text{O}_4$).



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

- Molecule 44 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
44	A	176	Total O 176 176	0	0
44	B	363	Total O 364 364	0	1
44	C	284	Total O 284 284	0	0
44	D	166	Total O 166 166	0	0
44	E	47	Total O 47 47	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
44	F	18	Total O 18 18	0	0
44	H	62	Total O 62 62	0	0
44	I	18	Total O 18 18	0	0
44	J	15	Total O 15 15	0	0
44	K	11	Total O 11 11	0	0
44	L	31	Total O 31 31	0	0
44	M	17	Total O 17 17	0	0
44	O	195	Total O 196 196	0	1
44	T	20	Total O 20 20	0	0
44	U	102	Total O 102 102	0	0
44	V	158	Total O 159 159	0	1
44	Y	9	Total O 9 9	0	0
44	X	16	Total O 16 16	0	0
44	a	164	Total O 164 164	0	0
44	b	323	Total O 325 325	0	2
44	c	273	Total O 275 275	0	2
44	d	157	Total O 157 157	0	0
44	e	29	Total O 29 29	0	0
44	f	11	Total O 11 11	0	0
44	h	45	Total O 45 45	0	0
44	i	10	Total O 10 10	0	0

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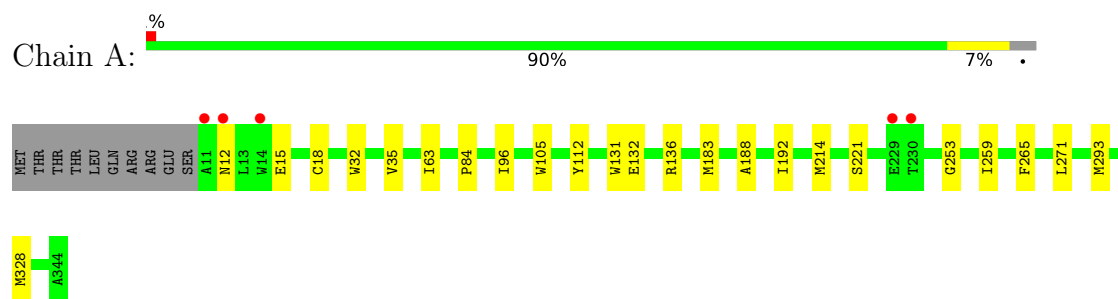
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
44	j	13	Total 13	O 13	0	0
44	k	11	Total 11	O 11	0	0
44	l	15	Total 15	O 15	0	0
44	m	26	Total 26	O 26	0	0
44	o	184	Total 184	O 184	0	0
44	t	18	Total 19	O 19	0	1
44	u	105	Total 106	O 106	0	1
44	v	106	Total 109	O 109	0	3
44	y	12	Total 12	O 12	0	0
44	x	18	Total 18	O 18	0	0
44	z	7	Total 7	O 7	0	0
44	R	2	Total 2	O 2	0	0

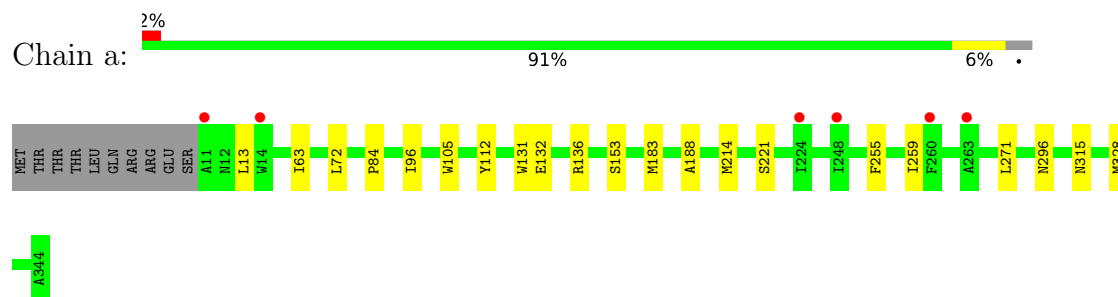
3 Residue-property plots [i](#)

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

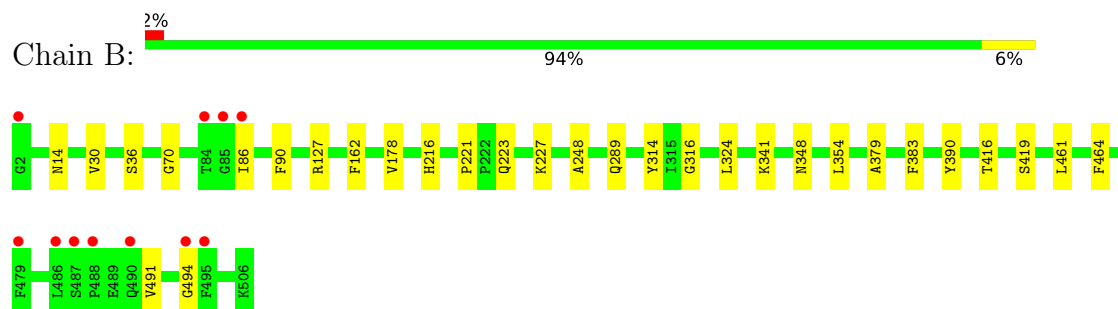
- Molecule 1: Photosystem II protein D1



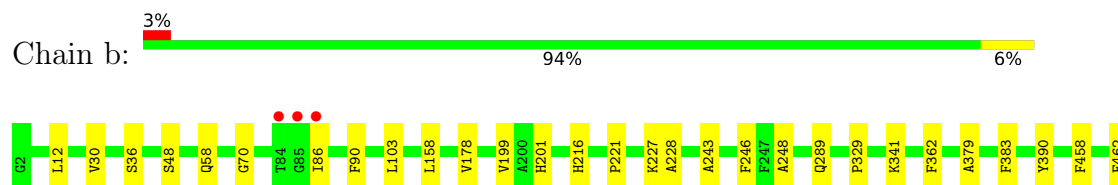
- Molecule 1: Photosystem II protein D1

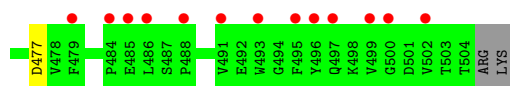


- Molecule 2: Photosystem II CP47 reaction center protein

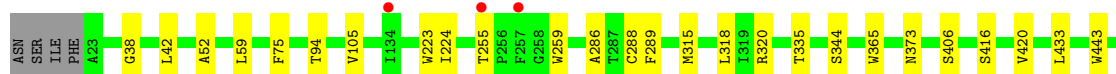
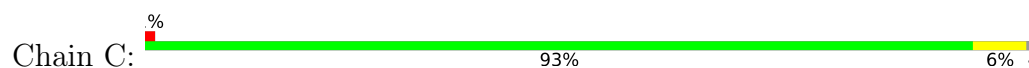


- Molecule 2: Photosystem II CP47 reaction center protein





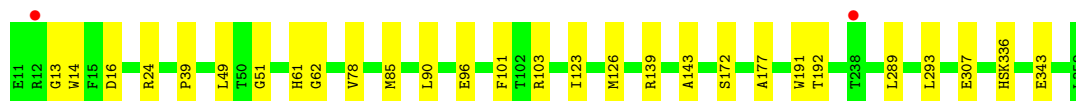
- Molecule 3: Photosystem II CP43 reaction center protein



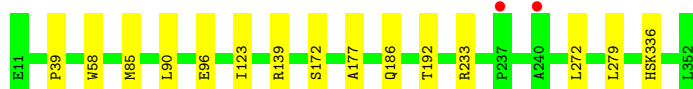
- Molecule 3: Photosystem II CP43 reaction center protein



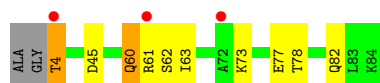
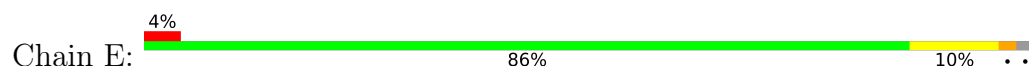
- Molecule 4: Photosystem II D2 protein



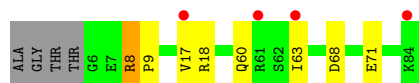
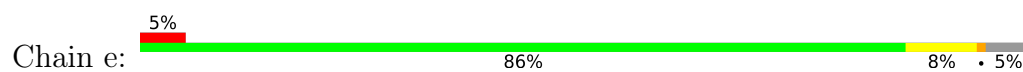
- Molecule 4: Photosystem II D2 protein



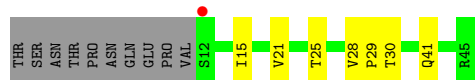
- Molecule 5: Cytochrome b559 subunit alpha



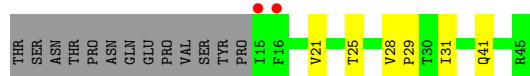
- Molecule 5: Cytochrome b559 subunit alpha



- Molecule 6: Cytochrome b559 subunit beta



- Molecule 6: Cytochrome b559 subunit beta



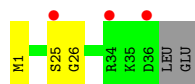
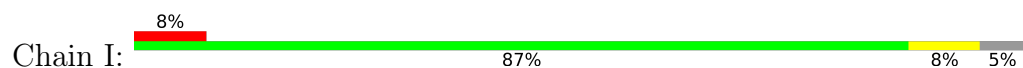
- Molecule 7: Photosystem II reaction center protein H



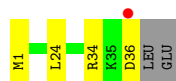
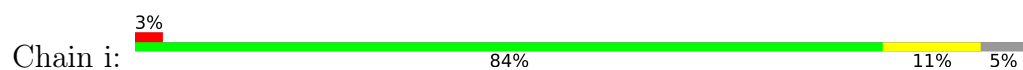
- Molecule 7: Photosystem II reaction center protein H



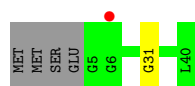
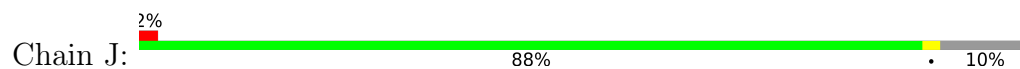
- Molecule 8: Photosystem II reaction center protein I



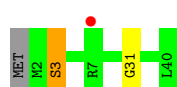
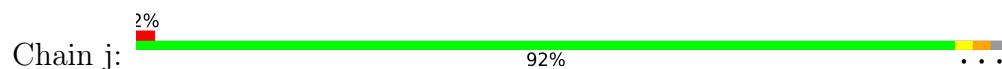
- Molecule 8: Photosystem II reaction center protein I



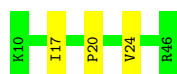
• Molecule 9: Photosystem II reaction center protein J



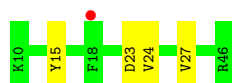
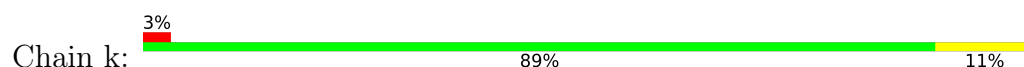
• Molecule 9: Photosystem II reaction center protein J



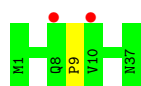
• Molecule 10: Photosystem II reaction center protein K



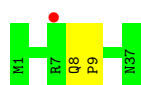
• Molecule 10: Photosystem II reaction center protein K



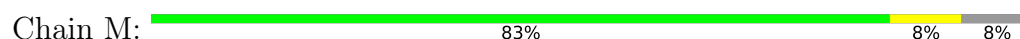
• Molecule 11: Photosystem II reaction center protein L

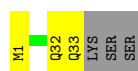


• Molecule 11: Photosystem II reaction center protein L



• Molecule 12: Photosystem II reaction center protein M





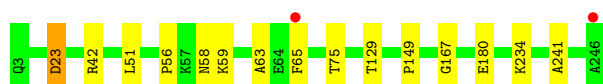
- Molecule 12: Photosystem II reaction center protein M

Chain m: 89% 6% 6%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O: 94% 6%



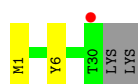
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o: 96% 2%



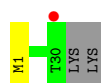
- Molecule 14: Photosystem II reaction center protein T

Chain T: 88% 3% 6%



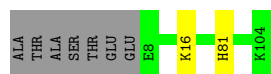
- Molecule 14: Photosystem II reaction center protein T

Chain t: 91% 3% 6%



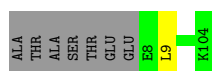
- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U: 91% 7%



- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u: 92% 7%



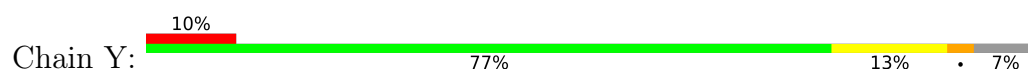
- Molecule 16: Cytochrome c-550



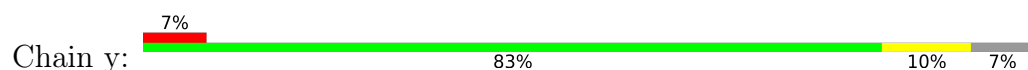
- Molecule 16: Cytochrome c-550



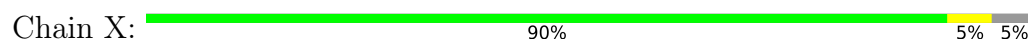
- Molecule 17: Photosystem II reaction center protein Ycf12



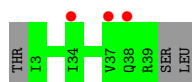
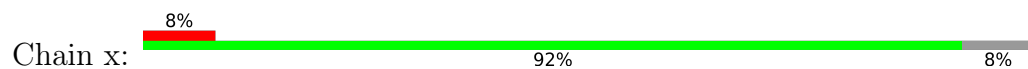
- Molecule 17: Photosystem II reaction center protein Ycf12



- Molecule 18: Photosystem II reaction center protein X

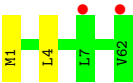


- Molecule 18: Photosystem II reaction center protein X

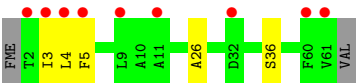
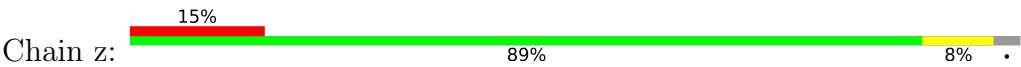


- Molecule 19: Photosystem II reaction center protein Z

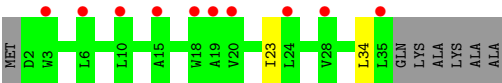
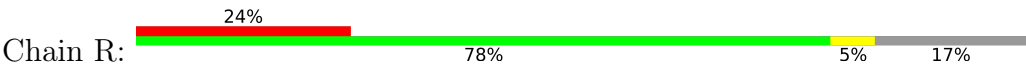




• Molecule 19: Photosystem II reaction center protein Z



• Molecule 20: Photosystem II protein Y



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	124.02Å 229.58Å 287.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.22 – 1.95 49.22 – 1.95	Depositor EDS
% Data completeness (in resolution range)	98.7 (49.22-1.95) 88.5 (49.22-1.95)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.94 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.8.0258, PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.153 , 0.181 0.157 , 0.184	Depositor DCC
R_{free} test set	29246 reflections (4.68%)	wwPDB-VP
Wilson B-factor (Å ²)	34.0	Xtriage
Anisotropy	0.640	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 66.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	55061	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.94% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HTG, DGD, CL, CLA, CA, SQD, HEM, BCR, LMG, HEC, MG, K3C, FME, FE2, LHG, PHO, BCT, LMT, DMS, RRX, OEX, UNL, PL9, GOL, HSK

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	0.35	0/2718	0.52	0/3707
1	a	0.34	0/2713	0.51	0/3700
2	B	0.33	1/4174 (0.0%)	0.48	0/5687
2	b	0.30	1/4158 (0.0%)	0.48	2/5667 (0.0%)
3	C	0.28	0/3613	0.44	0/4919
3	c	0.27	0/3636	0.43	0/4952
4	D	0.35	0/2809	0.50	0/3827
4	d	0.33	0/2819	0.47	0/3840
5	E	0.25	0/676	0.47	0/924
5	e	0.21	0/658	0.39	0/899
6	F	0.28	0/283	0.44	0/386
6	f	0.24	0/257	0.43	0/349
7	H	0.27	0/511	0.43	0/697
7	h	0.22	0/511	0.43	0/697
8	I	0.20	0/282	0.39	0/383
8	i	0.24	0/293	0.43	0/396
9	J	0.22	0/257	0.34	0/349
9	j	0.19	0/277	0.36	0/376
10	K	0.24	0/306	0.42	0/422
10	k	0.23	0/296	0.40	0/408
11	L	0.33	0/315	0.48	0/428
11	l	0.33	0/322	0.46	0/438
12	M	0.33	0/261	0.56	0/357
12	m	0.32	0/283	0.44	0/386
13	O	0.29	0/1933	0.49	0/2623
13	o	0.26	0/1917	0.49	0/2601
14	T	0.34	0/255	0.42	0/346
14	t	0.34	0/255	0.45	0/346
15	U	0.28	0/790	0.47	0/1071
15	u	0.30	0/794	0.48	0/1076
16	V	0.31	0/1090	0.45	0/1481

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.27	0/1084	0.43	0/1475
17	Y	0.20	0/199	0.42	0/266
17	y	0.18	0/197	0.41	0/264
18	X	0.19	0/282	0.31	0/381
18	x	0.16	0/279	0.30	0/377
19	Z	0.18	0/462	0.34	0/635
19	z	0.18	0/457	0.41	0/626
20	R	0.17	0/246	0.29	0/341
All	All	0.30	2/42668 (0.0%)	0.46	2/58103 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	221	PRO	CA-C	6.46	1.55	1.51
2	b	221	PRO	CA-C	-6.27	1.48	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	48	SER	CA-C-N	-6.24	115.26	122.00
2	b	48	SER	C-N-CA	-6.24	115.26	122.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2624	0	2525	16	0
1	a	2620	0	2527	15	0
2	B	4007	0	3875	23	0
2	b	3989	0	3850	24	0
3	C	3494	0	3418	19	0
3	c	3516	0	3430	21	0
4	D	2731	0	2631	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	d	2738	0	2643	12	0
5	E	657	0	637	8	0
5	e	639	0	617	5	0
6	F	274	0	279	5	0
6	f	250	0	261	4	0
7	H	498	0	518	2	0
7	h	498	0	518	4	0
8	I	285	0	291	2	0
8	i	296	0	311	1	0
9	J	251	0	257	1	0
9	j	271	0	270	3	0
10	K	293	0	303	2	0
10	k	286	0	285	3	0
11	L	305	0	323	1	0
11	l	309	0	332	1	0
12	M	265	0	286	1	0
12	m	281	0	310	3	0
13	O	1884	0	1856	11	0
13	o	1871	0	1841	6	0
14	T	256	0	256	1	0
14	t	256	0	256	0	0
15	U	776	0	777	2	0
15	u	780	0	781	0	0
16	V	1063	0	1069	2	0
16	v	1060	0	1053	5	0
17	Y	198	0	212	3	0
17	y	196	0	208	2	0
18	X	279	0	307	3	0
18	x	273	0	303	0	0
19	Z	461	0	483	0	0
19	z	446	0	457	2	0
20	R	240	0	218	1	0
21	A	10	0	0	0	0
21	a	10	0	0	0	0
22	A	1	0	0	0	0
22	a	1	0	0	0	0
23	A	2	0	0	0	0
23	a	2	0	0	0	0
24	A	260	0	288	8	0
24	B	1040	0	1152	24	0
24	C	845	0	936	24	0
24	D	130	0	144	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	a	260	0	288	4	0
24	b	1040	0	1152	31	0
24	c	845	0	936	22	0
24	d	130	0	144	3	0
25	A	64	0	74	0	0
25	D	64	0	74	2	0
25	a	64	0	74	0	0
25	d	64	0	74	2	0
26	A	40	0	56	3	0
26	B	160	0	224	10	0
26	C	80	0	112	3	0
26	D	40	0	56	3	0
26	K	40	0	56	2	0
26	T	40	0	56	3	0
26	Y	40	0	56	1	0
26	a	40	0	56	3	0
26	b	120	0	168	8	0
26	c	80	0	112	4	0
26	d	40	0	56	1	0
26	k	80	0	112	5	0
27	A	108	0	156	3	0
27	D	45	0	56	2	0
27	L	108	0	156	3	0
27	a	108	0	156	1	0
27	f	33	0	39	1	0
28	A	51	0	72	0	0
28	B	51	0	72	1	0
28	C	102	0	144	2	0
28	D	51	0	72	2	0
28	a	51	0	72	2	0
28	b	51	0	72	2	0
28	c	102	0	144	1	0
28	d	51	0	72	1	0
29	A	35	0	46	1	0
29	B	59	0	81	1	0
29	C	35	0	46	4	0
29	E	24	0	35	0	0
29	J	24	0	35	1	0
29	M	35	0	46	1	0
29	T	24	0	35	0	0
29	Z	35	0	46	0	0
29	a	35	0	46	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	b	25	0	35	1	0
29	c	35	0	46	2	0
29	f	35	0	46	1	0
29	m	105	0	138	1	0
29	z	32	0	33	2	0
30	A	12	0	16	0	0
30	B	36	0	48	0	0
30	C	30	0	40	2	0
30	E	6	0	8	0	0
30	L	6	0	8	0	0
30	M	6	0	8	0	0
30	O	6	0	8	0	0
30	T	12	0	16	1	0
30	V	24	0	30	0	0
30	a	24	0	32	3	0
30	b	24	0	32	0	0
30	c	24	0	32	1	0
30	d	12	0	16	2	0
30	h	6	0	8	0	0
30	k	6	0	8	0	0
30	o	12	0	16	1	0
30	u	6	0	8	0	0
30	v	36	0	46	1	0
31	A	74	0	0	0	0
31	B	99	0	0	0	0
31	C	73	0	0	0	0
31	D	68	0	0	0	0
31	E	30	0	0	0	0
31	H	8	0	0	0	0
31	I	47	0	0	0	0
31	J	31	0	0	0	0
31	T	9	0	0	0	0
31	X	16	0	0	0	0
31	Y	12	0	0	0	0
31	a	73	0	0	0	0
31	b	70	0	0	0	0
31	c	74	0	0	1	0
31	d	56	0	0	0	0
31	e	15	0	0	0	0
31	h	39	0	0	0	0
31	i	71	0	0	0	0
31	j	34	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	k	16	0	0	0	0
31	l	16	0	0	0	0
31	t	8	0	0	0	0
31	x	30	0	0	0	0
32	A	14	0	0	0	0
32	a	14	0	0	0	0
33	A	55	0	80	6	0
33	D	55	0	80	0	0
33	a	55	0	80	6	0
33	d	55	0	80	0	0
34	A	4	0	0	0	0
34	a	4	0	0	0	0
35	B	1	0	0	0	0
35	F	1	0	0	0	0
35	O	1	0	0	0	0
35	b	1	0	0	0	0
35	c	1	0	0	0	0
35	f	1	0	0	0	0
35	o	1	0	0	0	0
36	B	95	0	130	4	0
36	C	38	0	52	0	0
36	D	19	0	26	3	0
36	I	19	0	26	0	0
36	O	19	0	26	1	0
36	U	9	0	15	0	0
36	V	13	0	11	0	0
36	b	76	0	104	6	0
36	c	38	0	52	0	0
36	d	19	0	26	0	0
36	h	19	0	26	2	0
36	o	19	0	26	0	0
36	u	14	0	19	0	0
37	B	49	0	74	1	0
37	D	144	0	213	8	0
37	E	49	0	74	1	0
37	d	137	0	196	0	0
37	e	40	0	53	1	0
37	l	49	0	74	1	0
38	B	20	0	30	1	0
38	C	8	0	12	0	0
38	D	4	0	6	0	0
38	E	4	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	O	4	0	6	0	0
38	V	4	0	6	0	0
38	Y	4	0	6	0	0
38	a	4	0	6	0	0
38	b	12	0	18	3	0
38	c	20	0	30	2	0
38	d	8	0	12	0	0
38	i	4	0	6	0	0
38	o	20	0	30	1	0
38	v	4	0	6	0	0
38	z	4	0	6	0	0
39	C	186	0	246	4	0
39	D	53	0	71	6	0
39	H	62	0	82	1	0
39	c	186	0	246	5	0
39	h	62	0	82	1	0
40	F	43	0	30	1	0
40	f	43	0	30	3	0
41	H	41	0	56	3	0
41	h	41	0	56	5	0
42	J	1	0	0	0	0
42	j	1	0	0	0	0
43	V	43	0	30	0	0
43	v	43	0	30	0	0
44	A	176	0	0	0	0
44	B	364	0	0	2	0
44	C	284	0	0	1	0
44	D	166	0	0	2	0
44	E	47	0	0	0	0
44	F	18	0	0	0	0
44	H	62	0	0	1	0
44	I	18	0	0	0	0
44	J	15	0	0	0	0
44	K	11	0	0	0	0
44	L	31	0	0	1	0
44	M	17	0	0	0	0
44	O	196	0	0	2	0
44	R	2	0	0	0	0
44	T	20	0	0	0	0
44	U	102	0	0	2	0
44	V	159	0	0	1	0
44	X	16	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	Y	9	0	0	0	0
44	a	164	0	0	0	0
44	b	325	0	0	2	0
44	c	275	0	0	5	0
44	d	157	0	0	0	0
44	e	29	0	0	0	0
44	f	11	0	0	0	0
44	h	45	0	0	0	0
44	i	10	0	0	0	0
44	j	13	0	0	0	0
44	k	11	0	0	0	0
44	l	15	0	0	0	0
44	m	26	0	0	0	0
44	o	184	0	0	1	0
44	t	19	0	0	0	0
44	u	106	0	0	0	0
44	v	109	0	0	0	0
44	x	18	0	0	0	0
44	y	12	0	0	0	0
44	z	7	0	0	0	0
All	All	55061	0	52295	381	0

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

The worst 5 of 381 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)
39:D:407:DGD:HD62	5:E:45:ASP:HB3	1.59	0.85
4:d:192:THR:HG23	24:d:404:CLA:HBC2	1.71	0.72
39:c:519:DGD:HB62	28:c:521:LMG:H402	1.71	0.71
4:D:101:PHE:H	39:D:407:DGD:HB32	1.55	0.70
3:c:391[B]:ARG:NH2	44:c:601:HOH:O	2.24	0.69

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	335/344 (97%)	331 (99%)	3 (1%)	1 (0%)	36	28
1	a	335/344 (97%)	330 (98%)	4 (1%)	1 (0%)	36	28
2	B	512/505 (101%)	506 (99%)	6 (1%)	0	100	100
2	b	511/505 (101%)	505 (99%)	6 (1%)	0	100	100
3	C	451/455 (99%)	443 (98%)	7 (2%)	1 (0%)	43	36
3	c	455/455 (100%)	444 (98%)	10 (2%)	1 (0%)	43	36
4	D	340/342 (99%)	334 (98%)	6 (2%)	0	100	100
4	d	341/342 (100%)	334 (98%)	7 (2%)	0	100	100
5	E	79/83 (95%)	79 (100%)	0	0	100	100
5	e	77/83 (93%)	77 (100%)	0	0	100	100
6	F	32/44 (73%)	32 (100%)	0	0	100	100
6	f	29/44 (66%)	29 (100%)	0	0	100	100
7	H	61/63 (97%)	58 (95%)	3 (5%)	0	100	100
7	h	61/63 (97%)	58 (95%)	3 (5%)	0	100	100
8	I	34/38 (90%)	33 (97%)	1 (3%)	0	100	100
8	i	34/38 (90%)	33 (97%)	1 (3%)	0	100	100
9	J	34/40 (85%)	33 (97%)	1 (3%)	0	100	100
9	j	37/40 (92%)	37 (100%)	0	0	100	100
10	K	36/37 (97%)	36 (100%)	0	0	100	100
10	k	35/37 (95%)	35 (100%)	0	0	100	100
11	L	36/37 (97%)	36 (100%)	0	0	100	100
11	l	37/37 (100%)	37 (100%)	0	0	100	100
12	M	32/36 (89%)	32 (100%)	0	0	100	100
12	m	35/36 (97%)	35 (100%)	0	0	100	100
13	O	248/244 (102%)	244 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	o	246/244 (101%)	240 (98%)	6 (2%)	0	100	100
14	T	28/32 (88%)	28 (100%)	0	0	100	100
14	t	28/32 (88%)	28 (100%)	0	0	100	100
15	U	96/104 (92%)	93 (97%)	3 (3%)	0	100	100
15	u	96/104 (92%)	93 (97%)	3 (3%)	0	100	100
16	V	137/137 (100%)	135 (98%)	2 (2%)	0	100	100
16	v	136/137 (99%)	133 (98%)	3 (2%)	0	100	100
17	Y	26/30 (87%)	25 (96%)	1 (4%)	0	100	100
17	y	26/30 (87%)	26 (100%)	0	0	100	100
18	X	36/40 (90%)	35 (97%)	1 (3%)	0	100	100
18	x	36/40 (90%)	35 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
19	z	58/62 (94%)	56 (97%)	1 (2%)	1 (2%)	7	2
20	R	32/41 (78%)	32 (100%)	0	0	100	100
All	All	5258/5387 (98%)	5169 (98%)	84 (2%)	5 (0%)	48	41

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
19	z	3	ILE
3	C	416	SER
3	c	416	SER
1	a	259	ILE
1	A	259	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	270/279 (97%)	270 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	a	270/279 (97%)	270 (100%)	0	100	100
2	B	406/403 (101%)	404 (100%)	2 (0%)	81	82
2	b	405/403 (100%)	404 (100%)	1 (0%)	87	89
3	C	354/356 (99%)	352 (99%)	2 (1%)	78	79
3	c	353/356 (99%)	350 (99%)	3 (1%)	73	74
4	D	275/276 (100%)	274 (100%)	1 (0%)	84	85
4	d	277/276 (100%)	276 (100%)	1 (0%)	84	85
5	E	71/72 (99%)	69 (97%)	2 (3%)	38	30
5	e	68/72 (94%)	65 (96%)	3 (4%)	25	15
6	F	27/38 (71%)	27 (100%)	0	100	100
6	f	25/38 (66%)	25 (100%)	0	100	100
7	H	53/53 (100%)	53 (100%)	0	100	100
7	h	53/53 (100%)	53 (100%)	0	100	100
8	I	29/34 (85%)	29 (100%)	0	100	100
8	i	32/34 (94%)	30 (94%)	2 (6%)	16	6
9	J	23/28 (82%)	23 (100%)	0	100	100
9	j	25/28 (89%)	24 (96%)	1 (4%)	28	17
10	K	30/30 (100%)	29 (97%)	1 (3%)	33	24
10	k	28/30 (93%)	28 (100%)	0	100	100
11	L	35/35 (100%)	35 (100%)	0	100	100
11	l	36/35 (103%)	35 (97%)	1 (3%)	38	30
12	M	30/32 (94%)	30 (100%)	0	100	100
12	m	32/32 (100%)	30 (94%)	2 (6%)	16	6
13	O	209/207 (101%)	207 (99%)	2 (1%)	68	67
13	o	207/207 (100%)	206 (100%)	1 (0%)	81	82
14	T	25/28 (89%)	25 (100%)	0	100	100
14	t	25/28 (89%)	25 (100%)	0	100	100
15	U	84/89 (94%)	84 (100%)	0	100	100
15	u	85/89 (96%)	84 (99%)	1 (1%)	63	61
16	V	115/117 (98%)	115 (100%)	0	100	100
16	v	115/117 (98%)	115 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	Y	18/23 (78%)	17 (94%)	1 (6%)	19	8
17	y	18/23 (78%)	18 (100%)	0	100	100
18	X	30/33 (91%)	30 (100%)	0	100	100
18	x	29/33 (88%)	29 (100%)	0	100	100
19	Z	46/51 (90%)	45 (98%)	1 (2%)	45	40
19	z	44/51 (86%)	43 (98%)	1 (2%)	44	38
20	R	19/33 (58%)	18 (95%)	1 (5%)	20	9
All	All	4276/4401 (97%)	4246 (99%)	30 (1%)	76	76

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	c	289	PHE
15	u	9	LEU
5	e	8	ARG
20	R	34	LEU
12	m	16[A]	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
2	b	289	GLN
3	c	382	ASN
3	c	311	GLN
4	d	186	GLN
4	D	255	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

11 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
4	HSK	D	336[A]	-	9,10,12	20.10	1 (11%)	6,12,16	1.77	2 (33%)
14	FME	t	1	14	8,9,10	0.60	0	7,9,11	1.50	2 (28%)
4	HSK	D	336[B]	-	9,11,12	1.90	2 (22%)	6,14,16	3.74	4 (66%)
8	FME	I	1	8	8,9,10	0.63	0	7,9,11	1.86	4 (57%)
4	HSK	d	336[A]	-	9,10,12	3.65	1 (11%)	6,12,16	1.73	3 (50%)
8	FME	i	1	8	8,9,10	0.60	0	7,9,11	1.57	2 (28%)
12	FME	m	1	12	8,9,10	0.64	0	7,9,11	1.72	1 (14%)
4	HSK	d	336[B]	-	9,11,12	1.81	2 (22%)	6,14,16	3.80	4 (66%)
12	FME	M	1	12	8,9,10	0.60	0	7,9,11	1.50	1 (14%)
14	FME	T	1	14	8,9,10	0.56	0	7,9,11	1.84	3 (42%)
19	FME	Z	1	19	8,9,10	0.64	0	7,9,11	1.63	2 (28%)

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
4	HSK	D	336[A]	-	-	1/5/6/8	0/1/1/1
14	FME	t	1	14	-	1/7/9/11	-
4	HSK	D	336[B]	-	-	0/5/6/8	0/1/1/1
8	FME	I	1	8	-	2/7/9/11	-
4	HSK	d	336[A]	-	-	0/5/6/8	0/1/1/1
8	FME	i	1	8	-	0/7/9/11	-
12	FME	m	1	12	-	3/7/9/11	-
4	HSK	d	336[B]	-	-	0/5/6/8	0/1/1/1
12	FME	M	1	12	-	2/7/9/11	-
14	FME	T	1	14	-	2/7/9/11	-
19	FME	Z	1	19	-	3/7/9/11	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	336[A]	HSK	OM-ND1	-60.20	0.59	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	d	336[A]	HSK	OM-ND1	-10.34	1.25	1.38
4	D	336[B]	HSK	OM-ND1	4.29	1.44	1.38
4	d	336[B]	HSK	OM-ND1	3.98	1.43	1.38
4	d	336[B]	HSK	CE1-ND1	-2.41	1.33	1.37

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	336[B]	HSK	ND1-CE1-NE2	-5.83	104.46	111.75
4	d	336[B]	HSK	ND1-CE1-NE2	-5.82	104.47	111.75
4	d	336[B]	HSK	CE1-ND1-CG	5.54	114.46	107.37
4	D	336[B]	HSK	CE1-ND1-CG	5.50	114.41	107.37
12	m	1	FME	CE-SD-CG	3.48	112.35	100.40

There are no chirality outliers.

5 of 14 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
19	Z	1	FME	O1-CN-N-CA
14	t	1	FME	CB-CG-SD-CE
14	T	1	FME	CB-CG-SD-CE

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	m	1	FME	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 337 ligands modelled in this entry, 15 are monoatomic and 57 are unknown - leaving 265 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
34	BCT	a	407	22	2,3,3	0.64	0	2,3,3	0.68	0
30	GOL	v	1605	-	5,5,5	1.09	0	5,5,5	0.81	0
27	SQD	A	413	-	53,54,54	1.02	3 (5%)	62,65,65	1.30	10 (16%)
24	CLA	D	403	4	69,73,73	2.17	24 (34%)	83,113,113	2.72	32 (38%)
30	GOL	T	103	-	5,5,5	0.83	0	5,5,5	1.07	0
24	CLA	c	512	3	69,73,73	2.58	25 (36%)	83,113,113	2.45	26 (31%)
26	BCR	b	622	-	41,41,41	0.70	0	56,56,56	1.36	10 (17%)
36	HTG	B	623[B]	-	19,19,19	0.93	1 (5%)	23,24,24	1.47	2 (8%)
25	PHO	A	408	-	58,69,69	2.63	13 (22%)	56,99,99	2.86	15 (26%)
30	GOL	L	103	-	5,5,5	1.03	0	5,5,5	0.88	0
38	DMS	z	102	-	3,3,3	2.69	1 (33%)	3,3,3	0.58	0
30	GOL	B	630	-	5,5,5	0.59	0	5,5,5	1.04	0
27	SQD	A	411	-	53,54,54	0.96	3 (5%)	62,65,65	1.71	12 (19%)
26	BCR	k	302	-	41,41,41	0.76	1 (2%)	56,56,56	1.56	12 (21%)
24	CLA	B	610	2	69,73,73	2.54	23 (33%)	83,113,113	2.39	31 (37%)
24	CLA	d	404	4	69,73,73	2.29	22 (31%)	83,113,113	2.58	29 (34%)
30	GOL	B	633	-	5,5,5	0.87	0	5,5,5	0.98	0
30	GOL	h	1206	-	5,5,5	0.95	0	5,5,5	0.90	0
37	LHG	E	101	-	48,48,48	0.97	2 (4%)	51,54,54	1.13	3 (5%)
33	PL9	a	425[B]	-	55,55,55	0.60	2 (3%)	68,69,69	1.86	21 (30%)
32	K3C	A	421[A]	-	15,15,15	0.95	1 (6%)	19,20,20	0.88	1 (5%)
24	CLA	C	511	3	69,73,73	2.46	25 (36%)	83,113,113	2.48	28 (33%)
41	RRX	H	101	-	42,42,42	0.74	0	57,58,58	1.29	6 (10%)
27	SQD	D	408	-	44,45,54	1.10	3 (6%)	53,56,65	1.73	11 (20%)
26	BCR	K	101	-	41,41,41	0.75	0	56,56,56	1.51	11 (19%)
38	DMS	B	647	-	3,3,3	2.64	1 (33%)	3,3,3	0.41	0
36	HTG	U	201	-	8,8,19	0.37	0	7,7,24	1.01	1 (14%)
24	CLA	B	617	2	69,73,73	2.27	23 (33%)	83,113,113	2.54	27 (32%)
24	CLA	c	510	3	69,73,73	2.57	25 (36%)	83,113,113	2.53	28 (33%)
26	BCR	B	641	-	41,41,41	0.68	0	56,56,56	1.60	14 (25%)
30	GOL	A	416	-	5,5,5	1.00	0	5,5,5	0.90	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	LMT	z	101	-	32,32,36	0.55	1 (3%)	42,42,47	1.46	4 (9%)
36	HTG	D	413	-	19,19,19	1.11	2 (10%)	23,24,24	1.09	2 (8%)
24	CLA	C	509	3	69,73,73	2.53	24 (34%)	83,113,113	2.37	25 (30%)
26	BCR	B	620	-	41,41,41	0.71	0	56,56,56	1.24	4 (7%)
39	DGD	c	518	-	63,63,67	0.80	2 (3%)	77,77,81	1.11	7 (9%)
25	PHO	d	401	-	58,69,69	2.74	14 (24%)	56,99,99	2.87	17 (30%)
24	CLA	B	605	2	69,73,73	2.56	22 (31%)	83,113,113	2.53	28 (33%)
29	LMT	C	521	-	36,36,36	0.46	0	47,47,47	1.19	4 (8%)
39	DGD	C	518	-	63,63,67	0.85	2 (3%)	77,77,81	1.02	5 (6%)
30	GOL	V	204	-	5,5,5	1.12	0	5,5,5	0.90	0
30	GOL	C	530	-	5,5,5	1.20	0	5,5,5	1.14	1 (20%)
24	CLA	C	512	3	69,73,73	2.55	23 (33%)	83,113,113	2.42	27 (32%)
24	CLA	b	614	2	69,73,73	2.56	25 (36%)	83,113,113	2.39	28 (33%)
37	LHG	l	302	-	48,48,48	0.87	2 (4%)	51,54,54	0.85	1 (1%)
27	SQD	a	401	-	53,54,54	1.04	3 (5%)	62,65,65	1.26	7 (11%)
38	DMS	i	104	-	3,3,3	2.65	1 (33%)	3,3,3	0.60	0
36	HTG	c	524	-	19,19,19	0.99	2 (10%)	23,24,24	1.39	1 (4%)
28	LMG	A	412	-	51,51,55	0.93	2 (3%)	59,59,63	1.16	6 (10%)
39	DGD	h	1205	-	63,63,67	0.92	3 (4%)	77,77,81	0.99	4 (5%)
28	LMG	c	522	-	51,51,55	0.97	2 (3%)	59,59,63	1.24	5 (8%)
30	GOL	c	528	-	5,5,5	0.95	0	5,5,5	0.95	0
24	CLA	b	609	2	69,73,73	2.54	23 (33%)	83,113,113	2.38	27 (32%)
30	GOL	B	631	-	5,5,5	1.06	0	5,5,5	0.97	0
28	LMG	d	411	42	51,51,55	0.91	2 (3%)	59,59,63	0.92	2 (3%)
24	CLA	c	509	44	69,73,73	2.45	23 (33%)	83,113,113	2.59	30 (36%)
38	DMS	o	306	-	3,3,3	2.69	1 (33%)	3,3,3	0.50	0
38	DMS	o	308	-	3,3,3	2.69	1 (33%)	3,3,3	0.48	0
24	CLA	c	508	3	69,73,73	2.62	25 (36%)	83,113,113	2.41	32 (38%)
30	GOL	d	402	-	5,5,5	0.91	0	5,5,5	0.96	0
36	HTG	B	624	-	19,19,19	1.08	2 (10%)	23,24,24	1.75	2 (8%)
28	LMG	B	621	-	51,51,55	0.91	2 (3%)	59,59,63	1.05	3 (5%)
28	LMG	c	521	-	51,51,55	0.93	2 (3%)	59,59,63	0.99	4 (6%)
39	DGD	D	407	-	53,53,67	1.01	3 (5%)	60,61,81	1.41	6 (10%)
30	GOL	B	629	-	5,5,5	1.04	0	5,5,5	0.75	0
30	GOL	k	304	-	5,5,5	0.87	0	5,5,5	0.91	0
26	BCR	b	620	-	41,41,41	0.80	0	56,56,56	1.39	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	b	616	2	69,73,73	2.55	25 (36%)	83,113,113	2.56	27 (32%)
43	HEC	v	1603	16	50,50,50	1.88	8 (16%)	68,82,82	1.45	11 (16%)
36	HTG	b	602	-	19,19,19	1.09	2 (10%)	23,24,24	1.25	1 (4%)
24	CLA	c	511	3	69,73,73	2.55	23 (33%)	83,113,113	2.44	28 (33%)
37	LHG	D	409	-	48,48,48	0.86	3 (6%)	51,54,54	1.17	5 (9%)
38	DMS	c	536	-	3,3,3	2.65	1 (33%)	3,3,3	0.46	0
30	GOL	C	529	-	5,5,5	0.98	0	5,5,5	0.79	0
36	HTG	I	102	-	19,19,19	1.11	2 (10%)	23,24,24	1.89	4 (17%)
30	GOL	d	413	-	5,5,5	0.87	0	5,5,5	0.99	0
38	DMS	c	537	-	3,3,3	2.72	1 (33%)	3,3,3	0.56	0
24	CLA	b	619	2	69,73,73	2.42	23 (33%)	83,113,113	2.51	27 (32%)
25	PHO	D	401	-	58,69,69	2.72	13 (22%)	56,99,99	2.92	13 (23%)
38	DMS	d	416	-	3,3,3	2.72	1 (33%)	3,3,3	0.61	0
24	CLA	c	504	3	69,73,73	2.34	24 (34%)	83,113,113	2.52	25 (30%)
29	LMT	m	102	-	36,36,36	0.45	0	47,47,47	0.85	0
39	DGD	C	519	-	63,63,67	0.87	2 (3%)	77,77,81	1.08	4 (5%)
24	CLA	C	507	3	69,73,73	2.50	23 (33%)	83,113,113	2.53	31 (37%)
29	LMT	E	104	-	24,24,36	0.48	0	29,29,47	0.71	0
33	PL9	D	406	-	55,55,55	0.71	2 (3%)	68,69,69	1.54	14 (20%)
39	DGD	C	517	-	63,63,67	0.83	2 (3%)	77,77,81	1.05	8 (10%)
39	DGD	H	102	-	63,63,67	0.90	3 (4%)	77,77,81	0.92	5 (6%)
30	GOL	o	305	-	5,5,5	1.09	0	5,5,5	0.79	0
24	CLA	B	612	2	69,73,73	2.40	24 (34%)	83,113,113	2.55	30 (36%)
21	OEX	a	403	44,3,1	0,14,14	-	-	-	-	-
26	BCR	k	303	-	41,41,41	0.71	0	56,56,56	1.39	6 (10%)
29	LMT	m	103	-	36,36,36	0.46	0	47,47,47	0.85	0
38	DMS	b	636	-	3,3,3	2.68	1 (33%)	3,3,3	0.54	0
24	CLA	B	613	2	69,73,73	2.35	22 (31%)	83,113,113	2.61	26 (31%)
38	DMS	o	307	-	3,3,3	2.68	1 (33%)	3,3,3	0.53	0
24	CLA	c	506	44	69,73,73	2.27	25 (36%)	83,113,113	2.62	29 (34%)
36	HTG	C	523	-	19,19,19	0.98	2 (10%)	23,24,24	1.69	4 (17%)
29	LMT	B	642	-	24,24,36	0.56	1 (4%)	29,29,47	0.72	0
30	GOL	V	206	-	5,5,5	0.98	0	5,5,5	0.96	0
32	K3C	a	424[A]	-	15,15,15	0.94	1 (6%)	19,20,20	0.88	1 (5%)
28	LMG	C	520	-	51,51,55	0.95	2 (3%)	59,59,63	1.10	4 (6%)
24	CLA	c	507	3	69,73,73	2.60	24 (34%)	83,113,113	2.42	26 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	C	503	3	69,73,73	2.57	25 (36%)	83,113,113	2.42	25 (30%)
27	SQD	L	101	-	53,54,54	1.03	3 (5%)	62,65,65	1.37	9 (14%)
24	CLA	B	604	2	69,73,73	2.40	23 (33%)	83,113,113	2.67	26 (31%)
30	GOL	v	1606	-	5,5,5	0.76	0	5,5,5	1.08	0
37	LHG	e	101	-	39,39,48	1.03	2 (5%)	42,45,54	1.06	3 (7%)
24	CLA	b	606	2	69,73,73	2.46	25 (36%)	83,113,113	2.50	26 (31%)
30	GOL	C	528	-	5,5,5	0.74	0	5,5,5	1.12	1 (20%)
24	CLA	C	514	3	69,73,73	2.50	24 (34%)	83,113,113	2.48	24 (28%)
33	PL9	d	407	-	55,55,55	0.68	1 (1%)	68,69,69	1.50	13 (19%)
37	LHG	D	411	-	45,45,48	0.91	2 (4%)	48,51,54	0.99	3 (6%)
24	CLA	a	408	1	69,73,73	2.39	24 (34%)	83,113,113	2.53	27 (32%)
24	CLA	B	615	2	69,73,73	2.30	20 (28%)	83,113,113	2.67	29 (34%)
29	LMT	b	624	-	25,25,36	0.45	0	30,30,47	0.77	0
29	LMT	f	104	-	36,36,36	0.43	0	47,47,47	0.77	0
30	GOL	V	201	35	5,5,5	0.78	0	5,5,5	1.02	0
24	CLA	A	409	1	69,73,73	2.27	23 (33%)	83,113,113	2.63	29 (34%)
38	DMS	b	638	-	3,3,3	2.70	1 (33%)	3,3,3	0.55	0
30	GOL	v	1604	-	5,5,5	0.93	0	5,5,5	0.97	0
26	BCR	B	618	-	41,41,41	0.76	0	56,56,56	1.31	6 (10%)
30	GOL	T	101	-	5,5,5	0.96	0	5,5,5	0.81	0
30	GOL	A	415	-	5,5,5	0.82	0	5,5,5	1.06	1 (20%)
24	CLA	b	618	2	69,73,73	2.37	24 (34%)	83,113,113	2.37	28 (33%)
26	BCR	c	517	-	41,41,41	0.76	0	56,56,56	1.40	7 (12%)
30	GOL	b	627	-	5,5,5	0.96	0	5,5,5	0.84	0
30	GOL	o	302	-	5,5,5	1.06	0	5,5,5	0.79	0
24	CLA	a	412	1	69,73,73	2.23	21 (30%)	83,113,113	2.57	31 (37%)
38	DMS	D	416	-	3,3,3	2.70	1 (33%)	3,3,3	0.64	0
30	GOL	C	524	-	5,5,5	0.86	0	5,5,5	1.14	1 (20%)
38	DMS	c	533	-	3,3,3	2.70	1 (33%)	3,3,3	0.61	0
30	GOL	b	630	-	5,5,5	1.21	0	5,5,5	0.97	0
36	HTG	O	302	-	19,19,19	1.09	1 (5%)	23,24,24	0.98	1 (4%)
38	DMS	c	535	-	3,3,3	2.71	1 (33%)	3,3,3	0.64	0
21	OEX	A	401	44,3,1	0,14,14	-	-	-	-	-
24	CLA	a	410	44	69,73,73	2.40	24 (34%)	83,113,113	2.54	28 (33%)
30	GOL	M	102	-	5,5,5	0.59	0	5,5,5	1.17	1 (20%)
26	BCR	C	515	-	41,41,41	0.69	0	56,56,56	1.47	7 (12%)
24	CLA	b	604	44	69,73,73	2.48	24 (34%)	83,113,113	2.34	26 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	LMT	m	101	-	36,36,36	0.52	1 (2%)	47,47,47	0.85	0
24	CLA	B	606	2	69,73,73	2.36	24 (34%)	83,113,113	2.39	23 (27%)
28	LMG	a	415	-	51,51,55	0.94	2 (3%)	59,59,63	1.27	7 (11%)
38	DMS	o	309	-	3,3,3	2.68	1 (33%)	3,3,3	0.55	0
36	HTG	o	301	-	19,19,19	1.15	1 (5%)	23,24,24	1.19	1 (4%)
29	LMT	T	104	-	24,24,36	0.46	0	29,29,47	1.05	3 (10%)
38	DMS	O	304	-	3,3,3	2.73	1 (33%)	3,3,3	0.56	0
24	CLA	c	515	3	69,73,73	2.38	24 (34%)	83,113,113	2.39	25 (30%)
24	CLA	A	406	44	69,73,73	2.26	24 (34%)	83,113,113	2.67	29 (34%)
24	CLA	A	407	44	69,73,73	2.32	22 (31%)	83,113,113	2.58	28 (33%)
36	HTG	b	601	-	19,19,19	1.10	2 (10%)	23,24,24	1.52	2 (8%)
36	HTG	V	203	-	12,13,19	0.48	0	16,18,24	2.08	4 (25%)
24	CLA	C	513	3	69,73,73	2.64	23 (33%)	83,113,113	2.54	26 (31%)
38	DMS	Y	303	-	3,3,3	2.72	1 (33%)	3,3,3	0.64	0
37	LHG	d	408	-	48,48,48	0.84	2 (4%)	51,54,54	1.07	4 (7%)
38	DMS	B	644	-	3,3,3	2.68	1 (33%)	3,3,3	0.53	0
30	GOL	v	1607	-	5,5,5	0.83	0	5,5,5	0.95	0
34	BCT	A	423	22	2,3,3	0.61	0	2,3,3	0.79	0
38	DMS	E	106	-	3,3,3	2.67	1 (33%)	3,3,3	0.55	0
24	CLA	B	608	44	69,73,73	2.26	23 (33%)	83,113,113	2.53	25 (30%)
36	HTG	b	625	-	19,19,19	0.80	1 (5%)	23,24,24	1.15	2 (8%)
27	SQD	L	102	-	53,54,54	1.04	3 (5%)	62,65,65	1.63	11 (17%)
30	GOL	a	416	-	5,5,5	1.00	0	5,5,5	1.12	1 (20%)
24	CLA	B	611	44	69,73,73	2.54	25 (36%)	83,113,113	2.39	25 (30%)
30	GOL	a	418	-	5,5,5	0.91	0	5,5,5	0.94	0
24	CLA	B	607	2	69,73,73	2.39	23 (33%)	83,113,113	2.56	28 (33%)
24	CLA	B	614	2	69,73,73	2.42	23 (33%)	83,113,113	2.49	31 (37%)
36	HTG	d	414	-	19,19,19	1.03	2 (10%)	23,24,24	1.80	4 (17%)
29	LMT	M	101	-	36,36,36	0.40	0	47,47,47	0.90	0
37	LHG	D	410	-	48,48,48	0.86	2 (4%)	51,54,54	0.90	3 (5%)
38	DMS	C	525	-	3,3,3	2.67	1 (33%)	3,3,3	0.54	0
37	LHG	d	409	-	48,48,48	0.86	2 (4%)	51,54,54	0.97	3 (5%)
43	HEC	V	202	16	50,50,50	1.96	11 (22%)	68,82,82	1.56	10 (14%)
24	CLA	C	506	3	69,73,73	2.52	24 (34%)	83,113,113	2.34	23 (27%)
24	CLA	B	609	2	69,73,73	2.55	22 (31%)	83,113,113	2.44	29 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	PHO	a	411	-	58,69,69	2.64	13 (22%)	56,99,99	2.81	13 (23%)
36	HTG	b	626	-	19,19,19	1.06	1 (5%)	23,24,24	1.66	1 (4%)
38	DMS	a	426	-	3,3,3	2.69	1 (33%)	3,3,3	0.58	0
36	HTG	c	525	-	19,19,19	1.03	2 (10%)	23,24,24	1.48	3 (13%)
29	LMT	Z	101	-	36,36,36	0.44	0	47,47,47	0.83	1 (2%)
24	CLA	b	612	2	69,73,73	2.48	23 (33%)	83,113,113	2.39	26 (31%)
24	CLA	B	602	44	69,73,73	2.52	27 (39%)	83,113,113	2.41	24 (28%)
36	HTG	B	623[A]	-	19,19,19	1.02	1 (5%)	23,24,24	1.33	2 (8%)
24	CLA	b	607	2	69,73,73	2.59	24 (34%)	83,113,113	2.50	30 (36%)
24	CLA	b	615	2	69,73,73	2.34	23 (33%)	83,113,113	2.56	26 (31%)
26	BCR	D	405	-	41,41,41	0.83	1 (2%)	56,56,56	1.75	10 (17%)
24	CLA	C	510	3	69,73,73	2.41	24 (34%)	83,113,113	2.44	27 (32%)
38	DMS	B	646	-	3,3,3	2.70	1 (33%)	3,3,3	0.59	0
24	CLA	C	508	44	69,73,73	2.68	24 (34%)	83,113,113	2.46	29 (34%)
28	LMG	b	623	-	51,51,55	0.89	2 (3%)	59,59,63	1.06	3 (5%)
30	GOL	O	303	-	5,5,5	0.83	0	5,5,5	1.05	0
24	CLA	b	608	2	69,73,73	2.25	23 (33%)	83,113,113	2.60	29 (34%)
24	CLA	b	611	2	69,73,73	2.58	25 (36%)	83,113,113	2.36	25 (30%)
24	CLA	c	503	3	69,73,73	2.49	24 (34%)	83,113,113	2.66	27 (32%)
38	DMS	C	533	-	3,3,3	2.69	1 (33%)	3,3,3	0.51	0
30	GOL	v	1601	-	5,5,5	0.94	0	5,5,5	0.92	0
39	DGD	c	519	-	63,63,67	0.86	2 (3%)	77,77,81	0.97	4 (5%)
26	BCR	Y	302	-	41,41,41	0.78	0	56,56,56	1.61	10 (17%)
30	GOL	c	526	-	5,5,5	1.06	0	5,5,5	0.83	0
27	SQD	f	102	-	31,32,54	1.97	4 (12%)	34,36,65	1.44	3 (8%)
27	SQD	a	414	-	53,54,54	0.94	3 (5%)	62,65,65	1.69	10 (16%)
30	GOL	a	421	-	5,5,5	0.99	0	5,5,5	0.94	0
36	HTG	u	201	-	10,13,19	1.13	1 (10%)	13,14,24	1.72	1 (7%)
30	GOL	u	202	-	5,5,5	0.97	0	5,5,5	0.94	0
38	DMS	c	534	-	3,3,3	2.67	1 (33%)	3,3,3	0.44	0
40	HEM	f	101	5,6	50,50,50	1.88	8 (16%)	66,82,82	1.50	7 (10%)
30	GOL	b	628	-	5,5,5	0.85	0	5,5,5	0.94	0
38	DMS	V	207	-	3,3,3	2.66	1 (33%)	3,3,3	0.52	0
30	GOL	c	532	-	5,5,5	0.82	0	5,5,5	1.04	0
24	CLA	D	404	4	69,73,73	2.49	23 (33%)	83,113,113	2.45	27 (32%)
36	HTG	C	522	-	19,19,19	0.96	2 (10%)	23,24,24	1.16	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	BCR	b	621	-	41,41,41	0.77	0	56,56,56	1.17	6 (10%)
38	DMS	d	415	-	3,3,3	2.68	1 (33%)	3,3,3	0.53	0
24	CLA	C	504	3	69,73,73	2.45	23 (33%)	83,113,113	2.38	24 (28%)
29	LMT	c	523	-	36,36,36	0.49	1 (2%)	47,47,47	1.06	4 (8%)
36	HTG	B	625	-	19,19,19	1.03	2 (10%)	23,24,24	1.36	1 (4%)
38	DMS	B	645	-	3,3,3	2.68	1 (33%)	3,3,3	0.53	0
24	CLA	c	505	3	69,73,73	2.62	23 (33%)	83,113,113	2.30	26 (31%)
39	DGD	c	520	-	63,63,67	0.85	3 (4%)	77,77,81	0.96	5 (6%)
24	CLA	B	616	2	69,73,73	2.43	24 (34%)	83,113,113	2.60	31 (37%)
40	HEM	F	101	5,6	50,50,50	1.90	8 (16%)	66,82,82	1.59	11 (16%)
24	CLA	b	617	2	69,73,73	2.34	24 (34%)	83,113,113	2.62	28 (33%)
29	LMT	J	102	-	24,24,36	0.50	0	29,29,47	1.19	3 (10%)
30	GOL	v	1602	35	5,5,5	0.88	0	5,5,5	0.93	0
33	PL9	A	422[B]	-	55,55,55	0.66	2 (3%)	68,69,69	1.72	16 (23%)
30	GOL	V	205	-	5,5,5	0.86	0	5,5,5	0.99	0
41	RRX	h	1204	-	42,42,42	0.73	0	57,58,58	1.33	7 (12%)
36	HTG	h	1202	-	19,19,19	1.07	2 (10%)	23,24,24	1.81	1 (4%)
24	CLA	c	514	3	69,73,73	2.57	24 (34%)	83,113,113	2.63	30 (36%)
24	CLA	b	610	44	69,73,73	2.44	24 (34%)	83,113,113	2.38	29 (34%)
38	DMS	o	304	-	3,3,3	2.70	1 (33%)	3,3,3	0.57	0
26	BCR	B	619	-	41,41,41	0.83	0	56,56,56	1.20	4 (7%)
26	BCR	a	413	-	41,41,41	0.77	0	56,56,56	1.22	4 (7%)
24	CLA	d	405	4	69,73,73	2.43	25 (36%)	83,113,113	2.48	31 (37%)
24	CLA	B	603	2	69,73,73	2.53	24 (34%)	83,113,113	2.49	30 (36%)
24	CLA	b	605	2	69,73,73	2.45	24 (34%)	83,113,113	2.41	26 (31%)
26	BCR	A	410	-	41,41,41	0.77	0	56,56,56	1.30	6 (10%)
26	BCR	C	516	-	41,41,41	0.76	0	56,56,56	1.34	7 (12%)
26	BCR	T	102	-	41,41,41	0.72	0	56,56,56	1.55	15 (26%)
26	BCR	c	516	-	41,41,41	0.78	0	56,56,56	1.42	5 (8%)
30	GOL	B	628	-	5,5,5	1.01	0	5,5,5	0.89	0
30	GOL	c	527	-	5,5,5	1.03	0	5,5,5	0.88	0
38	DMS	B	643	-	3,3,3	2.67	1 (33%)	3,3,3	0.47	0
38	DMS	b	637	-	3,3,3	2.69	1 (33%)	3,3,3	0.65	0
37	LHG	B	640	-	48,48,48	0.93	3 (6%)	51,54,54	1.00	3 (5%)
30	GOL	E	105	-	5,5,5	0.89	0	5,5,5	1.01	0
29	LMT	a	402	-	36,36,36	0.43	0	47,47,47	0.88	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	LMT	B	622	-	36,36,36	0.40	0	47,47,47	1.17	4 (8%)
30	GOL	B	627	-	5,5,5	1.00	0	5,5,5	0.87	0
36	HTG	B	626	-	19,19,19	1.02	2 (10%)	23,24,24	1.83	5 (21%)
28	LMG	C	532	-	51,51,55	0.98	2 (3%)	59,59,63	1.30	4 (6%)
28	LMG	D	412	42	51,51,55	0.84	2 (3%)	59,59,63	0.89	3 (5%)
29	LMT	A	414	-	36,36,36	0.40	0	47,47,47	0.96	2 (4%)
30	GOL	C	527	-	5,5,5	0.83	0	5,5,5	1.06	0
30	GOL	a	417	-	5,5,5	1.05	0	5,5,5	0.92	0
37	LHG	d	410	-	38,38,48	1.07	2 (5%)	41,44,54	1.08	3 (7%)
24	CLA	C	502	3	69,73,73	2.34	25 (36%)	83,113,113	2.40	23 (27%)
24	CLA	b	613	44	69,73,73	2.51	25 (36%)	83,113,113	2.38	26 (31%)
24	CLA	C	505	44	69,73,73	2.34	23 (33%)	83,113,113	2.47	26 (31%)
26	BCR	d	406	-	41,41,41	0.80	0	56,56,56	1.82	13 (23%)
38	DMS	v	1608	-	3,3,3	2.69	1 (33%)	3,3,3	0.56	0
24	CLA	A	405	1	69,73,73	2.44	23 (33%)	83,113,113	2.31	27 (32%)
24	CLA	c	513	3	69,73,73	2.50	20 (28%)	83,113,113	2.47	32 (38%)
24	CLA	a	409	44	69,73,73	2.43	23 (33%)	83,113,113	2.72	30 (36%)
30	GOL	b	629	-	5,5,5	0.97	0	5,5,5	0.98	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	GOL	v	1605	-	-	2/4/4/4	-
27	SQD	A	413	-	-	11/49/69/69	0/1/1/1
24	CLA	D	403	4	-	3/39/115/115	-
30	GOL	T	103	-	-	0/4/4/4	-
24	CLA	c	512	3	-	5/39/115/115	-
26	BCR	b	622	-	-	1/29/63/63	0/2/2/2
36	HTG	B	623[B]	-	-	1/10/30/30	0/1/1/1
25	PHO	A	408	-	-	4/37/103/103	0/5/6/6
30	GOL	L	103	-	-	0/4/4/4	-
30	GOL	B	630	-	-	0/4/4/4	-
27	SQD	A	411	-	-	9/49/69/69	0/1/1/1
26	BCR	k	302	-	-	6/29/63/63	0/2/2/2
24	CLA	B	610	2	-	3/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	d	404	4	-	3/39/115/115	-
30	GOL	B	633	-	-	0/4/4/4	-
30	GOL	h	1206	-	-	0/4/4/4	-
37	LHG	E	101	-	-	26/53/53/53	-
33	PL9	a	425[B]	-	-	10/53/73/73	0/1/1/1
32	K3C	A	421[A]	-	-	4/4/17/17	0/2/2/2
24	CLA	C	511	3	-	4/39/115/115	-
41	RRX	H	101	-	-	3/29/65/65	0/2/2/2
27	SQD	D	408	-	-	15/40/60/69	0/1/1/1
26	BCR	K	101	-	-	1/29/63/63	0/2/2/2
36	HTG	U	201	-	-	3/6/6/30	-
24	CLA	B	617	2	-	11/39/115/115	-
24	CLA	c	510	3	-	3/39/115/115	-
26	BCR	B	641	-	-	1/29/63/63	0/2/2/2
30	GOL	A	416	-	-	1/4/4/4	-
29	LMT	z	101	-	-	5/15/55/61	0/2/2/2
36	HTG	D	413	-	-	1/10/30/30	0/1/1/1
24	CLA	C	509	3	-	5/39/115/115	-
26	BCR	B	620	-	-	0/29/63/63	0/2/2/2
39	DGD	c	518	-	-	15/51/91/95	0/2/2/2
25	PHO	d	401	-	-	1/37/103/103	0/5/6/6
24	CLA	B	605	2	-	5/39/115/115	-
29	LMT	C	521	-	-	12/21/61/61	0/2/2/2
39	DGD	C	518	-	-	19/51/91/95	0/2/2/2
30	GOL	V	204	-	-	2/4/4/4	-
30	GOL	C	530	-	-	0/4/4/4	-
24	CLA	C	512	3	-	3/39/115/115	-
24	CLA	b	614	2	-	5/39/115/115	-
37	LHG	l	302	-	-	13/53/53/53	-
27	SQD	a	401	-	-	12/49/69/69	0/1/1/1
36	HTG	c	524	-	-	1/10/30/30	0/1/1/1
28	LMG	A	412	-	-	21/46/66/70	0/1/1/1
39	DGD	h	1205	-	-	8/51/91/95	0/2/2/2
28	LMG	c	522	-	-	6/46/66/70	0/1/1/1
30	GOL	c	528	-	-	0/4/4/4	-
24	CLA	b	609	2	-	10/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	GOL	B	631	-	-	0/4/4/4	-
28	LMG	d	411	42	-	11/46/66/70	0/1/1/1
24	CLA	c	509	44	-	6/39/115/115	-
24	CLA	c	508	3	-	7/39/115/115	-
30	GOL	d	402	-	-	1/4/4/4	-
36	HTG	B	624	-	-	3/10/30/30	0/1/1/1
28	LMG	B	621	-	-	9/46/66/70	0/1/1/1
28	LMG	c	521	-	-	16/46/66/70	0/1/1/1
39	DGD	D	407	-	-	17/47/68/95	0/1/1/2
30	GOL	B	629	-	-	2/4/4/4	-
30	GOL	k	304	-	-	4/4/4/4	-
26	BCR	b	620	-	-	2/29/63/63	0/2/2/2
24	CLA	b	616	2	-	2/39/115/115	-
43	HEC	v	1603	16	1/1/3/7	6/14/54/54	-
36	HTG	b	602	-	-	1/10/30/30	0/1/1/1
24	CLA	c	511	3	-	11/39/115/115	-
37	LHG	D	409	-	-	10/53/53/53	-
30	GOL	C	529	-	-	0/4/4/4	-
36	HTG	I	102	-	-	5/10/30/30	0/1/1/1
30	GOL	d	413	-	-	2/4/4/4	-
24	CLA	b	619	2	-	9/39/115/115	-
25	PHO	D	401	-	-	1/37/103/103	0/5/6/6
24	CLA	c	504	3	-	9/39/115/115	-
29	LMT	m	102	-	-	1/21/61/61	0/2/2/2
39	DGD	C	519	-	-	11/51/91/95	0/2/2/2
24	CLA	C	507	3	-	14/39/115/115	-
29	LMT	E	104	-	-	6/15/35/61	0/1/1/2
33	PL9	D	406	-	-	5/53/73/73	0/1/1/1
39	DGD	C	517	-	-	13/51/91/95	0/2/2/2
39	DGD	H	102	-	-	9/51/91/95	0/2/2/2
30	GOL	o	305	-	-	2/4/4/4	-
24	CLA	B	612	2	-	2/39/115/115	-
26	BCR	k	303	-	-	1/29/63/63	0/2/2/2
29	LMT	m	103	-	-	2/21/61/61	0/2/2/2
24	CLA	B	613	2	-	3/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	c	506	44	-	5/39/115/115	-
36	HTG	C	523	-	-	4/10/30/30	0/1/1/1
29	LMT	B	642	-	-	7/15/35/61	0/1/1/2
30	GOL	V	206	-	-	0/4/4/4	-
32	K3C	a	424[A]	-	-	4/4/17/17	0/2/2/2
28	LMG	C	520	-	-	18/46/66/70	0/1/1/1
24	CLA	c	507	3	-	8/39/115/115	-
24	CLA	C	503	3	-	7/39/115/115	-
27	SQD	L	101	-	-	24/49/69/69	0/1/1/1
24	CLA	B	604	2	-	2/39/115/115	-
30	GOL	v	1606	-	-	2/4/4/4	-
37	LHG	e	101	-	-	23/44/44/53	-
24	CLA	b	606	2	-	5/39/115/115	-
30	GOL	C	528	-	-	0/4/4/4	-
24	CLA	C	514	3	-	4/39/115/115	-
33	PL9	d	407	-	-	6/53/73/73	0/1/1/1
37	LHG	D	411	-	-	11/50/50/53	-
24	CLA	a	408	1	-	4/39/115/115	-
24	CLA	B	615	2	-	10/39/115/115	-
29	LMT	b	624	-	-	4/17/37/61	0/1/1/2
29	LMT	f	104	-	-	7/21/61/61	0/2/2/2
30	GOL	V	201	35	-	0/4/4/4	-
24	CLA	A	409	1	-	7/39/115/115	-
30	GOL	v	1604	-	-	0/4/4/4	-
26	BCR	B	618	-	-	2/29/63/63	0/2/2/2
30	GOL	T	101	-	-	4/4/4/4	-
30	GOL	A	415	-	-	0/4/4/4	-
24	CLA	b	618	2	-	11/39/115/115	-
26	BCR	c	517	-	-	2/29/63/63	0/2/2/2
30	GOL	b	627	-	-	0/4/4/4	-
30	GOL	o	302	-	-	4/4/4/4	-
24	CLA	a	412	1	-	10/39/115/115	-
30	GOL	C	524	-	-	0/4/4/4	-
30	GOL	b	630	-	-	2/4/4/4	-
36	HTG	O	302	-	-	2/10/30/30	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	a	410	44	-	7/39/115/115	-
30	GOL	M	102	-	-	0/4/4/4	-
26	BCR	C	515	-	-	4/29/63/63	0/2/2/2
24	CLA	b	604	44	-	16/39/115/115	-
29	LMT	m	101	-	-	4/21/61/61	0/2/2/2
24	CLA	B	606	2	-	6/39/115/115	-
28	LMG	a	415	-	-	14/46/66/70	0/1/1/1
36	HTG	o	301	-	-	0/10/30/30	0/1/1/1
29	LMT	T	104	-	-	8/15/35/61	0/1/1/2
24	CLA	c	515	3	-	12/39/115/115	-
24	CLA	A	406	44	-	3/39/115/115	-
24	CLA	A	407	44	-	4/39/115/115	-
36	HTG	b	601	-	-	1/10/30/30	0/1/1/1
36	HTG	V	203	-	-	1/4/24/30	0/1/1/1
24	CLA	C	513	3	-	6/39/115/115	-
37	LHG	d	408	-	-	6/53/53/53	-
30	GOL	v	1607	-	-	4/4/4/4	-
24	CLA	B	608	44	-	4/39/115/115	-
36	HTG	b	625	-	-	5/10/30/30	0/1/1/1
27	SQD	L	102	-	-	25/49/69/69	0/1/1/1
30	GOL	a	416	-	-	2/4/4/4	-
24	CLA	B	611	44	-	8/39/115/115	-
30	GOL	a	418	-	-	2/4/4/4	-
24	CLA	B	607	2	-	5/39/115/115	-
24	CLA	B	614	2	-	3/39/115/115	-
36	HTG	d	414	-	-	1/10/30/30	0/1/1/1
29	LMT	M	101	-	-	1/21/61/61	0/2/2/2
37	LHG	D	410	-	-	8/53/53/53	-
43	HEC	V	202	16	1/1/3/7	6/14/54/54	-
37	LHG	d	409	-	-	12/53/53/53	-
24	CLA	C	506	3	-	2/39/115/115	-
24	CLA	B	609	2	-	2/39/115/115	-
25	PHO	a	411	-	-	5/37/103/103	0/5/6/6
36	HTG	b	626	-	-	3/10/30/30	0/1/1/1
36	HTG	c	525	-	-	0/10/30/30	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	LMT	Z	101	-	-	12/21/61/61	0/2/2/2
24	CLA	b	612	2	-	3/39/115/115	-
24	CLA	B	602	44	-	15/39/115/115	-
36	HTG	B	623[A]	-	-	1/10/30/30	0/1/1/1
24	CLA	b	607	2	-	4/39/115/115	-
24	CLA	b	615	2	-	0/39/115/115	-
26	BCR	D	405	-	-	8/29/63/63	0/2/2/2
24	CLA	C	510	3	-	4/39/115/115	-
24	CLA	C	508	44	-	11/39/115/115	-
28	LMG	b	623	-	-	19/46/66/70	0/1/1/1
30	GOL	O	303	-	-	0/4/4/4	-
24	CLA	b	608	2	-	3/39/115/115	-
24	CLA	b	611	2	-	3/39/115/115	-
24	CLA	c	503	3	-	4/39/115/115	-
30	GOL	v	1601	-	-	0/4/4/4	-
39	DGD	c	519	-	-	16/51/91/95	0/2/2/2
26	BCR	Y	302	-	-	6/29/63/63	0/2/2/2
30	GOL	c	526	-	-	4/4/4/4	-
27	SQD	f	102	-	-	10/33/33/69	-
27	SQD	a	414	-	-	12/49/69/69	0/1/1/1
30	GOL	a	421	-	-	4/4/4/4	-
36	HTG	u	201	-	-	2/12/14/30	-
30	GOL	u	202	-	-	2/4/4/4	-
40	HEM	f	101	5,6	-	3/14/54/54	-
30	GOL	b	628	-	-	0/4/4/4	-
30	GOL	c	532	-	-	0/4/4/4	-
24	CLA	D	404	4	-	5/39/115/115	-
36	HTG	C	522	-	-	1/10/30/30	0/1/1/1
26	BCR	b	621	-	-	0/29/63/63	0/2/2/2
24	CLA	C	504	3	-	6/39/115/115	-
29	LMT	c	523	-	-	6/21/61/61	0/2/2/2
36	HTG	B	625	-	-	3/10/30/30	0/1/1/1
24	CLA	c	505	3	-	4/39/115/115	-
39	DGD	c	520	-	-	14/51/91/95	0/2/2/2
24	CLA	B	616	2	-	6/39/115/115	-
40	HEM	F	101	5,6	-	2/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	b	617	2	-	9/39/115/115	-
29	LMT	J	102	-	-	2/15/35/61	0/1/1/2
30	GOL	v	1602	35	-	2/4/4/4	-
33	PL9	A	422[B]	-	-	13/53/73/73	0/1/1/1
30	GOL	V	205	-	-	0/4/4/4	-
41	RRX	h	1204	-	-	2/29/65/65	0/2/2/2
36	HTG	h	1202	-	-	4/10/30/30	0/1/1/1
24	CLA	c	514	3	-	8/39/115/115	-
24	CLA	b	610	44	-	3/39/115/115	-
26	BCR	B	619	-	-	0/29/63/63	0/2/2/2
26	BCR	a	413	-	-	0/29/63/63	0/2/2/2
24	CLA	d	405	4	-	5/39/115/115	-
24	CLA	B	603	2	-	4/39/115/115	-
24	CLA	b	605	2	-	2/39/115/115	-
26	BCR	A	410	-	-	1/29/63/63	0/2/2/2
26	BCR	C	516	-	-	1/29/63/63	0/2/2/2
26	BCR	T	102	-	-	1/29/63/63	0/2/2/2
26	BCR	c	516	-	-	0/29/63/63	0/2/2/2
30	GOL	B	628	-	-	0/4/4/4	-
30	GOL	c	527	-	-	0/4/4/4	-
37	LHG	B	640	-	-	12/53/53/53	-
30	GOL	E	105	-	-	0/4/4/4	-
29	LMT	a	402	-	-	8/21/61/61	0/2/2/2
29	LMT	B	622	-	-	8/21/61/61	0/2/2/2
30	GOL	B	627	-	-	2/4/4/4	-
36	HTG	B	626	-	-	3/10/30/30	0/1/1/1
28	LMG	C	532	-	-	10/46/66/70	0/1/1/1
28	LMG	D	412	42	-	10/46/66/70	0/1/1/1
29	LMT	A	414	-	-	5/21/61/61	0/2/2/2
30	GOL	C	527	-	-	1/4/4/4	-
30	GOL	a	417	-	-	3/4/4/4	-
37	LHG	d	410	-	-	8/43/43/53	-
24	CLA	C	502	3	-	4/39/115/115	-
24	CLA	b	613	44	-	7/39/115/115	-
24	CLA	C	505	44	-	7/39/115/115	-
26	BCR	d	406	-	-	8/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	A	405	1	-	2/39/115/115	-
24	CLA	c	513	3	-	0/39/115/115	-
24	CLA	a	409	44	-	4/39/115/115	-
30	GOL	b	629	-	-	1/4/4/4	-

The worst 5 of 1909 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	512	CLA	MG-NA	11.28	2.33	2.06
24	c	513	CLA	MG-NA	10.92	2.32	2.06
24	C	508	CLA	MG-NA	10.64	2.31	2.06
24	B	605	CLA	MG-ND	-10.09	1.85	2.05
24	c	505	CLA	MG-NA	9.46	2.28	2.06

The worst 5 of 2537 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	408	PHO	C2D-C1D-ND	12.44	118.11	109.53
25	D	401	PHO	C2D-C1D-ND	12.08	117.87	109.53
25	a	411	PHO	C2D-C1D-ND	11.69	117.60	109.53
25	d	401	PHO	C2D-C1D-ND	11.25	117.30	109.53
24	B	604	CLA	C1D-ND-C4D	-10.69	98.74	106.33

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
43	V	202	HEC	NA
43	v	1603	HEC	NA

5 of 1219 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	B	602	CLA	CHA-CBD-CGD-O1D
24	B	602	CLA	CHA-CBD-CGD-O2D
24	B	606	CLA	C2-C3-C5-C6
24	B	607	CLA	CHA-CBD-CGD-O1D
24	B	607	CLA	CHA-CBD-CGD-O2D

There are no ring outliers.

151 monomers are involved in 262 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	D	403	CLA	1	0
24	c	512	CLA	1	0
26	b	622	BCR	3	0
27	A	411	SQD	3	0
26	k	302	BCR	4	0
24	B	610	CLA	3	0
24	d	404	CLA	2	0
37	E	101	LHG	1	0
33	a	425[B]	PL9	6	0
24	C	511	CLA	3	0
41	H	101	RRX	3	0
27	D	408	SQD	2	0
26	K	101	BCR	2	0
24	B	617	CLA	4	0
24	c	510	CLA	3	0
26	B	641	BCR	4	0
29	z	101	LMT	2	0
36	D	413	HTG	3	0
24	C	509	CLA	4	0
26	B	620	BCR	2	0
39	c	518	DGD	1	0
25	d	401	PHO	2	0
24	B	605	CLA	3	0
29	C	521	LMT	4	0
39	C	518	DGD	2	0
30	C	530	GOL	2	0
24	C	512	CLA	3	0
37	l	302	LHG	1	0
39	h	1205	DGD	1	0
24	b	609	CLA	3	0
28	d	411	LMG	1	0
38	o	308	DMS	1	0
24	c	508	CLA	1	0
30	d	402	GOL	2	0
28	B	621	LMG	1	0
28	c	521	LMG	1	0
39	D	407	DGD	6	0
26	b	620	BCR	2	0
24	b	616	CLA	3	0
36	b	602	HTG	1	0
24	c	511	CLA	2	0
37	D	409	LHG	3	0
38	c	536	DMS	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	b	619	CLA	2	0
25	D	401	PHO	2	0
24	c	504	CLA	2	0
29	m	102	LMT	1	0
24	C	507	CLA	2	0
39	C	517	DGD	2	0
39	H	102	DGD	1	0
30	o	305	GOL	1	0
26	k	303	BCR	1	0
24	c	506	CLA	1	0
28	C	520	LMG	1	0
24	c	507	CLA	2	0
24	C	503	CLA	4	0
27	L	101	SQD	1	0
24	B	604	CLA	1	0
30	v	1606	GOL	1	0
37	e	101	LHG	1	0
24	b	606	CLA	3	0
24	C	514	CLA	1	0
37	D	411	LHG	5	0
24	a	408	CLA	3	0
29	b	624	LMT	1	0
29	f	104	LMT	1	0
24	A	409	CLA	2	0
38	b	638	DMS	3	0
26	B	618	BCR	1	0
30	T	101	GOL	1	0
24	b	618	CLA	4	0
26	c	517	BCR	2	0
38	c	533	DMS	1	0
36	O	302	HTG	1	0
24	a	410	CLA	1	0
26	C	515	BCR	2	0
24	b	604	CLA	4	0
24	B	606	CLA	5	0
28	a	415	LMG	2	0
24	c	515	CLA	3	0
24	A	406	CLA	4	0
24	A	407	CLA	1	0
36	b	601	HTG	1	0
24	C	513	CLA	2	0
36	b	625	HTG	4	0

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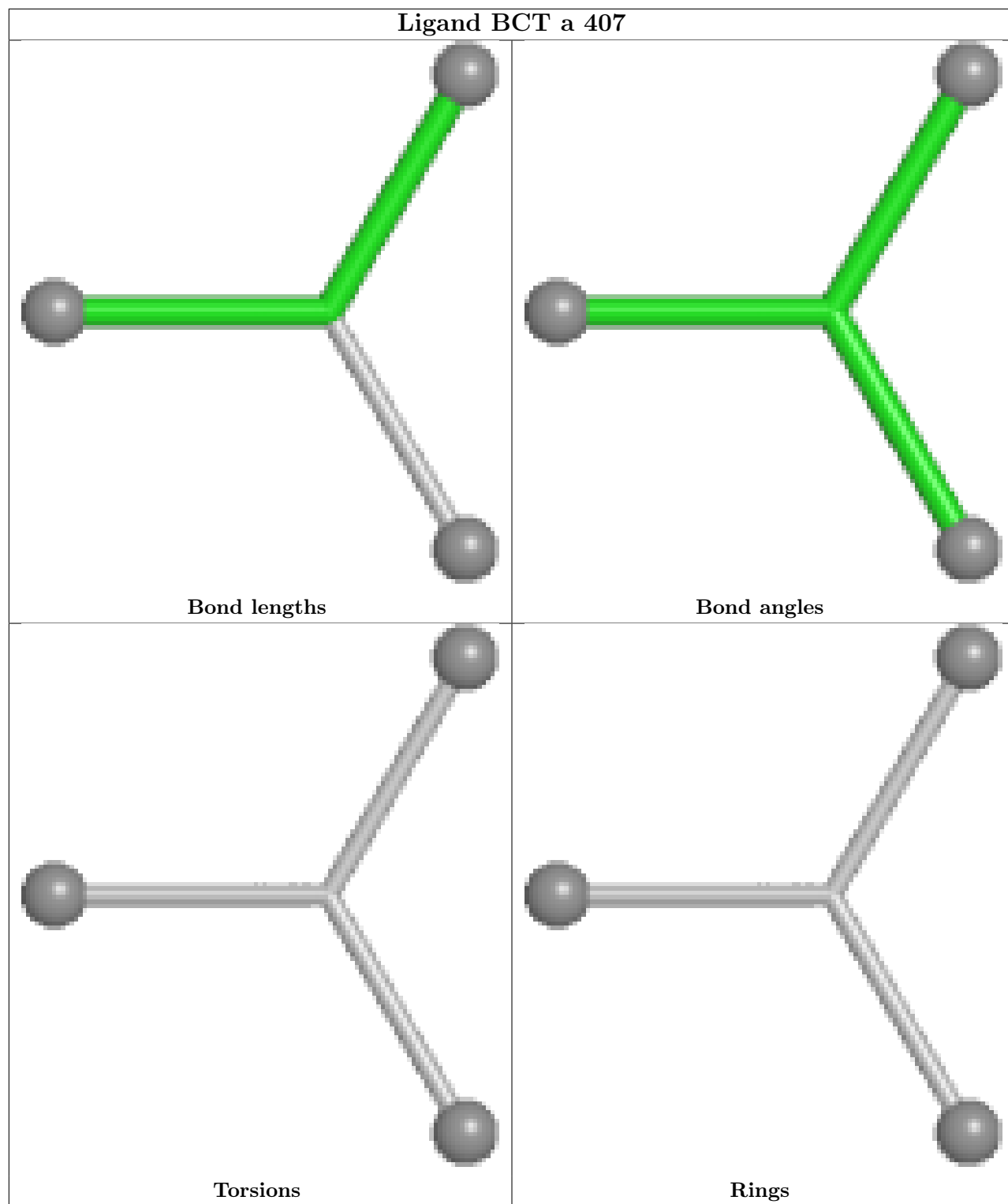
Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	L	102	SQD	2	0
24	B	611	CLA	3	0
30	a	418	GOL	1	0
24	B	607	CLA	2	0
24	B	614	CLA	1	0
29	M	101	LMT	1	0
24	C	506	CLA	2	0
36	b	626	HTG	1	0
24	b	612	CLA	4	0
24	B	602	CLA	1	0
36	B	623[A]	HTG	3	0
24	b	607	CLA	2	0
24	b	615	CLA	1	0
26	D	405	BCR	3	0
24	C	510	CLA	1	0
24	C	508	CLA	1	0
28	b	623	LMG	2	0
24	b	608	CLA	4	0
24	c	503	CLA	3	0
39	c	519	DGD	3	0
26	Y	302	BCR	1	0
27	f	102	SQD	1	0
27	a	414	SQD	1	0
40	f	101	HEM	3	0
24	D	404	CLA	1	0
26	b	621	BCR	3	0
24	C	504	CLA	2	0
29	c	523	LMT	2	0
36	B	625	HTG	1	0
24	c	505	CLA	4	0
39	c	520	DGD	2	0
24	B	616	CLA	8	0
40	F	101	HEM	1	0
24	b	617	CLA	1	0
29	J	102	LMT	1	0
33	A	422[B]	PL9	6	0
41	h	1204	RRX	5	0
36	h	1202	HTG	2	0
24	c	514	CLA	3	0
24	b	610	CLA	1	0
26	B	619	BCR	4	0
26	a	413	BCR	3	0

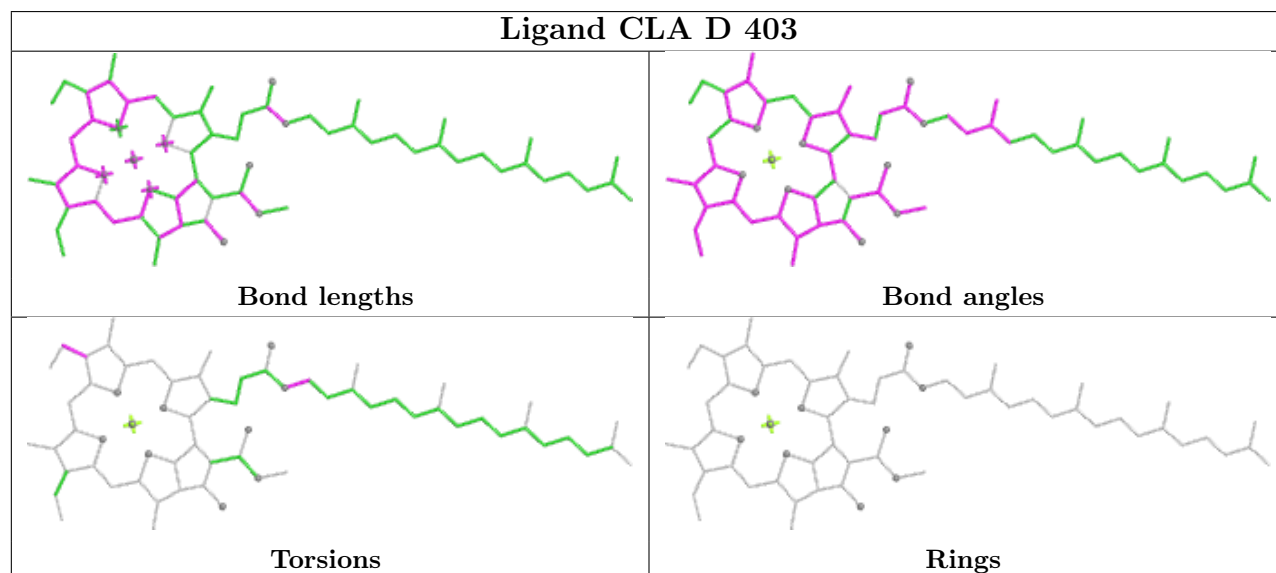
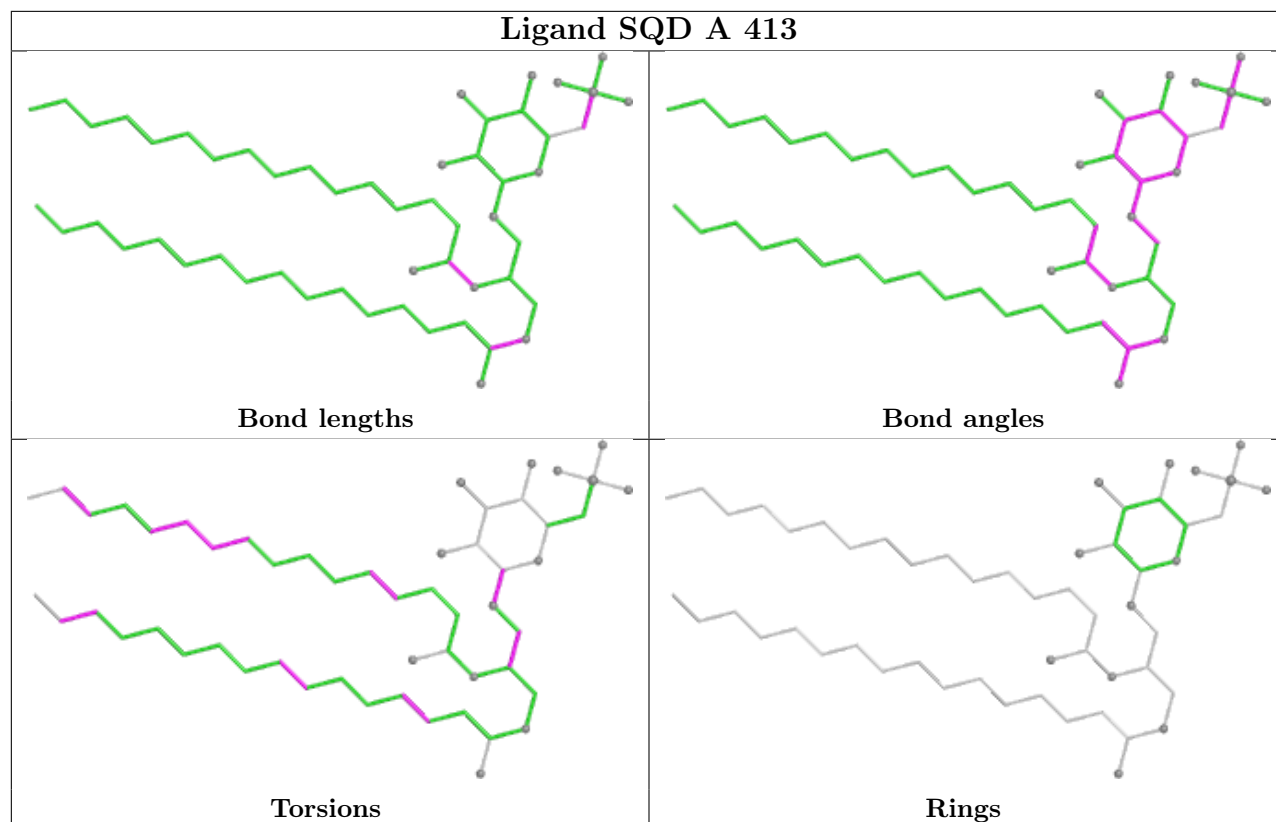
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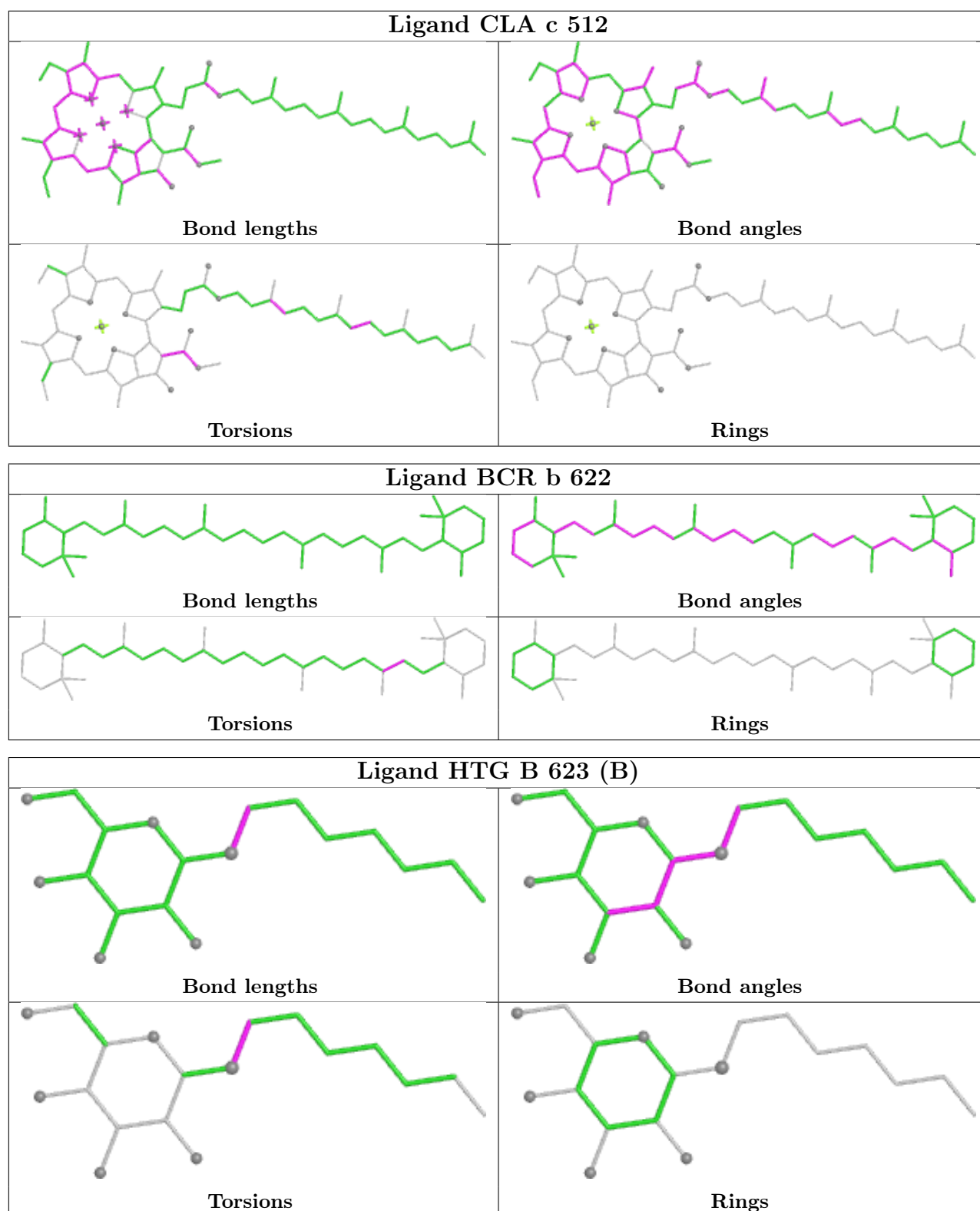
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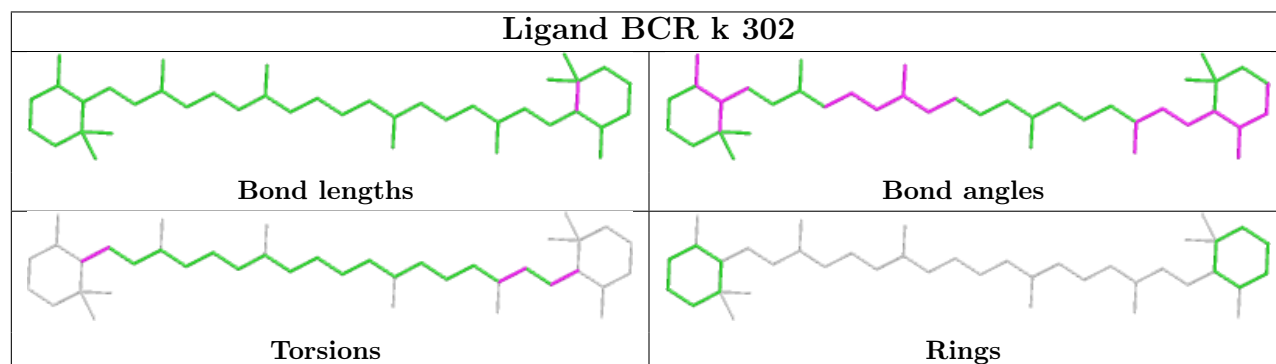
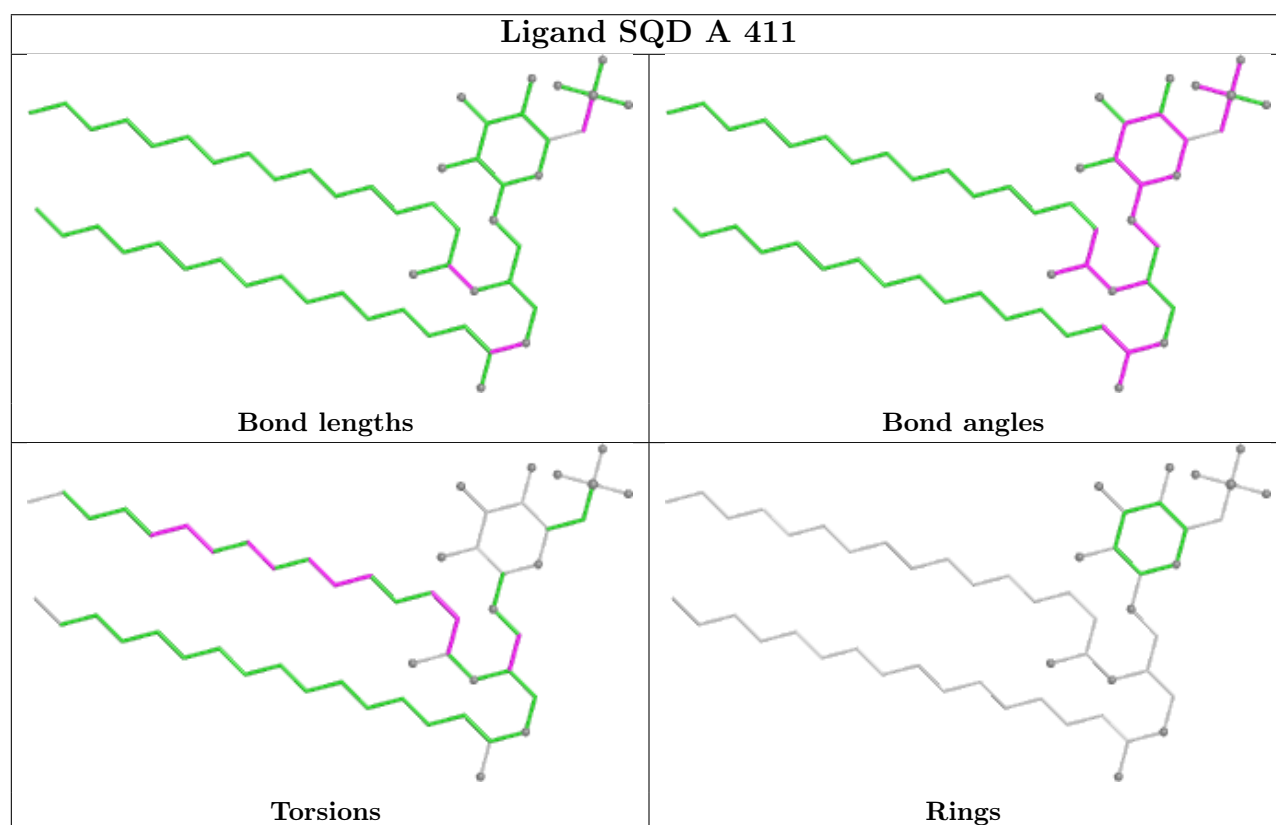
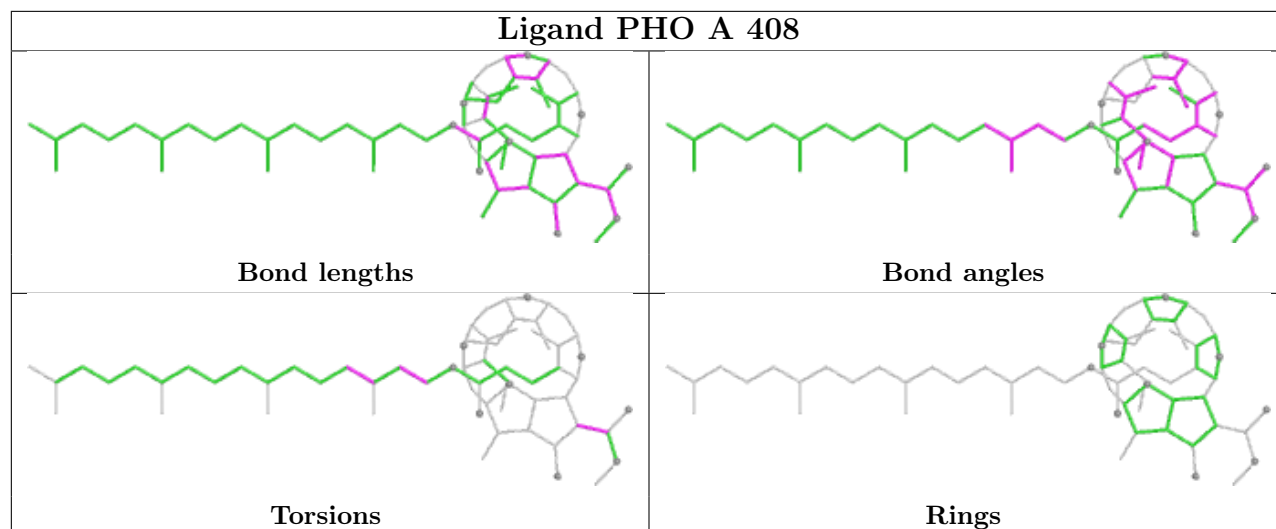
Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	d	405	CLA	1	0
24	B	603	CLA	2	0
24	b	605	CLA	2	0
26	A	410	BCR	3	0
26	C	516	BCR	1	0
26	T	102	BCR	3	0
26	c	516	BCR	2	0
30	c	527	GOL	1	0
38	B	643	DMS	1	0
37	B	640	LHG	1	0
29	a	402	LMT	1	0
29	B	622	LMT	1	0
36	B	626	HTG	1	0
28	C	532	LMG	1	0
28	D	412	LMG	2	0
29	A	414	LMT	1	0
30	a	417	GOL	2	0
24	C	502	CLA	5	0
24	b	613	CLA	3	0
24	C	505	CLA	1	0
26	d	406	BCR	1	0
24	A	405	CLA	2	0
24	c	513	CLA	3	0
24	a	409	CLA	1	0

