



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 15, 2026 – 02:50 PM UTC

PDB ID : 5H2F / pdb_00005h2f
Title : Crystal structure of the PsbM-deletion mutant of photosystem II
Authors : Uto, S.; Kawakami, K.; Umena, Y.; Iwai, M.; Ikeuchi, M.; Shen, J.R.; Kamiya, N.
Deposited on : 2016-10-15
Resolution : 2.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

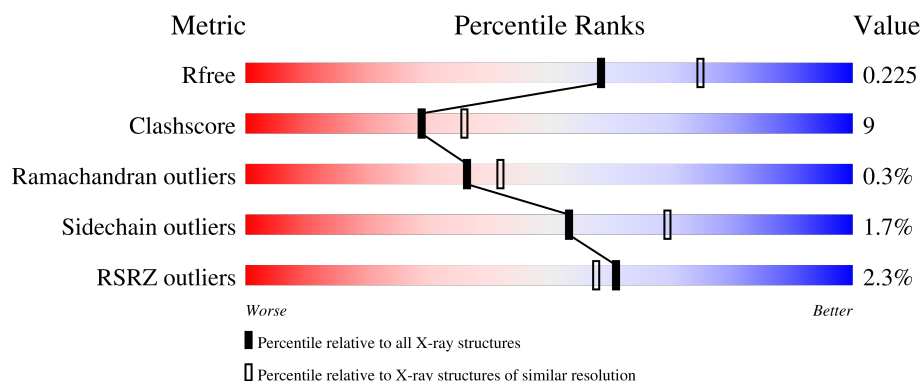
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

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



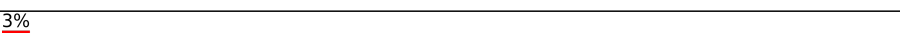
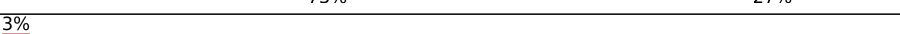
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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

Mol	Chain	Length	Quality of chain
1	A	334	2% 87% 13% .
1	a	334	10% 84% 16%
2	B	505	3% 86% 14%
2	b	505	% 82% 14% .
3	C	455	% 85% 15% .

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Mol	Chain	Length	Quality of chain
3	c	455	
4	D	342	
4	d	342	
5	E	80	
5	e	80	
6	F	33	
6	f	33	
7	H	63	
7	h	63	
8	I	36	
8	i	36	
9	J	40	
9	j	40	
10	K	37	
10	k	37	
11	L	35	
11	l	35	
12	O	243	
12	o	243	
13	T	30	
13	t	30	
14	U	97	
14	u	97	
15	V	137	
15	v	137	

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Mol	Chain	Length	Quality of chain
16	Y	29	
16	y	29	
17	X	37	
17	x	37	
18	Z	62	
18	z	62	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	A	405	X	-	-	-
22	CLA	A	408	X	-	-	-
22	CLA	B	602	X	-	-	-
22	CLA	B	603	X	-	-	-
22	CLA	B	604	X	-	-	-
22	CLA	B	605	X	-	-	-
22	CLA	B	607	X	-	-	-
22	CLA	B	608	X	-	-	-
22	CLA	B	610	X	-	-	-
22	CLA	B	611	X	-	-	-
22	CLA	B	612	X	-	-	-
22	CLA	B	613	X	-	-	-
22	CLA	B	614	X	-	-	-
22	CLA	B	615	X	-	-	-
22	CLA	B	616	X	-	-	-
22	CLA	B	617	X	-	-	-
22	CLA	C	502	X	-	-	-
22	CLA	C	503	X	-	-	-
22	CLA	C	506	X	-	-	-
22	CLA	C	507	X	-	-	-
22	CLA	C	508	X	-	-	-
22	CLA	C	509	X	-	-	-
22	CLA	C	510	X	-	-	-
22	CLA	C	511	X	-	-	-
22	CLA	C	513	X	-	-	-
22	CLA	D	403	X	-	-	-
22	CLA	D	404	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	a	407	X	-	-	-
22	CLA	a	408	X	-	-	-
22	CLA	b	602	X	-	-	-
22	CLA	b	603	X	-	-	-
22	CLA	b	604	X	-	-	-
22	CLA	b	605	X	-	-	-
22	CLA	b	606	X	-	-	-
22	CLA	b	607	X	-	-	-
22	CLA	b	608	X	-	-	-
22	CLA	b	611	X	-	-	-
22	CLA	b	613	X	-	-	-
22	CLA	b	614	X	-	-	-
22	CLA	b	615	X	-	-	-
22	CLA	b	616	X	-	-	-
22	CLA	b	617	X	-	-	-
22	CLA	c	902	X	-	-	-
22	CLA	c	903	X	-	-	-
22	CLA	c	906	X	-	-	-
22	CLA	c	907	X	-	-	-
22	CLA	c	908	X	-	-	-
22	CLA	c	910	X	-	-	-
22	CLA	c	911	X	-	-	-
22	CLA	c	913	X	-	-	-
22	CLA	d	402	X	-	-	-
31	DMS	B	631	-	-	X	-
31	DMS	B	638	-	-	X	-
31	DMS	O	303	-	-	X	-
31	DMS	O	304	-	-	X	-
31	DMS	O	312	-	-	X	-
31	DMS	V	212	-	-	X	-
31	DMS	a	425	-	-	X	-
31	DMS	b	638	-	-	X	-
31	DMS	c	924	-	-	X	-
31	DMS	d	415	-	-	X	-
31	DMS	f	103	-	-	X	-
31	DMS	o	304	-	-	X	-
31	DMS	o	308	-	-	X	-
31	DMS	u	205	-	-	X	-
34	HTG	D	415	-	-	X	-

2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 51892 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 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	1	0
			2598	1706	428	449	15			
1	a	334	Total	C	N	O	S	0	1	0
			2555	1675	427	438	15			

- 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	3	0
			3950	2596	661	680	13			
2	b	483	Total	C	N	O	S	0	1	0
			3780	2484	631	652	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	0	0
			3470	2274	580	603	13			
3	c	455	Total	C	N	O	S	0	1	0
			3521	2305	589	614	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	342	Total	C	N	O	S	0	3	0
			2732	1814	442	464	12			
4	d	341	Total	C	N	O	S	0	2	0
			2717	1805	441	459	12			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	79	Total	C	N	O	0	0	0
			635	417	101	117			
5	e	79	Total	C	N	O	0	0	0
			636	418	101	117			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	33	Total	C	N	O	S	0	0	0
			269	184	44	40	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	3	0
			522	347	87	86	2			
7	h	62	Total	C	N	O	S	0	1	0
			501	335	82	82	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	35	Total	C	N	O	S	0	0	0
			288	196	45	46	1			
8	i	36	Total	C	N	O	S	0	0	0
			293	199	46	47	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	40	Total	C	N	O	S	0	0	0
			277	186	41	49	1			

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

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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	k	37	Total	C	N	O	0	0	0
			286	198	42	46			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	L	35	Total	C	N	O	0	0	0
			287	192	46	49			
11	l	35	Total	C	N	O	0	0	0
			287	192	46	49			

- Molecule 12 is a protein called Photosystem II manganese-stabilizing polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	O	243	Total	C	N	O	S	0	1	0
			1853	1160	311	378	4			
12	o	243	Total	C	N	O	S	0	0	0
			1833	1149	305	375	4			

- Molecule 13 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	T	30	Total	C	N	O	S	0	0	0
			253	177	36	38	2			
13	t	30	Total	C	N	O	S	0	0	0
			253	177	36	38	2			

- Molecule 14 is a protein called Photosystem II 12 kDa extrinsic protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	U	97	Total	C	N	O	0	1	0
			782	496	132	154			
14	u	97	Total	C	N	O	0	0	0
			766	487	129	150			

- Molecule 15 is a protein called Cytochrome c-550.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	V	137	Total	C	N	O	S	0	1	0
			1066	677	177	208	4			
15	v	137	Total	C	N	O	S	0	1	0
			1058	671	175	208	4			

- Molecule 16 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	Y	29	Total	C	N	O	S	0	0	0
			215	142	37	33	3			
16	y	29	Total	C	N	O	S	0	0	0
			207	134	37	33	3			

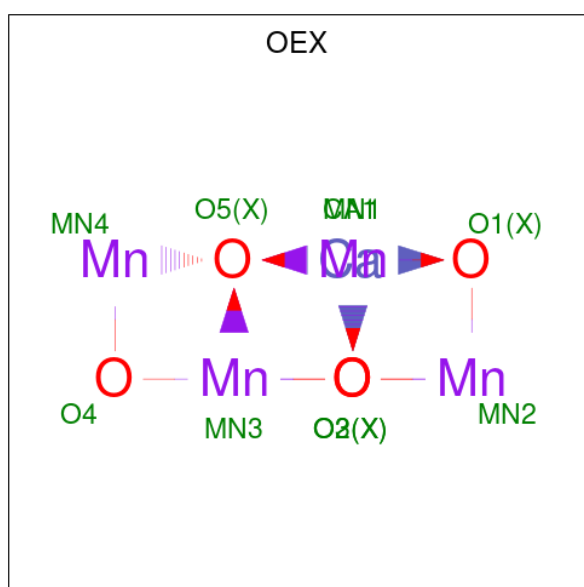
- Molecule 17 is a protein called Photosystem II reaction center X protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	X	37	Total	C	N	O	0	1	0
			269	183	40	46			
17	x	36	Total	C	N	O	0	0	0
			253	172	37	44			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	Z	62	Total	C	N	O	S	0	0	0
			453	311	68	72	2			
18	z	61	Total	C	N	O	S	0	0	0
			436	299	67	69	1			

- Molecule 19 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5).



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

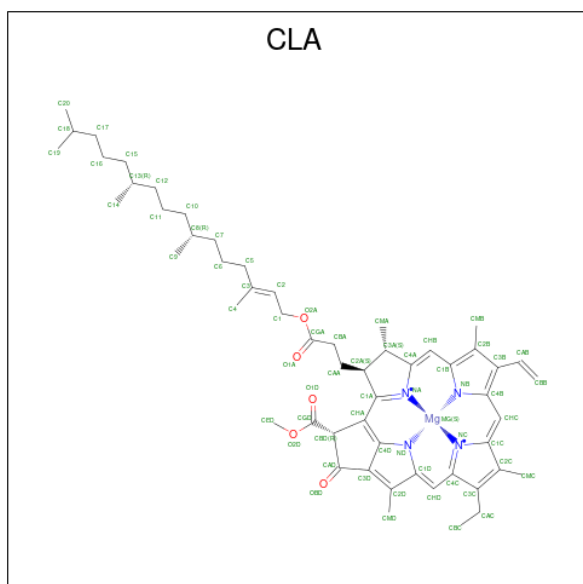
- Molecule 20 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

- Molecule 21 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 22 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	A	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	B	1	Total 61	C 51	Mg 1	N 4	O 5	0	0
22	B	1	Total 53	C 43	Mg 1	N 4	O 5	0	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	B	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	C	1	Total 56	C 46	Mg 1	N 4	O 5	0	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total 61	C 51	Mg 1	N 4	O 5	0	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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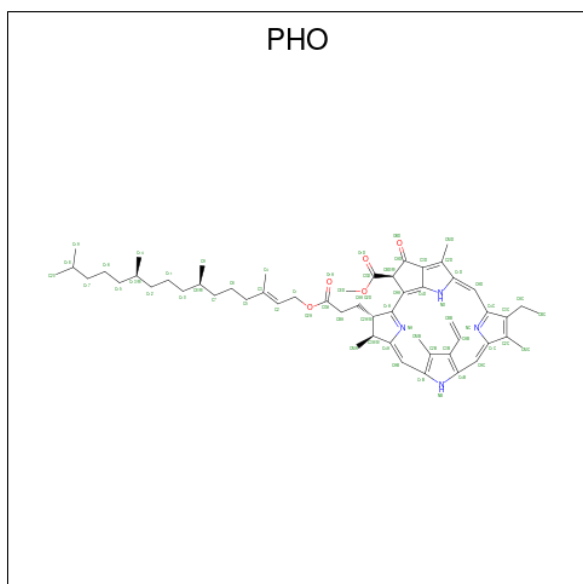
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 59	C 49	Mg 1	N 4	O 5	0	0
22	b	1	Total 52	C 42	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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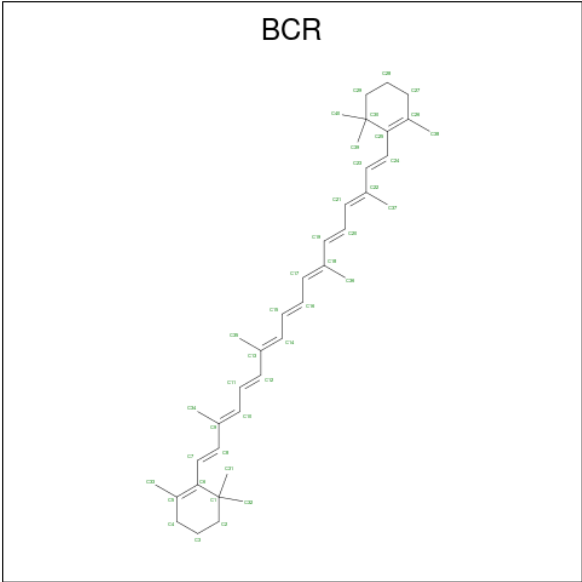
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 23 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



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

- Molecule 24 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



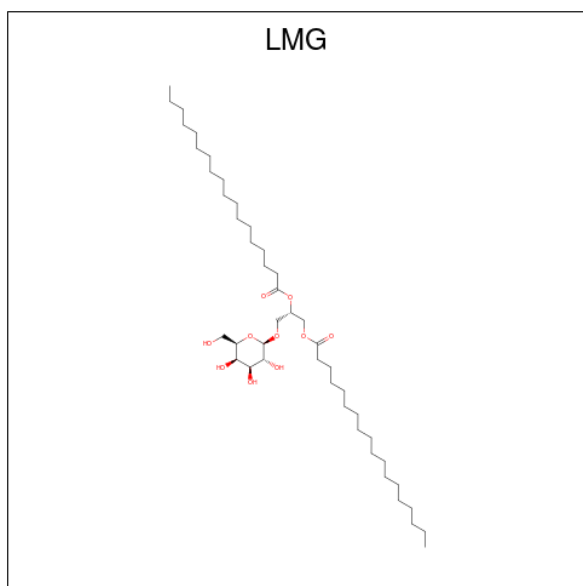
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	A	1	Total C 40 40	0	0
24	B	1	Total C 19 19	0	0
24	B	1	Total C 30 30	0	0
24	B	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	D	1	Total C 40 40	0	0
24	K	1	Total C 40 40	0	0
24	Y	1	Total C 39 39	0	0
24	a	1	Total C 40 40	0	0
24	b	1	Total C 20 20	0	0
24	b	1	Total C 31 31	0	0
24	b	1	Total C 40 40	0	0
24	c	1	Total C 40 40	0	0

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

- Molecule 25 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



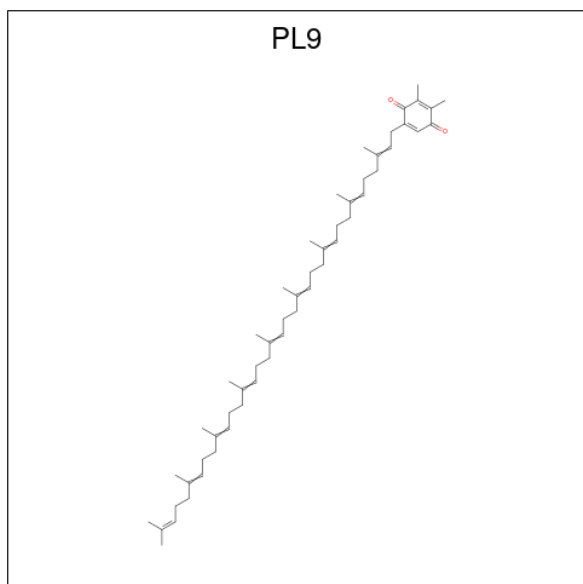
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C O 51 41 10	0	0
25	B	1	Total C O 40 30 10	0	0
25	C	1	Total C O 51 41 10	0	0
25	C	1	Total C O 40 30 10	0	0
25	D	1	Total C O 46 36 10	0	0
25	J	1	Total C O 45 35 10	0	0
25	b	1	Total C O 43 33 10	0	0

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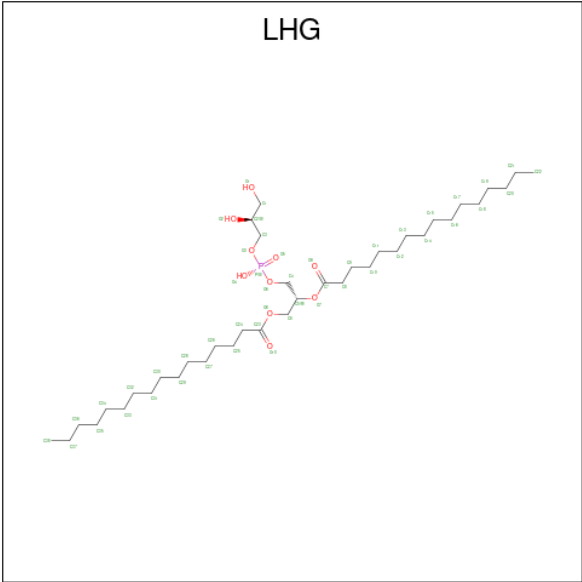
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	c	1	Total	C	O	0	0
			51	41	10		
25	c	1	Total	C	O	0	0
			49	39	10		
25	d	1	Total	C	O	0	0
			47	37	10		
25	i	1	Total	C	O	0	0
			51	41	10		
25	j	1	Total	C	O	0	0
			47	37	10		

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



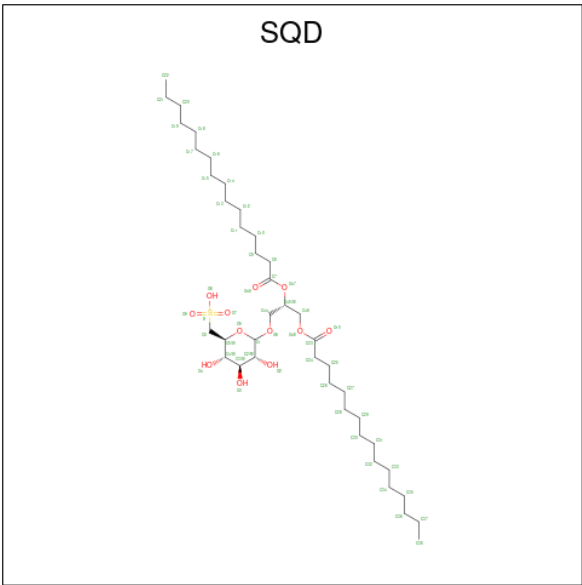
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	A	1	Total	C	O	0	0
			55	53	2		
26	D	1	Total	C	O	0	0
			55	53	2		
26	a	1	Total	C	O	0	0
			55	53	2		
26	d	1	Total	C	O	0	0
			55	53	2		

- Molecule 27 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



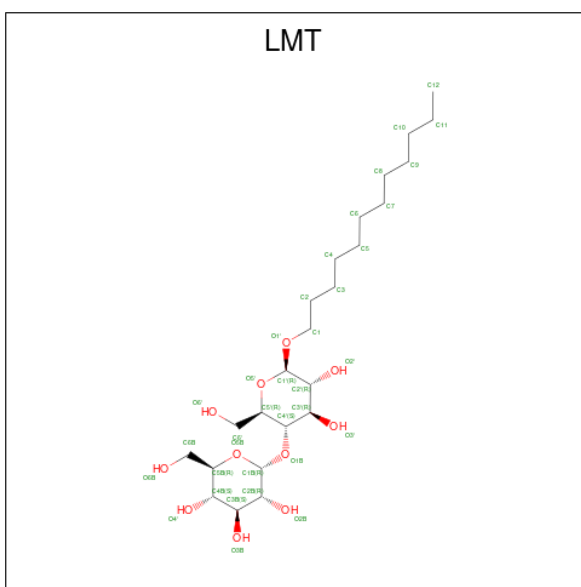
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	A	1	Total	C	O	P	0	0
			31	22	8	1		
27	C	1	Total	C	O	P	0	0
			30	21	8	1		
27	D	1	Total	C	O	P	0	0
			49	38	10	1		
27	D	1	Total	C	O	P	0	0
			49	38	10	1		
27	D	1	Total	C	O	P	0	0
			45	34	10	1		
27	L	1	Total	C	O	P	0	0
			40	29	10	1		
27	a	1	Total	C	O	P	0	0
			49	38	10	1		
27	a	1	Total	C	O	P	0	0
			45	34	10	1		
27	d	1	Total	C	O	P	0	0
			33	24	8	1		
27	d	1	Total	C	O	P	0	0
			49	38	10	1		
27	d	1	Total	C	O	P	0	0
			46	35	10	1		
27	l	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 28 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
28	A	1	Total	C	O	S	0	0
			49	36	12	1		
28	C	1	Total	C	O	S	0	0
			54	41	12	1		
28	D	1	Total	C	O	S	0	0
			20	9	10	1		
28	a	1	Total	C	O	S	0	0
			54	41	12	1		
28	a	1	Total	C	O	S	0	0
			51	38	12	1		
28	b	1	Total	C	O	S	0	0
			38	26	11	1		
28	f	1	Total	C	O	S	0	0
			14	6	7	1		
28	l	1	Total	C	O	S	0	0
			54	41	12	1		

- Molecule 29 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	A	1	Total 35	C 24	O 11	0	0
29	B	1	Total 24	C 18	O 6	0	0
29	E	1	Total 24	C 18	O 6	0	0
29	I	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	c	1	Total 35	C 24	O 11	0	0
29	c	1	Total 24	C 18	O 6	0	0
29	f	1	Total 25	C 19	O 6	0	0
29	t	1	Total 24	C 18	O 6	0	0

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

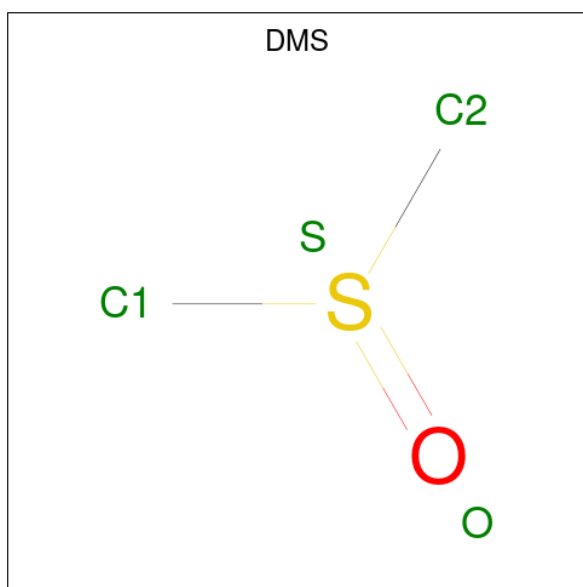
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	A	1	Total C 5 5	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	B	2	Total C 23 23	0	0
30	D	1	Total C 16 16	0	0
30	I	3	Total C 45 45	0	0
30	J	1	Total C 16 16	0	0
30	O	1	Total C 16 16	0	0
30	T	1	Total C 13 13	0	0
30	U	1	Total C 14 14	0	0
30	X	1	Total C 16 16	0	0
30	Z	1	Total C 9 9	0	0
30	a	2	Total C 16 16	0	0
30	b	2	Total C 27 27	0	0
30	c	1	Total C 10 10	0	0
30	d	1	Total C 16 16	0	0
30	i	4	Total C 58 58	0	0
30	j	1	Total C 16 16	0	0
30	t	1	Total C 16 16	0	0
30	u	1	Total C 11 11	0	0
30	x	1	Total C 15 15	0	0

- Molecule 31 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C₂H₆OS).



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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	B	1	Total 4	C 2	O 1	S 1	0	0
31	B	1	Total 4	C 2	O 1	S 1	0	0
31	B	1	Total 4	C 2	O 1	S 1	0	0
31	B	1	Total 4	C 2	O 1	S 1	0	0
31	B	1	Total 4	C 2	O 1	S 1	0	0
31	B	1	Total 4	C 2	O 1	S 1	0	0
31	C	1	Total 4	C 2	O 1	S 1	0	0
31	C	1	Total 4	C 2	O 1	S 1	0	0
31	C	1	Total 4	C 2	O 1	S 1	0	0
31	C	1	Total 4	C 2	O 1	S 1	0	0
31	C	1	Total 4	C 2	O 1	S 1	0	0
31	C	1	Total 4	C 2	O 1	S 1	0	0
31	C	1	Total 4	C 2	O 1	S 1	0	0
31	C	1	Total 4	C 2	O 1	S 1	0	0
31	C	1	Total 4	C 2	O 1	S 1	0	0
31	C	1	Total 4	C 2	O 1	S 1	0	0
31	C	1	Total 4	C 2	O 1	S 1	0	0
31	C	1	Total 4	C 2	O 1	S 1	0	0
31	C	1	Total 4	C 2	O 1	S 1	0	0
31	C	1	Total 4	C 2	O 1	S 1	0	0
31	C	1	Total 4	C 2	O 1	S 1	0	0
31	C	1	Total 4	C 2	O 1	S 1	0	0
31	C	1	Total 4	C 2	O 1	S 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	D	1	Total 4	C 2	O 1	S 1	0	0
31	D	1	Total 4	C 2	O 1	S 1	0	0
31	D	1	Total 4	C 2	O 1	S 1	0	0
31	F	1	Total 4	C 2	O 1	S 1	0	0
31	H	1	Total 4	C 2	O 1	S 1	0	0
31	I	1	Total 4	C 2	O 1	S 1	0	0
31	I	1	Total 4	C 2	O 1	S 1	0	0
31	L	1	Total 4	C 2	O 1	S 1	0	0
31	O	1	Total 4	C 2	O 1	S 1	0	0
31	O	1	Total 4	C 2	O 1	S 1	0	0
31	O	1	Total 4	C 2	O 1	S 1	0	0
31	O	1	Total 4	C 2	O 1	S 1	0	0
31	O	1	Total 4	C 2	O 1	S 1	0	0
31	O	1	Total 4	C 2	O 1	S 1	0	0
31	O	1	Total 4	C 2	O 1	S 1	0	0
31	O	1	Total 4	C 2	O 1	S 1	0	0
31	O	1	Total 4	C 2	O 1	S 1	0	0
31	O	1	Total 4	C 2	O 1	S 1	0	0
31	O	1	Total 4	C 2	O 1	S 1	0	0
31	O	1	Total 4	C 2	O 1	S 1	0	0
31	U	1	Total 4	C 2	O 1	S 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	U	1	Total 4	C 2	O 1	S 1	0	0
31	V	1	Total 4	C 2	O 1	S 1	0	0
31	V	1	Total 4	C 2	O 1	S 1	0	0
31	V	1	Total 4	C 2	O 1	S 1	0	0
31	V	1	Total 4	C 2	O 1	S 1	0	0
31	V	1	Total 4	C 2	O 1	S 1	0	0
31	V	1	Total 4	C 2	O 1	S 1	0	0
31	V	1	Total 4	C 2	O 1	S 1	0	0
31	V	1	Total 4	C 2	O 1	S 1	0	0
31	V	1	Total 4	C 2	O 1	S 1	0	0
31	V	1	Total 4	C 2	O 1	S 1	0	0
31	a	1	Total 4	C 2	O 1	S 1	0	0
31	a	1	Total 4	C 2	O 1	S 1	0	0
31	a	1	Total 4	C 2	O 1	S 1	0	0
31	a	1	Total 4	C 2	O 1	S 1	0	0
31	a	1	Total 4	C 2	O 1	S 1	0	0
31	b	1	Total 4	C 2	O 1	S 1	0	0
31	b	1	Total 4	C 2	O 1	S 1	0	0
31	b	1	Total 4	C 2	O 1	S 1	0	0
31	b	1	Total 4	C 2	O 1	S 1	0	0
31	b	1	Total 4	C 2	O 1	S 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	b	1	Total 4	C 2	O 1	S 1	0	0
31	b	1	Total 4	C 2	O 1	S 1	0	0
31	b	1	Total 4	C 2	O 1	S 1	0	0
31	b	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0

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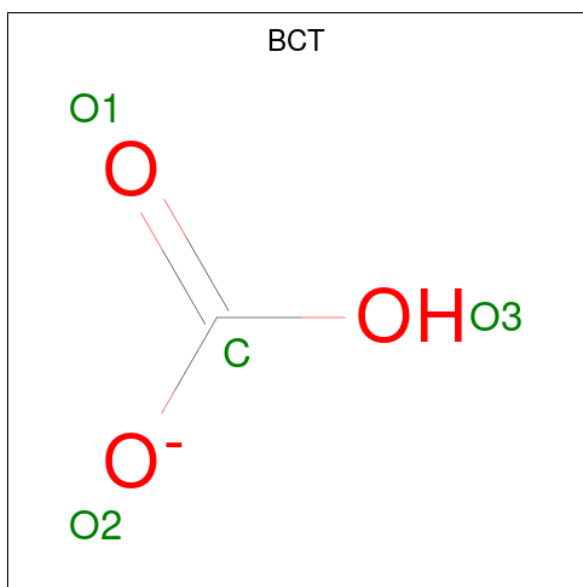
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	d	1	Total 4	C 2	O 1	S 1	0	0
31	d	1	Total 4	C 2	O 1	S 1	0	0
31	d	1	Total 4	C 2	O 1	S 1	0	0
31	d	1	Total 4	C 2	O 1	S 1	0	0
31	d	1	Total 4	C 2	O 1	S 1	0	0
31	f	1	Total 4	C 2	O 1	S 1	0	0
31	i	1	Total 4	C 2	O 1	S 1	0	0
31	l	1	Total 4	C 2	O 1	S 1	0	0
31	l	1	Total 4	C 2	O 1	S 1	0	0
31	l	1	Total 4	C 2	O 1	S 1	0	0
31	o	1	Total 4	C 2	O 1	S 1	0	0
31	o	1	Total 4	C 2	O 1	S 1	0	0
31	o	1	Total 4	C 2	O 1	S 1	0	0
31	o	1	Total 4	C 2	O 1	S 1	0	0
31	o	1	Total 4	C 2	O 1	S 1	0	0
31	o	1	Total 4	C 2	O 1	S 1	0	0
31	o	1	Total 4	C 2	O 1	S 1	0	0
31	t	1	Total 4	C 2	O 1	S 1	0	0
31	t	1	Total 4	C 2	O 1	S 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	t	1	Total 4	C 2	O 1	S 1	0	0
31	u	1	Total 4	C 2	O 1	S 1	0	0
31	u	1	Total 4	C 2	O 1	S 1	0	0
31	u	1	Total 4	C 2	O 1	S 1	0	0
31	u	1	Total 4	C 2	O 1	S 1	0	0
31	v	1	Total 4	C 2	O 1	S 1	0	0
31	v	1	Total 4	C 2	O 1	S 1	0	0
31	v	1	Total 4	C 2	O 1	S 1	0	0
31	v	1	Total 4	C 2	O 1	S 1	0	0
31	v	1	Total 4	C 2	O 1	S 1	0	0
31	v	1	Total 4	C 2	O 1	S 1	0	0
31	v	1	Total 4	C 2	O 1	S 1	0	0
31	v	1	Total 4	C 2	O 1	S 1	0	0
31	v	1	Total 4	C 2	O 1	S 1	0	0
31	v	1	Total 4	C 2	O 1	S 1	0	0

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

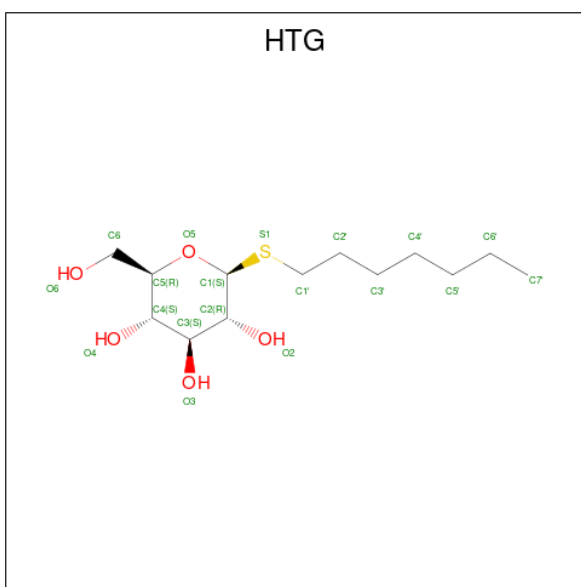


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	A	1	Total	C	O	0	1
			8	2	6		
32	a	1	Total	C	O	0	0
			4	1	3		

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

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

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

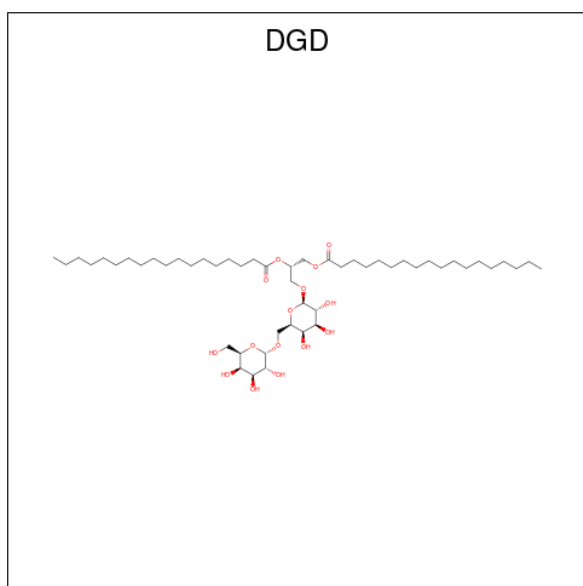
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	c	1	Total	C	O	S	0	0
			19	13	5	1		
34	l	1	Total	C	O	S	0	0
			19	13	5	1		
34	v	1	Total	C	O	S	0	0
			16	10	5	1		

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



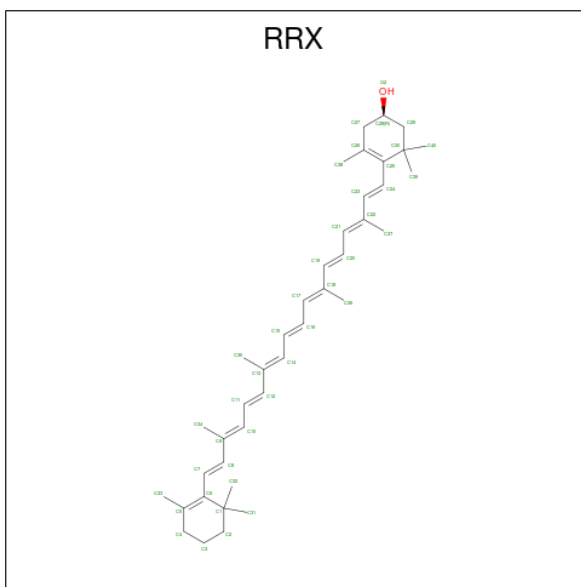
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
35	C	1	Total	C	O		0	0
			62	47	15			
35	C	1	Total	C	O		0	0
			62	47	15			
35	C	1	Total	C	O		0	0
			62	47	15			
35	D	1	Total	C	O		0	0
			50	41	9			
35	H	1	Total	C	O		0	0
			62	47	15			
35	c	1	Total	C	O		0	0
			62	47	15			
35	c	1	Total	C	O		0	0
			62	47	15			
35	c	1	Total	C	O		0	0
			62	47	15			

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
35	d	1	Total 43	C 37	O 6	0	0
35	h	1	Total 62	C 47	O 15	0	0

- # HEM

- Molecule 37 is (3R)-beta,beta-caroten-3-ol (CCD ID: RRX) (formula: C₄₀H₅₆O).

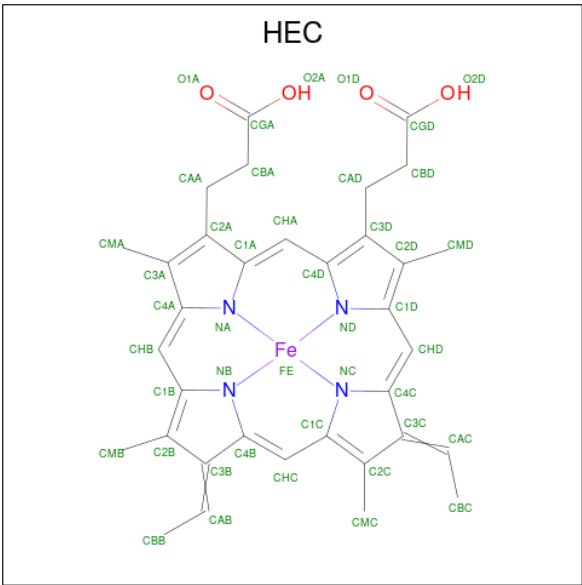


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
37	H	1	Total	C	O	0	0
			41	40	1		
37	h	1	Total	C	O	0	0
			41	40	1		

- Molecule 38 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	J	1	Total	Mg	0	0
			1	1		
38	K	1	Total	Mg	0	0
			1	1		
38	j	1	Total	Mg	0	0
			1	1		
38	k	1	Total	Mg	0	0
			1	1		

- Molecule 39 is HEME C (CCD ID: HEC) (formula: C₃₄H₃₄FeN₄O₄).



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

- Molecule 40 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	A	132	Total	O	0	0
			132	132		
40	B	256	Total	O	0	6
			262	262		
40	C	174	Total	O	0	4
			178	178		
40	D	130	Total	O	0	1
			131	131		
40	E	33	Total	O	0	2
			35	35		
40	F	4	Total	O	0	0
			4	4		
40	H	39	Total	O	0	0
			39	39		
40	I	5	Total	O	0	0
			5	5		
40	J	15	Total	O	0	1
			16	16		
40	K	7	Total	O	0	0
			7	7		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
40	L	18	Total O 19 19	0	1
40	O	161	Total O 166 166	0	5
40	T	12	Total O 12 12	0	0
40	U	72	Total O 74 74	0	2
40	V	110	Total O 113 113	0	3
40	Y	7	Total O 8 8	0	1
40	X	15	Total O 16 16	0	1
40	Z	5	Total O 5 5	0	0
40	a	122	Total O 123 123	0	1
40	b	251	Total O 261 261	0	10
40	c	216	Total O 220 220	0	4
40	d	115	Total O 115 115	0	0
40	e	16	Total O 17 17	0	1
40	f	4	Total O 4 4	0	0
40	h	31	Total O 31 31	0	0
40	i	5	Total O 5 5	0	0
40	j	10	Total O 10 10	0	0
40	k	9	Total O 10 10	0	1
40	l	14	Total O 15 15	0	1
40	o	153	Total O 156 156	0	3
40	t	10	Total O 10 10	0	0

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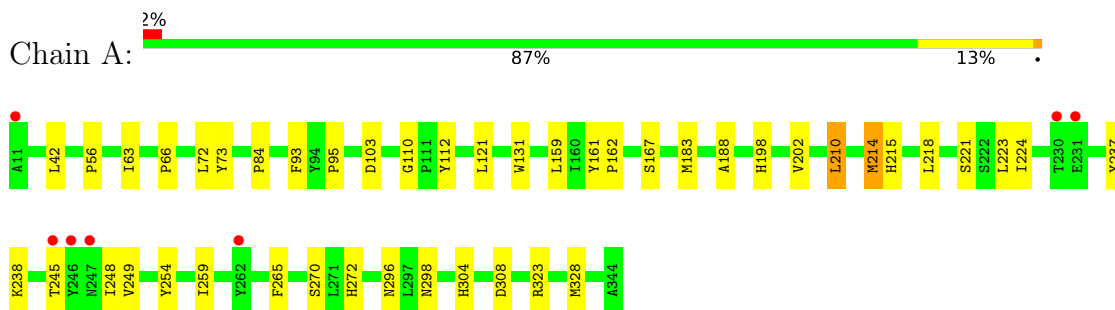
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	u	75	Total 75	O 75	0	0
40	v	77	Total 82	O 82	0	5
40	y	1	Total 1	O 1	0	0
40	x	5	Total 5	O 5	0	0
40	z	8	Total 8	O 8	0	0

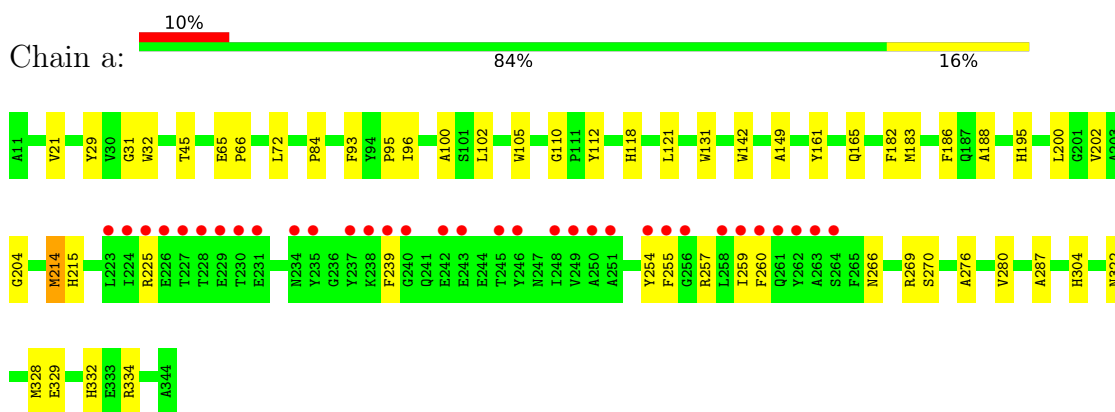
3 Residue-property plots

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

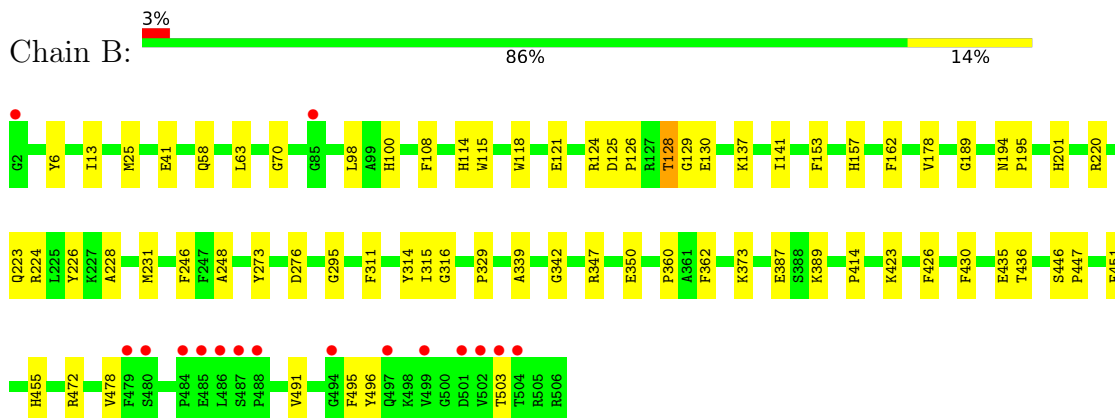
• Molecule 1: Photosystem II protein D1 1



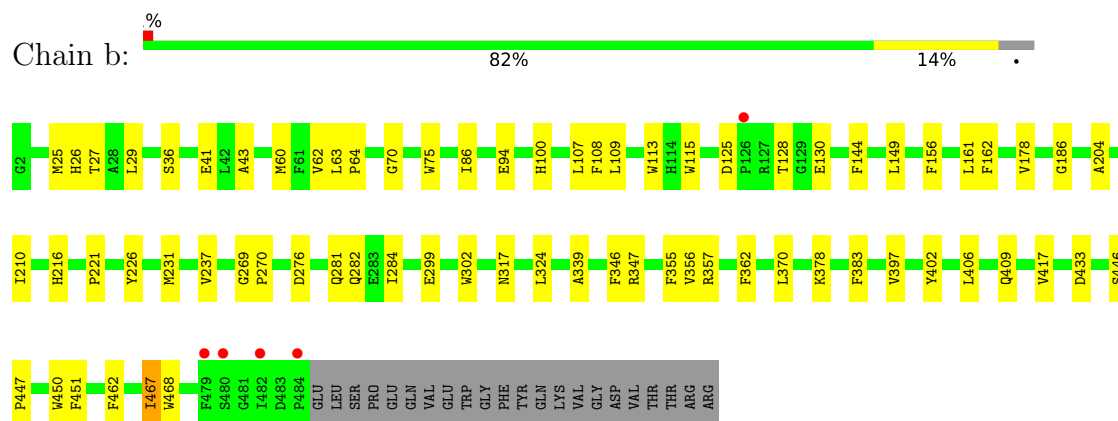
• Molecule 1: Photosystem II protein D1 1



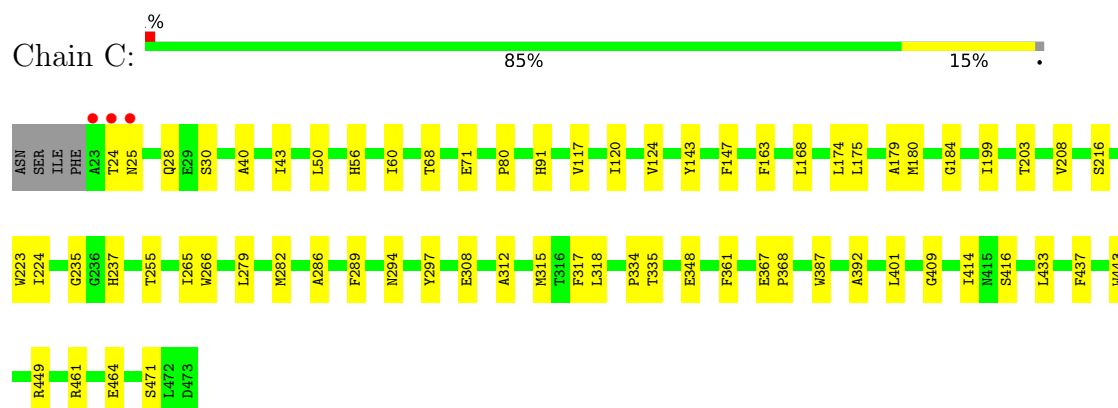
• Molecule 2: Photosystem II CP47 reaction center protein



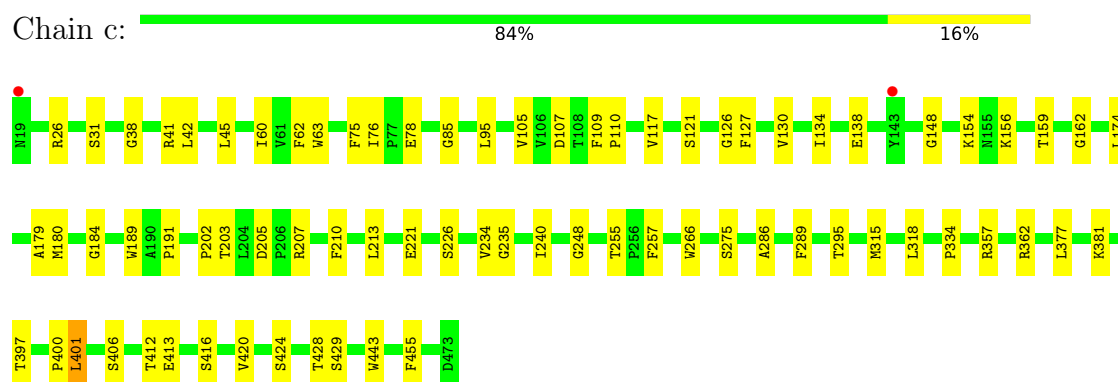
- Molecule 2: Photosystem II CP47 reaction center protein



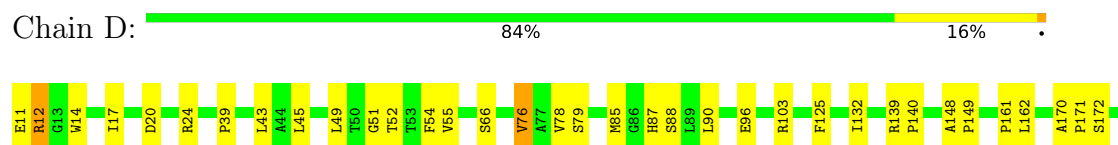
- Molecule 3: Photosystem II CP43 reaction center protein



- Molecule 3: Photosystem II CP43 reaction center protein

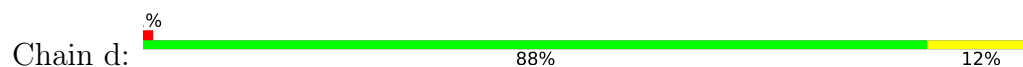


- Molecule 4: Photosystem II D2 protein

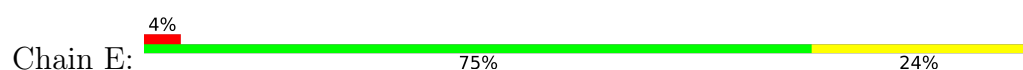




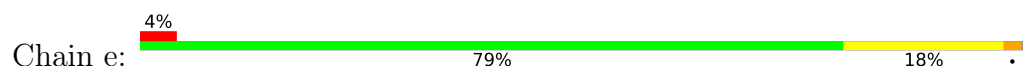
- Molecule 4: Photosystem II D2 protein



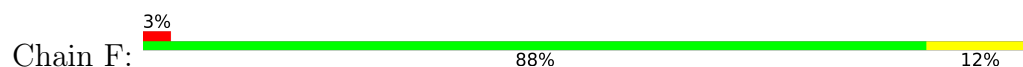
- Molecule 5: Cytochrome b559 subunit alpha



- Molecule 5: Cytochrome b559 subunit alpha



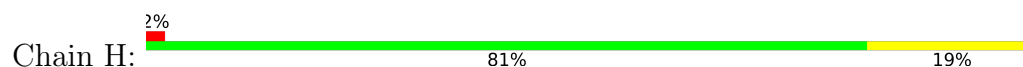
- Molecule 6: Cytochrome b559 subunit beta



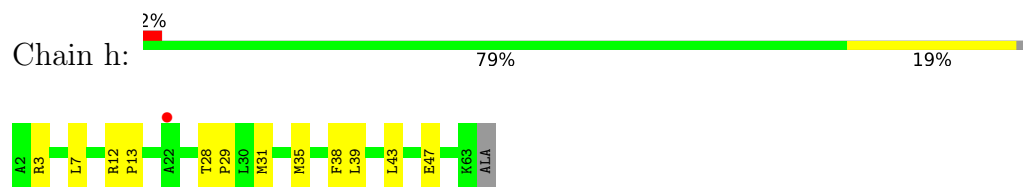
- Molecule 6: Cytochrome b559 subunit beta



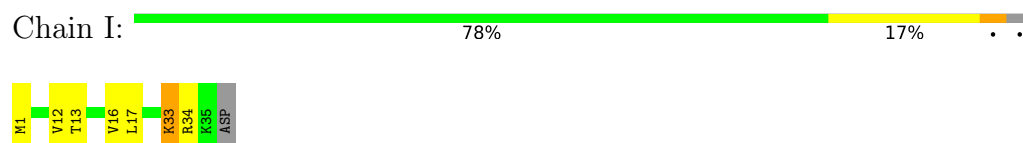
- Molecule 7: Photosystem II reaction center protein H



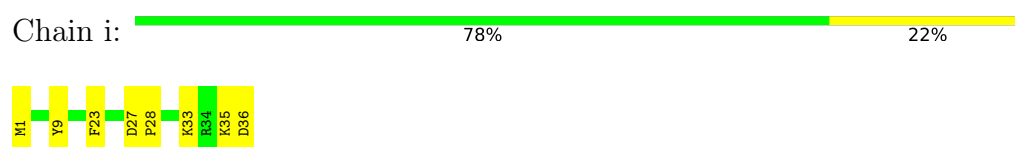
- Molecule 7: Photosystem II reaction center protein H



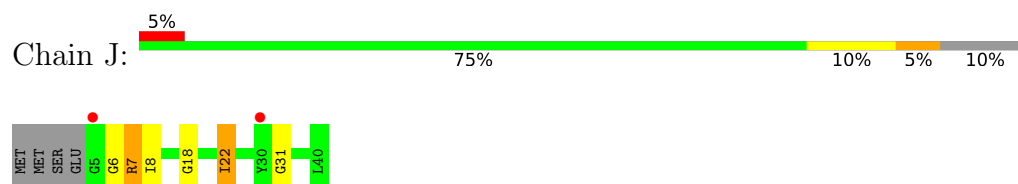
- Molecule 8: Photosystem II reaction center protein I



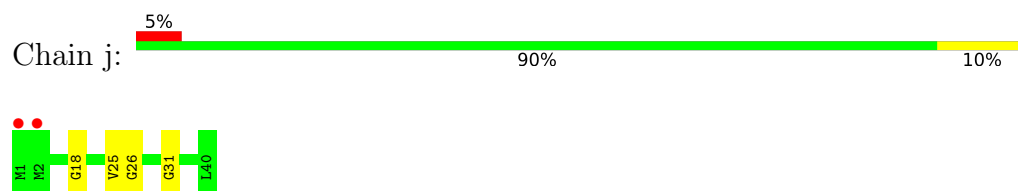
- Molecule 8: Photosystem II reaction center protein I



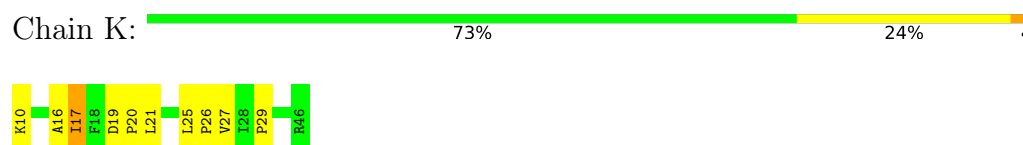
- Molecule 9: Photosystem II reaction center protein J



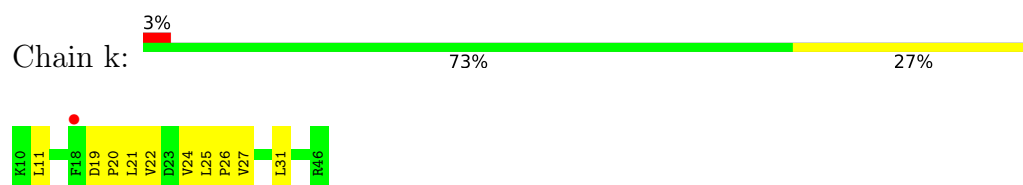
- Molecule 9: Photosystem II reaction center protein J



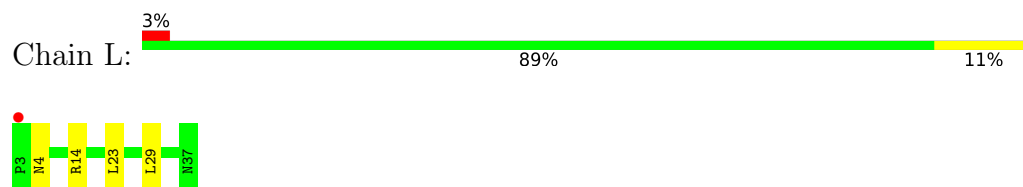
- Molecule 10: Photosystem II reaction center protein K



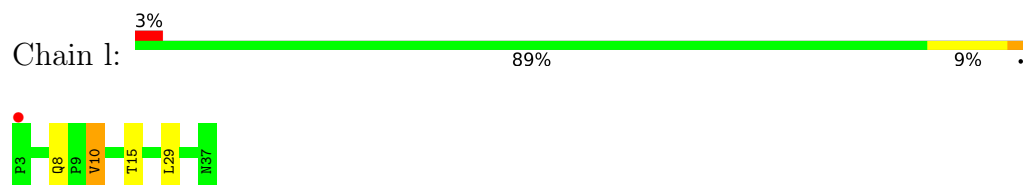
- Molecule 10: Photosystem II reaction center protein K



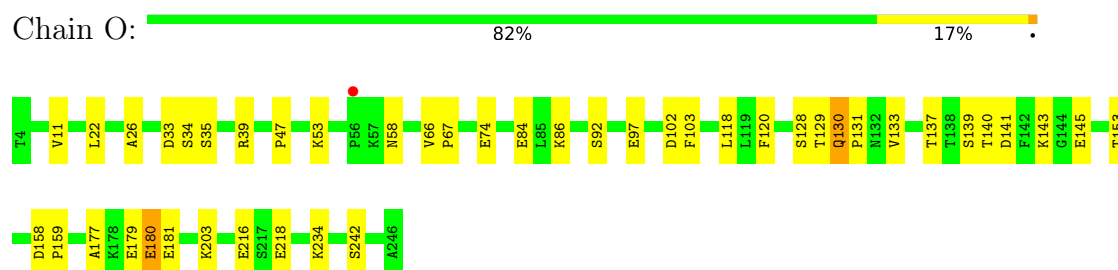
- Molecule 11: Photosystem II reaction center protein L



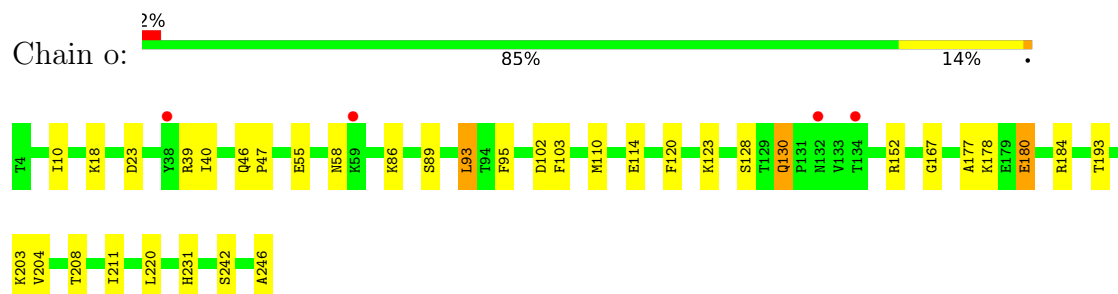
- Molecule 11: Photosystem II reaction center protein L



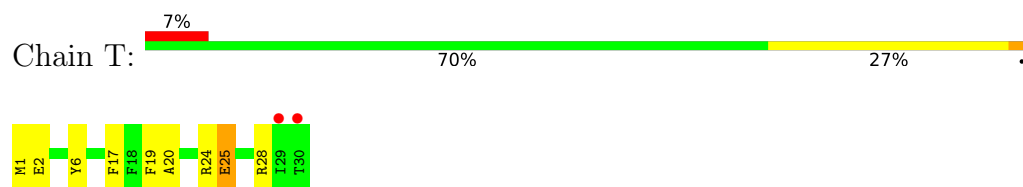
- Molecule 12: Photosystem II manganese-stabilizing polypeptide



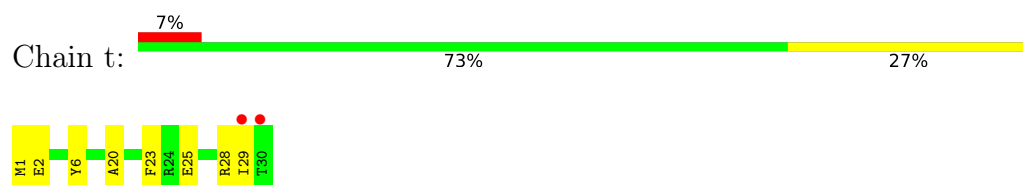
- Molecule 12: Photosystem II manganese-stabilizing polypeptide



- Molecule 13: Photosystem II reaction center protein T



- Molecule 13: Photosystem II reaction center protein T



- Molecule 14: Photosystem II 12 kDa extrinsic protein

Chain U:  88% 12%



- Molecule 14: Photosystem II 12 kDa extrinsic protein

Chain u:  85% 15%



- Molecule 15: Cytochrome c-550

Chain V:  87% 12%



- Molecule 15: Cytochrome c-550

Chain v:  82% 17%



- Molecule 16: Photosystem II reaction center protein Ycf12

Chain Y:  76% 24%



- Molecule 16: Photosystem II reaction center protein Ycf12

Chain y:  72% 28%

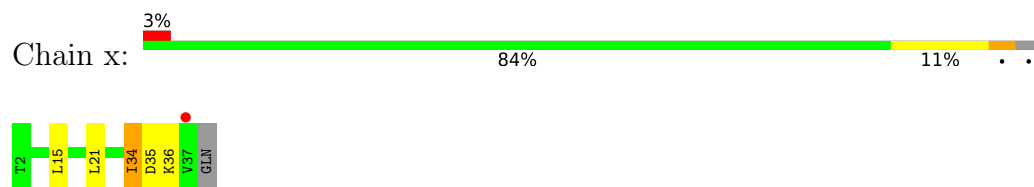


- Molecule 17: Photosystem II reaction center X protein

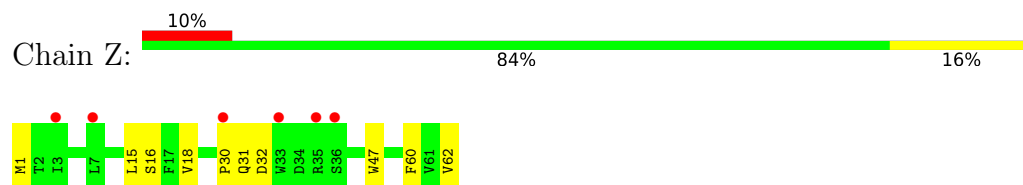
Chain X:  81% 16%



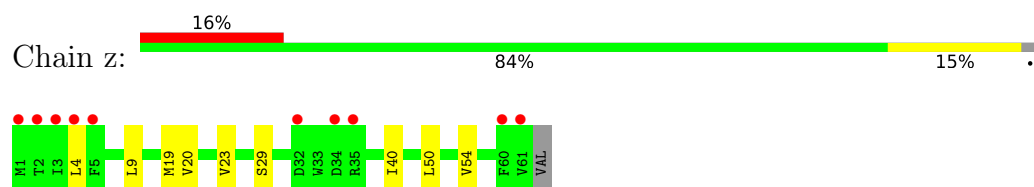
• Molecule 17: Photosystem II reaction center X protein



• Molecule 18: Photosystem II reaction center protein Z



• Molecule 18: Photosystem II reaction center protein Z



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	121.95Å 226.99Å 285.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20 50.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.2 (50.00-2.20) 96.3 (50.00-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.174 , 0.226 0.174 , 0.225	Depositor DCC
R_{free} test set	19357 reflections (3.10%)	wwPDB-VP
Wilson B-factor (Å ²)	35.7	Xtriage
Anisotropy	0.519	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 54.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	51892	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.17% 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: UNL, CLA, BCT, BCR, HEM, RRX, DMS, SQD, HEC, FME, LMT, CL, LHG, LMG, MG, PHO, HTG, PL9, OEX, CA, FE2, DGD

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	1.09	3/2686 (0.1%)	1.03	6/3666 (0.2%)
1	a	1.13	8/2640 (0.3%)	1.05	3/3604 (0.1%)
2	B	1.07	3/4099 (0.1%)	1.03	4/5591 (0.1%)
2	b	1.06	2/3917 (0.1%)	1.02	3/5342 (0.1%)
3	C	1.03	5/3583 (0.1%)	1.00	2/4880 (0.0%)
3	c	1.01	2/3638 (0.1%)	1.04	3/4953 (0.1%)
4	D	1.10	2/2836 (0.1%)	0.99	1/3866 (0.0%)
4	d	1.04	0/2818	1.00	4/3842 (0.1%)
5	E	0.91	0/654	1.04	1/895 (0.1%)
5	e	0.89	0/655	1.05	3/896 (0.3%)
6	F	0.99	0/278	0.87	0/379
6	f	0.90	0/257	0.94	0/349
7	H	0.90	0/541	0.94	1/737 (0.1%)
7	h	0.90	0/517	0.93	0/704
8	I	0.89	0/285	1.00	0/385
8	i	0.82	0/290	0.93	0/392
9	J	0.94	0/257	1.08	1/349 (0.3%)
9	j	0.88	0/283	1.01	0/384
10	K	0.90	0/303	1.13	2/416 (0.5%)
10	k	0.85	0/296	1.05	0/408
11	L	0.97	0/294	1.03	1/399 (0.3%)
11	l	0.93	0/294	1.08	0/399
12	O	0.95	0/1887	1.02	1/2561 (0.0%)
12	o	0.86	0/1864	1.03	5/2535 (0.2%)
13	T	0.92	0/252	1.04	2/342 (0.6%)
13	t	0.89	0/252	1.02	1/342 (0.3%)
14	U	0.96	0/796	1.01	1/1078 (0.1%)
14	u	0.94	0/777	1.07	1/1054 (0.1%)
15	V	1.05	1/1090 (0.1%)	1.04	0/1480
15	v	0.95	0/1082	1.03	2/1472 (0.1%)
16	Y	0.80	0/216	1.04	0/289

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	y	0.69	0/208	1.05	0/278
17	X	0.73	0/275	1.10	0/373
17	x	0.77	0/256	1.05	0/349
18	Z	0.83	0/463	1.04	0/636
18	z	0.75	0/447	1.06	0/614
All	All	1.01	26/41286 (0.1%)	1.02	48/56239 (0.1%)

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	87	HIS	CG-CD2	8.02	1.44	1.35
1	A	56	PRO	CA-C	6.77	1.58	1.52
1	a	195	HIS	ND1-CE1	6.00	1.38	1.32
1	A	159	LEU	CA-C	5.80	1.58	1.52
1	a	195	HIS	CG-CD2	5.78	1.42	1.35

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	142	TRP	N-CA-C	7.31	121.91	112.92
2	B	342	GLY	N-CA-C	-7.27	104.63	112.04
2	b	269	GLY	CA-C-N	6.76	127.15	119.92
2	b	269	GLY	C-N-CA	6.76	127.15	119.92
5	E	76	VAL	N-CA-C	-6.39	104.11	110.62

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2598	0	2484	42	0
1	a	2555	0	2420	41	0
2	B	3950	0	3776	54	0
2	b	3780	0	3636	70	0
3	C	3470	0	3380	46	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	c	3521	0	3439	60	0
4	D	2732	0	2640	57	0
4	d	2717	0	2628	37	0
5	E	635	0	613	12	0
5	e	636	0	609	9	0
6	F	269	0	277	3	0
6	f	250	0	261	12	0
7	H	522	0	547	13	0
7	h	501	0	526	12	0
8	I	288	0	307	3	0
8	i	293	0	309	7	0
9	J	251	0	257	8	0
9	j	277	0	277	4	0
10	K	293	0	305	9	0
10	k	286	0	285	9	0
11	L	287	0	299	3	0
11	l	287	0	299	6	0
12	O	1853	0	1819	36	0
12	o	1833	0	1783	29	0
13	T	253	0	247	5	0
13	t	253	0	247	3	0
14	U	782	0	786	7	0
14	u	766	0	765	12	0
15	V	1066	0	1075	22	0
15	v	1058	0	1053	18	0
16	Y	215	0	246	3	0
16	y	207	0	221	9	0
17	X	269	0	297	6	0
17	x	253	0	274	4	0
18	Z	453	0	471	5	0
18	z	436	0	431	5	0
19	A	10	0	0	0	0
19	a	10	0	0	0	0
20	A	1	0	0	0	0
20	a	1	0	0	0	0
21	A	2	0	0	0	0
21	a	2	0	0	0	0
22	A	185	0	193	10	0
22	B	1014	0	1091	25	0
22	C	836	0	915	32	0
22	D	195	0	216	5	0
22	a	256	0	277	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	b	1016	0	1096	47	0
22	c	845	0	936	32	0
22	d	130	0	144	3	0
23	A	64	0	74	0	0
23	D	64	0	74	5	0
23	a	128	0	148	10	0
24	A	40	0	56	1	0
24	B	89	0	121	4	0
24	C	80	0	112	5	0
24	D	40	0	56	1	0
24	K	40	0	56	0	0
24	Y	39	0	53	2	0
24	a	40	0	56	1	0
24	b	91	0	123	11	0
24	c	80	0	112	8	0
24	d	40	0	56	2	0
24	k	40	0	56	2	0
24	y	40	0	56	3	0
25	A	51	0	72	2	0
25	B	40	0	50	3	0
25	C	91	0	122	3	0
25	D	46	0	62	5	0
25	J	45	0	60	1	0
25	b	43	0	56	1	0
25	c	100	0	140	4	0
25	d	47	0	64	4	0
25	i	51	0	72	3	0
25	j	47	0	64	2	0
26	A	55	0	80	10	0
26	D	55	0	80	5	0
26	a	55	0	80	10	0
26	d	55	0	80	5	0
27	A	31	0	36	1	0
27	C	30	0	33	1	0
27	D	143	0	211	18	0
27	L	40	0	53	7	0
27	a	94	0	137	7	0
27	d	128	0	178	6	0
27	l	49	0	74	3	0
28	A	49	0	64	2	0
28	C	54	0	78	6	0
28	D	20	0	16	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	a	105	0	147	6	0
28	b	38	0	47	2	0
28	f	14	0	8	1	0
28	l	54	0	78	1	0
29	A	35	0	46	6	0
29	B	24	0	35	3	0
29	E	24	0	35	1	0
29	I	35	0	46	0	0
29	T	24	0	35	1	0
29	Z	35	0	46	1	0
29	a	35	0	46	7	0
29	c	59	0	81	1	0
29	f	25	0	35	0	0
29	t	24	0	35	2	0
30	A	5	0	0	0	0
30	B	23	0	0	0	0
30	D	16	0	0	0	0
30	I	45	0	0	1	0
30	J	16	0	0	0	0
30	O	16	0	0	0	0
30	T	13	0	0	0	0
30	U	14	0	0	1	0
30	X	16	0	0	1	0
30	Z	9	0	0	0	0
30	a	16	0	0	0	0
30	b	27	0	0	0	0
30	c	10	0	0	0	0
30	d	16	0	0	0	0
30	i	58	0	0	0	0
30	j	16	0	0	1	0
30	t	16	0	0	0	0
30	u	11	0	0	0	0
30	x	15	0	0	0	0
31	A	20	0	30	4	0
31	B	60	0	90	20	0
31	C	60	0	90	6	0
31	D	12	0	18	3	0
31	F	4	0	6	0	0
31	H	4	0	6	1	0
31	I	8	0	12	0	0
31	L	4	0	6	0	0
31	O	48	0	72	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	U	8	0	12	1	0
31	V	40	0	60	20	0
31	a	20	0	30	8	0
31	b	36	0	54	14	0
31	c	76	0	114	23	0
31	d	20	0	30	8	0
31	f	4	0	6	4	0
31	i	4	0	6	1	0
31	l	12	0	18	1	0
31	o	28	0	42	15	0
31	t	12	0	18	0	0
31	u	16	0	24	6	0
31	v	36	0	54	8	0
32	A	8	0	0	1	0
32	a	4	0	0	0	0
33	B	1	0	0	0	0
33	O	1	0	0	0	0
33	b	1	0	0	0	0
33	c	1	0	0	0	0
33	o	1	0	0	0	0
34	B	57	0	78	3	0
34	C	47	0	67	2	0
34	D	38	0	52	11	0
34	V	14	0	13	0	0
34	b	95	0	130	7	0
34	c	19	0	26	0	0
34	l	19	0	26	3	0
34	v	16	0	17	0	0
35	C	186	0	246	3	0
35	D	50	0	69	0	0
35	H	62	0	82	2	0
35	c	186	0	246	9	0
35	d	43	0	62	0	0
35	h	62	0	82	2	0
36	E	43	0	30	1	0
36	e	43	0	30	6	0
37	H	41	0	56	4	0
37	h	41	0	56	8	0
38	J	1	0	0	0	0
38	K	1	0	0	0	0
38	j	1	0	0	0	0
38	k	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	V	43	0	30	0	0
39	v	43	0	30	1	0
40	A	132	0	0	1	0
40	B	262	0	0	6	0
40	C	178	0	0	1	0
40	D	131	0	0	5	0
40	E	35	0	0	0	0
40	F	4	0	0	0	0
40	H	39	0	0	1	0
40	I	5	0	0	0	0
40	J	16	0	0	0	0
40	K	7	0	0	0	0
40	L	19	0	0	0	0
40	O	166	0	0	10	0
40	T	12	0	0	0	0
40	U	74	0	0	2	0
40	V	113	0	0	4	0
40	X	16	0	0	0	0
40	Y	8	0	0	0	0
40	Z	5	0	0	1	0
40	a	123	0	0	1	0
40	b	261	0	0	11	0
40	c	220	0	0	7	0
40	d	115	0	0	0	0
40	e	17	0	0	1	0
40	f	4	0	0	0	0
40	h	31	0	0	0	0
40	i	5	0	0	0	0
40	j	10	0	0	0	0
40	k	10	0	0	0	0
40	l	15	0	0	0	0
40	o	156	0	0	5	0
40	t	10	0	0	0	0
40	u	75	0	0	3	0
40	v	82	0	0	4	0
40	x	5	0	0	0	0
40	y	1	0	0	0	0
40	z	8	0	0	0	0
All	All	51892	0	50274	868	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 9.

The worst 5 of 868 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)
3:c:362:ARG:HD3	31:c:924:DMS:H22	1.29	1.13
1:a:214:MET:HG2	26:a:415:PL9:H102	1.31	1.12
22:b:608:CLA:H92	22:b:608:CLA:H52	1.14	1.10
2:b:347[B]:ARG:NH2	40:b:845[B]:HOH:O	1.79	1.07
3:c:362:ARG:HH11	31:c:924:DMS:H23	1.19	1.07

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	333/334 (100%)	326 (98%)	6 (2%)	1 (0%)	36	42
1	a	333/334 (100%)	321 (96%)	11 (3%)	1 (0%)	36	42
2	B	506/505 (100%)	495 (98%)	11 (2%)	0	100	100
2	b	482/505 (95%)	465 (96%)	17 (4%)	0	100	100
3	C	449/455 (99%)	434 (97%)	13 (3%)	2 (0%)	30	34
3	c	454/455 (100%)	435 (96%)	18 (4%)	1 (0%)	43	51
4	D	343/342 (100%)	336 (98%)	6 (2%)	1 (0%)	36	42
4	d	341/342 (100%)	333 (98%)	8 (2%)	0	100	100
5	E	77/80 (96%)	75 (97%)	1 (1%)	1 (1%)	9	8
5	e	77/80 (96%)	75 (97%)	2 (3%)	0	100	100
6	F	31/33 (94%)	31 (100%)	0	0	100	100
6	f	29/33 (88%)	29 (100%)	0	0	100	100
7	H	64/63 (102%)	60 (94%)	4 (6%)	0	100	100
7	h	61/63 (97%)	58 (95%)	3 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	I	33/36 (92%)	31 (94%)	2 (6%)	0	100	100
8	i	34/36 (94%)	30 (88%)	4 (12%)	0	100	100
9	J	34/40 (85%)	33 (97%)	0	1 (3%)	3	2
9	j	38/40 (95%)	37 (97%)	1 (3%)	0	100	100
10	K	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
10	k	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
11	L	33/35 (94%)	33 (100%)	0	0	100	100
11	l	33/35 (94%)	33 (100%)	0	0	100	100
12	O	242/243 (100%)	228 (94%)	12 (5%)	2 (1%)	16	16
12	o	241/243 (99%)	231 (96%)	10 (4%)	0	100	100
13	T	28/30 (93%)	28 (100%)	0	0	100	100
13	t	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
14	U	96/97 (99%)	92 (96%)	4 (4%)	0	100	100
14	u	95/97 (98%)	91 (96%)	4 (4%)	0	100	100
15	V	136/137 (99%)	131 (96%)	5 (4%)	0	100	100
15	v	136/137 (99%)	126 (93%)	9 (7%)	1 (1%)	18	19
16	Y	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
16	y	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
17	X	36/37 (97%)	35 (97%)	1 (3%)	0	100	100
17	x	34/37 (92%)	31 (91%)	1 (3%)	2 (6%)	1	0
18	Z	60/62 (97%)	56 (93%)	1 (2%)	3 (5%)	1	0
18	z	59/62 (95%)	55 (93%)	4 (7%)	0	100	100
All	All	5100/5190 (98%)	4921 (96%)	163 (3%)	16 (0%)	36	42

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	12	ARG
3	C	24	THR
3	C	416	SER
5	E	6	GLY
18	Z	31	GLN

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	263/270 (97%)	259 (98%)	4 (2%)	57	73
1	a	252/270 (93%)	251 (100%)	1 (0%)	84	92
2	B	391/403 (97%)	385 (98%)	6 (2%)	57	73
2	b	378/403 (94%)	375 (99%)	3 (1%)	73	85
3	C	347/356 (98%)	343 (99%)	4 (1%)	63	78
3	c	356/356 (100%)	350 (98%)	6 (2%)	53	69
4	D	278/277 (100%)	278 (100%)	0	100	100
4	d	276/277 (100%)	275 (100%)	1 (0%)	84	92
5	E	68/71 (96%)	66 (97%)	2 (3%)	37	51
5	e	67/71 (94%)	65 (97%)	2 (3%)	36	49
6	F	27/27 (100%)	27 (100%)	0	100	100
6	f	25/27 (93%)	24 (96%)	1 (4%)	28	38
7	H	56/53 (106%)	56 (100%)	0	100	100
7	h	54/53 (102%)	54 (100%)	0	100	100
8	I	31/32 (97%)	30 (97%)	1 (3%)	34	47
8	i	31/32 (97%)	31 (100%)	0	100	100
9	J	23/28 (82%)	22 (96%)	1 (4%)	26	35
9	j	25/28 (89%)	25 (100%)	0	100	100
10	K	30/30 (100%)	27 (90%)	3 (10%)	7	7
10	k	28/30 (93%)	27 (96%)	1 (4%)	31	42
11	L	33/33 (100%)	33 (100%)	0	100	100
11	l	33/33 (100%)	32 (97%)	1 (3%)	36	49
12	O	203/206 (98%)	196 (97%)	7 (3%)	32	44
12	o	199/206 (97%)	194 (98%)	5 (2%)	42	56
13	T	24/26 (92%)	23 (96%)	1 (4%)	26	36
13	t	24/26 (92%)	22 (92%)	2 (8%)	10	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	U	85/84 (101%)	84 (99%)	1 (1%)	63	78
14	u	82/84 (98%)	81 (99%)	1 (1%)	63	78
15	V	117/117 (100%)	114 (97%)	3 (3%)	40	55
15	v	115/117 (98%)	111 (96%)	4 (4%)	32	43
16	Y	22/22 (100%)	18 (82%)	4 (18%)	2	1
16	y	19/22 (86%)	19 (100%)	0	100	100
17	X	29/30 (97%)	27 (93%)	2 (7%)	14	16
17	x	27/30 (90%)	26 (96%)	1 (4%)	30	41
18	Z	45/52 (86%)	45 (100%)	0	100	100
18	z	40/52 (77%)	38 (95%)	2 (5%)	22	28
All	All	4103/4234 (97%)	4033 (98%)	70 (2%)	53	69

5 of 70 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	o	93	LEU
12	o	242	SER
15	v	28	GLU
12	O	130	GLN
12	O	118	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 45 such sidechains are listed below:

Mol	Chain	Res	Type
2	b	179	GLN
11	l	6	ASN
2	b	281	GLN
4	d	186	GLN
12	o	104	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	FME	I	1	8	8,9,10	0.93	0	8,9,11	1.23	1 (12%)
13	FME	T	1	13	8,9,10	0.62	0	8,9,11	1.24	1 (12%)
8	FME	i	1	8	8,9,10	0.56	0	8,9,11	1.23	1 (12%)
13	FME	t	1	13	8,9,10	0.62	0	8,9,11	1.65	2 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	FME	I	1	8	-	1/7/9/11	-
13	FME	T	1	13	-	2/7/9/11	-
8	FME	i	1	8	-	2/7/9/11	-
13	FME	t	1	13	-	2/7/9/11	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	t	1	FME	CB-CA-N	-3.07	104.92	110.52
13	t	1	FME	CE-SD-CG	2.61	113.85	100.32
8	i	1	FME	O-C-CA	-2.36	118.69	124.77
13	T	1	FME	C-CA-N	2.03	113.42	109.50
8	I	1	FME	O-C-CA	-2.03	119.54	124.77

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	I	1	FME	O1-CN-N-CA
13	T	1	FME	O1-CN-N-CA
13	t	1	FME	O1-CN-N-CA
13	T	1	FME	CA-CB-CG-SD
13	t	1	FME	CA-CB-CG-SD

