



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 5, 2026 – 04:27 AM JST

PDB ID : 4YUU / pdb_00004yuu
Title : Crystal structure of oxygen-evolving photosystem II from a red alga
Authors : Ago, H.; Shen, J.-R.
Deposited on : 2015-03-19
Resolution : 2.77 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

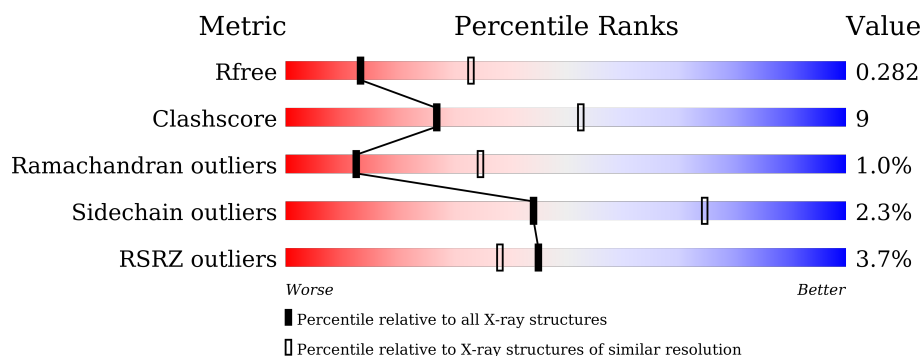
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.77 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	5248 (2.80-2.76)
Clashscore	190562	5693 (2.80-2.76)
Ramachandran outliers	187476	5590 (2.80-2.76)
Sidechain outliers	187428	5592 (2.80-2.76)
RSRZ outliers	180081	5251 (2.80-2.76)

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	A1	344	% 80% 19% .
1	A2	344	2% 81% 15% ..
1	a1	344	% 78% 18% ..
1	a2	344	% 80% 16% ..
2	B1	509	% 79% 14% . 5%
2	B2	509	2% 84% 13% ..

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Mol	Chain	Length	Quality of chain
2	b1	509	
2	b2	509	
3	C1	460	
3	C2	460	
3	c1	460	
3	c2	460	
4	D1	351	
4	D2	351	
4	d1	351	
4	d2	351	
5	E1	84	
5	E2	84	
5	e1	84	
5	e2	84	
6	F1	43	
6	F2	43	
6	f1	43	
6	f2	43	
7	H1	67	
7	H2	67	
7	h1	67	
7	h2	67	
8	I1	38	
8	I2	38	
8	i1	38	

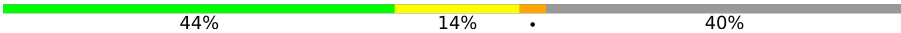
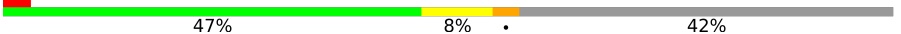
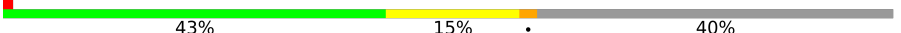
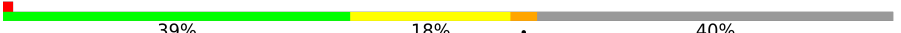
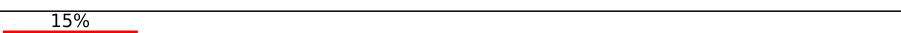
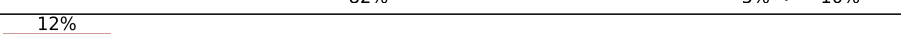
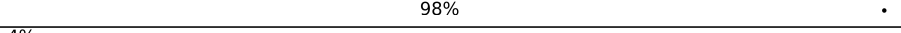
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Mol	Chain	Length	Quality of chain
8	i2	38	
9	J1	39	
9	J2	39	
9	j1	39	
9	j2	39	
10	K1	41	
10	K2	41	
10	k1	41	
10	k2	41	
11	L1	38	
11	L2	38	
11	l1	38	
11	l2	38	
12	M1	108	
12	M2	108	
12	m1	108	
12	m2	108	
13	O1	329	
13	O2	329	
13	o1	329	
13	o2	329	
14	T1	32	
14	T2	32	
14	t1	32	
14	t2	32	

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Mol	Chain	Length	Quality of chain
15	U1	155	
15	U2	155	
15	u1	155	
15	u2	155	
16	V1	155	
16	V2	155	
16	v1	155	
16	v2	155	
17	Y1	35	
17	Y2	35	
17	y1	35	
17	y2	35	
18	X1	40	
18	X2	40	
18	x1	40	
18	x2	40	
19	S1	46	
19	S2	46	
19	s1	46	
19	s2	46	
20	W1	25	
20	W2	25	
20	w1	25	
20	w2	25	
21	Q2	218	

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Mol	Chain	Length	Quality of chain
21	q1	218	8% 43% 5% 52%
22	Z2	62	21% 90% 5% 5%
22	z2	62	6% 82% 13% 5%

2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 92765 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A1	344	Total	C	N	O	S	0	0	0
			2609	1708	425	462	14			
1	a1	334	Total	C	N	O	S	0	0	0
			2564	1676	421	454	13			
1	A2	332	Total	C	N	O	S	0	1	0
			2475	1607	411	444	13			
1	a2	334	Total	C	N	O	S	0	0	0
			2513	1638	410	452	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B1	483	Total	C	N	O	S	0	0	0
			3703	2426	624	641	12			
2	b1	503	Total	C	N	O	S	0	1	0
			3881	2549	646	674	12			
2	B2	503	Total	C	N	O	S	0	0	0
			3770	2460	645	654	11			
2	b2	481	Total	C	N	O	S	0	0	0
			3681	2418	620	631	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C1	449	Total	C	N	O	S	0	0	0
			3392	2215	573	594	10			
3	c1	449	Total	C	N	O	S	0	2	0
			3439	2241	577	611	10			
3	C2	444	Total	C	N	O	S	0	0	0
			3145	2028	545	564	8			
3	c2	448	Total	C	N	O	S	0	0	0
			3386	2201	578	597	10			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D1	337	Total	C	N	O	S	0	0	0
			2615	1736	422	447	10			
4	d1	339	Total	C	N	O	S	0	0	0
			2678	1775	433	460	10			
4	D2	340	Total	C	N	O	S	0	0	0
			2585	1713	422	440	10			
4	d2	340	Total	C	N	O	S	0	0	0
			2643	1756	425	452	10			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E1	61	Total	C	N	O	0	0	0
			405	264	68	73			
5	e1	57	Total	C	N	O	0	0	0
			427	280	71	76			
5	E2	63	Total	C	N	O	0	0	0
			430	279	72	79			
5	e2	60	Total	C	N	O	0	0	0
			421	279	71	71			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F1	28	Total	C	N	O	S	0	0	0
			213	144	36	32	1			
6	f1	29	Total	C	N	O	S	0	0	0
			227	158	36	32	1			
6	F2	31	Total	C	N	O	S	0	0	0
			229	153	41	34	1			
6	f2	29	Total	C	N	O	S	0	0	0
			225	157	34	33	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H1	60	Total	C	N	O	S	0	0	0
			433	289	69	73	2			
7	h1	62	Total	C	N	O	S	0	0	0
			470	317	71	80	2			
7	H2	62	Total	C	N	O	S	0	0	0
			443	294	72	75	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	h2	62	Total	C	N	O	S	0	0	0
			450	302	69	77	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I1	34	Total	C	N	O	S	0	0	0
			274	184	42	45	3			
8	i1	34	Total	C	N	O	S	0	0	0
			280	188	44	45	3			
8	I2	35	Total	C	N	O	S	0	0	0
			265	177	41	45	2			
8	i2	33	Total	C	N	O	S	0	0	0
			261	174	40	44	3			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	J1	32	Total	C	N	O	0	0	0
			220	148	33	39			
9	j1	32	Total	C	N	O	0	0	0
			224	152	33	39			
9	J2	35	Total	C	N	O	0	0	0
			231	154	36	41			
9	j2	33	Total	C	N	O	0	0	0
			228	153	34	41			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	K1	37	Total	C	N	O	S	0	0	0
			279	195	39	44	1			
10	k1	37	Total	C	N	O	S	0	0	0
			280	198	39	42	1			
10	K2	37	Total	C	N	O		0	0	0
			250	171	39	40				
10	k2	37	Total	C	N	O	S	0	0	0
			269	185	40	43	1			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	L1	37	Total	C	N	O	0	0	0
			292	197	46	49			
11	l1	37	Total	C	N	O	0	0	0
			299	203	47	49			
11	L2	37	Total	C	N	O	0	0	0
			299	202	46	51			
11	l2	37	Total	C	N	O	0	0	0
			299	202	46	51			

- Molecule 12 is a protein called PHOTOSYSTEM II REACTION CENTER PROTEIN M.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M1	40	Total	C	N	O	S	0	0	0
			285	189	44	50	2			
12	m1	40	Total	C	N	O	S	0	0	0
			285	189	44	50	2			
12	M2	40	Total	C	N	O	S	0	0	0
			284	188	46	48	2			
12	m2	40	Total	C	N	O	S	0	0	0
			287	189	46	50	2			

- Molecule 13 is a protein called PHOTOSYSTEM II MANGANESE-STABILIZING POLYPEPTIDE, PSBO.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O1	240	Total	C	N	O	S	0	0	0
			1674	1074	276	316	8			
13	o1	238	Total	C	N	O	S	0	0	0
			1692	1070	282	332	8			
13	O2	205	Total	C	N	O	S	0	0	0
			1376	870	237	262	7			
13	o2	245	Total	C	N	O	S	0	0	0
			1768	1123	296	341	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T1	30	Total	C	N	O	S	0	0	0
			241	168	36	36	1			
14	t1	30	Total	C	N	O	S	0	0	0
			246	173	36	36	1			
14	T2	30	Total	C	N	O	S	0	0	0
			240	170	33	36	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	t2	29	Total	C	N	O	S	0	0	0
			235	167	32	35	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	U1	93	Total	C	N	O	S	0	0	0
			691	445	116	129	1			
15	u1	93	Total	C	N	O	S	0	0	0
			703	449	119	134	1			
15	U2	90	Total	C	N	O	S	0	0	0
			577	355	103	118	1			
15	u2	93	Total	C	N	O	S	0	0	0
			708	455	120	132	1			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U1	-51	MET	-	initiating methionine	UNP Q9ZQS5
u1	-51	MET	-	initiating methionine	UNP Q9ZQS5
U2	-51	MET	-	initiating methionine	UNP Q9ZQS5
u2	-51	MET	-	initiating methionine	UNP Q9ZQS5

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V1	129	Total	C	N	O	S	0	0	0
			917	579	159	175	4			
16	v1	129	Total	C	N	O	S	0	0	0
			921	577	163	177	4			
16	V2	129	Total	C	N	O	S	0	0	0
			845	521	152	168	4			
16	v2	129	Total	C	N	O	S	0	0	0
			963	608	168	183	4			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	Y1	27	Total	C	N	O	0	0	0
			170	111	29	30			
17	y1	27	Total	C	N	O	0	0	0
			195	133	30	32			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	Y2	25	Total	C	N	O	0	0	0
			159	104	27	28			
17	y2	27	Total	C	N	O	0	0	0
			188	126	30	32			

- Molecule 18 is a protein called PHOTOSYSTEM II REACTION CENTER PROTEIN X.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	X1	29	Total	C	N	O	0	0	0
			197	135	30	32			
18	x1	36	Total	C	N	O	0	0	0
			255	174	38	42			
18	X2	31	Total	C	N	O	0	0	0
			215	149	33	32			
18	x2	32	Total	C	N	O	0	0	0
			218	147	35	36			

- Molecule 19 is a protein called PEPTIDE CHAIN UNASSIGNED.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	S1	25	Total	C	N	O	0	0	0
			164	113	26	25			
19	s1	40	Total	C	N	O	0	0	0
			263	182	41	40			
19	S2	30	Total	C	N	O	0	0	0
			191	130	31	30			
19	s2	46	Total	C	N	O	0	0	0
			281	188	47	46			

- Molecule 20 is a protein called PEPTIDE CHAIN UNASSIGNED.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	W1	21	Total	C	N	O	0	0	0
			134	91	21	22			
20	w1	25	Total	C	N	O	0	0	0
			152	101	25	26			
20	W2	21	Total	C	N	O	0	0	0
			129	86	21	22			
20	w2	20	Total	C	N	O	0	0	0
			127	86	20	21			

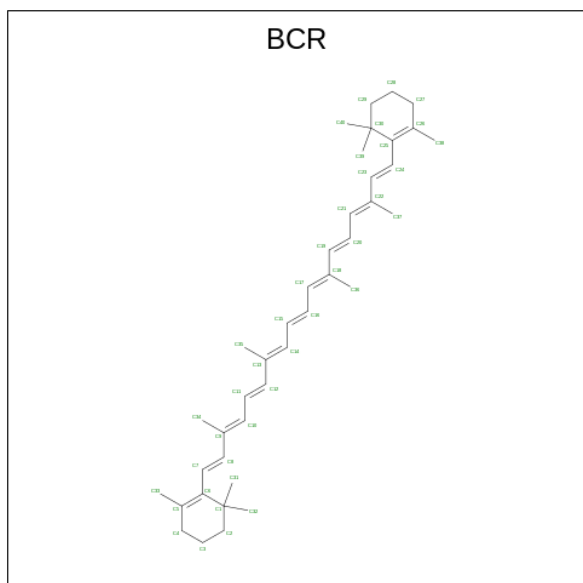
- Molecule 21 is a protein called Extrinsic protein in photosystem II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	q1	105	Total	C	N	O	S	0	0	0
			645	399	115	127	4			
21	Q2	111	Total	C	N	O	S	0	0	0
			676	417	123	133	3			

- Molecule 22 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	Z2	59	Total	C	N	O	S	0	0	0
			351	224	61	65	1			
22	z2	59	Total	C	N	O	S	0	0	0
			381	250	63	67	1			

- Molecule 23 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	A1	1	Total	C	0	0
			40	40		
23	B1	1	Total	C	0	0
			40	40		
23	B1	1	Total	C	0	0
			40	40		
23	B1	1	Total	C	0	0
			40	40		
23	C1	1	Total	C	0	0
			40	40		
23	C1	1	Total	C	0	0
			40	40		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	D1	1	Total C 40 40	0	0
23	H1	1	Total C 22 22	0	0
23	J1	1	Total C 40 40	0	0
23	K1	1	Total C 31 31	0	0
23	a1	1	Total C 40 40	0	0
23	b1	1	Total C 40 40	0	0
23	b1	1	Total C 40 40	0	0
23	b1	1	Total C 40 40	0	0
23	c1	1	Total C 40 40	0	0
23	c1	1	Total C 40 40	0	0
23	d1	1	Total C 40 40	0	0
23	h1	1	Total C 40 40	0	0
23	k1	1	Total C 40 40	0	0
23	A2	1	Total C 40 40	0	0
23	B2	1	Total C 40 40	0	0
23	B2	1	Total C 40 40	0	0
23	B2	1	Total C 40 40	0	0
23	C2	1	Total C 40 40	0	0
23	F2	1	Total C 40 40	0	0
23	H2	1	Total C 24 24	0	0
23	K2	1	Total C 40 40	0	0

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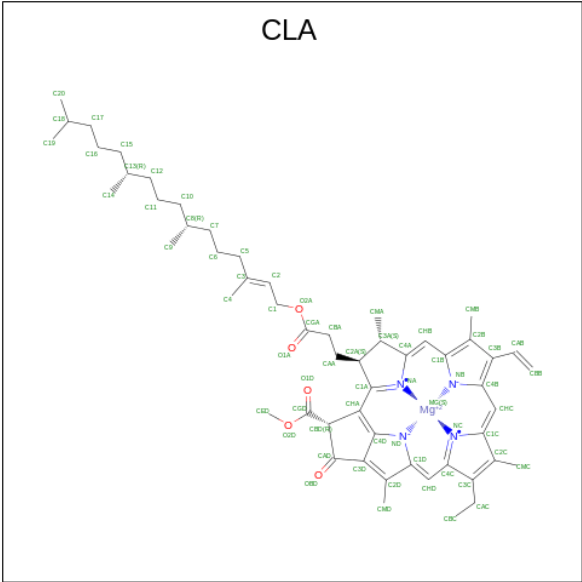
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	K2	1	Total C 29 29	0	0
23	a2	1	Total C 40 40	0	0
23	b2	1	Total C 40 40	0	0
23	b2	1	Total C 40 40	0	0
23	b2	1	Total C 40 40	0	0
23	c2	1	Total C 40 40	0	0
23	d2	1	Total C 40 40	0	0
23	h2	1	Total C 40 40	0	0
23	j2	1	Total C 40 40	0	0
23	k2	1	Total C 40 40	0	0
23	z2	1	Total C 40 40	0	0

- Molecule 24 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	A1	1	Total Cl 1 1	0	0
24	a1	1	Total Cl 1 1	0	0
24	A2	1	Total Cl 1 1	0	0
24	a2	1	Total Cl 1 1	0	0

- Molecule 25 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	A1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	A1	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
25	A1	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
25	A1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B1	1	Total	C	Mg	N	O	0	0
			42	34	1	4	3		
25	B1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B1	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
25	B1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B1	1	Total	C	Mg	N	O	0	0
			62	52	1	4	5		
25	B1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	B1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B1	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
25	B1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C1	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
25	C1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C1	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
25	C1	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
25	D1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	D1	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	a1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	a1	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
25	a1	1	Total 50	C 40	Mg 1	N 4	O 5	0	0
25	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b1	1	Total 59	C 49	Mg 1	N 4	O 5	0	0
25	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	c1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c1	1	Total 50	C 40	Mg 1	N 4	O 5	0	0
25	c1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c1	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
25	c1	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
25	c1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	d1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	d1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	d1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	A2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	A2	1	Total 61	C 51	Mg 1	N 4	O 5	0	0
25	A2	1	Total 51	C 41	Mg 1	N 4	O 5	0	0
25	B2	1	Total 41	C 33	Mg 1	N 4	O 3	0	0
25	B2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	B2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	B2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	B2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	B2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	B2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	B2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	B2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	B2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	B2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	B2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	B2	1	Total 54	C 44	Mg 1	N 4	O 5	0	0
25	B2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	B2	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
25	B2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	C2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	C2	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
25	C2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	C2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	C2	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
25	C2	1	Total 50	C 40	Mg 1	N 4	O 5	0	0
25	C2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	C2	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
25	C2	1	Total 50	C 40	Mg 1	N 4	O 5	0	0

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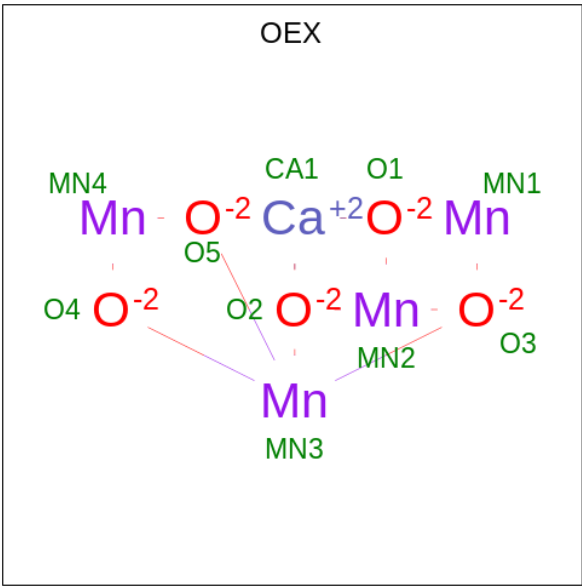
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	C2	1	Total 53	C 43	Mg 1	N 4	O 5	0	0
25	C2	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
25	C2	1	Total 41	C 33	Mg 1	N 4	O 3	0	0
25	D2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	D2	1	Total 61	C 51	Mg 1	N 4	O 5	0	0
25	D2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	K2	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
25	a2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	a2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	a2	1	Total 50	C 40	Mg 1	N 4	O 5	0	0
25	b2	1	Total 42	C 34	Mg 1	N 4	O 3	0	0
25	b2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b2	1	Total 61	C 51	Mg 1	N 4	O 5	0	0
25	b2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b2	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
25	b2	1	Total 60	C 50	Mg 1	N 4	O 5	0	0

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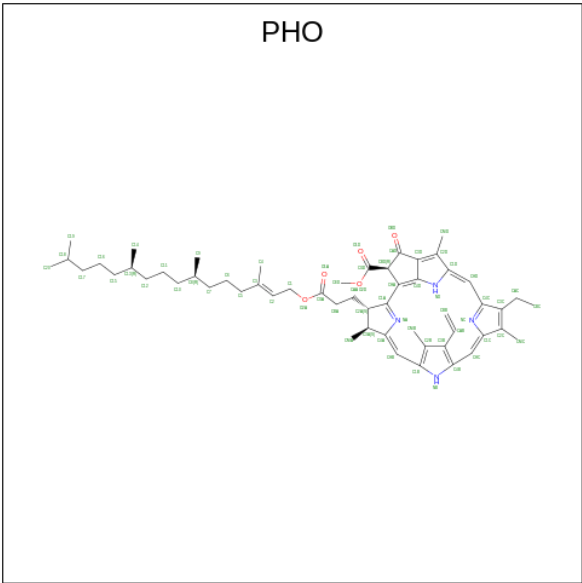
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	b2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b2	1	Total 59	C 49	Mg 1	N 4	O 5	0	0
25	b2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c2	1	Total 61	C 51	Mg 1	N 4	O 5	0	0
25	c2	1	Total 54	C 44	Mg 1	N 4	O 5	0	0
25	c2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c2	1	Total 54	C 44	Mg 1	N 4	O 5	0	0
25	c2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c2	1	Total 54	C 44	Mg 1	N 4	O 5	0	0
25	c2	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
25	d2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	d2	1	Total 50	C 40	Mg 1	N 4	O 5	0	0
25	d2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

- Molecule 26 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	A1	1	Total	Ca	Mn	O	0	0
			10	1	4	5		
26	a1	1	Total	Ca	Mn	O	0	0
			10	1	4	5		
26	A2	1	Total	Ca	Mn	O	0	0
			10	1	4	5		
26	a2	1	Total	Ca	Mn	O	0	0
			10	1	4	5		

- Molecule 27 is PHEOPHYTIN A (CCD ID: PHO) (formula: $\text{C}_{55}\text{H}_{74}\text{N}_4\text{O}_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	A1	1	Total	C	N	O	0	0
			64	55	4	5		
27	D1	1	Total	C	N	O	0	0
			63	54	4	5		
27	a1	1	Total	C	N	O	0	0
			64	55	4	5		
27	d1	1	Total	C	N	O	0	0
			64	55	4	5		
27	A2	1	Total	C	N	O	0	0
			64	55	4	5		
27	D2	1	Total	C	N	O	0	0
			64	55	4	5		
27	a2	1	Total	C	N	O	0	0
			64	55	4	5		
27	d2	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 28 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

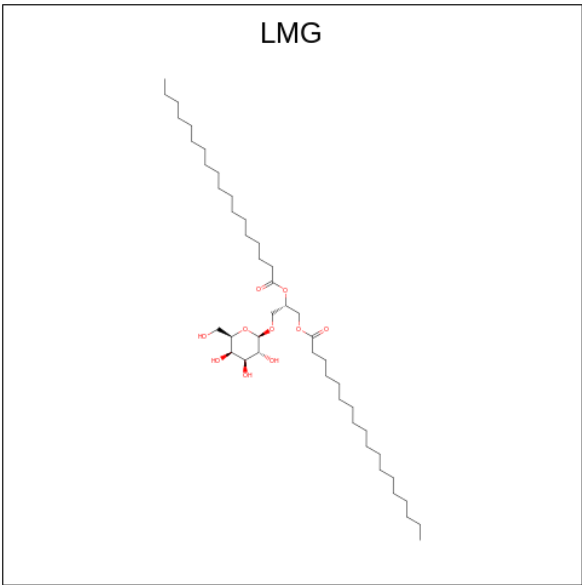
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	A1	1	Total	C	0	0
			14	14		
28	B1	3	Total	C	0	0
			41	41		
28	D1	1	Total	C	0	0
			6	6		
28	a1	1	Total	C	0	0
			11	11		
28	b1	7	Total	C	0	0
			92	92		
28	d1	1	Total	C	0	0
			12	12		
28	j1	1	Total	C	0	0
			17	17		
28	l1	1	Total	C	0	0
			12	12		
28	m1	1	Total	C	0	0
			6	6		
28	t1	2	Total	C	0	0
			27	27		
28	x1	1	Total	C	0	0
			15	15		
28	A2	2	Total	C	0	0
			28	28		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	B2	4	Total C 58 58	0	0
28	C2	2	Total C 24 24	0	0
28	F2	1	Total C 16 16	0	0
28	H2	1	Total C 5 5	0	0
28	I2	2	Total C 31 31	0	0
28	J2	1	Total C 10 10	0	0
28	K2	1	Total C 5 5	0	0
28	M2	1	Total C 11 11	0	0
28	X2	1	Total C 7 7	0	0
28	W2	1	Total C 9 9	0	0
28	a2	4	Total C 55 55	0	0
28	b2	1	Total C 12 12	0	0
28	c2	1	Total C 15 15	0	0
28	d2	2	Total C 25 25	0	0
28	i2	1	Total C 14 14	0	0
28	k2	4	Total C 30 30	0	0
28	m2	2	Total C 36 36	0	0

- Molecule 29 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	A1	1	Total	C	O	0	0
			43	33	10		
29	A1	1	Total	C	O	0	0
			41	31	10		
29	B1	1	Total	C	O	0	0
			31	21	10		
29	B1	1	Total	C	O	0	0
			48	38	10		
29	C1	1	Total	C	O	0	0
			48	38	10		
29	D1	1	Total	C	O	0	0
			35	25	10		
29	M1	1	Total	C	O	0	0
			31	27	4		
29	a1	1	Total	C	O	0	0
			51	41	10		
29	b1	1	Total	C	O	0	0
			38	28	10		
29	b1	1	Total	C	O	0	0
			39	29	10		
29	b1	1	Total	C	O	0	0
			40	30	10		
29	c1	1	Total	C	O	0	0
			55	45	10		
29	d1	1	Total	C	O	0	0
			33	23	10		
29	d1	1	Total	C	O	0	0
			35	30	5		

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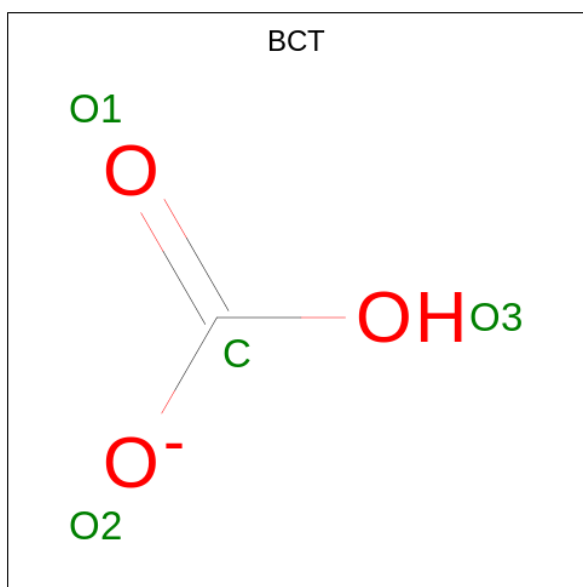
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	A2	1	Total	C	O	0	0
			29	19	10		
29	B2	1	Total	C	O	0	0
			40	30	10		
29	B2	1	Total	C	O	0	0
			37	27	10		
29	C2	1	Total	C	O	0	0
			24	14	10		
29	F2	1	Total	C	O	0	0
			35	25	10		
29	I2	1	Total	C	O	0	0
			34	24	10		
29	a2	1	Total	C	O	0	0
			44	34	10		
29	b2	1	Total	C	O	0	0
			39	29	10		
29	c2	1	Total	C	O	0	0
			26	16	10		
29	d2	1	Total	C	O	0	0
			27	17	10		
29	j2	1	Total	C	O	0	0
			50	40	10		

- Molecule 30 is FE (III) ION (CCD ID: FE) (formula: Fe).

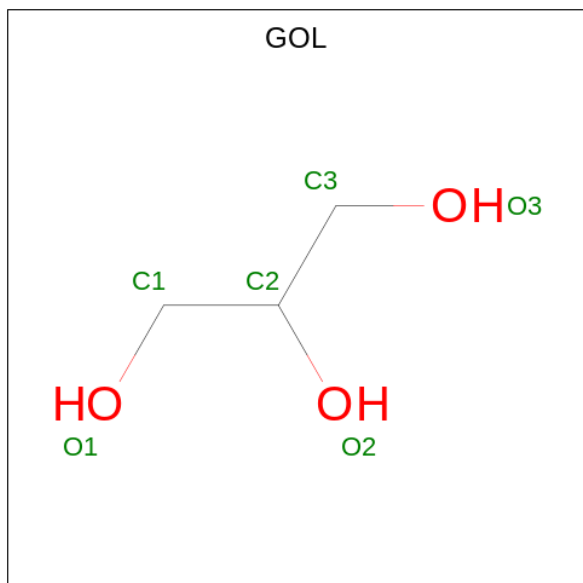
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	A1	1	Total	Fe	0	0
			1	1		
30	a1	1	Total	Fe	0	0
			1	1		
30	A2	1	Total	Fe	0	0
			1	1		
30	a2	1	Total	Fe	0	0
			1	1		

- Molecule 31 is BICARBONATE ION (CCD ID: BCT) (formula: CHO₃).



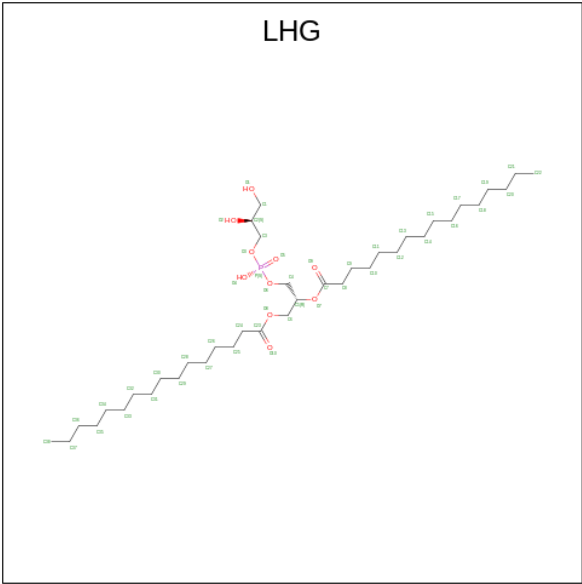
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	A1	1	Total	C	O	0	0
			4	1	3		
31	a1	1	Total	C	O	0	0
			4	1	3		
31	A2	1	Total	C	O	0	0
			4	1	3		
31	a2	1	Total	C	O	0	0
			4	1	3		

- Molecule 32 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	B1	1	Total	C	O	0	0
			6	3	3		
32	C1	1	Total	C	O	0	0
			6	3	3		
32	a1	1	Total	C	O	0	0
			6	3	3		
32	b1	1	Total	C	O	0	0
			6	3	3		
32	c1	1	Total	C	O	0	0
			6	3	3		
32	i1	1	Total	C	O	0	0
			6	3	3		
32	C2	1	Total	C	O	0	0
			6	3	3		
32	a2	1	Total	C	O	0	0
			6	3	3		
32	c2	1	Total	C	O	0	0
			6	3	3		

- Molecule 33 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



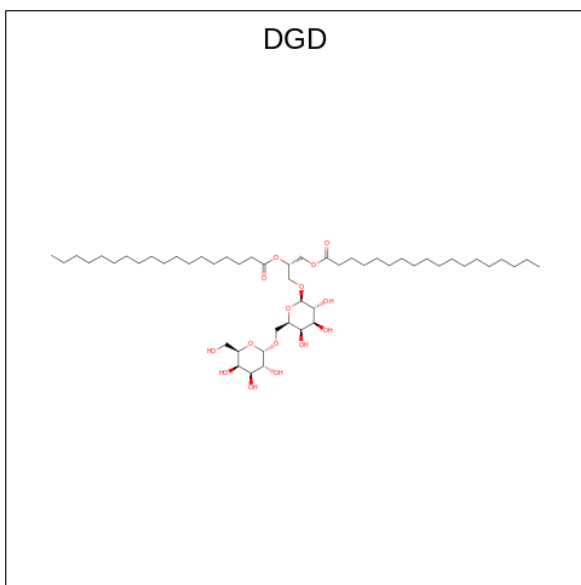
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	B1	1	Total	C	O	P	0	0
			49	38	10	1		
33	D1	1	Total	C	O	P	0	0
			49	38	10	1		

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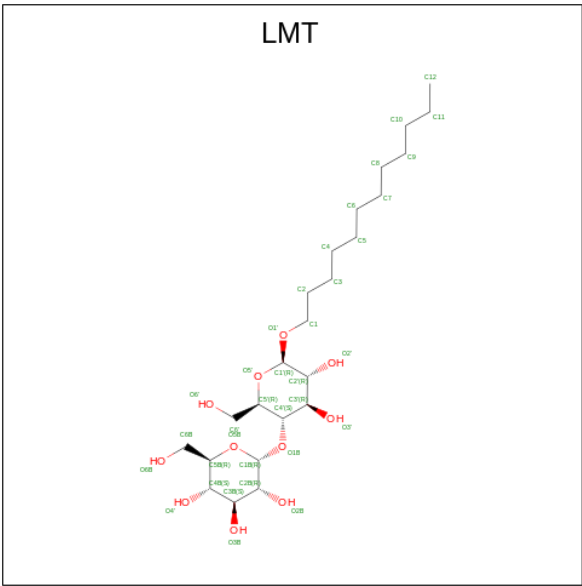
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	D1	1	Total	C	O	P	0	0
			49	38	10	1		
33	L1	1	Total	C	O	P	0	0
			41	30	10	1		
33	a1	1	Total	C	O	P	0	0
			43	32	10	1		
33	b1	1	Total	C	O	P	0	0
			49	38	10	1		
33	d1	1	Total	C	O	P	0	0
			32	21	10	1		
33	d1	1	Total	C	O	P	0	0
			49	38	10	1		
33	l1	1	Total	C	O	P	0	0
			49	38	10	1		
33	A2	1	Total	C	O	P	0	0
			33	22	10	1		
33	B2	1	Total	C	O	P	0	0
			42	31	10	1		
33	D2	1	Total	C	O	P	0	0
			49	38	10	1		
33	D2	1	Total	C	O	P	0	0
			49	38	10	1		
33	L2	1	Total	C	O	P	0	0
			49	38	10	1		
33	a2	1	Total	C	O	P	0	0
			30	19	10	1		
33	b2	1	Total	C	O	P	0	0
			43	32	10	1		
33	d2	1	Total	C	O	P	0	0
			49	38	10	1		
33	d2	1	Total	C	O	P	0	0
			49	38	10	1		
33	l2	1	Total	C	O	P	0	0
			44	33	10	1		

- Molecule 34 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	C1	1	Total	C	O	0	0
			52	37	15		
34	C1	1	Total	C	O	0	0
			62	47	15		
34	C1	1	Total	C	O	0	0
			64	49	15		
34	H1	1	Total	C	O	0	0
			62	47	15		
34	c1	1	Total	C	O	0	0
			51	36	15		
34	c1	1	Total	C	O	0	0
			62	47	15		
34	c1	1	Total	C	O	0	0
			62	47	15		
34	h1	1	Total	C	O	0	0
			62	47	15		
34	C2	1	Total	C	O	0	0
			33	18	15		
34	H2	1	Total	C	O	0	0
			62	47	15		
34	c2	1	Total	C	O	0	0
			62	47	15		
34	c2	1	Total	C	O	0	0
			52	37	15		
34	c2	1	Total	C	O	0	0
			62	47	15		
34	h2	1	Total	C	O	0	0
			62	47	15		

- Molecule 35 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



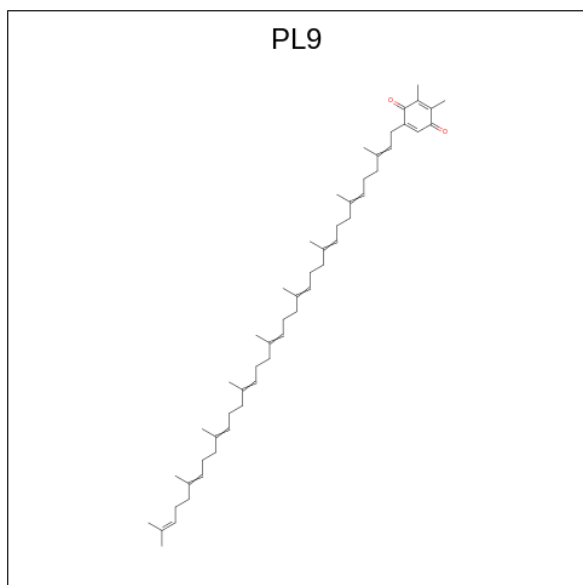
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	C1	1	Total C O 35 24 11	0	0
35	L1	1	Total C 12 12	0	0
35	M1	1	Total C 11 11	0	0
35	M1	1	Total C O 24 18 6	0	0
35	T1	1	Total C 12 12	0	0
35	c1	1	Total C O 33 22 11	0	0
35	l1	1	Total C O 24 18 6	0	0
35	m1	1	Total C O 35 24 11	0	0
35	a2	1	Total C O 35 24 11	0	0
35	b2	1	Total C O 35 24 11	0	0
35	b2	1	Total C O 35 24 11	0	0
35	i2	1	Total C 7 7	0	0
35	m2	1	Total C O 30 19 11	0	0

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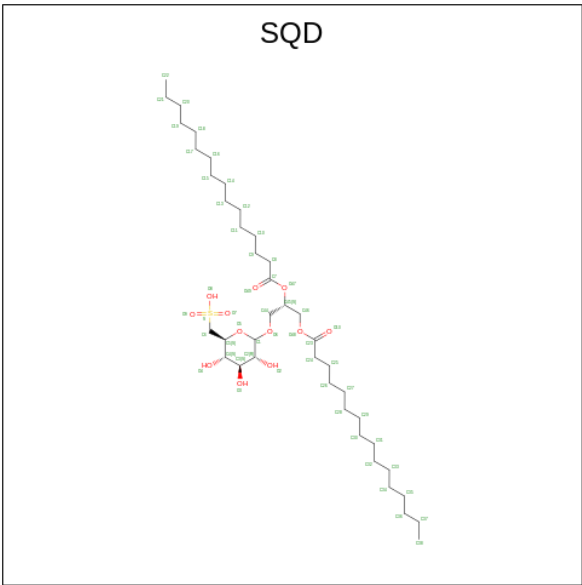
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
35	m2	1	Total	C	O	0	0
			29	18	11		

- Molecule 36 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: C₅₃H₈₀O₂).



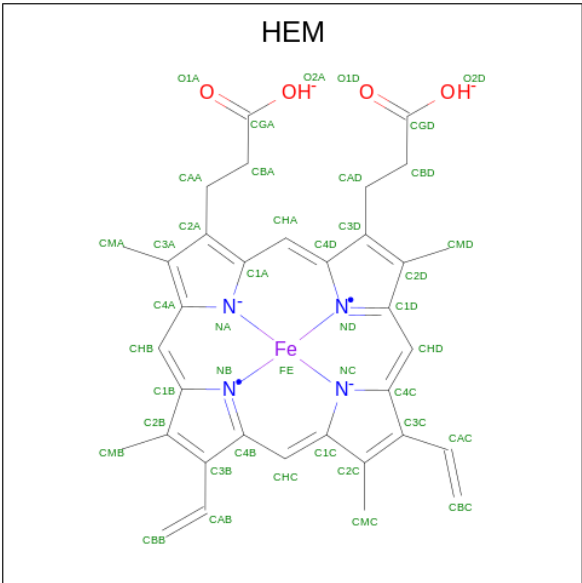
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
36	D1	1	Total	C	O	0	0
			55	53	2		
36	d1	1	Total	C	O	0	0
			55	53	2		
36	D2	1	Total	C	O	0	0
			55	53	2		
36	d2	1	Total	C	O	0	0
			55	53	2		

- Molecule 37 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
37	D1	1	Total	C	O	S	0	0
			35	22	12	1		
37	B2	1	Total	C	O	S	0	0
			45	32	12	1		
37	D2	1	Total	C	O	S	0	0
			25	12	12	1		
37	b2	1	Total	C	O	S	0	0
			45	32	12	1		

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
38	E1	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
38	V1	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
38	f1	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
38	v1	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
38	E2	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
38	V2	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
38	e2	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
38	v2	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 39 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	O1	1	Total 1	Ca 1	0	0
39	o2	1	Total 1	Ca 1	0	0

- Molecule 40 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	A1	2	Total 2	O 2	0	0
40	B1	1	Total 1	O 1	0	0
40	a1	4	Total 4	O 4	0	0
40	c1	2	Total 2	O 2	0	0
40	A2	2	Total 2	O 2	0	0
40	a2	4	Total 4	O 4	0	0
40	b2	1	Total 1	O 1	0	0
40	c2	1	Total 1	O 1	0	0

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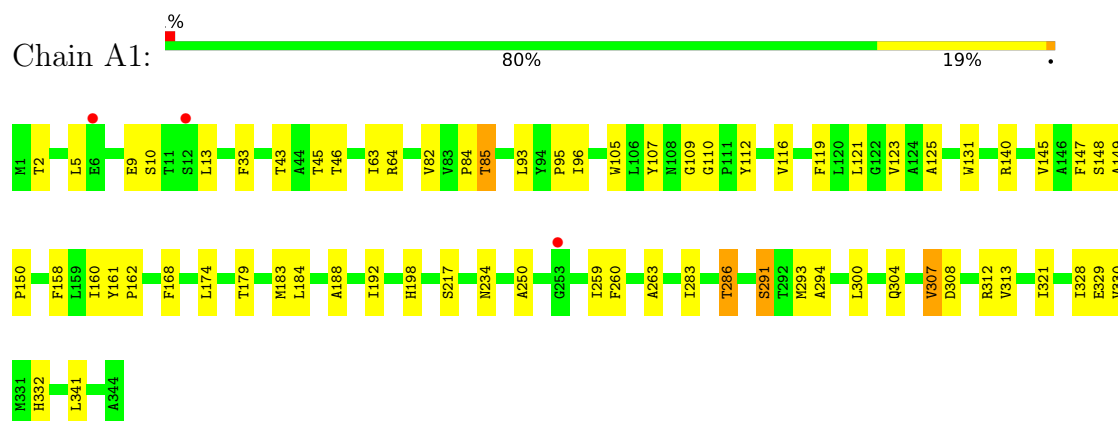
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	d2	1	Total	O	0	0
			1	1		

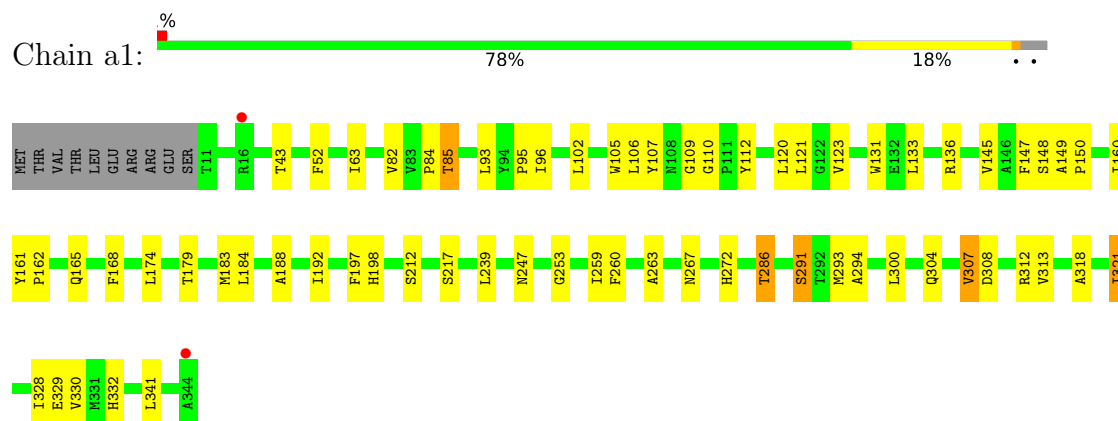
3 Residue-property plots

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.

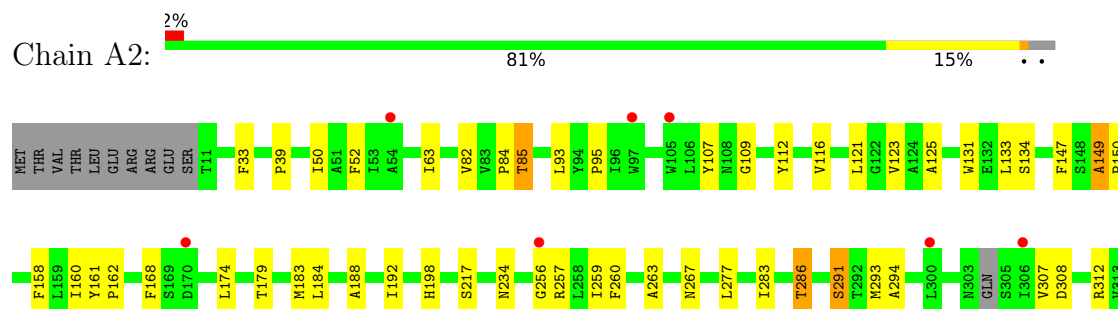
• Molecule 1: Photosystem II protein D1

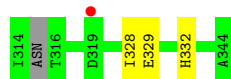


• Molecule 1: Photosystem II protein D1



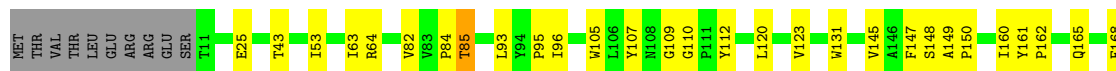
• Molecule 1: Photosystem II protein D1





- Molecule 1: Photosystem II protein D1

Chain a2: 80% 16% ..



- Molecule 2: Photosystem II CP47 reaction center protein

Chain B1: % 79% 14% 5%



- Molecule 2: Photosystem II CP47 reaction center protein

Chain b1: 83% 14% ..



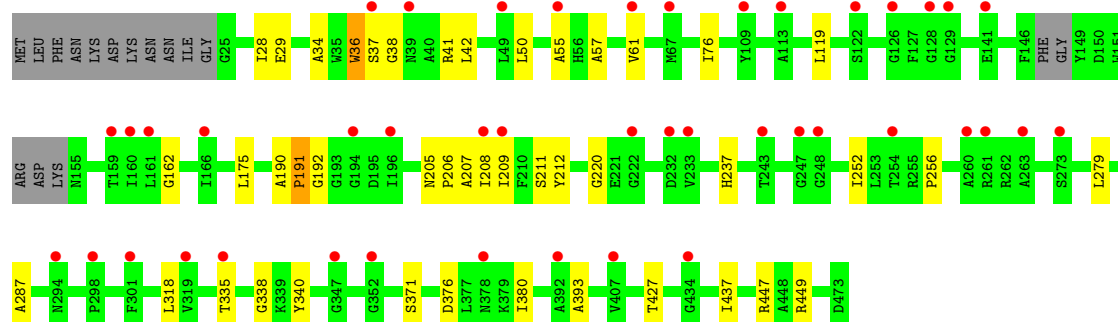
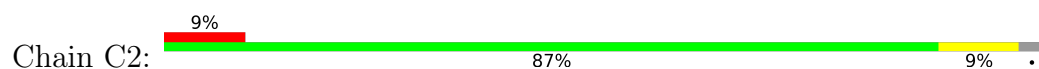
- Molecule 2: Photosystem II CP47 reaction center protein

Chain B2: 2% 84% 13% ..

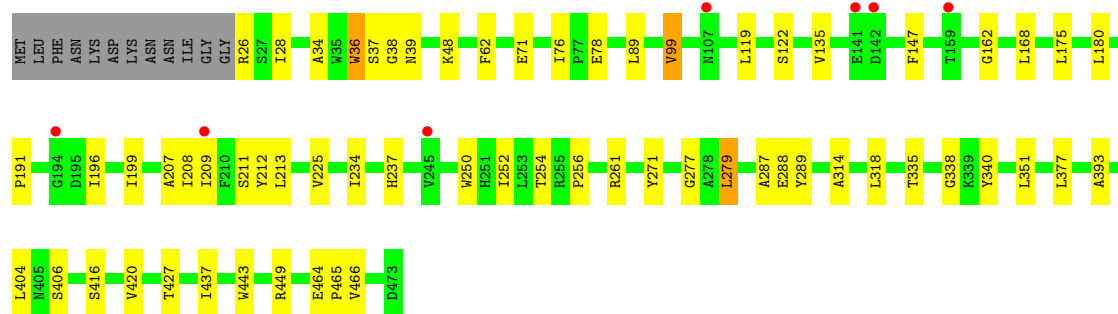
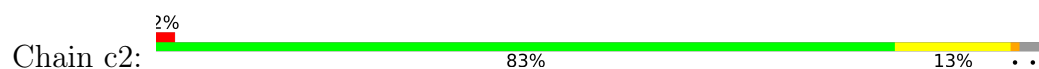




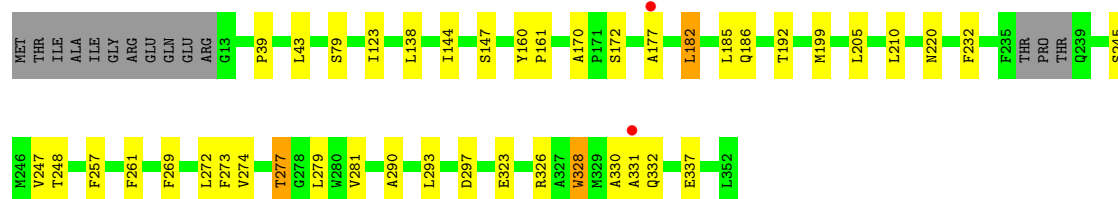
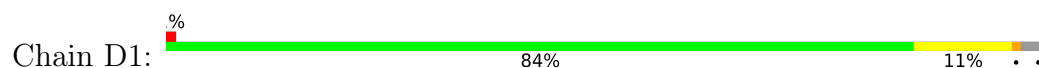
• Molecule 3: Photosystem II CP43 reaction center protein



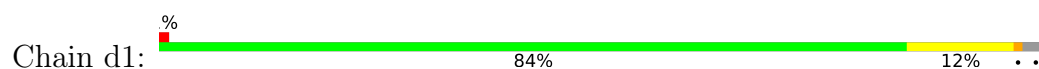
• Molecule 3: Photosystem II CP43 reaction center protein



• Molecule 4: Photosystem II D2 protein

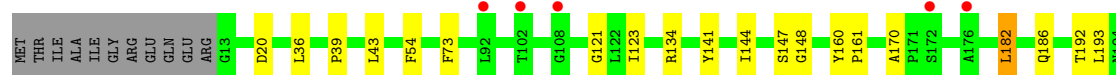
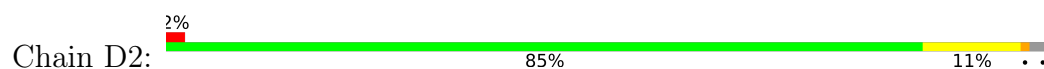


• Molecule 4: Photosystem II D2 protein

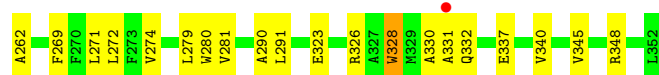
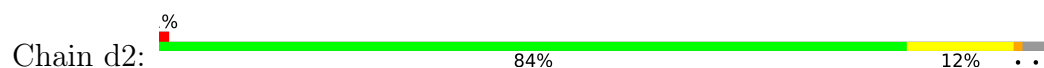




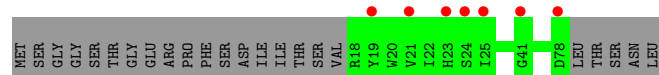
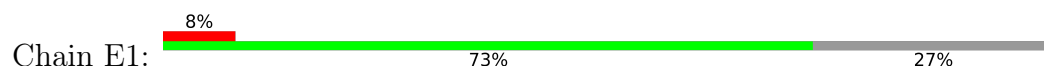
• Molecule 4: Photosystem II D2 protein



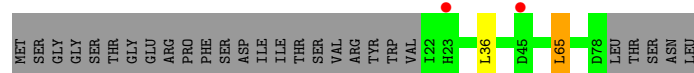
• Molecule 4: Photosystem II D2 protein



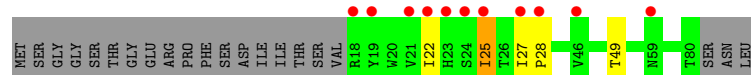
• Molecule 5: Cytochrome b559 subunit alpha



• Molecule 5: Cytochrome b559 subunit alpha

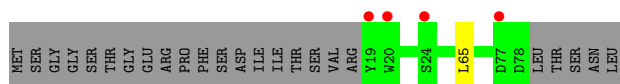


• Molecule 5: Cytochrome b559 subunit alpha

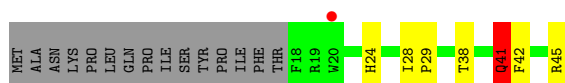


• Molecule 5: Cytochrome b559 subunit alpha





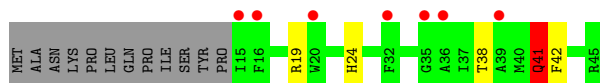
- Molecule 6: Cytochrome b559 subunit beta



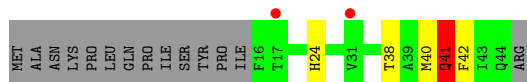
- Molecule 6: Cytochrome b559 subunit beta



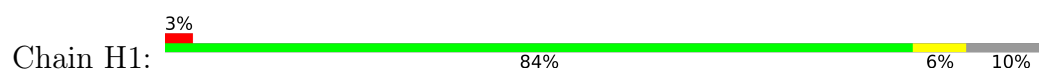
- Molecule 6: Cytochrome b559 subunit beta



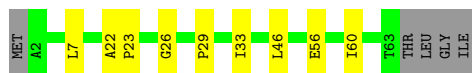
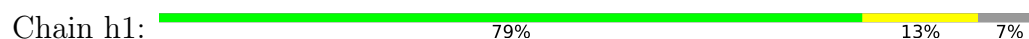
- Molecule 6: Cytochrome b559 subunit beta



- Molecule 7: Photosystem II reaction center protein H

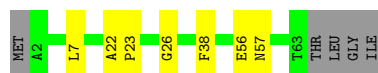


- Molecule 7: Photosystem II reaction center protein H



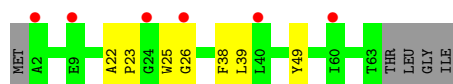
- Molecule 7: Photosystem II reaction center protein H

Chain H2:  82% 10% 7%



- Molecule 7: Photosystem II reaction center protein H

Chain h2:  9% 82% 10% 7%



- Molecule 8: Photosystem II reaction center protein I

Chain I1:  74% 16% 11%



- Molecule 8: Photosystem II reaction center protein I

Chain i1:  68% 21% 11%



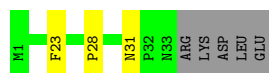
- Molecule 8: Photosystem II reaction center protein I

Chain I2:  3% 79% 13% 8%



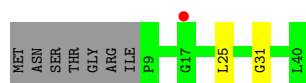
- Molecule 8: Photosystem II reaction center protein I

Chain i2:  79% 8% 13%



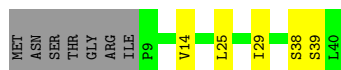
- Molecule 9: Photosystem II reaction center protein J

Chain J1:  3% 77% 5% 18%



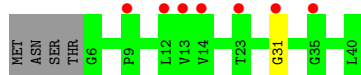
- Molecule 9: Photosystem II reaction center protein J

Chain j1:  69% 13% 18%



- Molecule 9: Photosystem II reaction center protein J

Chain J2:  18% 87% 10%



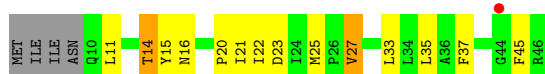
- Molecule 9: Photosystem II reaction center protein J

Chain j2:  3% 67% 15% 15%



- Molecule 10: Photosystem II reaction center protein K

Chain K1:  2% 56% 29% 5% 10%



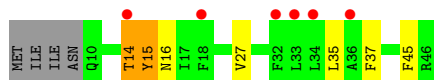
- Molecule 10: Photosystem II reaction center protein K

Chain k1:  61% 24% 5% 10%



- Molecule 10: Photosystem II reaction center protein K

Chain K2:  15% 73% 12% 5% 10%



- Molecule 10: Photosystem II reaction center protein K

Chain k2:  5% 61% 27% 10%



- Molecule 11: Photosystem II reaction center protein L

Chain L1:  74% 24% .



- Molecule 11: Photosystem II reaction center protein L

Chain l1:  71% 26% .



- Molecule 11: Photosystem II reaction center protein L

Chain L2:  74% 24% .



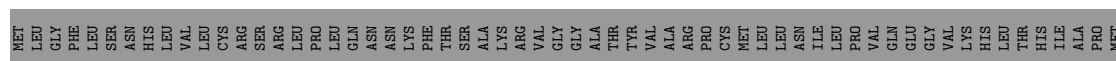
- Molecule 11: Photosystem II reaction center protein L

Chain l2:  71% 26% .



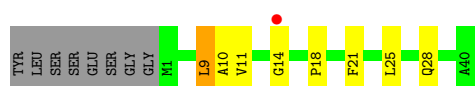
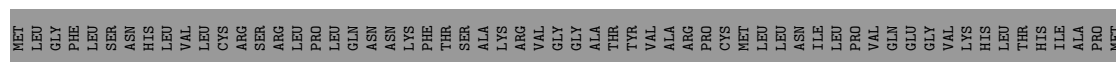
- Molecule 12: PHOTOSYSTEM II REACTION CENTER PROTEIN M

Chain M1:  27% 10% 63%



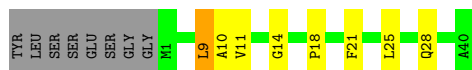
- Molecule 12: PHOTOSYSTEM II REACTION CENTER PROTEIN M

Chain m1:  30% 6% 63%

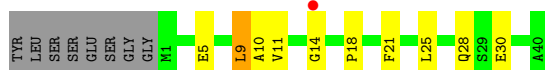


- Molecule 12: PHOTOSYSTEM II REACTION CENTER PROTEIN M

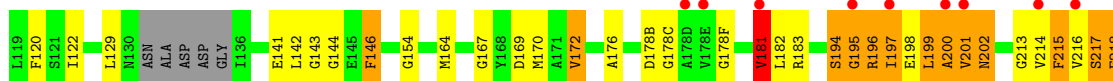
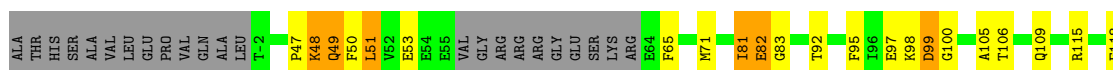
Chain M2:  30% 6% 63%



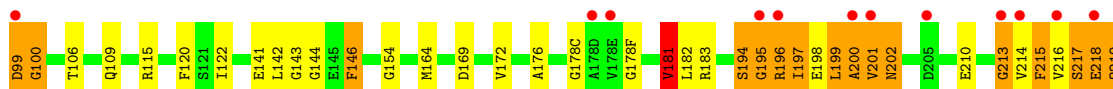
Chain m2: %



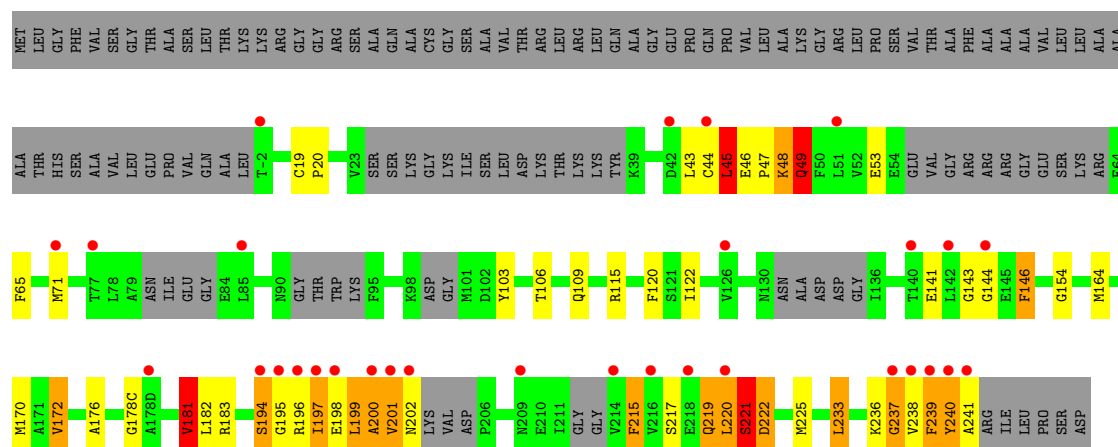
Chain O1:



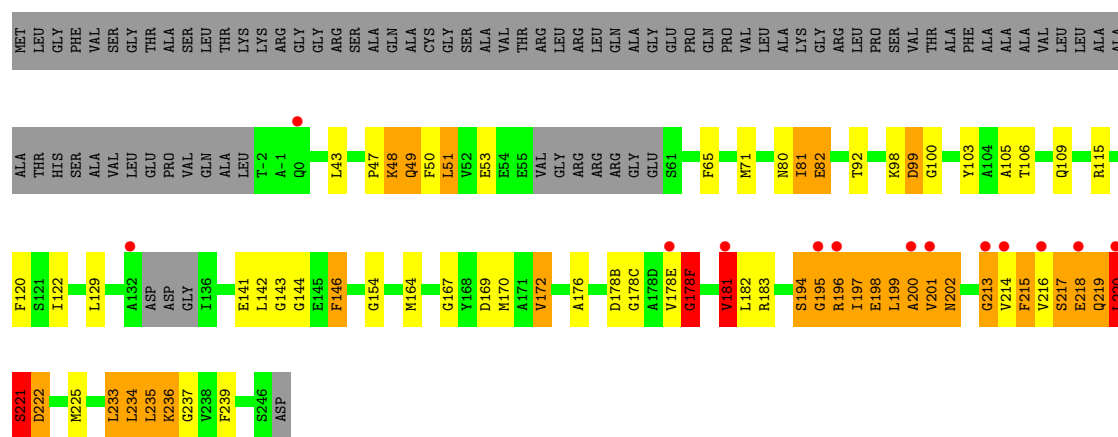
Chain 01: 5% 54% 9% 8% 28%



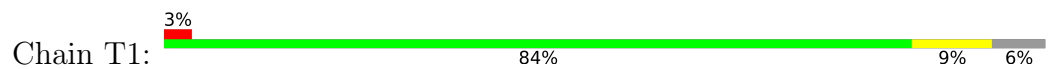
WORLDWIDE
PDB
PROTEIN DATA BANK



• Molecule 13: PHOTOSYSTEM II MANGANESE-STABILIZING POLYPEPTIDE, PSBO



• Molecule 14: Photosystem II reaction center protein T

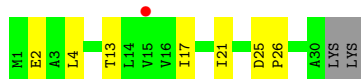


• Molecule 14: Photosystem II reaction center protein T



• Molecule 14: Photosystem II reaction center protein T





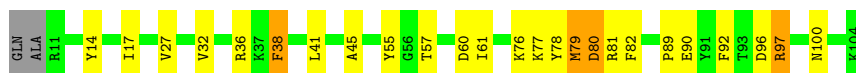
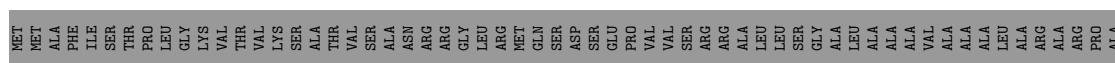
- Molecule 14: Photosystem II reaction center protein T

Chain t2: 72% 19% 9%



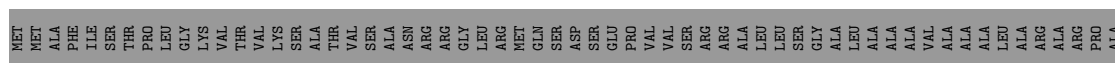
- Molecule 15: Photosystem II 12 kDa extrinsic protein, chloroplastic

Chain U1: 44% 14% 40%



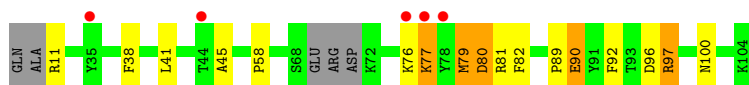
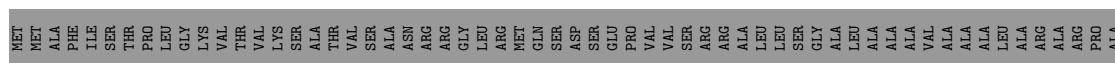
- Molecule 15: Photosystem II 12 kDa extrinsic protein, chloroplastic

Chain u1: 43% 15% 40%



- Molecule 15: Photosystem II 12 kDa extrinsic protein, chloroplastic

Chain U2: 3% 47% 8% 42%

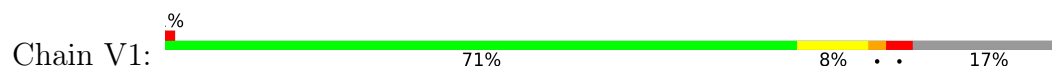


- Molecule 15: Photosystem II 12 kDa extrinsic protein, chloroplastic

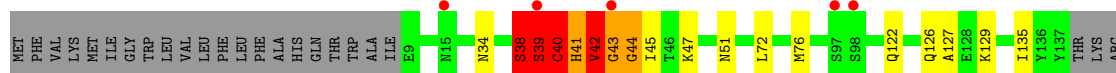
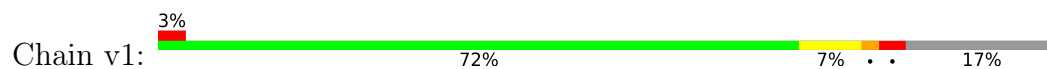
Chain u2: 39% 18% 40%



- Molecule 16: Cytochrome c-550

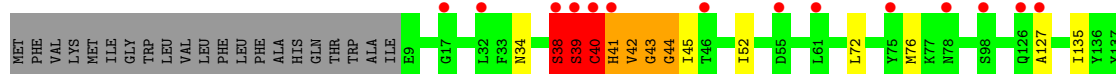
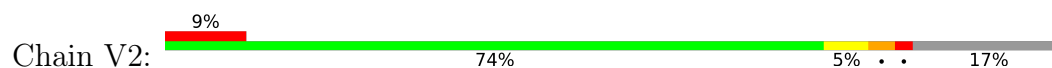


- Molecule 16: Cytochrome c-550



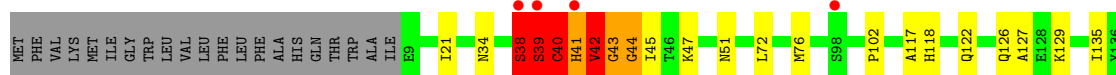
SER
MET

- Molecule 16: Cytochrome c-550



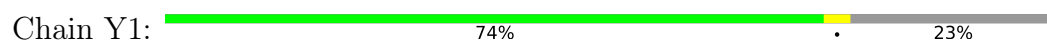
THR
LYS
ARG
SER
MET

- Molecule 16: Cytochrome c-550

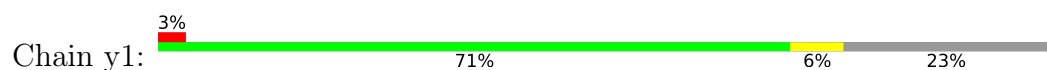


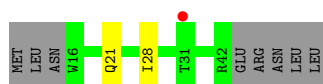
Y137
THR
LYS
ARG
SER
MET

- Molecule 17: Photosystem II reaction center protein Ycf12

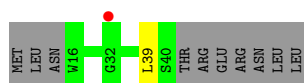


- Molecule 17: Photosystem II reaction center protein Ycf12





- Molecule 17: Photosystem II reaction center protein Ycf12



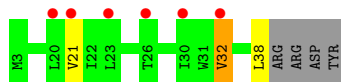
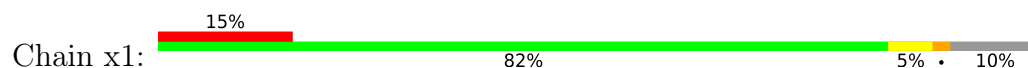
- Molecule 17: Photosystem II reaction center protein Ycf12



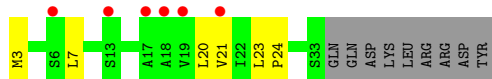
- Molecule 18: PHOTOSYSTEM II REACTION CENTER PROTEIN X



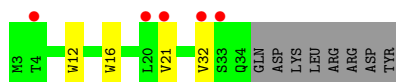
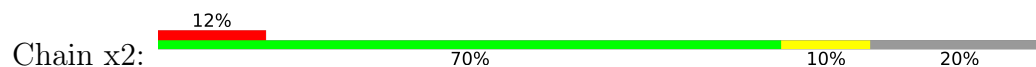
- Molecule 18: PHOTOSYSTEM II REACTION CENTER PROTEIN X



- Molecule 18: PHOTOSYSTEM II REACTION CENTER PROTEIN X

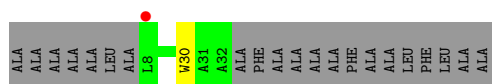


- Molecule 18: PHOTOSYSTEM II REACTION CENTER PROTEIN X

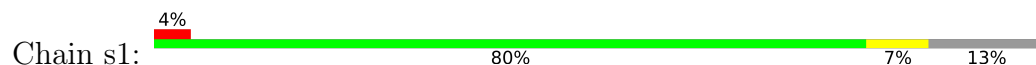


- Molecule 19: PEPTIDE CHAIN UNASSIGNED

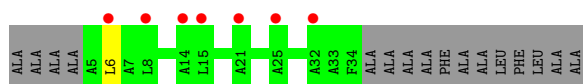




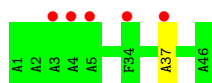
- Molecule 19: PEPTIDE CHAIN UNASSIGNED



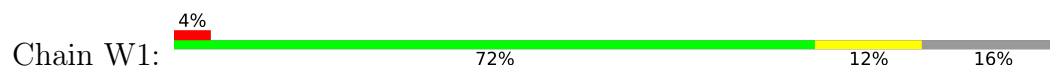
- Molecule 19: PEPTIDE CHAIN UNASSIGNED



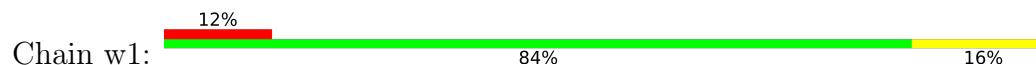
- Molecule 19: PEPTIDE CHAIN UNASSIGNED



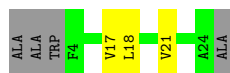
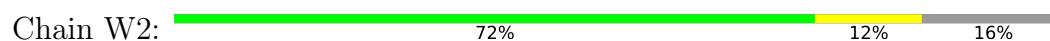
- Molecule 20: PEPTIDE CHAIN UNASSIGNED



- Molecule 20: PEPTIDE CHAIN UNASSIGNED

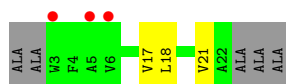


- Molecule 20: PEPTIDE CHAIN UNASSIGNED

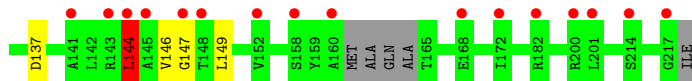
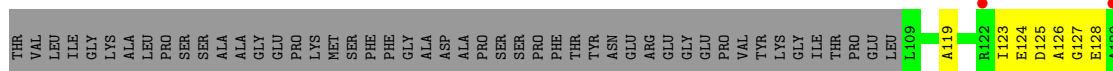
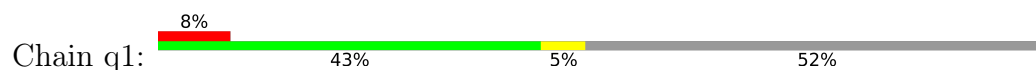


- Molecule 20: PEPTIDE CHAIN UNASSIGNED

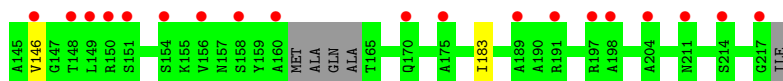
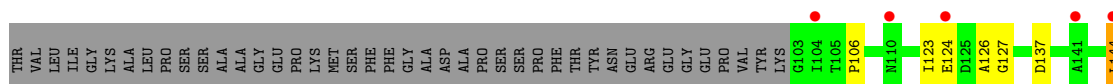




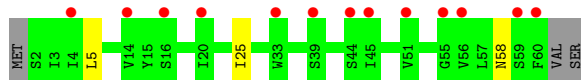
- Molecule 21: Extrinsic protein in photosystem II



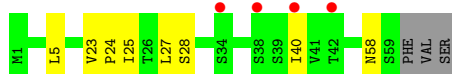
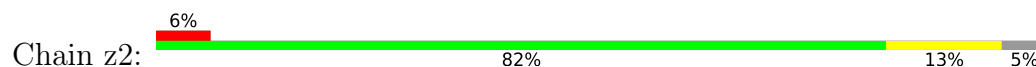
- Molecule 21: Extrinsic protein in photosystem II



- Molecule 22: Photosystem II reaction center protein Z



- Molecule 22: 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	210.44Å 240.31Å 300.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.77 10.00 – 2.77	Depositor EDS
% Data completeness (in resolution range)	99.7 (10.00-2.77) 97.5 (10.00-2.77)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 2.76Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.249 , 0.278 0.255 , 0.282	Depositor DCC
R_{free} test set	19164 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	68.0	Xtriage
Anisotropy	0.616	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 78.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	92765	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.84% 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: HEM, BCT, CA, PL9, PHO, OEX, UNL, FE, SQD, LMT, CLA, GOL, BCR, LHG, DGD, CL, LMG

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	A1	0.38	0/2685	0.77	1/3673 (0.0%)
1	A2	0.40	1/2548 (0.0%)	0.77	0/3481
1	a1	0.37	0/2642	0.76	0/3612
1	a2	0.37	0/2586	0.76	0/3538
2	B1	0.41	2/3830 (0.1%)	0.83	6/5227 (0.1%)
2	B2	0.41	2/3897 (0.1%)	0.83	6/5323 (0.1%)
2	b1	0.46	3/4015 (0.1%)	0.83	9/5473 (0.2%)
2	b2	0.41	2/3808 (0.1%)	0.83	6/5197 (0.1%)
3	C1	0.35	0/3501	0.77	2/4782 (0.0%)
3	C2	0.34	0/3242	0.79	2/4441 (0.0%)
3	c1	0.38	2/3555 (0.1%)	0.77	4/4850 (0.1%)
3	c2	0.34	0/3495	0.77	2/4773 (0.0%)
4	D1	0.44	1/2704 (0.0%)	0.77	2/3688 (0.1%)
4	D2	0.44	1/2675 (0.0%)	0.78	4/3655 (0.1%)
4	d1	0.44	1/2772 (0.0%)	0.78	2/3783 (0.1%)
4	d2	0.44	1/2736 (0.0%)	0.77	2/3734 (0.1%)
5	E1	0.33	0/418	0.74	0/577
5	E2	0.34	0/443	0.73	0/614
5	e1	0.32	0/440	0.69	0/603
5	e2	0.32	0/434	0.72	0/598
6	F1	0.67	0/220	0.95	3/299 (1.0%)
6	F2	0.61	0/236	0.95	3/320 (0.9%)
6	f1	0.64	0/235	0.92	3/319 (0.9%)
6	f2	0.63	0/234	0.92	3/318 (0.9%)
7	H1	0.29	0/443	0.70	0/606
7	H2	0.30	0/453	0.72	0/619
7	h1	0.29	0/481	0.71	0/657
7	h2	0.28	0/461	0.70	0/631
8	I1	0.30	0/283	0.68	0/381
8	I2	0.30	0/273	0.71	0/371
8	i1	0.29	0/289	0.69	0/389

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
8	i2	0.30	0/270	0.71	0/364
9	J1	0.27	0/225	0.70	0/307
9	J2	0.26	0/236	0.72	0/324
9	j1	0.26	0/229	0.70	0/313
9	j2	0.27	0/233	0.82	2/319 (0.6%)
10	K1	0.50	0/289	0.84	0/399
10	K2	0.54	0/258	0.87	0/359
10	k1	0.50	0/290	0.85	0/401
10	k2	0.53	0/278	0.85	0/385
11	L1	0.66	0/301	0.88	0/410
11	L2	0.64	0/308	0.87	0/419
11	l1	0.65	0/308	0.88	0/418
11	l2	0.65	0/308	0.87	0/418
12	M1	0.49	0/288	0.93	0/391
12	M2	0.48	0/287	0.93	0/390
12	m1	0.48	0/288	0.92	0/391
12	m2	0.46	0/290	0.93	0/394
13	O1	0.98	15/1700 (0.9%)	1.46	35/2315 (1.5%)
13	O2	0.89	9/1387 (0.6%)	1.35	27/1881 (1.4%)
13	o1	0.94	13/1716 (0.8%)	1.41	38/2330 (1.6%)
13	o2	0.95	14/1794 (0.8%)	1.46	40/2434 (1.6%)
14	T1	0.28	0/248	0.78	0/337
14	T2	0.28	0/247	0.77	0/337
14	t1	0.29	0/253	0.77	0/344
14	t2	0.29	0/242	0.77	0/330
15	U1	0.63	1/709 (0.1%)	1.03	7/970 (0.7%)
15	U2	0.67	2/588 (0.3%)	1.25	10/809 (1.2%)
15	u1	0.63	1/721 (0.1%)	1.02	5/981 (0.5%)
15	u2	0.62	2/726 (0.3%)	1.00	5/988 (0.5%)
16	V1	0.66	3/937 (0.3%)	0.98	8/1281 (0.6%)
16	V2	0.68	3/858 (0.3%)	0.98	8/1177 (0.7%)
16	v1	0.64	2/941 (0.2%)	0.98	8/1284 (0.6%)
16	v2	0.63	2/983 (0.2%)	0.96	8/1337 (0.6%)
17	Y1	0.61	0/171	1.00	0/236
17	Y2	0.62	0/159	1.05	0/219
17	y1	0.58	0/198	0.93	0/274
17	y2	0.59	0/191	0.98	0/264
18	X1	0.37	0/202	0.80	1/278 (0.4%)
18	X2	0.35	0/222	0.82	1/307 (0.3%)
18	x1	0.41	0/262	0.80	1/363 (0.3%)
18	x2	0.44	0/225	0.88	1/312 (0.3%)
19	S1	0.32	0/167	0.65	0/231
19	S2	0.32	0/194	0.66	0/268

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
19	s1	0.32	0/269	0.63	0/371
19	s2	0.33	0/285	0.68	0/395
20	W1	0.34	0/134	0.77	0/186
20	W2	0.35	0/129	0.81	0/179
20	w1	0.34	0/152	0.77	0/211
20	w2	0.32	0/127	0.79	0/176
21	Q2	0.55	1/682 (0.1%)	0.85	0/937
21	q1	0.55	1/650 (0.2%)	0.84	0/893
22	Z2	0.33	0/353	0.81	0/487
22	z2	0.34	0/387	0.77	0/532
All	All	0.50	85/79929 (0.1%)	0.88	265/109188 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
13	O1	0	2
13	O2	0	4
13	o1	0	3
13	o2	0	3
16	V1	0	3
16	V2	0	3
16	v1	0	3
16	v2	0	3
All	All	0	24

The worst 5 of 85 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	V2	42	VAL	CA-C	-11.01	1.38	1.52
13	O1	220	LEU	N-CA	10.34	1.57	1.45
13	o2	220	LEU	N-CA	10.33	1.57	1.45
13	o1	220	LEU	N-CA	10.19	1.57	1.45
13	O1	221	SER	N-CA	9.74	1.58	1.46

The worst 5 of 265 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	O1	219	GLN	N-CA-C	12.94	128.74	109.07
13	o2	219	GLN	N-CA-C	12.93	128.73	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	o1	219	GLN	N-CA-C	12.60	128.22	109.07
13	O1	215	PHE	CA-C-N	-12.49	102.53	122.64
13	O1	215	PHE	C-N-CA	-12.49	102.53	122.64

There are no chirality outliers.

5 of 24 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	O1	194	SER	Peptide
13	O1	220	LEU	Peptide
16	V1	38	SER	Peptide
16	V1	41	HIS	Peptide
16	V1	44	GLY	Peptide

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	A1	2609	0	2500	51	0
1	A2	2475	0	2296	41	0
1	a1	2564	0	2462	54	0
1	a2	2513	0	2376	46	0
2	B1	3703	0	3485	59	0
2	B2	3770	0	3462	47	0
2	b1	3881	0	3672	64	0
2	b2	3681	0	3452	59	0
3	C1	3392	0	3206	54	0
3	C2	3145	0	2751	34	0
3	c1	3439	0	3293	57	0
3	c2	3386	0	3189	50	0
4	D1	2615	0	2465	42	0
4	D2	2585	0	2371	41	0
4	d1	2678	0	2544	39	0
4	d2	2643	0	2489	40	0
5	E1	405	0	304	0	0
5	E2	430	0	345	3	0
5	e1	427	0	374	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	e2	421	0	354	0	0
6	F1	213	0	198	5	0
6	F2	229	0	204	5	0
6	f1	227	0	221	4	0
6	f2	225	0	205	4	0
7	H1	433	0	407	3	0
7	H2	443	0	414	4	0
7	h1	470	0	474	4	0
7	h2	450	0	432	5	0
8	I1	274	0	262	4	0
8	I2	265	0	236	4	0
8	i1	280	0	276	6	0
8	i2	261	0	238	1	0
9	J1	220	0	209	2	0
9	J2	231	0	208	1	0
9	j1	224	0	223	4	0
9	j2	228	0	220	6	0
10	K1	279	0	268	15	0
10	K2	250	0	218	6	0
10	k1	280	0	280	12	0
10	k2	269	0	252	10	0
11	L1	292	0	284	8	0
11	L2	299	0	297	11	0
11	l1	299	0	304	9	0
11	l2	299	0	294	12	0
12	M1	285	0	295	10	0
12	M2	284	0	296	9	0
12	m1	285	0	295	7	0
12	m2	287	0	298	9	0
13	O1	1674	0	1534	65	0
13	O2	1376	0	1198	57	0
13	o1	1692	0	1547	60	0
13	o2	1768	0	1663	71	0
14	T1	241	0	248	3	0
14	T2	240	0	253	6	0
14	t1	246	0	264	5	0
14	t2	235	0	248	4	0
15	U1	691	0	628	14	0
15	U2	577	0	435	10	0
15	u1	703	0	645	15	0
15	u2	708	0	671	19	0
16	V1	917	0	847	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	V2	845	0	719	15	0
16	v1	921	0	842	17	0
16	v2	963	0	937	22	0
17	Y1	170	0	141	1	0
17	Y2	159	0	148	1	0
17	y1	195	0	194	2	0
17	y2	188	0	174	7	0
18	X1	197	0	192	1	0
18	X2	215	0	197	3	0
18	x1	255	0	245	2	0
18	x2	218	0	191	1	0
19	S1	164	0	161	1	0
19	S2	191	0	184	1	0
19	s1	263	0	260	3	0
19	s2	281	0	276	1	0
20	W1	134	0	149	2	0
20	W2	129	0	136	3	0
20	w1	152	0	165	5	0
20	w2	127	0	137	2	0
21	Q2	676	0	484	4	0
21	q1	645	0	462	7	0
22	Z2	351	0	280	2	0
22	z2	381	0	335	6	0
23	A1	40	0	56	4	0
23	A2	40	0	56	6	0
23	B1	120	0	168	12	0
23	B2	120	0	168	13	0
23	C1	80	0	112	7	0
23	C2	40	0	56	3	0
23	D1	40	0	56	3	0
23	F2	40	0	56	4	0
23	H1	22	0	29	3	0
23	H2	24	0	30	4	0
23	J1	40	0	56	6	0
23	K1	31	0	40	4	0
23	K2	69	0	97	8	0
23	a1	40	0	56	7	0
23	a2	40	0	56	4	0
23	b1	120	0	168	10	0
23	b2	120	0	168	15	0
23	c1	80	0	112	11	0
23	c2	40	0	56	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	d1	40	0	56	4	0
23	d2	40	0	56	4	0
23	h1	40	0	56	3	0
23	h2	40	0	56	3	0
23	j2	40	0	56	9	0
23	k1	40	0	56	6	0
23	k2	40	0	56	8	0
23	z2	40	0	56	5	0
24	A1	1	0	0	0	0
24	A2	1	0	0	0	0
24	a1	1	0	0	0	0
24	a2	1	0	0	0	0
25	A1	236	0	234	16	0
25	A2	177	0	174	17	0
25	B1	1002	0	1072	45	0
25	B2	1000	0	1072	37	0
25	C1	816	0	873	34	0
25	C2	636	0	572	15	0
25	D1	116	0	113	3	0
25	D2	191	0	205	10	0
25	K2	55	0	49	4	0
25	a1	175	0	170	13	0
25	a2	180	0	183	9	0
25	b1	1034	0	1138	34	0
25	b2	997	0	1060	41	0
25	c1	815	0	867	36	0
25	c2	789	0	814	35	0
25	d1	195	0	216	16	0
25	d2	180	0	183	7	0
26	A1	10	0	0	0	0
26	A2	10	0	0	0	0
26	a1	10	0	0	0	0
26	a2	10	0	0	0	0
27	A1	64	0	74	2	0
27	A2	64	0	74	2	0
27	D1	63	0	70	1	0
27	D2	64	0	74	3	0
27	a1	64	0	74	4	0
27	a2	64	0	74	3	0
27	d1	64	0	74	2	0
27	d2	64	0	74	1	0
28	A1	14	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	A2	28	0	0	0	0
28	B1	41	0	0	0	0
28	B2	58	0	0	0	0
28	C2	24	0	0	1	0
28	D1	6	0	0	0	0
28	F2	16	0	0	0	0
28	H2	5	0	0	0	0
28	I2	31	0	0	0	0
28	J2	10	0	0	0	0
28	K2	5	0	0	0	0
28	M2	11	0	0	0	0
28	W2	9	0	0	0	0
28	X2	7	0	0	0	0
28	a1	11	0	0	0	0
28	a2	55	0	0	0	0
28	b1	92	0	0	0	0
28	b2	12	0	0	0	0
28	c2	15	0	0	0	0
28	d1	12	0	0	0	0
28	d2	25	0	0	0	0
28	i2	14	0	0	0	0
28	j1	17	0	0	0	0
28	k2	30	0	0	0	0
28	l1	12	0	0	0	0
28	m1	6	0	0	0	0
28	m2	36	0	0	0	0
28	t1	27	0	0	0	0
28	x1	15	0	0	0	0
29	A1	84	0	108	6	0
29	A2	29	0	28	1	0
29	B1	79	0	98	3	0
29	B2	77	0	94	3	0
29	C1	48	0	66	1	0
29	C2	24	0	18	0	0
29	D1	35	0	40	1	0
29	F2	35	0	40	1	0
29	I2	34	0	38	2	0
29	M1	31	0	43	2	0
29	a1	51	0	72	6	0
29	a2	44	0	58	0	0
29	b1	117	0	144	14	0
29	b2	39	0	48	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	c1	55	0	86	1	0
29	c2	26	0	24	0	0
29	d1	68	0	85	1	0
29	d2	27	0	24	2	0
29	j2	50	0	73	6	0
30	A1	1	0	0	0	0
30	A2	1	0	0	0	0
30	a1	1	0	0	0	0
30	a2	1	0	0	0	0
31	A1	4	0	0	0	0
31	A2	4	0	0	0	0
31	a1	4	0	0	0	0
31	a2	4	0	0	0	0
32	B1	6	0	8	0	0
32	C1	6	0	8	0	0
32	C2	6	0	8	0	0
32	a1	6	0	8	0	0
32	a2	6	0	8	0	0
32	b1	6	0	8	0	0
32	c1	6	0	8	0	0
32	c2	6	0	8	0	0
32	i1	6	0	8	1	0
33	A2	33	0	36	3	0
33	B1	49	0	74	8	0
33	B2	42	0	57	2	0
33	D1	98	0	148	10	0
33	D2	98	0	148	16	0
33	L1	41	0	55	1	0
33	L2	49	0	74	5	0
33	a1	43	0	59	3	0
33	a2	30	0	32	4	0
33	b1	49	0	74	4	0
33	b2	43	0	56	0	0
33	d1	81	0	108	6	0
33	d2	98	0	148	9	0
33	l1	49	0	74	3	0
33	l2	44	0	61	5	0
34	C1	178	0	233	10	0
34	C2	33	0	26	0	0
34	H1	62	0	82	1	0
34	H2	62	0	82	3	0
34	c1	175	0	224	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	c2	176	0	226	6	0
34	h1	62	0	82	4	0
34	h2	62	0	82	5	0
35	C1	35	0	46	1	0
35	L1	12	0	23	1	0
35	M1	35	0	56	1	0
35	T1	12	0	23	0	0
35	a2	35	0	46	2	0
35	b2	70	0	92	2	0
35	c1	33	0	39	0	0
35	i2	7	0	10	0	0
35	l1	24	0	35	1	0
35	m1	35	0	46	1	0
35	m2	59	0	64	3	0
36	D1	55	0	80	9	0
36	D2	55	0	80	11	0
36	d1	55	0	80	12	0
36	d2	55	0	80	7	0
37	B2	45	0	57	2	0
37	D1	35	0	34	1	0
37	D2	25	0	15	0	0
37	b2	45	0	54	2	0
38	E1	43	0	30	3	0
38	E2	43	0	30	4	0
38	V1	43	0	30	3	0
38	V2	43	0	30	4	0
38	e2	43	0	30	3	0
38	f1	43	0	30	3	0
38	v1	43	0	30	3	0
38	v2	43	0	30	3	0
39	O1	1	0	0	0	0
39	o2	1	0	0	0	0
40	A1	2	0	0	0	0
40	A2	2	0	0	0	0
40	B1	1	0	0	0	0
40	a1	4	0	0	1	0
40	a2	4	0	0	2	0
40	b2	1	0	0	0	0
40	c1	2	0	0	1	0
40	c2	1	0	0	1	0
40	d2	1	0	0	0	0
All	All	92765	0	88715	1661	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 1661 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)
13:O2:44:CYS:O	13:O2:240:TYR:N	1.70	1.25
23:c2:501:BCR:H361	23:c2:501:BCR:H21C	1.37	1.06
13:O2:201:VAL:HG12	13:O2:202:ASN:H	1.31	0.92
13:o1:195:GLY:CA	13:o1:220:LEU:H	1.86	0.89
13:O1:195:GLY:CA	13:O1:220:LEU:H	1.86	0.87

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	A1	342/344 (99%)	328 (96%)	14 (4%)	0	100	100
1	A2	327/344 (95%)	318 (97%)	9 (3%)	0	100	100
1	a1	332/344 (96%)	323 (97%)	9 (3%)	0	100	100
1	a2	332/344 (96%)	323 (97%)	9 (3%)	0	100	100
2	B1	481/509 (94%)	456 (95%)	23 (5%)	2 (0%)	30	57
2	B2	501/509 (98%)	474 (95%)	26 (5%)	1 (0%)	43	70
2	b1	502/509 (99%)	474 (94%)	26 (5%)	2 (0%)	30	57
2	b2	479/509 (94%)	454 (95%)	23 (5%)	2 (0%)	30	57
3	C1	447/460 (97%)	424 (95%)	20 (4%)	3 (1%)	18	44
3	C2	438/460 (95%)	416 (95%)	19 (4%)	3 (1%)	18	44
3	c1	449/460 (98%)	426 (95%)	19 (4%)	4 (1%)	14	37
3	c2	446/460 (97%)	424 (95%)	19 (4%)	3 (1%)	18	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D1	333/351 (95%)	318 (96%)	15 (4%)	0	100	100
4	D2	338/351 (96%)	322 (95%)	16 (5%)	0	100	100
4	d1	337/351 (96%)	321 (95%)	16 (5%)	0	100	100
4	d2	338/351 (96%)	323 (96%)	15 (4%)	0	100	100
5	E1	59/84 (70%)	57 (97%)	2 (3%)	0	100	100
5	E2	61/84 (73%)	59 (97%)	2 (3%)	0	100	100
5	e1	55/84 (66%)	54 (98%)	1 (2%)	0	100	100
5	e2	58/84 (69%)	57 (98%)	1 (2%)	0	100	100
6	F1	26/43 (60%)	26 (100%)	0	0	100	100
6	F2	29/43 (67%)	29 (100%)	0	0	100	100
6	f1	27/43 (63%)	27 (100%)	0	0	100	100
6	f2	27/43 (63%)	26 (96%)	1 (4%)	0	100	100
7	H1	56/67 (84%)	53 (95%)	2 (4%)	1 (2%)	6	21
7	H2	60/67 (90%)	54 (90%)	5 (8%)	1 (2%)	7	22
7	h1	60/67 (90%)	57 (95%)	2 (3%)	1 (2%)	7	22
7	h2	60/67 (90%)	56 (93%)	3 (5%)	1 (2%)	7	22
8	I1	32/38 (84%)	32 (100%)	0	0	100	100
8	I2	33/38 (87%)	32 (97%)	1 (3%)	0	100	100
8	i1	32/38 (84%)	32 (100%)	0	0	100	100
8	i2	31/38 (82%)	31 (100%)	0	0	100	100
9	J1	30/39 (77%)	30 (100%)	0	0	100	100
9	J2	33/39 (85%)	33 (100%)	0	0	100	100
9	j1	30/39 (77%)	30 (100%)	0	0	100	100
9	j2	31/39 (80%)	31 (100%)	0	0	100	100
10	K1	35/41 (85%)	31 (89%)	2 (6%)	2 (6%)	1	3
10	K2	35/41 (85%)	31 (89%)	2 (6%)	2 (6%)	1	3
10	k1	35/41 (85%)	31 (89%)	2 (6%)	2 (6%)	1	3
10	k2	35/41 (85%)	31 (89%)	2 (6%)	2 (6%)	1	3
11	L1	35/38 (92%)	33 (94%)	1 (3%)	1 (3%)	3	11
11	L2	35/38 (92%)	33 (94%)	1 (3%)	1 (3%)	3	11
11	l1	35/38 (92%)	33 (94%)	1 (3%)	1 (3%)	3	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	l2	35/38 (92%)	33 (94%)	1 (3%)	1 (3%)	3	11
12	M1	38/108 (35%)	30 (79%)	8 (21%)	0	100	100
12	M2	38/108 (35%)	30 (79%)	8 (21%)	0	100	100
12	m1	38/108 (35%)	30 (79%)	8 (21%)	0	100	100
12	m2	38/108 (35%)	30 (79%)	8 (21%)	0	100	100
13	O1	234/329 (71%)	210 (90%)	14 (6%)	10 (4%)	2	6
13	O2	187/329 (57%)	165 (88%)	14 (8%)	8 (4%)	2	6
13	o1	230/329 (70%)	204 (89%)	16 (7%)	10 (4%)	2	6
13	o2	239/329 (73%)	212 (89%)	15 (6%)	12 (5%)	1	4
14	T1	28/32 (88%)	28 (100%)	0	0	100	100
14	T2	28/32 (88%)	28 (100%)	0	0	100	100
14	t1	28/32 (88%)	28 (100%)	0	0	100	100
14	t2	27/32 (84%)	27 (100%)	0	0	100	100
15	U1	91/155 (59%)	85 (93%)	6 (7%)	0	100	100
15	U2	86/155 (56%)	81 (94%)	5 (6%)	0	100	100
15	u1	91/155 (59%)	87 (96%)	4 (4%)	0	100	100
15	u2	91/155 (59%)	85 (93%)	6 (7%)	0	100	100
16	V1	127/155 (82%)	115 (91%)	7 (6%)	5 (4%)	2	7
16	V2	127/155 (82%)	115 (91%)	7 (6%)	5 (4%)	2	7
16	v1	127/155 (82%)	115 (91%)	7 (6%)	5 (4%)	2	7
16	v2	127/155 (82%)	115 (91%)	7 (6%)	5 (4%)	2	7
17	Y1	25/35 (71%)	24 (96%)	1 (4%)	0	100	100
17	Y2	23/35 (66%)	22 (96%)	1 (4%)	0	100	100
17	y1	25/35 (71%)	24 (96%)	1 (4%)	0	100	100
17	y2	25/35 (71%)	24 (96%)	1 (4%)	0	100	100
18	X1	27/40 (68%)	27 (100%)	0	0	100	100
18	X2	29/40 (72%)	29 (100%)	0	0	100	100
18	x1	34/40 (85%)	33 (97%)	1 (3%)	0	100	100
18	x2	30/40 (75%)	30 (100%)	0	0	100	100
19	S1	23/46 (50%)	23 (100%)	0	0	100	100
19	S2	28/46 (61%)	27 (96%)	1 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	s1	38/46 (83%)	34 (90%)	4 (10%)	0	100	100
19	s2	44/46 (96%)	37 (84%)	7 (16%)	0	100	100
20	W1	19/25 (76%)	19 (100%)	0	0	100	100
20	W2	19/25 (76%)	19 (100%)	0	0	100	100
20	w1	23/25 (92%)	21 (91%)	2 (9%)	0	100	100
20	w2	18/25 (72%)	18 (100%)	0	0	100	100
21	Q2	107/218 (49%)	102 (95%)	3 (3%)	2 (2%)	6	19
21	q1	101/218 (46%)	97 (96%)	3 (3%)	1 (1%)	12	35
22	Z2	57/62 (92%)	55 (96%)	2 (4%)	0	100	100
22	z2	57/62 (92%)	55 (96%)	2 (4%)	0	100	100
All	All	10304/12316 (84%)	9726 (94%)	479 (5%)	99 (1%)	12	35

5 of 99 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C1	36	TRP
3	C1	37	SER
10	K1	14	THR
13	O1	49	GLN
13	O1	99	ASP

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	A1	261/282 (93%)	254 (97%)	7 (3%)	39	71
1	A2	239/282 (85%)	234 (98%)	5 (2%)	47	76
1	a1	261/282 (93%)	255 (98%)	6 (2%)	44	75
1	a2	249/282 (88%)	242 (97%)	7 (3%)	38	70
2	B1	360/415 (87%)	350 (97%)	10 (3%)	38	70
2	B2	351/415 (85%)	339 (97%)	12 (3%)	32	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	b1	380/415 (92%)	368 (97%)	12 (3%)	34	67
2	b2	352/415 (85%)	341 (97%)	11 (3%)	35	68
3	C1	320/364 (88%)	317 (99%)	3 (1%)	70	87
3	C2	261/364 (72%)	260 (100%)	1 (0%)	84	93
3	c1	338/364 (93%)	335 (99%)	3 (1%)	70	87
3	c2	323/364 (89%)	320 (99%)	3 (1%)	70	87
4	D1	255/283 (90%)	253 (99%)	2 (1%)	73	89
4	D2	238/283 (84%)	236 (99%)	2 (1%)	73	89
4	d1	267/283 (94%)	266 (100%)	1 (0%)	84	93
4	d2	258/283 (91%)	257 (100%)	1 (0%)	84	93
5	E1	28/75 (37%)	28 (100%)	0	100	100
5	E2	34/75 (45%)	33 (97%)	1 (3%)	37	70
5	e1	38/75 (51%)	36 (95%)	2 (5%)	20	49
5	e2	33/75 (44%)	32 (97%)	1 (3%)	36	69
6	F1	18/36 (50%)	17 (94%)	1 (6%)	19	46
6	F2	17/36 (47%)	16 (94%)	1 (6%)	18	44
6	f1	20/36 (56%)	18 (90%)	2 (10%)	7	21
6	f2	19/36 (53%)	18 (95%)	1 (5%)	20	49
7	H1	39/58 (67%)	39 (100%)	0	100	100
7	H2	38/58 (66%)	38 (100%)	0	100	100
7	h1	47/58 (81%)	45 (96%)	2 (4%)	26	57
7	h2	42/58 (72%)	42 (100%)	0	100	100
8	I1	30/36 (83%)	29 (97%)	1 (3%)	33	66
8	I2	26/36 (72%)	25 (96%)	1 (4%)	29	61
8	i1	32/36 (89%)	31 (97%)	1 (3%)	35	68
8	i2	28/36 (78%)	27 (96%)	1 (4%)	31	63
9	J1	20/32 (62%)	20 (100%)	0	100	100
9	J2	19/32 (59%)	19 (100%)	0	100	100
9	j1	22/32 (69%)	22 (100%)	0	100	100
9	j2	22/32 (69%)	22 (100%)	0	100	100
10	K1	26/36 (72%)	25 (96%)	1 (4%)	29	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	K2	18/36 (50%)	17 (94%)	1 (6%)	19	46
10	k1	27/36 (75%)	26 (96%)	1 (4%)	30	62
10	k2	24/36 (67%)	21 (88%)	3 (12%)	4	13
11	L1	31/35 (89%)	31 (100%)	0	100	100
11	L2	33/35 (94%)	33 (100%)	0	100	100
11	l1	33/35 (94%)	33 (100%)	0	100	100
11	l2	32/35 (91%)	32 (100%)	0	100	100
12	M1	26/88 (30%)	25 (96%)	1 (4%)	29	61
12	M2	26/88 (30%)	25 (96%)	1 (4%)	29	61
12	m1	26/88 (30%)	25 (96%)	1 (4%)	29	61
12	m2	27/88 (31%)	26 (96%)	1 (4%)	30	62
13	O1	148/266 (56%)	141 (95%)	7 (5%)	23	54
13	O2	110/266 (41%)	105 (96%)	5 (4%)	24	55
13	o1	156/266 (59%)	150 (96%)	6 (4%)	29	61
13	o2	168/266 (63%)	161 (96%)	7 (4%)	26	58
14	T1	24/28 (86%)	24 (100%)	0	100	100
14	T2	25/28 (89%)	25 (100%)	0	100	100
14	t1	26/28 (93%)	26 (100%)	0	100	100
14	t2	25/28 (89%)	24 (96%)	1 (4%)	28	60
15	U1	63/122 (52%)	59 (94%)	4 (6%)	16	41
15	U2	40/122 (33%)	37 (92%)	3 (8%)	12	34
15	u1	66/122 (54%)	62 (94%)	4 (6%)	17	43
15	u2	69/122 (57%)	64 (93%)	5 (7%)	13	35
16	V1	88/132 (67%)	86 (98%)	2 (2%)	44	75
16	V2	70/132 (53%)	68 (97%)	2 (3%)	37	70
16	v1	88/132 (67%)	86 (98%)	2 (2%)	44	75
16	v2	100/132 (76%)	99 (99%)	1 (1%)	68	86
17	Y1	11/33 (33%)	11 (100%)	0	100	100
17	Y2	13/33 (39%)	13 (100%)	0	100	100
17	y1	18/33 (54%)	18 (100%)	0	100	100
17	y2	16/33 (48%)	16 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	X1	17/34 (50%)	16 (94%)	1 (6%)	18	44
18	X2	16/34 (47%)	16 (100%)	0	100	100
18	x1	23/34 (68%)	22 (96%)	1 (4%)	26	57
18	x2	17/34 (50%)	16 (94%)	1 (6%)	18	44
19	S1	10/20 (50%)	10 (100%)	0	100	100
19	S2	10/20 (50%)	10 (100%)	0	100	100
19	s1	15/20 (75%)	15 (100%)	0	100	100
19	s2	13/20 (65%)	13 (100%)	0	100	100
20	W1	12/13 (92%)	12 (100%)	0	100	100
20	W2	10/13 (77%)	10 (100%)	0	100	100
20	w1	11/13 (85%)	11 (100%)	0	100	100
20	w2	11/13 (85%)	11 (100%)	0	100	100
21	Q2	35/175 (20%)	33 (94%)	2 (6%)	18	46
21	q1	33/175 (19%)	31 (94%)	2 (6%)	17	43
22	Z2	22/54 (41%)	22 (100%)	0	100	100
22	z2	28/54 (52%)	28 (100%)	0	100	100
All	All	7221/10010 (72%)	7054 (98%)	167 (2%)	44	75

5 of 167 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	O2	233	LEU
3	c2	279	LEU
16	V2	39	SER
2	b2	6	TYR
10	k2	38	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 71 such sidechains are listed below:

Mol	Chain	Res	Type
1	a2	181	ASN
2	b2	114	HIS
3	c2	385	GLN
2	b1	223	GLN
2	b1	216	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 353 ligands modelled in this entry, 10 are monoatomic and 52 are unknown - leaving 291 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
25	CLA	a1	403	1	69,73,73	1.32	8 (11%)	83,113,113	1.27	7 (8%)
32	GOL	c2	518	-	5,5,5	0.37	0	5,5,5	0.26	0
25	CLA	b1	610	2	69,73,73	1.27	8 (11%)	83,113,113	1.26	8 (9%)
27	PHO	d2	408	-	58,69,69	2.76	12 (20%)	56,99,99	2.62	16 (28%)
34	DGD	c2	517	-	63,63,67	0.89	2 (3%)	77,77,81	0.84	2 (2%)
25	CLA	B1	613	2	69,73,73	1.28	9 (13%)	83,113,113	1.33	6 (7%)
23	BCR	k2	501	-	41,41,41	0.68	0	56,56,56	2.04	16 (28%)
25	CLA	c1	513	3	64,68,73	1.32	7 (10%)	77,107,113	1.32	6 (7%)
25	CLA	c1	508	3	54,58,73	1.45	8 (14%)	65,95,113	1.41	9 (13%)
25	CLA	c1	512	3	69,73,73	1.28	8 (11%)	83,113,113	1.29	6 (7%)
25	CLA	A1	405	1	59,63,73	1.40	7 (11%)	71,101,113	1.37	8 (11%)
25	CLA	b2	610	2	69,73,73	1.26	7 (10%)	83,113,113	1.27	6 (7%)
25	CLA	b1	612	-	69,73,73	1.27	6 (8%)	83,113,113	1.31	7 (8%)
29	LMG	M1	101	-	30,30,55	1.20	3 (10%)	32,32,63	1.33	3 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	b2	618	2	69,73,73	1.27	7 (10%)	83,113,113	1.27	6 (7%)
25	CLA	c2	513	3	58,62,73	1.38	8 (13%)	69,99,113	1.37	6 (8%)
25	CLA	B1	607	2	64,68,73	1.33	8 (12%)	77,107,113	1.29	6 (7%)
23	BCR	A2	401	-	41,41,41	0.69	0	56,56,56	2.02	16 (28%)
32	GOL	a2	415	-	5,5,5	0.36	0	5,5,5	0.39	0
25	CLA	d1	406	4	69,73,73	1.26	6 (8%)	83,113,113	1.30	7 (8%)
25	CLA	C2	511	3	54,58,73	1.42	9 (16%)	65,95,113	1.49	8 (12%)
29	LMG	a2	412	-	44,44,55	1.01	2 (4%)	52,52,63	1.11	5 (9%)
25	CLA	c1	516	3	69,73,73	1.26	7 (10%)	83,113,113	1.27	7 (8%)
29	LMG	C1	520	-	48,48,55	0.97	2 (4%)	56,56,63	1.00	3 (5%)
34	DGD	H2	101	-	63,63,67	0.88	2 (3%)	77,77,81	0.91	3 (3%)
27	PHO	D1	407	-	57,68,69	2.78	12 (21%)	54,97,99	2.69	16 (29%)
25	CLA	B1	606	2	69,73,73	1.26	7 (10%)	83,113,113	1.28	6 (7%)
25	CLA	a2	404	1	69,73,73	1.29	8 (11%)	83,113,113	1.28	7 (8%)
35	LMT	M1	103	-	24,24,36	0.46	0	29,29,47	0.56	0
25	CLA	B2	605	2	69,73,73	1.27	6 (8%)	83,113,113	1.27	5 (6%)
36	PL9	d2	409	-	55,55,55	0.64	1 (1%)	68,69,69	1.72	16 (23%)
25	CLA	b2	614	2	69,73,73	1.25	8 (11%)	83,113,113	1.27	6 (7%)
35	LMT	m2	104	-	30,30,36	0.47	0	41,41,47	0.81	1 (2%)
25	CLA	C1	502	3	69,73,73	1.25	6 (8%)	83,113,113	1.31	7 (8%)
26	OEX	a1	408	3,40,1	0,14,14	-	-	-	-	-
25	CLA	c1	510	3	69,73,73	1.27	8 (11%)	83,113,113	1.34	6 (7%)
38	HEM	v1	201	16	50,50,50	1.92	7 (14%)	66,82,82	1.43	6 (9%)
33	LHG	l1	102	-	48,48,48	0.92	2 (4%)	51,54,54	1.07	4 (7%)
31	BCT	A1	413	30	2,3,3	0.94	0	2,3,3	0.26	0
32	GOL	i1	101	-	5,5,5	0.41	0	5,5,5	0.20	0
29	LMG	B2	621	-	37,37,55	0.95	3 (8%)	45,45,63	1.11	3 (6%)
29	LMG	B1	622	-	31,31,55	1.20	2 (6%)	39,39,63	1.19	4 (10%)
33	LHG	d1	407	-	48,48,48	0.91	2 (4%)	51,54,54	1.05	3 (5%)
25	CLA	B1	617	2	69,73,73	1.26	6 (8%)	83,113,113	1.27	6 (7%)
23	BCR	B2	601	-	41,41,41	0.70	0	56,56,56	1.92	15 (26%)
25	CLA	c2	503	3	69,73,73	1.27	8 (11%)	83,113,113	1.29	4 (4%)
25	CLA	C1	506	3	69,73,73	1.26	7 (10%)	83,113,113	1.28	6 (7%)
25	CLA	B2	607	2	69,73,73	1.29	8 (11%)	83,113,113	1.30	8 (9%)
25	CLA	C2	508	3	54,58,73	1.43	6 (11%)	65,95,113	1.42	7 (10%)
23	BCR	b2	601	-	41,41,41	0.70	0	56,56,56	1.97	16 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	B1	608	2	69,73,73	1.27	7 (10%)	83,113,113	1.27	5 (6%)
25	CLA	b2	624	2	69,73,73	1.26	7 (10%)	83,113,113	1.28	8 (9%)
26	OEX	a2	408	3,40,1	0,14,14	-	-	-		
29	LMG	d1	411	-	34,34,55	1.10	2 (5%)	36,36,63	1.14	3 (8%)
29	LMG	j2	101	-	50,50,55	0.94	2 (4%)	58,58,63	1.03	2 (3%)
34	DGD	C1	516	-	63,63,67	0.85	2 (3%)	77,77,81	1.00	4 (5%)
25	CLA	C2	510	3	49,53,73	1.49	7 (14%)	59,89,113	1.47	5 (8%)
37	SQD	B2	623	-	44,45,54	1.31	4 (9%)	53,56,65	1.22	6 (11%)
25	CLA	D1	402	4	69,73,73	1.25	7 (10%)	83,113,113	1.27	7 (8%)
25	CLA	B2	608	2	69,73,73	1.25	6 (8%)	83,113,113	1.29	7 (8%)
23	BCR	b1	602	-	41,41,41	0.69	0	56,56,56	2.05	18 (32%)
25	CLA	c2	507	3	58,62,73	1.39	8 (13%)	69,99,113	1.35	5 (7%)
23	BCR	z2	101	-	41,41,41	0.70	0	56,56,56	1.76	10 (17%)
23	BCR	c2	501	-	41,41,41	0.80	1 (2%)	56,56,56	3.50	20 (35%)
38	HEM	V2	201	16	50,50,50	1.96	7 (14%)	66,82,82	1.51	8 (12%)
23	BCR	H2	103	-	24,24,41	0.71	0	31,31,56	1.67	8 (25%)
25	CLA	C2	516	3	50,54,73	1.47	7 (14%)	60,90,113	1.43	6 (10%)
33	LHG	l2	101	-	43,43,48	1.00	2 (4%)	46,49,54	1.07	4 (8%)
25	CLA	D2	401	4	69,73,73	1.25	8 (11%)	83,113,113	1.29	6 (7%)
25	CLA	C1	511	3	69,73,73	1.28	7 (10%)	83,113,113	1.27	5 (6%)
25	CLA	B1	612	-	69,73,73	1.28	6 (8%)	83,113,113	1.29	7 (8%)
25	CLA	D2	404	4	65,69,73	1.31	7 (10%)	78,108,113	1.30	7 (8%)
29	LMG	C2	515	-	24,24,55	1.18	2 (8%)	32,32,63	1.05	2 (6%)
33	LHG	D1	405	-	48,48,48	0.93	2 (4%)	51,54,54	1.00	3 (5%)
29	LMG	b1	631	-	40,40,55	1.08	2 (5%)	48,48,63	1.23	5 (10%)
25	CLA	B2	604	-	45,49,73	1.55	6 (13%)	54,84,113	1.47	7 (12%)
29	LMG	c2	519	-	26,26,55	1.60	3 (11%)	32,33,63	1.30	2 (6%)
25	CLA	a1	404	1	64,68,73	1.34	7 (10%)	77,107,113	1.29	8 (10%)
25	CLA	B2	615	2	69,73,73	1.26	7 (10%)	83,113,113	1.25	6 (7%)
29	LMG	A2	412	-	29,29,55	1.07	2 (6%)	37,37,63	1.10	2 (5%)
23	BCR	K1	101	-	31,31,41	0.70	0	40,40,56	2.32	14 (35%)
27	PHO	a1	411	-	58,69,69	2.72	12 (20%)	56,99,99	2.56	16 (28%)
25	CLA	b2	615	2	64,68,73	1.31	7 (10%)	77,107,113	1.31	6 (7%)
37	SQD	D1	409	-	34,35,54	1.53	4 (11%)	43,46,65	1.41	6 (13%)
25	CLA	b2	611	-	69,73,73	1.27	6 (8%)	83,113,113	1.29	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	b2	617	2	69,73,73	1.27	7 (10%)	83,113,113	1.27	7 (8%)
25	CLA	B2	611	2	69,73,73	1.27	7 (10%)	83,113,113	1.27	6 (7%)
25	CLA	D1	403	4	55,59,73	1.42	7 (12%)	66,96,113	1.34	5 (7%)
23	BCR	b2	603	-	41,41,41	0.70	0	56,56,56	1.91	13 (23%)
29	LMG	b1	621	-	38,38,55	1.11	2 (5%)	46,46,63	1.07	2 (4%)
26	OEX	A1	407	3,40,1	0,14,14	-	-	-	-	-
33	LHG	D2	405	-	48,48,48	0.92	2 (4%)	51,54,54	1.02	4 (7%)
23	BCR	c1	501	-	41,41,41	0.70	0	56,56,56	2.10	13 (23%)
23	BCR	K2	102	-	41,41,41	0.72	0	56,56,56	2.07	16 (28%)
25	CLA	B2	606	2	69,73,73	1.28	7 (10%)	83,113,113	1.26	6 (7%)
35	LMT	C1	519	-	36,36,36	0.35	0	47,47,47	0.70	1 (2%)
25	CLA	c2	502	3	69,73,73	1.27	6 (8%)	83,113,113	1.27	6 (7%)
25	CLA	B2	614	2	69,73,73	1.24	8 (11%)	83,113,113	1.26	7 (8%)
33	LHG	a1	407	-	42,42,48	1.01	2 (4%)	45,48,54	1.09	3 (6%)
34	DGD	c1	520	-	63,63,67	0.87	2 (3%)	77,77,81	0.86	2 (2%)
25	CLA	c2	508	40	69,73,73	1.27	6 (8%)	83,113,113	1.24	5 (6%)
27	PHO	A2	407	-	58,69,69	2.72	12 (20%)	56,99,99	2.61	15 (26%)
32	GOL	b1	618	-	5,5,5	0.35	0	5,5,5	0.39	0
25	CLA	b1	604	-	69,73,73	1.29	7 (10%)	83,113,113	1.21	6 (7%)
23	BCR	b1	601	-	41,41,41	0.69	0	56,56,56	1.83	14 (25%)
25	CLA	c1	509	40	69,73,73	1.27	7 (10%)	83,113,113	1.27	4 (4%)
25	CLA	c2	505	-	69,73,73	1.25	6 (8%)	83,113,113	1.29	6 (7%)
25	CLA	B1	605	2	69,73,73	1.27	6 (8%)	83,113,113	1.23	6 (7%)
23	BCR	a2	402	-	41,41,41	0.67	0	56,56,56	1.64	12 (21%)
25	CLA	d1	401	4	69,73,73	1.25	7 (10%)	83,113,113	1.30	7 (8%)
25	CLA	B2	612	-	69,73,73	1.27	6 (8%)	83,113,113	1.29	8 (9%)
29	LMG	A1	412	-	41,41,55	1.06	2 (4%)	49,49,63	1.02	3 (6%)
25	CLA	C1	510	3	69,73,73	1.29	8 (11%)	83,113,113	1.23	6 (7%)
29	LMG	A1	410	-	43,43,55	1.03	2 (4%)	51,51,63	1.11	4 (7%)
33	LHG	A2	405	-	32,32,48	1.13	2 (6%)	35,38,54	1.07	2 (5%)
25	CLA	B1	610	2	69,73,73	1.28	8 (11%)	83,113,113	1.25	7 (8%)
33	LHG	B2	627	-	41,41,48	1.03	2 (4%)	44,47,54	1.08	3 (6%)
33	LHG	B1	621	-	48,48,48	0.92	2 (4%)	51,54,54	1.01	3 (5%)
25	CLA	c2	506	3	65,69,73	1.30	8 (12%)	78,108,113	1.37	7 (8%)
29	LMG	b1	624	-	39,39,55	1.08	2 (5%)	47,47,63	1.31	5 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	LMT	L1	102	-	11,11,36	0.25	0	10,10,47	0.56	0
25	CLA	B1	615	2	69,73,73	1.27	6 (8%)	83,113,113	1.25	5 (6%)
25	CLA	b1	611	2	69,73,73	1.27	7 (10%)	83,113,113	1.22	5 (6%)
25	CLA	C2	506	-	69,73,73	1.26	6 (8%)	83,113,113	1.27	7 (8%)
25	CLA	B2	617	2	69,73,73	1.26	7 (10%)	83,113,113	1.29	5 (6%)
25	CLA	C1	514	3	49,53,73	1.50	7 (14%)	59,89,113	1.44	6 (10%)
27	PHO	A1	408	-	58,69,69	2.71	12 (20%)	56,99,99	2.61	16 (28%)
38	HEM	v2	201	16	50,50,50	1.92	7 (14%)	66,82,82	1.45	7 (10%)
23	BCR	d2	401	-	41,41,41	0.70	0	56,56,56	2.11	16 (28%)
29	LMG	D1	406	-	35,35,55	1.11	2 (5%)	43,43,63	1.07	3 (6%)
23	BCR	K2	104	-	29,29,41	0.56	0	40,41,56	1.67	10 (25%)
35	LMT	a2	406	-	36,36,36	0.45	0	47,47,47	0.66	1 (2%)
38	HEM	E2	101	5	50,50,50	1.89	8 (16%)	66,82,82	1.43	6 (9%)
25	CLA	b2	608	2	69,73,73	1.28	7 (10%)	83,113,113	1.22	7 (8%)
25	CLA	C1	509	3	69,73,73	1.27	8 (11%)	83,113,113	1.38	8 (9%)
25	CLA	b2	616	2	64,68,73	1.34	8 (12%)	77,107,113	1.33	7 (9%)
23	BCR	j2	102	-	41,41,41	0.73	0	56,56,56	2.08	18 (32%)
25	CLA	B1	604	-	46,50,73	1.54	6 (13%)	55,85,113	1.43	5 (9%)
25	CLA	B1	619	40	69,73,73	1.26	6 (8%)	83,113,113	1.28	6 (7%)
25	CLA	b1	619	2	69,73,73	1.27	8 (11%)	83,113,113	1.27	6 (7%)
25	CLA	C1	508	-	69,73,73	1.27	7 (10%)	83,113,113	1.27	5 (6%)
23	BCR	a1	401	-	41,41,41	0.69	0	56,56,56	1.73	14 (25%)
23	BCR	B1	603	-	41,41,41	0.68	0	56,56,56	1.72	11 (19%)
25	CLA	c2	511	3	69,73,73	1.27	7 (10%)	83,113,113	1.27	5 (6%)
36	PL9	D1	408	-	55,55,55	0.64	2 (3%)	68,69,69	1.76	16 (23%)
25	CLA	B2	619	-	69,73,73	1.26	6 (8%)	83,113,113	1.27	7 (8%)
25	CLA	C1	503	3	64,68,73	1.31	7 (10%)	77,107,113	1.29	5 (6%)
25	CLA	B2	609	2	69,73,73	1.25	7 (10%)	83,113,113	1.33	7 (8%)
23	BCR	C1	521	-	41,41,41	0.69	0	56,56,56	1.94	13 (23%)
23	BCR	F2	401	-	41,41,41	0.72	0	56,56,56	2.18	18 (32%)
29	LMG	B2	620	-	40,40,55	1.07	3 (7%)	48,48,63	1.05	4 (8%)
25	CLA	C2	513	3	57,61,73	1.42	8 (14%)	68,98,113	1.34	6 (8%)
23	BCR	k1	101	-	41,41,41	0.71	0	56,56,56	2.03	15 (26%)
25	CLA	b1	613	2	69,73,73	1.28	9 (13%)	83,113,113	1.34	6 (7%)
29	LMG	I2	101	-	34,34,55	1.15	2 (5%)	42,42,63	1.13	3 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	c1	504	3	69,73,73	1.27	7 (10%)	83,113,113	1.26	7 (8%)
25	CLA	B1	611	2	66,70,73	1.31	6 (9%)	79,109,113	1.27	7 (8%)
25	CLA	b1	617	2	69,73,73	1.28	8 (11%)	83,113,113	1.27	5 (6%)
25	CLA	b1	607	2	69,73,73	1.30	7 (10%)	83,113,113	1.29	7 (8%)
29	LMG	d1	408	-	33,33,55	1.15	2 (6%)	41,41,63	1.10	3 (7%)
32	GOL	B1	620	-	5,5,5	0.35	0	5,5,5	0.32	0
23	BCR	b2	602	-	41,41,41	0.70	0	56,56,56	2.13	16 (28%)
25	CLA	b1	608	2	69,73,73	1.28	7 (10%)	83,113,113	1.30	7 (8%)
23	BCR	B2	602	-	41,41,41	0.68	0	56,56,56	2.02	14 (25%)
27	PHO	a2	416	-	58,69,69	2.71	12 (20%)	56,99,99	2.62	16 (28%)
25	CLA	c1	515	3	59,63,73	1.38	6 (10%)	71,101,113	1.34	6 (8%)
32	GOL	a1	406	-	5,5,5	0.35	0	5,5,5	0.28	0
33	LHG	d2	403	-	48,48,48	0.94	2 (4%)	51,54,54	1.02	3 (5%)
38	HEM	V1	201	16	50,50,50	1.93	7 (14%)	66,82,82	1.47	9 (13%)
31	BCT	a2	417	30	2,3,3	0.67	0	2,3,3	0.77	0
25	CLA	B1	618	2	62,66,73	1.34	8 (12%)	74,104,113	1.32	5 (6%)
25	CLA	B1	614	2	69,73,73	1.25	7 (10%)	83,113,113	1.26	7 (8%)
25	CLA	A2	402	1	69,73,73	1.32	8 (11%)	83,113,113	1.28	7 (8%)
23	BCR	B2	603	-	41,41,41	0.69	0	56,56,56	1.84	12 (21%)
32	GOL	C2	514	-	5,5,5	0.36	0	5,5,5	0.31	0
34	DGD	c1	514	-	52,52,67	0.96	2 (3%)	66,66,81	1.04	4 (6%)
25	CLA	c1	506	40	69,73,73	1.26	6 (8%)	83,113,113	1.31	8 (9%)
33	LHG	D1	404	-	48,48,48	0.93	2 (4%)	51,54,54	1.04	4 (7%)
34	DGD	c1	518	-	63,63,67	0.87	2 (3%)	77,77,81	1.00	5 (6%)
25	CLA	B2	616	2	58,62,73	1.38	7 (12%)	69,99,113	1.39	7 (10%)
25	CLA	B1	609	2	69,73,73	1.26	7 (10%)	83,113,113	1.51	10 (12%)
31	BCT	A2	413	30	2,3,3	0.68	0	2,3,3	0.74	0
34	DGD	H1	101	-	63,63,67	0.88	2 (3%)	77,77,81	0.92	3 (3%)
25	CLA	c2	504	3	69,73,73	1.27	6 (8%)	83,113,113	1.27	6 (7%)
34	DGD	c2	516	-	53,53,67	0.96	2 (3%)	67,67,81	1.03	3 (4%)
29	LMG	B1	626	-	48,48,55	0.98	2 (4%)	56,56,63	1.18	3 (5%)
23	BCR	H1	102	-	22,22,41	0.69	0	29,29,56	1.72	6 (20%)
25	CLA	d1	404	40	69,73,73	1.31	7 (10%)	83,113,113	1.31	7 (8%)
25	CLA	b2	619	2	63,67,73	1.34	7 (11%)	75,105,113	1.31	5 (6%)
25	CLA	a1	405	-	54,58,73	1.42	7 (12%)	65,95,113	1.49	8 (12%)
25	CLA	b2	612	2	69,73,73	1.29	10 (14%)	83,113,113	1.34	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	PHO	d1	403	-	58,69,69	2.76	12 (20%)	56,99,99	2.66	14 (25%)
32	GOL	c1	521	-	5,5,5	0.36	0	5,5,5	0.31	0
25	CLA	C1	504	3	69,73,73	1.29	7 (10%)	83,113,113	1.23	6 (7%)
25	CLA	b2	609	2	65,69,73	1.30	8 (12%)	78,108,113	1.33	5 (6%)
23	BCR	B1	601	-	41,41,41	0.69	0	56,56,56	1.90	15 (26%)
25	CLA	c2	512	3	69,73,73	1.27	6 (8%)	83,113,113	1.25	6 (7%)
33	LHG	L2	101	-	48,48,48	0.93	2 (4%)	51,54,54	1.10	4 (7%)
25	CLA	A2	404	-	55,59,73	1.46	8 (14%)	66,96,113	1.37	8 (12%)
25	CLA	b1	609	2	69,73,73	1.27	7 (10%)	83,113,113	1.26	6 (7%)
25	CLA	b1	614	2	69,73,73	1.24	8 (11%)	83,113,113	1.31	7 (8%)
37	SQD	D2	402	-	24,25,54	1.94	4 (16%)	31,35,65	1.66	6 (19%)
35	LMT	l1	101	-	24,24,36	0.47	0	29,29,47	0.83	2 (6%)
25	CLA	C2	504	3	50,54,73	1.48	7 (14%)	60,90,113	1.40	4 (6%)
25	CLA	C2	505	3	69,73,73	1.27	7 (10%)	83,113,113	1.27	5 (6%)
25	CLA	C1	512	3	69,73,73	1.26	8 (11%)	83,113,113	1.29	6 (7%)
34	DGD	c2	514	-	63,63,67	0.87	2 (3%)	77,77,81	0.97	4 (5%)
35	LMT	i2	102	-	6,6,36	0.28	0	5,5,47	0.44	0
32	GOL	C1	518	-	5,5,5	0.37	0	5,5,5	0.23	0
35	LMT	T1	101	-	11,11,36	0.25	0	10,10,47	0.58	0
25	CLA	B1	616	2	69,73,73	1.29	8 (11%)	83,113,113	1.26	7 (8%)
23	BCR	b1	603	-	41,41,41	0.72	0	56,56,56	1.75	11 (19%)
25	CLA	A1	403	1	69,73,73	1.31	9 (13%)	83,113,113	1.28	7 (8%)
35	LMT	c1	517	-	34,34,36	0.43	0	45,45,47	0.68	1 (2%)
25	CLA	c2	509	3	69,73,73	1.26	8 (11%)	83,113,113	1.37	9 (10%)
25	CLA	B2	618	2	64,68,73	1.34	7 (10%)	77,107,113	1.32	5 (6%)
25	CLA	d2	402	-	69,73,73	1.27	7 (10%)	83,113,113	1.34	8 (9%)
33	LHG	D2	403	-	48,48,48	0.92	2 (4%)	51,54,54	1.03	3 (5%)
37	SQD	b2	605	-	44,45,54	1.30	4 (9%)	53,56,65	1.16	4 (7%)
25	CLA	b2	613	2	69,73,73	1.27	6 (8%)	83,113,113	1.24	5 (6%)
25	CLA	d2	405	4	69,73,73	1.26	7 (10%)	83,113,113	1.23	6 (7%)
25	CLA	c1	503	3	69,73,73	1.24	7 (10%)	83,113,113	1.32	6 (7%)
23	BCR	J1	101	-	41,41,41	0.75	0	56,56,56	2.10	16 (28%)
23	BCR	h1	102	-	41,41,41	0.68	0	56,56,56	1.89	17 (30%)
25	CLA	C1	513	3	65,69,73	1.31	7 (10%)	78,108,113	1.28	5 (6%)
34	DGD	h2	102	-	63,63,67	0.87	2 (3%)	77,77,81	0.91	2 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	C2	518	3	45,49,73	1.53	6 (13%)	54,84,113	1.52	6 (11%)
38	HEM	f1	101	6	50,50,50	1.93	7 (14%)	66,82,82	1.43	6 (9%)
25	CLA	d2	404	4	54,58,73	1.43	6 (11%)	65,95,113	1.41	7 (10%)
29	LMG	a1	412	-	51,51,55	0.95	2 (3%)	59,59,63	1.07	4 (6%)
33	LHG	b2	625	-	42,42,48	1.00	2 (4%)	45,48,54	1.08	3 (6%)
25	CLA	c1	505	3	69,73,73	1.27	7 (10%)	83,113,113	1.25	5 (6%)
27	PHO	D2	407	-	58,69,69	2.77	12 (20%)	56,99,99	2.64	15 (26%)
25	CLA	b2	620	40	69,73,73	1.26	8 (11%)	83,113,113	1.31	6 (7%)
35	LMT	m1	101	-	36,36,36	0.42	0	47,47,47	0.68	0
33	LHG	d2	406	-	48,48,48	0.92	2 (4%)	51,54,54	1.00	4 (7%)
23	BCR	B1	602	-	41,41,41	0.69	0	56,56,56	1.95	12 (21%)
25	CLA	c2	515	3	50,54,73	1.46	7 (14%)	60,90,113	1.43	6 (10%)
25	CLA	b1	605	2	69,73,73	1.27	7 (10%)	83,113,113	1.29	4 (4%)
25	CLA	b1	606	2	69,73,73	1.26	7 (10%)	83,113,113	1.28	6 (7%)
26	OEX	A2	406	3,40,1	0,14,14	-	-	-	-	-
33	LHG	b1	622	-	48,48,48	0.92	2 (4%)	51,54,54	1.04	5 (9%)
35	LMT	M1	102	-	10,10,36	0.24	0	9,9,47	0.57	0
33	LHG	d1	402	-	31,31,48	1.16	2 (6%)	34,37,54	1.35	3 (8%)
36	PL9	d1	409	-	55,55,55	0.64	2 (3%)	68,69,69	1.78	20 (29%)
23	BCR	c1	502	-	41,41,41	0.75	0	56,56,56	2.09	14 (25%)
25	CLA	c2	510	3	58,62,73	1.40	7 (12%)	69,99,113	1.32	6 (8%)
23	BCR	C1	501	-	41,41,41	0.70	0	56,56,56	1.80	14 (25%)
36	PL9	D2	408	-	55,55,55	0.62	1 (1%)	68,69,69	1.73	19 (27%)
23	BCR	A1	401	-	41,41,41	0.68	0	56,56,56	1.74	11 (19%)
25	CLA	A1	406	-	69,73,73	1.29	7 (10%)	83,113,113	1.35	8 (9%)
25	CLA	a2	405	1	69,73,73	1.24	6 (8%)	83,113,113	1.29	8 (9%)
29	LMG	F2	402	-	35,35,55	1.13	2 (5%)	43,43,63	1.03	3 (6%)
34	DGD	C1	517	-	65,65,67	0.86	2 (3%)	79,79,81	0.85	3 (3%)
33	LHG	L1	101	-	40,40,48	1.01	2 (5%)	43,46,54	1.10	4 (9%)
29	LMG	c1	519	-	55,55,55	0.91	2 (3%)	63,63,63	0.95	2 (3%)
38	HEM	E1	101	5,6	50,50,50	1.93	8 (16%)	66,82,82	1.43	6 (9%)
25	CLA	A2	403	1	65,69,73	1.32	6 (9%)	78,108,113	1.27	7 (8%)
25	CLA	b1	616	2	69,73,73	1.26	6 (8%)	83,113,113	1.30	7 (8%)
25	CLA	c1	507	3	69,73,73	1.26	7 (10%)	83,113,113	1.27	5 (6%)
25	CLA	B2	610	2	69,73,73	1.27	7 (10%)	83,113,113	1.25	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	K2	101	-	59,63,73	1.37	8 (13%)	71,101,113	1.36	6 (8%)
23	BCR	D1	401	-	41,41,41	0.72	0	56,56,56	1.98	13 (23%)
25	CLA	b2	604	-	46,50,73	1.52	6 (13%)	55,85,113	1.43	4 (7%)
23	BCR	h2	101	-	41,41,41	0.68	0	56,56,56	1.79	14 (25%)
34	DGD	C2	512	-	34,34,67	1.16	2 (5%)	46,47,81	1.06	2 (4%)
35	LMT	m2	103	-	31,31,36	0.44	0	42,42,47	0.91	1 (2%)
33	LHG	a2	407	-	29,29,48	1.09	2 (6%)	30,34,54	1.02	1 (3%)
25	CLA	D2	406	-	69,73,73	1.27	6 (8%)	83,113,113	1.29	7 (8%)
35	LMT	b2	621	-	36,36,36	0.41	0	47,47,47	0.69	0
25	CLA	B2	613	2	69,73,73	1.28	9 (13%)	83,113,113	1.36	8 (9%)
25	CLA	b1	620	-	69,73,73	1.28	6 (8%)	83,113,113	1.30	6 (7%)
25	CLA	C2	507	3	49,53,73	1.50	7 (14%)	59,89,113	1.43	4 (6%)
25	CLA	c1	511	3	69,73,73	1.26	7 (10%)	83,113,113	1.29	7 (8%)
23	BCR	C2	502	-	41,41,41	0.70	0	56,56,56	1.88	12 (21%)
34	DGD	h1	101	-	63,63,67	0.88	2 (3%)	77,77,81	0.96	4 (5%)
25	CLA	b1	615	2	63,67,73	1.31	7 (11%)	75,105,113	1.32	7 (9%)
35	LMT	b2	623	-	36,36,36	0.38	0	47,47,47	0.84	0
25	CLA	C1	505	-	69,73,73	1.25	6 (8%)	83,113,113	1.31	5 (6%)
23	BCR	d1	405	-	41,41,41	0.71	0	56,56,56	1.86	12 (21%)
25	CLA	C2	509	-	69,73,73	1.27	7 (10%)	83,113,113	1.27	5 (6%)
25	CLA	a2	413	-	54,58,73	1.44	7 (12%)	65,95,113	1.38	9 (13%)
29	LMG	b2	622	-	39,39,55	1.07	2 (5%)	47,47,63	1.01	3 (6%)
34	DGD	C1	515	-	53,53,67	0.96	2 (3%)	67,67,81	1.02	4 (5%)
38	HEM	e2	101	5,6	50,50,50	1.92	8 (16%)	66,82,82	1.45	7 (10%)
29	LMG	d2	407	-	27,27,55	1.36	2 (7%)	35,35,63	1.29	3 (8%)
25	CLA	C1	507	3	69,73,73	1.28	9 (13%)	83,113,113	1.25	8 (9%)
25	CLA	A1	404	-	55,59,73	1.42	8 (14%)	66,96,113	1.42	7 (10%)
25	CLA	b2	606	2	69,73,73	1.26	8 (11%)	83,113,113	1.28	5 (6%)
25	CLA	C2	503	3	69,73,73	1.26	6 (8%)	83,113,113	1.32	5 (6%)
31	BCT	a1	413	30	2,3,3	0.67	0	2,3,3	0.72	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	CLA	a1	403	1	-	6/39/115/115	-
32	GOL	c2	518	-	-	2/4/4/4	-
25	CLA	b1	610	2	-	2/39/115/115	-
27	PHO	d2	408	-	-	0/37/103/103	0/5/6/6
34	DGD	c2	517	-	-	7/51/91/95	0/2/2/2
25	CLA	B1	613	2	-	15/39/115/115	-
23	BCR	k2	501	-	-	0/29/63/63	0/2/2/2
25	CLA	c1	513	3	-	5/33/109/115	-
25	CLA	c1	508	3	-	7/21/97/115	-
25	CLA	c1	512	3	-	15/39/115/115	-
25	CLA	A1	405	1	-	3/27/103/115	-
25	CLA	b2	610	2	-	9/39/115/115	-
25	CLA	b1	612	-	-	12/39/115/115	-
29	LMG	M1	101	-	-	4/31/31/70	-
25	CLA	b2	618	2	-	6/39/115/115	-
25	CLA	c2	513	3	-	7/26/102/115	-
25	CLA	B1	607	2	-	9/33/109/115	-
23	BCR	A2	401	-	-	0/29/63/63	0/2/2/2
32	GOL	a2	415	-	-	2/4/4/4	-
25	CLA	d1	406	4	-	15/39/115/115	-
25	CLA	C2	511	3	-	4/21/97/115	-
29	LMG	a2	412	-	-	6/39/59/70	0/1/1/1
25	CLA	c1	516	3	-	11/39/115/115	-
29	LMG	C1	520	-	-	8/43/63/70	0/1/1/1
34	DGD	H2	101	-	-	7/51/91/95	0/2/2/2
27	PHO	D1	407	-	-	3/35/101/103	0/5/6/6
25	CLA	B1	606	2	-	20/39/115/115	-
25	CLA	a2	404	1	-	7/39/115/115	-
35	LMT	M1	103	-	-	3/15/35/61	0/1/1/2
25	CLA	B2	605	2	-	9/39/115/115	-
36	PL9	d2	409	-	-	8/53/73/73	0/1/1/1
25	CLA	b2	614	2	-	17/39/115/115	-
35	LMT	m2	104	-	-	4/15/55/61	0/2/2/2
25	CLA	C1	502	3	-	17/39/115/115	-
25	CLA	c1	510	3	-	10/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	HEM	v1	201	16	-	4/14/54/54	-
33	LHG	l1	102	-	-	18/53/53/53	-
32	GOL	i1	101	-	-	2/4/4/4	-
29	LMG	B2	621	-	-	8/31/51/70	0/1/1/1
29	LMG	B1	622	-	-	2/26/46/70	0/1/1/1
33	LHG	d1	407	-	-	14/53/53/53	-
25	CLA	B1	617	2	-	12/39/115/115	-
23	BCR	B2	601	-	-	0/29/63/63	0/2/2/2
25	CLA	c2	503	3	-	15/39/115/115	-
25	CLA	C1	506	3	-	17/39/115/115	-
25	CLA	B2	607	2	-	7/39/115/115	-
25	CLA	C2	508	3	-	7/21/97/115	-
23	BCR	b2	601	-	-	0/29/63/63	0/2/2/2
25	CLA	B1	608	2	-	16/39/115/115	-
25	CLA	b2	624	2	-	9/39/115/115	-
29	LMG	d1	411	-	-	2/36/36/70	-
29	LMG	j2	101	-	-	7/45/65/70	0/1/1/1
34	DGD	C1	516	-	-	9/51/91/95	0/2/2/2
25	CLA	C2	510	3	-	6/15/91/115	-
37	SQD	B2	623	-	-	2/40/60/69	0/1/1/1
25	CLA	D1	402	4	-	9/39/115/115	-
25	CLA	B2	608	2	-	20/39/115/115	-
23	BCR	b1	602	-	-	3/29/63/63	0/2/2/2
25	CLA	c2	507	3	-	5/26/102/115	-
23	BCR	z2	101	-	-	0/29/63/63	0/2/2/2
23	BCR	c2	501	-	-	14/29/63/63	0/2/2/2
38	HEM	V2	201	16	-	3/14/54/54	-
23	BCR	H2	103	-	-	3/17/34/63	0/1/1/2
25	CLA	C2	516	3	-	8/17/93/115	-
33	LHG	l2	101	-	-	20/48/48/53	-
25	CLA	D2	401	4	-	7/39/115/115	-
25	CLA	C1	511	3	-	12/39/115/115	-
25	CLA	B1	612	-	-	10/39/115/115	-
25	CLA	D2	404	4	-	11/35/111/115	-
29	LMG	C2	515	-	-	0/18/38/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	LHG	D1	405	-	-	14/53/53/53	-
29	LMG	b1	631	-	-	7/35/55/70	0/1/1/1
25	CLA	B2	604	-	-	6/10/86/115	-
29	LMG	c2	519	-	-	3/20/40/70	0/1/1/1
25	CLA	a1	404	1	-	7/33/109/115	-
25	CLA	B2	615	2	-	11/39/115/115	-
29	LMG	A2	412	-	-	5/23/43/70	0/1/1/1
23	BCR	K1	101	-	-	5/26/43/63	0/1/1/2
27	PHO	a1	411	-	-	5/37/103/103	0/5/6/6
25	CLA	b2	615	2	-	8/33/109/115	-
37	SQD	D1	409	-	-	2/29/49/69	0/1/1/1
25	CLA	b2	611	-	-	7/39/115/115	-
25	CLA	b2	617	2	-	18/39/115/115	-
25	CLA	B2	611	2	-	10/39/115/115	-
25	CLA	D1	403	4	-	4/23/99/115	-
23	BCR	b2	603	-	-	0/29/63/63	0/2/2/2
29	LMG	b1	621	-	-	6/33/53/70	0/1/1/1
33	LHG	D2	405	-	-	16/53/53/53	-
23	BCR	c1	501	-	-	0/29/63/63	0/2/2/2
23	BCR	K2	102	-	-	7/29/63/63	0/2/2/2
25	CLA	B2	606	2	-	13/39/115/115	-
35	LMT	C1	519	-	-	2/21/61/61	0/2/2/2
25	CLA	c2	502	3	-	13/39/115/115	-
25	CLA	B2	614	2	-	12/39/115/115	-
33	LHG	a1	407	-	-	14/47/47/53	-
34	DGD	c1	520	-	-	8/51/91/95	0/2/2/2
25	CLA	c2	508	40	-	16/39/115/115	-
27	PHO	A2	407	-	-	8/37/103/103	0/5/6/6
32	GOL	b1	618	-	-	4/4/4/4	-
25	CLA	b1	604	-	-	16/39/115/115	-
23	BCR	b1	601	-	-	0/29/63/63	0/2/2/2
25	CLA	c1	509	40	-	17/39/115/115	-
25	CLA	c2	505	-	-	16/39/115/115	-
25	CLA	B1	605	2	-	11/39/115/115	-
23	BCR	a2	402	-	-	3/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	d1	401	4	-	12/39/115/115	-
25	CLA	B2	612	-	-	9/39/115/115	-
29	LMG	A1	412	-	-	7/36/56/70	0/1/1/1
25	CLA	C1	510	3	-	8/39/115/115	-
29	LMG	A1	410	-	-	4/38/58/70	0/1/1/1
33	LHG	A2	405	-	-	10/37/37/53	-
25	CLA	B1	610	2	-	13/39/115/115	-
33	LHG	B2	627	-	-	8/46/46/53	-
33	LHG	B1	621	-	-	11/53/53/53	-
25	CLA	c2	506	3	-	13/35/111/115	-
29	LMG	b1	624	-	-	3/34/54/70	0/1/1/1
35	LMT	L1	102	-	-	1/9/9/61	-
25	CLA	B1	615	2	-	15/39/115/115	-
25	CLA	b1	611	2	-	8/39/115/115	-
25	CLA	C2	506	-	-	14/39/115/115	-
25	CLA	B2	617	2	-	9/39/115/115	-
25	CLA	C1	514	3	-	4/15/91/115	-
27	PHO	A1	408	-	-	7/37/103/103	0/5/6/6
38	HEM	v2	201	16	-	2/14/54/54	-
23	BCR	d2	401	-	-	8/29/63/63	0/2/2/2
29	LMG	D1	406	-	-	4/30/50/70	0/1/1/1
23	BCR	K2	104	-	-	2/12/46/63	0/2/2/2
35	LMT	a2	406	-	-	5/21/61/61	0/2/2/2
38	HEM	E2	101	5	-	1/14/54/54	-
25	CLA	b2	608	2	-	14/39/115/115	-
25	CLA	C1	509	3	-	20/39/115/115	-
25	CLA	b2	616	2	-	11/33/109/115	-
23	BCR	j2	102	-	-	9/29/63/63	0/2/2/2
25	CLA	B1	604	-	-	6/12/88/115	-
25	CLA	B1	619	40	-	18/39/115/115	-
25	CLA	b1	619	2	-	17/39/115/115	-
25	CLA	C1	508	-	-	13/39/115/115	-
23	BCR	a1	401	-	-	2/29/63/63	0/2/2/2
23	BCR	B1	603	-	-	1/29/63/63	0/2/2/2
25	CLA	c2	511	3	-	16/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	PL9	D1	408	-	-	7/53/73/73	0/1/1/1
25	CLA	B2	619	-	-	17/39/115/115	-
25	CLA	C1	503	3	-	13/33/109/115	-
25	CLA	B2	609	2	-	11/39/115/115	-
23	BCR	C1	521	-	-	0/29/63/63	0/2/2/2
23	BCR	F2	401	-	-	9/29/63/63	0/2/2/2
29	LMG	B2	620	-	-	8/35/55/70	0/1/1/1
25	CLA	C2	513	3	-	2/25/101/115	-
23	BCR	k1	101	-	-	5/29/63/63	0/2/2/2
25	CLA	b1	613	2	-	8/39/115/115	-
29	LMG	I2	101	-	-	3/29/49/70	0/1/1/1
25	CLA	c1	504	3	-	7/39/115/115	-
25	CLA	B1	611	2	-	11/36/112/115	-
25	CLA	b1	617	2	-	5/39/115/115	-
25	CLA	b1	607	2	-	10/39/115/115	-
29	LMG	d1	408	-	-	2/28/48/70	0/1/1/1
32	GOL	B1	620	-	-	2/4/4/4	-
23	BCR	b2	602	-	-	6/29/63/63	0/2/2/2
25	CLA	b1	608	2	-	17/39/115/115	-
23	BCR	B2	602	-	-	2/29/63/63	0/2/2/2
27	PHO	a2	416	-	-	6/37/103/103	0/5/6/6
25	CLA	c1	515	3	-	9/27/103/115	-
32	GOL	a1	406	-	-	2/4/4/4	-
33	LHG	d2	403	-	-	13/53/53/53	-
38	HEM	V1	201	16	-	4/14/54/54	-
25	CLA	B1	618	2	-	3/31/107/115	-
25	CLA	B1	614	2	-	12/39/115/115	-
25	CLA	A2	402	1	-	10/39/115/115	-
23	BCR	B2	603	-	-	2/29/63/63	0/2/2/2
32	GOL	C2	514	-	-	2/4/4/4	-
34	DGD	c1	514	-	-	9/40/80/95	0/2/2/2
25	CLA	c1	506	40	-	15/39/115/115	-
33	LHG	D1	404	-	-	11/53/53/53	-
34	DGD	c1	518	-	-	10/51/91/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	B2	616	2	-	9/26/102/115	-
25	CLA	B1	609	2	-	12/39/115/115	-
34	DGD	H1	101	-	-	12/51/91/95	0/2/2/2
25	CLA	c2	504	3	-	12/39/115/115	-
34	DGD	c2	516	-	-	6/41/81/95	0/2/2/2
29	LMG	B1	626	-	-	12/43/63/70	0/1/1/1
23	BCR	H1	102	-	-	3/15/32/63	0/1/1/2
25	CLA	d1	404	40	-	8/39/115/115	-
25	CLA	b2	619	2	-	10/32/108/115	-
25	CLA	a1	405	-	-	8/21/97/115	-
25	CLA	b2	612	2	-	12/39/115/115	-
27	PHO	d1	403	-	-	3/37/103/103	0/5/6/6
32	GOL	c1	521	-	-	2/4/4/4	-
25	CLA	C1	504	3	-	8/39/115/115	-
25	CLA	b2	609	2	-	12/35/111/115	-
23	BCR	B1	601	-	-	0/29/63/63	0/2/2/2
25	CLA	c2	512	3	-	15/39/115/115	-
25	CLA	A2	404	-	-	9/23/99/115	-
25	CLA	b1	609	2	-	13/39/115/115	-
25	CLA	b1	614	2	-	14/39/115/115	-
37	SQD	D2	402	-	-	4/18/38/69	0/1/1/1
35	LMT	l1	101	-	-	3/15/35/61	0/1/1/2
25	CLA	C2	504	3	-	8/17/93/115	-
25	CLA	C2	505	3	-	17/39/115/115	-
25	CLA	C1	512	3	-	14/39/115/115	-
34	DGD	c2	514	-	-	16/51/91/95	0/2/2/2
35	LMT	i2	102	-	-	0/4/4/61	-
32	GOL	C1	518	-	-	2/4/4/4	-
35	LMT	T1	101	-	-	0/9/9/61	-
25	CLA	B1	616	2	-	10/39/115/115	-
23	BCR	b1	603	-	-	4/29/63/63	0/2/2/2
25	CLA	A1	403	1	-	10/39/115/115	-
35	LMT	c1	517	-	-	1/19/59/61	0/2/2/2
25	CLA	c2	509	3	-	11/39/115/115	-
25	CLA	B2	618	2	-	4/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	d2	402	-	-	12/39/115/115	-
33	LHG	D2	403	-	-	10/53/53/53	-
37	SQD	b2	605	-	-	10/40/60/69	0/1/1/1
25	CLA	b2	613	2	-	6/39/115/115	-
25	CLA	d2	405	4	-	11/39/115/115	-
25	CLA	c1	503	3	-	16/39/115/115	-
23	BCR	J1	101	-	-	9/29/63/63	0/2/2/2
23	BCR	h1	102	-	-	5/29/63/63	0/2/2/2
25	CLA	C1	513	3	-	15/35/111/115	-
34	DGD	h2	102	-	-	9/51/91/95	0/2/2/2
25	CLA	C2	518	3	-	4/10/86/115	-
38	HEM	f1	101	6	-	5/14/54/54	-
25	CLA	d2	404	4	-	4/21/97/115	-
29	LMG	a1	412	-	-	12/46/66/70	0/1/1/1
33	LHG	b2	625	-	-	5/47/47/53	-
25	CLA	c1	505	3	-	5/39/115/115	-
27	PHO	D2	407	-	-	6/37/103/103	0/5/6/6
25	CLA	b2	620	40	-	22/39/115/115	-
35	LMT	m1	101	-	-	8/21/61/61	0/2/2/2
33	LHG	d2	406	-	-	10/53/53/53	-
23	BCR	B1	602	-	-	5/29/63/63	0/2/2/2
25	CLA	c2	515	3	-	6/17/93/115	-
25	CLA	b1	605	2	-	7/39/115/115	-
25	CLA	b1	606	2	-	19/39/115/115	-
35	LMT	M1	102	-	-	1/8/8/61	-
33	LHG	b1	622	-	-	14/53/53/53	-
33	LHG	d1	402	-	-	12/36/36/53	-
36	PL9	d1	409	-	-	9/53/73/73	0/1/1/1
23	BCR	c1	502	-	-	5/29/63/63	0/2/2/2
25	CLA	c2	510	3	-	8/26/102/115	-
23	BCR	C1	501	-	-	4/29/63/63	0/2/2/2
36	PL9	D2	408	-	-	7/53/73/73	0/1/1/1
23	BCR	A1	401	-	-	2/29/63/63	0/2/2/2
25	CLA	A1	406	-	-	11/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	a2	405	1	-	15/39/115/115	-
29	LMG	F2	402	-	-	2/30/50/70	0/1/1/1
34	DGD	C1	517	-	-	6/53/93/95	0/2/2/2
33	LHG	L1	101	-	-	14/45/45/53	-
29	LMG	c1	519	-	-	9/50/70/70	0/1/1/1
38	HEM	E1	101	5,6	-	3/14/54/54	-
25	CLA	A2	403	1	-	7/35/111/115	-
25	CLA	b1	616	2	-	15/39/115/115	-
25	CLA	c1	507	3	-	18/39/115/115	-
25	CLA	B2	610	2	-	6/39/115/115	-
25	CLA	K2	101	-	-	13/27/103/115	-
23	BCR	D1	401	-	-	8/29/63/63	0/2/2/2
25	CLA	b2	604	-	-	6/12/88/115	-
23	BCR	h2	101	-	-	4/29/63/63	0/2/2/2
34	DGD	C2	512	-	-	1/20/60/95	0/2/2/2
35	LMT	m2	103	-	-	5/16/56/61	0/2/2/2
33	LHG	a2	407	-	-	11/33/33/53	-
25	CLA	D2	406	-	-	14/39/115/115	-
35	LMT	b2	621	-	-	1/21/61/61	0/2/2/2
25	CLA	B2	613	2	-	12/39/115/115	-
25	CLA	b1	620	-	-	18/39/115/115	-
25	CLA	C2	507	3	-	6/15/91/115	-
25	CLA	c1	511	3	-	10/39/115/115	-
23	BCR	C2	502	-	-	0/29/63/63	0/2/2/2
34	DGD	h1	101	-	-	9/51/91/95	0/2/2/2
25	CLA	b1	615	2	-	7/32/108/115	-
35	LMT	b2	623	-	-	1/21/61/61	0/2/2/2
25	CLA	C1	505	-	-	11/39/115/115	-
23	BCR	d1	405	-	-	8/29/63/63	0/2/2/2
25	CLA	C2	509	-	-	16/39/115/115	-
25	CLA	a2	413	-	-	7/21/97/115	-
29	LMG	b2	622	-	-	0/34/54/70	0/1/1/1
34	DGD	C1	515	-	-	10/41/81/95	0/2/2/2
38	HEM	e2	101	5,6	-	2/14/54/54	-
29	LMG	d2	407	-	-	3/21/41/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	C1	507	3	-	22/39/115/115	-
25	CLA	A1	404	-	-	9/23/99/115	-
25	CLA	b2	606	2	-	14/39/115/115	-
25	CLA	C2	503	3	-	16/39/115/115	-
33	LHG	L2	101	-	-	16/53/53/53	-

The worst 5 of 1291 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	d2	408	PHO	C1D-C2D	10.10	1.50	1.39
27	D1	407	PHO	C1D-C2D	10.06	1.50	1.39
27	D2	407	PHO	C1D-C2D	9.97	1.50	1.39
27	d1	403	PHO	C1D-C2D	9.94	1.50	1.39
27	A2	407	PHO	C1D-C2D	9.92	1.50	1.39

The worst 5 of 1879 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c2	501	BCR	C36-C18-C17	-10.87	107.70	122.92
23	c2	501	BCR	C24-C23-C22	-9.36	112.09	126.23
23	c2	501	BCR	C16-C17-C18	9.01	140.16	127.31
27	d1	403	PHO	C2B-C1B-NB	8.29	115.25	109.53
27	d2	408	PHO	C2B-C1B-NB	8.22	115.20	109.53

There are no chirality outliers.

