wwPDB X-ray Structure Validation Summary Report (i)

Sep 19, 2023 – 11:34 PM EDT

PDB ID	:	5KAF
Title	:	RT XFEL structure of Photosystem II in the dark state at 3.0 A resolution
Authors	:	Young, I.D.; Ibrahim, M.; Chatterjee, R.; Gul, S.; Koroidov, S.; Brewster, A.S.; Tran, R.; Alonso-Mori, R.; Fuller, F.; Kroll, T.; Michels-Clark, T.; Laksmono, H.; Sierra, R.G.; Stan, C.A.; Saracini, C.; Bean, M.A.; Seuffert, I.; Sokaras, D.; Weng, T.-C.; Hunter, M.S.; Aquila, A.; Koglin, J.E.; Robinson, J.; Liang, M.; Boutet, S.; Lyubimov, A.Y.; Uervirojnangkoorn, M.; Moriarty, N.W.; Liebschner, D.; Afonine, P.V.; Waterman, D.G.; Evans, G.; Dobbek, H.; Weis, W.I.; Brunger, A.T.; Zwart, P.H.; Adams, P.D.; Zouni, A.; Messinger, J.; Bergmann, U.; Sauter, N.K.; Kern, J.; Yachandra, V.K.; Yano, J.
Deposited on	:	2016-06-01
Resolution	:	3.00 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:

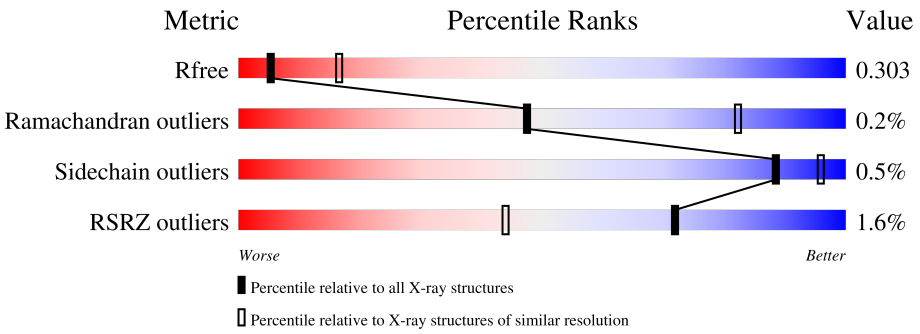
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)

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 3.00 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}	130704	2092 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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.

Mol	Chain	Length	Quality of chain
1	A	344	97%
1	a	344	97%
2	B	510	2% 99%

Continued on next page...

Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	b	510	%, 99%
3	C	461	%, 97%
3	c	461	%, 97%
4	D	352	%, 97%
4	d	352	97%
5	E	84	96%
5	e	84	4%, 98%
6	F	45	2%, 76%, 24%
6	f	45	76%, 24%
7	H	66	2%, 92%, 5%
7	h	66	2%, 94%, 5%
8	I	38	3%, 92%, 5%
8	i	38	8%, 95%, 5%
9	J	40	90%, 10%
9	j	40	5%, 90%, 10%
10	K	46	80%, 20%
10	k	46	80%, 20%
11	L	37	3%, 100%
11	l	37	3%, 100%
12	M	36	6%, 92%, 8%
12	m	36	8%, 92%, 8%
13	O	272	3%, 89%, 10%
13	o	272	2%, 89%, 10%
14	T	32	94%, 6%
14	t	32	94%, 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
15	U	134	72% 28%
15	u	134	72% 28%
16	V	163	84% 16%
16	v	163	% 83% 16%
17	Y	46	7% 63% 35%
17	y	46	4% 65% 35%
18	X	41	5% 93% 7%
18	x	41	5% 93% 7%
19	Z	62	8% 95% 5%
19	z	62	13% 98%
20	R	41	7% 83% 17%
20	r	41	80% 17%

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
25	CLA	A	606	X	-	-	-
25	CLA	A	607	X	-	-	-
25	CLA	A	609	X	-	-	-
25	CLA	A	615	X	-	-	-
25	CLA	B	601	X	-	-	-
25	CLA	B	602	X	-	-	-
25	CLA	B	603	X	-	-	-
25	CLA	B	604	X	-	-	-
25	CLA	B	606	X	-	-	-
25	CLA	B	607	X	-	-	-
25	CLA	B	608	X	-	-	-
25	CLA	B	610	X	-	-	-
25	CLA	B	611	X	-	-	-
25	CLA	B	612	X	-	-	-
25	CLA	B	613	X	-	-	-
25	CLA	B	614	X	-	-	-
25	CLA	B	615	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	B	616	X	-	-	-
25	CLA	C	501	X	-	-	-
25	CLA	C	503	X	-	-	-
25	CLA	C	504	X	-	-	-
25	CLA	C	507	X	-	-	-
25	CLA	C	508	X	-	-	-
25	CLA	C	509	X	-	-	-
25	CLA	C	510	X	-	-	-
25	CLA	C	512	X	-	-	-
25	CLA	C	513	X	-	-	-
25	CLA	D	403	X	-	-	-
25	CLA	a	606	X	-	-	-
25	CLA	a	607	X	-	-	-
25	CLA	a	609	X	-	-	-
25	CLA	a	612	X	-	-	-
25	CLA	b	604	X	-	-	-
25	CLA	b	605	X	-	-	-
25	CLA	b	606	X	-	-	-
25	CLA	b	607	X	-	-	-
25	CLA	b	609	X	-	-	-
25	CLA	b	610	X	-	-	-
25	CLA	b	611	X	-	-	-
25	CLA	b	613	X	-	-	-
25	CLA	b	614	X	-	-	-
25	CLA	b	615	X	-	-	-
25	CLA	b	616	X	-	-	-
25	CLA	b	617	X	-	-	-
25	CLA	b	618	X	-	-	-
25	CLA	b	619	X	-	-	-
25	CLA	c	503	X	-	-	-
25	CLA	c	505	X	-	-	-
25	CLA	c	506	X	-	-	-
25	CLA	c	508	X	-	-	-
25	CLA	c	509	X	-	-	-
25	CLA	c	510	X	-	-	-
25	CLA	c	511	X	-	-	-
25	CLA	c	512	X	-	-	-
25	CLA	c	513	X	-	-	-
25	CLA	c	514	X	-	-	-
25	CLA	c	515	X	-	-	-
25	CLA	d	404	X	-	-	-
29	LMG	b	625	-	-	-	X

2 Entry composition (i)

There are 36 unique types of molecules in this entry. The entry contains 50162 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
			Total	C	N	O	S			
1	A	334	2618	1715	431	457	15	0	0	0
1	a	334	2613	1713	428	457	15	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	504	3953	2596	658	686	13	0	0	0
2	b	504	3960	2600	658	689	13	3	1	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	341	2716	1800	444	460	12	0	0	0
4	d	341	2709	1798	441	458	12	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	E	81	657	429	106	122	0	0	0
5	e	82	665	434	108	123	0	0	0

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	1	FME	-	expression tag	UNP Q8DJZ6
i	1	FME	-	expression tag	UNP Q8DJZ6

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	J	36	257	174	40	42	1	0	0	0
9	j	36	257	174	40	42	1	0	0	0

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
11	L	37	301	200	48	53	0	0	0
11	l	37	301	200	48	53	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	M	33	256	171	37	47	1	0	0	0
12	m	33	256	171	37	47	1	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	1	FME	-	expression tag	UNP Q8DHA7
m	1	FME	-	expression tag	UNP Q8DHA7

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	O	244	1845	1154	309	378	4	0	0	0
13	o	244	1853	1160	312	377	4	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
14	T	30	258	181	36	39	2	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
14	t	30	258	181	36	39	2	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	1	FME	-	expression tag	UNP Q8DIQ0
t	1	FME	-	expression tag	UNP Q8DIQ0

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
17	Y	30	224	147	38	36	3	0	0	0
17	y	30	224	147	38	36	3	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
18	X	38	279	187	45	47	0	0	0
18	x	38	281	188	45	48	0	0	0

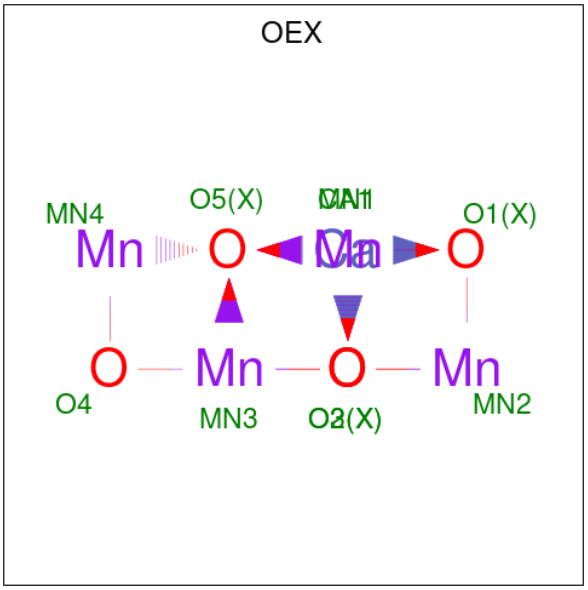
- Molecule 19 is a protein called Photosystem II reaction center protein Z.

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

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

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

- Molecule 21 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: $CaMn_4O_5$).



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

- Molecule 22 is FE (II) ION (three-letter code: FE2) (formula: Fe).

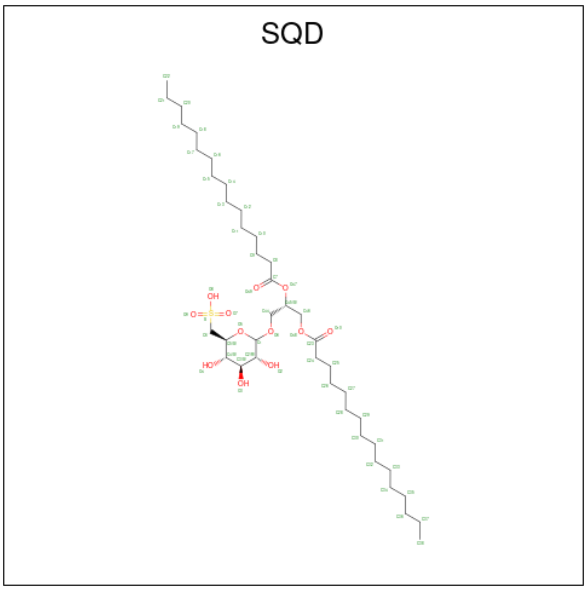
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Fe		
22	A	1	1	1	0	0

Continued on next page...

Continued from previous page...

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

- Molecule 23 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).

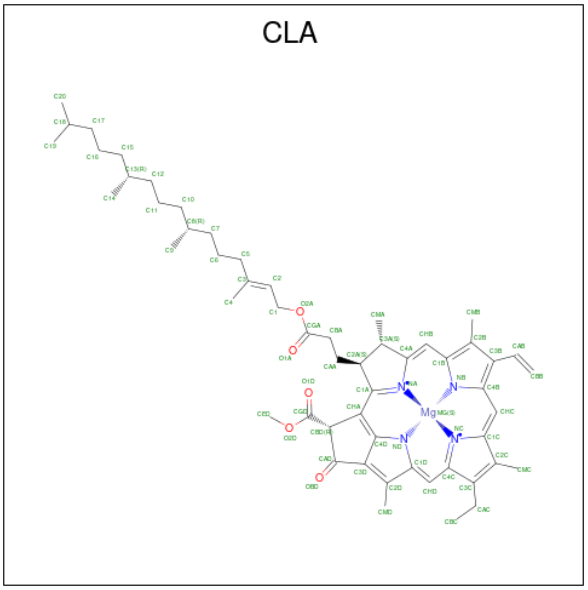


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	A	1	Total C O S 52 39 12 1	0	0
23	A	1	Total C O 40 35 5	0	0
23	B	1	Total C O S 54 41 12 1	0	0
23	D	1	Total C O S 47 34 12 1	0	0
23	D	1	Total C O S 43 30 12 1	0	0
23	I	1	Total C O 40 35 5	0	0
23	b	1	Total C O S 54 41 12 1	0	0
23	c	1	Total C O S 54 41 12 1	0	0
23	f	1	Total C O S 43 30 12 1	0	0

- Molecule 24 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 25 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
25	A	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
25	A	1	57	47	1	4	5	0	0
			Total	C	Mg	N	O		
25	A	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
25	A	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
25	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
25	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
25	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
25	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
25	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
25	B	1	65	55	1	4	5	0	0

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
25	C	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
25	C	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
25	D	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
25	D	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
25	a	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
25	a	1	59	49	1	4	5	0	0
			Total	C	Mg	N	O		
25	a	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
25	a	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
25	b	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
25	b	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
25	b	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
25	b	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
25	b	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
25	b	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
25	b	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
25	b	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
25	b	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
25	b	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
25	b	1	65	55	1	4	5	0	0

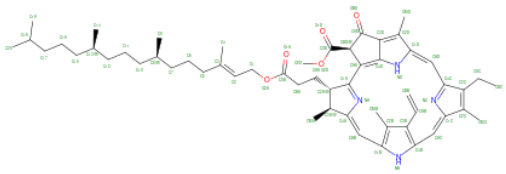
Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
25	b	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
25	b	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
25	b	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
25	c	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
25	c	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
25	c	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
25	c	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
25	c	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
25	c	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
25	c	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
25	c	1	58	48	1	4	5	0	0
			Total	C	Mg	N	O		
25	c	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
25	c	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
25	c	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
25	c	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
25	c	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
25	d	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
25	d	1	65	55	1	4	5	0	0

- Molecule 26 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).

