wwPDB X-ray Structure Validation Summary Report (i)

Aug 5, 2026 – 07:35 AM EDT

PDB ID	:	4RVY / pdb_00004rvy
Title	:	Serial Time resolved crystallography of Photosystem II using a femtosecond X-ray laser. The S state after two flashes (S3)
Authors	:	Kupitz, C.; Basu, S.; Grotjohann, I.; Fromme, R.; Zatsepin, N.; Rendek, K.N.; Hunter, M.; Shoeman, R.L.; White, T.A.; Wang, D.; James, D.; Yang, J.-H.; Cobb, D.E.; Reeder, B.; Sierra, R.G.; Liu, H.; Barty, A.; Aquila, A.; Deponte, D.; Kirian, R.; Bari, S.; Bergkamp, J.J.; Beyerlein, K.; Bogan, M.J.; Caleman, C.; Chao, T.-C.; Conrad, C.E.; Davis, K.M.; Fleckenstein, H.; Galli, L.; Hau-Riege, S.P.; Kassemeyer, S.; Laksmono, H.; Liang, M.; Lomb, L.; Marchesini, S.; Martin, A.V.; Messerschmidt, M.; Milathianaki, D.; Nass, K.; Ros, A.; Roy-Chowdhury, S.; Schmidt, K.; Seibert, M.; Steinbrener, J.; Stellato, F.; Yan, L.; Yoon, C.; Moore, T.A.; Moore, A.L.; Pushkar, Y.; Williams, G.J.; Boutet, S.; Doak, R.B.; Weierstall, U.; Frank, M.; Chapman, H.N.; Spence, J.C.H.; Fromme, P.
Deposited on	:	2014-11-29
Resolution	:	5.50 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 (i) 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 (i)) were used in the production of this report:

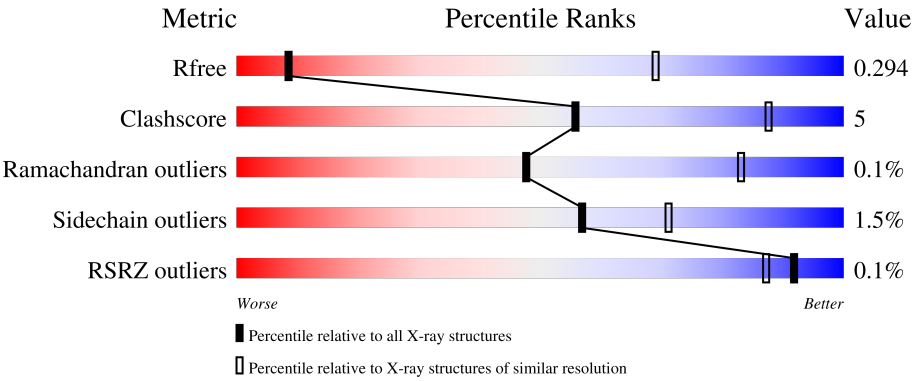
MolProbity : 4-5-2 with Phenix2.0

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 5.50 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	1088 (7.00-4.00)
Clashscore	190562	1147 (7.00-4.00)
Ramachandran outliers	187476	1012 (7.02-3.98)
Sidechain outliers	187428	1023 (7.04-3.96)
RSRZ outliers	180081	1081 (7.00-4.00)

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 <=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.

Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

Mol	Chain	Length	Quality of chain
1	A	334	95% 5%
1	a	334	93% 7%
2	B	504	93% 7%
2	b	504	92% 7%
3	C	461	92% 6% •
3	c	461	92% 6% •
4	D	342	94% 6%
4	d	342	94% 6%
5	E	81	94% 6%
5	e	81	94% 6%
6	F	34	85% 12% •
6	f	34	85% 12% •
7	H	65	92% 6% •
7	h	65	92% 6% •
8	I	38	87% 11% •
8	i	38	87% 11% •
9	J	40	92% • 5%
9	j	40	92% • 5%
10	K	37	89% 8% •
10	k	37	89% 8% •
11	L	37	86% 11% •
11	l	37	84% 14% •
12	M	34	3% 74% 26%
12	m	34	74% 26%
13	O	243	92% 7% •
13	o	243	91% 8% •

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Mol	Chain	Length	Quality of chain
14	T	30	77% 20%
14	t	30	77% 20%
15	U	97	99%
15	u	97	97%
16	V	137	95% 5%
16	v	137	96%
17	X	39	92% 8%
17	x	39	92% 8%
18	Y	29	86% 14%
18	y	29	86% 14%
19	Z	62	97%
19	z	62	97%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	BCR	K	102	-	X	-	-
24	BCR	k	102	-	X	-	-
26	CL	u	201	-	-	-	X

2 Entry composition (i)

There are 34 unique types of molecules in this entry. The entry contains 49594 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	0	0
			2620	1716	431	458	15			
1	a	334	Total	C	N	O	S	0	0	0
			2620	1716	431	458	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	286	ALA	THR	conflict	UNP P0A444
a	286	ALA	THR	conflict	UNP P0A444

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	504	Total	C	N	O	S	0	0	0
			3969	2605	661	690	13			
2	b	504	Total	C	N	O	S	0	0	0
			3969	2605	661	690	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	451	Total	C	N	O	S	0	0	0
			3486	2281	584	608	13			
3	c	451	Total	C	N	O	S	0	0	0
			3486	2281	584	608	13			

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	81	Total	C	N	O	0	0	0
			662	432	107	123			
5	e	81	Total	C	N	O	0	0	0
			662	432	107	123			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	34	Total	C	N	O	S	0	0	0
			275	187	45	42	1			
6	f	34	Total	C	N	O	S	0	0	0
			275	187	45	42	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	65	Total	C	N	O	S	0	0	0
			511	341	82	86	2			
7	h	65	Total	C	N	O	S	0	0	0
			511	341	82	86	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	38	Total	C	N	O	S	0	0	0
			312	210	48	53	1			
8	i	38	Total	C	N	O	S	0	0	0
			312	210	48	53	1			

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	34	Total	C	N	O	S	0	0	0
			267	178	40	48	1			
12	m	34	Total	C	N	O	S	0	0	0
			267	178	40	48	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	243	Total	C	N	O	S	0	0	0
			1865	1165	315	381	4			
13	o	243	Total	C	N	O	S	0	0	0
			1865	1165	315	381	4			

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	U	97	Total 774	C 491	N 129	O 154	0	0	0
15	u	97	Total 774	C 491	N 129	O 154	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total 1064	C 675	N 177	O 208	S 4	0	0	0
16	v	137	Total 1064	C 675	N 177	O 208	S 4	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	X	39	Total 287	C 191	N 46	O 50	0	0	0
17	x	39	Total 287	C 191	N 46	O 50	0	0	0

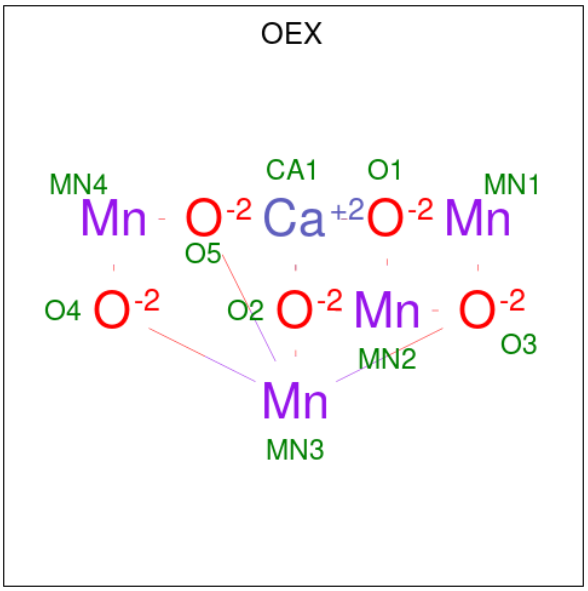
- Molecule 18 is a protein called Photosystem II reaction center protein Ycf12.

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

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

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

- Molecule 20 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: $CaMn_4O_5$).

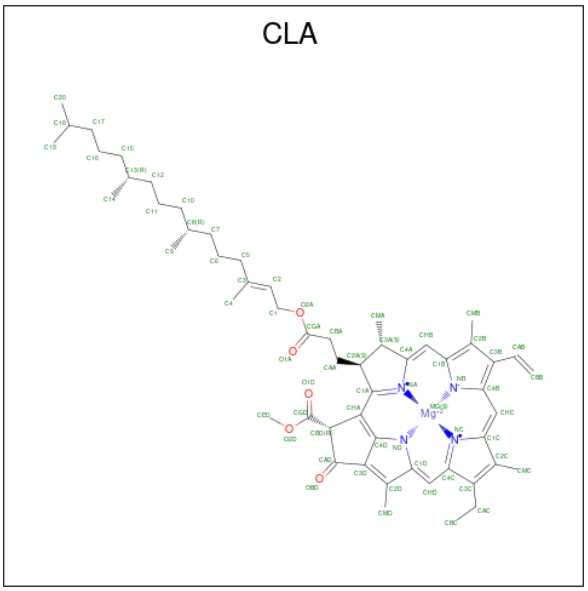


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	A	1	Total	Ca	Mn	O	0	0
			10	1	4	5		
20	a	1	Total	Ca	Mn	O	0	0
			10	1	4	5		

- Molecule 21 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

- Molecule 22 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



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

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

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

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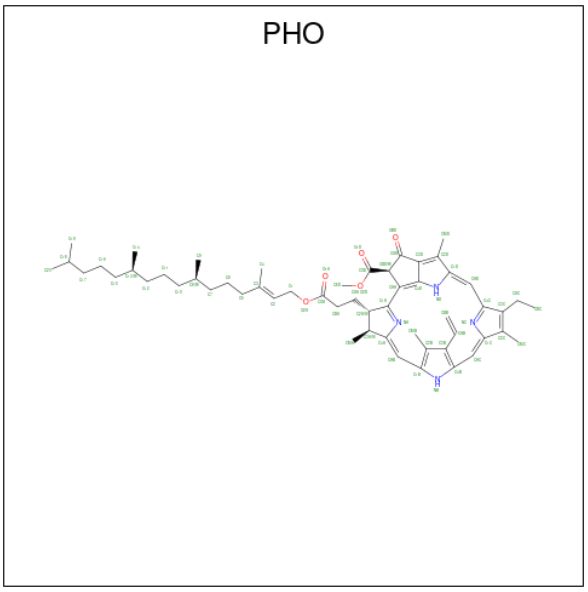
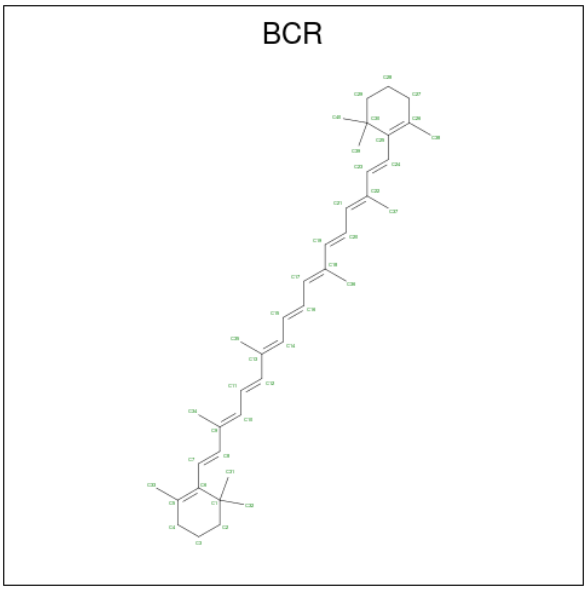
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

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



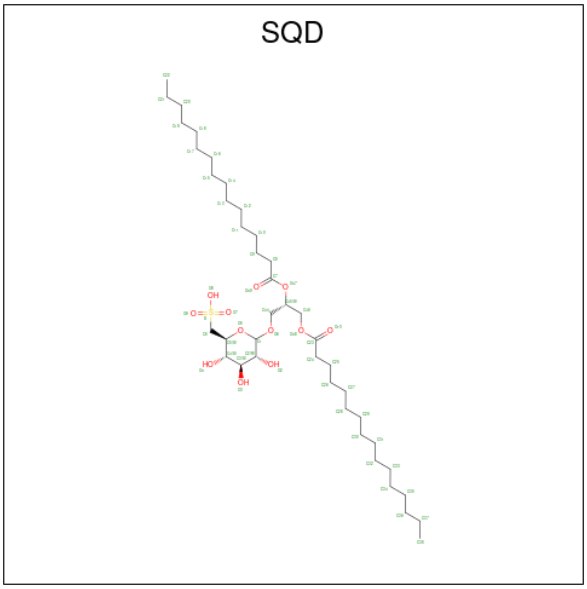
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
23	A	1	Total	C	N	O	0	0
			64	55	4	5		
23	A	1	Total	C	N	O	0	0
			64	55	4	5		
23	a	1	Total	C	N	O	0	0
			64	55	4	5		
23	a	1	Total	C	N	O	0	0
			64	55	4	5		

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



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

- Molecule 25 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).

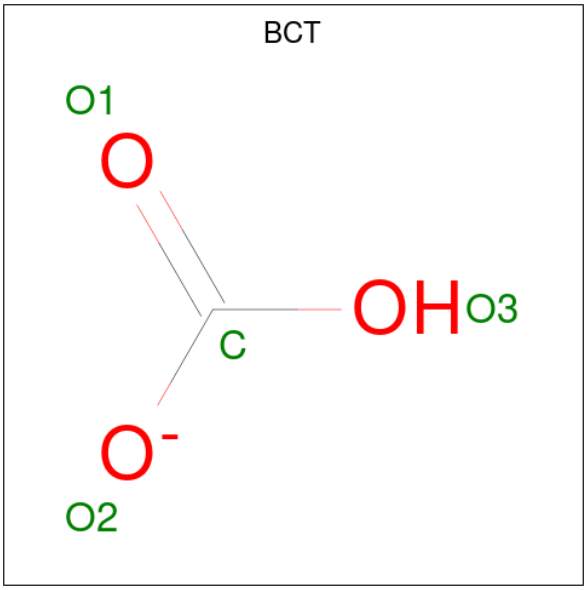


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	A	1	Total	C	O	S	0	0
			54	41	12	1		
25	a	1	Total	C	O	S	0	0
			54	41	12	1		
25	B	1	Total	C	O	S	0	0
			54	41	12	1		
25	b	1	Total	C	O	S	0	0
			54	41	12	1		
25	b	1	Total	C	O	S	0	0
			54	41	12	1		
25	D	1	Total	C	O	S	0	0
			43	30	12	1		
25	d	1	Total	C	O	S	0	0
			43	30	12	1		
25	L	1	Total	C	O	S	0	0
			54	41	12	1		
25	l	1	Total	C	O	S	0	0
			54	41	12	1		
25	l	1	Total	C	O	S	0	0
			54	41	12	1		

- Molecule 26 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

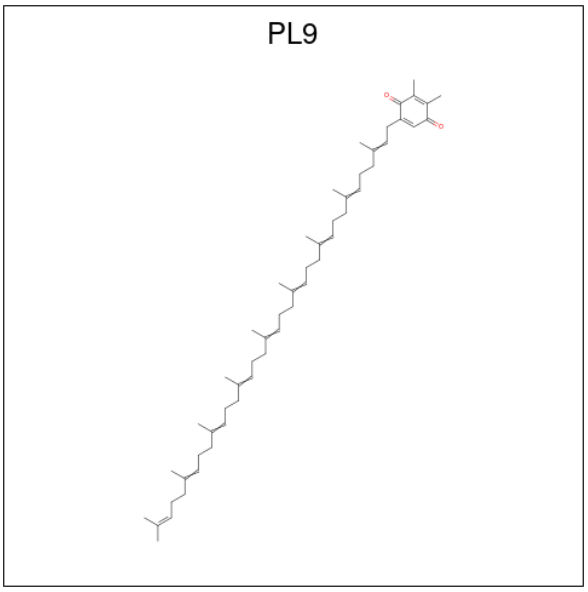
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	2	Total Cl 2 2	0	0
26	a	2	Total Cl 2 2	0	0
26	U	1	Total Cl 1 1	0	0
26	u	1	Total Cl 1 1	0	0

- Molecule 27 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



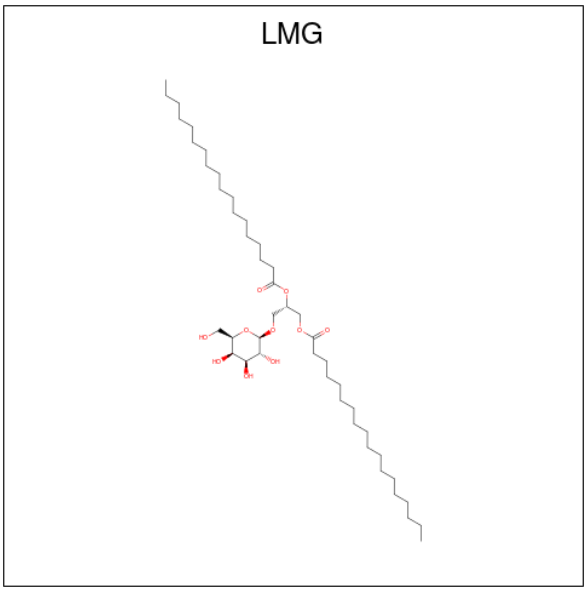
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	1	Total C O 4 1 3	0	0
27	a	1	Total C O 4 1 3	0	0

- Molecule 28 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: $C_{53}H_{80}O_2$).



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

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

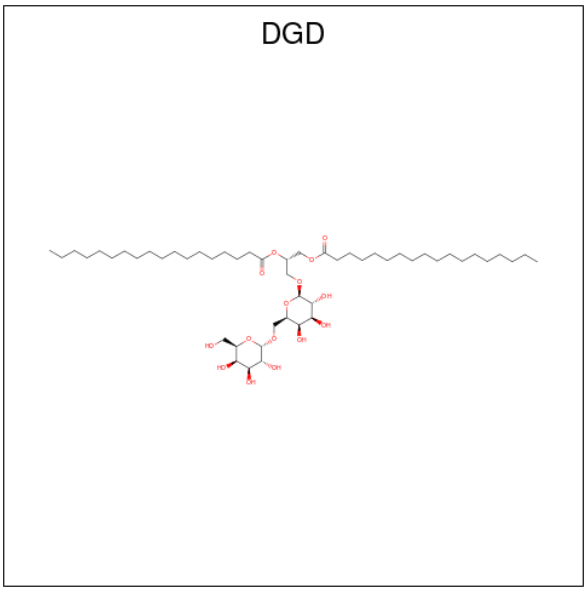


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	1	Total C O 51 41 10	0	0
29	a	1	Total C O 51 41 10	0	0
29	B	1	Total C O 51 41 10	0	0
29	b	1	Total C O 51 41 10	0	0
29	C	1	Total C O 51 41 10	0	0
29	C	1	Total C O 51 41 10	0	0
29	c	1	Total C O 51 41 10	0	0
29	c	1	Total C O 51 41 10	0	0
29	D	1	Total C O 51 41 10	0	0
29	d	1	Total C O 51 41 10	0	0
29	Z	1	Total C O 37 27 10	0	0
29	z	1	Total C O 37 27 10	0	0

- Molecule 30 is CALCIUM ION (CCD ID: CA) (formula: Ca).

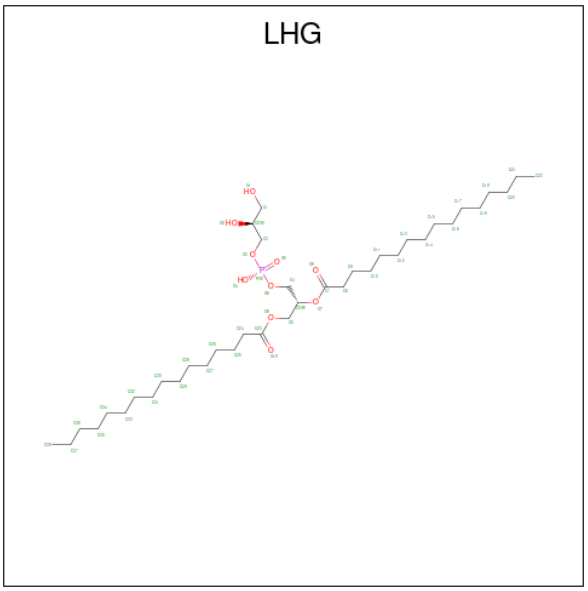
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	B	1	Total Ca 1 1	0	0
30	b	1	Total Ca 1 1	0	0
30	F	1	Total Ca 1 1	0	0
30	f	1	Total Ca 1 1	0	0
30	O	1	Total Ca 1 1	0	0
30	o	1	Total Ca 1 1	0	0

- Molecule 31 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



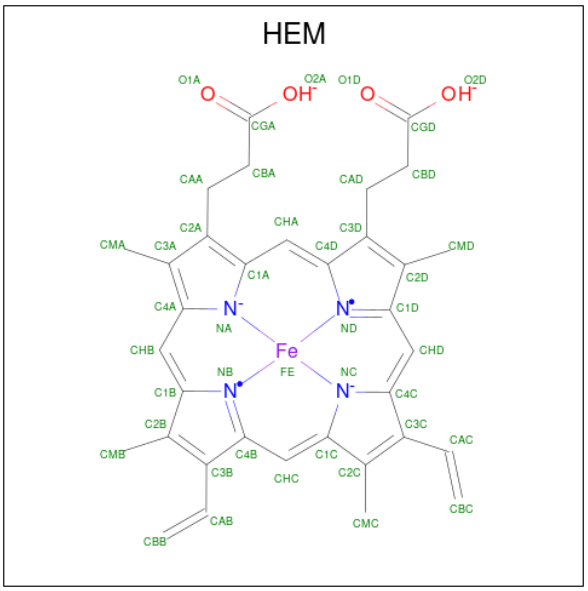
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	C	1	Total C O 62 47 15	0	0
31	C	1	Total C O 62 47 15	0	0
31	C	1	Total C O 62 47 15	0	0
31	c	1	Total C O 62 47 15	0	0
31	c	1	Total C O 62 47 15	0	0
31	c	1	Total C O 62 47 15	0	0
31	D	1	Total C O 62 47 15	0	0
31	d	1	Total C O 62 47 15	0	0
31	H	1	Total C O 62 47 15	0	0
31	h	1	Total C O 62 47 15	0	0

- Molecule 32 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	D	1	Total	C	O	P	0	0
			49	38	10	1		
32	D	1	Total	C	O	P	0	0
			49	38	10	1		
32	D	1	Total	C	O	P	0	0
			49	38	10	1		
32	d	1	Total	C	O	P	0	0
			49	38	10	1		
32	d	1	Total	C	O	P	0	0
			49	38	10	1		
32	d	1	Total	C	O	P	0	0
			49	38	10	1		
32	E	1	Total	C	O	P	0	0
			42	31	10	1		
32	e	1	Total	C	O	P	0	0
			42	31	10	1		
32	L	1	Total	C	O	P	0	0
			49	38	10	1		
32	l	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 33 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 34 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

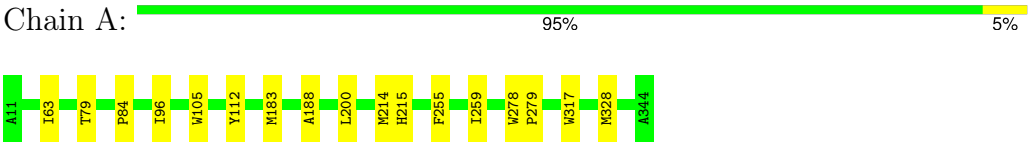
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	J	1	Total	Mg	0	0
			1	1		
34	j	1	Total	Mg	0	0
			1	1		

3 Residue-property plots (i)

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

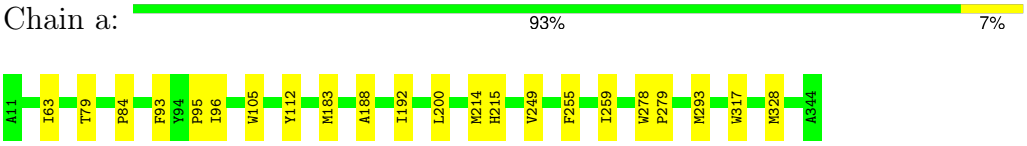
• Molecule 1: Photosystem II protein D1 1

Chain A:



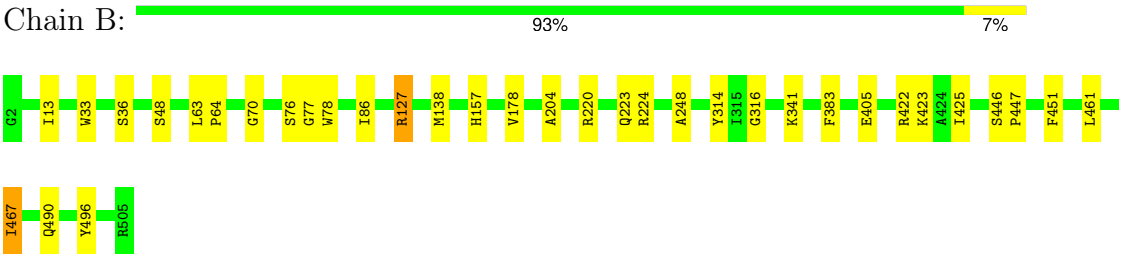
• Molecule 1: Photosystem II protein D1 1

Chain a:



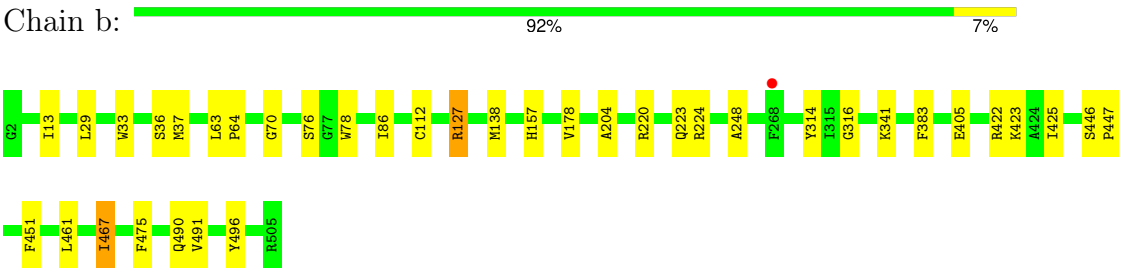
• Molecule 2: Photosystem II CP47 reaction center protein

Chain B:



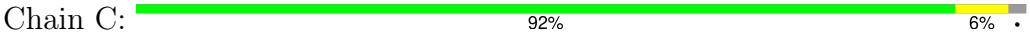
• Molecule 2: Photosystem II CP47 reaction center protein

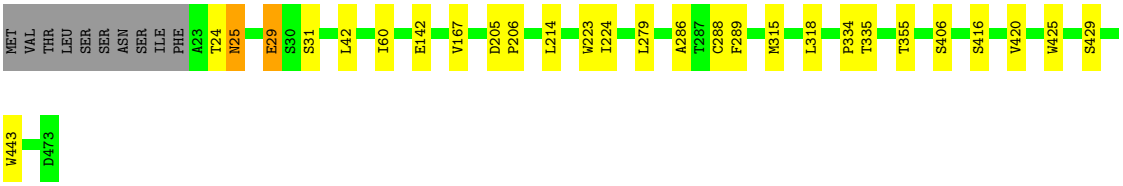
Chain b:



• Molecule 3: Photosystem II CP43 reaction center protein

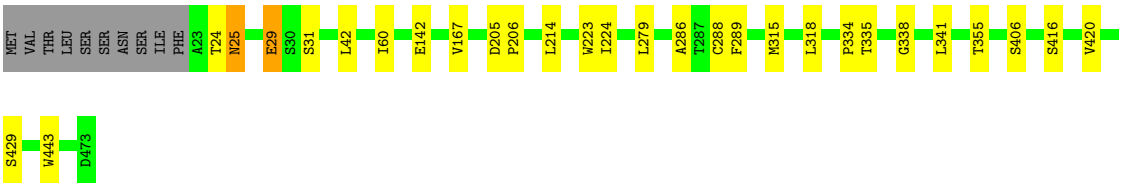
Chain C:





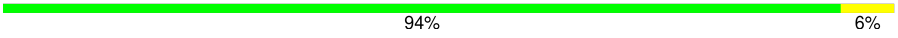
• Molecule 3: Photosystem II CP43 reaction center protein

Chain c:



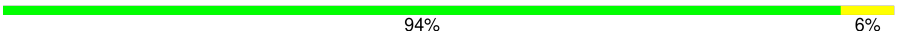
• Molecule 4: Photosystem II D2 protein

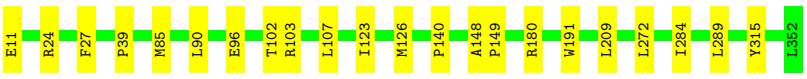
Chain D:



• Molecule 4: Photosystem II D2 protein

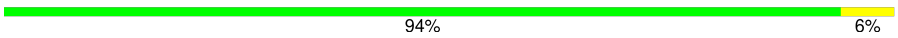
Chain d:





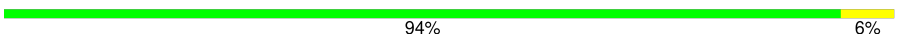
• Molecule 5: Cytochrome b559 subunit alpha

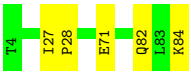
Chain E:



• Molecule 5: Cytochrome b559 subunit alpha

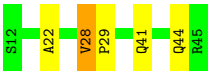
Chain e:





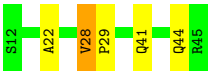
• Molecule 6: Cytochrome b559 subunit beta

Chain F:



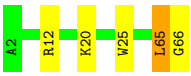
• Molecule 6: Cytochrome b559 subunit beta

Chain f:



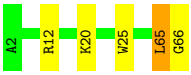
• Molecule 7: Photosystem II reaction center protein H

Chain H:



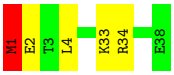
• Molecule 7: Photosystem II reaction center protein H

Chain h:



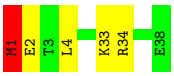
• Molecule 8: Photosystem II reaction center protein I

Chain I:



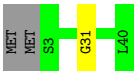
• Molecule 8: Photosystem II reaction center protein I

Chain i:



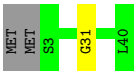
• Molecule 9: Photosystem II reaction center protein J

Chain J:



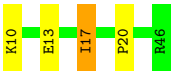
• Molecule 9: Photosystem II reaction center protein J

Chain j:



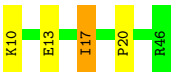
• Molecule 10: Photosystem II reaction center protein K

Chain K:



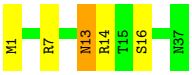
• Molecule 10: Photosystem II reaction center protein K

Chain k:



• Molecule 11: Photosystem II reaction center protein L

Chain L:



• Molecule 11: Photosystem II reaction center protein L

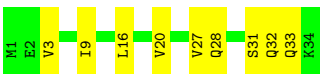
Chain l:

• Molecule 12: Photosystem II reaction center protein M

Chain M:

• Molecule 12: Photosystem II reaction center protein M

Chain m:

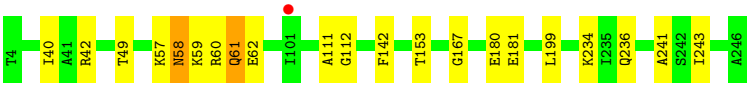


• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:

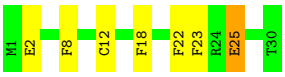
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:



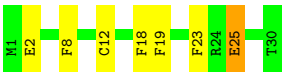
• Molecule 14: Photosystem II reaction center protein T

Chain T:



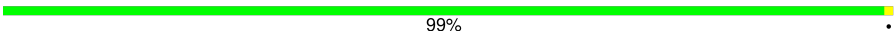
• Molecule 14: Photosystem II reaction center protein T

Chain t:



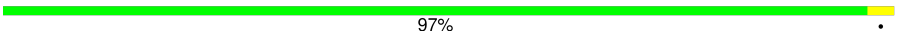
• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:



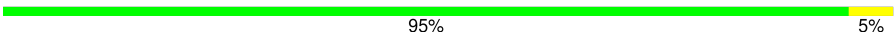
• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u:



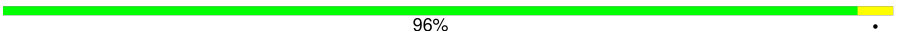
• Molecule 16: Cytochrome c-550

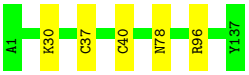
Chain V:



• Molecule 16: Cytochrome c-550

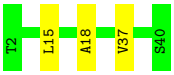
Chain v:





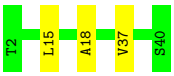
• Molecule 17: Photosystem II reaction center X protein

Chain X:



• Molecule 17: Photosystem II reaction center X protein

Chain x:



• Molecule 18: Photosystem II reaction center protein Ycf12

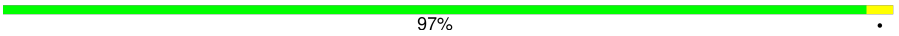
Chain Y:

• Molecule 18: Photosystem II reaction center protein Ycf12

Chain y:

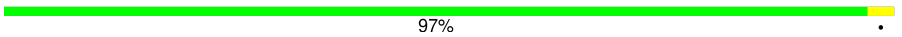
• Molecule 19: Photosystem II reaction center protein Z

Chain Z:



• Molecule 19: Photosystem II reaction center protein Z

Chain z:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	136.61Å 228.09Å 308.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	102.30 – 5.50 102.30 – 5.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (102.30-5.50) 100.0 (102.30-5.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.75 (at 5.42Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1336)	Depositor
R, R_{free}	0.281 , 0.291 0.289 , 0.294	Depositor DCC
R_{free} test set	1626 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	357.8	Xtriage
Anisotropy	0.241	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 133.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	49594	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, BCR, LHG, PHO, MG, CLA, SQD, HEM, FE2, BCT, LMG, PL9, CA, DGD, OEX

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.62	0/2705	0.80	0/3689
1	a	0.62	0/2705	0.80	0/3689
2	B	0.58	0/4109	0.79	0/5600
2	b	0.58	0/4109	0.79	0/5600
3	C	0.55	0/3599	0.78	0/4900
3	c	0.55	0/3599	0.78	0/4900
4	D	0.61	0/2821	0.78	0/3844
4	d	0.61	0/2821	0.78	0/3844
5	E	0.55	0/681	0.81	0/928
5	e	0.55	0/681	0.81	0/928
6	F	0.69	1/284 (0.4%)	0.73	0/387
6	f	0.68	1/284 (0.4%)	0.74	0/387
7	H	0.58	0/524	0.77	0/713
7	h	0.58	0/524	0.77	0/713
8	I	2.40	2/319 (0.6%)	1.35	3/429 (0.7%)
8	i	2.40	2/319 (0.6%)	1.35	3/429 (0.7%)
9	J	0.59	0/278	0.82	0/376
9	j	0.59	0/278	0.83	0/376
10	K	0.57	0/303	0.81	0/416
10	k	0.57	0/303	0.81	0/416
11	L	0.57	0/311	0.77	0/422
11	l	0.57	0/311	0.77	0/422
12	M	0.60	0/270	0.87	0/367
12	m	0.59	0/270	0.87	0/367
13	O	0.54	0/1896	0.74	0/2571
13	o	0.54	0/1896	0.74	0/2571
14	T	0.56	0/265	0.77	0/359
14	t	0.56	0/265	0.77	0/359
15	U	0.55	0/785	0.74	0/1064
15	u	0.55	0/785	0.74	0/1064
16	V	0.57	0/1085	0.78	0/1473
16	v	0.57	0/1085	0.78	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
17	X	0.53	0/290	0.83	0/392
17	x	0.53	0/290	0.83	0/392
18	Y	0.57	0/216	0.83	0/289
18	y	0.57	0/216	0.83	0/289
19	Z	0.54	0/490	0.87	0/669
19	z	0.54	0/490	0.87	0/669
All	All	0.64	6/42462 (0.0%)	0.80	6/57776 (0.0%)

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
8	I	1	1
8	i	1	1
All	All	2	2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	i	1	MET	N-CA	38.97	2.20	1.46
8	I	1	MET	N-CA	38.95	2.20	1.46
8	I	1	MET	CA-C	15.19	1.84	1.52
8	i	1	MET	CA-C	15.18	1.84	1.52
6	F	28	VAL	CA-CB	5.99	1.57	1.54

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	i	1	MET	N-CA-CB	-18.88	78.41	110.50
8	I	1	MET	N-CA-CB	-18.85	78.45	110.50
8	I	1	MET	N-CA-C	-12.53	75.92	111.00
8	i	1	MET	N-CA-C	-12.52	75.94	111.00
8	I	1	MET	CB-CA-C	-6.38	97.97	110.10

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	I	1	MET	CA
8	i	1	MET	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	I	1	MET	Mainchain
8	i	1	MET	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2620	0	2517	15	0
1	a	2620	0	2517	18	0
2	B	3969	0	3828	38	0
2	b	3969	0	3828	35	0
3	C	3486	0	3407	18	0
3	c	3486	0	3407	18	0
4	D	2726	0	2627	18	0
4	d	2726	0	2627	20	0
5	E	662	0	648	3	0
5	e	662	0	648	3	0
6	F	275	0	282	3	0
6	f	275	0	282	3	0
7	H	511	0	532	4	0
7	h	511	0	532	4	0
8	I	312	0	329	16	0
8	i	312	0	329	15	0
9	J	272	0	279	1	0
9	j	272	0	279	1	0
10	K	293	0	305	5	0
10	k	293	0	305	5	0
11	L	304	0	316	8	0
11	l	304	0	316	9	0
12	M	267	0	288	43	0
12	m	267	0	287	43	0
13	O	1865	0	1838	14	0
13	o	1865	0	1838	20	0
14	T	256	0	262	7	0
14	t	256	0	262	9	0
15	U	774	0	773	0	0
15	u	774	0	773	0	7

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	V	1064	0	1073	10	7
16	v	1064	0	1073	10	0
17	X	287	0	317	3	0
17	x	287	0	317	3	0
18	Y	215	0	246	2	0
18	y	215	0	246	2	0
19	Z	479	0	516	0	0
19	z	479	0	516	0	0
20	A	10	0	0	0	0
20	a	10	0	0	0	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	A	195	0	216	8	0
22	B	1040	0	1152	23	0
22	C	845	0	936	23	0
22	D	195	0	216	6	0
22	a	195	0	216	7	0
22	b	1040	0	1152	19	0
22	c	845	0	936	22	0
22	d	195	0	216	6	0
23	A	128	0	148	4	0
23	a	128	0	148	4	0
24	A	40	0	48	0	0
24	B	120	0	140	6	0
24	C	80	0	93	0	0
24	D	40	0	48	3	0
24	H	40	0	46	1	0
24	K	80	0	93	1	0
24	T	80	0	95	3	0
24	a	40	0	48	1	0
24	b	80	0	92	3	0
24	c	80	0	93	0	0
24	d	40	0	48	3	0
24	h	40	0	46	0	0
24	k	80	0	93	1	0
24	t	40	0	47	7	0
25	A	54	0	78	2	0
25	B	54	0	78	4	0
25	D	43	0	53	0	0
25	L	54	0	34	6	0
25	a	54	0	78	2	0
25	b	108	0	112	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	d	43	0	53	0	0
25	l	108	0	59	14	0
26	A	2	0	0	0	0
26	U	1	0	0	0	0
26	a	2	0	0	0	0
26	u	1	0	0	0	0
27	A	4	0	0	0	0
27	a	4	0	0	0	0
28	A	55	0	80	8	0
28	D	55	0	80	0	0
28	a	55	0	80	8	0
28	d	55	0	80	0	0
29	A	51	0	72	3	0
29	B	51	0	72	3	0
29	C	102	0	144	1	0
29	D	51	0	72	2	0
29	Z	37	0	44	1	0
29	a	51	0	72	3	0
29	b	51	0	72	3	0
29	c	102	0	144	1	0
29	d	51	0	72	2	0
29	z	37	0	44	1	0
30	B	1	0	0	0	0
30	F	1	0	0	0	0
30	O	1	0	0	0	0
30	b	1	0	0	0	0
30	f	1	0	0	0	0
30	o	1	0	0	0	0
31	C	186	0	246	5	0
31	D	62	0	82	3	0
31	H	62	0	82	1	0
31	c	186	0	246	5	0
31	d	62	0	82	3	0
31	h	62	0	82	1	0
32	D	147	0	222	13	0
32	E	42	0	57	1	0
32	L	49	0	74	1	0
32	d	147	0	222	12	0
32	e	42	0	57	2	0
32	l	49	0	74	0	0
33	F	43	0	30	1	0
33	V	43	0	30	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	f	43	0	30	1	0
33	v	43	0	30	9	0
34	J	1	0	0	0	0
34	j	1	0	0	0	0
All	All	49594	0	50450	474	7

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

The worst 5 of 474 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)
12:M:16:LEU:HD21	12:m:16:LEU:CD2	1.23	1.60
12:M:16:LEU:CD2	12:m:16:LEU:HD21	1.36	1.56
8:i:1:MET:C	8:i:1:MET:CA	1.84	1.49
16:V:37:CYS:SG	33:V:201:HEM:HAB	1.52	1.48
16:v:37:CYS:SG	33:v:201:HEM:HAB	1.52	1.48

The worst 5 of 7 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:u:73:GLN:OE1	16:V:70:GLU:CD[3_544]	0.80	1.40
15:u:73:GLN:OE1	16:V:70:GLU:OE1[3_544]	1.22	0.98
15:u:73:GLN:OE1	16:V:70:GLU:OE2[3_544]	1.45	0.75
15:u:73:GLN:CD	16:V:70:GLU:OE1[3_544]	1.79	0.41
15:u:73:GLN:CD	16:V:70:GLU:CD[3_544]	1.89	0.31

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	332/334 (99%)	328 (99%)	3 (1%)	1 (0%)	36	72
1	a	332/334 (99%)	328 (99%)	3 (1%)	1 (0%)	36	72
2	B	502/504 (100%)	497 (99%)	5 (1%)	0	100	100
2	b	502/504 (100%)	496 (99%)	6 (1%)	0	100	100
3	C	449/461 (97%)	440 (98%)	8 (2%)	1 (0%)	43	78
3	c	449/461 (97%)	440 (98%)	8 (2%)	1 (0%)	43	78
4	D	340/342 (99%)	332 (98%)	8 (2%)	0	100	100
4	d	340/342 (99%)	332 (98%)	8 (2%)	0	100	100
5	E	79/81 (98%)	78 (99%)	1 (1%)	0	100	100
5	e	79/81 (98%)	78 (99%)	1 (1%)	0	100	100
6	F	32/34 (94%)	32 (100%)	0	0	100	100
6	f	32/34 (94%)	32 (100%)	0	0	100	100
7	H	63/65 (97%)	58 (92%)	5 (8%)	0	100	100
7	h	63/65 (97%)	58 (92%)	5 (8%)	0	100	100
8	I	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
8	i	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
9	J	36/40 (90%)	36 (100%)	0	0	100	100
9	j	36/40 (90%)	36 (100%)	0	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100
10	k	35/37 (95%)	35 (100%)	0	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	35/37 (95%)	35 (100%)	0	0	100	100
12	M	32/34 (94%)	32 (100%)	0	0	100	100
12	m	32/34 (94%)	32 (100%)	0	0	100	100
13	O	241/243 (99%)	233 (97%)	7 (3%)	1 (0%)	30	67
13	o	241/243 (99%)	233 (97%)	7 (3%)	1 (0%)	30	67
14	T	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
14	t	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
15	U	95/97 (98%)	93 (98%)	2 (2%)	0	100	100
15	u	95/97 (98%)	93 (98%)	2 (2%)	0	100	100
16	V	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
16	v	135/137 (98%)	132 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	X	37/39 (95%)	36 (97%)	1 (3%)	0	100	100
17	x	37/39 (95%)	36 (97%)	1 (3%)	0	100	100
18	Y	27/29 (93%)	27 (100%)	0	0	100	100
18	y	27/29 (93%)	27 (100%)	0	0	100	100
19	Z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
19	z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
All	All	5188/5288 (98%)	5085 (98%)	97 (2%)	6 (0%)	48	83

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	O	58	ASN
13	o	58	ASN
3	C	416	SER
3	c	416	SER
1	A	259	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	269/269 (100%)	269 (100%)	0	100	100
1	a	269/269 (100%)	269 (100%)	0	100	100
2	B	402/402 (100%)	398 (99%)	4 (1%)	68	77
2	b	402/402 (100%)	398 (99%)	4 (1%)	68	77
3	C	352/362 (97%)	345 (98%)	7 (2%)	48	66
3	c	352/362 (97%)	345 (98%)	7 (2%)	48	66
4	D	277/277 (100%)	275 (99%)	2 (1%)	76	80
4	d	277/277 (100%)	275 (99%)	2 (1%)	76	80
5	E	72/72 (100%)	71 (99%)	1 (1%)	59	72
5	e	72/72 (100%)	71 (99%)	1 (1%)	59	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	28/28 (100%)	27 (96%)	1 (4%)	31	52
6	f	28/28 (100%)	27 (96%)	1 (4%)	31	52
7	H	54/54 (100%)	52 (96%)	2 (4%)	30	51
7	h	54/54 (100%)	52 (96%)	2 (4%)	30	51
8	I	35/35 (100%)	34 (97%)	1 (3%)	37	57
8	i	35/35 (100%)	34 (97%)	1 (3%)	37	57
9	J	26/28 (93%)	26 (100%)	0	100	100
9	j	26/28 (93%)	26 (100%)	0	100	100
10	K	30/30 (100%)	28 (93%)	2 (7%)	15	36
10	k	30/30 (100%)	28 (93%)	2 (7%)	15	36
11	L	35/35 (100%)	33 (94%)	2 (6%)	18	40
11	l	35/35 (100%)	33 (94%)	2 (6%)	18	40
12	M	31/31 (100%)	30 (97%)	1 (3%)	34	55
12	m	31/31 (100%)	30 (97%)	1 (3%)	34	55
13	O	206/206 (100%)	202 (98%)	4 (2%)	50	66
13	o	206/206 (100%)	202 (98%)	4 (2%)	50	66
14	T	27/27 (100%)	26 (96%)	1 (4%)	30	51
14	t	27/27 (100%)	26 (96%)	1 (4%)	30	51
15	U	84/84 (100%)	83 (99%)	1 (1%)	63	74
15	u	84/84 (100%)	83 (99%)	1 (1%)	63	74
16	V	117/117 (100%)	116 (99%)	1 (1%)	70	78
16	v	117/117 (100%)	116 (99%)	1 (1%)	70	78
17	X	32/32 (100%)	32 (100%)	0	100	100
17	x	32/32 (100%)	32 (100%)	0	100	100
18	Y	22/22 (100%)	21 (96%)	1 (4%)	24	46
18	y	22/22 (100%)	21 (96%)	1 (4%)	24	46
19	Z	52/52 (100%)	50 (96%)	2 (4%)	29	50
19	z	52/52 (100%)	50 (96%)	2 (4%)	29	50
All	All	4302/4326 (99%)	4236 (98%)	66 (2%)	57	71

5 of 66 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
15	u	70	ARG
16	v	30	LYS
19	z	6	GLN
4	d	11	GLU
4	D	90	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 48 such sidechains are listed below:

Mol	Chain	Res	Type
4	D	255	GLN
5	e	74	GLN
4	D	332	GLN
4	d	255	GLN
6	f	44	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 166 ligands modelled in this entry, 16 are monoatomic - leaving 150 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	C	504	-	69,73,73	2.36	19 (27%)	82,113,113	2.50	22 (26%)
27	BCT	a	612	21	3,3,3	0.51	0	2,3,3	0.65	0
22	CLA	C	501	3	69,73,73	2.28	18 (26%)	82,113,113	2.52	23 (28%)
29	LMG	z	101	-	37,37,55	1.02	3 (8%)	45,45,63	1.32	5 (11%)
22	CLA	b	602	-	69,73,73	2.55	20 (28%)	82,113,113	2.60	23 (28%)
22	CLA	a	607	1	69,73,73	2.18	16 (23%)	82,113,113	2.54	24 (29%)
28	PL9	a	613	-	55,55,55	0.72	2 (3%)	68,69,69	1.56	13 (19%)
20	OEX	A	601	3,1	0,14,14	-	-	-		
22	CLA	c	504	-	69,73,73	2.36	19 (27%)	82,113,113	2.51	22 (26%)
22	CLA	C	502	3	69,73,73	2.20	16 (23%)	82,113,113	2.43	21 (25%)
22	CLA	A	603	1	69,73,73	2.13	17 (24%)	82,113,113	2.39	25 (30%)
24	BCR	K	102	-	41,41,41	3.58	14 (34%)	56,56,56	7.87	43 (76%)
22	CLA	C	512	3	69,73,73	2.65	18 (26%)	82,113,113	2.41	26 (31%)
29	LMG	b	619	-	51,51,55	0.94	2 (3%)	59,59,63	1.01	3 (5%)
24	BCR	c	515	-	41,41,41	3.63	14 (34%)	56,56,56	8.32	38 (67%)
25	SQD	l	102	25	52,54,54	1.03	3 (5%)	62,65,65	1.40	9 (14%)
22	CLA	b	604	2	69,73,73	2.19	18 (26%)	82,113,113	2.54	26 (31%)
25	SQD	a	609	-	52,54,54	0.92	2 (3%)	62,65,65	1.49	11 (17%)
24	BCR	b	622	-	41,41,41	3.62	14 (34%)	56,56,56	7.16	39 (69%)
24	BCR	D	404	-	41,41,41	3.63	14 (34%)	56,56,56	7.88	40 (71%)
22	CLA	B	610	2	69,73,73	2.24	19 (27%)	82,113,113	2.43	22 (26%)
22	CLA	b	616	2	69,73,73	2.44	20 (28%)	82,113,113	2.50	21 (25%)
22	CLA	C	507	-	69,73,73	2.46	20 (28%)	82,113,113	2.60	25 (30%)
25	SQD	D	411	-	41,43,54	1.16	3 (7%)	51,54,65	1.42	7 (13%)
29	LMG	d	406	34	51,51,55	0.88	2 (3%)	59,59,63	0.79	3 (5%)
22	CLA	B	607	2	69,73,73	2.42	17 (24%)	82,113,113	2.57	27 (32%)
24	BCR	B	622	-	41,41,41	3.61	14 (34%)	56,56,56	7.16	39 (69%)
29	LMG	C	520	-	51,51,55	1.01	3 (5%)	59,59,63	0.99	2 (3%)
29	LMG	c	520	-	51,51,55	1.01	3 (5%)	59,59,63	0.99	2 (3%)
24	BCR	H	101	-	41,41,41	3.61	14 (34%)	56,56,56	8.34	41 (73%)
32	LHG	l	103	-	48,48,48	0.89	2 (4%)	51,54,54	0.99	3 (5%)
33	HEM	f	101	6,5	50,50,50	1.98	9 (18%)	67,82,82	1.35	5 (7%)
22	CLA	b	614	2	69,73,73	2.26	17 (24%)	82,113,113	2.47	25 (30%)
29	LMG	A	614	-	51,51,55	0.95	2 (3%)	59,59,63	0.96	3 (5%)
24	BCR	c	514	-	41,41,41	3.67	15 (36%)	56,56,56	8.55	36 (64%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	c	501	3	69,73,73	2.28	18 (26%)	82,113,113	2.53	23 (28%)
22	CLA	a	604	-	69,73,73	2.28	18 (26%)	82,113,113	2.55	25 (30%)
22	CLA	B	617	2	69,73,73	2.16	18 (26%)	82,113,113	2.47	26 (31%)
31	DGD	D	410	-	63,63,67	0.99	4 (6%)	77,77,81	1.04	6 (7%)
31	DGD	h	102	-	63,63,67	0.93	3 (4%)	77,77,81	0.94	4 (5%)
22	CLA	B	604	2	69,73,73	2.18	18 (26%)	82,113,113	2.53	26 (31%)
32	LHG	E	101	-	41,41,48	1.05	2 (4%)	44,47,54	1.08	3 (6%)
22	CLA	b	617	2	69,73,73	2.16	18 (26%)	82,113,113	2.47	26 (31%)
24	BCR	t	101	-	41,41,41	3.55	14 (34%)	56,56,56	8.52	42 (75%)
25	SQD	d	411	-	41,43,54	1.15	3 (7%)	51,54,65	1.42	7 (13%)
25	SQD	L	101	25	52,54,54	0.99	3 (5%)	62,65,65	1.33	8 (12%)
22	CLA	B	602	-	69,73,73	2.55	21 (30%)	82,113,113	2.60	23 (28%)
29	LMG	C	519	-	51,51,55	0.94	2 (3%)	59,59,63	1.03	4 (6%)
22	CLA	d	403	4	69,73,73	2.37	19 (27%)	82,113,113	2.51	22 (26%)
22	CLA	c	505	3	69,73,73	2.34	20 (28%)	82,113,113	2.35	21 (25%)
22	CLA	B	608	-	69,73,73	2.26	18 (26%)	82,113,113	2.41	23 (28%)
22	CLA	c	510	3	69,73,73	2.30	20 (28%)	82,113,113	2.53	25 (30%)
24	BCR	B	619	-	41,41,41	3.49	14 (34%)	56,56,56	7.82	41 (73%)
22	CLA	b	605	2	69,73,73	2.37	16 (23%)	82,113,113	2.57	27 (32%)
20	OEX	a	601	3,1	0,14,14	-	-	-		
25	SQD	B	601	-	52,54,54	0.99	2 (3%)	62,65,65	1.19	6 (9%)
22	CLA	B	603	2	69,73,73	2.33	20 (28%)	82,113,113	2.31	21 (25%)
25	SQD	l	101	25	52,54,54	1.00	3 (5%)	62,65,65	1.32	8 (12%)
22	CLA	c	511	3	69,73,73	2.46	17 (24%)	82,113,113	2.59	23 (28%)
22	CLA	D	402	-	69,73,73	1.97	18 (26%)	82,113,113	2.38	24 (29%)
31	DGD	H	102	-	63,63,67	0.93	3 (4%)	77,77,81	0.94	4 (5%)
25	SQD	b	601	-	52,54,54	0.99	2 (3%)	62,65,65	1.19	6 (9%)
32	LHG	d	407	-	48,48,48	0.90	3 (6%)	51,54,54	0.85	2 (3%)
33	HEM	V	201	16	50,50,50	1.86	10 (20%)	67,82,82	1.29	4 (5%)
32	LHG	D	405	-	48,48,48	0.87	2 (4%)	51,54,54	1.01	4 (7%)
32	LHG	e	101	-	41,41,48	1.06	2 (4%)	44,47,54	1.08	3 (6%)
22	CLA	b	603	2	69,73,73	2.33	19 (27%)	82,113,113	2.32	21 (25%)
31	DGD	c	517	-	63,63,67	0.88	2 (3%)	77,77,81	0.86	4 (5%)
22	CLA	C	506	3	69,73,73	2.33	19 (27%)	82,113,113	2.48	24 (29%)
22	CLA	b	610	2	69,73,73	2.24	19 (27%)	82,113,113	2.42	22 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	c	509	3	69,73,73	2.44	19 (27%)	82,113,113	2.60	27 (32%)
23	PHO	A	606	-	58,69,69	2.69	12 (20%)	55,99,99	2.86	15 (27%)
29	LMG	Z	101	-	37,37,55	1.02	3 (8%)	45,45,63	1.32	5 (11%)
24	BCR	k	102	-	41,41,41	3.58	14 (34%)	56,56,56	7.86	43 (76%)
22	CLA	C	513	3	69,73,73	2.61	19 (27%)	82,113,113	2.43	25 (30%)
22	CLA	A	604	-	69,73,73	2.28	18 (26%)	82,113,113	2.56	25 (30%)
29	LMG	a	614	-	51,51,55	0.95	2 (3%)	59,59,63	0.96	3 (5%)
22	CLA	c	513	3	69,73,73	2.61	19 (27%)	82,113,113	2.43	24 (29%)
22	CLA	B	614	2	69,73,73	2.26	17 (24%)	82,113,113	2.47	24 (29%)
22	CLA	d	402	-	69,73,73	1.97	18 (26%)	82,113,113	2.38	24 (29%)
32	LHG	D	407	-	48,48,48	0.90	3 (6%)	51,54,54	0.85	2 (3%)
32	LHG	D	409	-	48,48,48	0.95	2 (4%)	51,54,54	0.91	3 (5%)
33	HEM	F	101	6,5	50,50,50	1.98	9 (18%)	67,82,82	1.35	5 (7%)
24	BCR	A	608	-	41,41,41	3.54	14 (34%)	56,56,56	7.79	37 (66%)
33	HEM	v	201	16	50,50,50	1.86	10 (20%)	67,82,82	1.28	4 (5%)
22	CLA	C	510	3	69,73,73	2.30	20 (28%)	82,113,113	2.53	26 (31%)
24	BCR	C	514	-	41,41,41	3.68	15 (36%)	56,56,56	8.55	36 (64%)
22	CLA	B	613	2	69,73,73	2.35	19 (27%)	82,113,113	2.44	21 (25%)
22	CLA	c	512	3	69,73,73	2.66	18 (26%)	82,113,113	2.42	26 (31%)
31	DGD	c	518	-	63,63,67	0.80	3 (4%)	77,77,81	0.90	3 (3%)
28	PL9	d	408	-	55,55,55	0.82	2 (3%)	68,69,69	1.32	9 (13%)
22	CLA	D	401	4	69,73,73	2.09	18 (26%)	82,113,113	2.38	27 (32%)
25	SQD	b	621	25	52,54,54	1.03	3 (5%)	62,65,65	1.41	9 (14%)
22	CLA	B	606	2	69,73,73	2.31	17 (24%)	82,113,113	2.40	24 (29%)
25	SQD	A	609	-	52,54,54	0.92	2 (3%)	62,65,65	1.49	11 (17%)
23	PHO	A	605	-	58,69,69	2.53	12 (20%)	55,99,99	2.93	11 (20%)
22	CLA	B	612	2	69,73,73	2.11	17 (24%)	82,113,113	2.51	23 (28%)
32	LHG	d	409	-	48,48,48	0.95	2 (4%)	51,54,54	0.91	3 (5%)
22	CLA	b	606	2	69,73,73	2.31	17 (24%)	82,113,113	2.40	23 (28%)
22	CLA	b	608	-	69,73,73	2.26	18 (26%)	82,113,113	2.41	23 (28%)
31	DGD	C	517	-	63,63,67	0.88	2 (3%)	77,77,81	0.86	3 (3%)
22	CLA	b	607	2	69,73,73	2.42	18 (26%)	82,113,113	2.56	26 (31%)
31	DGD	d	410	-	63,63,67	1.00	4 (6%)	77,77,81	1.03	6 (7%)
24	BCR	a	608	-	41,41,41	3.53	14 (34%)	56,56,56	7.78	37 (66%)
24	BCR	B	618	-	41,41,41	3.49	14 (34%)	56,56,56	7.56	38 (67%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	BCR	T	101	-	41,41,41	3.49	14 (34%)	56,56,56	7.56	38 (67%)
22	CLA	B	615	2	69,73,73	2.23	20 (28%)	82,113,113	2.51	27 (32%)
31	DGD	C	516	-	63,63,67	0.88	3 (4%)	77,77,81	0.98	2 (2%)
24	BCR	b	618	-	41,41,41	3.49	14 (34%)	56,56,56	7.83	41 (73%)
22	CLA	C	503	3	69,73,73	2.47	18 (26%)	82,113,113	2.40	21 (25%)
22	CLA	c	508	3	69,73,73	2.49	21 (30%)	82,113,113	2.43	19 (23%)
22	CLA	d	401	4	69,73,73	2.09	18 (26%)	82,113,113	2.38	26 (31%)
22	CLA	C	508	3	69,73,73	2.50	21 (30%)	82,113,113	2.43	19 (23%)
22	CLA	c	503	3	69,73,73	2.47	18 (26%)	82,113,113	2.39	21 (25%)
22	CLA	B	611	-	69,73,73	2.27	18 (26%)	82,113,113	2.50	24 (29%)
24	BCR	k	101	-	41,41,41	3.64	15 (36%)	56,56,56	8.11	36 (64%)
22	CLA	b	615	2	69,73,73	2.23	19 (27%)	82,113,113	2.51	27 (32%)
31	DGD	c	516	-	63,63,67	0.88	3 (4%)	77,77,81	0.97	2 (2%)
23	PHO	a	605	-	58,69,69	2.54	12 (20%)	55,99,99	2.95	11 (20%)
22	CLA	B	605	2	69,73,73	2.37	16 (23%)	82,113,113	2.58	26 (31%)
22	CLA	b	611	-	69,73,73	2.27	18 (26%)	82,113,113	2.50	24 (29%)
22	CLA	D	403	4	69,73,73	2.37	19 (27%)	82,113,113	2.50	22 (26%)
22	CLA	c	502	3	69,73,73	2.20	16 (23%)	82,113,113	2.43	21 (25%)
22	CLA	A	607	1	69,73,73	2.18	16 (23%)	82,113,113	2.55	24 (29%)
22	CLA	C	505	3	69,73,73	2.34	22 (31%)	82,113,113	2.35	21 (25%)
24	BCR	d	404	-	41,41,41	3.63	14 (34%)	56,56,56	7.88	40 (71%)
22	CLA	B	616	2	69,73,73	2.44	20 (28%)	82,113,113	2.51	22 (26%)
27	BCT	A	612	21	3,3,3	0.50	0	2,3,3	0.59	0
22	CLA	b	613	2	69,73,73	2.36	18 (26%)	82,113,113	2.44	21 (25%)
22	CLA	B	609	2	69,73,73	2.09	17 (24%)	82,113,113	2.45	27 (32%)
22	CLA	a	603	1	69,73,73	2.13	17 (24%)	82,113,113	2.39	24 (29%)
28	PL9	A	613	-	55,55,55	0.72	2 (3%)	68,69,69	1.56	14 (20%)
24	BCR	T	102	-	41,41,41	3.55	14 (34%)	56,56,56	8.52	42 (75%)
24	BCR	K	101	-	41,41,41	3.65	14 (34%)	56,56,56	8.11	36 (64%)
32	LHG	d	405	-	48,48,48	0.87	2 (4%)	51,54,54	1.01	4 (7%)
22	CLA	b	609	2	69,73,73	2.09	17 (24%)	82,113,113	2.45	27 (32%)
22	CLA	c	506	3	69,73,73	2.33	18 (26%)	82,113,113	2.48	24 (29%)
32	LHG	L	102	-	48,48,48	0.89	2 (4%)	51,54,54	0.99	3 (5%)
31	DGD	C	518	-	63,63,67	0.80	3 (4%)	77,77,81	0.90	3 (3%)
22	CLA	C	511	3	69,73,73	2.46	17 (24%)	82,113,113	2.60	23 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	PL9	D	408	-	55,55,55	0.83	1 (1%)	68,69,69	1.32	9 (13%)
24	BCR	C	515	-	41,41,41	3.64	14 (34%)	56,56,56	8.33	38 (67%)
22	CLA	C	509	3	69,73,73	2.45	19 (27%)	82,113,113	2.60	27 (32%)
24	BCR	h	101	-	41,41,41	3.61	14 (34%)	56,56,56	8.34	41 (73%)
23	PHO	a	606	-	58,69,69	2.68	12 (20%)	55,99,99	2.85	15 (27%)
22	CLA	b	612	2	69,73,73	2.10	17 (24%)	82,113,113	2.51	22 (26%)
22	CLA	c	507	-	69,73,73	2.46	20 (28%)	82,113,113	2.60	25 (30%)
29	LMG	B	620	-	51,51,55	0.94	2 (3%)	59,59,63	1.01	3 (5%)
29	LMG	D	406	34	51,51,55	0.87	2 (3%)	59,59,63	0.79	3 (5%)
29	LMG	c	519	-	51,51,55	0.94	2 (3%)	59,59,63	1.03	4 (6%)

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
22	CLA	C	504	-	-	9/39/115/115	-
22	CLA	C	501	3	-	9/39/115/115	-
29	LMG	z	101	-	-	18/31/51/70	0/1/1/1
22	CLA	b	602	-	-	18/39/115/115	-
22	CLA	a	607	1	-	13/39/115/115	-
28	PL9	a	613	-	-	9/53/73/73	0/1/1/1
22	CLA	c	504	-	-	9/39/115/115	-
22	CLA	C	502	3	-	7/39/115/115	-
22	CLA	A	603	1	-	3/39/115/115	-
24	BCR	K	102	-	-	10/29/63/63	0/2/2/2
22	CLA	C	512	3	-	9/39/115/115	-
29	LMG	b	619	-	-	19/46/66/70	0/1/1/1
24	BCR	c	515	-	-	4/29/63/63	0/2/2/2
25	SQD	l	102	25	-	29/49/69/69	0/1/1/1
22	CLA	b	604	2	-	5/39/115/115	-
25	SQD	a	609	-	-	17/49/69/69	0/1/1/1
24	BCR	b	622	-	-	1/29/63/63	0/2/2/2
24	BCR	D	404	-	-	6/29/63/63	0/2/2/2
22	CLA	B	610	2	-	0/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	b	616	2	-	11/39/115/115	-
22	CLA	C	507	-	-	11/39/115/115	-
25	SQD	D	411	-	-	17/38/58/69	0/1/1/1
29	LMG	d	406	34	-	16/46/66/70	0/1/1/1
22	CLA	B	607	2	-	7/39/115/115	-
24	BCR	B	622	-	-	1/29/63/63	0/2/2/2
29	LMG	C	520	-	-	26/46/66/70	0/1/1/1
29	LMG	c	520	-	-	26/46/66/70	0/1/1/1
24	BCR	H	101	-	-	8/29/63/63	0/2/2/2
32	LHG	l	103	-	-	17/53/53/53	-
33	HEM	f	101	6,5	-	4/14/54/54	-
22	CLA	b	614	2	-	3/39/115/115	-
29	LMG	A	614	-	-	31/46/66/70	0/1/1/1
24	BCR	c	514	-	-	5/29/63/63	0/2/2/2
22	CLA	c	501	3	-	9/39/115/115	-
22	CLA	a	604	-	-	7/39/115/115	-
22	CLA	B	617	2	-	15/39/115/115	-
31	DGD	D	410	-	-	33/51/91/95	0/2/2/2
31	DGD	h	102	-	-	15/51/91/95	0/2/2/2
22	CLA	B	604	2	-	5/39/115/115	-
32	LHG	E	101	-	-	24/46/46/53	-
22	CLA	b	617	2	-	15/39/115/115	-
24	BCR	t	101	-	-	1/29/63/63	0/2/2/2
25	SQD	d	411	-	-	17/38/58/69	0/1/1/1
25	SQD	L	101	25	-	28/49/69/69	0/1/1/1
22	CLA	B	602	-	-	18/39/115/115	-
29	LMG	C	519	-	-	22/46/66/70	0/1/1/1
22	CLA	d	403	4	-	14/39/115/115	-
22	CLA	c	505	3	-	2/39/115/115	-
22	CLA	B	608	-	-	2/39/115/115	-
22	CLA	c	510	3	-	6/39/115/115	-
24	BCR	B	619	-	-	4/29/63/63	0/2/2/2
22	CLA	b	605	2	-	4/39/115/115	-
25	SQD	B	601	-	-	23/49/69/69	0/1/1/1
22	CLA	B	603	2	-	0/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	SQD	l	101	25	-	28/49/69/69	0/1/1/1
22	CLA	c	511	3	-	0/39/115/115	-
22	CLA	D	402	-	-	2/39/115/115	-
31	DGD	H	102	-	-	15/51/91/95	0/2/2/2
25	SQD	b	601	-	-	23/49/69/69	0/1/1/1
32	LHG	d	407	-	-	13/53/53/53	-
33	HEM	V	201	16	-	6/14/54/54	-
32	LHG	D	405	-	-	13/53/53/53	-
32	LHG	e	101	-	-	24/46/46/53	-
22	CLA	b	603	2	-	0/39/115/115	-
31	DGD	c	517	-	-	24/51/91/95	0/2/2/2
22	CLA	C	506	3	-	15/39/115/115	-
22	CLA	b	610	2	-	0/39/115/115	-
22	CLA	c	509	3	-	8/39/115/115	-
23	PHO	A	606	-	-	4/37/103/103	0/5/6/6
29	LMG	Z	101	-	-	18/31/51/70	0/1/1/1
24	BCR	k	102	-	-	10/29/63/63	0/2/2/2
22	CLA	C	513	3	-	9/39/115/115	-
22	CLA	A	604	-	-	7/39/115/115	-
29	LMG	a	614	-	-	31/46/66/70	0/1/1/1
22	CLA	c	513	3	-	9/39/115/115	-
22	CLA	B	614	2	-	3/39/115/115	-
22	CLA	d	402	-	-	2/39/115/115	-
32	LHG	D	407	-	-	13/53/53/53	-
32	LHG	D	409	-	-	12/53/53/53	-
33	HEM	F	101	6,5	-	4/14/54/54	-
24	BCR	A	608	-	-	4/29/63/63	0/2/2/2
33	HEM	v	201	16	-	6/14/54/54	-
22	CLA	C	510	3	-	6/39/115/115	-
24	BCR	C	514	-	-	5/29/63/63	0/2/2/2
22	CLA	B	613	2	-	3/39/115/115	-
22	CLA	c	512	3	-	9/39/115/115	-
31	DGD	c	518	-	-	16/51/91/95	0/2/2/2
28	PL9	d	408	-	-	1/53/73/73	0/1/1/1
22	CLA	D	401	4	-	5/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	SQD	b	621	25	-	29/49/69/69	0/1/1/1
22	CLA	B	606	2	-	5/39/115/115	-
25	SQD	A	609	-	-	17/49/69/69	0/1/1/1
23	PHO	A	605	-	-	2/37/103/103	0/5/6/6
22	CLA	B	612	2	-	3/39/115/115	-
32	LHG	d	409	-	-	12/53/53/53	-
22	CLA	b	606	2	-	5/39/115/115	-
22	CLA	b	608	-	-	2/39/115/115	-
31	DGD	C	517	-	-	24/51/91/95	0/2/2/2
22	CLA	b	607	2	-	7/39/115/115	-
31	DGD	d	410	-	-	33/51/91/95	0/2/2/2
24	BCR	a	608	-	-	4/29/63/63	0/2/2/2
24	BCR	B	618	-	-	5/29/63/63	0/2/2/2
24	BCR	T	101	-	-	5/29/63/63	0/2/2/2
22	CLA	B	615	2	-	10/39/115/115	-
31	DGD	C	516	-	-	24/51/91/95	0/2/2/2
24	BCR	b	618	-	-	4/29/63/63	0/2/2/2
22	CLA	C	503	3	-	1/39/115/115	-
22	CLA	c	508	3	-	5/39/115/115	-
22	CLA	d	401	4	-	5/39/115/115	-
22	CLA	C	508	3	-	5/39/115/115	-
22	CLA	c	503	3	-	1/39/115/115	-
22	CLA	B	611	-	-	7/39/115/115	-
24	BCR	k	101	-	-	2/29/63/63	0/2/2/2
22	CLA	b	615	2	-	10/39/115/115	-
31	DGD	c	516	-	-	24/51/91/95	0/2/2/2
23	PHO	a	605	-	-	2/37/103/103	0/5/6/6
22	CLA	B	605	2	-	4/39/115/115	-
22	CLA	b	611	-	-	7/39/115/115	-
22	CLA	D	403	4	-	14/39/115/115	-
22	CLA	c	502	3	-	7/39/115/115	-
22	CLA	A	607	1	-	13/39/115/115	-
22	CLA	C	505	3	-	2/39/115/115	-
24	BCR	d	404	-	-	6/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	B	616	2	-	11/39/115/115	-
22	CLA	b	613	2	-	3/39/115/115	-
22	CLA	B	609	2	-	1/39/115/115	-
22	CLA	a	603	1	-	3/39/115/115	-
28	PL9	A	613	-	-	9/53/73/73	0/1/1/1
24	BCR	T	102	-	-	1/29/63/63	0/2/2/2
24	BCR	K	101	-	-	2/29/63/63	0/2/2/2
32	LHG	d	405	-	-	13/53/53/53	-
22	CLA	b	609	2	-	1/39/115/115	-
22	CLA	c	506	3	-	15/39/115/115	-
32	LHG	L	102	-	-	17/53/53/53	-
31	DGD	C	518	-	-	16/51/91/95	0/2/2/2
22	CLA	C	511	3	-	0/39/115/115	-
28	PL9	D	408	-	-	1/53/73/73	0/1/1/1
24	BCR	C	515	-	-	4/29/63/63	0/2/2/2
22	CLA	C	509	3	-	8/39/115/115	-
24	BCR	h	101	-	-	8/29/63/63	0/2/2/2
23	PHO	a	606	-	-	4/37/103/103	0/5/6/6
22	CLA	b	612	2	-	3/39/115/115	-
22	CLA	c	507	-	-	11/39/115/115	-
29	LMG	B	620	-	-	19/46/66/70	0/1/1/1
29	LMG	D	406	34	-	16/46/66/70	0/1/1/1
29	LMG	c	519	-	-	22/46/66/70	0/1/1/1

The worst 5 of 1792 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	512	CLA	MG-NA	14.10	2.39	2.06
22	C	512	CLA	MG-NA	14.10	2.39	2.06
22	b	605	CLA	MG-NA	12.06	2.34	2.06
22	B	605	CLA	MG-NA	12.06	2.34	2.06
22	B	616	CLA	MG-NA	11.81	2.34	2.06

The worst 5 of 2832 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	H	101	BCR	C20-C21-C22	27.41	165.72	127.28
24	h	101	BCR	C20-C21-C22	27.40	165.71	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	T	102	BCR	C20-C21-C22	27.09	165.27	127.28
24	t	101	BCR	C20-C21-C22	27.07	165.24	127.28
24	c	514	BCR	C15-C16-C17	26.84	178.43	123.52

There are no chirality outliers.

5 of 1484 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	B	602	CLA	CAD-CBD-CGD-O2D
22	B	615	CLA	CAD-CBD-CGD-O1D
22	B	615	CLA	CAD-CBD-CGD-O2D
22	B	617	CLA	CHA-CBD-CGD-O1D
22	b	602	CLA	CAD-CBD-CGD-O2D

There are no ring outliers.