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 352 ligands modelled in this entry, 15 are monoatomic and 27 are unknown - leaving 310 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	$\# Z > 2$
22	CLA	b	612	-	69,73,73	2.17	20 (28%)	82,113,113	2.27	29 (35%)
22	CLA	a	412	-	69,73,73	2.28	22 (31%)	82,113,113	2.24	31 (37%)
31	DMS	u	204	-	3,3,3	2.86	1 (33%)	3,3,3	0.83	0
37	RRX	h	101	-	42,42,42	0.97	1 (2%)	56,58,58	1.21	5 (8%)
31	DMS	c	944	-	3,3,3	2.78	1 (33%)	3,3,3	0.81	0
22	CLA	c	914	-	69,73,73	2.35	19 (27%)	82,113,113	2.23	27 (32%)
22	CLA	B	617	-	59,63,73	2.20	16 (27%)	70,101,113	2.64	30 (42%)
27	LHG	d	407	-	48,48,48	0.76	2 (4%)	51,54,54	1.08	3 (5%)
31	DMS	V	201	-	3,3,3	2.70	1 (33%)	3,3,3	0.92	0
34	HTG	B	627	-	19,19,19	0.95	1 (5%)	23,24,24	1.83	3 (13%)
29	LMT	a	419	-	36,36,36	0.78	0	47,47,47	1.38	4 (8%)
31	DMS	b	636	-	3,3,3	2.73	1 (33%)	3,3,3	0.72	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	DMS	O	306	-	3,3,3	2.76	1 (33%)	3,3,3	0.78	0
35	DGD	c	918	-	63,63,67	0.94	5 (7%)	77,77,81	1.03	4 (5%)
22	CLA	C	510	-	69,73,73	2.15	18 (26%)	82,113,113	2.38	28 (34%)
24	BCR	d	404	-	41,41,41	1.06	3 (7%)	56,56,56	1.79	13 (23%)
25	LMG	D	412	-	46,46,55	1.14	3 (6%)	54,54,63	1.13	2 (3%)
27	LHG	L	101	-	39,39,48	1.05	2 (5%)	42,45,54	1.21	4 (9%)
28	SQD	l	101	-	52,54,54	1.09	3 (5%)	62,65,65	1.44	8 (12%)
23	PHO	D	402	-	58,69,69	2.83	10 (17%)	55,99,99	2.80	16 (29%)
35	DGD	C	517	-	63,63,67	0.85	3 (4%)	77,77,81	1.32	12 (15%)
39	HEC	V	202	15	46,50,50	2.05	8 (17%)	58,82,82	1.26	7 (12%)
24	BCR	B	619	-	30,30,41	0.94	0	39,39,56	1.33	8 (20%)
31	DMS	l	103	-	3,3,3	2.77	1 (33%)	3,3,3	0.68	0
22	CLA	b	609	-	69,73,73	2.22	19 (27%)	82,113,113	2.09	27 (32%)
35	DGD	c	917	-	63,63,67	0.97	3 (4%)	77,77,81	1.01	3 (3%)
22	CLA	b	615	-	56,60,73	2.73	21 (37%)	65,97,113	2.41	29 (44%)
31	DMS	I	101	-	3,3,3	2.77	1 (33%)	3,3,3	0.71	0
28	SQD	a	414	-	52,54,54	1.02	2 (3%)	62,65,65	1.96	12 (19%)
24	BCR	K	101	-	41,41,41	0.85	0	56,56,56	1.21	5 (8%)
31	DMS	B	639	-	3,3,3	2.82	1 (33%)	3,3,3	0.73	0
31	DMS	C	537	-	3,3,3	2.81	1 (33%)	3,3,3	0.72	0
22	CLA	b	606	-	69,73,73	2.23	19 (27%)	82,113,113	2.31	27 (32%)
24	BCR	c	916	-	41,41,41	0.87	0	56,56,56	1.55	10 (17%)
22	CLA	B	602	40	69,73,73	2.78	22 (31%)	82,113,113	2.35	28 (34%)
31	DMS	v	209	-	3,3,3	2.70	1 (33%)	3,3,3	0.65	0
31	DMS	v	207	-	3,3,3	2.78	1 (33%)	3,3,3	0.67	0
29	LMT	B	622	-	24,24,36	0.64	1 (4%)	29,29,47	0.85	1 (3%)
25	LMG	J	101	38	45,45,55	0.99	2 (4%)	53,53,63	1.03	6 (11%)
31	DMS	o	303	-	3,3,3	2.76	1 (33%)	3,3,3	0.83	0
31	DMS	c	924	-	3,3,3	2.88	1 (33%)	3,3,3	1.35	1 (33%)
31	DMS	o	308	-	3,3,3	2.85	1 (33%)	3,3,3	0.85	0
25	LMG	C	531	-	40,40,55	1.19	3 (7%)	48,48,63	1.14	3 (6%)
31	DMS	u	205	-	3,3,3	3.14	1 (33%)	3,3,3	1.22	0
29	LMT	Z	101	-	36,36,36	0.68	1 (2%)	47,47,47	1.16	3 (6%)
25	LMG	d	409	-	47,47,55	1.09	3 (6%)	55,55,63	1.48	9 (16%)
19	OEX	A	401	40,3,1	0,15,15	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	DMS	B	631	-	3,3,3	2.62	1 (33%)	3,3,3	0.63	0
34	HTG	D	415	-	19,19,19	1.09	1 (5%)	23,24,24	2.48	7 (30%)
31	DMS	V	212	-	3,3,3	2.84	1 (33%)	3,3,3	1.21	0
31	DMS	O	313	-	3,3,3	2.69	1 (33%)	3,3,3	0.49	0
31	DMS	C	533	-	3,3,3	2.80	1 (33%)	3,3,3	0.77	0
31	DMS	O	307	-	3,3,3	2.86	1 (33%)	3,3,3	0.93	0
31	DMS	d	412	-	3,3,3	2.62	1 (33%)	3,3,3	0.85	0
27	LHG	d	408	-	45,45,48	1.04	2 (4%)	48,51,54	0.74	0
22	CLA	B	612	-	69,73,73	2.16	17 (24%)	82,113,113	2.25	32 (39%)
22	CLA	b	607	-	69,73,73	2.24	23 (33%)	82,113,113	2.49	27 (32%)
31	DMS	b	630	-	3,3,3	2.72	1 (33%)	3,3,3	0.30	0
32	BCT	A	421[A]	20	3,3,3	1.52	1 (33%)	2,3,3	0.16	0
22	CLA	C	507	-	69,73,73	2.27	20 (28%)	82,113,113	2.18	23 (28%)
31	DMS	C	534	-	3,3,3	2.76	1 (33%)	3,3,3	0.57	0
31	DMS	I	106	-	3,3,3	2.75	1 (33%)	3,3,3	0.77	0
22	CLA	d	402	-	69,73,73	2.06	21 (30%)	82,113,113	2.36	28 (34%)
27	LHG	l	102	-	48,48,48	0.93	2 (4%)	51,54,54	1.09	3 (5%)
31	DMS	v	210	-	3,3,3	2.91	1 (33%)	3,3,3	0.81	0
31	DMS	c	938	-	3,3,3	2.83	1 (33%)	3,3,3	0.85	0
36	HEM	E	102	5,6	50,50,50	2.01	8 (16%)	67,82,82	1.50	10 (14%)
31	DMS	b	634	-	3,3,3	2.78	1 (33%)	3,3,3	0.60	0
22	CLA	B	615	-	57,61,73	2.63	19 (33%)	67,98,113	2.82	31 (46%)
31	DMS	V	211	-	3,3,3	2.88	1 (33%)	3,3,3	0.78	0
22	CLA	A	405	-	69,73,73	2.39	18 (26%)	82,113,113	2.05	25 (30%)
31	DMS	C	536	-	3,3,3	2.75	1 (33%)	3,3,3	0.47	0
25	LMG	j	101	38	47,47,55	1.01	2 (4%)	55,55,63	1.18	7 (12%)
31	DMS	c	941	-	3,3,3	2.66	1 (33%)	3,3,3	0.54	0
22	CLA	C	512	3	69,73,73	2.54	21 (30%)	82,113,113	2.28	31 (37%)
31	DMS	o	304	-	3,3,3	2.88	1 (33%)	3,3,3	1.17	0
31	DMS	C	525	-	3,3,3	2.50	1 (33%)	3,3,3	0.64	0
27	LHG	D	411	-	44,44,48	0.98	2 (4%)	47,50,54	1.05	3 (6%)
31	DMS	B	634	-	3,3,3	2.87	1 (33%)	3,3,3	0.67	0
31	DMS	c	943	-	3,3,3	2.76	1 (33%)	3,3,3	0.83	0
19	OEX	a	403	40,3,1	0,15,15	-	-	-	-	-
31	DMS	c	935	-	3,3,3	2.72	1 (33%)	3,3,3	0.91	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	BCR	a	413	-	41,41,41	1.15	2 (4%)	56,56,56	1.18	8 (14%)
34	HTG	C	521	-	19,19,19	0.87	2 (10%)	23,24,24	1.47	2 (8%)
34	HTG	D	414	-	19,19,19	0.81	1 (5%)	23,24,24	1.59	1 (4%)
31	DMS	v	211	-	3,3,3	2.82	1 (33%)	3,3,3	0.78	0
29	LMT	c	921	-	36,36,36	0.68	1 (2%)	47,47,47	1.04	4 (8%)
27	LHG	d	401	-	32,32,48	1.24	2 (6%)	35,37,54	1.17	4 (11%)
31	DMS	A	417	-	3,3,3	2.73	1 (33%)	3,3,3	0.49	0
22	CLA	C	505	40	69,73,73	3.00	22 (31%)	82,113,113	2.12	24 (29%)
22	CLA	D	401	40	69,73,73	1.89	17 (24%)	82,113,113	2.43	29 (35%)
37	RRX	H	101	-	42,42,42	0.84	0	56,58,58	1.52	9 (16%)
26	PL9	D	406	-	55,55,55	0.94	3 (5%)	68,69,69	1.54	14 (20%)
31	DMS	O	304	-	3,3,3	2.63	1 (33%)	3,3,3	0.43	0
31	DMS	u	202	-	3,3,3	2.68	1 (33%)	3,3,3	1.07	0
31	DMS	t	104	-	3,3,3	2.77	1 (33%)	3,3,3	0.61	0
31	DMS	V	210	-	3,3,3	2.83	1 (33%)	3,3,3	0.90	0
35	DGD	C	519	-	63,63,67	0.82	2 (3%)	77,77,81	1.21	10 (12%)
26	PL9	A	411	-	55,55,55	0.96	4 (7%)	68,69,69	1.71	13 (19%)
31	DMS	b	633	-	3,3,3	2.73	1 (33%)	3,3,3	0.57	0
31	DMS	V	205	-	3,3,3	2.68	1 (33%)	3,3,3	0.66	0
31	DMS	C	528	-	3,3,3	2.69	1 (33%)	3,3,3	0.59	0
31	DMS	C	539	-	3,3,3	2.75	1 (33%)	3,3,3	0.63	0
31	DMS	B	630	-	3,3,3	2.88	1 (33%)	3,3,3	0.94	0
31	DMS	c	923	-	3,3,3	2.56	1 (33%)	3,3,3	0.41	0
31	DMS	B	633	-	3,3,3	2.72	1 (33%)	3,3,3	0.48	0
25	LMG	i	101	-	51,51,55	0.99	2 (3%)	59,59,63	1.18	7 (11%)
29	LMT	A	414	-	36,36,36	0.79	0	47,47,47	1.14	3 (6%)
22	CLA	c	906	-	69,73,73	2.38	21 (30%)	82,113,113	2.08	25 (30%)
31	DMS	C	540	-	3,3,3	2.85	1 (33%)	3,3,3	0.91	0
22	CLA	B	607	-	69,73,73	2.36	19 (27%)	82,113,113	2.38	32 (39%)
31	DMS	D	417	-	3,3,3	2.82	1 (33%)	3,3,3	0.61	0
31	DMS	c	936	-	3,3,3	2.76	1 (33%)	3,3,3	0.60	0
27	LHG	C	522	-	29,29,48	1.31	2 (6%)	32,34,54	1.36	3 (9%)
31	DMS	B	638	-	3,3,3	2.71	1 (33%)	3,3,3	0.41	0
29	LMT	c	931	-	24,24,36	0.80	1 (4%)	29,29,47	0.87	2 (6%)
35	DGD	d	406	-	42,42,67	1.25	3 (7%)	44,45,81	1.10	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	DMS	D	418	-	3,3,3	2.46	1 (33%)	3,3,3	0.69	0
22	CLA	c	904	-	69,73,73	2.59	20 (28%)	82,113,113	2.39	30 (36%)
22	CLA	b	605	-	69,73,73	2.49	22 (31%)	82,113,113	2.22	22 (26%)
31	DMS	O	310	-	3,3,3	2.68	1 (33%)	3,3,3	0.87	0
31	DMS	d	411	-	3,3,3	2.77	1 (33%)	3,3,3	0.96	0
25	LMG	A	410	-	51,51,55	0.96	2 (3%)	59,59,63	1.10	5 (8%)
22	CLA	b	611	40	69,73,73	2.54	21 (30%)	82,113,113	2.22	26 (31%)
35	DGD	h	102	-	63,63,67	0.98	3 (4%)	77,77,81	1.14	4 (5%)
31	DMS	V	207	-	3,3,3	2.82	1 (33%)	3,3,3	0.92	0
31	DMS	O	314	-	3,3,3	2.80	1 (33%)	3,3,3	0.78	0
28	SQD	f	101	-	12,13,54	2.28	1 (8%)	14,16,65	1.13	2 (14%)
23	PHO	A	407	-	58,69,69	2.45	13 (22%)	55,99,99	2.74	16 (29%)
22	CLA	c	911	-	69,73,73	2.23	20 (28%)	82,113,113	2.15	28 (34%)
22	CLA	C	513	-	60,64,73	2.84	21 (35%)	71,102,113	2.39	24 (33%)
22	CLA	A	408	-	69,73,73	2.15	20 (28%)	82,113,113	2.23	31 (37%)
31	DMS	t	105	-	3,3,3	2.77	1 (33%)	3,3,3	0.63	0
24	BCR	C	516	-	41,41,41	0.93	0	56,56,56	1.37	7 (12%)
31	DMS	o	307	-	3,3,3	2.66	1 (33%)	3,3,3	0.60	0
34	HTG	C	523	-	8,8,19	0.40	0	7,7,24	1.02	1 (14%)
31	DMS	c	934	-	3,3,3	2.72	1 (33%)	3,3,3	0.69	0
35	DGD	c	919	-	63,63,67	0.99	4 (6%)	77,77,81	1.16	6 (7%)
31	DMS	C	538	-	3,3,3	2.73	1 (33%)	3,3,3	0.60	0
22	CLA	b	610	-	69,73,73	2.58	21 (30%)	82,113,113	2.05	27 (32%)
31	DMS	V	204	-	3,3,3	2.79	1 (33%)	3,3,3	0.84	0
22	CLA	c	907	-	69,73,73	2.36	20 (28%)	82,113,113	2.17	30 (36%)
27	LHG	a	423	-	44,44,48	1.02	2 (4%)	47,50,54	1.10	4 (8%)
31	DMS	t	103	-	3,3,3	2.77	1 (33%)	3,3,3	0.66	0
31	DMS	O	311	-	3,3,3	3.04	1 (33%)	3,3,3	0.93	0
31	DMS	V	209	-	3,3,3	2.71	1 (33%)	3,3,3	0.50	0
26	PL9	a	415	-	55,55,55	0.95	3 (5%)	68,69,69	1.48	9 (13%)
29	LMT	E	101	-	24,24,36	0.64	0	29,29,47	0.99	1 (3%)
31	DMS	v	204	-	3,3,3	2.73	1 (33%)	3,3,3	0.70	0
32	BCT	A	421[B]	20	3,3,3	1.54	1 (33%)	2,3,3	0.37	0
31	DMS	c	927	-	3,3,3	2.70	1 (33%)	3,3,3	0.43	0
31	DMS	f	103	-	3,3,3	2.77	1 (33%)	3,3,3	0.94	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	DMS	A	418	-	3,3,3	2.47	1 (33%)	3,3,3	1.28	0
31	DMS	l	105	-	3,3,3	2.80	1 (33%)	3,3,3	0.74	0
31	DMS	v	205	-	3,3,3	2.72	1 (33%)	3,3,3	0.86	0
31	DMS	d	413	-	3,3,3	2.60	1 (33%)	3,3,3	0.41	0
22	CLA	c	909	-	69,73,73	3.20	23 (33%)	82,113,113	2.24	25 (30%)
27	LHG	D	409	-	48,48,48	1.02	2 (4%)	51,54,54	1.39	5 (9%)
25	LMG	c	930	-	49,49,55	1.10	3 (6%)	57,57,63	1.07	4 (7%)
31	DMS	u	203	-	3,3,3	2.79	1 (33%)	3,3,3	0.78	0
34	HTG	B	623	-	19,19,19	1.07	1 (5%)	23,24,24	1.60	2 (8%)
24	BCR	k	101	-	41,41,41	0.92	0	56,56,56	1.25	6 (10%)
31	DMS	c	937	-	3,3,3	2.95	1 (33%)	3,3,3	0.84	0
31	DMS	C	535	-	3,3,3	2.80	1 (33%)	3,3,3	0.81	0
34	HTG	b	626	-	19,19,19	0.77	1 (5%)	23,24,24	1.47	4 (17%)
31	DMS	B	637	-	3,3,3	2.84	1 (33%)	3,3,3	0.73	0
24	BCR	C	515	-	41,41,41	0.82	1 (2%)	56,56,56	1.50	9 (16%)
31	DMS	O	308	-	3,3,3	2.85	1 (33%)	3,3,3	0.64	0
22	CLA	C	503	-	69,73,73	2.40	20 (28%)	82,113,113	2.20	22 (26%)
31	DMS	d	414	-	3,3,3	2.76	1 (33%)	3,3,3	0.60	0
34	HTG	B	626	-	19,19,19	0.69	0	23,24,24	1.65	5 (21%)
23	PHO	a	411	-	58,69,69	2.60	11 (18%)	55,99,99	3.14	13 (23%)
31	DMS	B	636	-	3,3,3	2.66	1 (33%)	3,3,3	0.65	0
31	DMS	c	942	-	3,3,3	2.80	1 (33%)	3,3,3	0.74	0
22	CLA	B	605	-	69,73,73	2.09	20 (28%)	82,113,113	2.36	36 (43%)
28	SQD	C	501	-	52,54,54	0.99	2 (3%)	62,65,65	1.87	12 (19%)
35	DGD	C	518	-	63,63,67	0.97	3 (4%)	77,77,81	1.27	10 (12%)
22	CLA	C	504	-	69,73,73	2.67	22 (31%)	82,113,113	2.28	30 (36%)
28	SQD	D	408	-	18,20,54	0.85	1 (5%)	26,29,65	1.87	7 (26%)
31	DMS	C	529	-	3,3,3	2.74	1 (33%)	3,3,3	0.56	0
31	DMS	b	635	-	3,3,3	2.82	1 (33%)	3,3,3	0.56	0
25	LMG	b	622	-	43,43,55	1.36	4 (9%)	51,51,63	1.90	12 (23%)
23	PHO	a	410	-	58,69,69	2.62	12 (20%)	55,99,99	2.66	12 (21%)
34	HTG	b	632	-	19,19,19	1.05	2 (10%)	23,24,24	2.36	7 (30%)
34	HTG	b	623	-	19,19,19	1.03	1 (5%)	23,24,24	1.28	4 (17%)
31	DMS	i	106	-	3,3,3	2.68	1 (33%)	3,3,3	0.56	0
22	CLA	c	908	40	69,73,73	2.71	17 (24%)	82,113,113	2.35	23 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	DMS	U	203	-	3,3,3	2.84	1 (33%)	3,3,3	1.25	0
24	BCR	c	915	-	41,41,41	0.86	1 (2%)	56,56,56	1.40	7 (12%)
22	CLA	B	606	-	69,73,73	2.79	19 (27%)	82,113,113	2.36	29 (35%)
22	CLA	C	509	-	69,73,73	2.40	19 (27%)	82,113,113	2.14	24 (29%)
24	BCR	B	618	-	19,19,41	0.95	1 (5%)	26,26,56	1.45	5 (19%)
22	CLA	C	508	40	69,73,73	2.27	20 (28%)	82,113,113	2.29	25 (30%)
22	CLA	B	609	-	69,73,73	2.56	21 (30%)	82,113,113	2.25	26 (31%)
31	DMS	a	401	-	3,3,3	2.81	1 (33%)	3,3,3	0.83	0
31	DMS	V	206	-	3,3,3	2.76	1 (33%)	3,3,3	0.56	0
31	DMS	b	638	-	3,3,3	3.05	1 (33%)	3,3,3	0.71	0
31	DMS	o	302	-	3,3,3	2.74	1 (33%)	3,3,3	0.96	0
29	LMT	T	102	-	24,24,36	0.73	1 (4%)	29,29,47	1.28	3 (10%)
24	BCR	b	619	-	30,31,41	1.02	1 (3%)	38,40,56	1.37	6 (15%)
24	BCR	D	405	-	41,41,41	1.00	1 (2%)	56,56,56	2.01	15 (26%)
34	HTG	C	532	-	19,19,19	1.06	2 (10%)	23,24,24	1.66	1 (4%)
27	LHG	D	410	-	48,48,48	0.80	2 (4%)	51,54,54	1.10	5 (9%)
22	CLA	B	604	-	69,73,73	2.23	18 (26%)	82,113,113	2.28	32 (39%)
31	DMS	C	526	-	3,3,3	2.66	1 (33%)	3,3,3	0.57	0
28	SQD	A	413	-	47,49,54	0.99	2 (4%)	57,60,65	1.71	9 (15%)
31	DMS	d	415	-	3,3,3	2.68	1 (33%)	3,3,3	0.61	0
31	DMS	o	306	-	3,3,3	2.71	1 (33%)	3,3,3	0.61	0
31	DMS	b	637	-	3,3,3	2.78	1 (33%)	3,3,3	0.63	0
22	CLA	b	613	-	69,73,73	2.56	20 (28%)	82,113,113	2.24	29 (35%)
28	SQD	b	621	-	36,38,54	0.98	1 (2%)	45,48,65	1.46	8 (17%)
35	DGD	H	102	-	63,63,67	1.03	3 (4%)	77,77,81	1.17	7 (9%)
32	BCT	a	422	20	3,3,3	1.80	1 (33%)	2,3,3	1.11	0
31	DMS	B	642	-	3,3,3	2.72	1 (33%)	3,3,3	1.04	0
34	HTG	c	922	-	19,19,19	0.78	1 (5%)	23,24,24	1.53	2 (8%)
22	CLA	C	511	-	69,73,73	2.35	19 (27%)	82,113,113	2.06	25 (30%)
24	BCR	B	620	-	41,41,41	0.99	3 (7%)	56,56,56	1.51	11 (19%)
22	CLA	B	608	40	69,73,73	2.18	20 (28%)	82,113,113	2.25	33 (40%)
22	CLA	b	603	-	69,73,73	2.79	19 (27%)	82,113,113	2.29	30 (36%)
31	DMS	F	101	-	3,3,3	2.72	1 (33%)	3,3,3	0.62	0
34	HTG	v	203	-	16,16,19	0.97	1 (6%)	20,21,24	2.82	7 (35%)
31	DMS	O	309	-	3,3,3	2.59	1 (33%)	3,3,3	0.61	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	DMS	D	416	-	3,3,3	2.56	1 (33%)	3,3,3	0.65	0
31	DMS	B	628	-	3,3,3	2.87	1 (33%)	3,3,3	0.78	0
31	DMS	V	208	-	3,3,3	2.66	1 (33%)	3,3,3	0.41	0
22	CLA	b	616	-	69,73,73	2.37	20 (28%)	82,113,113	2.14	27 (32%)
31	DMS	A	419	-	3,3,3	2.73	1 (33%)	3,3,3	0.84	0
22	CLA	c	905	40	69,73,73	2.64	20 (28%)	82,113,113	2.26	28 (34%)
31	DMS	a	425	-	3,3,3	3.08	1 (33%)	3,3,3	0.89	0
31	DMS	v	201	-	3,3,3	2.65	1 (33%)	3,3,3	0.88	0
29	LMT	I	102	-	36,36,36	0.69	1 (2%)	47,47,47	1.39	4 (8%)
31	DMS	c	929	-	3,3,3	2.87	1 (33%)	3,3,3	0.85	0
24	BCR	b	618	-	20,20,41	0.95	1 (5%)	27,27,56	1.76	5 (18%)
31	DMS	l	104	-	3,3,3	2.83	1 (33%)	3,3,3	0.59	0
22	CLA	C	514	-	69,73,73	2.64	20 (28%)	82,113,113	2.27	25 (30%)
24	BCR	A	409	-	41,41,41	1.09	2 (4%)	56,56,56	1.26	5 (8%)
31	DMS	O	303	-	3,3,3	2.81	1 (33%)	3,3,3	0.79	0
31	DMS	O	305	-	3,3,3	2.97	1 (33%)	3,3,3	0.86	0
25	LMG	C	520	-	51,51,55	1.08	2 (3%)	59,59,63	1.24	6 (10%)
31	DMS	v	208	-	3,3,3	2.69	1 (33%)	3,3,3	0.54	0
22	CLA	c	903	-	69,73,73	2.02	18 (26%)	82,113,113	2.30	26 (31%)
22	CLA	D	404	-	69,73,73	2.41	18 (26%)	82,113,113	2.03	23 (28%)
31	DMS	A	420	-	3,3,3	2.81	1 (33%)	3,3,3	1.37	0
22	CLA	c	910	-	69,73,73	2.17	18 (26%)	82,113,113	2.29	31 (37%)
31	DMS	b	629	-	3,3,3	2.33	1 (33%)	3,3,3	1.12	0
31	DMS	B	640	-	3,3,3	2.69	1 (33%)	3,3,3	0.62	0
31	DMS	c	925	-	3,3,3	2.72	1 (33%)	3,3,3	1.13	0
24	BCR	y	101	-	41,41,41	0.91	0	56,56,56	1.63	13 (23%)
22	CLA	b	608	40	69,73,73	2.42	21 (30%)	82,113,113	2.22	25 (30%)
31	DMS	B	635	-	3,3,3	2.84	1 (33%)	3,3,3	0.71	0
31	DMS	C	524	-	3,3,3	2.54	1 (33%)	3,3,3	0.87	0
31	DMS	a	421	-	3,3,3	2.72	1 (33%)	3,3,3	0.62	0
22	CLA	b	604	-	69,73,73	2.60	20 (28%)	82,113,113	2.27	27 (32%)
22	CLA	D	403	-	69,73,73	2.04	19 (27%)	82,113,113	2.43	28 (34%)
31	DMS	L	102	-	3,3,3	2.81	1 (33%)	3,3,3	0.97	0
27	LHG	A	412	-	30,30,48	1.41	2 (6%)	33,35,54	1.48	4 (12%)
31	DMS	A	416	-	3,3,3	2.73	1 (33%)	3,3,3	1.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	B	613	-	69,73,73	2.63	22 (31%)	82,113,113	2.09	32 (39%)
31	DMS	C	527	-	3,3,3	2.72	1 (33%)	3,3,3	0.58	0
31	DMS	U	202	-	3,3,3	2.84	1 (33%)	3,3,3	1.31	0
22	CLA	b	617	-	64,68,73	2.88	21 (32%)	76,107,113	2.49	31 (40%)
22	CLA	B	611	40	69,73,73	2.90	20 (28%)	82,113,113	2.32	23 (28%)
25	LMG	B	621	-	40,40,55	1.26	3 (7%)	48,48,63	1.40	8 (16%)
22	CLA	B	610	-	69,73,73	2.38	21 (30%)	82,113,113	2.14	24 (29%)
34	HTG	V	203	-	14,14,19	0.65	0	18,19,24	2.97	7 (38%)
29	LMT	t	101	-	24,24,36	0.45	0	29,29,47	1.33	3 (10%)
34	HTG	b	627	-	19,19,19	0.97	2 (10%)	23,24,24	1.66	3 (13%)
25	LMG	c	920	-	51,51,55	0.99	2 (3%)	59,59,63	1.10	6 (10%)
22	CLA	c	912	3	69,73,73	2.87	18 (26%)	82,113,113	2.11	25 (30%)
22	CLA	B	603	-	69,73,73	2.57	23 (33%)	82,113,113	2.36	35 (42%)
31	DMS	c	940	-	3,3,3	2.79	1 (33%)	3,3,3	0.59	0
22	CLA	a	407	-	69,73,73	2.32	20 (28%)	82,113,113	2.11	29 (35%)
22	CLA	a	408	40	69,73,73	2.55	20 (28%)	82,113,113	2.43	31 (37%)
31	DMS	B	632	-	3,3,3	2.72	1 (33%)	3,3,3	0.61	0
31	DMS	b	631	-	3,3,3	2.74	1 (33%)	3,3,3	0.56	0
22	CLA	B	616	-	69,73,73	2.64	21 (30%)	82,113,113	2.20	26 (31%)
22	CLA	b	602	40	69,73,73	3.32	19 (27%)	82,113,113	2.39	23 (28%)
22	CLA	b	614	-	63,67,73	2.36	19 (30%)	74,105,113	2.39	25 (33%)
22	CLA	d	403	-	69,73,73	2.89	21 (30%)	82,113,113	2.12	26 (31%)
22	CLA	C	506	-	69,73,73	2.57	19 (27%)	82,113,113	2.15	24 (29%)
22	CLA	c	902	-	69,73,73	2.45	19 (27%)	82,113,113	2.36	24 (29%)
35	DGD	D	407	-	50,50,67	1.18	3 (6%)	58,58,81	1.32	6 (10%)
31	DMS	c	939	-	3,3,3	2.83	1 (33%)	3,3,3	0.67	0
27	LHG	a	416	-	48,48,48	1.13	2 (4%)	51,54,54	1.20	4 (7%)
31	DMS	o	305	-	3,3,3	2.66	1 (33%)	3,3,3	0.68	0
22	CLA	C	502	-	69,73,73	2.11	21 (30%)	82,113,113	2.29	26 (31%)
31	DMS	C	530	-	3,3,3	2.74	1 (33%)	3,3,3	0.86	0
24	BCR	Y	101	-	40,40,41	0.91	1 (2%)	52,54,56	1.73	15 (28%)
22	CLA	B	614	-	65,69,73	2.30	17 (26%)	77,108,113	2.09	26 (33%)
34	HTG	l	106	-	19,19,19	0.93	2 (10%)	23,24,24	1.85	3 (13%)
31	DMS	O	312	-	3,3,3	2.69	1 (33%)	3,3,3	0.98	0
26	PL9	d	405	-	55,55,55	1.05	4 (7%)	68,69,69	1.45	8 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	A	406	40	59,63,73	2.29	21 (35%)	70,101,113	2.58	32 (45%)
31	DMS	B	629	-	3,3,3	2.60	1 (33%)	3,3,3	1.21	0
31	DMS	c	933	-	3,3,3	2.90	1 (33%)	3,3,3	0.94	0
22	CLA	c	913	-	69,73,73	2.49	24 (34%)	82,113,113	2.17	27 (32%)
28	SQD	a	418	-	49,51,54	1.10	2 (4%)	59,62,65	1.47	8 (13%)
36	HEM	e	101	5,6	50,50,50	2.05	9 (18%)	67,82,82	1.34	6 (8%)
31	DMS	c	926	-	3,3,3	2.66	1 (33%)	3,3,3	0.80	0
31	DMS	B	641	-	3,3,3	2.82	1 (33%)	3,3,3	0.86	0
39	HEC	v	202	15	46,50,50	2.11	7 (15%)	58,82,82	1.37	8 (13%)
22	CLA	a	409	40	65,69,73	2.15	20 (30%)	77,108,113	2.59	33 (42%)
29	LMT	f	102	-	25,25,36	1.02	1 (4%)	30,30,47	1.25	5 (16%)
31	DMS	a	424	-	3,3,3	2.78	1 (33%)	3,3,3	1.05	0
31	DMS	c	928	-	3,3,3	2.76	1 (33%)	3,3,3	0.79	0
31	DMS	v	206	-	3,3,3	2.75	1 (33%)	3,3,3	0.75	0
34	HTG	b	624	-	19,19,19	1.00	1 (5%)	23,24,24	1.99	6 (26%)
24	BCR	b	620	-	41,41,41	0.86	1 (2%)	56,56,56	1.37	8 (14%)
31	DMS	H	103	-	3,3,3	2.98	1 (33%)	3,3,3	1.22	0
31	DMS	a	402	-	3,3,3	2.44	1 (33%)	3,3,3	0.74	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
25	LMG	C	520	-	-	19/46/66/70	0/1/1/1
25	LMG	j	101	38	-	13/42/62/70	0/1/1/1
22	CLA	c	903	-	1/1/15/20	9/39/115/115	-
22	CLA	D	404	-	1/1/15/20	9/39/115/115	-
34	HTG	b	626	-	-	6/10/30/30	0/1/1/1
22	CLA	b	612	-	-	9/39/115/115	-
22	CLA	C	512	3	-	1/39/115/115	-
22	CLA	a	412	-	-	13/39/115/115	-
24	BCR	C	515	-	-	3/29/63/63	0/2/2/2
22	CLA	C	503	-	1/1/15/20	8/39/115/115	-
27	LHG	D	411	-	-	11/49/49/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	RRX	h	101	-	-	8/29/65/65	0/2/2/2
22	CLA	c	914	-	-	15/39/115/115	-
24	BCR	a	413	-	-	1/29/63/63	0/2/2/2
22	CLA	B	617	-	1/1/13/20	4/27/103/115	-
22	CLA	c	910	-	1/1/15/20	16/39/115/115	-
34	HTG	B	626	-	-	2/10/30/30	0/1/1/1
34	HTG	C	521	-	-	4/10/30/30	0/1/1/1
27	LHG	d	407	-	-	19/53/53/53	-
34	HTG	B	627	-	-	7/10/30/30	0/1/1/1
34	HTG	D	414	-	-	3/10/30/30	0/1/1/1
29	LMT	a	419	-	-	14/21/61/61	0/2/2/2
23	PHO	a	411	-	-	6/37/103/103	0/5/6/6
29	LMT	c	921	-	-	11/21/61/61	0/2/2/2
35	DGD	c	918	-	-	22/51/91/95	0/2/2/2
27	LHG	d	401	-	-	15/34/34/53	-
24	BCR	y	101	-	-	4/29/63/63	0/2/2/2
22	CLA	b	608	40	1/1/15/20	15/39/115/115	-
22	CLA	C	505	40	-	4/39/115/115	-
22	CLA	D	401	40	-	4/39/115/115	-
37	RRX	H	101	-	-	1/29/65/65	0/2/2/2
26	PL9	D	406	-	-	5/53/73/73	0/1/1/1
22	CLA	B	605	-	1/1/15/20	8/39/115/115	-
22	CLA	C	510	-	1/1/15/20	11/39/115/115	-
24	BCR	d	404	-	-	4/29/63/63	0/2/2/2
25	LMG	D	412	-	-	15/41/61/70	0/1/1/1
27	LHG	L	101	-	-	18/44/44/53	-
28	SQD	C	501	-	-	26/49/69/69	0/1/1/1
22	CLA	b	604	-	1/1/15/20	10/39/115/115	-
28	SQD	l	101	-	-	32/49/69/69	0/1/1/1
35	DGD	C	518	-	-	22/51/91/95	0/2/2/2
35	DGD	C	519	-	-	28/51/91/95	0/2/2/2
23	PHO	D	402	-	-	6/37/103/103	0/5/6/6
22	CLA	D	403	-	1/1/15/20	0/39/115/115	-
35	DGD	C	517	-	-	17/51/91/95	0/2/2/2
22	CLA	C	504	-	-	2/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	SQD	D	408	-	-	2/12/32/69	0/1/1/1
39	HEC	V	202	15	-	6/14/54/54	-
24	BCR	B	619	-	-	0/24/41/63	0/1/1/2
22	CLA	b	609	-	-	7/39/115/115	-
35	DGD	c	917	-	-	21/51/91/95	0/2/2/2
22	CLA	b	615	-	1/1/12/20	4/24/100/115	-
27	LHG	A	412	-	-	14/33/33/53	-
26	PL9	A	411	-	-	12/53/73/73	0/1/1/1
28	SQD	a	414	-	-	27/49/69/69	0/1/1/1
25	LMG	b	622	-	-	20/38/58/70	0/1/1/1
22	CLA	B	613	-	1/1/15/20	4/39/115/115	-
23	PHO	a	410	-	-	1/37/103/103	0/5/6/6
34	HTG	b	632	-	-	5/10/30/30	0/1/1/1
34	HTG	b	623	-	-	6/10/30/30	0/1/1/1
24	BCR	K	101	-	-	3/29/63/63	0/2/2/2
22	CLA	b	606	-	1/1/15/20	4/39/115/115	-
22	CLA	b	617	-	1/1/14/20	8/33/109/115	-
22	CLA	c	908	40	1/1/15/20	12/39/115/115	-
22	CLA	B	611	40	1/1/15/20	9/39/115/115	-
24	BCR	c	916	-	-	4/29/63/63	0/2/2/2
24	BCR	c	915	-	-	1/29/63/63	0/2/2/2
22	CLA	B	602	40	1/1/15/20	23/39/115/115	-
22	CLA	B	606	-	-	10/39/115/115	-
25	LMG	i	101	-	-	26/46/66/70	0/1/1/1
29	LMT	A	414	-	-	14/21/61/61	0/2/2/2
22	CLA	C	509	-	1/1/15/20	9/39/115/115	-
22	CLA	c	906	-	1/1/15/20	8/39/115/115	-
29	LMT	B	622	-	-	8/15/35/61	0/1/1/2
25	LMG	B	621	-	-	23/35/55/70	0/1/1/1
22	CLA	B	610	-	1/1/15/20	2/39/115/115	-
24	BCR	B	618	-	-	0/11/28/63	0/1/1/2
25	LMG	J	101	38	-	9/40/60/70	0/1/1/1
22	CLA	C	508	40	1/1/15/20	10/39/115/115	-
22	CLA	B	609	-	-	2/39/115/115	-
34	HTG	V	203	-	-	0/5/25/30	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	LMT	t	101	-	-	10/15/35/61	0/1/1/2
22	CLA	B	607	-	1/1/15/20	12/39/115/115	-
29	LMT	T	102	-	-	10/15/35/61	0/1/1/2
27	LHG	C	522	-	-	14/31/31/53	-
24	BCR	b	619	-	-	4/26/43/63	0/1/1/2
29	LMT	c	931	-	-	11/15/35/61	0/1/1/2
34	HTG	b	627	-	-	3/10/30/30	0/1/1/1
35	DGD	d	406	-	-	31/44/44/95	-
25	LMG	c	920	-	-	21/46/66/70	0/1/1/1
22	CLA	c	912	3	-	4/39/115/115	-
22	CLA	c	904	-	-	6/39/115/115	-
24	BCR	D	405	-	-	4/29/63/63	0/2/2/2
34	HTG	C	532	-	-	6/10/30/30	0/1/1/1
22	CLA	B	603	-	1/1/15/20	4/39/115/115	-
27	LHG	D	410	-	-	10/53/53/53	-
22	CLA	b	605	-	1/1/15/20	11/39/115/115	-
22	CLA	B	604	-	1/1/15/20	6/39/115/115	-
25	LMG	C	531	-	-	13/35/55/70	0/1/1/1
25	LMG	A	410	-	-	27/46/66/70	0/1/1/1
22	CLA	b	611	40	1/1/15/20	6/39/115/115	-
35	DGD	h	102	-	-	18/51/91/95	0/2/2/2
22	CLA	a	407	-	1/1/15/20	6/39/115/115	-
28	SQD	A	413	-	-	26/44/64/69	0/1/1/1
29	LMT	Z	101	-	-	8/21/61/61	0/2/2/2
22	CLA	a	408	40	1/1/15/20	4/39/115/115	-
28	SQD	f	101	-	-	4/12/12/69	-
25	LMG	d	409	-	-	28/42/62/70	0/1/1/1
22	CLA	B	616	-	1/1/15/20	12/39/115/115	-
23	PHO	A	407	-	-	2/37/103/103	0/5/6/6
22	CLA	c	911	-	1/1/15/20	7/39/115/115	-
22	CLA	b	602	40	1/1/15/20	22/39/115/115	-
34	HTG	D	415	-	-	8/10/30/30	0/1/1/1
22	CLA	b	614	-	1/1/13/20	5/32/108/115	-
22	CLA	b	613	-	1/1/15/20	4/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	d	403	-	-	10/39/115/115	-
28	SQD	b	621	-	-	16/32/52/69	0/1/1/1
35	DGD	H	102	-	-	17/51/91/95	0/2/2/2
22	CLA	C	506	-	1/1/15/20	5/39/115/115	-
22	CLA	C	513	-	1/1/13/20	9/29/105/115	-
22	CLA	A	408	-	1/1/15/20	13/39/115/115	-
22	CLA	c	902	-	1/1/15/20	4/39/115/115	-
35	DGD	D	407	-	-	30/44/64/95	0/1/1/2
24	BCR	C	516	-	-	0/29/63/63	0/2/2/2
34	HTG	C	523	-	-	1/6/6/30	-
35	DGD	c	919	-	-	18/51/91/95	0/2/2/2
27	LHG	a	416	-	-	27/53/53/53	-
27	LHG	d	408	-	-	17/50/50/53	-
22	CLA	B	612	-	1/1/15/20	10/39/115/115	-
22	CLA	C	502	-	1/1/15/20	6/39/115/115	-
22	CLA	b	607	-	1/1/15/20	5/39/115/115	-
24	BCR	Y	101	-	-	6/29/60/63	0/2/2/2
22	CLA	B	614	-	1/1/14/20	6/35/111/115	-
34	HTG	l	106	-	-	6/10/30/30	0/1/1/1
22	CLA	b	610	-	-	3/39/115/115	-
26	PL9	d	405	-	-	6/53/73/73	0/1/1/1
34	HTG	c	922	-	-	6/10/30/30	0/1/1/1
22	CLA	A	406	40	-	3/27/103/115	-
22	CLA	C	507	-	1/1/15/20	10/39/115/115	-
22	CLA	C	511	-	1/1/15/20	10/39/115/115	-
22	CLA	c	907	-	1/1/15/20	10/39/115/115	-
24	BCR	B	620	-	-	0/29/63/63	0/2/2/2
27	LHG	a	423	-	-	20/49/49/53	-
22	CLA	B	608	40	1/1/15/20	5/39/115/115	-
22	CLA	b	603	-	1/1/15/20	3/39/115/115	-
34	HTG	v	203	-	-	4/7/27/30	0/1/1/1
26	PL9	a	415	-	-	17/53/73/73	0/1/1/1
29	LMT	E	101	-	-	9/15/35/61	0/1/1/2
22	CLA	c	913	-	1/1/15/20	20/39/115/115	-
22	CLA	d	402	-	1/1/15/20	9/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	SQD	a	418	-	-	22/46/66/69	0/1/1/1
36	HEM	e	101	5,6	-	7/14/54/54	-
22	CLA	b	616	-	1/1/15/20	9/39/115/115	-
27	LHG	l	102	-	-	26/53/53/53	-
36	HEM	E	102	5,6	-	1/14/54/54	-
22	CLA	c	905	40	-	14/39/115/115	-
39	HEC	v	202	15	-	6/14/54/54	-
22	CLA	a	409	40	-	8/35/111/115	-
29	LMT	f	102	-	-	10/17/37/61	0/1/1/2
22	CLA	B	615	-	1/1/12/20	9/25/101/115	-
22	CLA	c	909	-	-	10/39/115/115	-
27	LHG	D	409	-	-	14/53/53/53	-
29	LMT	I	102	-	-	11/21/61/61	0/2/2/2
25	LMG	c	930	-	-	12/44/64/70	0/1/1/1
22	CLA	A	405	-	1/1/15/20	6/39/115/115	-
24	BCR	b	618	-	-	7/13/30/63	0/1/1/2
34	HTG	b	624	-	-	4/10/30/30	0/1/1/1
22	CLA	C	514	-	-	18/39/115/115	-
24	BCR	A	409	-	-	2/29/63/63	0/2/2/2
24	BCR	b	620	-	-	0/29/63/63	0/2/2/2
34	HTG	B	623	-	-	3/10/30/30	0/1/1/1
24	BCR	k	101	-	-	4/29/63/63	0/2/2/2

The worst 5 of 1770 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	602	CLA	MG-NA	19.40	2.52	2.06
22	B	606	CLA	MG-NA	15.87	2.44	2.06
22	b	617	CLA	MG-NA	15.18	2.42	2.06
22	c	912	CLA	MG-NA	14.71	2.41	2.06
22	B	602	CLA	MG-NA	14.39	2.40	2.06

The worst 5 of 2581 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	602	CLA	C4A-NA-C1A	11.60	111.97	106.68
22	C	506	CLA	C4A-NA-C1A	11.09	111.74	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	602	CLA	C4A-NA-C1A	10.85	111.63	106.68
23	a	410	PHO	C3B-C4B-NB	10.46	114.28	107.46
22	c	912	CLA	C4A-NA-C1A	10.25	111.36	106.68

5 of 51 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	A	405	CLA	ND
22	A	408	CLA	ND
22	B	602	CLA	ND
22	B	603	CLA	ND
22	B	604	CLA	ND

5 of 1705 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	B	602	CLA	CAD-CBD-CGD-O2D
22	B	602	CLA	C11-C10-C8-C9
22	B	606	CLA	C4B-C3B-CAB-CBB
22	B	610	CLA	C4B-C3B-CAB-CBB
22	B	615	CLA	C2-C1-O2A-CGA

There are no ring outliers.

211 monomers are involved in 519 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	b	612	CLA	2	0
22	a	412	CLA	2	0
37	h	101	RRX	8	0
22	c	914	CLA	2	0
27	d	407	LHG	1	0
31	V	201	DMS	1	0
29	a	419	LMT	7	0
31	b	636	DMS	1	0
31	O	306	DMS	2	0
35	c	918	DGD	3	0
22	C	510	CLA	2	0
24	d	404	BCR	2	0
25	D	412	LMG	5	0
27	L	101	LHG	7	0
28	l	101	SQD	1	0
23	D	402	PHO	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	b	609	CLA	5	0
35	c	917	DGD	3	0
22	b	615	CLA	5	0
28	a	414	SQD	6	0
22	b	606	CLA	5	0
24	c	916	BCR	6	0
29	B	622	LMT	3	0
25	J	101	LMG	1	0
31	o	303	DMS	2	0
31	c	924	DMS	7	0
31	o	308	DMS	4	0
25	C	531	LMG	2	0
31	u	205	DMS	5	0
29	Z	101	LMT	1	0
25	d	409	LMG	4	0
31	B	631	DMS	4	0
34	D	415	HTG	9	0
31	V	212	DMS	11	0
27	d	408	LHG	5	0
22	B	612	CLA	1	0
22	b	607	CLA	1	0
31	b	630	DMS	2	0
22	C	507	CLA	5	0
22	d	402	CLA	2	0
27	l	102	LHG	3	0
31	v	210	DMS	2	0
36	E	102	HEM	1	0
22	A	405	CLA	4	0
31	C	536	DMS	1	0
25	j	101	LMG	2	0
31	o	304	DMS	4	0
27	D	411	LHG	8	0
31	c	935	DMS	2	0
24	a	413	BCR	1	0
34	C	521	HTG	1	0
34	D	414	HTG	2	0
22	C	505	CLA	4	0
22	D	401	CLA	4	0
37	H	101	RRX	4	0
26	D	406	PL9	5	0
31	O	304	DMS	6	0
31	u	202	DMS	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	C	519	DGD	2	0
26	A	411	PL9	10	0
31	b	633	DMS	1	0
31	V	205	DMS	2	0
31	B	630	DMS	1	0
31	B	633	DMS	1	0
25	i	101	LMG	3	0
29	A	414	LMT	6	0
22	c	906	CLA	2	0
31	C	540	DMS	1	0
22	B	607	CLA	5	0
27	C	522	LHG	1	0
31	B	638	DMS	5	0
29	c	931	LMT	1	0
22	c	904	CLA	8	0
22	b	605	CLA	2	0
31	O	310	DMS	3	0
31	d	411	DMS	3	0
25	A	410	LMG	2	0
22	b	611	CLA	4	0
35	h	102	DGD	2	0
31	V	207	DMS	3	0
28	f	101	SQD	1	0
22	c	911	CLA	2	0
22	C	513	CLA	5	0
22	A	408	CLA	3	0
24	C	516	BCR	1	0
31	o	307	DMS	1	0
31	c	934	DMS	2	0
35	c	919	DGD	4	0
22	b	610	CLA	4	0
27	a	423	LHG	6	0
31	O	311	DMS	3	0
26	a	415	PL9	10	0
29	E	101	LMT	1	0
32	A	421[B]	BCT	1	0
31	c	927	DMS	1	0
31	f	103	DMS	4	0
31	v	205	DMS	2	0
22	c	909	CLA	2	0
27	D	409	LHG	7	0
25	c	930	LMG	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	u	203	DMS	2	0
34	B	623	HTG	3	0
24	k	101	BCR	2	0
31	c	937	DMS	1	0
34	b	626	HTG	2	0
24	C	515	BCR	4	0
22	C	503	CLA	5	0
23	a	411	PHO	8	0
31	B	636	DMS	1	0
31	c	942	DMS	1	0
22	B	605	CLA	1	0
28	C	501	SQD	6	0
35	C	518	DGD	1	0
22	C	504	CLA	2	0
25	b	622	LMG	1	0
23	a	410	PHO	2	0
34	b	632	HTG	2	0
34	b	623	HTG	3	0
31	i	106	DMS	1	0
22	c	908	CLA	2	0
31	U	203	DMS	1	0
24	c	915	BCR	2	0
22	B	606	CLA	7	0
22	C	509	CLA	3	0
24	B	618	BCR	3	0
22	C	508	CLA	2	0
31	a	401	DMS	1	0
31	V	206	DMS	3	0
31	b	638	DMS	9	0
31	o	302	DMS	1	0
29	T	102	LMT	1	0
24	b	619	BCR	1	0
24	D	405	BCR	1	0
34	C	532	HTG	1	0
27	D	410	LHG	3	0
22	B	604	CLA	1	0
28	A	413	SQD	2	0
31	d	415	DMS	5	0
28	b	621	SQD	2	0
35	H	102	DGD	2	0
31	B	642	DMS	1	0
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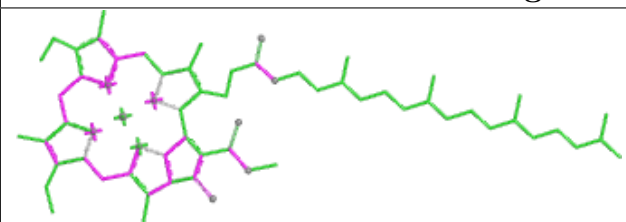
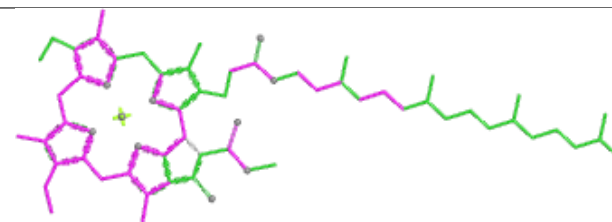
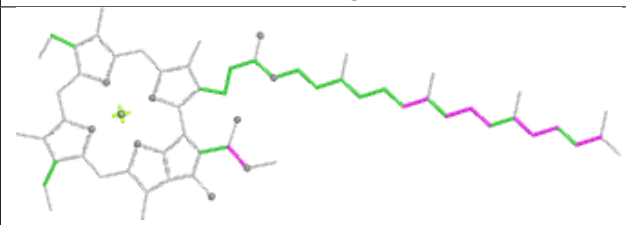
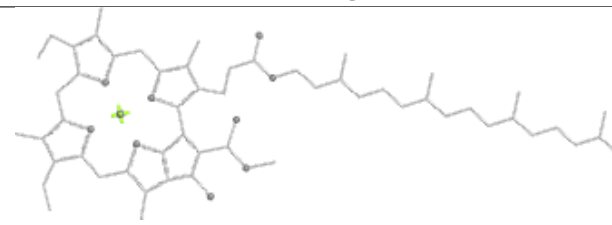
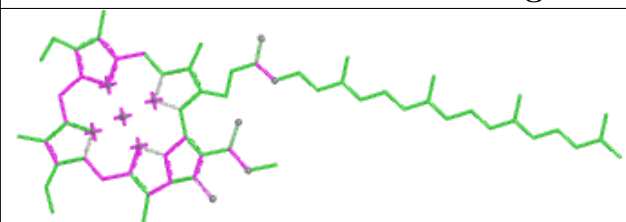
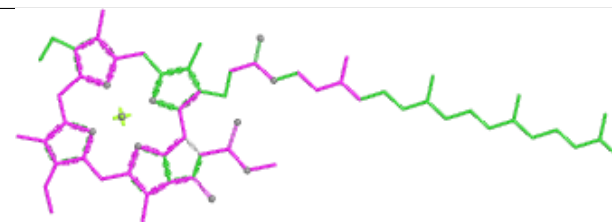
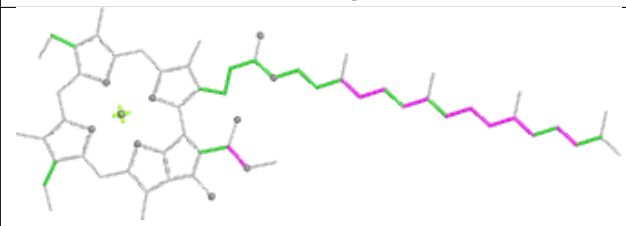
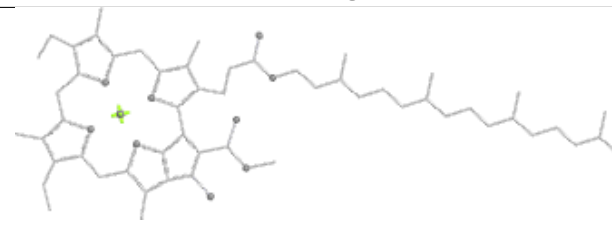
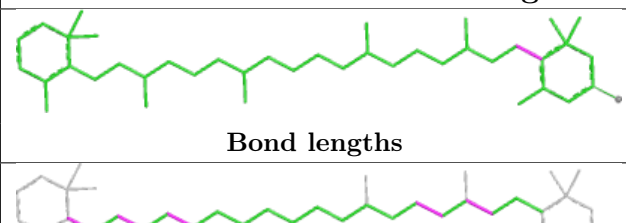
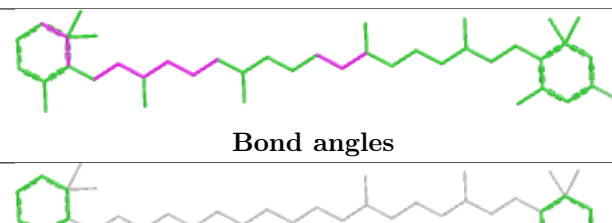
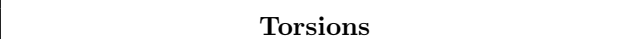
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22	B	608	CLA	6	0
22	b	603	CLA	2	0
31	D	416	DMS	3	0
31	B	628	DMS	3	0
22	b	616	CLA	2	0
31	A	419	DMS	2	0
22	c	905	CLA	2	0
31	a	425	DMS	7	0
31	v	201	DMS	1	0
31	c	929	DMS	2	0
24	b	618	BCR	7	0
31	l	104	DMS	1	0
22	C	514	CLA	5	0
24	A	409	BCR	1	0
31	O	303	DMS	4	0
25	C	520	LMG	1	0
22	c	903	CLA	3	0
31	A	420	DMS	2	0
22	c	910	CLA	3	0
31	b	629	DMS	1	0
31	B	640	DMS	1	0
31	c	925	DMS	2	0
24	y	101	BCR	3	0
22	b	608	CLA	7	0
31	B	635	DMS	1	0
22	b	604	CLA	1	0
22	D	403	CLA	1	0
27	A	412	LHG	1	0
22	B	613	CLA	1	0
31	C	527	DMS	2	0
22	b	617	CLA	2	0
22	B	611	CLA	6	0
25	B	621	LMG	3	0
22	B	610	CLA	1	0
29	t	101	LMT	2	0
34	b	627	HTG	1	0
25	c	920	LMG	1	0
22	c	912	CLA	4	0
22	B	603	CLA	1	0
31	c	940	DMS	2	0
22	a	407	CLA	2	0

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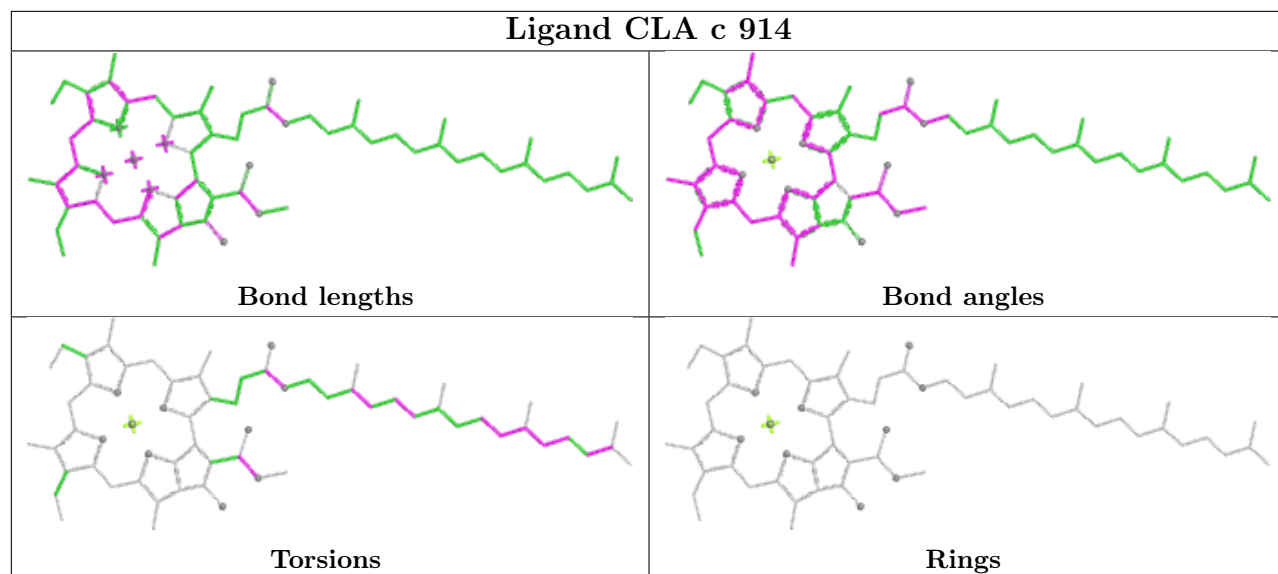
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
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31	B	632	DMS	1	0
22	b	602	CLA	5	0
22	b	614	CLA	4	0
22	d	403	CLA	1	0
22	C	506	CLA	1	0
22	c	902	CLA	4	0
31	c	939	DMS	2	0
27	a	416	LHG	1	0
31	o	305	DMS	3	0
31	C	530	DMS	2	0
24	Y	101	BCR	2	0
22	B	614	CLA	2	0
34	l	106	HTG	3	0
31	O	312	DMS	4	0
26	d	405	PL9	5	0
22	A	406	CLA	3	0
31	B	629	DMS	1	0
31	c	933	DMS	2	0
22	c	913	CLA	3	0
36	e	101	HEM	6	0
31	B	641	DMS	1	0
39	v	202	HEC	1	0
22	a	409	CLA	3	0
31	v	206	DMS	3	0
24	b	620	BCR	3	0
31	H	103	DMS	1	0

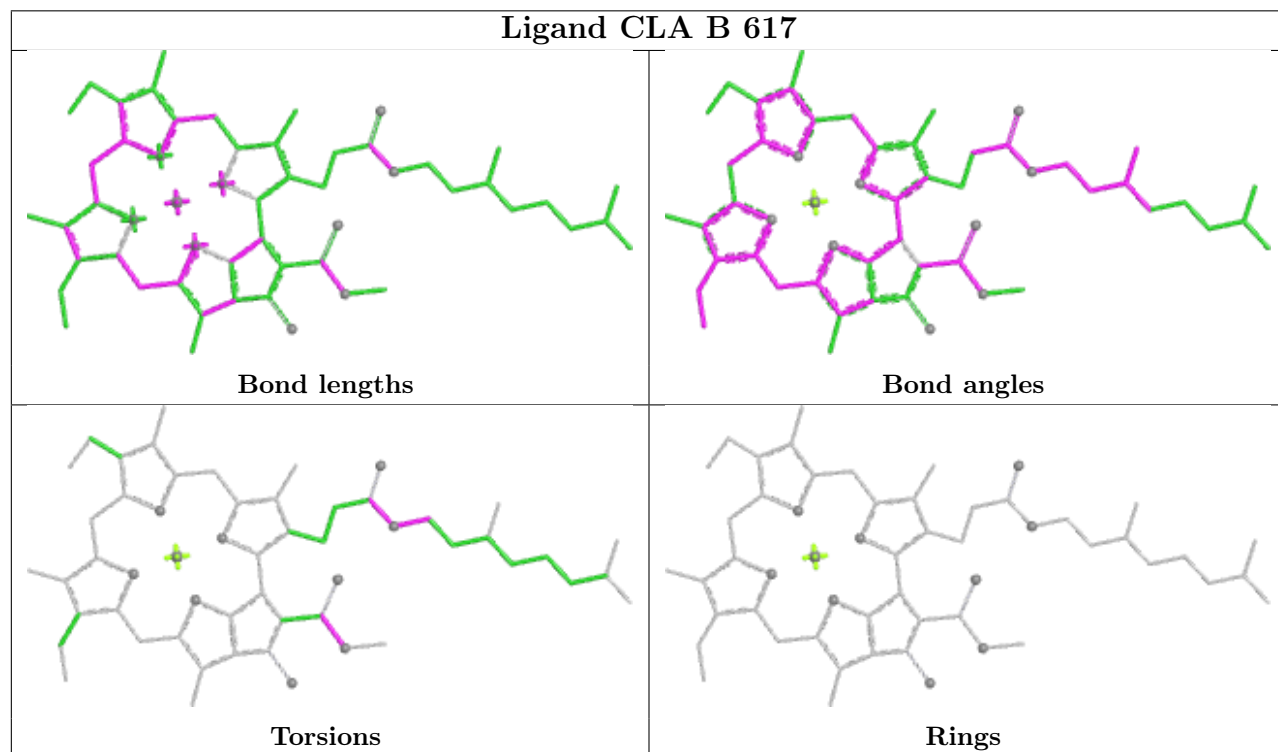
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

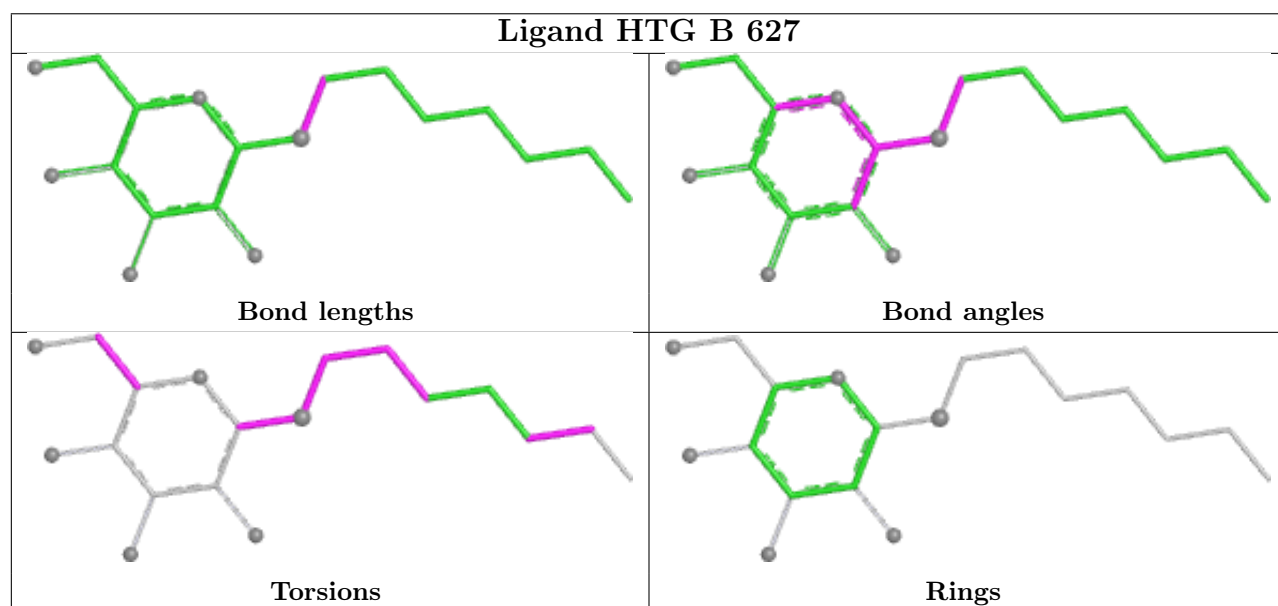
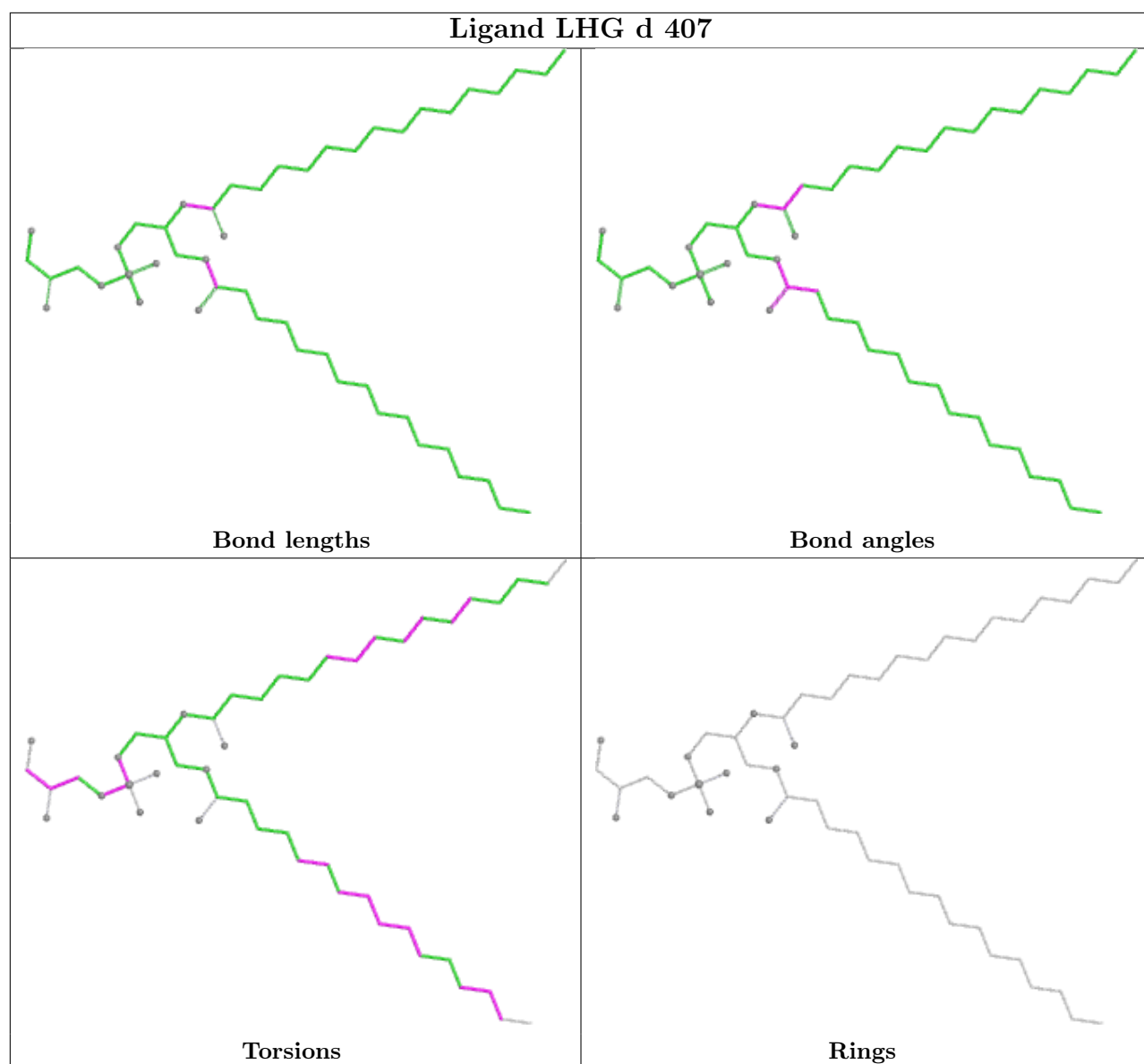
Ligand CLA b 612	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand CLA a 412	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand RRX h 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

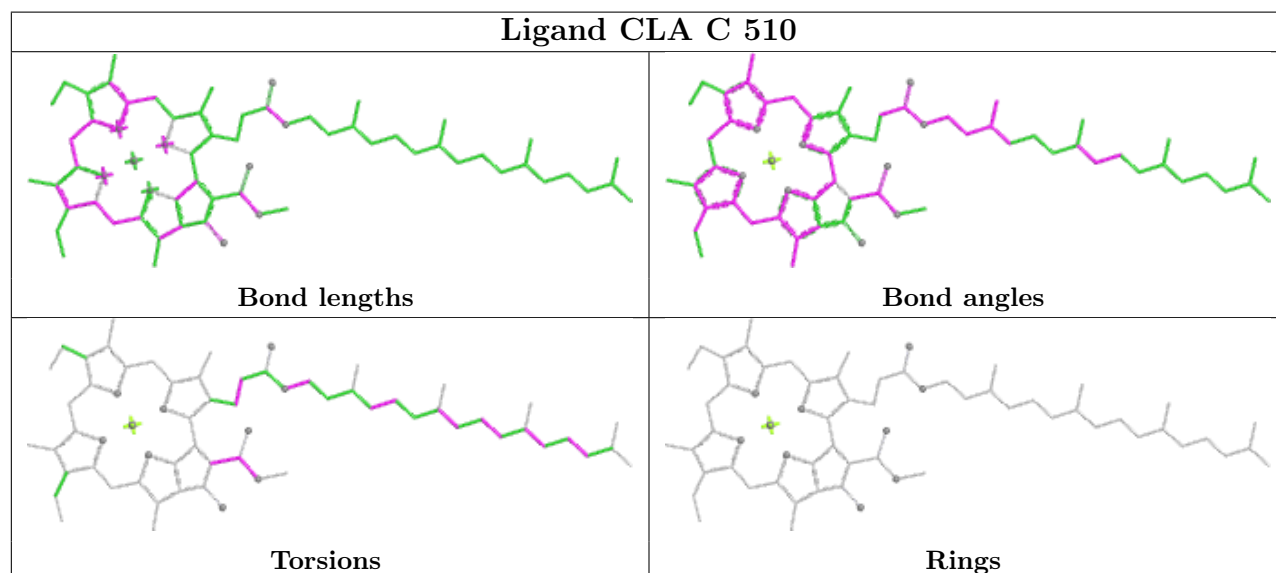
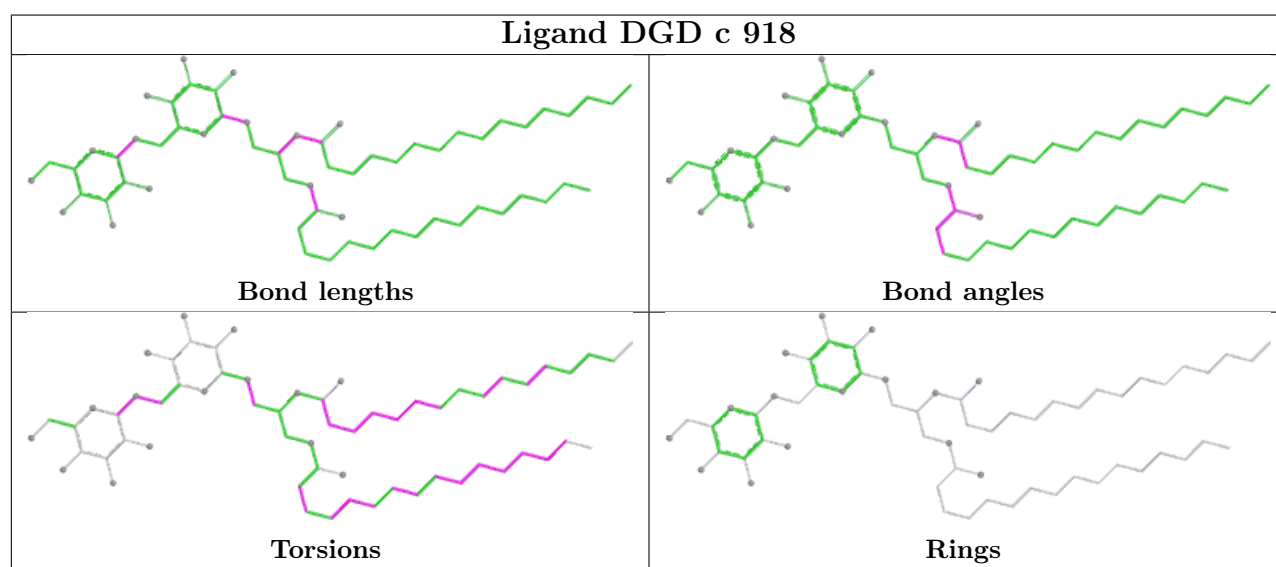
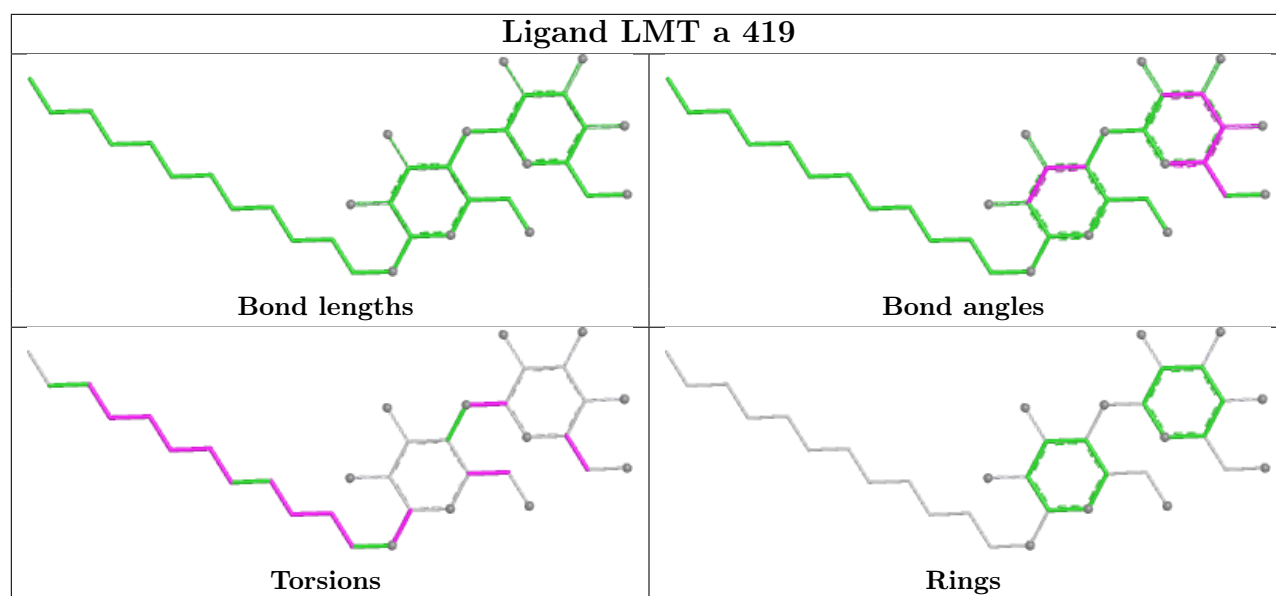
Ligand CLA c 914

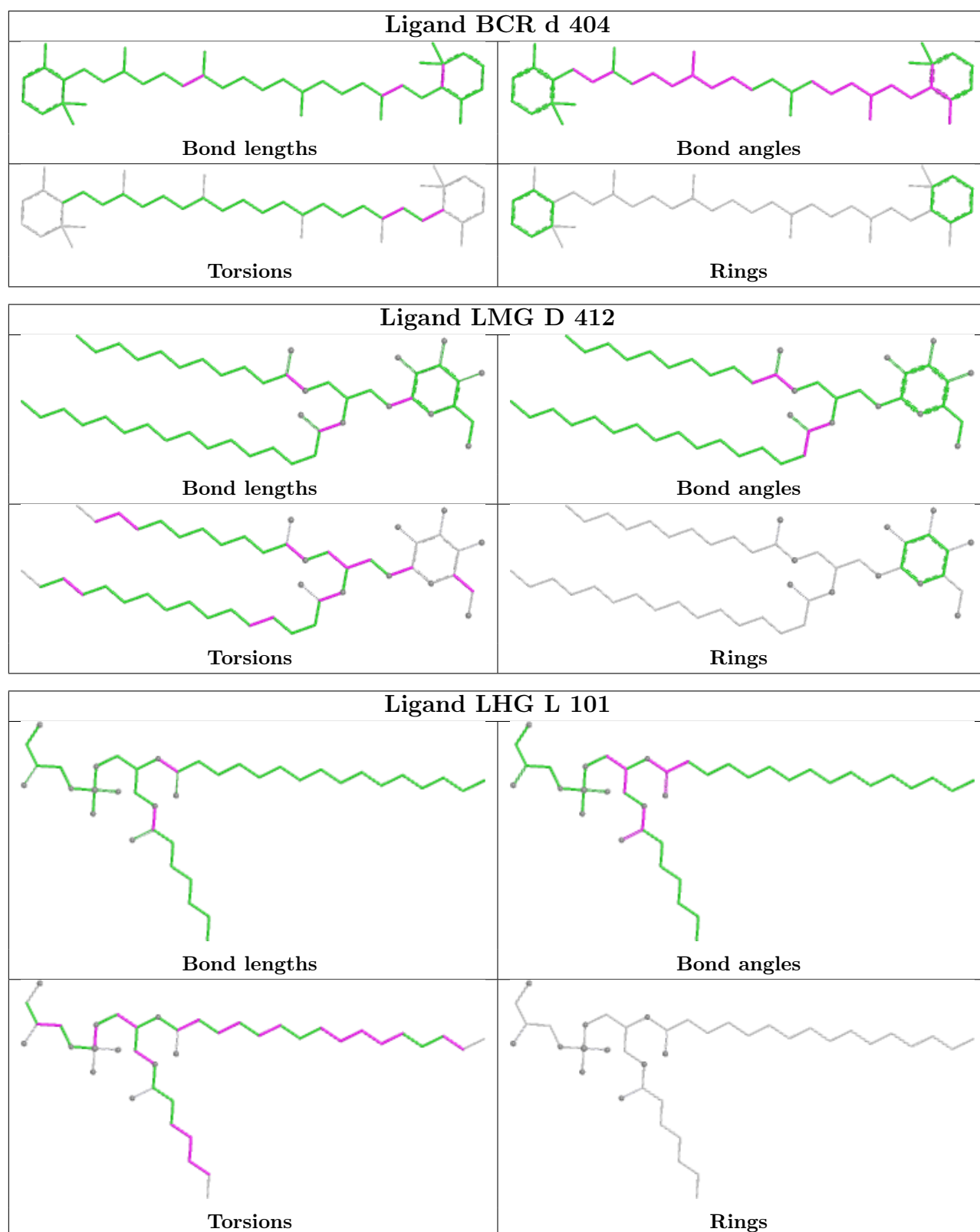


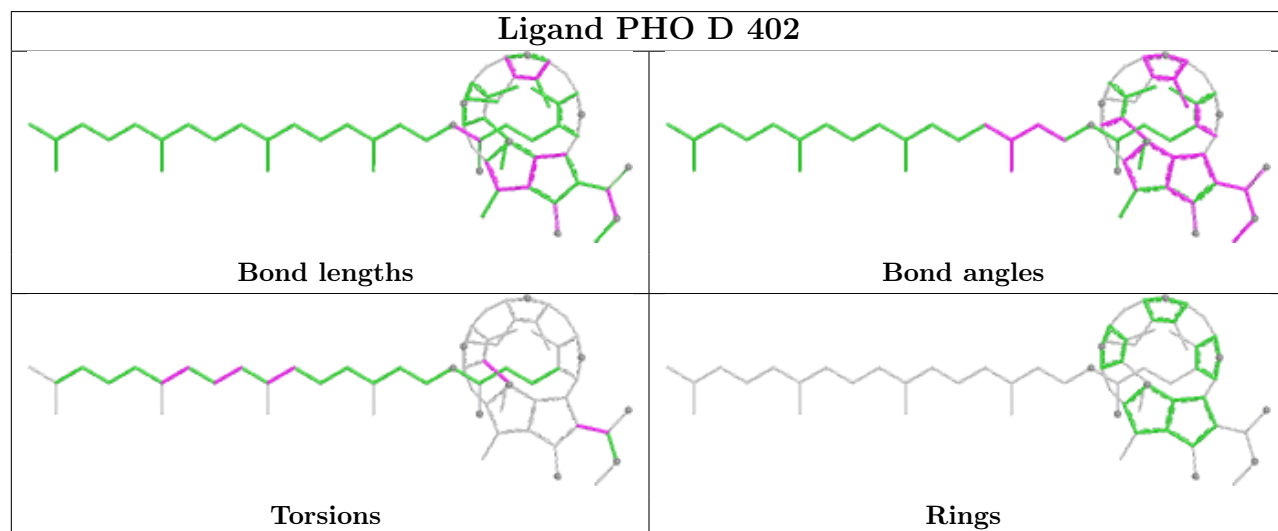
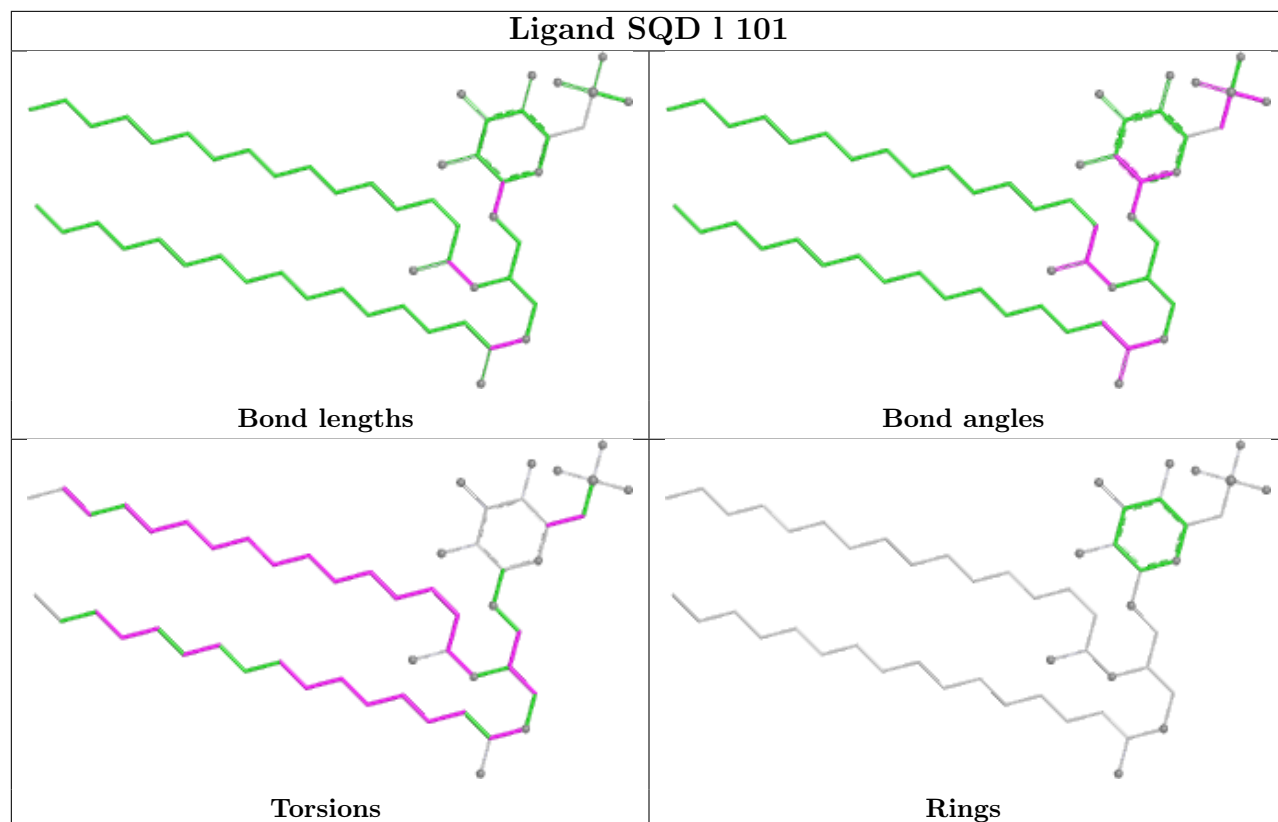
Ligand CLA B 617

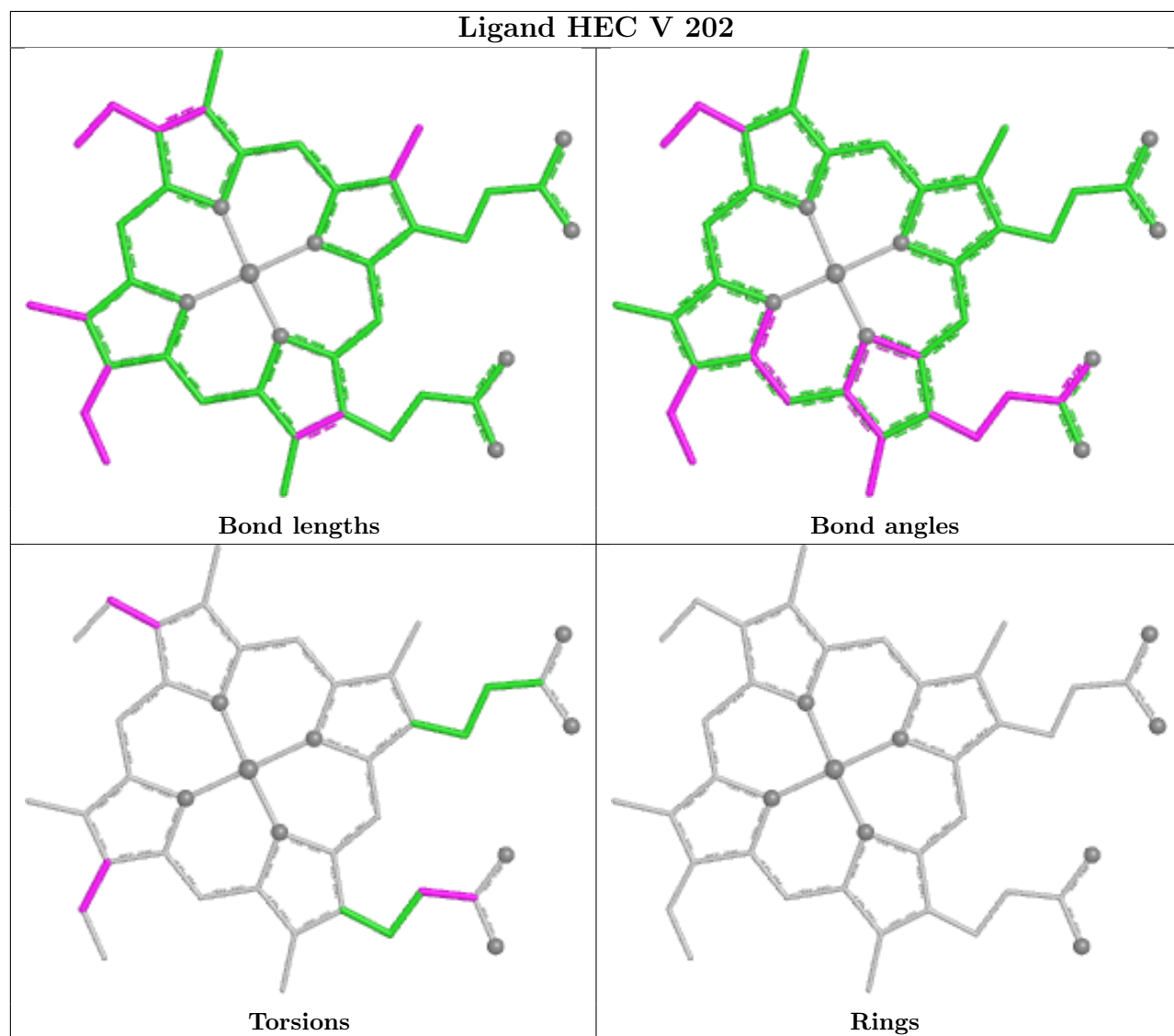
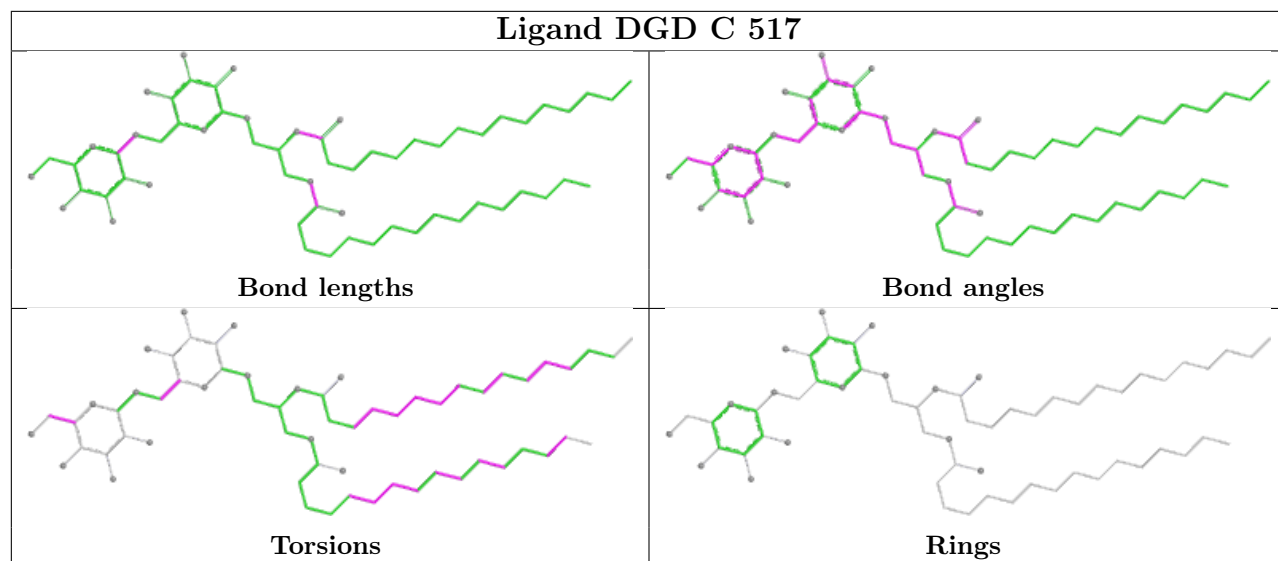


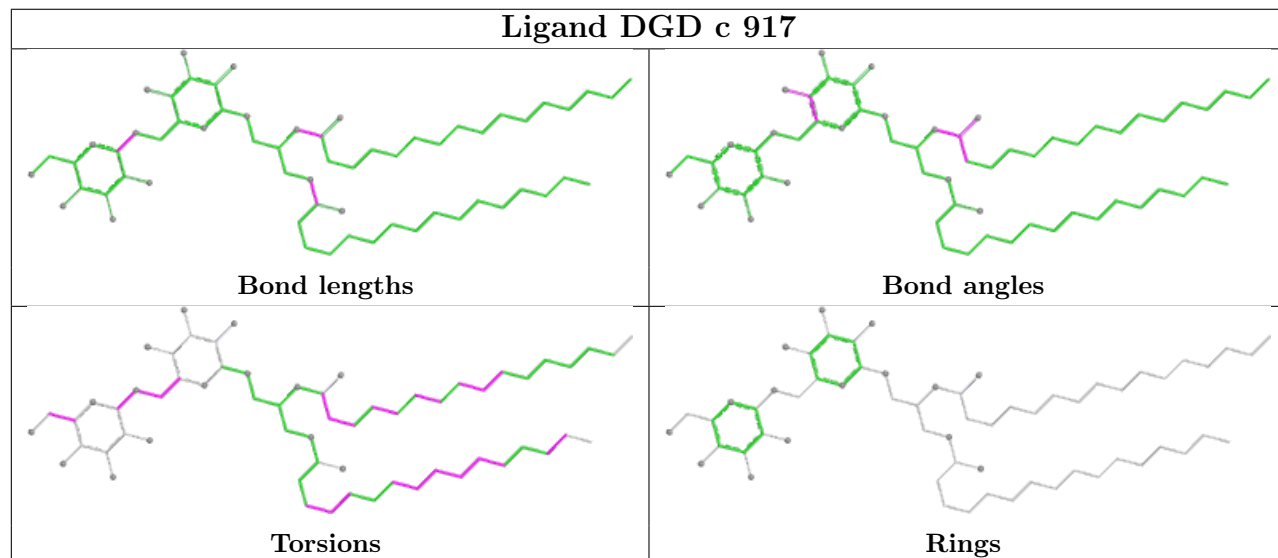
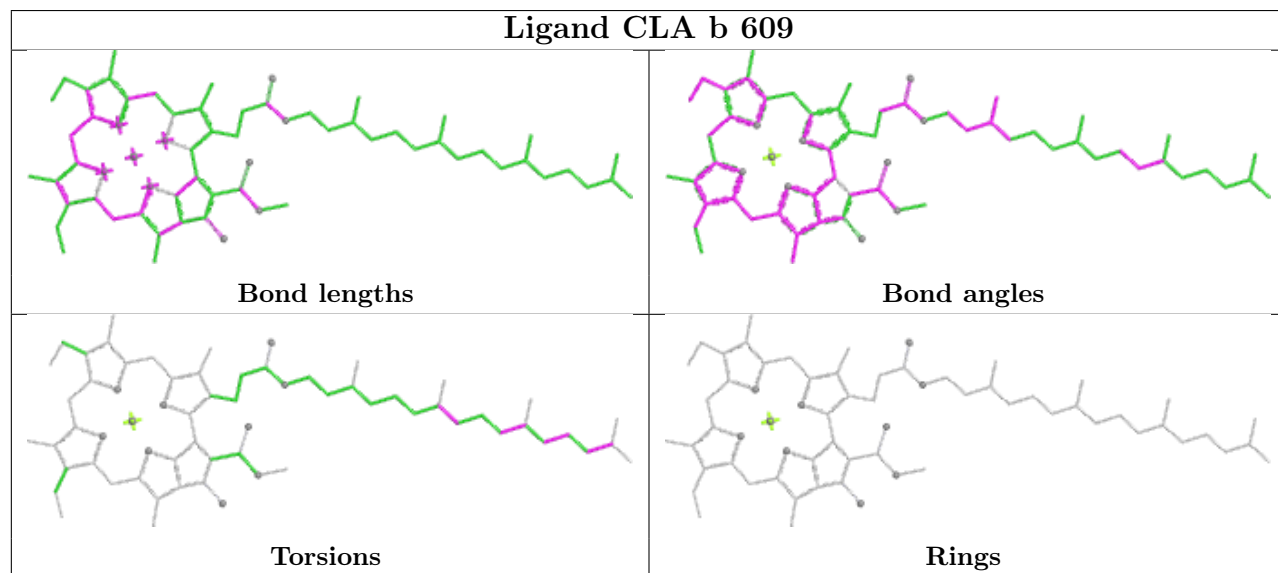
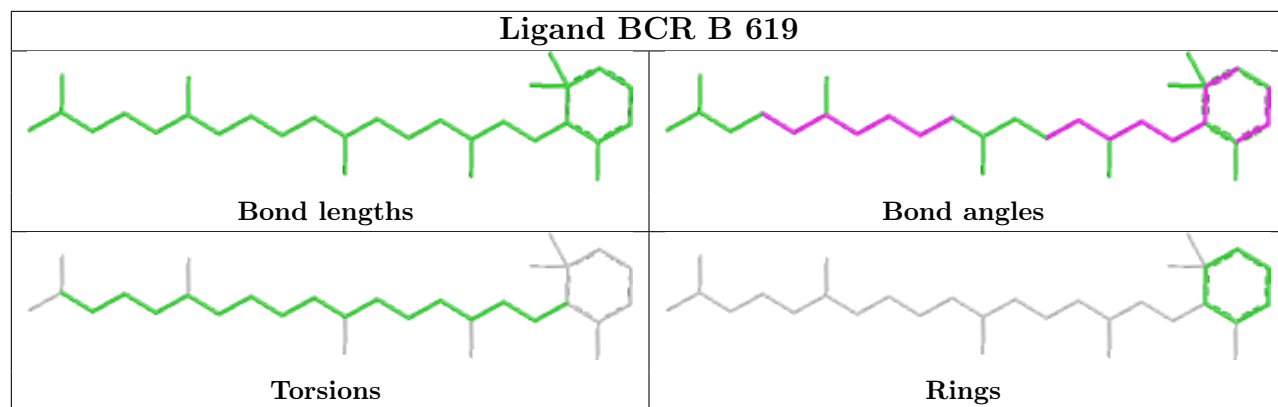




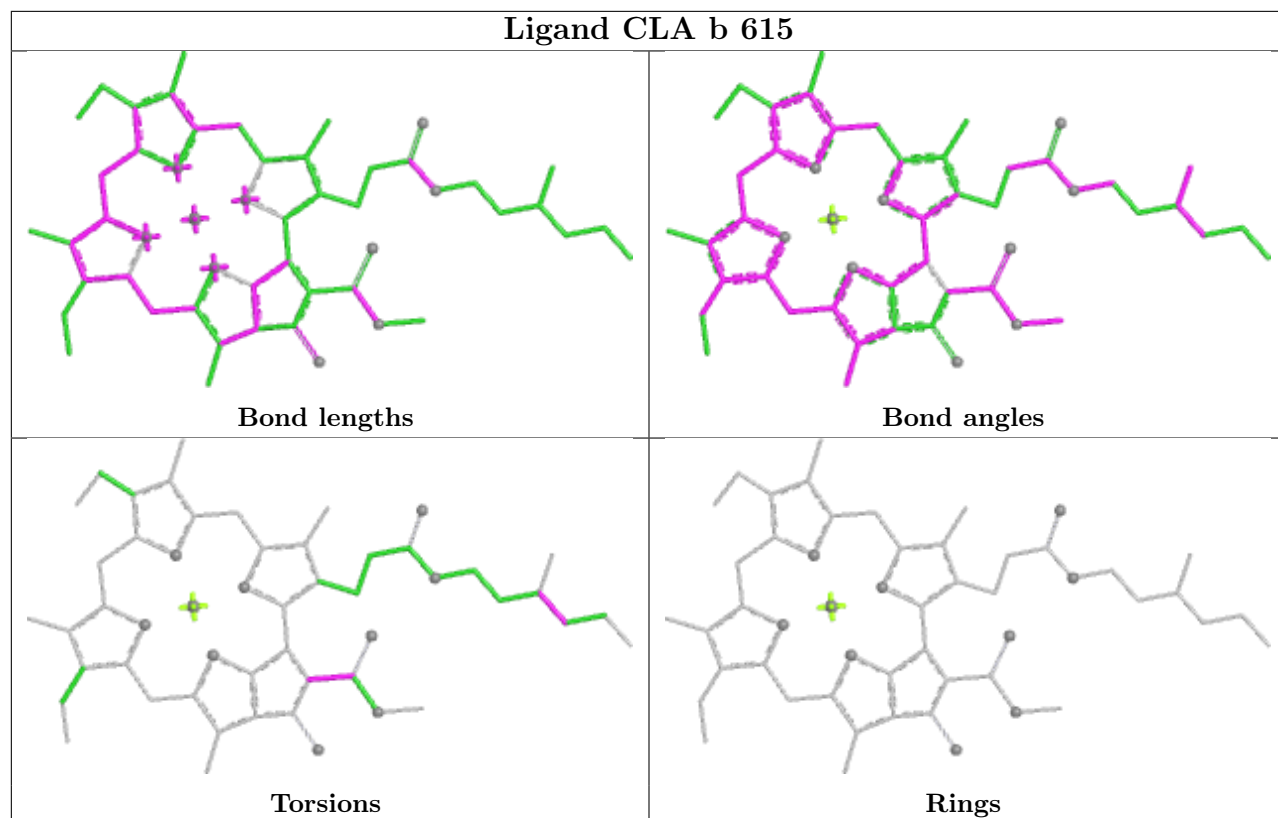




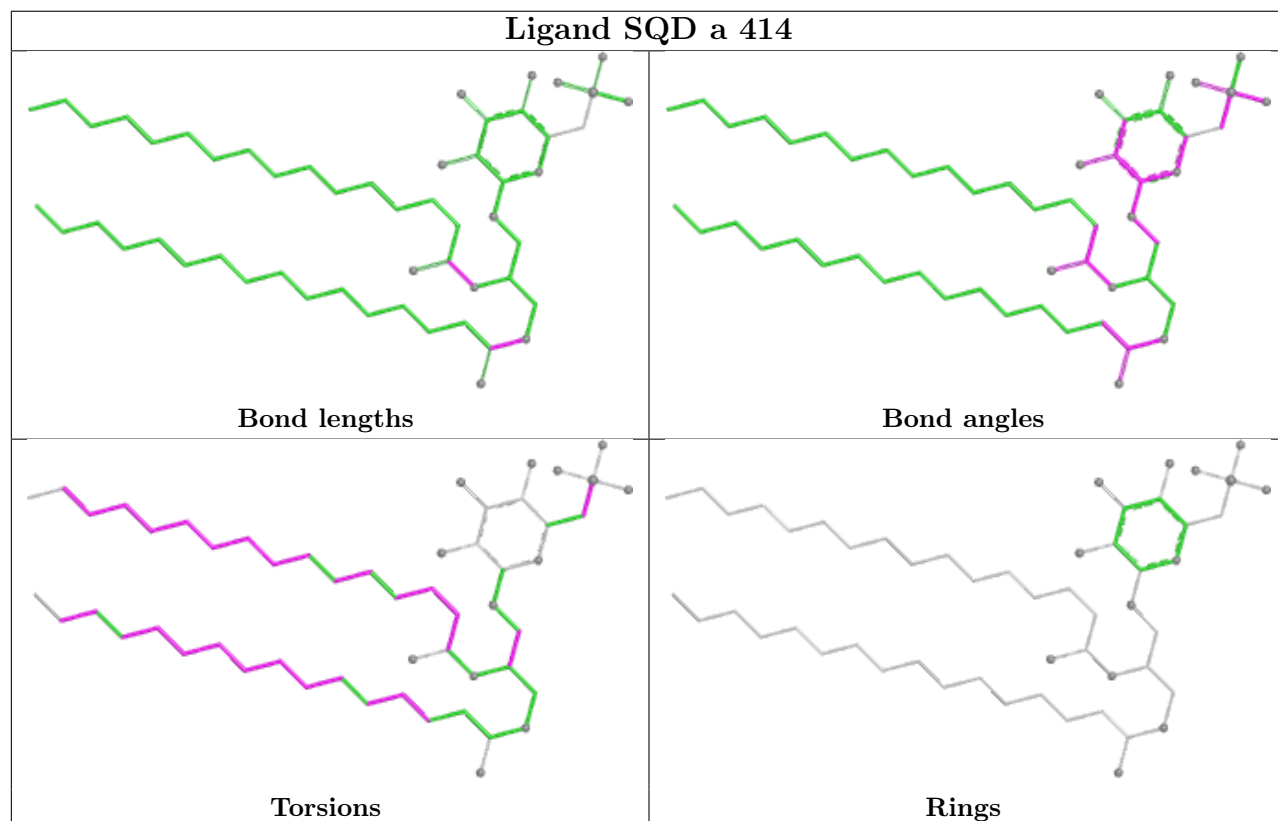


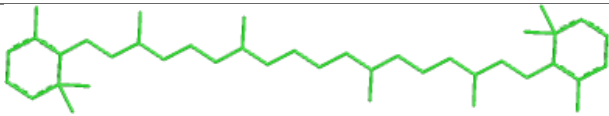
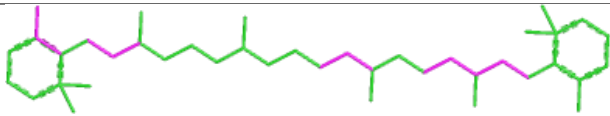
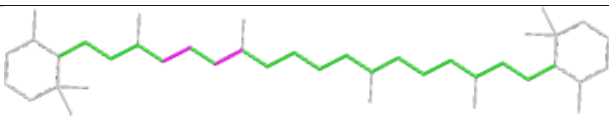
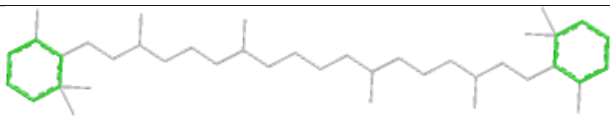


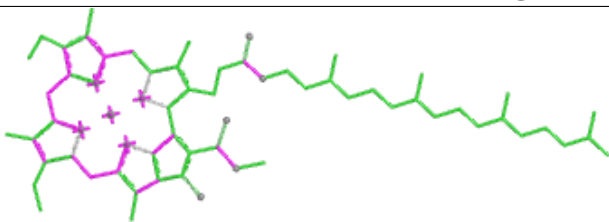
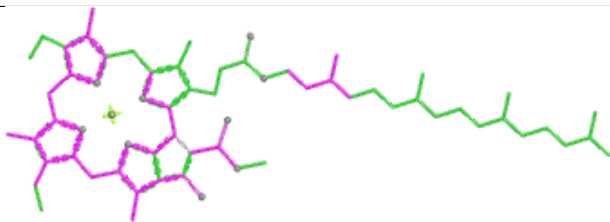
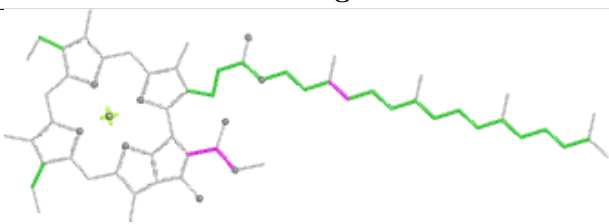
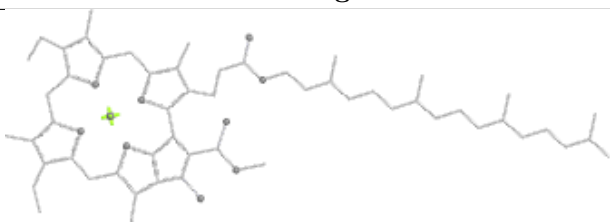
Ligand CLA b 615

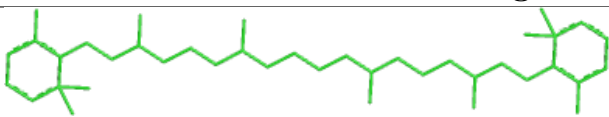
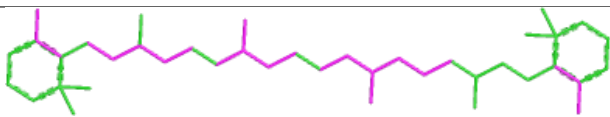
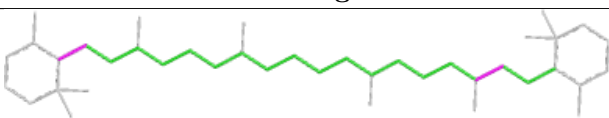
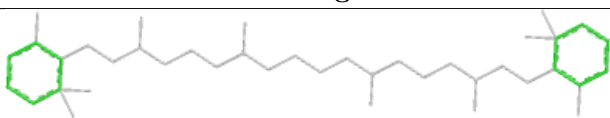


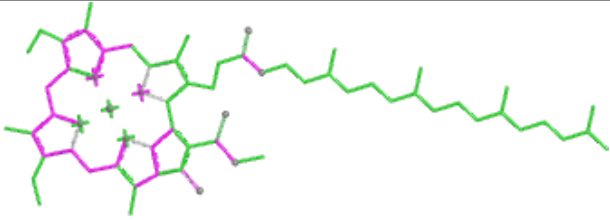
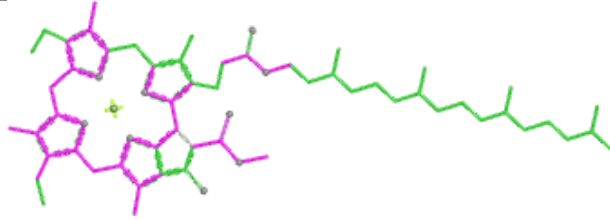
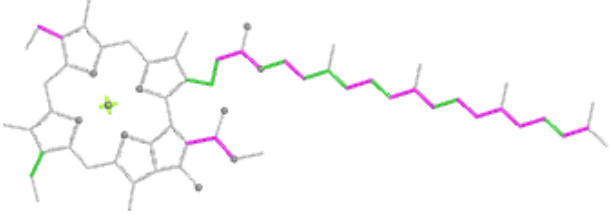
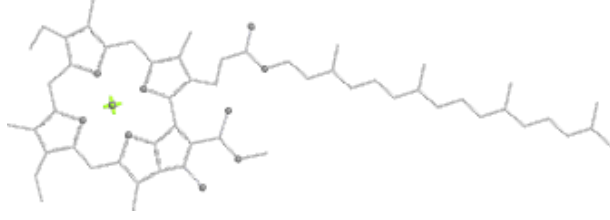
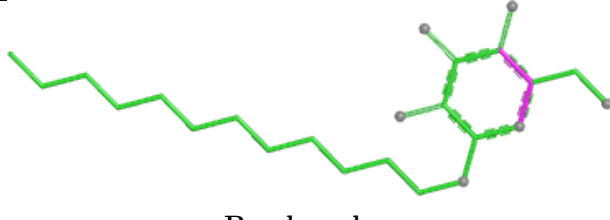
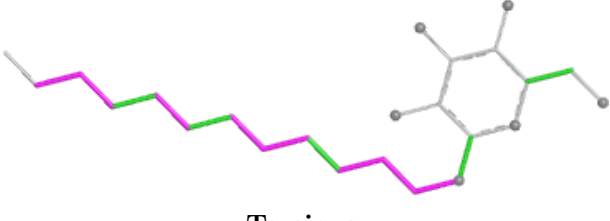
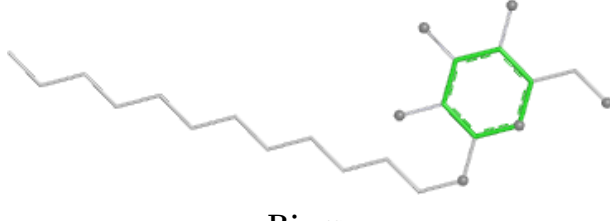
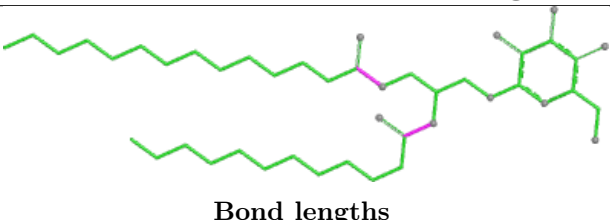
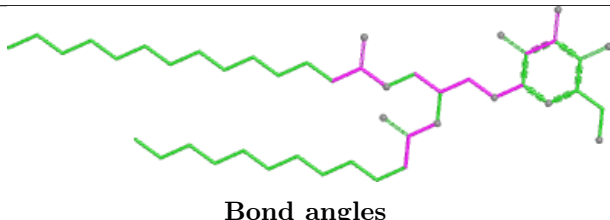
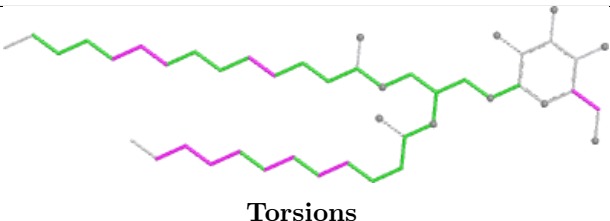
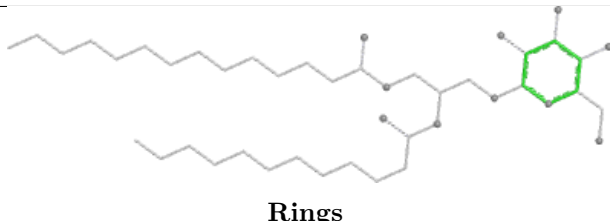
Ligand SQD a 414

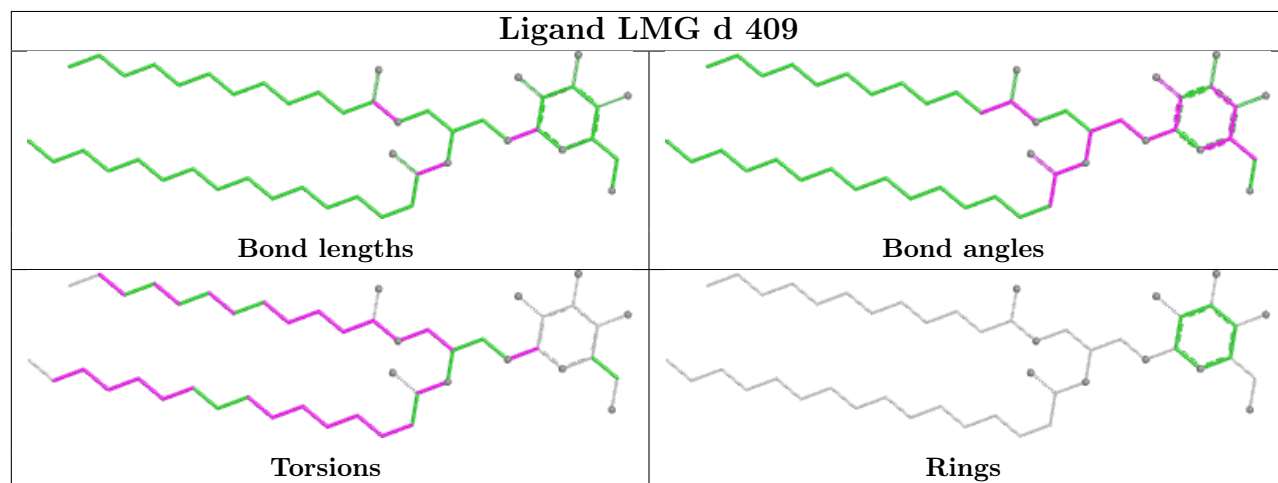
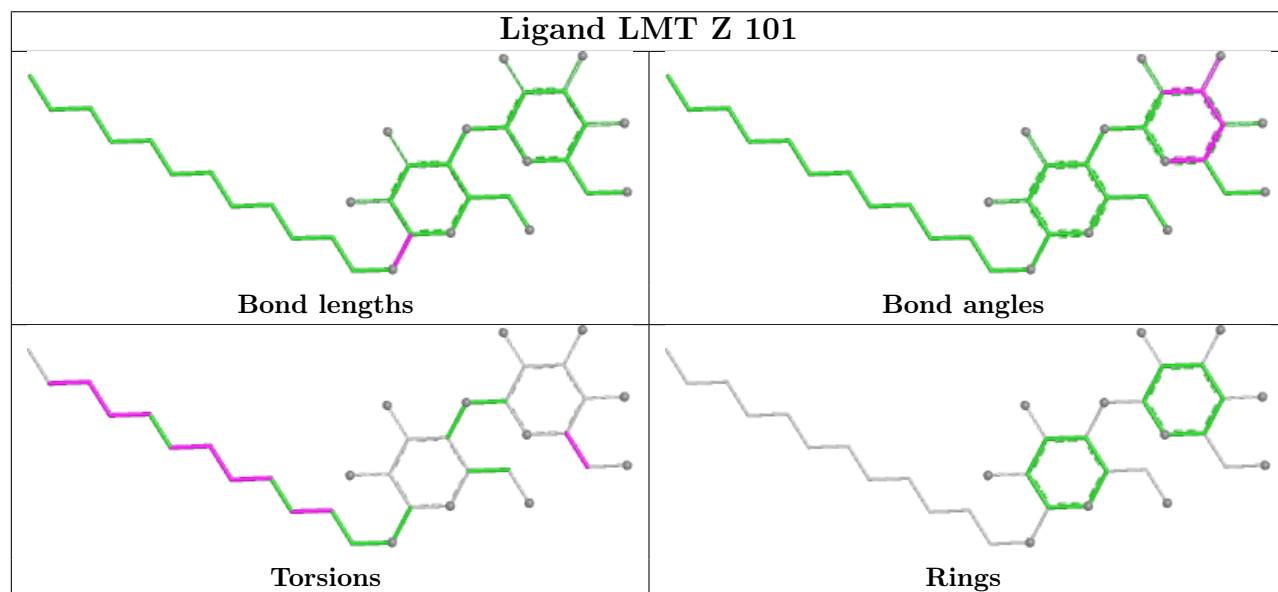
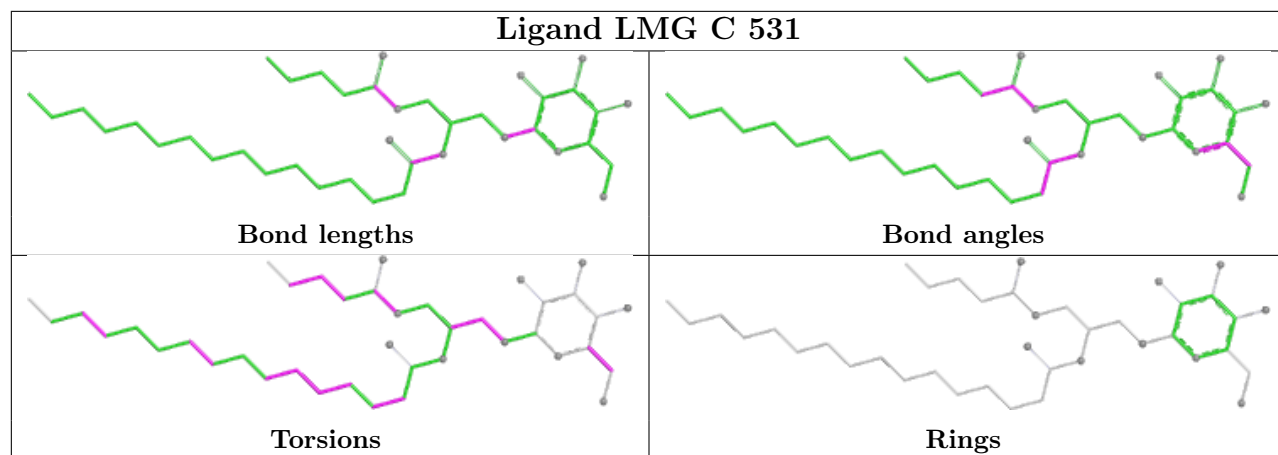