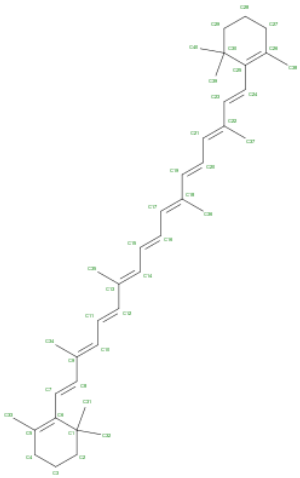
PHO



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

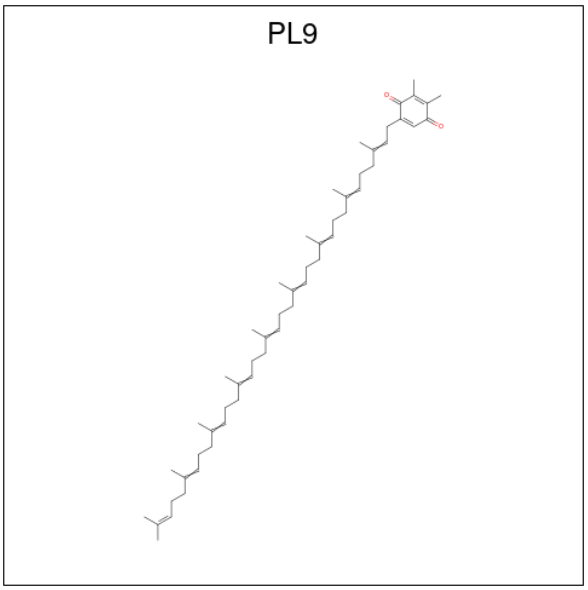
- Molecule 27 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).

BCR



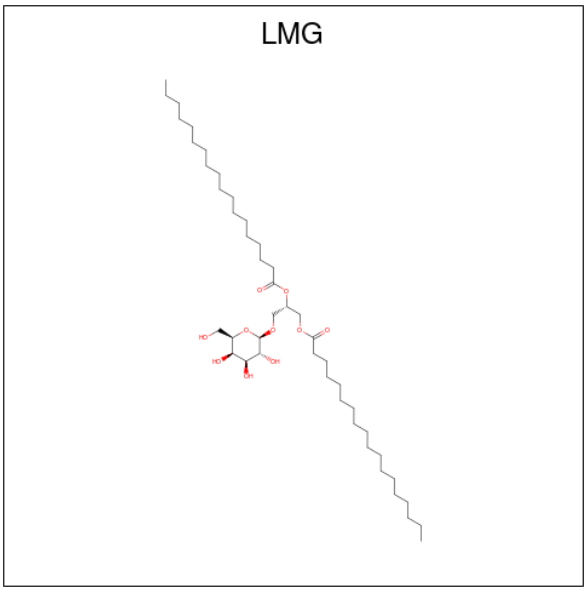
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	C		
27	A	1	40	40	0	0
27	B	1	40	40	0	0
27	B	1	40	40	0	0
27	B	1	40	40	0	0
27	B	1	40	40	0	0
27	C	1	40	40	0	0
27	C	1	40	40	0	0
27	D	1	40	40	0	0
27	H	1	40	40	0	0
27	K	1	40	40	0	0
27	T	1	40	40	0	0
27	Y	1	40	40	0	0
27	a	1	40	40	0	0
27	b	1	40	40	0	0
27	b	1	40	40	0	0
27	b	1	40	40	0	0
27	c	1	40	40	0	0
27	c	1	40	40	0	0
27	d	1	40	40	0	0
27	h	1	40	40	0	0
27	k	1	40	40	0	0
27	y	1	40	40	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 (three-letter code: PL9) (formula: $C_{53}H_{80}O_2$).



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

- Molecule 29 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: 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	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	D	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	b	1	Total C 9 9	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

Continued on next page...

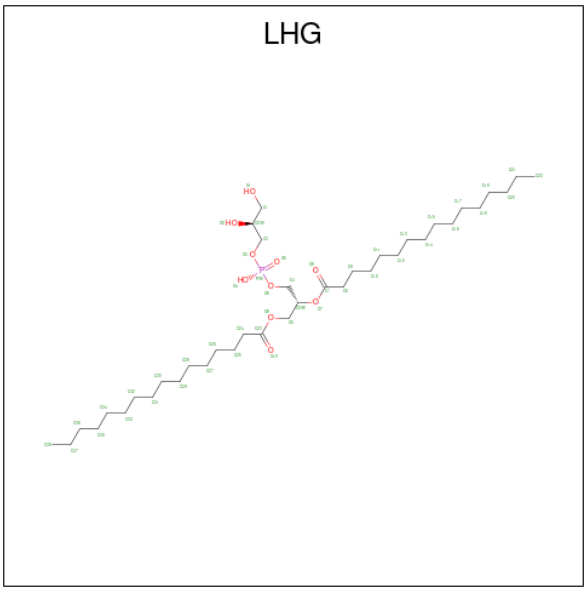
Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
29	d	1	42	32	10	0	0
			Total	C	O		
29	d	1	40	35	5	0	0

- Molecule 30 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

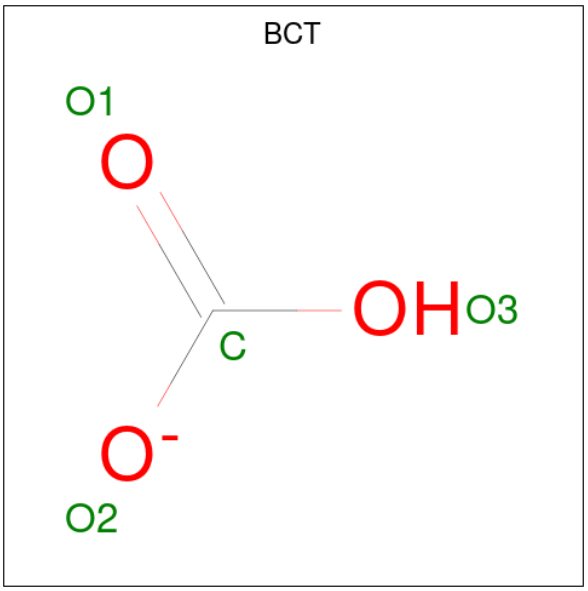
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	C		
30	A	1	7	7	0	0
			Total	C		
30	B	3	28	28	0	0
			Total	C		
30	C	1	9	9	0	0
			Total	C		
30	H	1	8	8	0	0
			Total	C		
30	M	2	23	23	0	0
			Total	C		
30	b	2	26	26	0	0
			Total	C		
30	d	1	22	22	0	0
			Total	C		
30	i	1	12	12	0	0
			Total	C		
30	j	1	9	9	0	0
			Total	C		
30	m	2	21	21	0	0
			Total	C		
30	t	1	10	10	0	0
			Total	C		
30	z	1	11	11	0	0

- Molecule 31 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



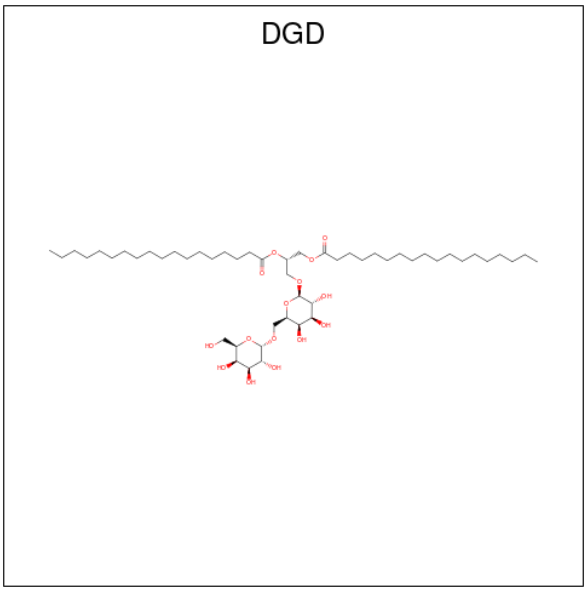
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
31	A	1	49	38	10	1	0	0
			Total	C	O	P		
31	A	1	49	38	10	1	0	0
			Total	C	O	P		
31	A	1	49	38	10	1	0	0
			Total	C	O	P		
31	D	1	49	38	10	1	0	0
			Total	C	O	P		
31	L	1	49	38	10	1	0	0
			Total	C	O	P		
31	a	1	49	38	10	1	0	0
			Total	C	O	P		
31	a	1	35	24	10	1	0	0
			Total	C	O	P		
31	a	1	42	31	10	1	0	0
			Total	C	O	P		
31	d	1	49	38	10	1	0	0
			Total	C	O	P		
31	l	1	49	38	10	1	0	0

- Molecule 32 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



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

- Molecule 33 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



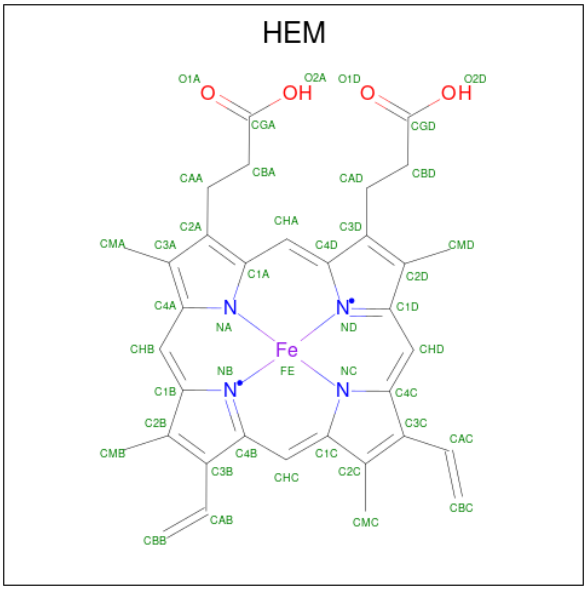
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
33	C	1	62	47	15	0	0

Continued on next page...

Continued from previous page...

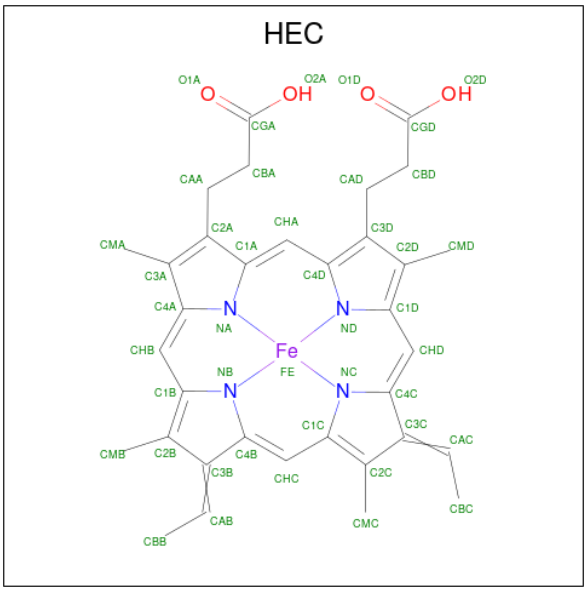
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
33	C	1	62	47	15		0	0
			Total	C	O			
33	C	1	62	47	15		0	0
			Total	C	O			
33	H	1	62	47	15		0	0
			Total	C	O			
33	c	1	62	47	15		0	0
			Total	C	O			
33	c	1	62	47	15		0	0
			Total	C	O			
33	c	1	62	47	15		0	0
			Total	C	O			
33	h	1	62	47	15		0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

- Molecule 34 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 35 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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

- Molecule 36 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
36	A	10	10	10	0	0
			Total	O		
36	B	17	17	17	0	0
			Total	O		
36	C	11	11	11	0	0
			Total	O		
36	D	9	9	9	0	0
			Total	O		
36	E	3	3	3	0	0
			Total	O		
36	L	2	2	2	0	0
			Total	O		
36	M	2	2	2	0	0
			Total	O		
36	O	5	5	5	0	0
			Total	O		
36	T	1	1	1	0	0
			Total	O		
36	V	2	2	2	0	0

Continued on next page...

Continued from previous page...