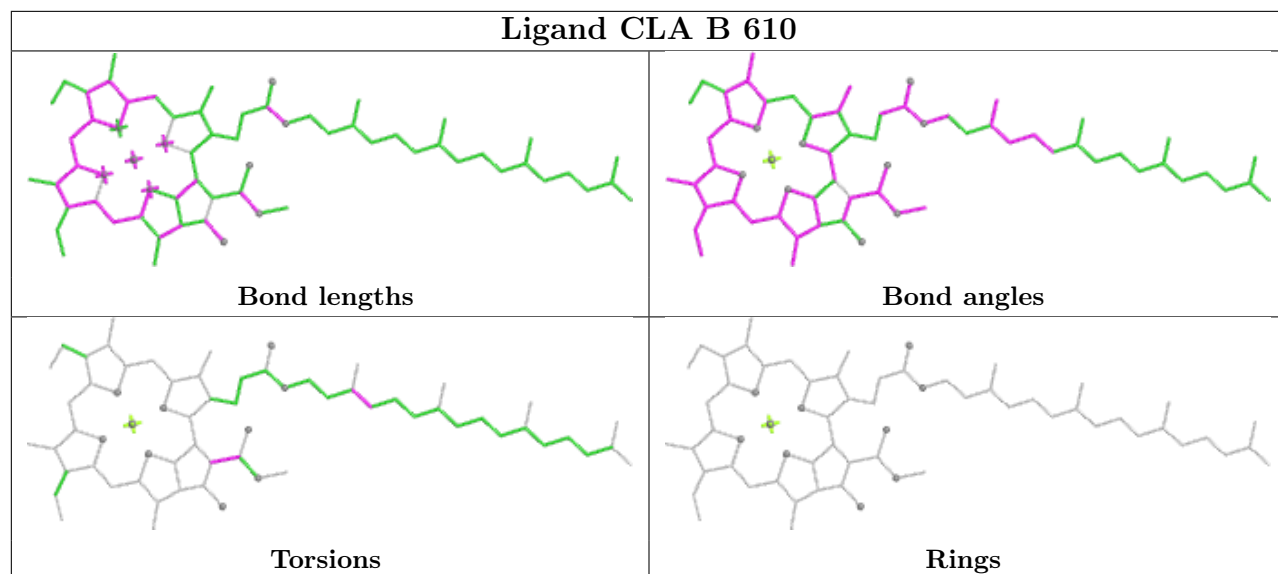
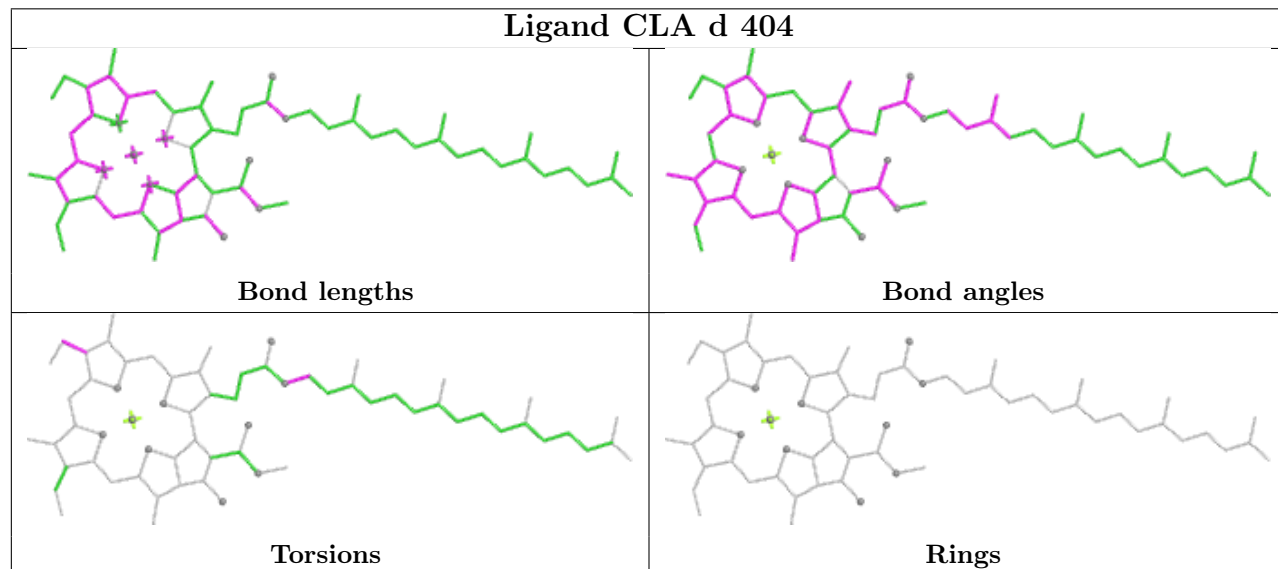
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

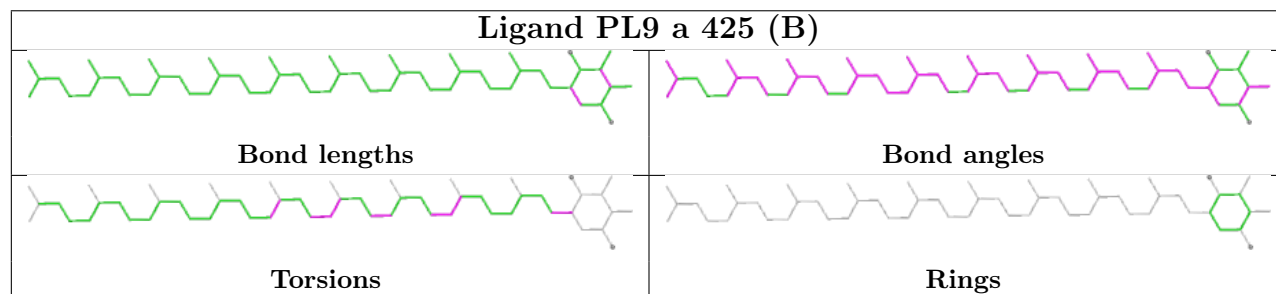
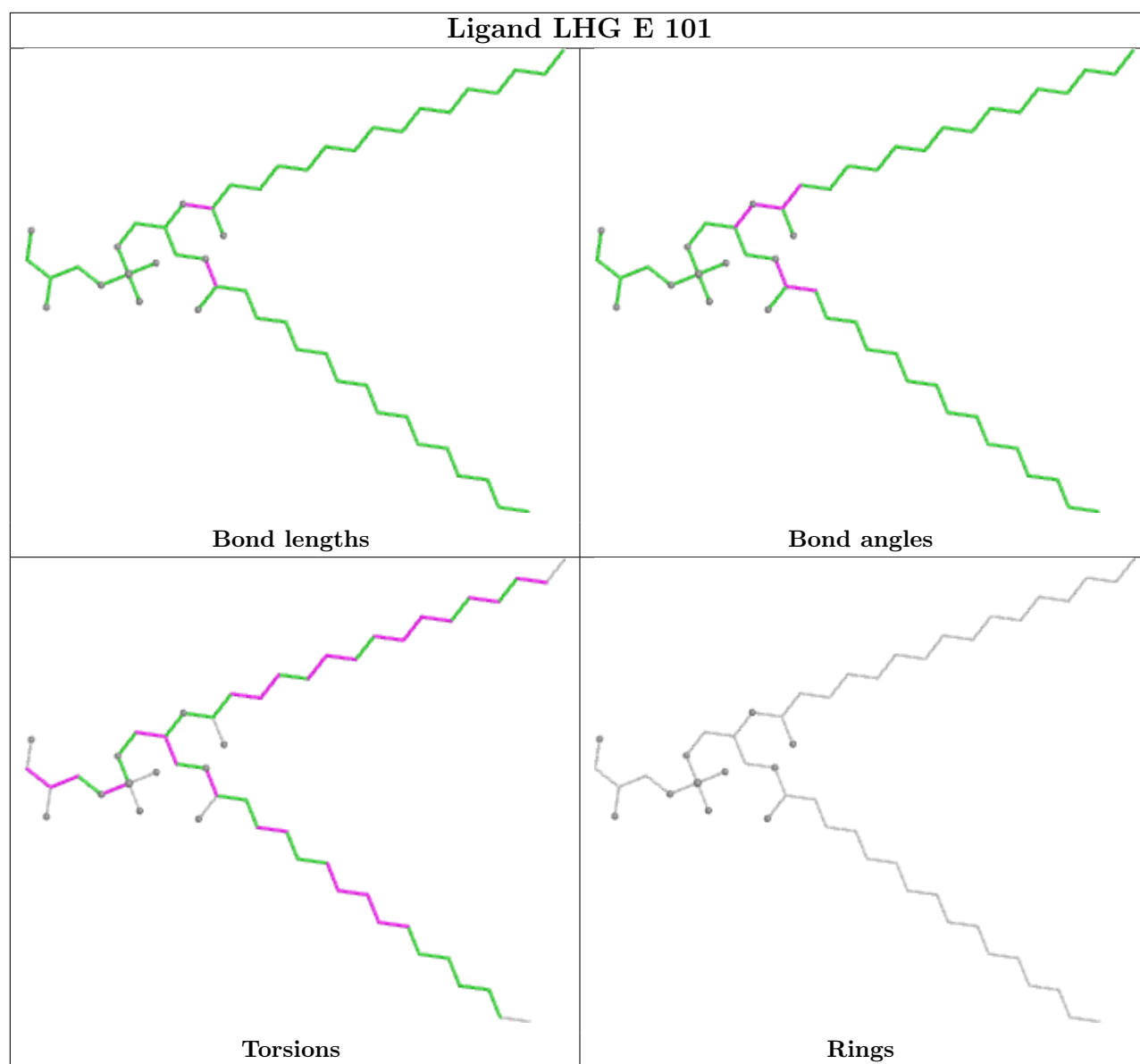




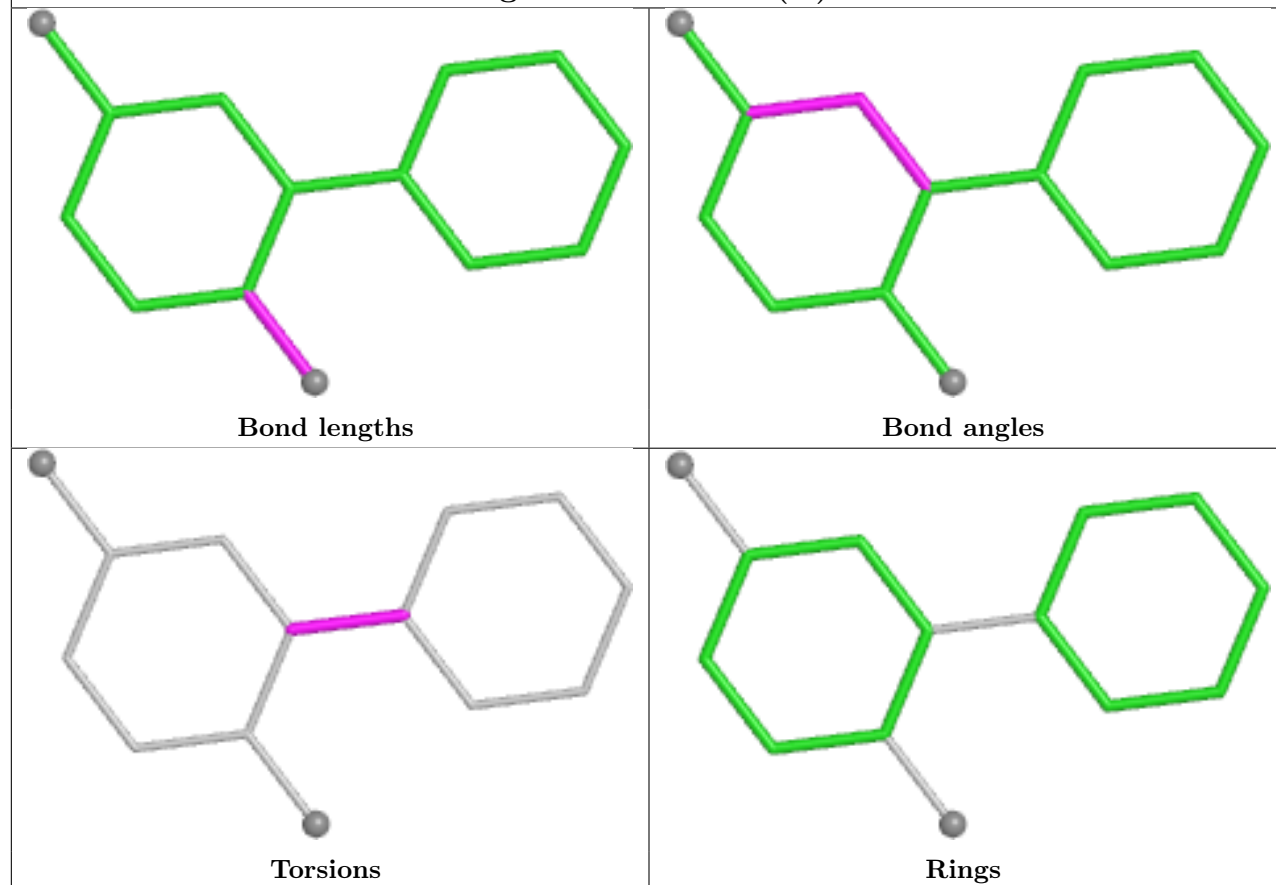




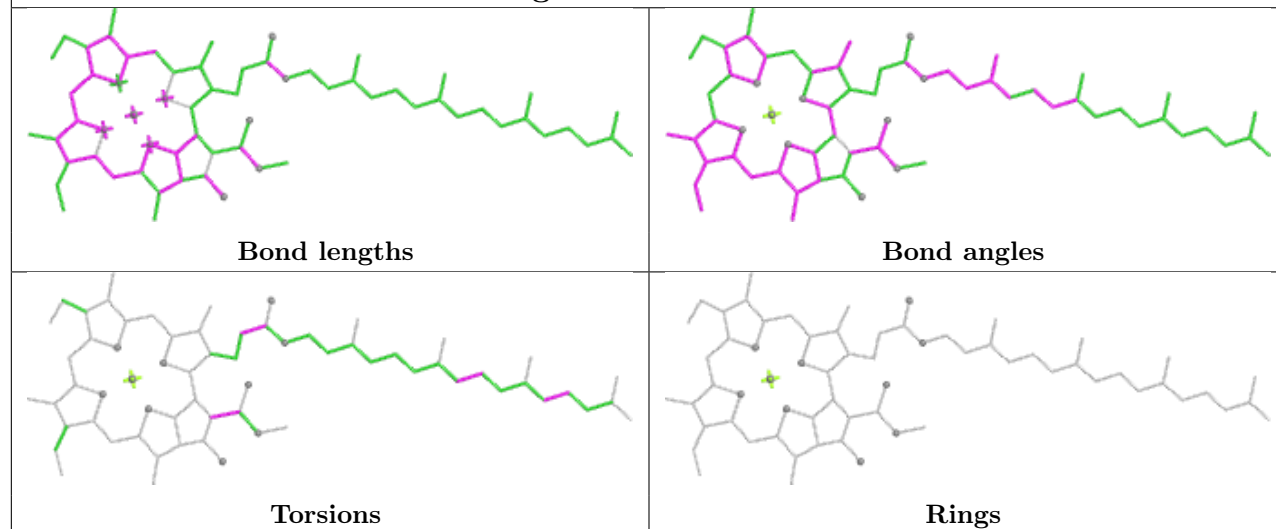
Ligand CLA B 610**Ligand CLA d 404**

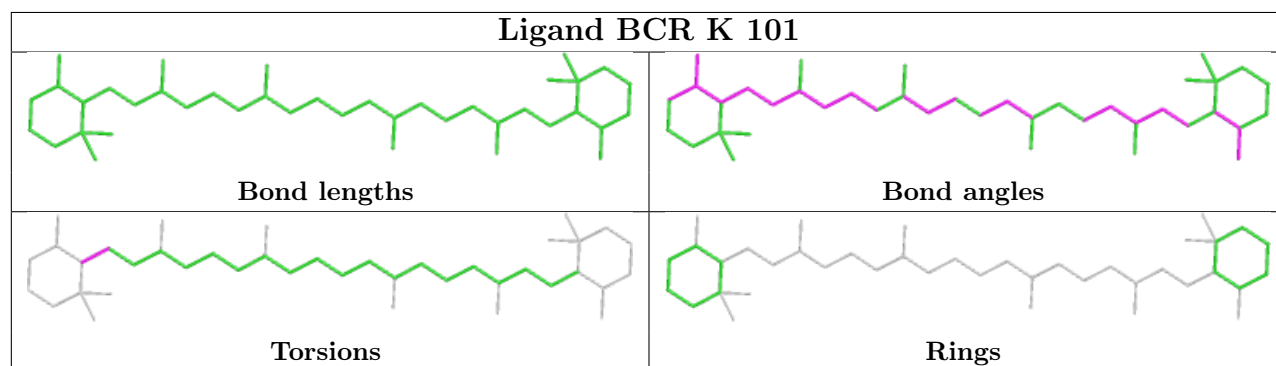
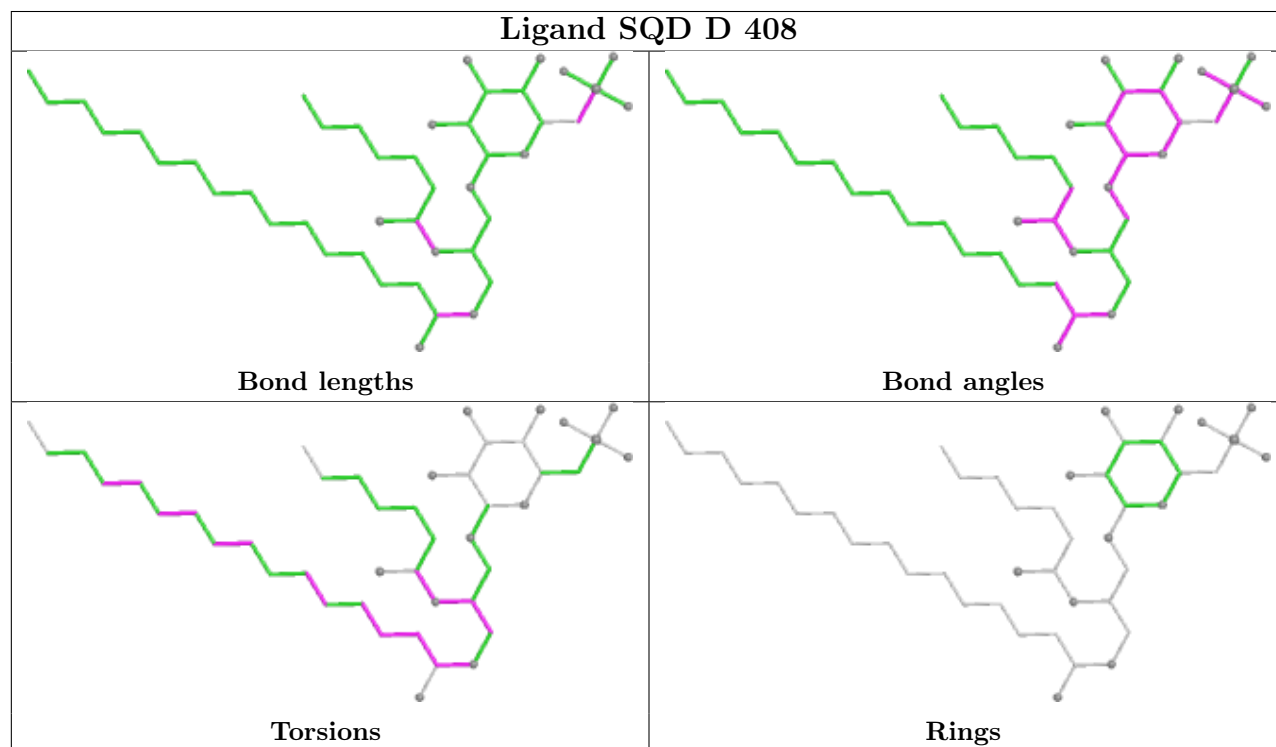
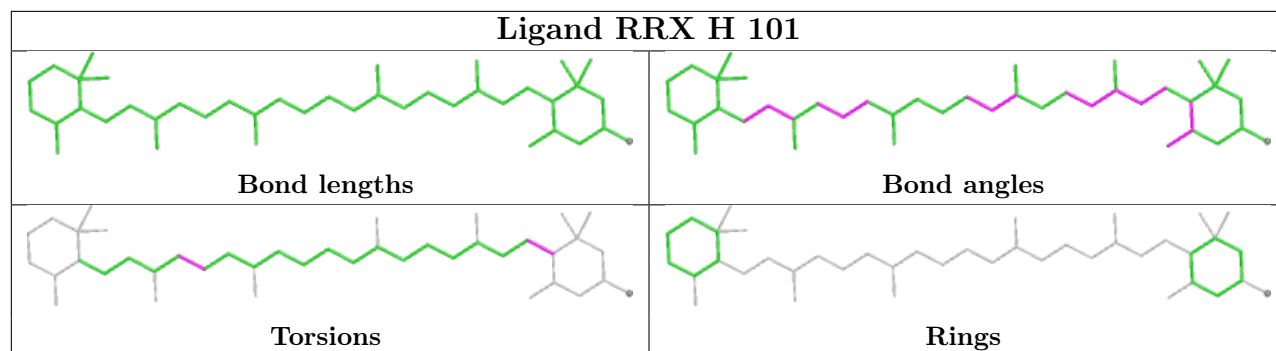


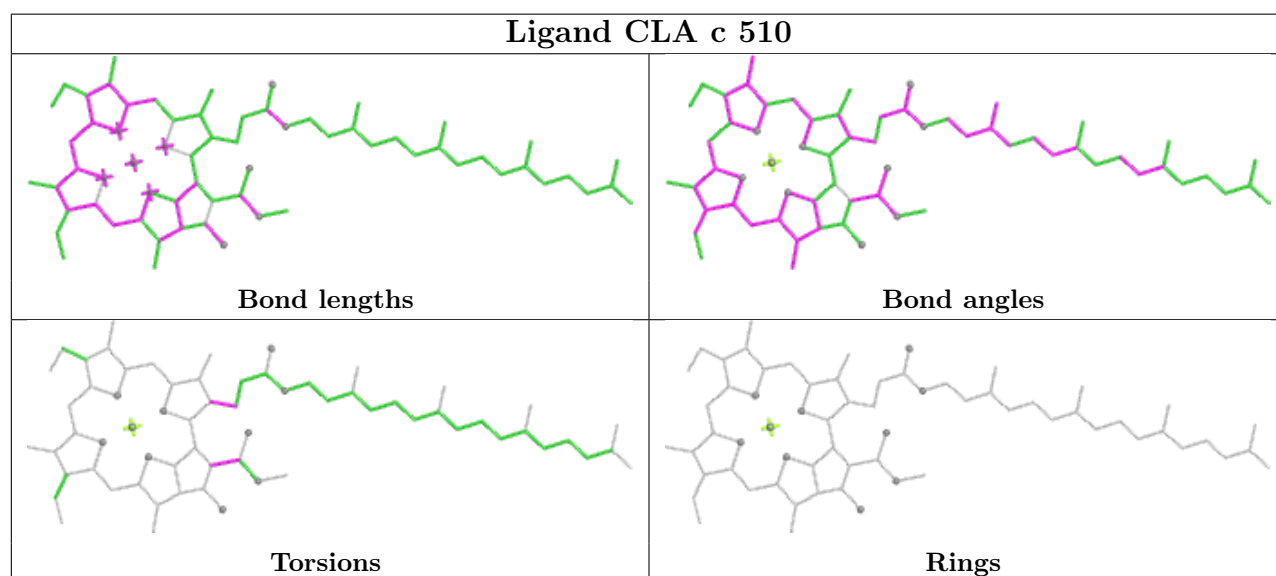
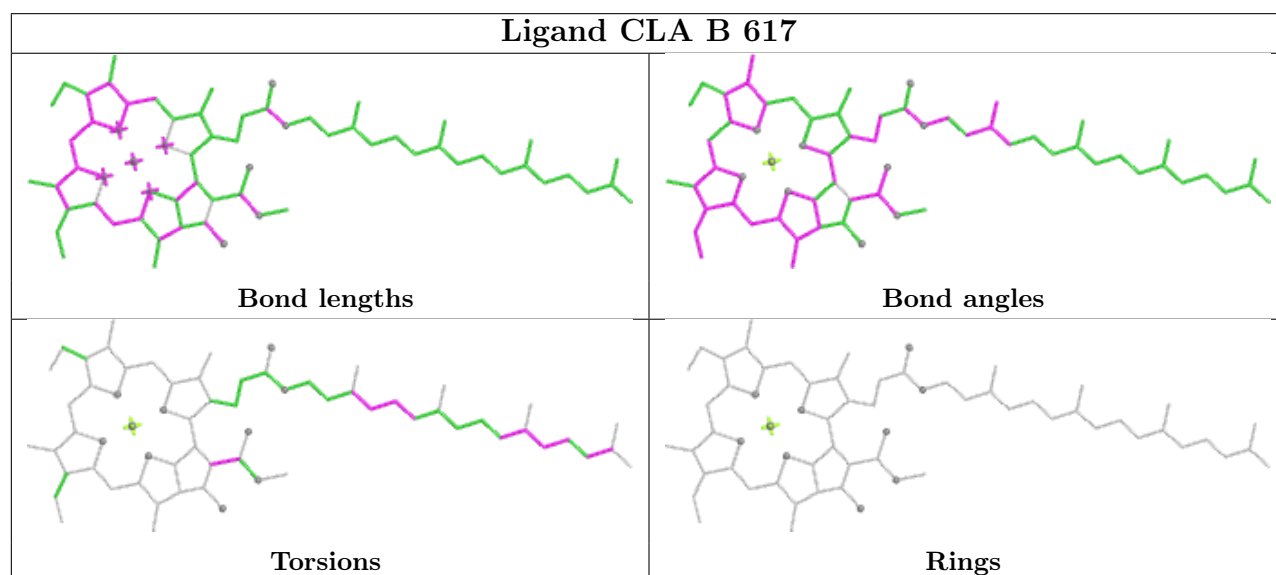
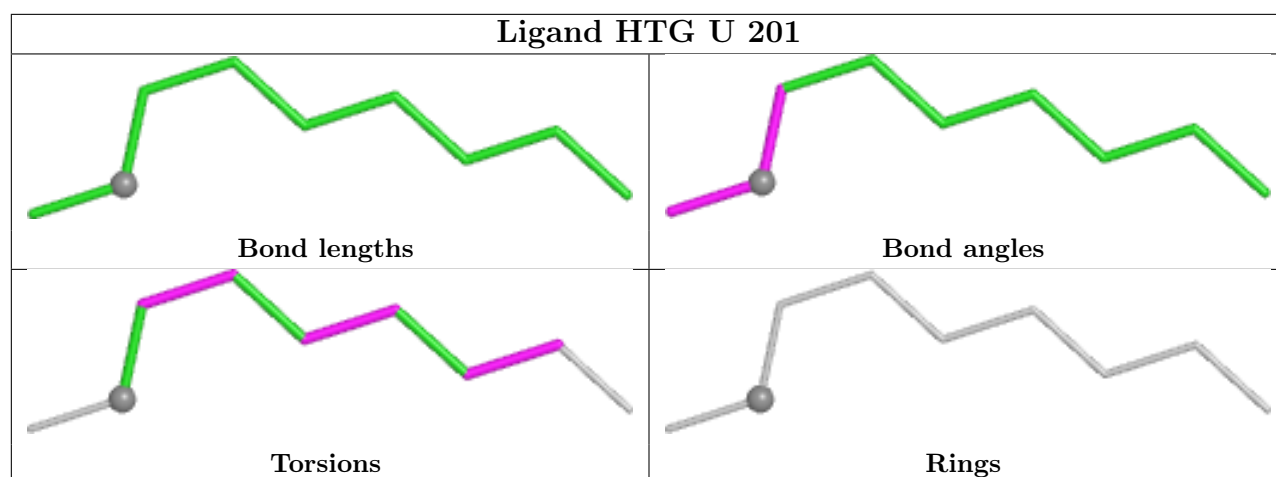
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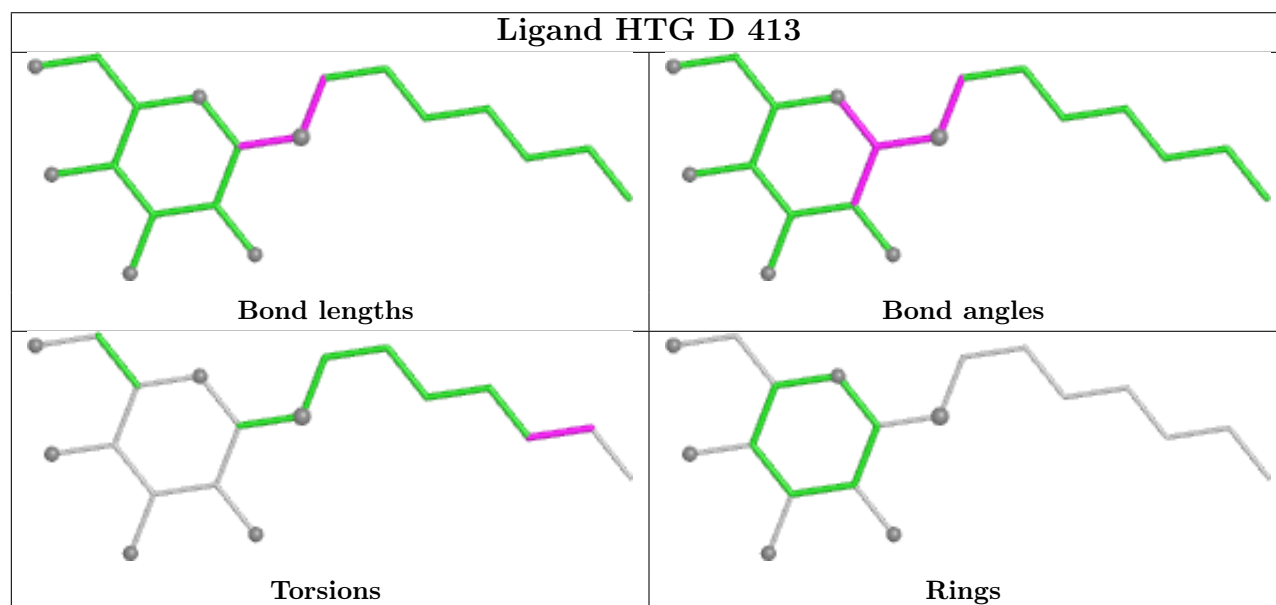
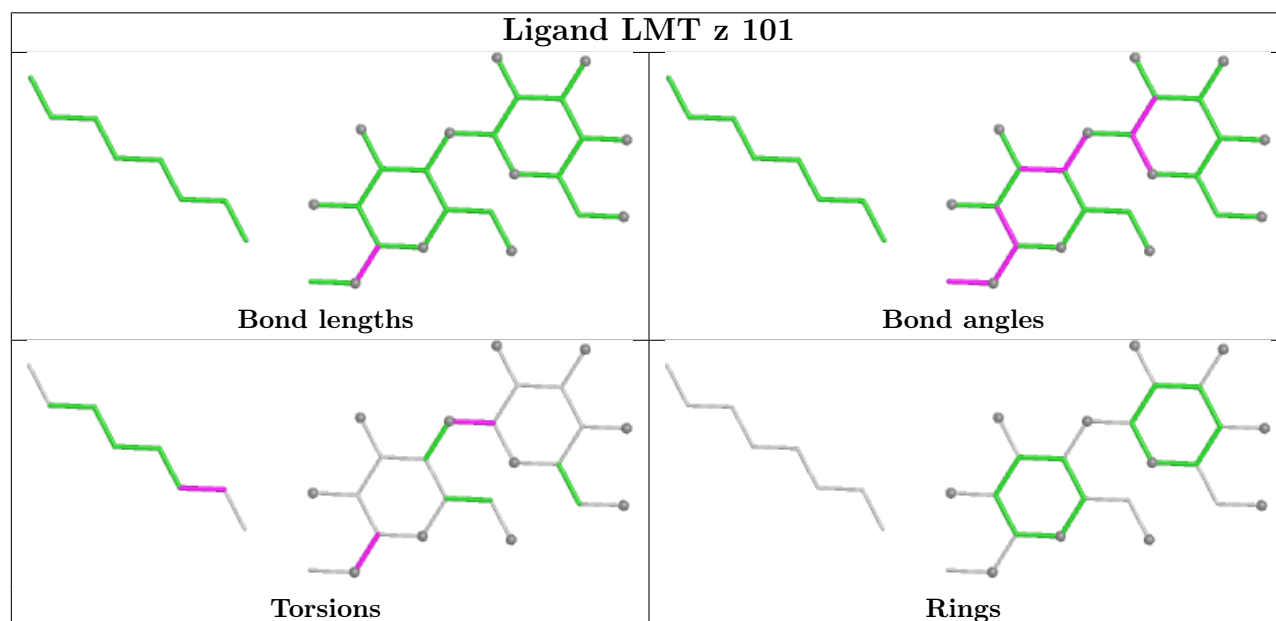
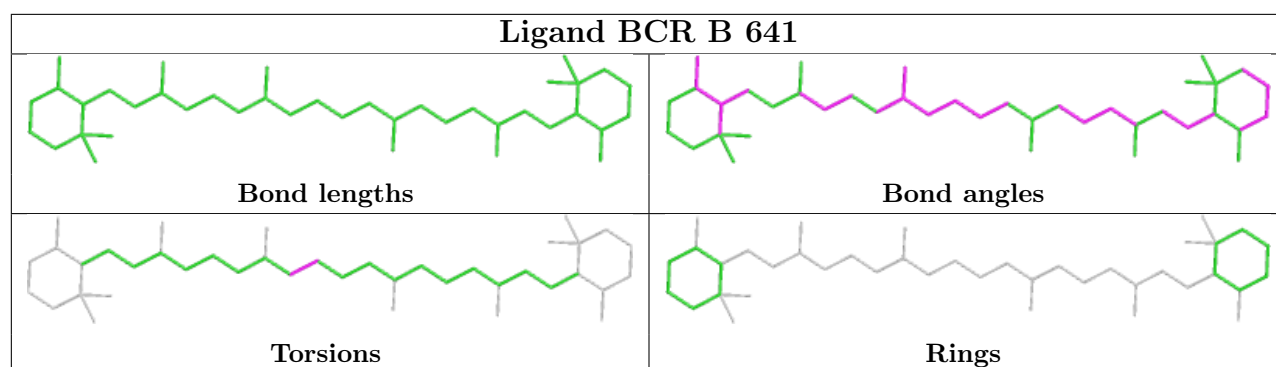


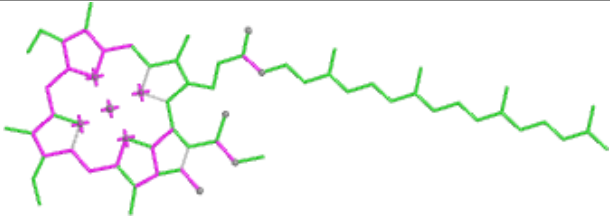
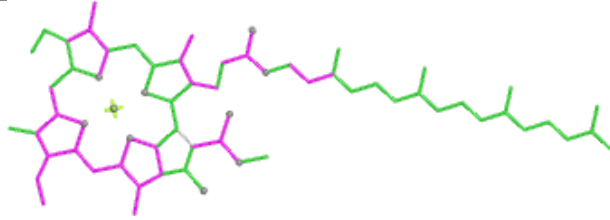
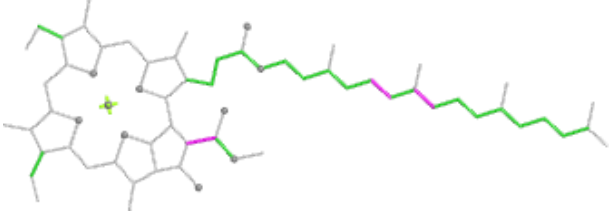
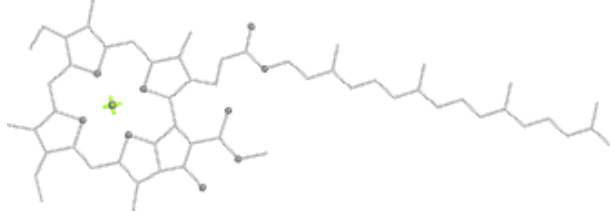
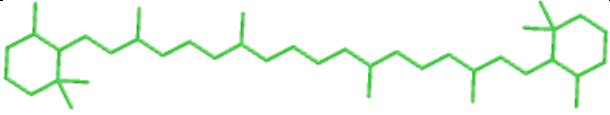
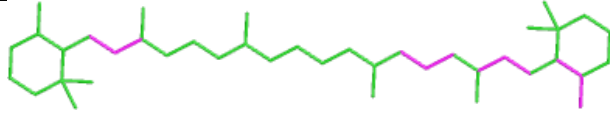
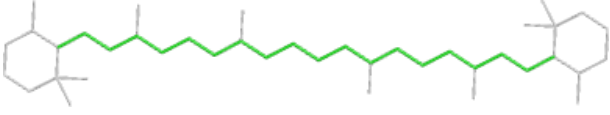
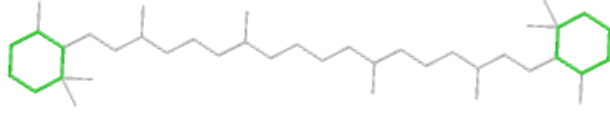
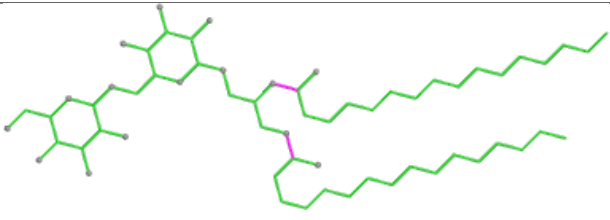
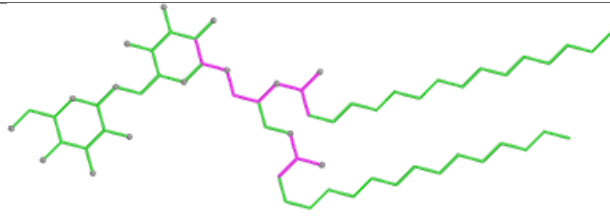
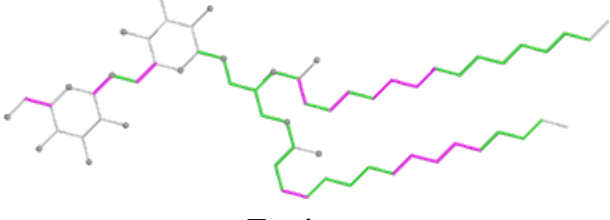
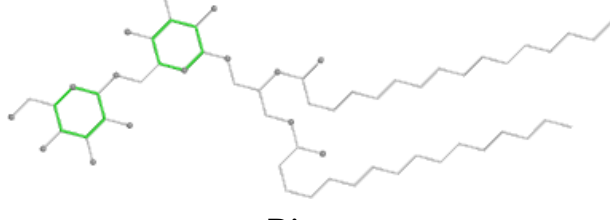
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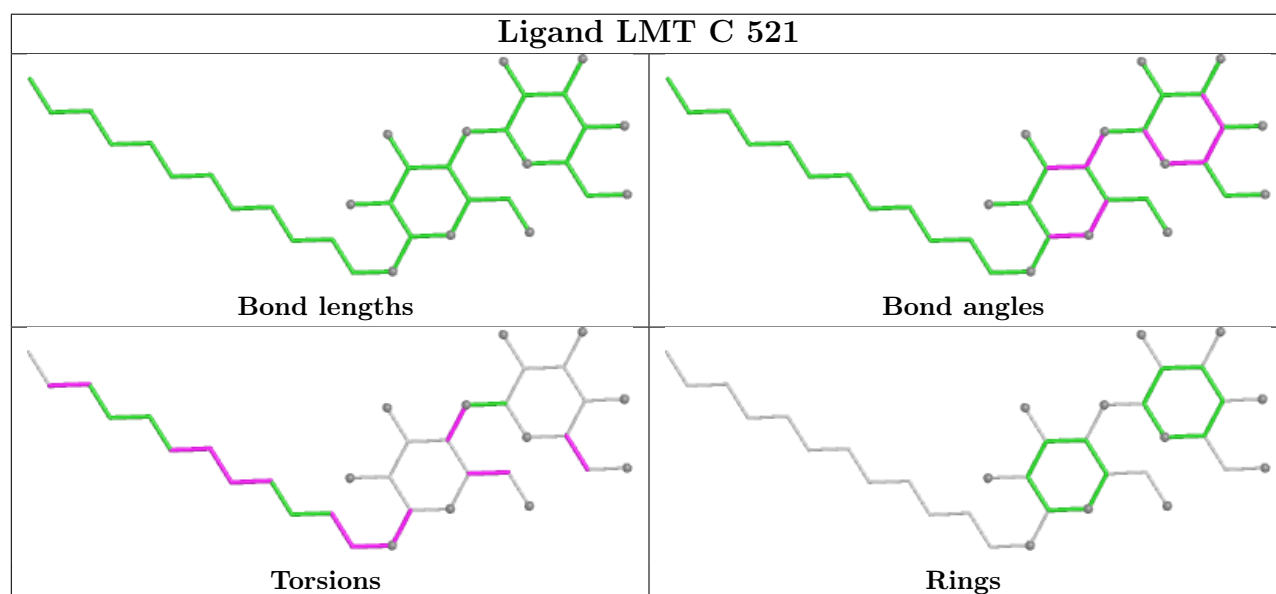
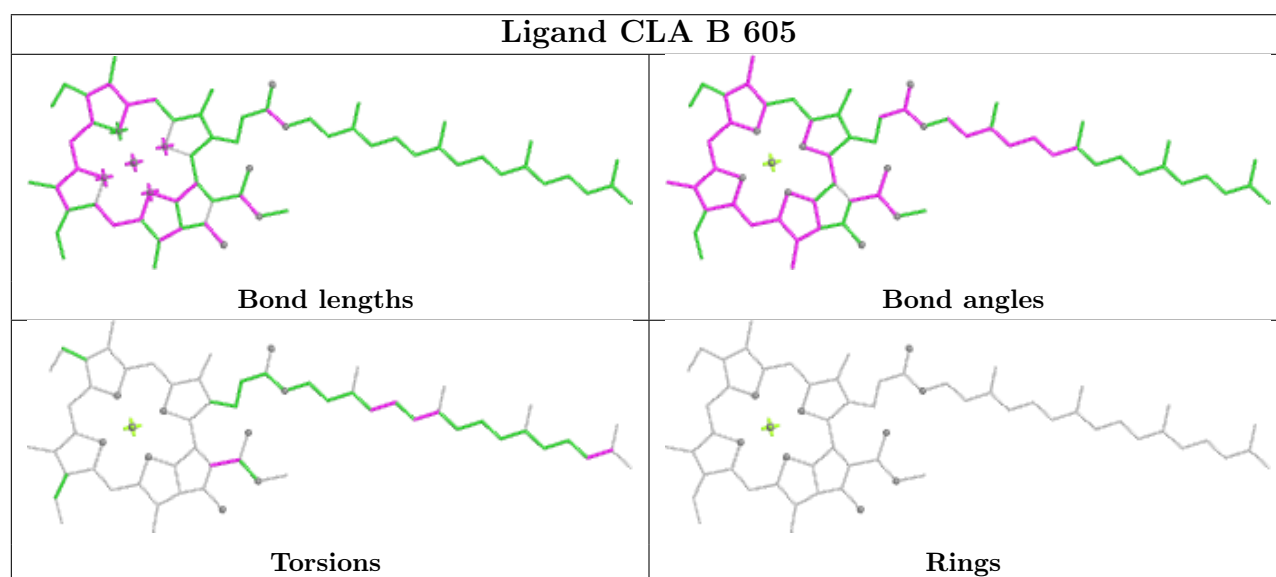
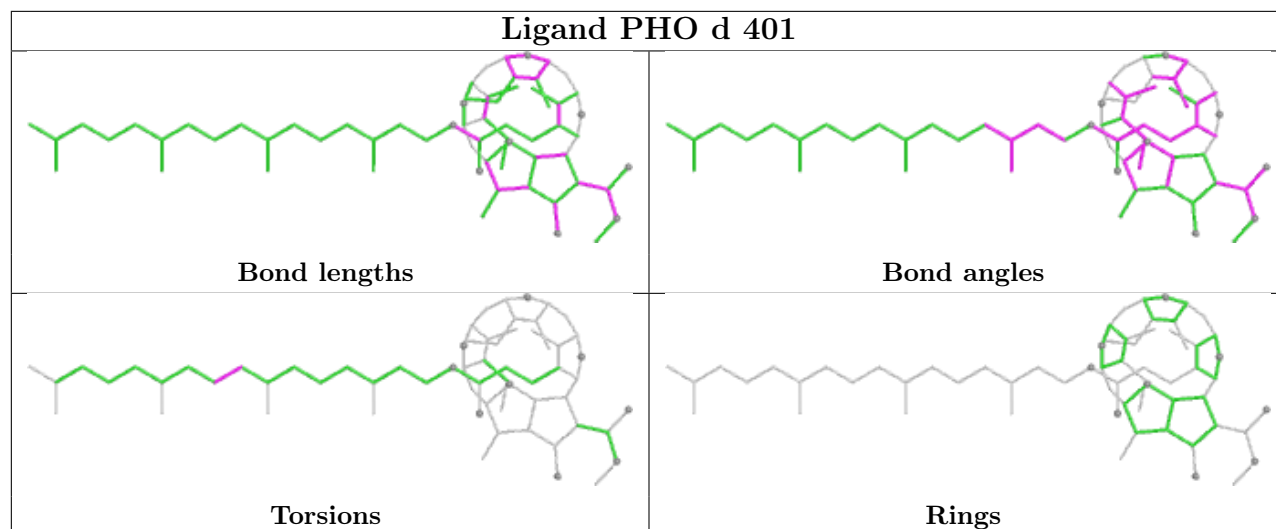


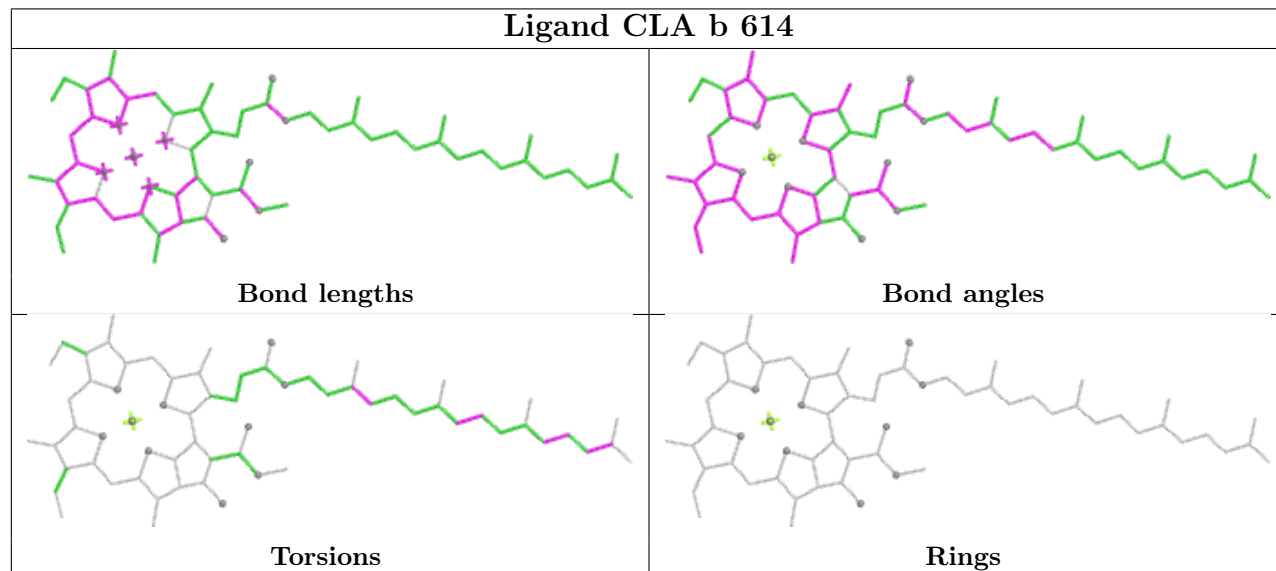
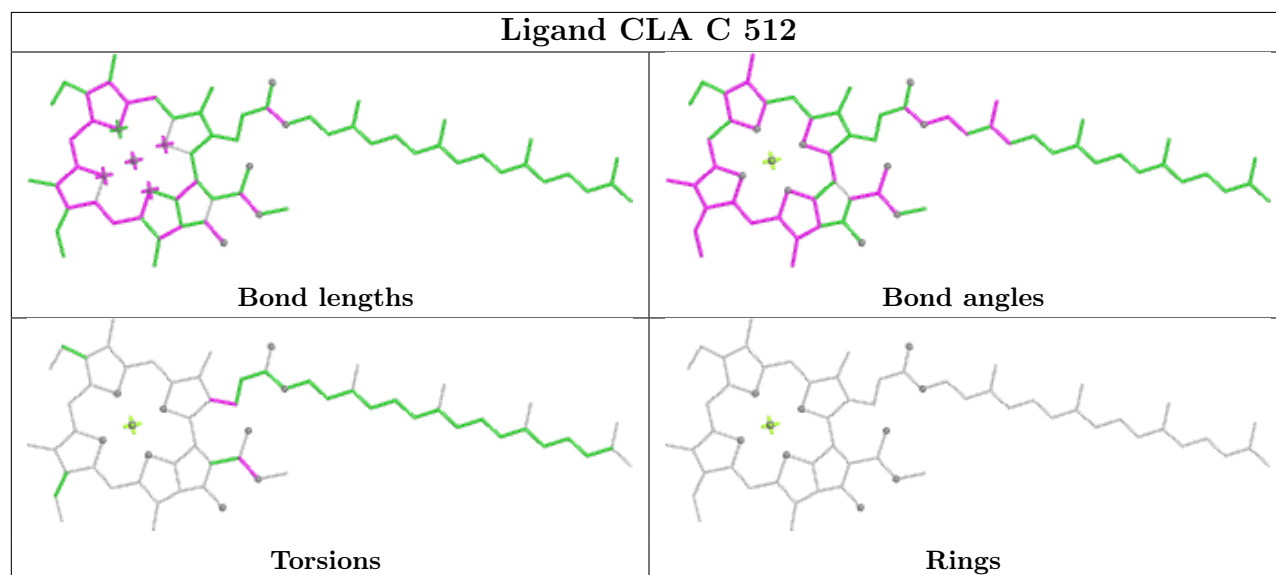
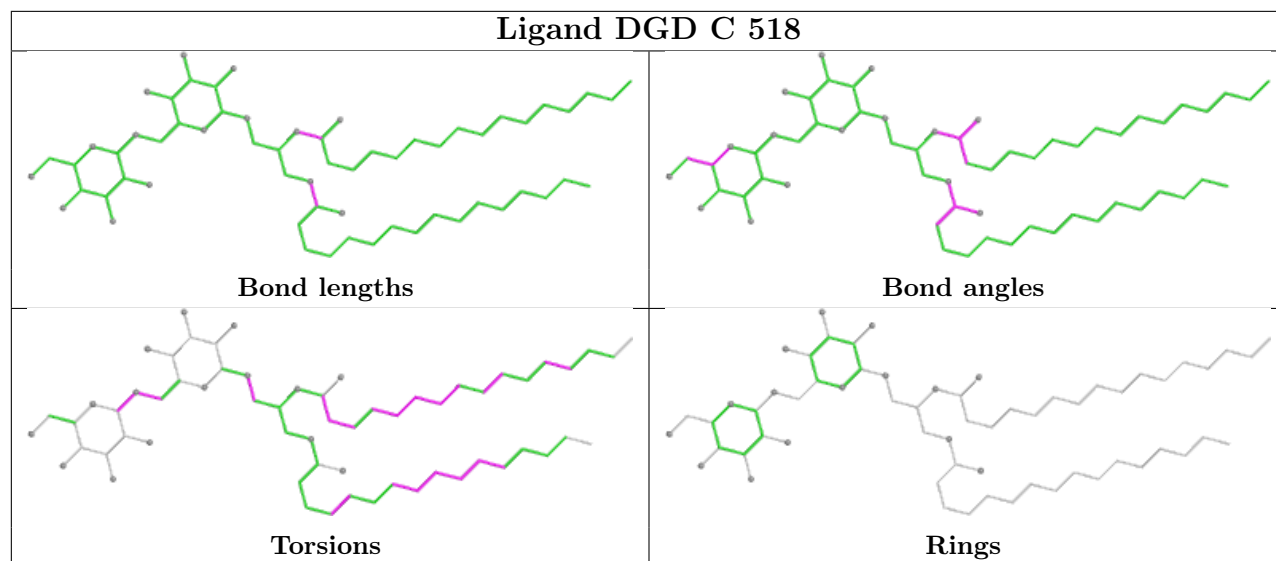


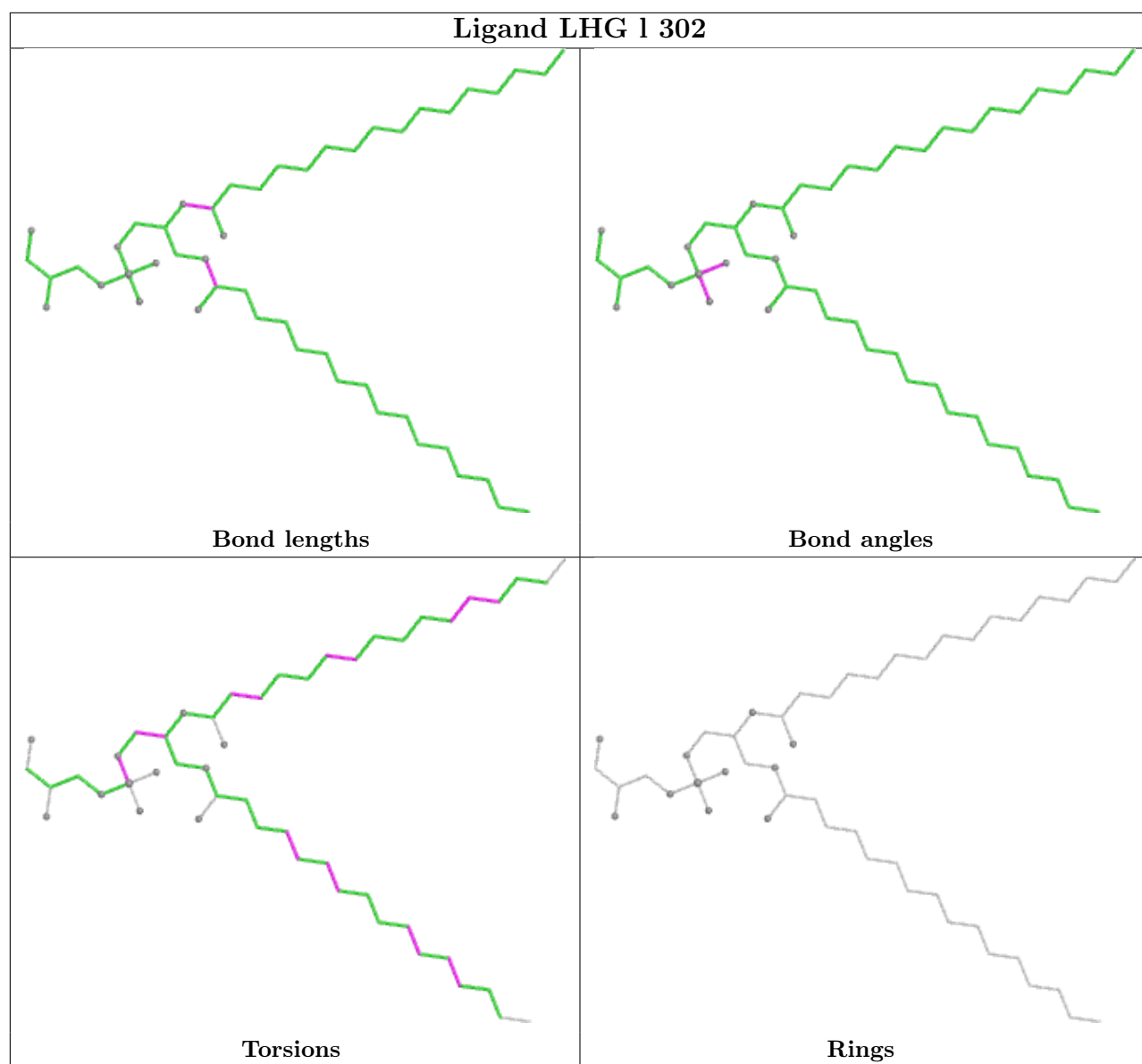


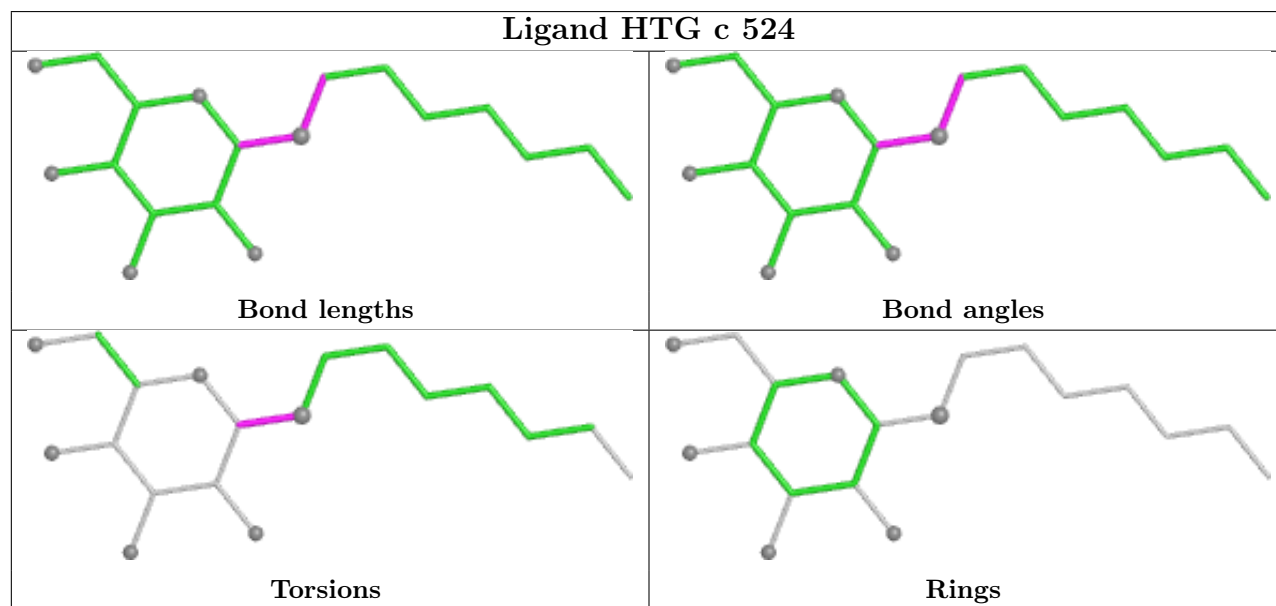
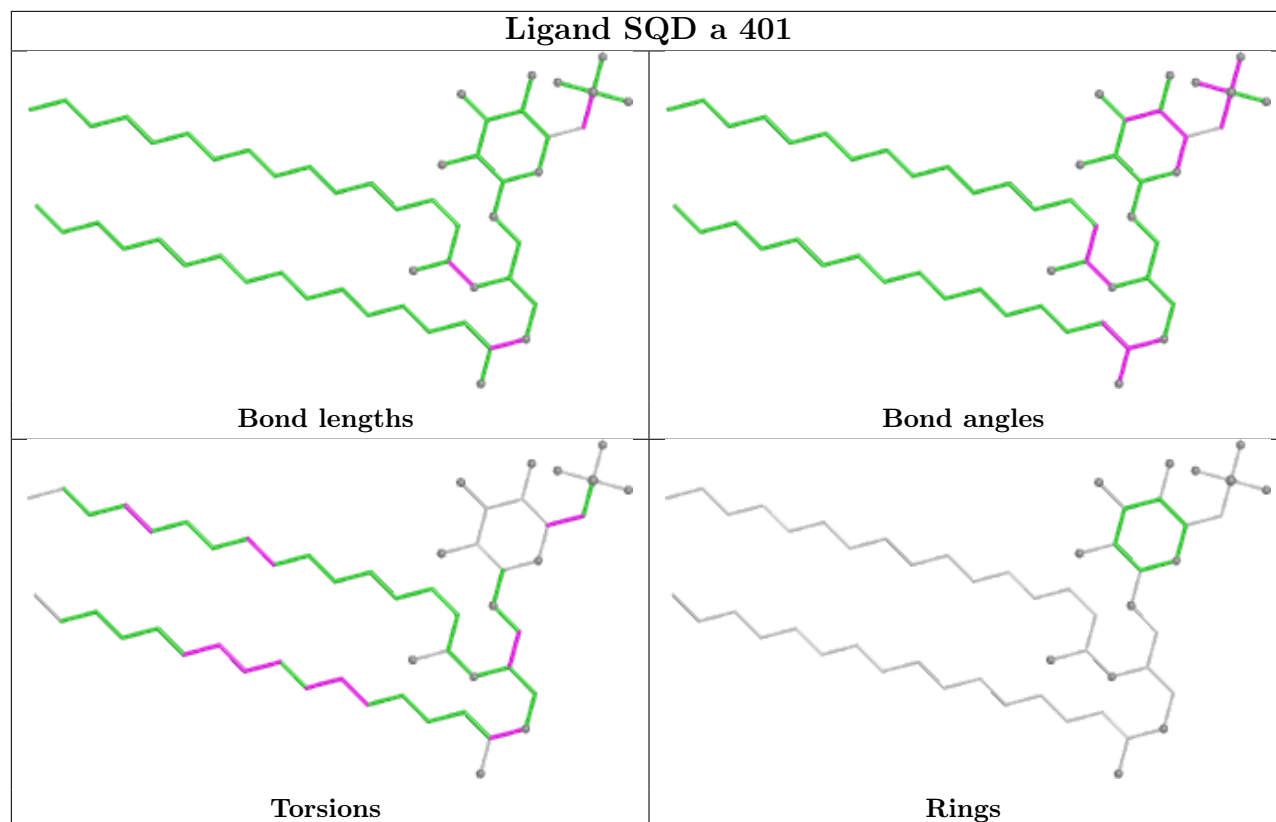


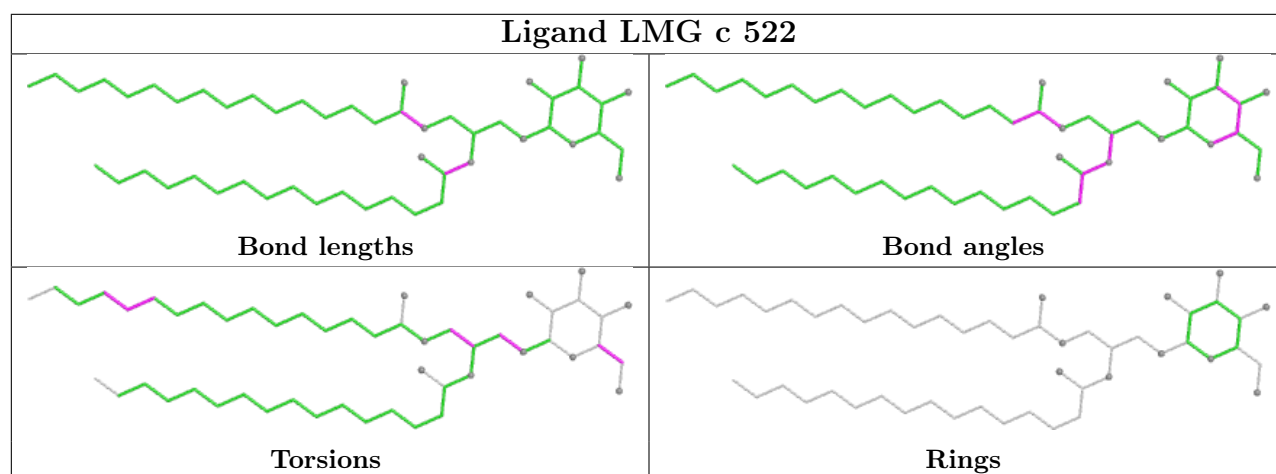
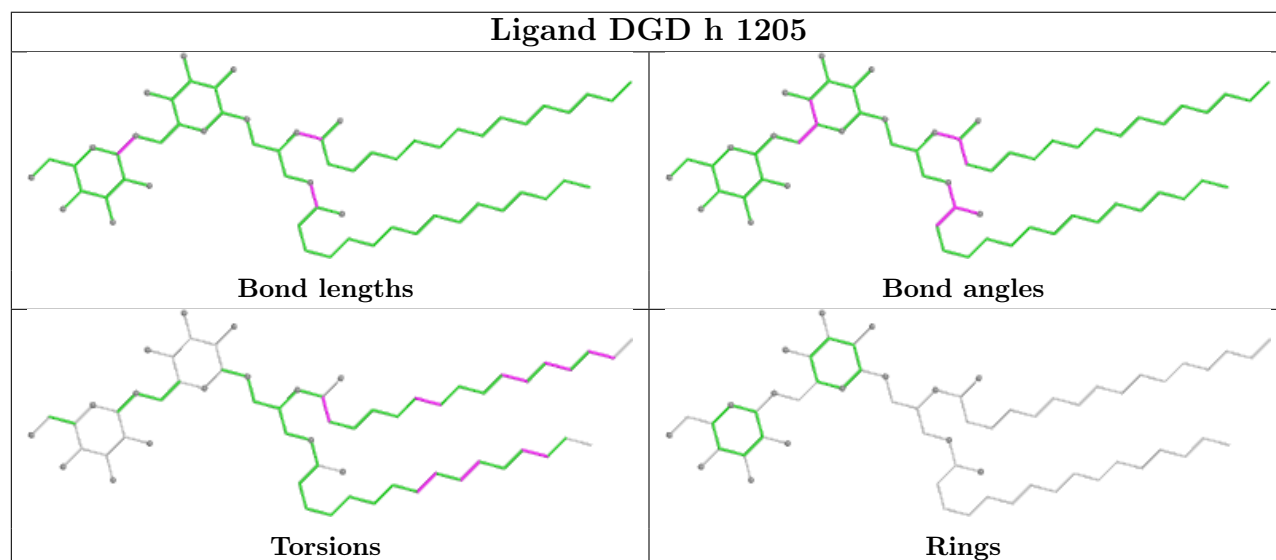
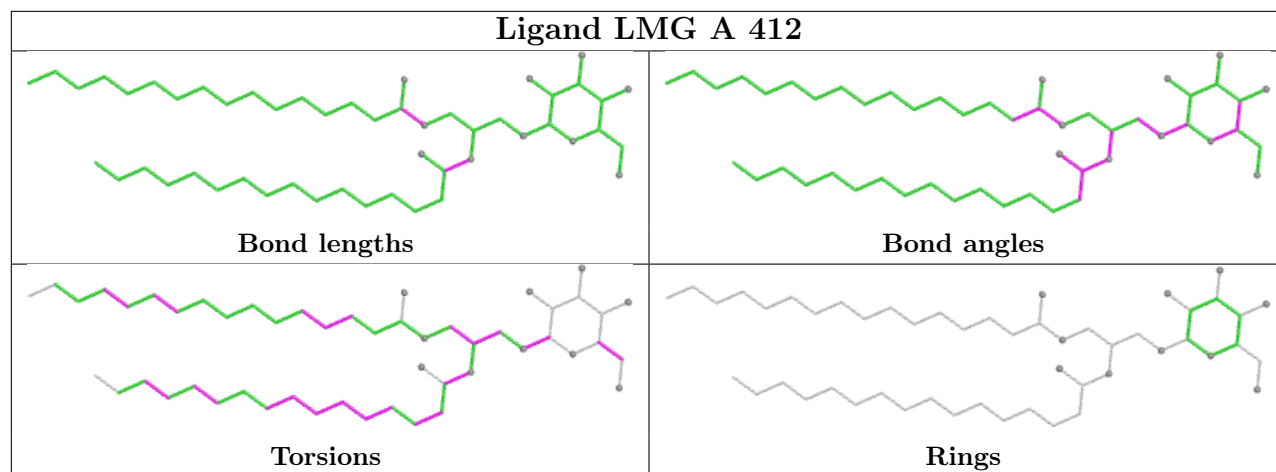
Ligand CLA C 509	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR B 620	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand DGD c 518	
 Bond lengths	 Bond angles
 Torsions	 Rings

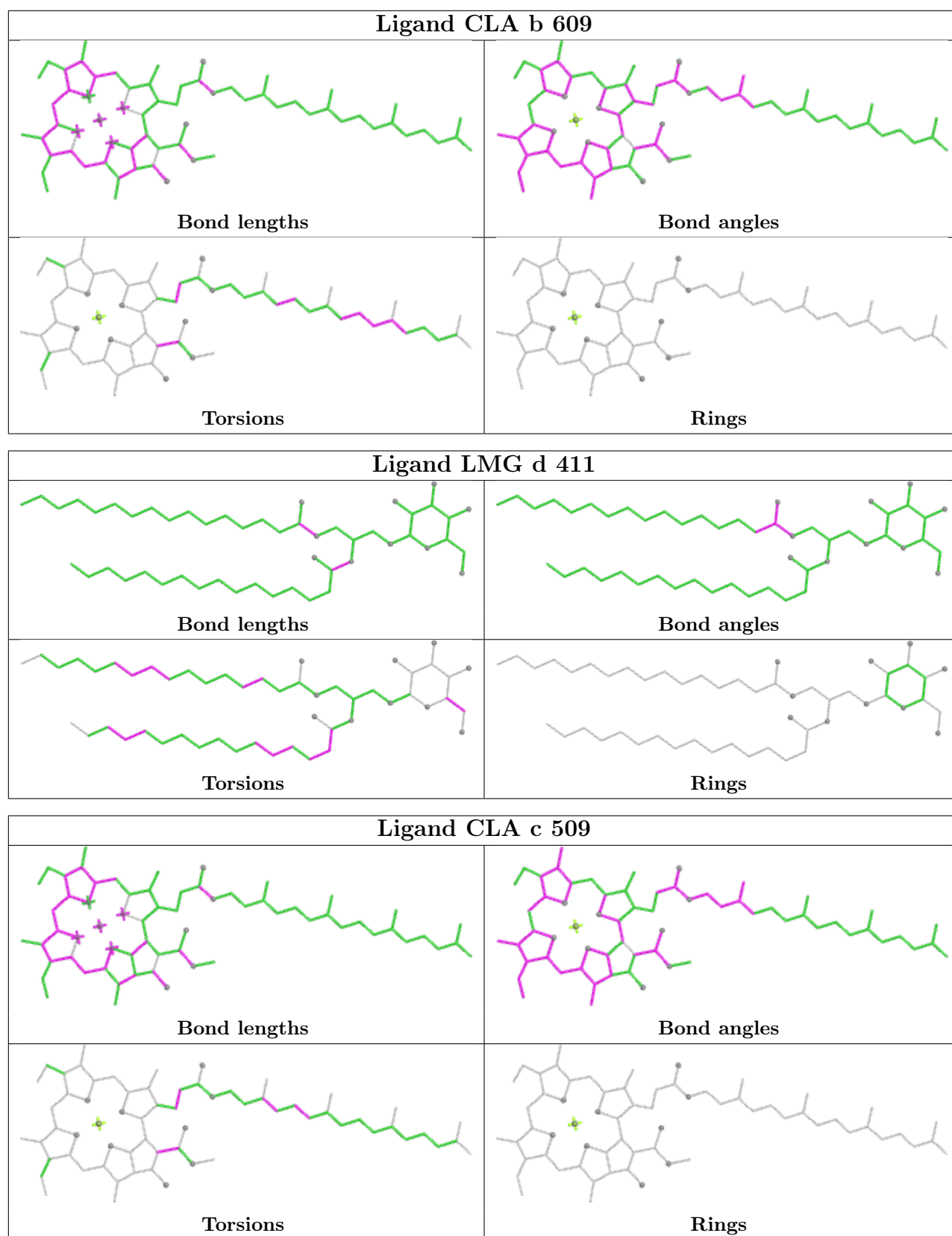


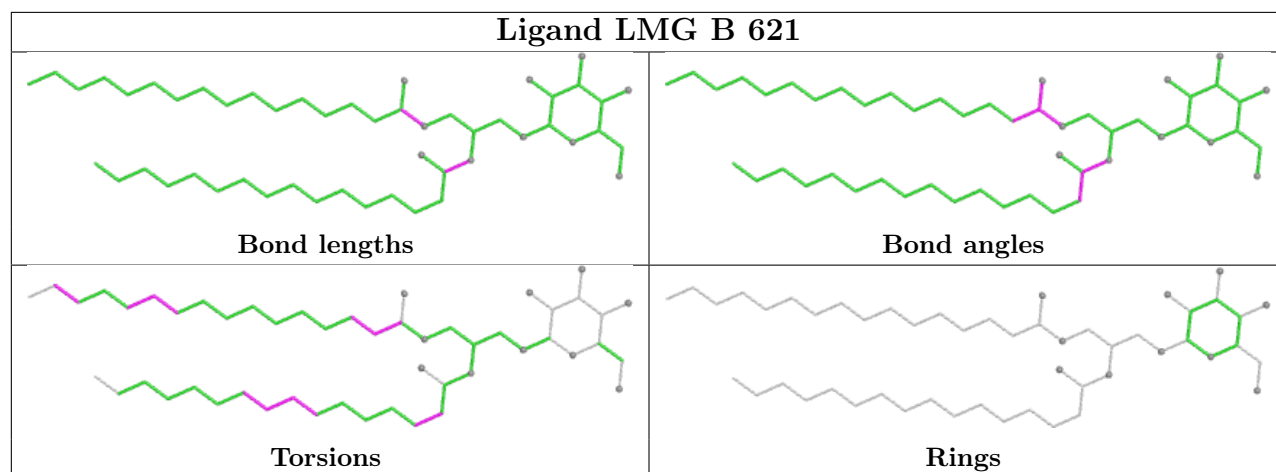
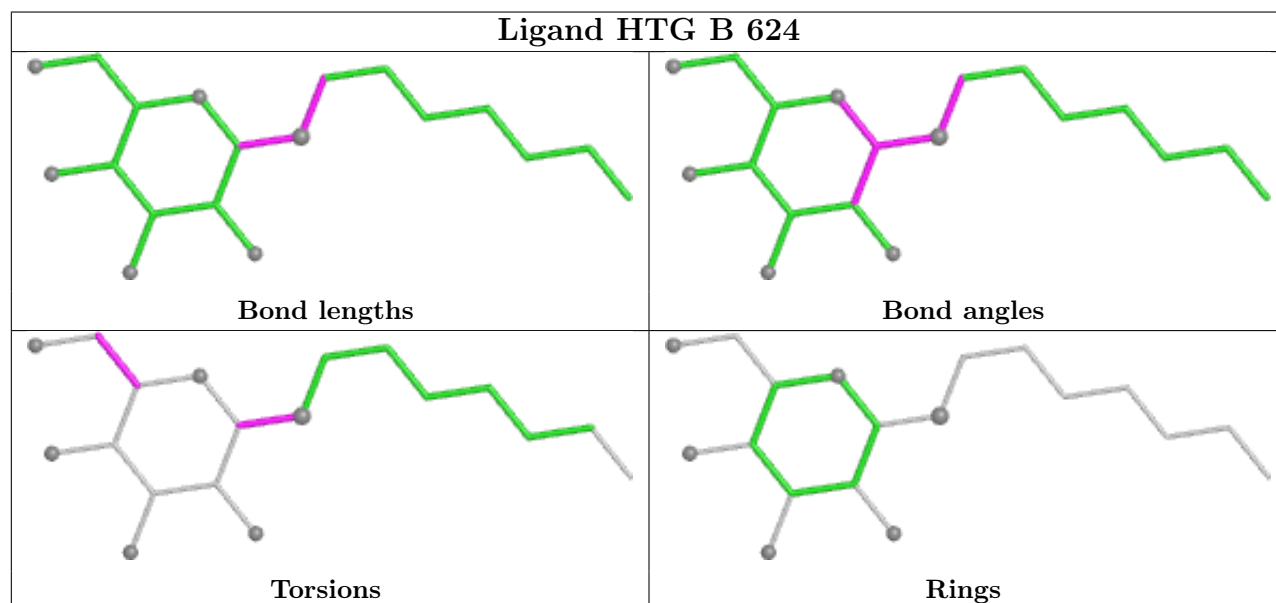
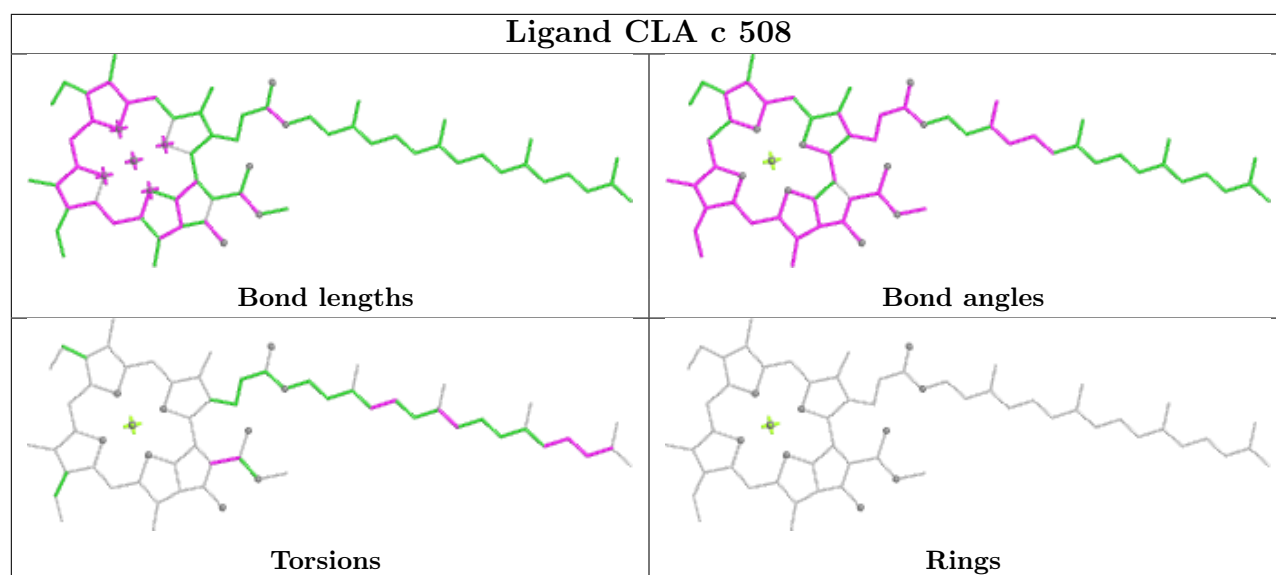


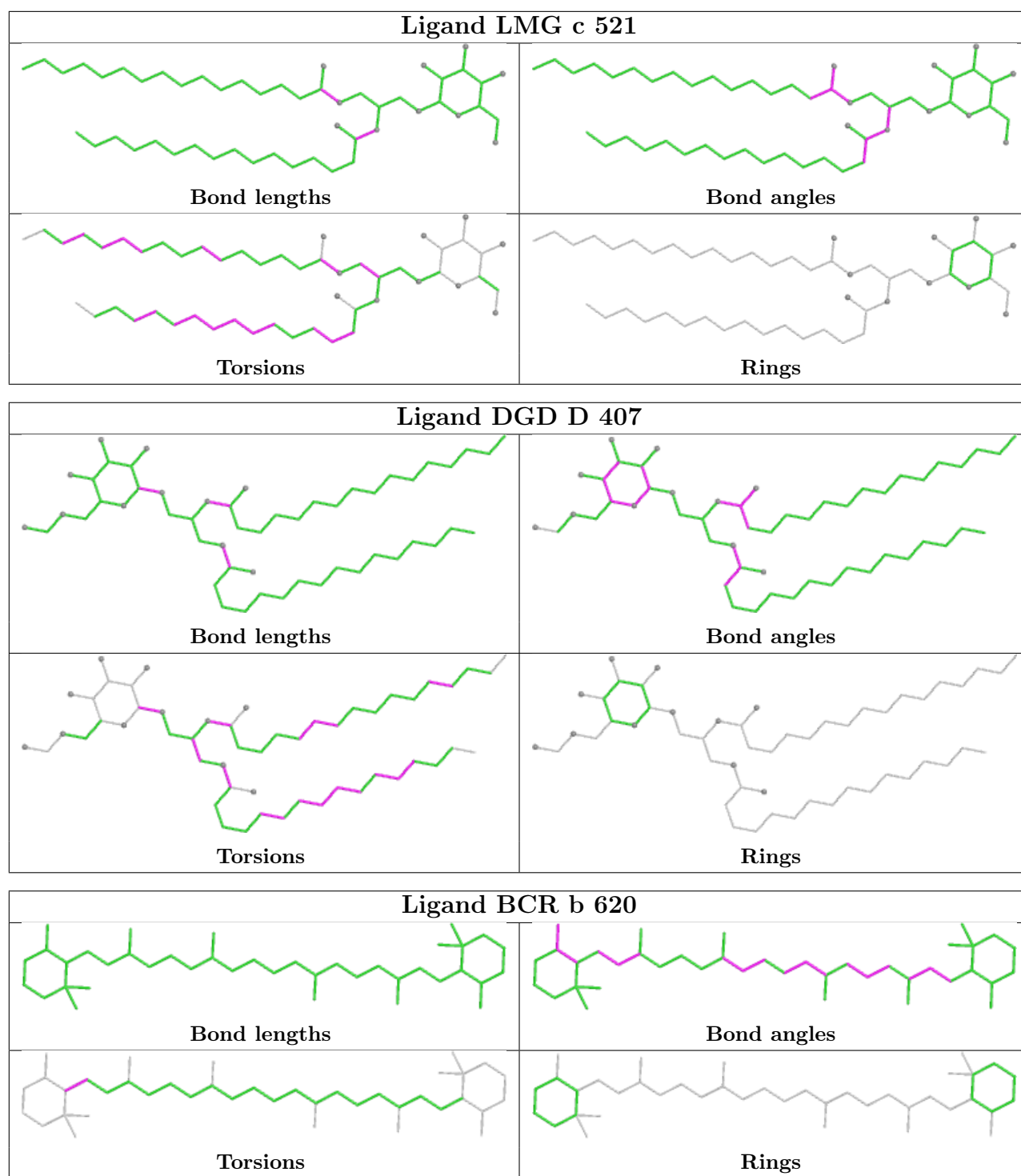


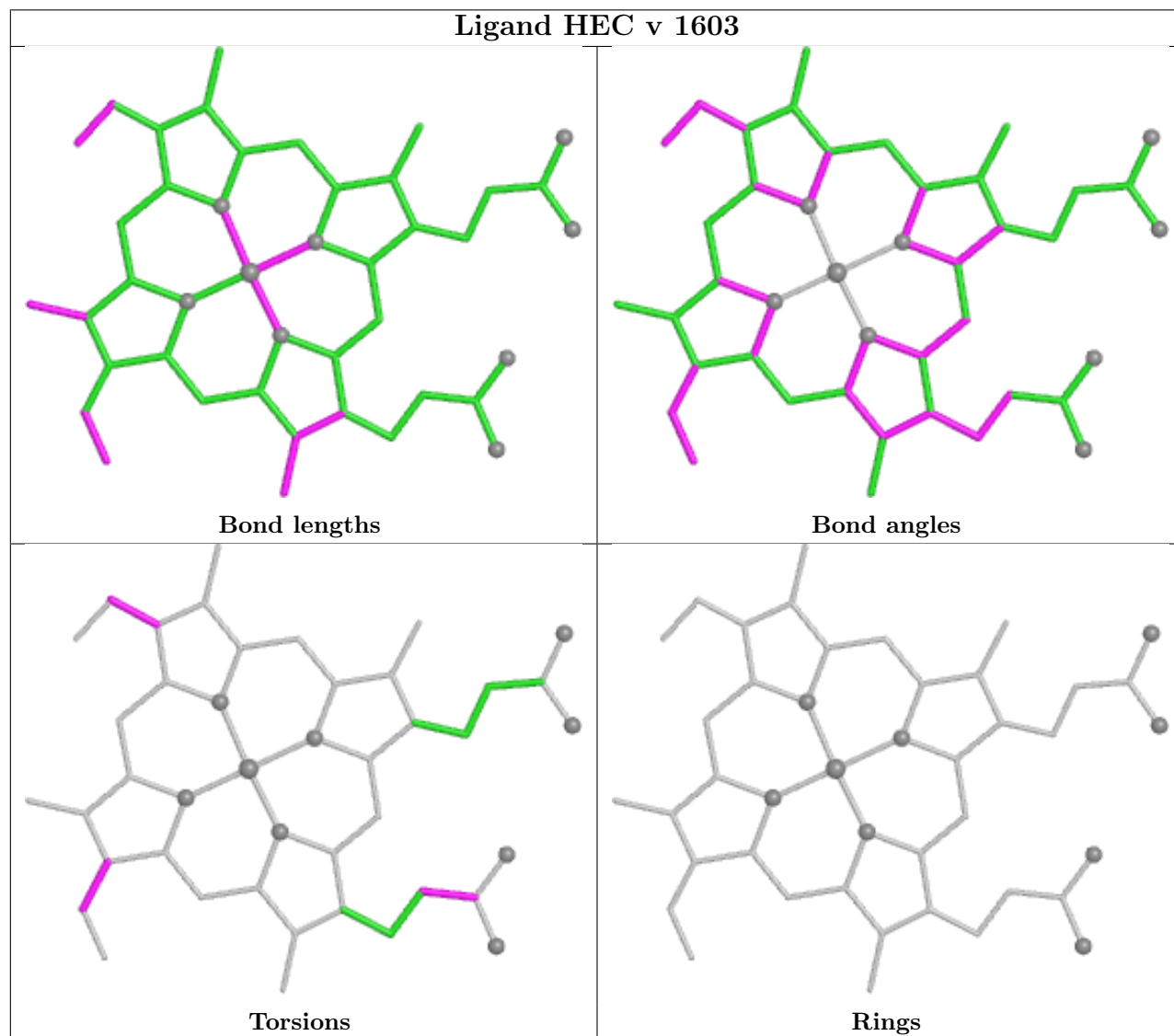
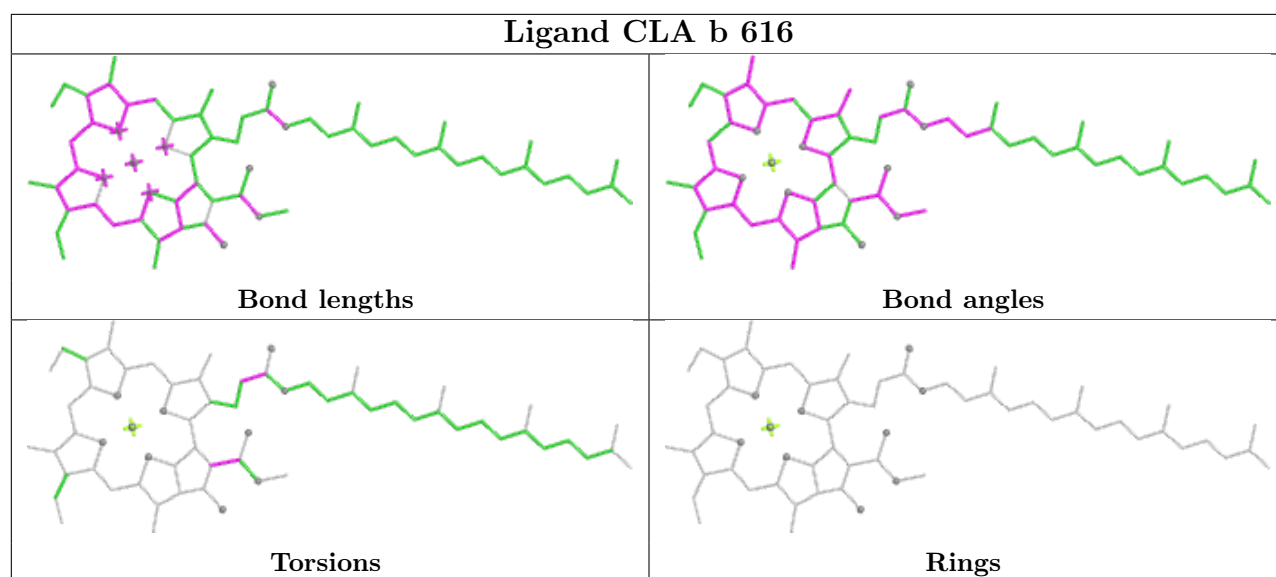


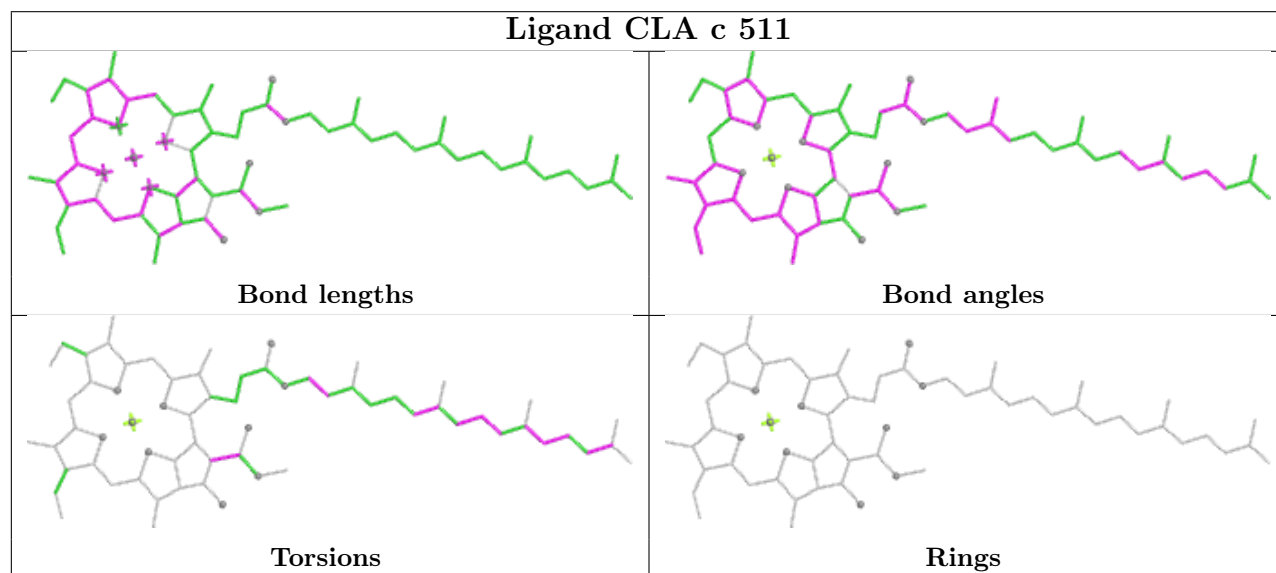
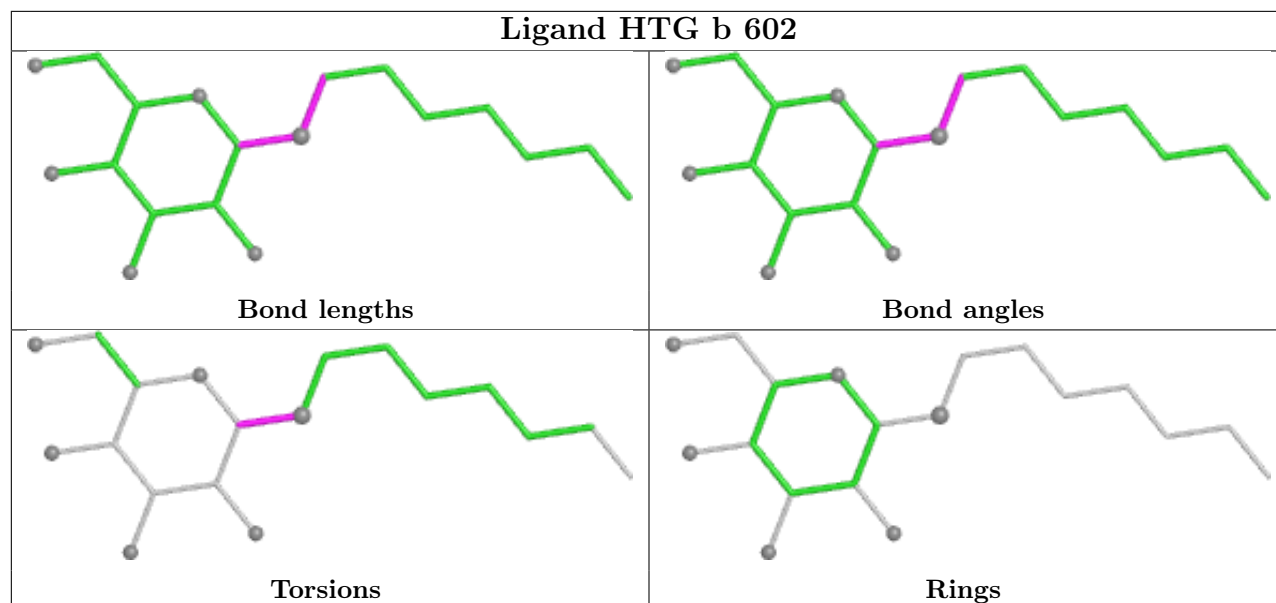