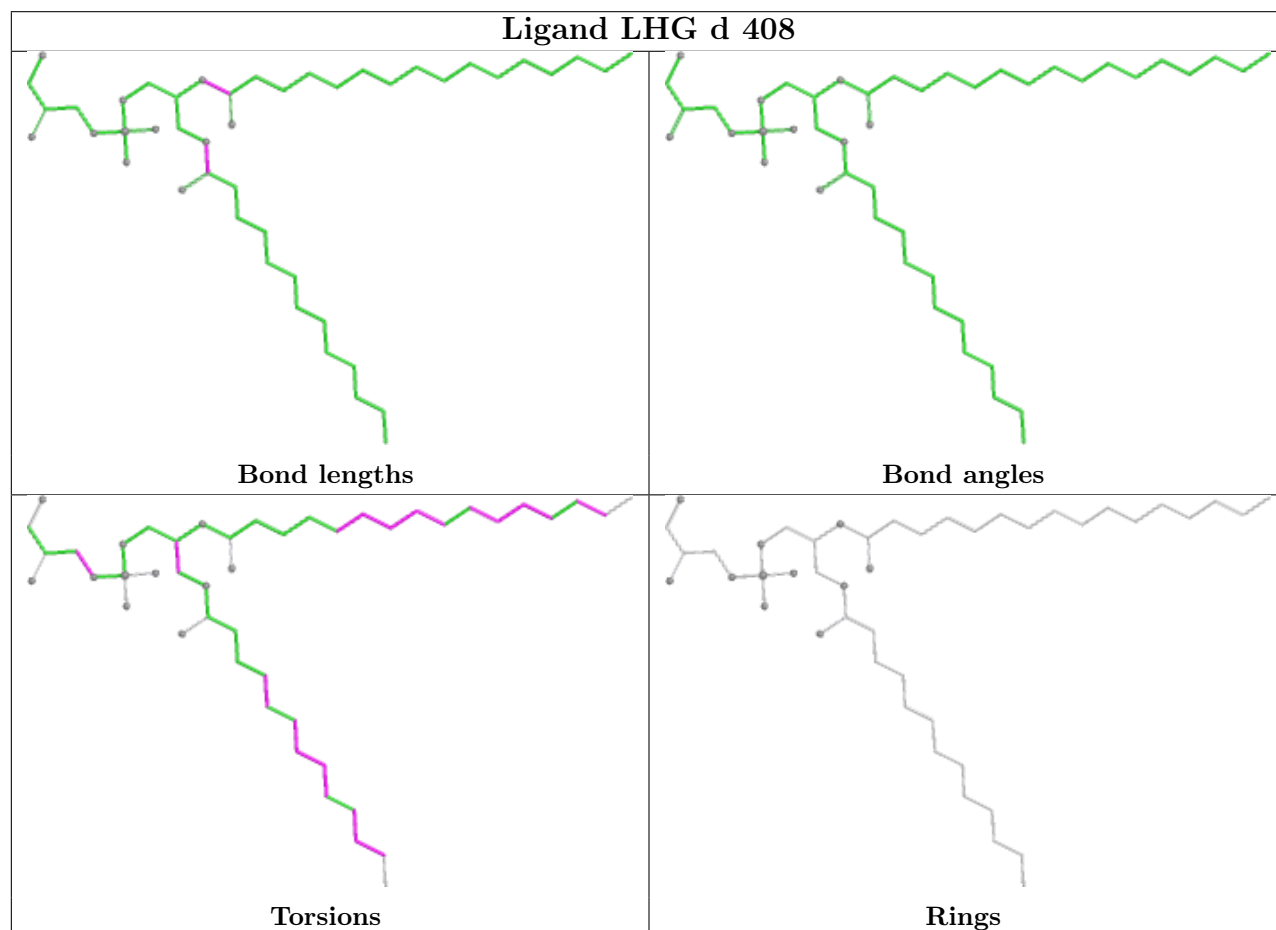
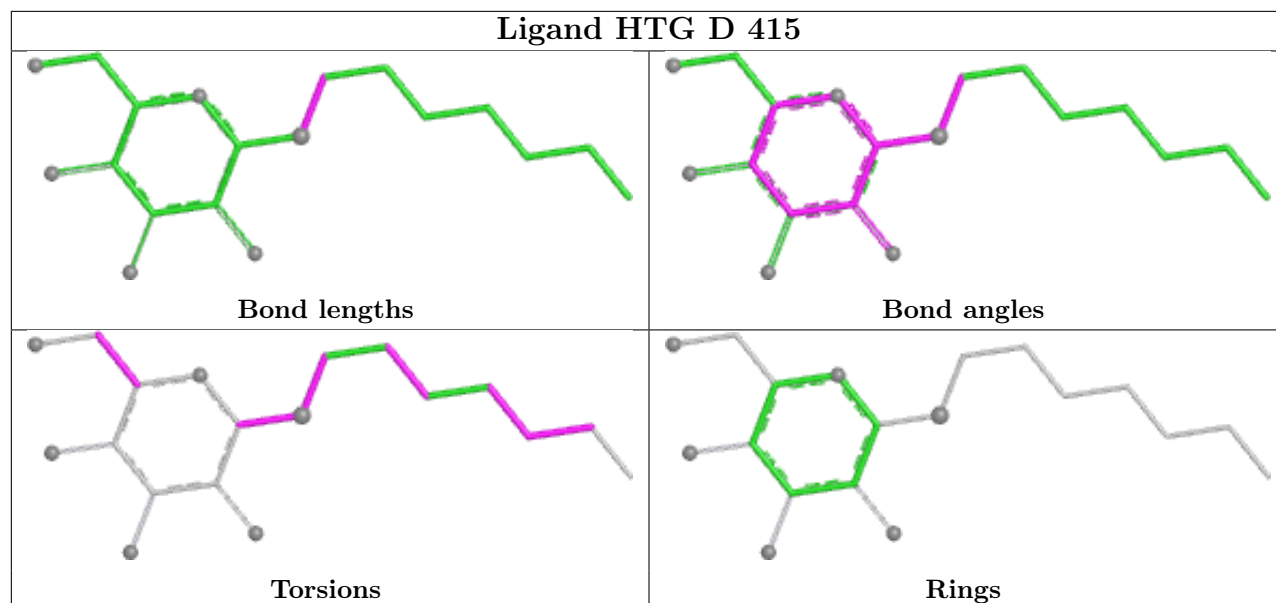
Ligand BCR K 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

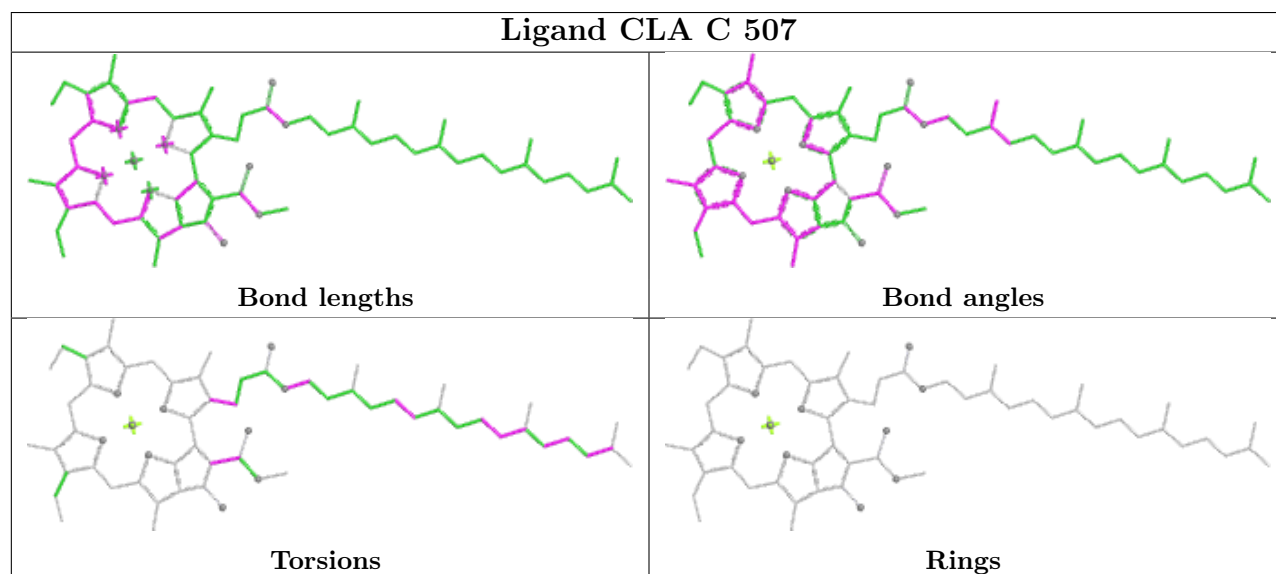
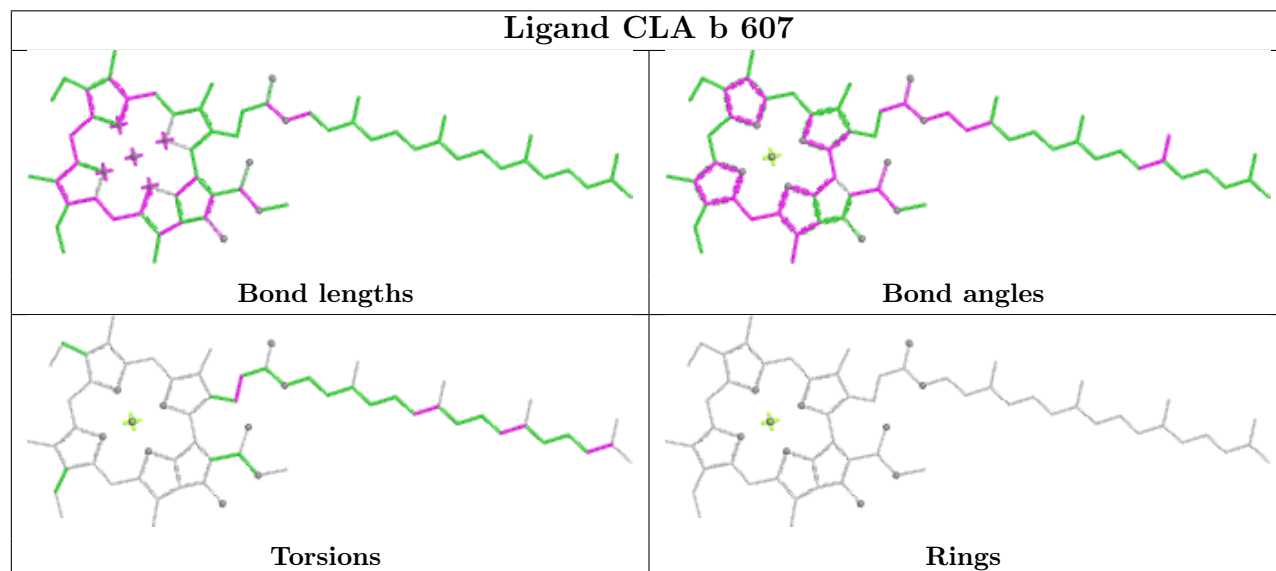
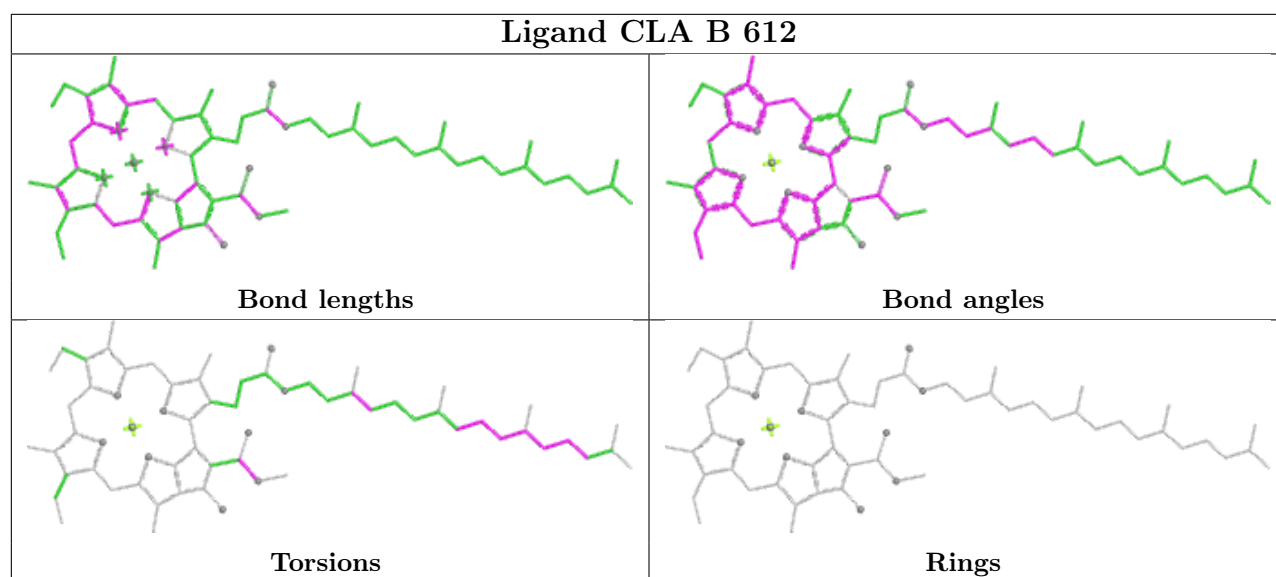
Ligand CLA b 606	
	
Bond lengths	Bond angles
	
Torsions	Rings

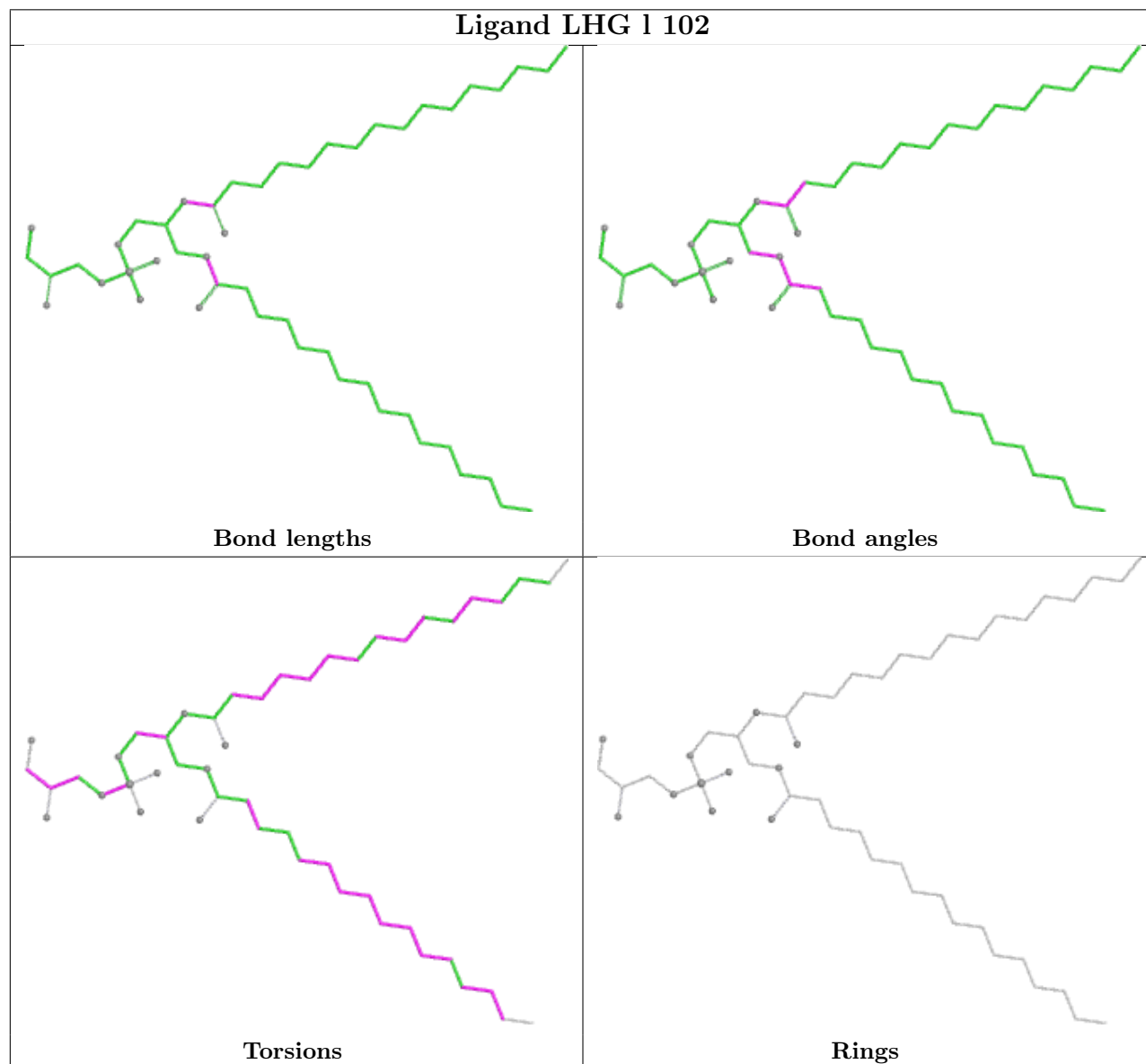
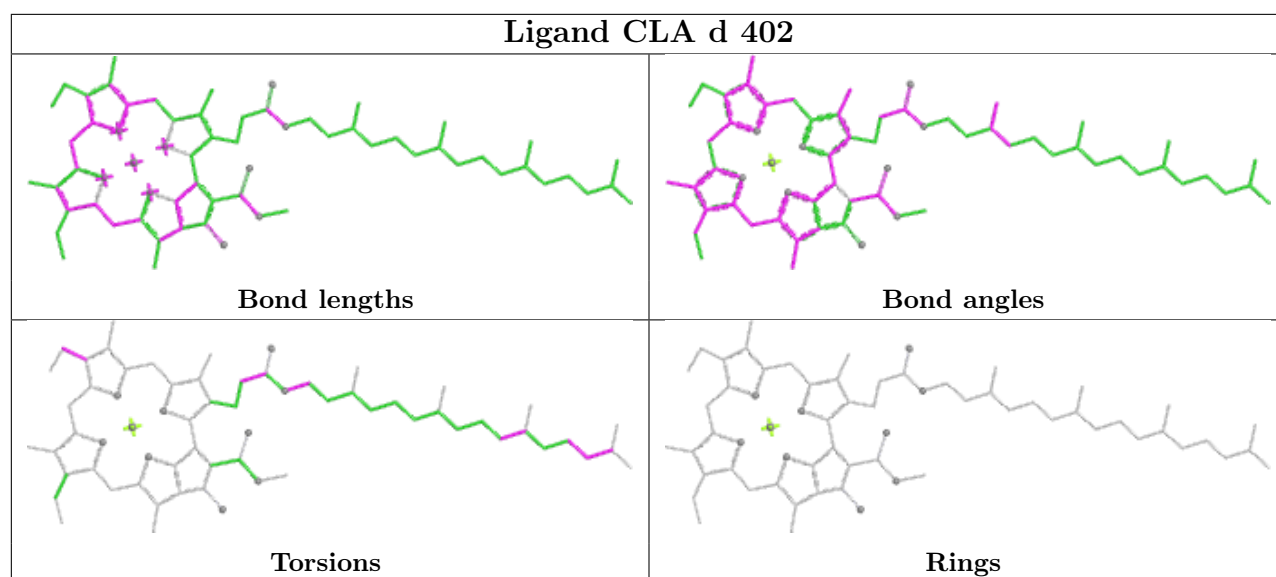
Ligand BCR c 916	
	
Bond lengths	Bond angles
	
Torsions	Rings

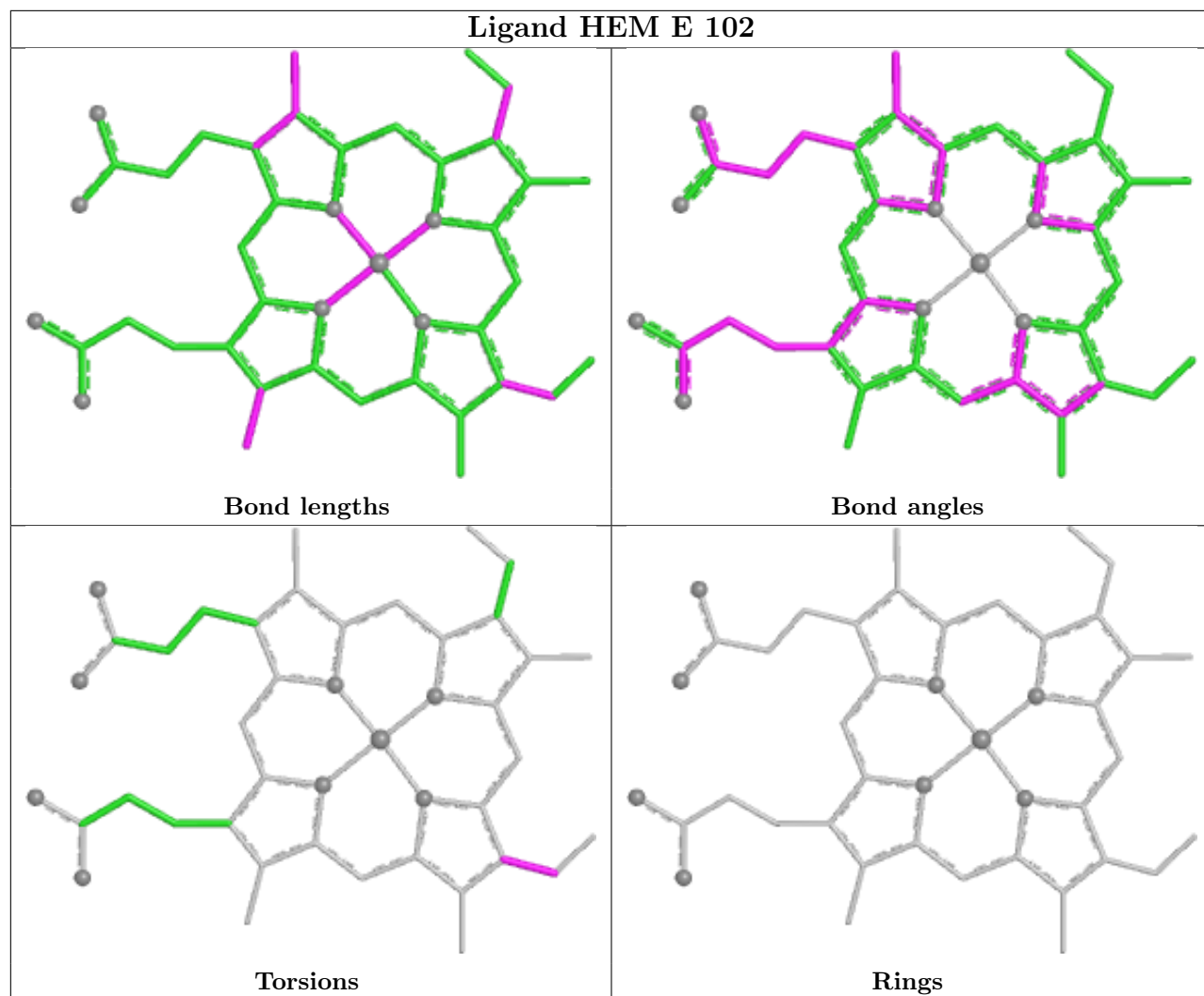
Ligand CLA B 602	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMT B 622	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG J 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

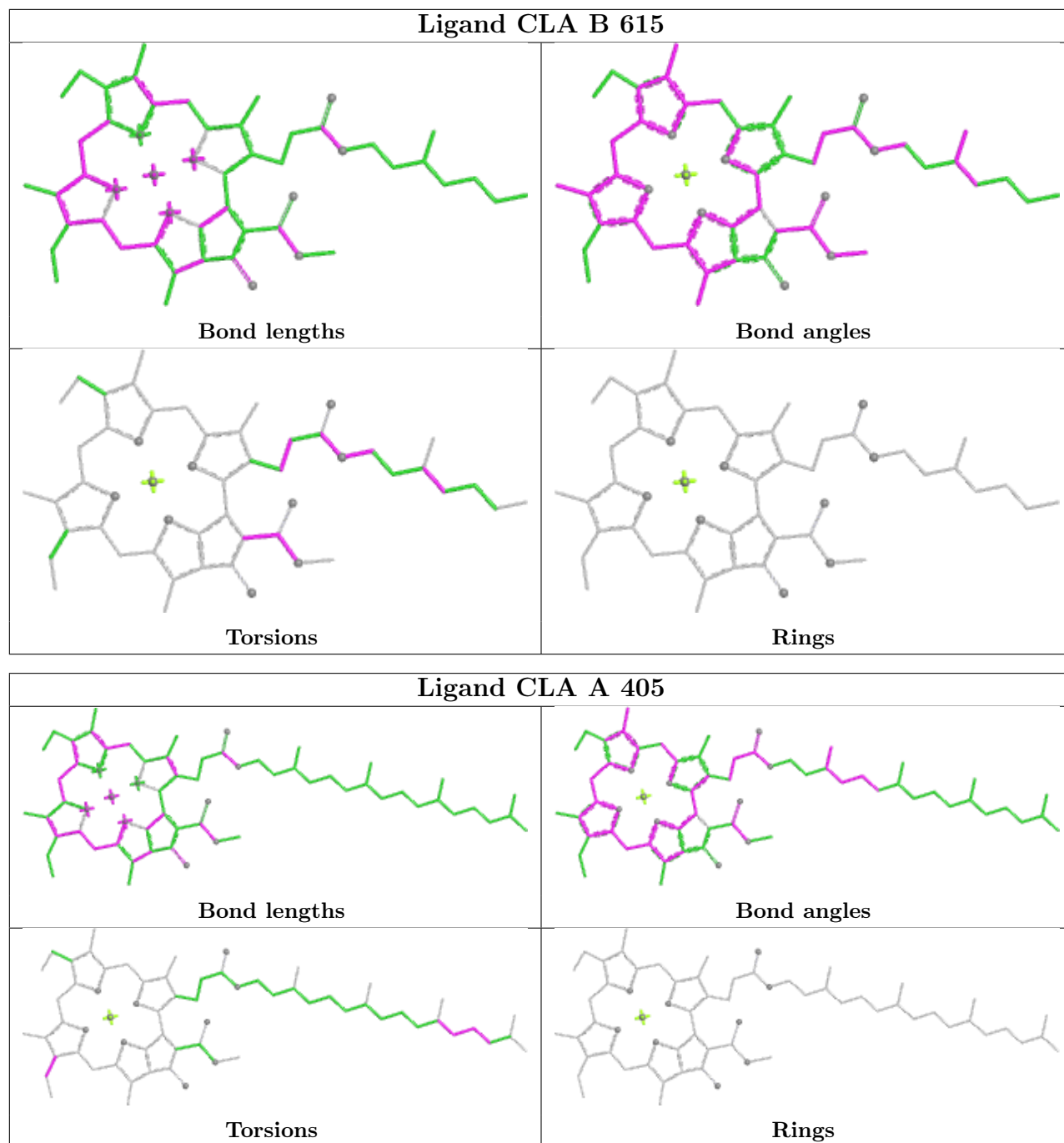


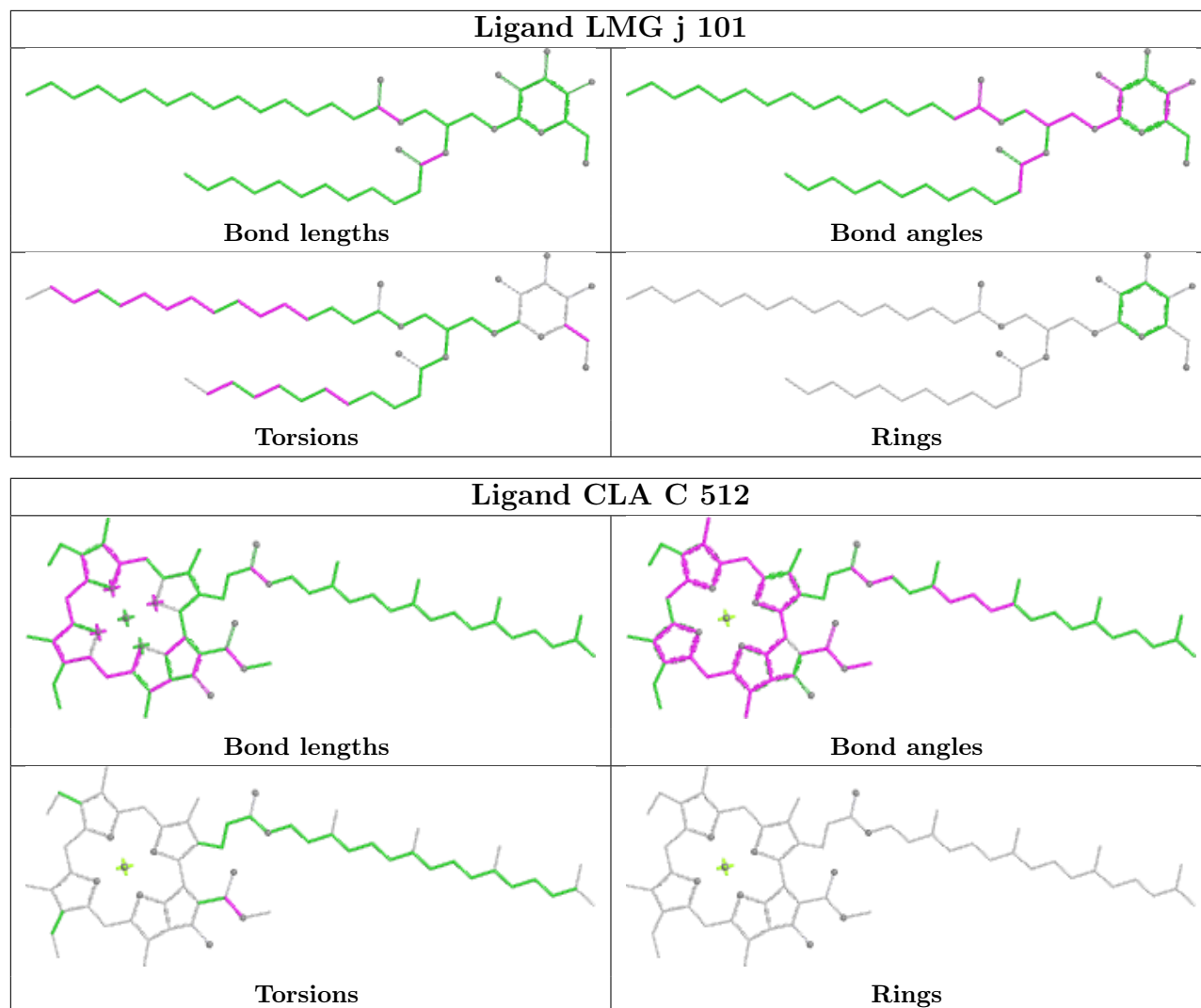


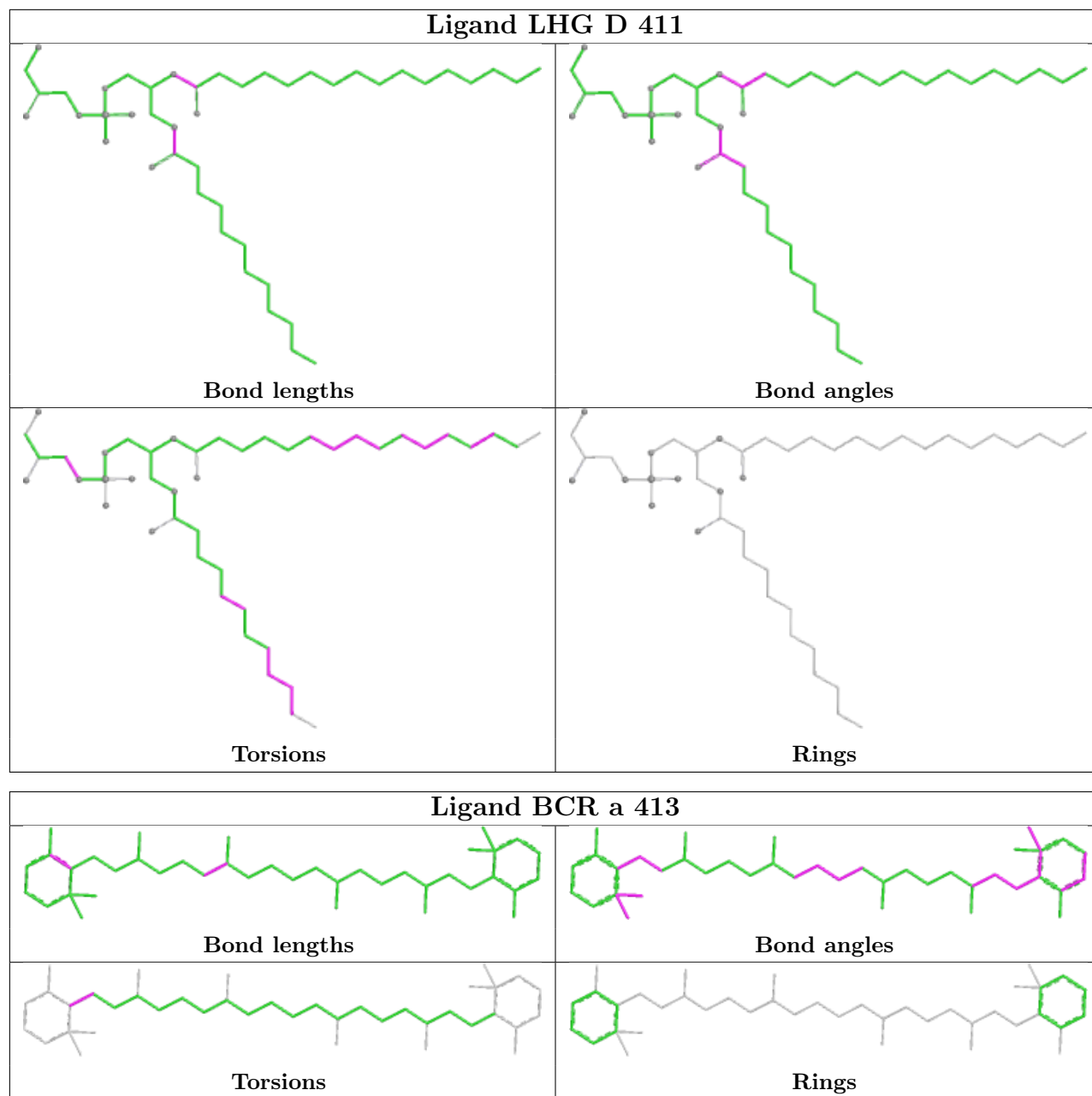


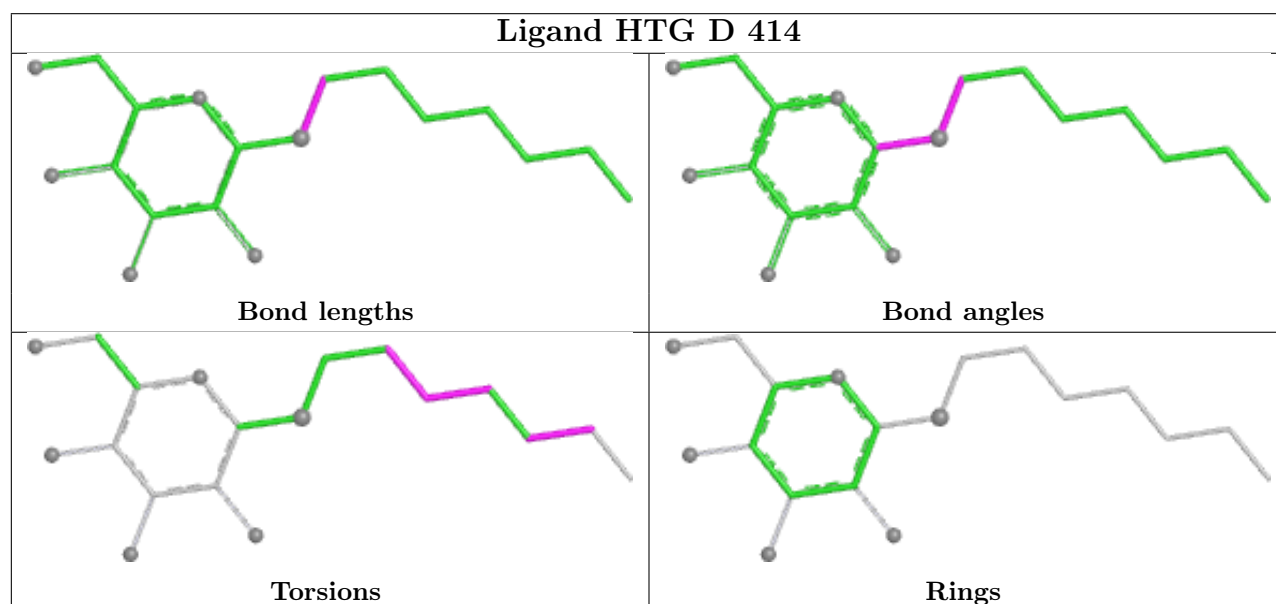
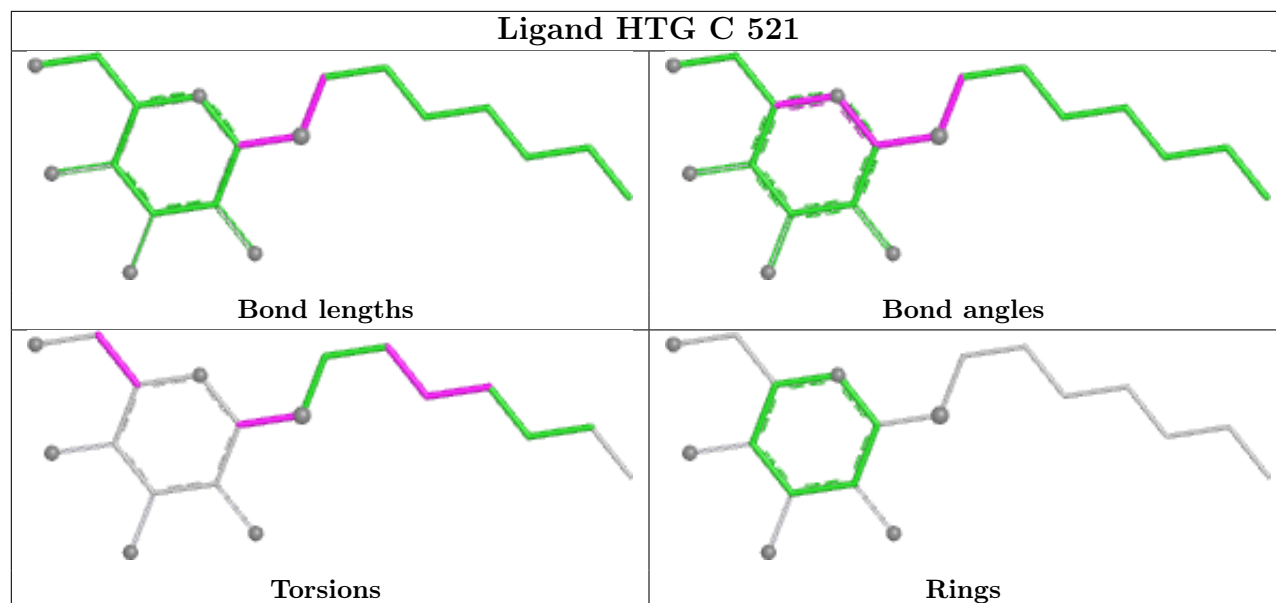


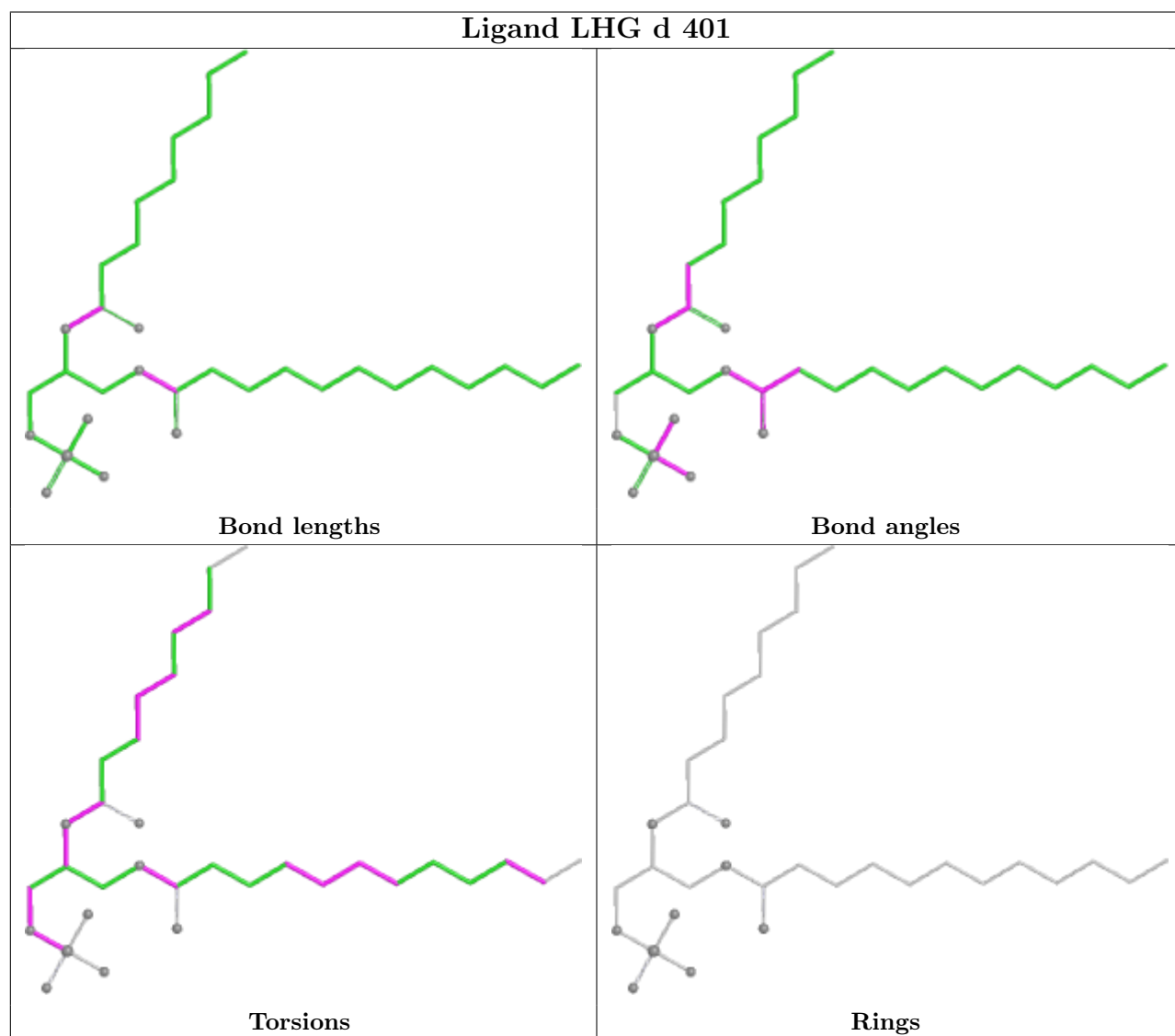
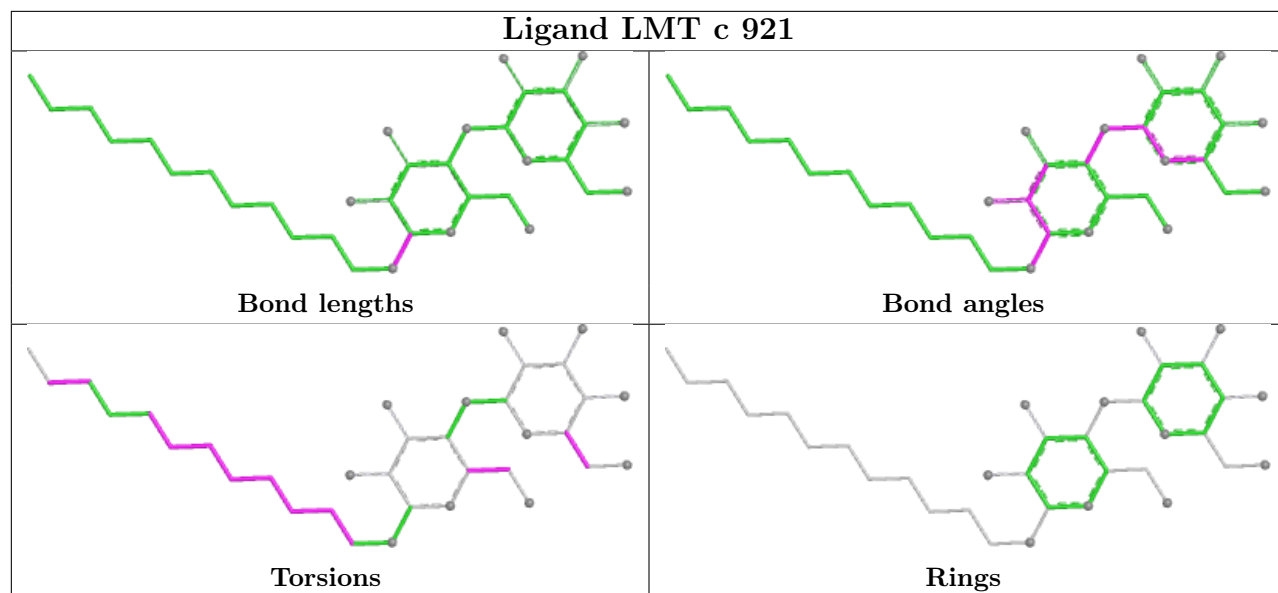


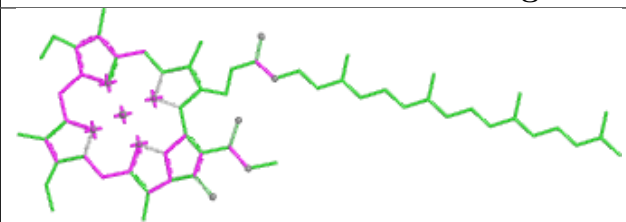
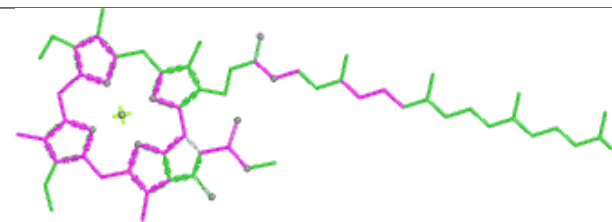
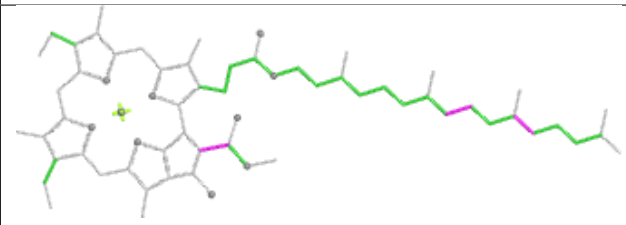
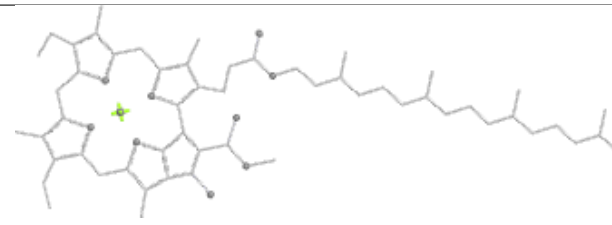


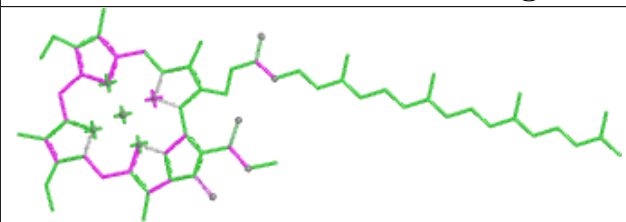
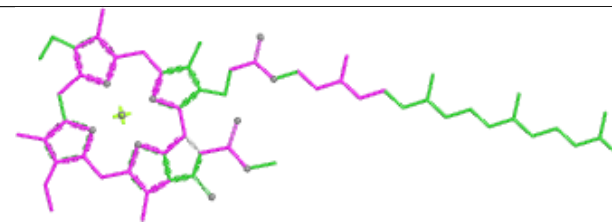
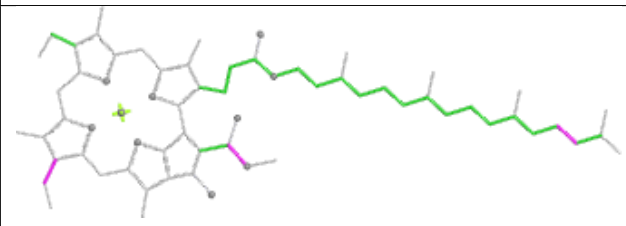
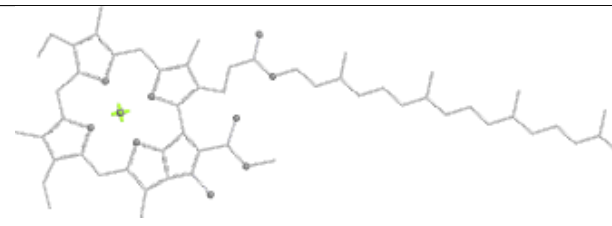


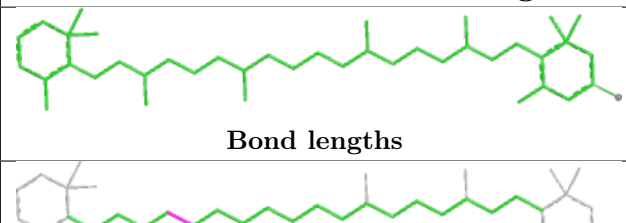
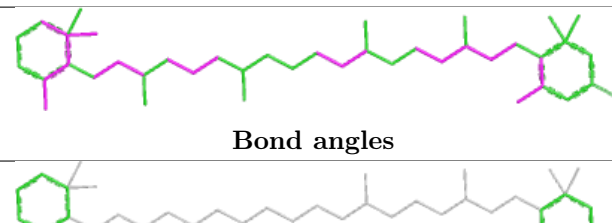
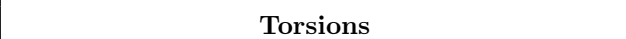


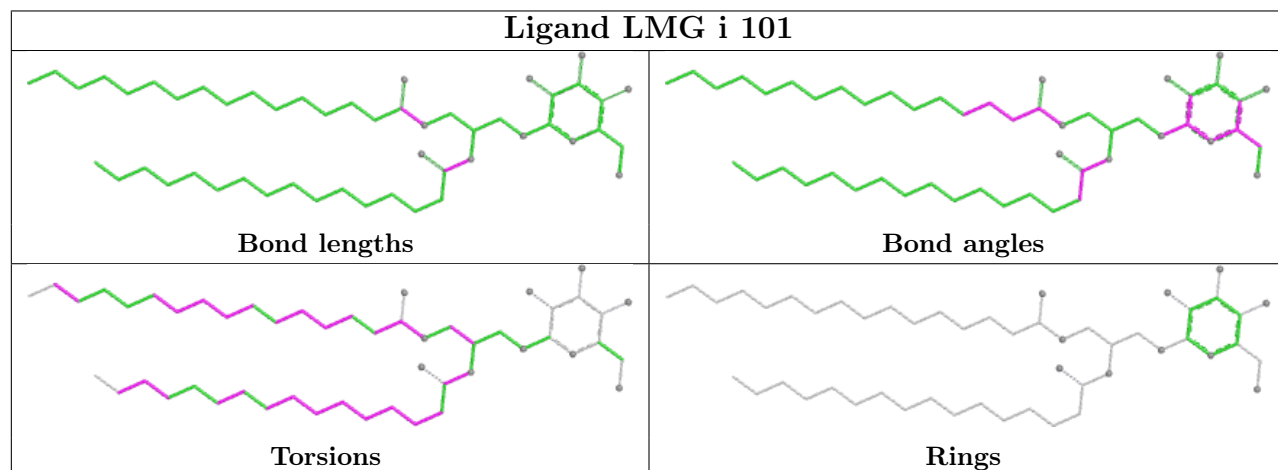
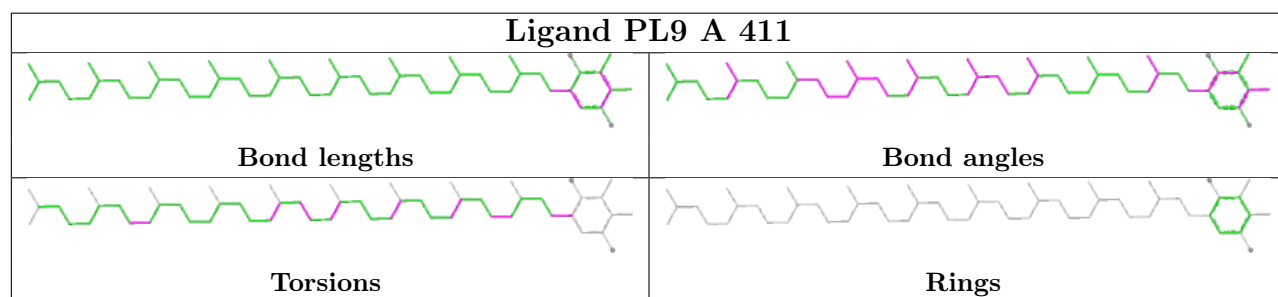
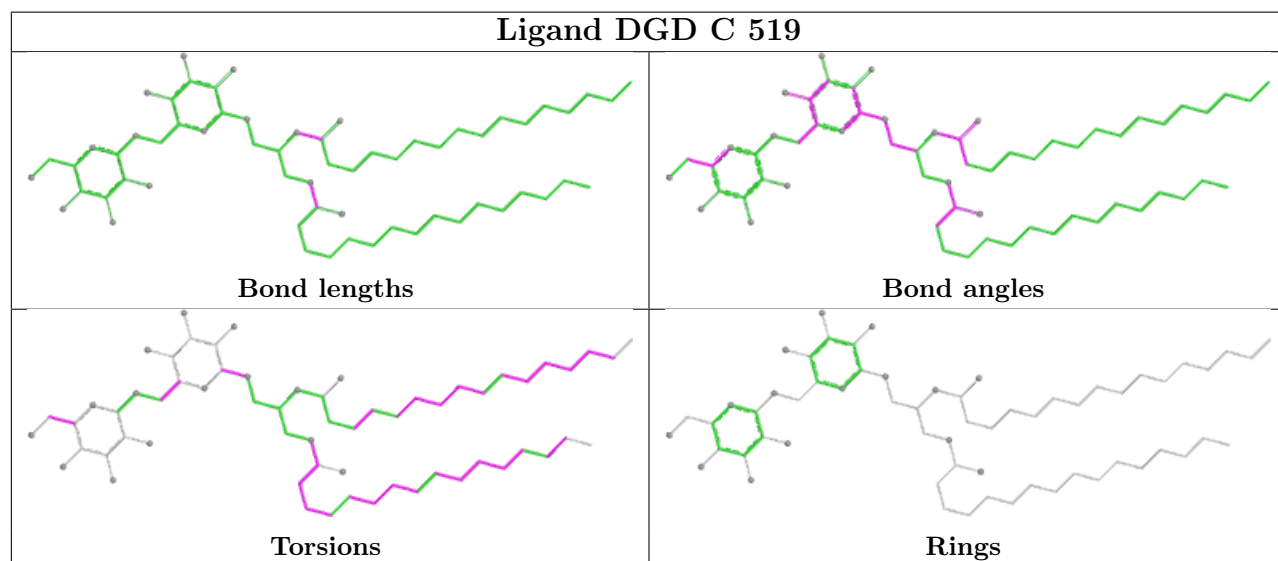
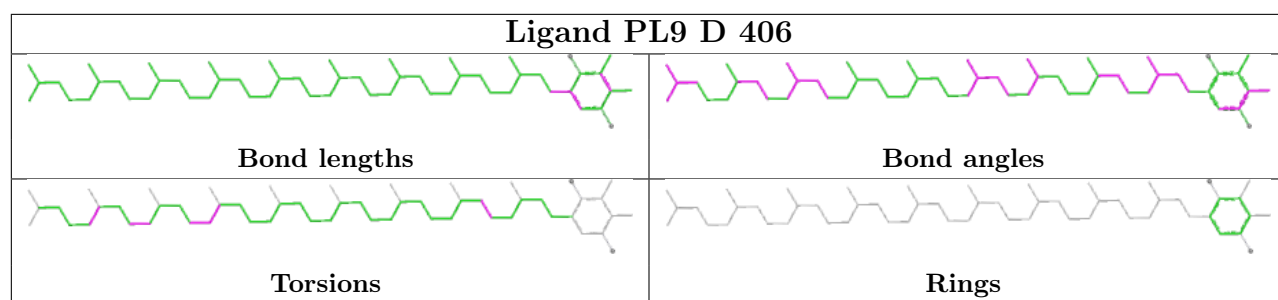


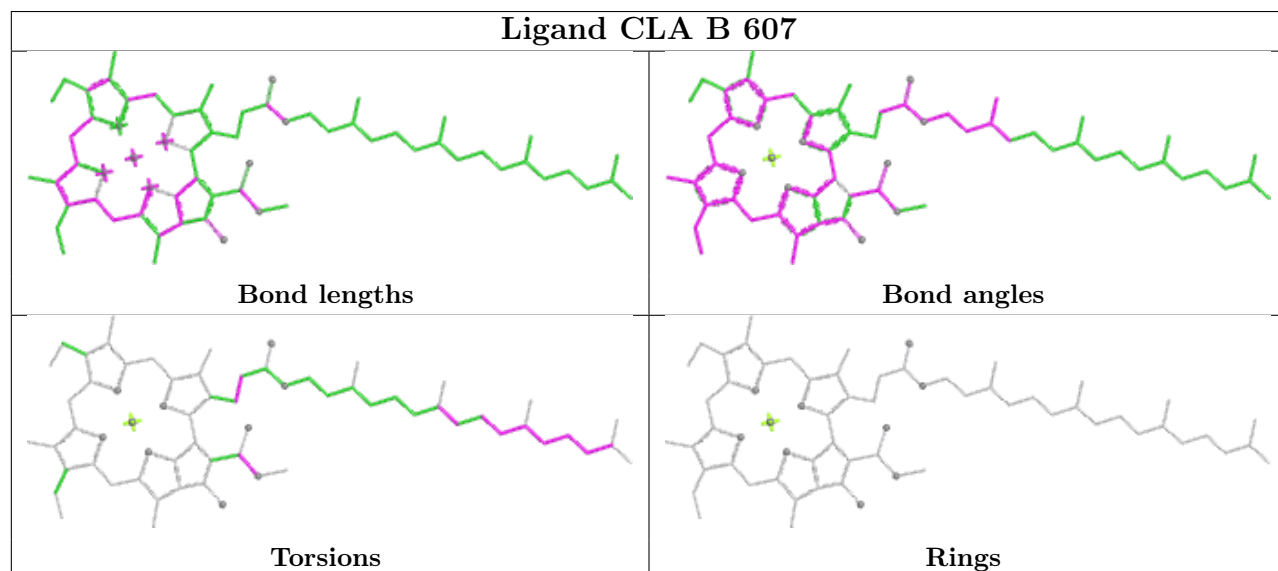
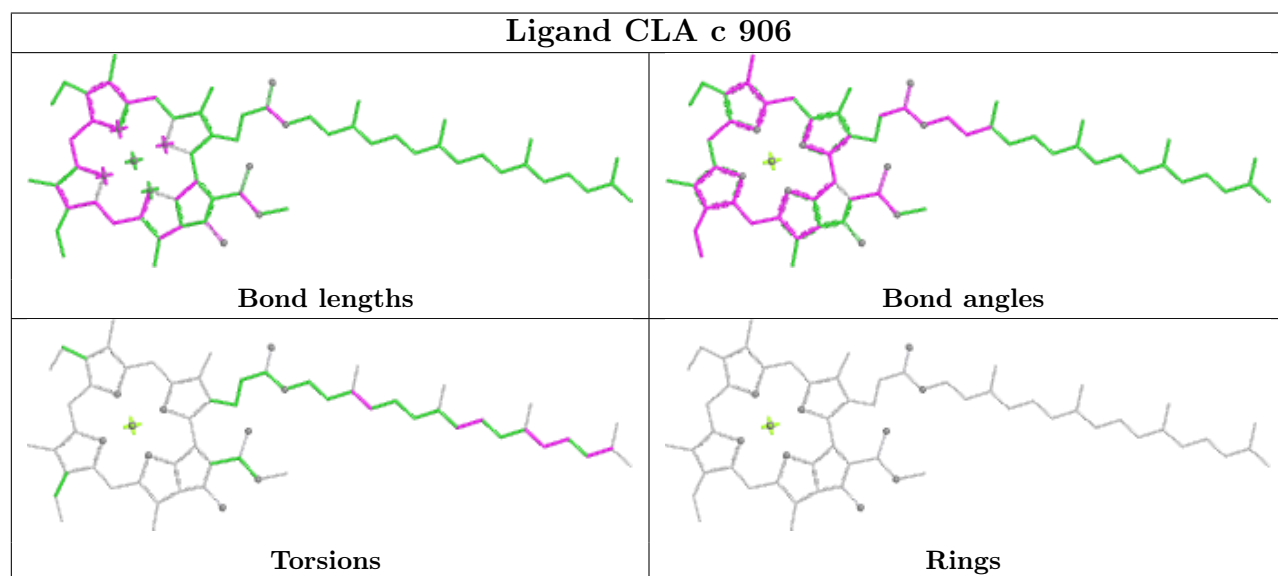
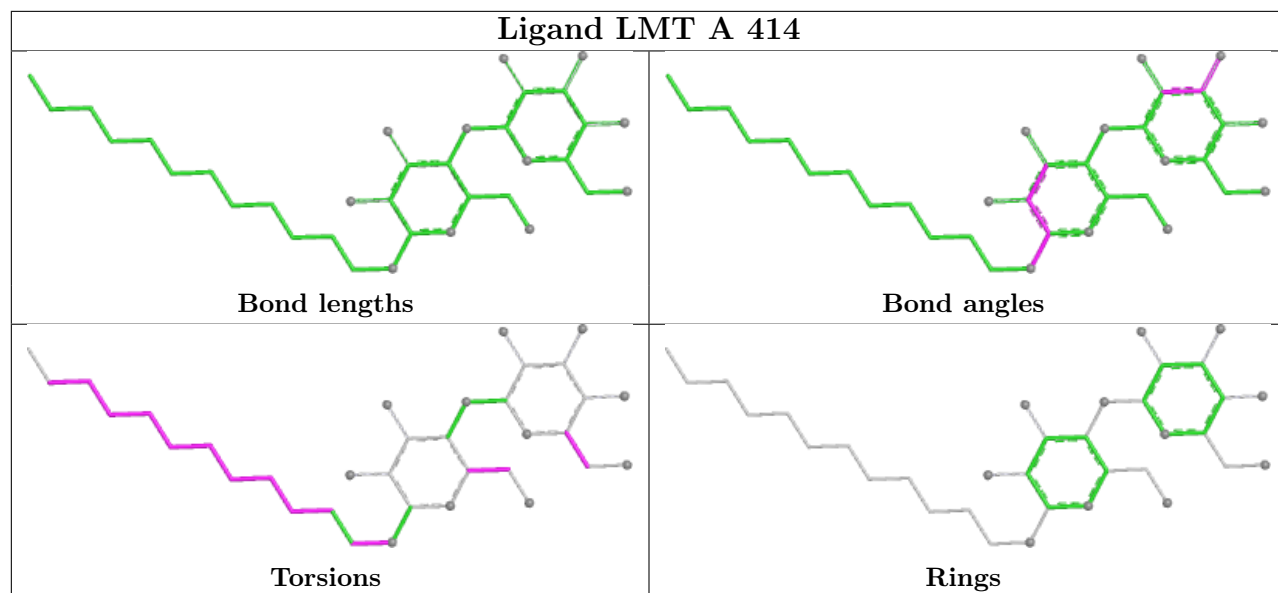


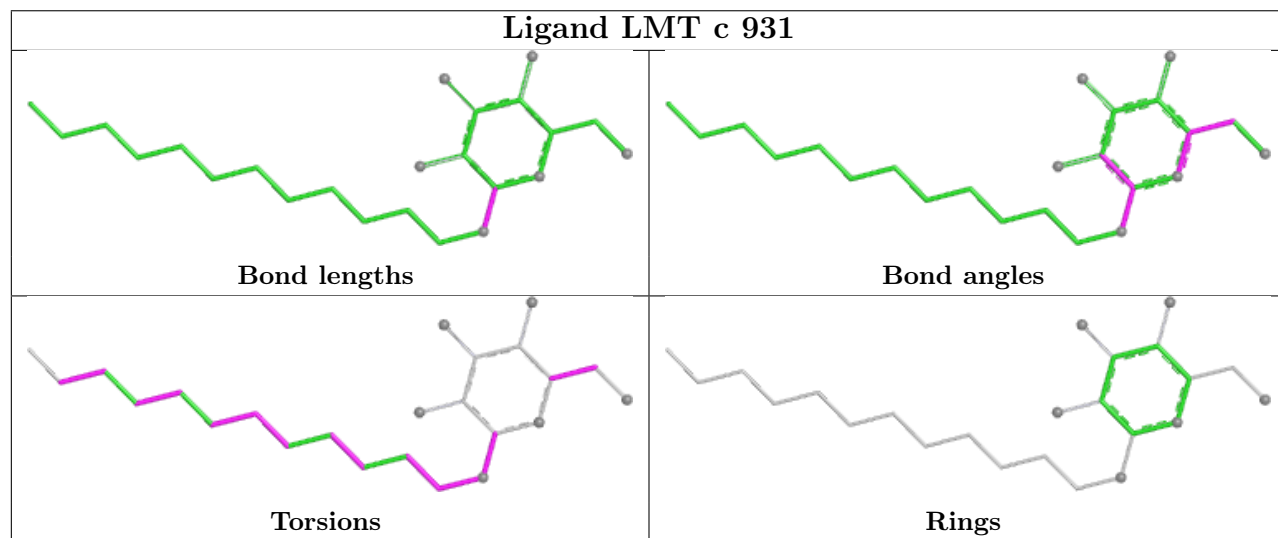
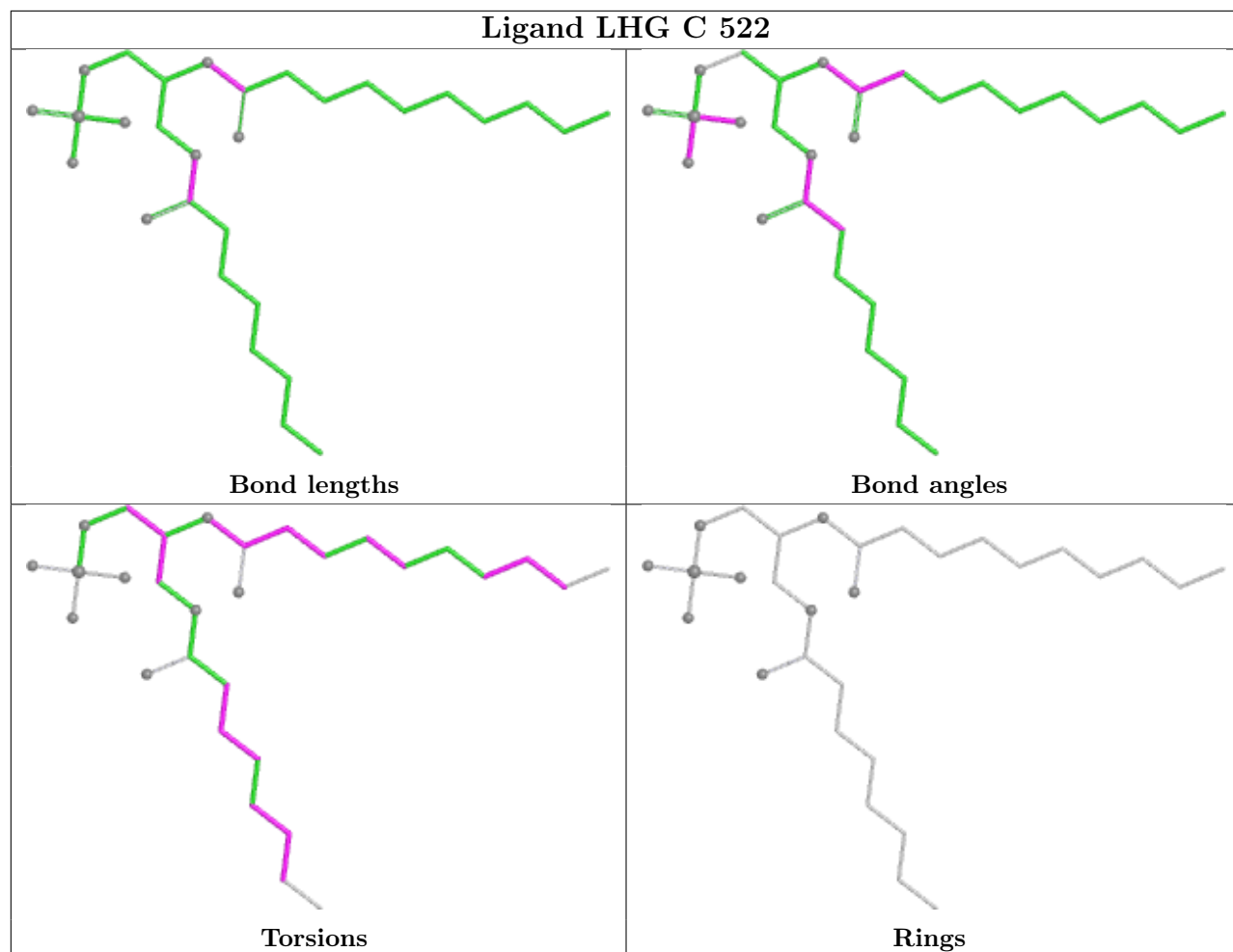
Ligand CLA C 505	
	
Bond lengths	Bond angles
	
Torsions	Rings

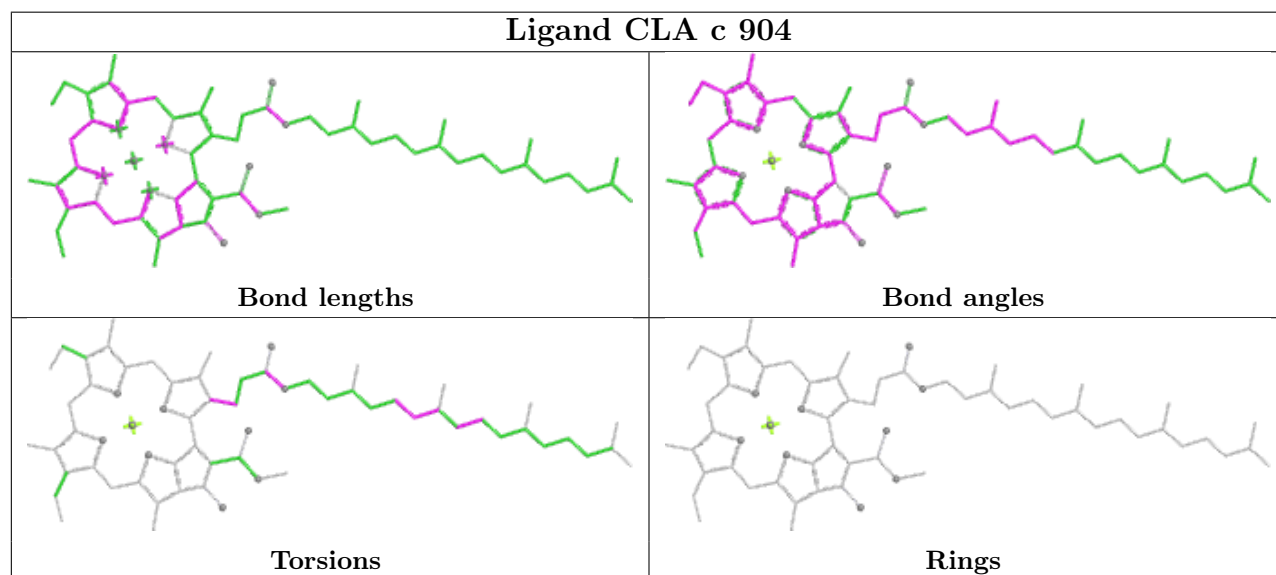
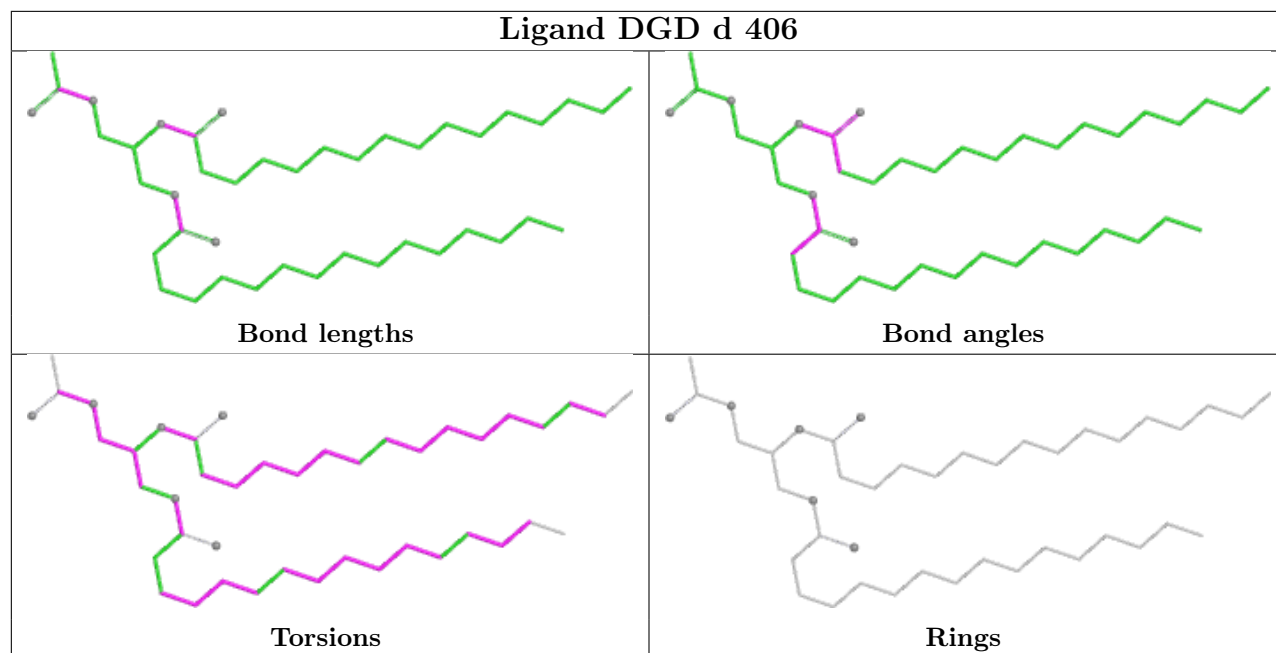
Ligand CLA D 401	
	
Bond lengths	Bond angles
	
Torsions	Rings

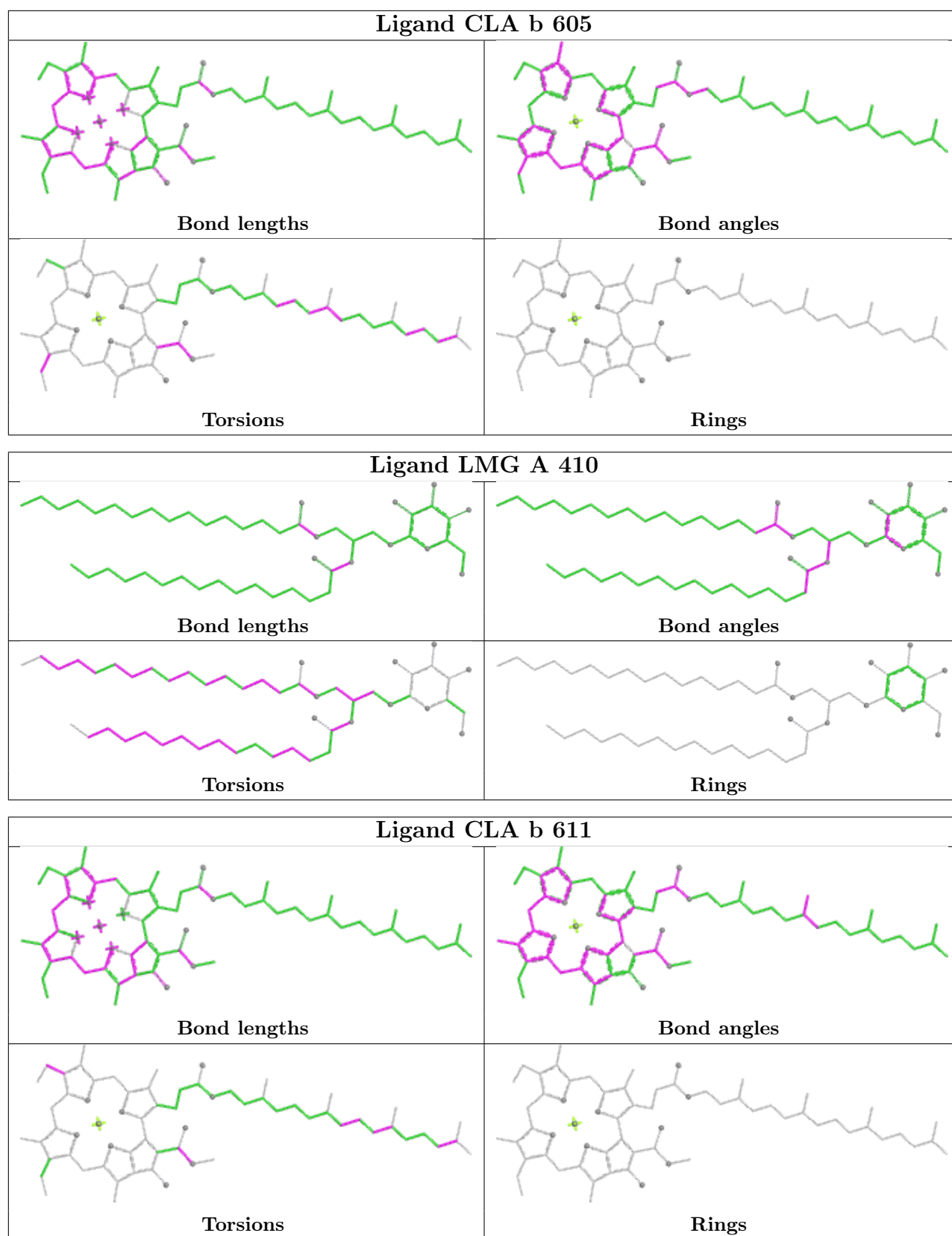
Ligand RRX H 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

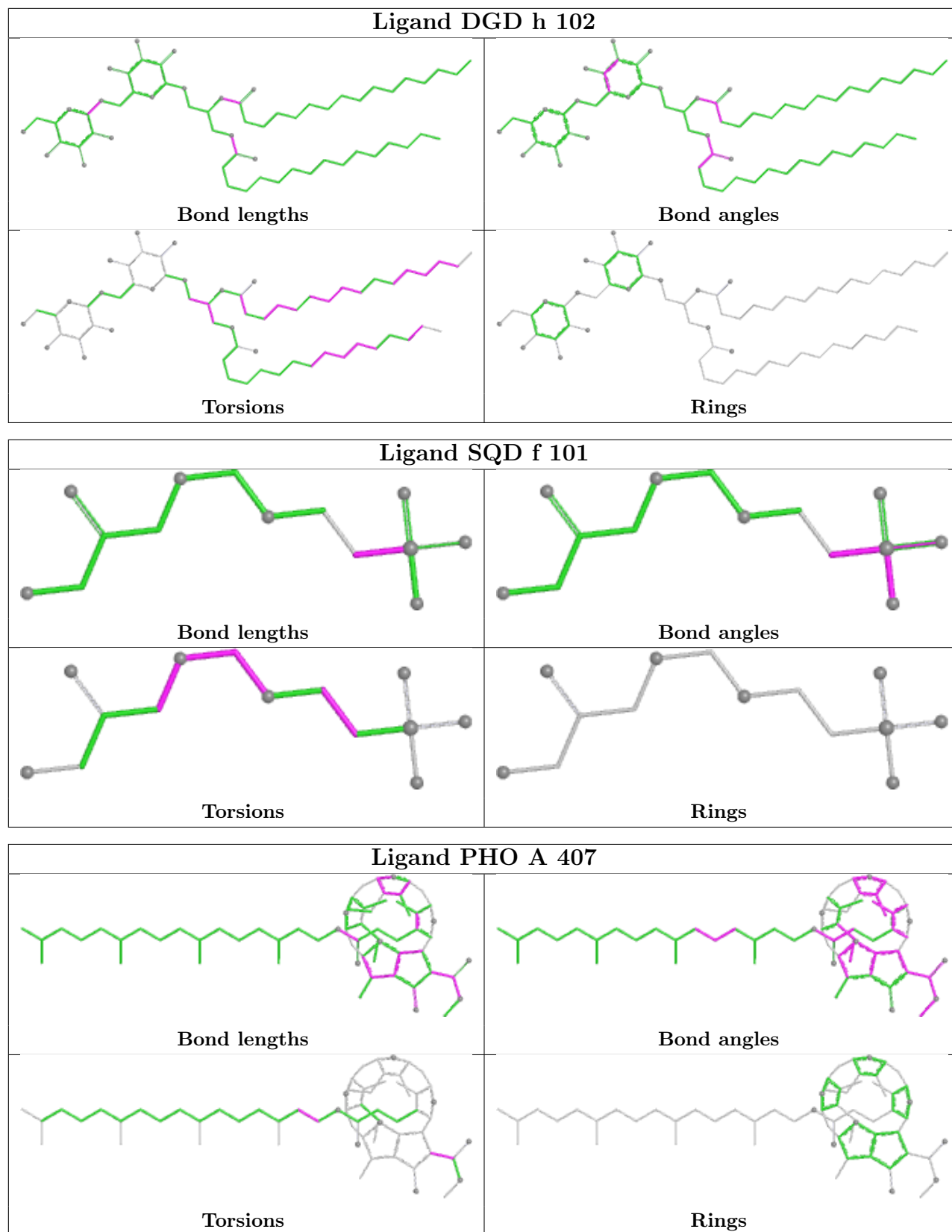




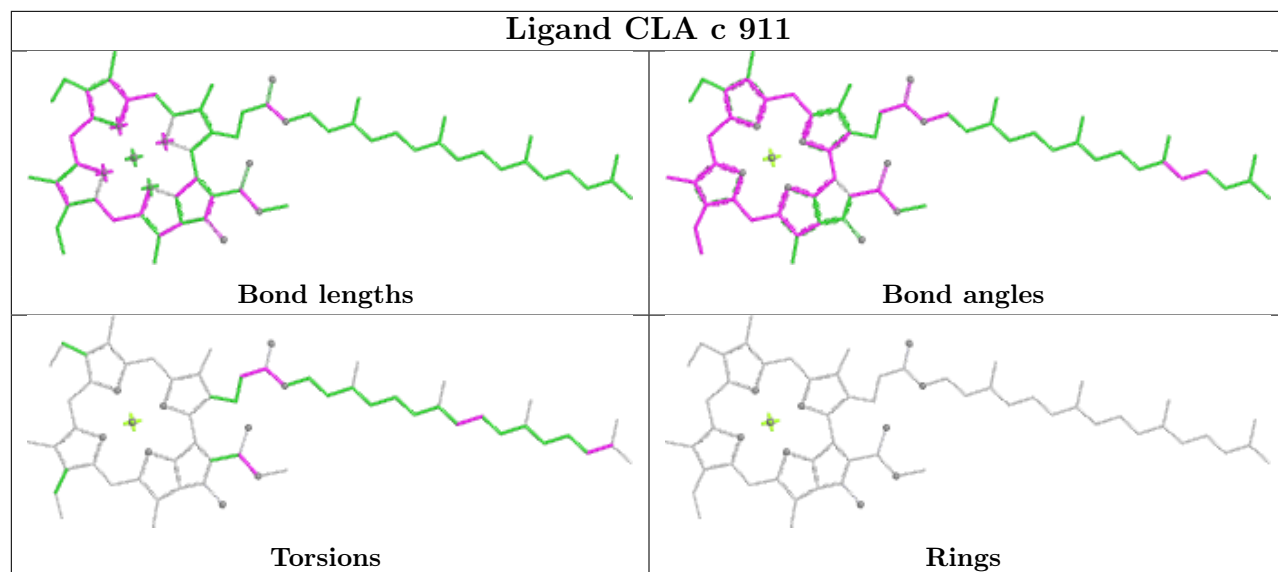




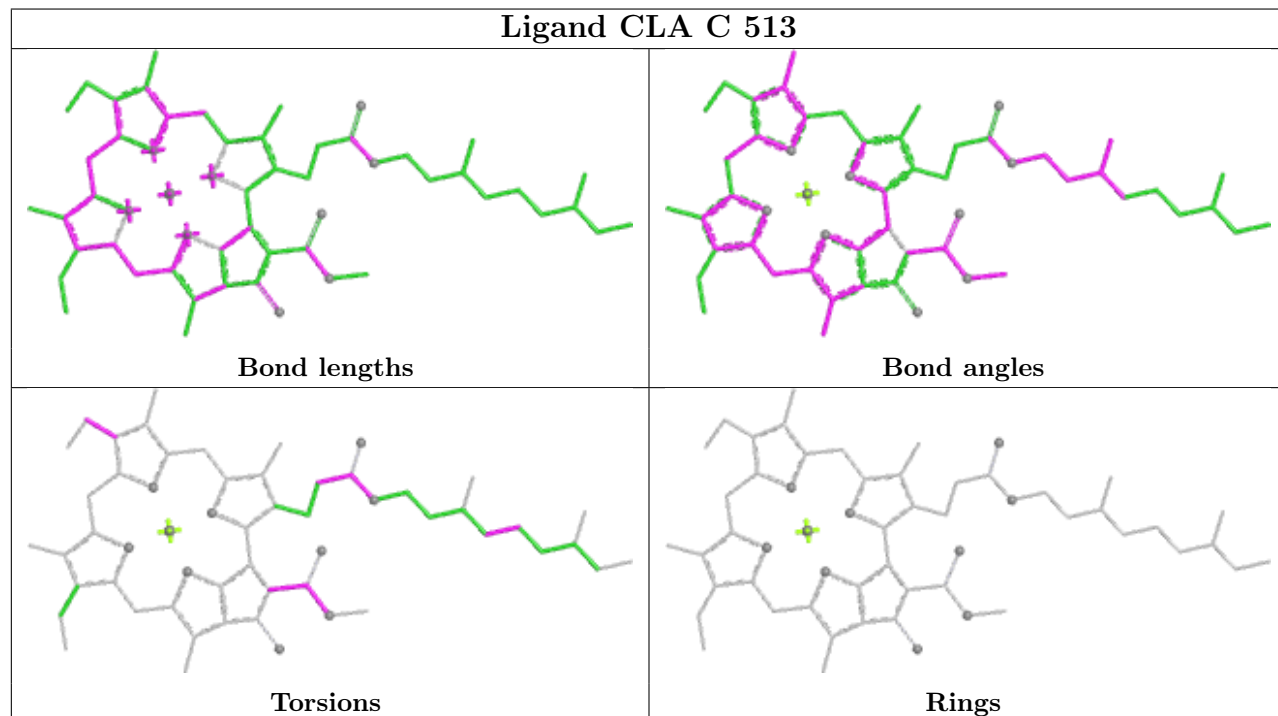


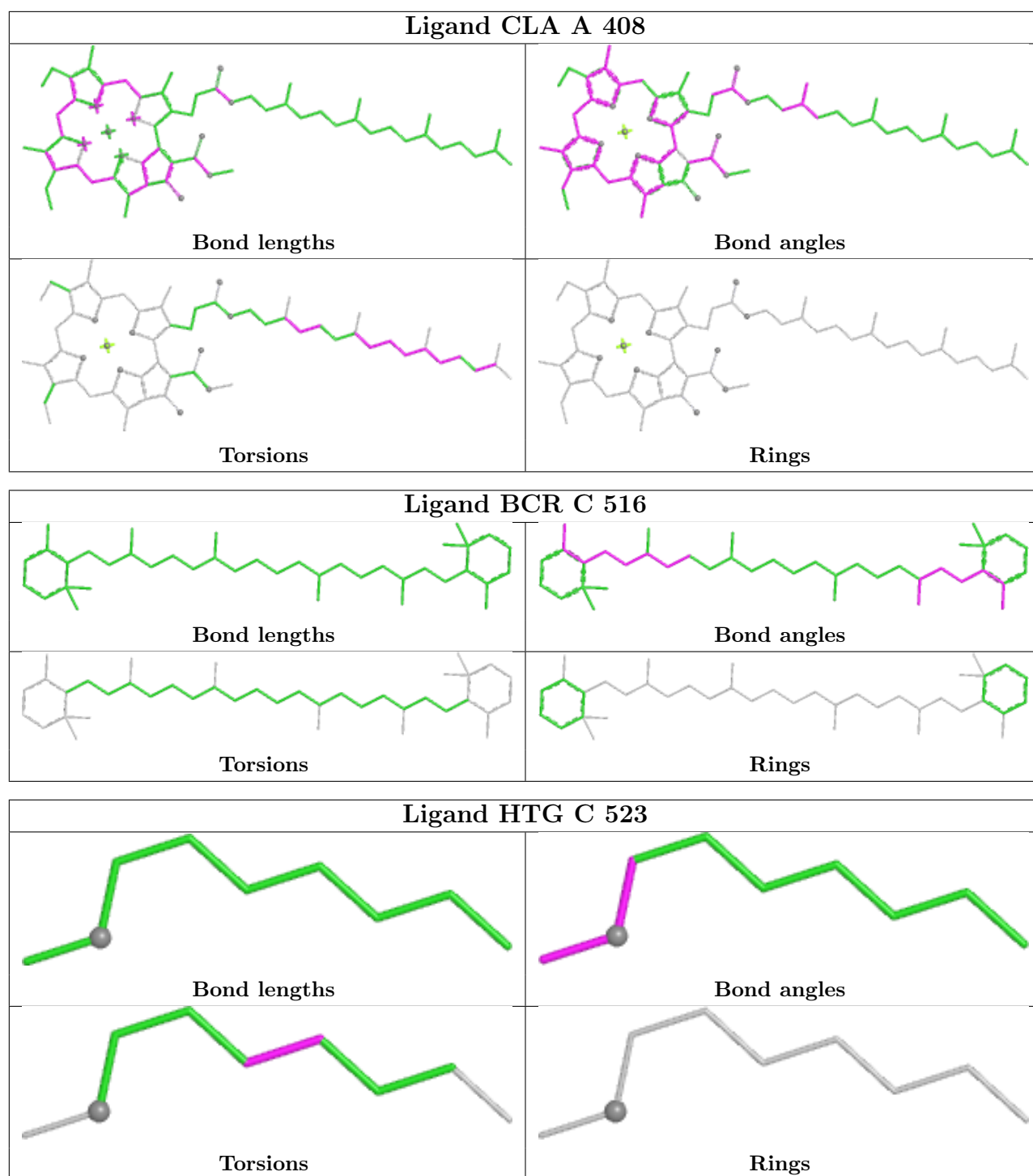


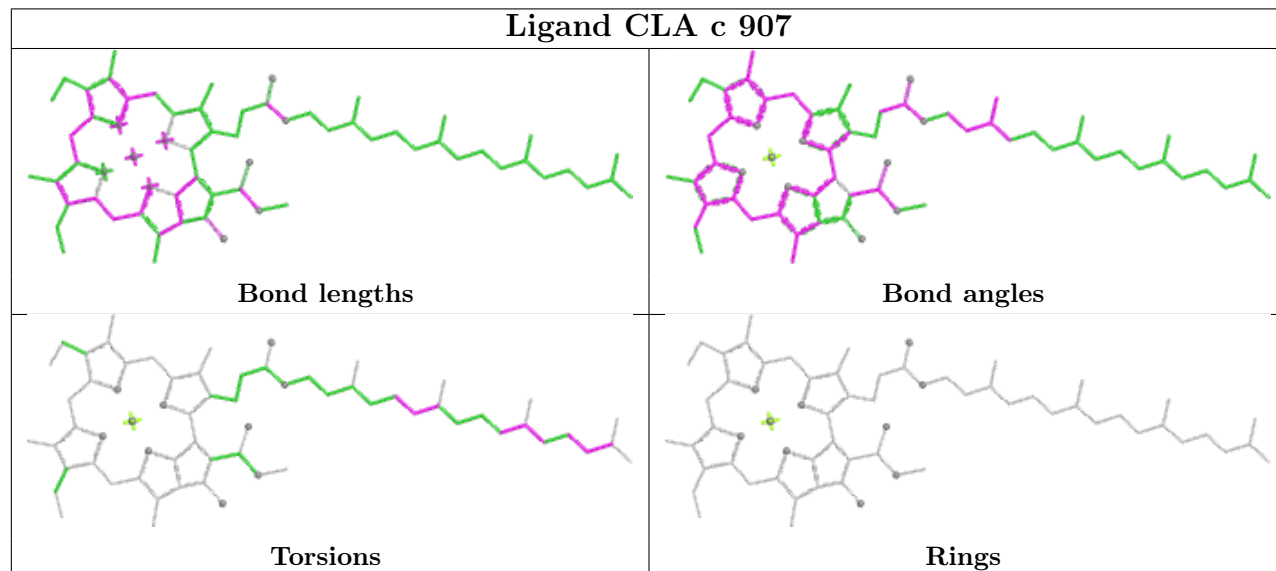
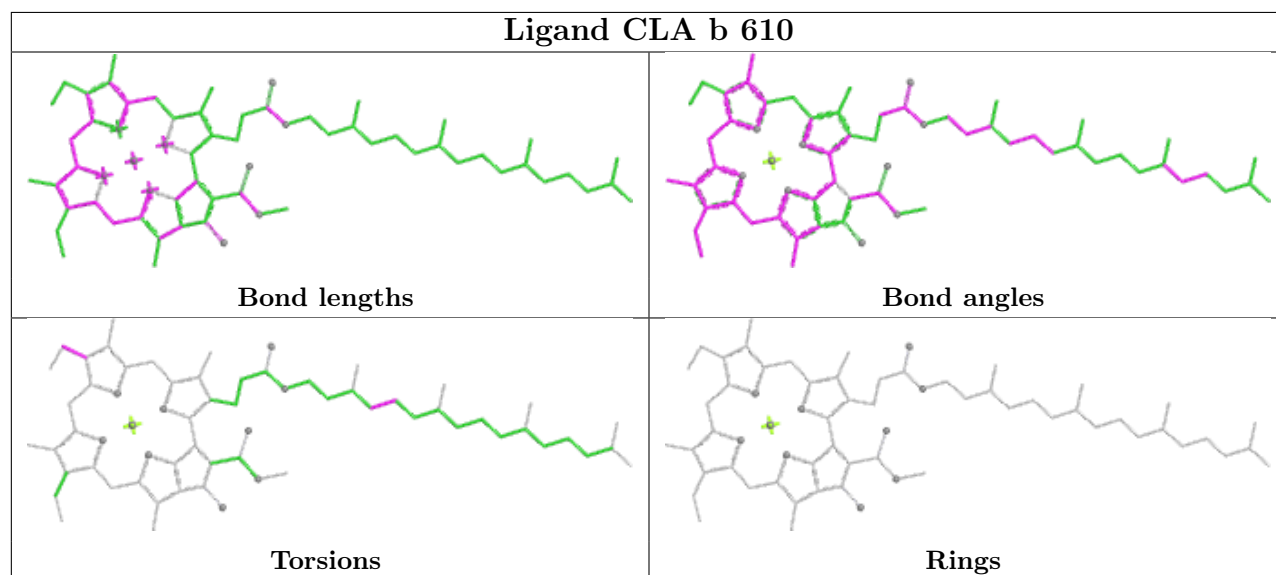
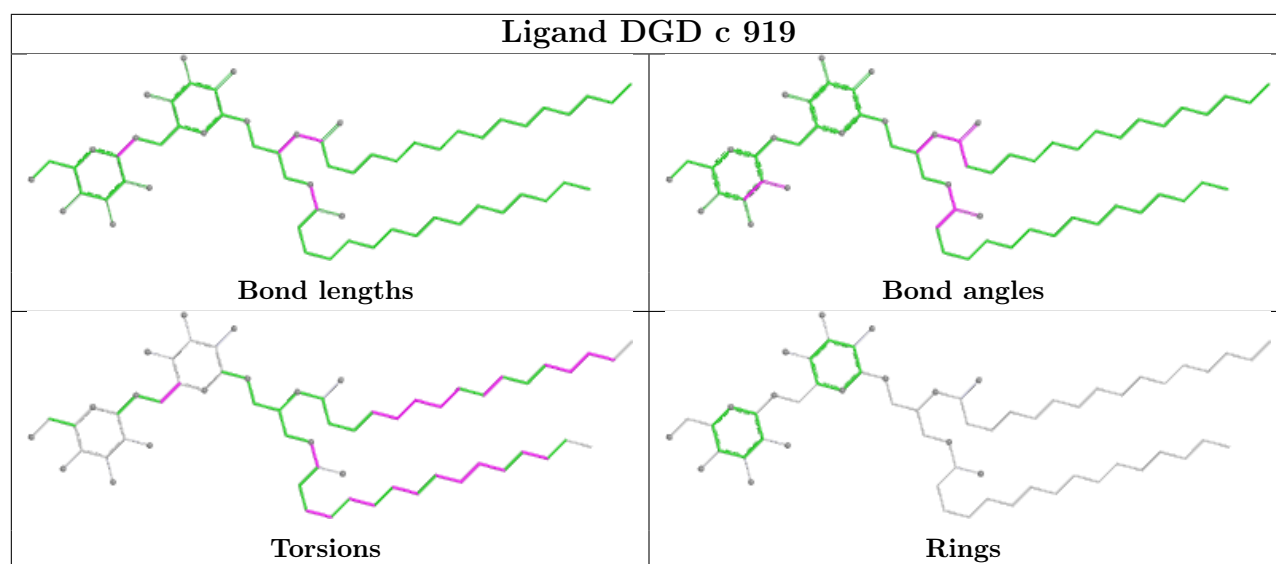
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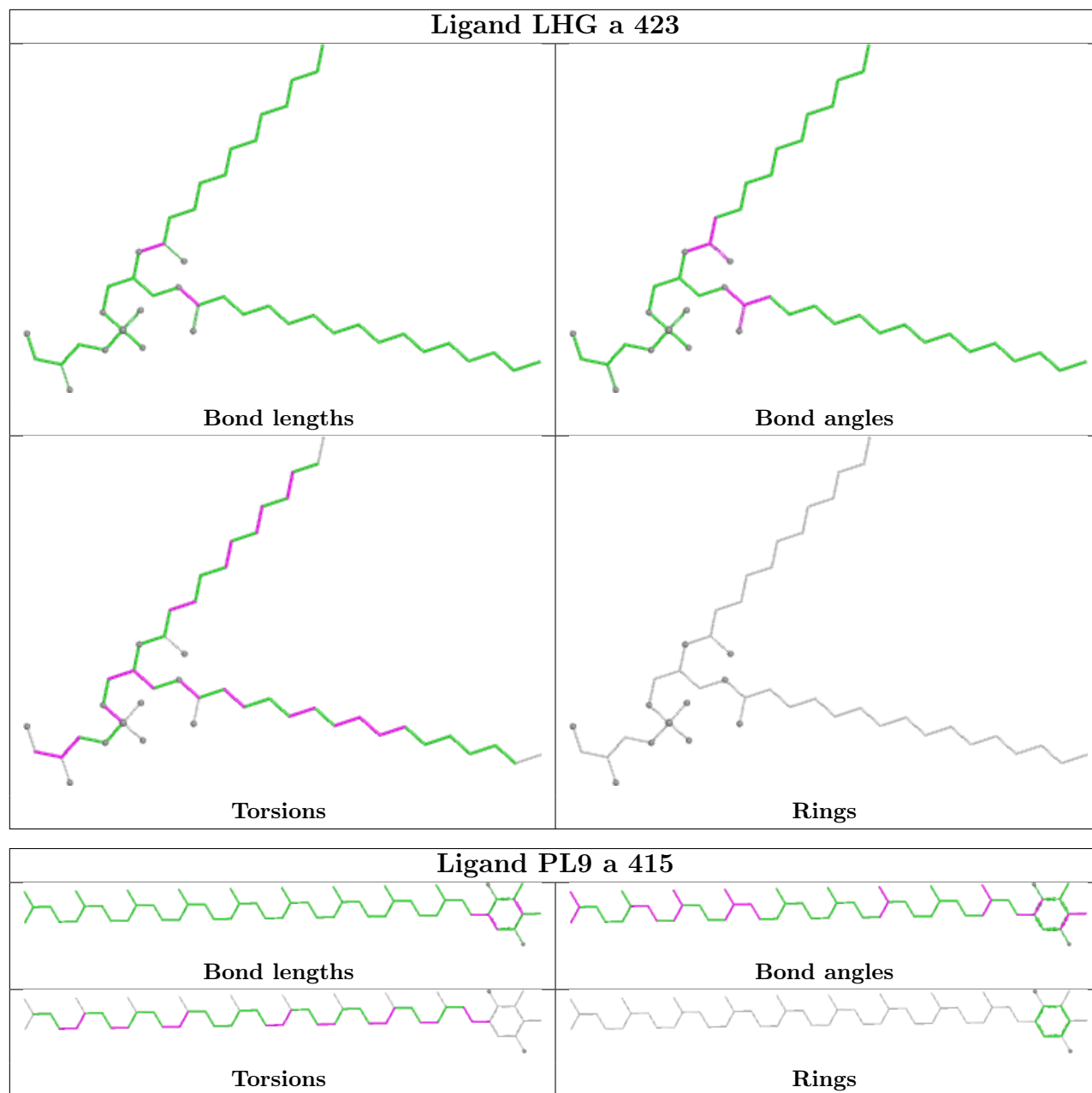