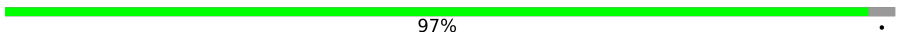
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	X	1	Total O 1 1	0	0
36	Z	1	Total O 1 1	0	0
36	a	11	Total O 11 11	0	0
36	b	12	Total O 12 12	0	0
36	c	11	Total O 11 11	0	0
36	d	9	Total O 9 9	0	0
36	i	1	Total O 1 1	0	0
36	l	2	Total O 2 2	0	0
36	o	9	Total O 9 9	0	0
36	u	2	Total O 2 2	0	0
36	v	3	Total O 3 3	0	0

3 Residue-property plots (i)

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

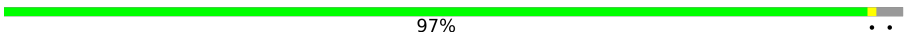
• Molecule 1: Photosystem II protein D1 1

Chain A:



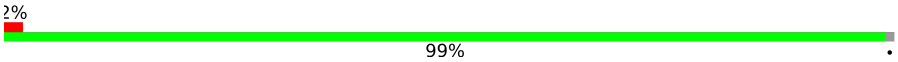
• Molecule 1: Photosystem II protein D1 1

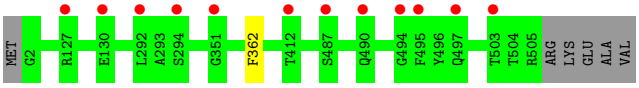
Chain a:



• Molecule 2: Photosystem II CP47 reaction center protein

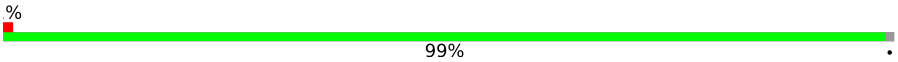
Chain B:

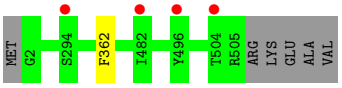




• Molecule 2: Photosystem II CP47 reaction center protein

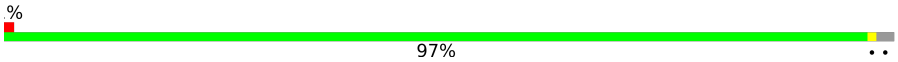
Chain b:

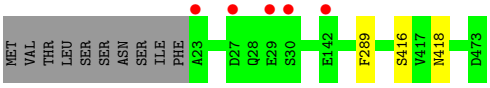




• Molecule 3: Photosystem II CP43 reaction center protein

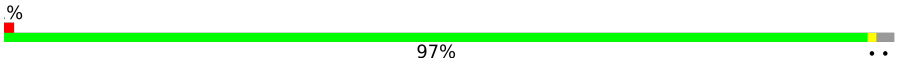
Chain C:

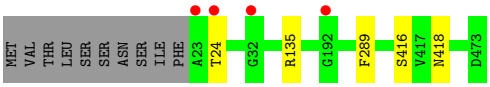




• Molecule 3: Photosystem II CP43 reaction center protein

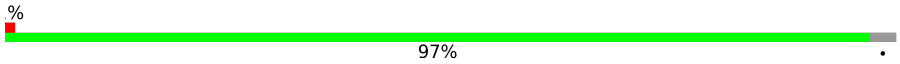
Chain c:

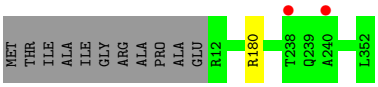




• Molecule 4: Photosystem II D2 protein

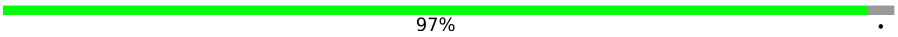
Chain D:





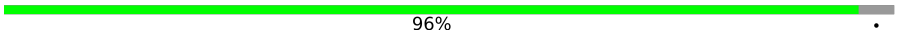
• Molecule 4: Photosystem II D2 protein

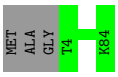
Chain d:



• Molecule 5: Cytochrome b559 subunit alpha

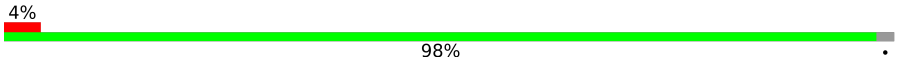
Chain E:

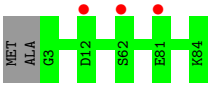




• Molecule 5: Cytochrome b559 subunit alpha

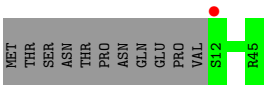
Chain e:





• Molecule 6: Cytochrome b559 subunit beta

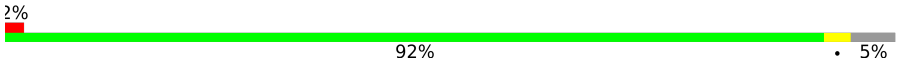
Chain F:

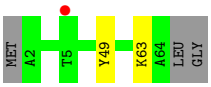


• Molecule 6: Cytochrome b559 subunit beta

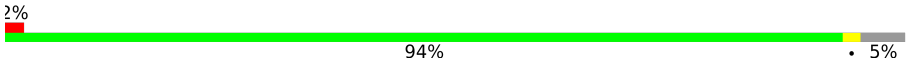
Chain f:

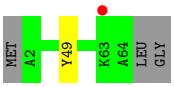
• Molecule 7: Photosystem II reaction center protein H

Chain H: 

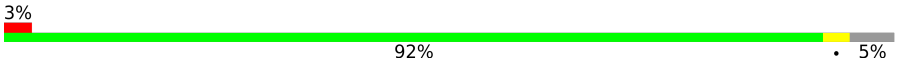


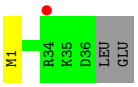
• Molecule 7: Photosystem II reaction center protein H

Chain h: 

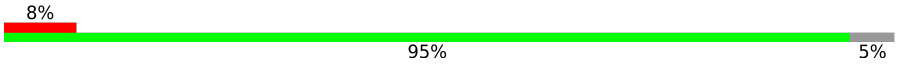


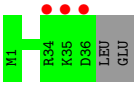
• Molecule 8: Photosystem II reaction center protein I

Chain I: 



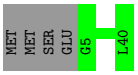
• Molecule 8: Photosystem II reaction center protein I

Chain i: 

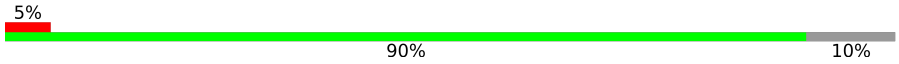


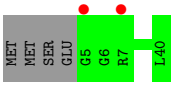
• Molecule 9: Photosystem II reaction center protein J

Chain J:



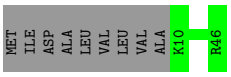
• Molecule 9: Photosystem II reaction center protein J

Chain j: 



• Molecule 10: Photosystem II reaction center protein K

Chain K:

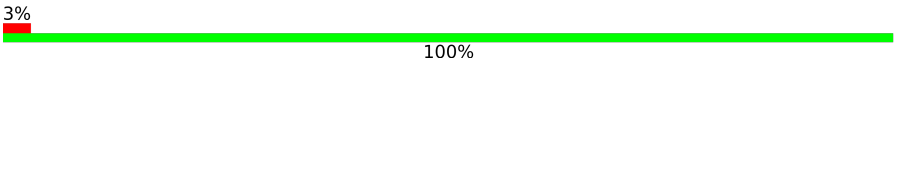


• Molecule 10: Photosystem II reaction center protein K

Chain k:

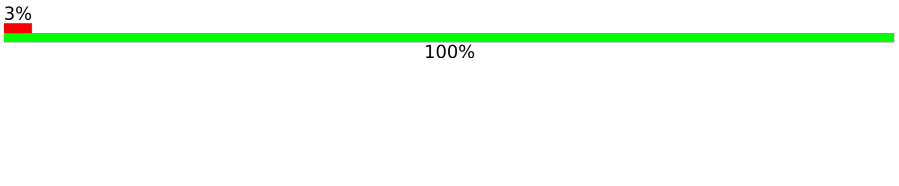
• Molecule 11: Photosystem II reaction center protein L

Chain L:



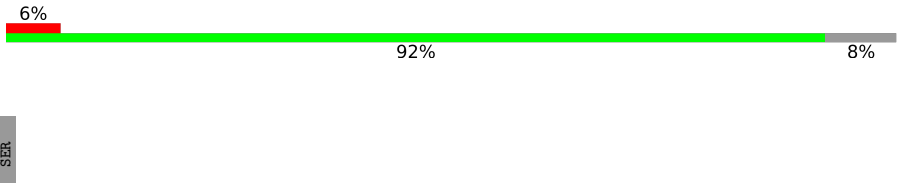
• Molecule 11: Photosystem II reaction center protein L

Chain l:



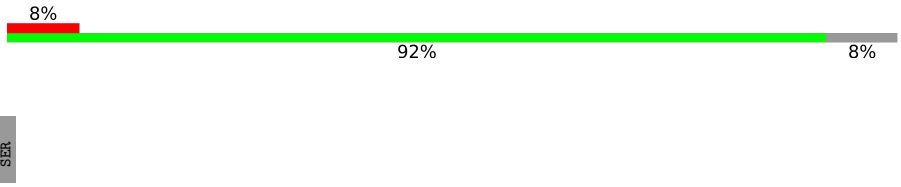
• Molecule 12: Photosystem II reaction center protein M

Chain M:



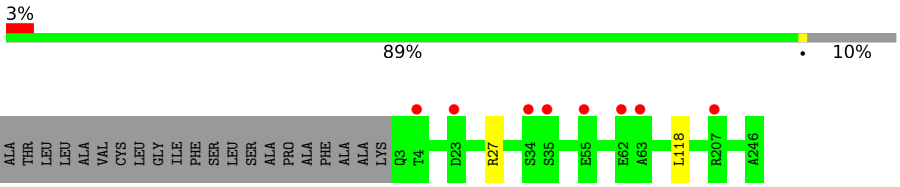
• Molecule 12: Photosystem II reaction center protein M

Chain m:



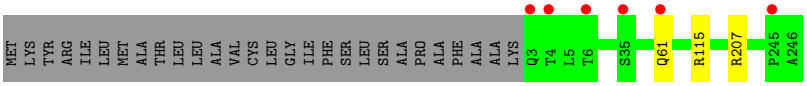
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:



• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:



• Molecule 14: Photosystem II reaction center protein T

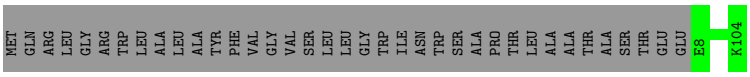
Chain T: 94% 6%

• Molecule 14: Photosystem II reaction center protein T

Chain t: 94% 6%

• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U: 72% 28%



• Molecule 15: Photosystem II 12 kDa extrinsic protein

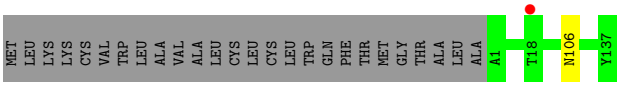
Chain u: 72% 28%

• Molecule 16: Cytochrome c-550

Chain V: 84% 16%

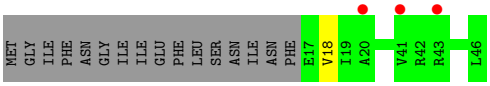
• Molecule 16: Cytochrome c-550

Chain v: % 83% 16%



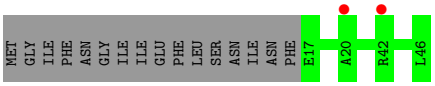
• Molecule 17: Photosystem II reaction center protein Ycf12

Chain Y: 7% 63% 35%



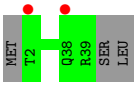
• Molecule 17: Photosystem II reaction center protein Ycf12

Chain y: 4% 65% 35%



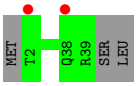
• Molecule 18: Photosystem II reaction center X protein

Chain X: 5% 93% 7%



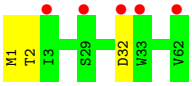
• Molecule 18: Photosystem II reaction center X protein

Chain x: 5% 93% 7%



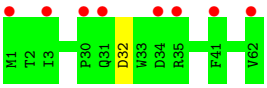
• Molecule 19: Photosystem II reaction center protein Z

Chain Z: 8% 95% 5%



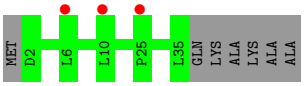
• Molecule 19: Photosystem II reaction center protein Z

Chain z: 13% 98%



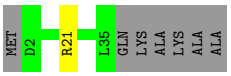
• Molecule 20: Photosystem II protein Y

Chain R: 7% 83% 17%



• Molecule 20: Photosystem II protein Y

Chain r:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	117.73Å 223.81Å 330.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.12 – 3.00 43.12 – 3.00	Depositor EDS
% Data completeness (in resolution range)	96.0 (43.12-3.00) 86.3 (43.12-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.43 (at 3.01Å)	Xtriage
Refinement program	PHENIX dev_2411	Depositor
R, R_{free}	0.264 , 0.303 0.264 , 0.303	Depositor DCC
R_{free} test set	1446 reflections (0.85%)	wwPDB-VP
Wilson B-factor (Å^2)	48.4	Xtriage
Anisotropy	0.294	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 56.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	50162	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.20% 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, LHG, HEM, PL9, UNL, DGD, HEC, FME, PHO, CLA, FE2, BCR, LMG, SQD, OEX, BCT

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	0.24	0/2703	0.39	0/3687
1	a	0.24	0/2698	0.39	0/3681
2	B	0.25	0/4093	0.39	0/5580
2	b	0.25	0/4103	0.39	0/5593
3	C	0.24	0/3599	0.39	0/4900
3	c	0.24	0/3599	0.38	0/4900
4	D	0.25	0/2811	0.39	0/3830
4	d	0.25	0/2804	0.39	0/3821
5	E	0.30	0/676	0.39	0/924
5	e	0.23	0/684	0.39	0/933
6	F	0.24	0/283	0.37	0/386
6	f	0.24	0/283	0.37	0/386
7	H	0.24	0/511	0.41	0/697
7	h	0.24	0/511	0.40	0/697
8	I	0.24	0/293	0.37	0/396
8	i	0.25	0/293	0.38	0/396
9	J	0.24	0/263	0.37	0/356
9	j	0.24	0/263	0.38	0/356
10	K	0.25	0/303	0.40	0/416
10	k	0.25	0/303	0.37	0/416
11	L	0.24	0/308	0.37	0/419
11	l	0.23	0/308	0.36	0/419
12	M	0.24	0/249	0.35	0/341
12	m	0.24	0/249	0.35	0/341
13	O	0.24	0/1876	0.45	0/2549
13	o	0.24	0/1884	0.45	0/2557
14	T	0.26	0/257	0.35	0/349
14	t	0.26	0/257	0.36	0/349
15	U	0.23	0/785	0.40	0/1064
15	u	0.24	0/785	0.41	0/1064
16	V	0.23	0/1085	0.40	0/1473
16	v	0.22	0/1085	0.41	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	Y	0.27	0/225	0.54	0/301
17	y	0.24	0/225	0.37	0/301
18	X	0.23	0/282	0.35	0/381
18	x	0.24	0/284	0.37	0/384
19	Z	0.23	0/490	0.34	0/669
19	z	0.24	0/490	0.36	0/669
20	R	0.21	0/279	0.36	0/383
20	r	0.22	0/279	0.39	0/383
All	All	0.24	0/42758	0.39	0/58220