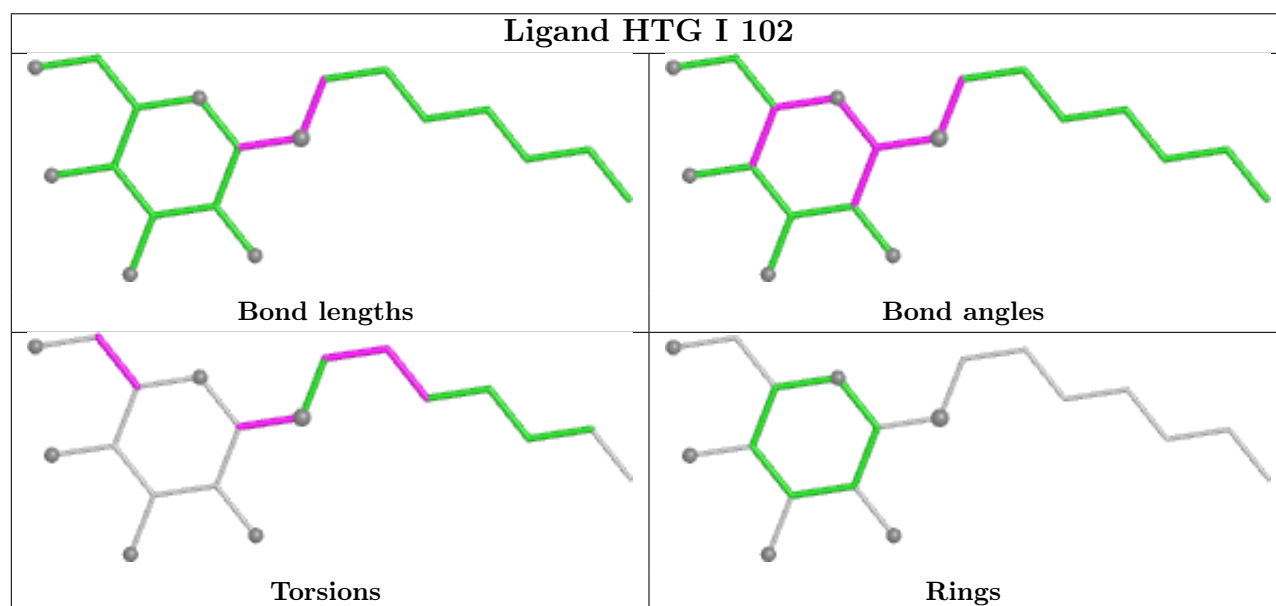
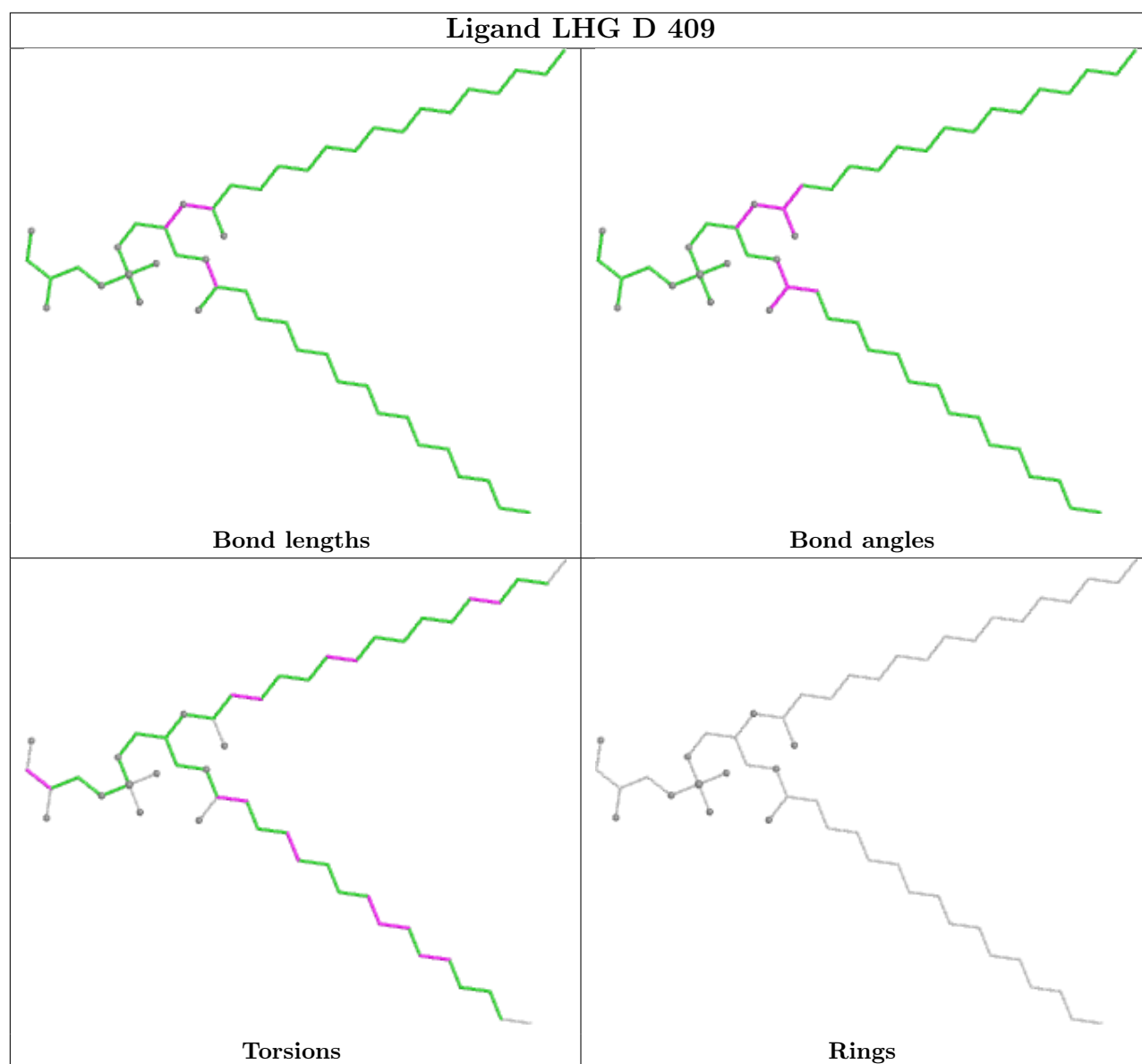


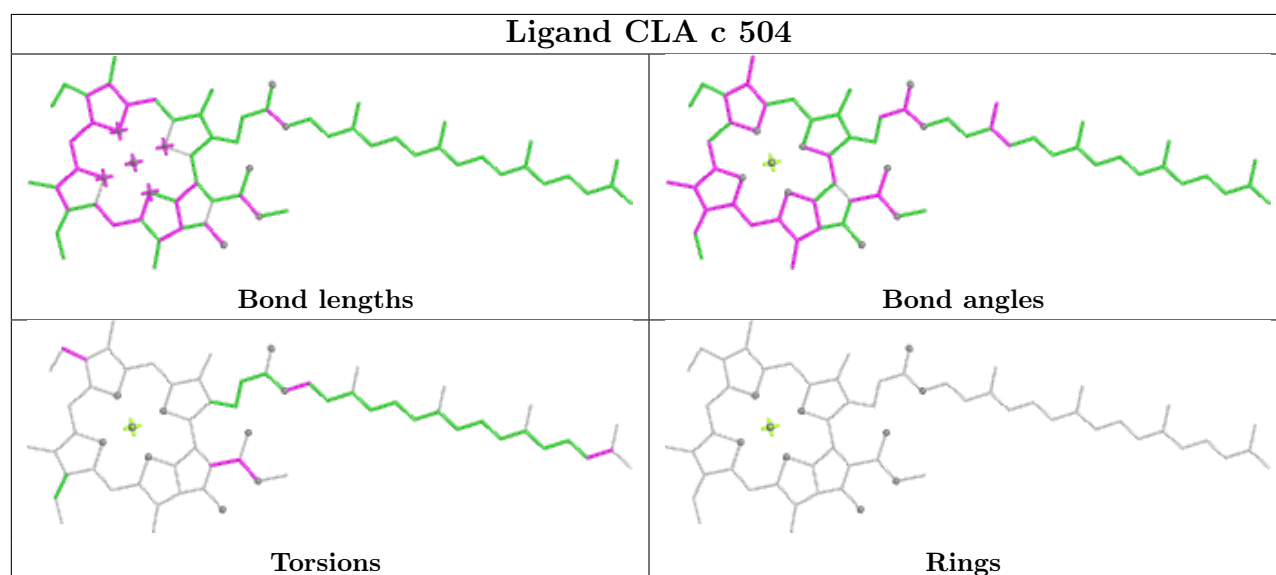
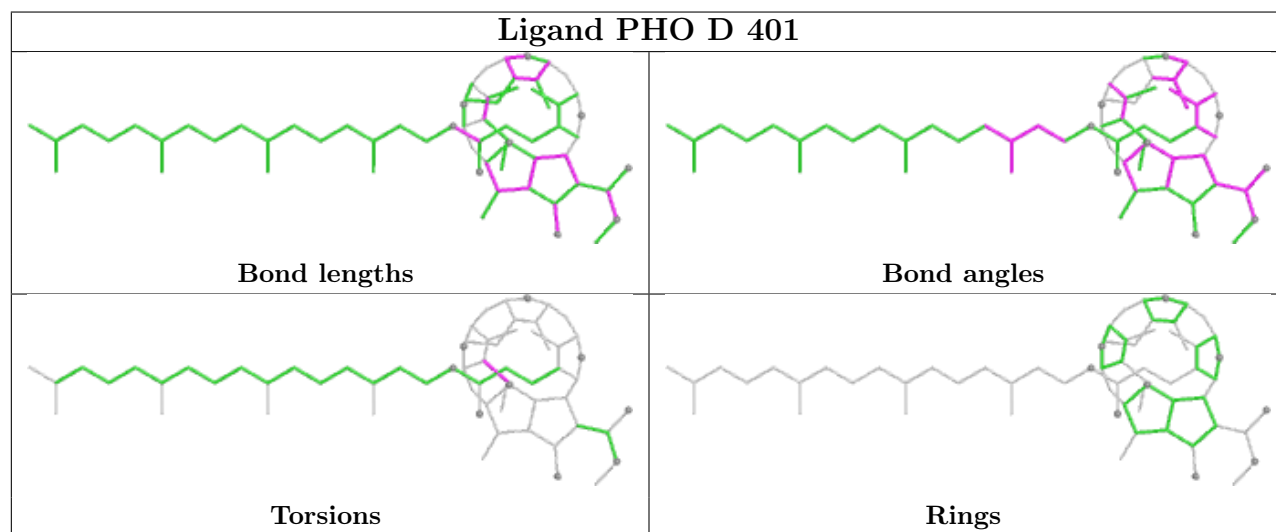
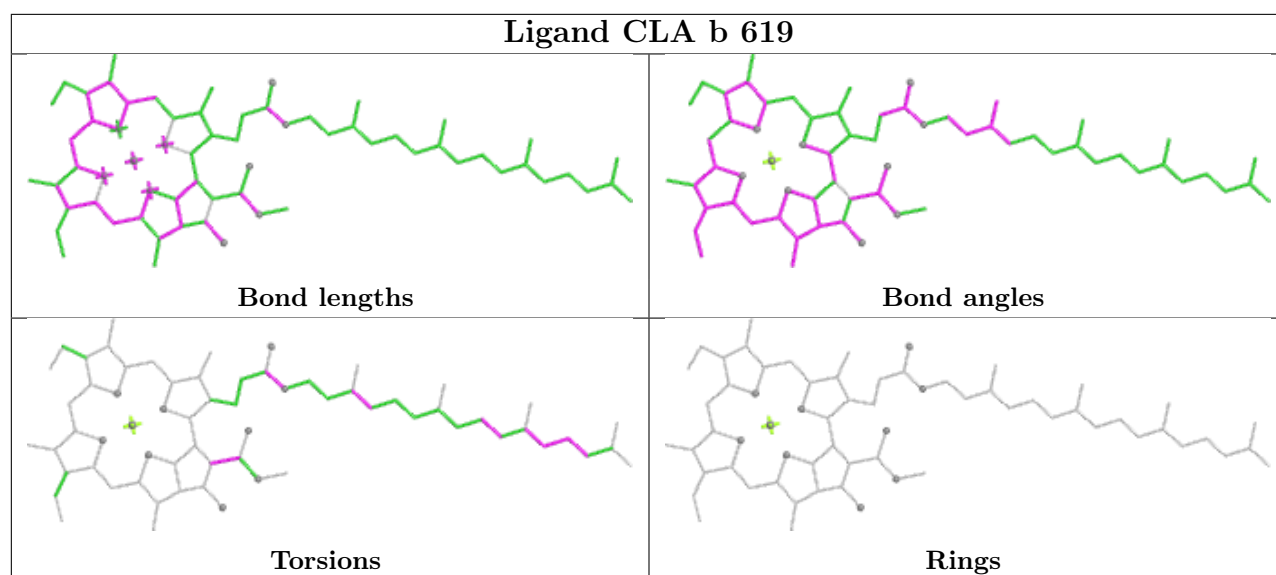


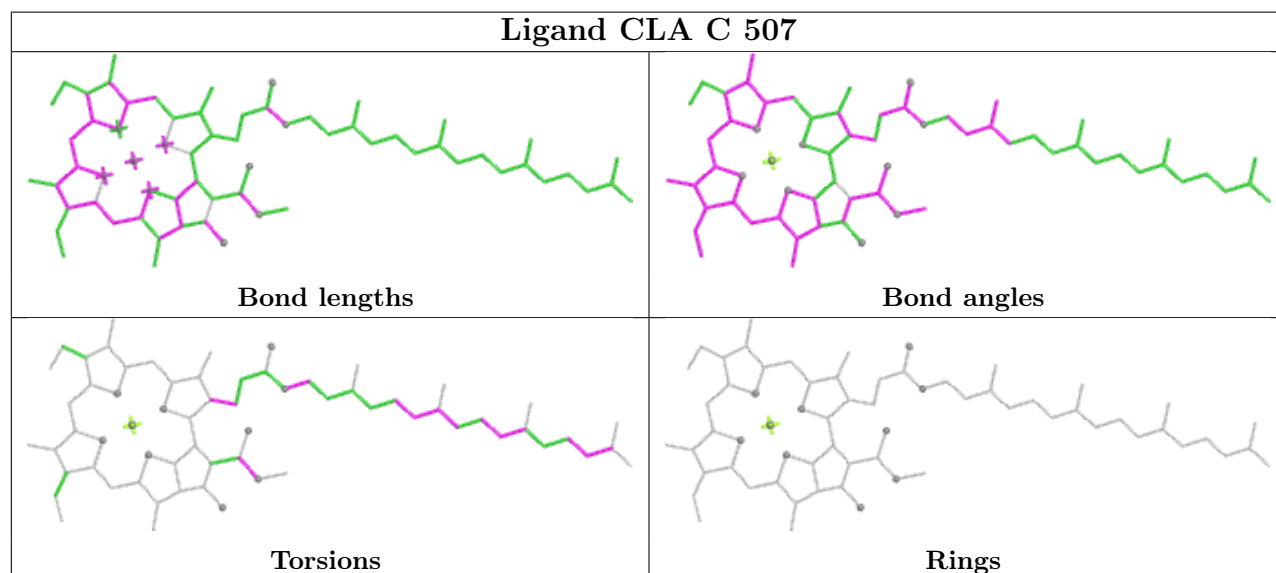
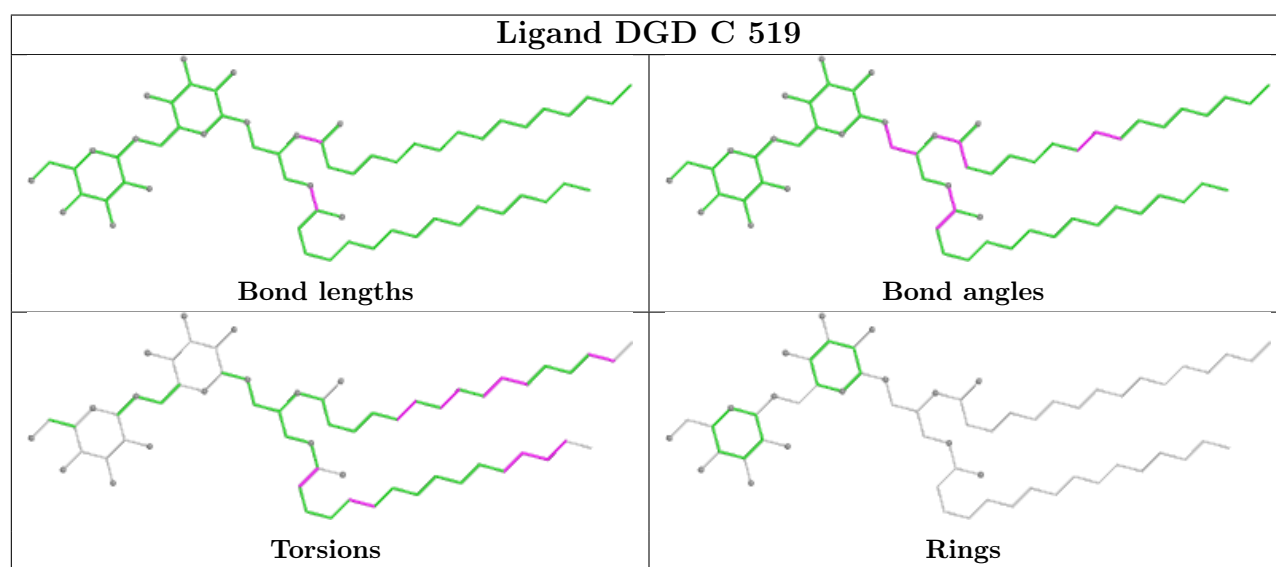
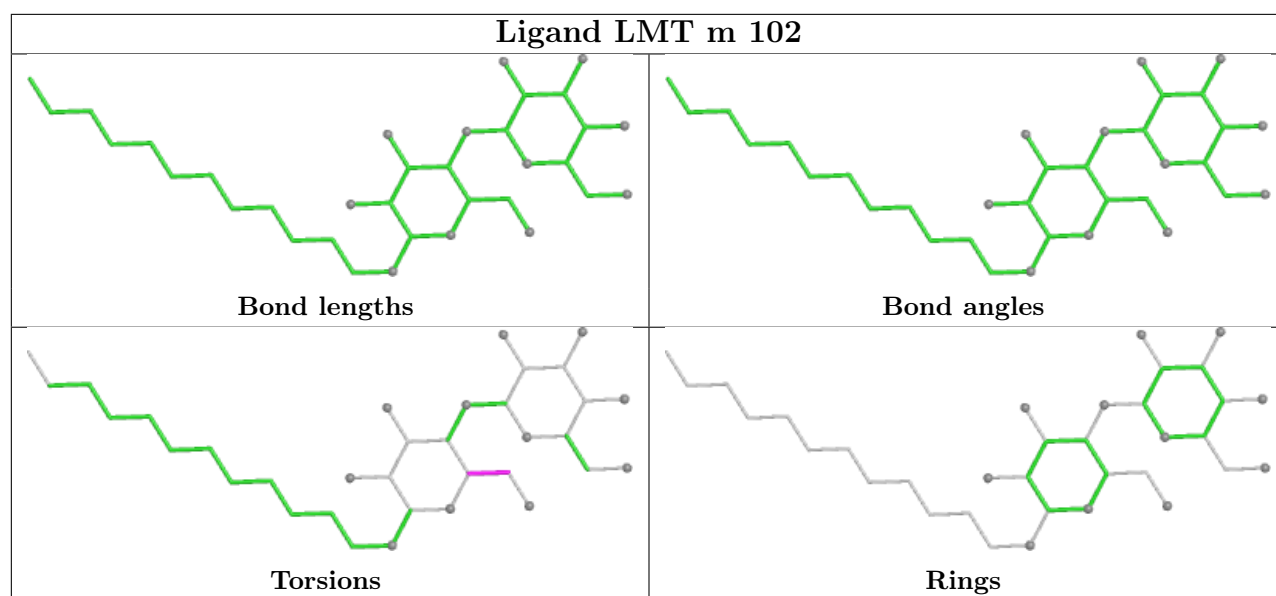


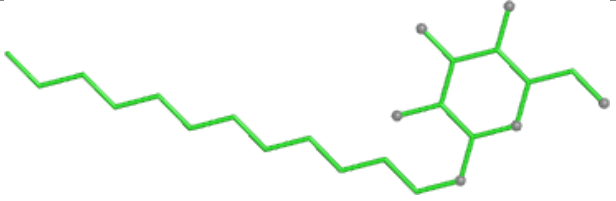
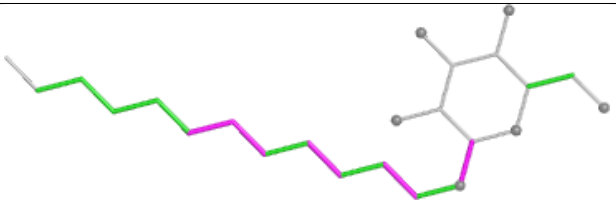
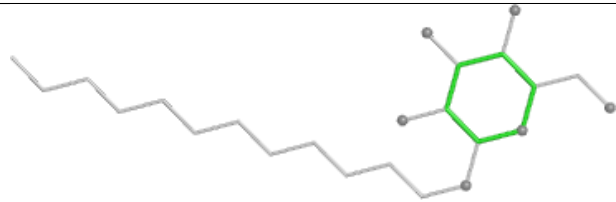
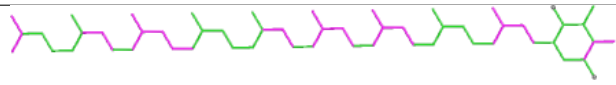
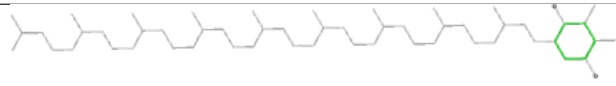
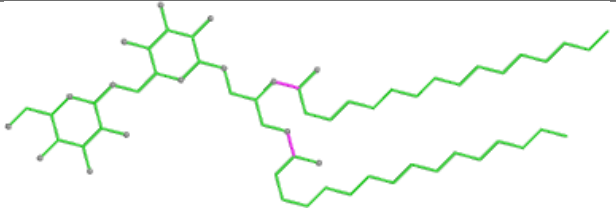
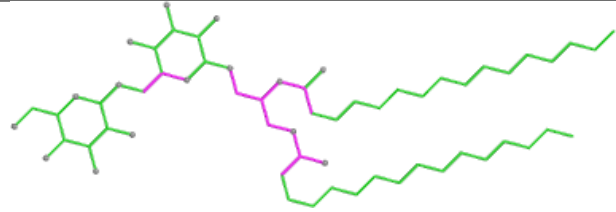
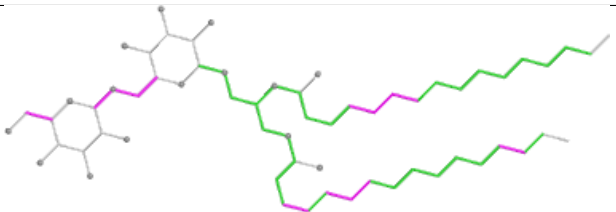
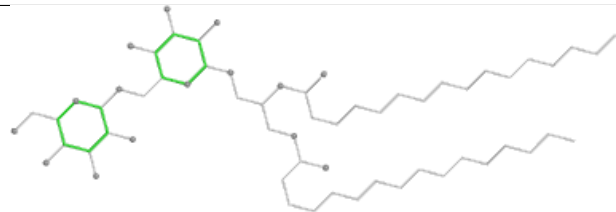


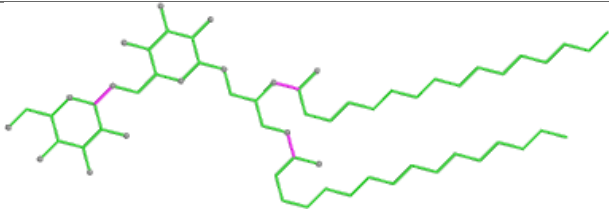
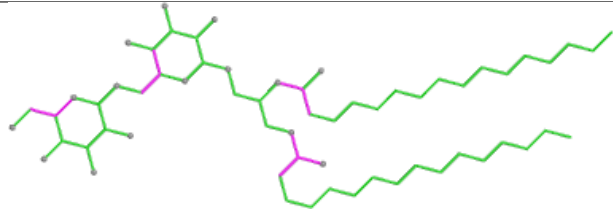
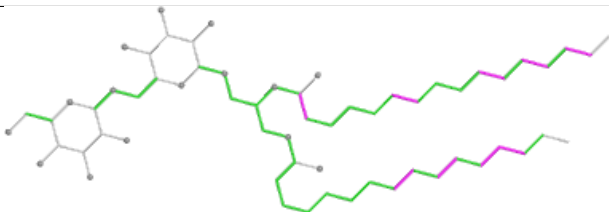
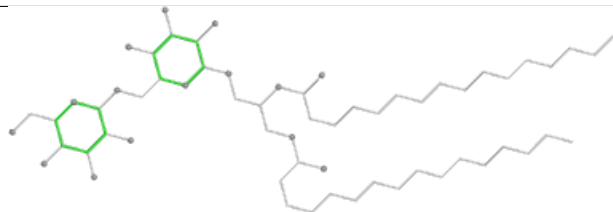


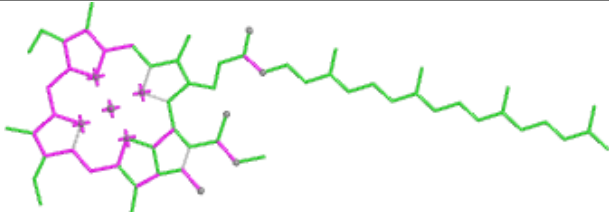
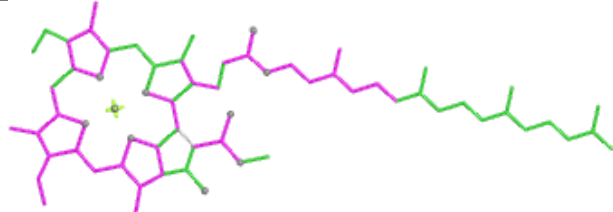
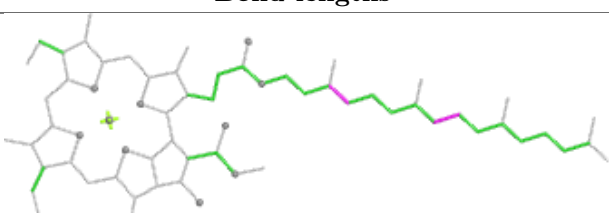
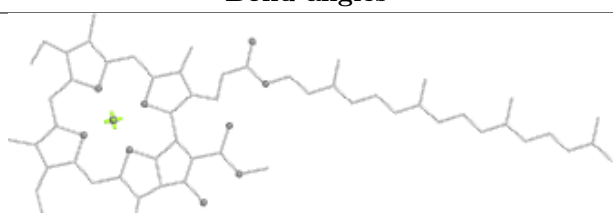


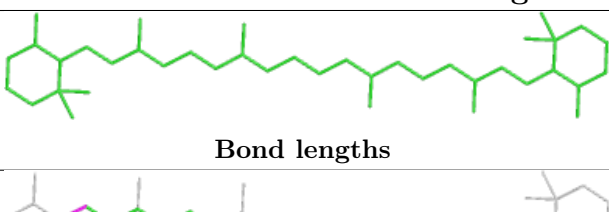
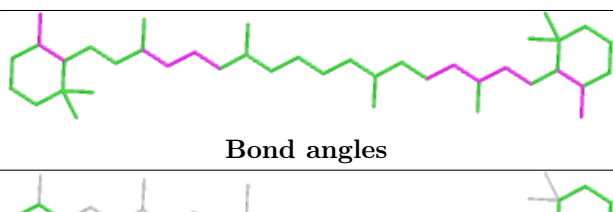


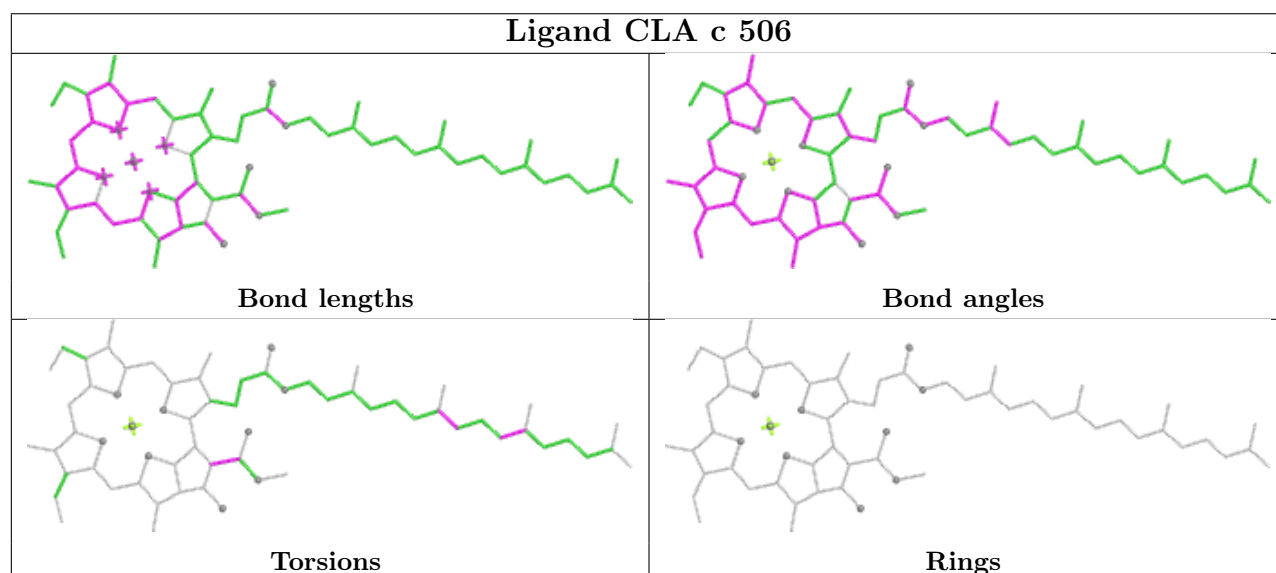
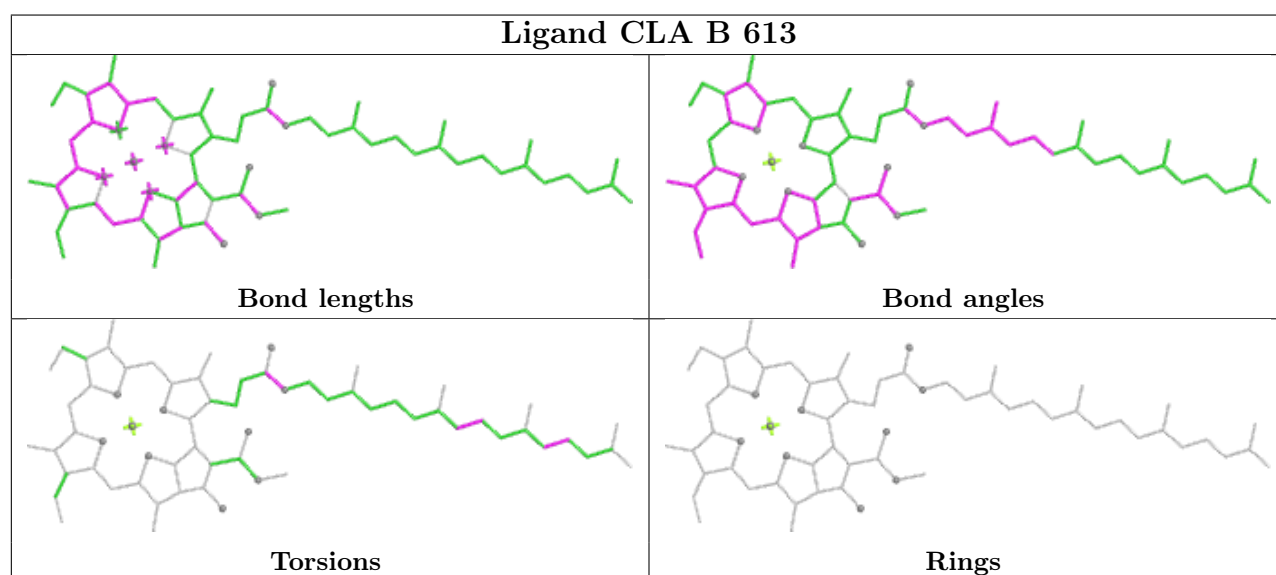
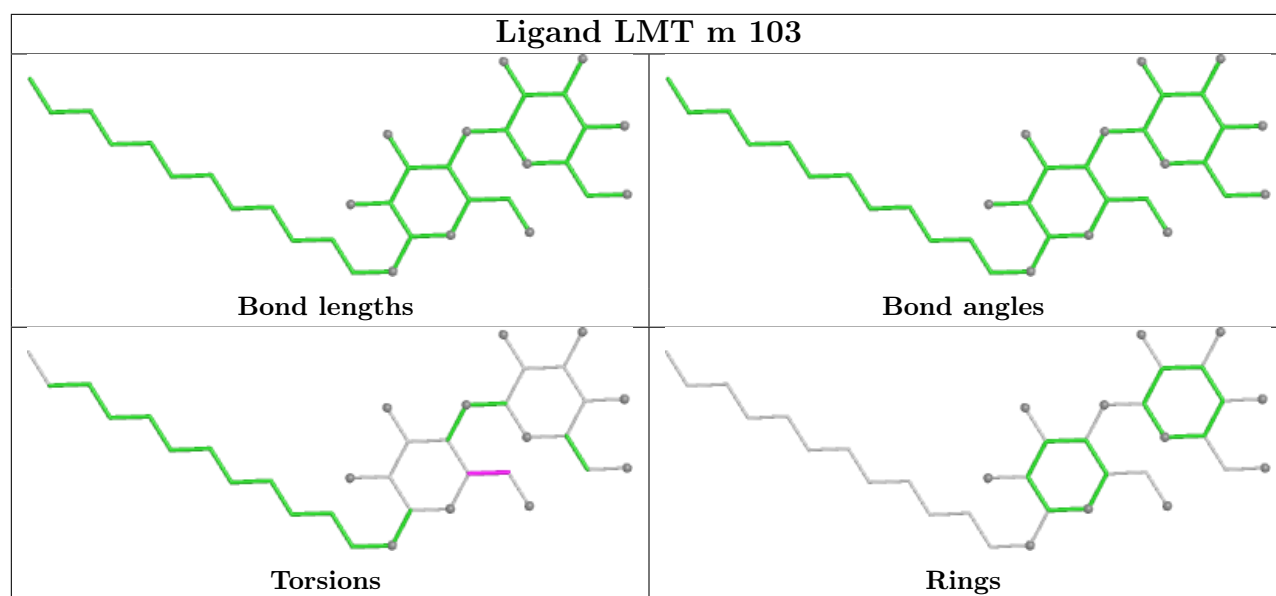


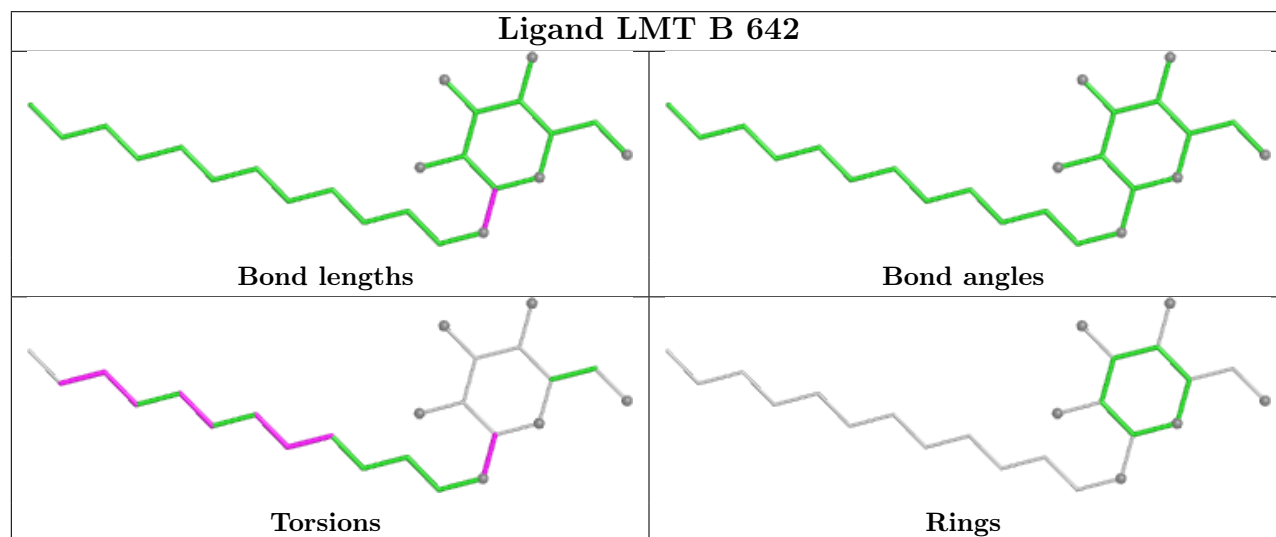
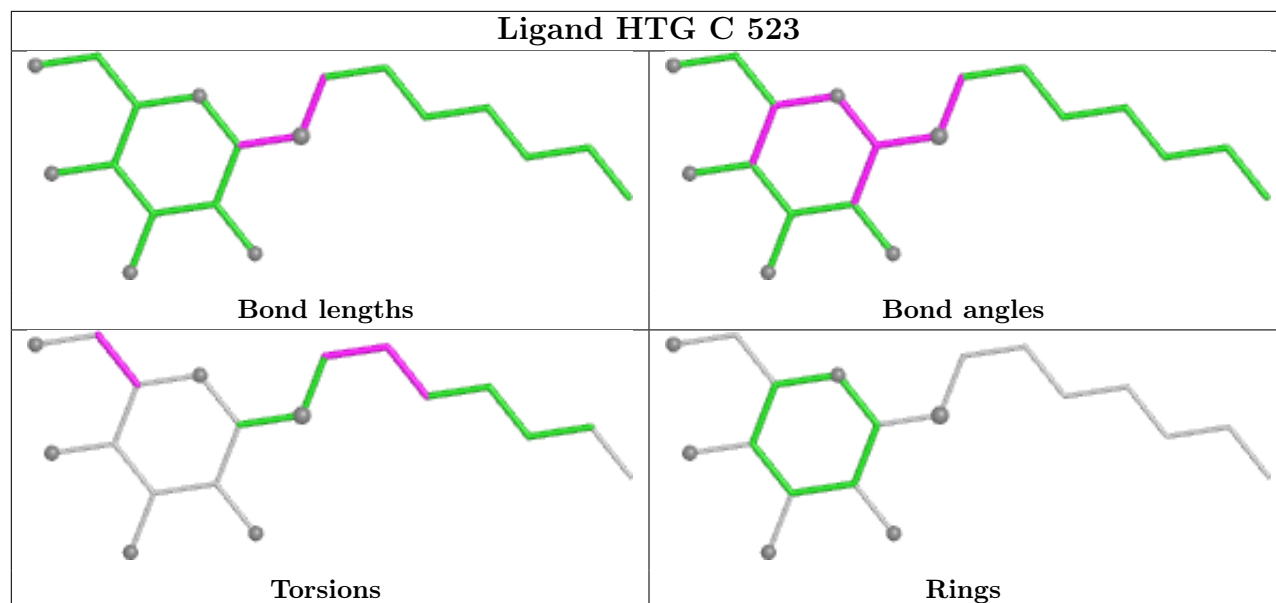
Ligand LMT E 104	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PL9 D 406	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand DGD C 517	
 Bond lengths	 Bond angles
 Torsions	 Rings

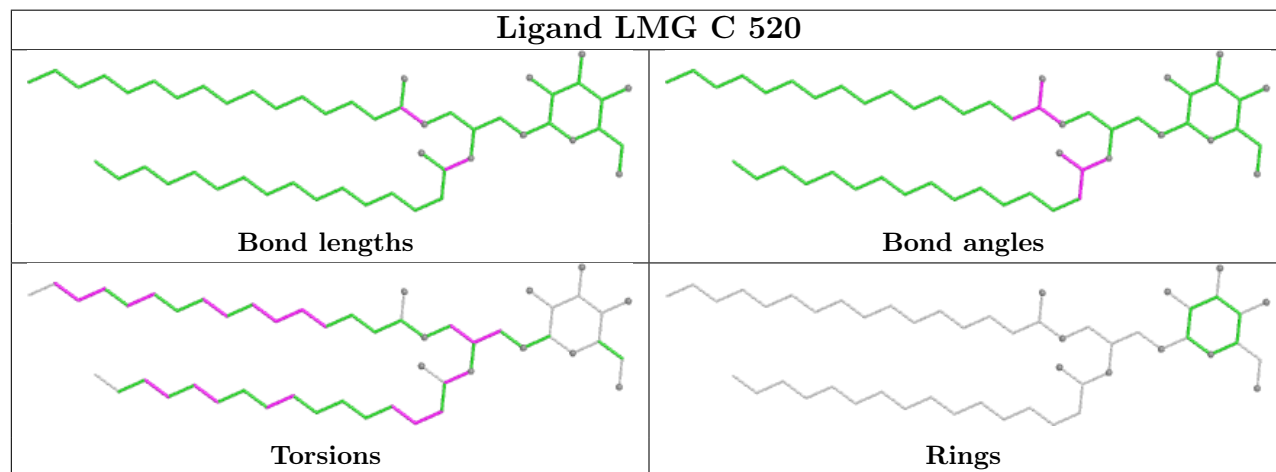
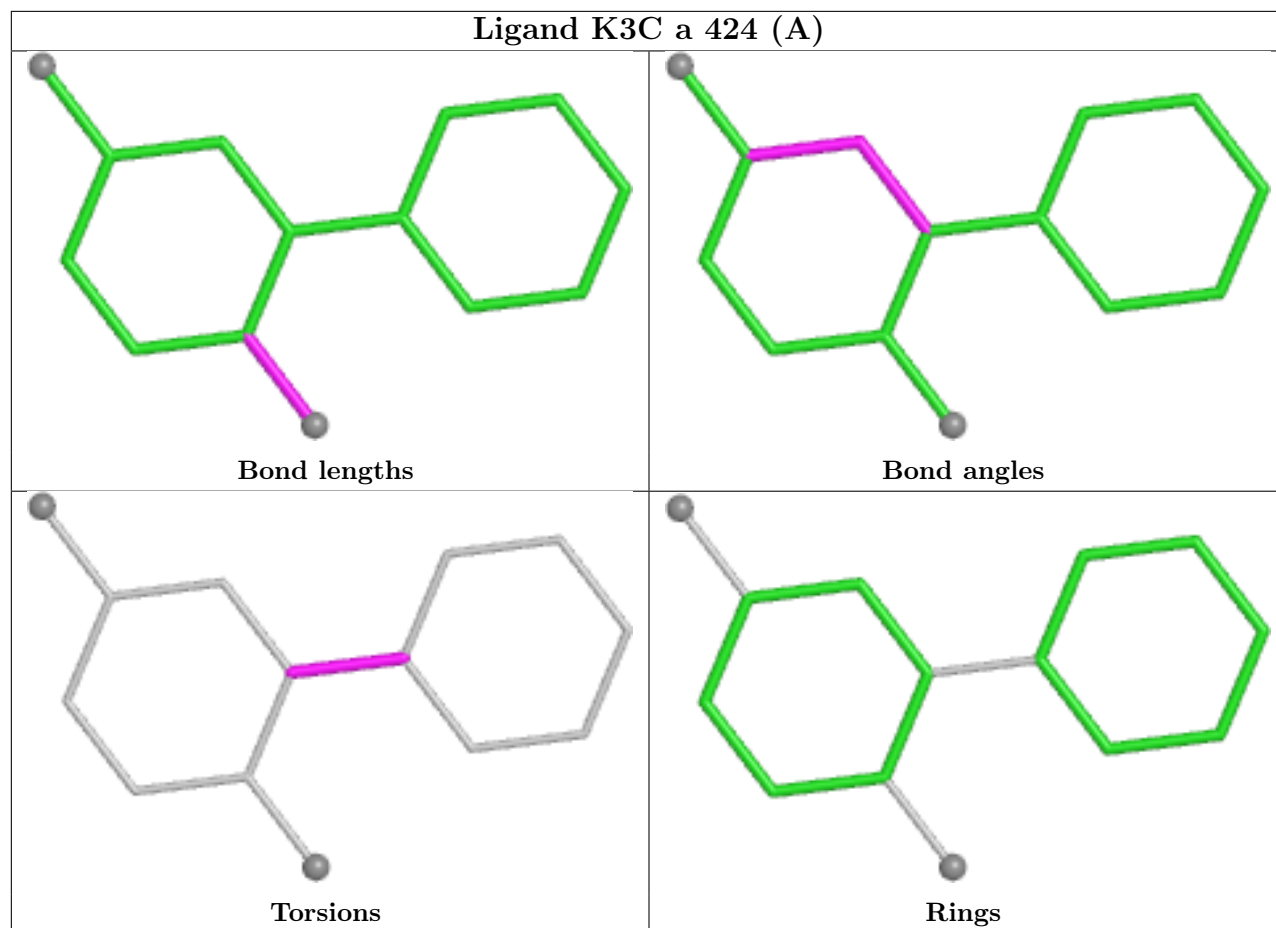
Ligand DGD H 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

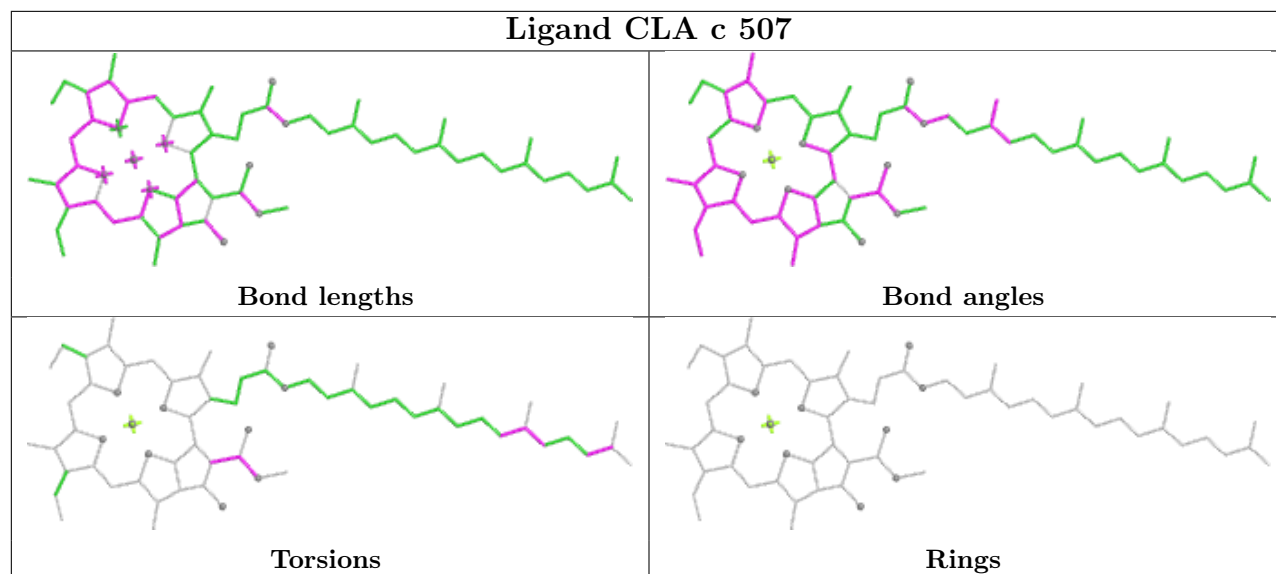
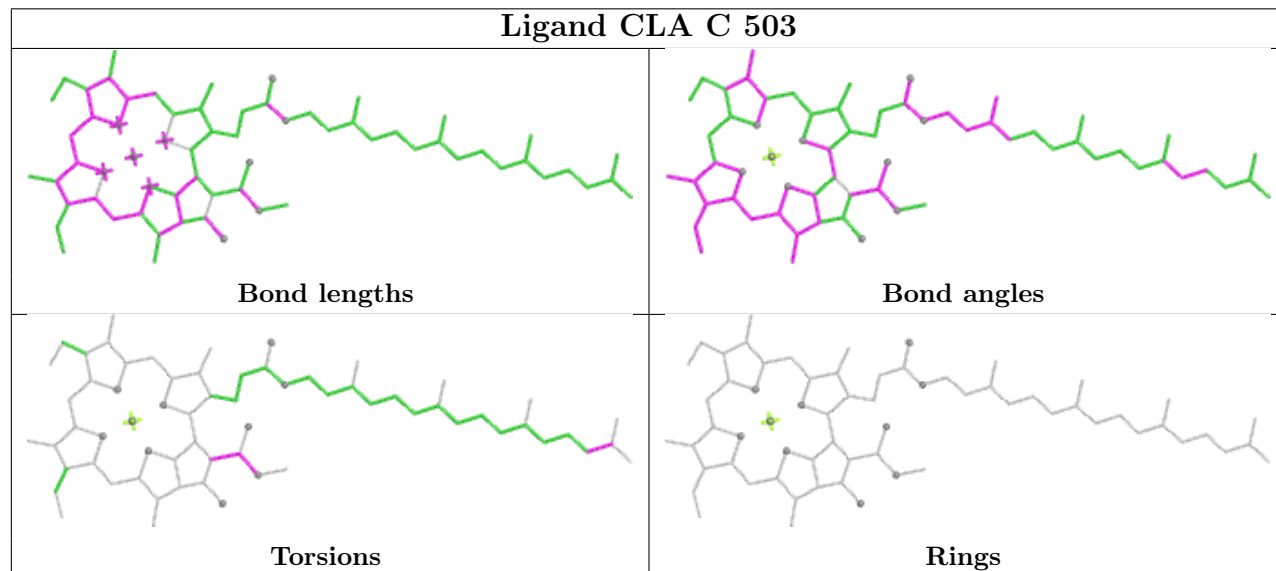
Ligand CLA B 612	
	
Bond lengths	Bond angles
	
Torsions	Rings

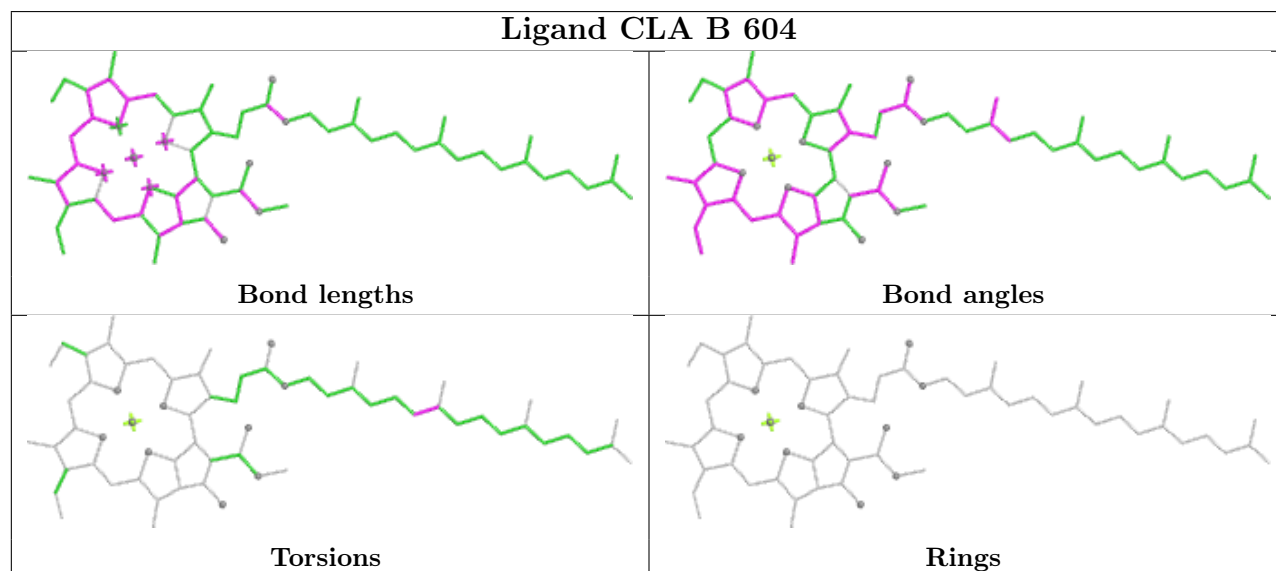
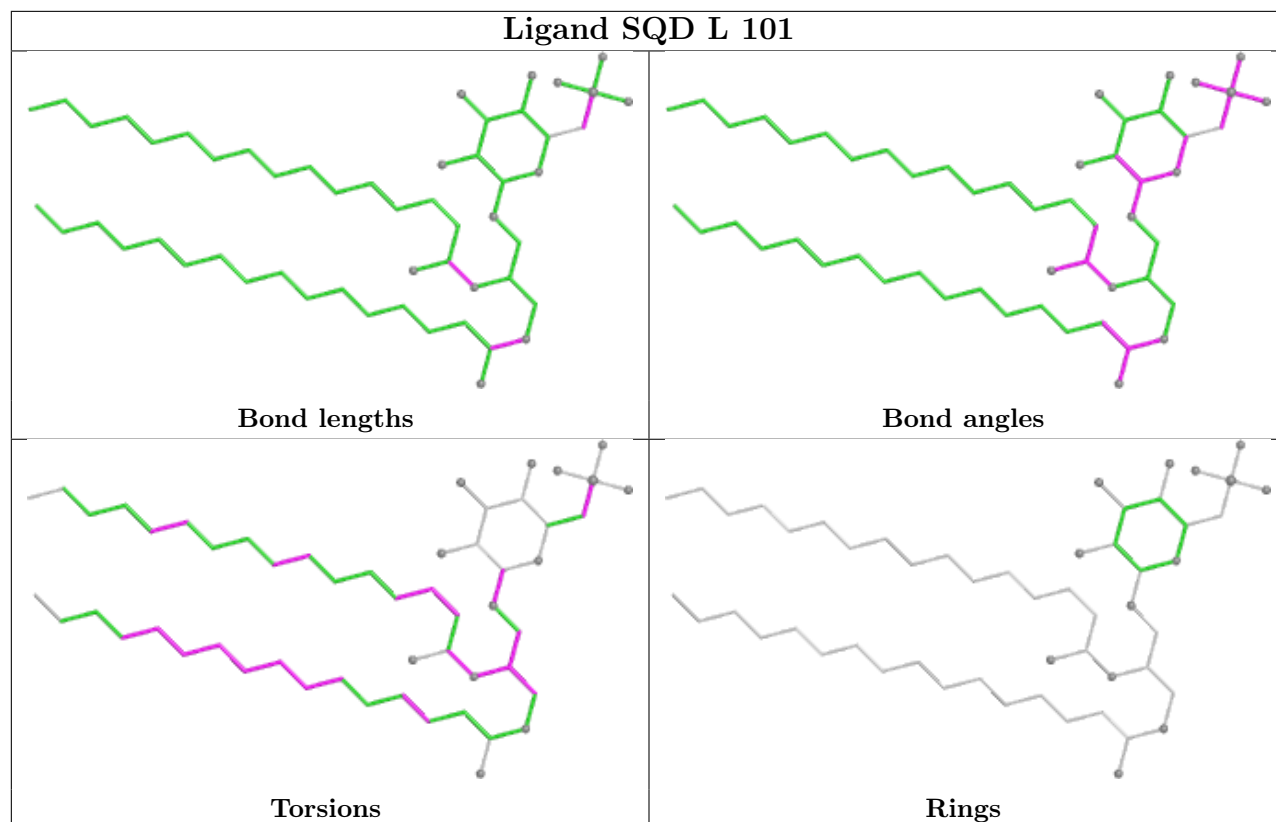
Ligand BCR k 303	
	
Bond lengths	Bond angles
	
Torsions	Rings

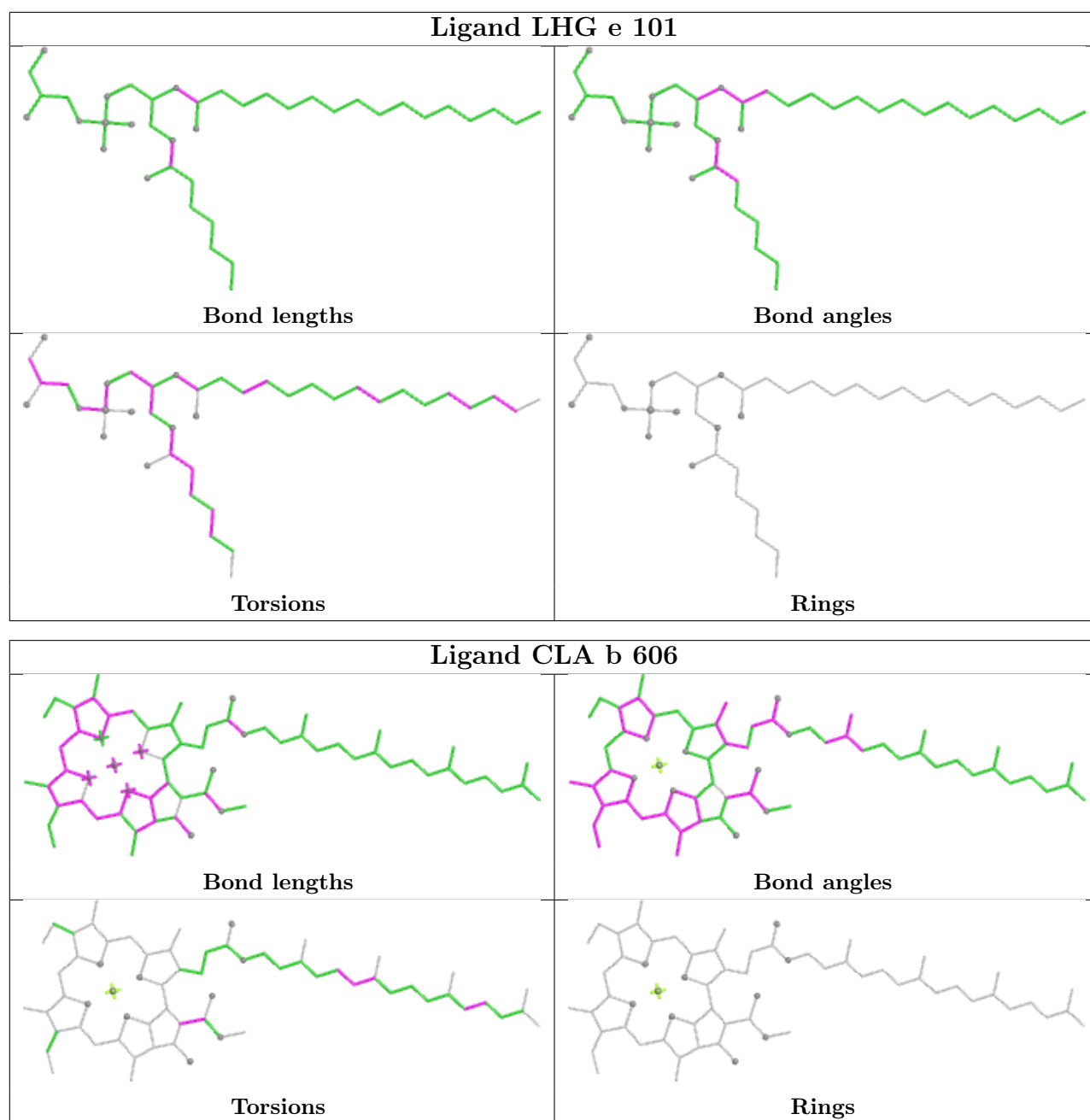


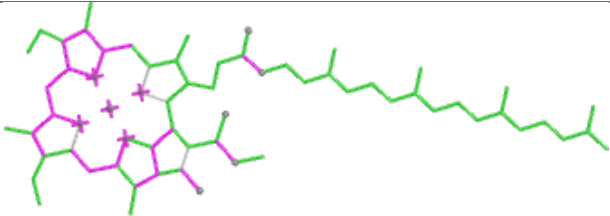
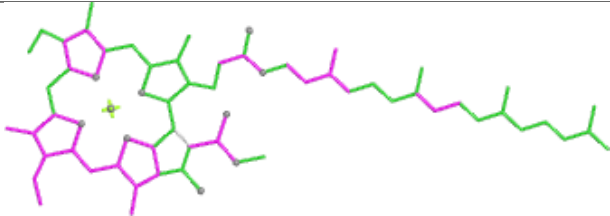
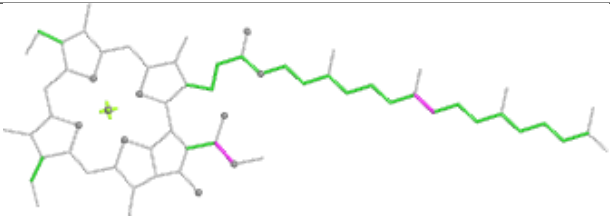
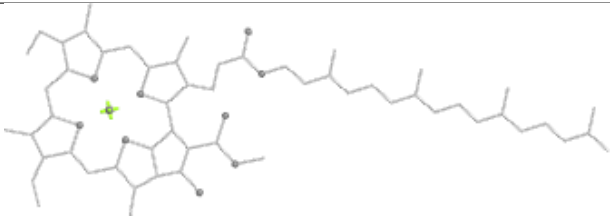
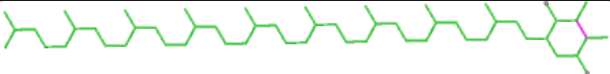
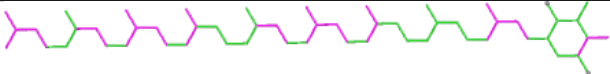
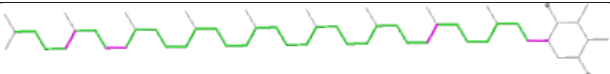
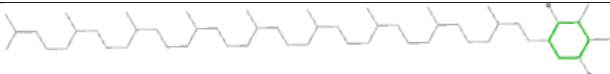


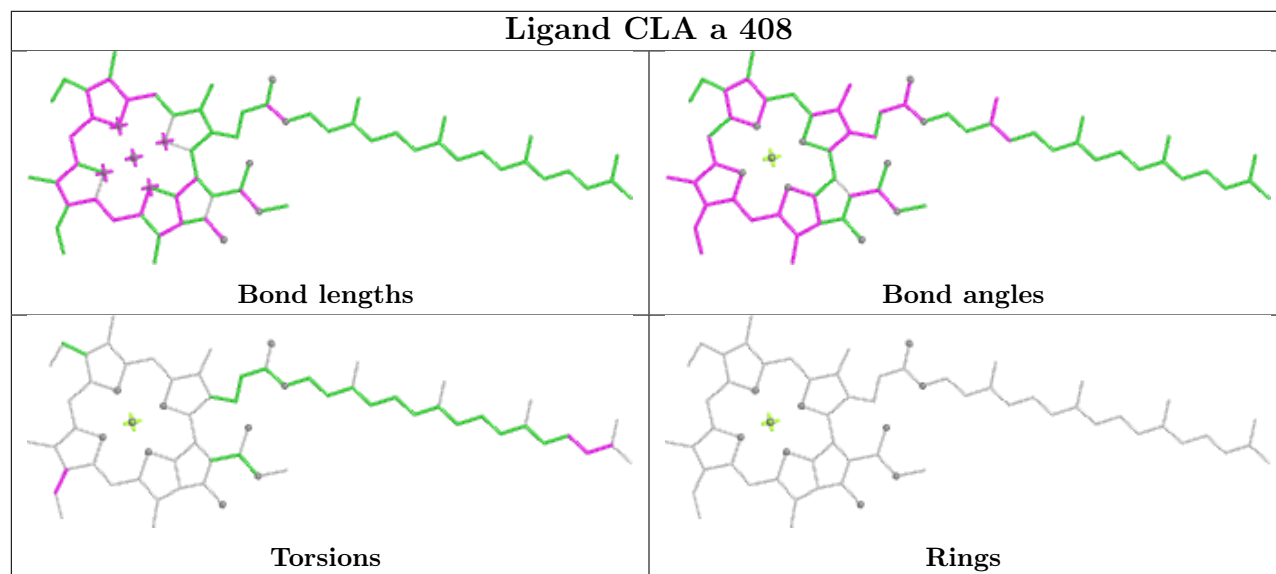
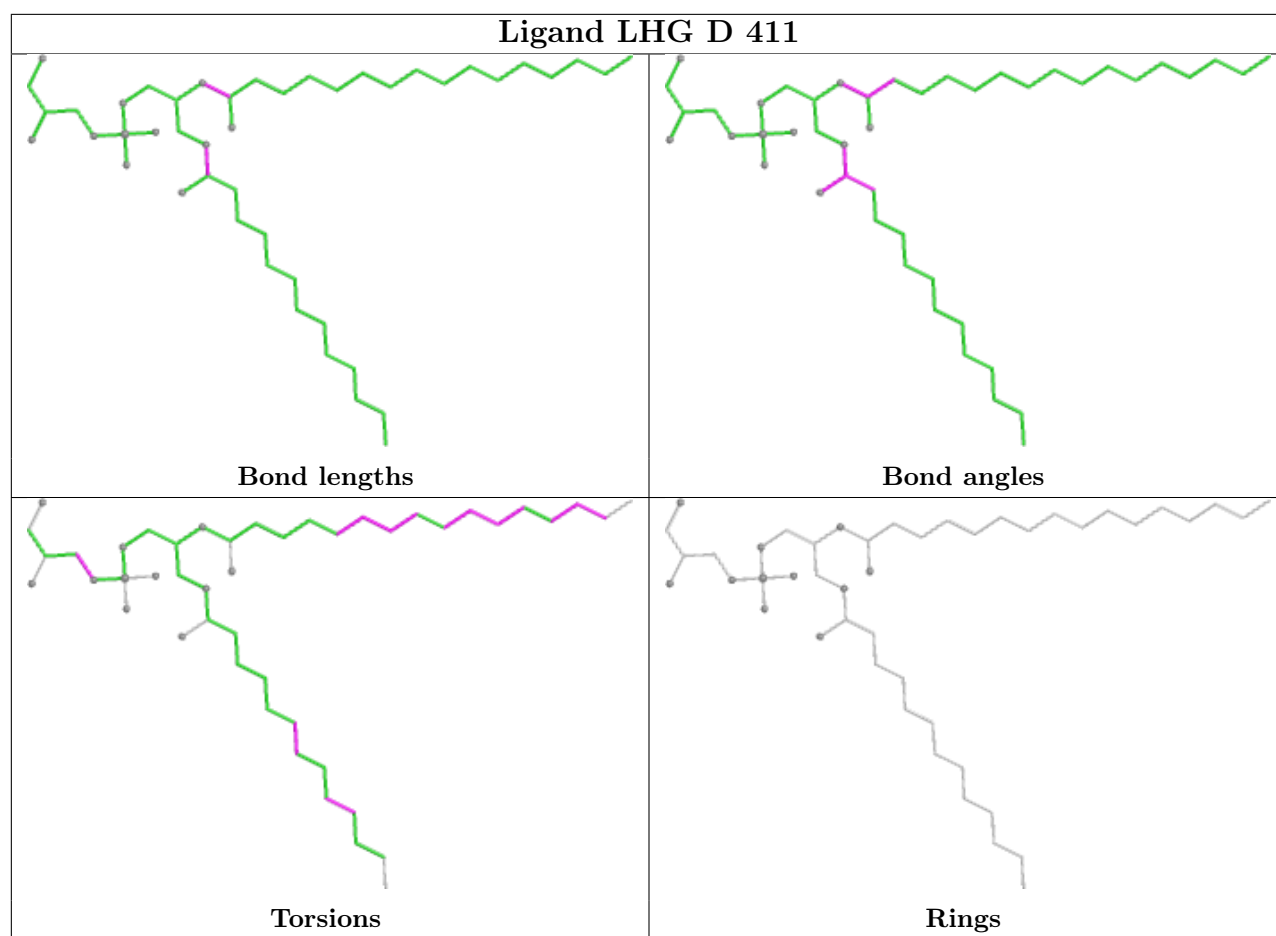


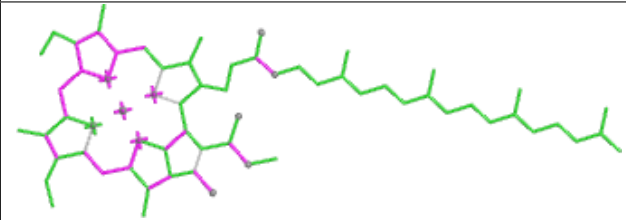
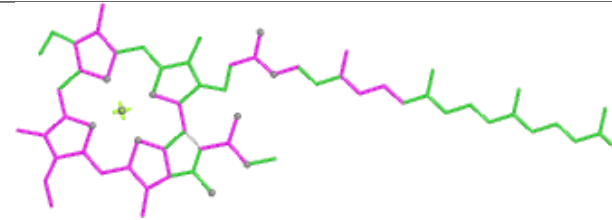
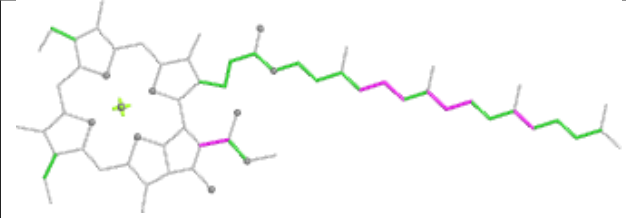
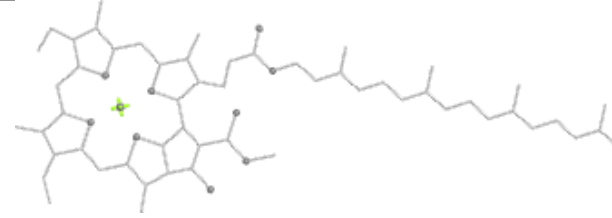
Ligand CLA c 507**Ligand CLA C 503**

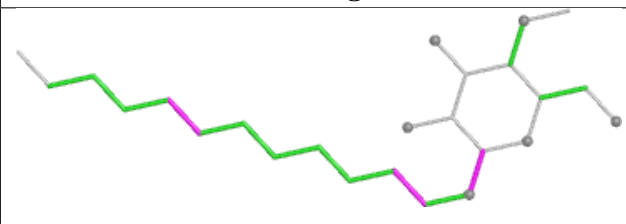
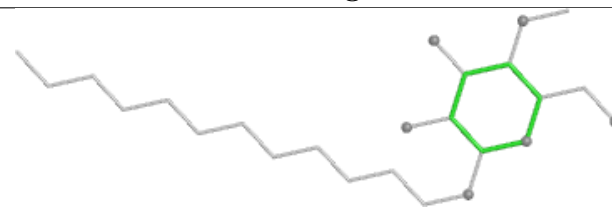


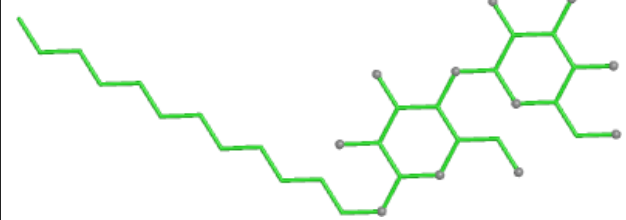
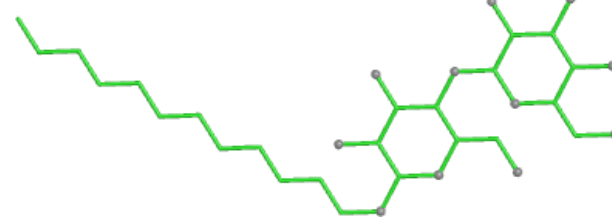
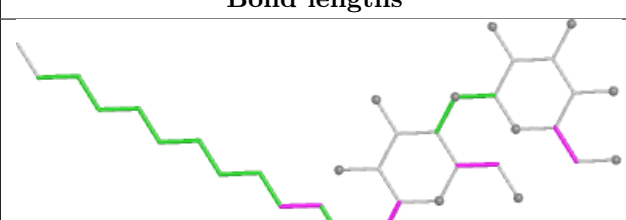
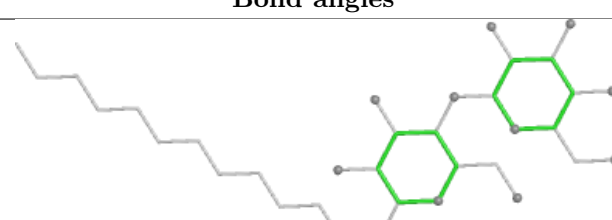


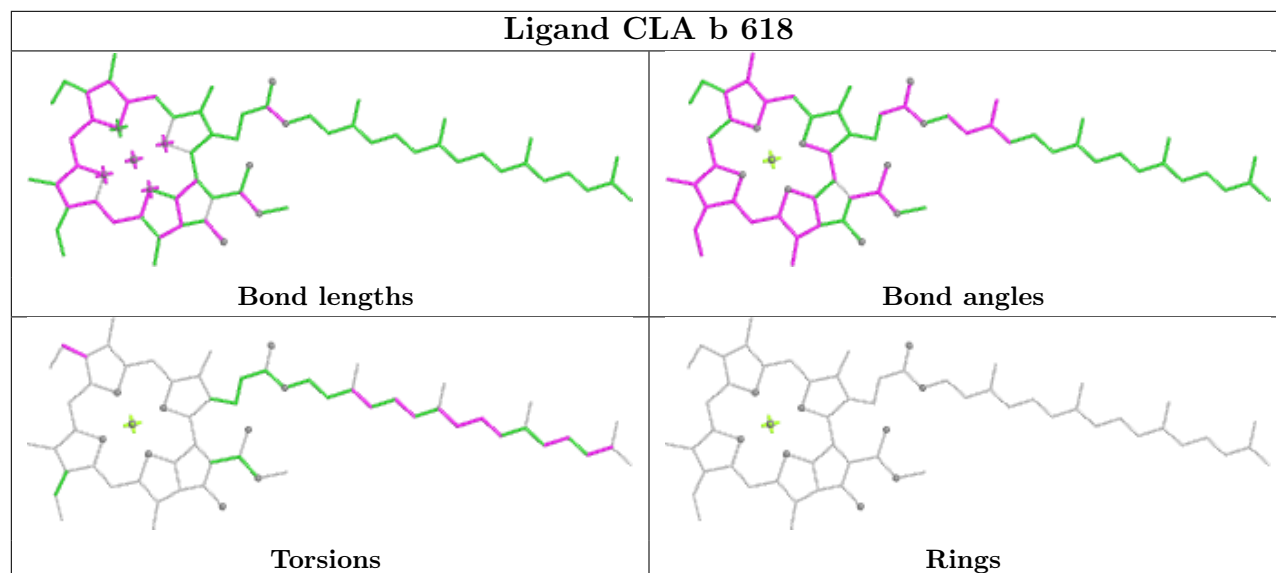
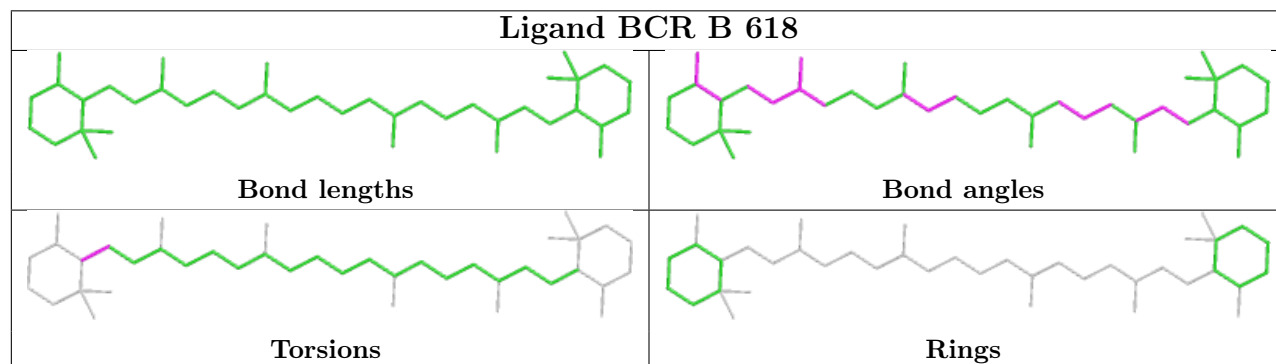
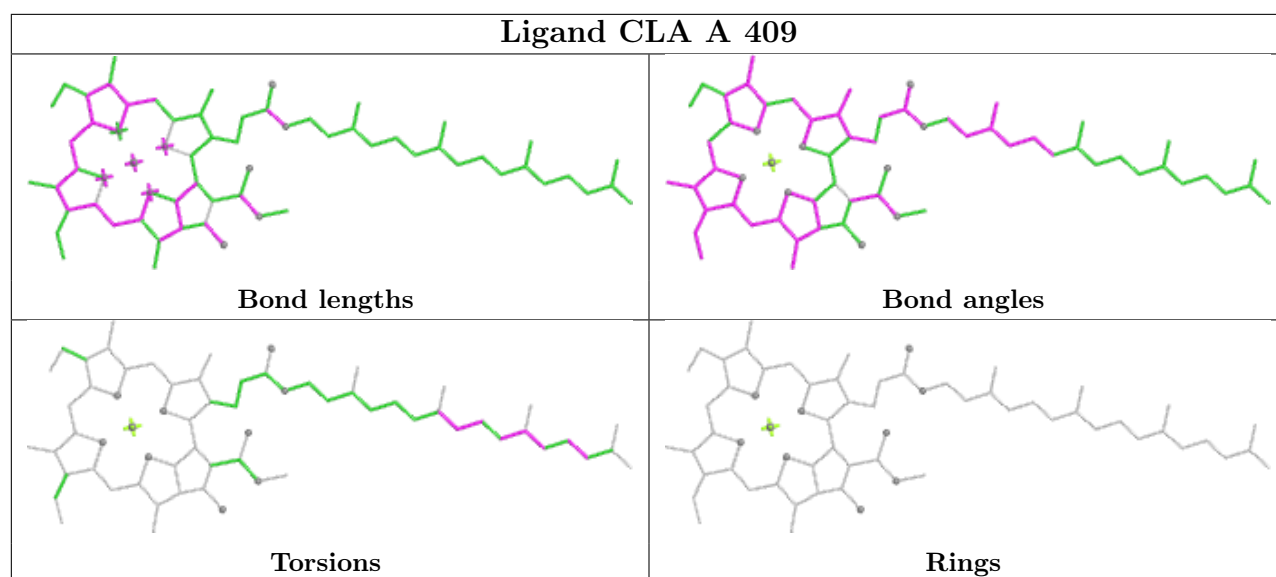
Ligand CLA C 514	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PL9 d 407	
 Bond lengths	 Bond angles
 Torsions	 Rings



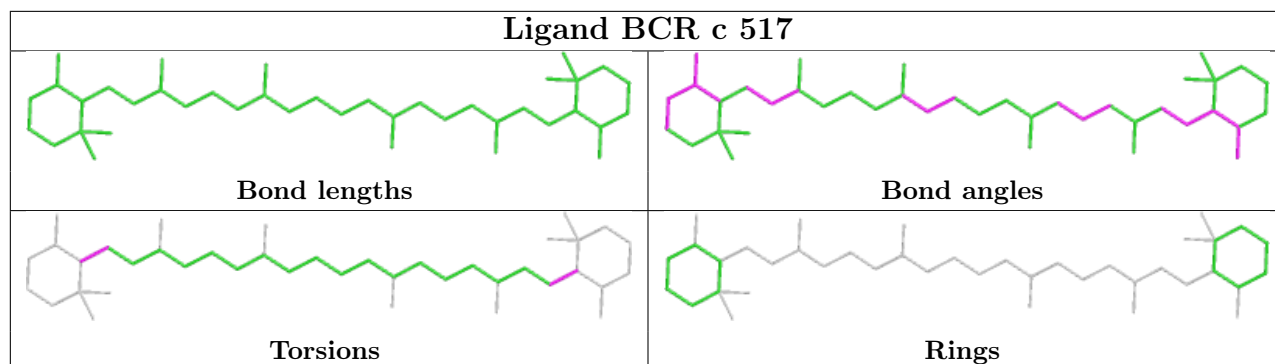
Ligand CLA B 615	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LMT b 624	
	
Bond lengths	Bond angles
	
Torsions	Rings

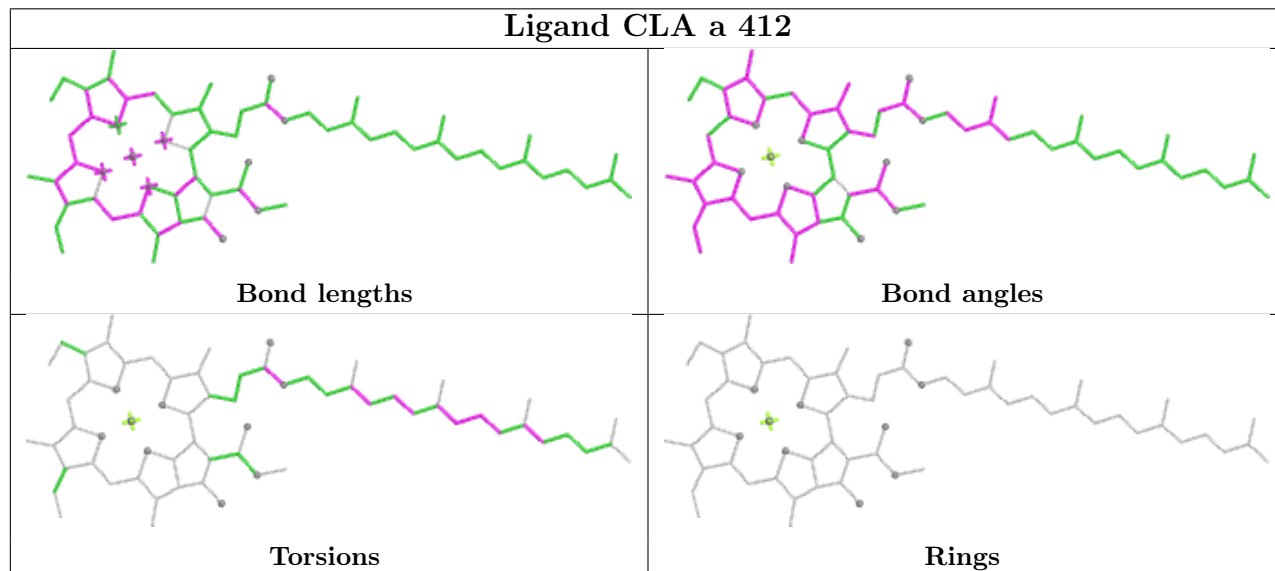
Ligand LMT f 104	
	
Bond lengths	Bond angles
	
Torsions	Rings



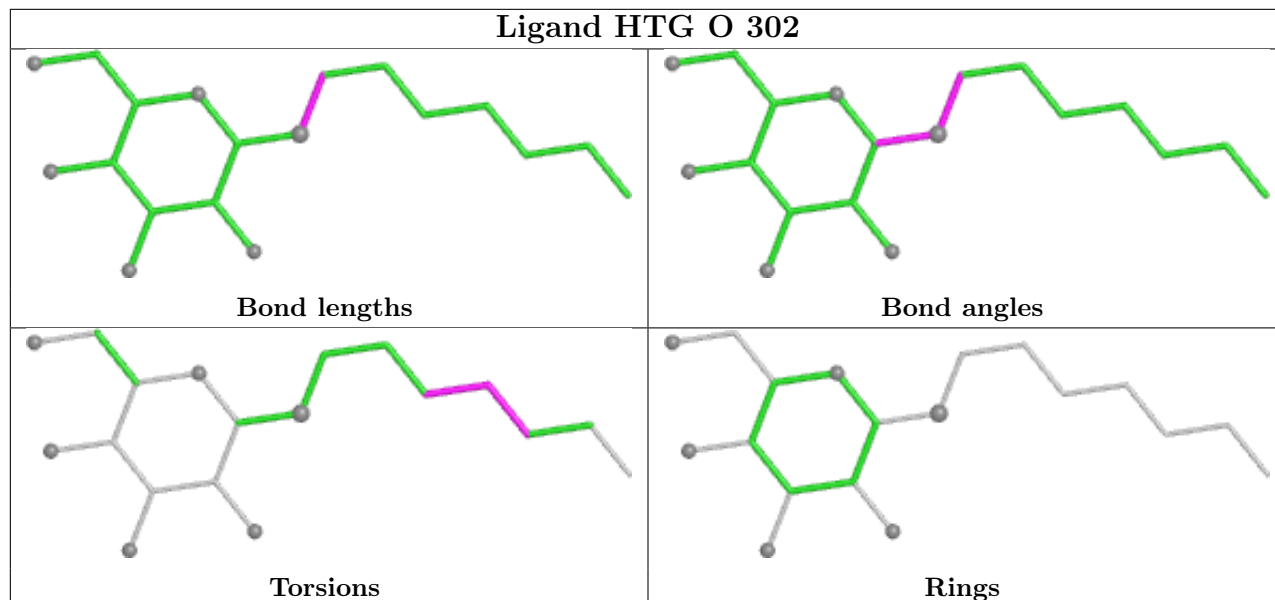
Ligand BCR c 517

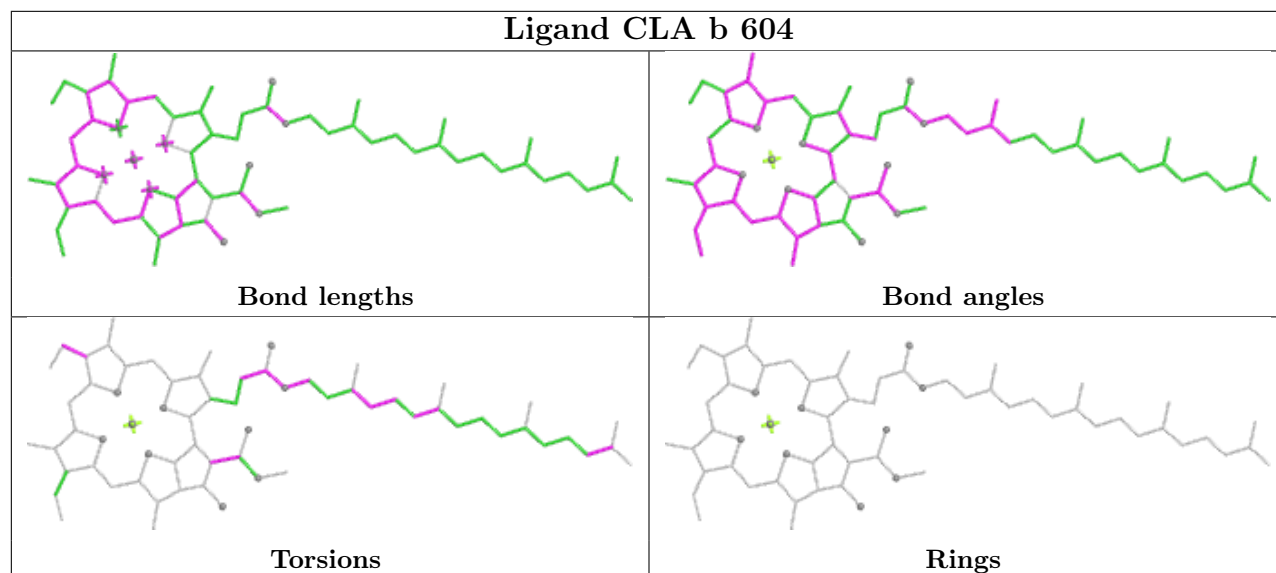
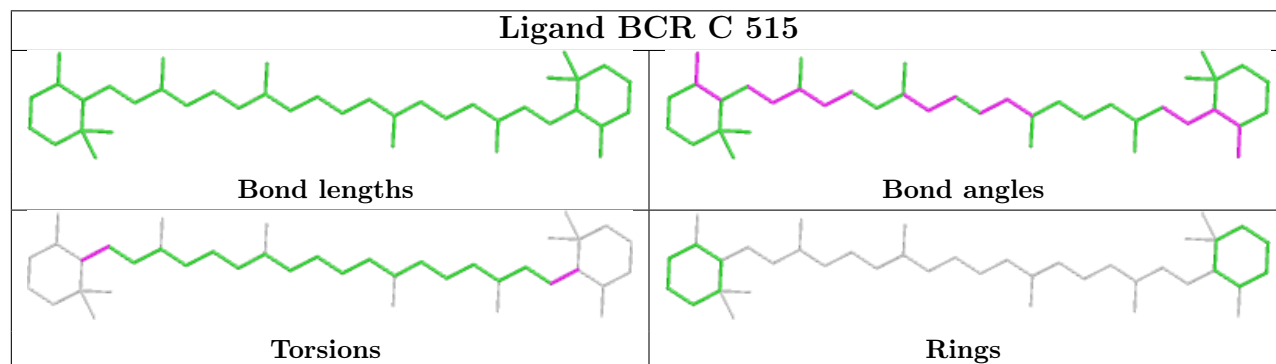
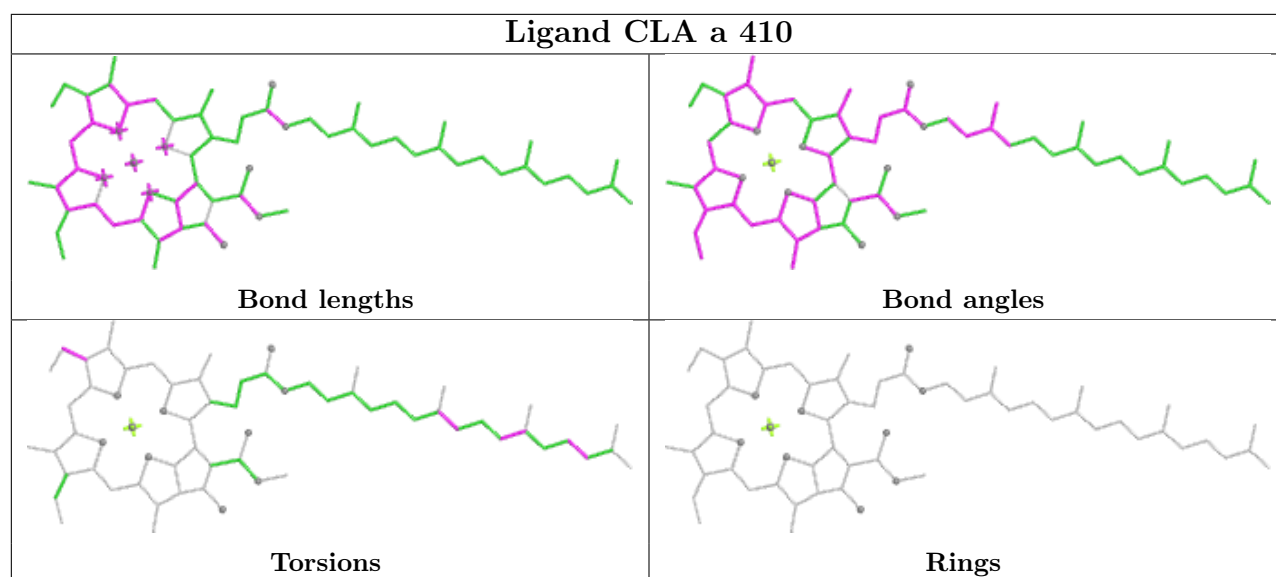


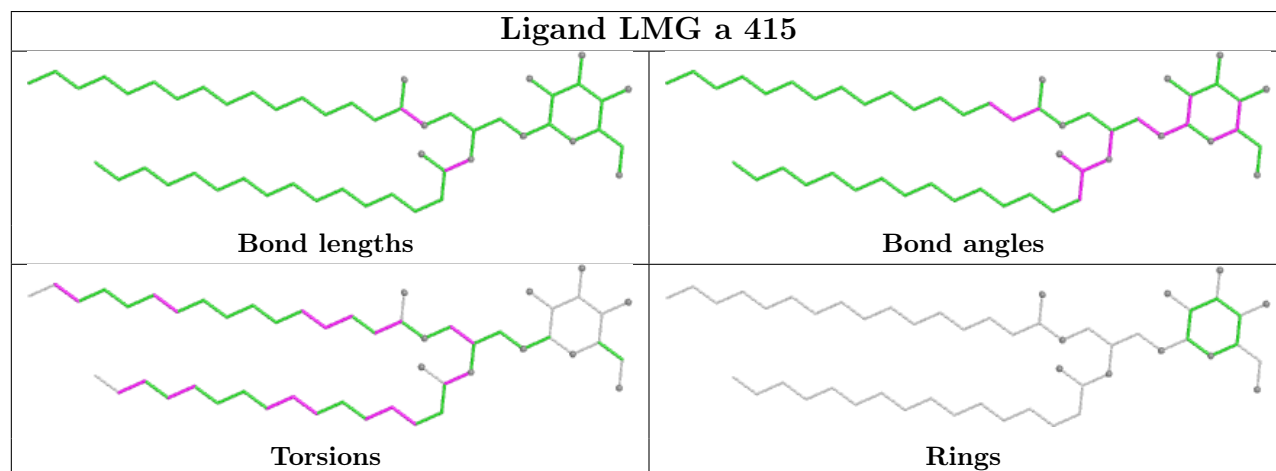
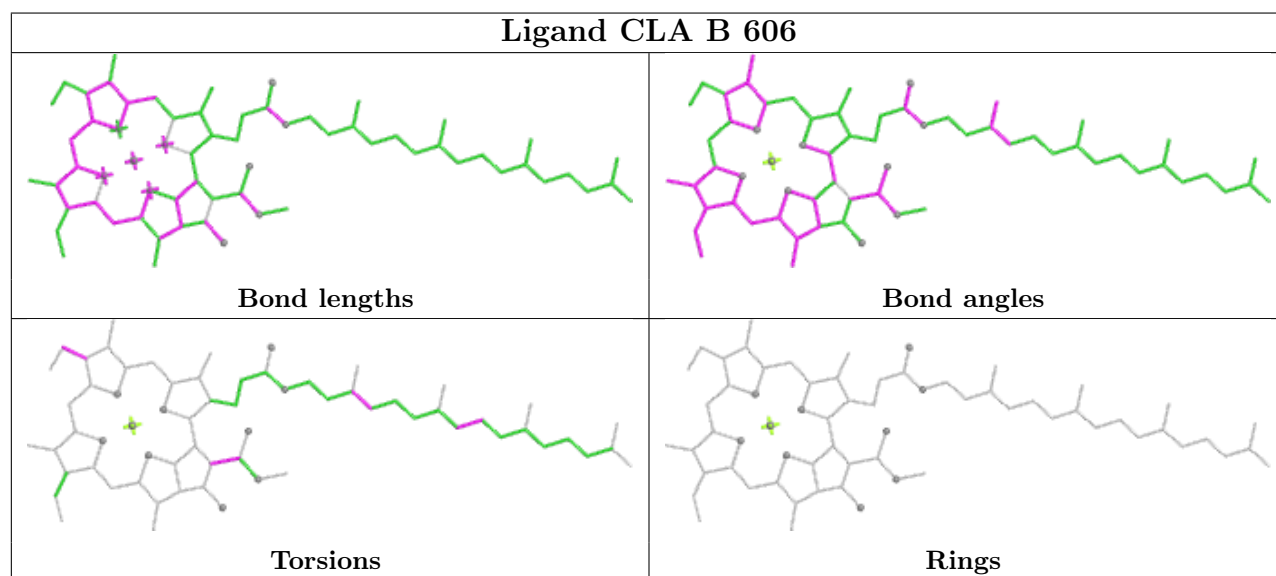
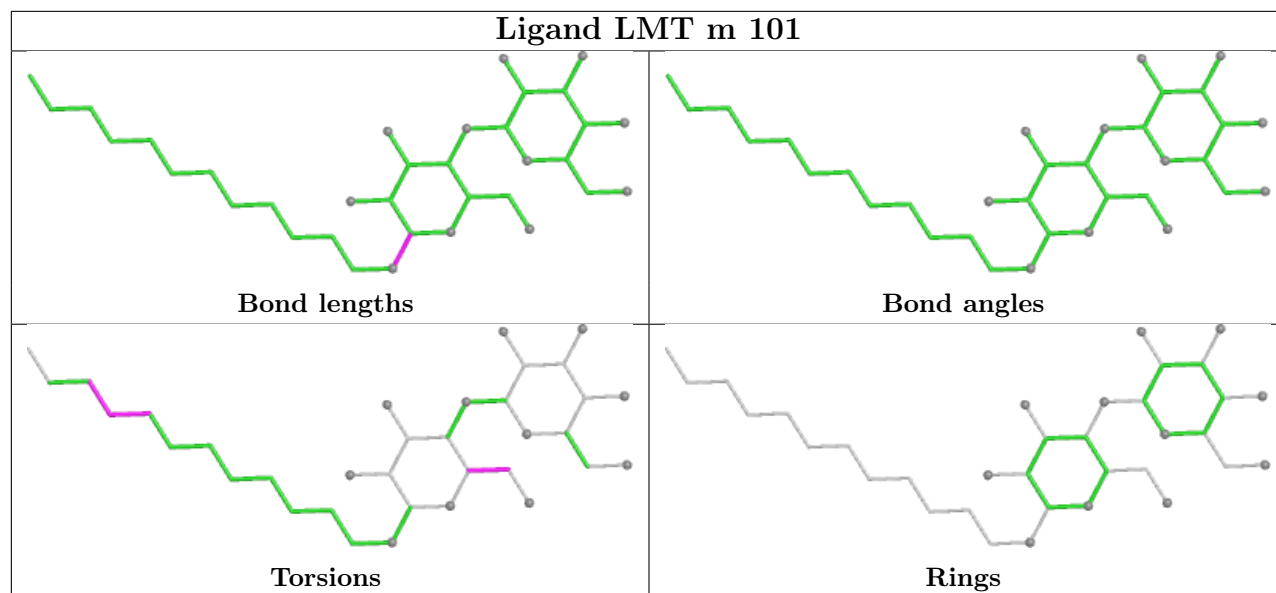
Ligand CLA a 412

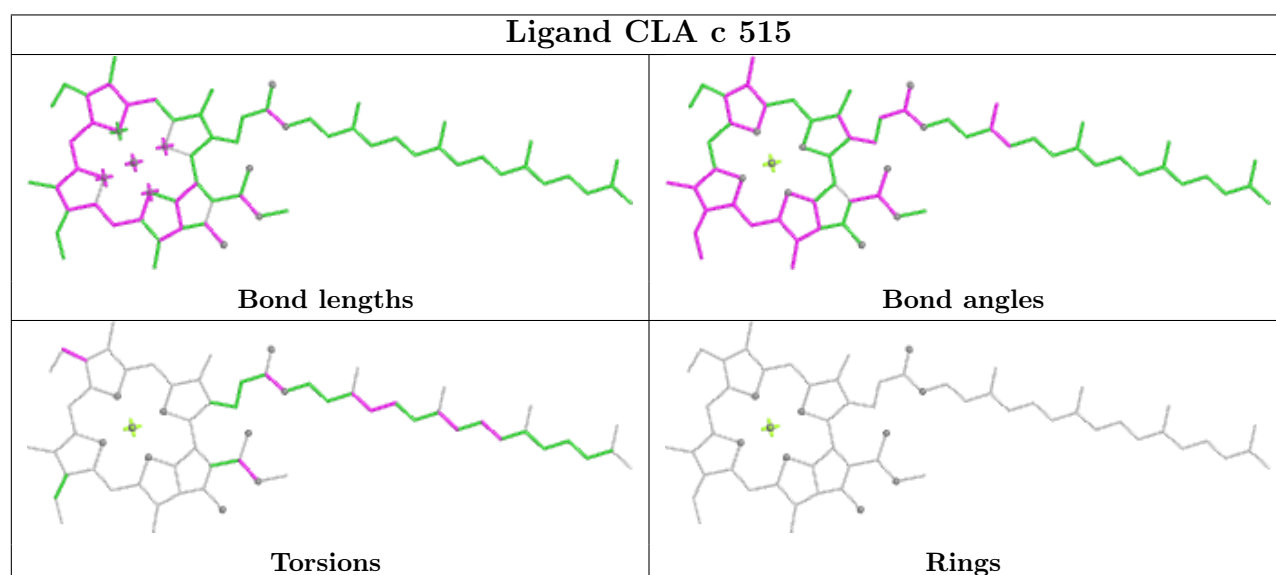
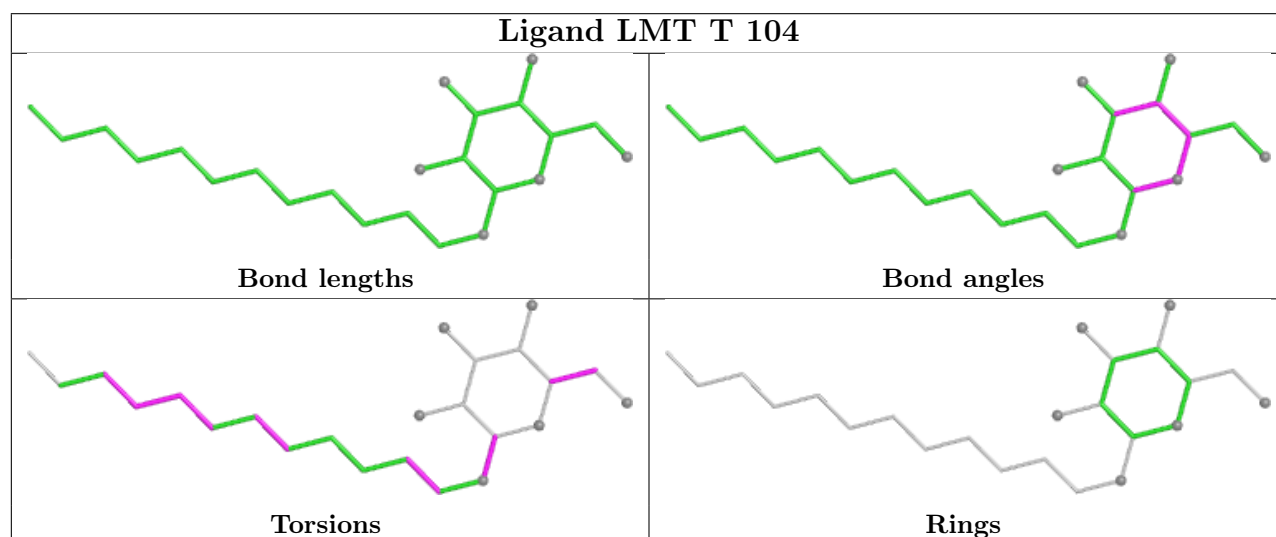
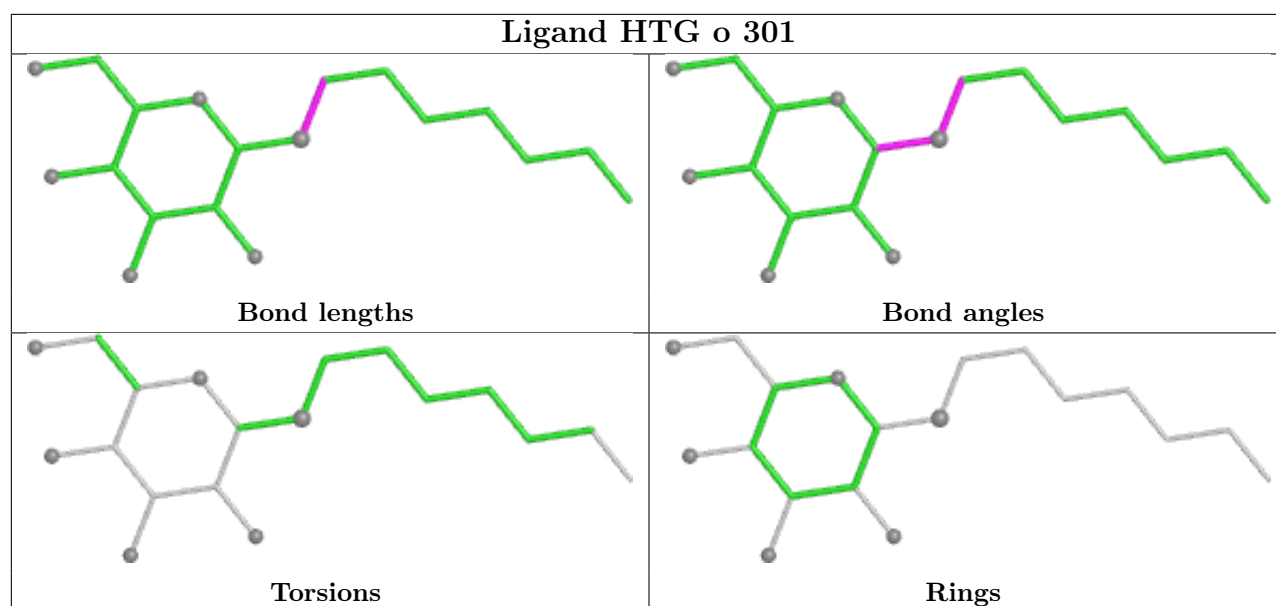