5 of 2327 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	C1	501	BCR	C7-C8-C9-C10
23	C1	501	BCR	C7-C8-C9-C34
23	D1	401	BCR	C7-C8-C9-C10
23	D1	401	BCR	C7-C8-C9-C34
23	K1	101	BCR	C1-C6-C7-C8

There are no ring outliers.

250 monomers are involved in 721 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	a1	403	CLA	5	0
27	d2	408	PHO	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	c2	517	DGD	2	0
25	B1	613	CLA	3	0
23	k2	501	BCR	8	0
25	c1	513	CLA	3	0
25	c1	508	CLA	6	0
25	c1	512	CLA	5	0
25	A1	405	CLA	6	0
25	b2	610	CLA	7	0
25	b1	612	CLA	3	0
29	M1	101	LMG	2	0
25	b2	618	CLA	2	0
25	B1	607	CLA	2	0
23	A2	401	BCR	6	0
25	d1	406	CLA	2	0
25	C2	511	CLA	1	0
25	c1	516	CLA	1	0
29	C1	520	LMG	1	0
34	H2	101	DGD	3	0
27	D1	407	PHO	1	0
25	B1	606	CLA	5	0
25	a2	404	CLA	7	0
25	B2	605	CLA	2	0
36	d2	409	PL9	7	0
25	b2	614	CLA	1	0
35	m2	104	LMT	1	0
25	C1	502	CLA	2	0
25	c1	510	CLA	4	0
38	v1	201	HEM	3	0
33	l1	102	LHG	3	0
32	i1	101	GOL	1	0
29	B2	621	LMG	2	0
29	B1	622	LMG	1	0
33	d1	407	LHG	4	0
25	B1	617	CLA	5	0
23	B2	601	BCR	5	0
25	c2	503	CLA	4	0
25	C1	506	CLA	4	0
25	B2	607	CLA	2	0
25	C2	508	CLA	1	0
23	b2	601	BCR	4	0
25	B1	608	CLA	3	0
25	b2	624	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	j2	101	LMG	6	0
34	C1	516	DGD	7	0
25	C2	510	CLA	1	0
37	B2	623	SQD	2	0
25	D1	402	CLA	3	0
25	B2	608	CLA	6	0
23	b1	602	BCR	2	0
25	c2	507	CLA	2	0
23	z2	101	BCR	5	0
23	c2	501	BCR	8	0
38	V2	201	HEM	4	0
23	H2	103	BCR	4	0
25	C2	516	CLA	1	0
33	l2	101	LHG	5	0
25	D2	401	CLA	3	0
25	C1	511	CLA	4	0
25	B1	612	CLA	3	0
25	D2	404	CLA	3	0
33	D1	405	LHG	6	0
29	b1	631	LMG	2	0
25	B2	604	CLA	1	0
25	a1	404	CLA	7	0
25	B2	615	CLA	2	0
29	A2	412	LMG	1	0
23	K1	101	BCR	4	0
27	a1	411	PHO	4	0
25	b2	615	CLA	4	0
37	D1	409	SQD	1	0
25	b2	611	CLA	1	0
25	B2	611	CLA	5	0
23	b2	603	BCR	8	0
29	b1	621	LMG	3	0
33	D2	405	LHG	7	0
23	c1	501	BCR	7	0
23	K2	102	BCR	5	0
25	B2	606	CLA	3	0
35	C1	519	LMT	1	0
25	c2	502	CLA	5	0
25	B2	614	CLA	5	0
33	a1	407	LHG	3	0
34	c1	520	DGD	1	0
25	c2	508	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	A2	407	PHO	2	0
25	b1	604	CLA	2	0
23	b1	601	BCR	4	0
25	c1	509	CLA	4	0
25	c2	505	CLA	3	0
25	B1	605	CLA	2	0
23	a2	402	BCR	4	0
25	d1	401	CLA	7	0
25	B2	612	CLA	2	0
29	A1	412	LMG	3	0
25	C1	510	CLA	3	0
29	A1	410	LMG	3	0
33	A2	405	LHG	3	0
25	B1	610	CLA	6	0
33	B2	627	LHG	2	0
33	B1	621	LHG	8	0
25	c2	506	CLA	4	0
29	b1	624	LMG	9	0
35	L1	102	LMT	1	0
25	B1	615	CLA	2	0
25	b1	611	CLA	3	0
25	B2	617	CLA	3	0
25	C1	514	CLA	2	0
27	A1	408	PHO	2	0
38	v2	201	HEM	3	0
23	d2	401	BCR	4	0
29	D1	406	LMG	1	0
23	K2	104	BCR	3	0
35	a2	406	LMT	2	0
38	E2	101	HEM	4	0
25	b2	608	CLA	5	0
25	C1	509	CLA	7	0
25	b2	616	CLA	2	0
23	j2	102	BCR	9	0
25	B1	604	CLA	2	0
25	B1	619	CLA	4	0
25	b1	619	CLA	1	0
25	C1	508	CLA	2	0
23	a1	401	BCR	7	0
23	B1	603	BCR	3	0
25	c2	511	CLA	3	0
36	D1	408	PL9	9	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	B2	619	CLA	1	0
25	C1	503	CLA	2	0
25	B2	609	CLA	2	0
23	C1	521	BCR	3	0
23	F2	401	BCR	4	0
29	B2	620	LMG	1	0
25	C2	513	CLA	2	0
23	k1	101	BCR	6	0
25	b1	613	CLA	4	0
29	I2	101	LMG	2	0
25	c1	504	CLA	4	0
25	B1	611	CLA	6	0
25	b1	607	CLA	2	0
29	d1	408	LMG	1	0
23	b2	602	BCR	3	0
25	b1	608	CLA	3	0
23	B2	602	BCR	6	0
27	a2	416	PHO	3	0
25	c1	515	CLA	1	0
33	d2	403	LHG	4	0
38	V1	201	HEM	3	0
25	B1	614	CLA	1	0
25	A2	402	CLA	6	0
23	B2	603	BCR	3	0
34	c1	514	DGD	6	0
25	c1	506	CLA	5	0
33	D1	404	LHG	4	0
34	c1	518	DGD	7	0
25	B2	616	CLA	3	0
25	B1	609	CLA	2	0
34	H1	101	DGD	1	0
25	c2	504	CLA	4	0
34	c2	516	DGD	1	0
29	B1	626	LMG	2	0
23	H1	102	BCR	3	0
25	d1	404	CLA	7	0
25	b2	619	CLA	2	0
25	a1	405	CLA	1	0
25	b2	612	CLA	5	0
27	d1	403	PHO	2	0
25	C1	504	CLA	5	0
25	b2	609	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	B1	601	BCR	6	0
25	c2	512	CLA	4	0
33	L2	101	LHG	5	0
25	A2	404	CLA	1	0
25	b1	609	CLA	7	0
25	b1	614	CLA	4	0
35	l1	101	LMT	1	0
25	C2	505	CLA	4	0
25	C1	512	CLA	3	0
34	c2	514	DGD	3	0
25	B1	616	CLA	5	0
23	b1	603	BCR	4	0
25	A1	403	CLA	4	0
25	c2	509	CLA	5	0
25	B2	618	CLA	1	0
25	d2	402	CLA	4	0
33	D2	403	LHG	9	0
37	b2	605	SQD	2	0
25	b2	613	CLA	2	0
25	d2	405	CLA	3	0
25	c1	503	CLA	4	0
23	J1	101	BCR	6	0
23	h1	102	BCR	3	0
25	C1	513	CLA	4	0
34	h2	102	DGD	5	0
38	f1	101	HEM	3	0
29	a1	412	LMG	6	0
25	c1	505	CLA	1	0
27	D2	407	PHO	3	0
25	b2	620	CLA	6	0
35	m1	101	LMT	1	0
33	d2	406	LHG	5	0
23	B1	602	BCR	5	0
25	c2	515	CLA	3	0
25	b1	605	CLA	1	0
25	b1	606	CLA	5	0
33	b1	622	LHG	4	0
35	M1	102	LMT	1	0
33	d1	402	LHG	2	0
36	d1	409	PL9	12	0
23	c1	502	BCR	4	0
25	c2	510	CLA	3	0

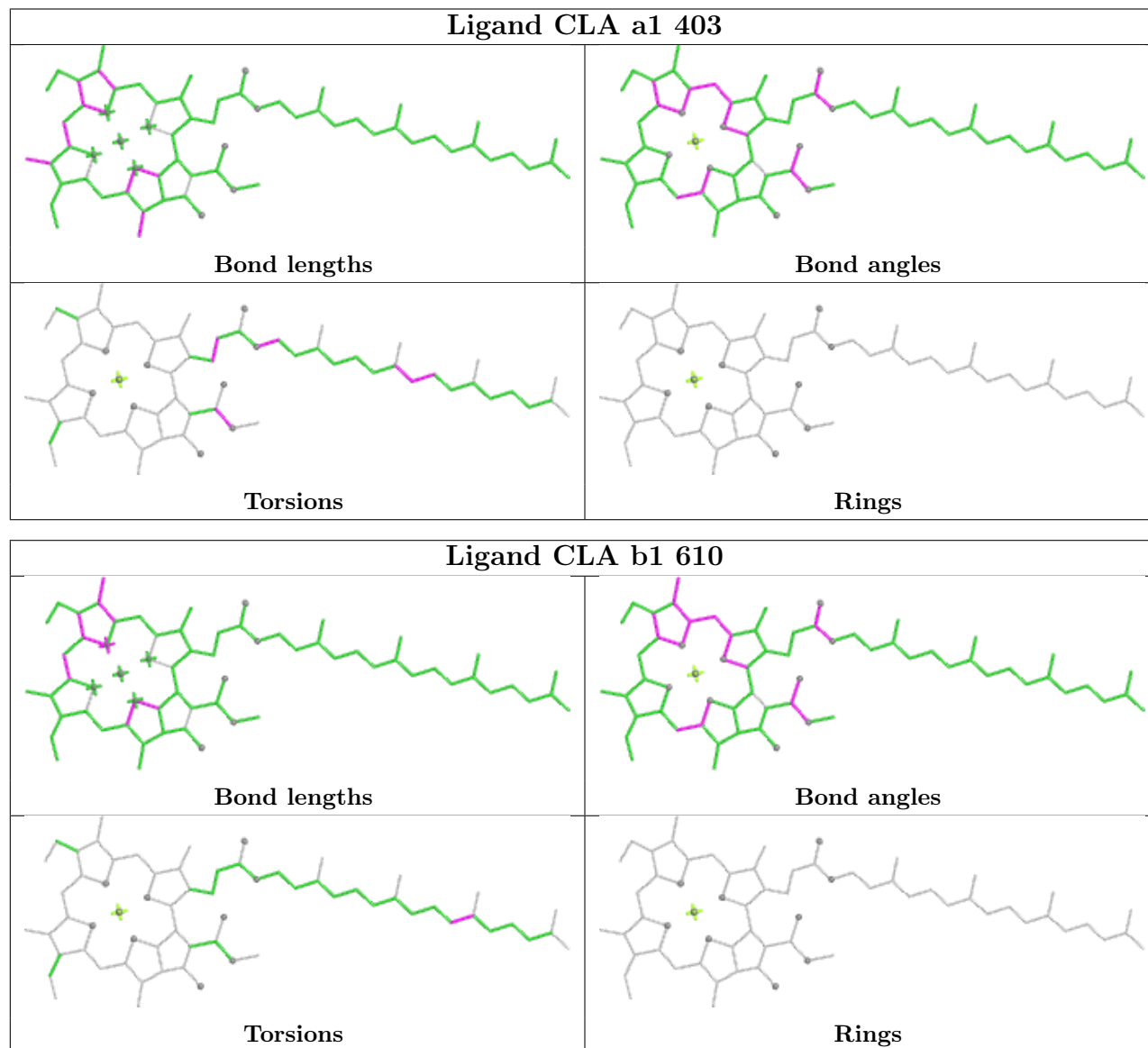
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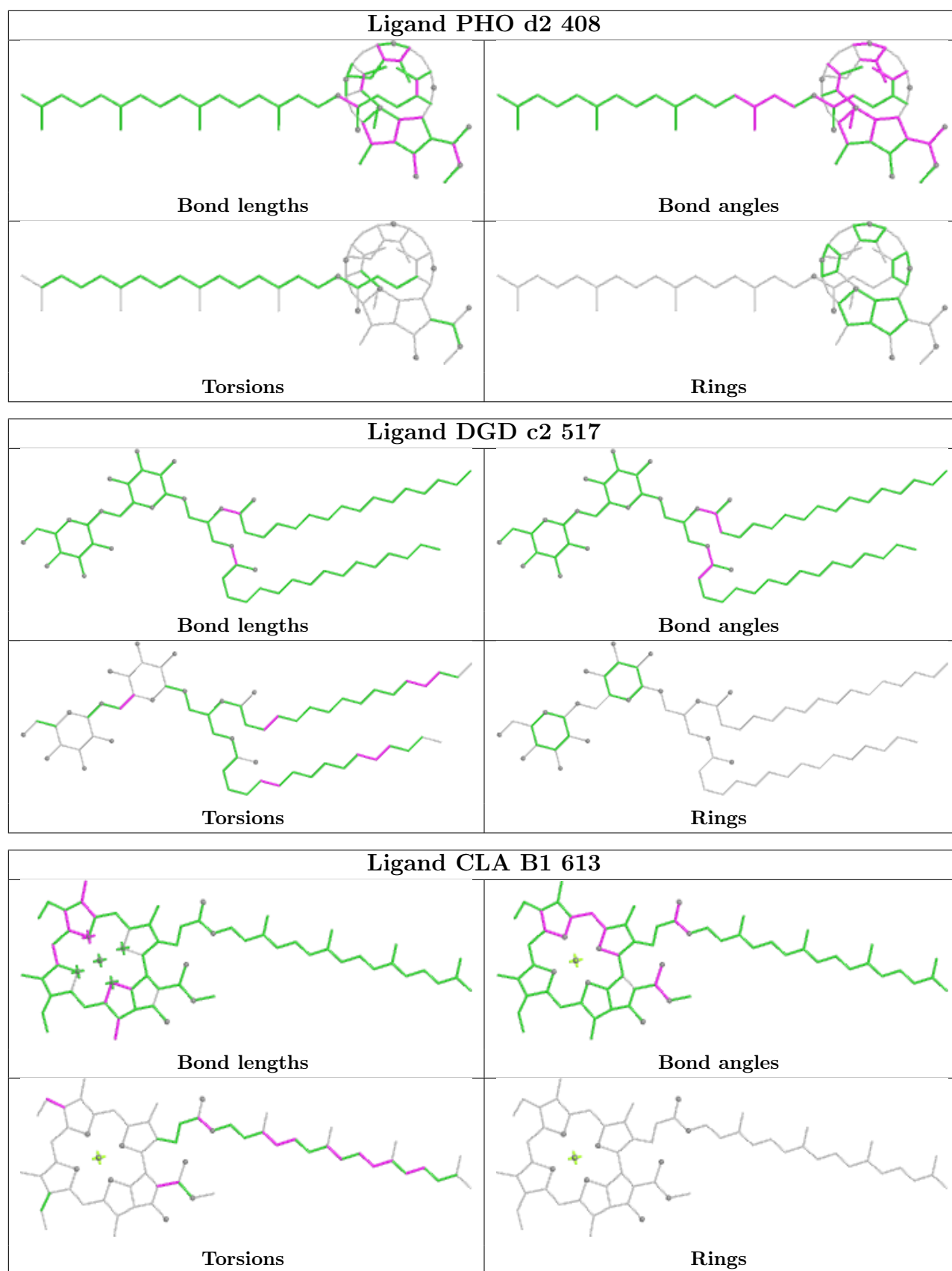
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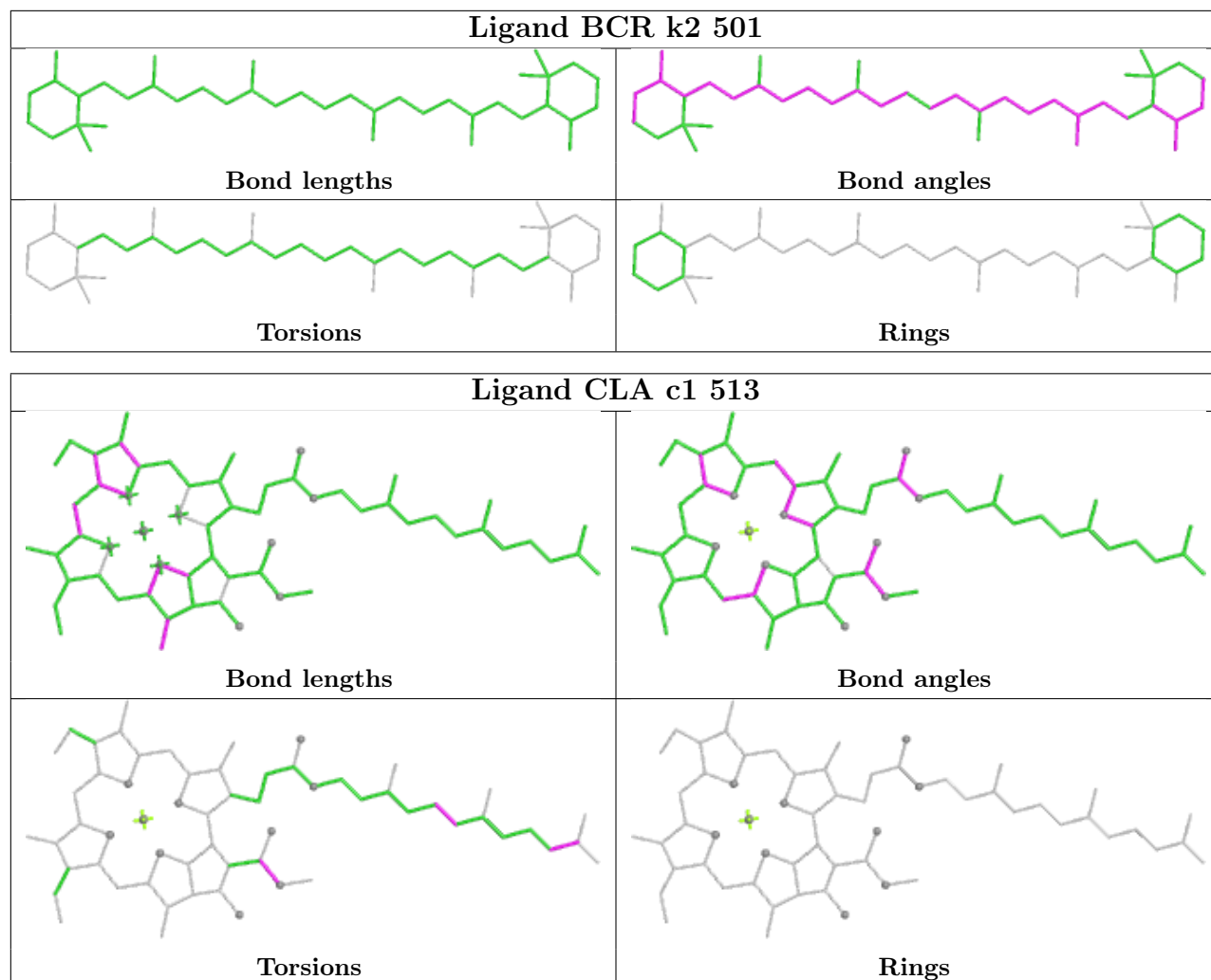
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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36	D2	408	PL9	11	0
23	A1	401	BCR	4	0
25	A1	406	CLA	5	0
25	a2	405	CLA	2	0
29	F2	402	LMG	1	0
34	C1	517	DGD	1	0
33	L1	101	LHG	1	0
29	c1	519	LMG	1	0
38	E1	101	HEM	3	0
25	A2	403	CLA	10	0
25	b1	616	CLA	3	0
25	c1	507	CLA	5	0
25	B2	610	CLA	2	0
25	K2	101	CLA	4	0
23	D1	401	BCR	3	0
23	h2	101	BCR	3	0
35	m2	103	LMT	2	0
33	a2	407	LHG	4	0
25	D2	406	CLA	4	0
25	B2	613	CLA	4	0
25	b1	620	CLA	1	0
25	C2	507	CLA	2	0
25	c1	511	CLA	1	0
23	C2	502	BCR	3	0
34	h1	101	DGD	4	0
35	b2	623	LMT	2	0
25	C1	505	CLA	2	0
23	d1	405	BCR	4	0
25	C2	509	CLA	3	0
29	b2	622	LMG	3	0
34	C1	515	DGD	2	0
38	e2	101	HEM	3	0
29	d2	407	LMG	2	0
25	C1	507	CLA	1	0
25	A1	404	CLA	1	0
25	b2	606	CLA	7	0
25	C2	503	CLA	4	0

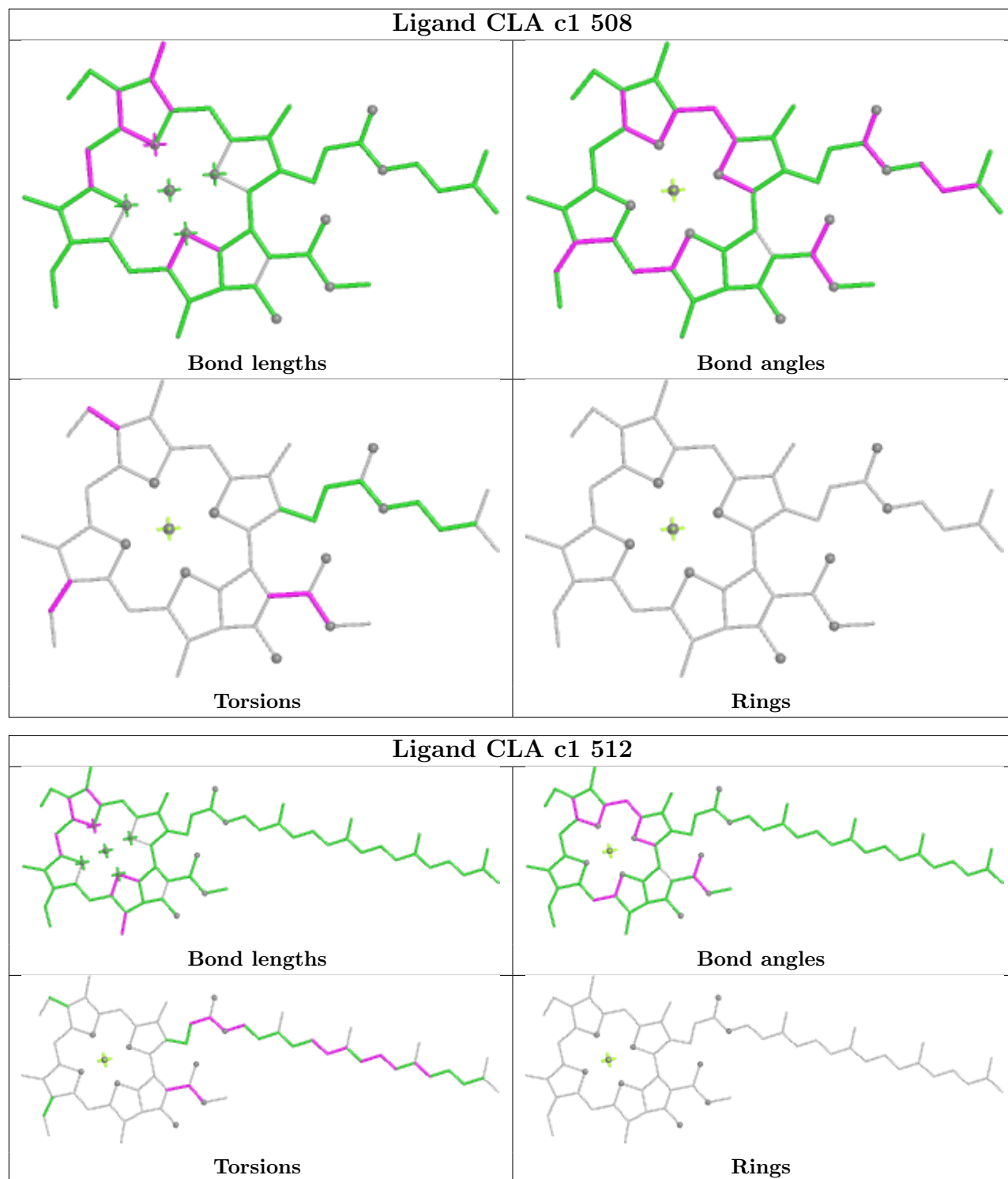
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

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

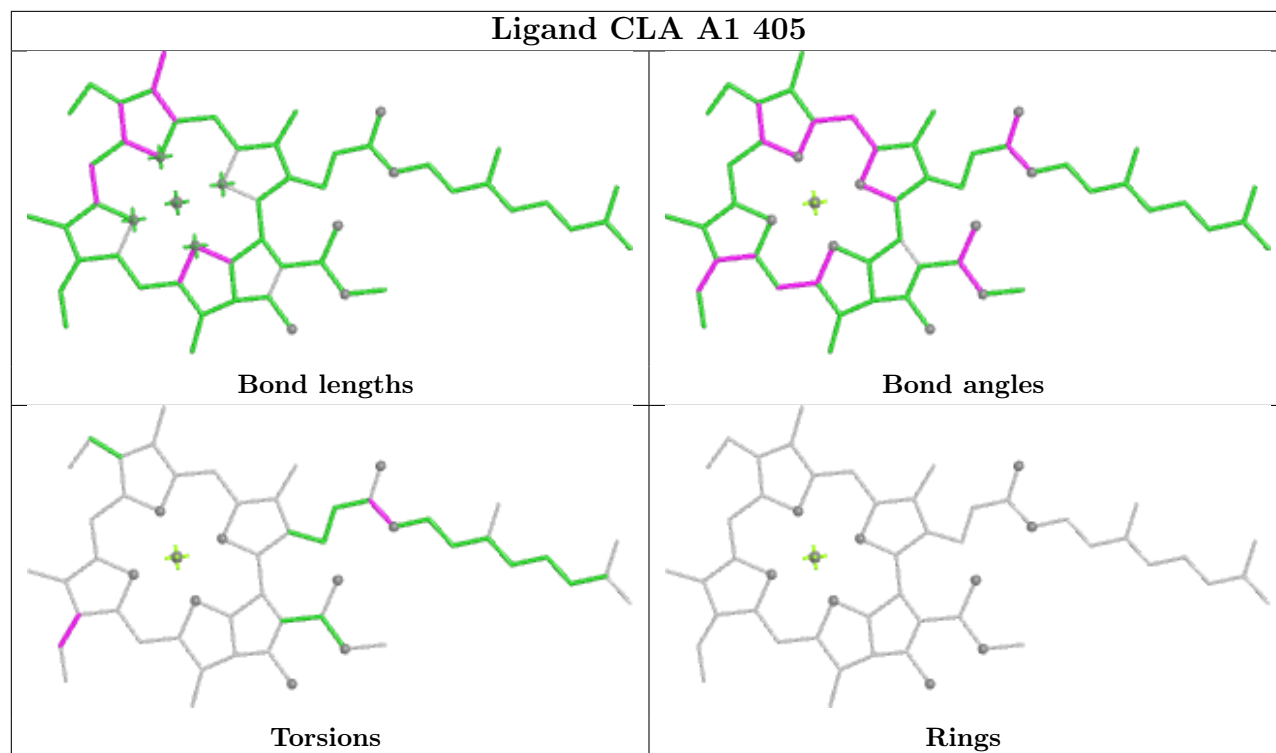




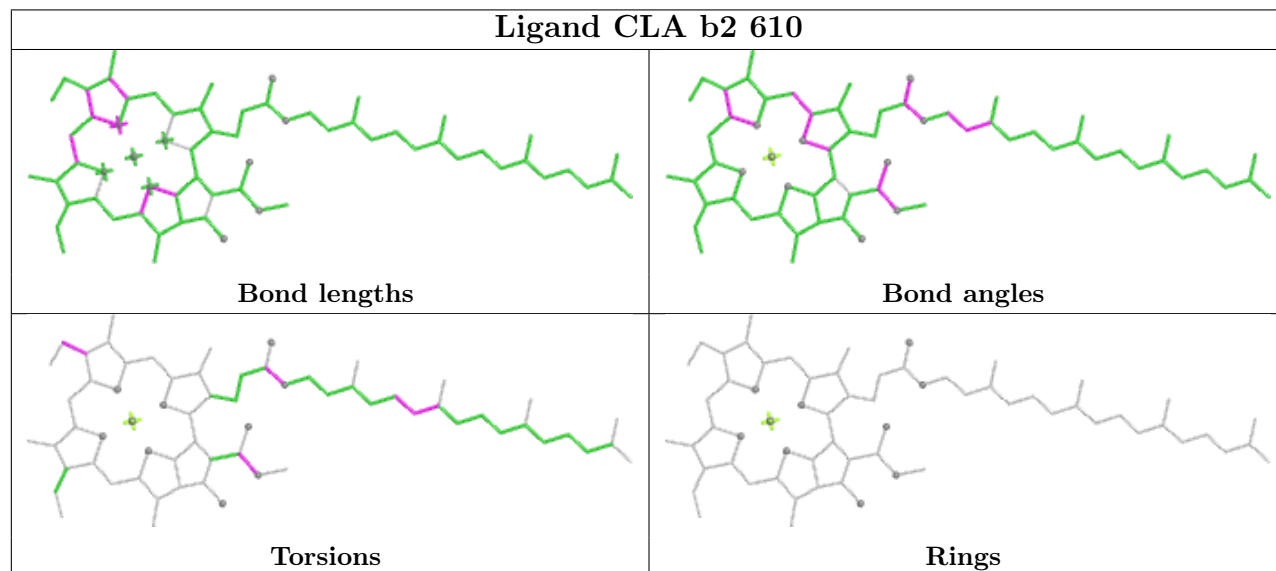


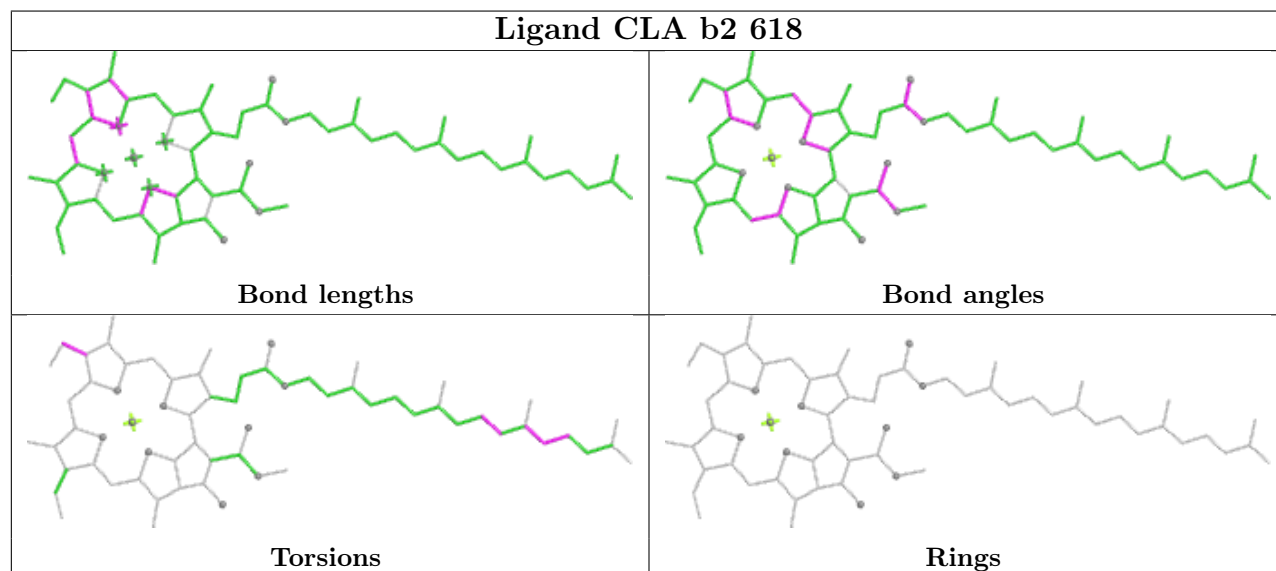
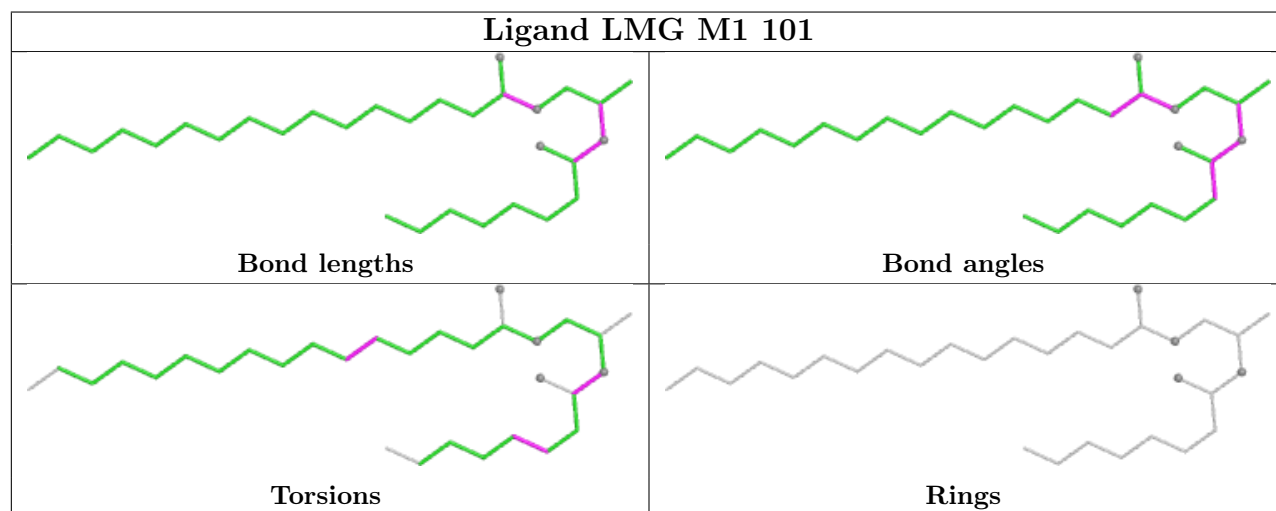
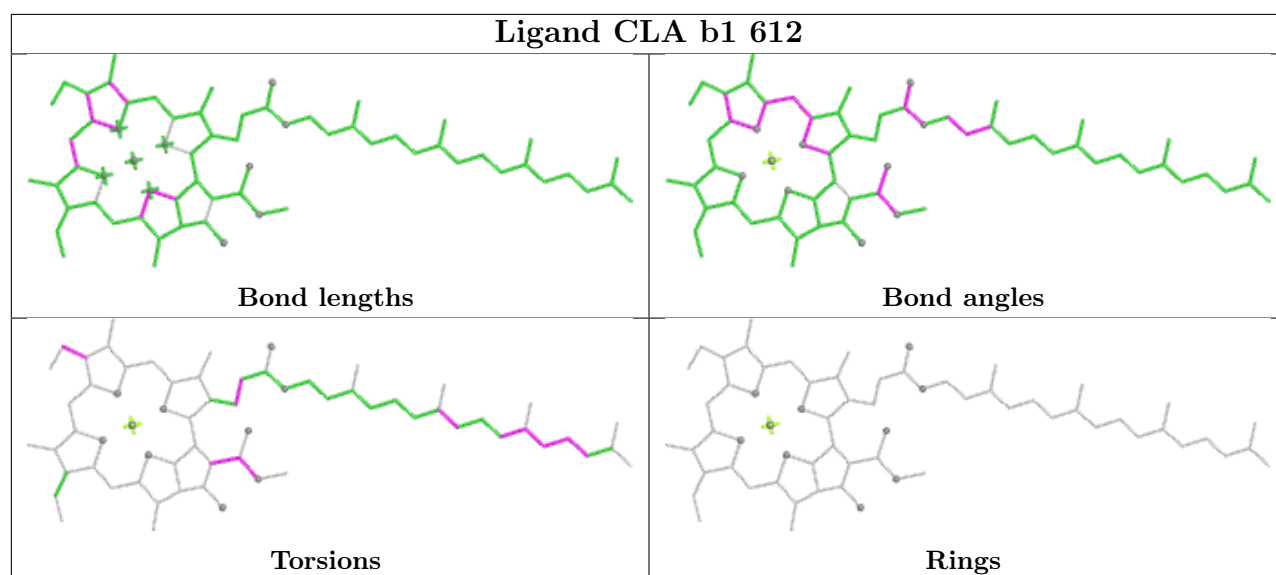


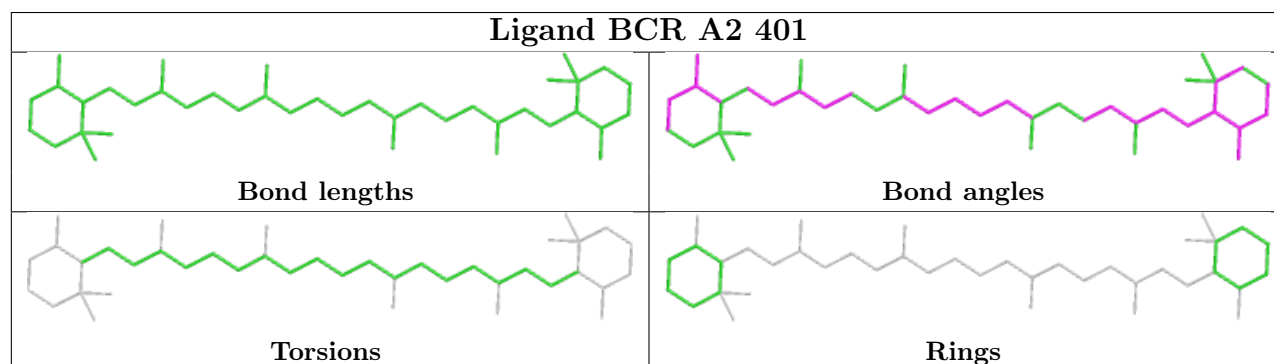
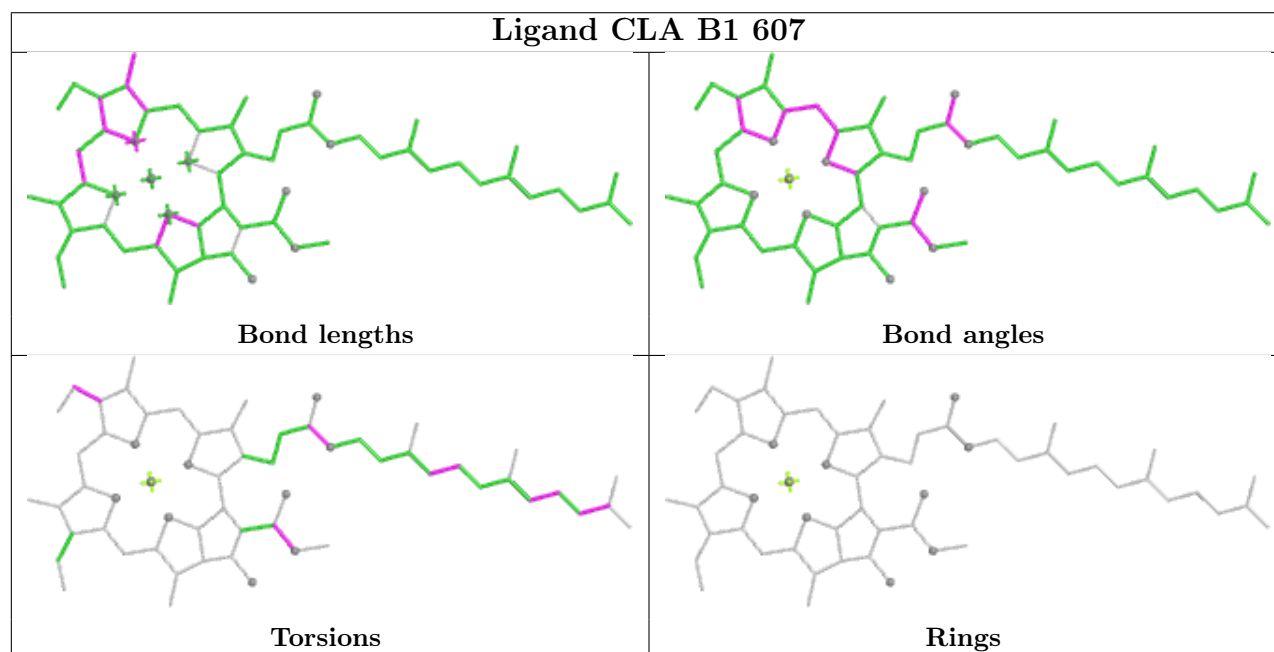
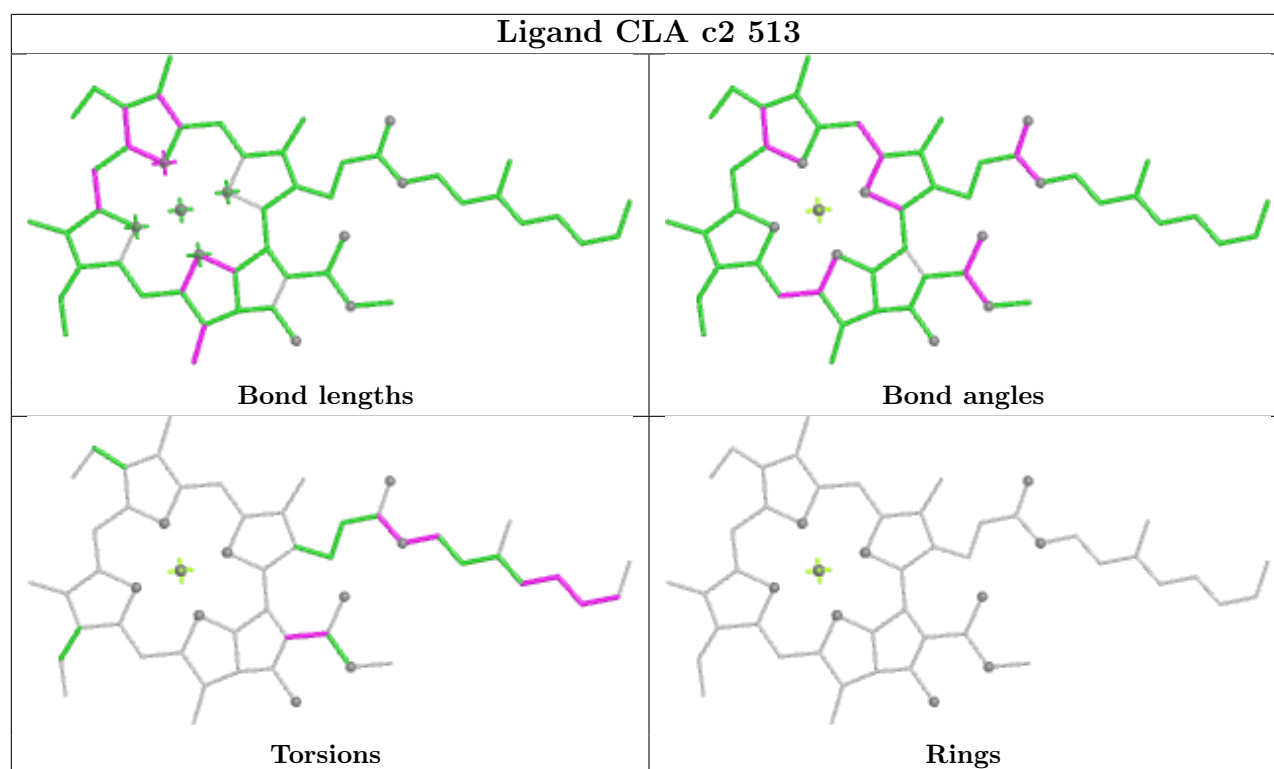
Ligand CLA A1 405

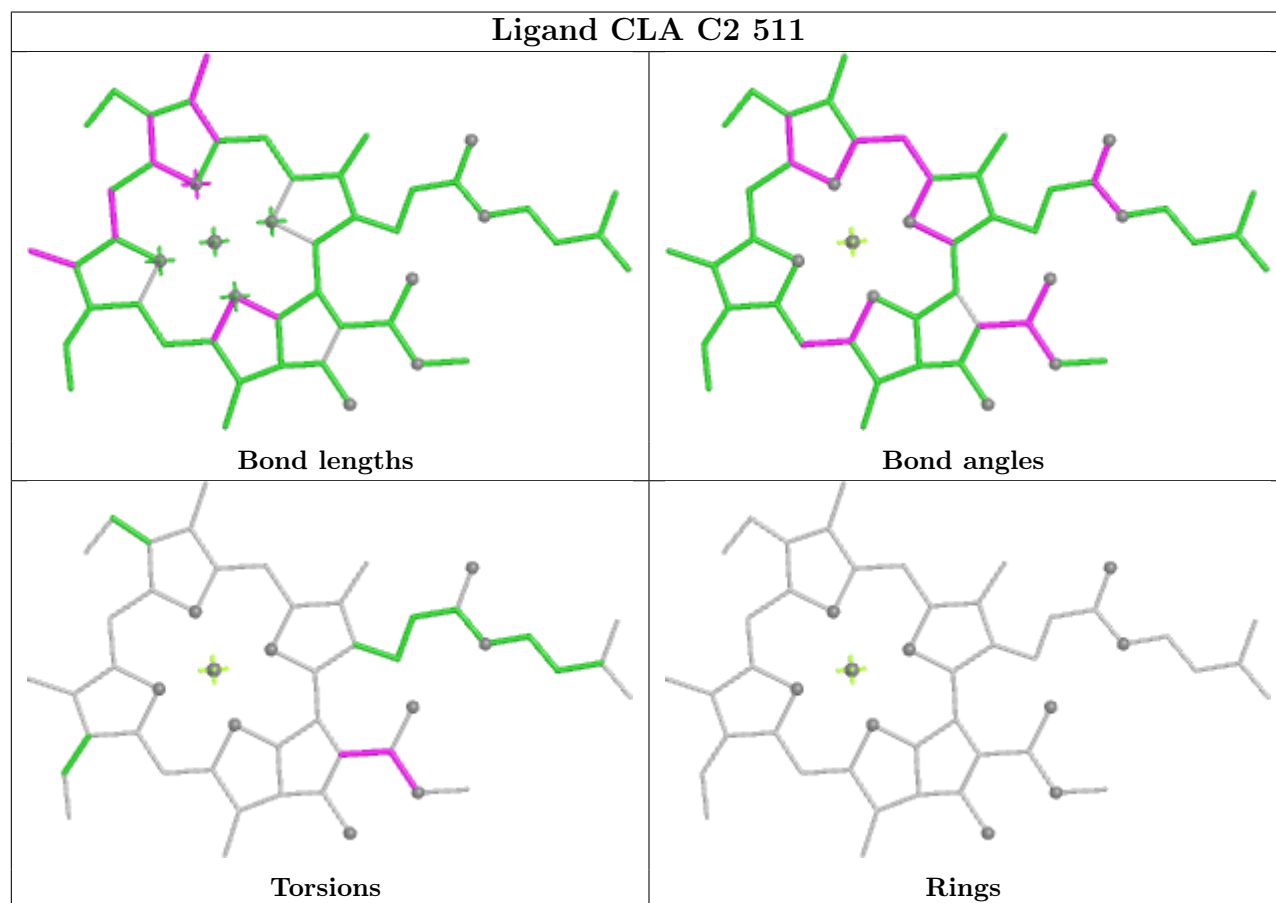
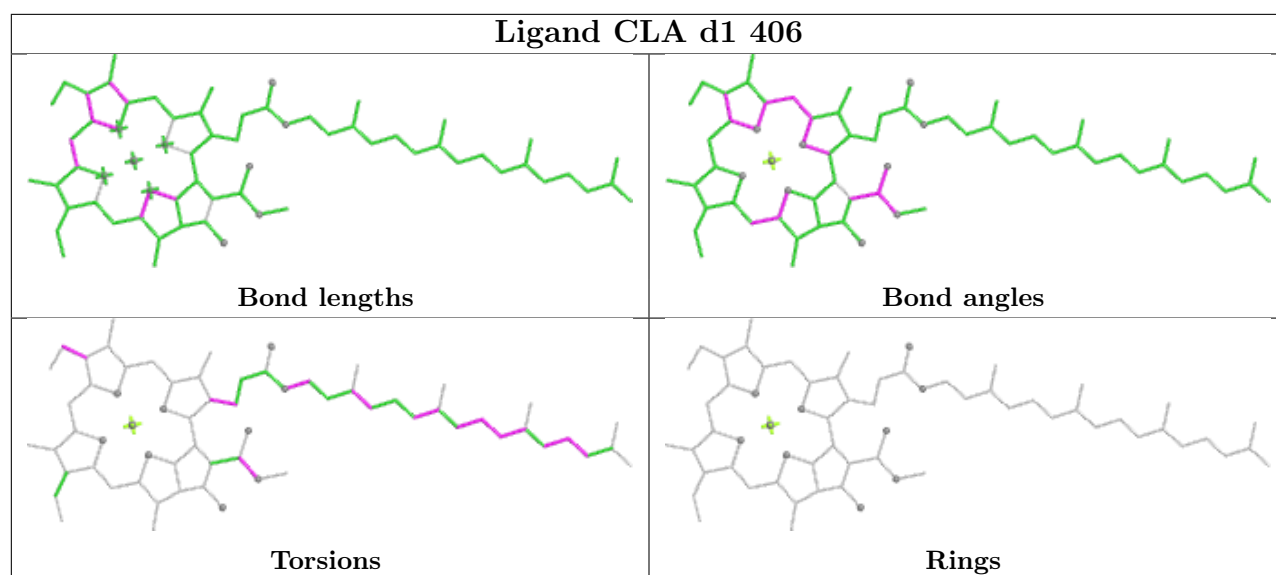


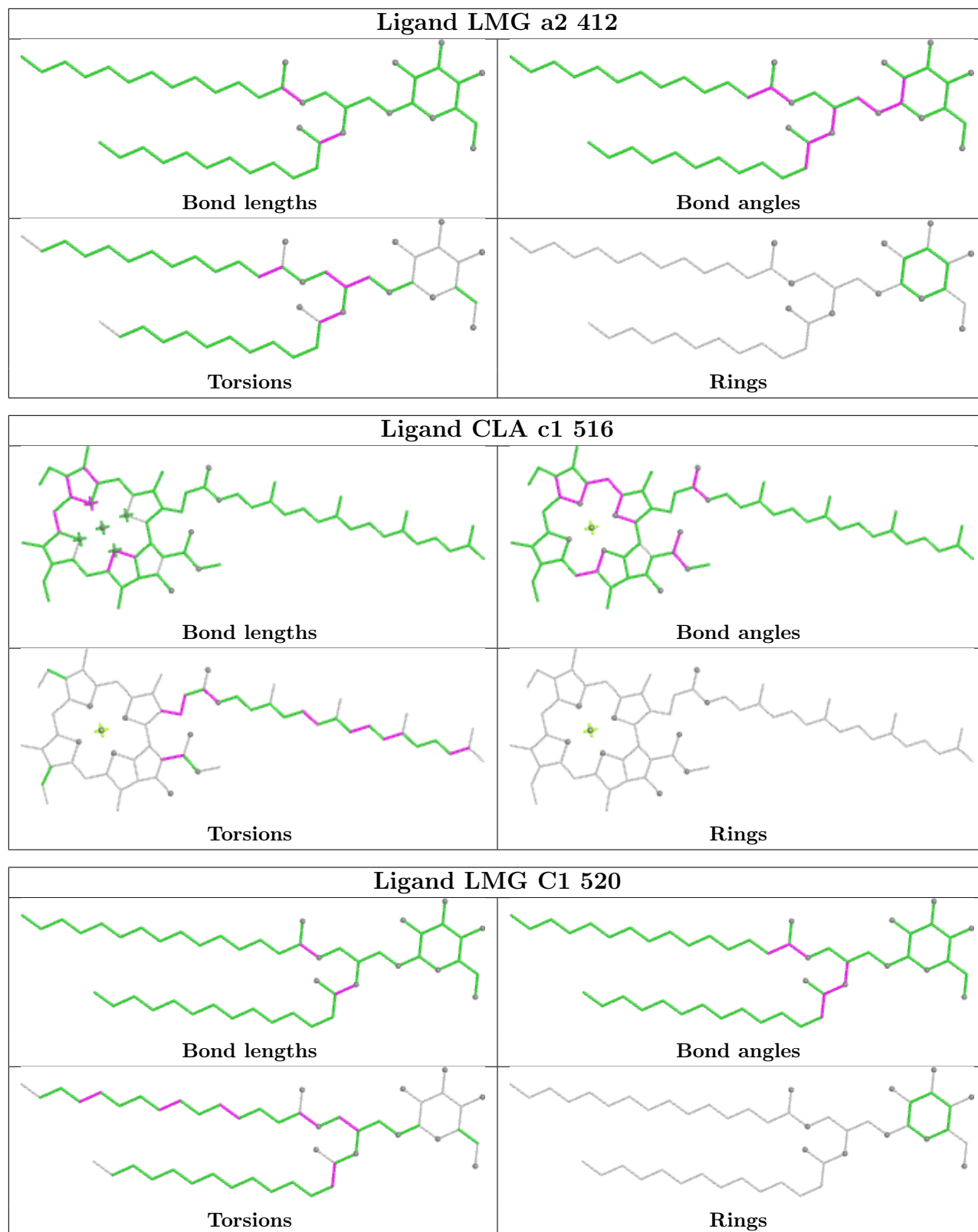
Ligand CLA b2 610

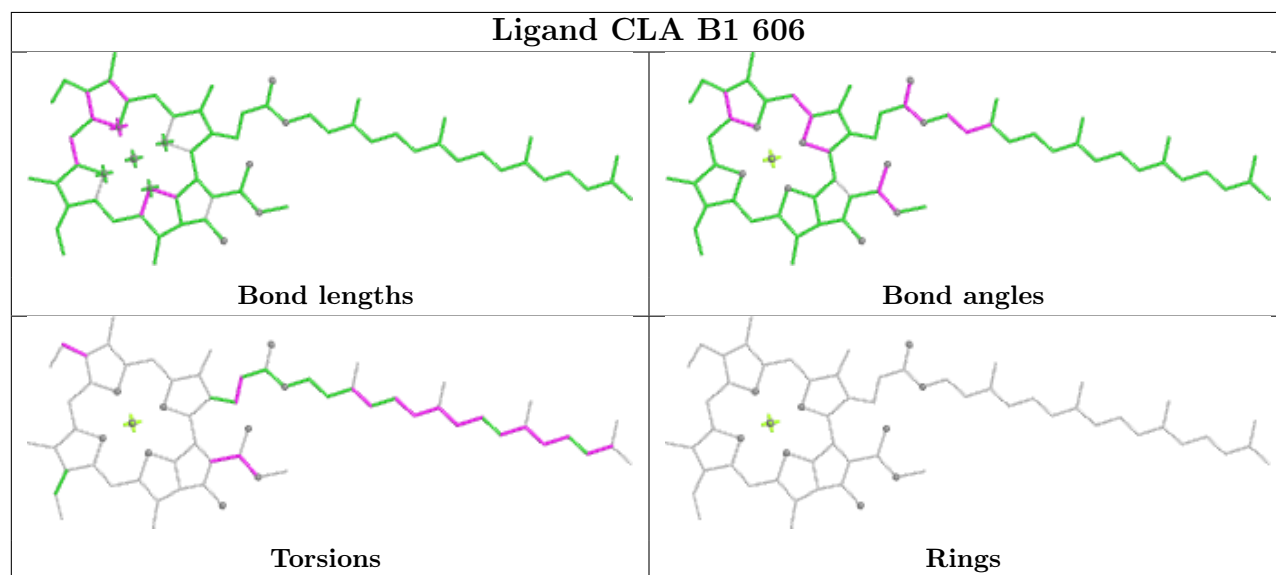
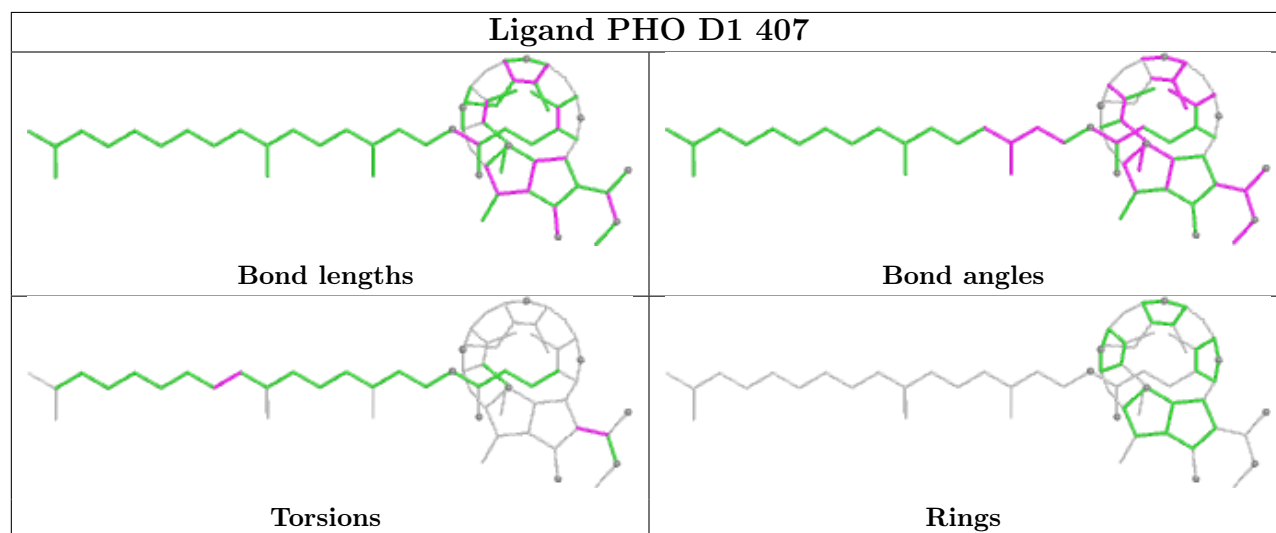
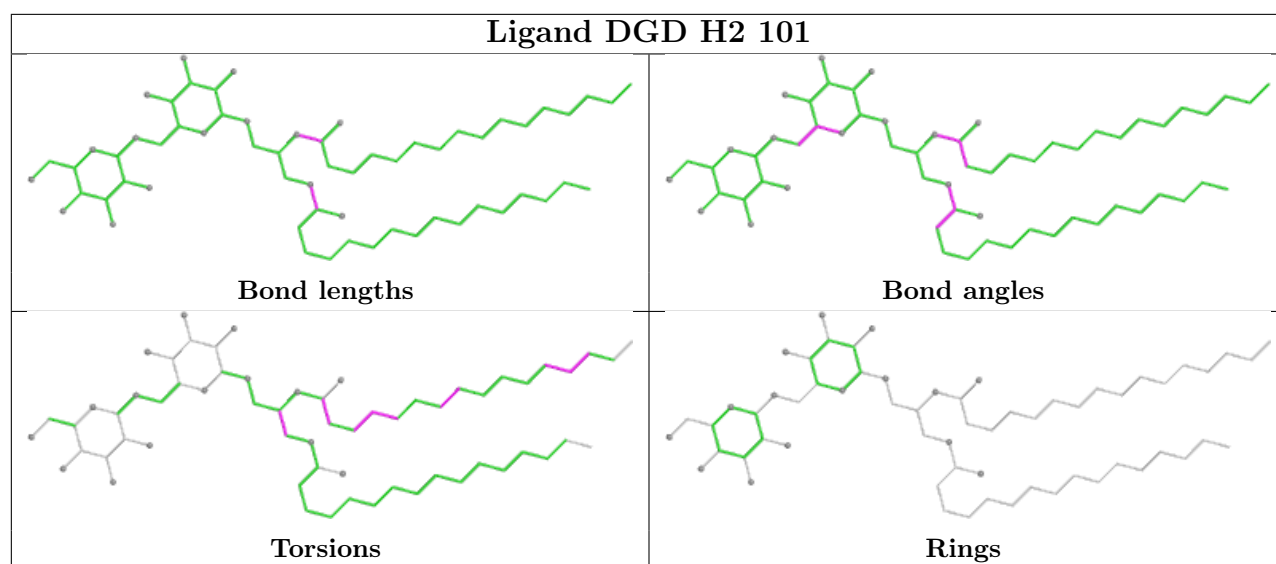


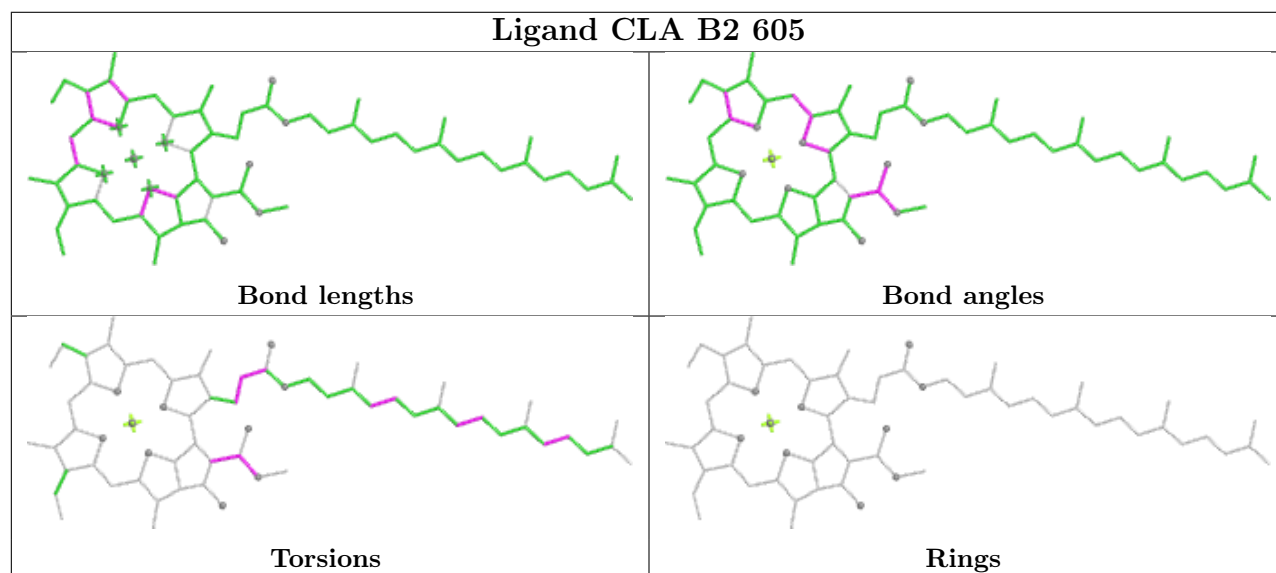
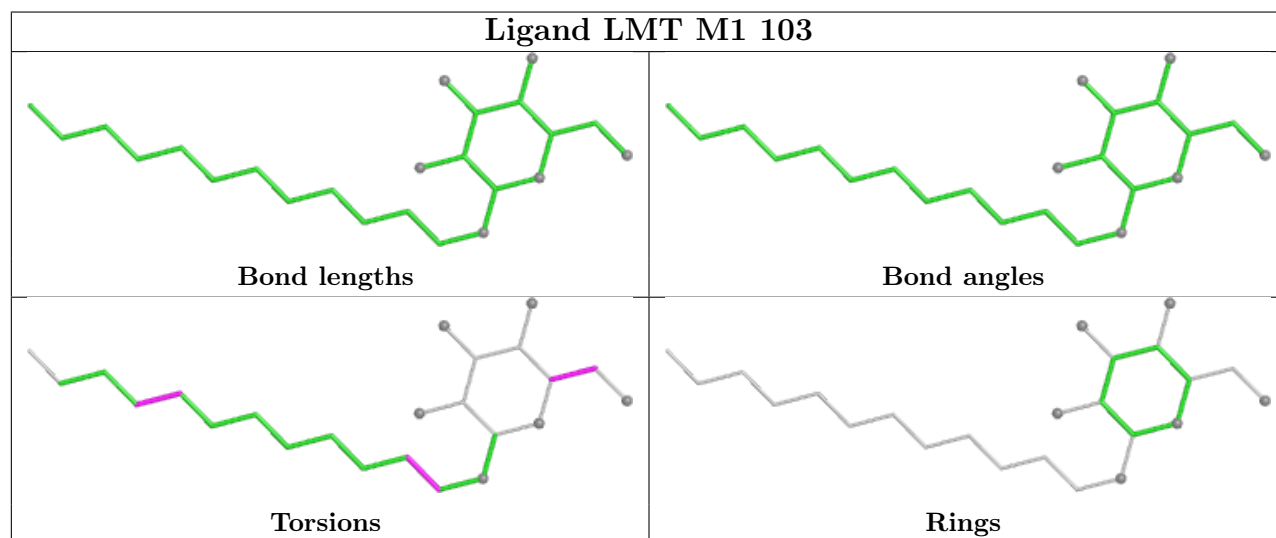
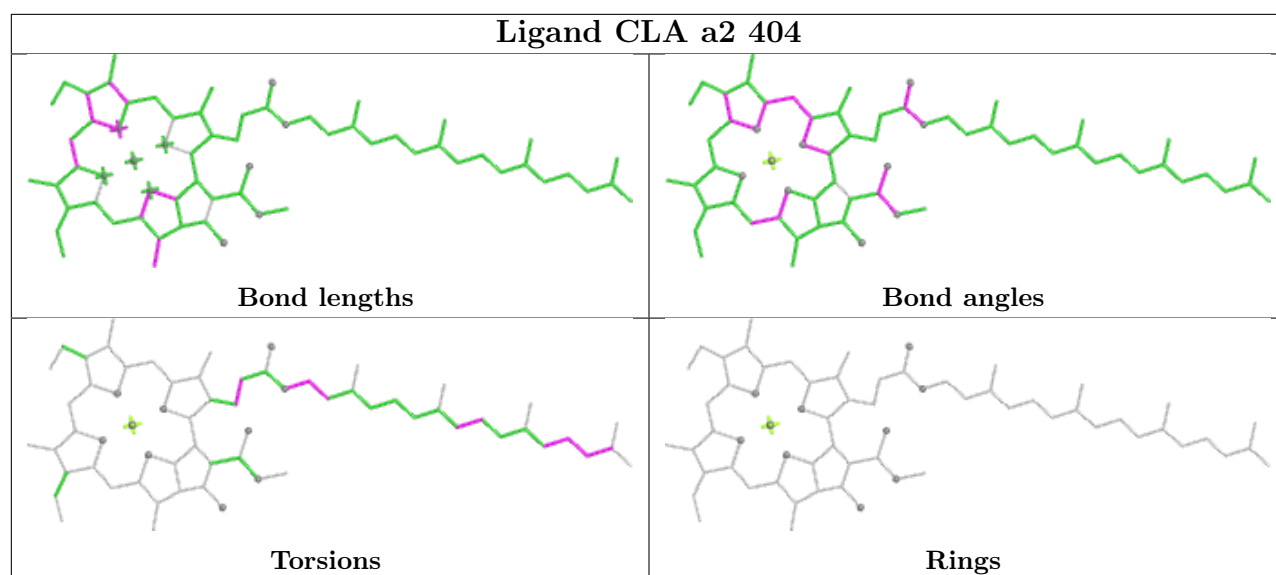


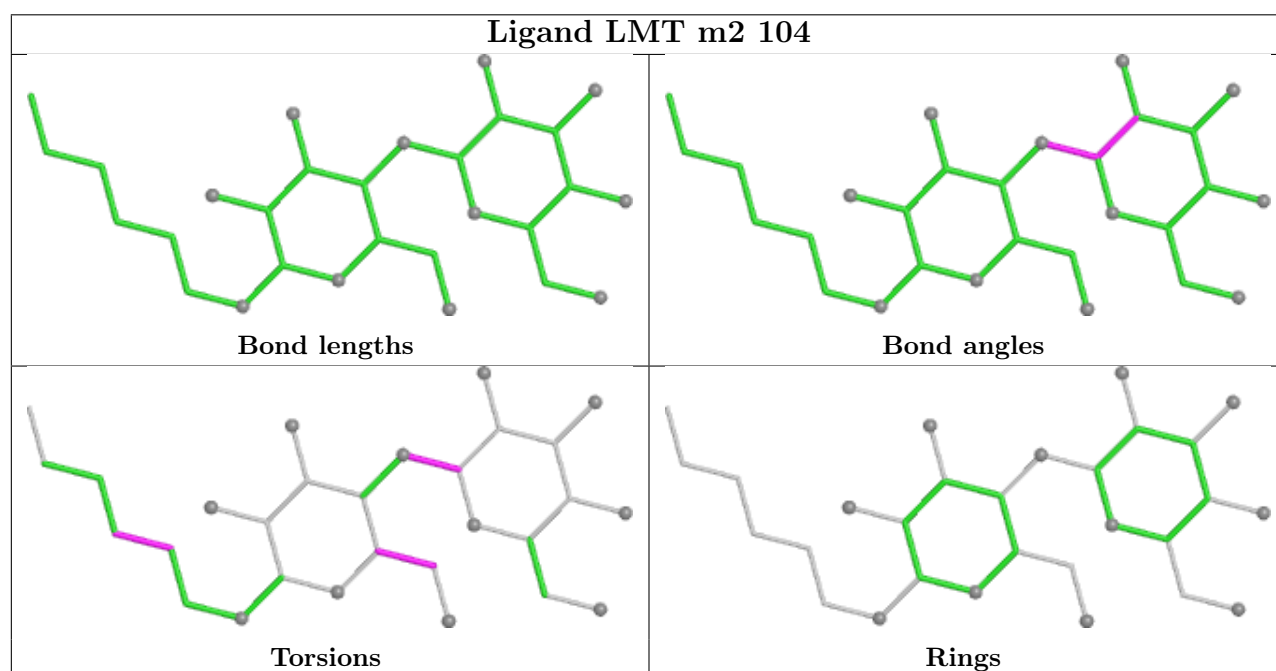
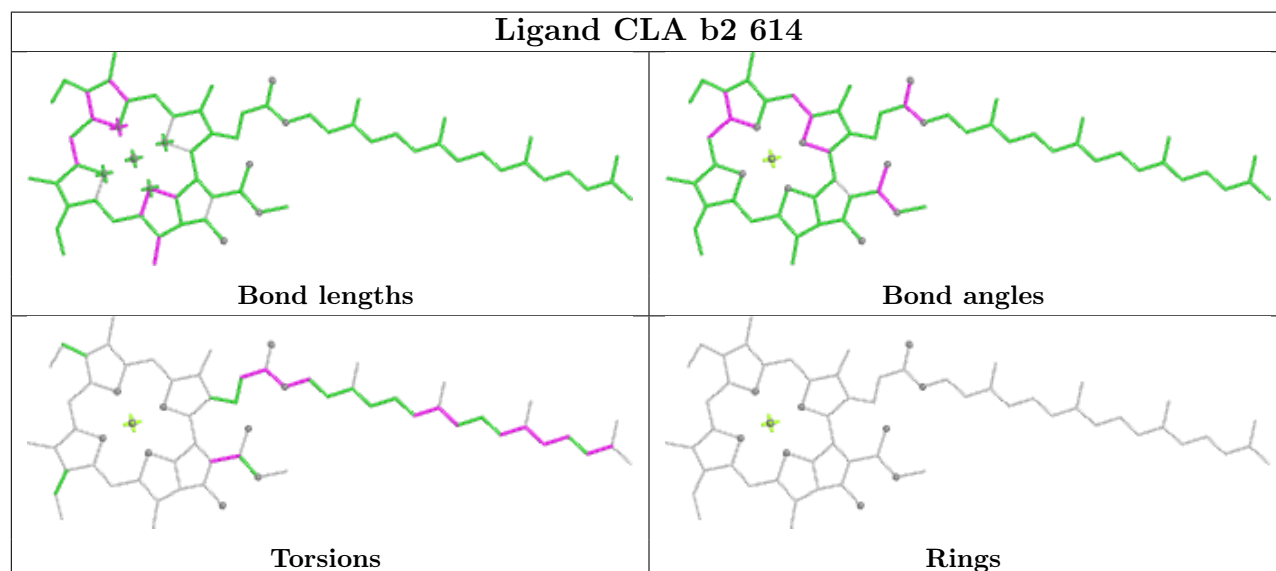
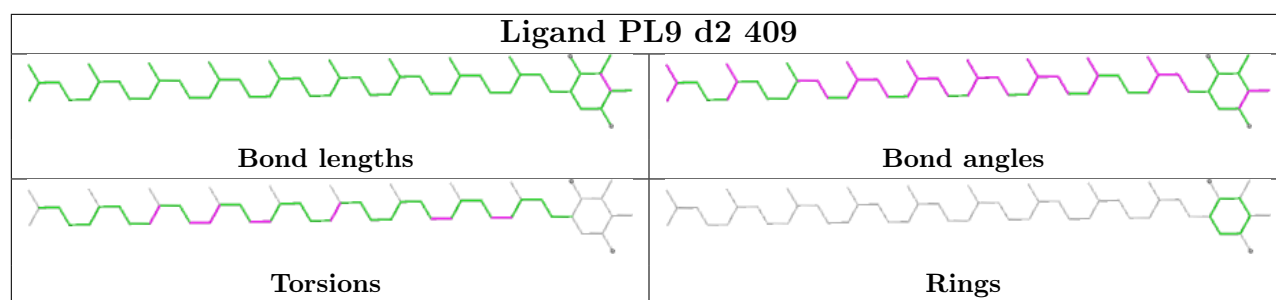


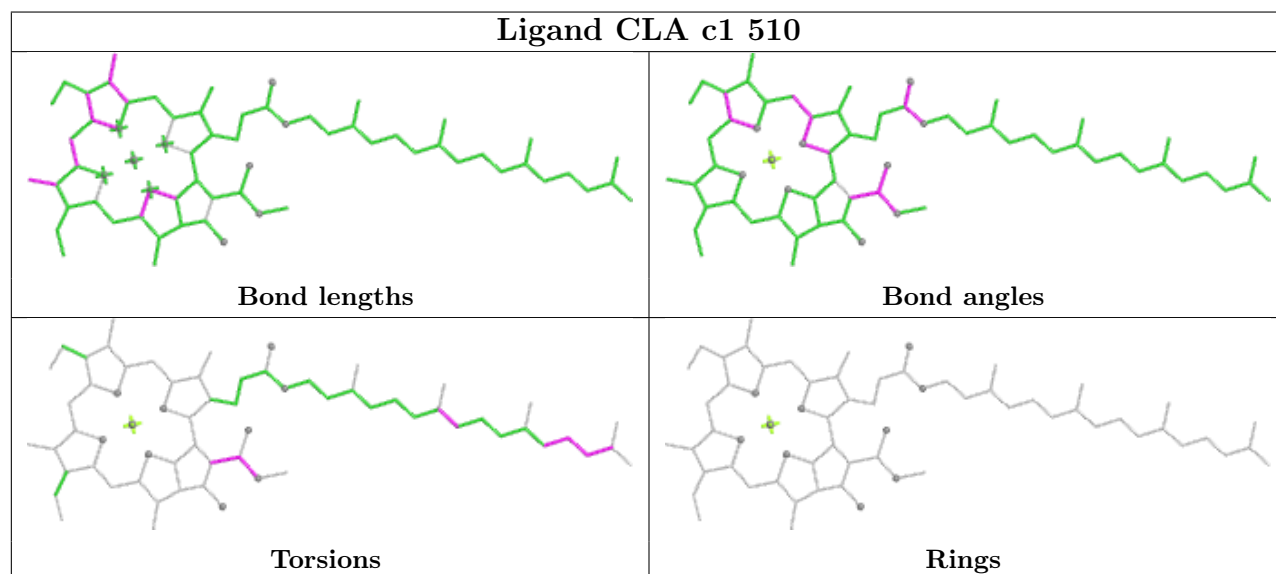
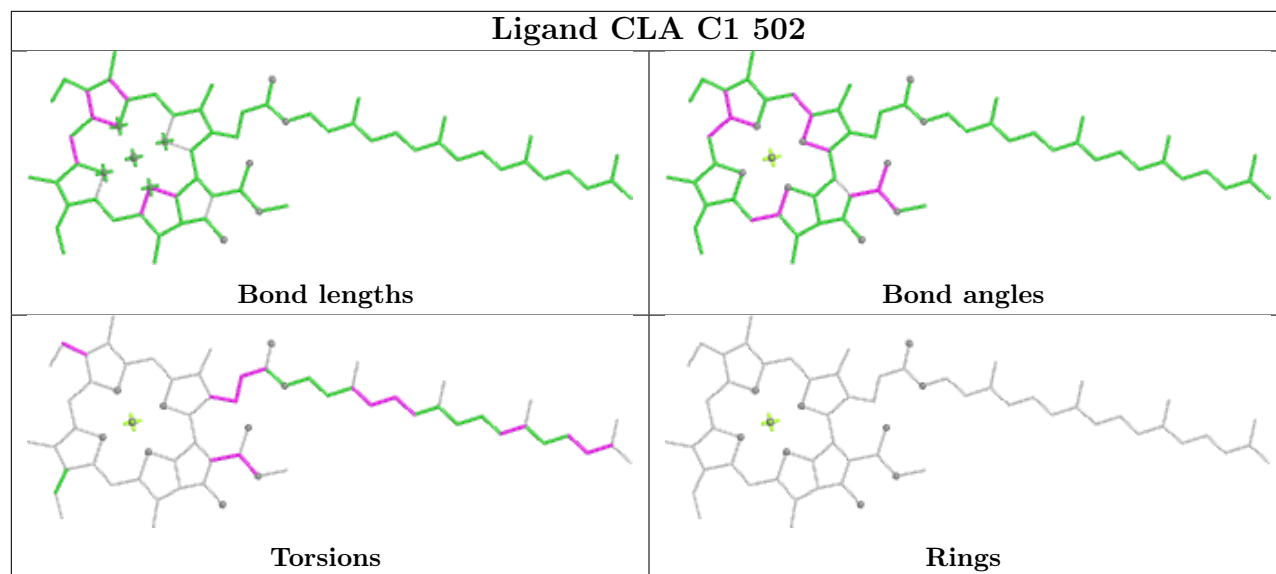


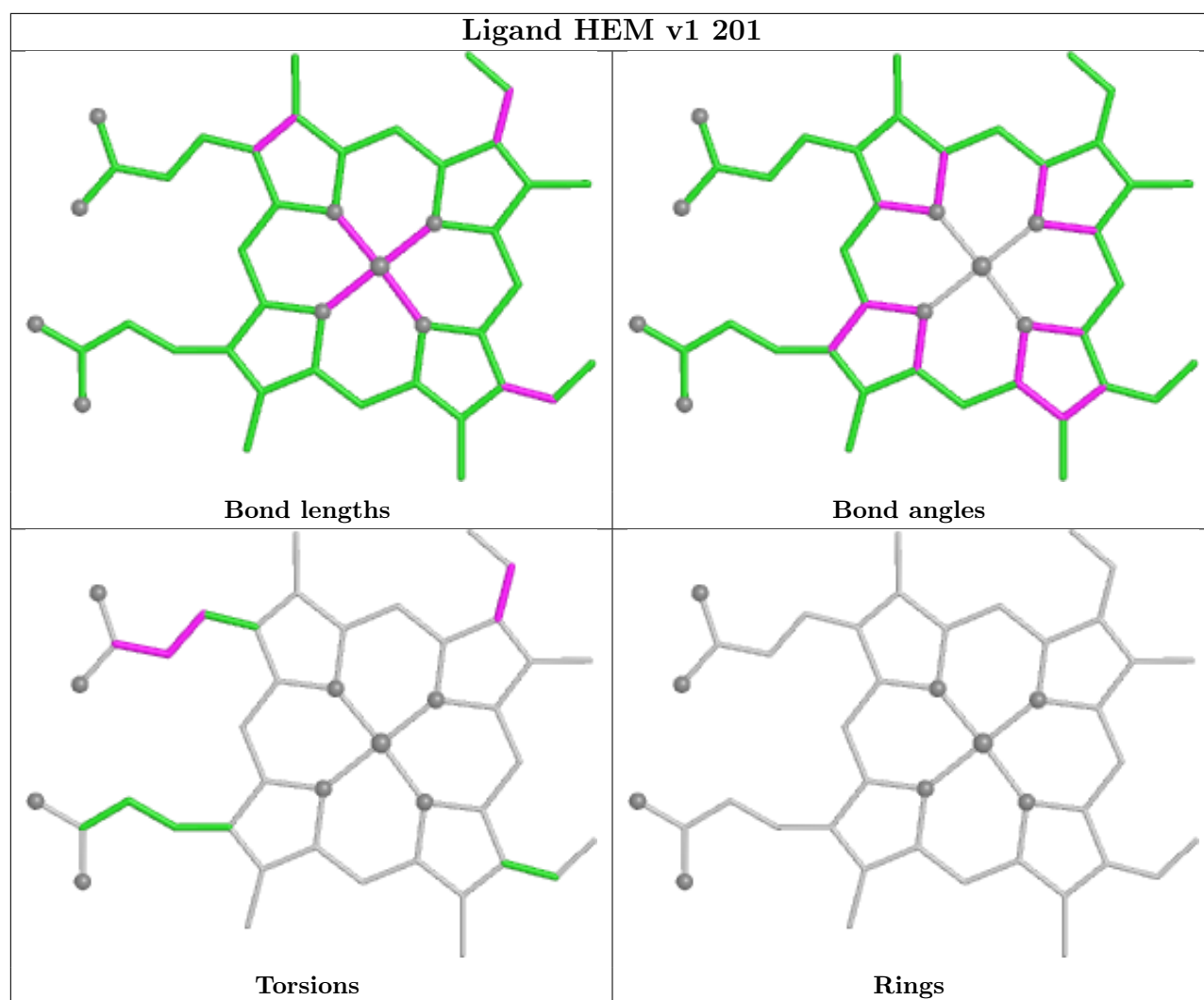


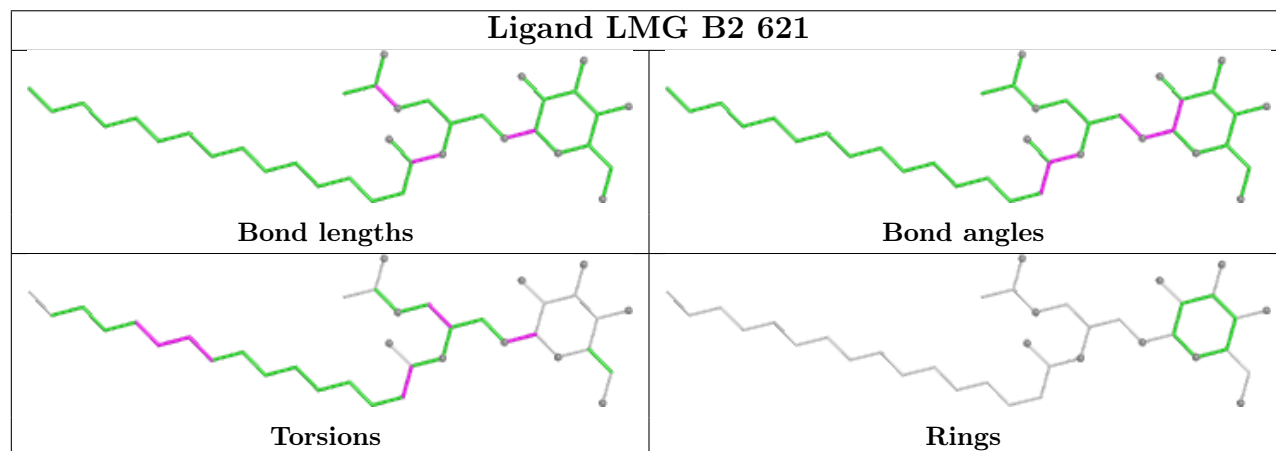
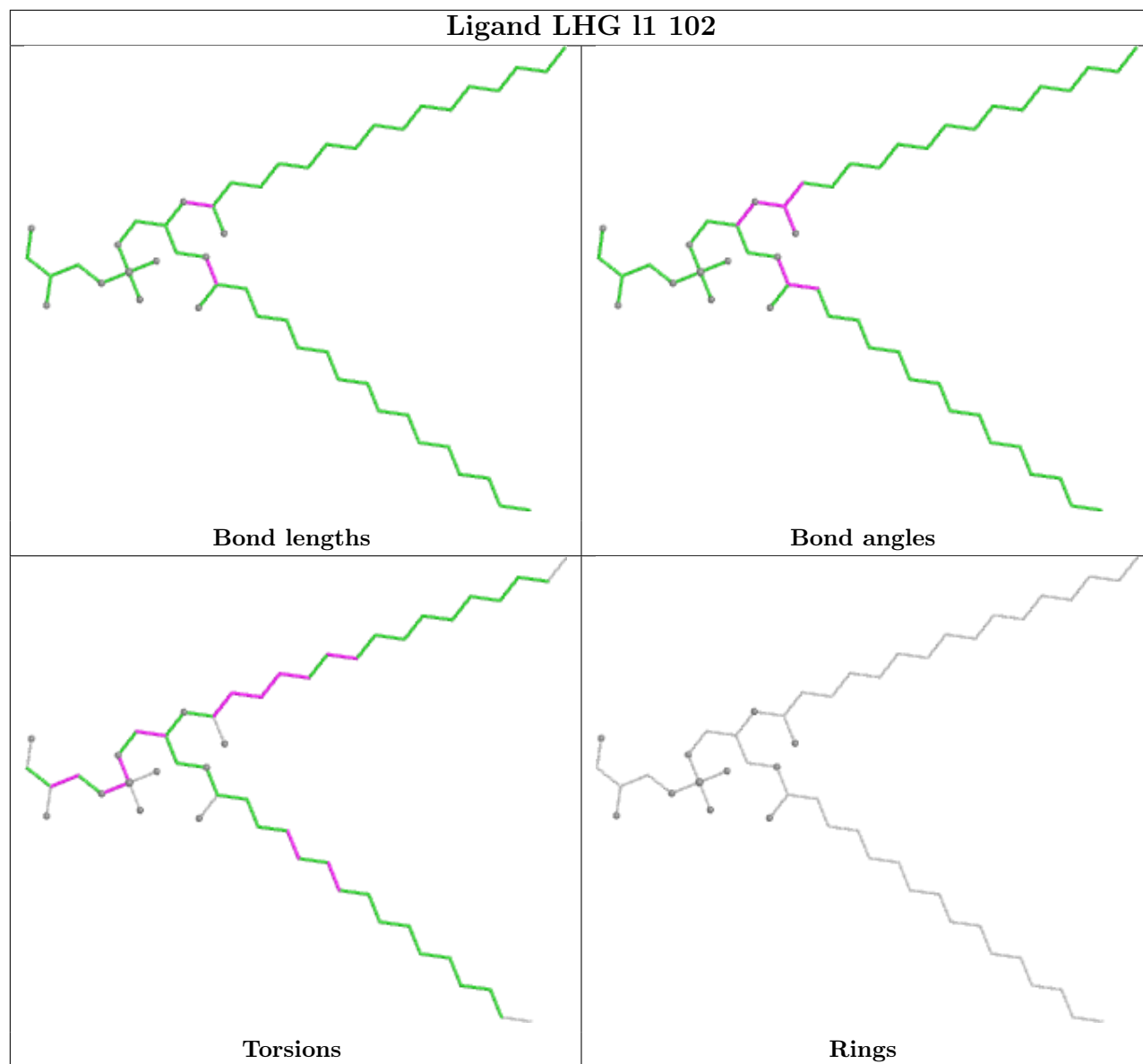


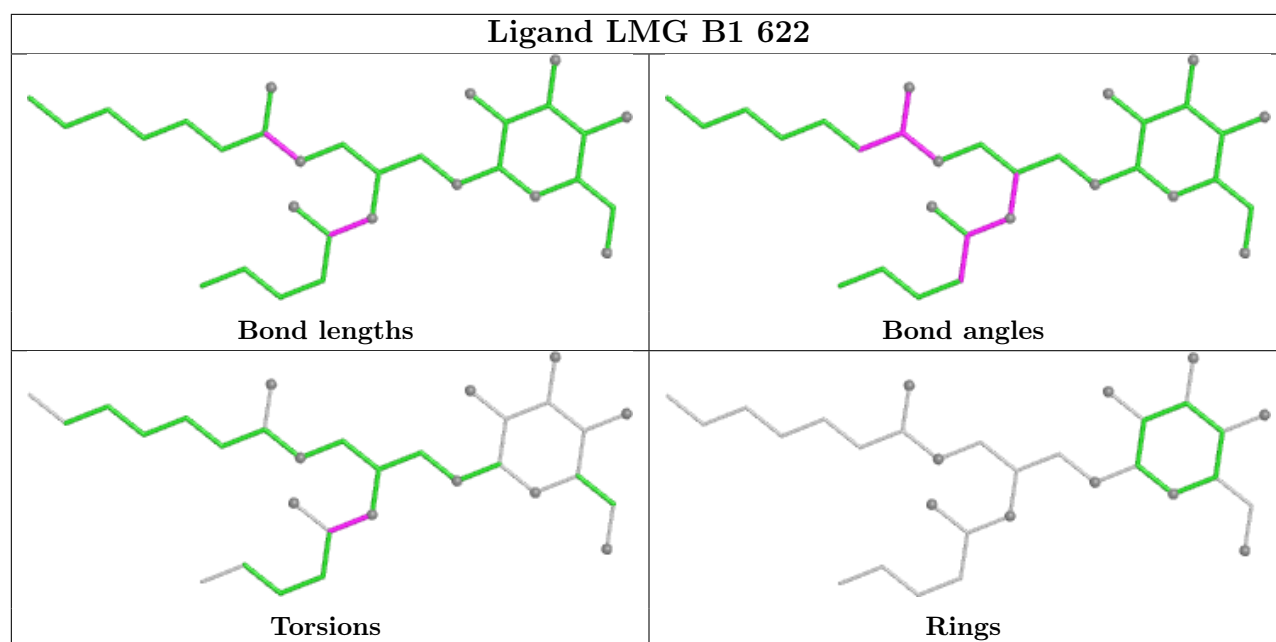


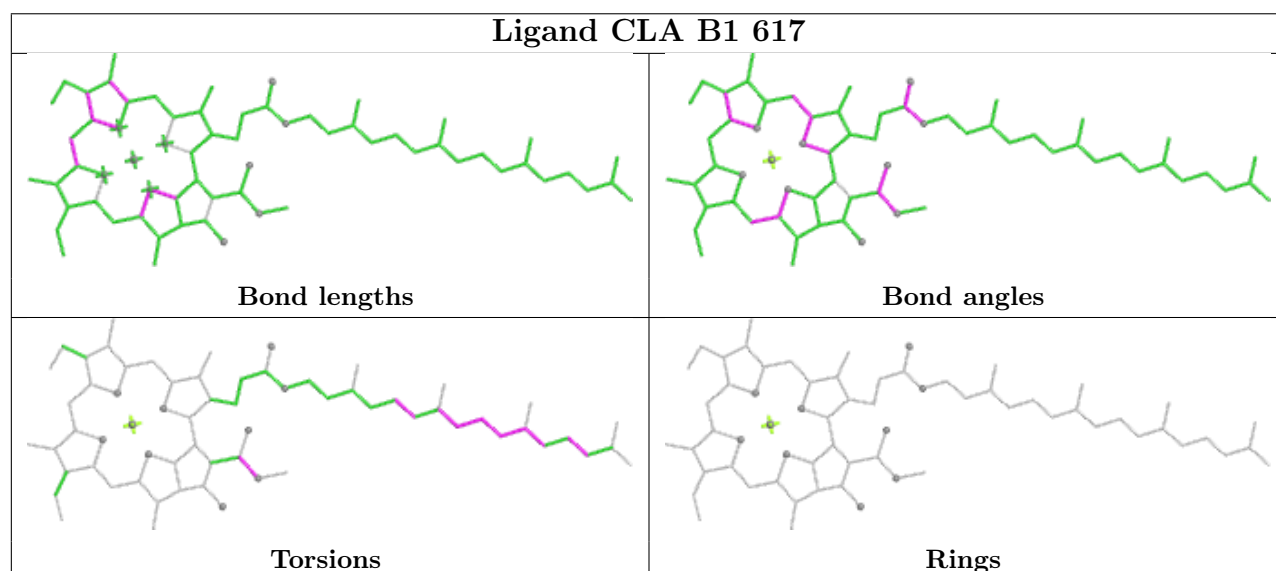
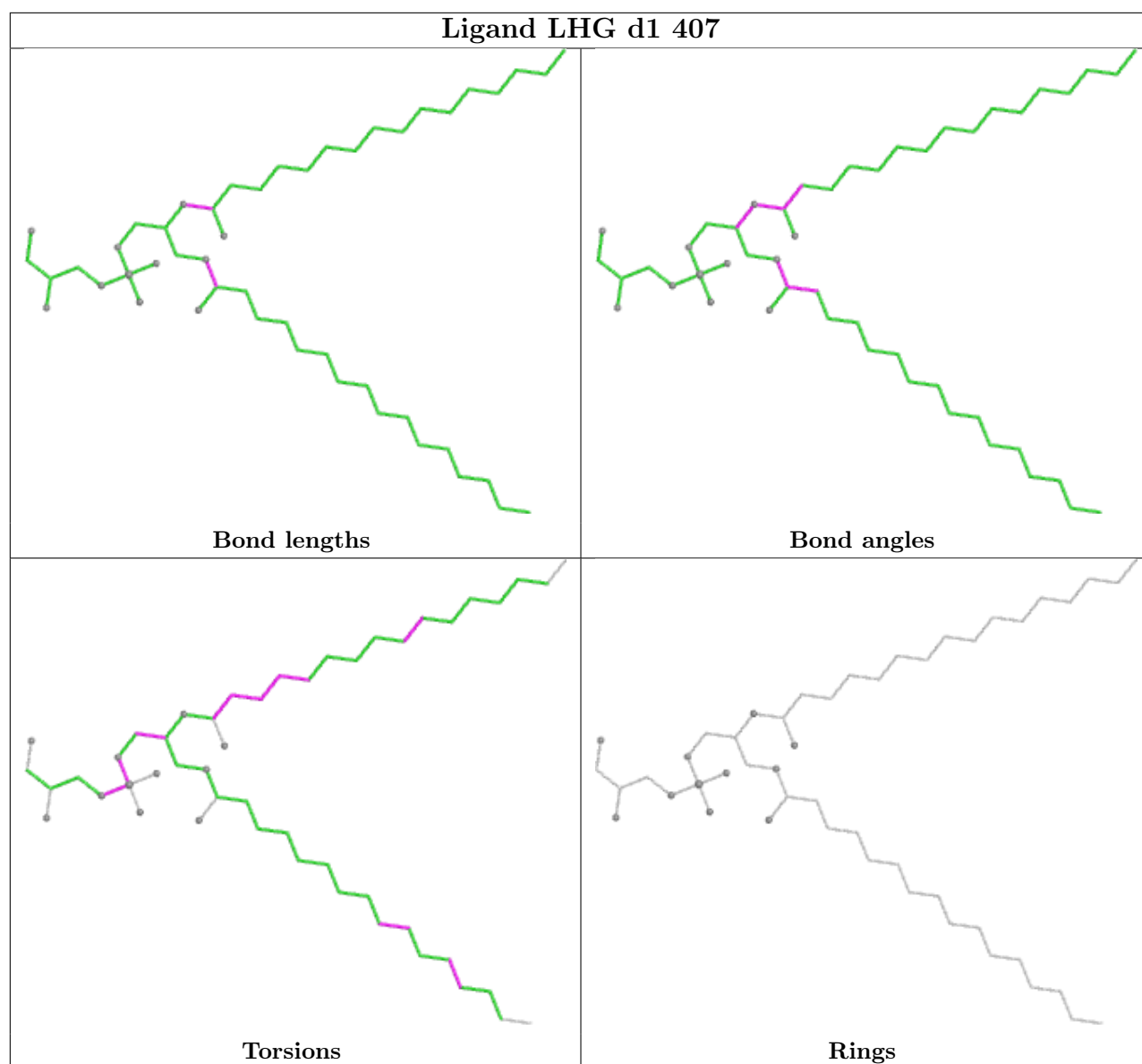


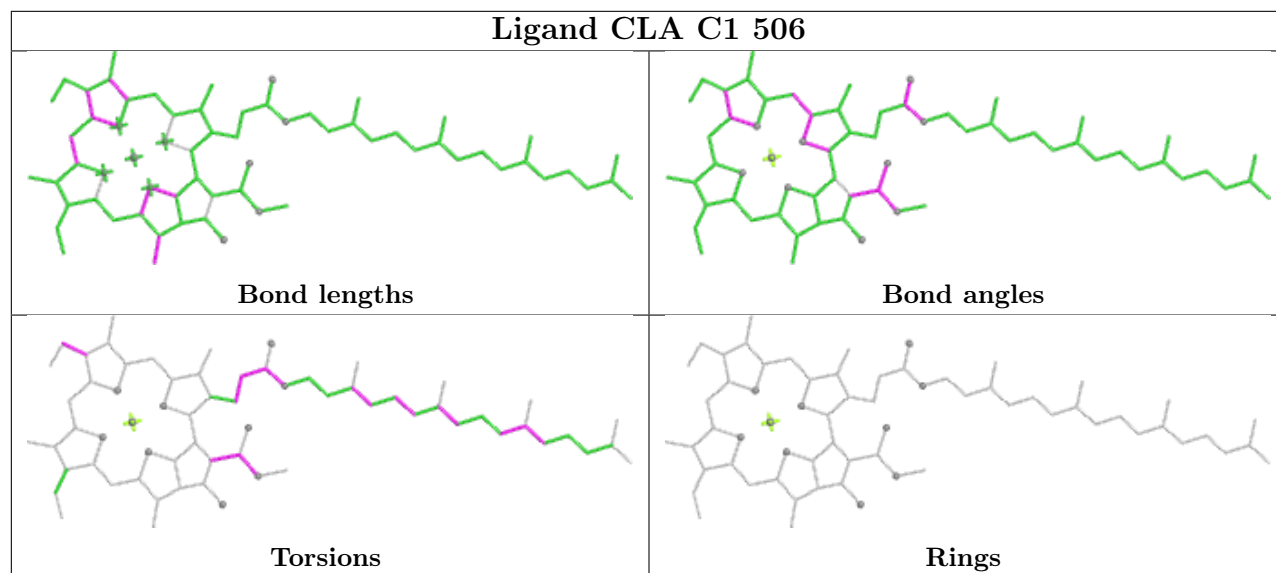
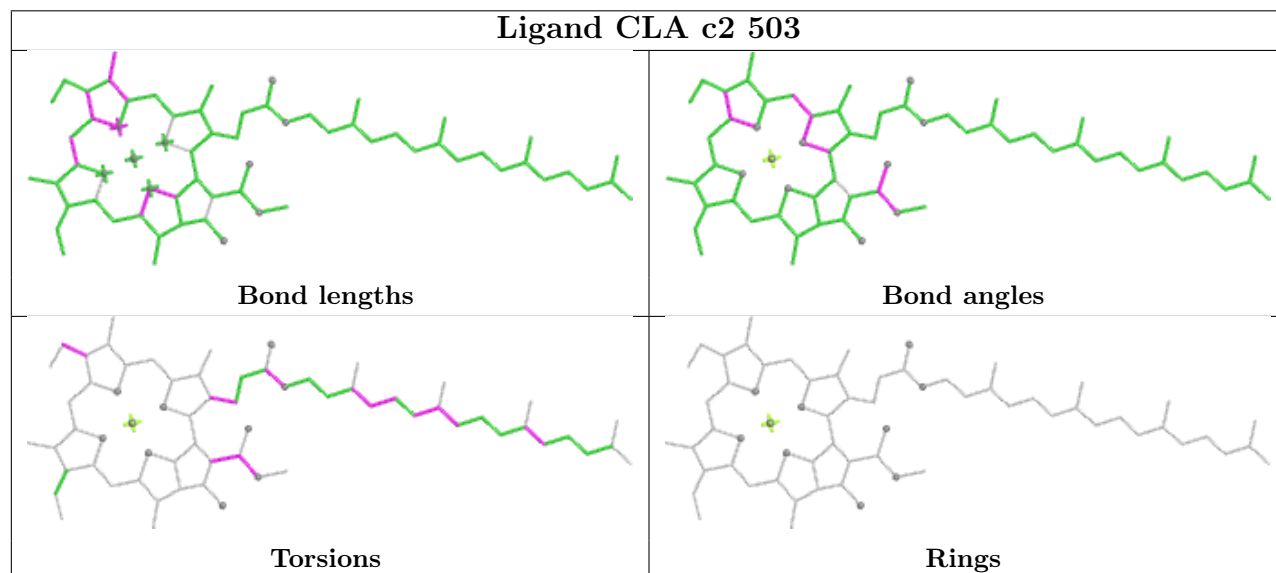
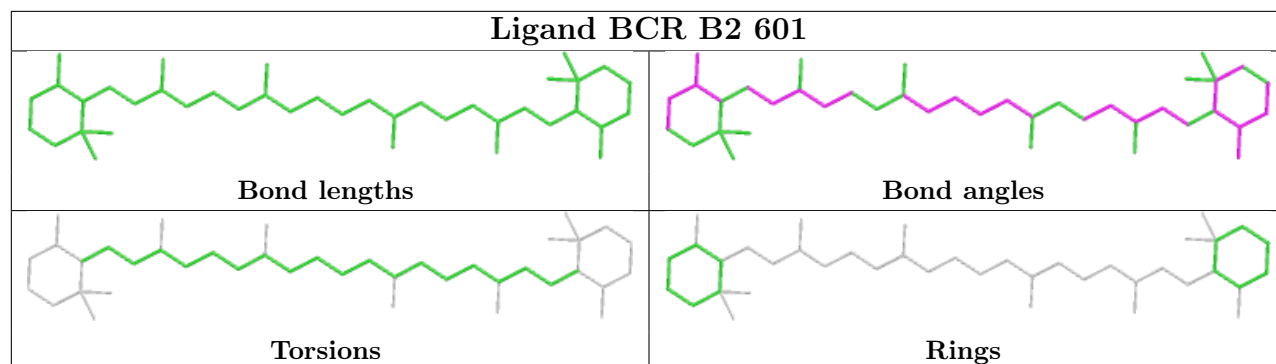


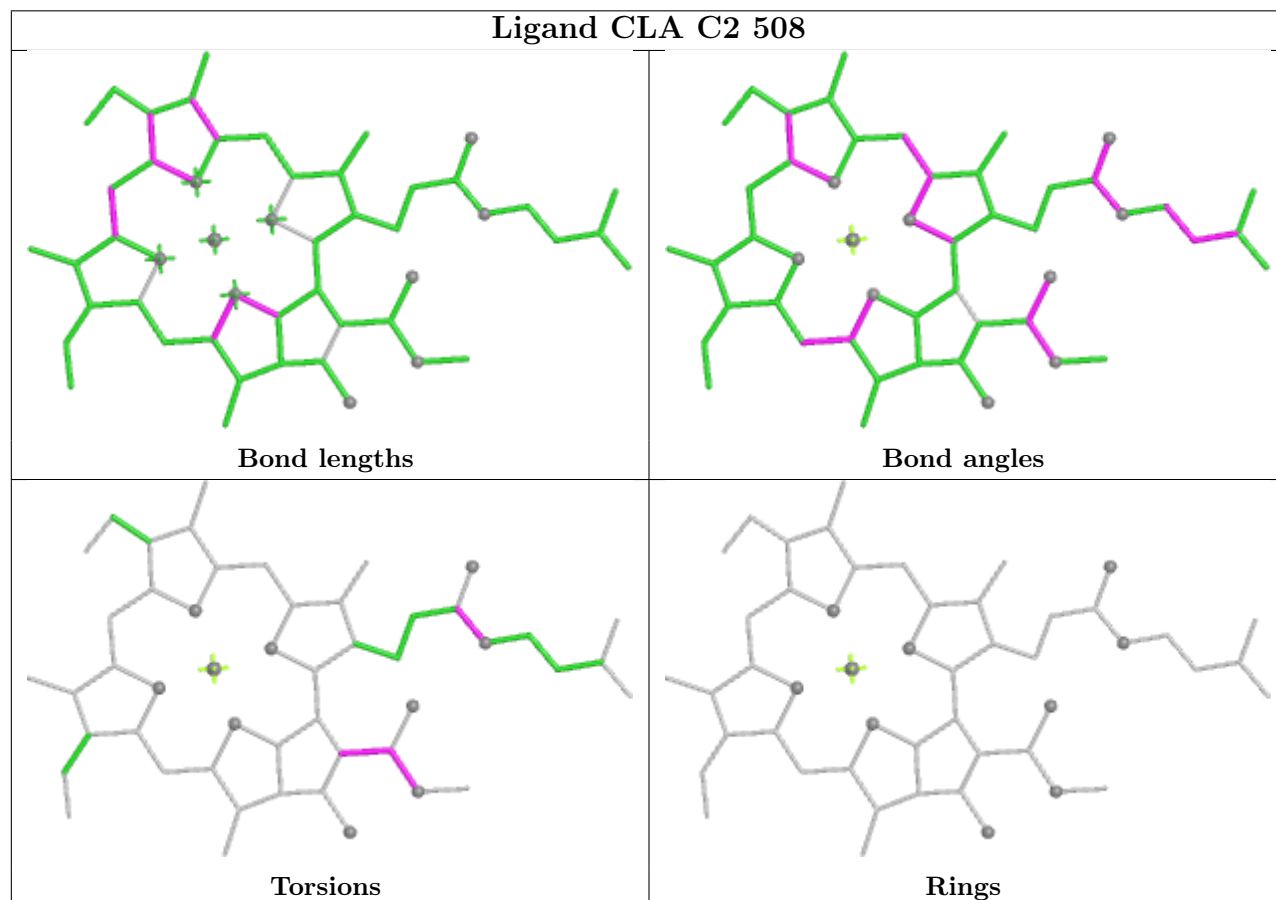
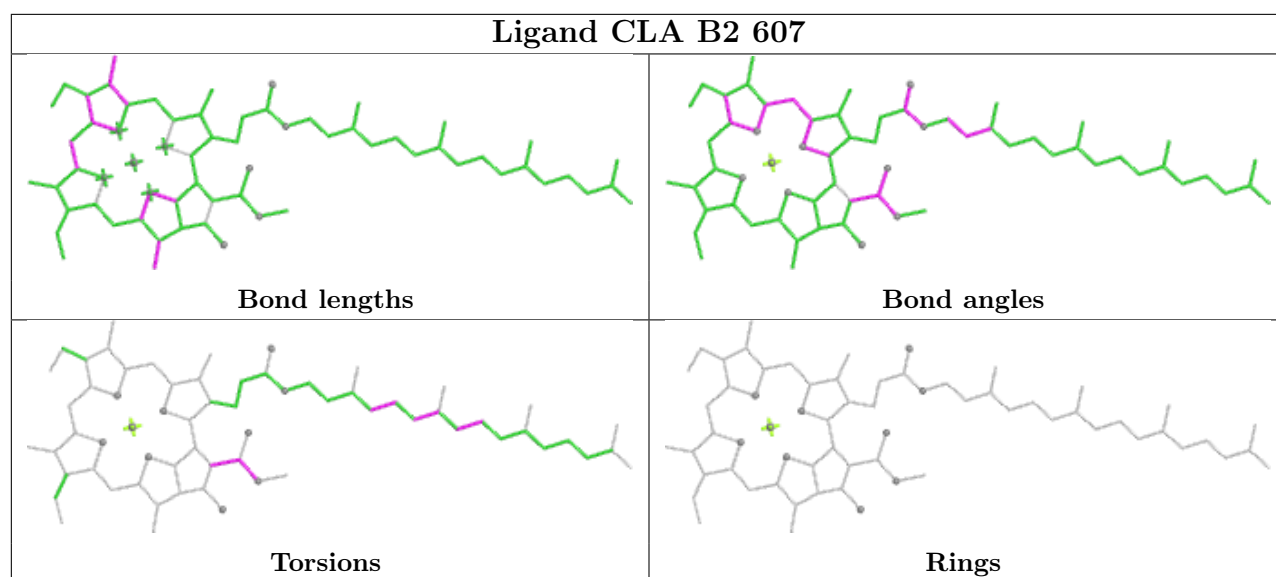


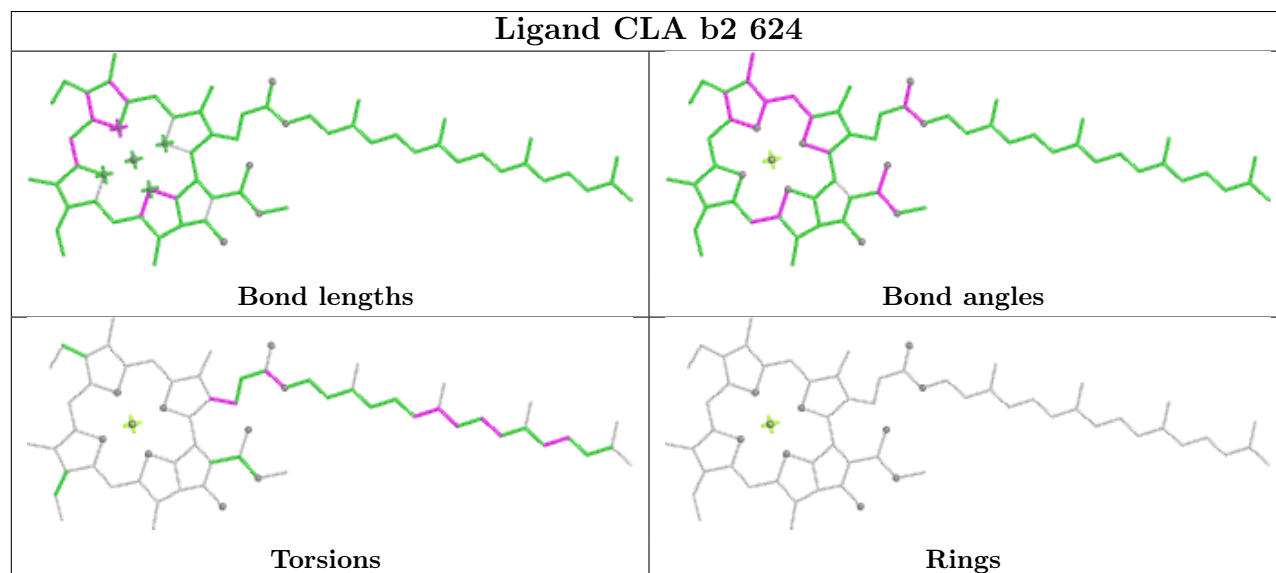
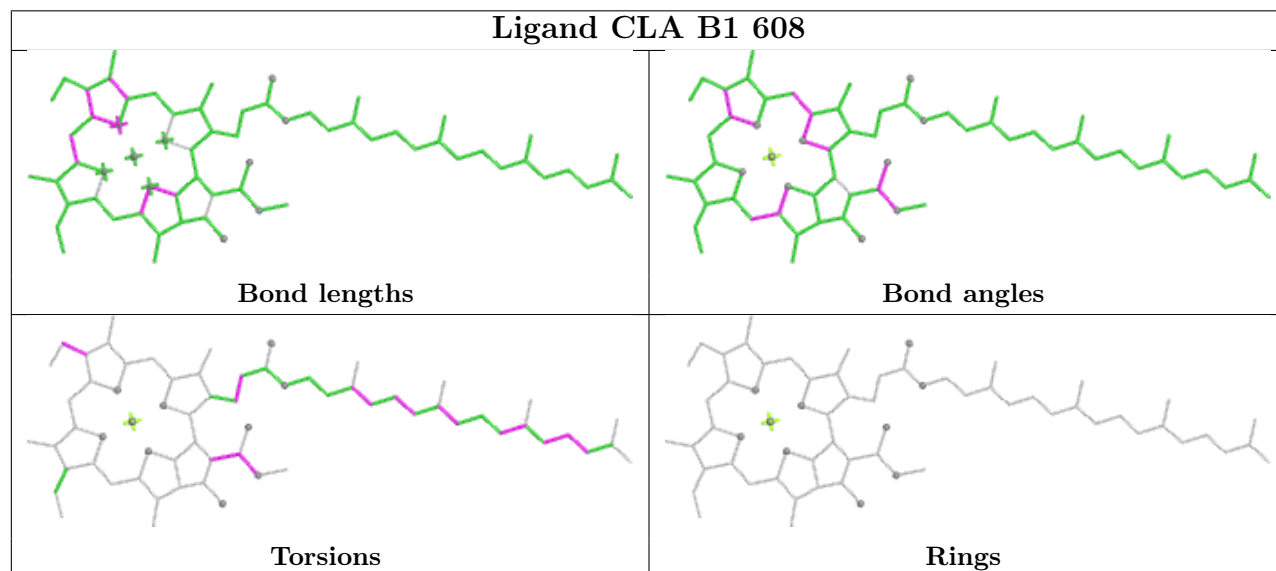
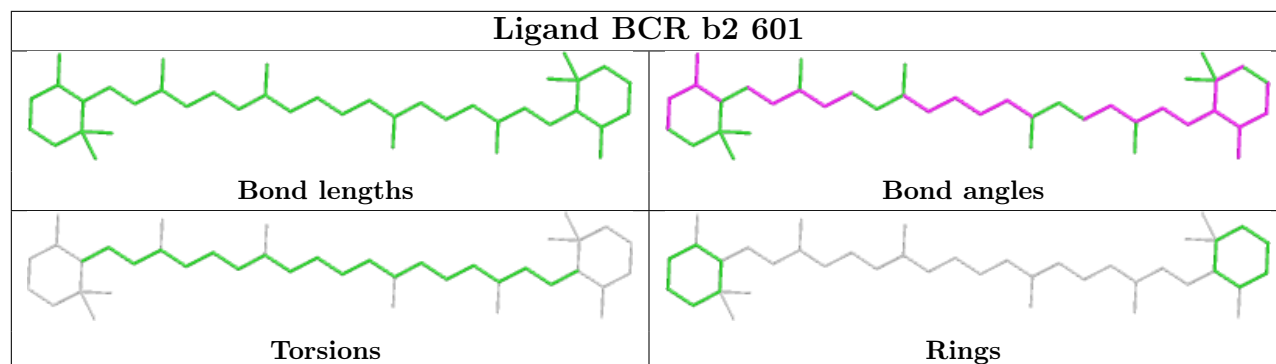


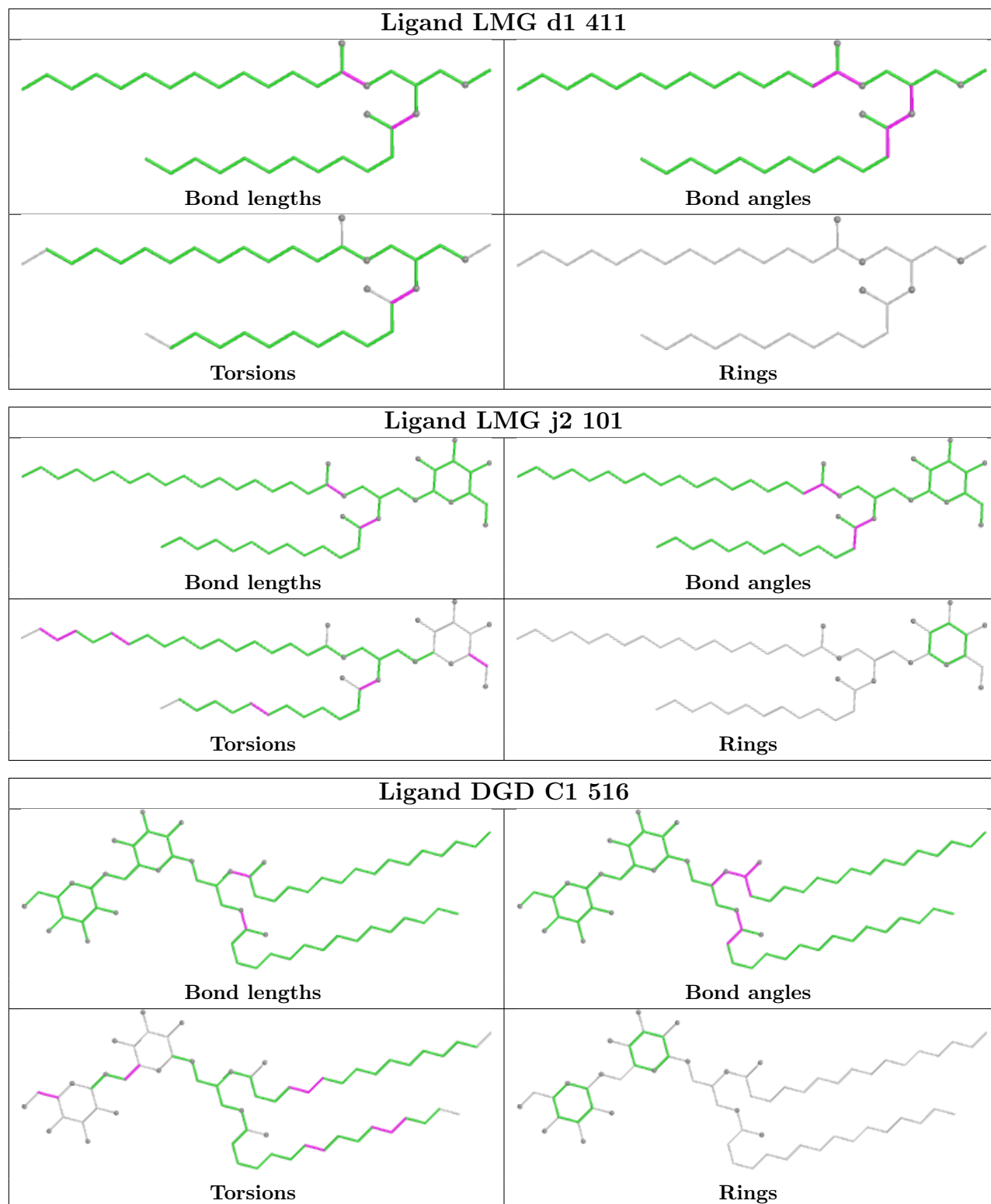




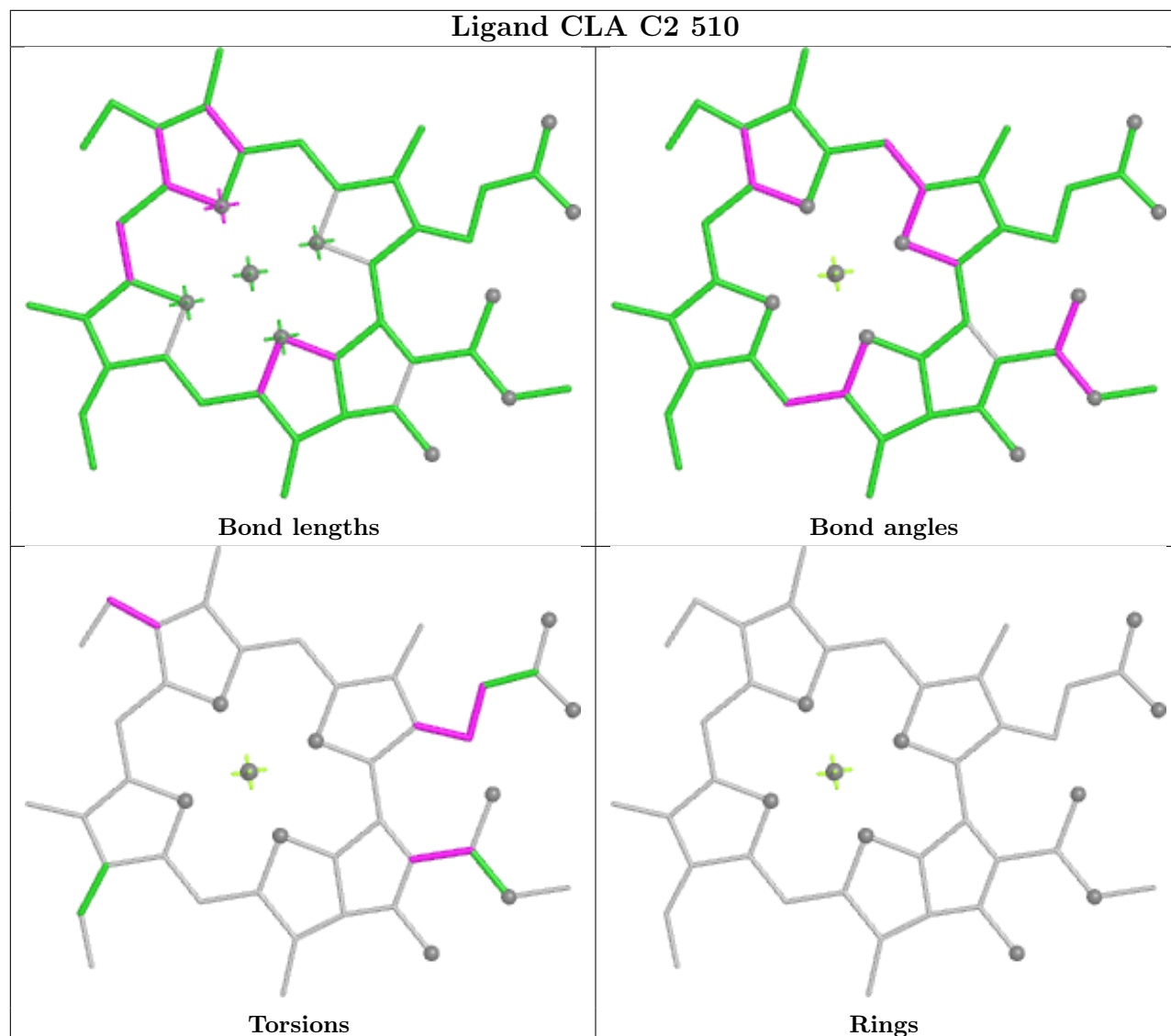


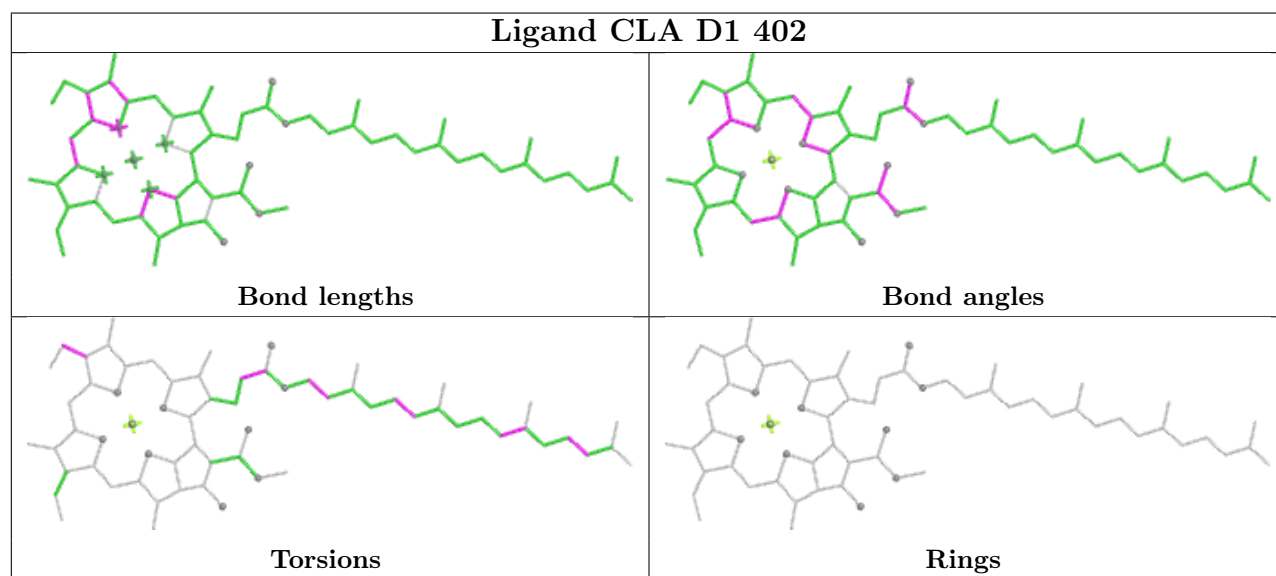
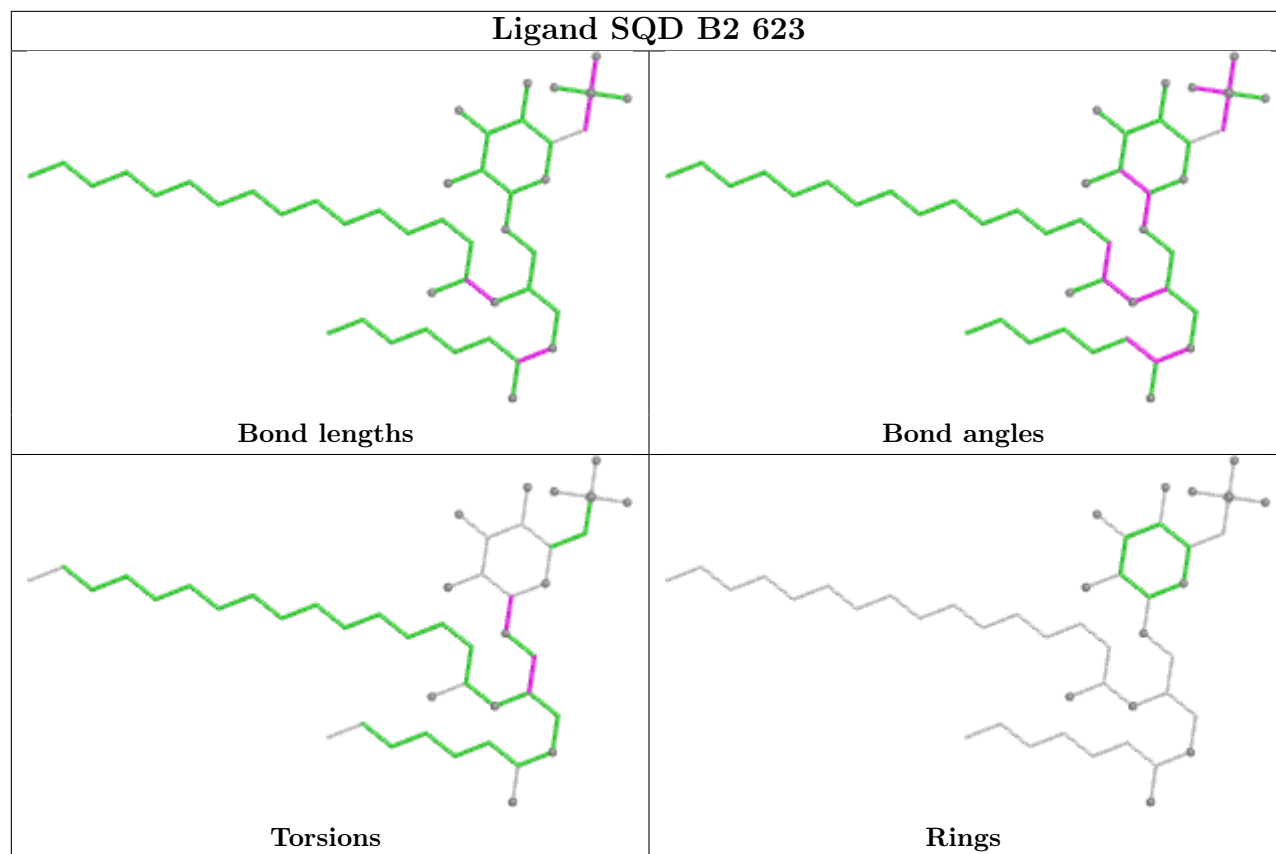


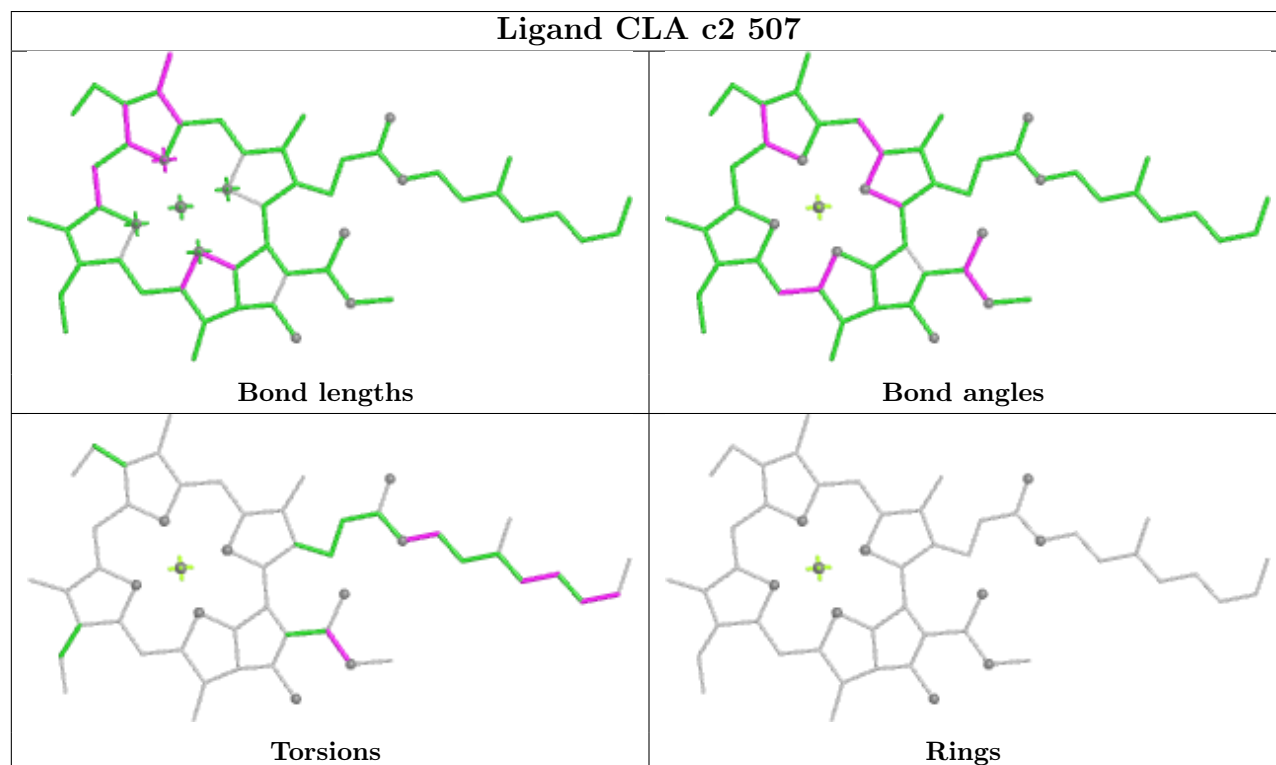
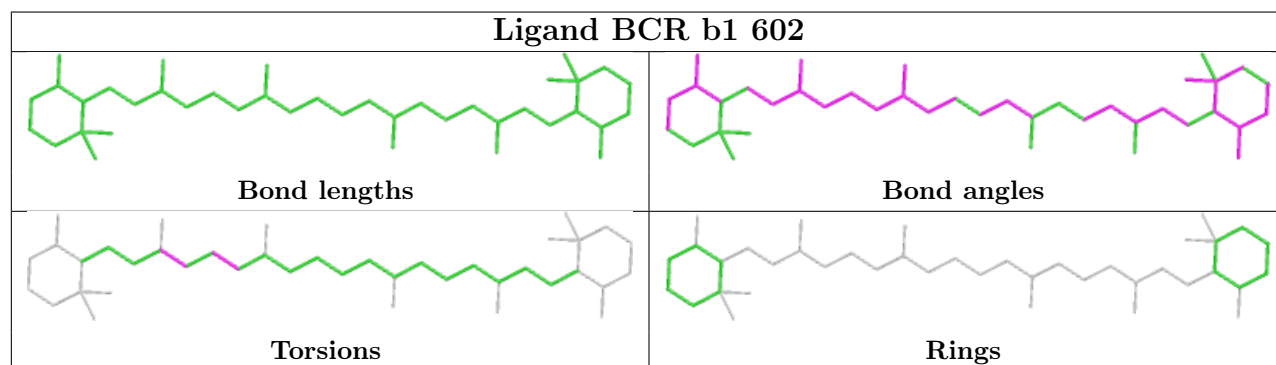
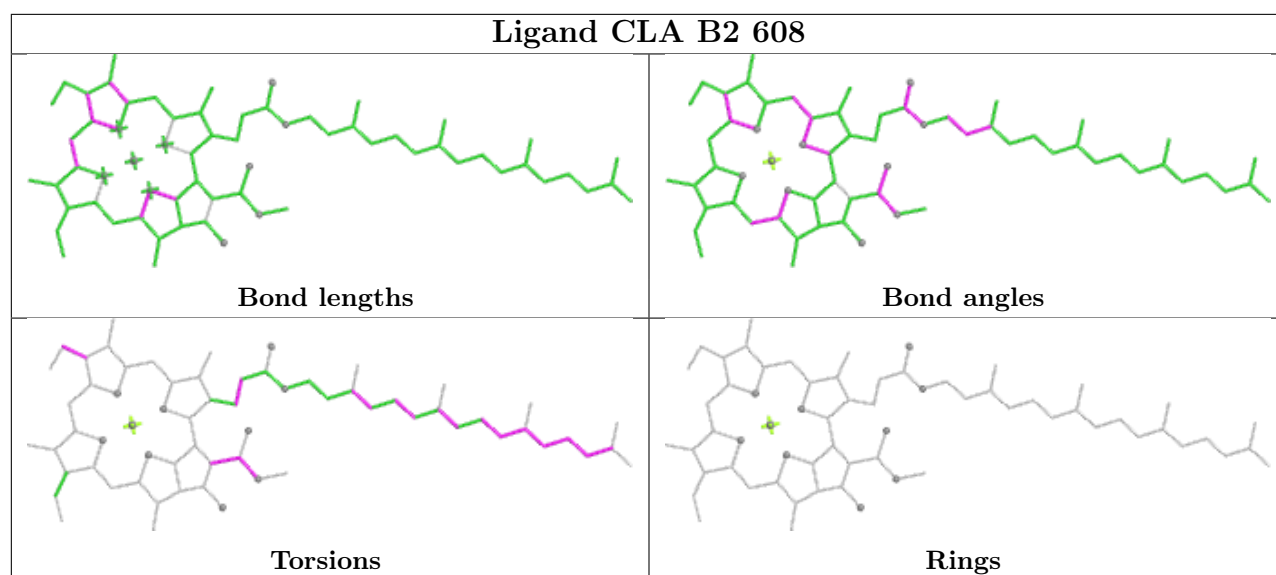


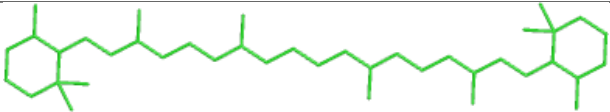
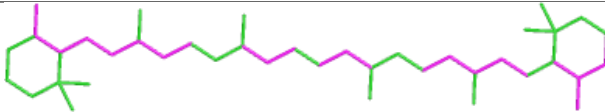
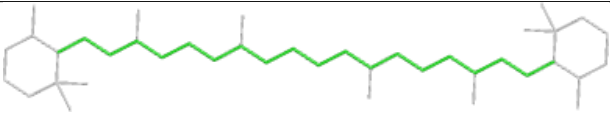
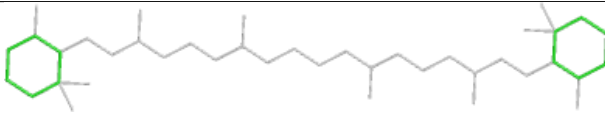


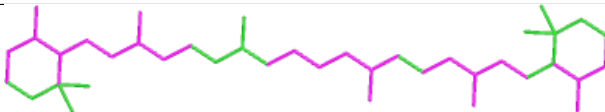
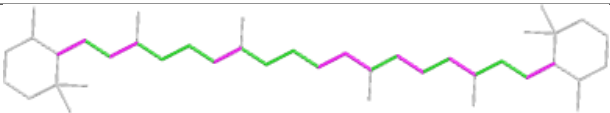
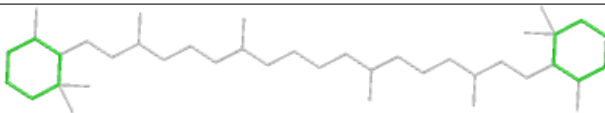
Ligand CLA C2 510



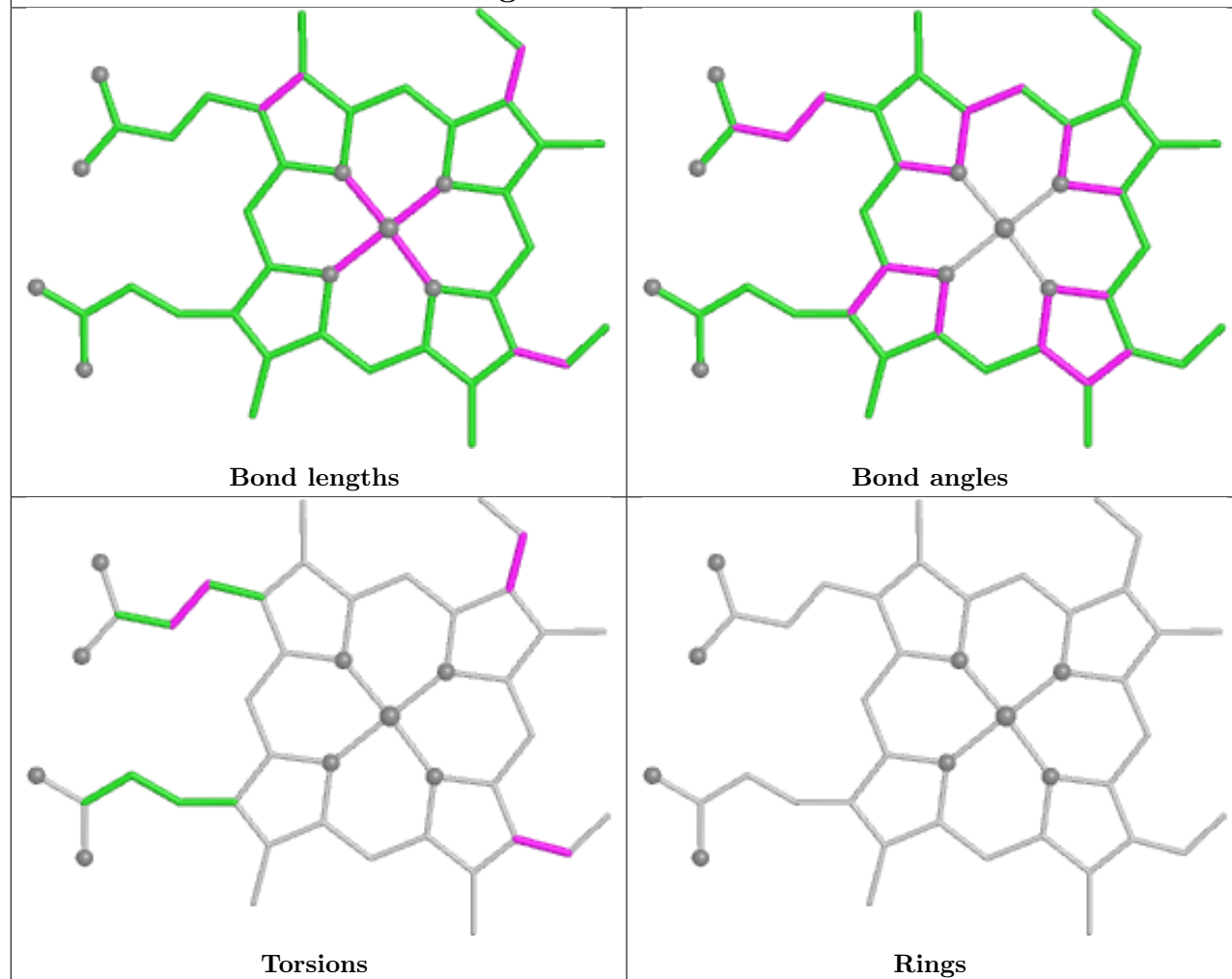




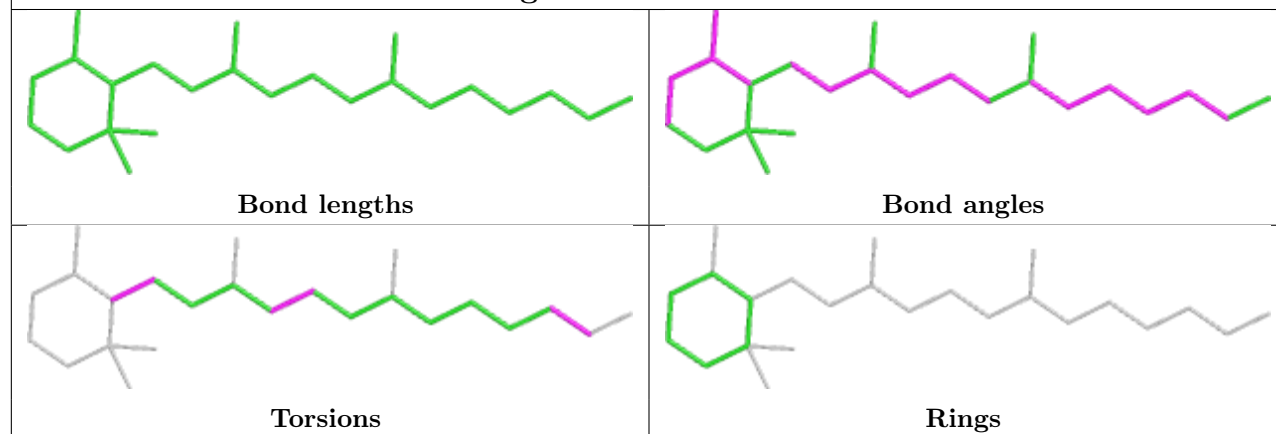
Ligand BCR z2 101			
			
Bond lengths	Bond angles		
			
Torsions	Rings		

Ligand BCR c2 501			
			
Bond lengths	Bond angles		
			
Torsions	Rings		

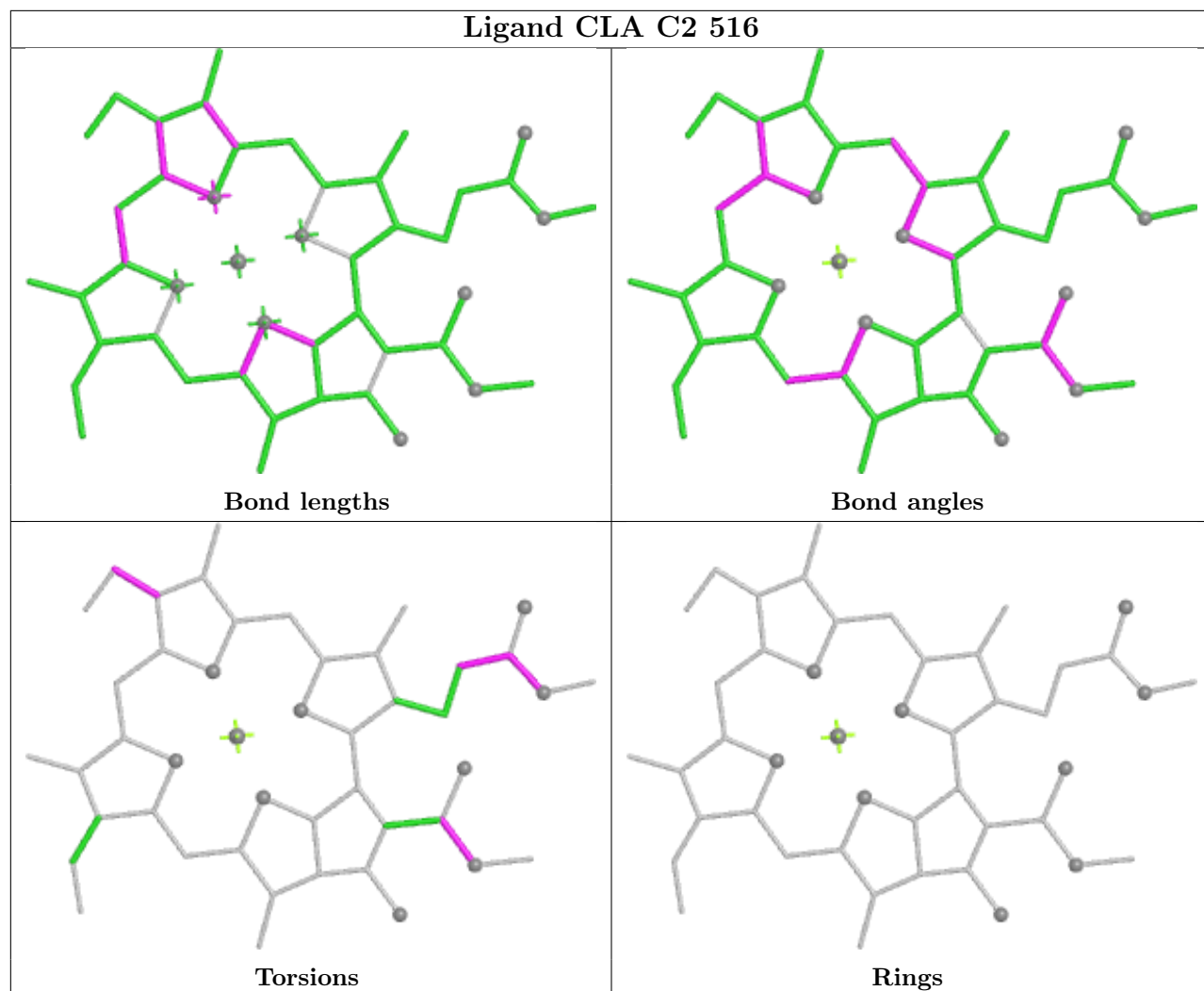
Ligand HEM V2 201

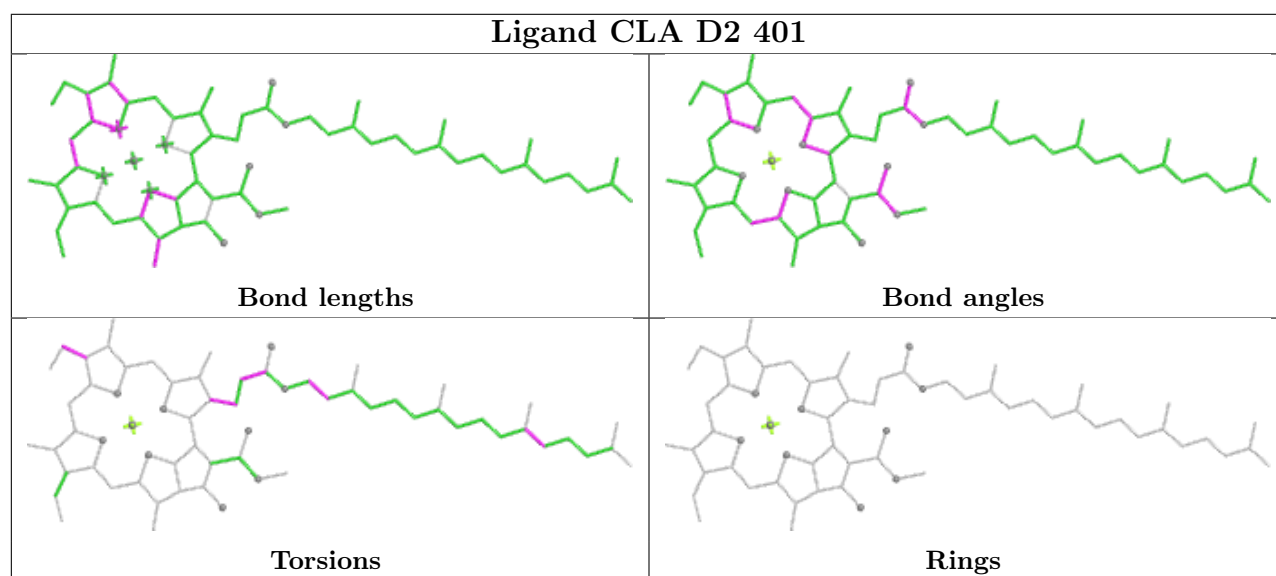
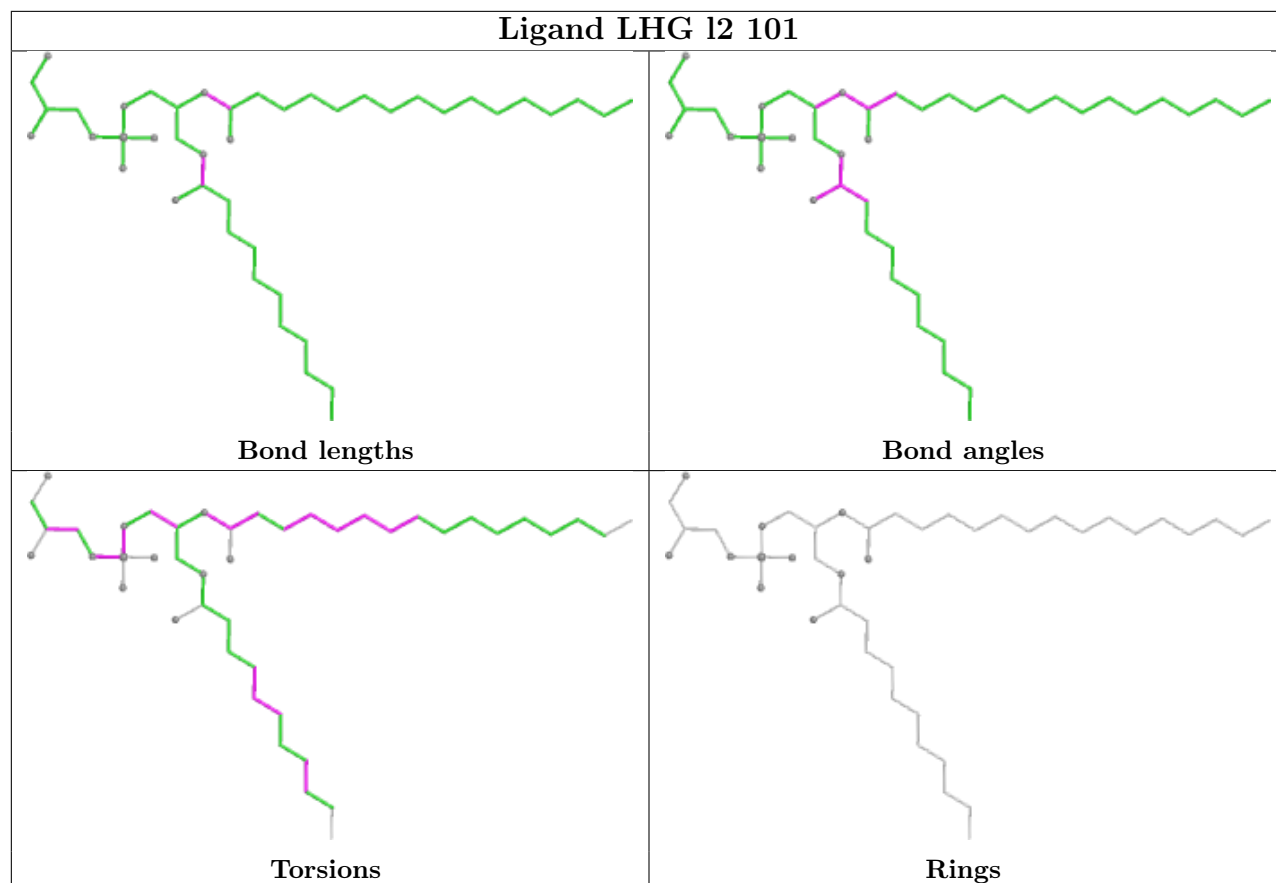