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	332/344 (96%)	320 (96%)	11 (3%)	1 (0%)	41	76
1	a	332/344 (96%)	320 (96%)	11 (3%)	1 (0%)	41	76
2	B	502/510 (98%)	483 (96%)	19 (4%)	0	100	100
2	b	503/510 (99%)	486 (97%)	17 (3%)	0	100	100
3	C	449/461 (97%)	436 (97%)	12 (3%)	1 (0%)	47	82
3	c	449/461 (97%)	430 (96%)	17 (4%)	2 (0%)	34	72

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	339/352 (96%)	328 (97%)	11 (3%)	0	100	100
4	d	339/352 (96%)	324 (96%)	15 (4%)	0	100	100
5	E	79/84 (94%)	78 (99%)	1 (1%)	0	100	100
5	e	80/84 (95%)	78 (98%)	2 (2%)	0	100	100
6	F	32/45 (71%)	32 (100%)	0	0	100	100
6	f	32/45 (71%)	32 (100%)	0	0	100	100
7	H	61/66 (92%)	57 (93%)	3 (5%)	1 (2%)	9	40
7	h	61/66 (92%)	58 (95%)	3 (5%)	0	100	100
8	I	34/38 (90%)	32 (94%)	2 (6%)	0	100	100
8	i	34/38 (90%)	31 (91%)	3 (9%)	0	100	100
9	J	34/40 (85%)	32 (94%)	2 (6%)	0	100	100
9	j	34/40 (85%)	33 (97%)	1 (3%)	0	100	100
10	K	35/46 (76%)	35 (100%)	0	0	100	100
10	k	35/46 (76%)	35 (100%)	0	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
12	M	31/36 (86%)	30 (97%)	1 (3%)	0	100	100
12	m	31/36 (86%)	30 (97%)	1 (3%)	0	100	100
13	O	242/272 (89%)	228 (94%)	14 (6%)	0	100	100
13	o	242/272 (89%)	232 (96%)	9 (4%)	1 (0%)	34	72
14	T	28/32 (88%)	27 (96%)	1 (4%)	0	100	100
14	t	28/32 (88%)	28 (100%)	0	0	100	100
15	U	95/134 (71%)	91 (96%)	4 (4%)	0	100	100
15	u	95/134 (71%)	90 (95%)	5 (5%)	0	100	100
16	V	135/163 (83%)	128 (95%)	7 (5%)	0	100	100
16	v	135/163 (83%)	130 (96%)	5 (4%)	0	100	100
17	Y	28/46 (61%)	25 (89%)	2 (7%)	1 (4%)	3	19
17	y	28/46 (61%)	28 (100%)	0	0	100	100
18	X	36/41 (88%)	36 (100%)	0	0	100	100
18	x	36/41 (88%)	32 (89%)	4 (11%)	0	100	100
19	Z	60/62 (97%)	55 (92%)	3 (5%)	2 (3%)	4	21

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	z	60/62 (97%)	57 (95%)	3 (5%)	0	100	100
20	R	32/41 (78%)	32 (100%)	0	0	100	100
20	r	32/41 (78%)	32 (100%)	0	0	100	100
All	All	5240/5700 (92%)	5040 (96%)	190 (4%)	10 (0%)	47	82

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
17	Y	18	VAL
19	Z	32	ASP
13	o	61	GLN
3	C	416	SER
7	H	63	LYS

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	269/280 (96%)	269 (100%)	0	100	100
1	a	268/280 (96%)	267 (100%)	1 (0%)	91	97
2	B	398/407 (98%)	397 (100%)	1 (0%)	92	97
2	b	400/407 (98%)	399 (100%)	1 (0%)	92	97
3	C	352/362 (97%)	350 (99%)	2 (1%)	86	95
3	c	352/362 (97%)	349 (99%)	3 (1%)	78	92
4	D	276/283 (98%)	275 (100%)	1 (0%)	91	97
4	d	274/283 (97%)	273 (100%)	1 (0%)	91	97
5	E	71/73 (97%)	71 (100%)	0	100	100
5	e	72/73 (99%)	72 (100%)	0	100	100
6	F	27/39 (69%)	27 (100%)	0	100	100
6	f	27/39 (69%)	27 (100%)	0	100	100
7	H	53/55 (96%)	52 (98%)	1 (2%)	57	84

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	h	53/55 (96%)	52 (98%)	1 (2%)	57	84
8	I	32/34 (94%)	32 (100%)	0	100	100
8	i	32/34 (94%)	32 (100%)	0	100	100
9	J	24/28 (86%)	24 (100%)	0	100	100
9	j	24/28 (86%)	24 (100%)	0	100	100
10	K	30/37 (81%)	30 (100%)	0	100	100
10	k	30/37 (81%)	30 (100%)	0	100	100
11	L	34/35 (97%)	34 (100%)	0	100	100
11	l	34/35 (97%)	34 (100%)	0	100	100
12	M	28/32 (88%)	28 (100%)	0	100	100
12	m	28/32 (88%)	28 (100%)	0	100	100
13	O	200/228 (88%)	198 (99%)	2 (1%)	76	91
13	o	202/228 (89%)	200 (99%)	2 (1%)	76	91
14	T	26/28 (93%)	26 (100%)	0	100	100
14	t	26/28 (93%)	26 (100%)	0	100	100
15	U	84/112 (75%)	84 (100%)	0	100	100
15	u	84/112 (75%)	83 (99%)	1 (1%)	71	90
16	V	117/138 (85%)	117 (100%)	0	100	100
16	v	117/138 (85%)	116 (99%)	1 (1%)	78	92
17	Y	23/37 (62%)	23 (100%)	0	100	100
17	y	23/37 (62%)	23 (100%)	0	100	100
18	X	30/34 (88%)	30 (100%)	0	100	100
18	x	31/34 (91%)	31 (100%)	0	100	100
19	Z	52/52 (100%)	51 (98%)	1 (2%)	57	84
19	z	52/52 (100%)	51 (98%)	1 (2%)	57	84
20	R	29/33 (88%)	29 (100%)	0	100	100
20	r	29/33 (88%)	28 (97%)	1 (3%)	37	72
All	All	4313/4654 (93%)	4292 (100%)	21 (0%)	88	96

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	h	49	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
15	u	86	GLU
20	r	21	ARG
16	v	106	ASN
13	o	207	ARG

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

Mol	Chain	Res	Type
2	b	216	HIS
2	b	289	GLN
16	v	118	HIS
12	m	5	GLN
13	o	104	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)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
14	FME	t	1	14	8,9,10	0.94	0	7,9,11	0.87	0
8	FME	I	1	8	8,9,10	0.85	0	7,9,11	1.74	2 (28%)
8	FME	i	1	8	8,9,10	0.93	0	7,9,11	0.86	0
12	FME	m	1	12	8,9,10	0.93	0	7,9,11	0.87	0
14	FME	T	1	14	8,9,10	0.93	0	7,9,11	0.94	0
12	FME	M	1	12	8,9,10	0.94	0	7,9,11	0.81	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	FME	t	1	14	-	0/7/9/11	-
8	FME	I	1	8	-	2/7/9/11	-
8	FME	i	1	8	-	2/7/9/11	-
12	FME	m	1	12	-	2/7/9/11	-
14	FME	T	1	14	-	1/7/9/11	-
12	FME	M	1	12	-	1/7/9/11	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	I	1	FME	C-CA-N	3.53	116.10	109.73
8	I	1	FME	CA-N-CN	2.44	126.57	122.82

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	I	1	FME	O-C-CA-CB
8	i	1	FME	CB-CA-N-CN
12	m	1	FME	N-CA-CB-CG
12	m	1	FME	C-CA-CB-CG
14	T	1	FME	CA-CB-CG-SD