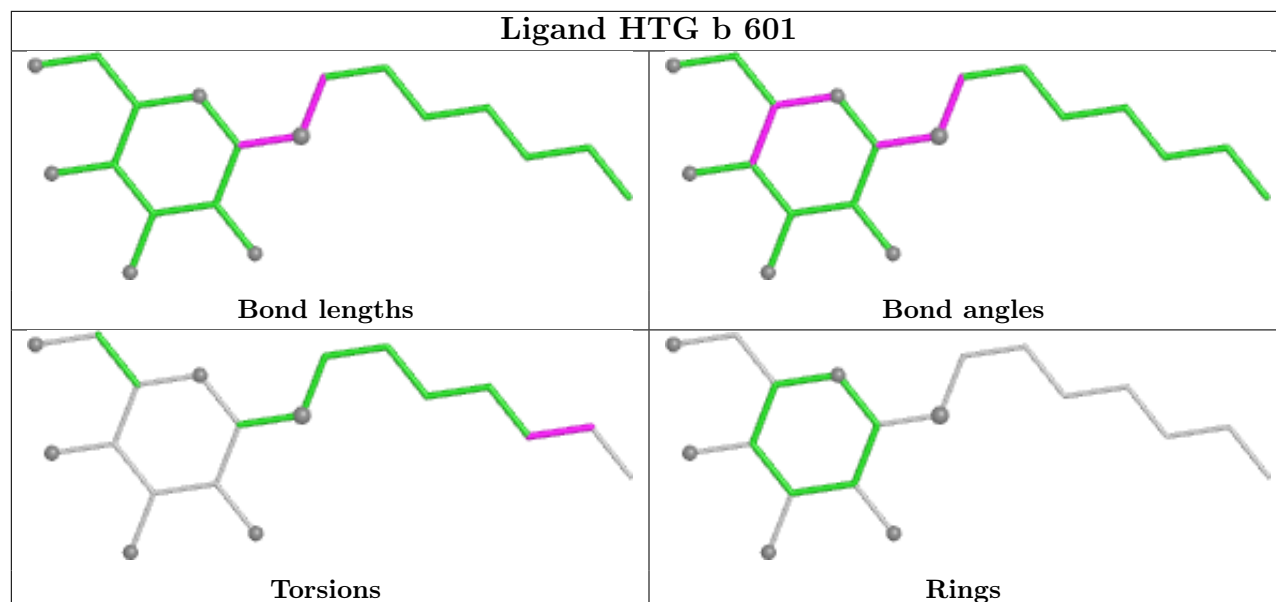
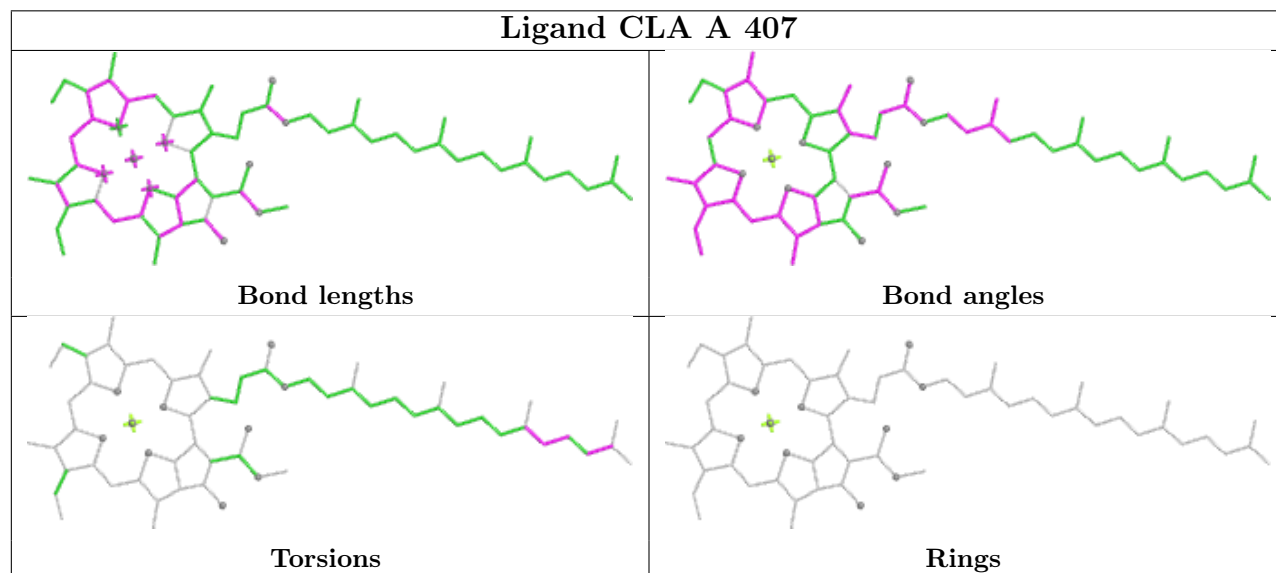
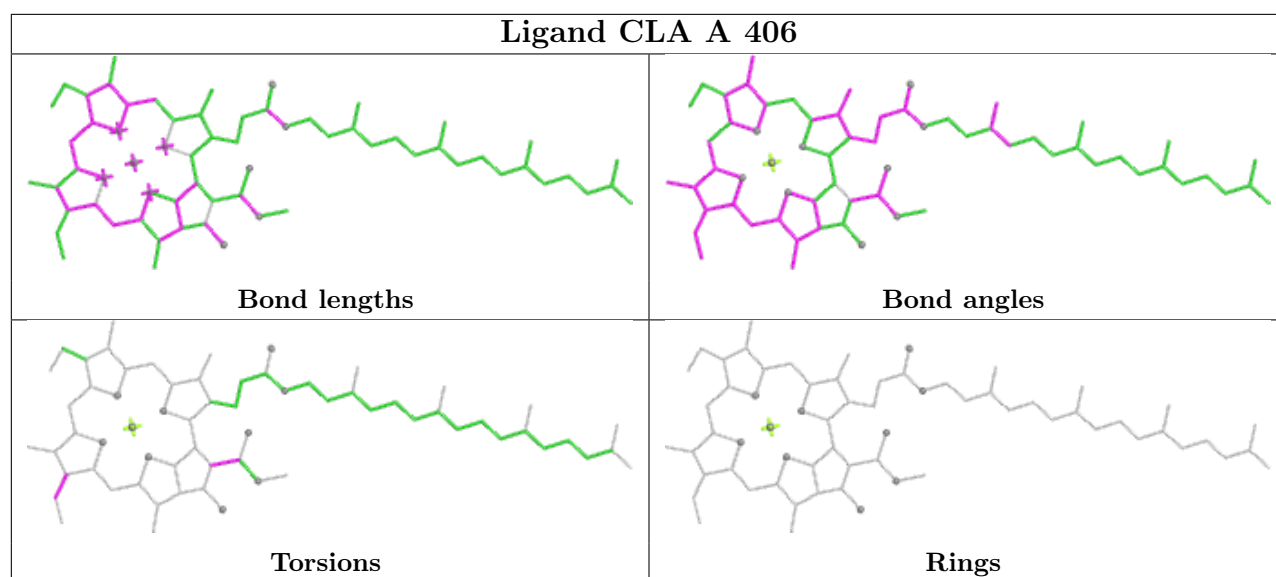
Ligand HTG O 302

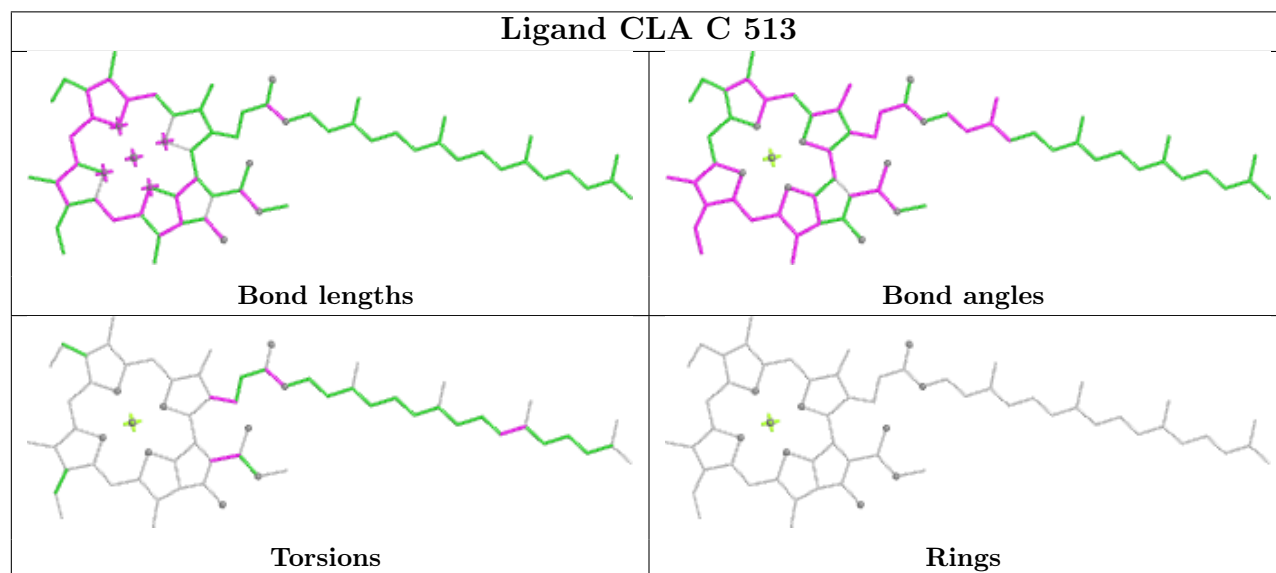
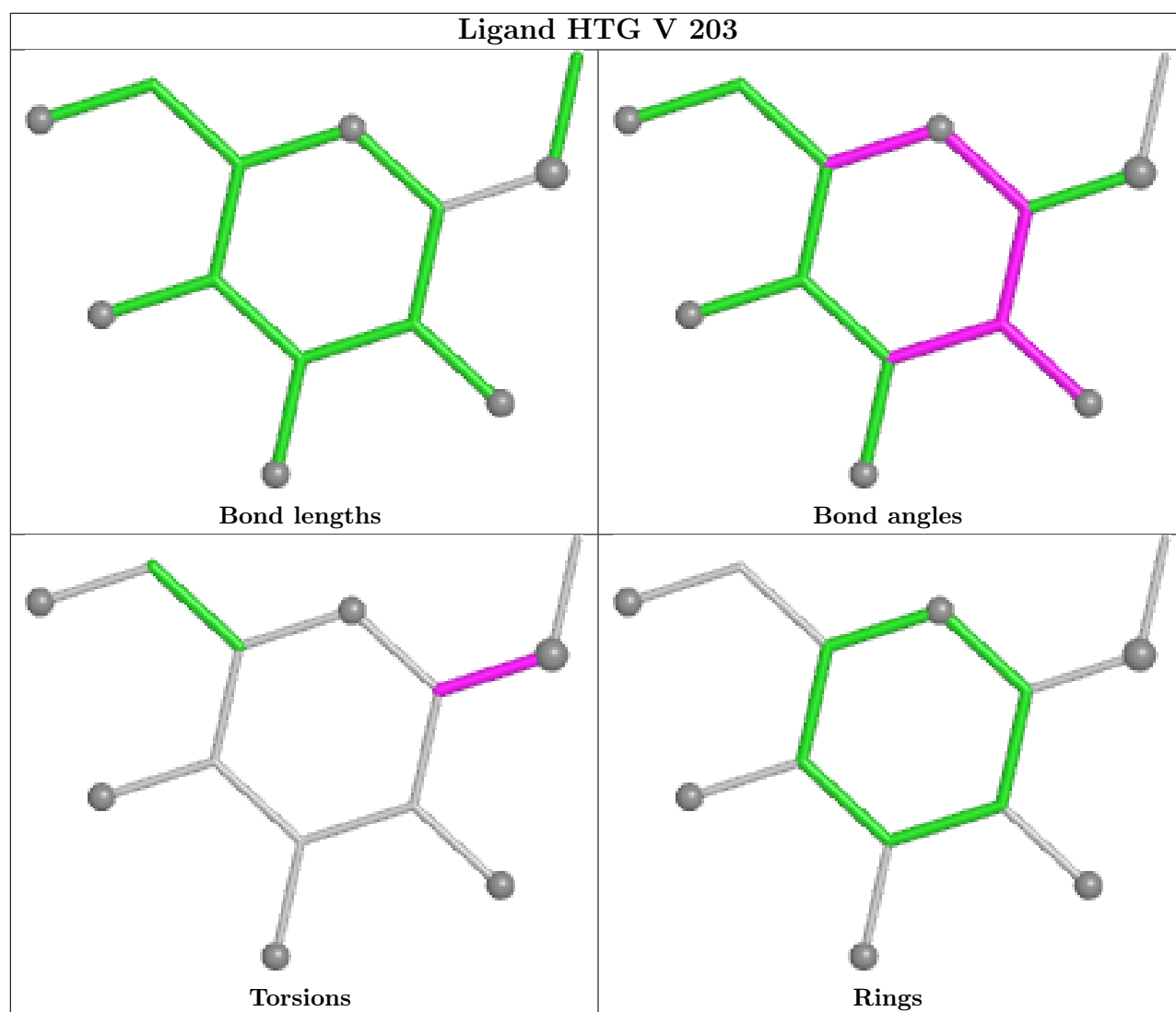


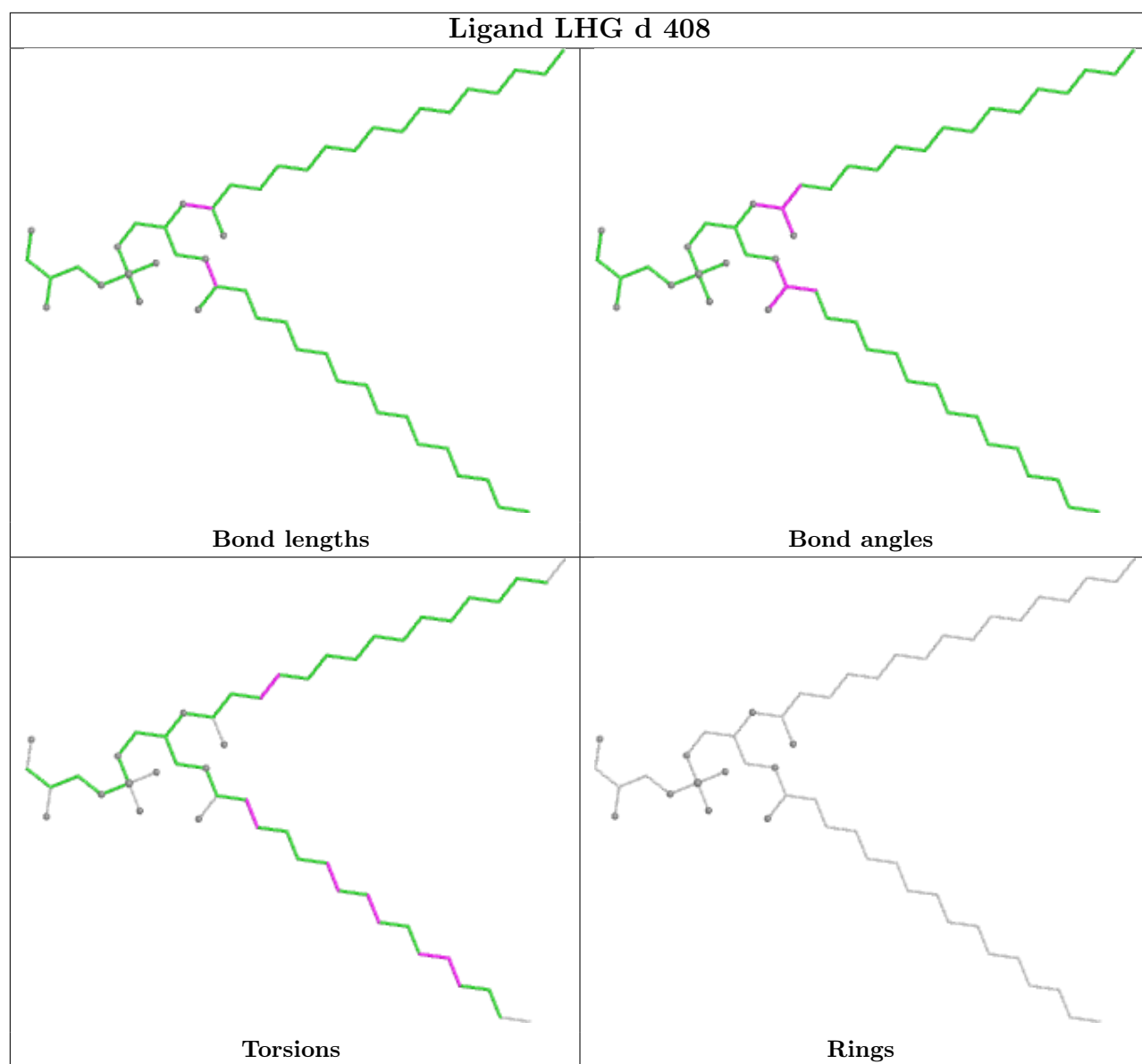


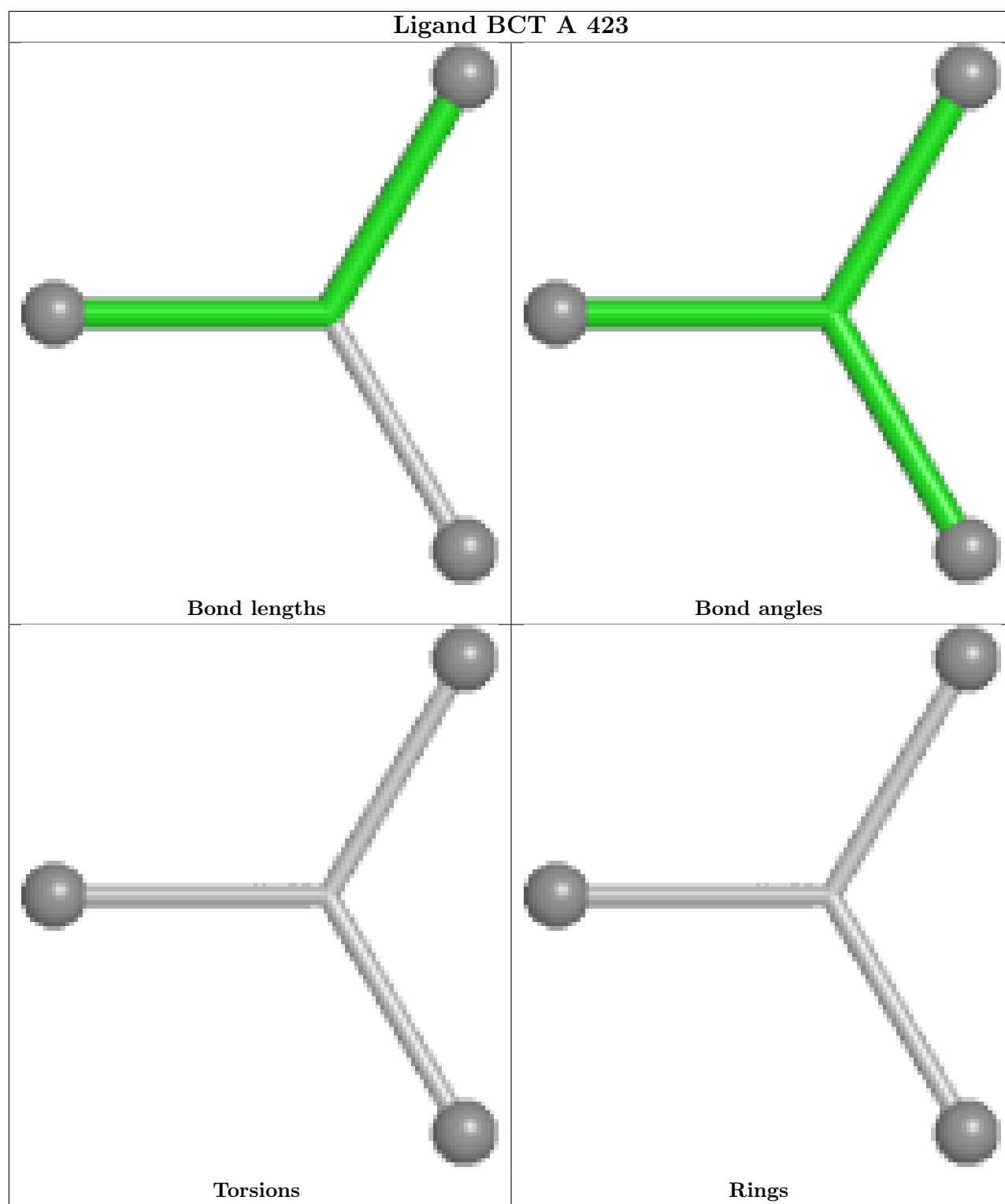


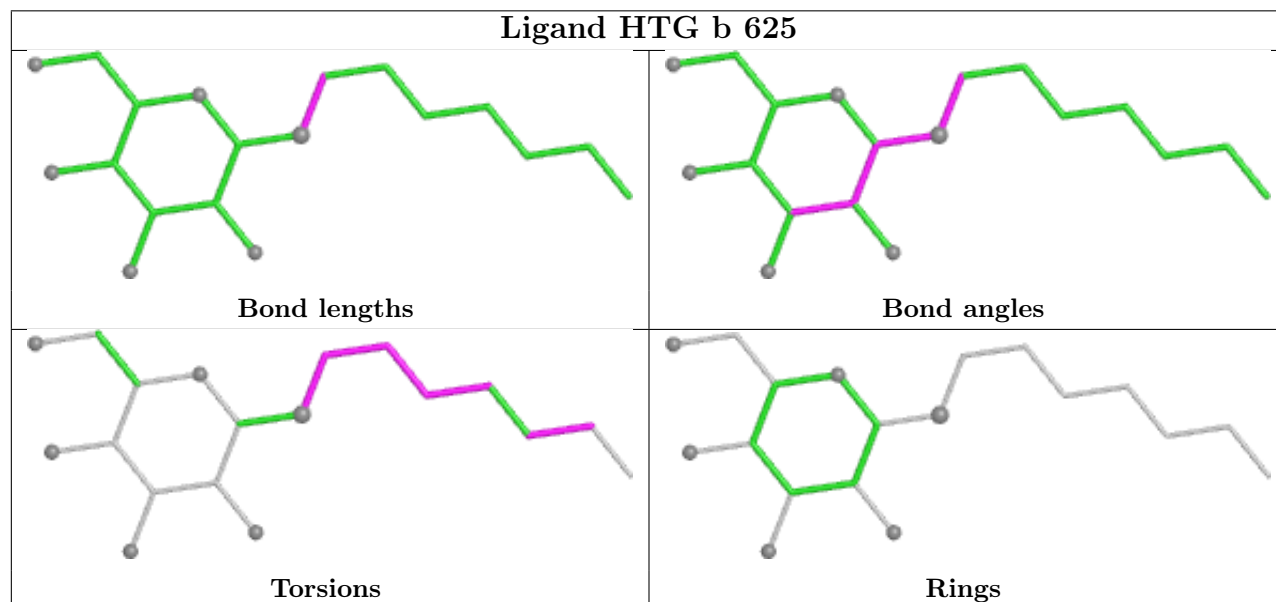
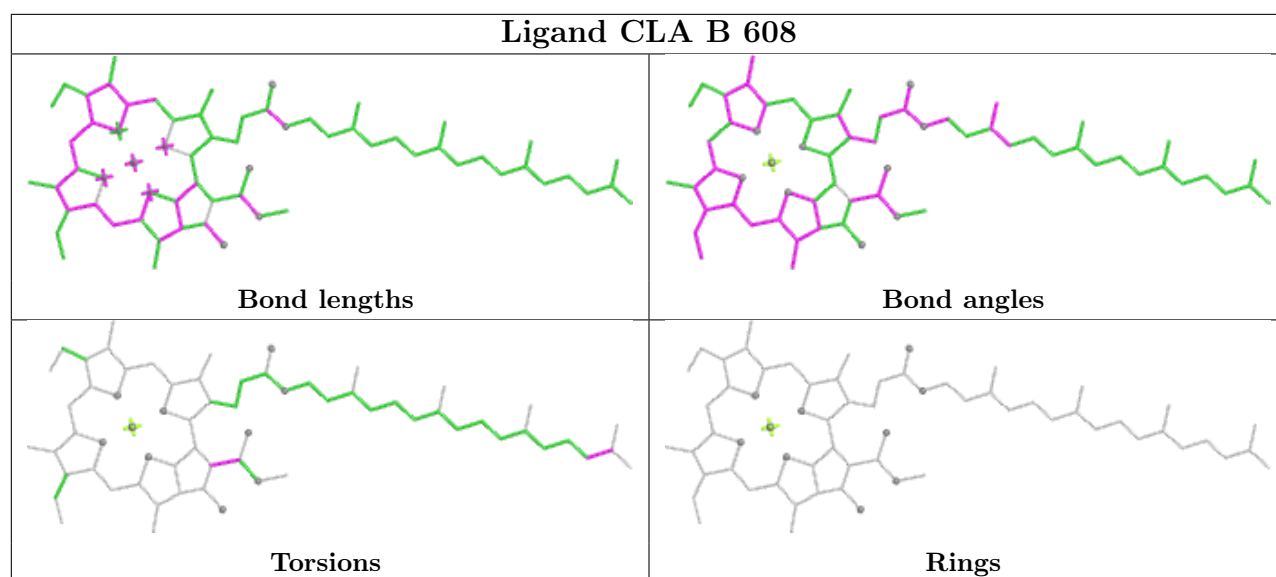


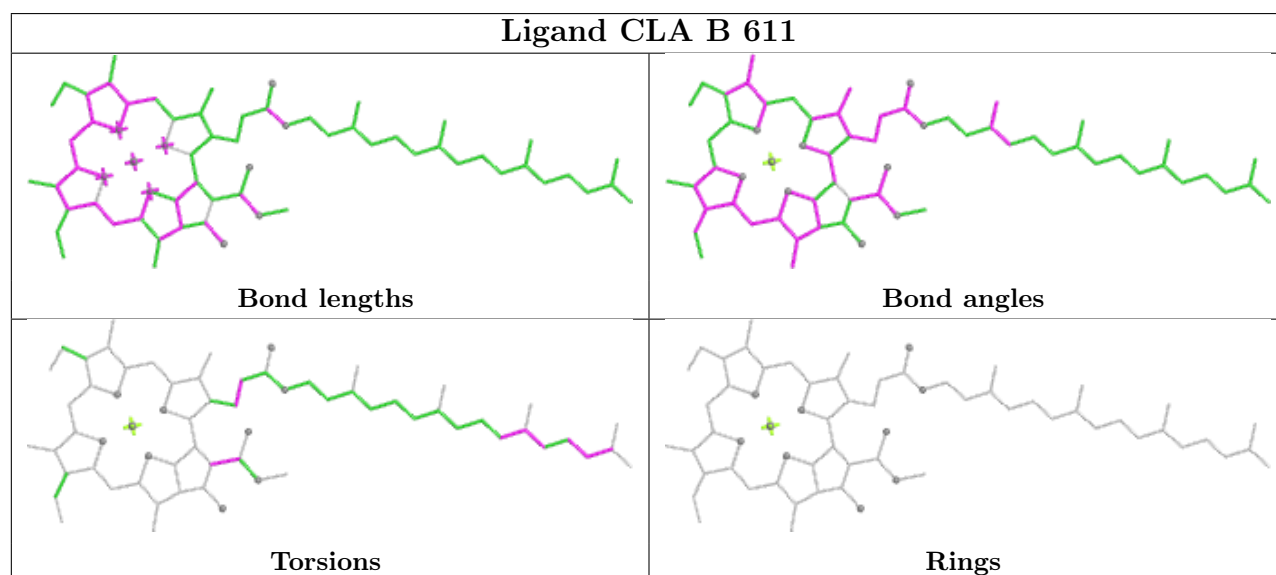
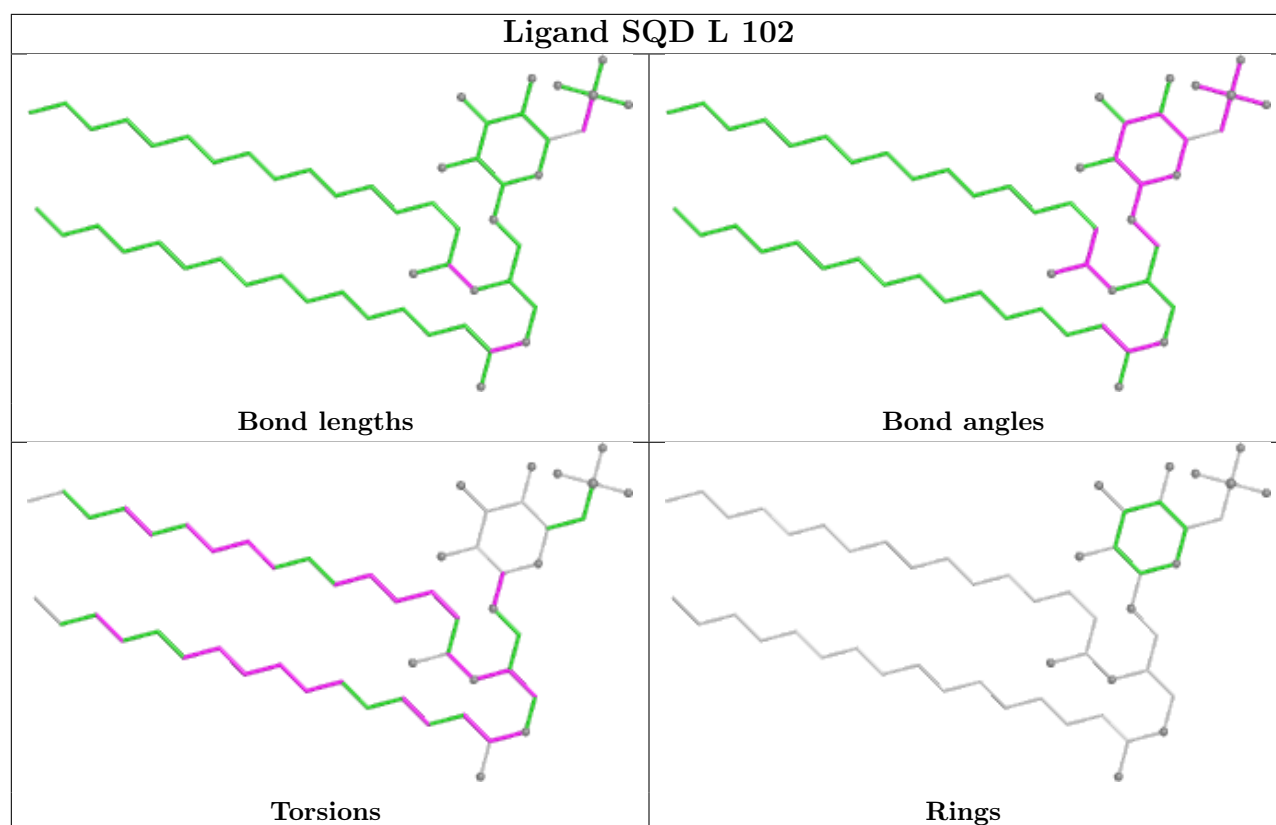




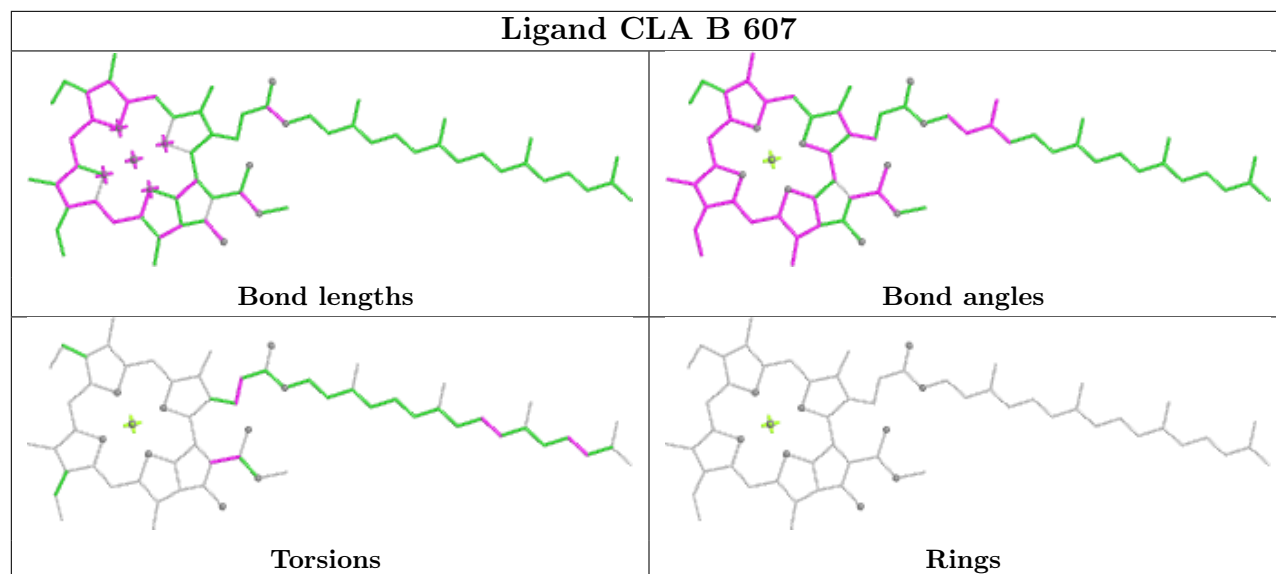




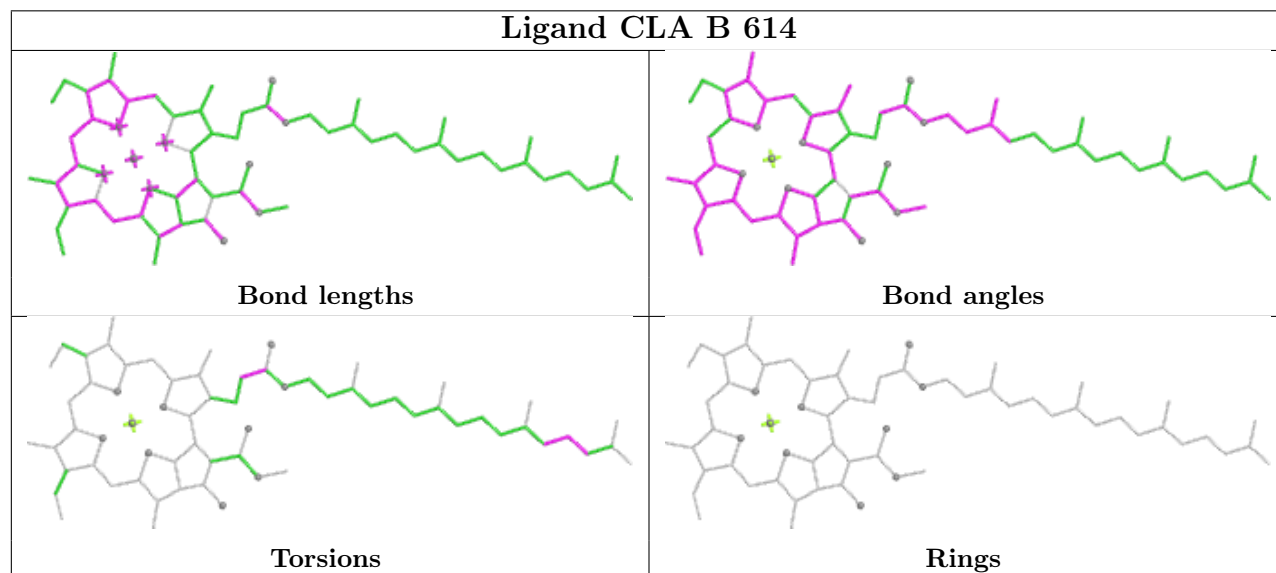




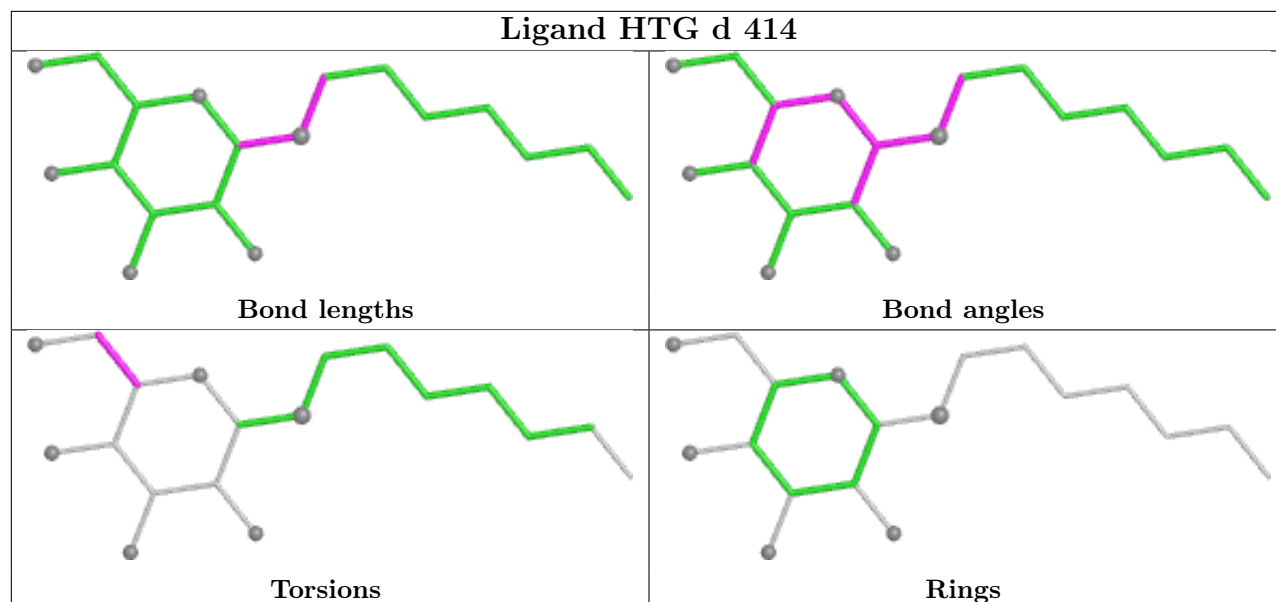
Ligand CLA B 607

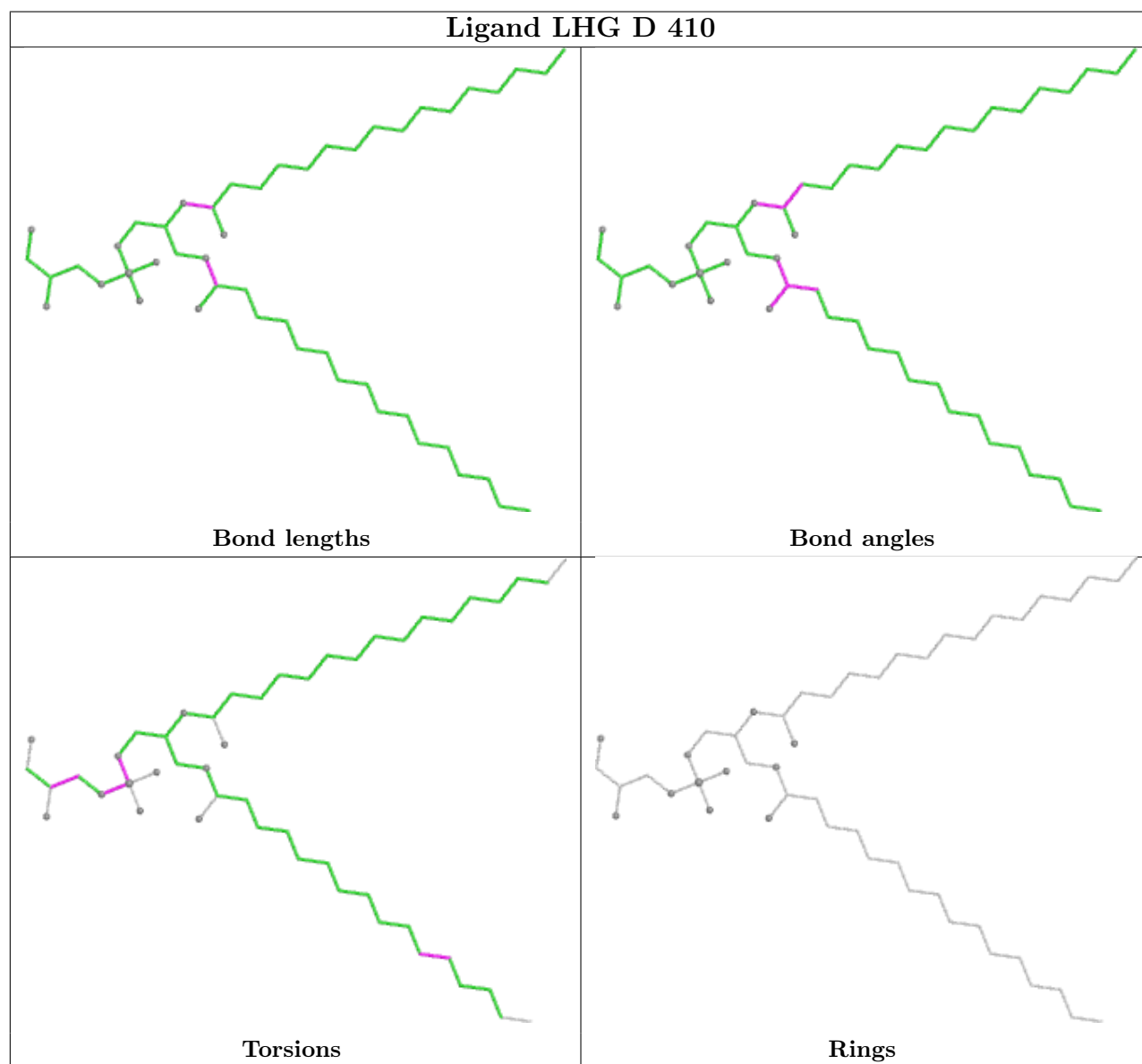
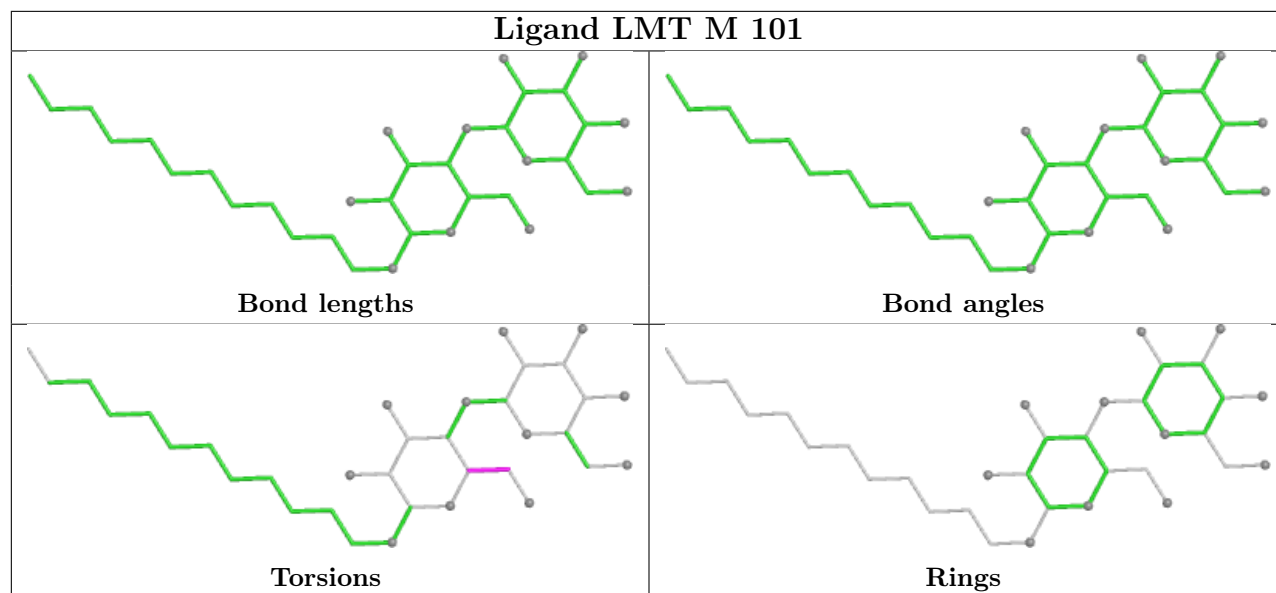


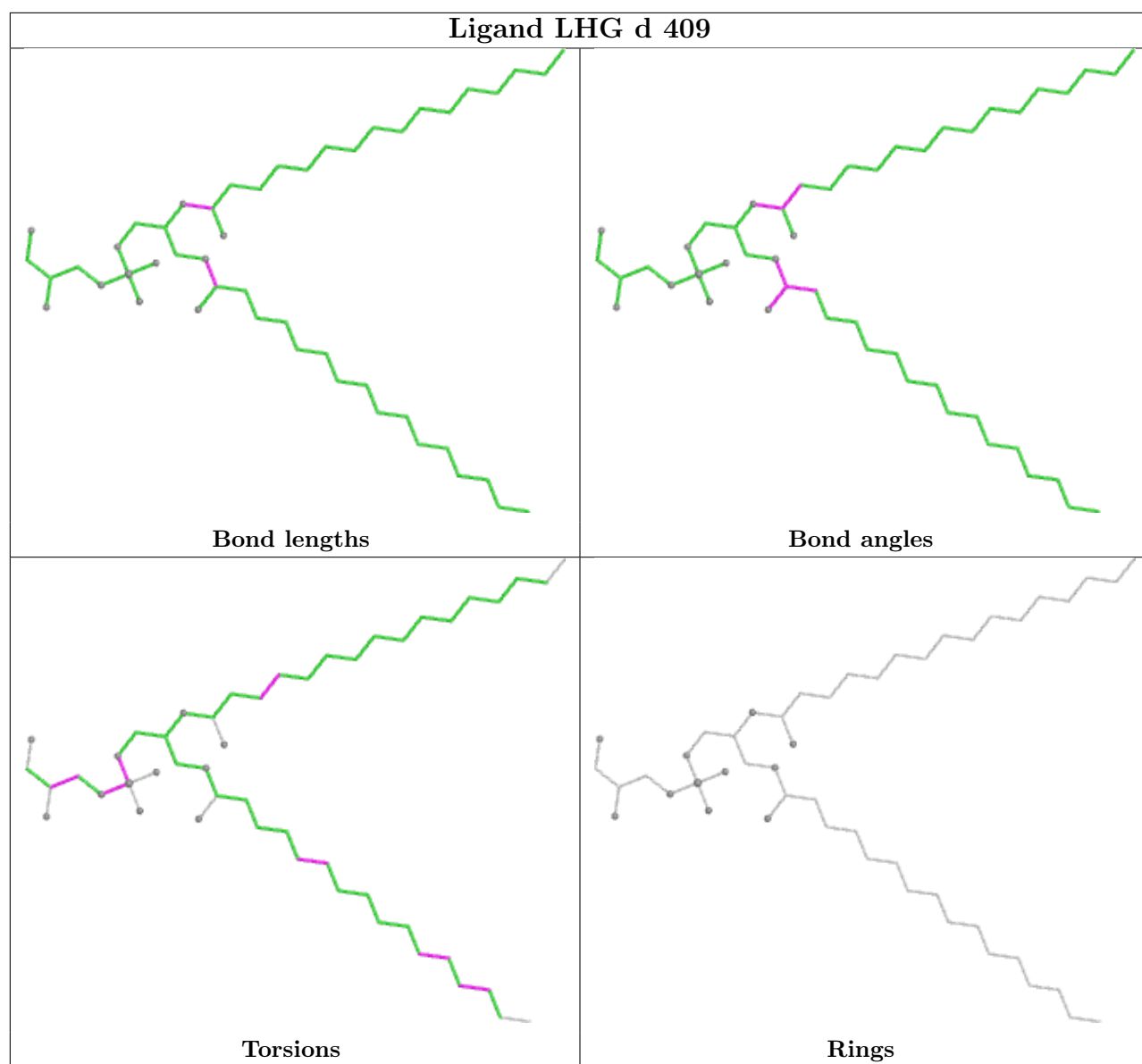
Ligand CLA B 614



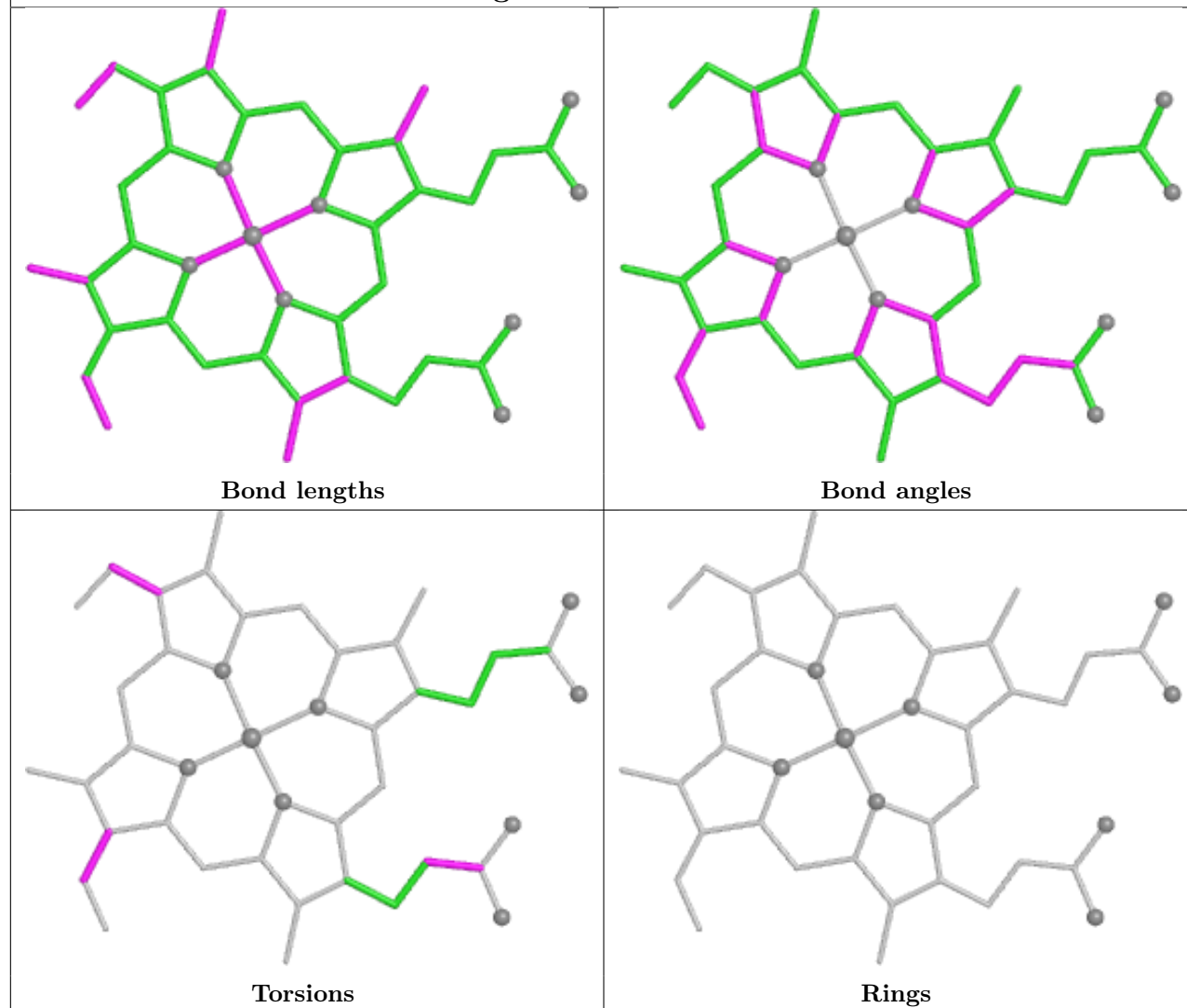
Ligand HTG d 414



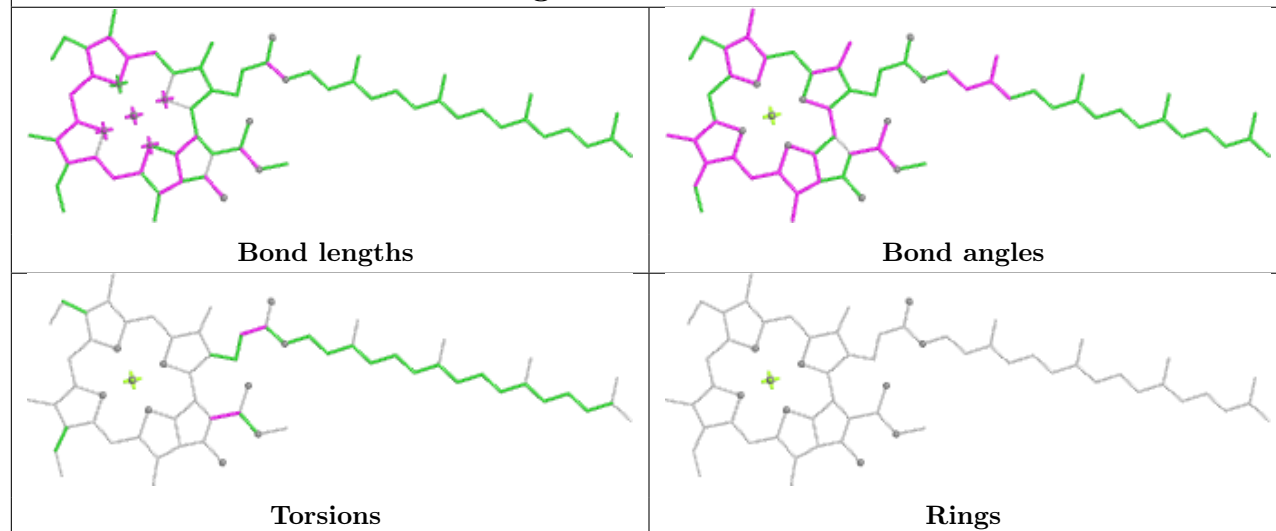


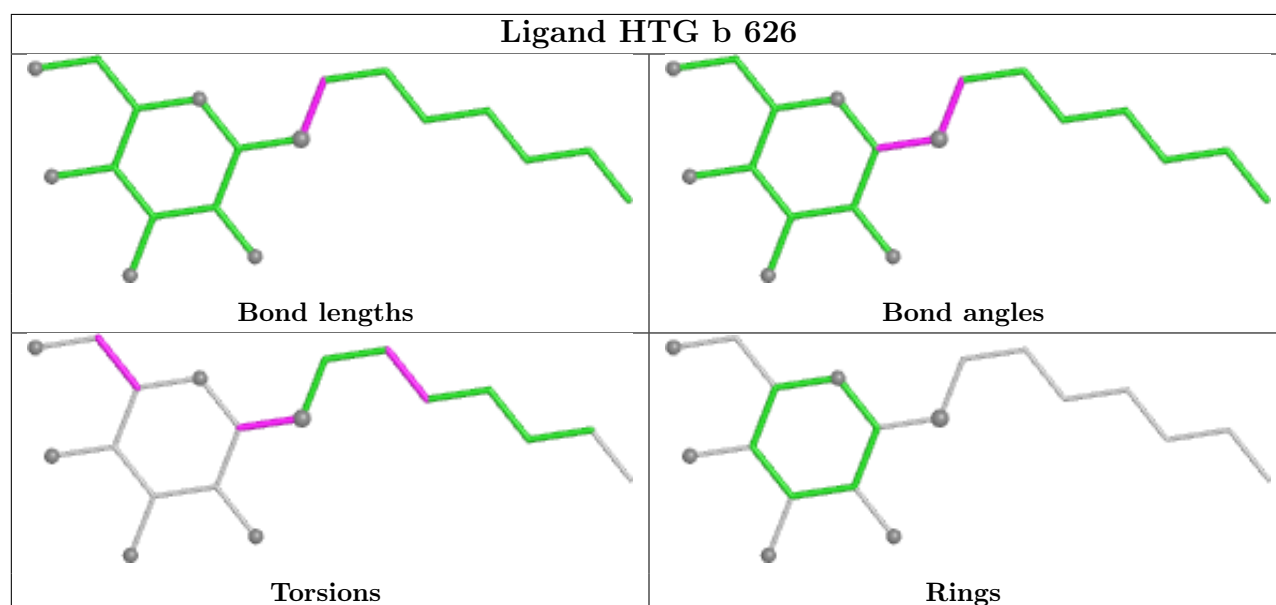
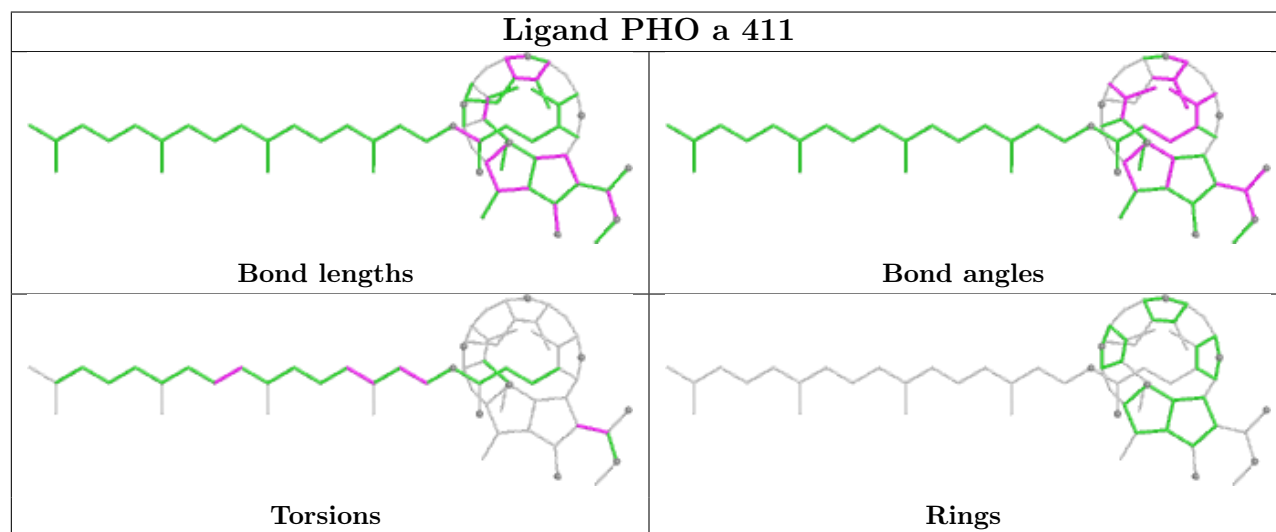
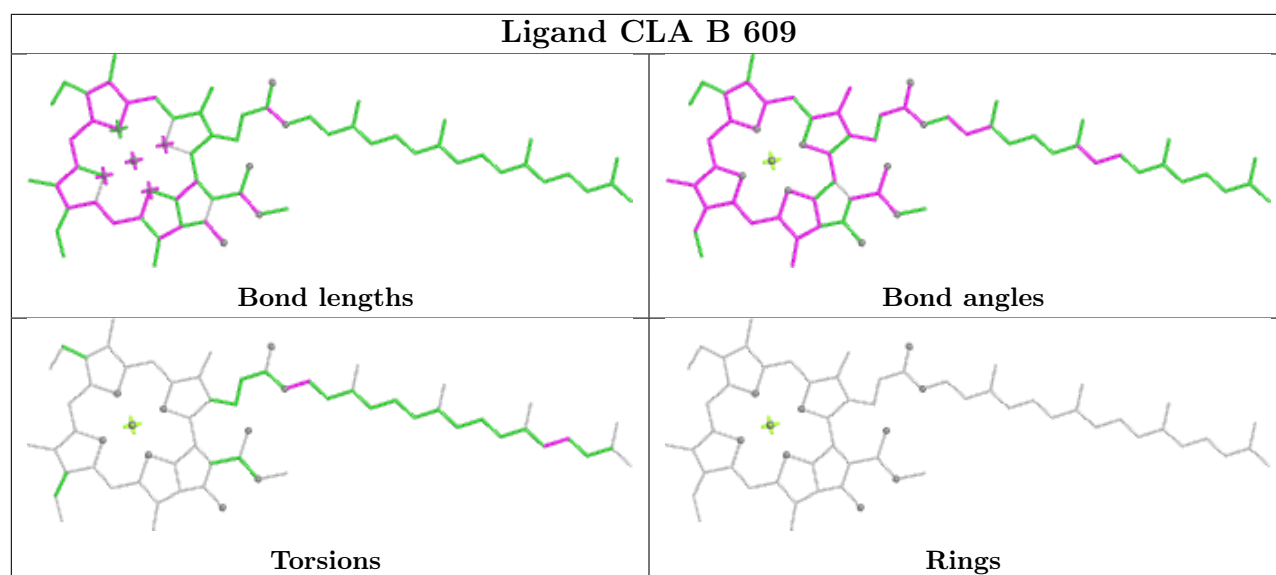


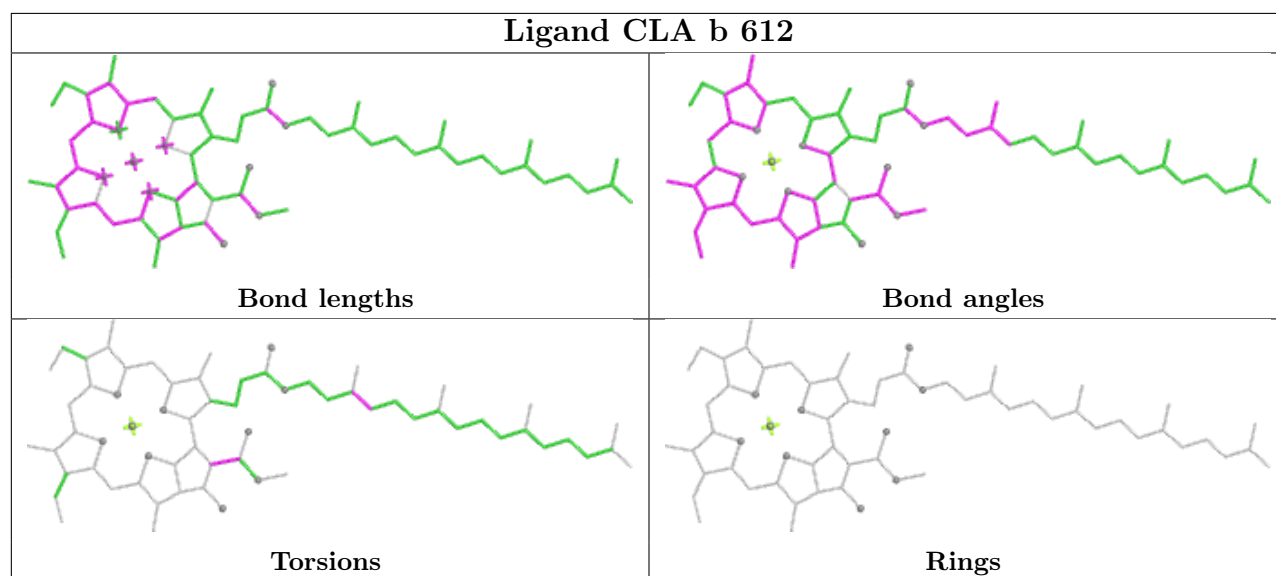
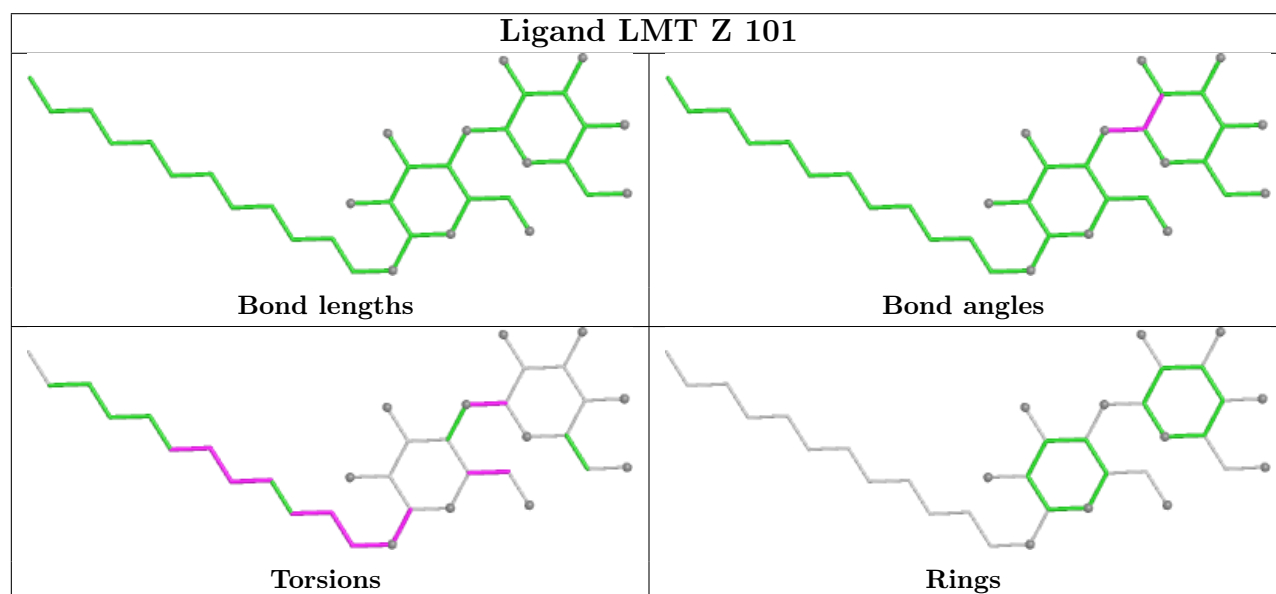
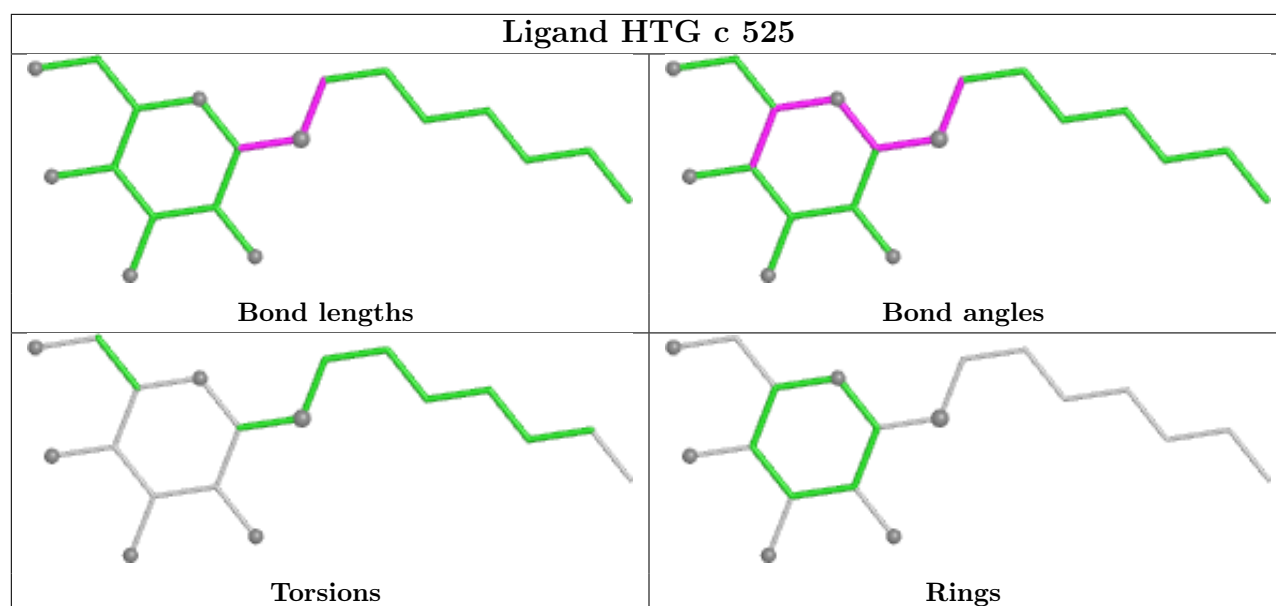
Ligand HEC V 202

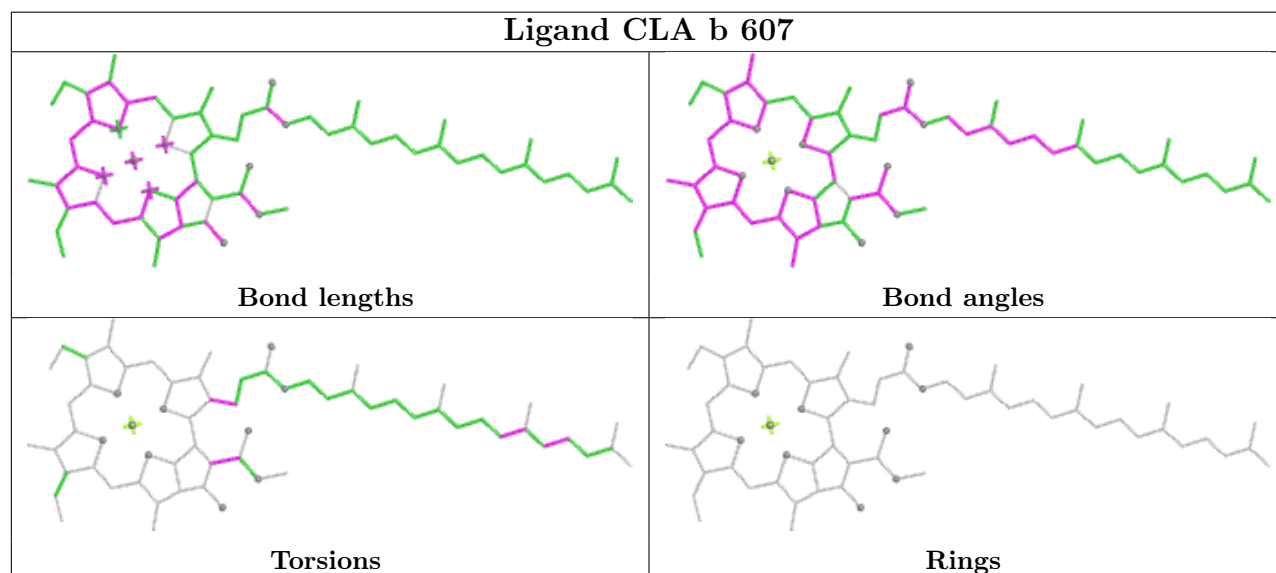
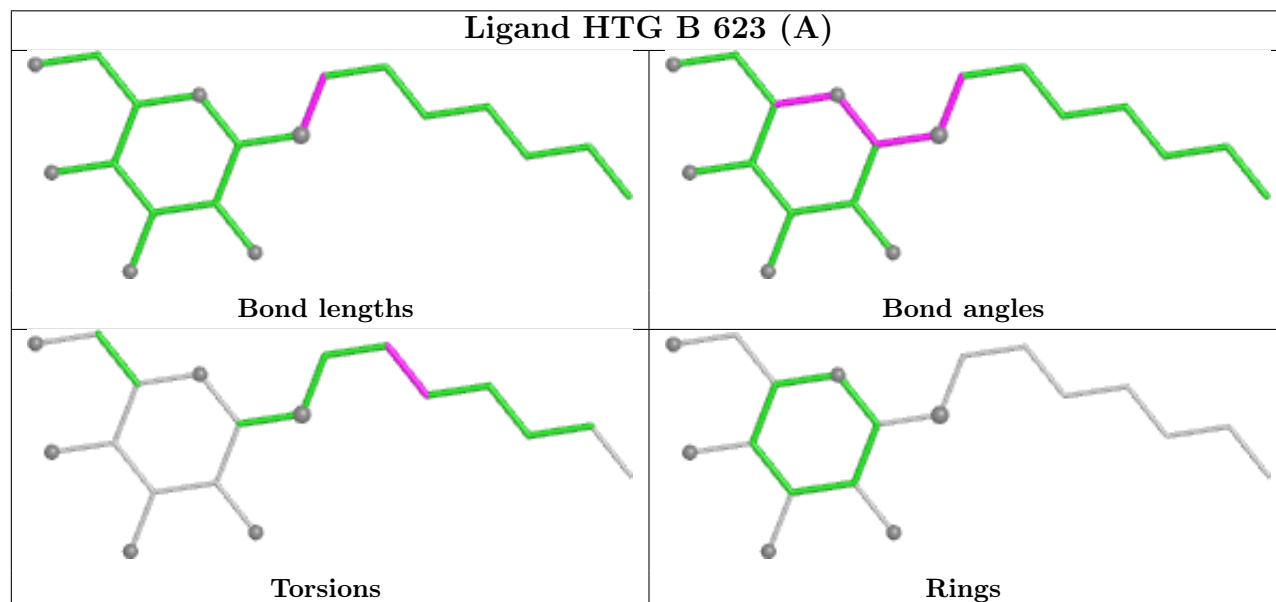
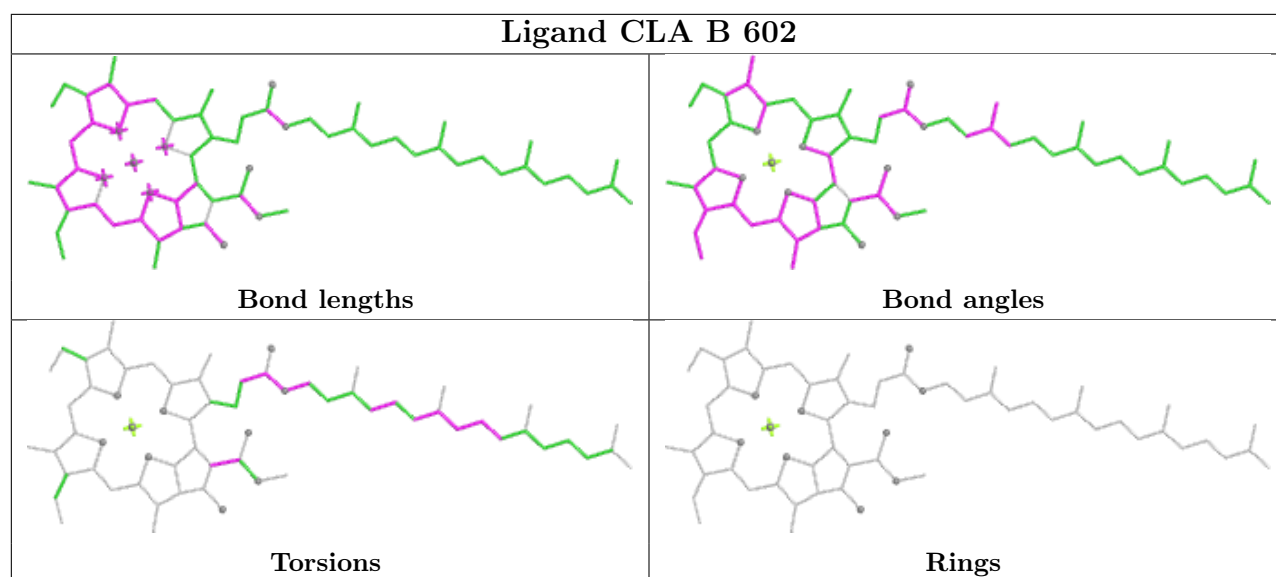


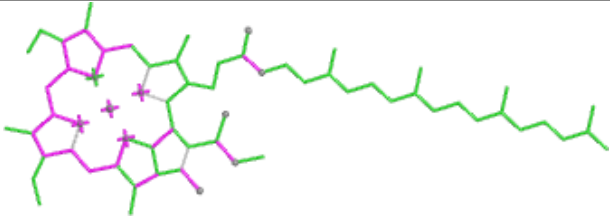
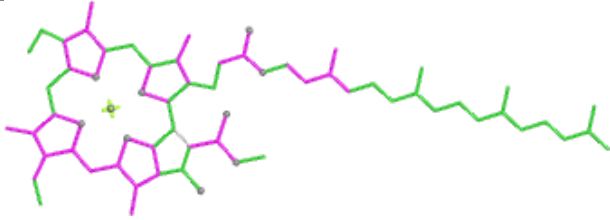
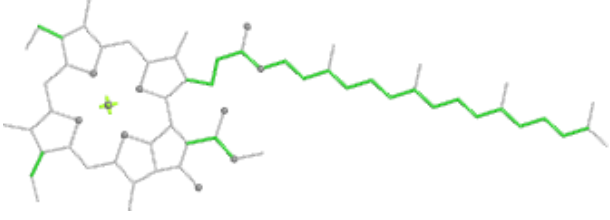
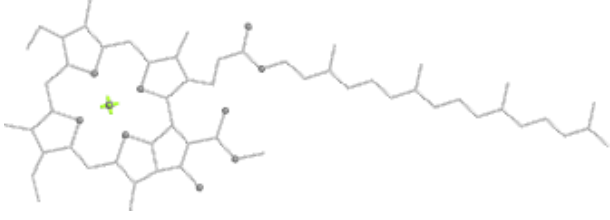
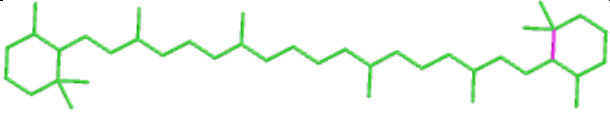
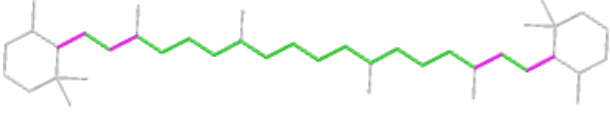
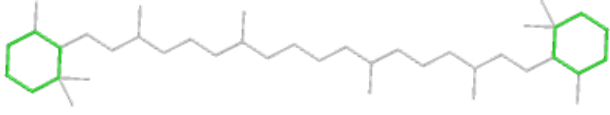
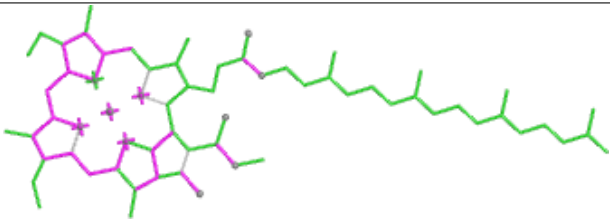
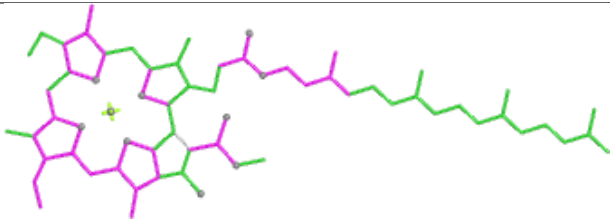
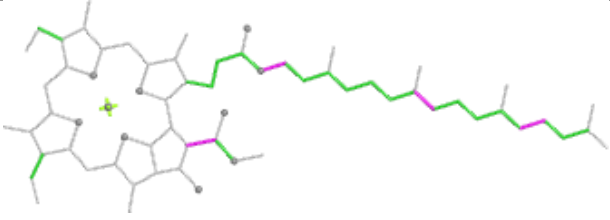
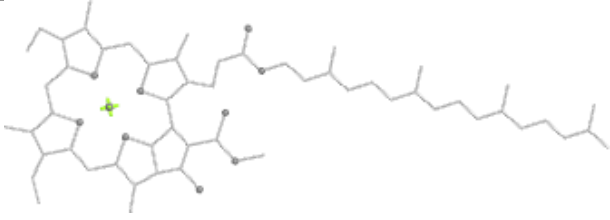
Ligand CLA C 506

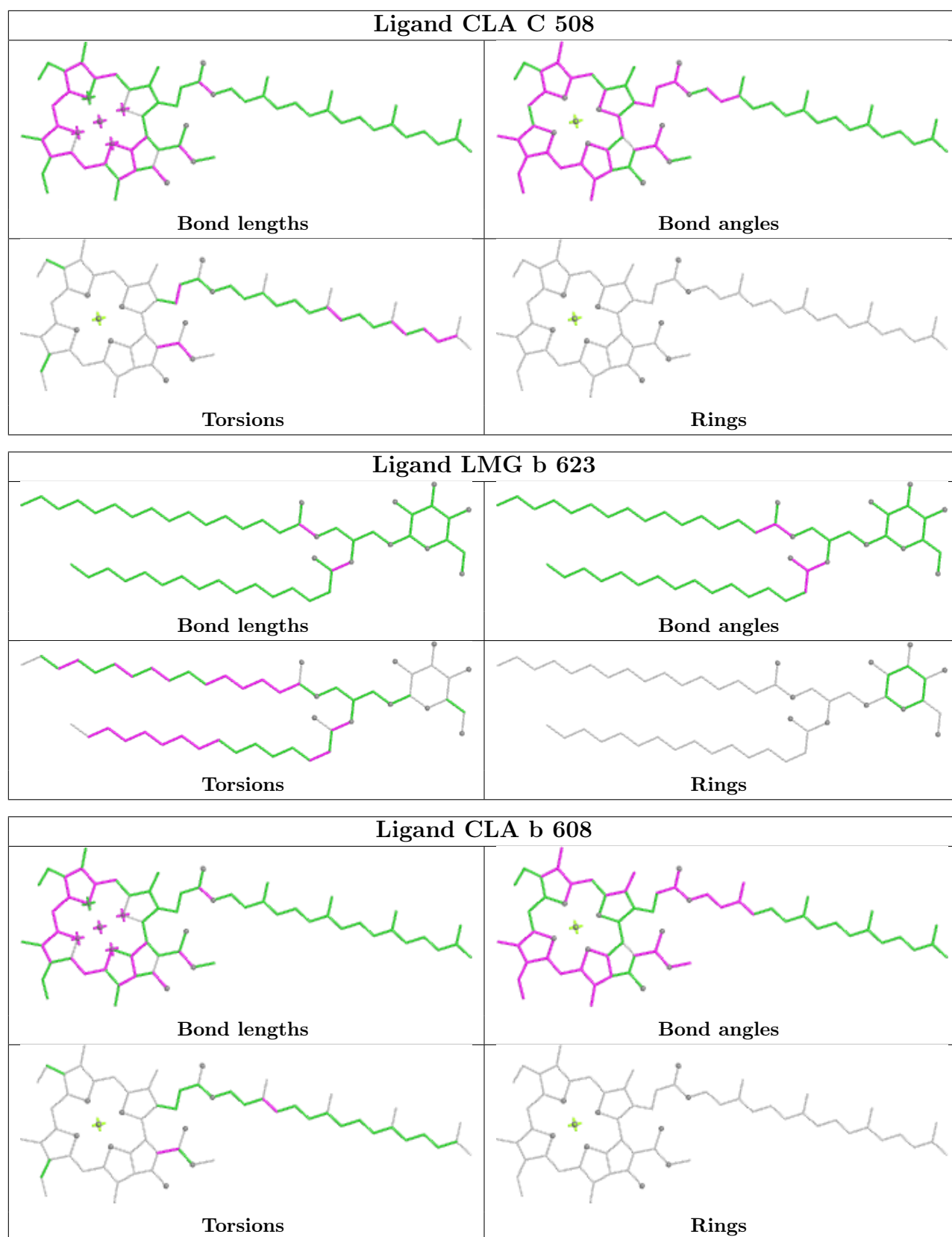


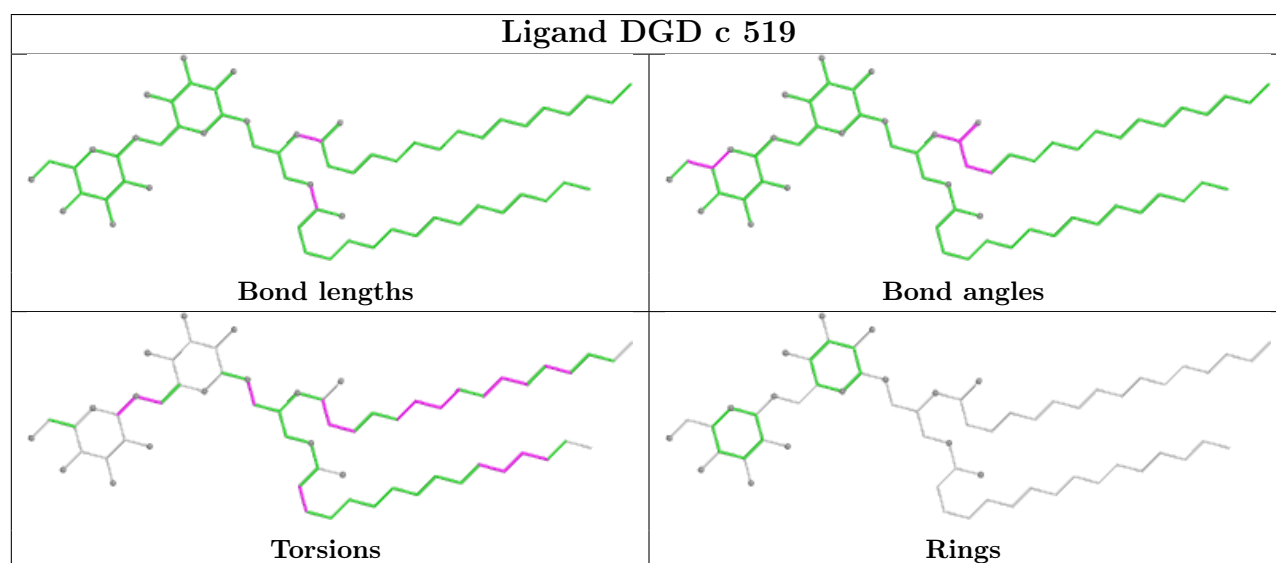
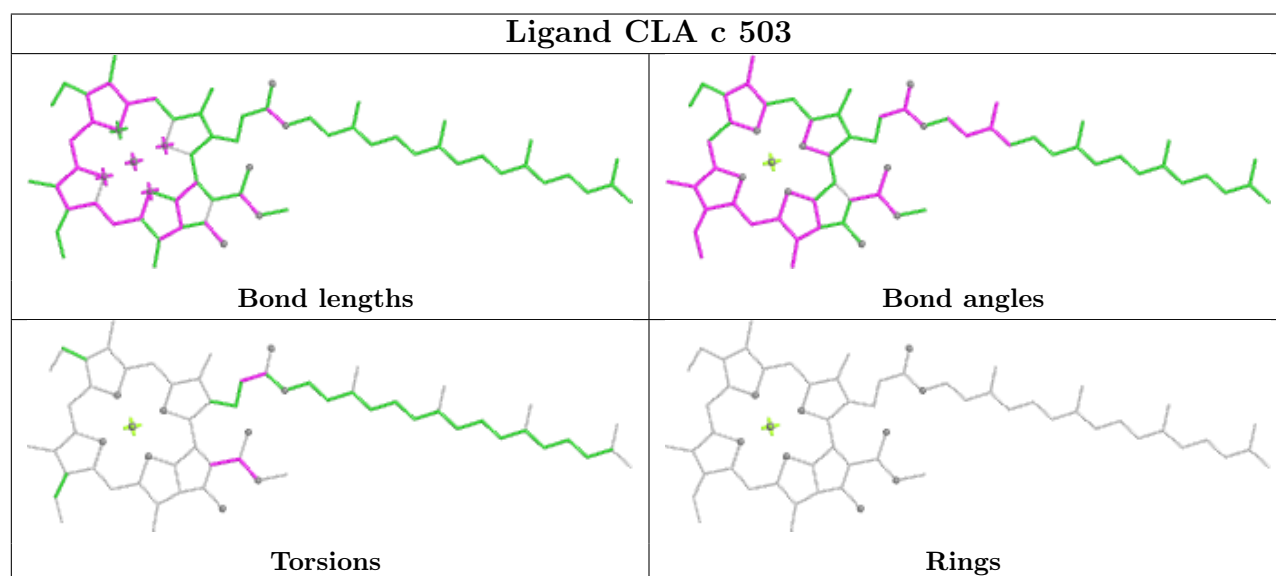
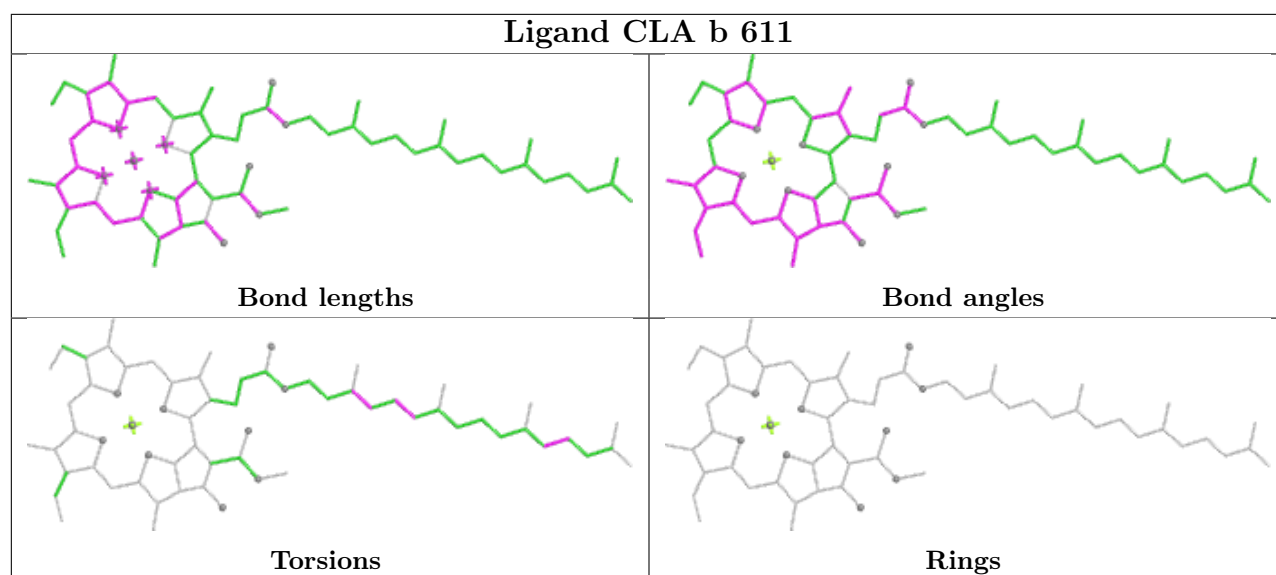


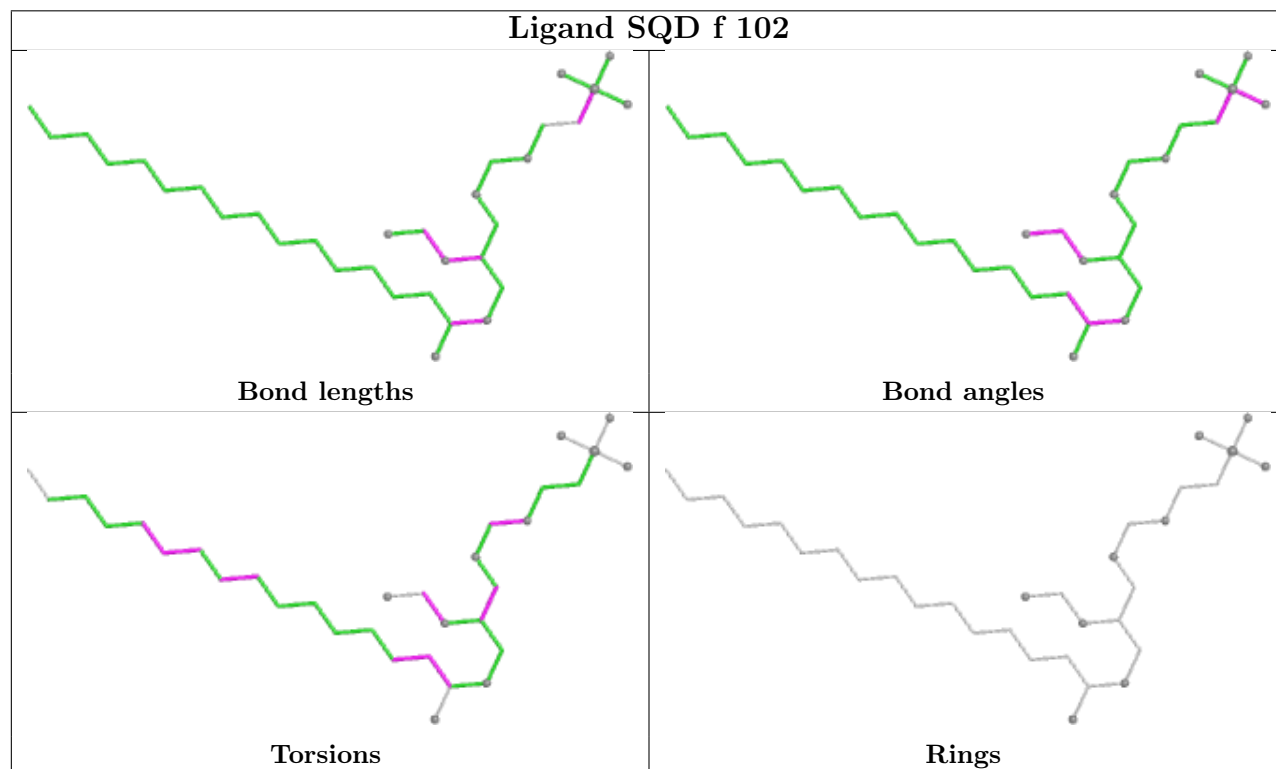
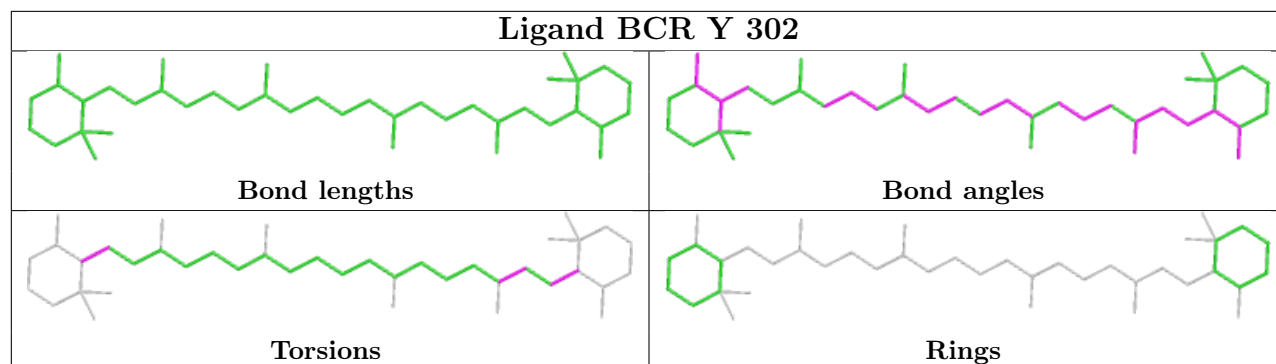


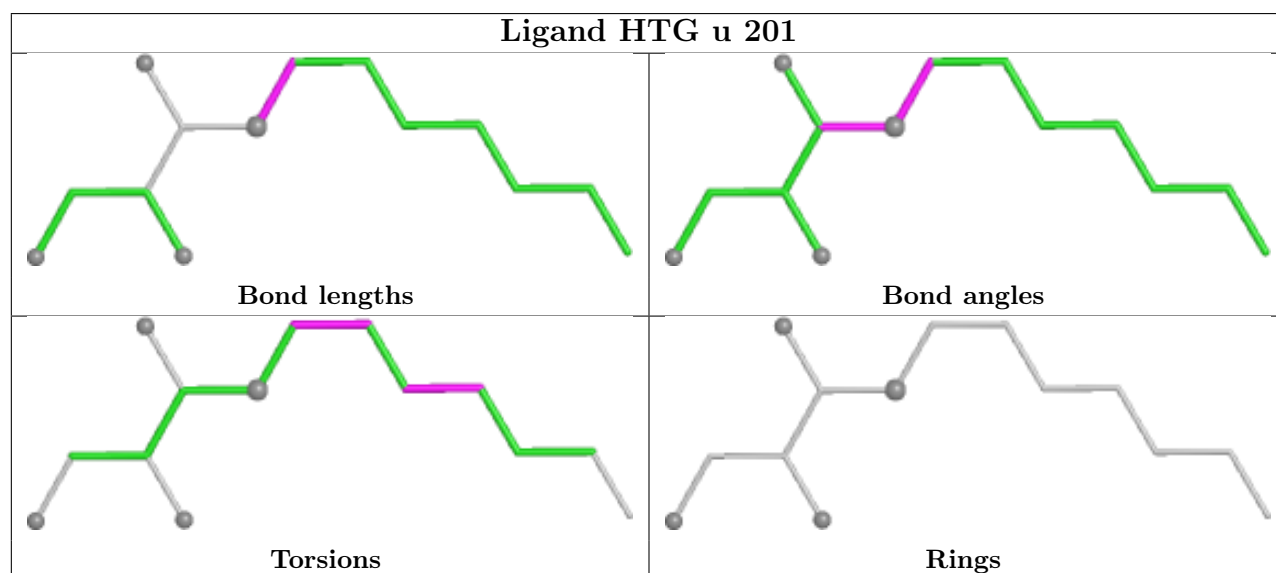
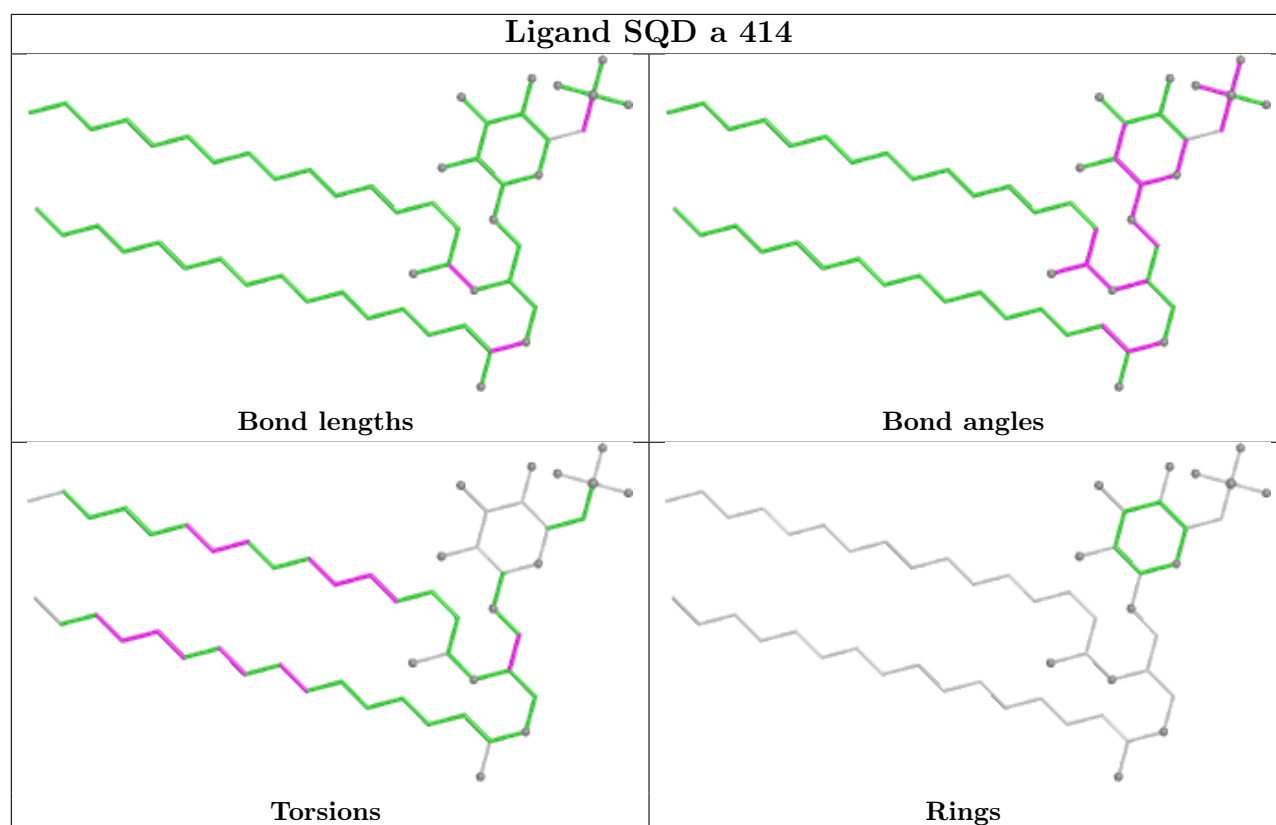