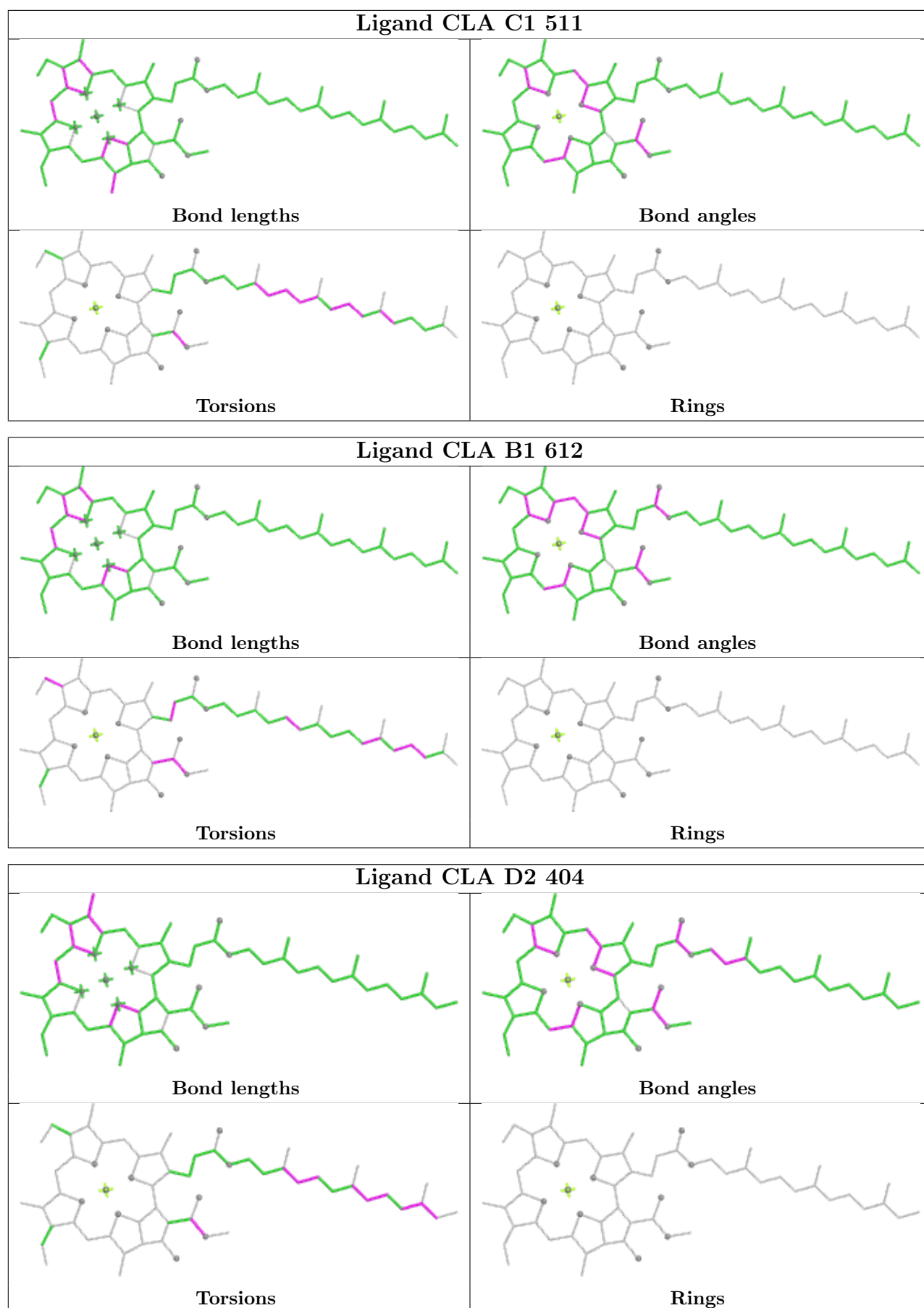
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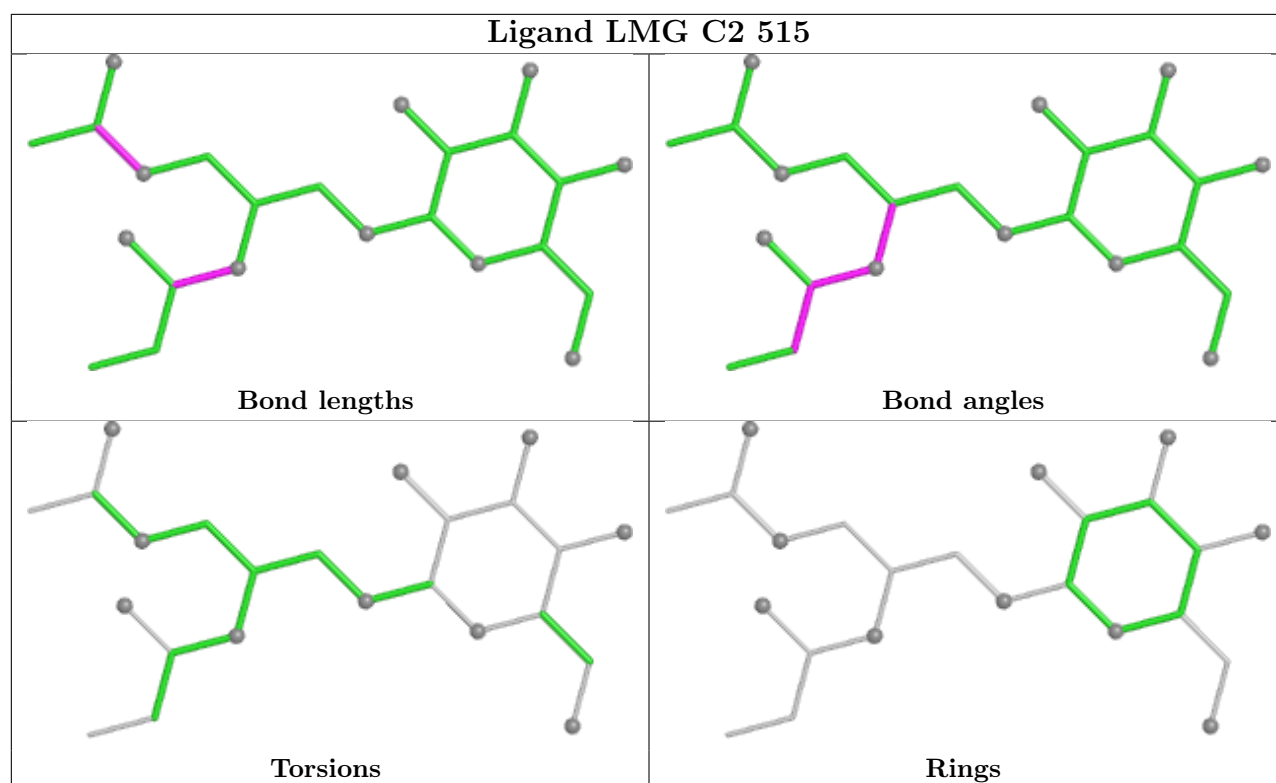


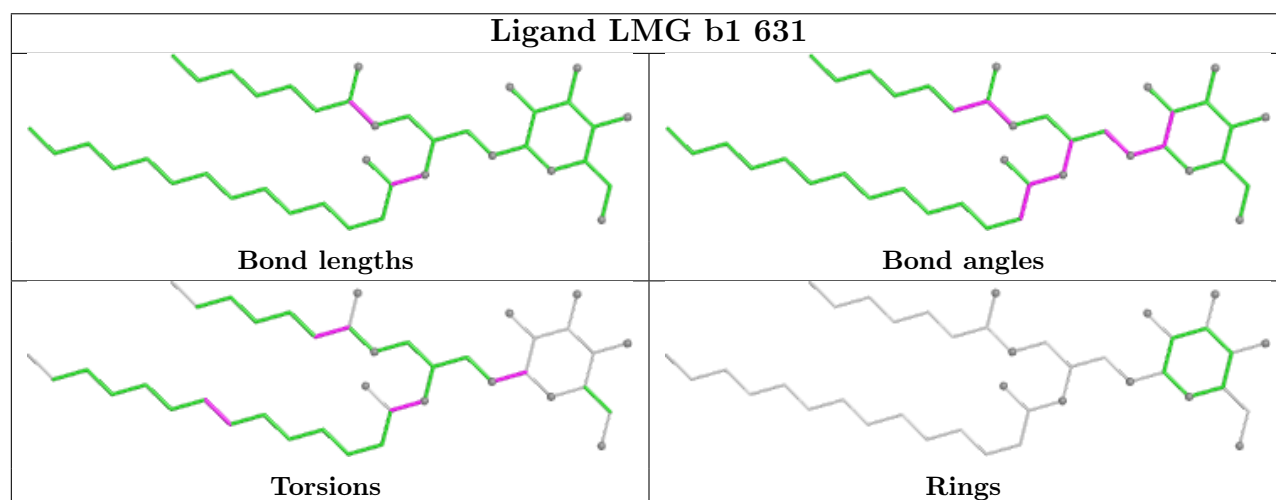
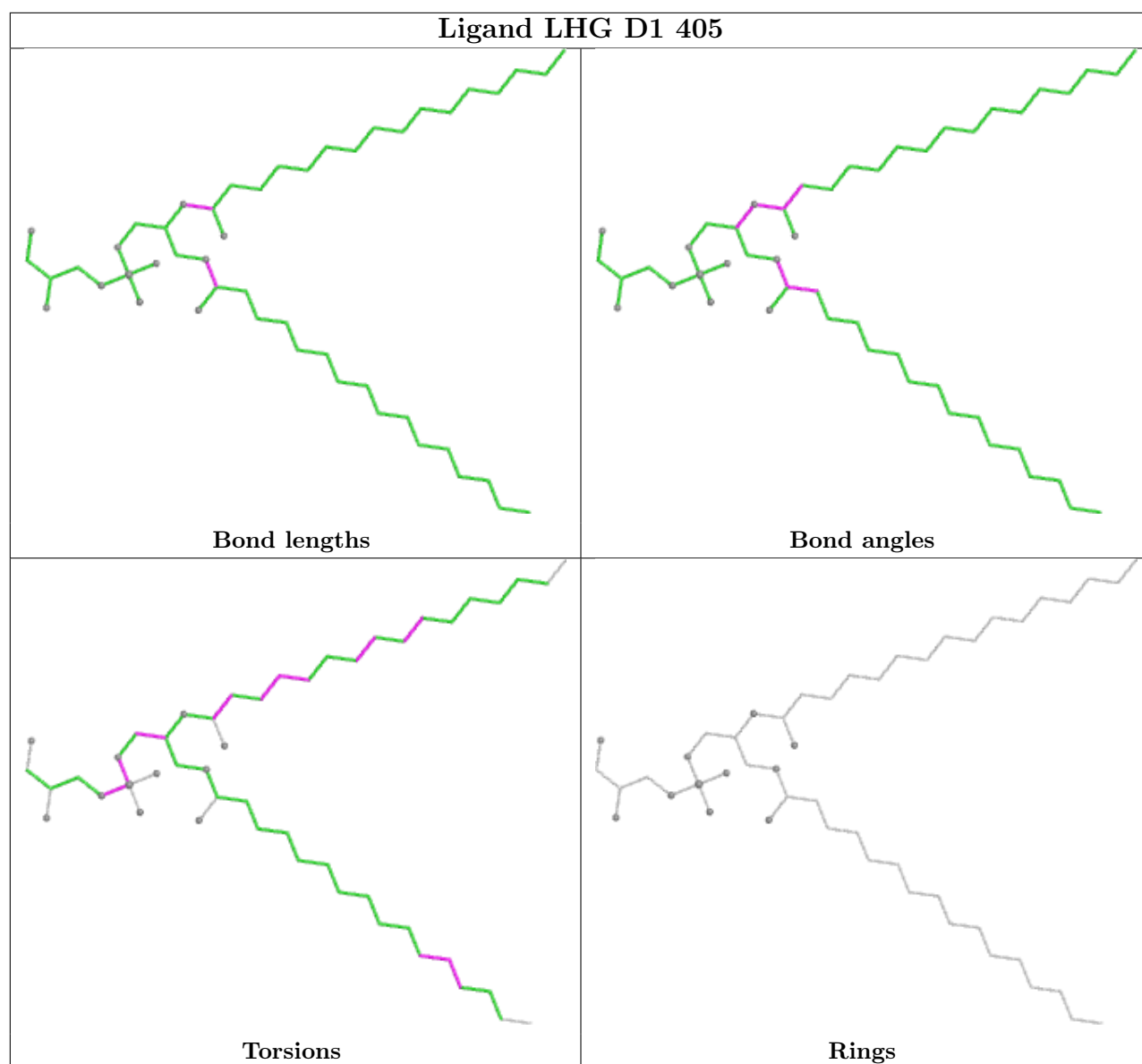
Ligand CLA C2 516



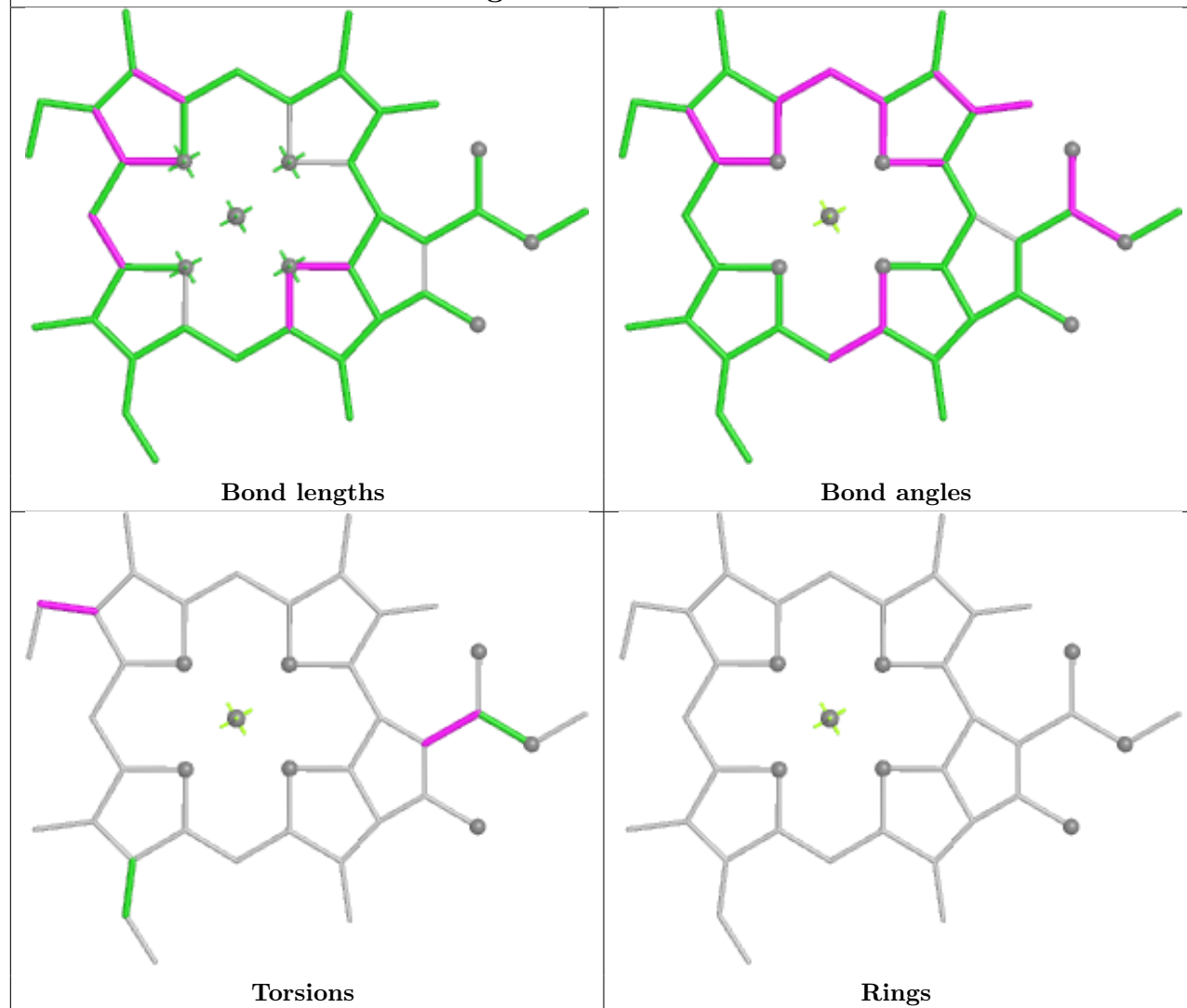




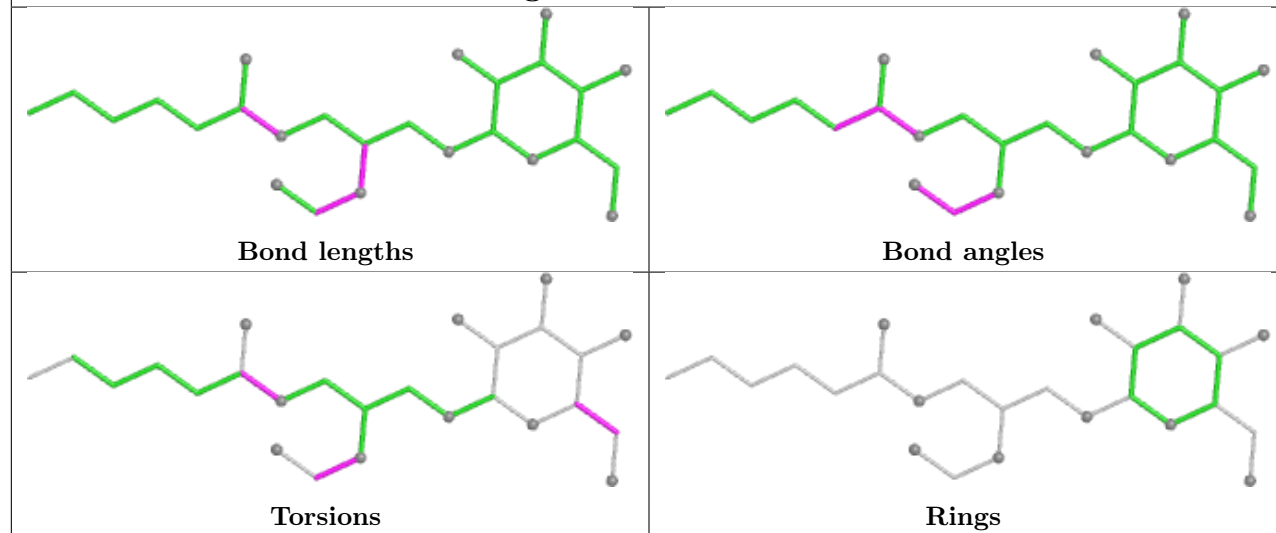


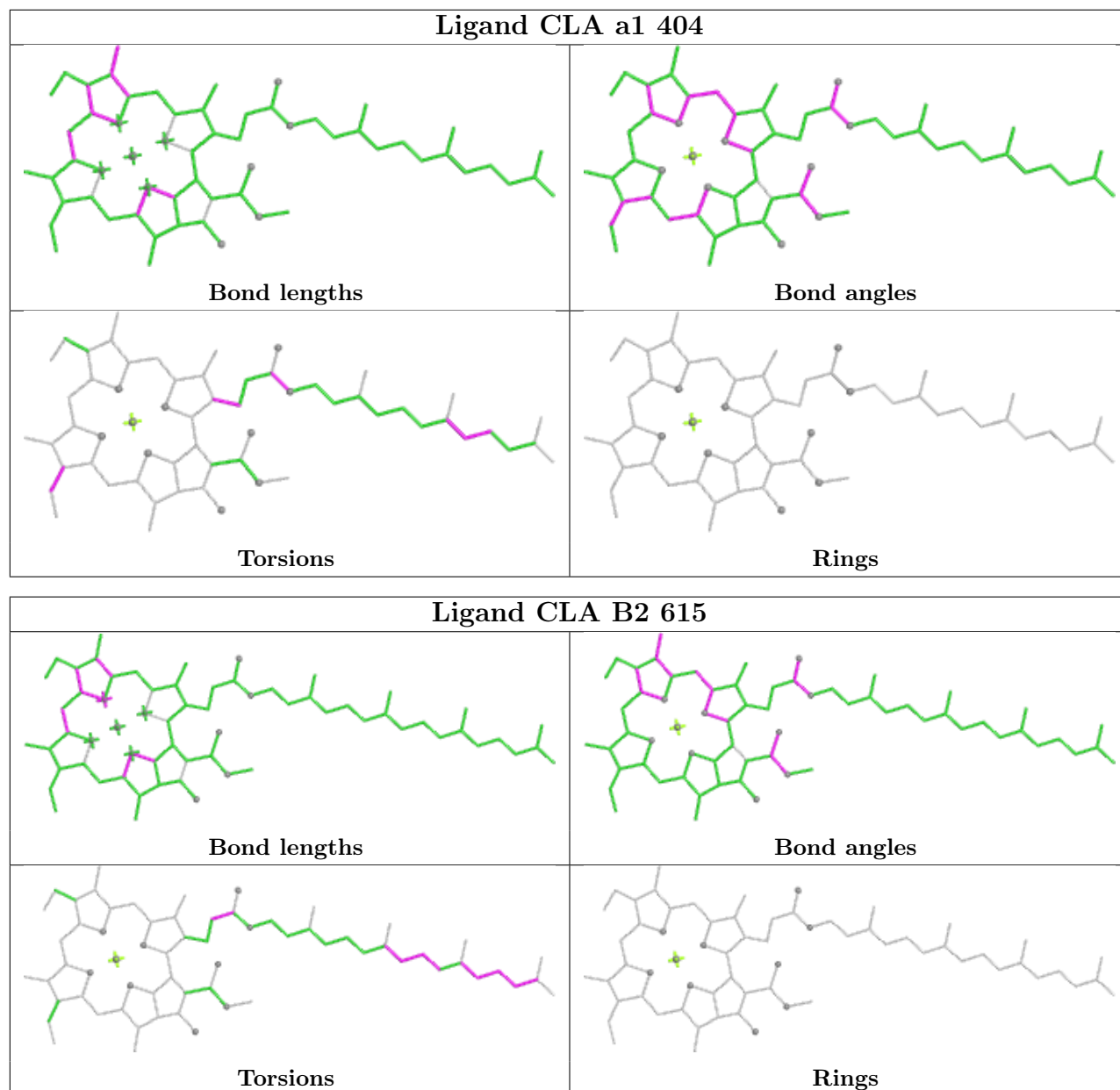


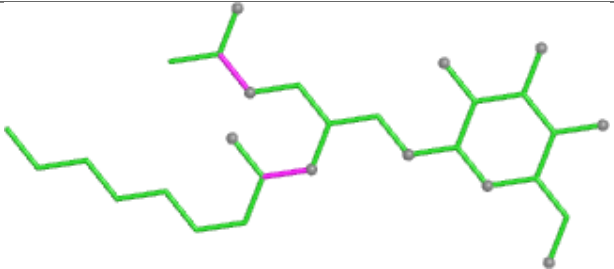
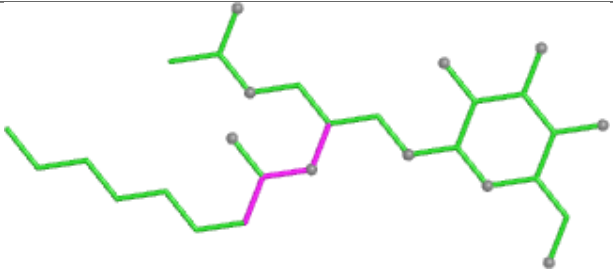
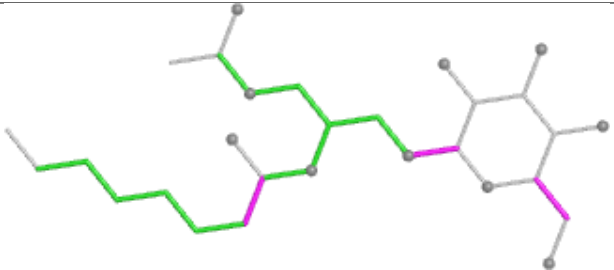
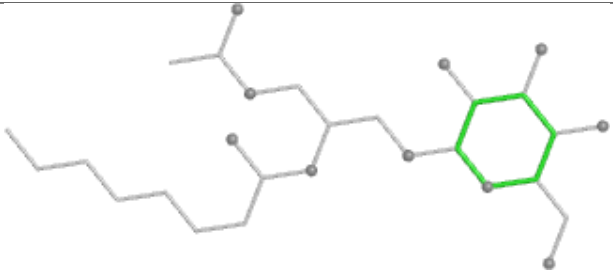
Ligand CLA B2 604

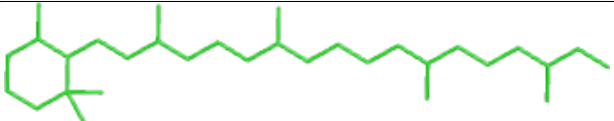
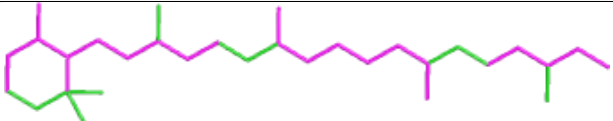
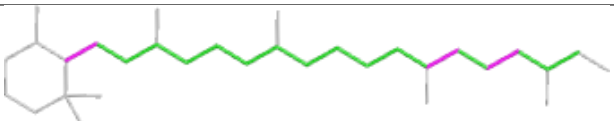
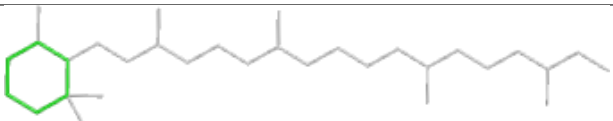


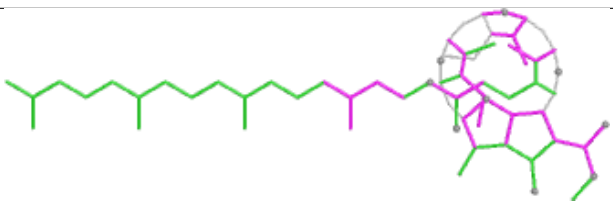
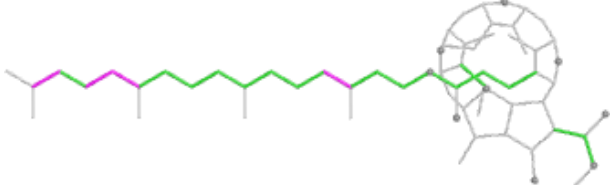
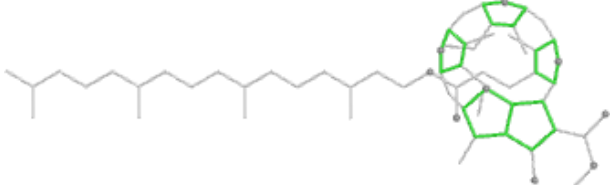
Ligand LMG c2 519

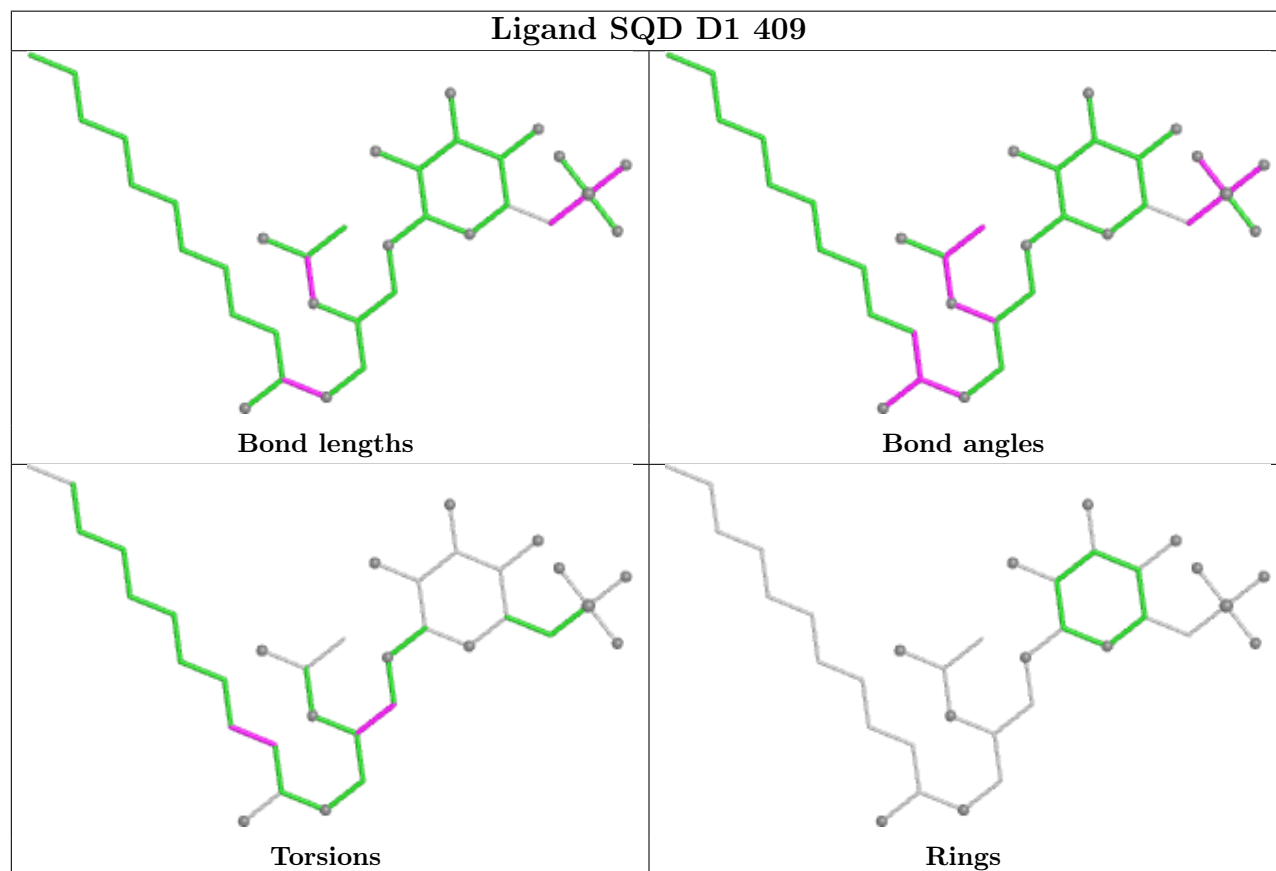
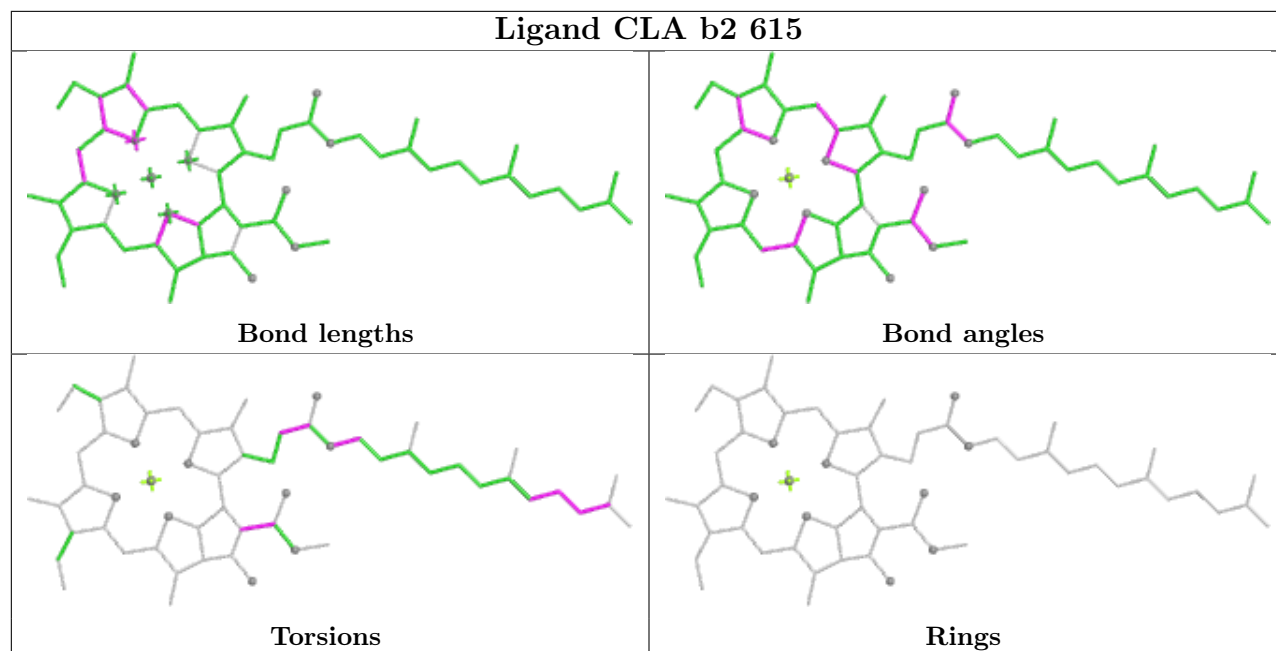


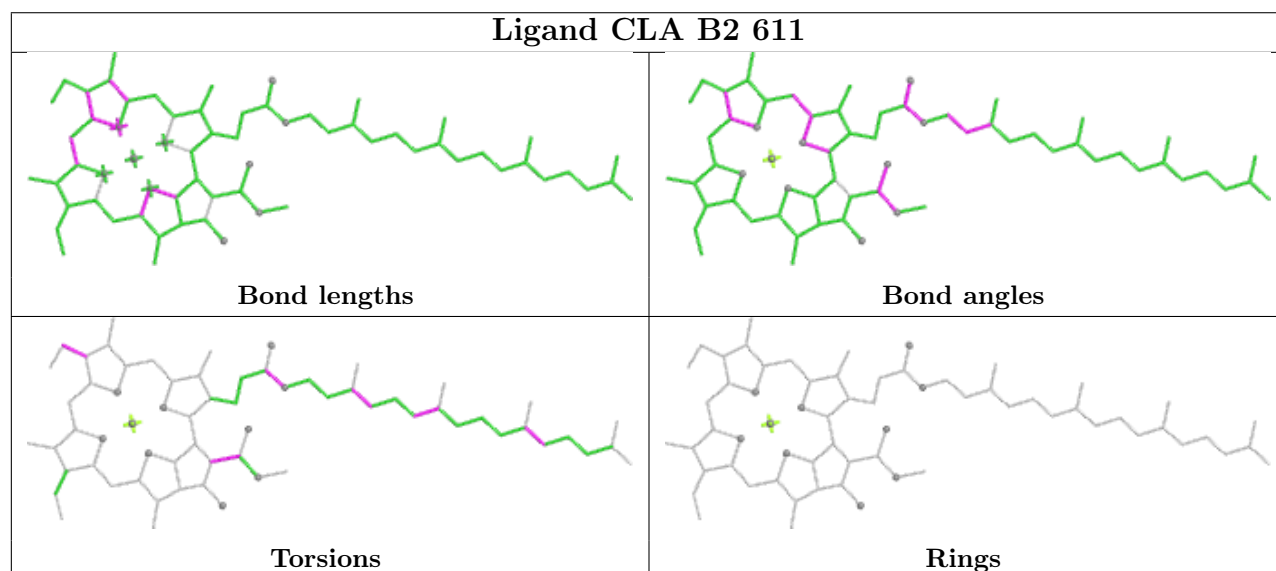
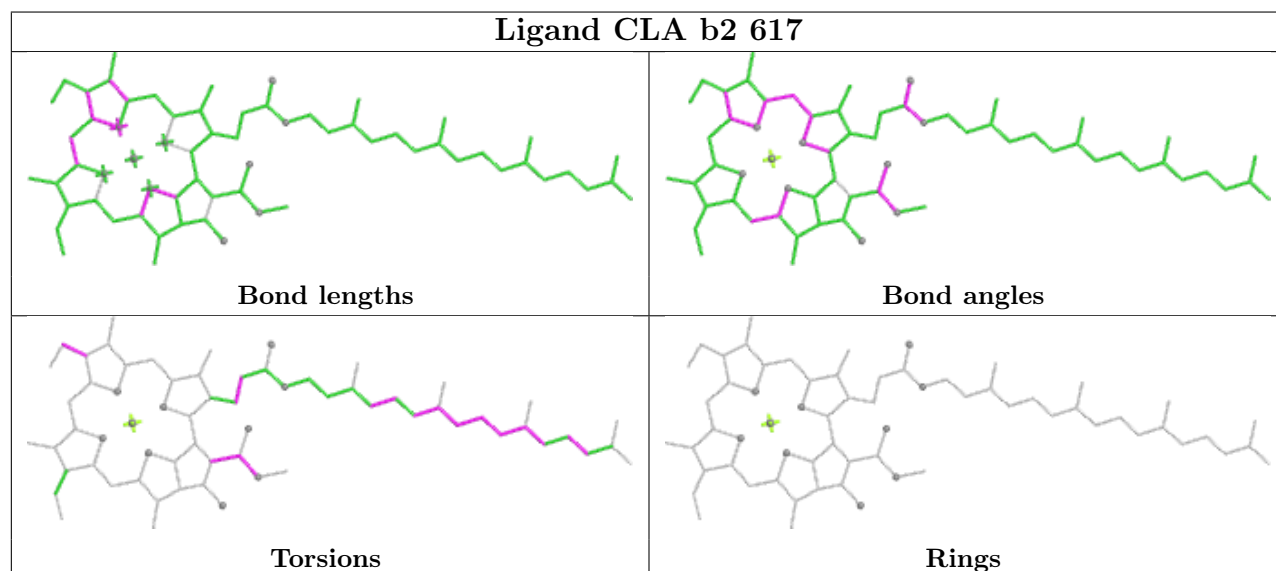
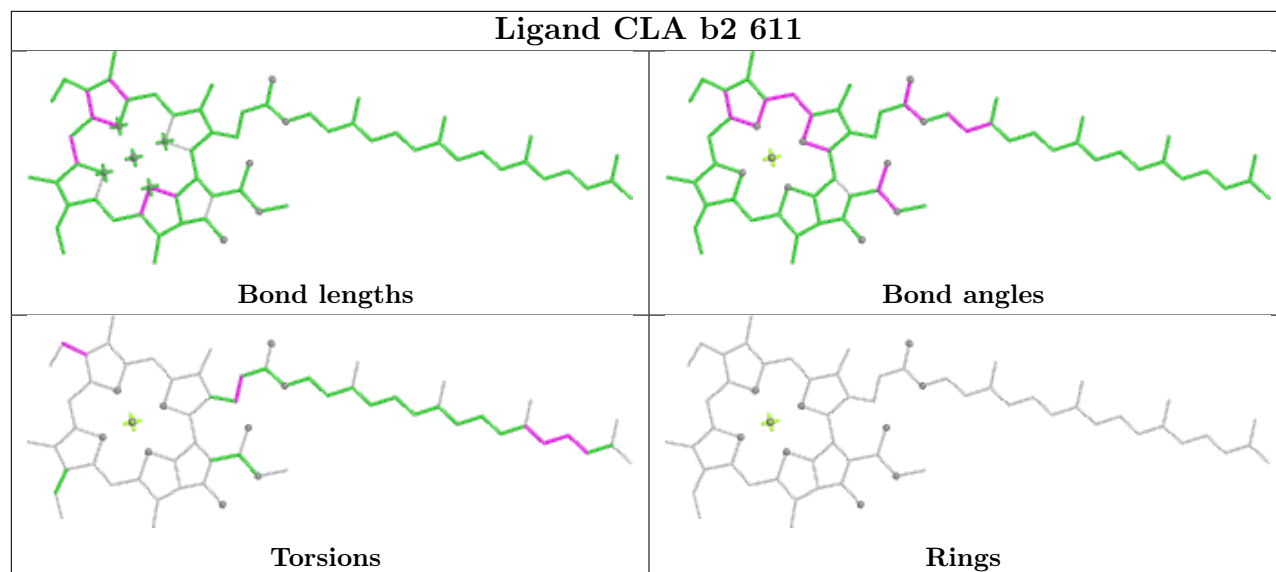


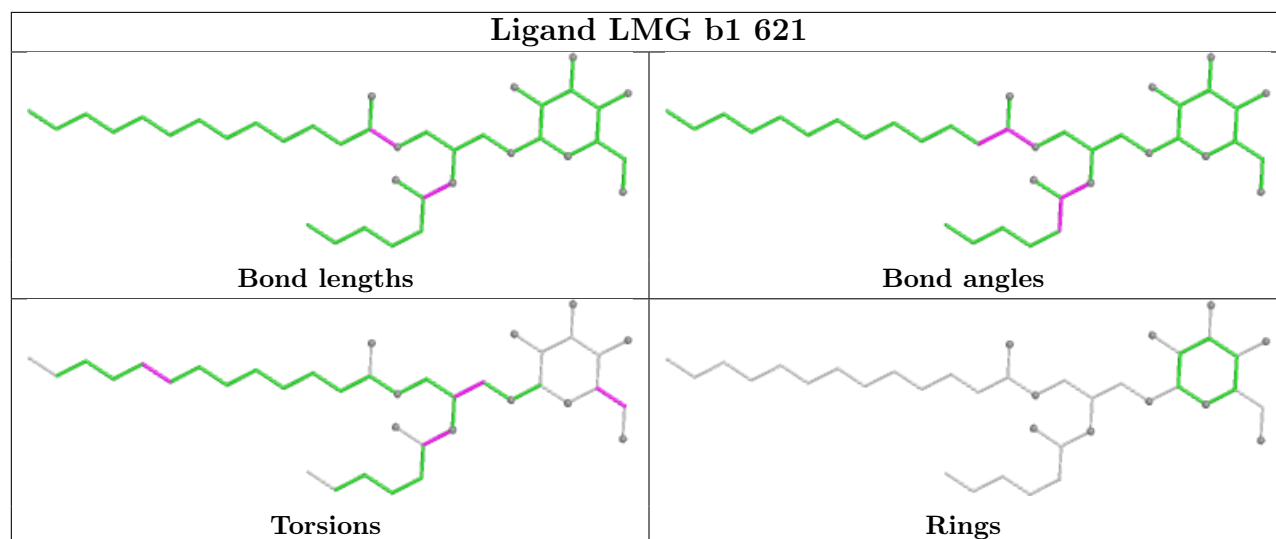
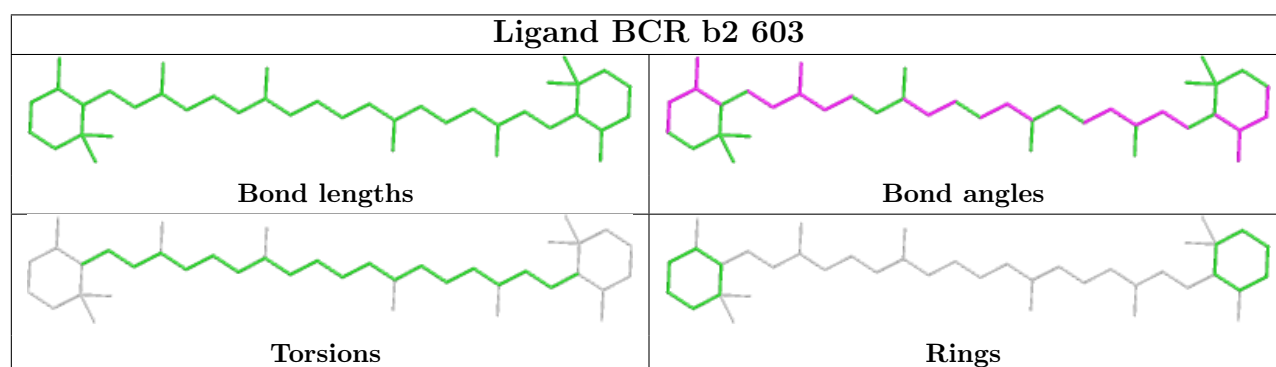
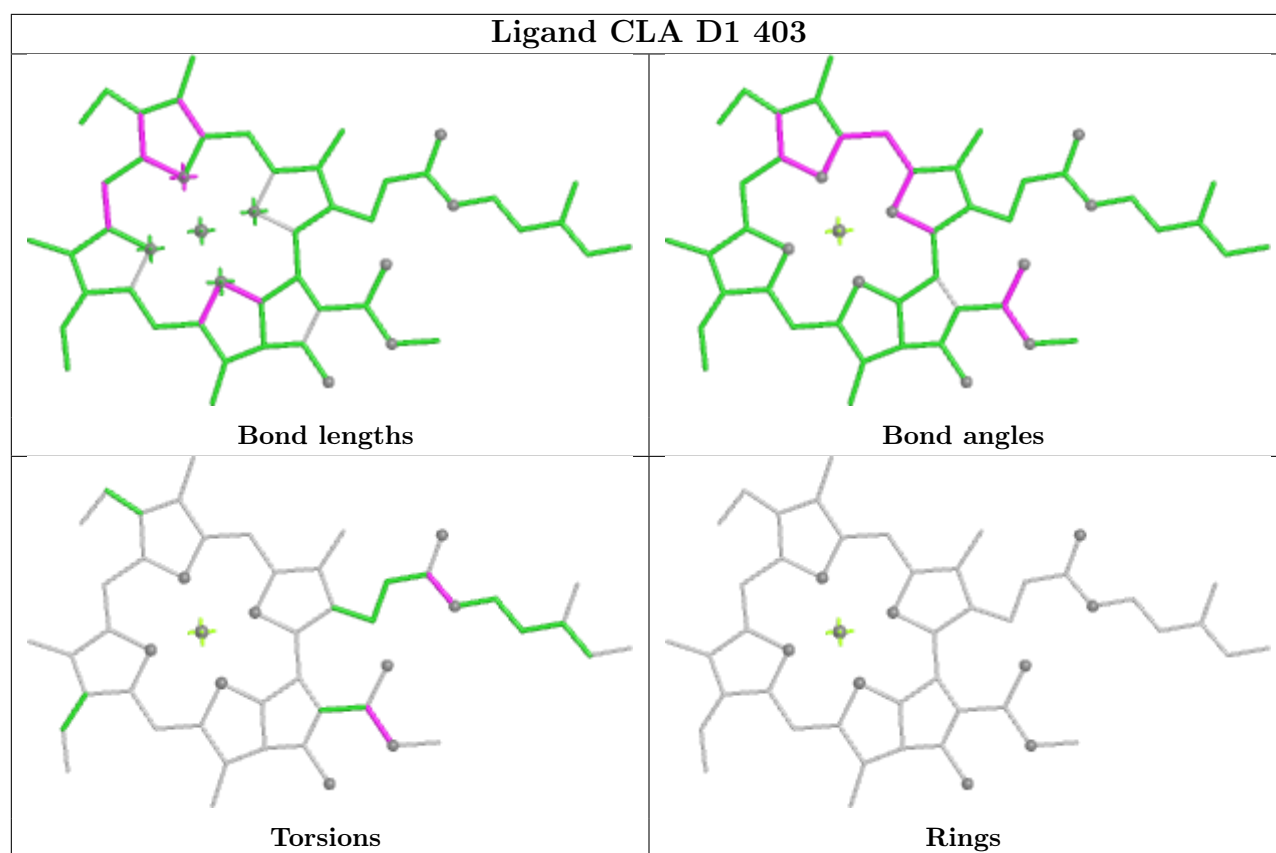
Ligand LMG A2 412	
	
Bond lengths	Bond angles
	
Torsions	Rings

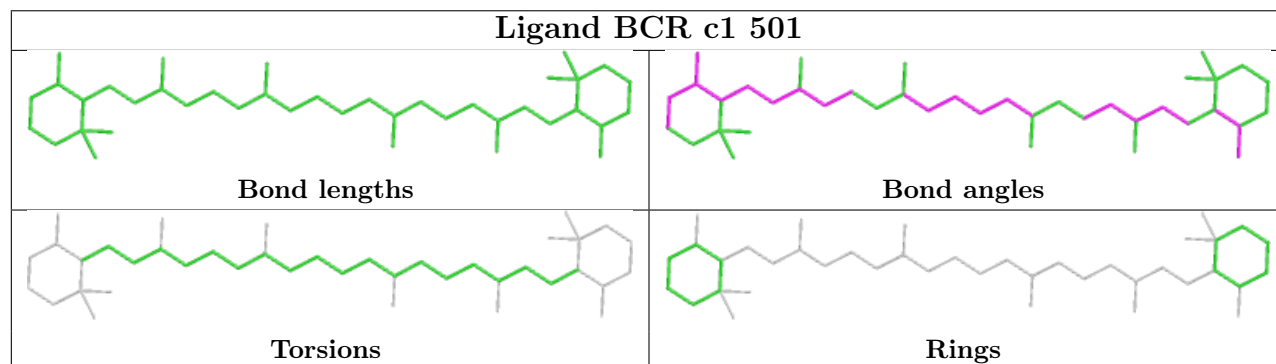
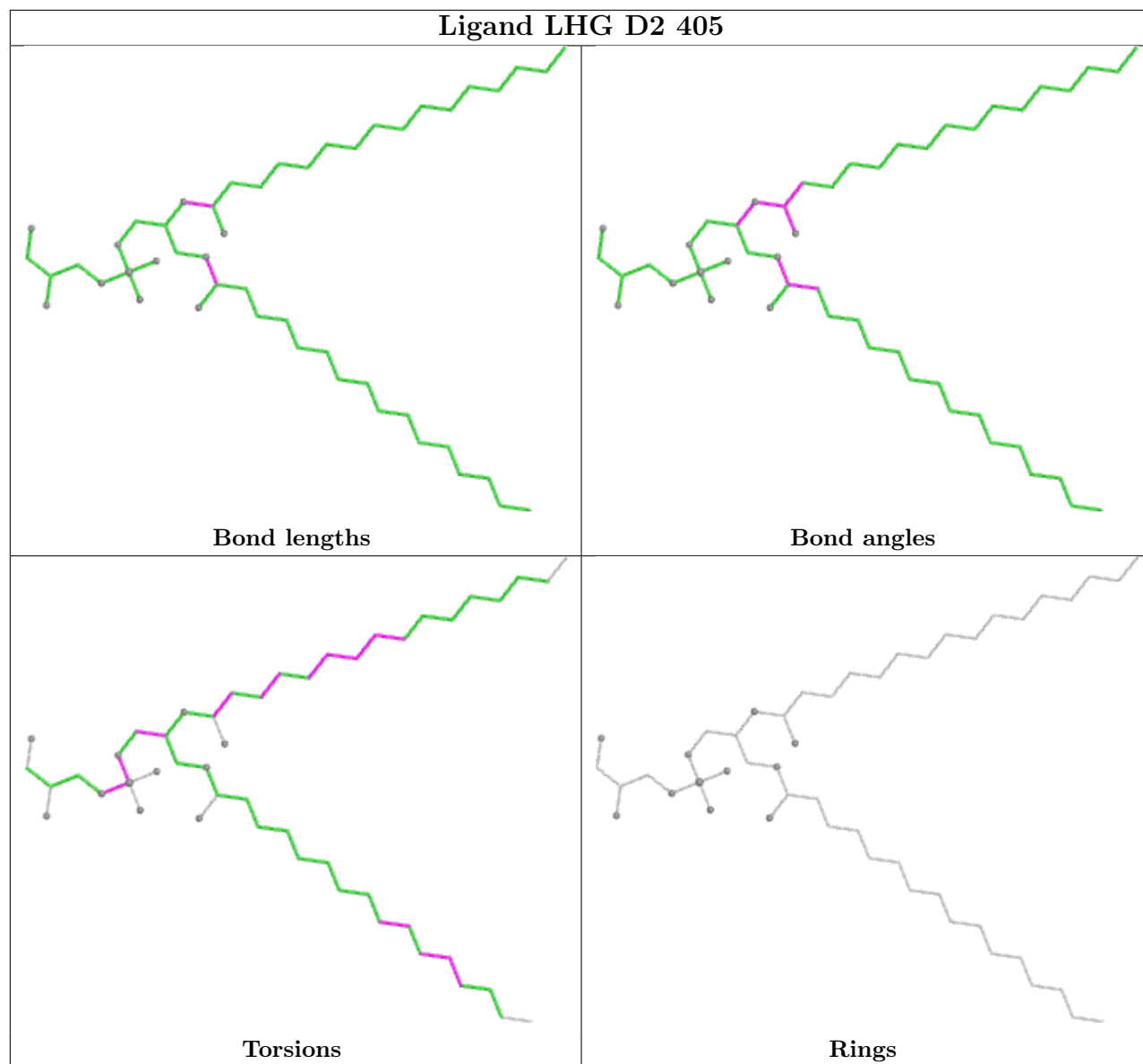
Ligand BCR K1 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

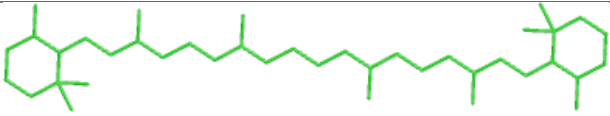
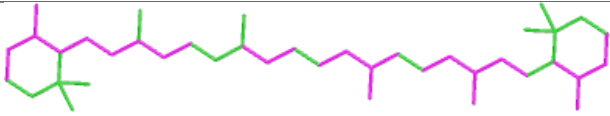
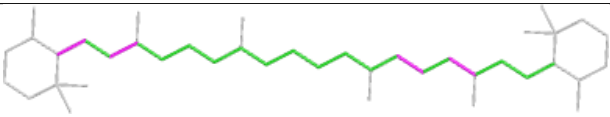
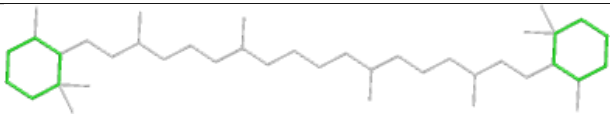
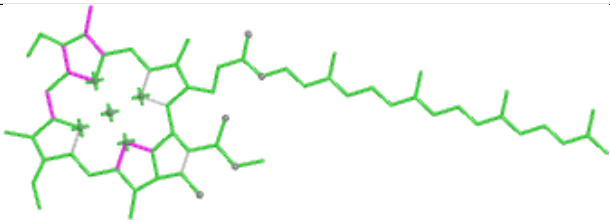
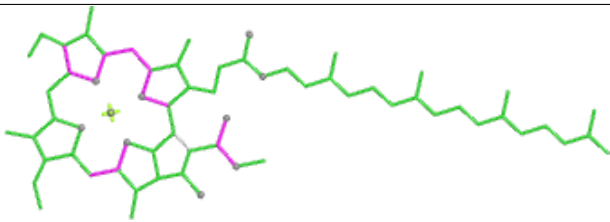
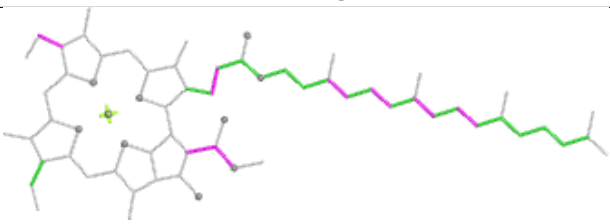
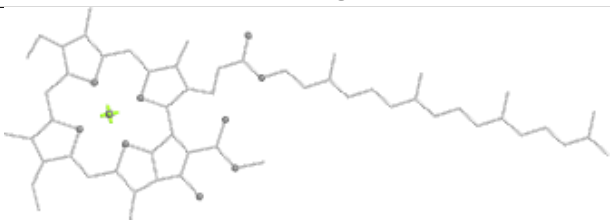
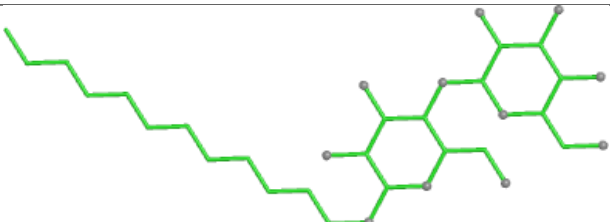
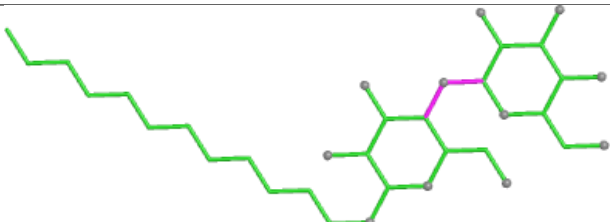
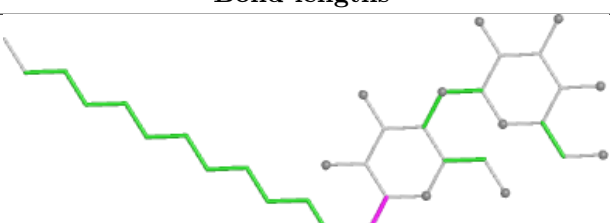
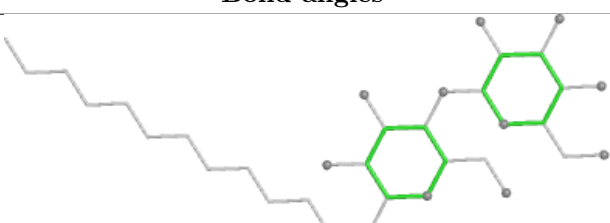
Ligand PHO a1 411	
	
Bond lengths	Bond angles
	
Torsions	Rings

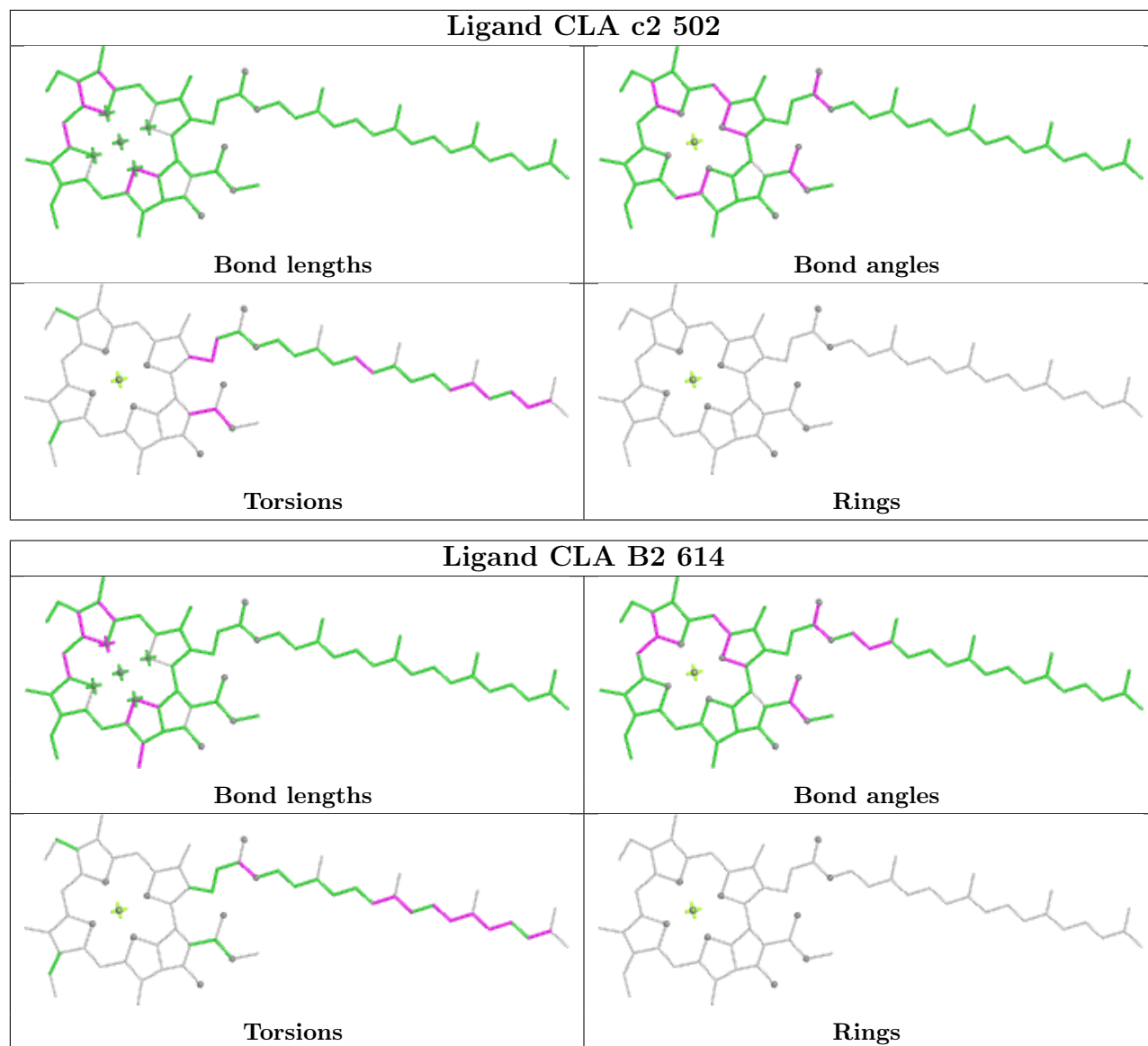


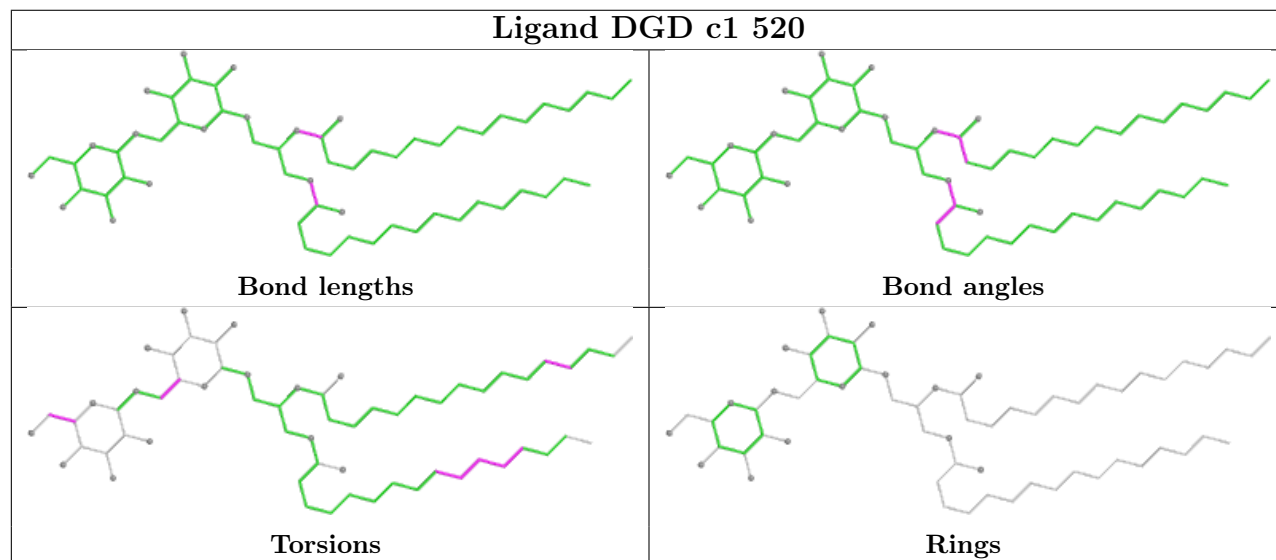
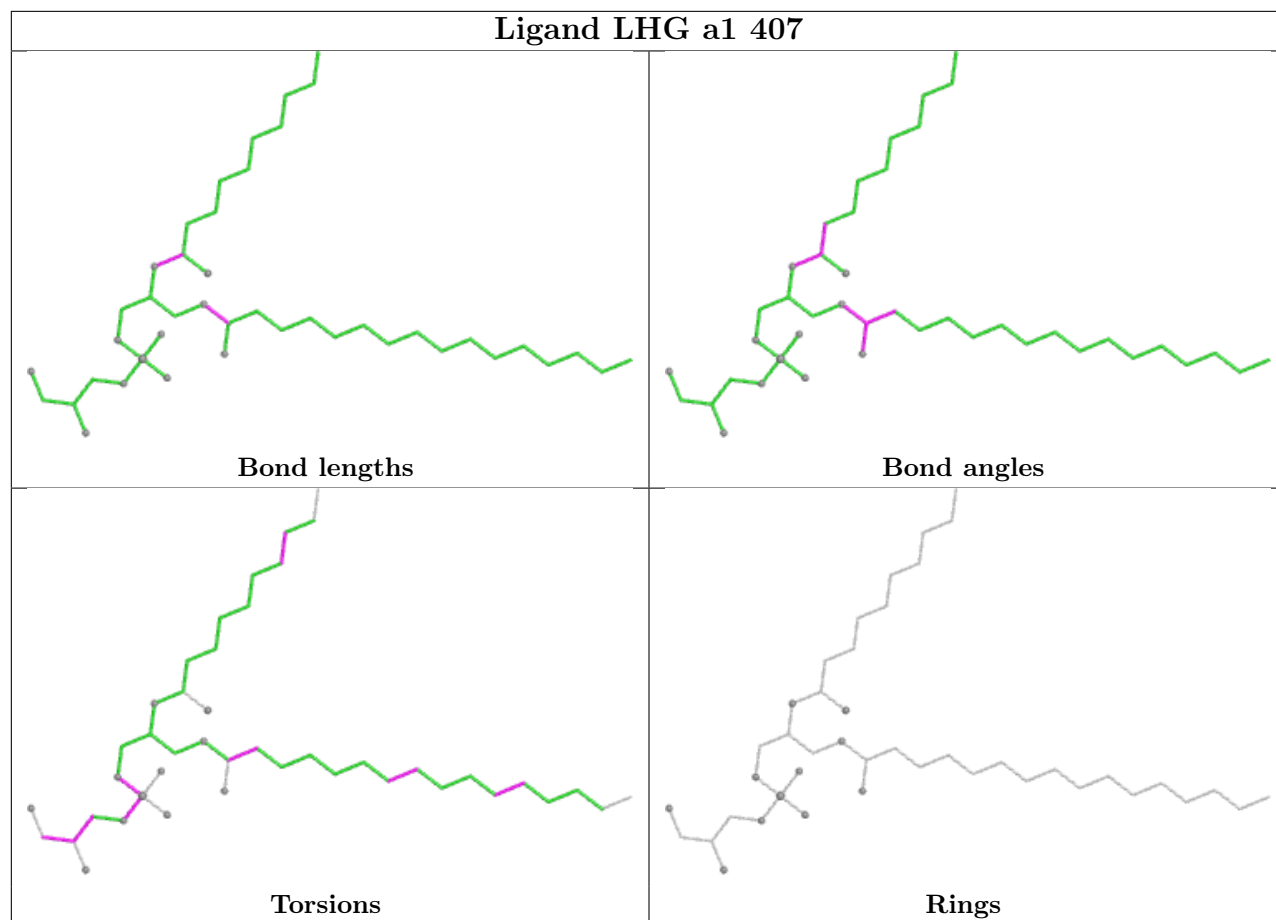


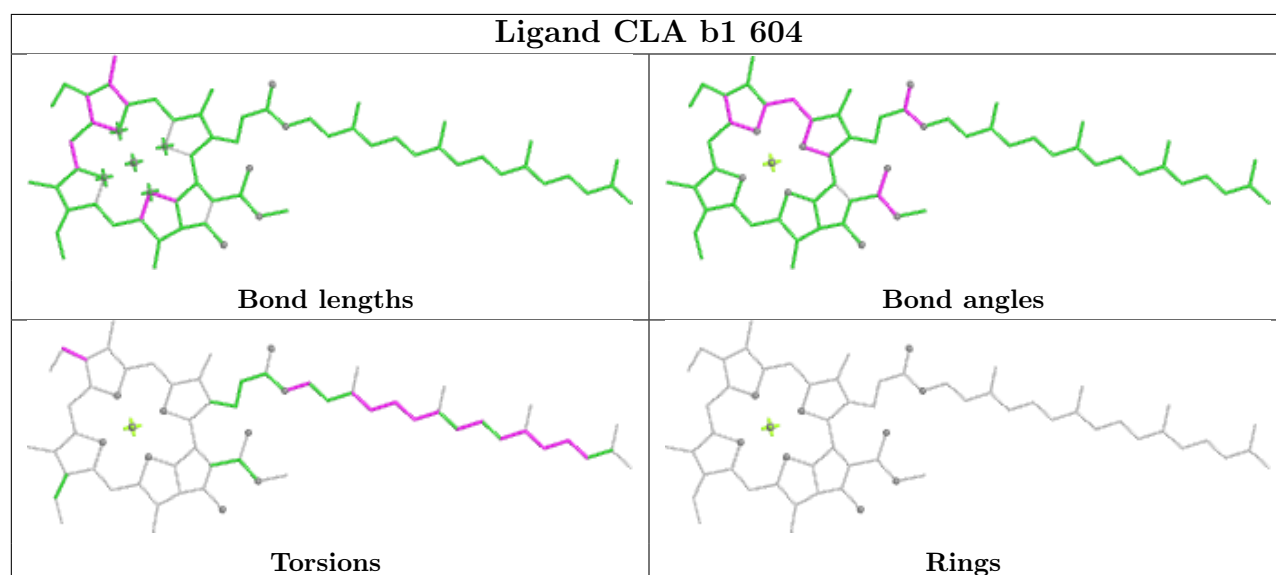
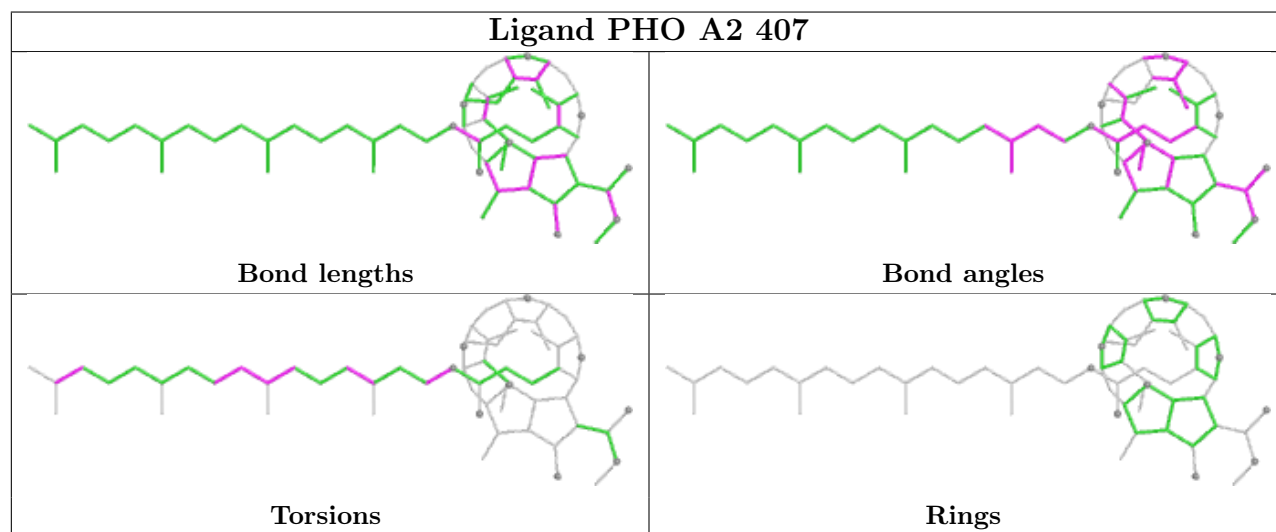
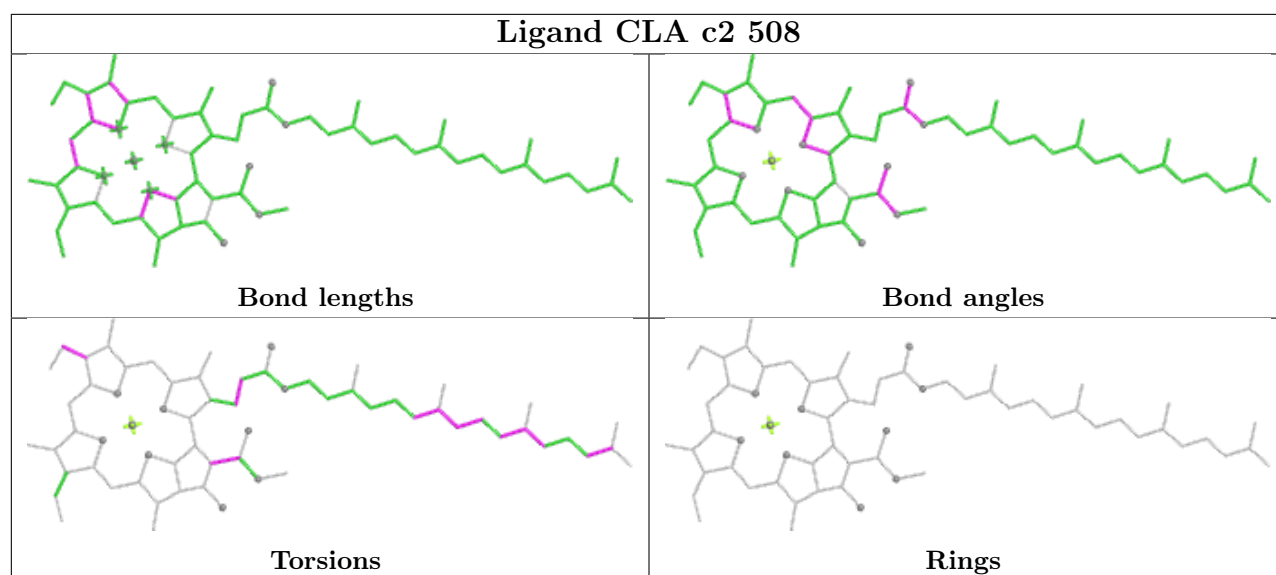


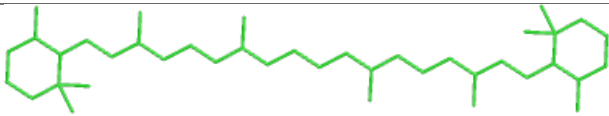
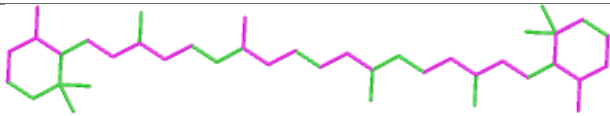
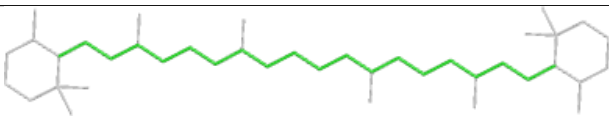
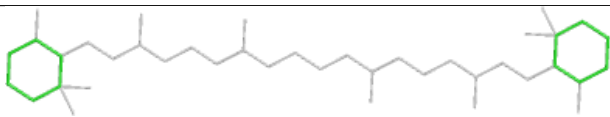


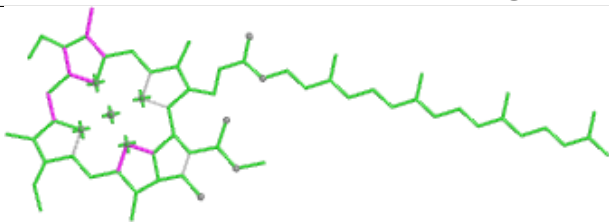
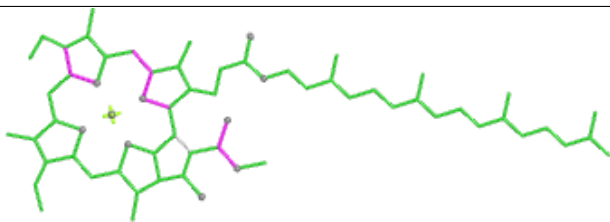
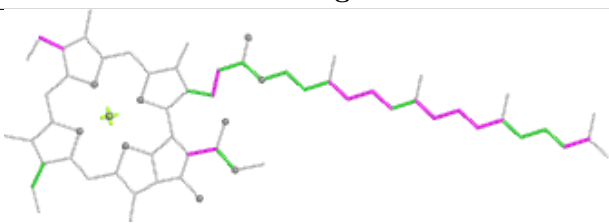
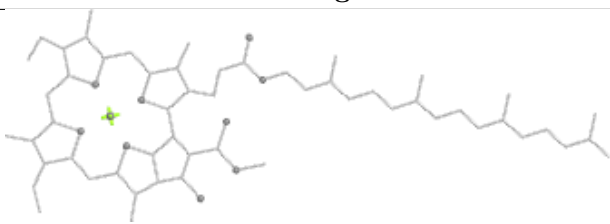
Ligand BCR K2 102	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA B2 606	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMT C1 519	
 Bond lengths	 Bond angles
 Torsions	 Rings

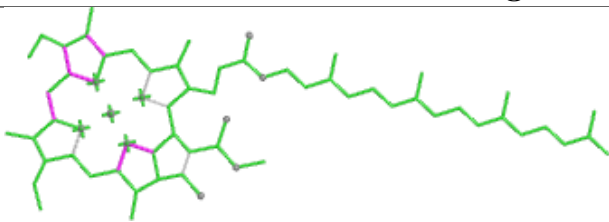
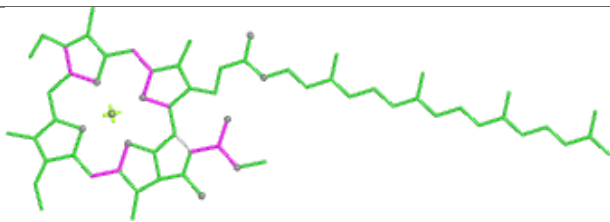
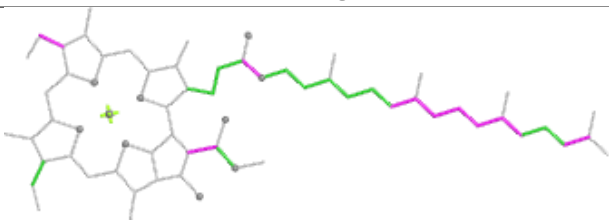
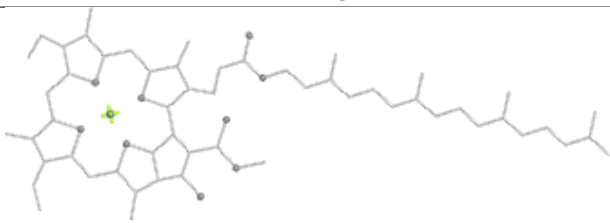


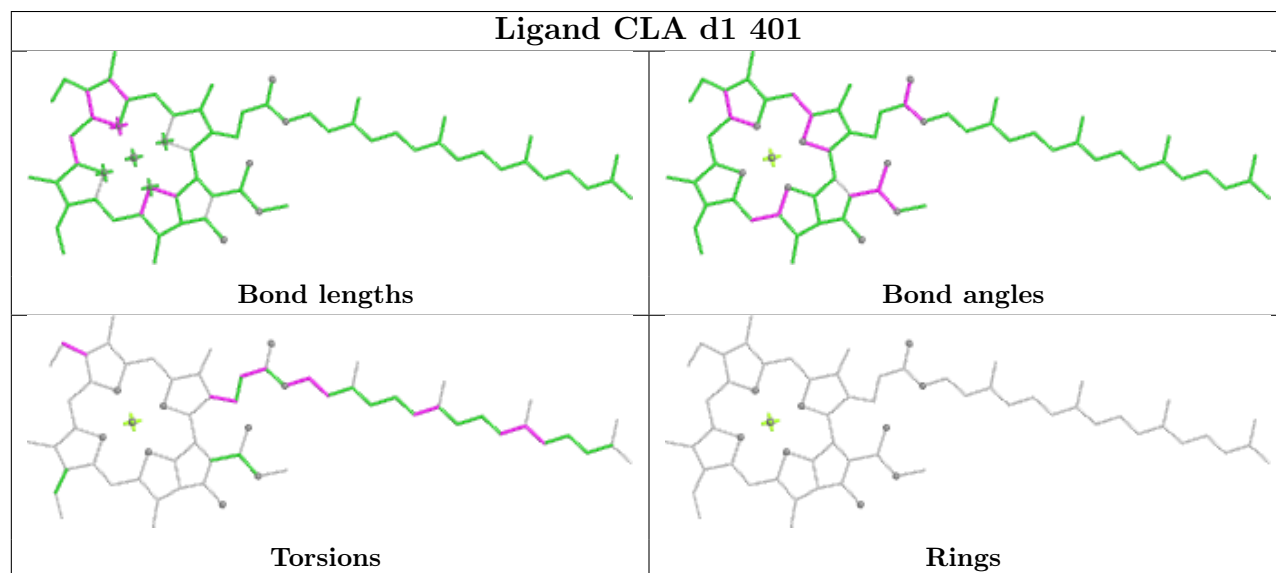
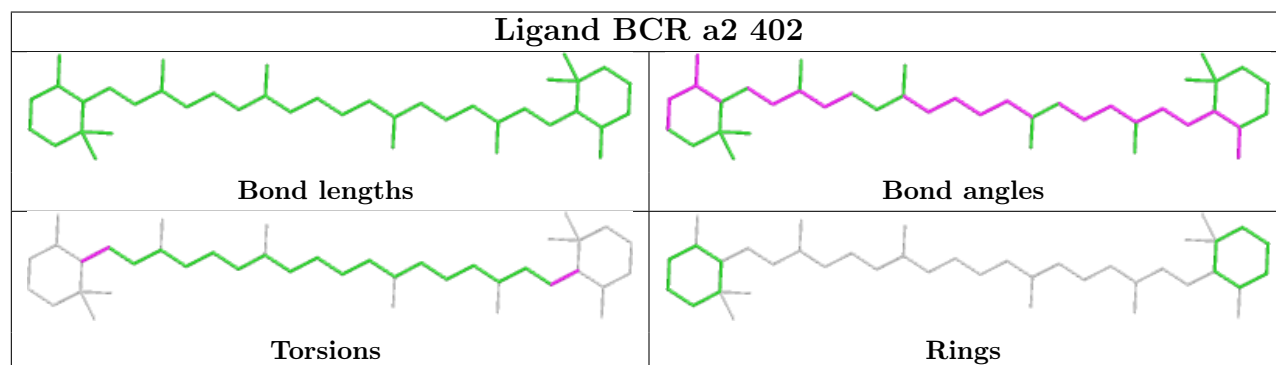
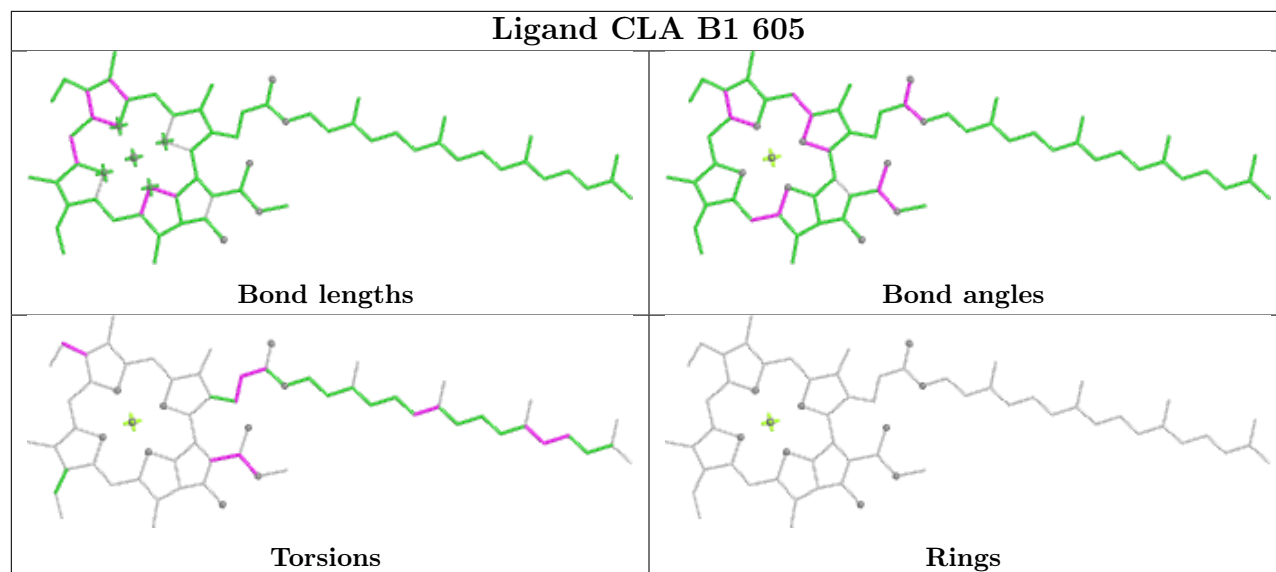


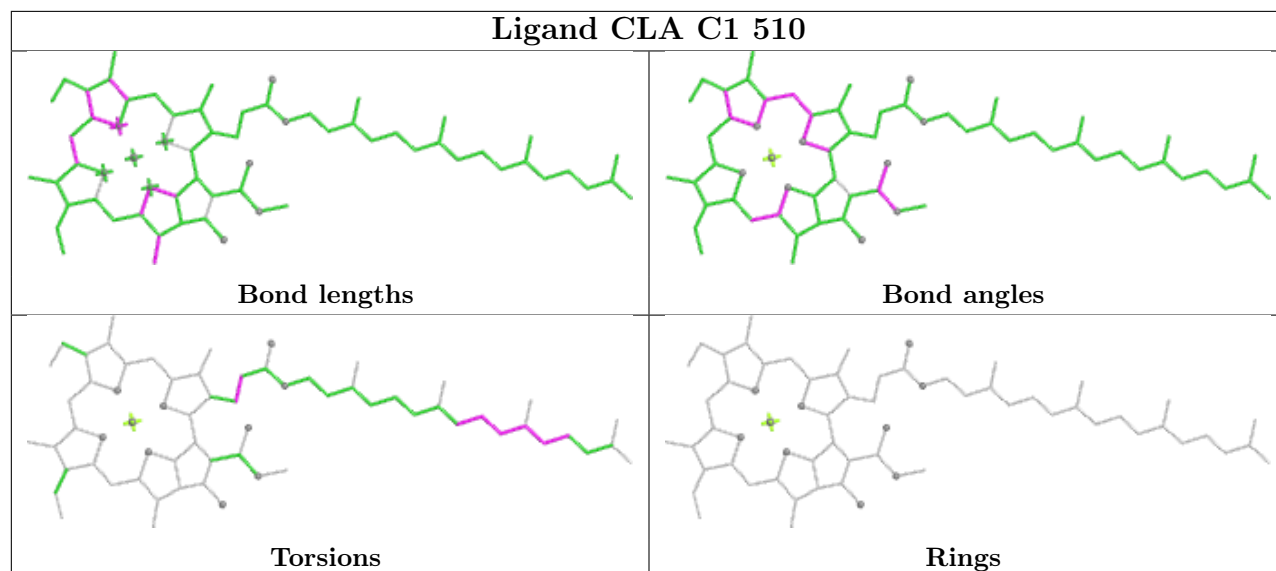
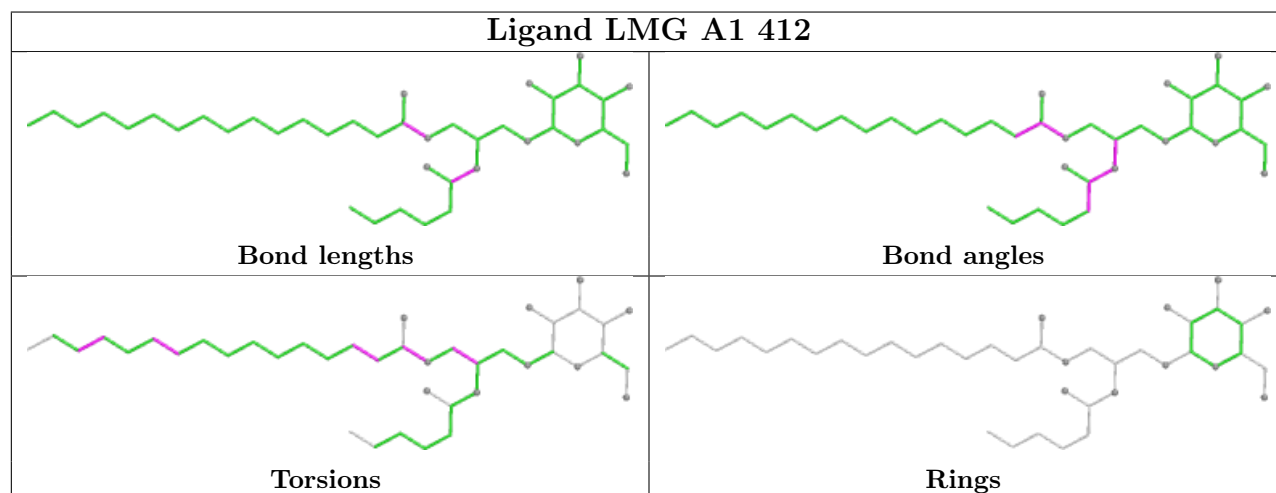
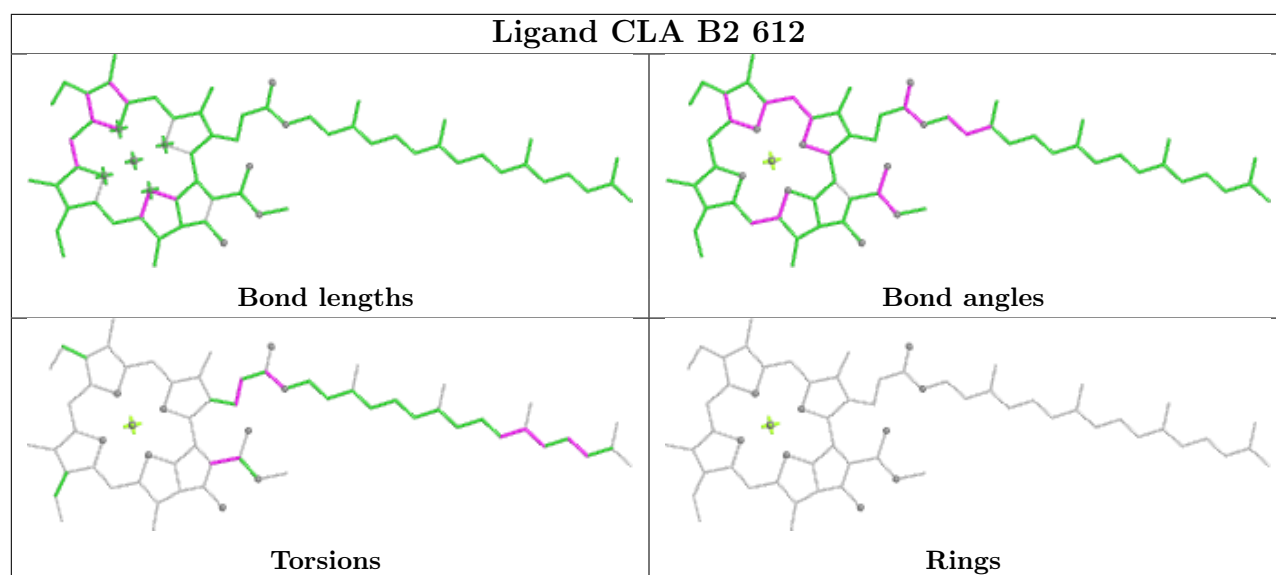


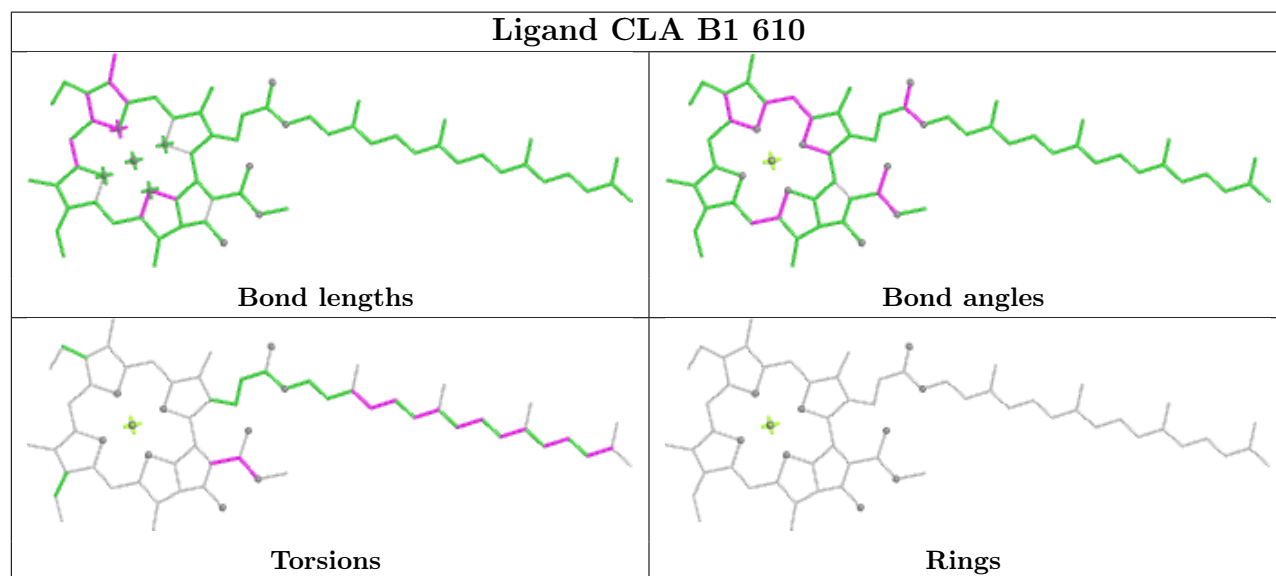
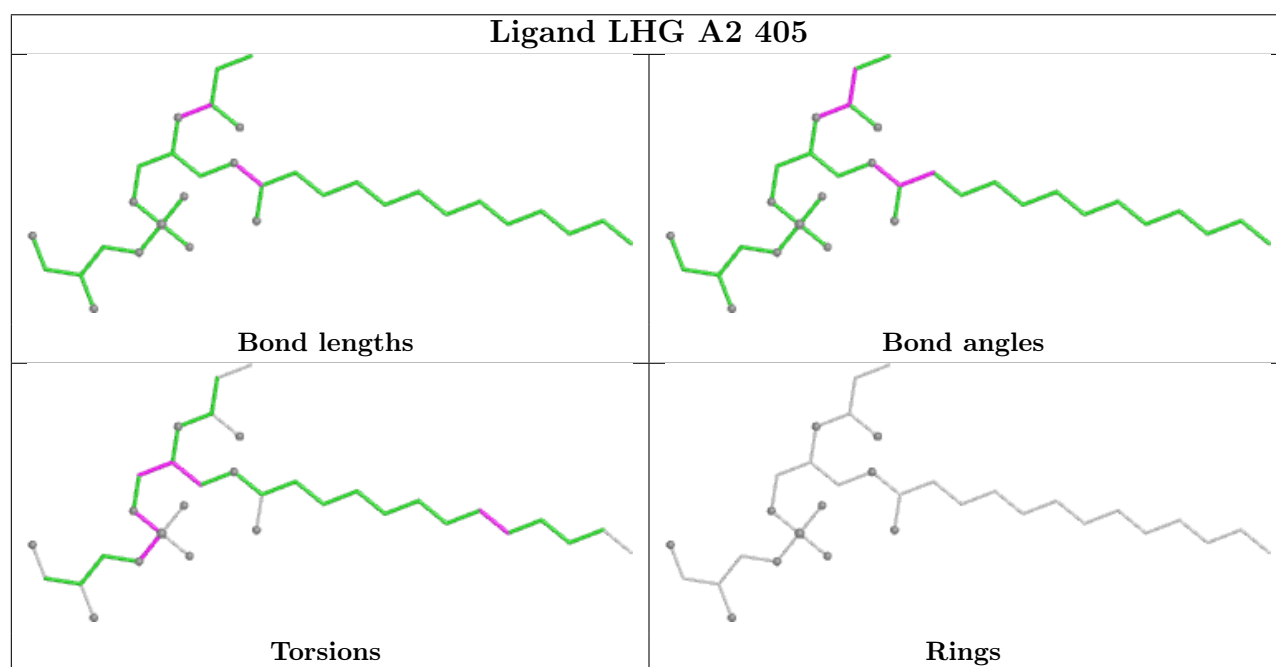
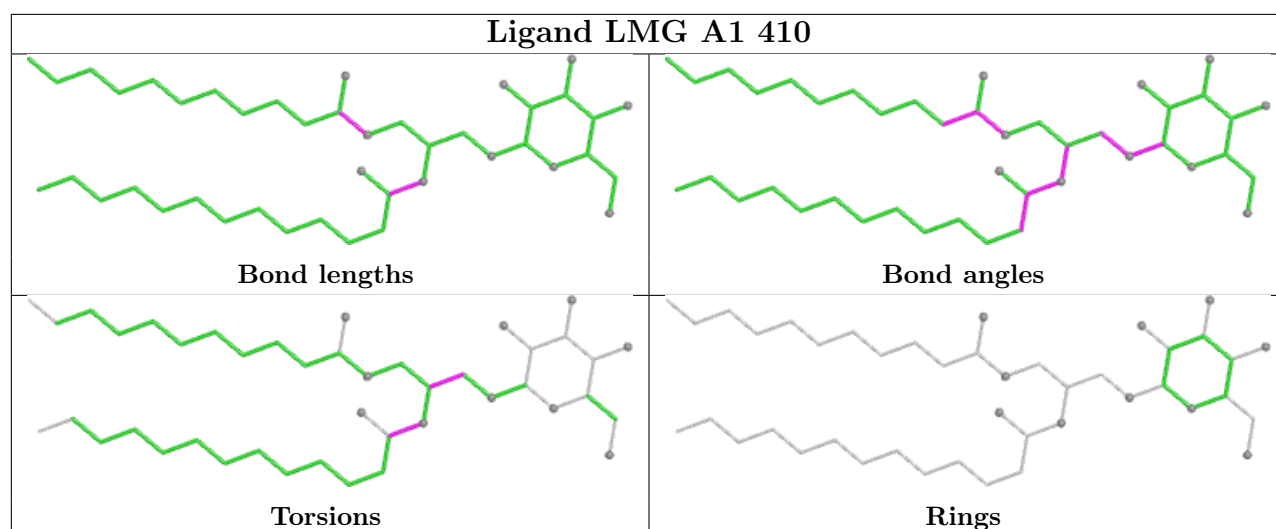
Ligand BCR b1 601	
	
Bond lengths	Bond angles
	
Torsions	Rings

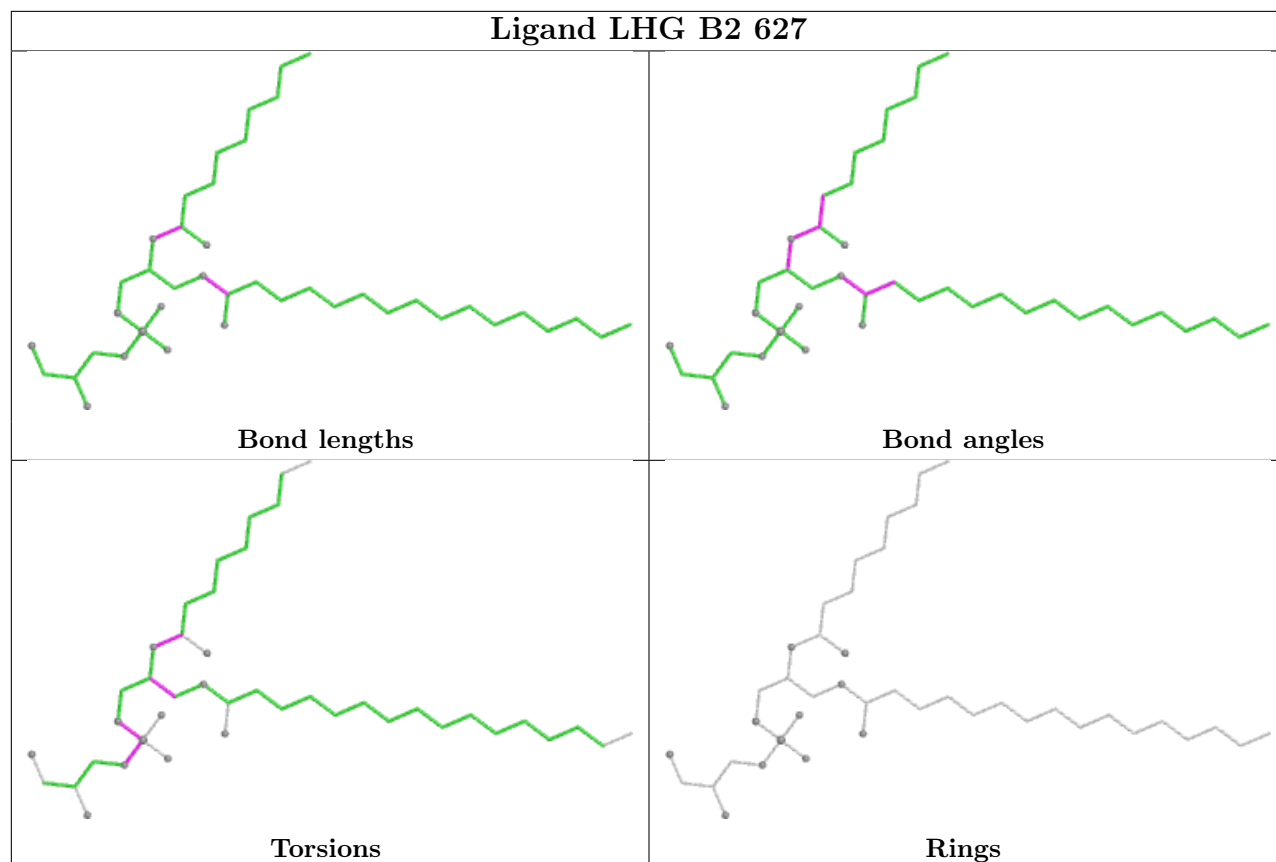
Ligand CLA c1 509	
	
Bond lengths	Bond angles
	
Torsions	Rings

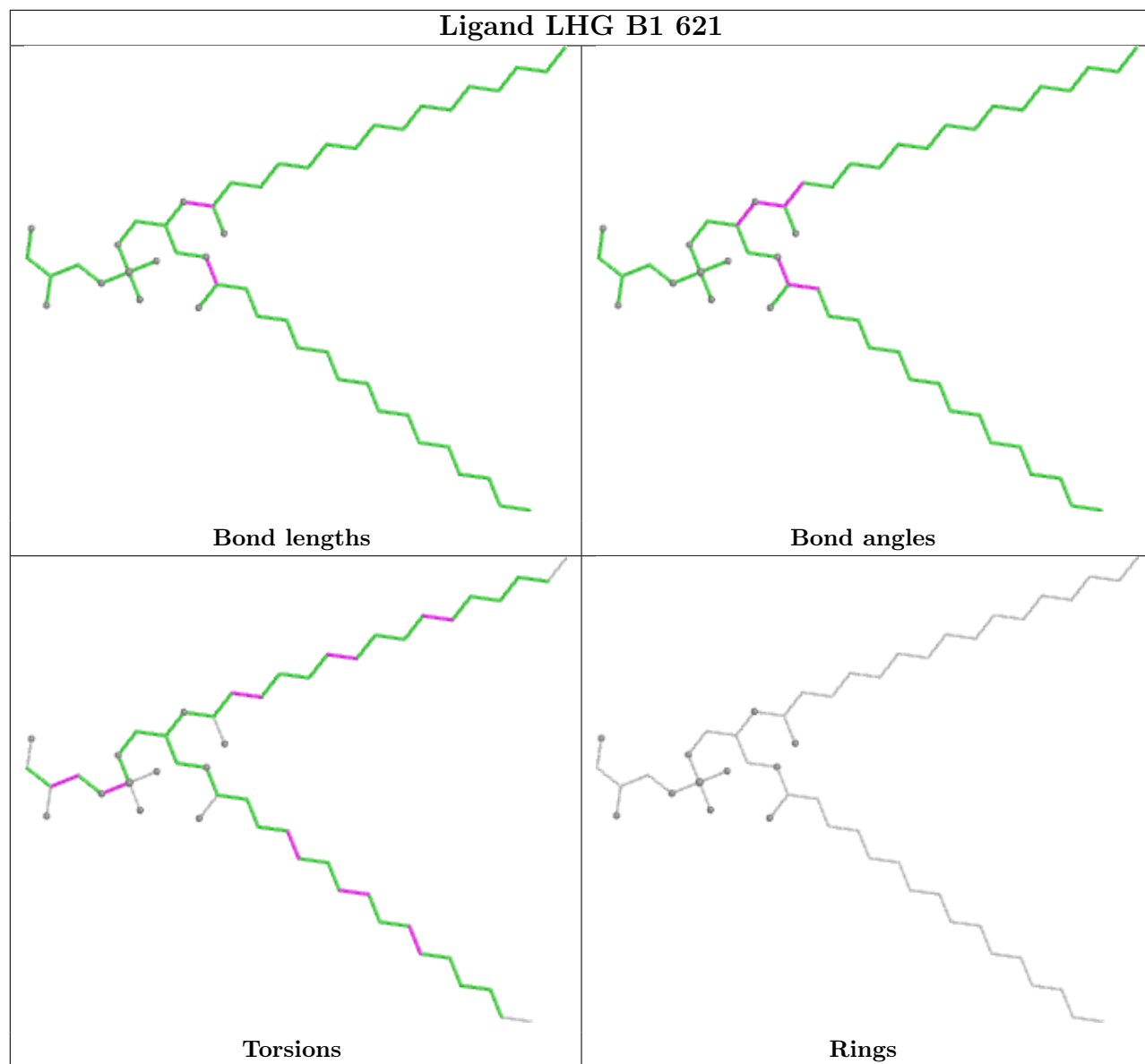
Ligand CLA c2 505	
	
Bond lengths	Bond angles
	
Torsions	Rings

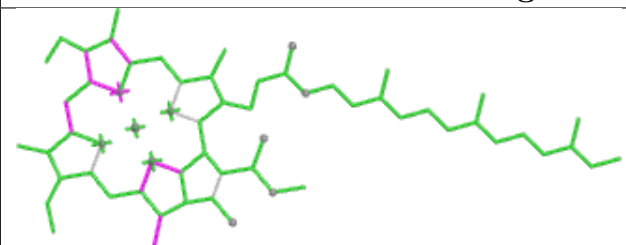
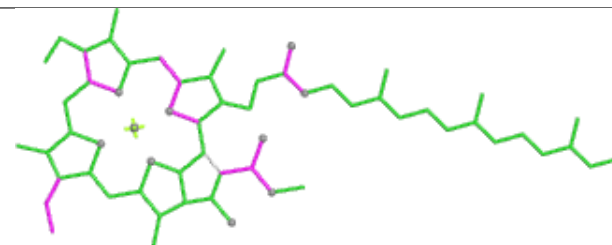
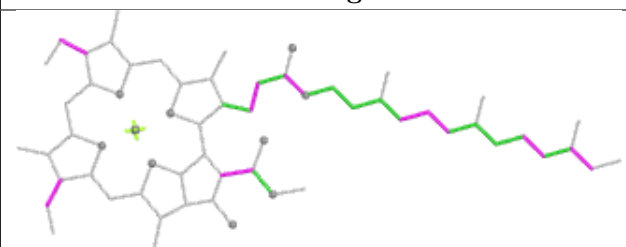
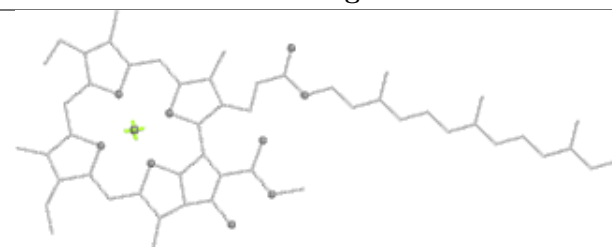


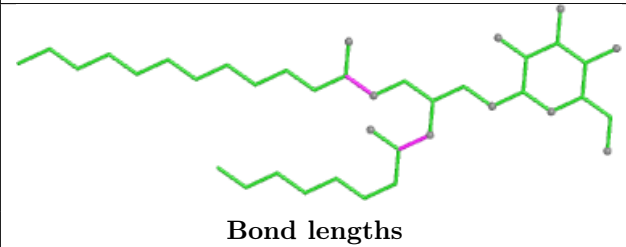
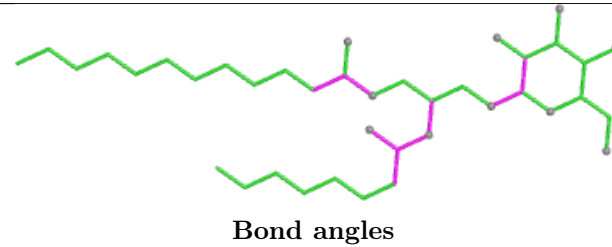
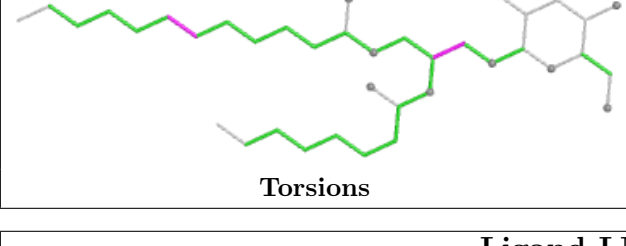
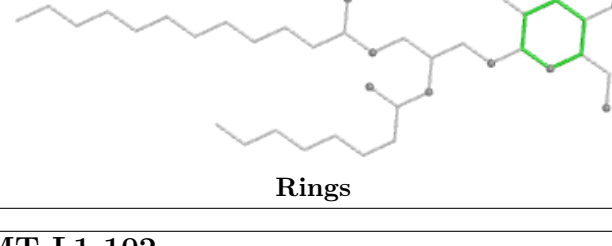


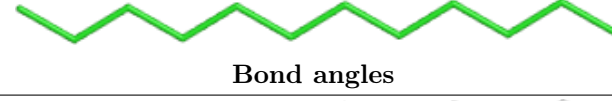
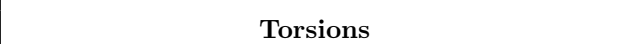


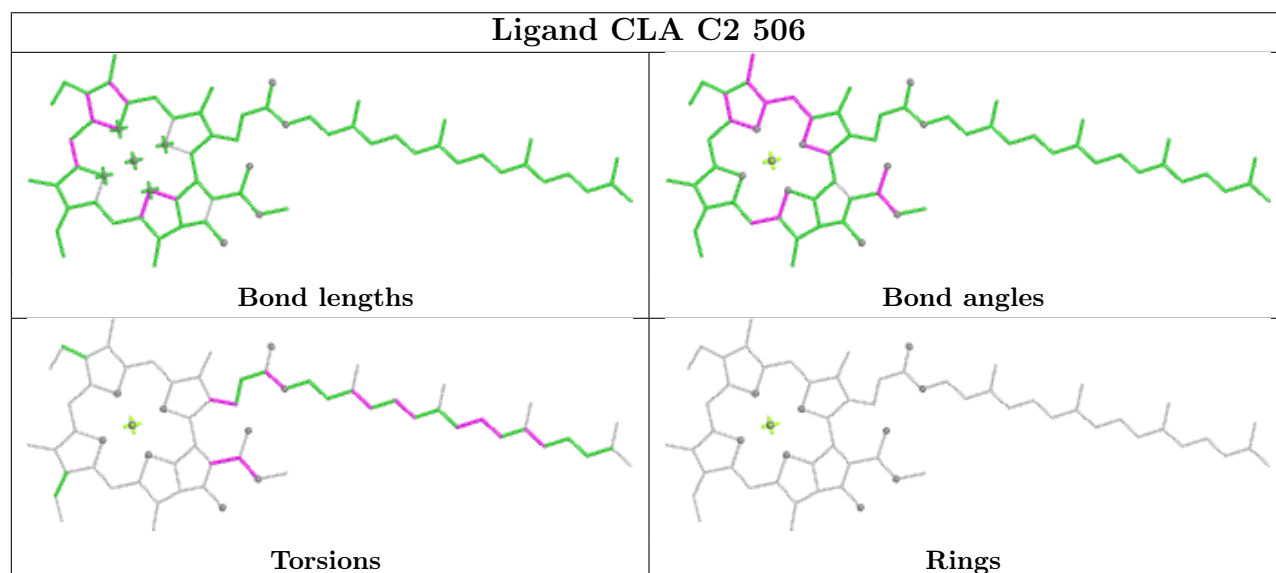
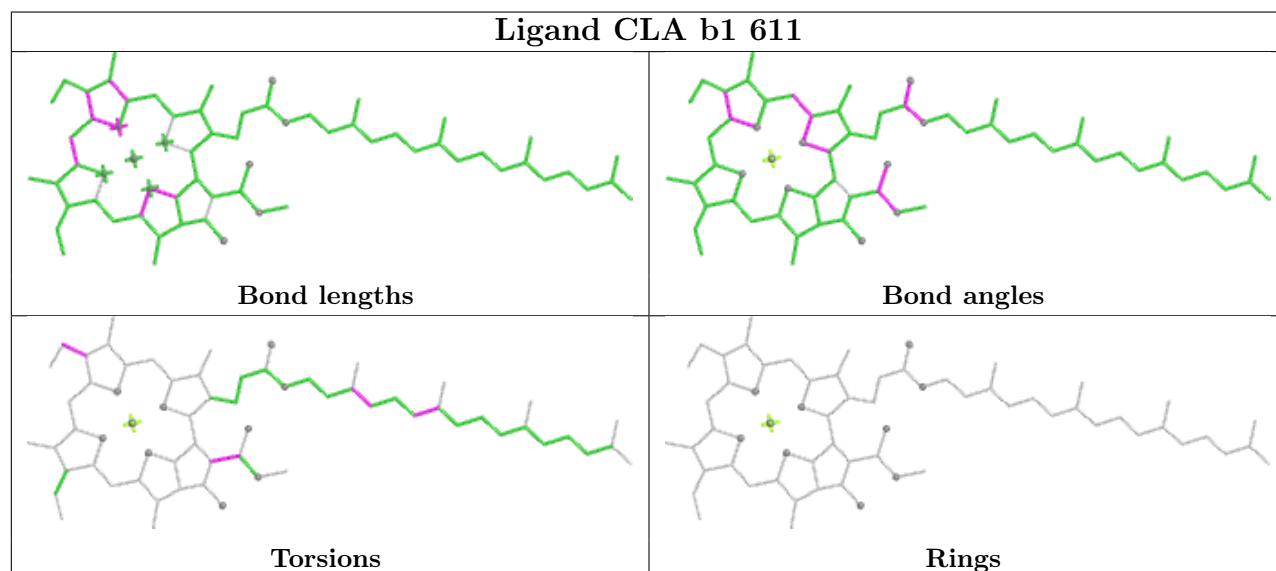
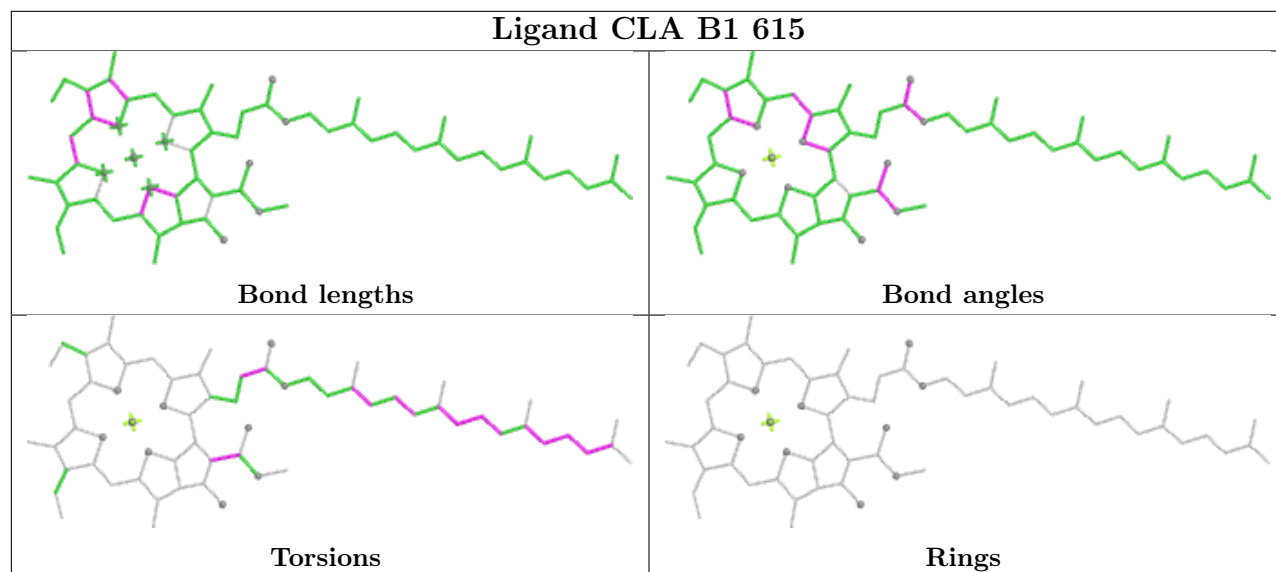


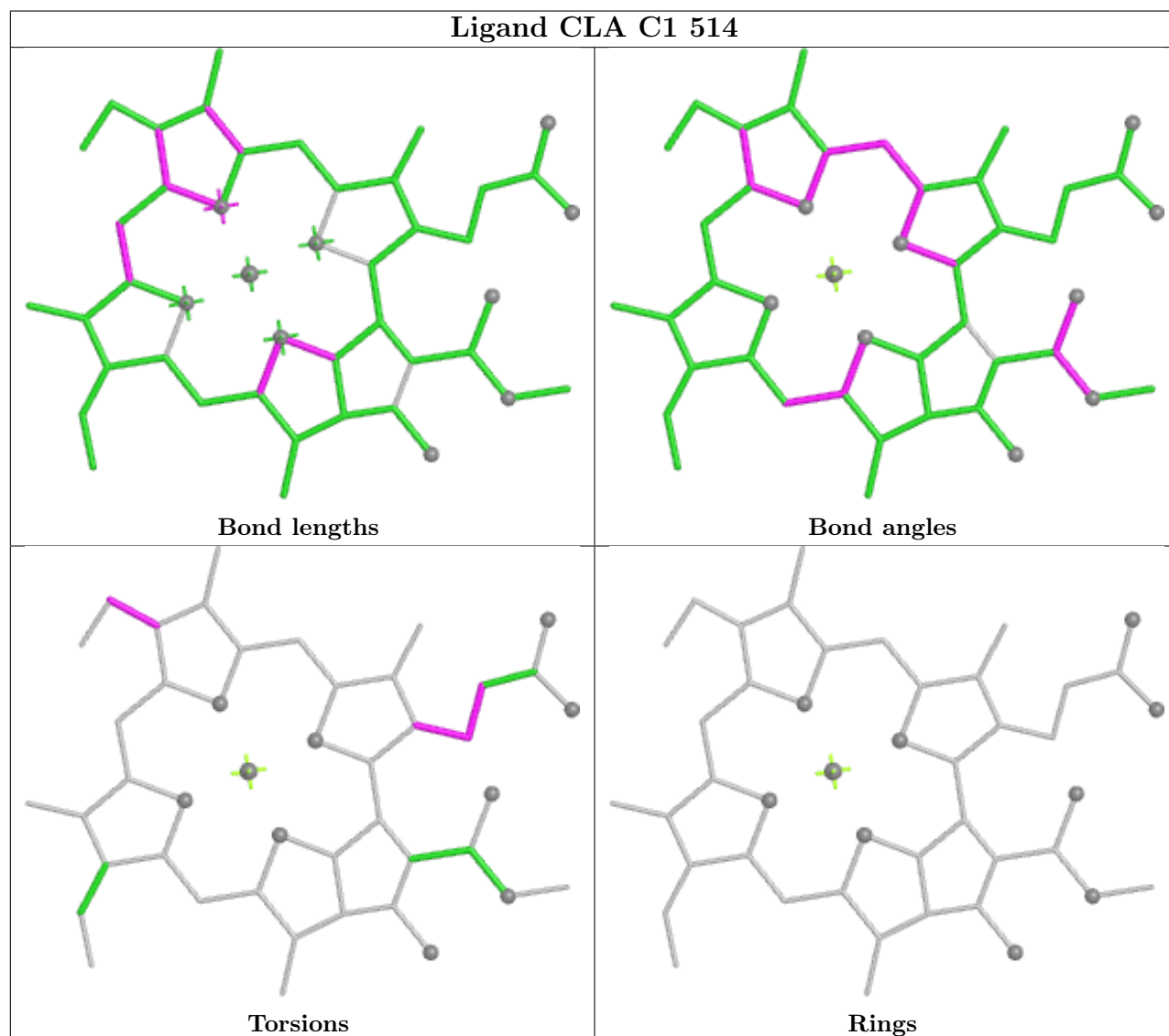
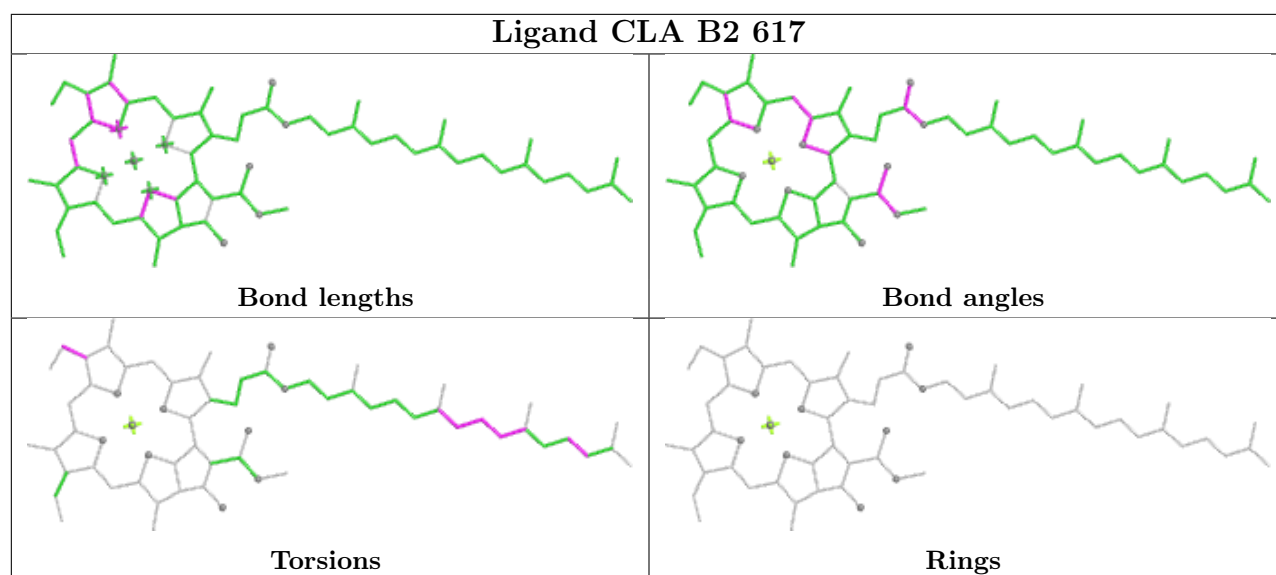


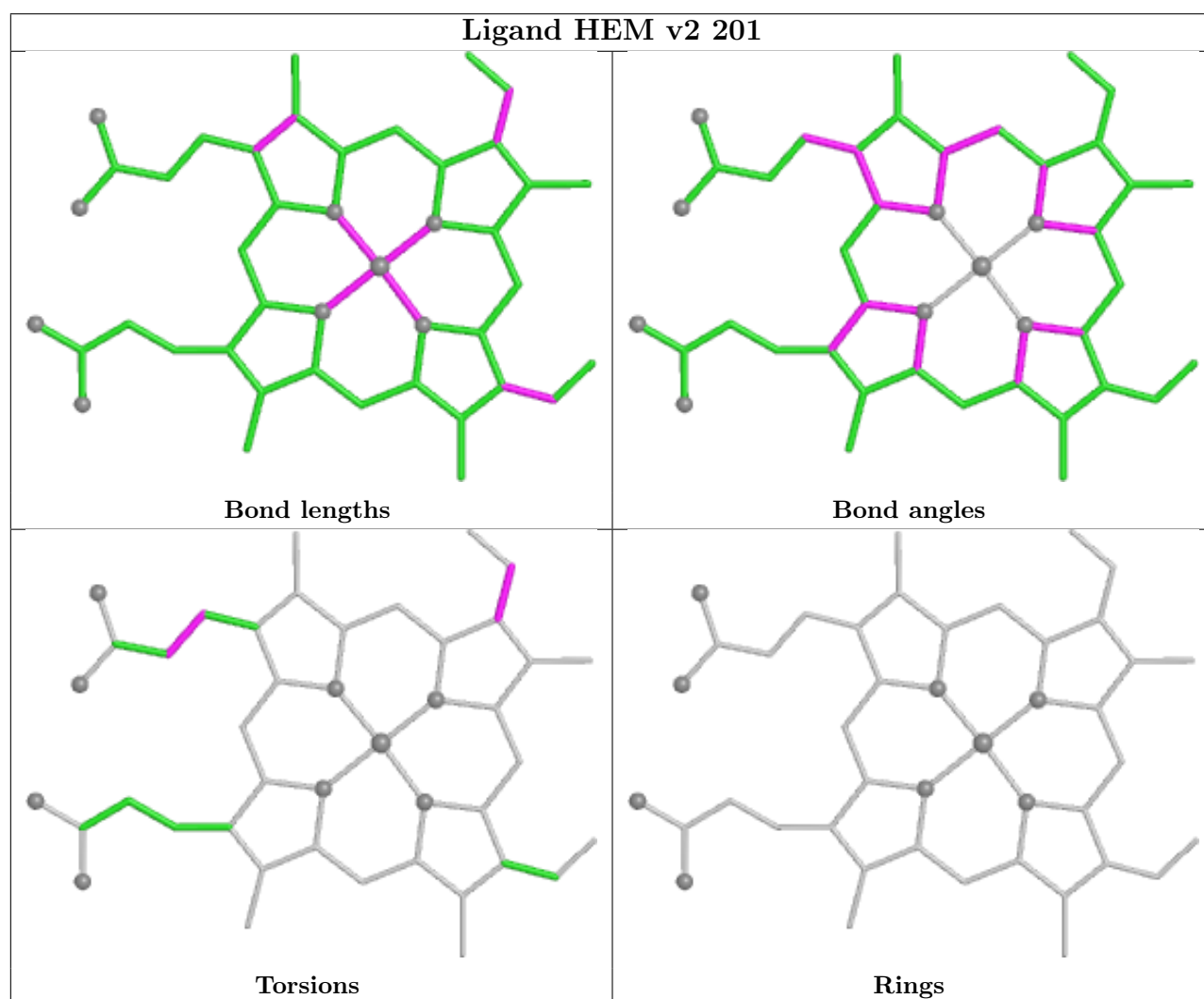
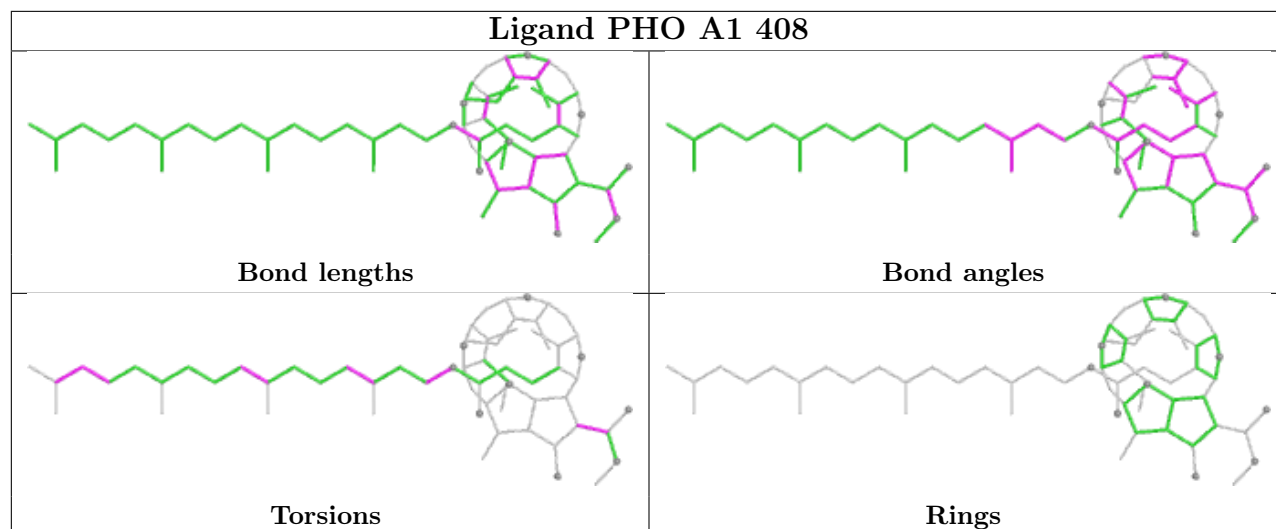
Ligand CLA c2 506	
	
Bond lengths	Bond angles
	
Torsions	Rings

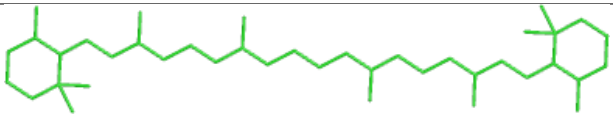
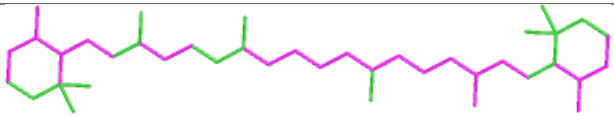
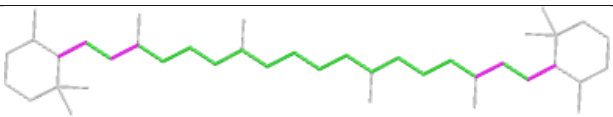
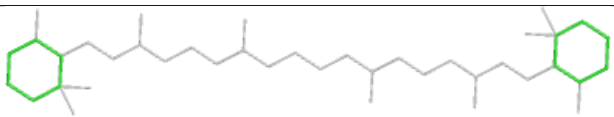
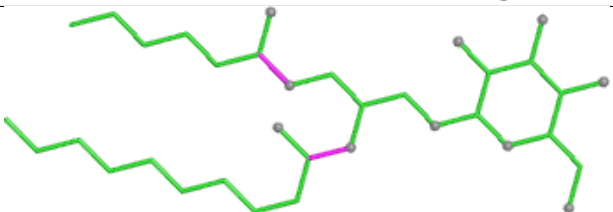
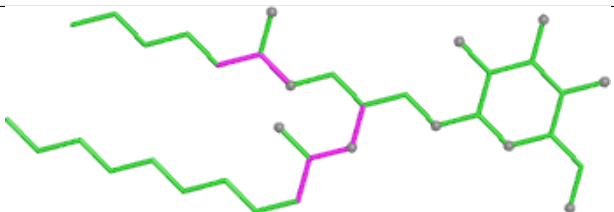
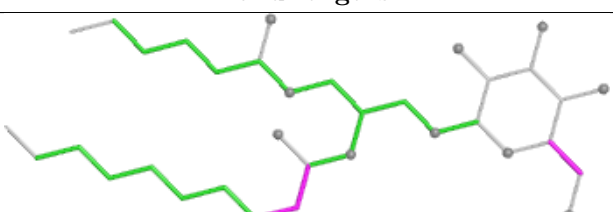
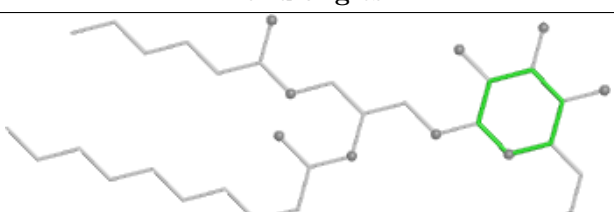
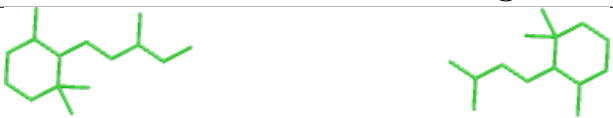
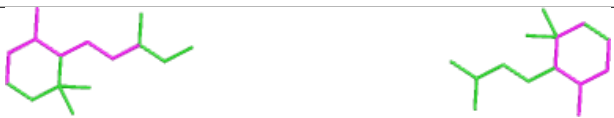
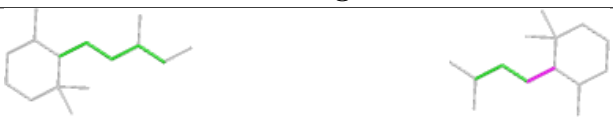
Ligand LMG b1 624	
	
Bond lengths	Bond angles
	
Torsions	Rings

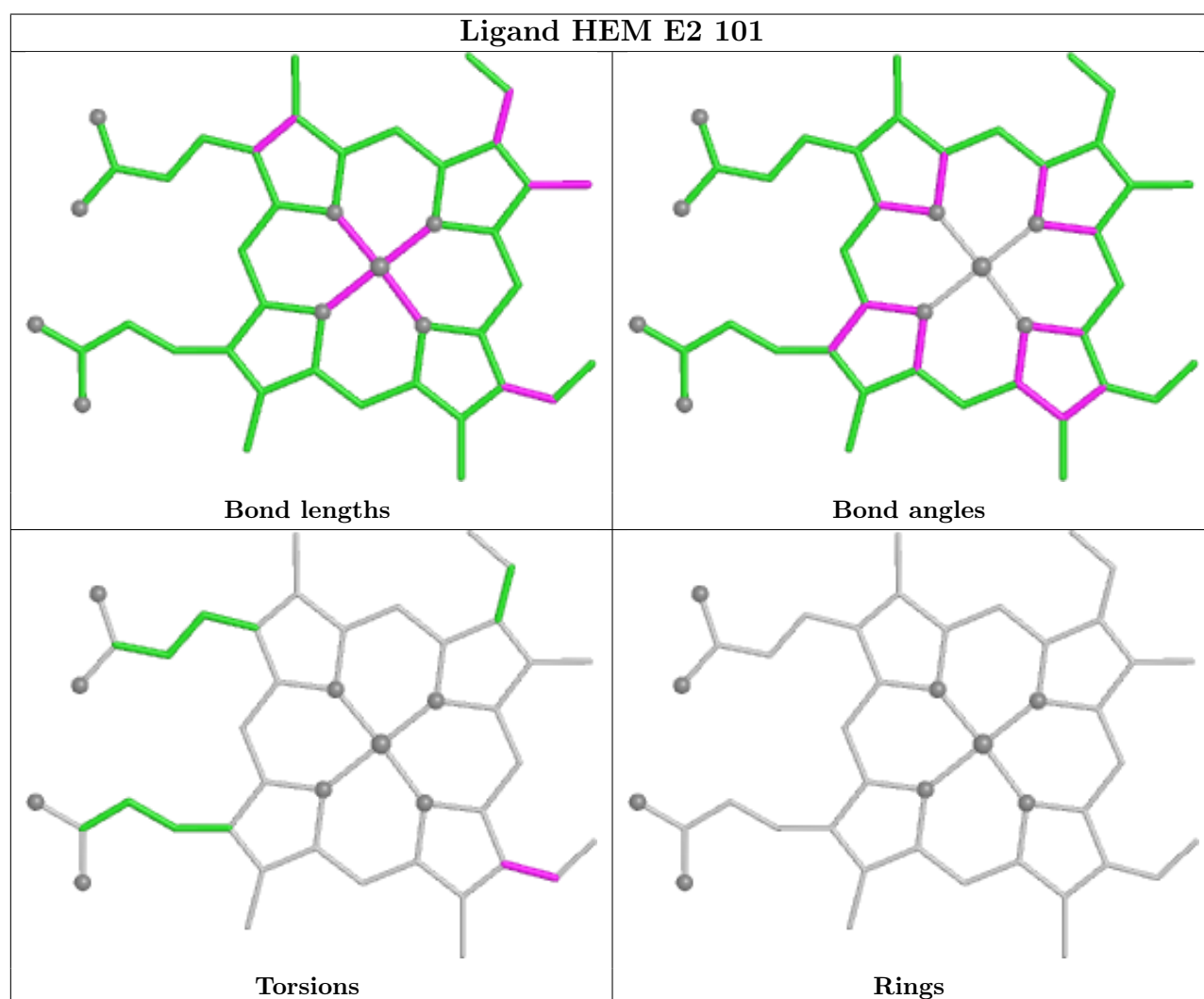
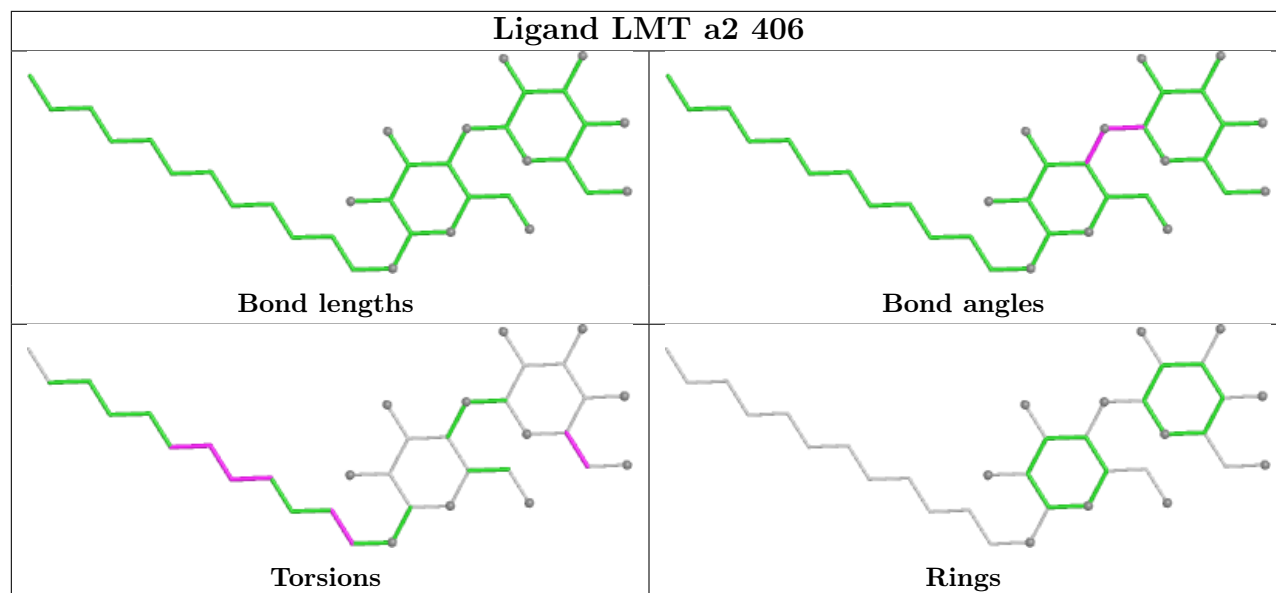
Ligand LMT L1 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