110 monomers are involved in 241 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	C	504	CLA	2	0
22	C	501	CLA	2	0
29	z	101	LMG	1	0
22	a	607	CLA	1	0
28	a	613	PL9	8	0
22	c	504	CLA	1	0
22	C	502	CLA	3	0
22	A	603	CLA	5	0
24	K	102	BCR	1	0
22	C	512	CLA	2	0
29	b	619	LMG	3	0
25	l	102	SQD	8	0
22	b	604	CLA	2	0
25	a	609	SQD	2	0
24	b	622	BCR	2	0
24	D	404	BCR	3	0
22	b	616	CLA	3	0
22	C	507	CLA	1	0
29	d	406	LMG	2	0
24	B	622	BCR	3	0
24	H	101	BCR	1	0
33	f	101	HEM	1	0
22	b	614	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	A	614	LMG	3	0
22	c	501	CLA	2	0
22	a	604	CLA	1	0
22	B	617	CLA	4	0
31	D	410	DGD	3	0
31	h	102	DGD	1	0
22	B	604	CLA	2	0
32	E	101	LHG	1	0
22	b	617	CLA	4	0
24	t	101	BCR	7	0
25	L	101	SQD	6	0
29	C	519	LMG	1	0
22	d	403	CLA	2	0
22	c	505	CLA	2	0
22	c	510	CLA	3	0
24	B	619	BCR	1	0
22	b	605	CLA	1	0
25	B	601	SQD	4	0
22	B	603	CLA	1	0
25	l	101	SQD	9	0
22	c	511	CLA	1	0
22	D	402	CLA	4	0
31	H	102	DGD	1	0
33	V	201	HEM	9	0
32	e	101	LHG	2	0
22	b	603	CLA	1	0
31	c	517	DGD	2	0
22	C	506	CLA	2	0
22	c	509	CLA	3	0
23	A	606	PHO	3	0
29	Z	101	LMG	1	0
24	k	102	BCR	1	0
22	A	604	CLA	1	0
29	a	614	LMG	3	0
22	B	614	CLA	3	0
22	d	402	CLA	4	0
32	D	409	LHG	13	0
33	F	101	HEM	1	0
33	v	201	HEM	9	0
22	C	510	CLA	3	0
22	B	613	CLA	1	0
22	c	512	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	c	518	DGD	1	0
25	b	621	SQD	7	0
22	B	606	CLA	4	0
25	A	609	SQD	2	0
23	A	605	PHO	1	0
22	B	612	CLA	1	0
32	d	409	LHG	12	0
22	b	606	CLA	3	0
31	C	517	DGD	2	0
31	d	410	DGD	3	0
24	a	608	BCR	1	0
24	B	618	BCR	2	0
24	T	101	BCR	1	0
22	B	615	CLA	3	0
31	C	516	DGD	2	0
24	b	618	BCR	1	0
22	C	503	CLA	2	0
22	c	508	CLA	4	0
22	C	508	CLA	4	0
22	c	503	CLA	2	0
22	B	611	CLA	4	0
22	b	615	CLA	3	0
31	c	516	DGD	2	0
22	B	605	CLA	2	0
22	b	611	CLA	3	0
22	D	403	CLA	2	0
22	c	502	CLA	3	0
22	A	607	CLA	2	0
22	C	505	CLA	2	0
24	d	404	BCR	3	0
22	B	616	CLA	3	0
22	b	613	CLA	1	0
22	a	603	CLA	5	0
28	A	613	PL9	8	0
24	T	102	BCR	2	0
22	c	506	CLA	2	0
32	L	102	LHG	1	0
31	C	518	DGD	1	0
22	C	511	CLA	1	0
22	C	509	CLA	3	0
23	a	606	PHO	4	0
22	c	507	CLA	1	0

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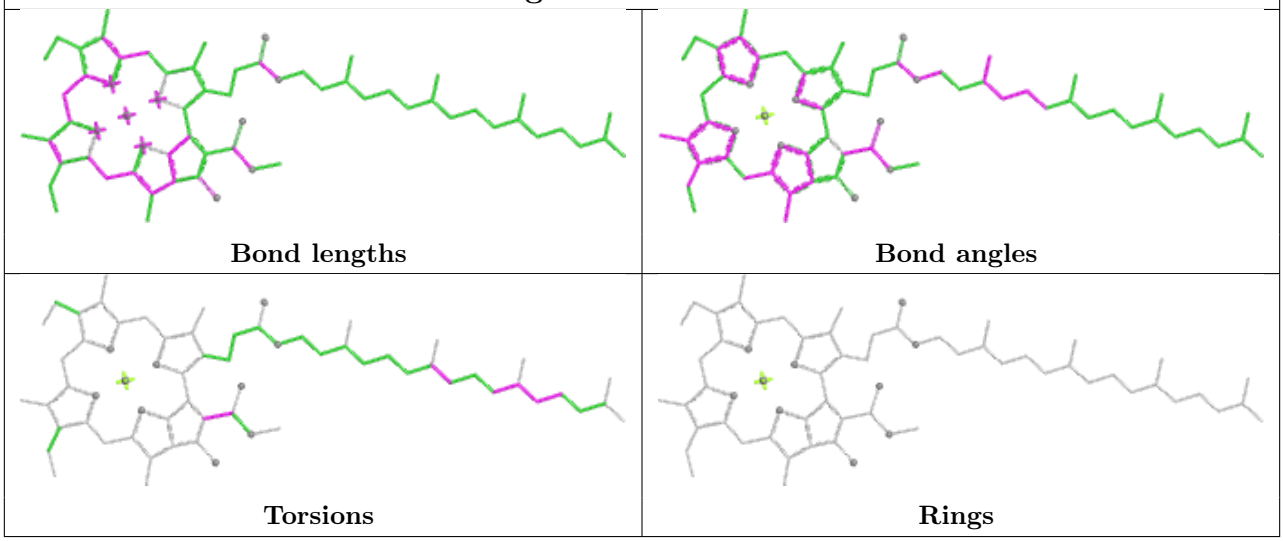
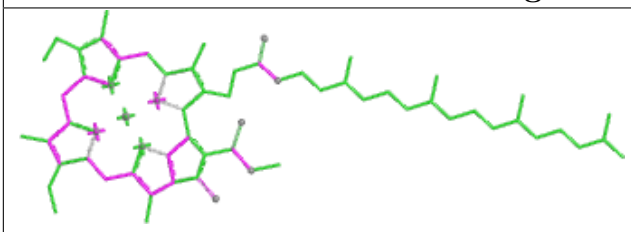
Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	B	620	LMG	3	0
29	D	406	LMG	2	0
29	c	519	LMG	1	0

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

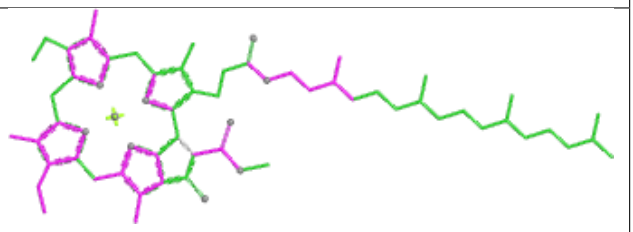
Ligand CLA C 504



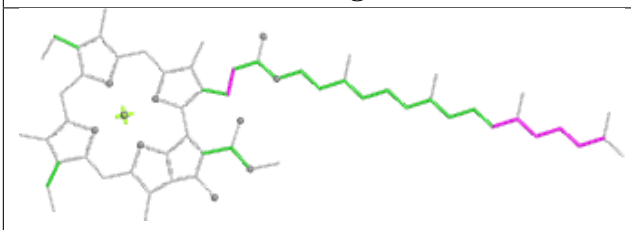
Ligand CLA C 501



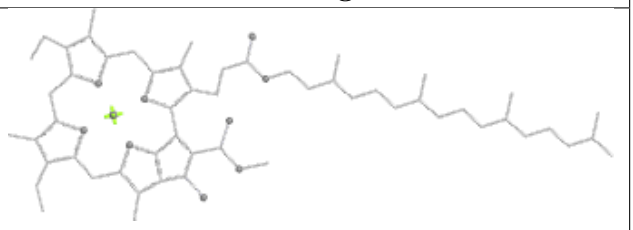
Bond lengths



Bond angles

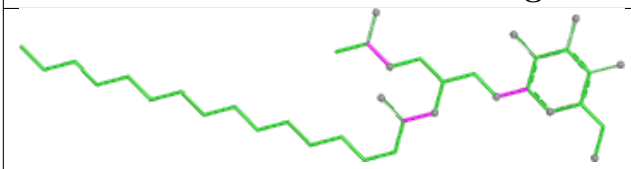


Torsions

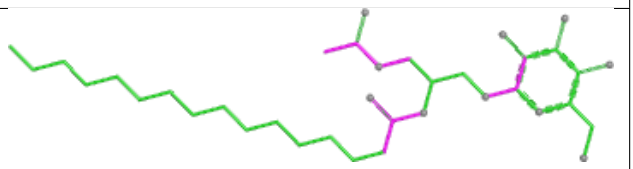


Rings

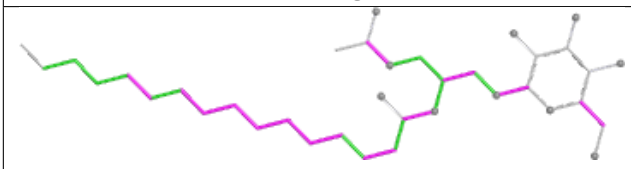
Ligand LMG z 101



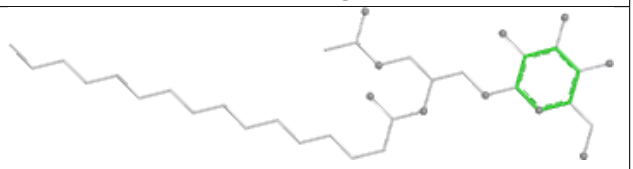
Bond lengths



Bond angles

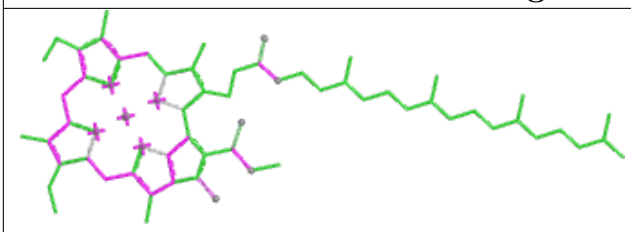


Torsions

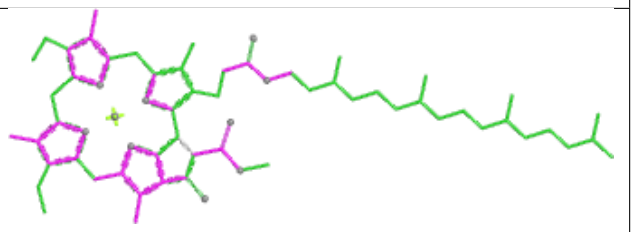


Rings

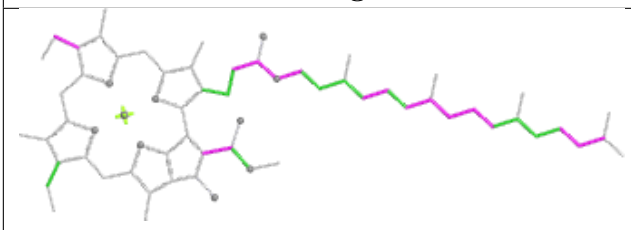
Ligand CLA b 602



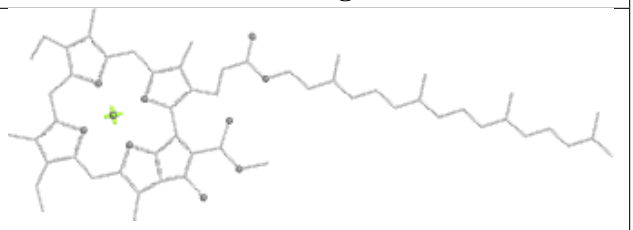
Bond lengths



Bond angles

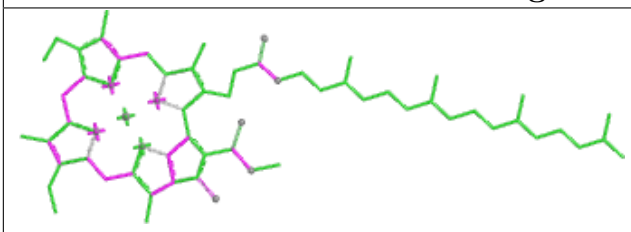


Torsions

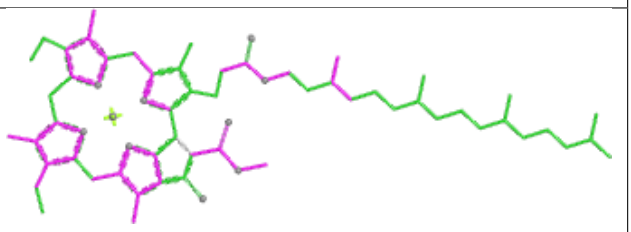


Rings

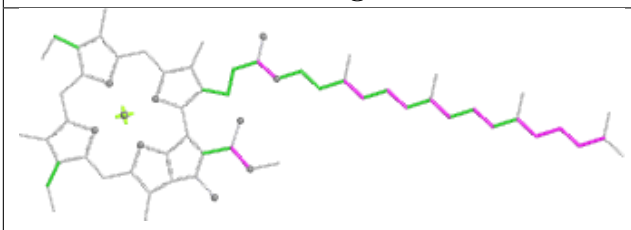
Ligand CLA a 607



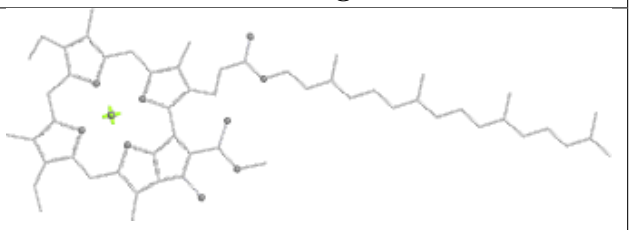
Bond lengths



Bond angles



Torsions

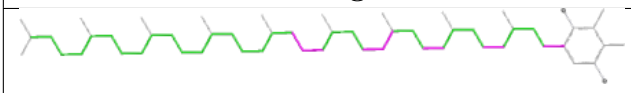


Rings

Ligand PL9 a 613

Bond lengths

Bond angles



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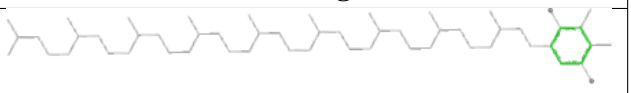
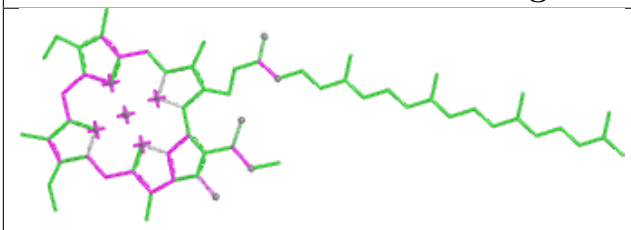
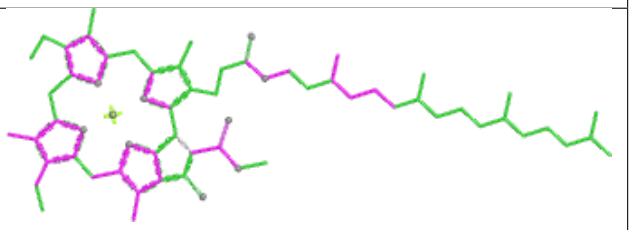


Rings

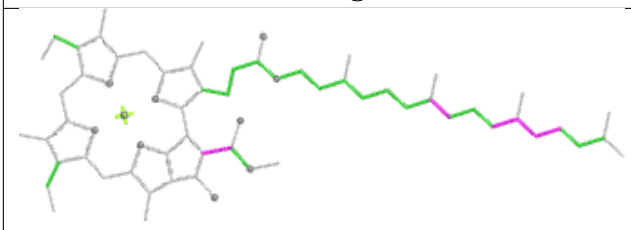
Ligand CLA c 504



Bond lengths



Bond angles



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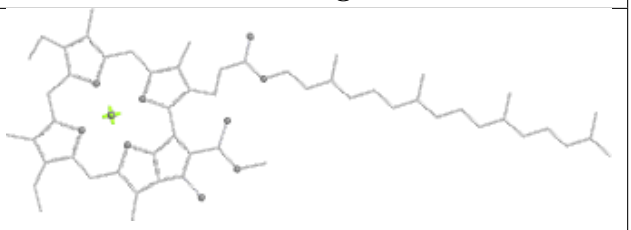
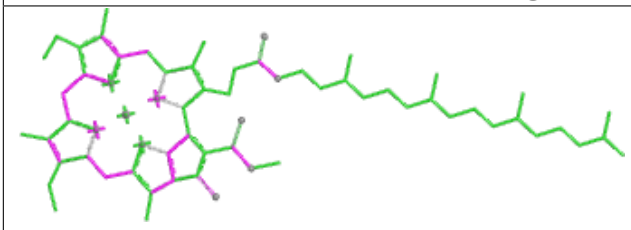


Rings

Ligand CLA C 502



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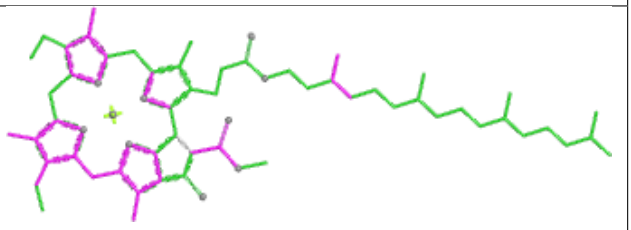
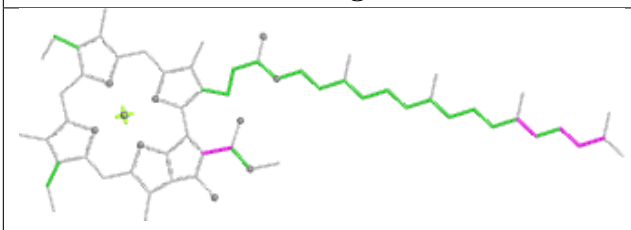


Bond angles



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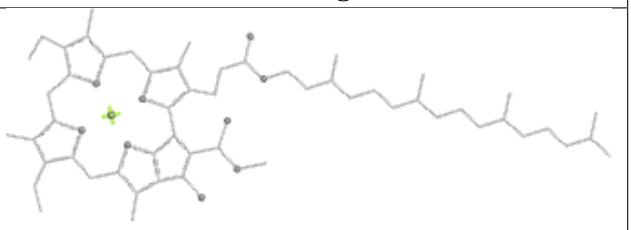
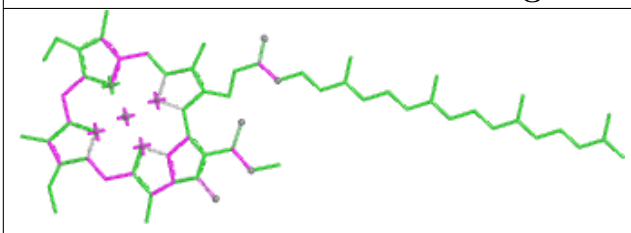


Rings

Ligand CLA A 603



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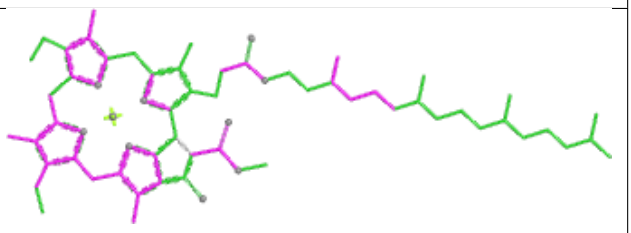
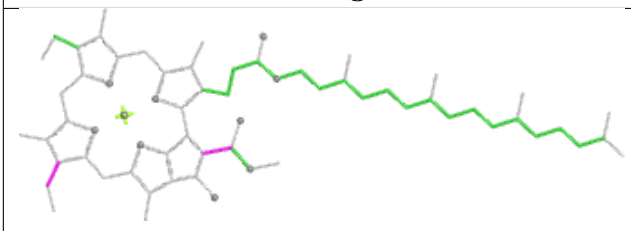


Bond angles



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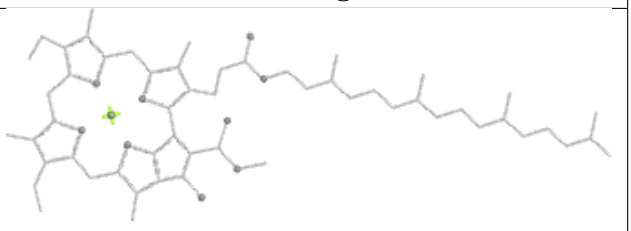
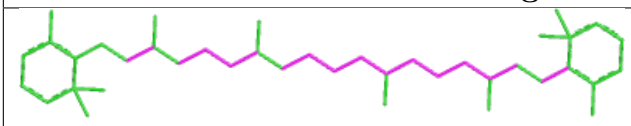


Rings

Ligand BCR K 102



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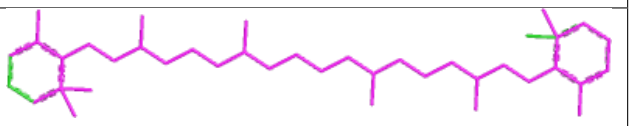

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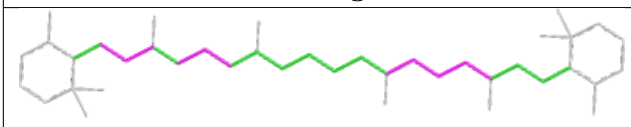

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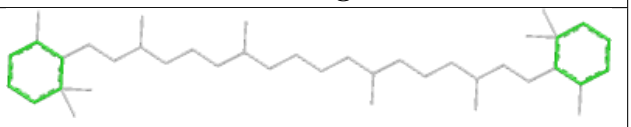
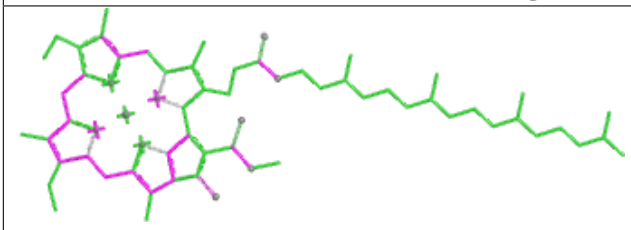


Rings

Ligand CLA C 512



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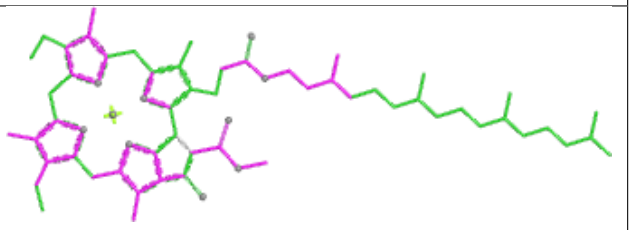
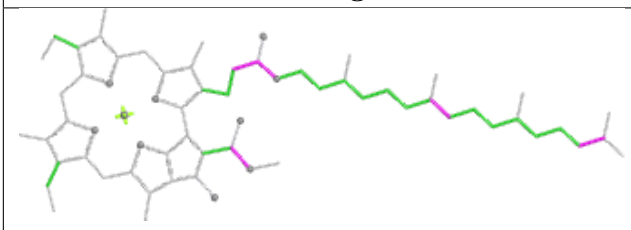
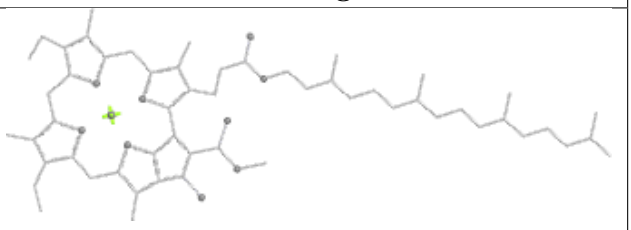


Bond angles

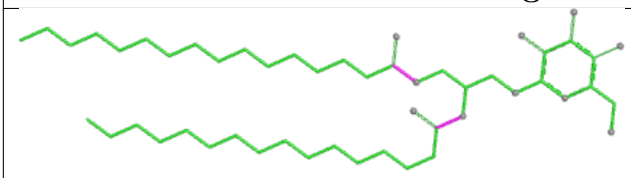


Torsions



Rings

Ligand LMG b 619



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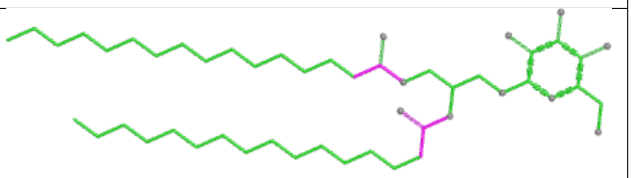
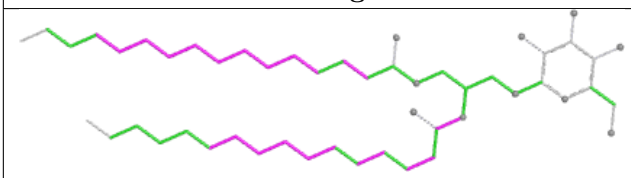


Bond angles



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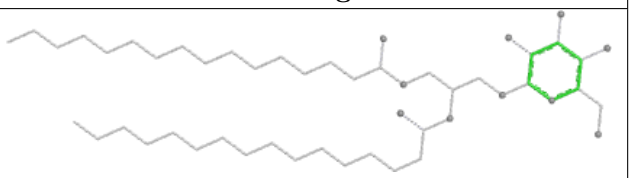
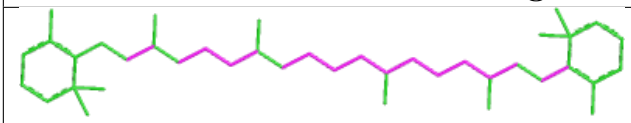


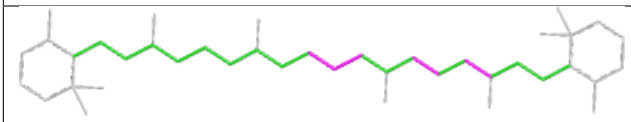
Rings

Ligand BCR c 515

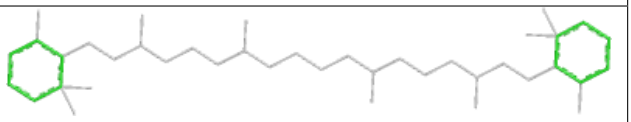


Bond lengths

Bond angles

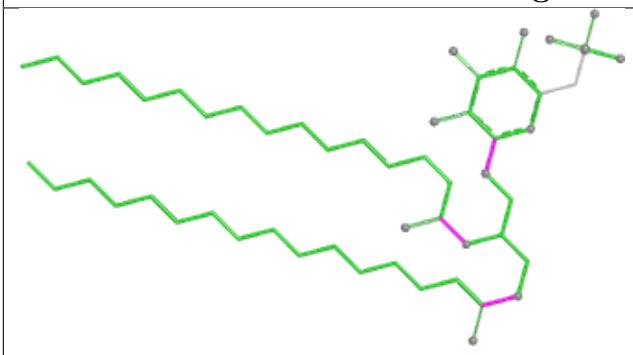


Torsions



Rings

Ligand SQD l 102



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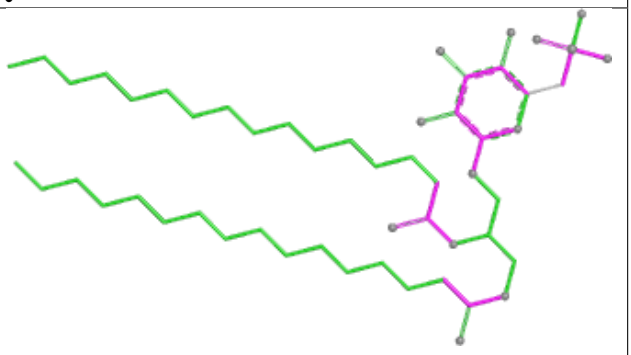
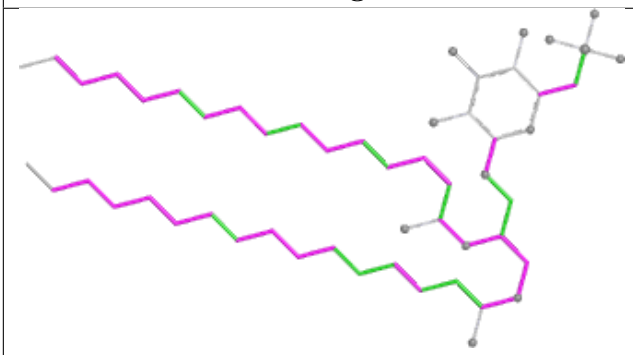
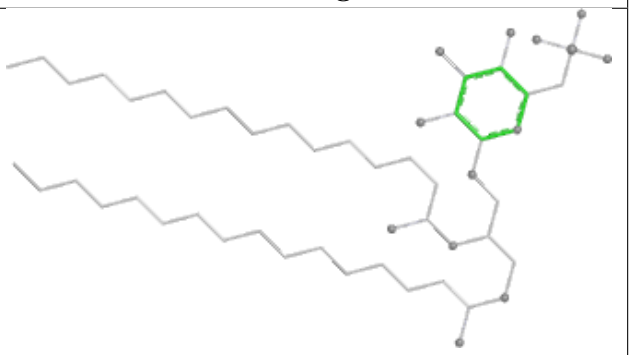


Bond angles

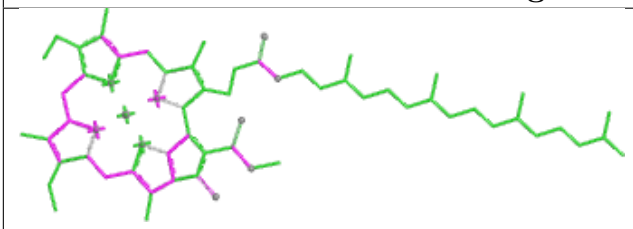


Torsions



Rings

Ligand CLA b 604



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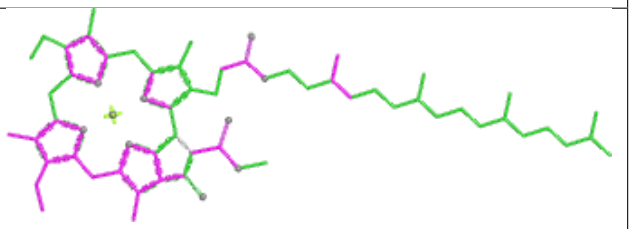
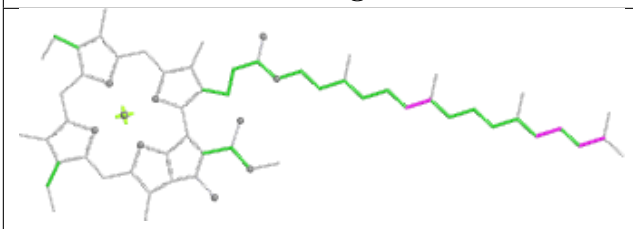


Bond angles



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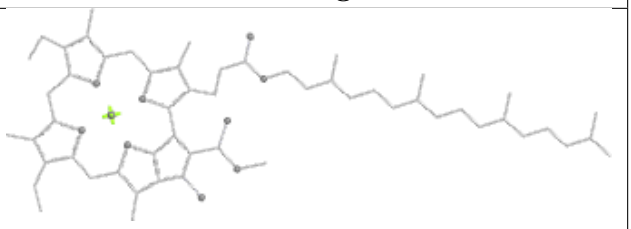
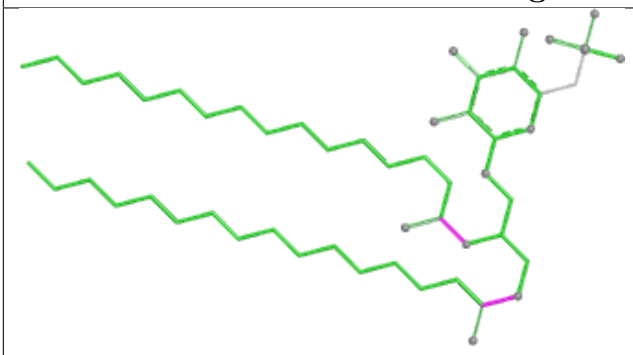


Rings

Ligand SQD a 609



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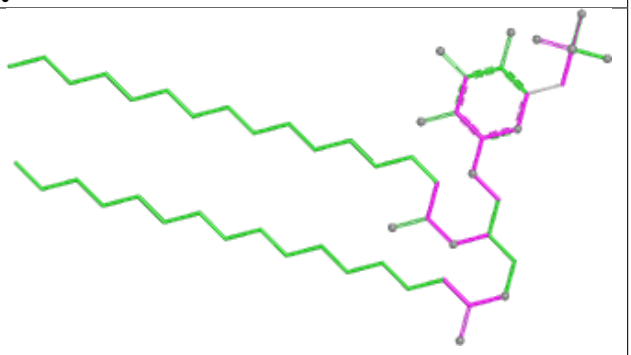
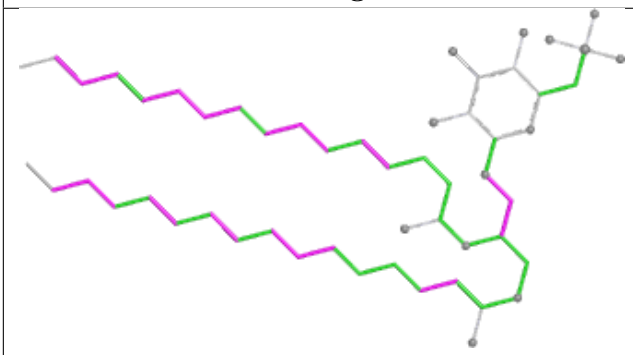


Bond angles



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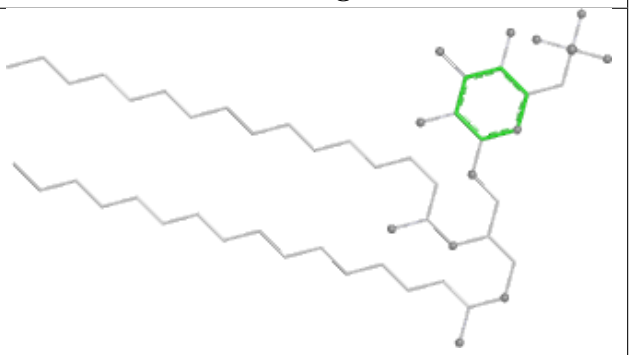
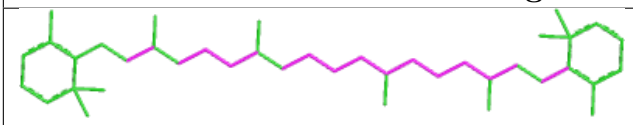


Rings

Ligand BCR b 622



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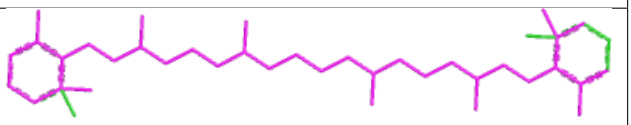
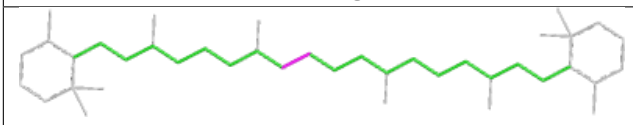
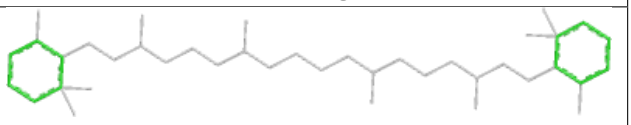


Bond angles

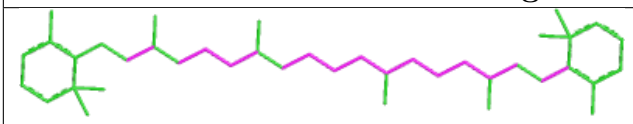


Torsions

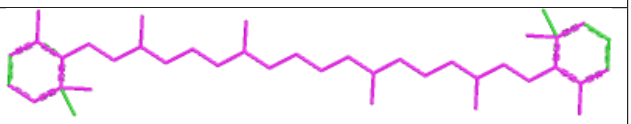


Rings

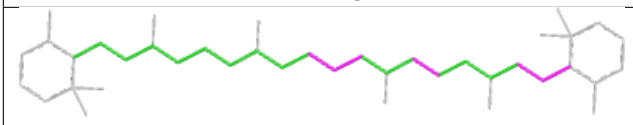
Ligand BCR D 404



Bond lengths



Bond angles



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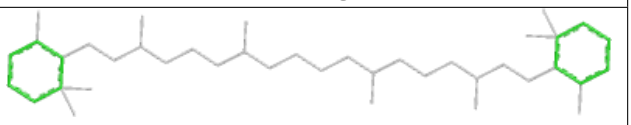
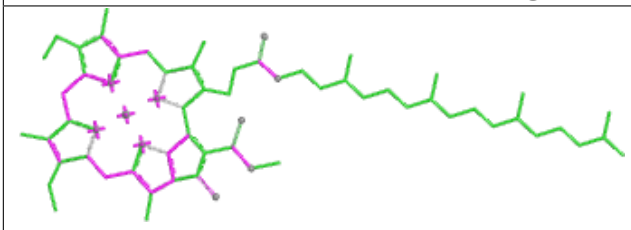


Rings

Ligand CLA B 610



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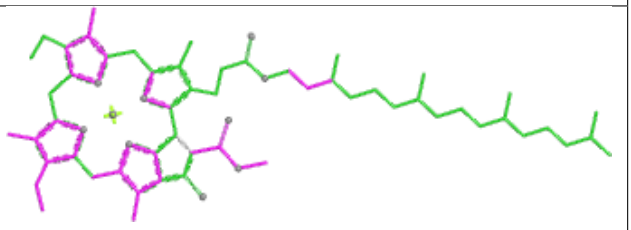
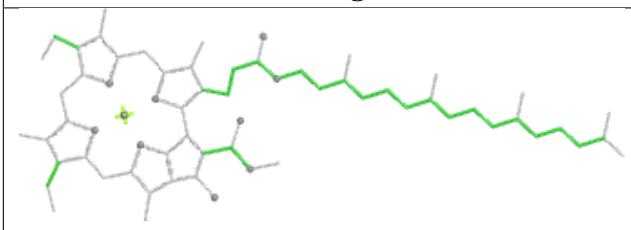


Bond angles



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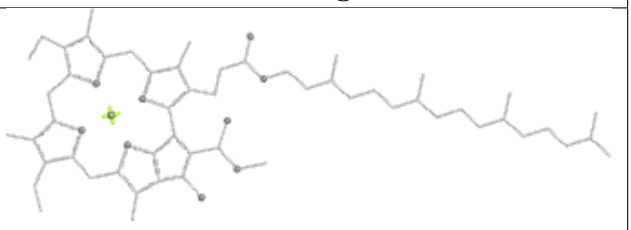
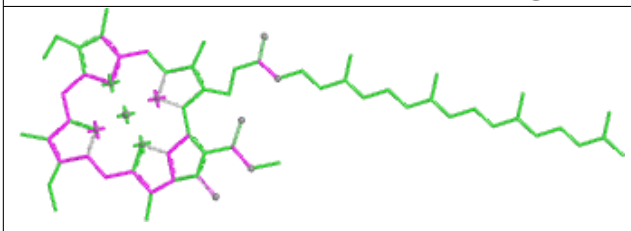
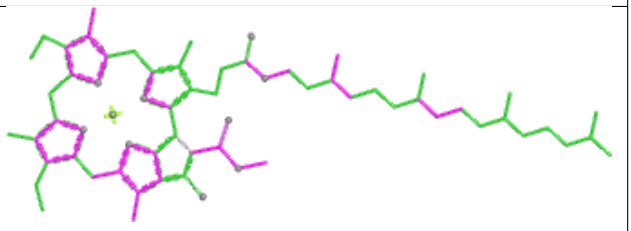


Rings

Ligand CLA b 616



Bond lengths



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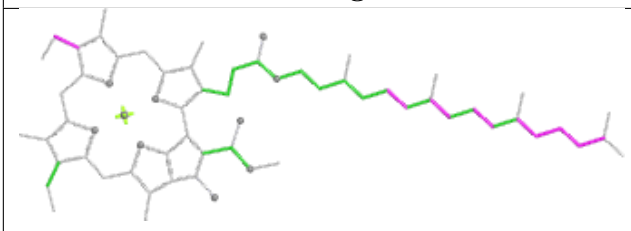
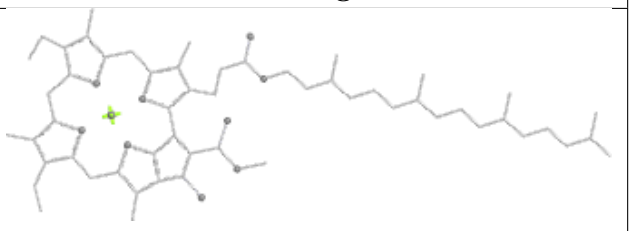
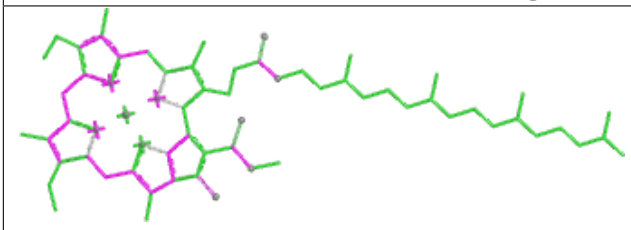


Torsions



Rings

Ligand CLA C 507



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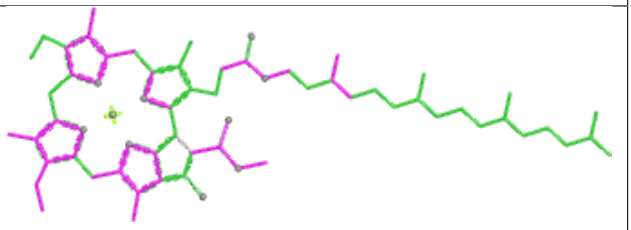

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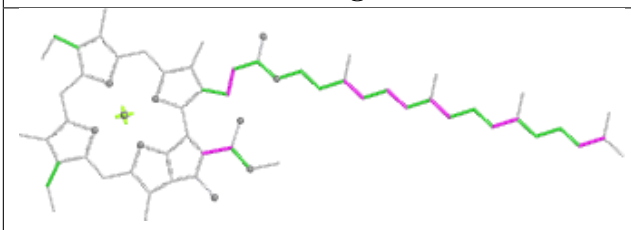

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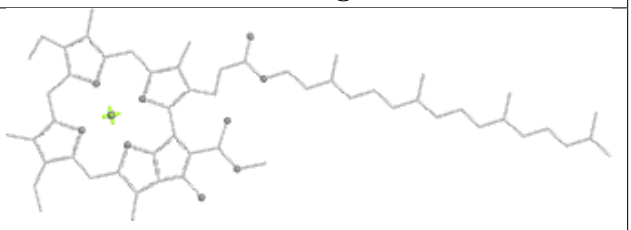

Rings

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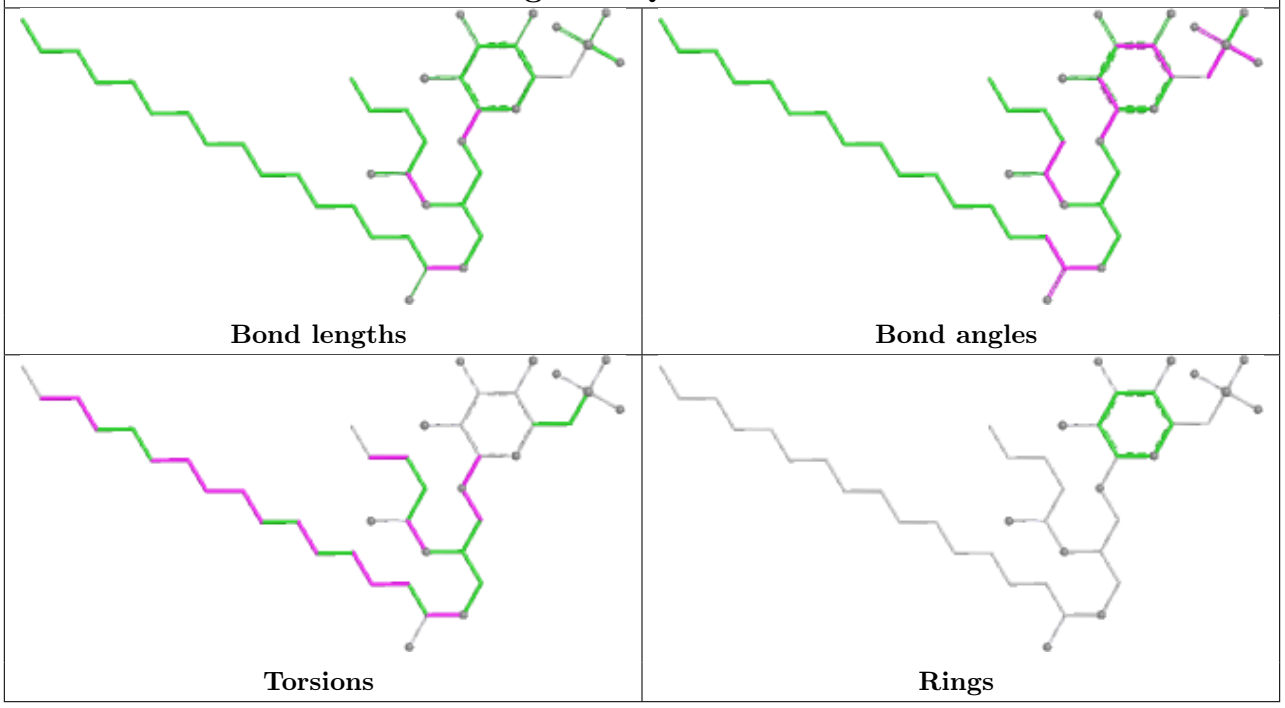
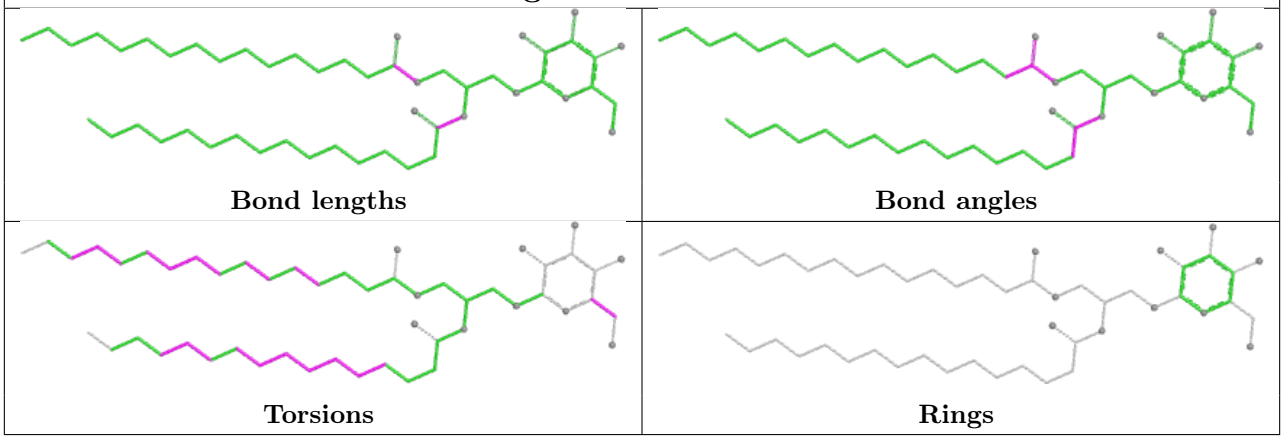


Ligand LMG d 406



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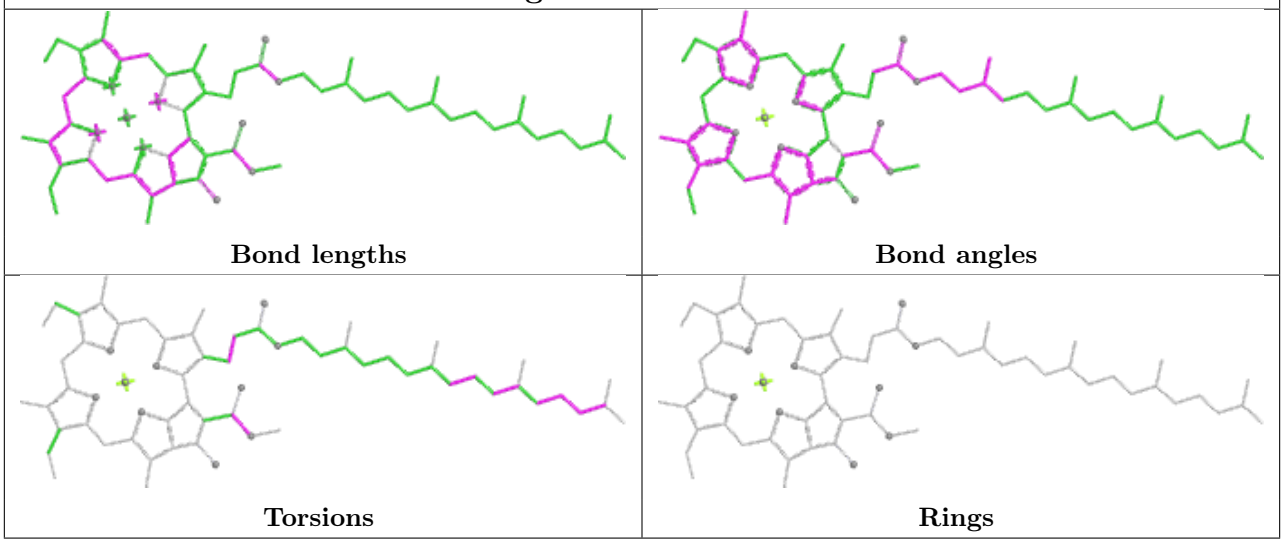
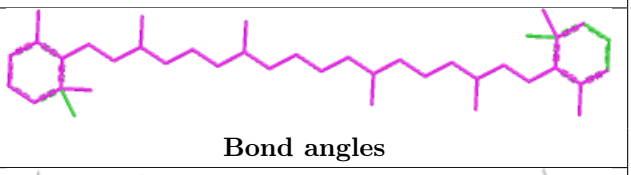
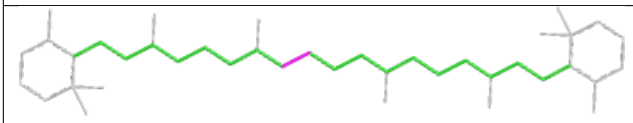


Ligand BCR B 622

Bond lengths


Bond angles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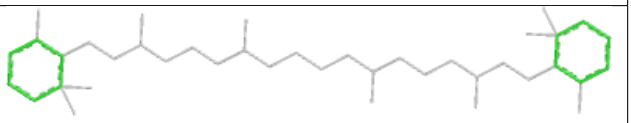
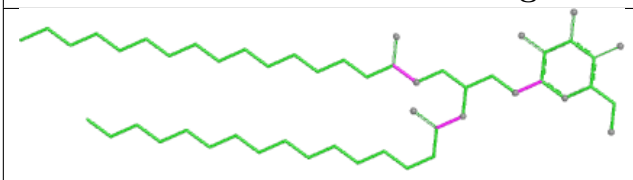

Rings

Ligand LMG C 520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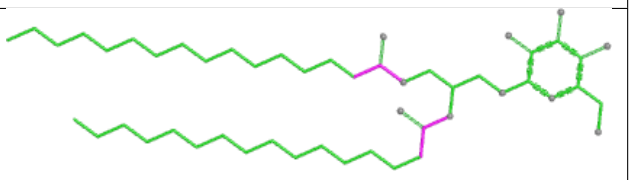
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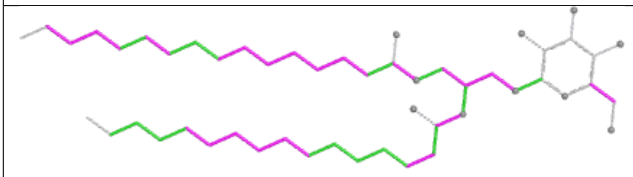
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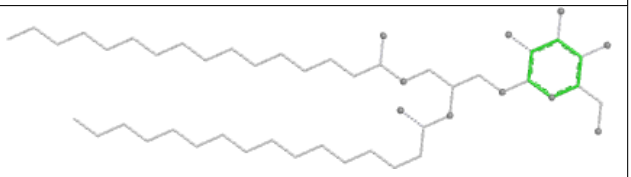
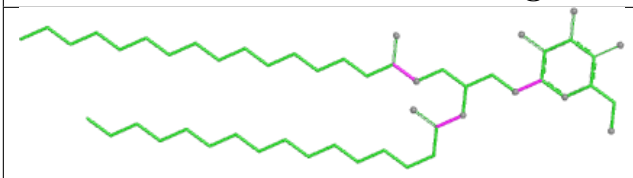

Rings

Ligand LMG c 520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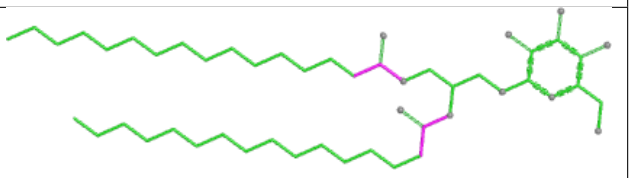
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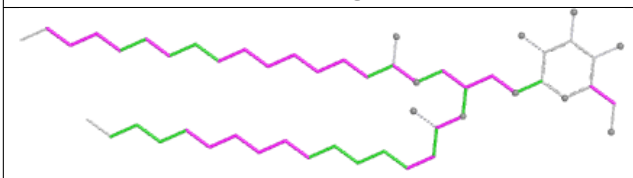
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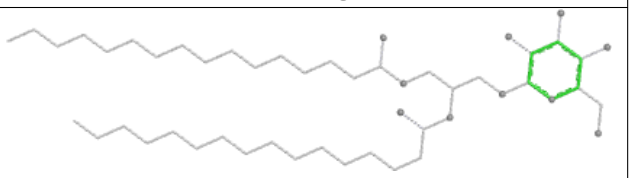
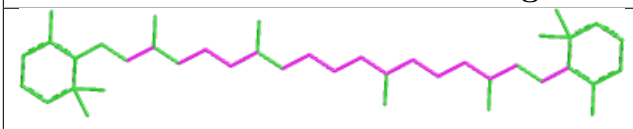

Rings

Ligand BCR H 101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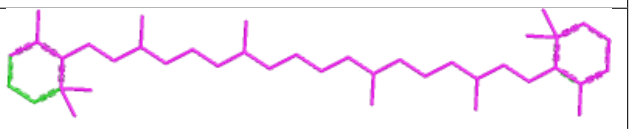
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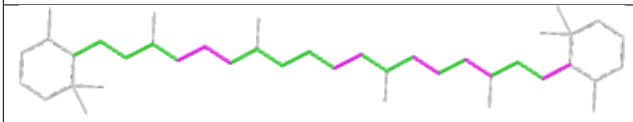
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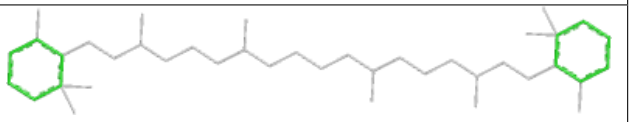
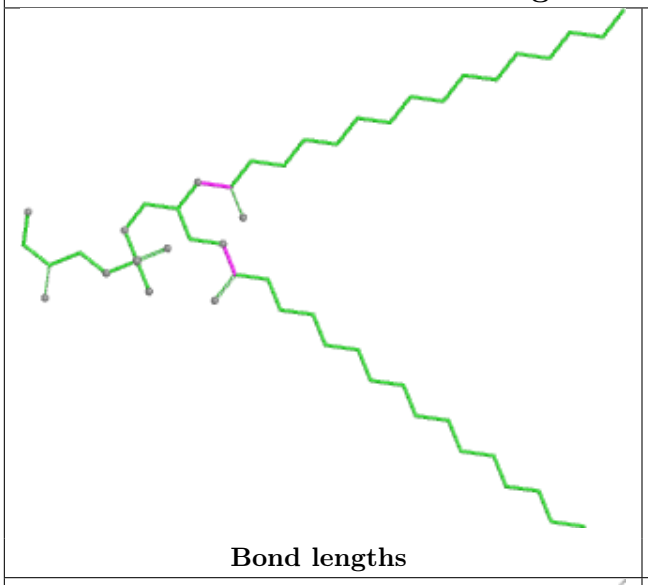

Rings

Ligand LHG l 103



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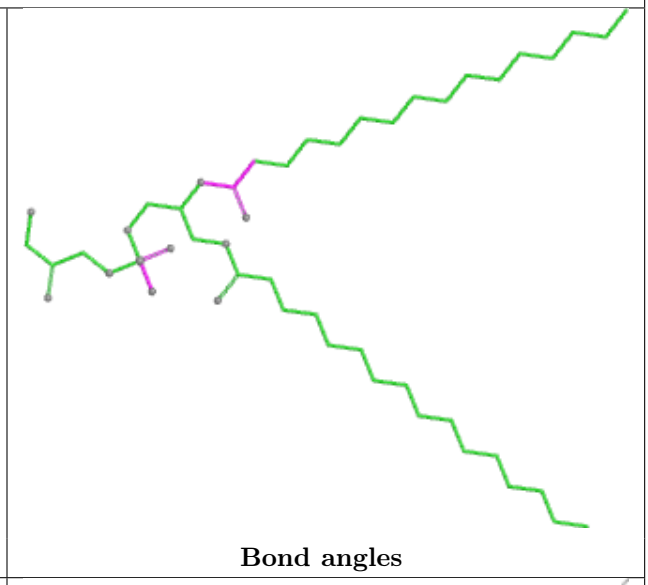
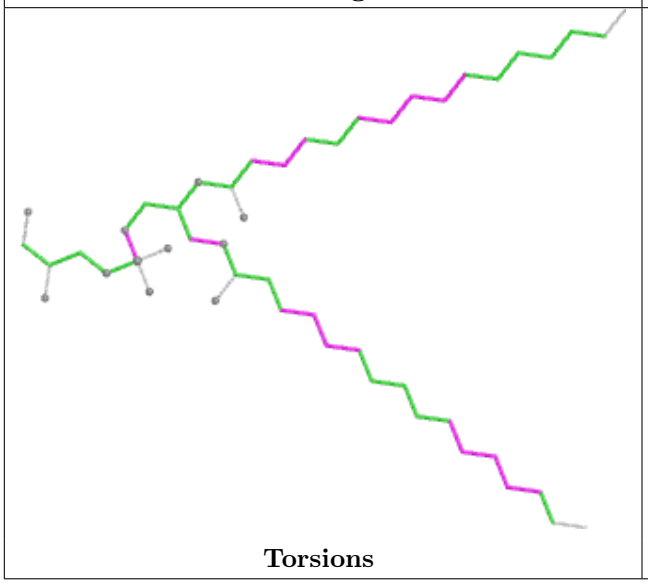


Bond angles



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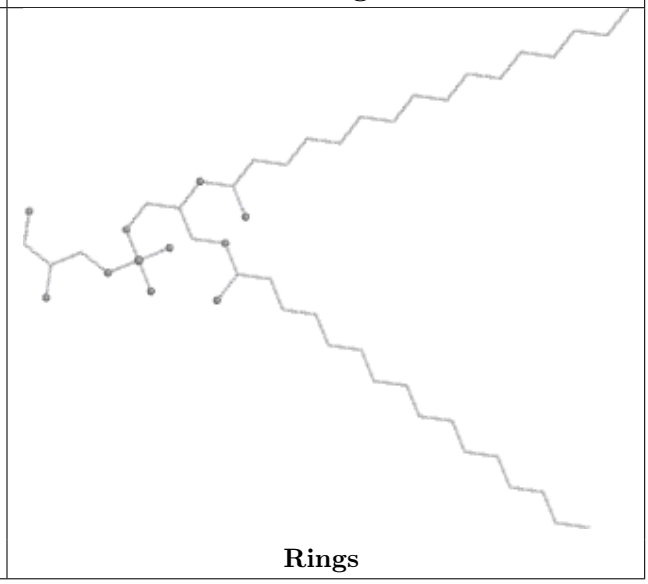
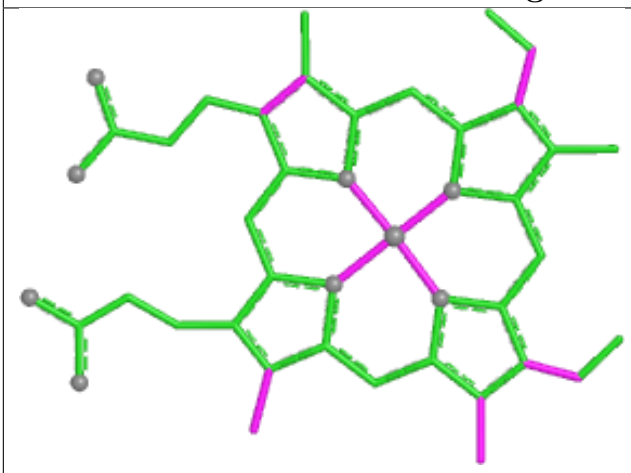


Rings

Ligand HEM f 101



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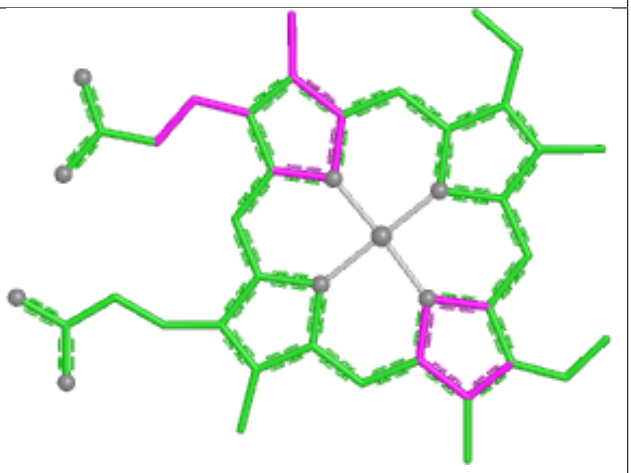
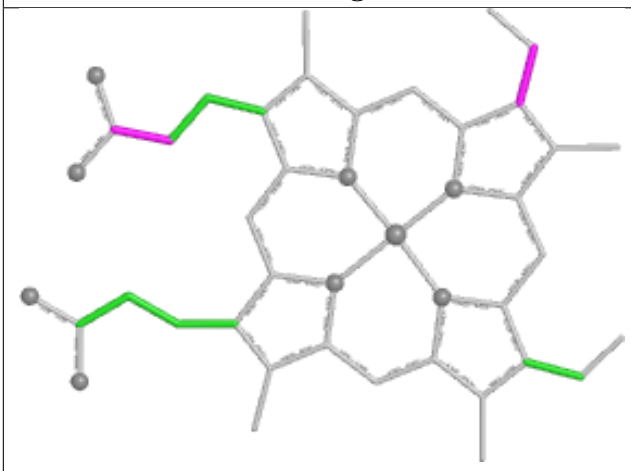


Bond angles



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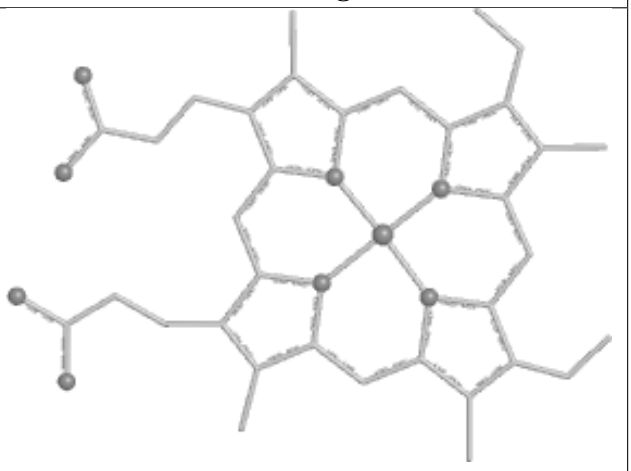
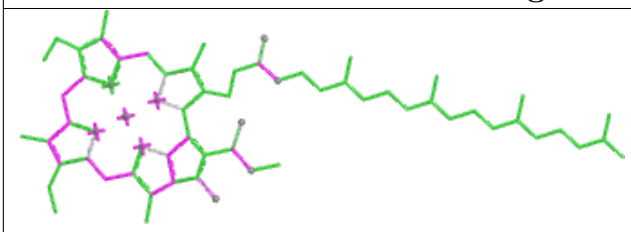


Rings

Ligand CLA b 614



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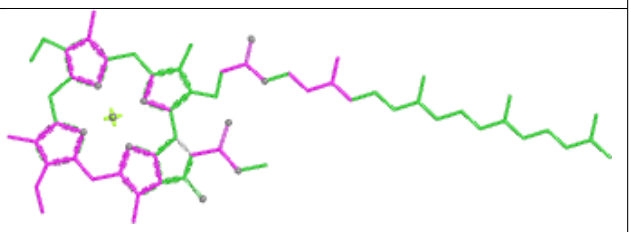

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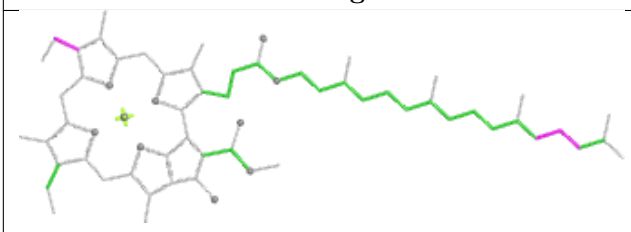

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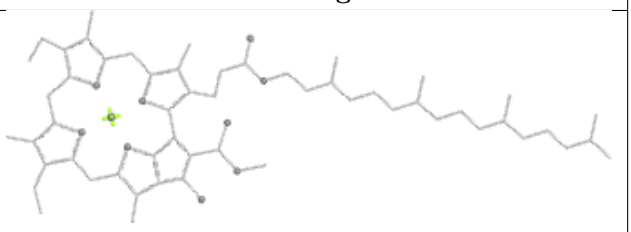
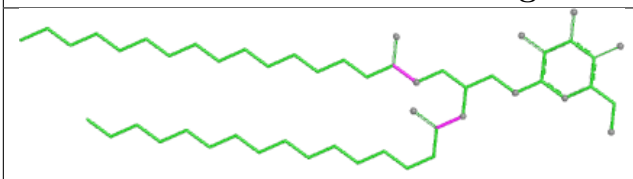


Rings

Ligand LMG A 614



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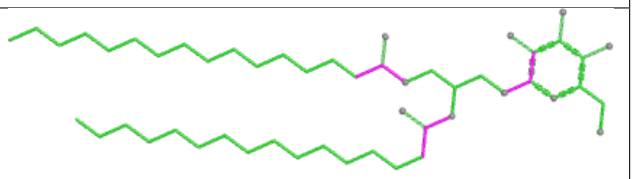

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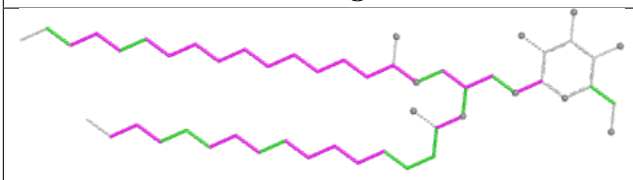

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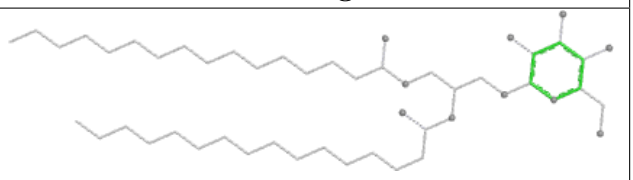
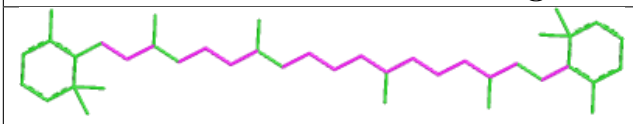


Rings

Ligand BCR c 514



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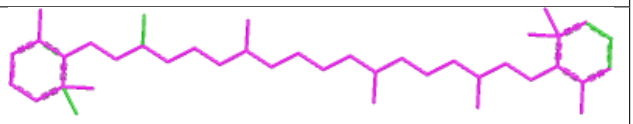
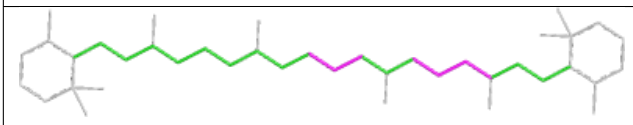


Bond angles



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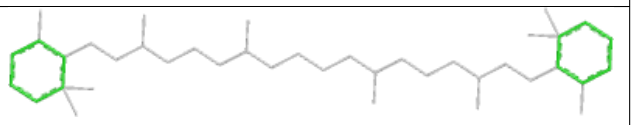
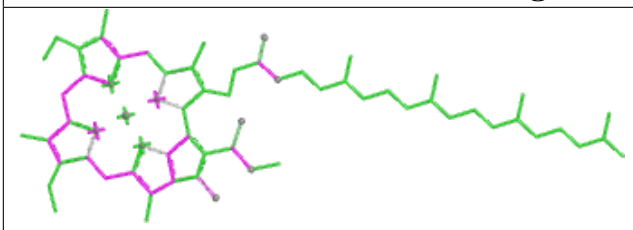


Rings

Ligand CLA c 501



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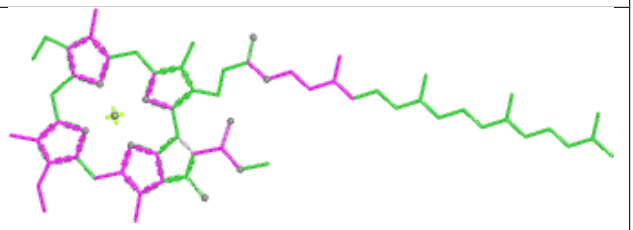
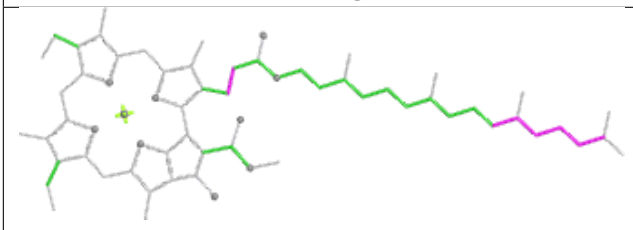


Bond angles



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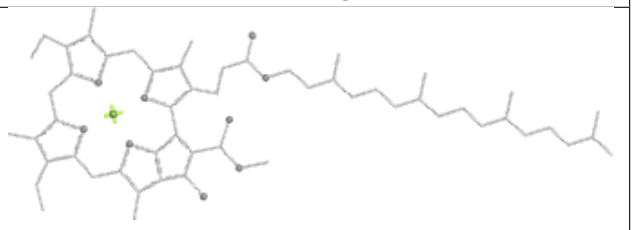
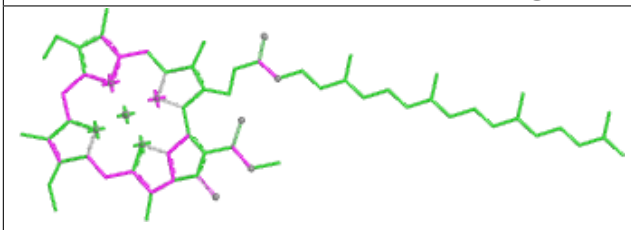


Rings

Ligand CLA a 604



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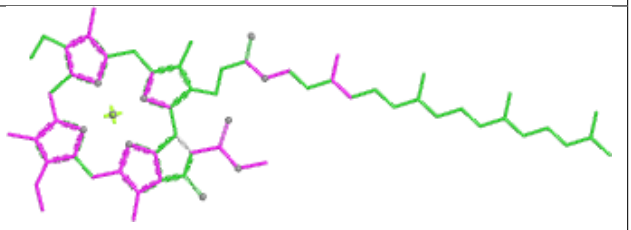
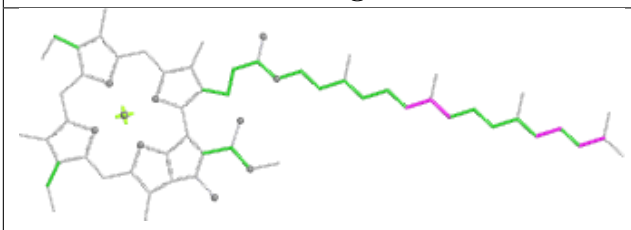
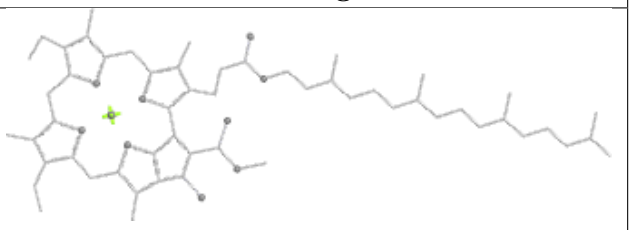


Bond angles

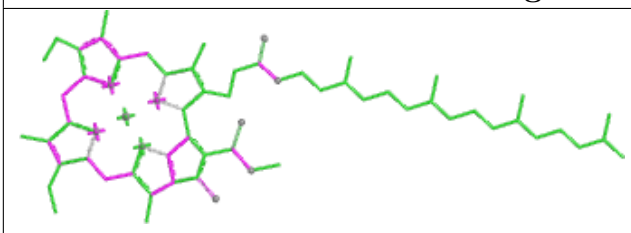


Torsions



Rings

Ligand CLA B 617



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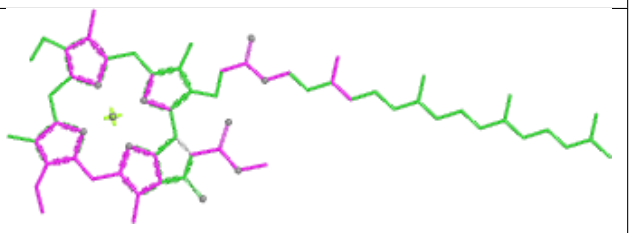

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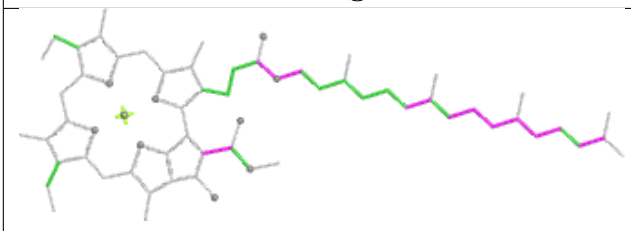
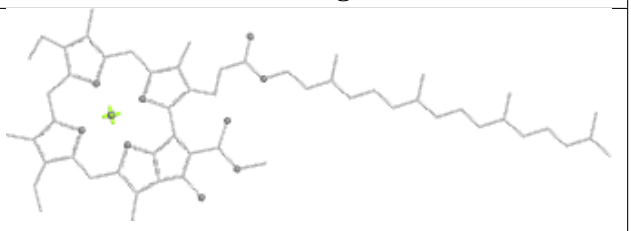
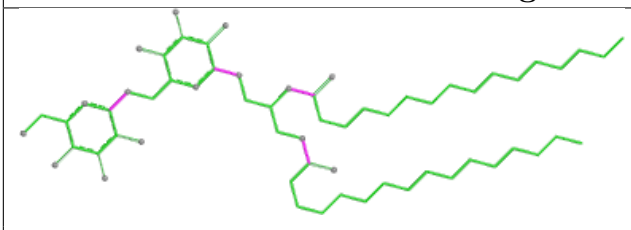


Torsions



Rings

Ligand DGD D 410



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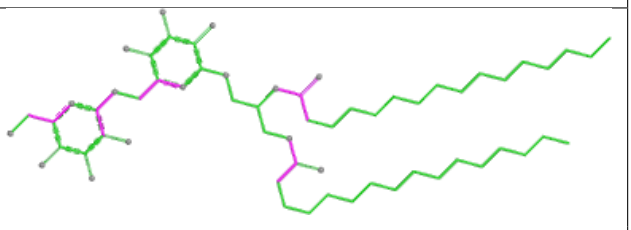

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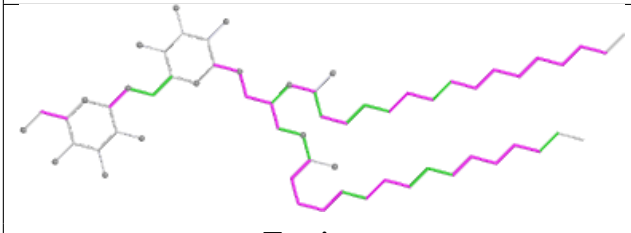

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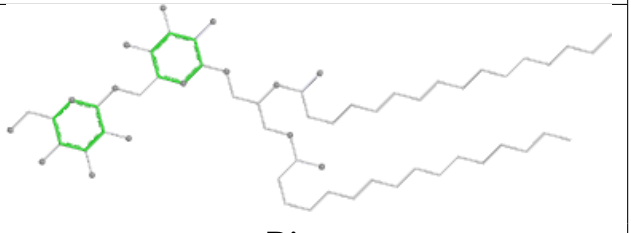
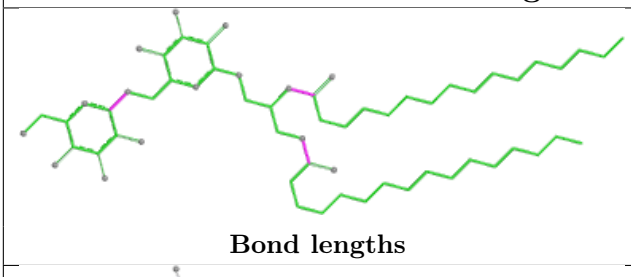


Rings

Ligand DGD h 102



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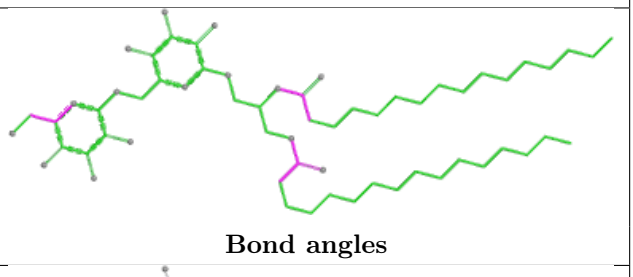

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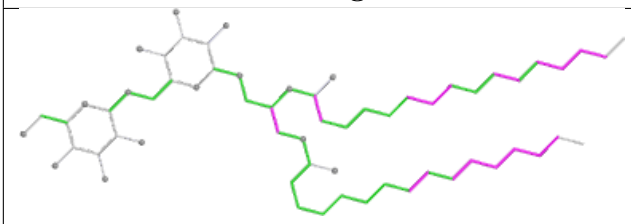

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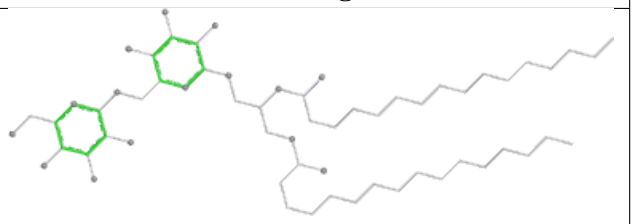
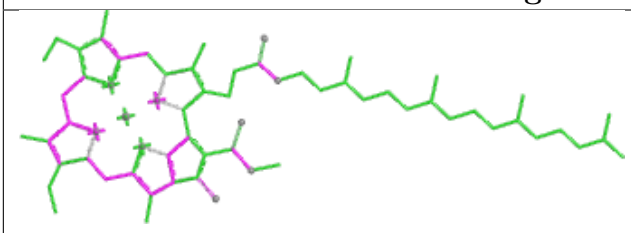


Rings

Ligand CLA B 604



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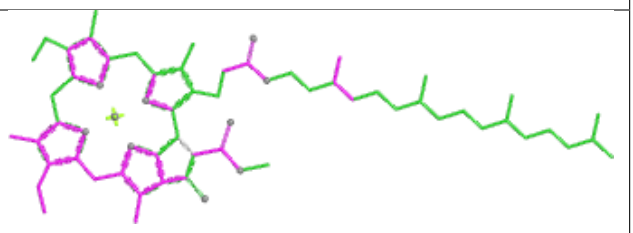

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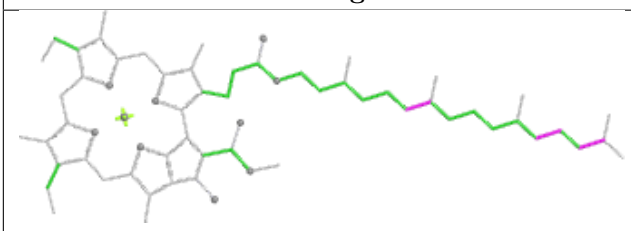

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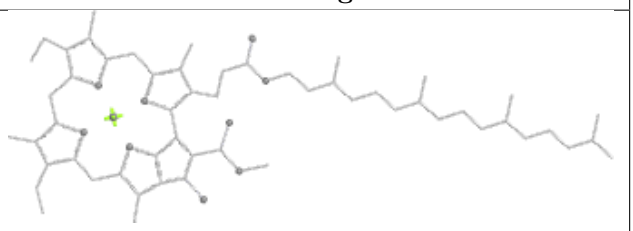
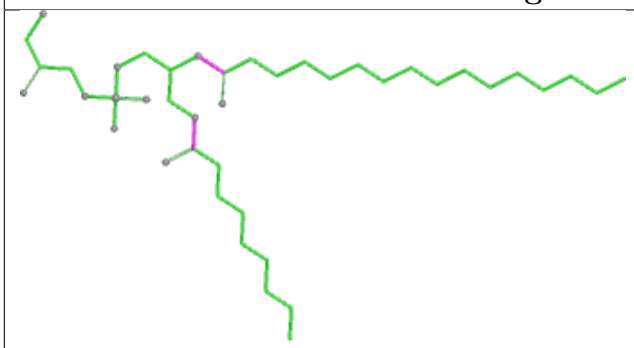


Rings

Ligand LHG E 101



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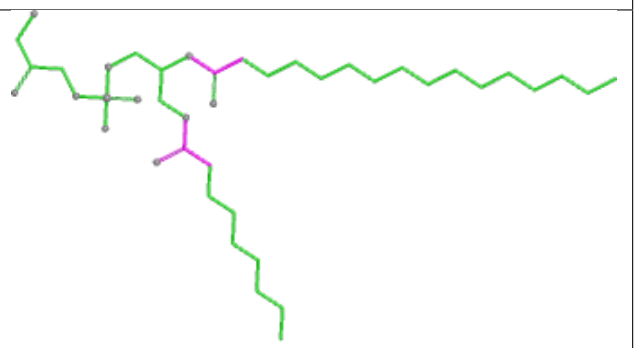

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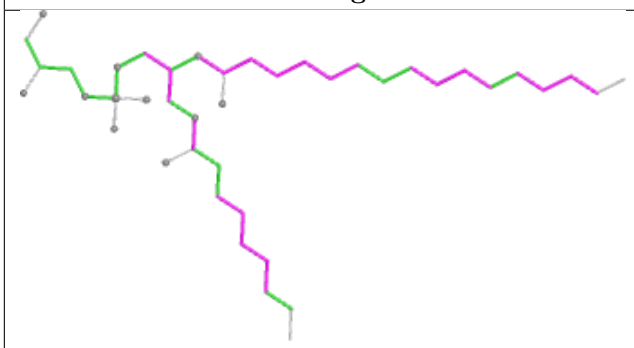

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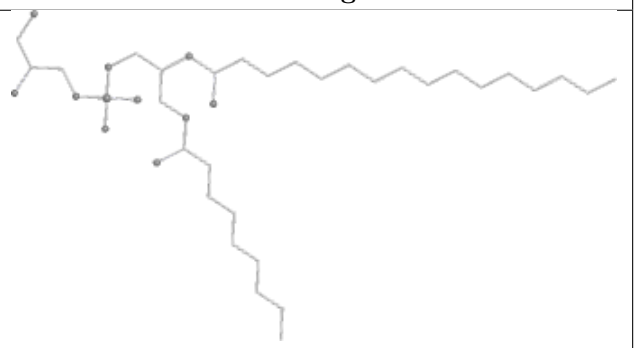
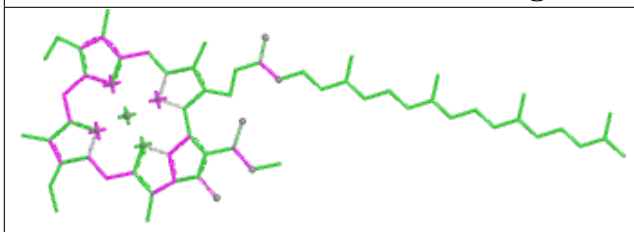


Rings

Ligand CLA b 617



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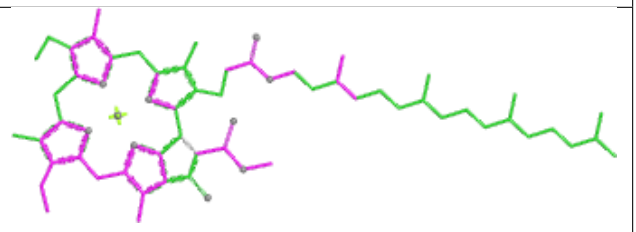

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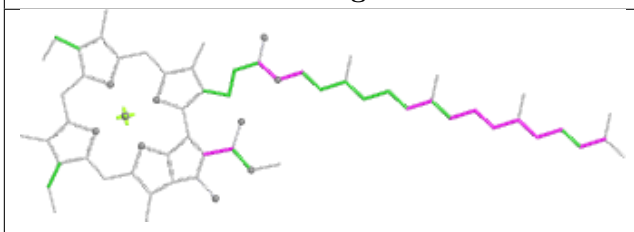