Ligand CLA b 615	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR D 405	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA C 510	
 Bond lengths	 Bond angles
 Torsions	 Rings

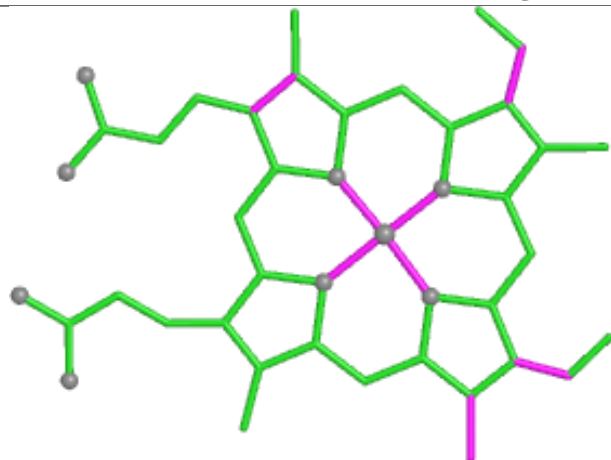




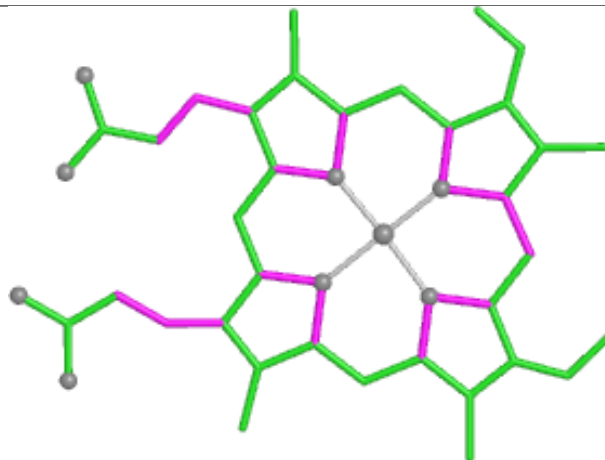




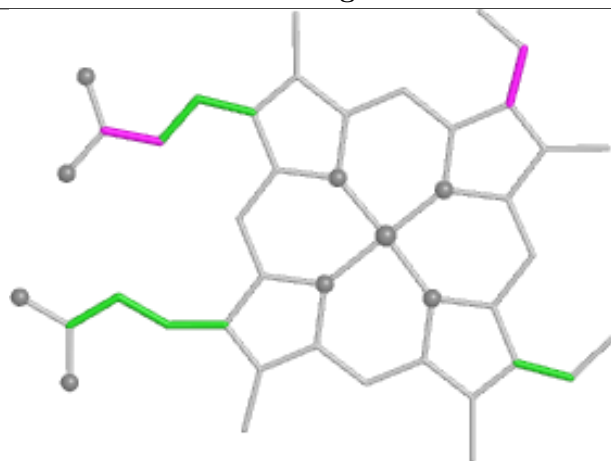
Ligand HEM f 101



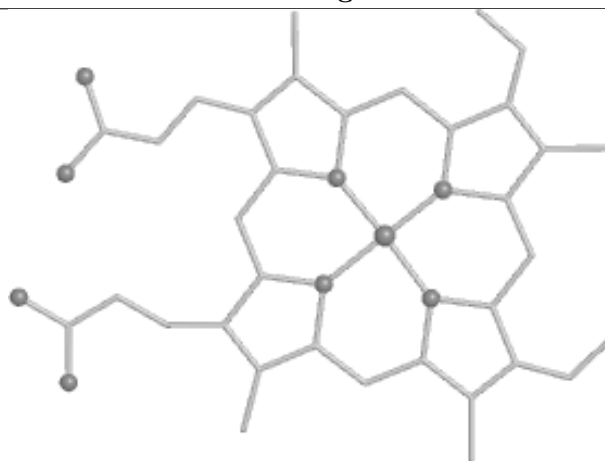
Bond lengths



Bond angles

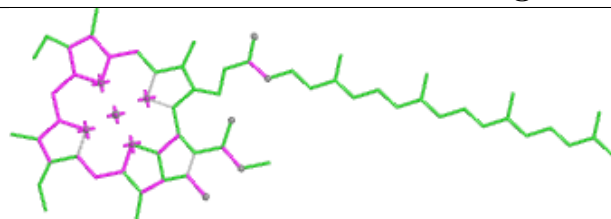


Torsions

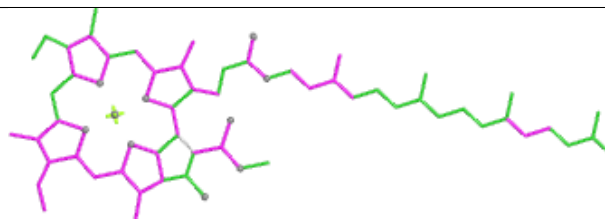


Rings

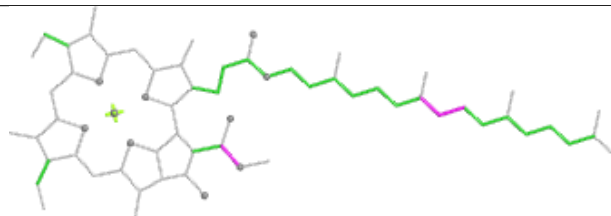
Ligand CLA D 404



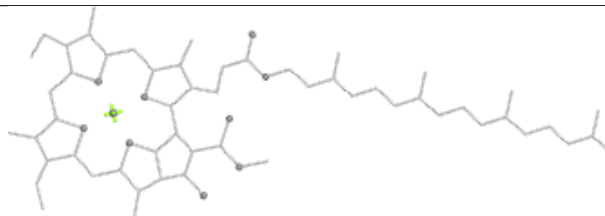
Bond lengths



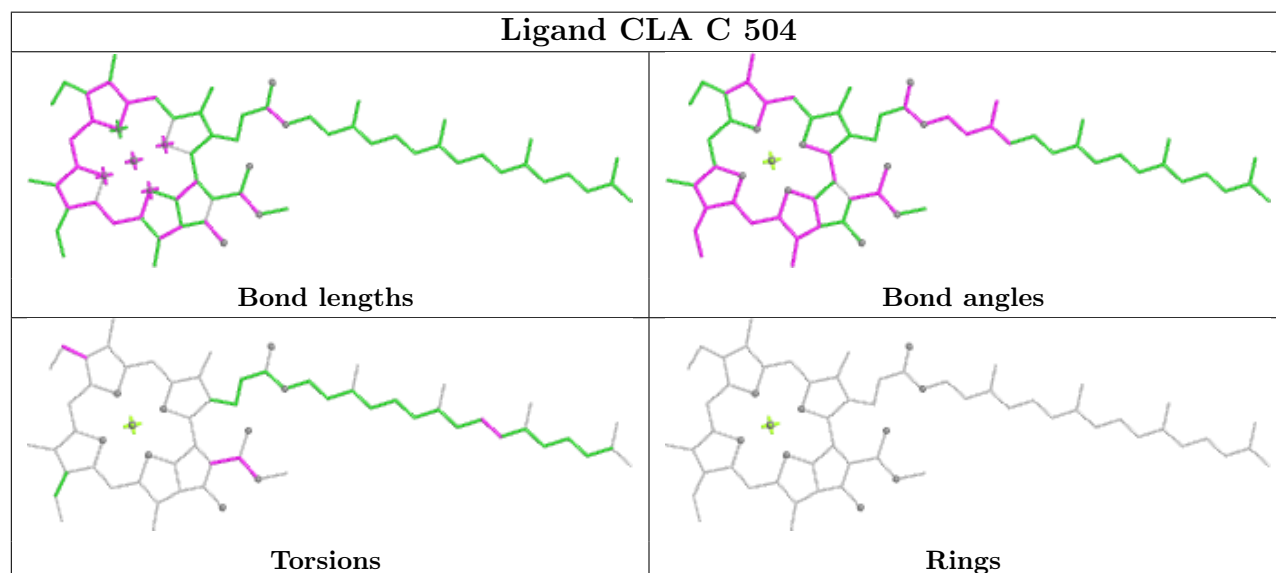
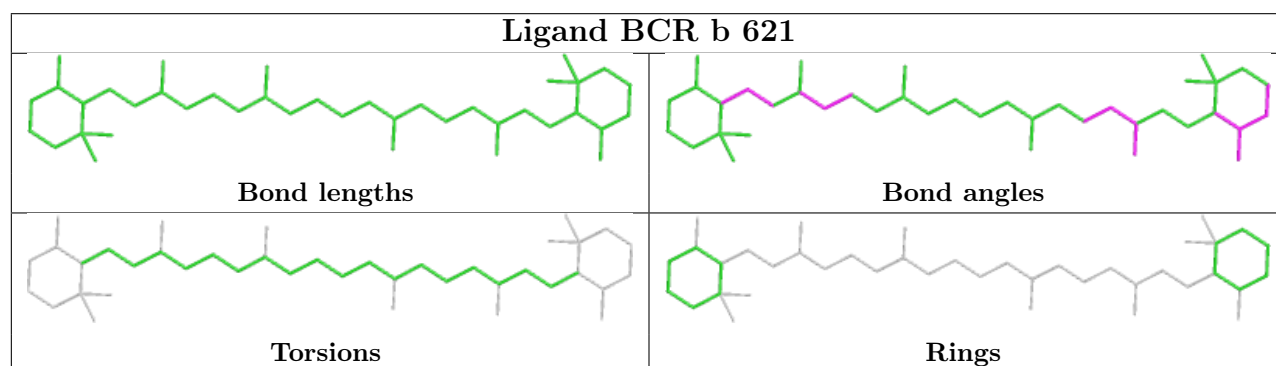
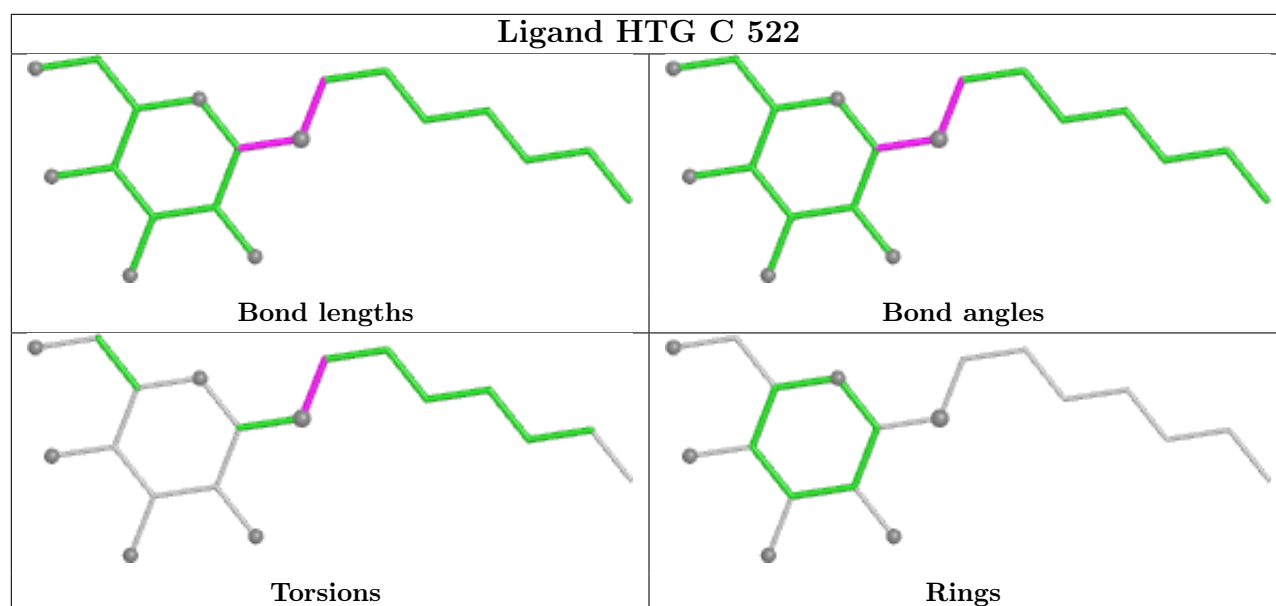
Bond angles

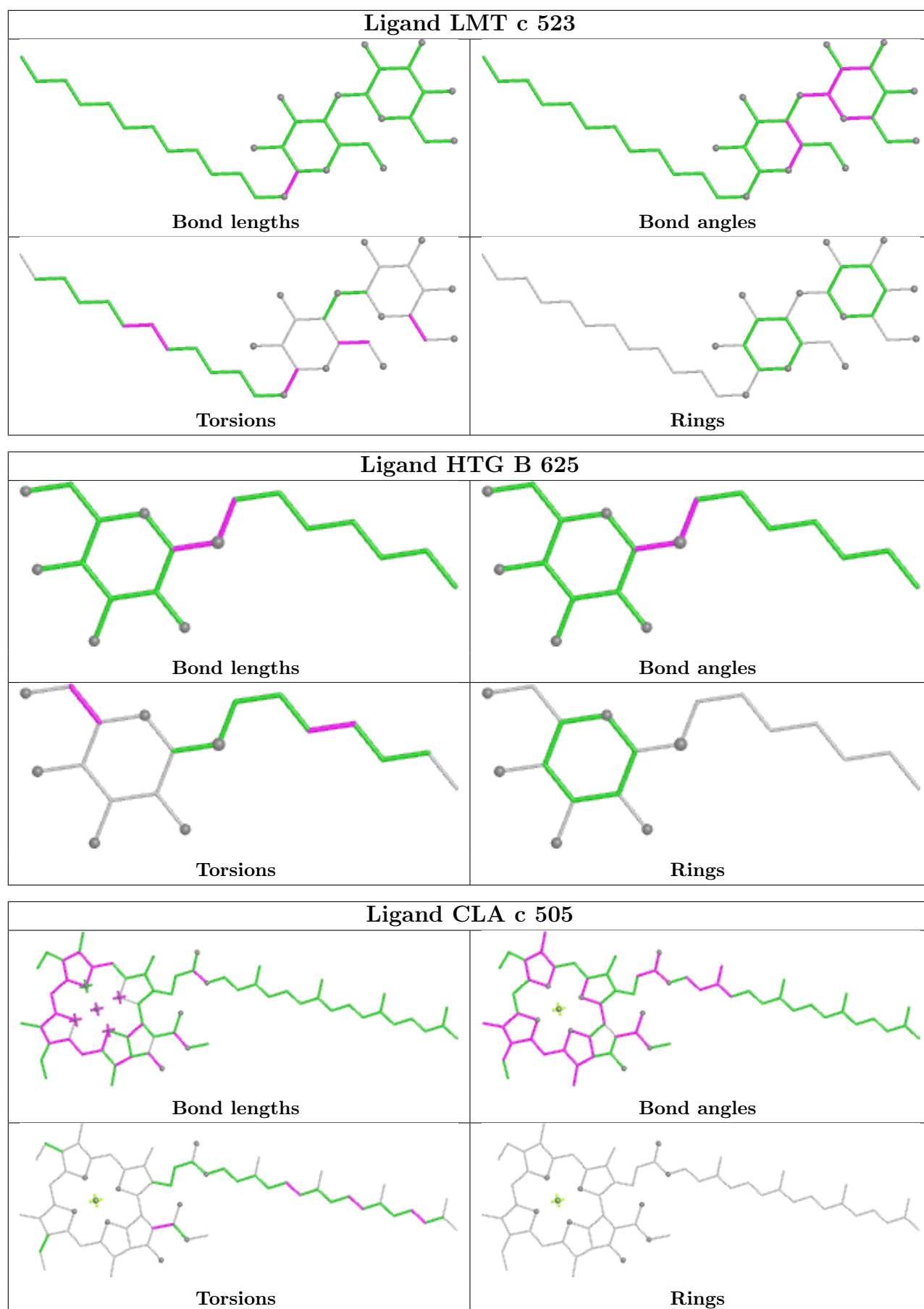


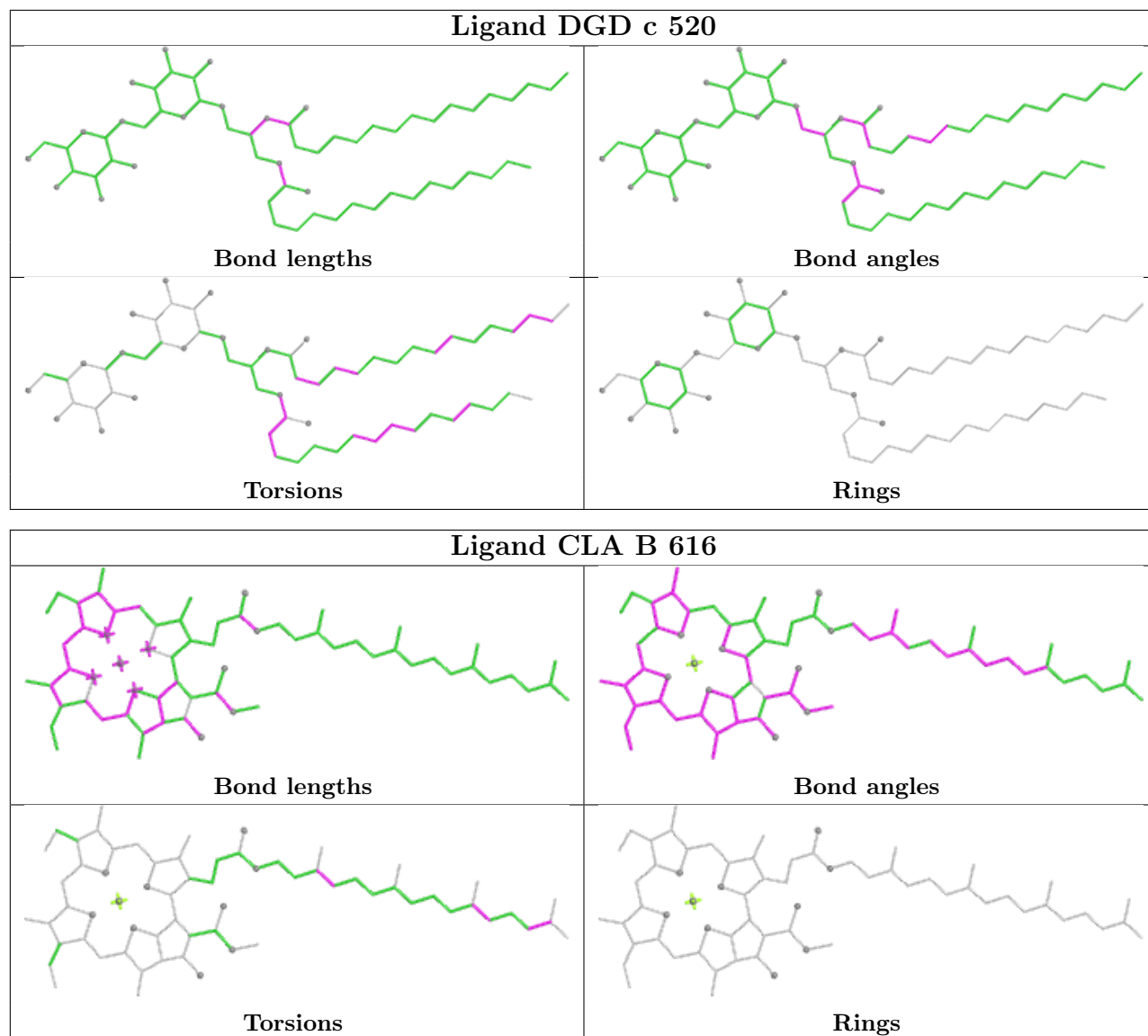
Torsions

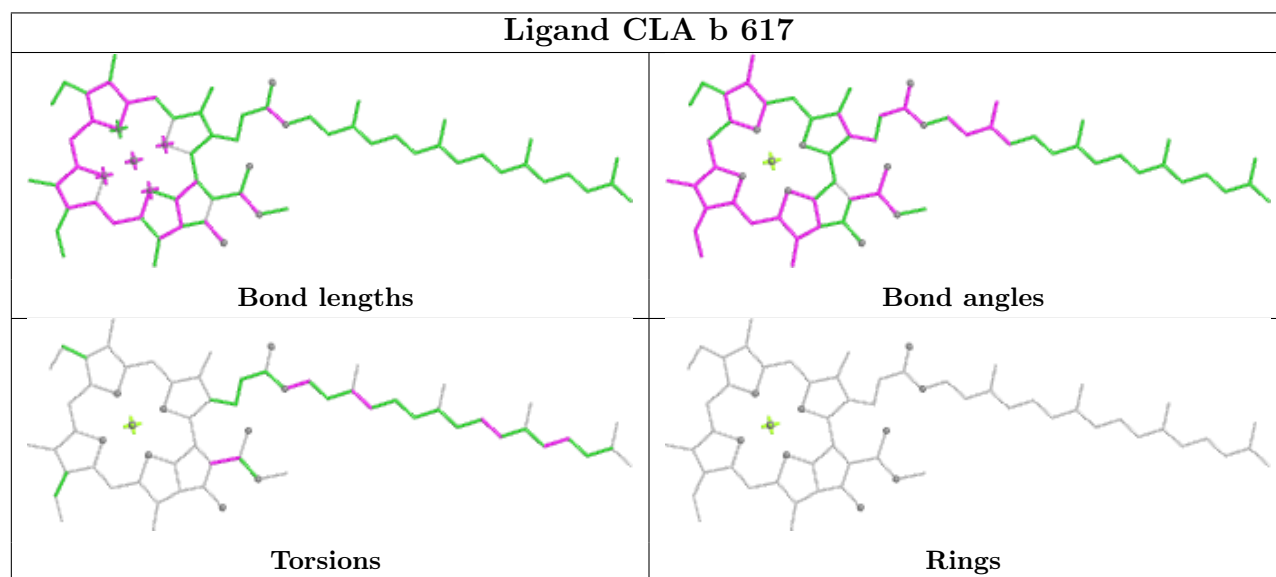
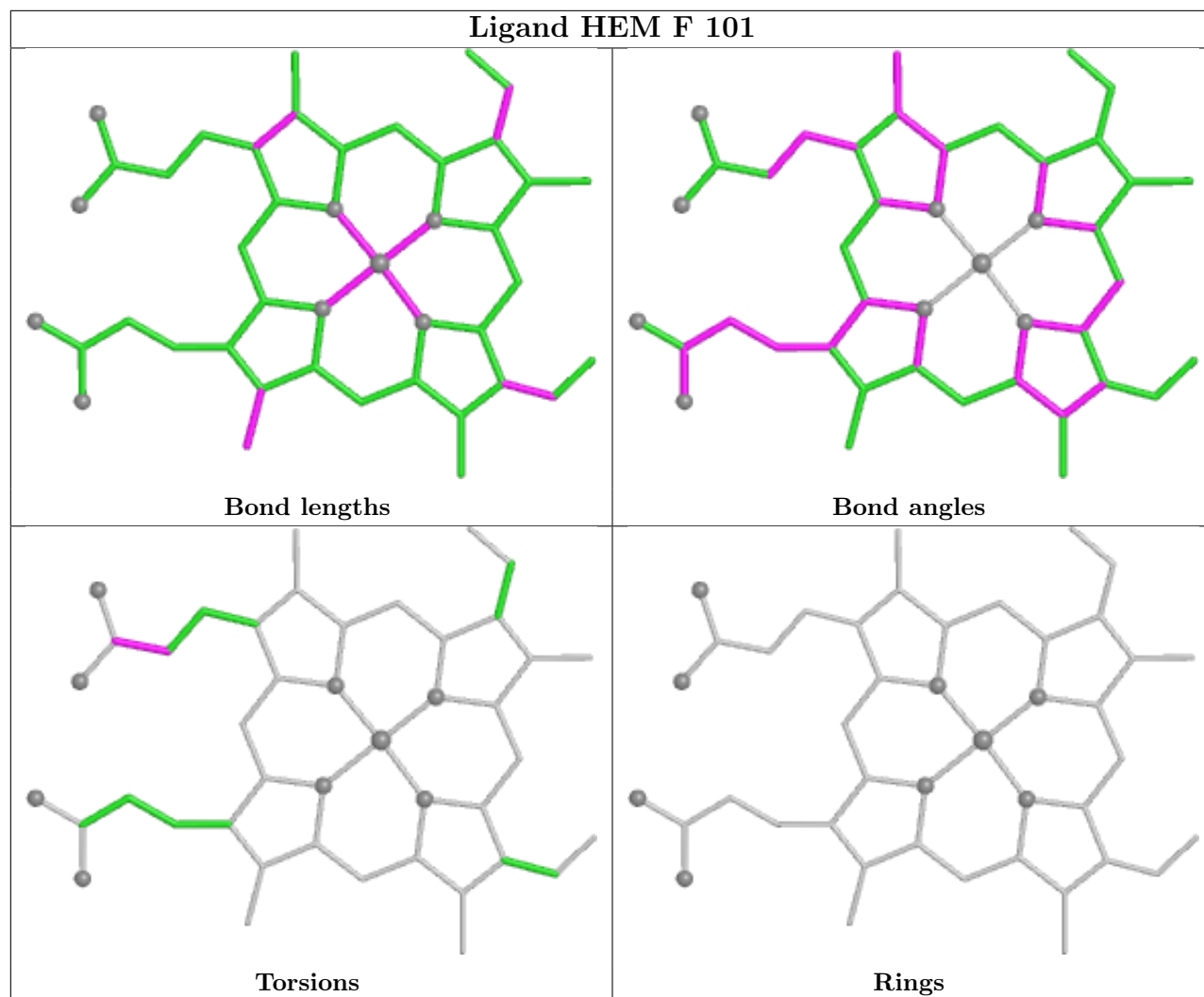


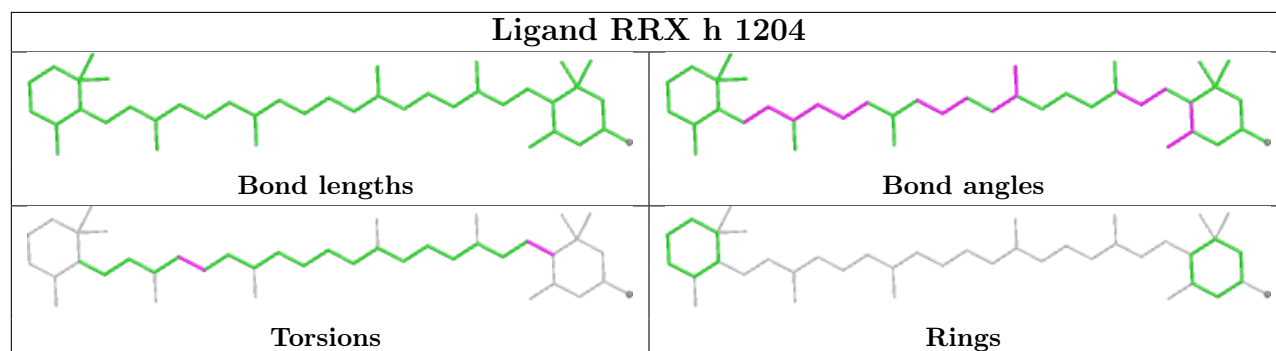
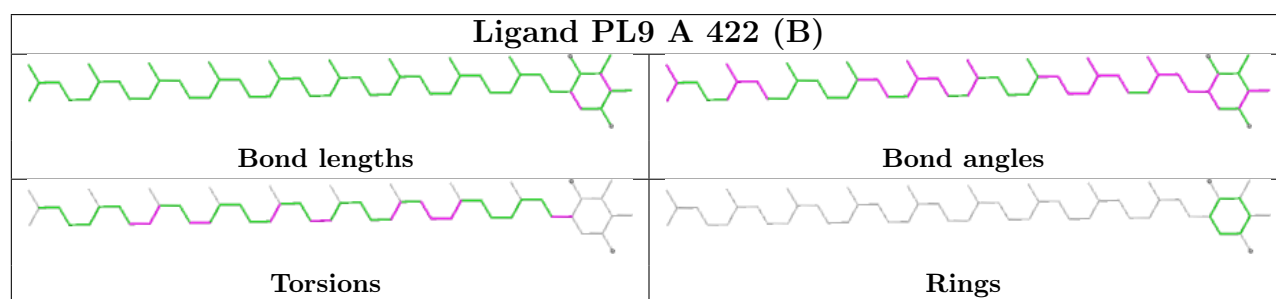
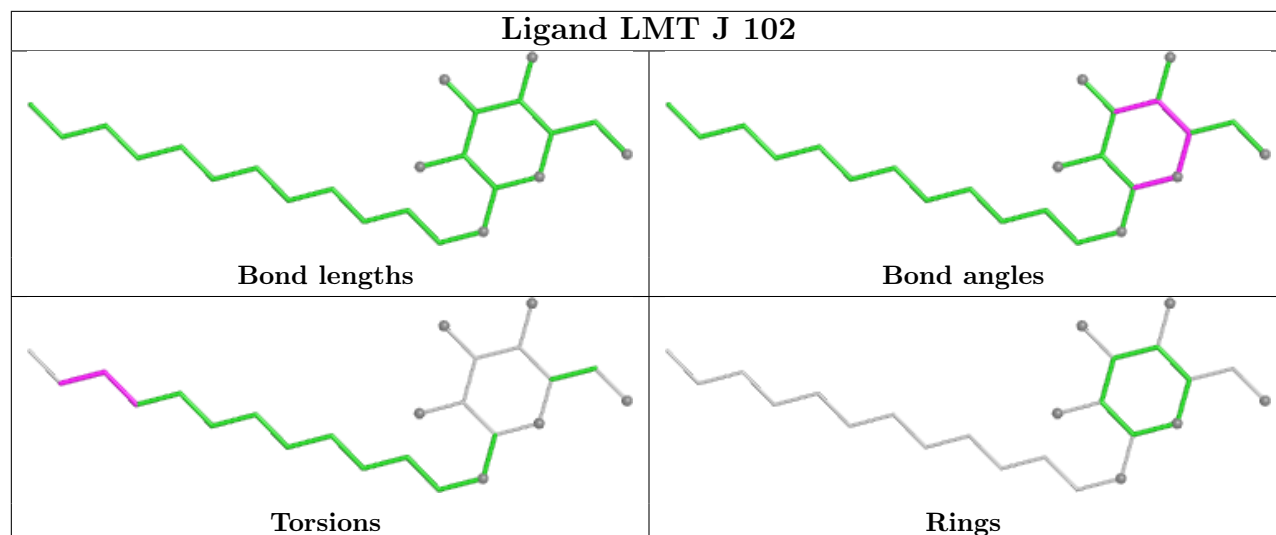
Rings

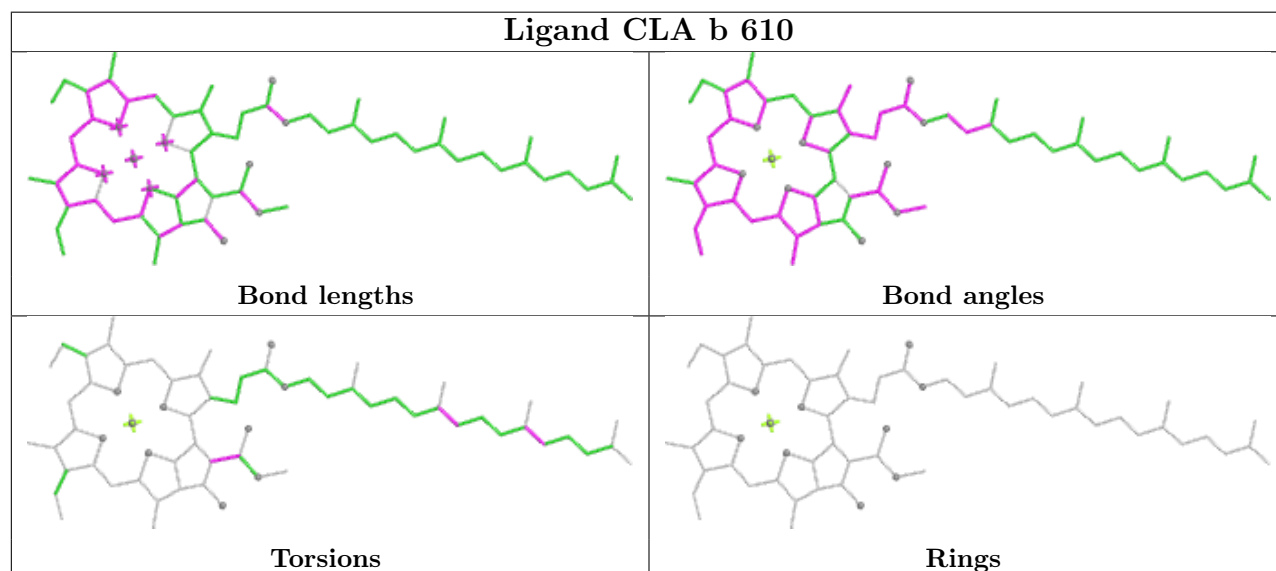
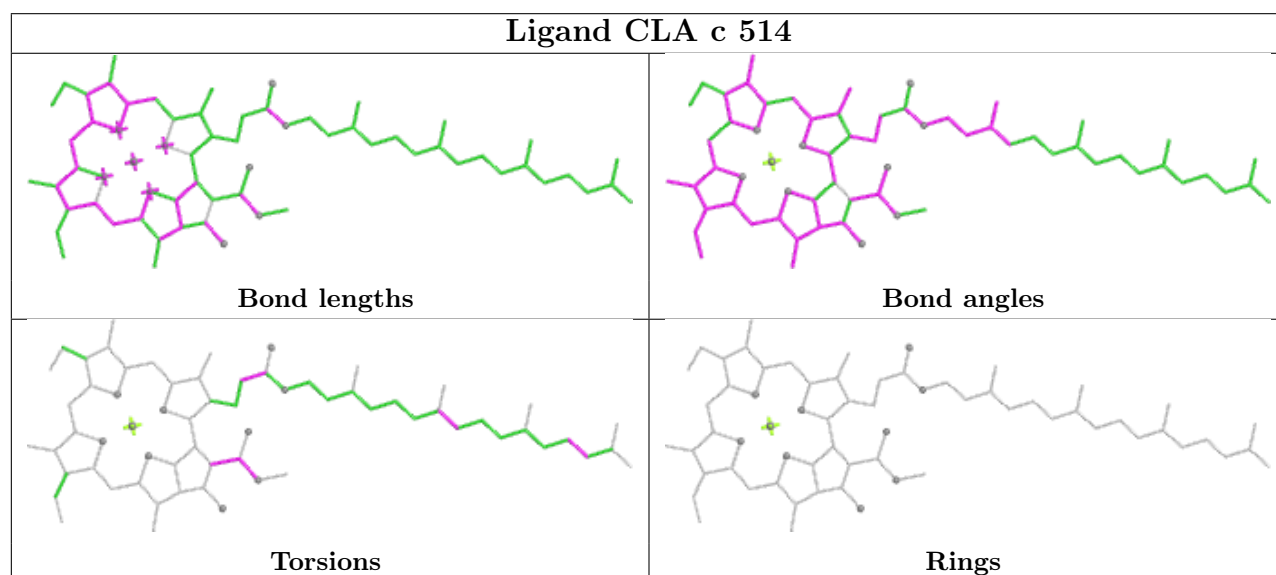
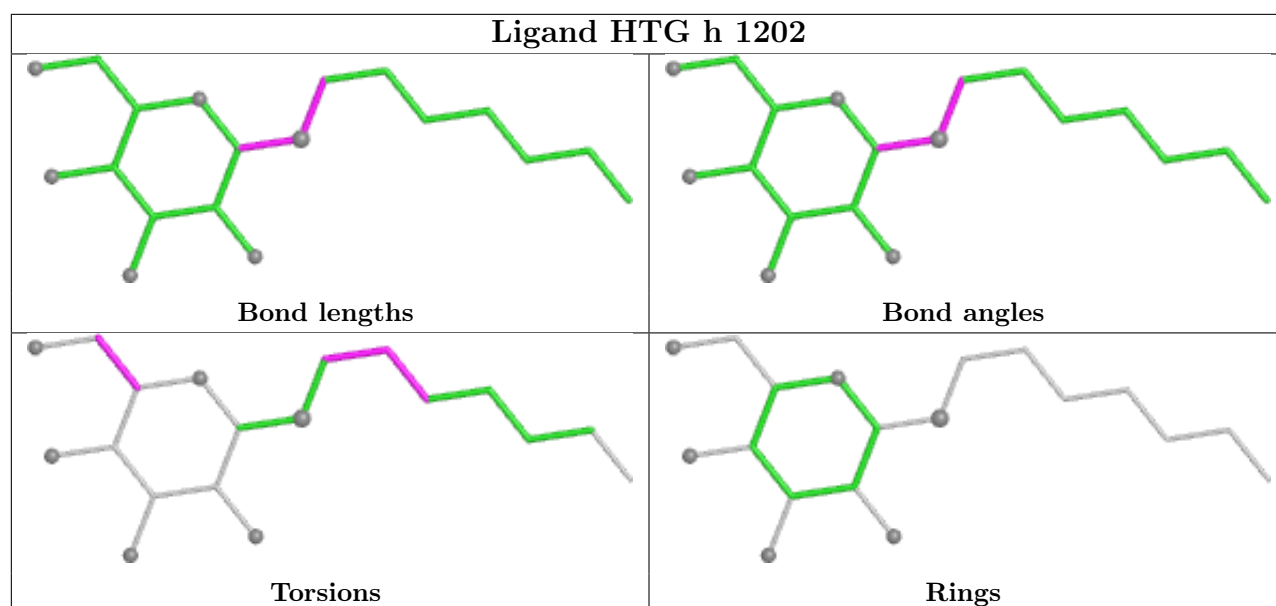


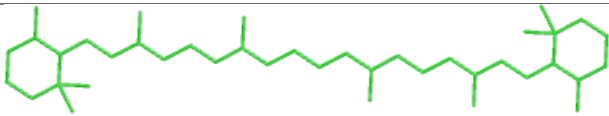
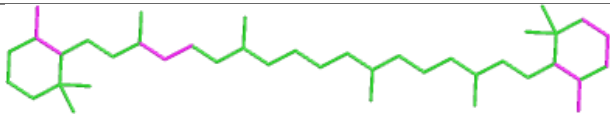
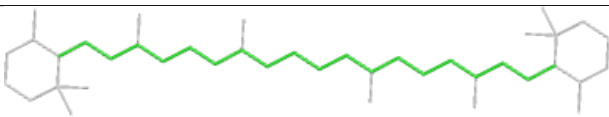
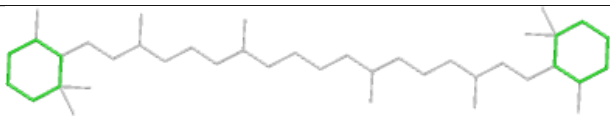


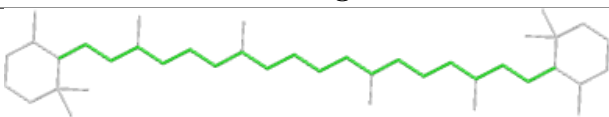
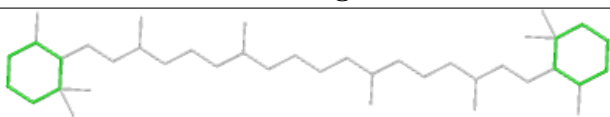


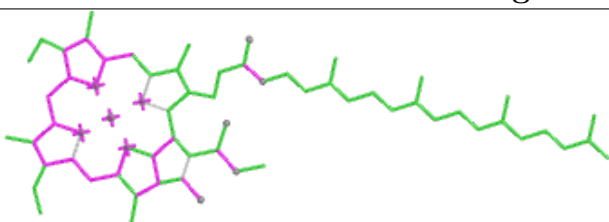
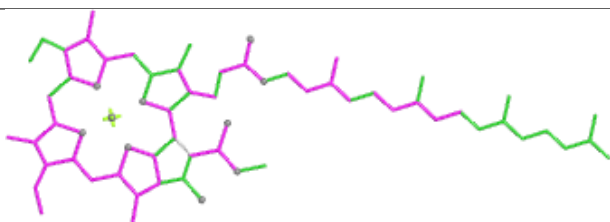
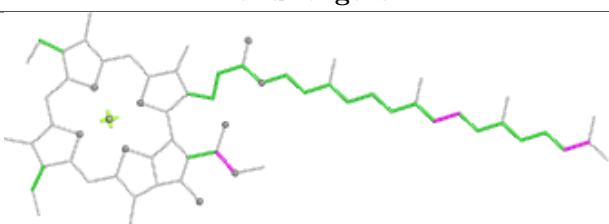
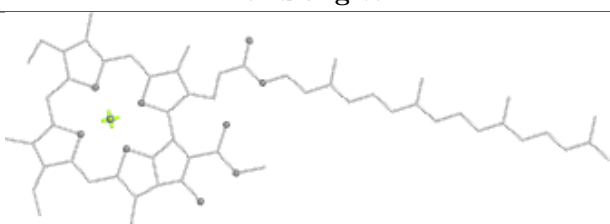


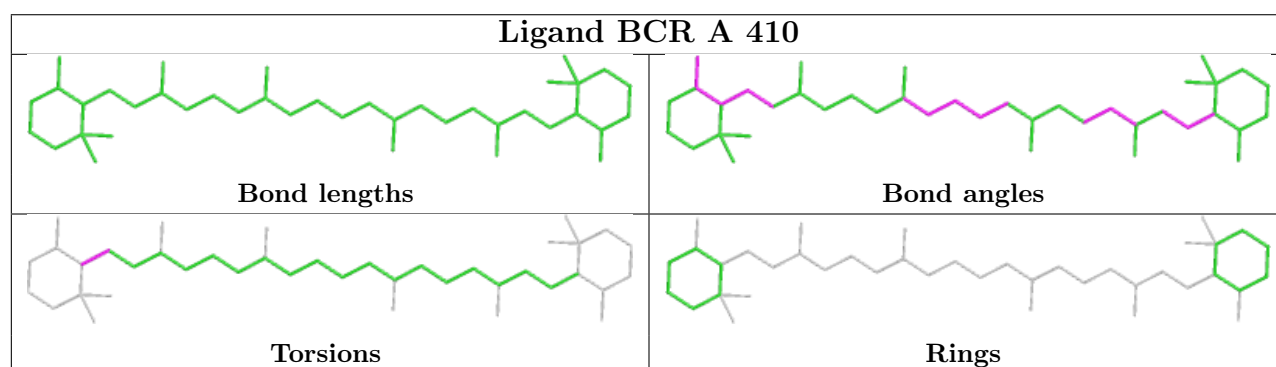
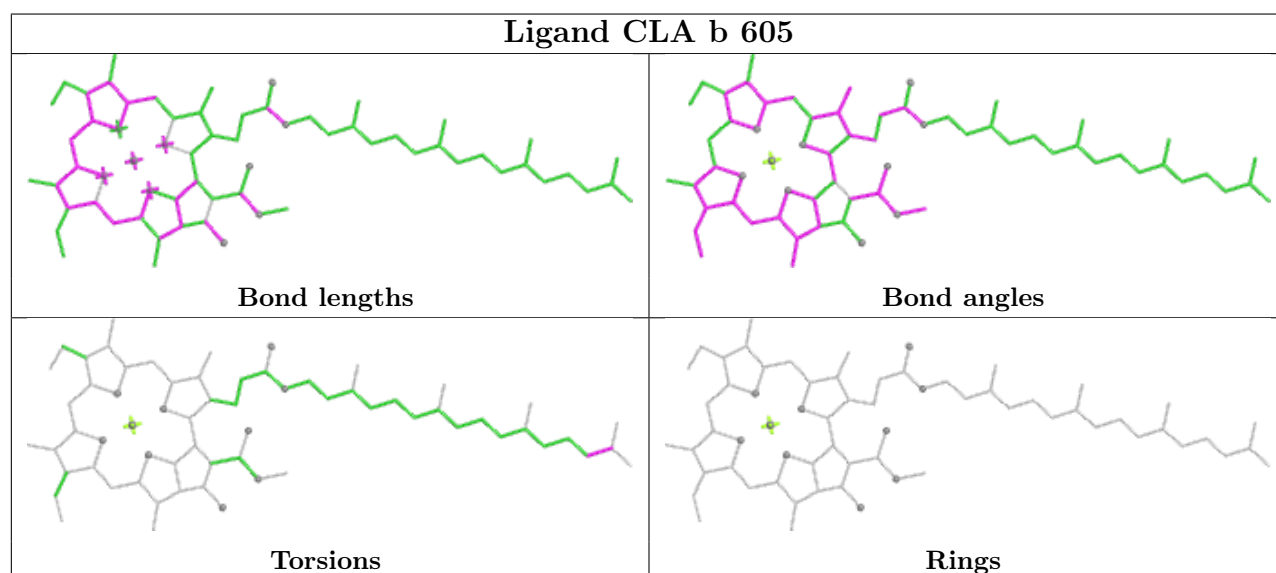
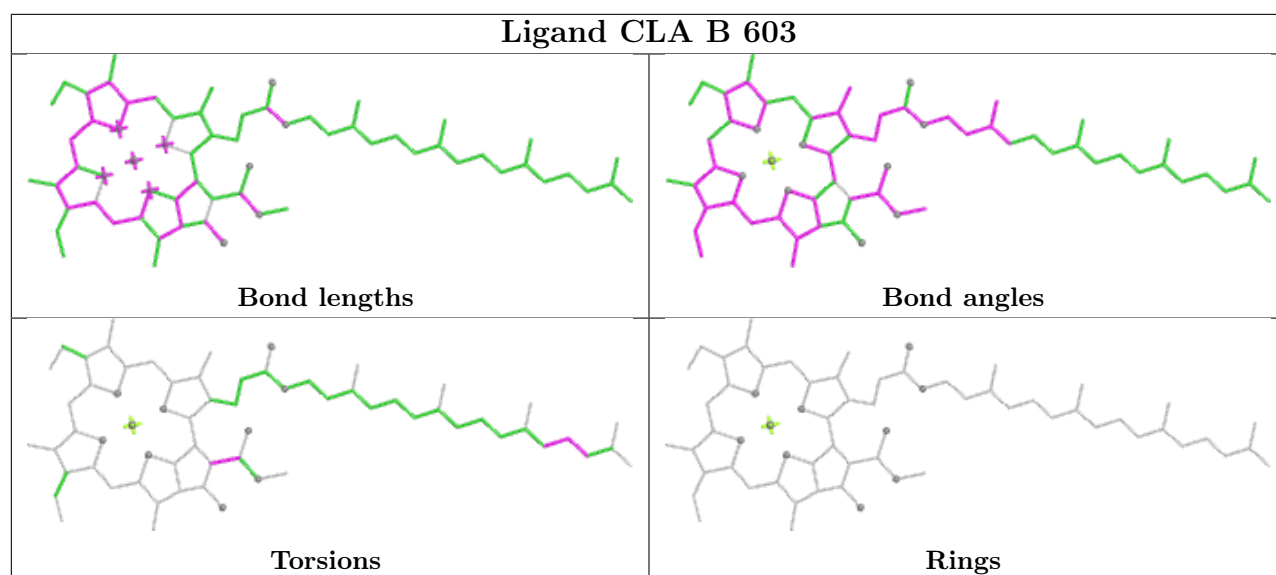


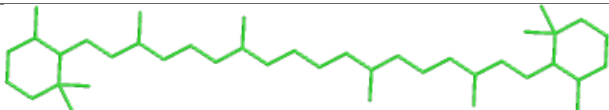
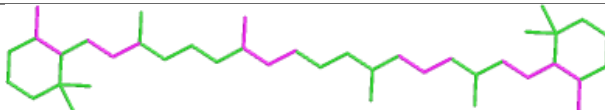
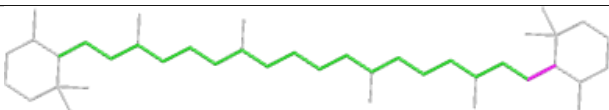
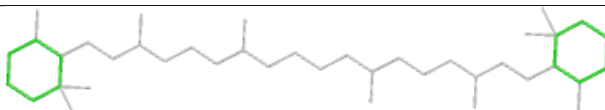


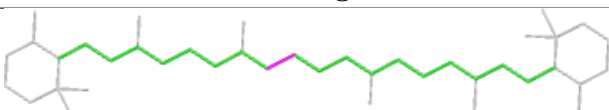
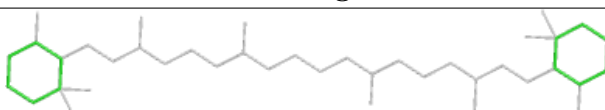
Ligand BCR B 619	
	
Bond lengths	Bond angles
	
Torsions	Rings

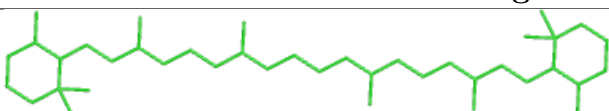
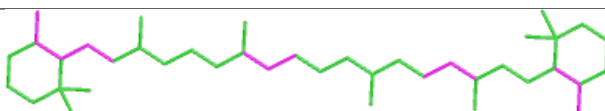
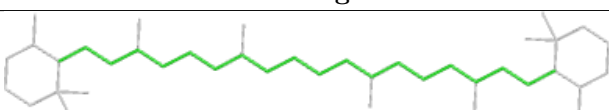
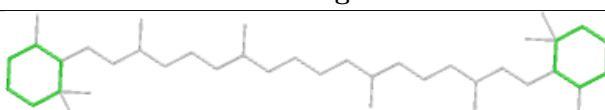
Ligand BCR a 413	
	
Bond lengths	Bond angles
	
Torsions	Rings

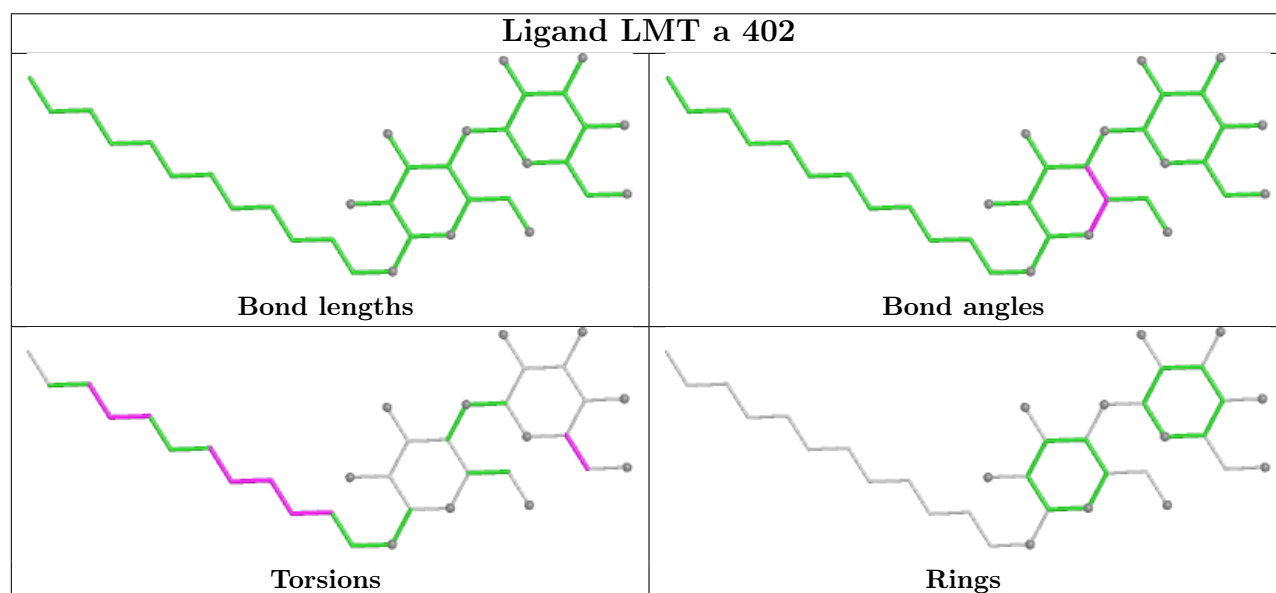
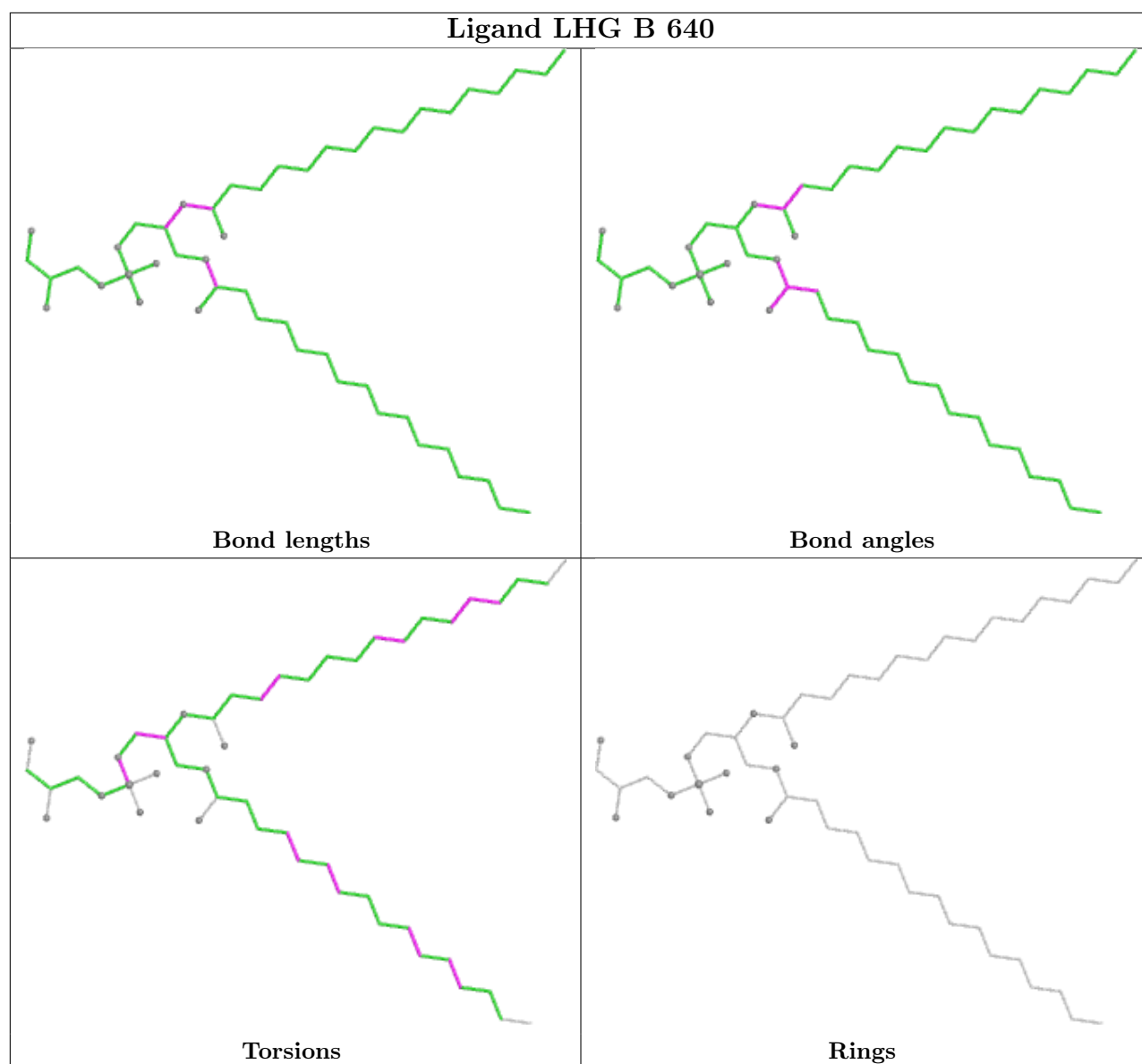
Ligand CLA d 405	
	
Bond lengths	Bond angles
	
Torsions	Rings

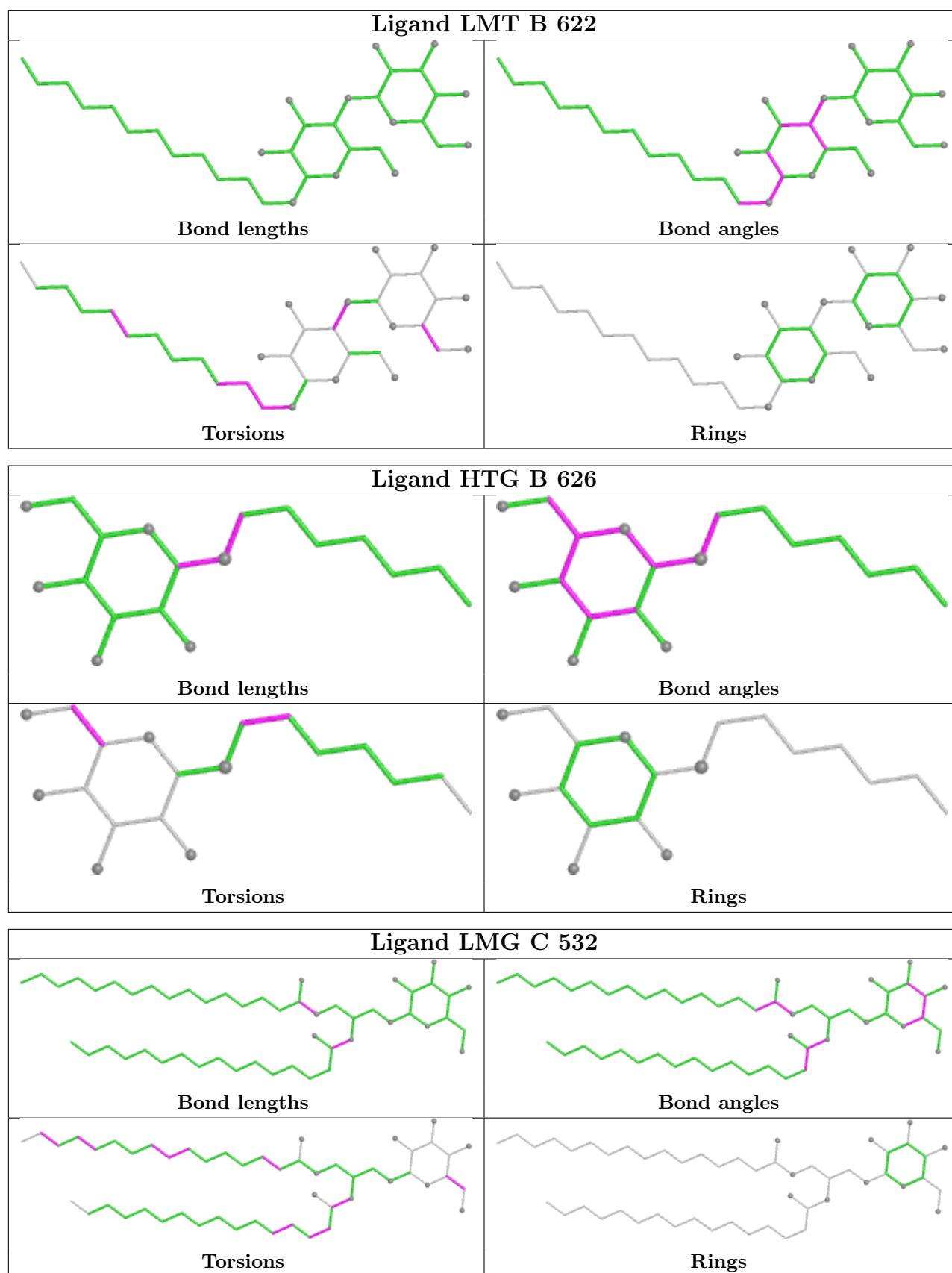


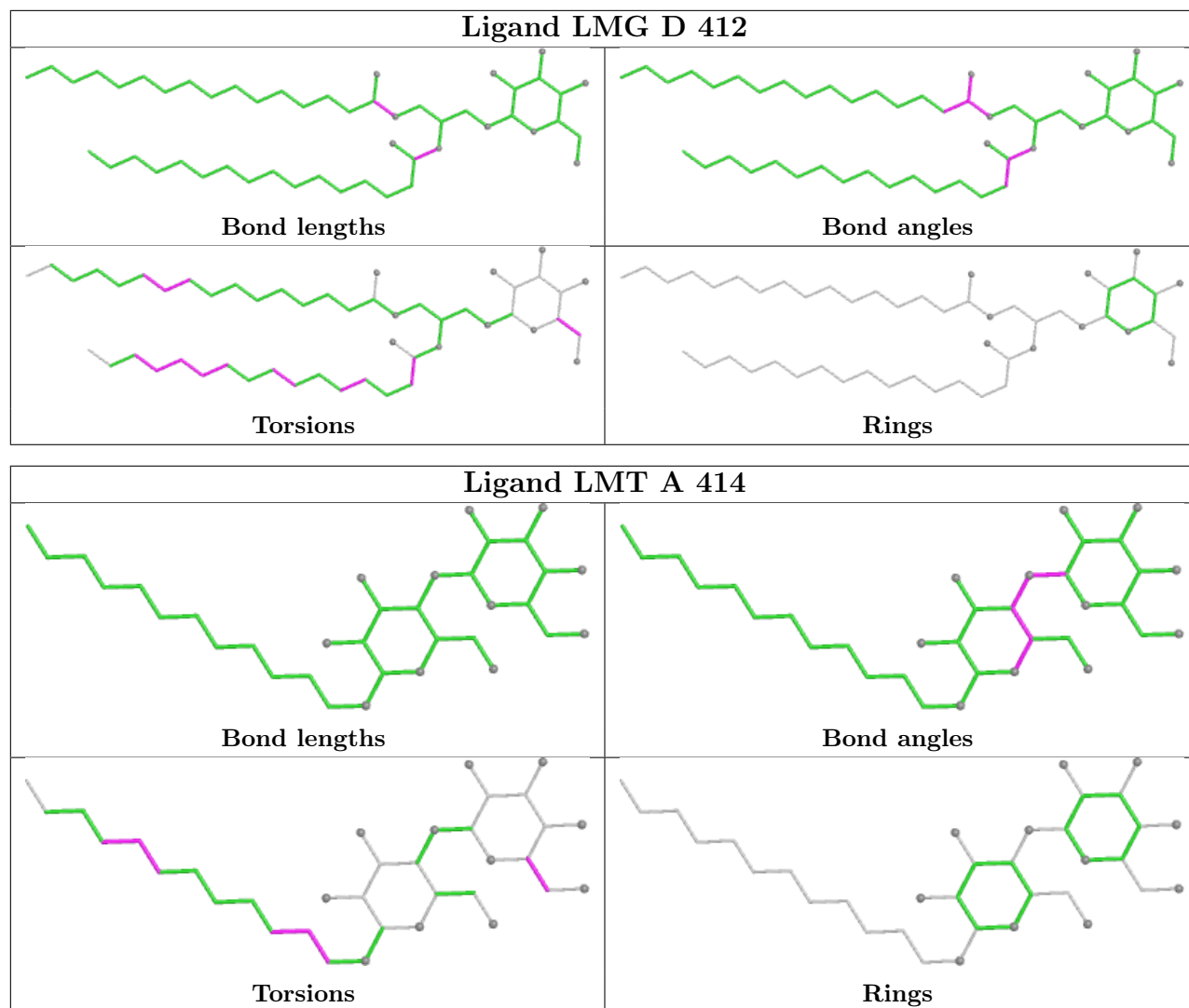
Ligand BCR C 516	
	
Bond lengths	Bond angles
	
Torsions	Rings

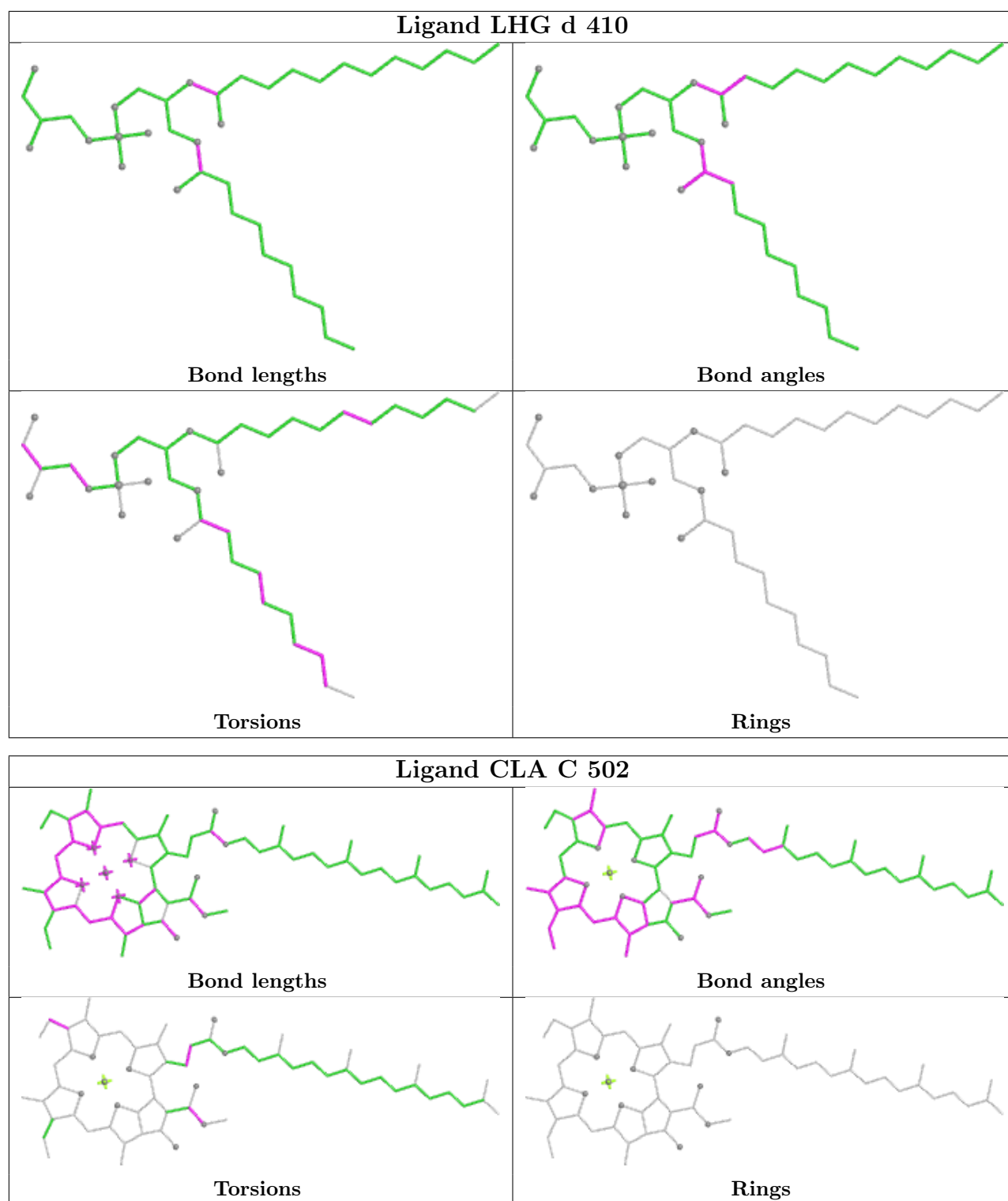
Ligand BCR T 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

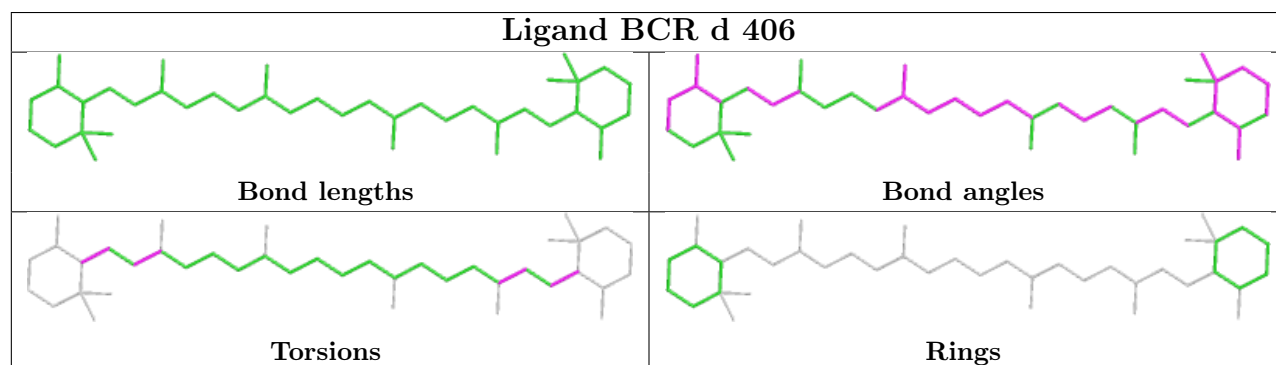
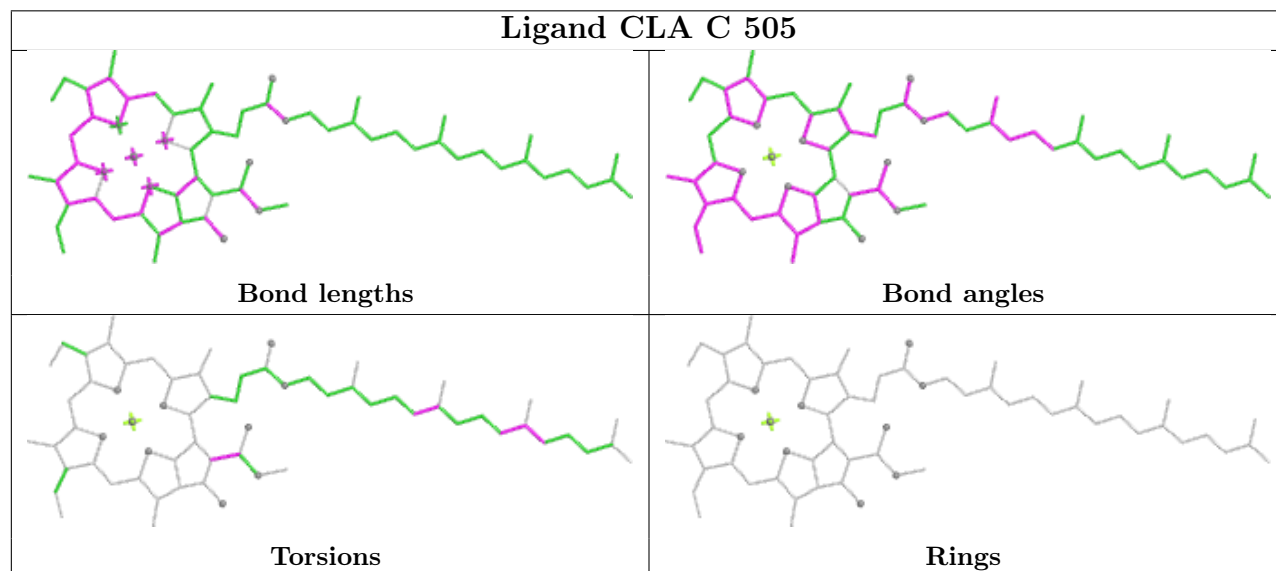
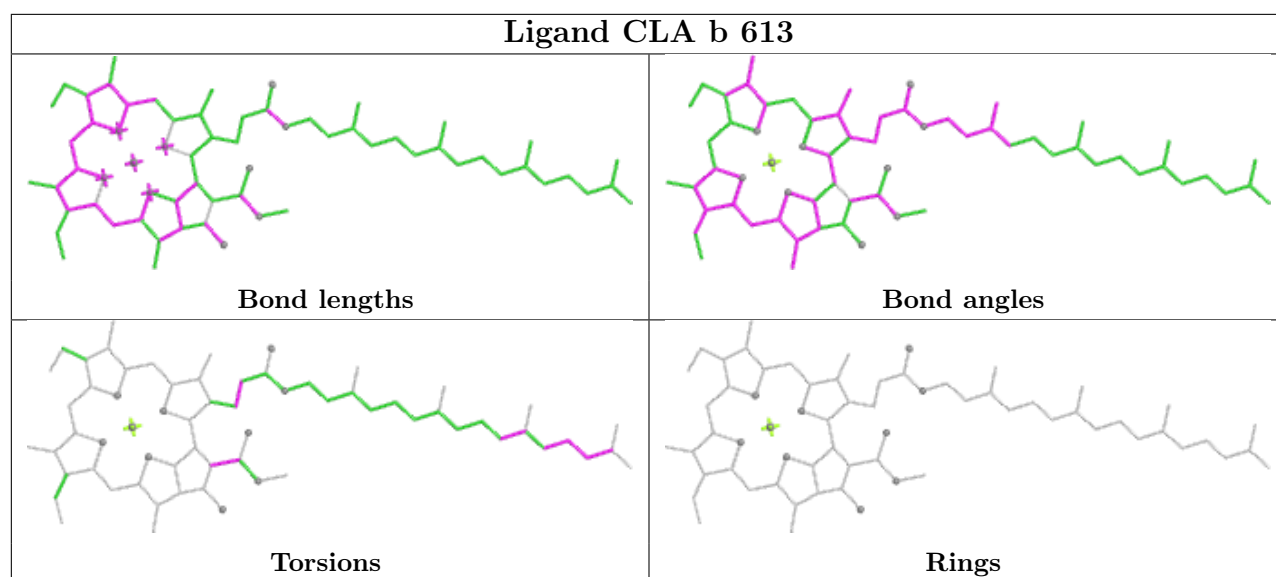
Ligand BCR c 516	
	
Bond lengths	Bond angles
	
Torsions	Rings

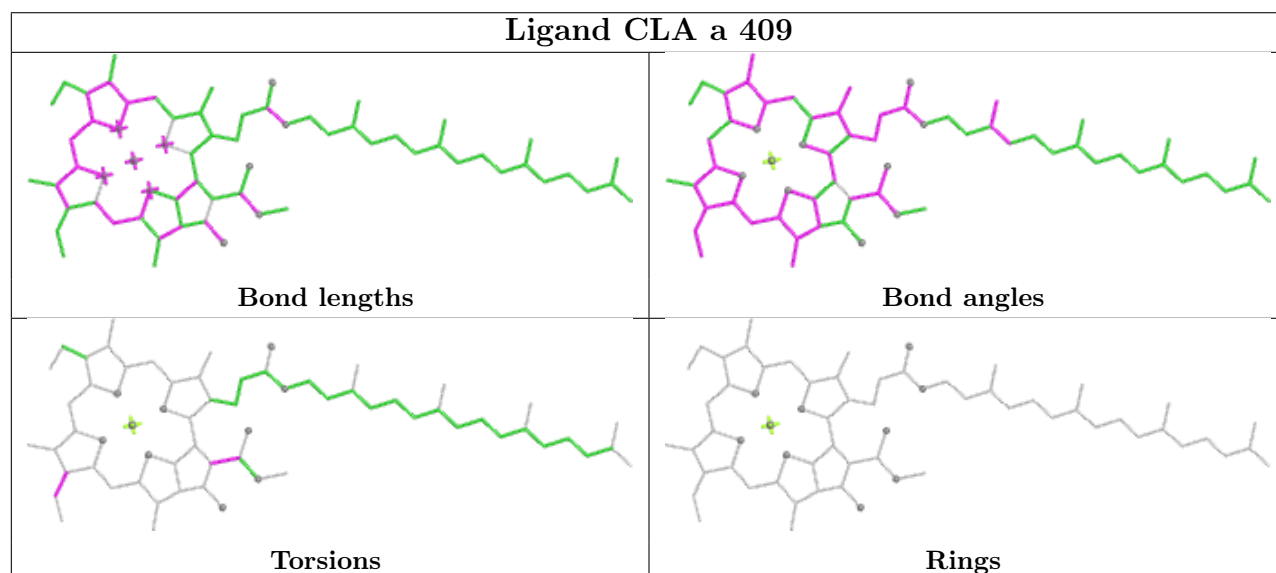
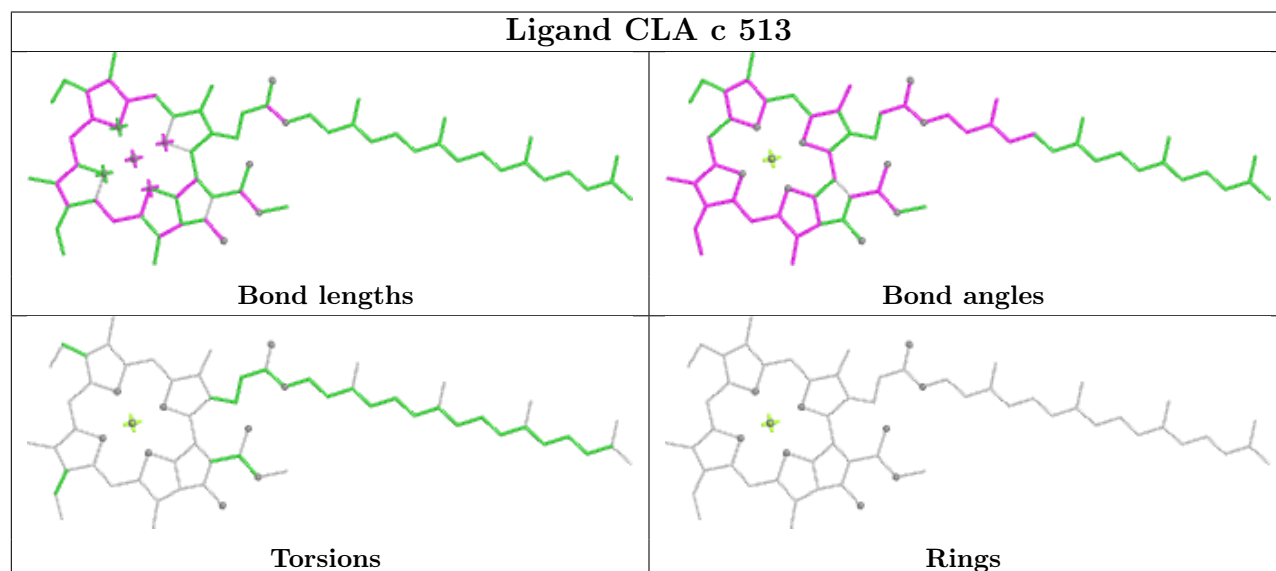
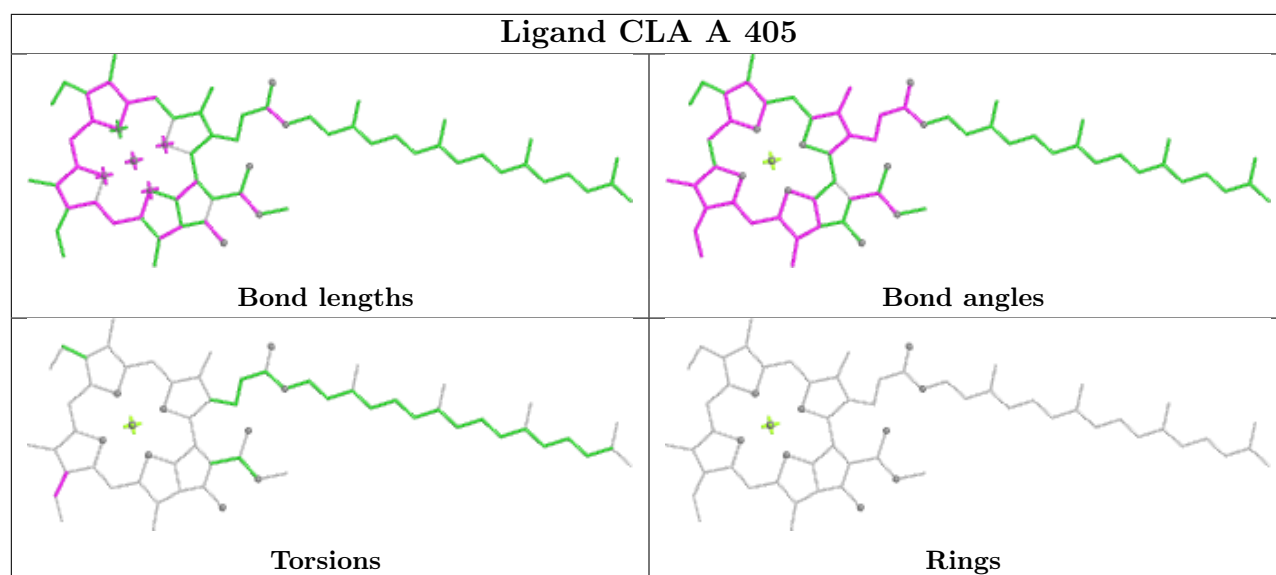












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	334/344 (97%)	-0.08	5 (1%) 72 78	24, 37, 60, 107	3 (0%)
1	a	334/344 (97%)	-0.07	6 (1%) 67 75	26, 39, 72, 113	3 (0%)
2	B	505/505 (100%)	-0.04	11 (2%) 62 69	24, 41, 67, 98	9 (1%)
2	b	503/505 (99%)	0.07	16 (3%) 50 56	27, 45, 79, 146	10 (1%)
3	C	451/455 (99%)	0.02	3 (0%) 84 88	33, 47, 64, 116	2 (0%)
3	c	455/455 (100%)	0.11	7 (1%) 72 78	31, 51, 67, 121	2 (0%)
4	D	341/342 (99%)	-0.14	2 (0%) 85 89	19, 38, 53, 116	1 (0%)
4	d	341/342 (99%)	-0.14	2 (0%) 85 89	22, 42, 63, 115	2 (0%)
5	E	81/83 (97%)	0.36	3 (3%) 45 52	41, 54, 77, 107	0
5	e	79/83 (95%)	0.51	4 (5%) 33 39	49, 63, 102, 131	0
6	F	34/44 (77%)	-0.07	1 (2%) 53 60	41, 46, 66, 88	0
6	f	31/44 (70%)	0.24	2 (6%) 25 28	47, 54, 71, 107	0
7	H	63/63 (100%)	0.20	2 (3%) 50 56	39, 48, 62, 106	0
7	h	63/63 (100%)	0.32	2 (3%) 50 56	43, 54, 69, 103	0
8	I	35/38 (92%)	0.69	3 (8%) 16 19	44, 53, 98, 126	0
8	i	35/38 (92%)	0.21	1 (2%) 53 60	42, 51, 89, 144	0
9	J	36/40 (90%)	0.27	1 (2%) 55 62	39, 51, 83, 101	0
9	j	39/40 (97%)	0.44	1 (2%) 57 64	46, 60, 129, 148	0
10	K	37/37 (100%)	-0.03	0 100 100	34, 52, 68, 82	1 (2%)
10	k	37/37 (100%)	0.30	1 (2%) 56 62	49, 59, 74, 90	0
11	L	37/37 (100%)	-0.05	2 (5%) 31 37	19, 36, 83, 113	1 (2%)
11	l	37/37 (100%)	-0.13	1 (2%) 56 62	21, 36, 85, 112	2 (5%)
12	M	32/36 (88%)	-0.16	0 100 100	22, 37, 54, 85	1 (3%)
12	m	33/36 (91%)	-0.14	0 100 100	22, 37, 59, 88	3 (9%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/244 (100%)	0.08	2 (0%) 82 86	28, 50, 90, 139	6 (2%)
13	o	243/244 (99%)	0.20	4 (1%) 70 77	25, 50, 96, 134	5 (2%)
14	T	29/32 (90%)	-0.09	1 (3%) 48 54	32, 37, 71, 108	0
14	t	29/32 (90%)	0.05	1 (3%) 48 54	32, 37, 67, 88	0
15	U	97/104 (93%)	0.00	0 100 100	37, 49, 73, 80	1 (1%)
15	u	97/104 (93%)	0.02	0 100 100	36, 51, 71, 102	1 (1%)
16	V	137/137 (100%)	-0.11	1 (0%) 84 88	25, 46, 62, 85	2 (1%)
16	v	137/137 (100%)	0.05	0 100 100	31, 56, 77, 107	1 (0%)
17	Y	28/30 (93%)	0.85	3 (10%) 11 12	50, 62, 117, 138	0
17	y	28/30 (93%)	0.94	2 (7%) 22 25	59, 75, 110, 127	0
18	X	38/40 (95%)	0.30	0 100 100	46, 56, 69, 91	0
18	x	37/40 (92%)	0.51	3 (8%) 18 21	36, 63, 101, 124	1 (2%)
19	Z	61/62 (98%)	0.46	2 (3%) 49 55	52, 64, 100, 117	0
19	z	60/62 (96%)	1.00	9 (15%) 5 6	61, 74, 107, 118	0
20	R	34/41 (82%)	1.57	10 (29%) 1 1	68, 92, 107, 117	0
All	All	5272/5387 (97%)	0.07	114 (2%) 62 69	19, 46, 80, 148	57 (1%)

The worst 5 of 114 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
18	x	37	VAL	5.7
2	b	486	LEU	5.6
2	B	86	ILE	5.3
2	B	479	PHE	4.9
2	b	484	PRO	4.3

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
19	FME	Z	1	10/11	0.79	0.14	88,100,114,119	0
14	FME	t	1	10/11	0.93	0.10	34,38,57,70	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	0.94	0.08	37,44,64,68	0
12	FME	m	1	10/11	0.95	0.11	42,50,78,87	0
12	FME	M	1	10/11	0.95	0.09	44,51,79,81	0
4	HSK	d	336[A]	10/12	0.96	0.08	46,49,54,56	7
4	HSK	d	336[B]	11/12	0.96	0.08	46,49,55,57	8
8	FME	i	1	10/11	0.96	0.08	43,48,54,55	0
4	HSK	D	336[B]	11/12	0.96	0.08	40,41,43,45	8
4	HSK	D	336[A]	10/12	0.96	0.08	40,42,44,46	7
8	FME	I	1	10/11	0.98	0.06	44,49,54,54	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
38	DMS	a	426	4/4	0.42	0.16	144,146,147,147	0
38	DMS	Y	303	4/4	0.47	0.19	141,143,145,146	0
38	DMS	o	309	4/4	0.50	0.21	140,142,142,143	0
38	DMS	z	102	4/4	0.58	0.19	141,143,143,144	0
31	UNL	b	635	15/-	0.61	0.23	89,106,109,110	0
38	DMS	b	636	4/4	0.62	0.25	134,135,138,139	0
38	DMS	C	525	4/4	0.65	0.21	111,114,116,117	0
38	DMS	o	307	4/4	0.65	0.23	121,123,123,124	0
31	UNL	D	415	12/-	0.67	0.26	79,86,92,94	0
29	LMT	C	521	35/35	0.67	0.17	76,138,158,160	0
30	GOL	h	1206	6/6	0.67	0.14	95,104,105,109	0
29	LMT	f	104	35/35	0.68	0.16	90,115,143,147	0
31	UNL	B	635	13/-	0.71	0.20	78,94,106,107	0
31	UNL	B	638	9/-	0.72	0.25	67,73,84,86	0
38	DMS	c	536	4/4	0.72	0.18	105,108,109,111	0
30	GOL	k	304	6/6	0.72	0.14	101,105,108,118	0
31	UNL	a	423	10/-	0.72	0.22	94,98,104,104	0
31	UNL	b	632	15/-	0.72	0.21	71,86,107,108	0
38	DMS	c	535	4/4	0.73	0.15	112,112,112,113	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
38	DMS	B	645	4/4	0.73	0.22	129,130,130,130	0
38	DMS	d	415	4/4	0.73	0.21	114,118,118,119	0
30	GOL	u	202	6/6	0.74	0.16	76,100,104,106	0
31	UNL	A	419	10/-	0.74	0.22	79,90,94,95	0
38	DMS	B	644	4/4	0.74	0.27	136,138,138,138	0
29	LMT	c	523	35/35	0.74	0.15	103,134,152,153	0
38	DMS	B	647	4/4	0.74	0.15	122,122,122,123	0
36	HTG	D	413	19/19	0.75	0.20	71,120,132,134	0
31	UNL	A	420	9/-	0.75	0.19	98,100,108,110	0
31	UNL	b	633	15/-	0.76	0.26	80,90,106,106	0
31	UNL	I	103	16/-	0.77	0.18	66,83,91,91	0
36	HTG	b	625	19/19	0.77	0.21	47,59,82,86	0
36	HTG	h	1202	19/19	0.77	0.18	89,109,120,121	0
31	UNL	I	104	15/-	0.77	0.20	87,94,102,103	0
39	DGD	D	407	53/66	0.77	0.17	76,89,137,139	0
31	UNL	B	639	15/-	0.78	0.26	88,95,108,108	0
38	DMS	o	304	4/4	0.78	0.24	101,113,115,116	0
31	UNL	a	422	11/-	0.78	0.15	87,91,95,96	0
37	LHG	e	101	40/49	0.79	0.17	90,135,148,150	0
31	UNL	h	1203	12/-	0.79	0.21	80,88,90,93	0
31	UNL	a	419	40/-	0.79	0.19	78,107,124,132	0
36	HTG	u	201	14/19	0.79	0.17	73,89,104,111	0
30	GOL	E	105	6/6	0.80	0.11	100,107,109,110	0
31	UNL	h	1201	15/-	0.80	0.18	87,104,123,123	0
38	DMS	B	643	4/4	0.80	0.22	87,99,102,103	0
30	GOL	c	532	6/6	0.80	0.16	59,87,90,93	0
31	UNL	h	1207	12/-	0.80	0.19	67,87,101,103	0
31	UNL	i	103	40/-	0.80	0.16	73,93,120,123	0
31	UNL	E	103	15/-	0.80	0.23	76,79,90,95	0
38	DMS	v	1608	4/4	0.80	0.26	118,122,124,126	0
30	GOL	d	413	6/6	0.80	0.13	74,93,98,99	0
31	UNL	A	417	40/-	0.80	0.19	74,94,119,122	0
31	UNL	B	637	10/-	0.81	0.17	89,96,99,100	0
31	UNL	E	102	15/-	0.81	0.23	77,85,99,99	0
29	LMT	m	103	35/35	0.81	0.14	57,74,104,105	0
31	UNL	k	301	16/-	0.81	0.29	82,118,131,131	0
31	UNL	c	501	40/-	0.81	0.19	76,101,136,137	0
38	DMS	o	306	4/4	0.81	0.24	113,116,117,117	0
31	UNL	e	102	15/-	0.81	0.20	76,82,97,98	0
36	HTG	b	626	19/19	0.81	0.15	74,133,142,142	0
38	DMS	C	533	4/4	0.81	0.22	99,102,107,111	0
36	HTG	d	414	19/19	0.81	0.18	71,103,114,118	19