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 174 ligands modelled in this entry, 6 are monoatomic and 17 are unknown - leaving 151 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
25	CLA	c	508	-	65,73,73	1.49	5 (7%)	76,113,113	1.29	8 (10%)
35	HEC	V	201	16	32,50,50	2.10	5 (15%)	24,82,82	1.56	4 (16%)
29	LMG	B	621	-	51,51,55	0.73	0	59,59,63	1.39	6 (10%)
27	BCR	h	101	-	41,41,41	1.09	2 (4%)	56,56,56	1.29	8 (14%)
25	CLA	B	603	-	65,73,73	1.49	6 (9%)	76,113,113	1.26	8 (10%)
25	CLA	B	602	-	65,73,73	1.48	5 (7%)	76,113,113	1.25	8 (10%)
33	DGD	C	516	-	63,63,67	0.86	2 (3%)	77,77,81	1.43	9 (11%)
25	CLA	B	601	36	65,73,73	1.47	5 (7%)	76,113,113	1.32	8 (10%)
25	CLA	D	402	-	65,73,73	1.50	6 (9%)	76,113,113	1.27	7 (9%)
26	PHO	a	608	-	51,69,69	1.00	4 (7%)	47,99,99	1.12	4 (8%)
25	CLA	A	609	-	65,73,73	1.48	5 (7%)	76,113,113	1.34	9 (11%)
25	CLA	b	618	-	65,73,73	1.48	5 (7%)	76,113,113	1.35	8 (10%)
29	LMG	B	625	-	51,51,55	0.83	3 (5%)	59,59,63	1.40	8 (13%)
31	LHG	l	101	-	48,48,48	0.62	1 (2%)	51,54,54	1.24	6 (11%)
25	CLA	C	501	-	65,73,73	1.46	5 (7%)	76,113,113	1.32	8 (10%)
29	LMG	C	519	-	51,51,55	0.72	1 (1%)	59,59,63	1.33	6 (10%)
27	BCR	c	516	-	41,41,41	1.09	2 (4%)	56,56,56	1.26	6 (10%)
27	BCR	b	621	-	41,41,41	1.10	2 (4%)	56,56,56	1.18	4 (7%)
23	SQD	f	101	-	42,43,54	1.07	5 (11%)	51,54,65	1.65	11 (21%)
27	BCR	H	102	-	41,41,41	1.07	2 (4%)	56,56,56	1.24	7 (12%)
27	BCR	K	101	-	41,41,41	1.10	2 (4%)	56,56,56	1.25	7 (12%)
33	DGD	H	103	-	63,63,67	0.87	1 (1%)	77,77,81	1.34	7 (9%)
27	BCR	C	514	-	41,41,41	1.12	2 (4%)	56,56,56	1.23	7 (12%)
26	PHO	d	401	-	51,69,69	0.99	3 (5%)	47,99,99	1.13	4 (8%)
29	LMG	c	522	-	51,51,55	0.79	1 (1%)	59,59,63	1.37	6 (10%)
25	CLA	a	607	36	59,67,73	1.55	6 (10%)	68,105,113	1.34	8 (11%)
26	PHO	A	608	-	51,69,69	1.00	4 (7%)	47,99,99	1.10	4 (8%)
25	CLA	c	511	-	65,73,73	1.46	5 (7%)	76,113,113	1.35	8 (10%)
27	BCR	C	515	-	41,41,41	1.12	2 (4%)	56,56,56	1.22	7 (12%)
25	CLA	B	608	-	65,73,73	1.48	5 (7%)	76,113,113	1.29	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
27	BCR	B	619	-	41,41,41	1.11	2 (4%)	56,56,56	1.23	8 (14%)
23	SQD	A	603	-	51,52,54	0.97	5 (9%)	60,63,65	1.59	11 (18%)
31	LHG	A	618	-	48,48,48	0.65	1 (2%)	51,54,54	1.24	7 (13%)
25	CLA	b	610	36	65,73,73	1.47	5 (7%)	76,113,113	1.28	7 (9%)
27	BCR	b	620	-	41,41,41	1.13	2 (4%)	56,56,56	1.21	6 (10%)
31	LHG	a	614	-	34,34,48	0.72	0	37,40,54	1.19	3 (8%)
25	CLA	c	514	-	65,73,73	1.46	5 (7%)	76,113,113	1.39	8 (10%)
25	CLA	c	509	36	65,73,73	1.49	5 (7%)	76,113,113	1.35	7 (9%)
25	CLA	B	610	36	65,73,73	1.48	5 (7%)	76,113,113	1.22	8 (10%)
23	SQD	B	626	-	53,54,54	0.95	4 (7%)	62,65,65	1.65	12 (19%)
25	CLA	b	617	-	65,73,73	1.48	6 (9%)	76,113,113	1.29	7 (9%)
27	BCR	Y	101	-	41,41,41	1.10	2 (4%)	56,56,56	1.15	4 (7%)
25	CLA	C	507	36	65,73,73	1.47	5 (7%)	76,113,113	1.36	7 (9%)
25	CLA	C	506	-	65,73,73	1.50	5 (7%)	76,113,113	1.30	9 (11%)
25	CLA	c	515	-	65,73,73	1.47	5 (7%)	76,113,113	1.30	8 (10%)
29	LMG	C	520	-	51,51,55	0.78	1 (1%)	59,59,63	1.36	7 (11%)
33	DGD	h	102	-	63,63,67	0.87	1 (1%)	77,77,81	1.32	8 (10%)
33	DGD	c	520	-	63,63,67	0.87	2 (3%)	77,77,81	1.40	10 (12%)
25	CLA	b	619	-	65,73,73	1.45	6 (9%)	76,113,113	1.32	7 (9%)
32	BCT	a	605	22	2,3,3	1.24	0	2,3,3	2.55	1 (50%)
25	CLA	c	507	-	65,73,73	1.49	6 (9%)	76,113,113	1.30	7 (9%)
25	CLA	C	502	-	65,73,73	1.47	5 (7%)	76,113,113	1.31	8 (10%)
25	CLA	b	606	-	65,73,73	1.49	6 (9%)	76,113,113	1.25	8 (10%)
29	LMG	A	613	-	51,51,55	0.70	0	59,59,63	1.48	9 (15%)
25	CLA	b	614	-	65,73,73	1.47	5 (7%)	76,113,113	1.33	9 (11%)
25	CLA	B	609	-	65,73,73	1.51	5 (7%)	76,113,113	1.28	8 (10%)
29	LMG	B	620	-	51,51,55	0.73	0	59,59,63	1.34	6 (10%)
23	SQD	D	408	-	46,47,54	1.00	4 (8%)	55,58,65	1.78	11 (20%)
33	DGD	c	519	-	63,63,67	0.89	2 (3%)	77,77,81	1.38	8 (10%)
25	CLA	b	604	36	65,73,73	1.47	5 (7%)	76,113,113	1.33	8 (10%)
25	CLA	c	505	-	65,73,73	1.48	5 (7%)	76,113,113	1.34	8 (10%)
29	LMG	b	623	-	51,51,55	0.72	0	59,59,63	1.35	7 (11%)
25	CLA	B	614	-	65,73,73	1.47	6 (9%)	76,113,113	1.28	7 (9%)
27	BCR	D	404	-	41,41,41	1.11	2 (4%)	56,56,56	1.20	7 (12%)
25	CLA	A	607	36	57,65,73	1.56	6 (10%)	66,103,113	1.38	9 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
27	BCR	T	101	-	41,41,41	1.11	2 (4%)	56,56,56	1.26	6 (10%)
28	PL9	D	407	-	55,55,55	0.99	4 (7%)	68,69,69	1.53	13 (19%)
25	CLA	B	605	-	65,73,73	1.49	6 (9%)	76,113,113	1.28	7 (9%)
27	BCR	y	101	-	41,41,41	1.12	2 (4%)	56,56,56	1.15	5 (8%)
25	CLA	B	607	36	65,73,73	1.47	5 (7%)	76,113,113	1.24	8 (10%)
25	CLA	a	606	-	65,73,73	1.46	6 (9%)	76,113,113	1.30	8 (10%)
23	SQD	b	601	-	53,54,54	0.96	5 (9%)	62,65,65	1.45	9 (14%)
29	LMG	d	409	-	39,39,55	0.56	0	41,41,63	1.29	3 (7%)
25	CLA	b	616	-	65,73,73	1.47	5 (7%)	76,113,113	1.33	8 (10%)
33	DGD	C	518	-	63,63,67	0.87	2 (3%)	77,77,81	1.40	8 (10%)
35	HEC	v	201	16	32,50,50	2.12	4 (12%)	24,82,82	1.55	3 (12%)
25	CLA	C	504	36	65,73,73	1.46	5 (7%)	76,113,113	1.30	7 (9%)
25	CLA	a	612	36	65,73,73	1.47	5 (7%)	76,113,113	1.30	7 (9%)
25	CLA	b	609	-	65,73,73	1.47	5 (7%)	76,113,113	1.31	7 (9%)
27	BCR	b	622	-	41,41,41	1.09	2 (4%)	56,56,56	1.22	7 (12%)
31	LHG	A	617	-	48,48,48	0.61	0	51,54,54	1.24	6 (11%)
25	CLA	C	508	-	65,73,73	1.48	5 (7%)	76,113,113	1.31	9 (11%)
31	LHG	D	406	-	48,48,48	0.62	1 (2%)	51,54,54	1.24	6 (11%)
25	CLA	c	503	-	65,73,73	1.46	5 (7%)	76,113,113	1.32	9 (11%)
31	LHG	a	615	-	41,41,48	0.67	1 (2%)	44,47,54	1.30	6 (13%)
23	SQD	A	619	-	39,39,54	0.88	2 (5%)	41,41,65	1.17	2 (4%)
27	BCR	k	101	-	41,41,41	1.08	2 (4%)	56,56,56	1.22	6 (10%)
32	BCT	A	620	22	2,3,3	1.26	0	2,3,3	2.67	2 (100%)
25	CLA	C	511	3	65,73,73	1.48	5 (7%)	76,113,113	1.35	8 (10%)
26	PHO	D	401	-	51,69,69	0.98	3 (5%)	47,99,99	1.13	4 (8%)
25	CLA	c	513	3	65,73,73	1.47	5 (7%)	76,113,113	1.37	8 (10%)
29	LMG	b	624	-	51,51,55	0.75	0	59,59,63	1.30	6 (10%)
29	LMG	b	625	-	8,8,55	0.14	0	7,7,63	0.92	0
25	CLA	B	616	-	65,73,73	1.46	6 (9%)	76,113,113	1.35	8 (10%)
25	CLA	B	615	-	65,73,73	1.49	5 (7%)	76,113,113	1.33	8 (10%)
27	BCR	B	627	-	41,41,41	1.11	2 (4%)	56,56,56	1.27	7 (12%)
29	LMG	d	406	-	42,42,55	0.79	0	50,50,63	1.31	6 (12%)
25	CLA	C	509	-	65,73,73	1.45	5 (7%)	76,113,113	1.34	7 (9%)
28	PL9	d	408	-	55,55,55	0.99	4 (7%)	68,69,69	1.51	13 (19%)
25	CLA	b	611	-	65,73,73	1.48	5 (7%)	76,113,113	1.28	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
25	CLA	c	510	-	58,66,73	1.56	5 (8%)	67,104,113	1.38	9 (13%)
31	LHG	a	613	-	48,48,48	0.62	1 (2%)	51,54,54	1.28	6 (11%)
21	OEX	A	601	3,36,1	0,15,15	-	-	-		
23	SQD	D	409	-	42,43,54	1.07	5 (11%)	51,54,65	1.62	11 (21%)
31	LHG	A	616	-	48,48,48	0.62	2 (4%)	51,54,54	1.27	6 (11%)
25	CLA	b	612	-	65,73,73	1.49	5 (7%)	76,113,113	1.30	8 (10%)
25	CLA	c	504	-	65,73,73	1.47	5 (7%)	76,113,113	1.31	8 (10%)
25	CLA	A	615	36	65,73,73	1.46	5 (7%)	76,113,113	1.29	7 (9%)
25	CLA	b	608	-	65,73,73	1.49	6 (9%)	76,113,113	1.29	8 (10%)
25	CLA	C	510	-	65,73,73	1.47	6 (9%)	76,113,113	1.28	8 (10%)
25	CLA	a	609	-	65,73,73	1.49	5 (7%)	76,113,113	1.27	9 (11%)
25	CLA	C	505	-	65,73,73	1.49	6 (9%)	76,113,113	1.30	8 (10%)
25	CLA	c	512	-	65,73,73	1.46	5 (7%)	76,113,113	1.32	8 (10%)
25	CLA	B	611	-	65,73,73	1.48	5 (7%)	76,113,113	1.33	9 (11%)
27	BCR	B	617	-	41,41,41	1.14	2 (4%)	56,56,56	1.25	7 (12%)
34	HEM	e	101	6,5	41,50,50	1.47	4 (9%)	45,82,82	1.41	7 (15%)
25	CLA	B	612	-	65,73,73	1.45	6 (9%)	76,113,113	1.34	9 (11%)
21	OEX	a	601	3,36,1	0,15,15	-	-	-		
28	PL9	a	611	-	55,55,55	0.94	3 (5%)	68,69,69	1.52	12 (17%)
27	BCR	d	405	-	41,41,41	1.09	2 (4%)	56,56,56	1.20	5 (8%)
33	DGD	C	517	-	63,63,67	0.90	2 (3%)	77,77,81	1.36	8 (10%)
23	SQD	I	101	-	39,39,54	0.86	2 (5%)	41,41,65	1.19	2 (4%)
25	CLA	b	613	36	65,73,73	1.47	5 (7%)	76,113,113	1.24	8 (10%)
25	CLA	b	607	-	65,73,73	1.47	6 (9%)	76,113,113	1.39	9 (11%)
25	CLA	b	615	-	65,73,73	1.47	7 (10%)	76,113,113	1.33	8 (10%)
25	CLA	d	404	-	65,73,73	1.46	5 (7%)	76,113,113	1.33	8 (10%)
25	CLA	B	604	-	65,73,73	1.47	5 (7%)	76,113,113	1.38	8 (10%)
25	CLA	c	506	36	65,73,73	1.46	5 (7%)	76,113,113	1.32	7 (9%)
29	LMG	c	521	-	51,51,55	0.71	0	59,59,63	1.33	6 (10%)
25	CLA	B	606	-	65,73,73	1.48	5 (7%)	76,113,113	1.33	9 (11%)
27	BCR	A	610	-	41,41,41	1.10	2 (4%)	56,56,56	1.18	6 (10%)
25	CLA	D	403	-	65,73,73	1.48	5 (7%)	76,113,113	1.31	8 (10%)
25	CLA	b	605	-	65,73,73	1.49	5 (7%)	76,113,113	1.26	8 (10%)
25	CLA	C	503	-	65,73,73	1.47	6 (9%)	76,113,113	1.34	8 (10%)
29	LMG	A	612	-	51,51,55	0.72	0	59,59,63	1.31	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
29	LMG	c	502	-	51,51,55	0.77	1 (1%)	59,59,63	1.33	6 (10%)
33	DGD	c	518	-	63,63,67	0.86	2 (3%)	77,77,81	1.42	8 (10%)
25	CLA	C	512	-	65,73,73	1.50	6 (9%)	76,113,113	1.35	8 (10%)
25	CLA	d	403	-	65,73,73	1.49	5 (7%)	76,113,113	1.28	7 (9%)
25	CLA	C	513	-	65,73,73	1.46	5 (7%)	76,113,113	1.28	8 (10%)
27	BCR	c	517	-	41,41,41	1.11	2 (4%)	56,56,56	1.19	6 (10%)
28	PL9	A	611	-	55,55,55	1.02	3 (5%)	68,69,69	1.53	13 (19%)
29	LMG	D	405	-	51,51,55	0.73	0	59,59,63	1.32	6 (10%)
27	BCR	a	610	-	41,41,41	1.10	2 (4%)	56,56,56	1.18	5 (8%)
31	LHG	L	101	-	48,48,48	0.63	1 (2%)	51,54,54	1.24	6 (11%)
25	CLA	A	606	-	65,73,73	1.46	5 (7%)	76,113,113	1.30	8 (10%)
23	SQD	c	501	-	53,54,54	0.95	5 (9%)	62,65,65	1.51	9 (14%)
34	HEM	E	101	6,5	41,50,50	1.47	5 (12%)	45,82,82	1.36	7 (15%)
27	BCR	B	618	-	41,41,41	1.11	2 (4%)	56,56,56	1.20	5 (8%)
25	CLA	B	613	-	65,73,73	1.46	5 (7%)	76,113,113	1.35	8 (10%)
31	LHG	d	407	-	48,48,48	0.62	1 (2%)	51,54,54	1.26	6 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	c	508	-	1/1/15/20	19/37/115/115	-
35	HEC	V	201	16	-	1/10/54/54	-
29	LMG	B	621	-	-	18/46/66/70	0/1/1/1
27	BCR	h	101	-	-	5/29/63/63	0/2/2/2
25	CLA	B	603	-	1/1/15/20	8/37/115/115	-
25	CLA	B	602	-	1/1/15/20	12/37/115/115	-
33	DGD	C	516	-	-	12/51/91/95	0/2/2/2
25	CLA	B	601	36	1/1/15/20	14/37/115/115	-
25	CLA	D	402	-	-	8/37/115/115	-
26	PHO	a	608	-	-	8/37/103/103	0/5/6/6
25	CLA	A	609	-	1/1/15/20	7/37/115/115	-
25	CLA	b	618	-	1/1/15/20	10/37/115/115	-
29	LMG	B	625	-	-	21/46/66/70	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LHG	l	101	-	-	20/53/53/53	-
25	CLA	C	501	-	1/1/15/20	5/37/115/115	-
29	LMG	C	519	-	-	21/46/66/70	0/1/1/1
27	BCR	c	516	-	-	7/29/63/63	0/2/2/2
27	BCR	b	621	-	-	6/29/63/63	0/2/2/2
23	SQD	f	101	-	-	19/38/58/69	0/1/1/1
27	BCR	H	102	-	-	5/29/63/63	0/2/2/2
27	BCR	K	101	-	-	6/29/63/63	0/2/2/2
33	DGD	H	103	-	-	13/51/91/95	0/2/2/2
27	BCR	C	514	-	-	4/29/63/63	0/2/2/2
26	PHO	d	401	-	-	6/37/103/103	0/5/6/6
29	LMG	c	522	-	-	15/46/66/70	0/1/1/1
25	CLA	a	607	36	1/1/13/20	8/30/108/115	-
26	PHO	A	608	-	-	9/37/103/103	0/5/6/6
25	CLA	c	511	-	1/1/15/20	8/37/115/115	-
27	BCR	C	515	-	-	6/29/63/63	0/2/2/2
25	CLA	B	608	-	1/1/15/20	2/37/115/115	-
27	BCR	B	619	-	-	4/29/63/63	0/2/2/2
23	SQD	A	603	-	-	15/47/67/69	0/1/1/1
31	LHG	A	618	-	-	24/53/53/53	-
25	CLA	b	610	36	1/1/15/20	10/37/115/115	-
27	BCR	b	620	-	-	5/29/63/63	0/2/2/2
31	LHG	a	614	-	-	16/39/39/53	-
25	CLA	c	514	-	1/1/15/20	10/37/115/115	-
25	CLA	c	509	36	1/1/15/20	10/37/115/115	-
25	CLA	B	610	36	1/1/15/20	8/37/115/115	-
25	CLA	b	617	-	1/1/15/20	8/37/115/115	-
23	SQD	B	626	-	-	26/49/69/69	0/1/1/1
27	BCR	Y	101	-	-	10/29/63/63	0/2/2/2
25	CLA	C	507	36	1/1/15/20	5/37/115/115	-
25	CLA	C	506	-	-	17/37/115/115	-
25	CLA	c	515	-	1/1/15/20	4/37/115/115	-
29	LMG	C	520	-	-	16/46/66/70	0/1/1/1
33	DGD	h	102	-	-	10/51/91/95	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	DGD	c	520	-	-	12/51/91/95	0/2/2/2
25	CLA	b	619	-	1/1/15/20	15/37/115/115	-
25	CLA	c	507	-	-	13/37/115/115	-
25	CLA	C	502	-	-	6/37/115/115	-
25	CLA	b	606	-	1/1/15/20	7/37/115/115	-
29	LMG	A	613	-	-	15/46/66/70	0/1/1/1
25	CLA	b	614	-	1/1/15/20	5/37/115/115	-
25	CLA	B	609	-	-	12/37/115/115	-
29	LMG	B	620	-	-	16/46/66/70	0/1/1/1
23	SQD	D	408	-	-	20/42/62/69	0/1/1/1
33	DGD	c	519	-	-	19/51/91/95	0/2/2/2
25	CLA	b	604	36	1/1/15/20	18/37/115/115	-
25	CLA	c	505	-	1/1/15/20	5/37/115/115	-
29	LMG	b	623	-	-	11/46/66/70	0/1/1/1
25	CLA	B	614	-	1/1/15/20	19/37/115/115	-
27	BCR	D	404	-	-	6/29/63/63	0/2/2/2
25	CLA	A	607	36	1/1/13/20	9/28/106/115	-
27	BCR	T	101	-	-	11/29/63/63	0/2/2/2
28	PL9	D	407	-	-	9/53/73/73	0/1/1/1
27	BCR	y	101	-	-	6/29/63/63	0/2/2/2
25	CLA	B	607	36	1/1/15/20	11/37/115/115	-
25	CLA	a	606	-	1/1/15/20	3/37/115/115	-
23	SQD	b	601	-	-	18/49/69/69	0/1/1/1
29	LMG	d	409	-	-	22/41/41/70	-
25	CLA	b	616	-	1/1/15/20	9/37/115/115	-
33	DGD	C	518	-	-	15/51/91/95	0/2/2/2
35	HEC	v	201	16	-	2/10/54/54	-
25	CLA	C	504	36	1/1/15/20	7/37/115/115	-
25	CLA	a	612	36	1/1/15/20	2/37/115/115	-
25	CLA	b	609	-	1/1/15/20	8/37/115/115	-
27	BCR	b	622	-	-	6/29/63/63	0/2/2/2
31	LHG	A	617	-	-	16/53/53/53	-
25	CLA	C	508	-	1/1/15/20	6/37/115/115	-
31	LHG	D	406	-	-	20/53/53/53	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	c	503	-	1/1/15/20	6/37/115/115	-
31	LHG	a	615	-	-	21/46/46/53	-
23	SQD	A	619	-	-	28/41/41/69	-
27	BCR	k	101	-	-	5/29/63/63	0/2/2/2
25	CLA	C	511	3	-	4/37/115/115	-
26	PHO	D	401	-	-	7/37/103/103	0/5/6/6
25	CLA	c	513	3	1/1/15/20	4/37/115/115	-
29	LMG	b	624	-	-	23/46/66/70	0/1/1/1
29	LMG	b	625	-	-	1/6/6/70	-
25	CLA	B	616	-	1/1/15/20	15/37/115/115	-
25	CLA	B	615	-	1/1/15/20	4/37/115/115	-
27	BCR	B	627	-	-	10/29/63/63	0/2/2/2
29	LMG	d	406	-	-	4/37/57/70	0/1/1/1
25	CLA	C	509	-	1/1/15/20	11/37/115/115	-
28	PL9	d	408	-	-	10/53/73/73	0/1/1/1
25	CLA	b	611	-	1/1/15/20	3/37/115/115	-
25	CLA	c	510	-	1/1/13/20	6/29/107/115	-
31	LHG	a	613	-	-	19/53/53/53	-
23	SQD	D	409	-	-	17/38/58/69	0/1/1/1
31	LHG	A	616	-	-	17/53/53/53	-
25	CLA	b	612	-	-	10/37/115/115	-
25	CLA	c	504	-	-	5/37/115/115	-
25	CLA	A	615	36	1/1/15/20	3/37/115/115	-
25	CLA	b	608	-	-	7/37/115/115	-
25	CLA	C	510	-	1/1/15/20	7/37/115/115	-
25	CLA	a	609	-	1/1/15/20	9/37/115/115	-
25	CLA	c	512	-	1/1/15/20	9/37/115/115	-
25	CLA	C	505	-	-	14/37/115/115	-
25	CLA	B	611	-	1/1/15/20	4/37/115/115	-
27	BCR	B	617	-	-	5/29/63/63	0/2/2/2
34	HEM	e	101	6,5	-	3/12/54/54	-
25	CLA	B	612	-	1/1/15/20	8/37/115/115	-
28	PL9	a	611	-	-	15/53/73/73	0/1/1/1
27	BCR	d	405	-	-	6/29/63/63	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	DGD	C	517	-	-	17/51/91/95	0/2/2/2
23	SQD	I	101	-	-	22/41/41/69	-
25	CLA	b	613	36	1/1/15/20	8/37/115/115	-
25	CLA	b	607	-	1/1/15/20	8/37/115/115	-
25	CLA	b	615	-	1/1/15/20	12/37/115/115	-
25	CLA	d	404	-	1/1/15/20	6/37/115/115	-
25	CLA	B	604	-	1/1/15/20	8/37/115/115	-
25	CLA	c	506	36	1/1/15/20	7/37/115/115	-
29	LMG	c	521	-	-	24/46/66/70	0/1/1/1
25	CLA	B	606	-	1/1/15/20	7/37/115/115	-
25	CLA	B	613	-	1/1/15/20	3/37/115/115	-
27	BCR	A	610	-	-	5/29/63/63	0/2/2/2
25	CLA	D	403	-	1/1/15/20	5/37/115/115	-
25	CLA	b	605	-	1/1/15/20	8/37/115/115	-
25	CLA	C	503	-	1/1/15/20	1/37/115/115	-
29	LMG	A	612	-	-	17/46/66/70	0/1/1/1
29	LMG	c	502	-	-	27/46/66/70	0/1/1/1
33	DGD	c	518	-	-	15/51/91/95	0/2/2/2
25	CLA	C	512	-	1/1/15/20	14/37/115/115	-
25	CLA	d	403	-	-	8/37/115/115	-
25	CLA	C	513	-	1/1/15/20	5/37/115/115	-
27	BCR	c	517	-	-	6/29/63/63	0/2/2/2
28	PL9	A	611	-	-	10/53/73/73	0/1/1/1
29	LMG	D	405	-	-	14/46/66/70	0/1/1/1
27	BCR	a	610	-	-	5/29/63/63	0/2/2/2
31	LHG	L	101	-	-	19/53/53/53	-
25	CLA	A	606	-	1/1/15/20	3/37/115/115	-
23	SQD	c	501	-	-	19/49/69/69	0/1/1/1
34	HEM	E	101	6,5	-	5/12/54/54	-
27	BCR	B	618	-	-	4/29/63/63	0/2/2/2
25	CLA	B	605	-	-	9/37/115/115	-
31	LHG	d	407	-	-	15/53/53/53	-