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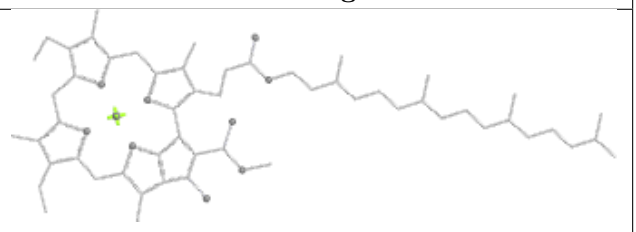
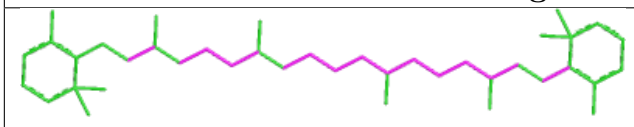


Rings

Ligand BCR t 101



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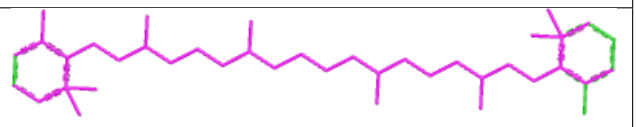

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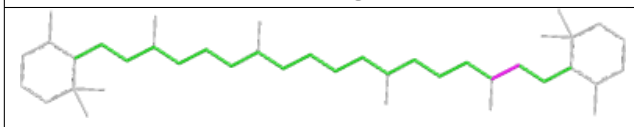

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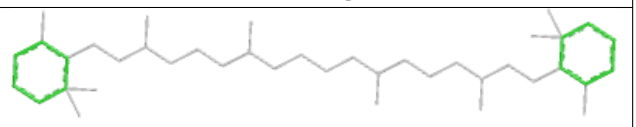
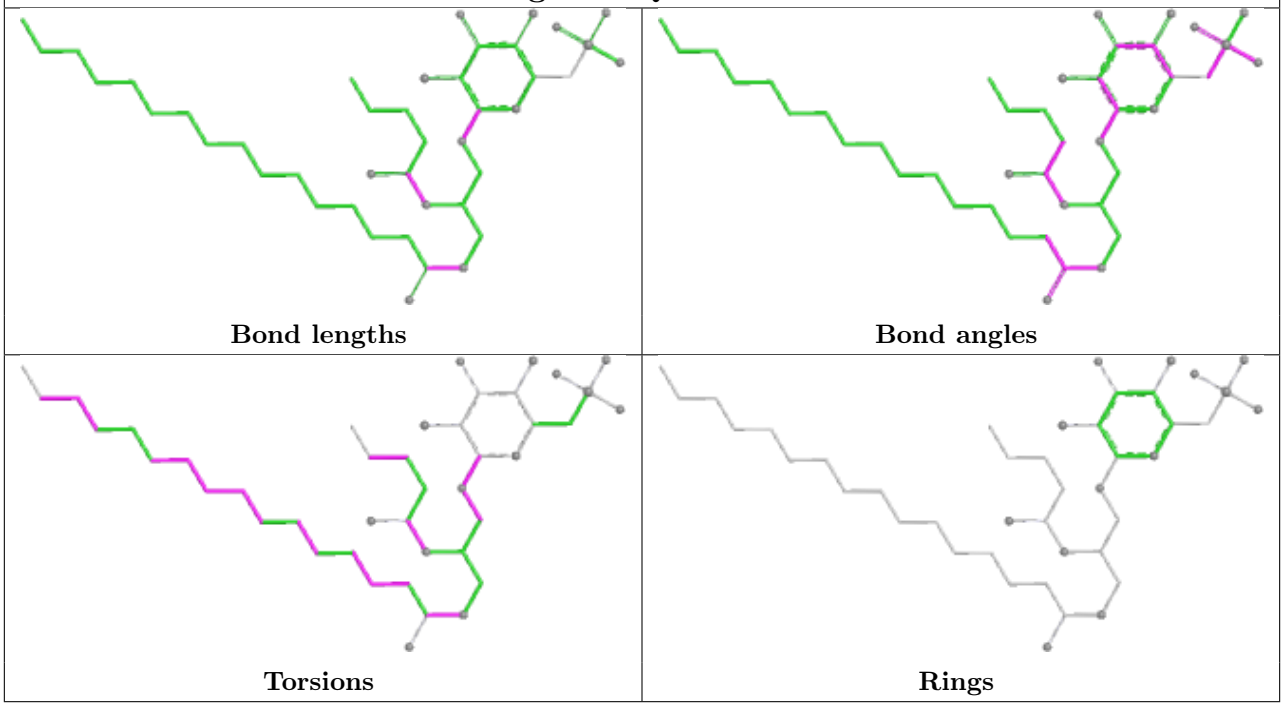


Rings

Ligand SQD d 411



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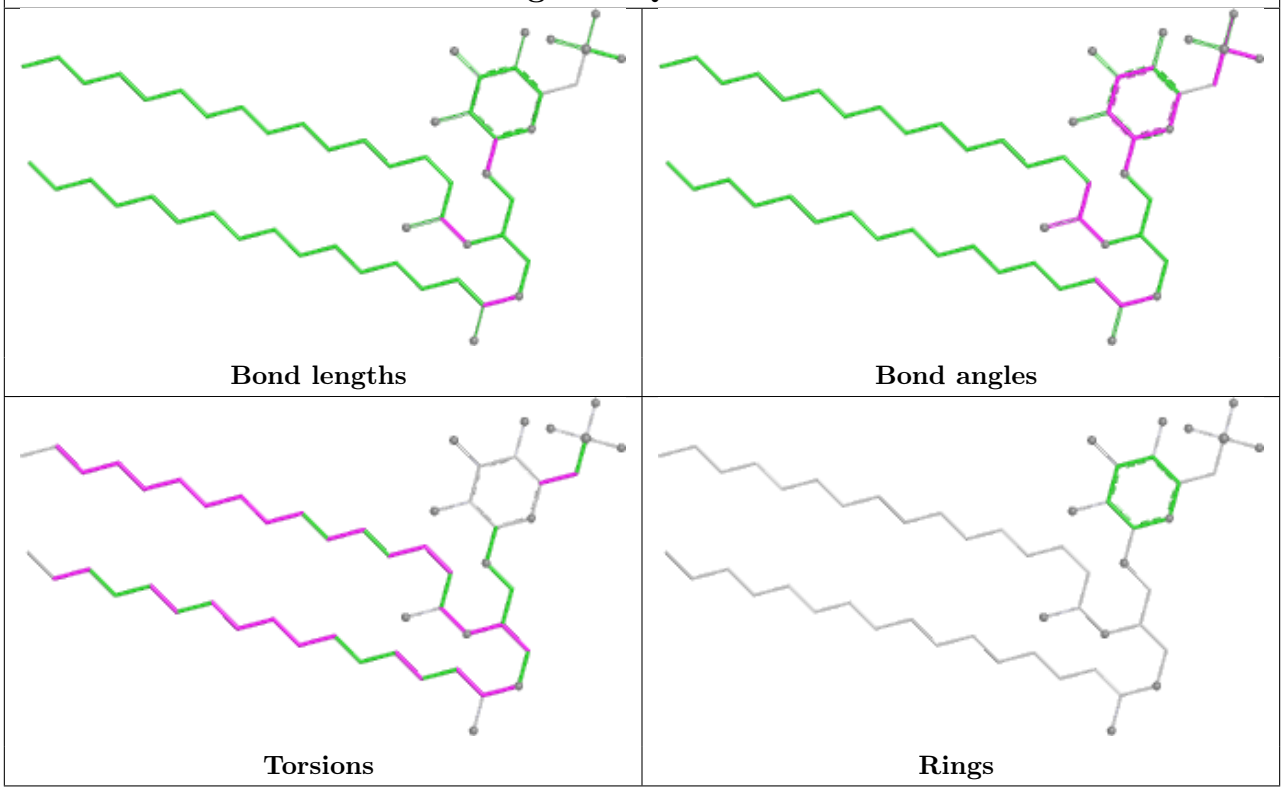

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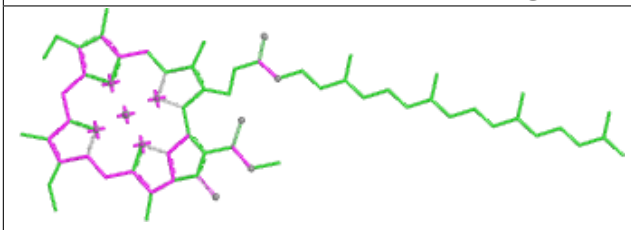

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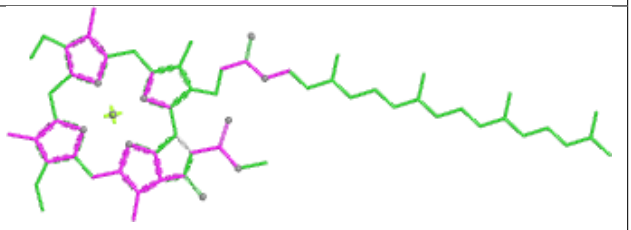
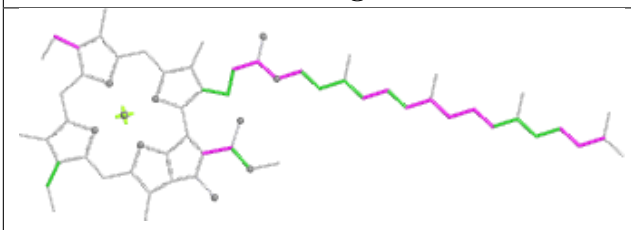


Bond angles



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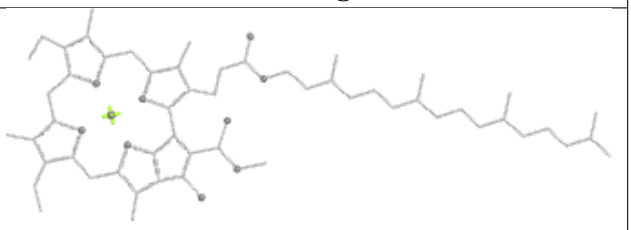
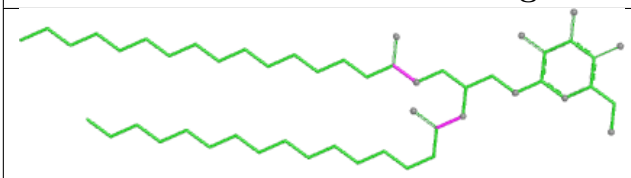


Rings

Ligand LMG C 519



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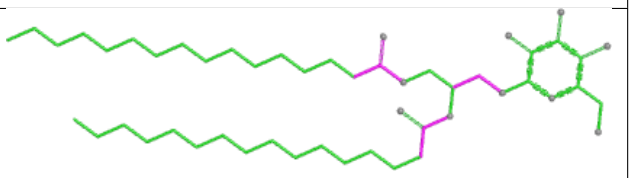

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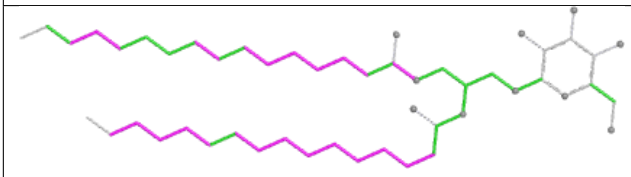

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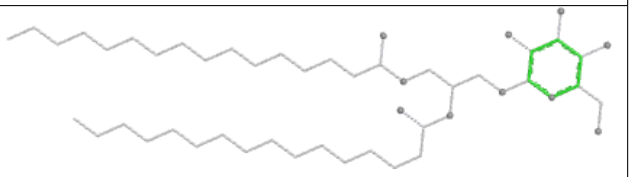
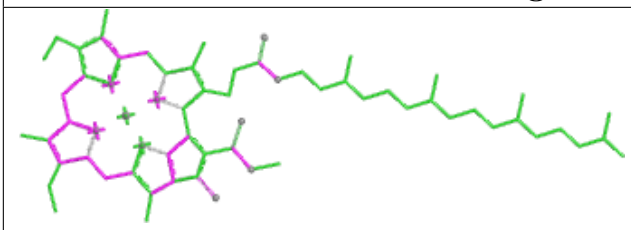


Rings

Ligand CLA d 403



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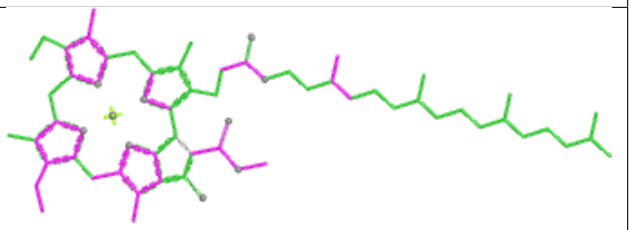

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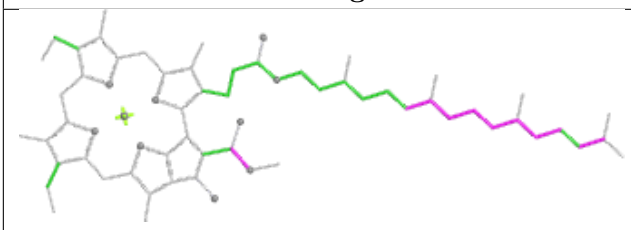

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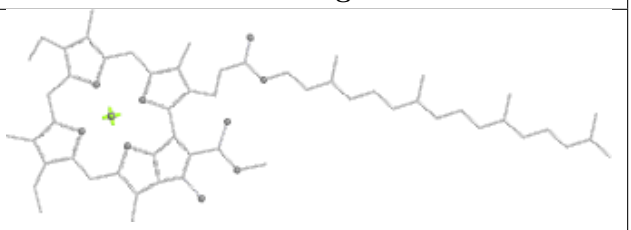
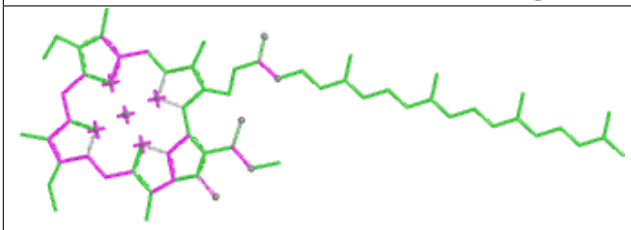


Rings

Ligand CLA c 505



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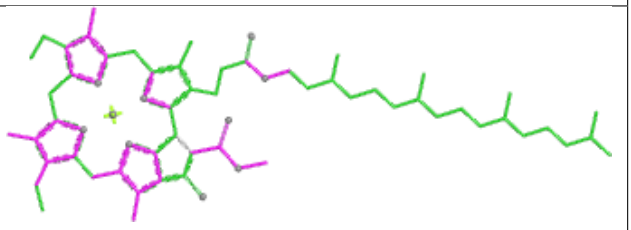
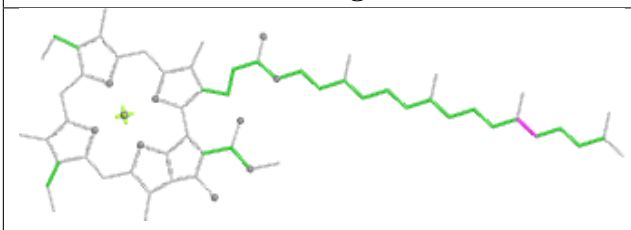


Bond angles



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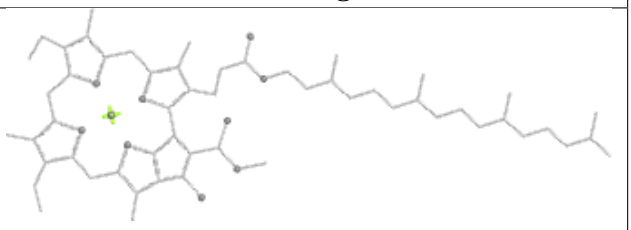
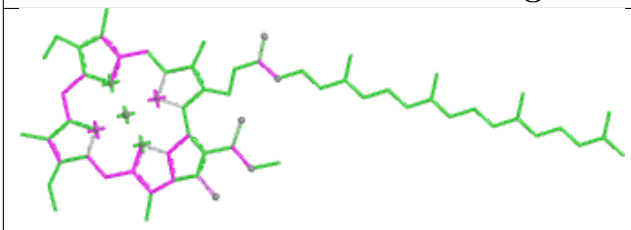


Rings

Ligand CLA B 608



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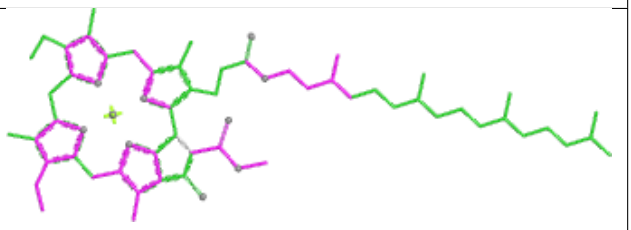
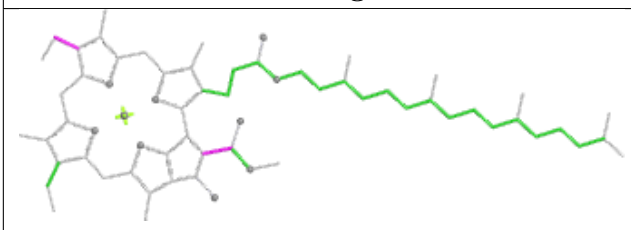
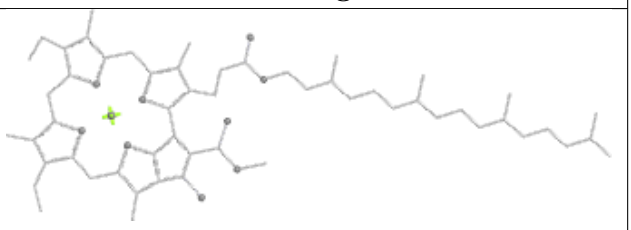


Bond angles

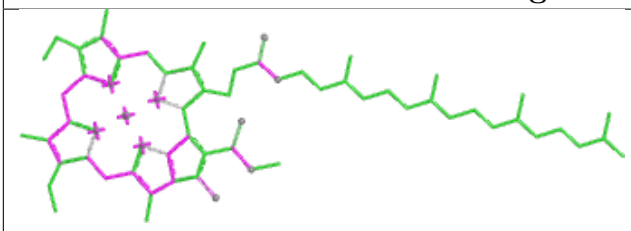


Torsions



Rings

Ligand CLA c 510



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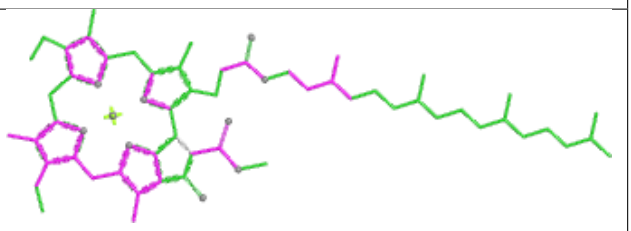
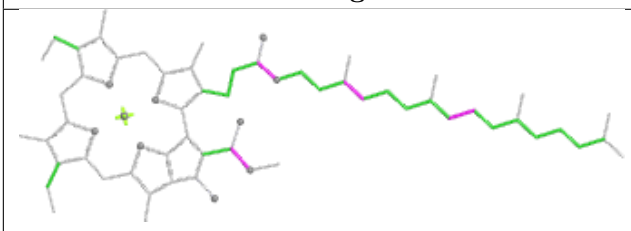


Bond angles



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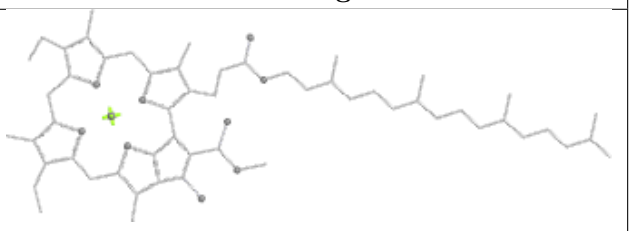
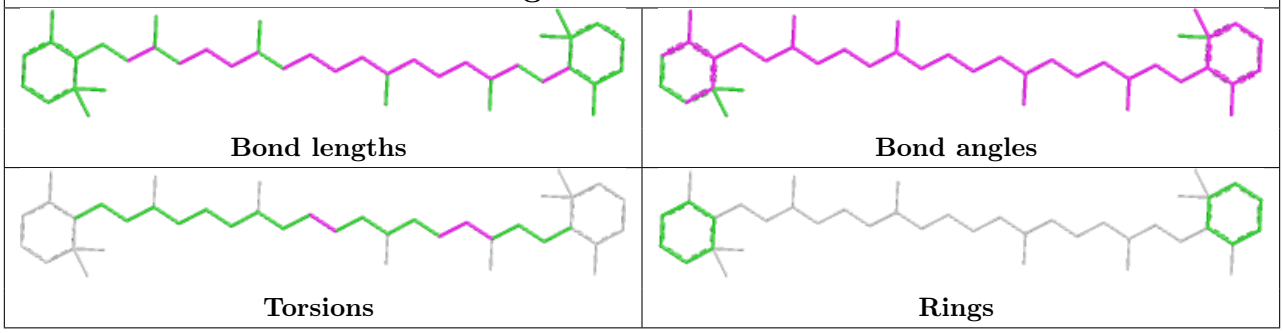
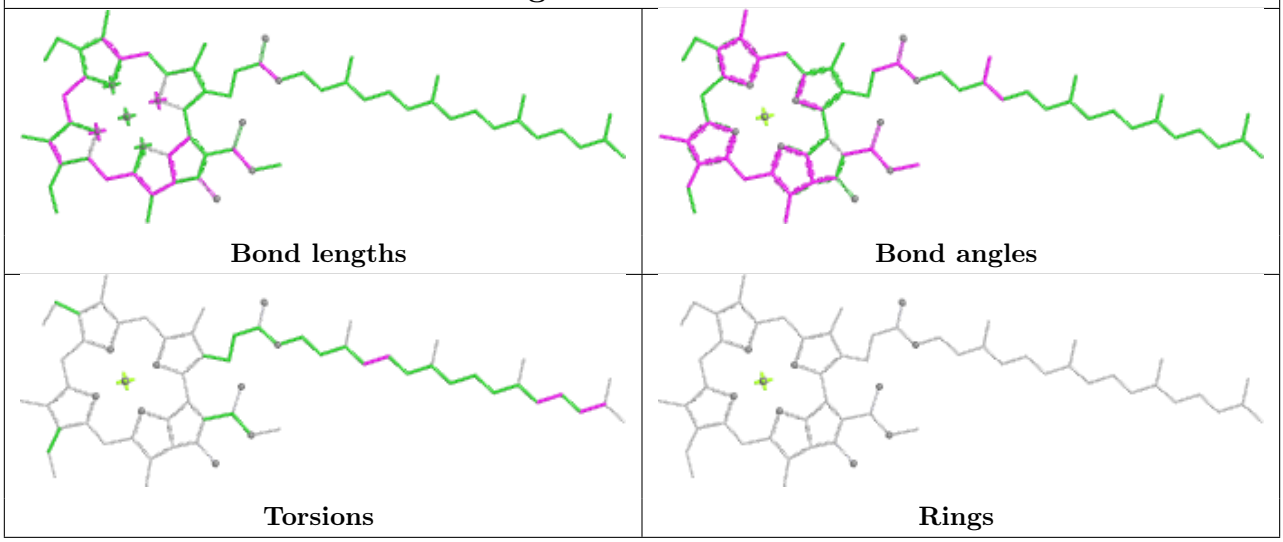


Rings

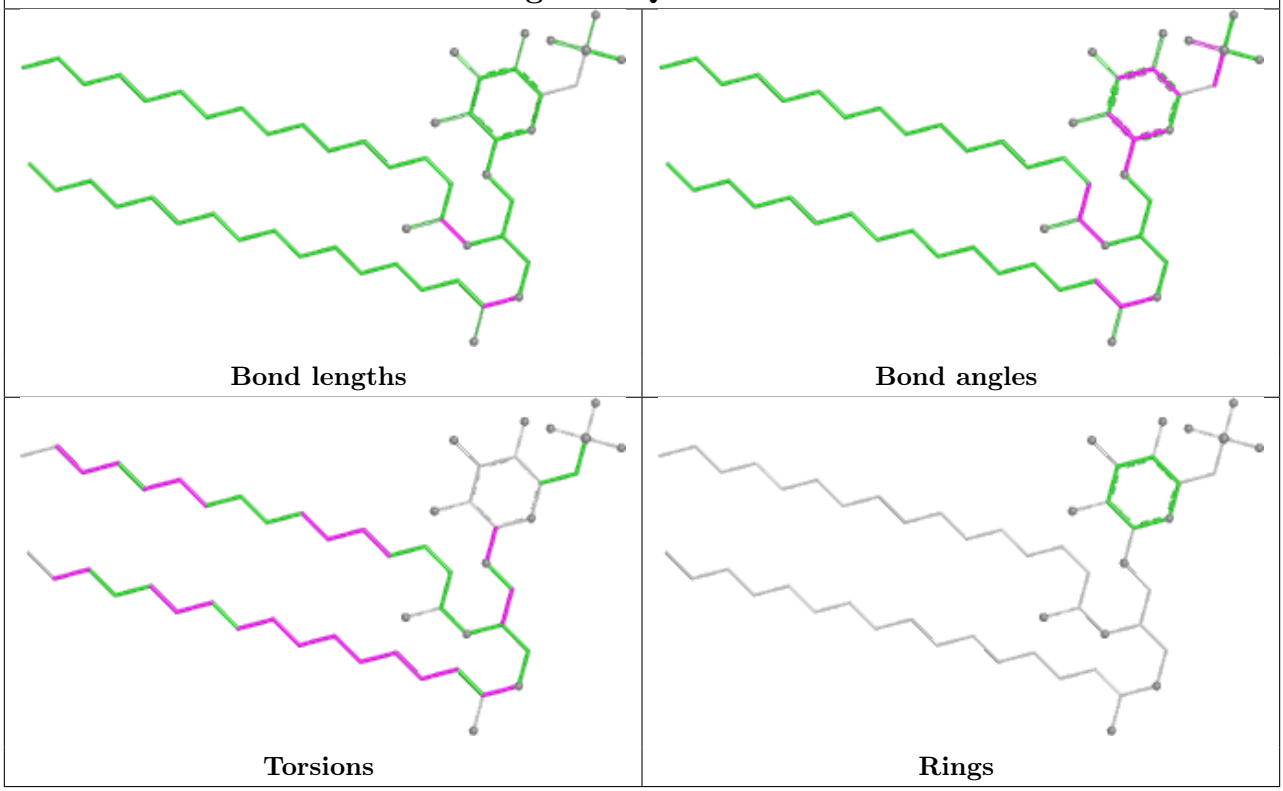
Ligand BCR B 619



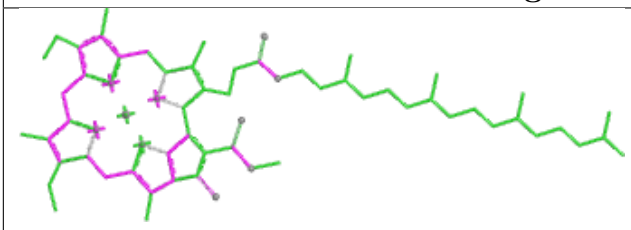
Ligand CLA b 605



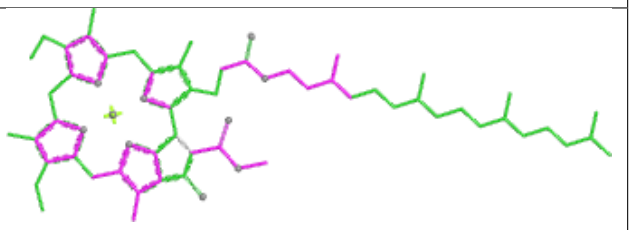
Ligand SQD B 601



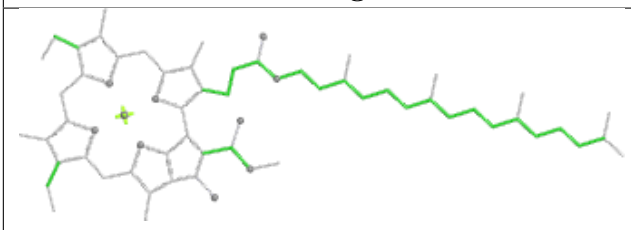
Ligand CLA B 603



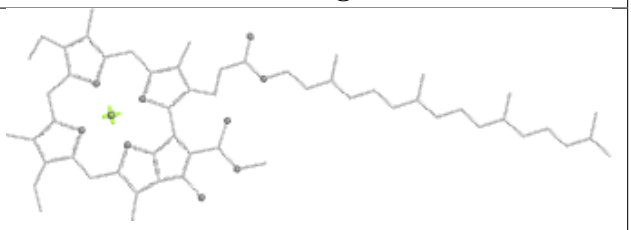
Bond lengths



Bond angles

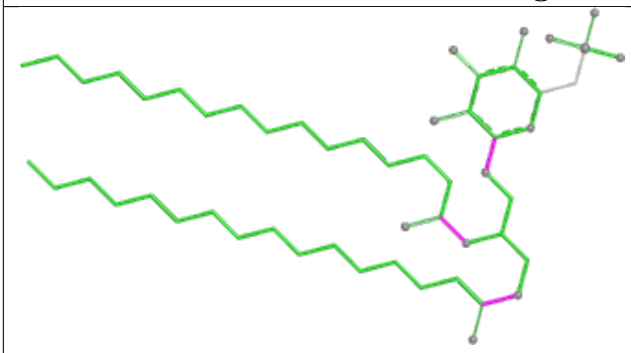


Torsions



Rings

Ligand SQD l 101



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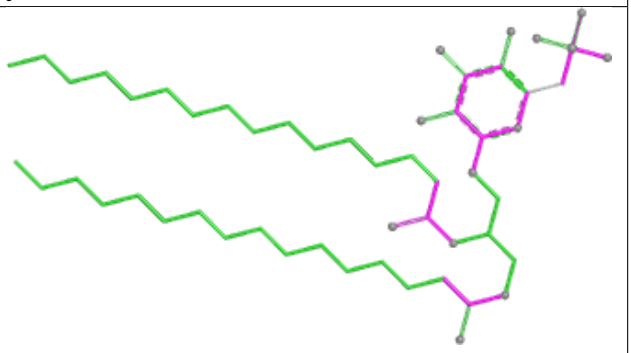
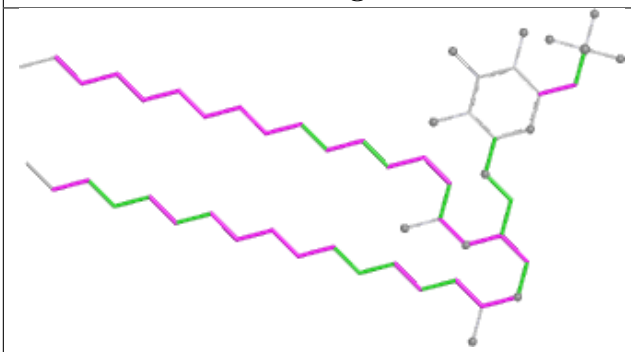
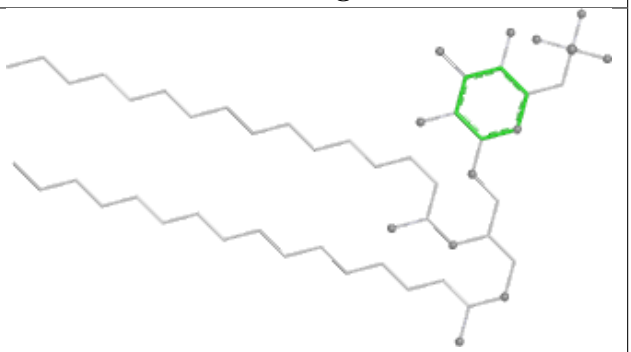


Bond angles

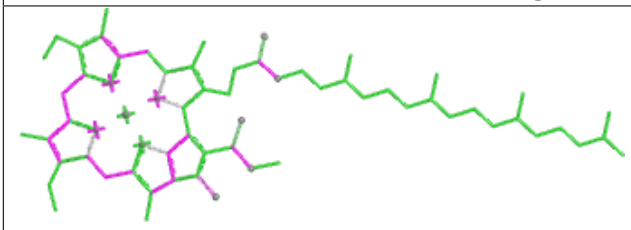


Torsions

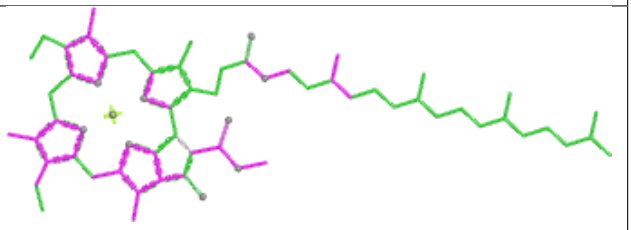


Rings

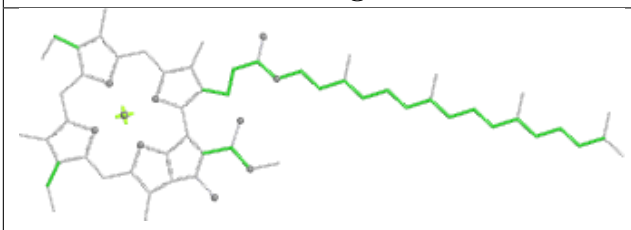
Ligand CLA c 511



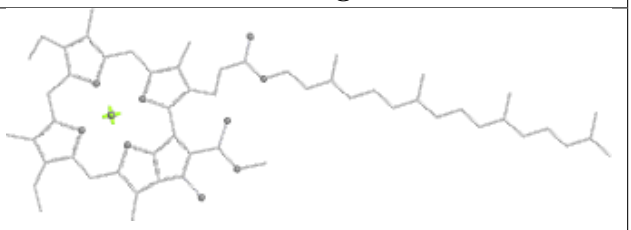
Bond lengths



Bond angles

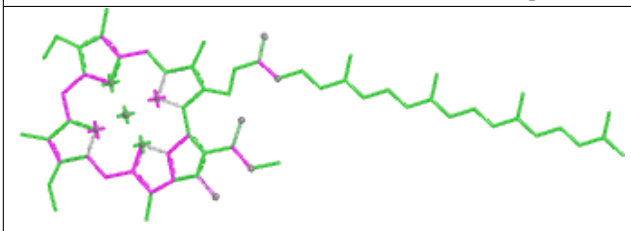


Torsions

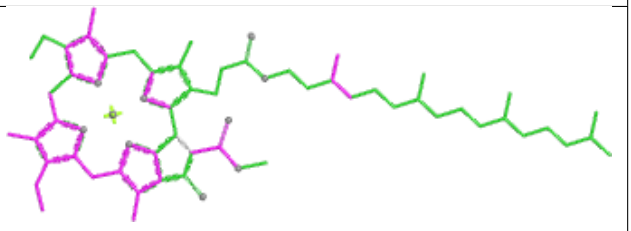


Rings

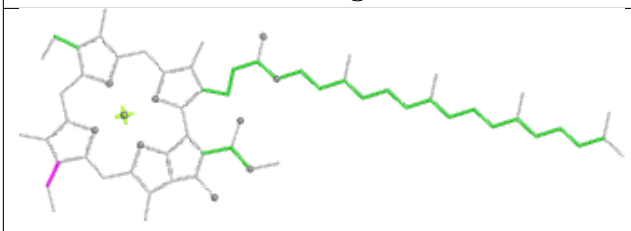
Ligand CLA D 402



Bond lengths



Bond angles



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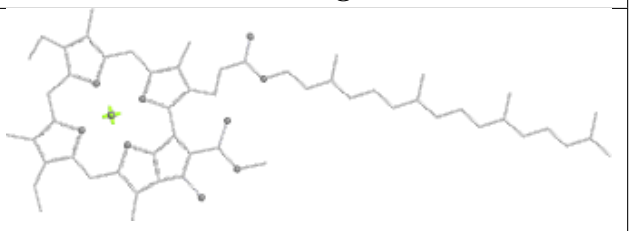
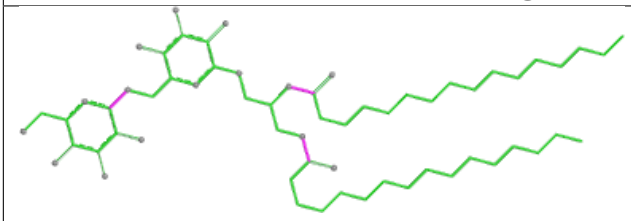


Rings

Ligand DGD H 102



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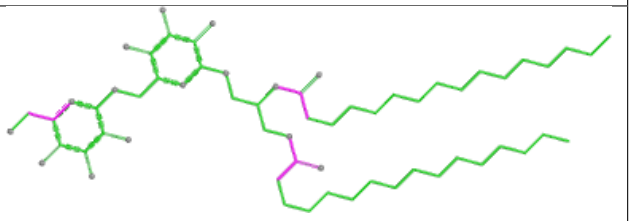
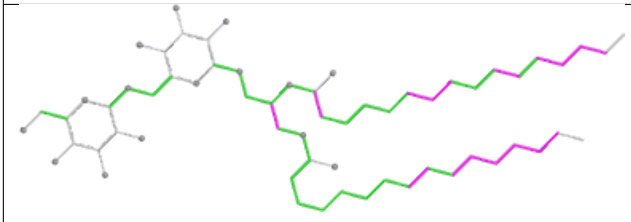
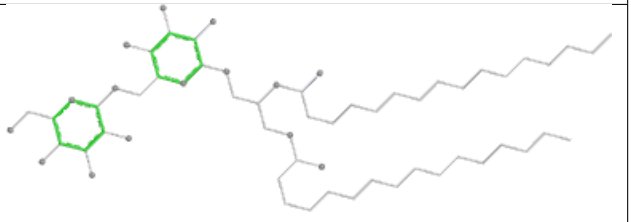


Bond angles

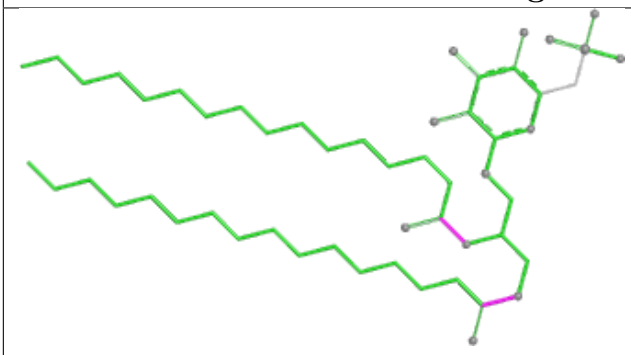


Torsions



Rings

Ligand SQD b 601



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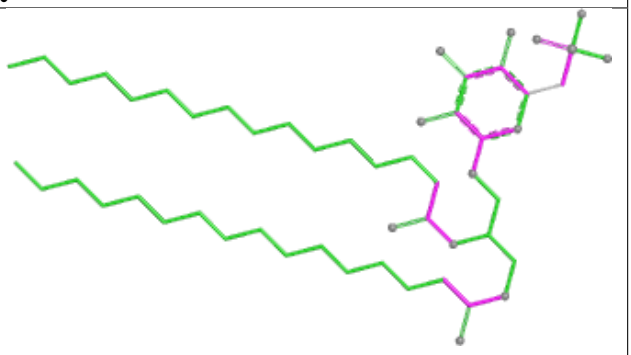
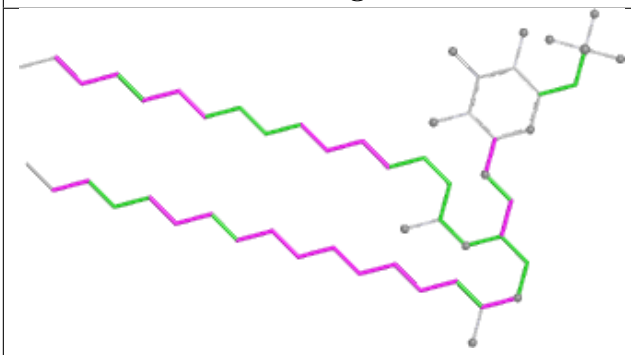


Bond angles



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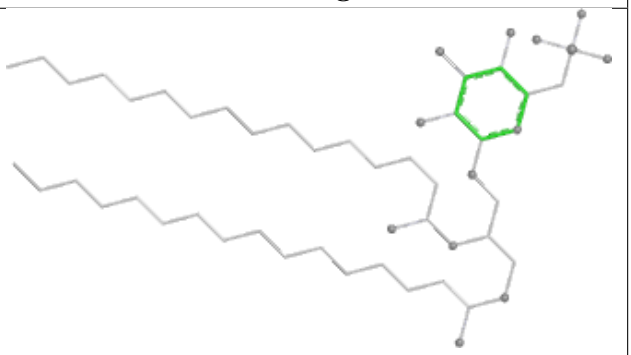
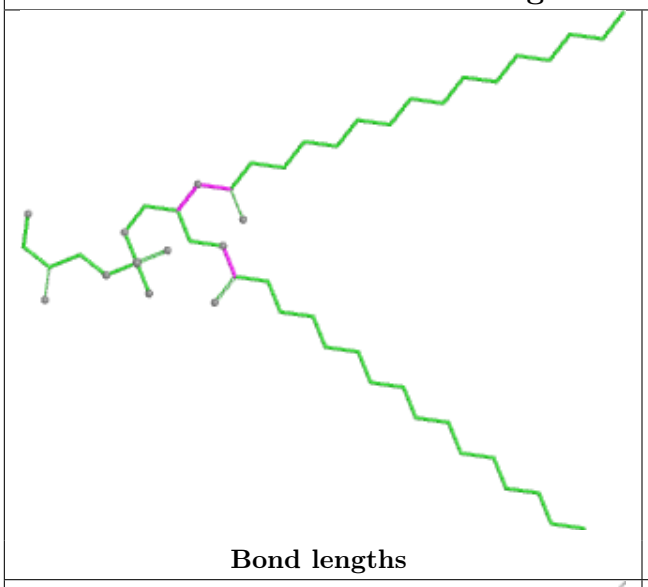
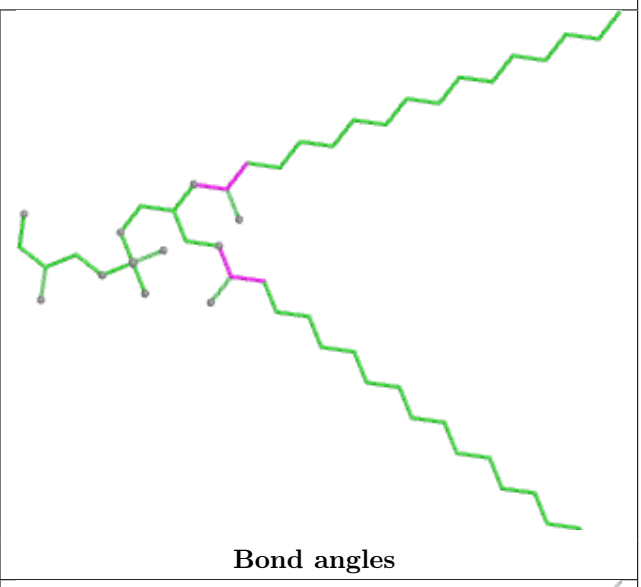


Rings

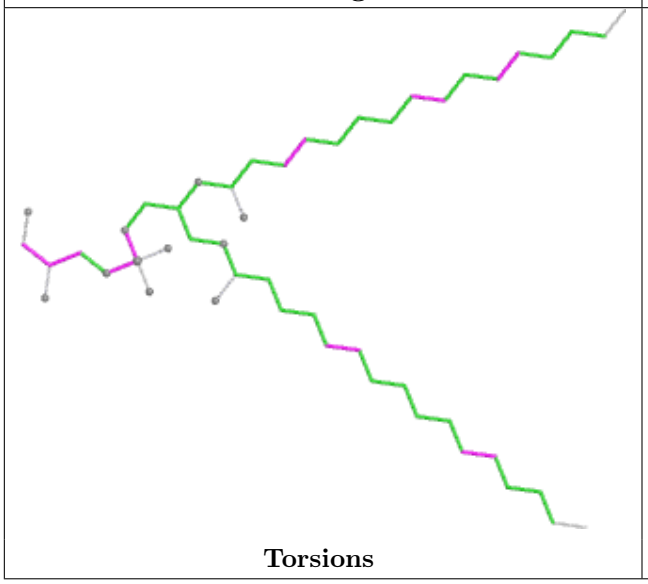
Ligand LHG d 407



Bond lengths



Bond angles



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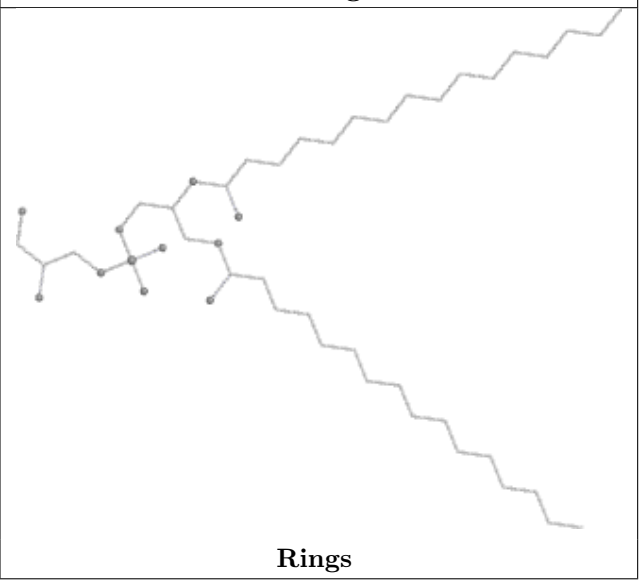
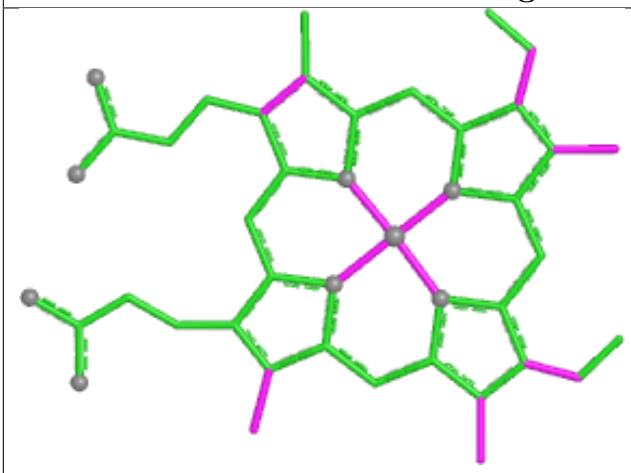


Rings

Ligand HEM V 201



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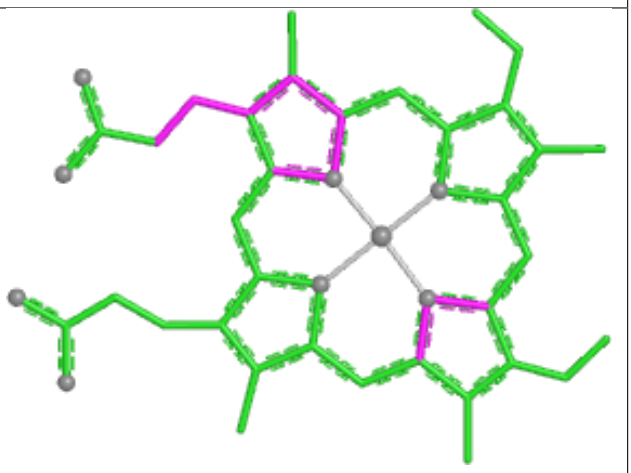
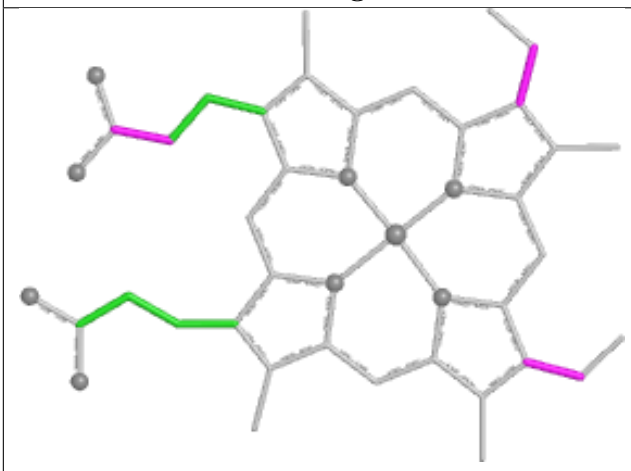
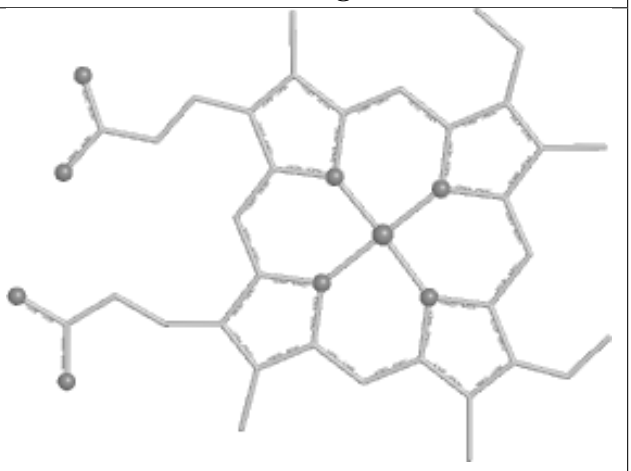


Bond angles

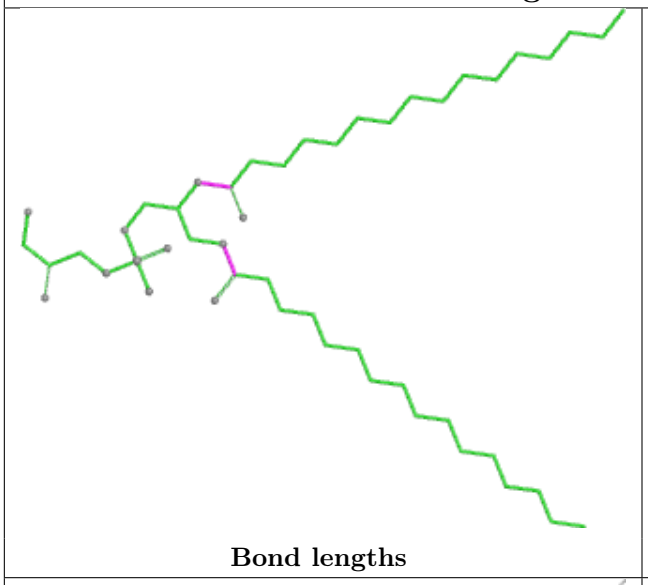


Torsions



Rings

Ligand LHG D 405



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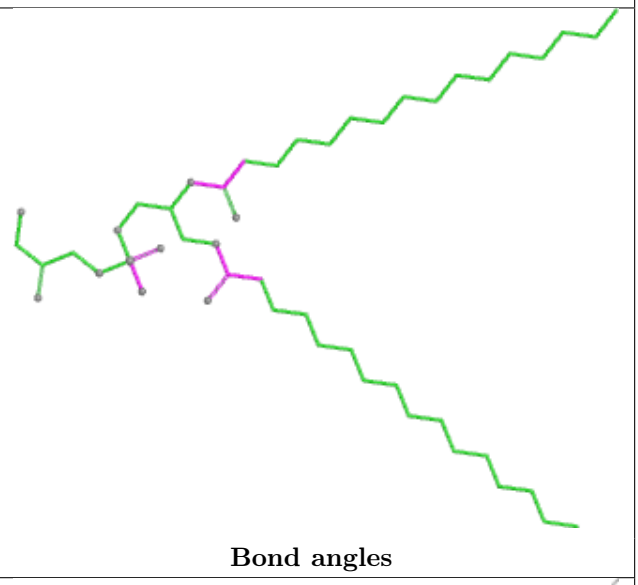
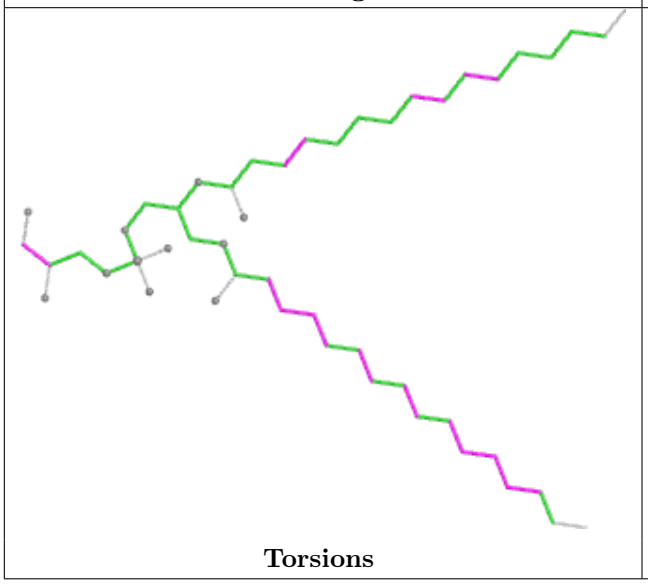
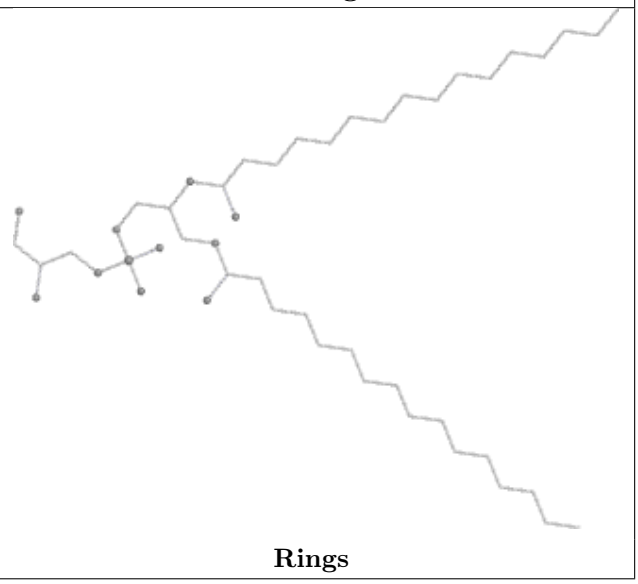


Bond angles

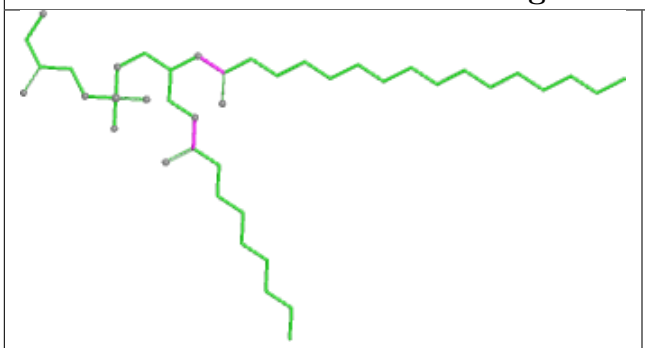


Torsions



Rings

Ligand LHG e 101



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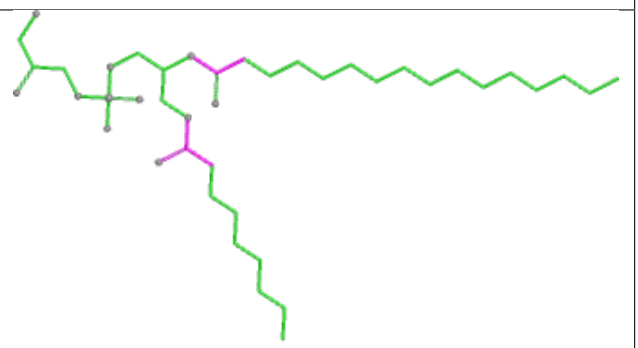
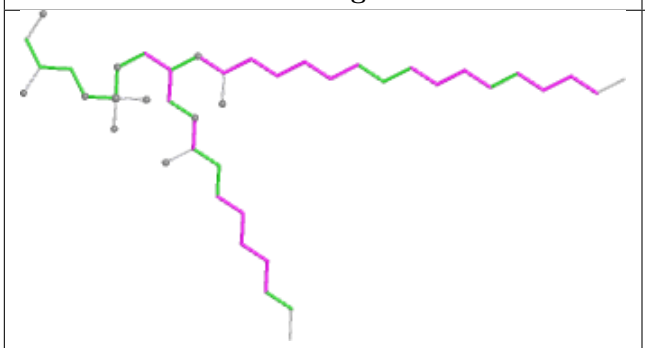


Bond angles



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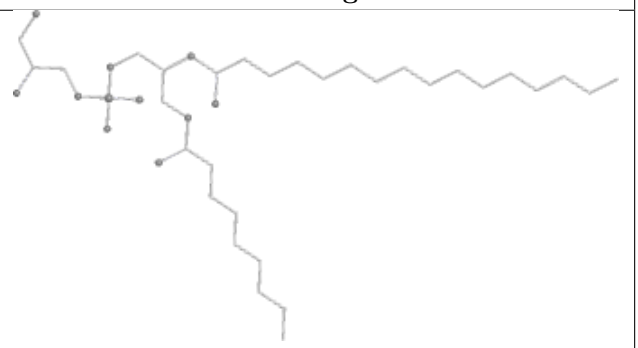
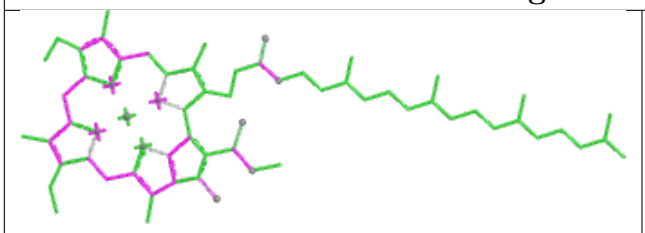


Rings

Ligand CLA b 603



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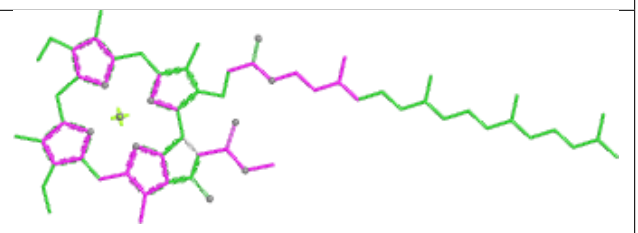
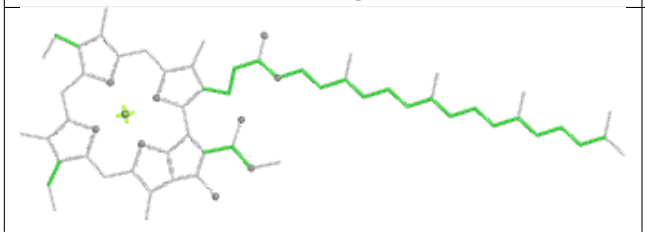


Bond angles



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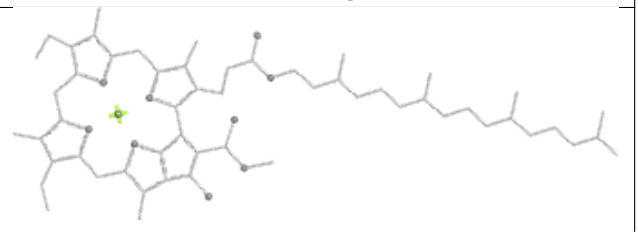
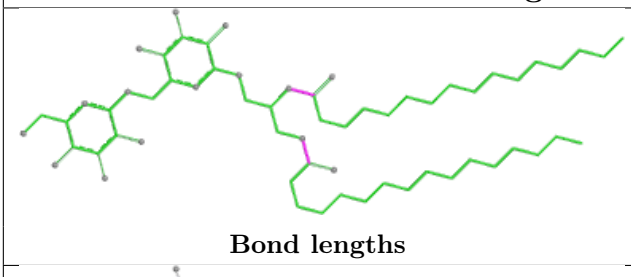


Rings

Ligand DGD c 517



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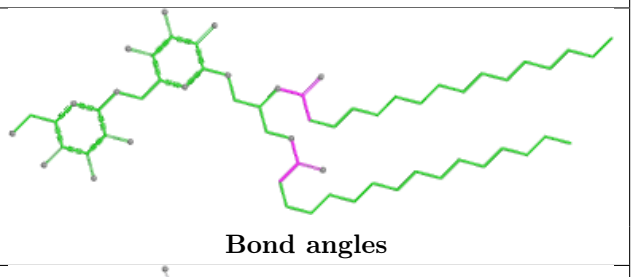
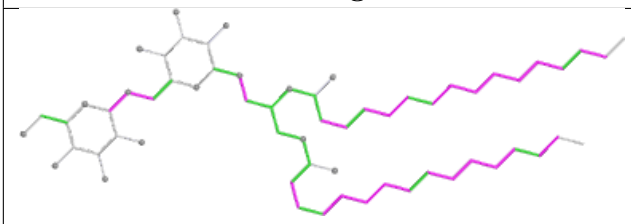


Bond angles



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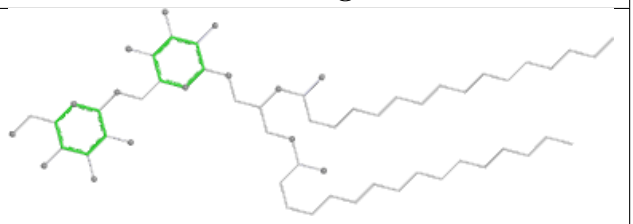
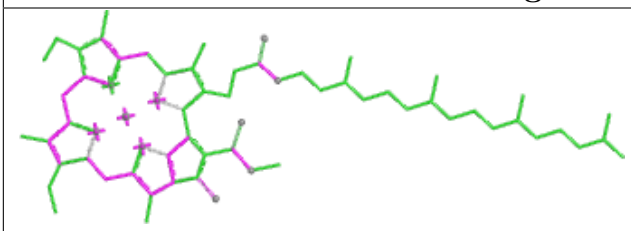


Rings

Ligand CLA C 506



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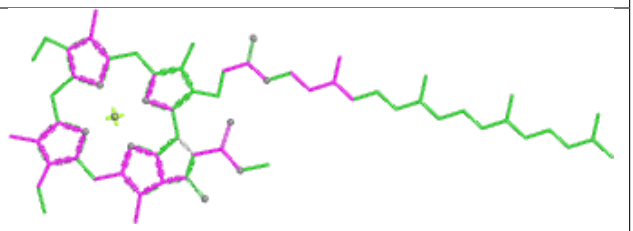
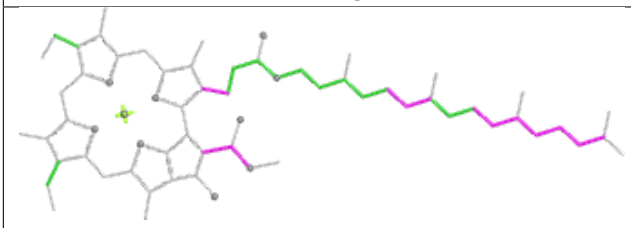


Bond angles



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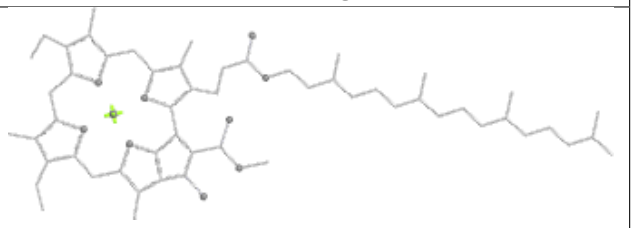
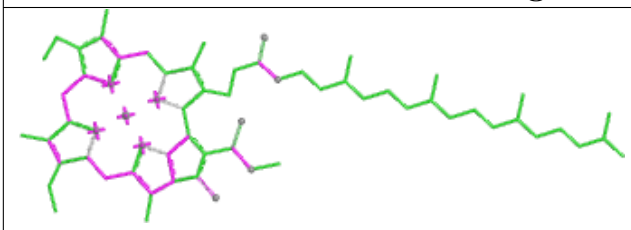
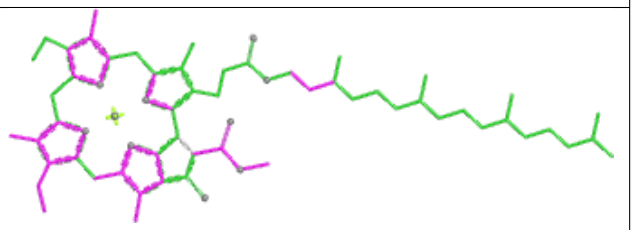


Rings

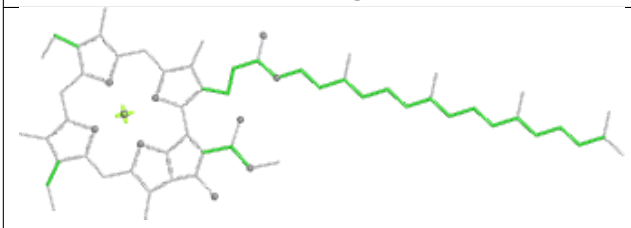
Ligand CLA b 610



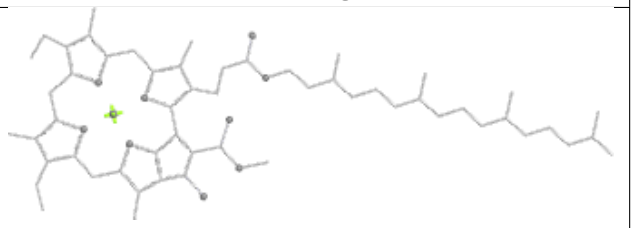
Bond lengths



Bond angles

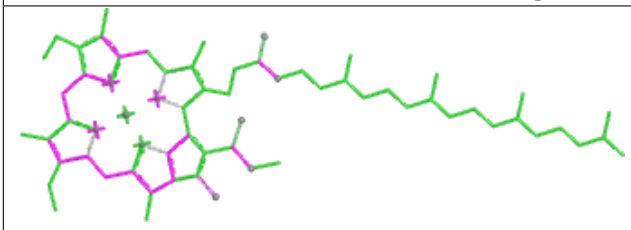


Torsions



Rings

Ligand CLA c 509



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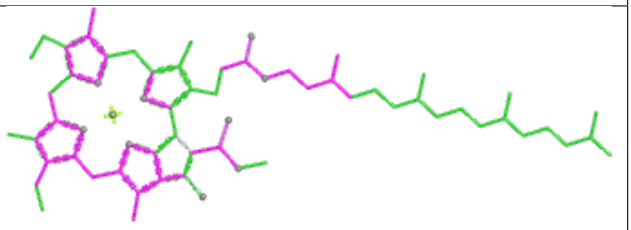

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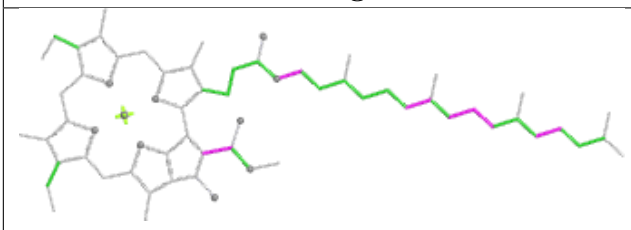

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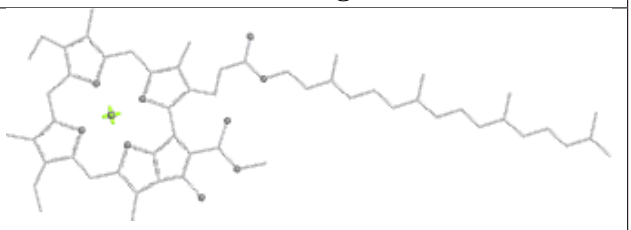
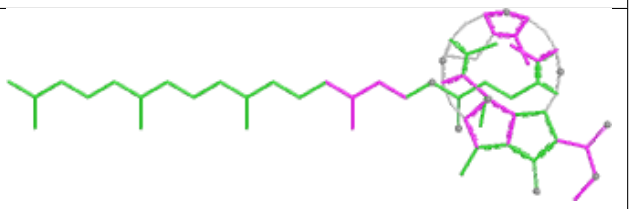


Rings

Ligand PHO A 606

Bond lengths



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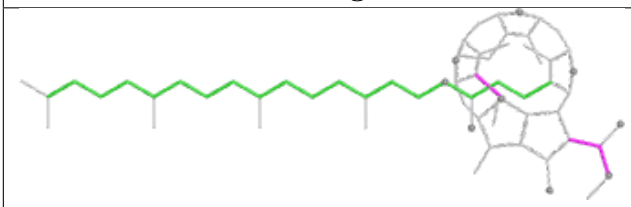

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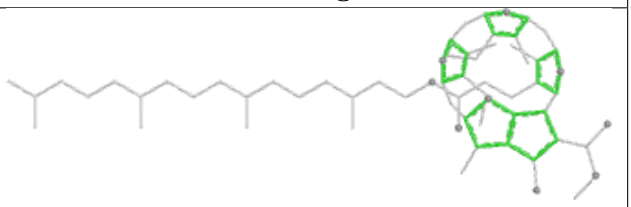
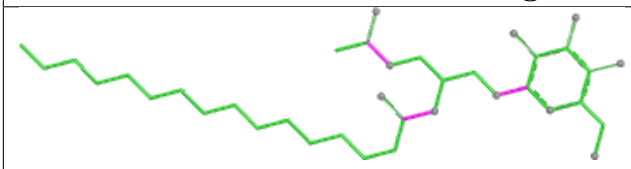


Rings

Ligand LMG Z 101



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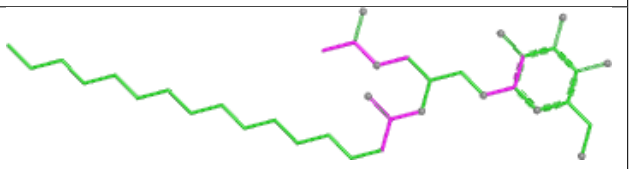

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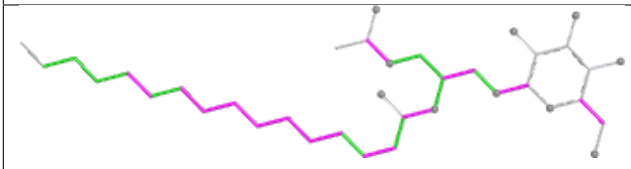

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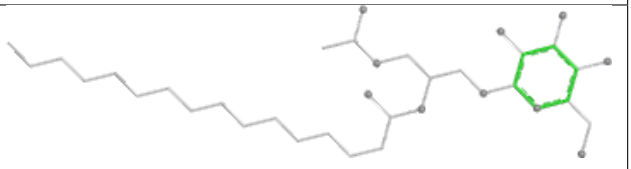

Rings

Ligand BCR k 102

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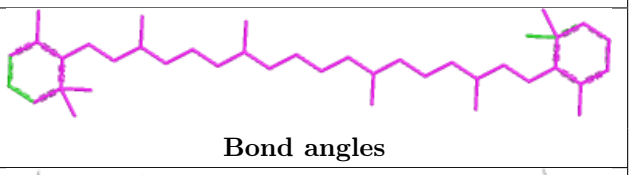
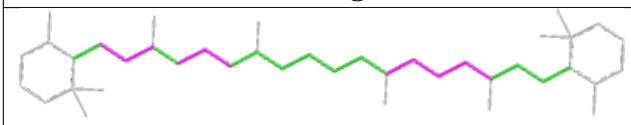


Bond angles



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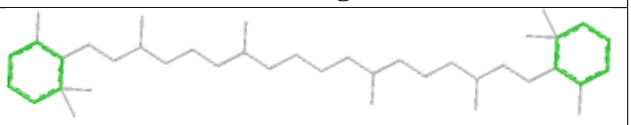
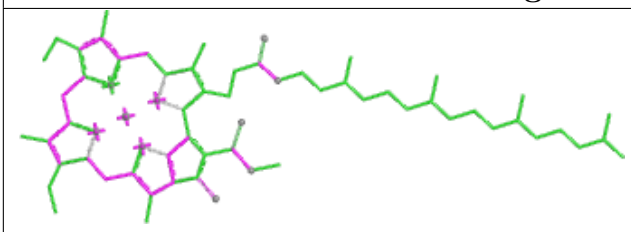


Rings

Ligand CLA C 513



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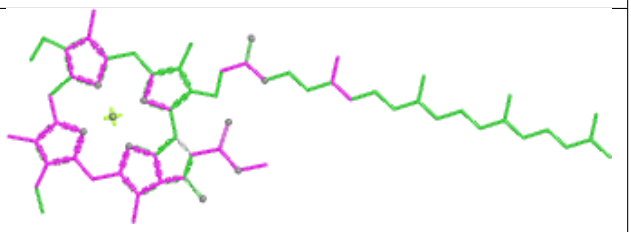

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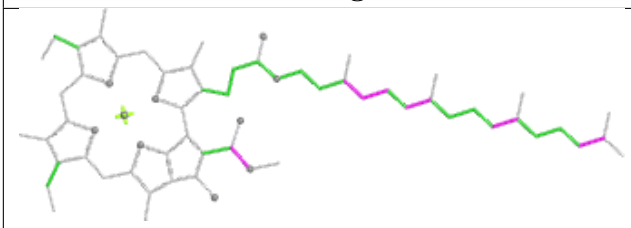

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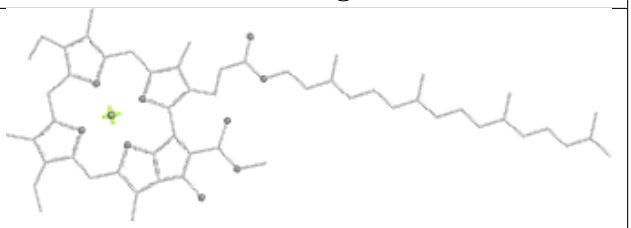
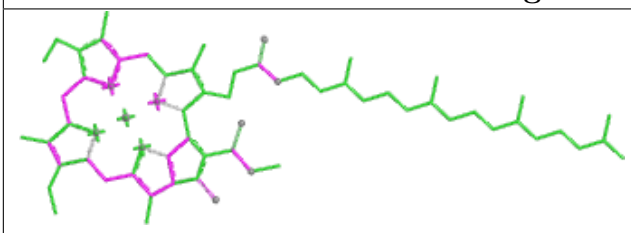


Rings

Ligand CLA A 604



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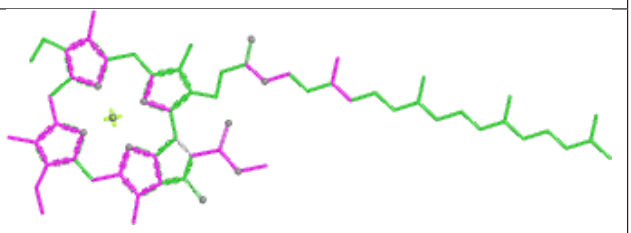

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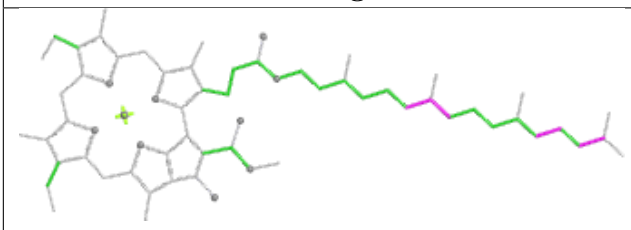

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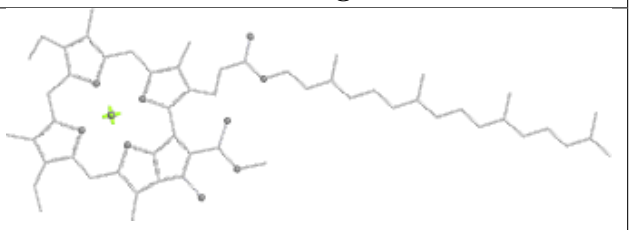
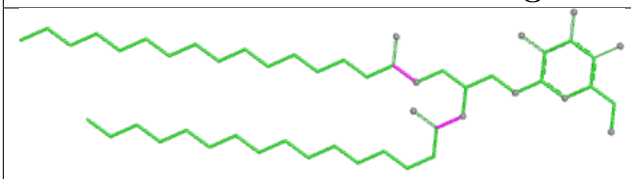


Rings

Ligand LMG a 614



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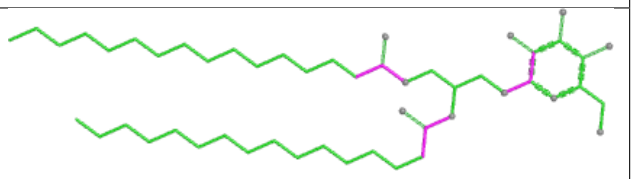
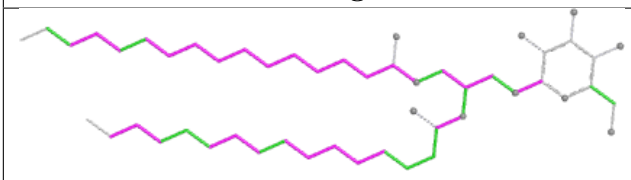


Bond angles



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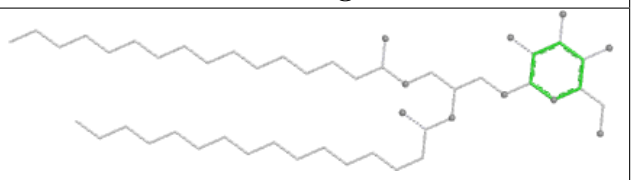
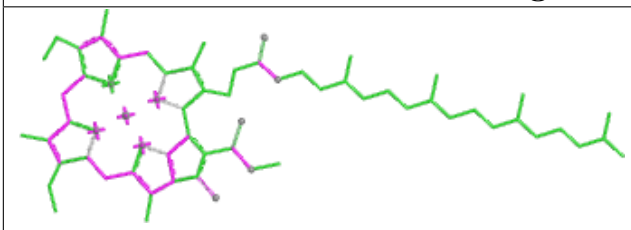


Rings

Ligand CLA c 513



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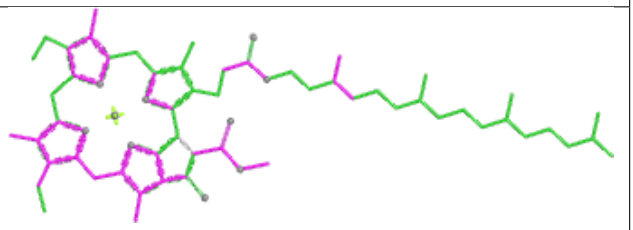

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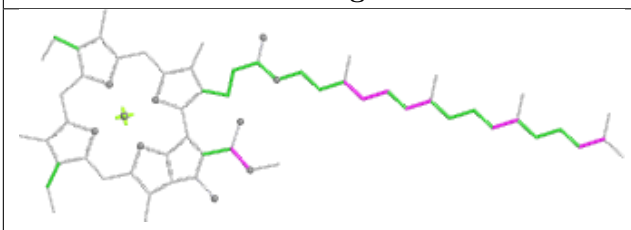

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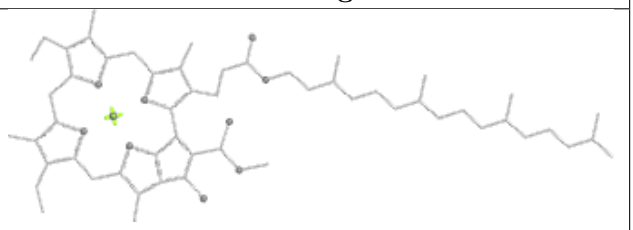

Rings

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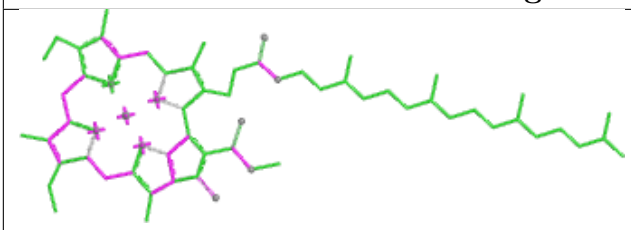