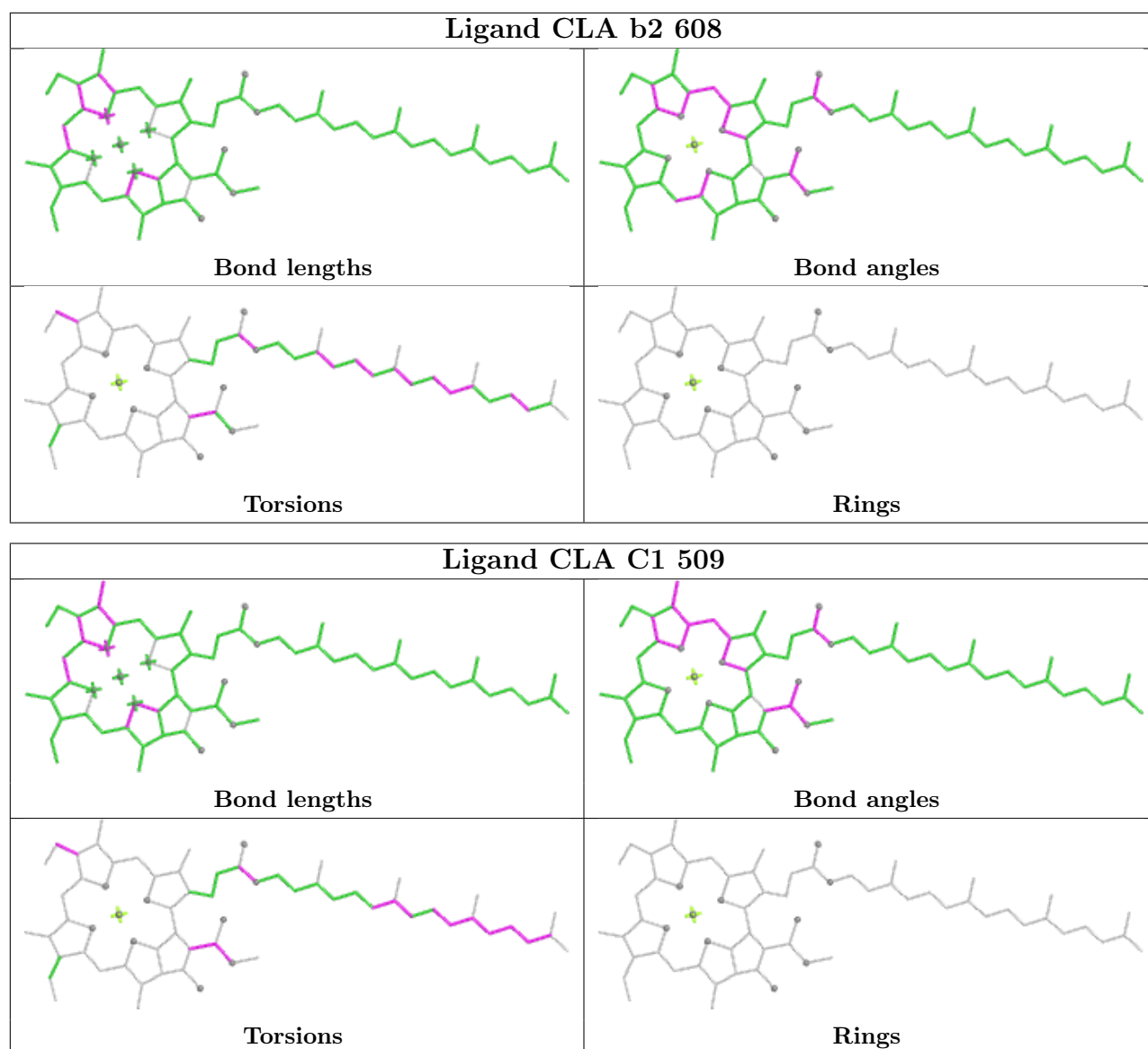


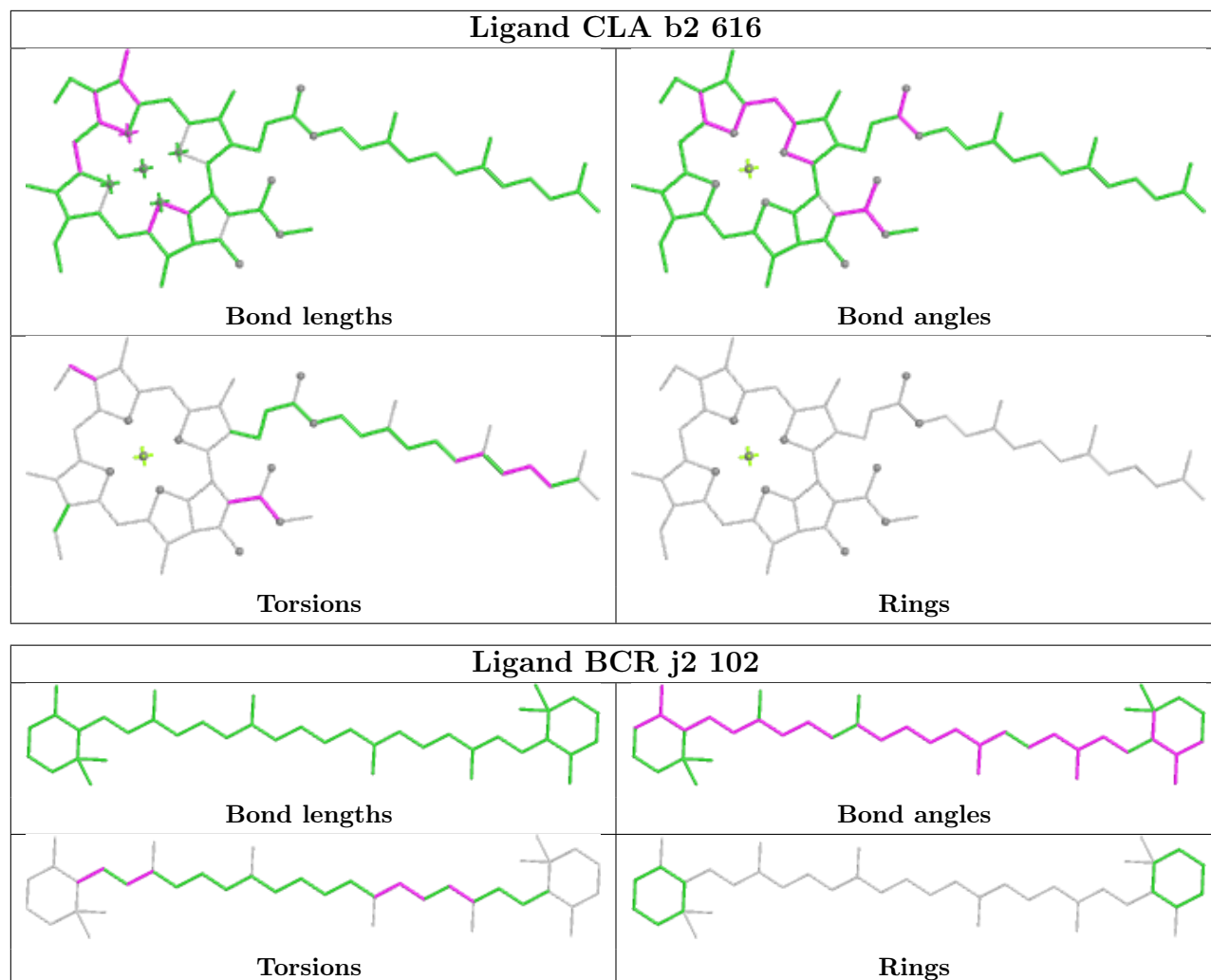


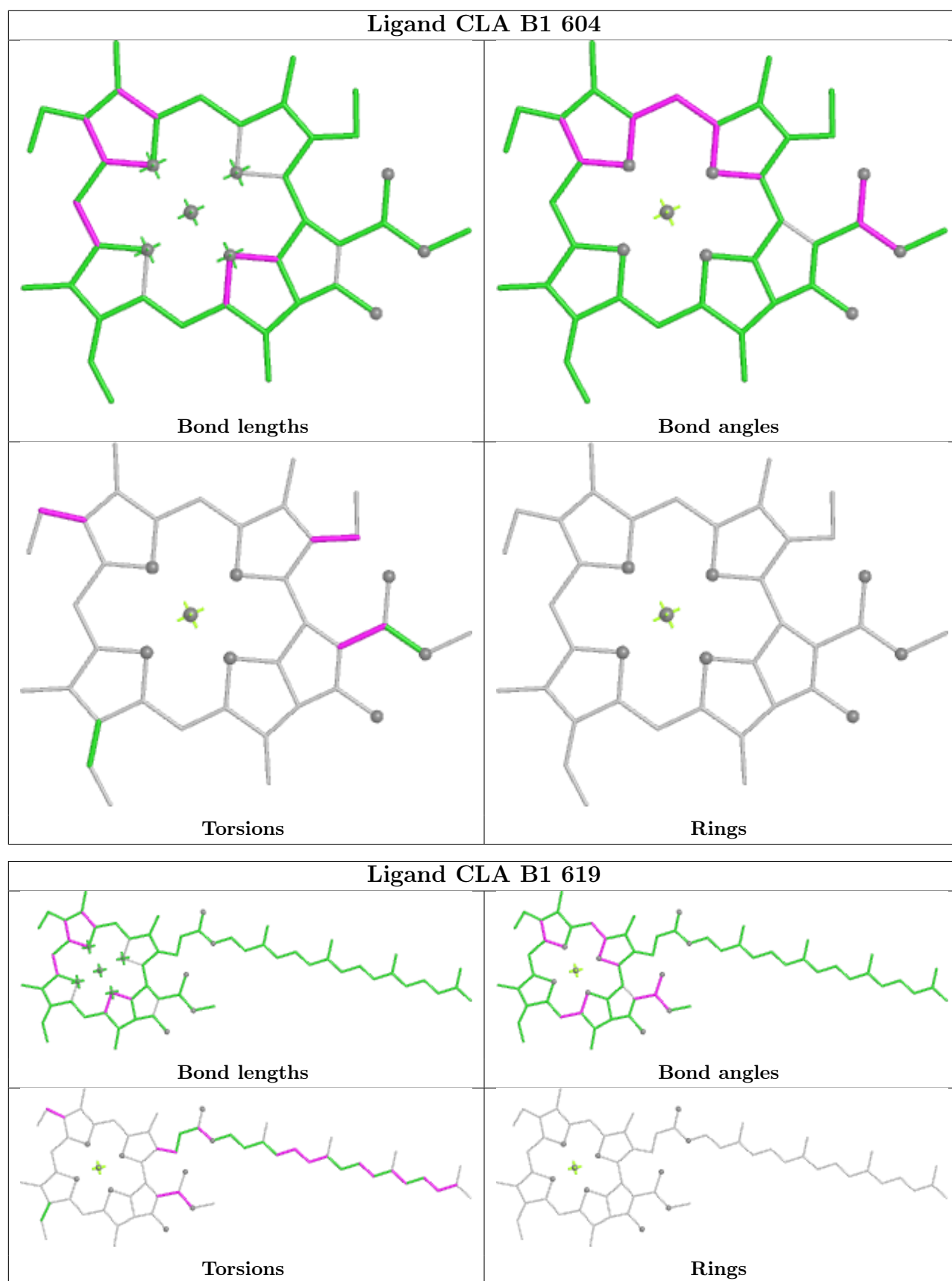


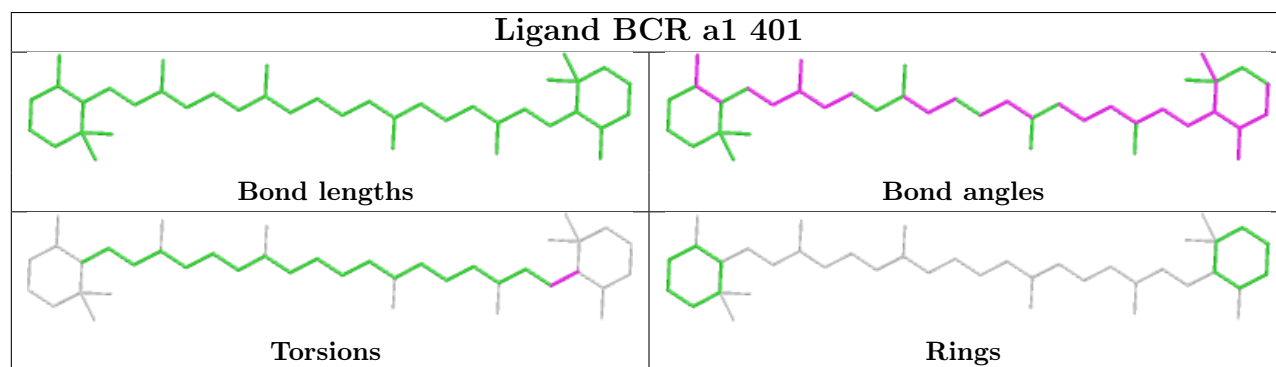
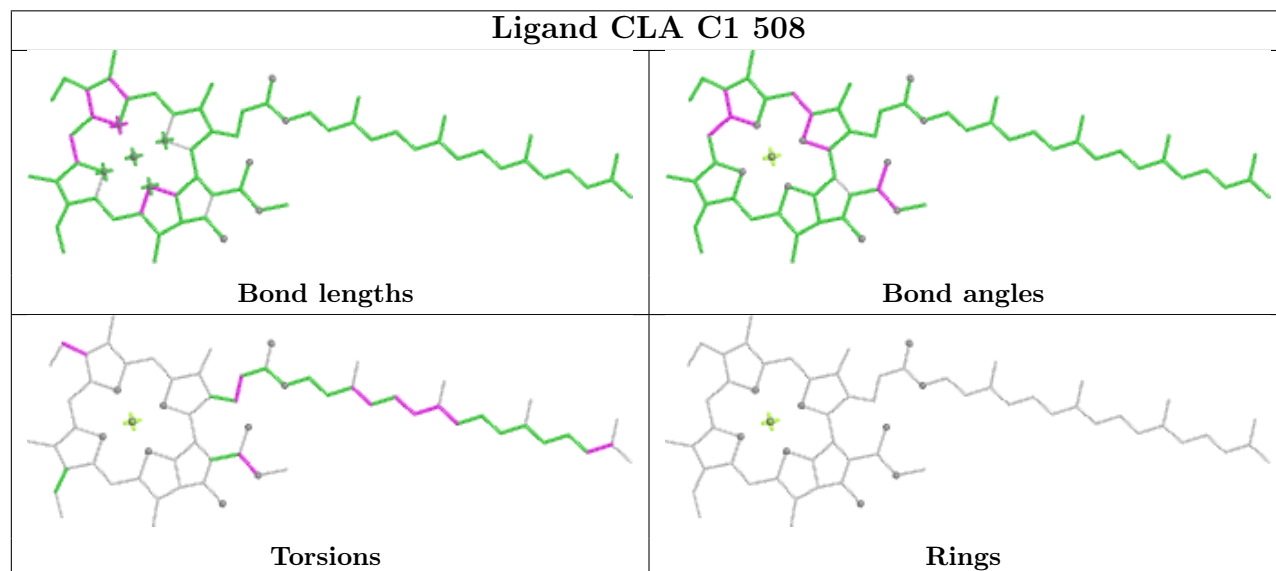
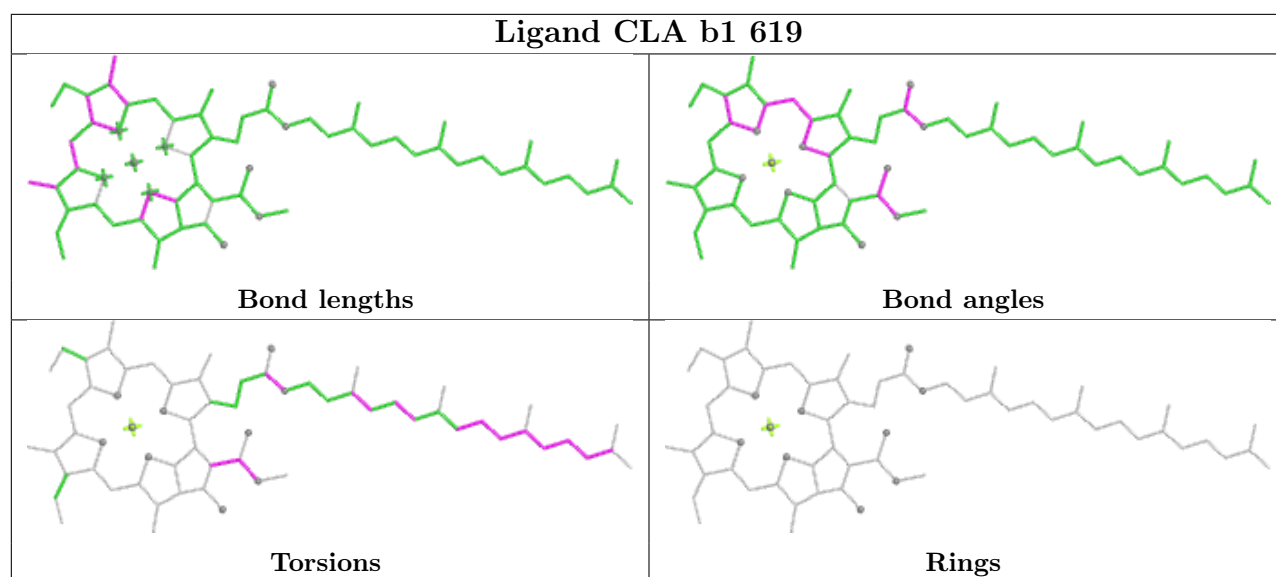
Ligand BCR d2 401			
 Bond lengths		 Bond angles	
 Torsions		 Rings	
Ligand LMG D1 406			
 Bond lengths		 Bond angles	
 Torsions		 Rings	
Ligand BCR K2 104			
 Bond lengths		 Bond angles	
 Torsions		 Rings	

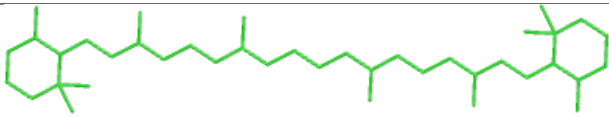
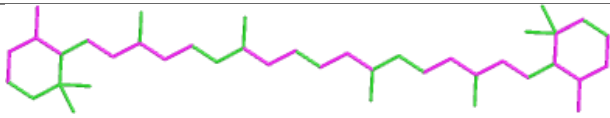
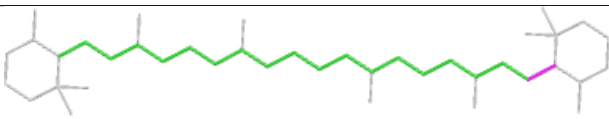
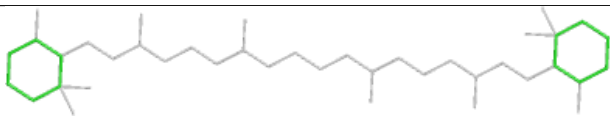


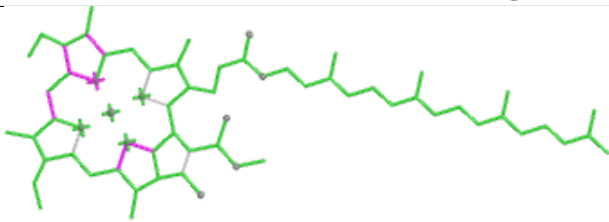
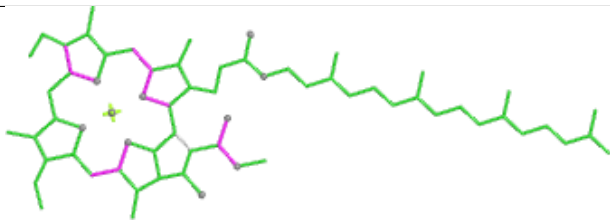
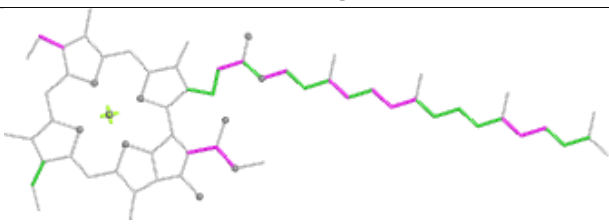
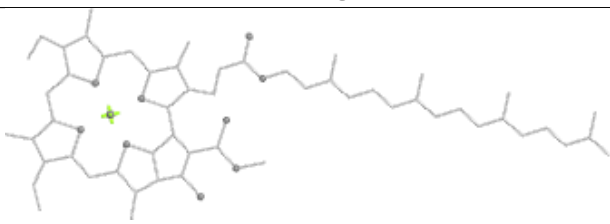


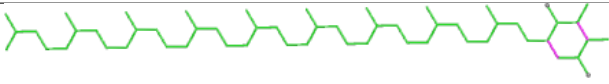
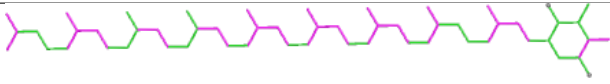
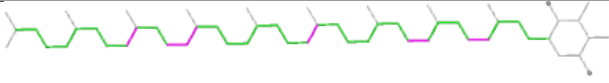
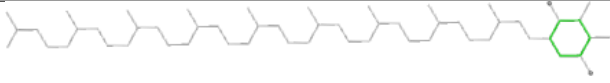


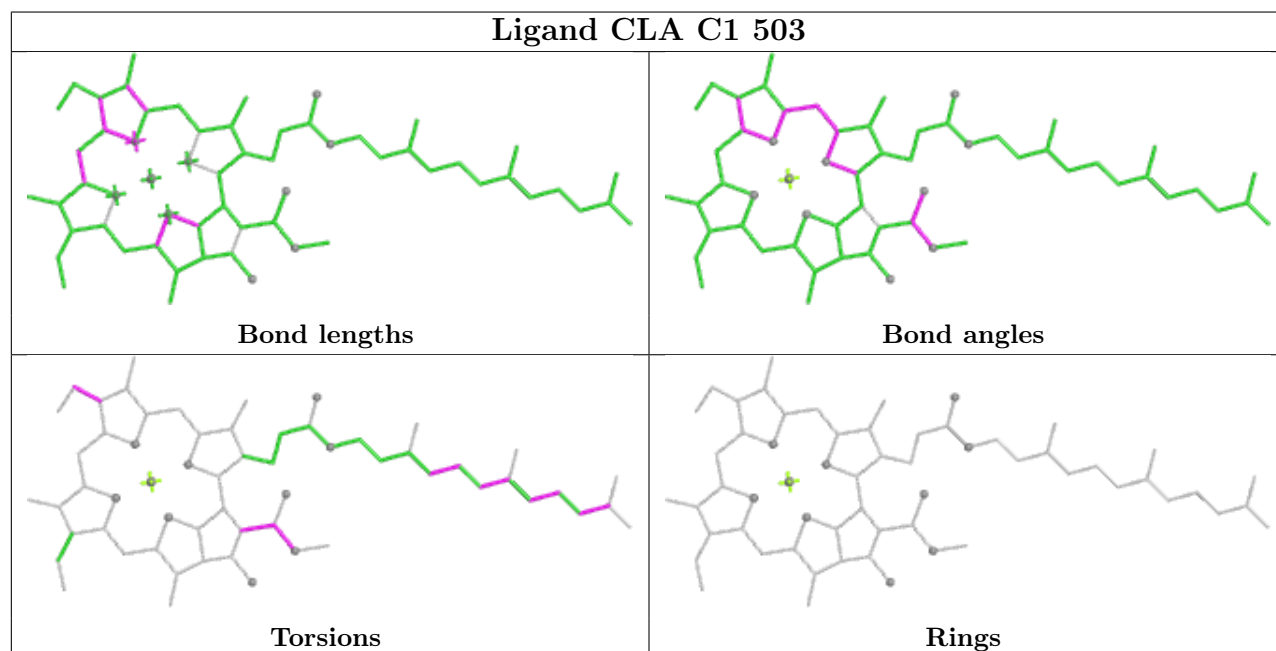
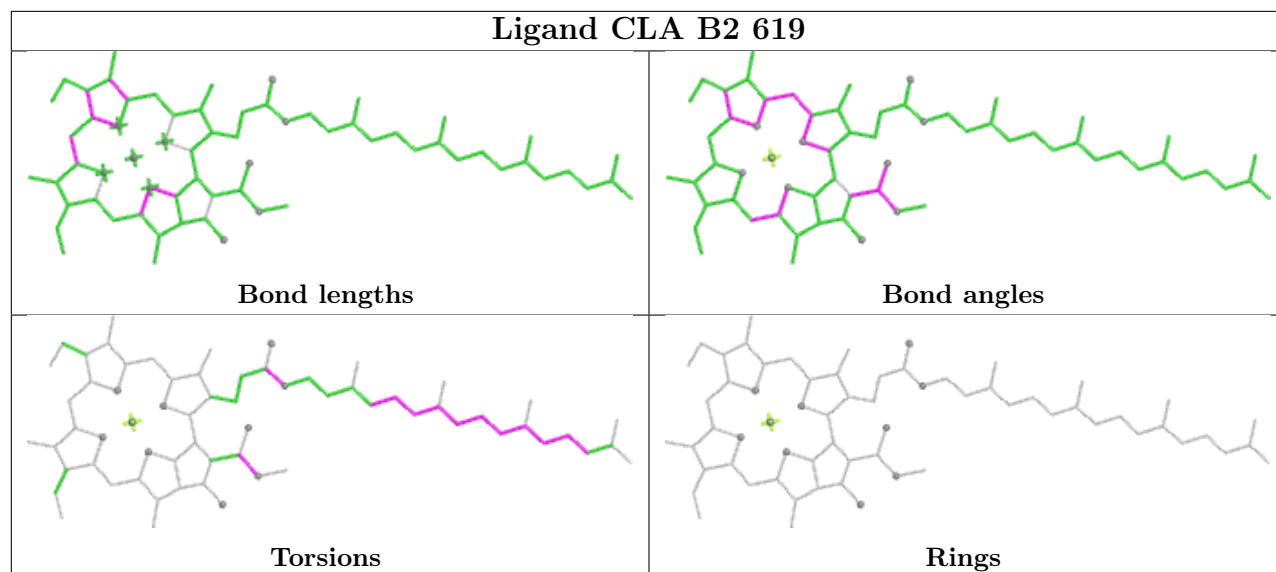


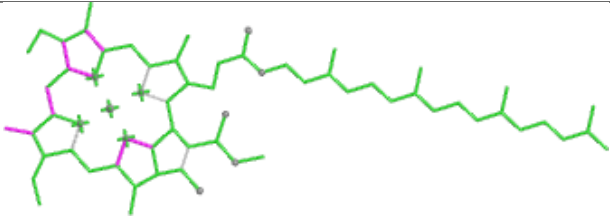
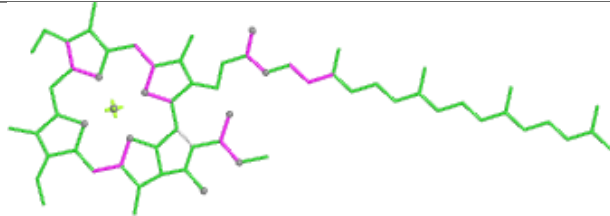
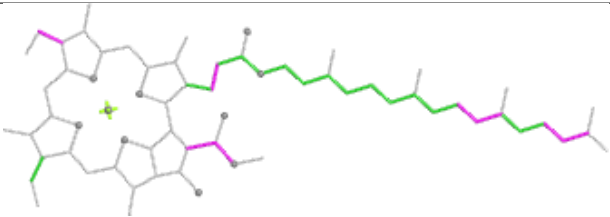
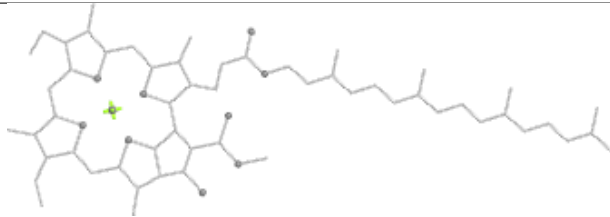
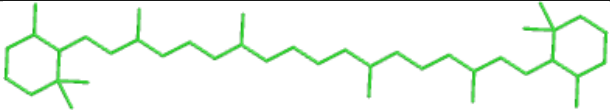
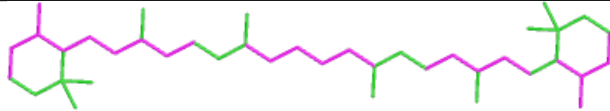
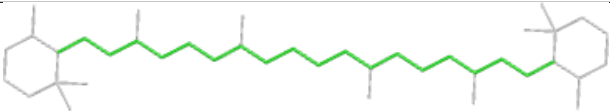
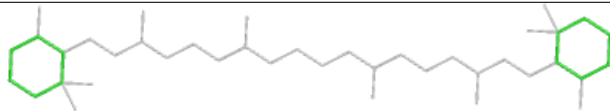
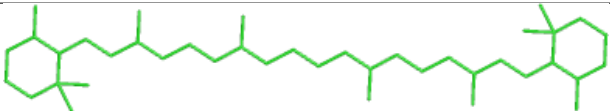
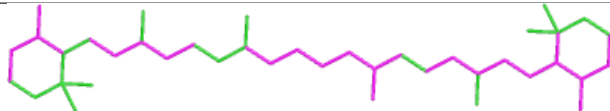
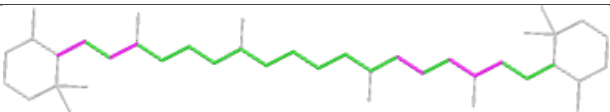
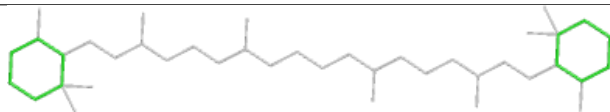


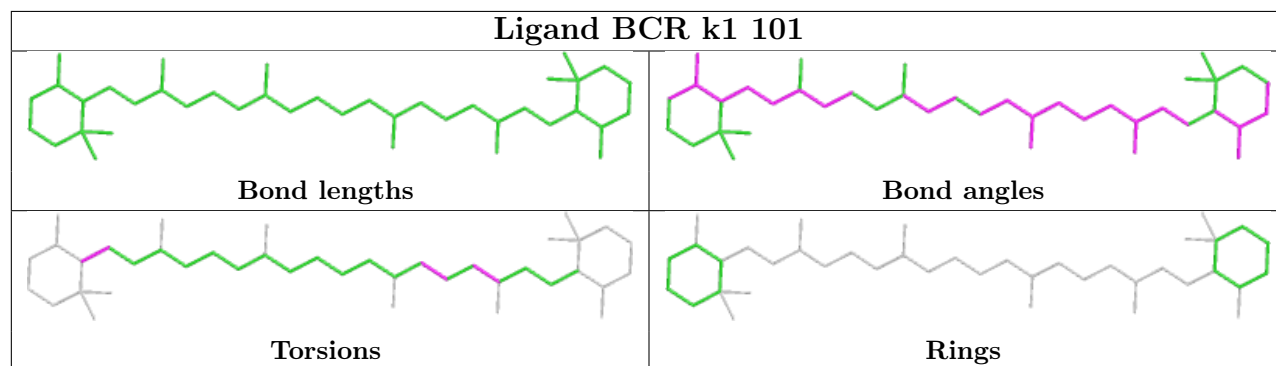
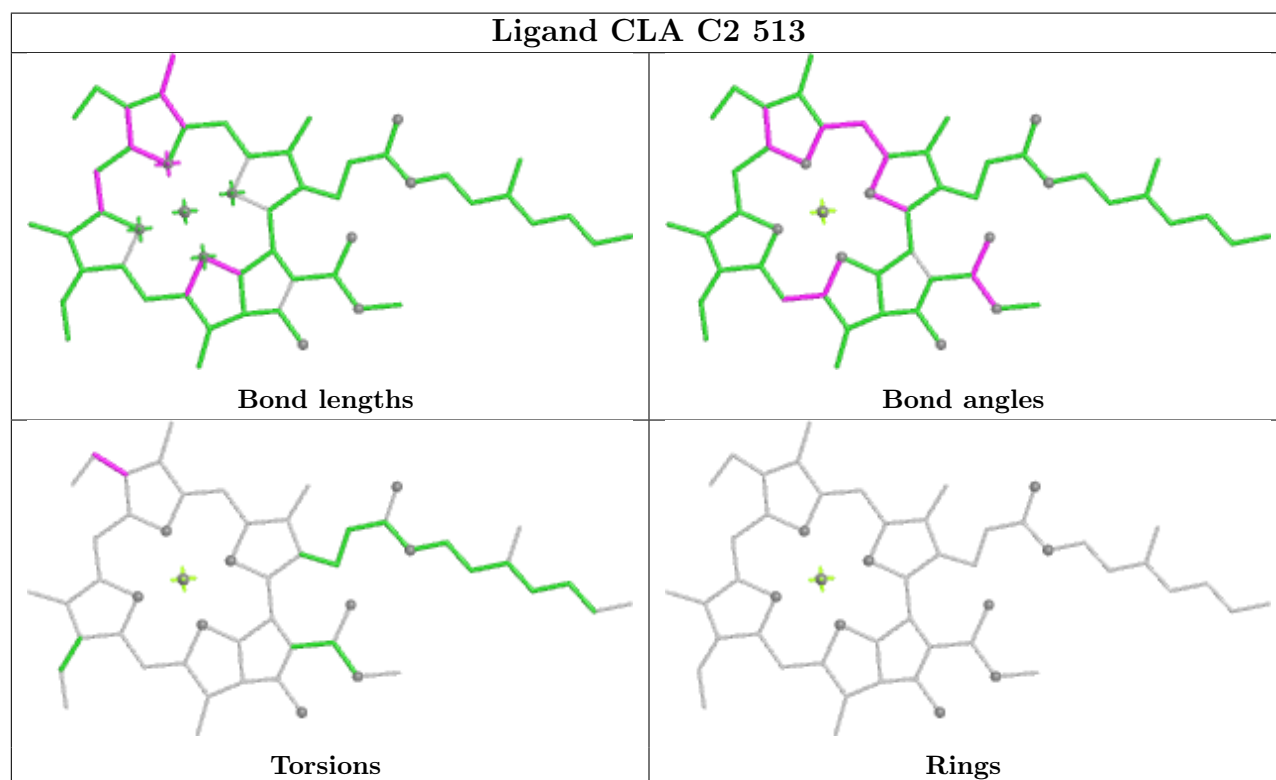
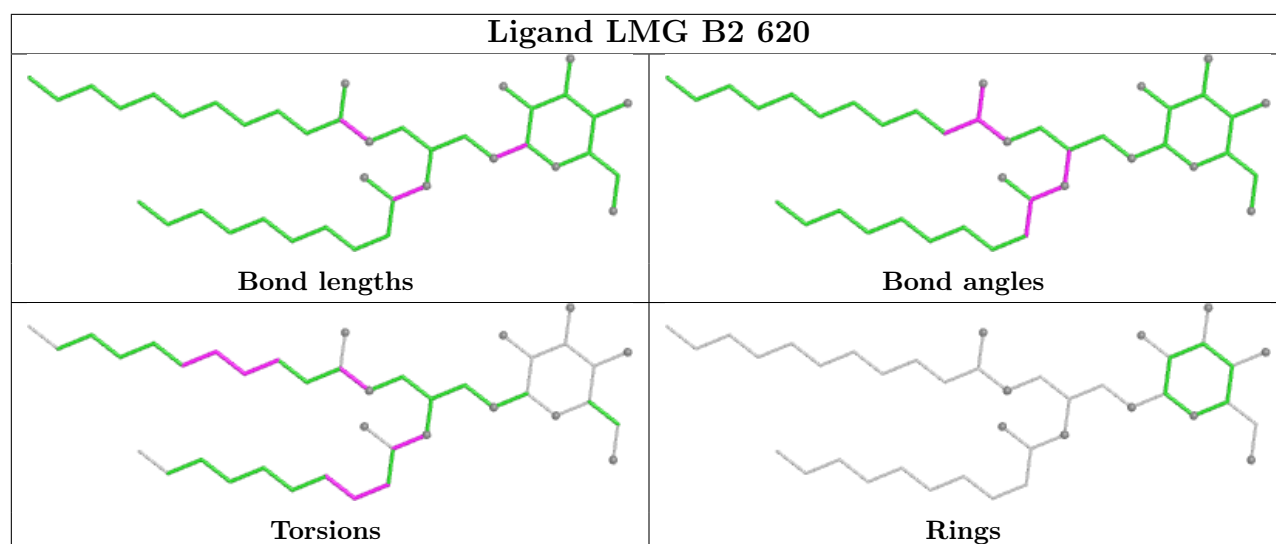
Ligand BCR B1 603	
	
Bond lengths	Bond angles
	
Torsions	Rings

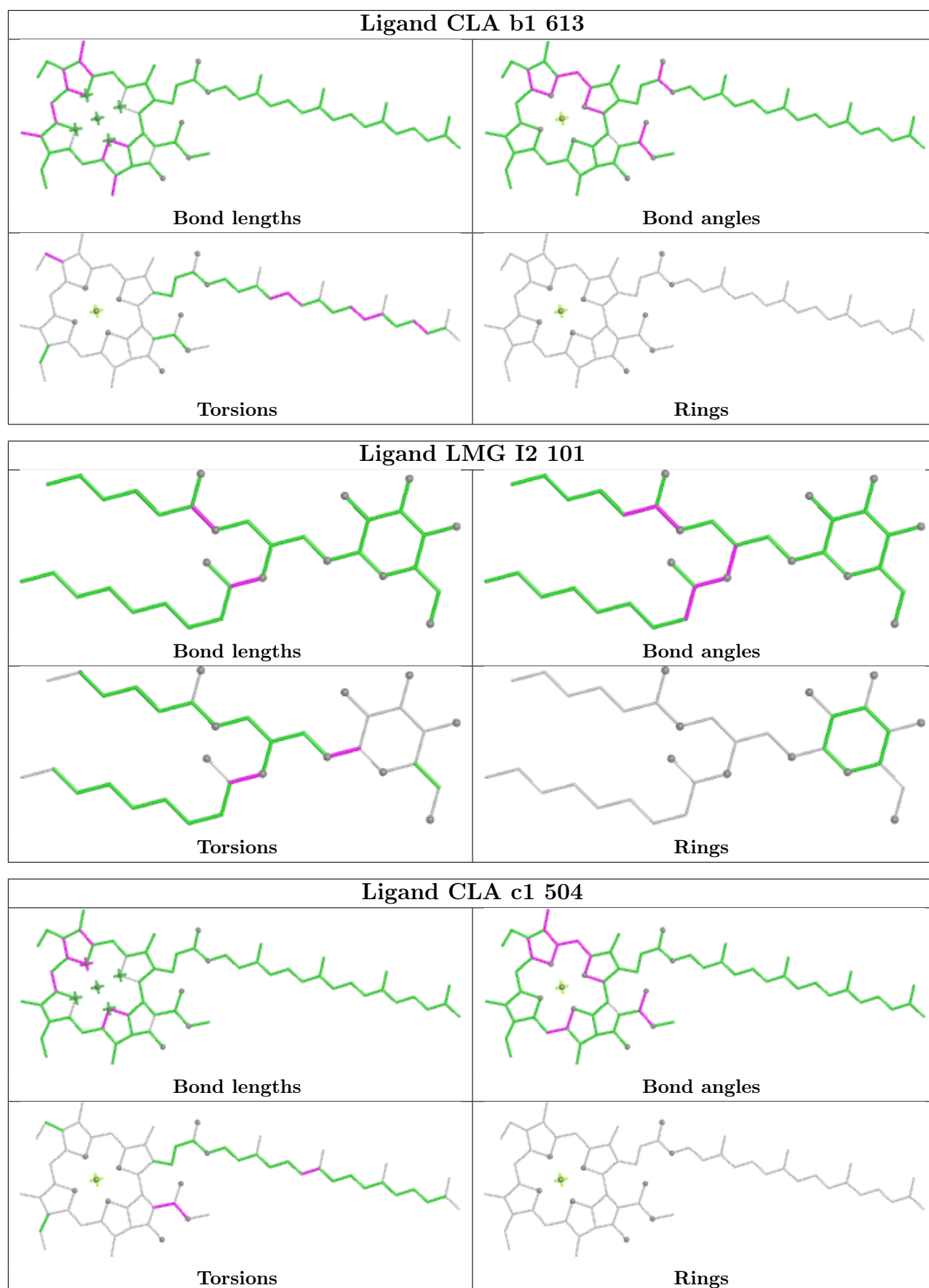
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Bond lengths	Bond angles
	
Torsions	Rings

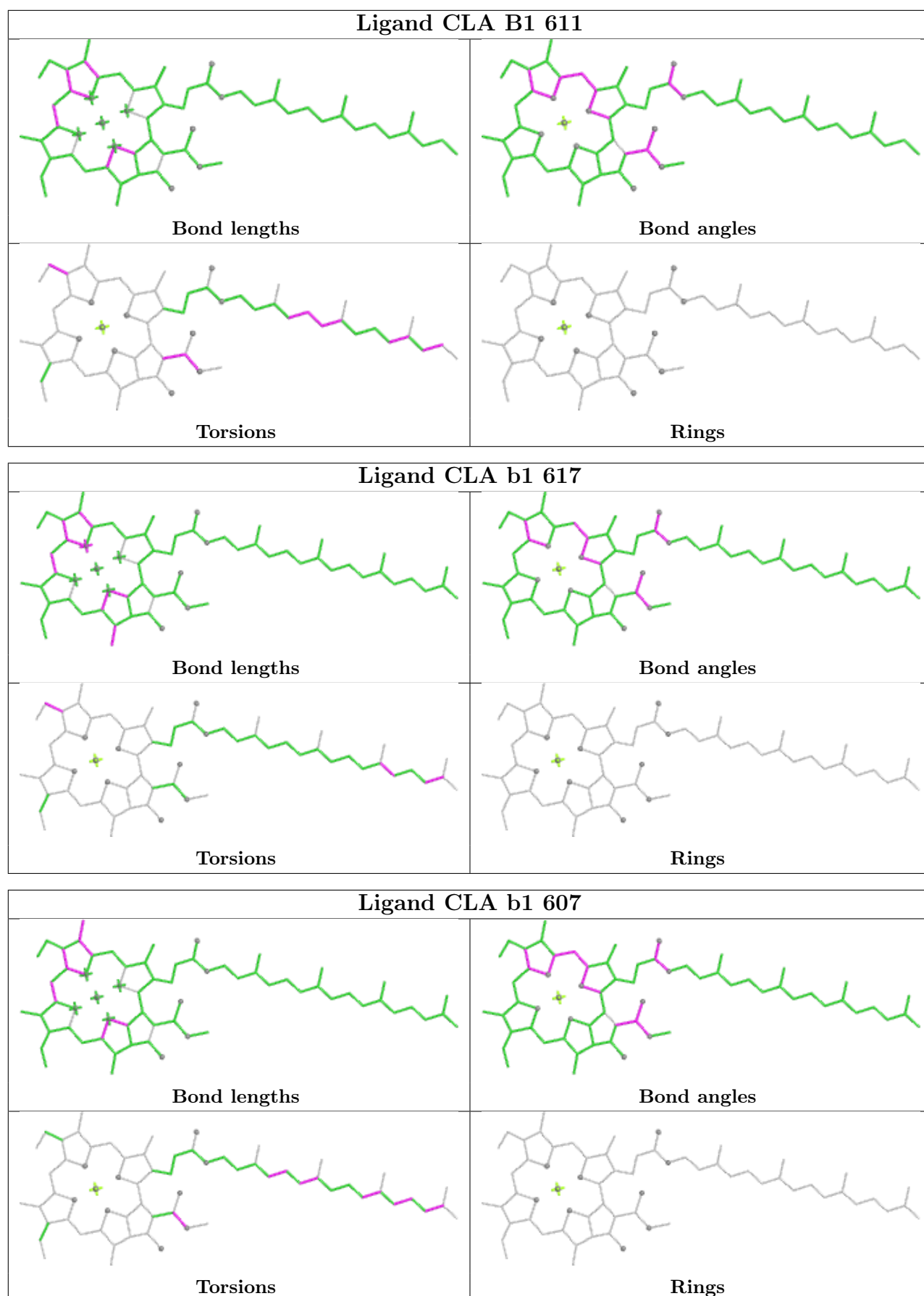
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Bond lengths	Bond angles
	
Torsions	Rings

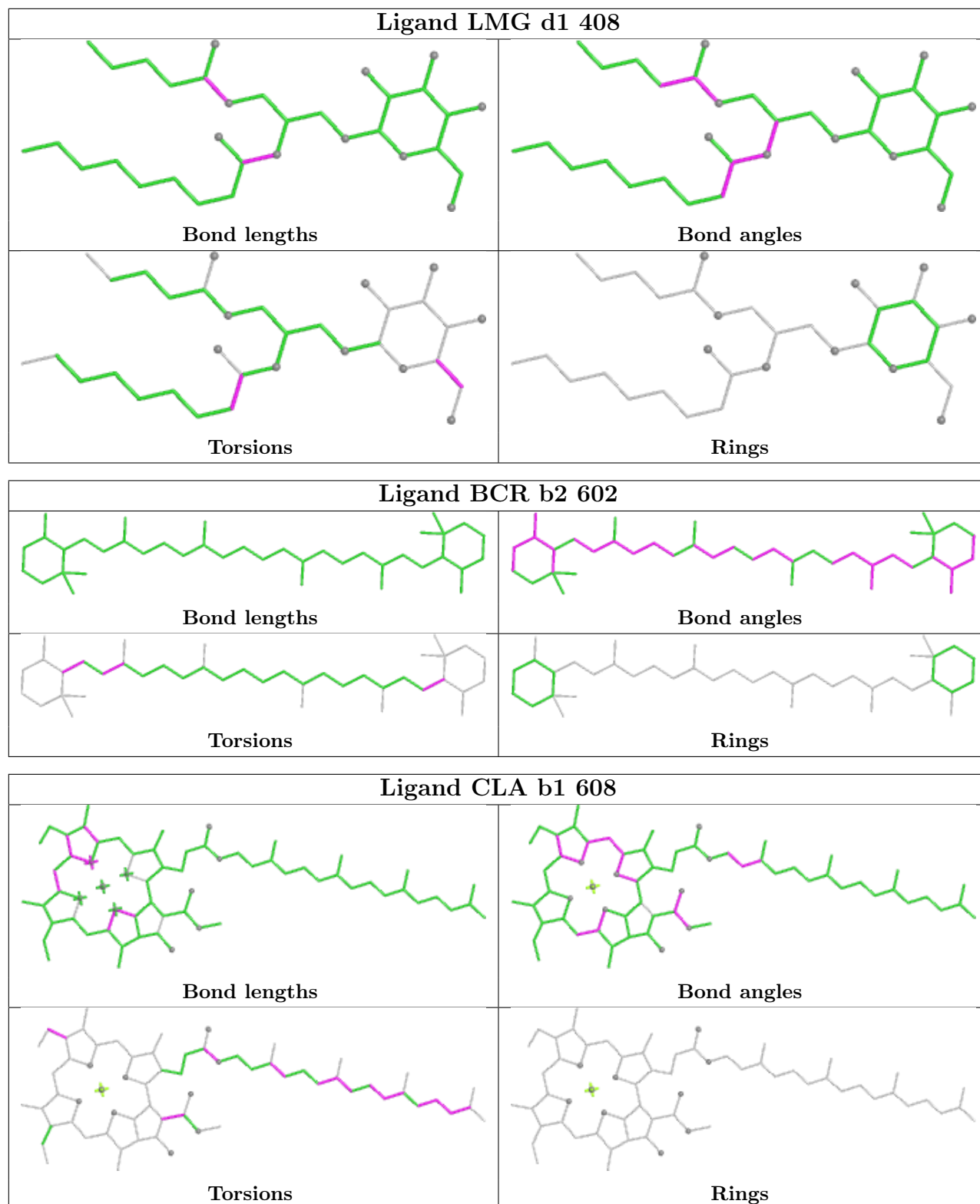


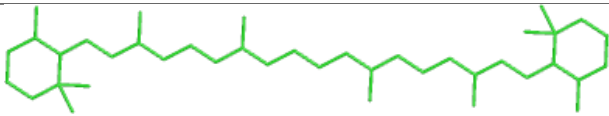
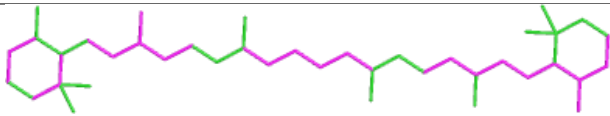
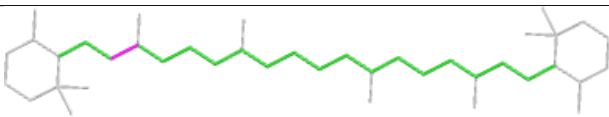
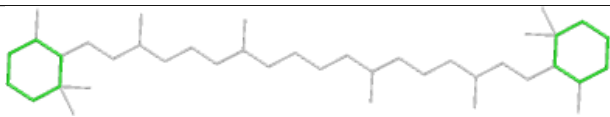
Ligand CLA B2 609	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR C1 521	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR F2 401	
 Bond lengths	 Bond angles
 Torsions	 Rings

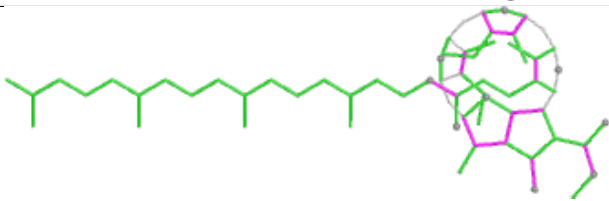
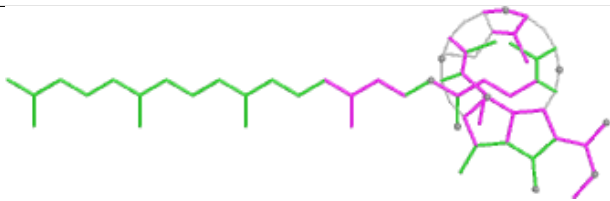
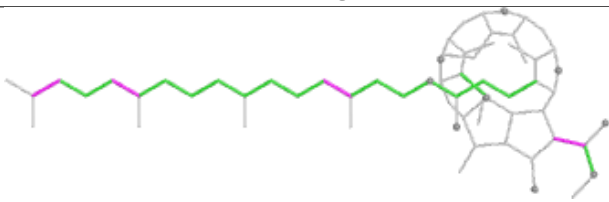
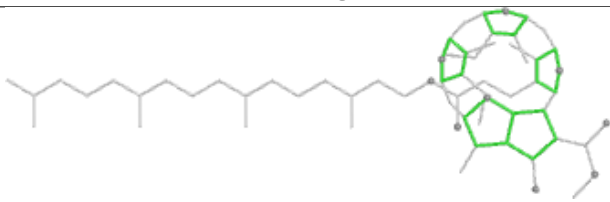


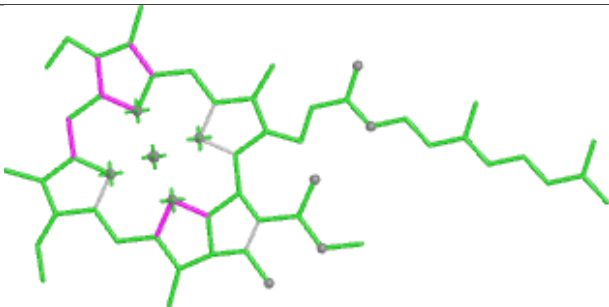
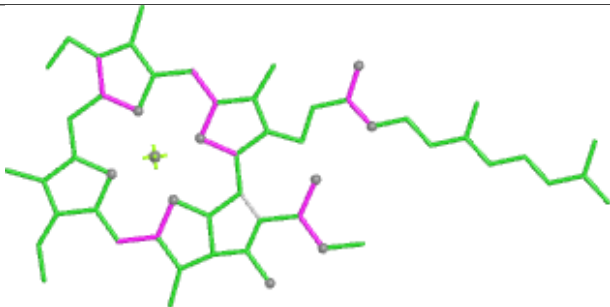
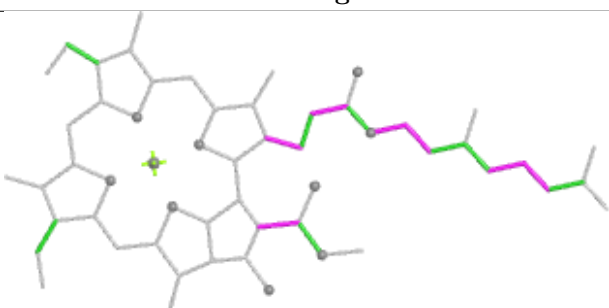
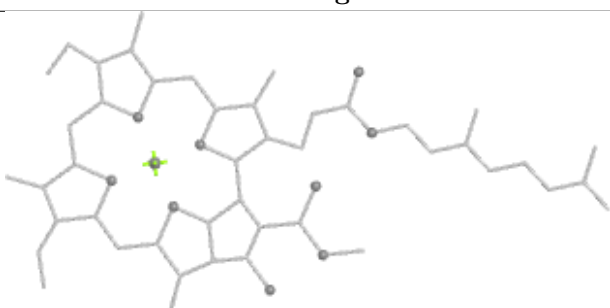


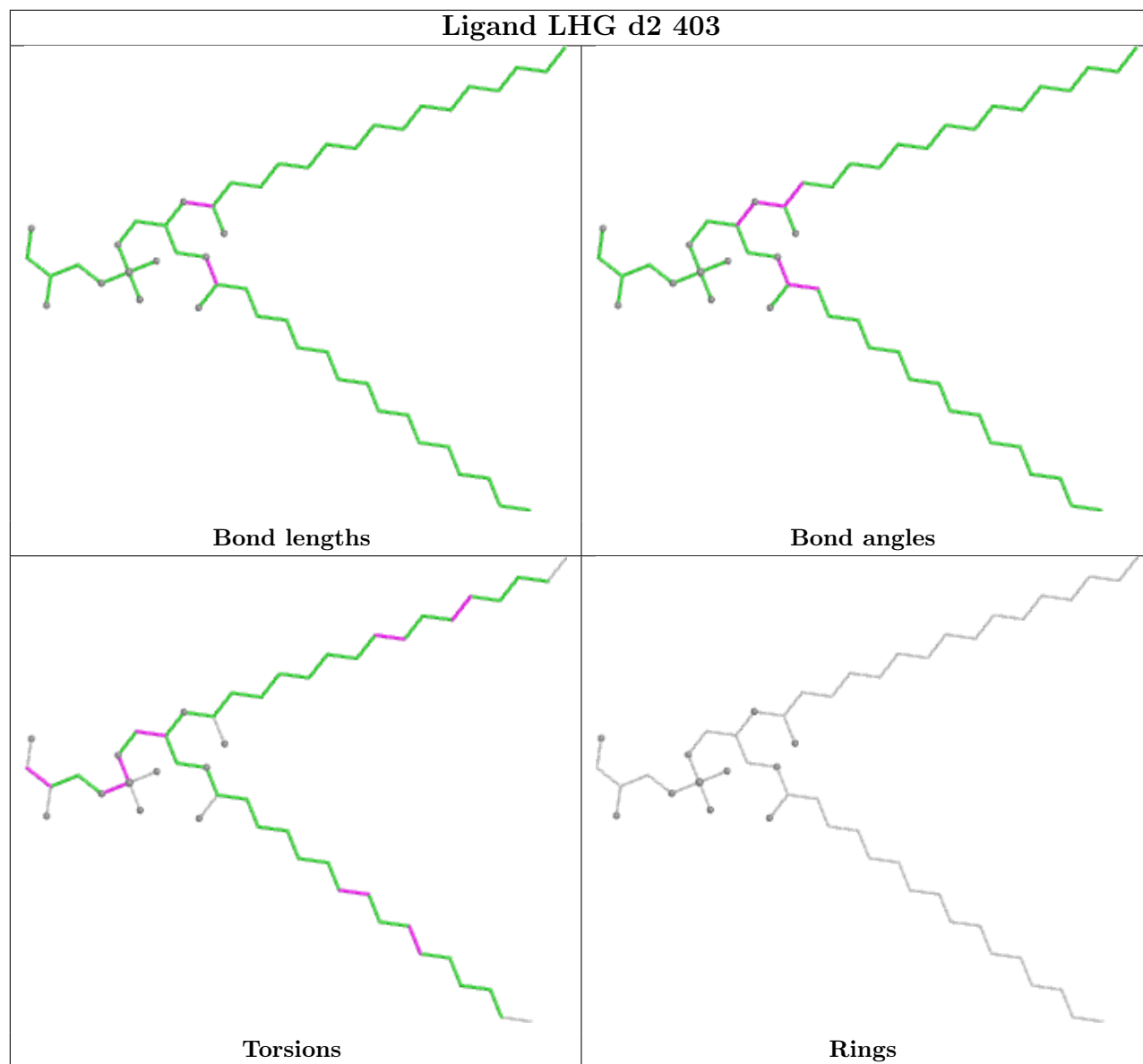




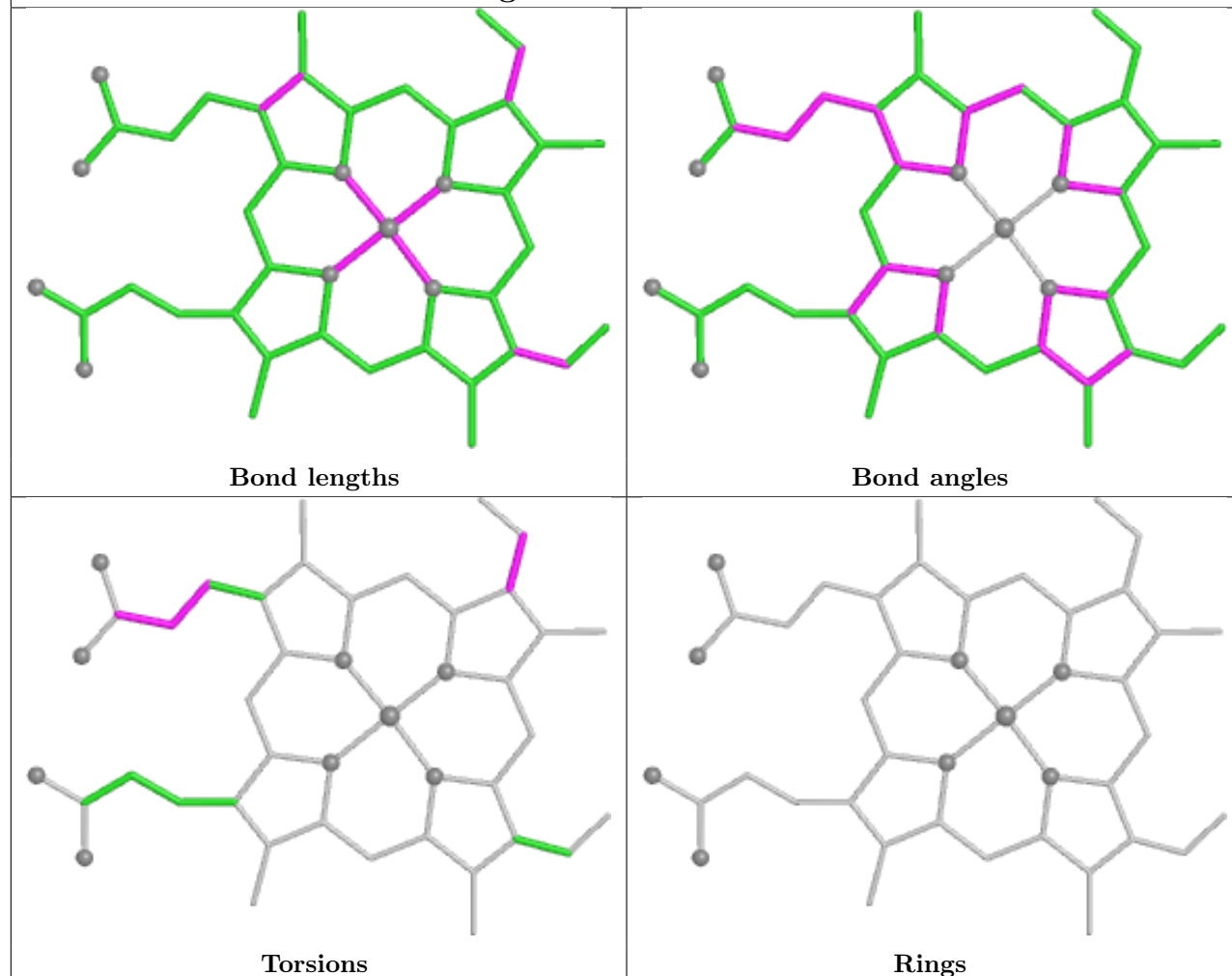
Ligand BCR B2 602	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PHO a2 416	
	
Bond lengths	Bond angles
	
Torsions	Rings

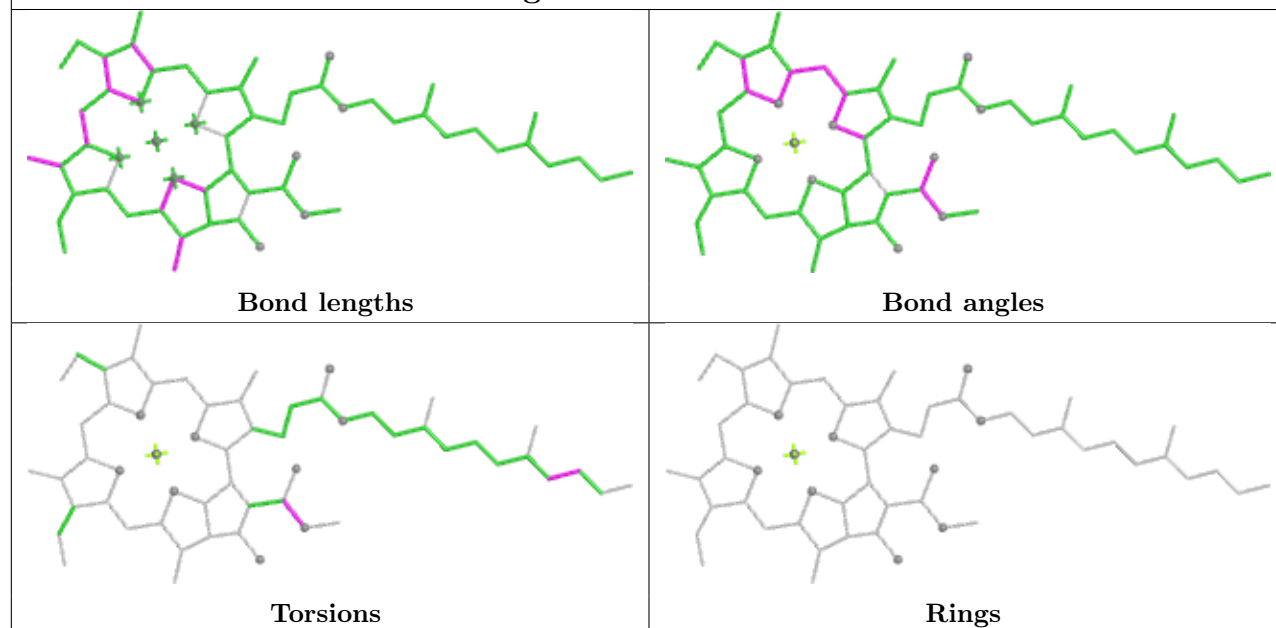
Ligand CLA c1 515	
	
Bond lengths	Bond angles
	
Torsions	Rings

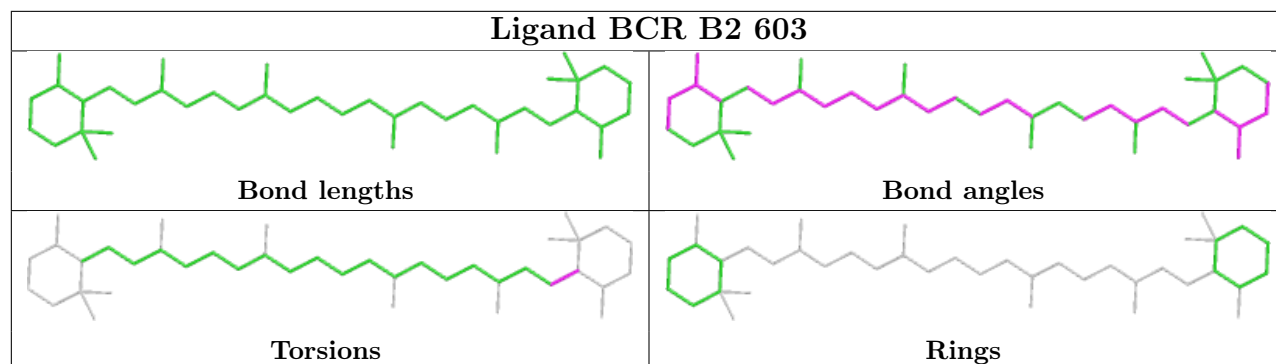
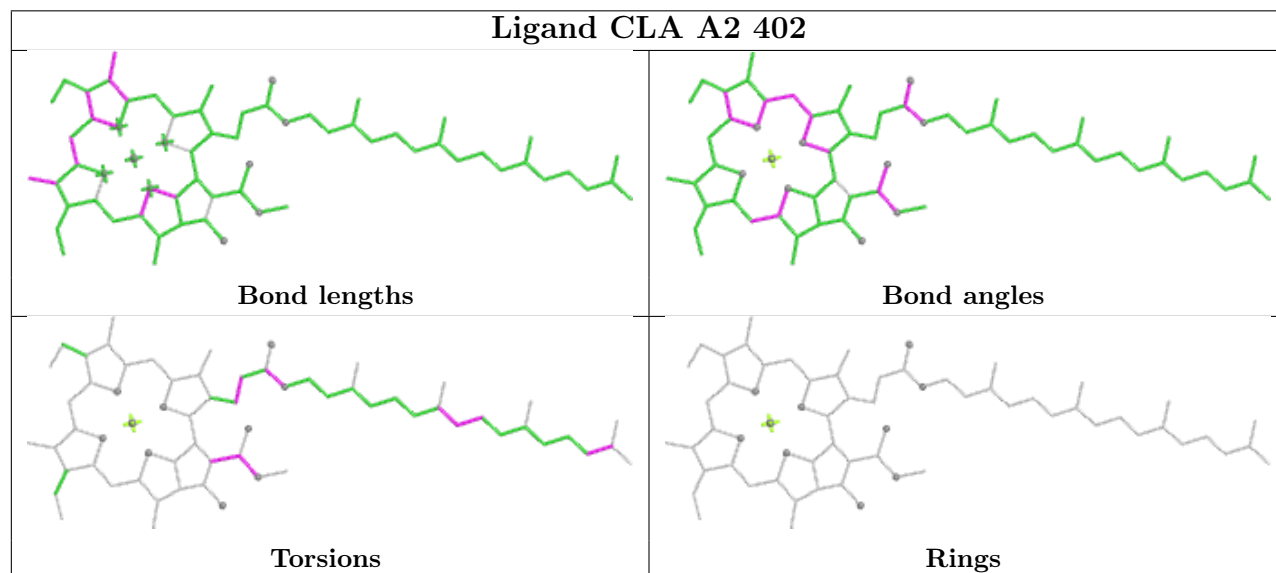
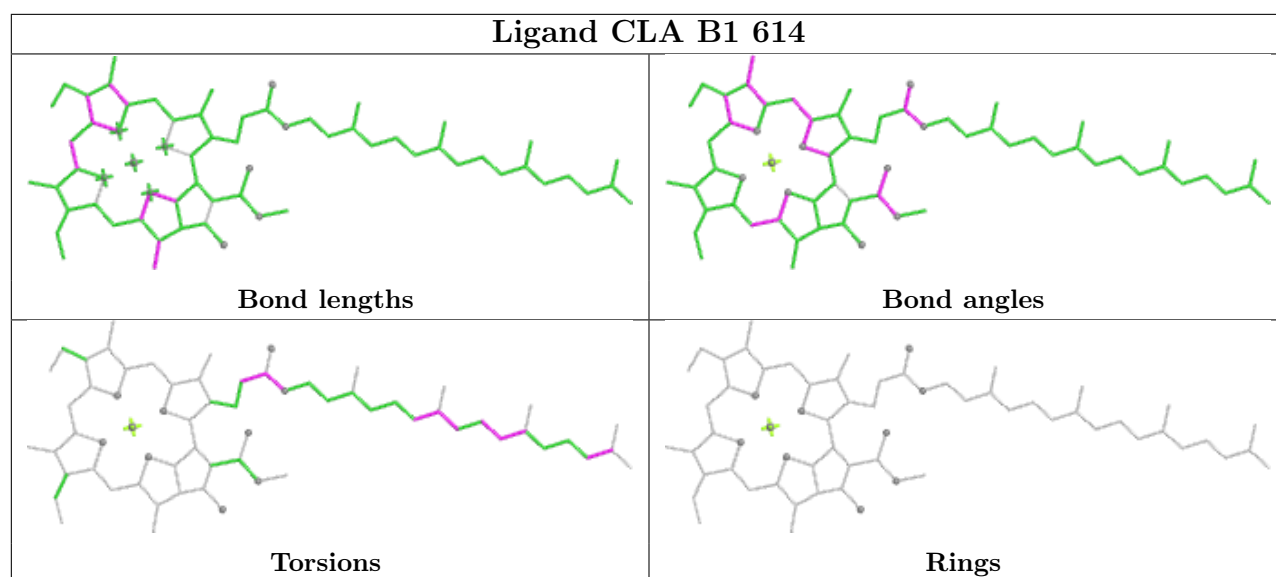


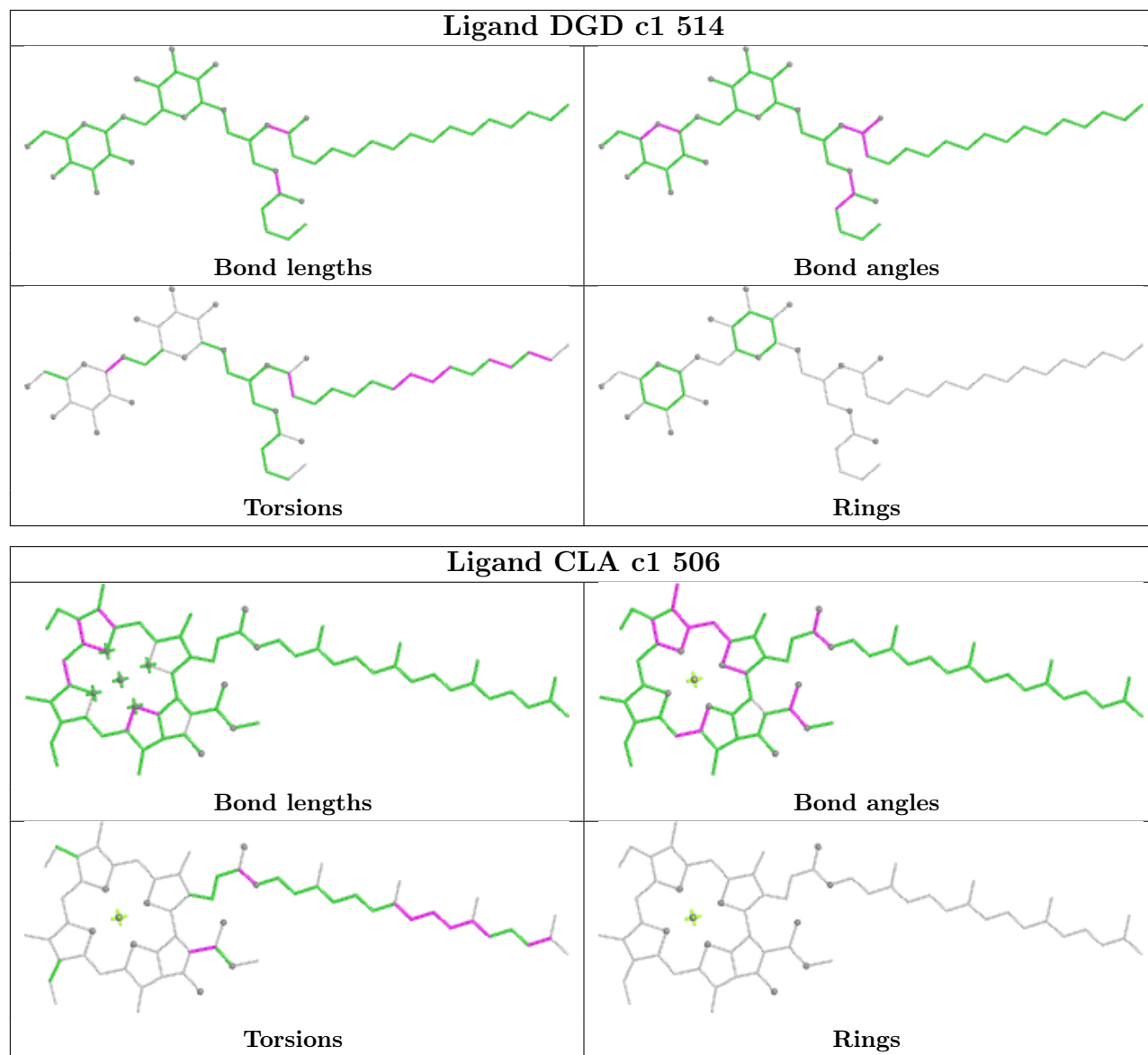
Ligand HEM V1 201

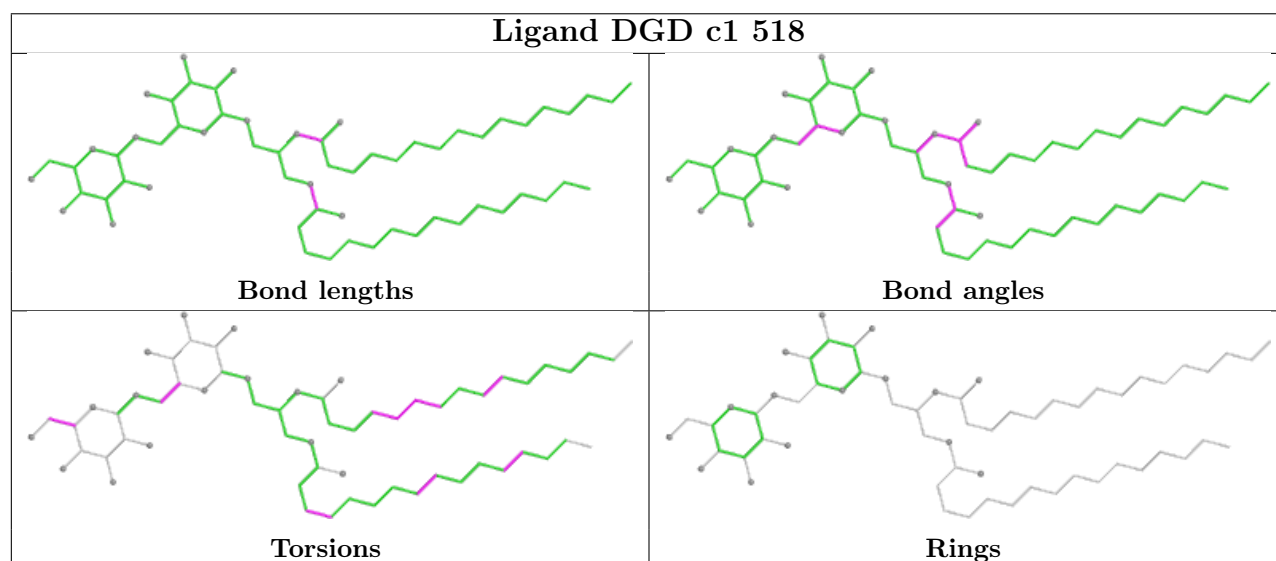
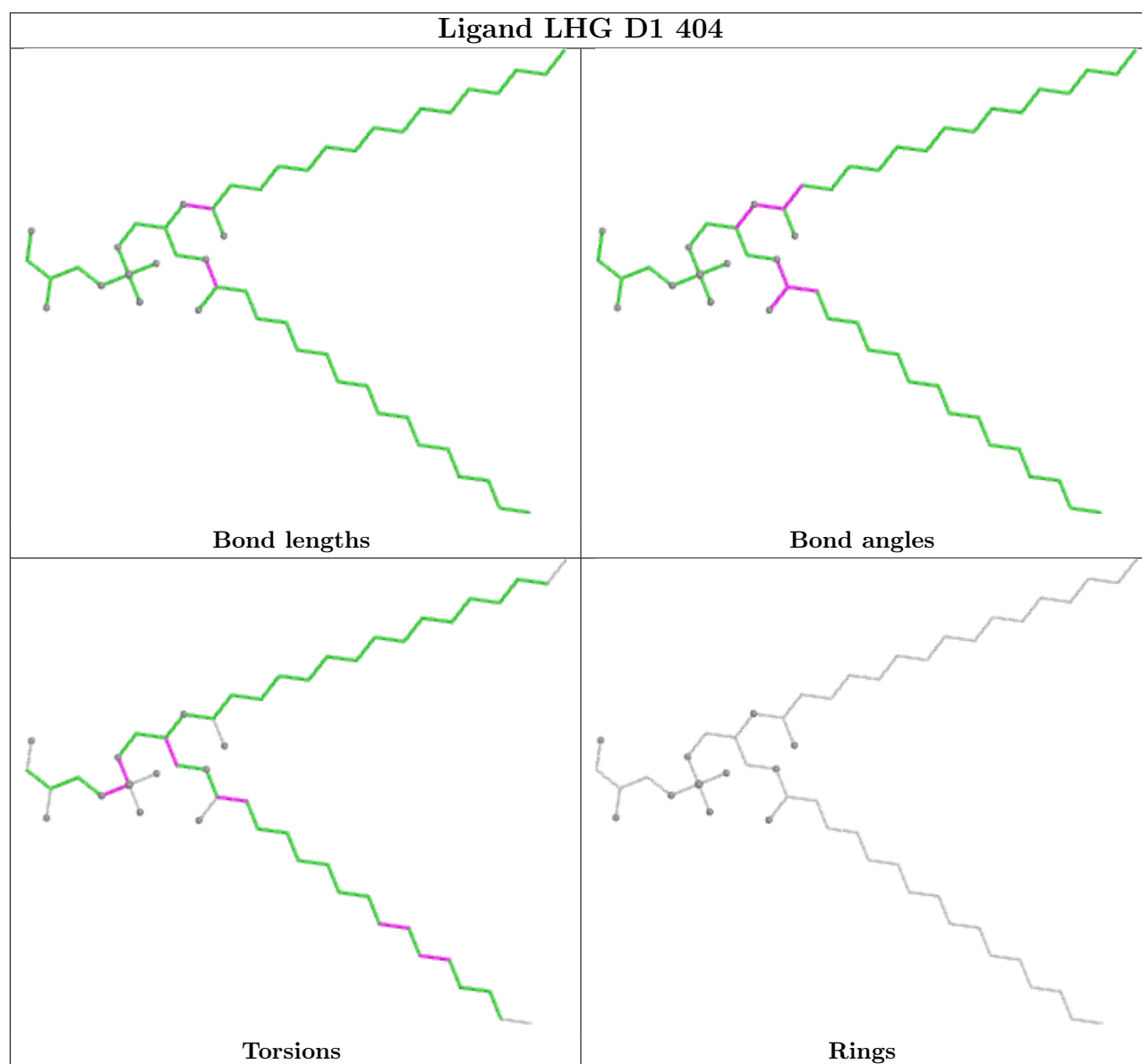


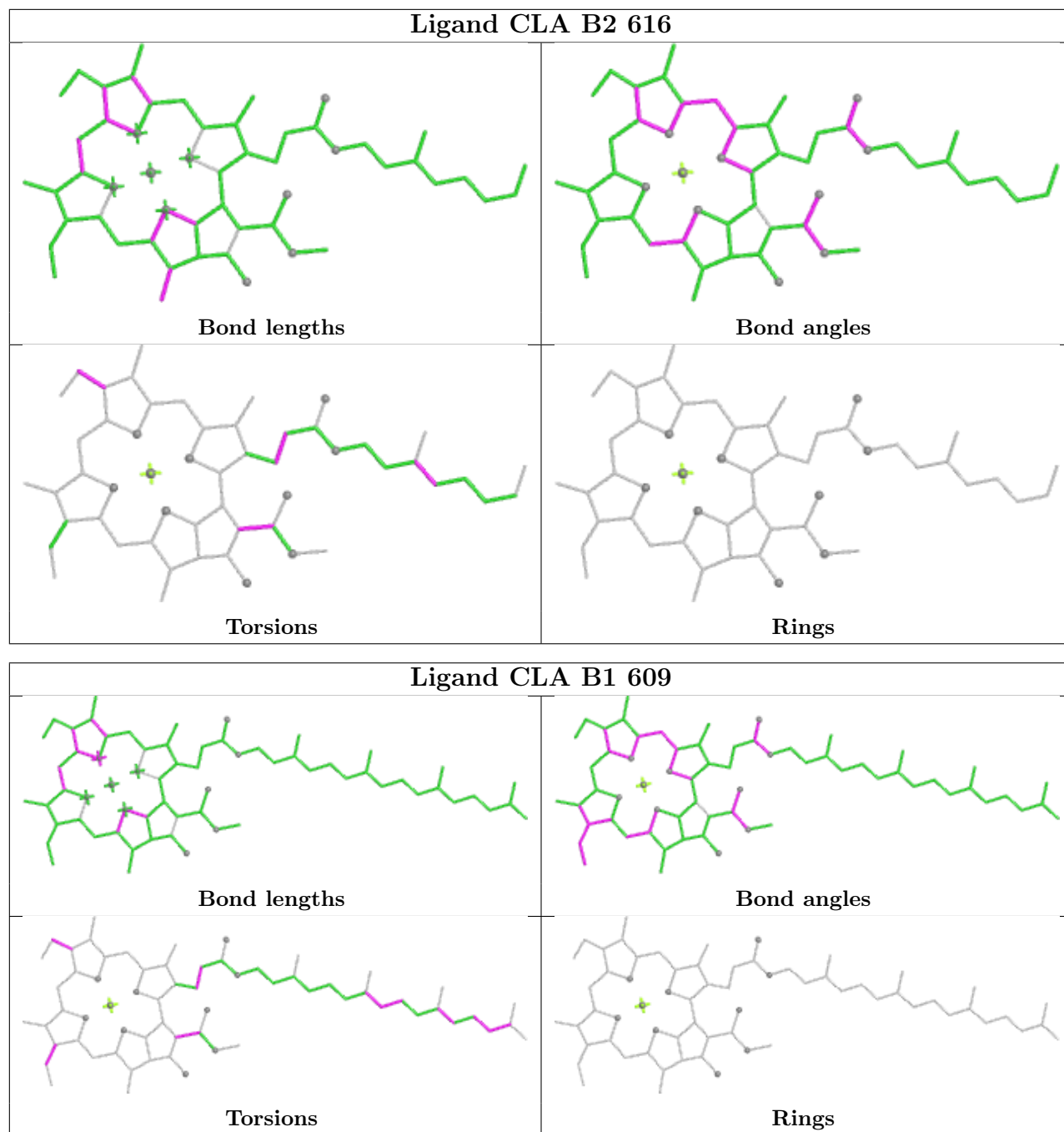
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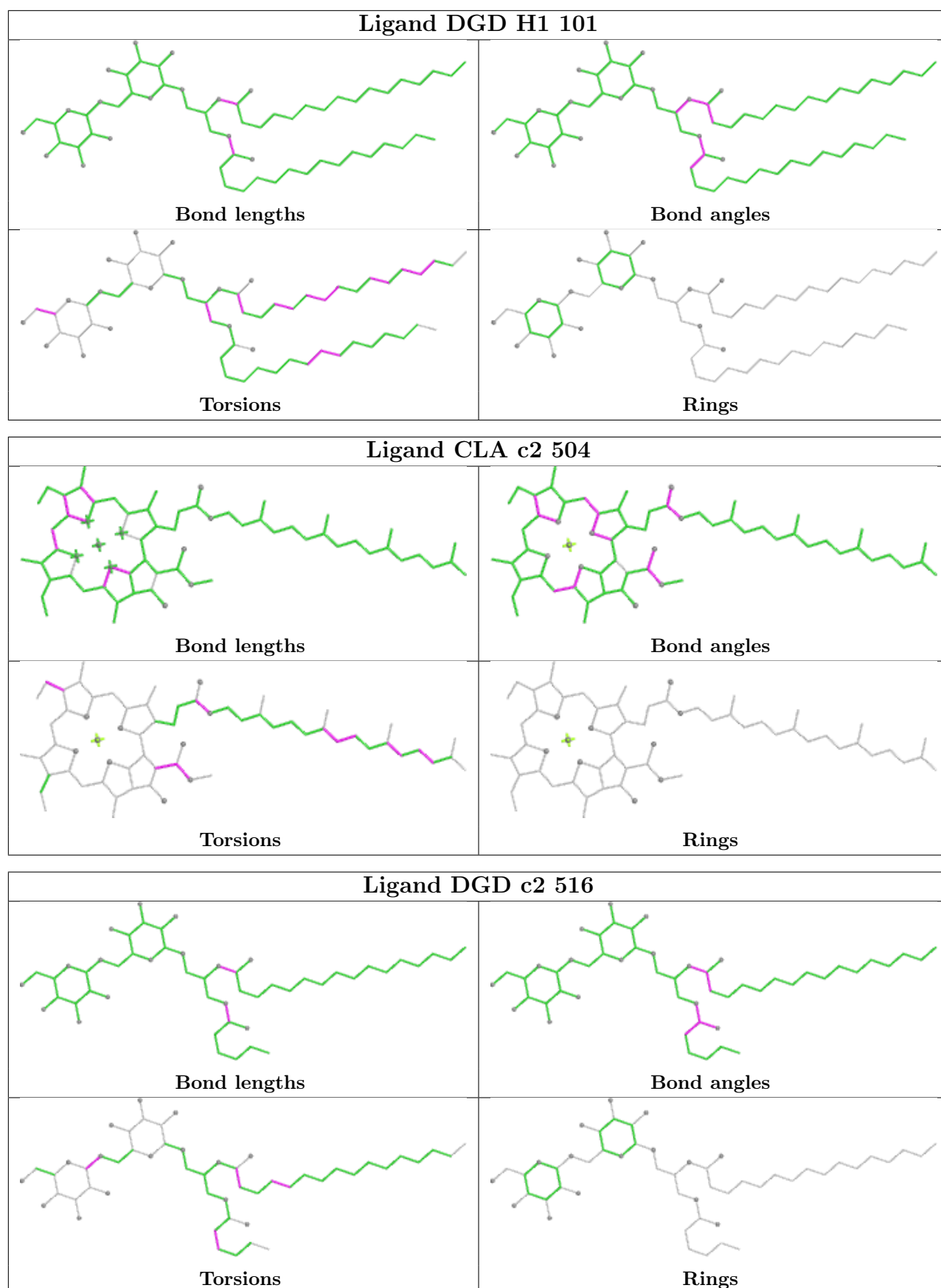


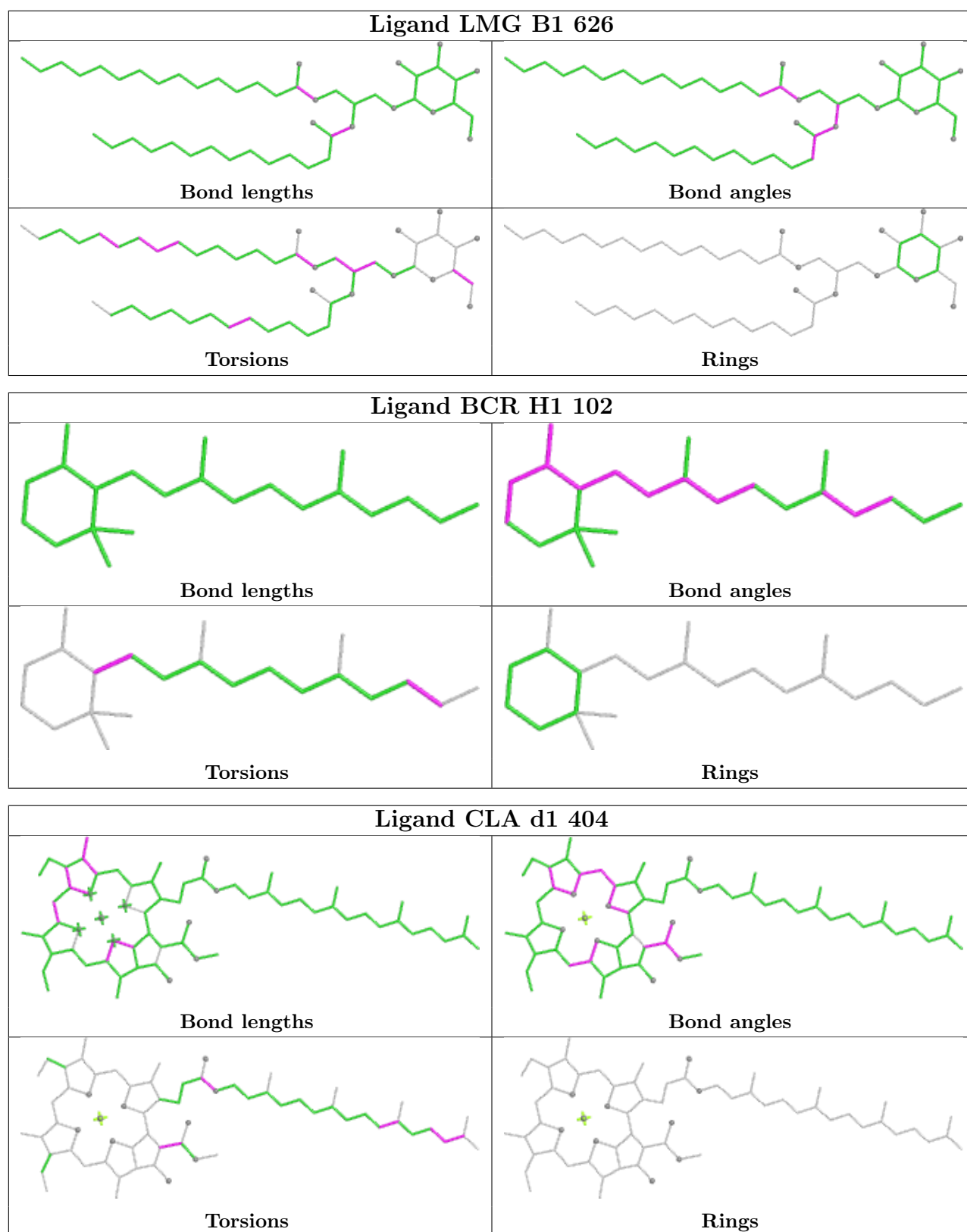


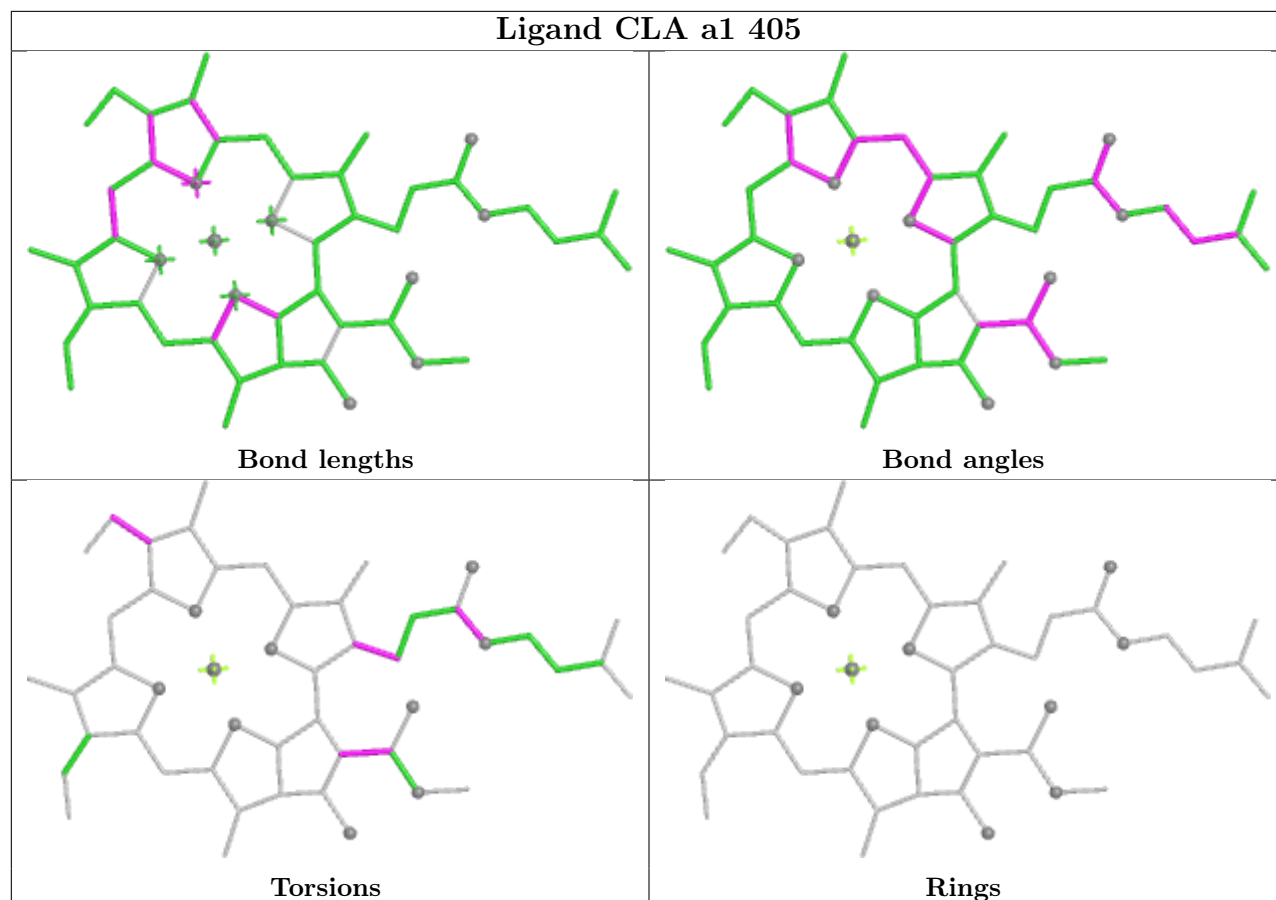
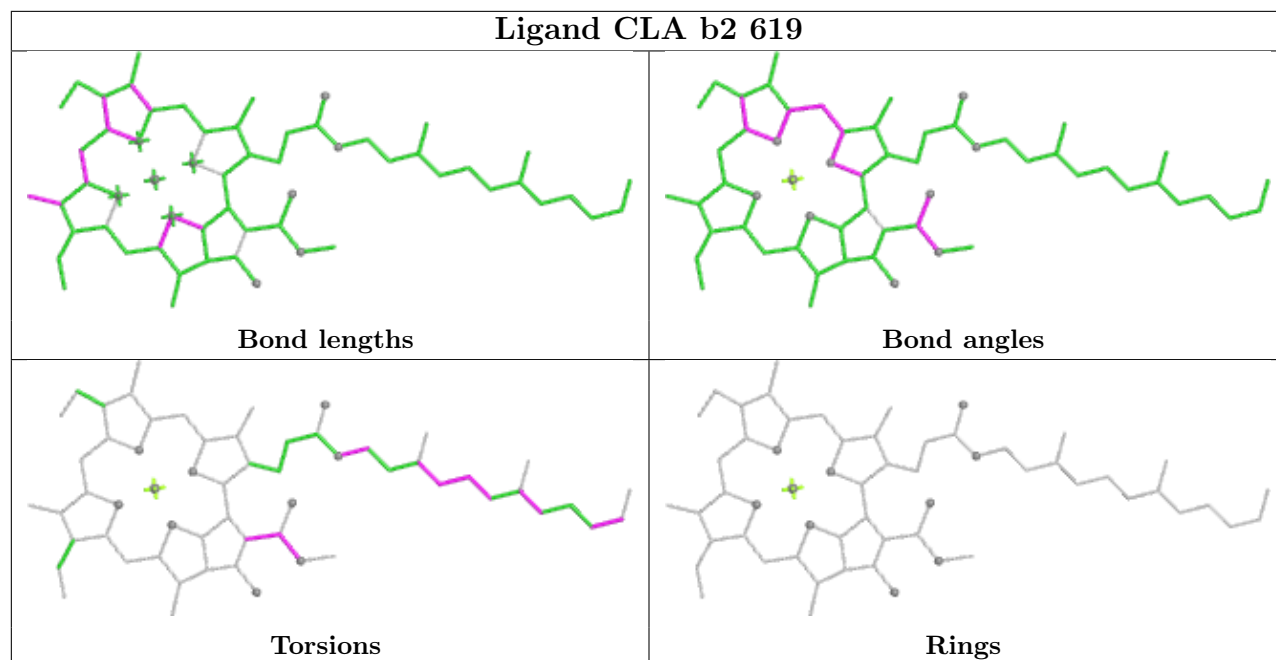


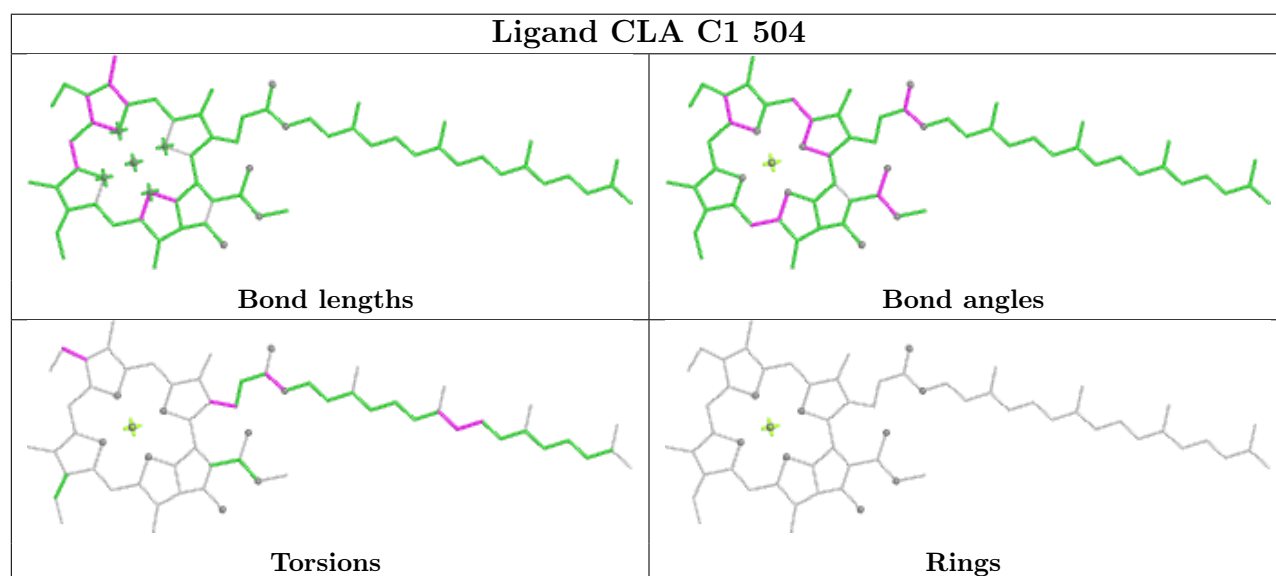
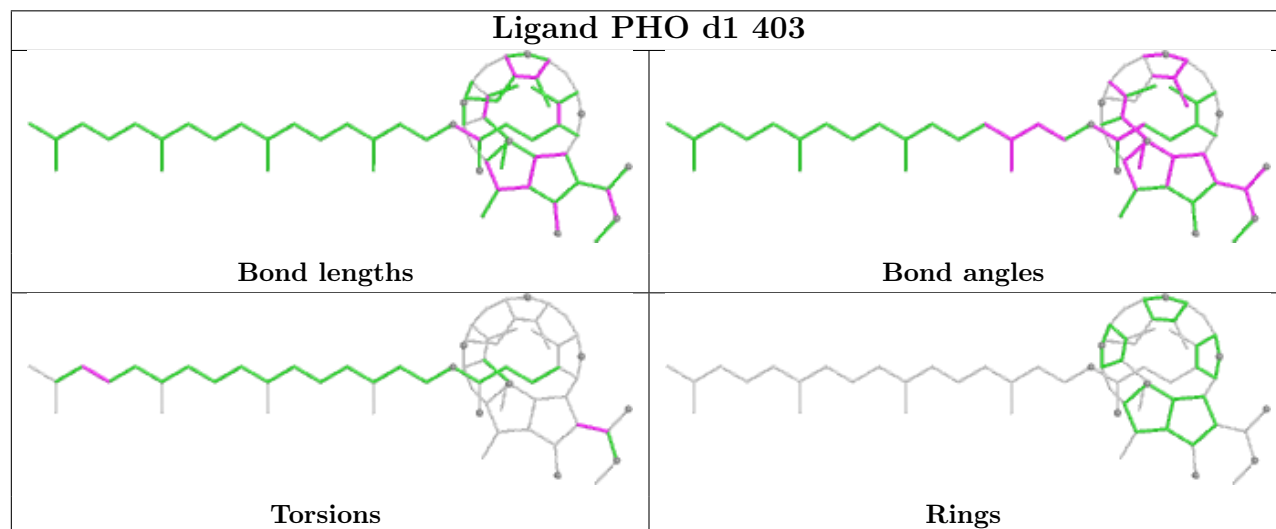
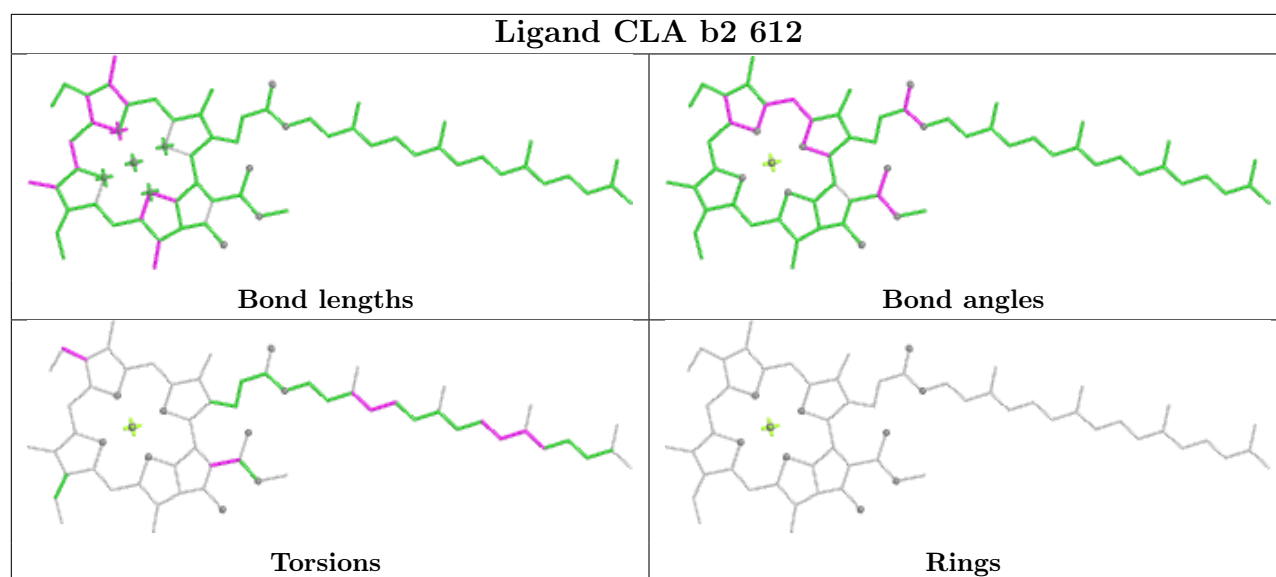


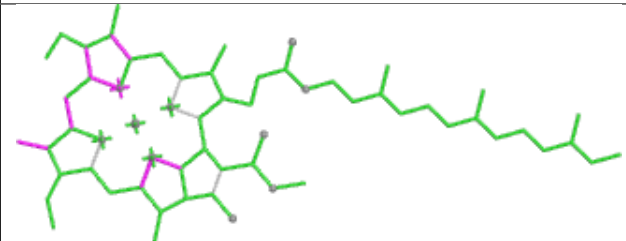
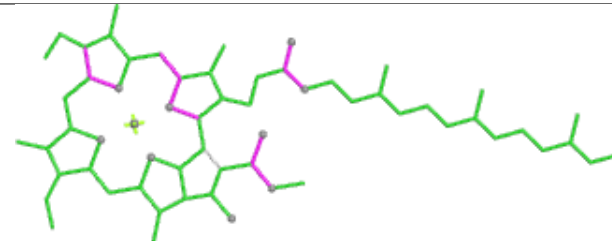
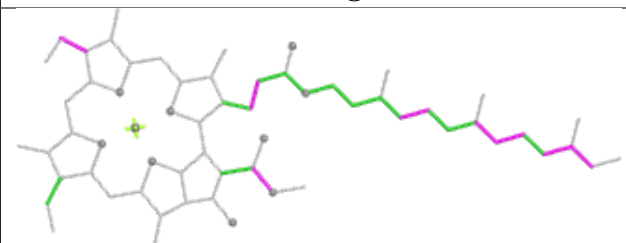
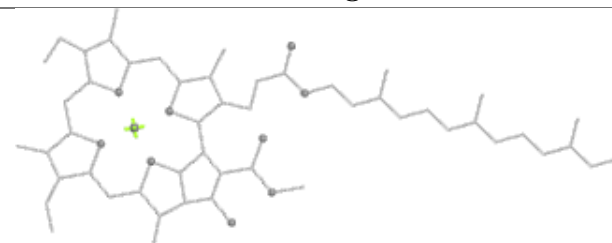


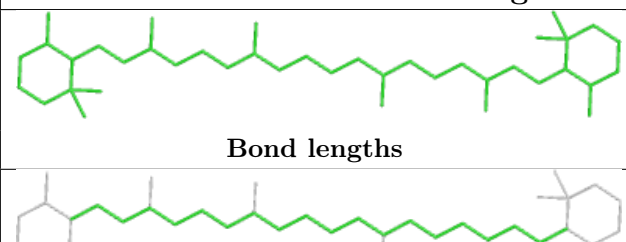
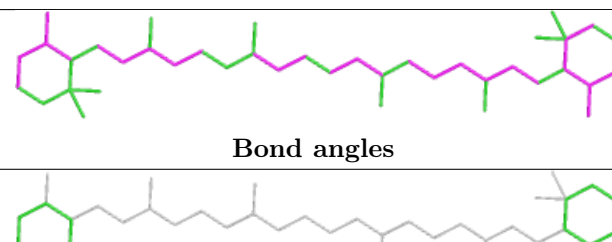
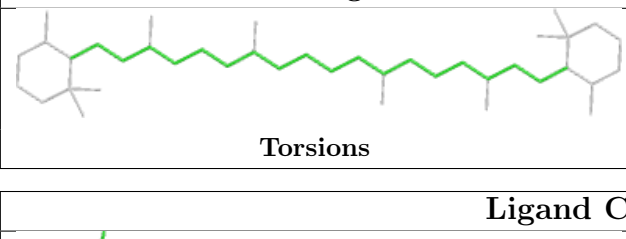
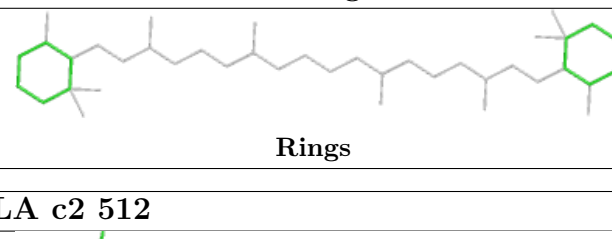


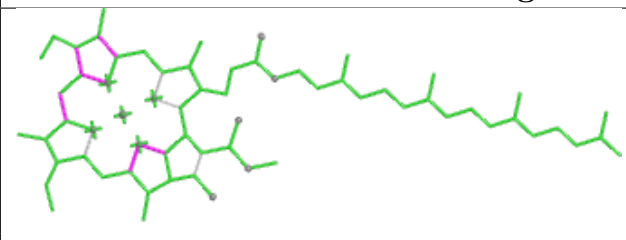
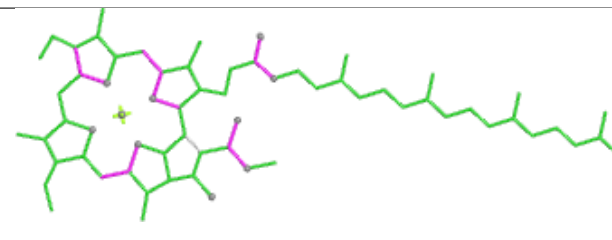
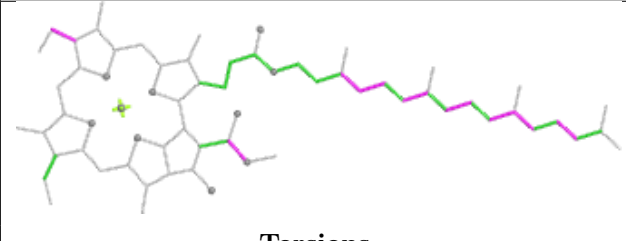
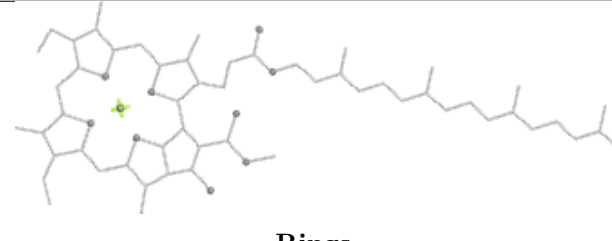


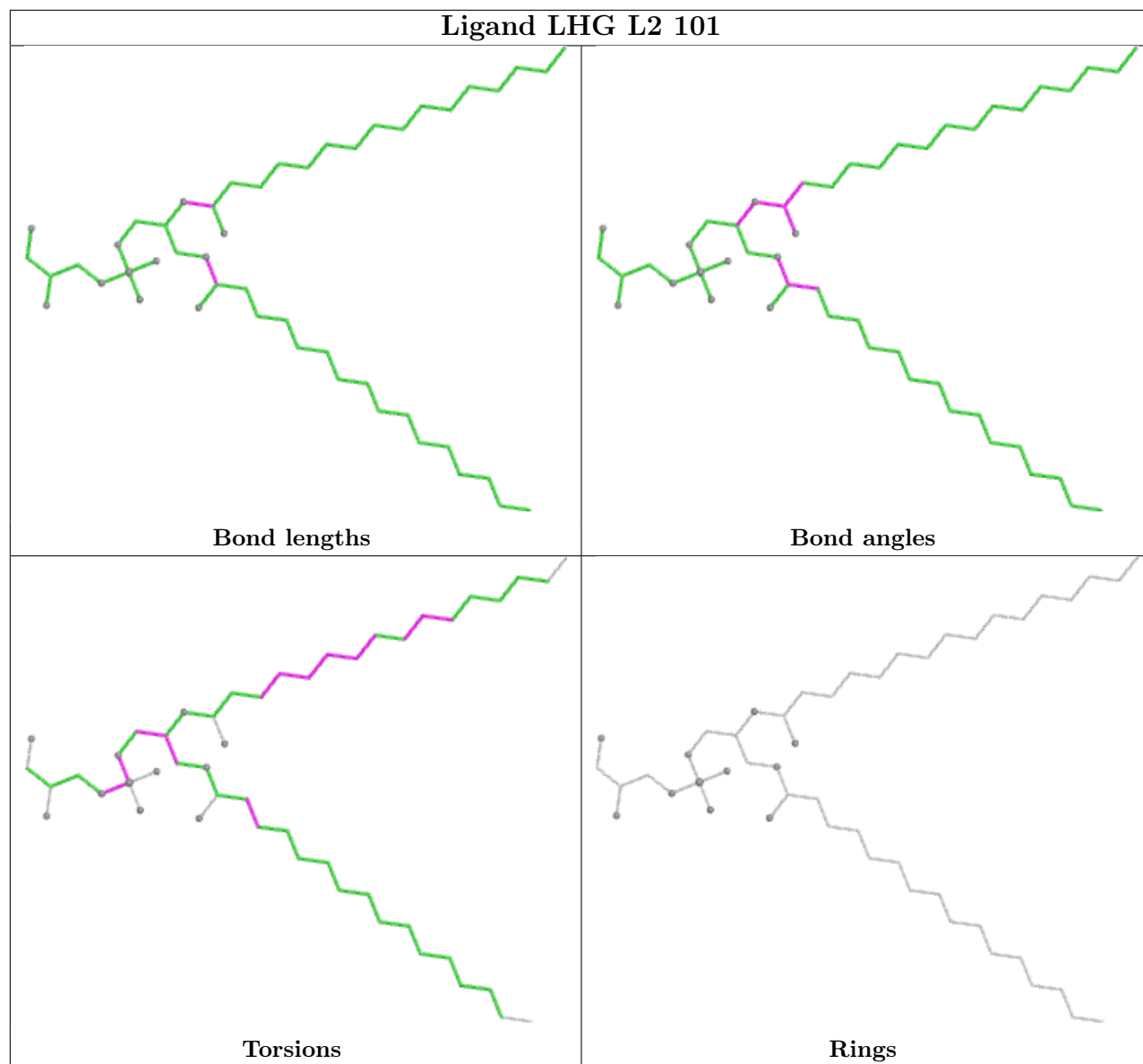


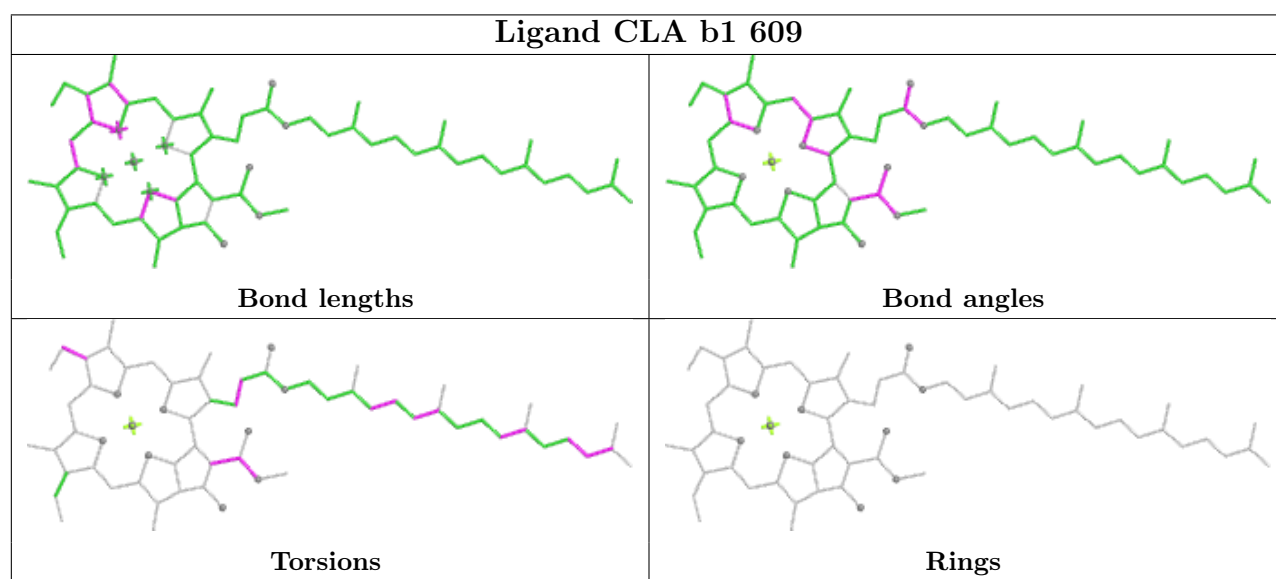
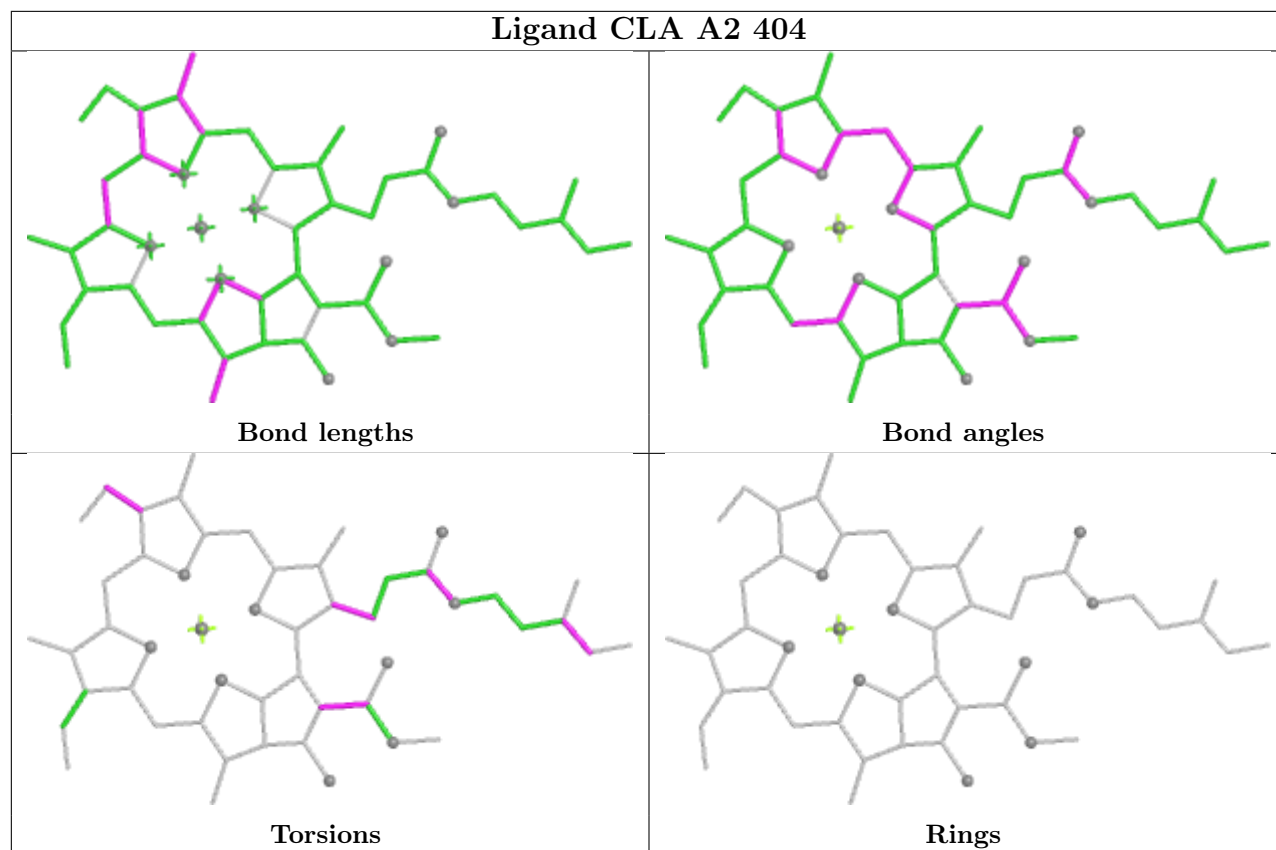


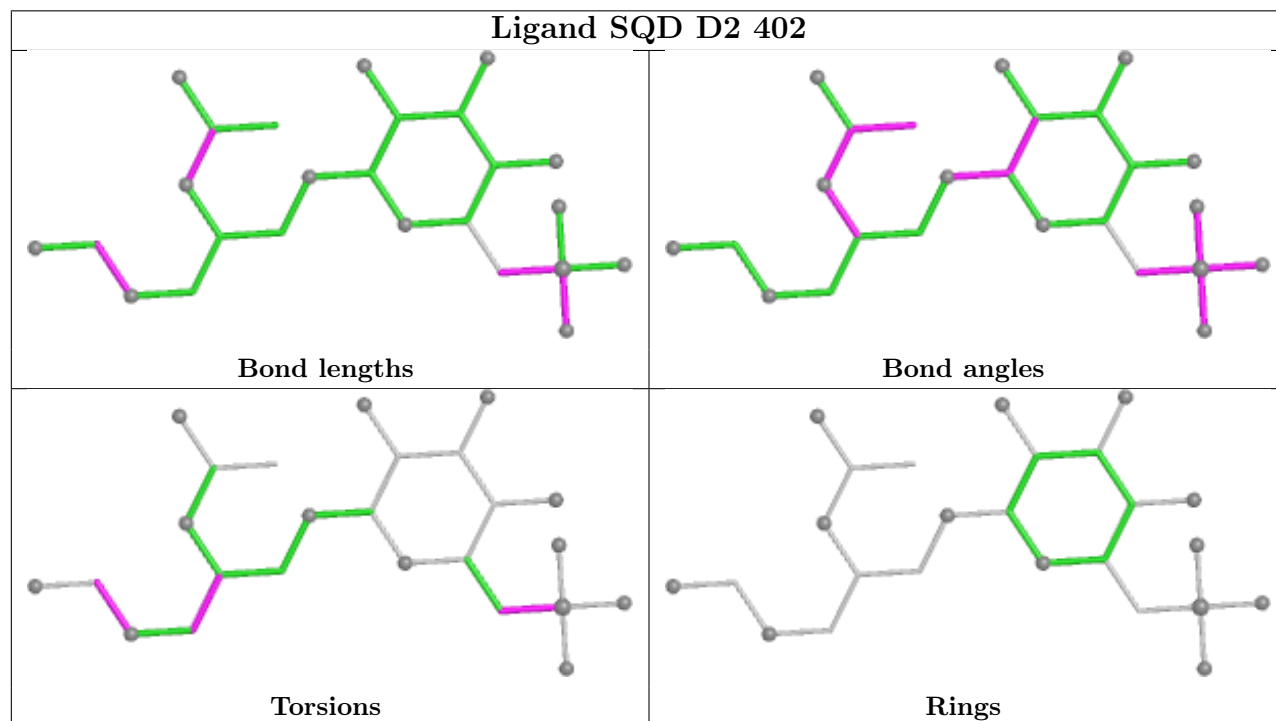
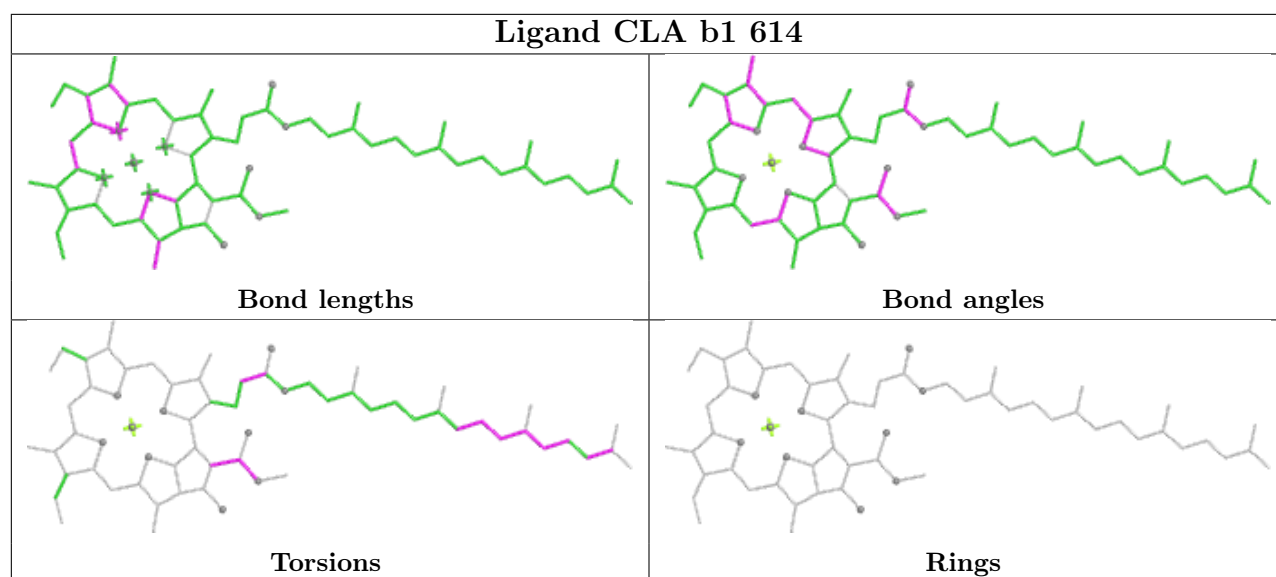
Ligand CLA b2 609	
	
Bond lengths	Bond angles
	
Torsions	Rings

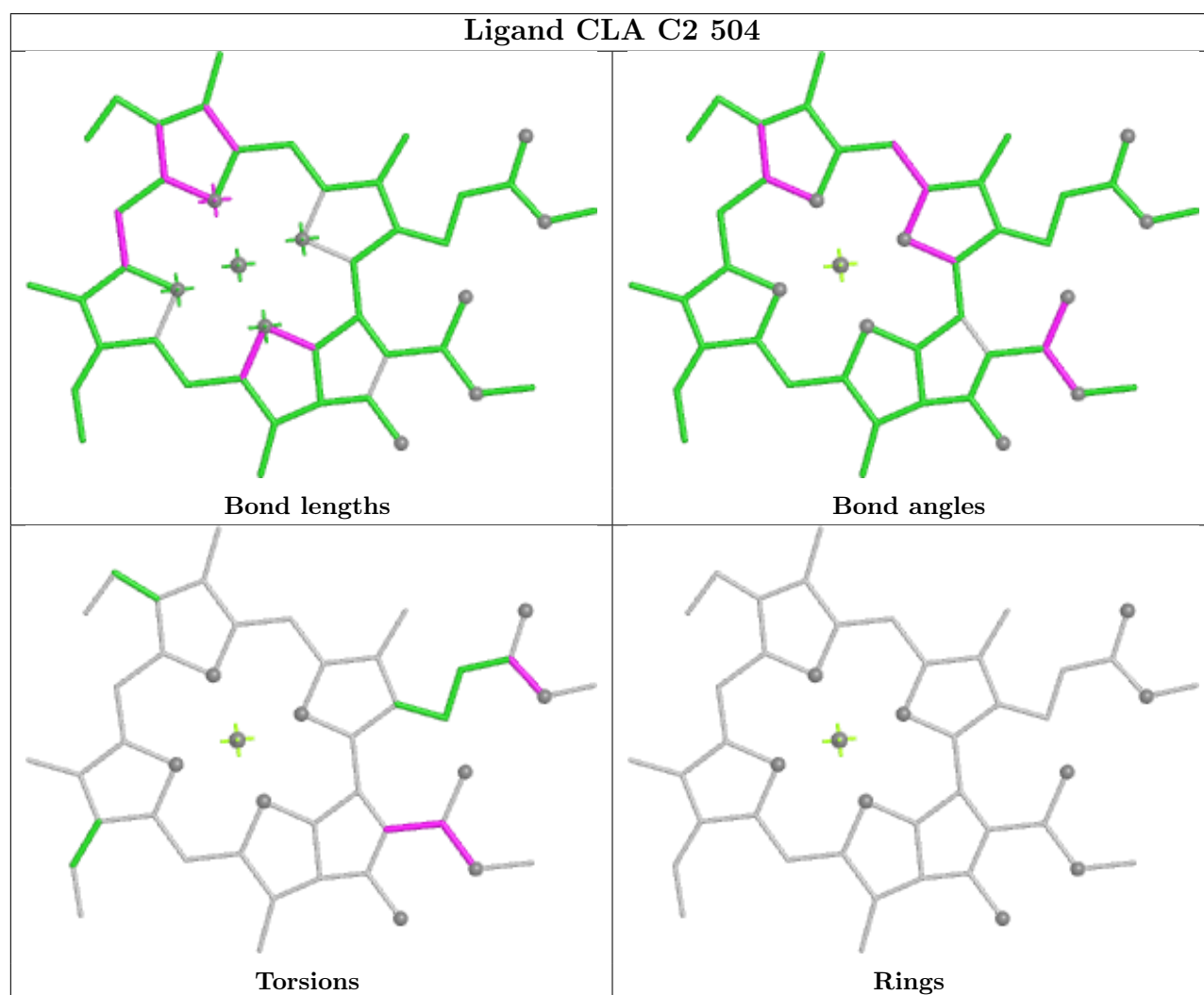
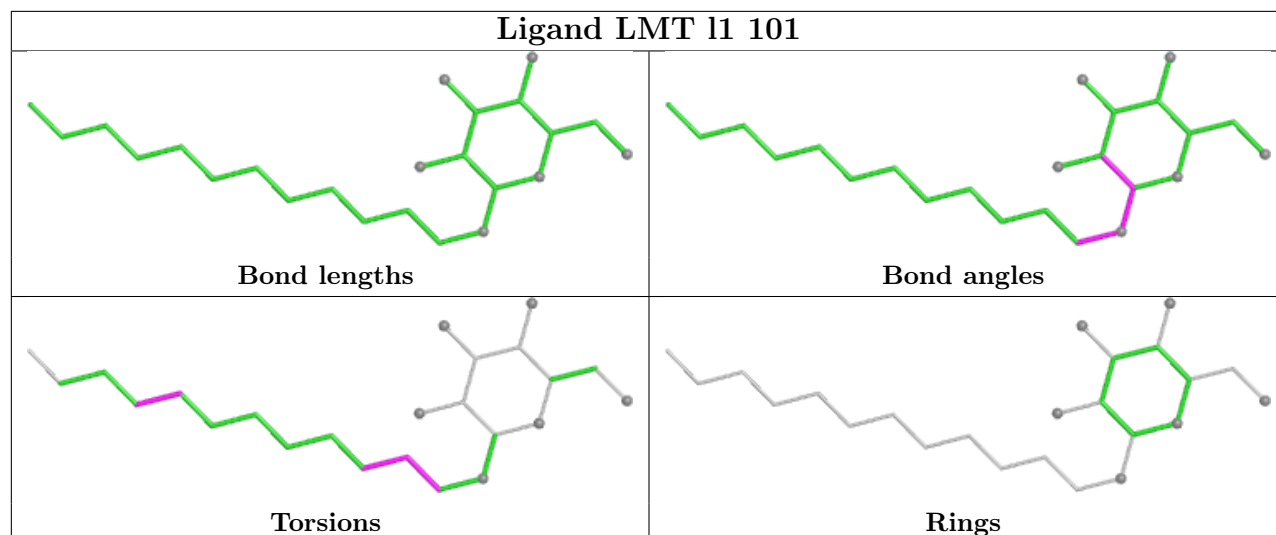
Ligand BCR B1 601	
	
Bond lengths	Bond angles
	
Torsions	Rings

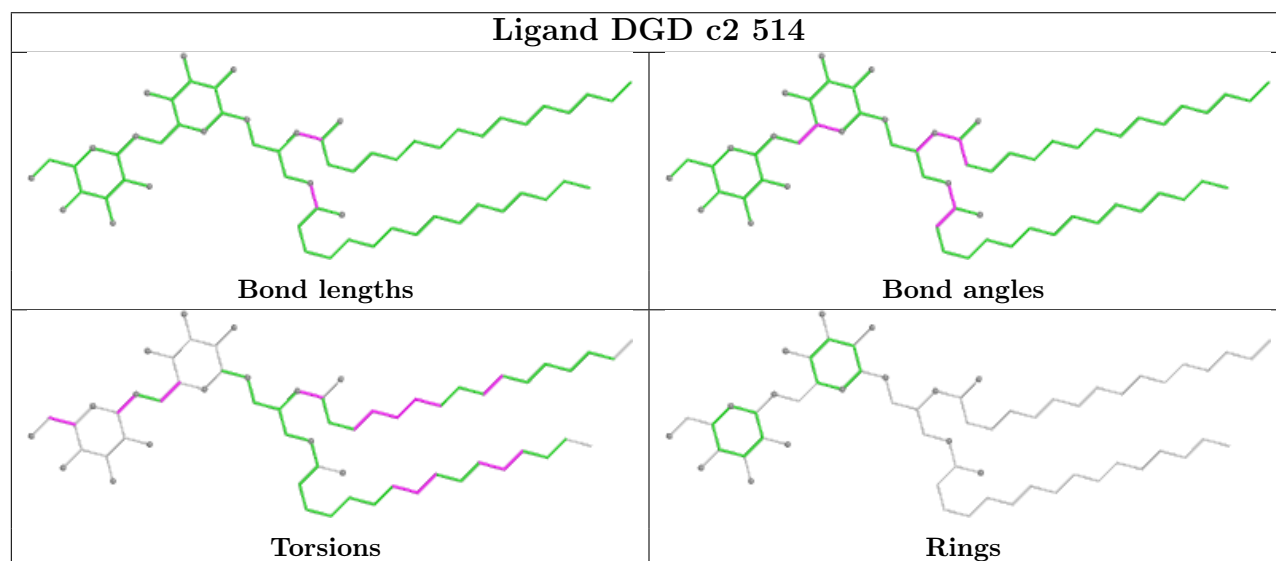
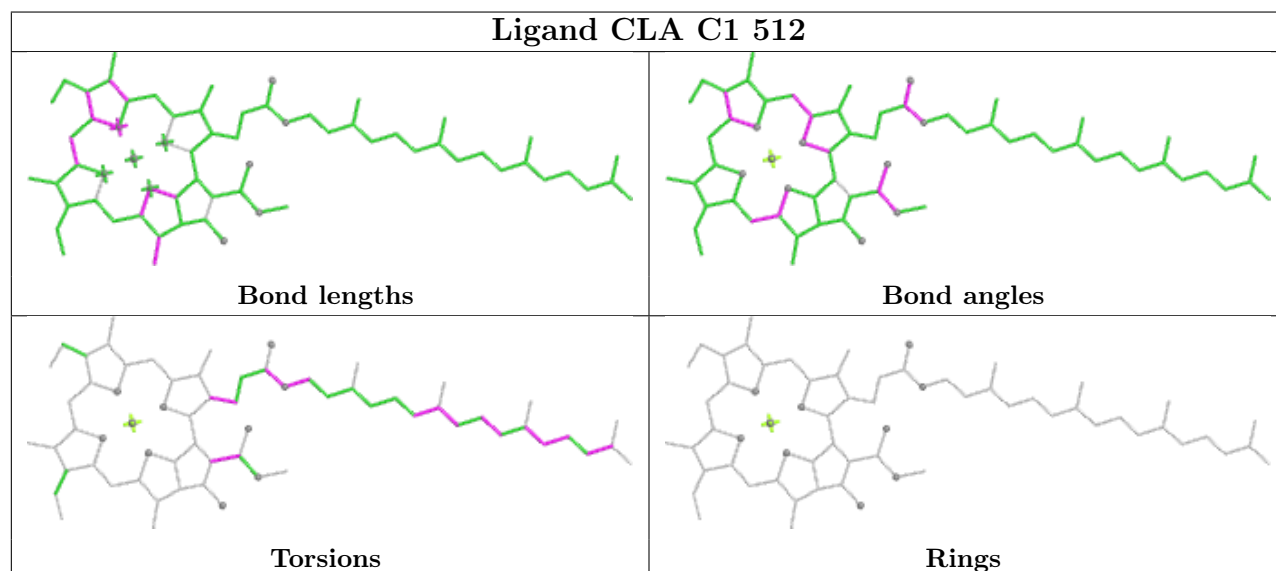
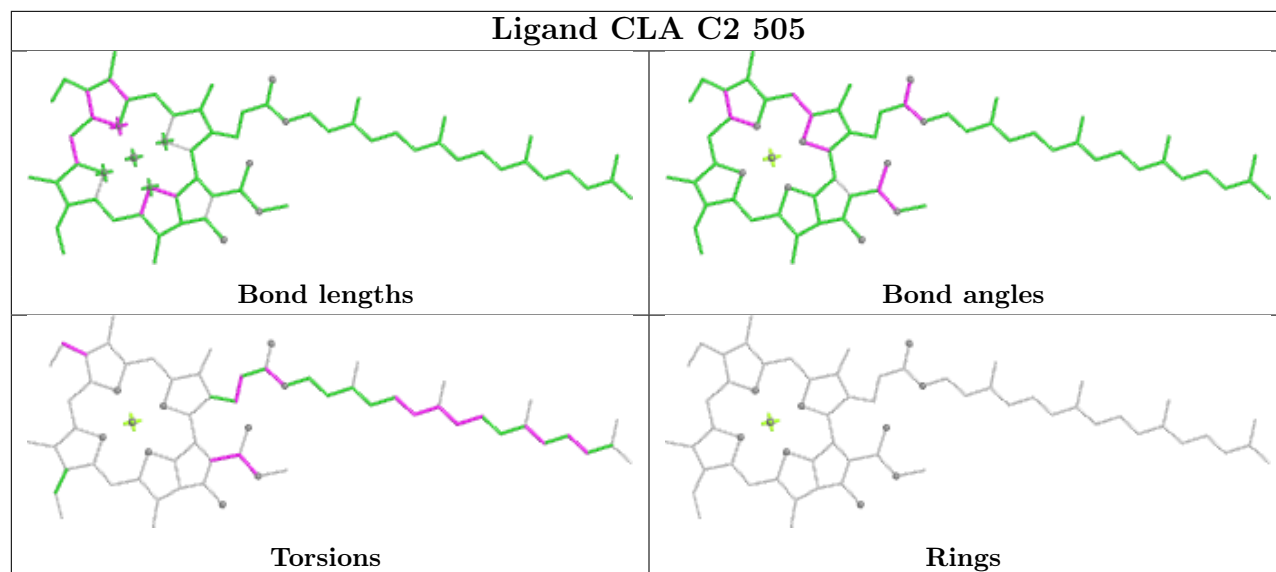
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Bond lengths	Bond angles
	
Torsions	Rings

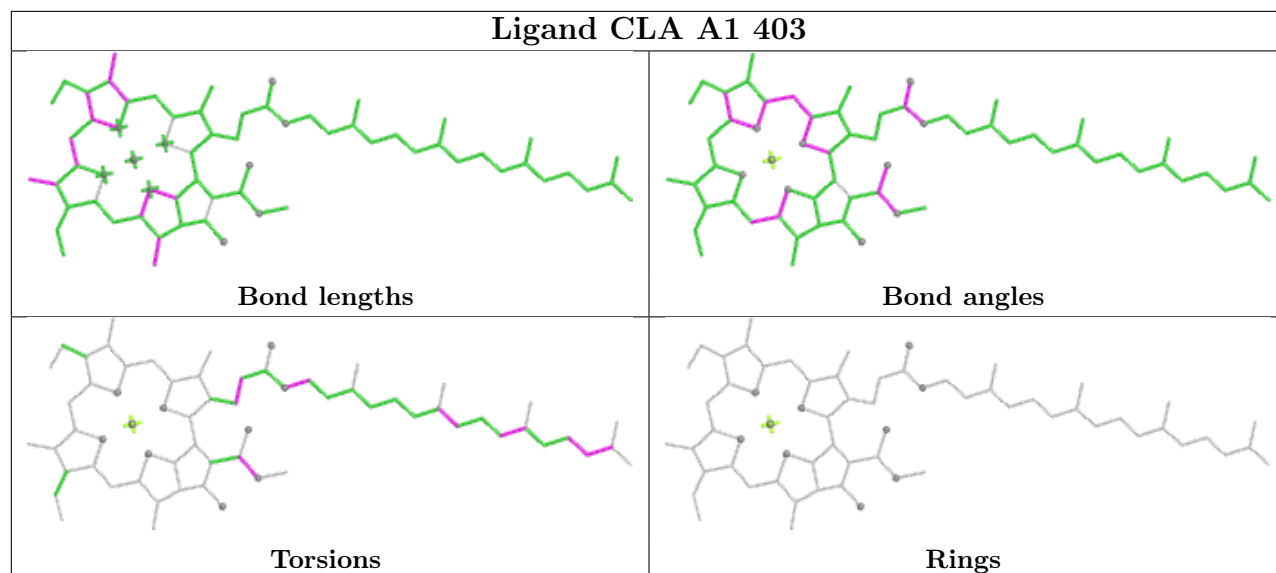
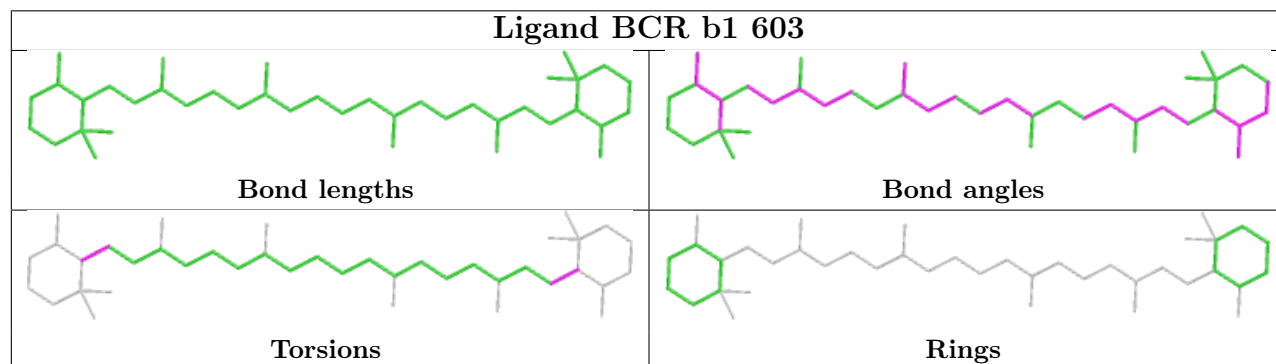
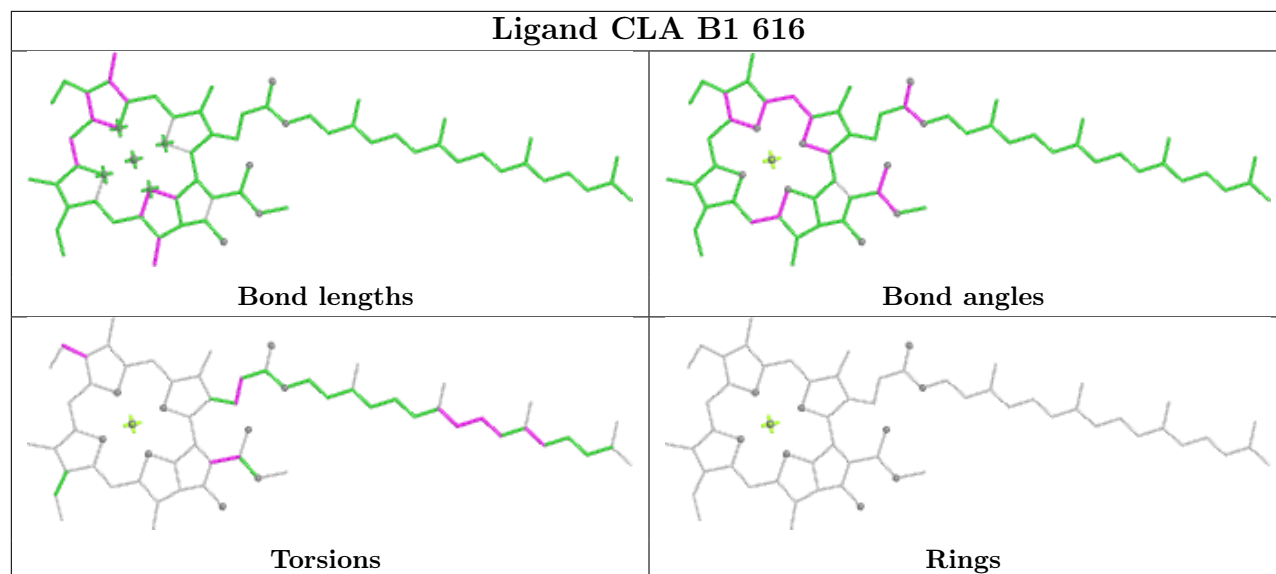


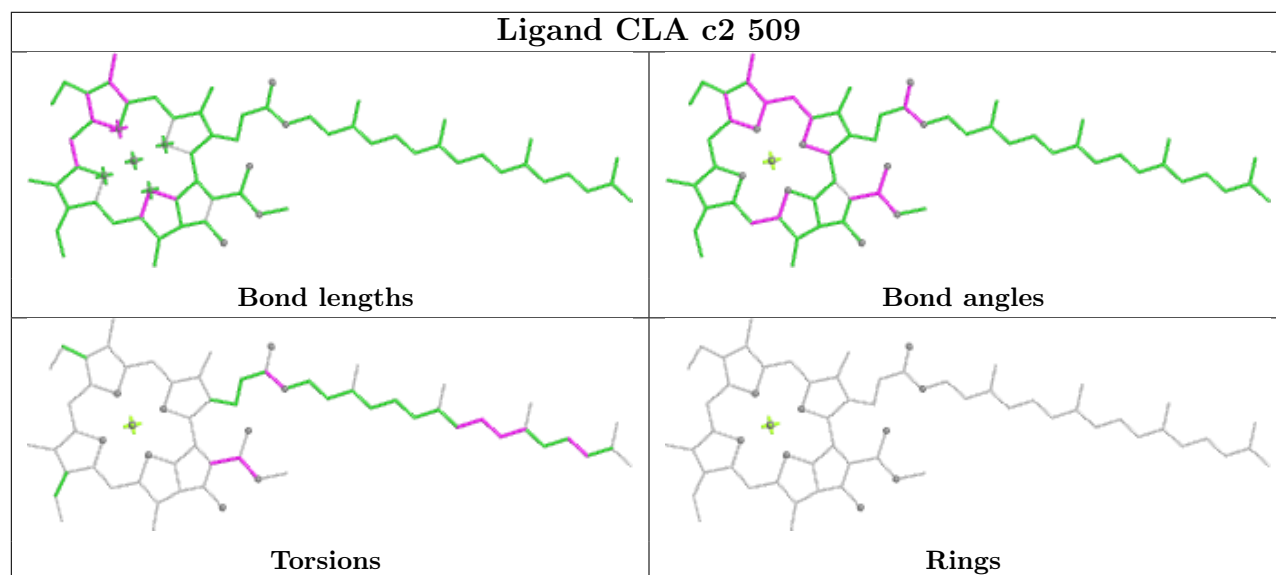
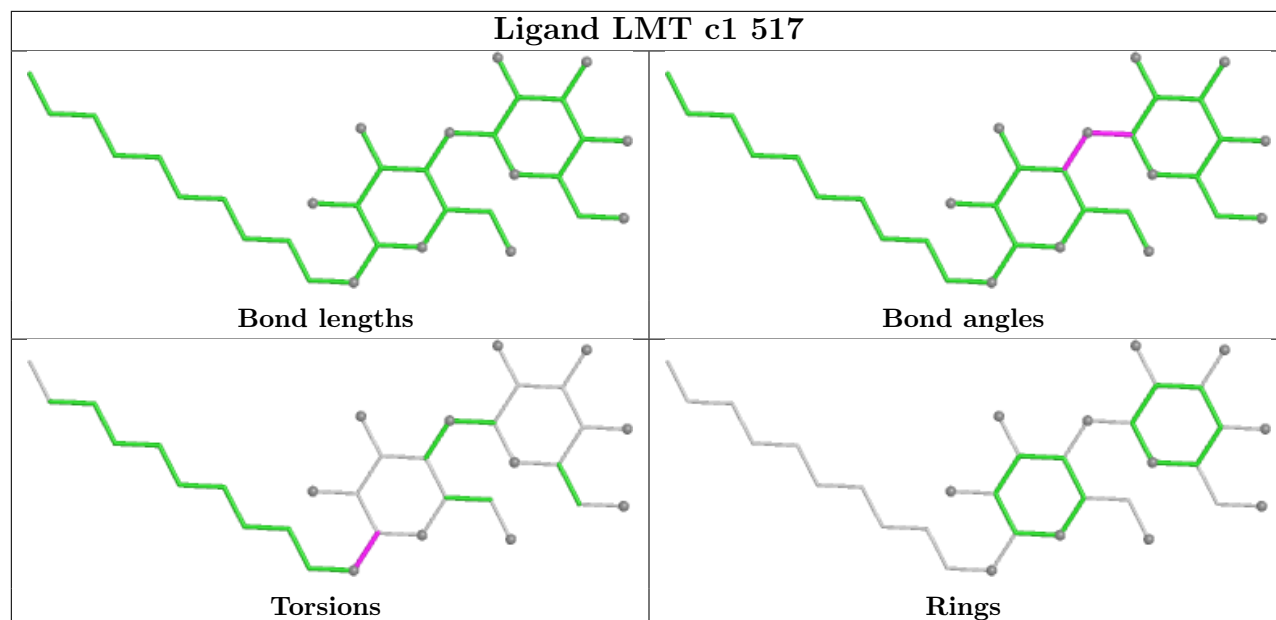


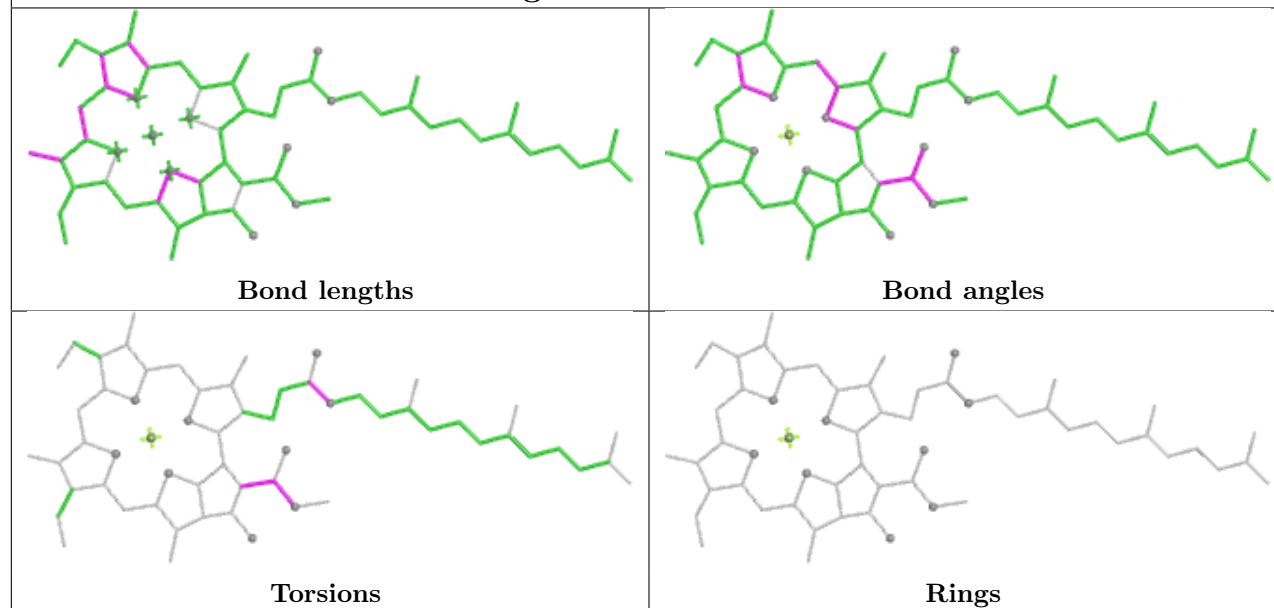
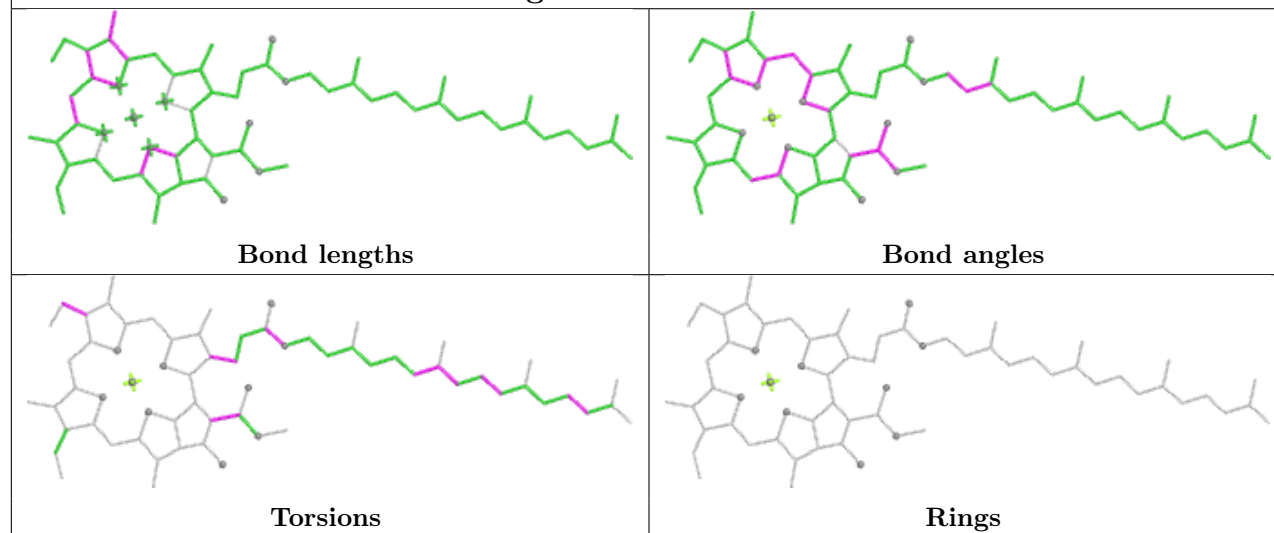