The worst 5 of 528 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	609	CLA	C4B-NB	7.81	1.42	1.35
25	C	512	CLA	C4B-NB	7.70	1.42	1.35
25	D	402	CLA	C4B-NB	7.70	1.42	1.35
25	C	506	CLA	C4B-NB	7.67	1.42	1.35
25	d	403	CLA	C4B-NB	7.66	1.42	1.35

The worst 5 of 1077 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	C	507	CLA	C4A-NA-C1A	6.39	109.58	106.71
25	C	503	CLA	C4A-NA-C1A	6.28	109.53	106.71
25	B	604	CLA	C4A-NA-C1A	6.28	109.53	106.71
25	b	607	CLA	C4A-NA-C1A	6.26	109.52	106.71
25	c	513	CLA	C4A-NA-C1A	6.25	109.51	106.71

5 of 58 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
25	A	606	CLA	ND
25	A	607	CLA	ND
25	A	609	CLA	ND
25	A	615	CLA	ND
25	B	601	CLA	ND

5 of 1536 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	A	603	SQD	C5-C6-S-O7
23	A	603	SQD	C5-C6-S-O8
23	A	603	SQD	C5-C6-S-O9
23	A	619	SQD	O6-C44-C45-C46
23	B	626	SQD	C2-C1-O6-C44

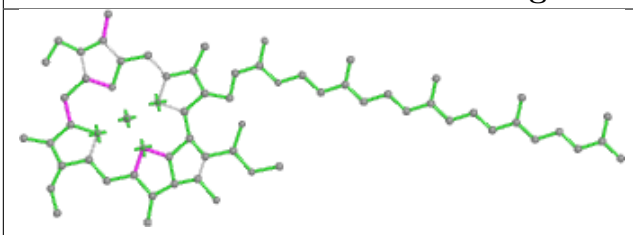
There are no ring outliers.

No monomer is involved in short contacts.

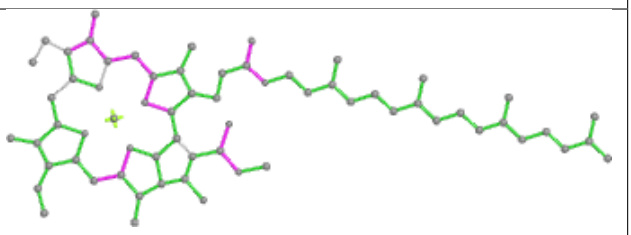
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