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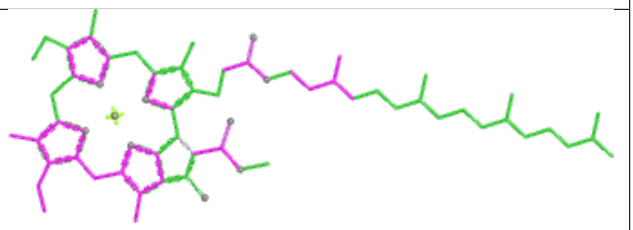

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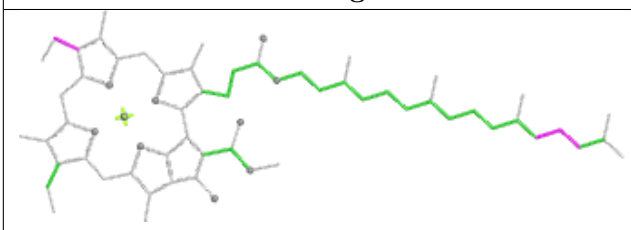

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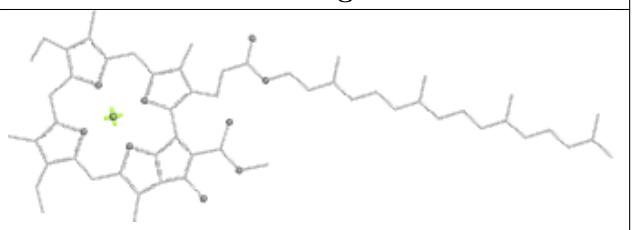
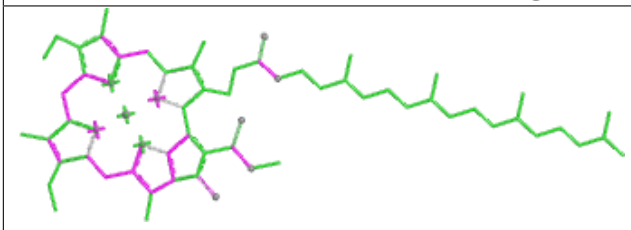


Rings

Ligand CLA d 402



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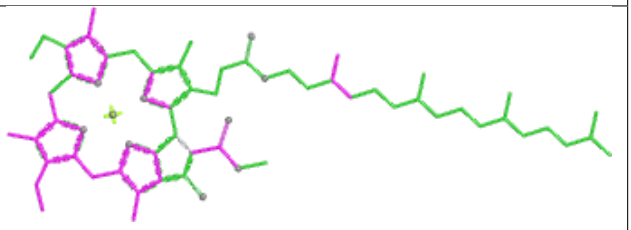
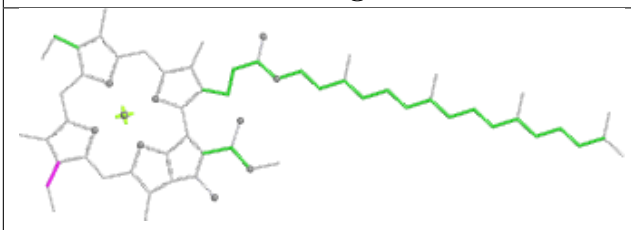


Bond angles



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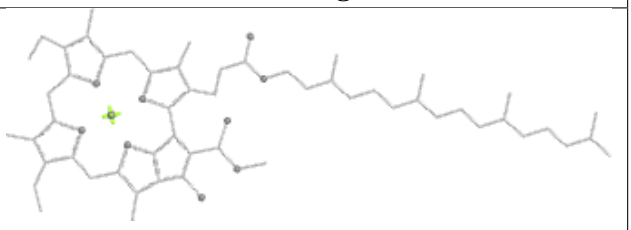
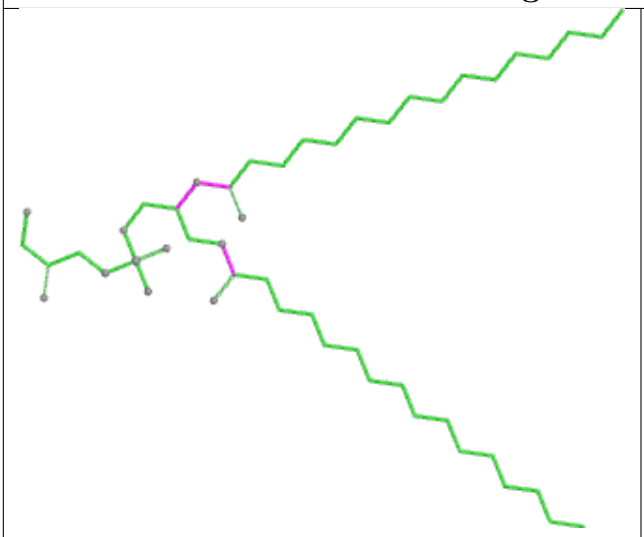


Rings

Ligand LHG D 407



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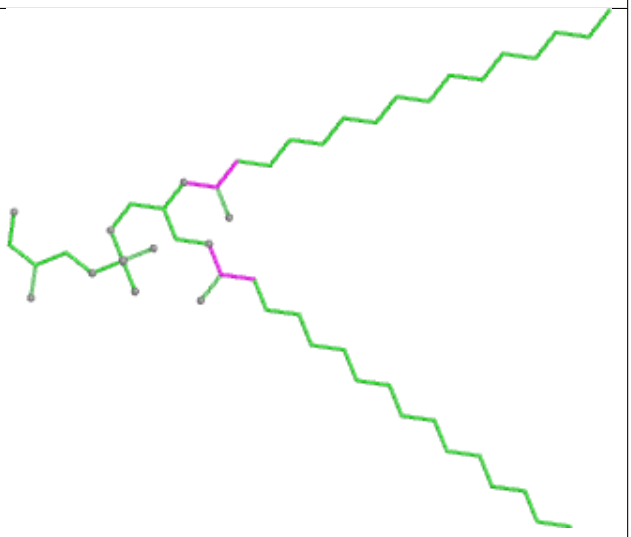
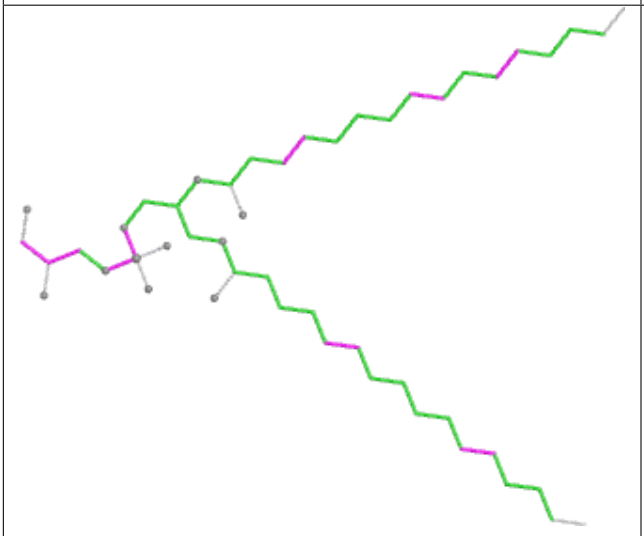


Bond angles



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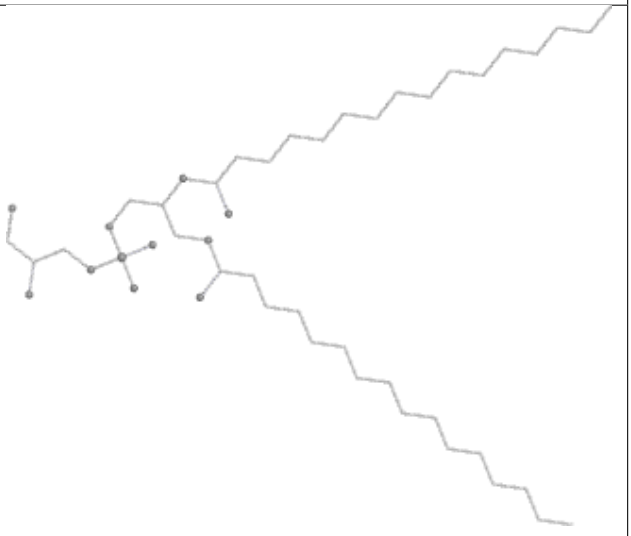
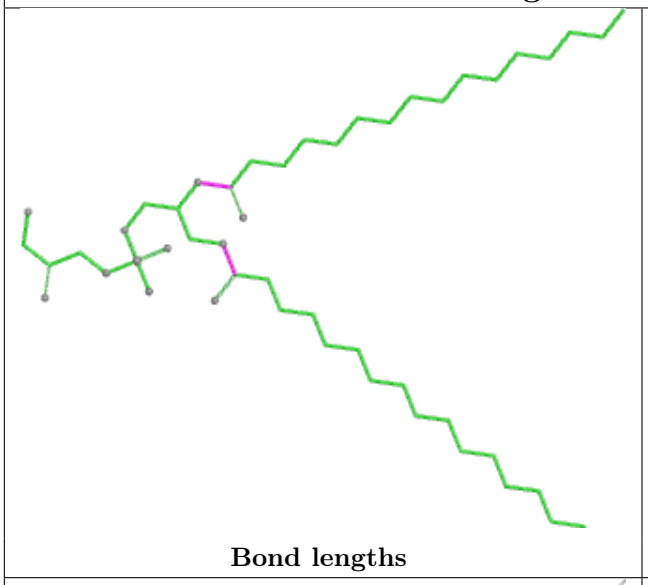


Rings

Ligand LHG D 409



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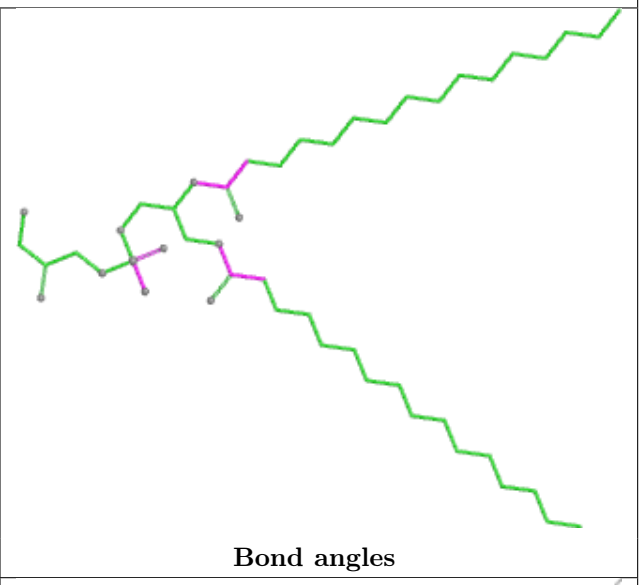
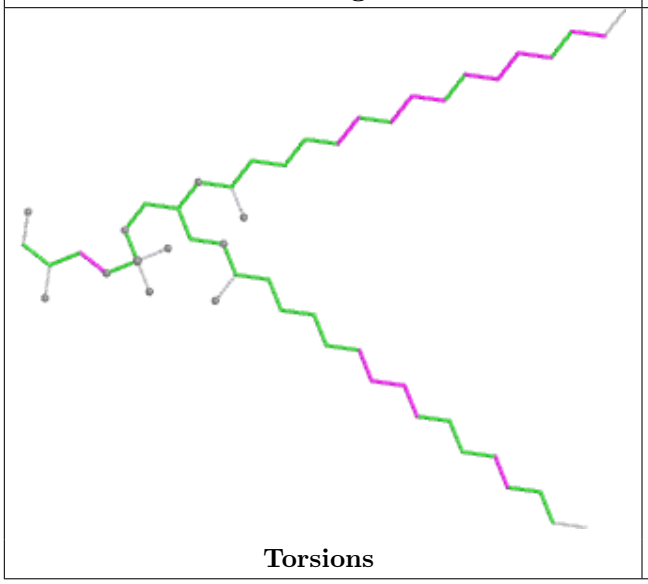
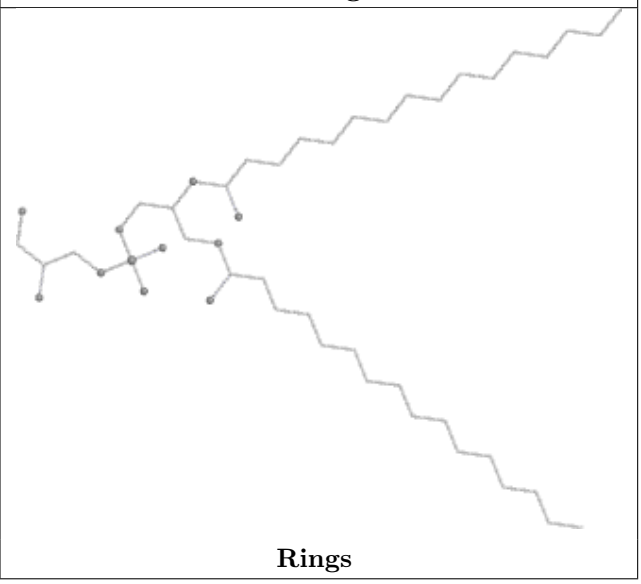


Bond angles

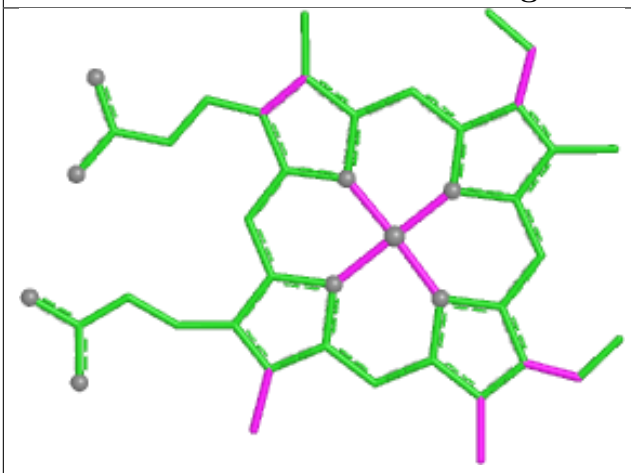


Torsions



Rings

Ligand HEM F 101



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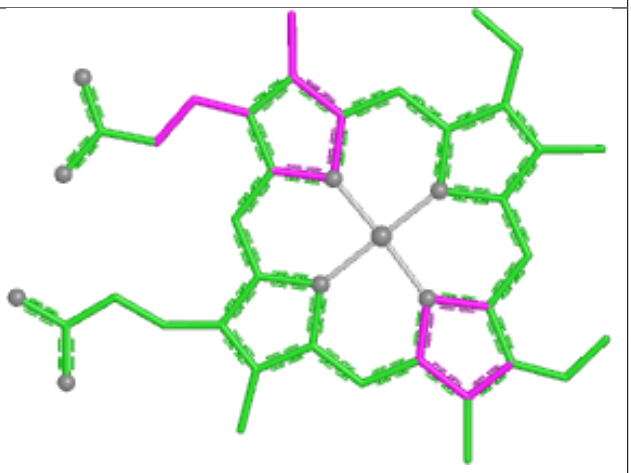
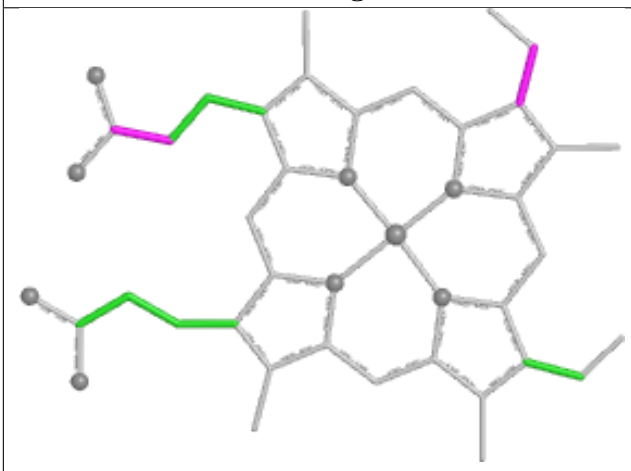


Bond angles



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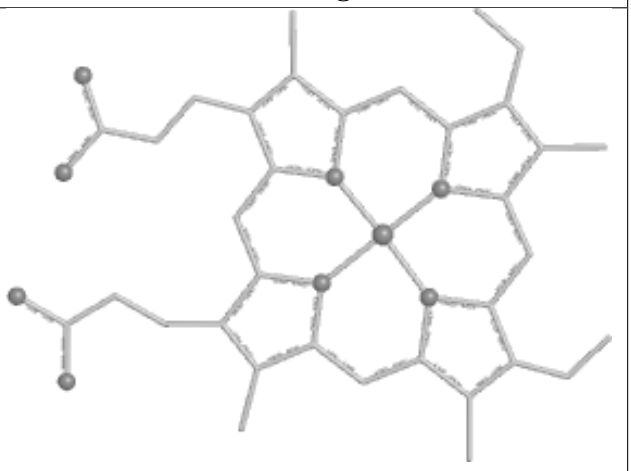
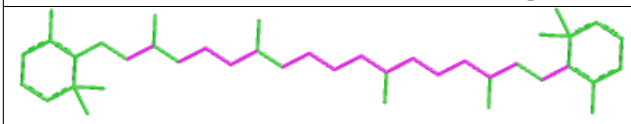
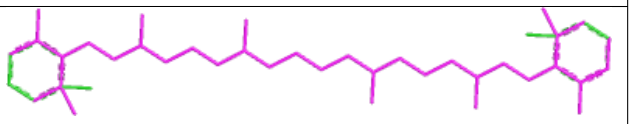


Rings

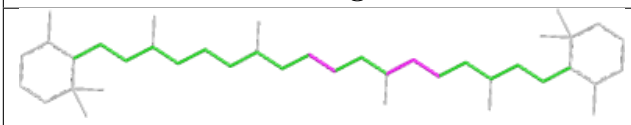
Ligand BCR A 608



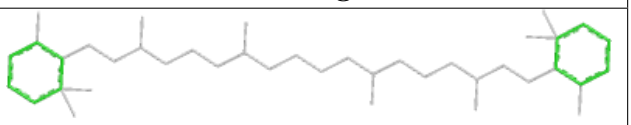
Bond lengths



Bond angles

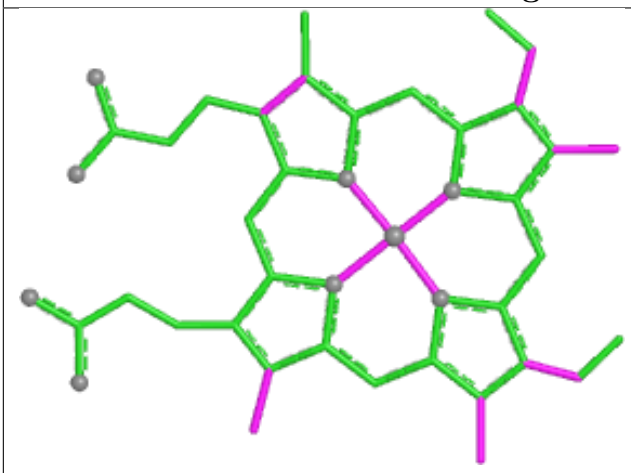


Torsions



Rings

Ligand HEM v 201



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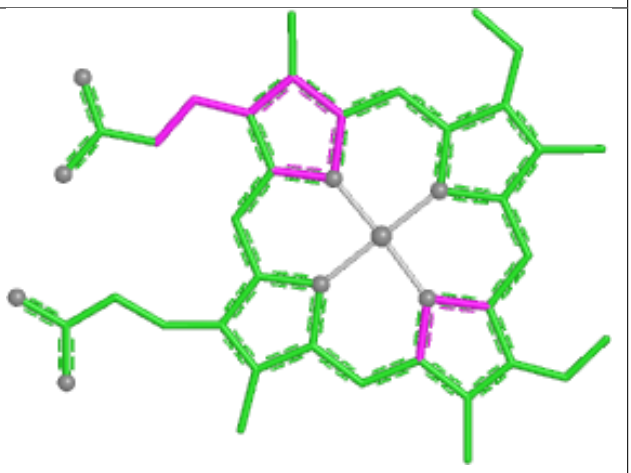

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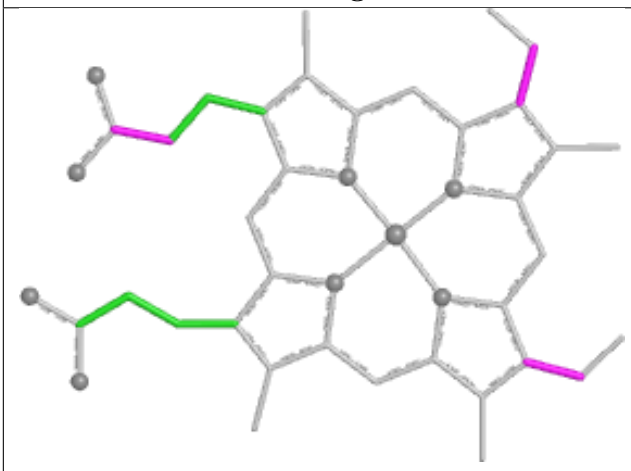

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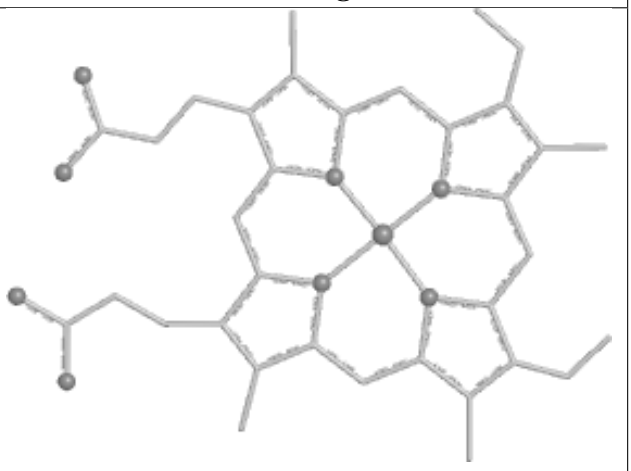
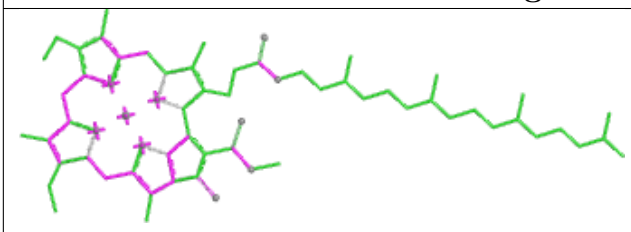


Rings

Ligand CLA C 510



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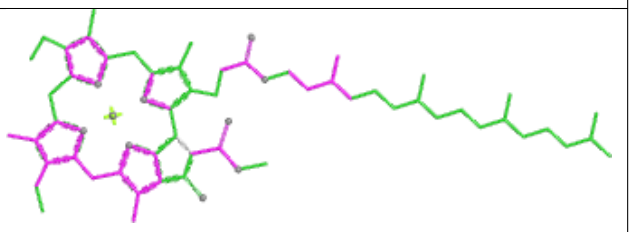

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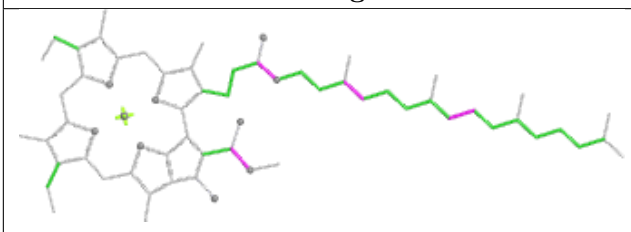

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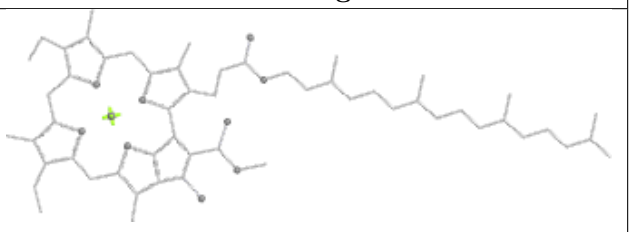

Rings

Ligand BCR C 514

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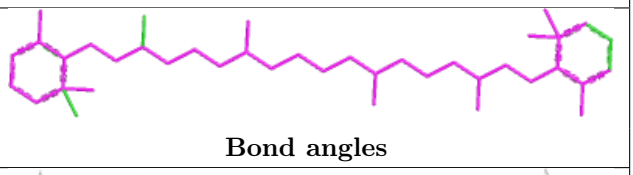
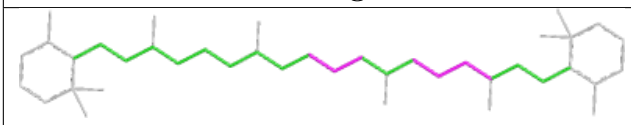


Bond angles



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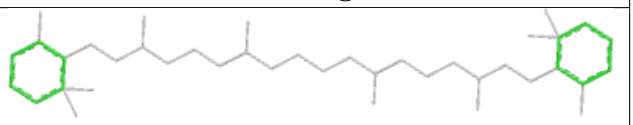
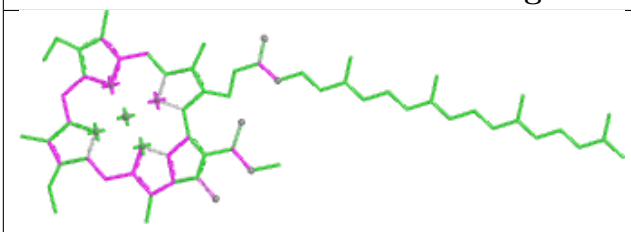


Rings

Ligand CLA B 613



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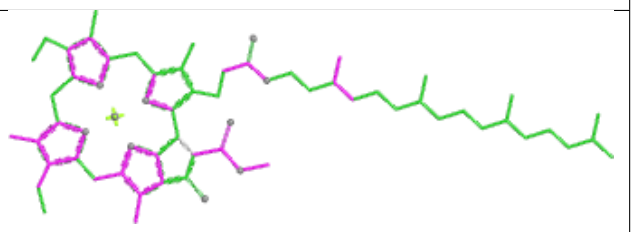
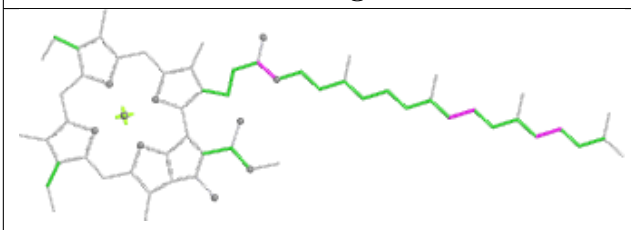


Bond angles



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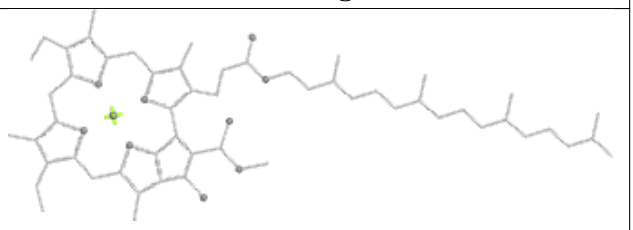
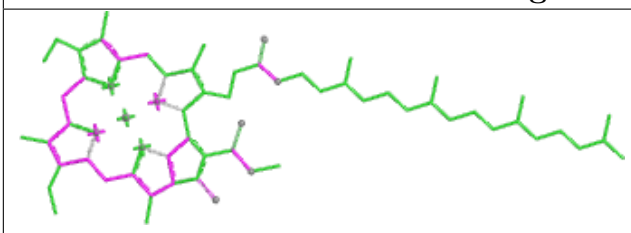


Rings

Ligand CLA c 512



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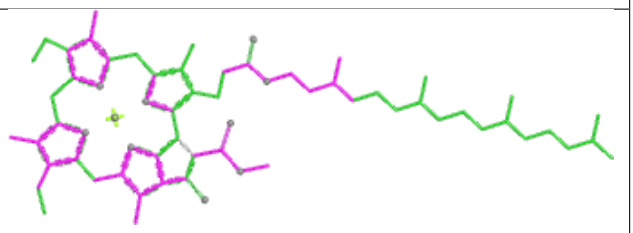
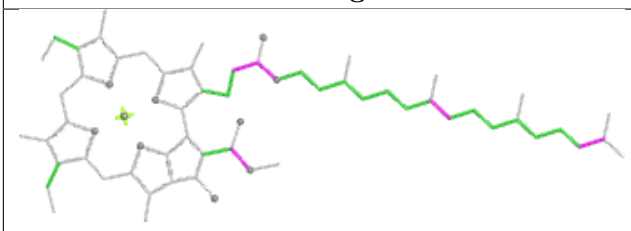


Bond angles



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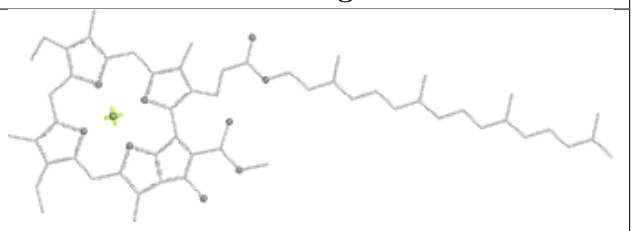
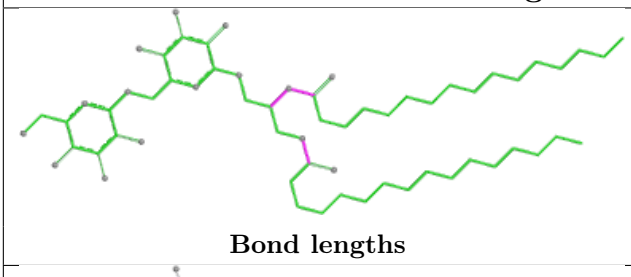


Rings

Ligand DGD c 518



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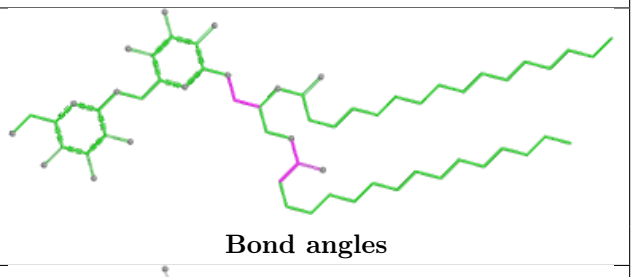

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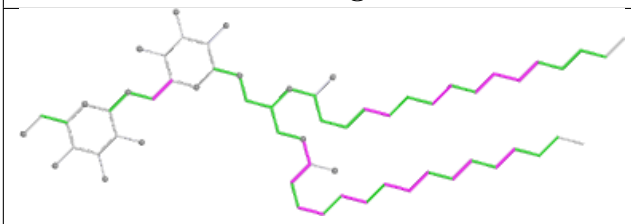

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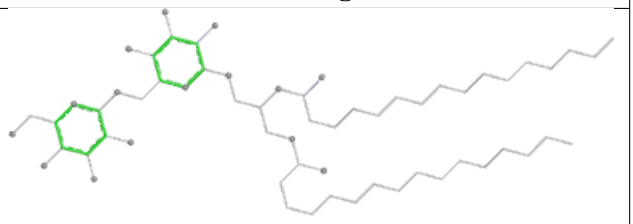

Rings

Ligand PL9 d 408

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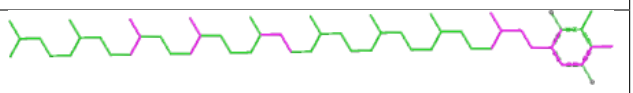
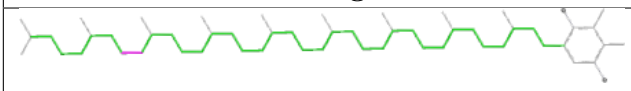


Bond angles



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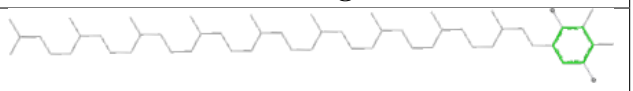
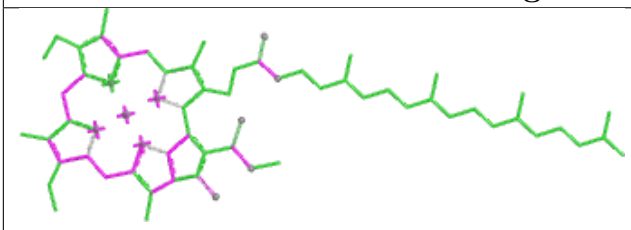


Rings

Ligand CLA D 401



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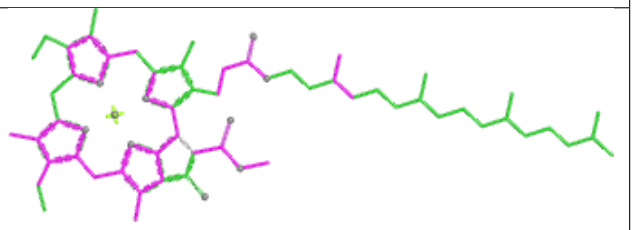
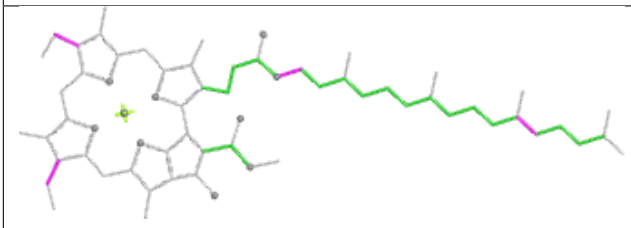


Bond angles



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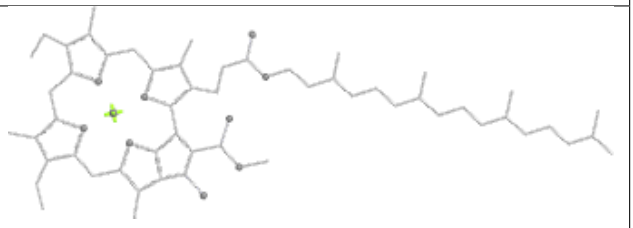
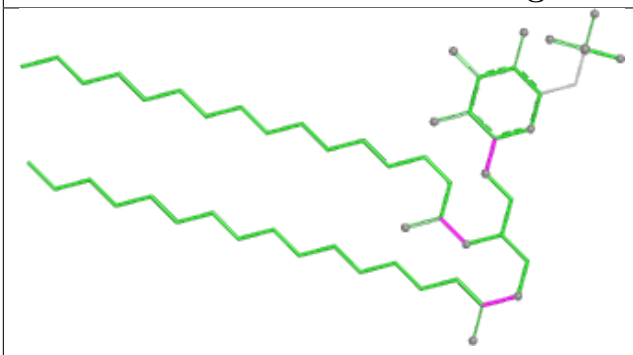


Rings

Ligand SQD b 621



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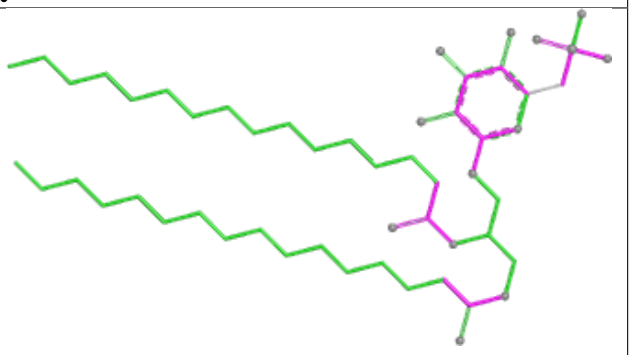
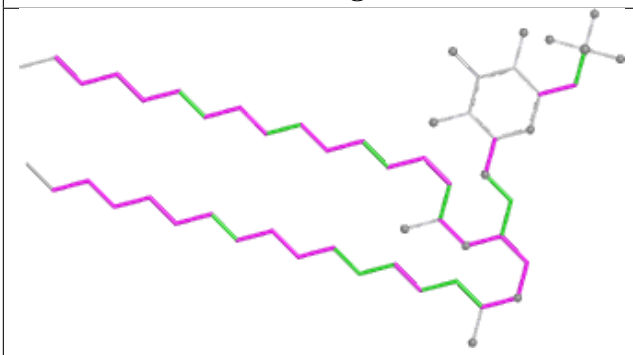


Bond angles



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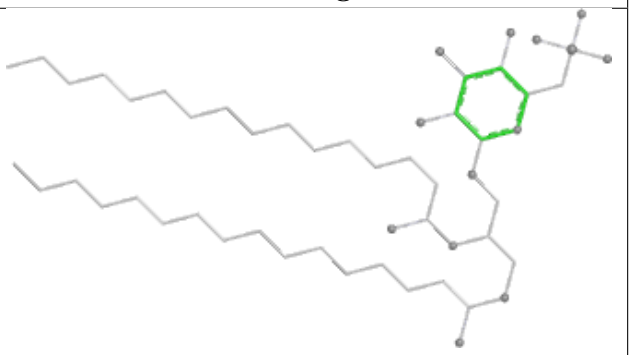
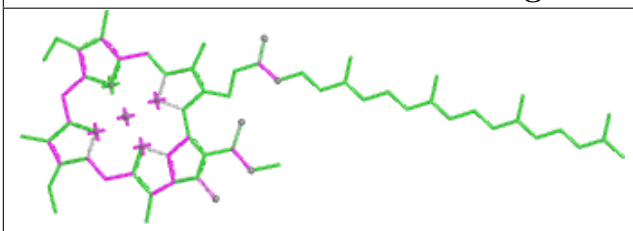


Rings

Ligand CLA B 606



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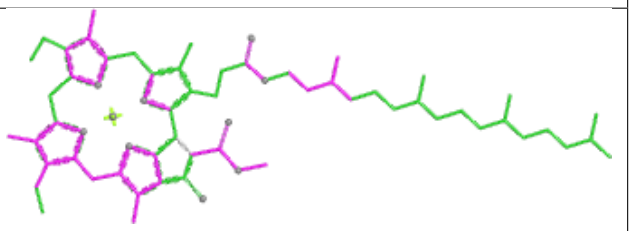

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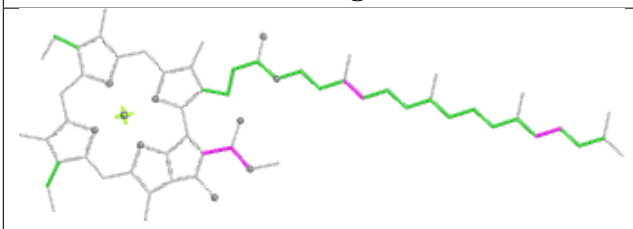

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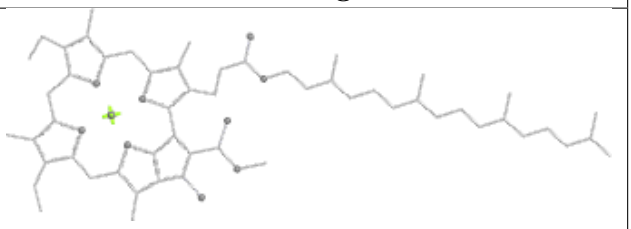
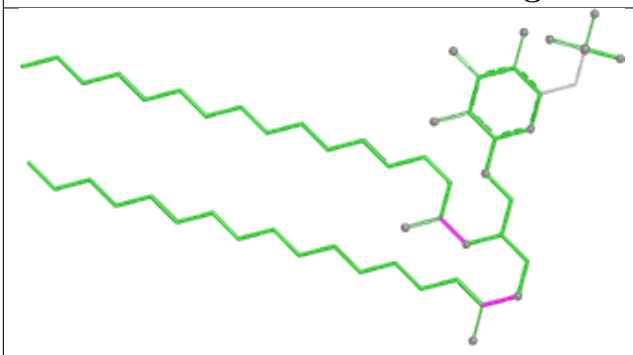


Rings

Ligand SQD A 609



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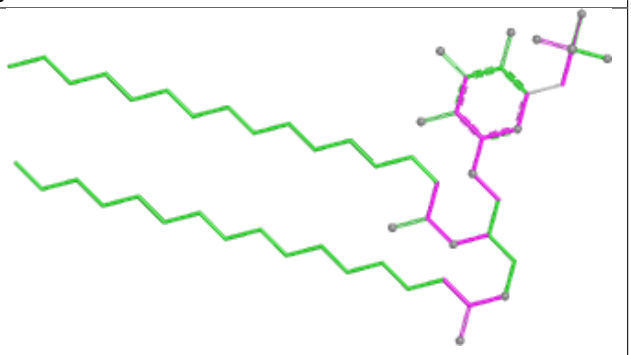
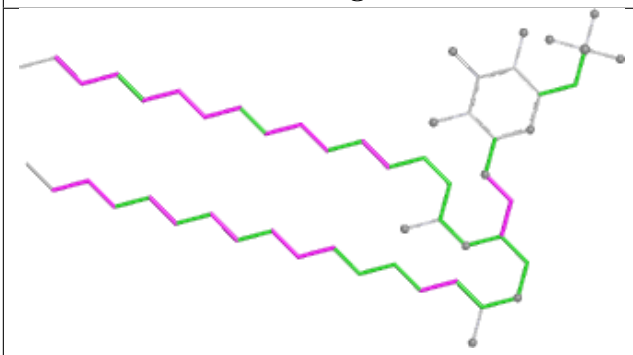
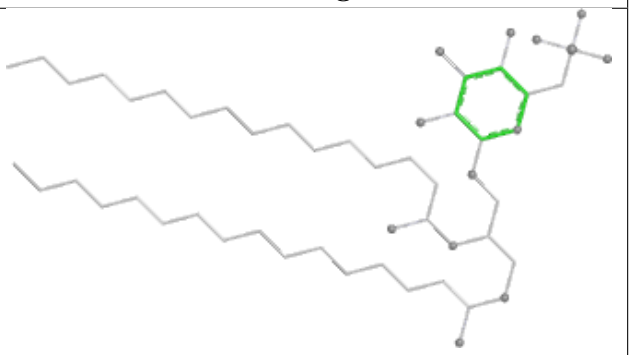


Bond angles

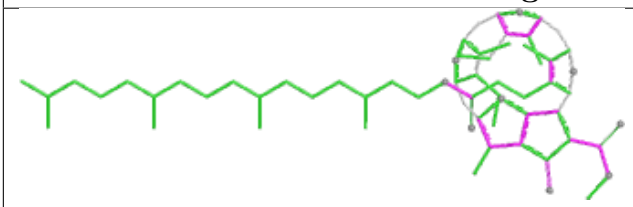


Torsions



Rings

Ligand PHO A 605



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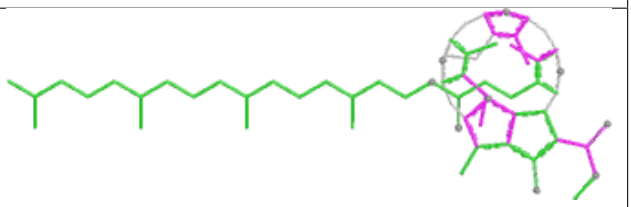
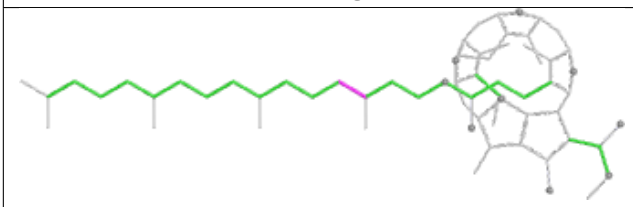
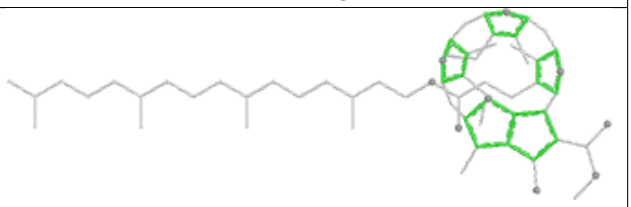


Bond angles

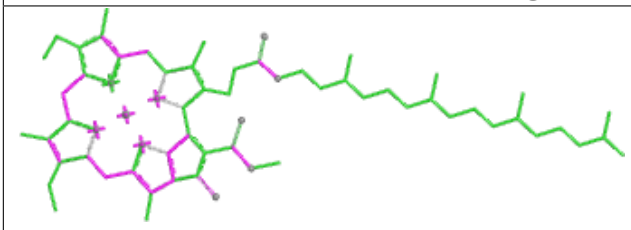


Torsions



Rings

Ligand CLA B 612



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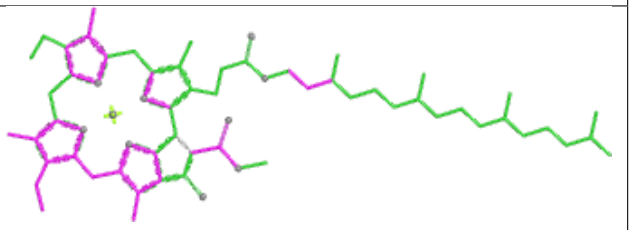
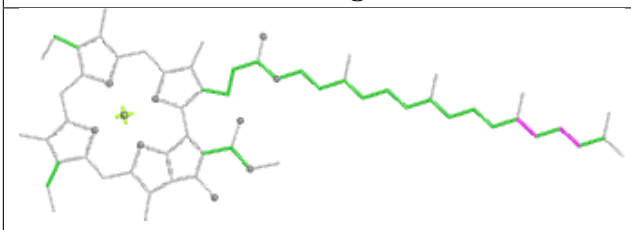
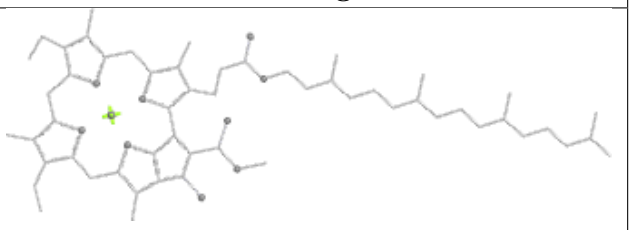


Bond angles

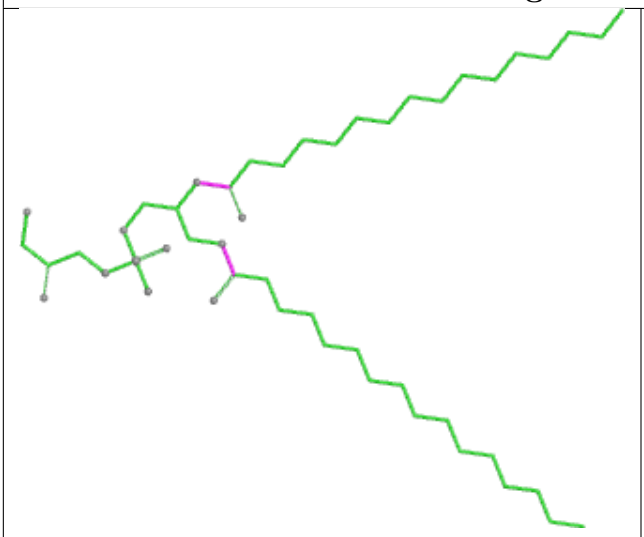


Torsions

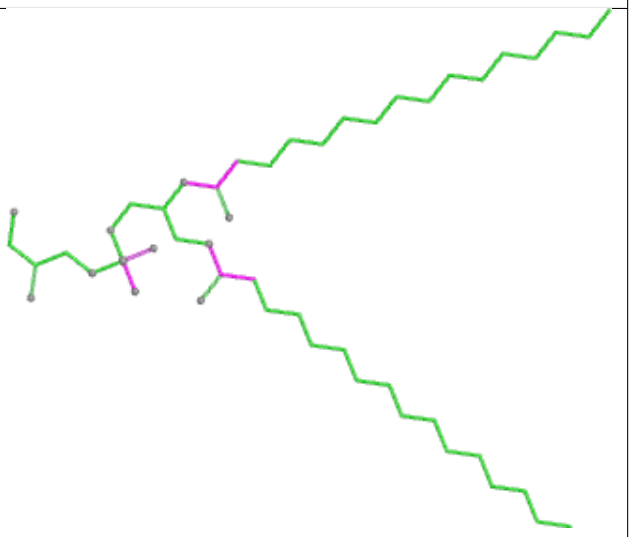


Rings

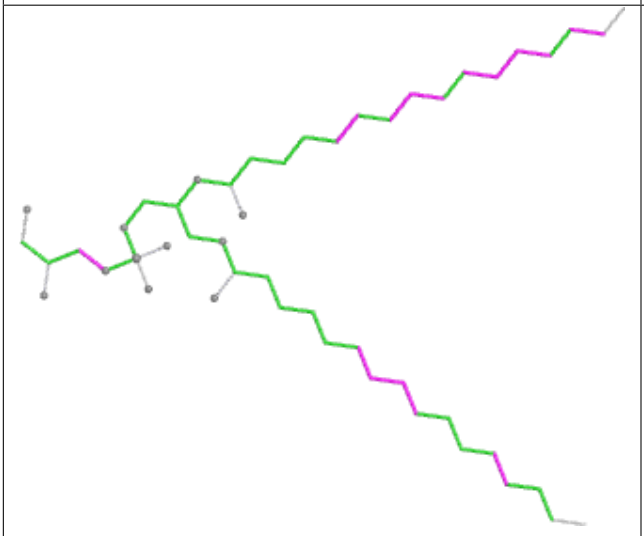
Ligand LHG d 409



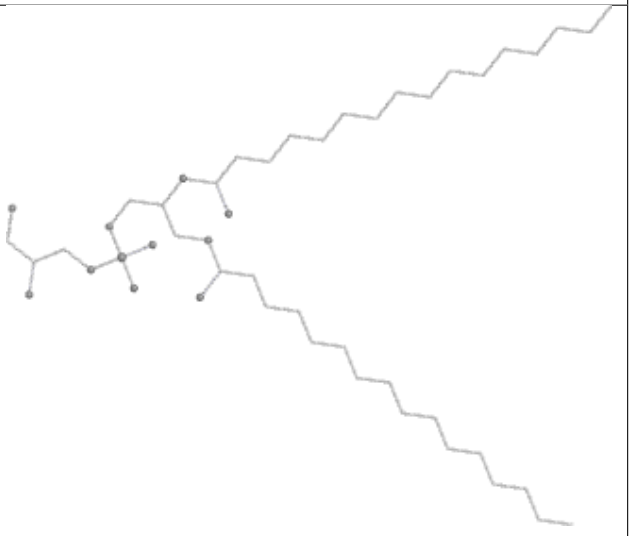
Bond lengths



Bond angles

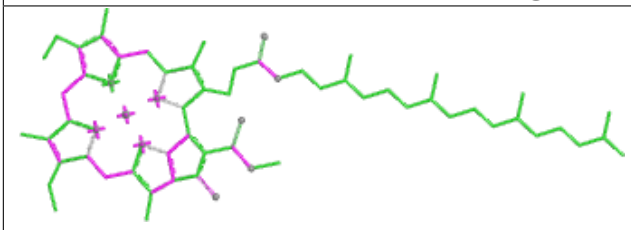


Torsions



Rings

Ligand CLA b 606



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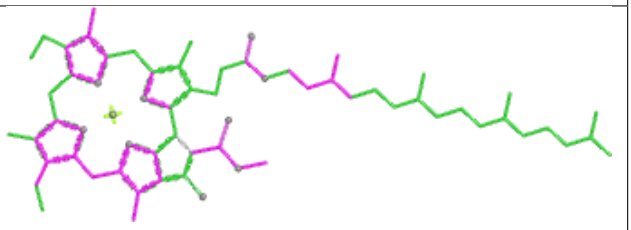
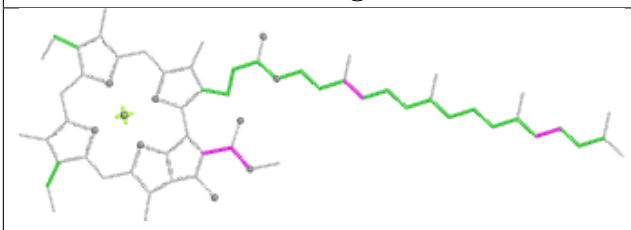


Bond angles



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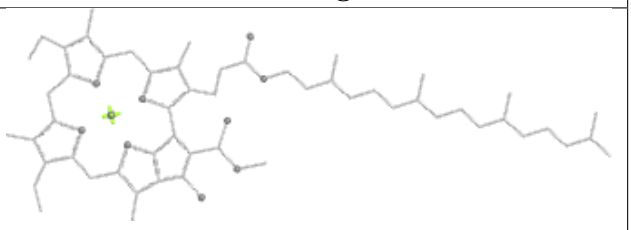
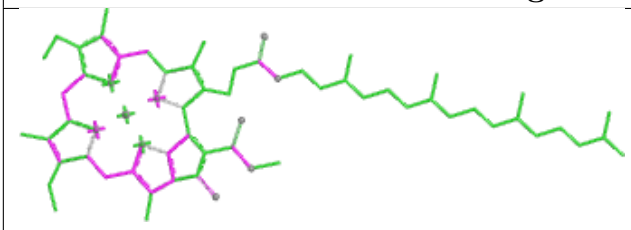


Rings

Ligand CLA b 608



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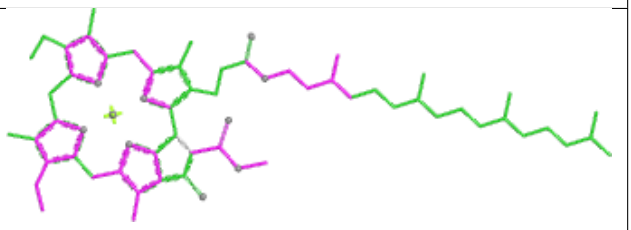
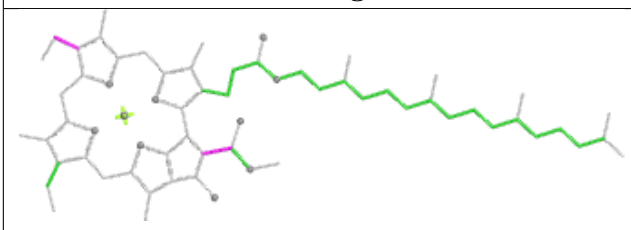


Bond angles



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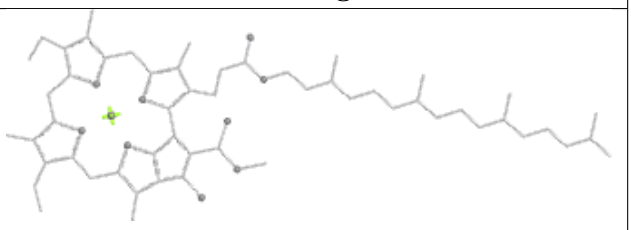
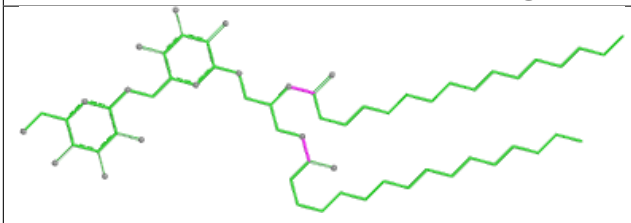


Rings

Ligand DGD C 517



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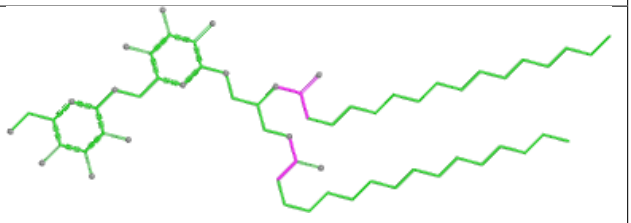

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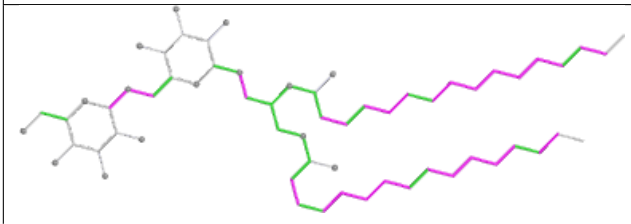

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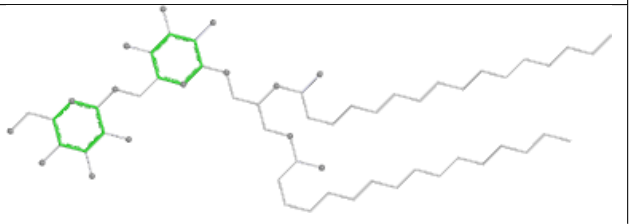
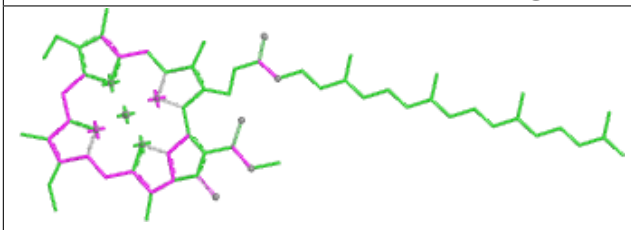


Rings

Ligand CLA b 607



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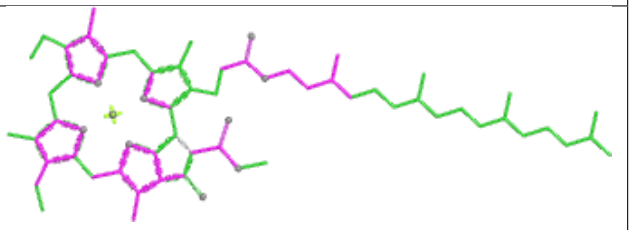
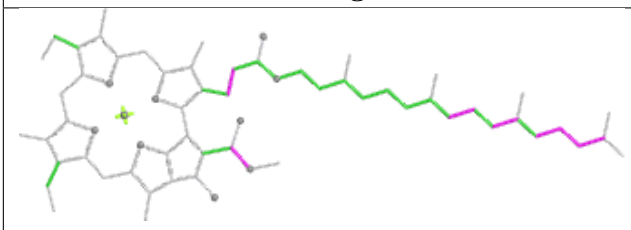


Bond angles



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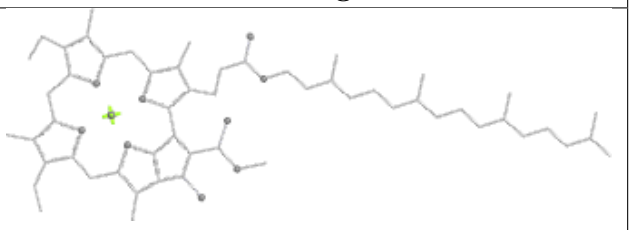
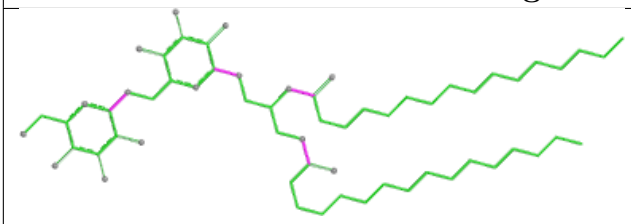


Rings

Ligand DGD d 410



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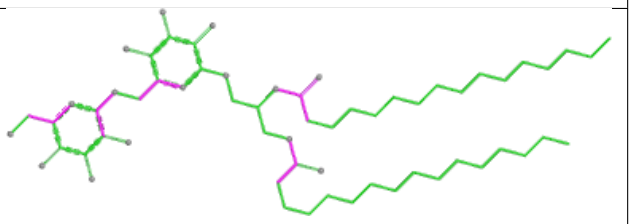
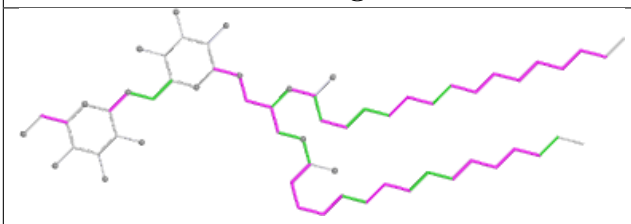


Bond angles



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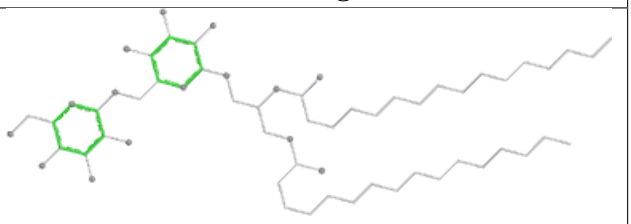
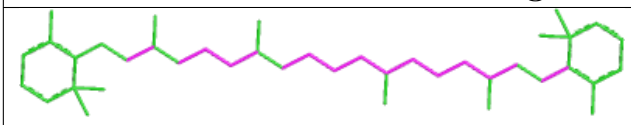


Rings

Ligand BCR a 608



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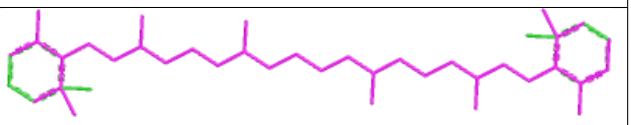
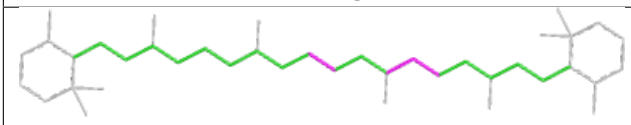


Bond angles



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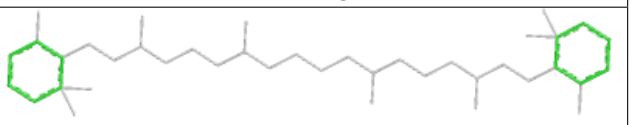
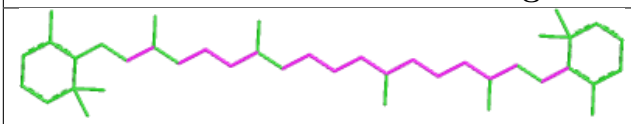
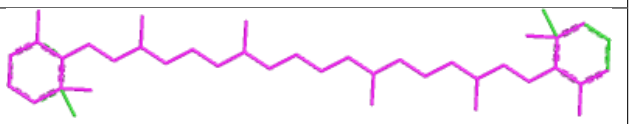
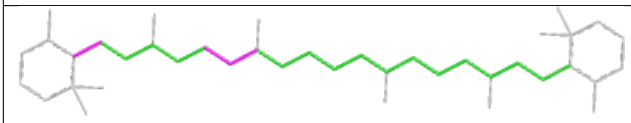
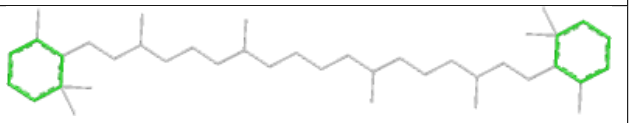
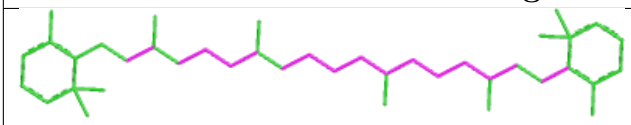
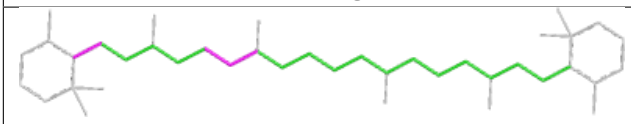
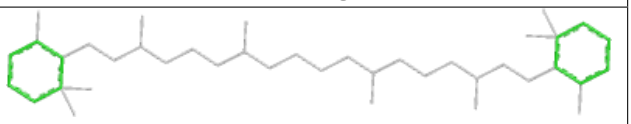


Rings

Ligand BCR B 618	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR T 101	
 Bond lengths	Bond angles
 Torsions	 Rings

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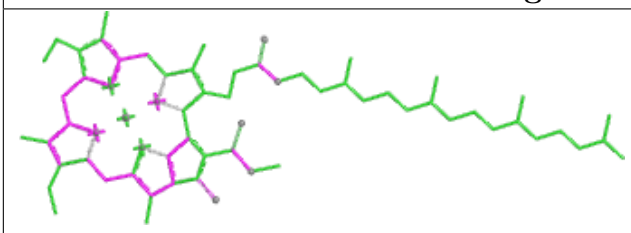
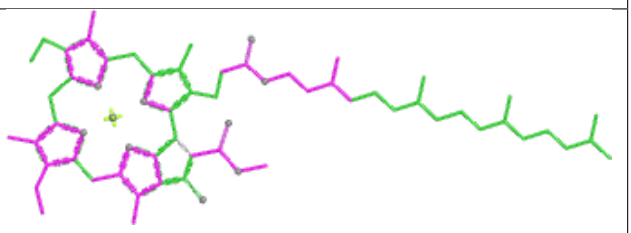
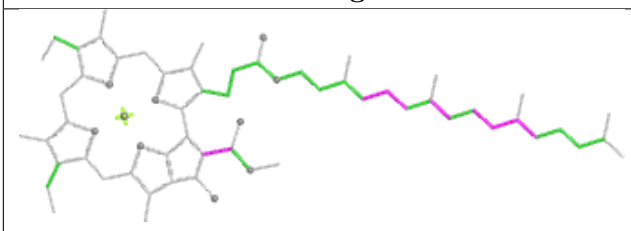
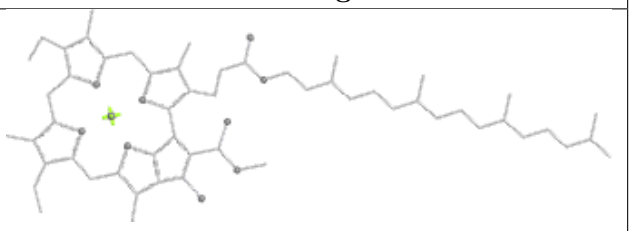
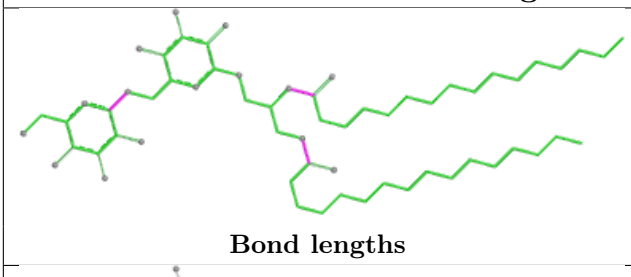
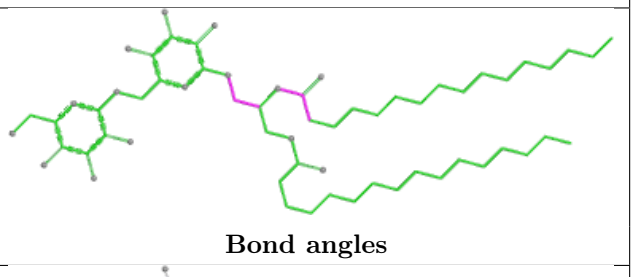
 Bond lengths	 Bond angles
 Torsions	 Rings

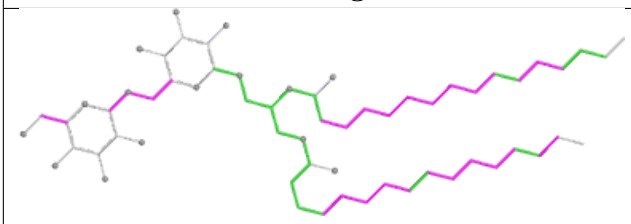
Ligand DGD C 516



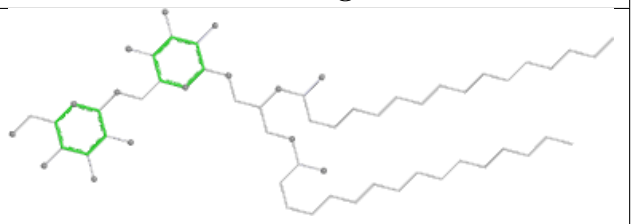
Bond lengths



Bond angles

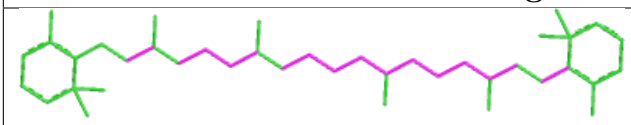


Torsions



Rings

Ligand BCR b 618



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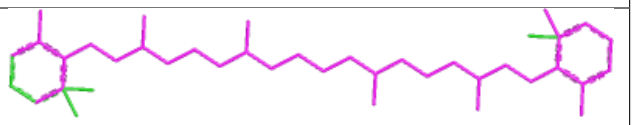
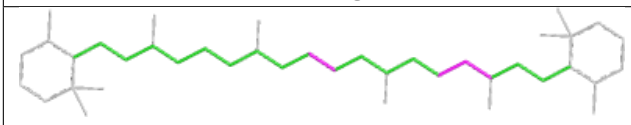


Bond angles



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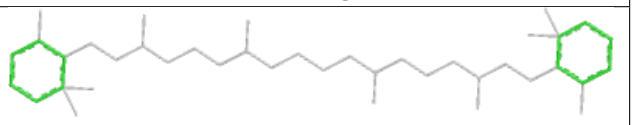
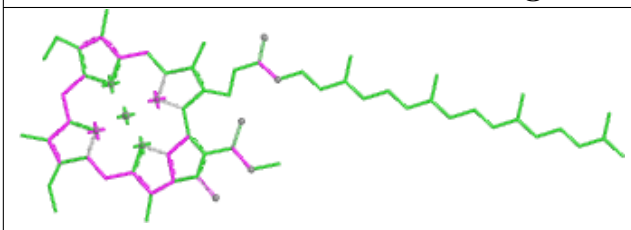
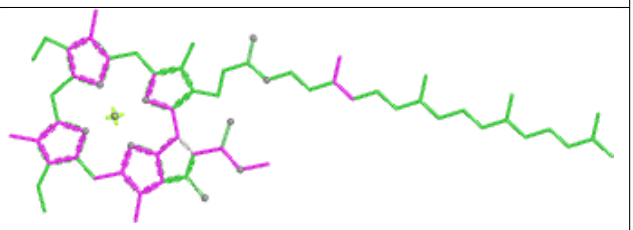


Rings

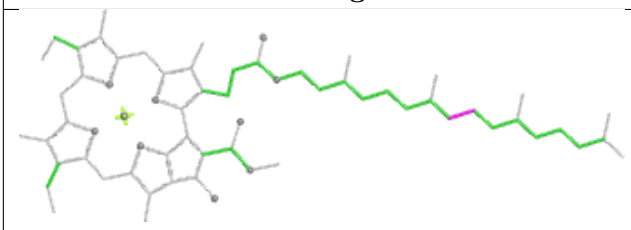
Ligand CLA C 503



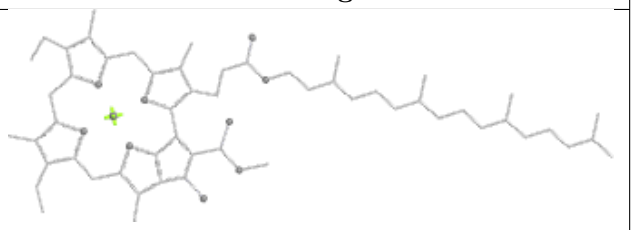
Bond lengths



Bond angles

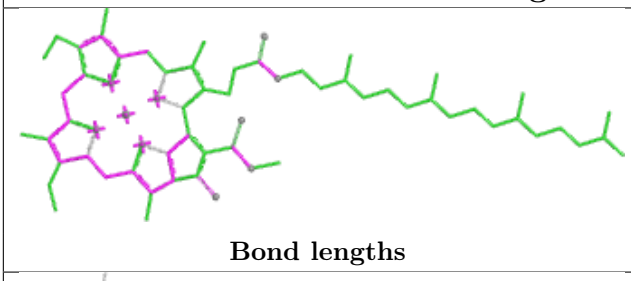


Torsions



Rings

Ligand CLA c 508



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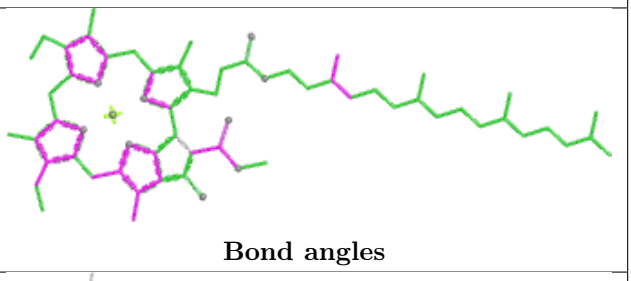
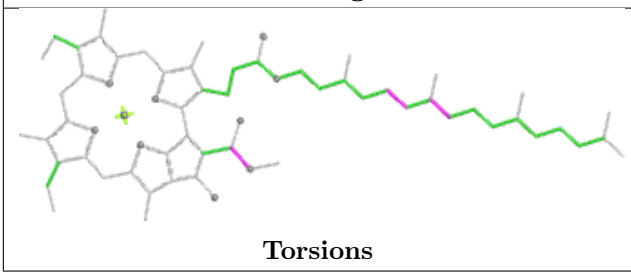


Bond angles



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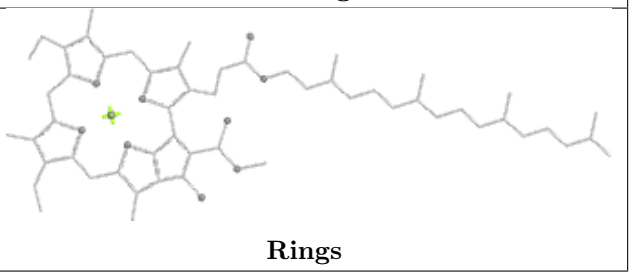
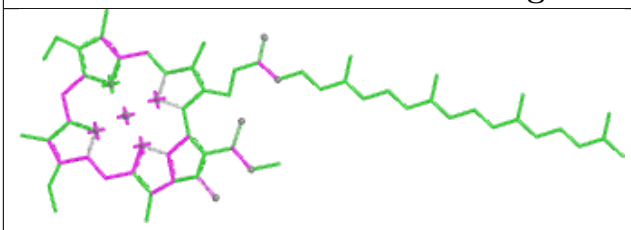


Rings

Ligand CLA d 401



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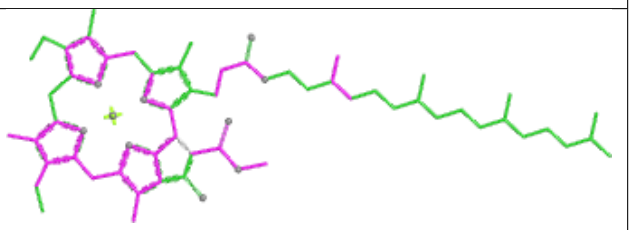
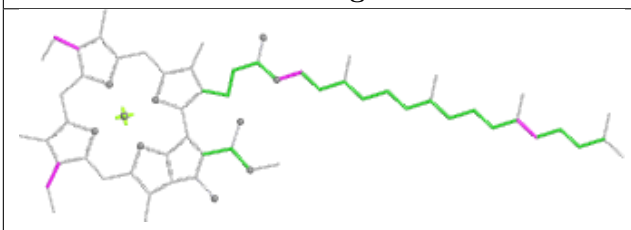
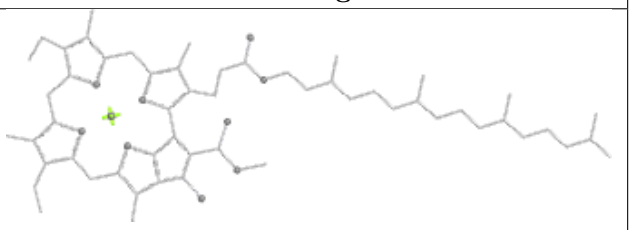


Bond angles

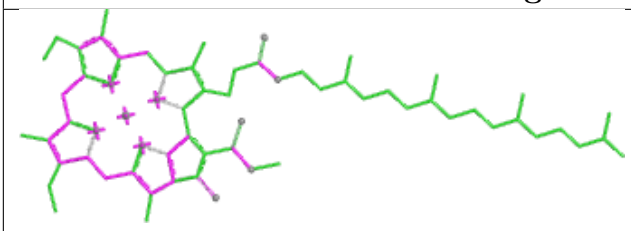


Torsions



Rings

Ligand CLA C 508



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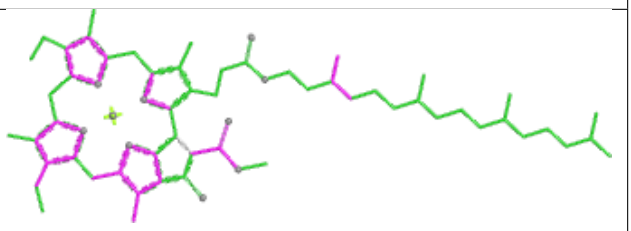

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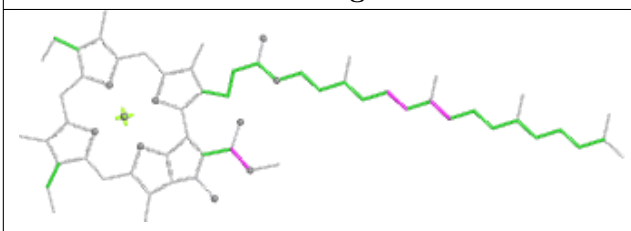

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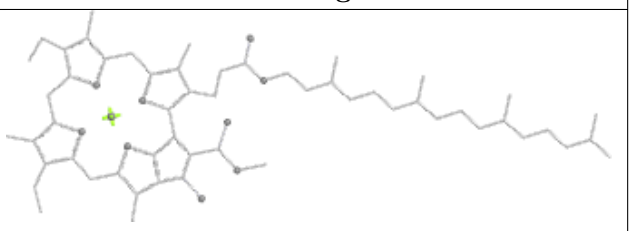

Rings

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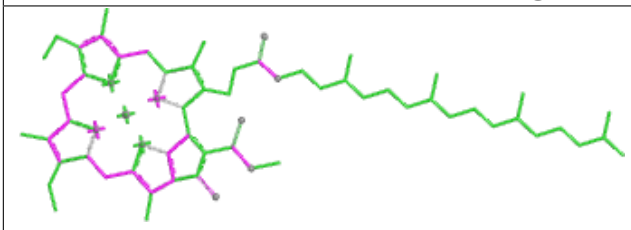

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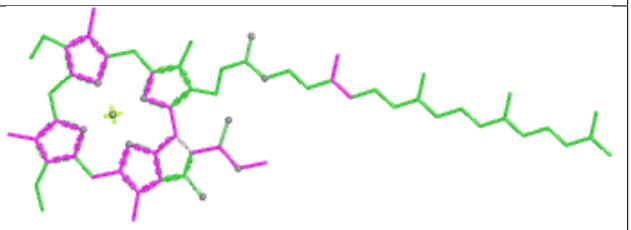

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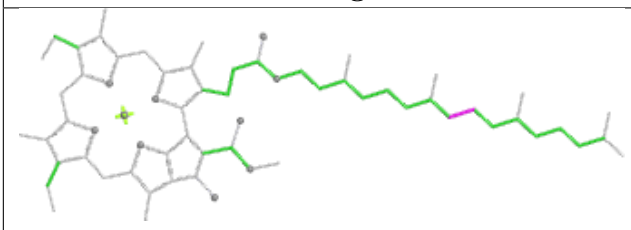

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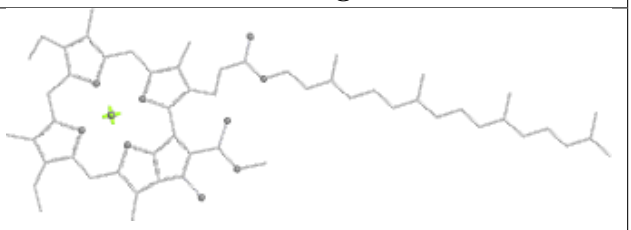

Rings

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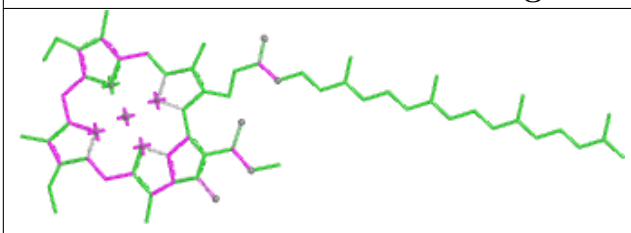