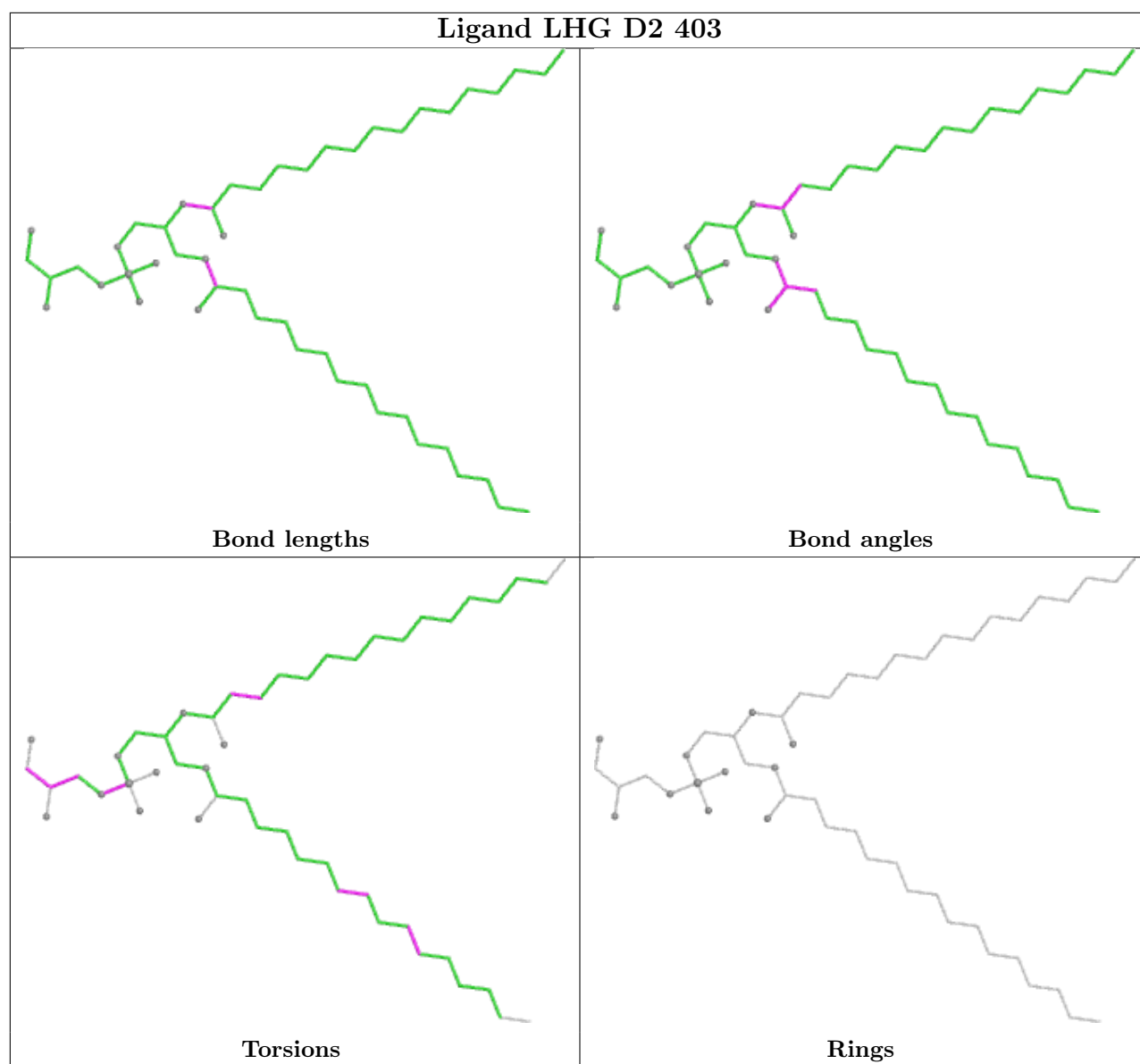


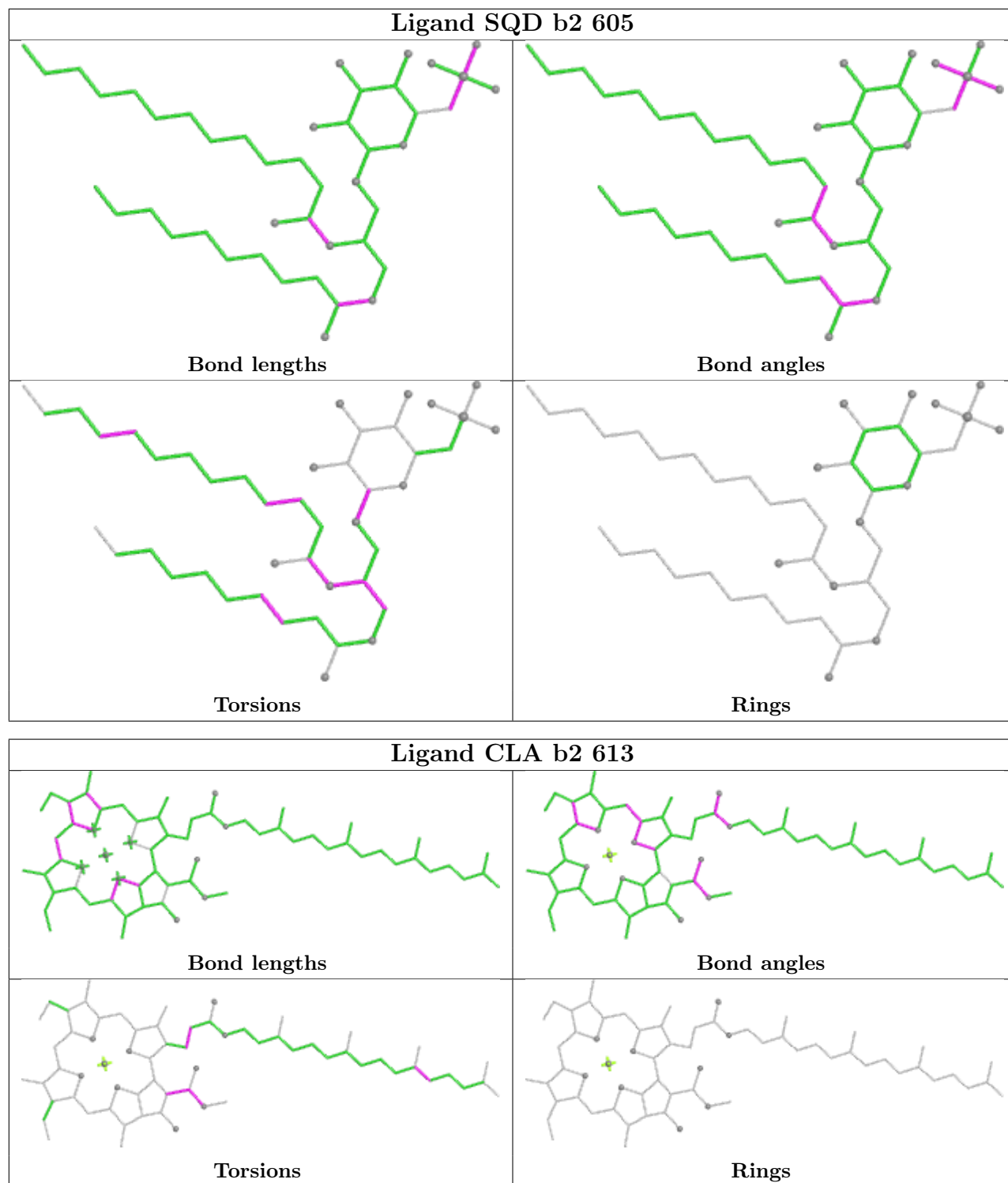


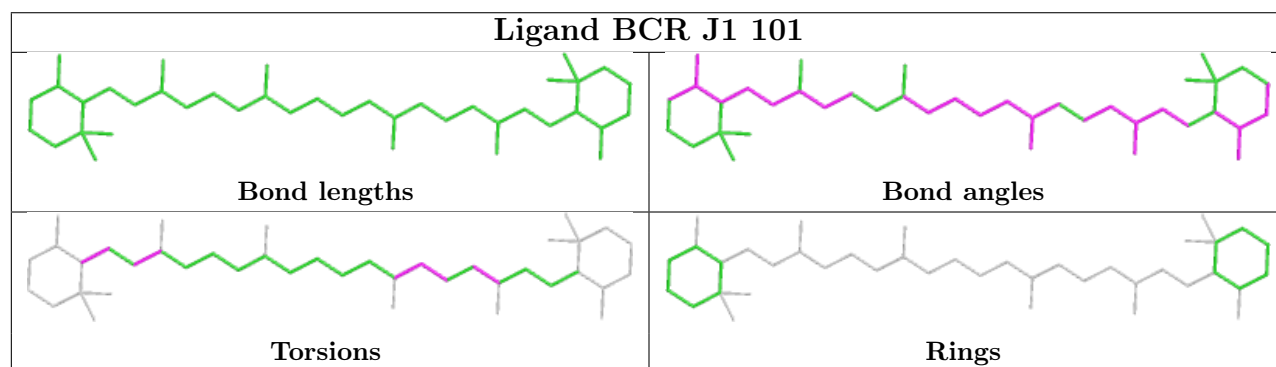
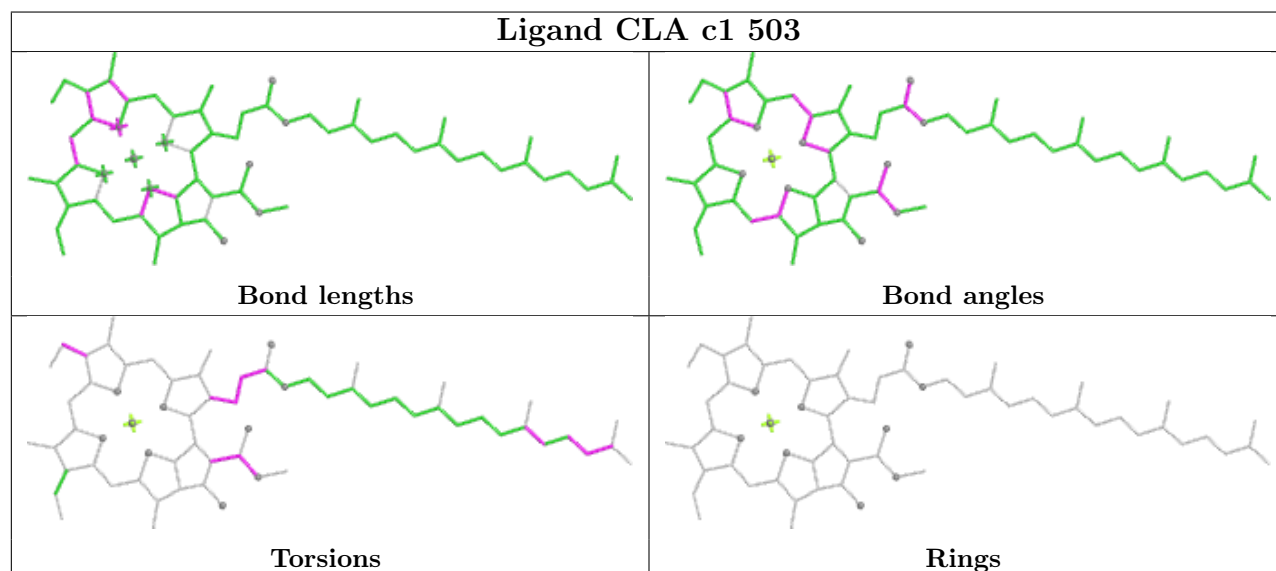
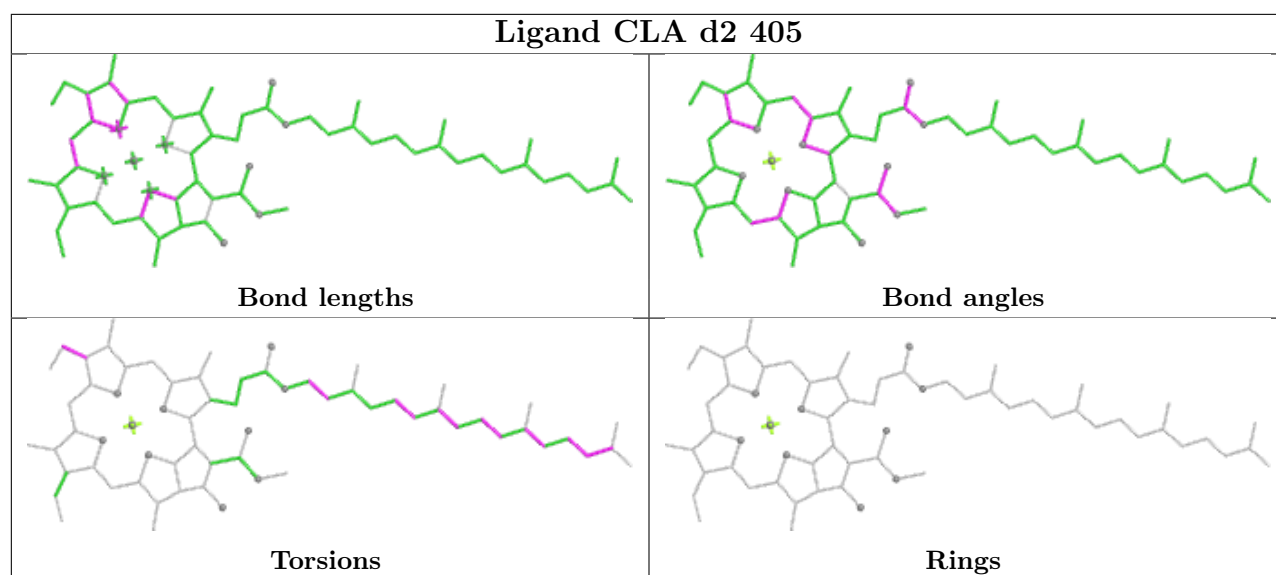


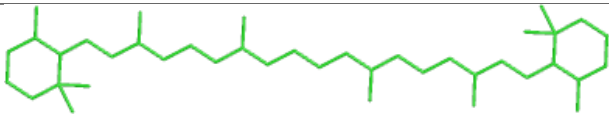
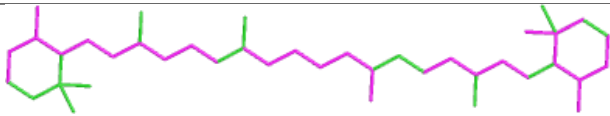
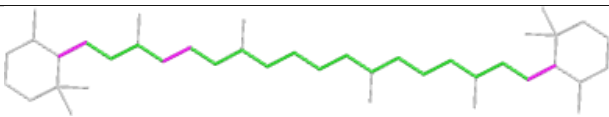
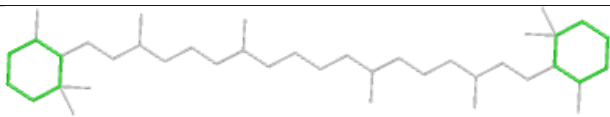


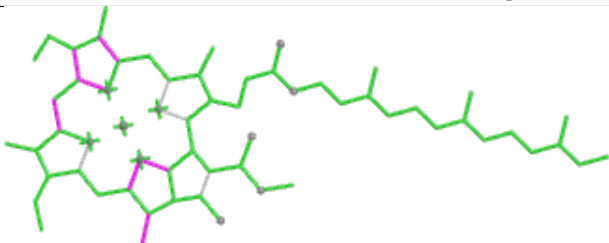
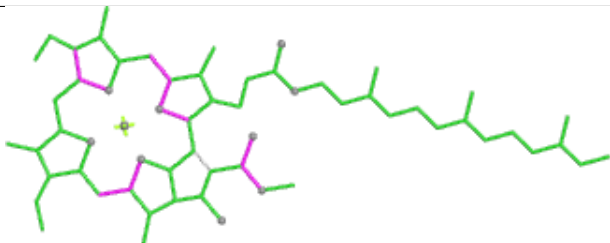
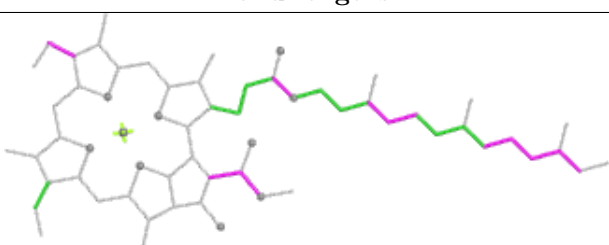
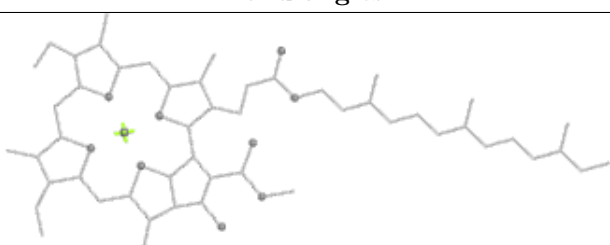
Ligand CLA B2 618**Ligand CLA d2 402**

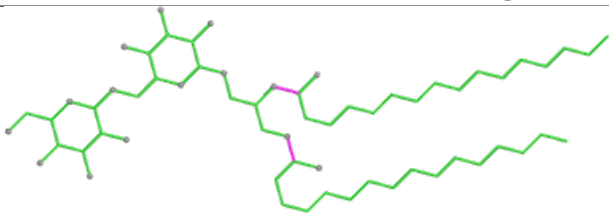
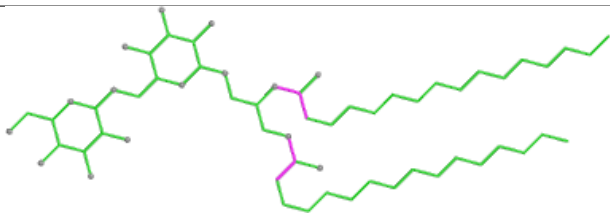
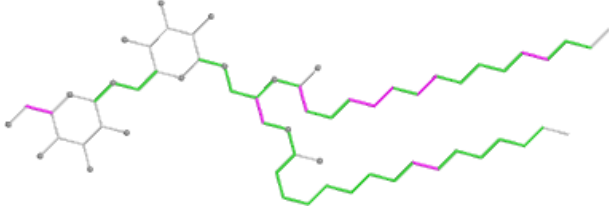
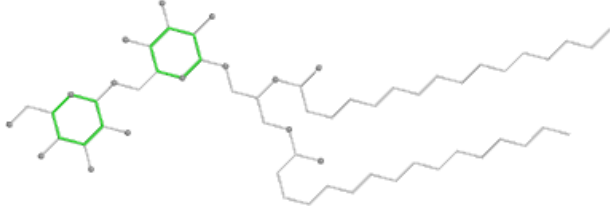


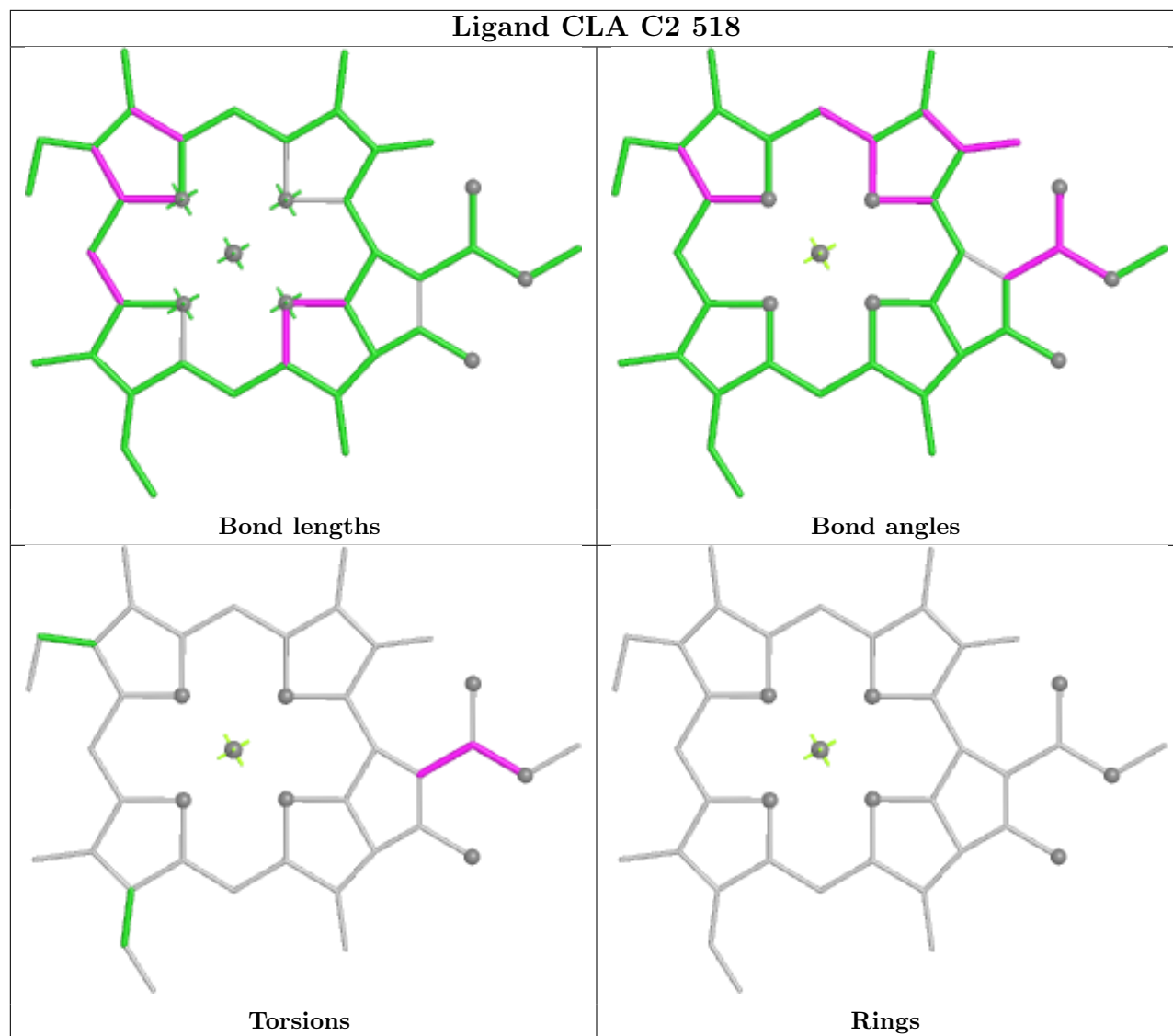


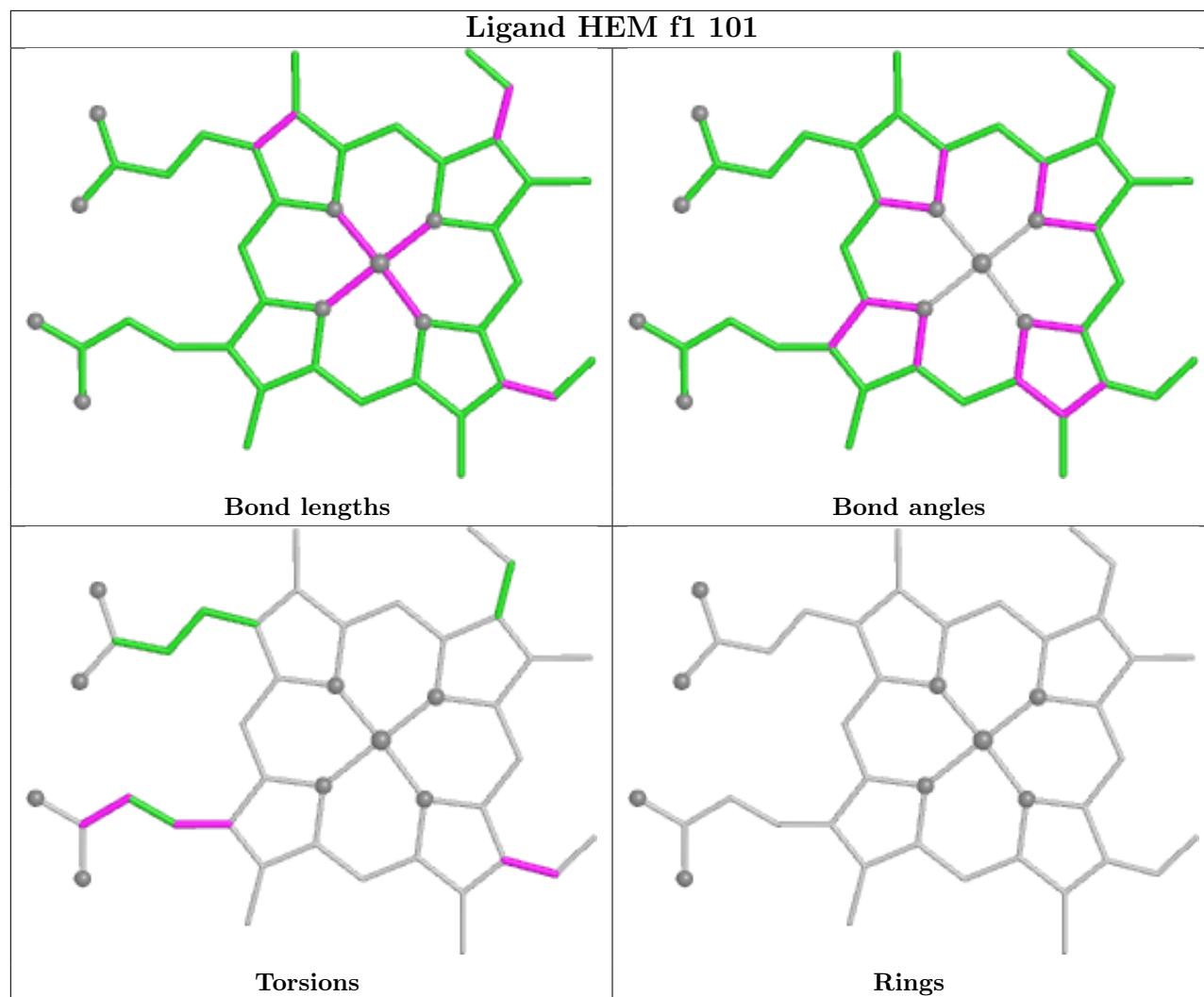


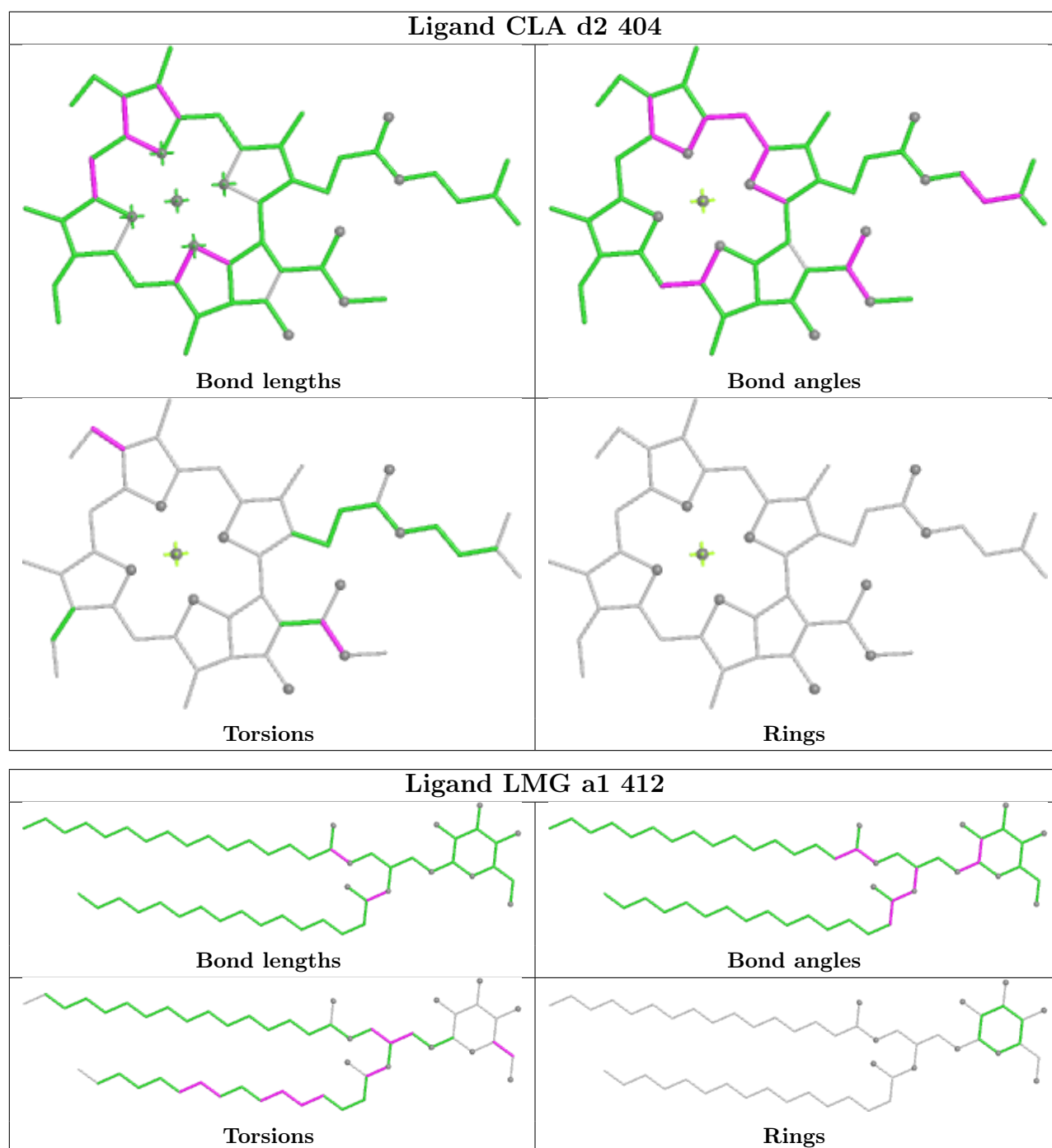
Ligand BCR h1 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

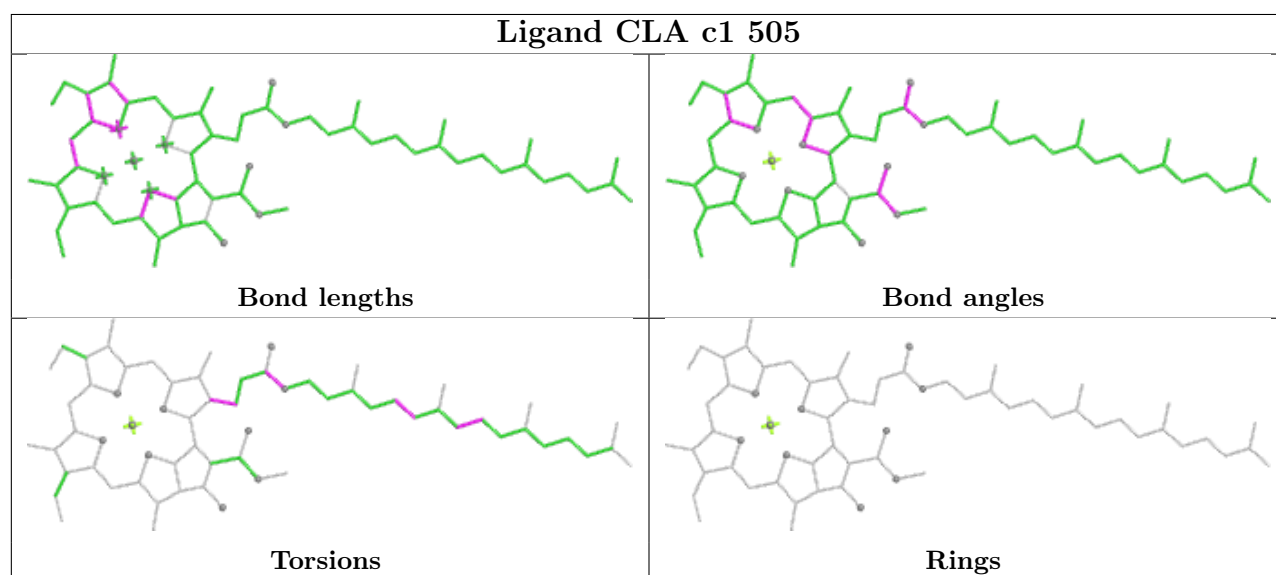
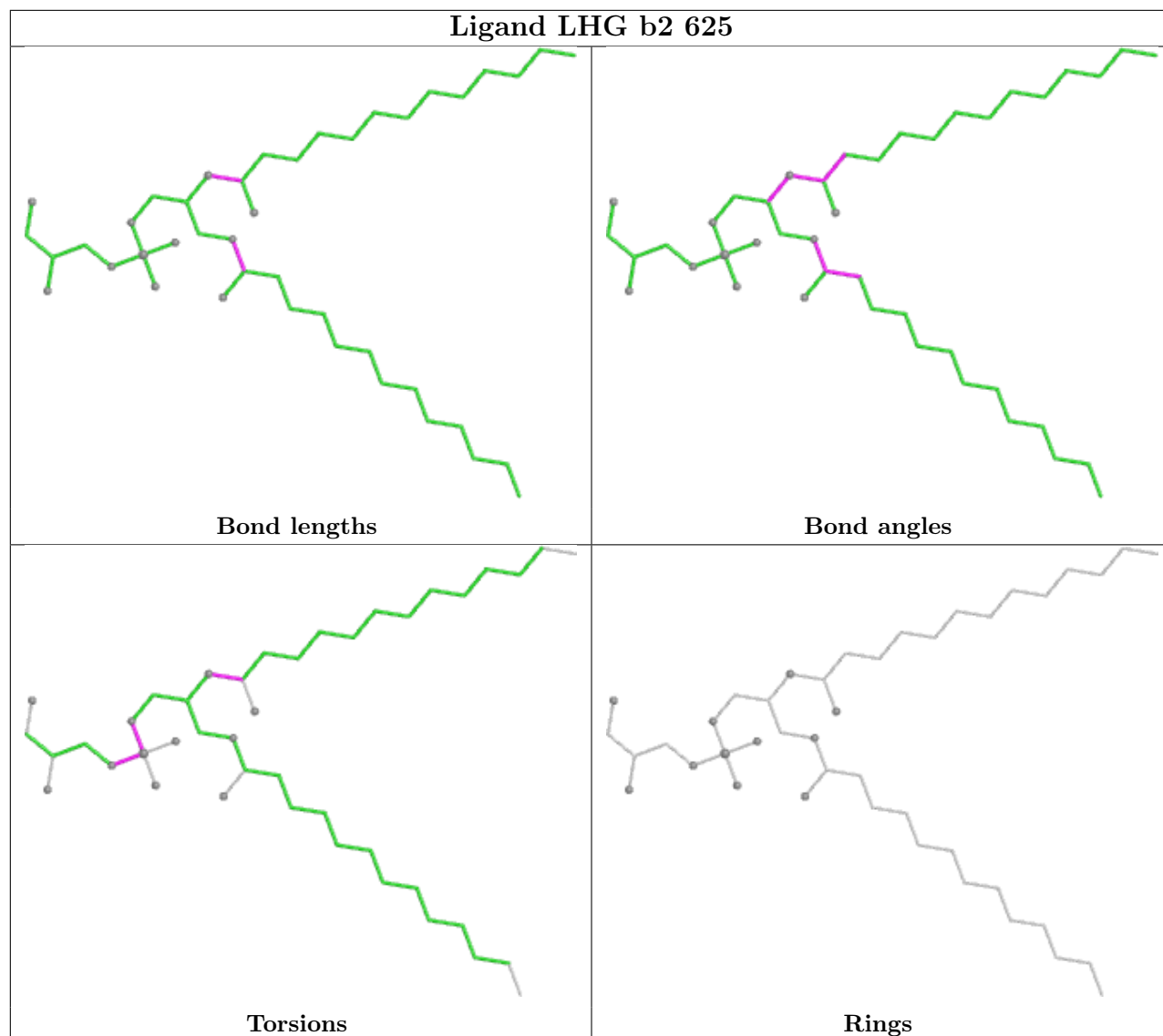
Ligand CLA C1 513	
	
Bond lengths	Bond angles
	
Torsions	Rings

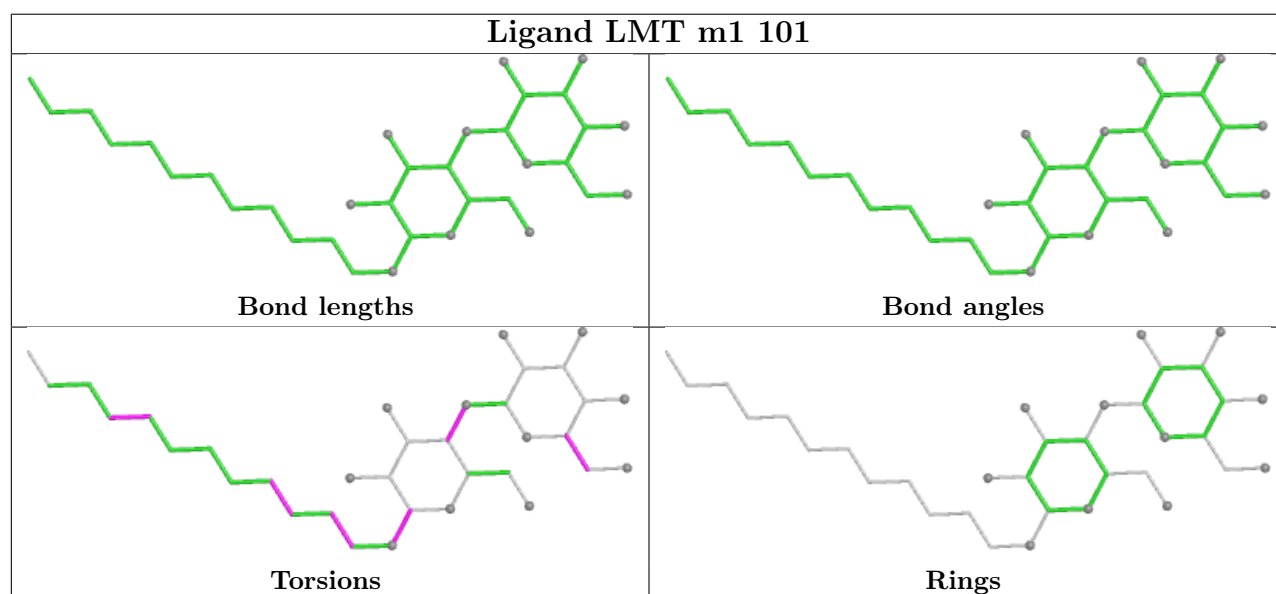
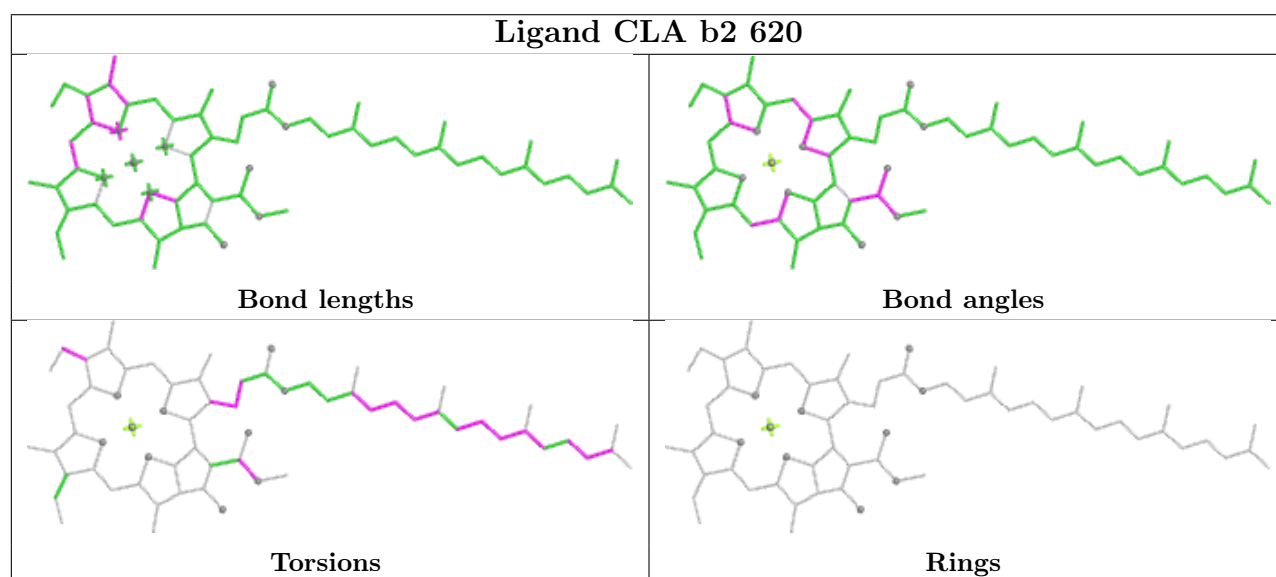
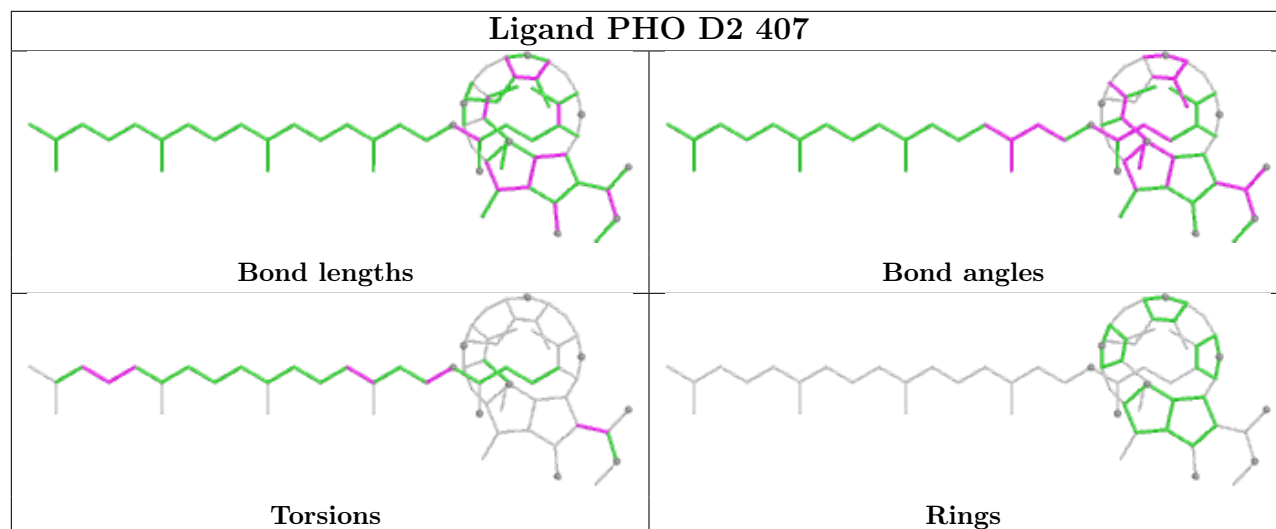
Ligand DGD h2 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

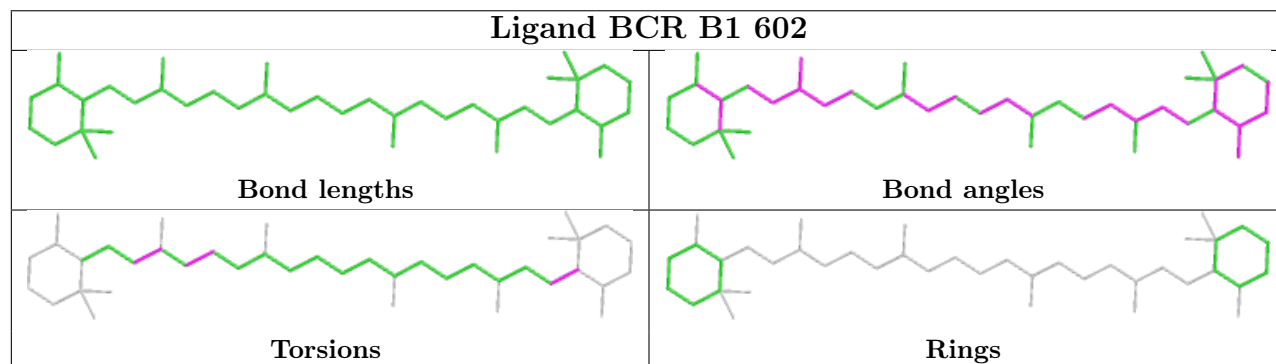
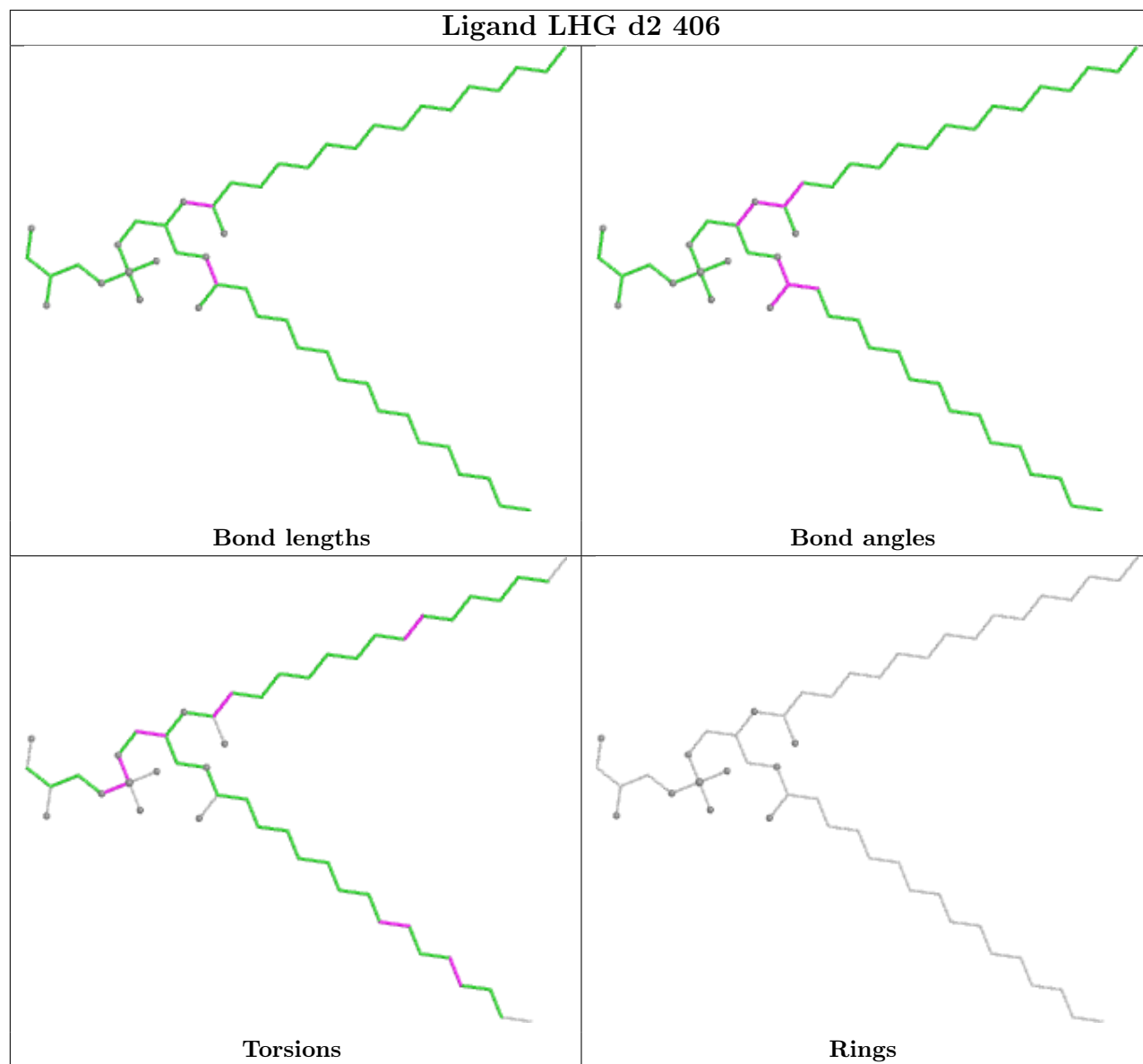


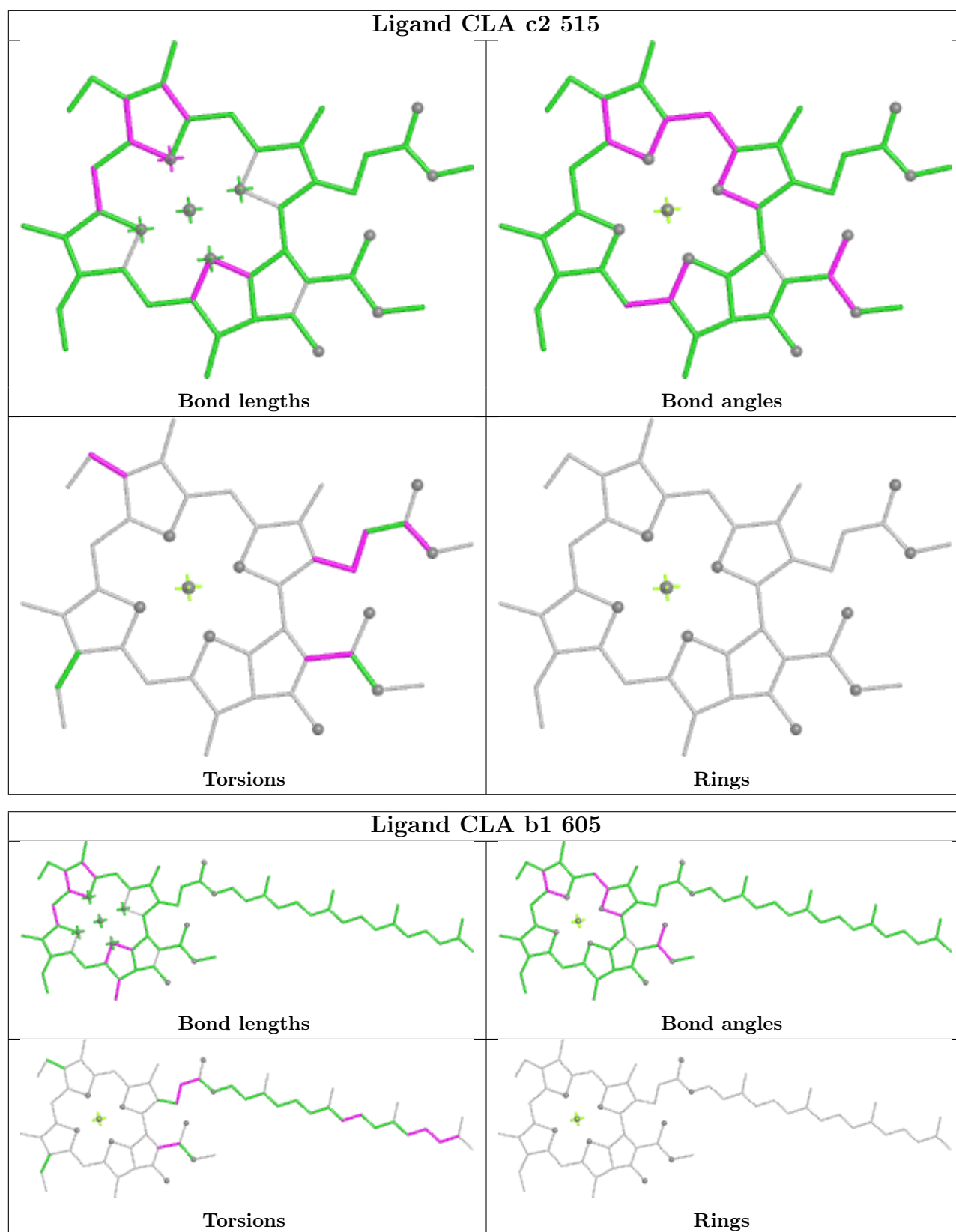


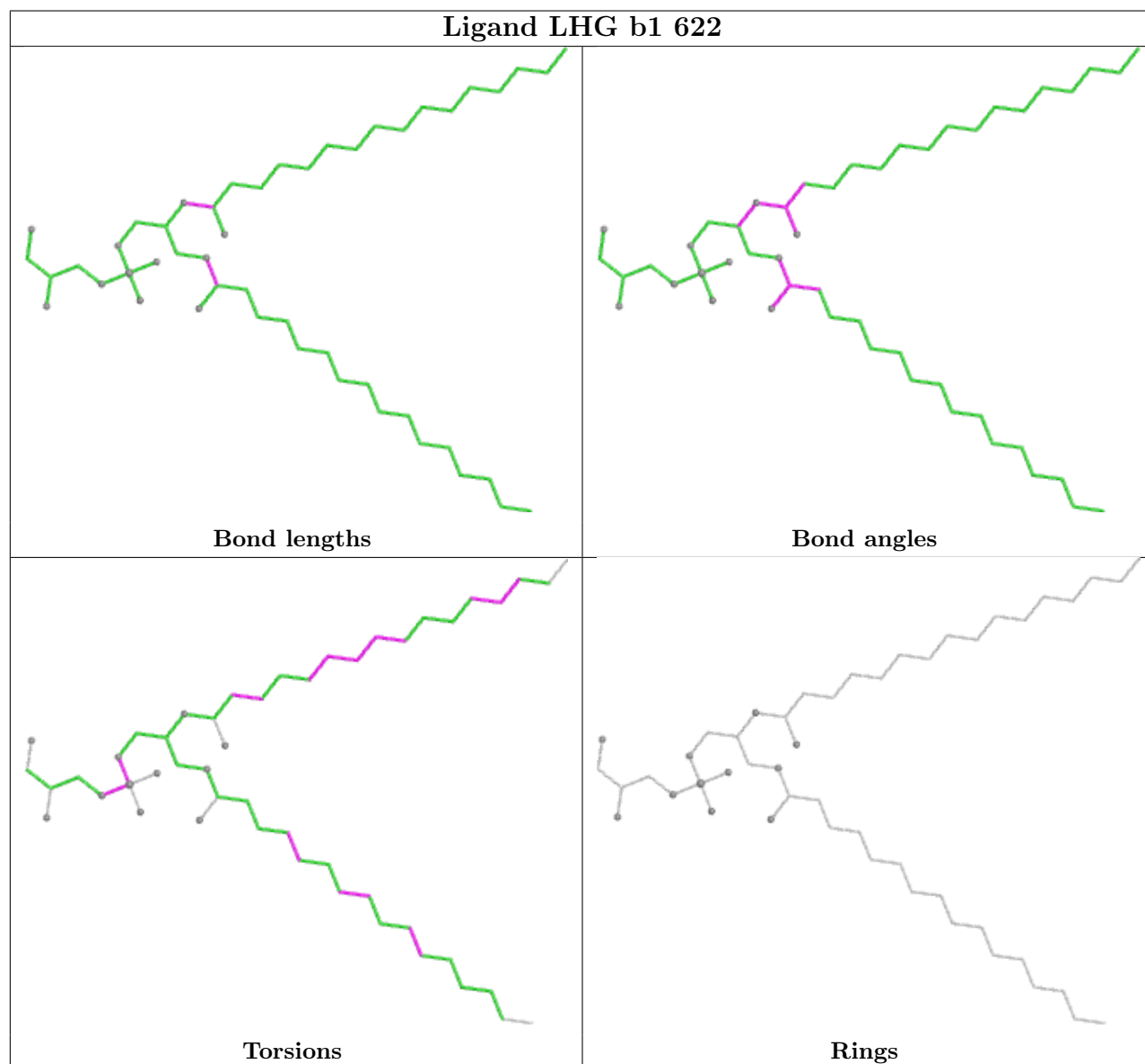
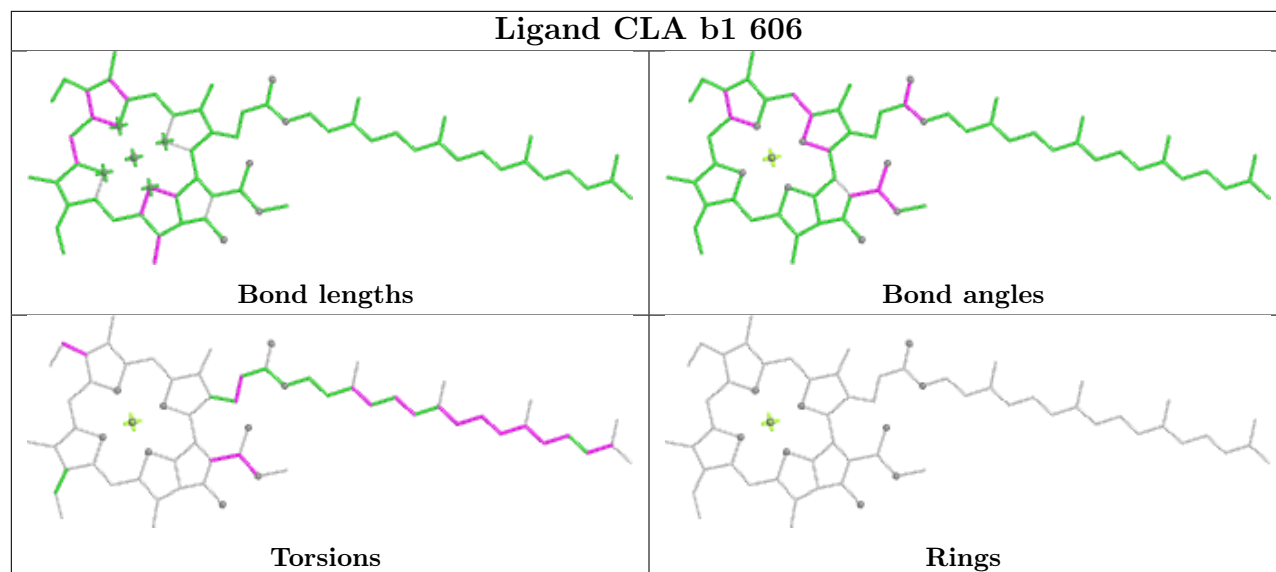


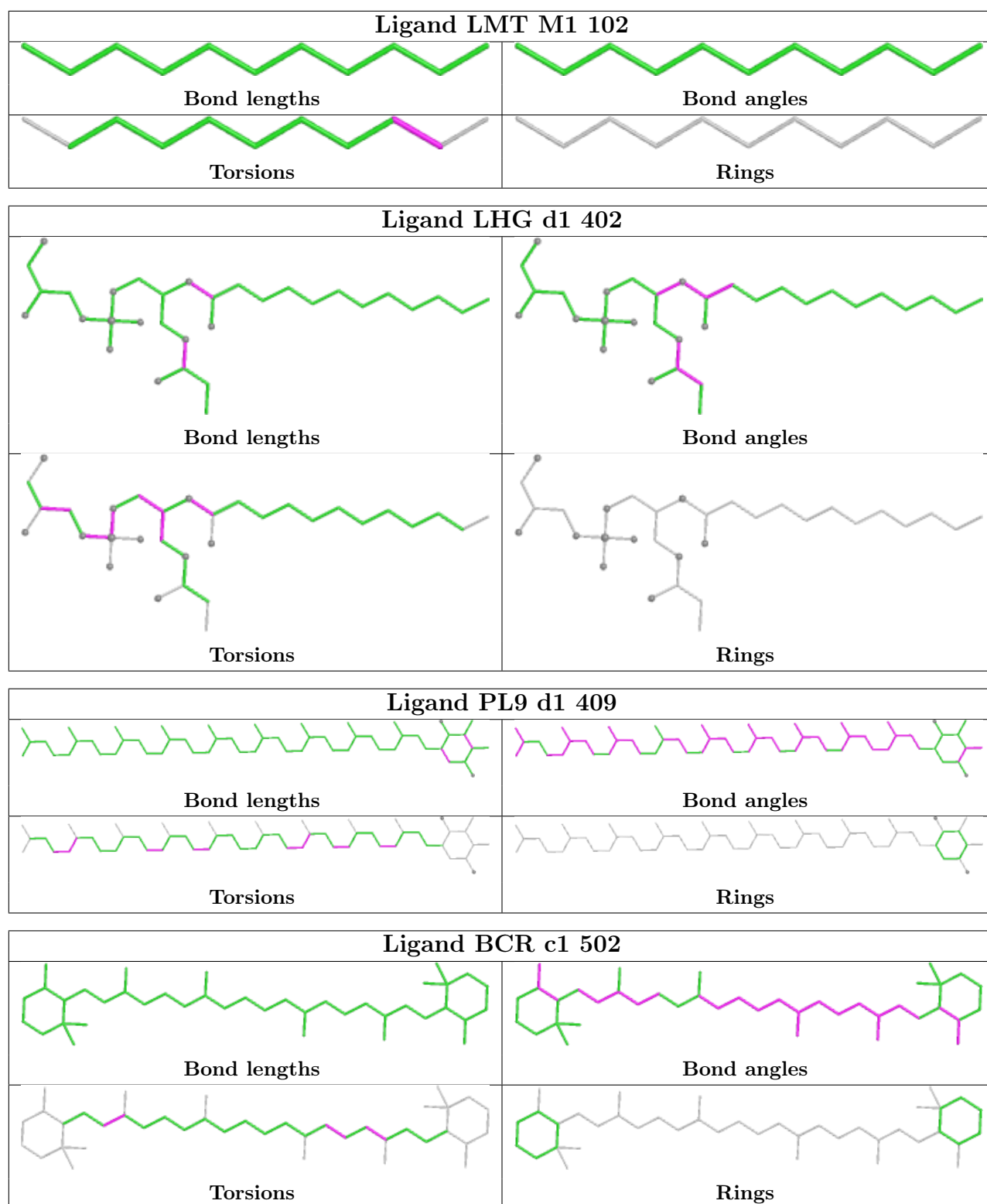


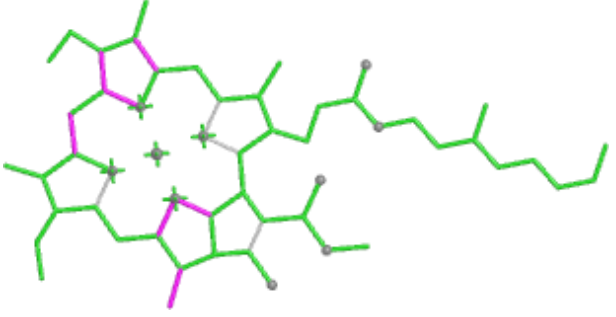
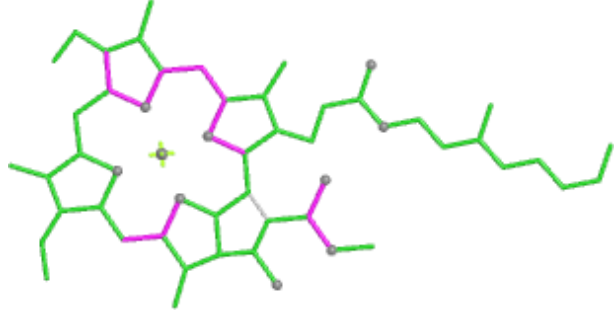
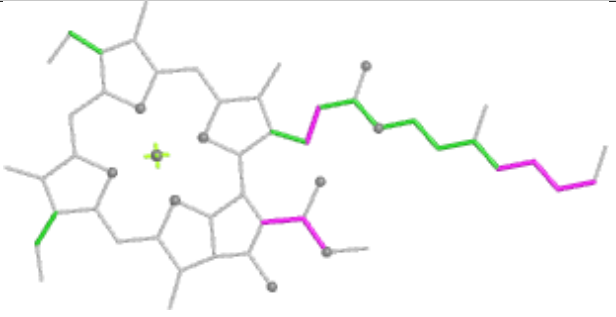
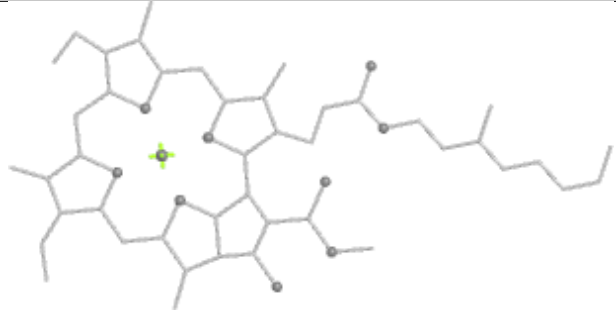
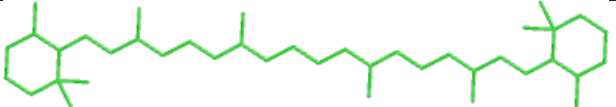
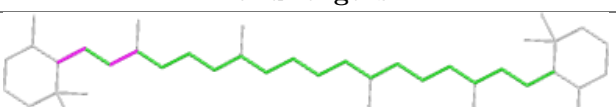
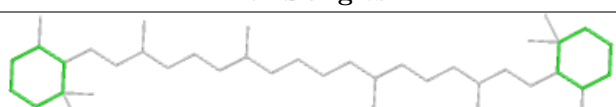
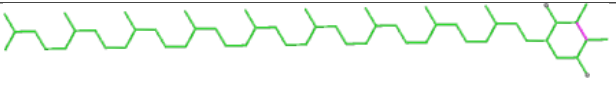
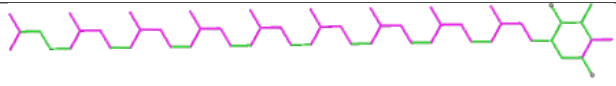
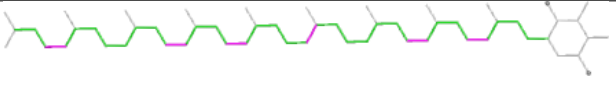
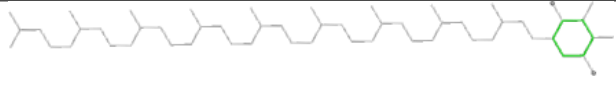


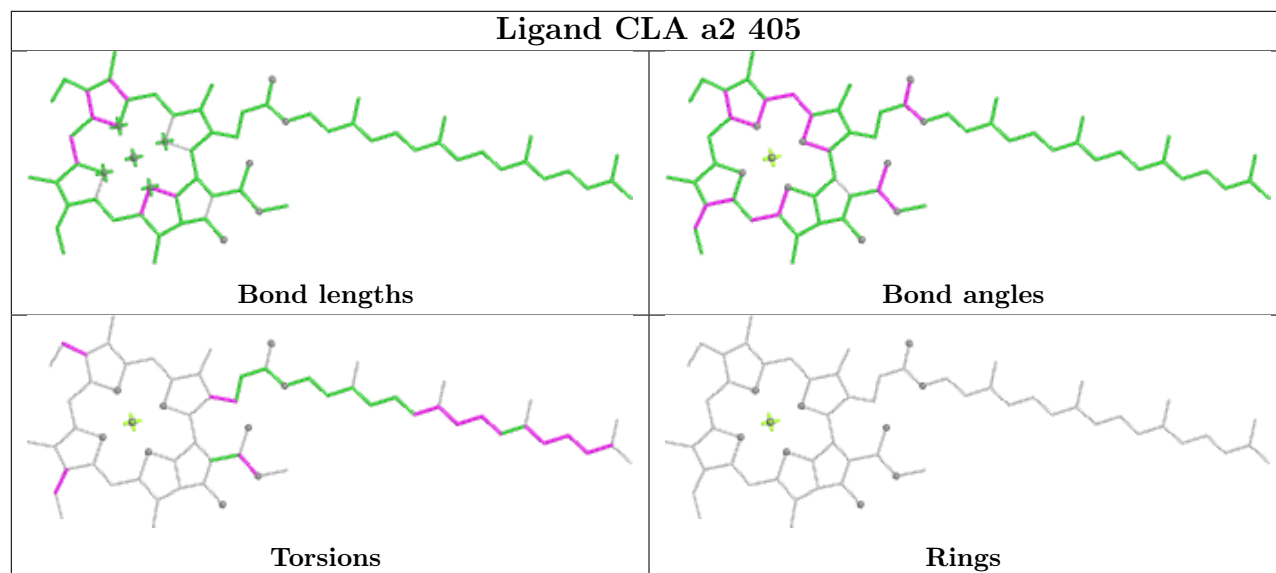
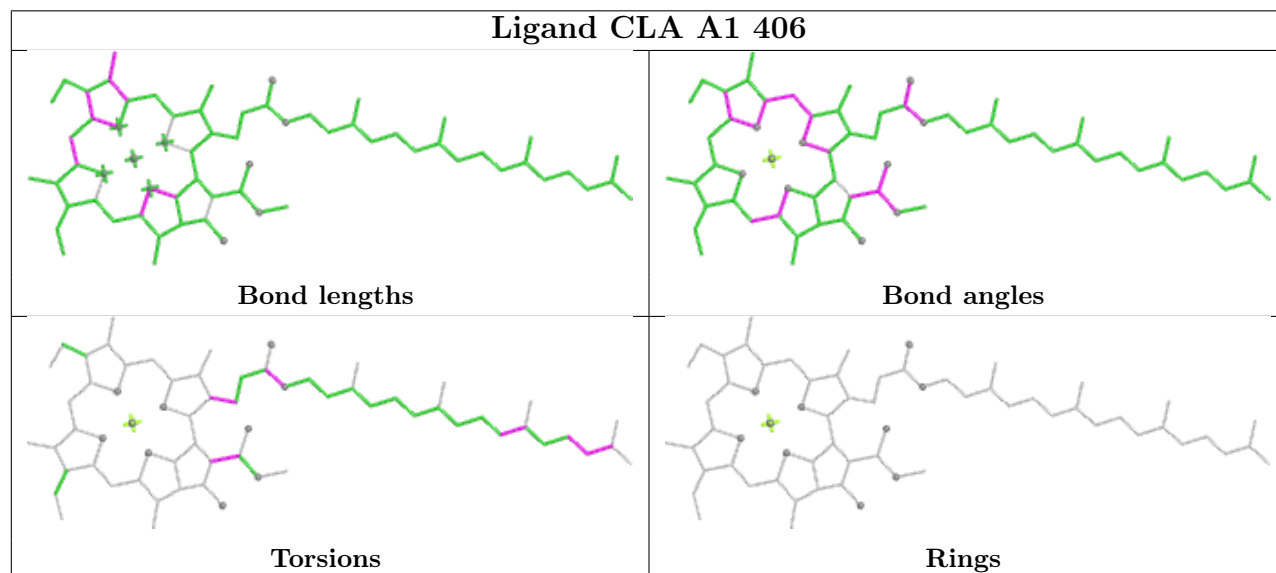
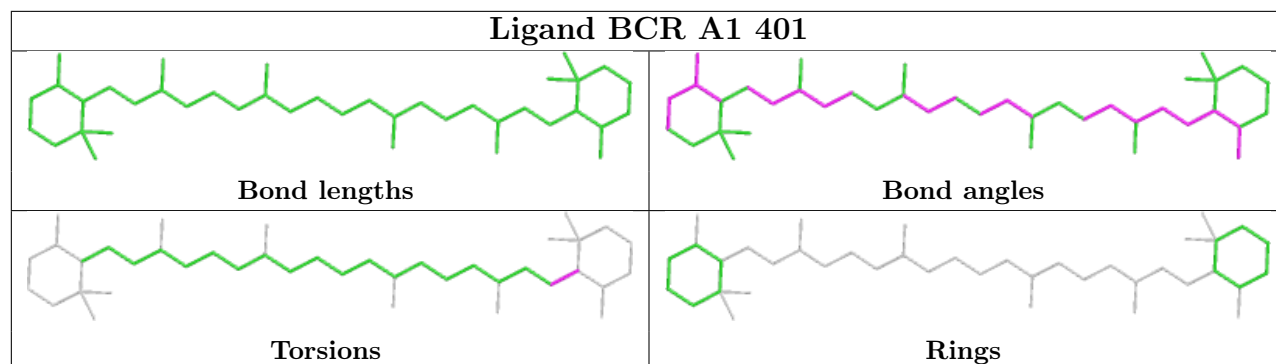


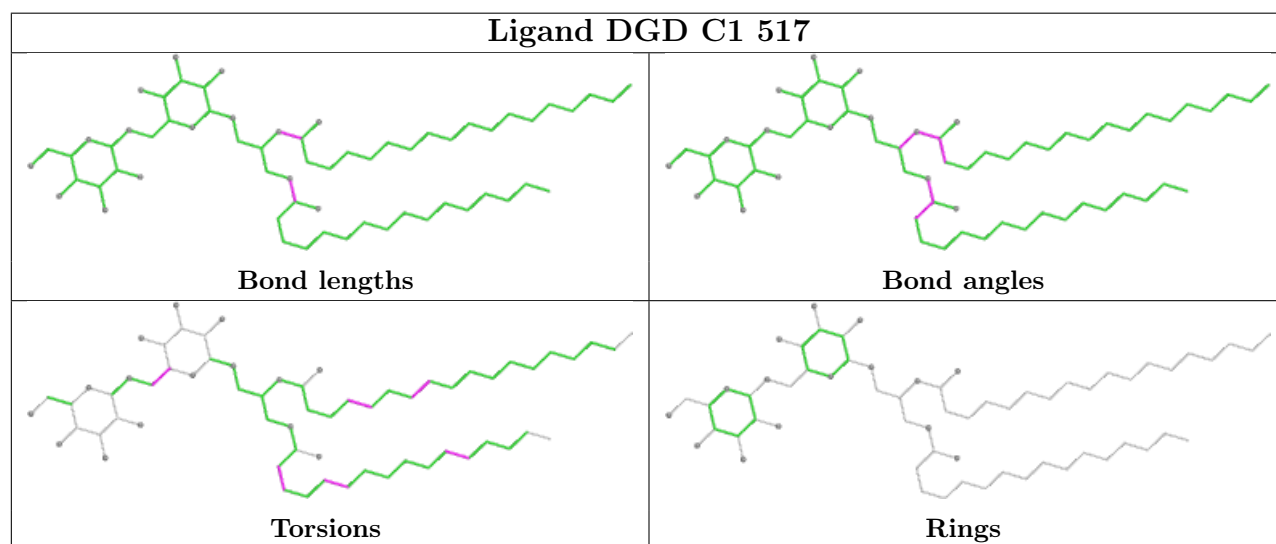
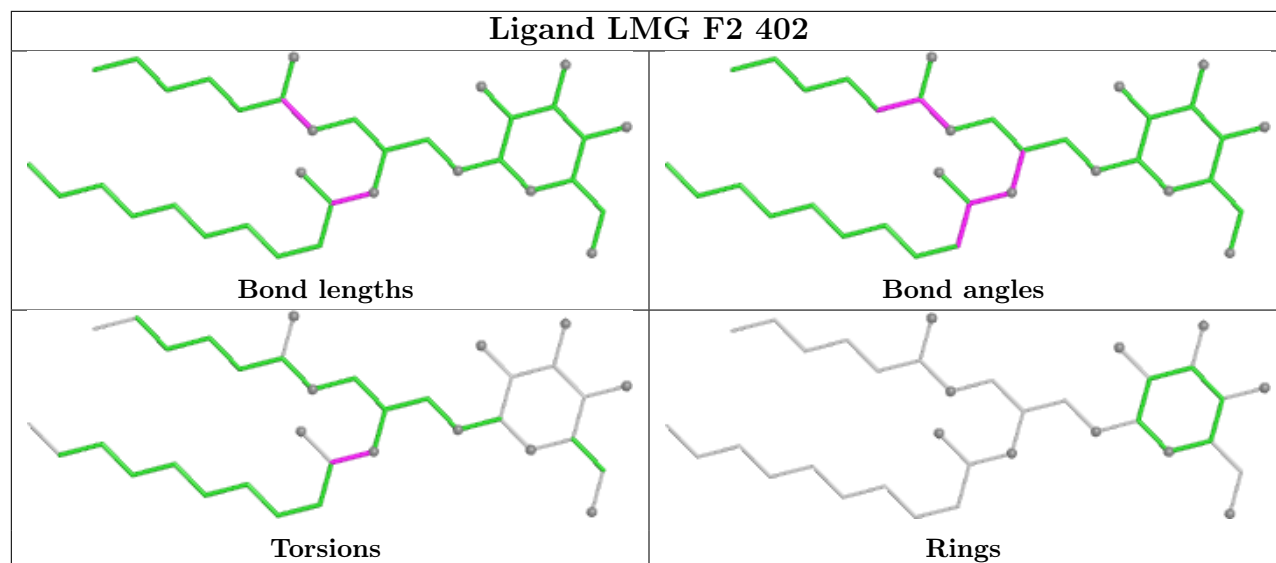


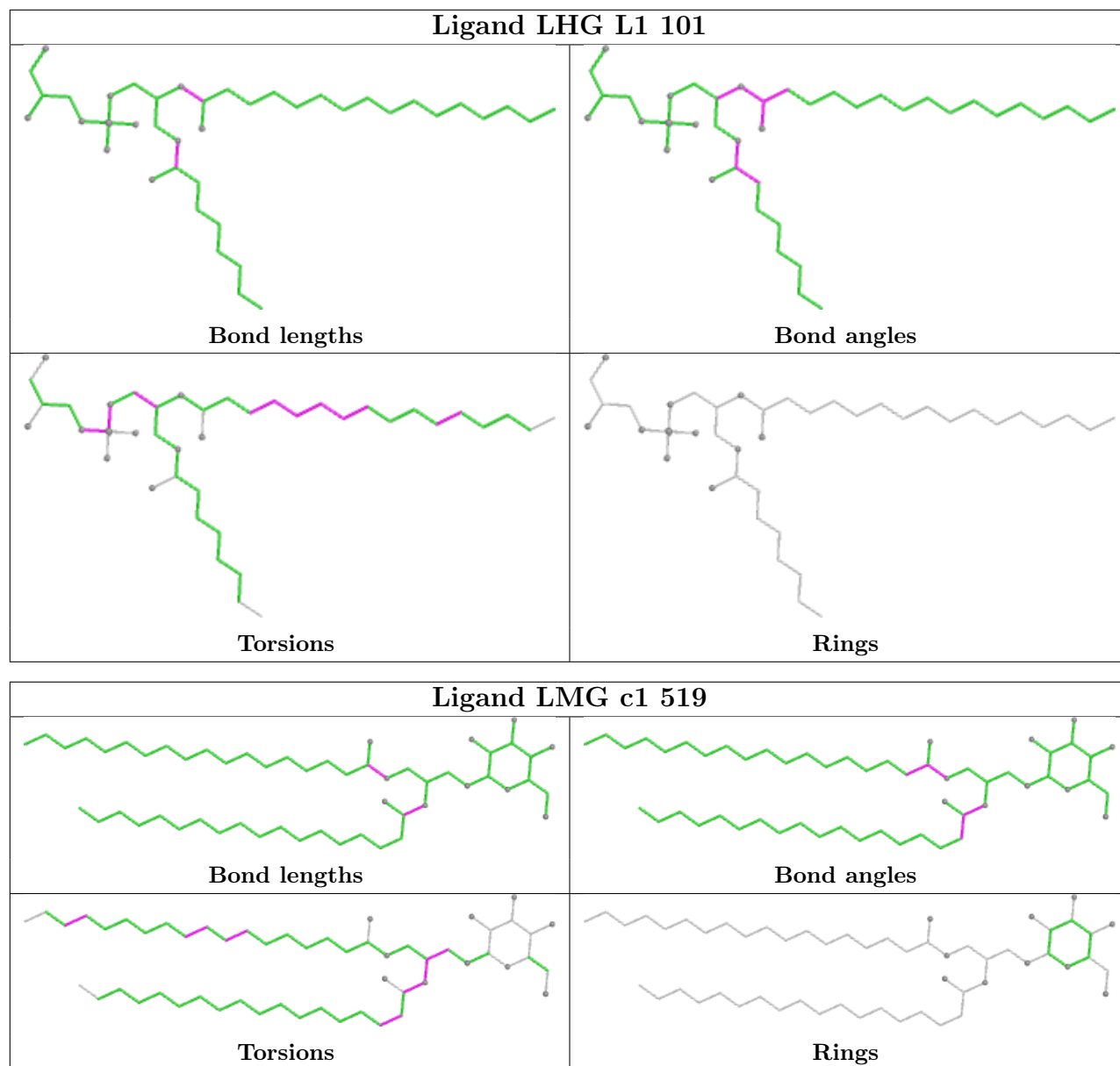




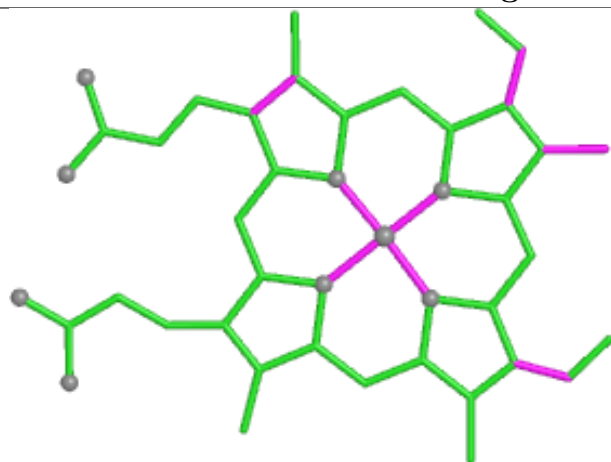
Ligand CLA c2 510	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR C1 501	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PL9 D2 408	
 Bond lengths	 Bond angles
 Torsions	 Rings



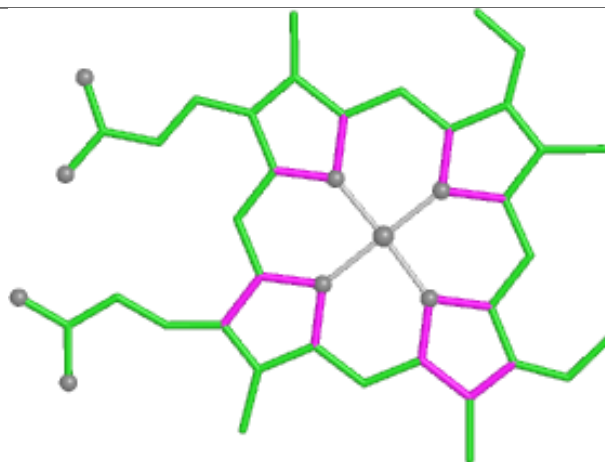




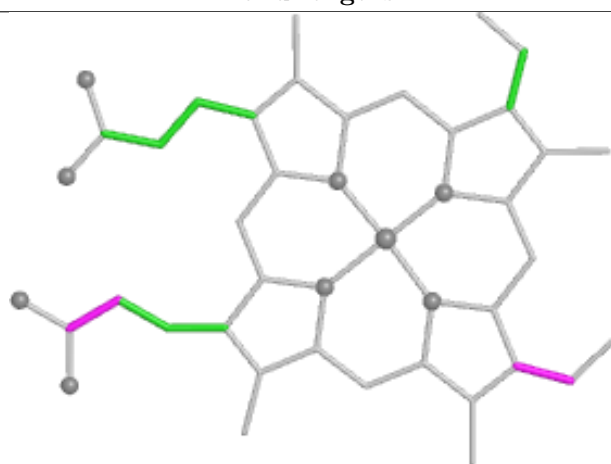
Ligand HEM E1 101



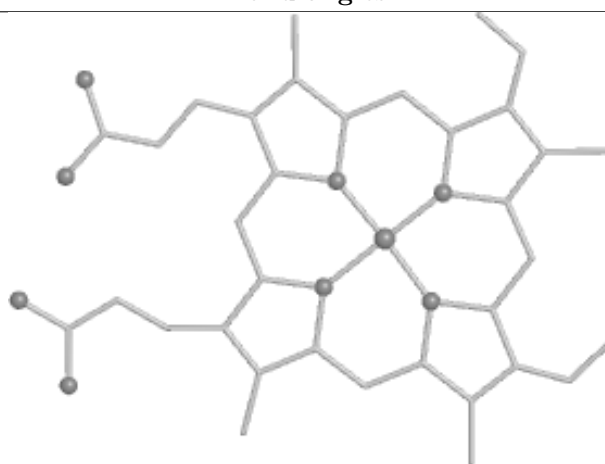
Bond lengths



Bond angles

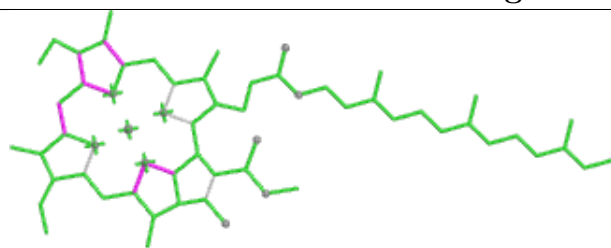


Torsions

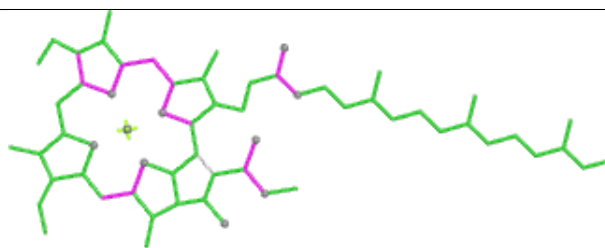


Rings

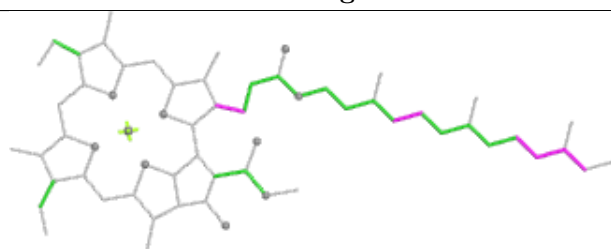
Ligand CLA A2 403



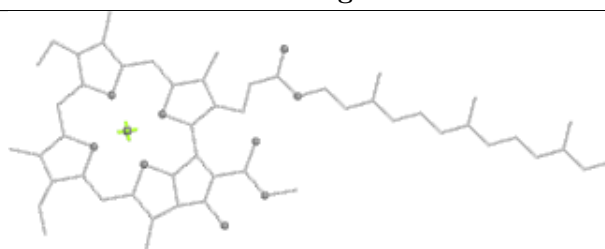
Bond lengths



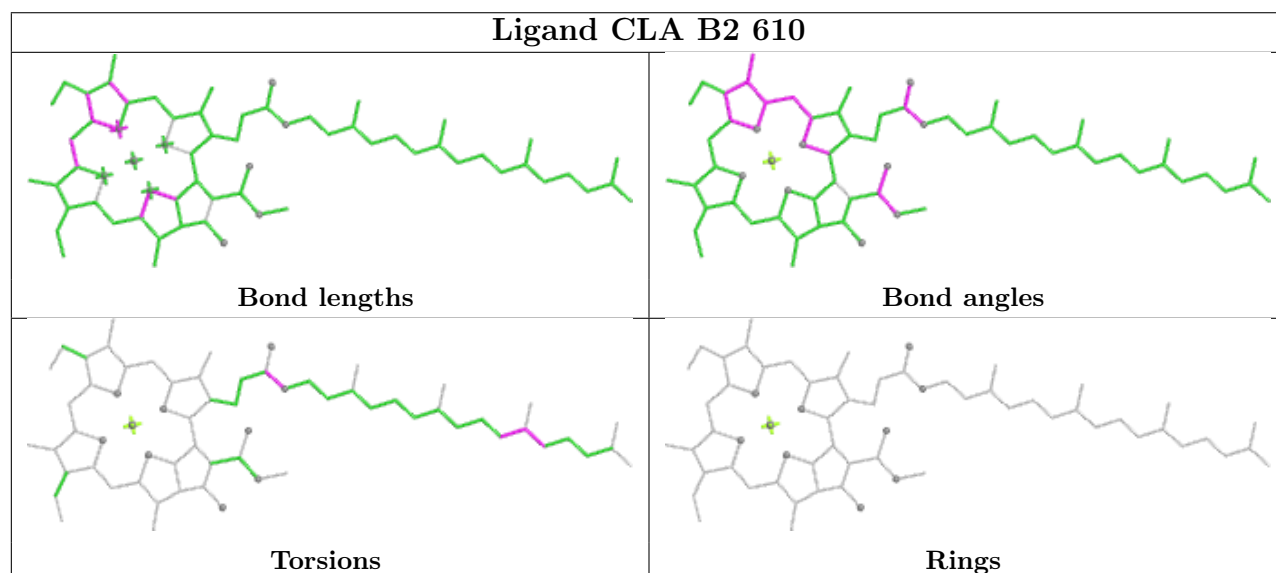
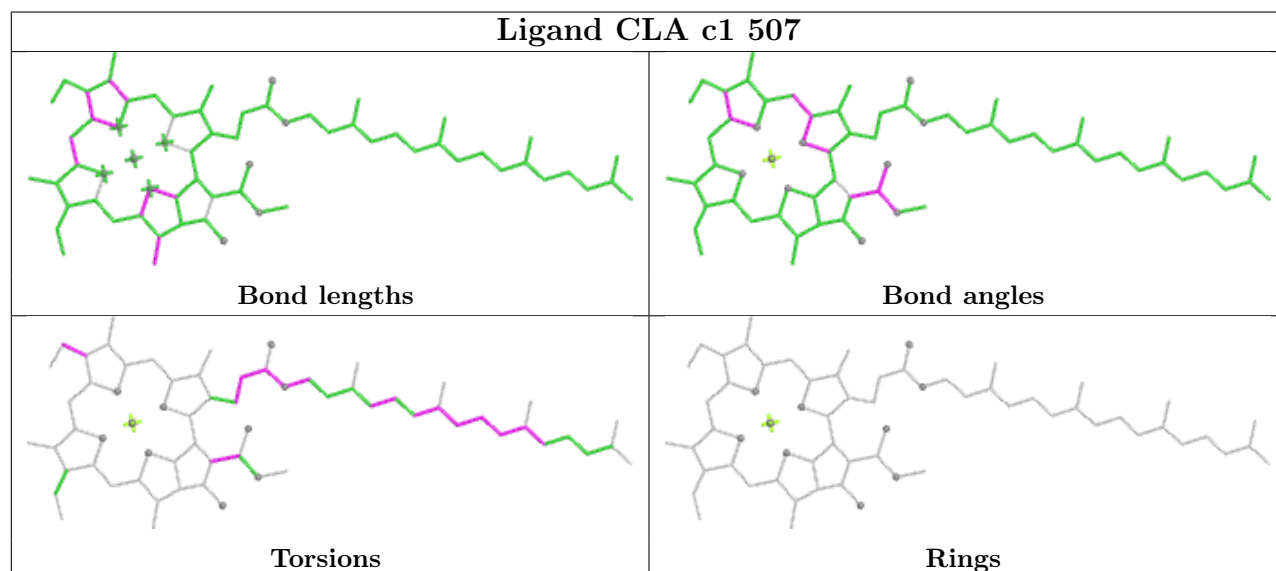
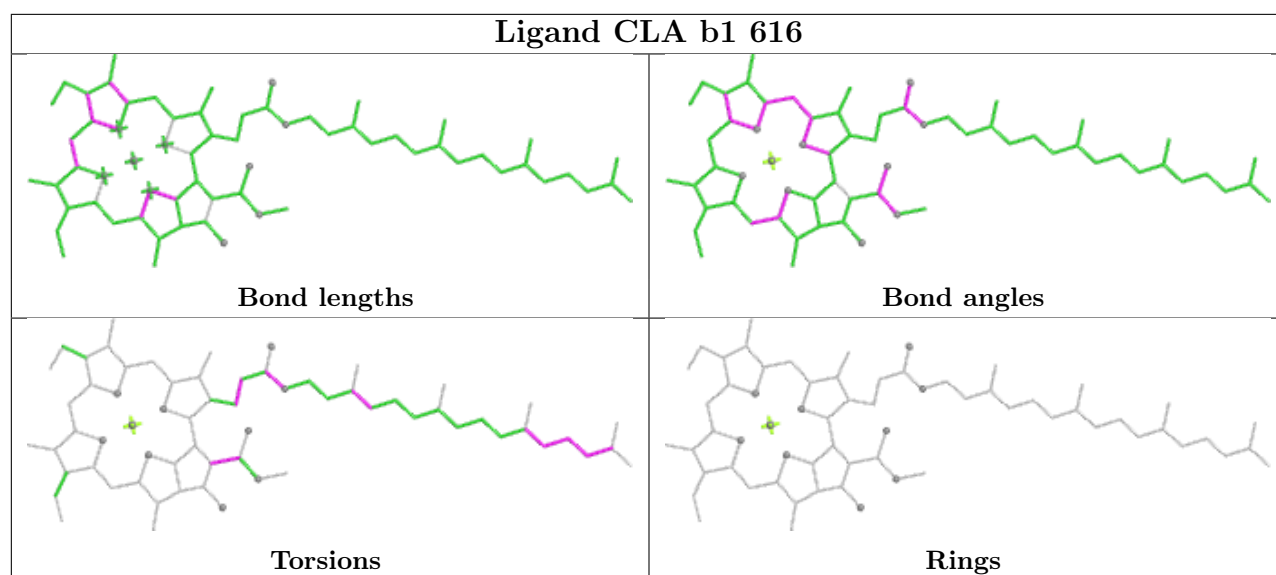
Bond angles

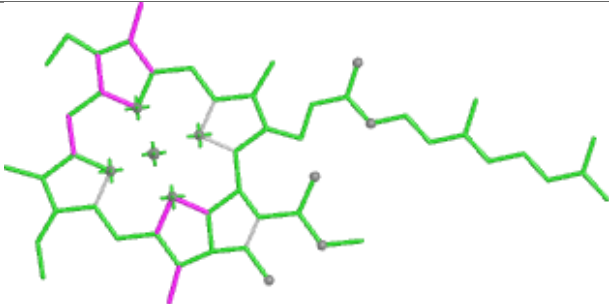
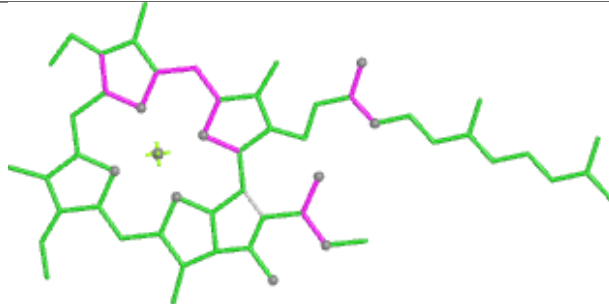
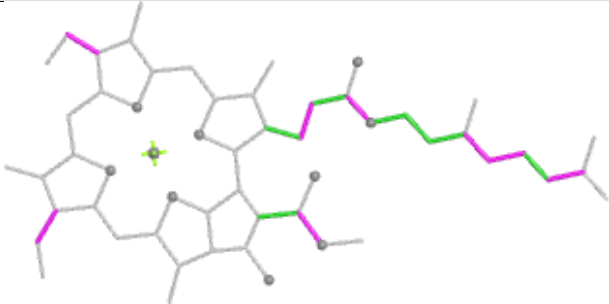
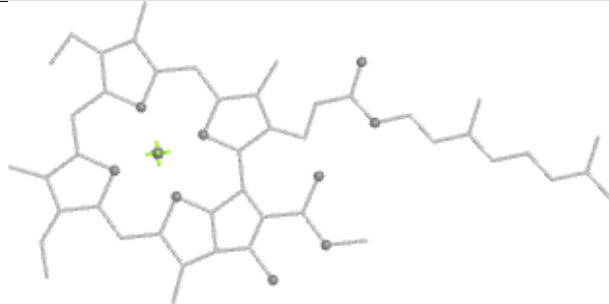


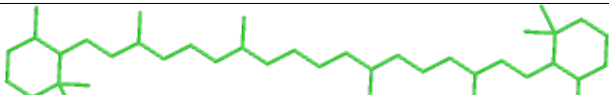
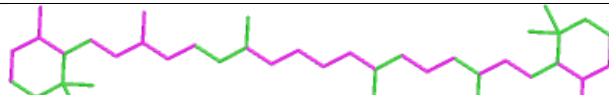
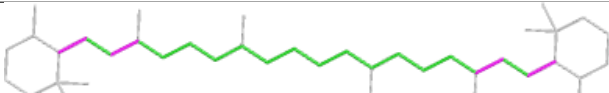
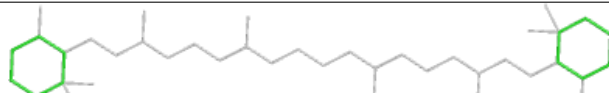
Torsions

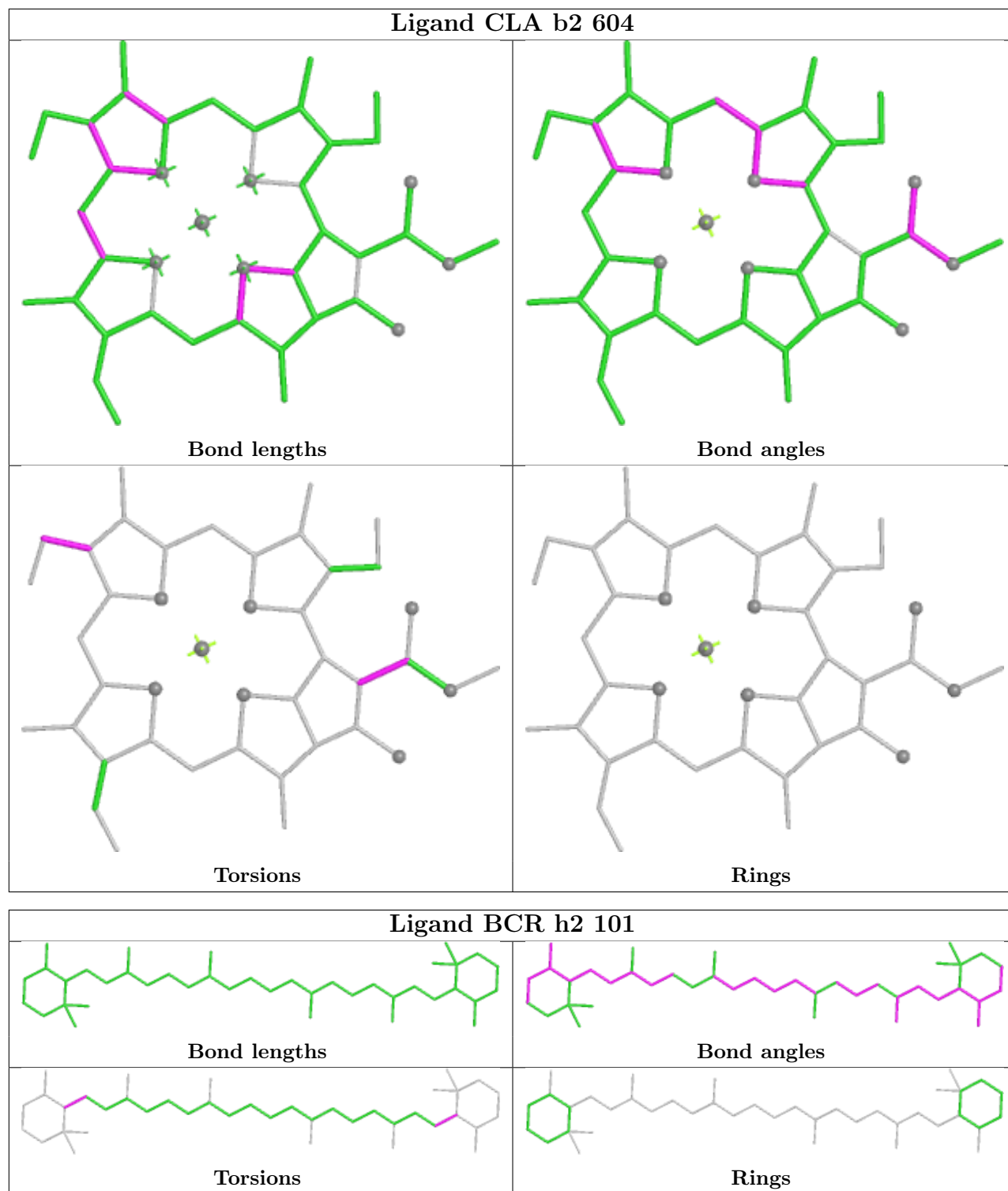


Rings

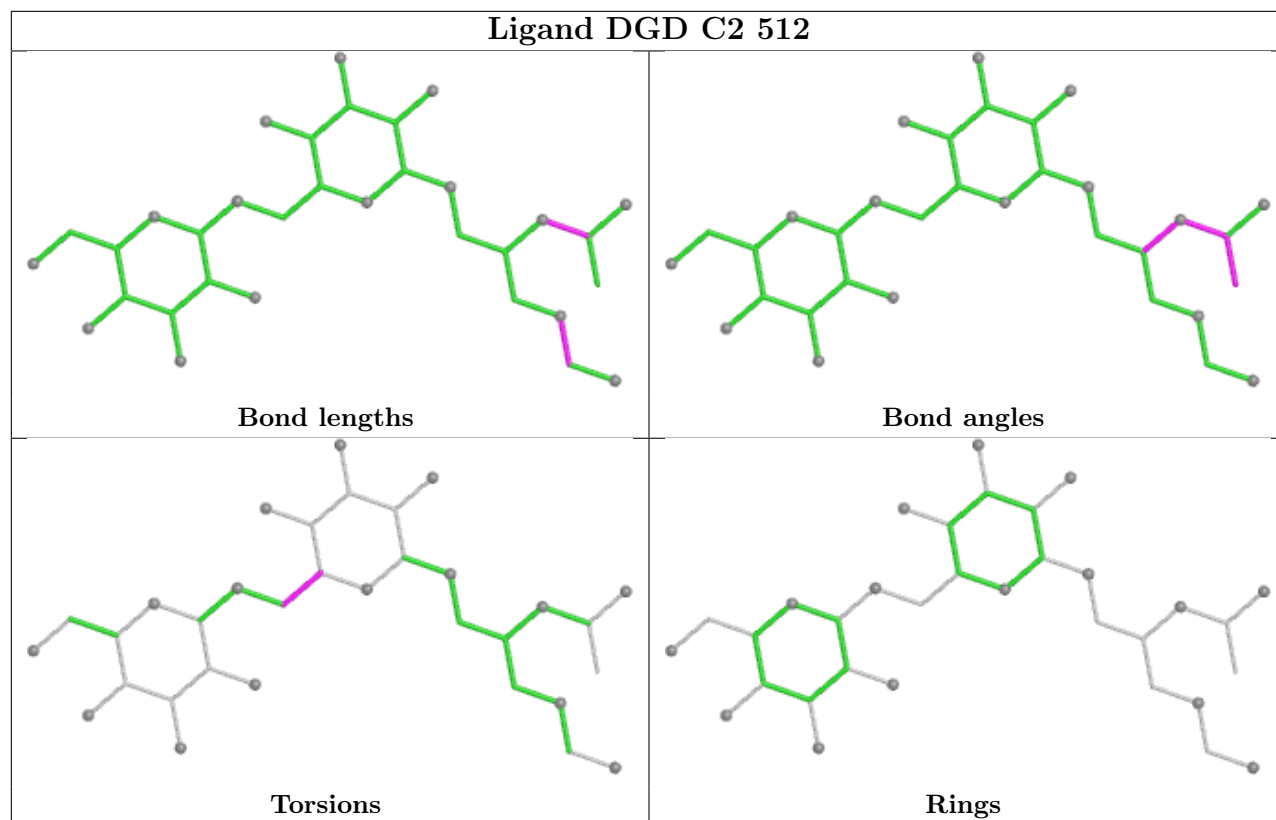


Ligand CLA K2 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

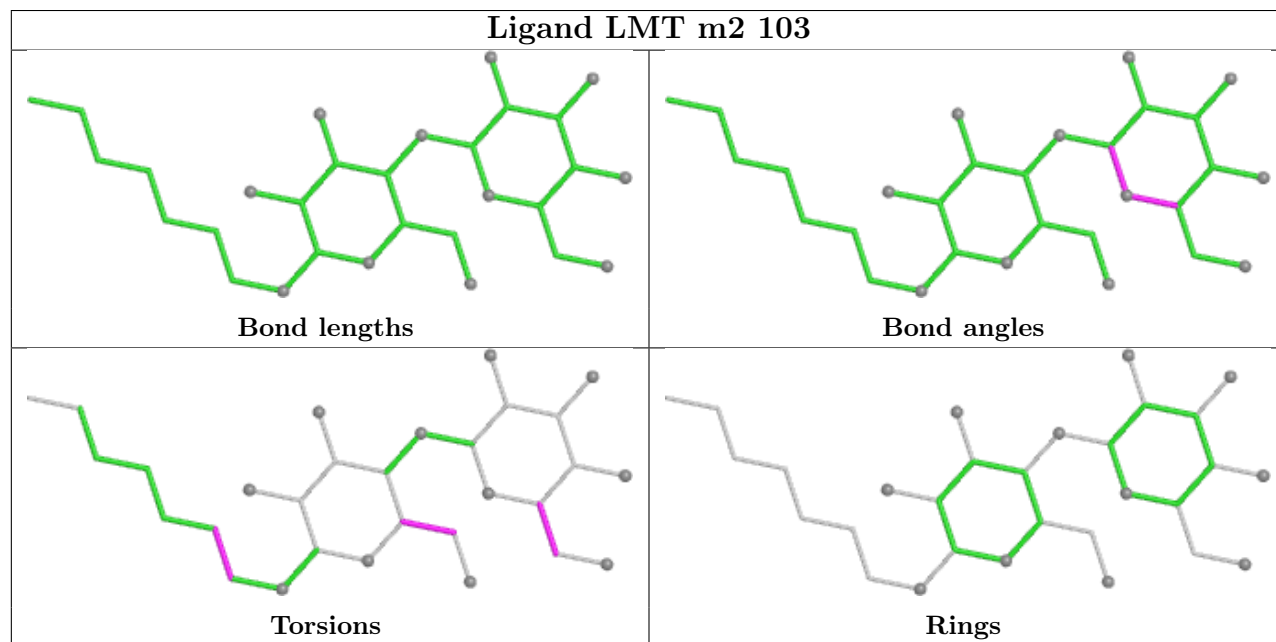
Ligand BCR D1 401	
	
Bond lengths	Bond angles
	
Torsions	Rings

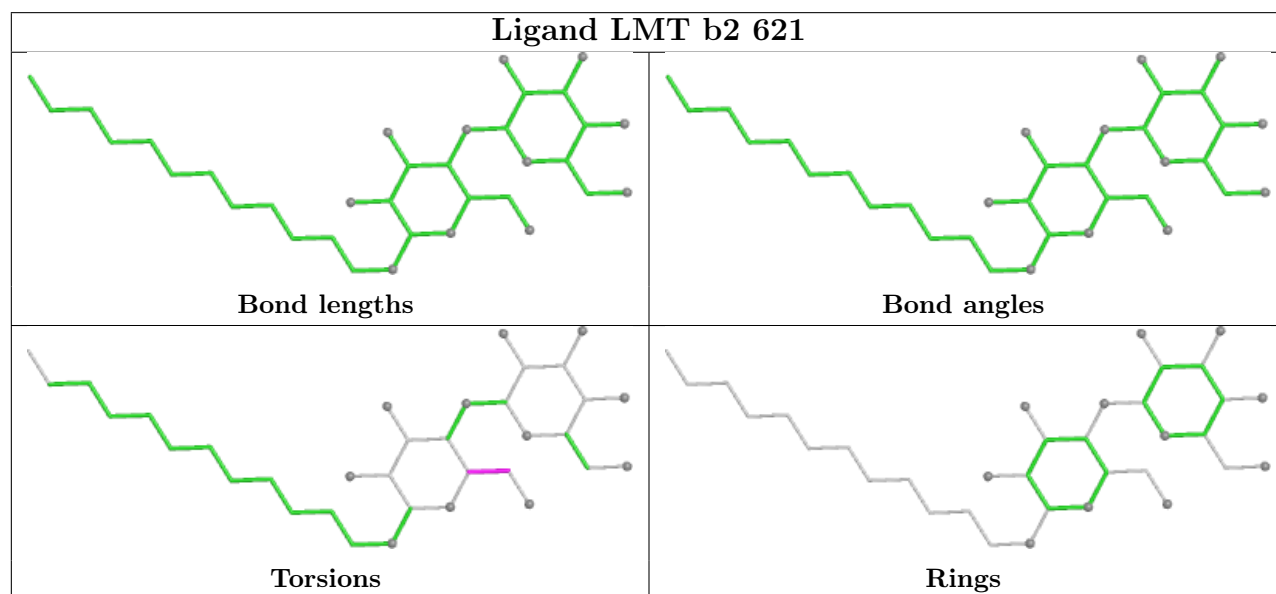
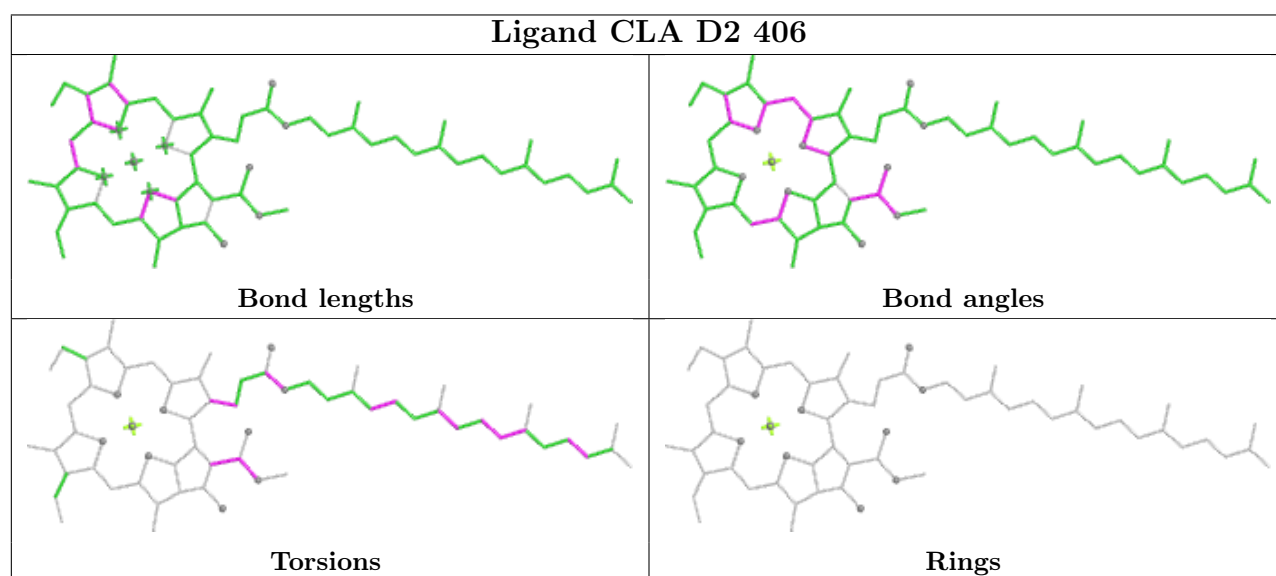
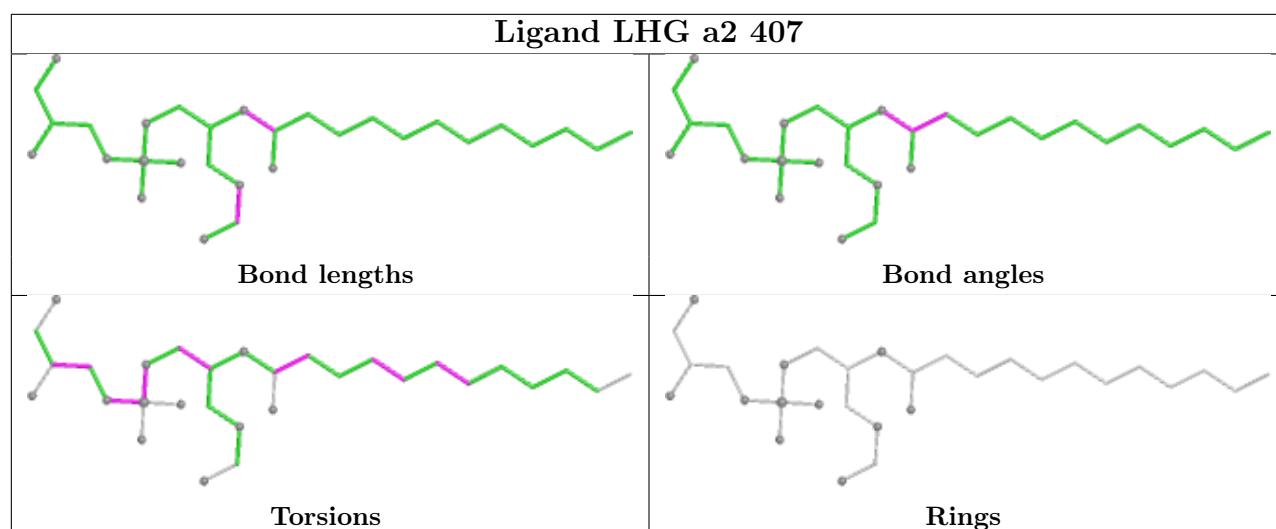


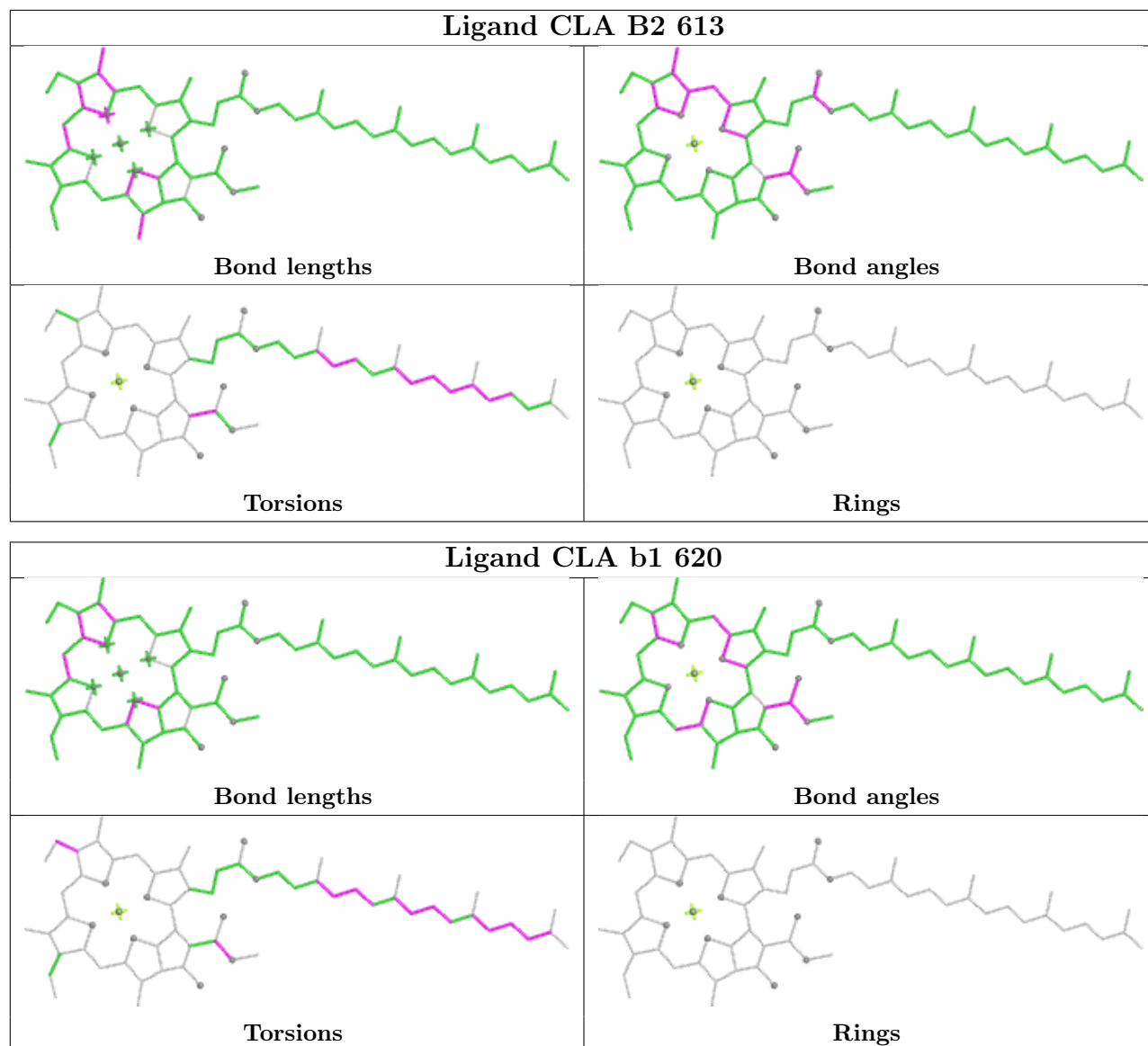
Ligand DGD C2 512



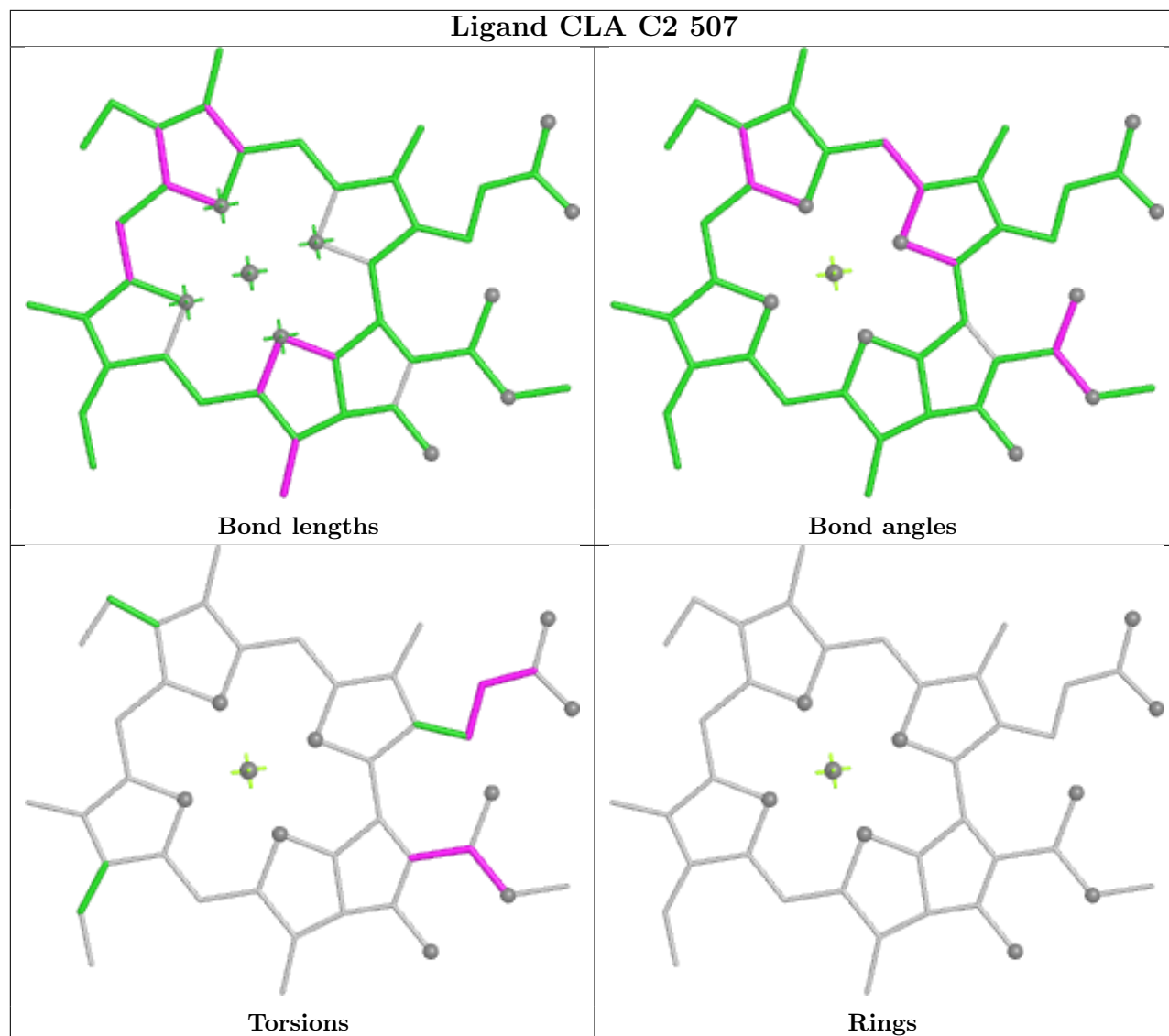
Ligand LMT m2 103



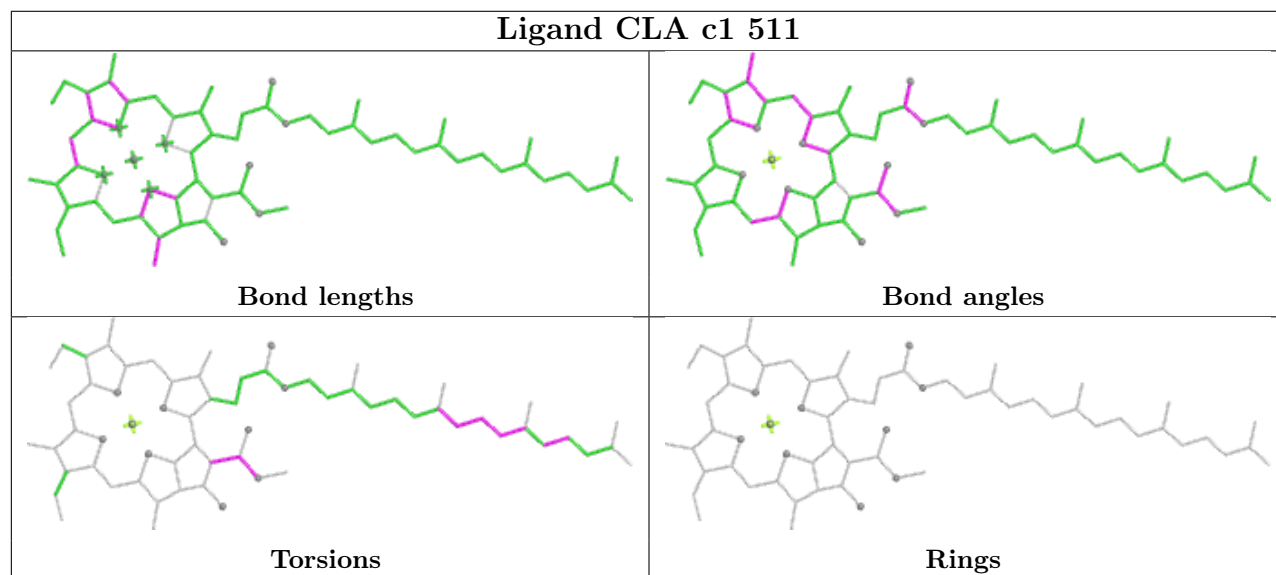


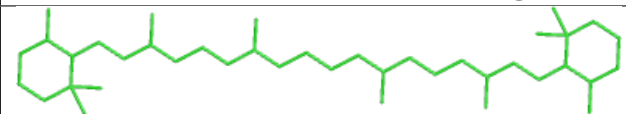
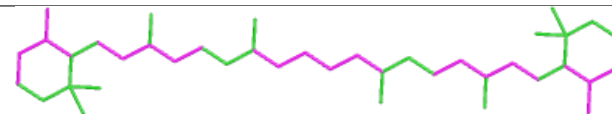
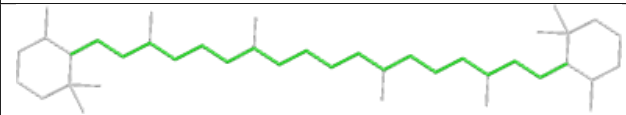
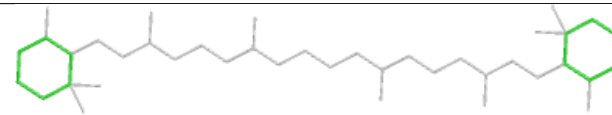


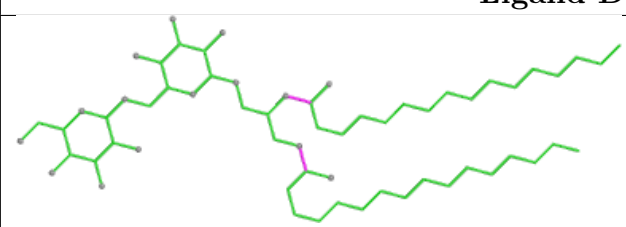
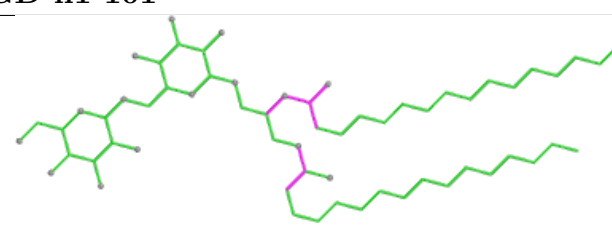
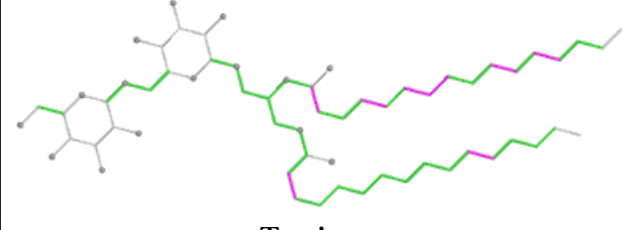
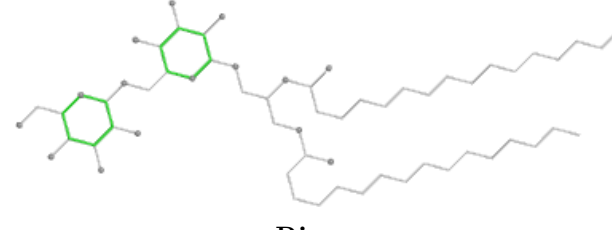
Ligand CLA C2 507

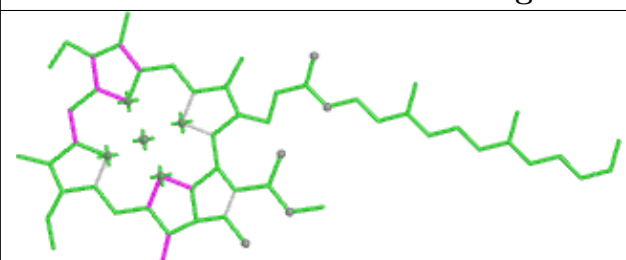
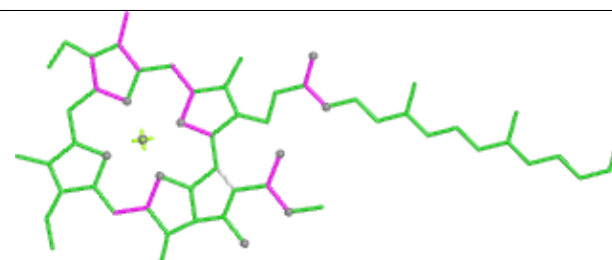
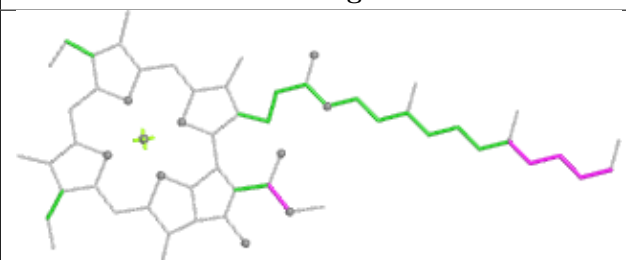
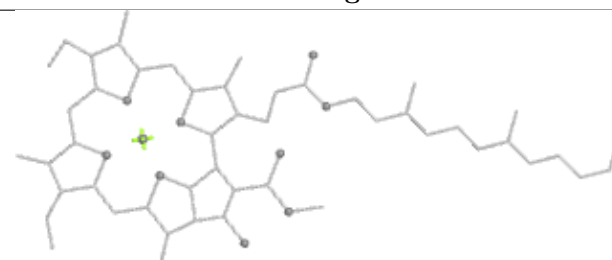


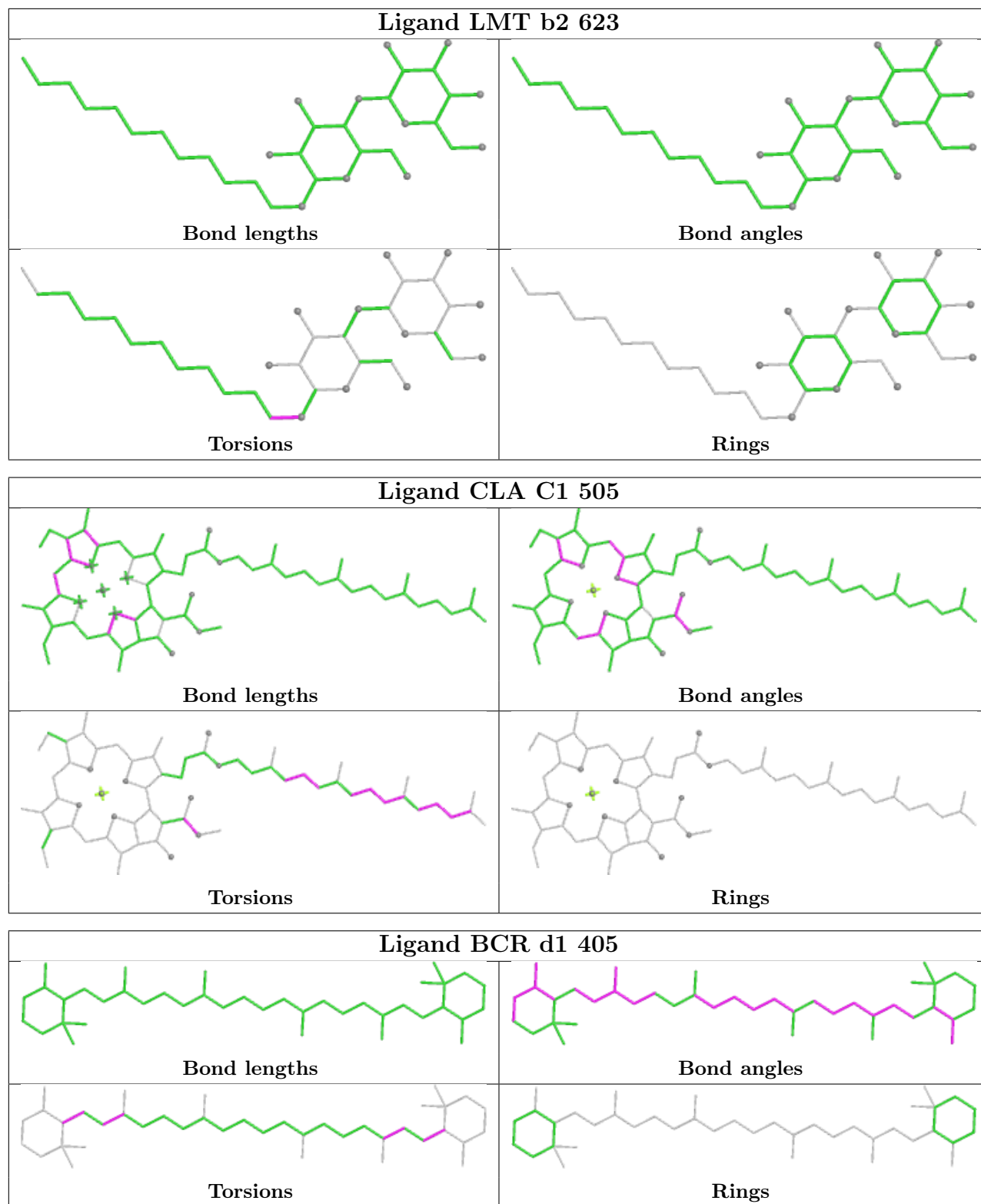
Ligand CLA c1 511



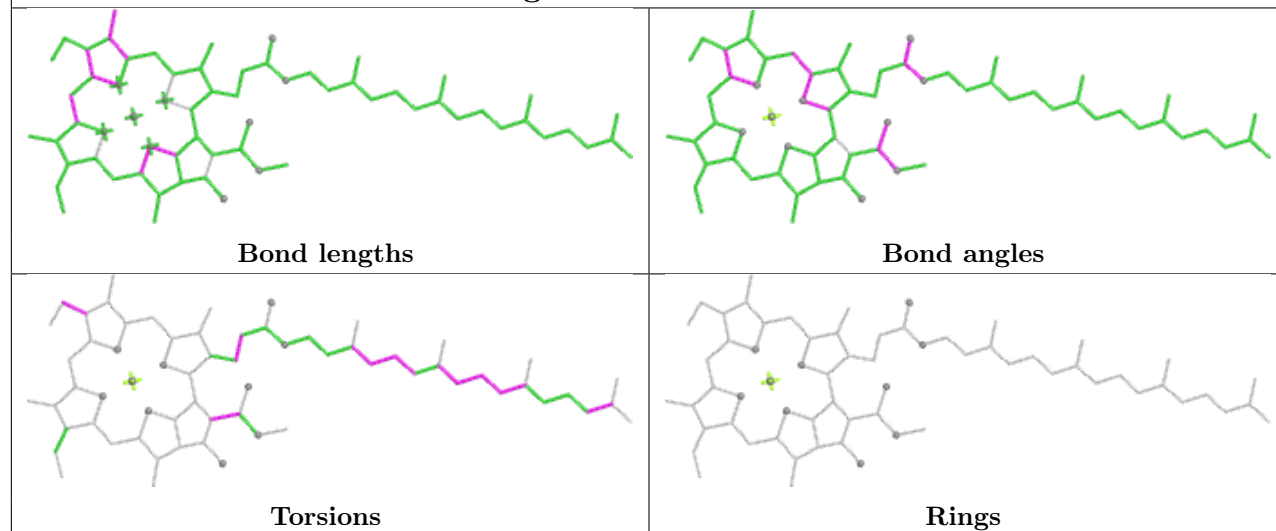
Ligand BCR C2 502	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand DGD h1 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

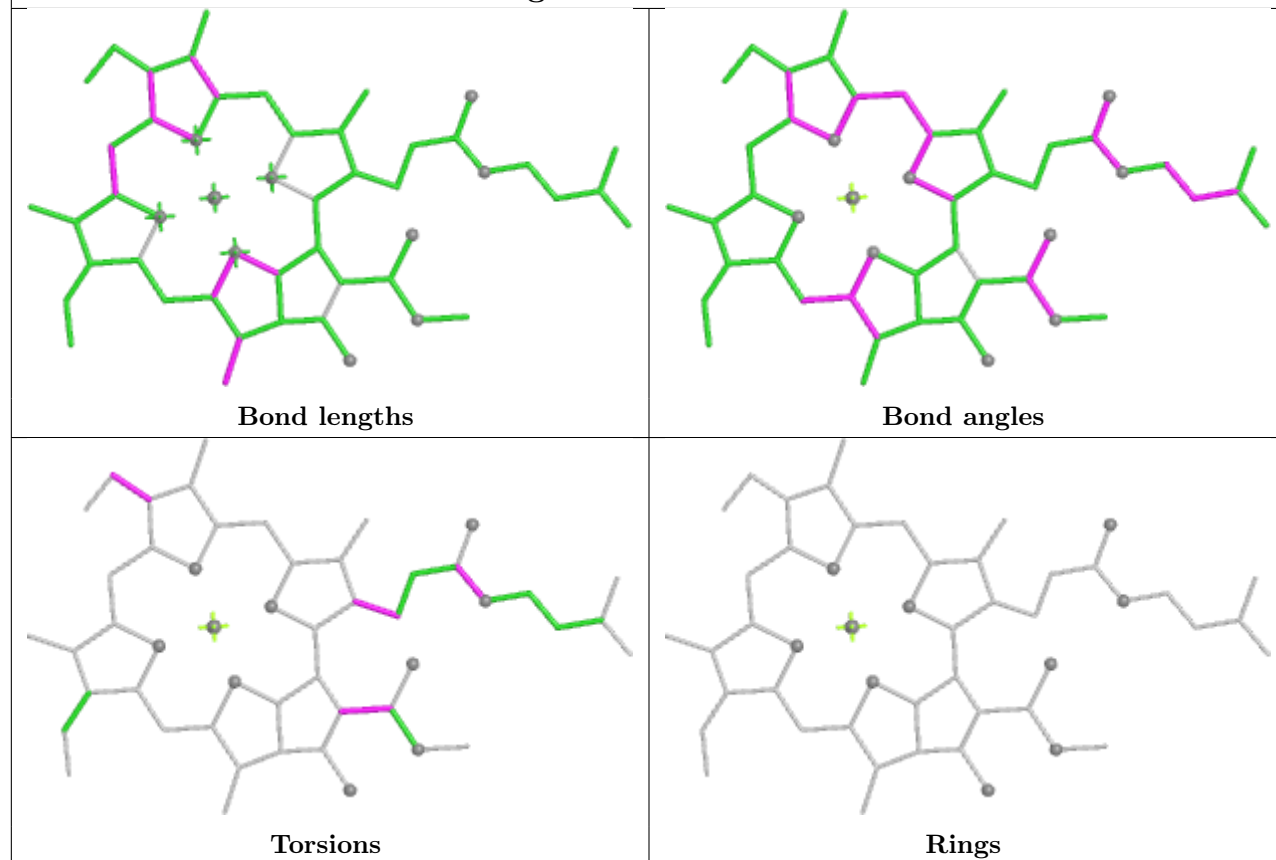
Ligand CLA b1 615	
	
Bond lengths	Bond angles
	
Torsions	Rings

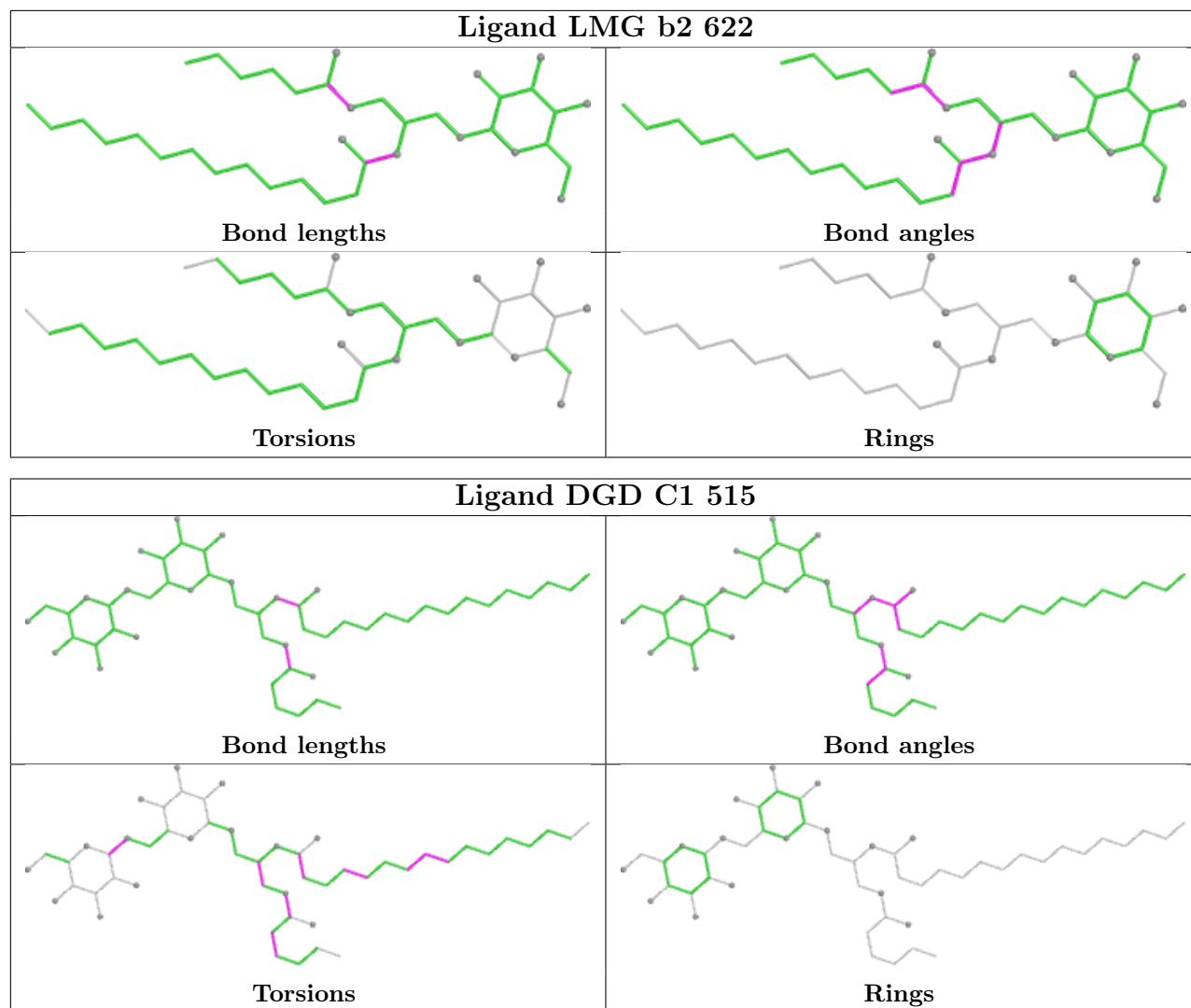


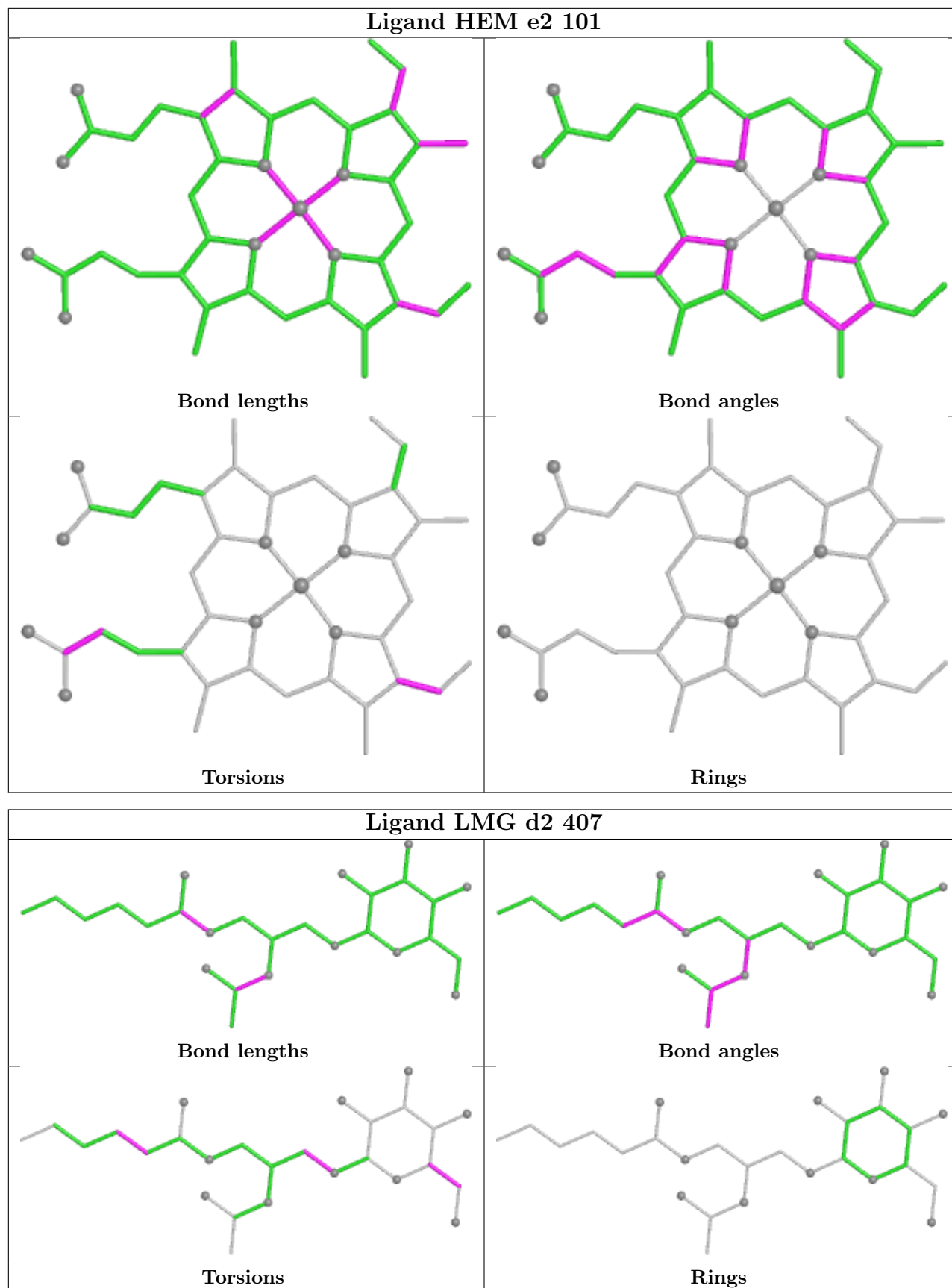
Ligand CLA C2 509



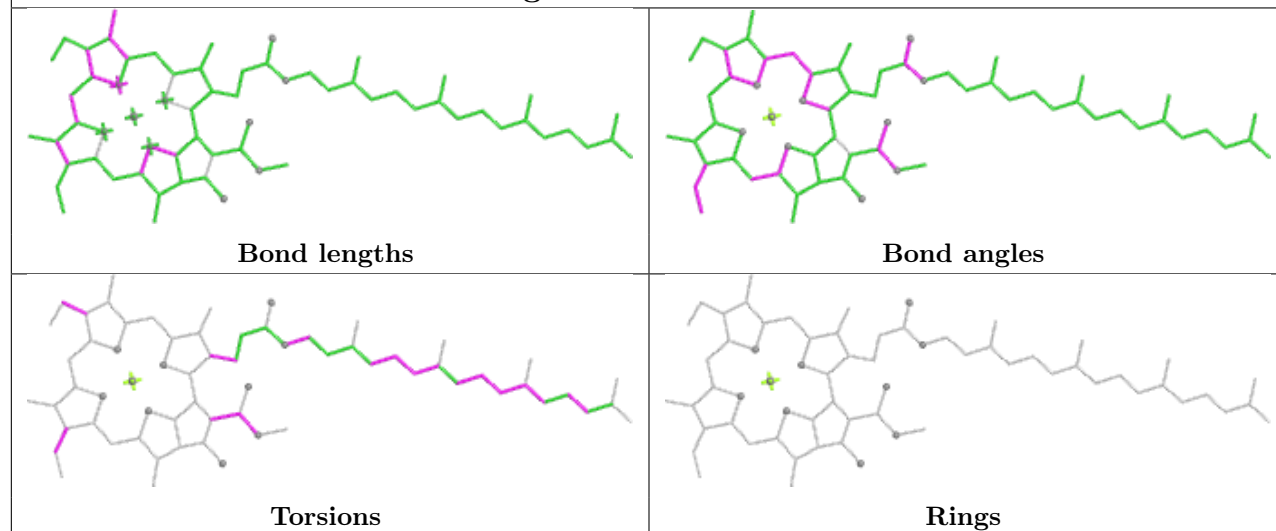
Ligand CLA a2 413



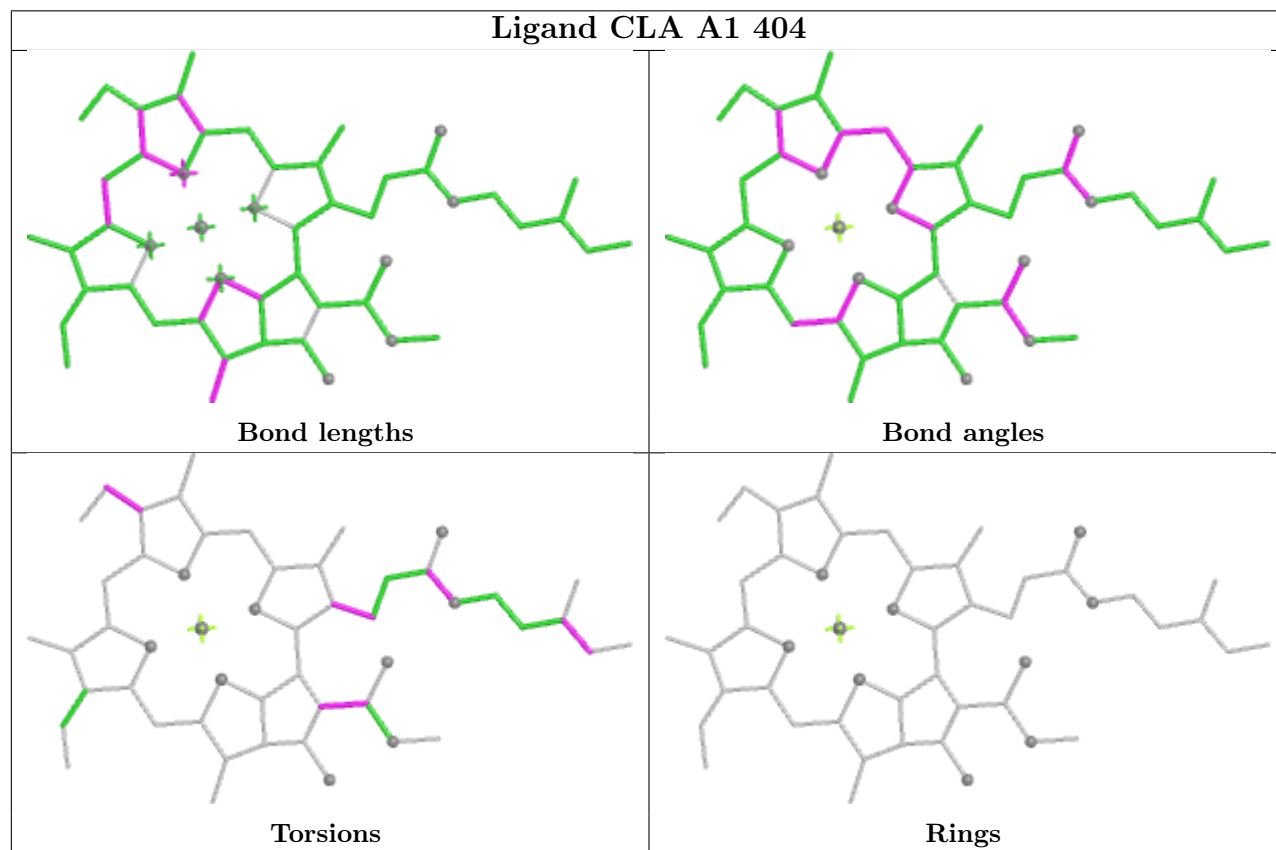


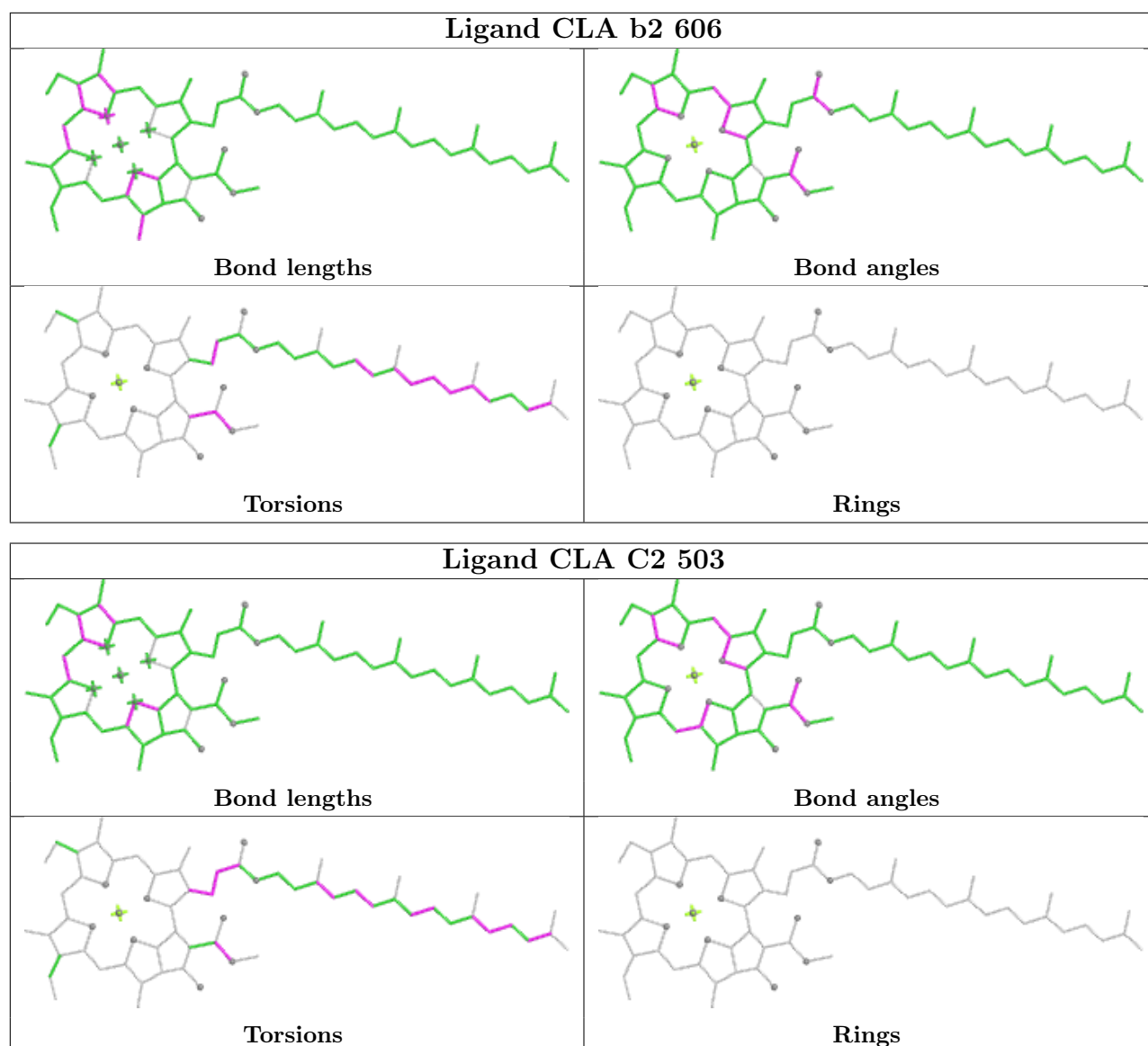


Ligand CLA C1 507



Ligand CLA A1 404





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A1	344/344 (100%)	-0.17	3 (0%) 81 76	31, 48, 79, 104	0
1	A2	332/344 (96%)	0.34	8 (2%) 59 52	48, 75, 91, 112	1 (0%)
1	a1	334/344 (97%)	-0.20	2 (0%) 85 81	36, 48, 68, 105	0
1	a2	334/344 (97%)	-0.21	1 (0%) 90 88	34, 50, 83, 107	0
2	B1	483/509 (94%)	0.11	6 (1%) 76 70	40, 63, 93, 108	0
2	B2	503/509 (98%)	0.14	8 (1%) 70 63	46, 65, 93, 112	0
2	b1	503/509 (98%)	-0.11	1 (0%) 91 89	36, 53, 80, 99	1 (0%)
2	b2	481/509 (94%)	0.25	14 (2%) 53 46	43, 70, 99, 115	0
3	C1	449/460 (97%)	-0.04	8 (1%) 67 60	33, 59, 78, 93	0
3	C2	444/460 (96%)	0.85	43 (9%) 13 10	73, 97, 117, 128	0
3	c1	449/460 (97%)	0.14	4 (0%) 81 76	41, 62, 84, 101	2 (0%)
3	c2	448/460 (97%)	0.13	7 (1%) 70 63	39, 70, 93, 110	0
4	D1	337/351 (96%)	-0.14	2 (0%) 85 81	36, 56, 88, 94	0
4	D2	340/351 (96%)	0.24	6 (1%) 67 60	51, 69, 85, 96	0
4	d1	339/351 (96%)	-0.30	2 (0%) 85 81	34, 45, 65, 94	0
4	d2	340/351 (96%)	-0.11	2 (0%) 85 81	36, 56, 88, 118	0
5	E1	61/84 (72%)	0.56	7 (11%) 9 7	64, 87, 141, 158	0
5	E2	63/84 (75%)	1.11	11 (17%) 4 3	77, 98, 131, 144	0
5	e1	57/84 (67%)	0.26	2 (3%) 47 40	49, 65, 87, 91	0
5	e2	60/84 (71%)	0.49	4 (6%) 24 19	59, 80, 144, 159	0
6	F1	28/43 (65%)	0.28	1 (3%) 46 39	62, 75, 123, 131	0
6	F2	31/43 (72%)	1.19	7 (22%) 2 1	81, 92, 144, 146	0
6	f1	29/43 (67%)	0.08	1 (3%) 48 41	50, 60, 95, 108	0
6	f2	29/43 (67%)	0.50	2 (6%) 23 18	64, 73, 128, 149	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
7	H1	60/67 (89%)	0.46	2 (3%) 49 42	70, 84, 93, 101	0
7	H2	62/67 (92%)	0.36	0 100 100	63, 75, 92, 124	0
7	h1	62/67 (92%)	-0.10	0 100 100	47, 67, 78, 84	0
7	h2	62/67 (92%)	0.55	6 (9%) 13 10	72, 87, 98, 122	0
8	I1	34/38 (89%)	-0.06	0 100 100	53, 61, 70, 71	0
8	I2	35/38 (92%)	0.63	1 (2%) 53 46	82, 93, 105, 109	0
8	i1	34/38 (89%)	0.03	0 100 100	54, 61, 71, 76	0
8	i2	33/38 (86%)	0.15	0 100 100	60, 67, 75, 77	0
9	J1	32/39 (82%)	0.16	1 (3%) 51 44	51, 65, 89, 105	0
9	J2	35/39 (89%)	1.06	7 (20%) 3 2	75, 87, 125, 136	0
9	j1	32/39 (82%)	0.10	0 100 100	49, 63, 74, 81	0
9	j2	33/39 (84%)	0.23	1 (3%) 52 45	54, 70, 88, 110	0
10	K1	37/41 (90%)	0.15	1 (2%) 56 48	56, 66, 78, 79	0
10	K2	37/41 (90%)	1.06	6 (16%) 4 4	86, 96, 111, 117	0
10	k1	37/41 (90%)	0.23	0 100 100	56, 67, 81, 81	0
10	k2	37/41 (90%)	0.69	2 (5%) 31 26	67, 76, 89, 92	0
11	L1	37/38 (97%)	-0.26	0 100 100	39, 43, 67, 77	0
11	L2	37/38 (97%)	-0.03	0 100 100	49, 56, 61, 73	0
11	l1	37/38 (97%)	-0.16	0 100 100	36, 43, 63, 73	0
11	l2	37/38 (97%)	-0.15	0 100 100	43, 47, 73, 79	0
12	M1	40/108 (37%)	-0.11	0 100 100	32, 46, 62, 66	0
12	M2	40/108 (37%)	-0.10	0 100 100	45, 54, 67, 69	0
12	m1	40/108 (37%)	-0.05	1 (2%) 58 50	34, 44, 65, 67	0
12	m2	40/108 (37%)	-0.00	1 (2%) 58 50	44, 51, 65, 71	0
13	O1	240/329 (72%)	0.19	10 (4%) 40 34	38, 61, 96, 107	0
13	O2	205/329 (62%)	0.91	30 (14%) 6 5	54, 91, 119, 151	0
13	o1	238/329 (72%)	0.42	15 (6%) 26 21	38, 76, 121, 145	0
13	o2	245/329 (74%)	0.24	13 (5%) 32 26	41, 64, 103, 127	0
14	T1	30/32 (93%)	-0.24	1 (3%) 49 42	37, 44, 60, 68	0
14	T2	30/32 (93%)	0.10	1 (3%) 49 42	54, 63, 76, 82	0
14	t1	30/32 (93%)	-0.23	0 100 100	40, 46, 60, 76	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
14	t2	29/32 (90%)	-0.31	0 100 100	38, 48, 68, 84	0
15	U1	93/155 (60%)	-0.11	0 100 100	44, 59, 75, 104	0
15	U2	90/155 (58%)	0.48	5 (5%) 30 25	74, 91, 104, 115	0
15	u1	93/155 (60%)	0.03	1 (1%) 78 72	53, 68, 88, 95	0
15	u2	93/155 (60%)	-0.17	1 (1%) 78 72	44, 58, 71, 86	0
16	V1	129/155 (83%)	0.15	1 (0%) 82 77	47, 62, 87, 93	0
16	V2	129/155 (83%)	0.89	14 (10%) 10 8	75, 96, 114, 127	0
16	v1	129/155 (83%)	0.37	5 (3%) 43 36	47, 69, 108, 124	0
16	v2	129/155 (83%)	0.08	4 (3%) 51 44	47, 63, 90, 105	0
17	Y1	27/35 (77%)	0.18	0 100 100	64, 74, 103, 118	0
17	Y2	25/35 (71%)	1.00	1 (4%) 42 36	96, 100, 107, 109	0
17	y1	27/35 (77%)	0.64	1 (3%) 45 38	64, 71, 105, 107	0
17	y2	27/35 (77%)	0.52	0 100 100	72, 79, 92, 106	0
18	X1	29/40 (72%)	1.32	5 (17%) 4 3	98, 113, 130, 135	0
18	X2	31/40 (77%)	1.42	6 (19%) 3 2	83, 101, 114, 121	0
18	x1	36/40 (90%)	0.90	6 (16%) 4 3	61, 83, 96, 102	0
18	x2	32/40 (80%)	0.96	5 (15%) 5 4	83, 104, 122, 126	0
19	S1	25/46 (54%)	0.63	1 (4%) 42 36	72, 79, 85, 98	0
19	S2	30/46 (65%)	1.39	7 (23%) 2 1	98, 114, 120, 122	0
19	s1	40/46 (86%)	0.75	2 (5%) 34 28	54, 78, 94, 95	0
19	s2	46/46 (100%)	0.95	5 (10%) 10 8	75, 90, 106, 112	0
20	W1	21/25 (84%)	0.64	1 (4%) 35 30	71, 79, 86, 90	0
20	W2	21/25 (84%)	0.52	0 100 100	66, 76, 84, 89	0
20	w1	25/25 (100%)	0.85	3 (12%) 9 7	73, 79, 96, 101	0
20	w2	20/25 (80%)	0.88	3 (15%) 5 4	91, 96, 103, 111	0
21	Q2	111/218 (50%)	1.29	24 (21%) 2 2	122, 132, 145, 151	0
21	q1	105/218 (48%)	1.08	18 (17%) 4 3	103, 125, 138, 144	0
22	Z2	59/62 (95%)	1.22	13 (22%) 2 2	108, 121, 134, 140	0
22	z2	59/62 (95%)	0.87	4 (6%) 23 18	83, 101, 116, 127	0
All	All	10516/12316 (85%)	0.21	387 (3%) 45 38	31, 66, 113, 159	4 (0%)