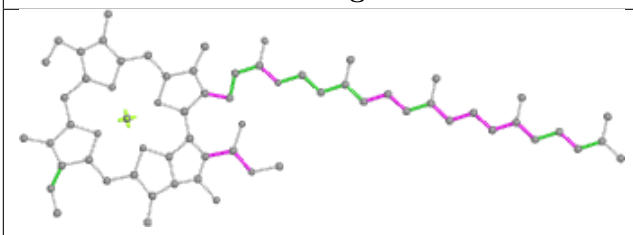
Ligand CLA c 508



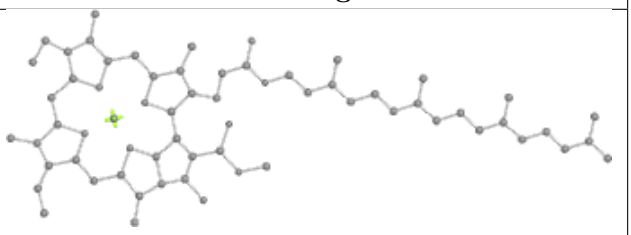
Bond lengths



Bond angles

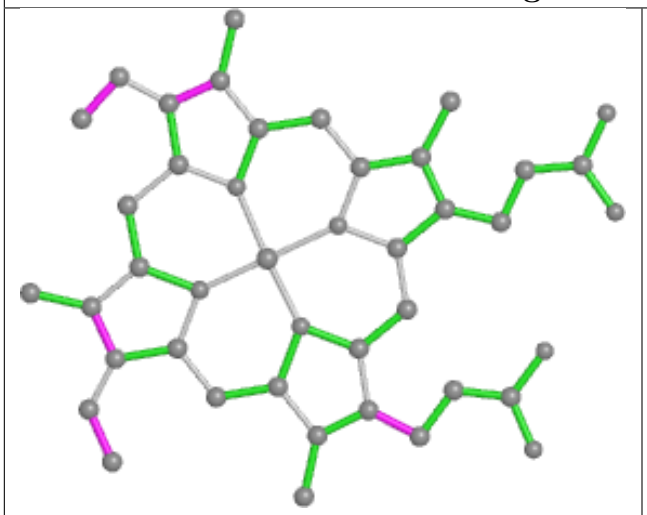


Torsions

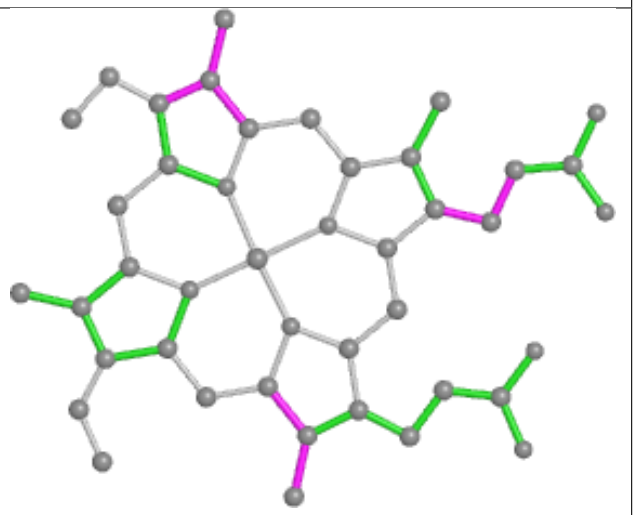


Rings

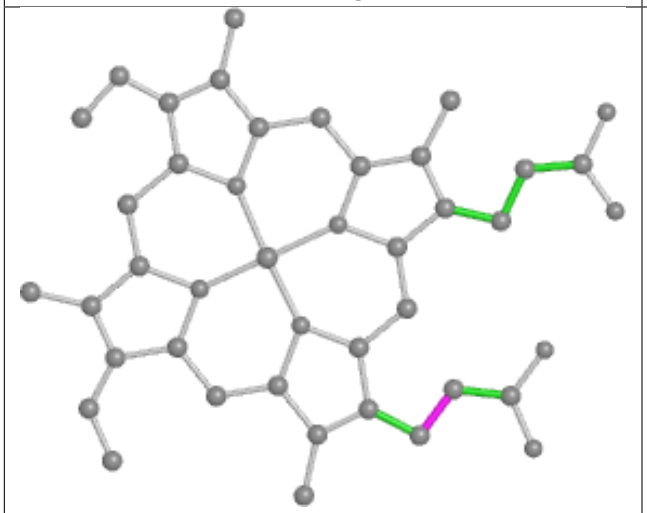
Ligand HEC V 201



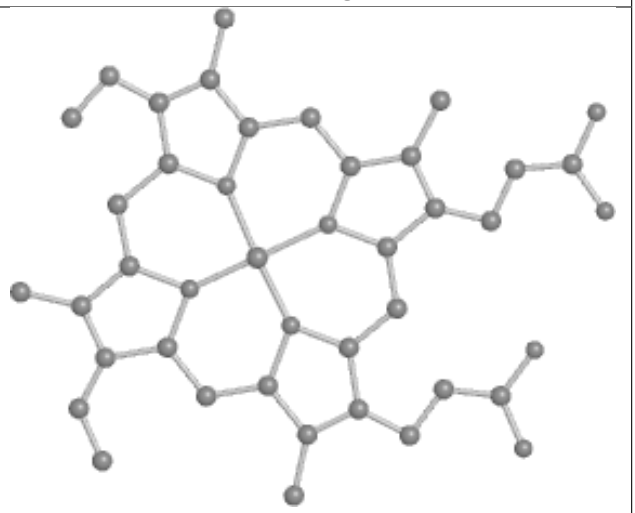
Bond lengths



Bond angles

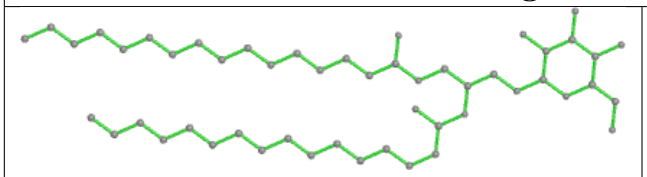


Torsions

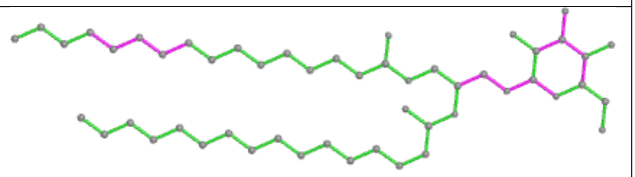


Rings

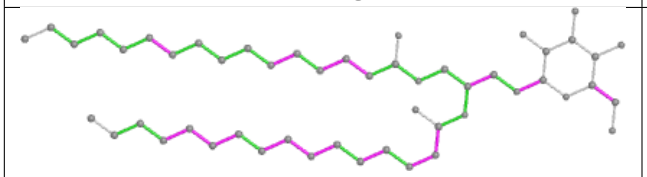
Ligand LMG B 621



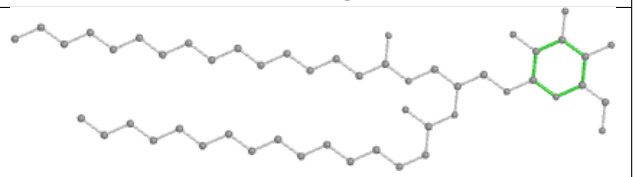
Bond lengths



Bond angles

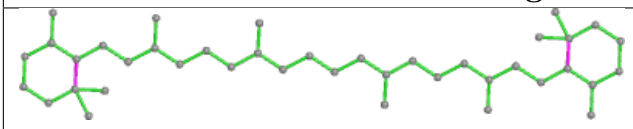


Torsions

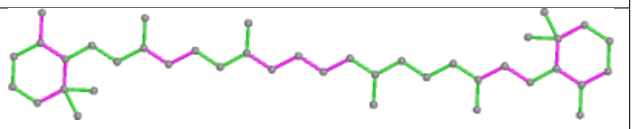


Rings

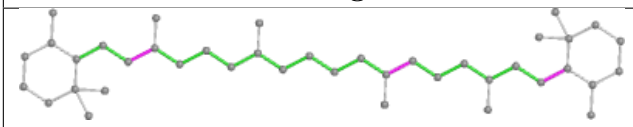
Ligand BCR h 101



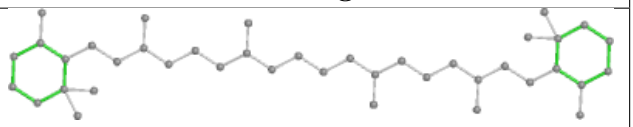
Bond lengths



Bond angles

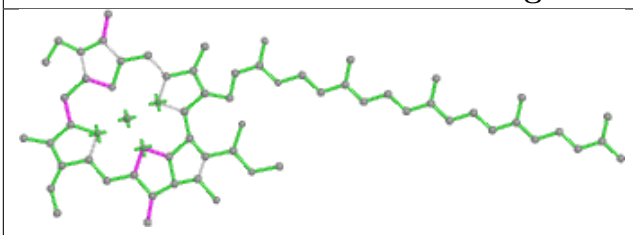


Torsions

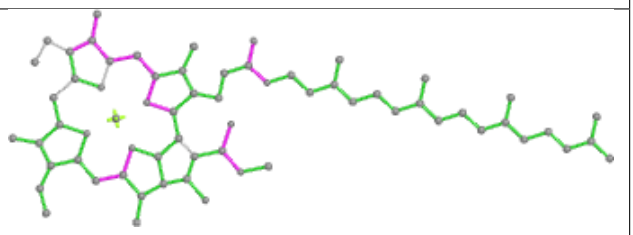


Rings

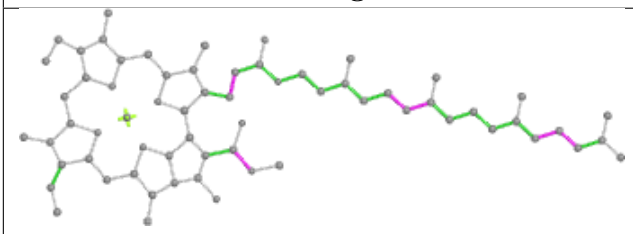
Ligand CLA B 603



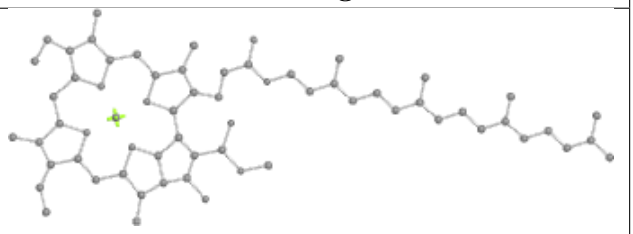
Bond lengths



Bond angles

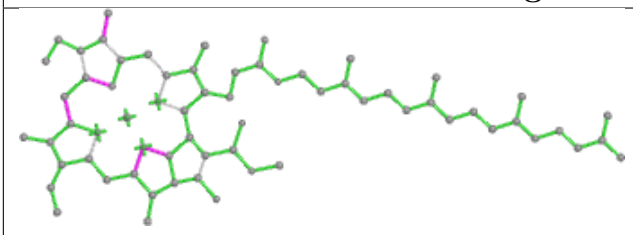


Torsions

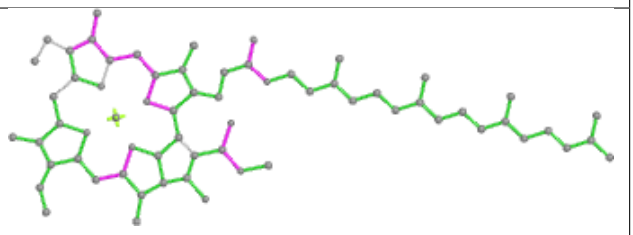


Rings

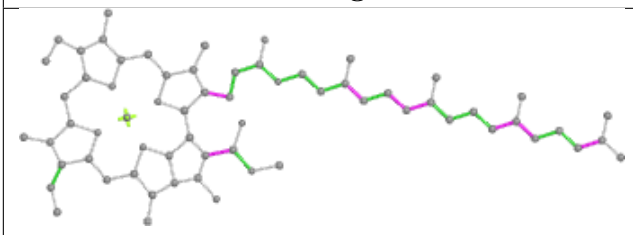
Ligand CLA B 602



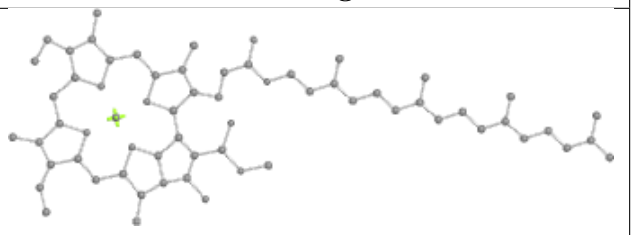
Bond lengths



Bond angles

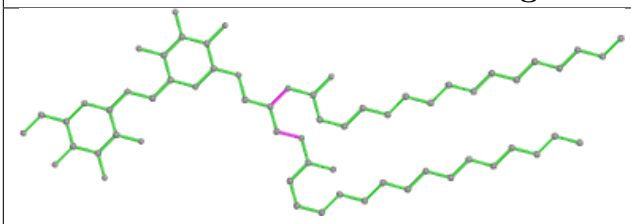


Torsions

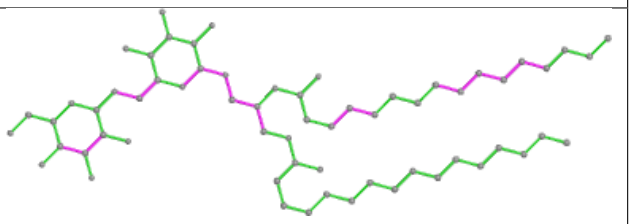


Rings