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	GOL	v	1607	6/6	0.81	0.15	56,68,79,84	0
31	UNL	c	531	11/-	0.82	0.20	84,96,105,106	0
38	DMS	b	638	4/4	0.82	0.18	79,91,95,98	0
37	LHG	E	101	49/49	0.82	0.18	53,87,108,115	0
36	HTG	B	626	19/19	0.82	0.14	55,122,127,128	0
38	DMS	c	537	4/4	0.82	0.18	93,100,100,103	0
36	HTG	C	523	19/19	0.82	0.12	72,102,110,111	0
38	DMS	d	416	4/4	0.82	0.25	88,90,90,93	0
31	UNL	J	104	16/-	0.82	0.25	76,87,94,96	0
36	HTG	I	102	19/19	0.82	0.12	73,112,128,132	0
36	HTG	V	203	13/19	0.82	0.12	65,71,107,111	0
31	UNL	C	501	40/-	0.82	0.17	68,92,106,108	0
29	LMT	m	101	35/35	0.82	0.14	49,71,97,101	0
31	UNL	J	103	15/-	0.82	0.23	76,86,98,99	0
31	UNL	c	529	12/-	0.82	0.24	93,97,103,105	0
31	UNL	x	801	12/-	0.83	0.16	77,89,94,95	0
29	LMT	E	104	24/35	0.83	0.15	84,98,107,112	0
30	GOL	L	103	6/6	0.83	0.15	58,69,79,82	0
38	DMS	D	416	4/4	0.83	0.16	91,98,102,102	0
31	UNL	A	418	15/-	0.83	0.21	85,88,97,98	0
30	GOL	C	529	6/6	0.83	0.18	93,95,101,107	0
38	DMS	o	308	4/4	0.83	0.24	77,78,84,97	0
30	GOL	d	402	6/6	0.83	0.11	83,103,103,106	0
31	UNL	j	1302	16/-	0.83	0.18	69,82,99,100	0
31	UNL	b	631	16/-	0.83	0.18	58,63,74,76	0
38	DMS	B	646	4/4	0.83	0.20	108,110,113,115	0
31	UNL	b	634	9/-	0.84	0.21	67,85,95,96	0
36	HTG	U	201	9/19	0.84	0.18	71,84,122,126	0
38	DMS	O	304	4/4	0.84	0.19	83,99,100,102	0
31	UNL	i	101	16/-	0.84	0.22	59,67,82,84	0
33	PL9	a	425[B]	55/55	0.84	0.36	41,71,125,126	55
28	LMG	C	532	51/55	0.85	0.18	64,117,127,130	0
31	UNL	Y	301	12/-	0.85	0.23	82,91,97,98	0
35	CA	B	601	1/1	0.85	0.10	110,110,110,110	0
30	GOL	o	305	6/6	0.85	0.13	60,85,88,89	0
30	GOL	b	630	6/6	0.85	0.19	57,75,76,76	0
29	LMT	Z	101	35/35	0.85	0.16	54,108,130,136	0
31	UNL	B	634	18/-	0.85	0.15	73,82,96,99	0
31	UNL	C	531	18/-	0.85	0.17	69,93,106,107	0
38	DMS	E	106	4/4	0.85	0.19	109,113,116,119	0
30	GOL	a	418	6/6	0.86	0.15	69,82,85,86	0
29	LMT	M	101	35/35	0.86	0.13	47,71,83,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	GOL	c	527	6/6	0.86	0.16	65,68,78,86	0
36	HTG	B	624	19/19	0.86	0.12	62,98,106,108	19
28	LMG	c	522	51/55	0.86	0.16	58,121,129,132	0
29	LMT	z	101	32/35	0.86	0.14	63,112,129,131	0
29	LMT	b	624	25/35	0.86	0.16	69,95,125,130	0
27	SQD	f	102	33/54	0.86	0.15	74,97,122,123	0
27	SQD	L	101	54/54	0.86	0.15	55,83,128,132	0
30	GOL	O	303	6/6	0.86	0.09	73,77,82,88	0
30	GOL	T	101	6/6	0.86	0.15	37,55,59,63	0
30	GOL	v	1601	6/6	0.86	0.22	70,85,94,98	0
36	HTG	c	525	19/19	0.86	0.13	69,92,102,104	19
31	UNL	D	402	40/-	0.86	0.19	55,72,101,107	0
30	GOL	T	103	6/6	0.86	0.18	116,117,119,120	0
36	HTG	b	602	19/19	0.87	0.13	70,114,131,134	0
31	UNL	d	403	40/-	0.87	0.19	57,83,114,117	0
31	UNL	l	301	16/-	0.87	0.21	58,76,110,111	0
36	HTG	c	524	19/19	0.87	0.11	87,102,108,110	0
30	GOL	b	629	6/6	0.87	0.13	58,68,71,77	0
31	UNL	H	103	8/-	0.87	0.20	71,78,81,83	0
38	DMS	c	533	4/4	0.87	0.17	100,104,104,105	0
29	LMT	T	104	24/35	0.87	0.17	44,71,113,118	0
36	HTG	B	623[A]	19/19	0.87	0.17	39,52,67,67	19
36	HTG	B	623[B]	19/19	0.87	0.17	31,50,67,70	19
27	SQD	a	401	54/54	0.88	0.14	54,73,95,98	0
27	SQD	A	413	54/54	0.88	0.13	54,72,100,102	0
38	DMS	i	104	4/4	0.88	0.20	107,108,109,109	0
30	GOL	B	627	6/6	0.88	0.16	53,58,67,78	0
30	GOL	B	630	6/6	0.88	0.13	51,60,67,75	0
29	LMT	J	102	24/35	0.88	0.14	65,86,117,122	0
31	UNL	C	526	15/-	0.88	0.18	80,91,111,112	0
29	LMT	A	414	35/35	0.88	0.13	52,73,95,108	0
31	UNL	B	632	16/-	0.88	0.20	59,74,97,97	0
29	LMT	B	622	35/35	0.88	0.13	59,89,115,120	0
31	UNL	a	420	12/-	0.88	0.20	75,89,106,107	0
33	PL9	A	422[B]	55/55	0.89	0.22	54,80,96,98	55
27	SQD	L	102	54/54	0.89	0.14	52,76,113,120	0
38	DMS	V	207	4/4	0.89	0.18	97,105,106,109	0
30	GOL	c	526	6/6	0.89	0.15	58,80,93,98	0
30	GOL	B	631	6/6	0.89	0.15	49,60,67,73	0
31	UNL	c	530	11/-	0.89	0.17	85,92,105,108	0
31	UNL	j	1301	18/-	0.89	0.14	66,81,110,112	0
29	LMT	B	642	24/35	0.89	0.17	51,69,117,121	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	UNL	T	105	9/-	0.89	0.19	72,78,85,88	0
30	GOL	A	416	6/6	0.89	0.14	55,78,82,86	0
29	LMT	m	102	35/35	0.89	0.12	39,58,71,73	0
30	GOL	A	415	6/6	0.90	0.12	44,54,55,58	0
30	GOL	a	421	6/6	0.90	0.13	90,97,107,111	0
29	LMT	a	402	35/35	0.90	0.13	49,68,83,93	0
30	GOL	C	528	6/6	0.90	0.14	66,81,86,93	0
27	SQD	D	408	45/54	0.90	0.13	50,85,118,127	0
31	UNL	t	101	8/-	0.90	0.18	70,80,85,86	0
30	GOL	C	530	6/6	0.90	0.13	44,50,54,61	6
30	GOL	a	416	6/6	0.90	0.14	43,53,57,59	0
30	GOL	v	1606	6/6	0.90	0.10	74,86,91,98	0
31	UNL	B	636	18/-	0.90	0.14	56,74,98,108	0
35	CA	b	603	1/1	0.90	0.10	142,142,142,142	0
31	UNL	i	102	15/-	0.90	0.17	70,79,106,106	0
30	GOL	o	302	6/6	0.91	0.11	61,71,78,85	0
30	GOL	C	527	6/6	0.91	0.18	80,86,90,90	0
28	LMG	a	415	51/55	0.91	0.13	58,75,87,90	0
31	UNL	X	101	16/-	0.91	0.16	55,63,78,84	0
36	HTG	b	601	19/19	0.91	0.12	57,68,82,86	0
30	GOL	b	627	6/6	0.91	0.14	64,66,69,84	0
28	LMG	C	520	51/55	0.91	0.14	43,80,103,106	0
38	DMS	b	637	4/4	0.91	0.21	89,93,97,99	0
36	HTG	B	625	19/19	0.91	0.12	52,73,95,96	0
24	CLA	B	602	65/65	0.91	0.10	38,58,106,113	0
36	HTG	C	522	19/19	0.91	0.11	82,86,95,97	0
30	GOL	B	633	6/6	0.91	0.12	41,52,57,58	6
26	BCR	T	102	40/40	0.92	0.09	35,47,58,59	0
30	GOL	a	417	6/6	0.92	0.12	54,63,66,70	0
24	CLA	b	604	65/65	0.92	0.11	48,66,112,120	0
30	GOL	v	1602	6/6	0.92	0.10	64,75,79,86	0
28	LMG	c	521	51/55	0.92	0.14	48,80,115,117	0
31	UNL	x	802	18/-	0.92	0.14	60,74,107,110	0
30	GOL	V	204	6/6	0.92	0.12	42,53,56,57	0
31	UNL	d	412	16/-	0.93	0.18	54,71,95,97	0
28	LMG	d	411	51/55	0.93	0.12	45,53,108,114	0
26	BCR	K	101	40/40	0.93	0.10	39,49,56,59	0
27	SQD	a	414	54/54	0.93	0.12	54,73,92,96	0
37	LHG	D	409	49/49	0.93	0.11	40,49,57,62	0
38	DMS	c	534	4/4	0.93	0.13	62,74,78,78	0
24	CLA	C	507	65/65	0.93	0.11	43,58,101,104	0
28	LMG	A	412	51/55	0.93	0.13	51,73,97,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	UNL	D	414	16/-	0.93	0.16	46,62,78,84	0
28	LMG	B	621	51/55	0.93	0.11	45,52,69,84	0
26	BCR	b	622	40/40	0.93	0.09	41,49,61,68	0
24	CLA	b	619	65/65	0.93	0.10	40,47,113,115	0
24	CLA	c	508	65/65	0.93	0.12	47,57,86,89	0
31	UNL	I	101	16/-	0.93	0.13	50,63,75,76	0
30	GOL	B	629	6/6	0.93	0.14	50,65,76,78	0
30	GOL	V	205	6/6	0.93	0.09	72,87,90,100	0
28	LMG	b	623	51/55	0.93	0.13	45,56,76,79	0
32	K3C	a	424[A]	14/14	0.93	0.23	116,122,125,126	14
24	CLA	c	515	65/65	0.93	0.11	50,64,103,106	0
26	BCR	B	641	40/40	0.93	0.09	35,47,61,62	0
41	RRX	h	1204	41/41	0.93	0.09	41,53,65,73	0
30	GOL	M	102	6/6	0.94	0.08	36,38,61,71	0
24	CLA	b	609	65/65	0.94	0.09	36,46,76,79	0
24	CLA	b	617	65/65	0.94	0.11	32,41,97,106	0
26	BCR	c	516	40/40	0.94	0.11	58,70,74,76	0
30	GOL	V	201	6/6	0.94	0.09	56,73,76,84	0
30	GOL	B	628	6/6	0.94	0.09	44,49,50,52	0
37	LHG	d	408	49/49	0.94	0.10	38,52,66,74	0
26	BCR	d	406	40/40	0.94	0.10	42,51,76,82	0
37	LHG	l	302	49/49	0.94	0.10	38,47,66,78	0
30	GOL	V	206	6/6	0.94	0.07	55,56,63,63	0
26	BCR	k	303	40/40	0.94	0.10	49,56,65,67	0
27	SQD	A	411	54/54	0.94	0.12	40,69,91,94	0
30	GOL	v	1605	6/6	0.94	0.12	46,56,63,65	0
24	CLA	B	617	65/65	0.94	0.12	35,45,111,116	0
24	CLA	B	607	65/65	0.94	0.09	33,41,67,79	0
24	CLA	C	513	65/65	0.94	0.10	45,57,86,95	0
24	CLA	d	405	65/65	0.94	0.10	43,49,94,101	0
24	CLA	C	514	65/65	0.94	0.10	46,59,99,100	0
32	K3C	A	421[A]	14/14	0.94	0.21	84,85,87,88	14
26	BCR	D	405	40/40	0.94	0.10	36,45,76,77	0
39	DGD	h	1205	62/66	0.94	0.10	41,49,62,76	0
24	CLA	B	615	65/65	0.94	0.11	28,38,94,99	0
25	PHO	D	401	64/64	0.95	0.07	28,36,44,47	0
35	CA	f	103	1/1	0.95	0.08	86,86,86,86	0
26	BCR	B	618	40/40	0.95	0.07	34,40,47,48	0
26	BCR	B	619	40/40	0.95	0.07	34,41,56,63	0
26	BCR	B	620	40/40	0.95	0.07	38,44,58,60	0
24	CLA	C	504	65/65	0.95	0.08	40,47,56,67	0
26	BCR	C	515	40/40	0.95	0.09	47,62,66,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
26	BCR	C	516	40/40	0.95	0.09	42,52,57,59	0
24	CLA	D	404	65/65	0.95	0.09	36,42,98,100	0
24	CLA	c	506	65/65	0.95	0.09	40,48,77,80	0
30	GOL	v	1604	6/6	0.95	0.09	49,57,59,60	0
36	HTG	O	302	19/19	0.95	0.10	42,46,68,71	0
24	CLA	a	412	65/65	0.95	0.10	33,41,113,114	0
26	BCR	Y	302	40/40	0.95	0.08	44,50,58,64	0
28	LMG	D	412	51/55	0.95	0.11	37,51,102,112	0
26	BCR	a	413	40/40	0.95	0.07	29,39,45,46	0
26	BCR	b	620	40/40	0.95	0.08	37,43,49,51	0
26	BCR	b	621	40/40	0.95	0.08	34,46,59,63	0
24	CLA	c	509	65/65	0.95	0.10	41,49,68,77	0
24	CLA	c	510	65/65	0.95	0.09	38,47,105,126	0
30	GOL	b	628	6/6	0.95	0.09	47,58,62,64	0
26	BCR	c	517	40/40	0.95	0.09	45,52,66,72	0
36	HTG	o	301	19/19	0.95	0.10	40,48,64,67	0
24	CLA	c	514	65/65	0.95	0.10	49,60,88,94	0
26	BCR	k	302	40/40	0.95	0.09	48,56,67,70	0
37	LHG	D	411	46/49	0.95	0.11	36,44,100,104	0
24	CLA	B	610	65/65	0.95	0.07	37,42,47,54	0
33	PL9	D	406	55/55	0.95	0.07	31,37,47,49	0
37	LHG	d	409	49/49	0.95	0.09	34,41,59,70	0
37	LHG	d	410	39/49	0.95	0.11	40,46,97,100	0
39	DGD	C	518	62/66	0.95	0.10	36,47,91,102	0
30	GOL	c	528	6/6	0.95	0.08	38,45,47,47	0
39	DGD	H	102	62/66	0.95	0.10	36,46,58,64	0
39	DGD	c	518	62/66	0.95	0.10	38,49,91,96	0
39	DGD	c	519	62/66	0.95	0.11	43,53,110,123	0
33	PL9	d	407	55/55	0.95	0.08	30,39,49,52	0
41	RRX	H	101	41/41	0.95	0.08	40,50,61,71	0
24	CLA	B	611	65/65	0.95	0.09	35,41,52,64	0
34	BCT	a	407	4/4	0.96	0.08	45,48,53,58	0
26	BCR	A	410	40/40	0.96	0.07	32,40,45,47	0
35	CA	F	102	1/1	0.96	0.09	77,77,77,77	0
24	CLA	B	612	65/65	0.96	0.07	28,35,51,61	0
24	CLA	B	606	65/65	0.96	0.07	30,37,51,54	0
24	CLA	a	410	65/65	0.96	0.10	34,40,104,109	0
24	CLA	B	616	65/65	0.96	0.08	36,42,65,71	0
24	CLA	A	409	65/65	0.96	0.10	33,39,118,122	0
24	CLA	b	605	65/65	0.96	0.08	39,46,56,58	0
24	CLA	b	608	65/65	0.96	0.08	33,39,56,62	0
24	CLA	C	502	65/65	0.96	0.07	38,47,64,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	CLA	b	610	65/65	0.96	0.07	30,38,49,52	0
24	CLA	b	611	65/65	0.96	0.07	37,44,52,58	0
24	CLA	b	612	65/65	0.96	0.07	41,48,55,60	0
24	CLA	b	613	65/65	0.96	0.08	35,46,54,70	0
24	CLA	b	615	65/65	0.96	0.07	34,40,51,58	0
24	CLA	b	616	65/65	0.96	0.07	32,38,68,71	0
24	CLA	C	503	65/65	0.96	0.07	36,42,59,65	0
24	CLA	b	618	65/65	0.96	0.08	34,47,69,75	0
24	CLA	B	608	65/65	0.96	0.07	28,34,48,53	0
24	CLA	c	503	65/65	0.96	0.09	41,50,64,71	0
24	CLA	c	504	65/65	0.96	0.08	38,47,62,70	0
24	CLA	c	505	65/65	0.96	0.07	41,51,59,71	0
24	CLA	C	505	65/65	0.96	0.09	36,43,80,86	0
24	CLA	c	507	65/65	0.96	0.07	35,45,62,67	0
24	CLA	B	603	65/65	0.96	0.07	34,41,47,53	0
24	CLA	C	508	65/65	0.96	0.08	41,49,68,71	0
37	LHG	B	640	49/49	0.96	0.09	37,46,65,67	0
24	CLA	C	509	65/65	0.96	0.08	35,43,95,116	0
37	LHG	D	410	49/49	0.96	0.08	32,42,65,78	0
39	DGD	C	517	62/66	0.96	0.10	36,47,90,91	0
24	CLA	c	512	65/65	0.96	0.08	39,48,60,71	0
39	DGD	C	519	62/66	0.96	0.09	34,43,85,94	0
24	CLA	C	510	65/65	0.96	0.08	39,46,70,77	0
24	CLA	C	511	65/65	0.96	0.07	38,44,61,72	0
24	CLA	C	512	65/65	0.96	0.07	39,50,56,58	0
25	PHO	A	408	64/64	0.96	0.06	28,34,38,40	0
39	DGD	c	520	62/66	0.96	0.10	39,50,80,95	0
24	CLA	B	604	65/65	0.96	0.08	32,40,49,53	0
40	HEM	f	101	43/43	0.96	0.09	55,66,96,113	0
25	PHO	a	411	64/64	0.96	0.06	31,37,41,47	0
34	BCT	A	423	4/4	0.96	0.07	38,39,48,52	0
24	CLA	d	404	65/65	0.97	0.07	28,36,58,65	0
24	CLA	B	605	65/65	0.97	0.07	27,35,72,80	0
24	CLA	A	406	65/65	0.97	0.06	26,32,38,53	0
24	CLA	A	407	65/65	0.97	0.08	29,35,98,100	0
24	CLA	b	606	65/65	0.97	0.07	37,44,54,57	0
25	PHO	d	401	64/64	0.97	0.06	33,41,50,54	0
24	CLA	b	607	65/65	0.97	0.08	29,39,83,87	0
24	CLA	B	613	65/65	0.97	0.07	28,37,46,53	0
24	CLA	B	614	65/65	0.97	0.07	30,36,67,81	0
24	CLA	C	506	65/65	0.97	0.08	36,46,65,70	0
24	CLA	D	403	65/65	0.97	0.07	25,32,50,54	0

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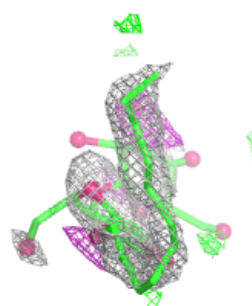
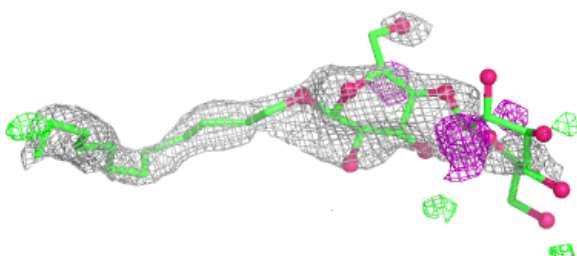
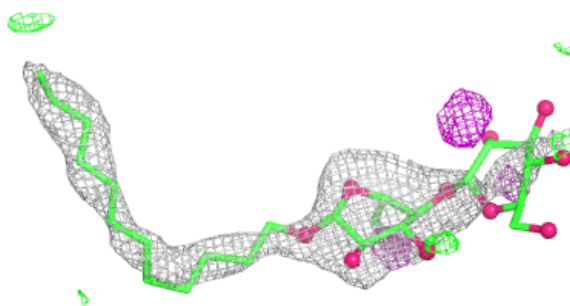
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	CLA	A	405	65/65	0.97	0.06	27,32,41,63	0
24	CLA	a	408	65/65	0.97	0.06	31,35,43,64	0
24	CLA	c	511	65/65	0.97	0.08	42,50,66,70	0
24	CLA	b	614	65/65	0.97	0.07	32,38,57,65	0
24	CLA	c	513	65/65	0.97	0.07	42,53,62,67	0
24	CLA	a	409	65/65	0.97	0.06	29,34,43,53	0
24	CLA	B	609	65/65	0.97	0.06	31,39,47,50	0
42	MG	J	101	1/1	0.97	0.08	43,43,43,43	0
30	GOL	C	524	6/6	0.98	0.05	36,41,43,44	0
35	CA	o	303	1/1	0.98	0.04	67,67,67,67	0
40	HEM	F	101	43/43	0.98	0.06	42,52,61,65	0
23	CL	a	406	1/1	0.98	0.05	41,41,41,41	0
23	CL	A	403	1/1	0.98	0.06	38,38,38,38	0
23	CL	a	405	1/1	0.98	0.11	44,44,44,44	0
35	CA	c	502	1/1	0.98	0.04	61,61,61,61	0
43	HEC	v	1603	43/43	0.98	0.07	40,49,54,55	0
21	OEX	a	403	10/10	0.99	0.03	38,40,42,42	0
22	FE2	A	402	1/1	0.99	0.02	39,39,39,39	0
35	CA	O	301	1/1	0.99	0.09	70,70,70,70	0
21	OEX	A	401	10/10	0.99	0.03	35,37,41,42	0
42	MG	j	1303	1/1	0.99	0.11	52,52,52,52	0
43	HEC	V	202	43/43	0.99	0.05	36,42,45,49	0
23	CL	A	404	1/1	0.99	0.04	38,38,38,38	0
22	FE2	a	404	1/1	1.00	0.02	42,42,42,42	0

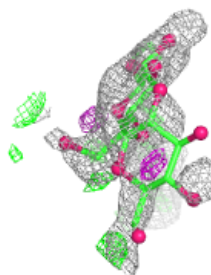
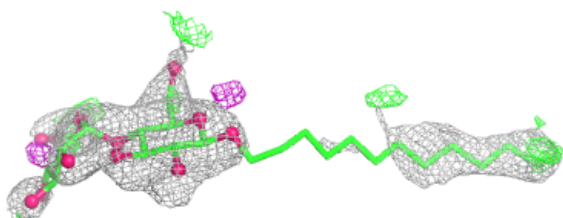
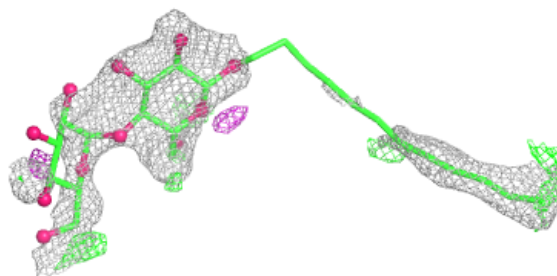
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LMT 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)

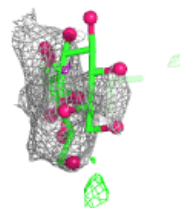
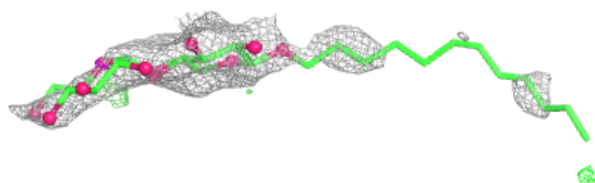
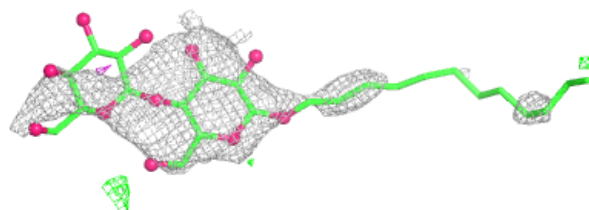
**Electron density around LMT f 104:**

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

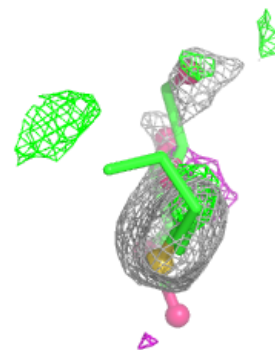
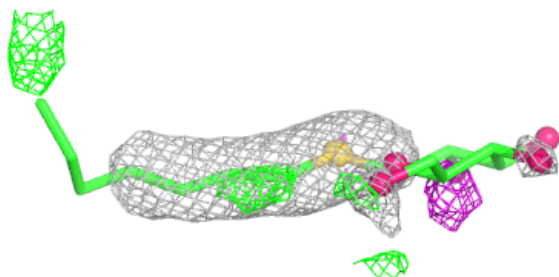
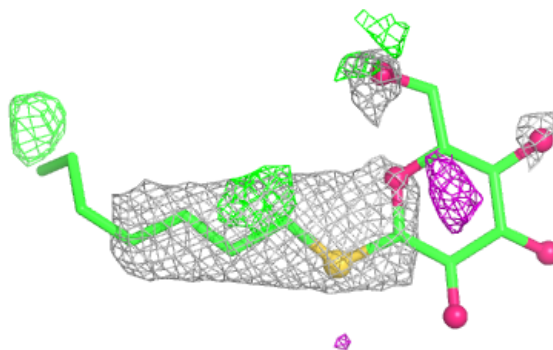


Electron density around LMT c 523:

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

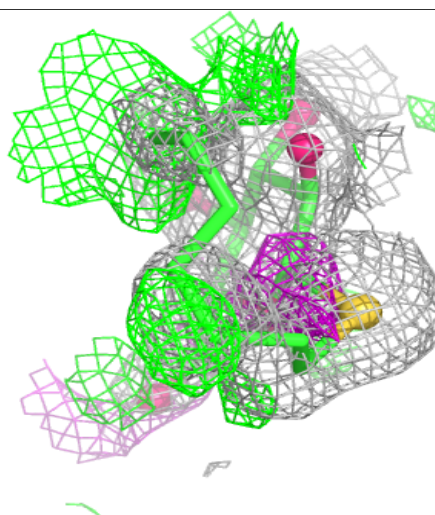
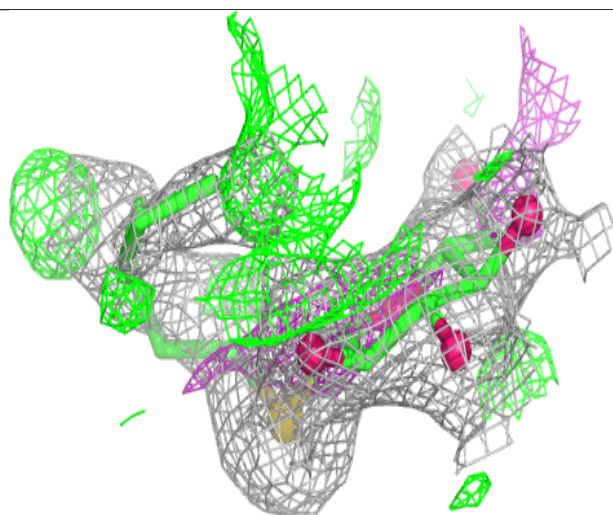
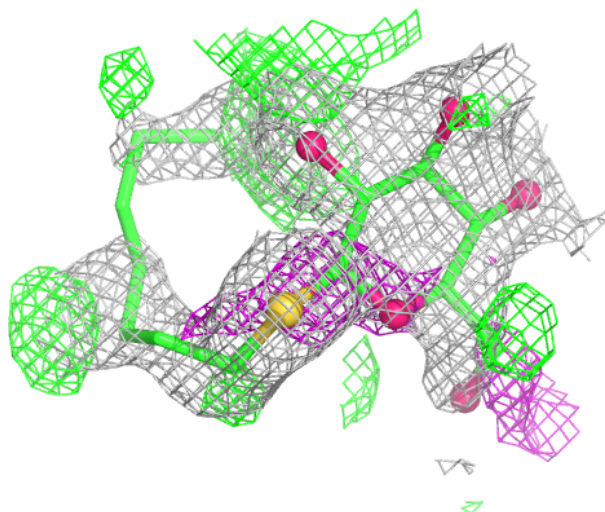
**Electron density around HTG D 413:**

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



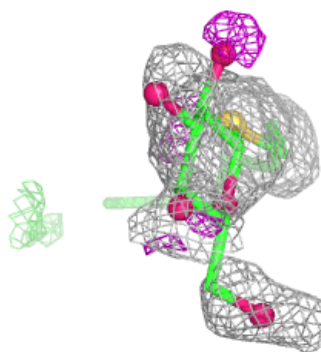
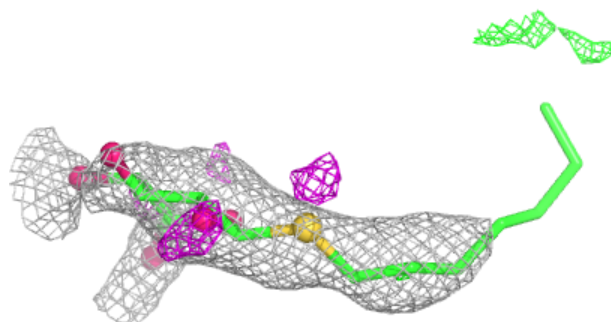
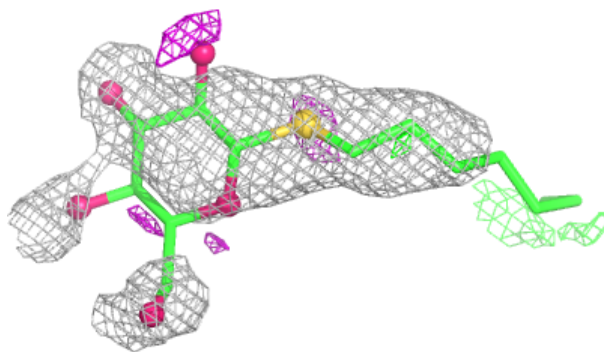
Electron density around HTG b 625:

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

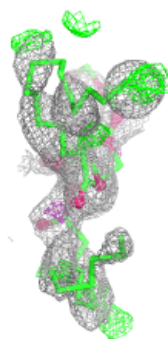
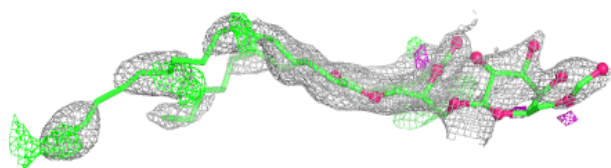
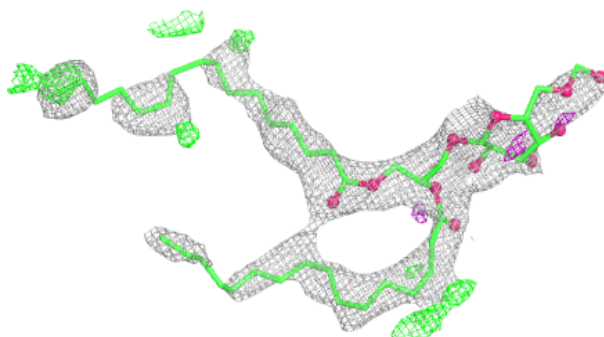


Electron density around HTG h 1202:

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

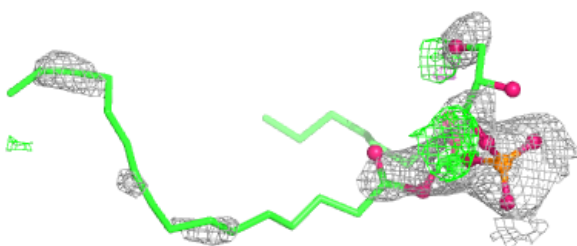
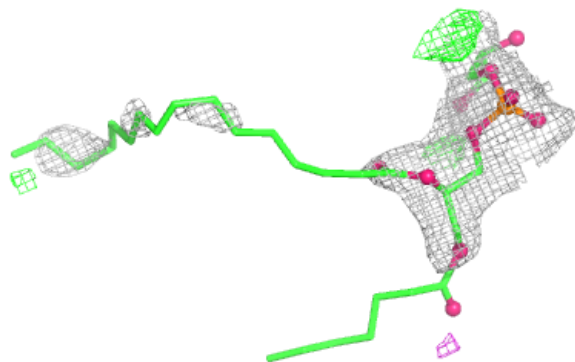
**Electron density around DGD D 407:**

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

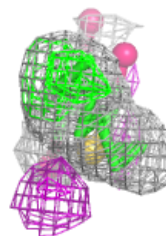
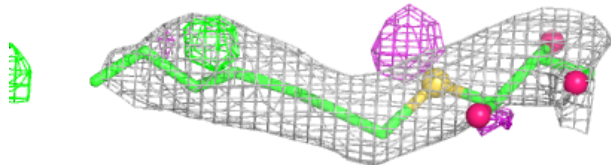
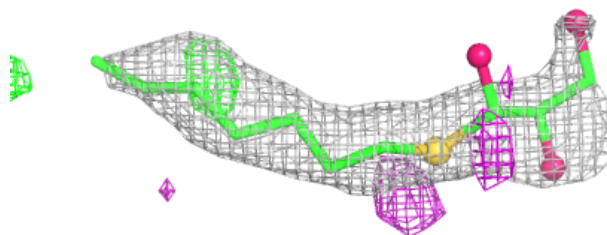


Electron density around LHG e 101:

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

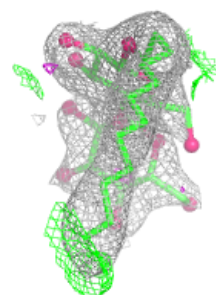
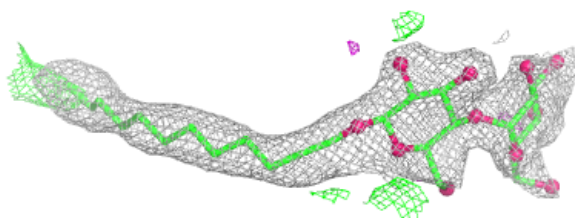
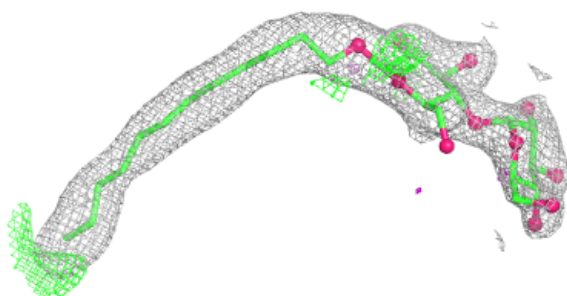
**Electron density around HTG u 201:**

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

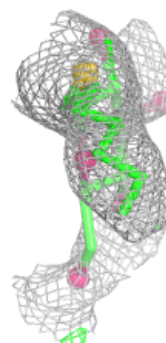
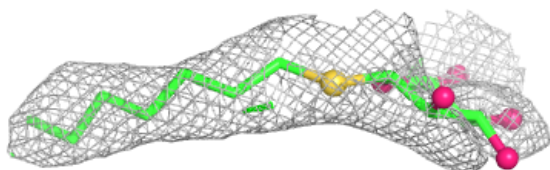
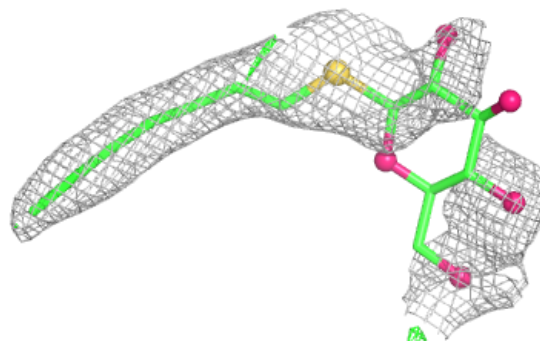


Electron density around LMT m 103:

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

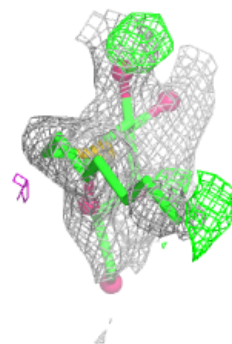
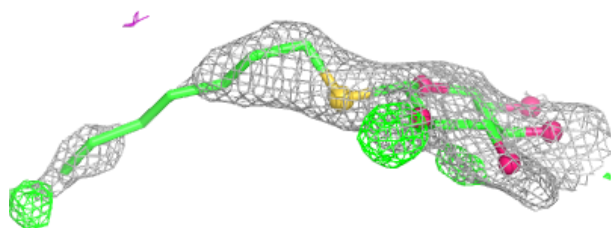
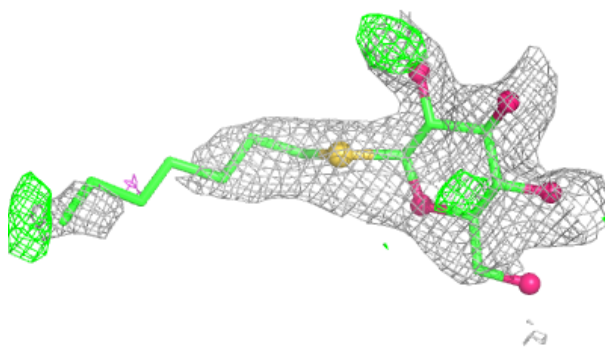
**Electron density around HTG b 626:**

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



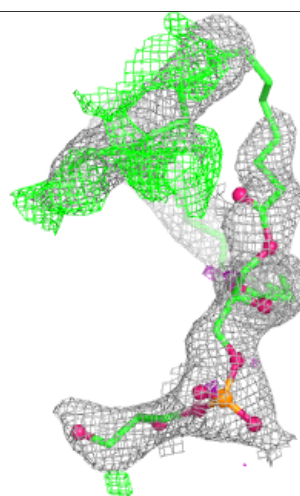
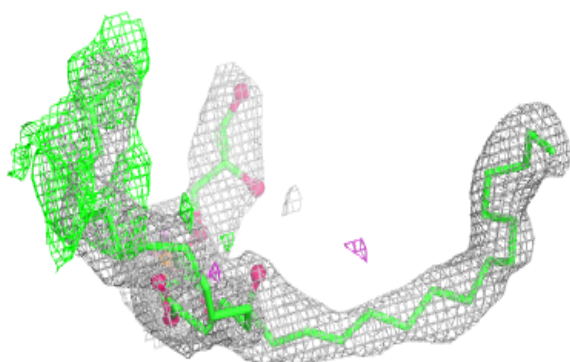
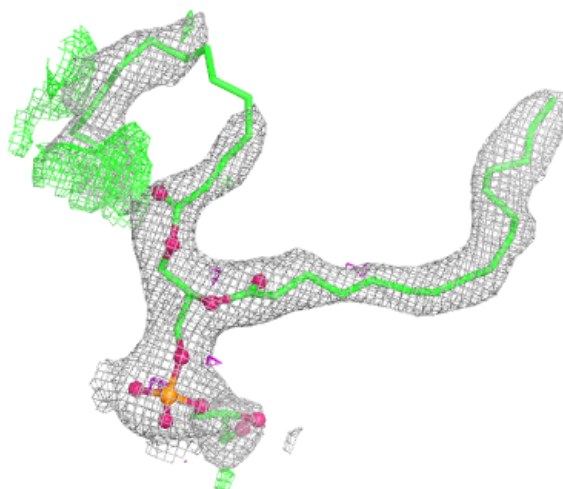
Electron density around HTG d 414:

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



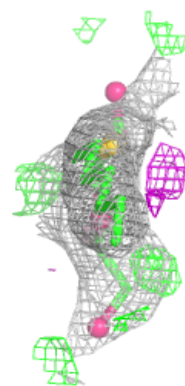
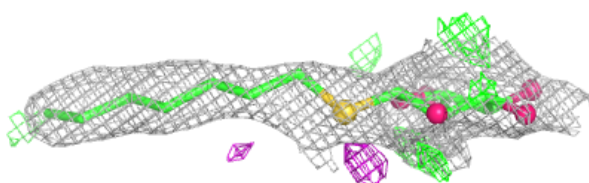
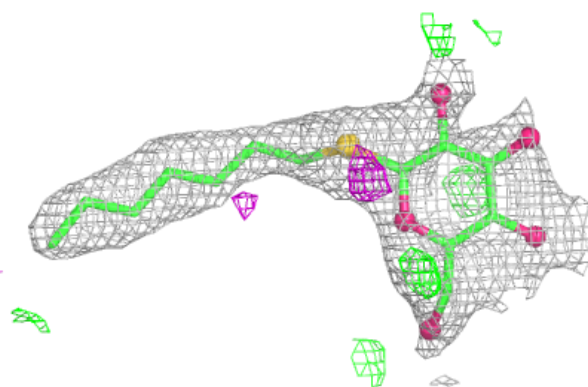
Electron density around LHG E 101:

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

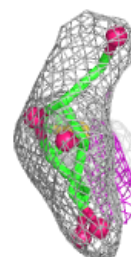
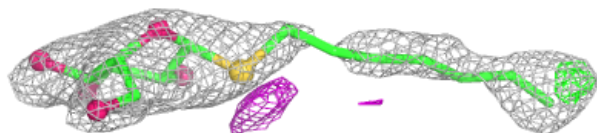
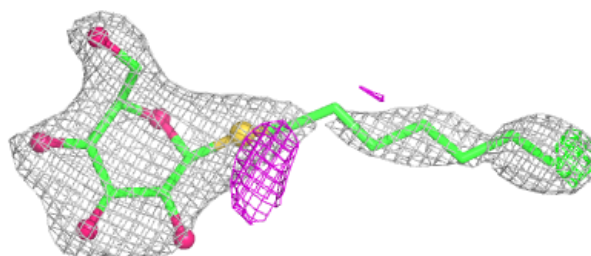


Electron density around HTG B 626:

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

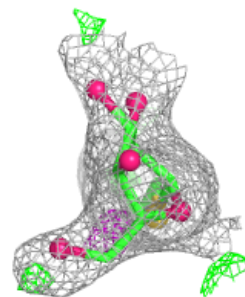
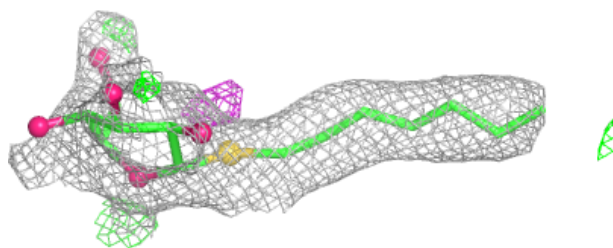
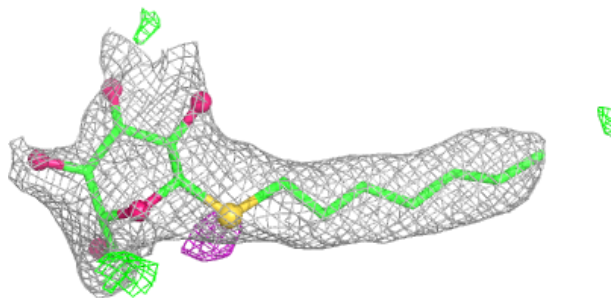
**Electron density around HTG C 523:**

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



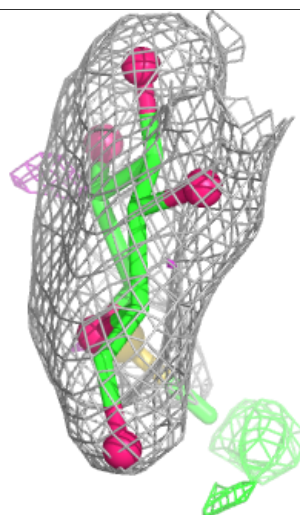
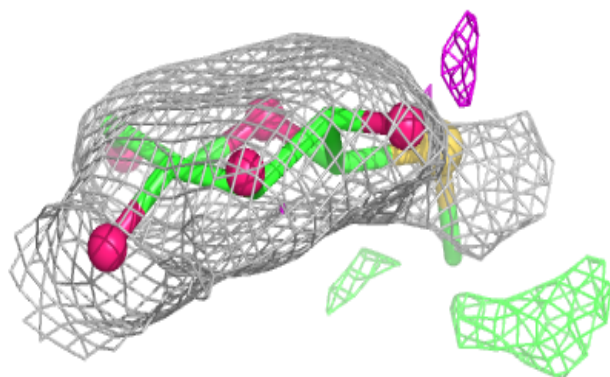
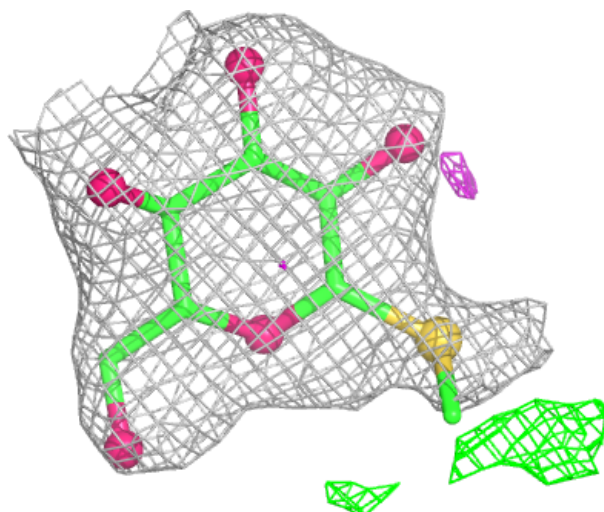
Electron density around HTG I 102:

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



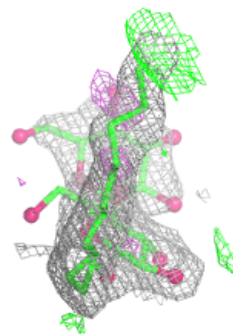
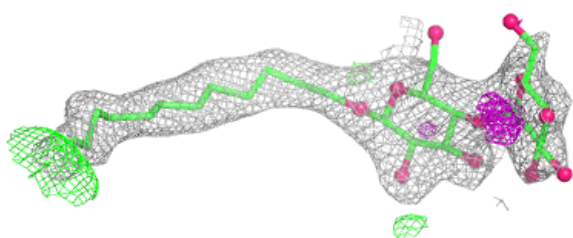
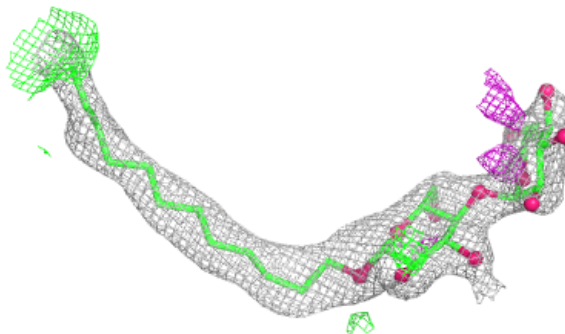
Electron density around HTG V 203:

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

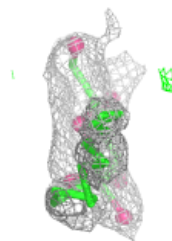
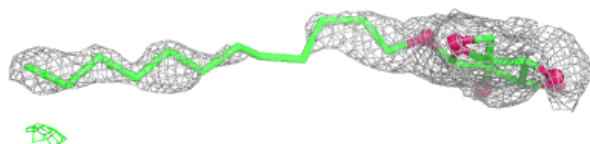
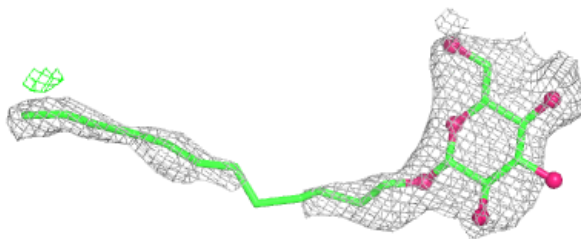


Electron density around LMT m 101:

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

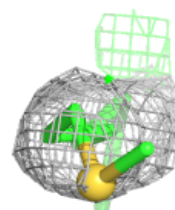
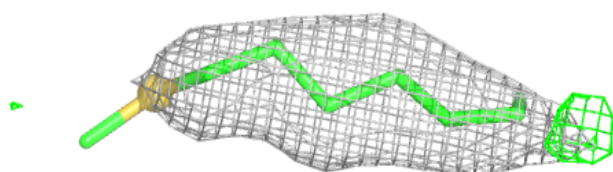
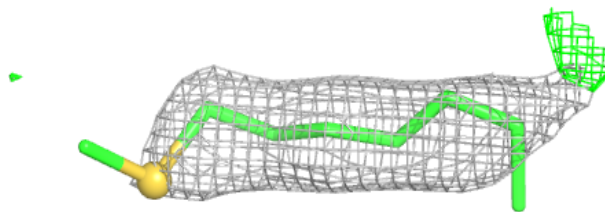
**Electron density around LMT E 104:**

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

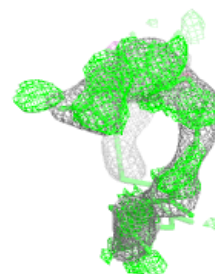
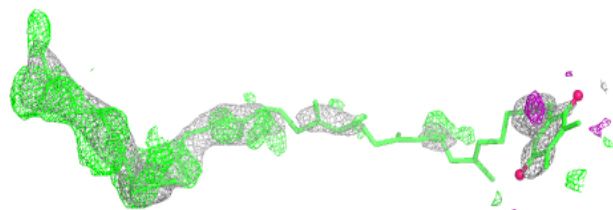
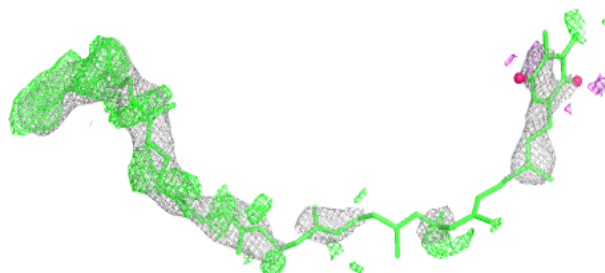


Electron density around HTG U 201:

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

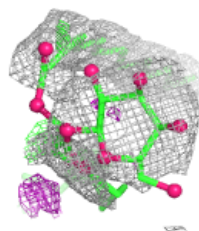
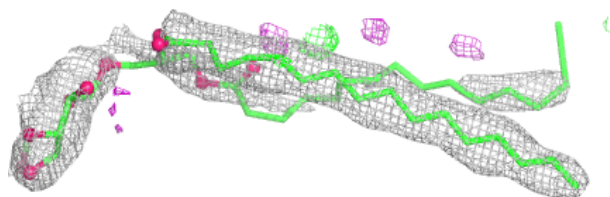
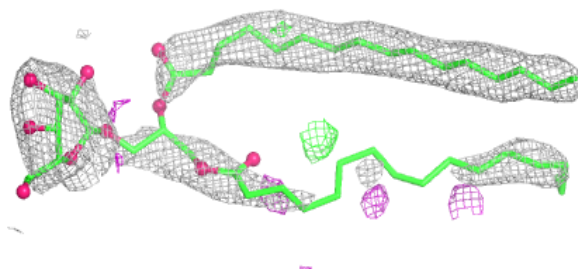
**Electron density around PL9 a 425 (B):**

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

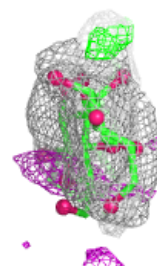
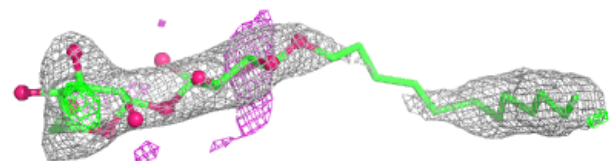
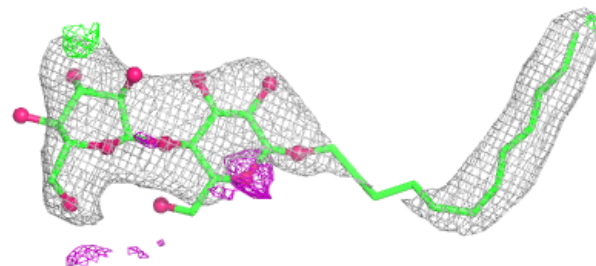


Electron density around LMG C 532:

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

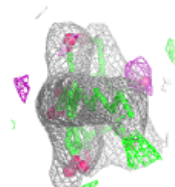
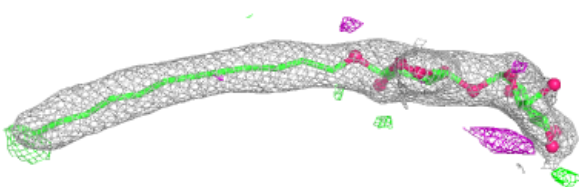
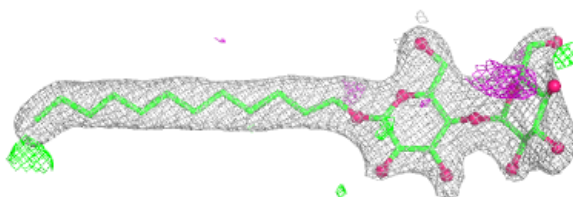
**Electron density around LMT Z 101:**

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

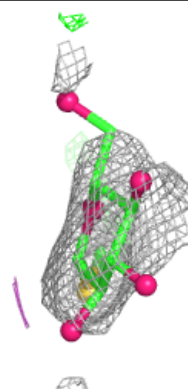
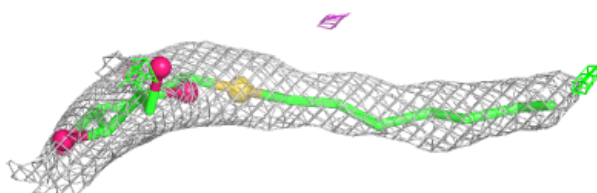
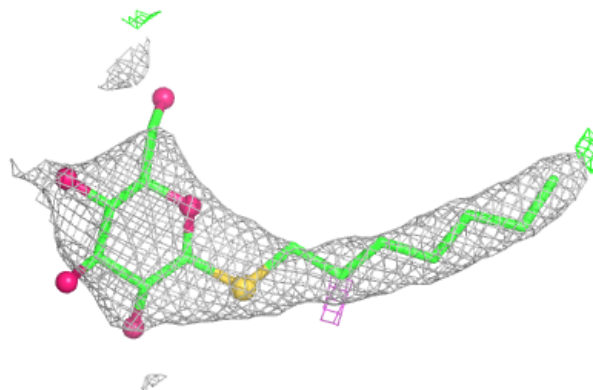


Electron density around LMT M 101:

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

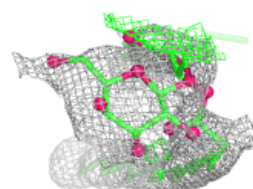
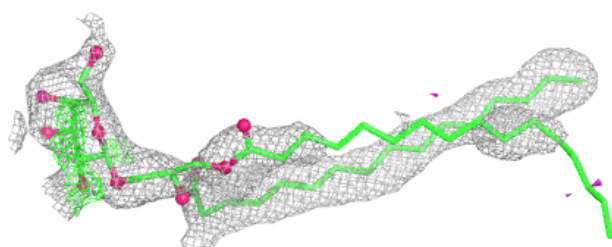
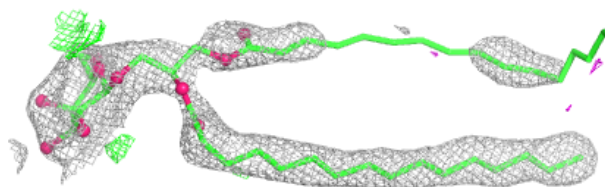
**Electron density around HTG B 624:**

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

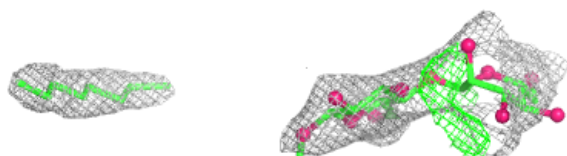
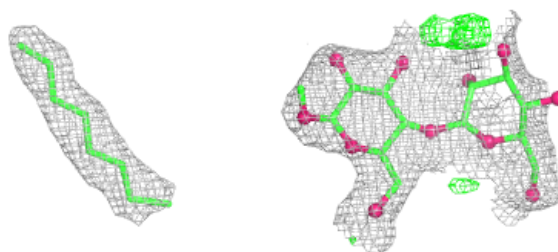


Electron density around LMG c 522:

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

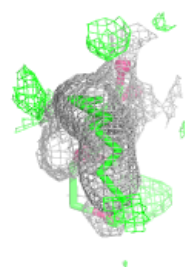
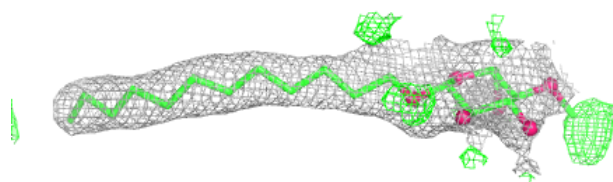
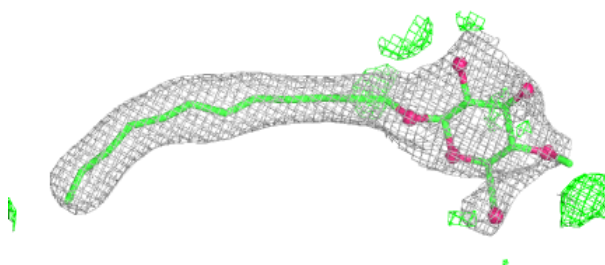
**Electron density around LMT z 101:**

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

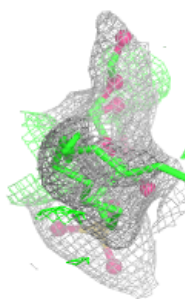
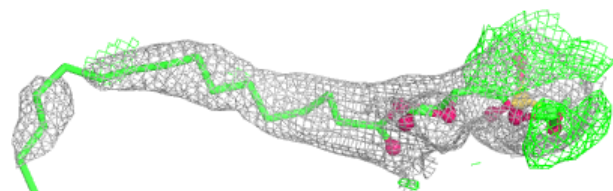
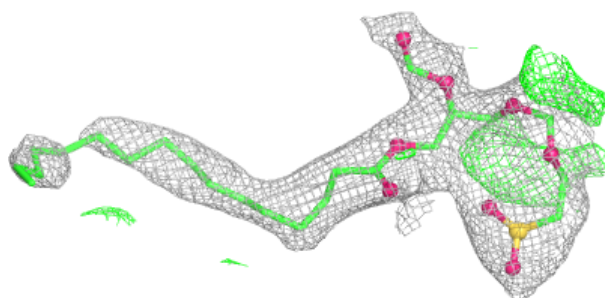


Electron density around LMT b 624:

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

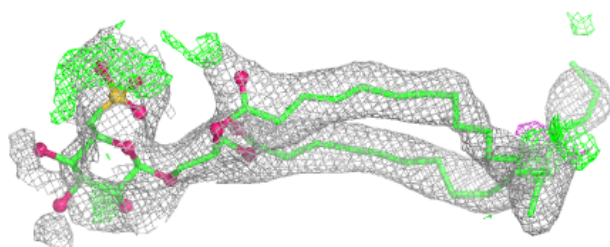
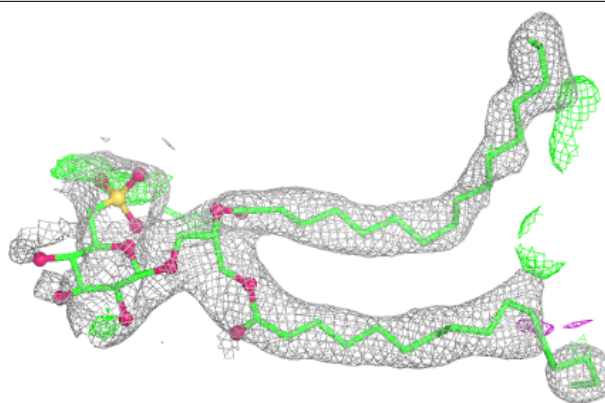
**Electron density around SQD f 102:**

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

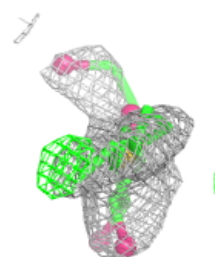
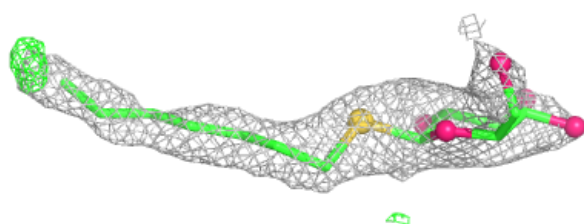
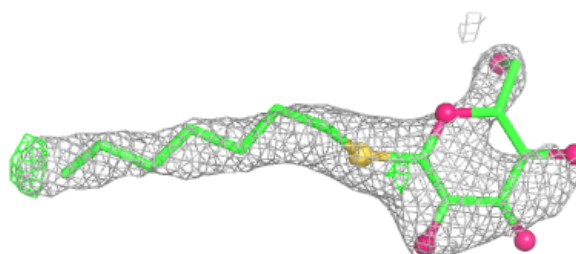


Electron density around SQD L 101:

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

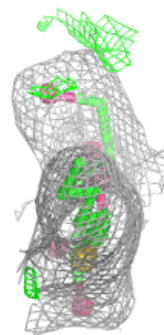
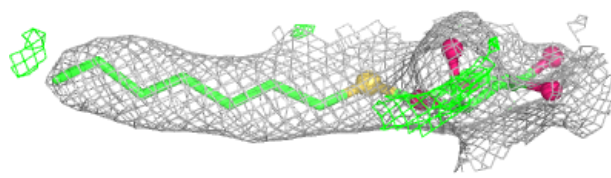
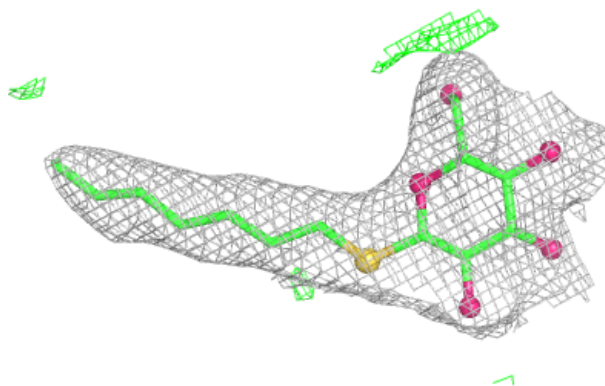
**Electron density around HTG c 525:**

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

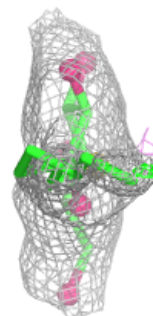
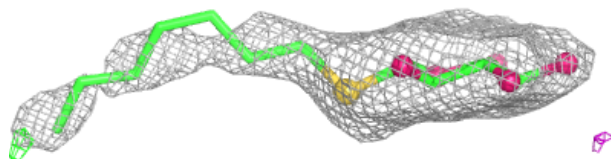
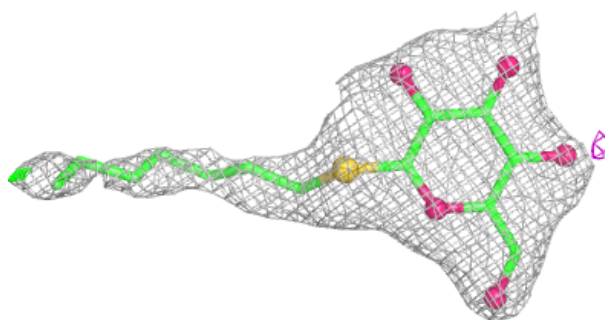


Electron density around HTG b 602:

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

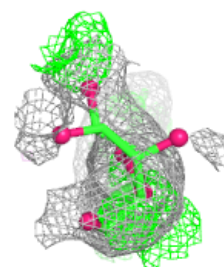
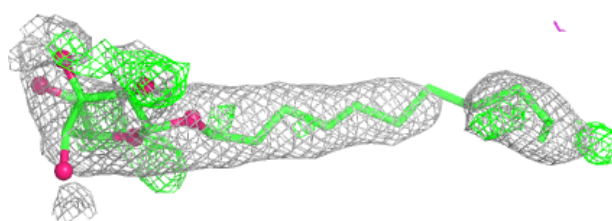
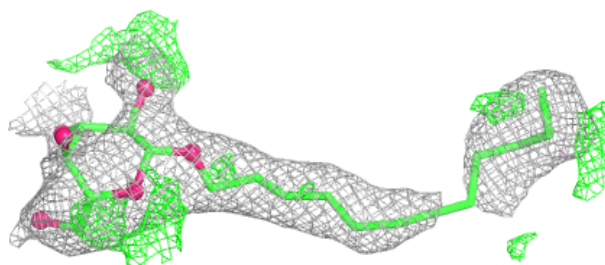
**Electron density around HTG c 524:**

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

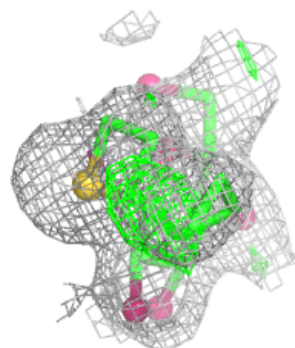
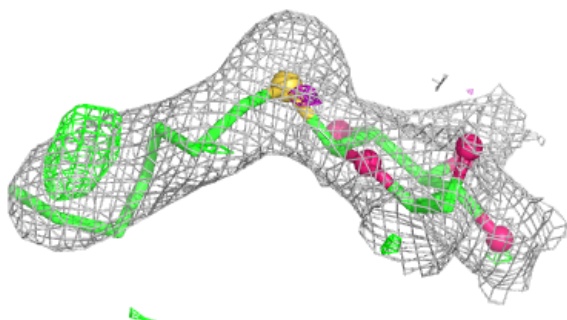
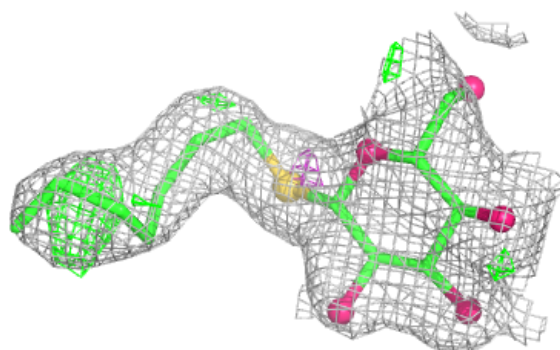


Electron density around LMT T 104:

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

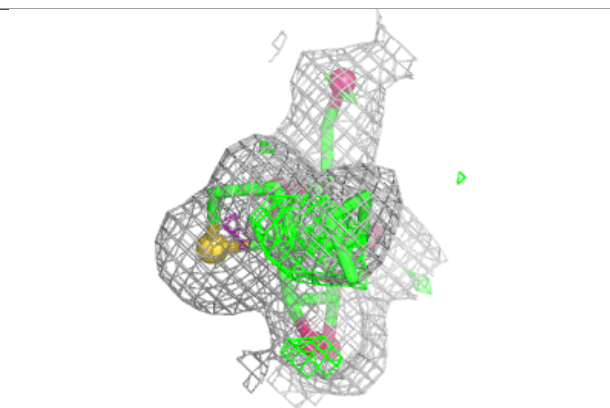
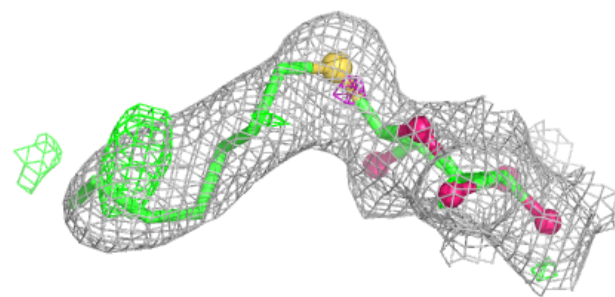
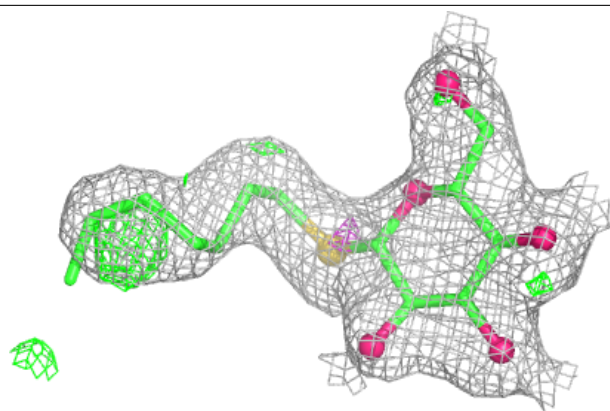
**Electron density around HTG B 623 (A):**

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

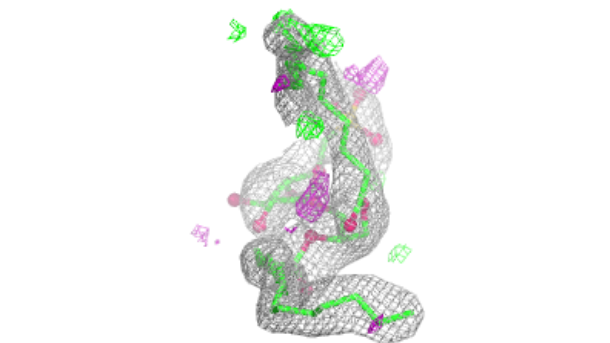
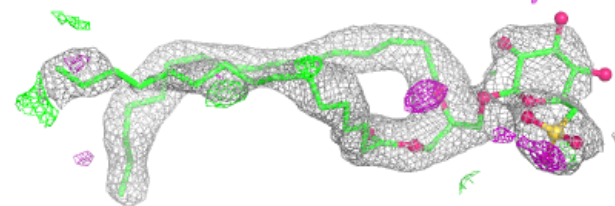
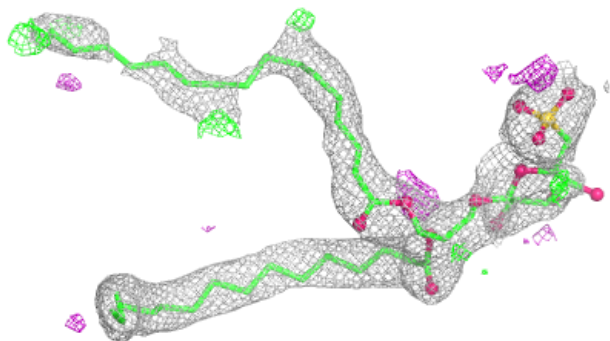


Electron density around HTG B 623 (B):

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

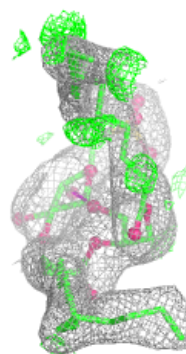
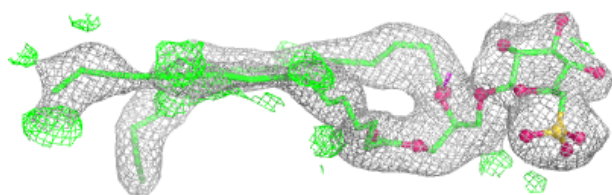
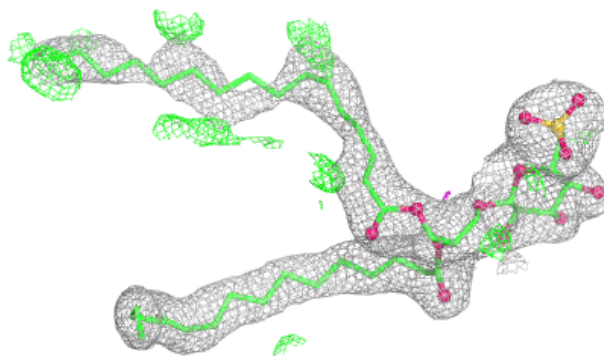
**Electron density around SQD a 401:**

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

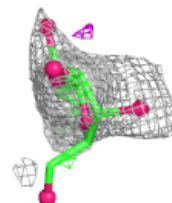
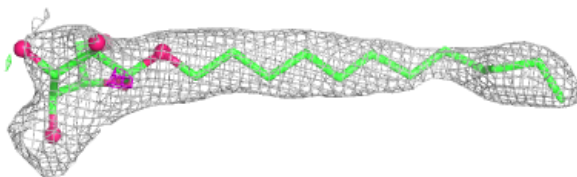
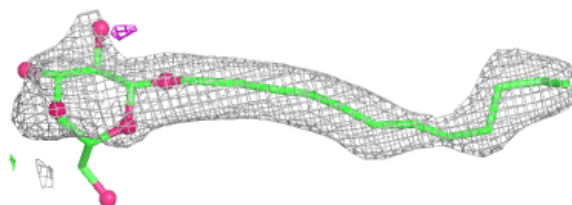


Electron density around SQD A 413:

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

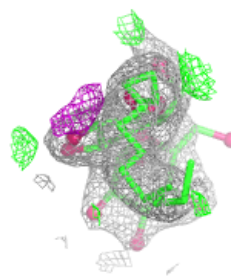
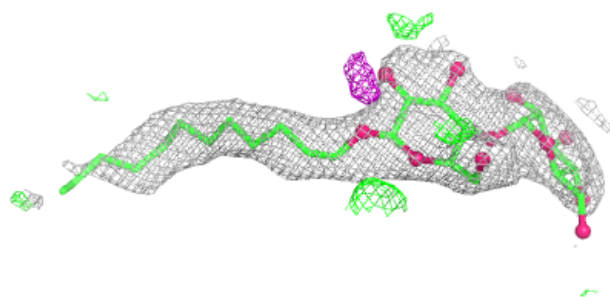
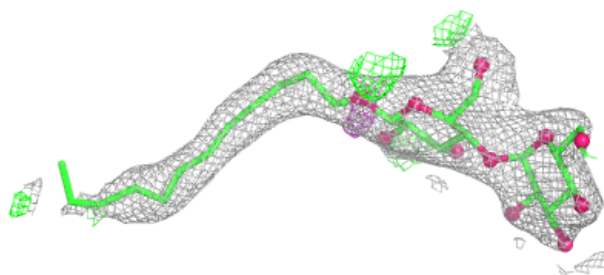
**Electron density around LMT J 102:**

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

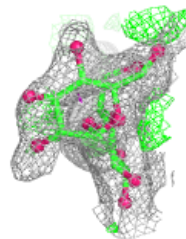
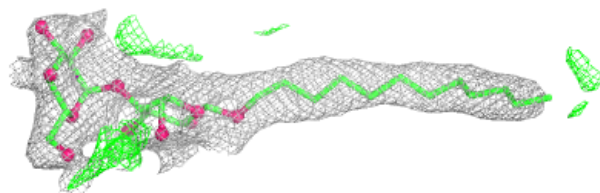
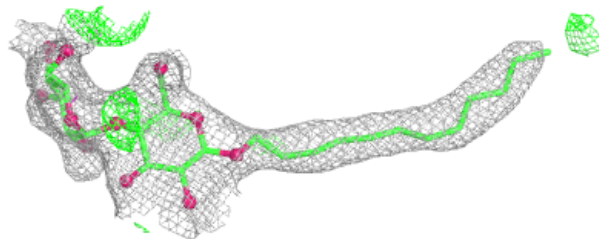


Electron density around LMT A 414:

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

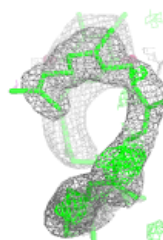
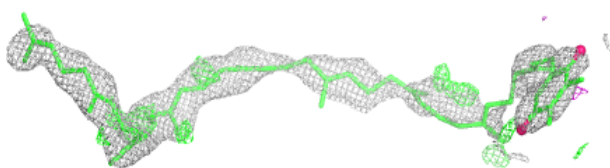
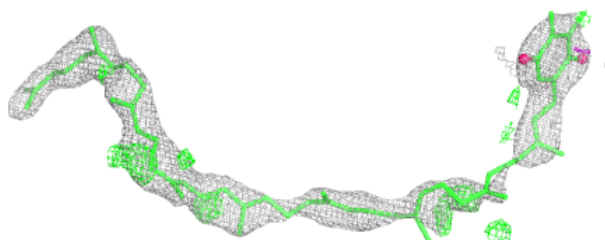
**Electron density around LMT B 622:**

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

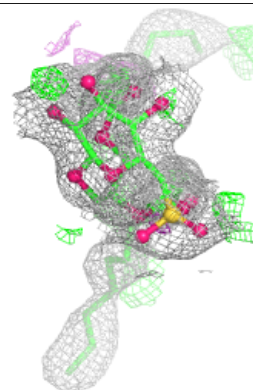
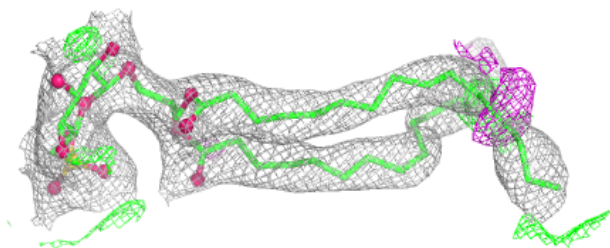
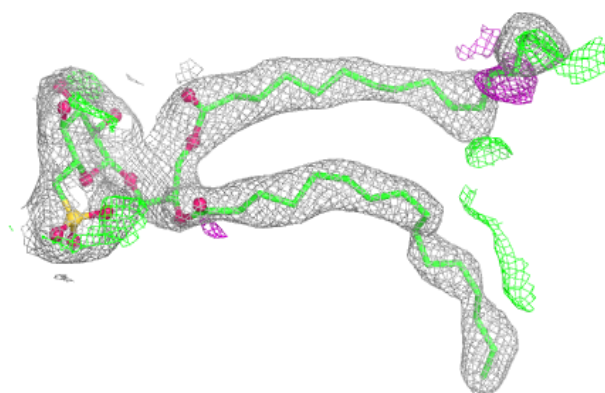


Electron density around PL9 A 422 (B):

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

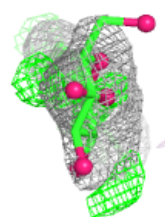
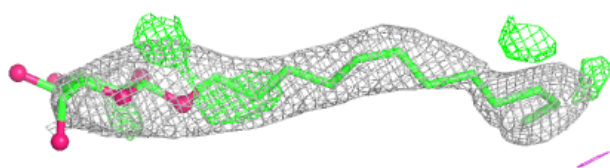
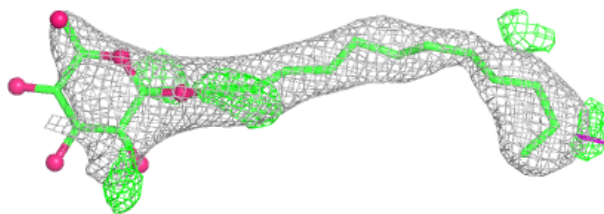
**Electron density around SQD L 102:**

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

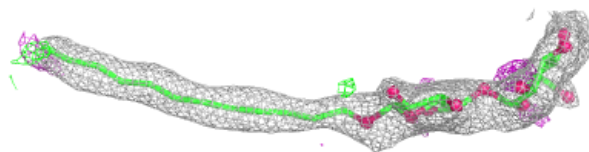
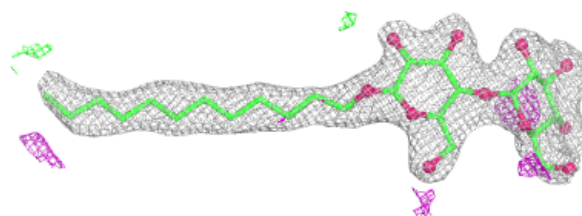


Electron density around LMT B 642:

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

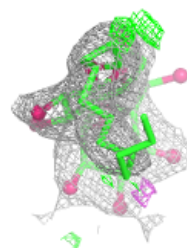
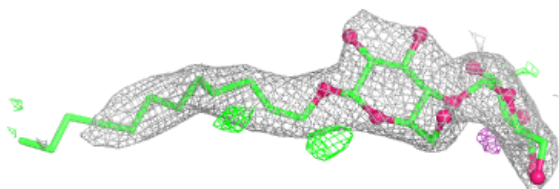
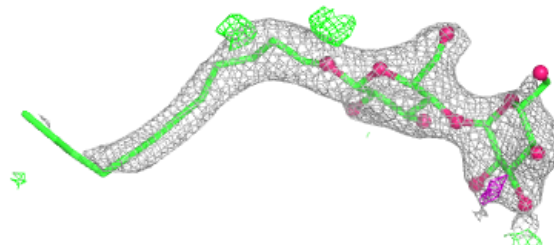
**Electron density around LMT m 102:**

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

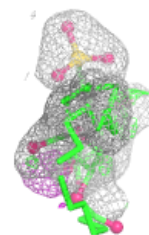
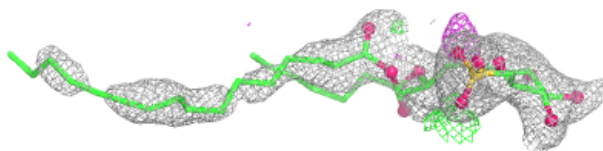
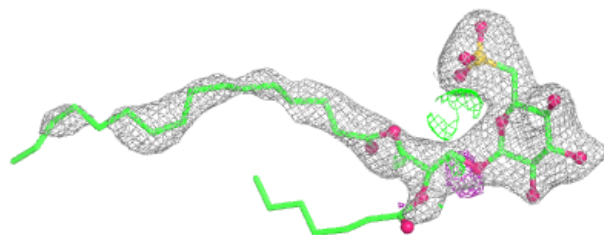


Electron density around LMT a 402:

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

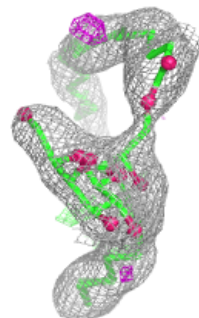
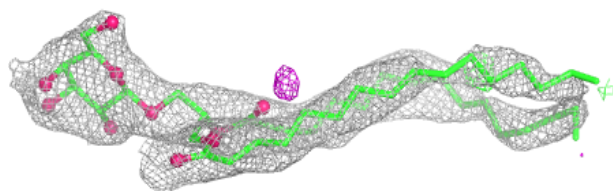
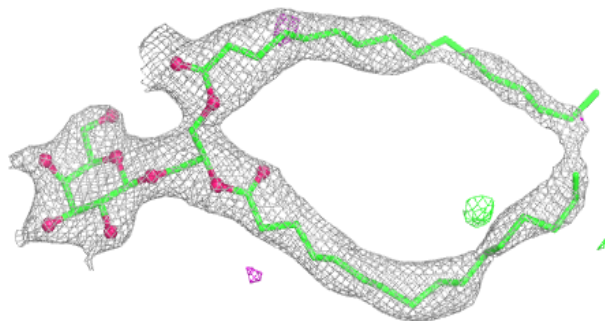
**Electron density around SQD D 408:**

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

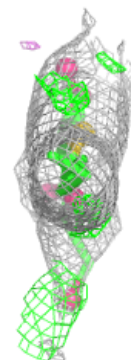
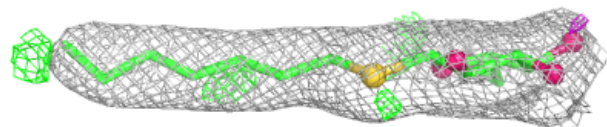
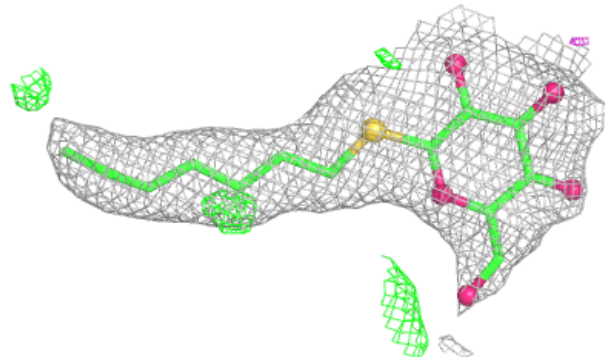


Electron density around LMG a 415:

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

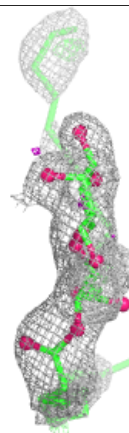
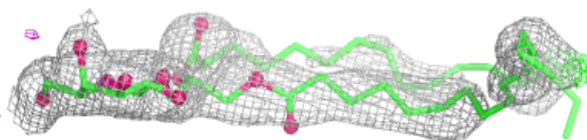
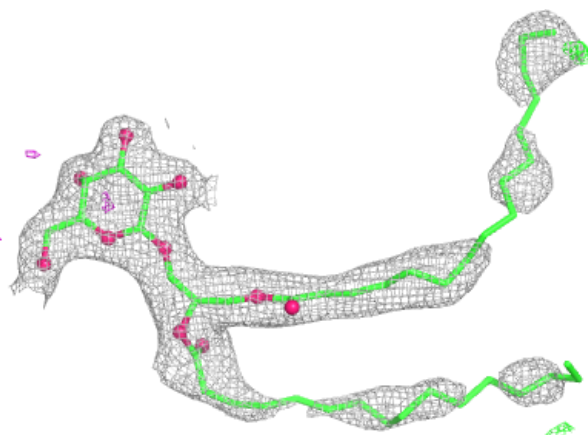
**Electron density around HTG b 601:**

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



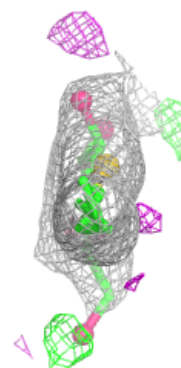
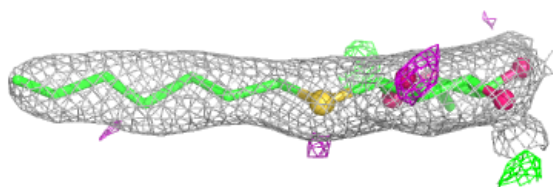
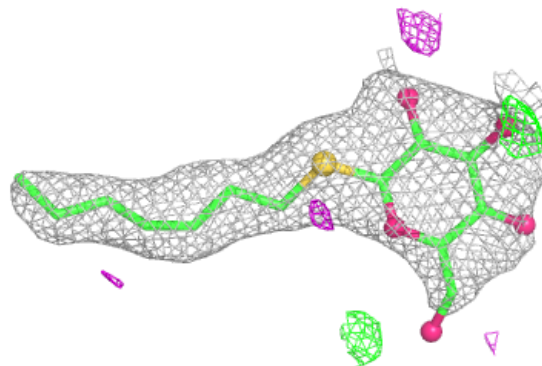
Electron density around LMG C 520:

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

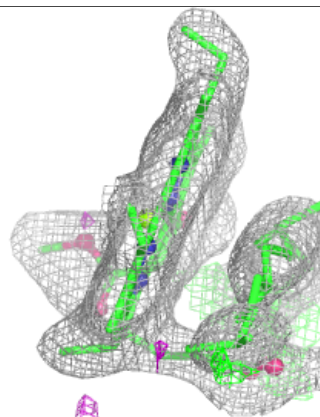
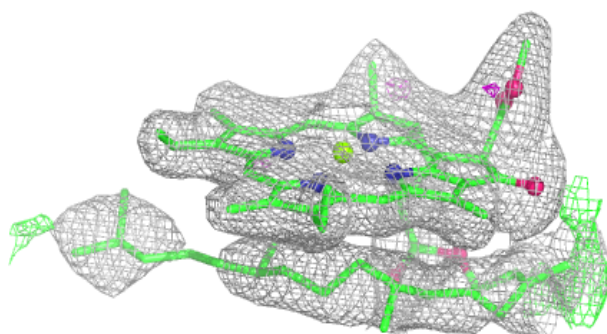
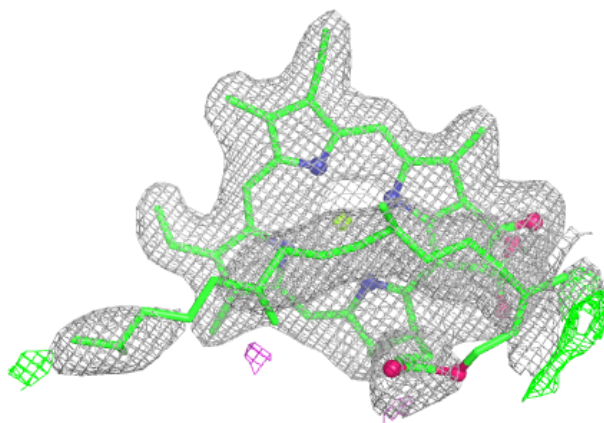


Electron density around HTG B 625:

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

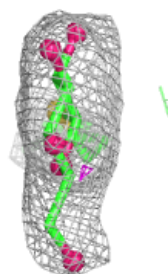
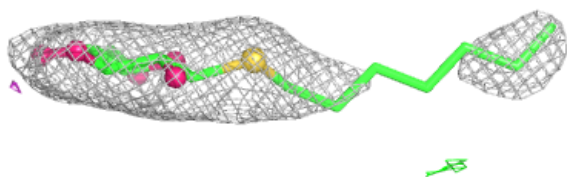
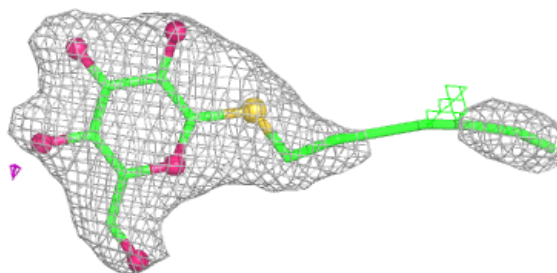
**Electron density around CLA B 602:**

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

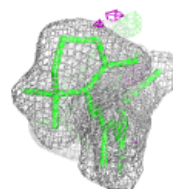
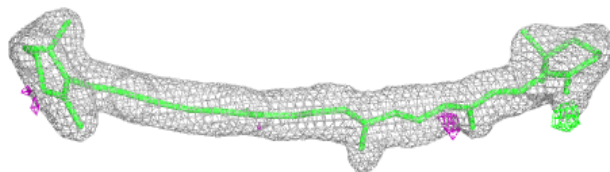
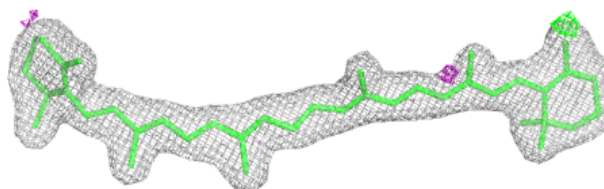


Electron density around HTG C 522:

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

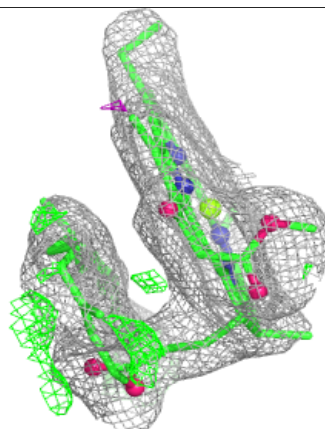
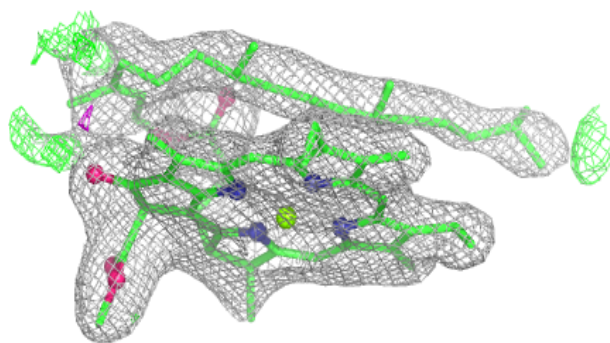
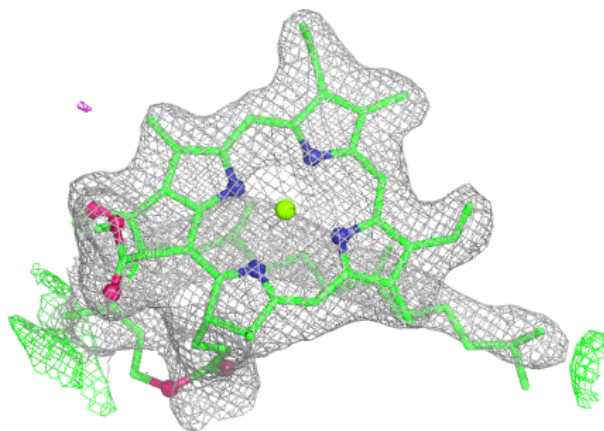
**Electron density around BCR T 102:**

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



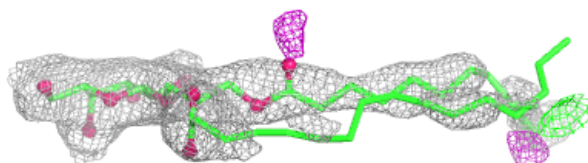
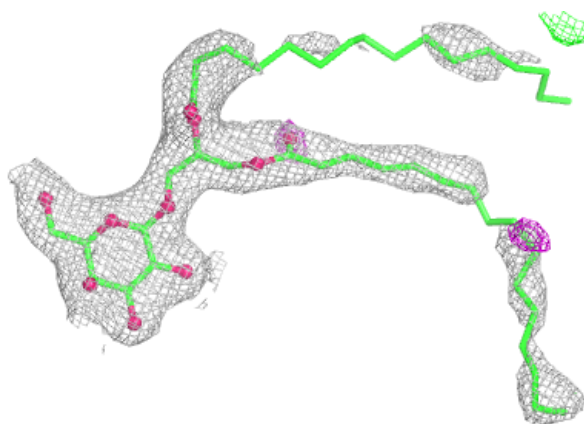
Electron density around CLA b 604:

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

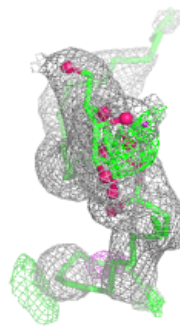
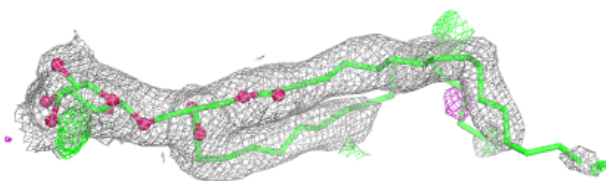
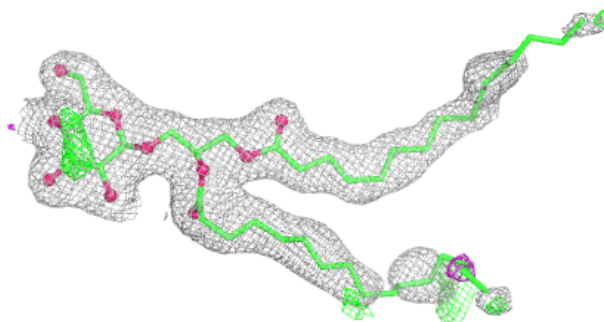


Electron density around LMG c 521:

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

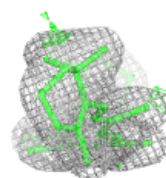
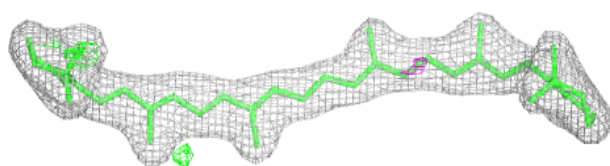
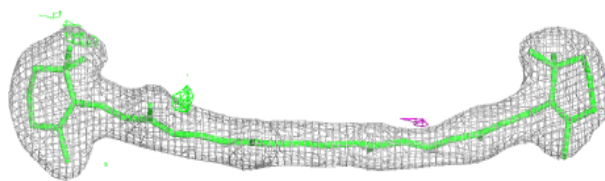
**Electron density around LMG d 411:**

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



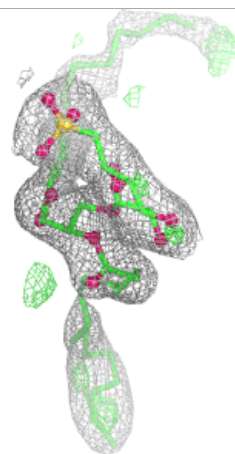
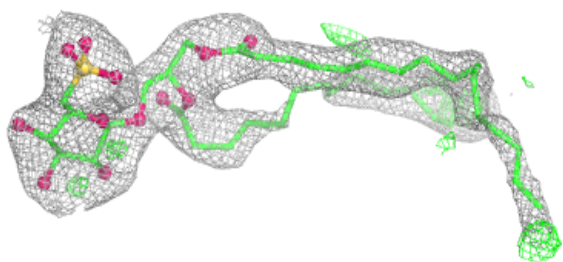
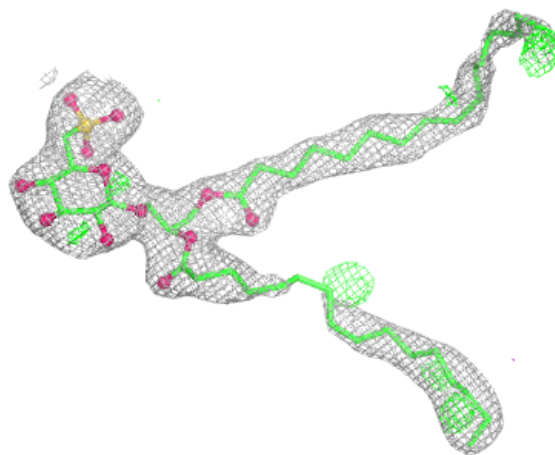
Electron density around BCR K 101:

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



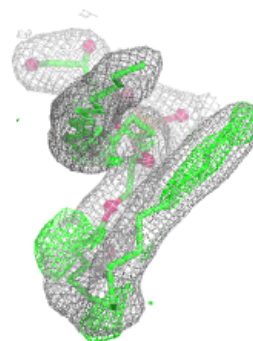
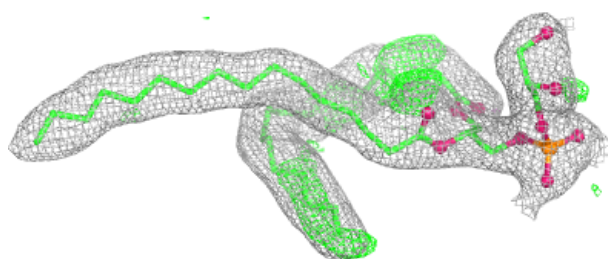
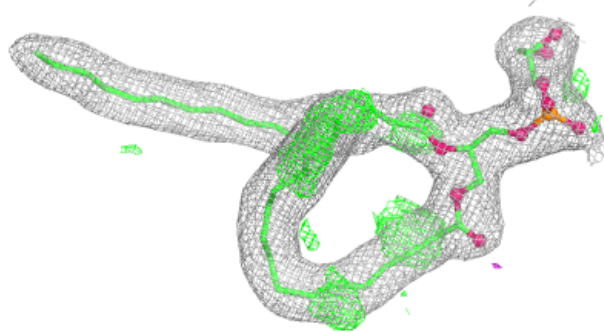
Electron density around SQD a 414:

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

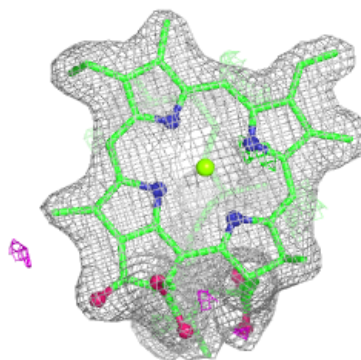
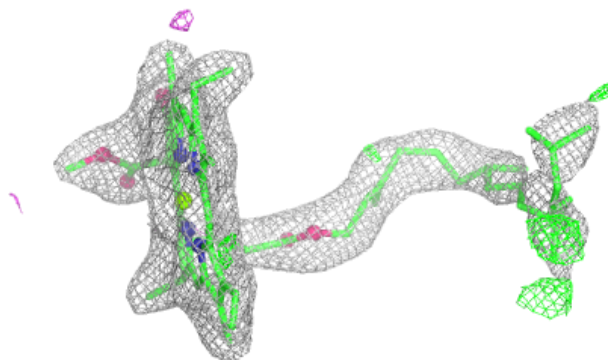
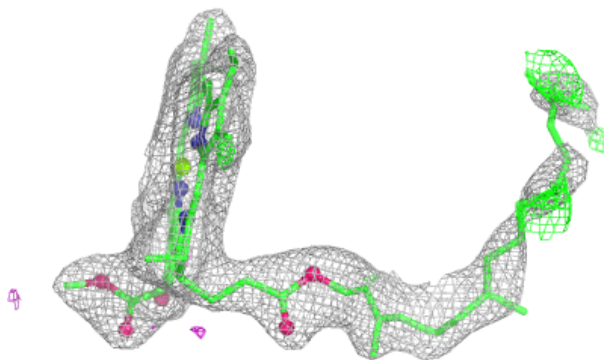


Electron density around LHG D 409:

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

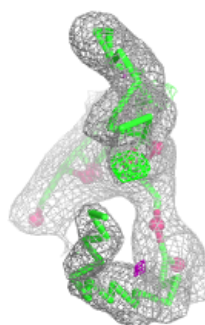
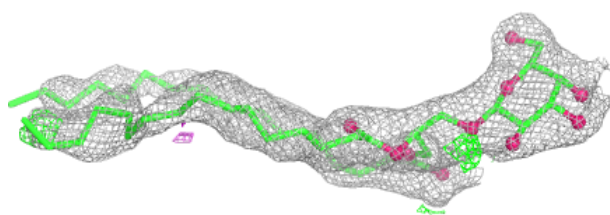
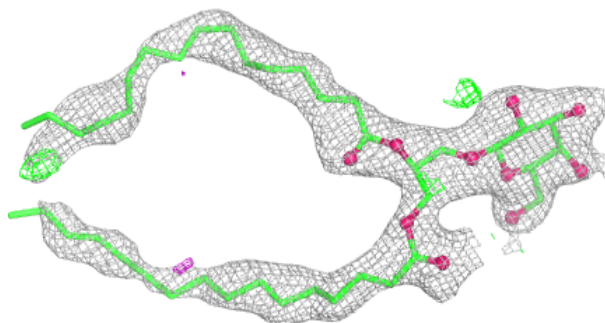
**Electron density around CLA C 507:**

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

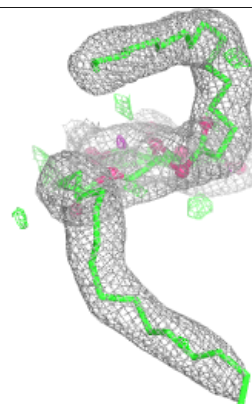
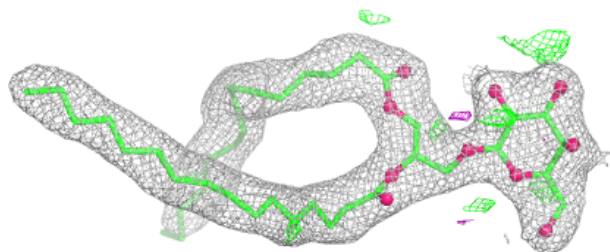
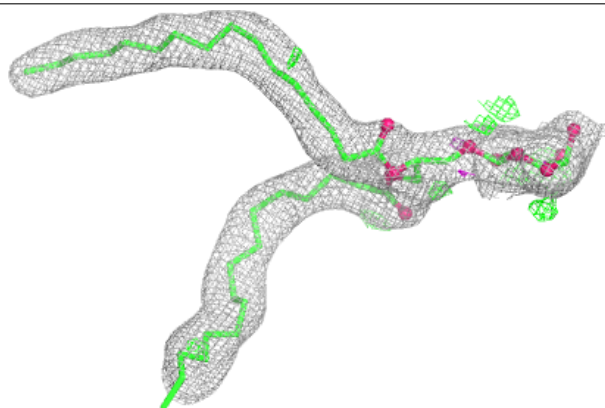


Electron density around LMG A 412:

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

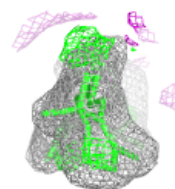
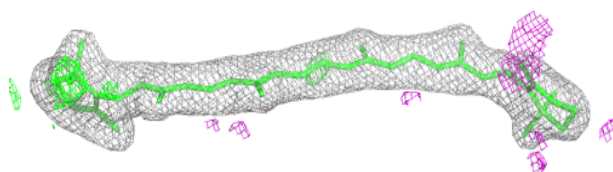
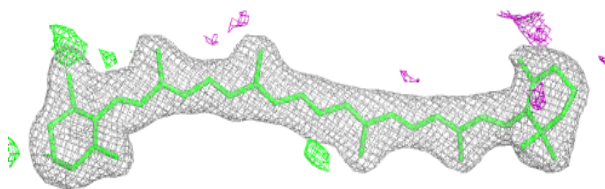
**Electron density around LMG B 621:**