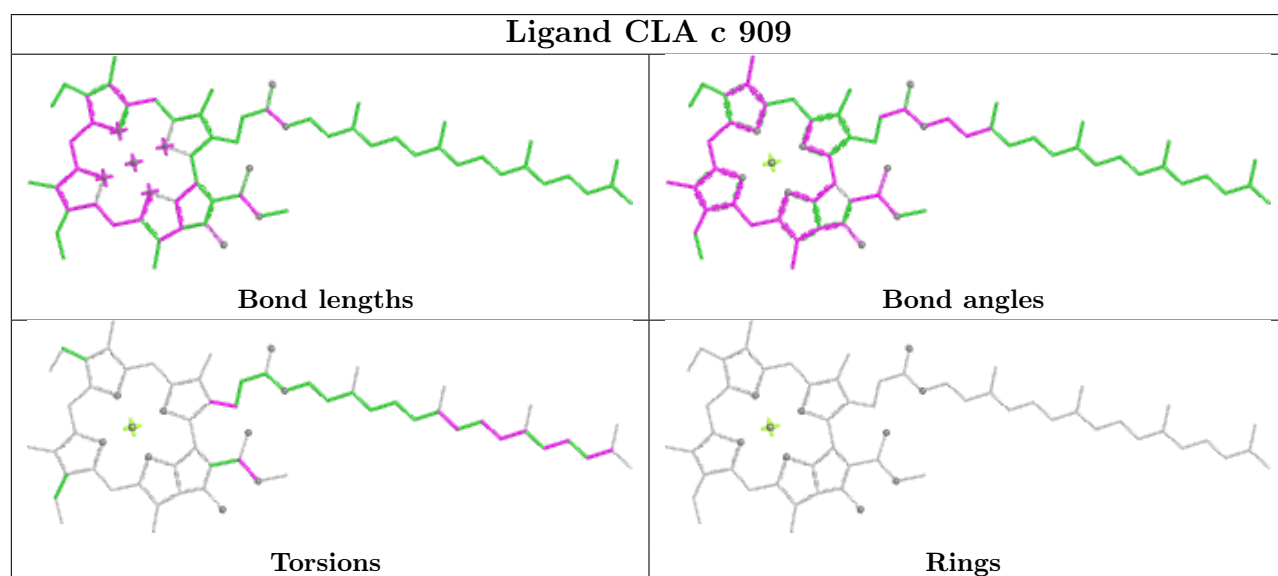
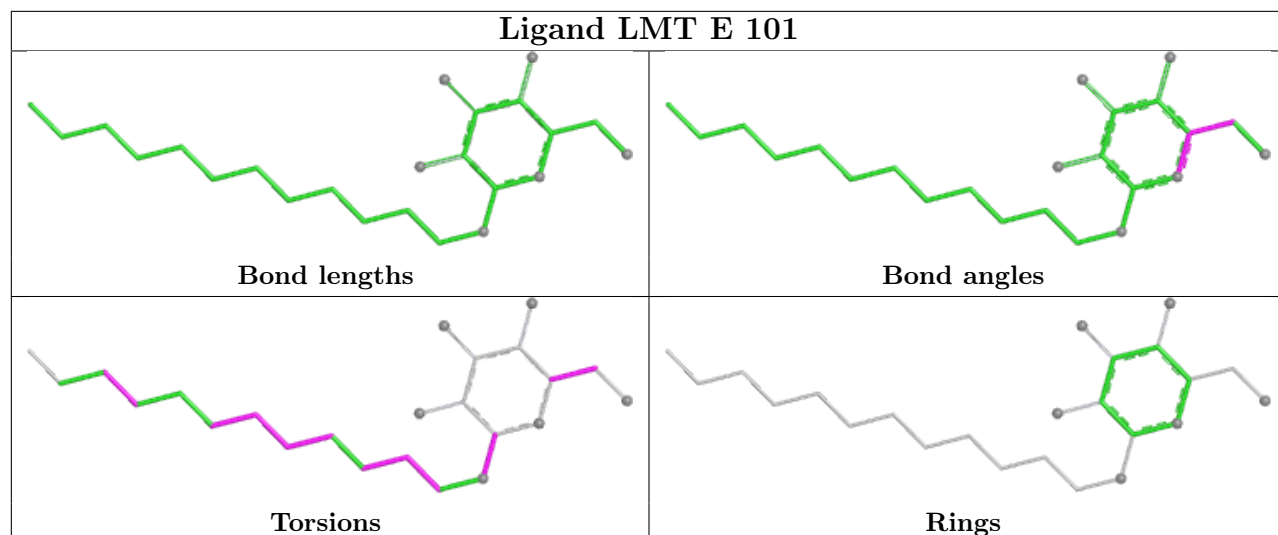
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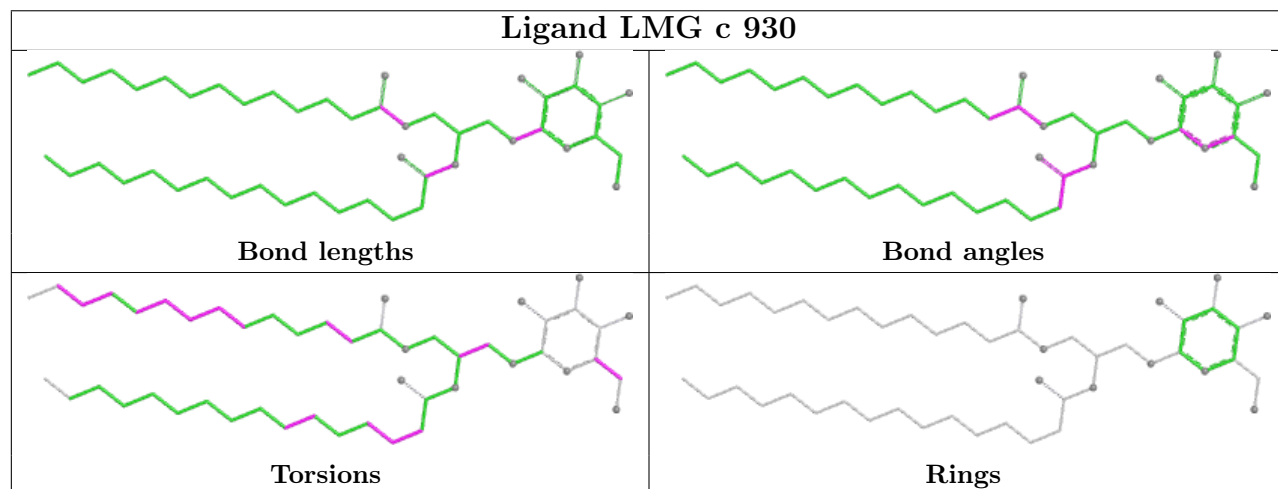
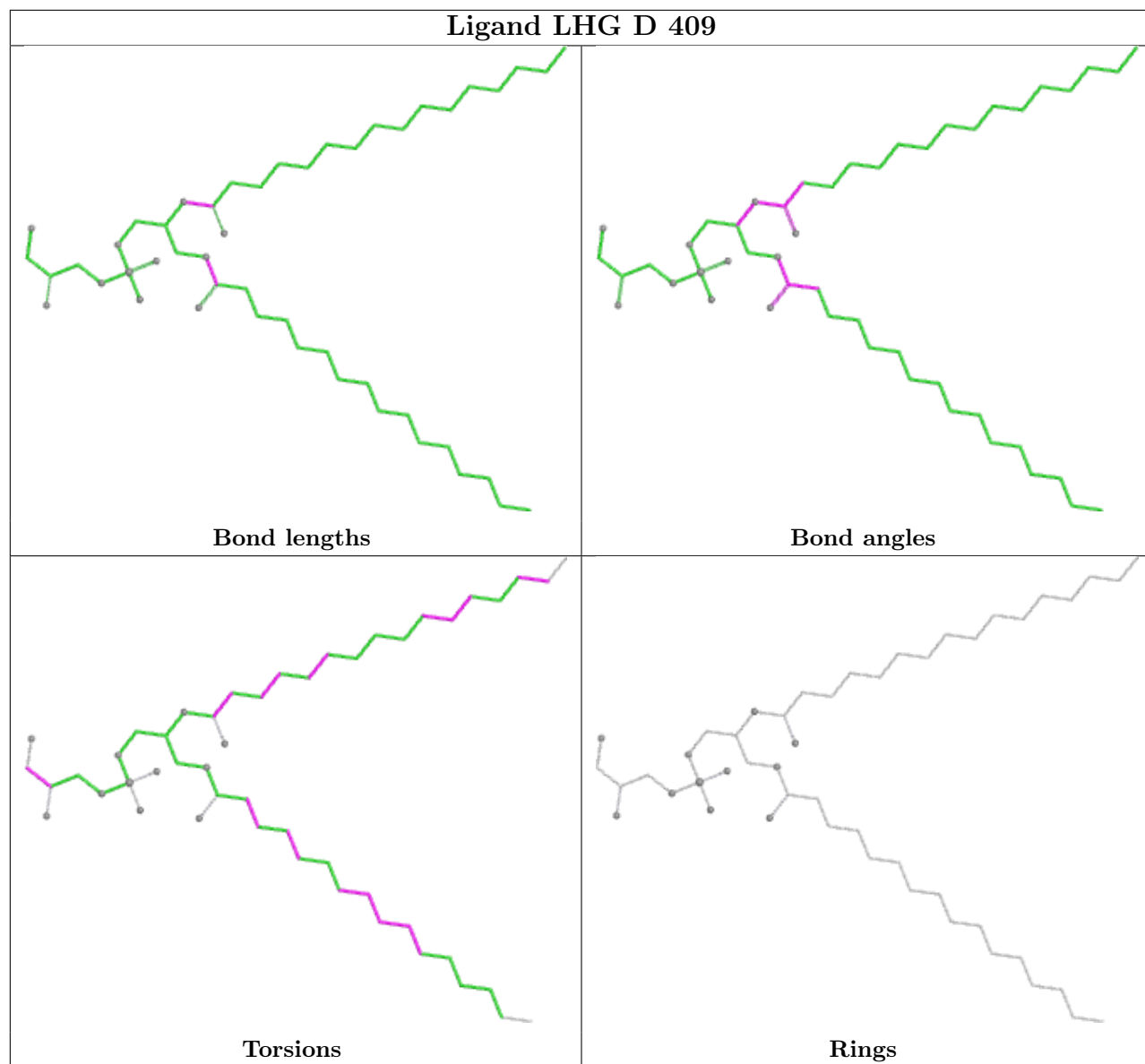


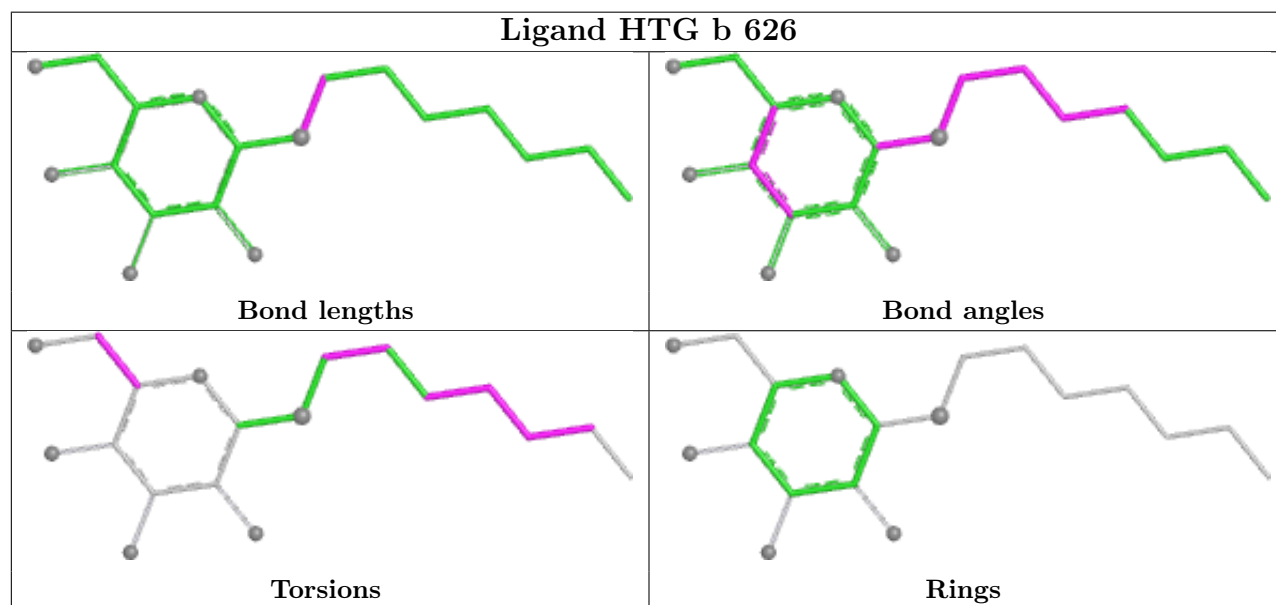
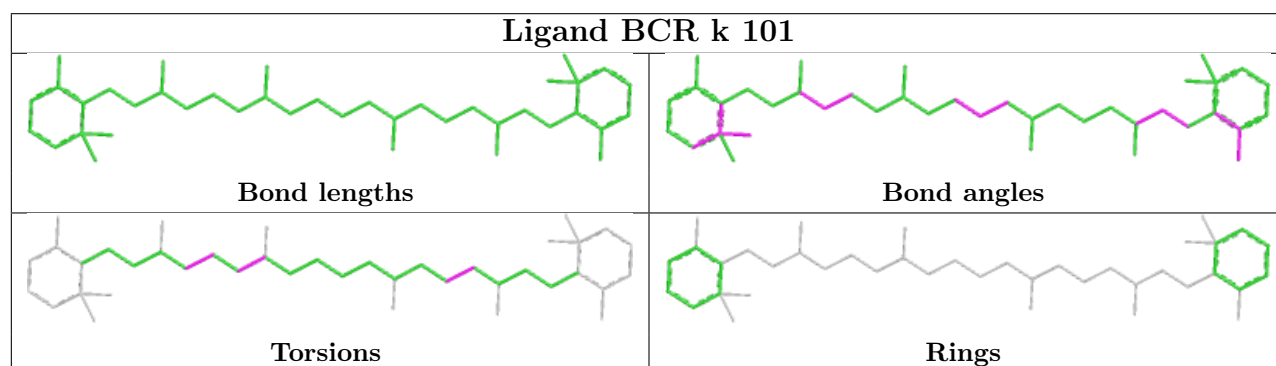
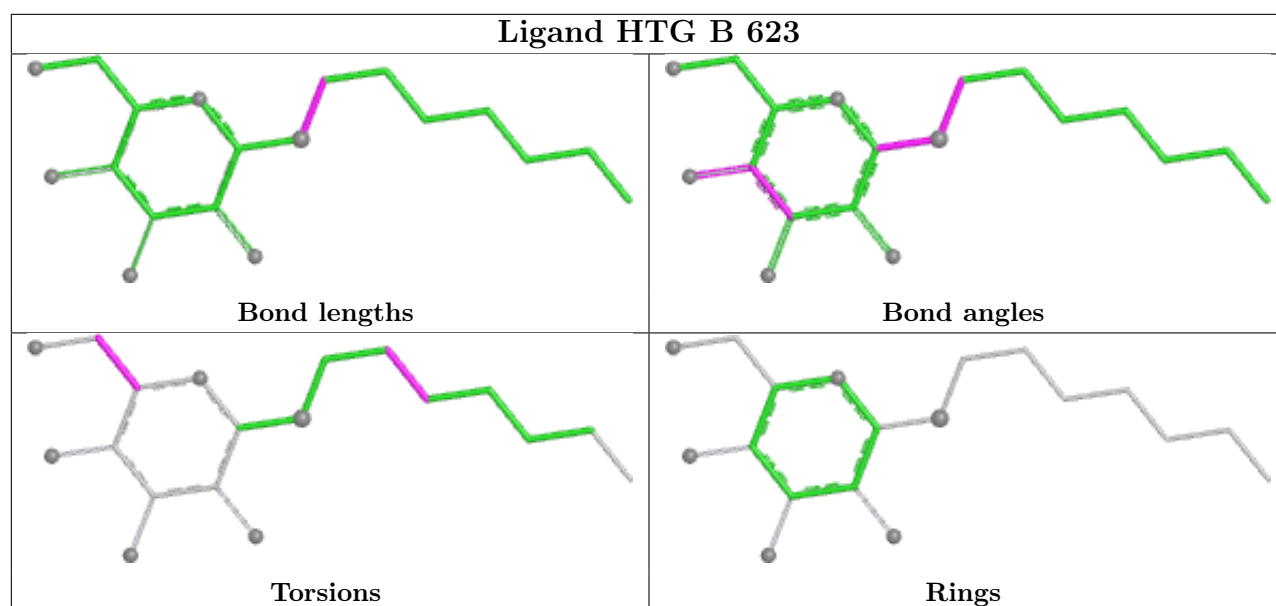


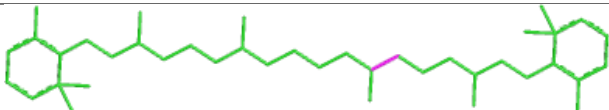
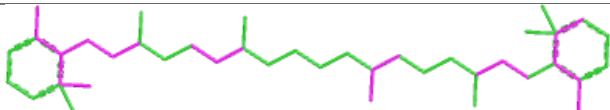
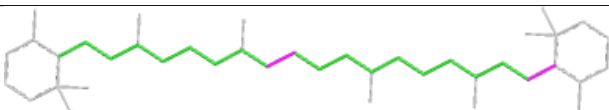
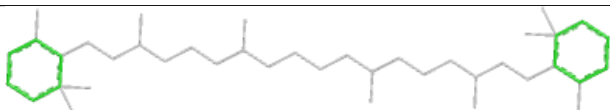


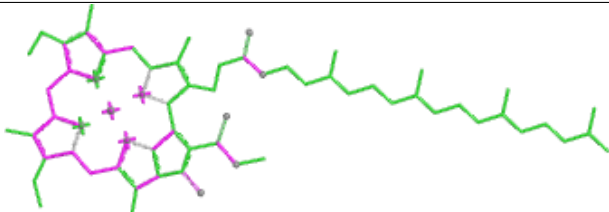
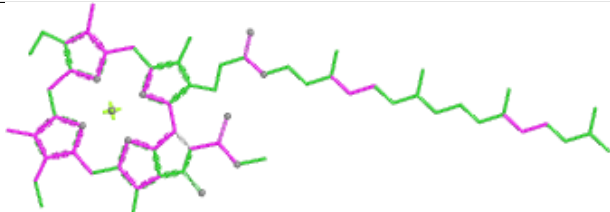
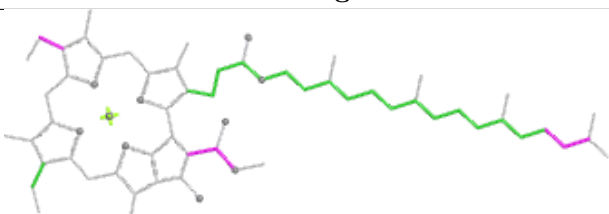
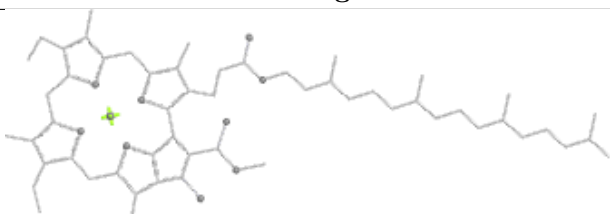


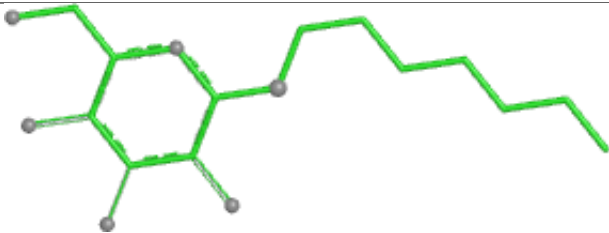
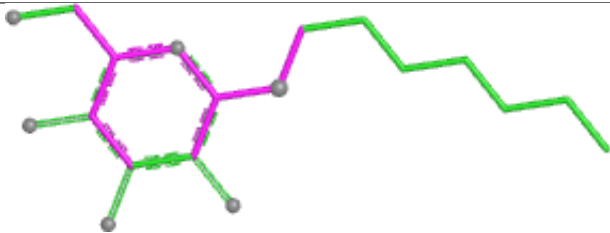
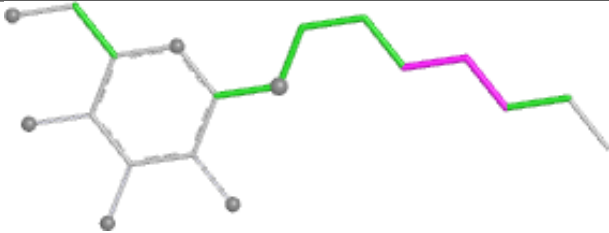
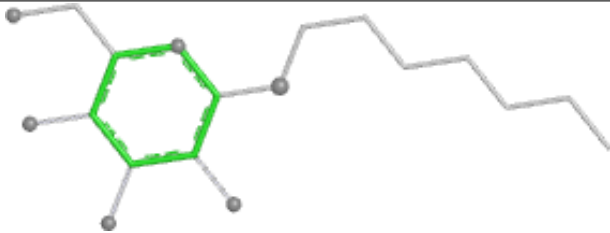


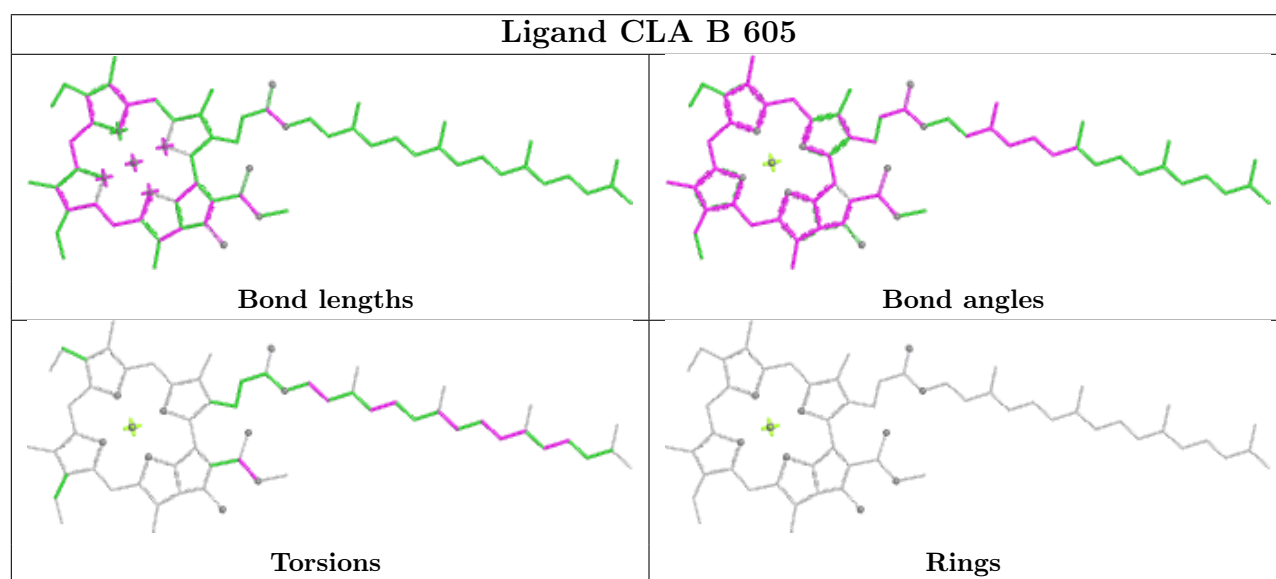
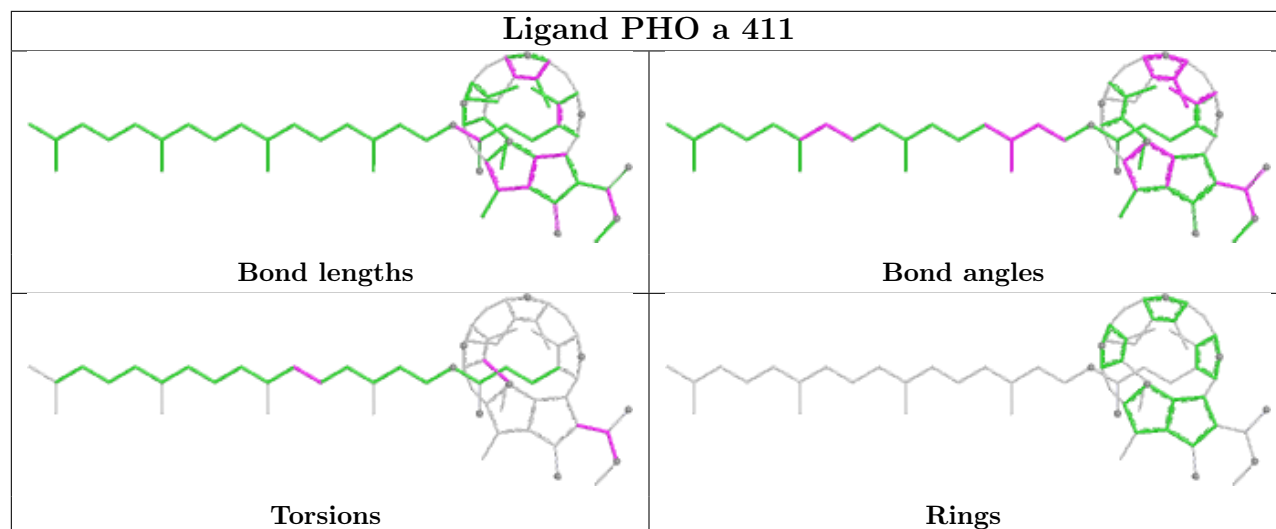


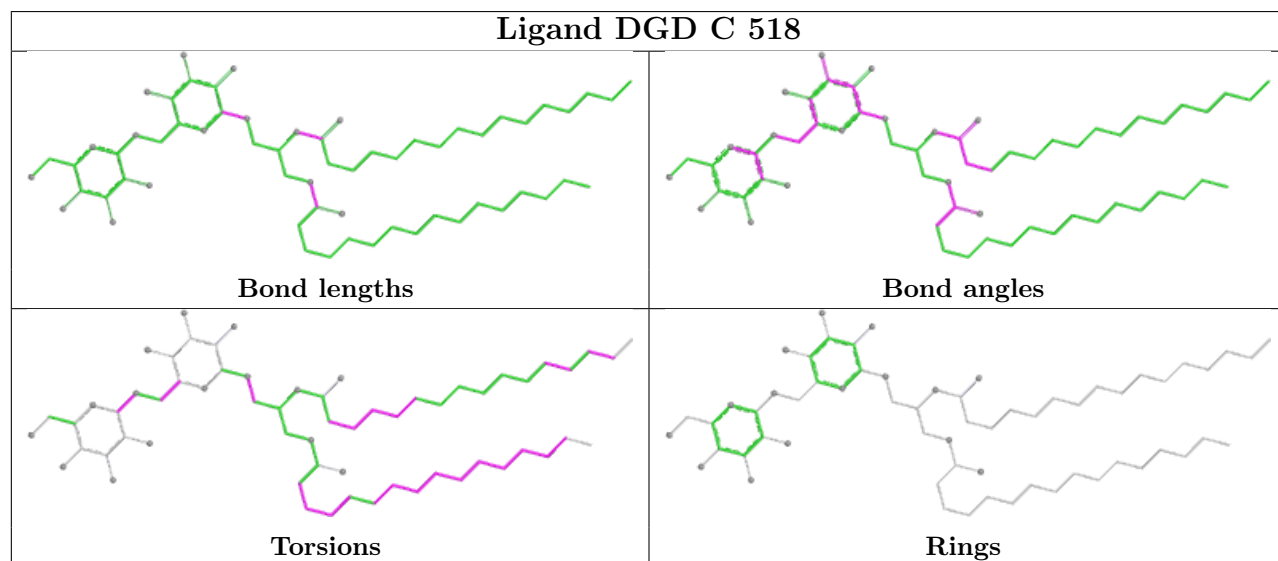
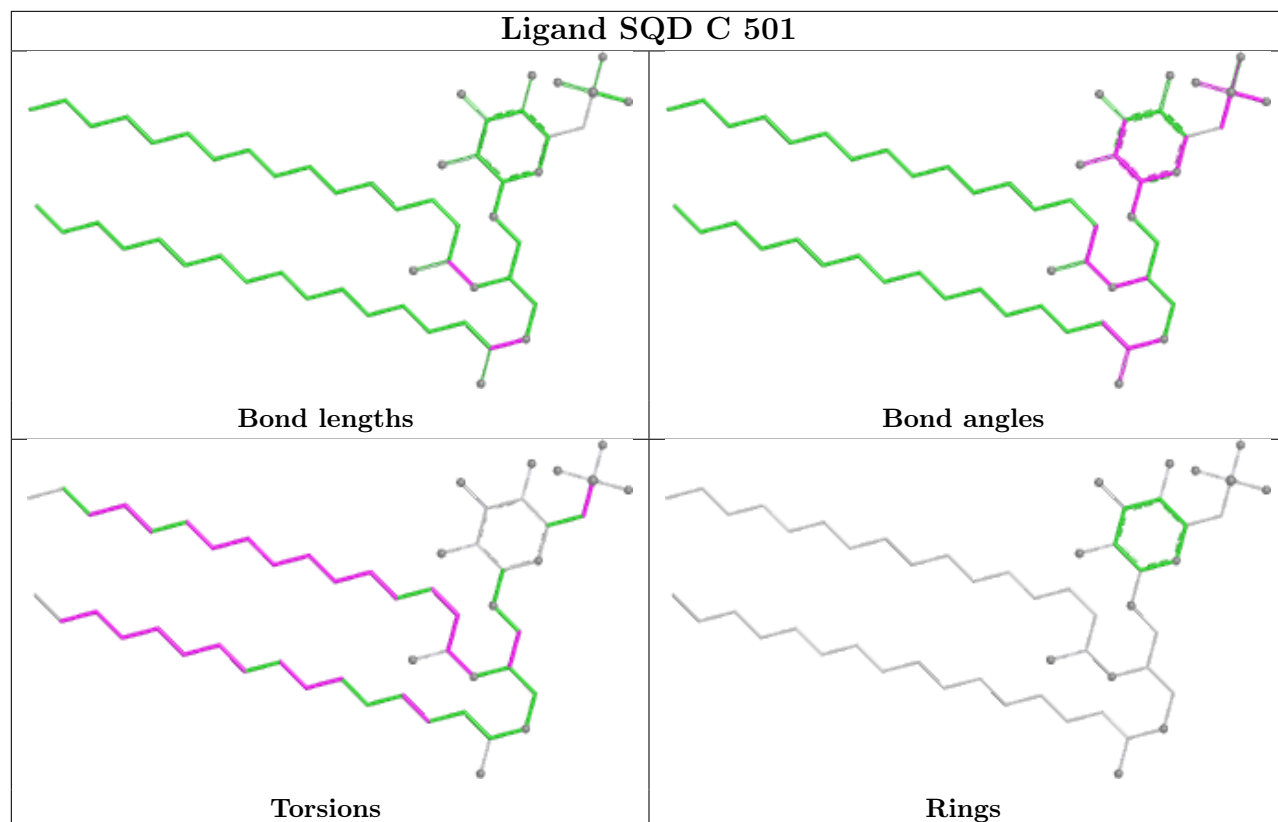


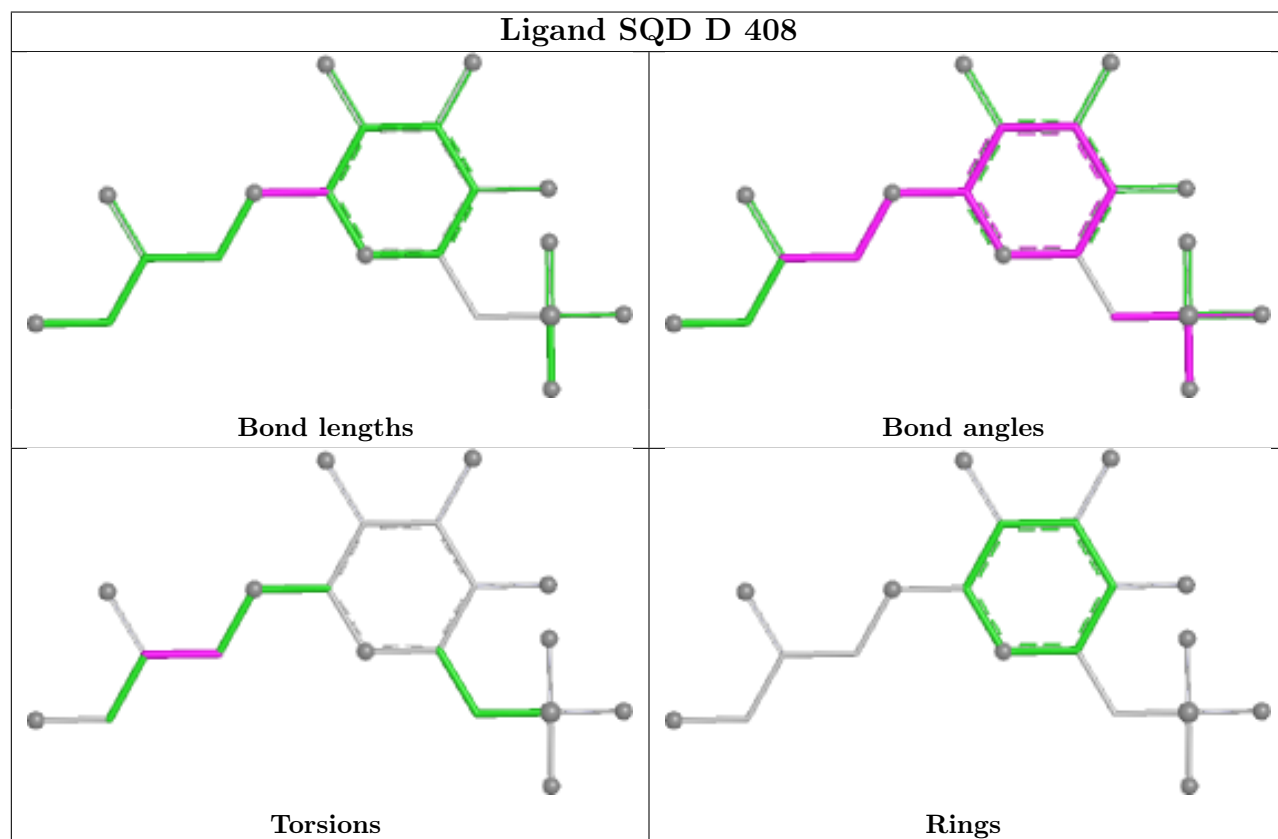
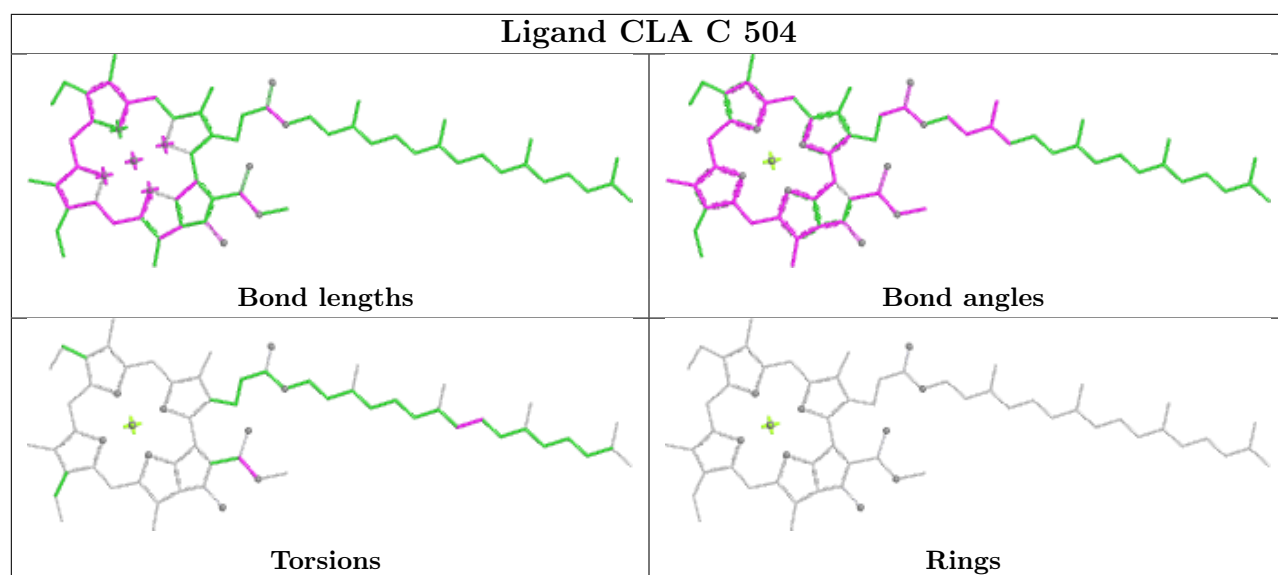
Ligand BCR C 515	
	
Bond lengths	Bond angles
	
Torsions	Rings

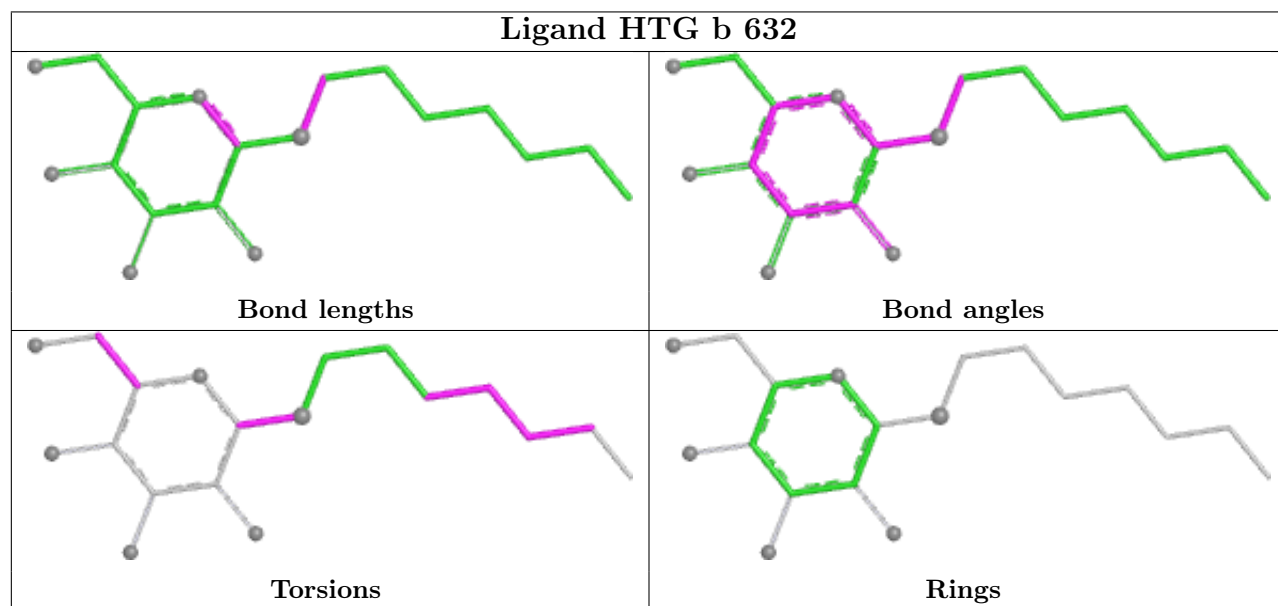
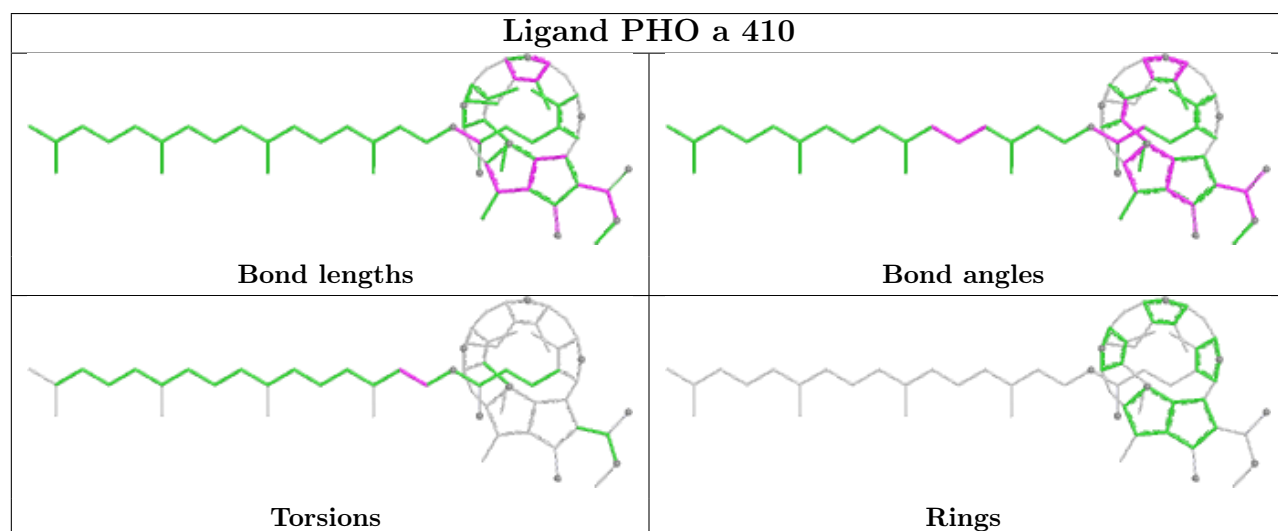
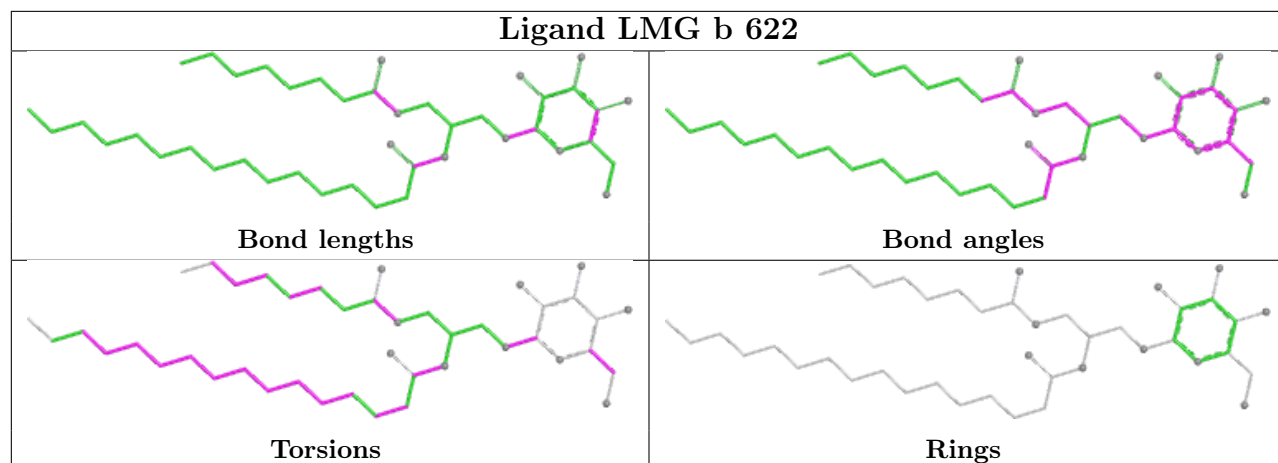
Ligand CLA C 503	
	
Bond lengths	Bond angles
	
Torsions	Rings

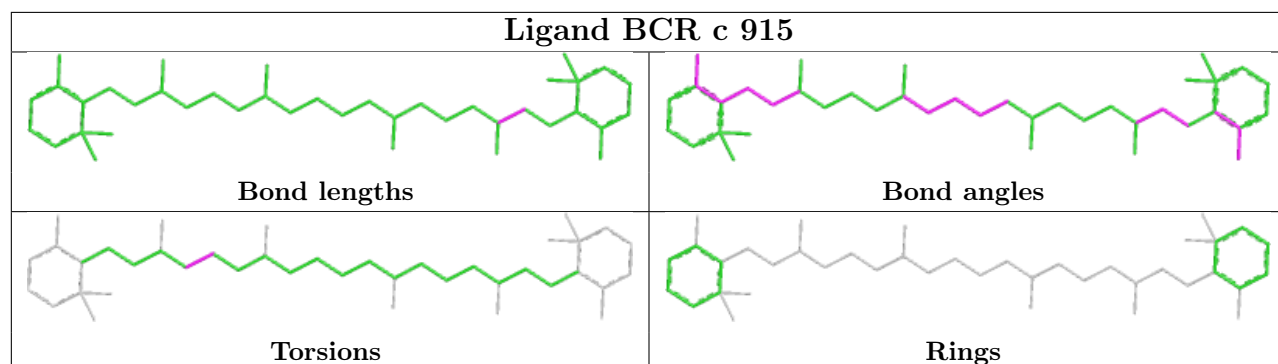
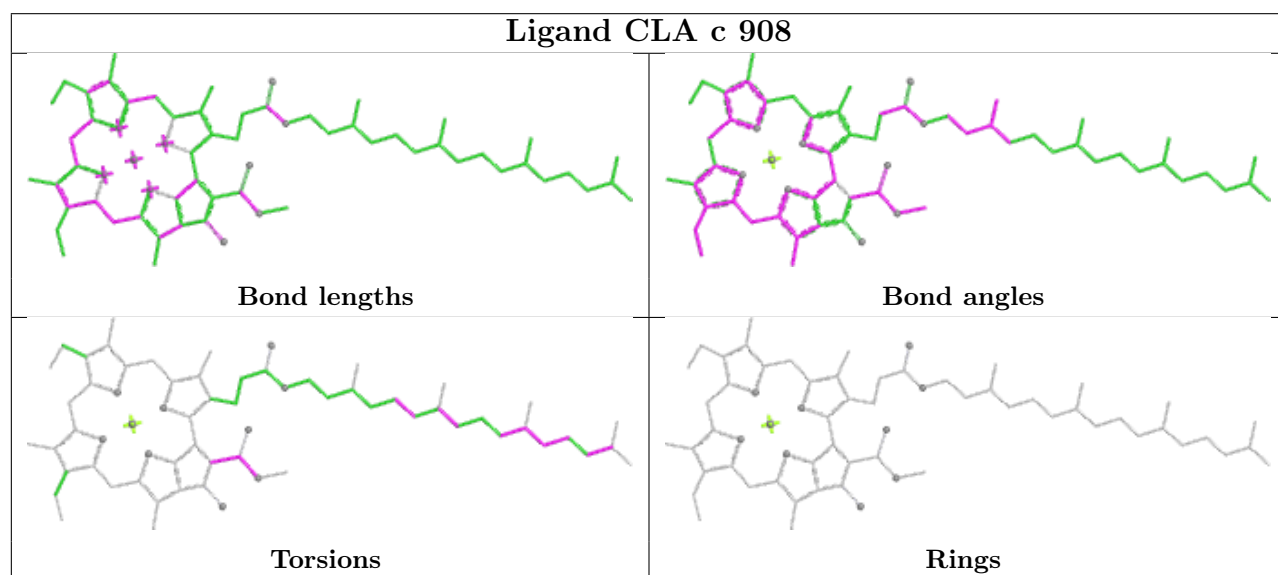
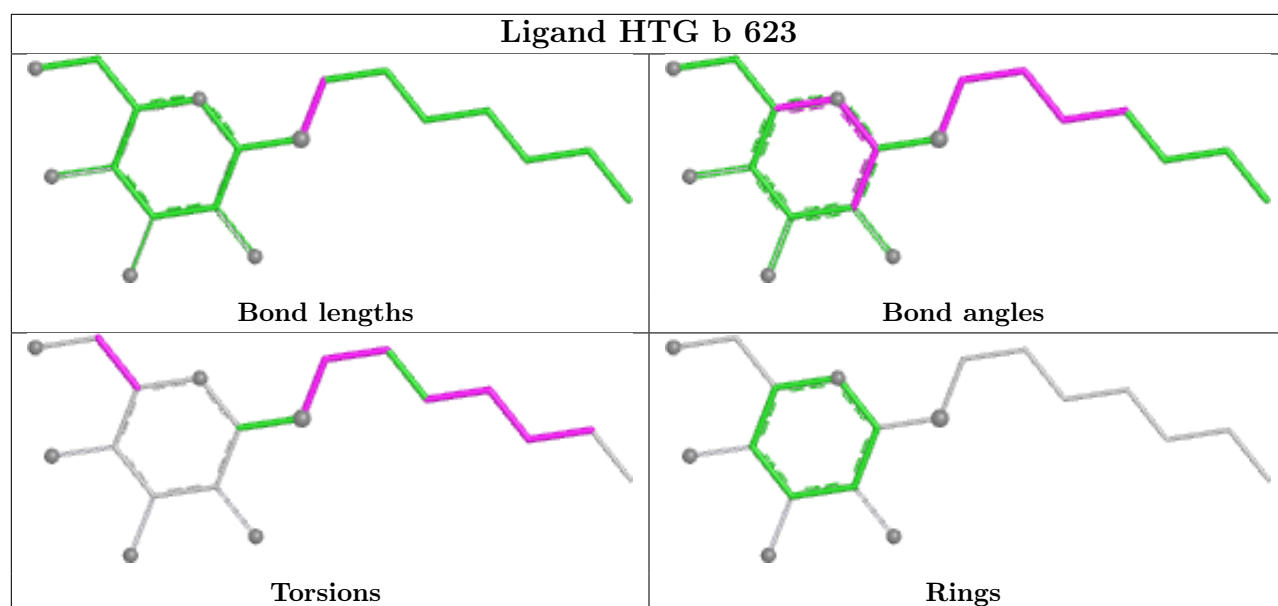
Ligand HTG B 626	
	
Bond lengths	Bond angles
	
Torsions	Rings

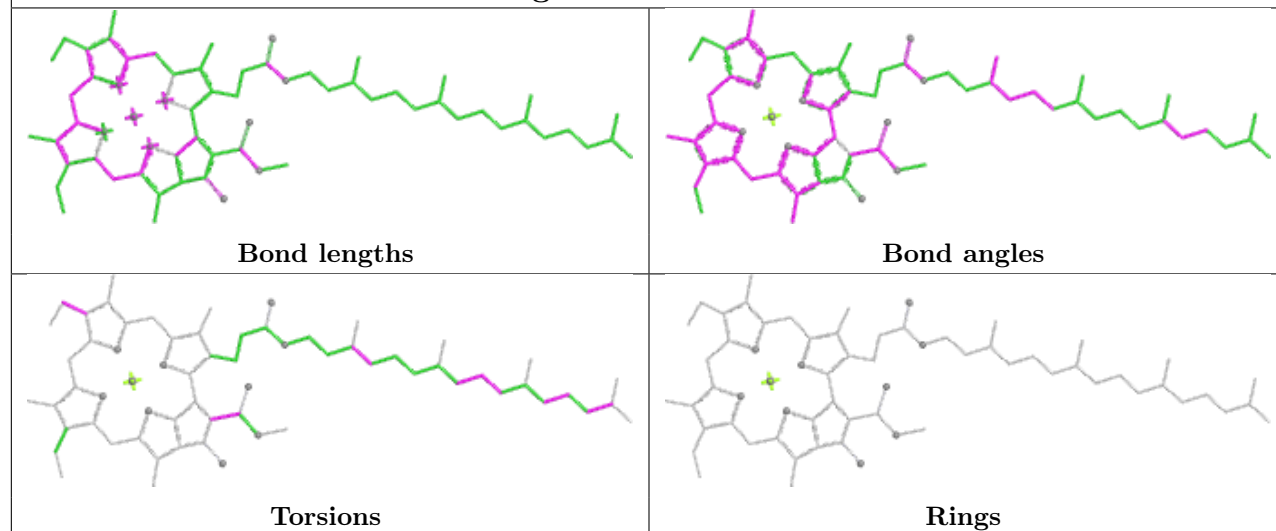
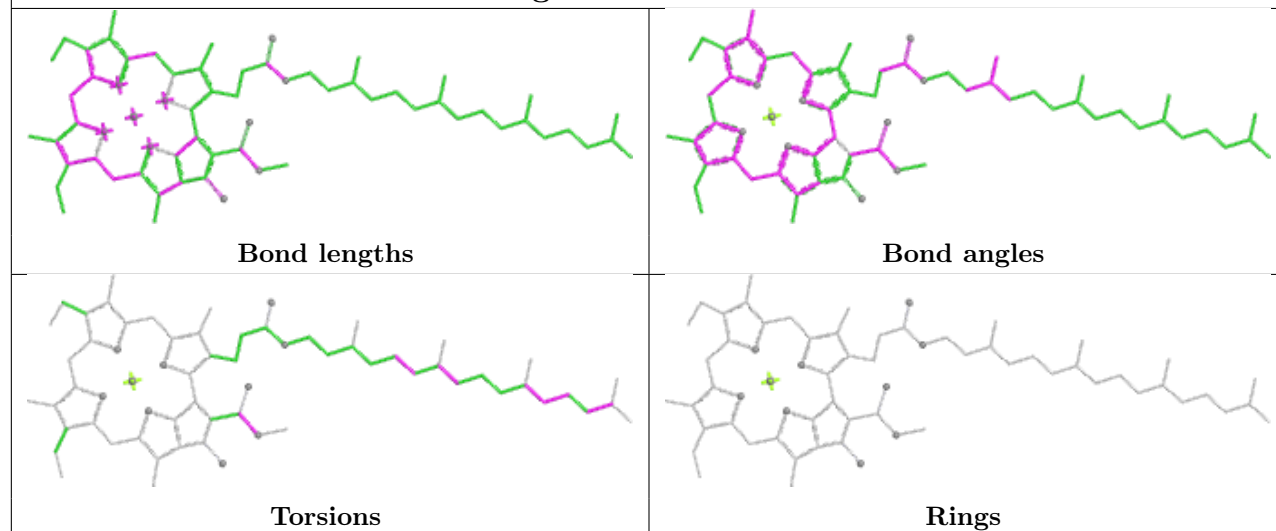


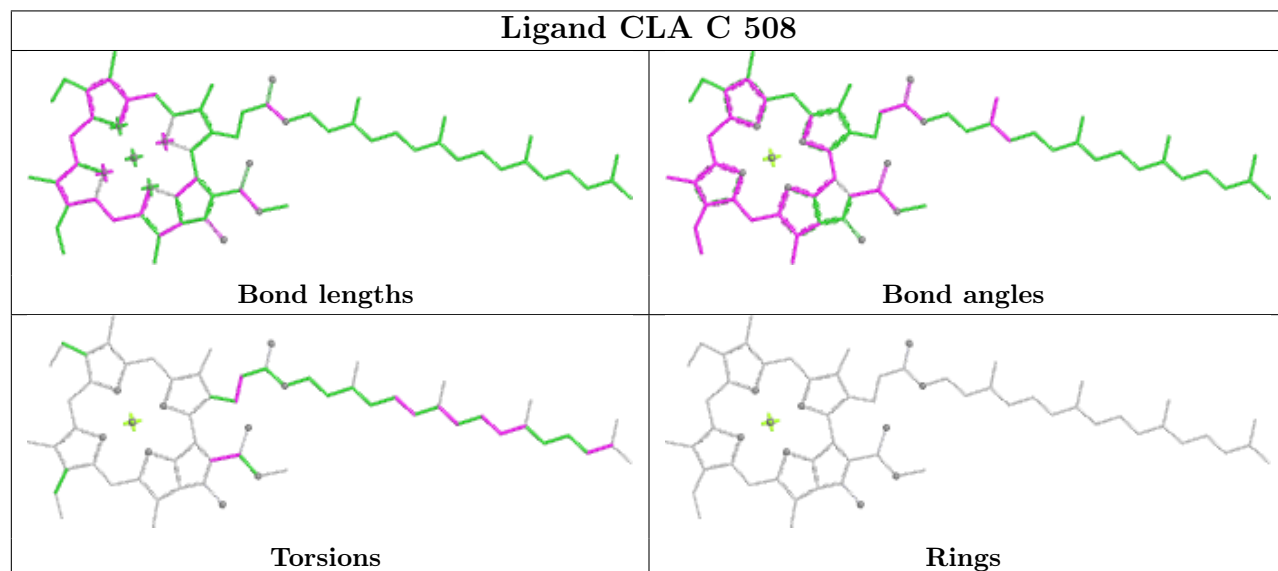
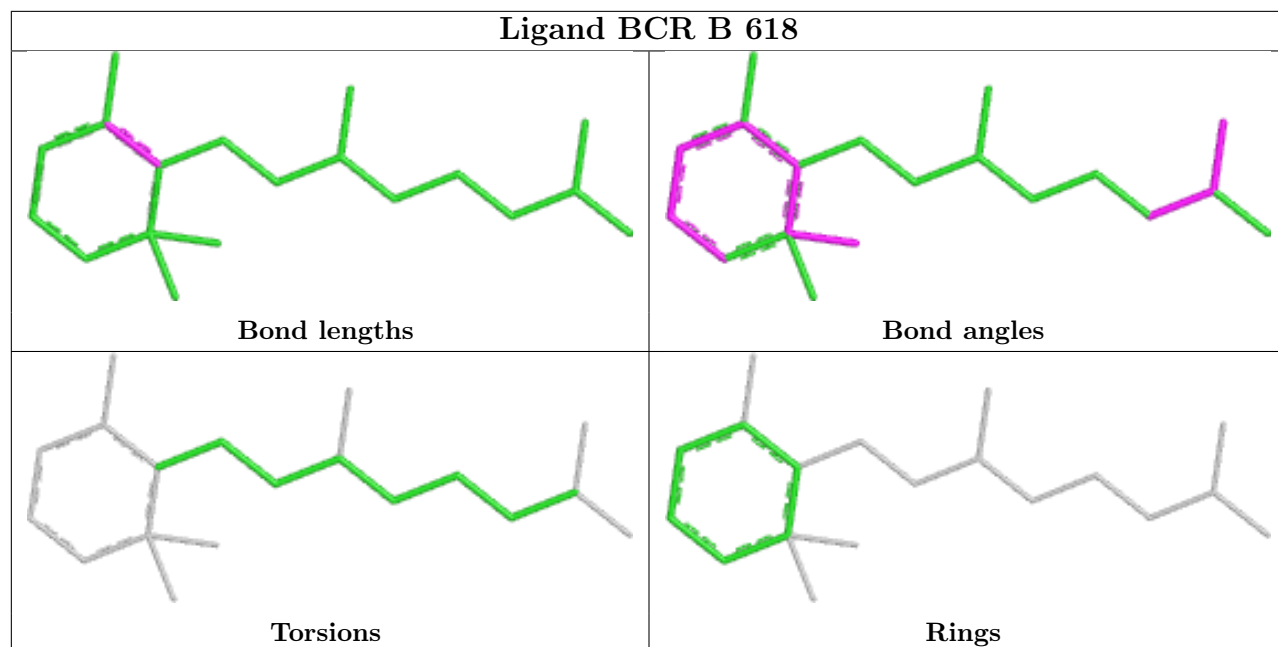


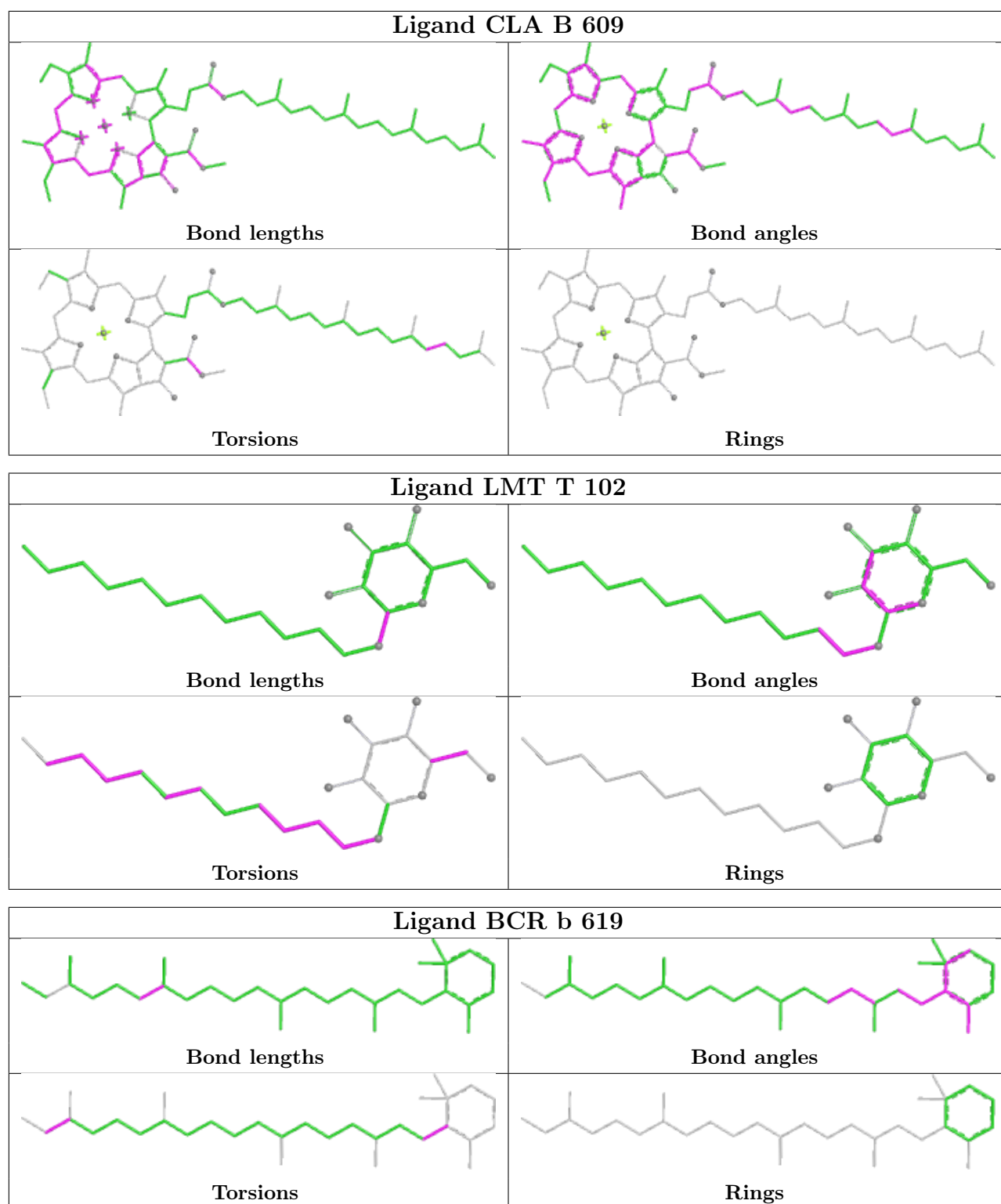


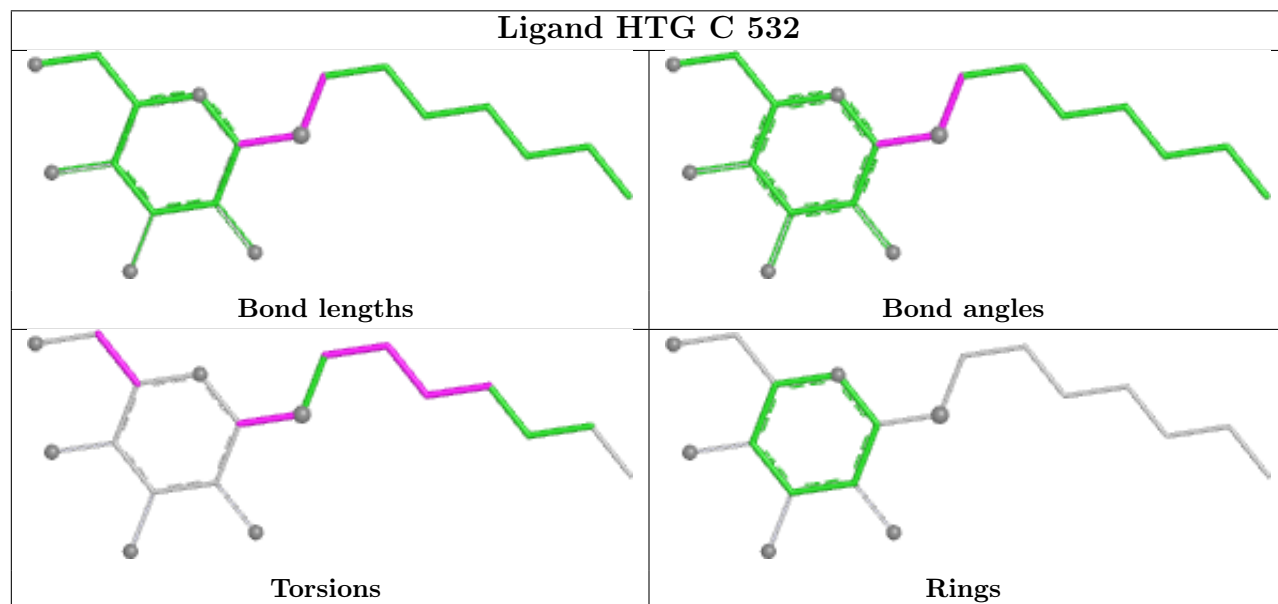
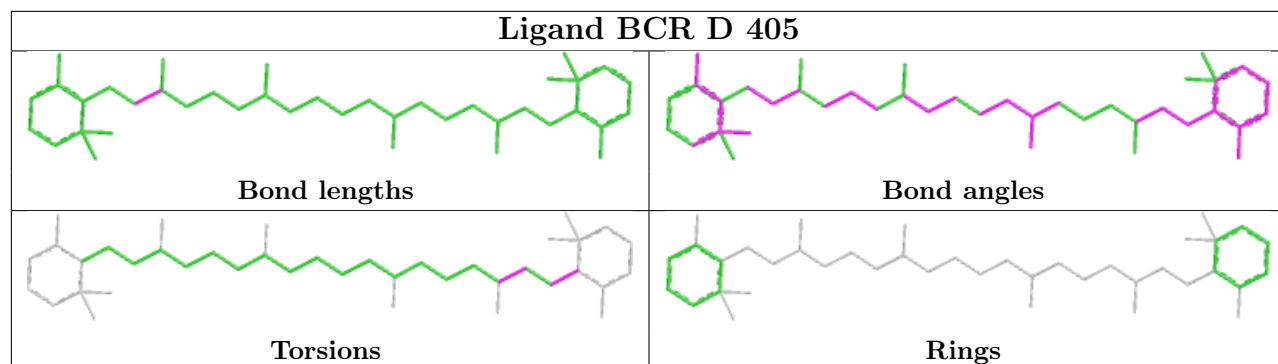


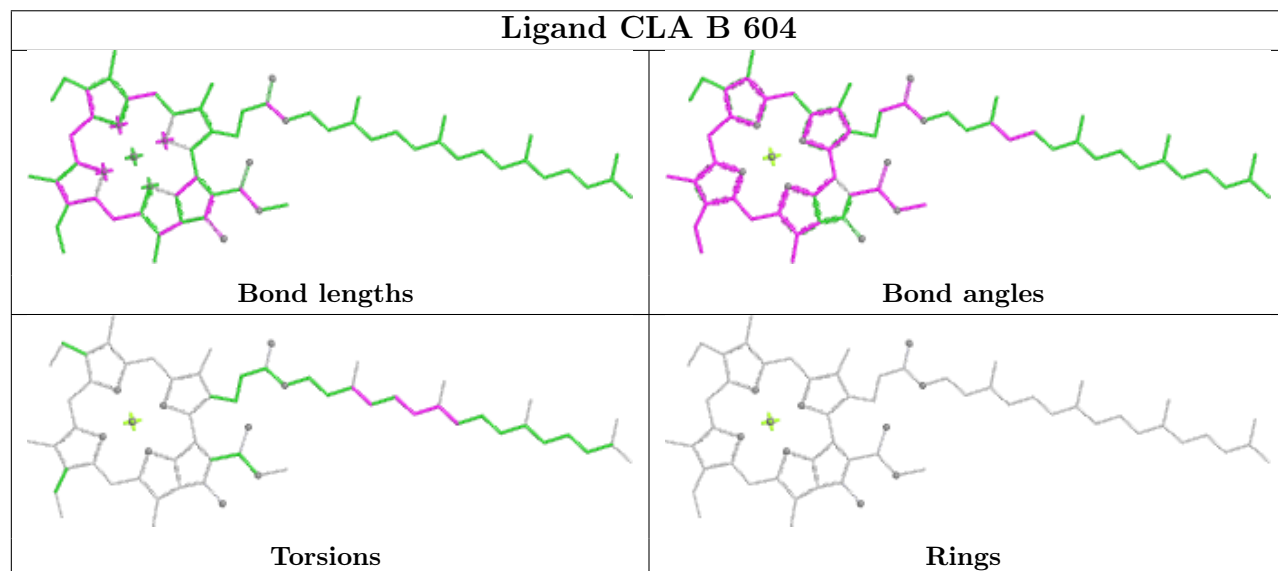
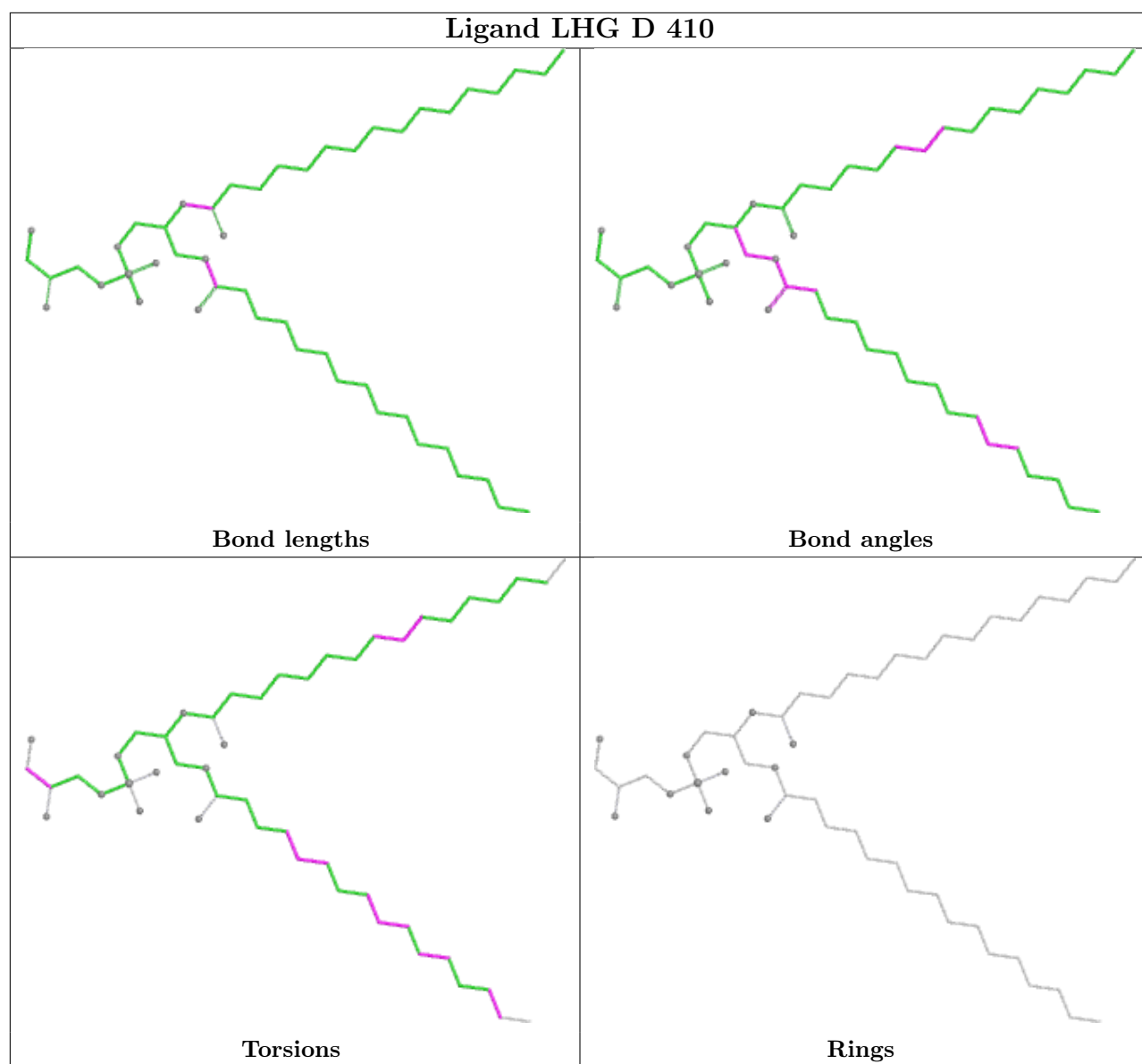


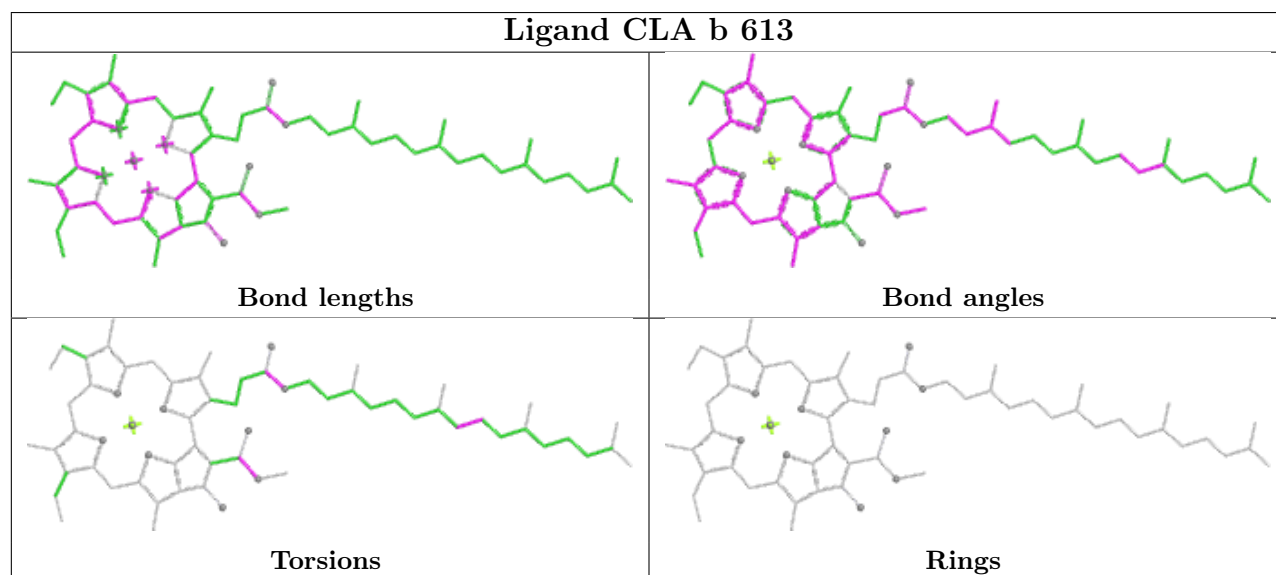
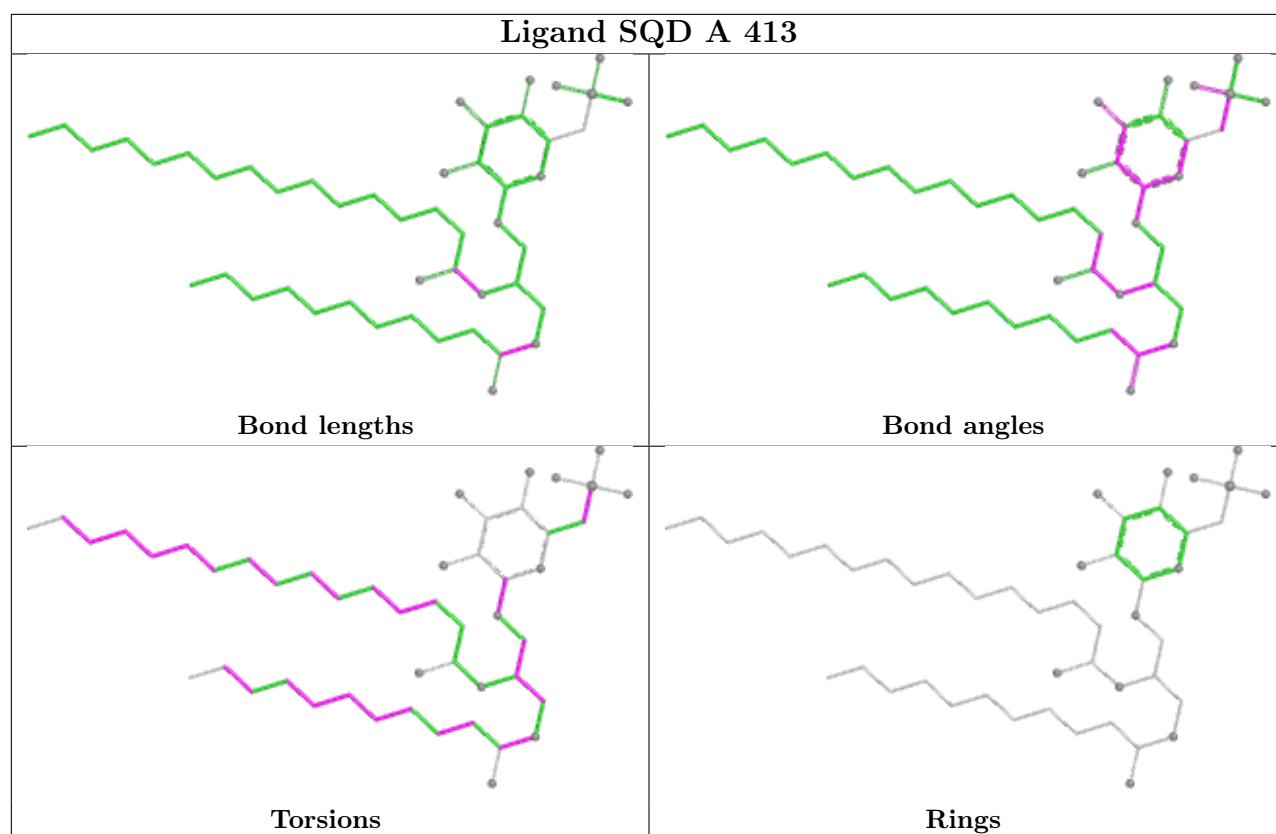
Ligand CLA B 606**Ligand CLA C 509**

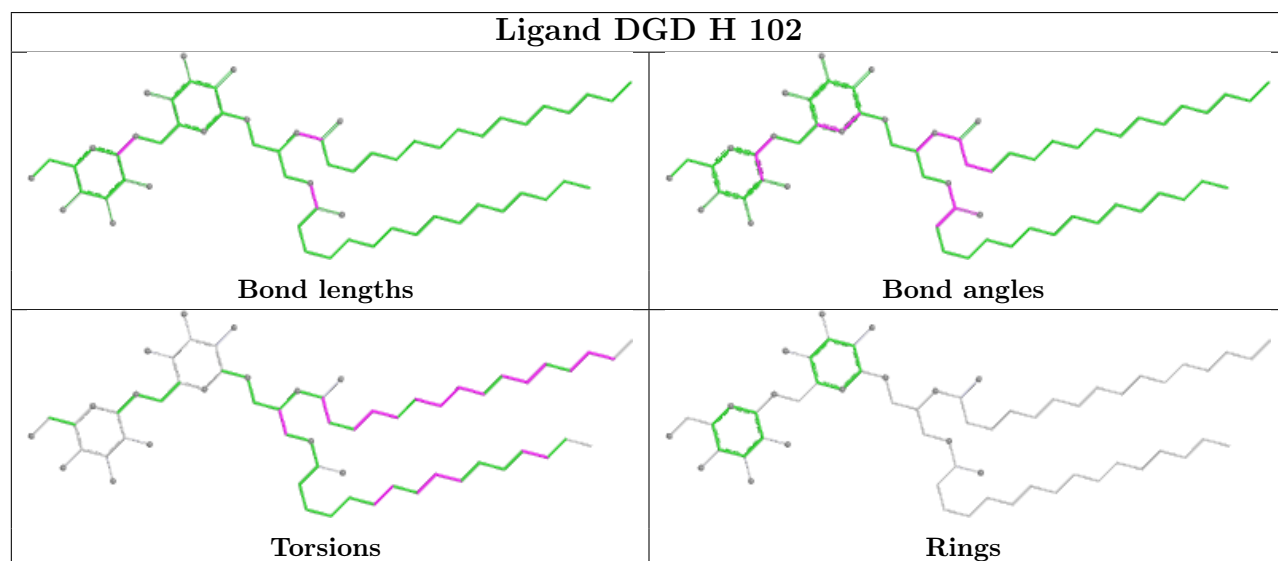
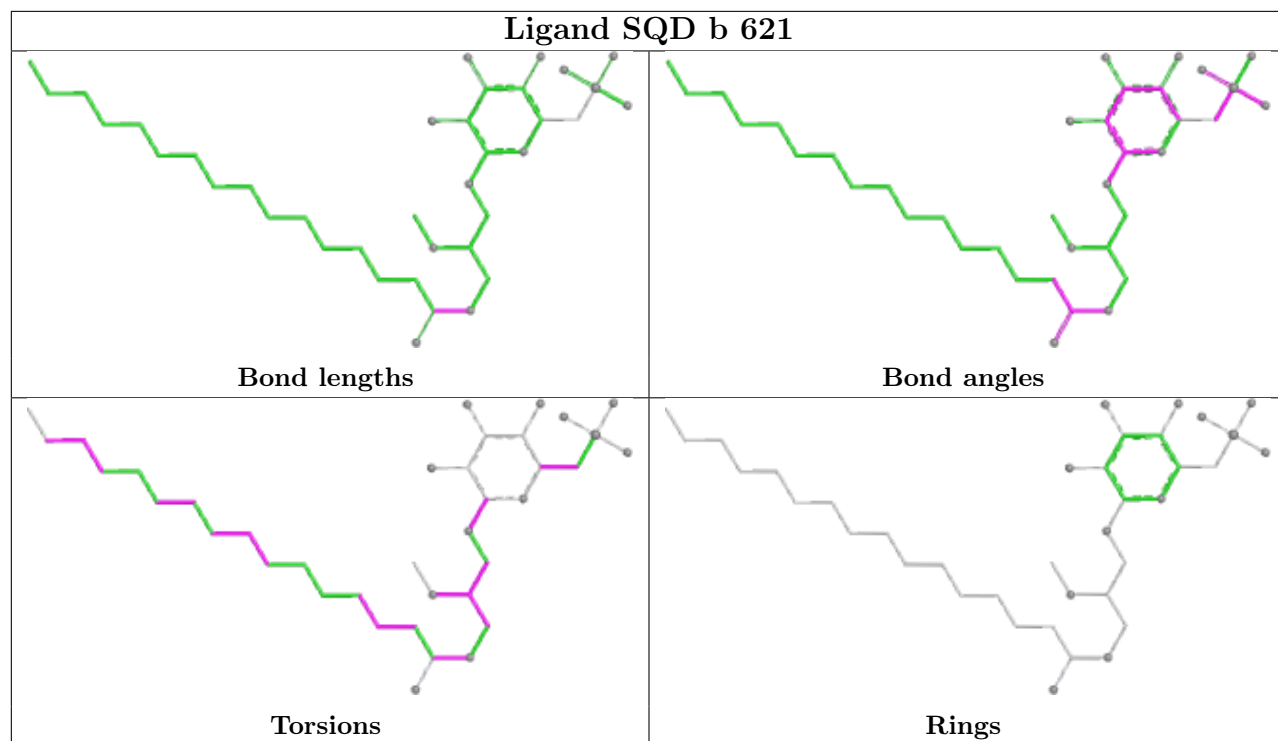


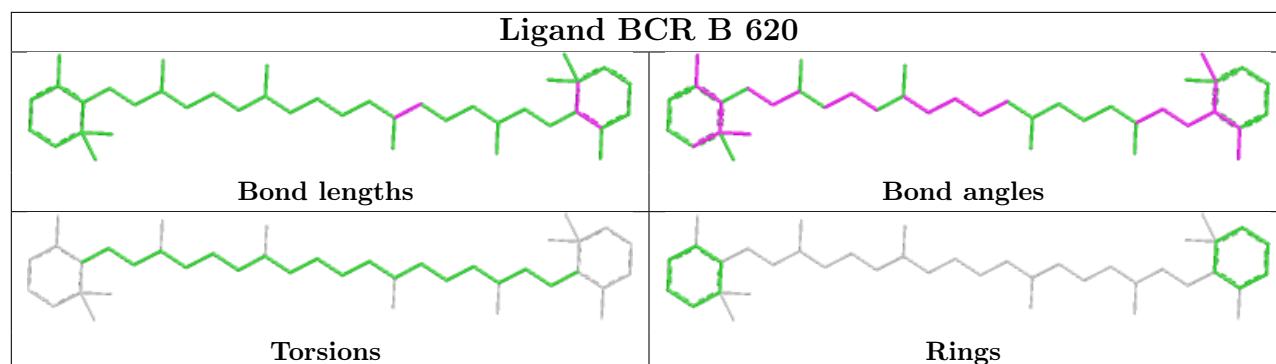
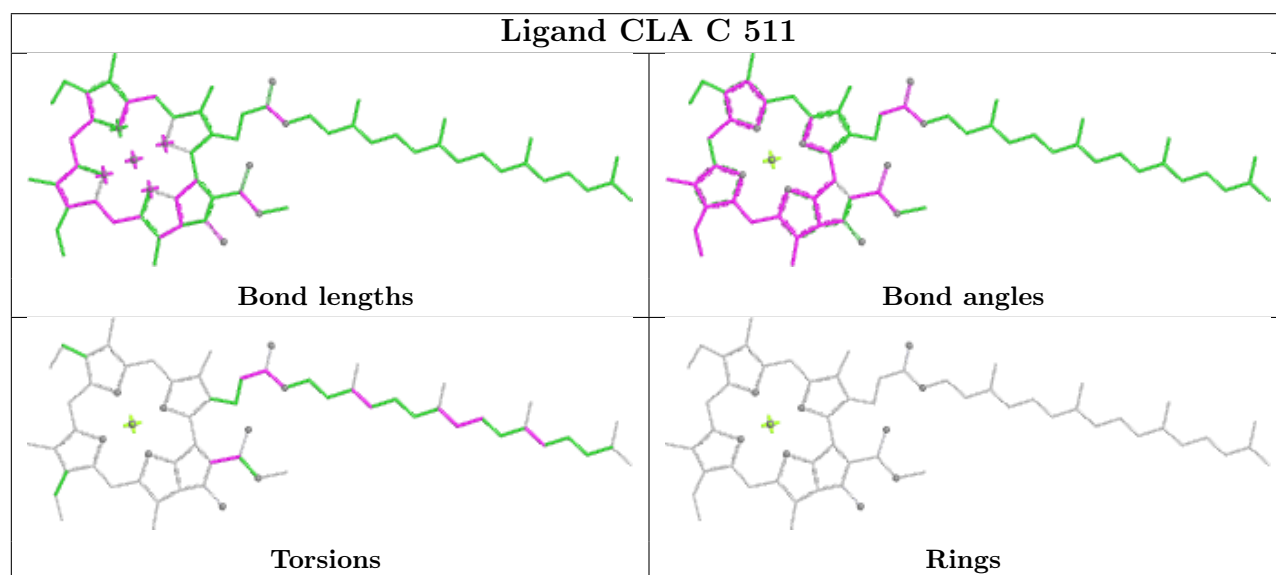
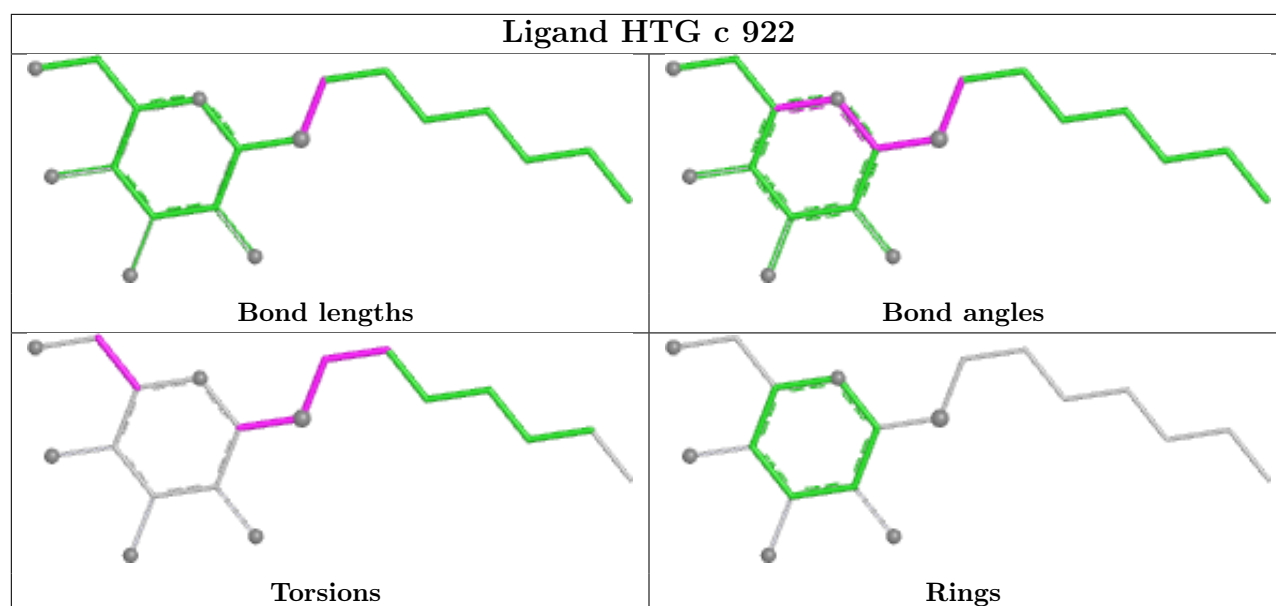


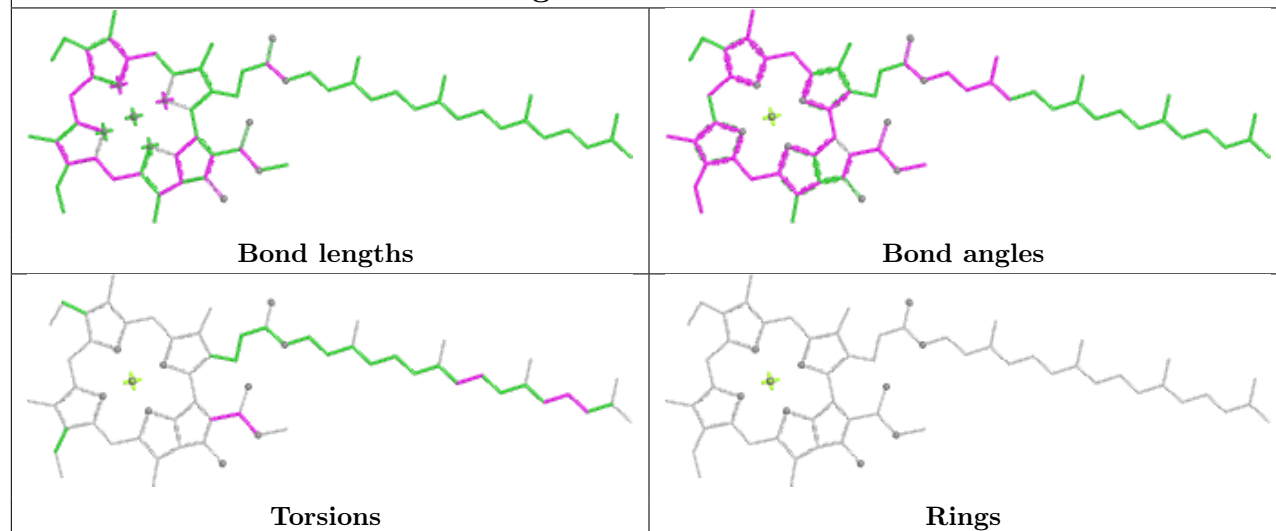
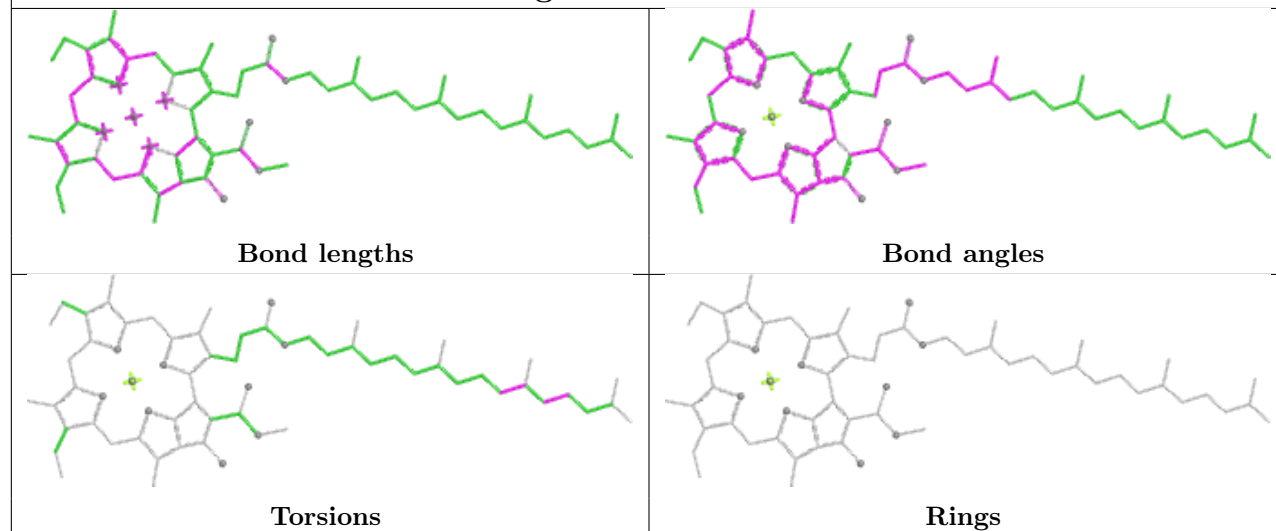