The worst 5 of 387 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C2	392	ALA	8.1
13	o2	195	GLY	7.6
13	o1	195	GLY	6.6
18	X2	17	ALA	6.2
13	O1	195	GLY	6.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

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
28	UNL	I2	102	17/-	0.49	0.11	80,92,102,103	0
28	UNL	k2	505	6/-	0.51	0.10	70,80,84,87	0
28	UNL	I2	103	14/-	0.55	0.10	62,93,102,104	0
32	GOL	a1	406	6/6	0.55	0.11	68,75,86,90	0
28	UNL	a2	409	18/-	0.57	0.10	61,74,86,90	0
28	UNL	C2	501	6/-	0.57	0.10	72,74,78,87	0
28	UNL	J2	101	10/-	0.57	0.12	71,82,86,88	0
28	UNL	b1	623	11/-	0.58	0.12	59,74,83,84	0
23	BCR	K1	101	31/40	0.59	0.12	64,82,93,96	0
28	UNL	D1	410	6/-	0.59	0.14	59,62,66,66	0
28	UNL	F2	403	16/-	0.59	0.15	51,76,86,89	0
28	UNL	A2	409	10/-	0.60	0.14	72,82,85,87	0
28	UNL	c2	520	15/-	0.60	0.12	86,97,106,108	0
28	UNL	B1	624	18/-	0.61	0.10	43,71,79,81	0
28	UNL	H2	102	5/-	0.62	0.14	72,81,84,85	0
28	UNL	K2	103	5/-	0.63	0.16	79,83,88,90	0
25	CLA	b2	604	42/65	0.63	0.13	82,109,116,127	0
25	CLA	C2	518	41/65	0.63	0.12	105,121,127,134	0
28	UNL	d2	410	13/-	0.63	0.12	74,92,108,111	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
28	UNL	C2	517	18/-	0.63	0.13	74,83,87,89	0
28	UNL	b1	629	15/-	0.63	0.10	46,59,71,83	0
28	UNL	m2	102	18/-	0.64	0.09	46,65,79,79	0
29	LMG	C2	515	24/55	0.64	0.10	82,97,104,105	0
28	UNL	k2	502	9/-	0.64	0.09	72,78,84,86	0
28	UNL	d1	410	12/-	0.65	0.13	49,72,77,79	0
28	UNL	X2	101	7/-	0.65	0.24	83,85,91,93	0
28	UNL	B2	626	15/-	0.66	0.10	79,83,92,95	0
29	LMG	I2	101	34/55	0.66	0.13	82,103,109,114	0
25	CLA	C2	510	45/65	0.66	0.14	107,116,121,126	0
33	LHG	B2	627	42/49	0.66	0.10	67,88,120,132	0
35	LMT	m2	104	29/35	0.66	0.12	49,104,119,122	0
23	BCR	K2	102	40/40	0.67	0.13	84,99,113,115	0
33	LHG	b2	625	43/49	0.68	0.10	62,87,109,126	0
32	GOL	C1	518	6/6	0.68	0.11	65,73,77,81	0
39	CA	o2	401	1/1	0.68	0.18	101,101,101,101	0
32	GOL	B1	620	6/6	0.69	0.10	63,75,81,82	0
28	UNL	t1	101	18/-	0.69	0.10	43,60,66,67	0
35	LMT	b2	621	35/35	0.69	0.11	69,110,123,123	0
28	UNL	B1	623	16/-	0.69	0.09	53,68,72,74	0
33	LHG	d1	402	32/49	0.69	0.14	45,63,76,86	0
29	LMG	j2	101	50/55	0.70	0.12	60,78,97,107	0
29	LMG	F2	402	35/55	0.70	0.11	68,81,91,92	0
28	UNL	j1	101	17/-	0.70	0.11	60,69,71,77	0
33	LHG	a2	407	30/49	0.70	0.13	55,75,94,102	0
28	UNL	a2	401	18/-	0.71	0.11	46,56,70,86	0
24	CL	A2	410	1/1	0.71	0.09	87,87,87,87	0
28	UNL	a2	410	8/-	0.71	0.10	61,68,70,76	0
28	UNL	b2	607	12/-	0.71	0.12	64,75,80,87	0
25	CLA	C2	503	65/65	0.71	0.12	94,104,112,116	0
25	CLA	D2	404	61/65	0.71	0.11	67,87,113,120	0
25	CLA	K2	101	55/65	0.71	0.10	86,98,104,109	0
28	UNL	k2	504	9/-	0.71	0.09	66,74,80,88	0
28	UNL	i2	101	14/-	0.72	0.07	62,66,73,75	0
28	UNL	M2	101	11/-	0.72	0.07	59,68,73,74	0
35	LMT	c1	517	33/35	0.72	0.12	63,100,117,119	0
25	CLA	c2	513	54/65	0.73	0.10	75,94,102,105	0
23	BCR	c2	501	40/40	0.73	0.13	66,82,89,92	0
28	UNL	b1	626	13/-	0.73	0.08	53,64,83,86	0
32	GOL	C2	514	6/6	0.73	0.09	87,93,100,101	0
35	LMT	m2	103	30/35	0.73	0.14	52,89,111,113	0
23	BCR	K2	104	29/40	0.73	0.10	92,100,109,112	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
28	UNL	b1	630	17/-	0.73	0.09	48,57,74,75	0
29	LMG	d1	411	35/55	0.74	0.11	58,76,94,99	0
23	BCR	z2	101	40/40	0.74	0.12	80,95,100,101	0
28	UNL	m2	101	18/-	0.74	0.09	44,57,79,85	0
28	UNL	B2	625	18/-	0.74	0.09	37,56,68,68	0
29	LMG	A1	412	41/55	0.74	0.11	50,75,96,100	0
29	LMG	b1	621	38/55	0.74	0.10	52,63,76,82	0
23	BCR	F2	401	40/40	0.75	0.11	67,81,107,113	0
29	LMG	B2	621	37/55	0.75	0.10	53,68,80,96	0
25	CLA	C2	505	65/65	0.75	0.12	78,100,112,118	0
28	UNL	A2	408	18/-	0.75	0.10	62,83,92,93	0
23	BCR	B1	602	40/40	0.75	0.11	49,62,74,78	0
33	LHG	A2	405	33/49	0.75	0.10	70,80,90,97	0
23	BCR	C2	502	40/40	0.75	0.13	95,106,118,120	0
28	UNL	k2	503	6/-	0.76	0.09	67,76,79,80	0
23	BCR	J1	101	40/40	0.76	0.10	50,70,86,88	0
35	LMT	i2	102	7/35	0.76	0.08	68,71,76,79	0
29	LMG	A2	412	29/55	0.76	0.10	86,94,100,102	0
32	GOL	b1	618	6/6	0.76	0.08	60,69,80,80	0
25	CLA	C2	509	65/65	0.76	0.12	90,101,106,108	0
35	LMT	C1	519	35/35	0.77	0.10	57,76,85,93	0
35	LMT	M1	103	24/35	0.77	0.10	42,68,97,101	0
35	LMT	T1	101	12/35	0.77	0.10	46,51,54,56	0
25	CLA	C2	511	50/65	0.77	0.11	85,93,100,104	0
23	BCR	k1	101	40/40	0.77	0.11	56,70,82,85	0
25	CLA	B1	604	42/65	0.77	0.11	83,98,107,113	0
28	UNL	B2	622	17/-	0.77	0.09	57,71,76,78	0
25	CLA	C1	512	65/65	0.77	0.10	63,82,102,121	0
25	CLA	c1	516	65/65	0.77	0.11	66,82,104,109	0
35	LMT	a2	406	35/35	0.78	0.11	43,80,92,94	0
28	UNL	b1	627	16/-	0.78	0.09	42,56,75,77	0
25	CLA	B1	611	62/65	0.78	0.10	58,78,87,89	0
25	CLA	c1	515	55/65	0.78	0.10	69,82,90,94	0
29	LMG	b1	624	39/55	0.78	0.12	58,73,84,87	0
37	SQD	D1	409	35/54	0.78	0.11	61,75,92,97	0
28	UNL	W2	101	9/-	0.78	0.08	64,77,83,87	0
25	CLA	C2	504	46/65	0.79	0.11	72,88,95,96	0
25	CLA	C1	513	61/65	0.79	0.10	49,68,74,78	0
28	UNL	a2	411	11/-	0.79	0.07	51,55,65,67	0
25	CLA	C2	507	45/65	0.79	0.11	73,93,102,113	0
23	BCR	b2	603	40/40	0.80	0.10	60,74,102,104	0
23	BCR	H2	103	24/40	0.80	0.12	65,76,82,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	BCR	j2	102	40/40	0.80	0.11	59,75,86,87	0
25	CLA	c2	515	46/65	0.80	0.11	81,100,104,109	0
29	LMG	C1	520	48/55	0.80	0.08	59,69,78,86	0
29	LMG	a1	412	51/55	0.80	0.10	54,67,77,91	0
25	CLA	C2	513	53/65	0.80	0.11	78,91,106,110	0
23	BCR	H1	102	22/40	0.80	0.12	75,88,95,100	0
23	BCR	D1	401	40/40	0.80	0.10	54,67,89,95	0
23	BCR	b2	602	40/40	0.81	0.10	51,70,78,82	0
25	CLA	C2	506	65/65	0.81	0.10	78,90,97,100	0
23	BCR	b1	602	40/40	0.81	0.10	35,57,65,73	0
25	CLA	C2	508	50/65	0.81	0.13	87,103,112,115	0
34	DGD	H2	101	62/66	0.81	0.09	51,74,83,85	0
25	CLA	C2	516	46/65	0.81	0.10	70,92,97,100	0
28	UNL	d2	411	12/-	0.81	0.08	55,67,73,79	0
39	CA	O1	401	1/1	0.81	0.06	82,82,82,82	0
29	LMG	b2	622	39/55	0.81	0.10	47,60,85,90	0
32	GOL	c2	518	6/6	0.82	0.11	50,55,59,64	0
25	CLA	d2	404	50/65	0.82	0.10	57,74,83,88	0
35	LMT	m1	101	35/35	0.82	0.11	44,80,103,112	0
25	CLA	B2	604	41/65	0.82	0.09	68,79,92,97	0
28	UNL	x1	101	15/-	0.82	0.09	55,73,79,82	0
25	CLA	c2	509	65/65	0.82	0.08	54,70,82,85	0
23	BCR	C1	521	40/40	0.82	0.10	59,68,80,84	0
34	DGD	C2	512	33/66	0.82	0.10	63,77,83,93	0
29	LMG	B1	622	31/55	0.82	0.11	66,74,81,83	0
37	SQD	B2	623	45/54	0.82	0.10	58,79,89,96	0
37	SQD	b2	605	45/54	0.82	0.08	54,83,114,124	0
29	LMG	B1	626	48/55	0.82	0.09	55,70,89,94	0
25	CLA	C1	514	45/65	0.82	0.10	73,84,92,96	0
23	BCR	B2	602	40/40	0.83	0.10	47,59,80,86	0
29	LMG	B2	620	40/55	0.83	0.09	62,74,97,98	0
25	CLA	c1	503	65/65	0.83	0.10	55,66,71,75	0
25	CLA	C1	502	65/65	0.83	0.09	51,63,68,70	0
35	LMT	b2	623	35/35	0.83	0.08	63,90,98,101	0
28	UNL	B1	625	7/-	0.83	0.08	45,52,55,63	0
25	CLA	b2	618	65/65	0.83	0.10	68,82,90,92	0
23	BCR	h2	101	40/40	0.83	0.10	71,85,107,109	0
28	UNL	b1	625	10/-	0.83	0.10	50,62,68,69	0
23	BCR	c1	502	40/40	0.83	0.10	57,66,72,72	0
29	LMG	b1	631	40/55	0.83	0.10	29,52,85,92	0
38	HEM	E1	101	43/43	0.83	0.13	108,134,152,155	0
29	LMG	c1	519	55/55	0.83	0.08	47,70,84,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	CLA	B2	611	65/65	0.83	0.10	51,73,81,86	0
28	UNL	a1	409	11/-	0.84	0.06	43,51,60,63	0
25	CLA	c2	512	65/65	0.84	0.09	61,76,86,93	0
23	BCR	d2	401	40/40	0.84	0.09	48,67,81,85	0
25	CLA	B2	606	65/65	0.84	0.09	53,67,75,78	0
23	BCR	k2	501	40/40	0.84	0.09	61,84,95,98	0
25	CLA	b2	610	65/65	0.84	0.09	60,82,90,92	0
25	CLA	b1	604	65/65	0.84	0.10	52,78,110,115	0
37	SQD	D2	402	25/54	0.84	0.09	85,90,96,98	0
25	CLA	c2	502	65/65	0.84	0.09	60,78,85,90	0
35	LMT	l1	101	24/35	0.84	0.08	42,55,89,90	0
38	HEM	V2	201	43/43	0.84	0.12	83,98,102,107	0
38	HEM	e2	101	43/43	0.84	0.11	126,145,163,171	0
25	CLA	A2	403	61/65	0.84	0.11	80,89,98,102	0
28	UNL	m1	102	6/-	0.84	0.08	54,55,63,66	0
29	LMG	a2	412	44/55	0.85	0.09	55,70,78,93	0
25	CLA	b2	609	61/65	0.85	0.10	77,89,95,100	0
25	CLA	A2	404	51/65	0.85	0.08	47,58,70,73	0
25	CLA	C1	509	65/65	0.85	0.09	48,59,71,80	0
28	UNL	B2	624	8/-	0.85	0.07	46,51,54,55	0
25	CLA	b2	619	59/65	0.85	0.10	71,80,106,109	0
23	BCR	c1	501	40/40	0.85	0.08	56,66,79,82	0
32	GOL	i1	101	6/6	0.85	0.12	55,57,60,64	0
25	CLA	c2	506	61/65	0.85	0.10	55,70,77,83	0
32	GOL	a2	415	6/6	0.85	0.14	47,55,59,63	0
25	CLA	c2	508	65/65	0.85	0.10	68,78,84,88	0
28	UNL	b1	628	10/-	0.85	0.08	51,57,61,67	0
25	CLA	B2	610	65/65	0.85	0.09	44,59,82,86	0
25	CLA	c1	508	50/65	0.85	0.10	57,66,77,81	0
25	CLA	c1	510	65/65	0.85	0.08	41,54,62,72	0
25	CLA	c1	513	60/65	0.85	0.07	49,59,71,72	0
34	DGD	c1	520	62/66	0.85	0.09	36,59,73,87	0
25	CLA	B1	609	65/65	0.85	0.10	54,71,81,90	0
25	CLA	C1	506	65/65	0.85	0.09	49,62,70,73	0
25	CLA	D1	403	51/65	0.85	0.09	64,74,88,90	0
34	DGD	c2	517	62/66	0.86	0.08	45,57,70,75	0
25	CLA	c1	509	65/65	0.86	0.10	51,62,68,72	0
29	LMG	A1	410	43/55	0.86	0.08	52,59,65,76	0
25	CLA	a2	405	65/65	0.86	0.09	51,60,81,87	0
25	CLA	c1	505	65/65	0.86	0.09	47,70,79,88	0
28	UNL	t1	102	9/-	0.86	0.08	45,57,68,69	0
34	DGD	C1	517	64/66	0.86	0.08	38,55,75,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
38	HEM	E2	101	43/43	0.86	0.13	116,132,146,152	0
25	CLA	B1	606	65/65	0.86	0.10	60,71,77,82	0
29	LMG	d2	407	27/55	0.86	0.09	49,60,64,70	0
25	CLA	c2	504	65/65	0.86	0.10	46,78,92,100	0
34	DGD	c2	516	52/66	0.86	0.10	37,63,71,75	0
23	BCR	b2	601	40/40	0.87	0.09	51,61,69,72	0
34	DGD	c1	514	51/66	0.87	0.09	46,54,62,64	0
25	CLA	b1	609	65/65	0.87	0.10	42,58,84,104	0
25	CLA	b2	624	65/65	0.87	0.08	47,60,75,82	0
25	CLA	b1	619	65/65	0.87	0.10	48,62,81,85	0
27	PHO	D2	407	64/64	0.87	0.08	58,68,81,83	0
25	CLA	b2	606	65/65	0.87	0.11	68,77,84,90	0
25	CLA	C1	511	65/65	0.87	0.10	45,56,62,68	0
35	LMT	L1	102	12/35	0.87	0.07	35,45,59,62	0
29	LMG	M1	101	31/55	0.87	0.09	41,52,63,70	0
25	CLA	c2	507	54/65	0.87	0.10	76,81,86,92	0
25	CLA	B1	618	58/65	0.87	0.10	53,64,80,86	0
29	LMG	c2	519	26/55	0.87	0.07	58,67,73,74	0
28	UNL	l1	103	12/-	0.87	0.08	35,47,53,55	0
25	CLA	b2	613	65/65	0.87	0.10	59,84,96,99	0
25	CLA	c1	507	65/65	0.88	0.09	49,62,72,80	0
23	BCR	B2	603	40/40	0.88	0.08	46,59,76,81	0
25	CLA	B2	612	65/65	0.88	0.10	58,64,71,83	0
25	CLA	c2	511	65/65	0.88	0.10	54,65,72,75	0
25	CLA	B2	619	65/65	0.88	0.07	46,55,63,71	0
25	CLA	B1	605	65/65	0.88	0.09	60,75,87,88	0
25	CLA	C1	505	65/65	0.88	0.08	43,55,64,68	0
34	DGD	C1	515	52/66	0.88	0.09	36,58,67,71	0
25	CLA	c1	512	65/65	0.88	0.10	36,50,57,60	0
36	PL9	D2	408	55/55	0.88	0.09	43,59,64,74	0
27	PHO	D1	407	63/64	0.88	0.08	40,56,63,67	0
23	BCR	C1	501	40/40	0.88	0.08	47,61,72,75	0
25	CLA	C1	507	65/65	0.88	0.09	46,67,86,105	0
25	CLA	b2	616	60/65	0.88	0.09	51,64,82,82	0
25	CLA	b1	616	65/65	0.88	0.09	39,46,57,69	0
23	BCR	A2	401	40/40	0.88	0.12	58,84,90,91	0
23	BCR	d1	405	40/40	0.88	0.09	38,51,94,99	0
25	CLA	B1	617	65/65	0.88	0.08	59,67,74,75	0
25	CLA	B2	605	65/65	0.88	0.07	63,71,77,82	0
25	CLA	c1	506	65/65	0.88	0.08	40,54,68,73	0
25	CLA	B2	614	65/65	0.89	0.08	46,58,66,68	0
25	CLA	B2	616	54/65	0.89	0.08	43,51,57,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
34	DGD	c1	518	62/66	0.89	0.07	41,61,69,79	0
25	CLA	B2	617	65/65	0.89	0.08	52,63,70,74	0
25	CLA	B2	618	60/65	0.89	0.08	59,65,80,85	0
36	PL9	d1	409	55/55	0.89	0.09	28,41,50,61	0
25	CLA	b2	617	65/65	0.89	0.08	47,58,65,72	0
36	PL9	d2	409	55/55	0.89	0.09	33,44,56,57	0
25	CLA	B1	610	65/65	0.89	0.09	46,58,73,76	0
25	CLA	a1	404	60/65	0.89	0.10	49,57,82,89	0
23	BCR	B1	603	40/40	0.89	0.07	45,56,78,85	0
33	LHG	D1	404	49/49	0.89	0.09	48,60,84,90	0
25	CLA	B1	607	60/65	0.89	0.09	45,56,68,72	0
28	UNL	A1	409	14/-	0.89	0.06	44,48,57,68	0
23	BCR	B1	601	40/40	0.89	0.08	41,55,65,65	0
25	CLA	c2	505	65/65	0.89	0.08	48,61,71,80	0
25	CLA	d1	406	65/65	0.89	0.08	44,58,94,99	0
25	CLA	C1	508	65/65	0.89	0.09	47,66,76,80	0
25	CLA	c2	503	65/65	0.90	0.10	53,62,83,89	0
23	BCR	B2	601	40/40	0.90	0.07	41,56,66,68	0
29	LMG	D1	406	35/55	0.90	0.08	50,57,71,74	0
33	LHG	D2	405	49/49	0.90	0.07	52,60,66,68	0
33	LHG	L2	101	49/49	0.90	0.08	42,57,70,78	0
25	CLA	B1	616	65/65	0.90	0.08	39,49,58,66	0
23	BCR	b1	603	40/40	0.90	0.08	40,58,69,77	0
33	LHG	d2	403	49/49	0.90	0.08	42,59,69,73	0
25	CLA	b2	611	65/65	0.90	0.10	66,72,80,83	0
34	DGD	C1	516	62/66	0.90	0.07	44,53,60,61	0
31	BCT	a1	413	4/4	0.90	0.07	43,48,48,50	0
34	DGD	H1	101	62/66	0.90	0.08	50,71,84,89	0
25	CLA	b2	612	65/65	0.90	0.08	39,54,64,70	0
25	CLA	A1	405	55/65	0.90	0.08	38,46,59,65	0
25	CLA	c2	510	54/65	0.90	0.10	64,69,77,79	0
25	CLA	B2	607	65/65	0.90	0.08	49,59,73,78	0
25	CLA	B2	609	65/65	0.90	0.08	51,67,76,82	0
34	DGD	c2	514	62/66	0.90	0.07	47,59,67,69	0
25	CLA	b1	611	65/65	0.90	0.08	37,59,68,73	0
25	CLA	B1	619	65/65	0.90	0.08	32,50,57,73	0
25	CLA	A2	402	65/65	0.90	0.09	47,57,69,77	0
33	LHG	B1	621	49/49	0.90	0.08	41,57,67,73	0
25	CLA	b1	617	65/65	0.90	0.07	47,56,65,68	0
25	CLA	b2	614	65/65	0.91	0.08	51,66,73,75	0
25	CLA	d1	401	65/65	0.91	0.08	30,36,44,47	0
25	CLA	B2	615	65/65	0.91	0.07	44,56,73,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	CLA	d2	405	65/65	0.91	0.08	34,44,61,77	0
25	CLA	B1	615	65/65	0.91	0.08	35,47,73,80	0
33	LHG	d2	406	49/49	0.91	0.07	36,50,59,66	0
25	CLA	c1	504	65/65	0.91	0.09	36,53,83,98	0
25	CLA	b2	620	65/65	0.91	0.09	42,56,63,72	0
25	CLA	D2	401	65/65	0.91	0.08	43,53,71,76	0
23	BCR	a1	401	40/40	0.91	0.08	47,56,64,65	0
36	PL9	D1	408	55/55	0.91	0.08	28,42,52,63	0
25	CLA	D2	406	65/65	0.91	0.07	45,57,65,67	0
24	CL	a1	402	1/1	0.91	0.05	49,49,49,49	0
23	BCR	h1	102	40/40	0.91	0.08	53,60,67,69	0
25	CLA	b1	606	65/65	0.91	0.09	44,53,61,63	0
29	LMG	d1	408	33/55	0.91	0.08	41,50,61,63	0
25	CLA	A1	404	51/65	0.91	0.07	37,48,58,70	0
25	CLA	C1	510	65/65	0.91	0.09	47,59,77,82	0
25	CLA	B1	612	65/65	0.91	0.10	52,66,71,77	0
38	HEM	f1	101	43/43	0.91	0.11	62,82,124,136	0
38	HEM	v1	201	43/43	0.91	0.10	60,66,72,75	0
34	DGD	h2	102	62/66	0.91	0.08	47,67,82,96	0
25	CLA	C1	503	60/65	0.91	0.07	38,53,67,73	0
25	CLA	C1	504	65/65	0.91	0.07	49,64,74,77	0
35	LMT	M1	102	11/35	0.91	0.08	47,52,56,58	0
25	CLA	b1	620	65/65	0.91	0.08	31,43,56,60	0
33	LHG	D2	403	49/49	0.92	0.07	45,60,68,73	0
25	CLA	b2	608	65/65	0.92	0.08	65,77,85,86	0
25	CLA	d1	404	65/65	0.92	0.07	31,43,49,51	0
27	PHO	d1	403	64/64	0.92	0.07	32,41,50,54	0
27	PHO	A2	407	64/64	0.92	0.08	53,64,72,80	0
32	GOL	c1	521	6/6	0.92	0.08	54,56,60,65	0
25	CLA	b1	615	59/65	0.92	0.08	31,43,58,64	0
27	PHO	d2	408	64/64	0.92	0.08	45,56,62,64	0
25	CLA	b1	607	65/65	0.92	0.08	33,46,69,76	0
23	BCR	a2	402	40/40	0.92	0.07	33,51,62,67	0
25	CLA	b1	610	65/65	0.92	0.07	37,47,56,63	0
25	CLA	B1	613	65/65	0.92	0.08	38,49,57,64	0
33	LHG	b1	622	49/49	0.92	0.09	36,49,57,69	0
25	CLA	B2	613	65/65	0.92	0.07	41,52,68,70	0
34	DGD	h1	101	62/66	0.92	0.07	37,48,59,65	0
25	CLA	b1	612	65/65	0.92	0.07	45,54,60,68	0
31	BCT	A2	413	4/4	0.92	0.07	65,69,71,72	0
25	CLA	c1	511	65/65	0.93	0.08	38,53,71,78	0
31	BCT	A1	413	4/4	0.93	0.06	54,60,62,63	0

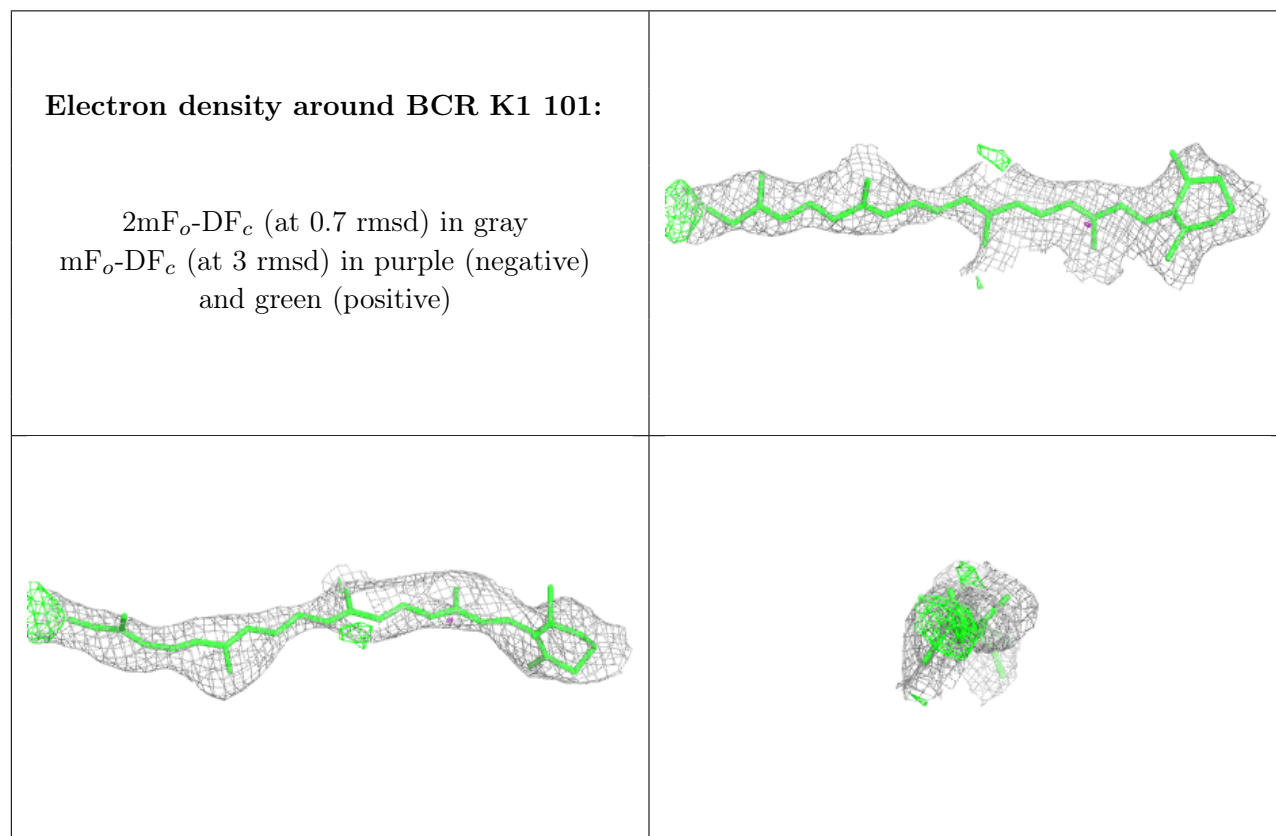
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
33	LHG	d1	407	49/49	0.93	0.07	34,44,53,67	0
26	OEX	A2	406	10/10	0.93	0.09	68,84,93,94	0
25	CLA	a1	405	50/65	0.93	0.07	25,33,49,55	0
23	BCR	b1	601	40/40	0.93	0.07	36,47,56,57	0
25	CLA	b1	613	65/65	0.93	0.07	36,44,54,68	0
25	CLA	a2	404	65/65	0.93	0.07	30,42,52,53	0
27	PHO	a2	416	64/64	0.93	0.07	35,46,53,62	0
25	CLA	b1	605	65/65	0.93	0.07	38,52,60,66	0
25	CLA	a2	413	50/65	0.93	0.06	33,46,57,66	0
24	CL	A1	402	1/1	0.93	0.12	39,39,39,39	0
38	HEM	V1	201	43/43	0.93	0.08	35,61,66,71	0
33	LHG	l2	101	44/49	0.93	0.06	36,53,66,72	0
25	CLA	B2	608	65/65	0.93	0.07	43,53,70,76	0
25	CLA	D1	402	65/65	0.93	0.06	31,40,58,63	0
23	BCR	A1	401	40/40	0.93	0.07	36,48,54,58	0
25	CLA	B1	614	65/65	0.93	0.07	43,55,62,67	0
33	LHG	L1	101	41/49	0.93	0.06	30,46,61,85	0
33	LHG	a1	407	43/49	0.93	0.06	36,52,66,70	0
25	CLA	d2	402	65/65	0.94	0.06	24,37,48,52	0
25	CLA	b2	615	60/65	0.94	0.07	45,54,67,74	0
25	CLA	a1	403	65/65	0.94	0.07	29,37,48,51	0
25	CLA	A1	406	65/65	0.94	0.07	28,37,46,55	0
33	LHG	l1	102	49/49	0.94	0.07	25,43,67,75	0
27	PHO	A1	408	64/64	0.94	0.07	30,42,50,56	0
25	CLA	B1	608	65/65	0.94	0.07	46,58,71,81	0
27	PHO	a1	411	64/64	0.94	0.06	33,41,47,50	0
38	HEM	v2	201	43/43	0.94	0.09	47,60,66,78	0
33	LHG	D1	405	49/49	0.94	0.06	35,45,54,56	0
25	CLA	b1	614	65/65	0.94	0.08	35,45,54,56	0
25	CLA	A1	403	65/65	0.95	0.06	27,37,49,54	0
25	CLA	b1	608	65/65	0.95	0.07	37,48,58,63	0
31	BCT	a2	417	4/4	0.96	0.05	59,65,67,73	0
26	OEX	A1	407	10/10	0.97	0.08	45,49,63,68	0
30	FE	A1	411	1/1	0.97	0.02	52,52,52,52	0
30	FE	a1	410	1/1	0.98	0.07	49,49,49,49	0
30	FE	a2	414	1/1	0.98	0.03	57,57,57,57	0
26	OEX	a2	408	10/10	0.98	0.07	42,49,58,61	0
26	OEX	a1	408	10/10	0.98	0.08	39,49,62,70	0
24	CL	a2	403	1/1	0.98	0.03	37,37,37,37	0
30	FE	A2	411	1/1	0.99	0.04	63,63,63,63	0

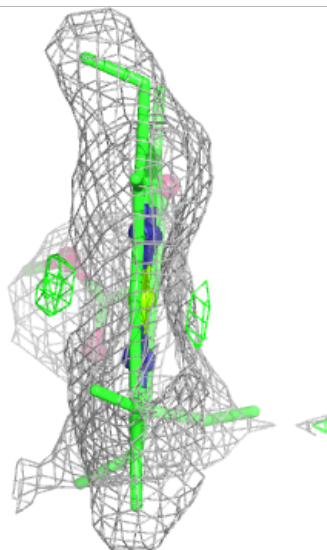
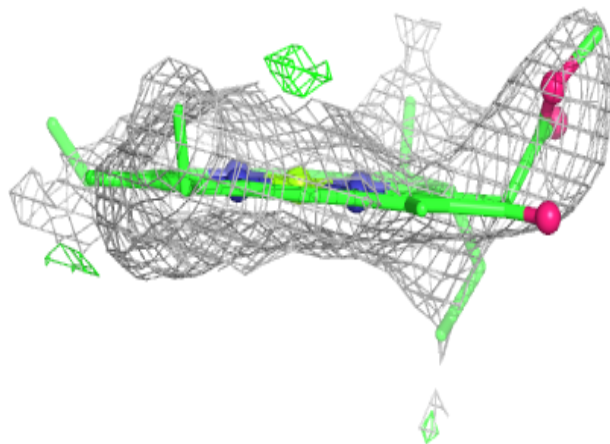
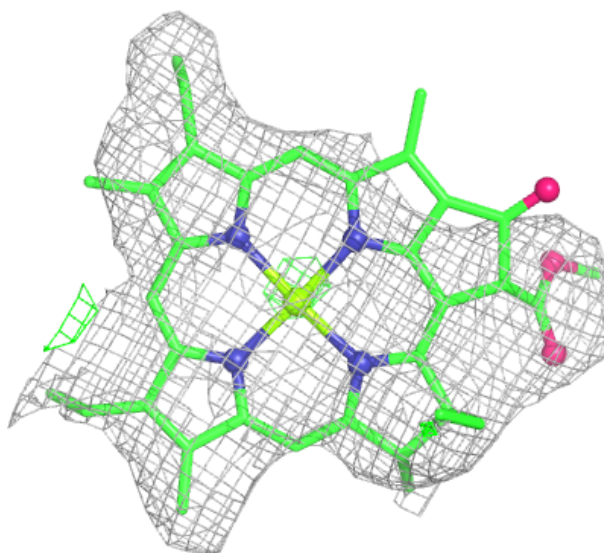
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

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



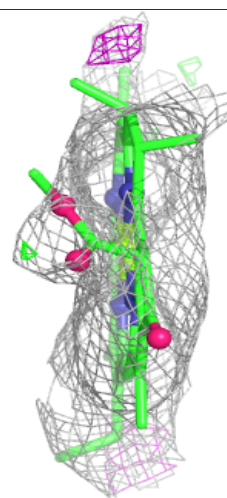
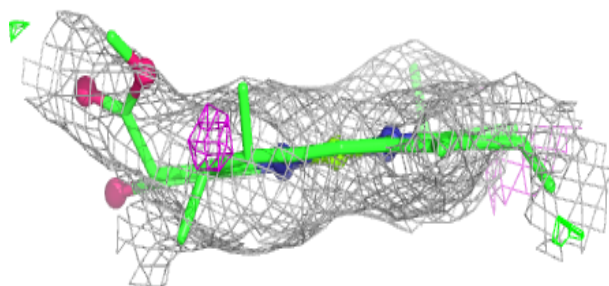
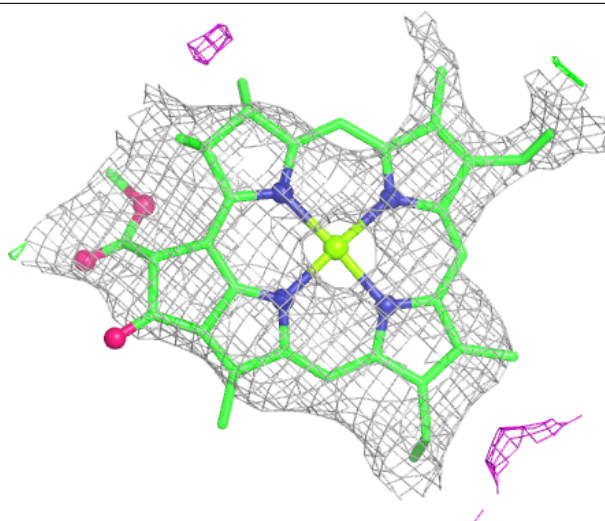
Electron density around CLA b2 604:

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



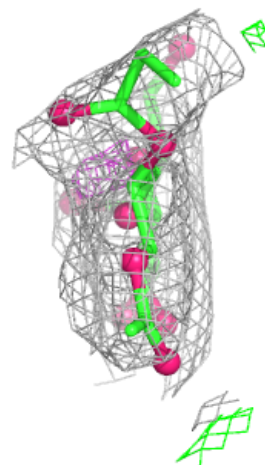
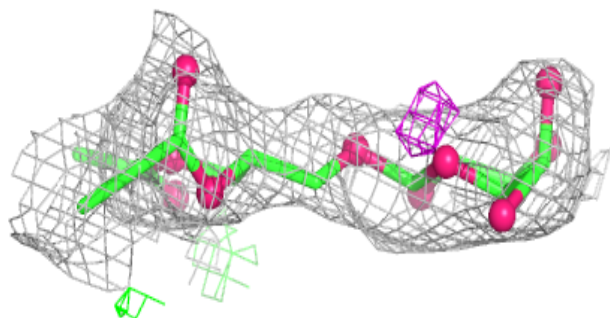
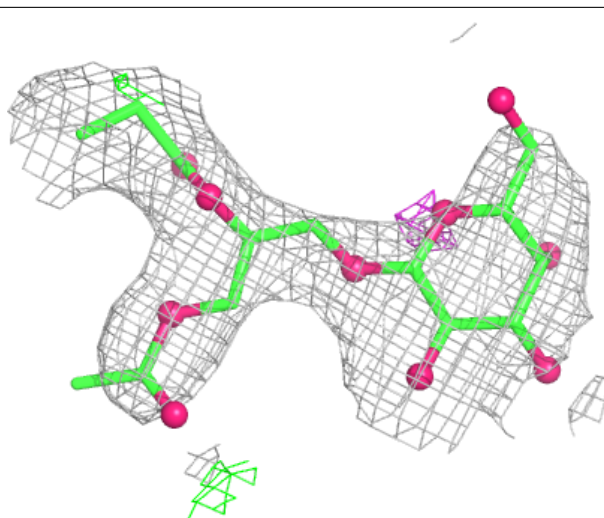
Electron density around CLA C2 518:

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



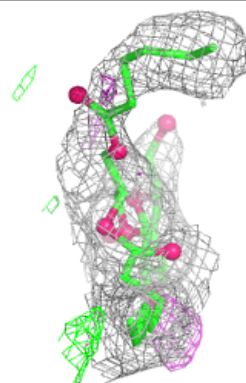
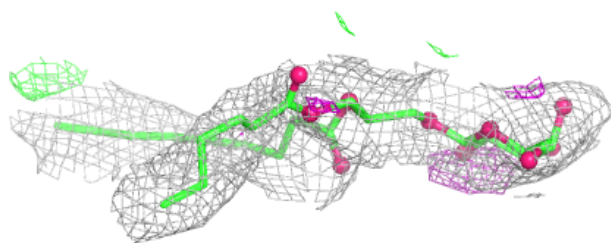
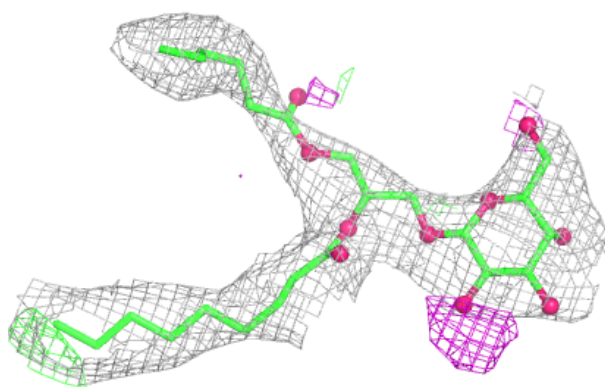
Electron density around LMG C2 515:

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



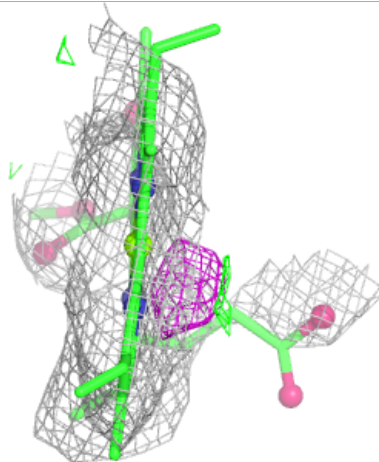
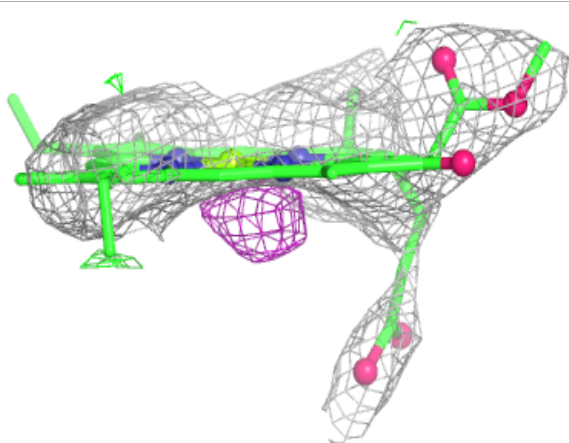
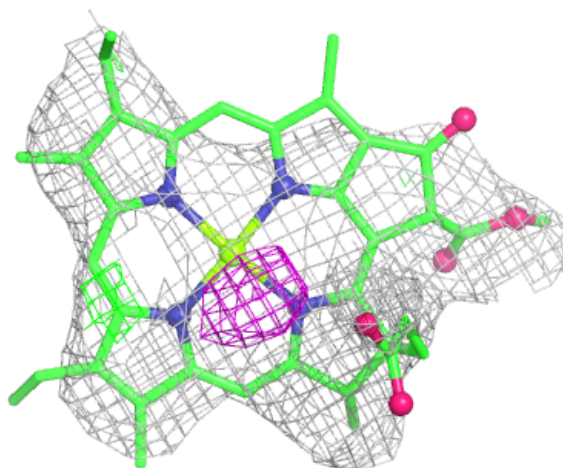
Electron density around LMG I2 101:

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



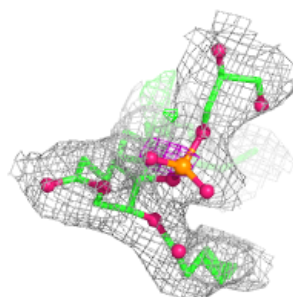
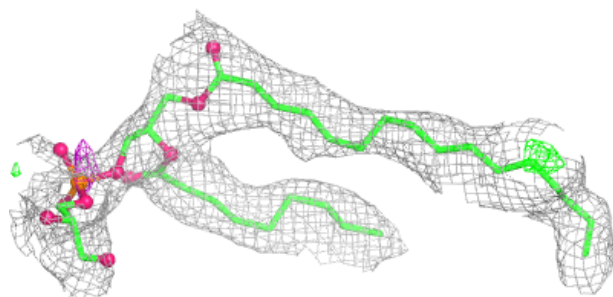
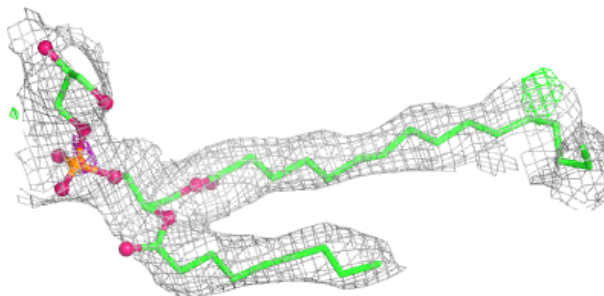
Electron density around CLA C2 510:

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

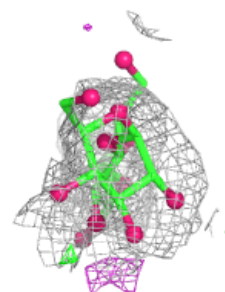
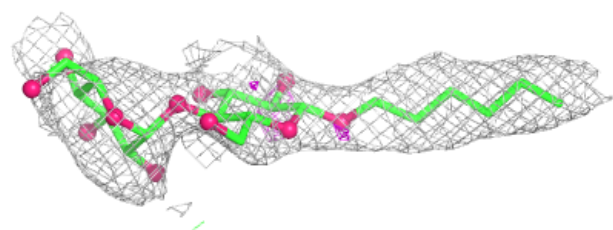
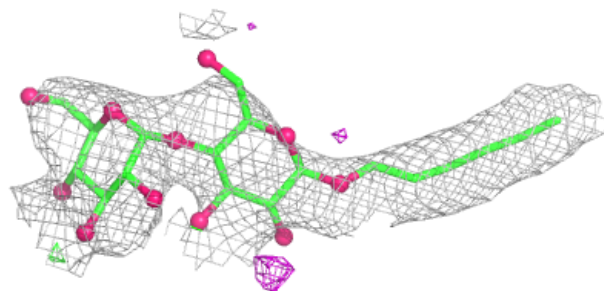


Electron density around LHG B2 627:

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

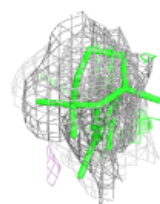
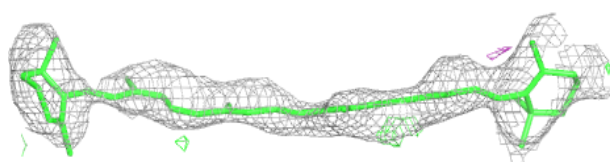
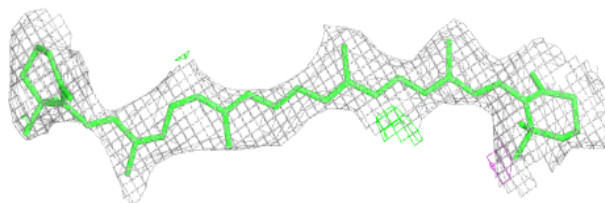
**Electron density around LMT m2 104:**

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

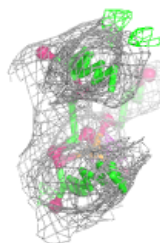
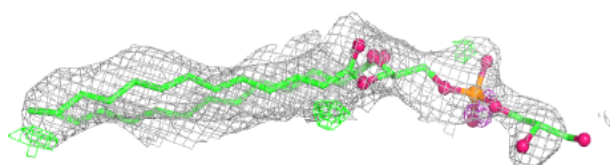
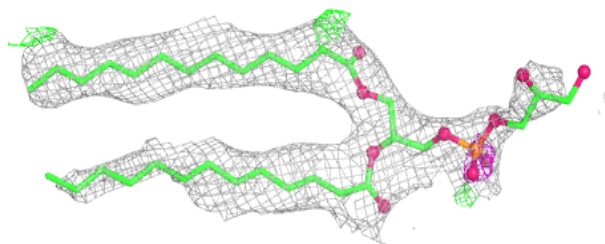


Electron density around BCR K2 102:

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

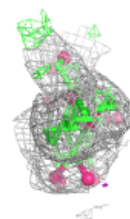
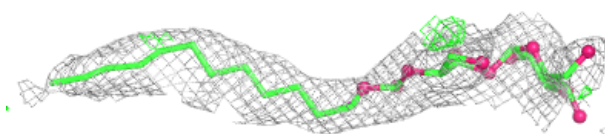
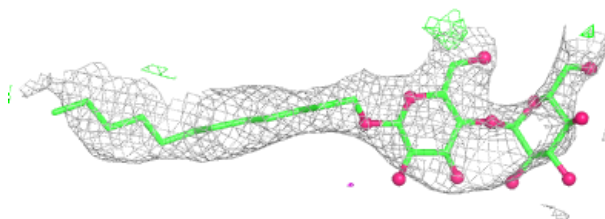
**Electron density around LHG b2 625:**

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

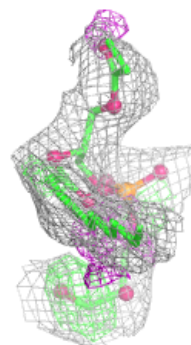
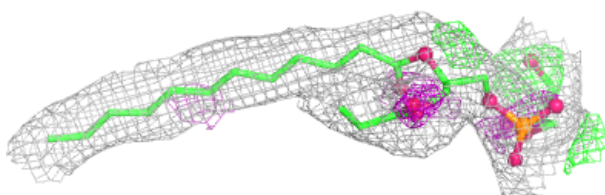
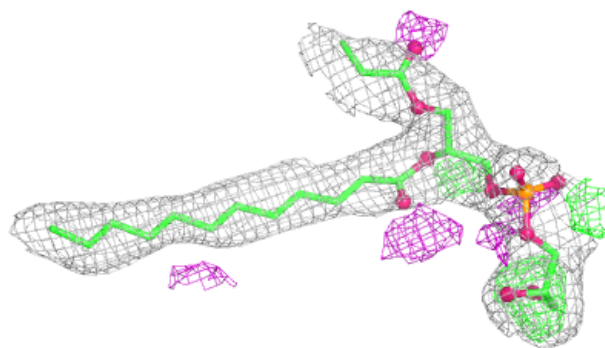


Electron density around LMT b2 621:

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

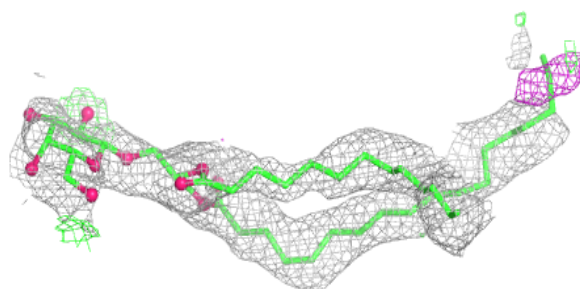
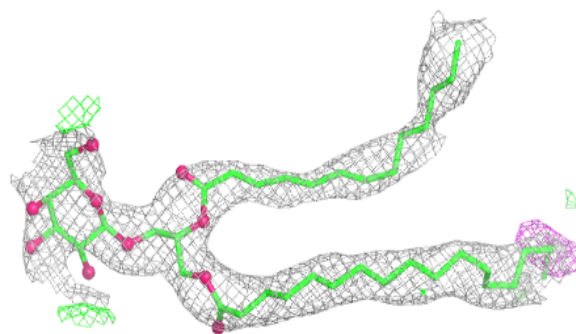
**Electron density around LHG d1 402:**

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

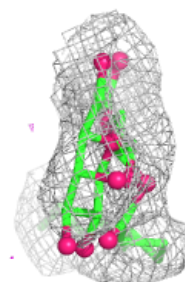
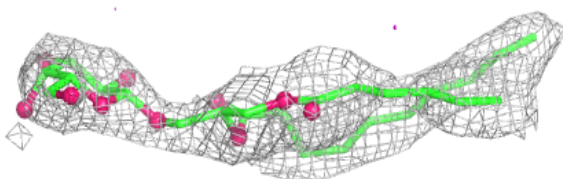
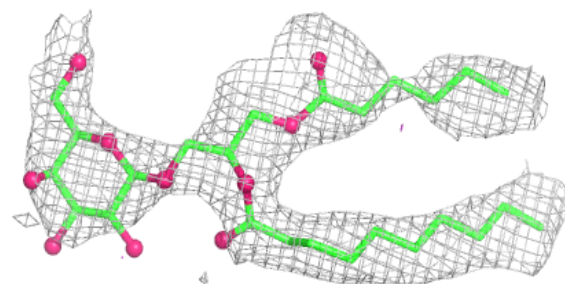


Electron density around LMG j2 101:

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

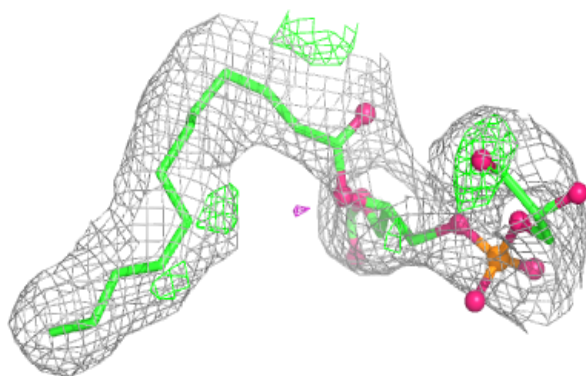
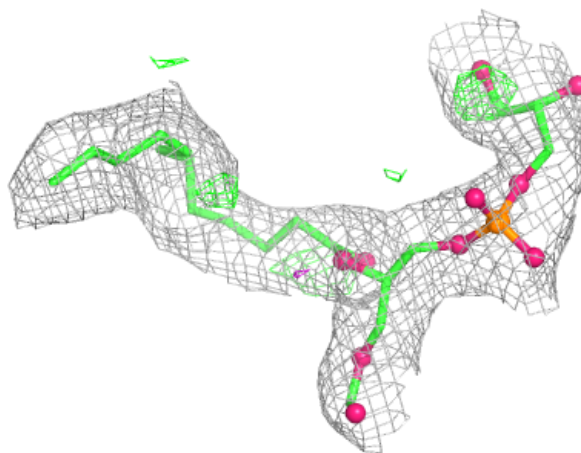
**Electron density around LMG F2 402:**

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



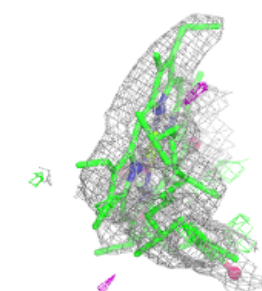
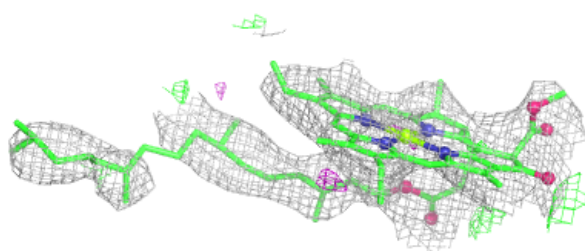
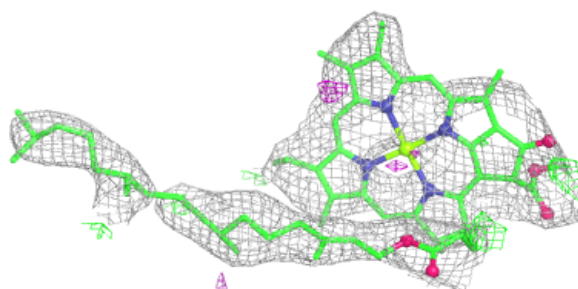
Electron density around LHG a2 407:

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

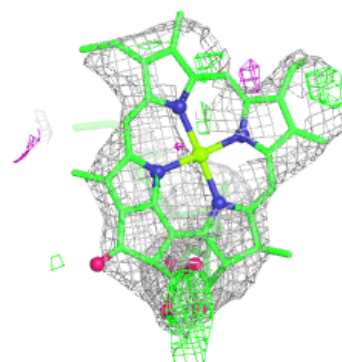
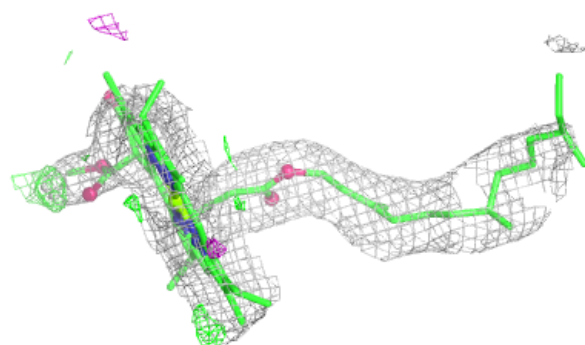
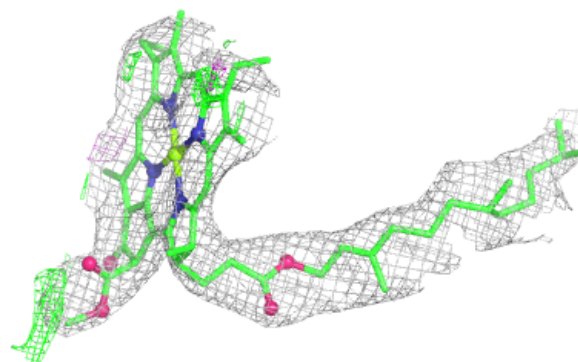


Electron density around CLA C2 503:

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

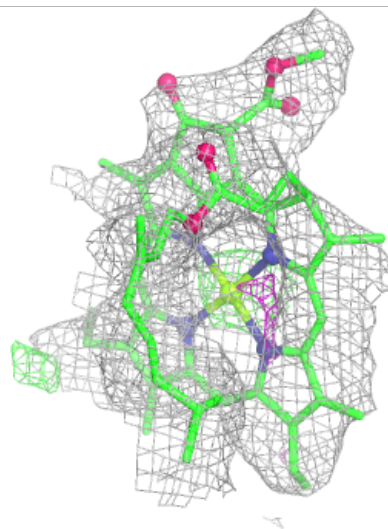
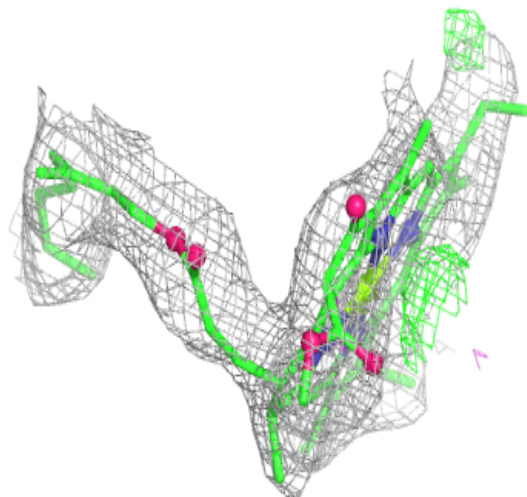
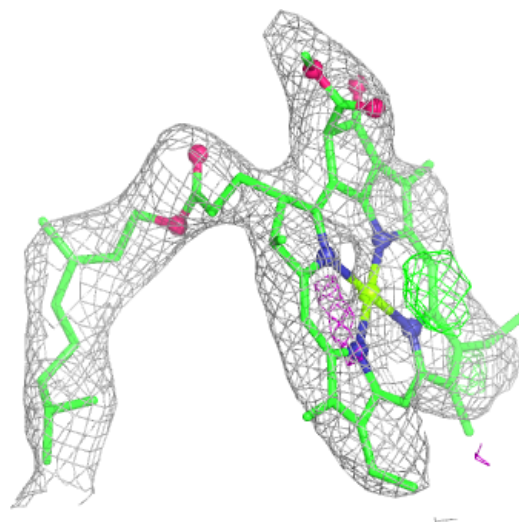
**Electron density around CLA D2 404:**

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



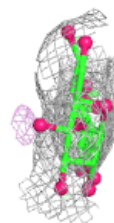
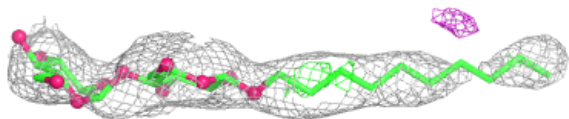
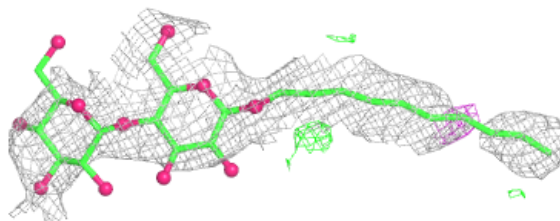
Electron density around CLA K2 101:

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



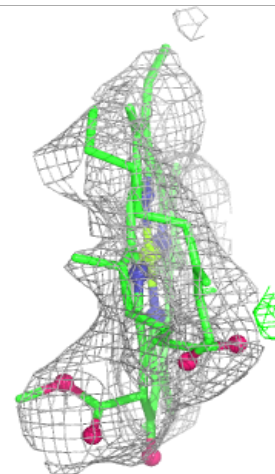
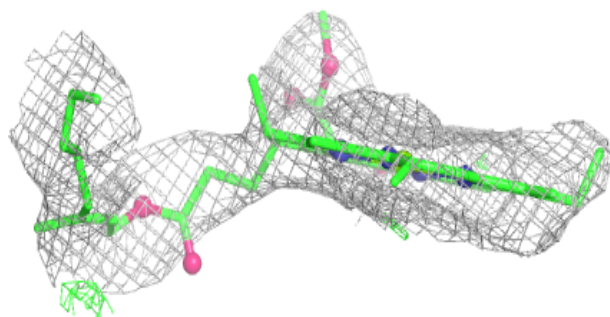
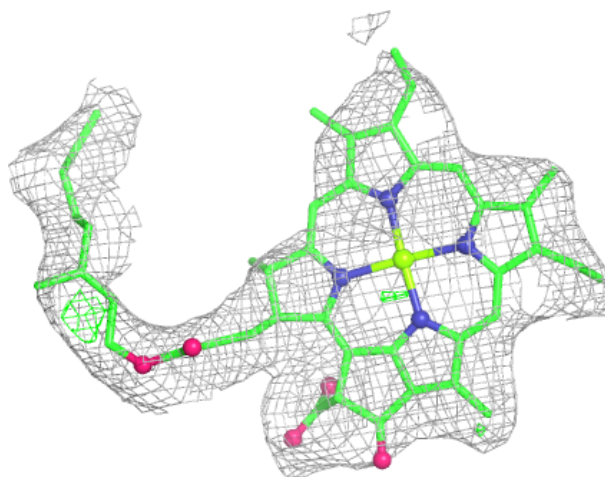
Electron density around LMT c1 517:

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



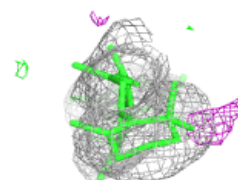
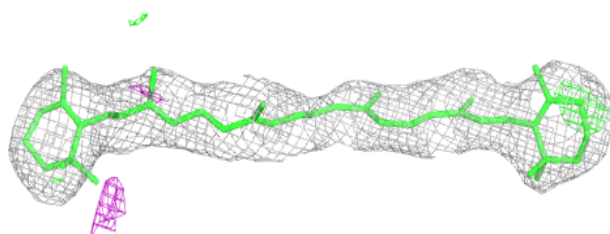
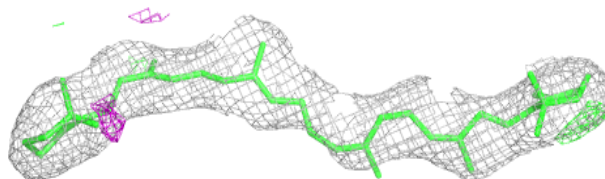
Electron density around CLA c2 513:

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

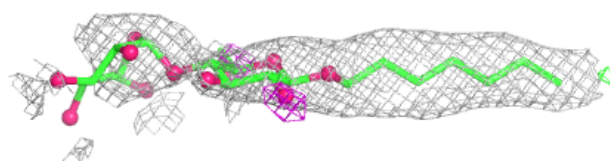
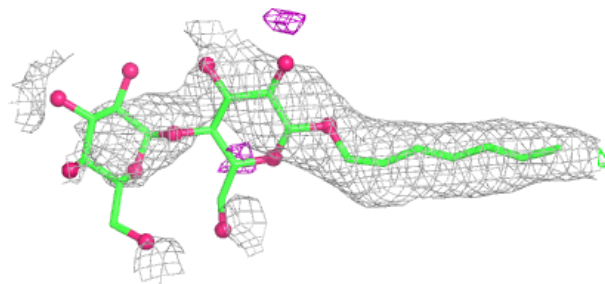


Electron density around BCR c2 501:

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

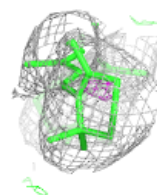
**Electron density around LMT m2 103:**

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

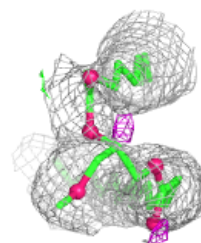
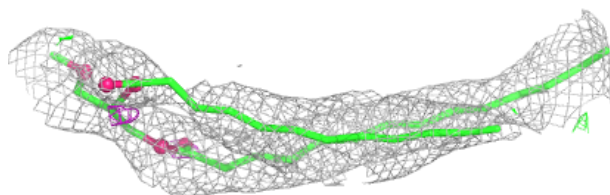
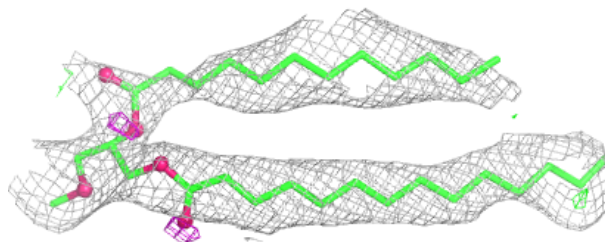


Electron density around BCR K2 104:

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

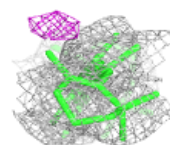
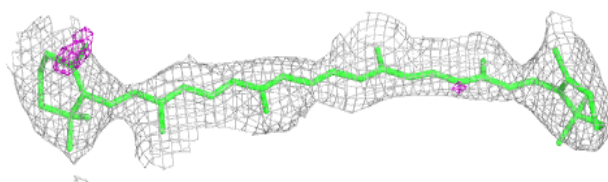
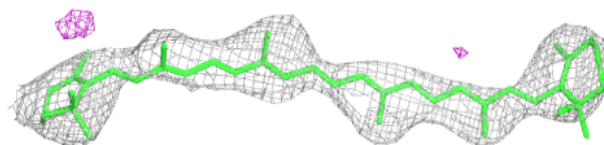
**Electron density around LMG d1 411:**

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

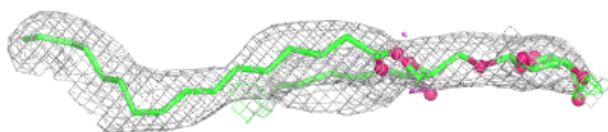
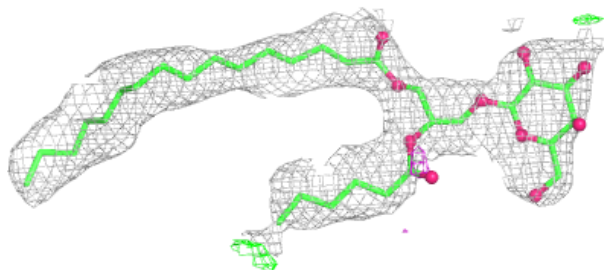


Electron density around BCR z2 101:

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

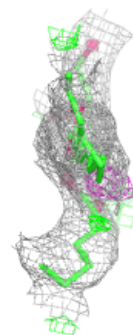
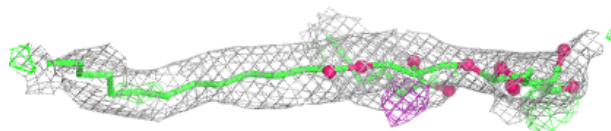
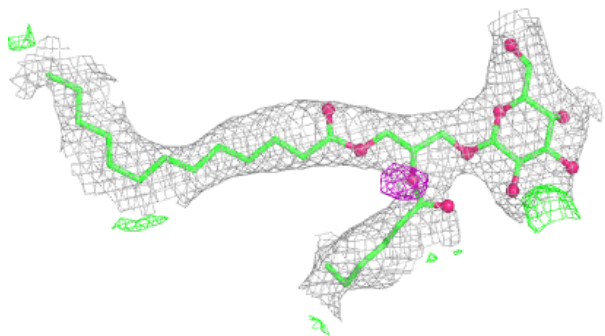
**Electron density around LMG A1 412:**

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

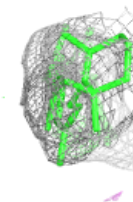
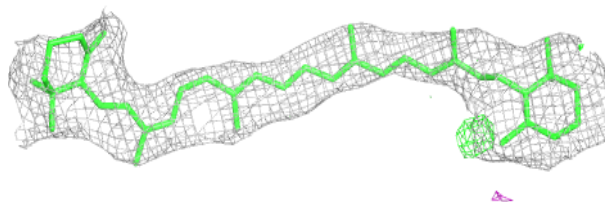


Electron density around LMG b1 621:

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

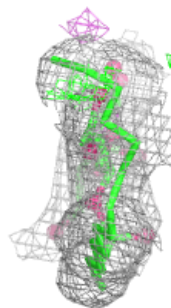
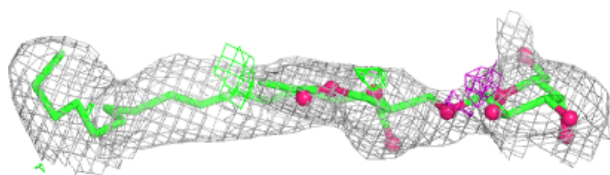
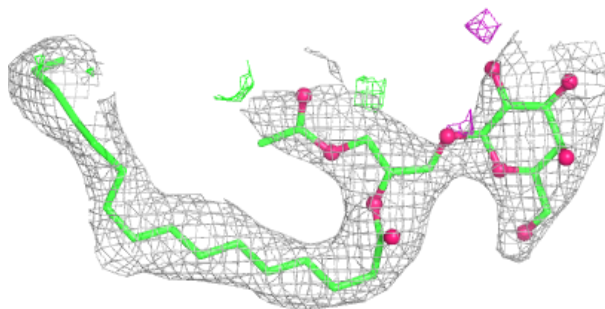
**Electron density around BCR F2 401:**

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



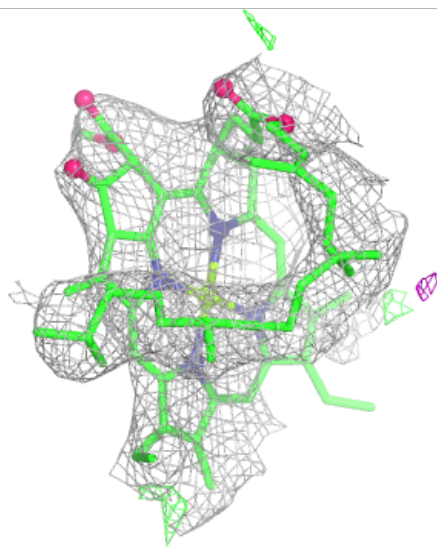
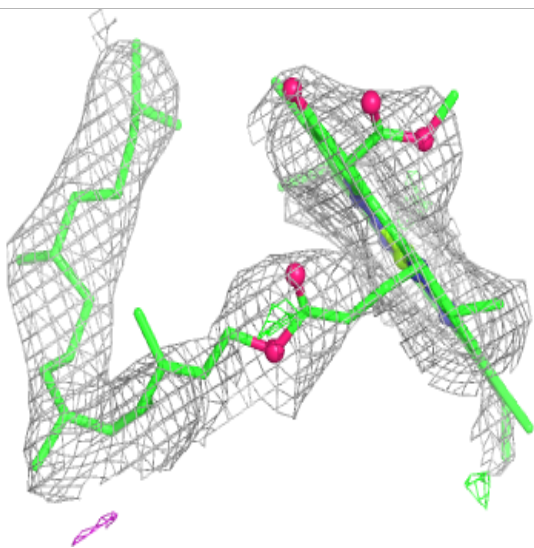
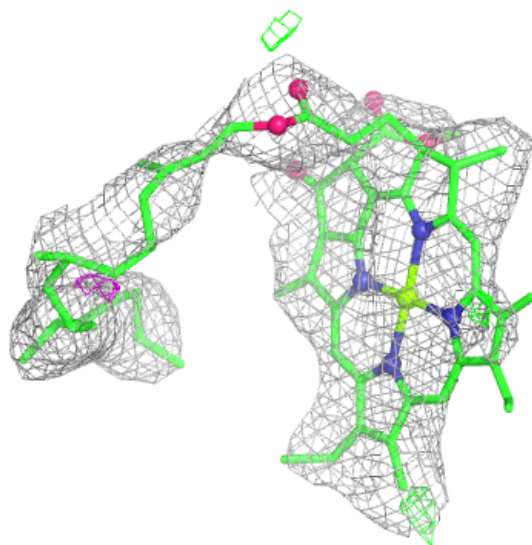
Electron density around LMG B2 621:

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



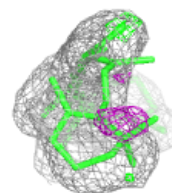
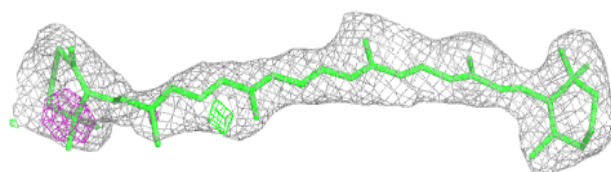
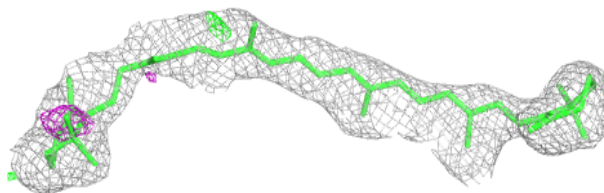
Electron density around CLA C2 505:

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



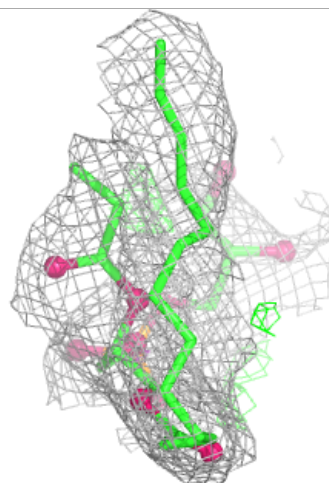
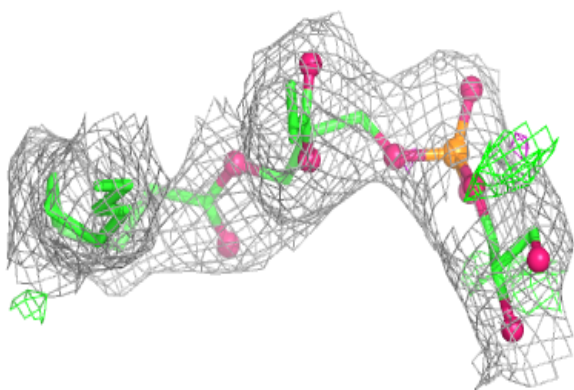
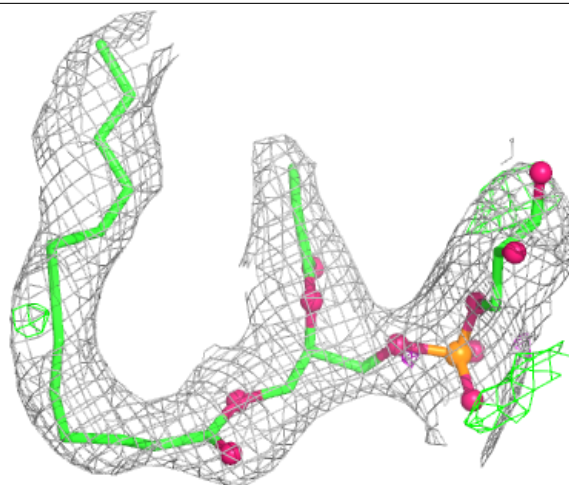
Electron density around BCR B1 602:

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



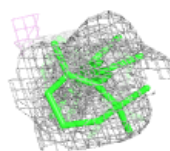
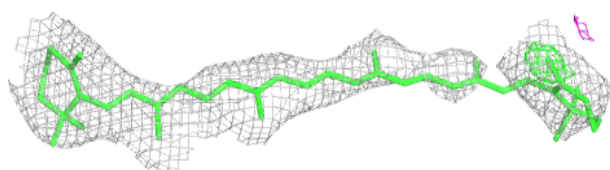
Electron density around LHG A2 405:

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

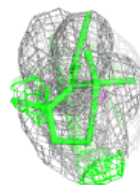
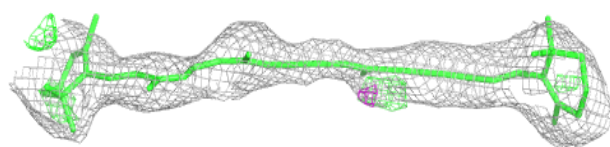
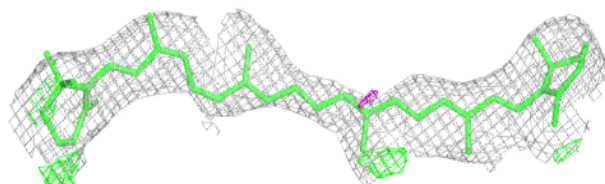


Electron density around BCR C2 502:

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

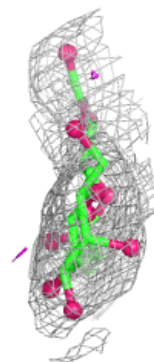
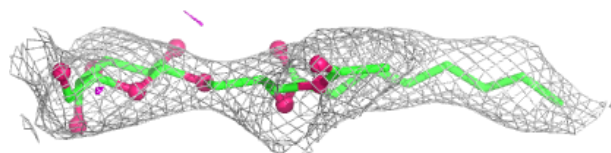
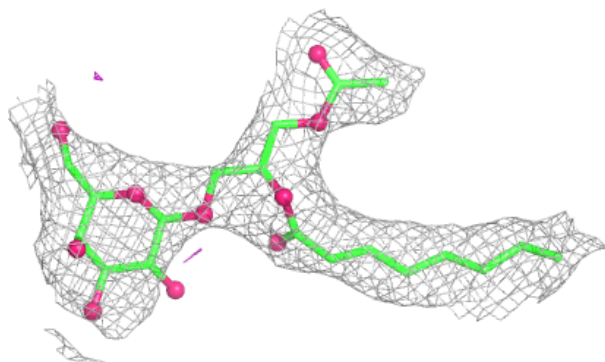
**Electron density around BCR J1 101:**

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



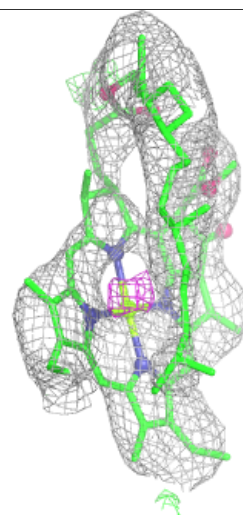
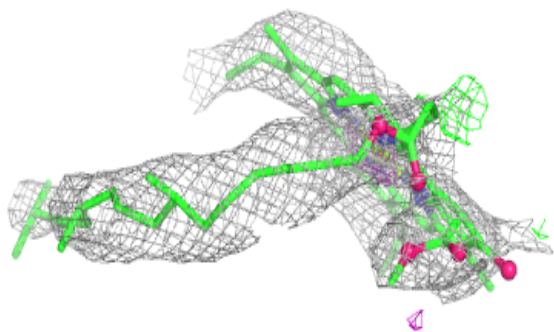
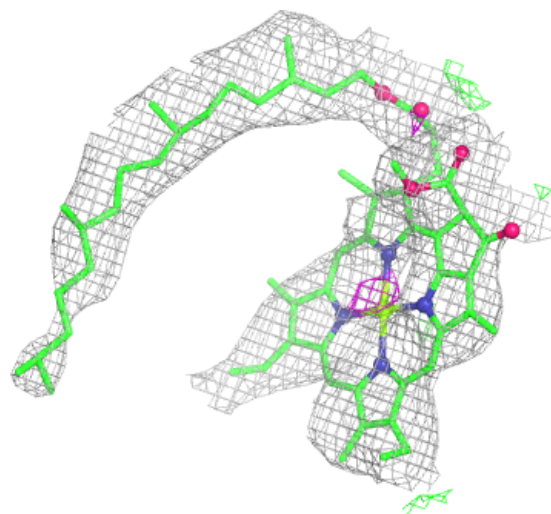
Electron density around LMG A2 412:

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



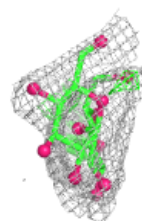
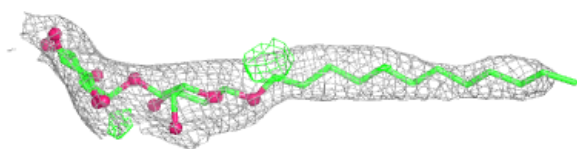
Electron density around CLA C2 509:

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

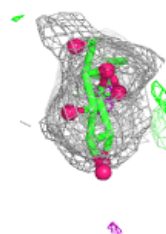
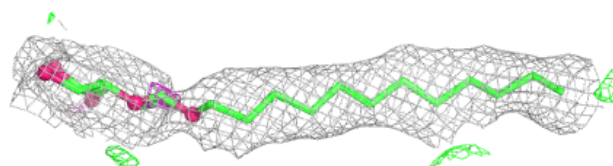
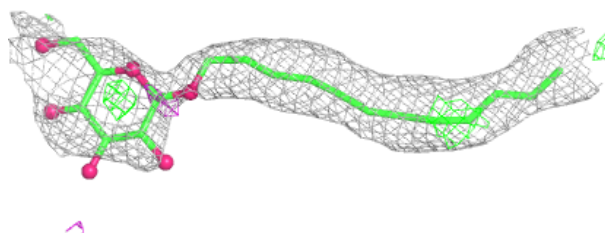


Electron density around LMT C1 519:

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

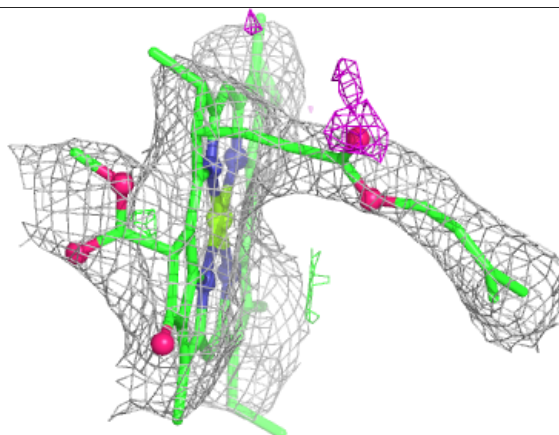
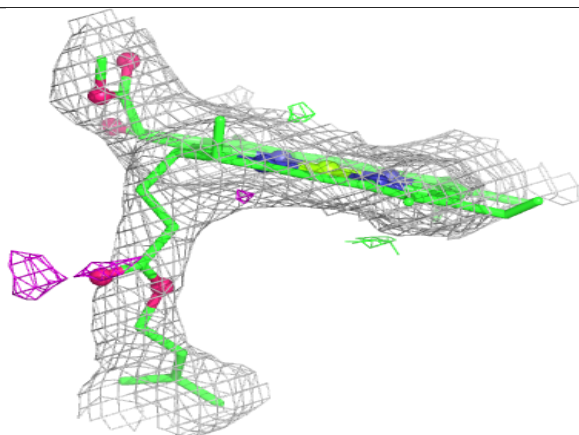
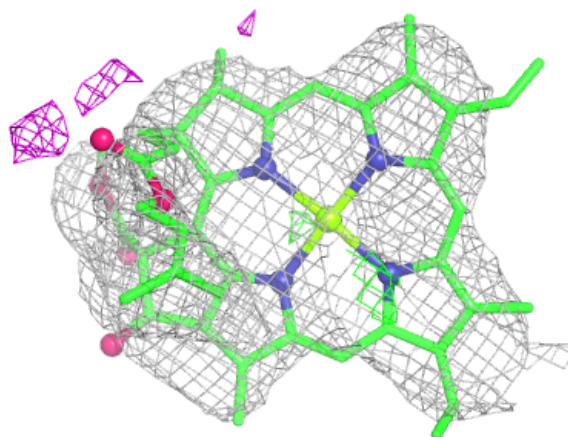
**Electron density around LMT M1 103:**

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

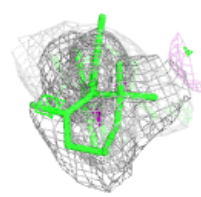
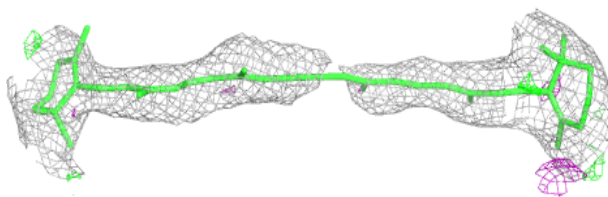
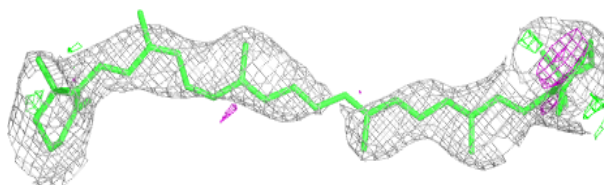


Electron density around CLA C2 511:

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

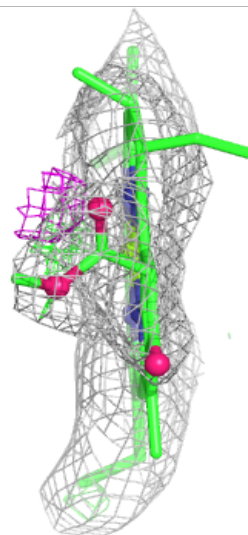
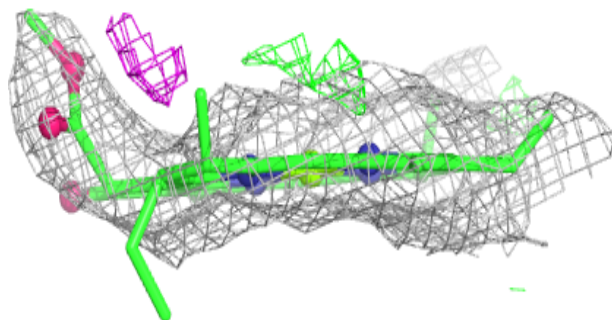
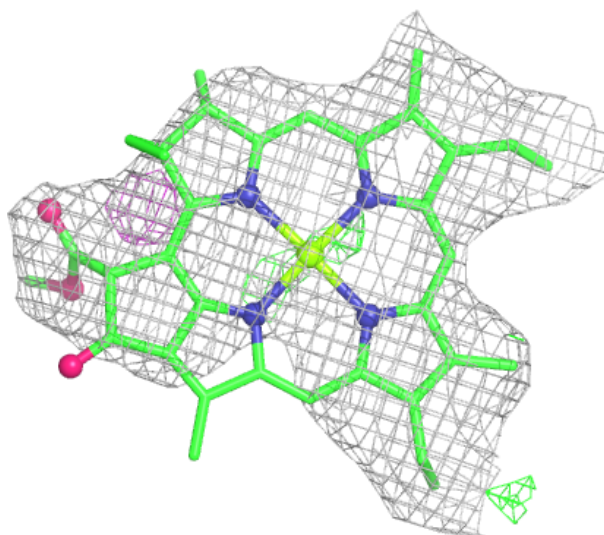
**Electron density around BCR k1 101:**

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



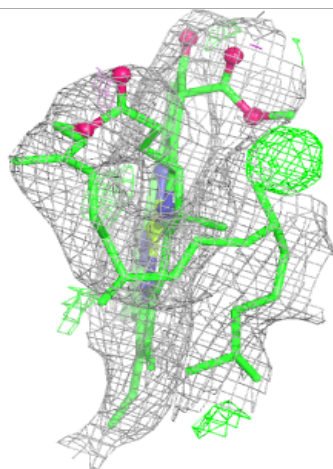
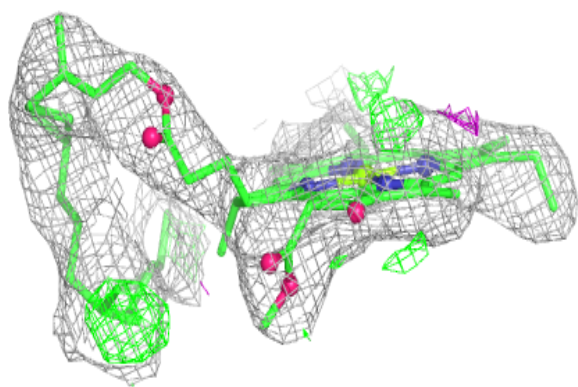
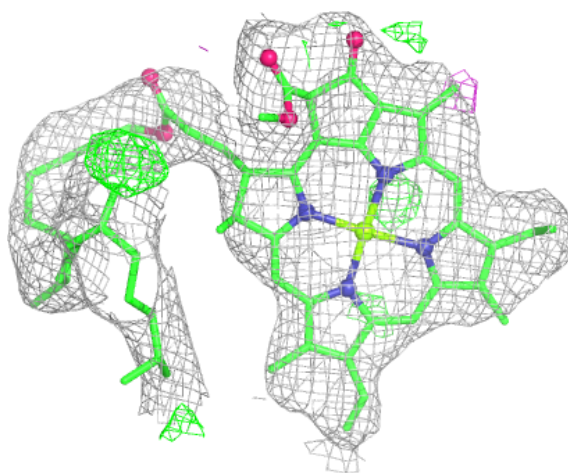
Electron density around CLA B1 604:

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



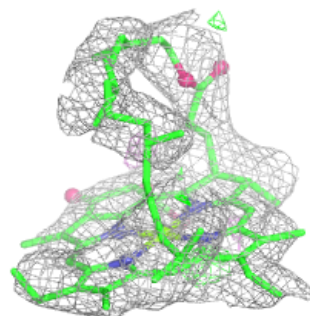
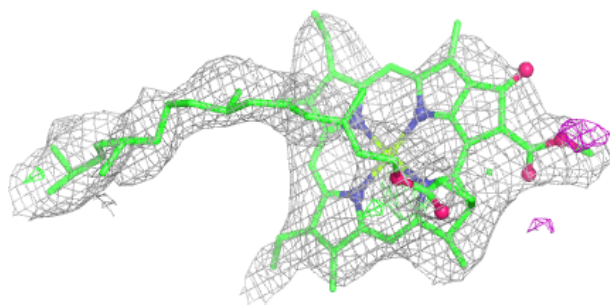
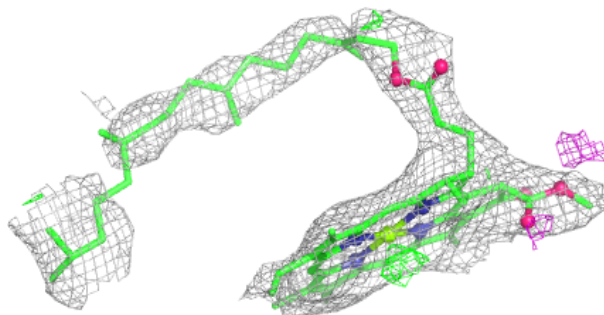
Electron density around CLA C1 512:

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

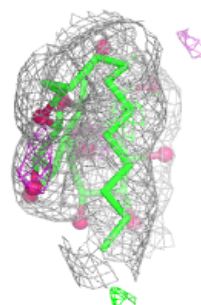
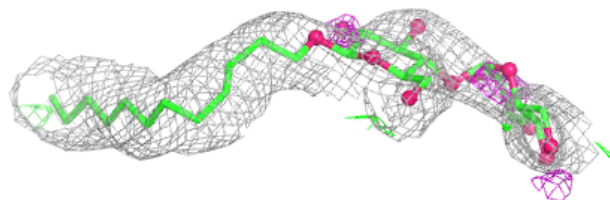
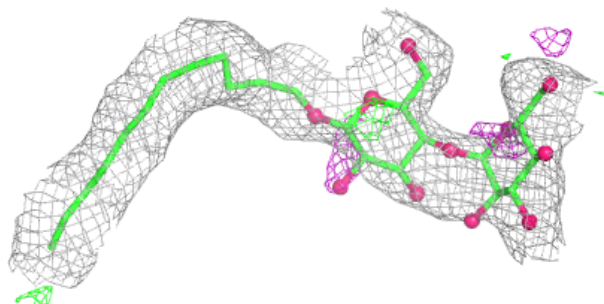


Electron density around CLA c1 516:

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

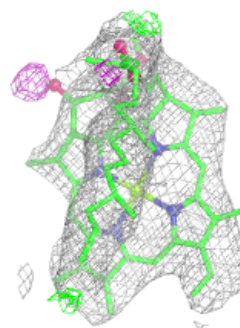
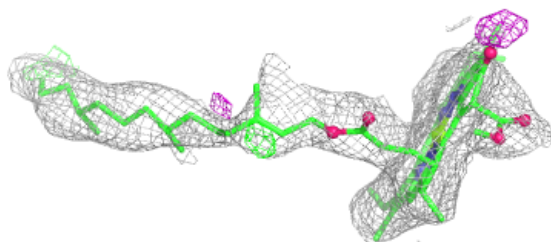
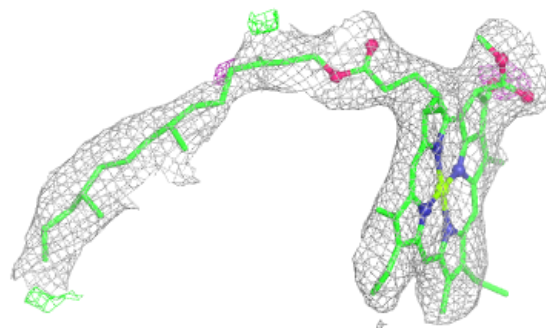
**Electron density around LMT a2 406:**

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



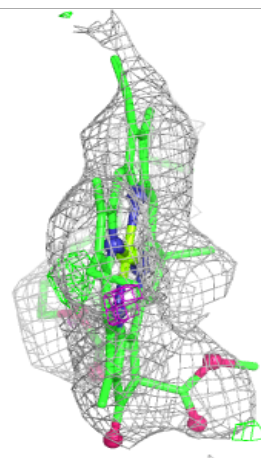
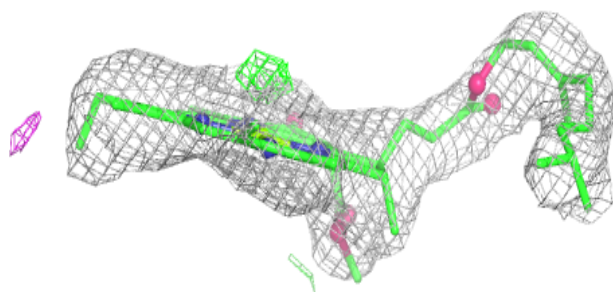
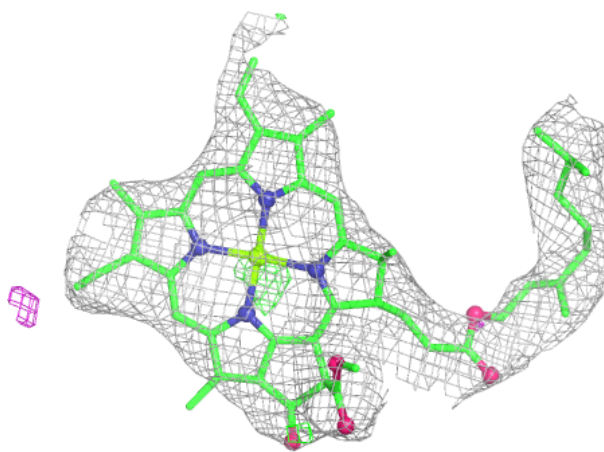
Electron density around CLA B1 611:

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



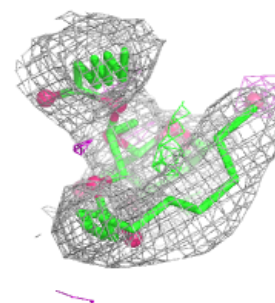
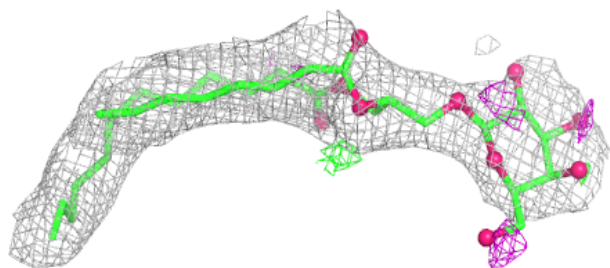
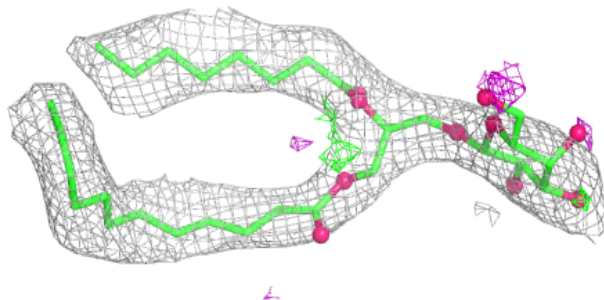
Electron density around CLA c1 515:

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

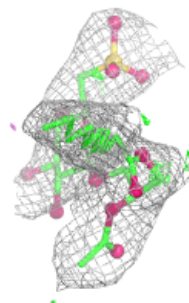
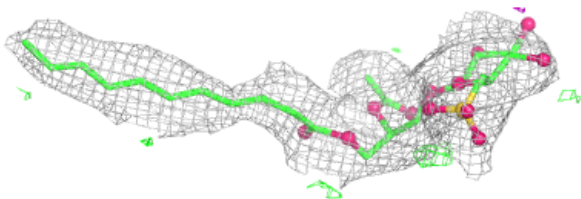
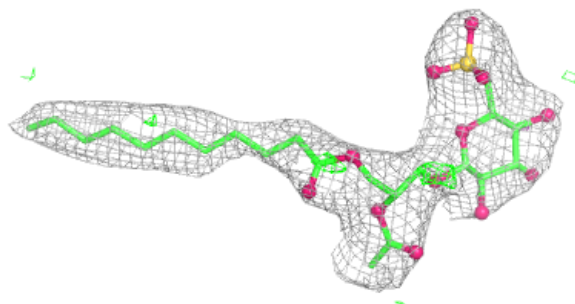


Electron density around LMG b1 624:

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

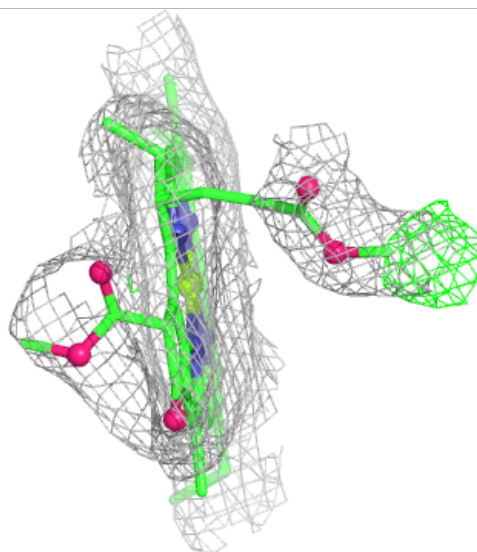
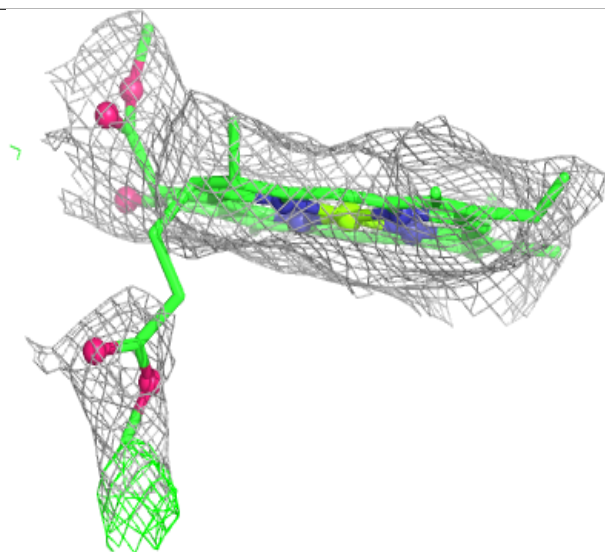
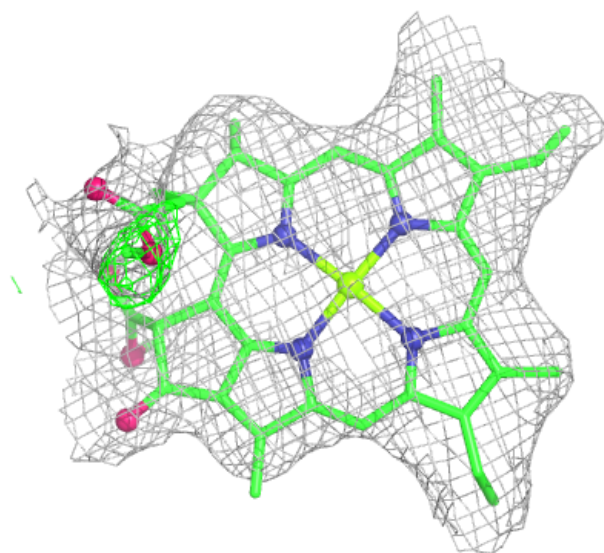
**Electron density around SQD D1 409:**

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



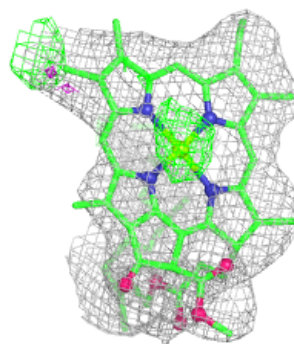
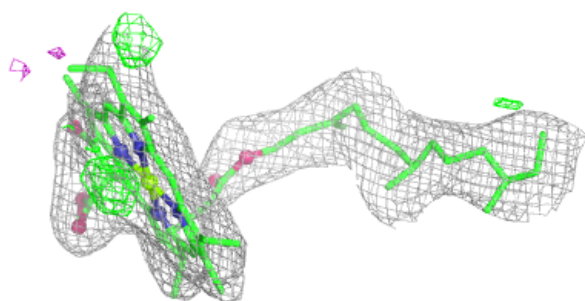
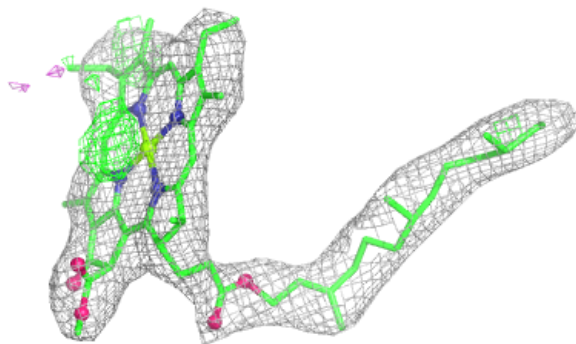
Electron density around CLA C2 504:

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



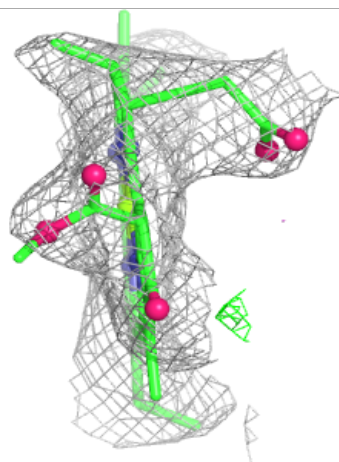
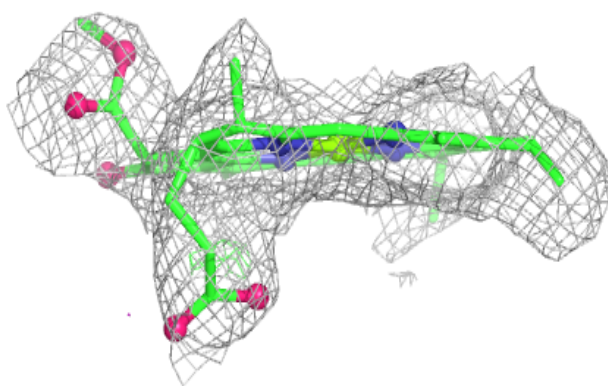
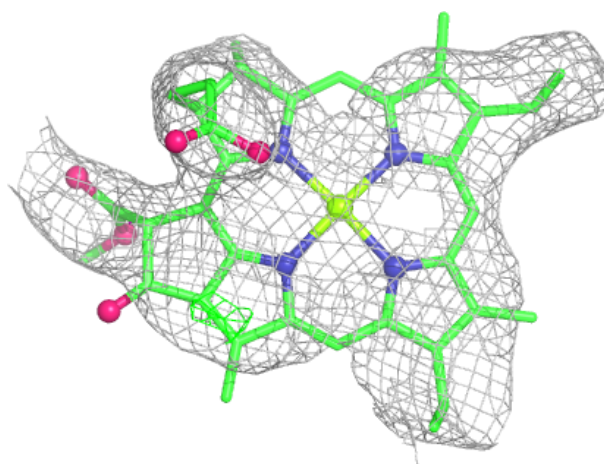
Electron density around CLA C1 513:

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



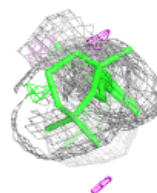
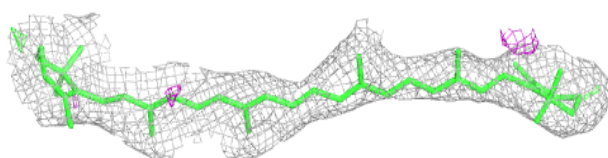
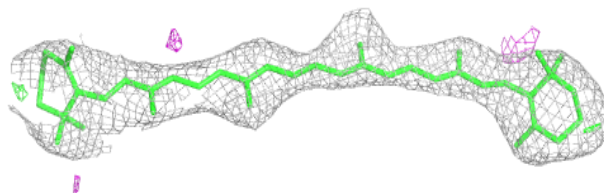
Electron density around CLA C2 507:

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

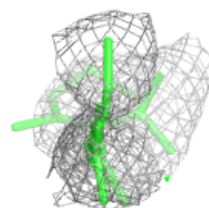
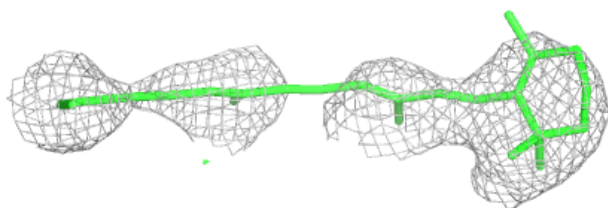
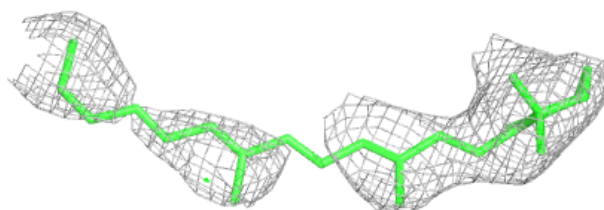


Electron density around BCR b2 603:

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

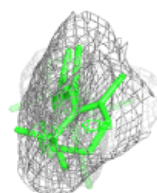
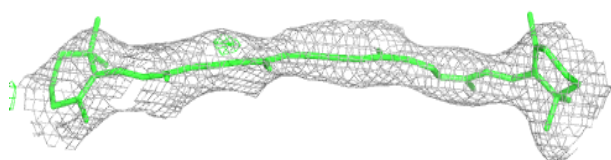
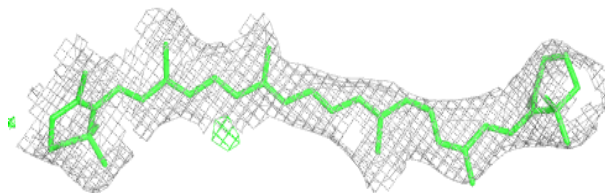
**Electron density around BCR H2 103:**

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

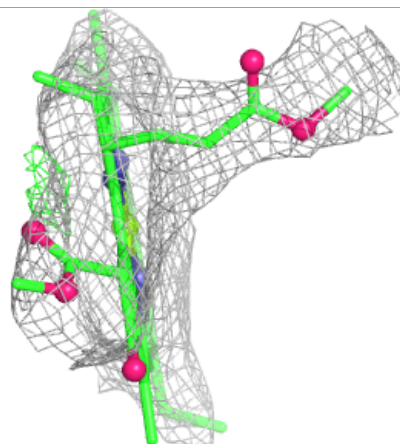
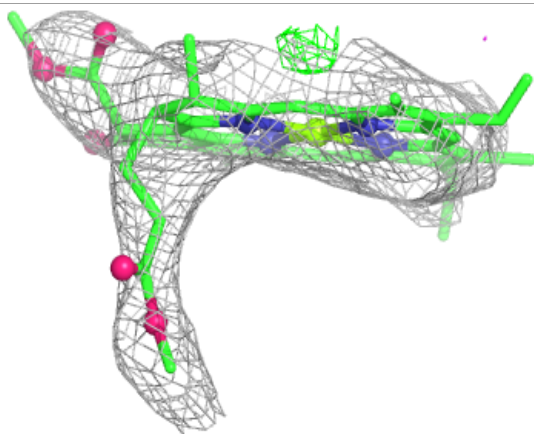
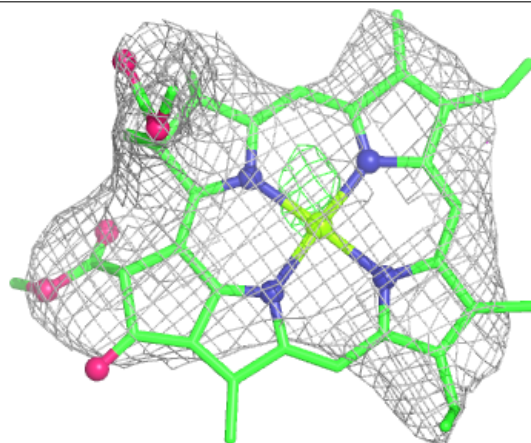


Electron density around BCR j2 102:

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

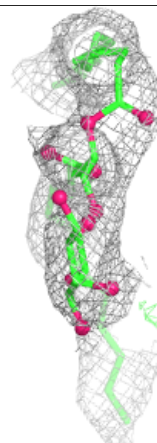
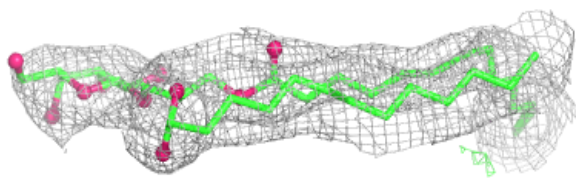
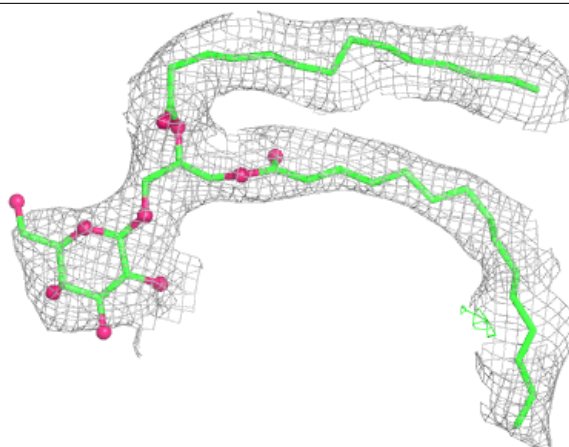
**Electron density around CLA c2 515:**

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

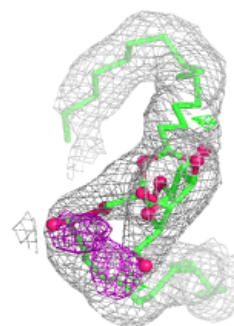
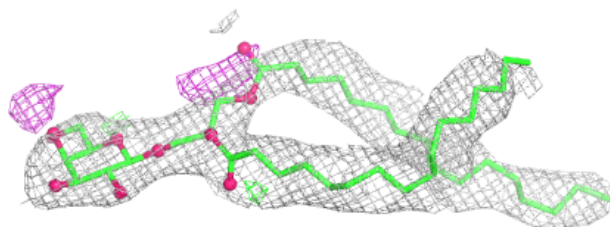
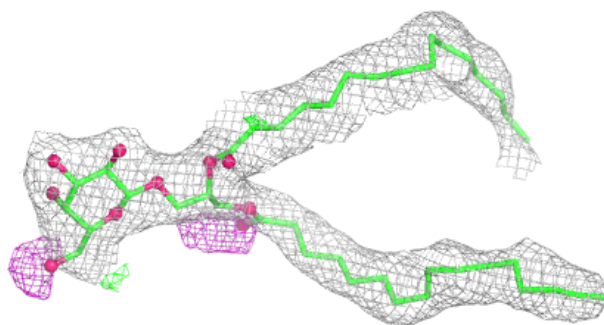


Electron density around LMG C1 520:

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

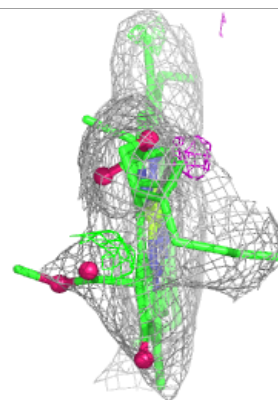
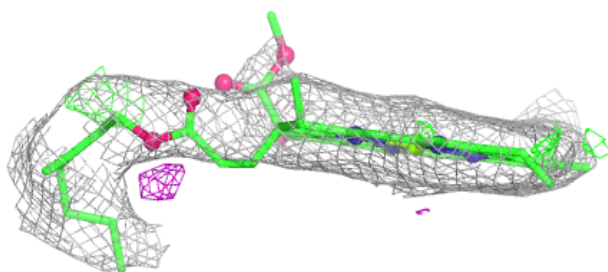
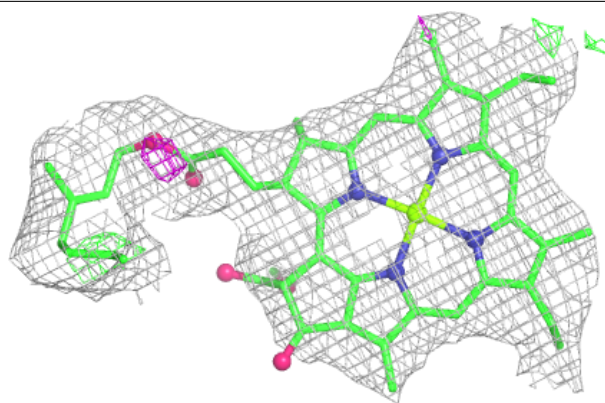
**Electron density around LMG a1 412:**

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

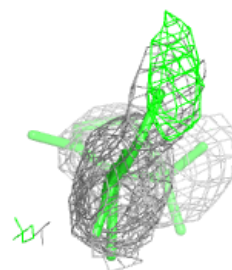
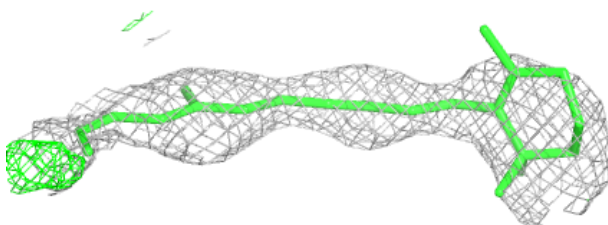
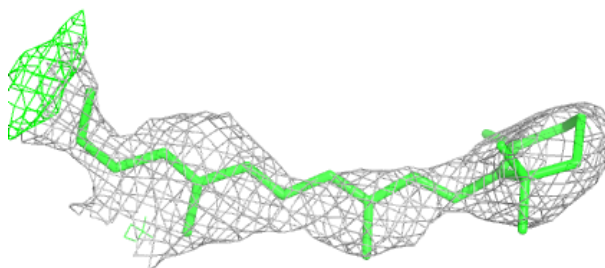


Electron density around CLA C2 513:

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

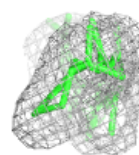
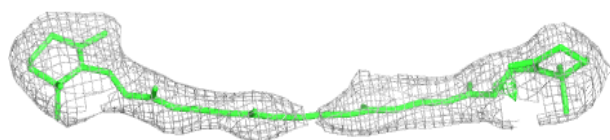
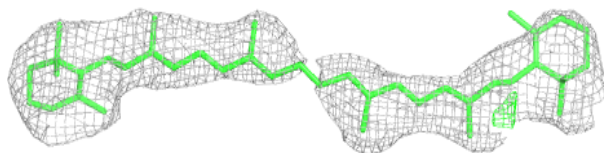
**Electron density around BCR H1 102:**

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

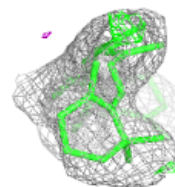
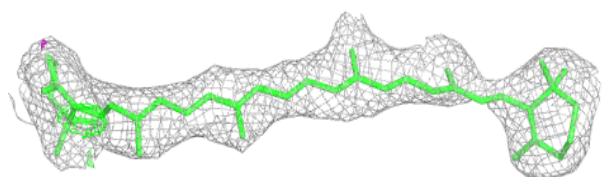
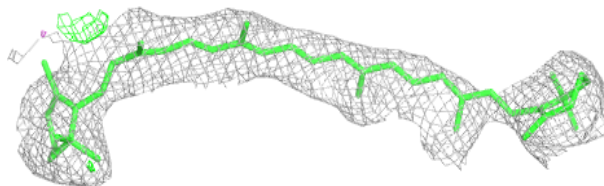


Electron density around BCR D1 401:

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

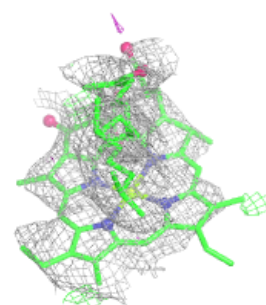
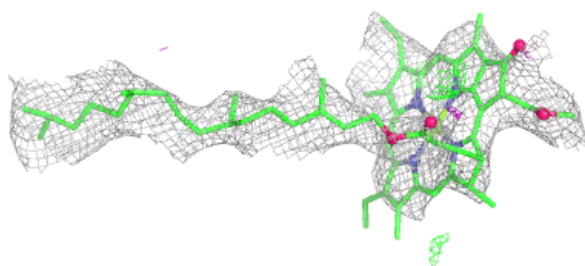
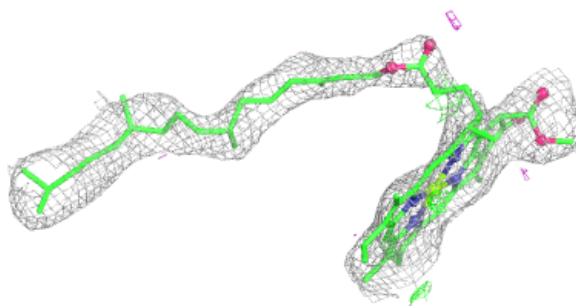
**Electron density around BCR b2 602:**

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

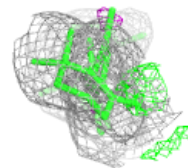
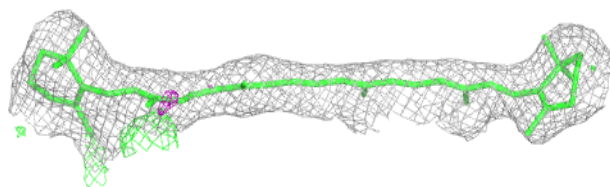
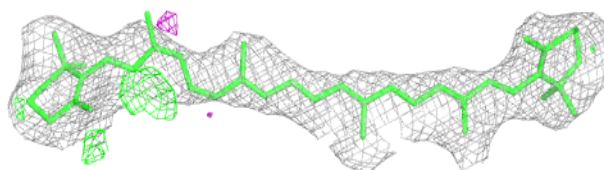


Electron density around CLA C2 506:

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

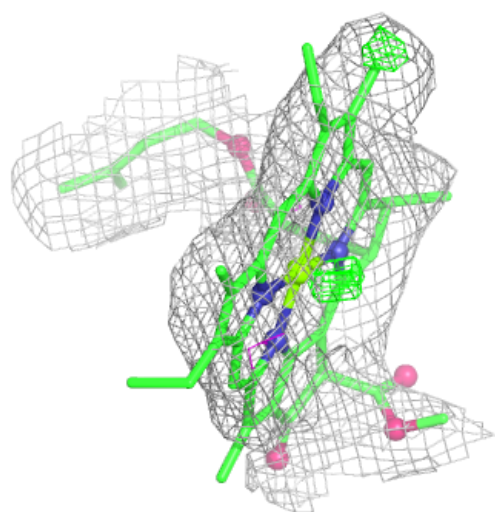
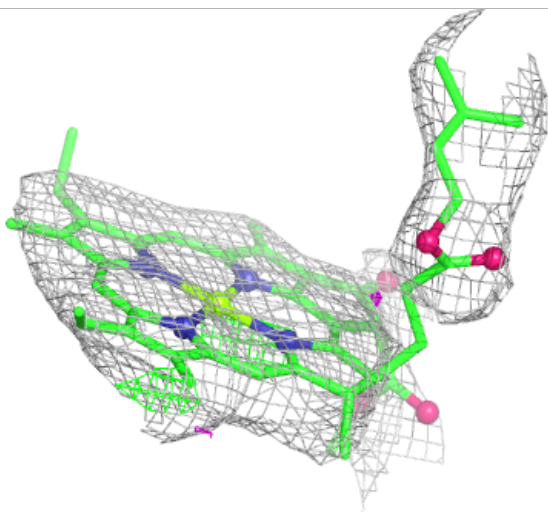
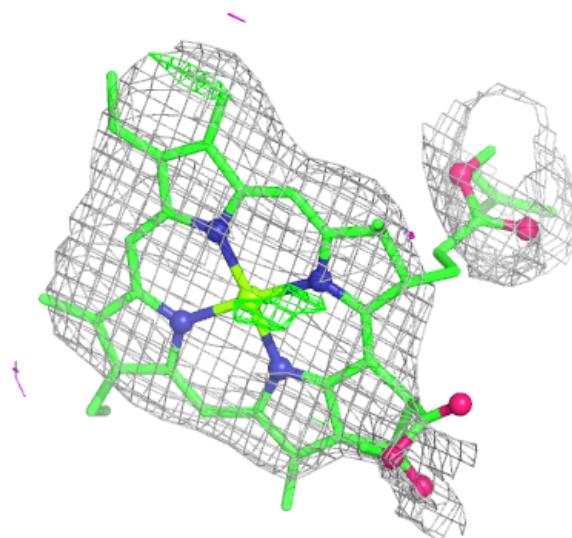
**Electron density around BCR b1 602:**

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



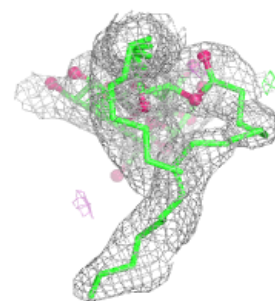
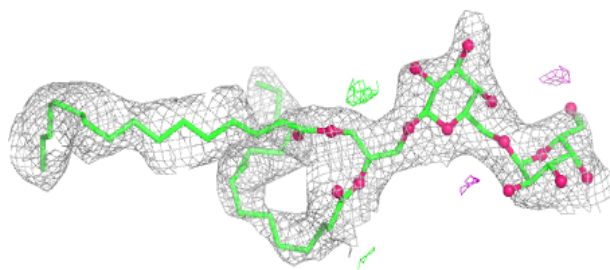
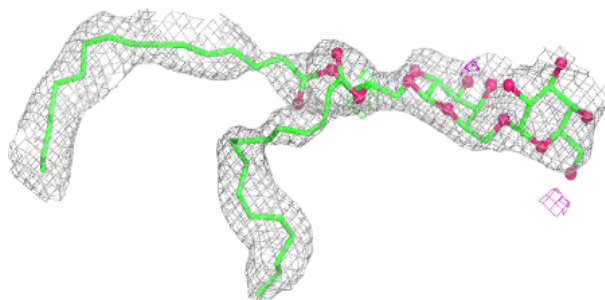
Electron density around CLA C2 508:

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



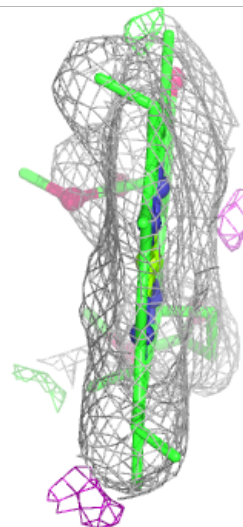
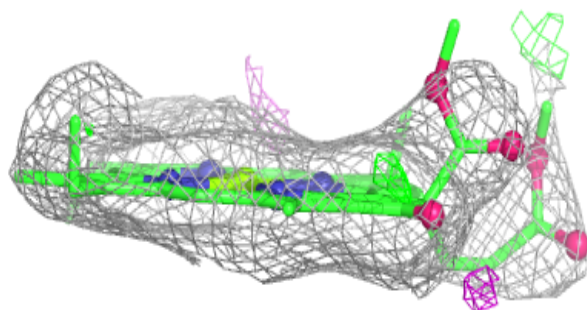
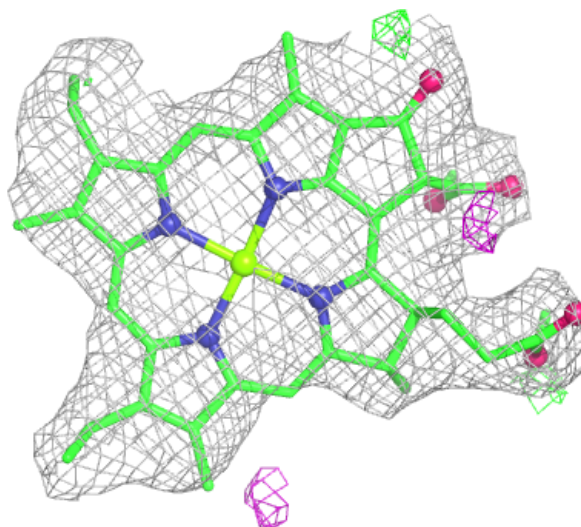
Electron density around DGD H2 101:

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



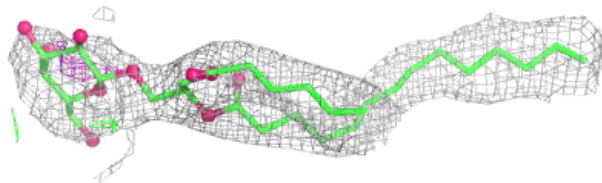
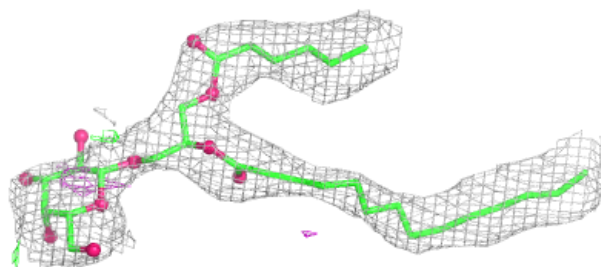
Electron density around CLA C2 516:

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



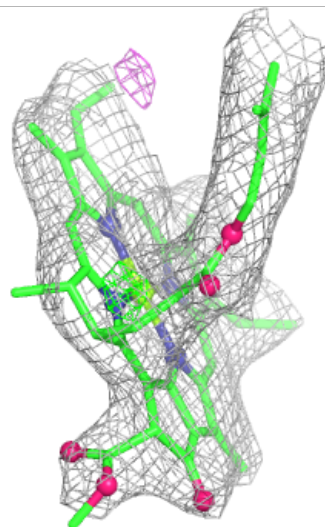
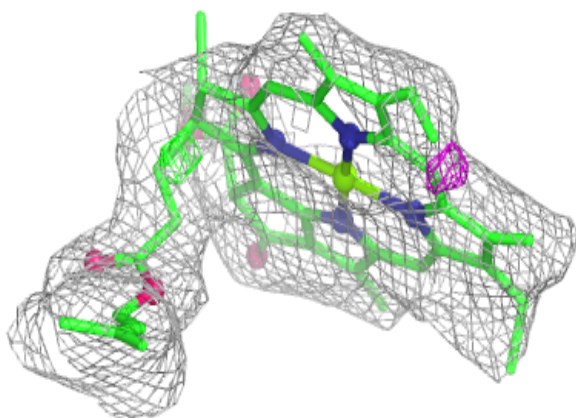
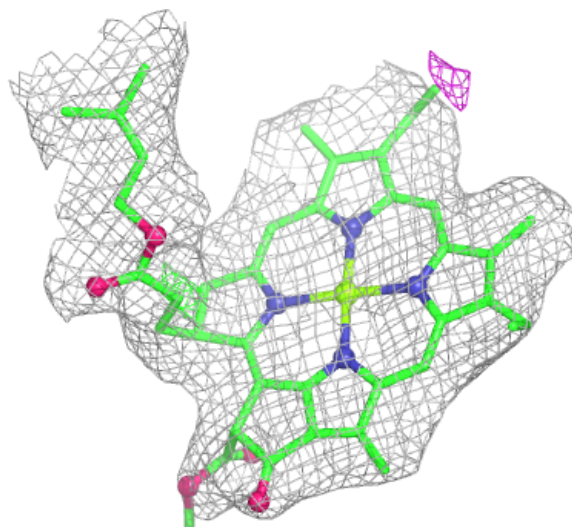
Electron density around LMG b2 622:

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



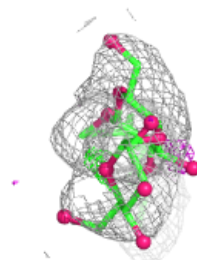
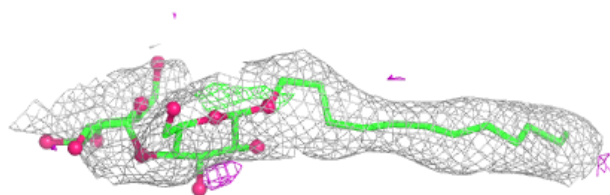
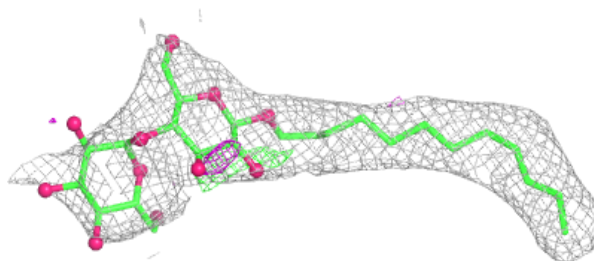
Electron density around CLA d2 404:

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



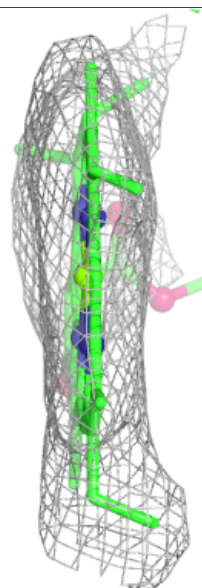
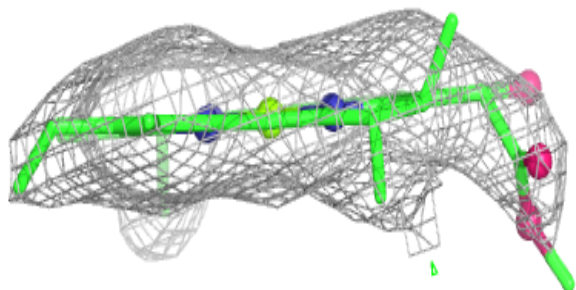
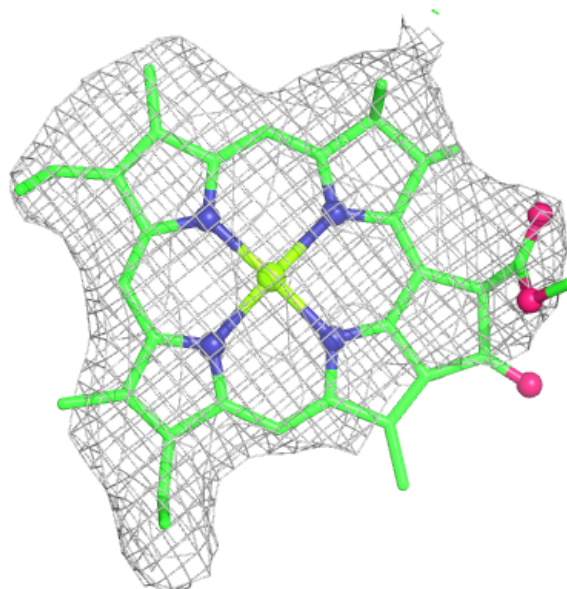
Electron density around LMT m1 101:

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



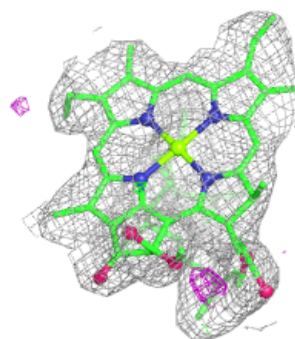
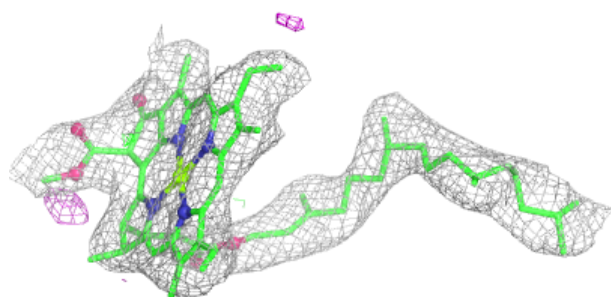
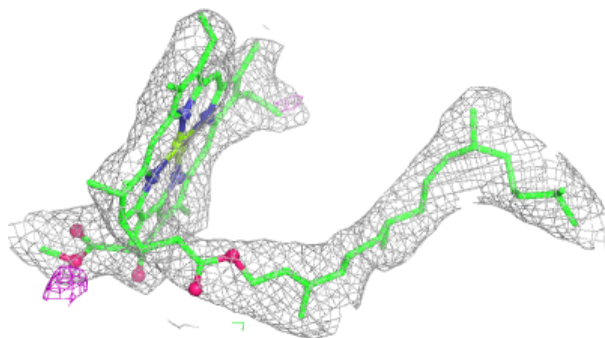
Electron density around CLA B2 604:

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

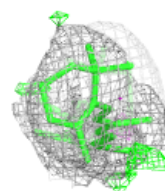
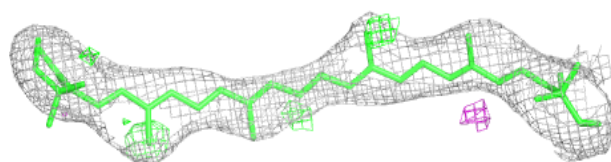
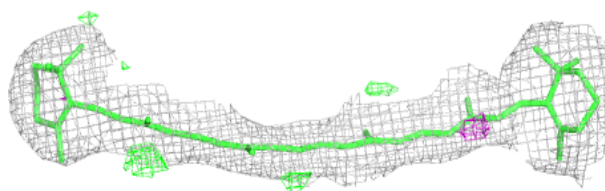


Electron density around CLA c2 509:

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

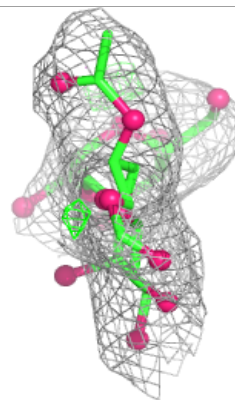
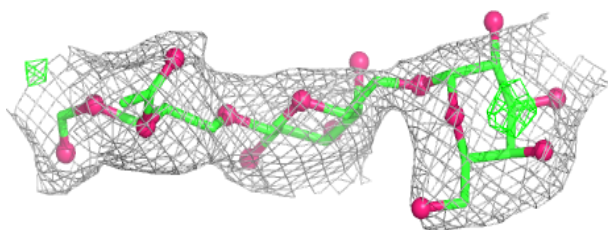
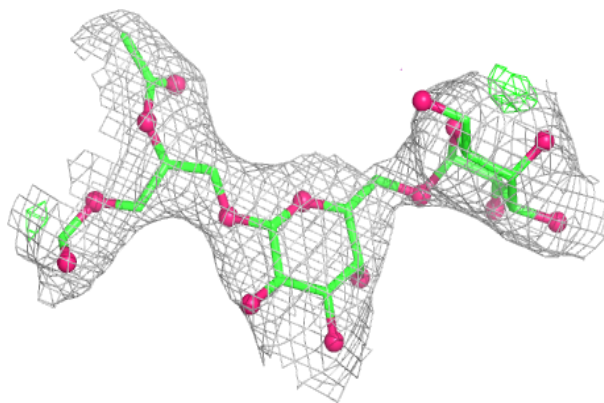
**Electron density around BCR C1 521:**

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

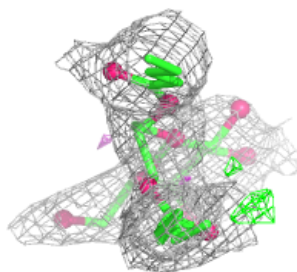
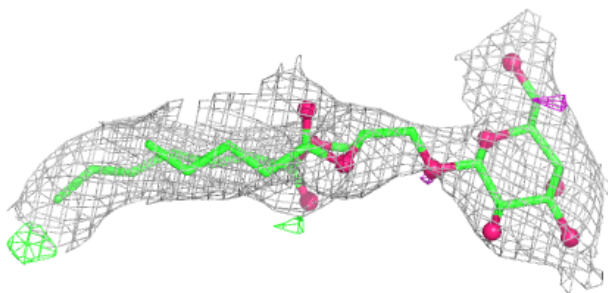
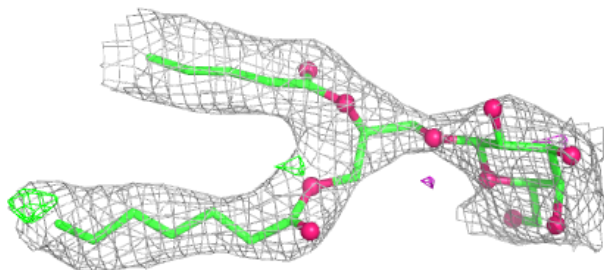


Electron density around DGD C2 512:

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

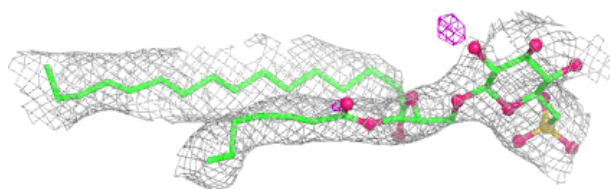
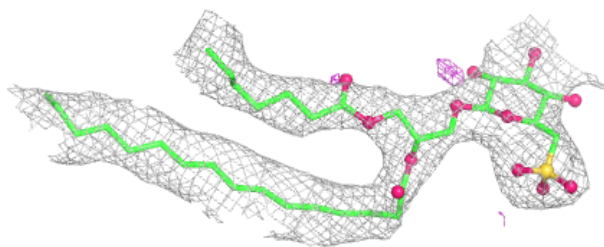
**Electron density around LMG B1 622:**

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

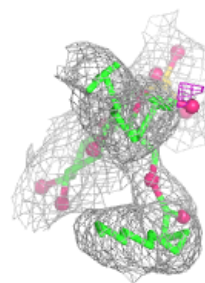
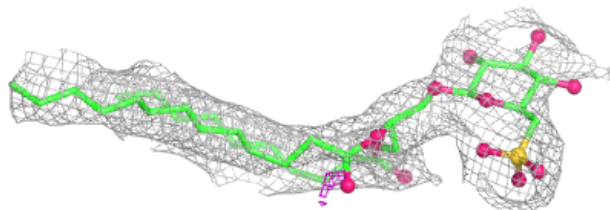
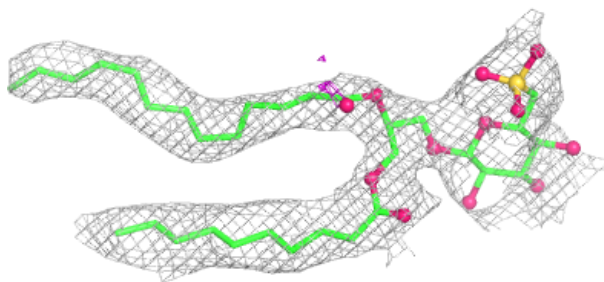


Electron density around SQD B2 623:

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

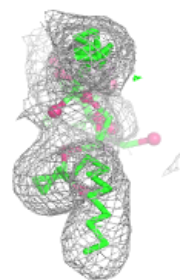
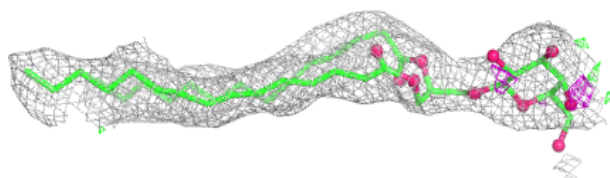
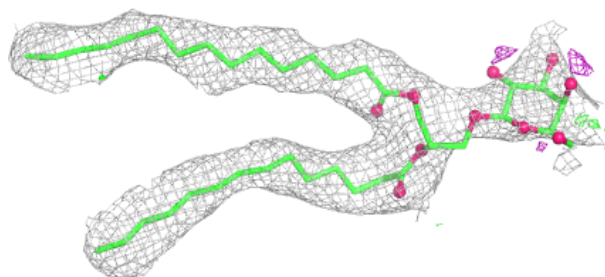
**Electron density around SQD b2 605:**

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



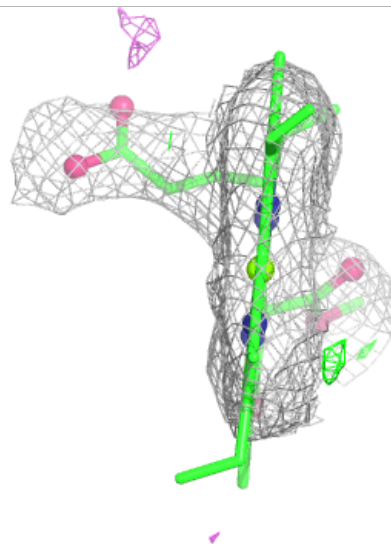
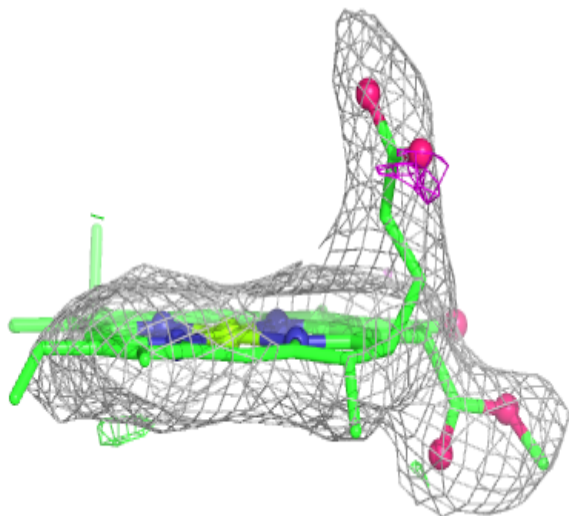
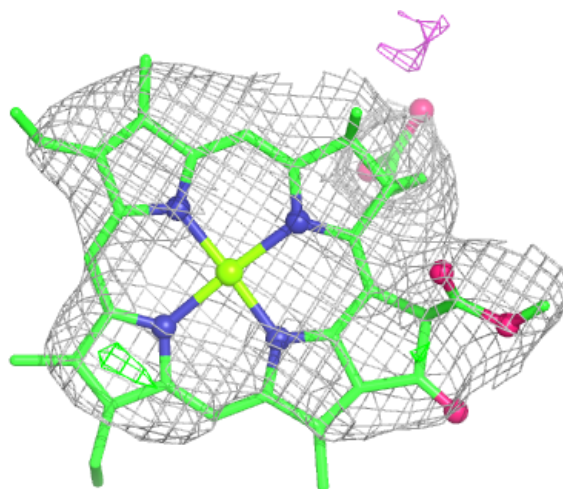
Electron density around LMG B1 626:

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



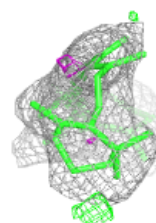
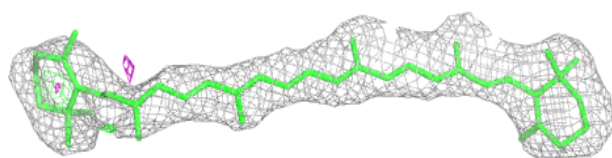
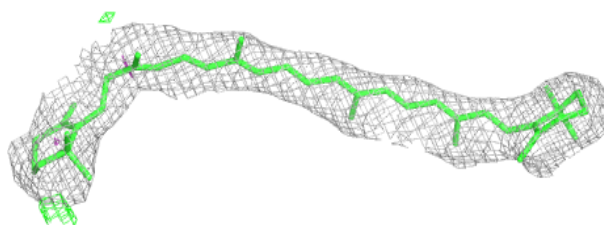
Electron density around CLA C1 514:

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

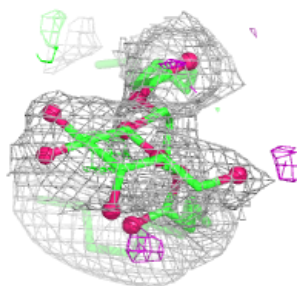
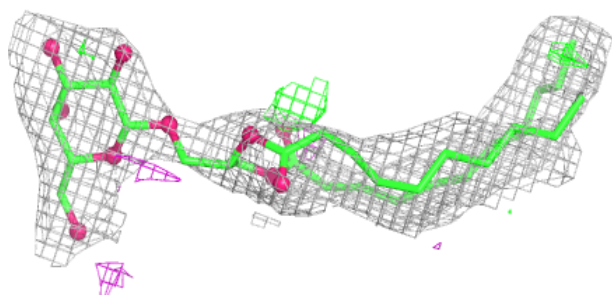
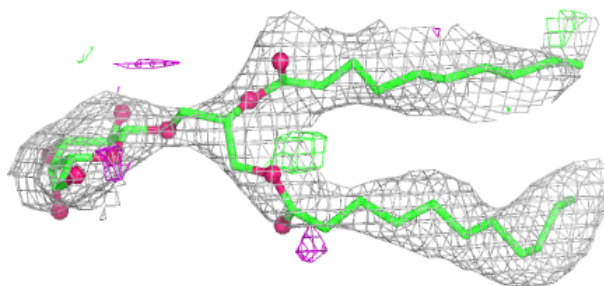