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



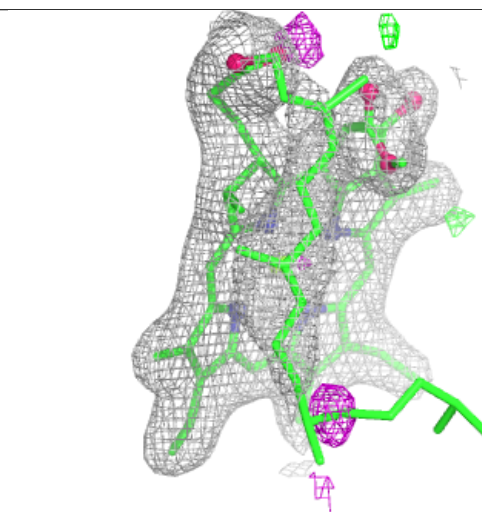
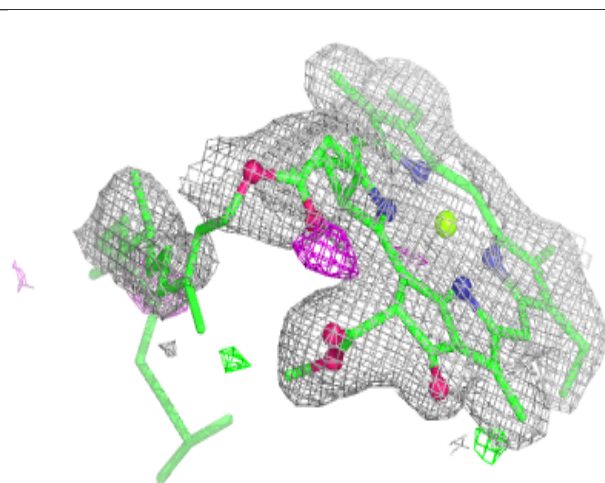
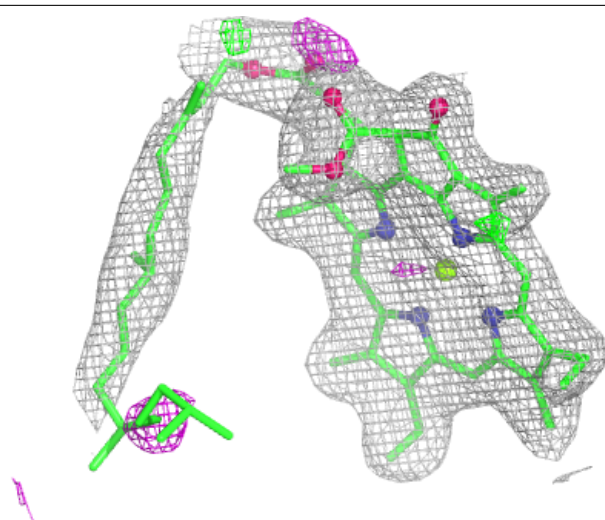
Electron density around BCR b 622:

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



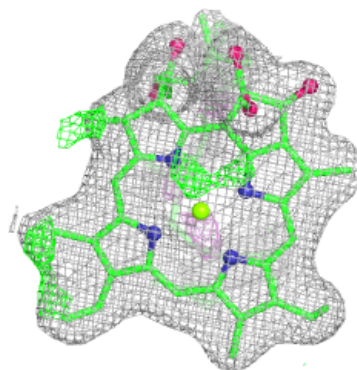
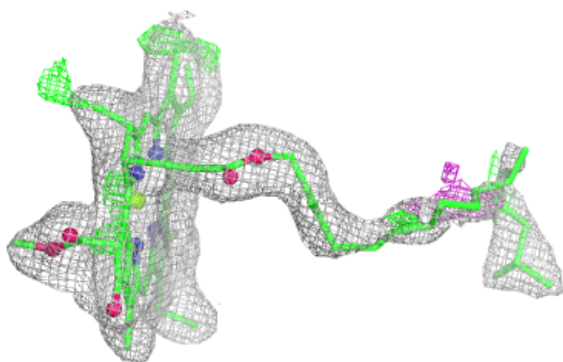
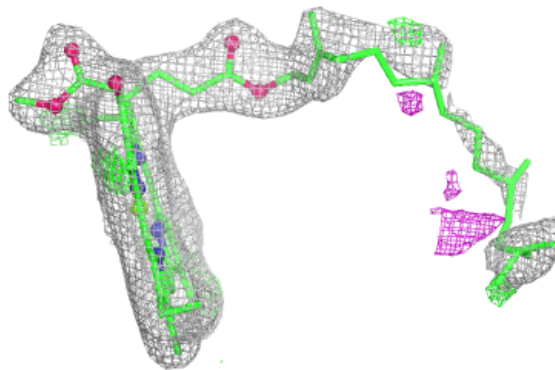
Electron density around CLA b 619:

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

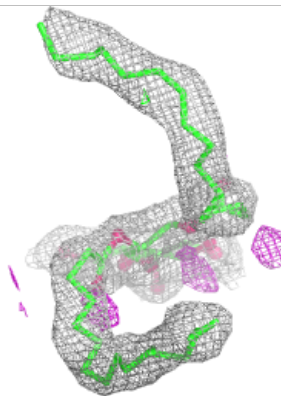
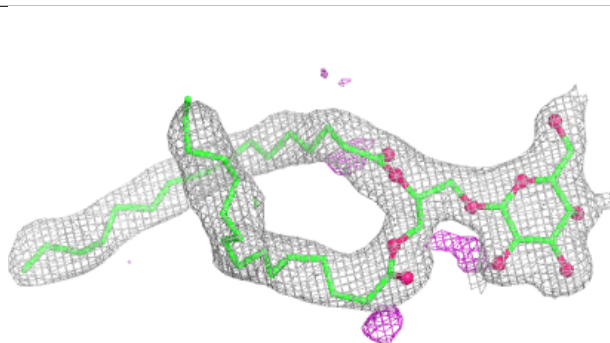
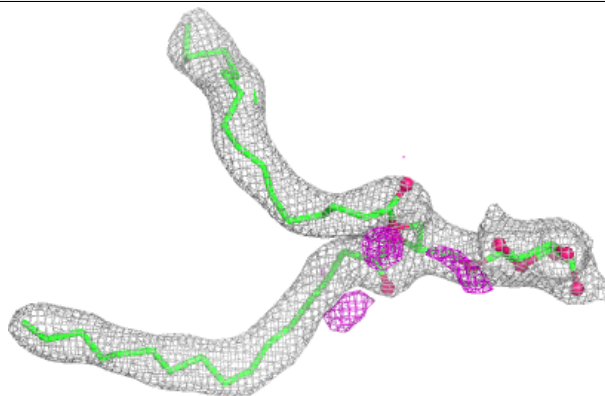


Electron density around CLA c 508:

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

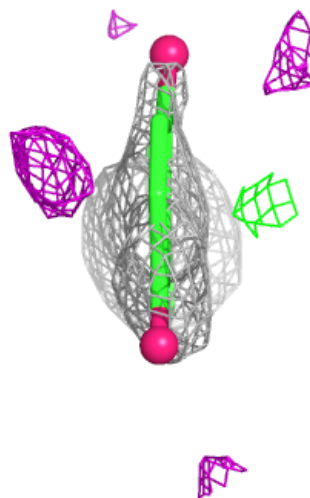
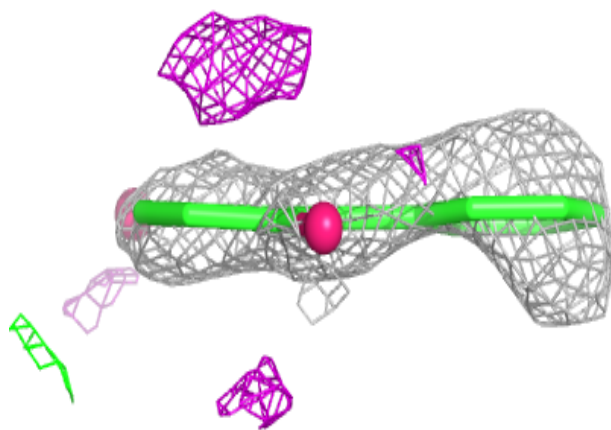
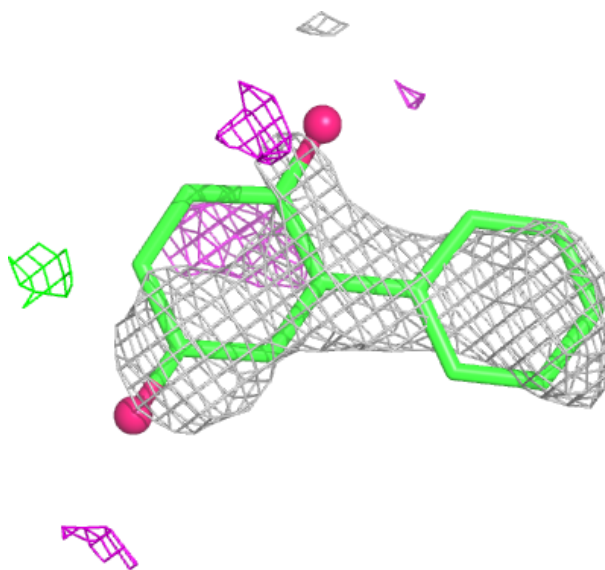
**Electron density around LMG b 623:**

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



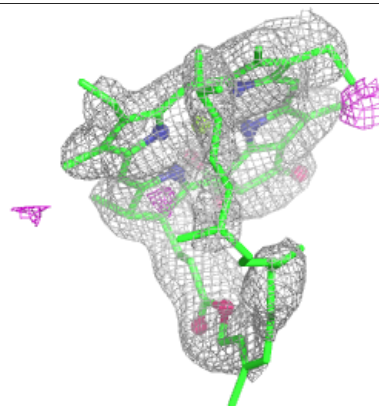
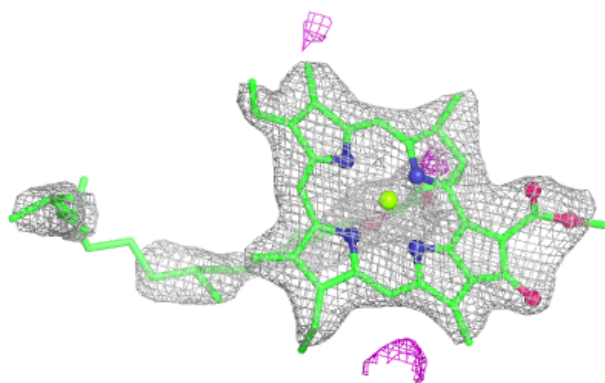
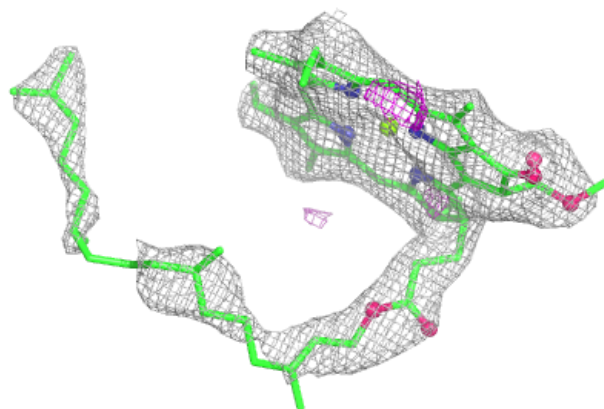
Electron density around K3C a 424 (A):

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

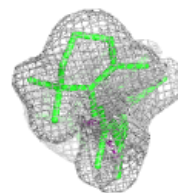
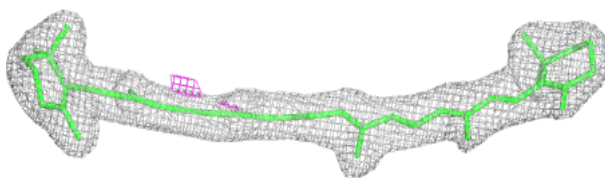
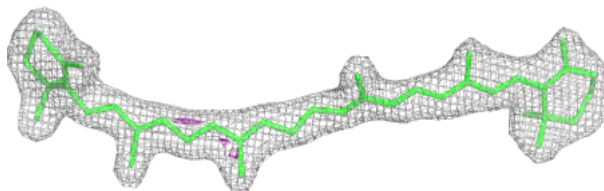


Electron density around CLA c 515:

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

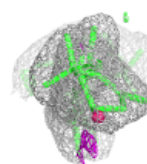
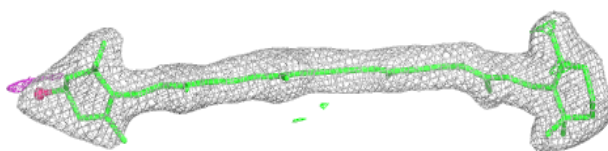
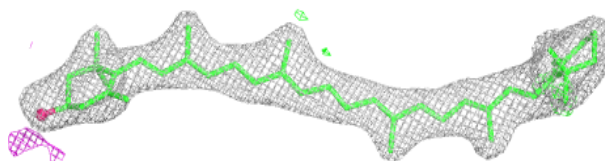
**Electron density around BCR B 641:**

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



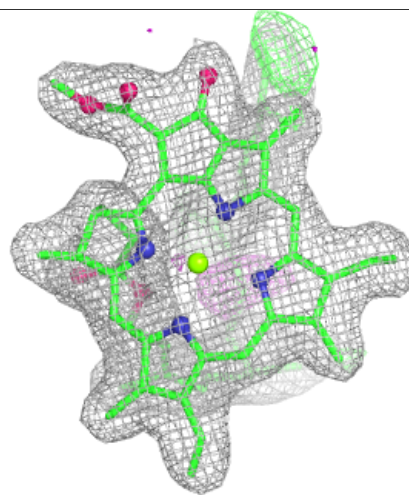
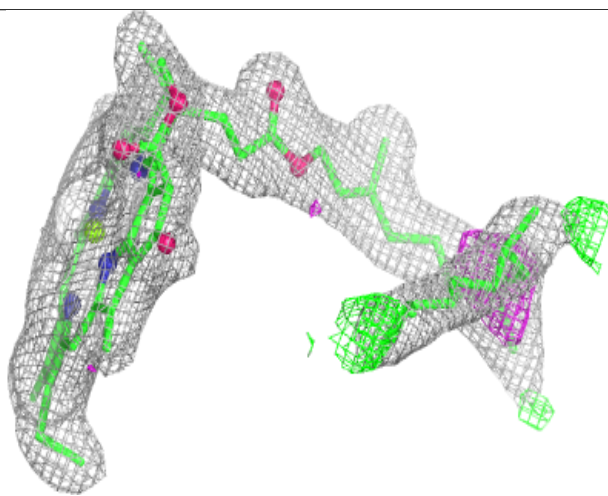
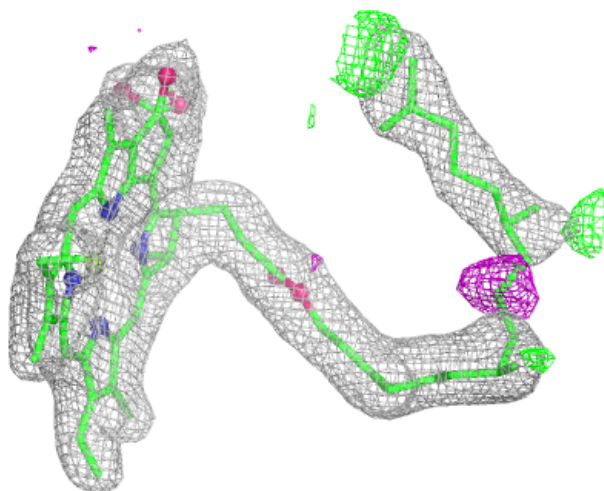
Electron density around RRX h 1204:

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



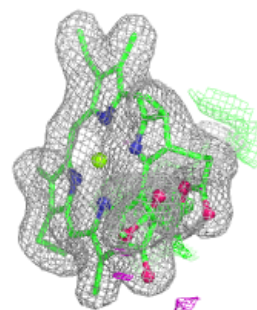
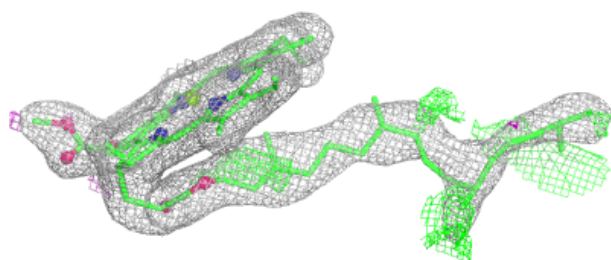
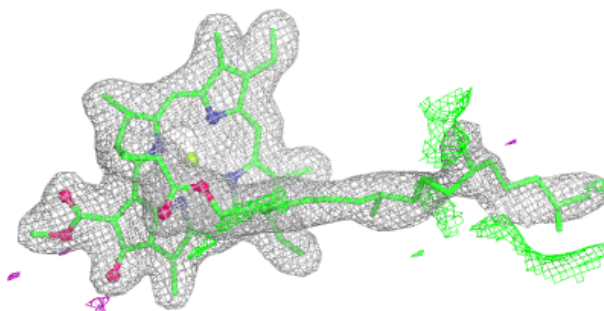
Electron density around CLA b 609:

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

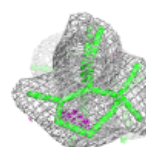
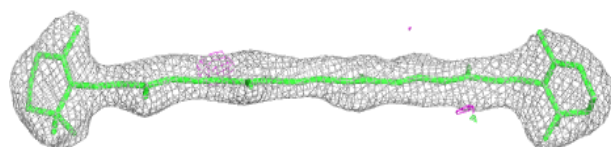
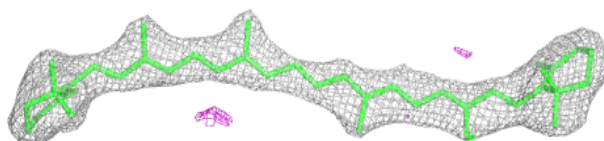


Electron density around CLA b 617:

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

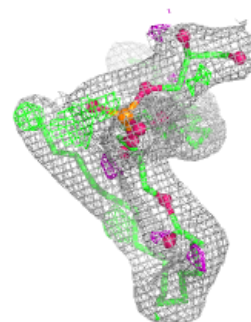
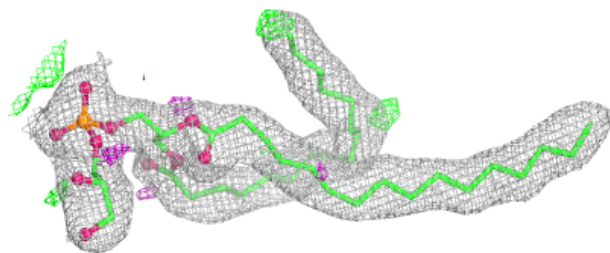
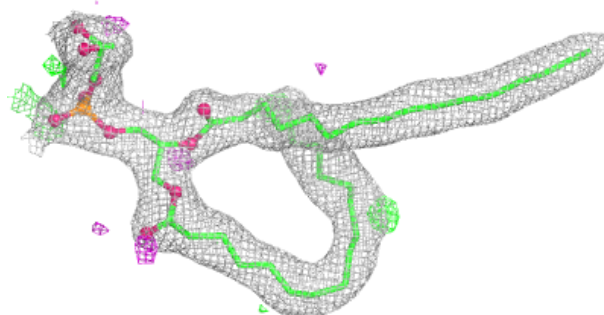
**Electron density around BCR c 516:**

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

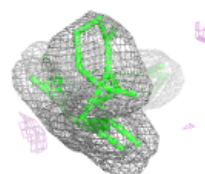
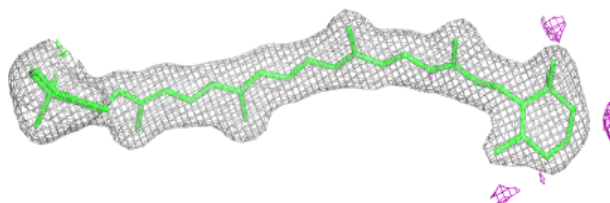
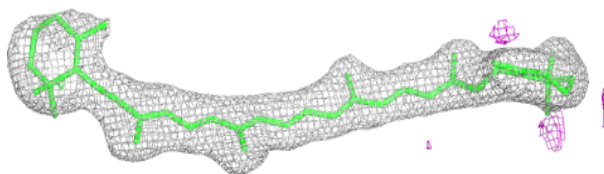


Electron density around LHG d 408:

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

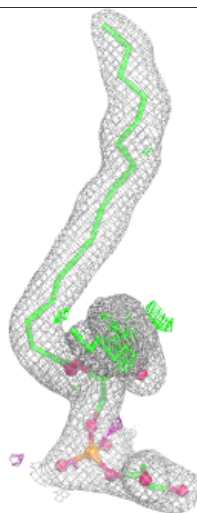
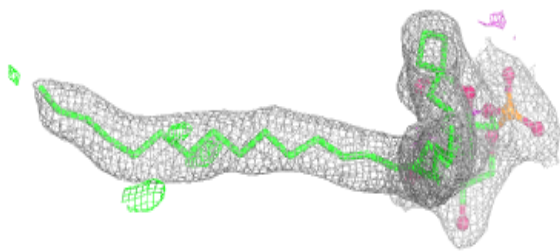
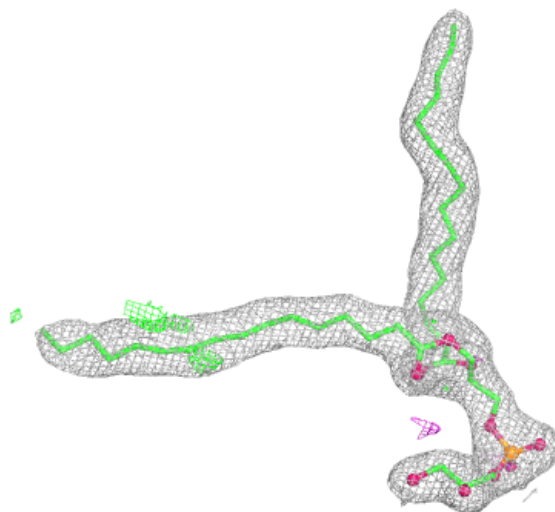
**Electron density around BCR d 406:**

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



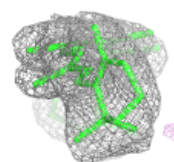
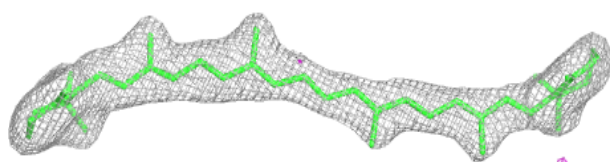
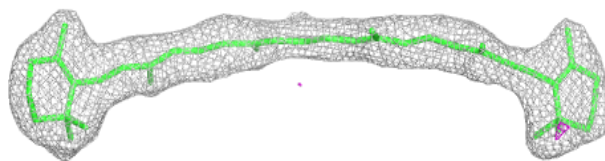
Electron density around LHG 1 302:

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



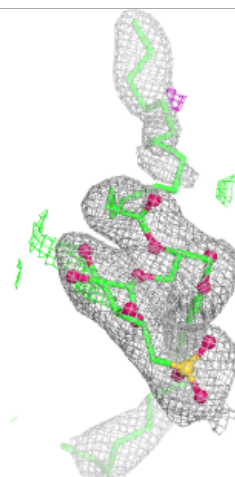
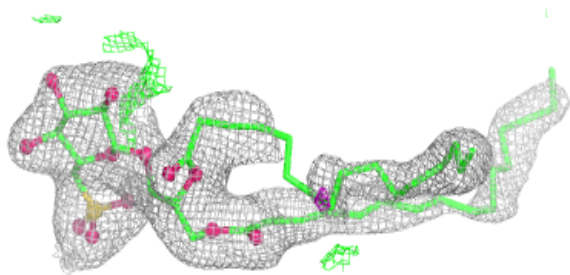
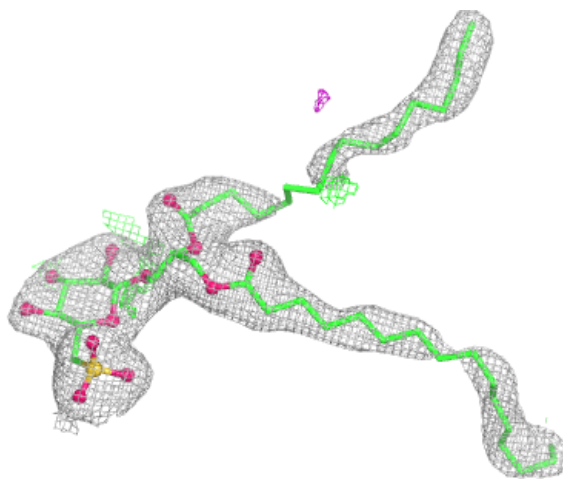
Electron density around BCR k 303:

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



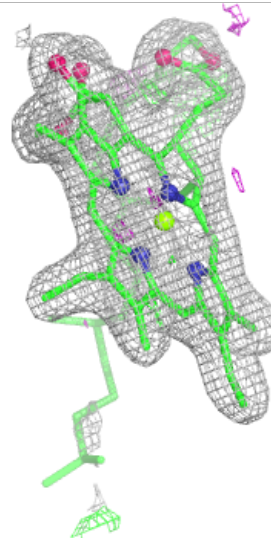
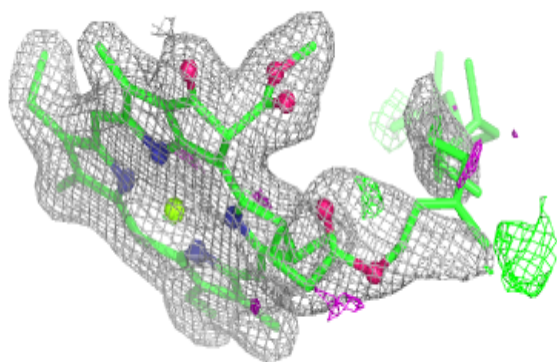
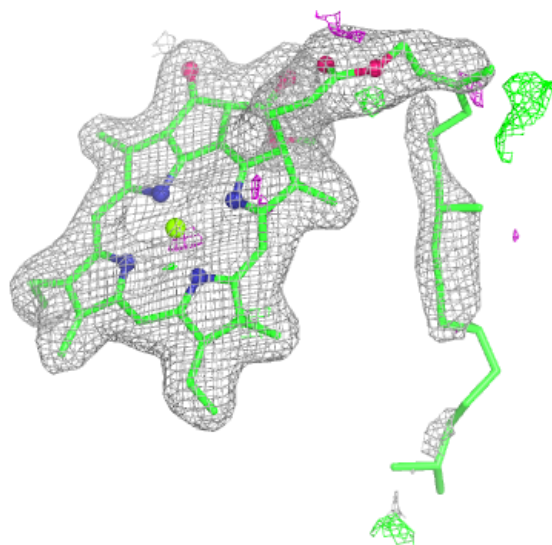
Electron density around SQD A 411:

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



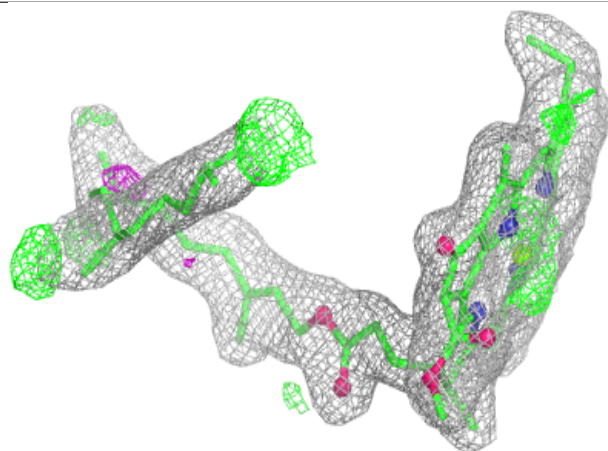
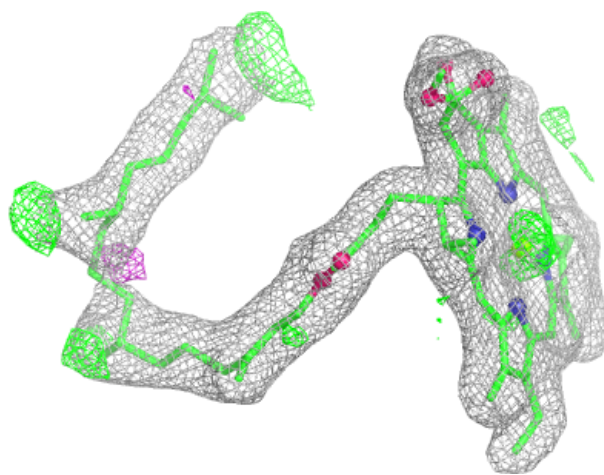
Electron density around CLA B 617:

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



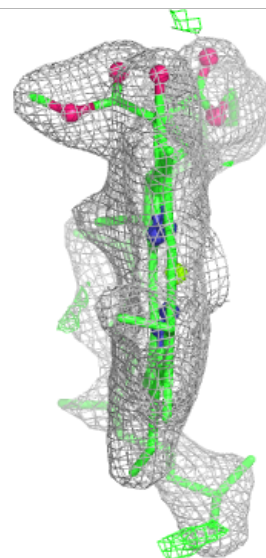
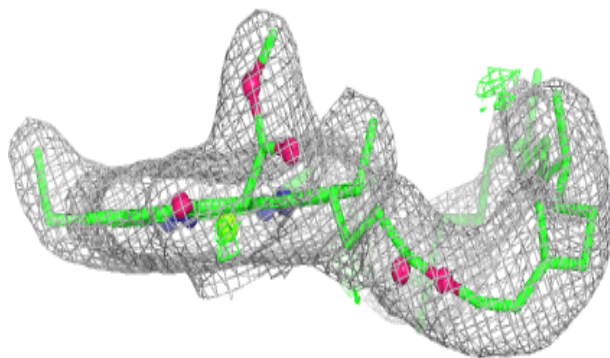
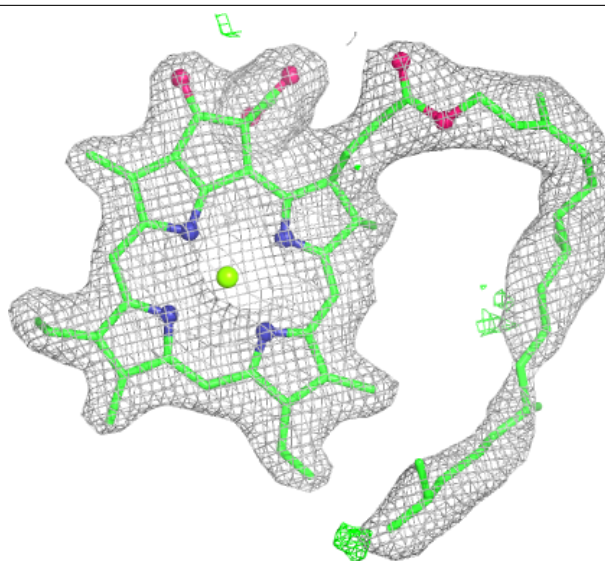
Electron density around CLA B 607:

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



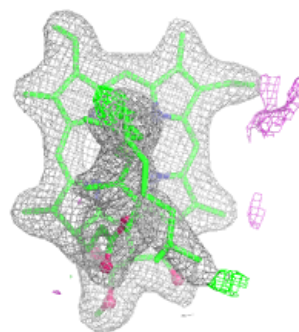
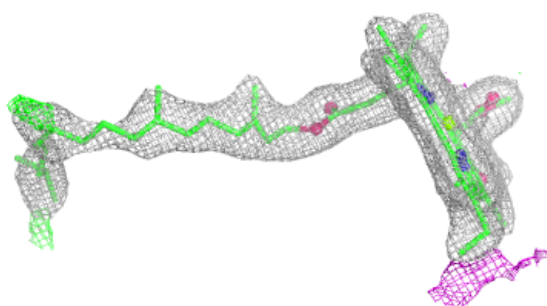
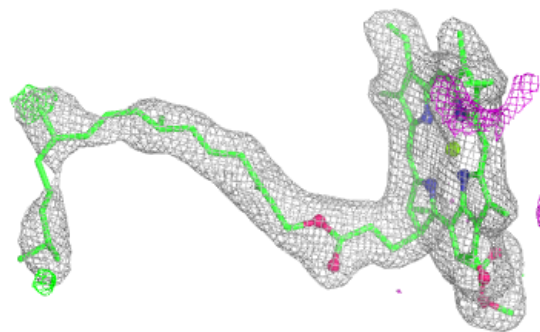
Electron density around CLA C 513:

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

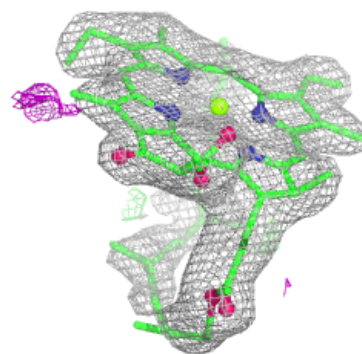
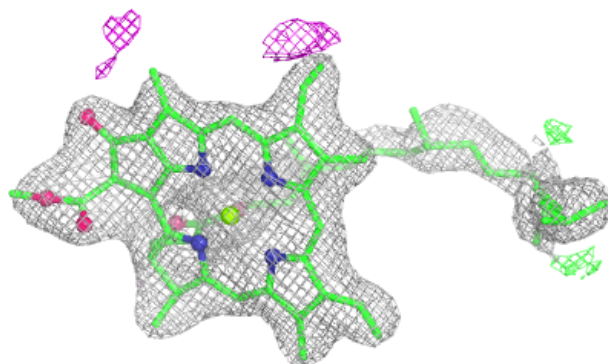
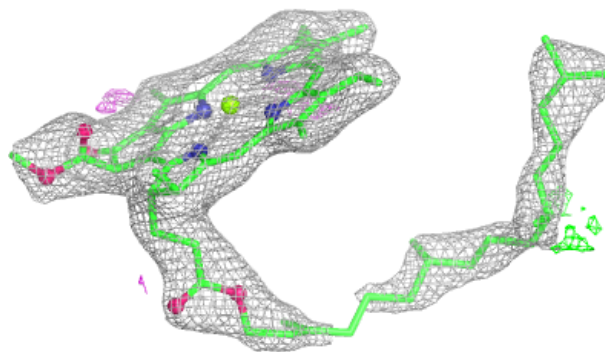


Electron density around CLA d 405:

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

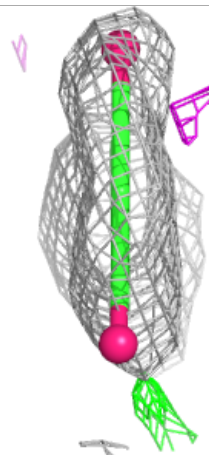
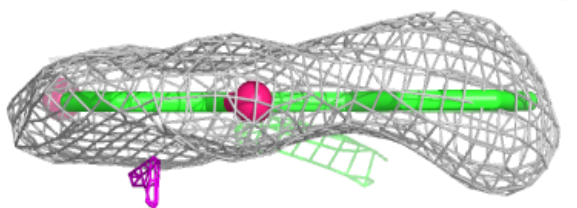
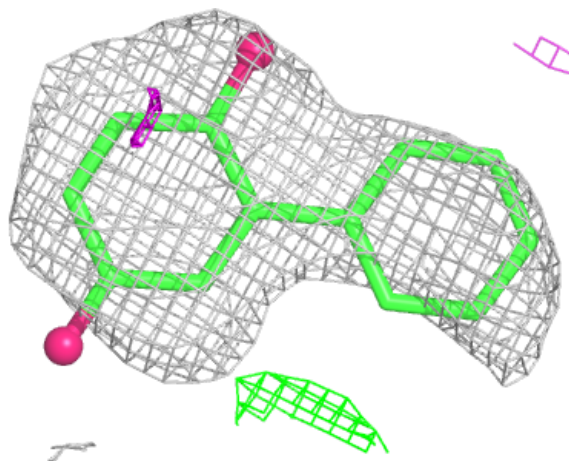
**Electron density around CLA C 514:**

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



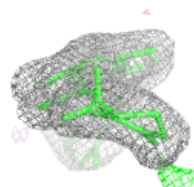
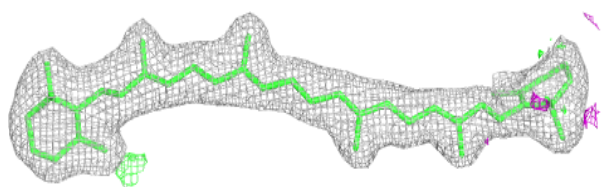
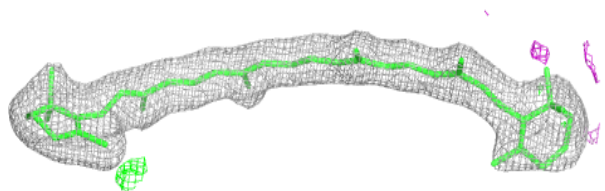
Electron density around K3C A 421 (A):

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

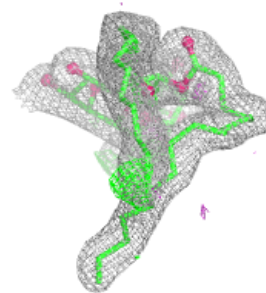
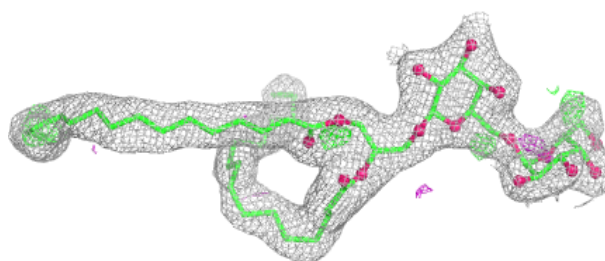
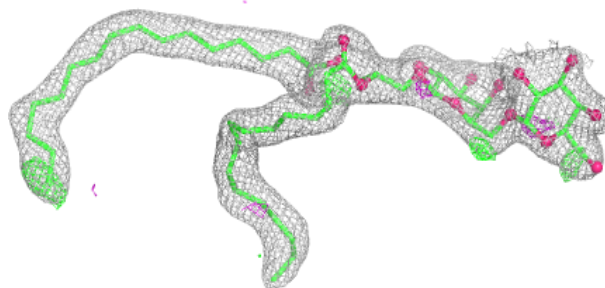


Electron density around BCR D 405:

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

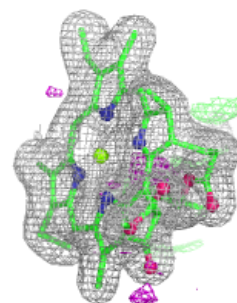
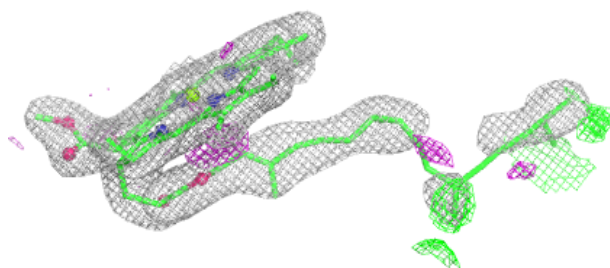
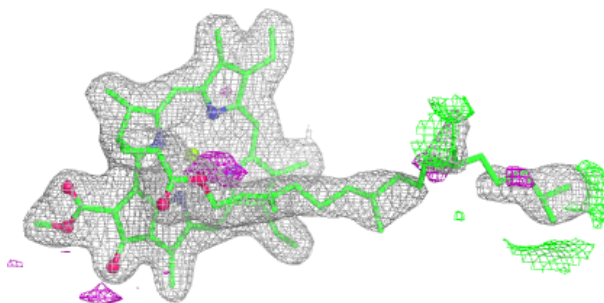
**Electron density around DGD h 1205:**

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

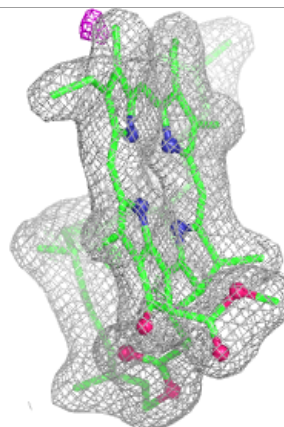
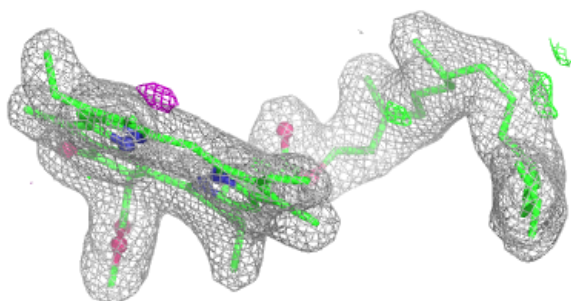
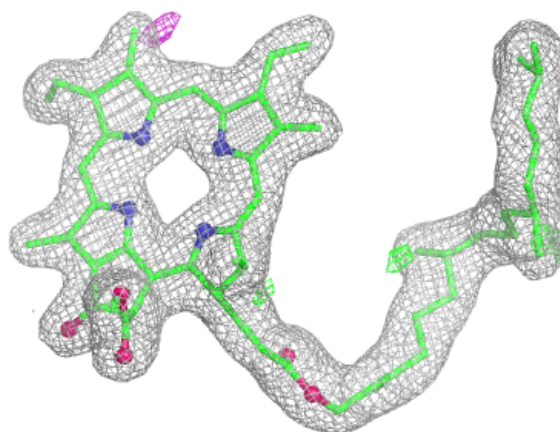


Electron density around CLA B 615:

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

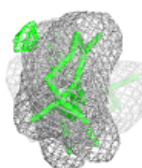
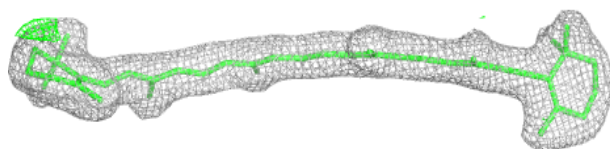
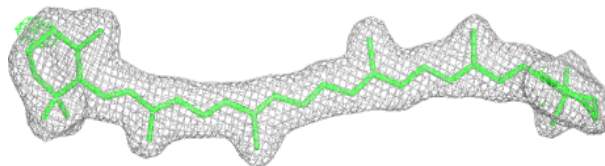
**Electron density around PHO D 401:**

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

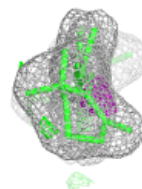
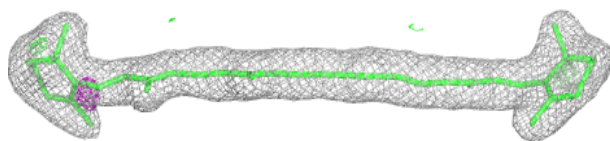
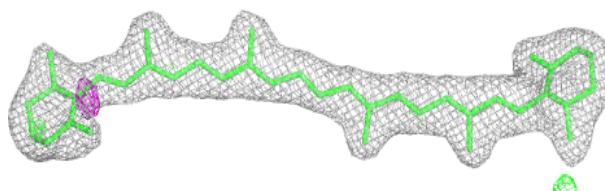


Electron density around BCR B 618:

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

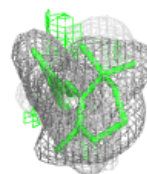
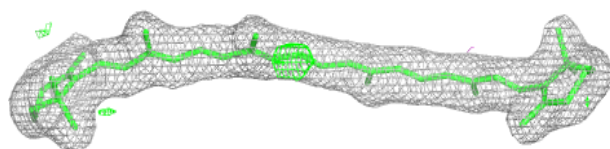
**Electron density around BCR B 619:**

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



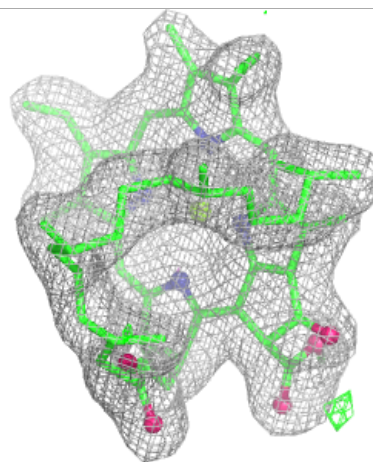
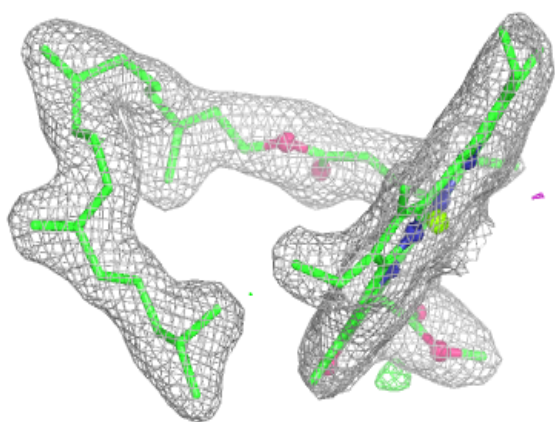
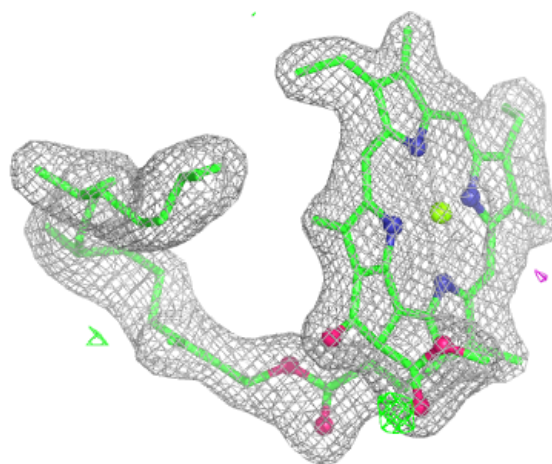
Electron density around BCR B 620:

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



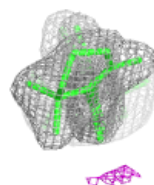
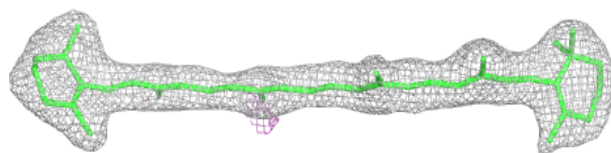
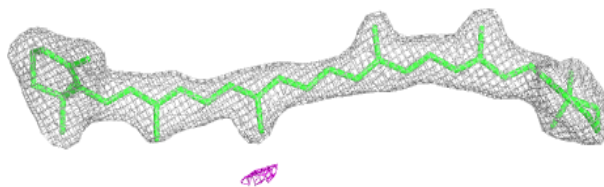
Electron density around CLA C 504:

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

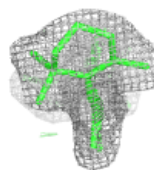
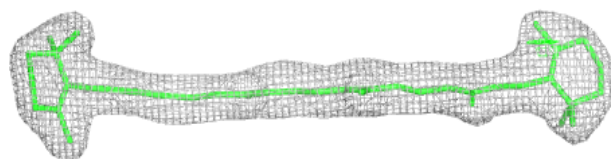
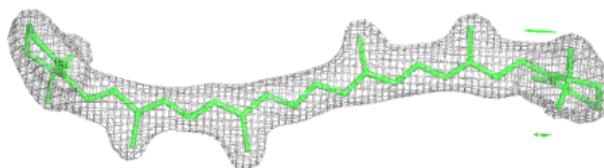


Electron density around BCR C 515:

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

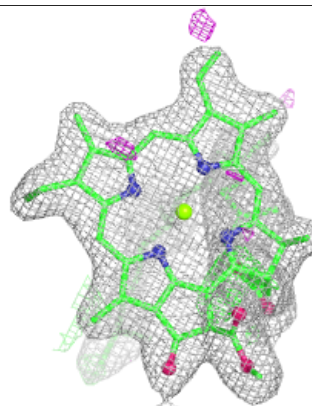
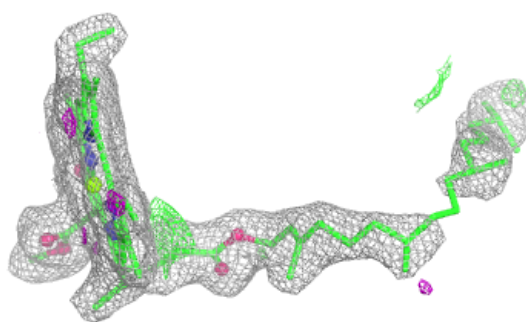
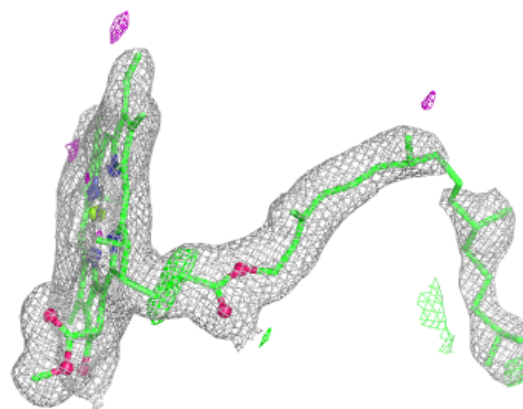
**Electron density around BCR C 516:**

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

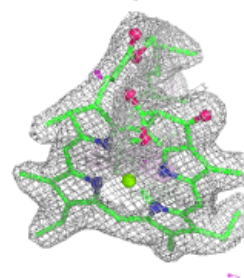
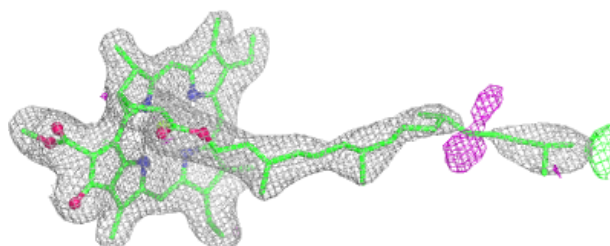
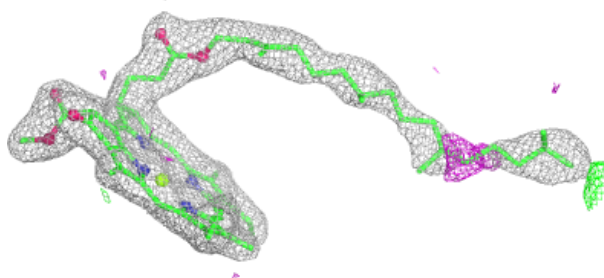


Electron density around CLA D 404:

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

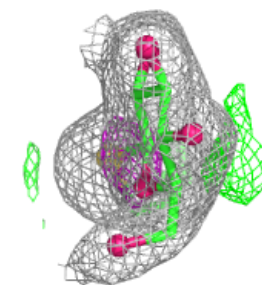
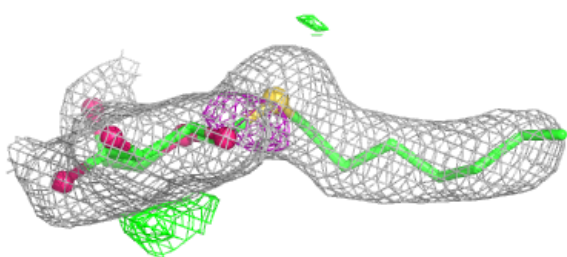
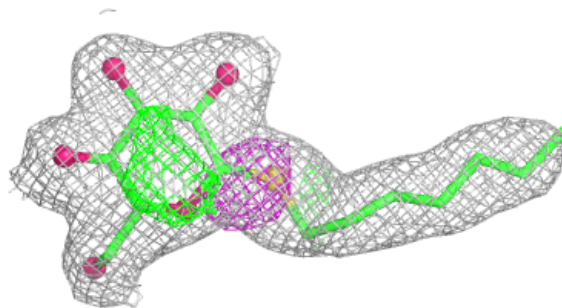
**Electron density around CLA c 506:**

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

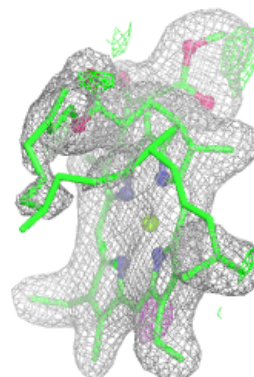
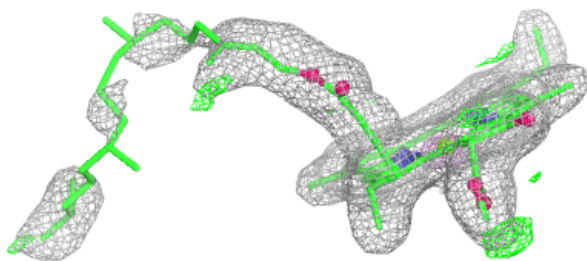
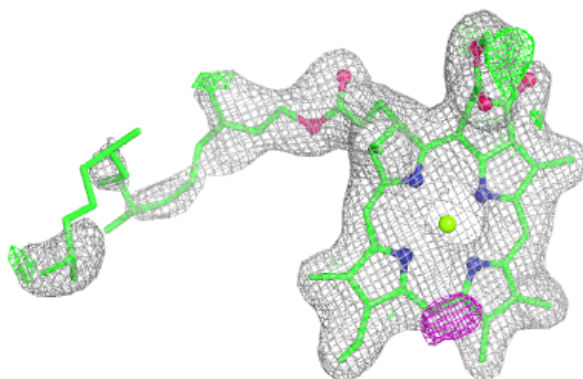


Electron density around HTG O 302:

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

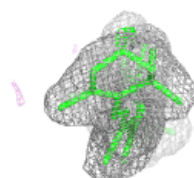
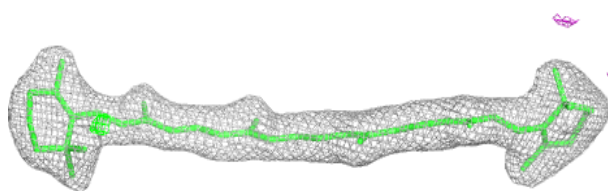
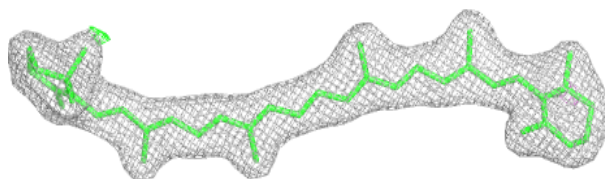
**Electron density around CLA a 412:**

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

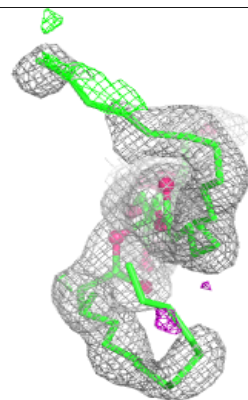
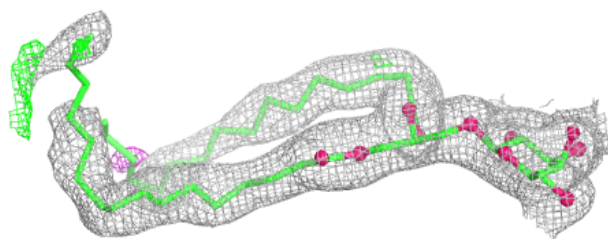
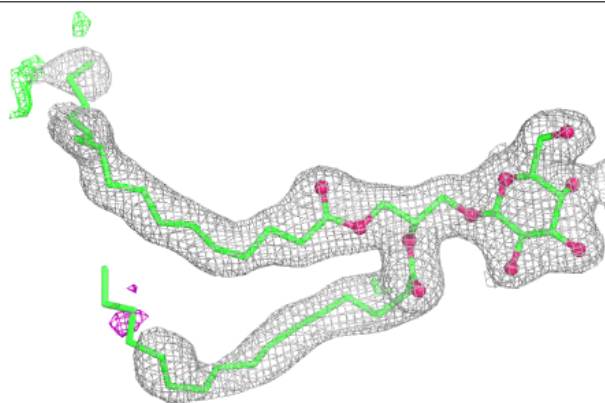


Electron density around BCR Y 302:

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

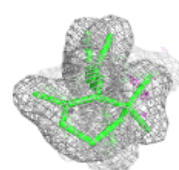
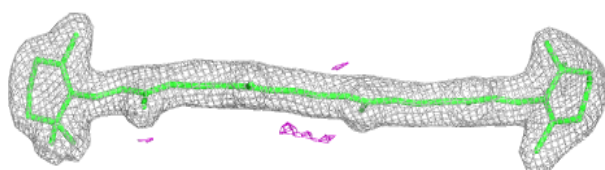
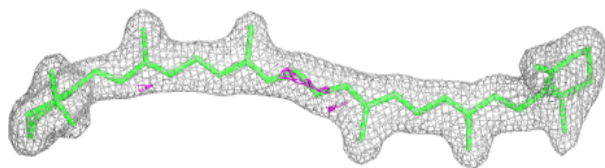
**Electron density around LMG D 412:**

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

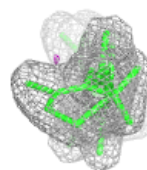
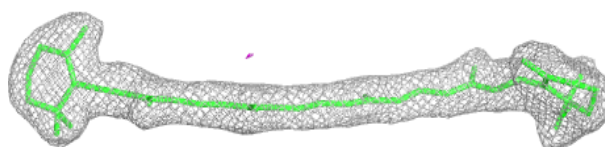
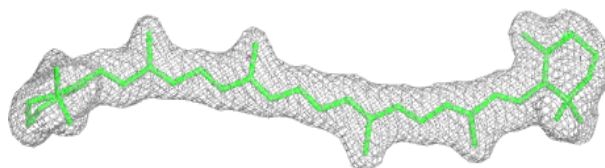


Electron density around BCR a 413:

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

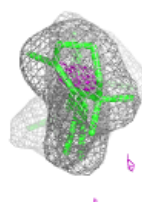
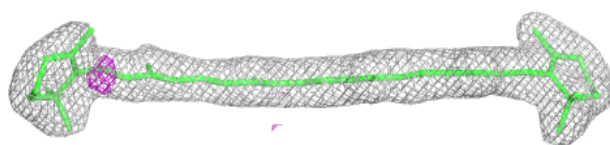
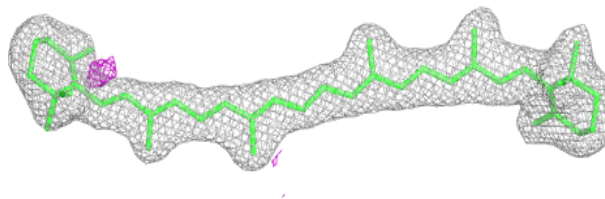
**Electron density around BCR b 620:**

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

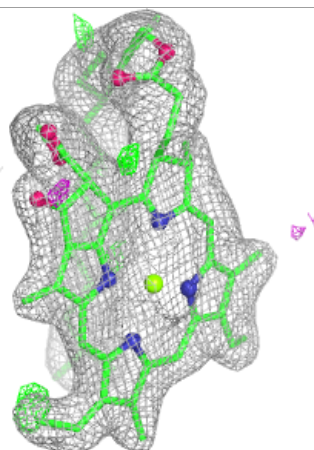
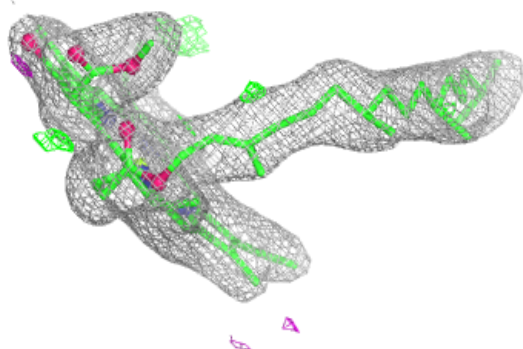
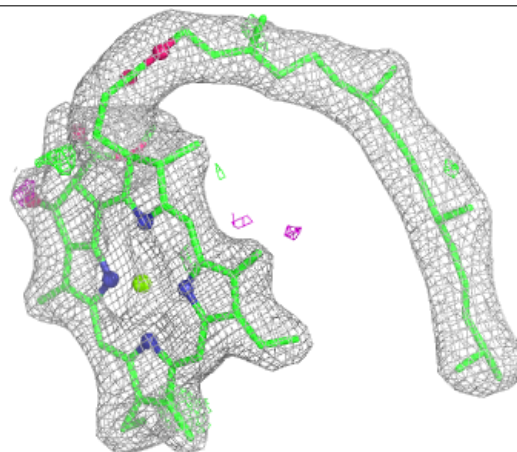


Electron density around BCR b 621:

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

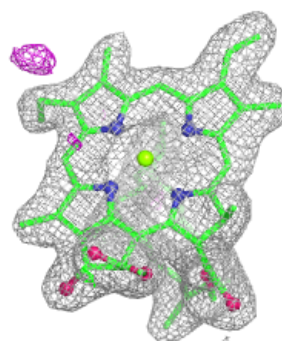
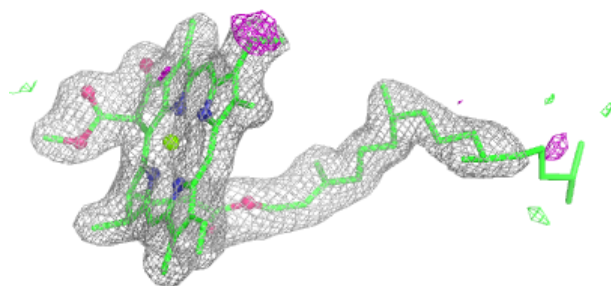
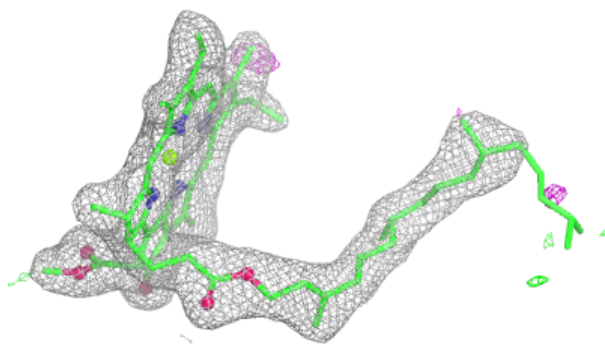
**Electron density around CLA c 509:**

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

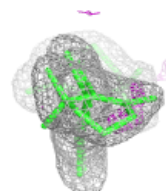
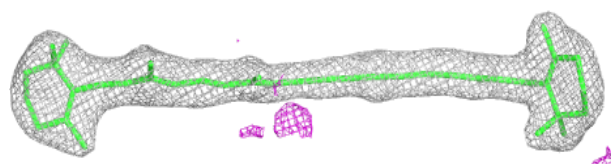
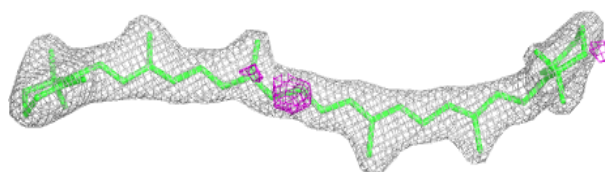


Electron density around CLA c 510:

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

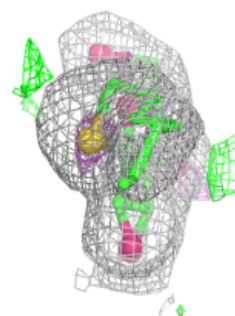
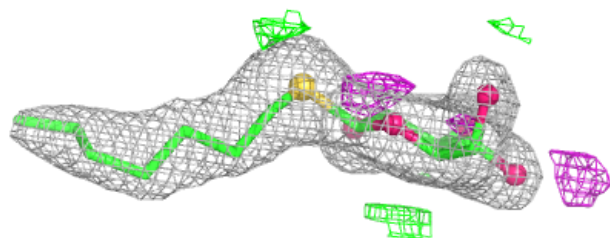
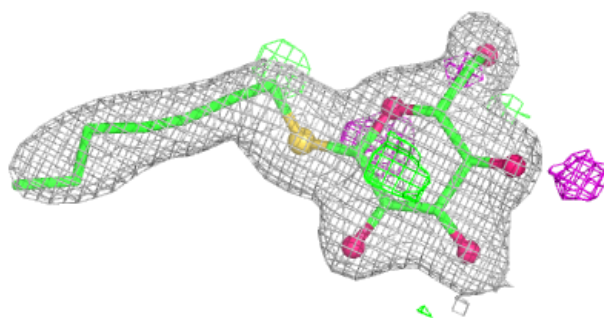
**Electron density around BCR c 517:**

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



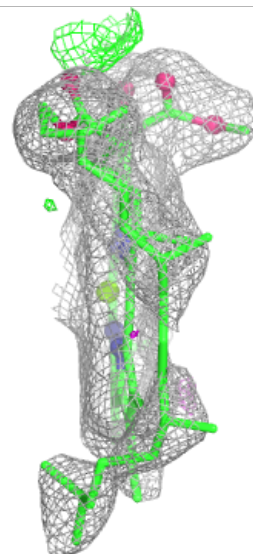
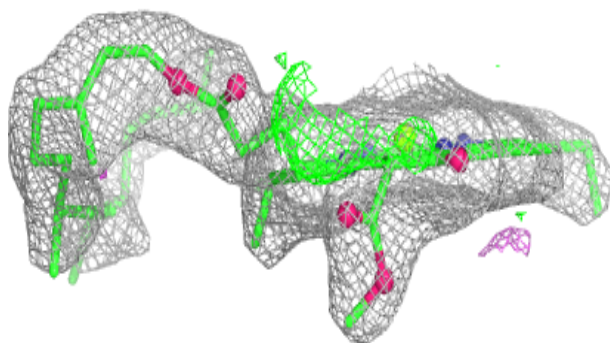
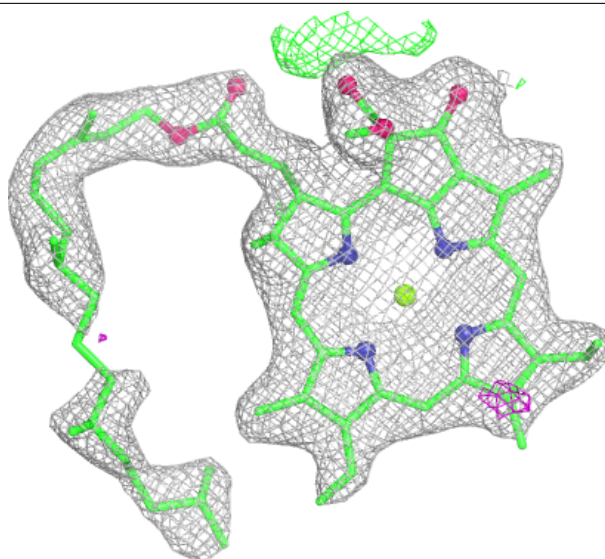
Electron density around HTG o 301:

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



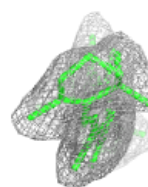
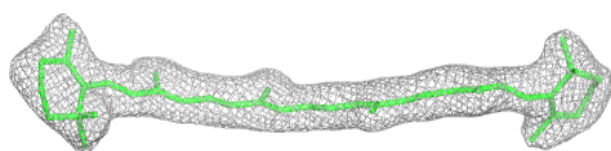
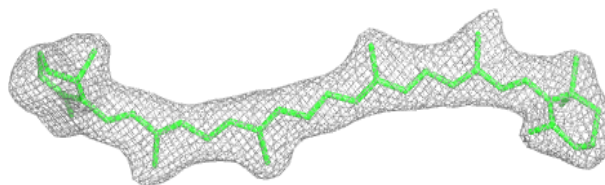
Electron density around CLA c 514:

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

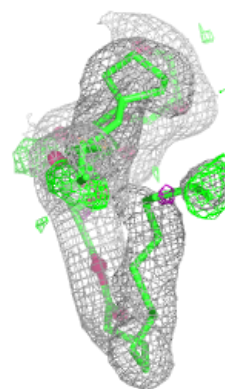
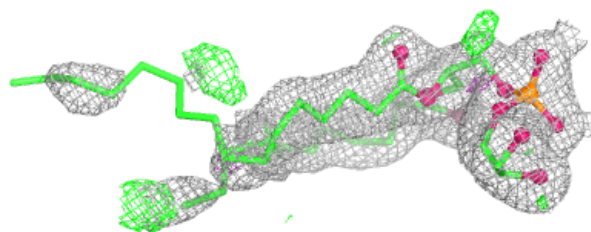
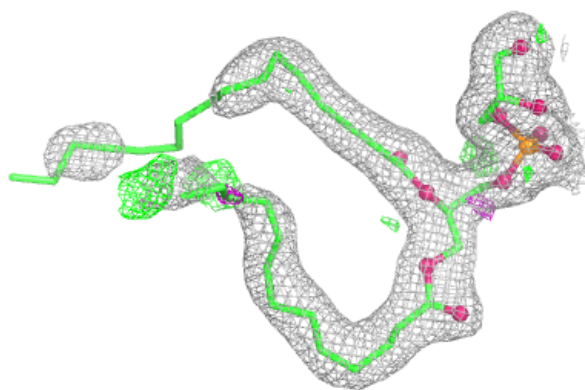


Electron density around BCR k 302:

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

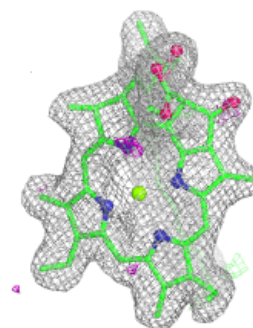
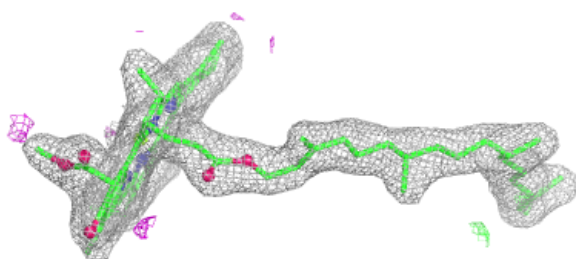
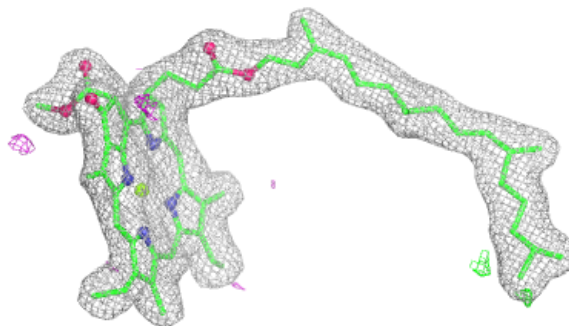
**Electron density around LHG D 411:**

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

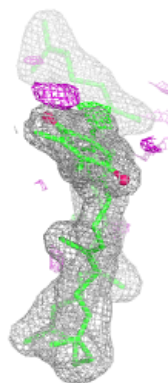
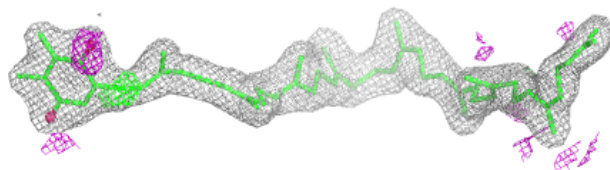
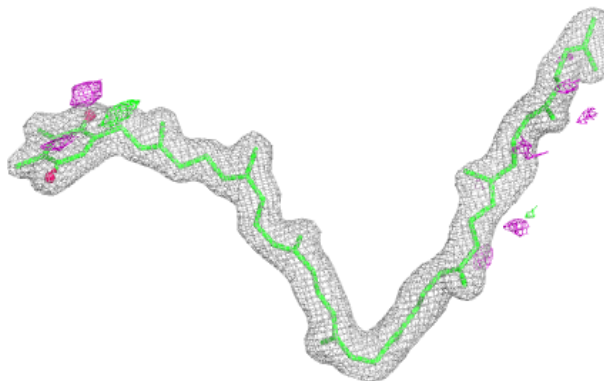


Electron density around CLA B 610:

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

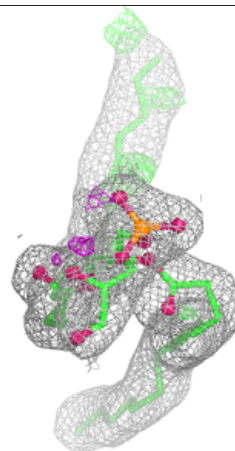
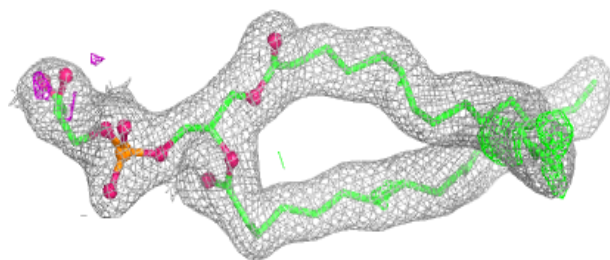
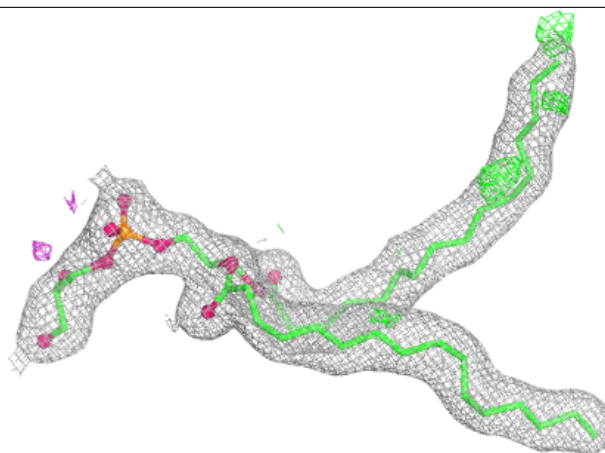
**Electron density around PL9 D 406:**

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



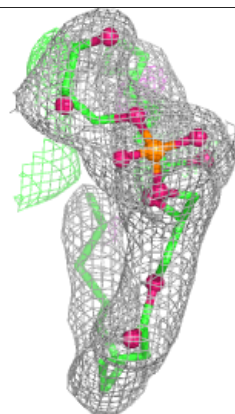
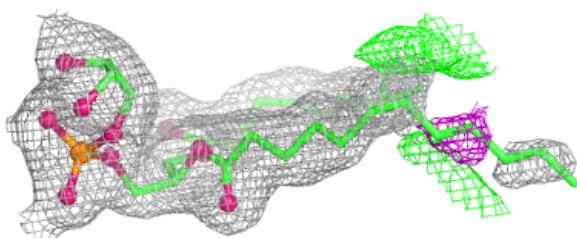
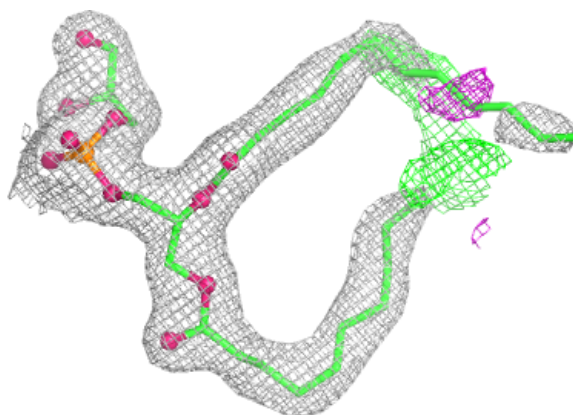
Electron density around LHG d 409:

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

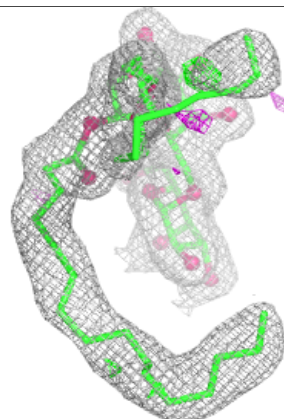
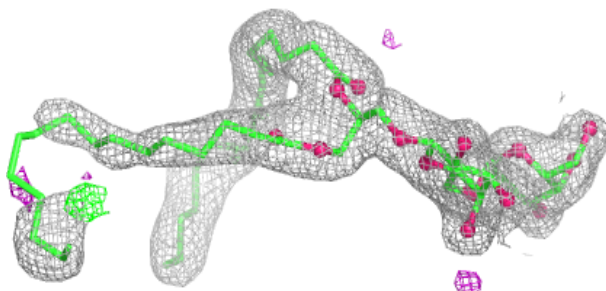
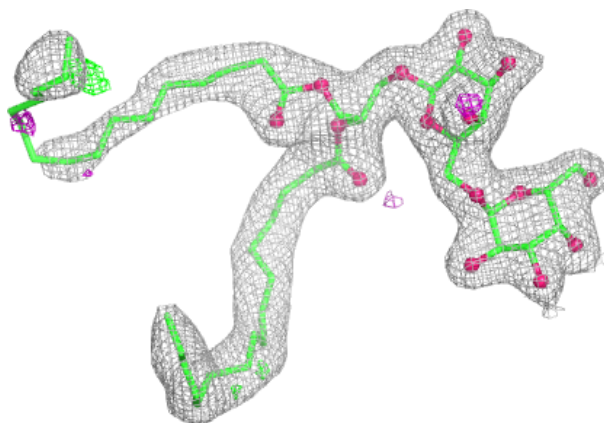


Electron density around LHG d 410:

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

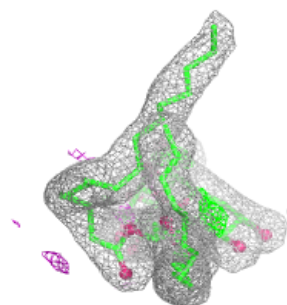
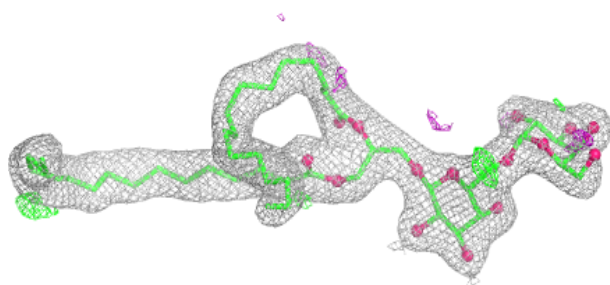
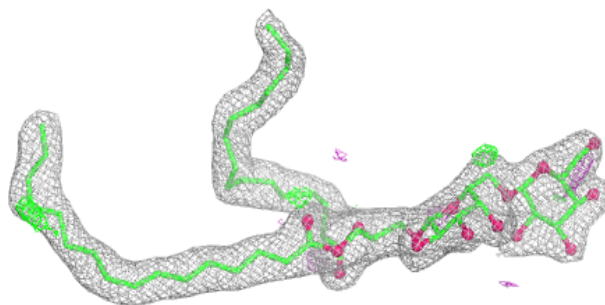
**Electron density around DGD C 518:**

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

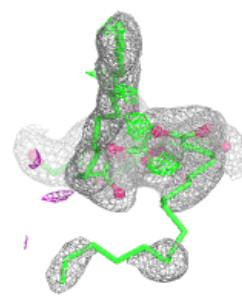
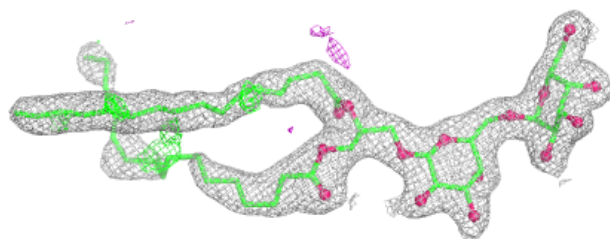
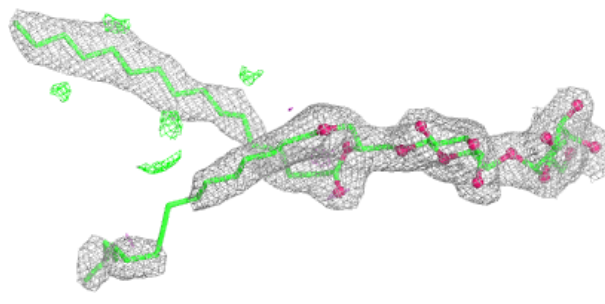


Electron density around DGD H 102:

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

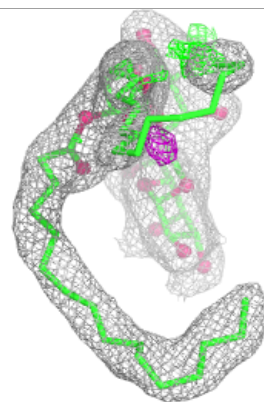
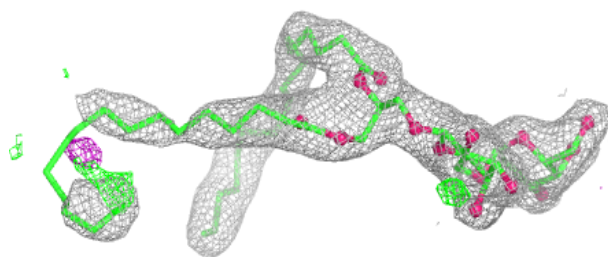
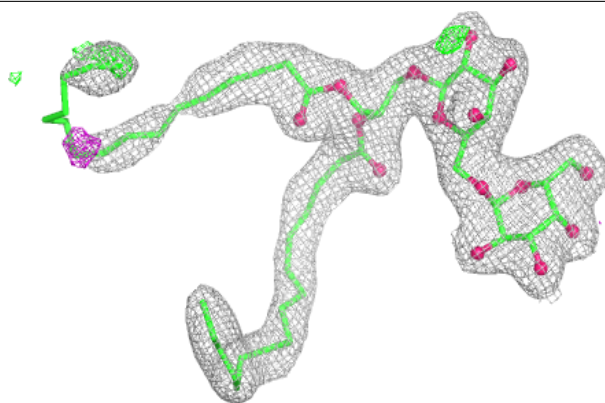
**Electron density around DGD c 518:**

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

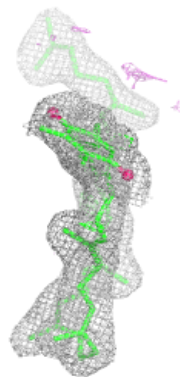
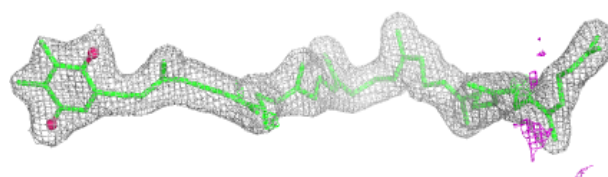
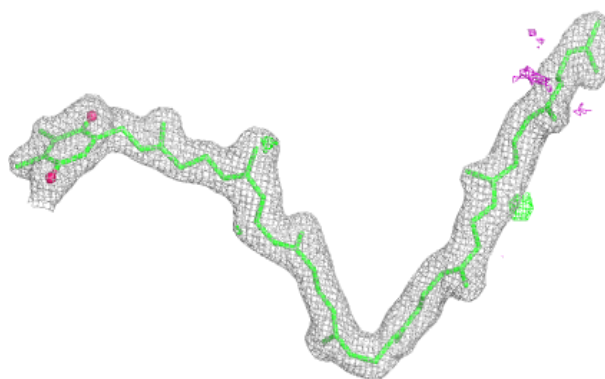


Electron density around DGD c 519:

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

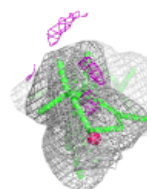
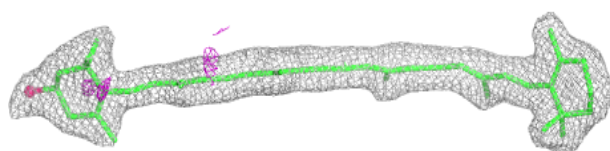
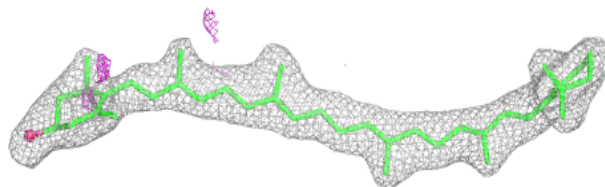
**Electron density around PL9 d 407:**

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

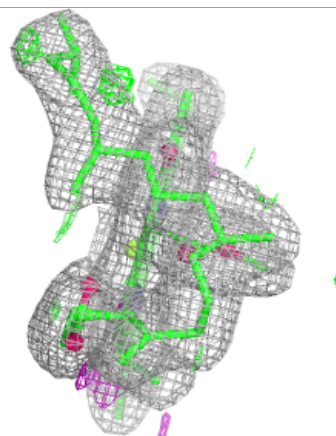
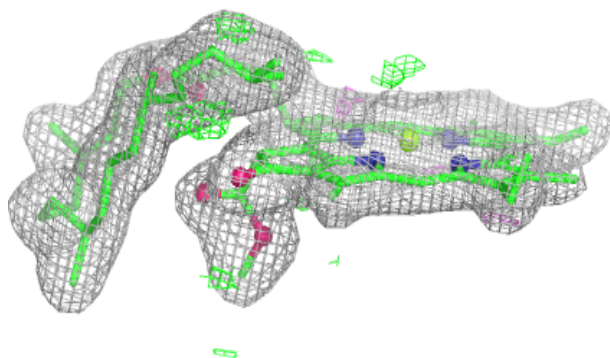
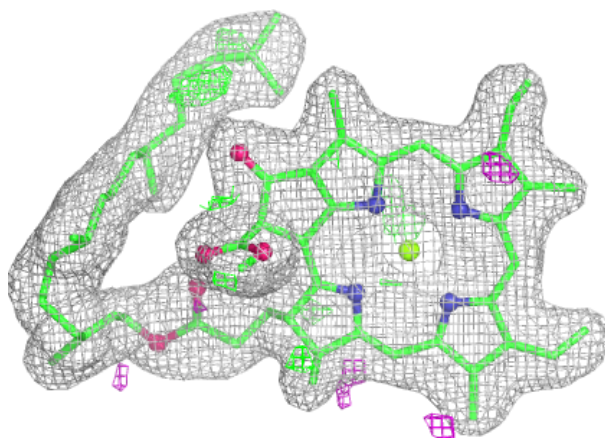


Electron density around RRX H 101:

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

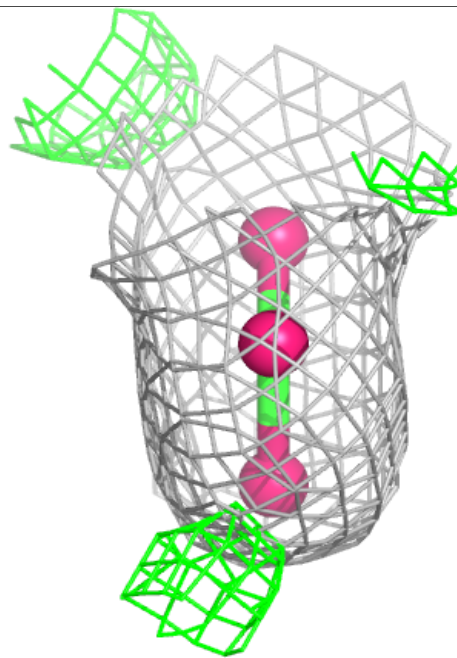
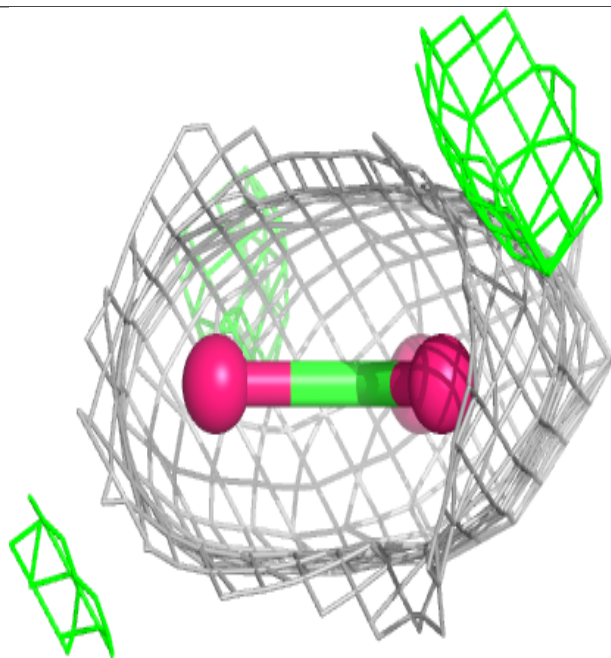
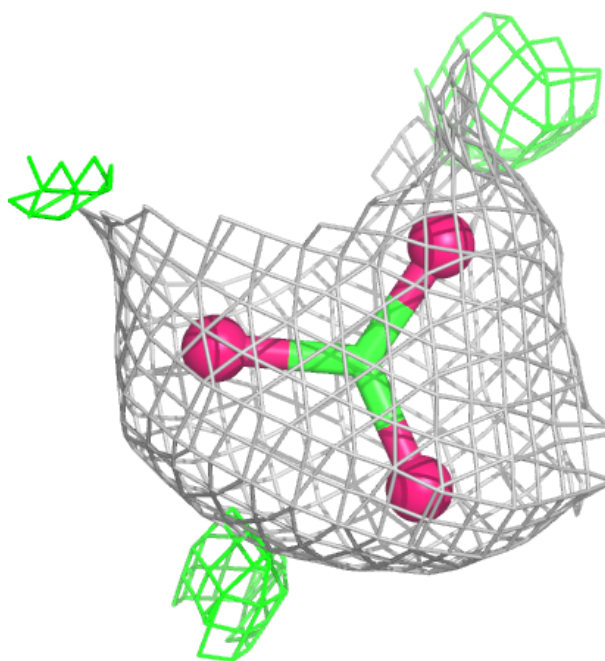
**Electron density around CLA B 611:**

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



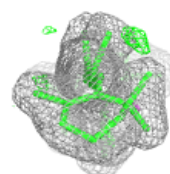
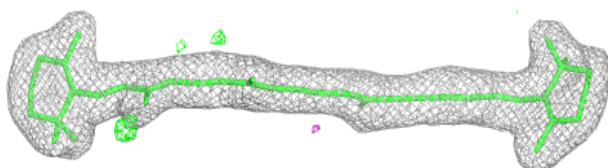
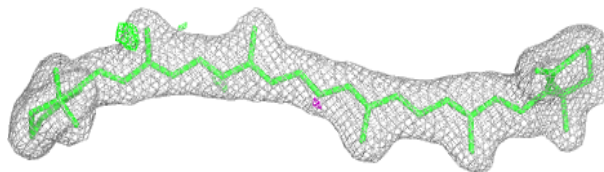
Electron density around BCT a 407:

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



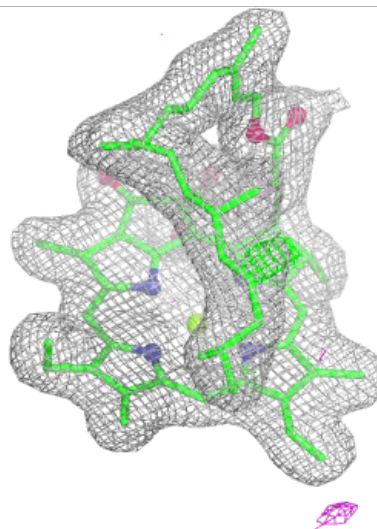
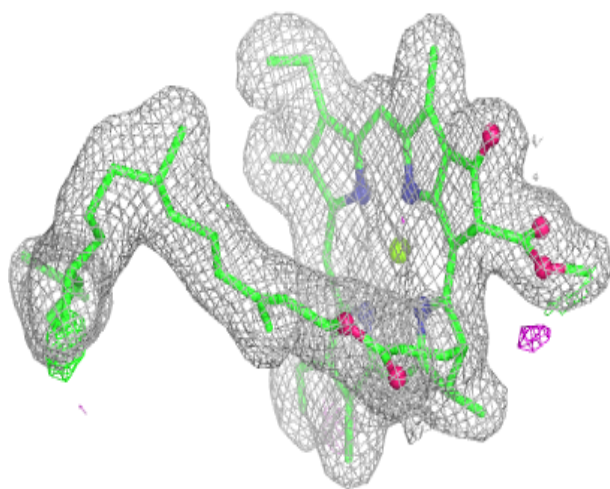
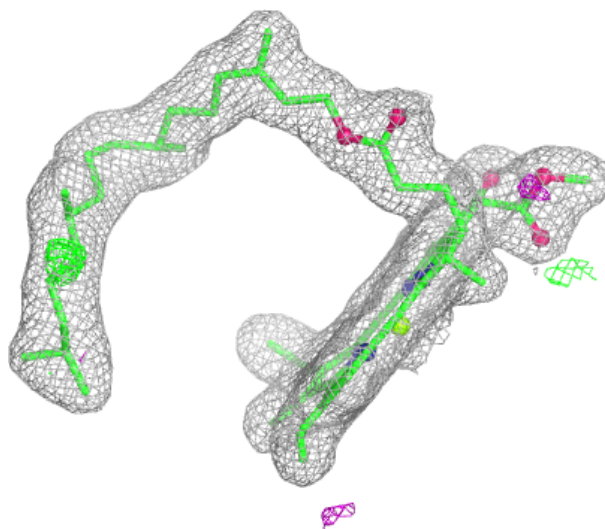
Electron density around BCR A 410:

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



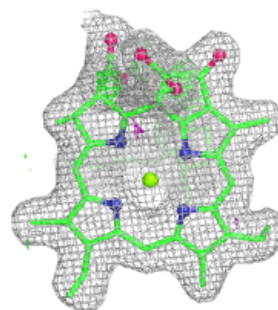
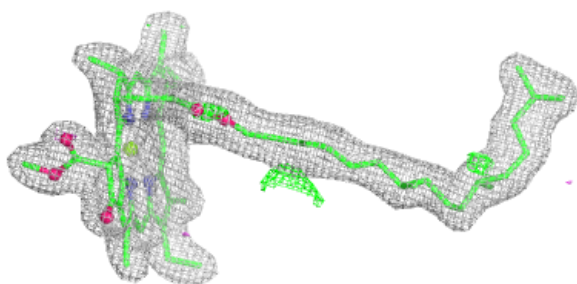
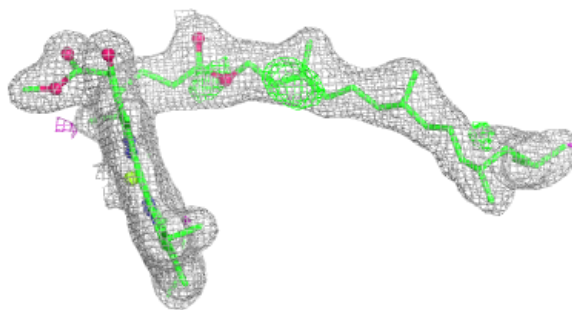
Electron density around CLA B 612:

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

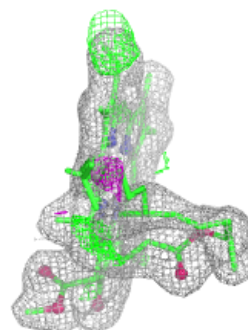
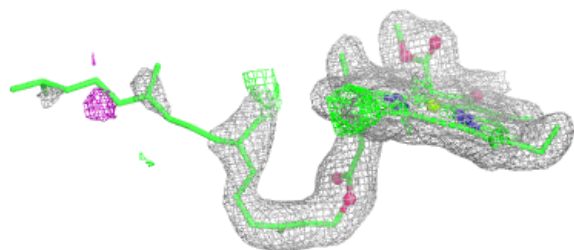
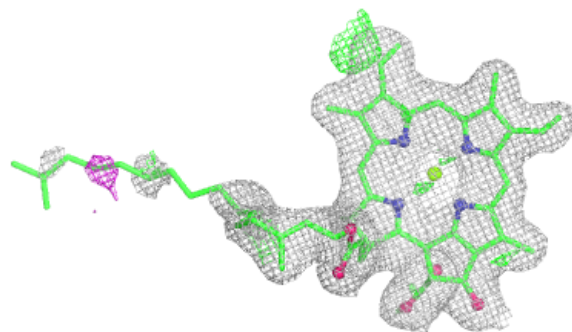


Electron density around CLA B 606:

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

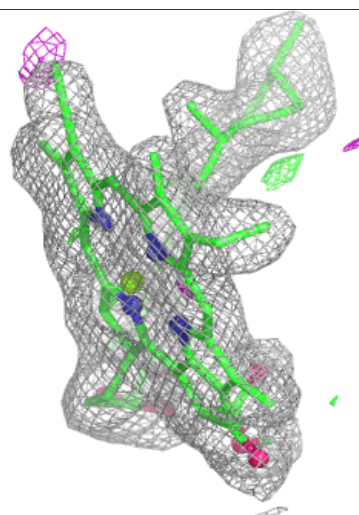
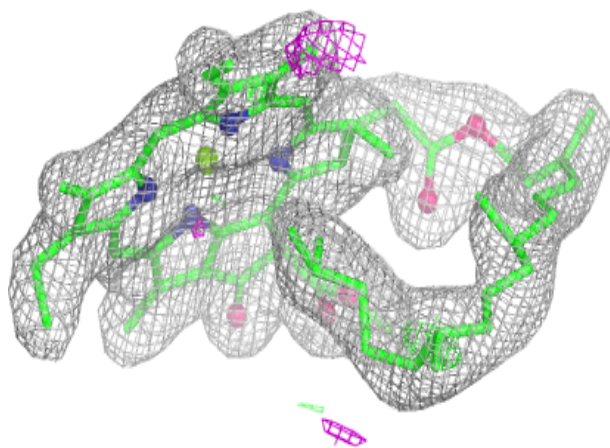
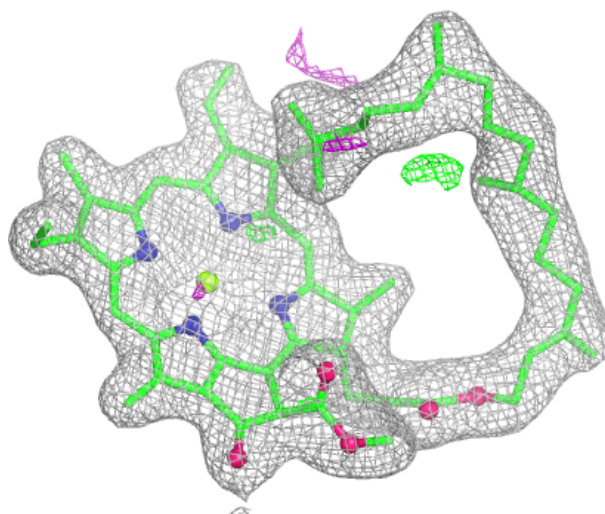
**Electron density around CLA a 410:**

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



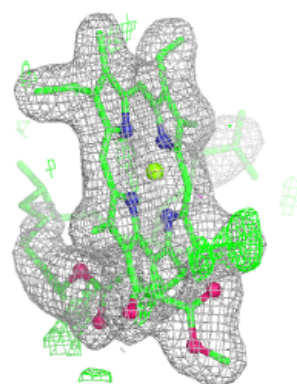
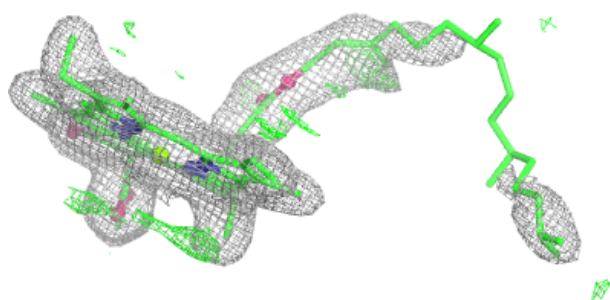
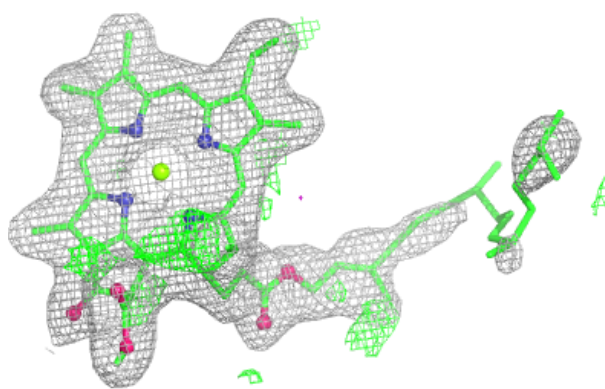
Electron density around CLA B 616:

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

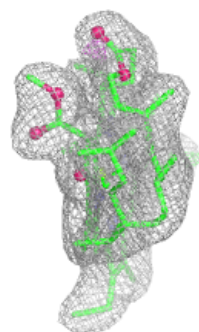
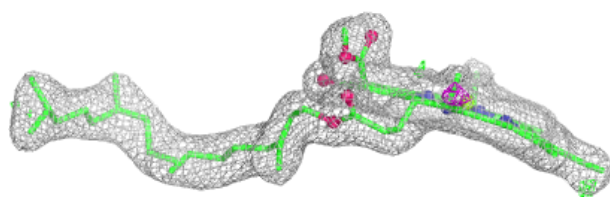
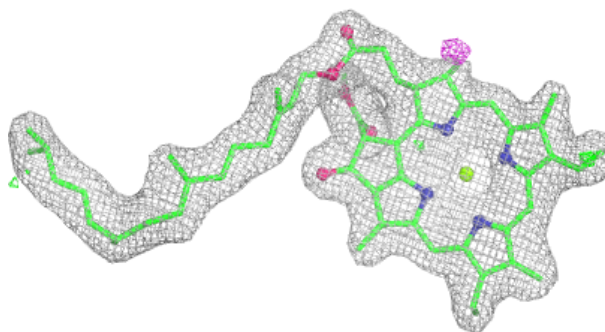