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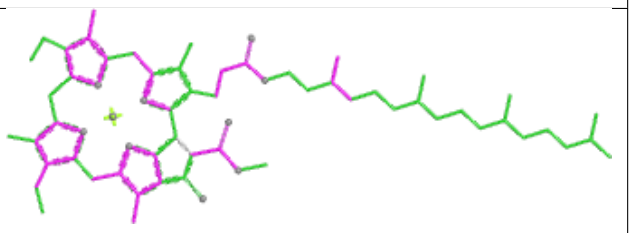

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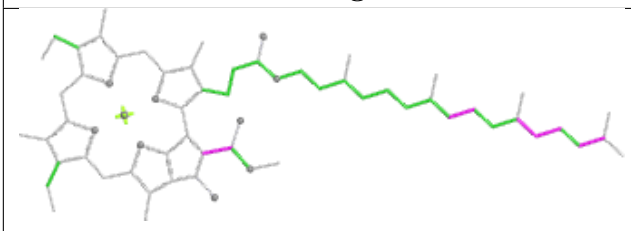

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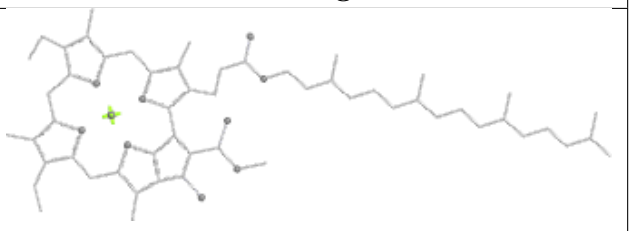

Rings

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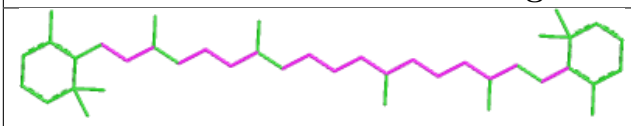

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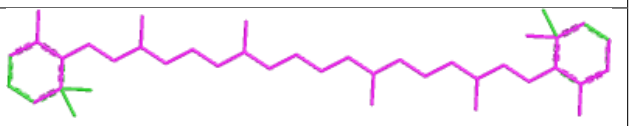

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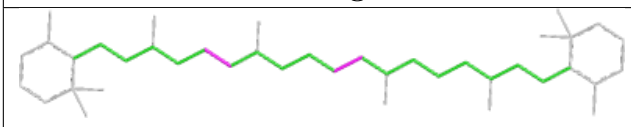

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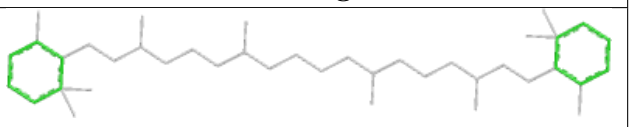

Rings

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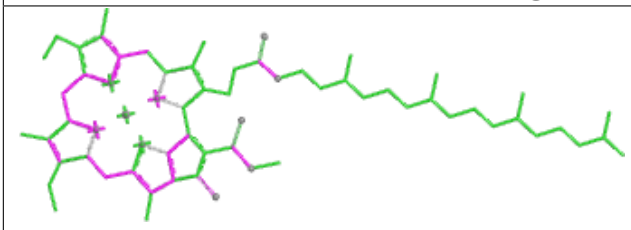

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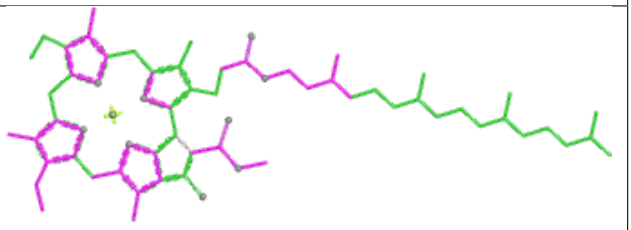
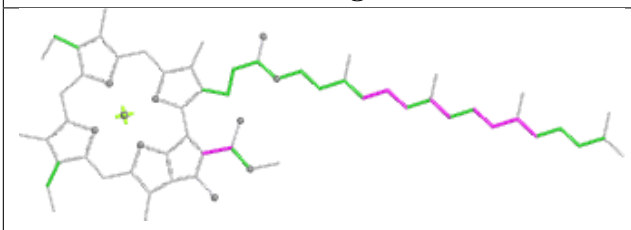


Bond angles



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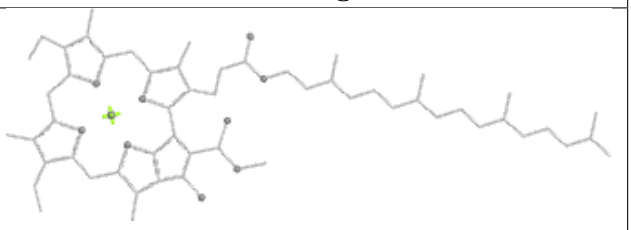

Rings

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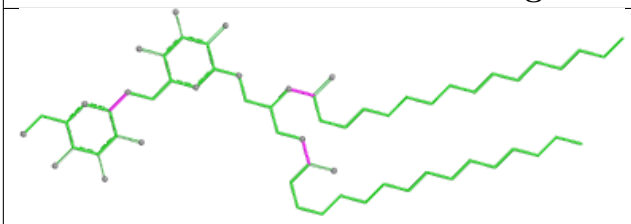

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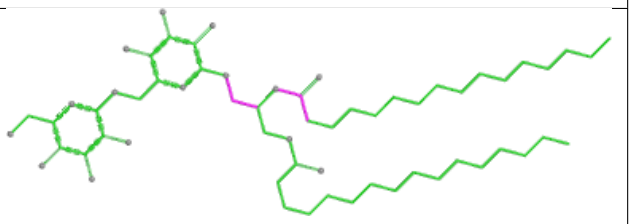

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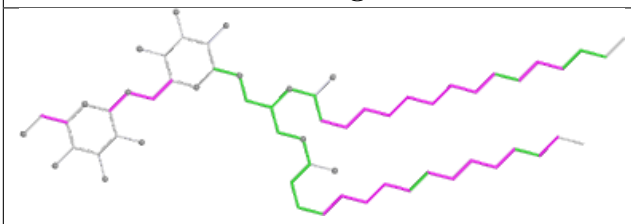

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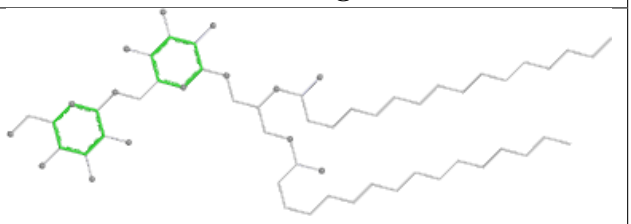

Rings

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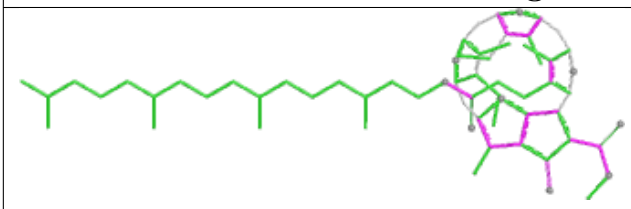

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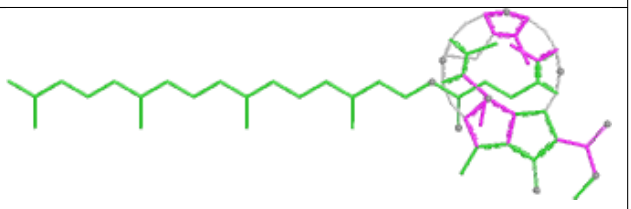
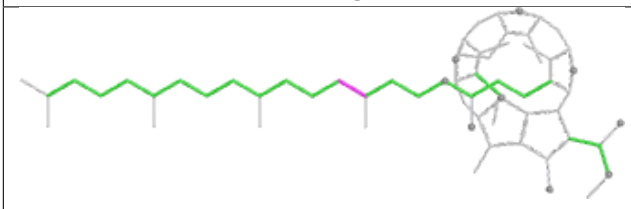


Bond angles



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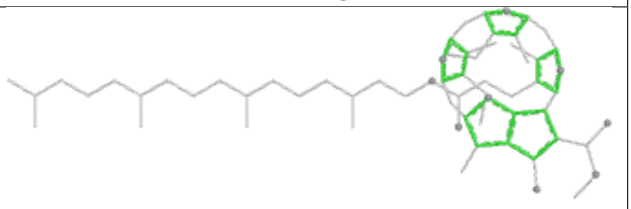

Rings

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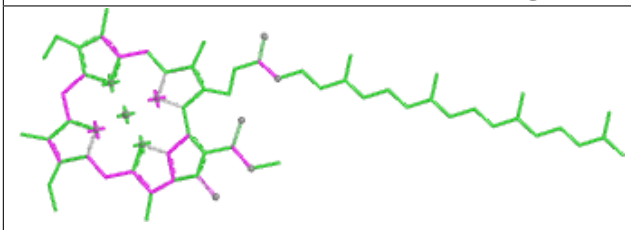

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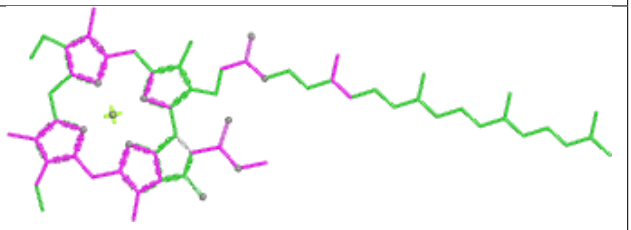

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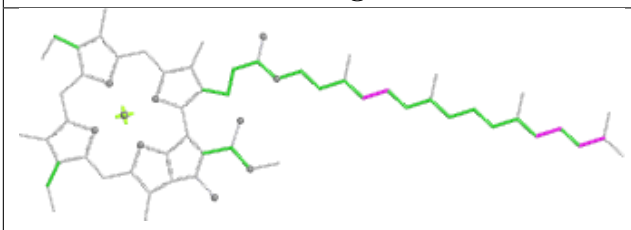

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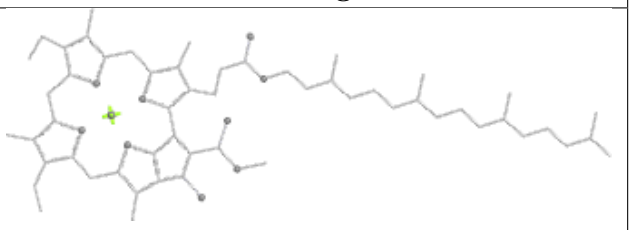

Rings

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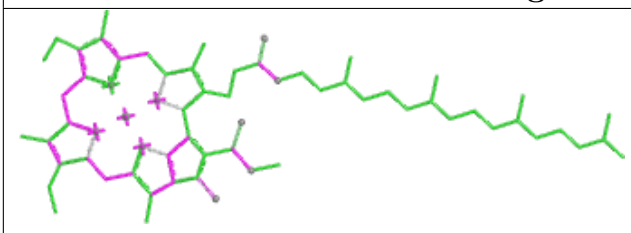

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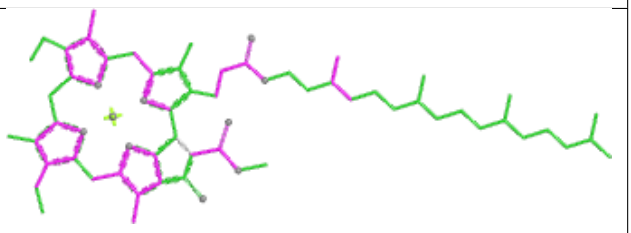

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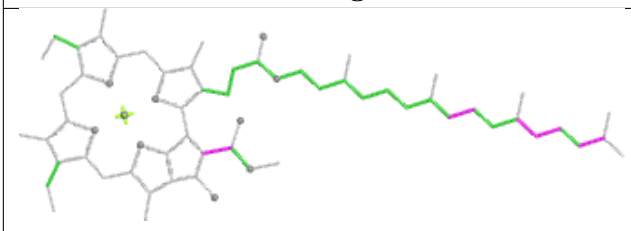

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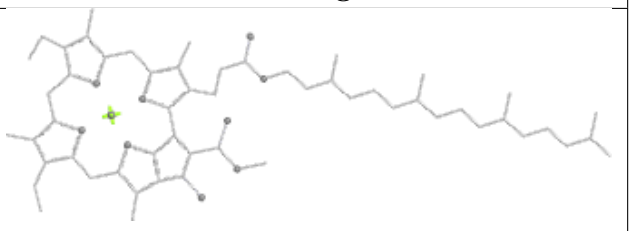

Rings

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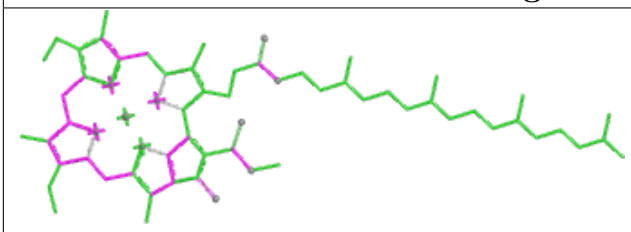

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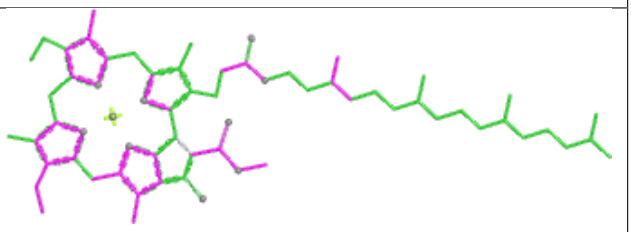

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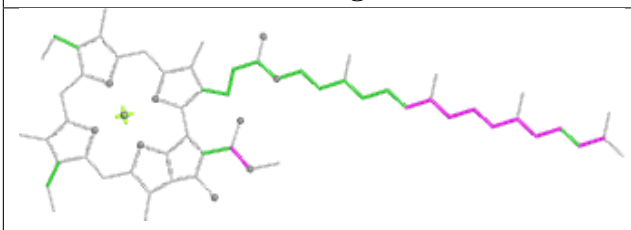

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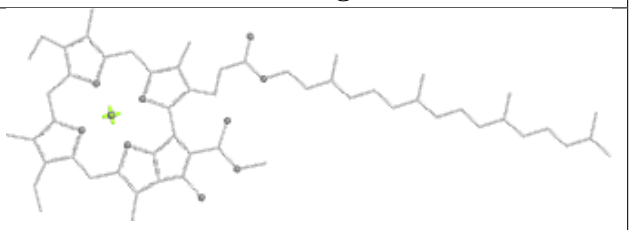

Rings

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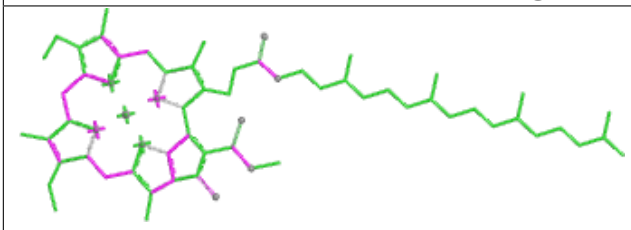

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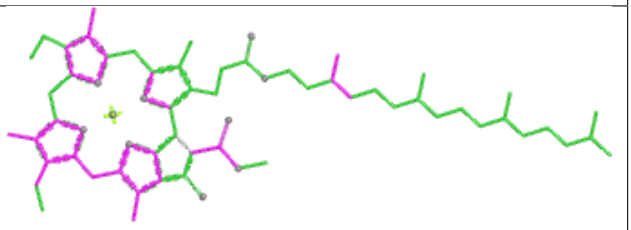

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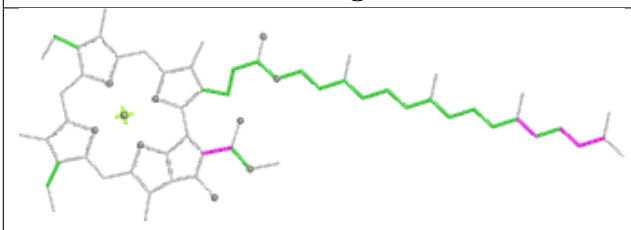

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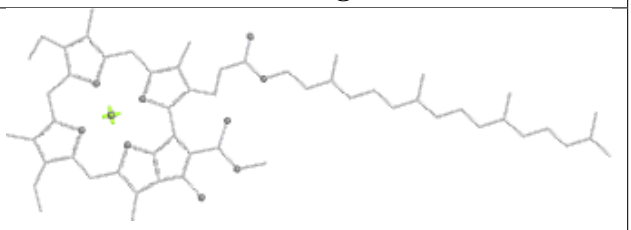

Rings

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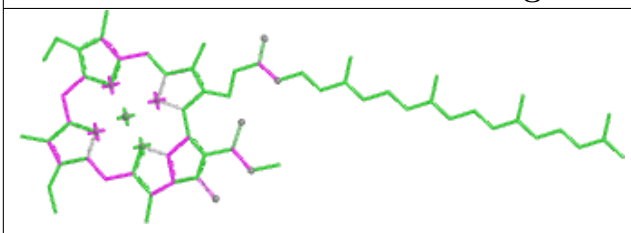

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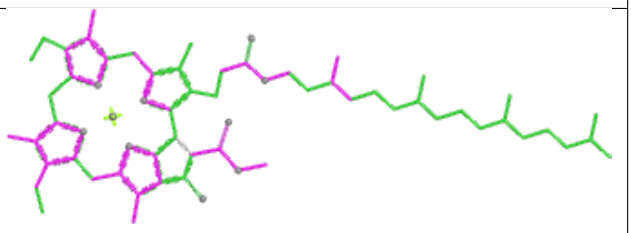
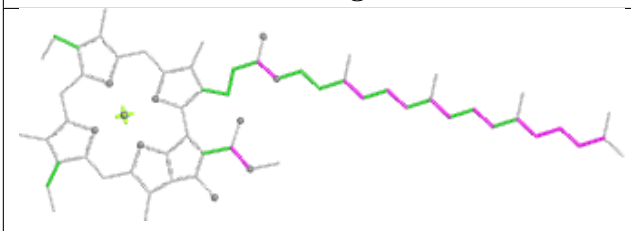


Bond angles



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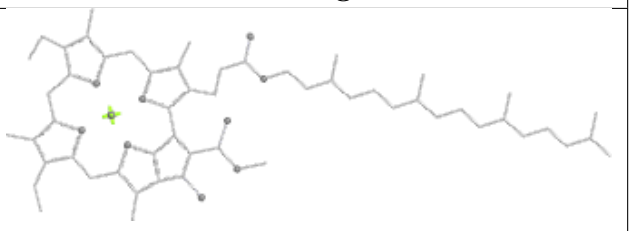

Rings

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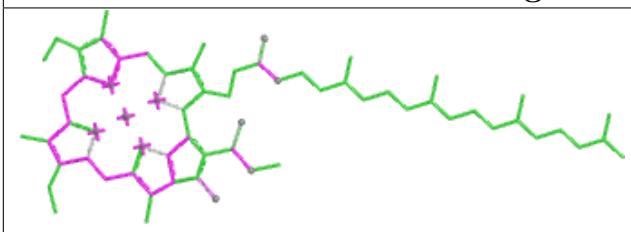

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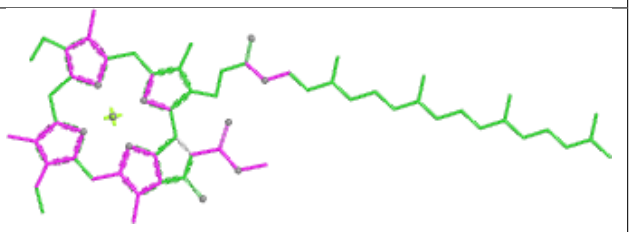
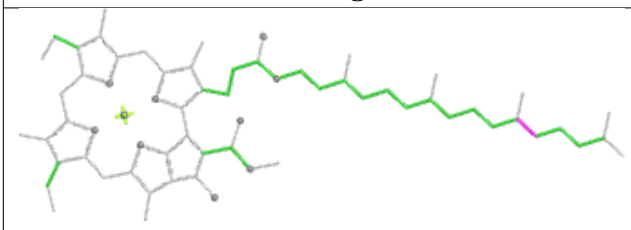
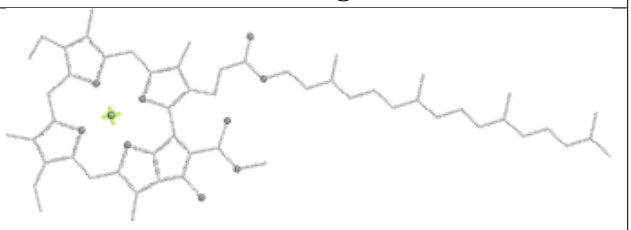


Bond angles



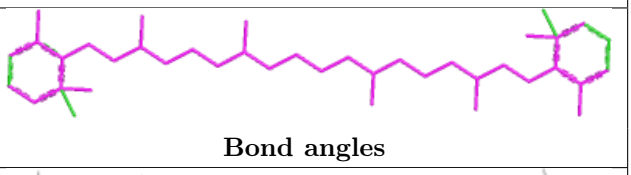
Torsions



Rings

Ligand BCR d 404

Bond lengths



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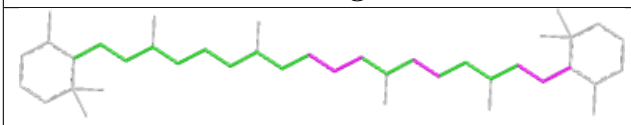

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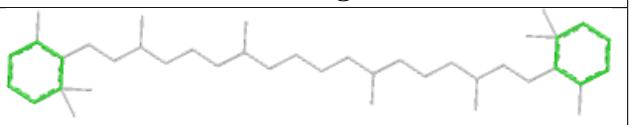
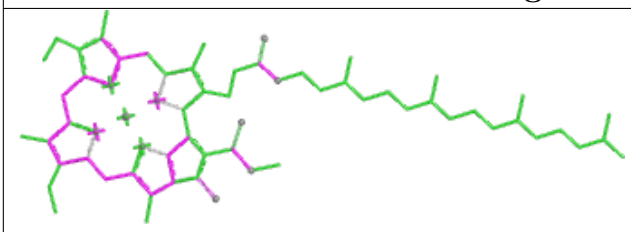


Rings

Ligand CLA B 616



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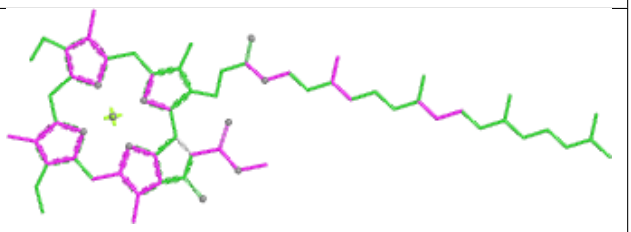
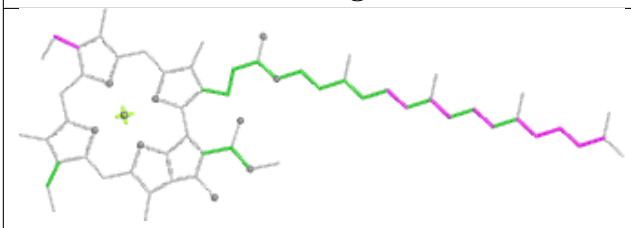


Bond angles



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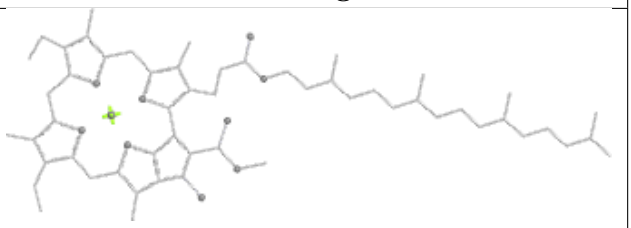
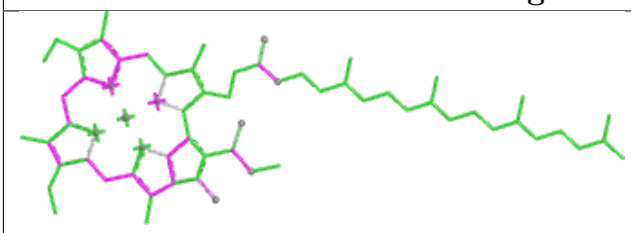


Rings

Ligand CLA b 613



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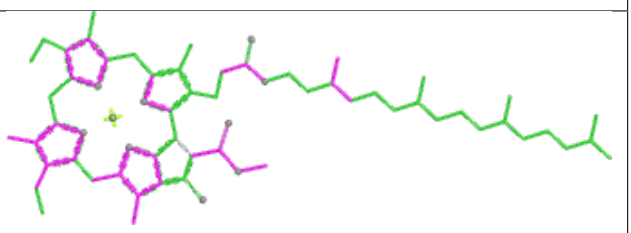

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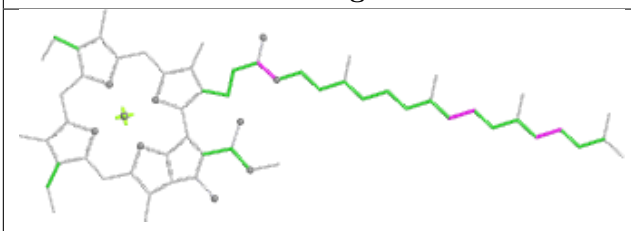

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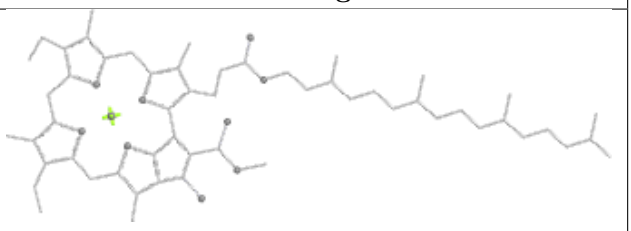
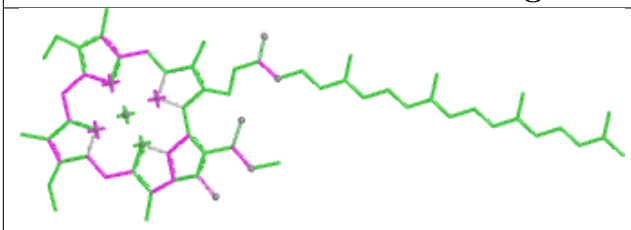


Rings

Ligand CLA B 609



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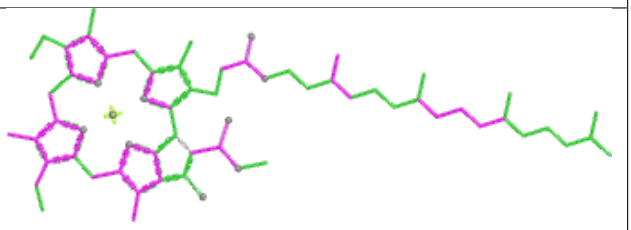

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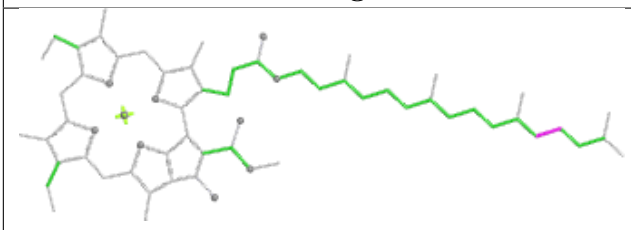

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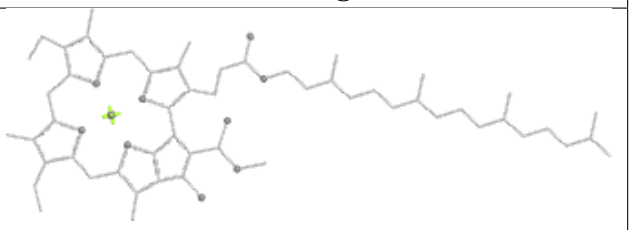
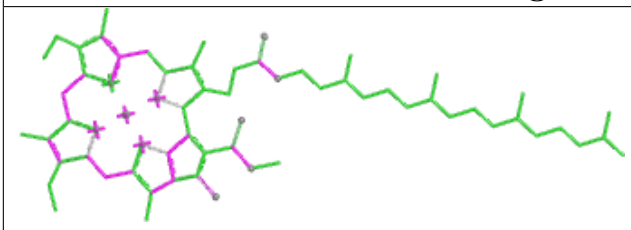


Rings

Ligand CLA a 603



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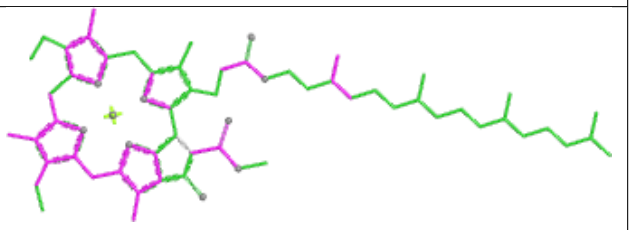
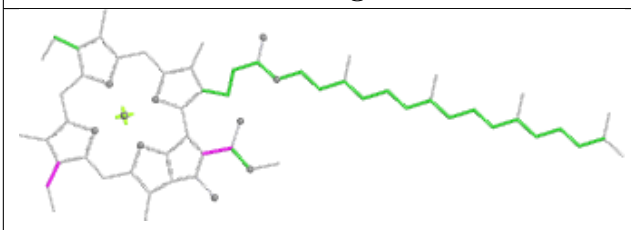


Bond angles



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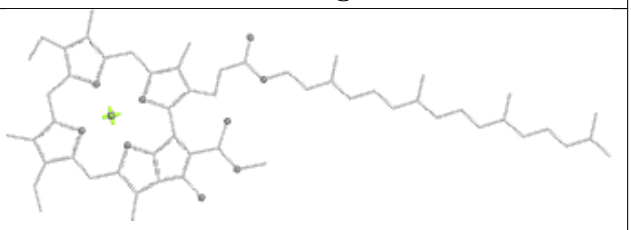
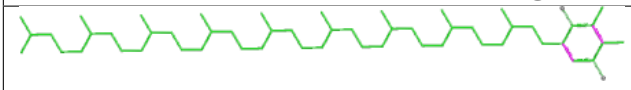


Rings

Ligand PL9 A 613



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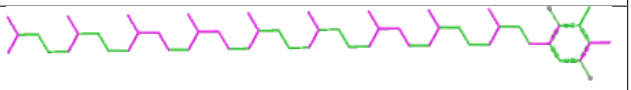
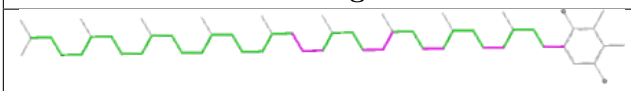


Bond angles



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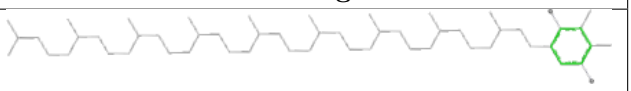
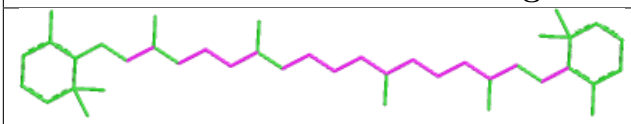
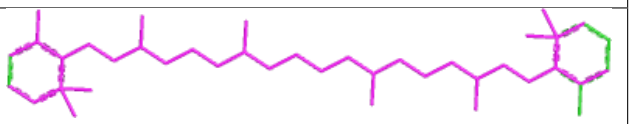
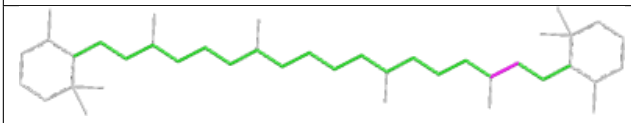
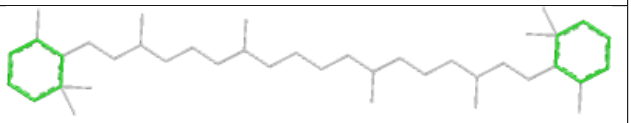


Rings

Ligand BCR T 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

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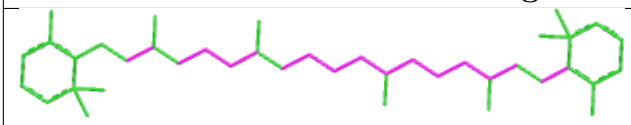
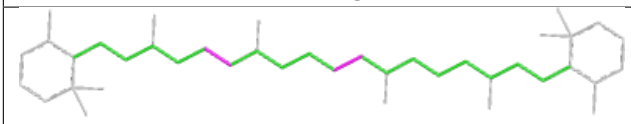
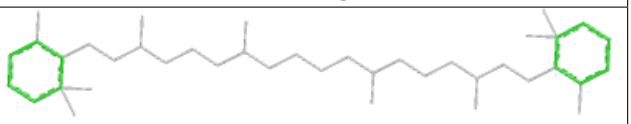
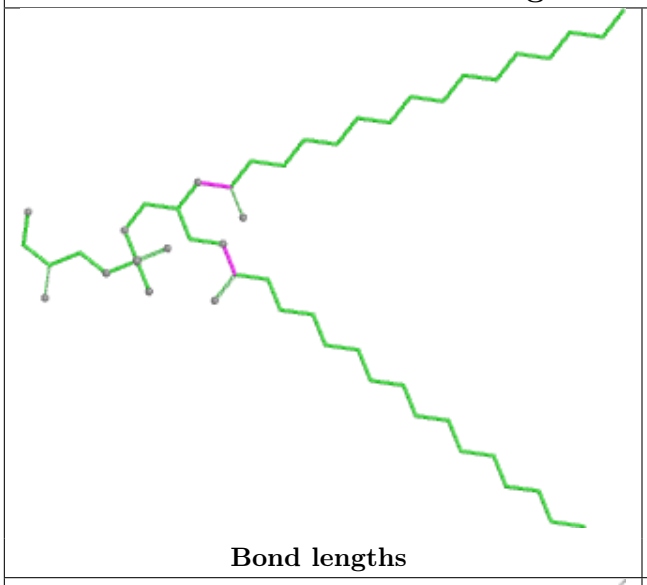
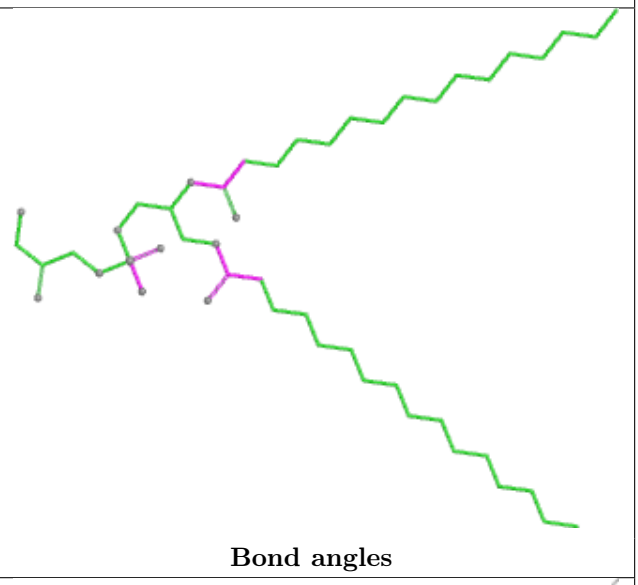
 Bond lengths	Bond angles
 Torsions	 Rings

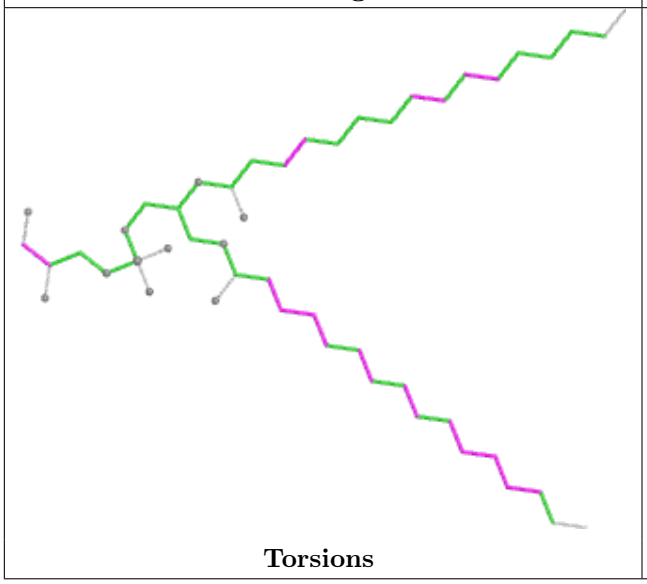
Ligand LHG d 405



Bond lengths



Bond angles



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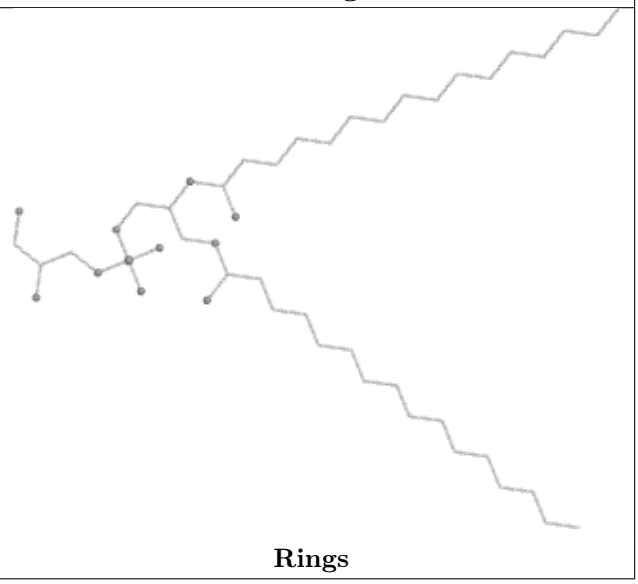
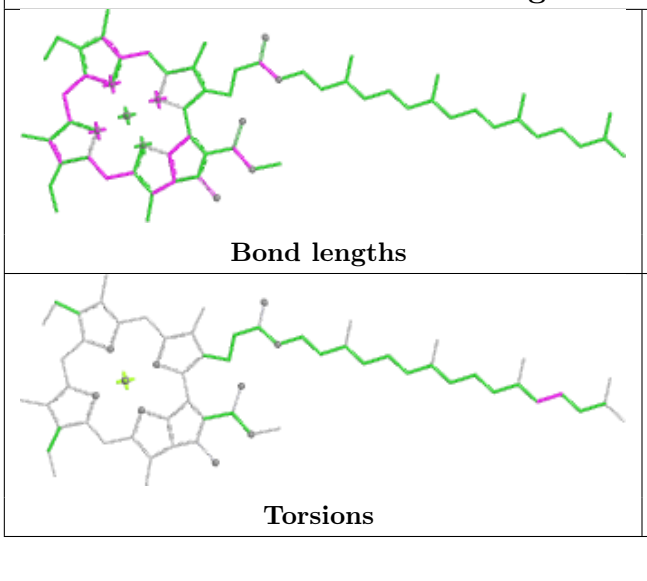


Rings

Ligand CLA b 609



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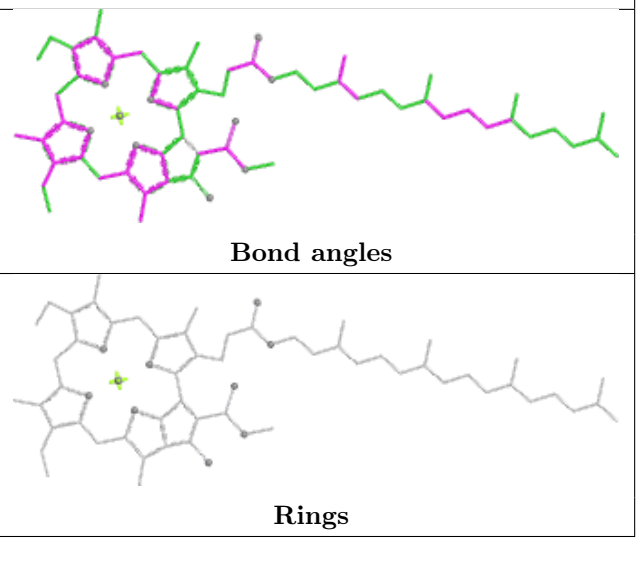
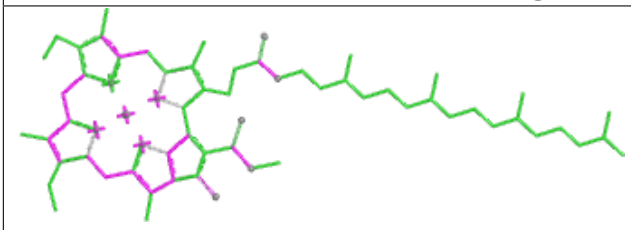


Bond angles

Torsions

Rings

Ligand CLA c 506



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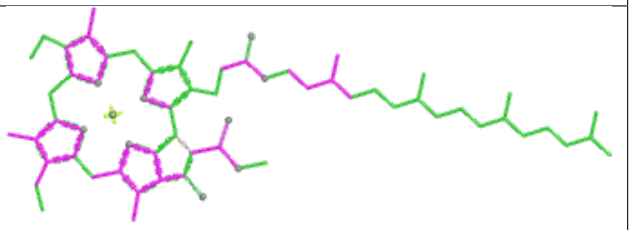
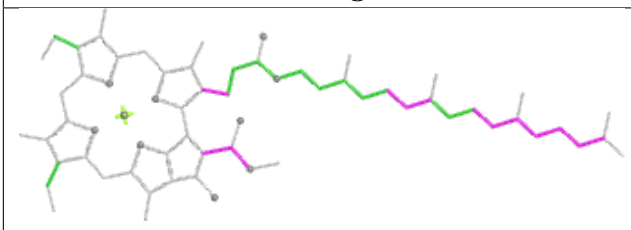
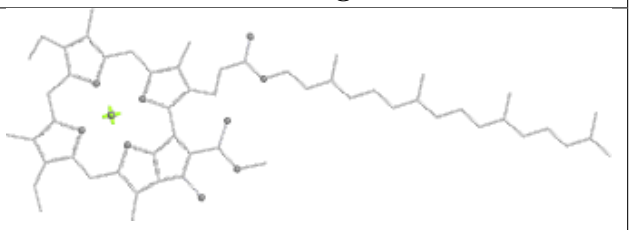


Bond angles

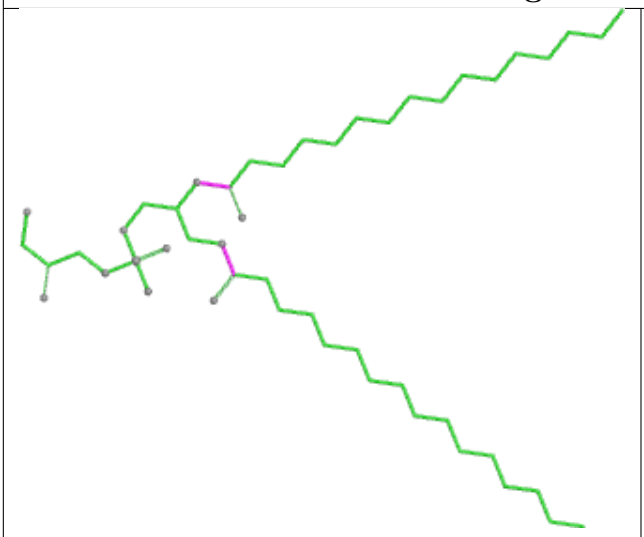


Torsions



Rings

Ligand LHG L 102



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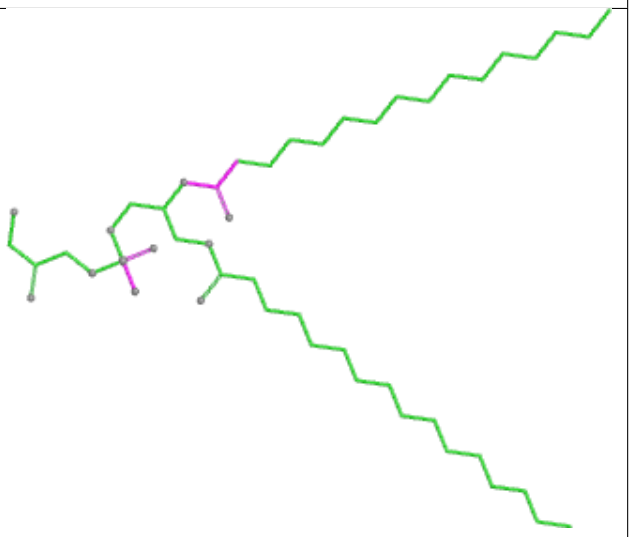
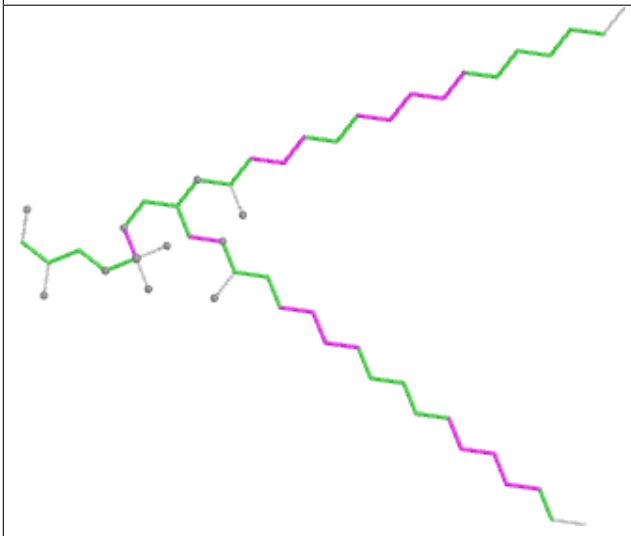


Bond angles



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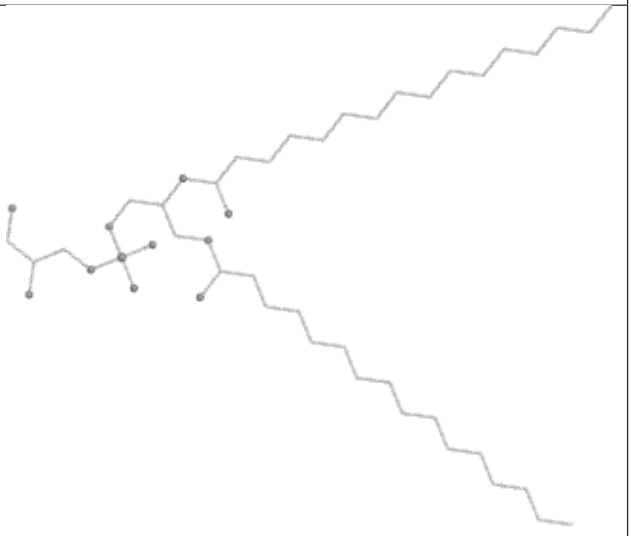
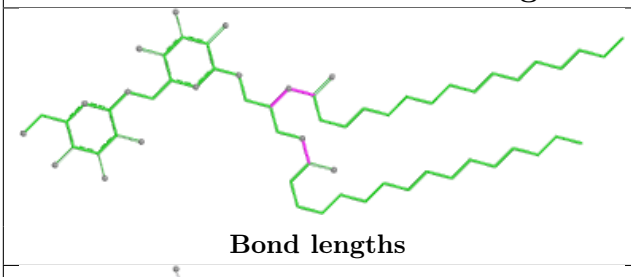
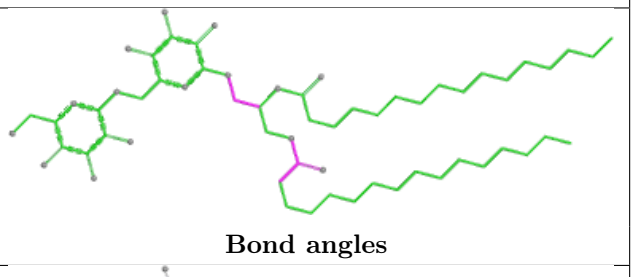


Rings

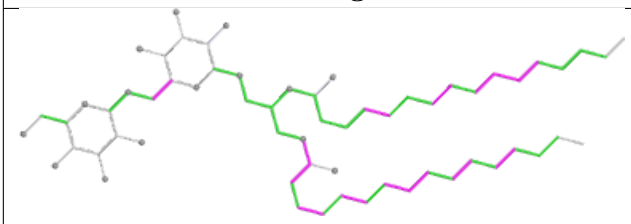
Ligand DGD C 518



Bond lengths



Bond angles



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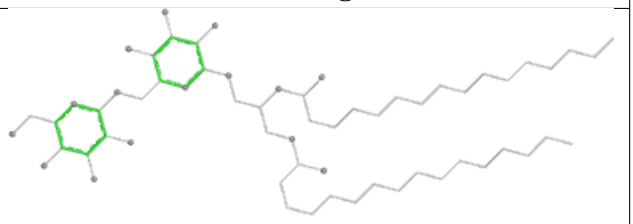
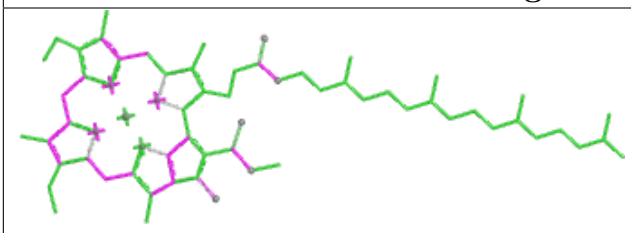
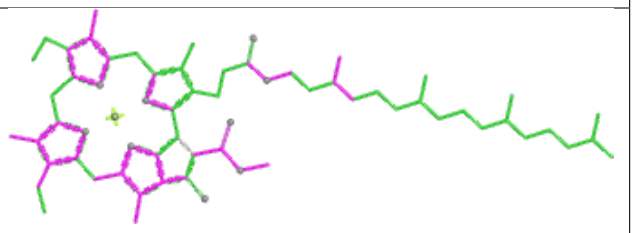


Rings

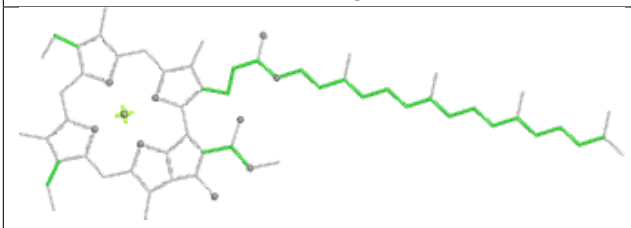
Ligand CLA C 511



Bond lengths



Bond angles



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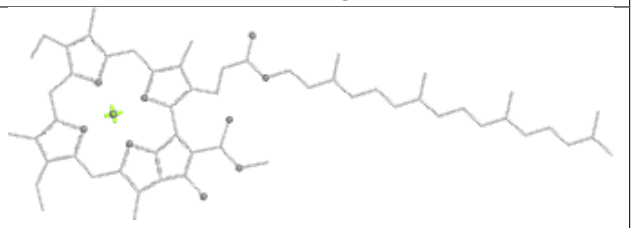
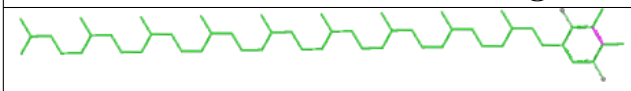
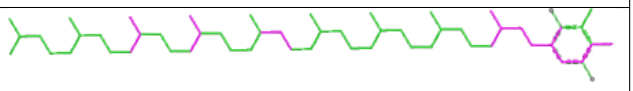


Rings

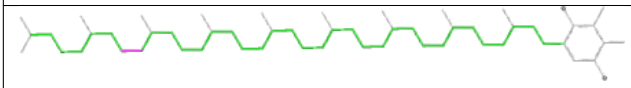
Ligand PL9 D 408



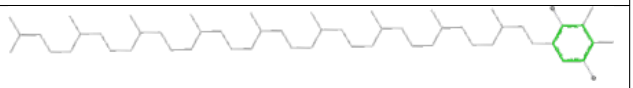
Bond lengths



Bond angles

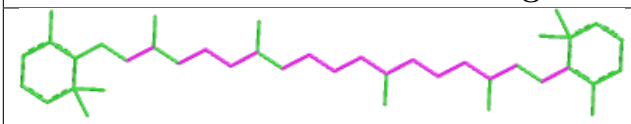


Torsions

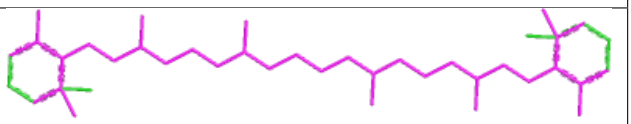


Rings

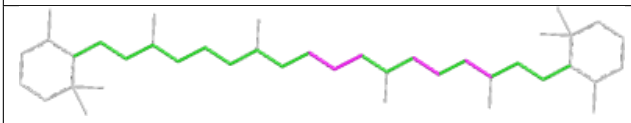
Ligand BCR C 515



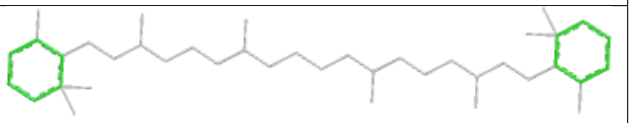
Bond lengths



Bond angles

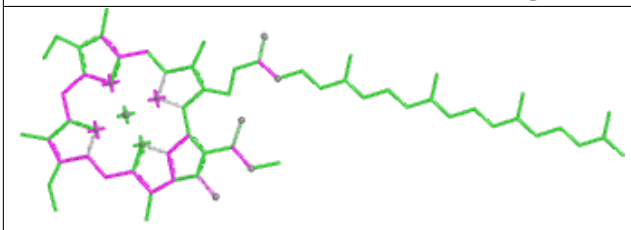


Torsions

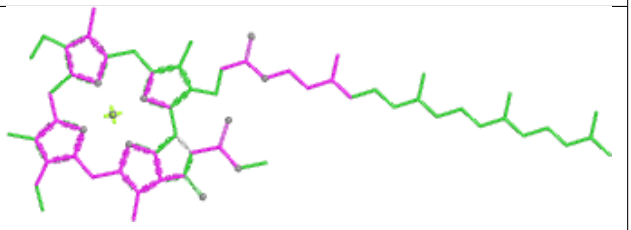


Rings

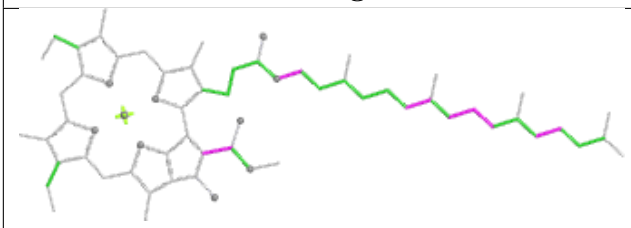
Ligand CLA C 509



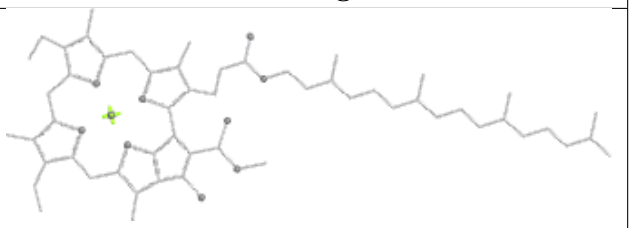
Bond lengths



Bond angles

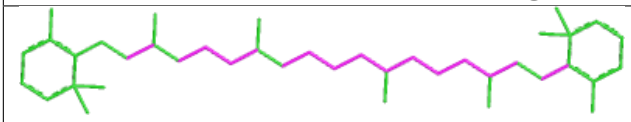


Torsions

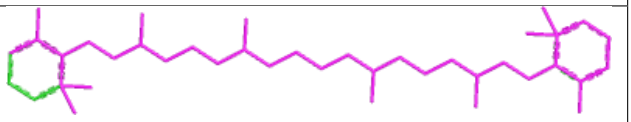


Rings

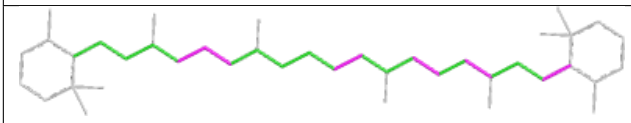
Ligand BCR h 101



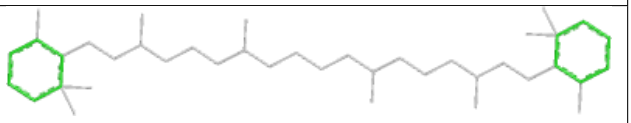
Bond lengths



Bond angles

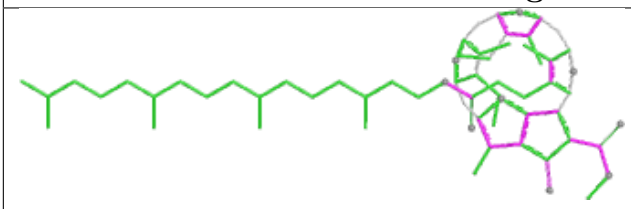


Torsions

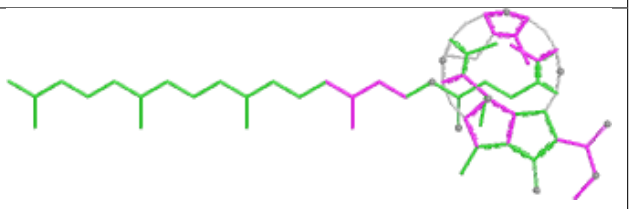


Rings

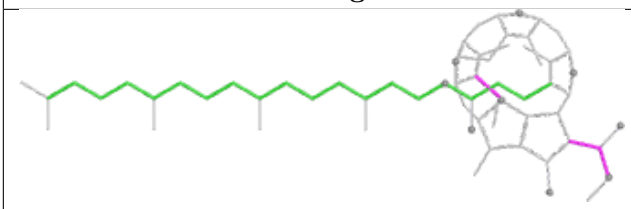
Ligand PHO a 606



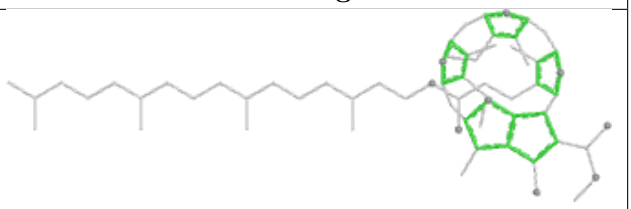
Bond lengths



Bond angles

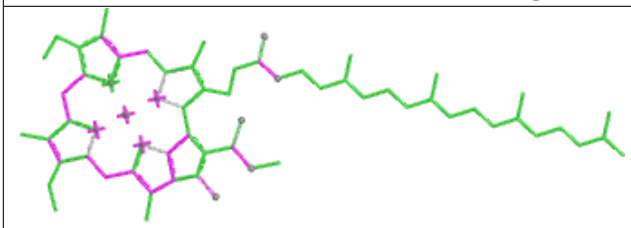


Torsions

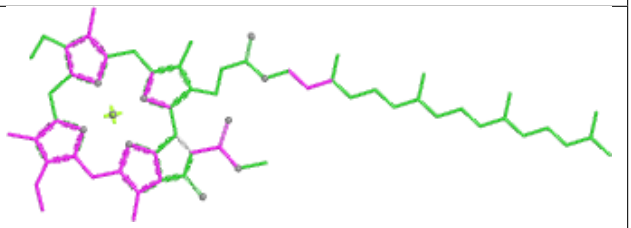


Rings

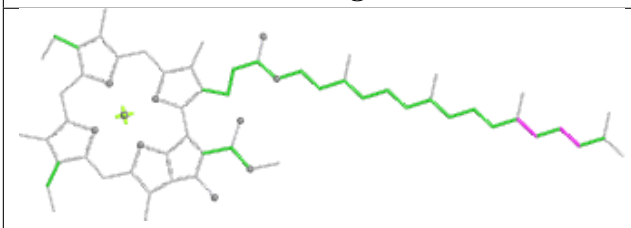
Ligand CLA b 612



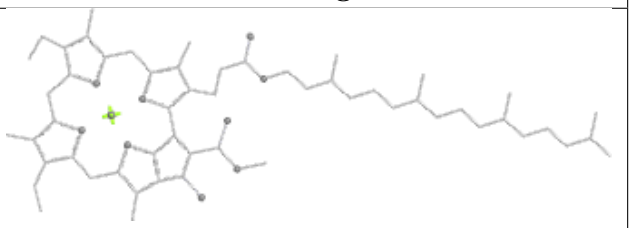
Bond lengths



Bond angles

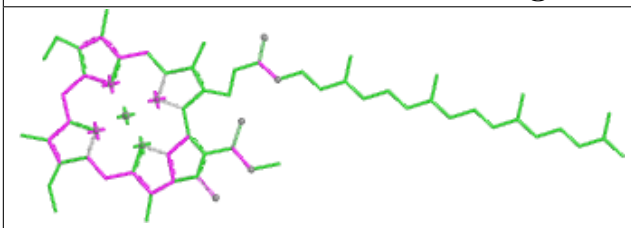


Torsions

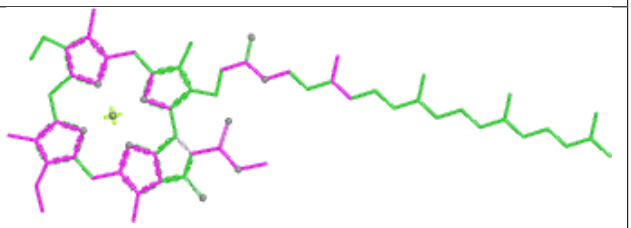


Rings

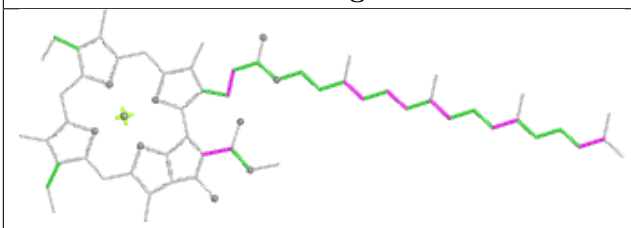
Ligand CLA c 507



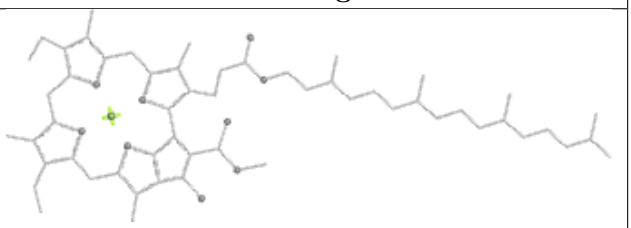
Bond lengths



Bond angles

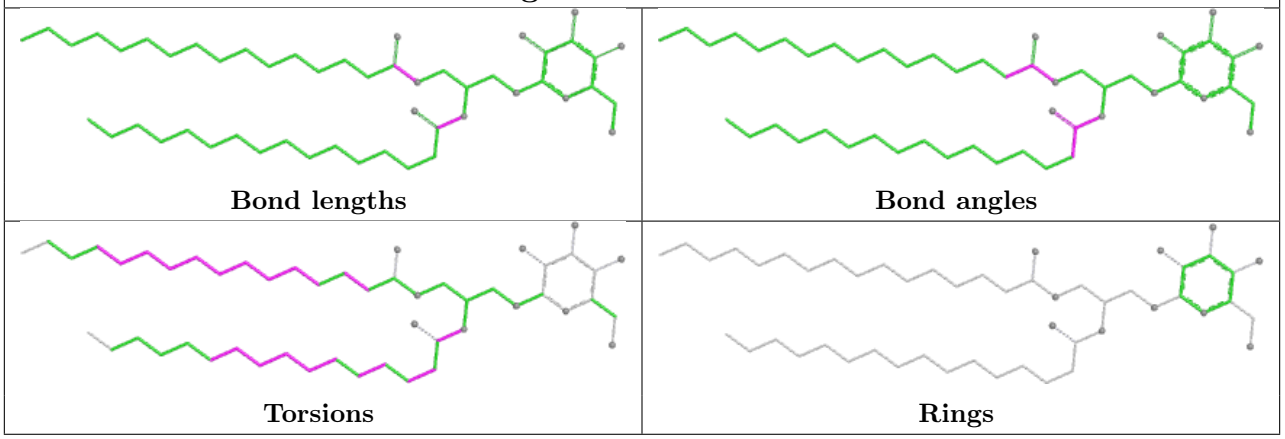


Torsions

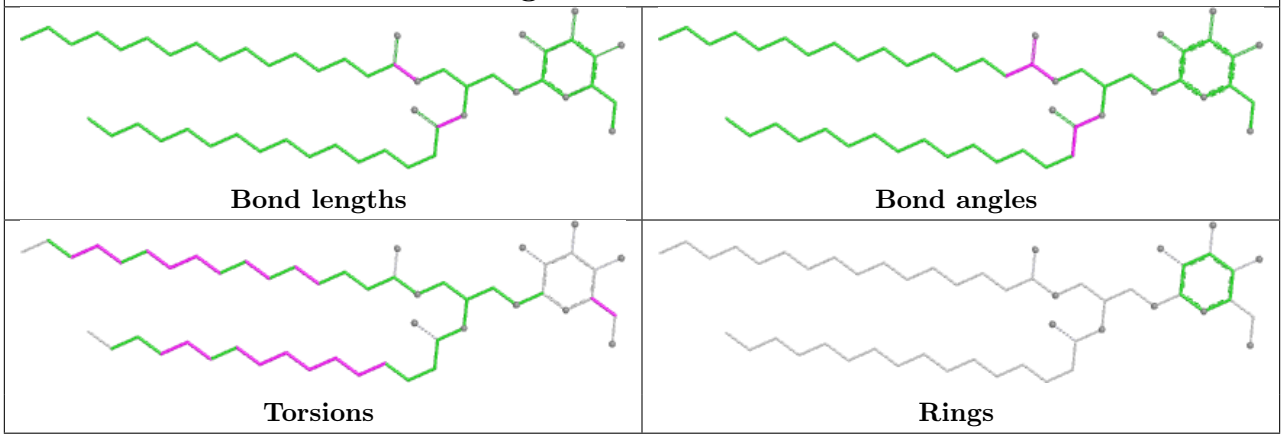


Rings

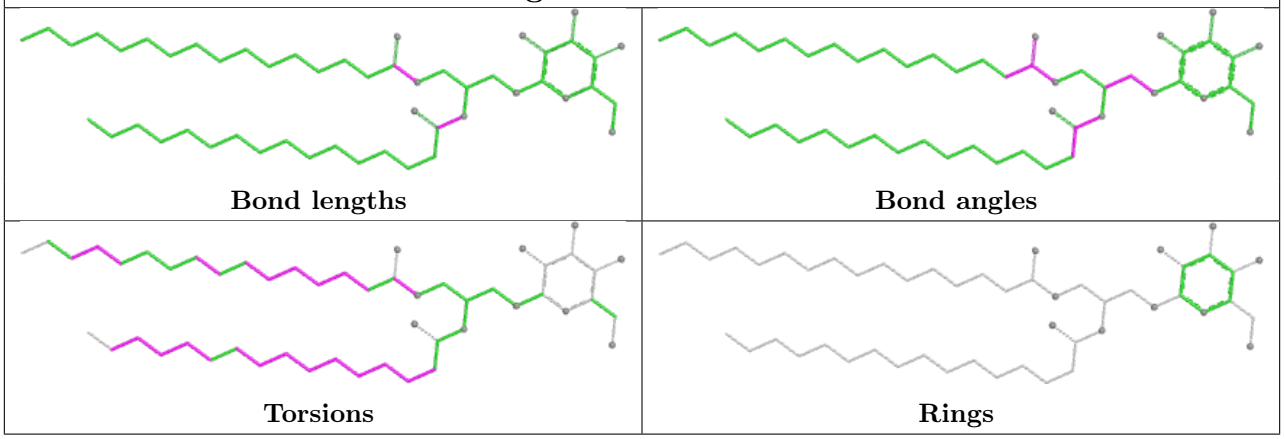
Ligand LMG B 620



Ligand LMG D 406



Ligand LMG c 519



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	334/334 (100%)	-0.59	0 100 100	16, 22, 43, 53	0
1	a	334/334 (100%)	-0.63	0 100 100	16, 22, 43, 53	0
2	B	504/504 (100%)	-0.62	0 100 100	18, 27, 49, 70	0
2	b	504/504 (100%)	-0.63	1 (0%) 91 84	18, 27, 49, 70	0
3	C	451/461 (97%)	-0.64	0 100 100	21, 31, 44, 56	0
3	c	451/461 (97%)	-0.75	0 100 100	21, 31, 44, 56	0
4	D	342/342 (100%)	-0.63	1 (0%) 90 81	17, 23, 39, 61	0
4	d	342/342 (100%)	-0.62	0 100 100	17, 23, 39, 61	0
5	E	81/81 (100%)	-0.65	0 100 100	27, 40, 57, 63	0
5	e	81/81 (100%)	-0.70	0 100 100	27, 40, 57, 63	0
6	F	34/34 (100%)	-0.65	0 100 100	28, 33, 58, 61	0
6	f	34/34 (100%)	-0.67	0 100 100	28, 33, 58, 61	0
7	H	65/65 (100%)	-0.59	0 100 100	23, 34, 40, 58	0
7	h	65/65 (100%)	-0.54	0 100 100	23, 34, 40, 58	0
8	I	38/38 (100%)	-0.54	0 100 100	30, 34, 65, 68	0
8	i	38/38 (100%)	-0.93	0 100 100	30, 34, 65, 68	0
9	J	38/40 (95%)	-0.95	0 100 100	26, 37, 68, 72	0
9	j	38/40 (95%)	-0.81	0 100 100	26, 37, 68, 72	0
10	K	37/37 (100%)	-0.77	0 100 100	33, 38, 45, 47	0
10	k	37/37 (100%)	-0.48	0 100 100	33, 38, 45, 47	0
11	L	37/37 (100%)	-0.54	0 100 100	17, 22, 50, 59	0
11	l	37/37 (100%)	-0.67	0 100 100	17, 22, 50, 59	0
12	M	34/34 (100%)	-0.26	1 (2%) 53 46	21, 23, 36, 52	0
12	m	34/34 (100%)	-0.32	0 100 100	21, 23, 36, 52	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	O	243/243 (100%)	-0.63	0 100 100	18, 32, 55, 71	0
13	o	243/243 (100%)	-0.64	1 (0%) 88 78	18, 32, 55, 71	0
14	T	30/30 (100%)	-0.17	0 100 100	19, 23, 44, 52	0
14	t	30/30 (100%)	-0.53	0 100 100	19, 23, 44, 52	0
15	U	97/97 (100%)	-0.58	0 100 100	23, 30, 48, 50	0
15	u	97/97 (100%)	-0.59	0 100 100	23, 30, 48, 50	0
16	V	137/137 (100%)	-0.69	0 100 100	23, 28, 39, 48	0
16	v	137/137 (100%)	-0.70	0 100 100	23, 28, 39, 48	0
17	X	39/39 (100%)	-0.73	0 100 100	33, 40, 66, 68	0
17	x	39/39 (100%)	-0.83	0 100 100	33, 40, 66, 68	0
18	Y	29/29 (100%)	-0.72	0 100 100	42, 48, 75, 77	0
18	y	29/29 (100%)	-0.51	0 100 100	42, 48, 75, 77	0
19	Z	62/62 (100%)	-0.72	0 100 100	39, 48, 68, 72	0
19	z	62/62 (100%)	-0.48	0 100 100	39, 48, 68, 72	0
All	All	5264/5288 (99%)	-0.64	4 (0%) 92 87	16, 28, 51, 77	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	183	LEU	2.5
12	M	23	ILE	2.4
2	b	268	PHE	2.4
13	o	101	ILE	2.0

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

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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
30	CA	F	102	1/1	0.11	0.12	56,56,56,56	0
30	CA	B	621	1/1	0.28	0.13	76,76,76,76	0
30	CA	f	102	1/1	0.41	0.16	56,56,56,56	0
27	BCT	a	612	4/4	0.43	0.31	39,39,40,42	0
26	CL	u	201	1/1	0.59	0.52	50,50,50,50	0
25	SQD	b	621	54/54	0.63	0.13	58,66,80,80	0
25	SQD	l	102	54/54	0.66	0.13	58,66,80,80	0
25	SQD	l	101	54/54	0.66	0.13	57,69,84,85	0
25	SQD	L	101	54/54	0.71	0.12	57,69,84,85	0
24	BCR	T	102	40/40	0.71	0.13	27,33,39,39	0
22	CLA	b	602	65/65	0.75	0.12	32,41,66,66	0
24	BCR	t	101	40/40	0.77	0.12	27,33,39,39	0
29	LMG	c	520	51/55	0.78	0.15	43,76,81,82	0
26	CL	a	610	1/1	0.78	0.17	24,24,24,24	0
22	CLA	b	607	65/65	0.79	0.12	24,28,40,41	0
29	LMG	b	619	51/55	0.79	0.18	29,39,51,54	0
22	CLA	a	604	65/65	0.80	0.15	19,21,63,65	0
29	LMG	C	520	51/55	0.80	0.13	43,76,81,82	0
24	BCR	A	608	40/40	0.82	0.13	22,27,32,32	0
22	CLA	b	608	65/65	0.82	0.14	17,20,32,34	0
32	LHG	E	101	42/49	0.82	0.15	69,83,86,86	0
24	BCR	T	101	40/40	0.83	0.13	23,27,28,29	0
22	CLA	C	513	65/65	0.83	0.12	39,45,64,64	0
24	BCR	C	514	40/40	0.83	0.11	37,43,47,47	0
25	SQD	a	609	54/54	0.83	0.14	49,57,66,67	0
26	CL	A	611	1/1	0.83	0.08	21,21,21,21	0
28	PL9	A	613	55/55	0.84	0.17	52,69,78,78	0
23	PHO	A	606	64/64	0.84	0.08	19,22,28,32	0
28	PL9	d	408	55/55	0.85	0.13	19,23,29,32	0
29	LMG	A	614	51/55	0.85	0.14	53,59,64,65	0
26	CL	A	610	1/1	0.85	0.10	24,24,24,24	0
24	BCR	d	404	40/40	0.85	0.12	25,30,48,49	0
24	BCR	k	101	40/40	0.85	0.12	34,38,39,39	0
26	CL	U	201	1/1	0.85	0.13	50,50,50,50	0
22	CLA	a	603	65/65	0.85	0.11	15,19,25,34	0
24	BCR	C	515	40/40	0.85	0.11	30,37,40,41	0
24	BCR	c	514	40/40	0.85	0.12	37,43,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
24	BCR	a	608	40/40	0.86	0.14	22,27,32,32	0
27	BCT	A	612	4/4	0.86	0.10	39,39,40,42	0
22	CLA	C	507	65/65	0.86	0.11	29,33,52,53	0
29	LMG	Z	101	37/55	0.86	0.08	55,84,88,88	0
22	CLA	C	508	65/65	0.87	0.12	25,29,54,58	0
22	CLA	C	511	65/65	0.87	0.09	29,34,37,38	0
25	SQD	A	609	54/54	0.87	0.12	49,57,66,67	0
22	CLA	A	604	65/65	0.87	0.15	19,21,63,65	0
28	PL9	D	408	55/55	0.87	0.15	19,23,29,32	0
24	BCR	B	618	40/40	0.87	0.10	23,27,28,29	0
22	CLA	c	501	65/65	0.87	0.11	29,32,44,46	0
31	DGD	C	516	62/66	0.87	0.14	23,33,61,62	0
32	LHG	d	409	49/49	0.87	0.13	26,33,62,64	0
29	LMG	B	620	51/55	0.87	0.14	29,39,51,54	0
22	CLA	D	403	65/65	0.88	0.14	24,27,65,67	0
29	LMG	z	101	37/55	0.88	0.09	55,84,88,88	0
22	CLA	A	603	65/65	0.88	0.12	15,19,25,34	0
22	CLA	B	602	65/65	0.88	0.08	32,41,66,66	0
22	CLA	B	607	65/65	0.88	0.10	24,28,40,41	0
22	CLA	b	613	65/65	0.88	0.12	20,24,30,31	0
31	DGD	d	410	62/66	0.88	0.12	77,89,103,103	0
32	LHG	D	407	49/49	0.88	0.16	24,28,37,40	0
24	BCR	b	622	40/40	0.88	0.12	25,37,44,45	0
22	CLA	b	617	65/65	0.88	0.10	22,29,77,78	0
24	BCR	K	102	40/40	0.89	0.11	29,33,37,37	0
29	LMG	C	519	51/55	0.89	0.16	31,57,72,73	0
22	CLA	B	613	65/65	0.89	0.12	20,24,30,31	0
22	CLA	C	504	65/65	0.89	0.11	25,28,54,54	0
29	LMG	d	406	51/55	0.89	0.14	26,35,65,67	0
22	CLA	b	614	65/65	0.89	0.10	19,22,45,47	0
24	BCR	b	618	40/40	0.89	0.13	21,28,40,40	0
22	CLA	c	512	65/65	0.89	0.10	37,41,62,63	0
30	CA	b	620	1/1	0.89	0.13	76,76,76,76	0
22	CLA	b	615	65/65	0.89	0.12	20,24,60,61	0
22	CLA	d	403	65/65	0.89	0.12	24,27,65,67	0
25	SQD	d	411	43/54	0.89	0.10	67,74,78,79	0
31	DGD	D	410	62/66	0.89	0.11	77,89,103,103	0
22	CLA	C	509	65/65	0.89	0.09	29,32,46,47	0
23	PHO	a	606	64/64	0.89	0.08	19,22,28,32	0
32	LHG	D	409	49/49	0.89	0.13	26,33,62,64	0
29	LMG	a	614	51/55	0.89	0.11	53,59,64,65	0
24	BCR	K	101	40/40	0.89	0.10	34,38,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
24	BCR	c	515	40/40	0.90	0.12	30,37,40,41	0
31	DGD	C	517	62/66	0.90	0.11	23,35,62,63	0
31	DGD	C	518	62/66	0.90	0.11	22,31,52,56	0
31	DGD	c	516	62/66	0.90	0.12	23,33,61,62	0
24	BCR	D	404	40/40	0.90	0.12	25,30,48,49	0
24	BCR	B	622	40/40	0.90	0.12	25,37,44,45	0
22	CLA	b	612	65/65	0.90	0.10	19,21,32,34	0
28	PL9	a	613	55/55	0.90	0.14	52,69,78,78	0
32	LHG	d	407	49/49	0.90	0.13	24,28,37,40	0
26	CL	a	611	1/1	0.90	0.05	21,21,21,21	0
22	CLA	c	503	65/65	0.90	0.09	27,31,35,36	0
22	CLA	c	502	65/65	0.91	0.10	24,26,39,42	0
24	BCR	H	101	40/40	0.91	0.13	26,33,42,42	0
31	DGD	c	518	62/66	0.91	0.11	22,31,52,56	0
22	CLA	C	512	65/65	0.91	0.10	37,41,62,63	0
25	SQD	D	411	43/54	0.91	0.10	67,74,78,79	0
22	CLA	C	501	65/65	0.91	0.11	29,32,44,46	0
22	CLA	c	513	65/65	0.91	0.09	39,45,64,64	0
22	CLA	D	401	65/65	0.91	0.10	13,18,34,35	0
22	CLA	D	402	65/65	0.91	0.11	14,18,29,35	0
22	CLA	b	603	65/65	0.91	0.09	23,26,32,32	0
32	LHG	l	103	49/49	0.91	0.12	23,31,43,44	0
24	BCR	B	619	40/40	0.92	0.11	21,28,40,40	0
22	CLA	d	402	65/65	0.92	0.11	14,18,29,35	0
22	CLA	c	511	65/65	0.92	0.09	29,34,37,38	0
22	CLA	B	611	65/65	0.92	0.09	21,25,32,37	0
22	CLA	B	615	65/65	0.92	0.10	20,24,60,61	0
22	CLA	B	616	65/65	0.92	0.10	25,27,45,46	0
22	CLA	B	617	65/65	0.92	0.10	22,29,77,78	0
32	LHG	e	101	42/49	0.92	0.10	69,83,86,86	0
22	CLA	c	510	65/65	0.92	0.07	24,28,35,37	0
22	CLA	B	609	65/65	0.93	0.09	20,24,31,31	0
22	CLA	B	606	65/65	0.93	0.08	19,23,34,35	0
29	LMG	D	406	51/55	0.93	0.11	26,35,65,67	0
24	BCR	k	102	40/40	0.93	0.08	29,33,37,37	0
22	CLA	C	506	65/65	0.93	0.09	31,38,74,75	0
32	LHG	D	405	49/49	0.93	0.13	29,34,41,41	0
22	CLA	B	608	65/65	0.93	0.09	17,20,32,34	0
23	PHO	a	605	64/64	0.93	0.10	16,21,25,26	0
22	CLA	c	507	65/65	0.93	0.07	29,33,52,53	0
24	BCR	h	101	40/40	0.93	0.09	26,33,42,42	0
25	SQD	B	601	54/54	0.93	0.12	50,63,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
25	SQD	b	601	54/54	0.93	0.12	50,63,68,68	0
22	CLA	c	508	65/65	0.93	0.09	25,29,54,58	0
22	CLA	b	616	65/65	0.94	0.07	25,27,45,46	0
22	CLA	b	604	65/65	0.94	0.08	18,22,31,35	0
22	CLA	b	610	65/65	0.94	0.09	23,28,31,32	0
32	LHG	d	405	49/49	0.94	0.10	29,34,41,41	0
22	CLA	B	612	65/65	0.94	0.08	19,21,32,34	0
29	LMG	c	519	51/55	0.94	0.13	31,57,72,73	0
23	PHO	A	605	64/64	0.94	0.07	16,21,25,26	0
22	CLA	c	509	65/65	0.94	0.07	29,32,46,47	0
32	LHG	L	102	49/49	0.94	0.11	23,31,43,44	0
31	DGD	h	102	62/66	0.94	0.14	26,32,38,40	0
33	HEM	F	101	43/43	0.94	0.09	39,42,45,47	0
33	HEM	f	101	43/43	0.94	0.09	39,42,45,47	0
31	DGD	c	517	62/66	0.95	0.07	23,35,62,63	0
22	CLA	b	609	65/65	0.95	0.09	20,24,31,31	0
22	CLA	C	510	65/65	0.95	0.05	24,28,35,37	0
30	CA	O	301	1/1	0.95	0.03	49,49,49,49	0
31	DGD	H	102	62/66	0.95	0.09	26,32,38,40	0
22	CLA	A	607	65/65	0.95	0.08	21,24,71,72	0
22	CLA	c	506	65/65	0.95	0.08	31,38,74,75	0
22	CLA	b	605	65/65	0.95	0.08	19,22,50,51	0
22	CLA	C	502	65/65	0.95	0.09	24,26,39,42	0
22	CLA	c	504	65/65	0.96	0.07	25,28,54,54	0
22	CLA	c	505	65/65	0.96	0.07	28,30,44,45	0
22	CLA	b	606	65/65	0.96	0.06	19,23,34,35	0
22	CLA	C	503	65/65	0.96	0.08	27,31,35,36	0
22	CLA	a	607	65/65	0.96	0.07	21,24,71,72	0
22	CLA	C	505	65/65	0.96	0.07	28,30,44,45	0
22	CLA	d	401	65/65	0.96	0.06	13,18,34,35	0
22	CLA	B	603	65/65	0.96	0.08	23,26,32,32	0
34	MG	j	101	1/1	0.96	0.06	27,27,27,27	0
22	CLA	B	614	65/65	0.97	0.08	19,22,45,47	0
30	CA	o	301	1/1	0.97	0.03	49,49,49,49	0
22	CLA	b	611	65/65	0.97	0.06	21,25,32,37	0
22	CLA	B	610	65/65	0.97	0.07	23,28,31,32	0
33	HEM	V	201	43/43	0.97	0.08	23,24,27,29	0
33	HEM	v	201	43/43	0.97	0.09	23,24,27,29	0
22	CLA	B	605	65/65	0.97	0.07	19,22,50,51	0
22	CLA	B	604	65/65	0.98	0.07	18,22,31,35	0
21	FE2	a	602	1/1	0.99	0.19	26,26,26,26	0
20	OEX	A	601	10/10	0.99	0.06	22,23,26,26	0

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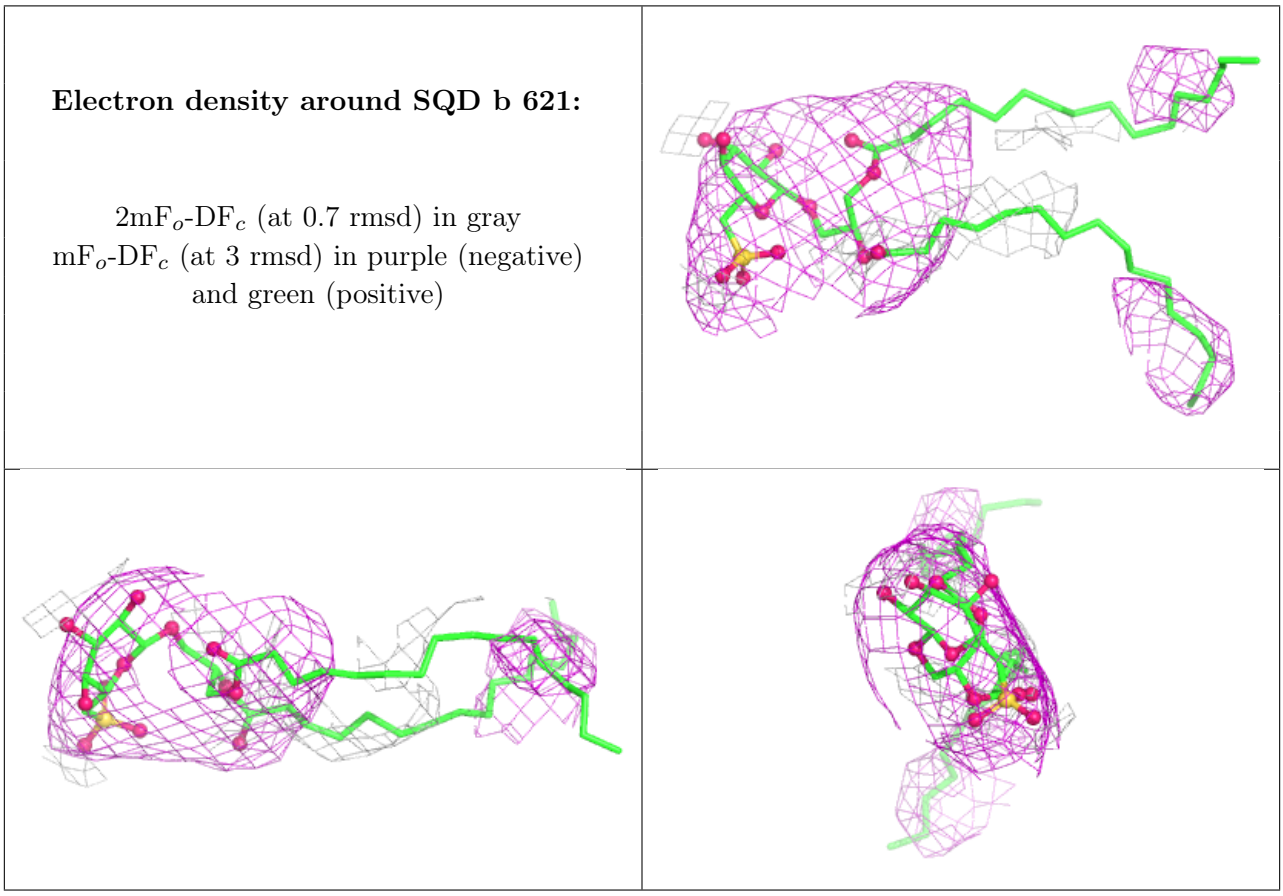
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
20	OEX	a	601	10/10	0.99	0.06	22,23,26,26	0
34	MG	J	101	1/1	1.00	0.04	27,27,27,27	0
21	FE2	A	602	1/1	1.00	0.04	26,26,26,26	0

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.