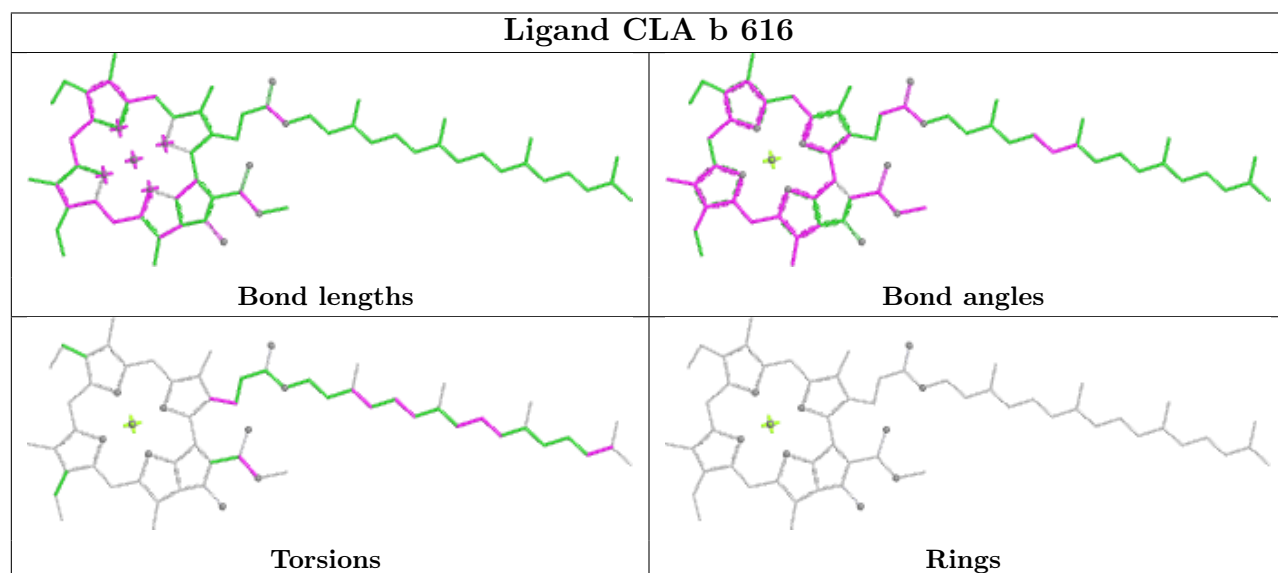
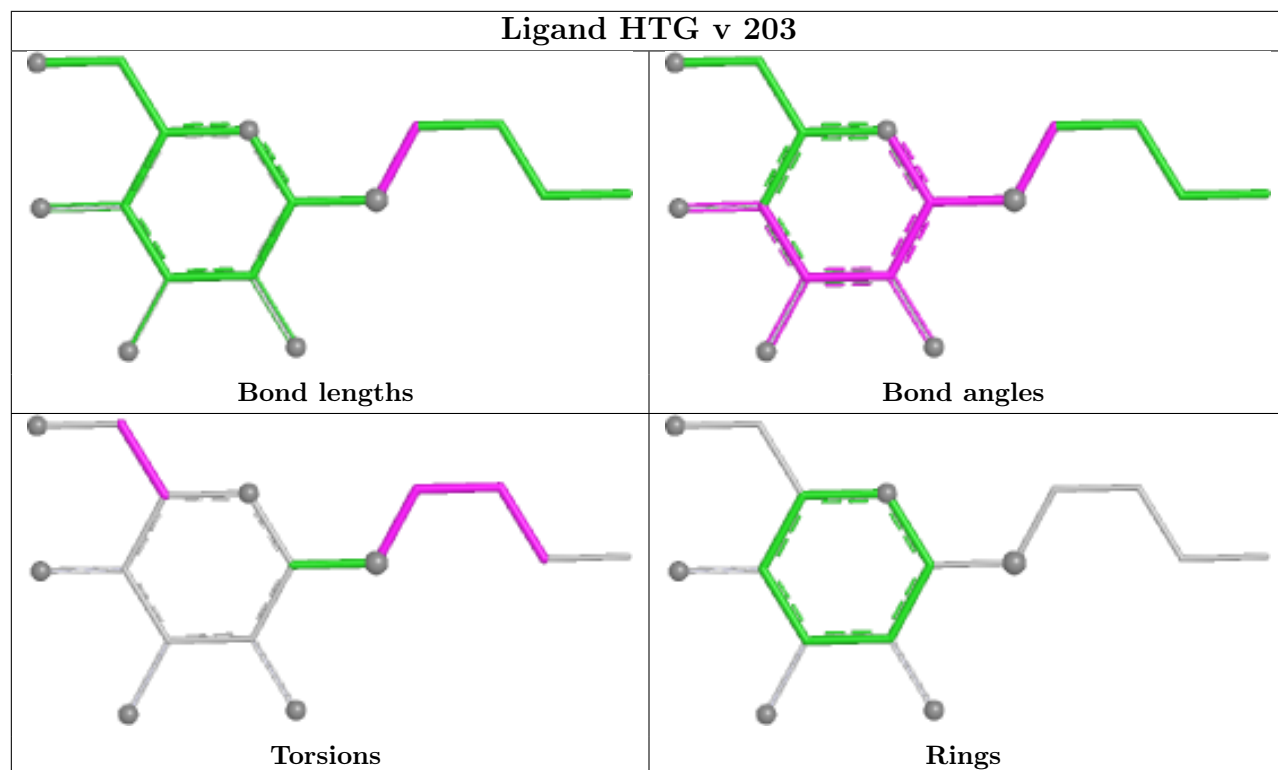


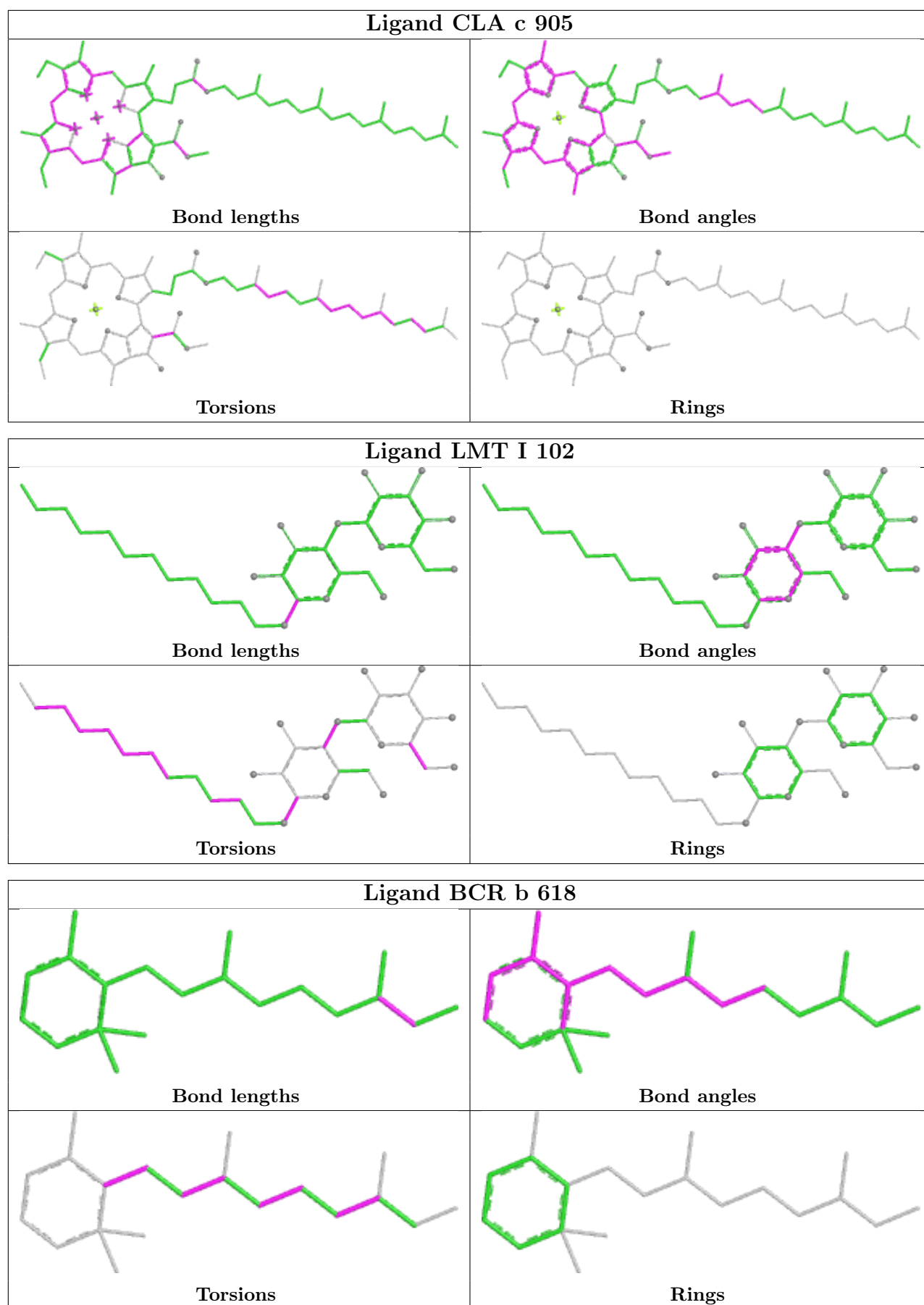


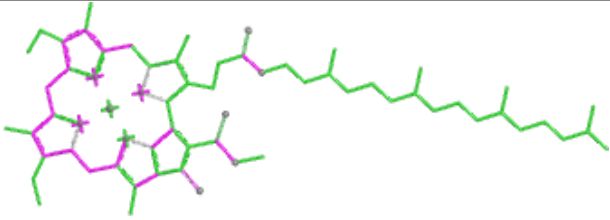
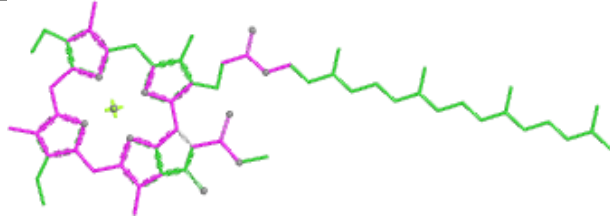
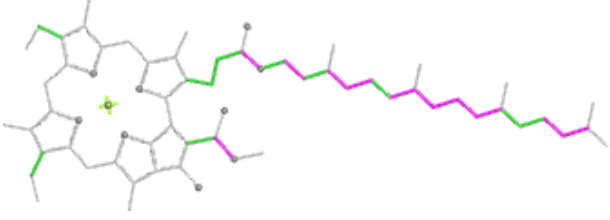
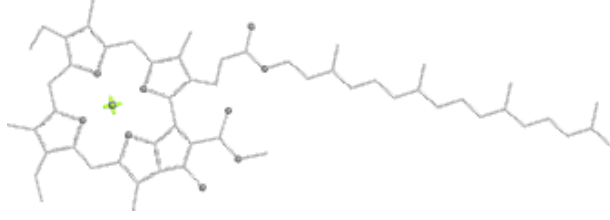
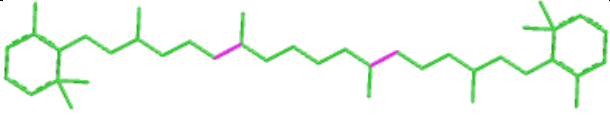
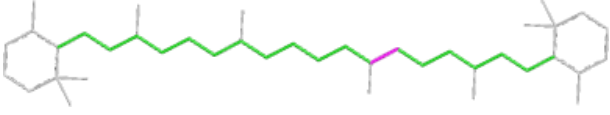
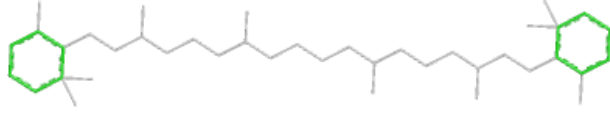
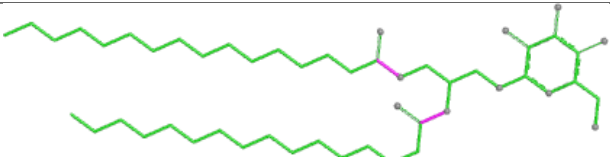
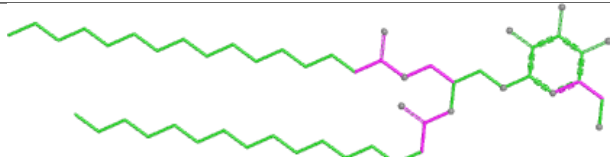
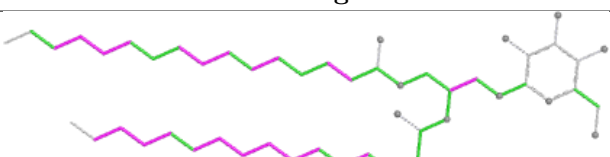
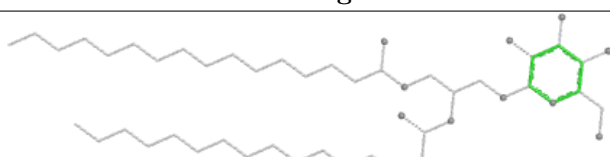


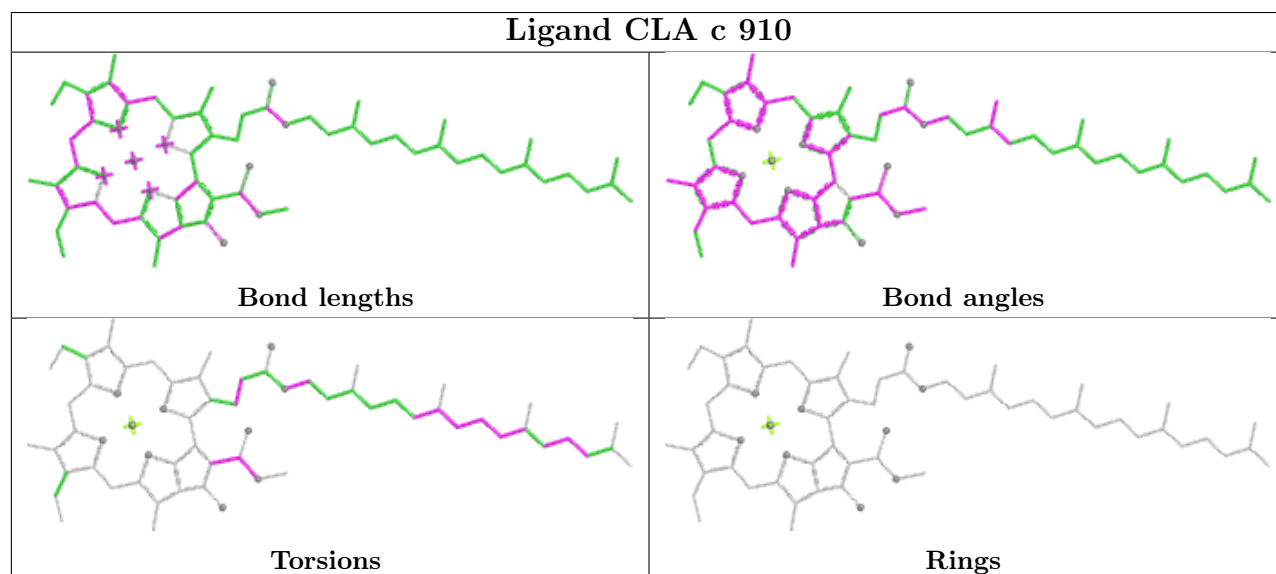
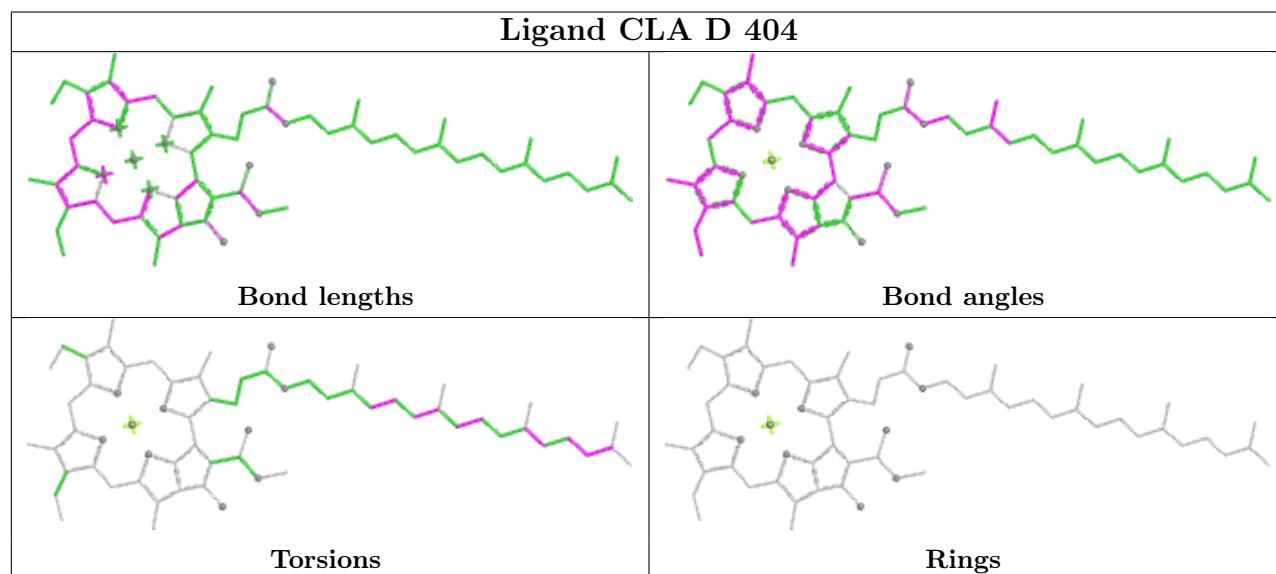
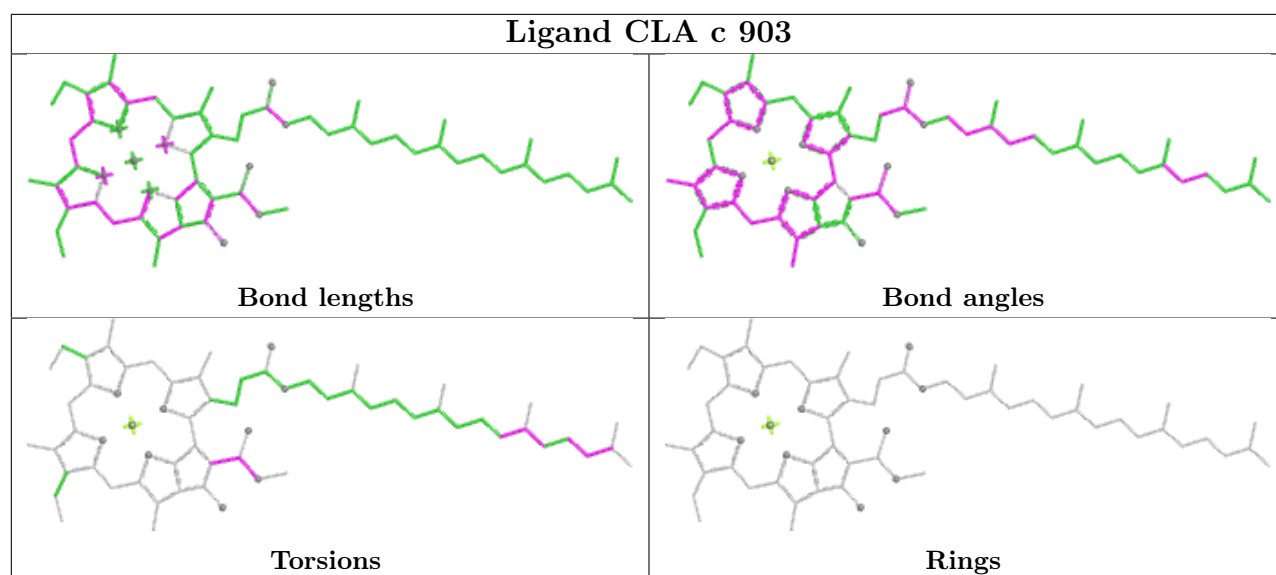


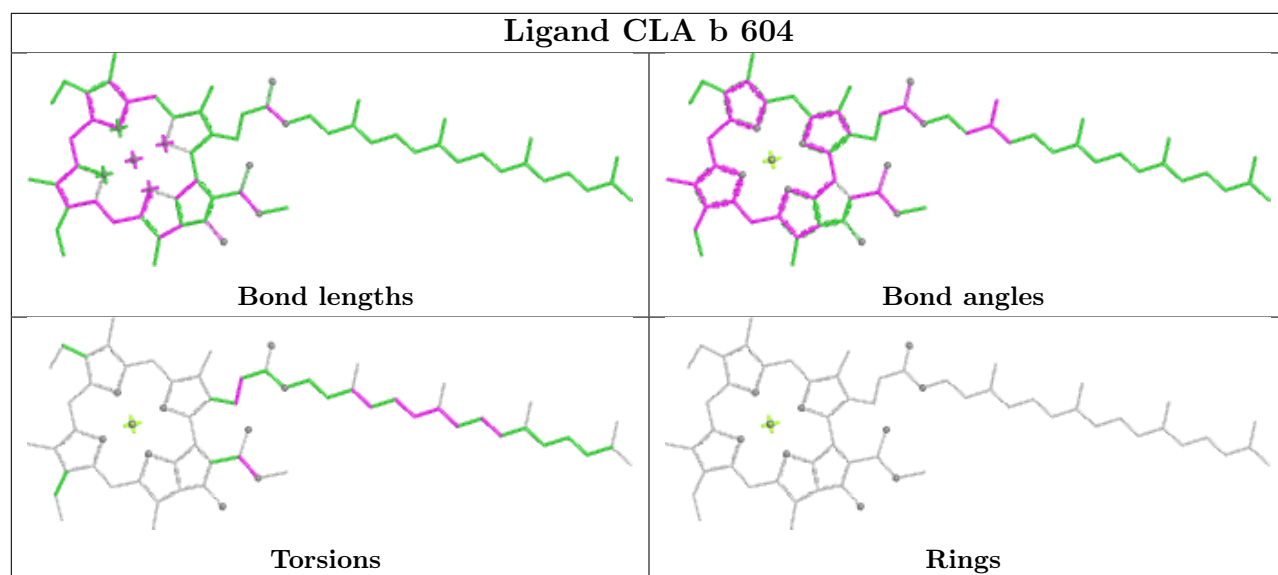
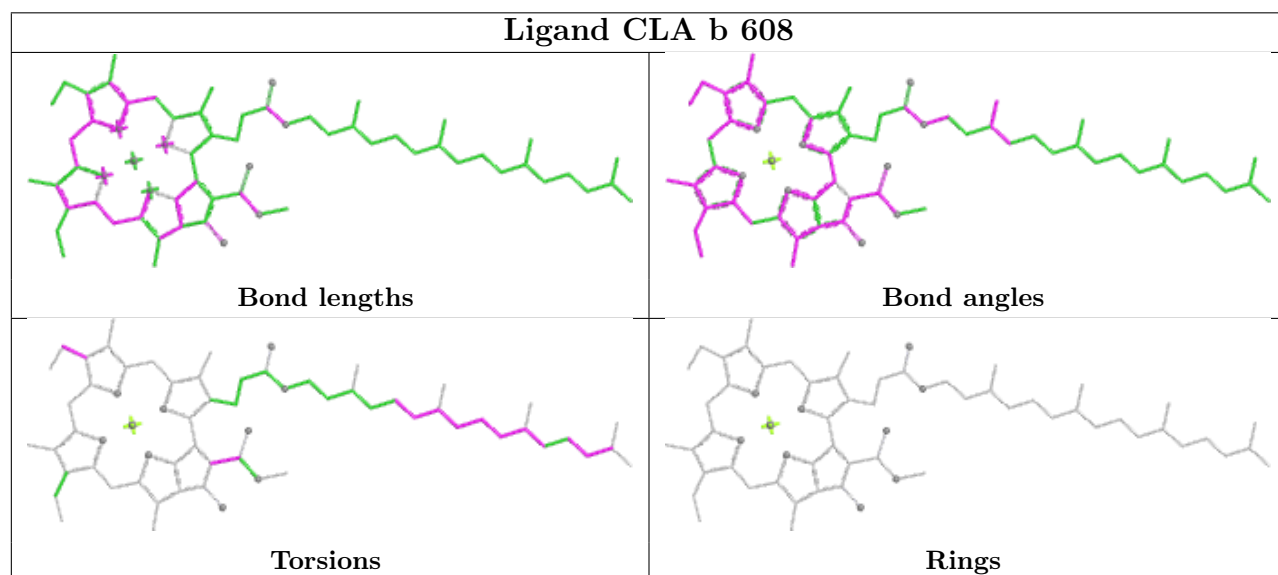
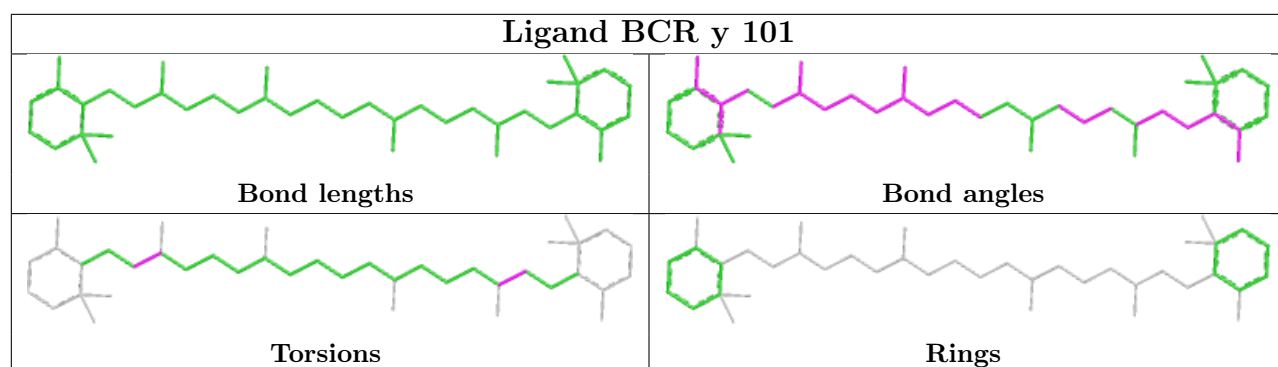
Ligand CLA B 608**Ligand CLA b 603**

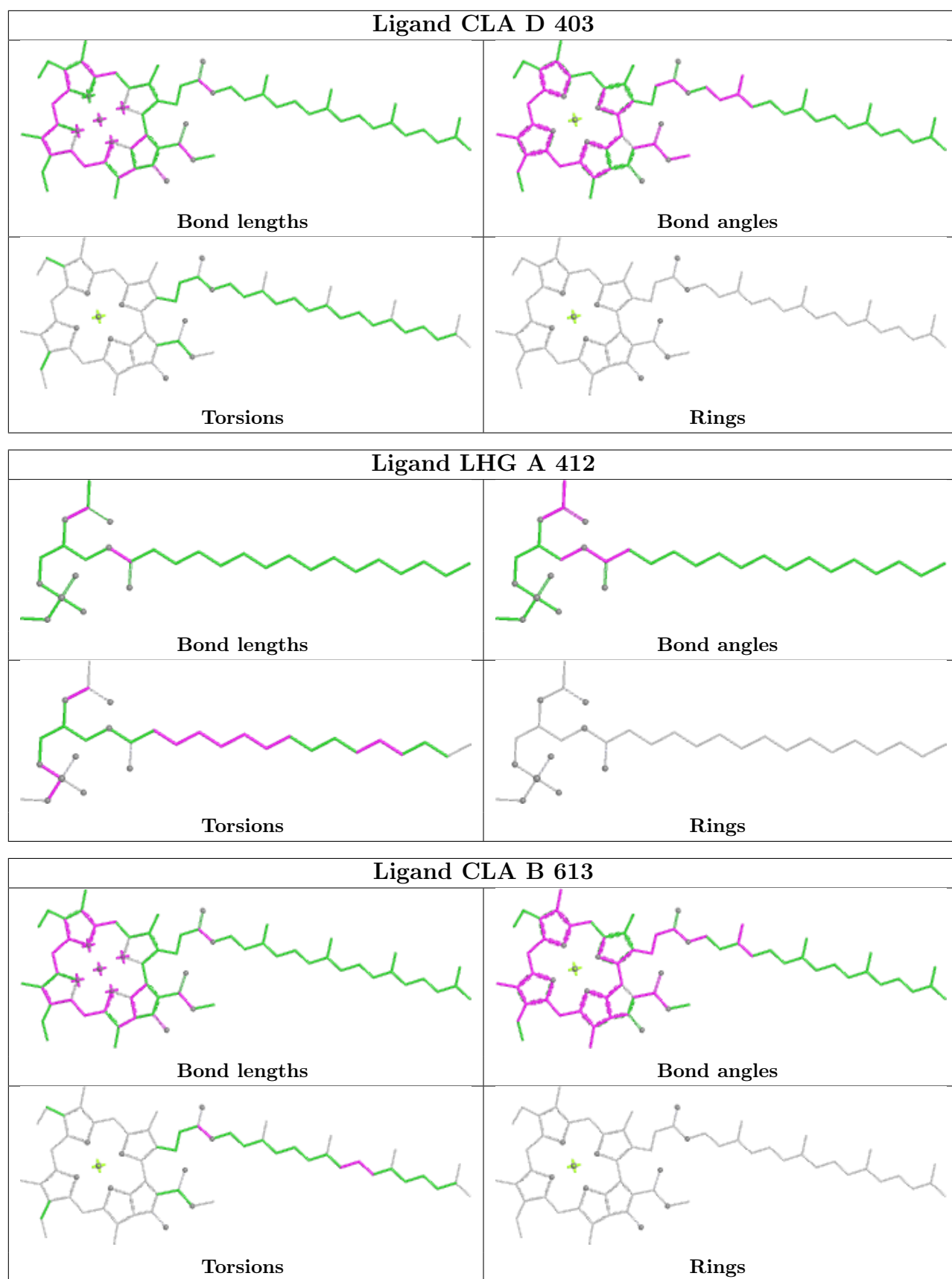


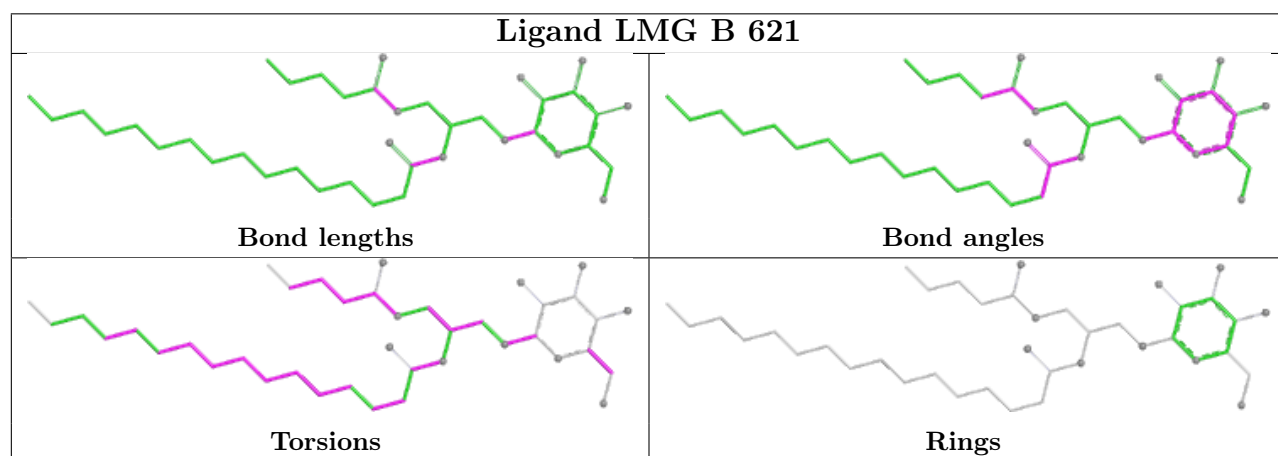
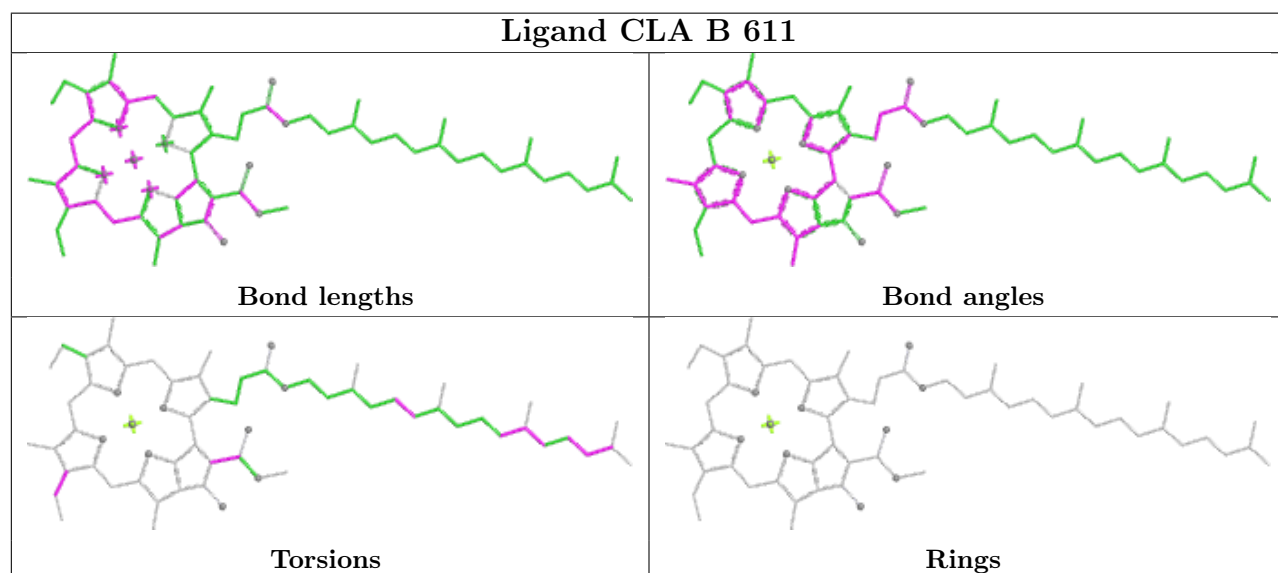
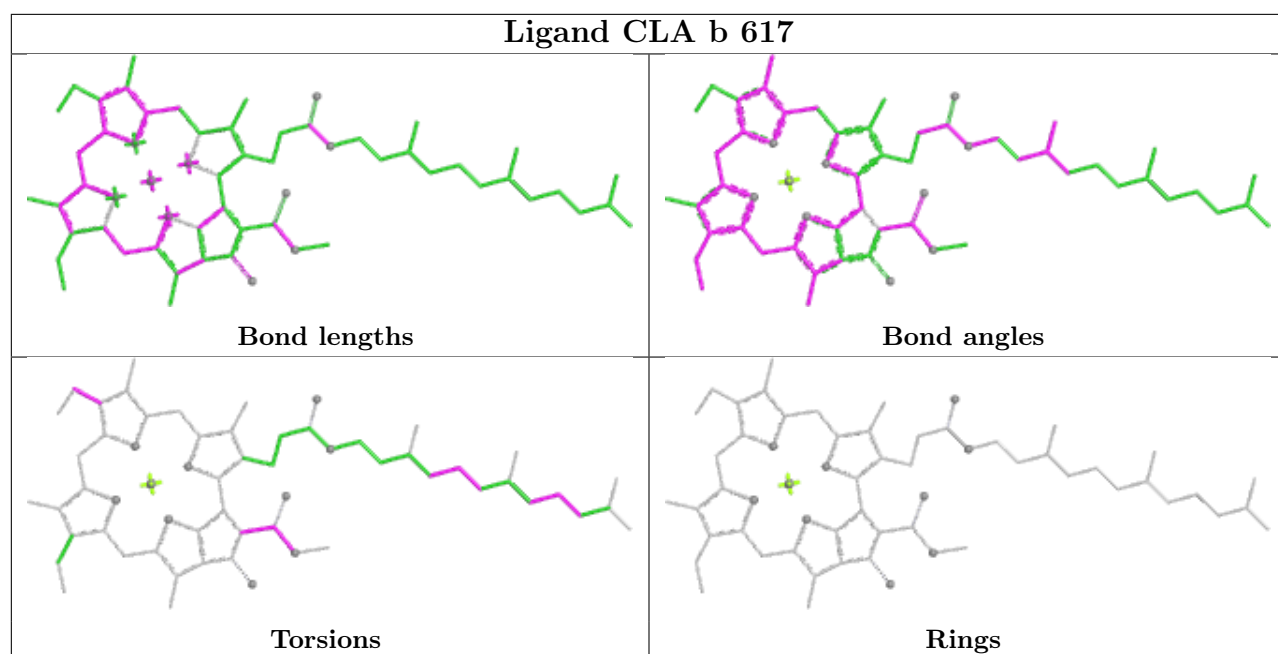


Ligand CLA C 514	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR A 409	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG C 520	
 Bond lengths	 Bond angles
 Torsions	 Rings

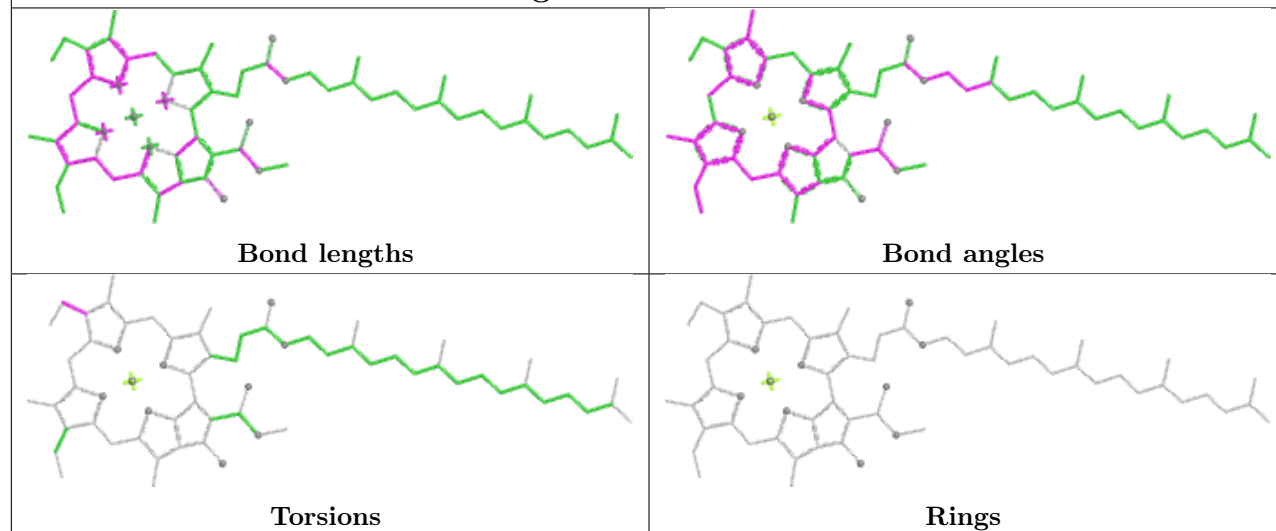




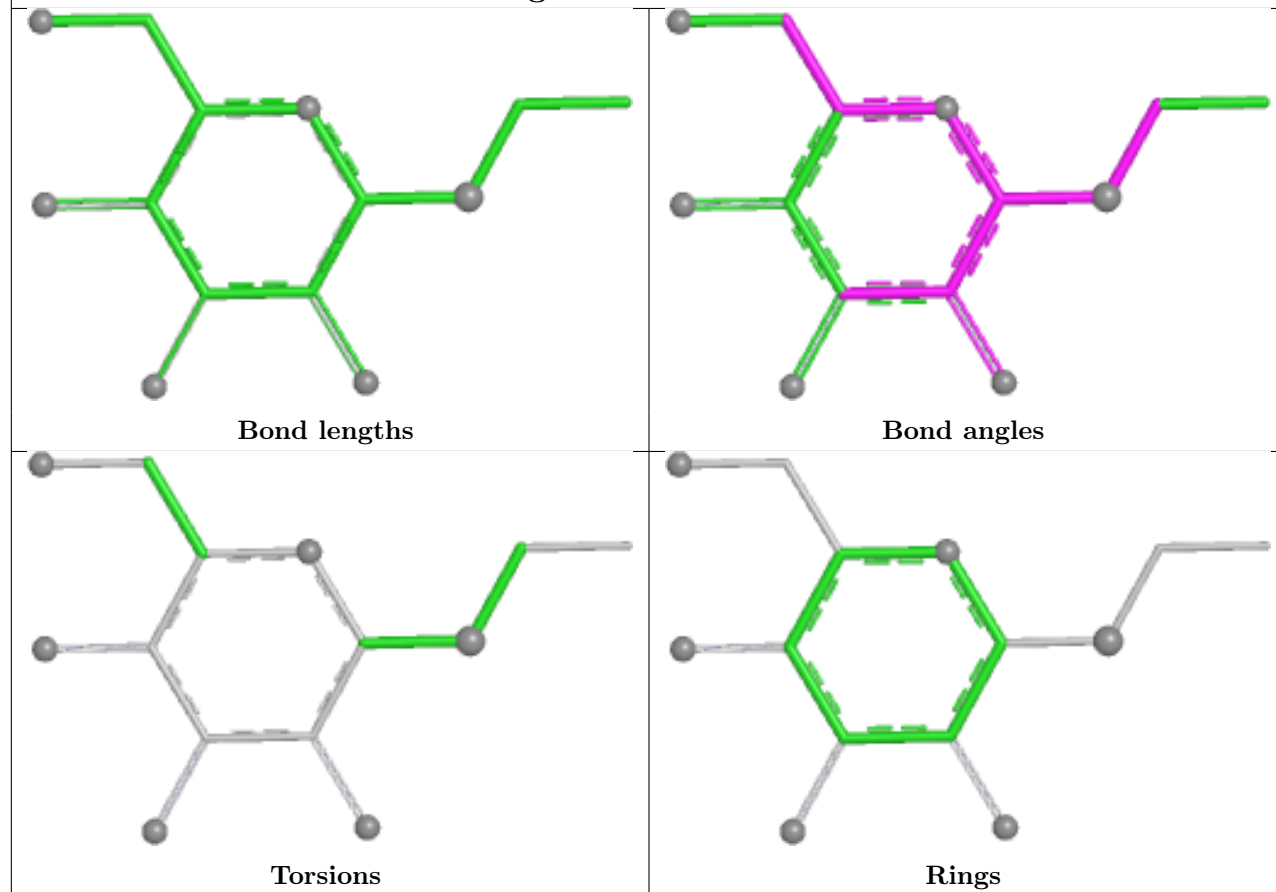


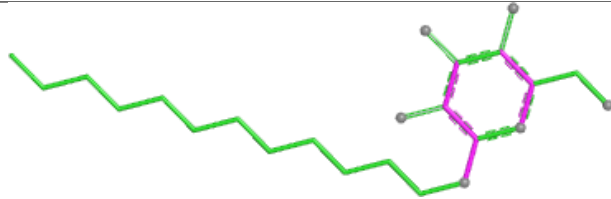


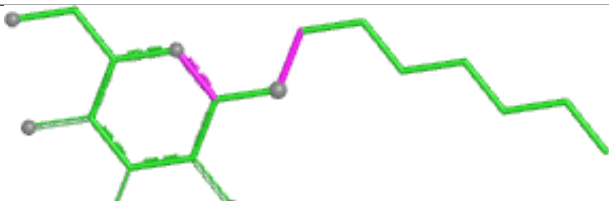
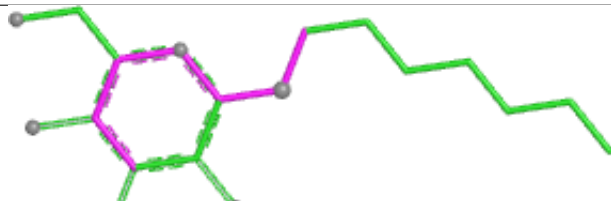
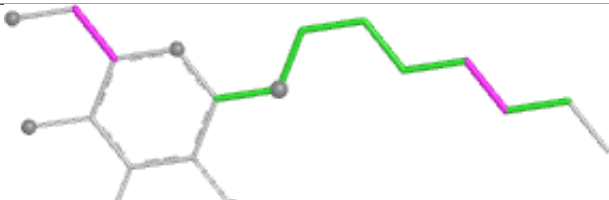
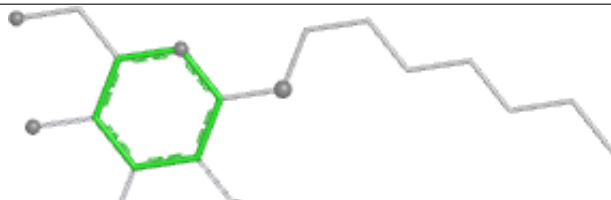
Ligand CLA B 610

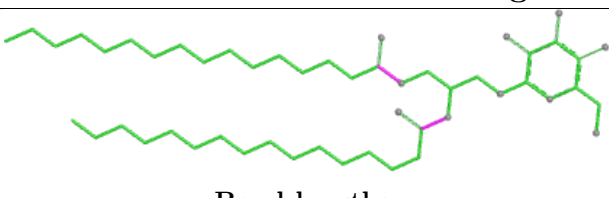
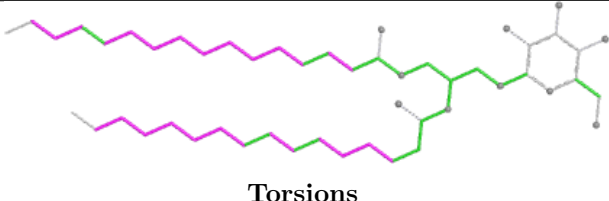
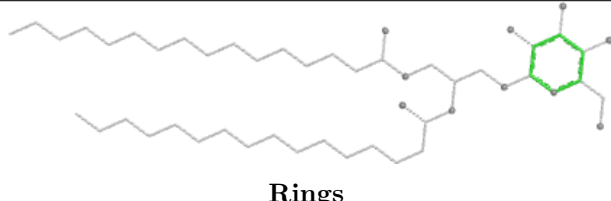


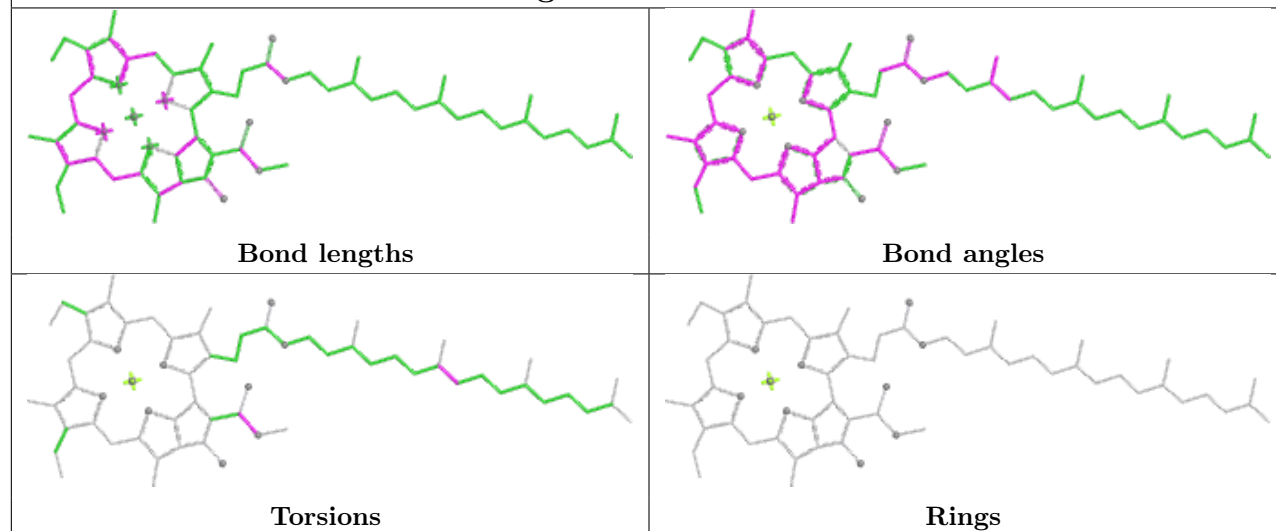
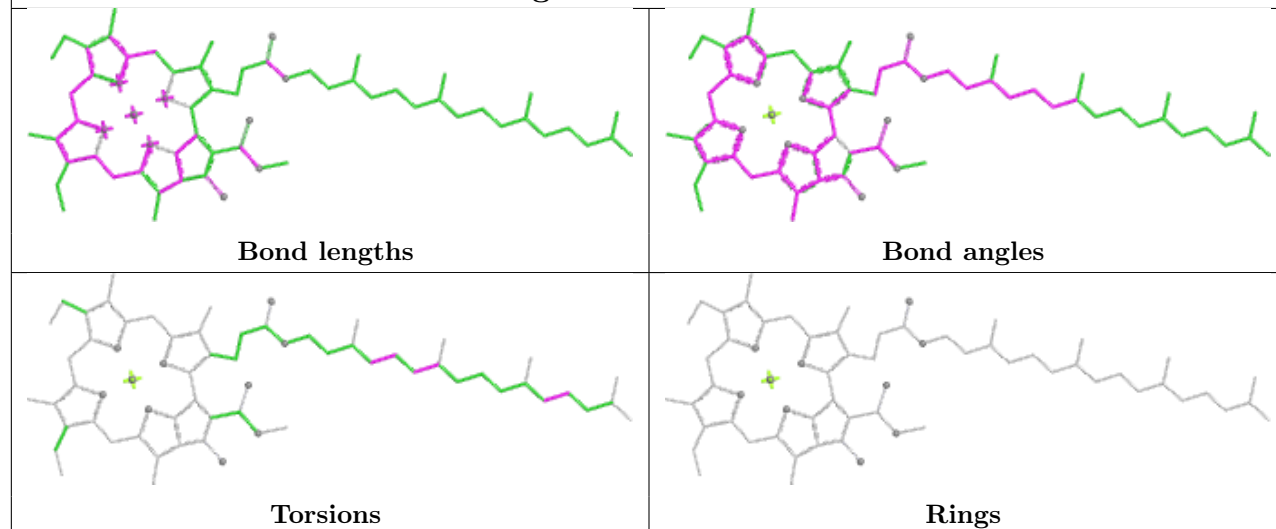
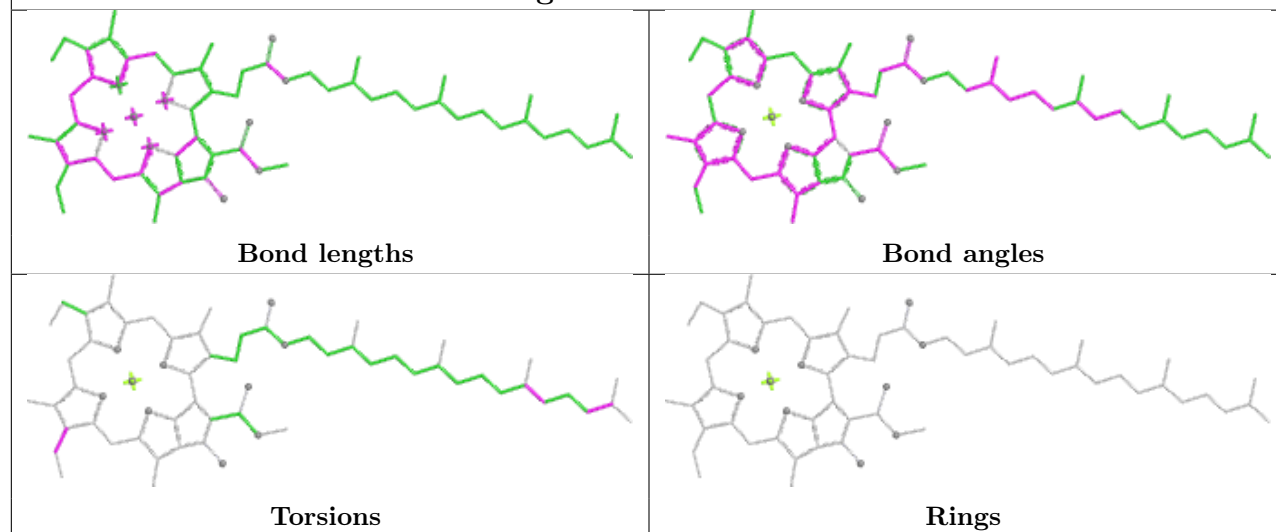
Ligand HTG V 203

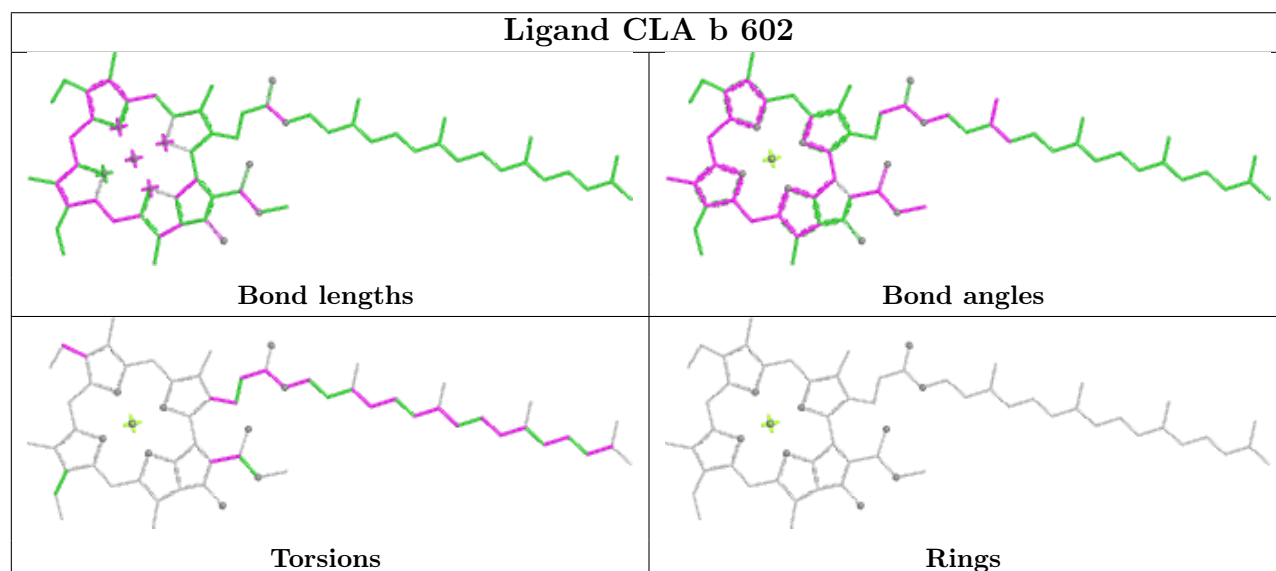
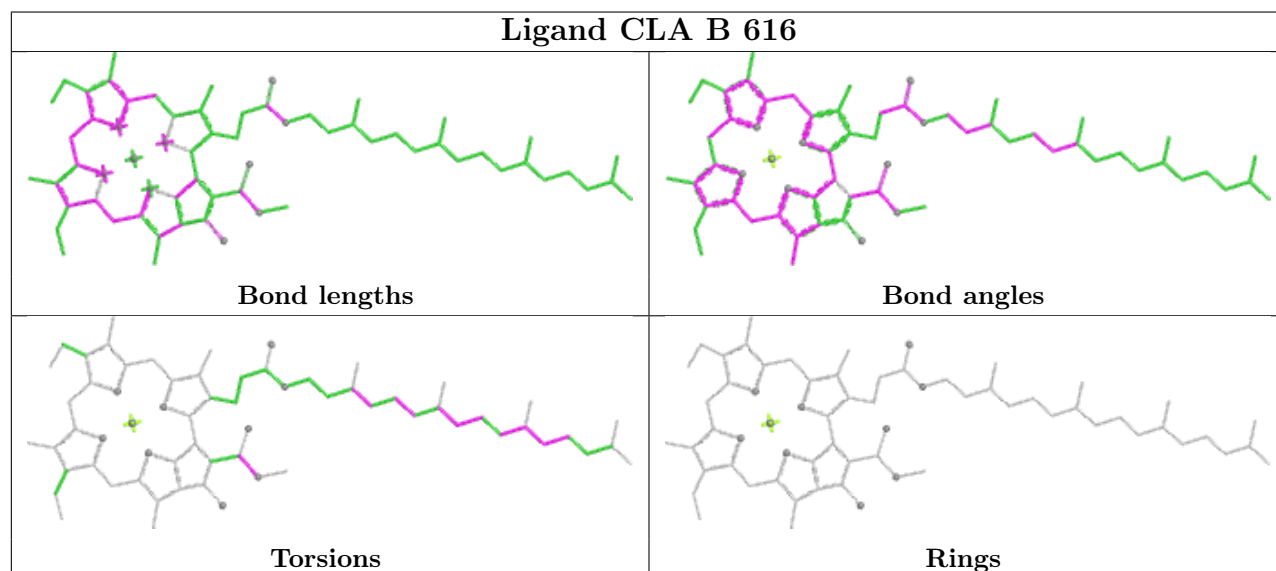
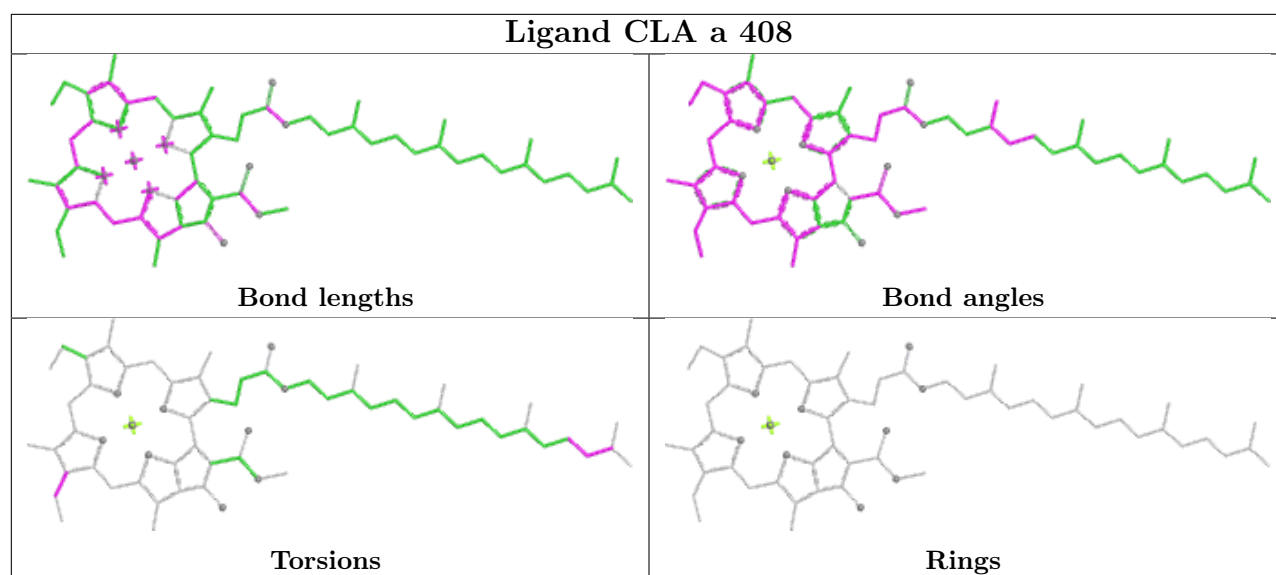


Ligand LMT t 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

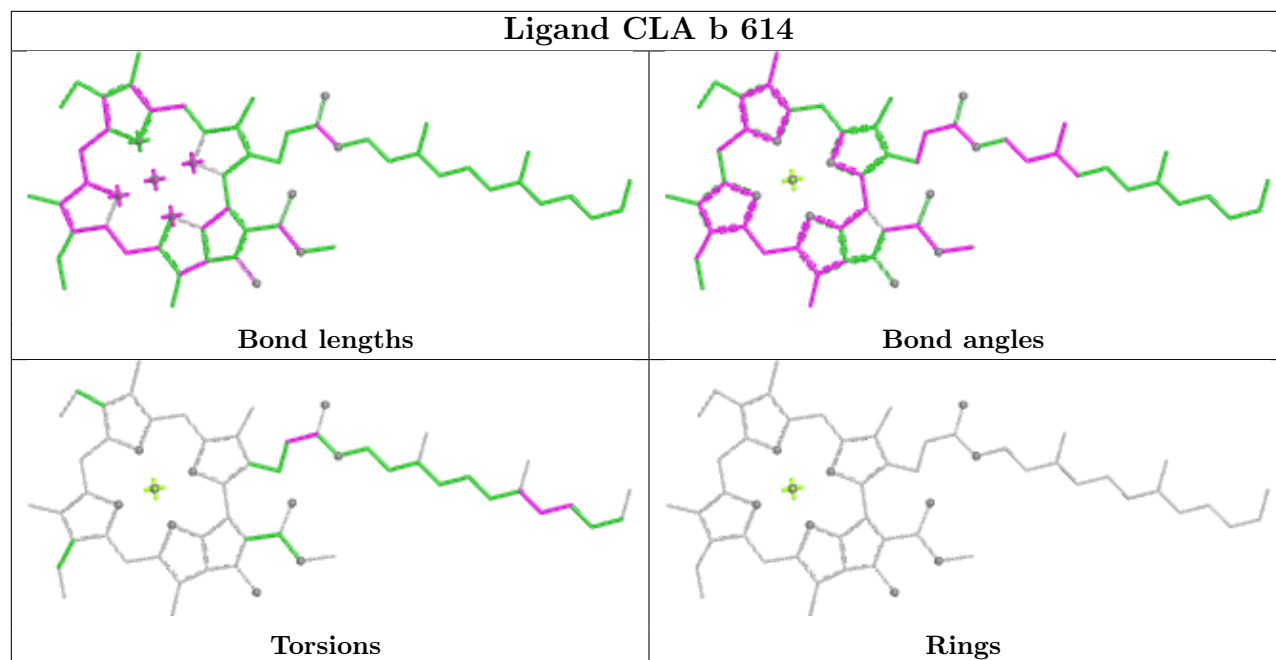
Ligand HTG b 627	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LMG c 920	
	
Bond lengths	Bond angles
	
Torsions	Rings

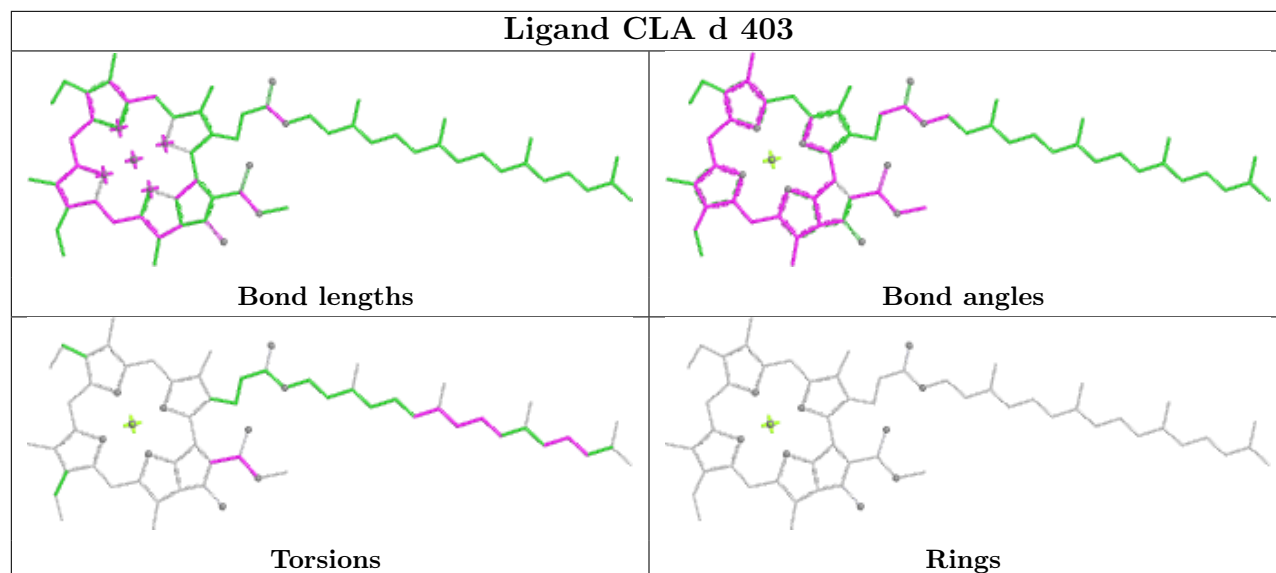
Ligand CLA c 912**Ligand CLA B 603****Ligand CLA a 407**

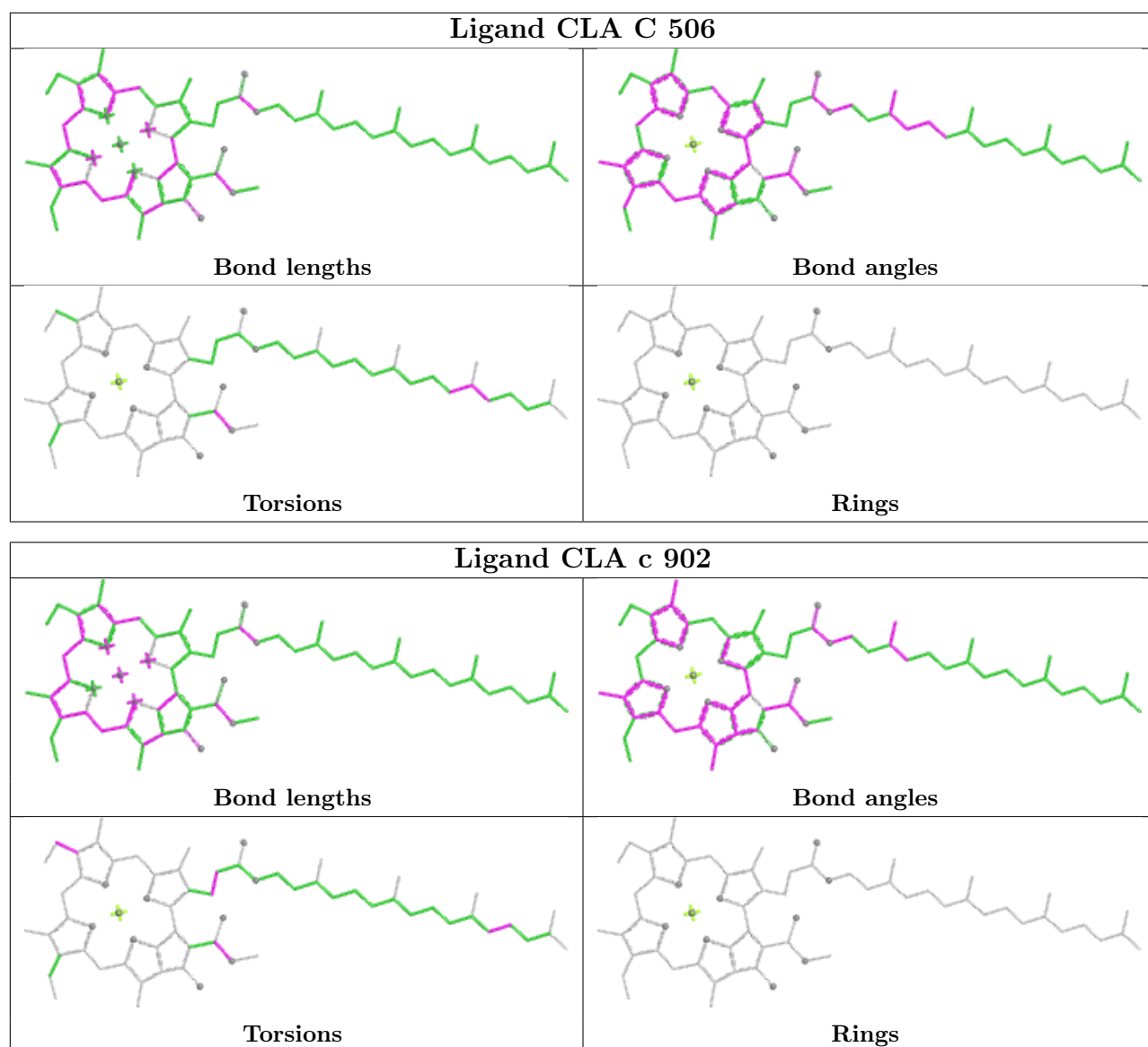


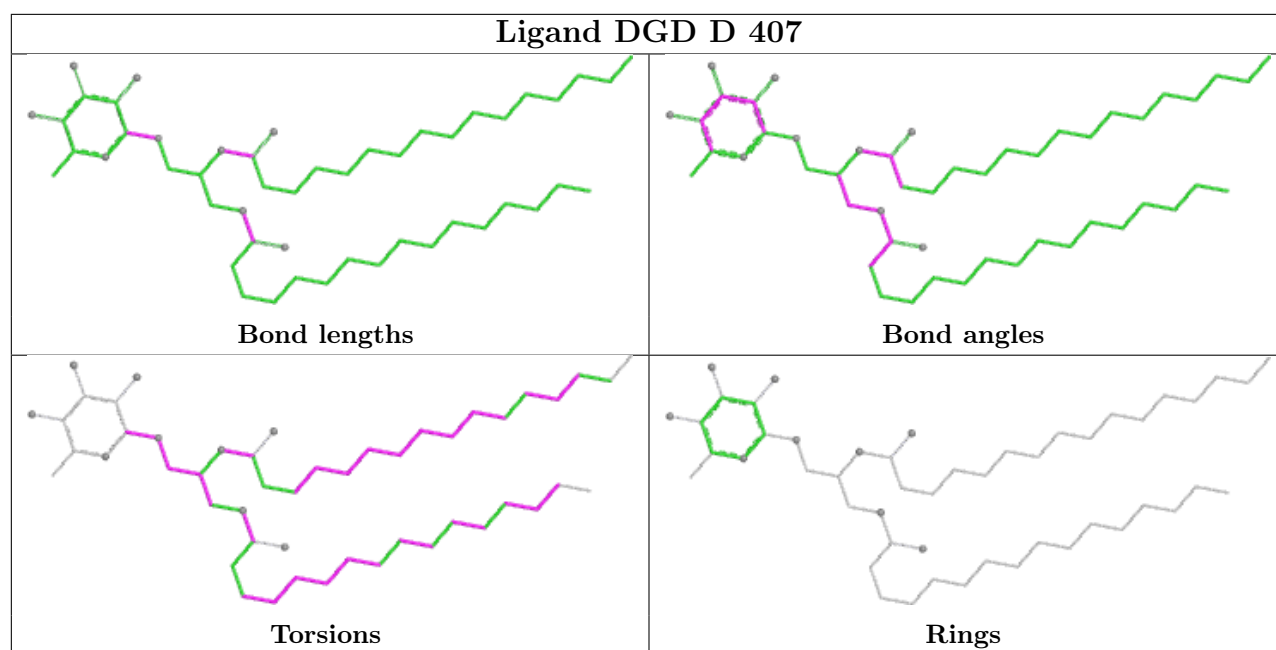
Ligand CLA b 614

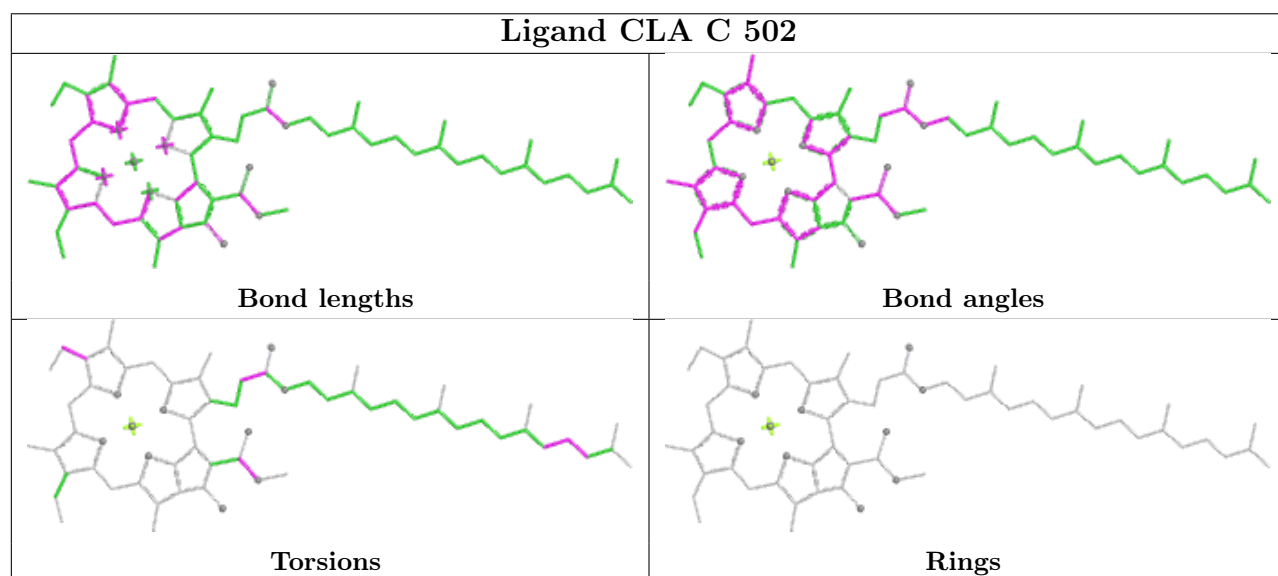
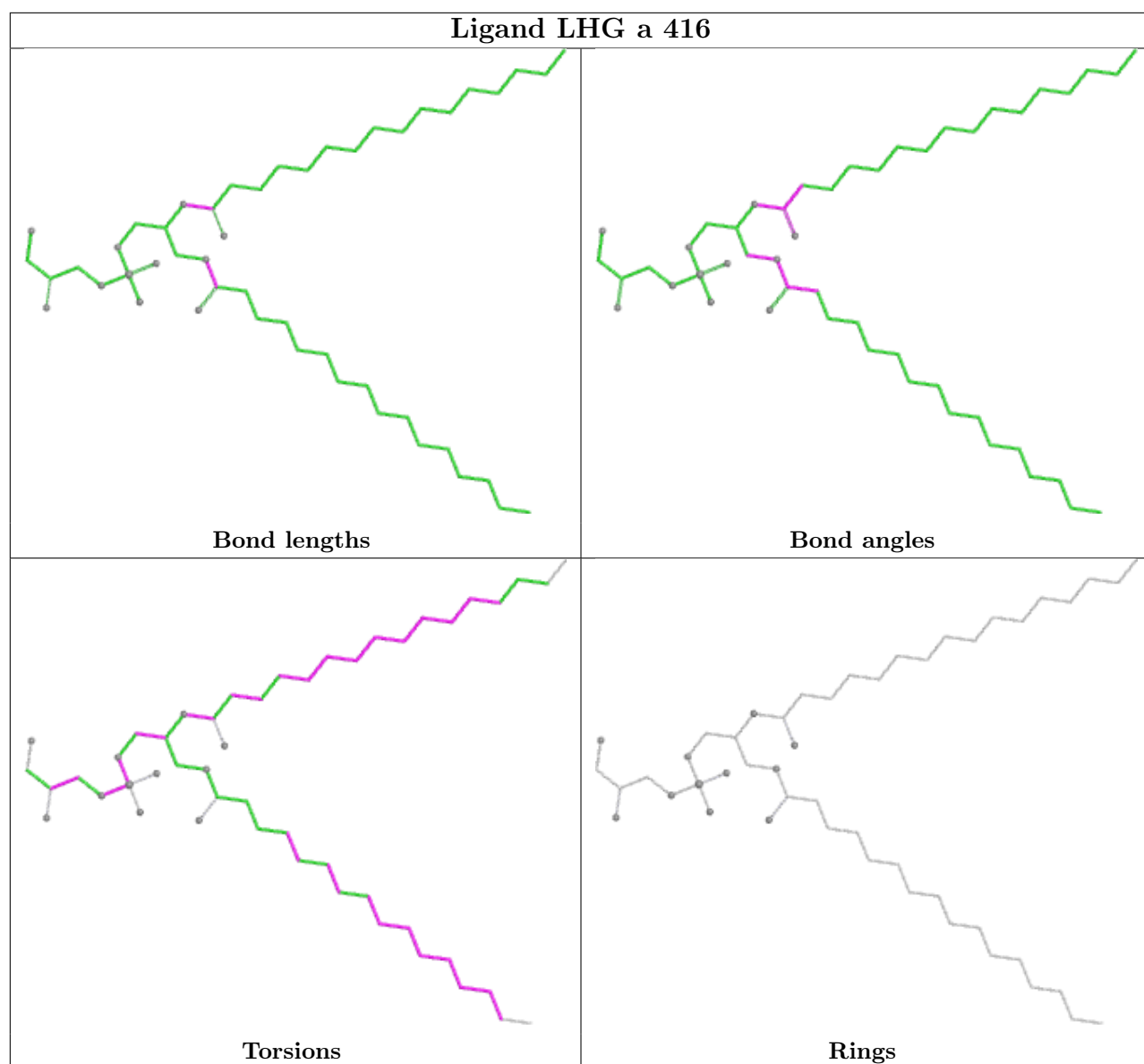


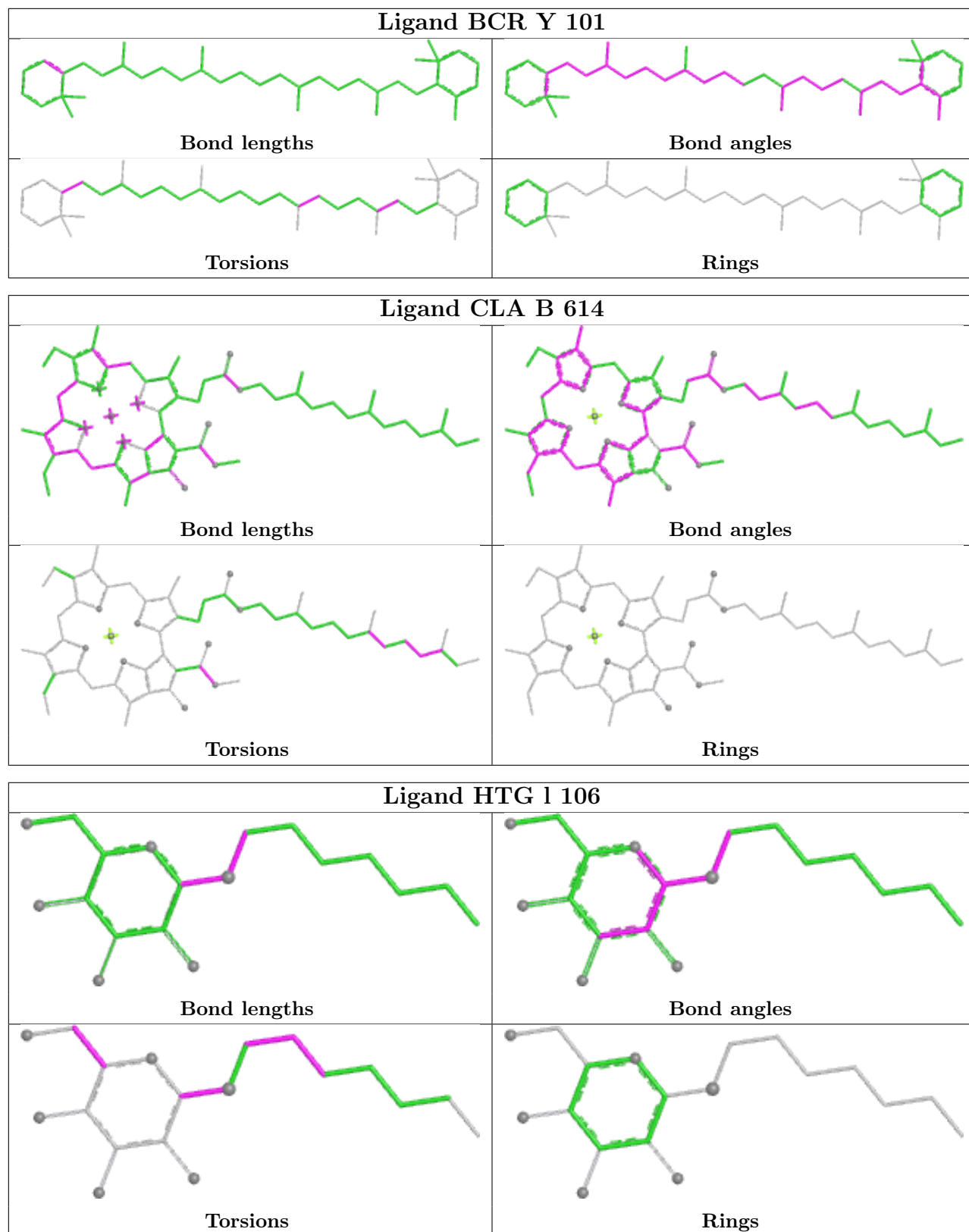
Ligand CLA d 403

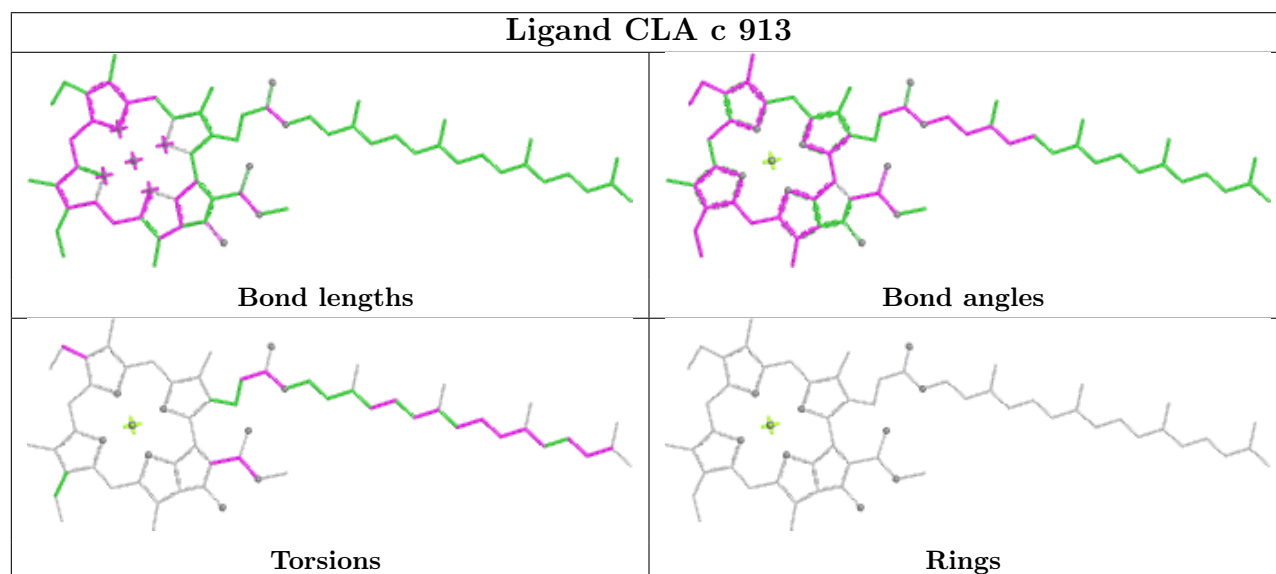
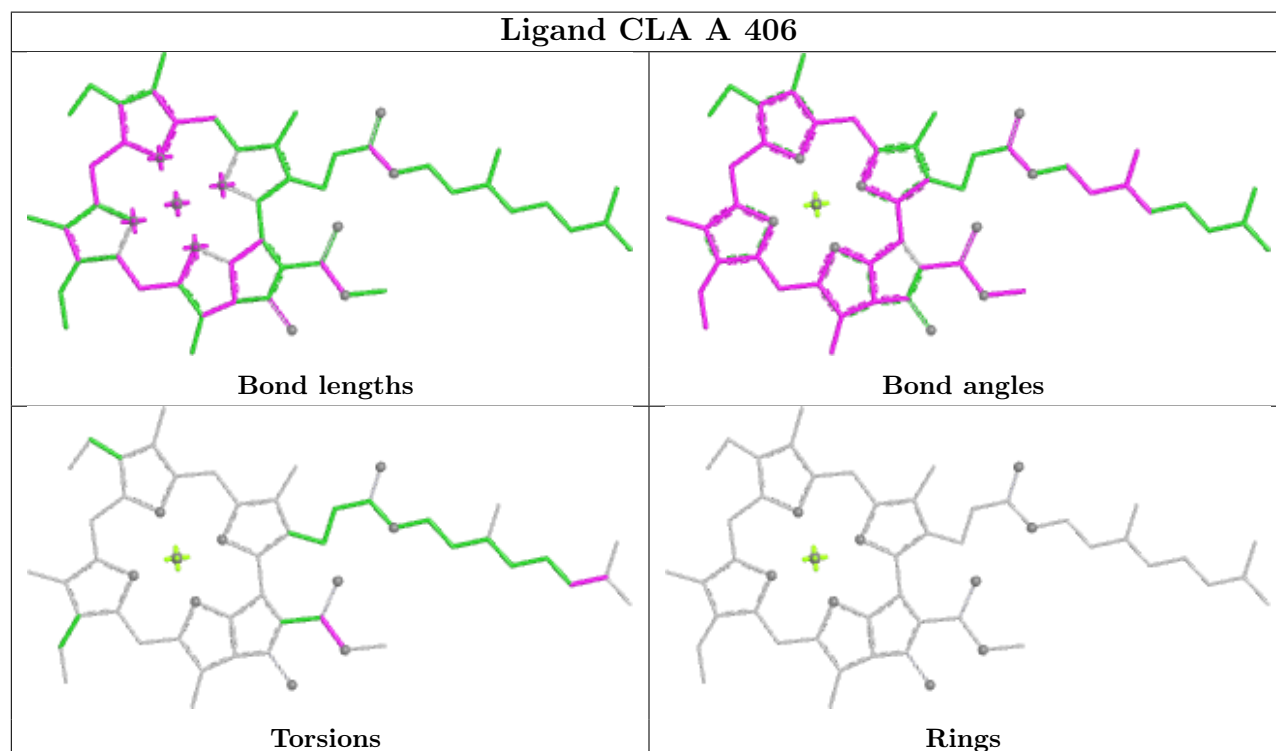
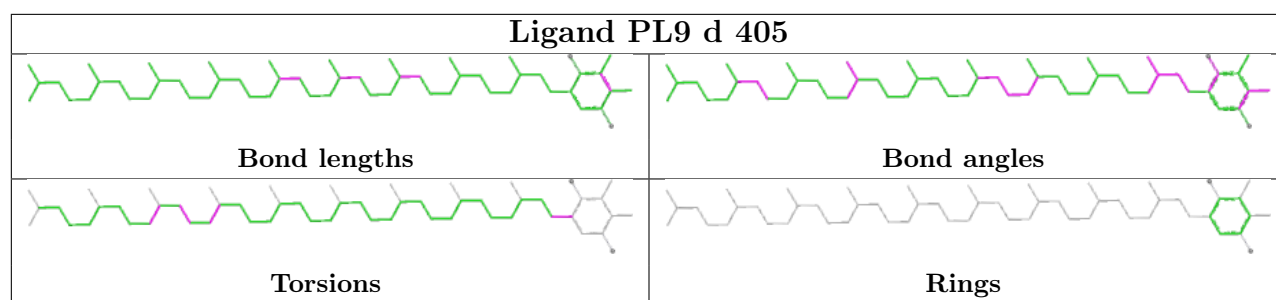


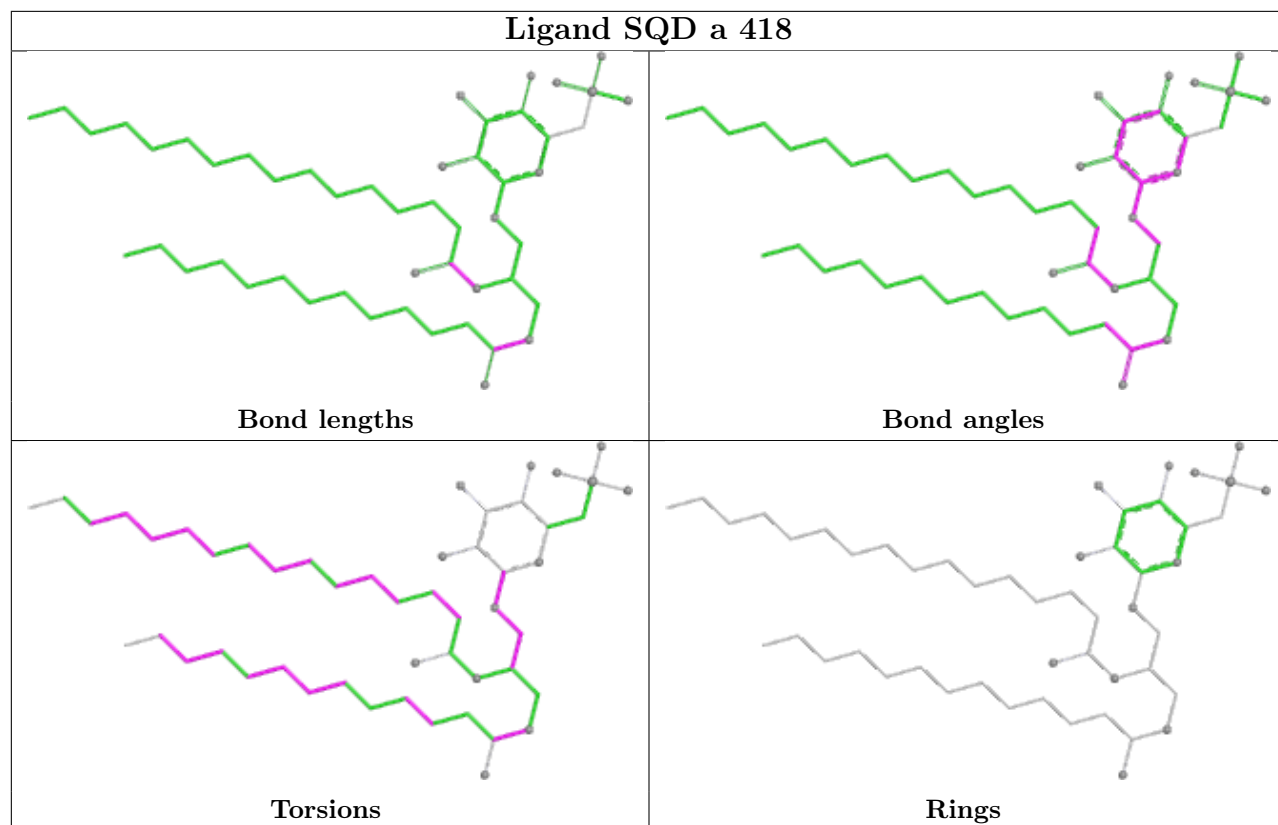




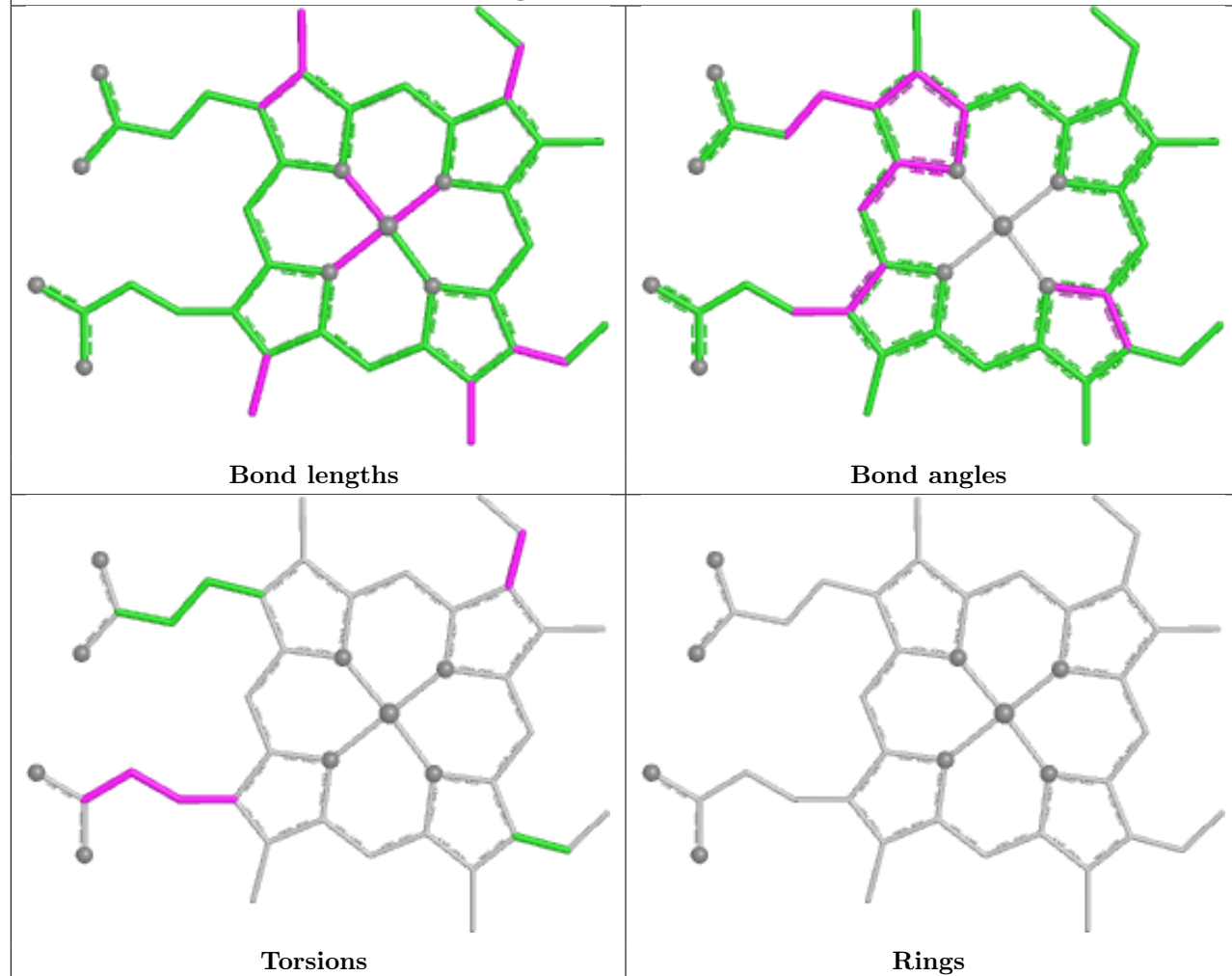




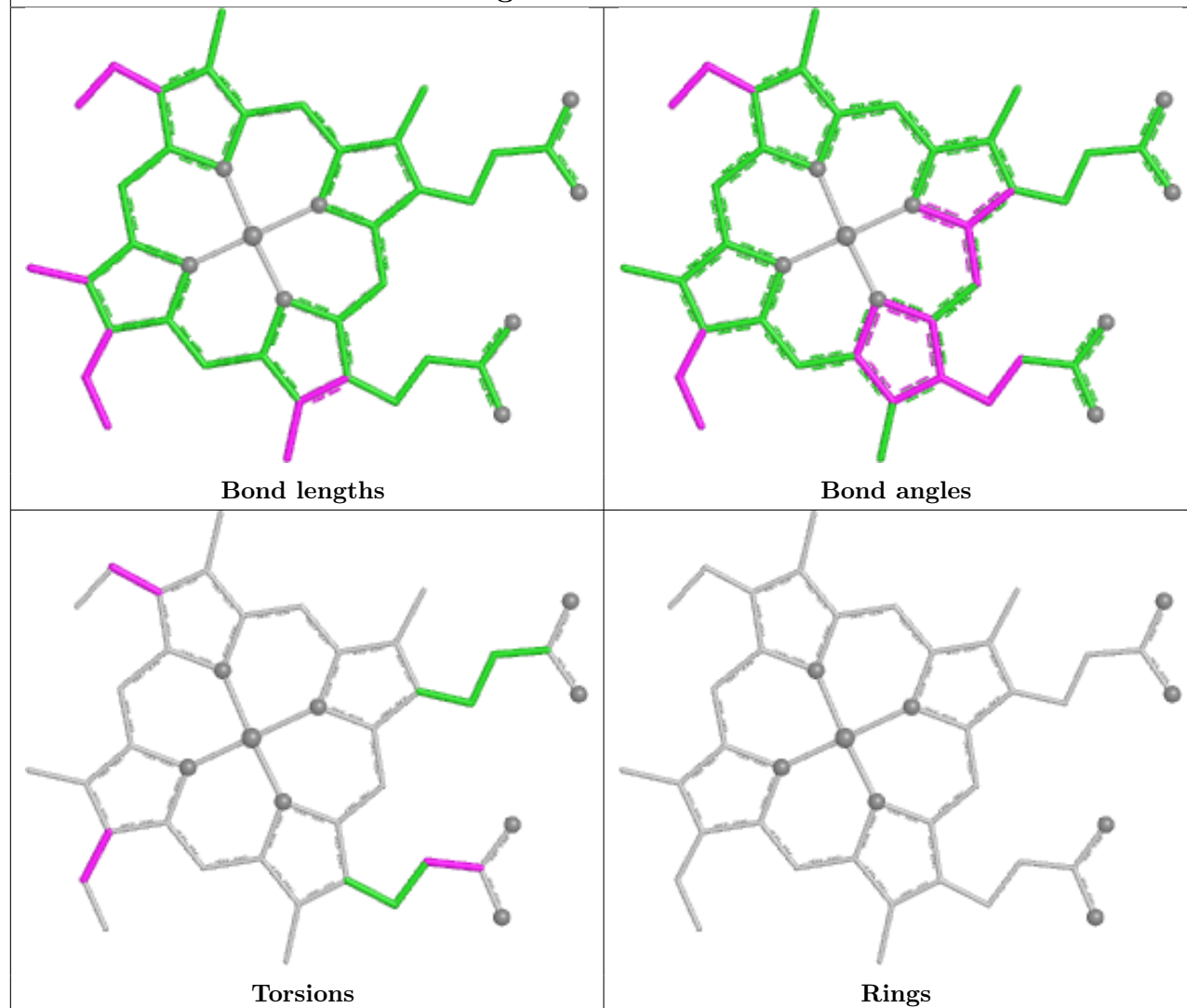




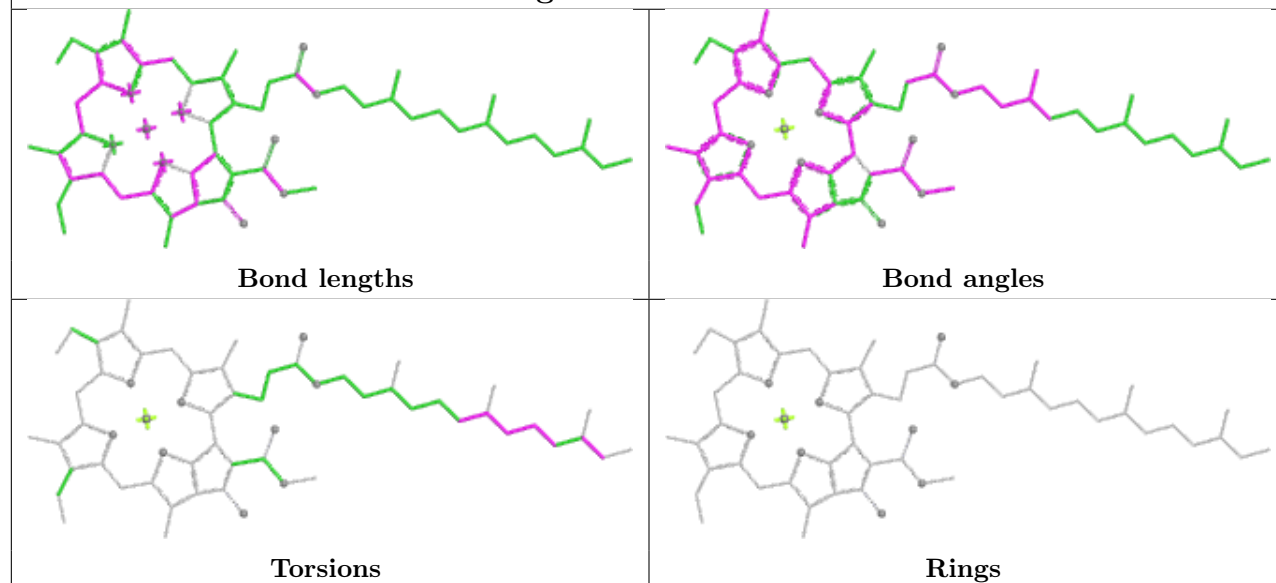
Ligand HEM e 101

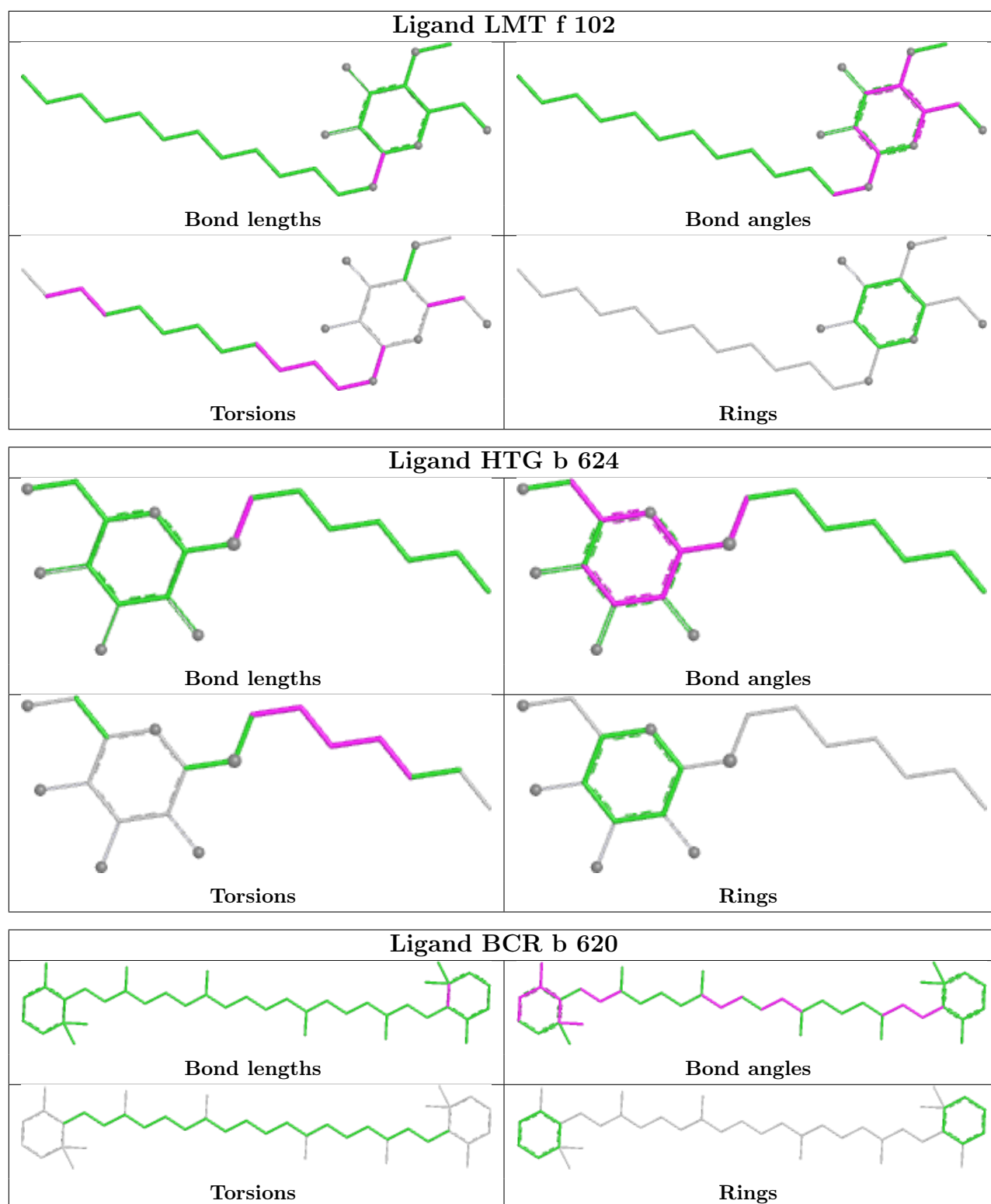


Ligand HEC v 202



Ligand CLA a 409





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	334/334 (100%)	-0.48	7 (2%) 63 60	17, 28, 66, 87	1 (0%)
1	a	334/334 (100%)	-0.18	33 (9%) 13 10	17, 30, 96, 135	1 (0%)
2	B	505/505 (100%)	-0.32	16 (3%) 50 47	21, 33, 67, 109	3 (0%)
2	b	483/505 (95%)	-0.32	5 (1%) 79 77	19, 35, 57, 124	1 (0%)
3	C	451/455 (99%)	-0.29	3 (0%) 84 82	24, 37, 55, 106	0
3	c	455/455 (100%)	-0.14	2 (0%) 88 87	27, 41, 57, 89	1 (0%)
4	D	342/342 (100%)	-0.55	0 100 100	14, 29, 51, 86	3 (0%)
4	d	341/342 (99%)	-0.41	4 (1%) 76 74	16, 32, 59, 85	2 (0%)
5	E	79/80 (98%)	0.19	3 (3%) 44 41	30, 53, 77, 89	0
5	e	79/80 (98%)	0.43	3 (3%) 44 41	35, 54, 91, 96	0
6	F	33/33 (100%)	0.03	1 (3%) 52 49	32, 38, 68, 87	0
6	f	31/33 (93%)	0.18	1 (3%) 50 47	34, 42, 62, 95	0
7	H	63/63 (100%)	0.11	1 (1%) 70 67	22, 41, 51, 104	3 (4%)
7	h	62/63 (98%)	0.31	1 (1%) 70 67	26, 48, 62, 74	1 (1%)
8	I	34/36 (94%)	-0.08	0 100 100	33, 42, 60, 78	0
8	i	35/36 (97%)	-0.19	0 100 100	34, 43, 71, 95	0
9	J	36/40 (90%)	0.02	2 (5%) 30 27	29, 46, 73, 82	0
9	j	40/40 (100%)	0.25	2 (5%) 34 31	34, 47, 81, 92	0
10	K	37/37 (100%)	-0.11	0 100 100	36, 44, 55, 70	0
10	k	37/37 (100%)	0.18	1 (2%) 56 53	39, 47, 68, 81	0
11	L	35/35 (100%)	-0.25	1 (2%) 53 50	23, 32, 66, 78	0
11	l	35/35 (100%)	-0.04	1 (2%) 53 50	25, 35, 75, 92	0
12	O	243/243 (100%)	-0.20	1 (0%) 88 87	20, 39, 69, 104	1 (0%)
12	o	243/243 (100%)	-0.19	4 (1%) 70 67	24, 42, 71, 102	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	T	29/30 (96%)	-0.24	2 (6%) 23 20	26, 32, 59, 89	0
13	t	29/30 (96%)	-0.16	2 (6%) 23 20	27, 34, 66, 98	0
14	U	97/97 (100%)	-0.32	0 100 100	26, 36, 58, 89	1 (1%)
14	u	97/97 (100%)	-0.31	1 (1%) 79 77	28, 37, 51, 76	0
15	V	137/137 (100%)	-0.53	0 100 100	22, 34, 50, 70	1 (0%)
15	v	137/137 (100%)	-0.11	0 100 100	24, 44, 61, 84	1 (0%)
16	Y	29/29 (100%)	0.28	1 (3%) 48 45	40, 54, 69, 81	0
16	y	29/29 (100%)	0.53	1 (3%) 48 45	51, 62, 70, 74	0
17	X	37/37 (100%)	0.31	1 (2%) 56 53	27, 50, 72, 83	1 (2%)
17	x	36/37 (97%)	0.63	1 (2%) 55 52	41, 54, 88, 89	0
18	Z	62/62 (100%)	0.70	6 (9%) 13 10	42, 54, 88, 106	0
18	z	61/62 (98%)	1.04	10 (16%) 4 3	49, 64, 98, 102	0
All	All	5147/5190 (99%)	-0.21	117 (2%) 61 58	14, 37, 70, 135	21 (0%)