Electron density around CLA A 409:

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

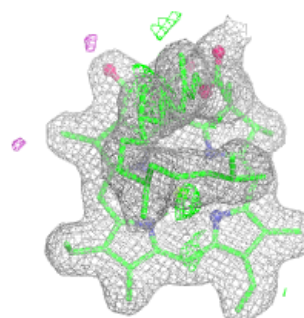
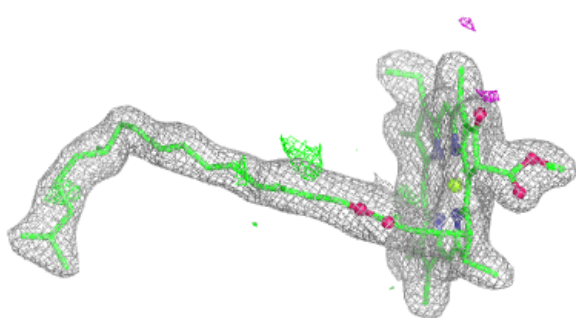
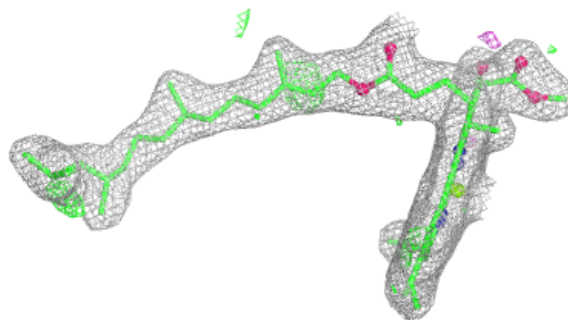
**Electron density around CLA b 605:**

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

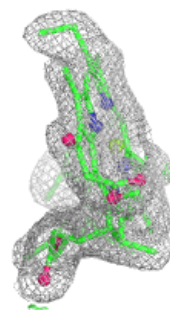
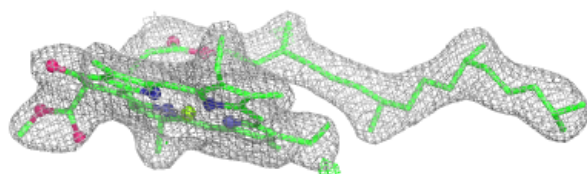
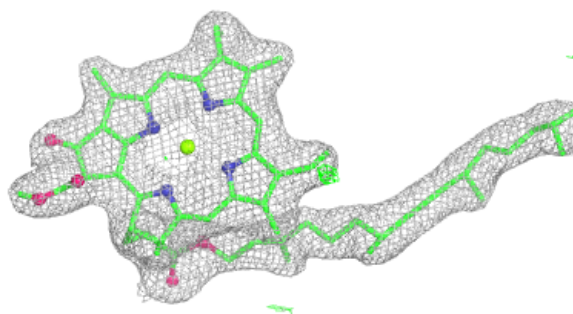


Electron density around CLA b 608:

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

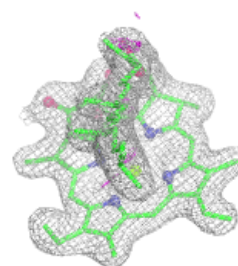
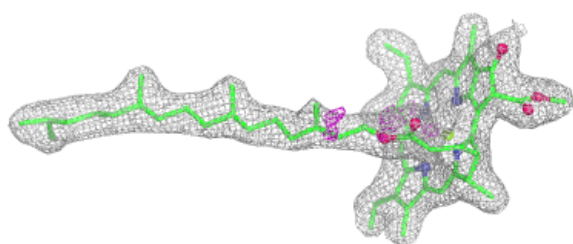
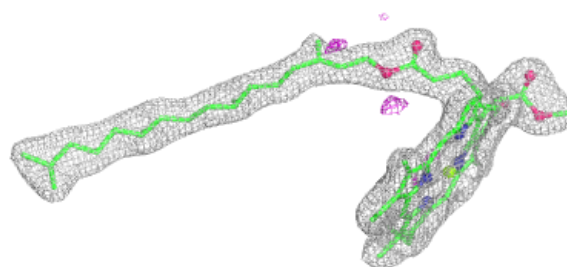
**Electron density around CLA C 502:**

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

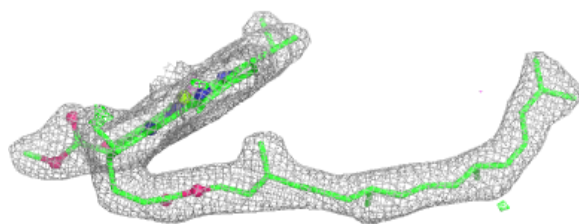
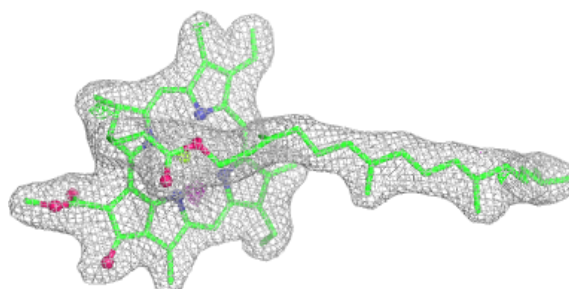


Electron density around CLA b 610:

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

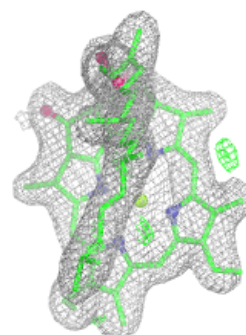
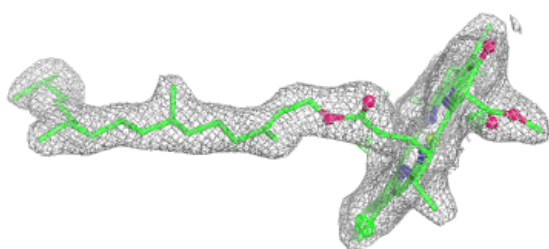
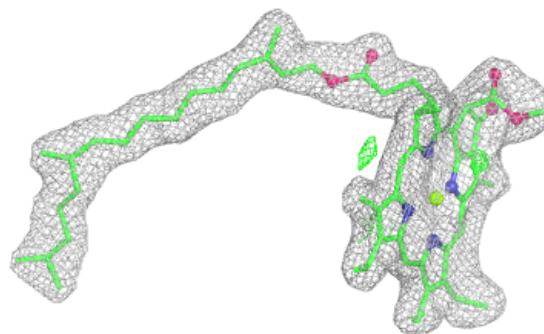
**Electron density around CLA b 611:**

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

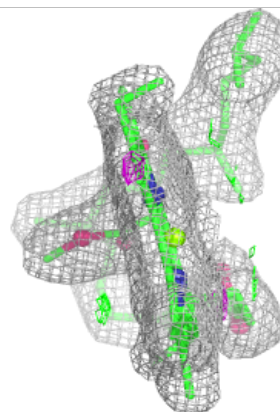
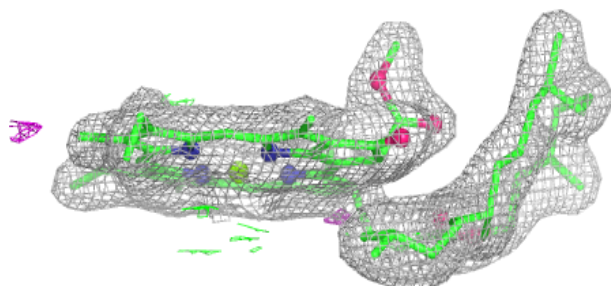
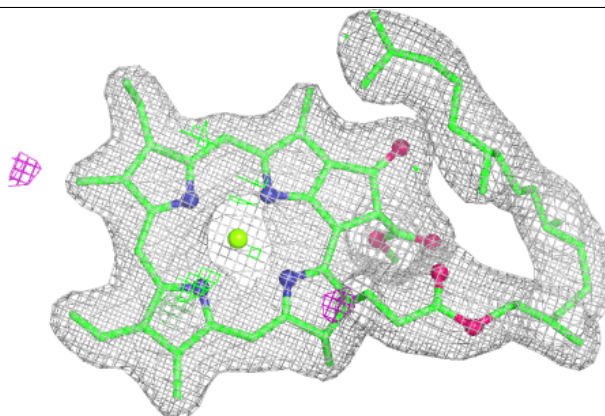


Electron density around CLA b 612:

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

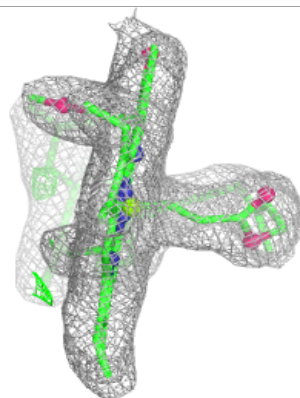
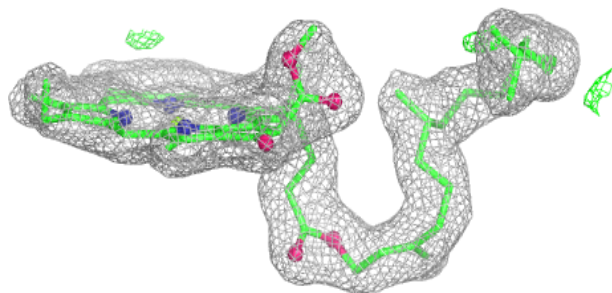
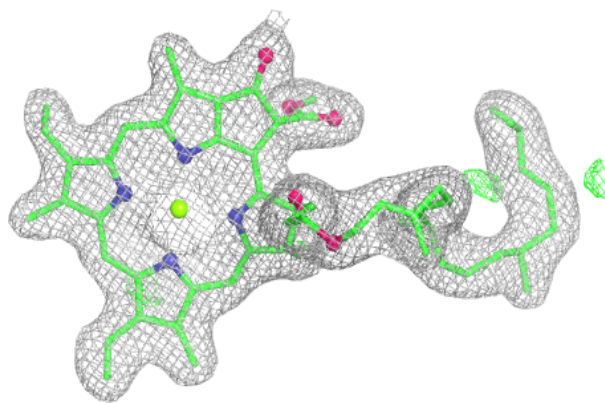
**Electron density around CLA b 613:**

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



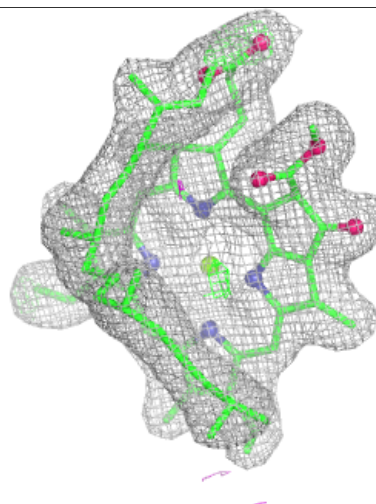
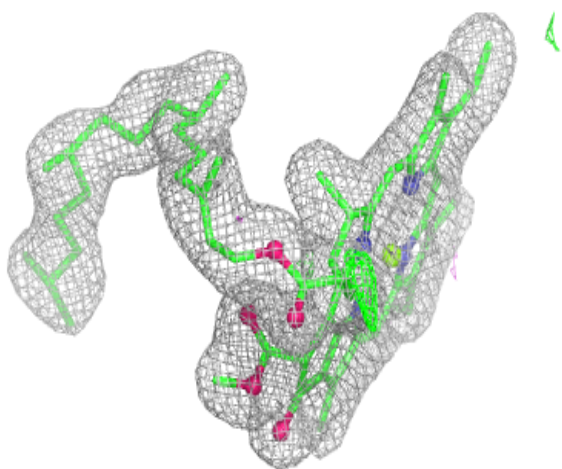
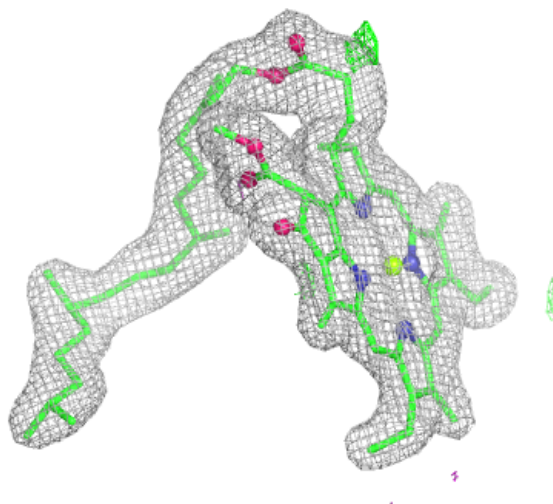
Electron density around CLA b 615:

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



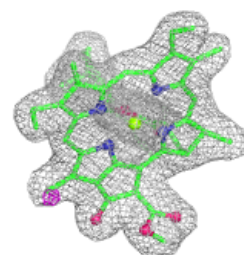
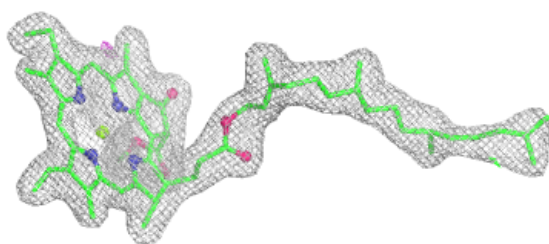
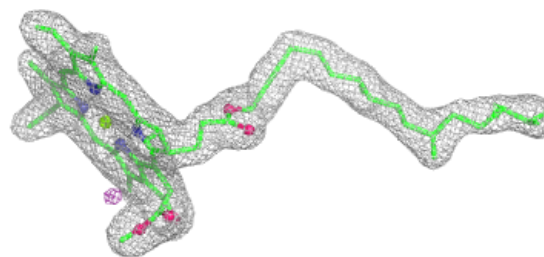
Electron density around CLA b 616:

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



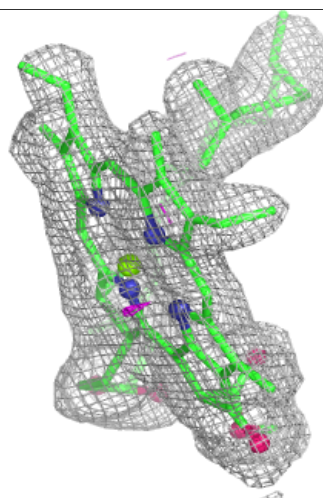
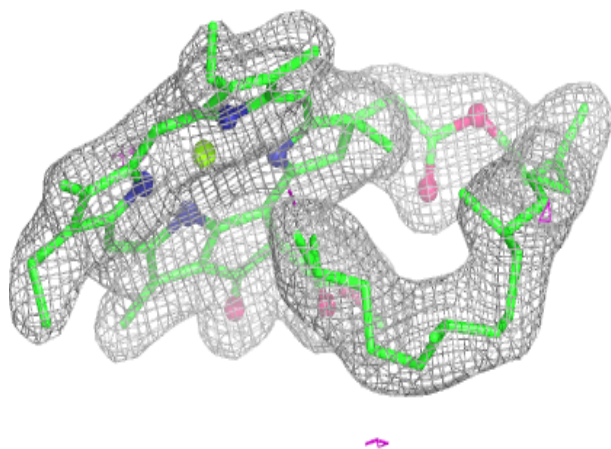
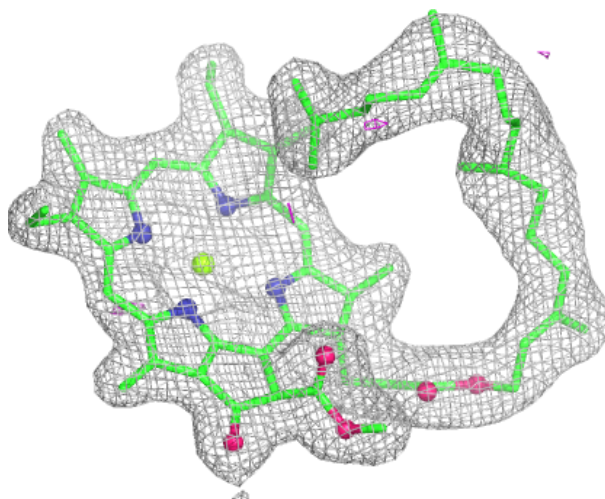
Electron density around CLA C 503:

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



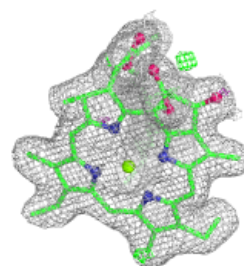
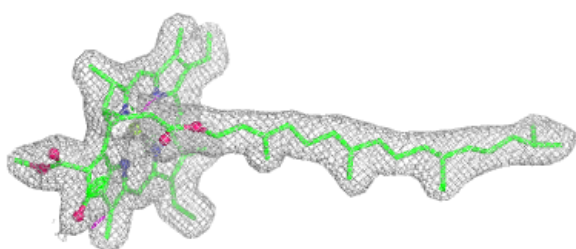
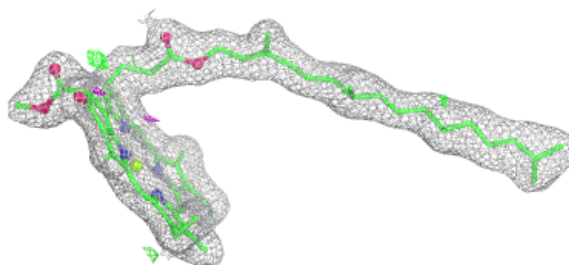
Electron density around CLA b 618:

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

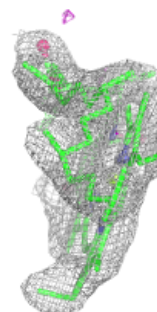
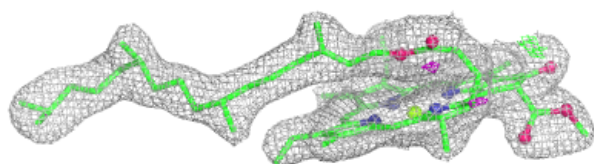
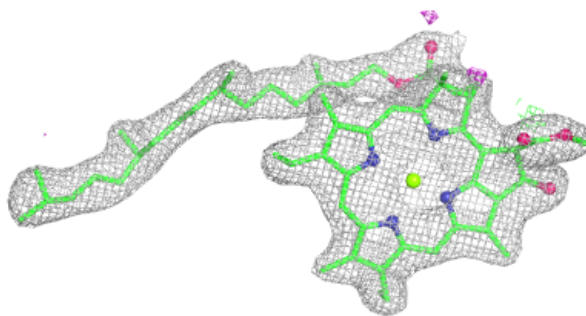


Electron density around CLA B 608:

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

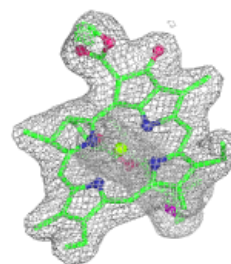
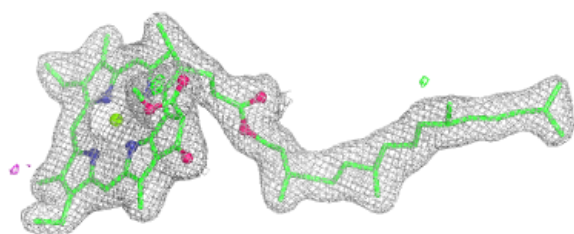
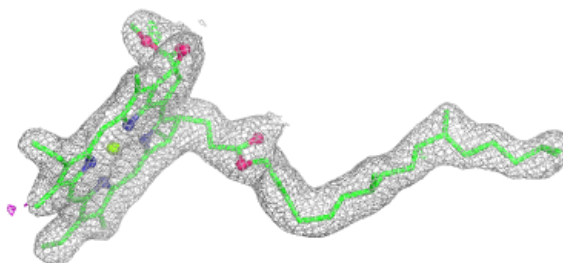
**Electron density around CLA c 503:**

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



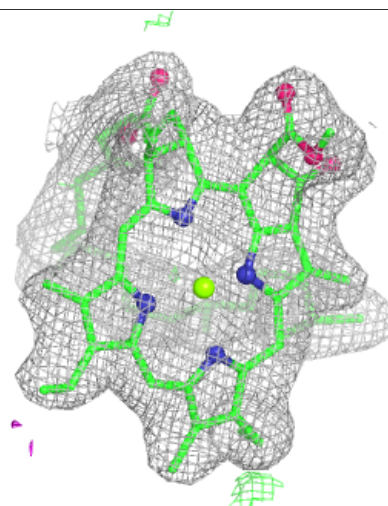
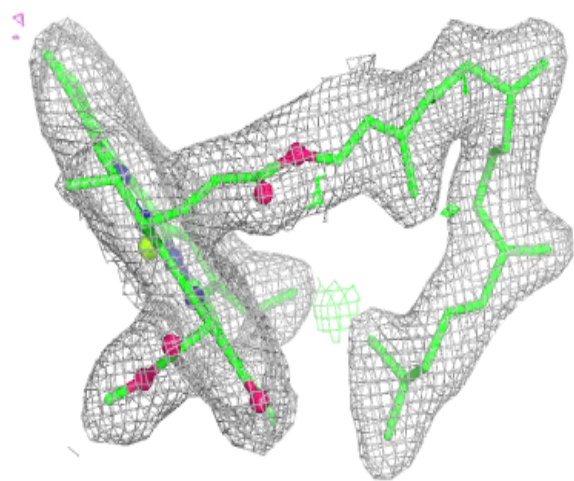
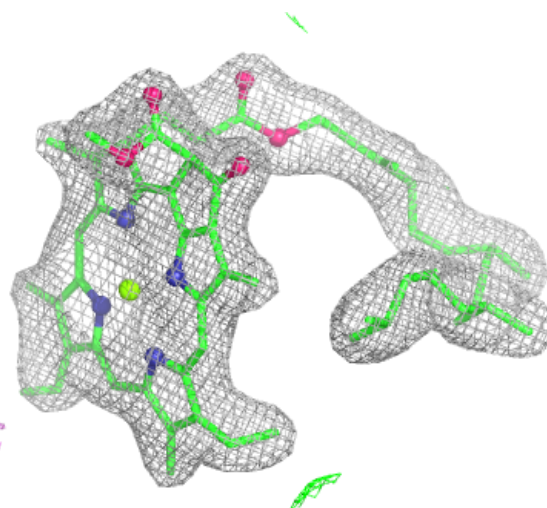
Electron density around CLA c 504:

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



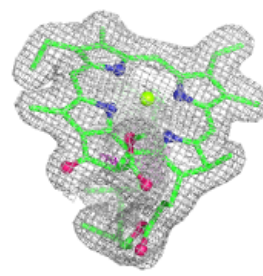
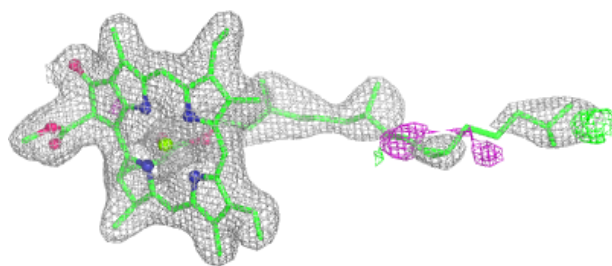
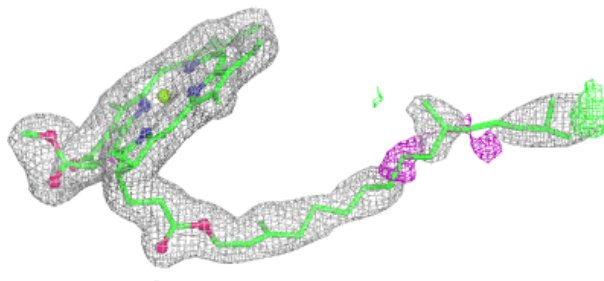
Electron density around CLA c 505:

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

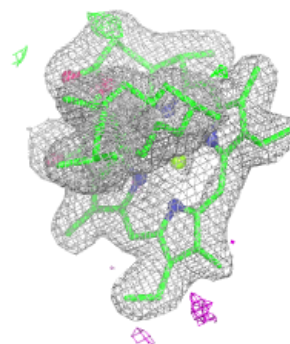
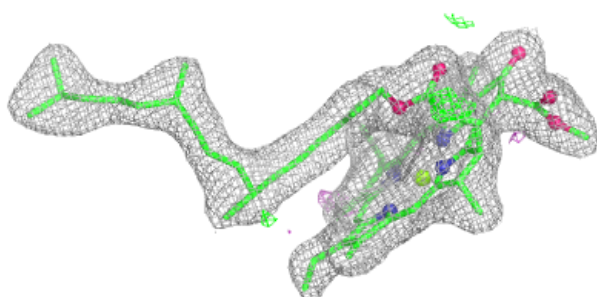
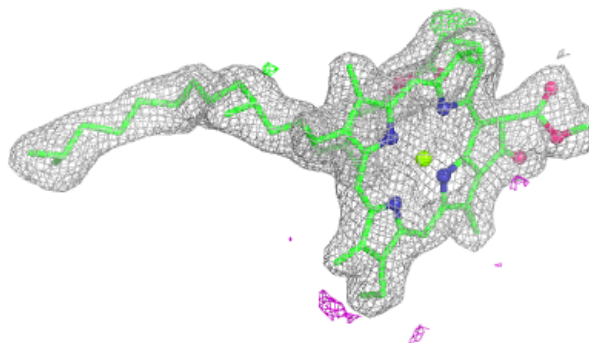


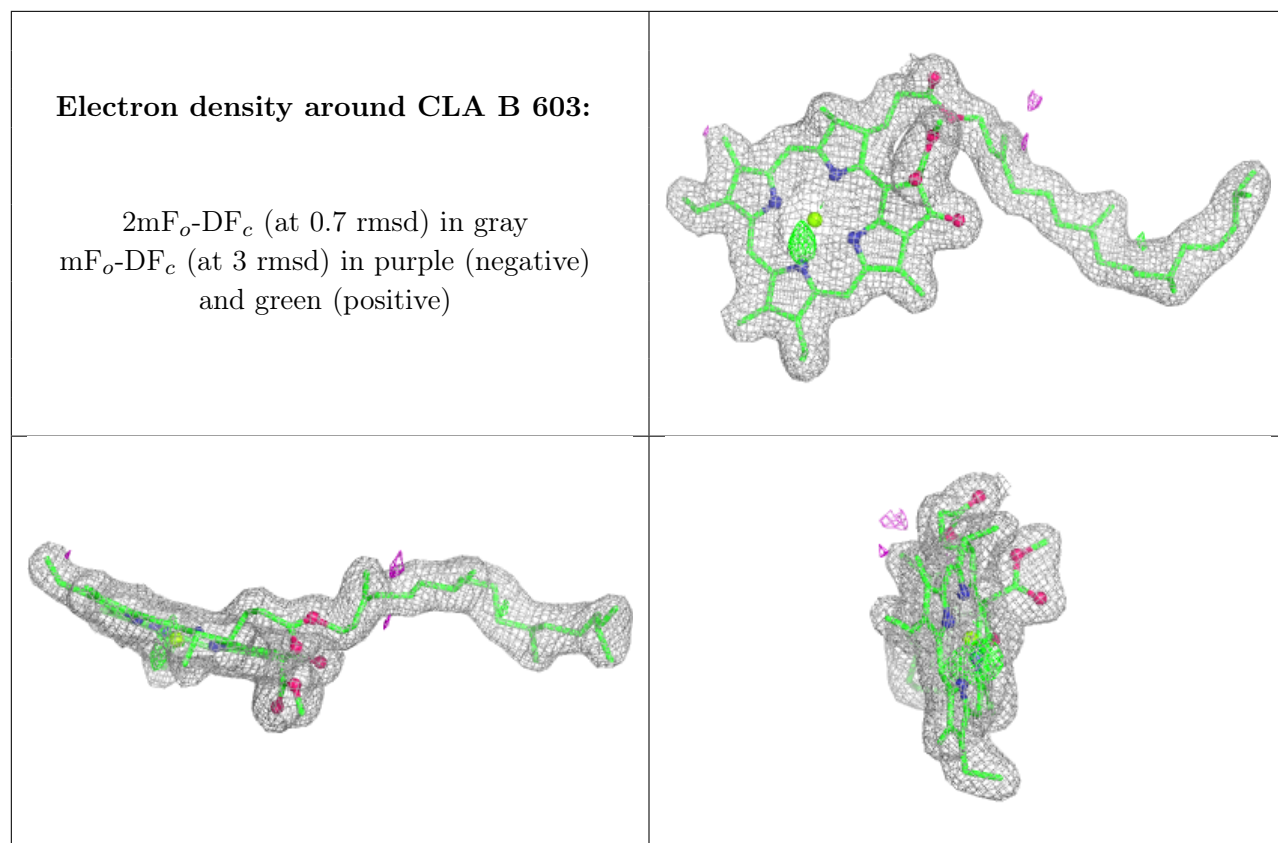
Electron density around CLA C 505:

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

**Electron density around CLA c 507:**

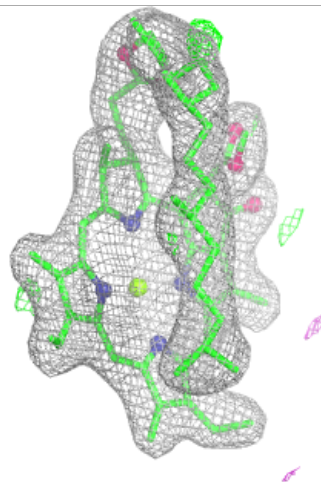
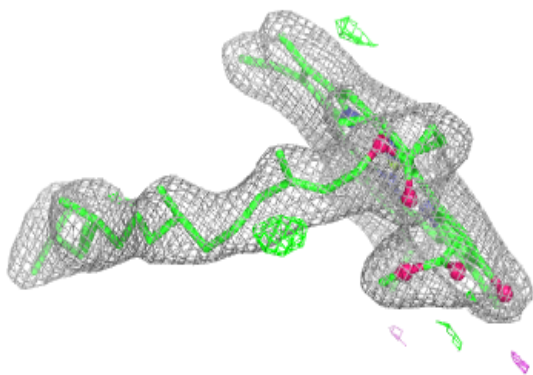
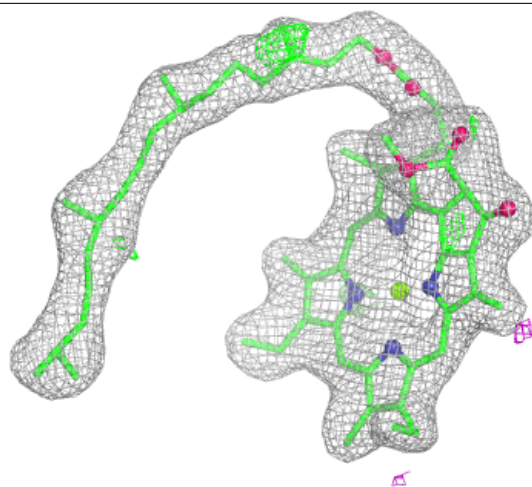
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





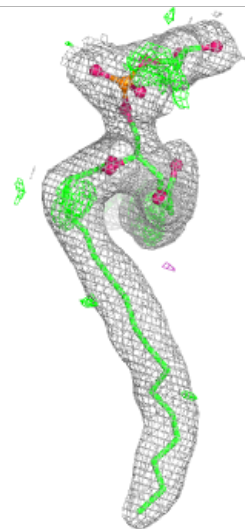
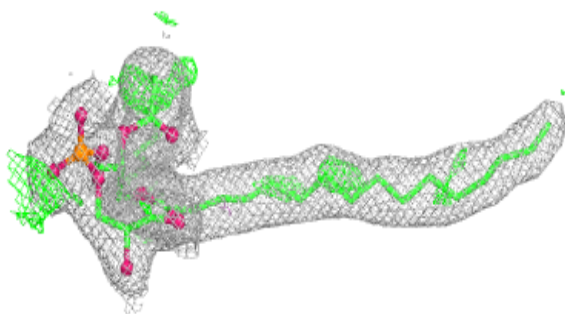
Electron density around CLA C 508:

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



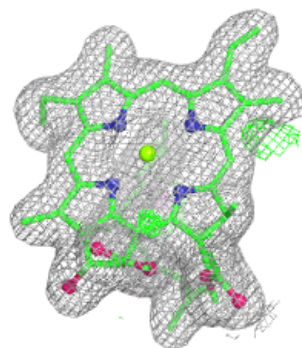
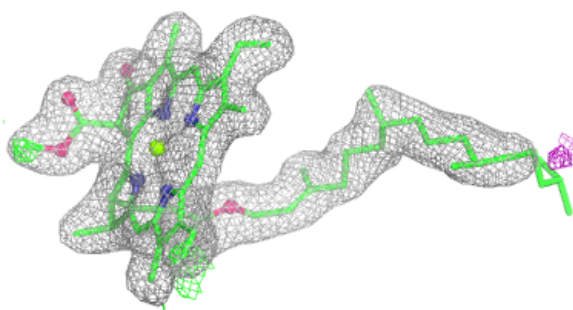
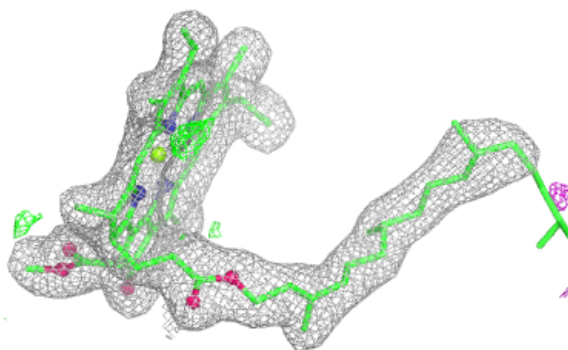
Electron density around LHG B 640:

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



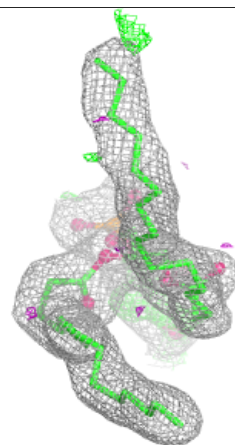
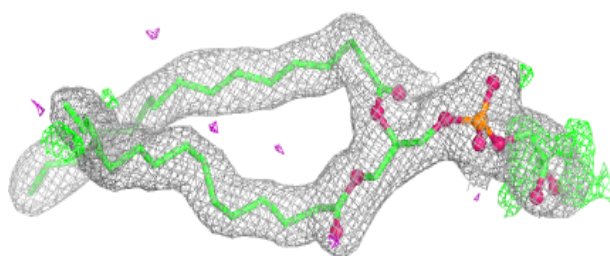
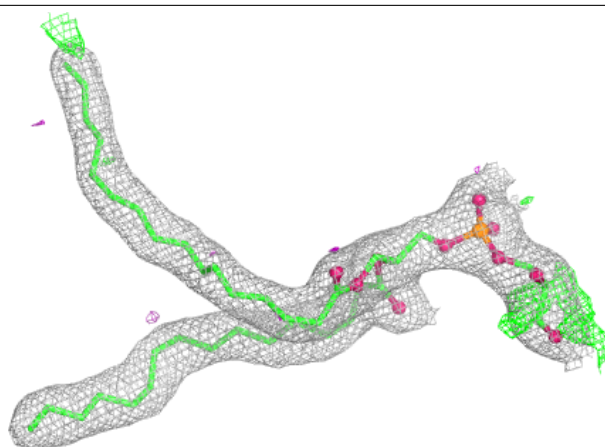
Electron density around CLA C 509:

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

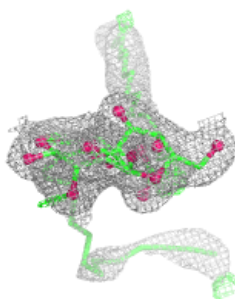
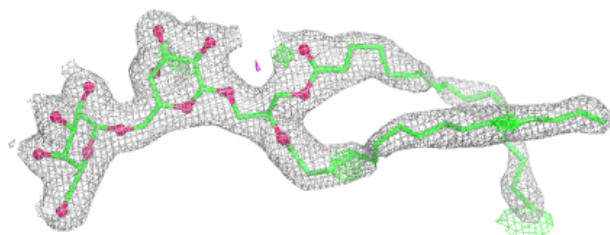
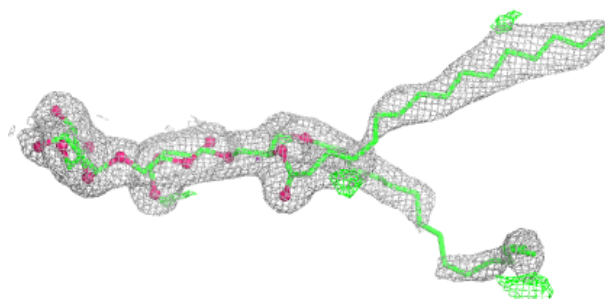


Electron density around LHG D 410:

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

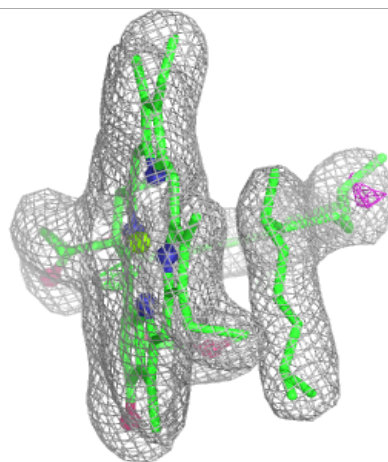
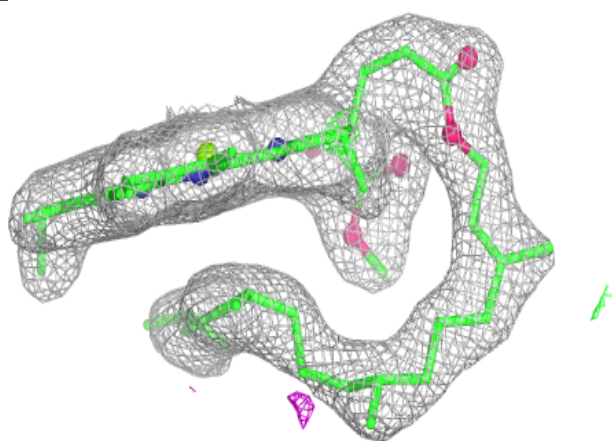
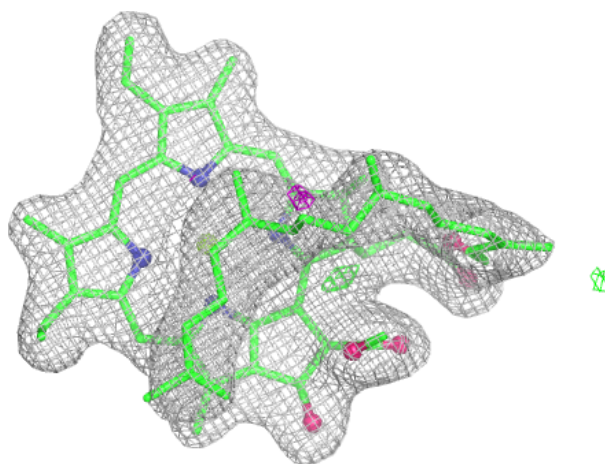
**Electron density around DGD C 517:**

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



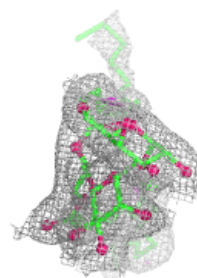
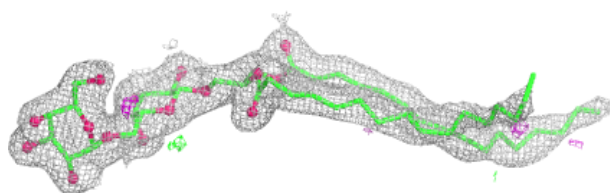
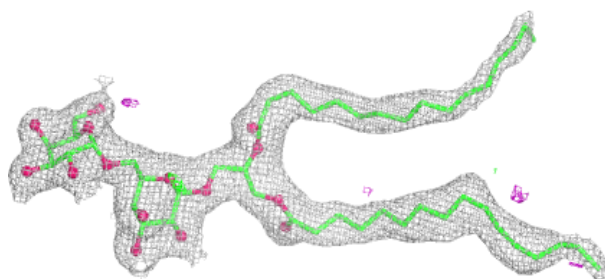
Electron density around CLA c 512:

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



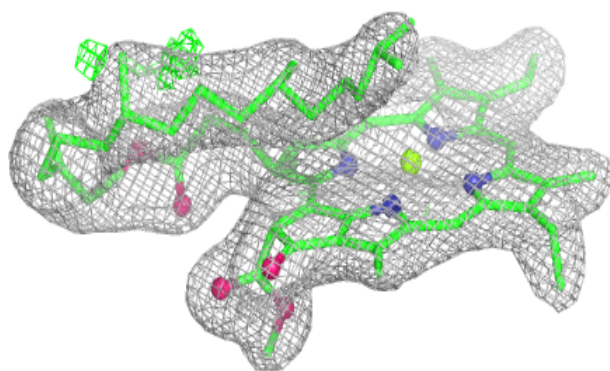
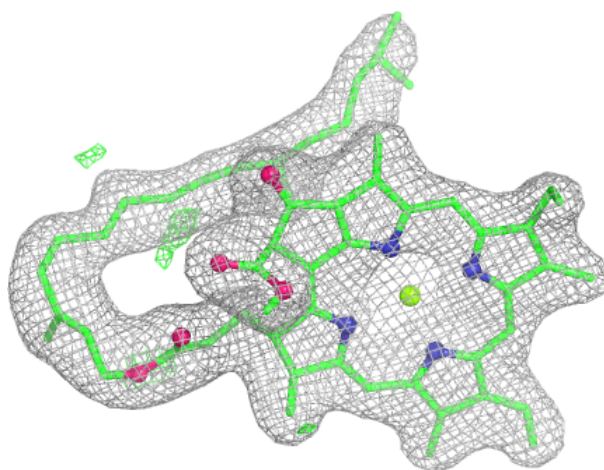
Electron density around DGD C 519:

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



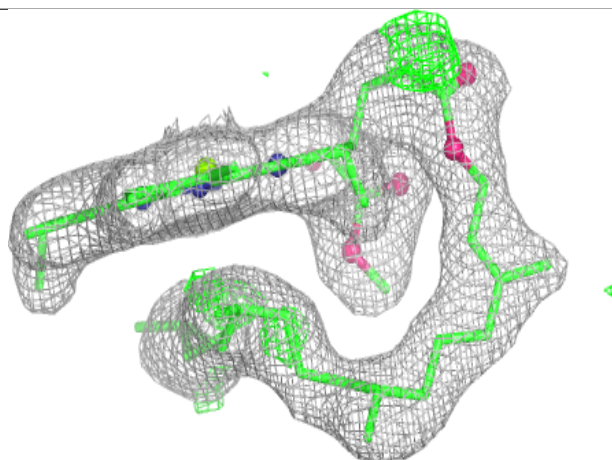
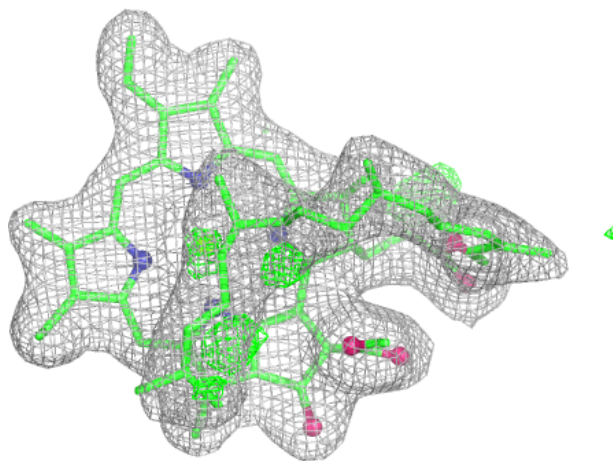
Electron density around CLA C 510:

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



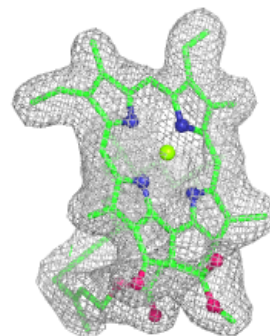
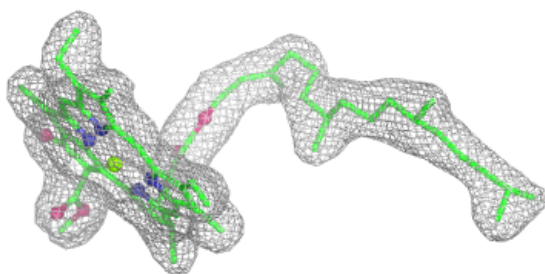
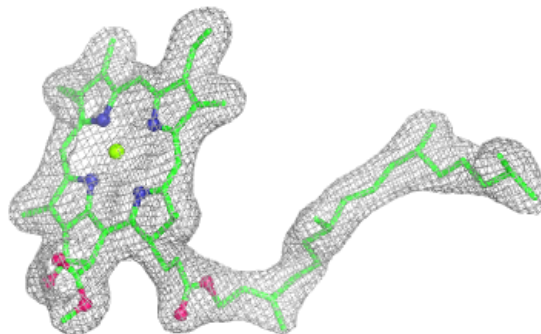
Electron density around CLA C 511:

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



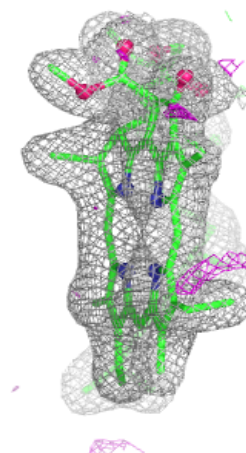
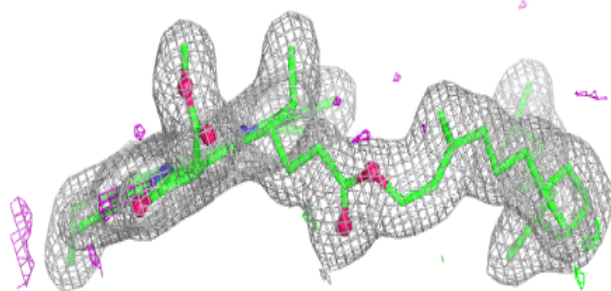
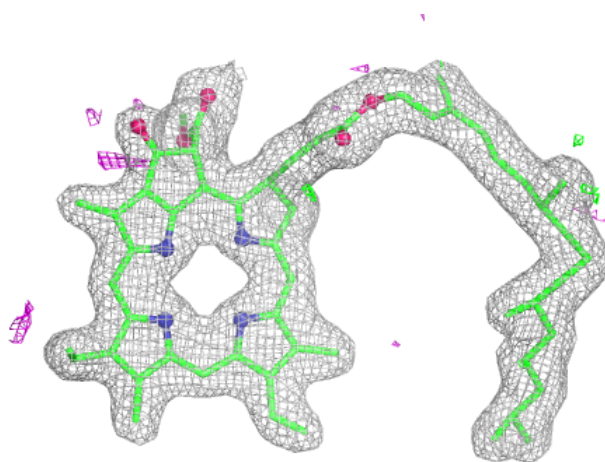
Electron density around CLA C 512:

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



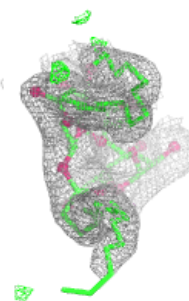
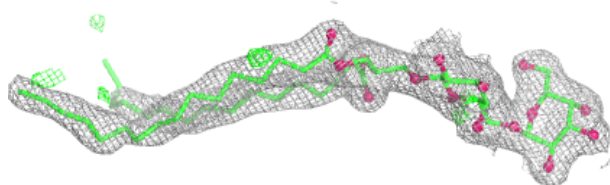
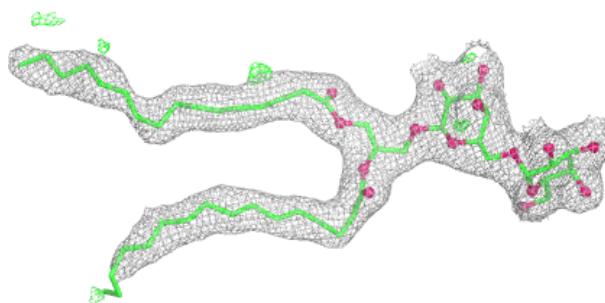
Electron density around PHO A 408:

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

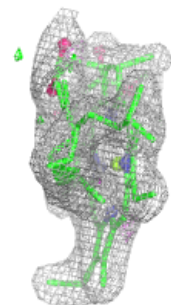
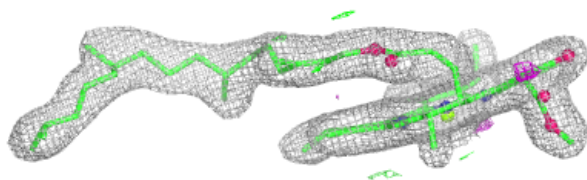
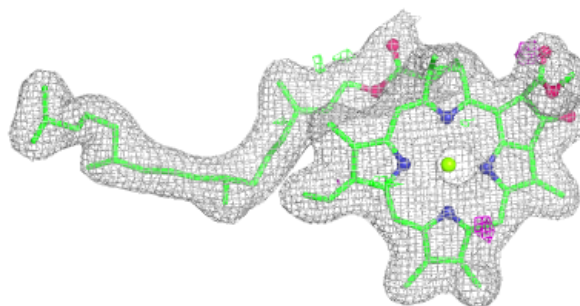


Electron density around DGD c 520:

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

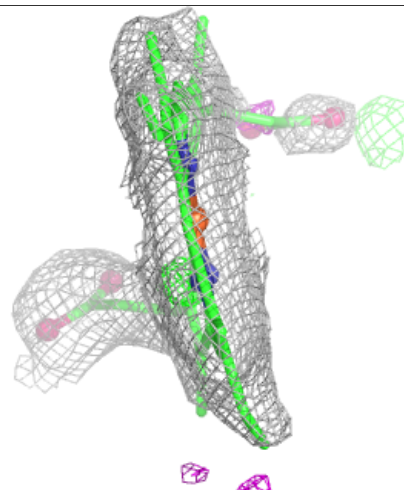
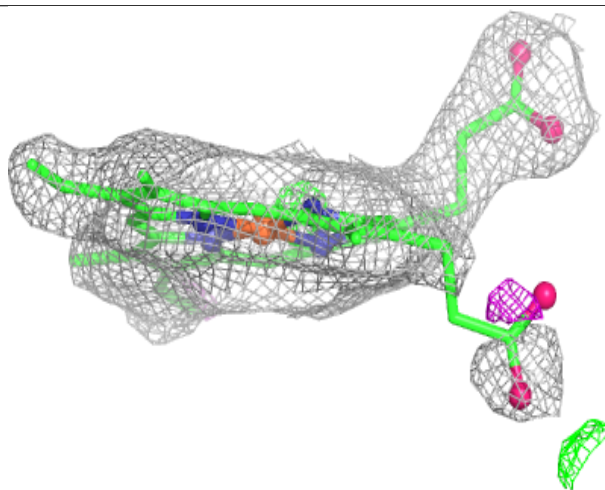
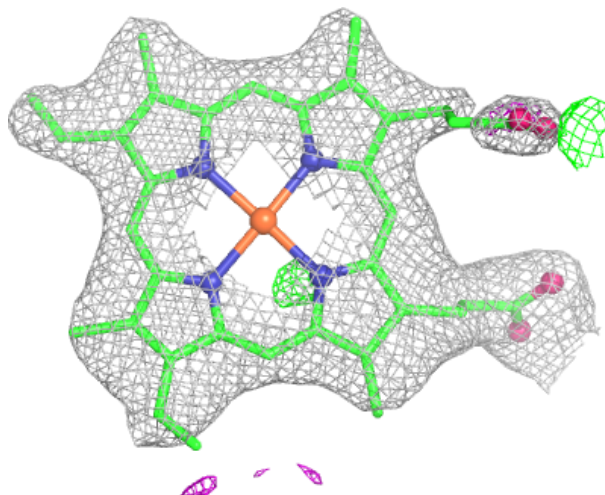
**Electron density around CLA B 604:**

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



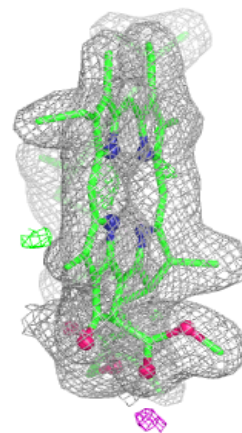
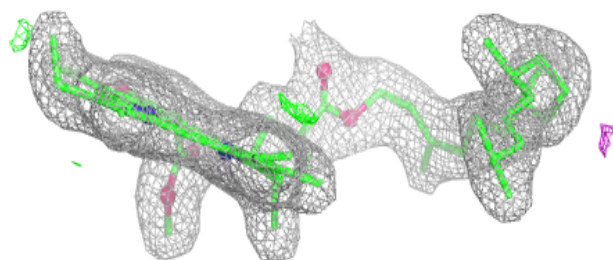
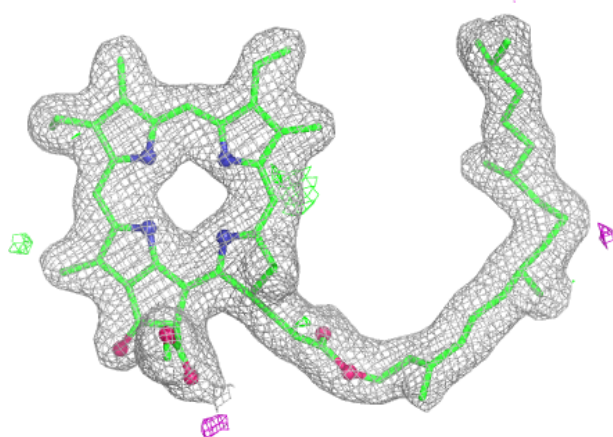
Electron density around HEM f 101:

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



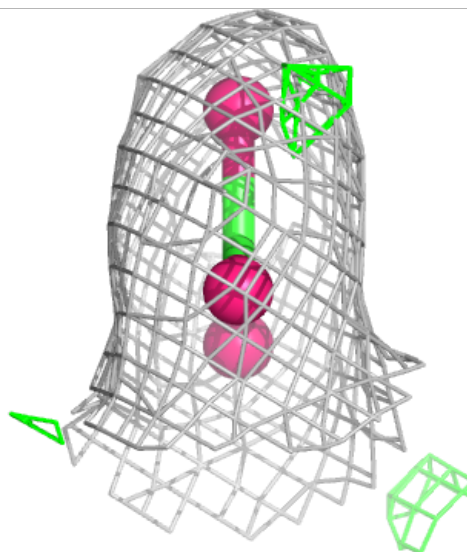
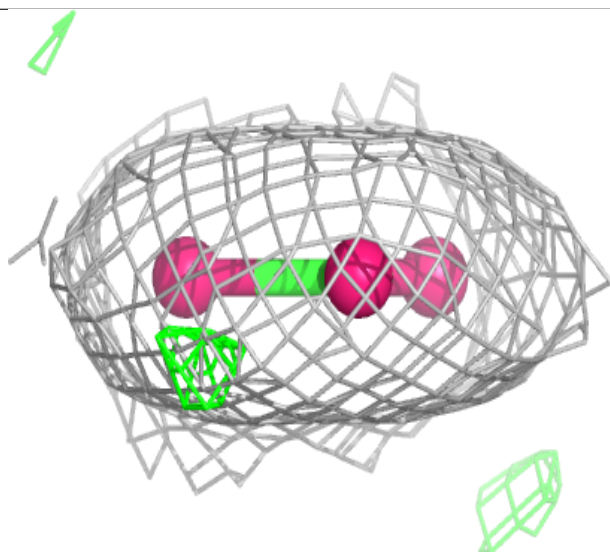
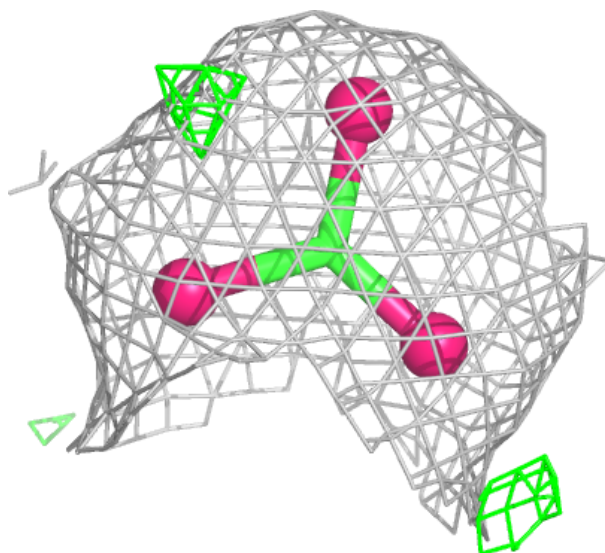
Electron density around PHO a 411:

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



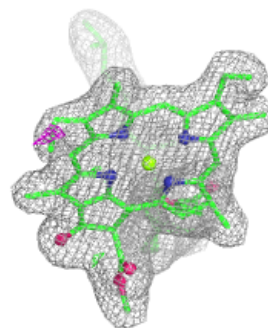
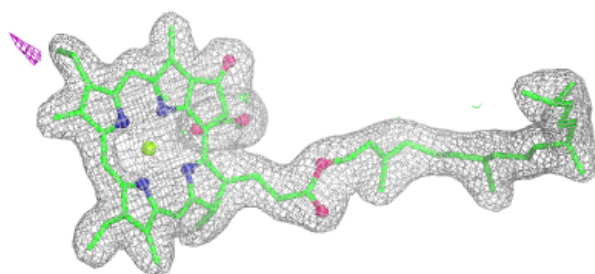
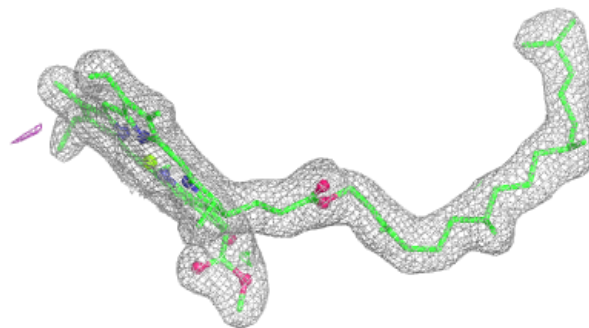
Electron density around BCT A 423:

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

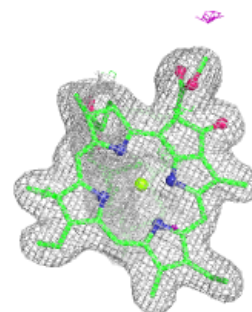
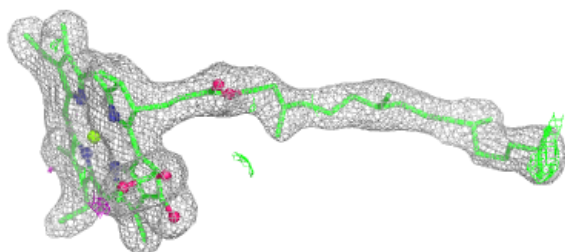
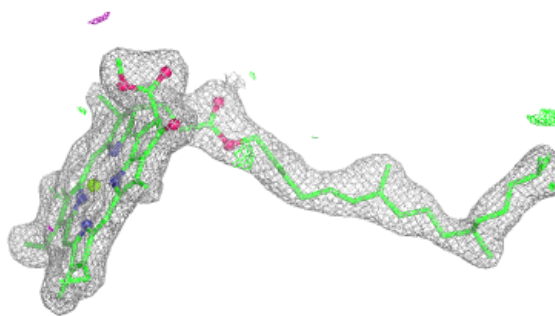


Electron density around CLA d 404:

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

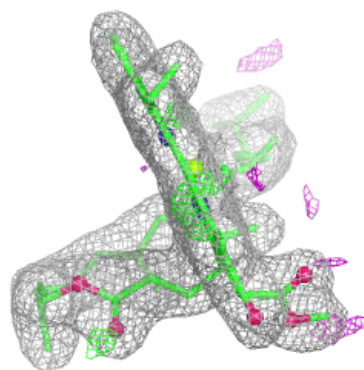
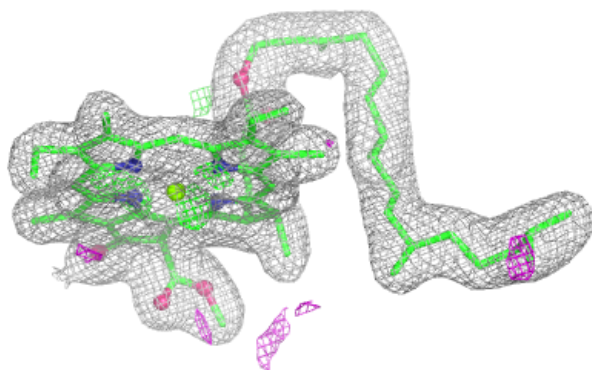
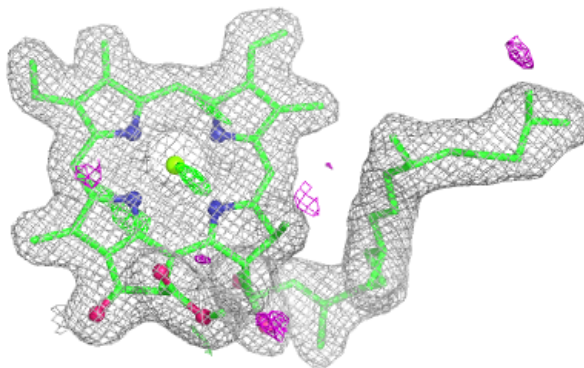
**Electron density around CLA B 605:**

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

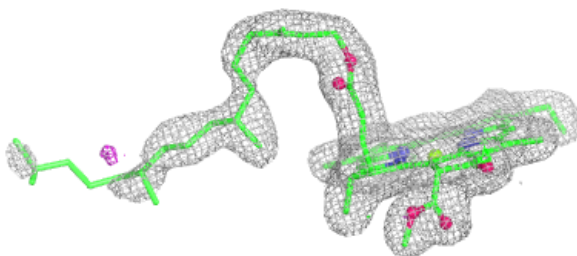
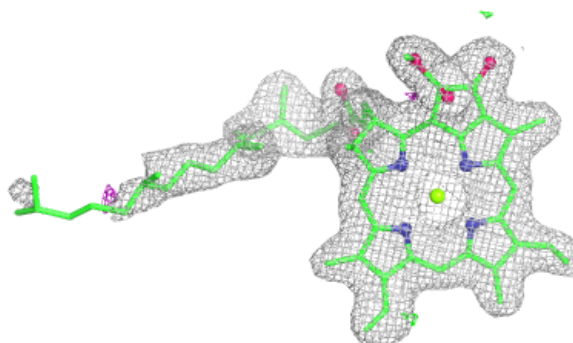


Electron density around CLA A 406:

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

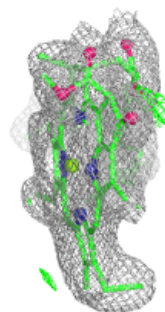
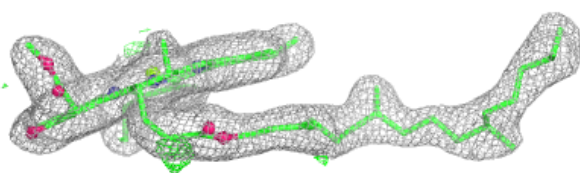
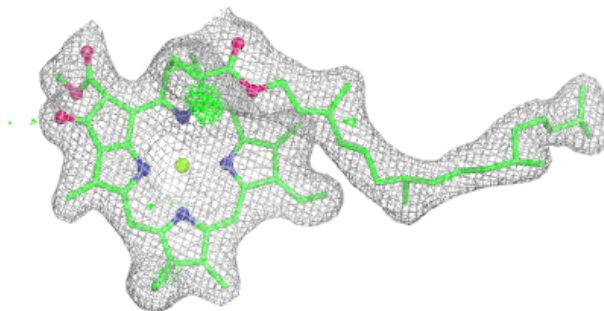
**Electron density around CLA A 407:**

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

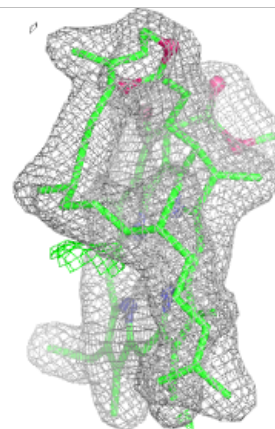
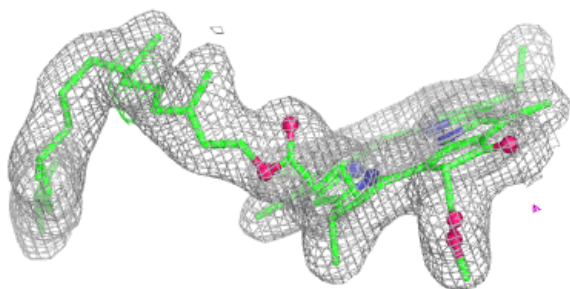
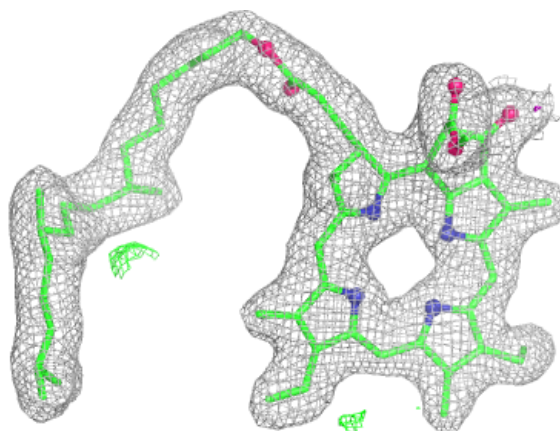


Electron density around CLA b 606:

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

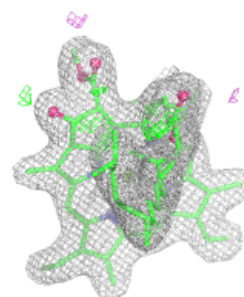
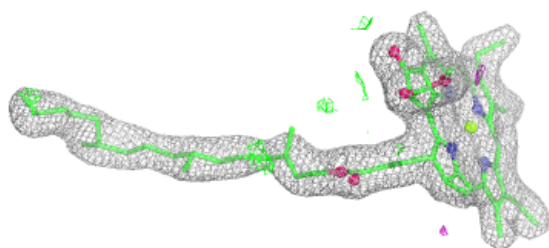
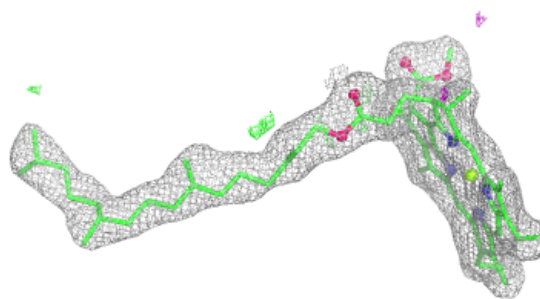
**Electron density around PHO d 401:**

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

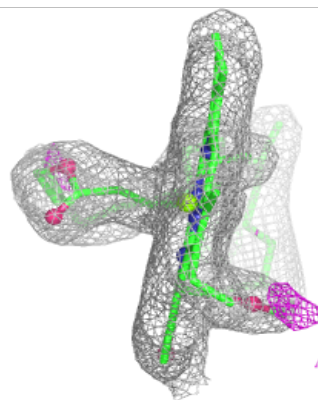
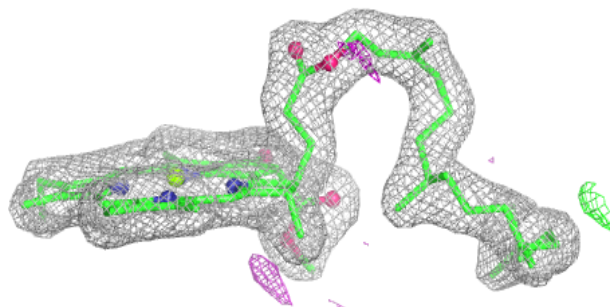
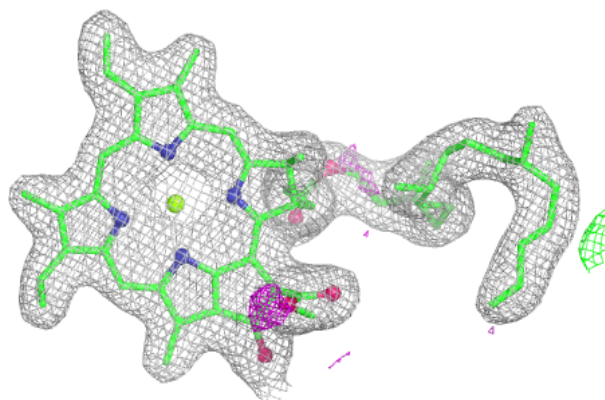


Electron density around CLA b 607:

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

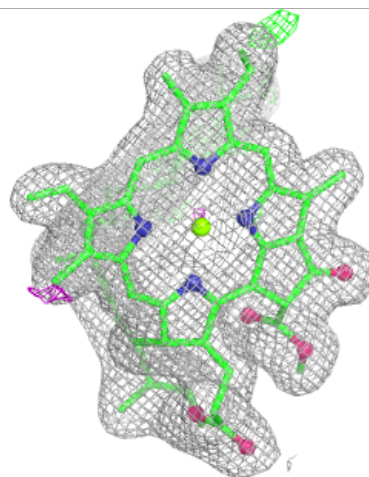
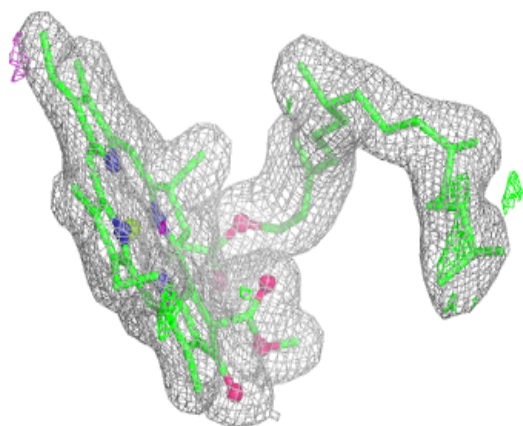
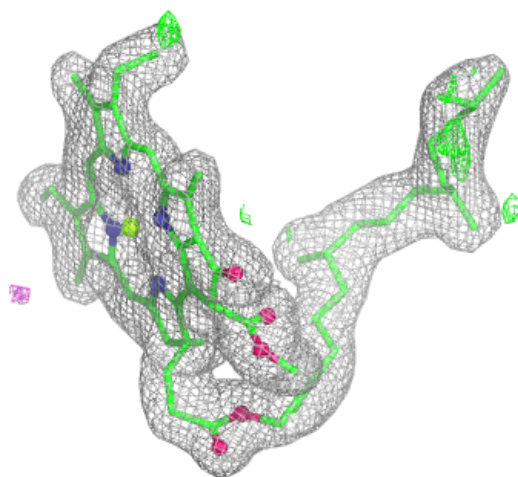
**Electron density around CLA B 613:**

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



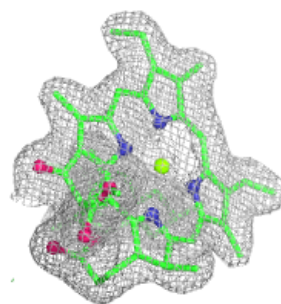
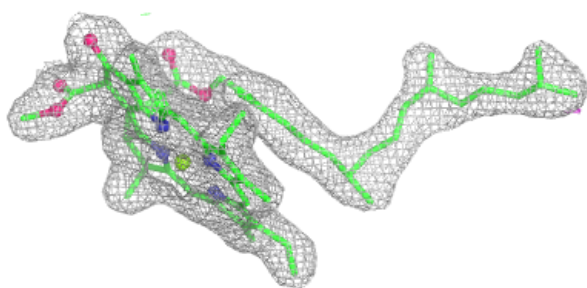
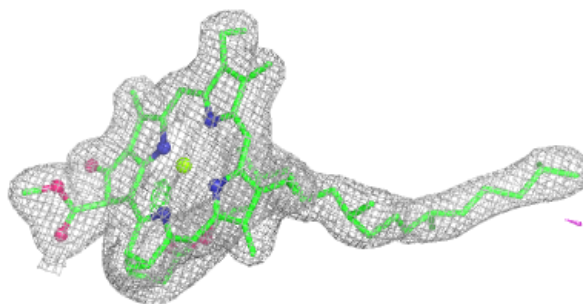
Electron density around CLA B 614:

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

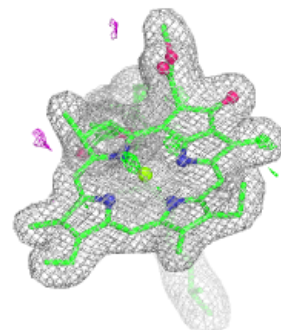
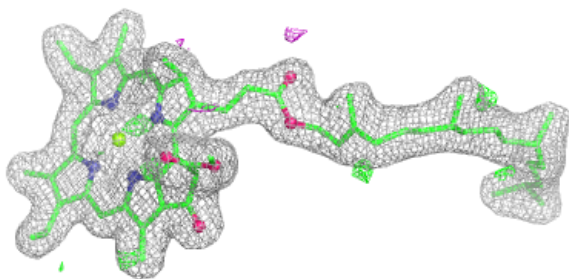
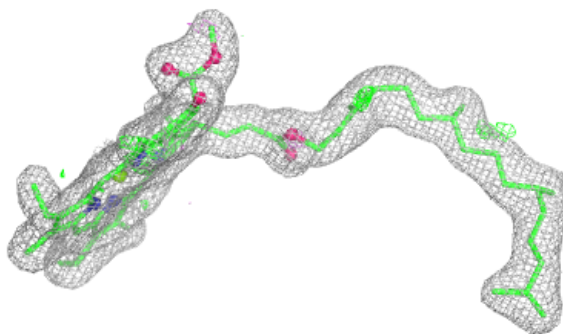


Electron density around CLA C 506:

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

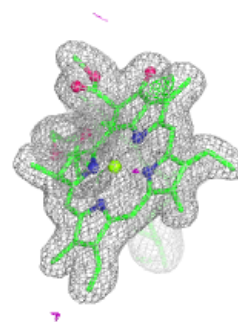
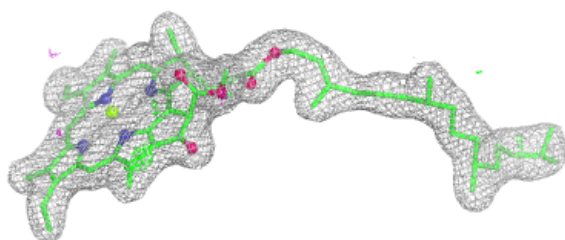
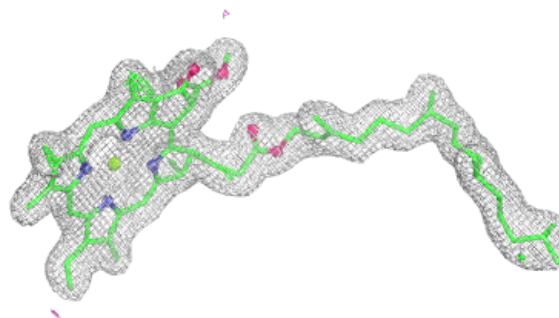
**Electron density around CLA D 403:**

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

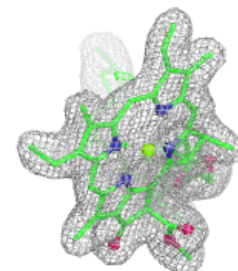
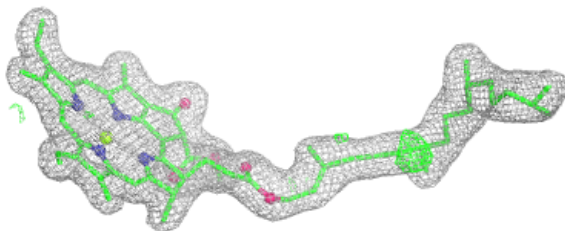
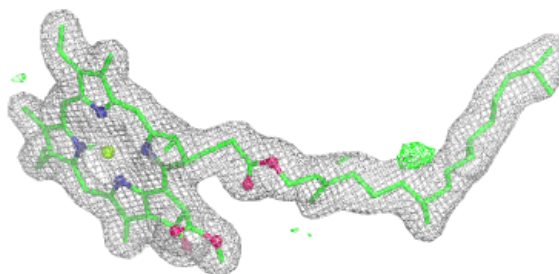


Electron density around CLA A 405:

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

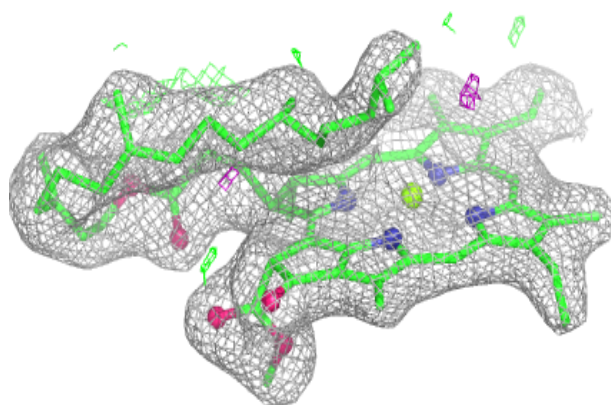
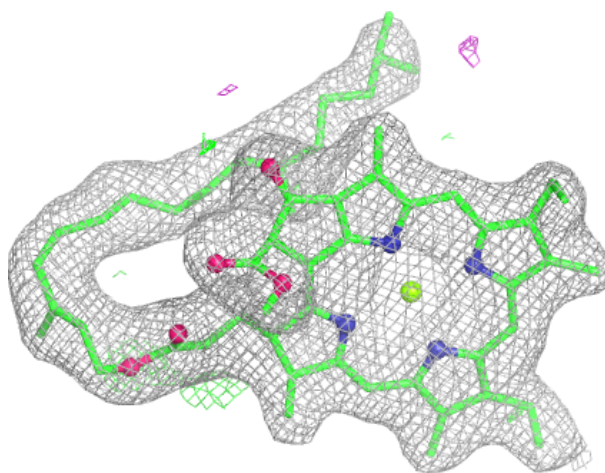
**Electron density around CLA a 408:**

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



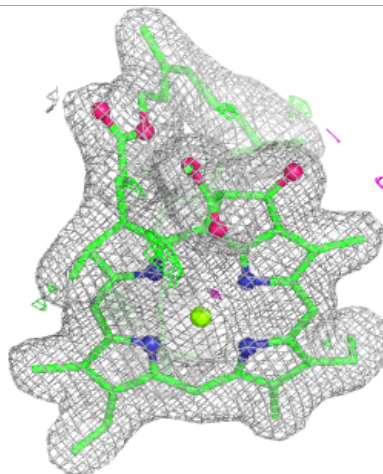
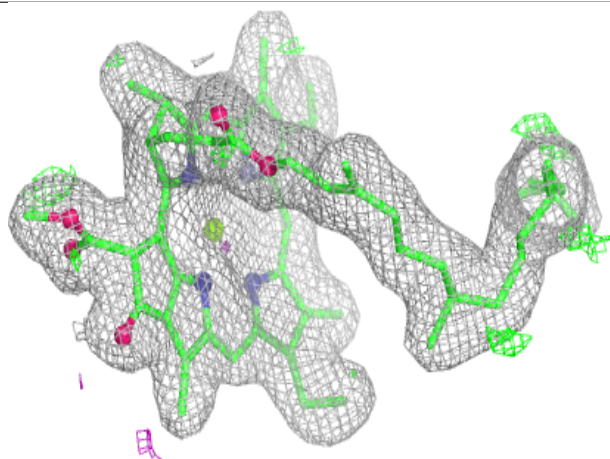
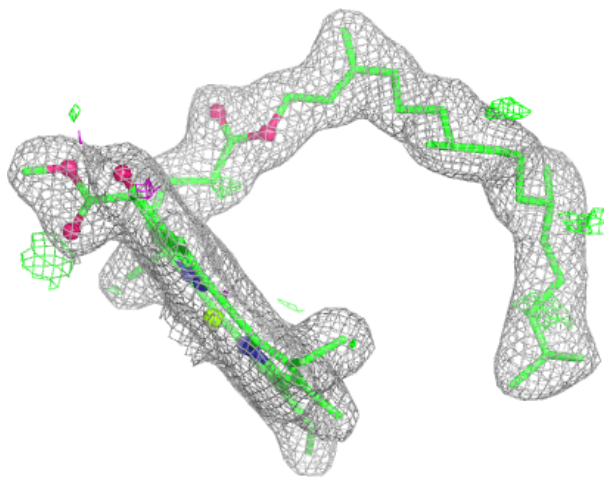
Electron density around CLA c 511:

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



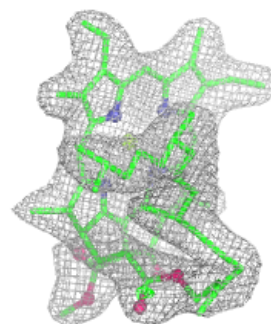
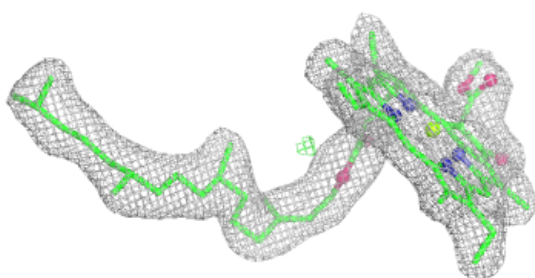
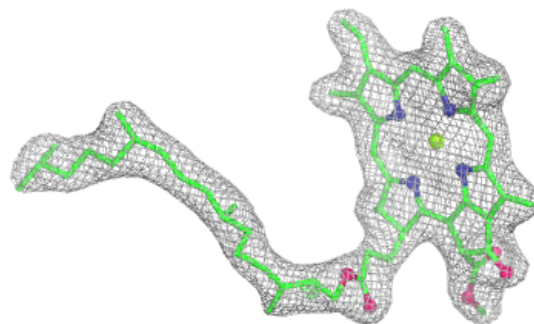
Electron density around CLA b 614:

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

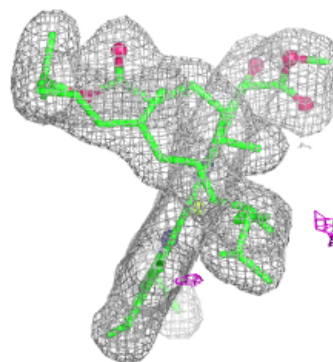
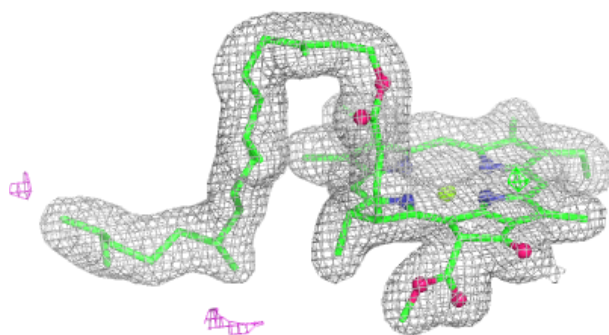
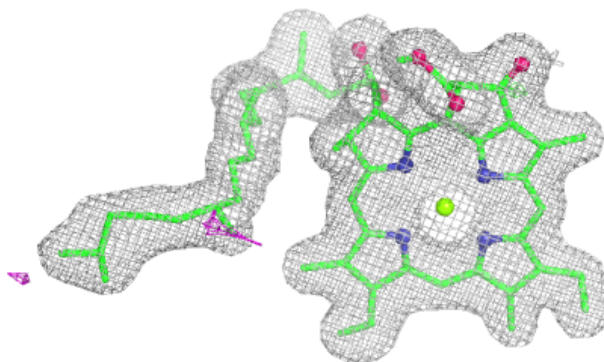


Electron density around CLA c 513:

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

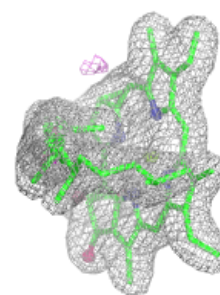
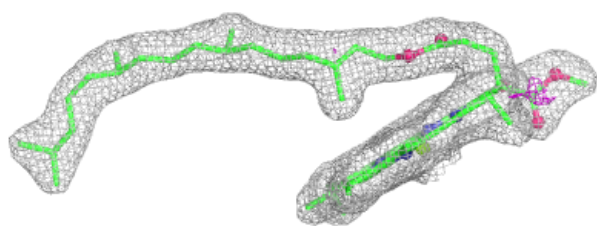
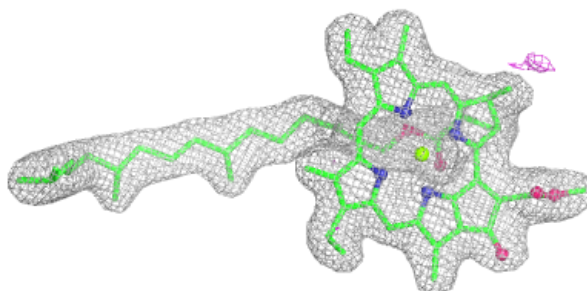
**Electron density around CLA a 409:**

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



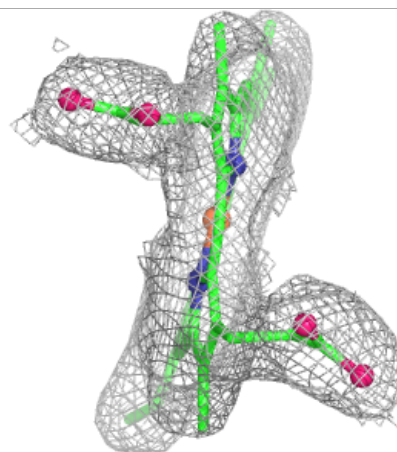
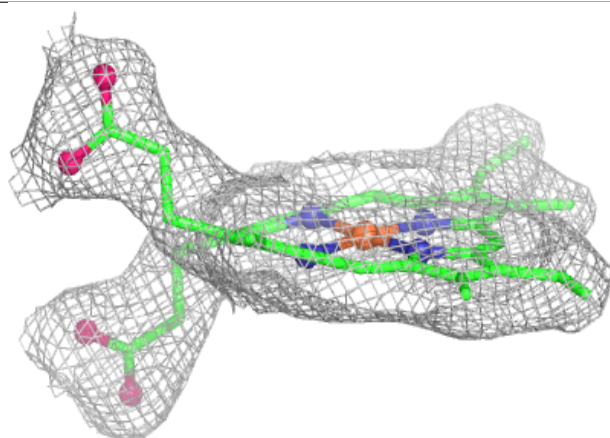
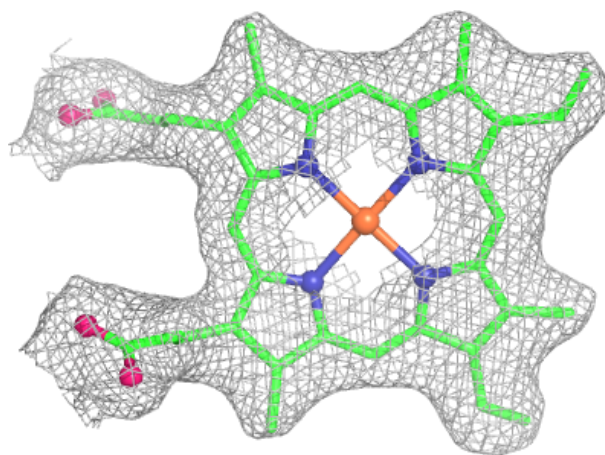
Electron density around CLA B 609:

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



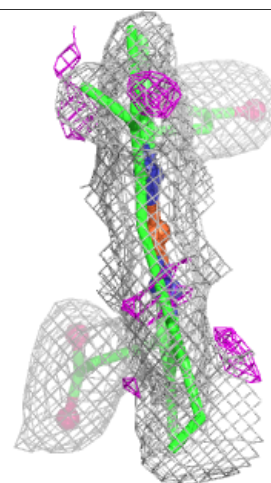
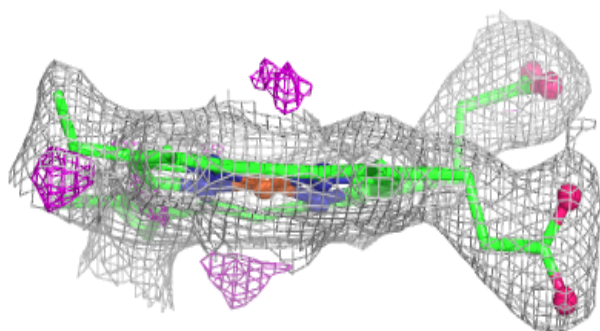
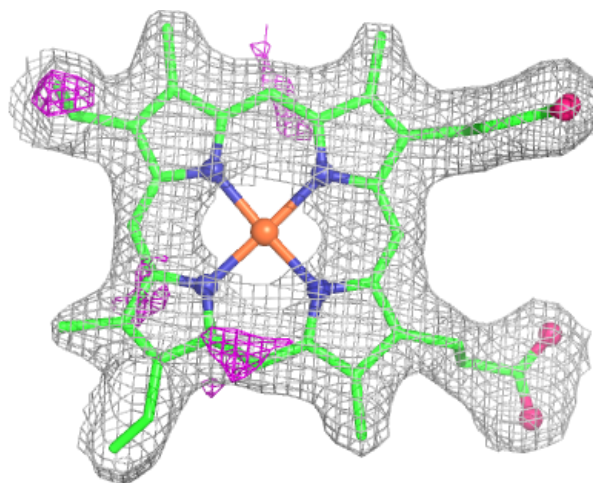
Electron density around HEM F 101:

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



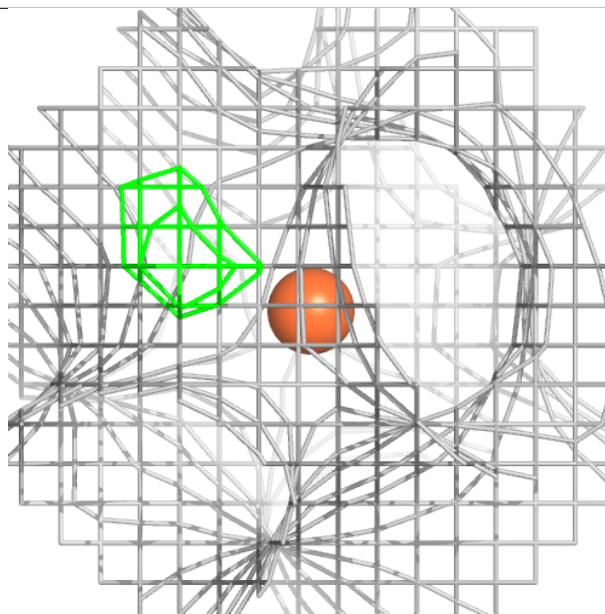
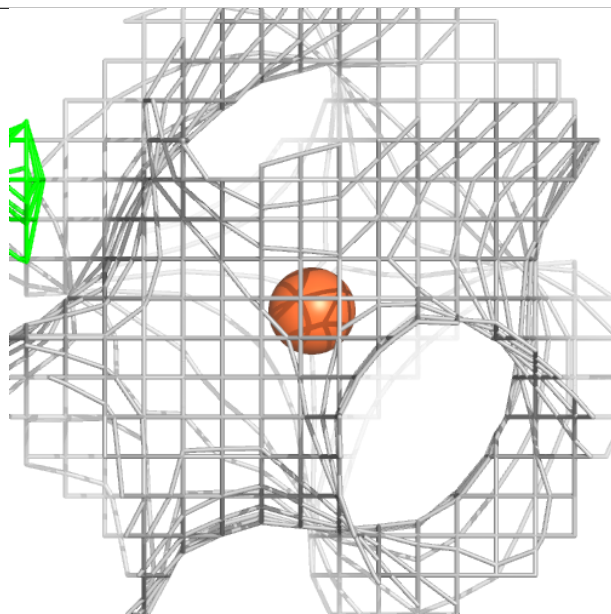
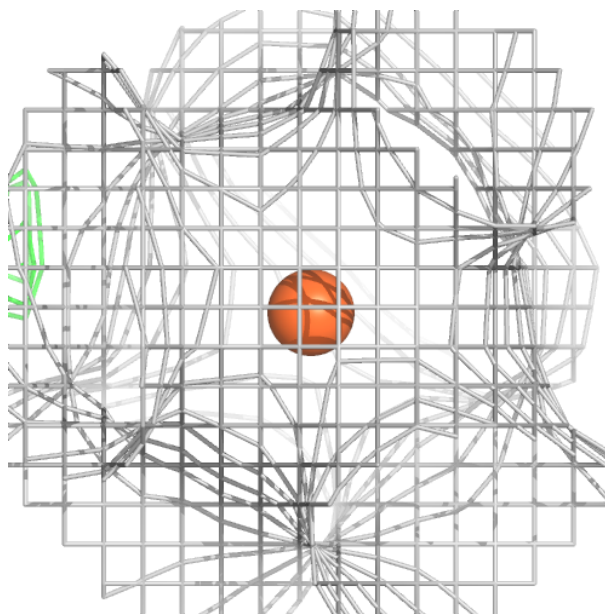
Electron density around HEC v 1603:

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



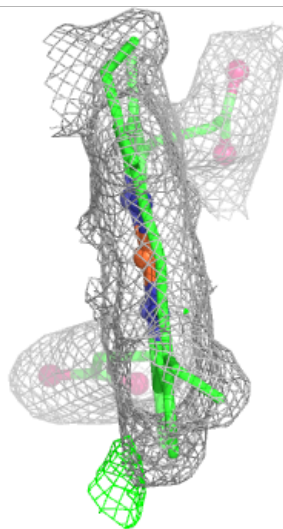
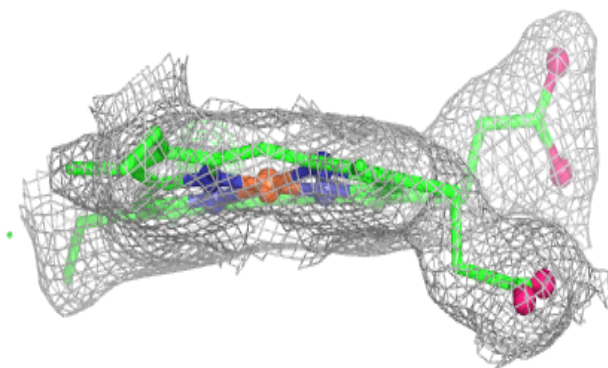
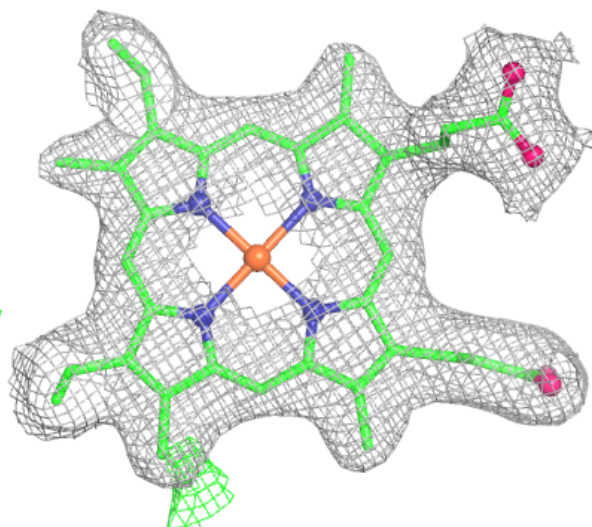
Electron density around FE2 A 402:

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



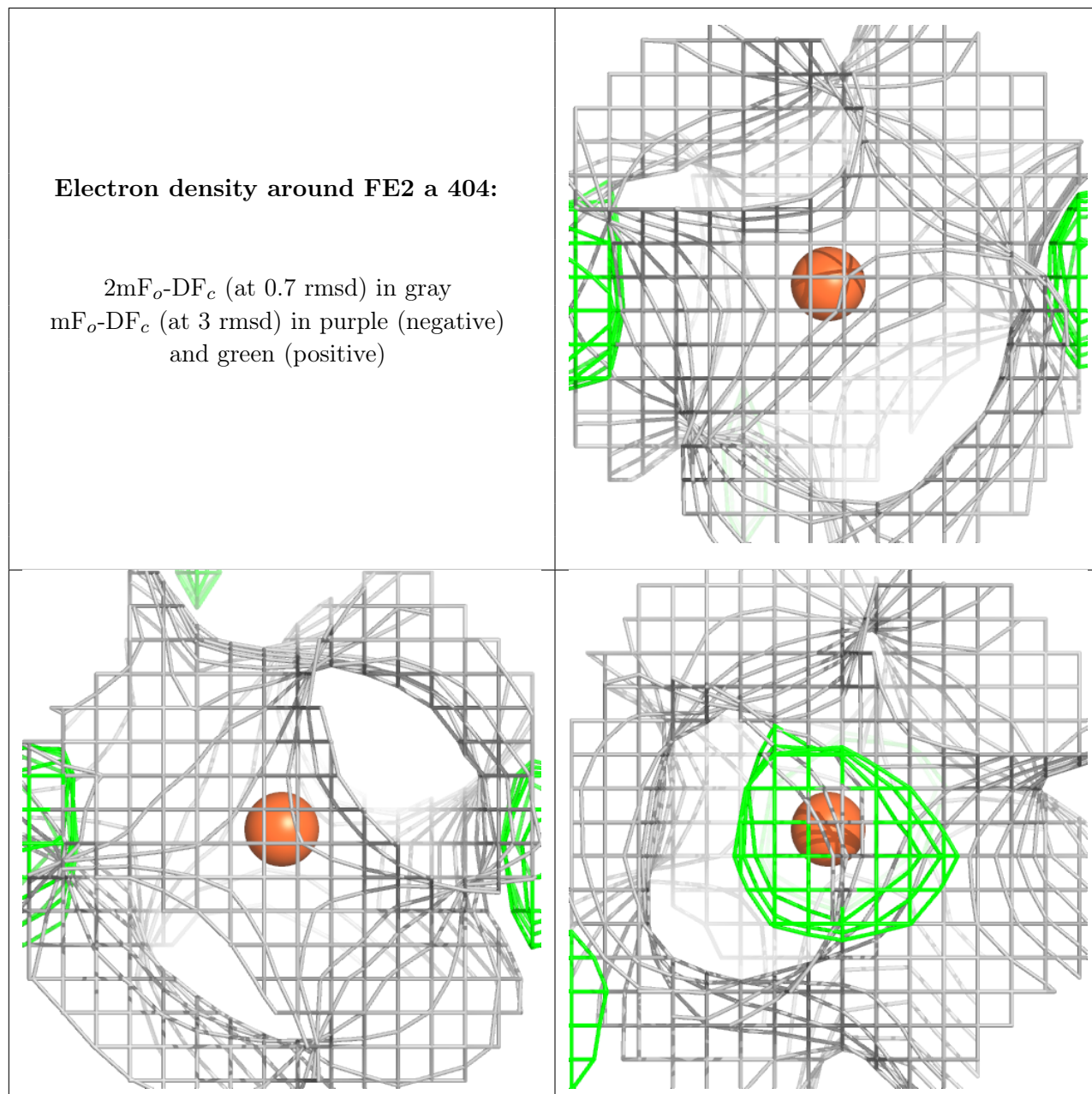
Electron density around HEC V 202:

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



Electron density around FE2 a 404:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.