Electron density around BCR B2 602:

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

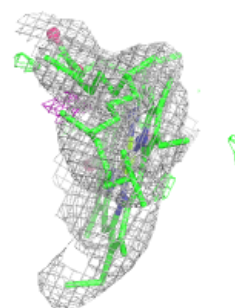
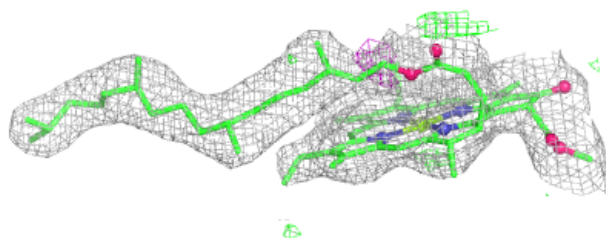
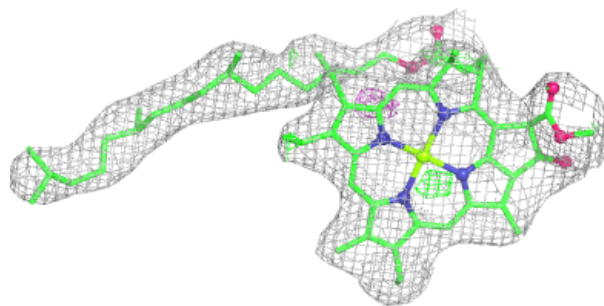
**Electron density around LMG B2 620:**

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

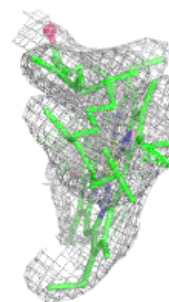
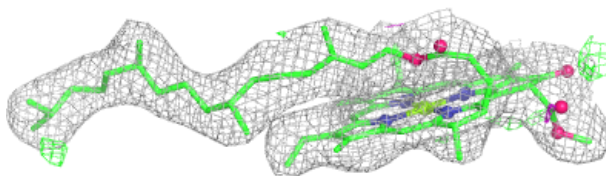
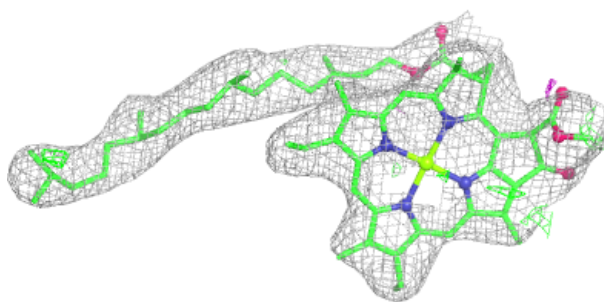


Electron density around CLA c1 503:

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

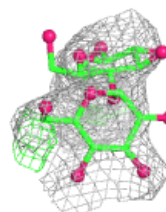
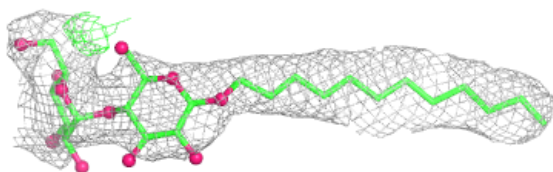
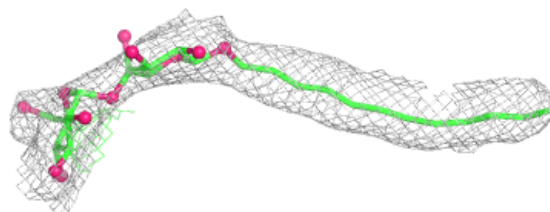
**Electron density around CLA C1 502:**

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



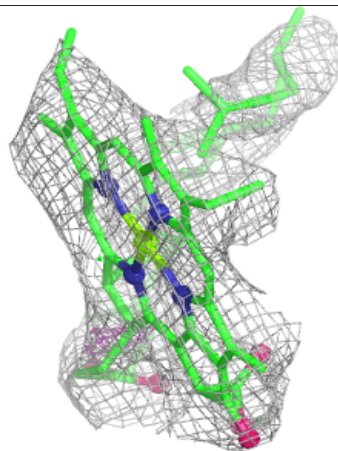
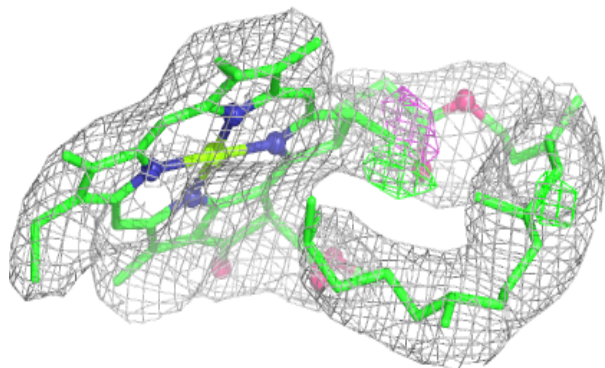
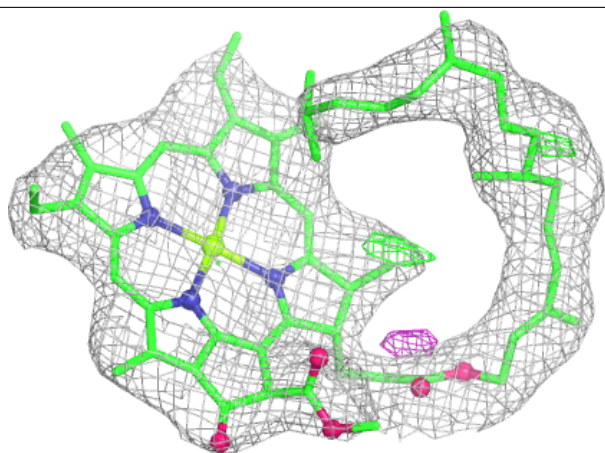
Electron density around LMT b2 623:

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

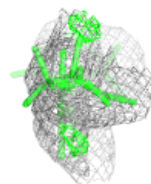
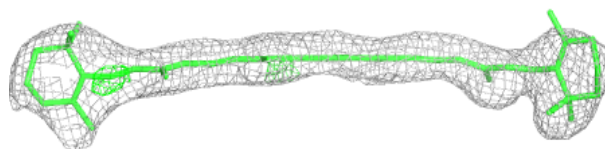
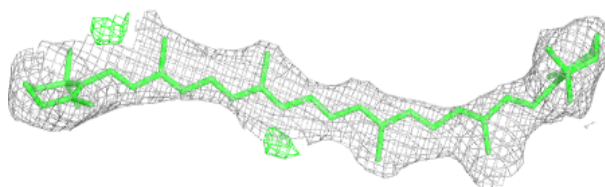


Electron density around CLA b2 618:

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

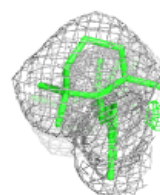
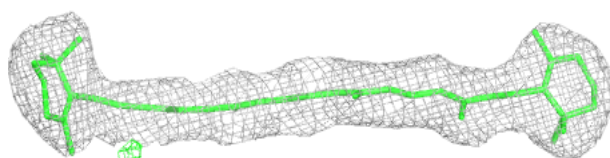
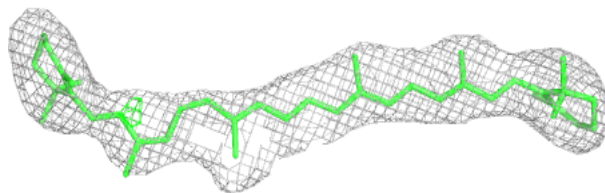
**Electron density around BCR h2 101:**

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

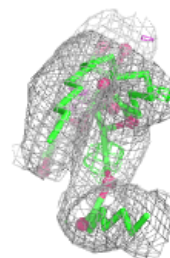
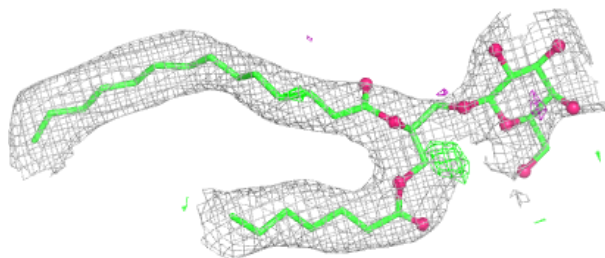


Electron density around BCR c1 502:

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

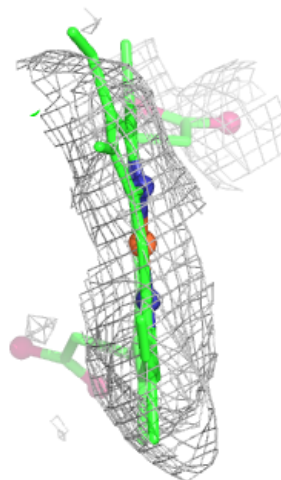
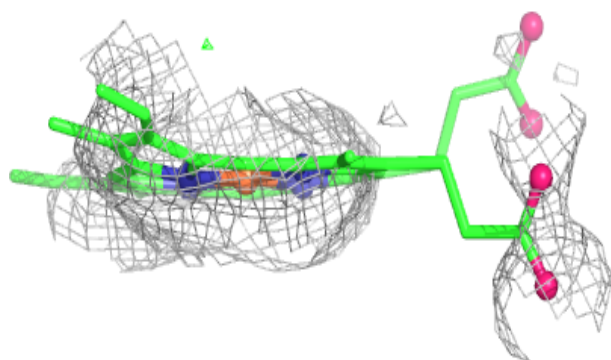
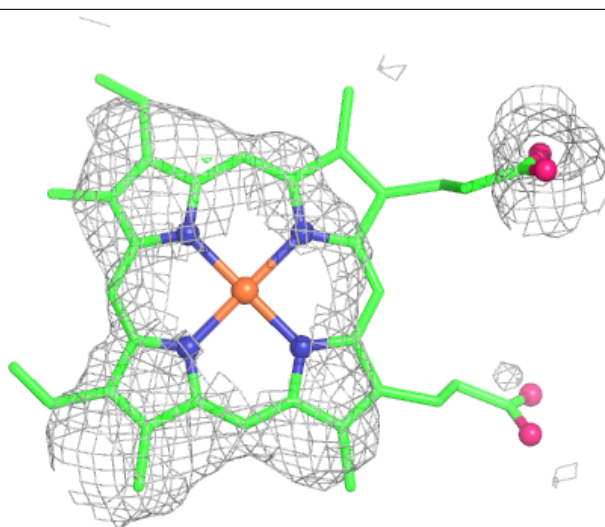
**Electron density around LMG b1 631:**

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



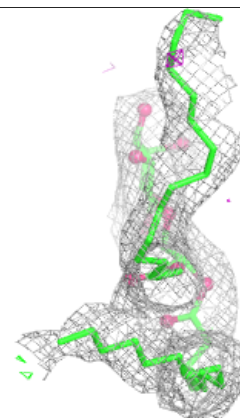
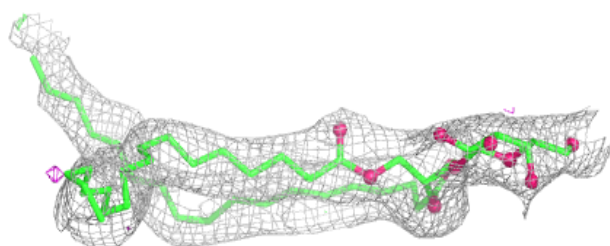
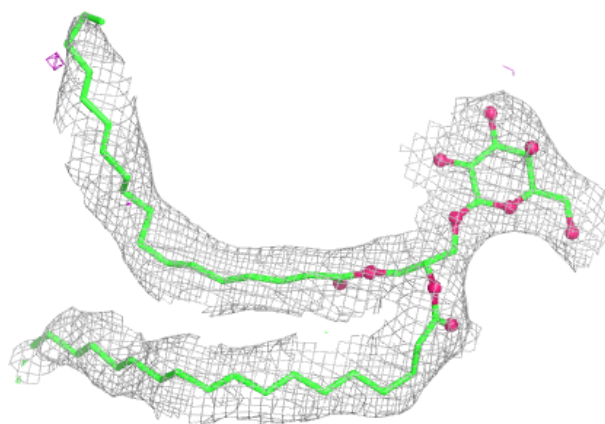
Electron density around HEM E1 101:

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

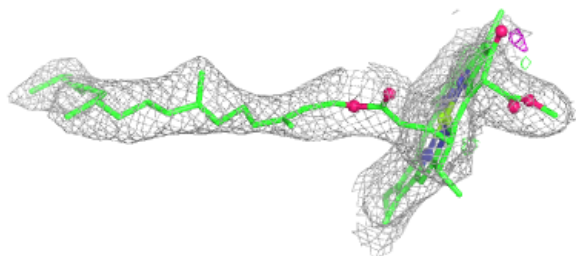
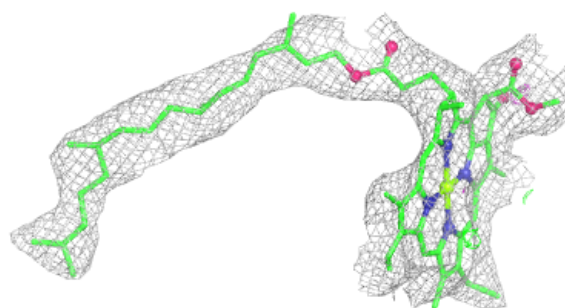


Electron density around LMG c1 519:

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

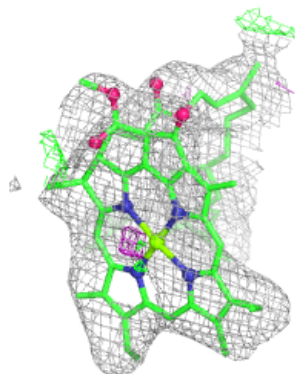
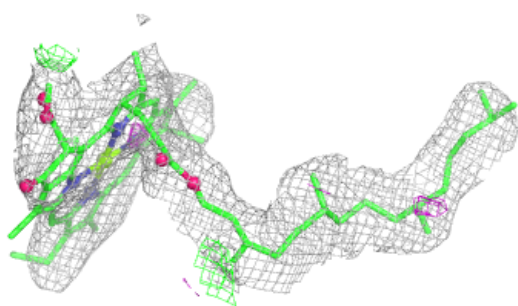
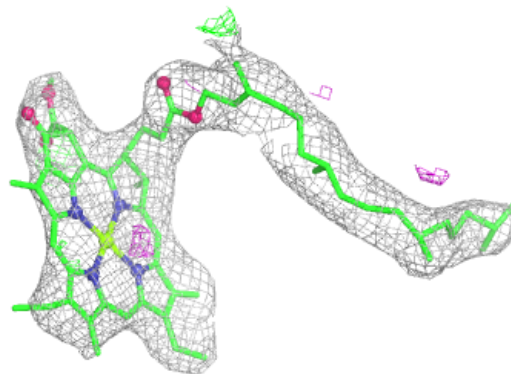
**Electron density around CLA B2 611:**

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

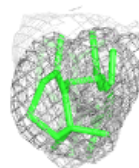
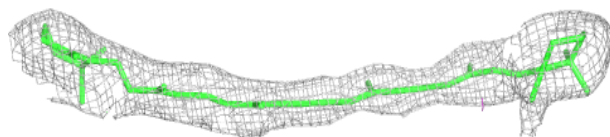
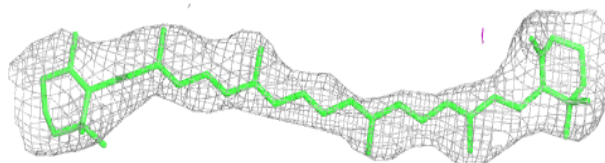


Electron density around CLA c2 512:

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

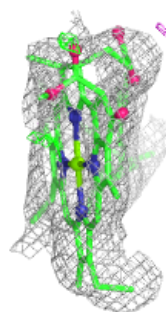
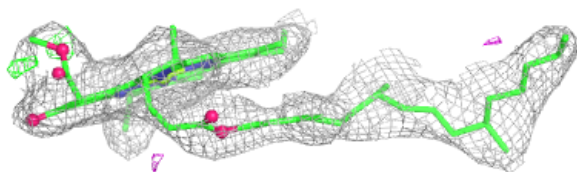
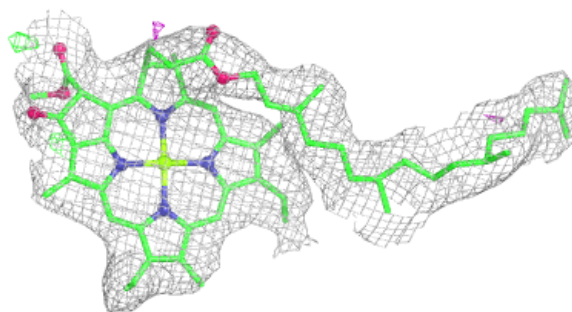
**Electron density around BCR d2 401:**

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

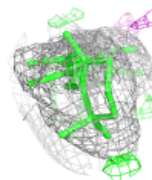
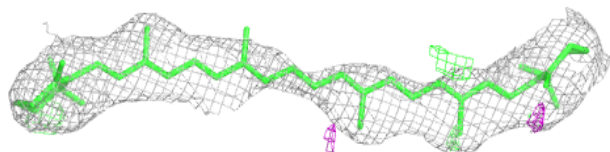
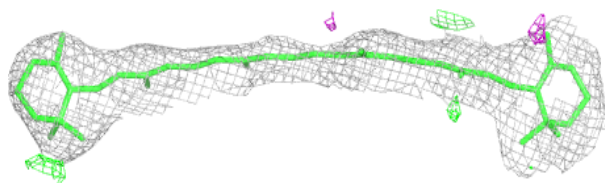


Electron density around CLA B2 606:

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

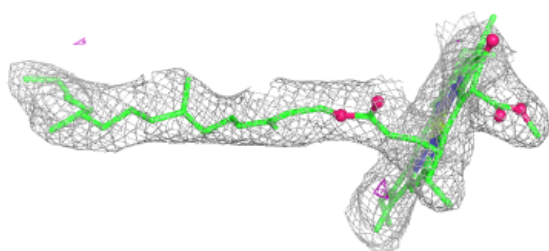
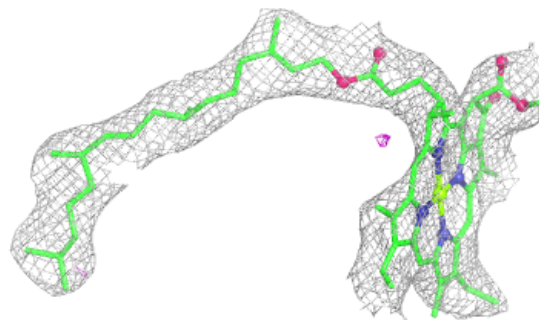
**Electron density around BCR k2 501:**

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

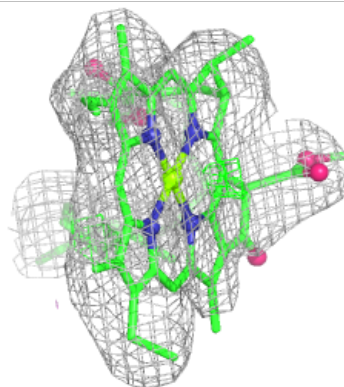
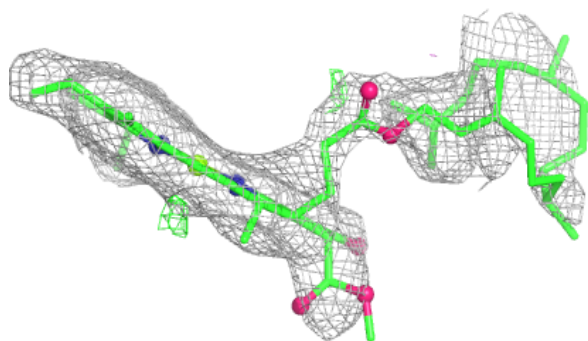
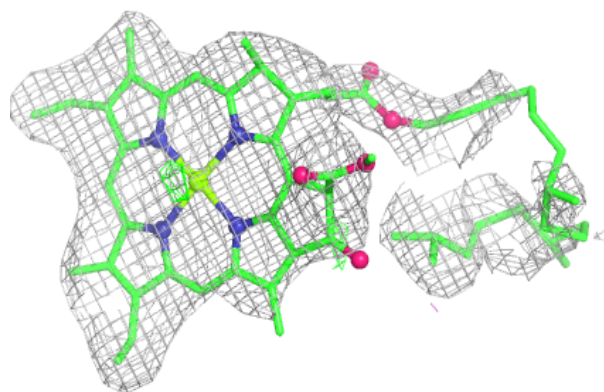


Electron density around CLA b2 610:

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

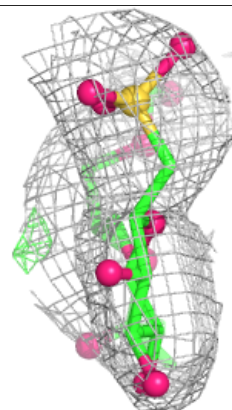
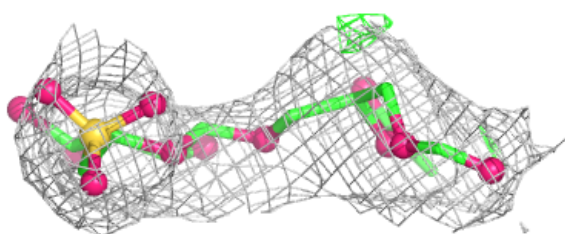
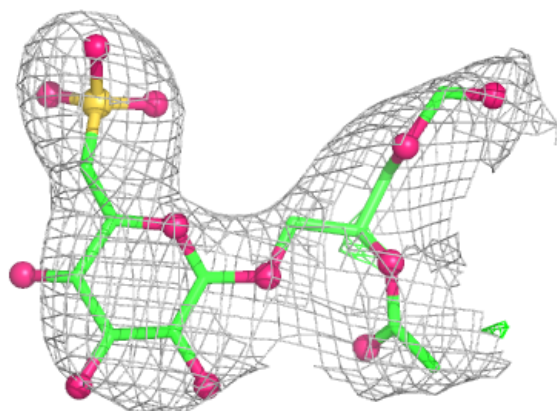
**Electron density around CLA b1 604:**

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

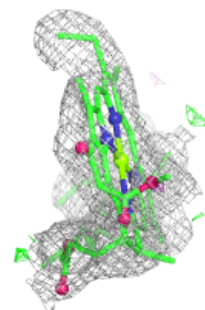
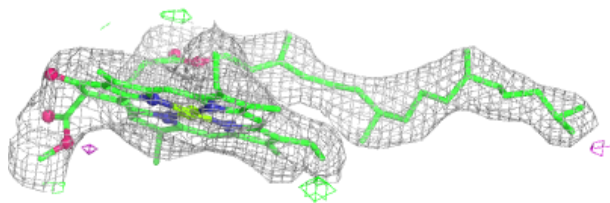
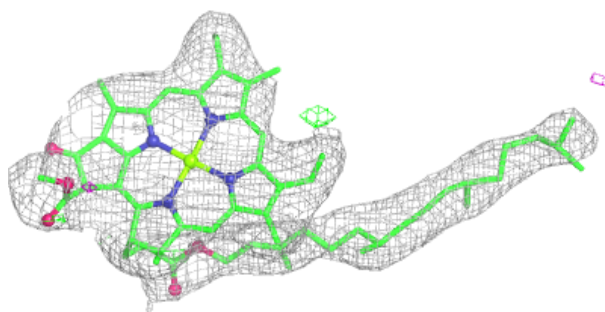


Electron density around SQD D2 402:

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

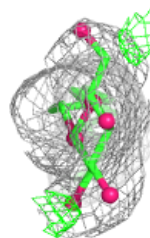
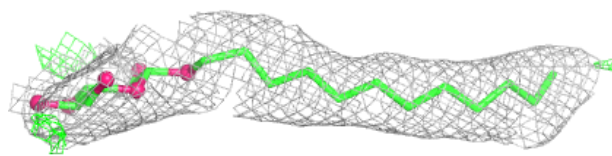
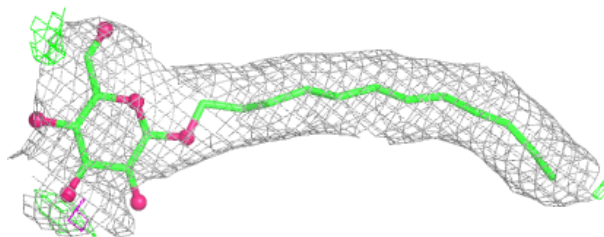
**Electron density around CLA c2 502:**

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



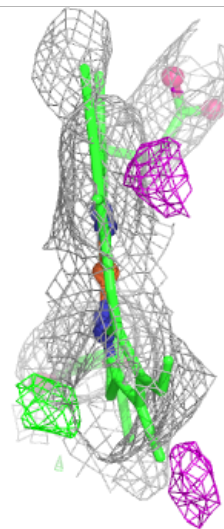
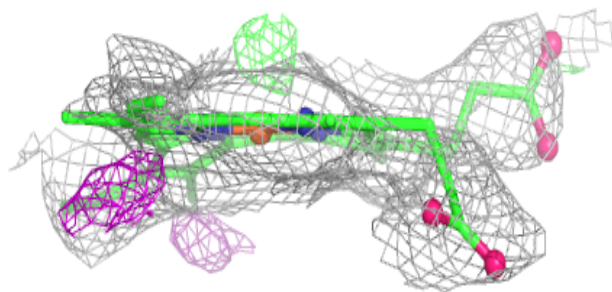
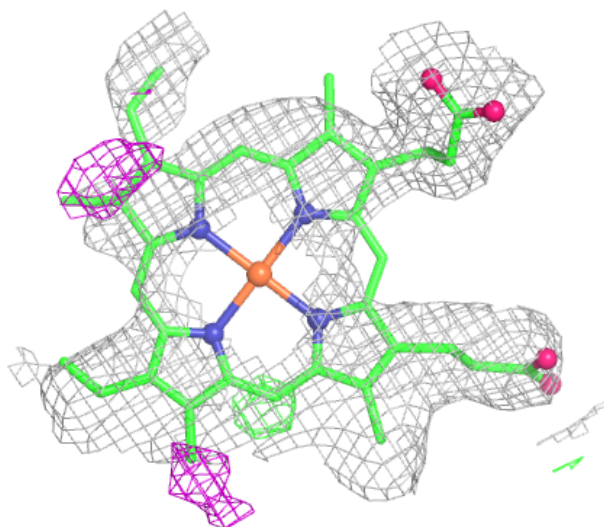
Electron density around LMT 11 101:

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



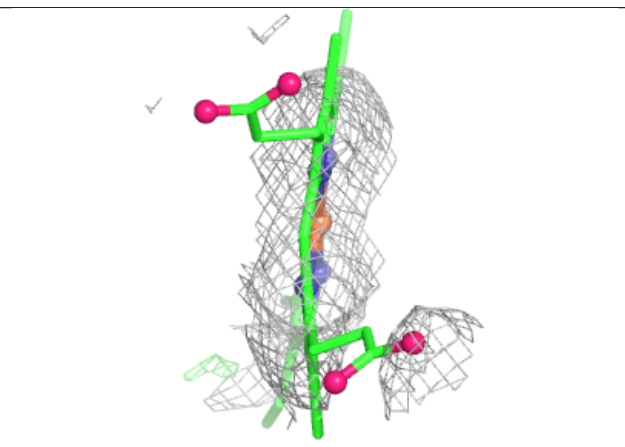
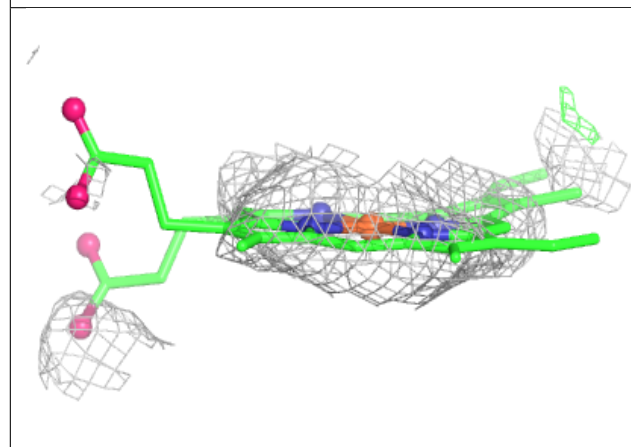
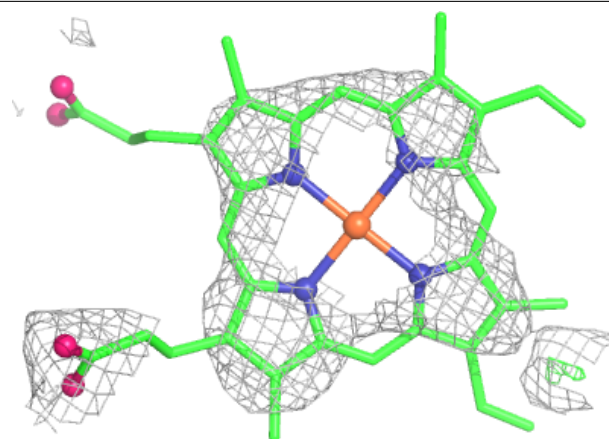
Electron density around HEM V2 201:

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



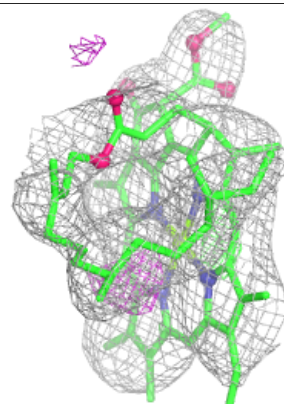
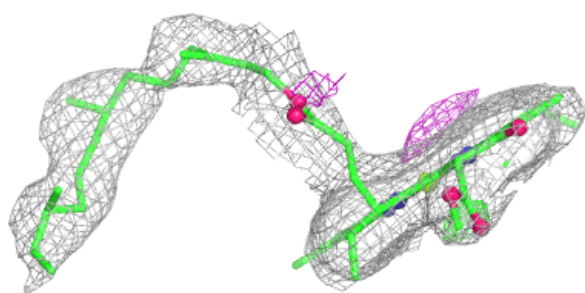
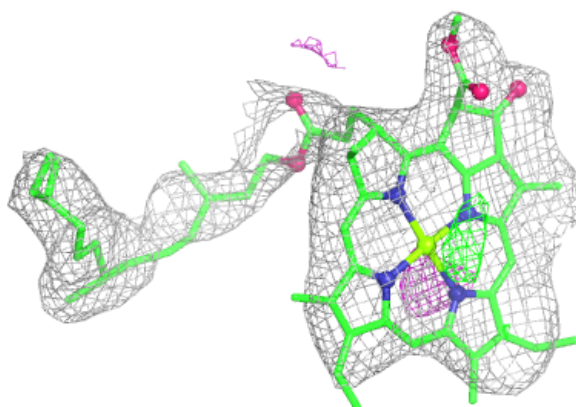
Electron density around HEM e2 101:

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

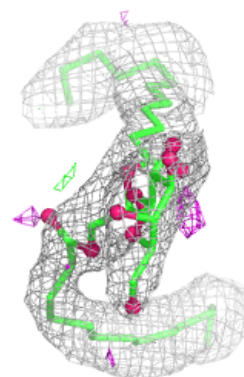
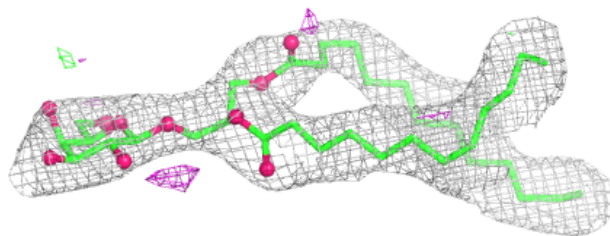
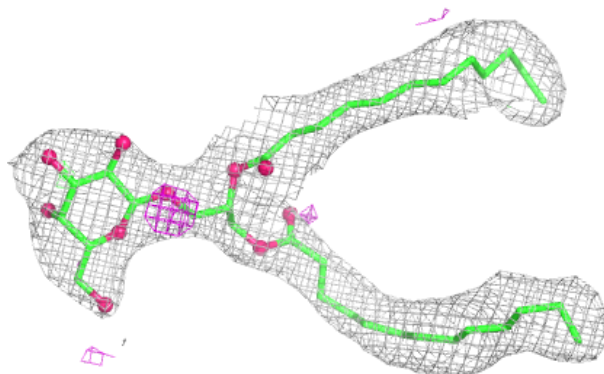


Electron density around CLA A2 403:

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

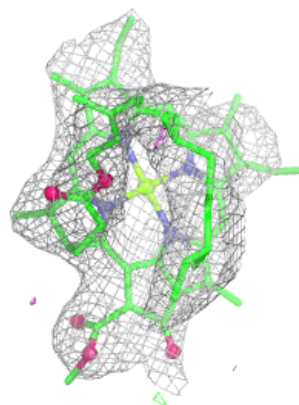
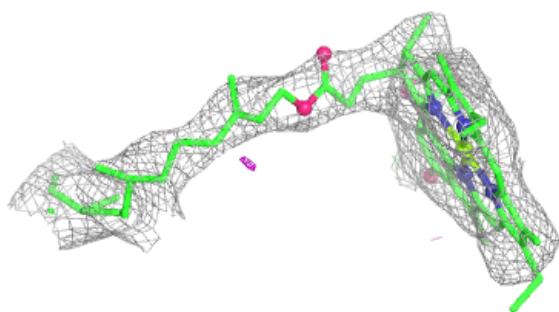
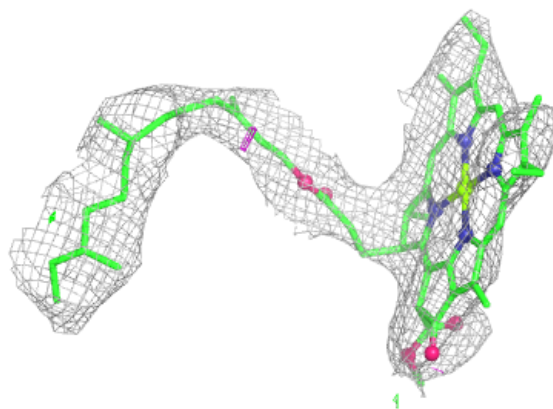
**Electron density around LMG a2 412:**

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



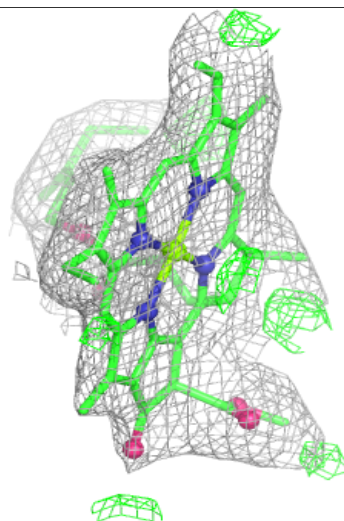
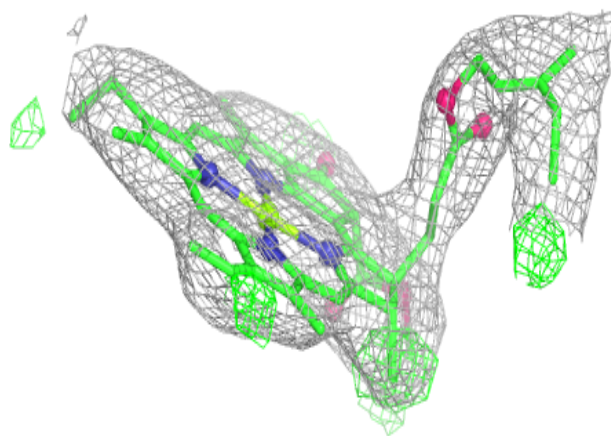
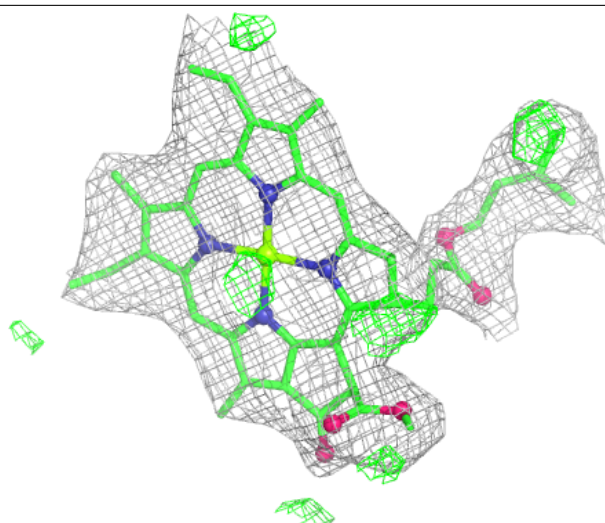
Electron density around CLA b2 609:

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



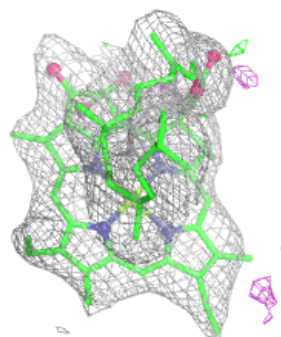
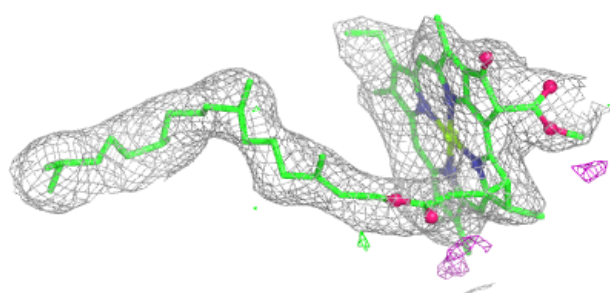
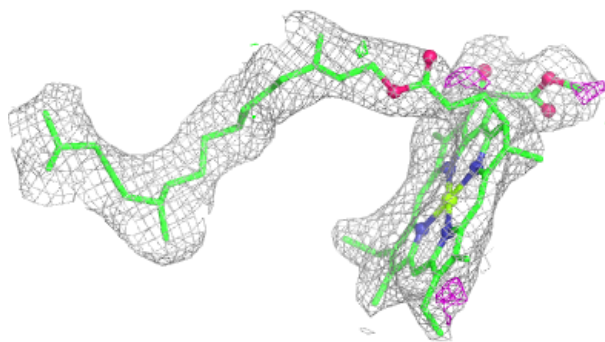
Electron density around CLA A2 404:

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

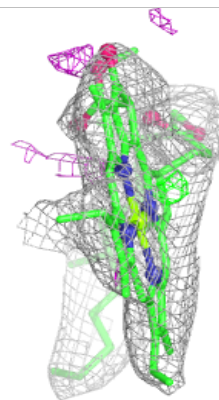
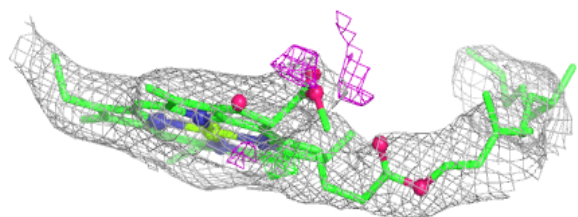
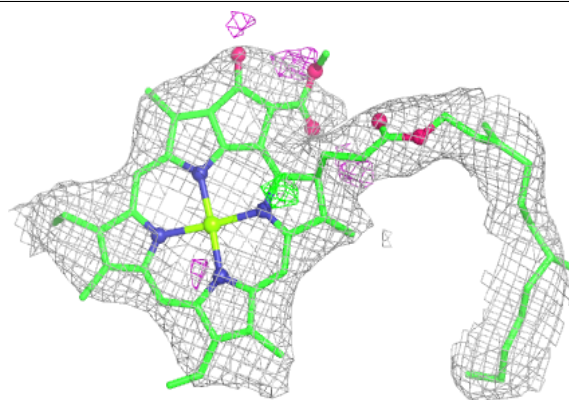


Electron density around CLA C1 509:

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

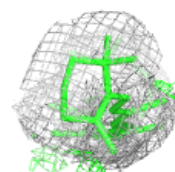
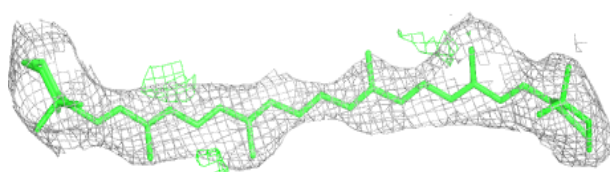
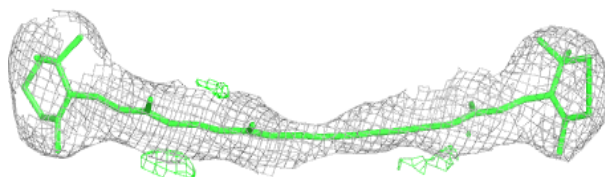
**Electron density around CLA b2 619:**

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

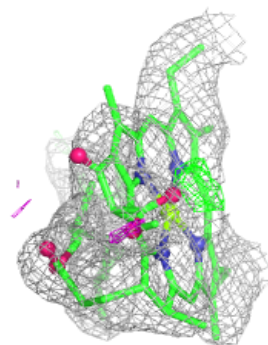
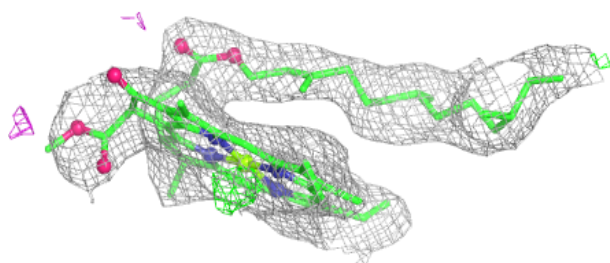
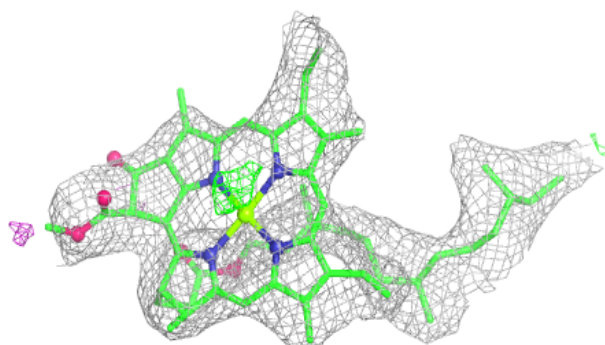


Electron density around BCR c1 501:

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

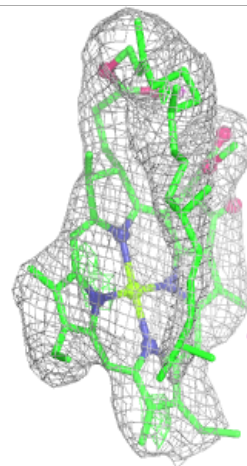
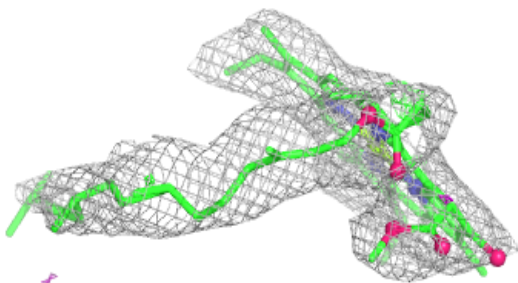
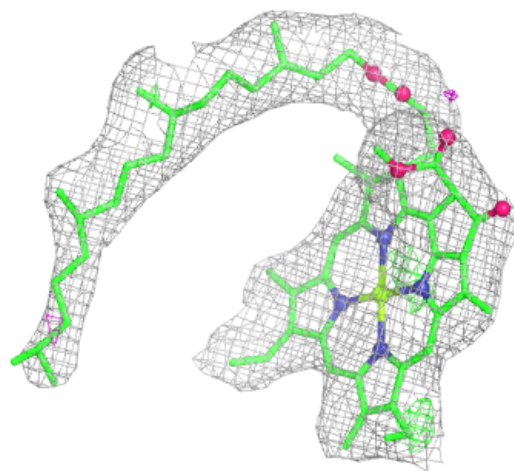
**Electron density around CLA c2 506:**

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



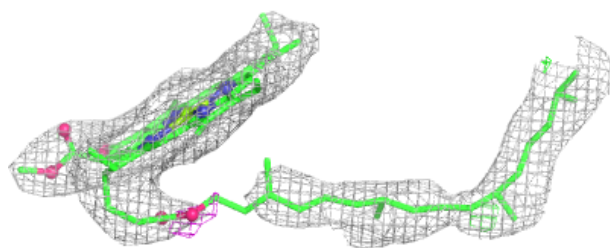
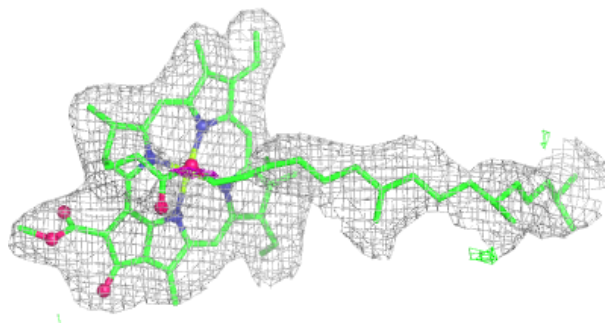
Electron density around CLA c2 508:

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



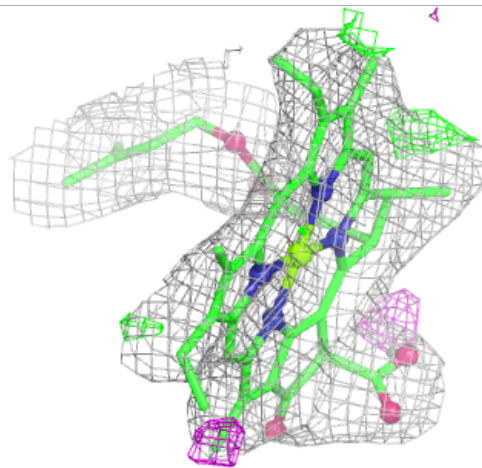
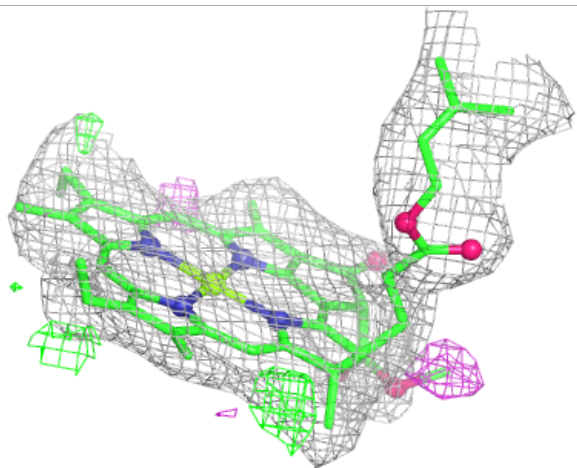
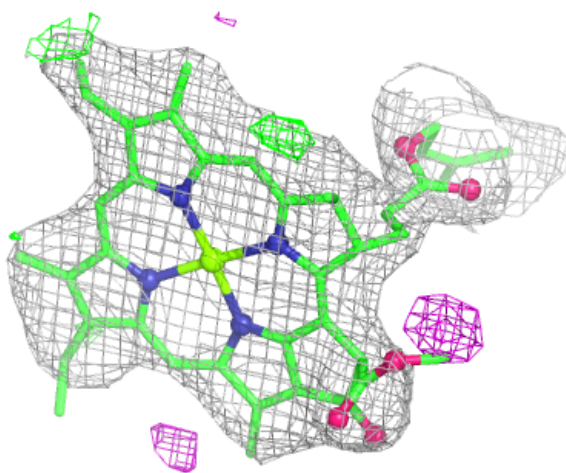
Electron density around CLA B2 610:

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



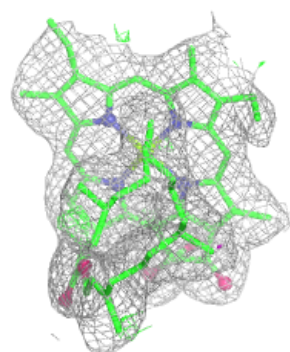
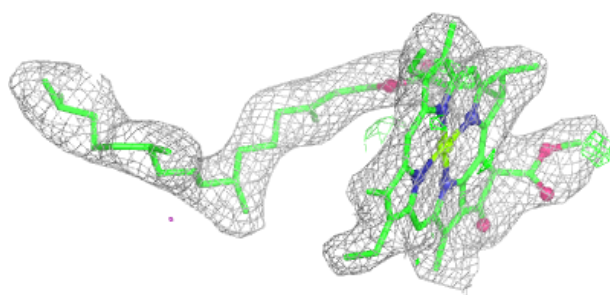
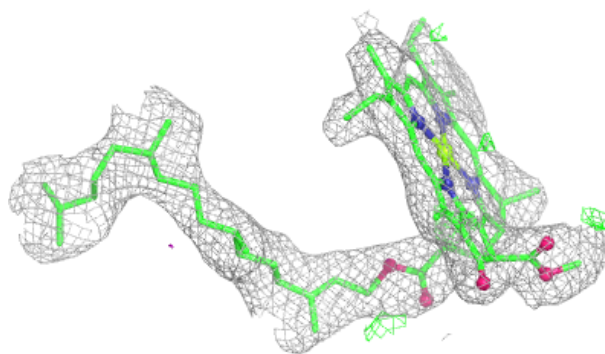
Electron density around CLA c1 508:

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

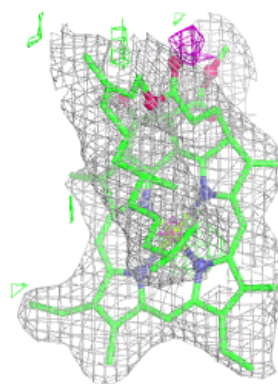
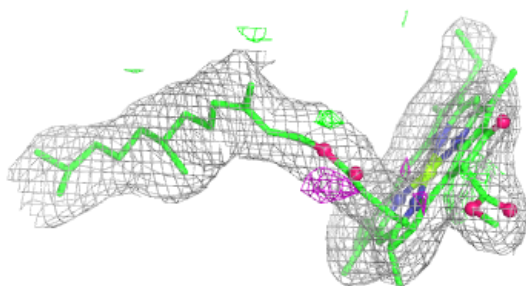
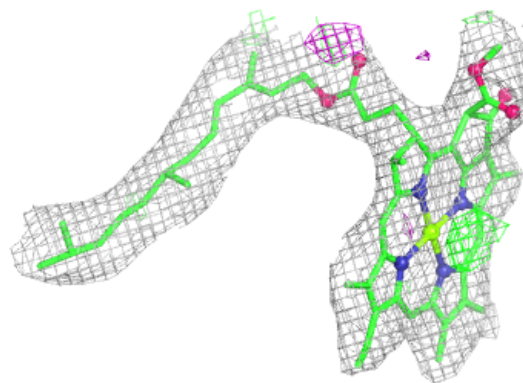


Electron density around CLA c1 510:

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

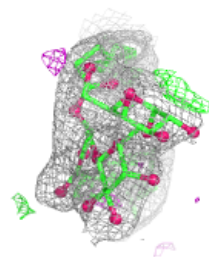
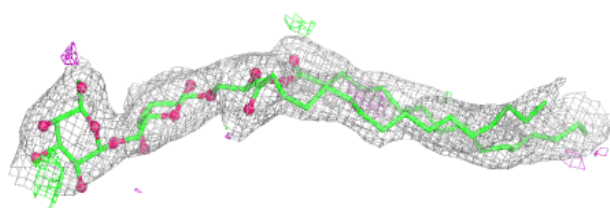
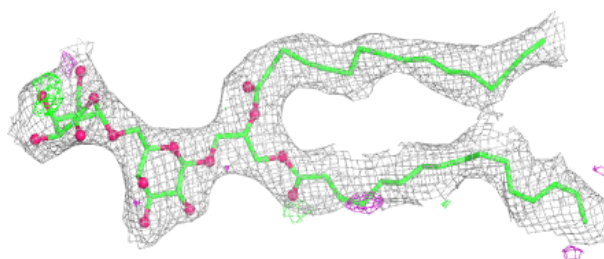
**Electron density around CLA c1 513:**

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

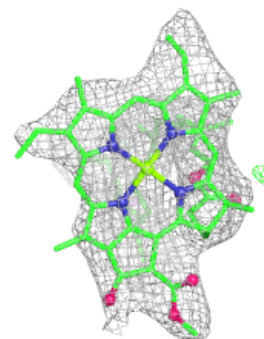
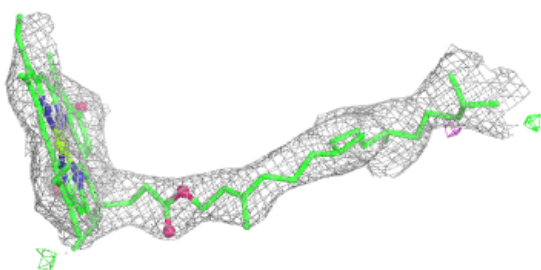
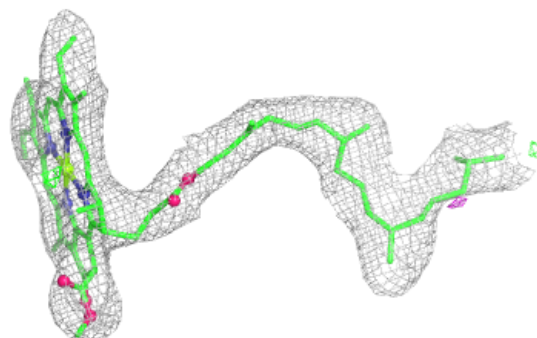


Electron density around DGD c1 520:

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

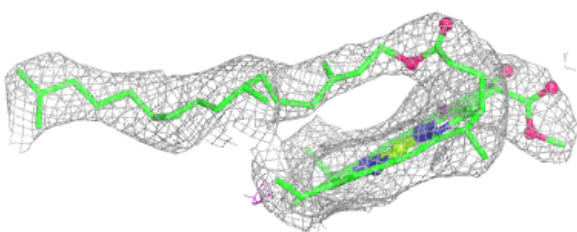
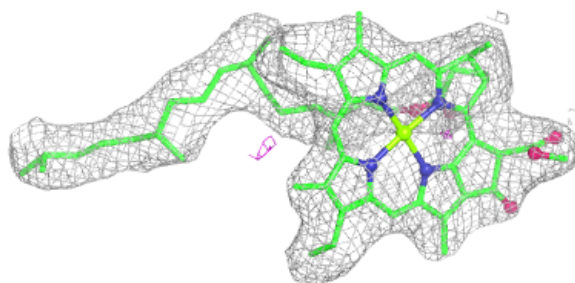
**Electron density around CLA B1 609:**

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



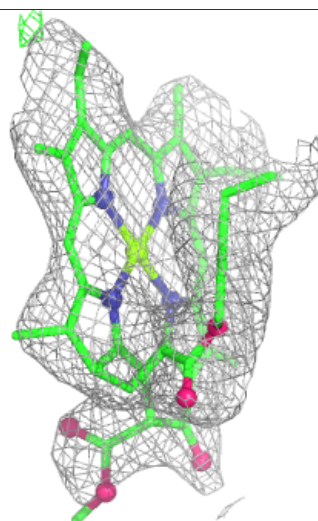
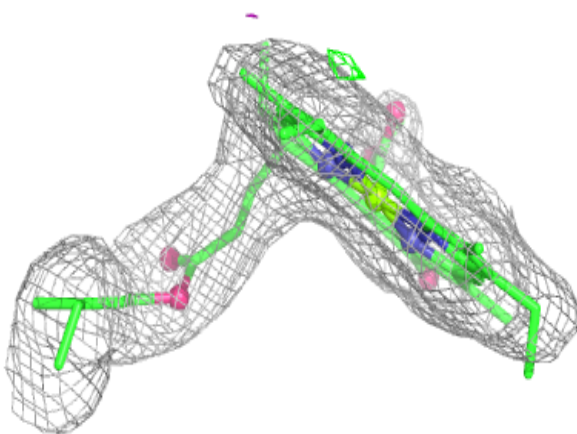
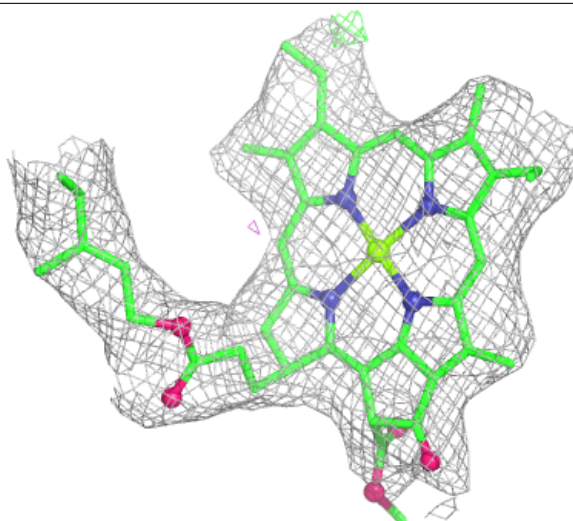
Electron density around CLA C1 506:

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



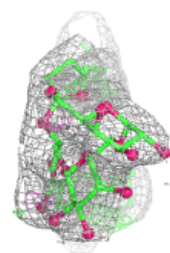
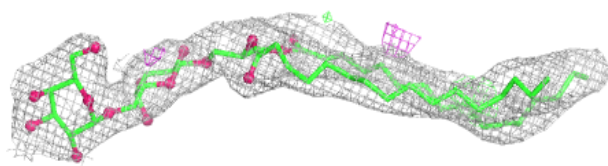
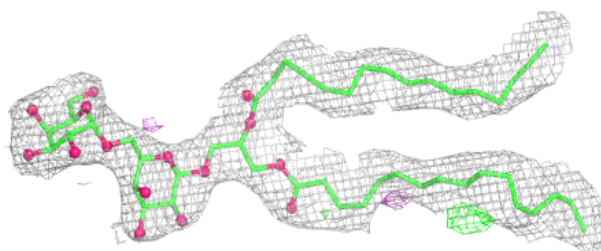
Electron density around CLA D1 403:

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



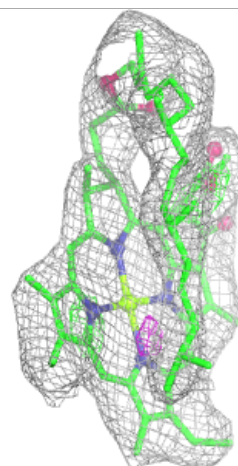
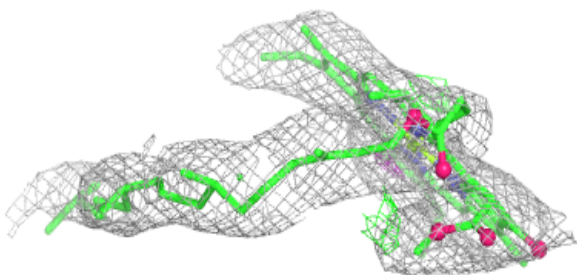
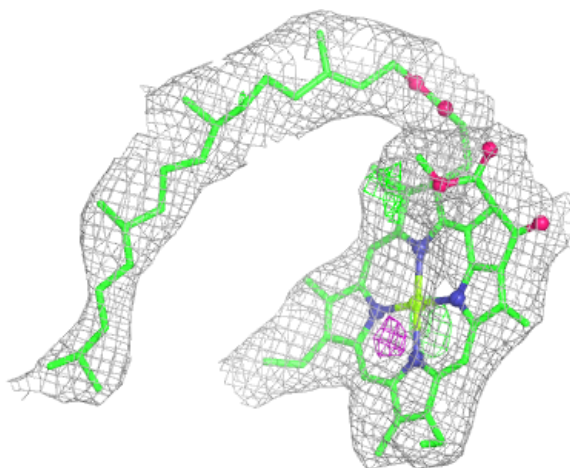
Electron density around DGD c2 517:

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



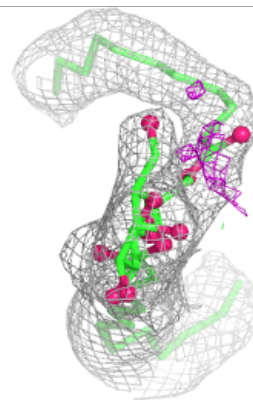
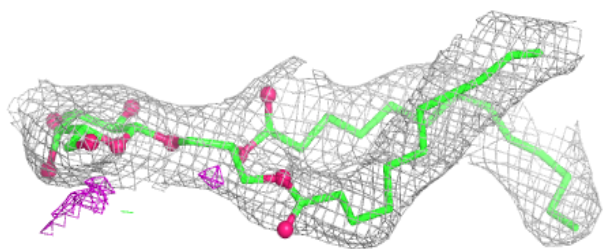
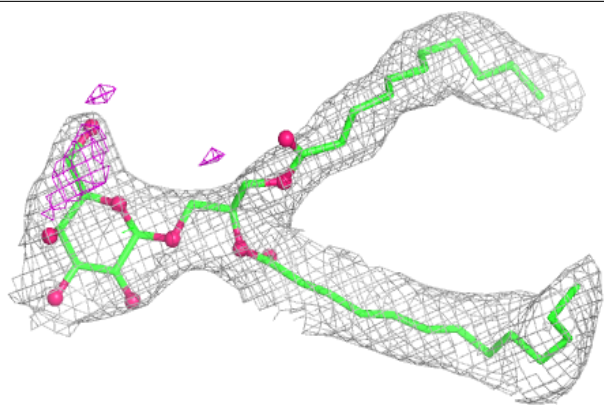
Electron density around CLA c1 509:

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

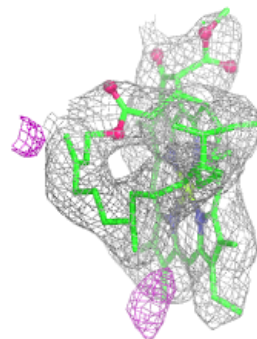
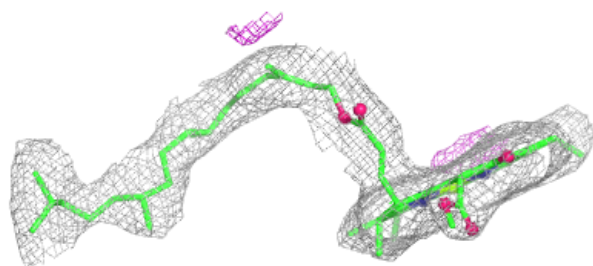
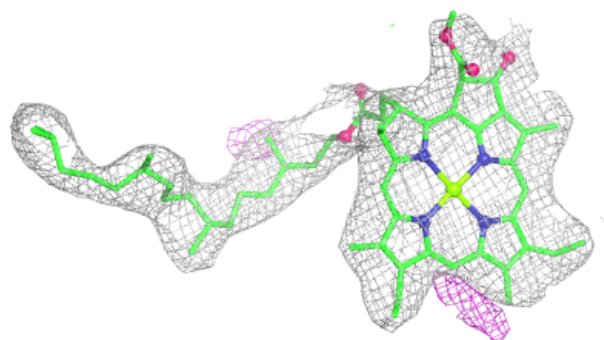


Electron density around LMG A1 410:

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

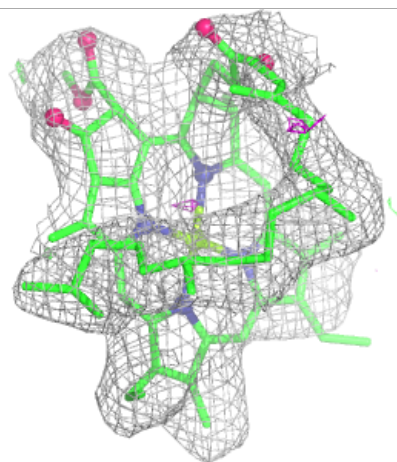
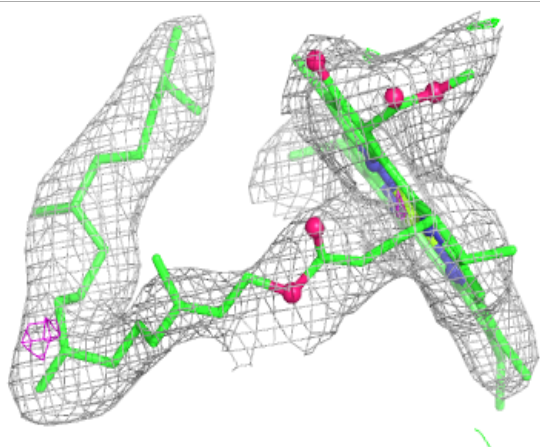
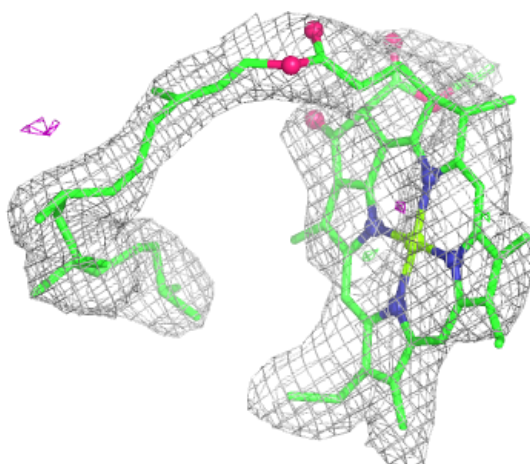
**Electron density around CLA a2 405:**

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



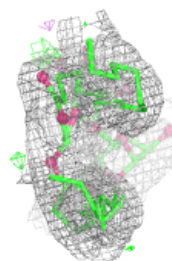
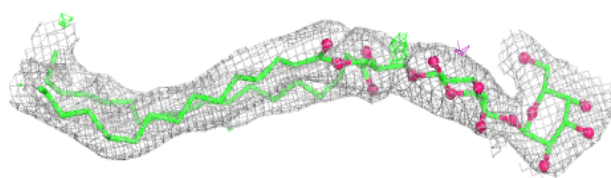
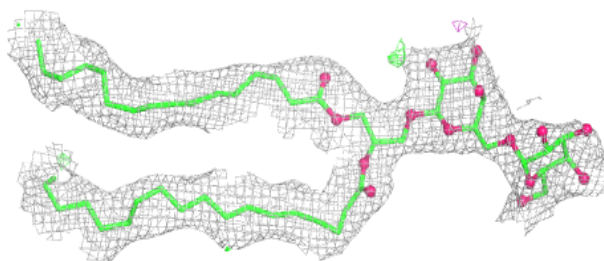
Electron density around CLA c1 505:

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



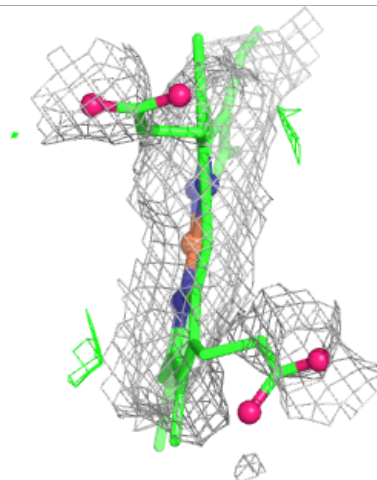
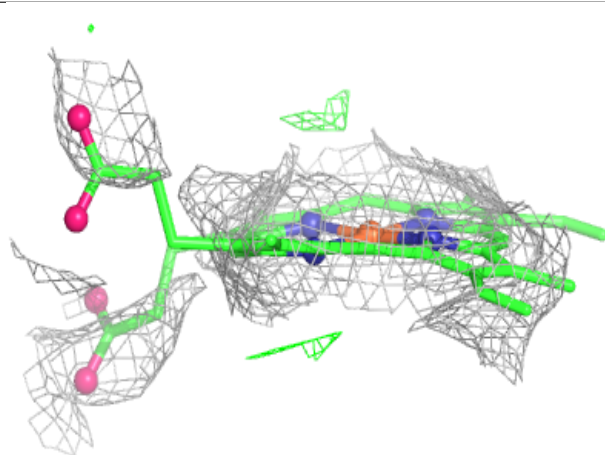
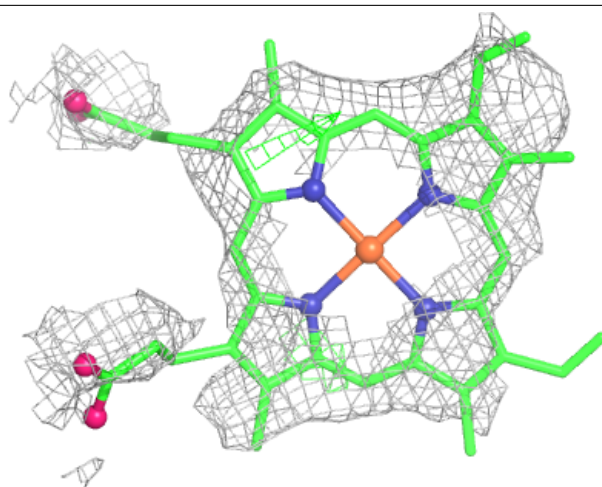
Electron density around DGD C1 517:

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



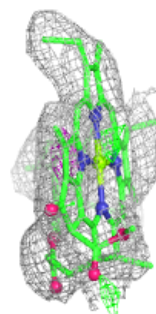
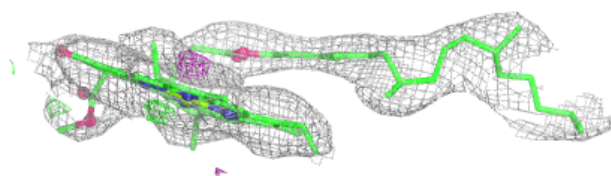
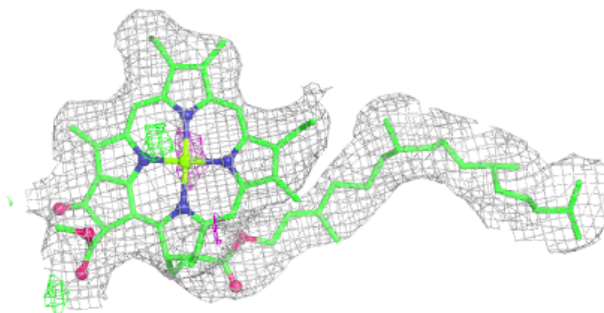
Electron density around HEM E2 101:

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

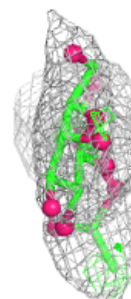
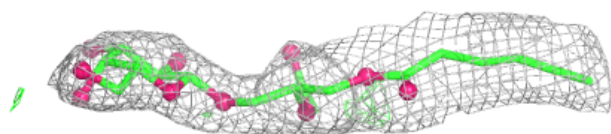
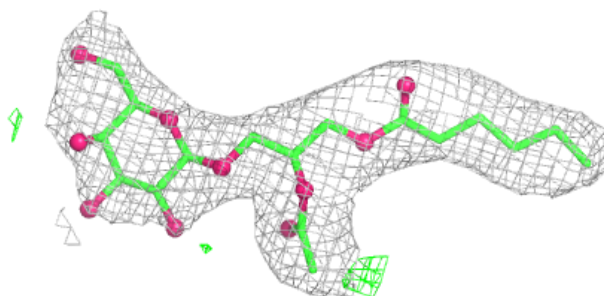


Electron density around CLA B1 606:

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

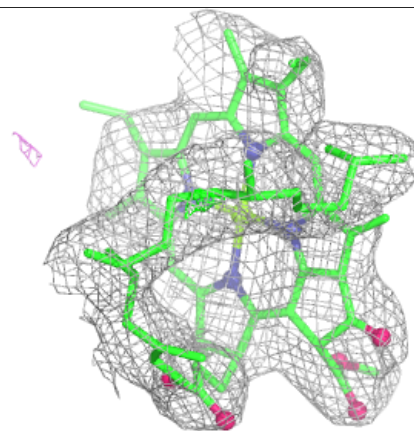
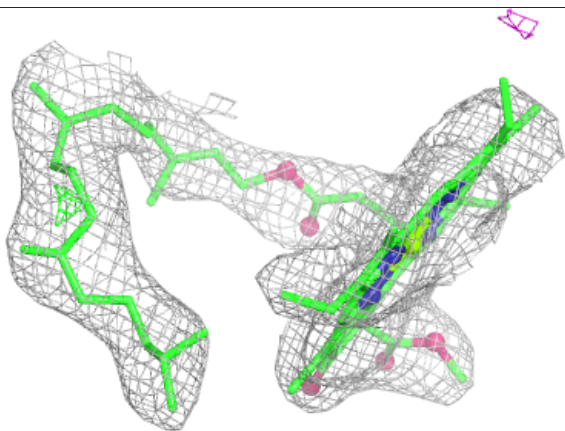
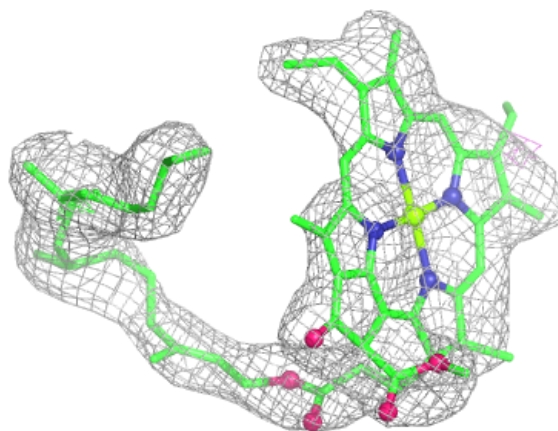
**Electron density around LMG d2 407:**

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



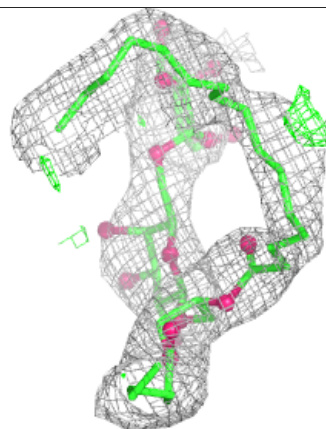
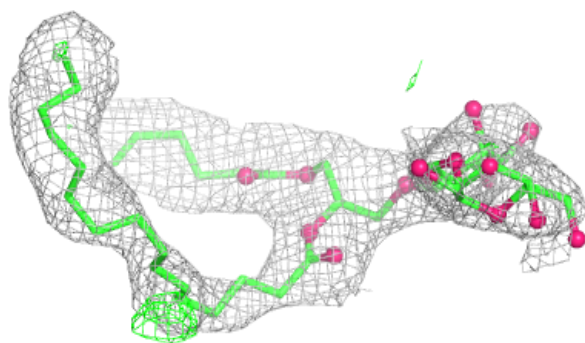
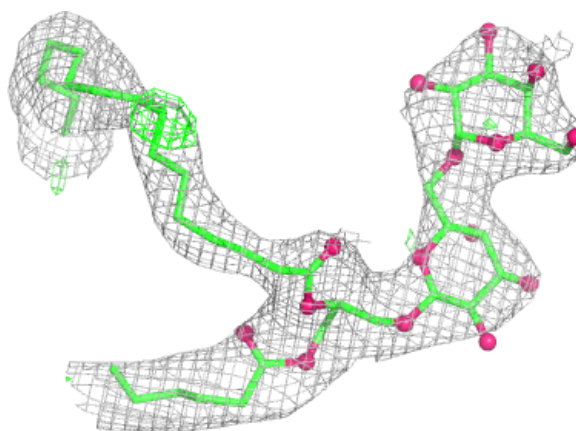
Electron density around CLA c2 504:

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

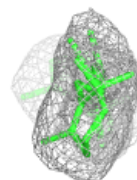
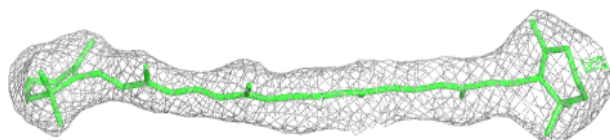
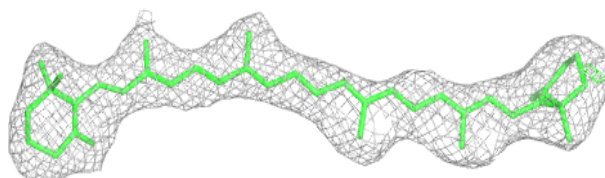


Electron density around DGD c2 516:

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

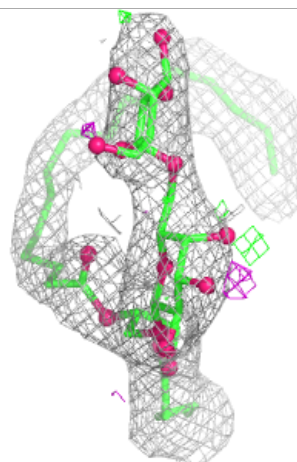
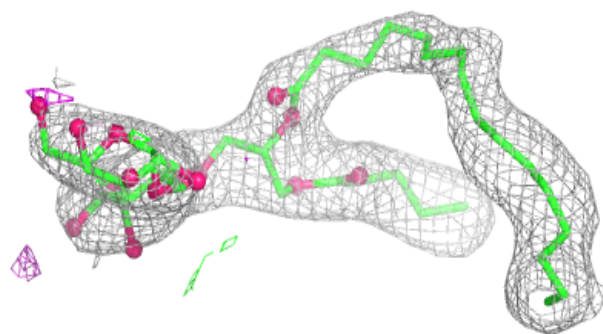
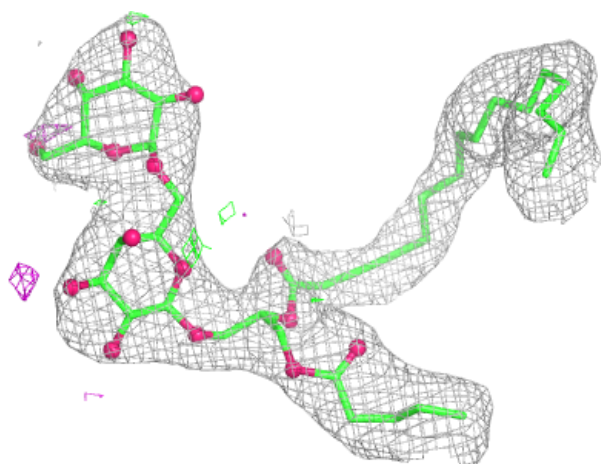
**Electron density around BCR b2 601:**

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



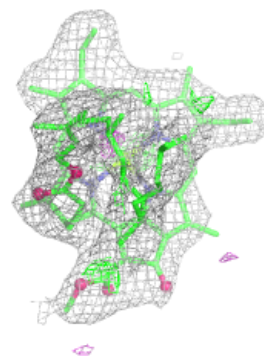
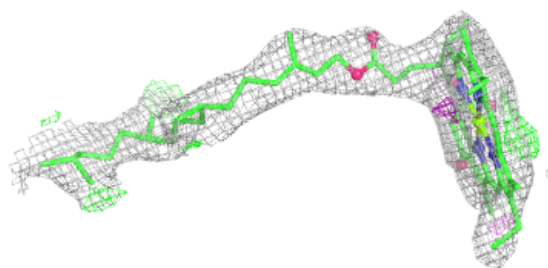
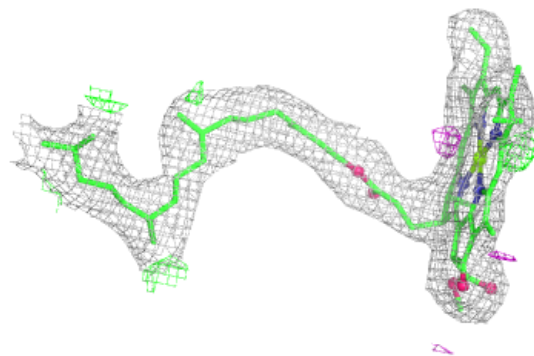
Electron density around DGD c1 514:

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

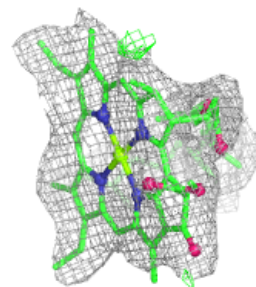
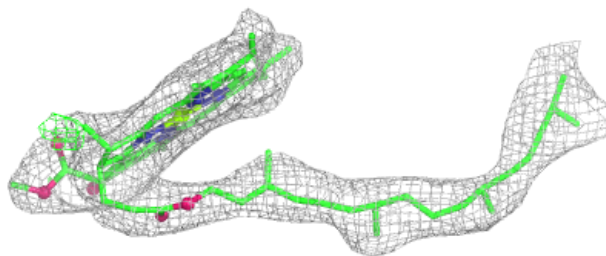
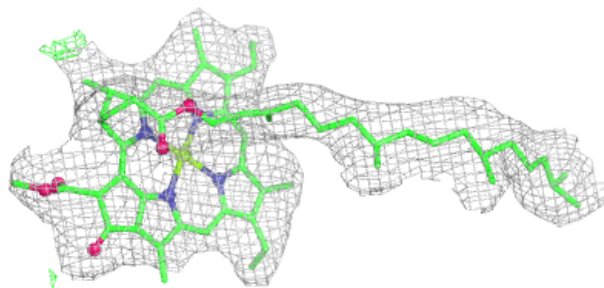


Electron density around CLA b1 609:

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

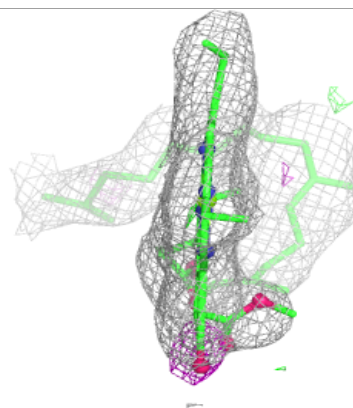
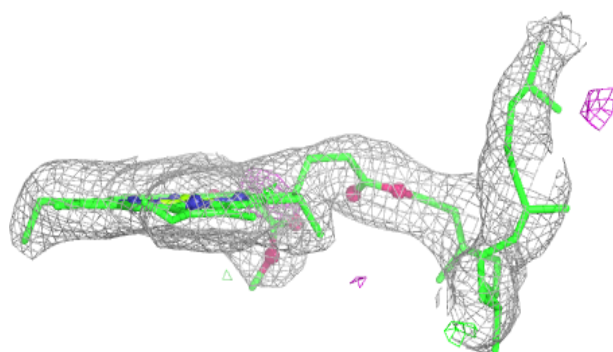
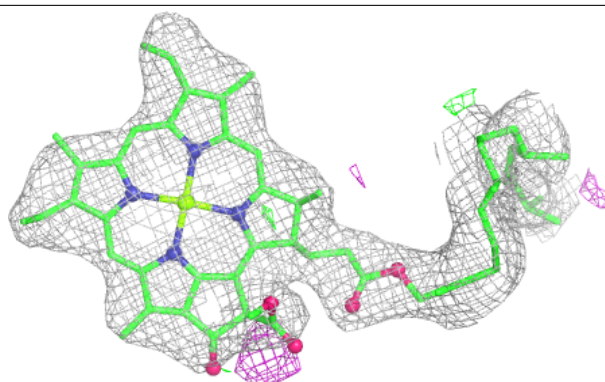
**Electron density around CLA b2 624:**

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

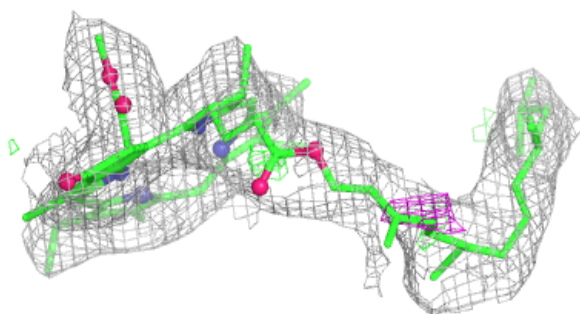
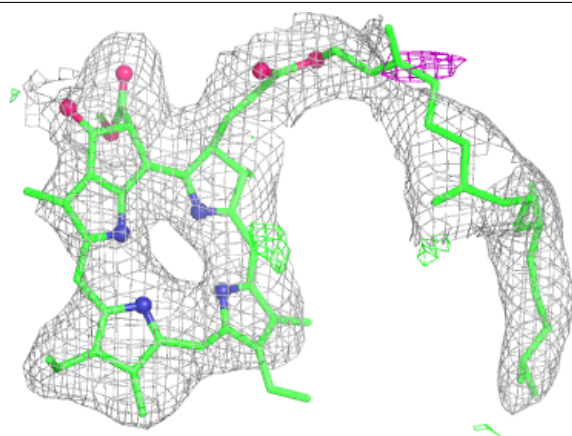


Electron density around CLA b1 619:

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

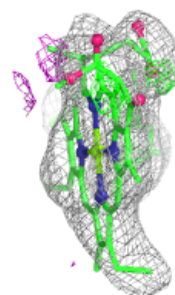
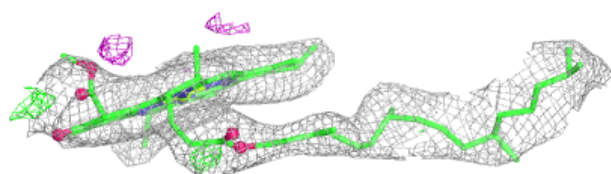
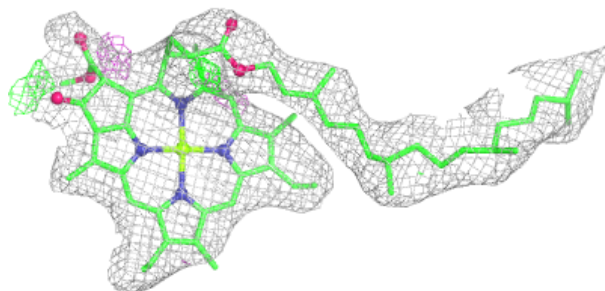
**Electron density around PHO D2 407:**

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



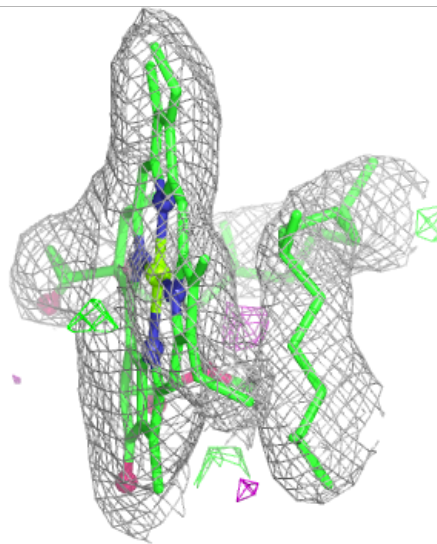
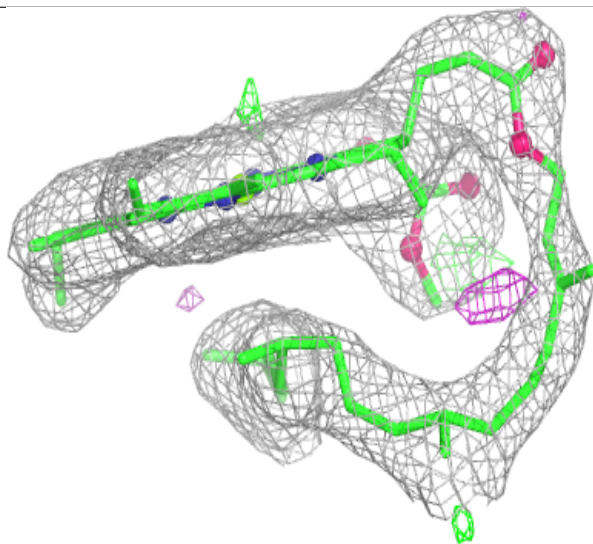
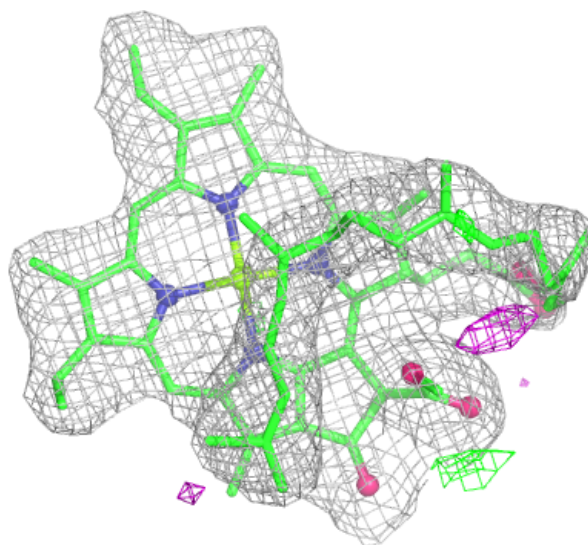
Electron density around CLA b2 606:

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



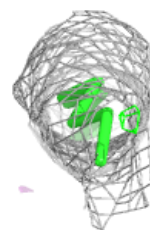
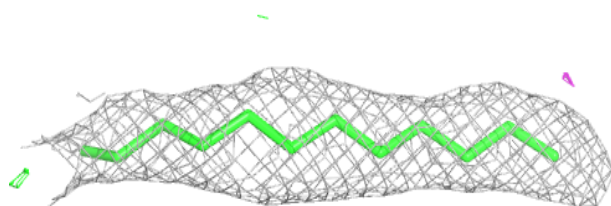
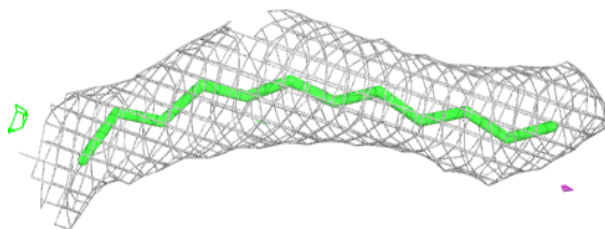
Electron density around CLA C1 511:

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

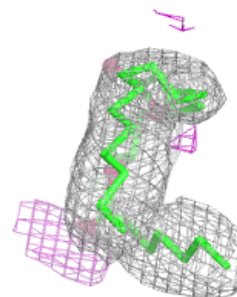
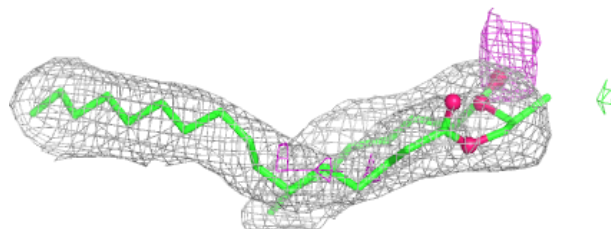
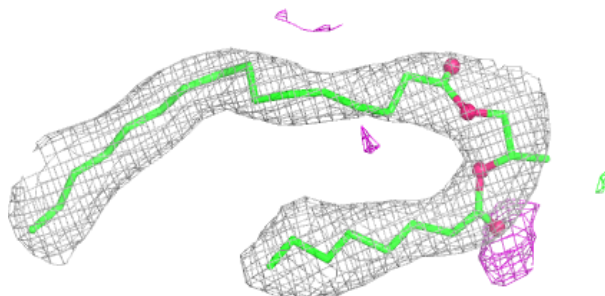


Electron density around LMT L1 102:

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

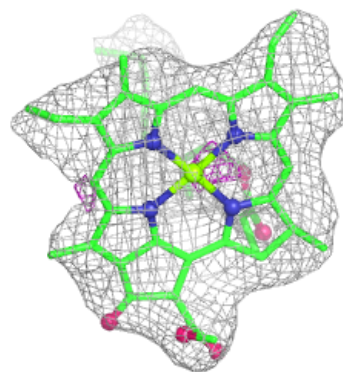
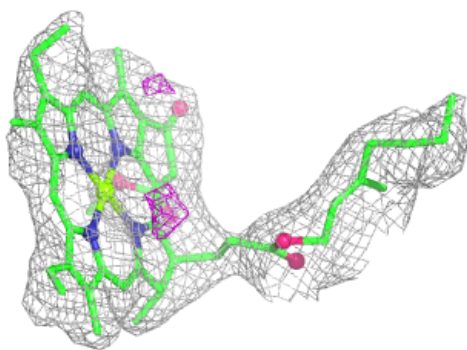
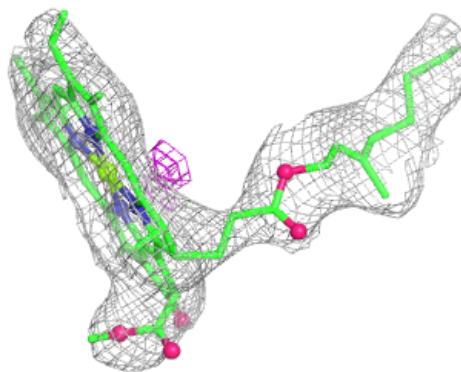
**Electron density around LMG M1 101:**

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

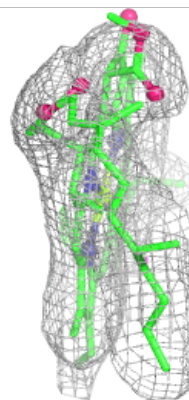
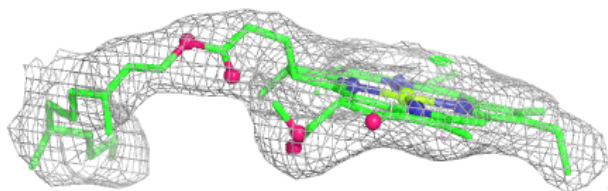
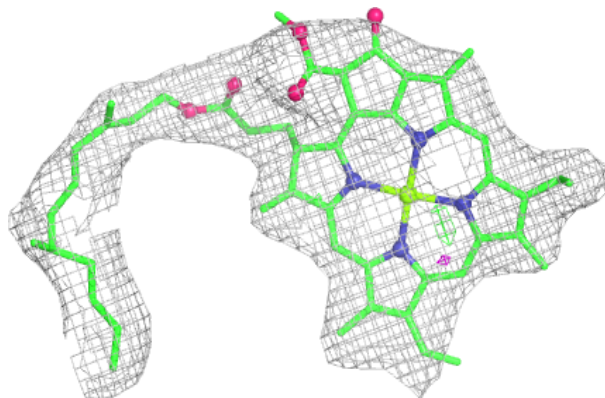


Electron density around CLA c2 507:

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

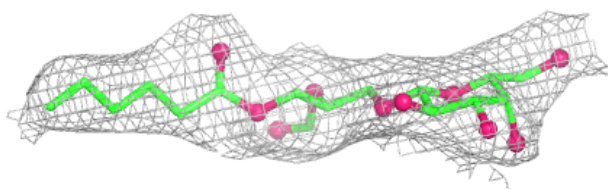
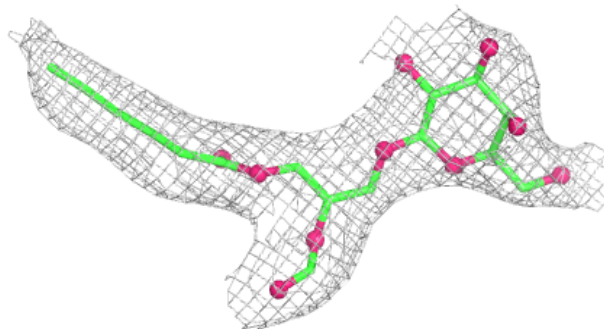
**Electron density around CLA B1 618:**

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

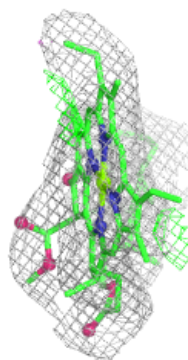
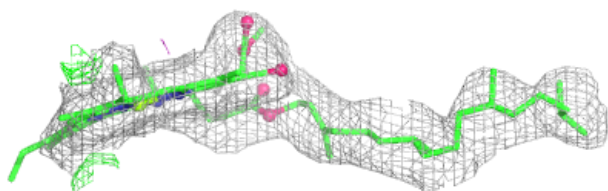
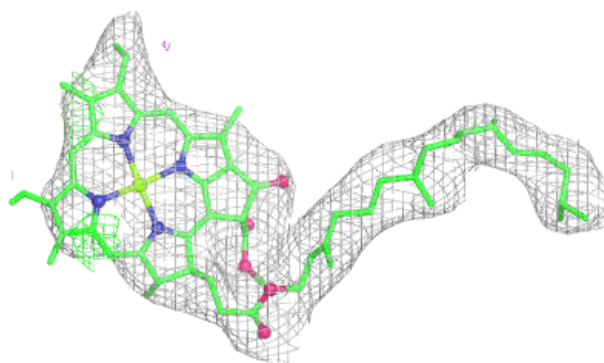


Electron density around LMG c2 519:

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

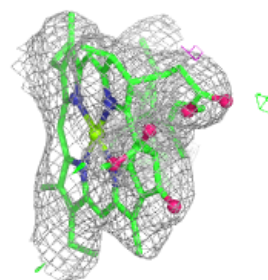
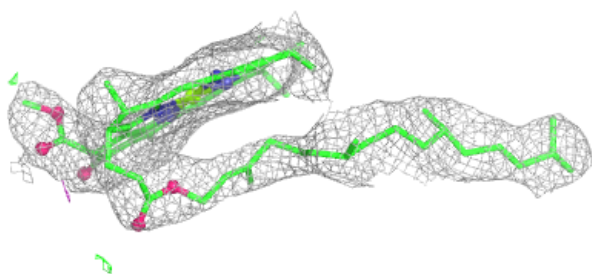
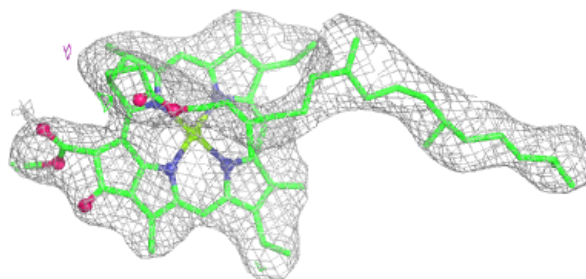
**Electron density around CLA b2 613:**

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

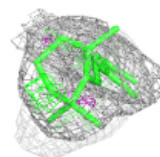
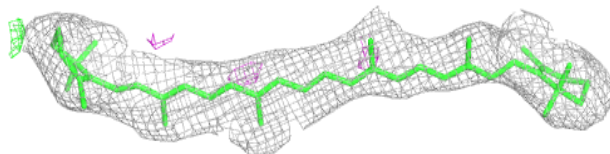
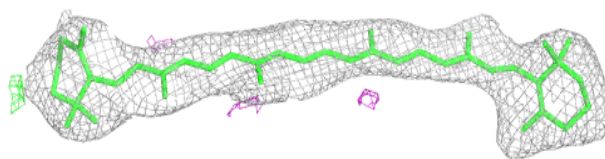


Electron density around CLA c1 507:

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

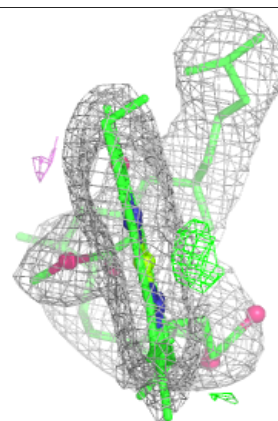
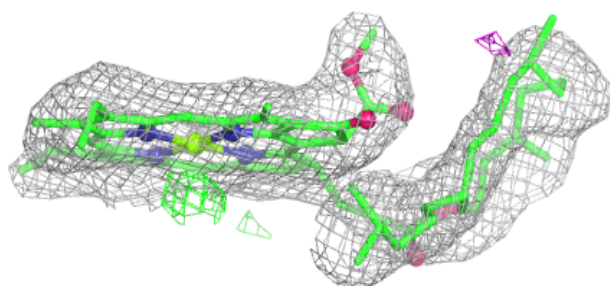
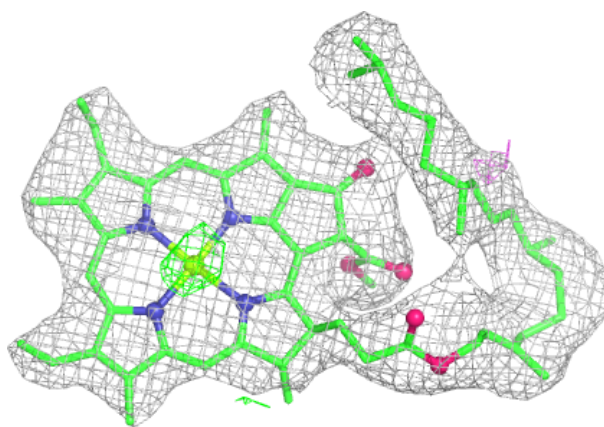
**Electron density around BCR B2 603:**

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



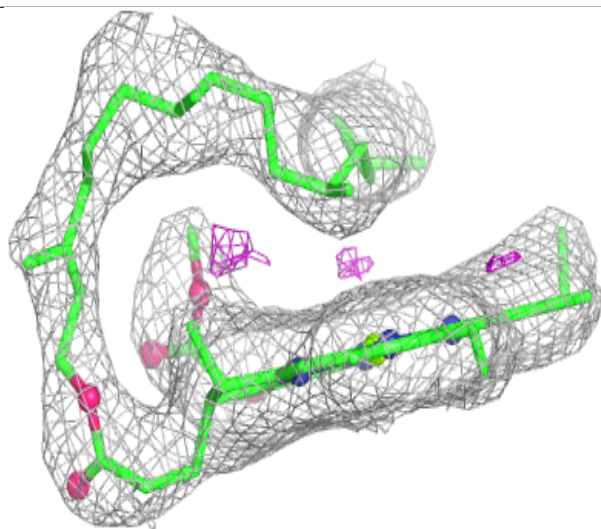
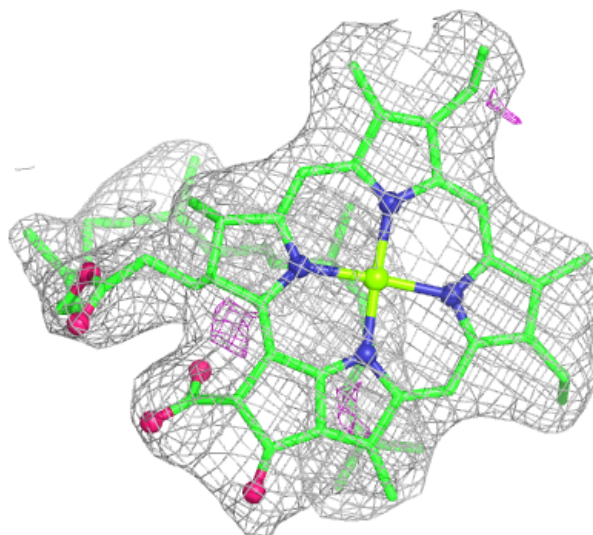
Electron density around CLA B2 612:

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



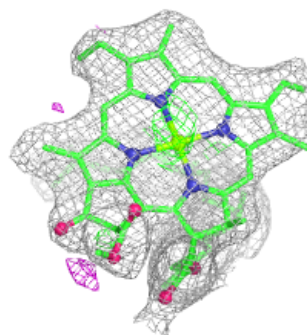
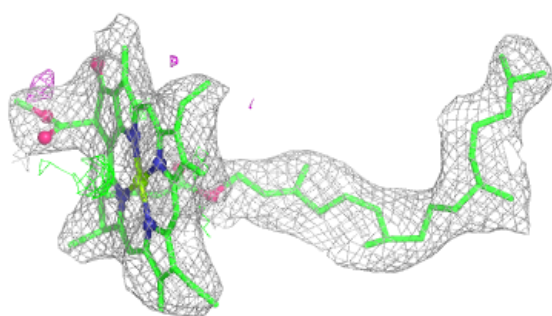
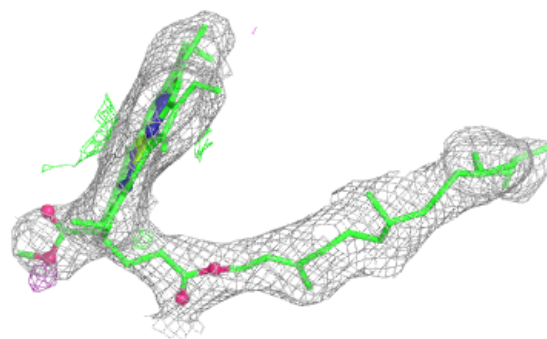
Electron density around CLA c2 511:

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

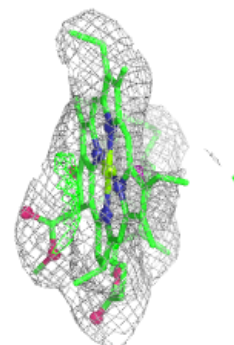
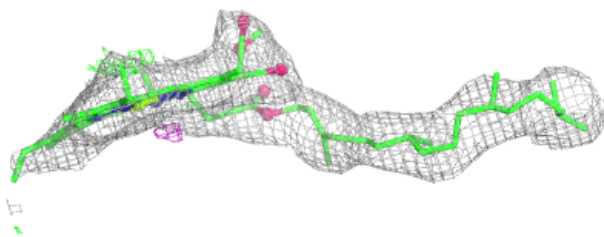
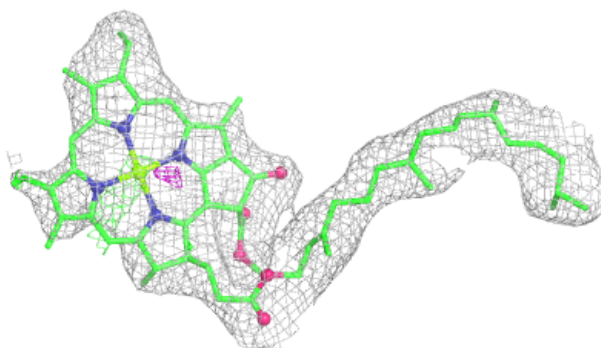


Electron density around CLA B2 619:

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

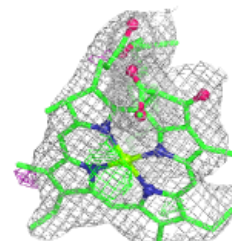
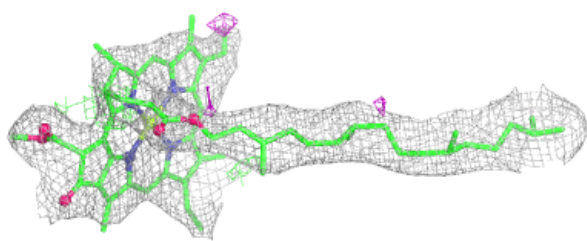
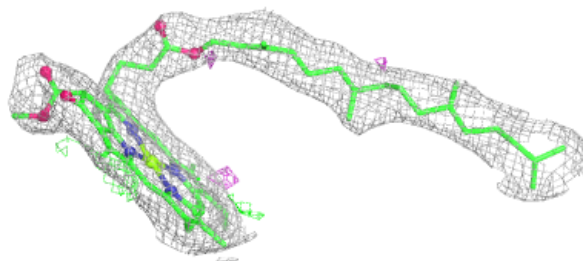
**Electron density around CLA B1 605:**

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



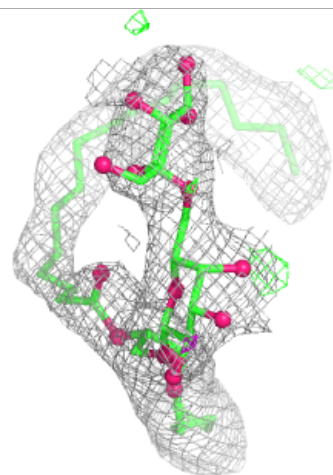
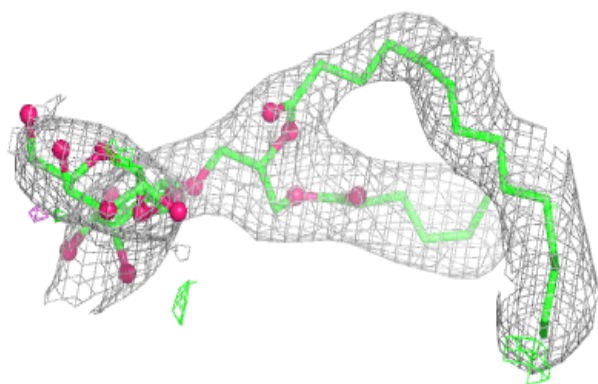
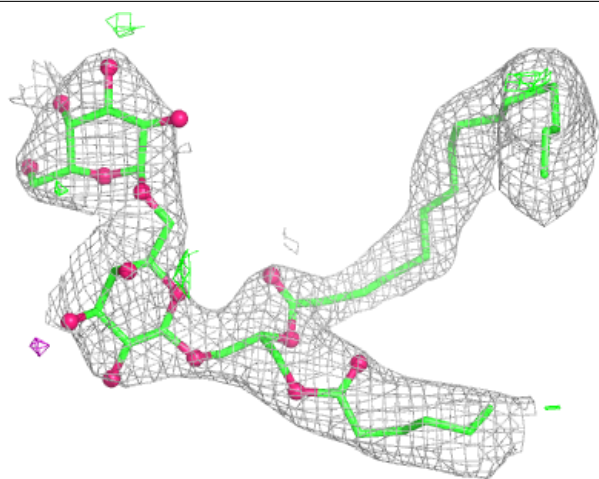
Electron density around CLA C1 505:

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



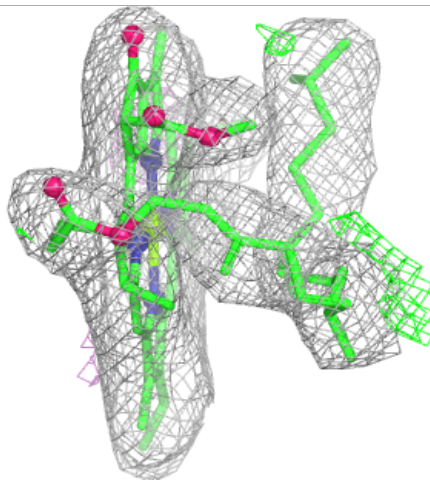
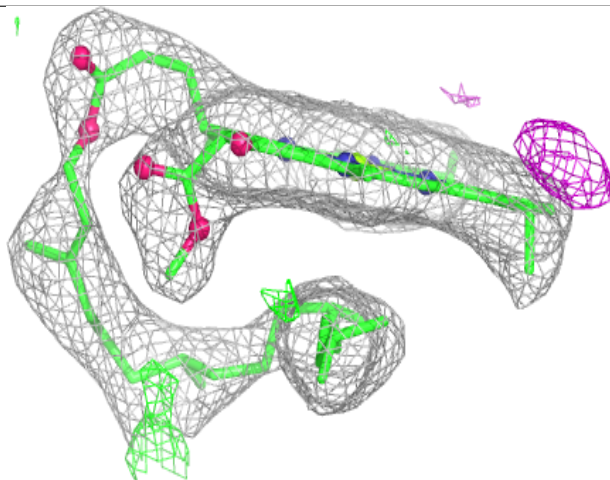
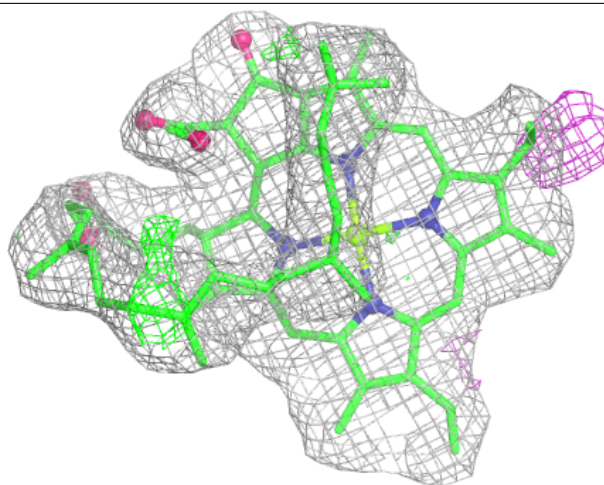
Electron density around DGD C1 515:

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



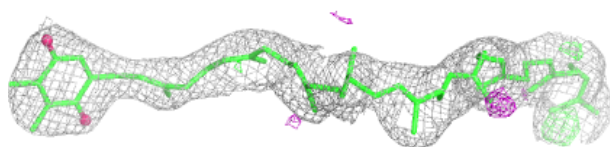
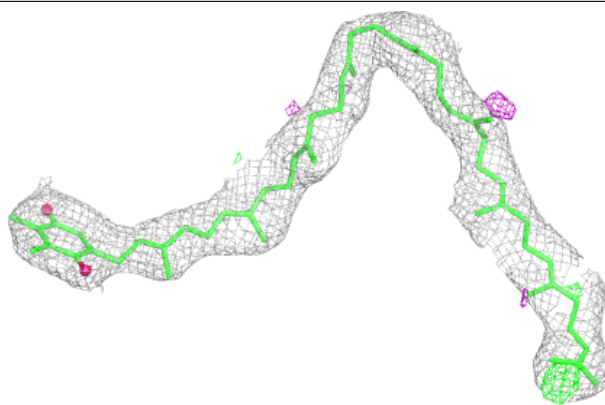
Electron density around CLA c1 512:

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

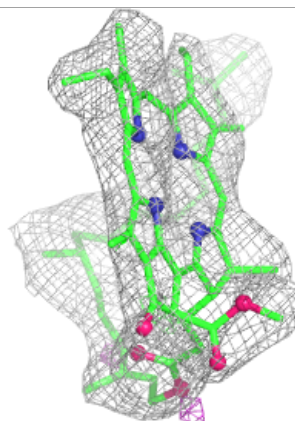
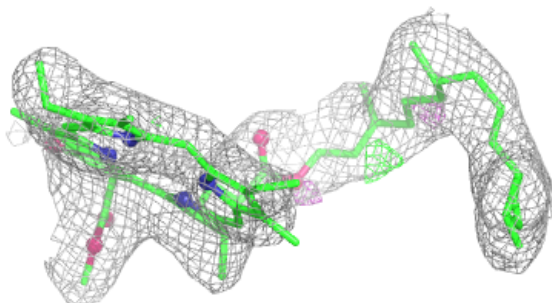
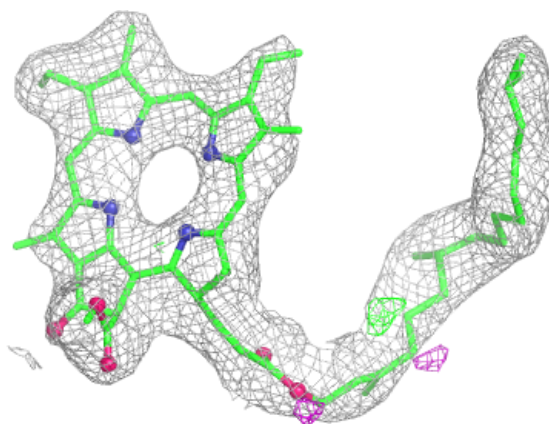


Electron density around PL9 D2 408:

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

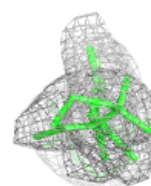
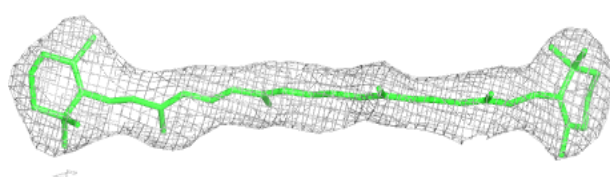
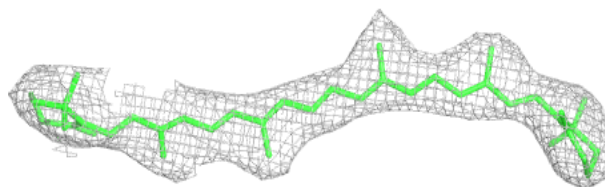
**Electron density around PHO D1 407:**

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

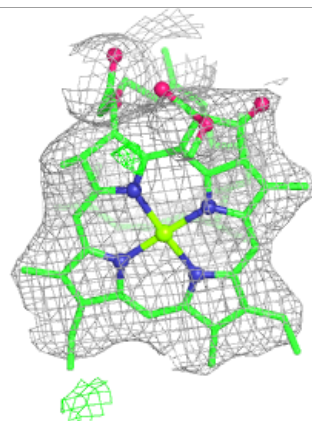
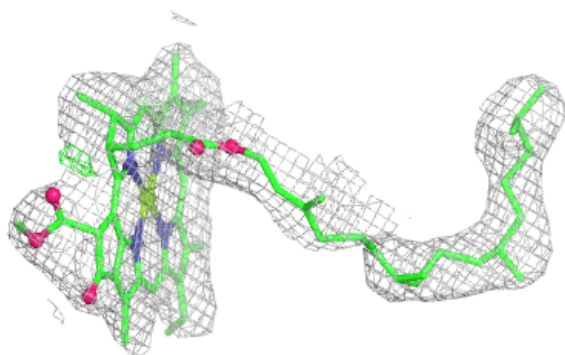
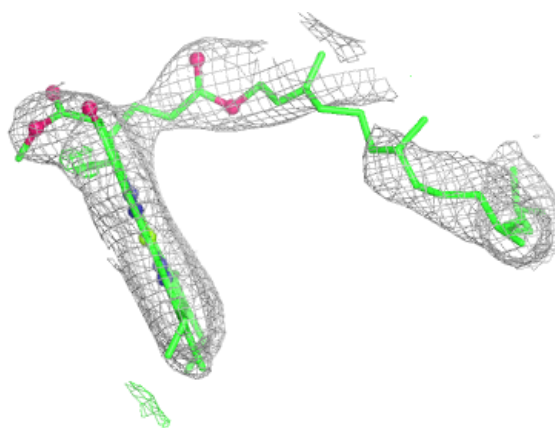


Electron density around BCR C1 501:

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

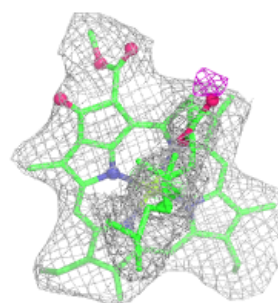
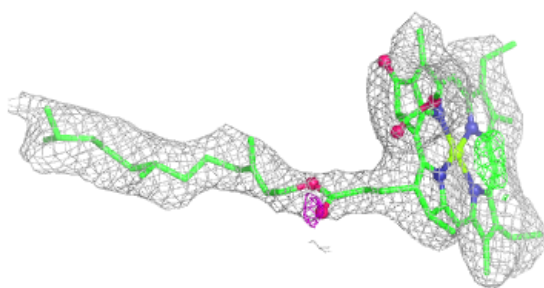
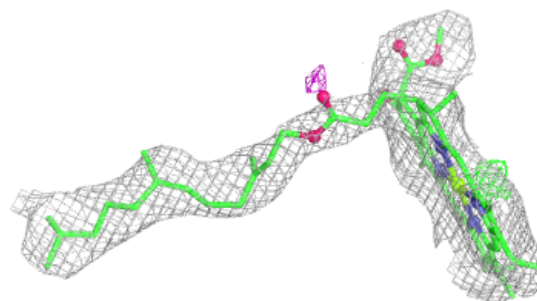
**Electron density around CLA C1 507:**

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

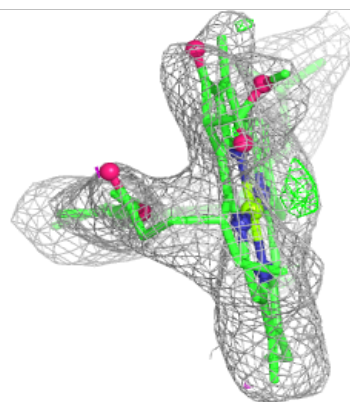
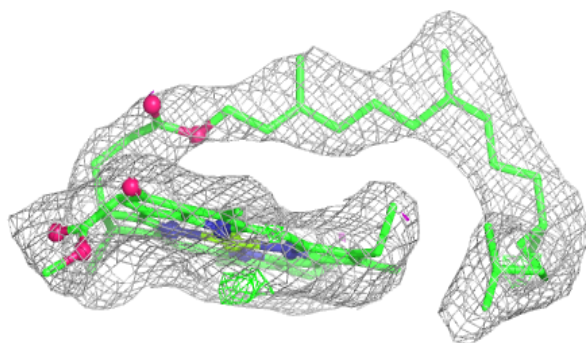
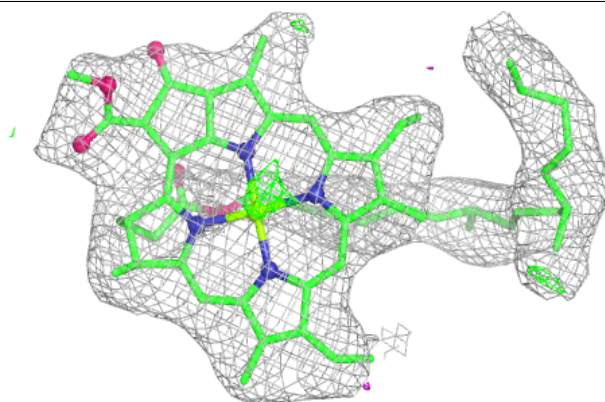


Electron density around CLA b2 616:

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

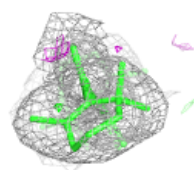
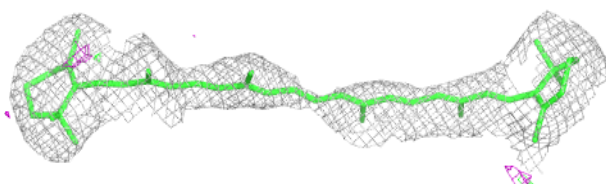
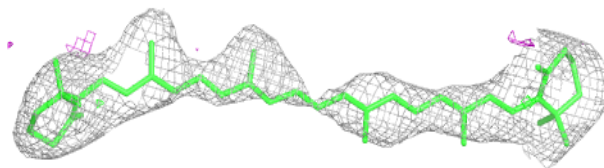
**Electron density around CLA b1 616:**

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

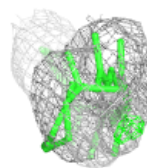
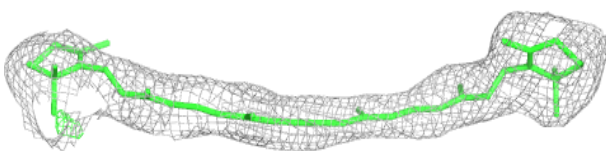
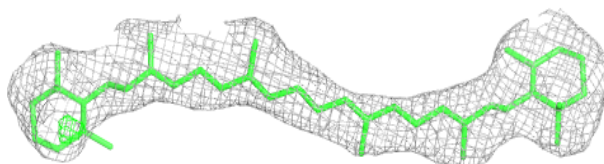


Electron density around BCR A2 401:

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

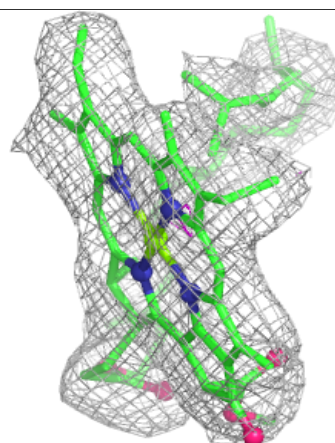
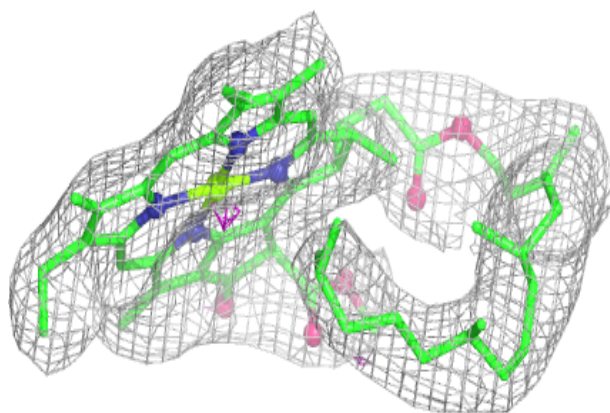
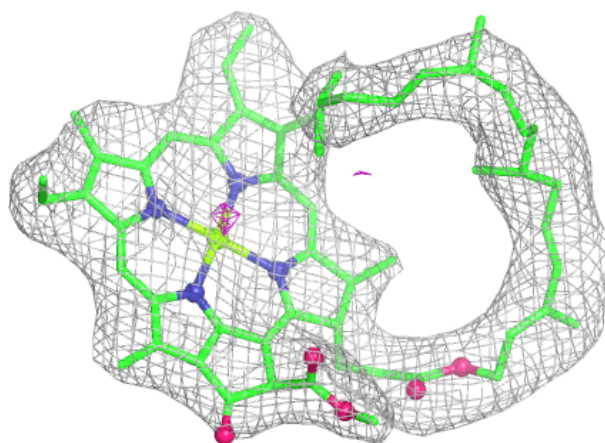
**Electron density around BCR d1 405:**

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



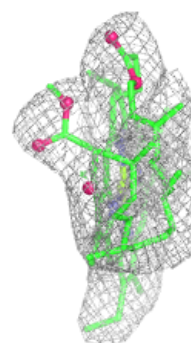
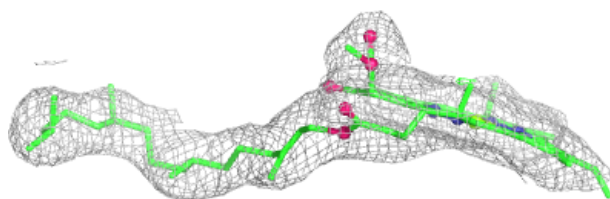
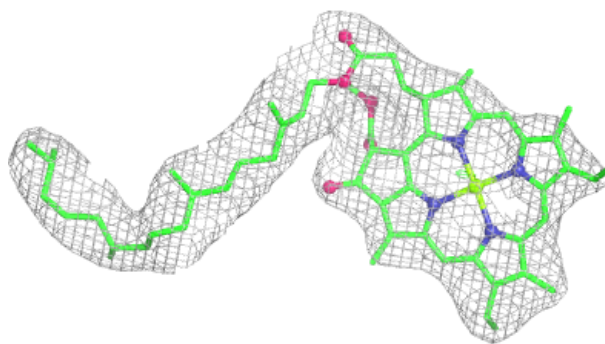
Electron density around CLA B1 617:

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

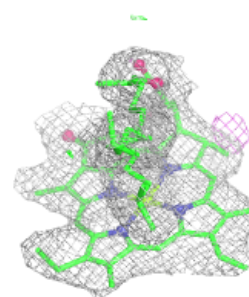
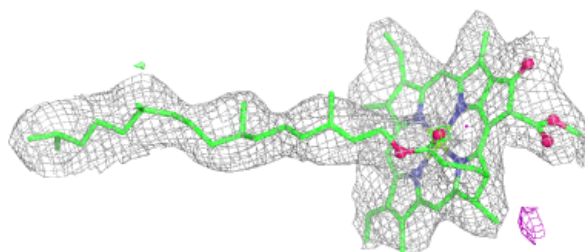
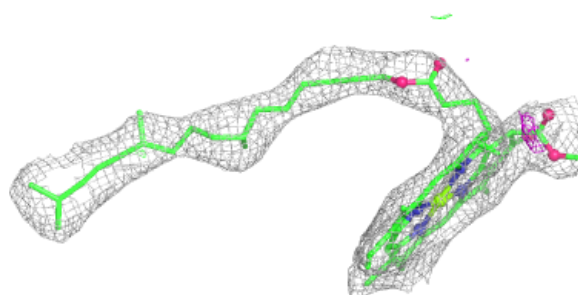


Electron density around CLA B2 605:

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

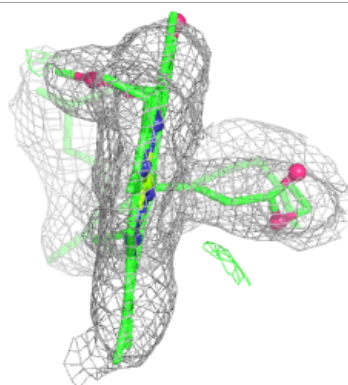
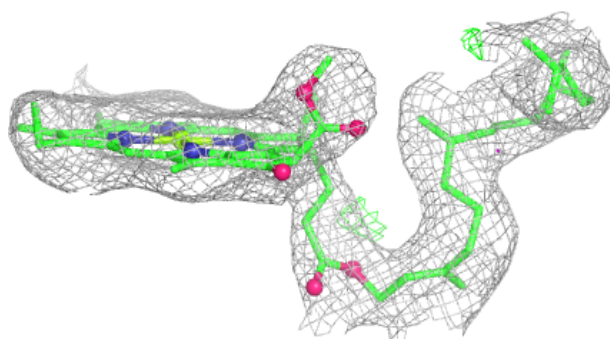
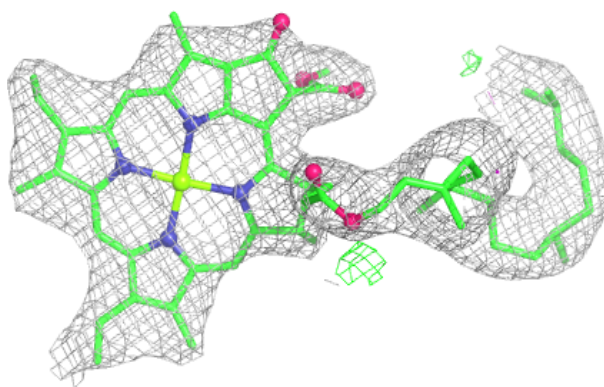
**Electron density around CLA c1 506:**

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

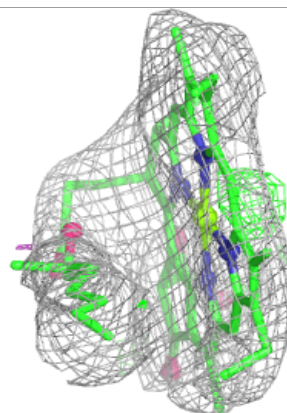
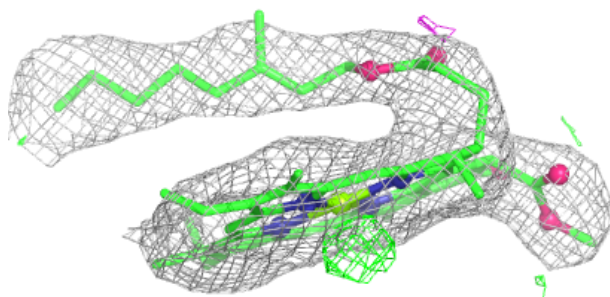
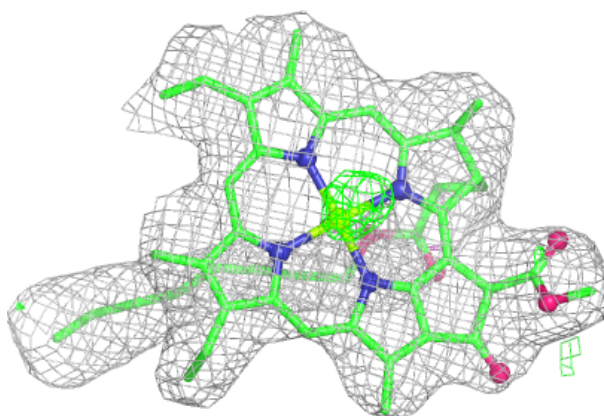


Electron density around CLA B2 614:

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

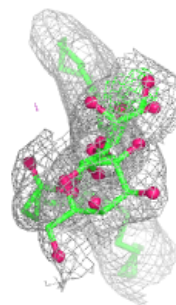
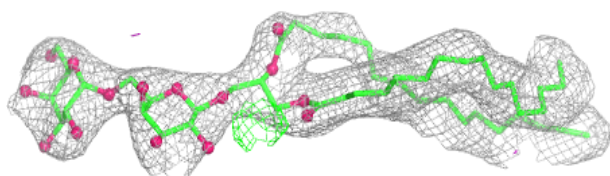
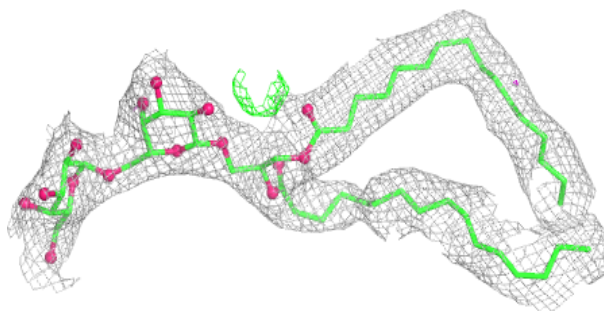
**Electron density around CLA B2 616:**

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



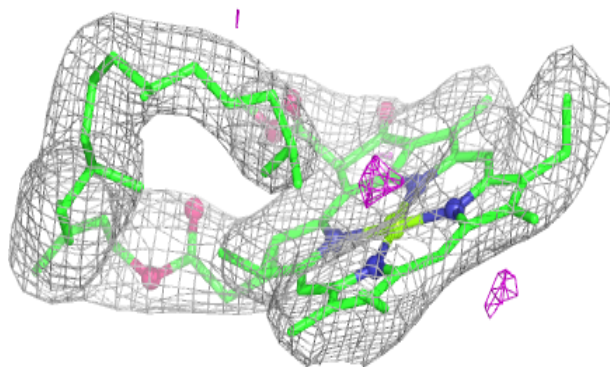
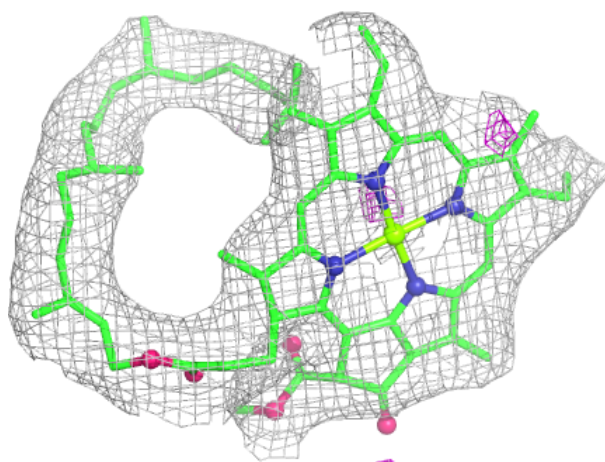
Electron density around DGD c1 518:

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



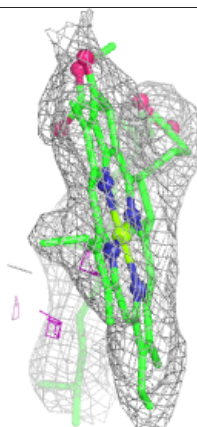
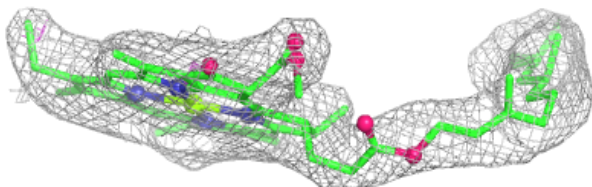
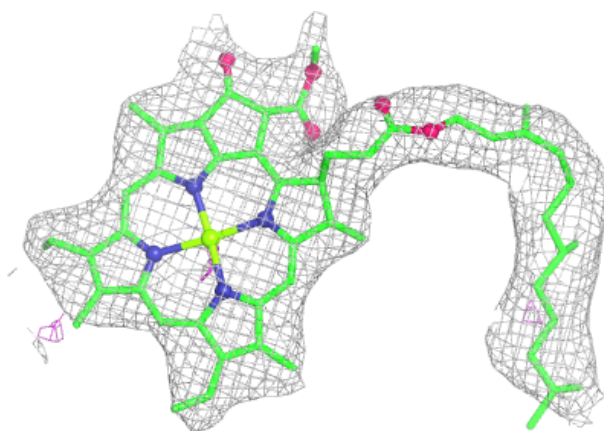
Electron density around CLA B2 617:

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

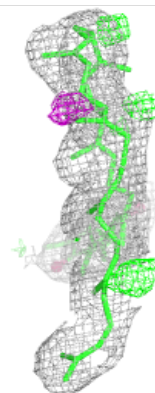
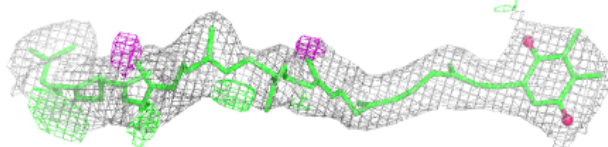
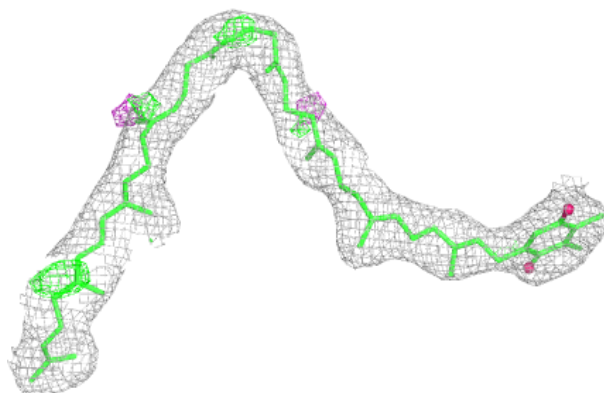


Electron density around CLA B2 618:

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

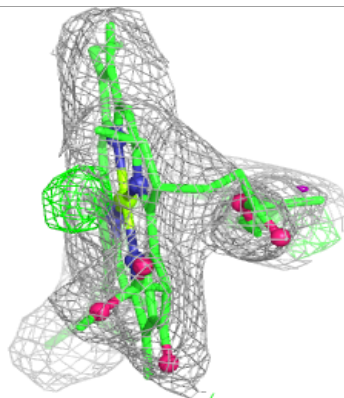
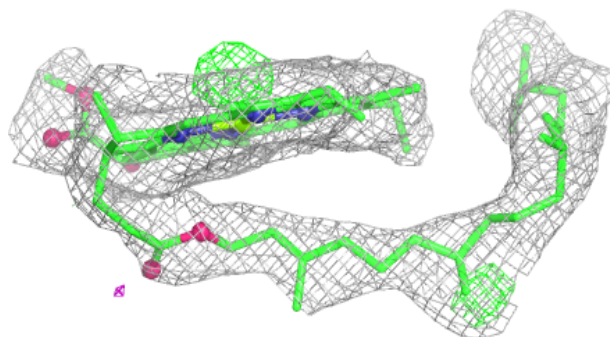
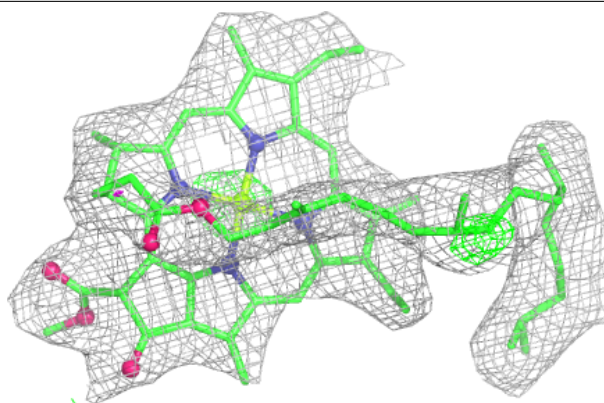
**Electron density around PL9 d1 409:**

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

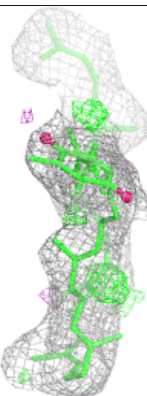
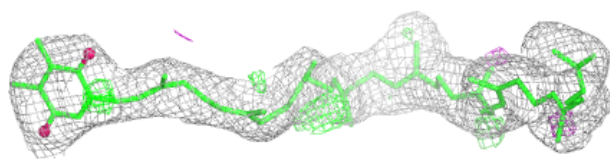
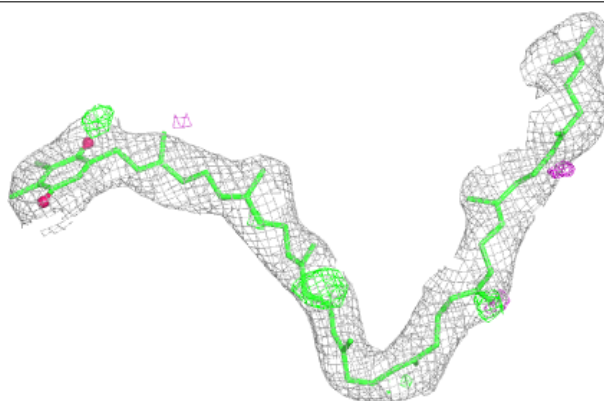


Electron density around CLA b2 617:

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

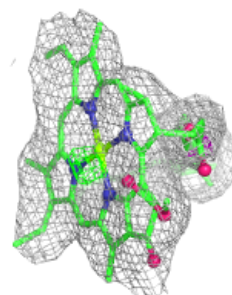
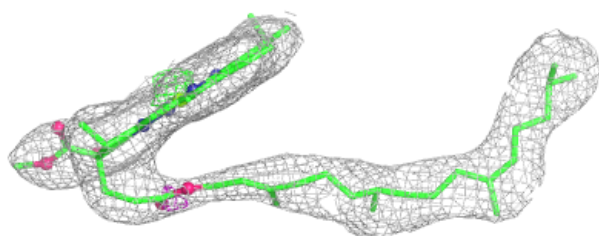
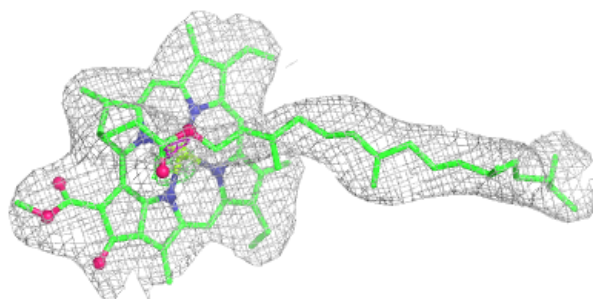
**Electron density around PL9 d2 409:**

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

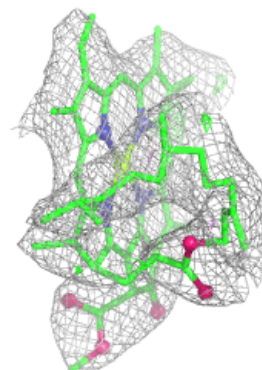
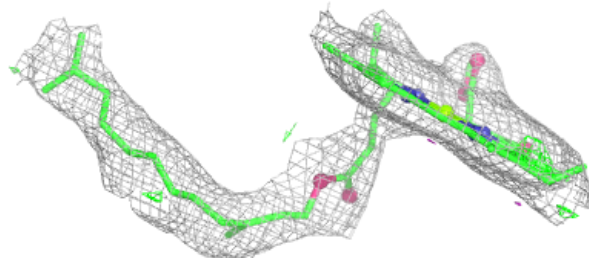
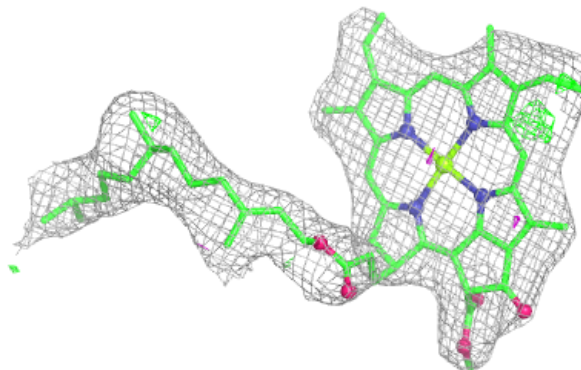


Electron density around CLA B1 610:

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

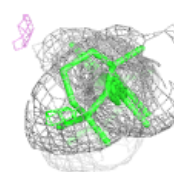
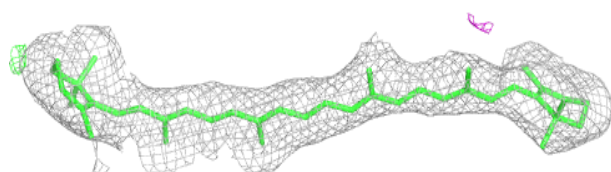
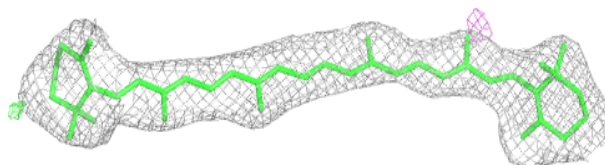
**Electron density around CLA a1 404:**

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

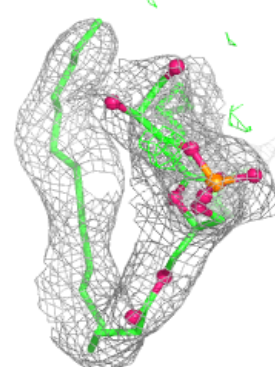
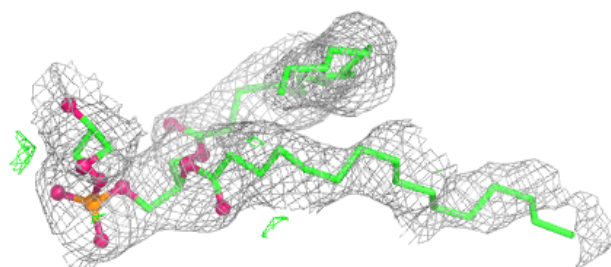
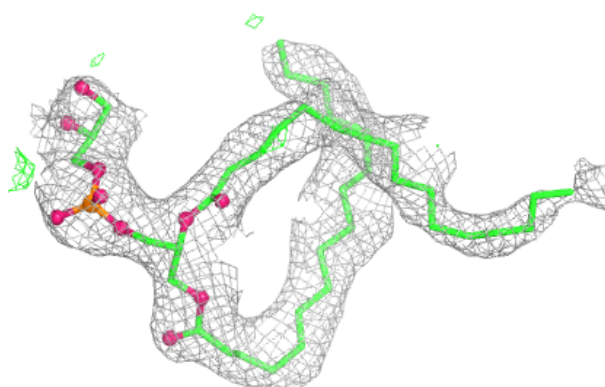


Electron density around BCR B1 603:

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

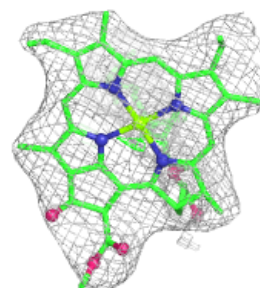
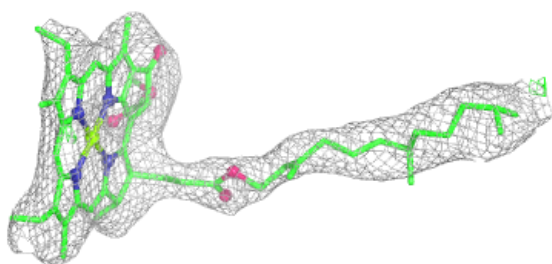
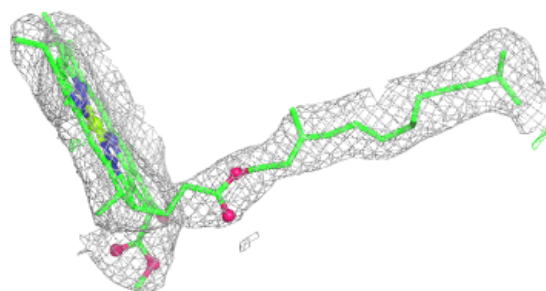
**Electron density around LHG D1 404:**

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

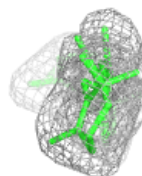
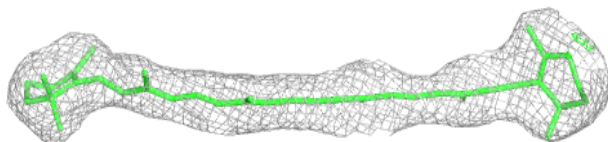
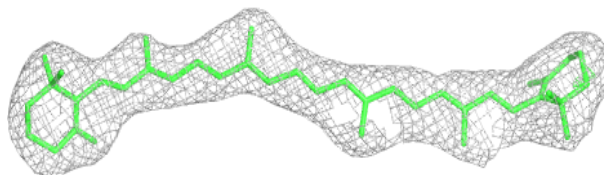


Electron density around CLA B1 607:

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

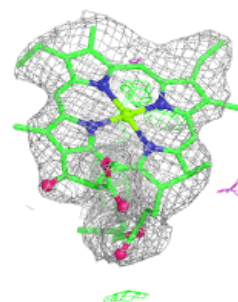
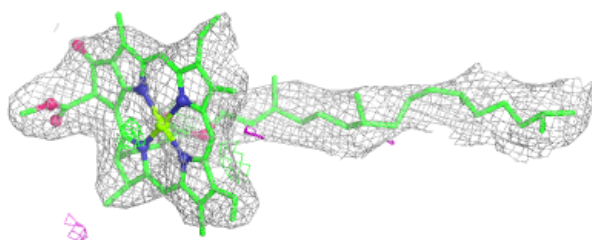
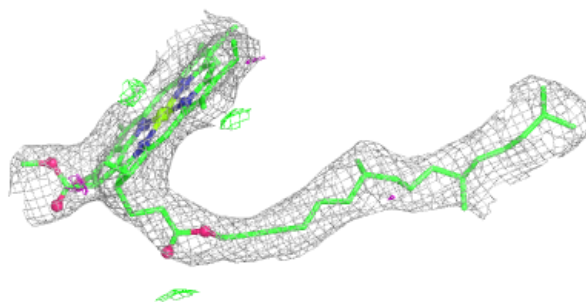
**Electron density around BCR B1 601:**

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

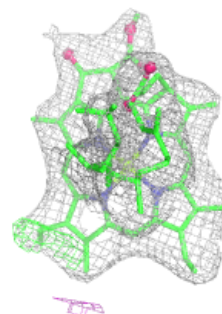
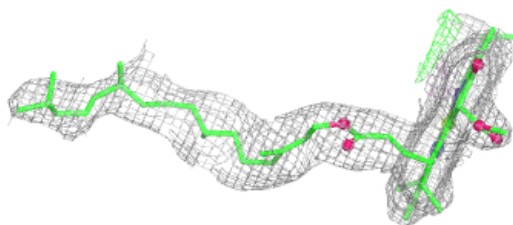
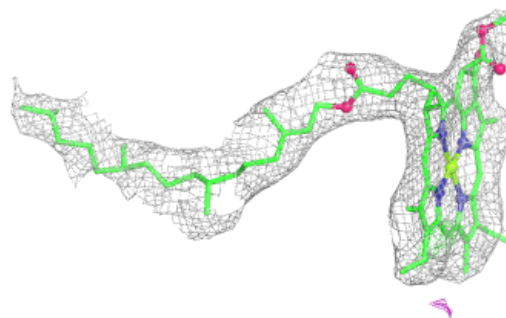


Electron density around CLA c2 505:

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

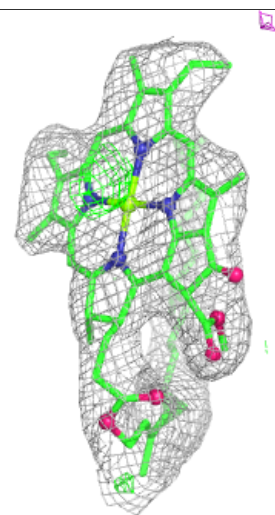
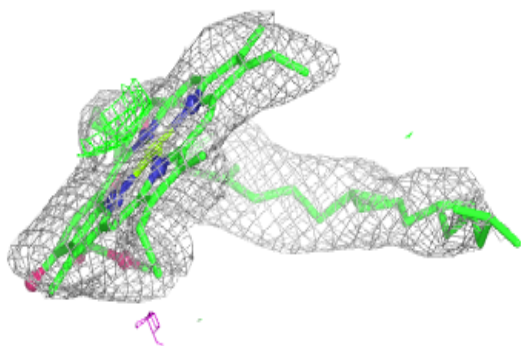
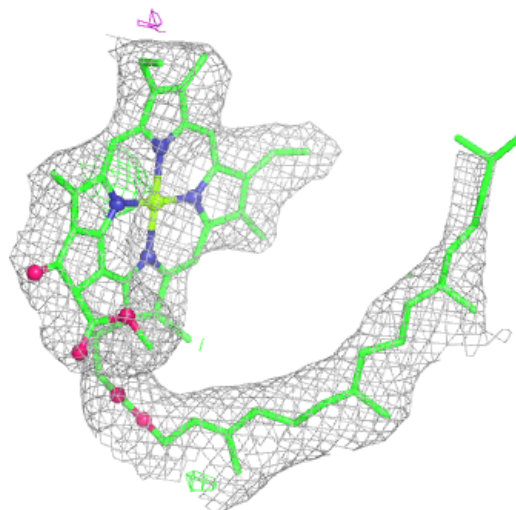
**Electron density around CLA d1 406:**

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



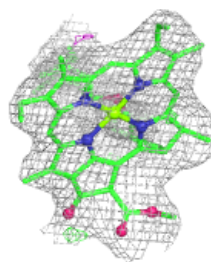
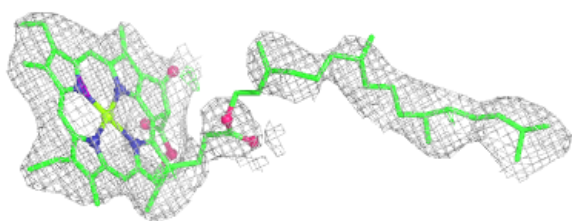
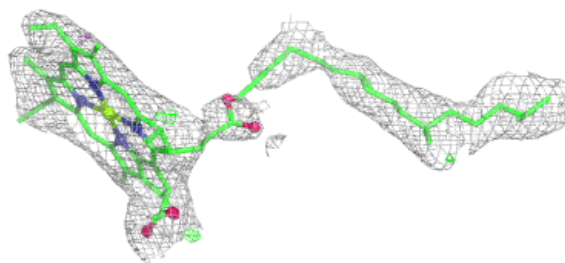
Electron density around CLA C1 508:

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

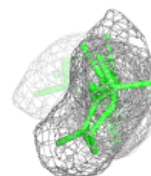
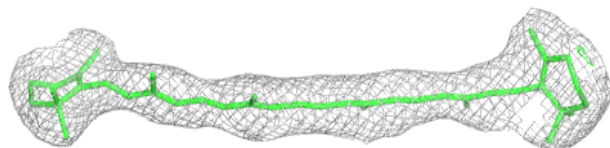
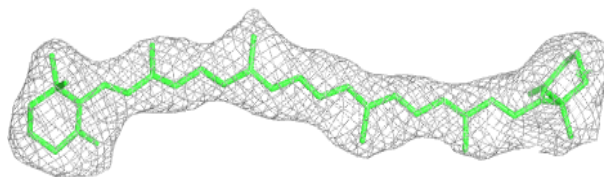


Electron density around CLA c2 503:

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

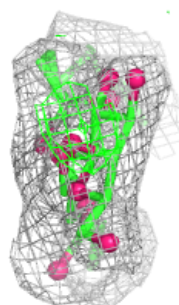
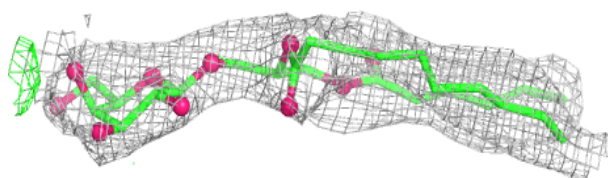
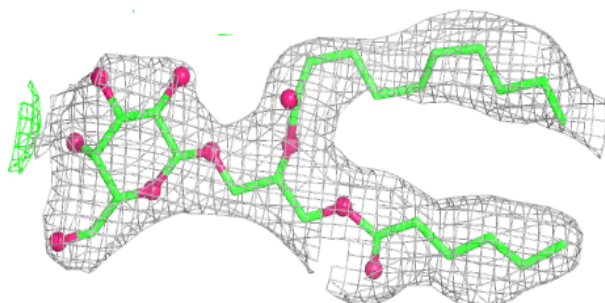
**Electron density around BCR B2 601:**

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

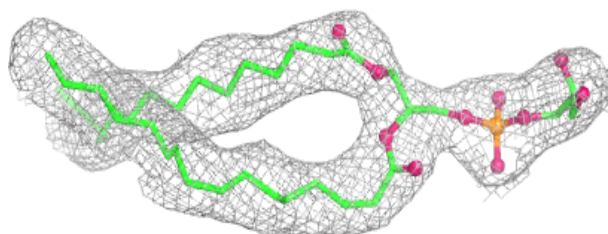
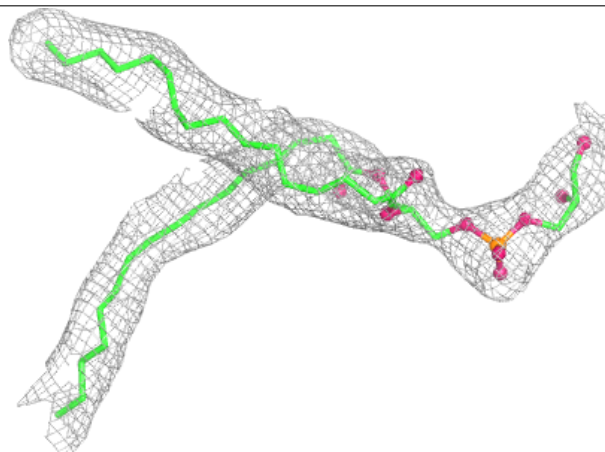


Electron density around LMG D1 406:

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

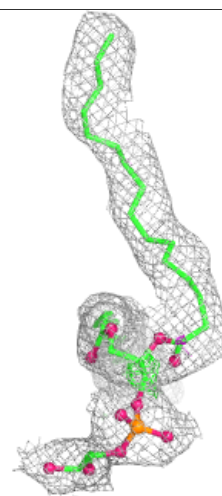
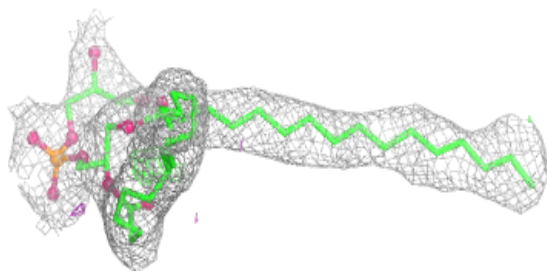
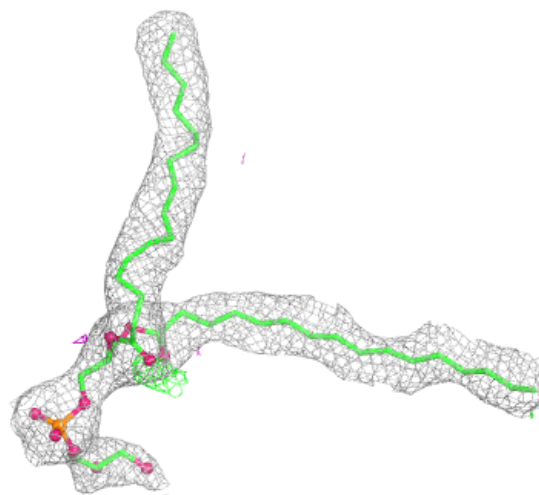
**Electron density around LHG D2 405:**

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



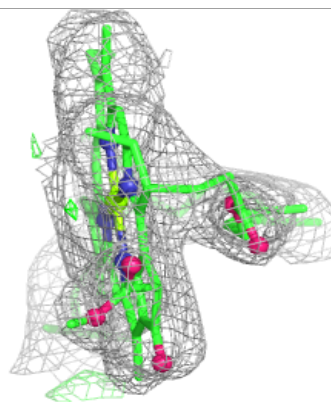
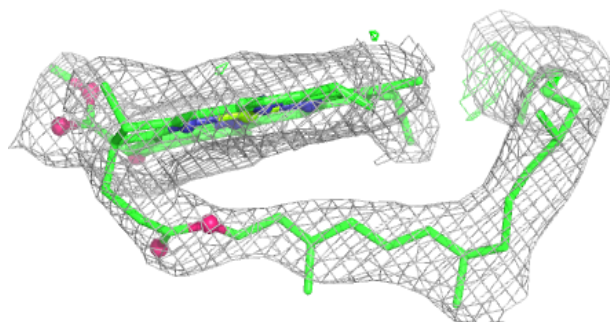
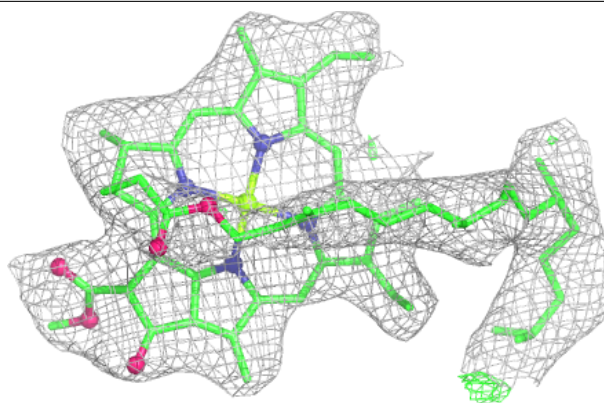
Electron density around LHG L2 101:

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

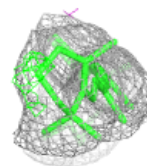
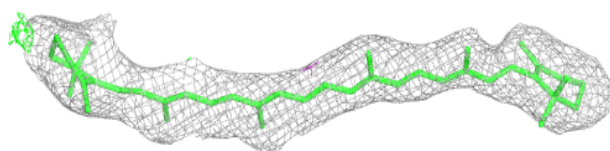
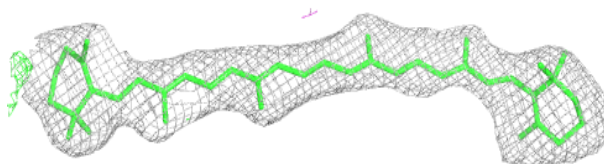


Electron density around CLA B1 616:

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

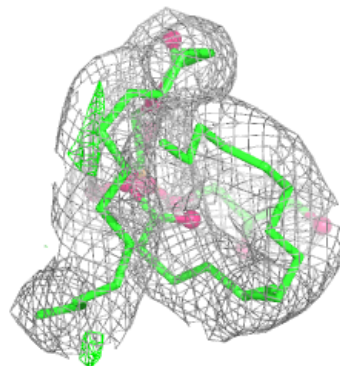
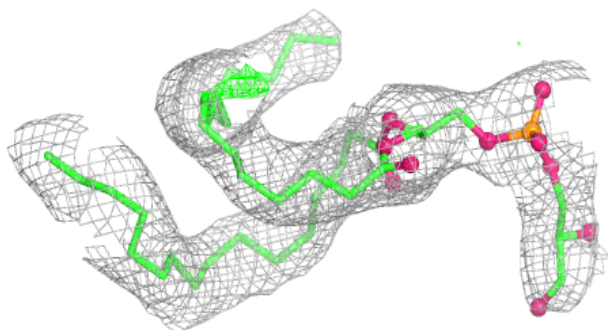
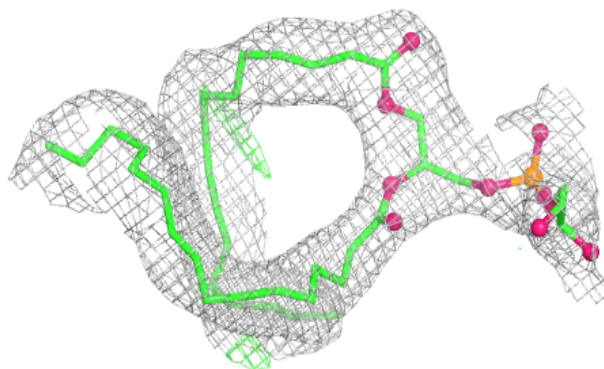
**Electron density around BCR b1 603:**

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

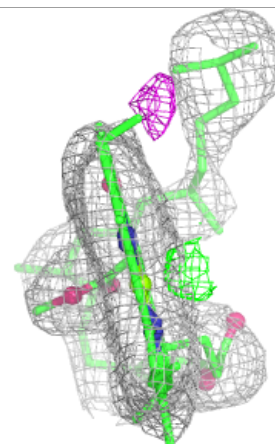
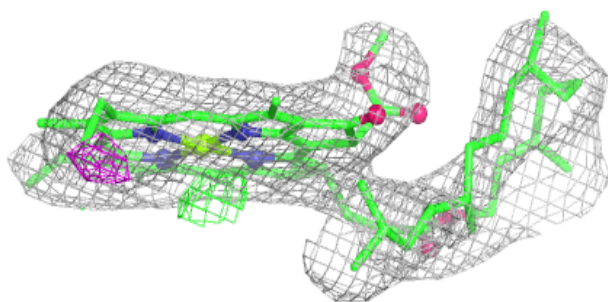
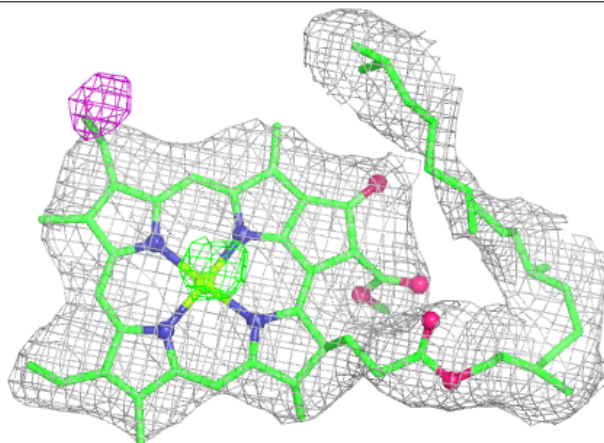


Electron density around LHG d2 403:

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

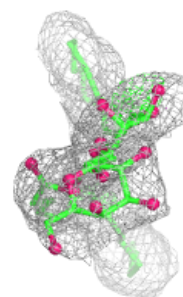
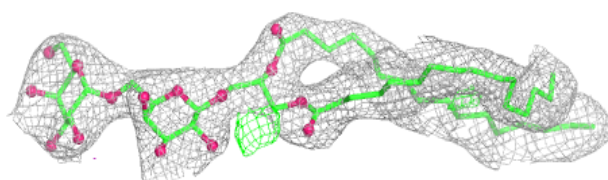
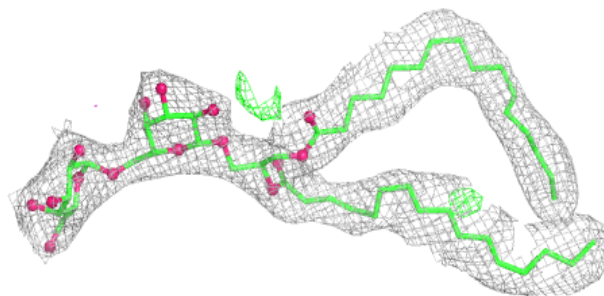
**Electron density around CLA b2 611:**

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

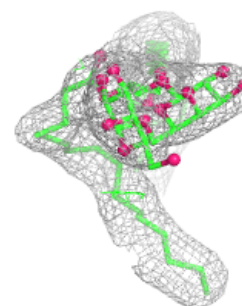
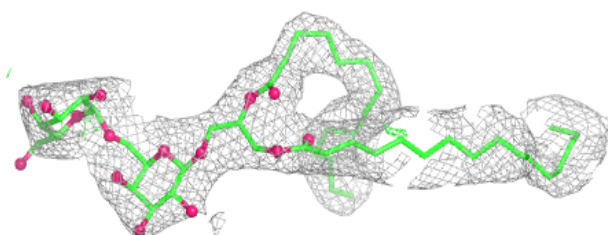
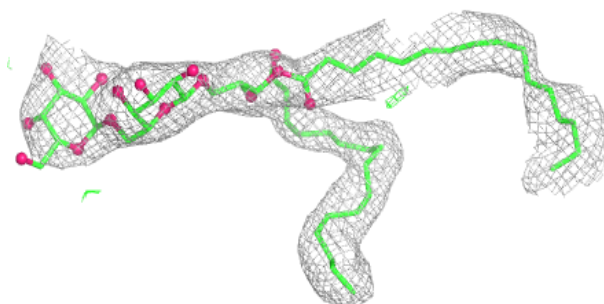


Electron density around DGD C1 516:

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

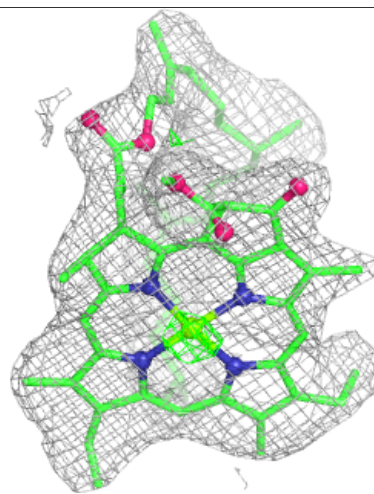
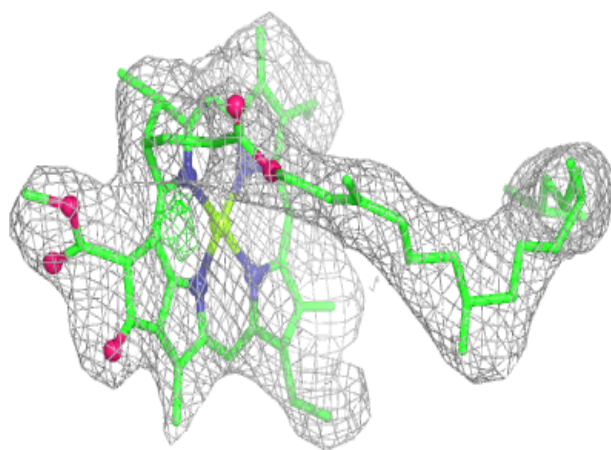
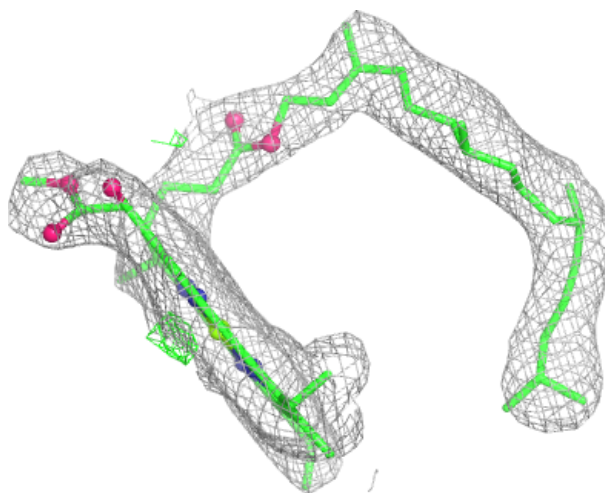
**Electron density around DGD H1 101:**

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



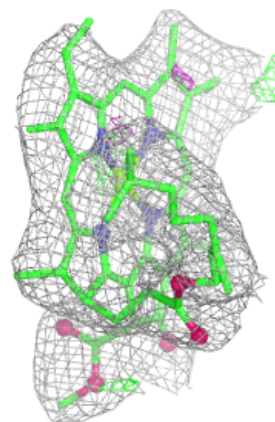
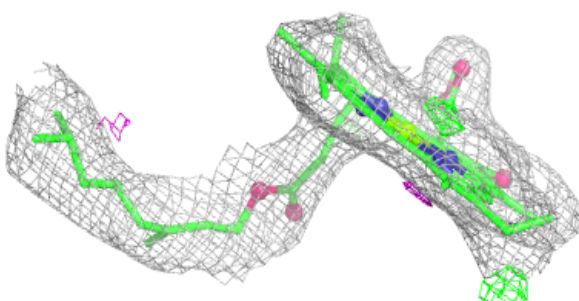
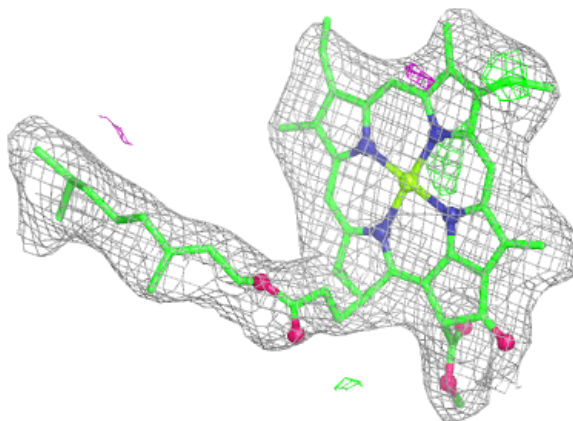
Electron density around CLA b2 612:

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

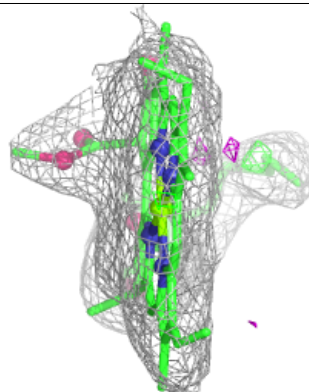
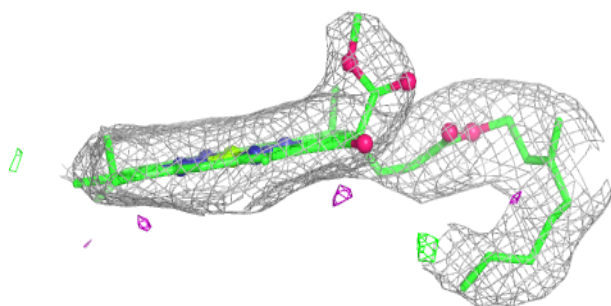
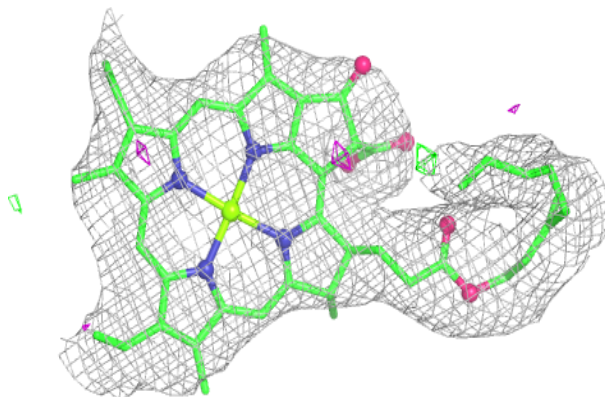


Electron density around CLA A1 405:

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

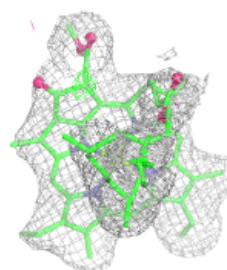
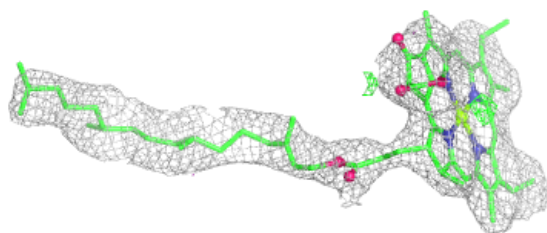
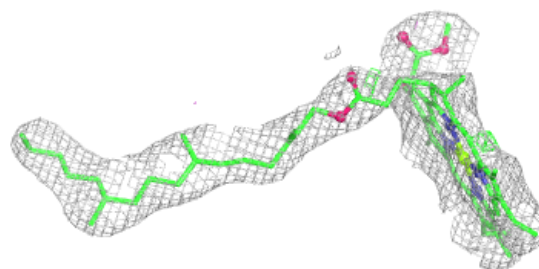
**Electron density around CLA c2 510:**

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

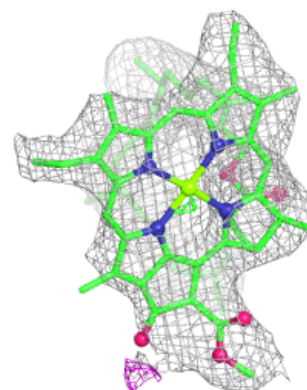
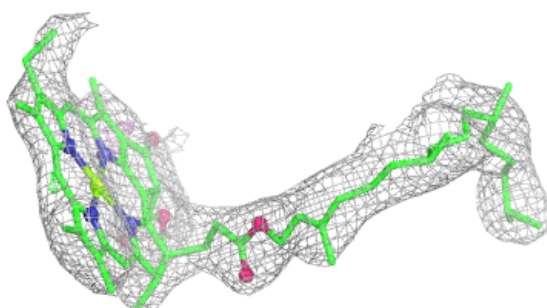
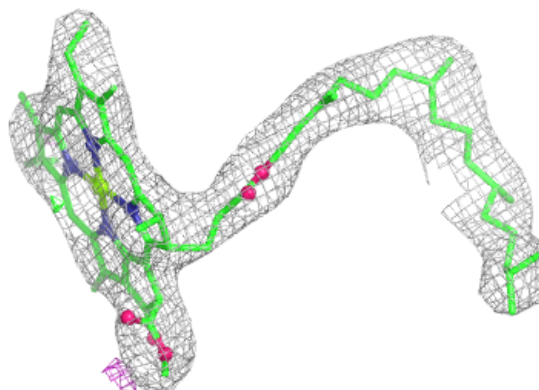


Electron density around CLA B2 607:

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

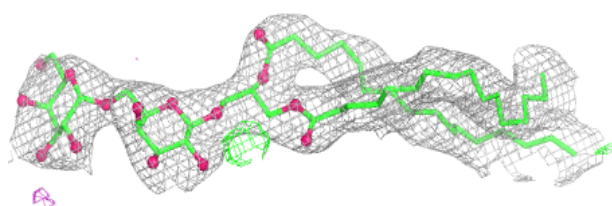
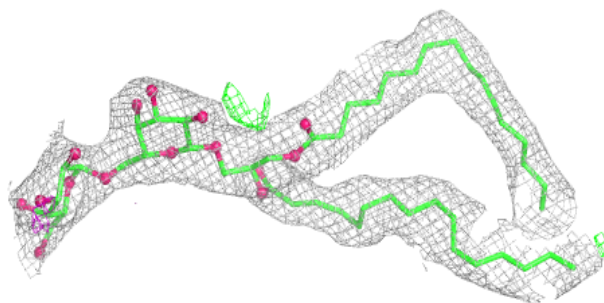
**Electron density around CLA B2 609:**

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

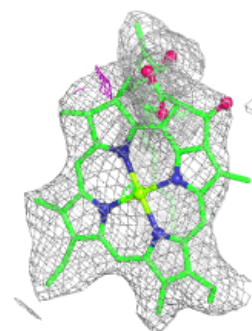
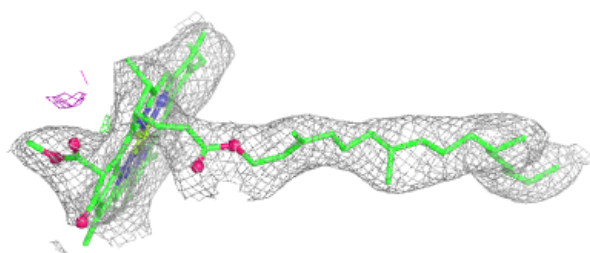
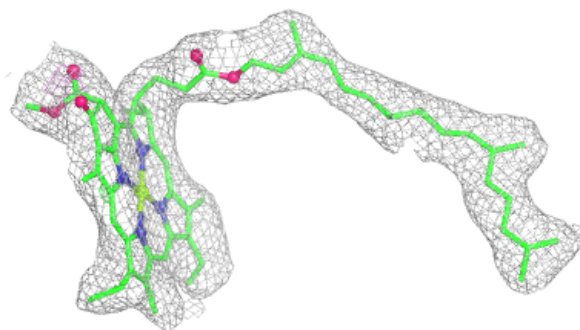


Electron density around DGD c2 514:

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

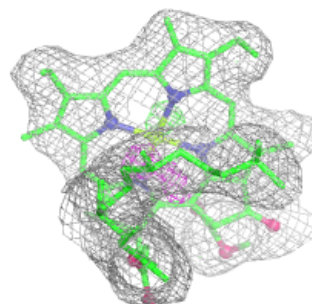
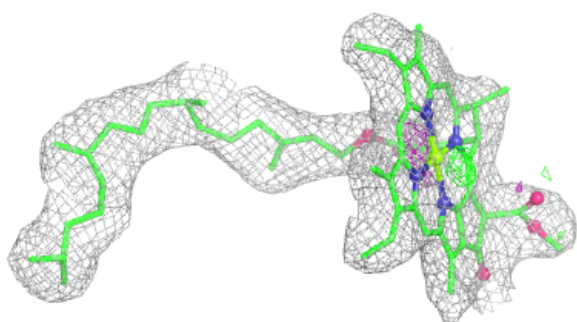
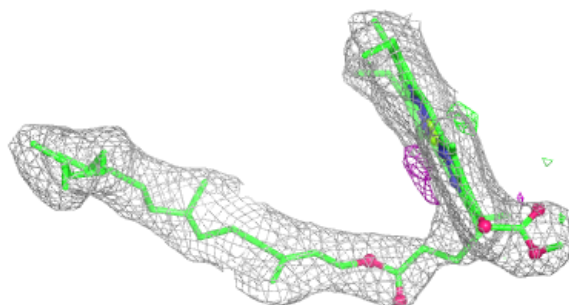
**Electron density around CLA b1 611:**

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

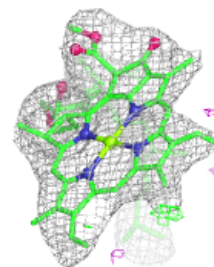
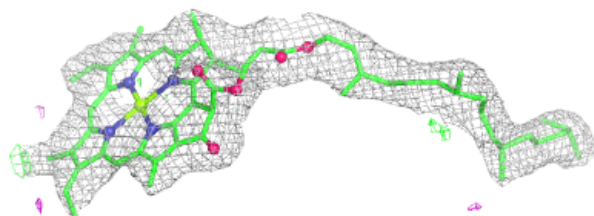
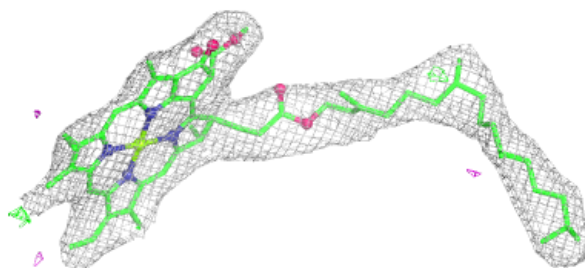


Electron density around CLA B1 619:

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

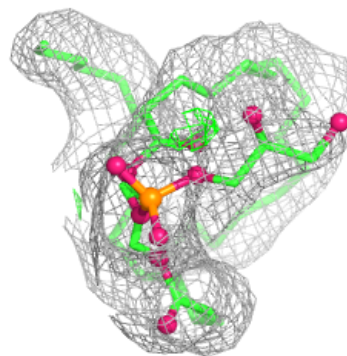
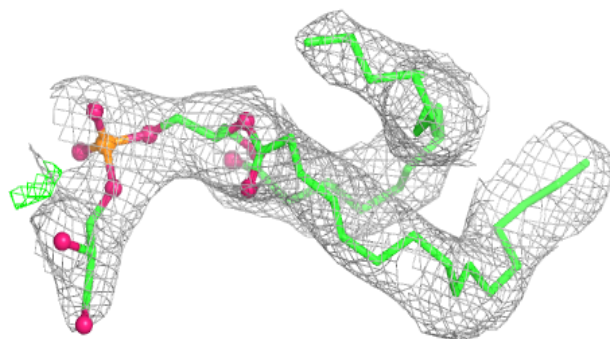
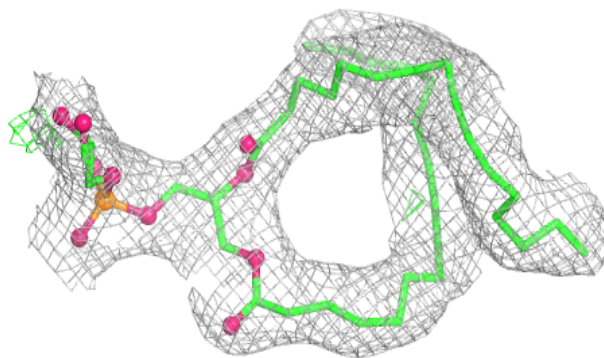
**Electron density around CLA A2 402:**

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



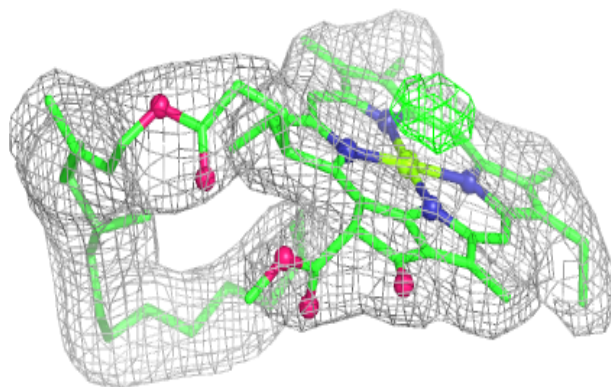
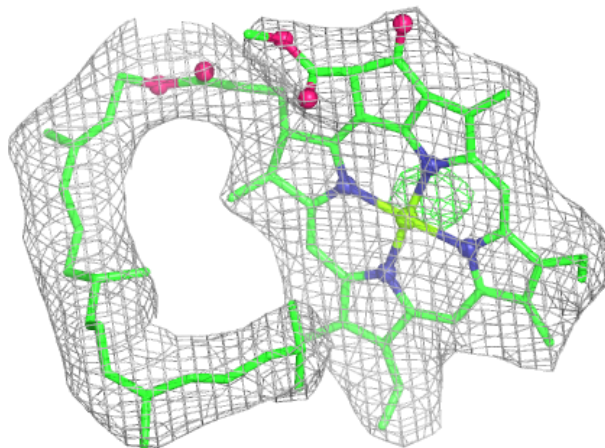
Electron density around LHG B1 621:

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



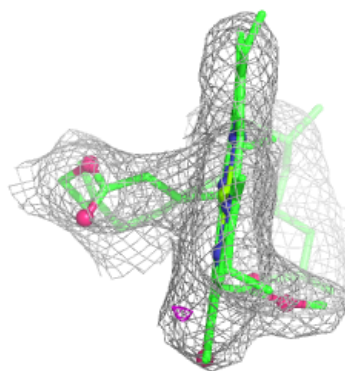
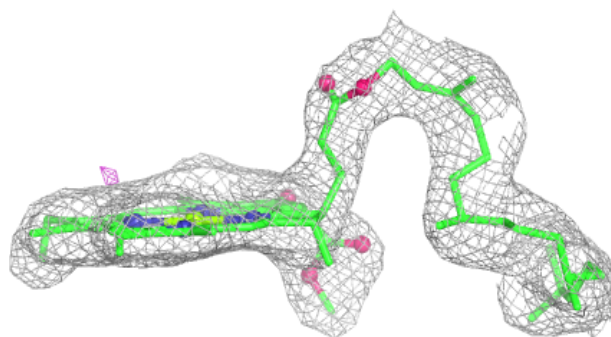
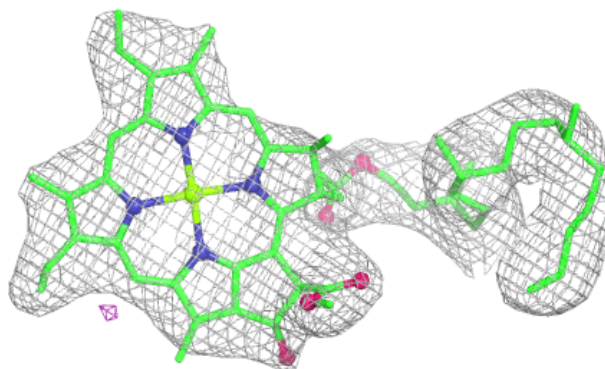
Electron density around CLA b1 617:

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

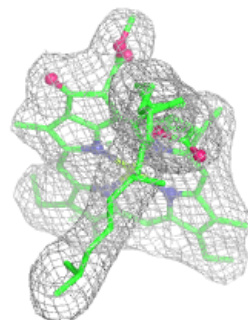
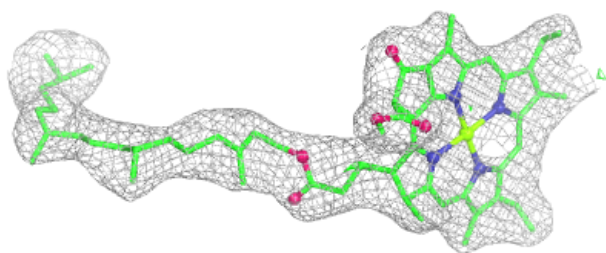
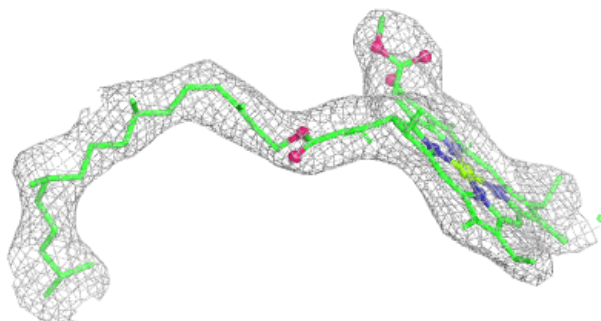


Electron density around CLA b2 614:

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

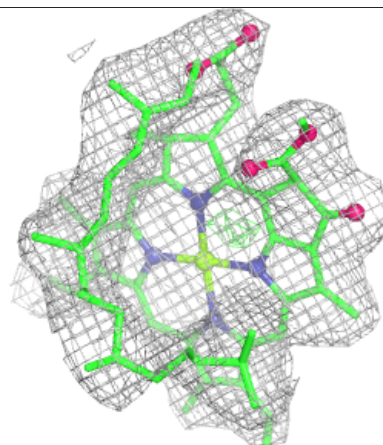
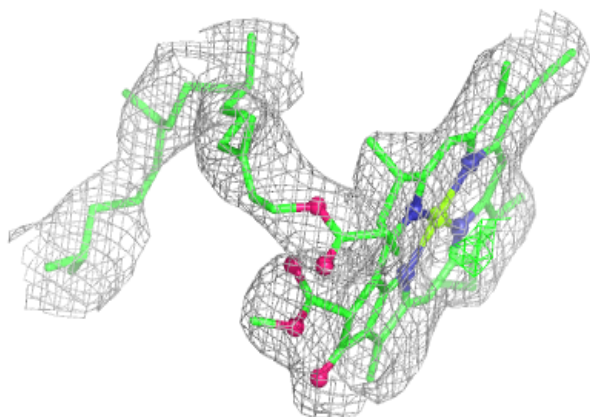
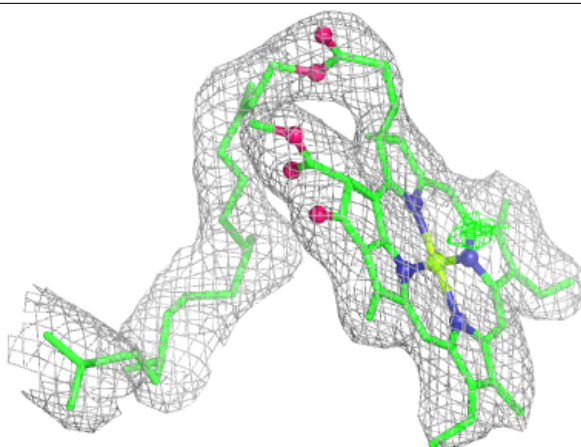
**Electron density around CLA d1 401:**

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



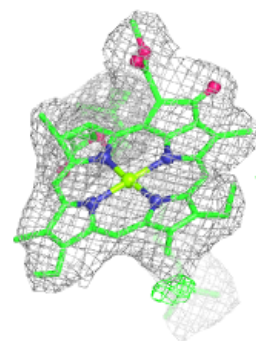
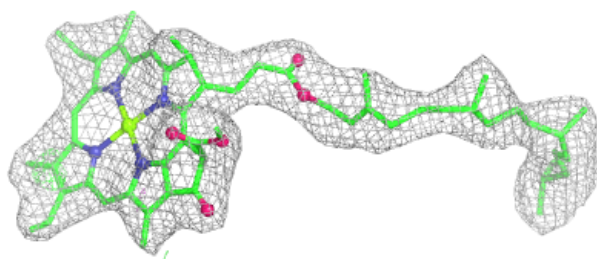
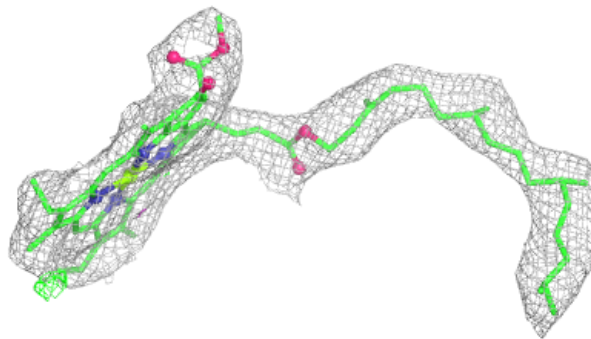
Electron density around CLA B2 615:

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



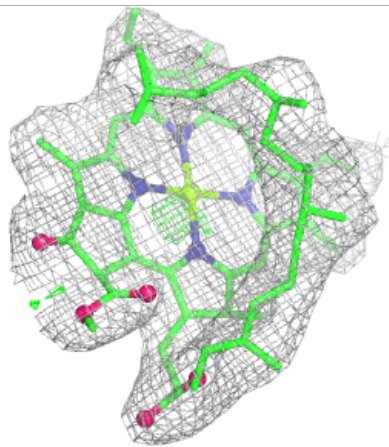
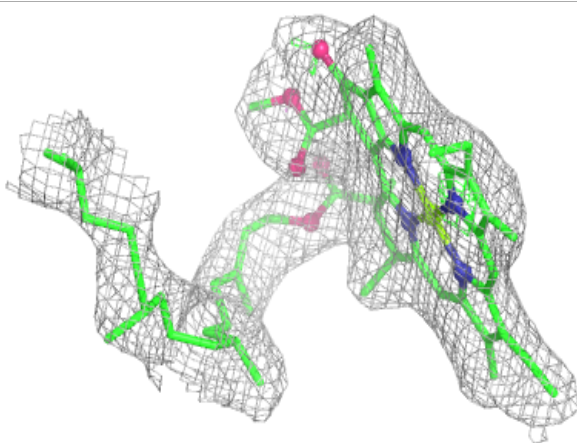
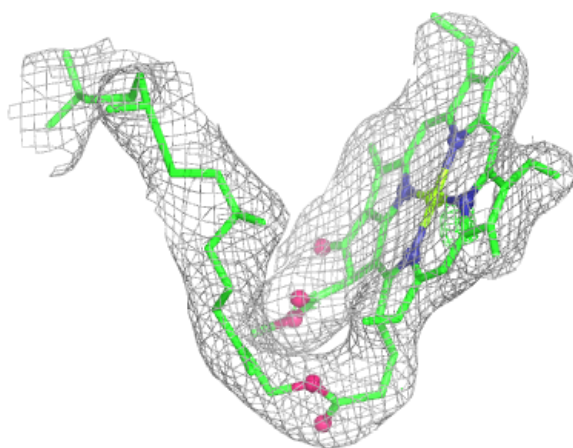
Electron density around CLA d2 405:

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



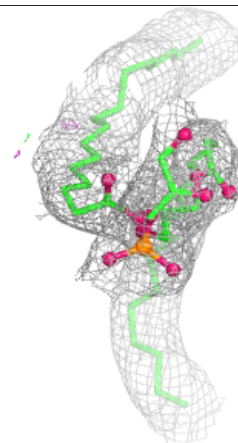
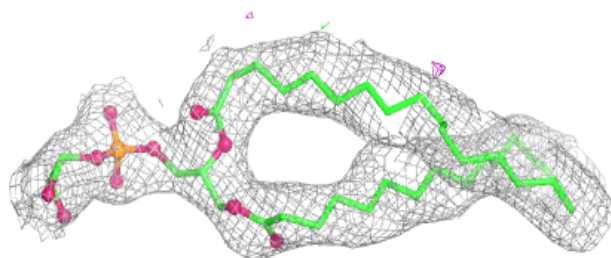
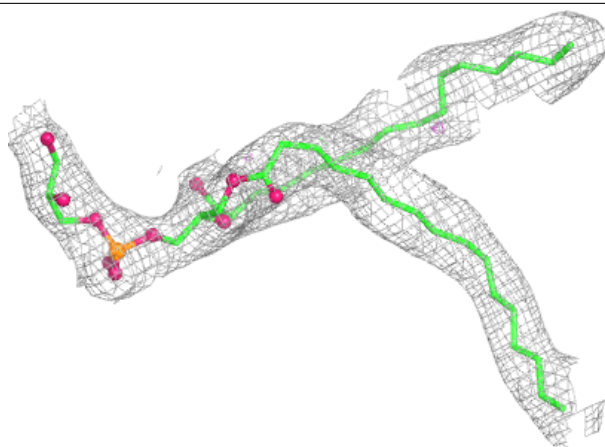
Electron density around CLA B1 615:

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



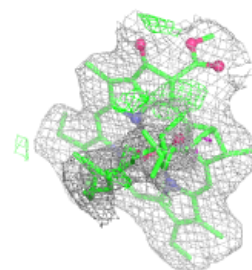
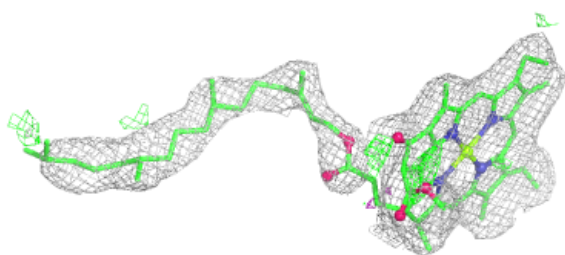
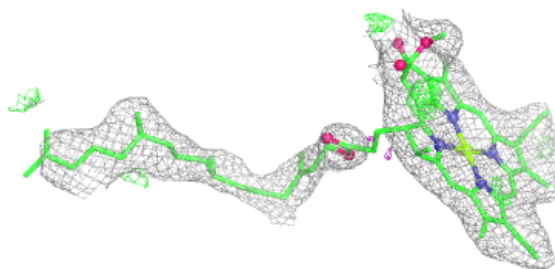
Electron density around LHG d2 406:

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

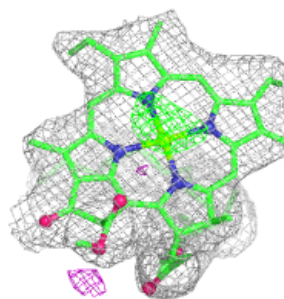
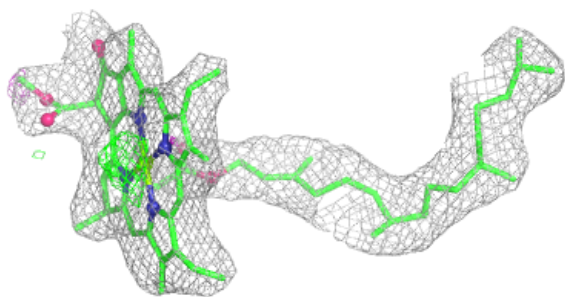
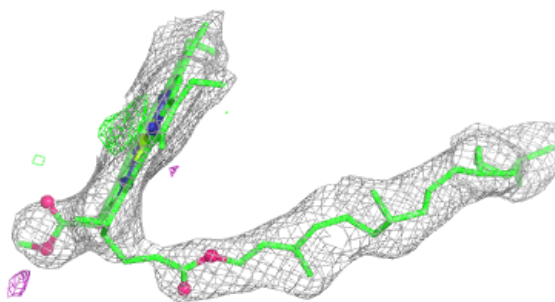


Electron density around CLA c1 504:

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

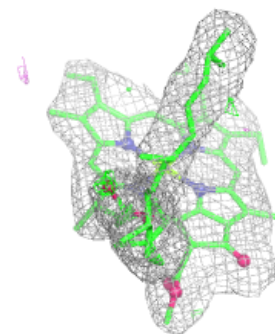
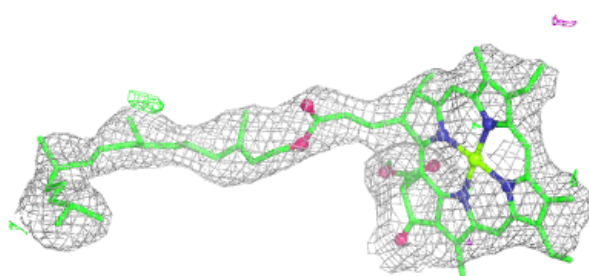
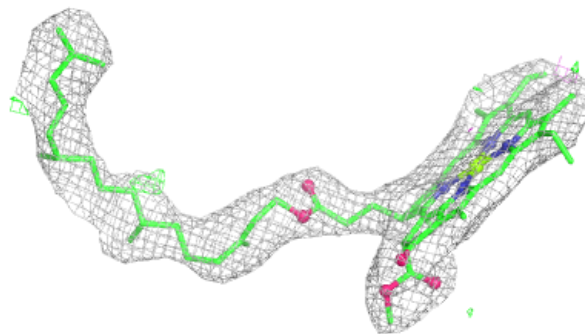
**Electron density around CLA b2 620:**

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

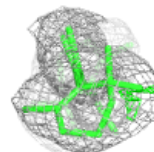
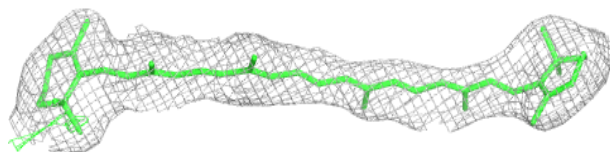
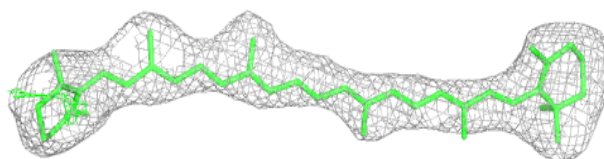


Electron density around CLA D2 401:

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

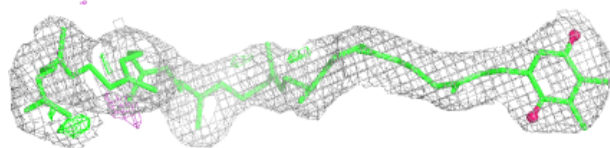
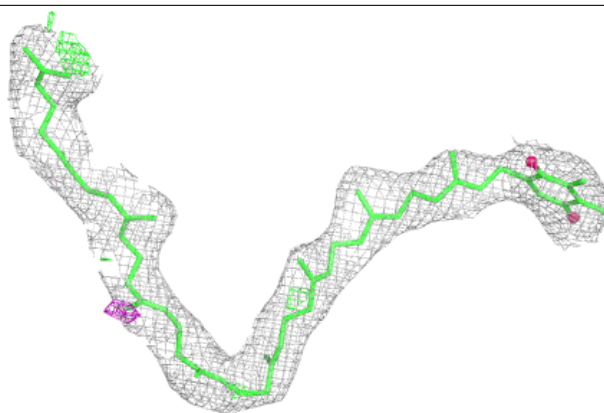
**Electron density around BCR a1 401:**

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

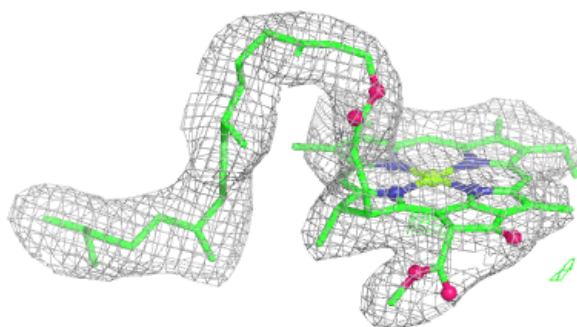
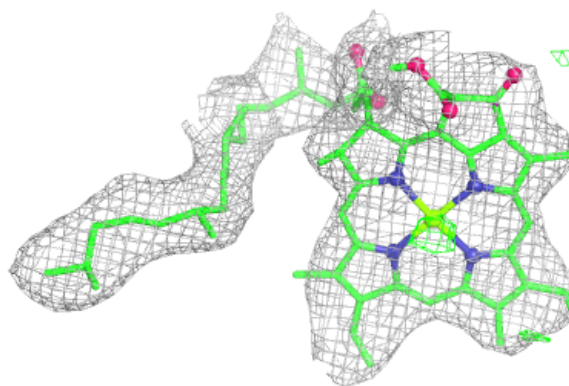


Electron density around PL9 D1 408:

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

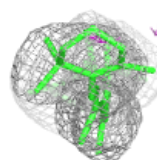
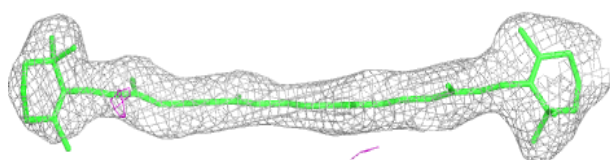
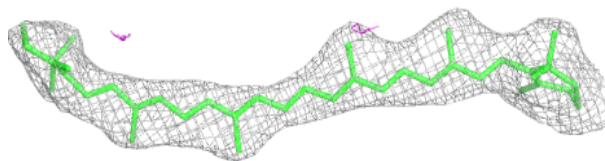
**Electron density around CLA D2 406:**

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

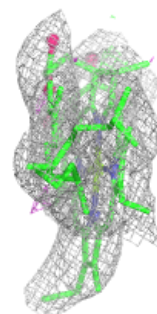
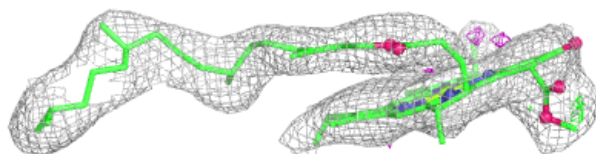
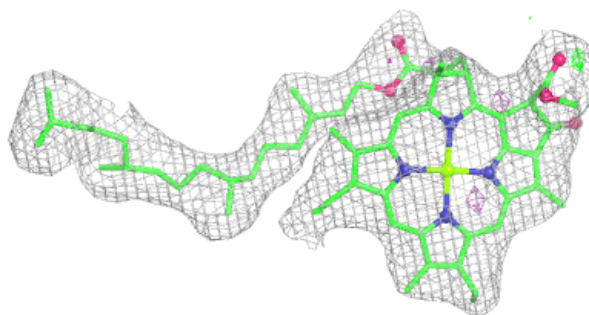


Electron density around BCR h1 102:

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

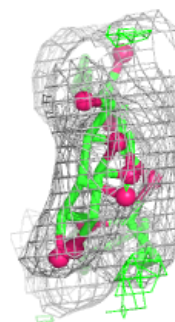
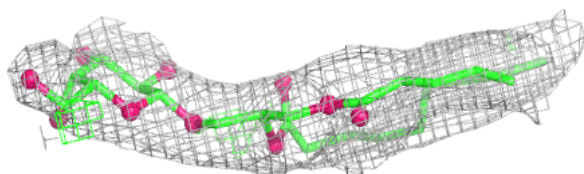
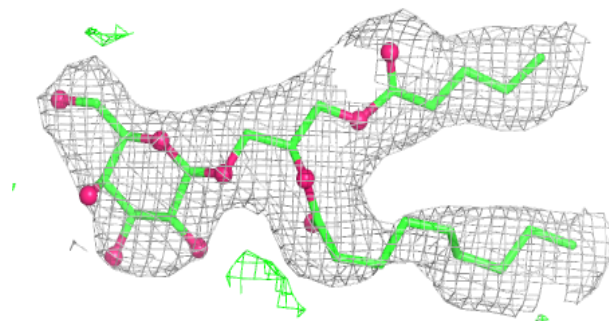
**Electron density around CLA b1 606:**

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



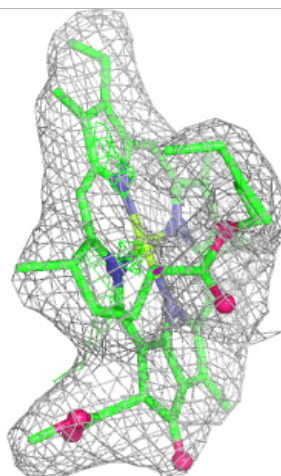
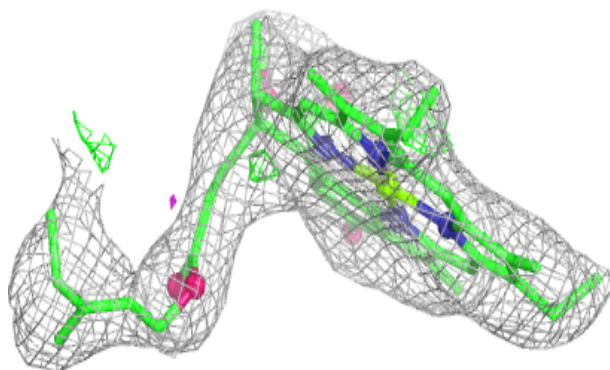
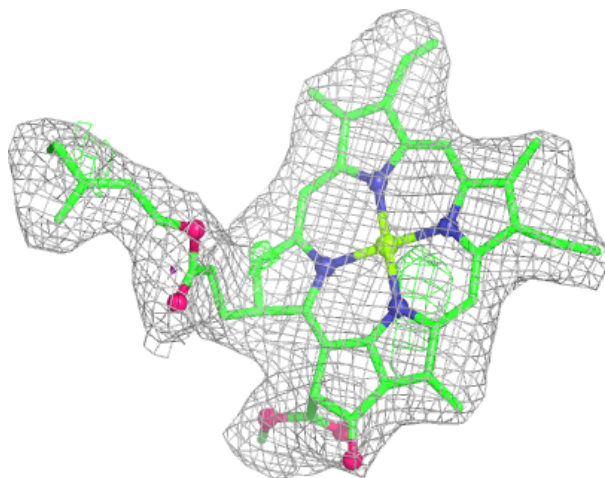
Electron density around LMG d1 408:

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



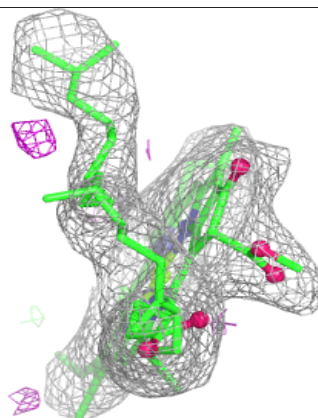
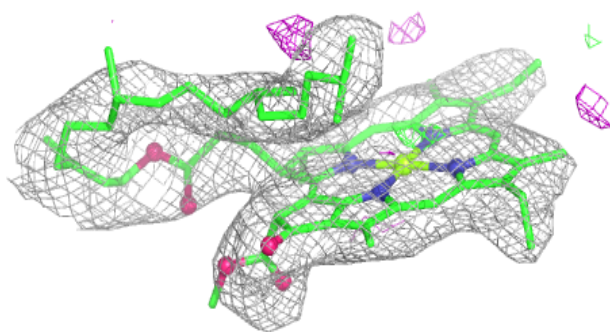
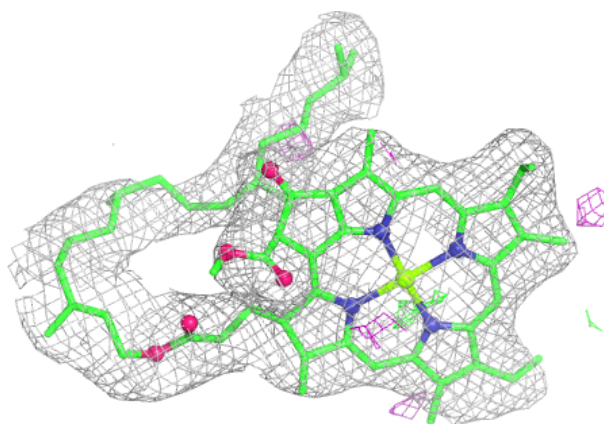
Electron density around CLA A1 404:

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



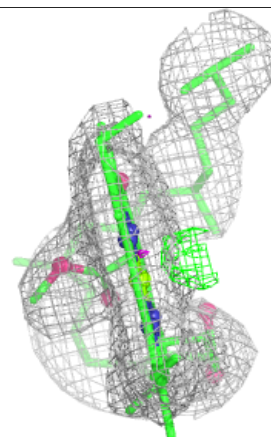
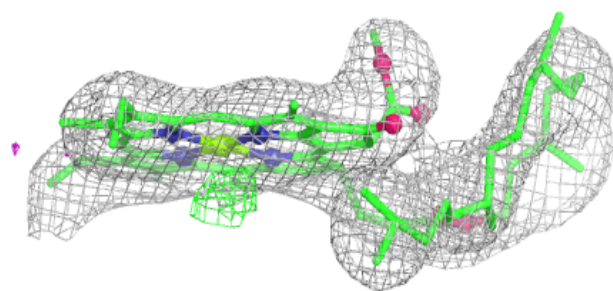
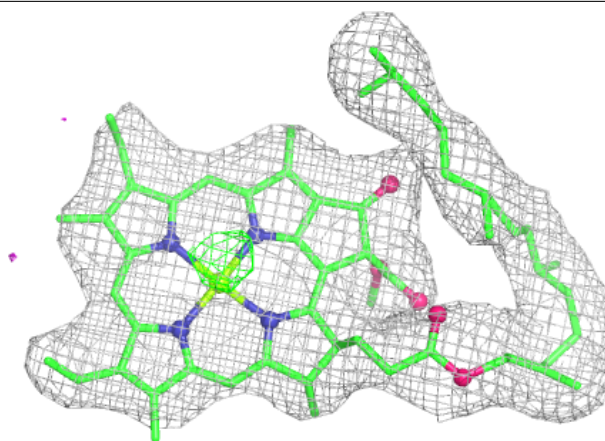
Electron density around CLA C1 510:

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



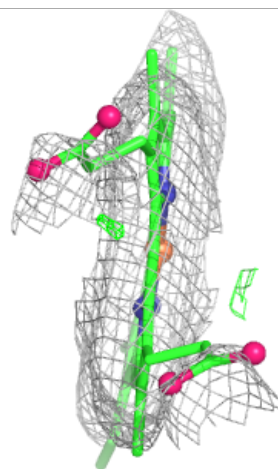
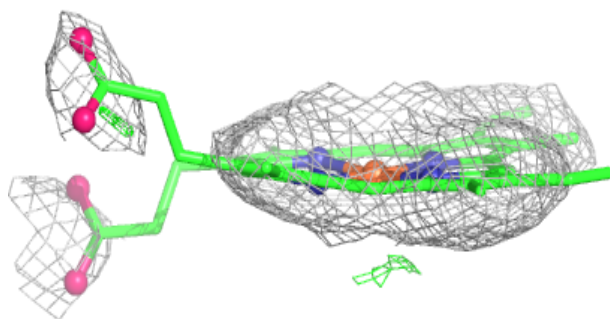
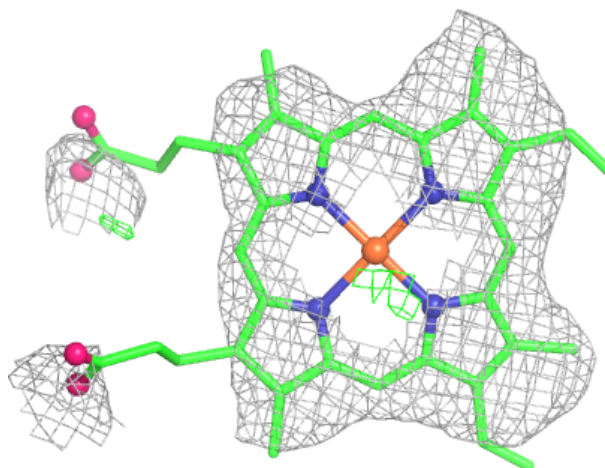
Electron density around CLA B1 612:

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



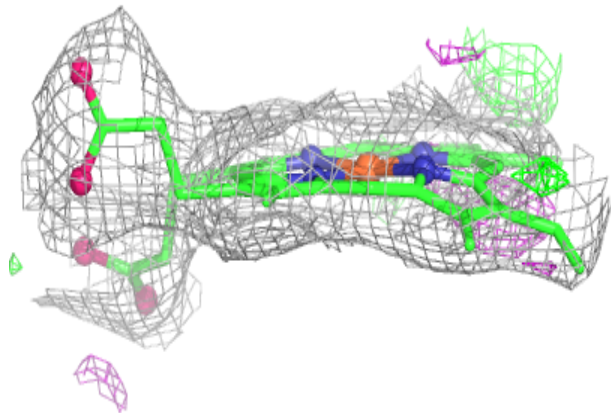
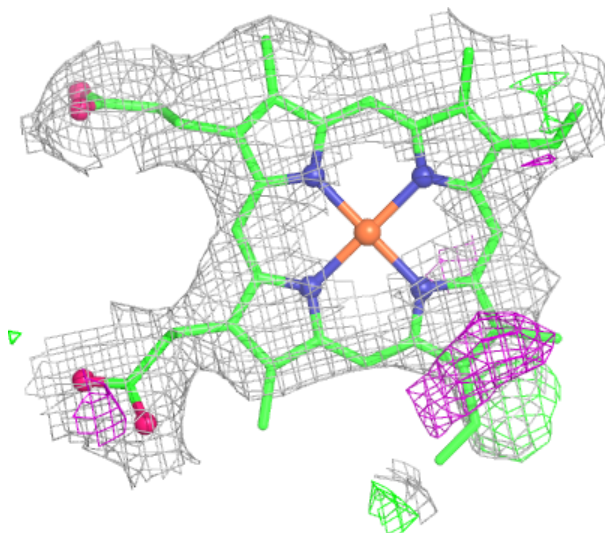
Electron density around HEM f1 101:

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



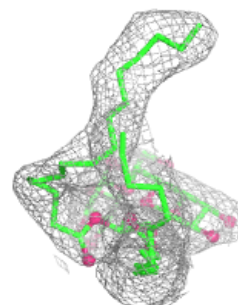
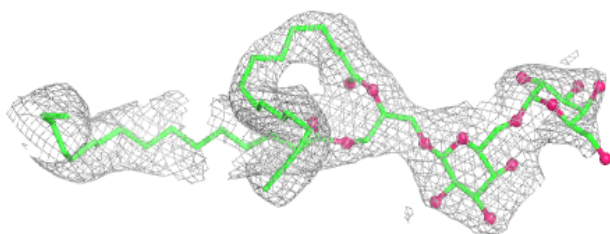
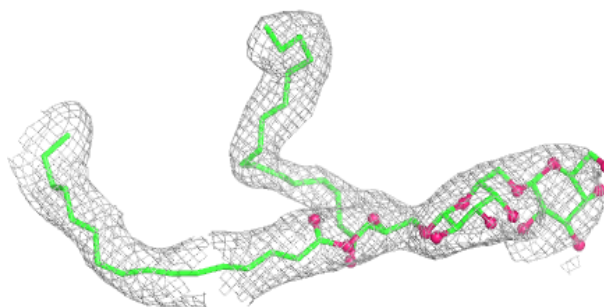
Electron density around HEM v1 201:

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

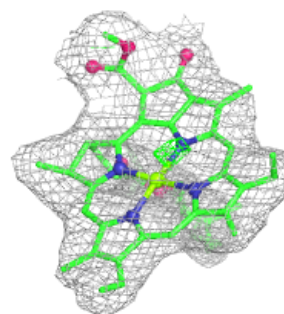
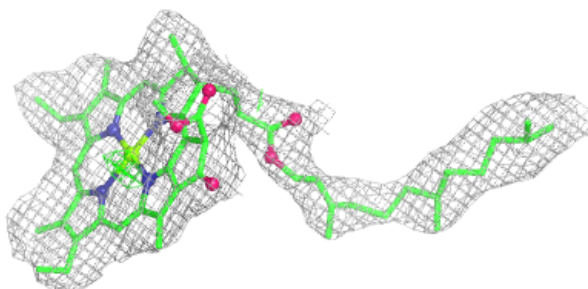
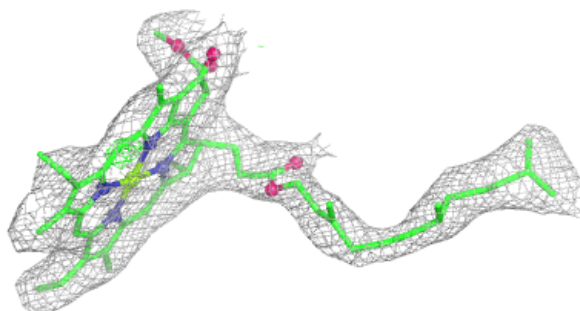


Electron density around DGD h2 102:

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

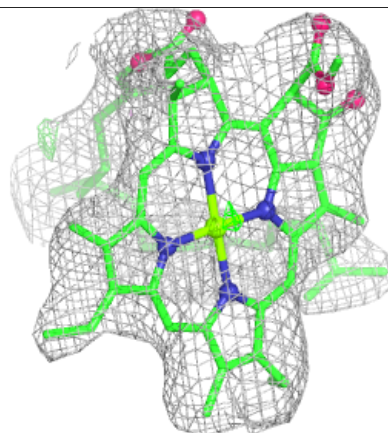
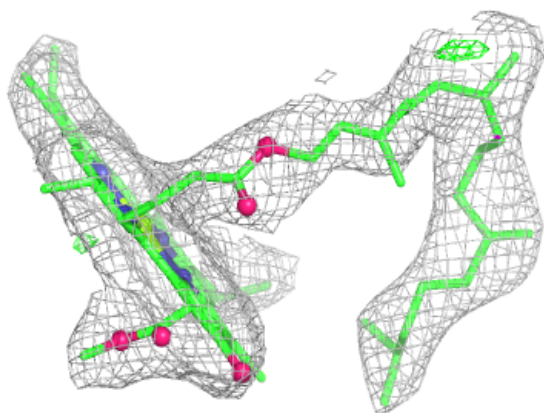
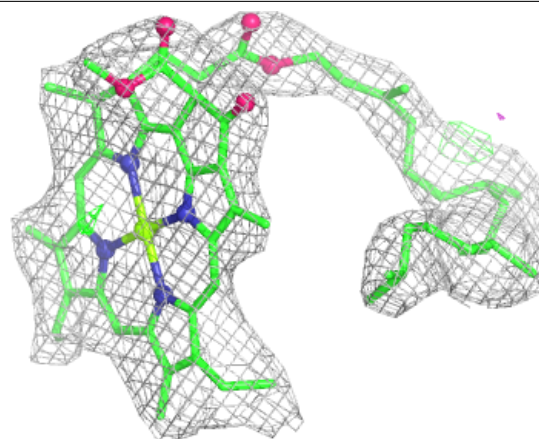
**Electron density around CLA C1 503:**

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

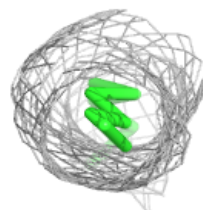
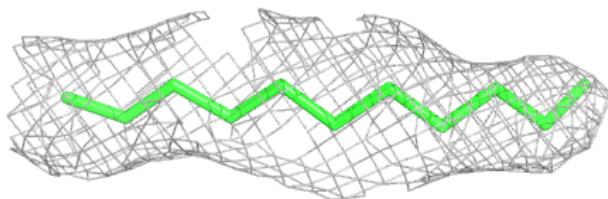
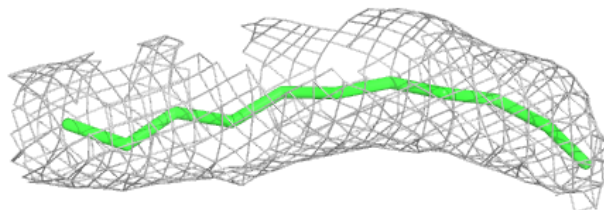


Electron density around CLA C1 504:

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

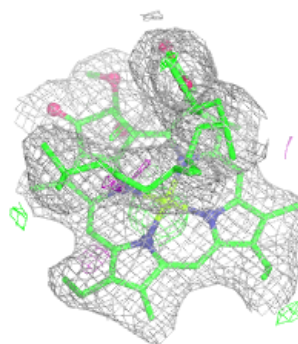
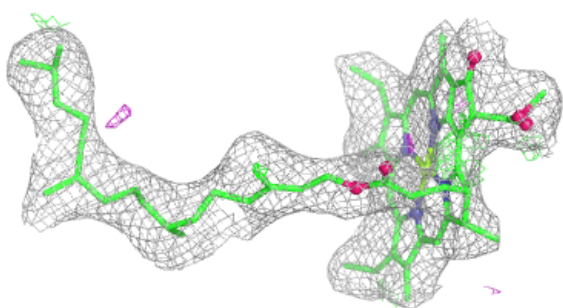
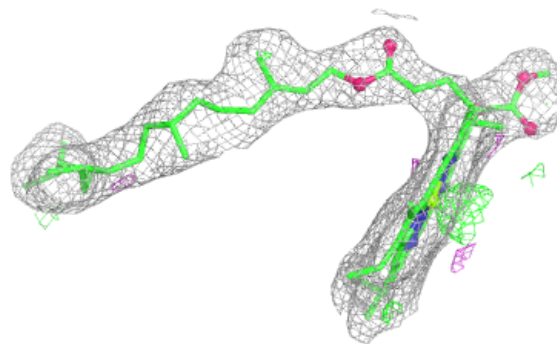
**Electron density around LMT M1 102:**

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

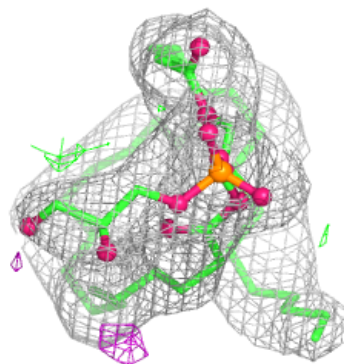
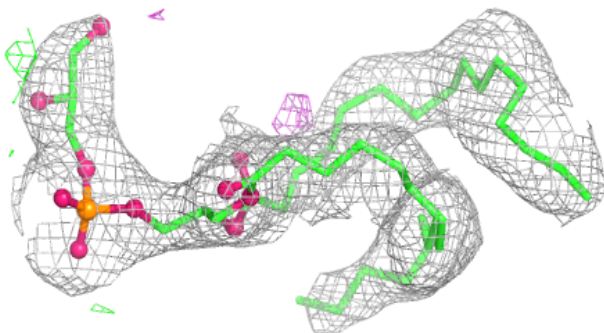
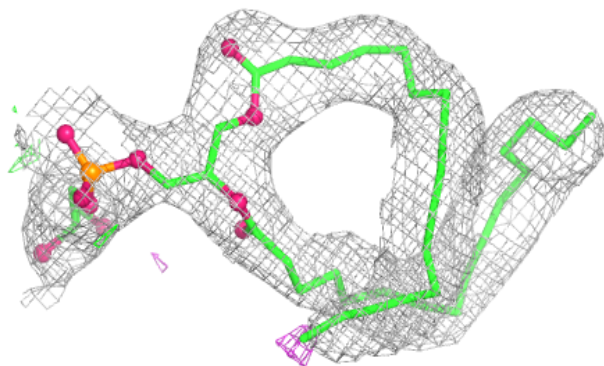


Electron density around CLA b1 620:

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

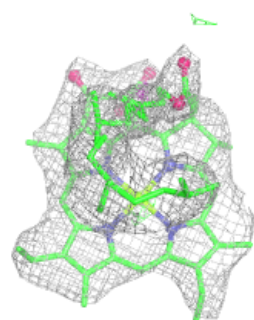
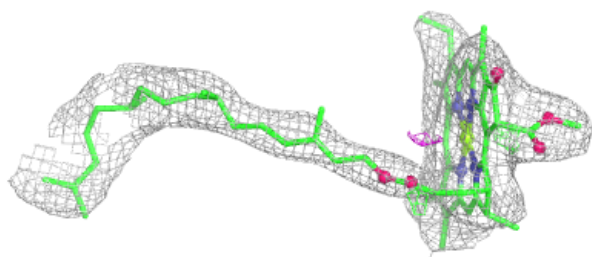
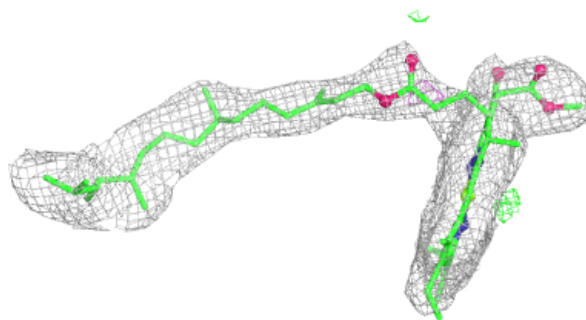
**Electron density around LHG D2 403:**

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

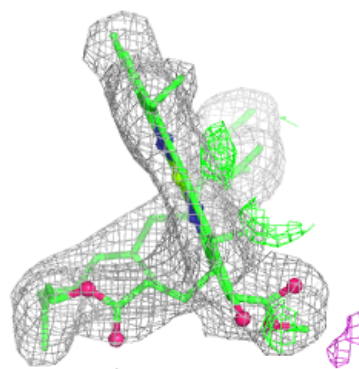
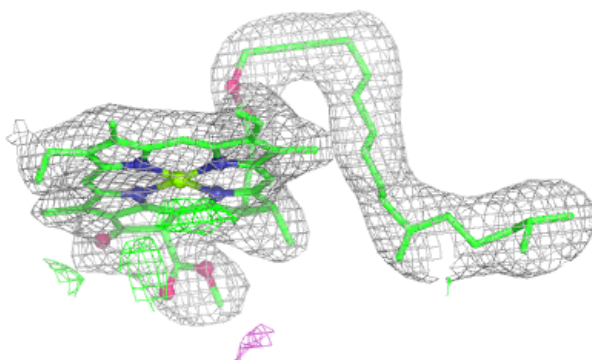
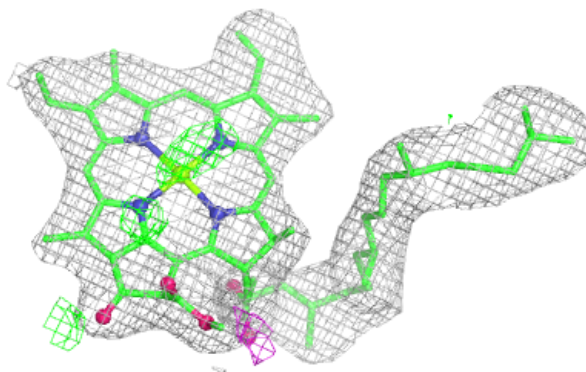


Electron density around CLA b2 608:

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

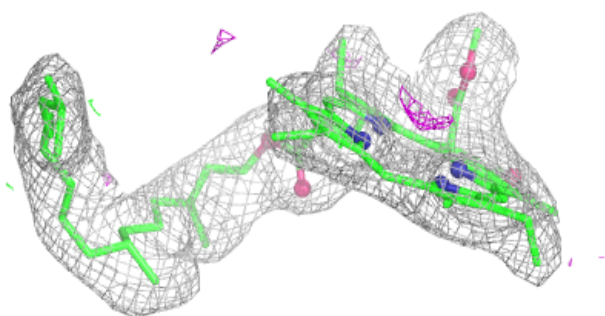
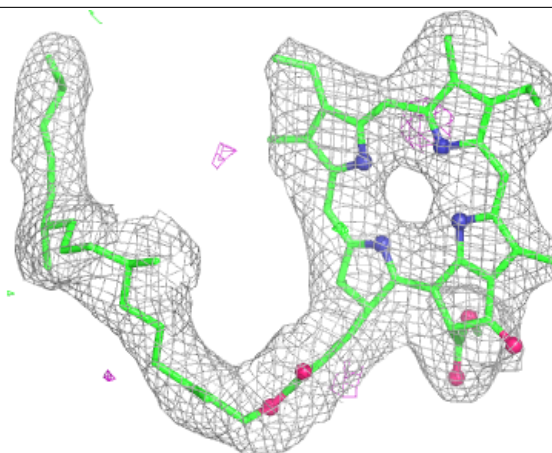
**Electron density around CLA d1 404:**

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

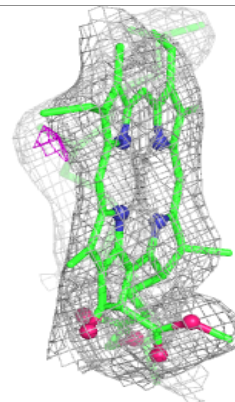
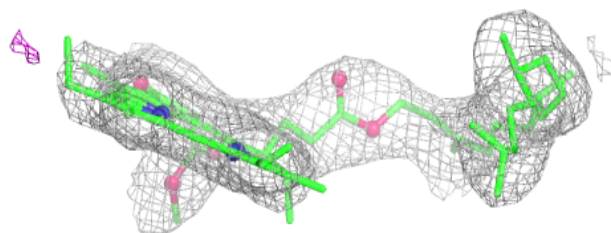
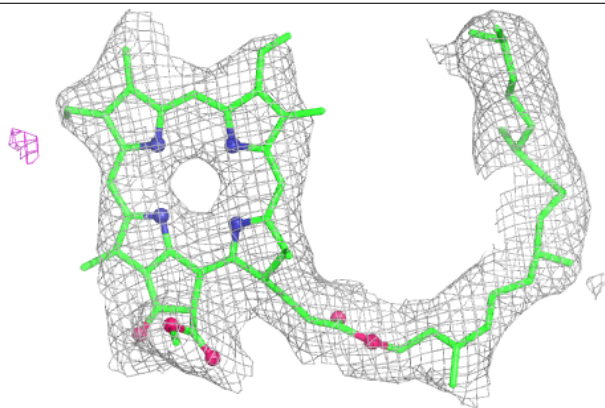


Electron density around PHO d1 403:

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

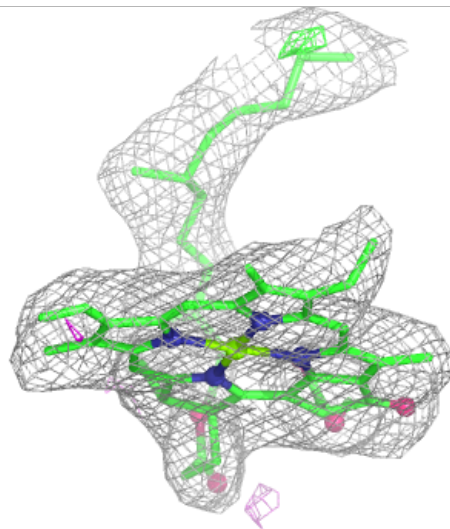
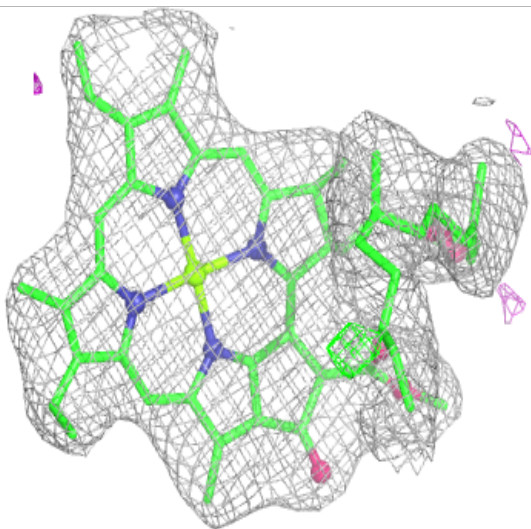
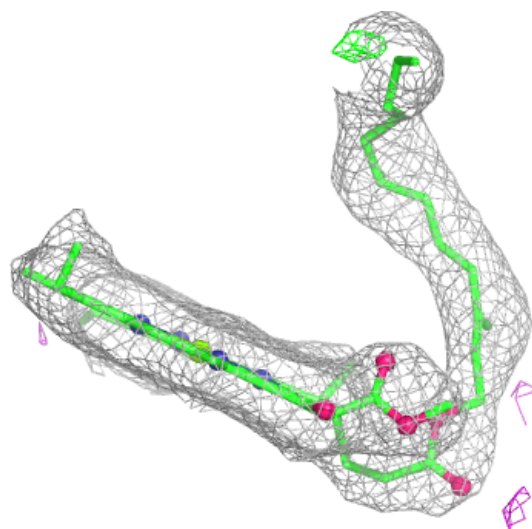
**Electron density around PHO A2 407:**

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



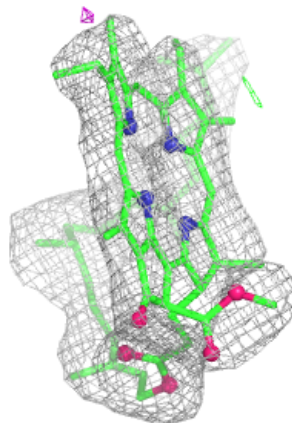
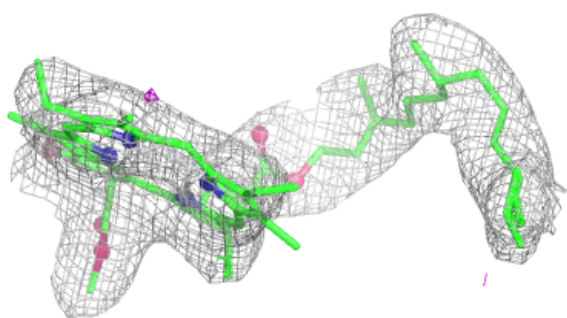
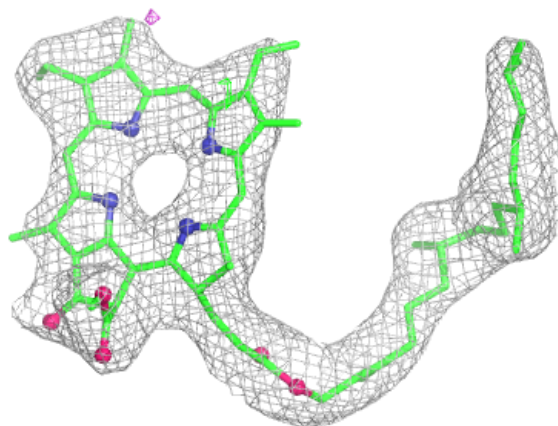
Electron density around CLA b1 615:

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



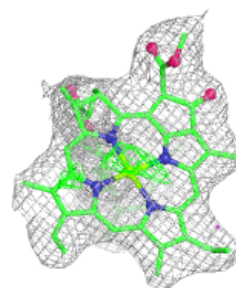
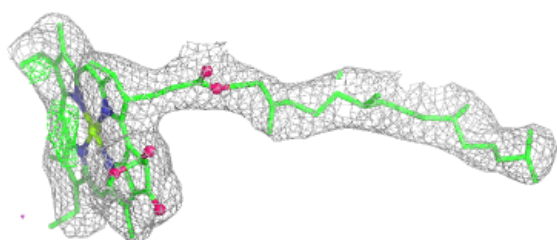
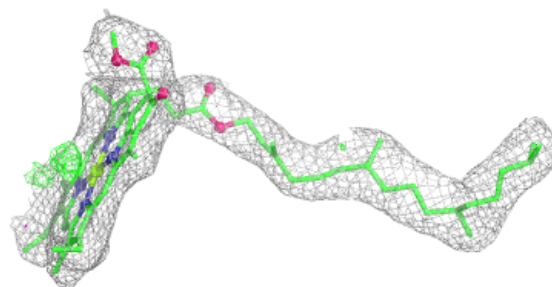
Electron density around PHO d2 408:

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

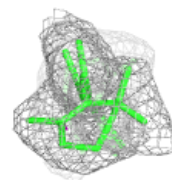
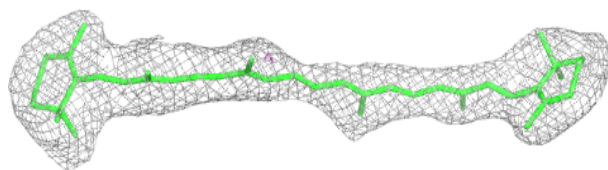
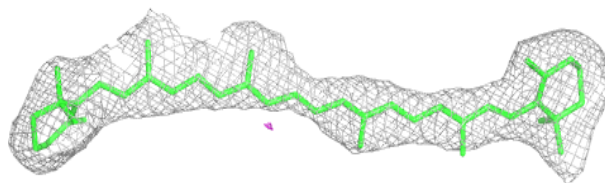


Electron density around CLA b1 607:

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

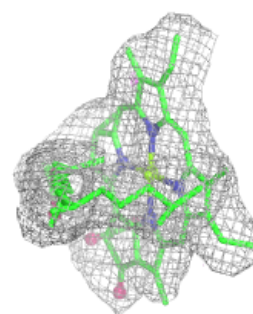
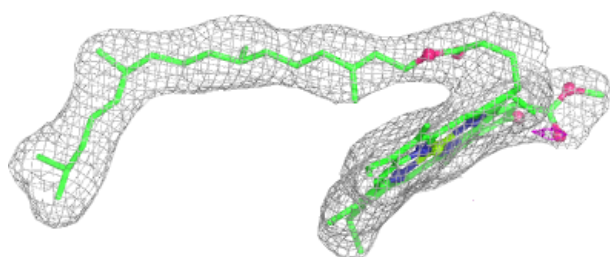
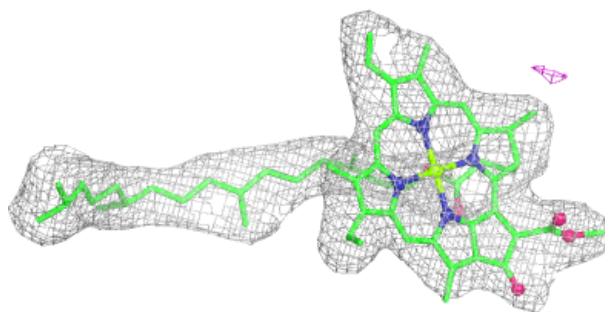
**Electron density around BCR a2 402:**

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



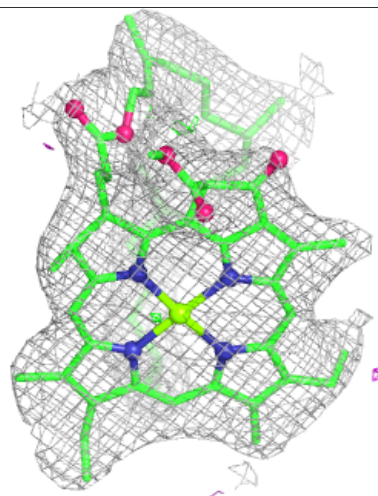
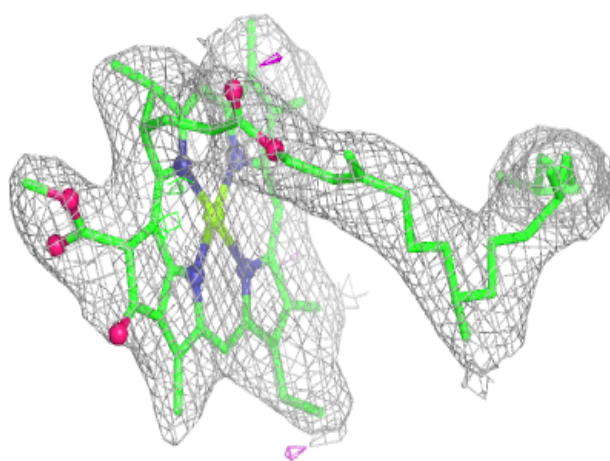
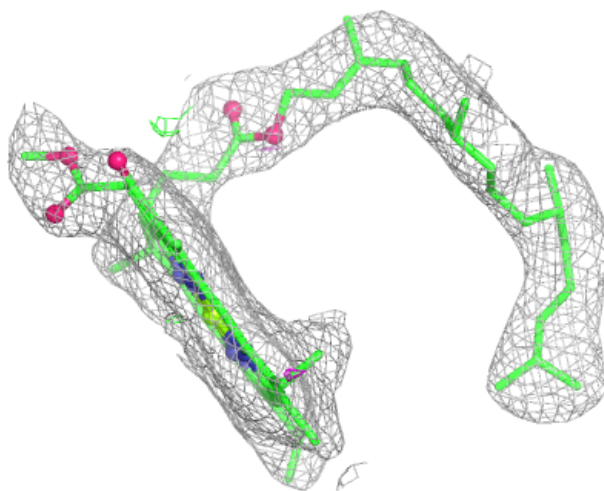
Electron density around CLA b1 610:

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



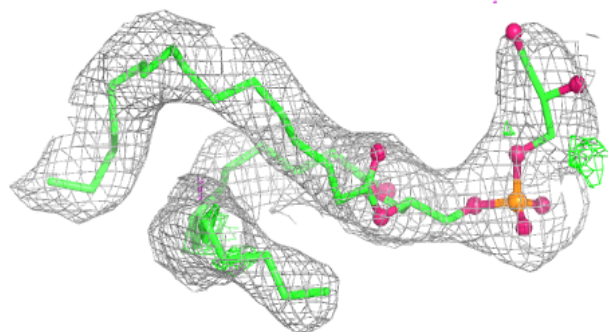
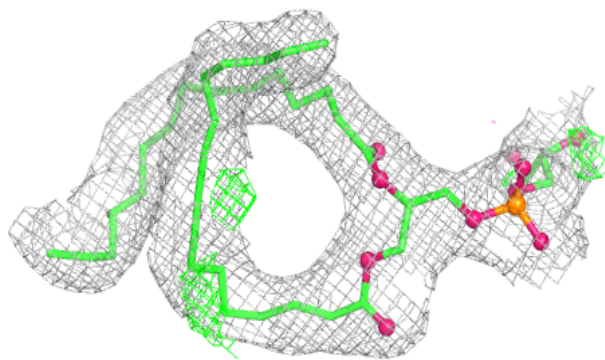
Electron density around CLA B1 613:

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



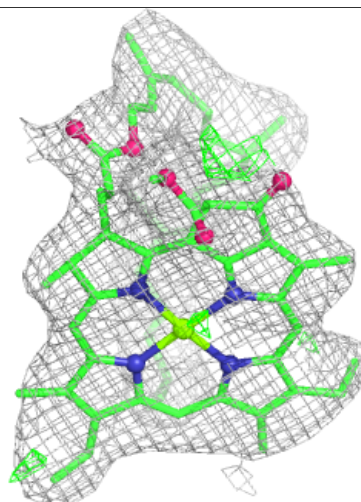
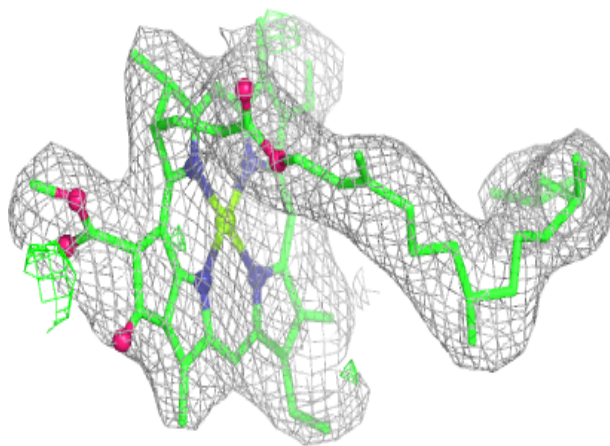
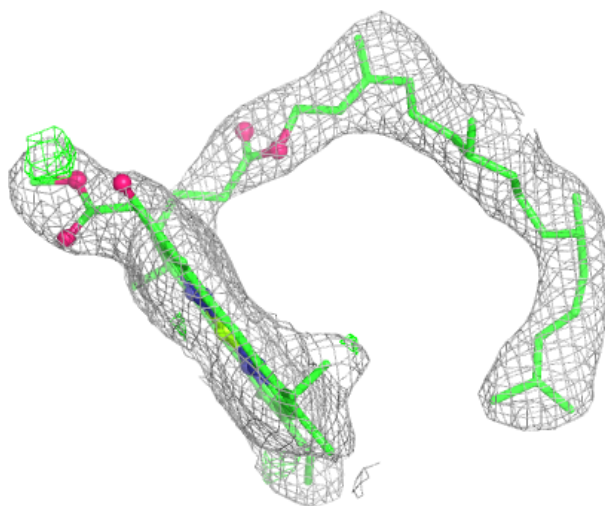
Electron density around LHG b1 622:

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



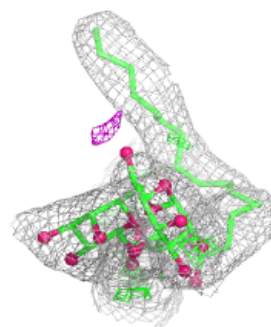
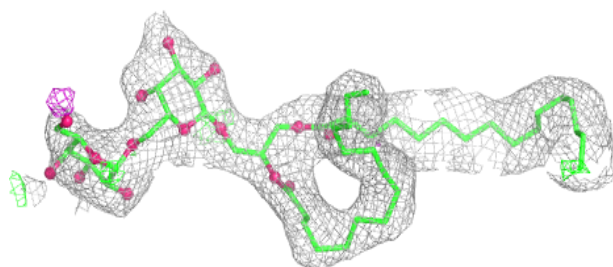
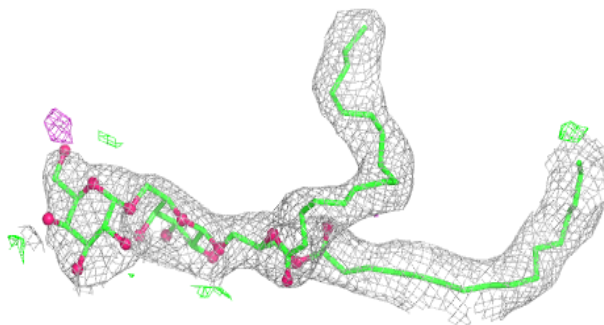
Electron density around CLA B2 613:

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



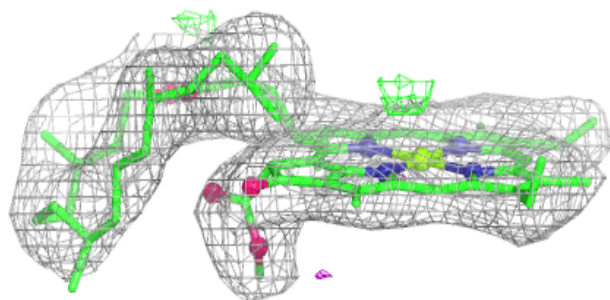
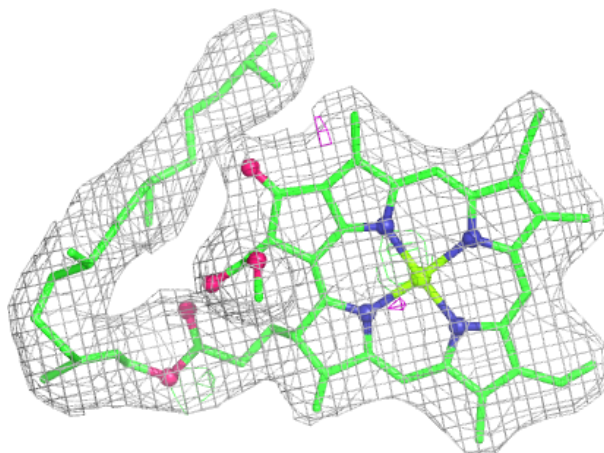
Electron density around DGD h1 101:

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



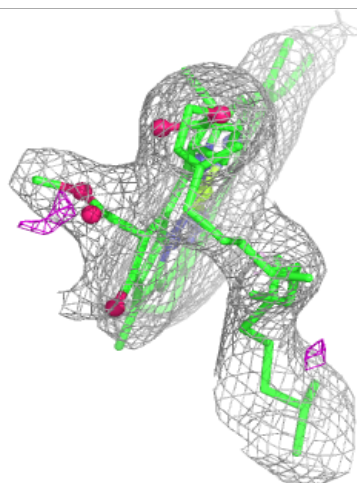
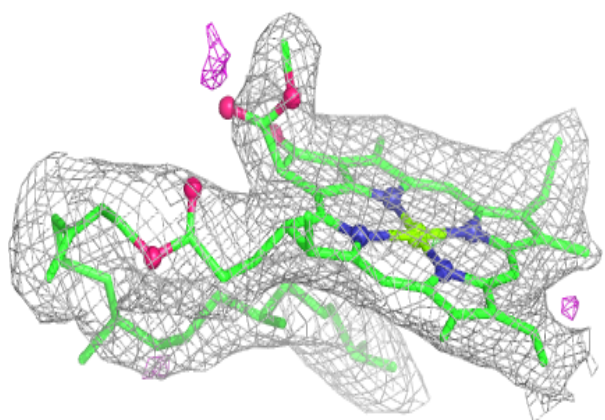
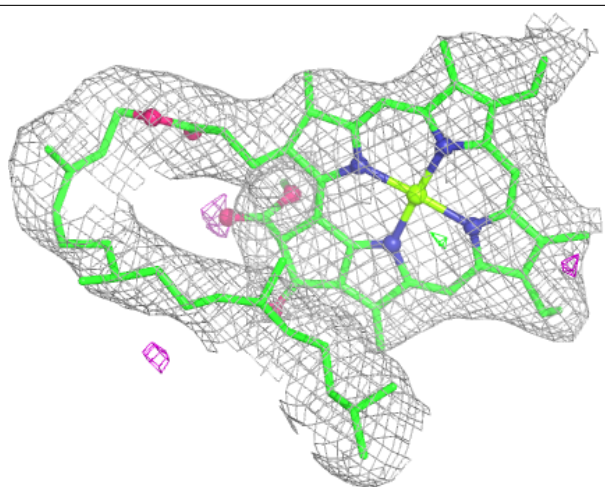
Electron density around CLA b1 612:

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



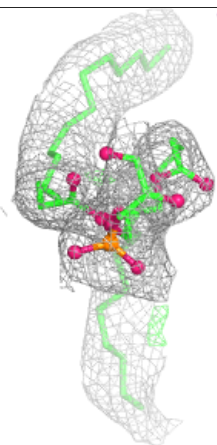
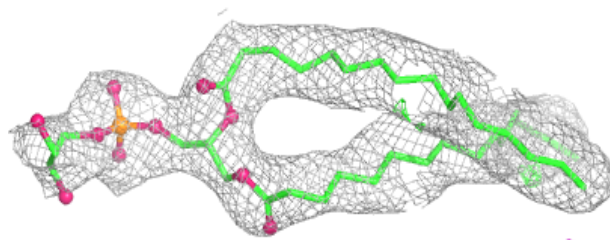
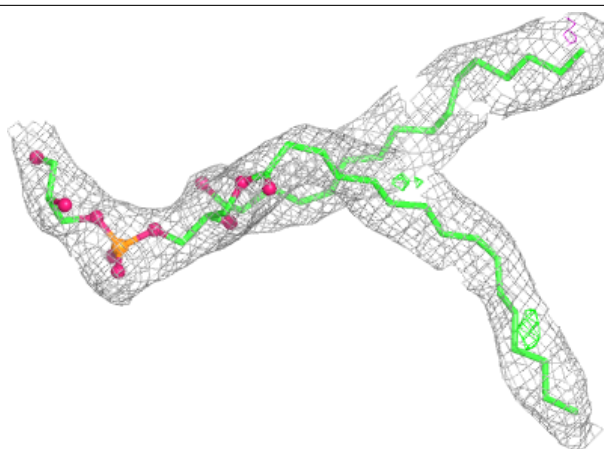
Electron density around CLA c1 511:

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



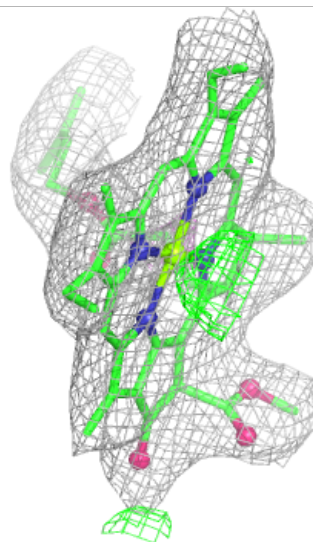
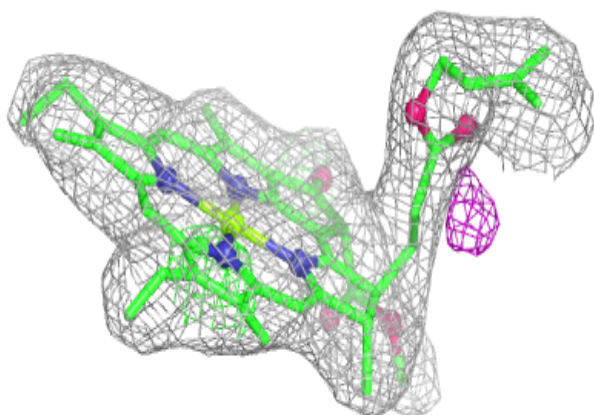
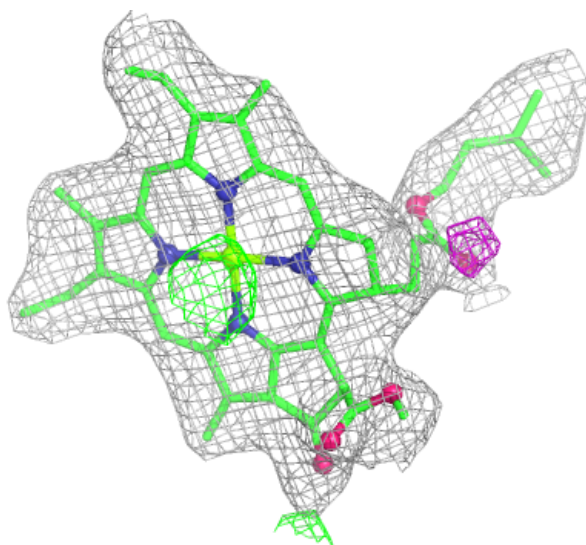
Electron density around LHG d1 407:

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



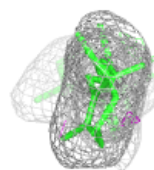
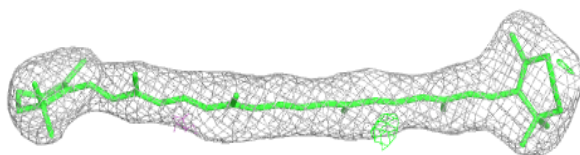
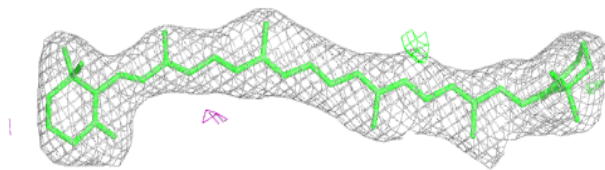
Electron density around CLA a1 405:

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



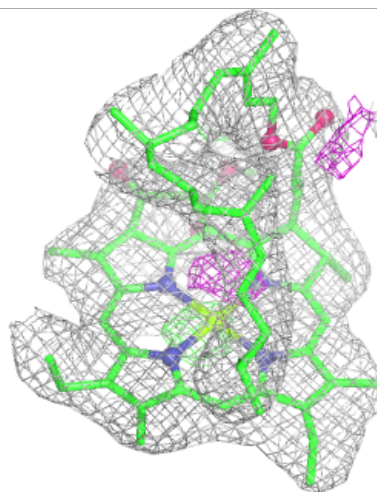
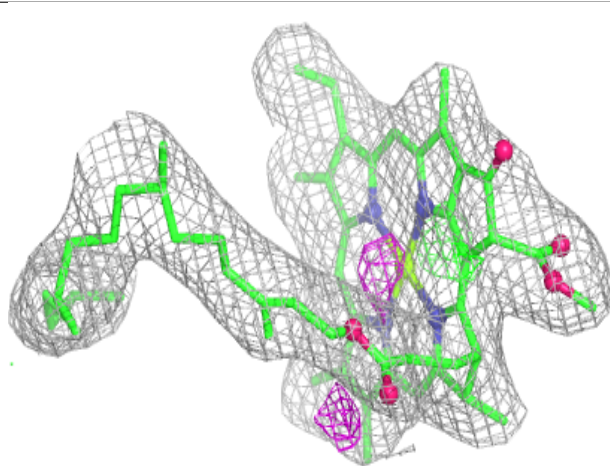
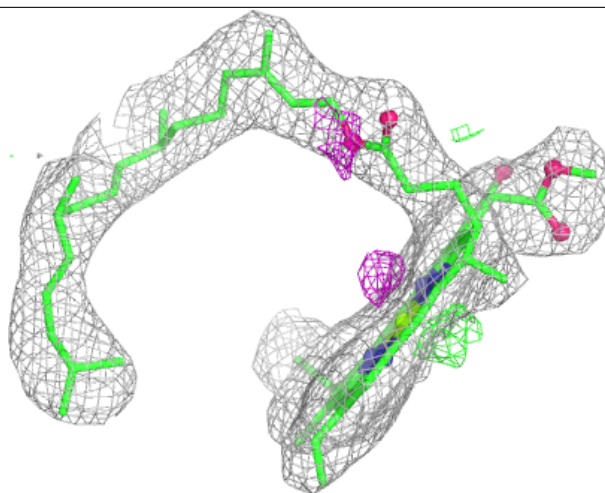
Electron density around BCR b1 601:

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



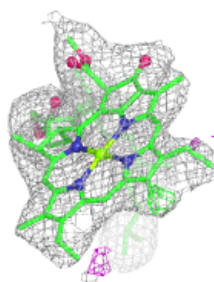
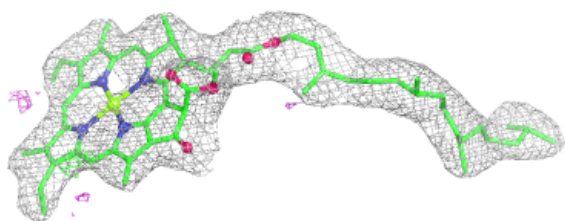
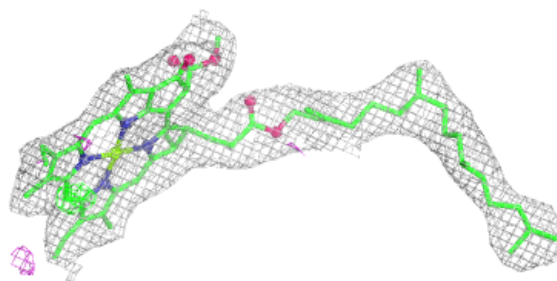
Electron density around CLA b1 613:

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



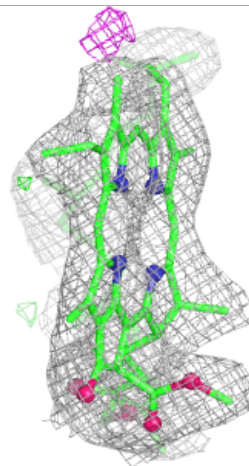
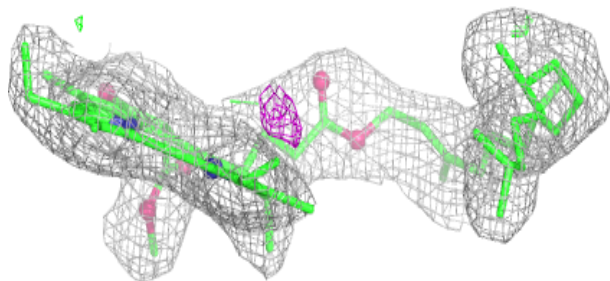
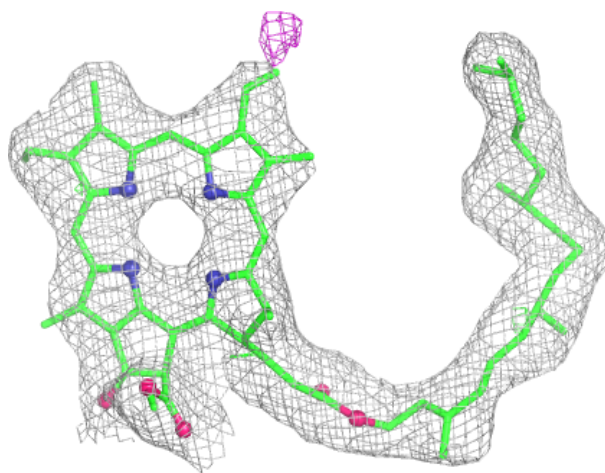
Electron density around CLA a2 404:

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



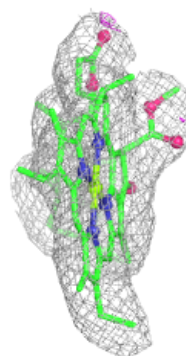
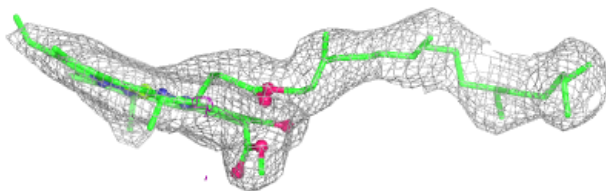
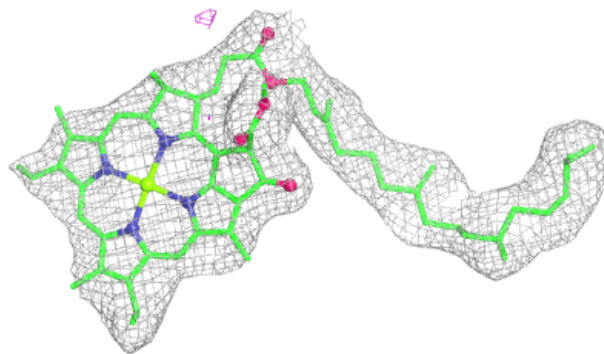
Electron density around PHO a2 416:

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



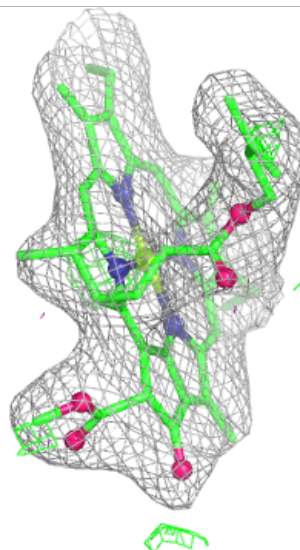
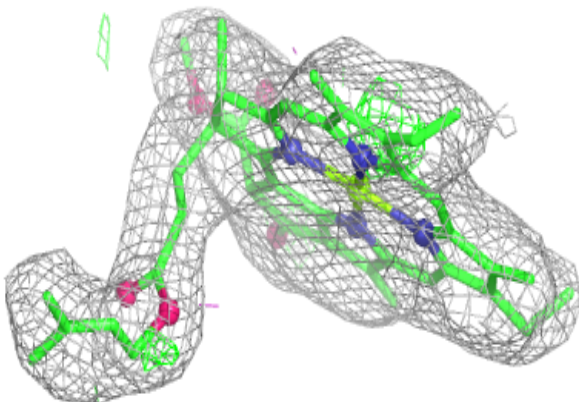
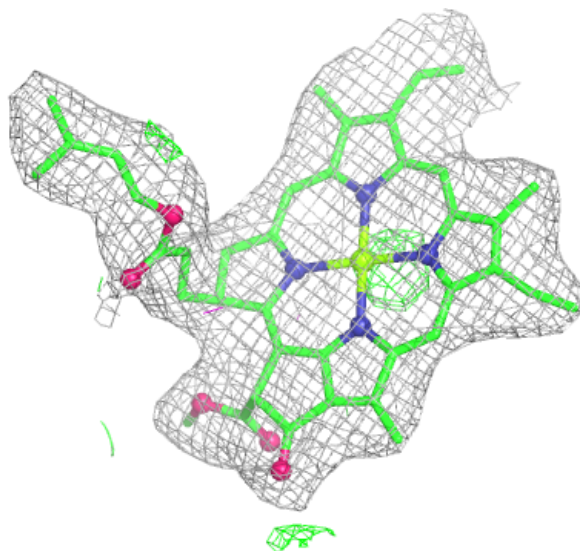
Electron density around CLA b1 605:

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



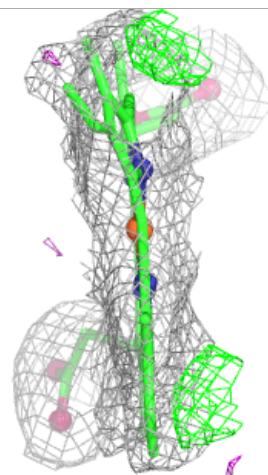
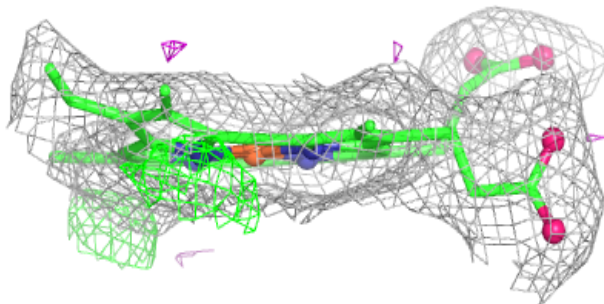
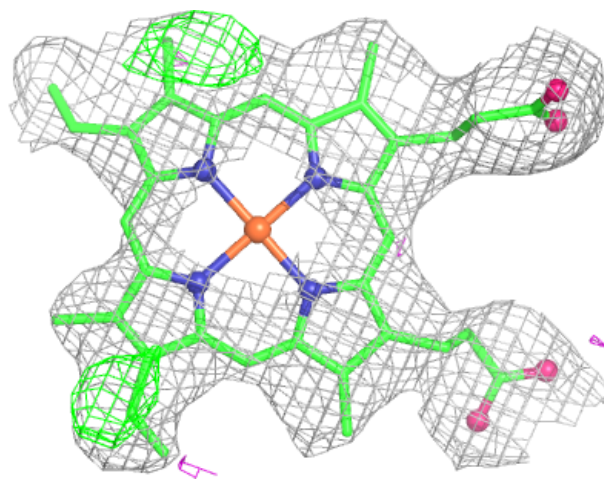
Electron density around CLA a2 413:

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



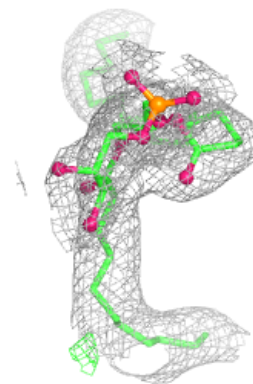
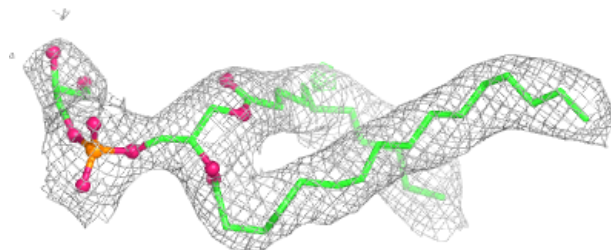
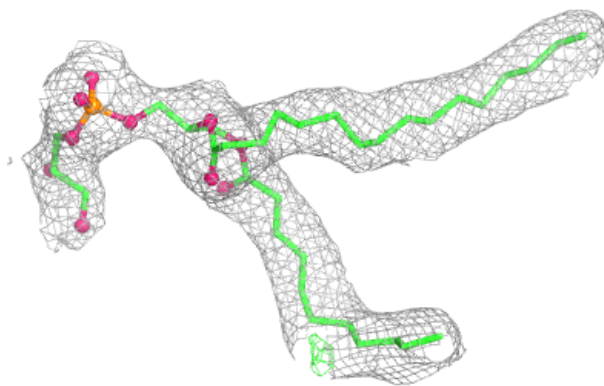
Electron density around HEM V1 201:

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

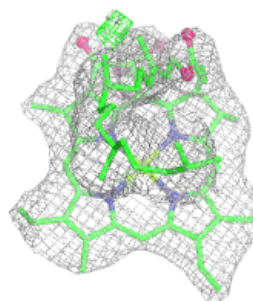
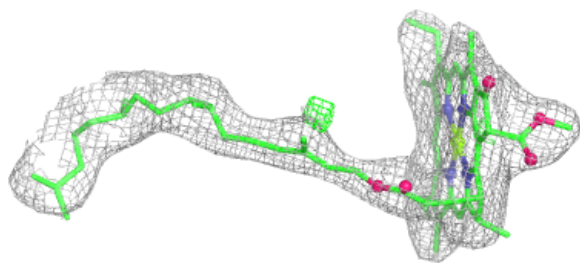
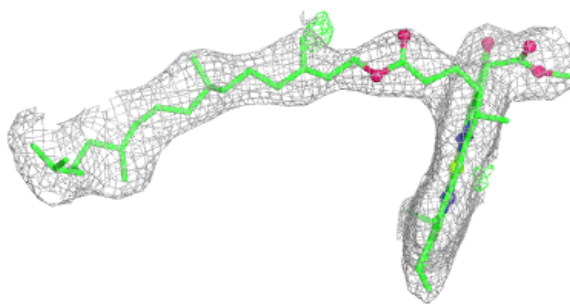


Electron density around LHG 12 101:

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

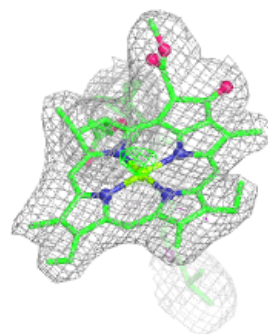
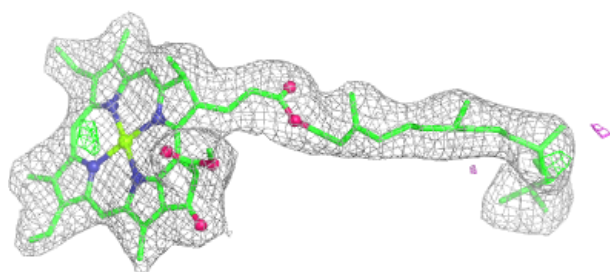
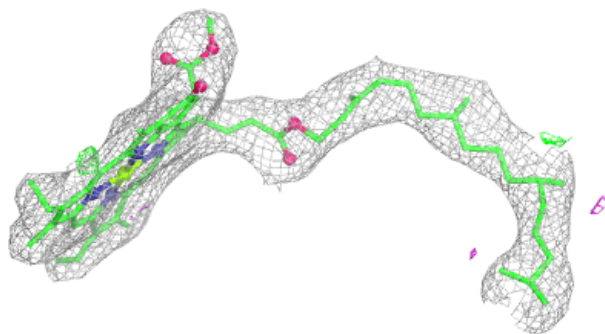
**Electron density around CLA B2 608:**

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

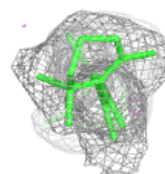
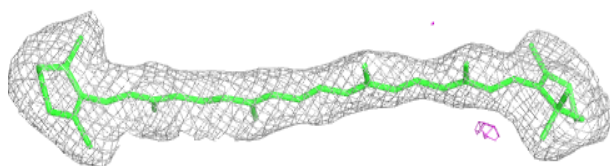
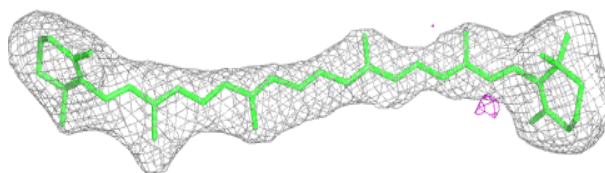


Electron density around CLA D1 402:

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

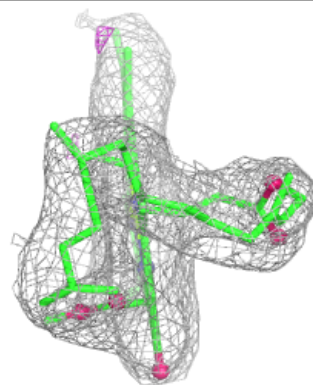
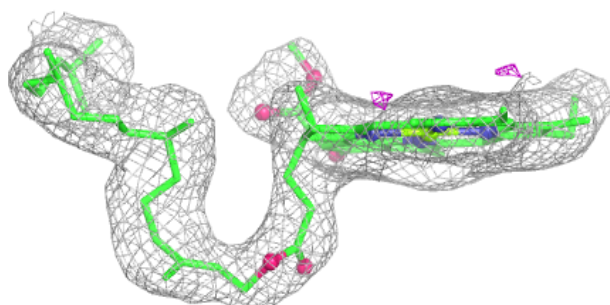
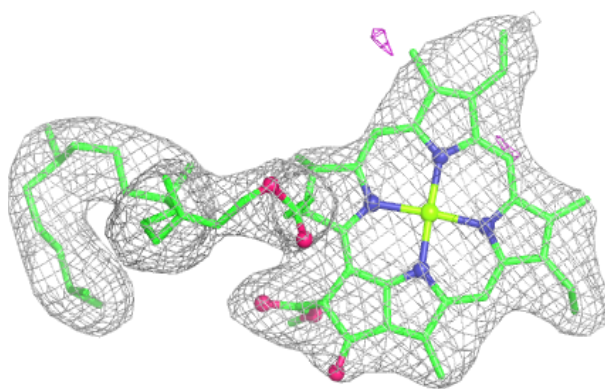
**Electron density around BCR A1 401:**

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

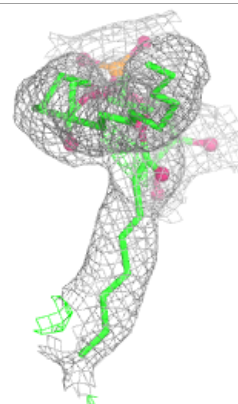
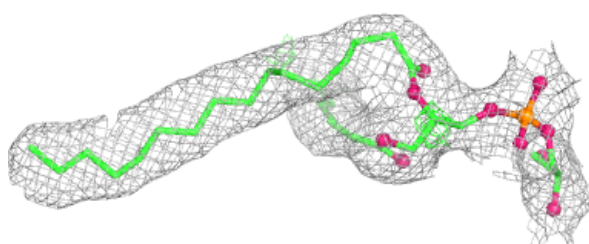
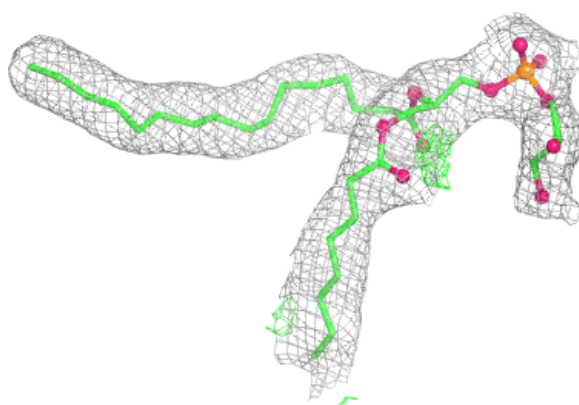


Electron density around CLA B1 614:

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

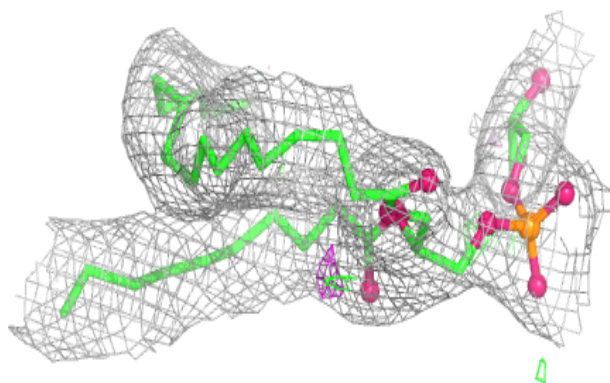
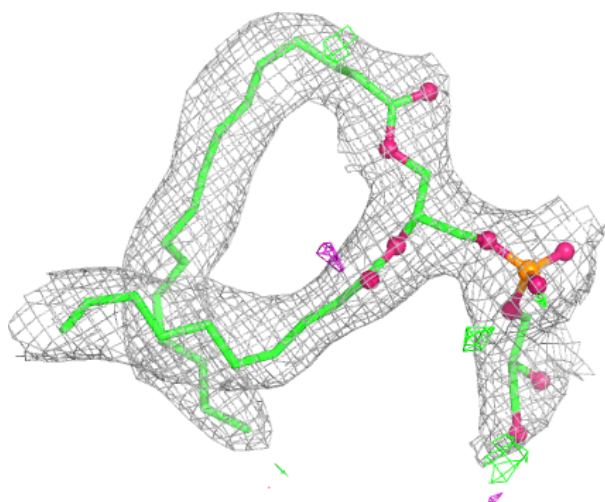
**Electron density around LHG L1 101:**

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



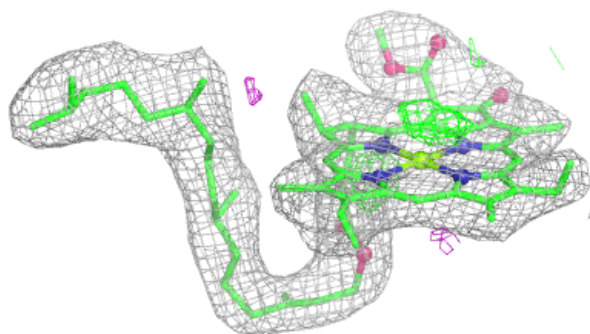
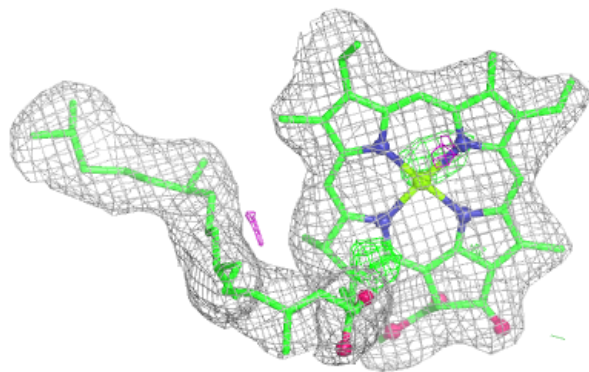
Electron density around LHG a1 407:

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



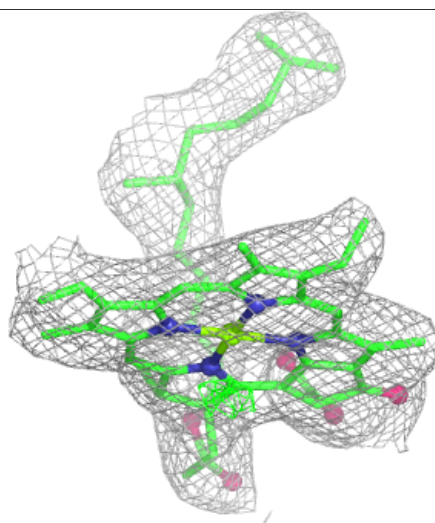
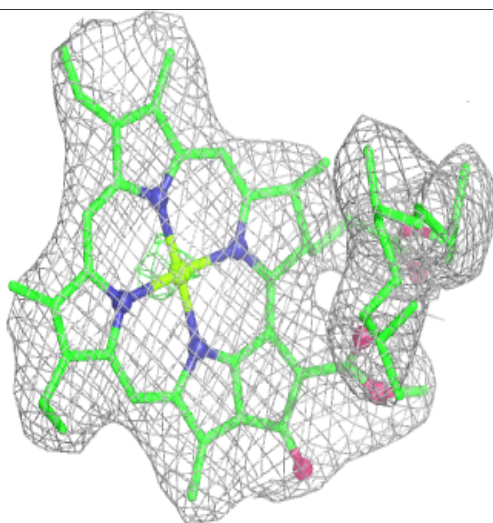
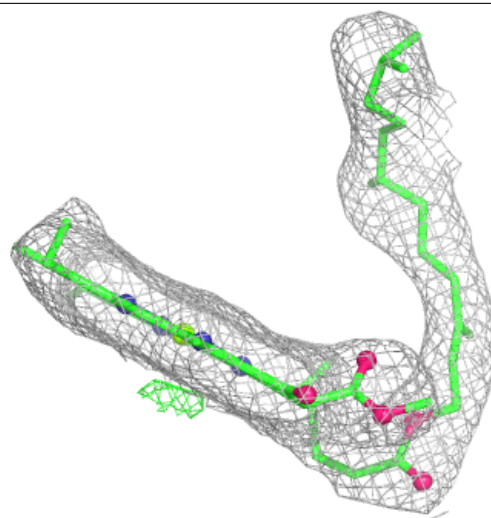
Electron density around CLA d2 402:

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



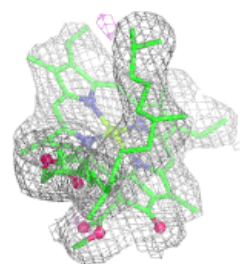
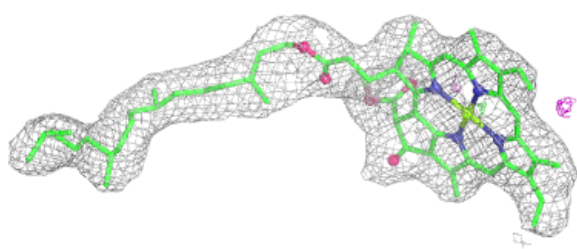
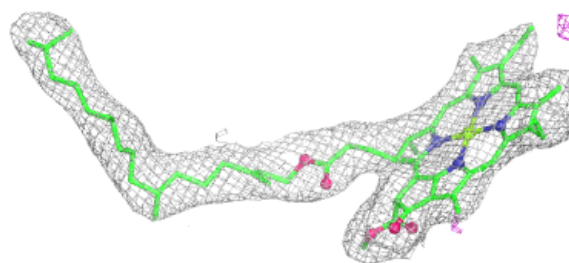
Electron density around CLA b2 615:

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

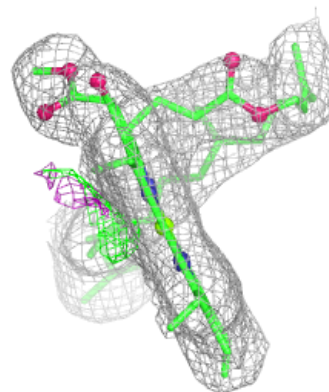
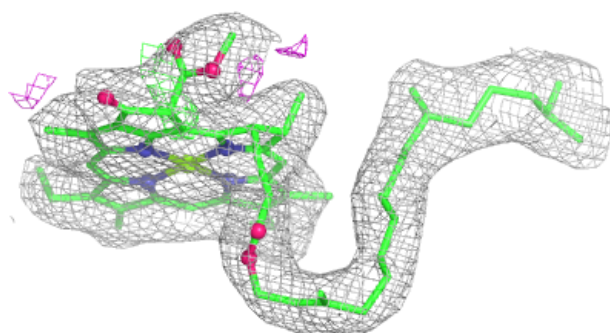
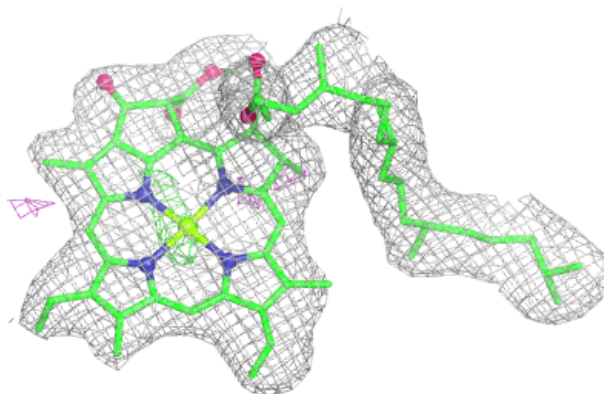


Electron density around CLA a1 403:

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

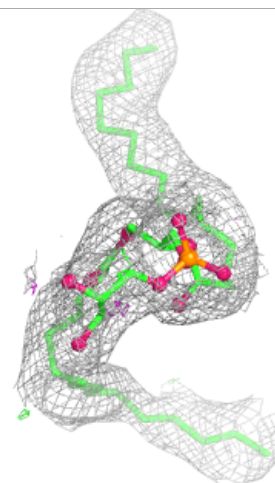
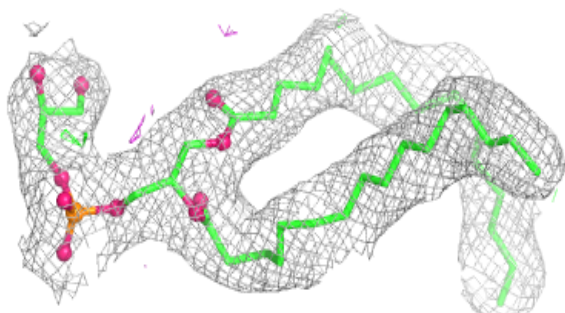
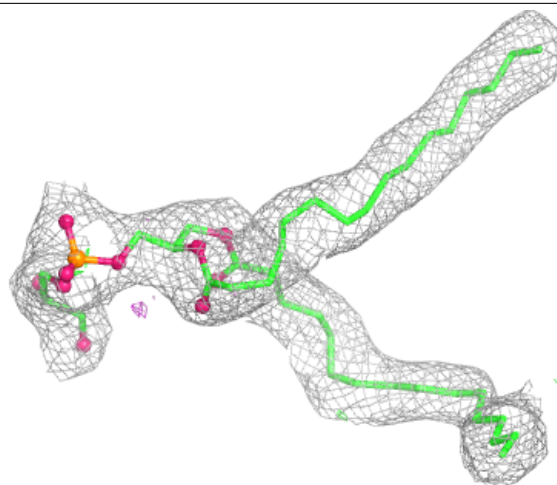
**Electron density around CLA A1 406:**

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



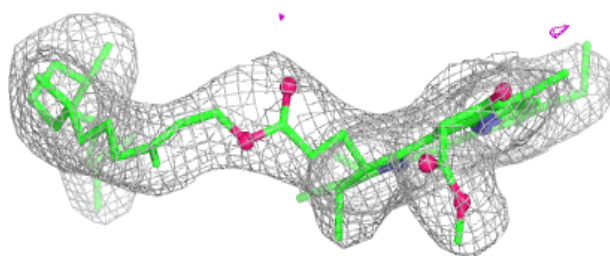
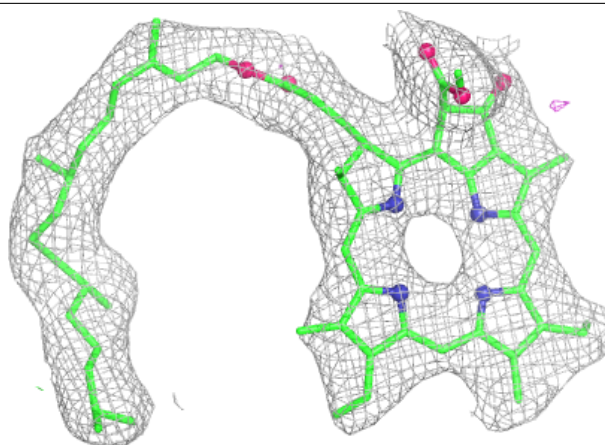
Electron density around LHG l1 102:

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



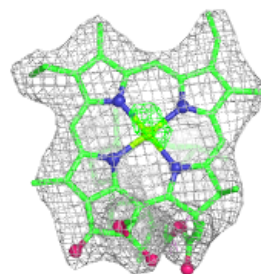
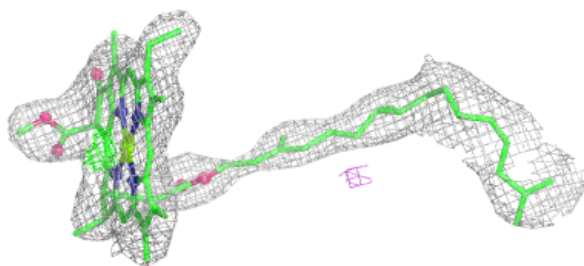
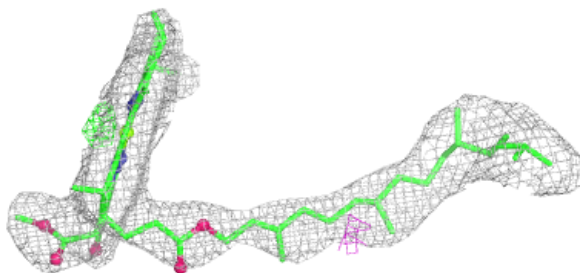
Electron density around PHO A1 408:

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



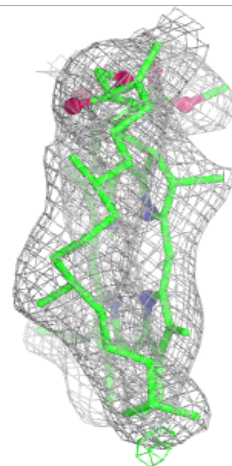
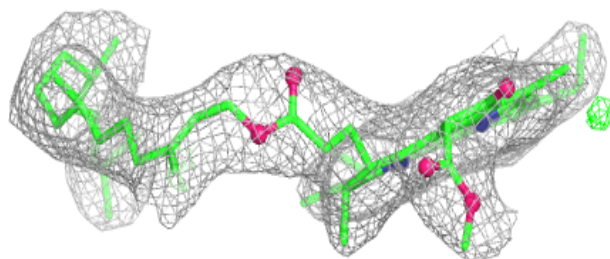
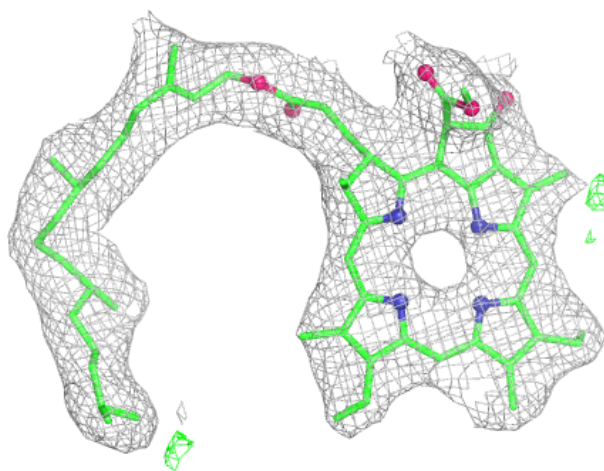
Electron density around CLA B1 608:

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



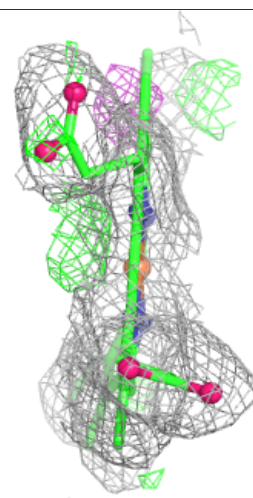
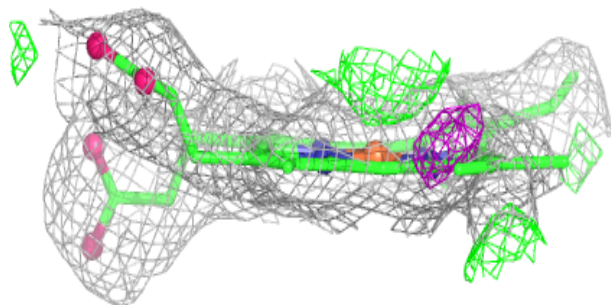
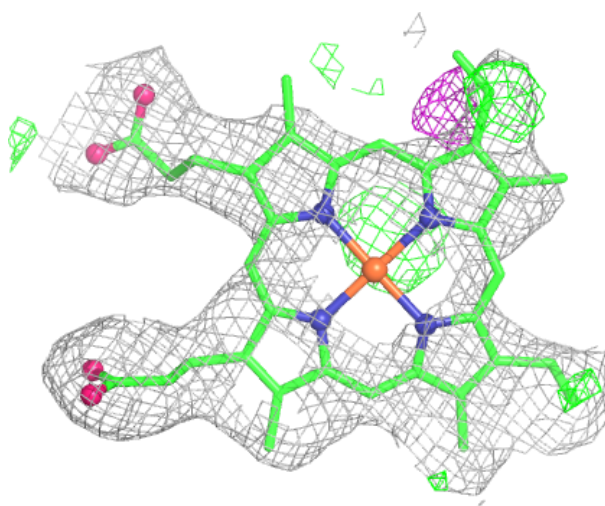
Electron density around PHO a1 411:

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



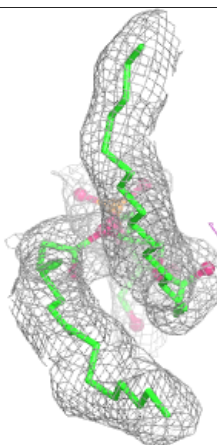
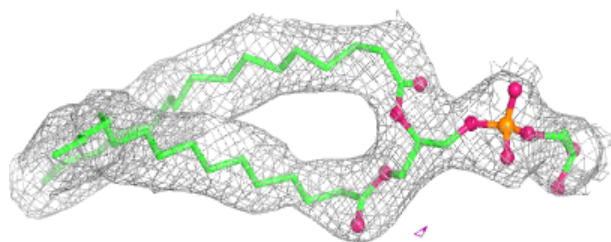
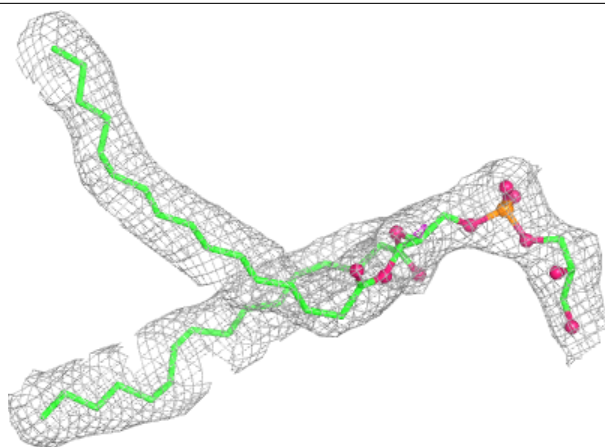
Electron density around HEM v2 201:

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

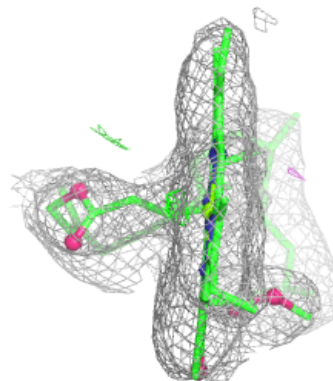
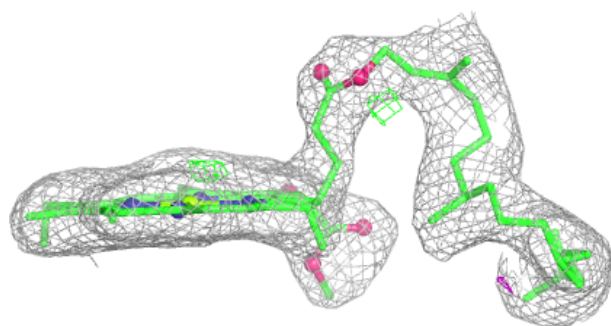
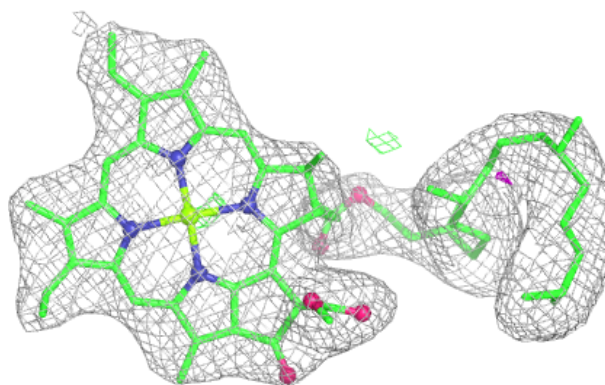


Electron density around LHG D1 405:

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

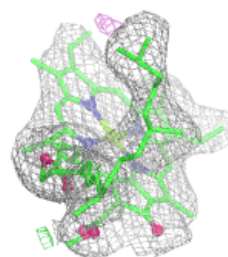
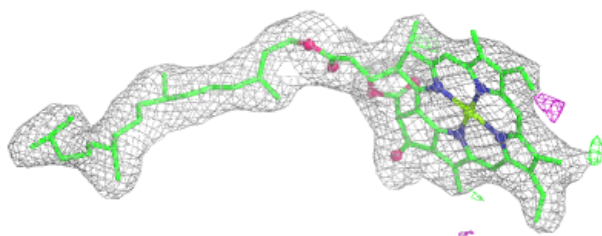
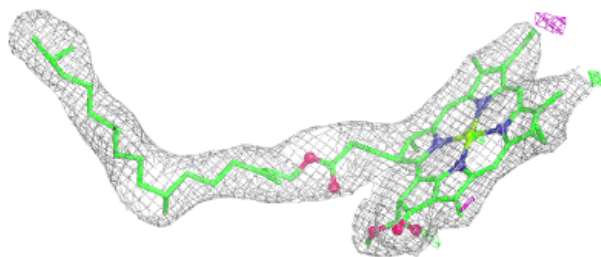
**Electron density around CLA b1 614:**

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

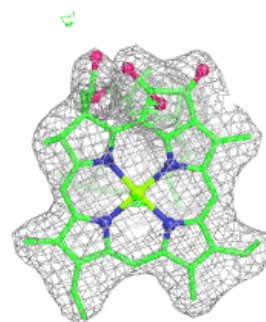
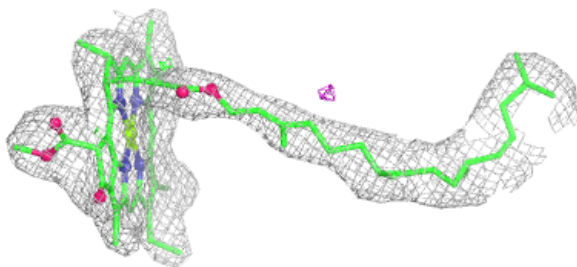
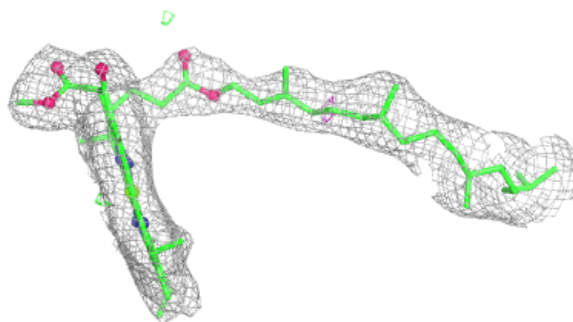


Electron density around CLA A1 403:

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

**Electron density around CLA b1 608:**

$2mF_o-DF_c$ (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.