The worst 5 of 117 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	486	LEU	5.6
1	a	230	THR	5.5
17	x	37	VAL	5.2
7	H	64	ALA	4.8
1	A	246	TYR	4.6

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
13	FME	T	1	10/11	0.88	0.14	38,42,72,75	0
13	FME	t	1	10/11	0.92	0.10	33,38,80,91	0
8	FME	I	1	10/11	0.96	0.09	33,37,40,41	0
8	FME	i	1	10/11	0.97	0.09	36,41,45,48	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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
31	DMS	c	942	4/4	0.60	0.24	101,103,111,117	0
31	DMS	c	936	4/4	0.64	0.22	106,116,116,124	0
31	DMS	C	537	4/4	0.67	0.29	88,103,104,113	0
30	UNL	c	932	10/-	0.70	0.23	56,74,80,83	0
31	DMS	O	307	4/4	0.70	0.24	84,97,98,104	0
30	UNL	i	104	16/-	0.70	0.23	67,76,87,89	0
31	DMS	c	937	4/4	0.70	0.25	80,90,91,100	0
31	DMS	B	639	4/4	0.70	0.20	72,87,90,102	0
34	HTG	b	624	19/19	0.70	0.18	69,97,109,110	0
31	DMS	O	305	4/4	0.71	0.20	68,70,79,99	0
29	LMT	f	102	25/35	0.71	0.21	61,93,105,108	0
34	HTG	c	922	19/19	0.71	0.16	70,93,109,112	0
30	UNL	t	102	16/-	0.72	0.16	59,71,78,80	0
30	UNL	i	105	10/-	0.72	0.22	67,78,86,87	0
31	DMS	u	205	4/4	0.73	0.26	64,67,73,83	0
31	DMS	b	637	4/4	0.73	0.20	90,97,101,112	0
30	UNL	a	417	10/-	0.73	0.24	75,80,84,87	0
30	UNL	Z	102	9/-	0.74	0.17	57,71,79,81	0
34	HTG	b	627	19/19	0.74	0.16	50,92,108,109	0
34	HTG	D	415	19/19	0.74	0.19	39,69,80,87	0
35	DGD	d	406	43/66	0.74	0.22	58,85,139,146	0
34	HTG	D	414	19/19	0.75	0.18	63,103,114,115	0
34	HTG	b	632	19/19	0.75	0.20	56,74,91,92	0
31	DMS	b	636	4/4	0.75	0.23	88,95,109,113	0
31	DMS	c	938	4/4	0.75	0.20	86,91,98,103	0
34	HTG	B	627	19/19	0.76	0.16	51,104,113,116	0
31	DMS	v	207	4/4	0.76	0.31	84,93,97,117	0
29	LMT	I	102	35/35	0.77	0.15	76,88,100,102	0
31	DMS	d	414	4/4	0.77	0.28	102,112,113,120	0
30	UNL	I	105	16/-	0.77	0.20	70,82,88,90	0
30	UNL	a	420	6/-	0.77	0.20	56,59,60,60	0
30	UNL	b	628	11/-	0.77	0.16	58,63,78,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	DMS	V	211	4/4	0.77	0.23	77,84,85,85	0
31	DMS	u	204	4/4	0.78	0.20	50,68,69,75	0
27	LHG	A	412	31/49	0.78	0.19	66,83,107,117	0
31	DMS	v	204	4/4	0.78	0.19	87,88,90,91	0
31	DMS	a	401	4/4	0.78	0.28	75,84,85,104	0
30	UNL	u	201	11/-	0.78	0.20	47,53,69,69	0
34	HTG	v	203	16/19	0.78	0.15	52,69,81,97	0
35	DGD	D	407	50/66	0.78	0.20	60,87,120,123	0
31	DMS	l	105	4/4	0.78	0.26	100,103,110,115	0
31	DMS	c	943	4/4	0.79	0.21	77,82,87,92	0
22	CLA	b	602	65/65	0.79	0.16	49,67,89,98	0
31	DMS	l	103	4/4	0.79	0.24	91,95,97,99	0
31	DMS	c	935	4/4	0.79	0.16	71,78,81,84	0
31	DMS	u	203	4/4	0.79	0.21	56,68,72,84	0
29	LMT	A	414	35/35	0.79	0.17	59,86,109,114	0
31	DMS	C	540	4/4	0.79	0.22	82,83,91,97	0
31	DMS	H	103	4/4	0.79	0.21	63,67,69,74	0
31	DMS	v	205	4/4	0.79	0.19	70,72,78,80	0
31	DMS	L	102	4/4	0.79	0.23	79,80,91,100	0
29	LMT	T	102	24/35	0.80	0.17	42,80,98,101	0
31	DMS	f	103	4/4	0.80	0.24	87,89,90,100	0
31	DMS	O	313	4/4	0.80	0.26	89,100,100,107	0
27	LHG	a	416	49/49	0.80	0.17	60,84,100,108	0
34	HTG	V	203	14/19	0.81	0.15	48,52,79,84	0
31	DMS	c	944	4/4	0.81	0.20	79,82,89,92	0
29	LMT	Z	101	35/35	0.81	0.16	40,105,123,128	0
31	DMS	C	539	4/4	0.81	0.23	88,90,93,95	0
25	LMG	D	412	46/55	0.81	0.19	41,68,138,142	0
31	DMS	B	634	4/4	0.81	0.23	57,68,73,95	0
30	UNL	j	103	16/-	0.81	0.16	59,67,71,74	0
31	DMS	C	534	4/4	0.81	0.17	105,111,112,121	0
31	DMS	B	631	4/4	0.82	0.19	78,80,84,87	0
28	SQD	D	408	20/54	0.82	0.15	65,97,105,108	0
31	DMS	B	637	4/4	0.82	0.20	69,76,80,88	0
34	HTG	l	106	19/19	0.82	0.17	63,97,108,109	0
31	DMS	U	203	4/4	0.82	0.23	62,73,74,76	0
30	UNL	T	101	13/-	0.82	0.16	63,71,77,79	0
24	BCR	B	618	19/40	0.82	0.15	50,59,74,77	0
30	UNL	I	104	16/-	0.83	0.18	60,71,84,86	0
34	HTG	C	532	19/19	0.83	0.14	69,98,111,112	0
26	PL9	A	411	55/55	0.83	0.20	61,73,87,92	0
28	SQD	l	101	54/54	0.83	0.16	53,82,119,123	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	UNL	U	201	14/-	0.83	0.17	44,57,65,66	0
27	LHG	d	401	33/49	0.83	0.14	62,94,138,142	0
31	DMS	t	105	4/4	0.83	0.23	89,93,101,108	0
29	LMT	a	419	35/35	0.83	0.18	46,69,93,100	0
29	LMT	E	101	24/35	0.83	0.17	61,82,97,113	0
29	LMT	t	101	24/35	0.83	0.13	50,71,109,119	0
31	DMS	c	940	4/4	0.83	0.19	74,74,75,80	0
30	UNL	I	103	13/-	0.83	0.17	53,57,77,82	0
31	DMS	C	533	4/4	0.83	0.19	79,84,85,89	0
29	LMT	c	931	24/35	0.84	0.18	50,84,95,98	0
28	SQD	b	621	38/54	0.84	0.16	58,90,110,112	0
31	DMS	C	536	4/4	0.84	0.20	77,80,94,95	0
25	LMG	b	622	43/55	0.84	0.17	48,78,88,98	0
31	DMS	d	415	4/4	0.84	0.17	60,63,67,79	0
31	DMS	C	538	4/4	0.84	0.14	79,86,86,87	0
30	UNL	b	625	16/-	0.84	0.15	43,52,64,67	0
34	HTG	C	523	9/19	0.84	0.17	63,69,81,86	0
31	DMS	V	207	4/4	0.84	0.18	64,71,71,76	0
29	LMT	c	921	35/35	0.84	0.15	74,90,99,103	0
31	DMS	o	308	4/4	0.85	0.16	76,77,82,91	0
31	DMS	V	210	4/4	0.85	0.19	70,73,78,88	0
26	PL9	a	415	55/55	0.85	0.22	64,84,106,111	0
25	LMG	c	930	49/55	0.85	0.13	44,78,96,106	0
31	DMS	b	634	4/4	0.85	0.15	68,76,79,86	0
28	SQD	f	101	14/54	0.85	0.12	77,89,96,96	0
27	LHG	C	522	30/49	0.85	0.14	55,79,127,134	0
31	DMS	c	929	4/4	0.85	0.25	69,73,76,78	0
31	DMS	O	314	4/4	0.85	0.19	78,80,86,91	0
25	LMG	d	409	47/55	0.85	0.15	49,76,113,114	0
25	LMG	C	531	40/55	0.85	0.14	37,81,103,107	0
31	DMS	V	209	4/4	0.86	0.21	76,87,89,93	0
30	UNL	x	101	15/-	0.86	0.11	43,50,56,58	0
31	DMS	o	305	4/4	0.86	0.17	78,82,86,87	0
30	UNL	B	624	7/-	0.86	0.18	30,45,51,56	0
31	DMS	t	103	4/4	0.86	0.17	89,102,103,103	0
28	SQD	a	418	51/54	0.86	0.14	47,70,91,97	0
31	DMS	c	941	4/4	0.86	0.15	73,79,87,88	0
31	DMS	O	308	4/4	0.86	0.17	64,72,73,80	0
31	DMS	B	636	4/4	0.86	0.14	60,62,67,69	0
25	LMG	B	621	40/55	0.86	0.16	47,82,108,112	0
31	DMS	c	927	4/4	0.86	0.21	87,89,91,97	0
30	UNL	A	415	5/-	0.86	0.18	68,72,73,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	UNL	i	103	16/-	0.86	0.14	53,64,79,82	0
31	DMS	a	421	4/4	0.87	0.19	85,87,87,94	0
31	DMS	o	302	4/4	0.87	0.17	59,64,71,75	0
31	DMS	o	303	4/4	0.87	0.21	60,77,80,83	0
31	DMS	D	417	4/4	0.87	0.16	72,72,77,86	0
31	DMS	b	635	4/4	0.87	0.16	62,69,76,86	0
31	DMS	U	202	4/4	0.87	0.21	42,49,58,67	0
24	BCR	b	618	20/40	0.87	0.18	57,65,70,71	0
27	LHG	l	102	49/49	0.87	0.14	38,61,91,95	0
30	UNL	J	103	16/-	0.87	0.13	44,57,77,77	0
31	DMS	B	642	4/4	0.87	0.16	65,66,75,82	0
31	DMS	C	529	4/4	0.87	0.16	72,78,78,86	0
29	LMT	B	622	24/35	0.87	0.12	57,67,73,78	0
31	DMS	l	104	4/4	0.87	0.20	79,80,86,87	0
31	DMS	v	210	4/4	0.87	0.25	63,71,80,91	0
31	DMS	t	104	4/4	0.88	0.15	101,101,104,111	0
30	UNL	i	102	16/-	0.88	0.15	41,51,80,81	0
24	BCR	b	619	31/40	0.88	0.11	47,54,63,67	0
31	DMS	A	416	4/4	0.88	0.19	60,67,69,72	0
31	DMS	C	535	4/4	0.88	0.16	70,79,83,86	0
31	DMS	A	417	4/4	0.88	0.15	76,82,83,85	0
31	DMS	V	204	4/4	0.88	0.16	66,73,76,76	0
31	DMS	O	303	4/4	0.88	0.15	68,71,78,79	0
31	DMS	b	638	4/4	0.88	0.20	49,52,54,70	0
28	SQD	A	413	49/54	0.88	0.15	46,65,91,95	0
34	HTG	C	521	19/19	0.88	0.12	55,80,93,96	0
31	DMS	C	528	4/4	0.88	0.21	88,89,90,90	0
31	DMS	V	212	4/4	0.89	0.17	51,54,55,72	0
27	LHG	D	409	49/49	0.89	0.15	38,56,85,97	0
31	DMS	v	206	4/4	0.89	0.17	69,72,72,77	0
31	DMS	C	530	4/4	0.89	0.17	71,79,82,83	0
31	DMS	b	631	4/4	0.89	0.16	68,72,79,80	0
31	DMS	V	205	4/4	0.89	0.13	64,66,67,71	0
31	DMS	O	311	4/4	0.89	0.15	48,56,59,61	0
31	DMS	B	632	4/4	0.89	0.14	49,57,67,69	0
30	UNL	D	413	16/-	0.89	0.12	38,46,52,58	0
30	UNL	O	301	16/-	0.89	0.16	39,47,73,74	0
37	RRX	h	101	41/41	0.89	0.12	40,49,75,82	0
31	DMS	c	928	4/4	0.90	0.15	73,74,74,80	0
30	UNL	B	625	16/-	0.90	0.12	40,47,59,59	0
22	CLA	B	602	65/65	0.90	0.11	39,56,101,107	0
24	BCR	B	619	30/40	0.90	0.10	44,51,61,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	DMS	i	106	4/4	0.90	0.19	72,76,79,89	0
28	SQD	a	414	54/54	0.90	0.13	36,69,81,87	0
31	DMS	V	208	4/4	0.90	0.15	73,74,77,78	0
31	DMS	c	939	4/4	0.90	0.15	88,92,95,102	0
30	UNL	X	101	16/-	0.90	0.12	35,53,62,64	0
31	DMS	I	101	4/4	0.90	0.19	64,69,74,76	0
31	DMS	o	304	4/4	0.90	0.18	70,70,70,74	0
34	HTG	B	626	19/19	0.90	0.12	42,69,81,87	0
31	DMS	I	106	4/4	0.90	0.18	64,74,78,80	0
22	CLA	c	914	65/65	0.90	0.12	47,60,95,108	0
25	LMG	i	101	51/55	0.91	0.12	45,57,80,81	0
25	LMG	c	920	51/55	0.91	0.13	37,61,87,91	0
31	DMS	d	412	4/4	0.91	0.13	58,59,66,66	0
31	DMS	F	101	4/4	0.91	0.16	69,70,74,77	0
31	DMS	B	638	4/4	0.91	0.16	81,82,86,93	0
31	DMS	u	202	4/4	0.91	0.15	47,53,55,68	0
31	DMS	A	420	4/4	0.91	0.16	37,39,39,57	0
31	DMS	B	641	4/4	0.91	0.14	46,49,61,66	0
31	DMS	a	425	4/4	0.91	0.17	39,47,51,62	0
25	LMG	C	520	51/55	0.91	0.12	34,60,90,92	0
27	LHG	a	423	45/49	0.91	0.11	39,58,72,74	0
31	DMS	O	304	4/4	0.91	0.15	74,80,84,88	0
24	BCR	c	915	40/40	0.91	0.11	43,59,68,69	0
31	DMS	v	208	4/4	0.91	0.17	88,90,91,94	0
31	DMS	v	209	4/4	0.91	0.14	72,74,76,81	0
31	DMS	O	306	4/4	0.91	0.15	69,69,70,81	0
31	DMS	v	211	4/4	0.91	0.14	65,77,82,90	0
30	UNL	d	410	16/-	0.92	0.10	40,49,57,60	0
25	LMG	A	410	51/55	0.92	0.11	47,62,83,91	0
27	LHG	L	101	40/49	0.92	0.11	37,53,63,66	0
27	LHG	d	408	46/49	0.92	0.13	29,41,93,97	0
31	DMS	O	309	4/4	0.92	0.16	61,70,70,74	0
34	HTG	b	626	19/19	0.92	0.11	47,69,86,90	0
22	CLA	c	913	65/65	0.92	0.11	42,54,96,98	0
24	BCR	d	404	40/40	0.93	0.09	27,38,63,66	0
31	DMS	d	413	4/4	0.93	0.24	67,69,73,80	0
31	DMS	o	306	4/4	0.93	0.15	66,71,74,83	0
24	BCR	k	101	40/40	0.93	0.09	36,45,51,52	0
24	BCR	y	101	40/40	0.93	0.09	32,41,51,53	0
24	BCR	Y	101	39/40	0.93	0.08	34,40,48,50	0
31	DMS	C	527	4/4	0.93	0.16	74,80,80,81	0
32	BCT	a	422	4/4	0.93	0.10	51,52,56,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	CLA	C	507	65/65	0.93	0.11	37,45,85,88	0
31	DMS	c	926	4/4	0.93	0.14	63,64,67,68	0
31	DMS	B	635	4/4	0.93	0.15	61,63,66,73	0
35	DGD	c	918	62/66	0.93	0.10	34,42,98,113	0
22	CLA	b	617	60/65	0.93	0.10	32,41,75,80	0
37	RRX	H	101	41/41	0.93	0.10	32,42,58,62	0
22	CLA	C	514	65/65	0.93	0.10	44,55,83,86	0
22	CLA	B	615	53/65	0.94	0.09	31,36,71,84	0
22	CLA	b	607	65/65	0.94	0.08	29,37,58,65	0
31	DMS	a	424	4/4	0.94	0.12	38,47,50,65	0
24	BCR	C	515	40/40	0.94	0.09	37,50,58,59	0
31	DMS	B	633	4/4	0.94	0.17	65,71,71,73	0
22	CLA	b	615	52/65	0.94	0.09	36,42,71,76	0
22	CLA	B	617	55/65	0.94	0.09	28,35,72,76	0
34	HTG	b	623	19/19	0.94	0.09	42,46,54,63	0
22	CLA	c	904	65/65	0.94	0.08	32,44,50,54	0
22	CLA	c	907	65/65	0.94	0.11	39,47,102,108	0
24	BCR	c	916	40/40	0.94	0.08	33,42,48,49	0
22	CLA	c	908	65/65	0.94	0.09	34,39,53,61	0
31	DMS	B	640	4/4	0.94	0.17	47,53,57,63	0
28	SQD	C	501	54/54	0.94	0.11	32,64,83,89	0
25	LMG	j	101	47/55	0.94	0.10	33,43,69,74	0
35	DGD	C	518	62/66	0.94	0.10	29,40,89,109	0
31	DMS	c	934	4/4	0.94	0.11	64,73,74,77	0
22	CLA	B	607	65/65	0.94	0.08	28,34,56,65	0
22	CLA	B	608	65/65	0.94	0.09	24,29,64,79	0
35	DGD	h	102	62/66	0.94	0.09	28,42,53,58	0
22	CLA	d	403	65/65	0.94	0.10	35,40,85,90	0
31	DMS	A	419	4/4	0.94	0.17	58,60,70,72	0
31	DMS	c	933	4/4	0.95	0.12	57,64,66,70	0
22	CLA	b	614	59/65	0.95	0.08	26,32,76,82	0
31	DMS	O	310	4/4	0.95	0.14	66,68,68,73	0
24	BCR	B	620	40/40	0.95	0.07	30,37,49,50	0
22	CLA	C	509	65/65	0.95	0.09	29,35,81,102	0
24	BCR	C	516	40/40	0.95	0.08	32,39,47,54	0
24	BCR	D	405	40/40	0.95	0.08	26,35,62,66	0
24	BCR	K	101	40/40	0.95	0.08	31,39,43,43	0
31	DMS	V	201	4/4	0.95	0.10	46,48,54,58	0
32	BCT	A	421[A]	4/4	0.95	0.10	34,36,39,39	4
32	BCT	A	421[B]	4/4	0.95	0.10	27,29,30,34	4
26	PL9	D	406	55/55	0.95	0.07	21,30,37,51	0
33	CA	B	601	1/1	0.95	0.05	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
33	CA	O	302	1/1	0.95	0.06	59,59,59,59	0
34	HTG	B	623	19/19	0.95	0.09	41,47,64,66	0
22	CLA	C	512	65/65	0.95	0.08	31,39,48,51	0
26	PL9	d	405	55/55	0.95	0.07	23,32,39,43	0
24	BCR	a	413	40/40	0.95	0.07	26,31,38,39	0
22	CLA	c	902	65/65	0.95	0.08	34,39,50,51	0
22	CLA	C	513	56/65	0.95	0.08	37,48,62,65	0
27	LHG	D	411	45/49	0.95	0.10	31,39,90,94	0
24	BCR	b	620	40/40	0.95	0.07	33,39,48,49	0
22	CLA	c	906	65/65	0.95	0.08	30,40,50,54	0
31	DMS	D	416	4/4	0.95	0.12	55,59,60,69	0
22	CLA	B	611	65/65	0.95	0.08	26,33,41,46	0
22	CLA	D	404	65/65	0.95	0.09	30,37,94,104	0
31	DMS	b	630	4/4	0.95	0.15	56,63,63,64	0
31	DMS	B	629	4/4	0.95	0.14	48,52,58,65	0
31	DMS	b	633	4/4	0.95	0.14	68,68,70,78	0
22	CLA	c	909	65/65	0.95	0.08	31,37,80,97	0
22	CLA	c	910	65/65	0.95	0.09	28,38,58,64	0
22	CLA	c	912	65/65	0.95	0.08	35,45,50,53	0
35	DGD	C	519	62/66	0.95	0.09	23,36,76,85	0
22	CLA	a	412	65/65	0.95	0.11	27,32,102,116	0
35	DGD	H	102	62/66	0.95	0.08	28,37,46,50	0
22	CLA	B	604	65/65	0.95	0.08	26,30,40,47	0
35	DGD	c	919	62/66	0.95	0.09	29,40,73,79	0
22	CLA	C	508	65/65	0.95	0.08	32,42,55,59	0
23	PHO	a	411	64/64	0.95	0.06	26,33,40,48	0
25	LMG	J	101	45/55	0.95	0.09	28,36,71,79	0
22	CLA	b	610	65/65	0.95	0.08	32,41,45,54	0
22	CLA	A	408	65/65	0.96	0.09	19,29,99,110	0
27	LHG	d	407	49/49	0.96	0.07	28,36,56,63	0
31	DMS	d	411	4/4	0.96	0.12	60,62,64,64	0
22	CLA	b	608	65/65	0.96	0.08	27,31,73,74	0
31	DMS	B	630	4/4	0.96	0.13	63,67,68,75	0
22	CLA	b	609	65/65	0.96	0.06	27,34,42,45	0
23	PHO	A	407	64/64	0.96	0.06	20,25,30,32	0
23	PHO	D	402	64/64	0.96	0.06	25,29,35,39	0
23	PHO	a	410	64/64	0.96	0.06	21,28,32,36	0
22	CLA	B	614	61/65	0.96	0.07	25,31,70,83	0
24	BCR	A	409	40/40	0.96	0.06	25,30,37,38	0
22	CLA	b	611	65/65	0.96	0.07	28,35,40,43	0
22	CLA	b	612	65/65	0.96	0.08	27,31,72,83	0
22	CLA	B	606	65/65	0.96	0.07	24,30,42,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	CLA	C	510	65/65	0.96	0.09	31,36,59,64	0
22	CLA	b	616	65/65	0.96	0.07	30,37,53,57	0
31	DMS	c	924	4/4	0.96	0.14	37,42,47,49	0
31	DMS	c	925	4/4	0.96	0.11	51,58,60,61	0
22	CLA	C	511	65/65	0.96	0.06	31,36,41,46	0
22	CLA	B	610	65/65	0.96	0.06	30,37,42,46	0
31	DMS	O	312	4/4	0.96	0.14	37,51,56,59	0
22	CLA	C	502	65/65	0.96	0.07	33,39,52,62	0
22	CLA	c	905	65/65	0.96	0.08	30,35,62,66	0
35	DGD	C	517	62/66	0.96	0.09	24,35,80,88	0
22	CLA	C	503	65/65	0.96	0.07	28,32,47,56	0
22	CLA	C	504	65/65	0.96	0.06	29,37,42,51	0
31	DMS	v	201	4/4	0.96	0.16	42,48,50,51	0
22	CLA	C	505	65/65	0.96	0.07	28,34,58,60	0
35	DGD	c	917	62/66	0.96	0.08	26,42,81,94	0
27	LHG	D	410	49/49	0.96	0.07	29,36,51,61	0
22	CLA	C	506	65/65	0.96	0.07	30,37,50,54	0
31	DMS	V	206	4/4	0.96	0.09	45,48,51,62	0
22	CLA	b	603	65/65	0.96	0.07	29,36,46,49	0
36	HEM	E	102	43/43	0.96	0.09	48,56,62,65	0
22	CLA	c	911	65/65	0.96	0.06	29,38,46,52	0
22	CLA	b	604	65/65	0.96	0.07	26,32,45,50	0
38	MG	J	102	1/1	0.96	0.06	30,30,30,30	0
22	CLA	B	609	65/65	0.97	0.06	25,30,38,39	0
31	DMS	C	526	4/4	0.97	0.09	48,48,50,51	0
22	CLA	B	616	65/65	0.97	0.06	30,36,50,57	0
22	CLA	A	406	55/65	0.97	0.06	21,27,49,60	0
31	DMS	b	629	4/4	0.97	0.09	29,31,36,45	0
22	CLA	a	408	65/65	0.97	0.05	20,26,35,41	0
22	CLA	a	409	61/65	0.97	0.07	25,29,80,87	0
22	CLA	B	603	65/65	0.97	0.06	27,36,43,47	0
22	CLA	b	613	65/65	0.97	0.06	26,32,37,40	0
22	CLA	B	612	65/65	0.97	0.06	23,29,55,60	0
22	CLA	B	613	65/65	0.97	0.06	24,30,37,40	0
22	CLA	A	405	65/65	0.97	0.06	18,23,36,54	0
22	CLA	b	605	65/65	0.97	0.07	23,29,63,65	0
22	CLA	d	402	65/65	0.97	0.05	21,27,42,50	0
36	HEM	e	101	43/43	0.97	0.09	43,55,85,93	0
31	DMS	o	307	4/4	0.97	0.19	48,56,62,64	0
22	CLA	b	606	65/65	0.97	0.06	24,28,40,40	0
22	CLA	c	903	65/65	0.97	0.07	27,34,54,65	0
38	MG	k	102	1/1	0.97	0.07	48,48,48,48	0

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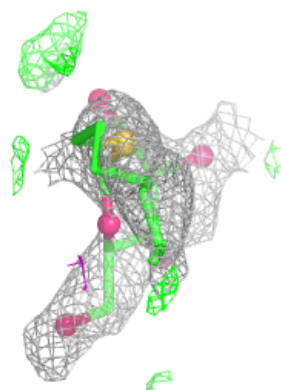
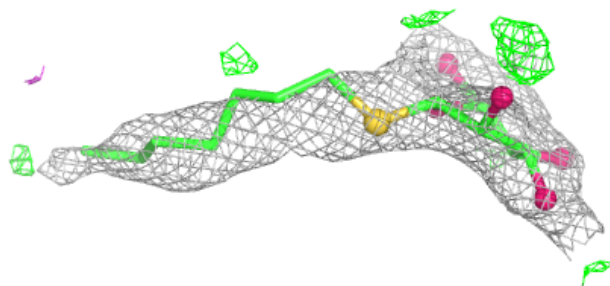
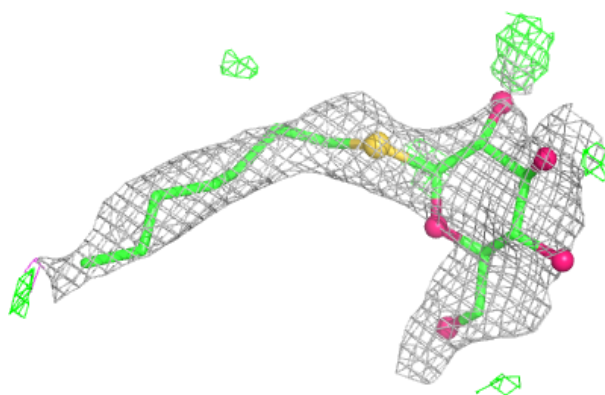
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	DMS	c	923	4/4	0.98	0.09	37,40,42,43	0
22	CLA	B	605	65/65	0.98	0.06	24,28,60,66	0
31	DMS	B	628	4/4	0.98	0.07	27,29,32,38	0
31	DMS	D	418	4/4	0.98	0.06	35,39,42,43	0
31	DMS	C	525	4/4	0.98	0.08	34,35,38,40	0
22	CLA	a	407	65/65	0.98	0.05	23,26,45,61	0
21	CL	A	404	1/1	0.98	0.04	28,28,28,28	0
22	CLA	D	401	65/65	0.98	0.05	19,23,31,36	0
31	DMS	A	418	4/4	0.98	0.05	29,30,31,31	0
38	MG	K	102	1/1	0.98	0.05	51,51,51,51	0
22	CLA	D	403	65/65	0.98	0.05	18,24,45,52	0
39	HEC	V	202	43/43	0.98	0.06	23,29,36,40	0
39	HEC	v	202	43/43	0.98	0.06	33,37,42,46	0
21	CL	a	406	1/1	0.99	0.03	32,32,32,32	0
33	CA	b	601	1/1	0.99	0.03	59,59,59,59	0
33	CA	c	901	1/1	0.99	0.05	48,48,48,48	0
33	CA	o	301	1/1	0.99	0.04	55,55,55,55	0
31	DMS	a	402	4/4	0.99	0.07	30,32,34,34	0
38	MG	j	102	1/1	0.99	0.08	40,40,40,40	0
31	DMS	C	524	4/4	0.99	0.06	38,42,43,43	0
21	CL	A	403	1/1	0.99	0.04	29,29,29,29	0
21	CL	a	405	1/1	0.99	0.04	31,31,31,31	0
19	OEX	A	401	10/10	1.00	0.05	25,27,31,32	0
19	OEX	a	403	10/10	1.00	0.03	29,31,32,33	0
20	FE2	A	402	1/1	1.00	0.01	39,39,39,39	0
20	FE2	a	404	1/1	1.00	0.01	42,42,42,42	0

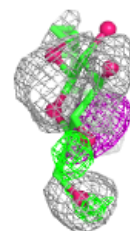
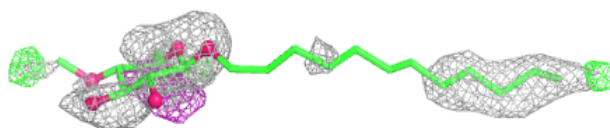
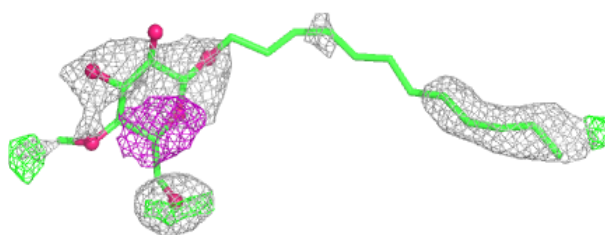
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HTG b 624:

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

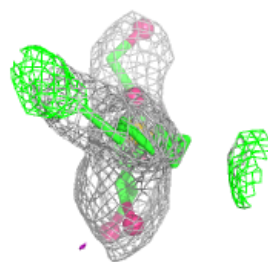
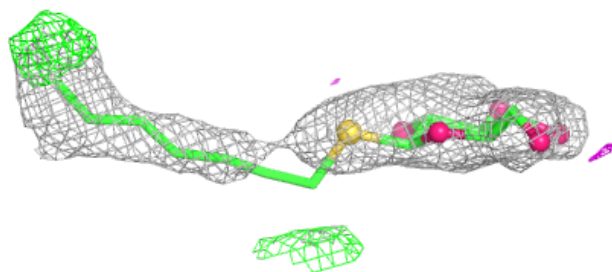
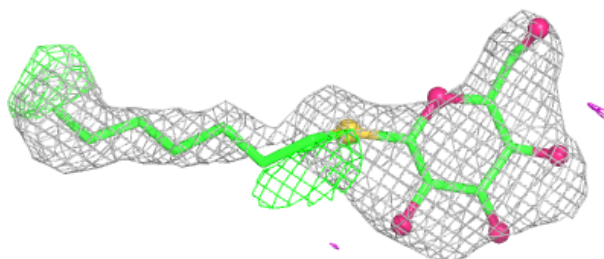
**Electron density around LMT f 102:**

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

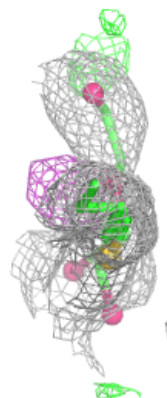
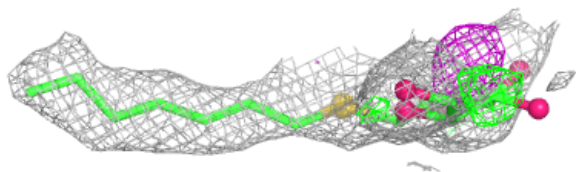
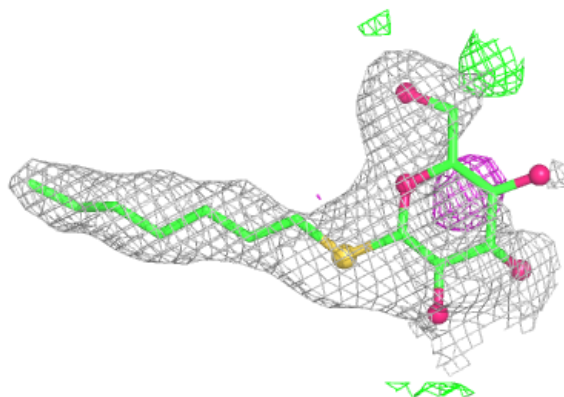


Electron density around HTG c 922:

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

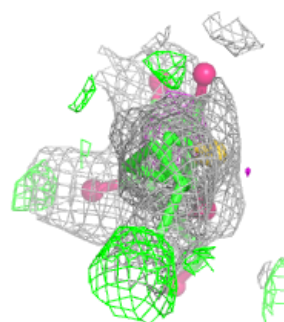
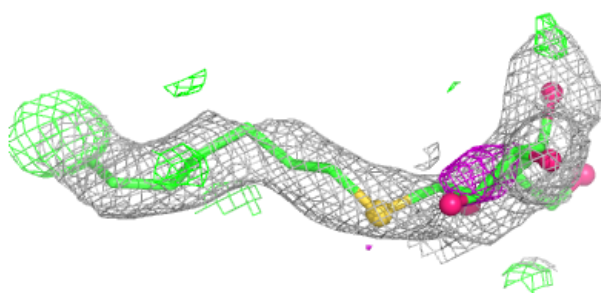
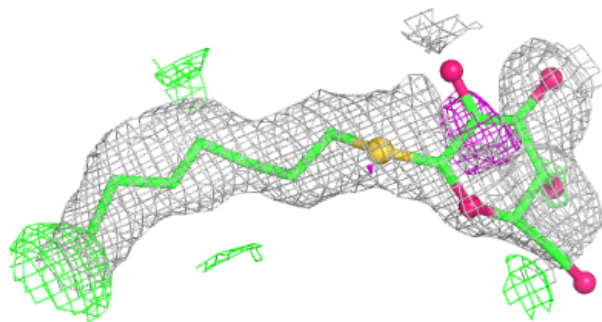
**Electron density around HTG b 627:**

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

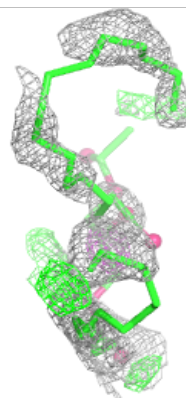
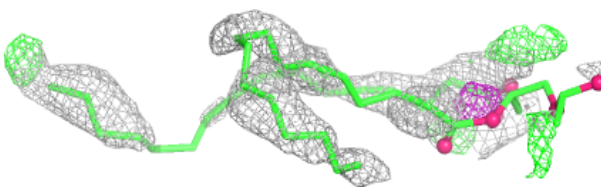
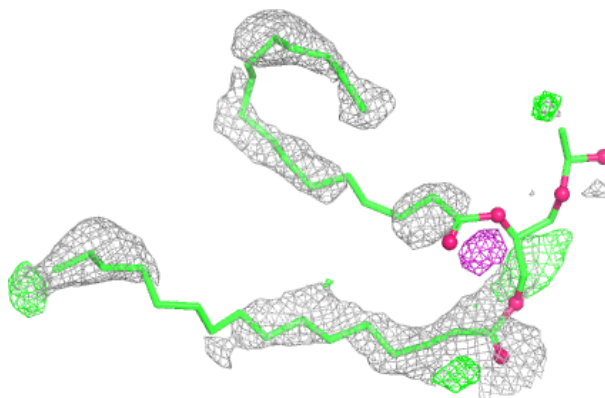


Electron density around HTG D 415:

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

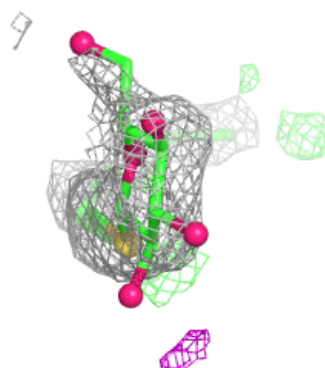
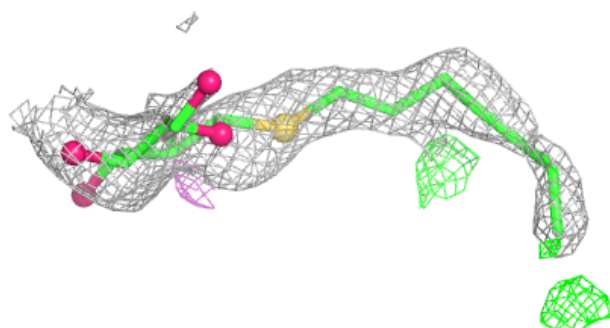
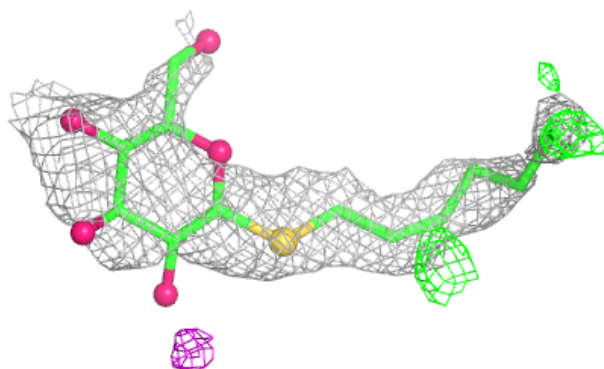
**Electron density around DGD d 406:**

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

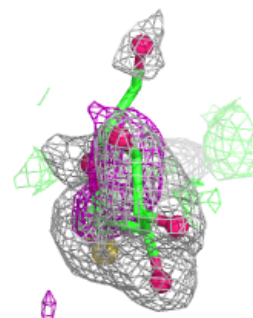
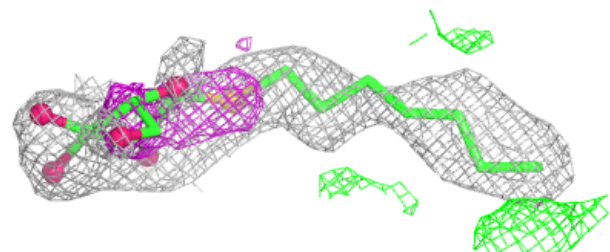
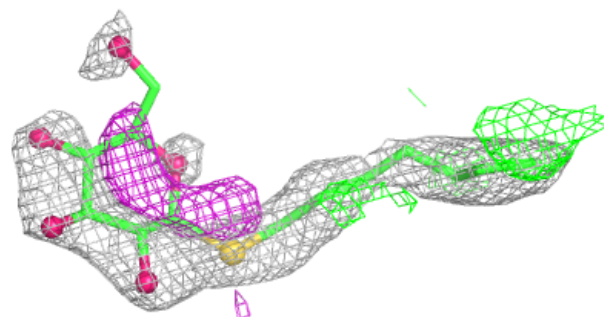


Electron density around HTG D 414:

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

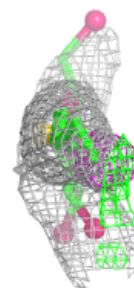
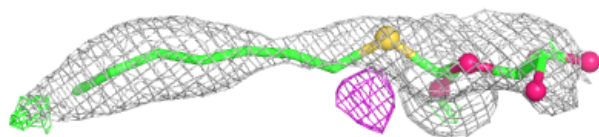
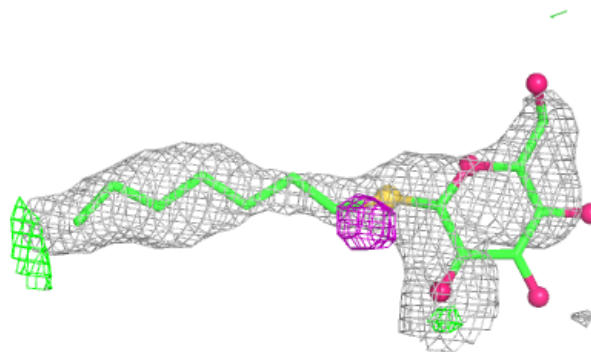
**Electron density around HTG b 632:**

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

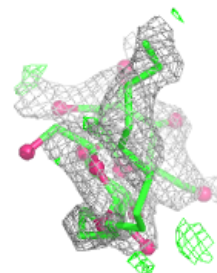
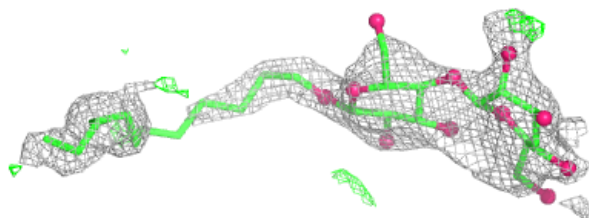
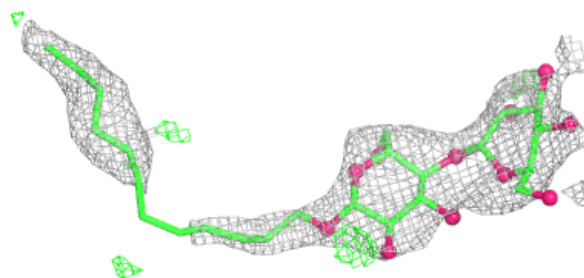


Electron density around HTG B 627:

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

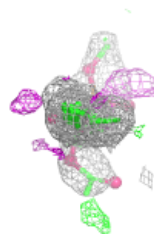
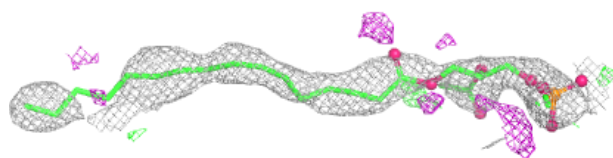
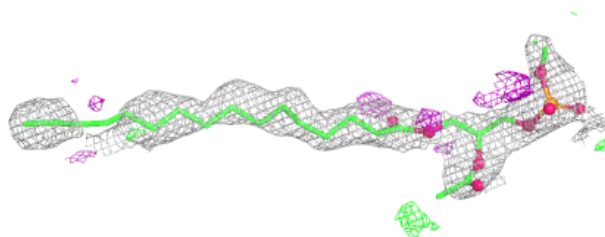
**Electron density around LMT I 102:**

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



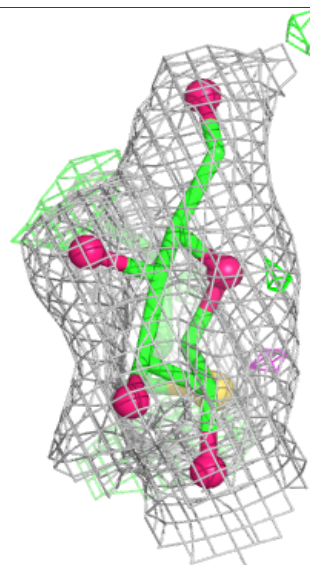
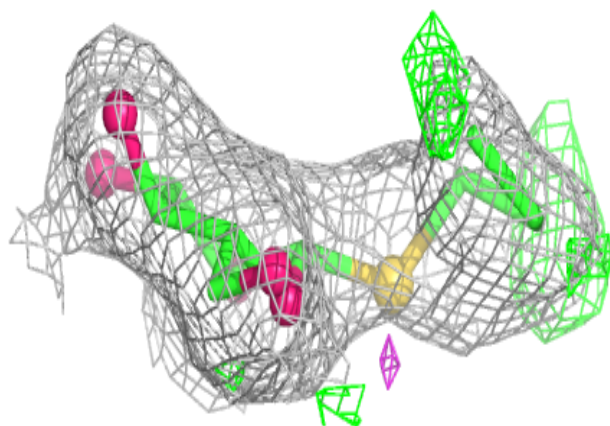
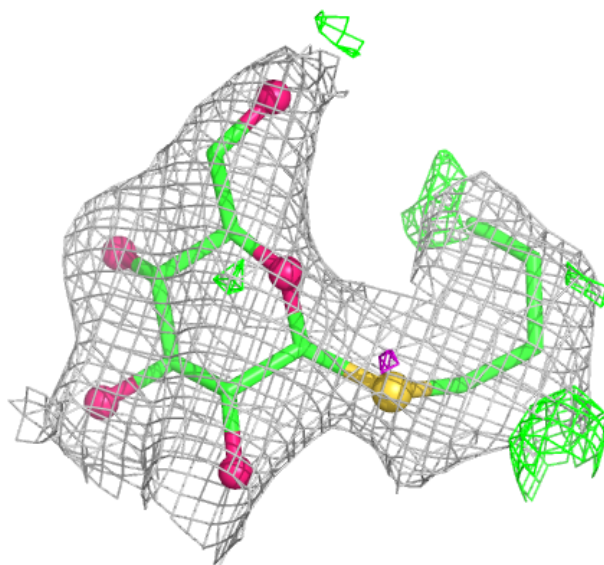
Electron density around LHG A 412:

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



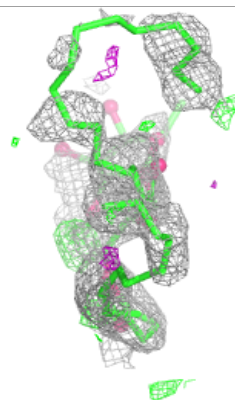
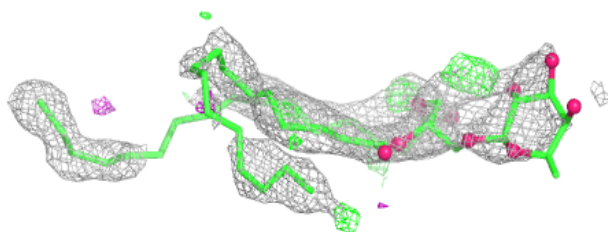
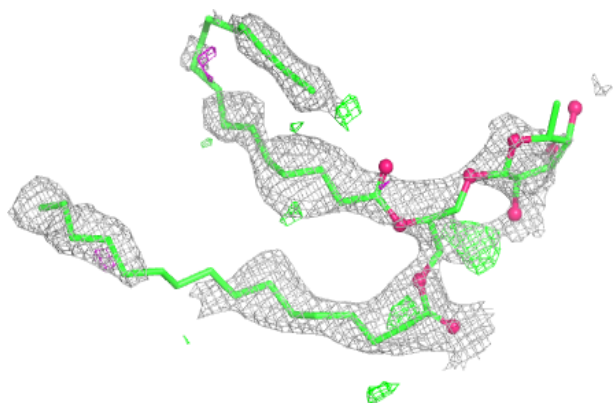
Electron density around HTG v 203:

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

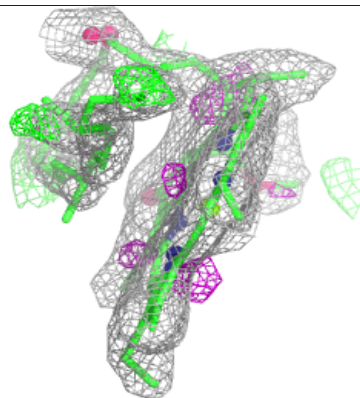
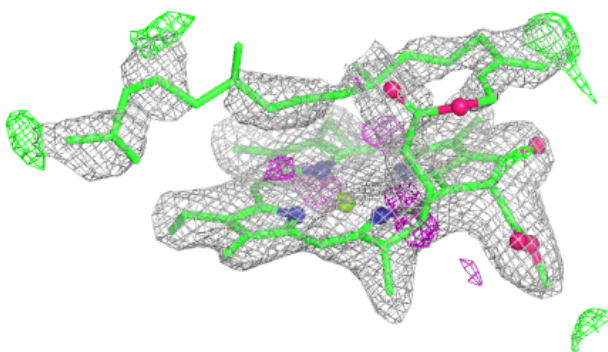
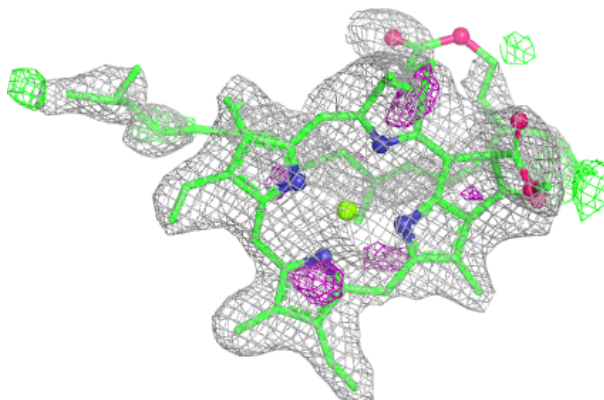


Electron density around DGD D 407:

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

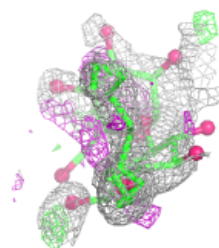
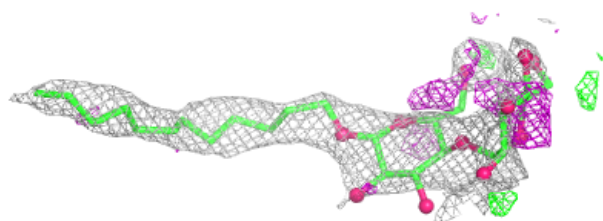
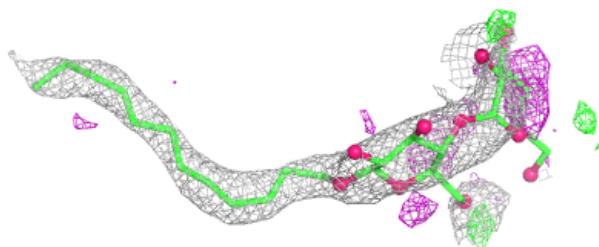
**Electron density around CLA b 602:**

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

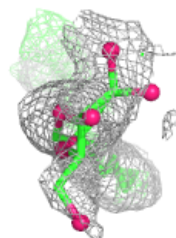
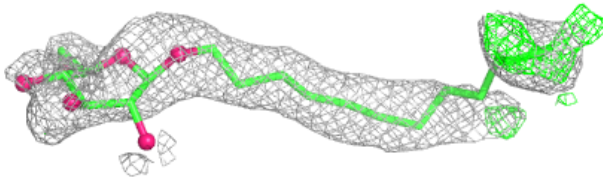
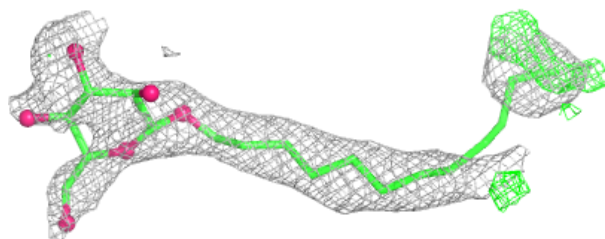


Electron density around LMT A 414:

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

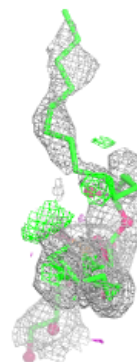
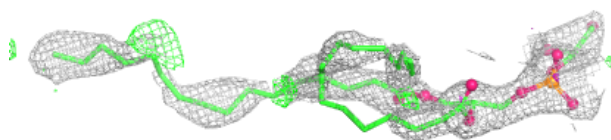
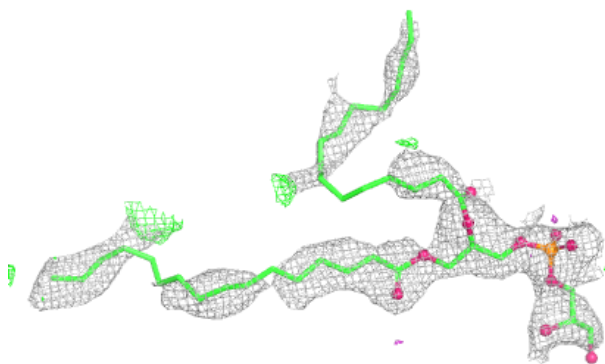
**Electron density around LMT T 102:**

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



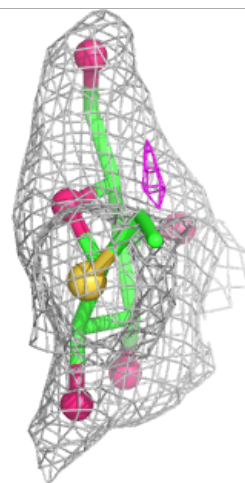
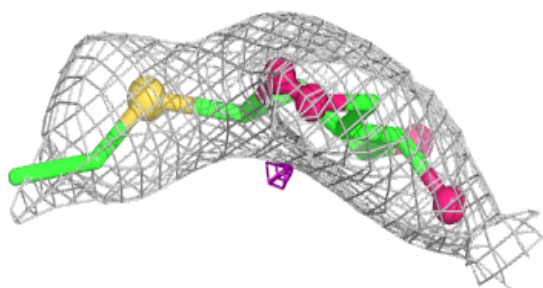
Electron density around LHG a 416:

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



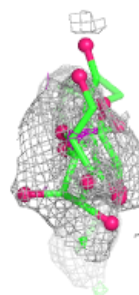
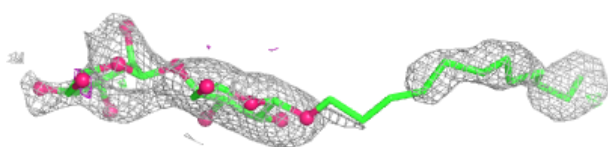
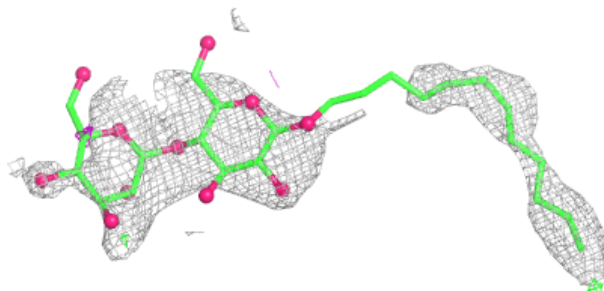
Electron density around HTG V 203:

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

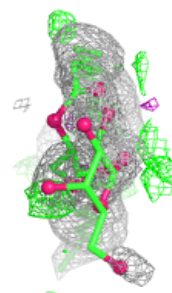
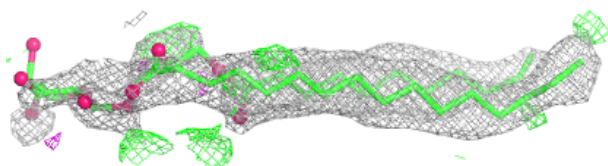
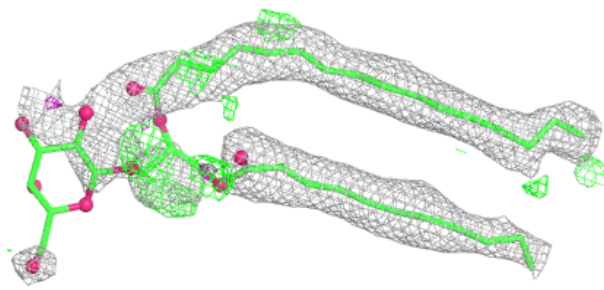


Electron density around LMT Z 101:

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

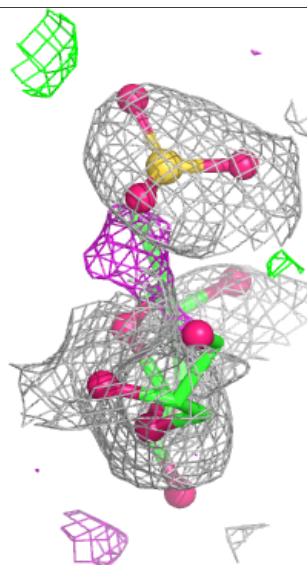
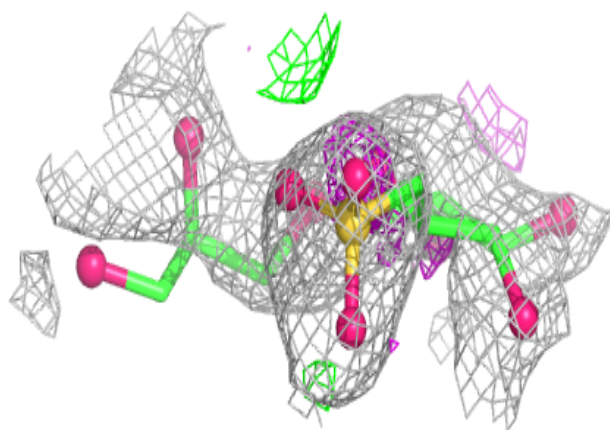
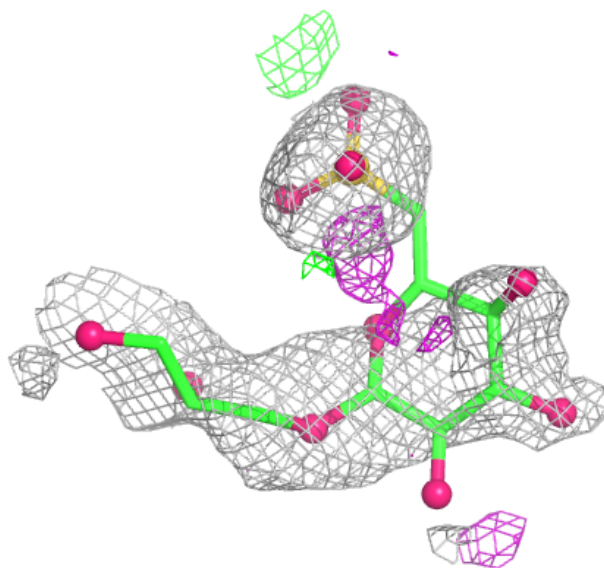
**Electron density around LMG D 412:**

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



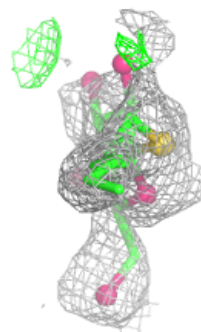
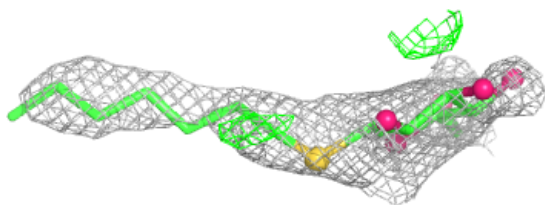
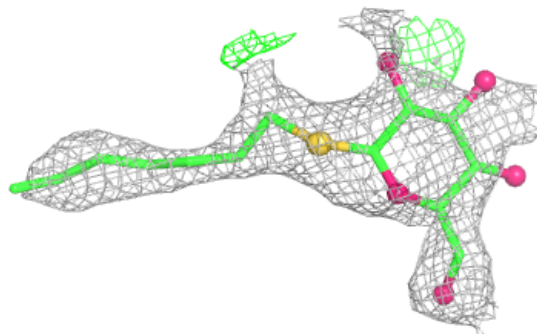
Electron density around SQD D 408:

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

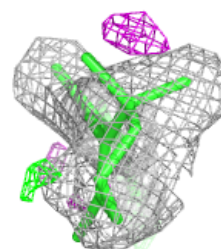
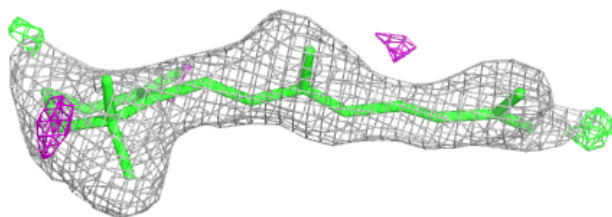
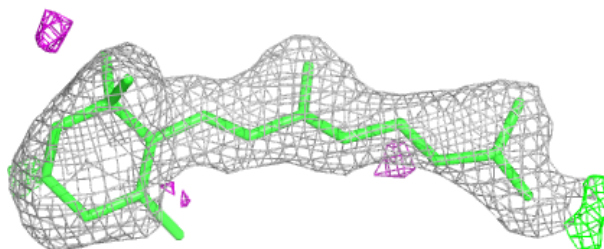


Electron density around HTG 1 106:

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

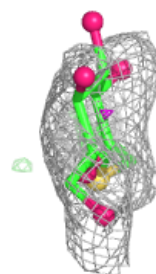
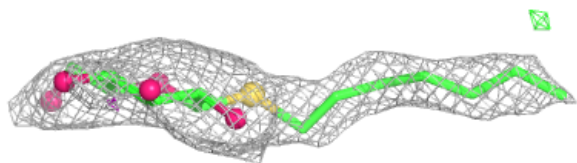
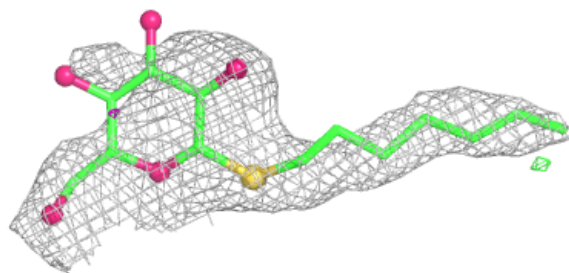
**Electron density around BCR B 618:**

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

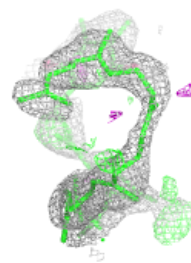
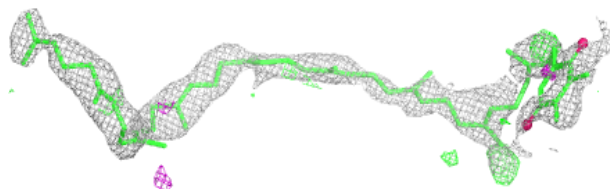
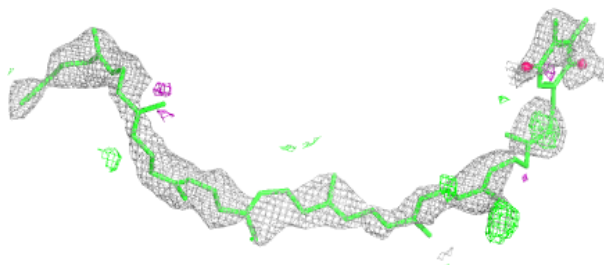


Electron density around HTG C 532:

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

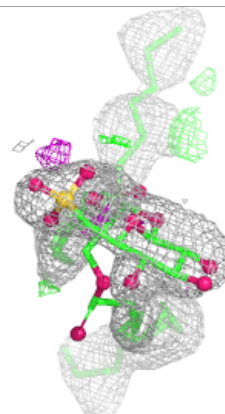
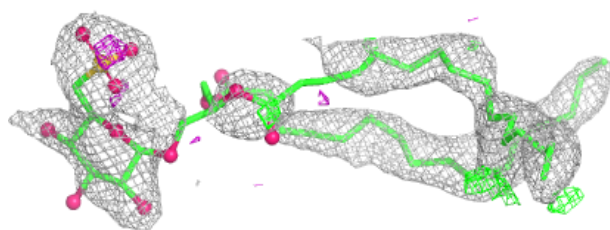
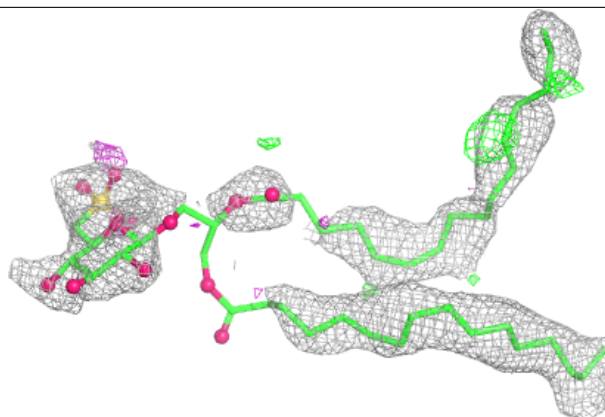
**Electron density around PL9 A 411:**

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

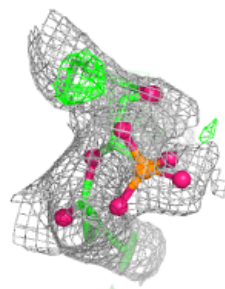
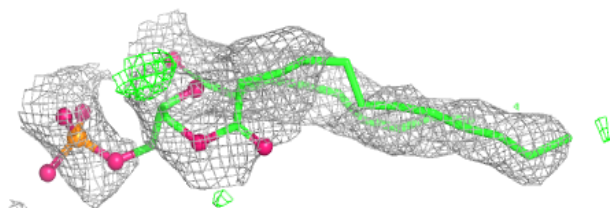
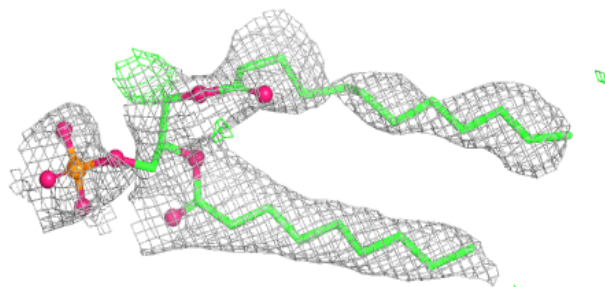


Electron density around SQD 1 101:

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

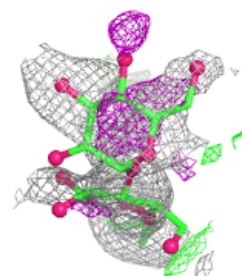
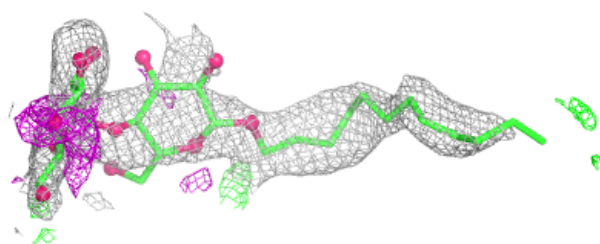
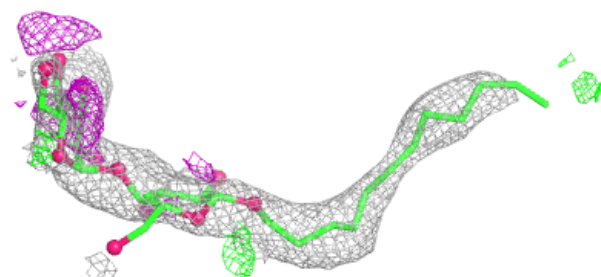
**Electron density around LHG d 401:**

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

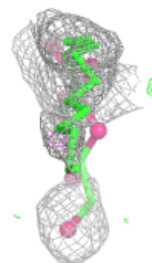
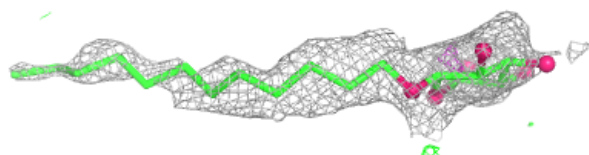
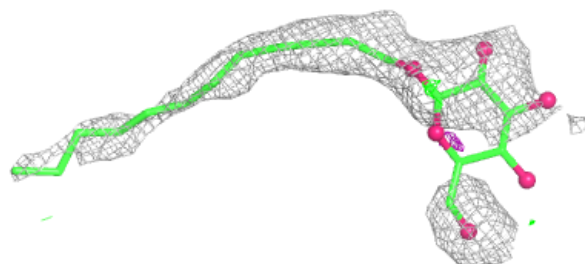


Electron density around LMT a 419:

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

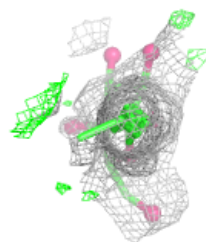
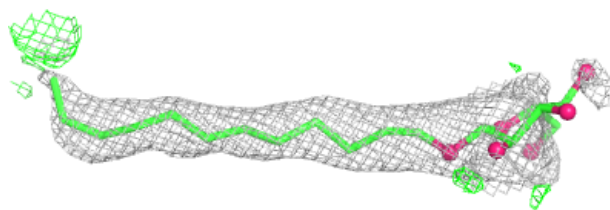
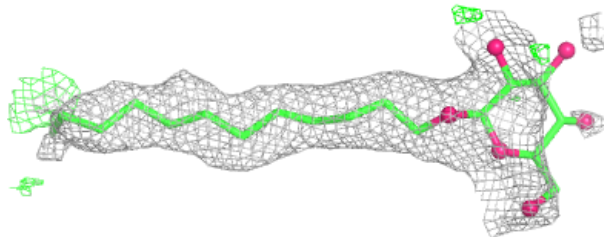
**Electron density around LMT E 101:**

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

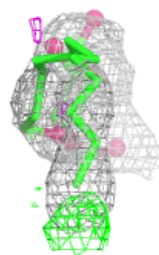
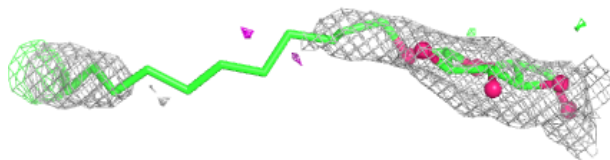
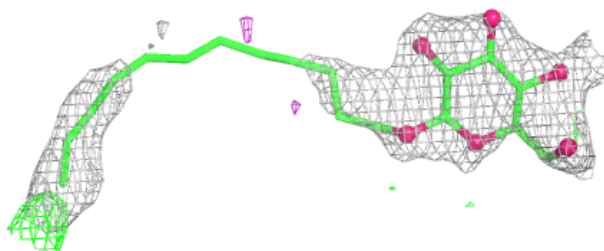


Electron density around LMT t 101:

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

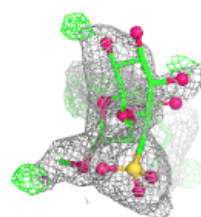
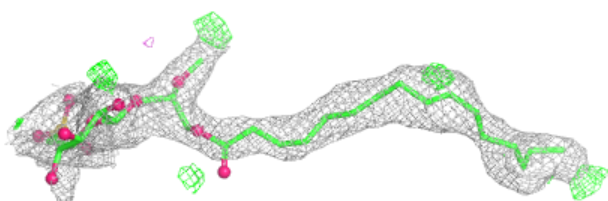
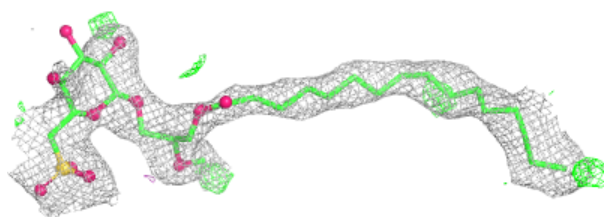
**Electron density around LMT c 931:**

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

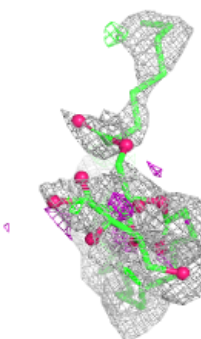
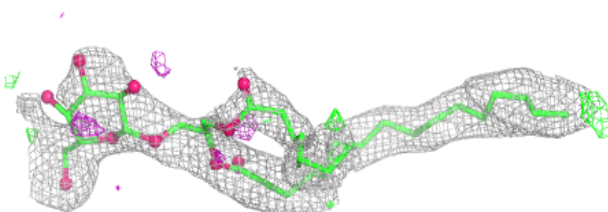
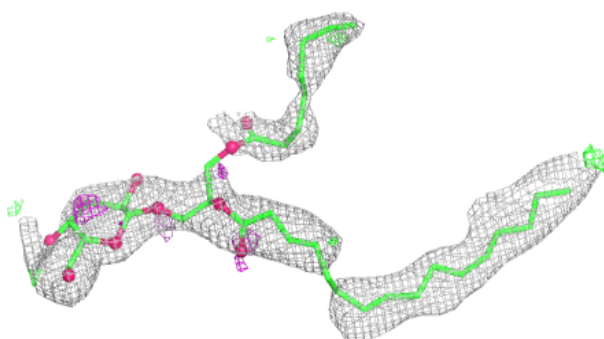


Electron density around SQD b 621:

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

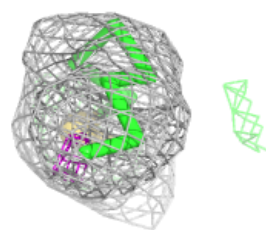
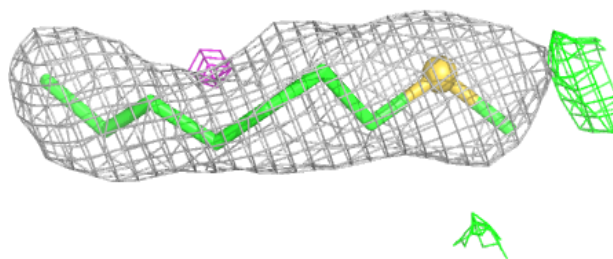
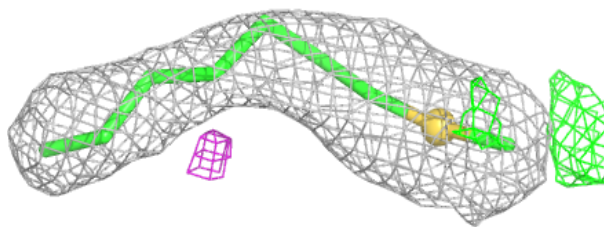
**Electron density around LMG b 622:**

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

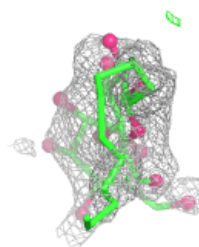
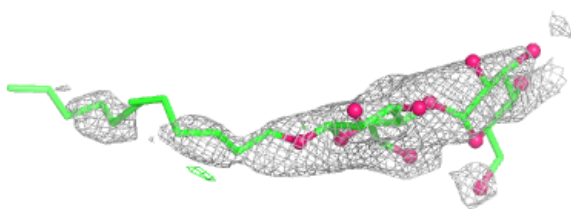
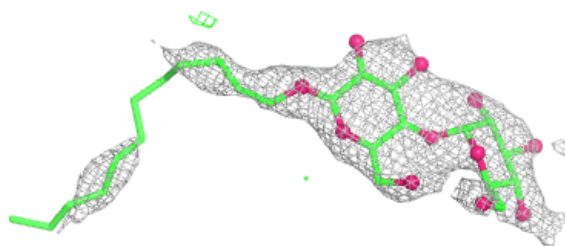


Electron density around HTG C 523:

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

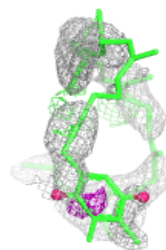
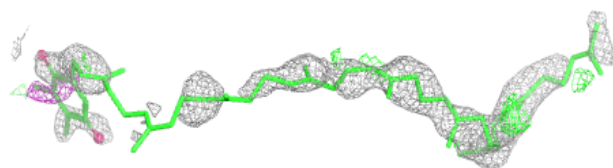
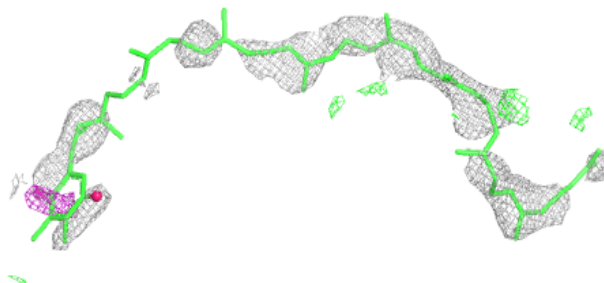
**Electron density around LMT c 921:**

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

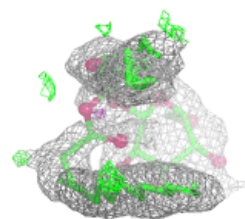
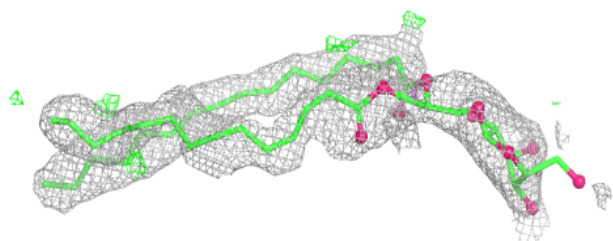
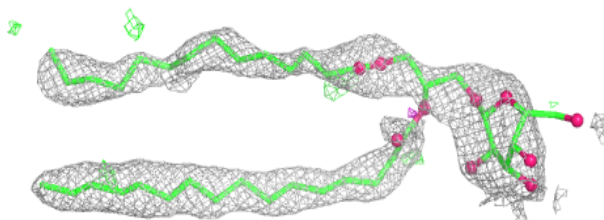


Electron density around PL9 a 415:

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

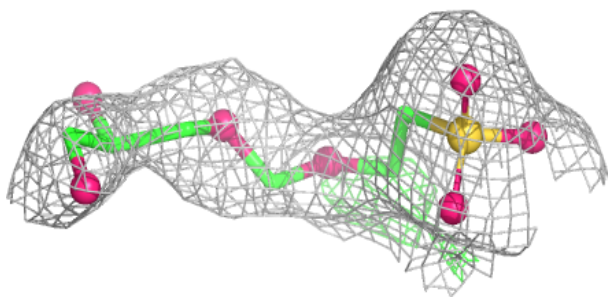
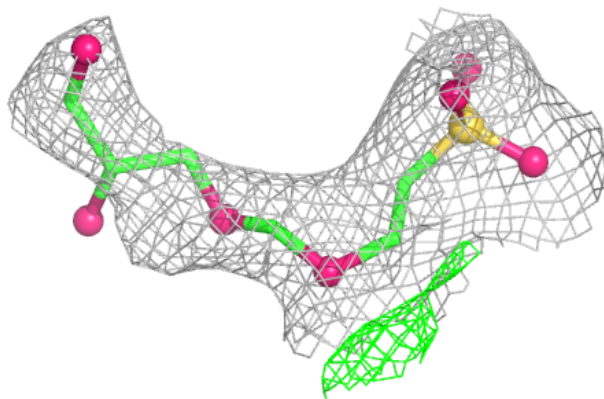
**Electron density around LMG c 930:**

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

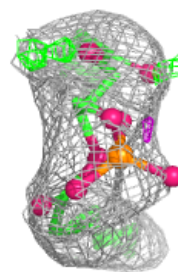
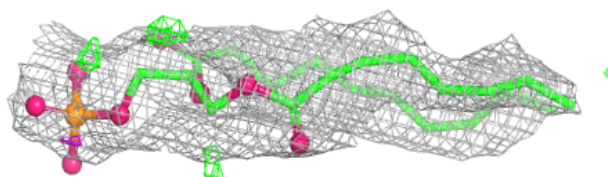
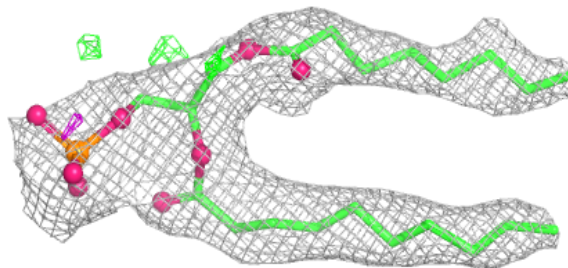


Electron density around SQD f 101:

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

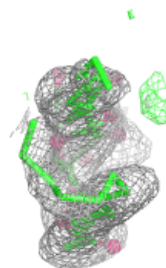
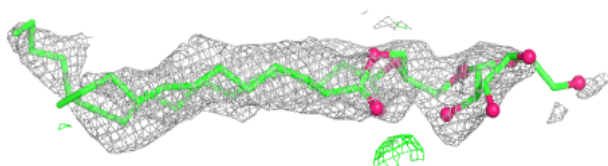
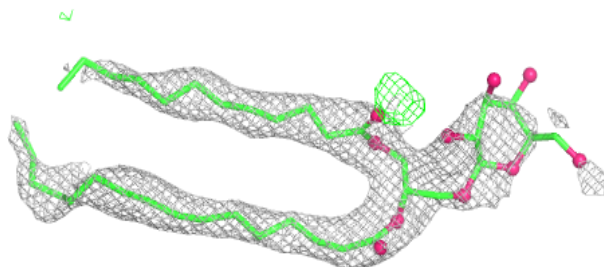
**Electron density around LHG C 522:**

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

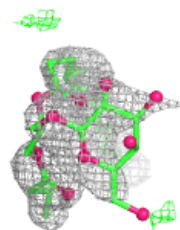
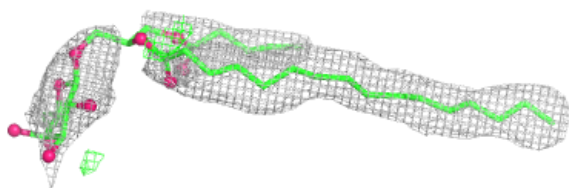
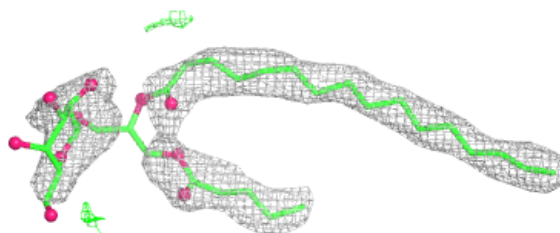


Electron density around LMG d 409:

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

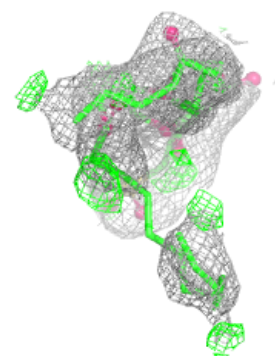
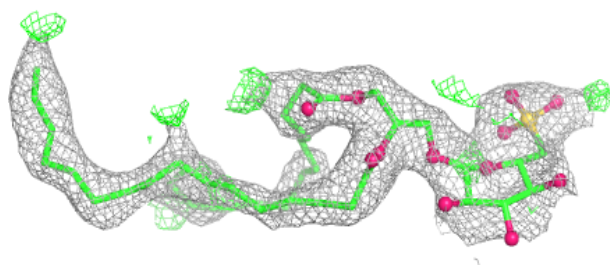
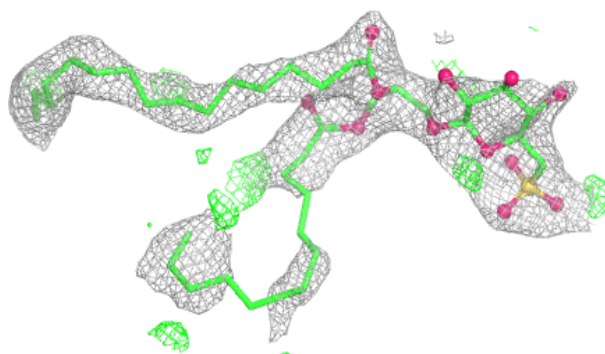
**Electron density around LMG C 531:**

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

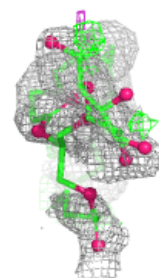
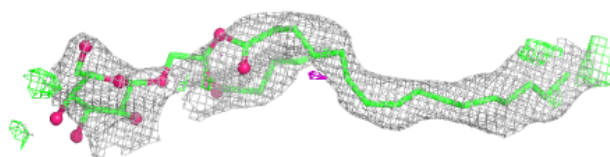
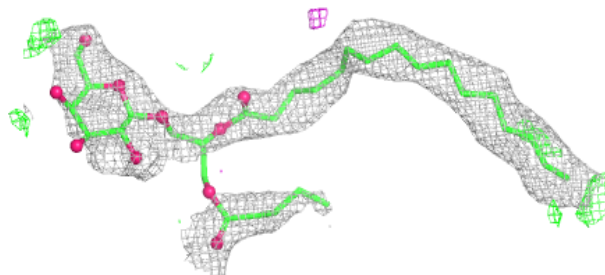


Electron density around SQD a 418:

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

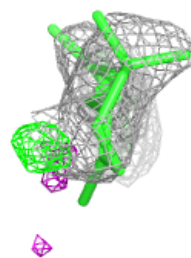
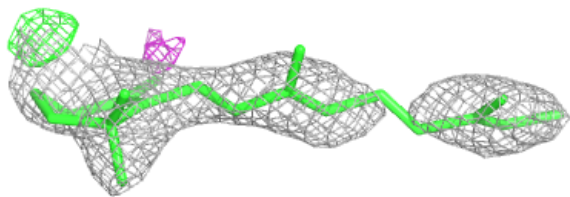
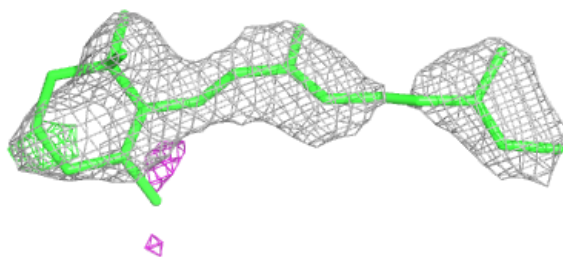
**Electron density around LMG B 621:**

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



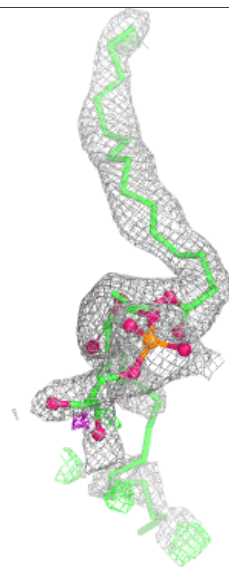
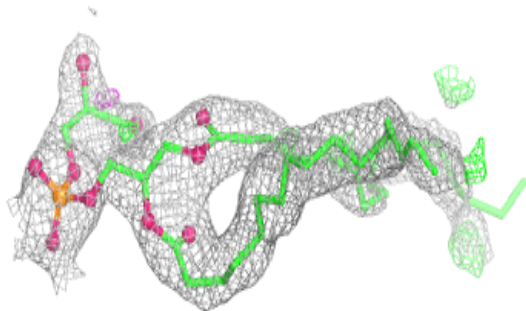
Electron density around BCR b 618:

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



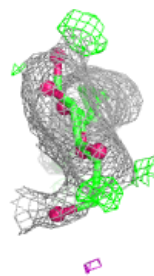
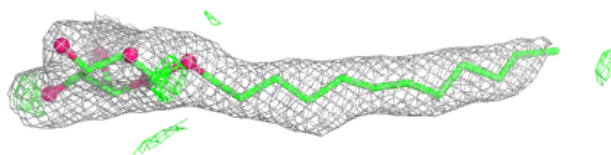
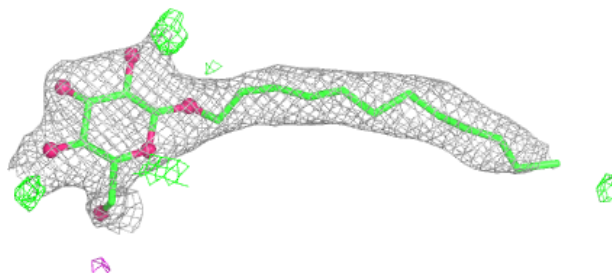
Electron density around LHG 1 102:

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

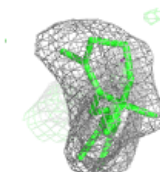
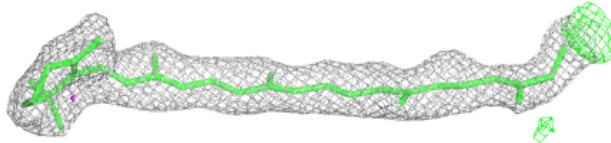
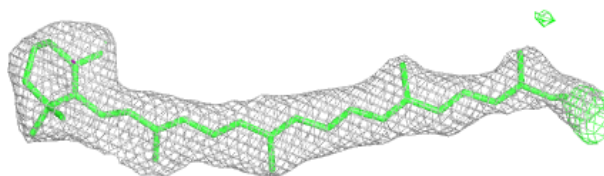


Electron density around LMT B 622:

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

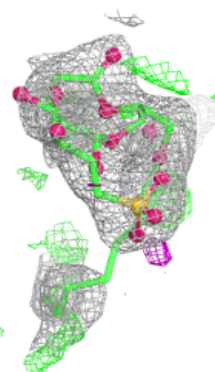
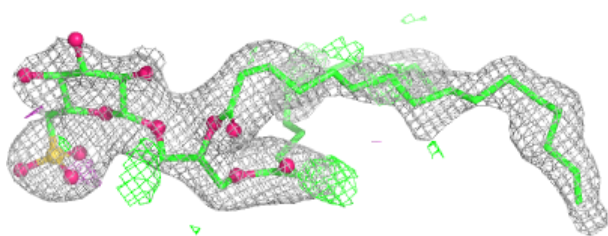
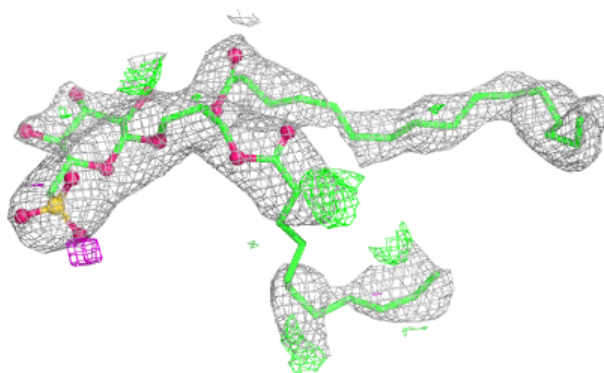
**Electron density around BCR b 619:**

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

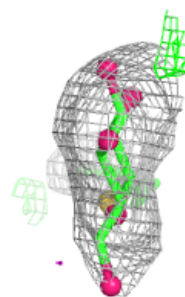
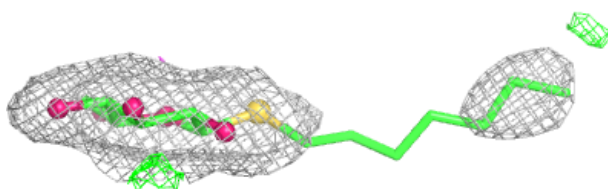
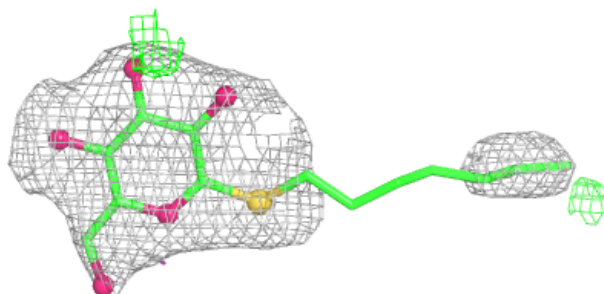


Electron density around SQD A 413:

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

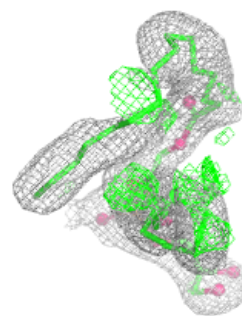
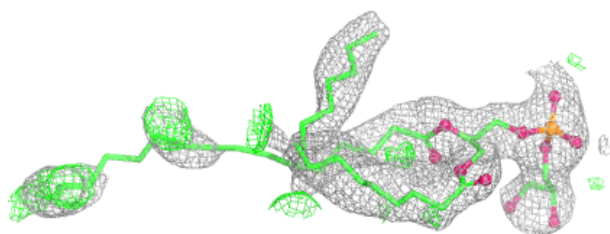
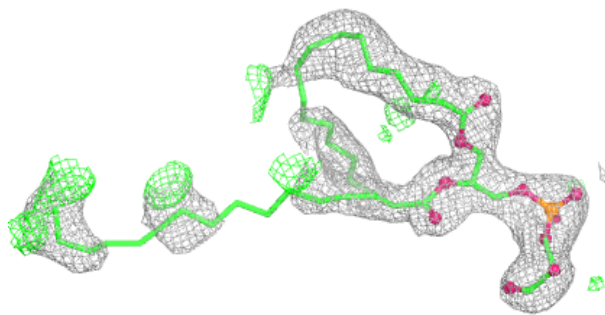
**Electron density around HTG C 521:**

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

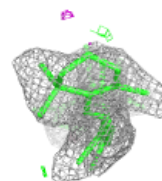
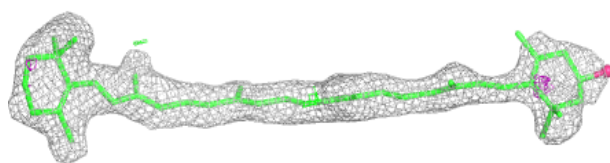
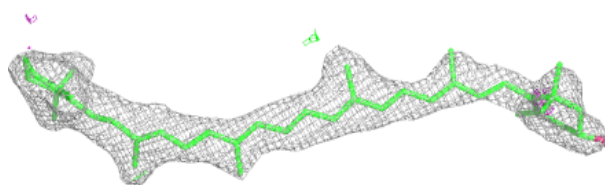


Electron density around LHG D 409:

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

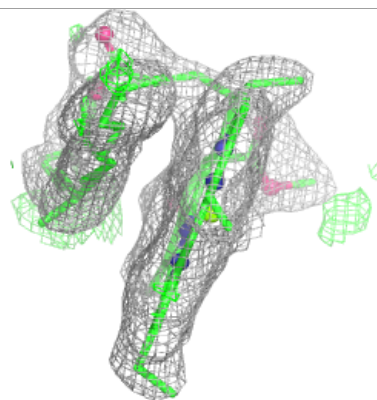
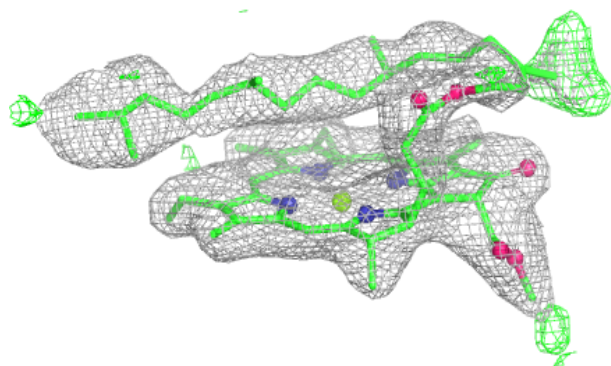
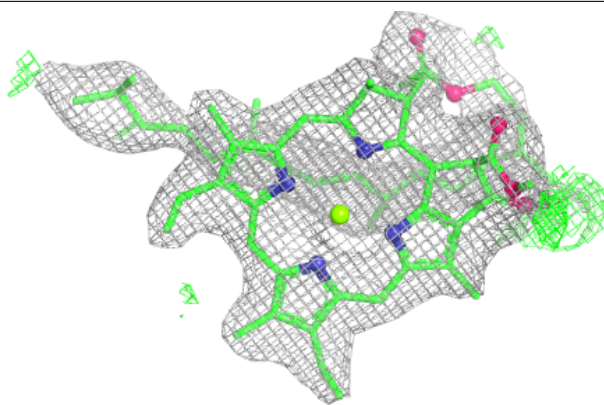
**Electron density around RRX h 101:**

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

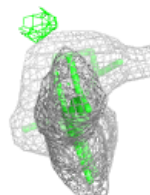
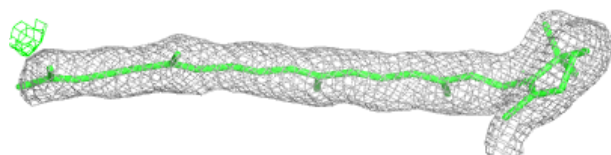
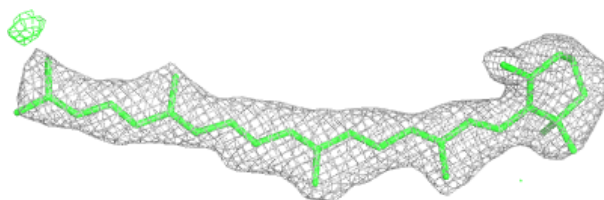


Electron density around CLA B 602:

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

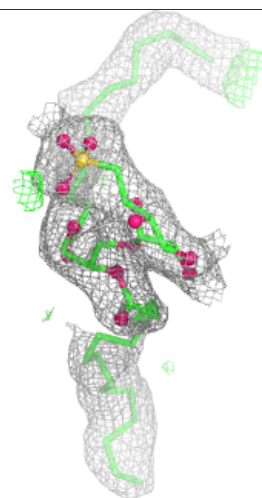
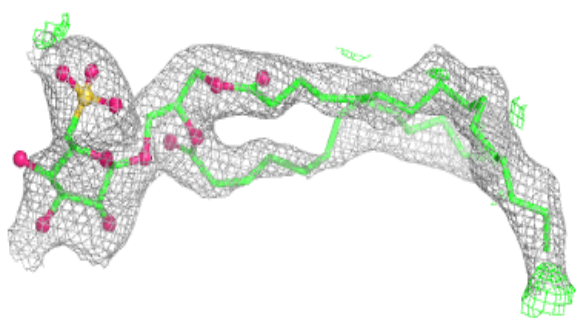
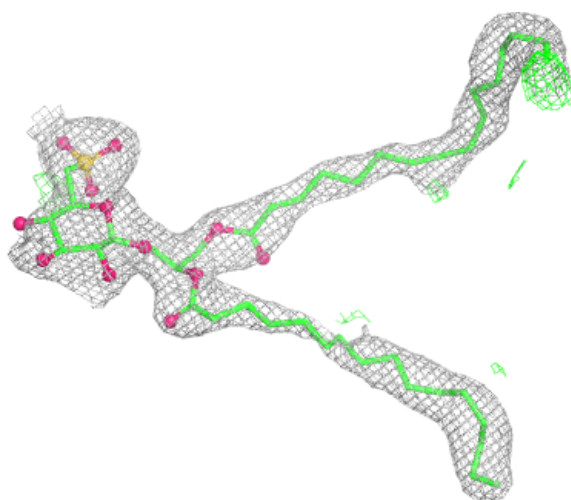
**Electron density around BCR B 619:**

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



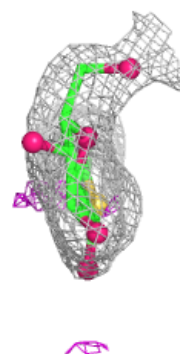
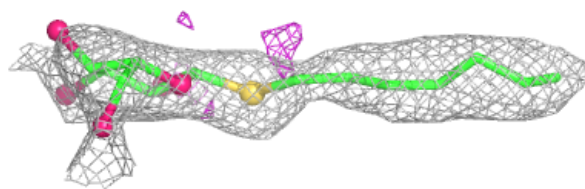
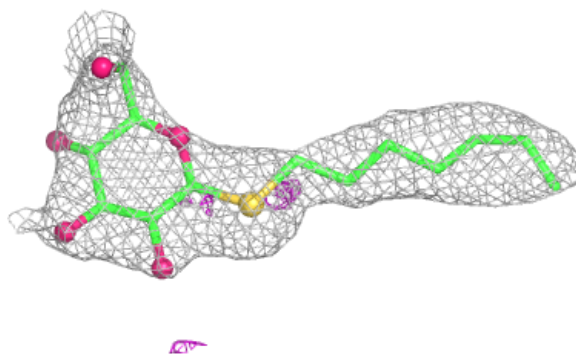
Electron density around SQD a 414:

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

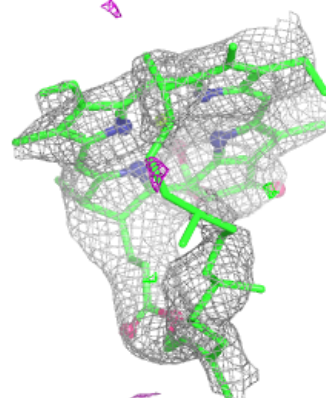
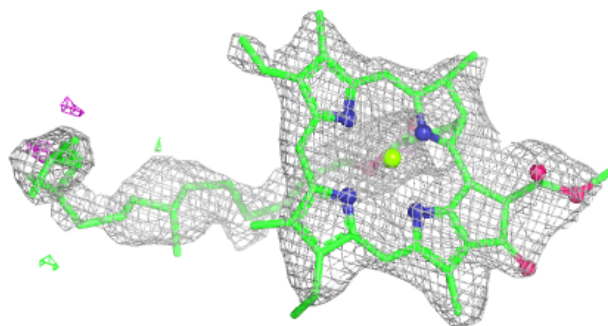
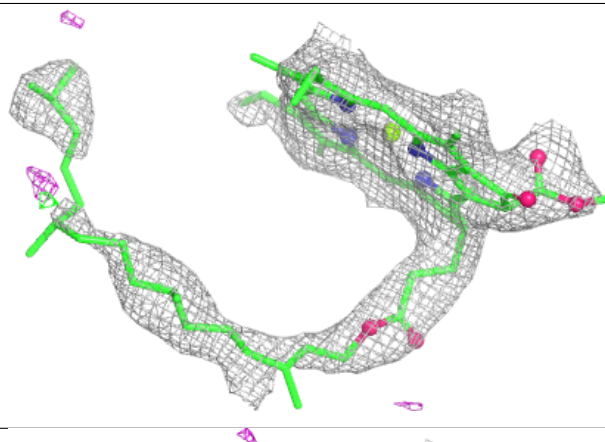


Electron density around HTG B 626:

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

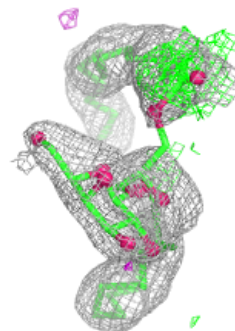
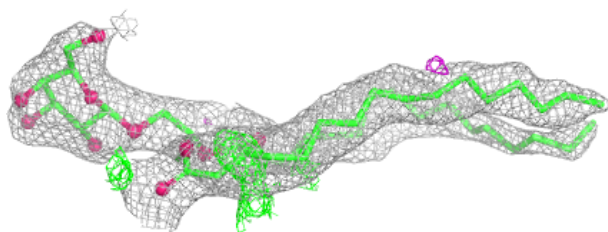
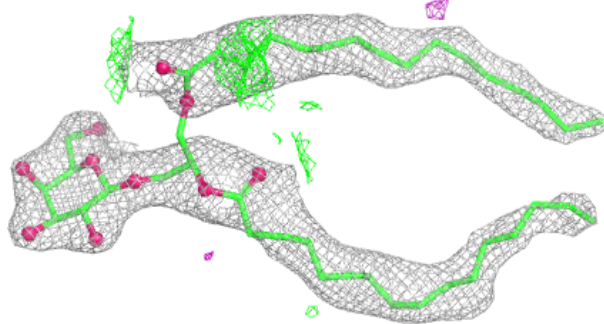
**Electron density around CLA c 914:**

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



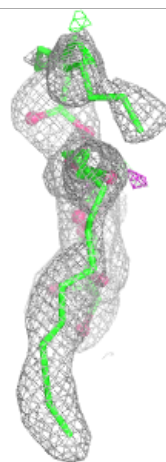
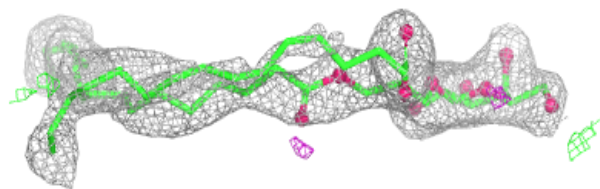
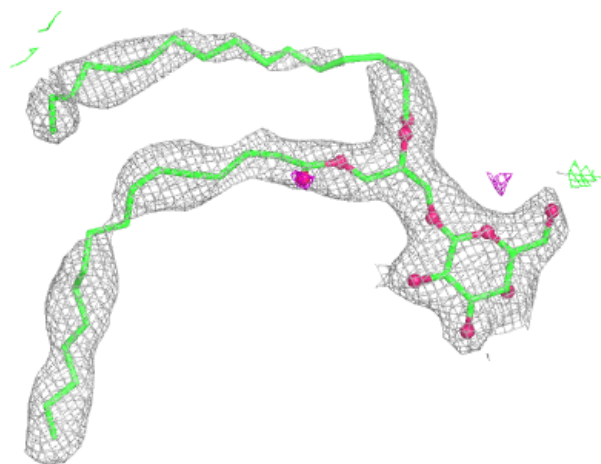
Electron density around LMG i 101:

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



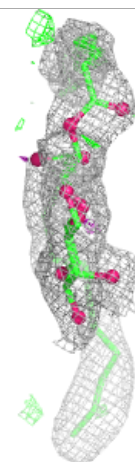
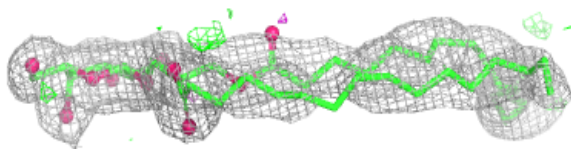
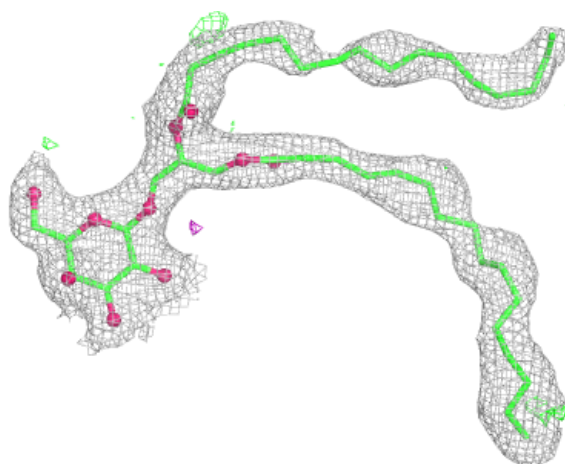
Electron density around LMG c 920:

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



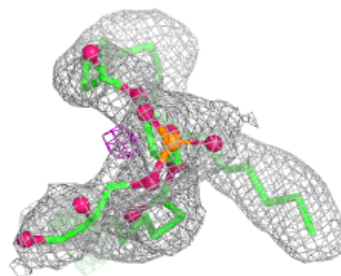
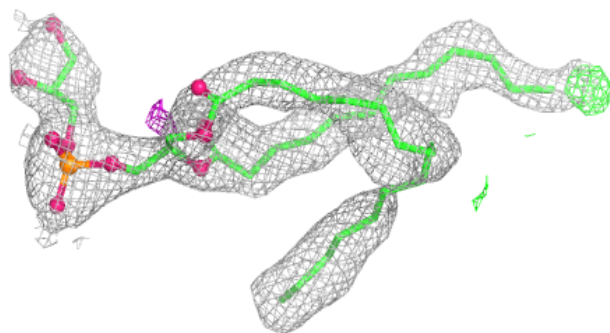
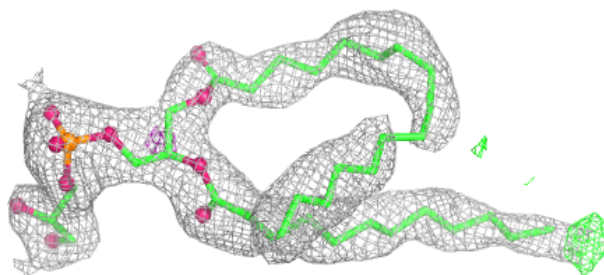
Electron density around LMG C 520:

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

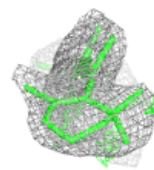
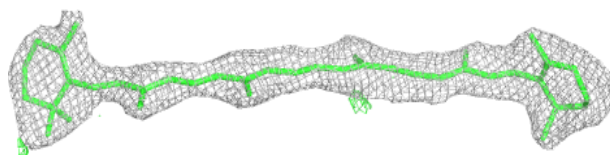
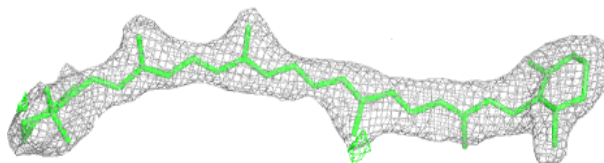


Electron density around LHG a 423:

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

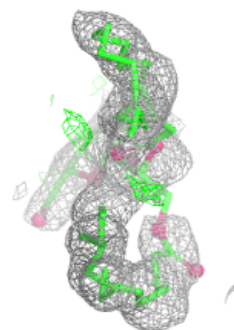
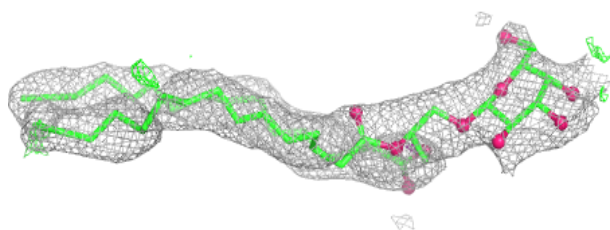
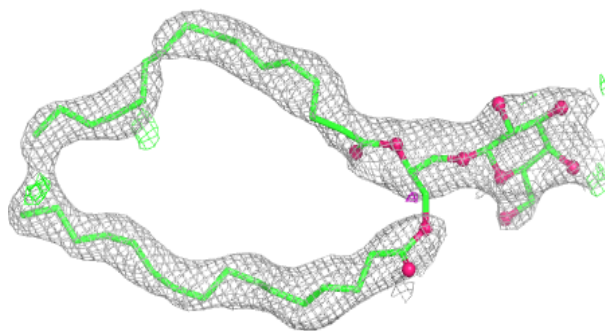
**Electron density around BCR c 915:**

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

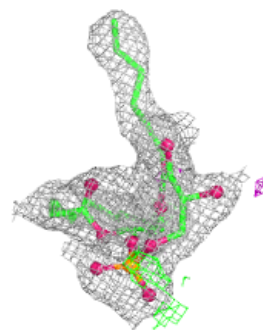
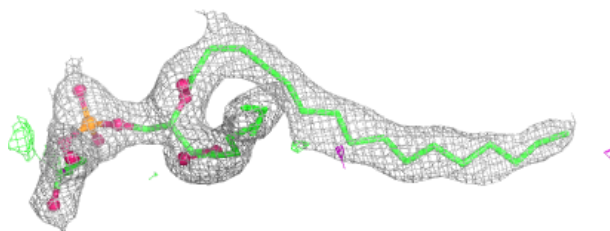
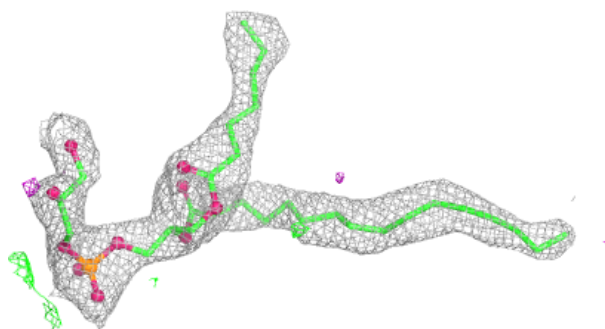


Electron density around LMG A 410:

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

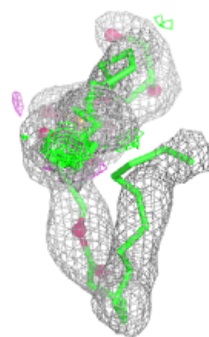
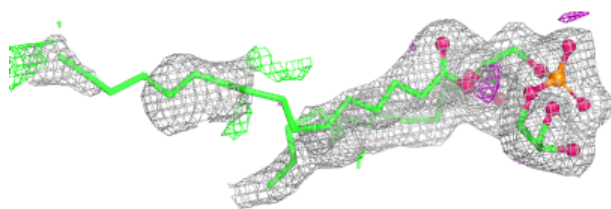
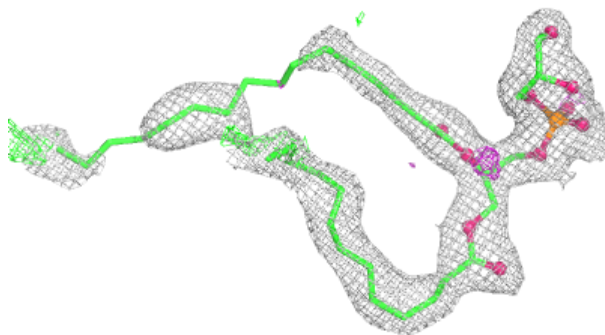
**Electron density around LHG L 101:**

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

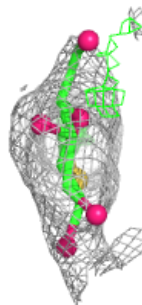
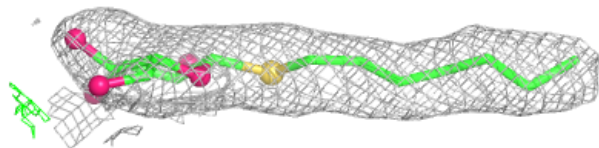
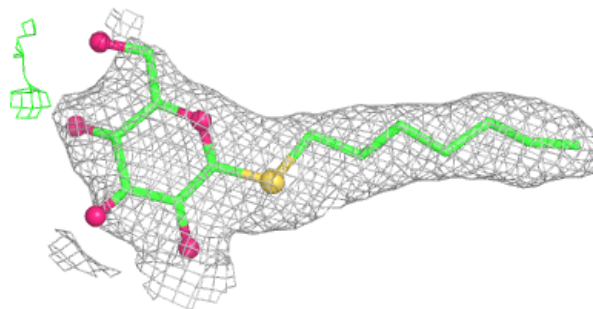


Electron density around LHG d 408:

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

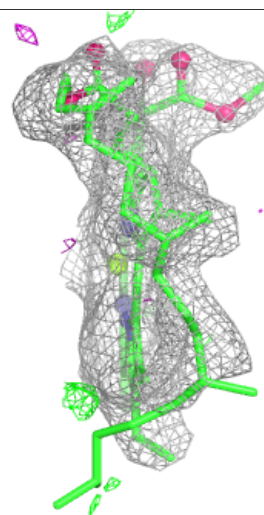
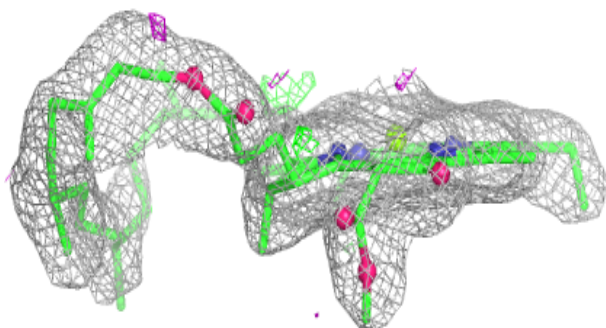
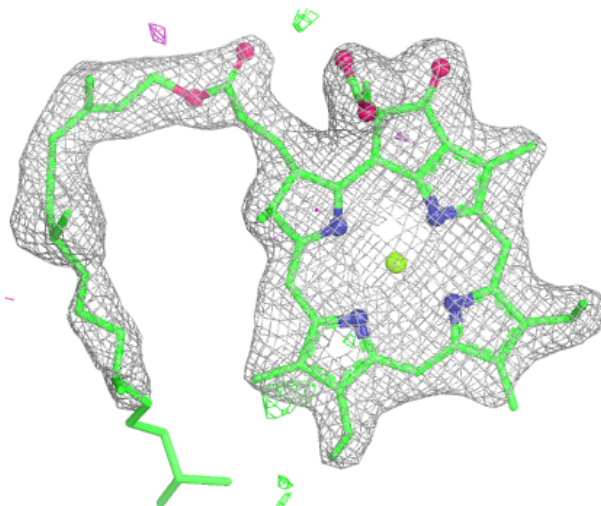
**Electron density around HTG b 626:**

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



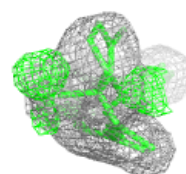
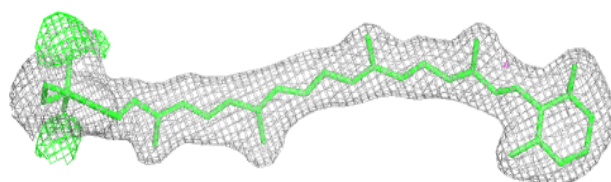
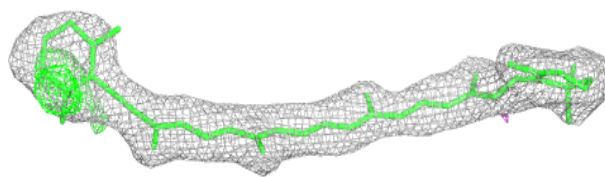
Electron density around CLA c 913:

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

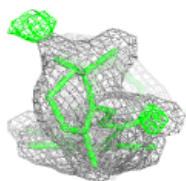
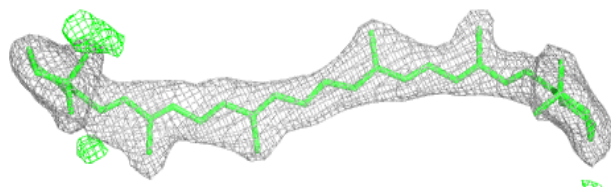
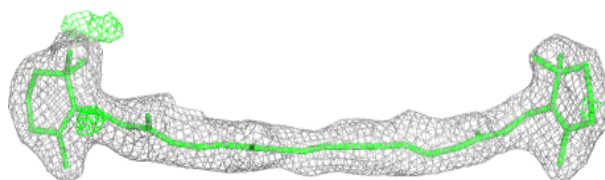


Electron density around BCR d 404:

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

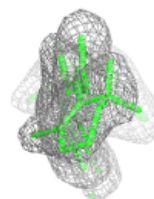
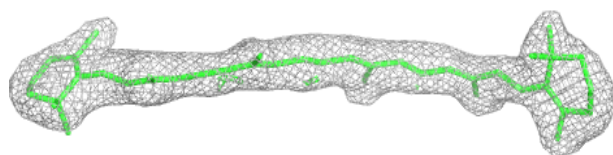
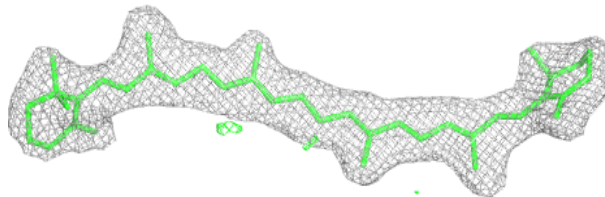
**Electron density around BCR k 101:**

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

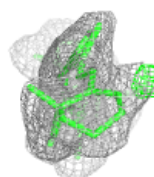
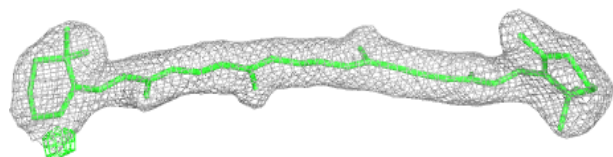
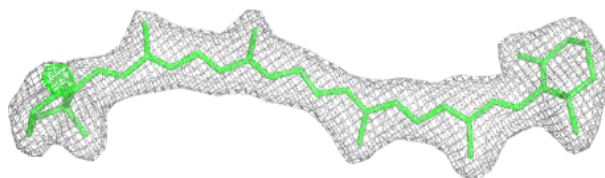


Electron density around BCR y 101:

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

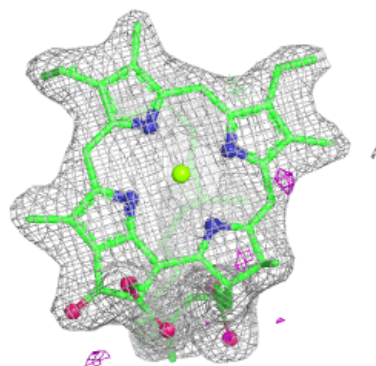
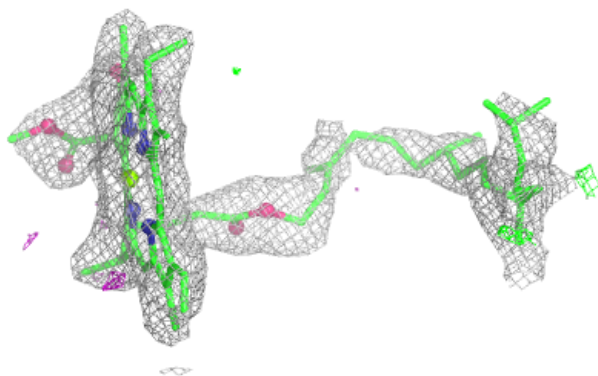
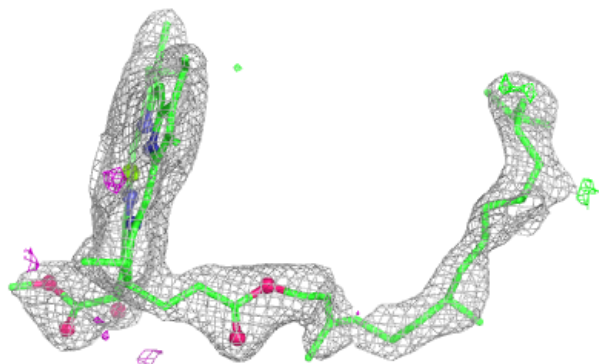
**Electron density around BCR Y 101:**

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

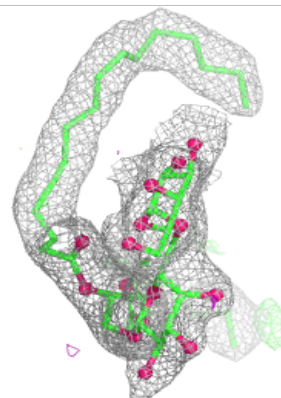
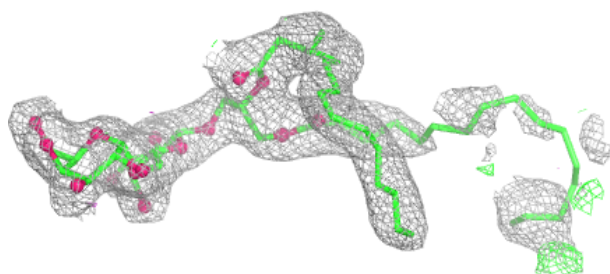
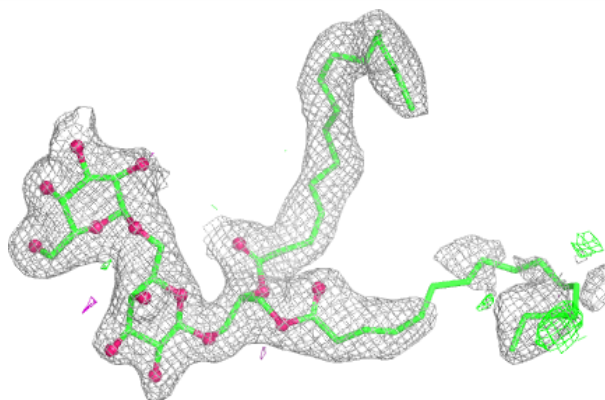


Electron density around CLA C 507:

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

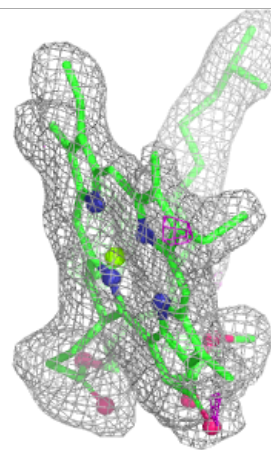
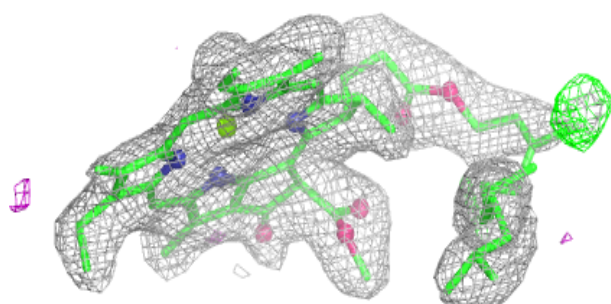
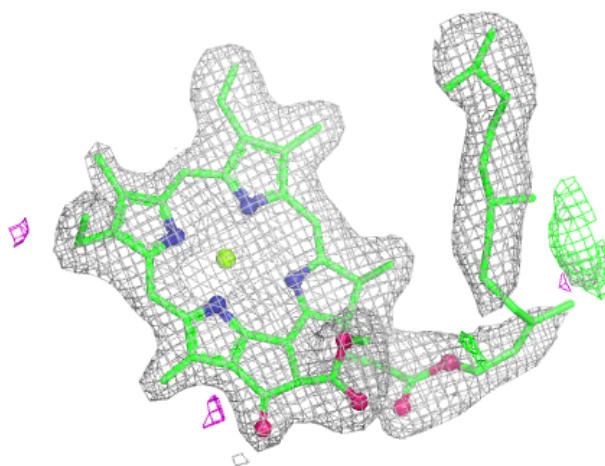
**Electron density around DGD c 918:**

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



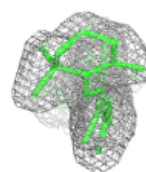
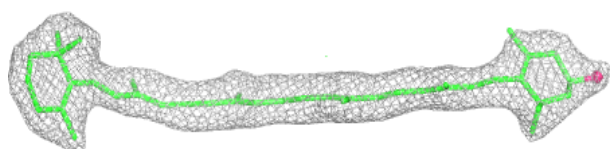
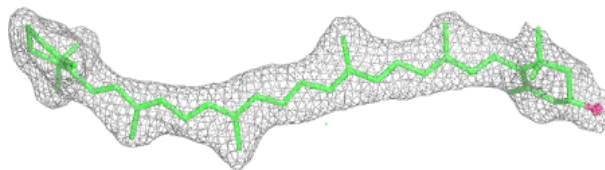
Electron density around CLA b 617:

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

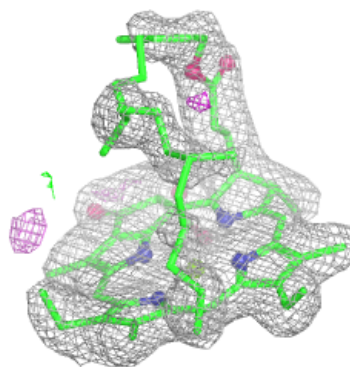
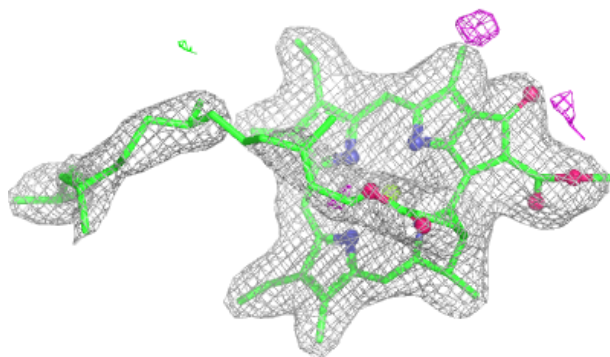
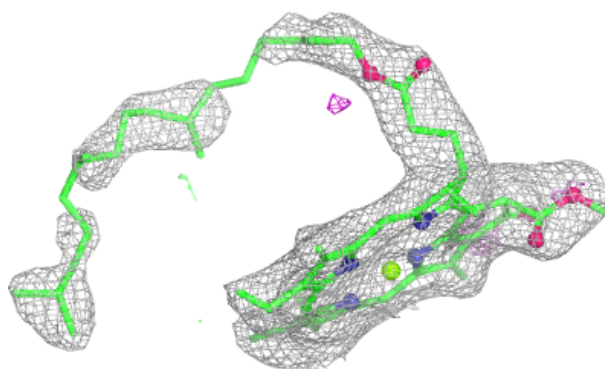


Electron density around RRX H 101:

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

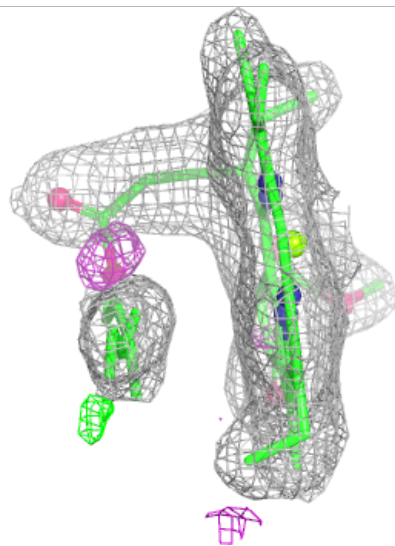
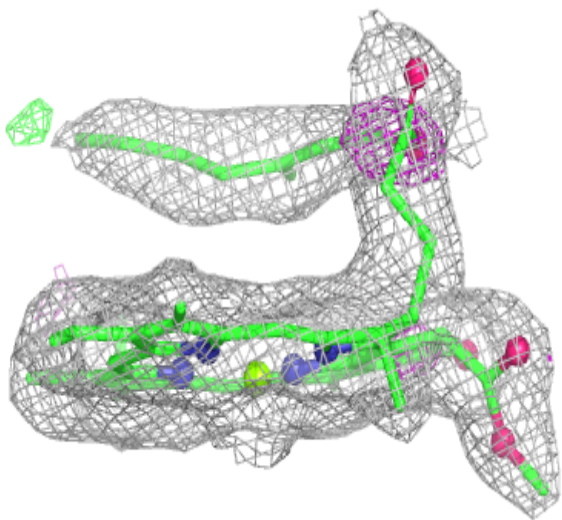
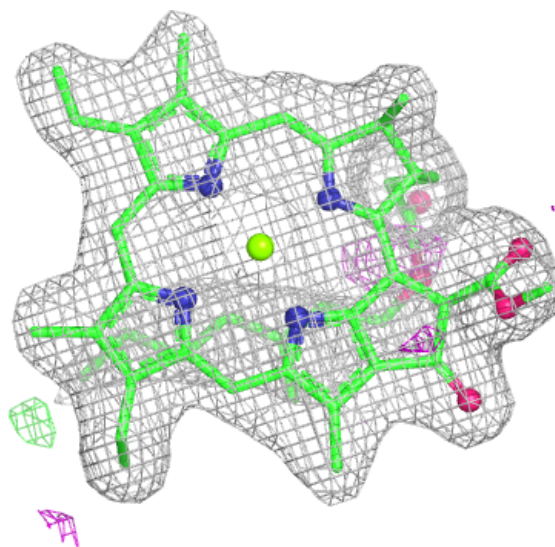
**Electron density around CLA C 514:**

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



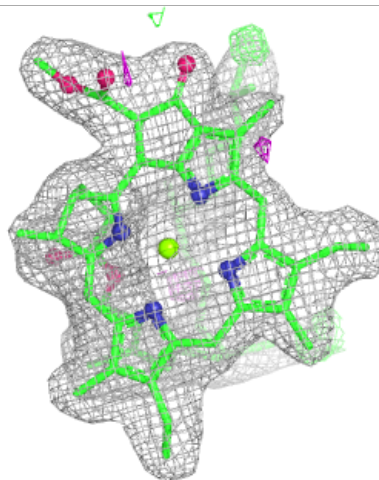
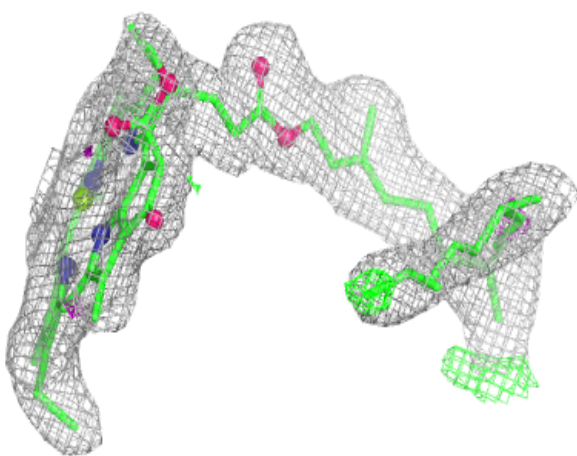
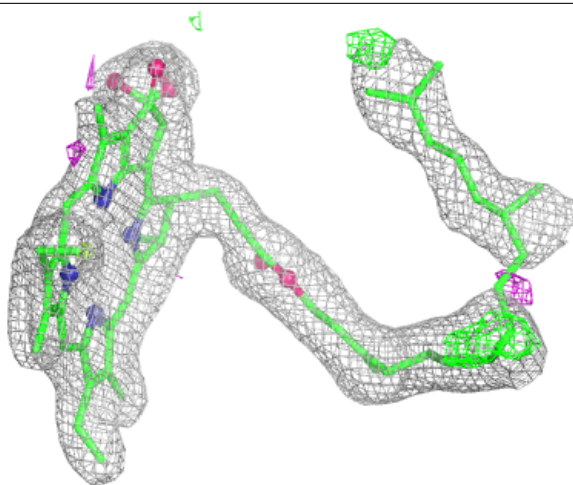
Electron density around CLA B 615:

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



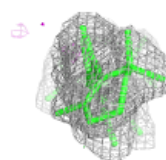
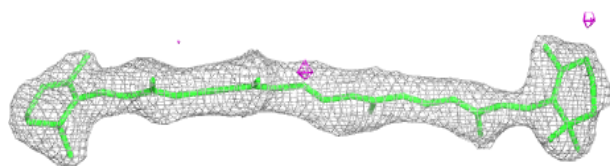
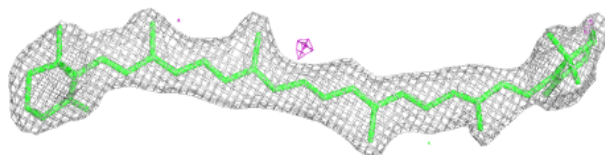
Electron density around CLA b 607:

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

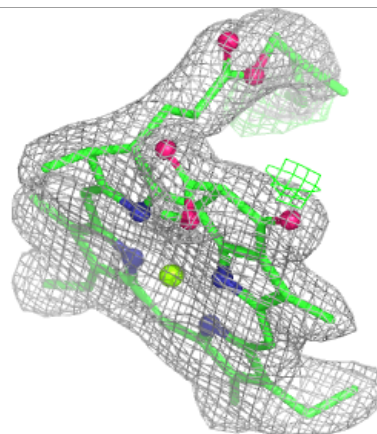
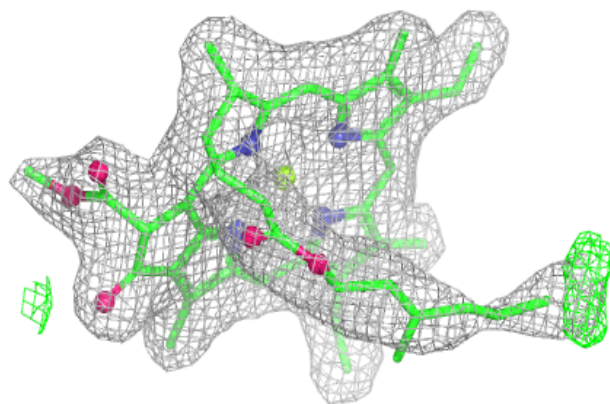
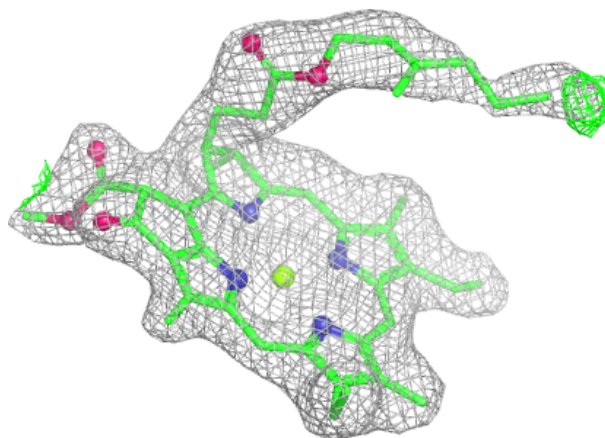


Electron density around BCR C 515:

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

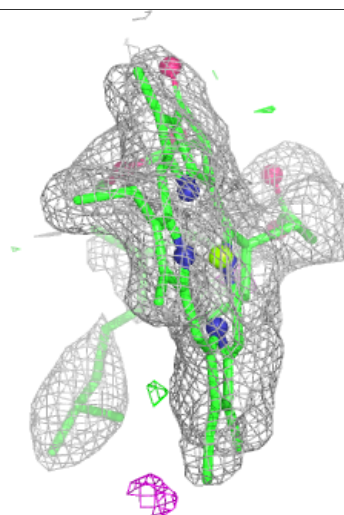
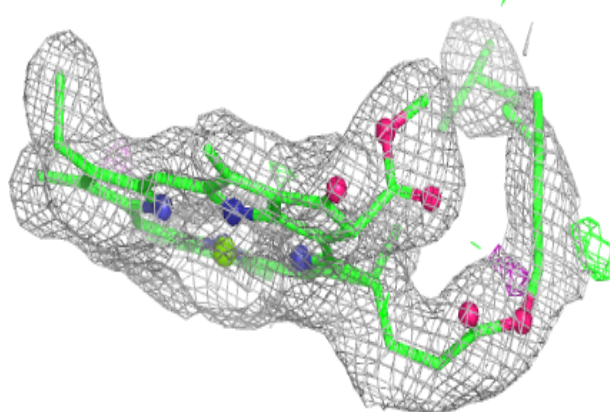
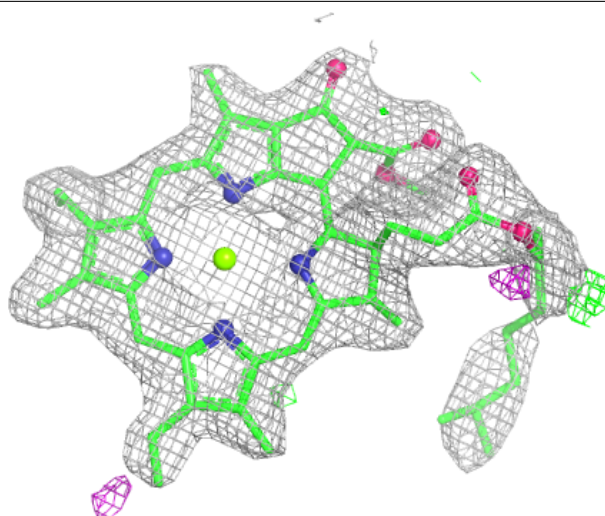
**Electron density around CLA b 615:**

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



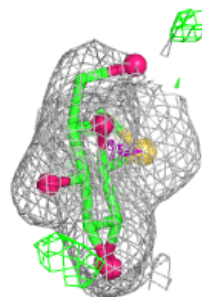
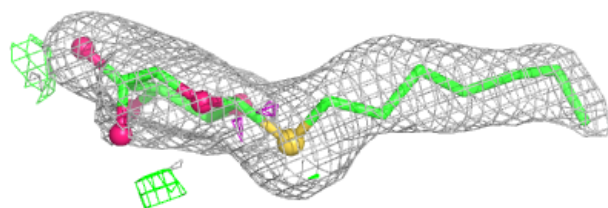
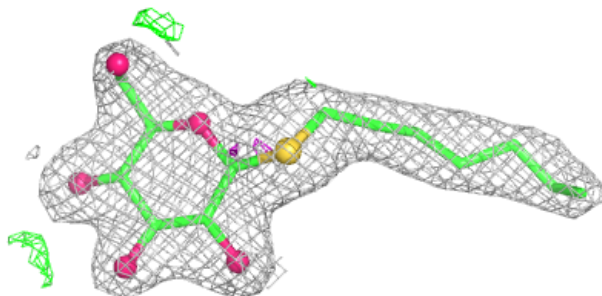
Electron density around CLA B 617:

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



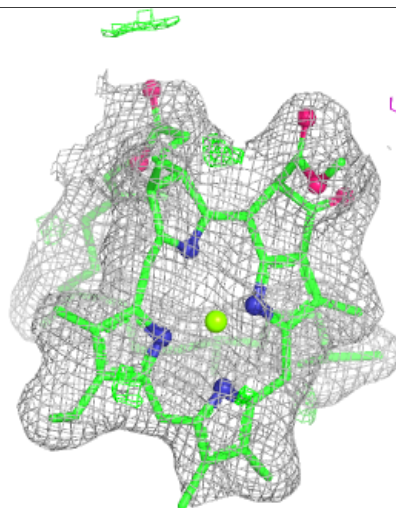
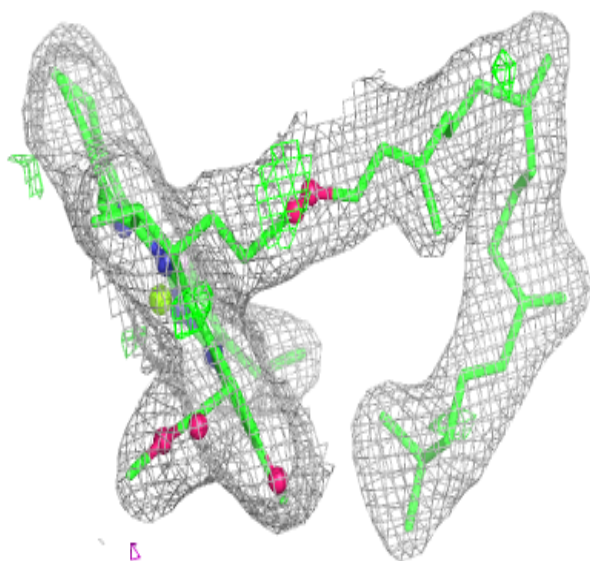
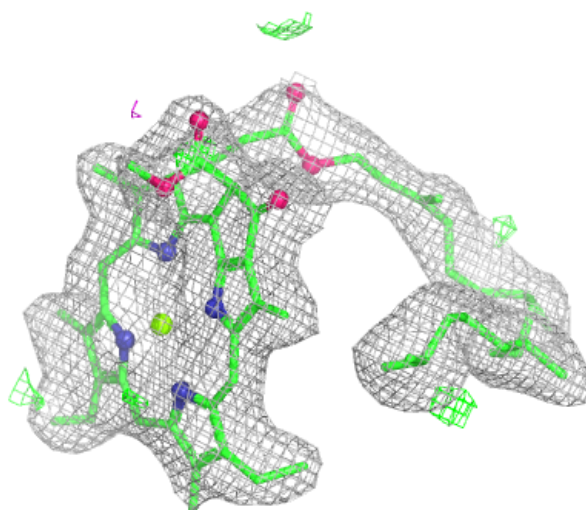
Electron density around HTG b 623:

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



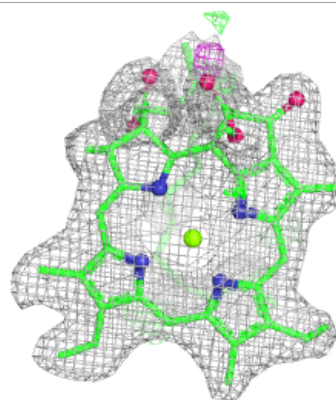
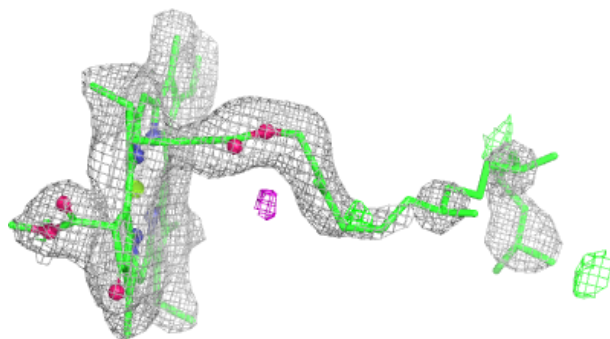
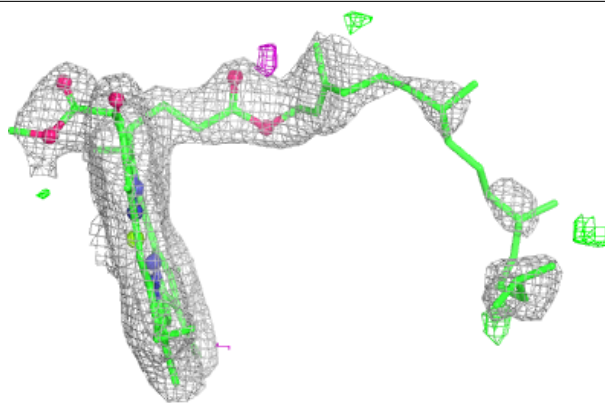
Electron density around CLA c 904:

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

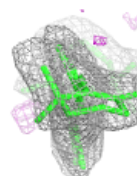
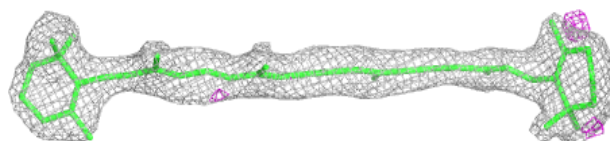
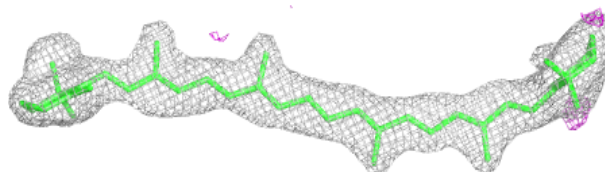


Electron density around CLA c 907:

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

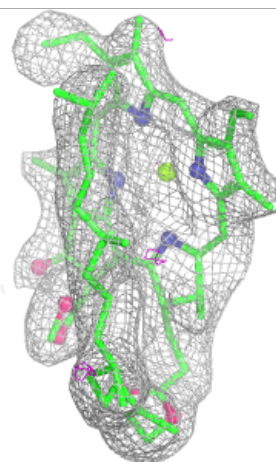
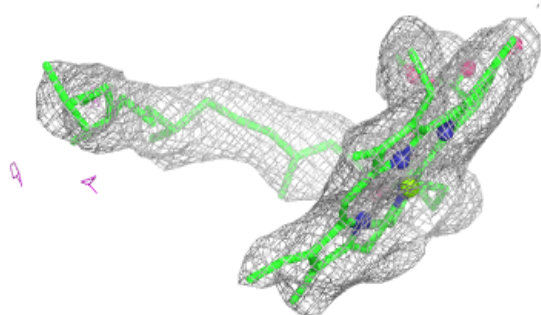
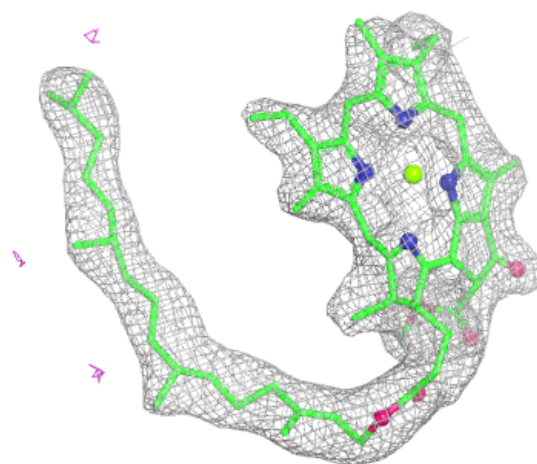
**Electron density around BCR c 916:**

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



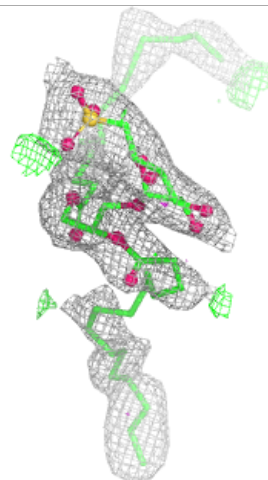
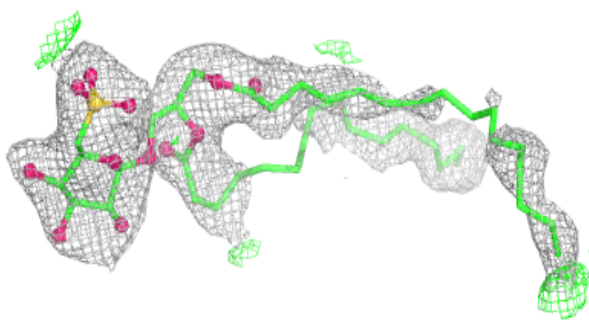
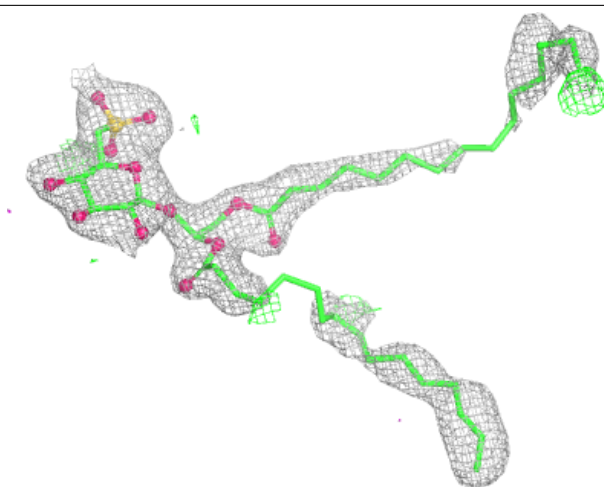
Electron density around CLA c 908:

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



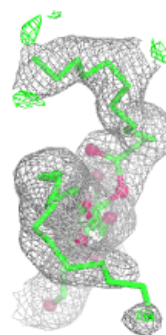
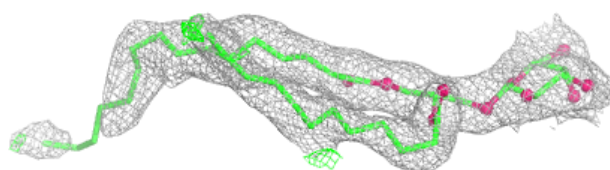
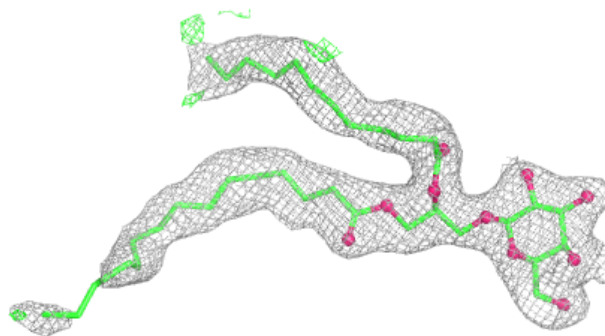
Electron density around SQD C 501:

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

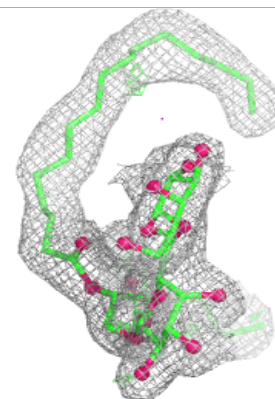
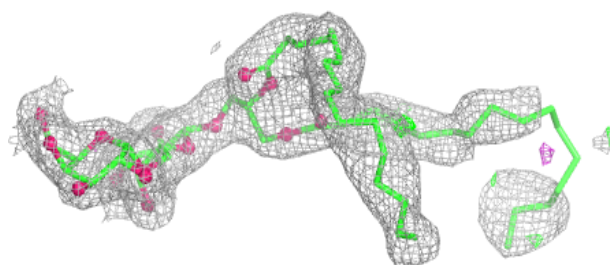
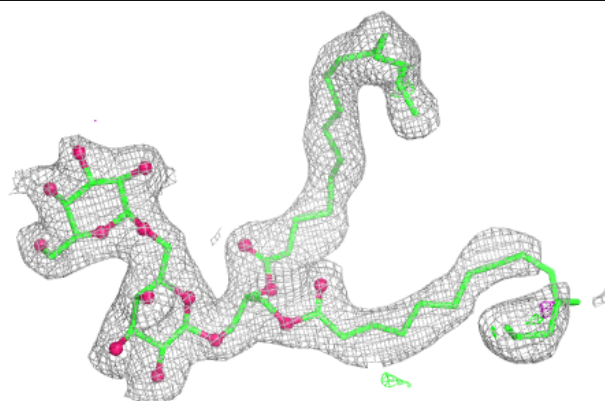


Electron density around LMG j 101:

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

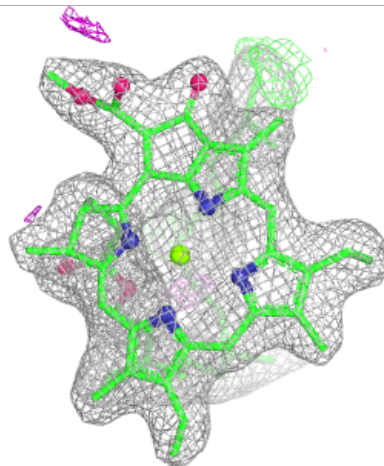
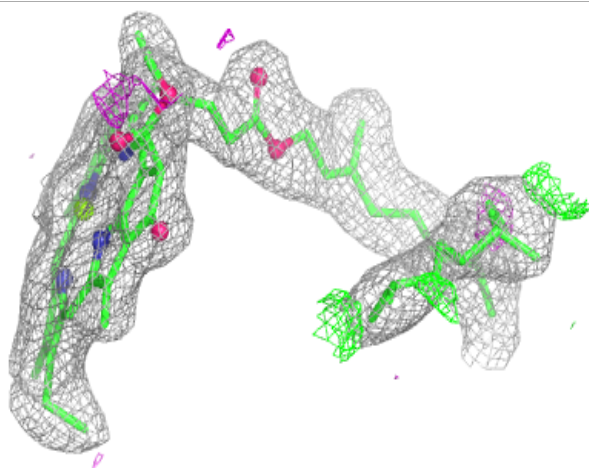
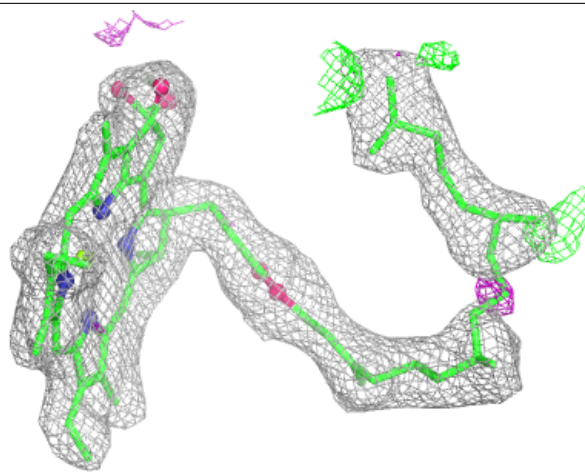
**Electron density around DGD C 518:**

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



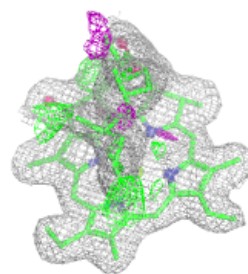
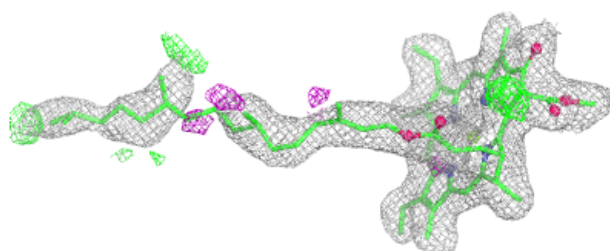
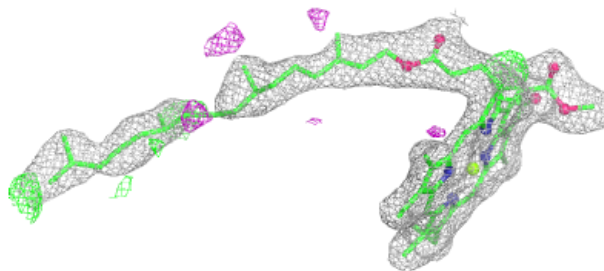
Electron density around CLA B 607:

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

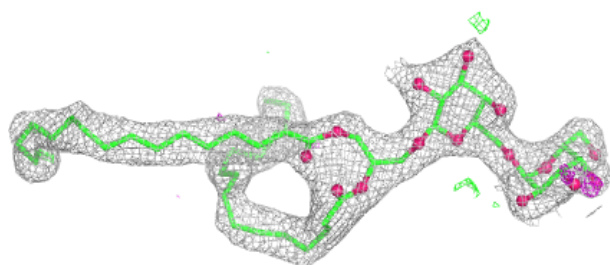
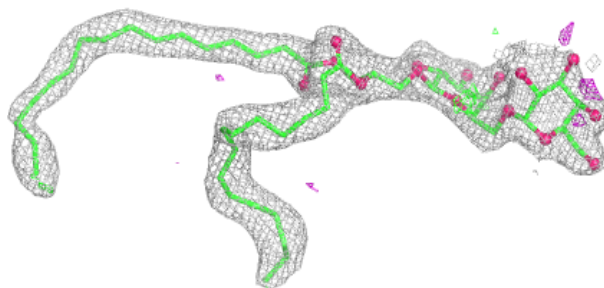


Electron density around CLA B 608:

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

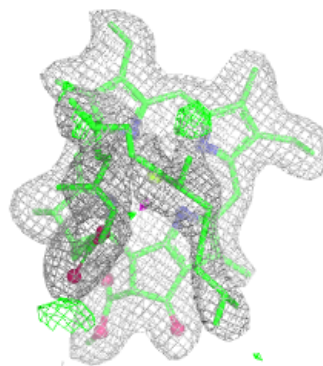
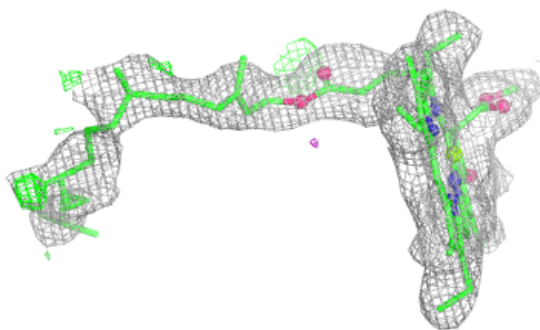
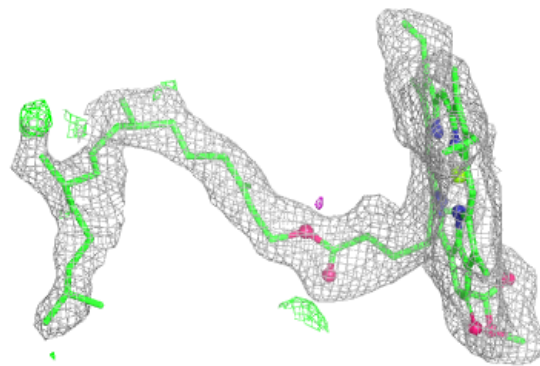
**Electron density around DGD h 102:**

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



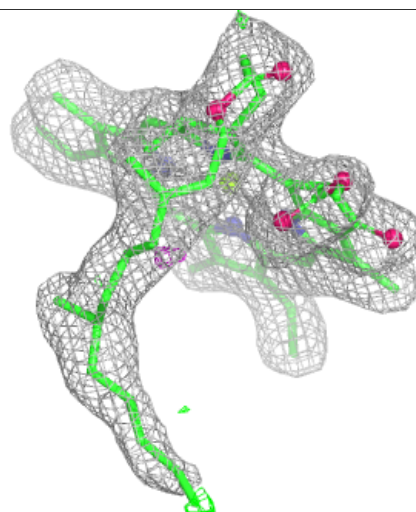
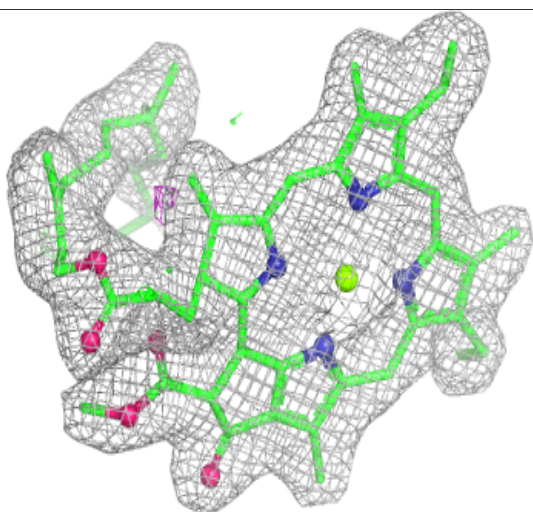
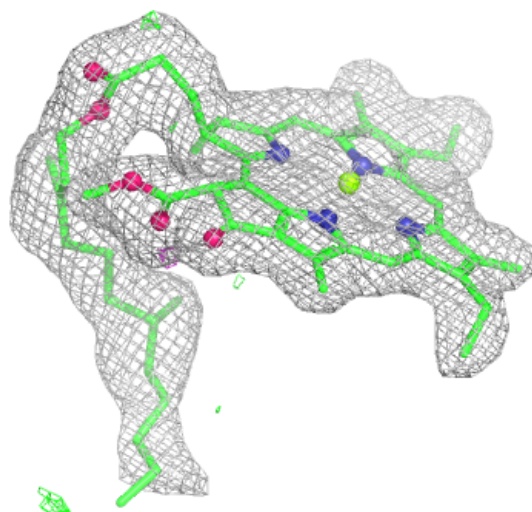
Electron density around CLA d 403:

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



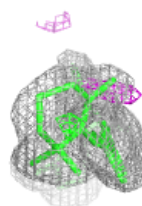
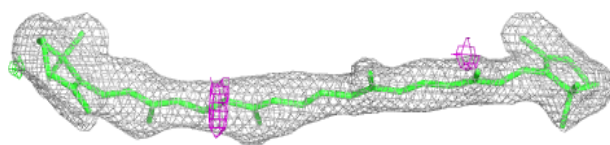
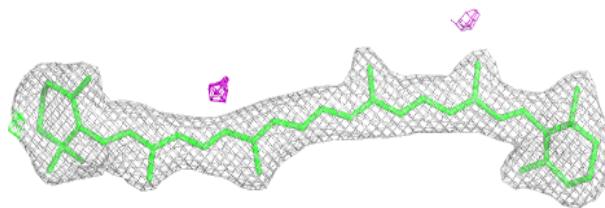
Electron density around CLA b 614:

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

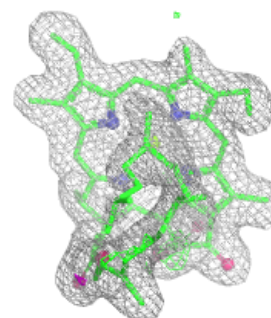
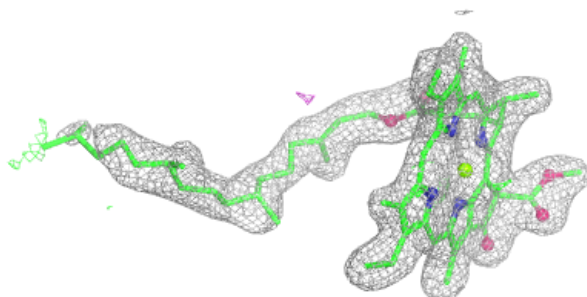
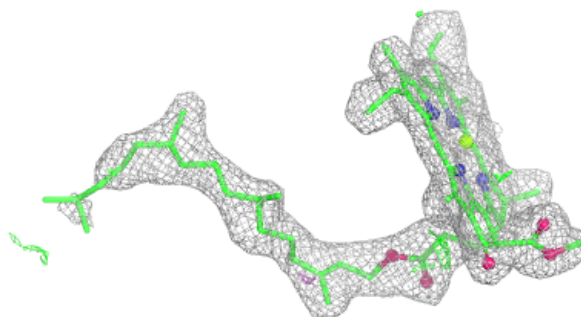


Electron density around BCR B 620:

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

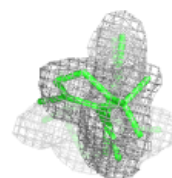
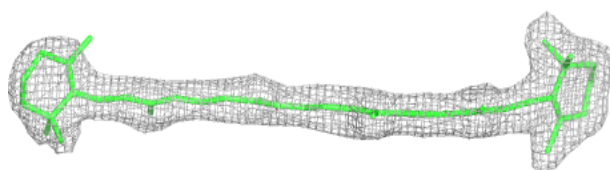
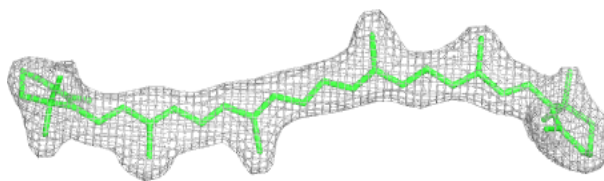
**Electron density around CLA C 509:**

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

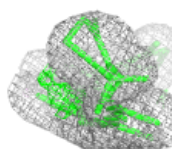
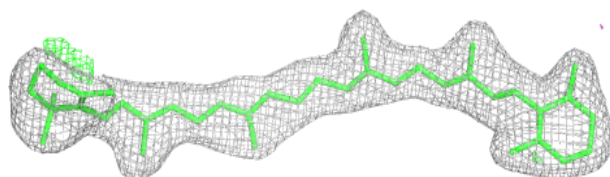
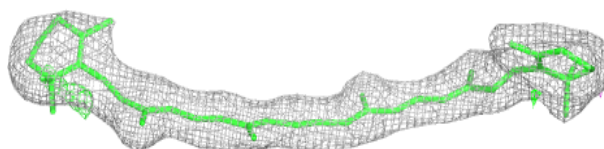


Electron density around BCR C 516:

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

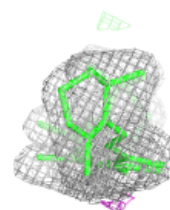
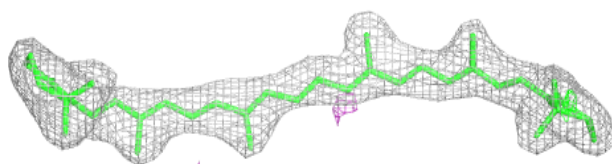
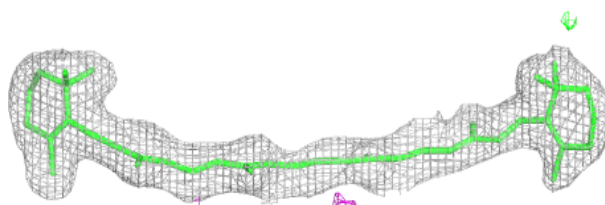
**Electron density around BCR D 405:**

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

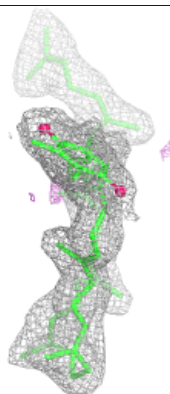
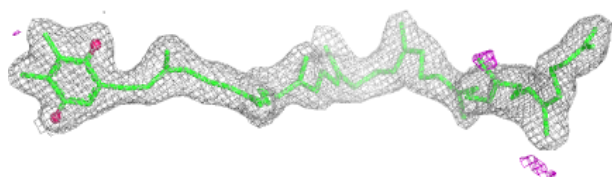
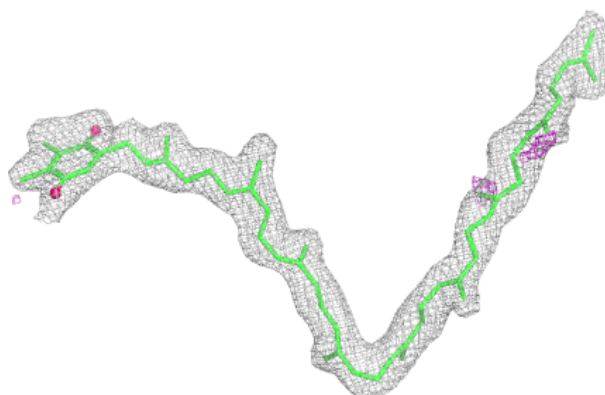


Electron density around BCR K 101:

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

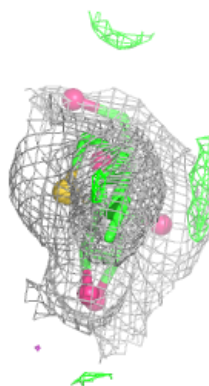
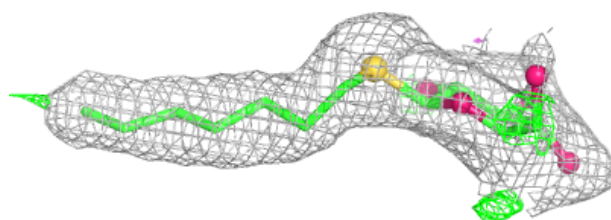
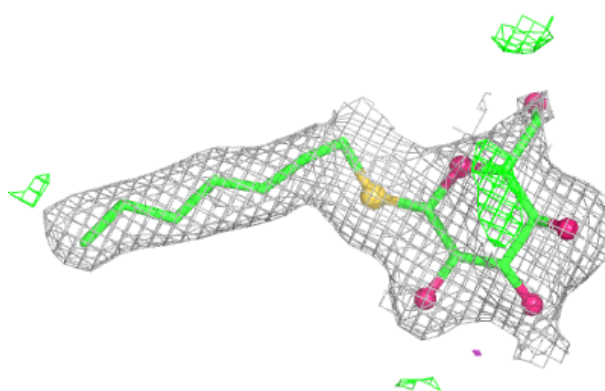
**Electron density around PL9 D 406:**

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

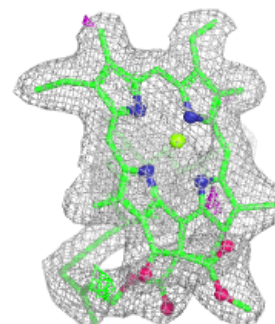
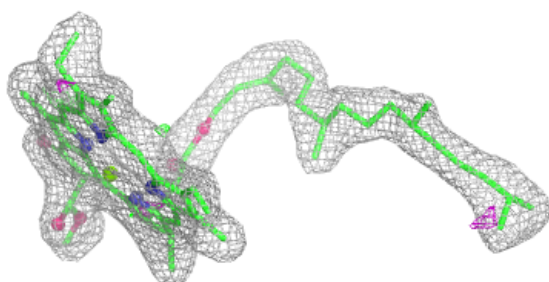
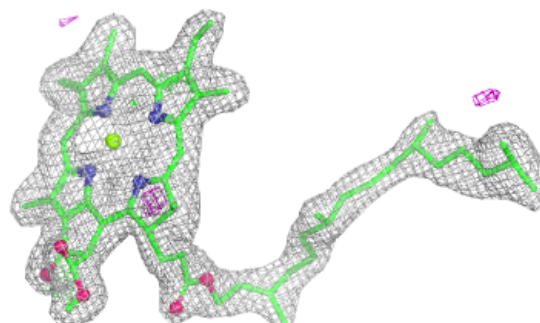


Electron density around HTG B 623:

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

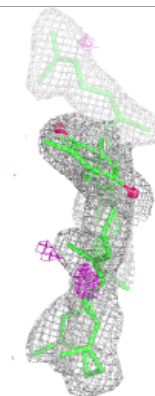
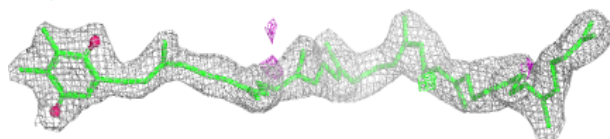
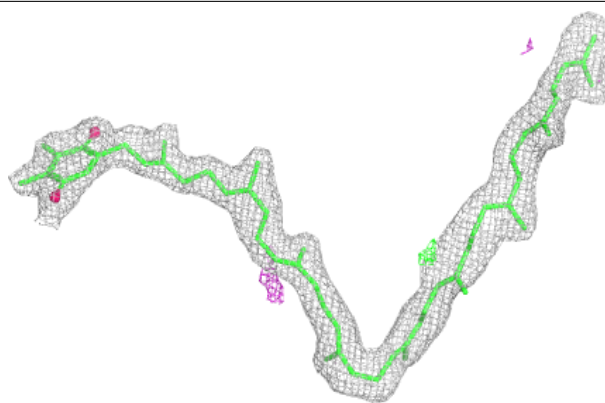
**Electron density around CLA C 512:**

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

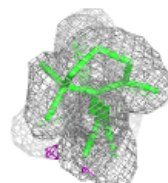
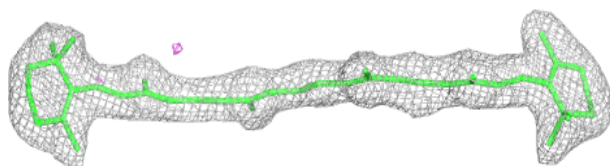
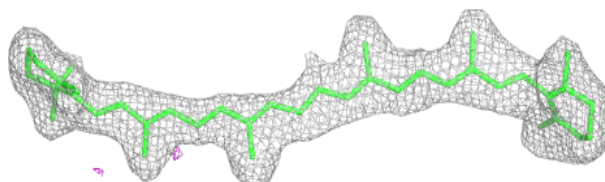


Electron density around PL9 d 405:

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

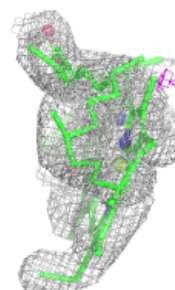
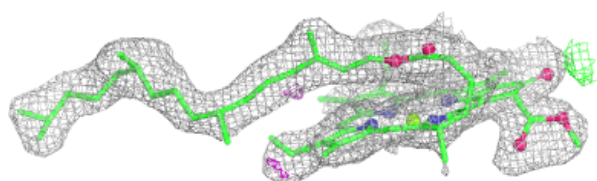
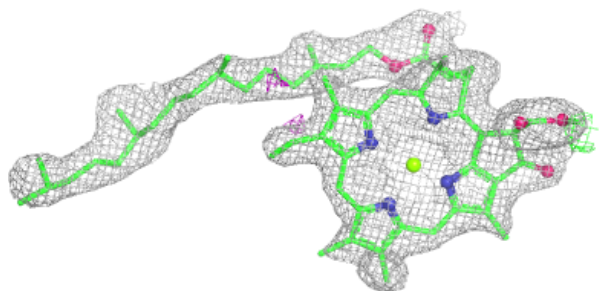
**Electron density around BCR a 413:**

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



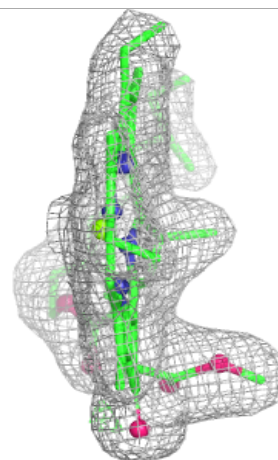
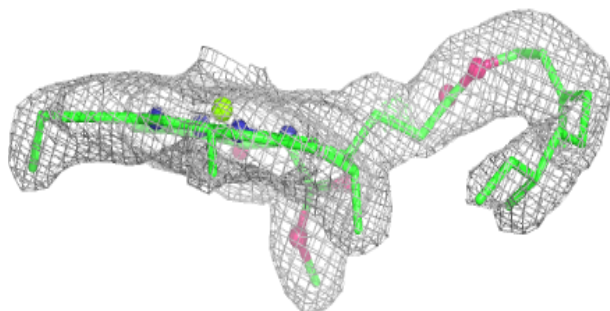
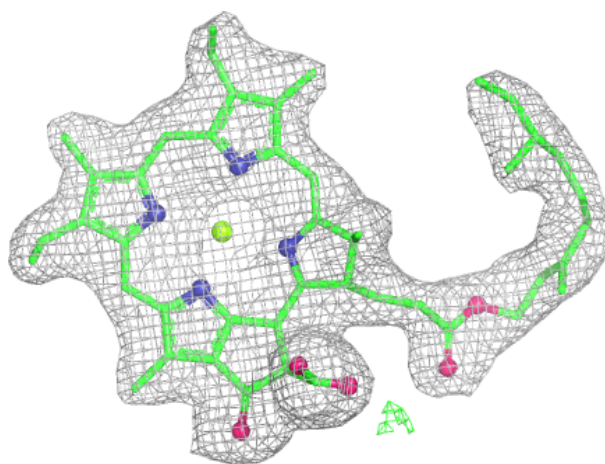
Electron density around CLA c 902:

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



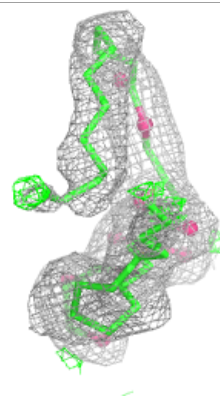
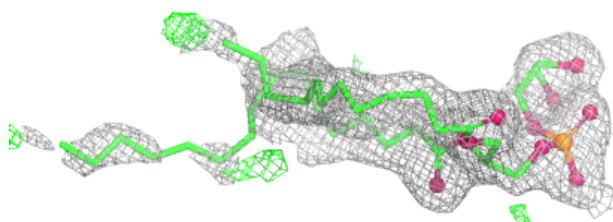
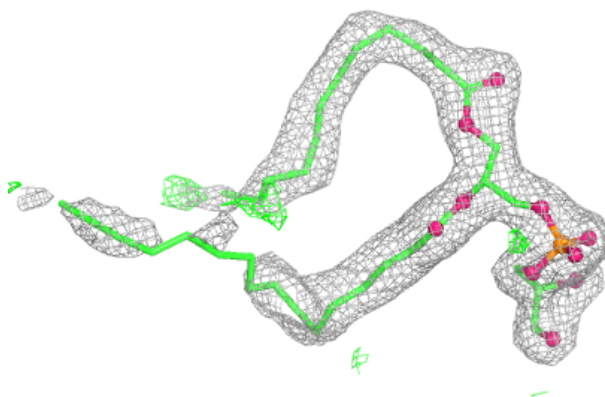
Electron density around CLA C 513:

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

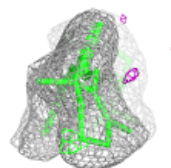
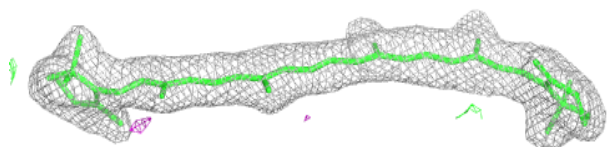
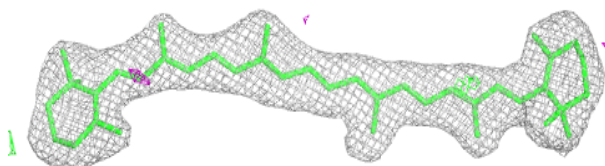


Electron density around LHG D 411:

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

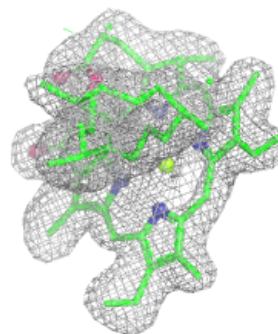
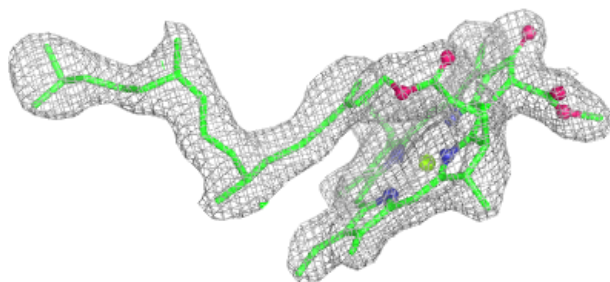
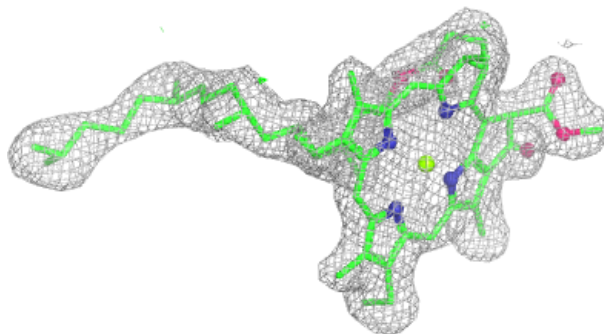
**Electron density around BCR b 620:**

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



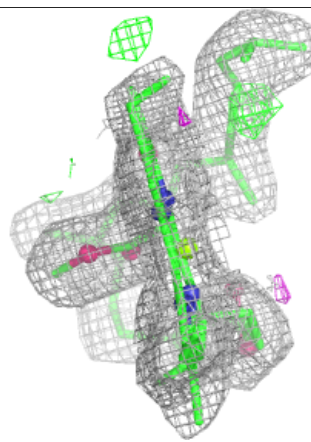
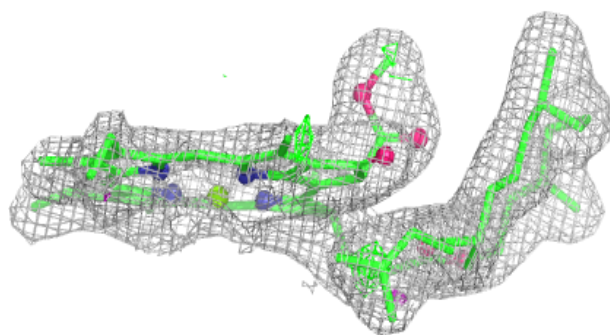
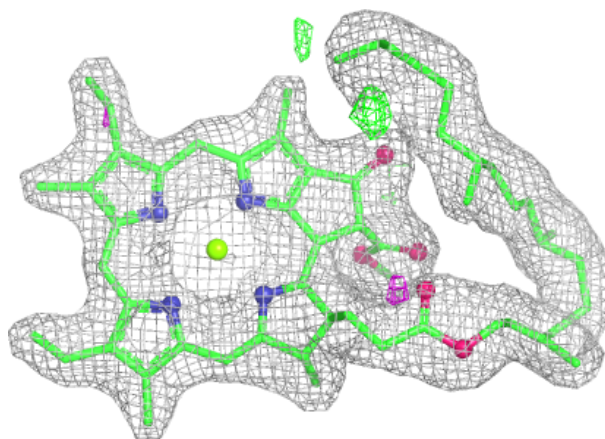
Electron density around CLA c 906:

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



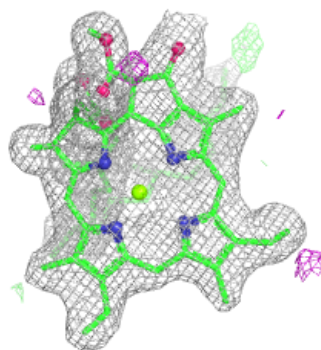
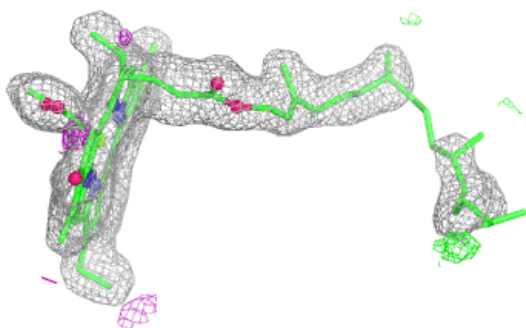
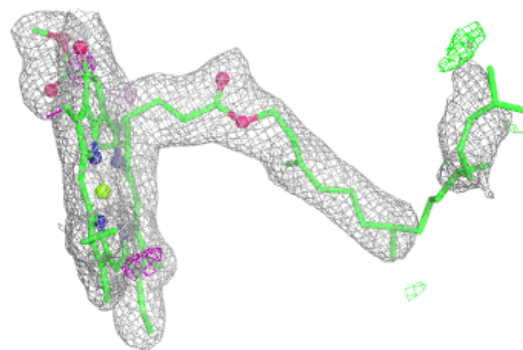
Electron density around CLA B 611:

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

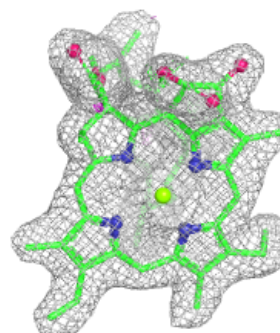
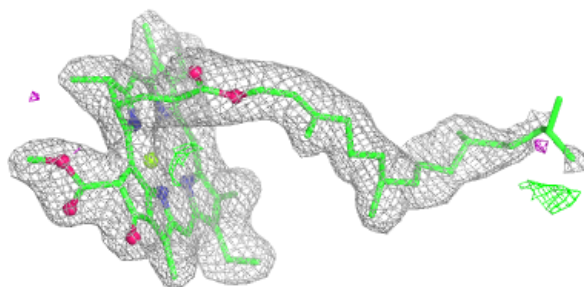
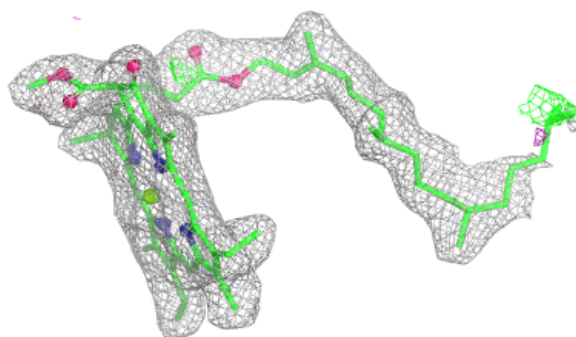


Electron density around CLA D 404:

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

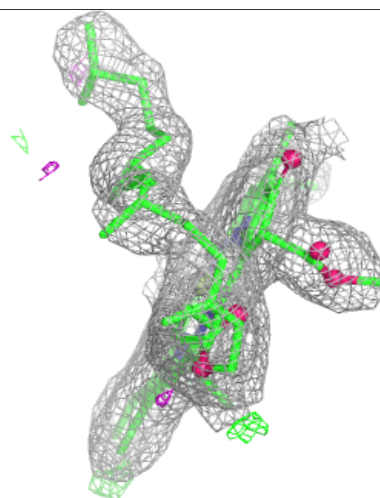
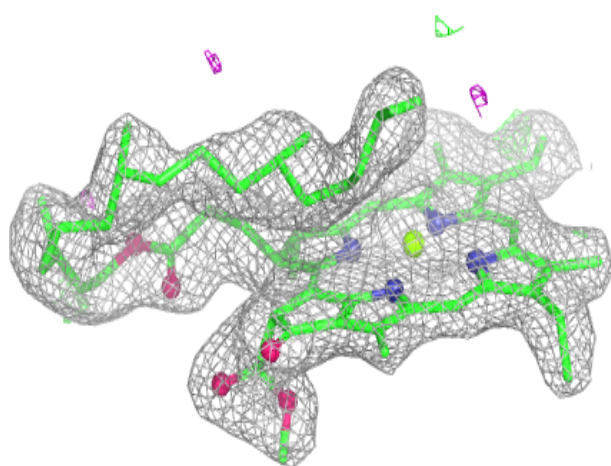
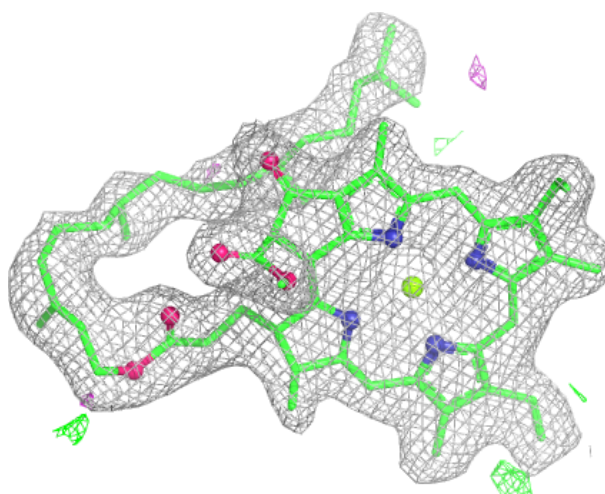
**Electron density around CLA c 909:**

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



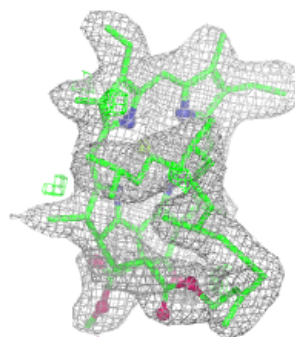
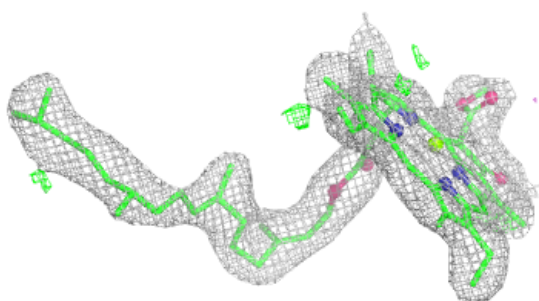
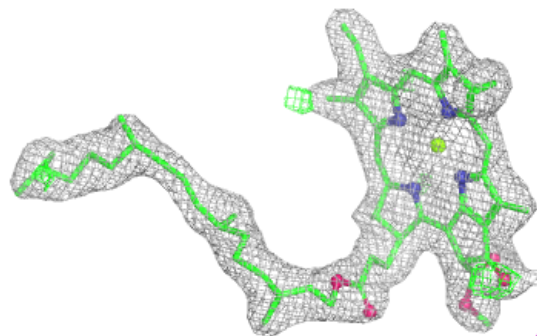
Electron density around CLA c 910:

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

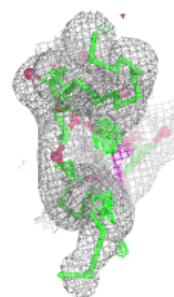
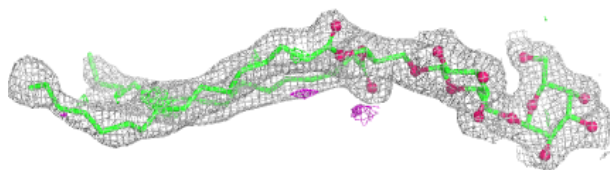
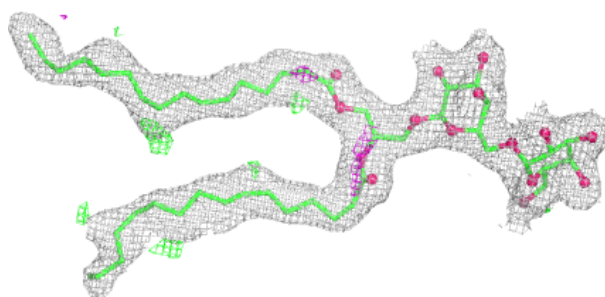


Electron density around CLA c 912:

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

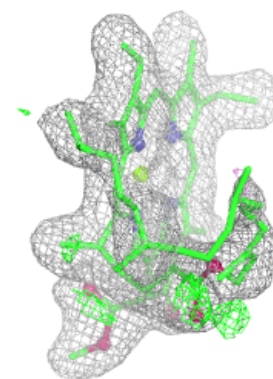
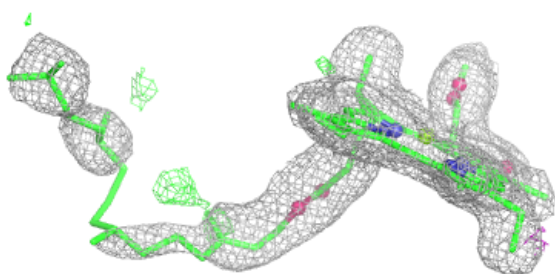
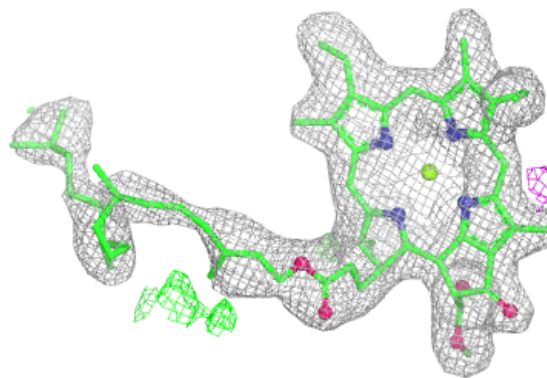
**Electron density around DGD C 519:**

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

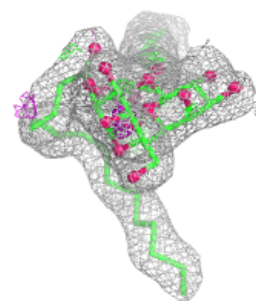
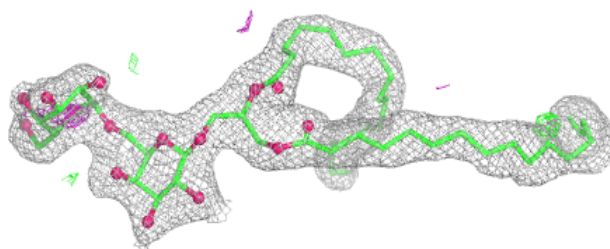
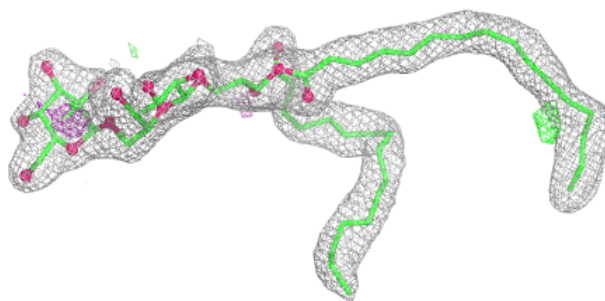


Electron density around CLA a 412:

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

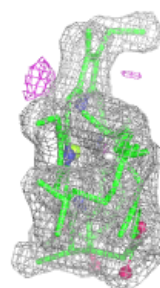
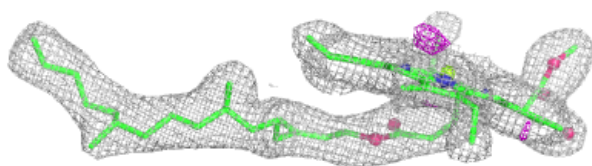
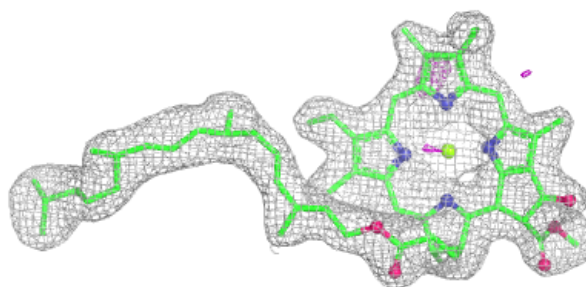
**Electron density around DGD H 102:**

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

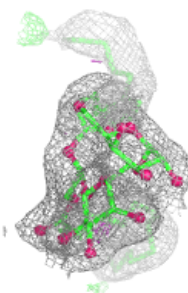
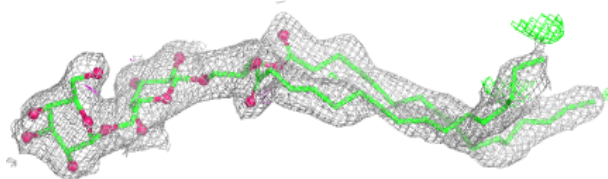
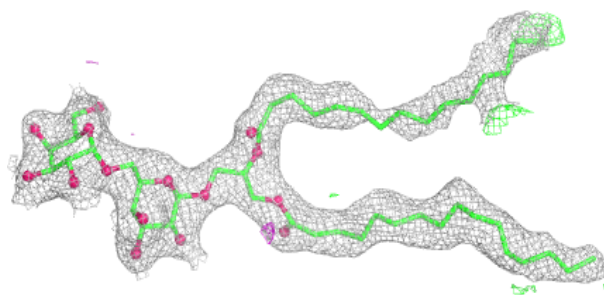


Electron density around CLA B 604:

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

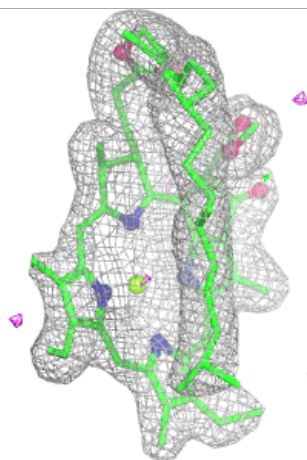
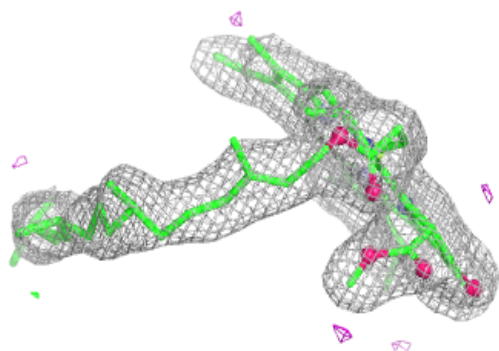
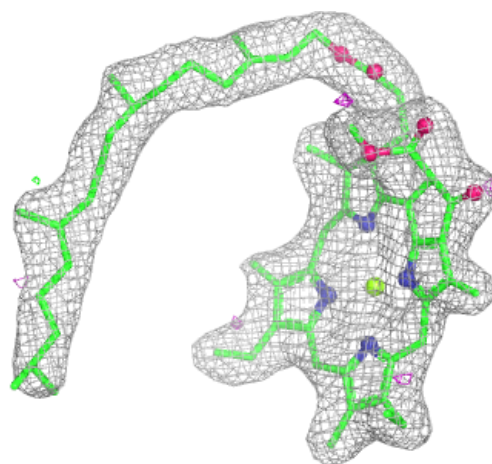
**Electron density around DGD c 919:**

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



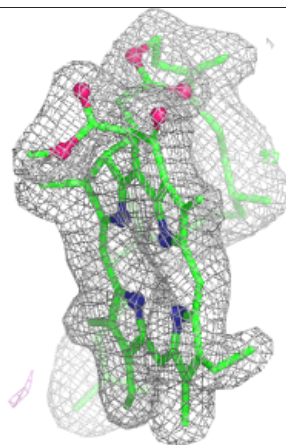
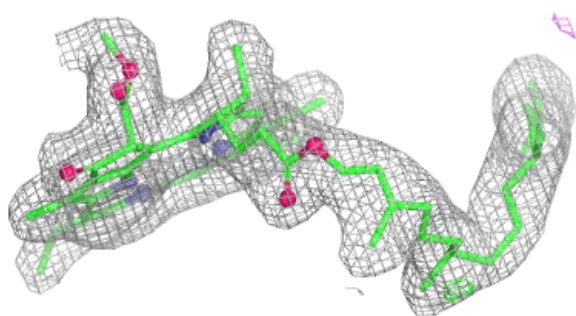
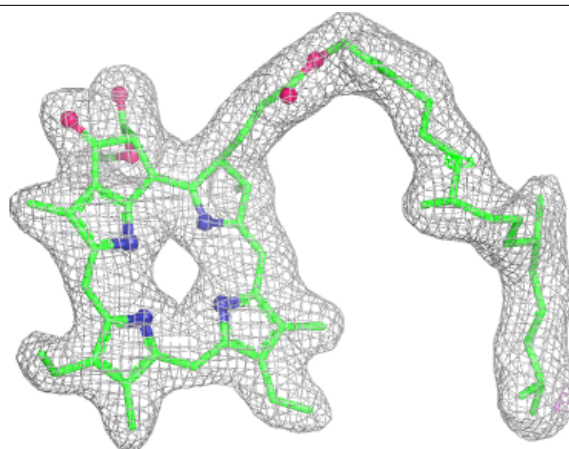
Electron density around CLA C 508:

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

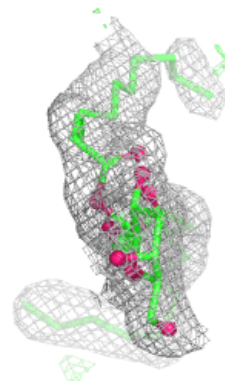
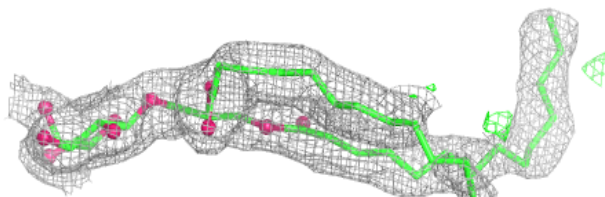
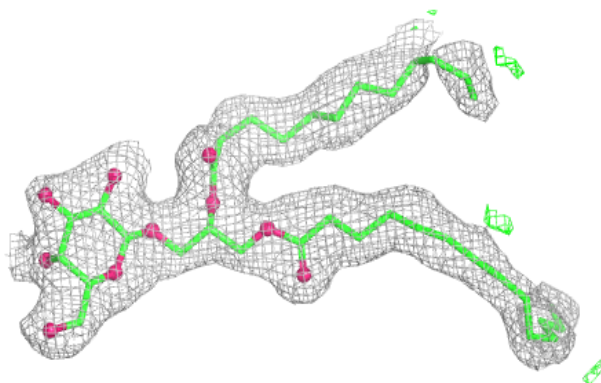


Electron density around PHO a 411:

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

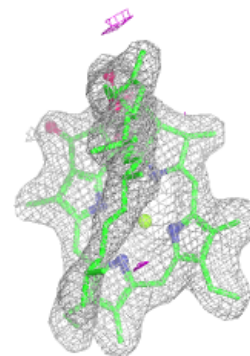
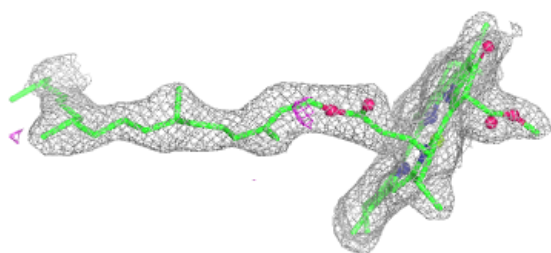
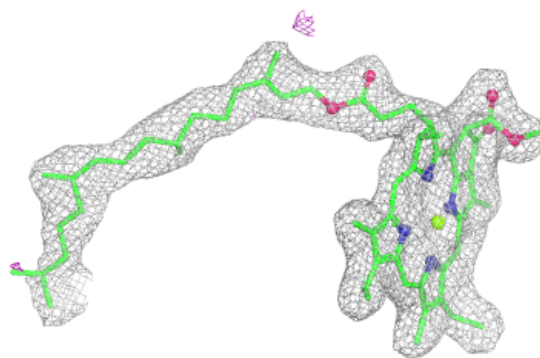
**Electron density around LMG J 101:**

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

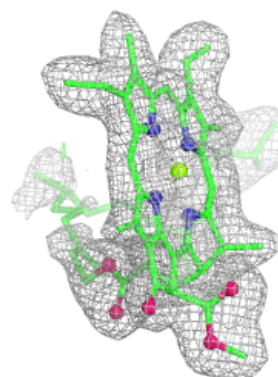
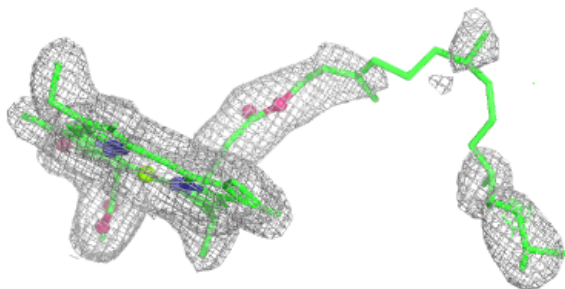
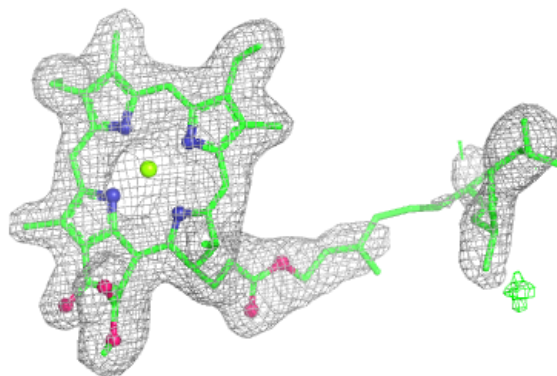


Electron density around CLA b 610:

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

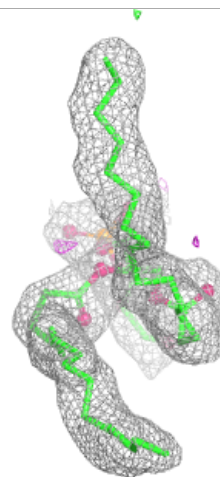
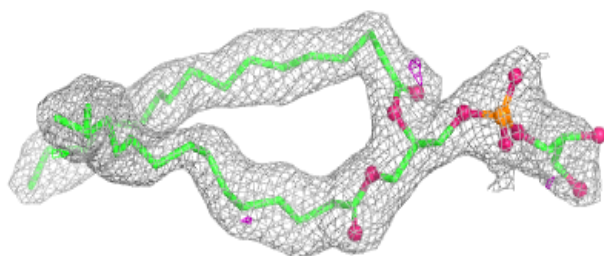
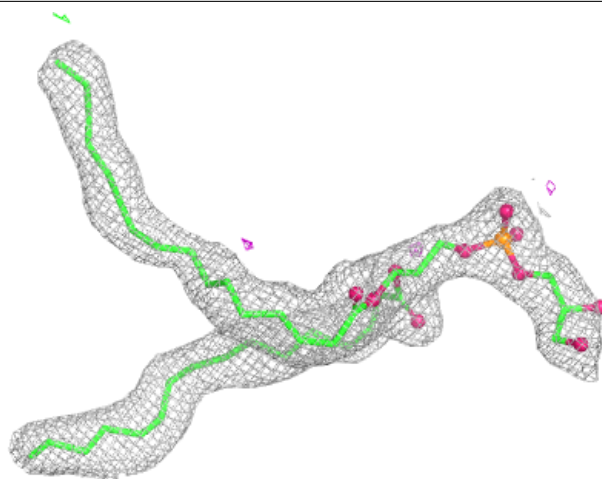
**Electron density around CLA A 408:**

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



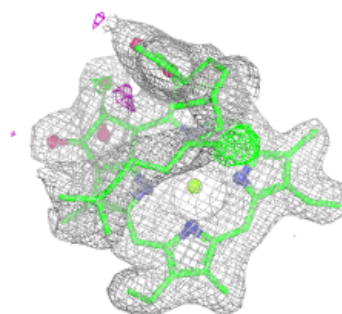
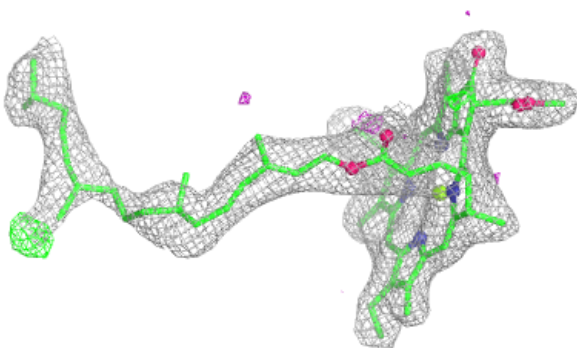
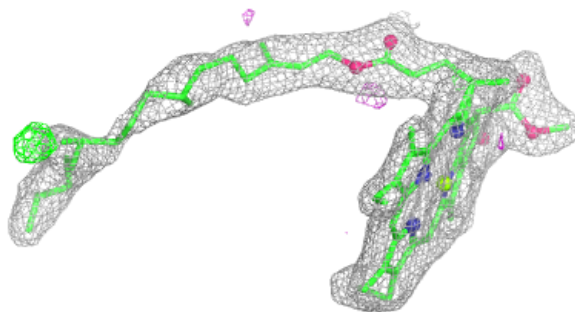
Electron density around LHG d 407:

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

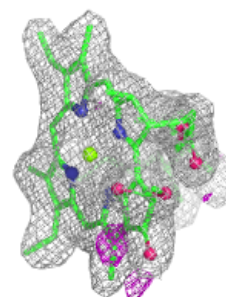
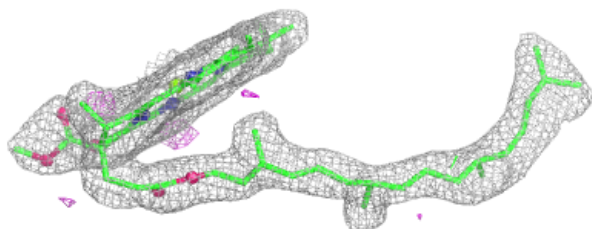
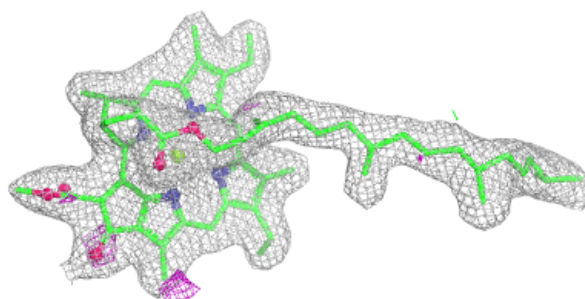


Electron density around CLA b 608:

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

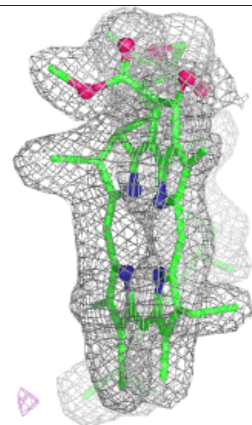
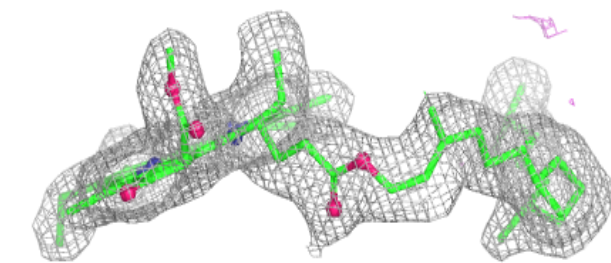
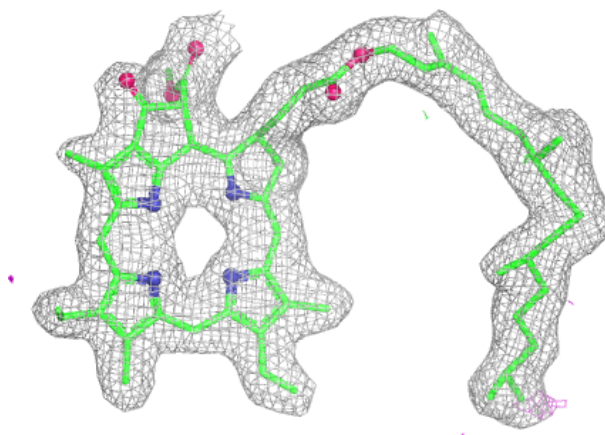
**Electron density around CLA b 609:**

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



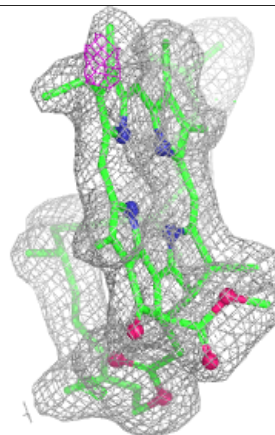
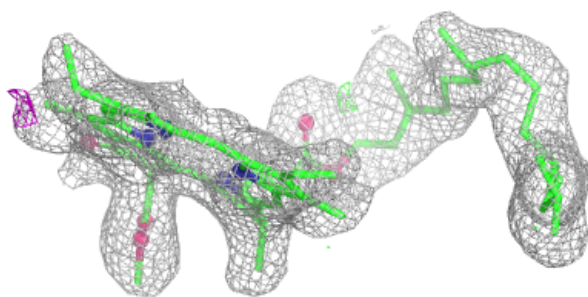
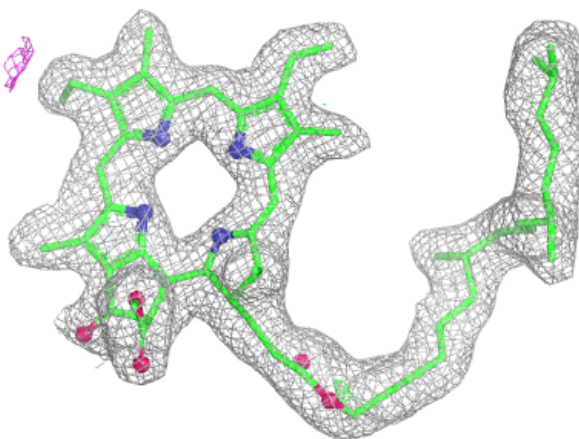
Electron density around PHO A 407:

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



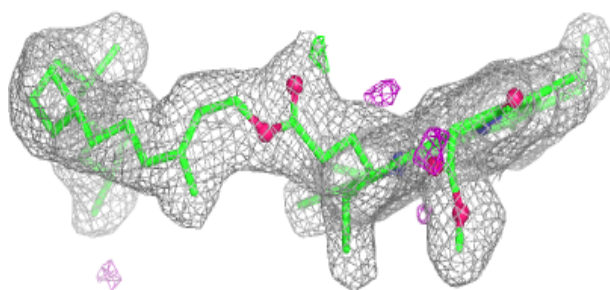
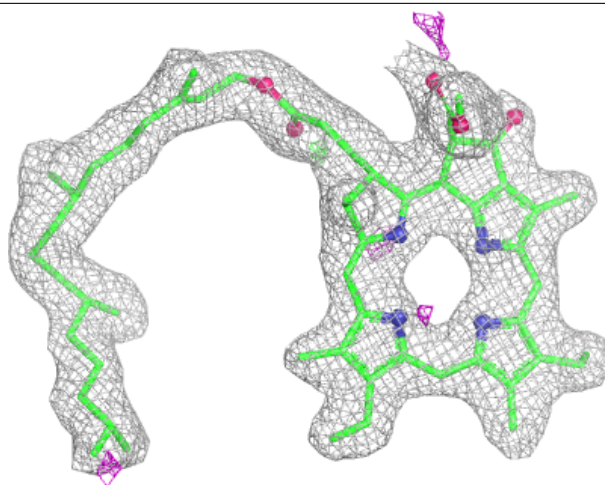
Electron density around PHO D 402:

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



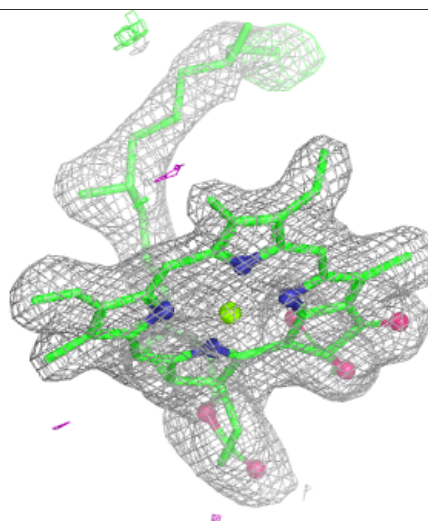
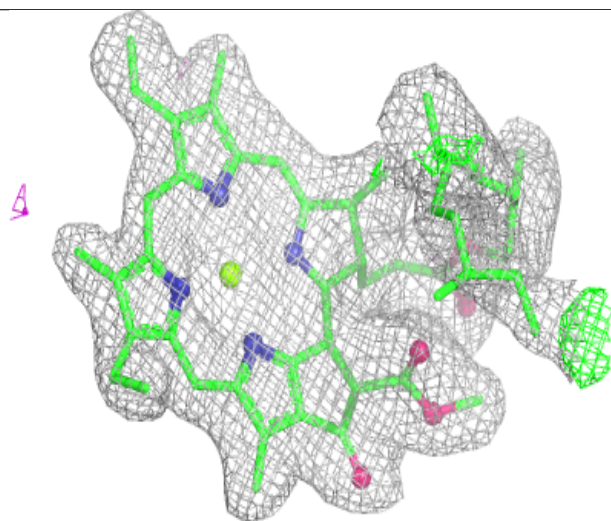
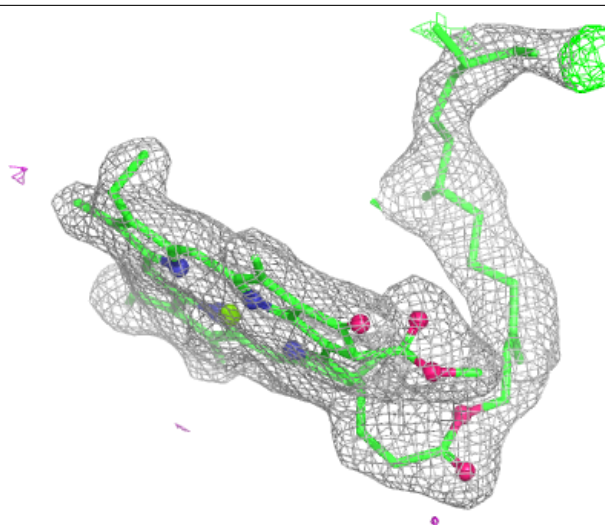
Electron density around PHO a 410:

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



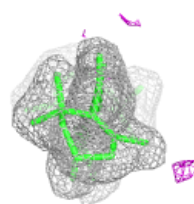
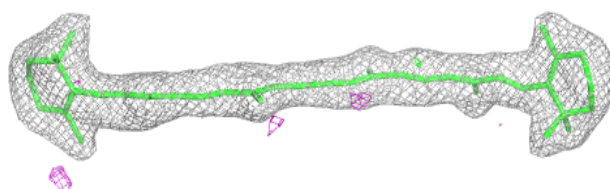
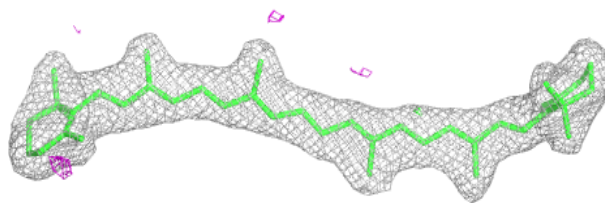
Electron density around CLA B 614:

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



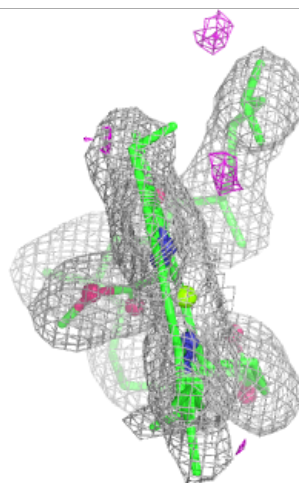
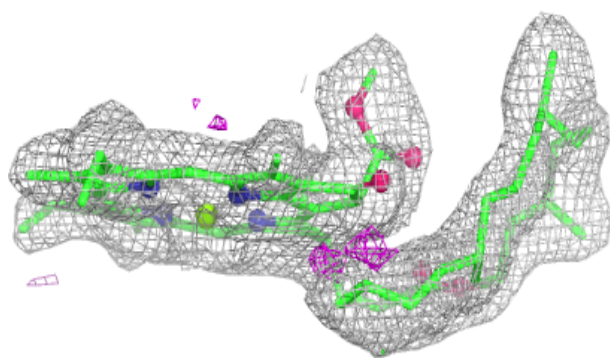
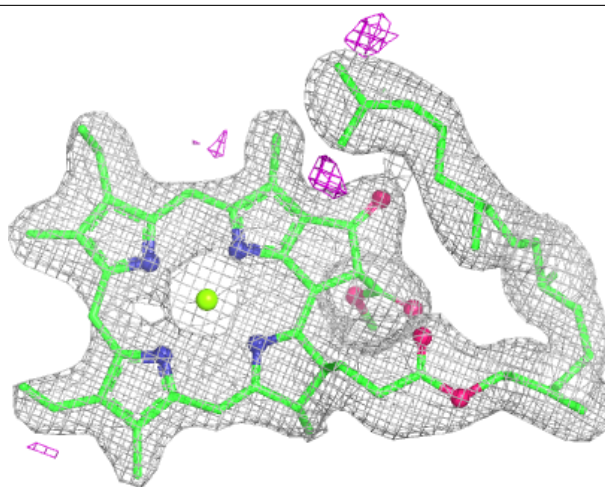
Electron density around BCR A 409:

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



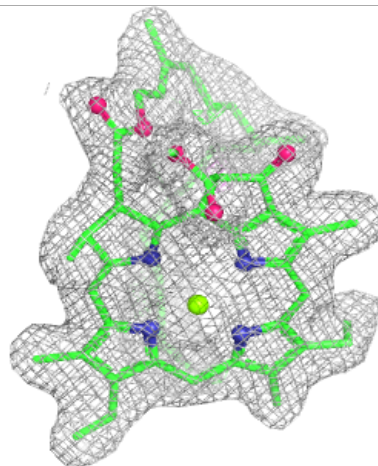
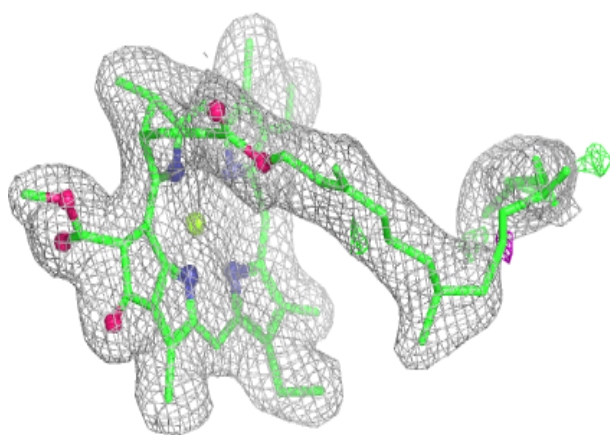
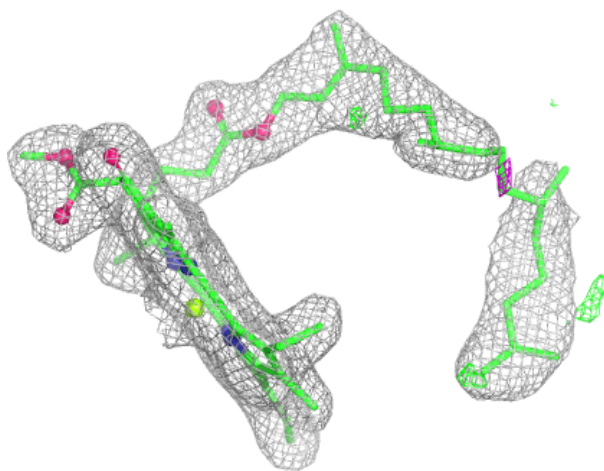
Electron density around CLA b 611:

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



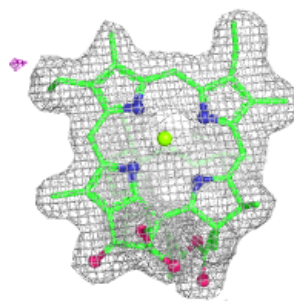
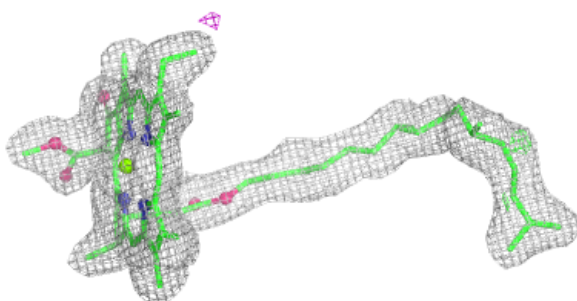
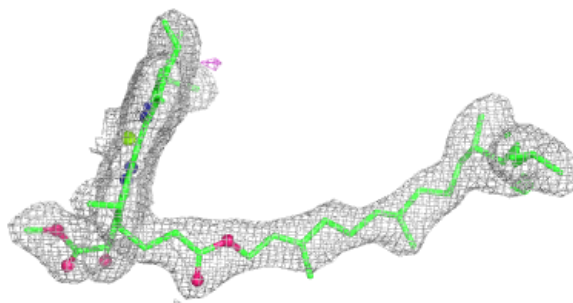
Electron density around CLA b 612:

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



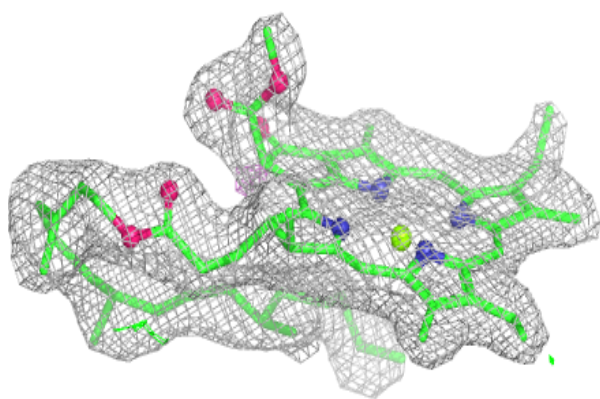
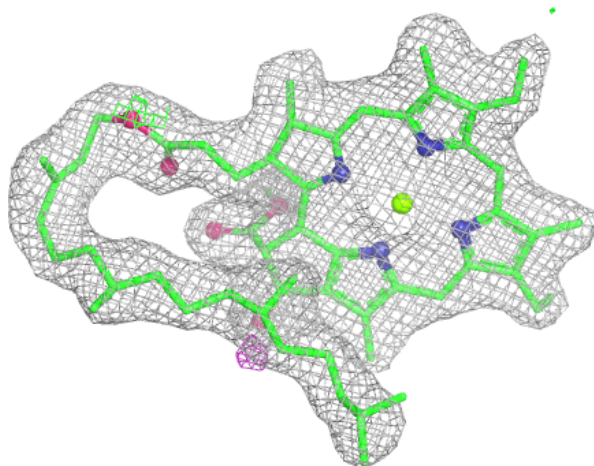
Electron density around CLA B 606:

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



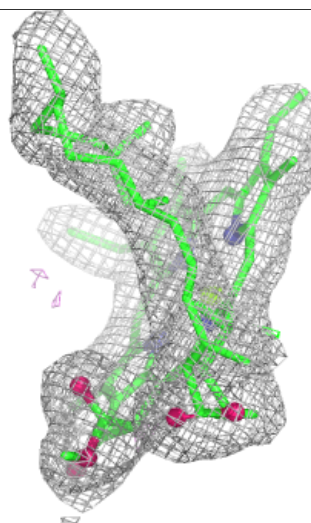
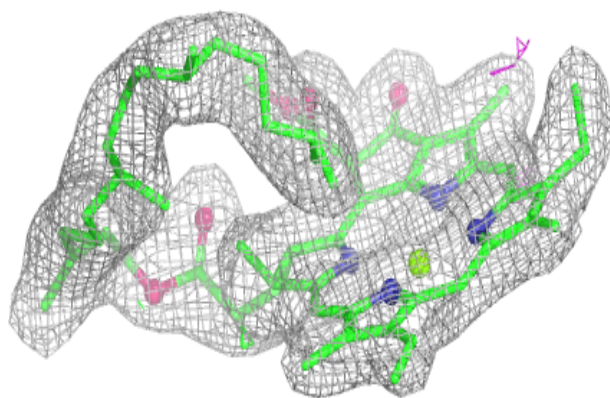
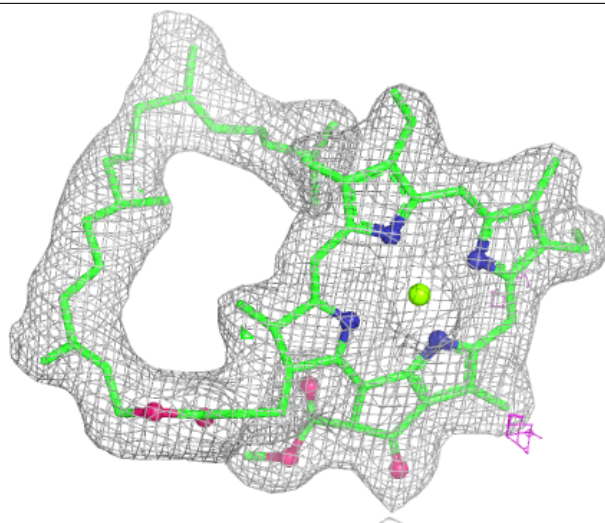
Electron density around CLA C 510:

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



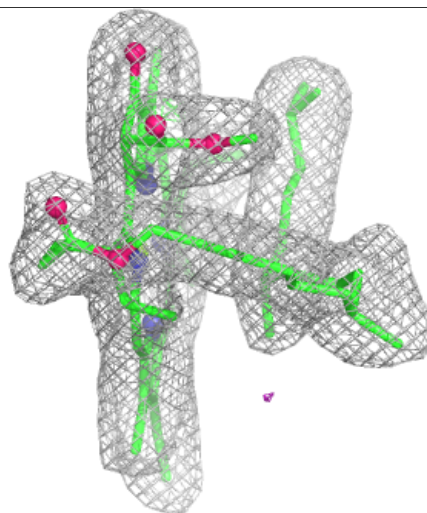
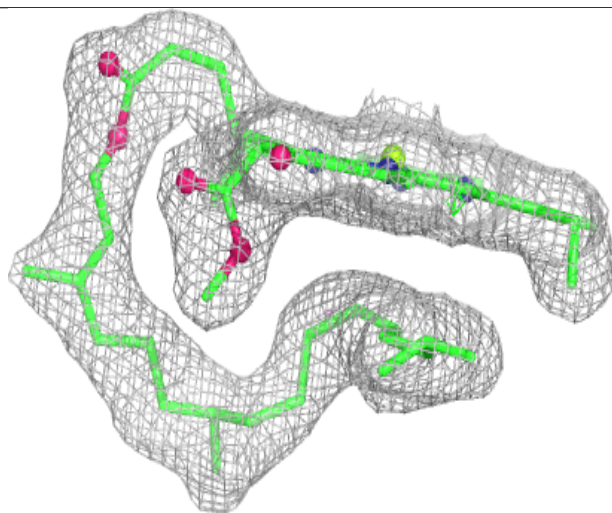
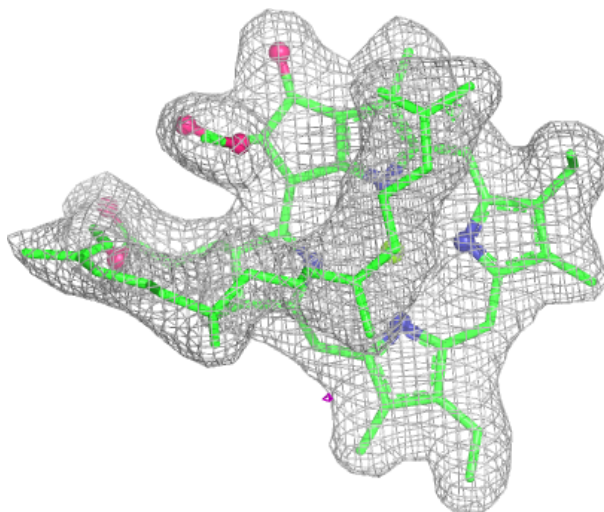
Electron density around CLA b 616:

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



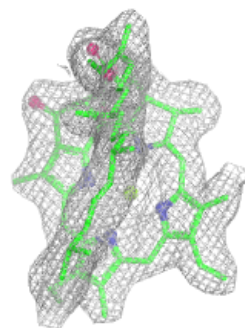
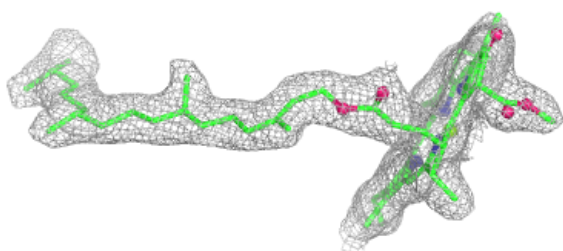
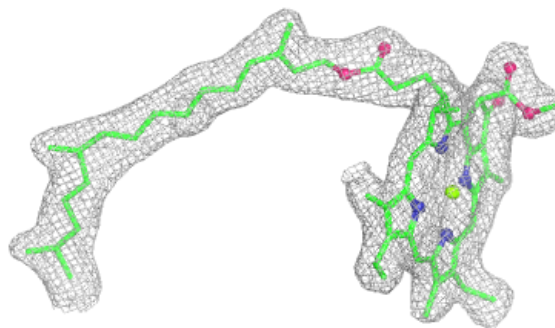
Electron density around CLA C 511:

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

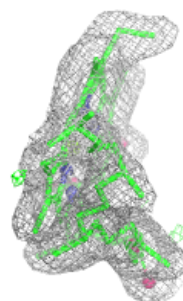
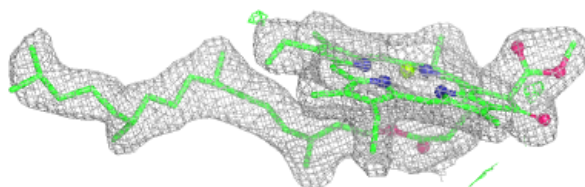
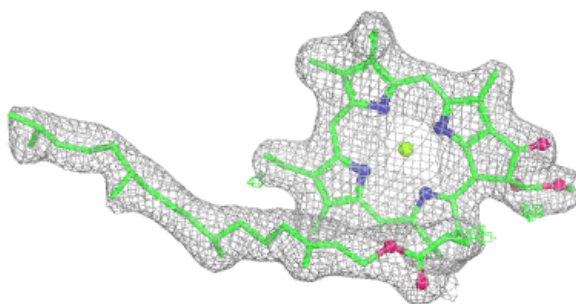


Electron density around CLA B 610:

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

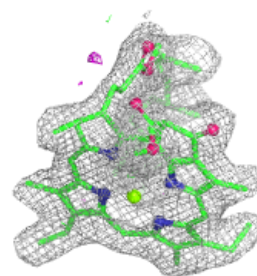
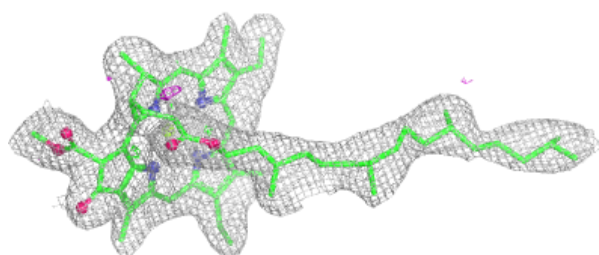
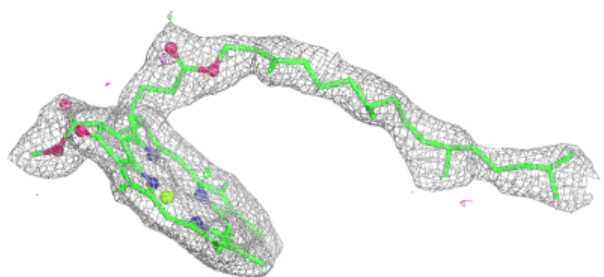
**Electron density around CLA C 502:**

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

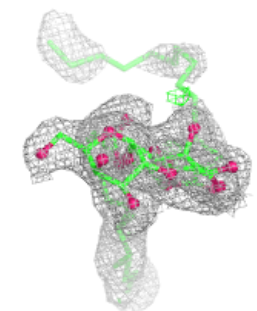
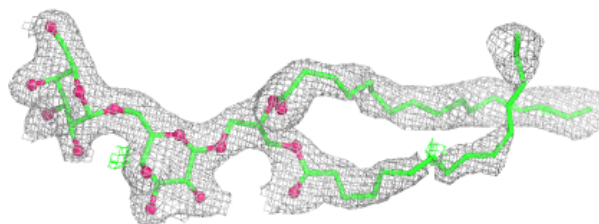
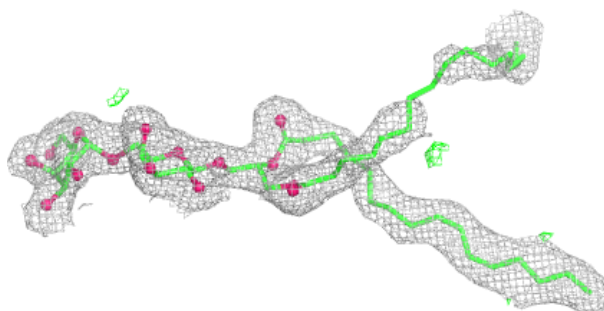


Electron density around CLA c 905:

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

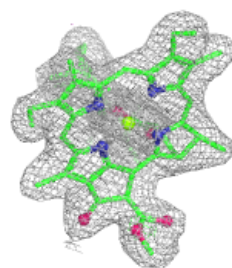
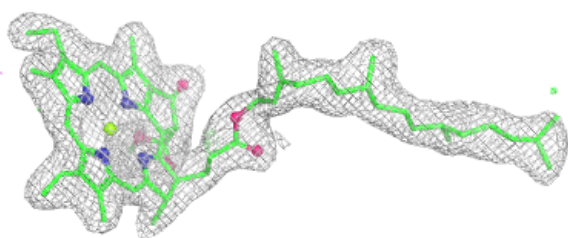
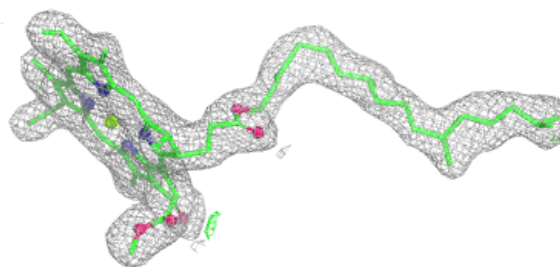
**Electron density around DGD C 517:**

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



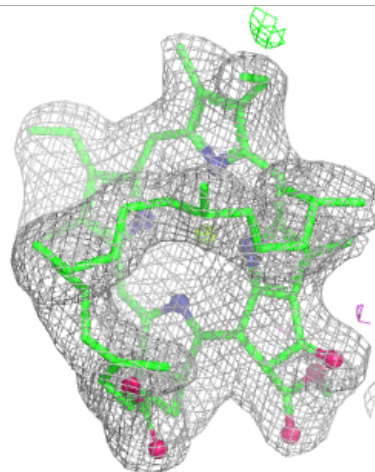
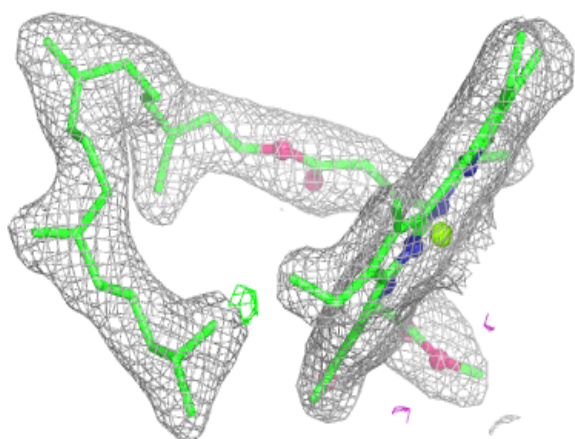
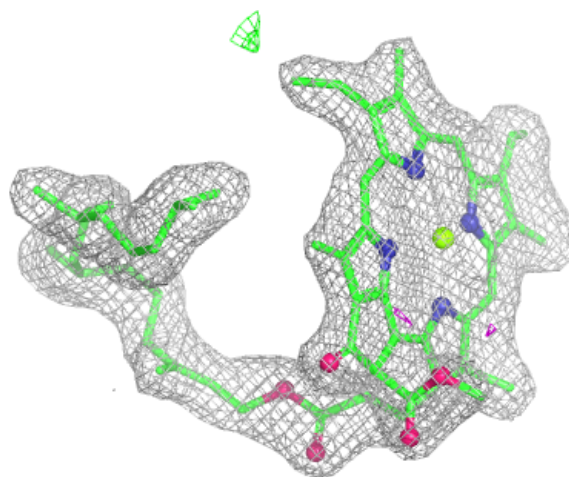
Electron density around CLA C 503:

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



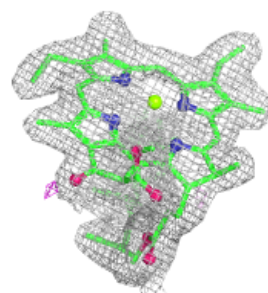
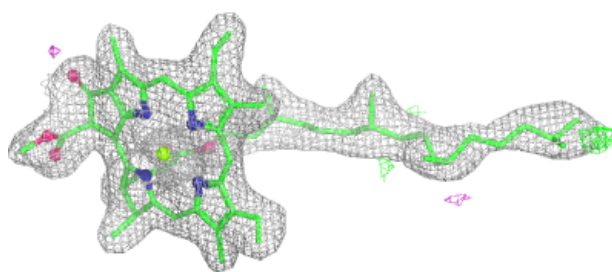
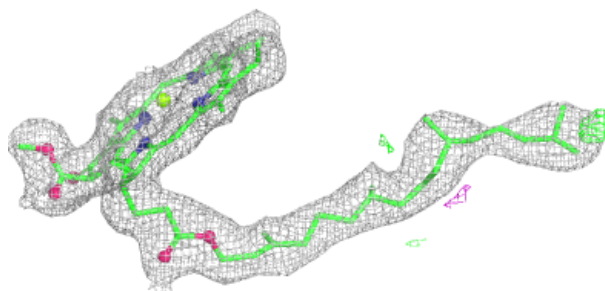
Electron density around CLA C 504:

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

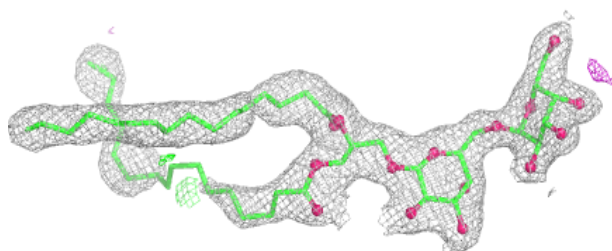
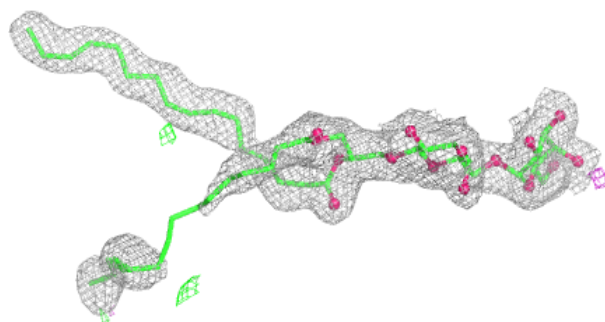


Electron density around CLA C 505:

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

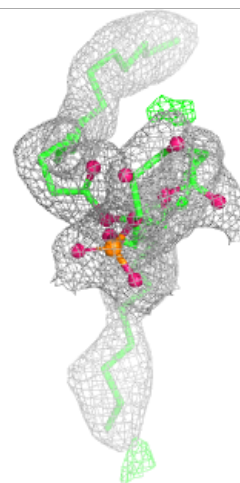
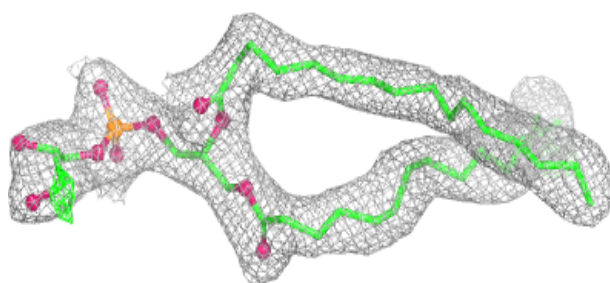
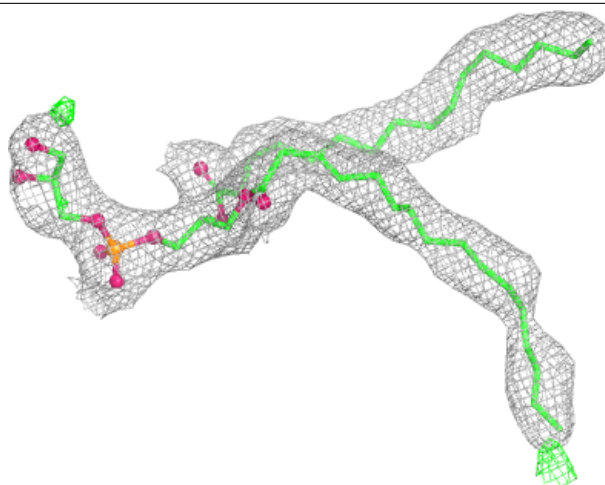
**Electron density around DGD c 917:**

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



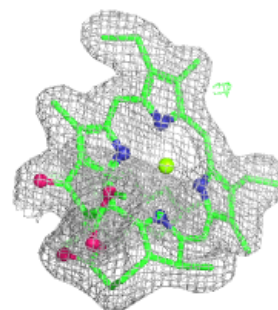
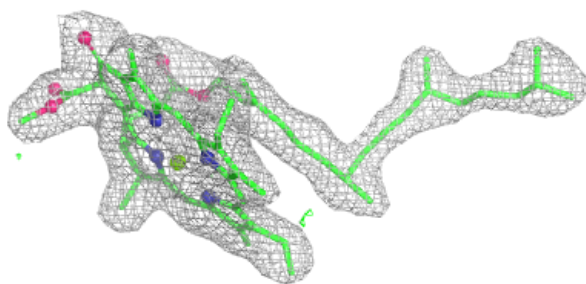
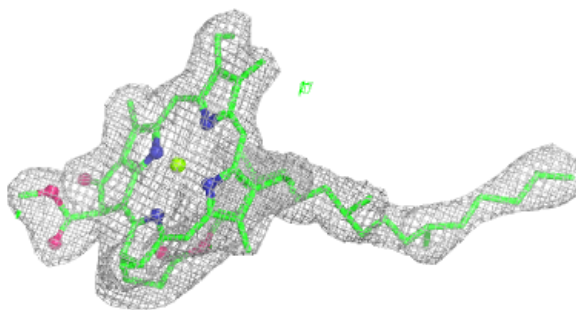
Electron density around LHG D 410:

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

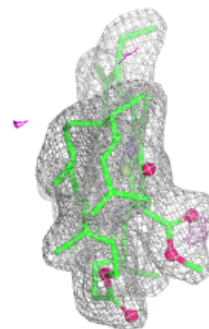
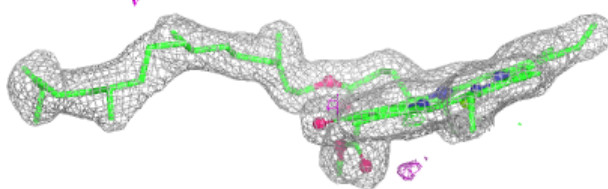
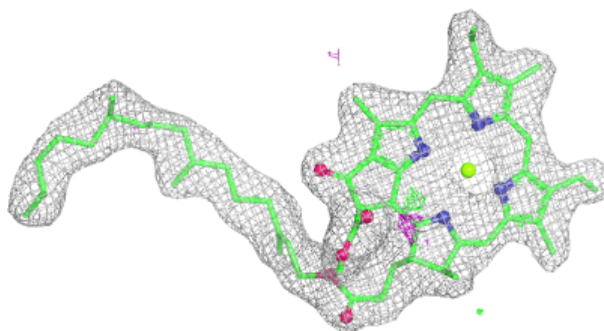


Electron density around CLA C 506:

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

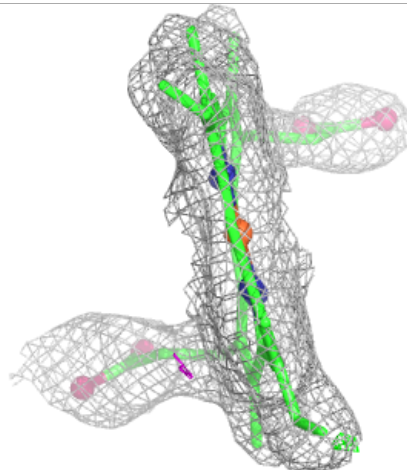
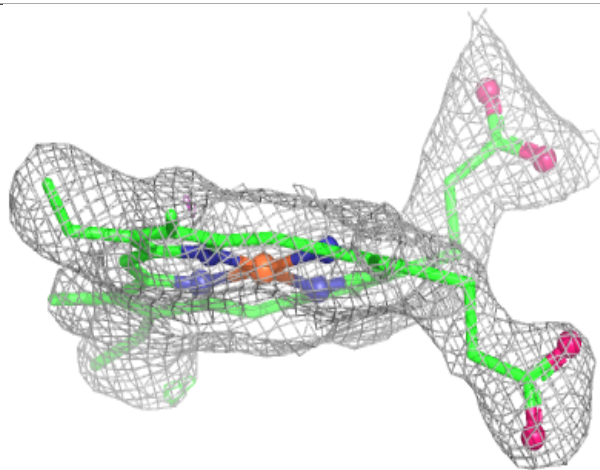
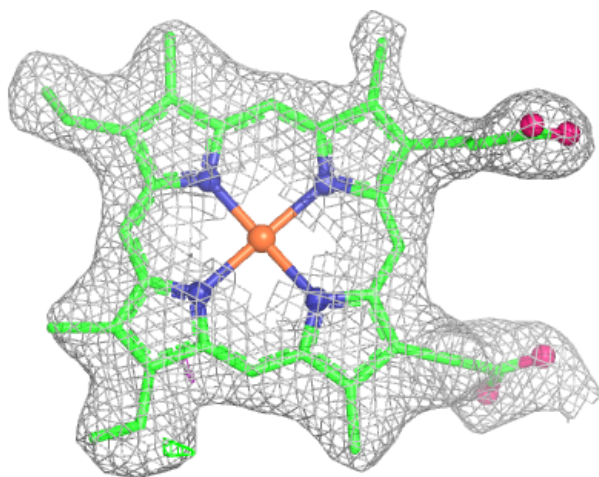
**Electron density around CLA b 603:**

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



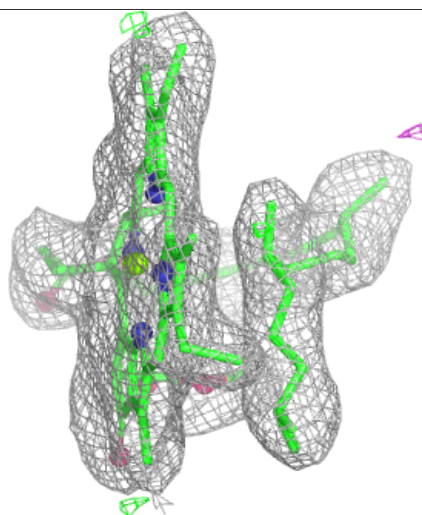
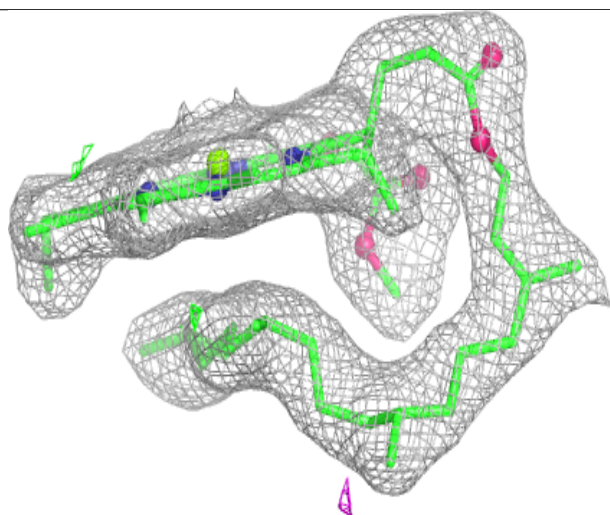
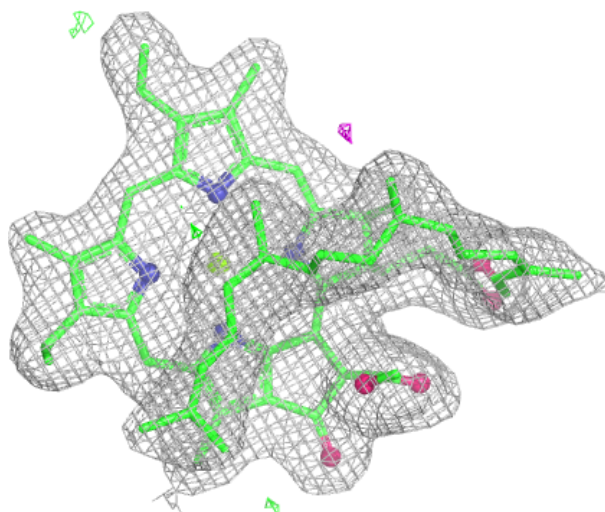
Electron density around HEM E 102:

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



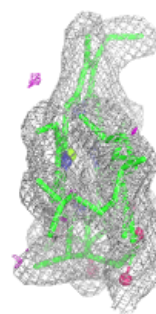
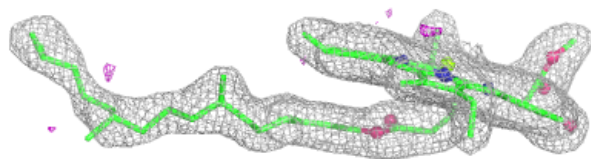
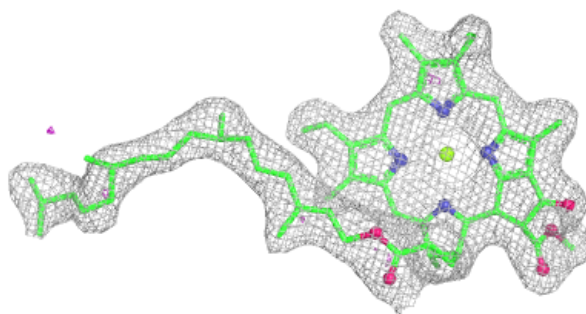
Electron density around CLA c 911:

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

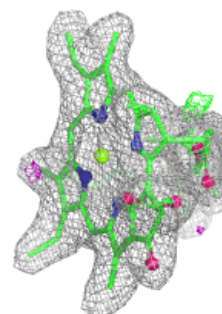
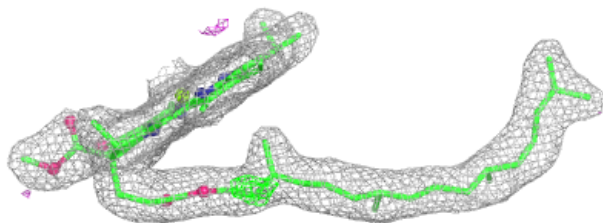
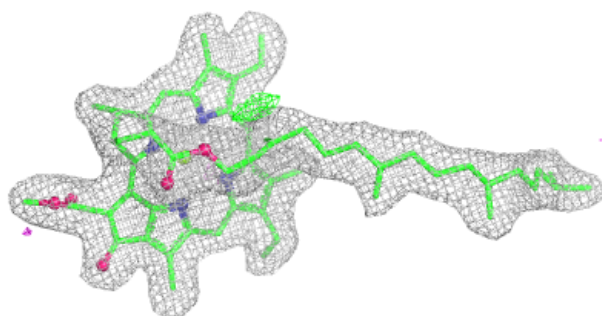


Electron density around CLA b 604:

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

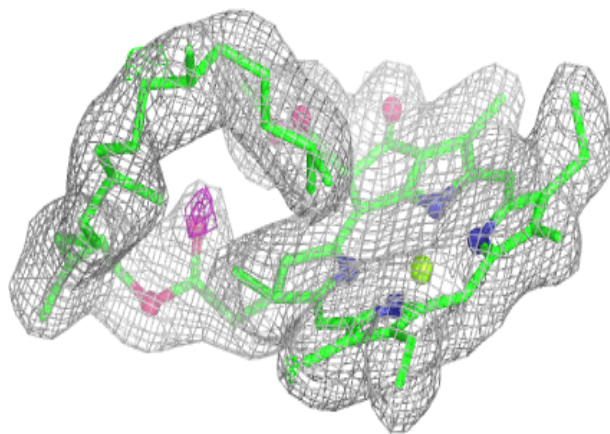
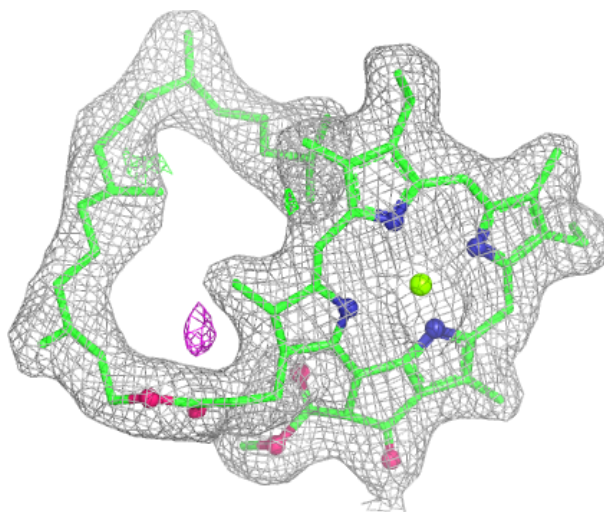
**Electron density around CLA B 609:**

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



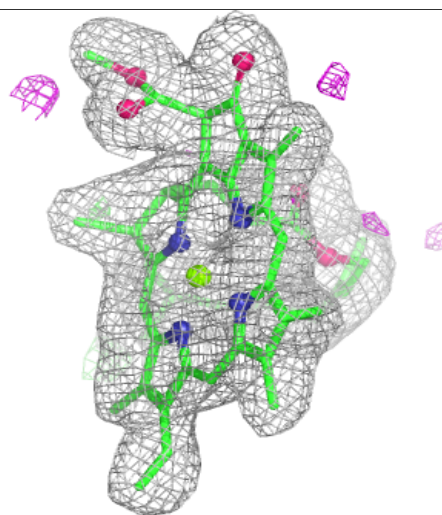
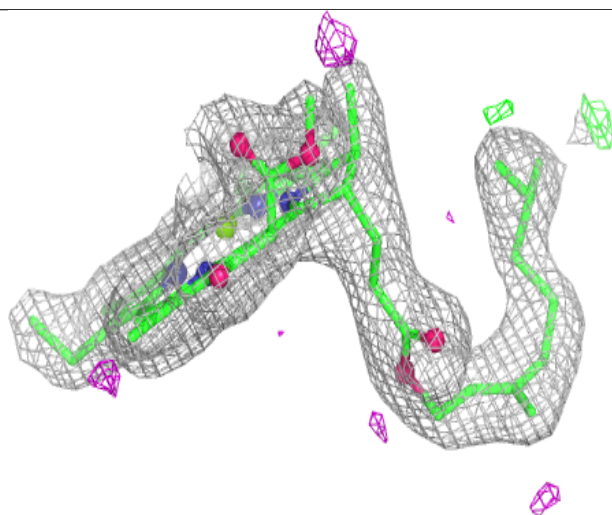
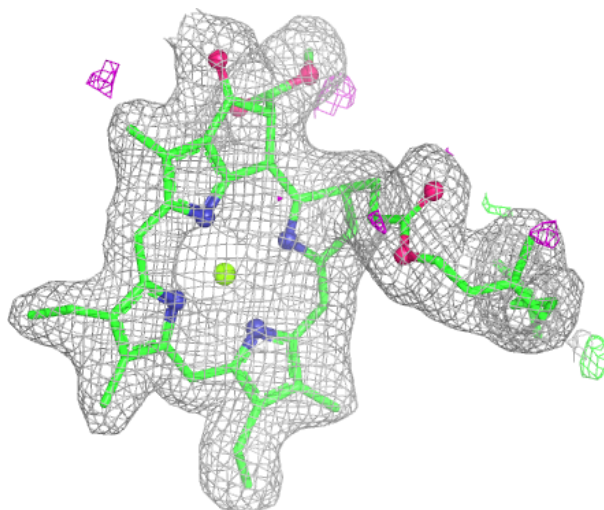
Electron density around CLA B 616:

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



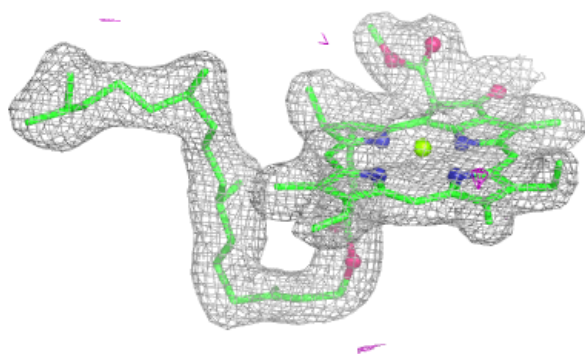
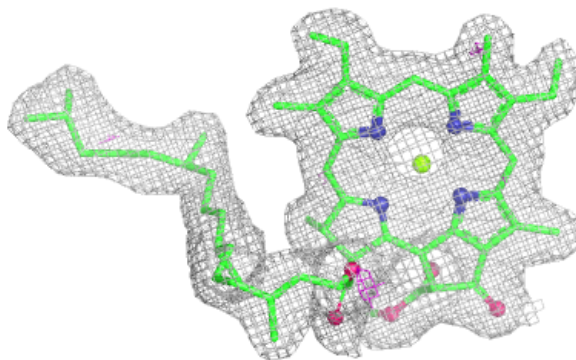
Electron density around CLA A 406:

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

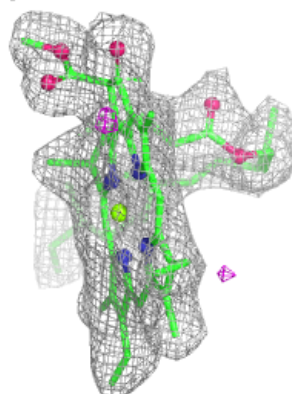
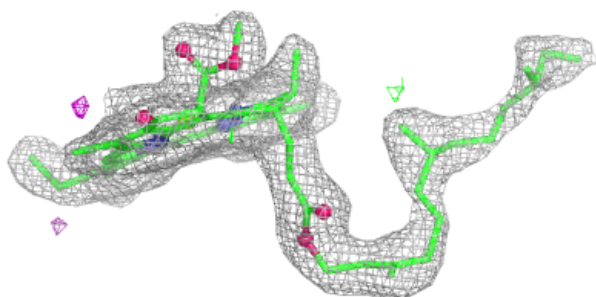
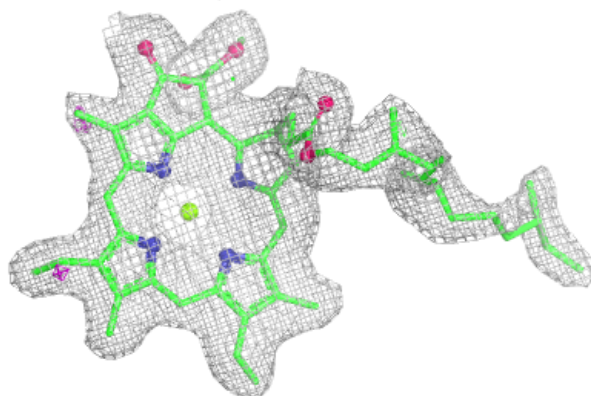


Electron density around CLA a 408:

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

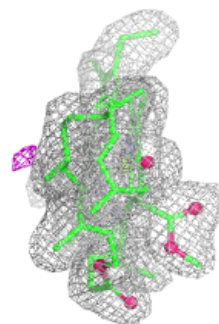
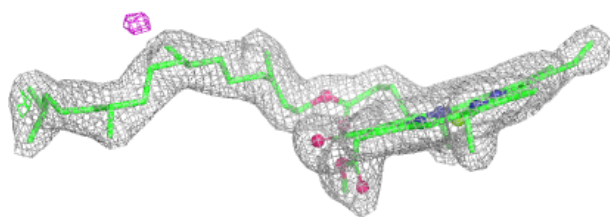
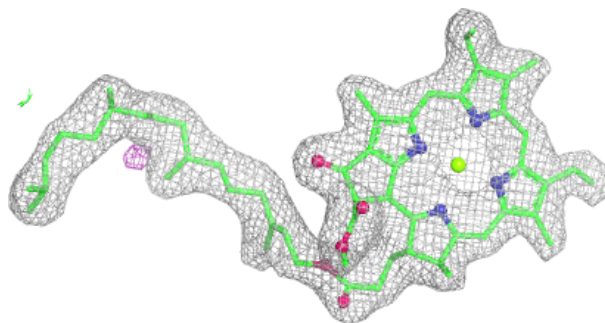
**Electron density around CLA a 409:**

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

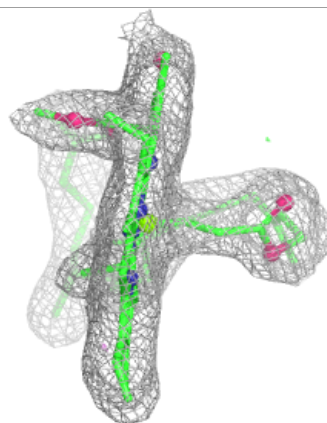
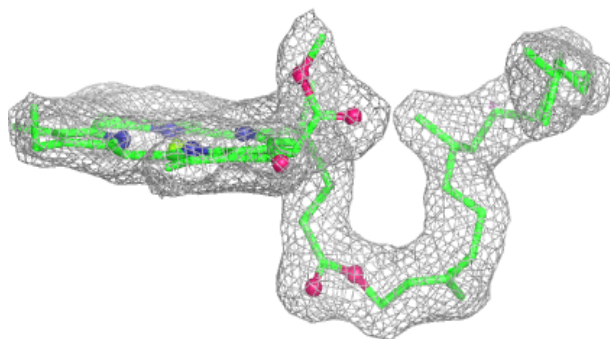
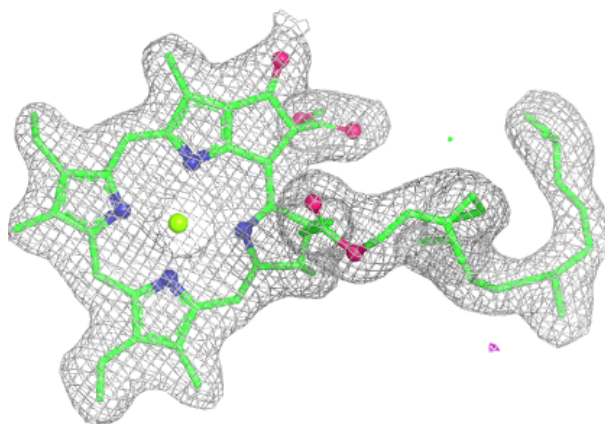


Electron density around CLA B 603:

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

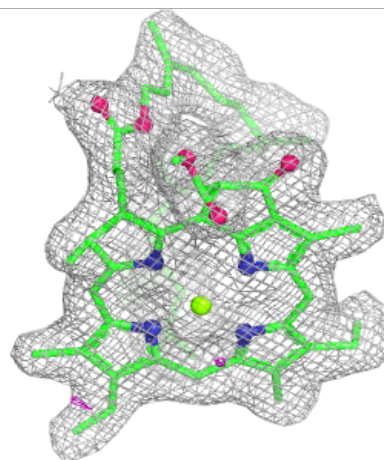
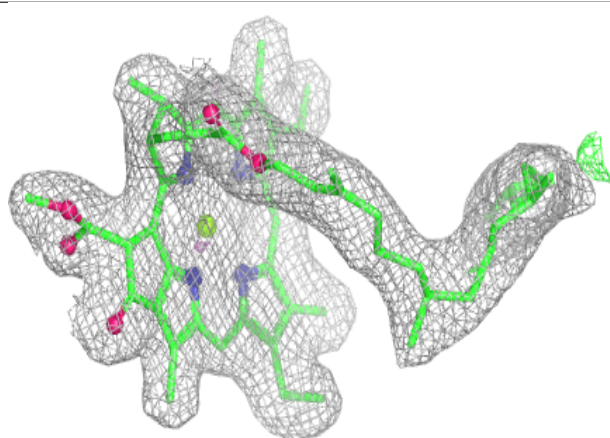
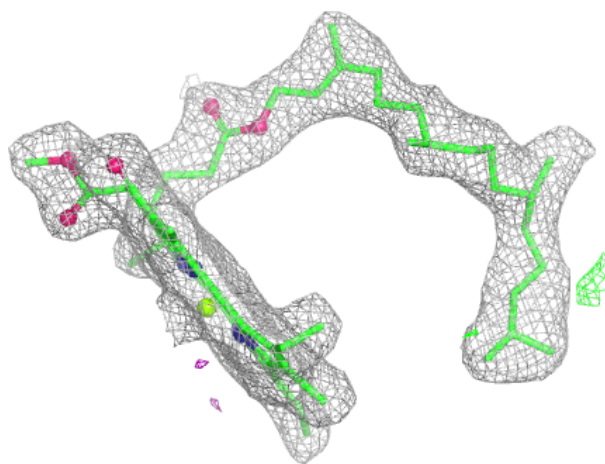
**Electron density around CLA b 613:**

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



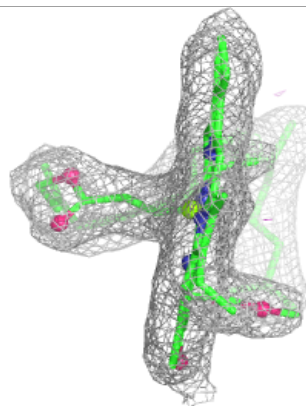
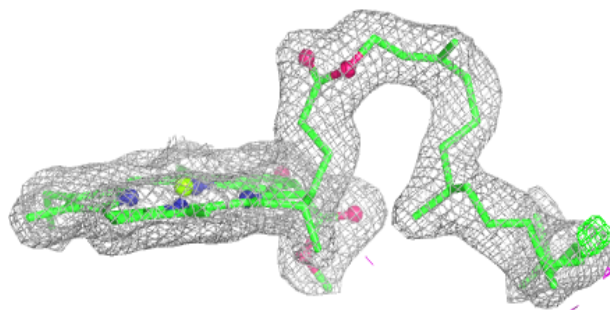
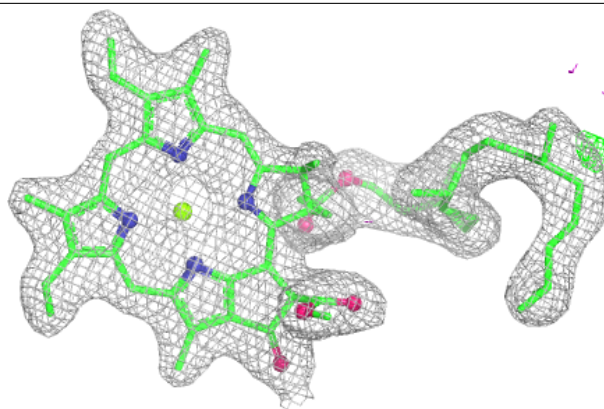
Electron density around CLA B 612:

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

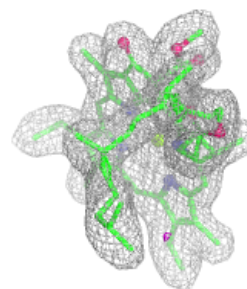
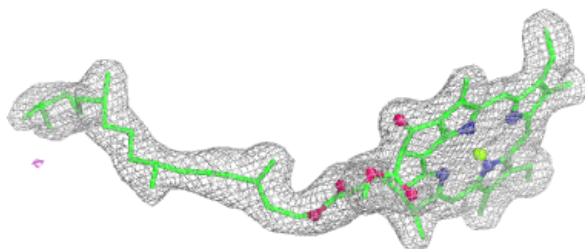
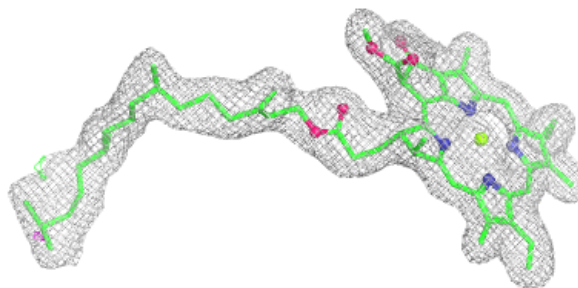


Electron density around CLA B 613:

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

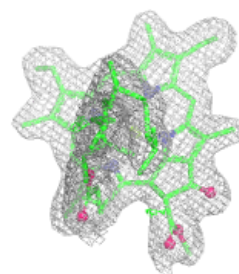
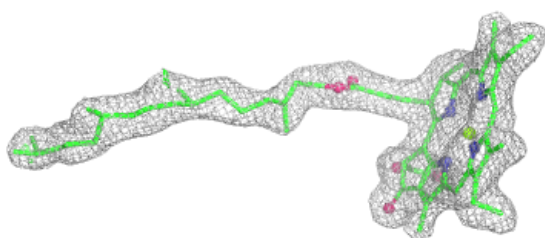
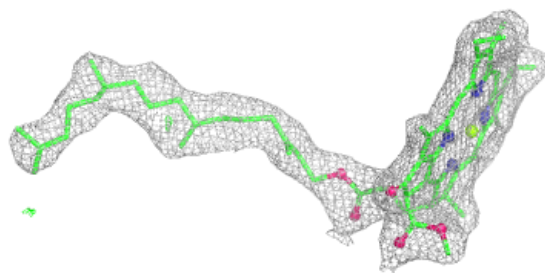
**Electron density around CLA A 405:**

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

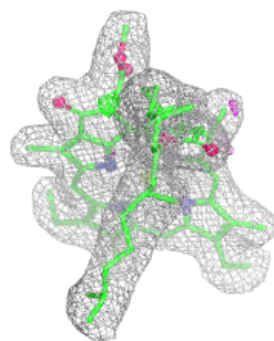
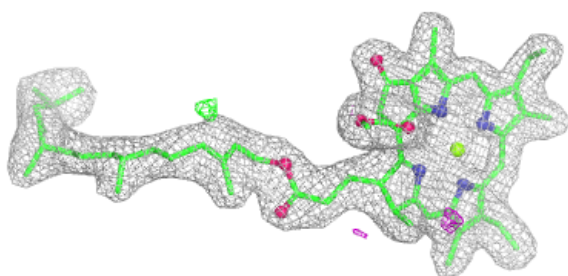
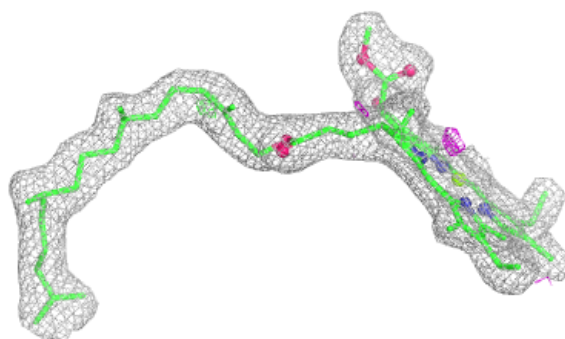


Electron density around CLA b 605:

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

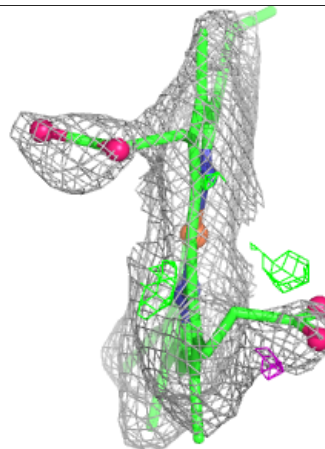
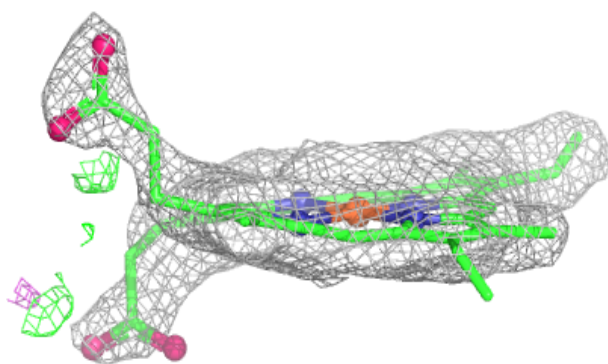
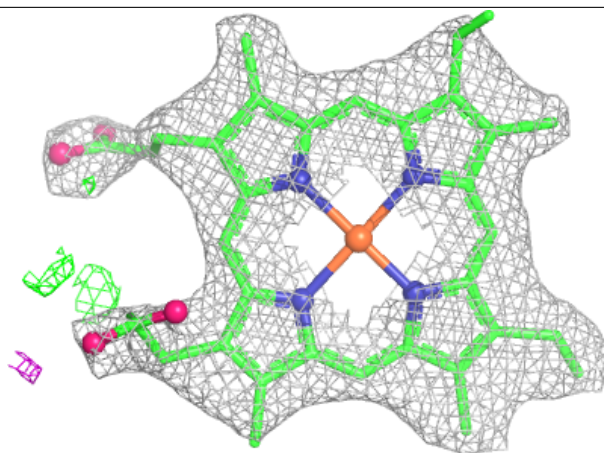
**Electron density around CLA d 402:**

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



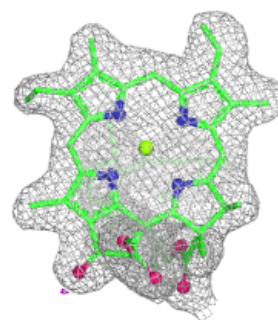
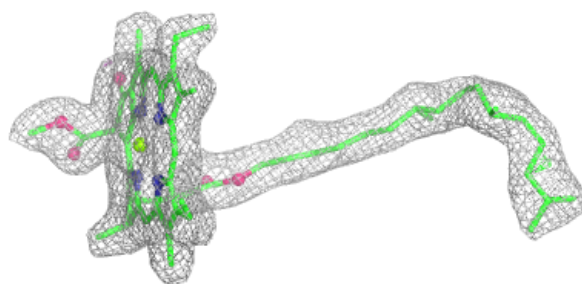
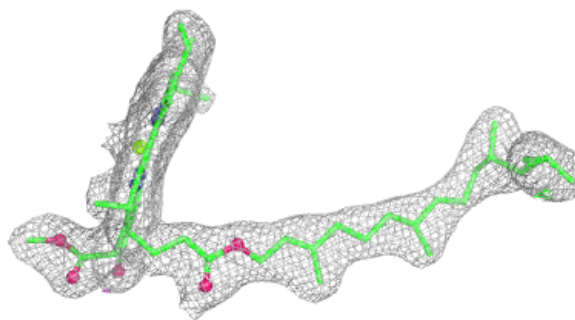
Electron density around HEM e 101:

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

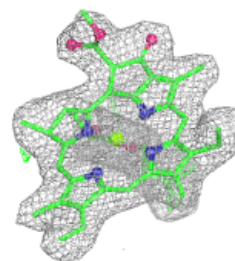
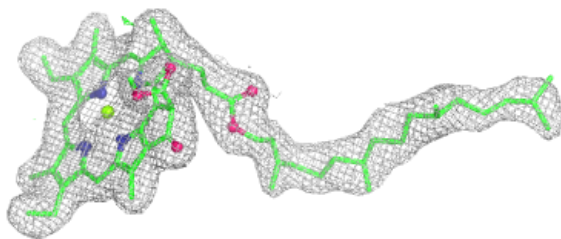
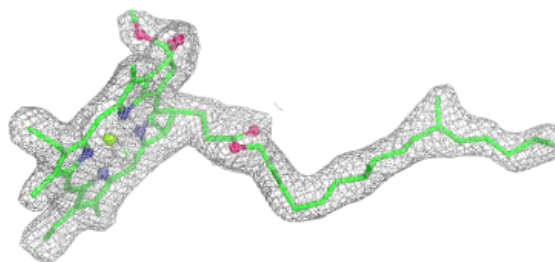


Electron density around CLA b 606:

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

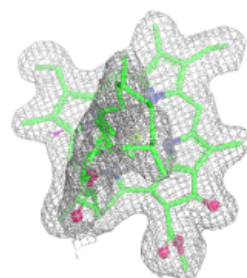
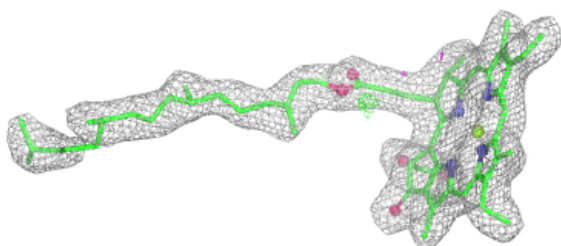
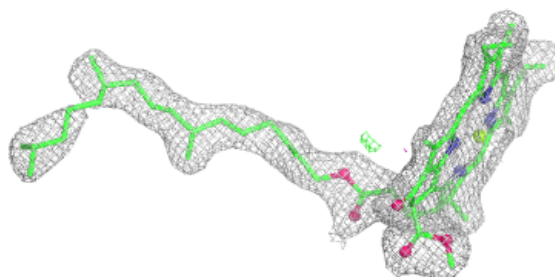
**Electron density around CLA c 903:**

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

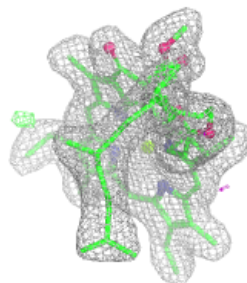
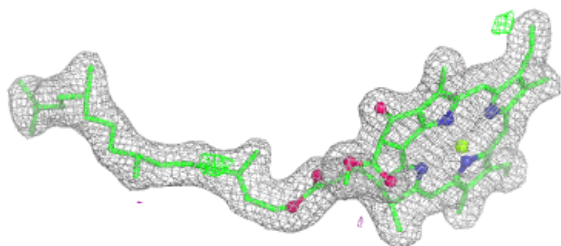
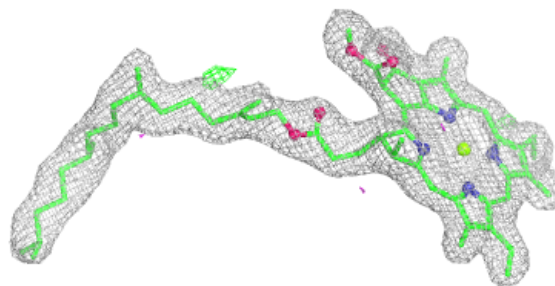


Electron density around CLA B 605:

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

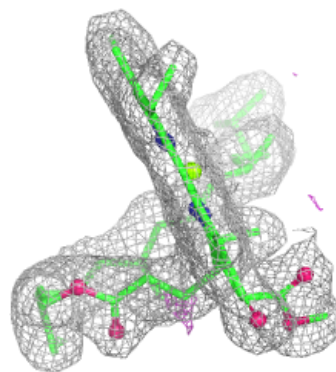
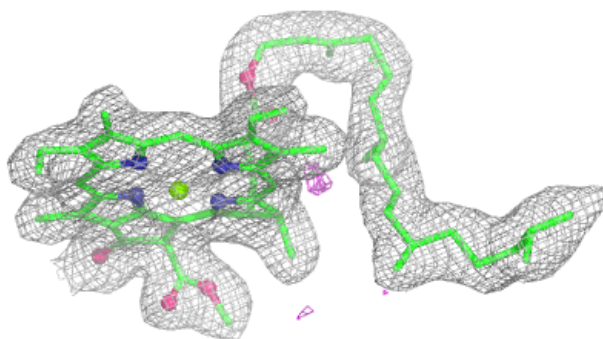
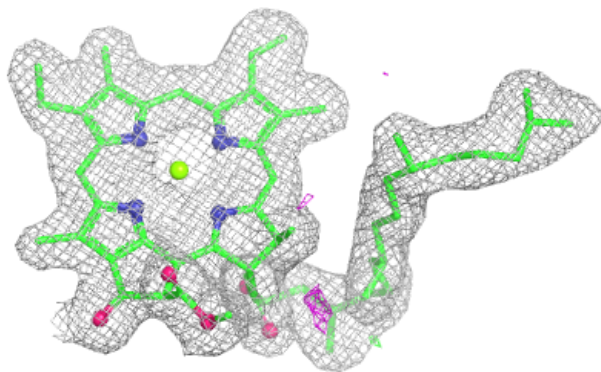
**Electron density around CLA a 407:**

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

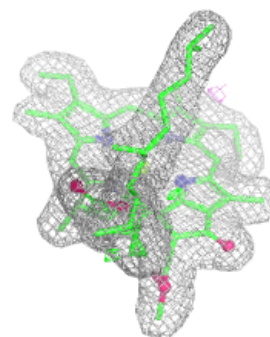
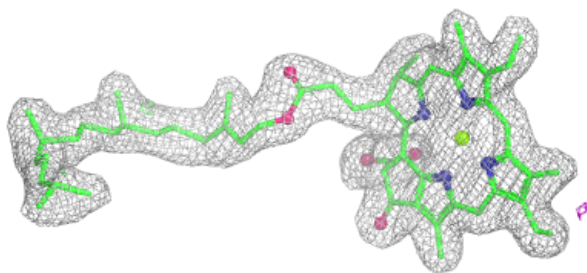
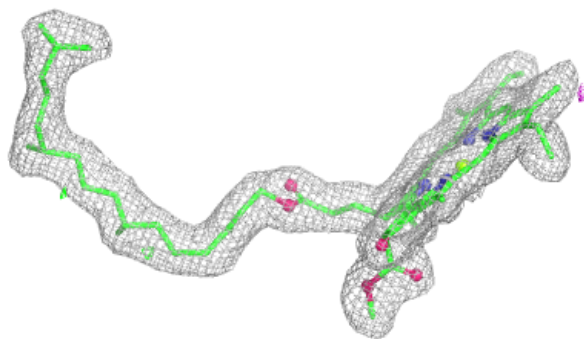


Electron density around CLA D 401:

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

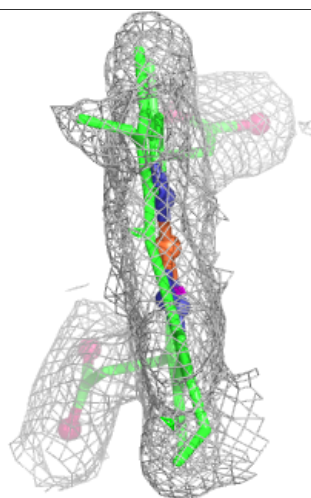
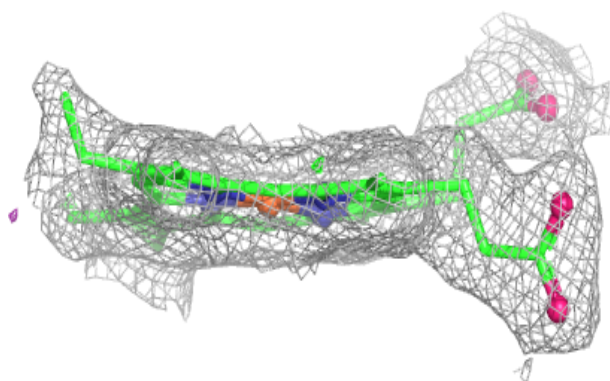
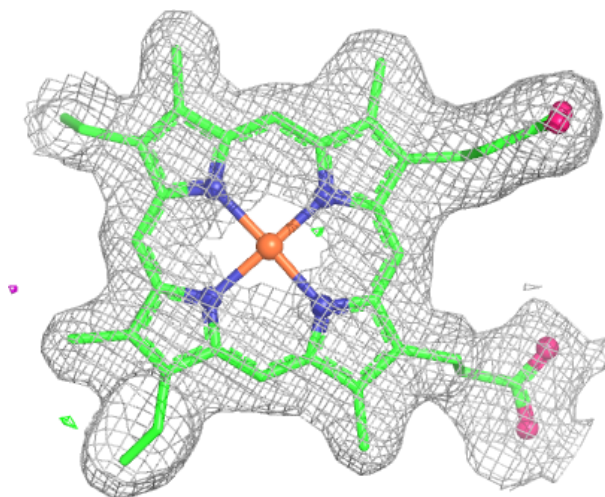
**Electron density around CLA D 403:**

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



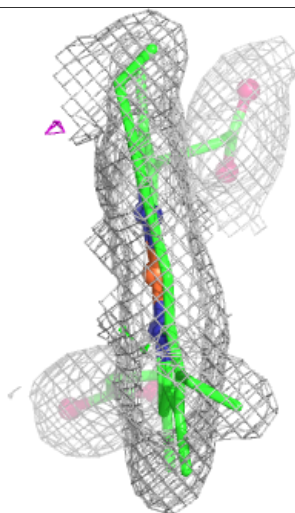
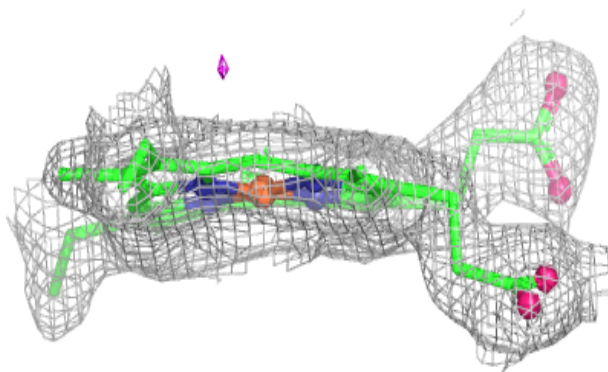
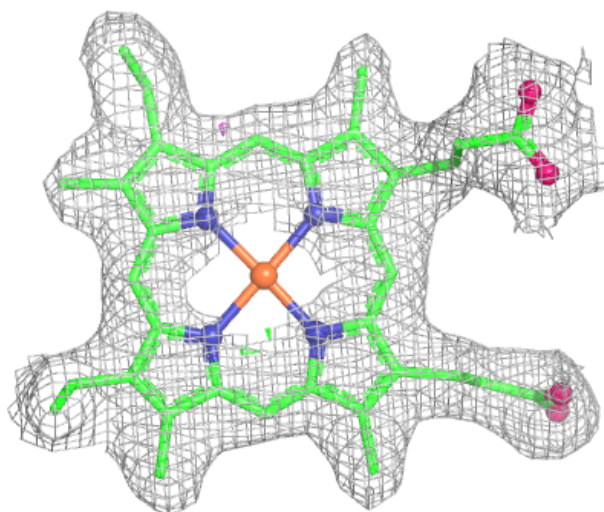
Electron density around HEC V 202:

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



Electron density around 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.