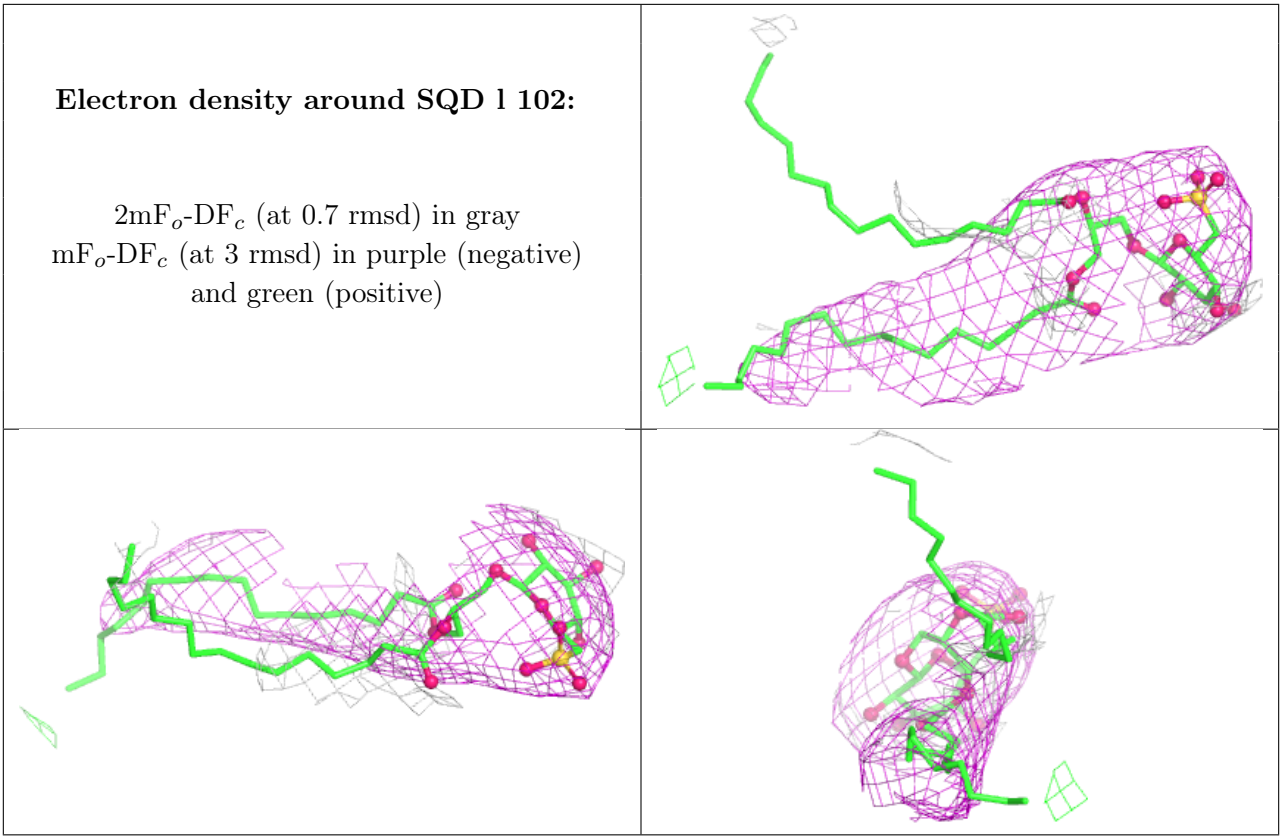
Electron density around SQD b 621:

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



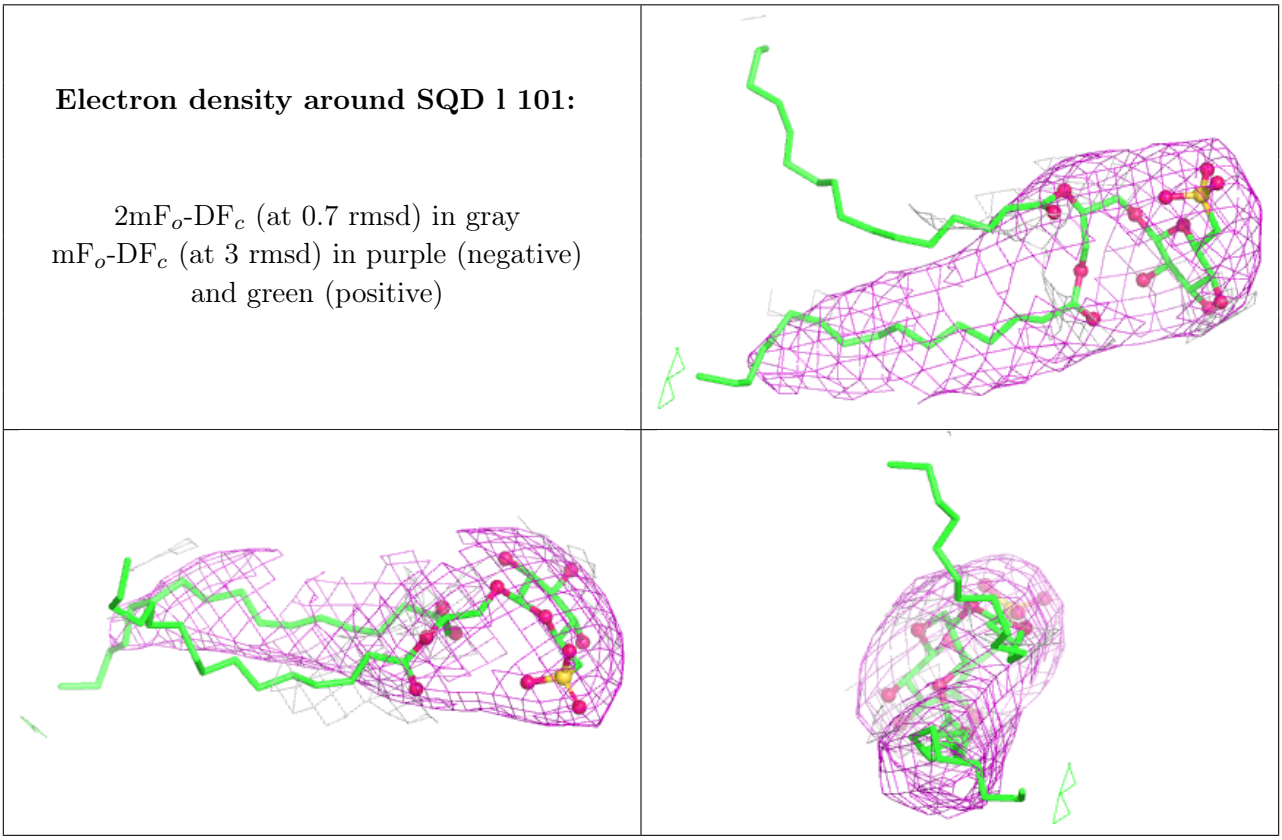
Electron density around SQD l 102:

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



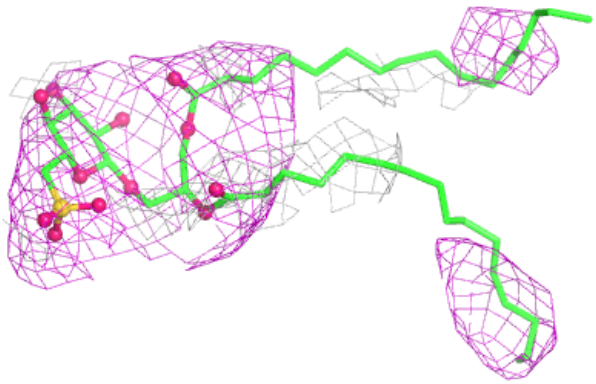
Electron density around SQD l 101:

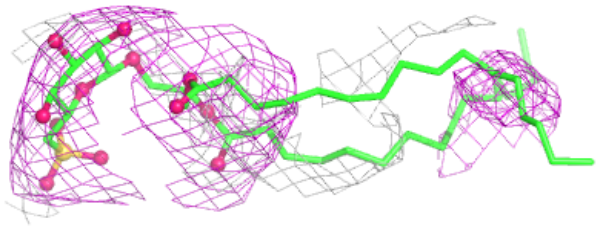
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

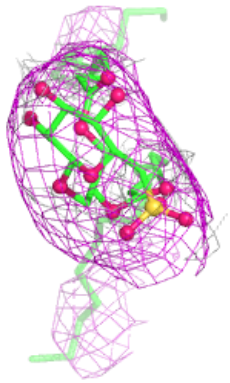


Electron density around SQD L 101:

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

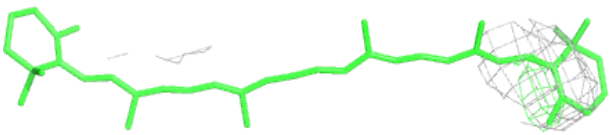


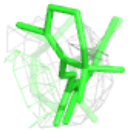




Electron density around BCR T 102:

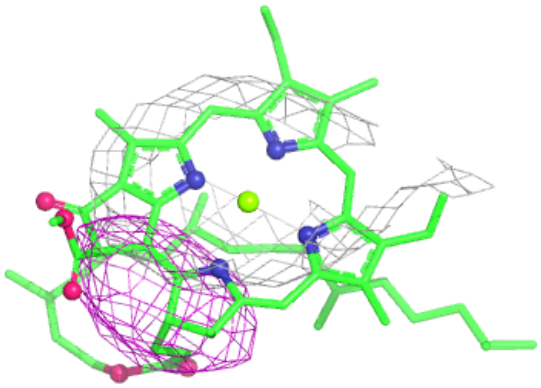
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

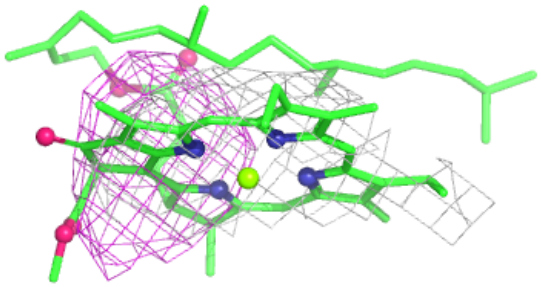


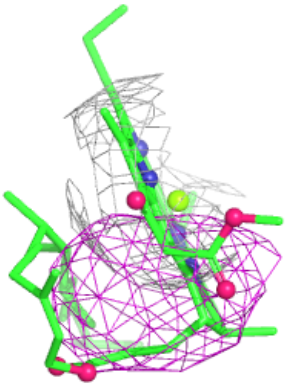


Electron density around CLA b 602:

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

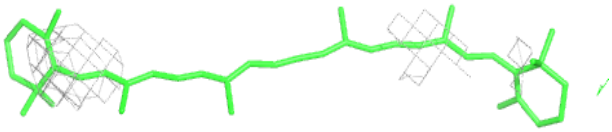


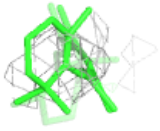




Electron density around BCR t 101:

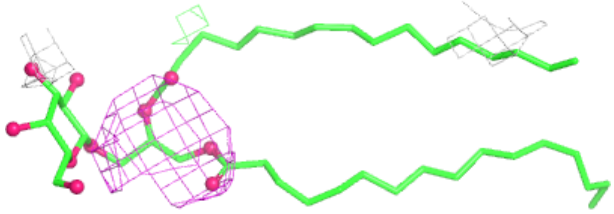
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

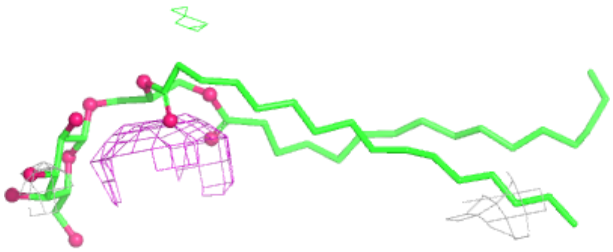


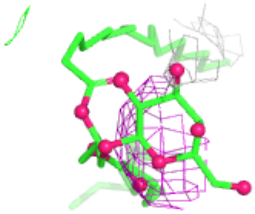


Electron density around LMG c 520:

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

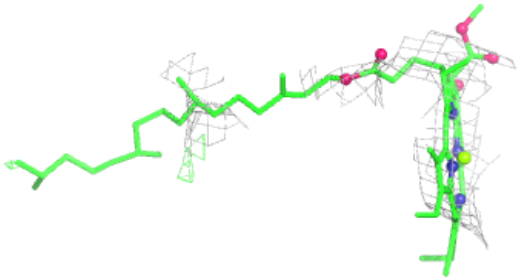


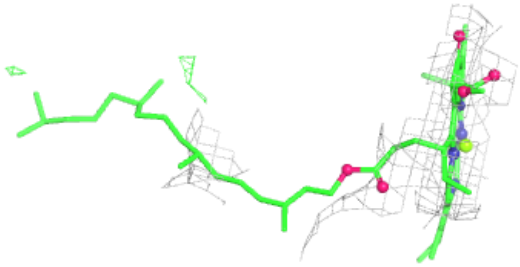


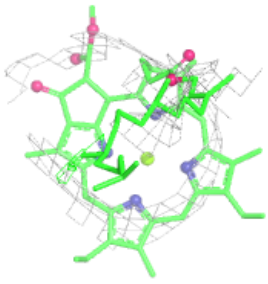


Electron density around CLA b 607:

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

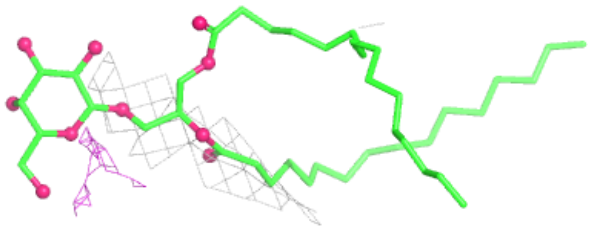






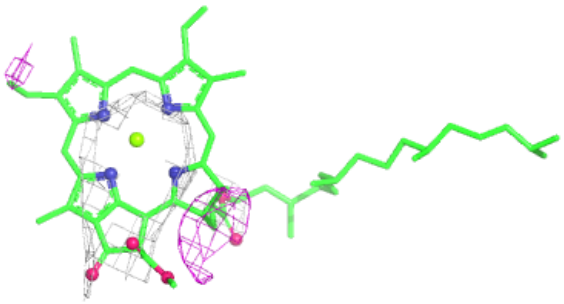
Electron density around LMG b 619:

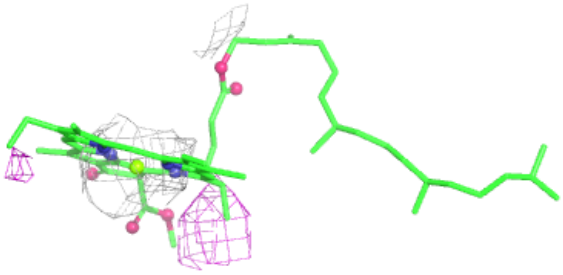
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

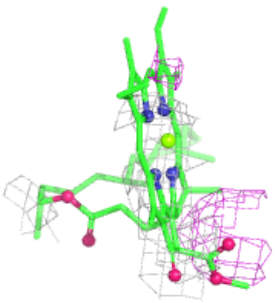


Electron density around CLA a 604:

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

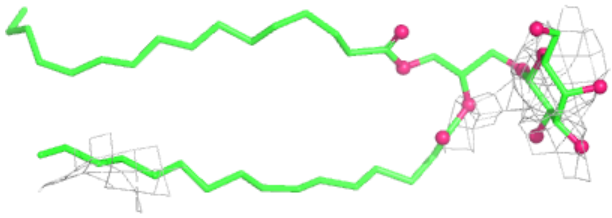


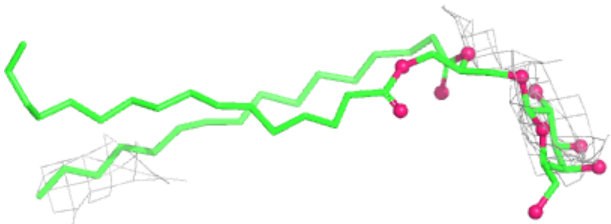


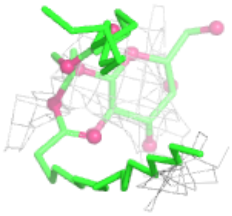


Electron density around LMG C 520:

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

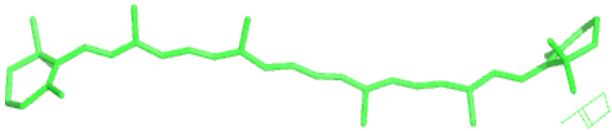


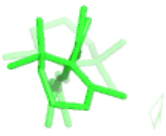




Electron density around BCR A 608:

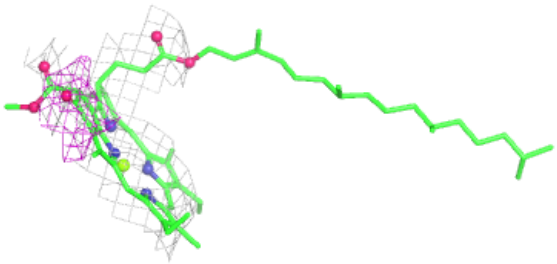
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

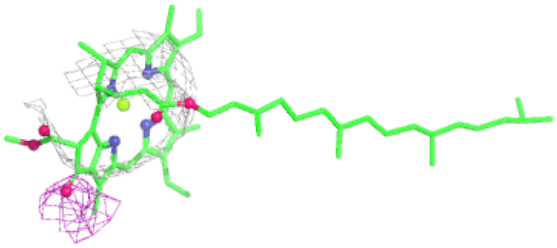


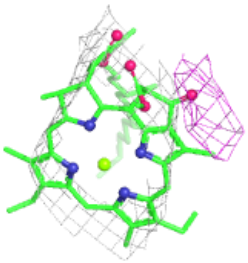


Electron density around CLA b 608:

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

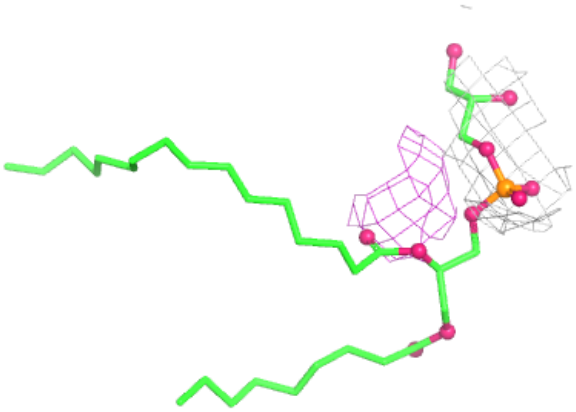


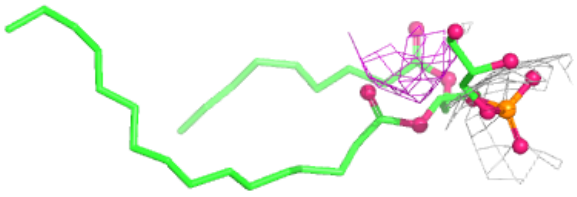




Electron density around LHG E 101:

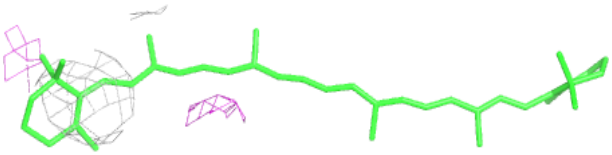
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

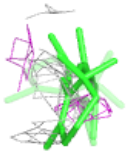




Electron density around BCR T 101:

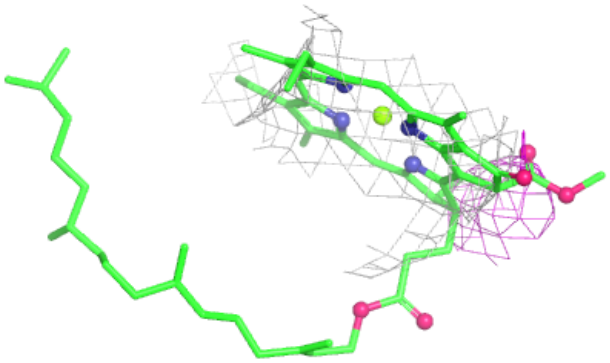
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

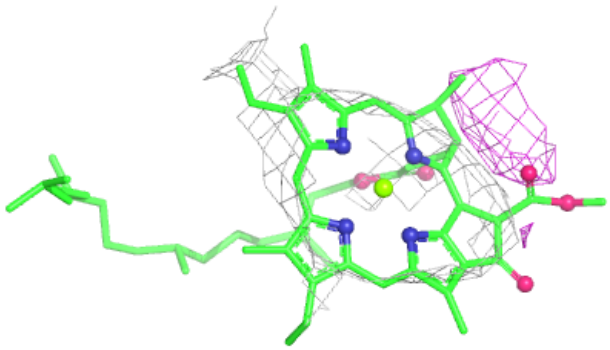


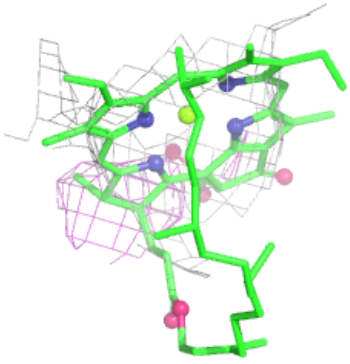


Electron density around CLA C 513:

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

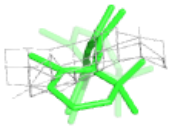






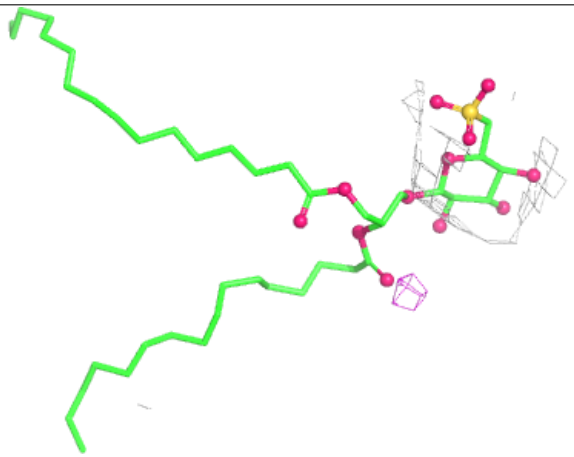
Electron density around BCR C 514:

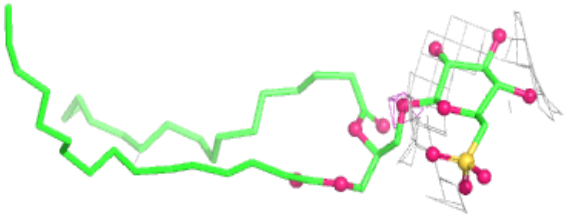
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around SQD a 609:

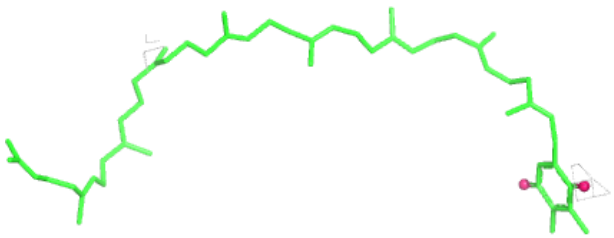
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

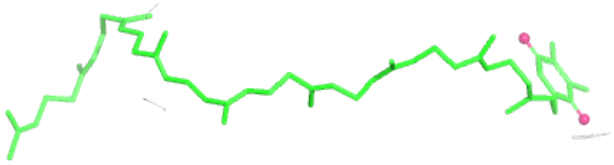


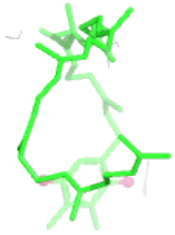


Electron density around PL9 A 613:

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

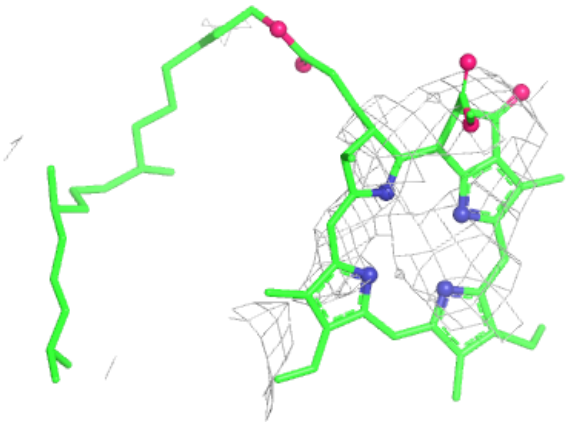


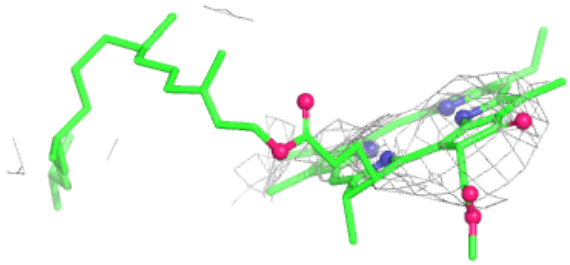




Electron density around PHO A 606:

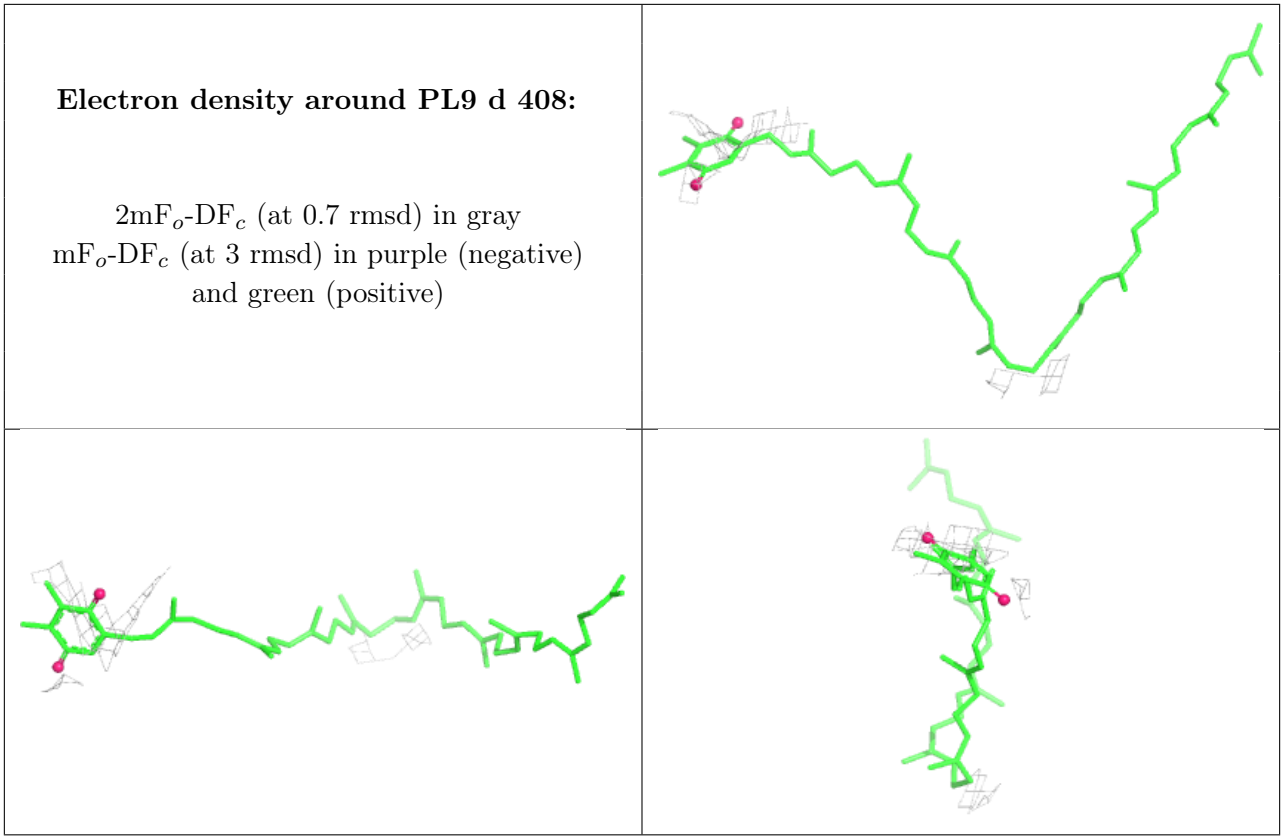
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





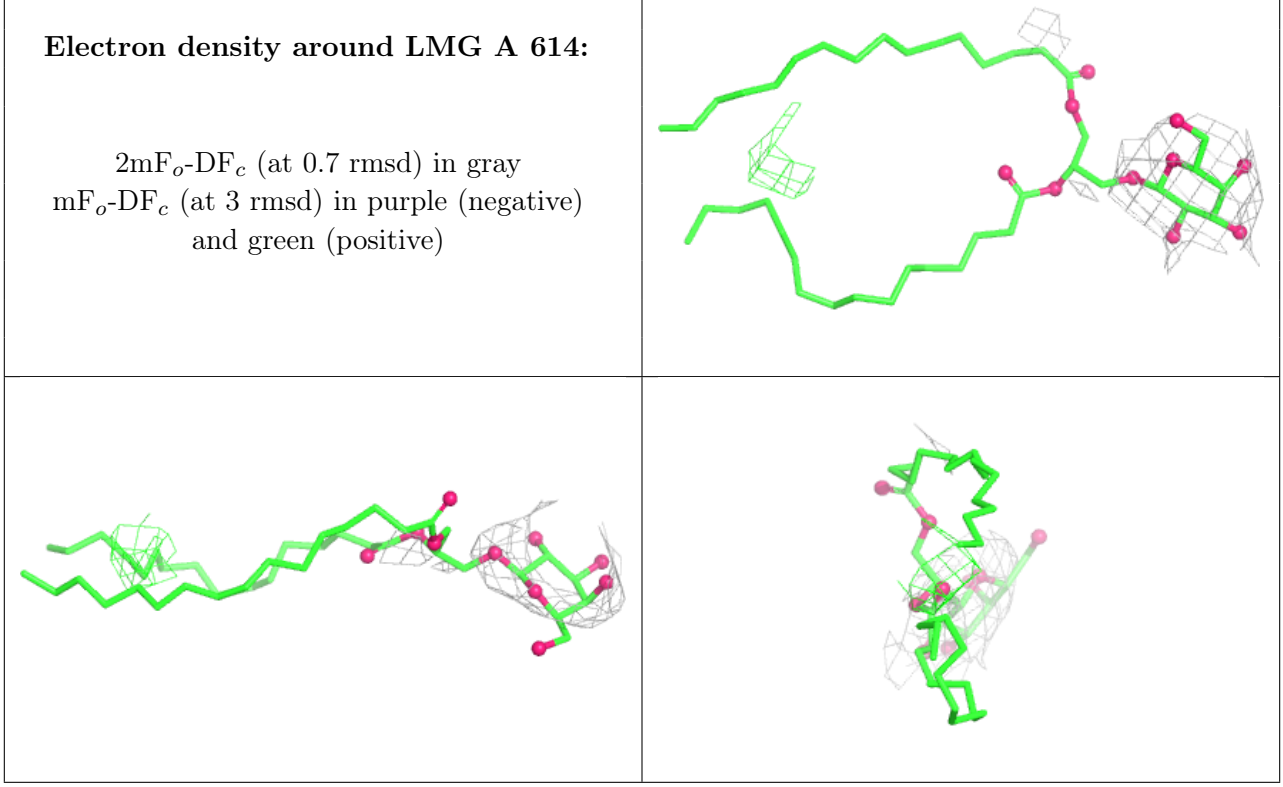
Electron density around PL9 d 408:

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



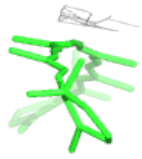
Electron density around LMG A 614:

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



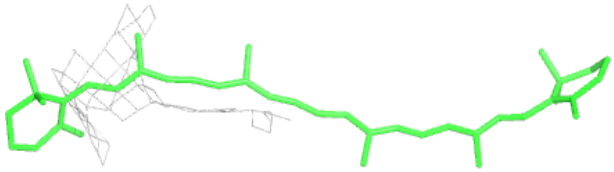
Electron density around BCR d 404:

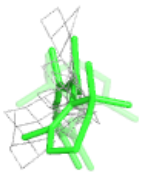
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around BCR k 101:

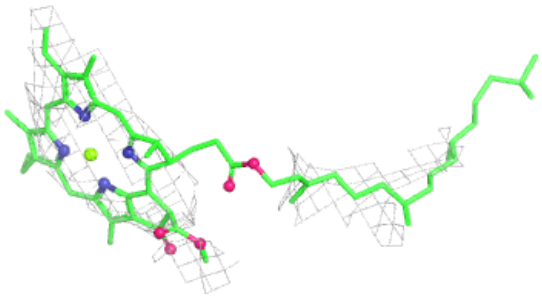
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

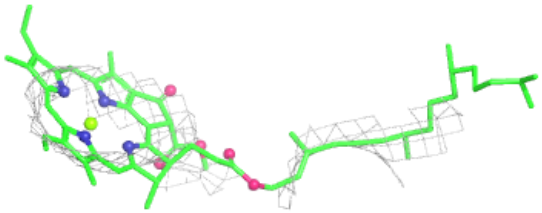


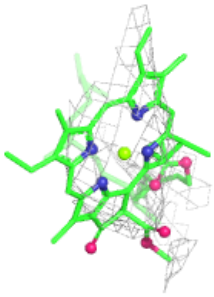


Electron density around CLA a 603:

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

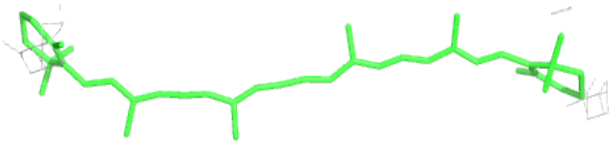


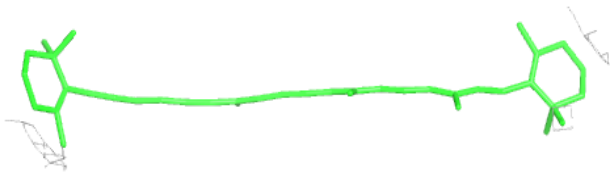




Electron density around BCR C 515:

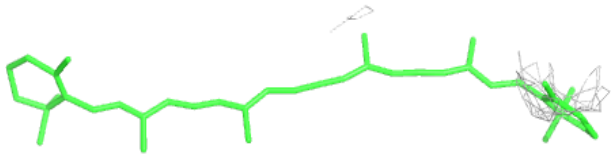
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

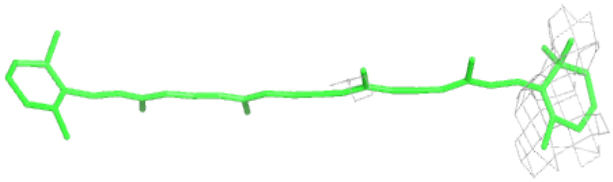


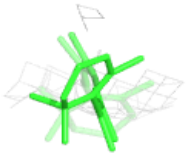


Electron density around BCR c 514:

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

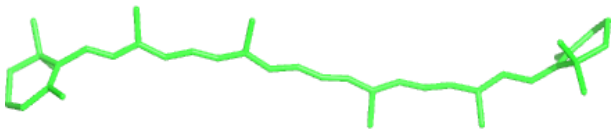


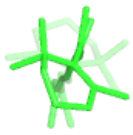




Electron density around BCR a 608:

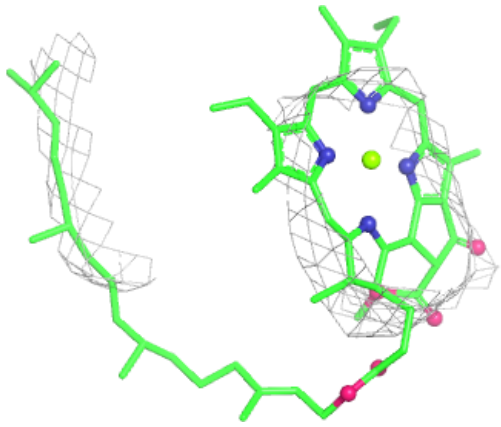
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

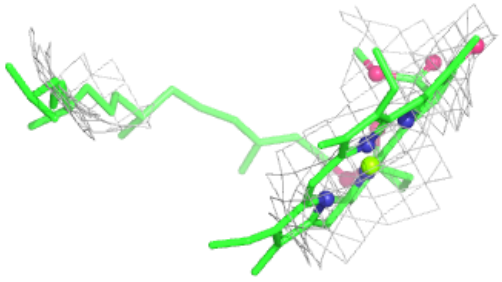




Electron density around CLA C 507:

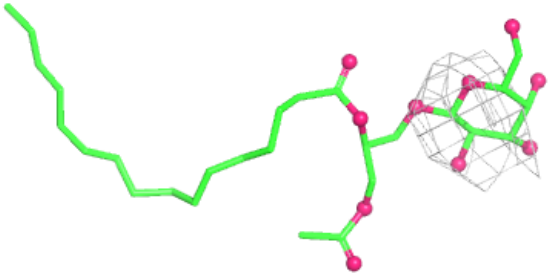
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

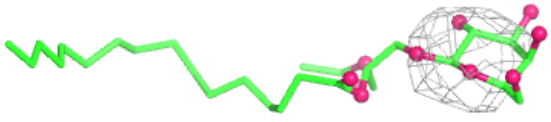


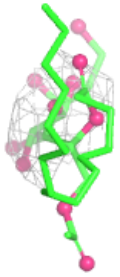


Electron density around LMG Z 101:

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

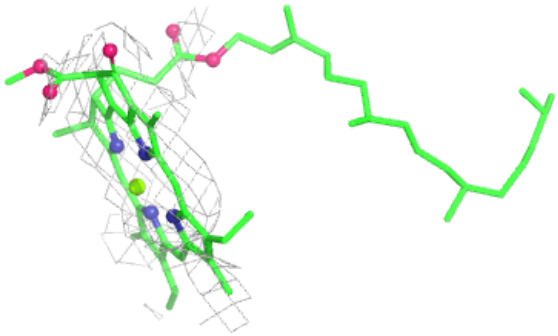


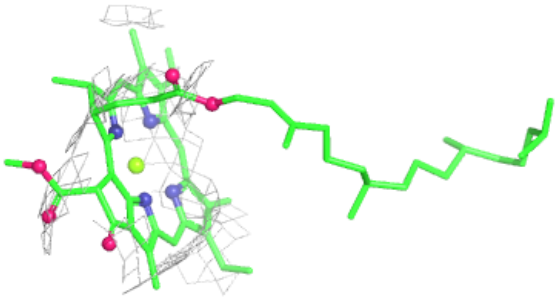


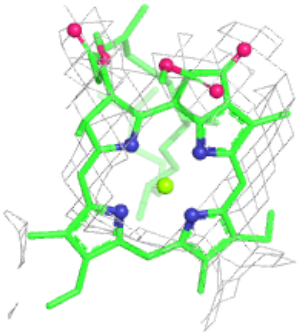


Electron density around CLA C 508:

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

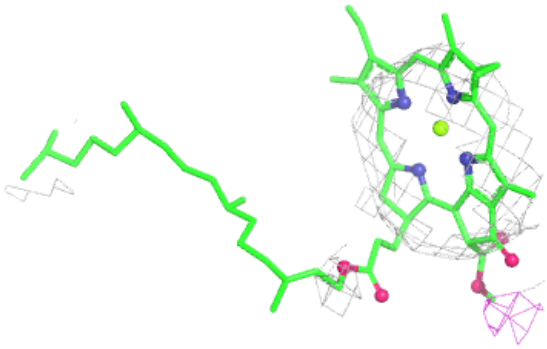


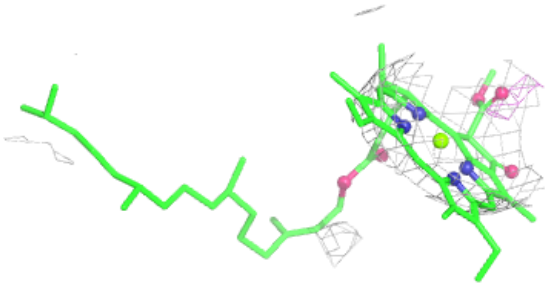




Electron density around CLA C 511:

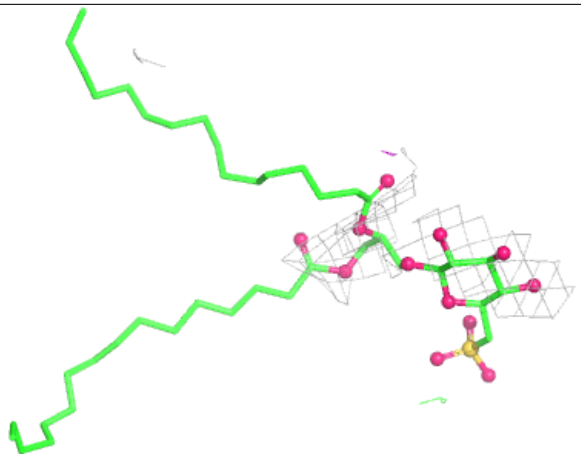
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

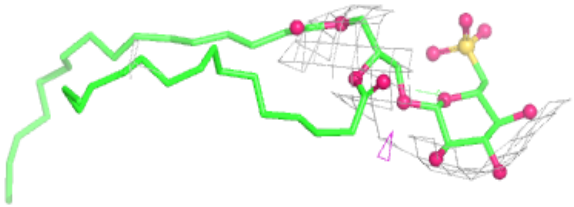


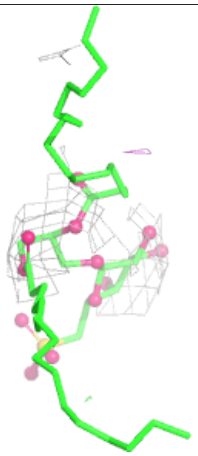


Electron density around SQD A 609:

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

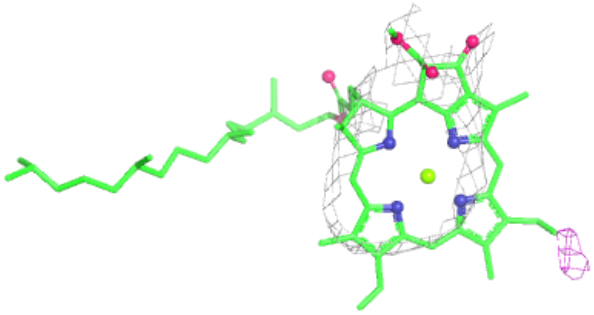


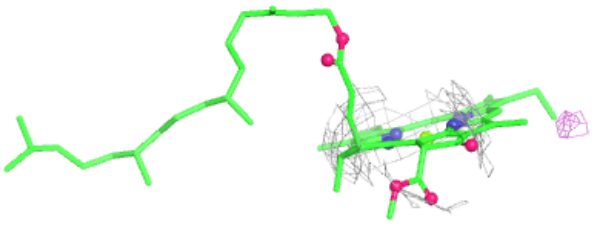


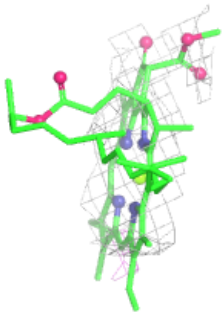


Electron density around CLA A 604:

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

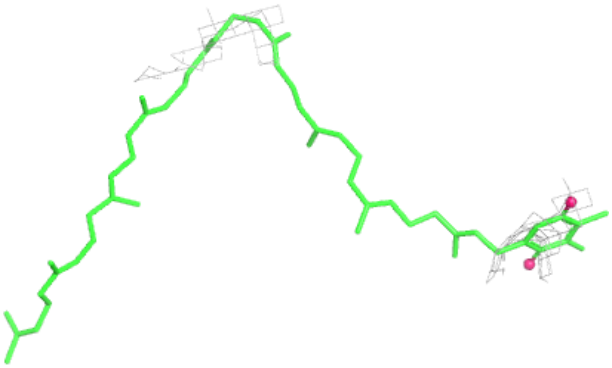


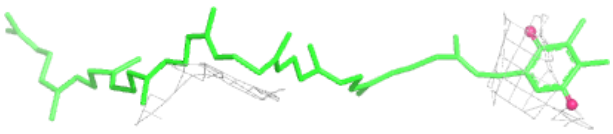




Electron density around PL9 D 408:

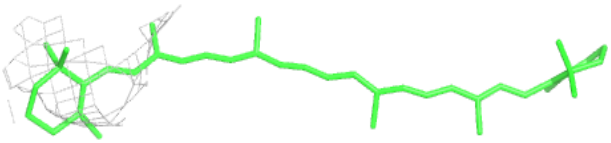
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

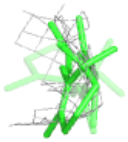




Electron density around BCR B 618:

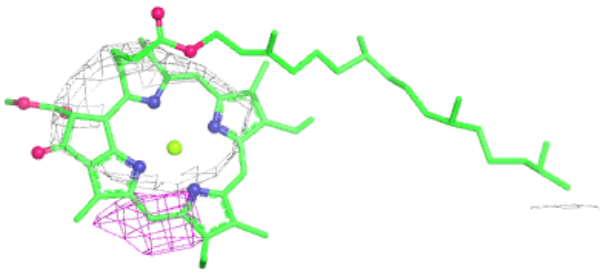
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

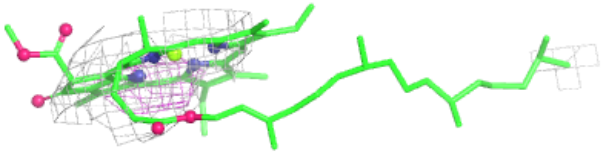


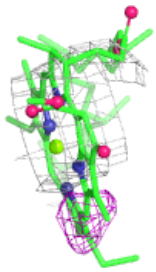


Electron density around CLA c 501:

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

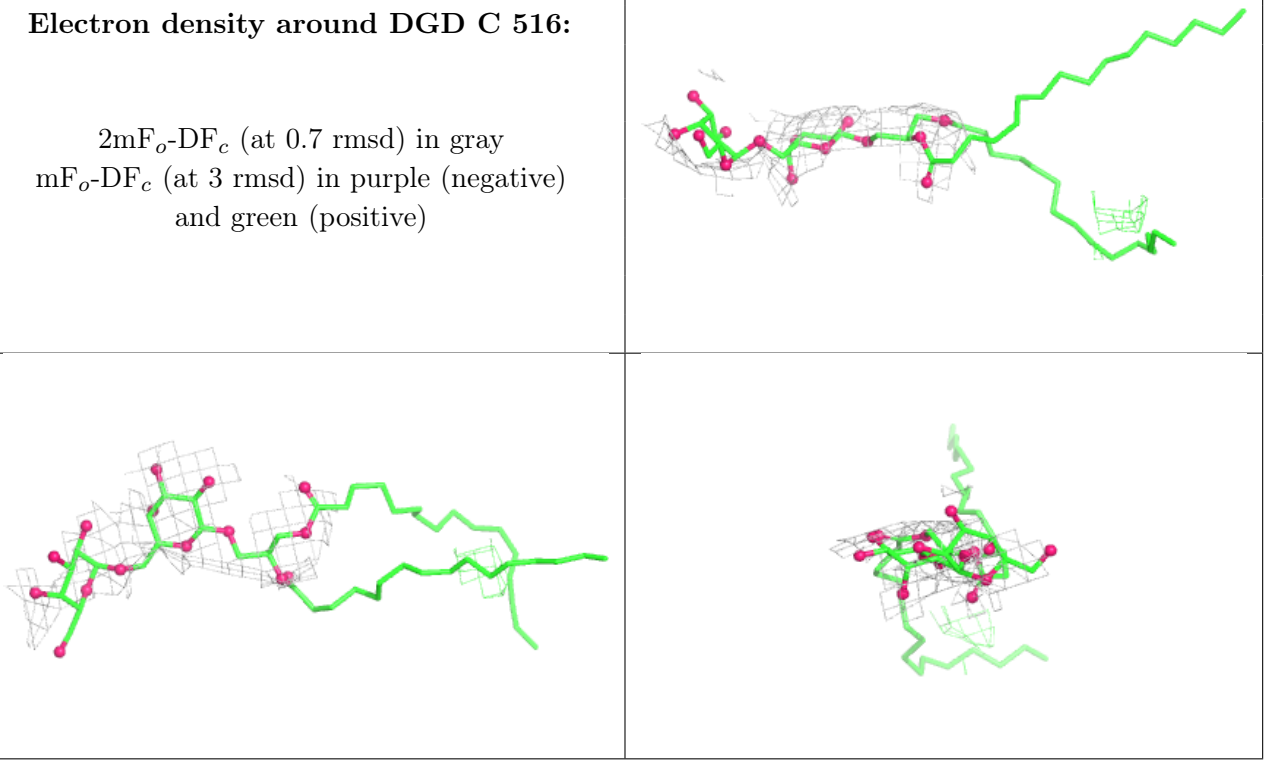






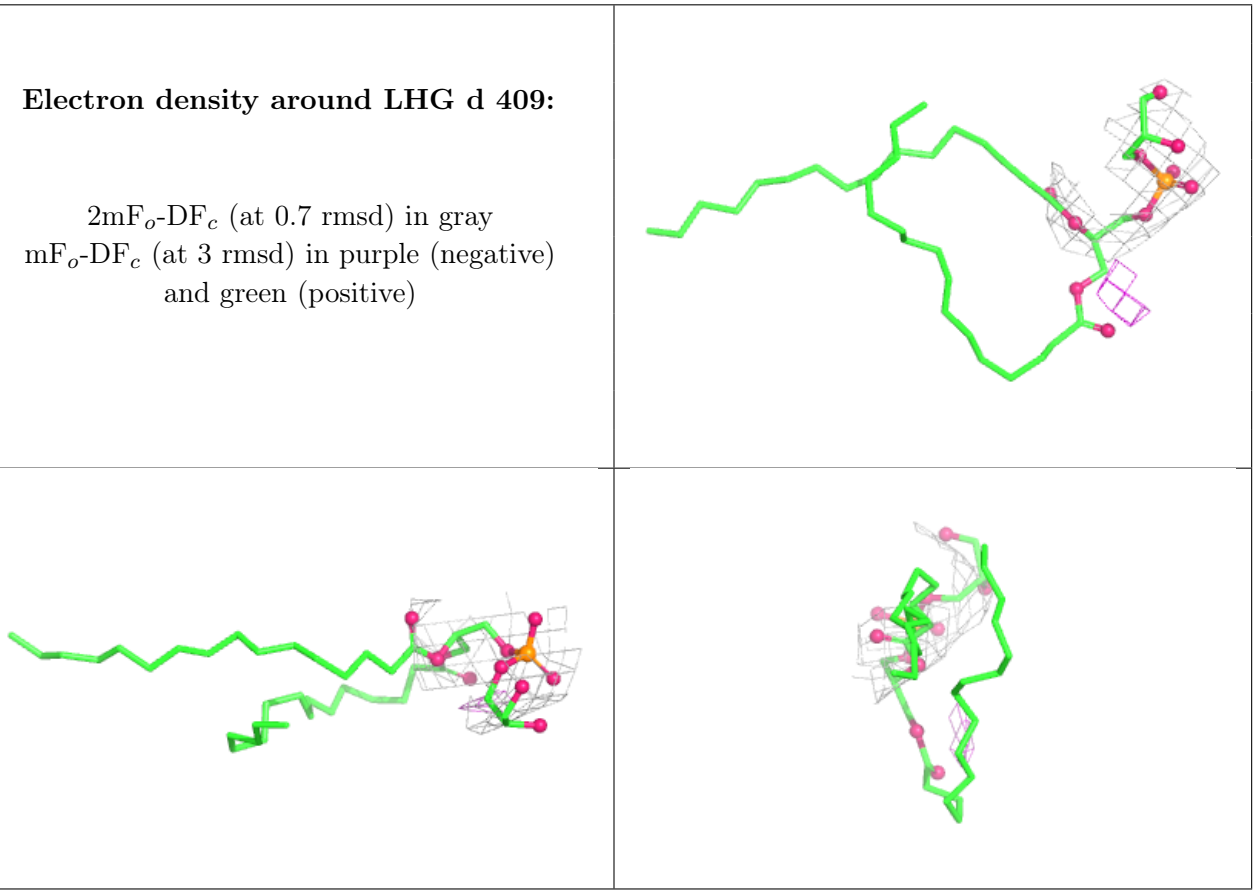
Electron density around DGD C 516:

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



Electron density around LHG d 409:

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

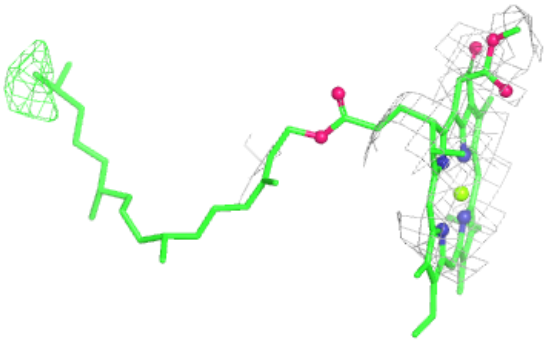


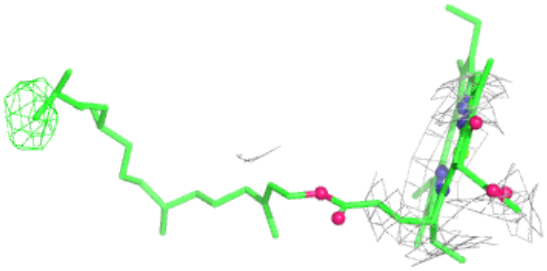
Electron density around LMG B 620:

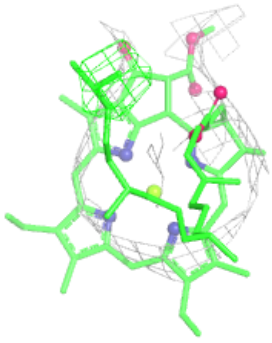
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

Electron density around CLA D 403:

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

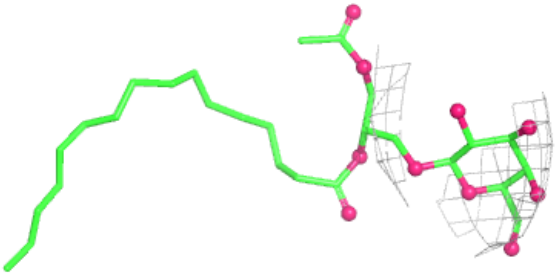


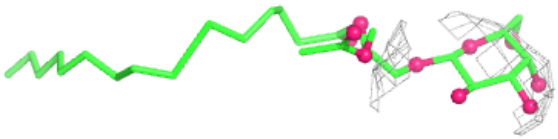




Electron density around LMG z 101:

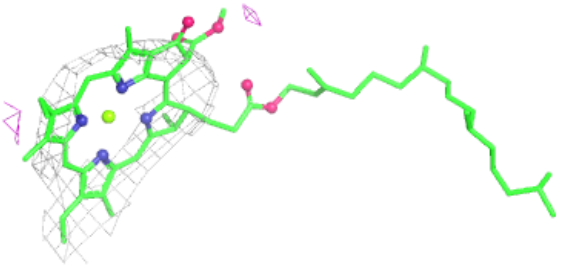
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





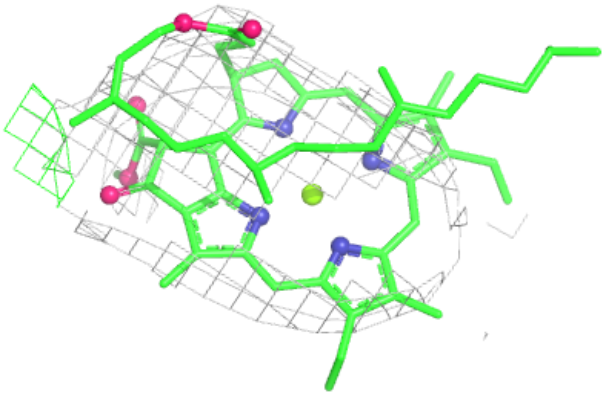
Electron density around CLA A 603:

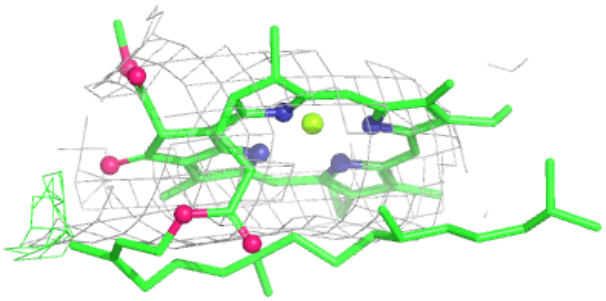
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CLA B 602:

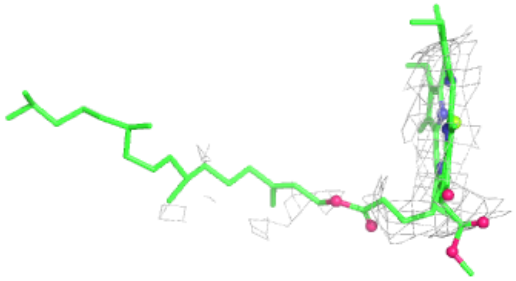
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

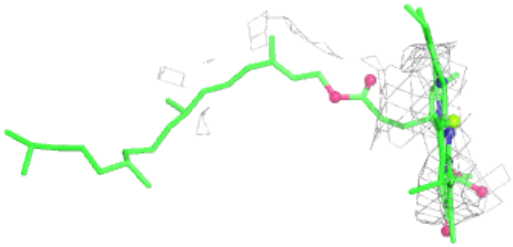


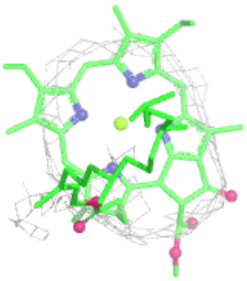


Electron density around CLA B 607:

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

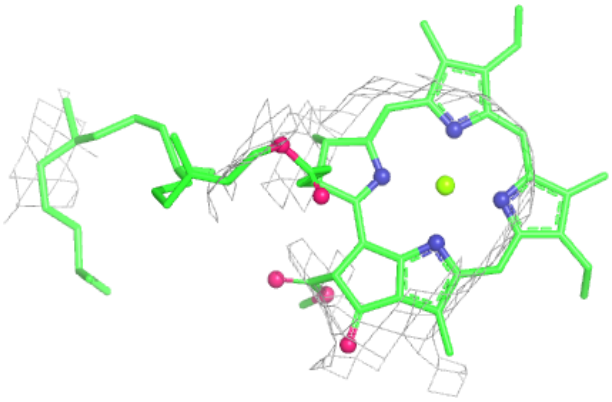


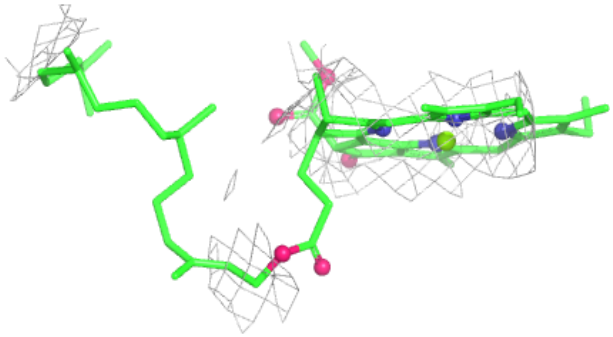


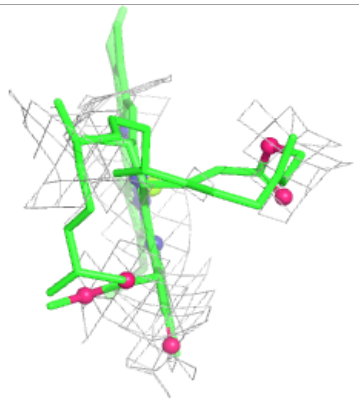


Electron density around CLA b 613:

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

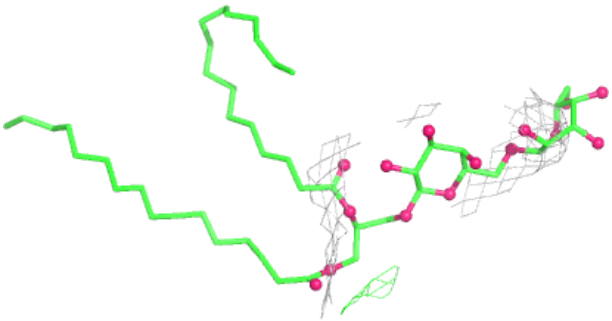


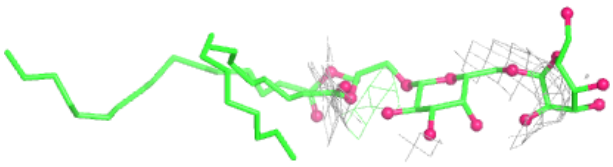


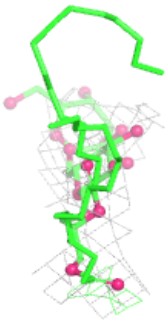


Electron density around DGD d 410:

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

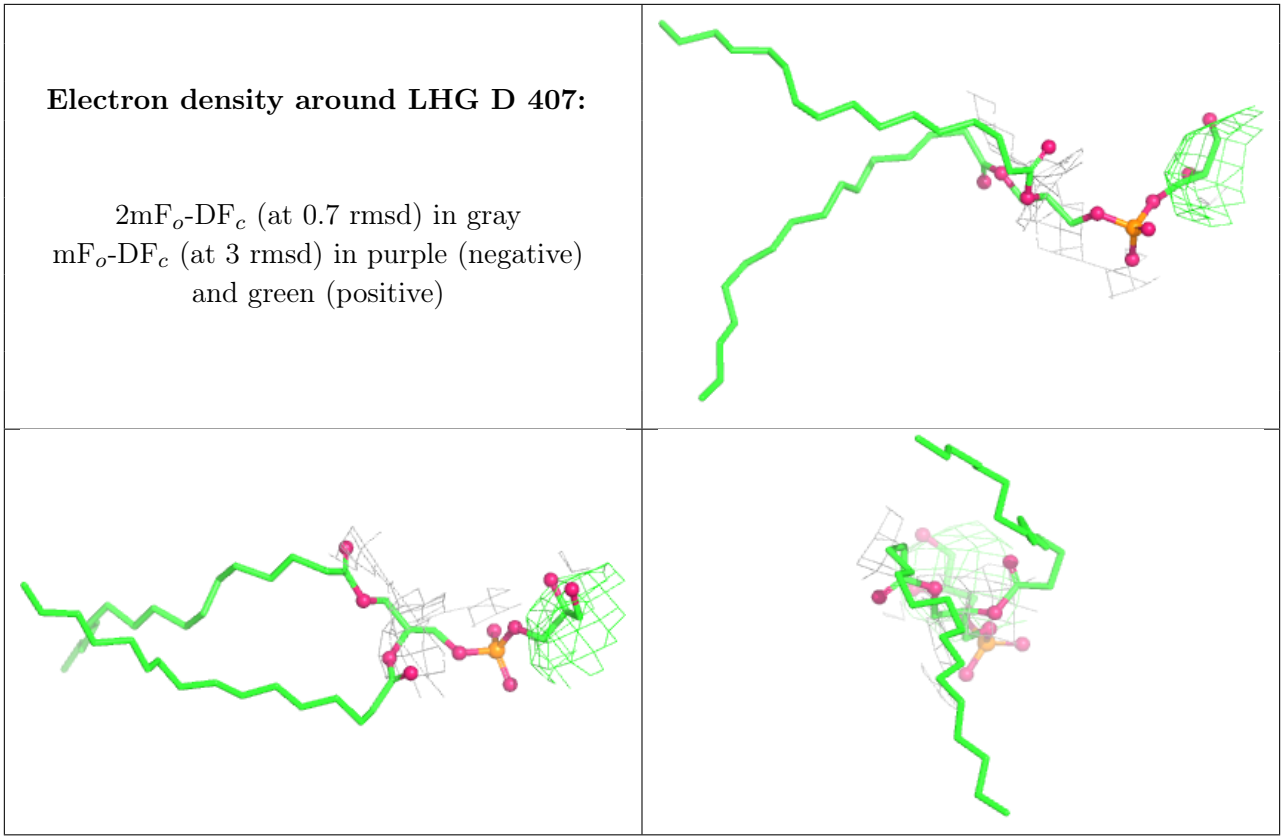






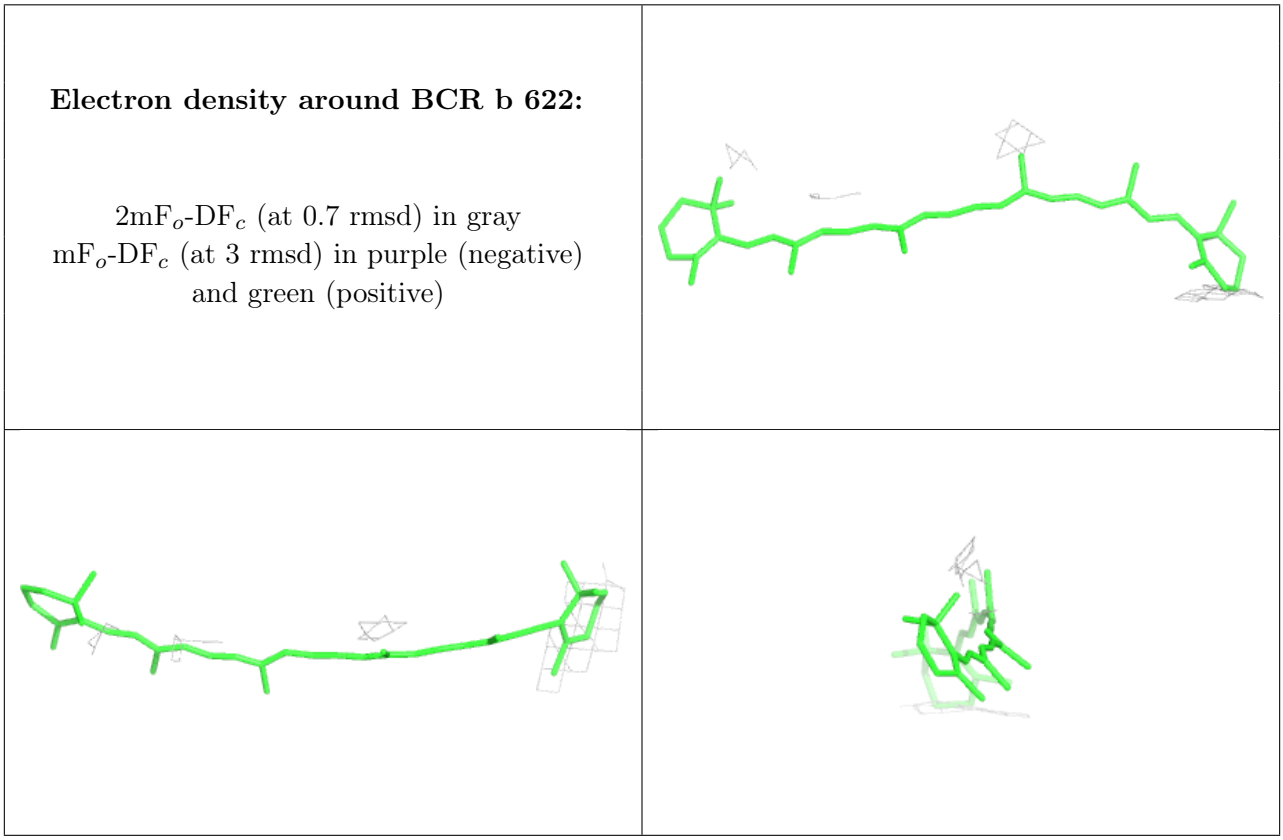
Electron density around LHG D 407:

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



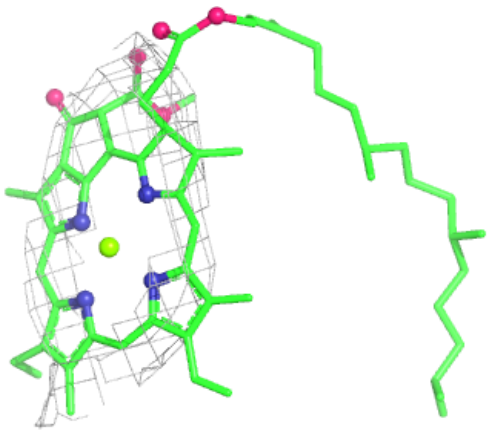
Electron density around BCR b 622:

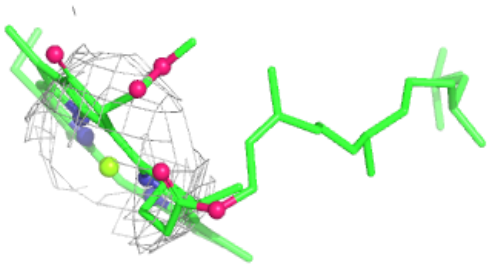
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

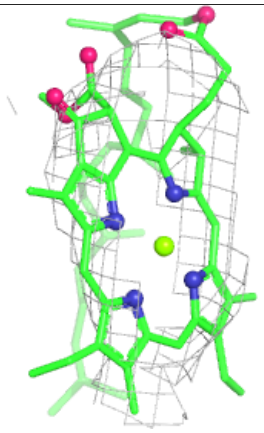


Electron density around CLA b 617:

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

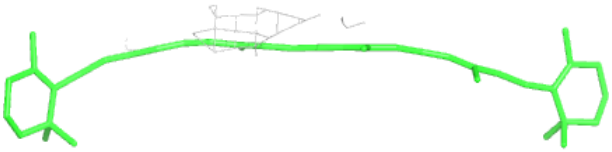


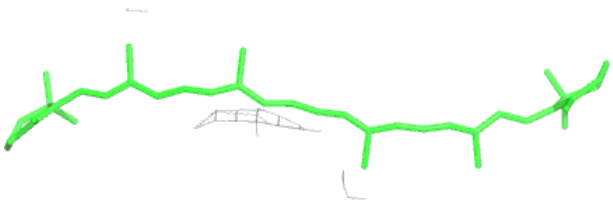


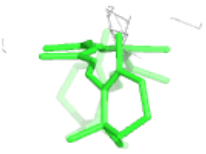


Electron density around BCR K 102:

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

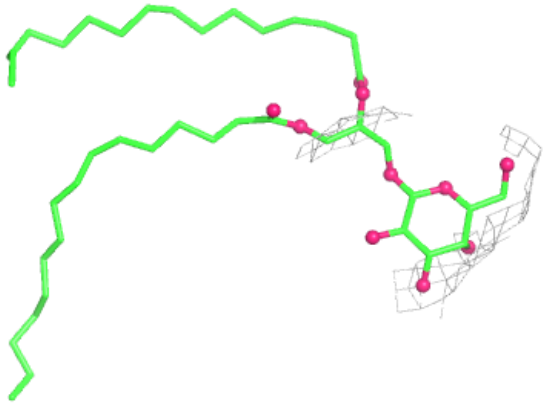


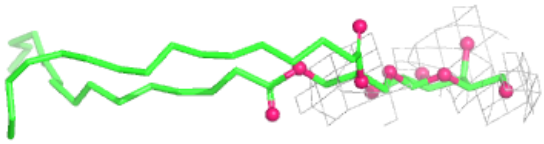




Electron density around LMG C 519:

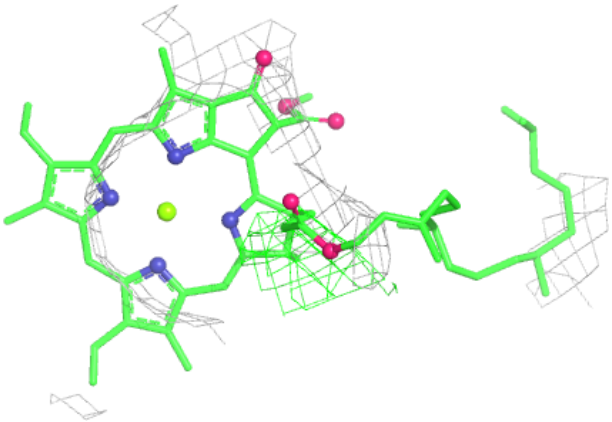
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

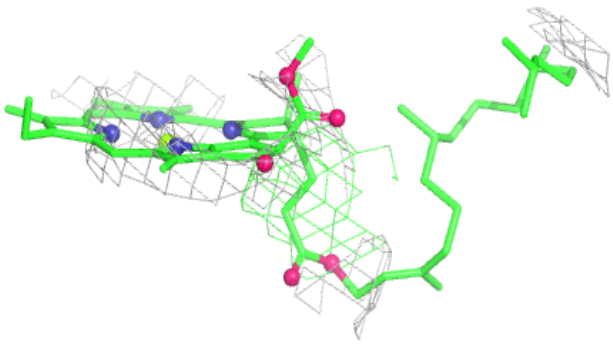


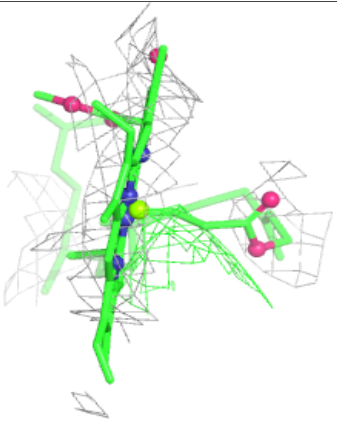


Electron density around CLA B 613:

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

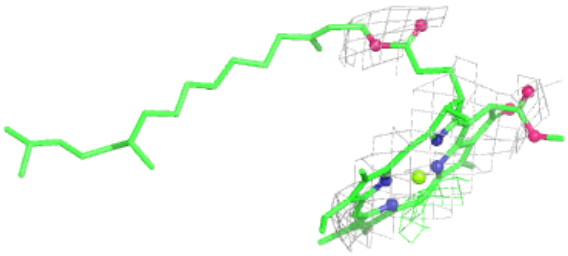


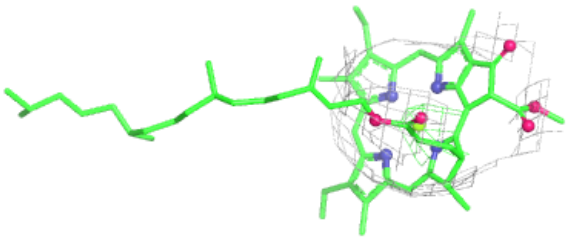


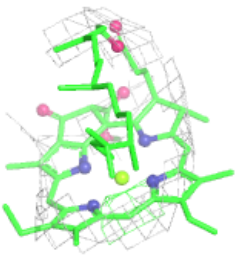


Electron density around CLA C 504:

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

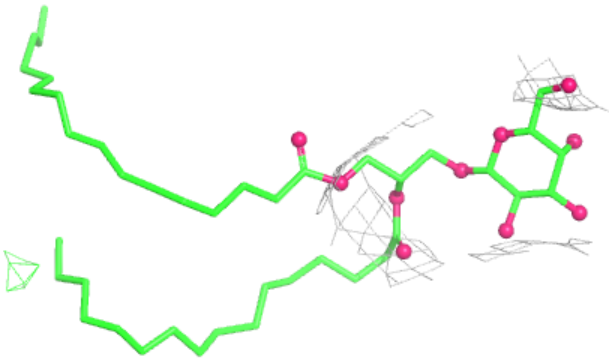


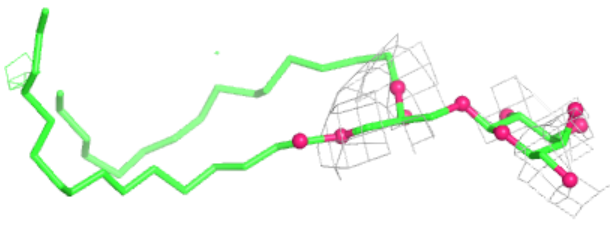




Electron density around LMG d 406:

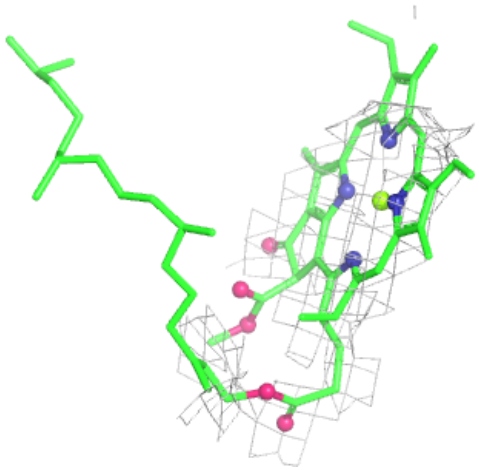
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

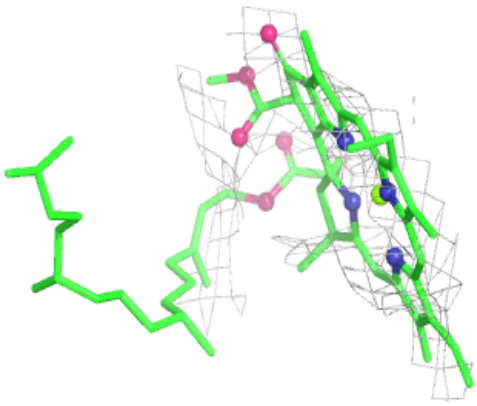


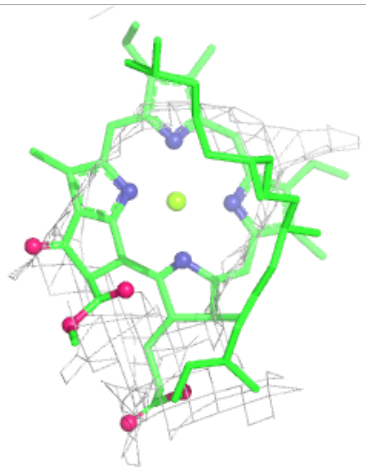


Electron density around CLA b 614:

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

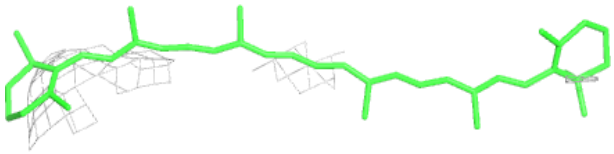


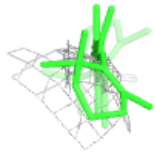




Electron density around BCR b 618:

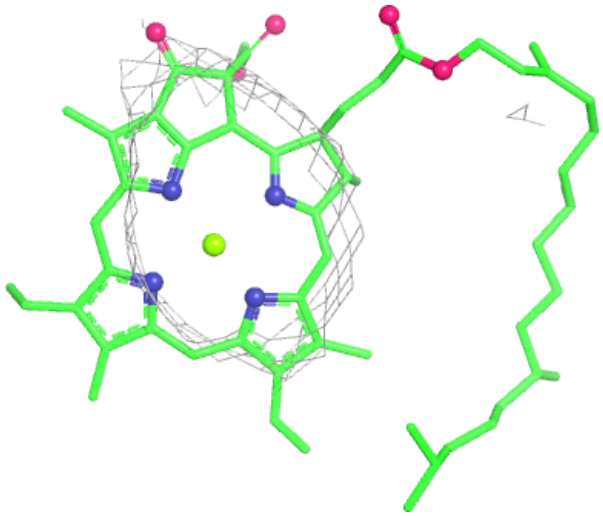
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

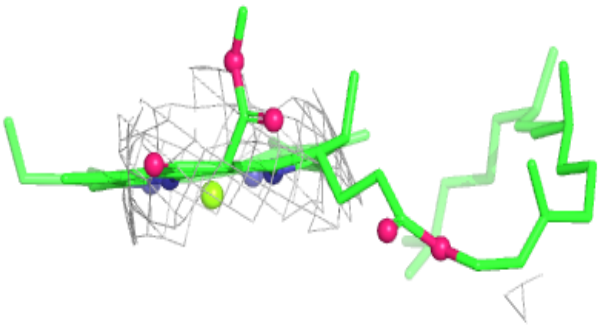




Electron density around CLA c 512:

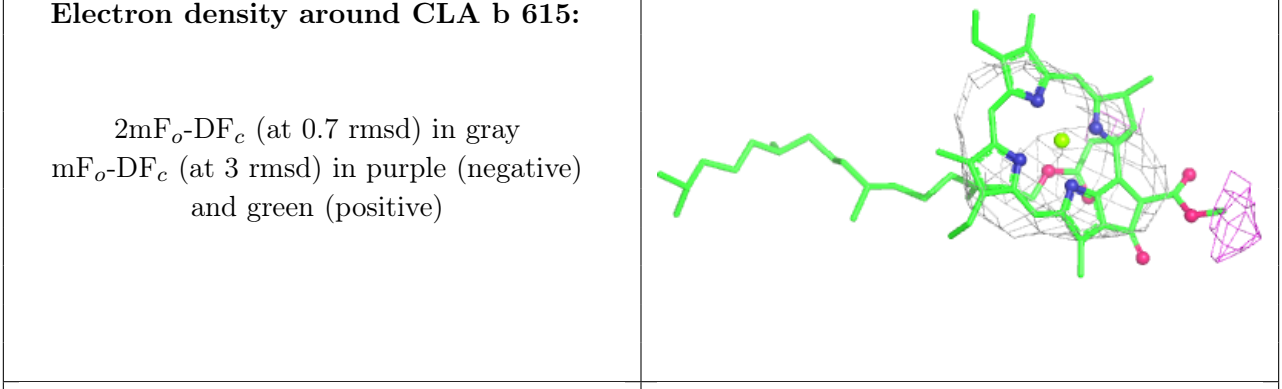
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





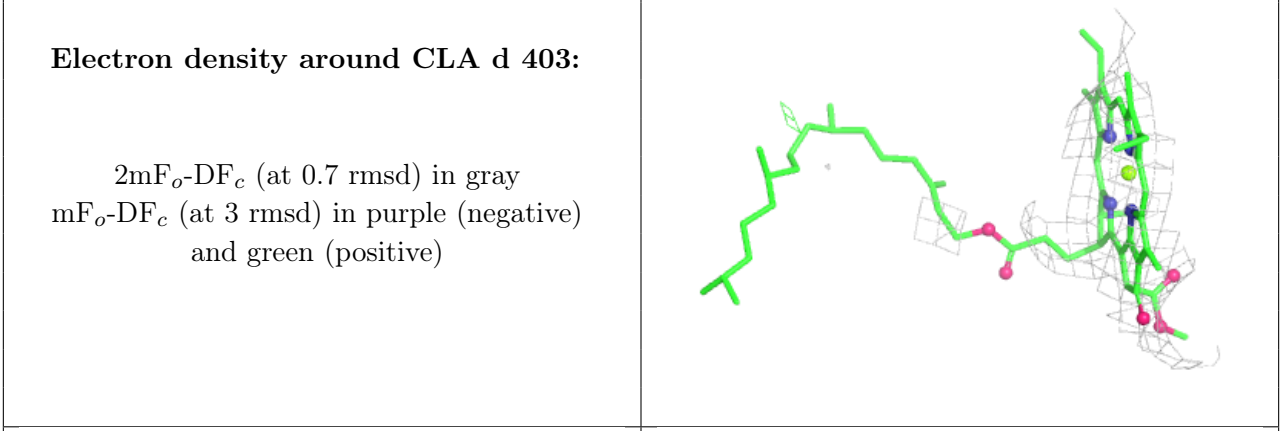
Electron density around CLA b 615:

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



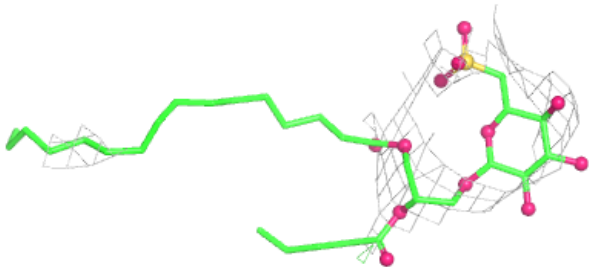
Electron density around CLA d 403:

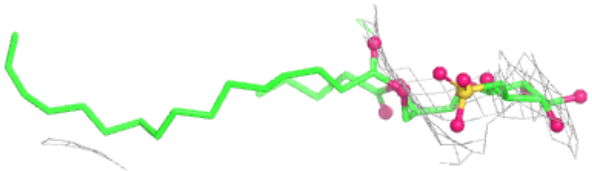
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

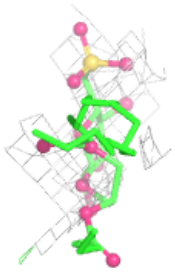


Electron density around SQD d 411:

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

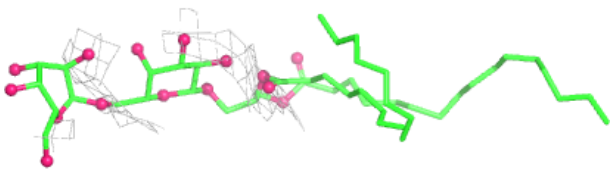


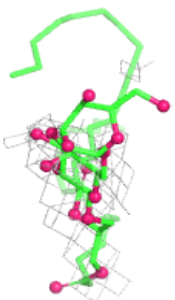




Electron density around DGD D 410:

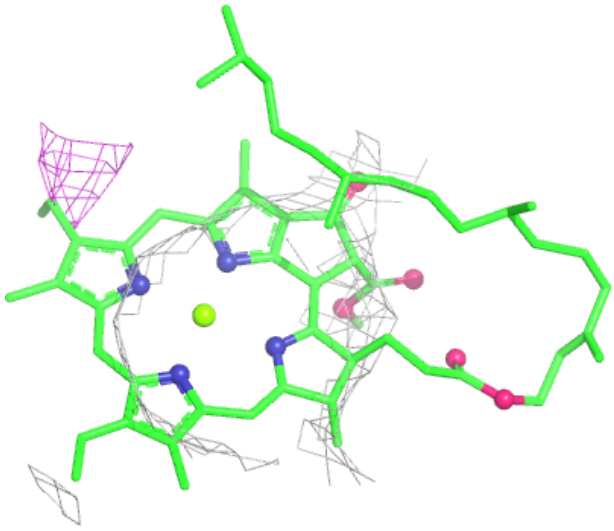
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

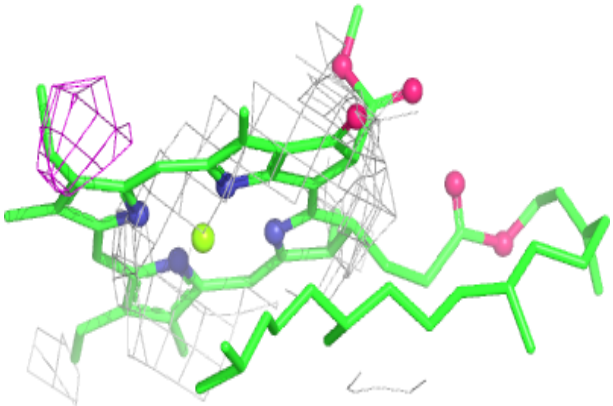




Electron density around CLA C 509:

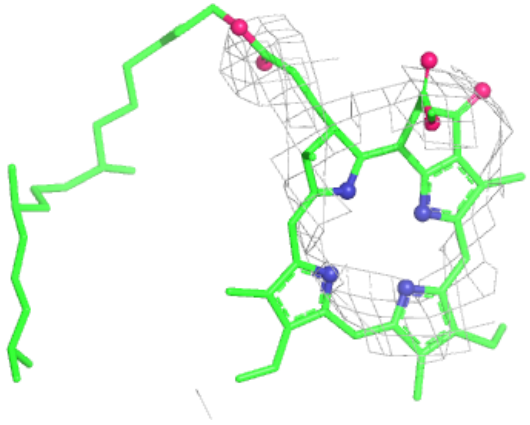
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

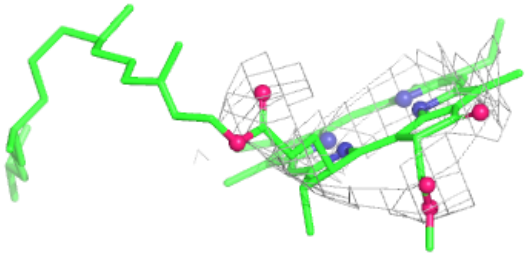




Electron density around PHO a 606:

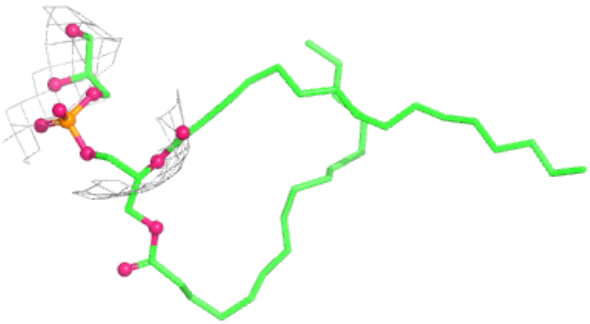
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

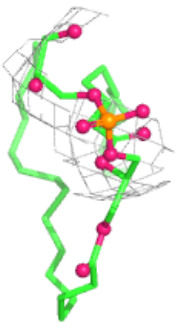




Electron density around LHG D 409:

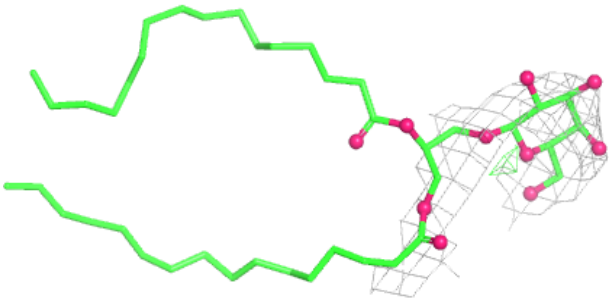
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

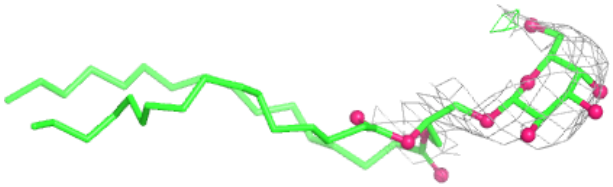


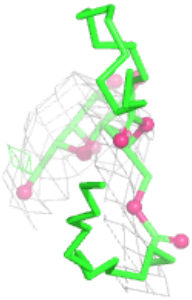


Electron density around LMG a 614:

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

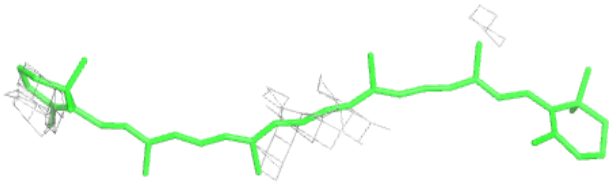


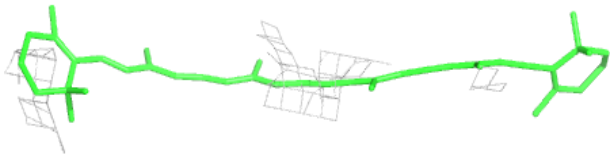




Electron density around BCR K 101:

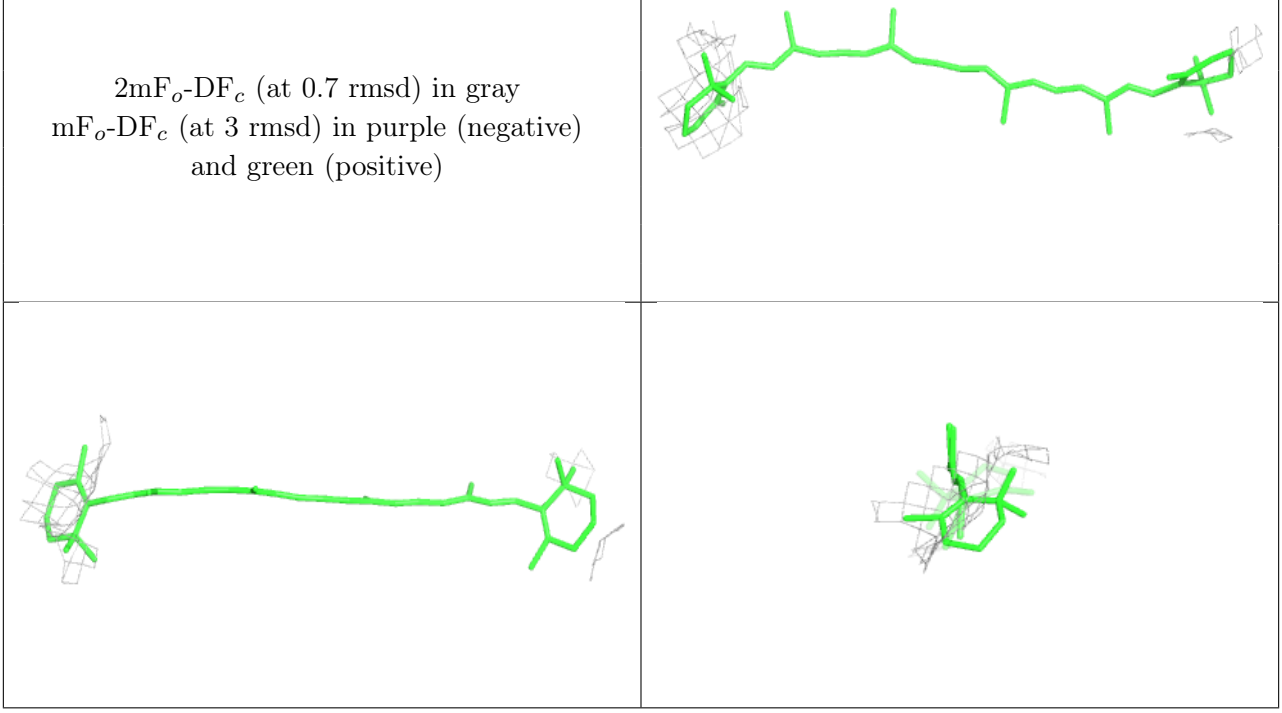
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





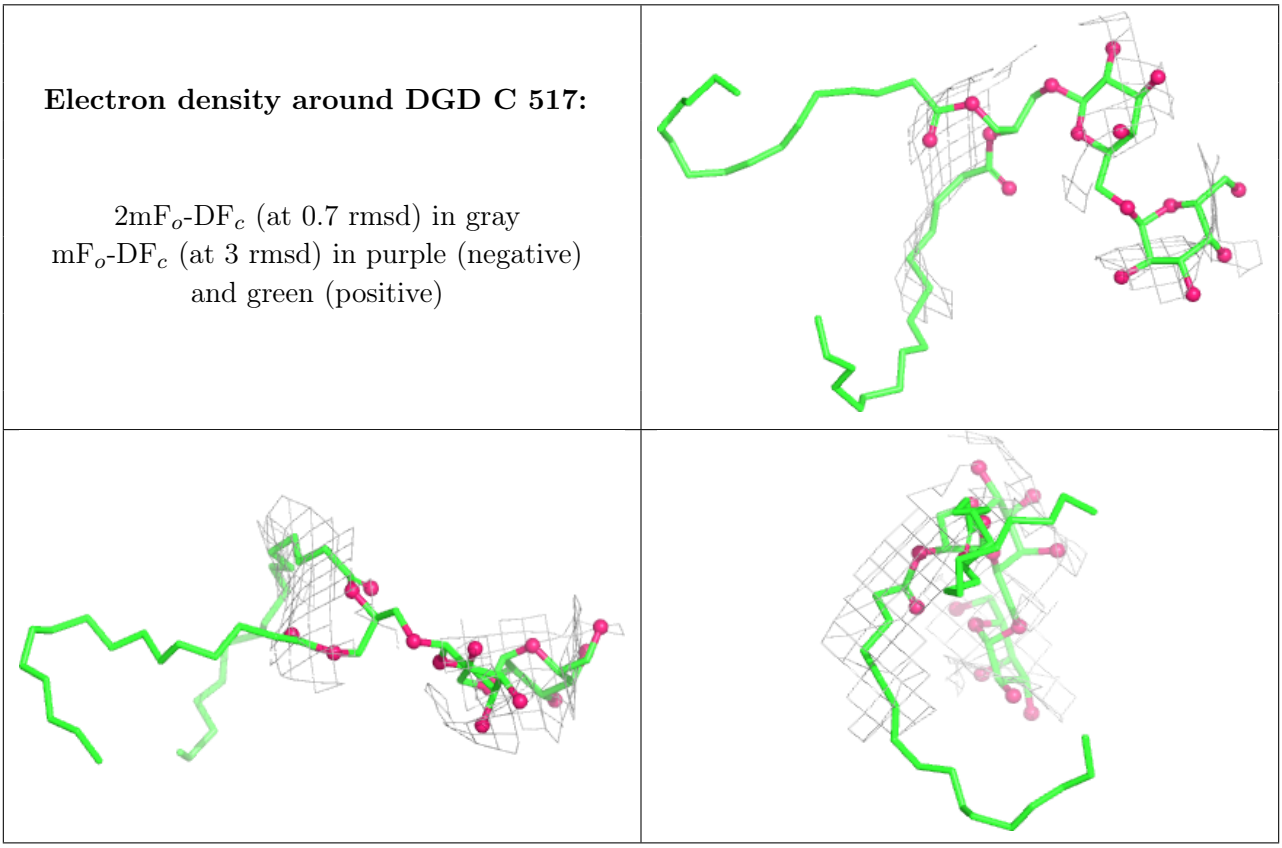
Electron density around BCR c 515:

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



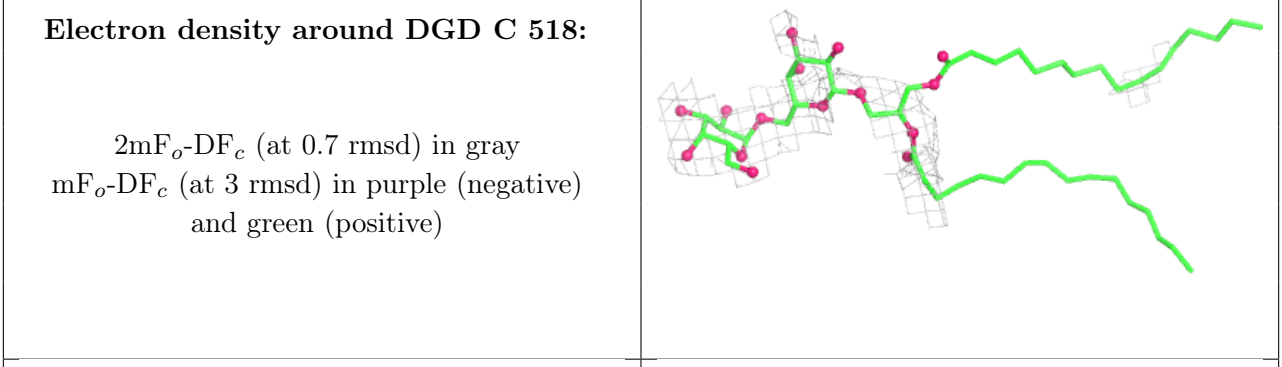
Electron density around DGD C 517:

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



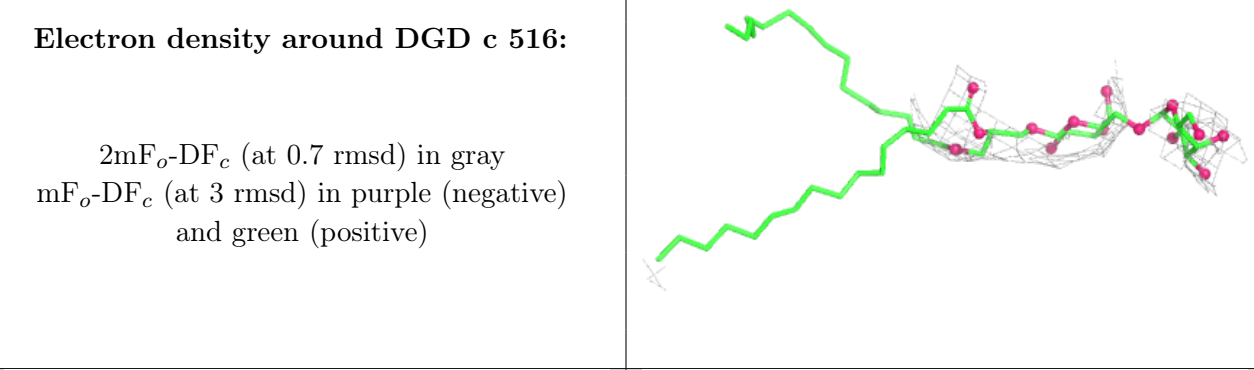
Electron density around DGD C 518:

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



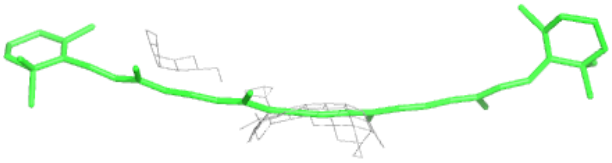
Electron density around DGD c 516:

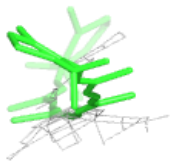
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around BCR D 404:

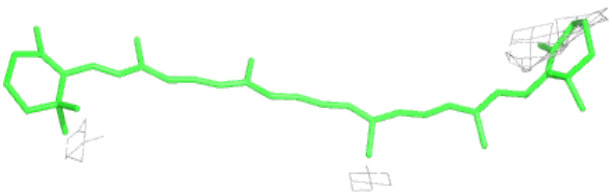
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

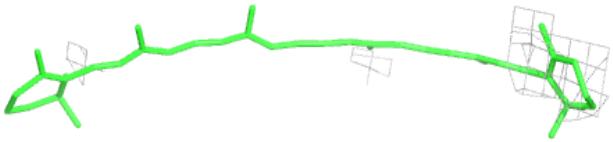


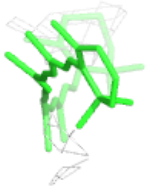


Electron density around BCR B 622:

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

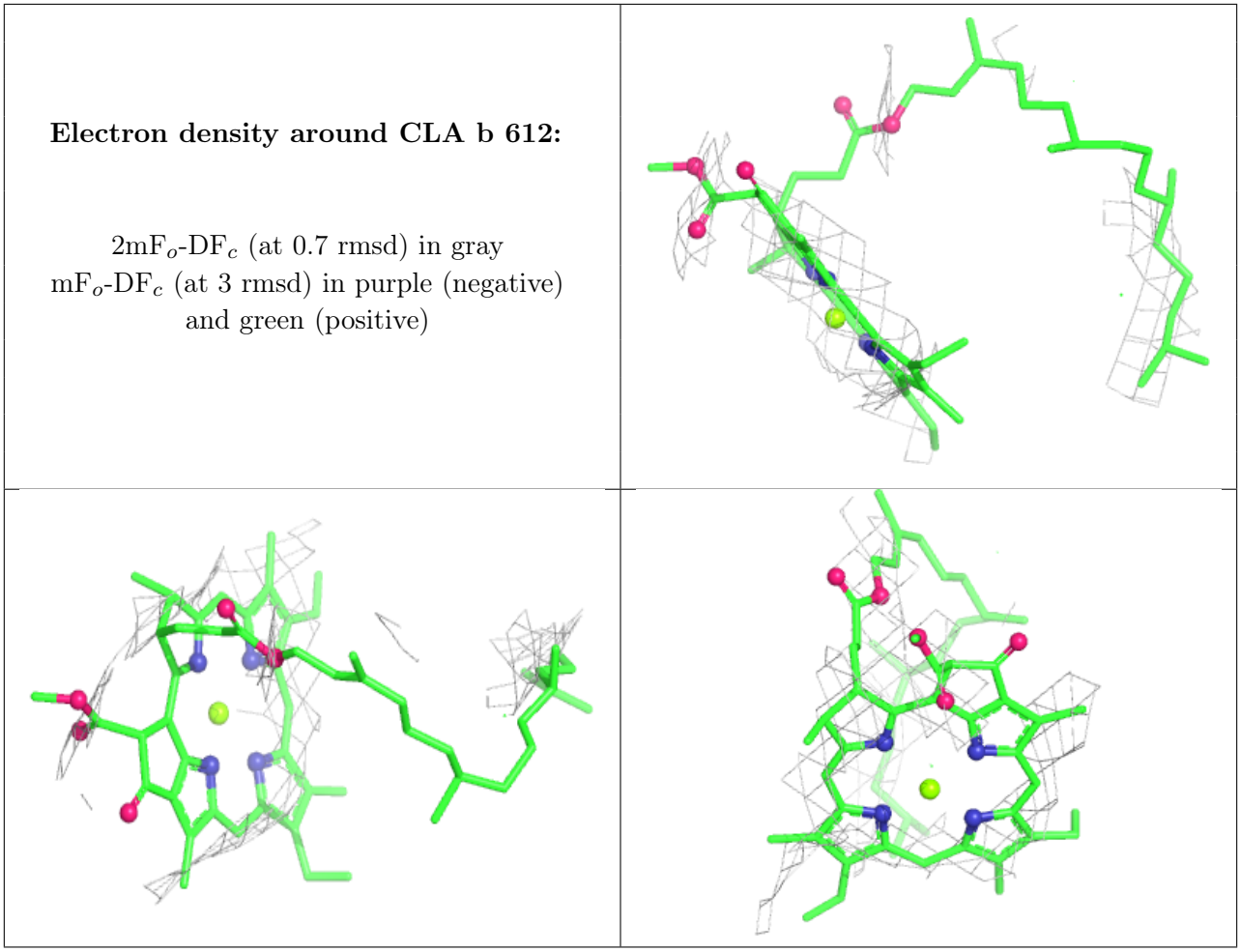






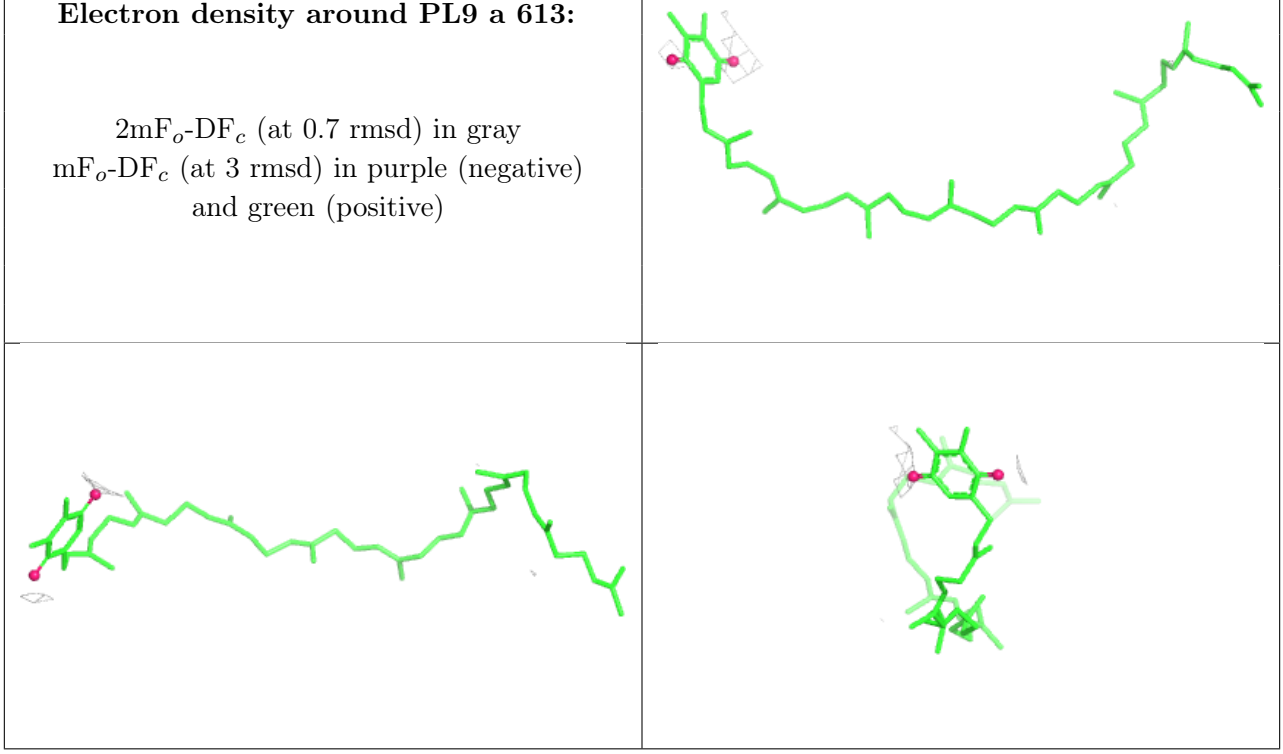
Electron density around CLA b 612:

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



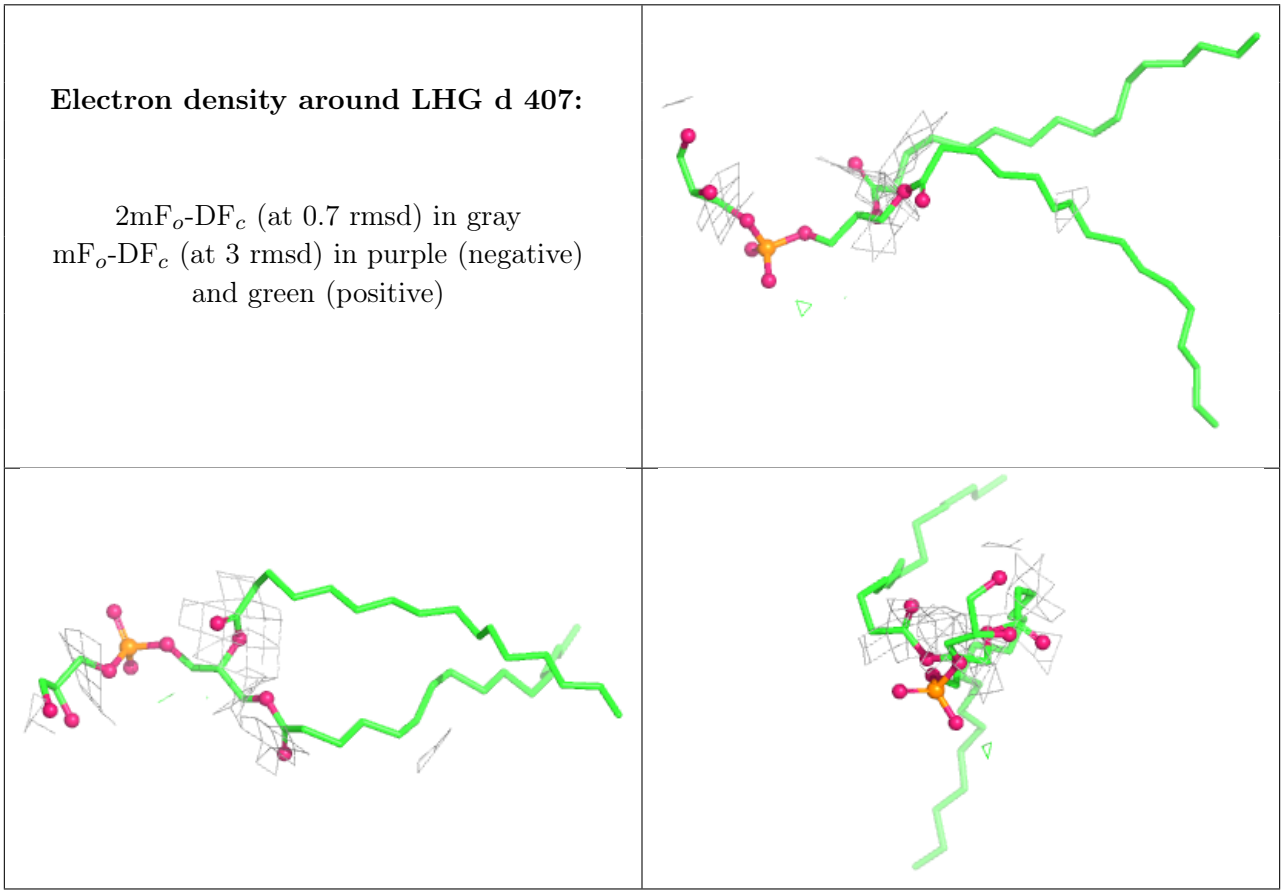
Electron density around PL9 a 613:

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



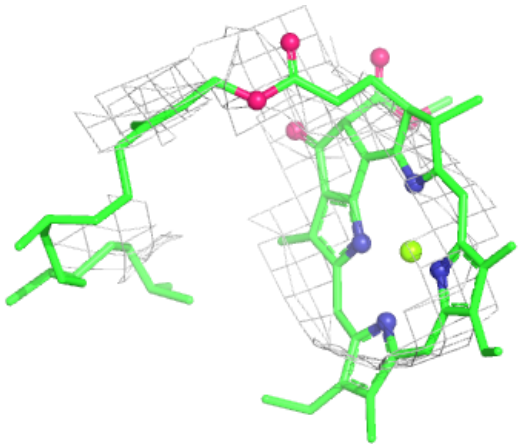
Electron density around LHG d 407:

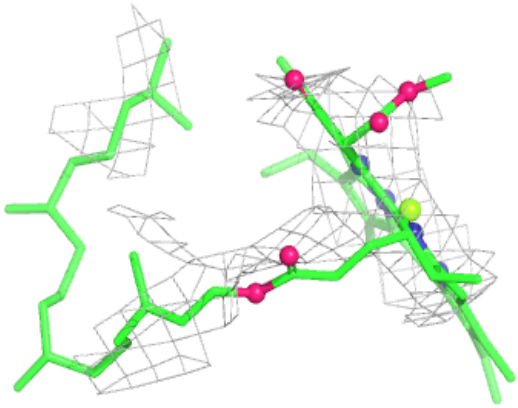
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

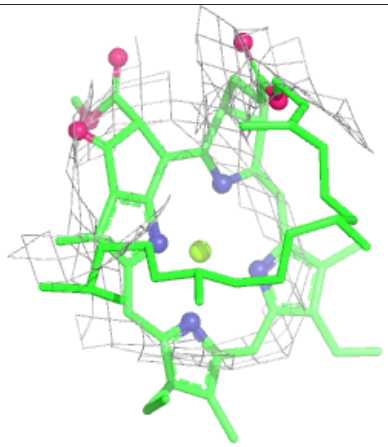


Electron density around CLA c 503:

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

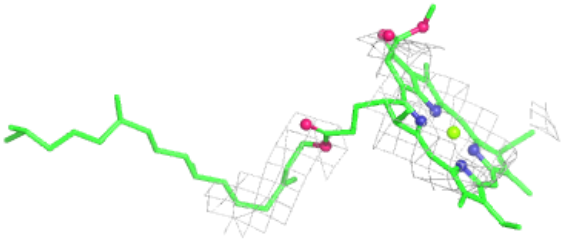


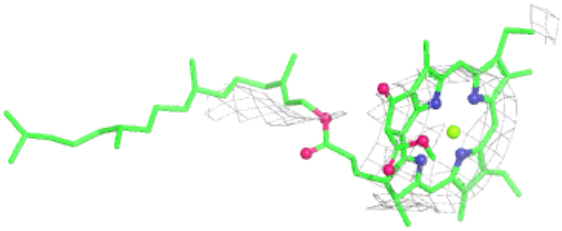


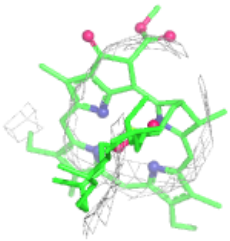


Electron density around CLA c 502:

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

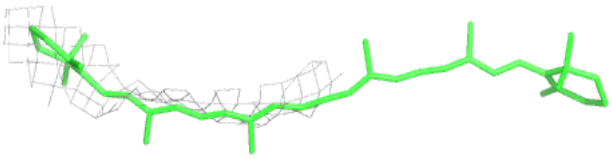


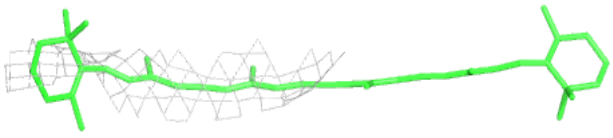


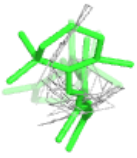


Electron density around BCR H 101:

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

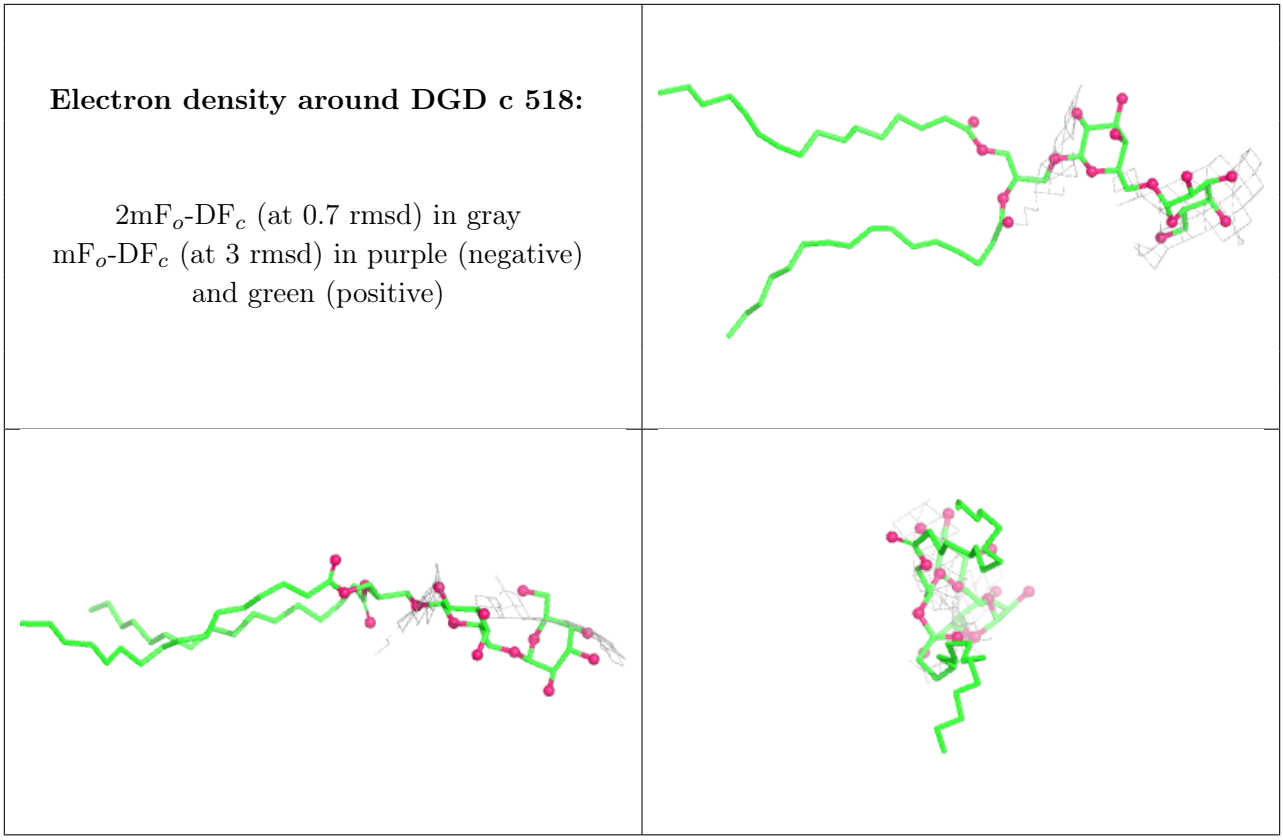






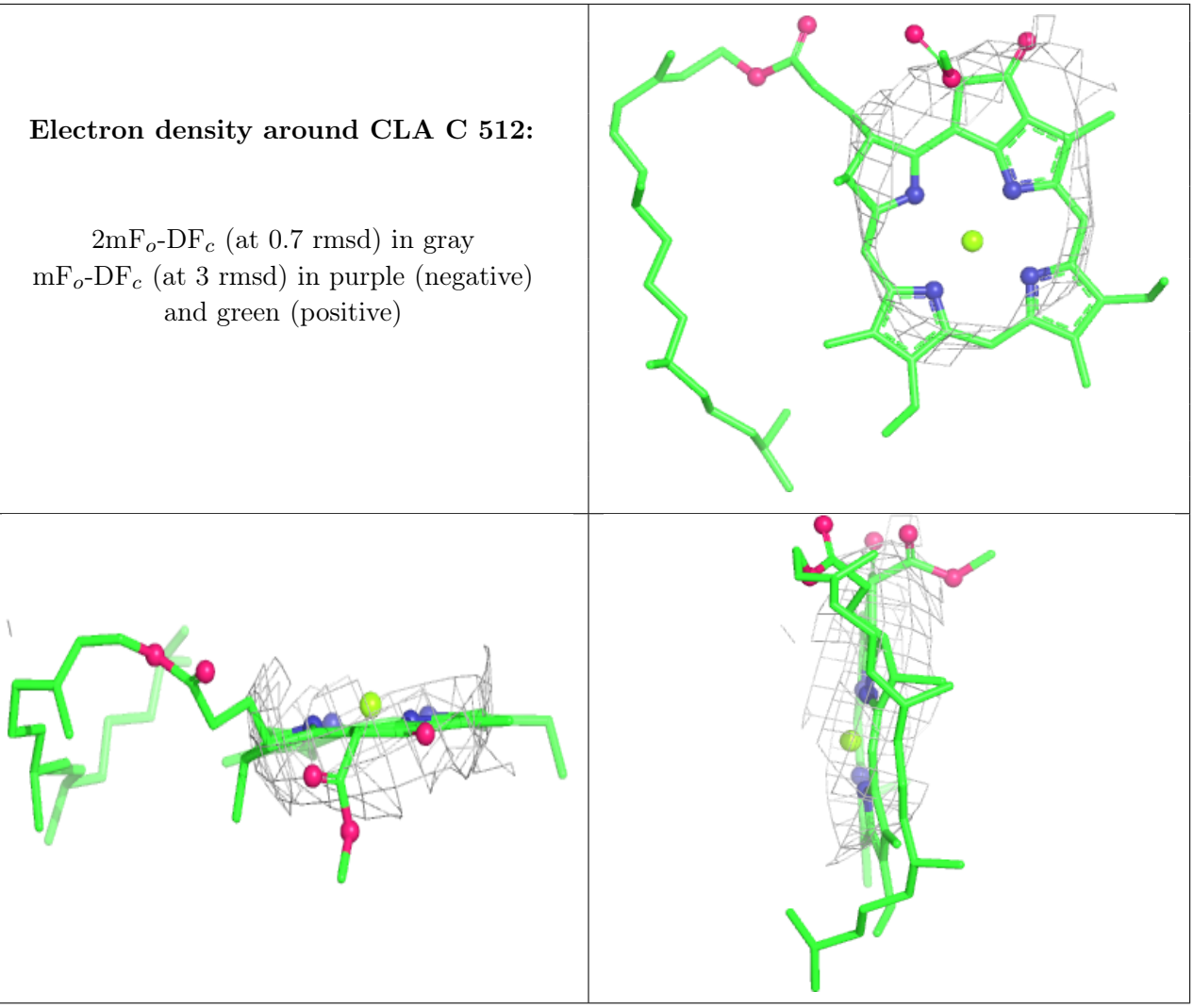
Electron density around DGD c 518:

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



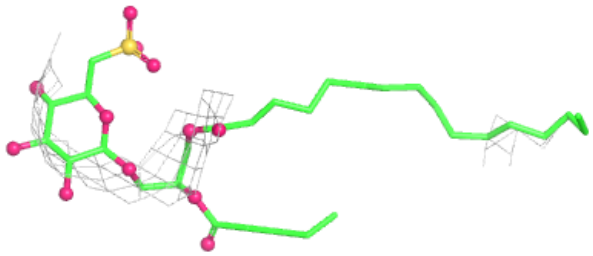
Electron density around CLA C 512:

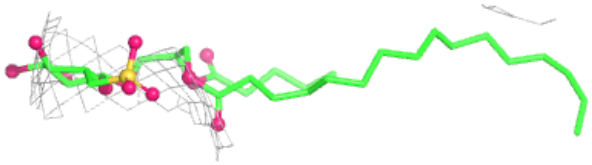
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around SQD D 411:

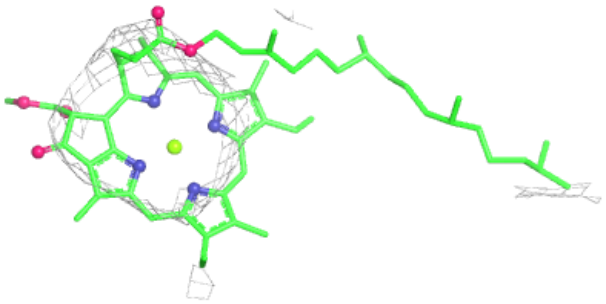
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

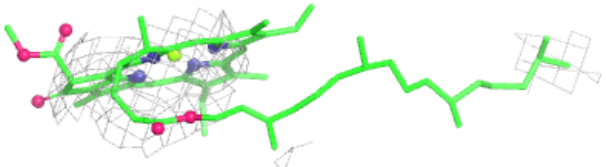


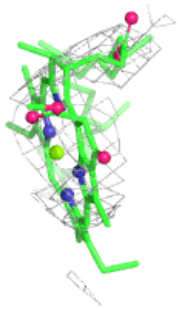


Electron density around CLA C 501:

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

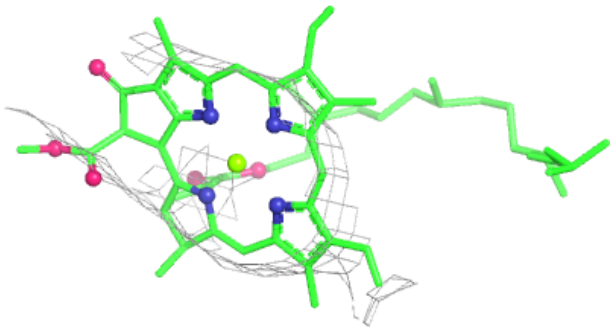


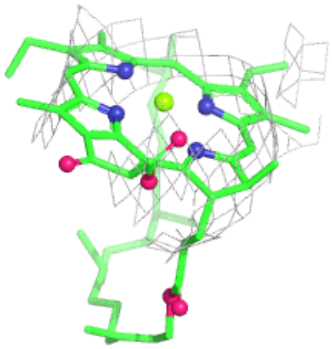




Electron density around CLA c 513:

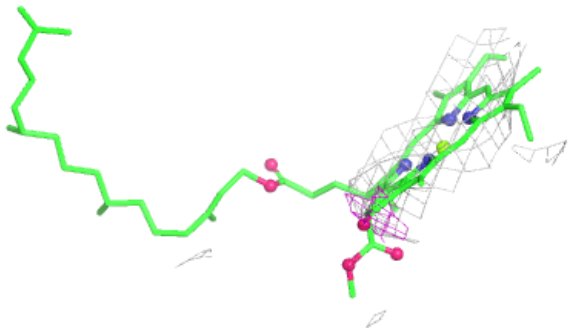
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

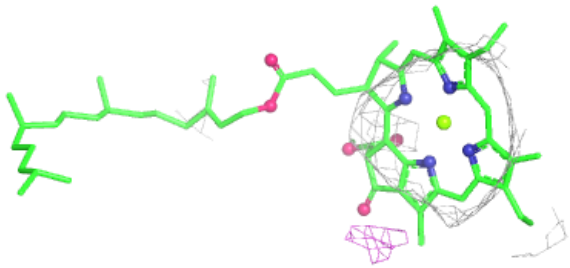


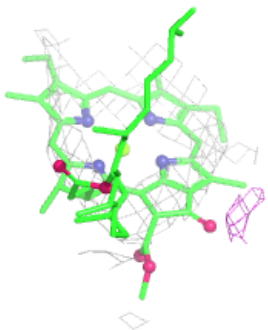


Electron density around CLA D 401:

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

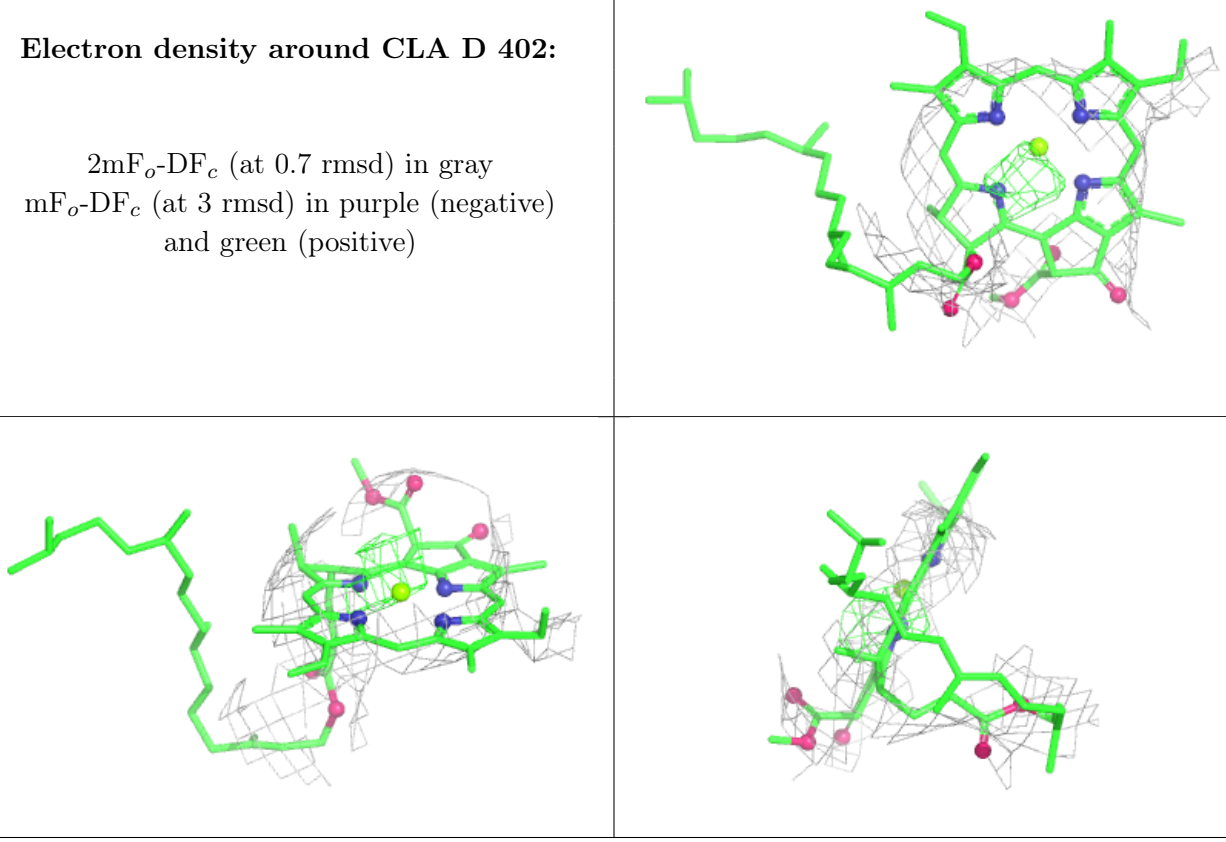






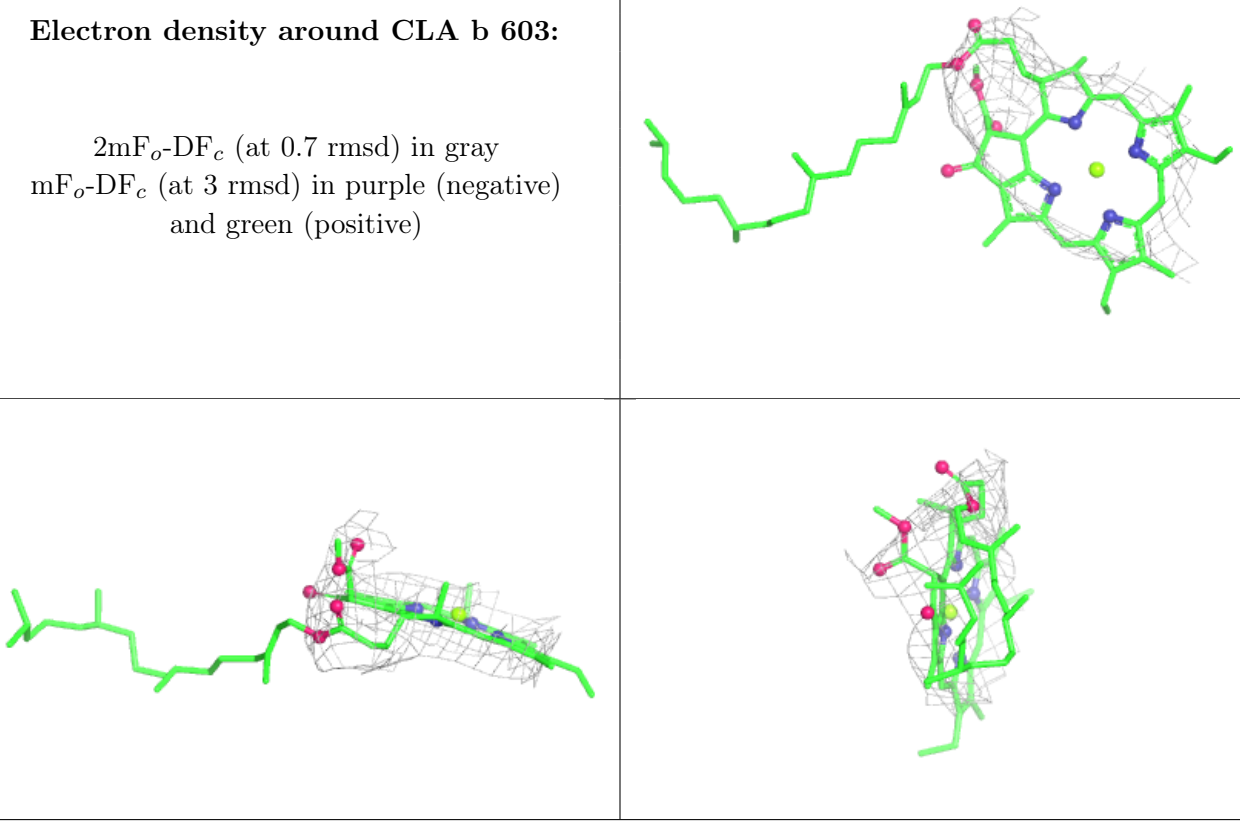
Electron density around CLA D 402:

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



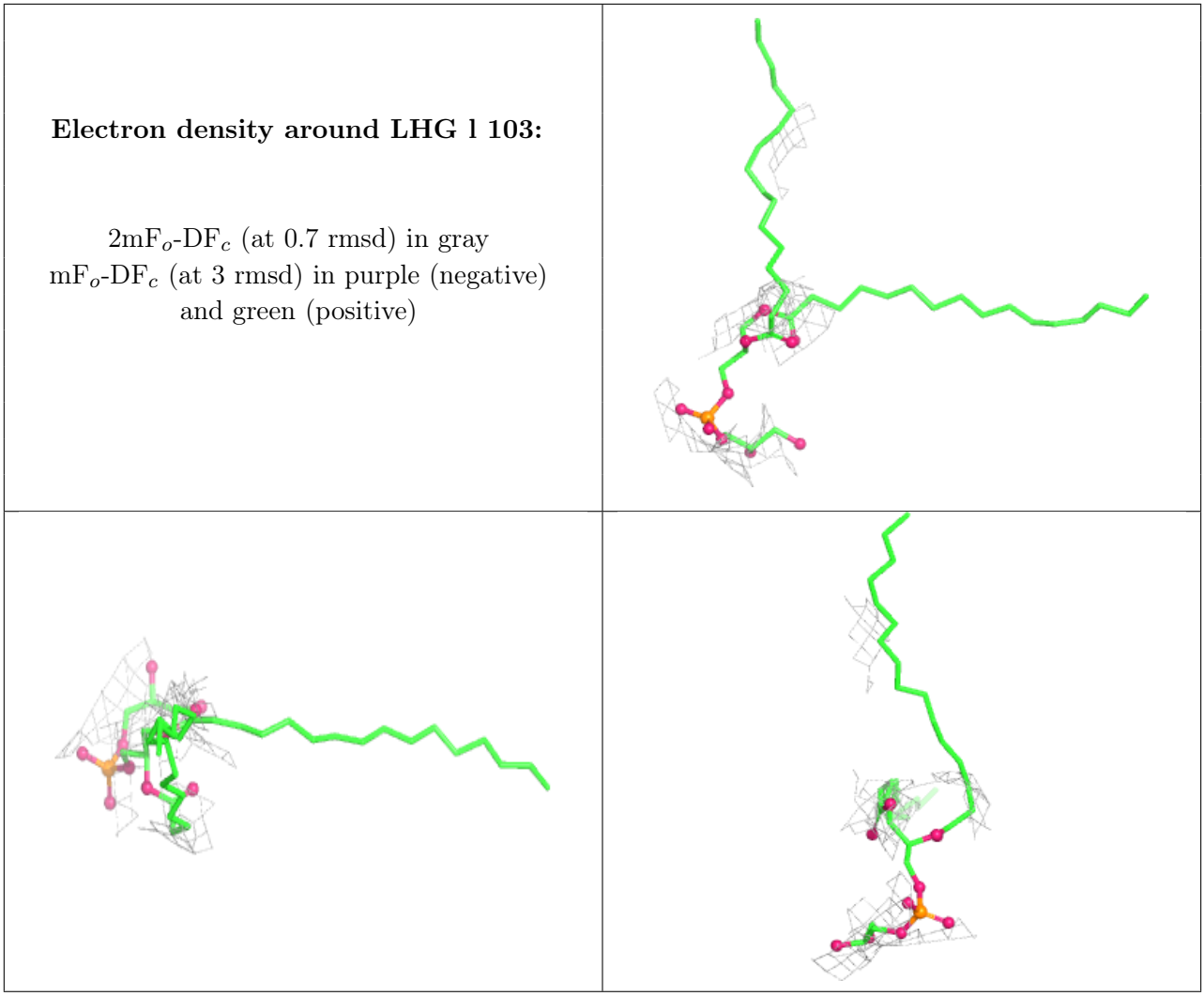
Electron density around CLA b 603:

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



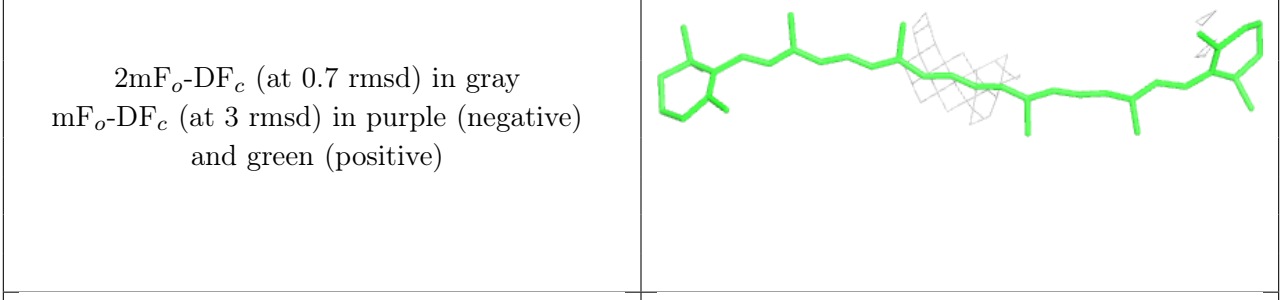
Electron density around LHG l 103:

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



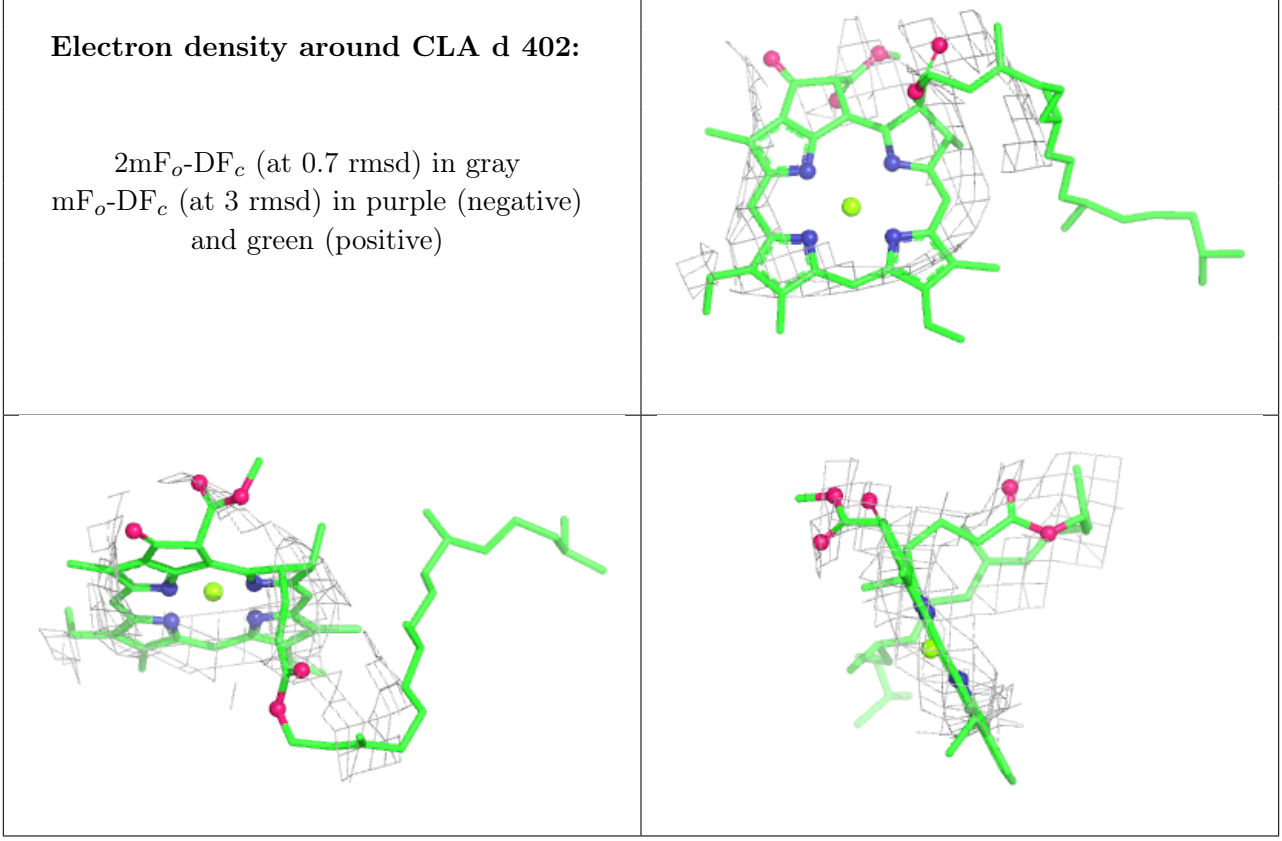
Electron density around BCR B 619:

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



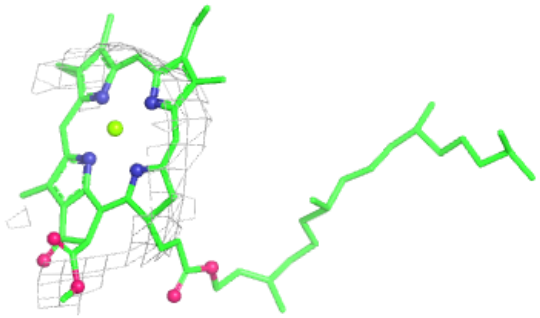
Electron density around CLA d 402:

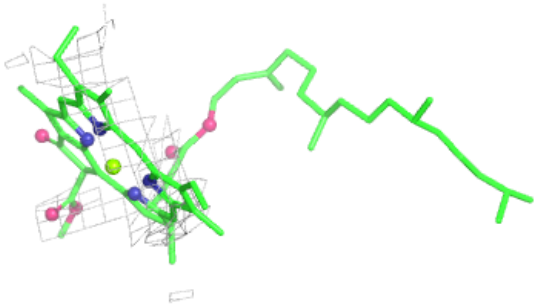
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

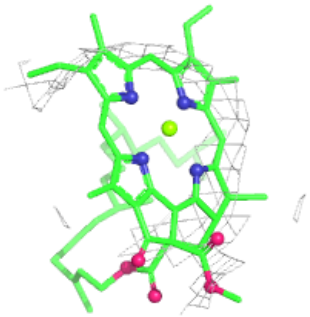


Electron density around CLA c 511:

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

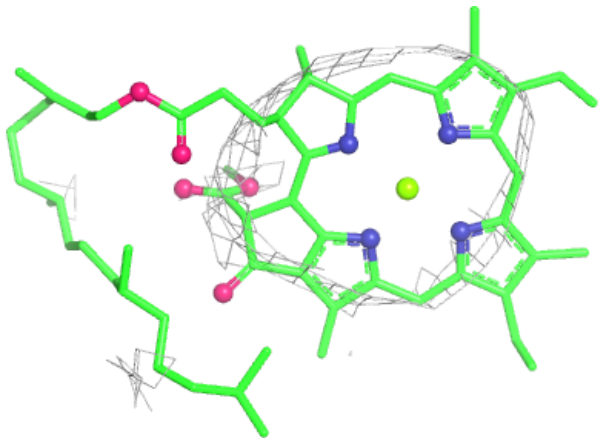


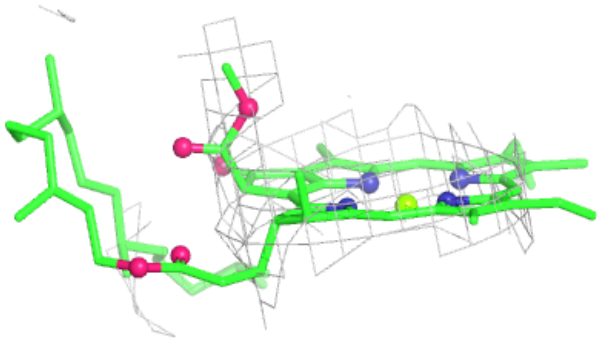


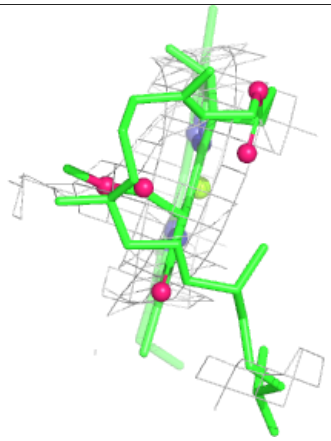


Electron density around CLA B 611:

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

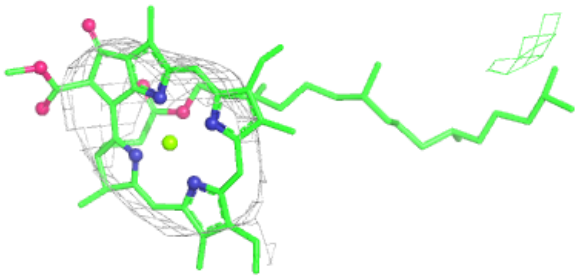


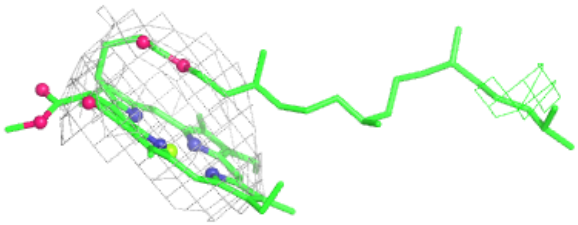


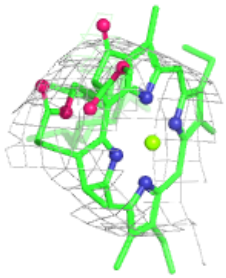


Electron density around CLA B 615:

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

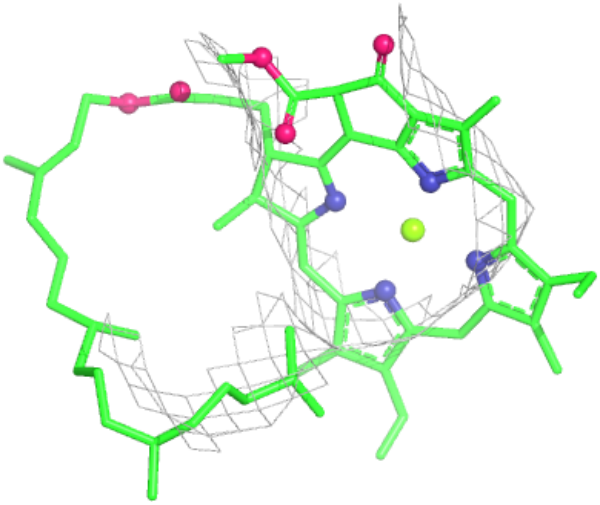


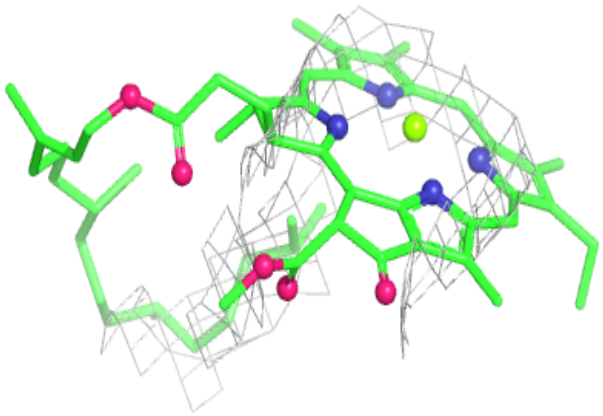


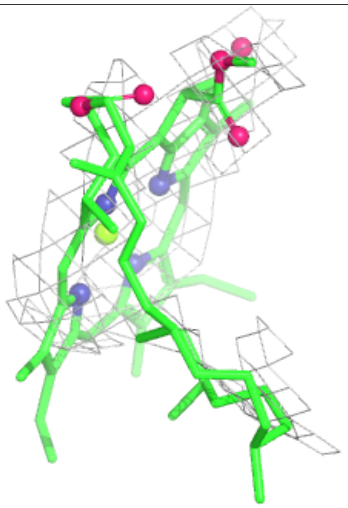


Electron density around CLA B 616:

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

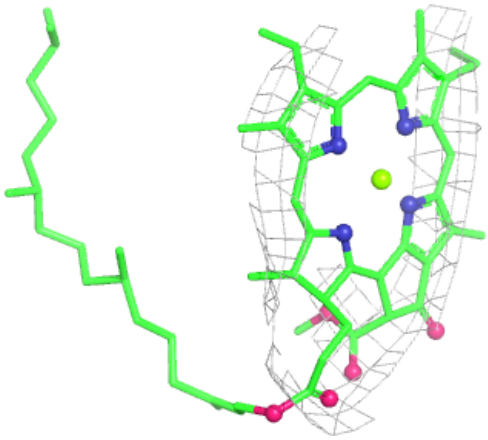


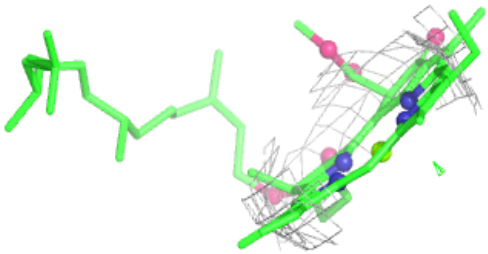


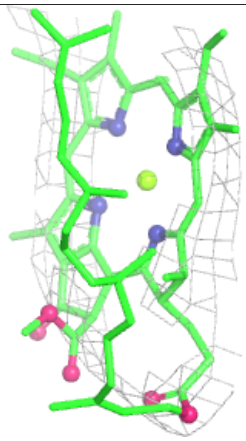


Electron density around CLA B 617:

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

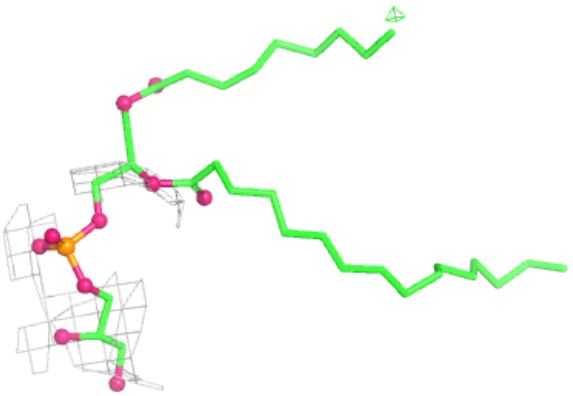


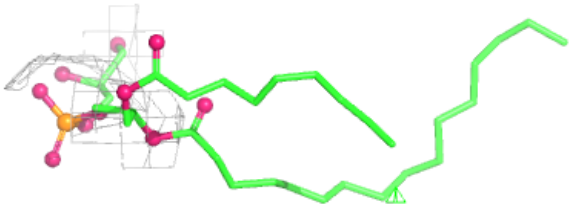


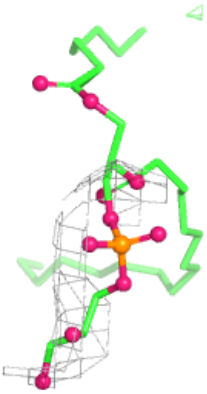


Electron density around LHG e 101:

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

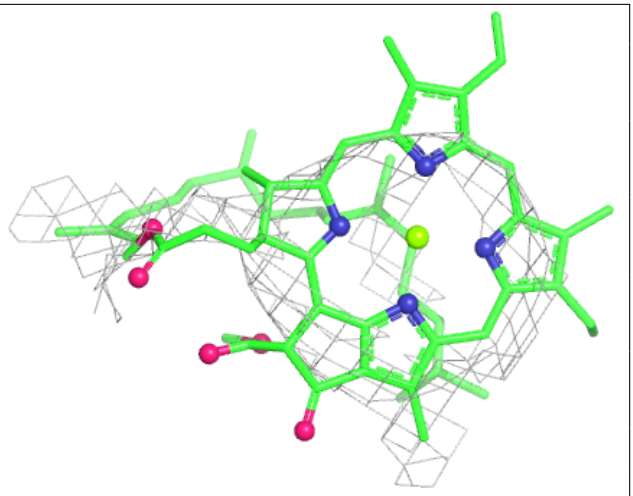


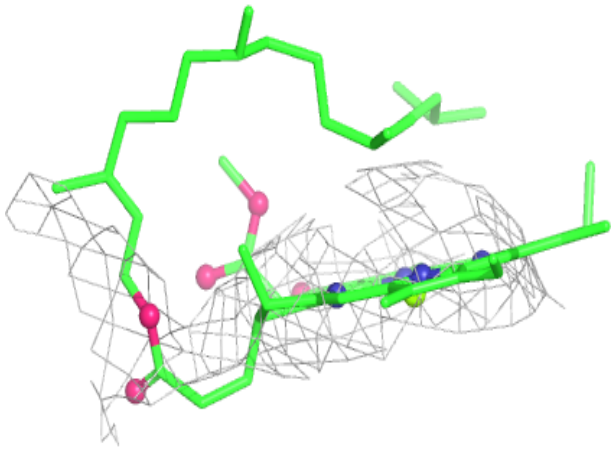




Electron density around CLA c 510:

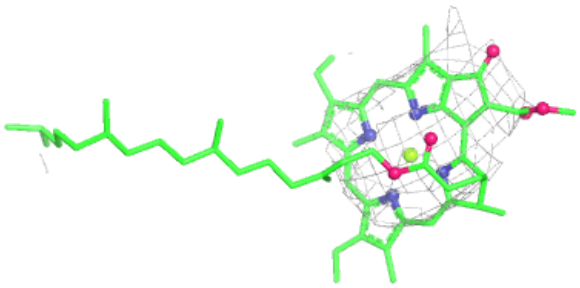
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

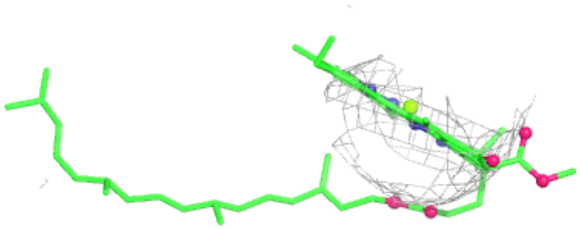


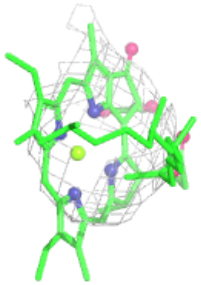


Electron density around CLA B 609:

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

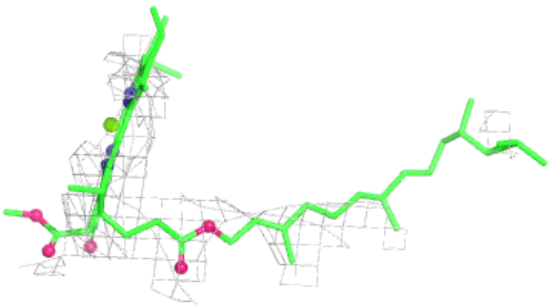


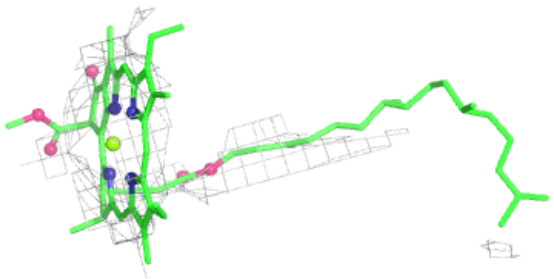


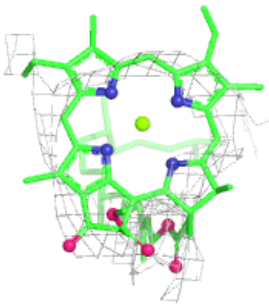


Electron density around CLA B 606:

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

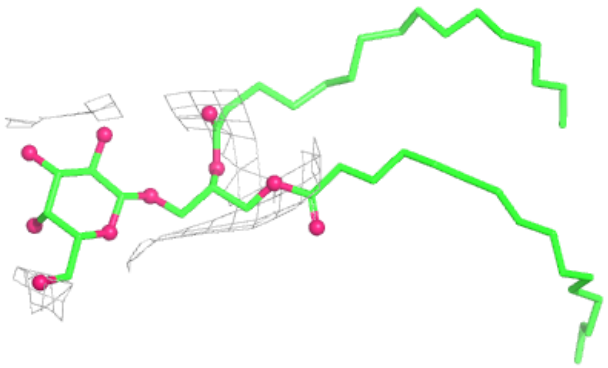


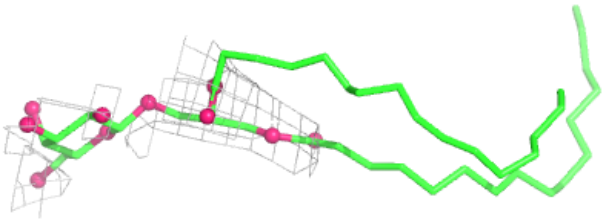


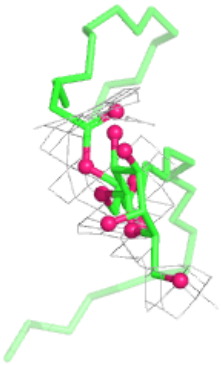


Electron density around LMG D 406:

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

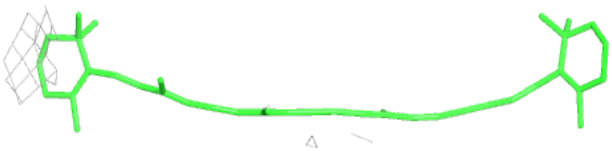


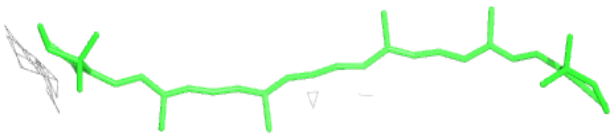


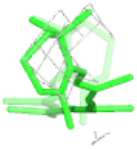


Electron density around BCR k 102:

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

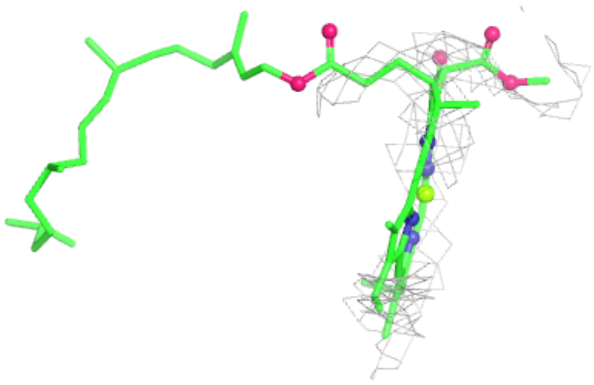


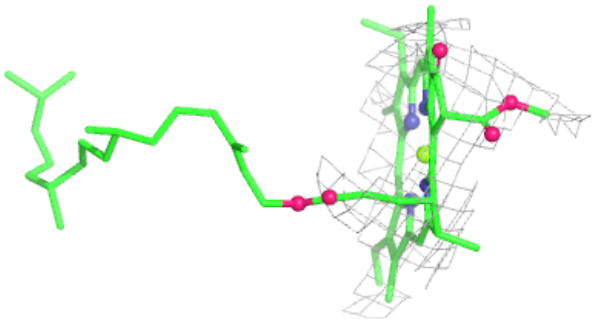




Electron density around CLA C 506:

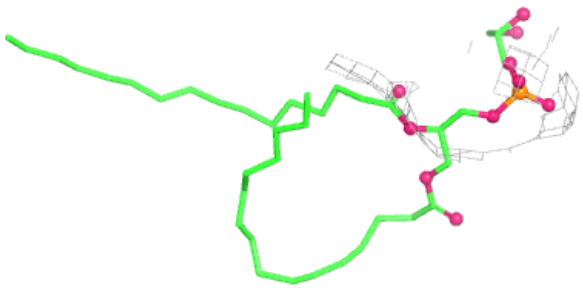
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





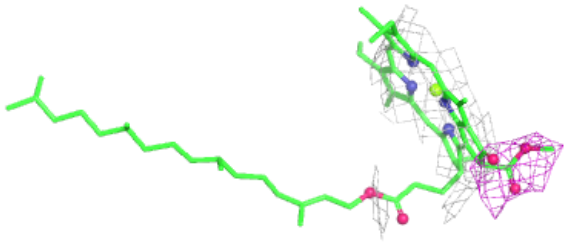
Electron density around LHG D 405:

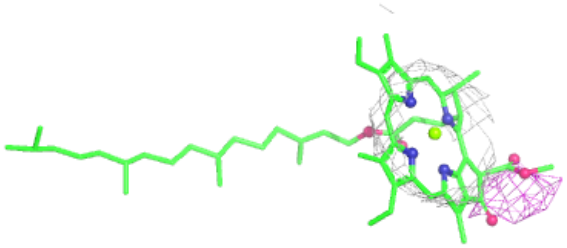
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CLA B 608:

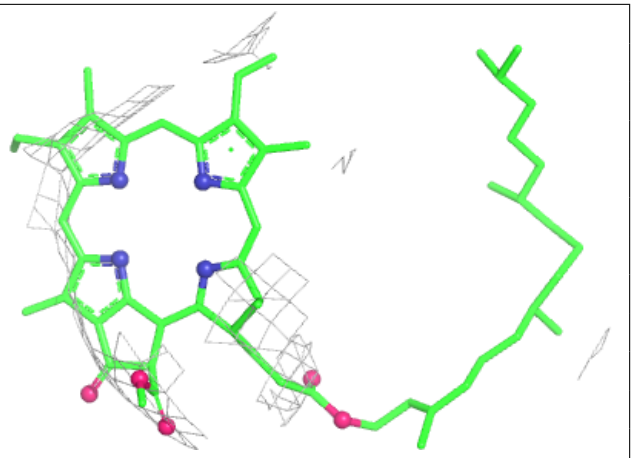
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

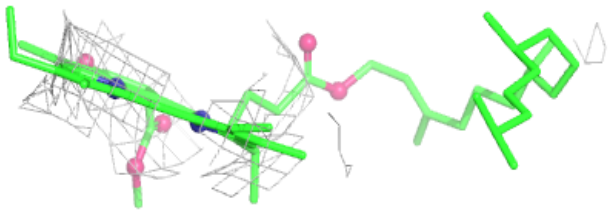


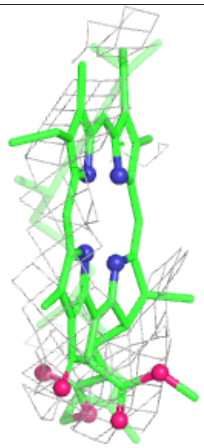


Electron density around PHO a 605:

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

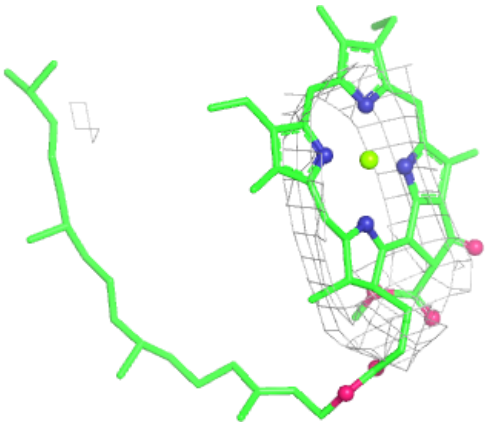


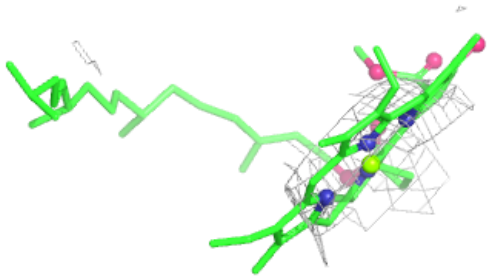




Electron density around CLA c 507:

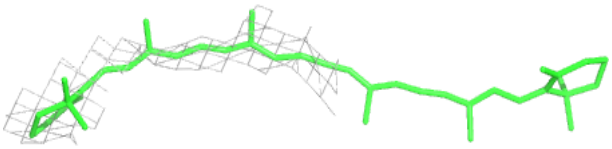
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

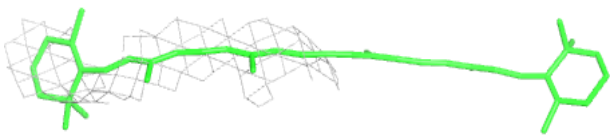


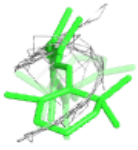


Electron density around BCR h 101:

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

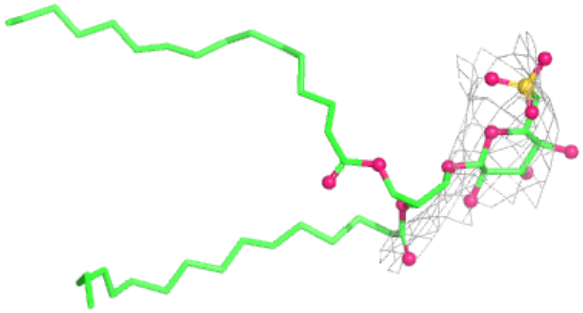


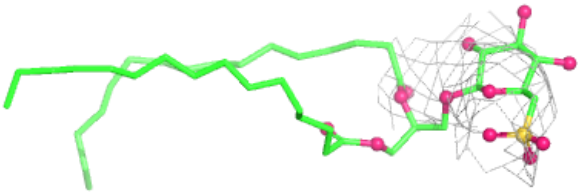


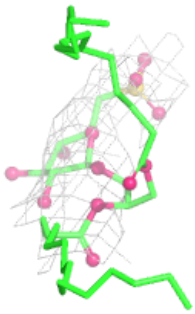


Electron density around SQD B 601:

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

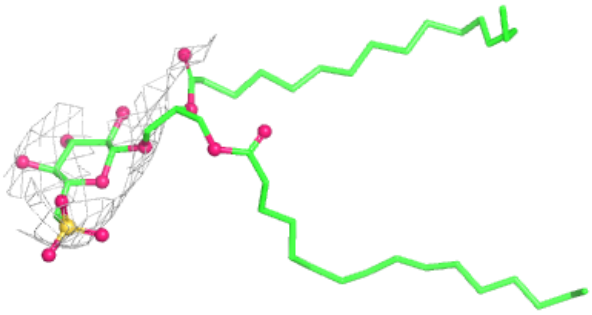


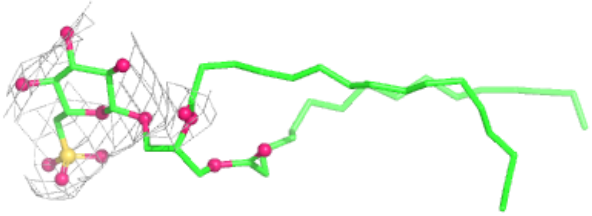


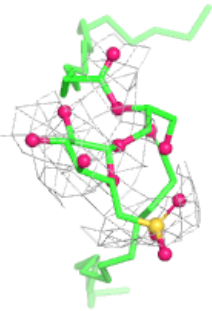


Electron density around SQD b 601:

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

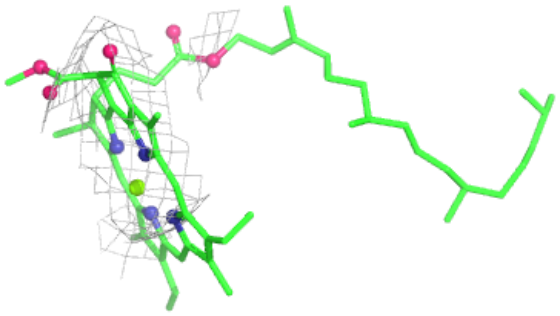


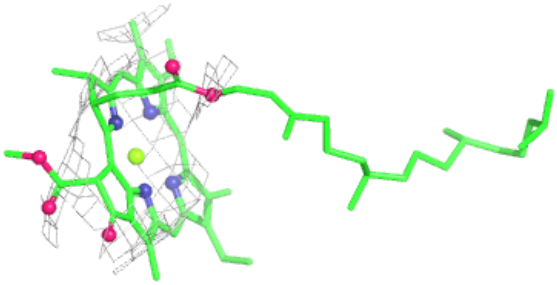


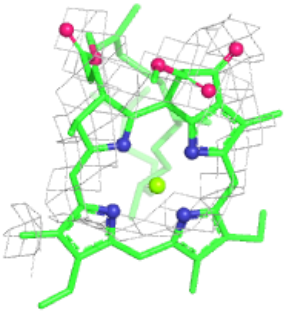


Electron density around CLA c 508:

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

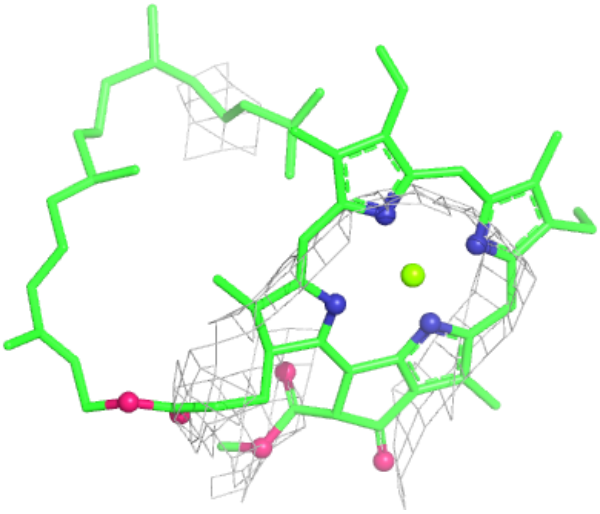


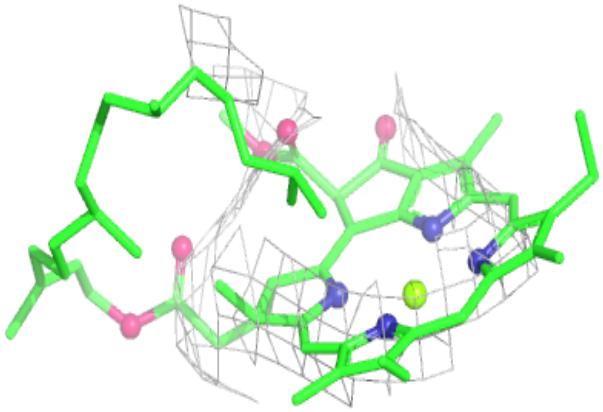


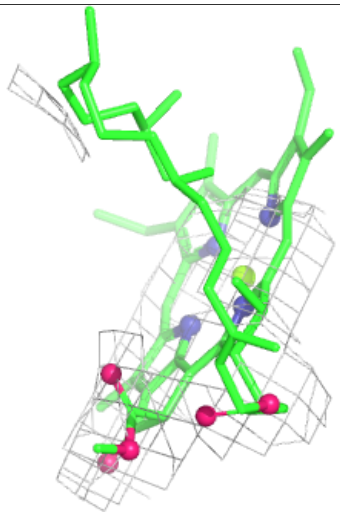


Electron density around CLA b 616:

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

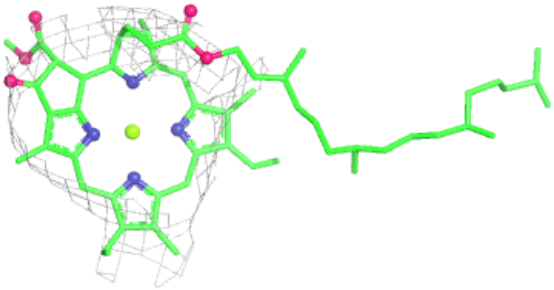


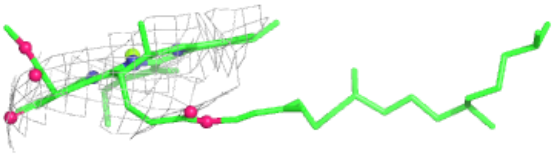


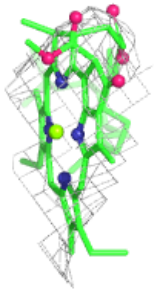


Electron density around CLA b 604:

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

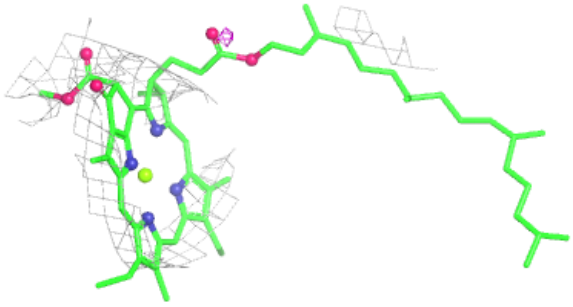


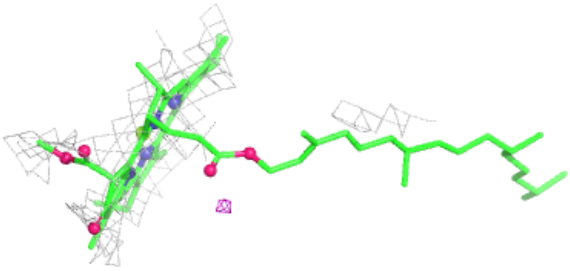


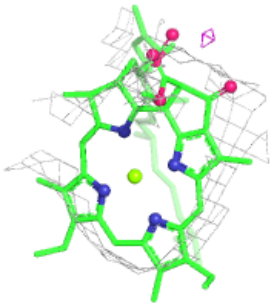


Electron density around CLA b 610:

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

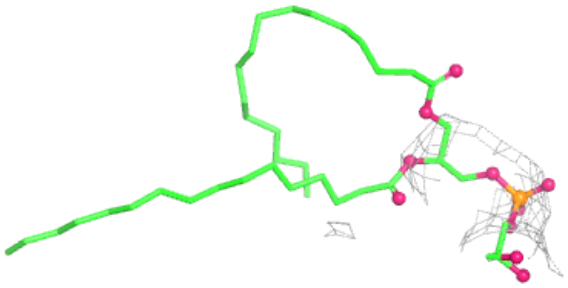


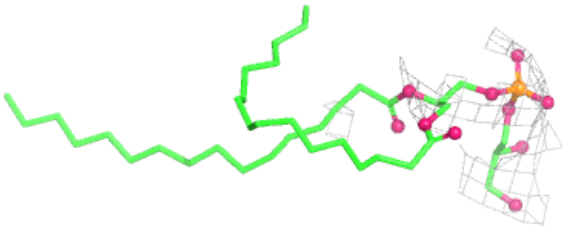




Electron density around LHG d 405:

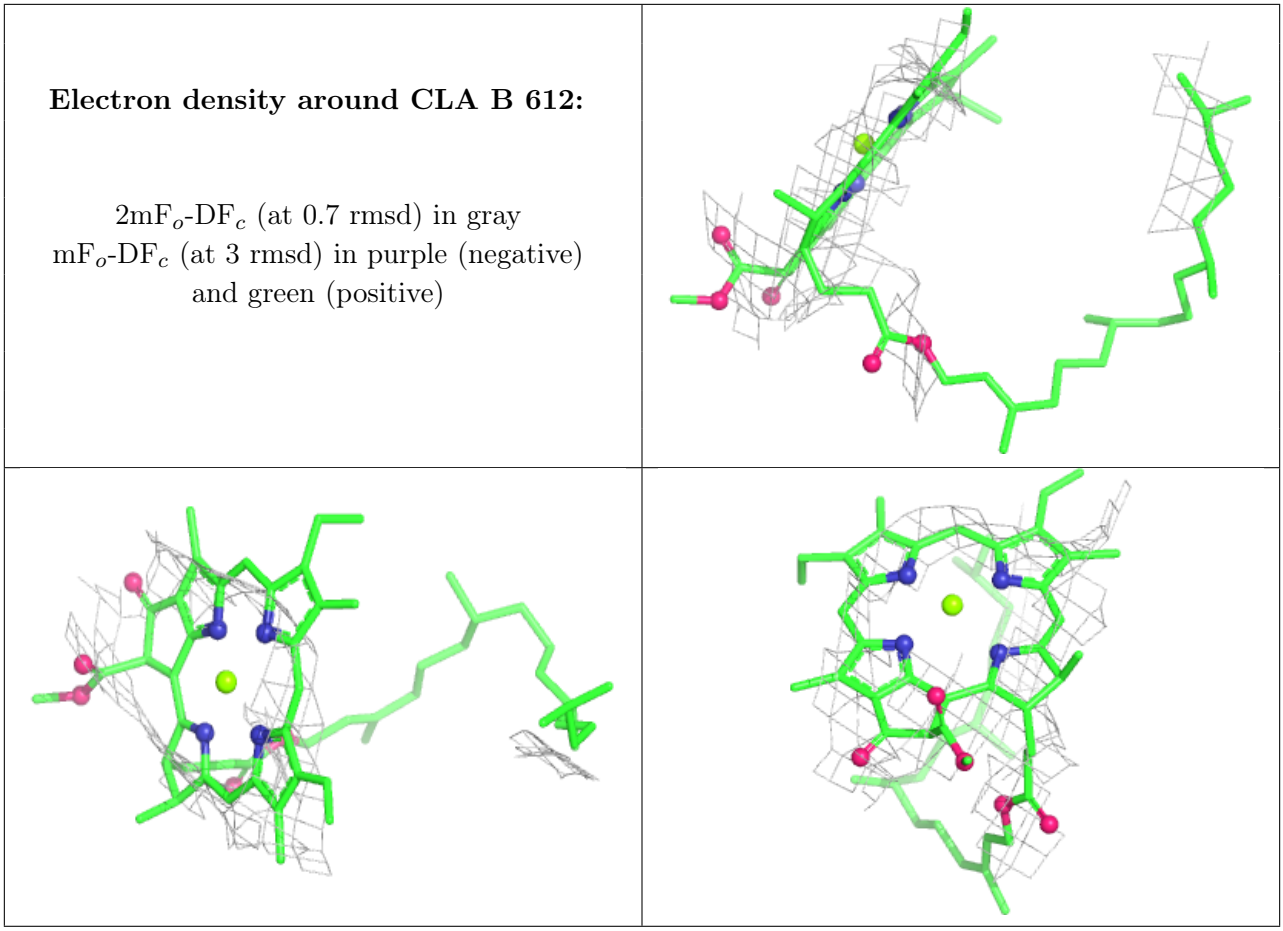
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





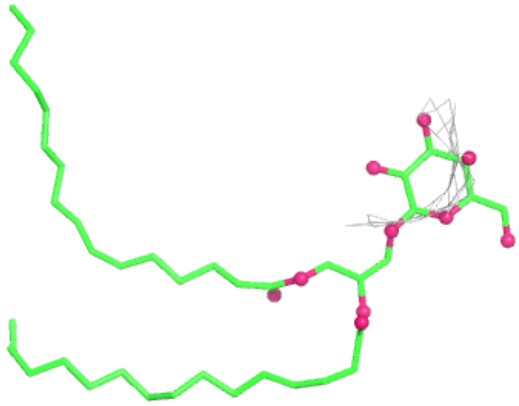
Electron density around CLA B 612:

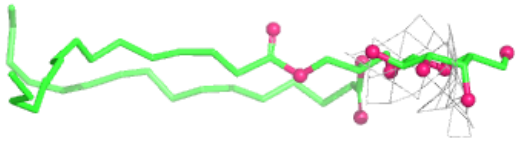
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around LMG c 519:

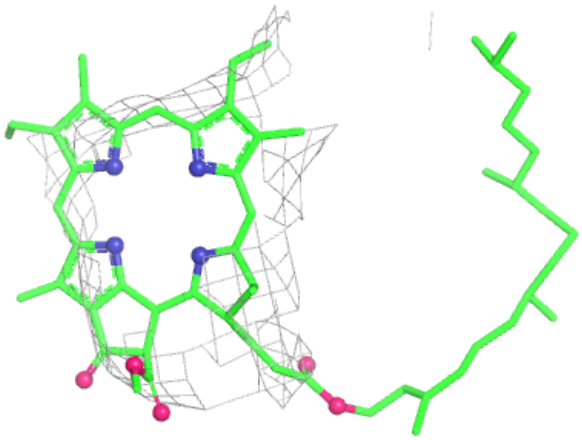
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

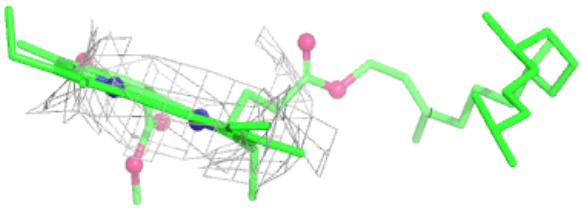


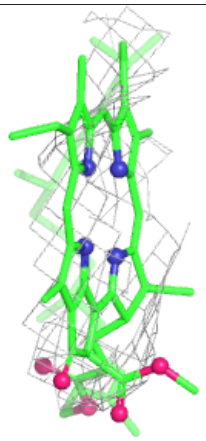


Electron density around PHO A 605:

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

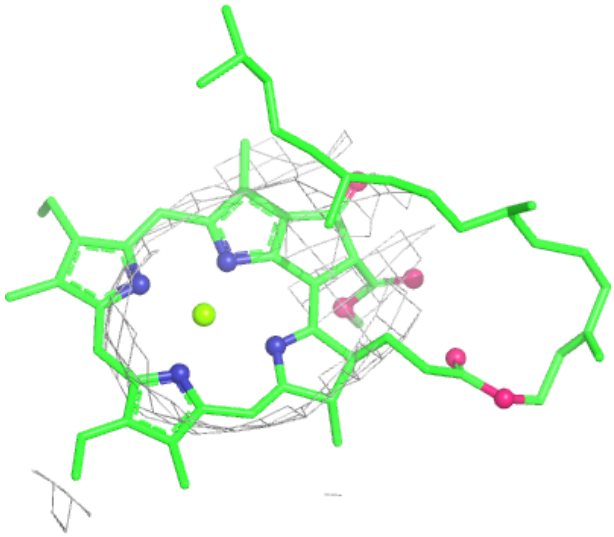


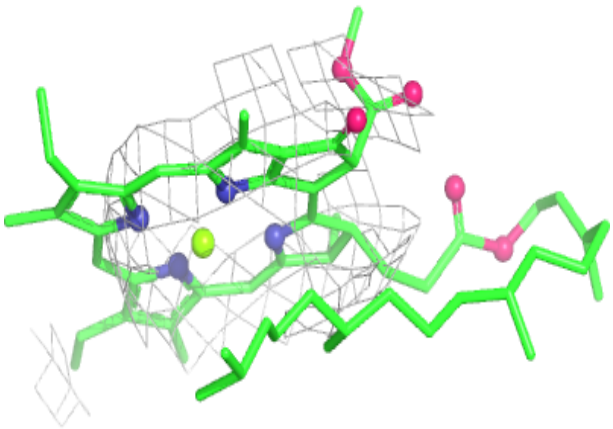


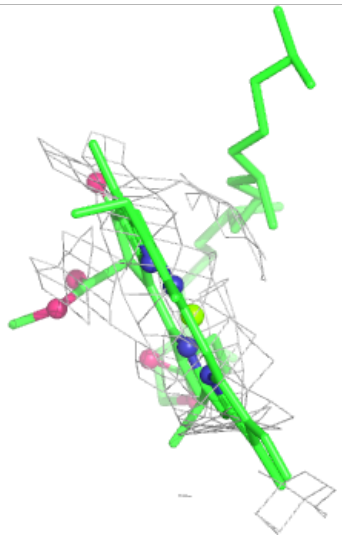


Electron density around CLA c 509:

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

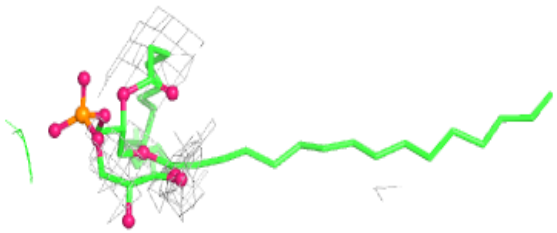


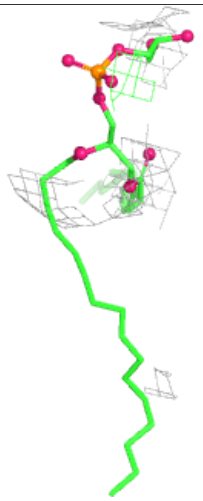




Electron density around LHG L 102:

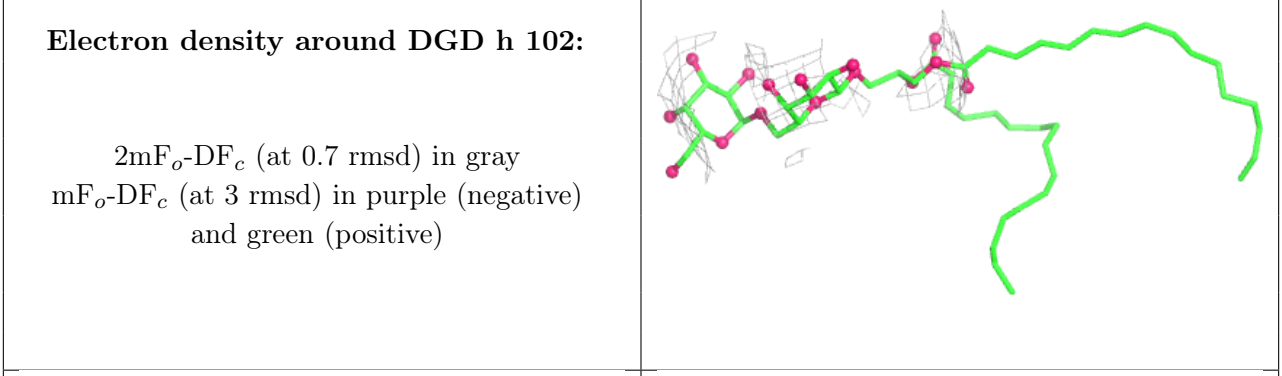
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

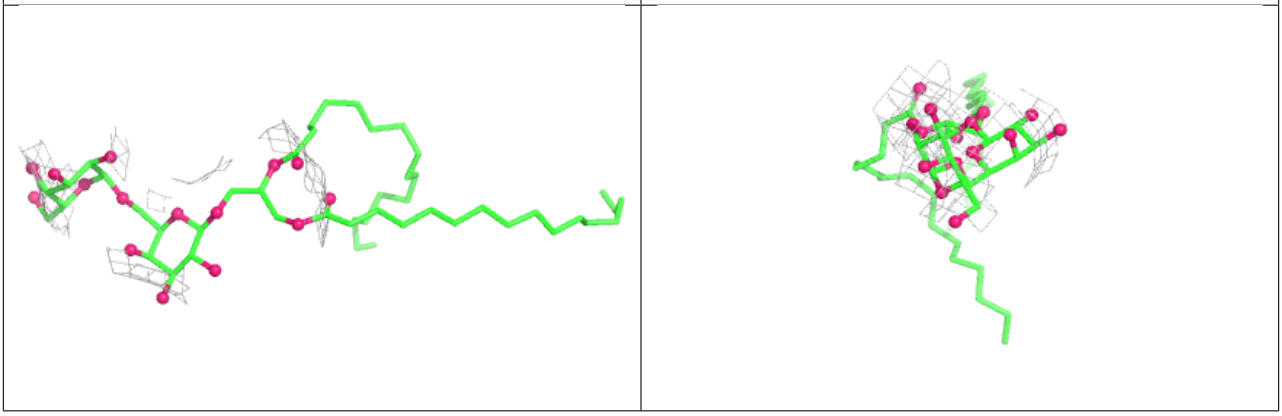




Electron density around DGD h 102:

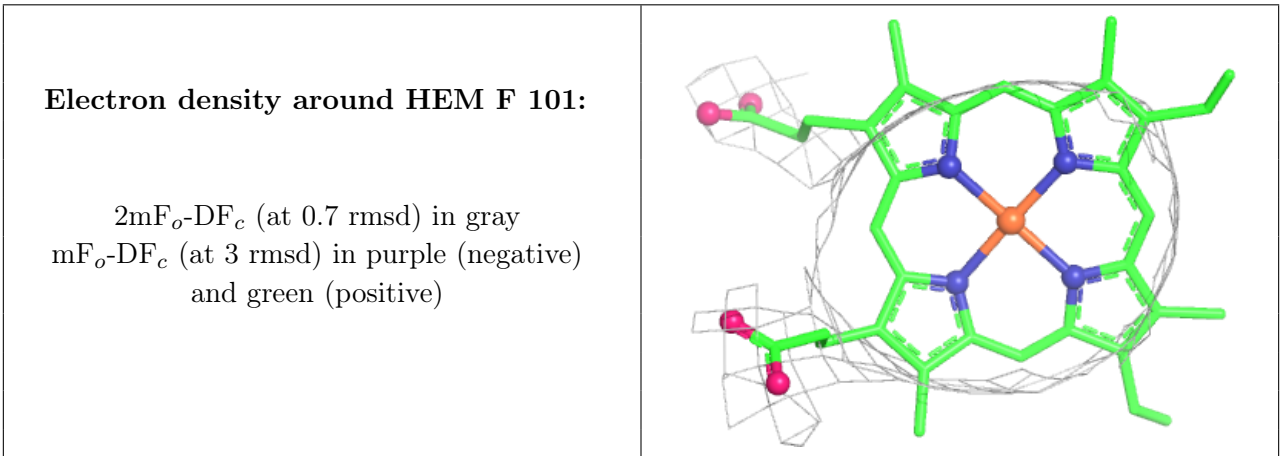
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

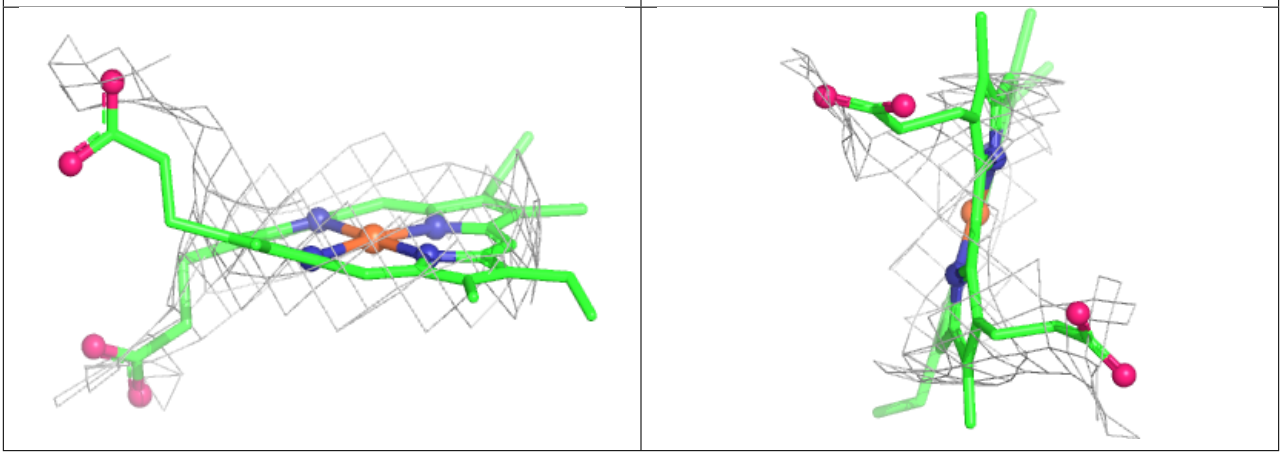




Electron density around HEM F 101:

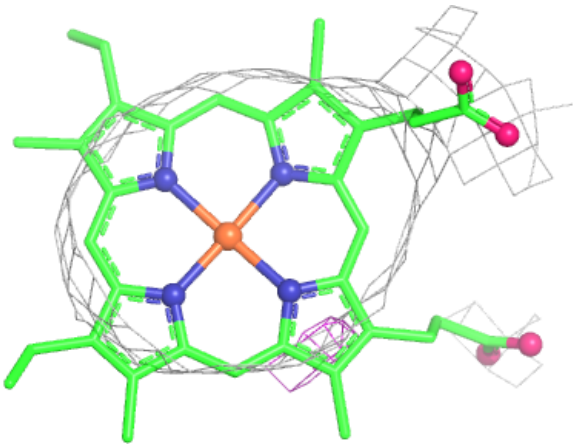
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

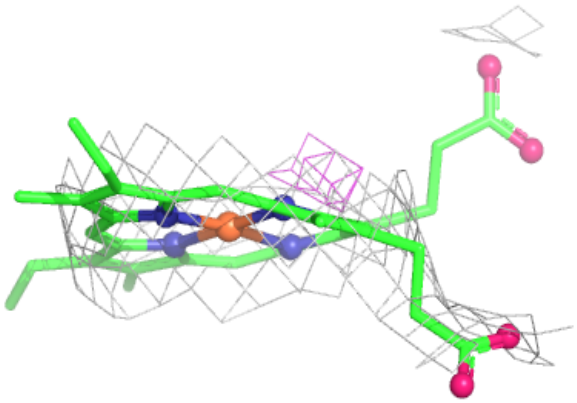




Electron density around HEM f 101:

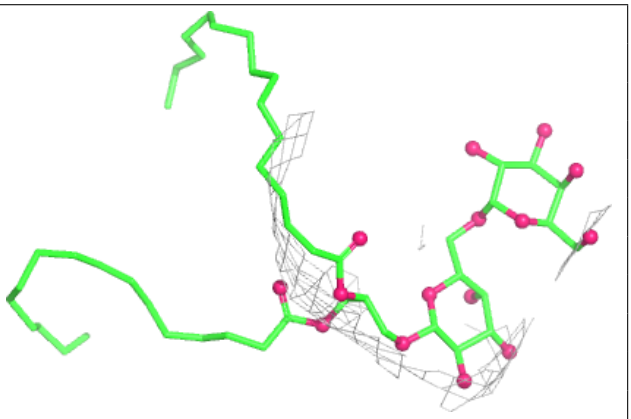
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





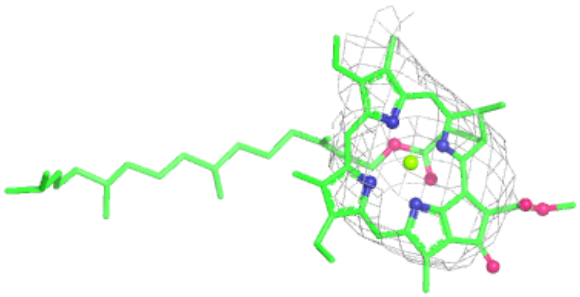
Electron density around DGD c 517:

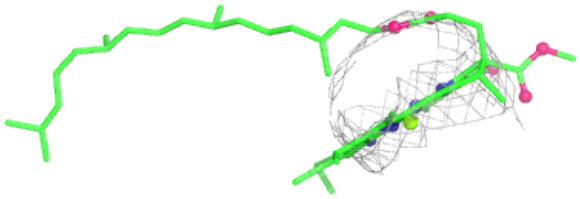
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

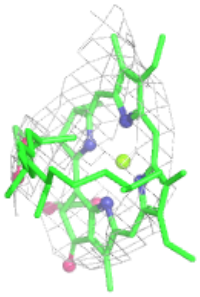


Electron density around CLA b 609:

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

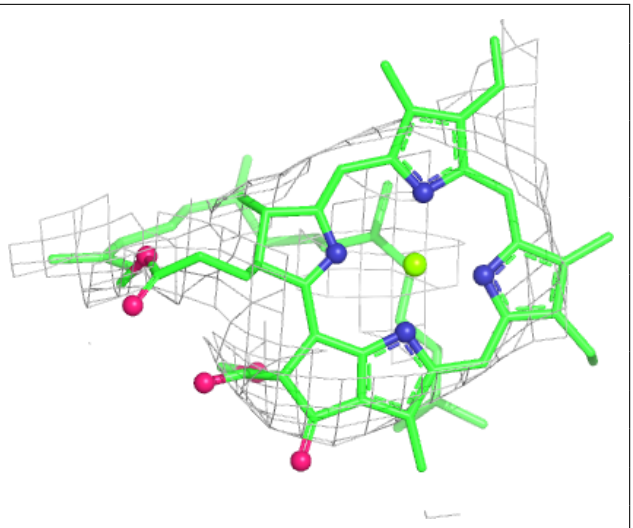


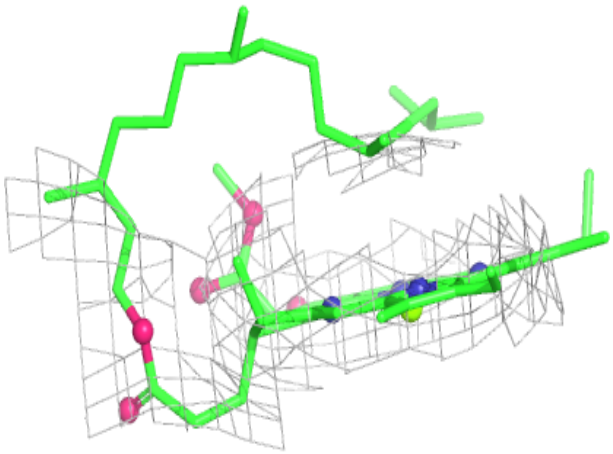


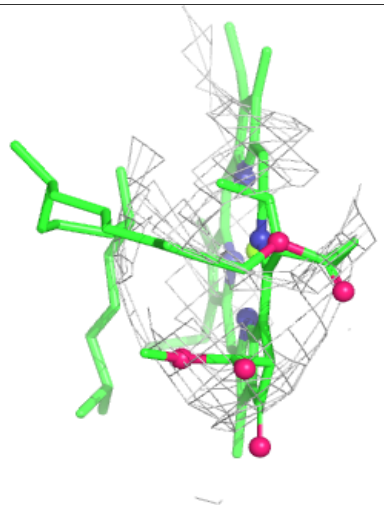


Electron density around CLA C 510:

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

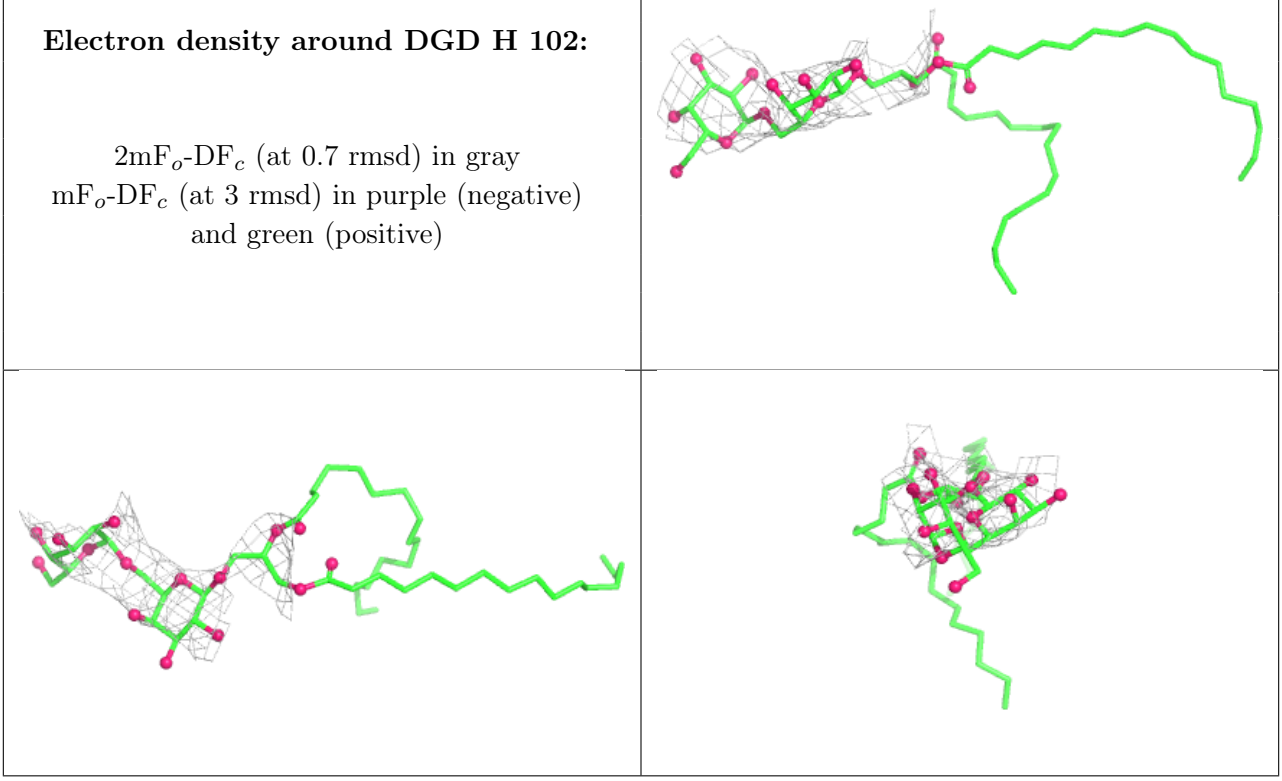






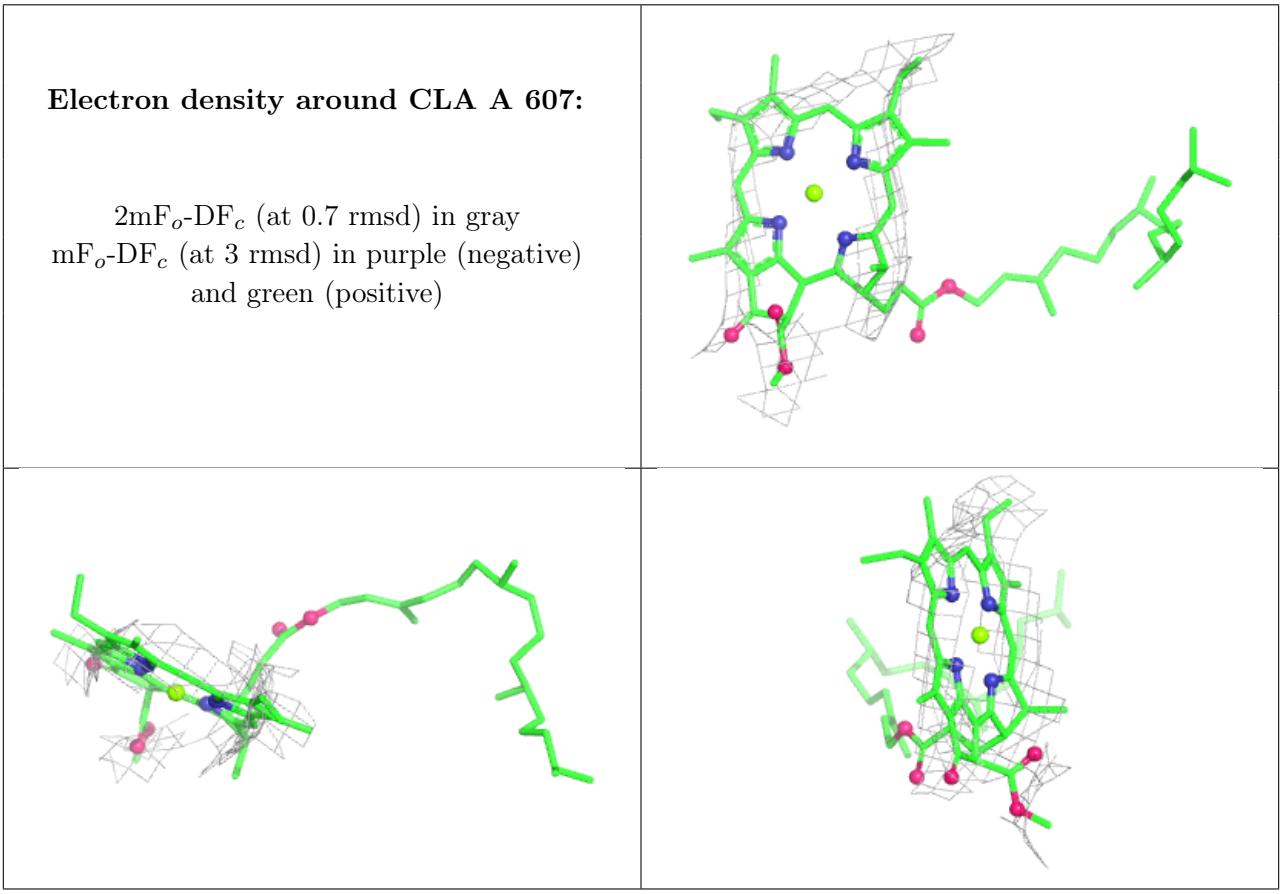
Electron density around DGD H 102:

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



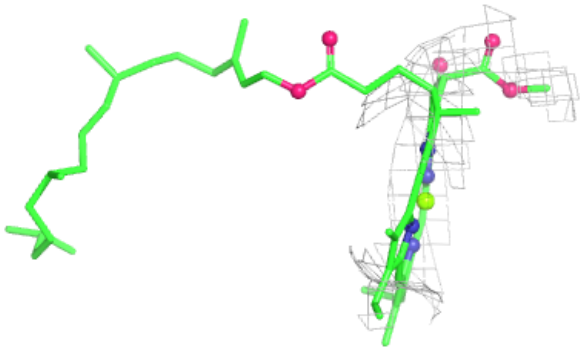
Electron density around CLA A 607:

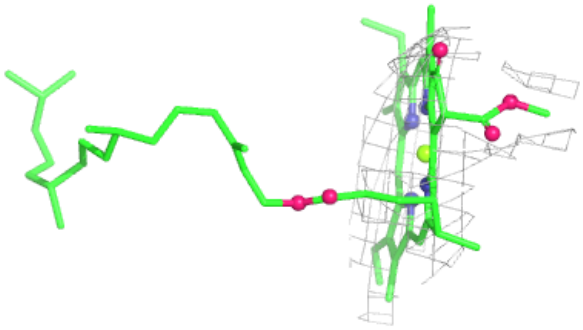
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

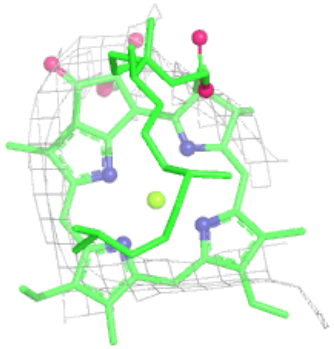


Electron density around CLA c 506:

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

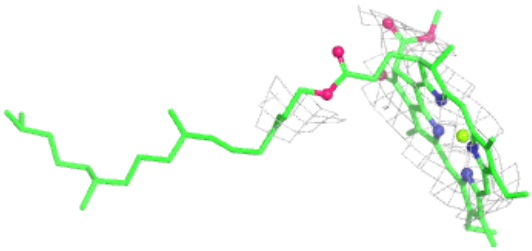


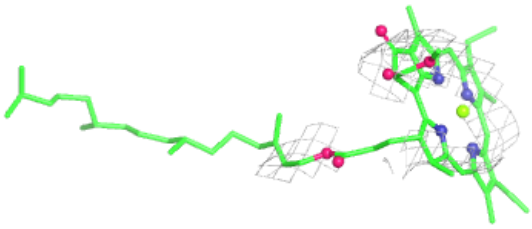


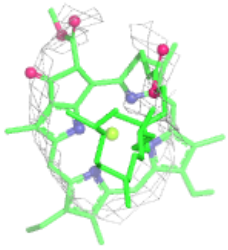


Electron density around CLA b 605:

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

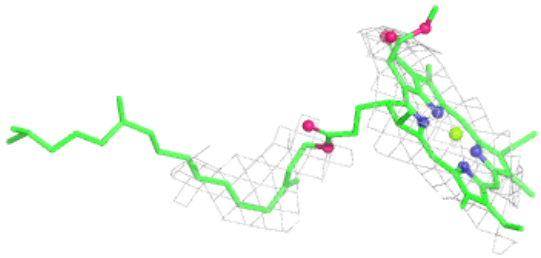


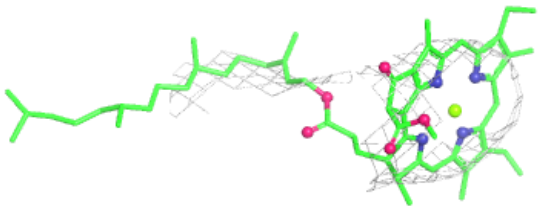


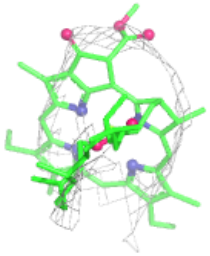


Electron density around CLA C 502:

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

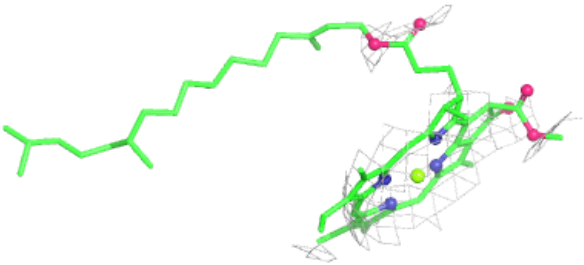






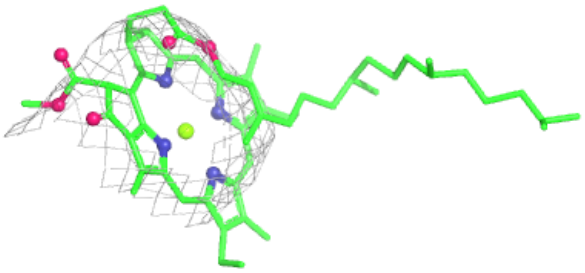
Electron density around CLA c 504:

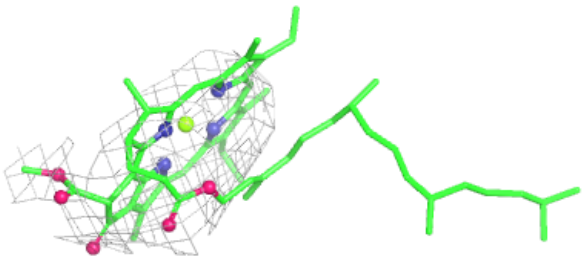
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

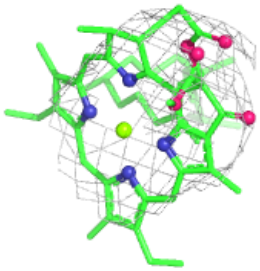


Electron density around CLA c 505:

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

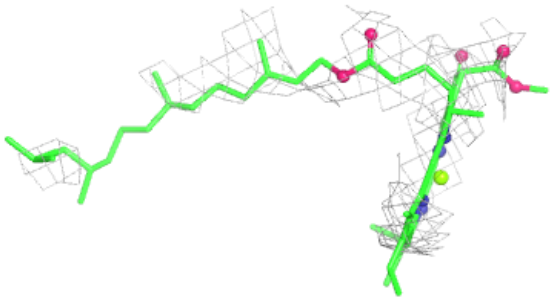


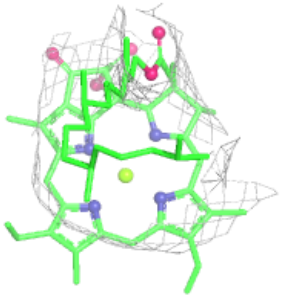




Electron density around CLA b 606:

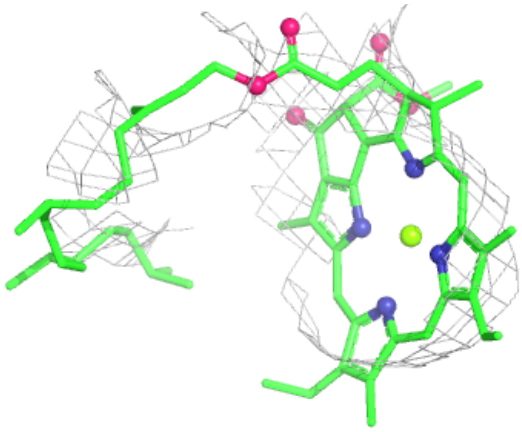
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

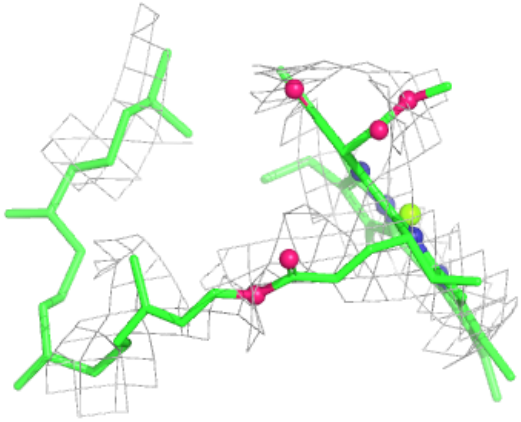


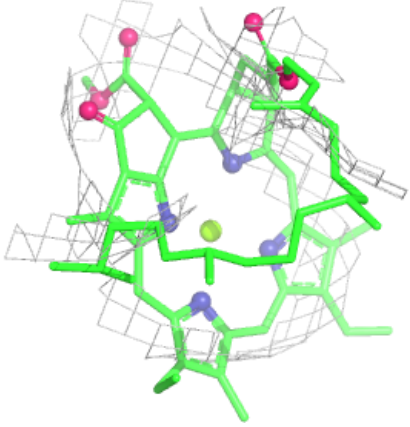


Electron density around CLA C 503:

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

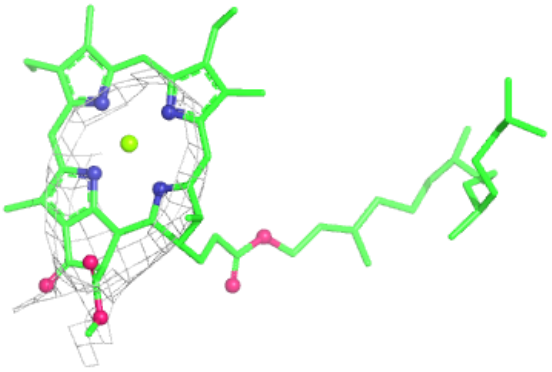


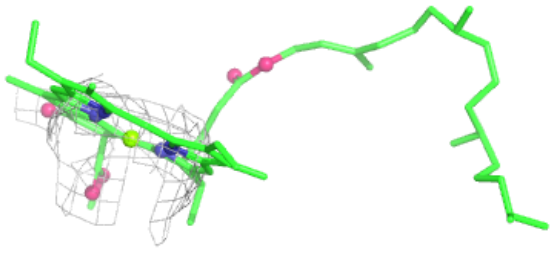




Electron density around CLA a 607:

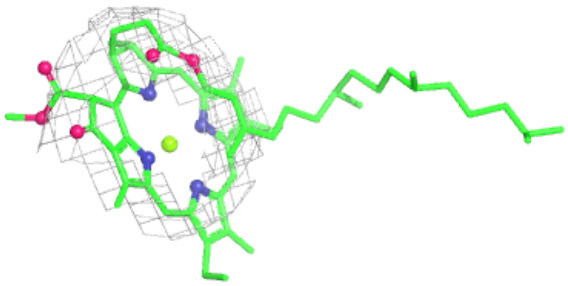
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

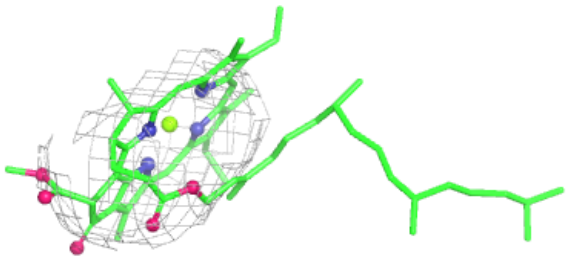


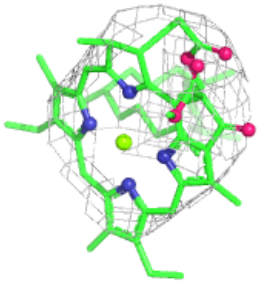


Electron density around CLA C 505:

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

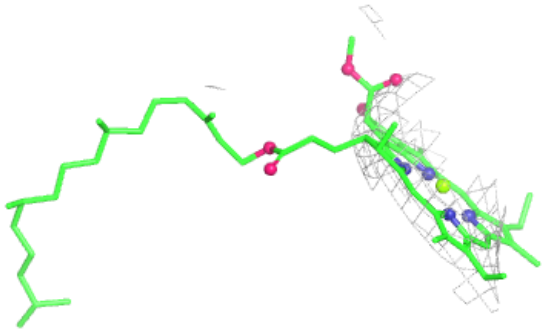


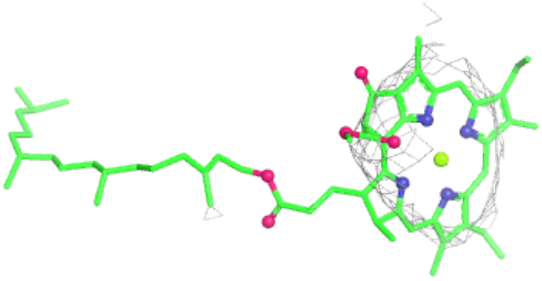


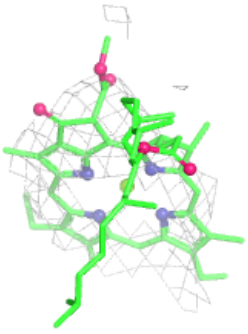


Electron density around CLA d 401:

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

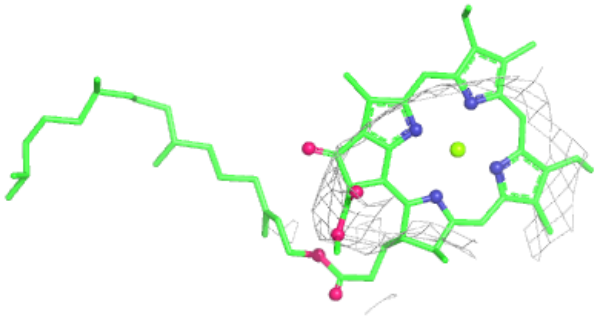


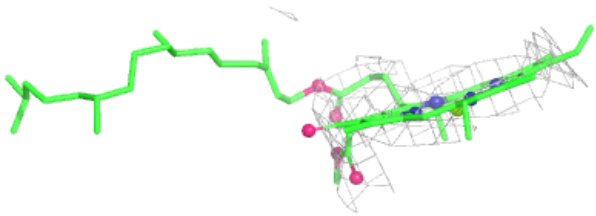




Electron density around CLA B 603:

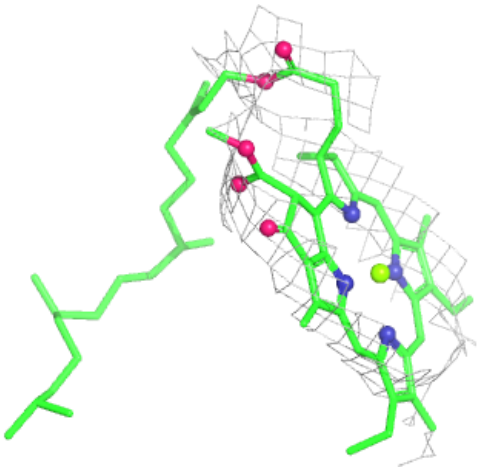
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

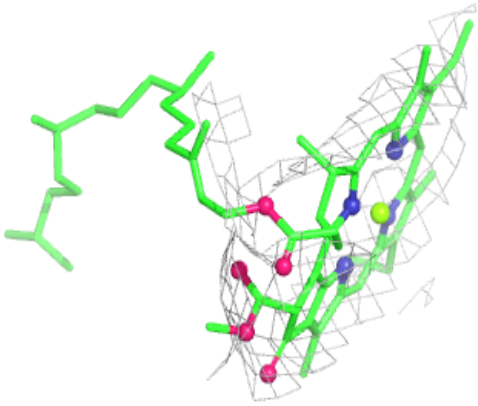


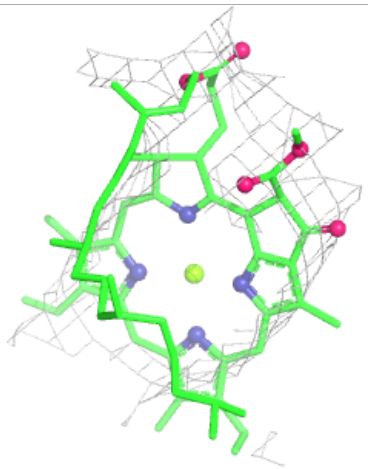


Electron density around CLA B 614:

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

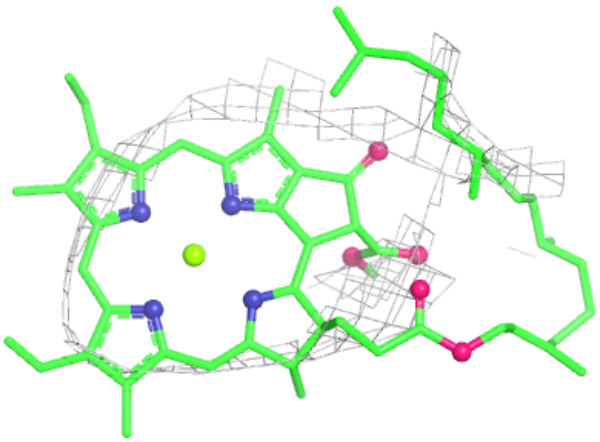


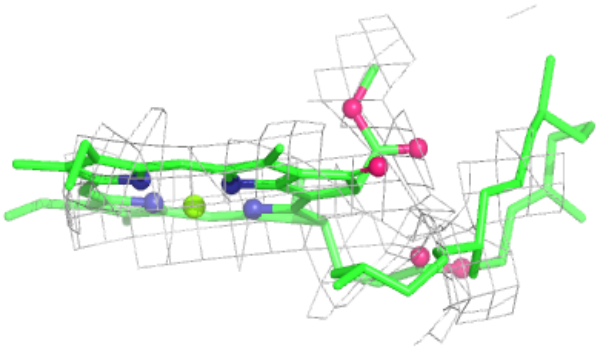


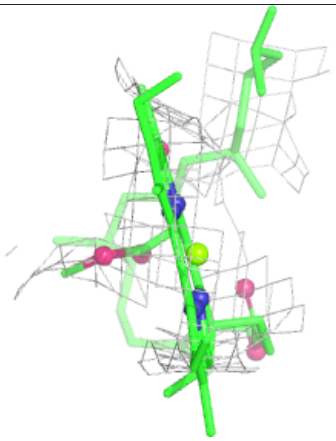


Electron density around CLA b 611:

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

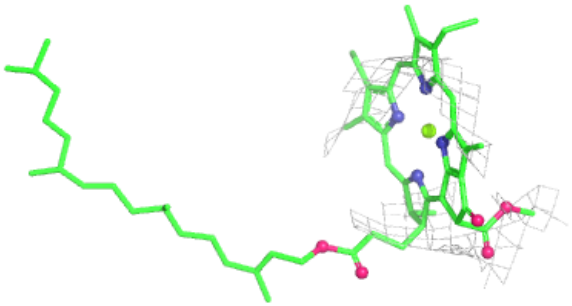


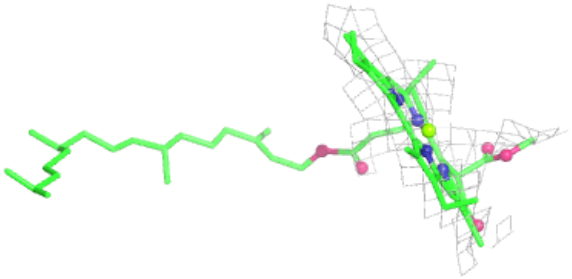


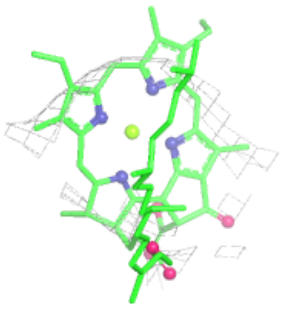


Electron density around CLA B 610:

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

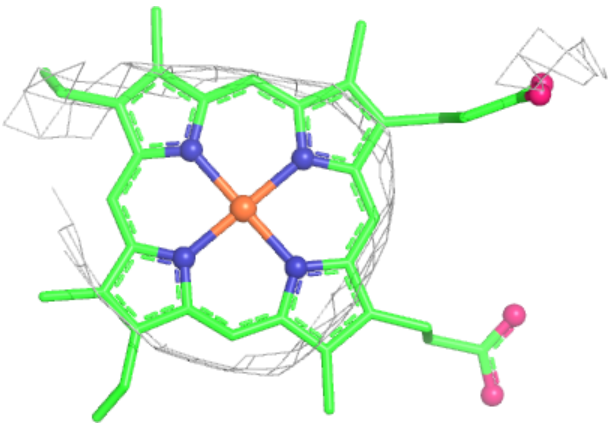


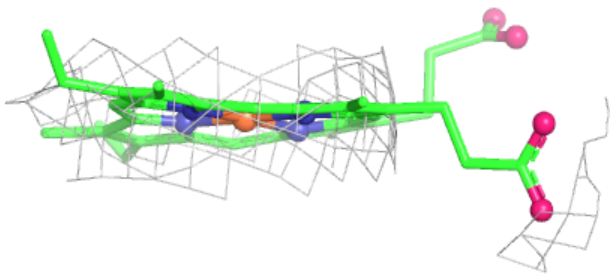


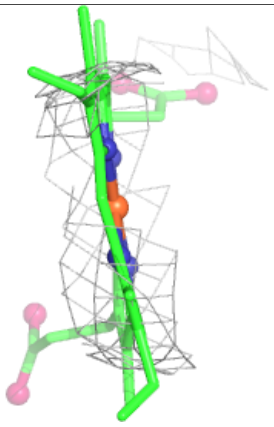


Electron density around HEM V 201:

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

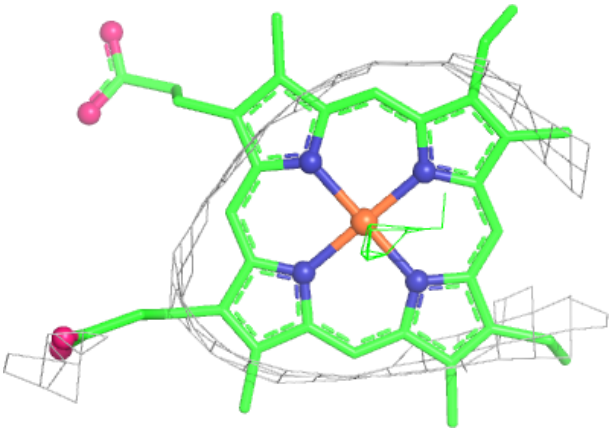


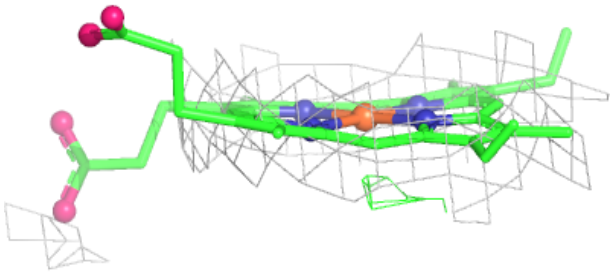


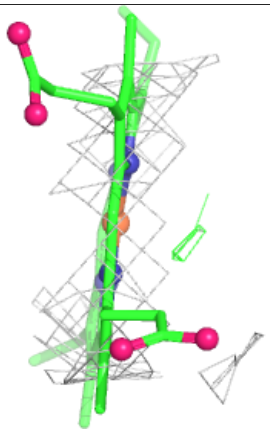


Electron density around HEM v 201:

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

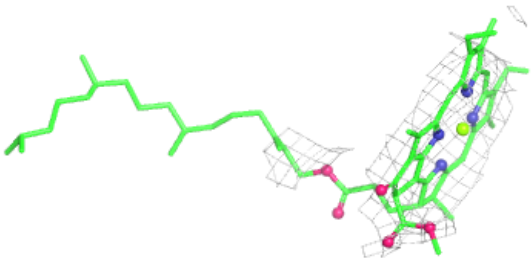


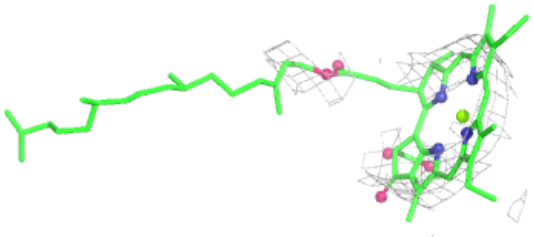


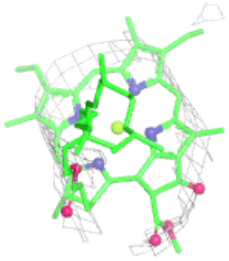


Electron density around CLA B 605:

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

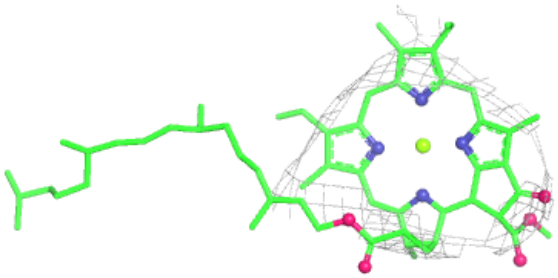


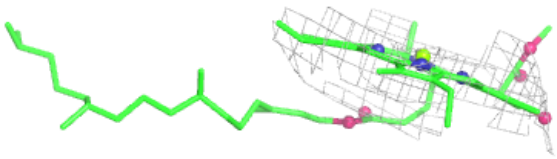


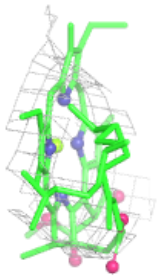


Electron density around CLA B 604:

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







6.5 Other polymers

There are no such residues in this entry.