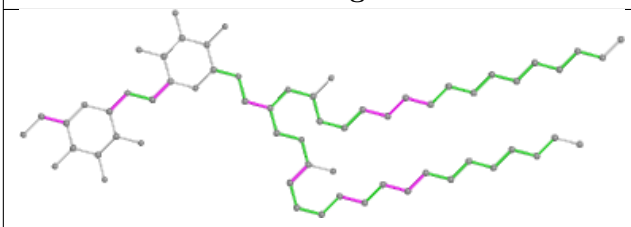
Ligand DGD C 516



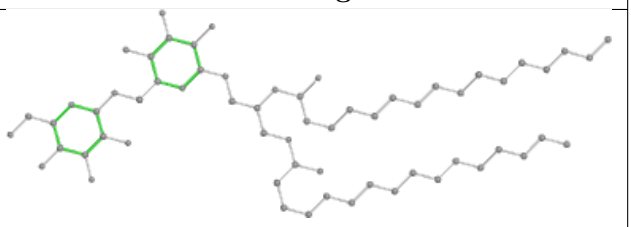
Bond lengths



Bond angles

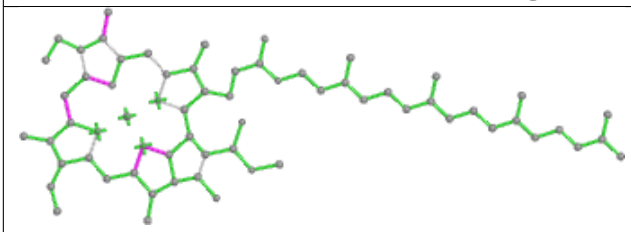


Torsions

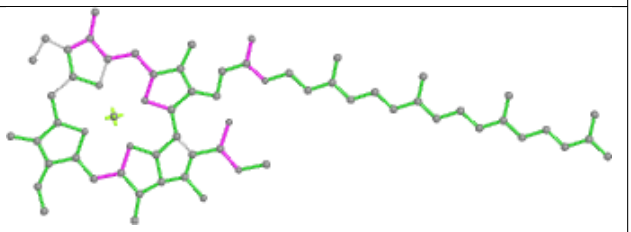


Rings

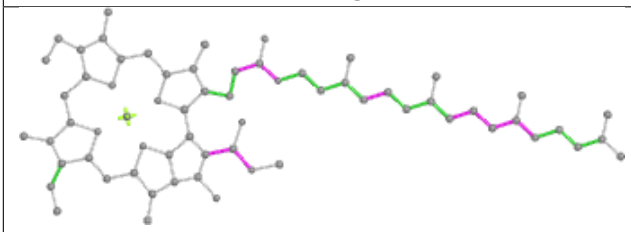
Ligand CLA B 601



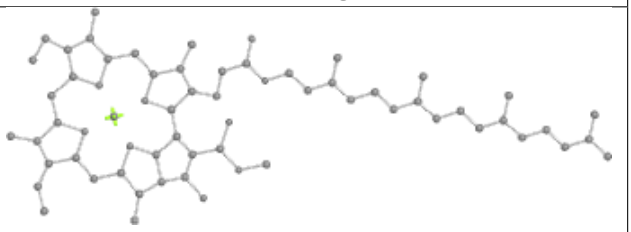
Bond lengths



Bond angles

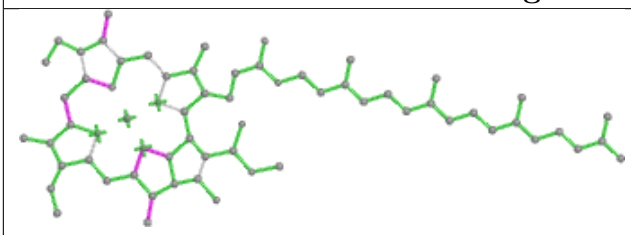


Torsions

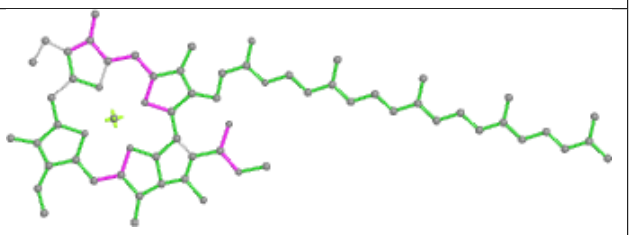


Rings

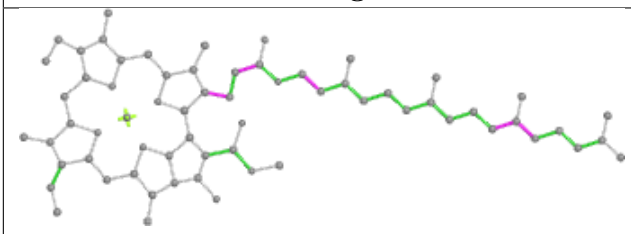
Ligand CLA D 402



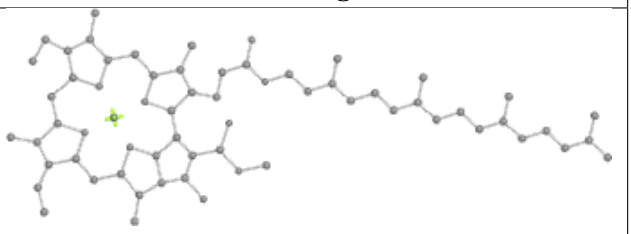
Bond lengths



Bond angles

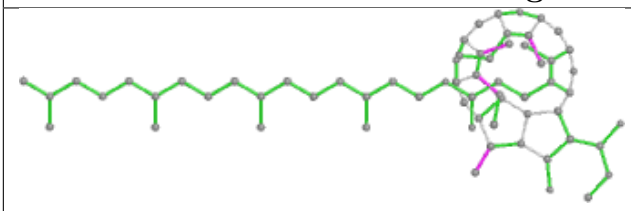


Torsions

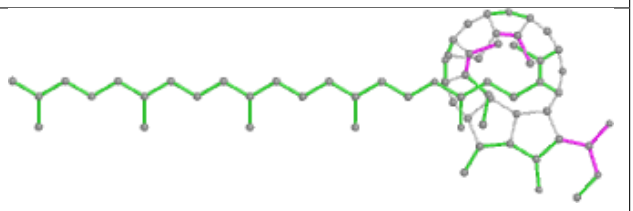


Rings

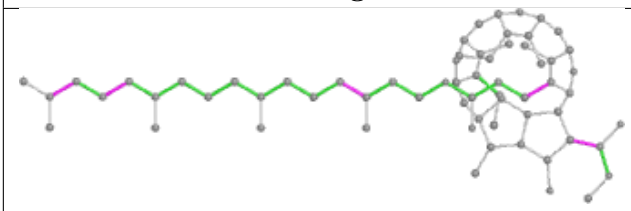
Ligand PHO a 608



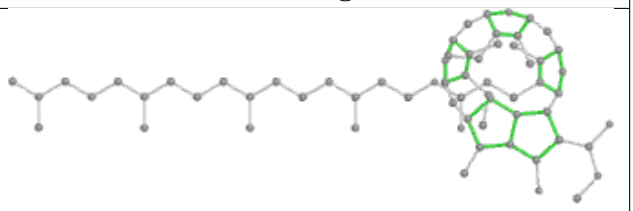
Bond lengths



Bond angles

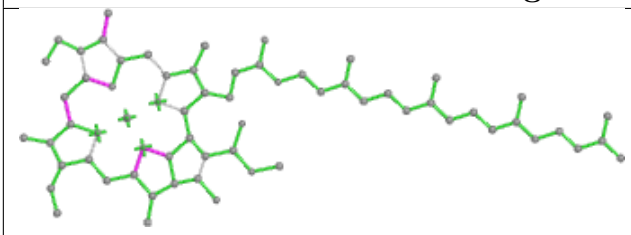


Torsions

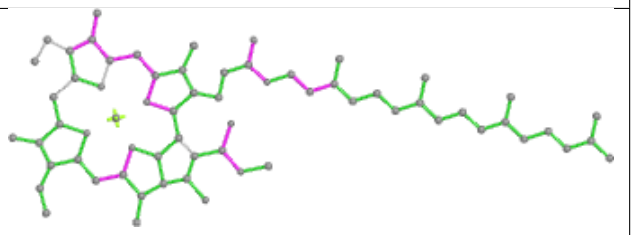


Rings

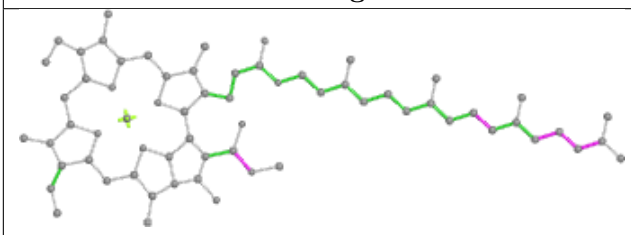
Ligand CLA A 609



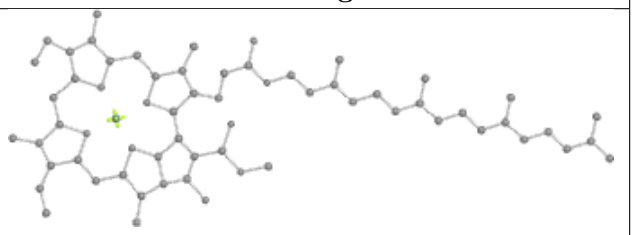
Bond lengths



Bond angles

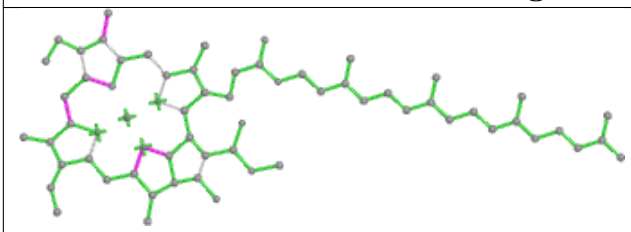


Torsions

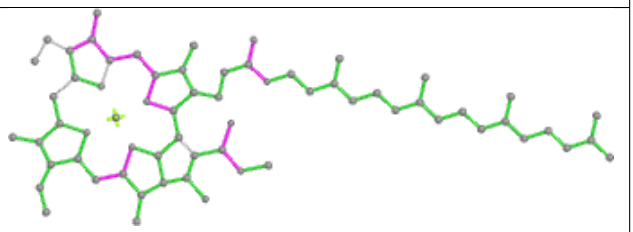


Rings

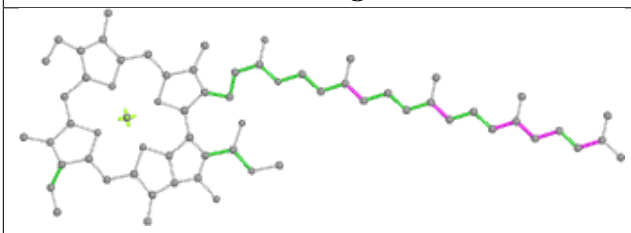
Ligand CLA b 618



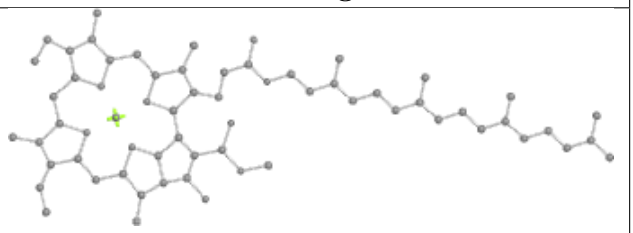
Bond lengths



Bond angles

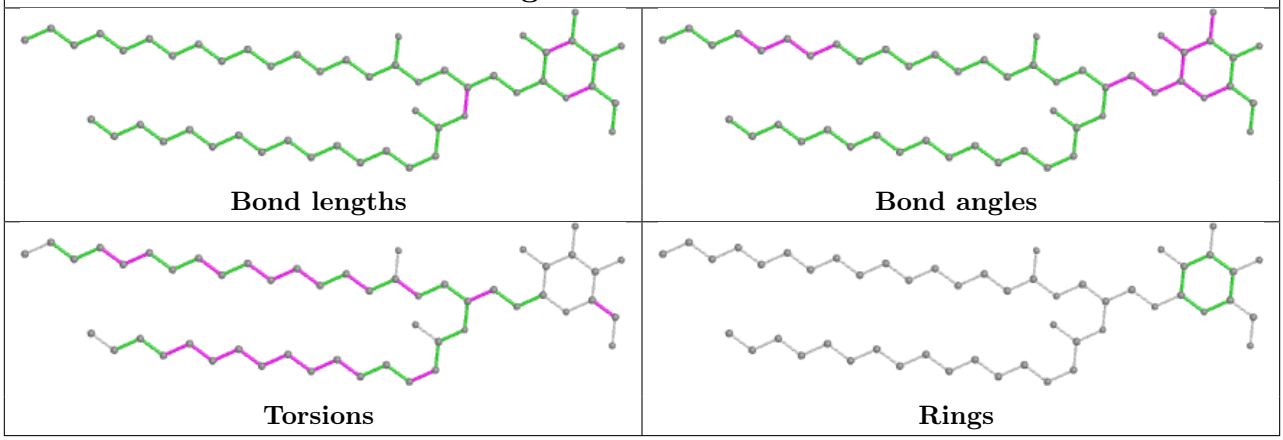


Torsions

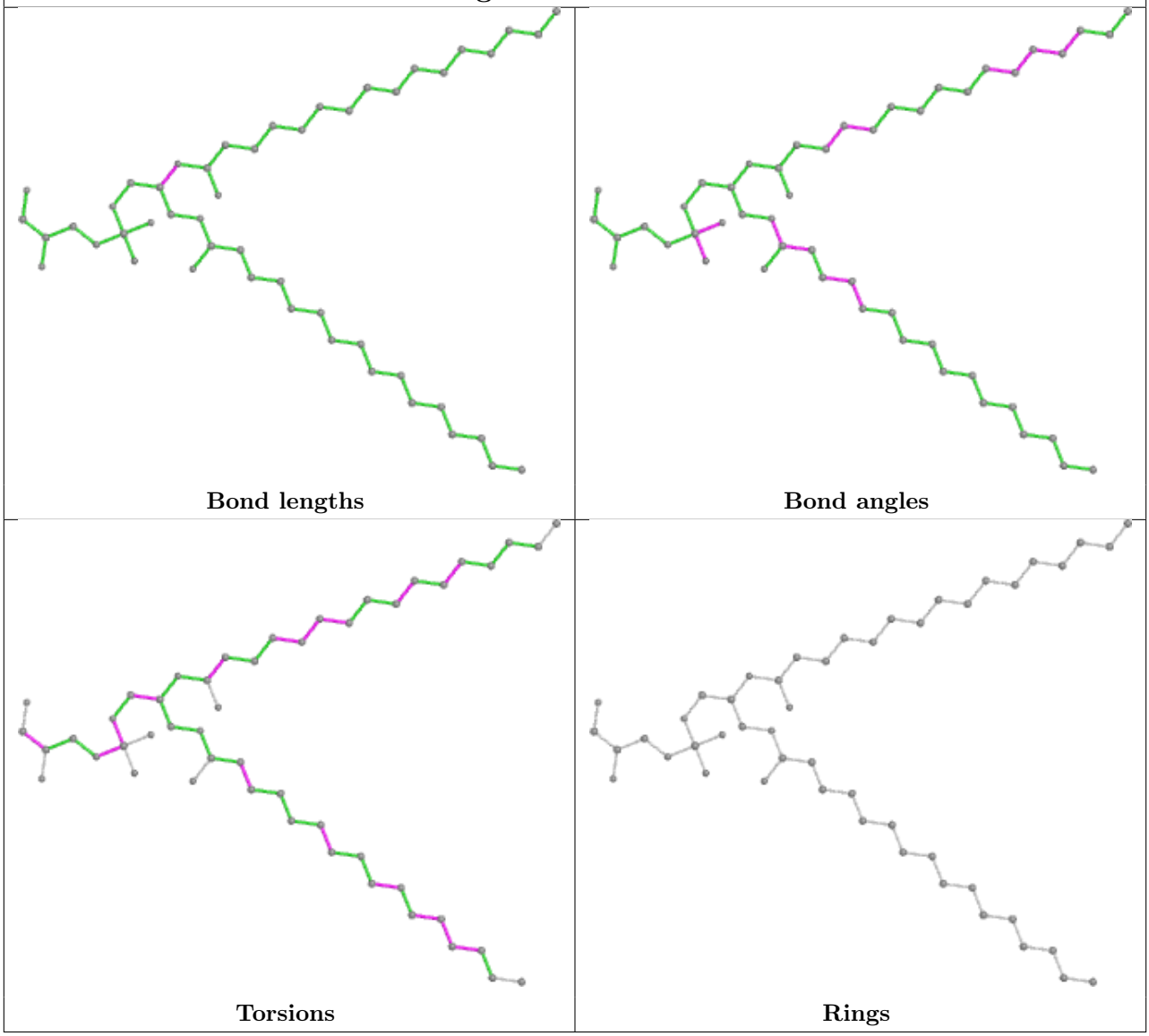


Rings

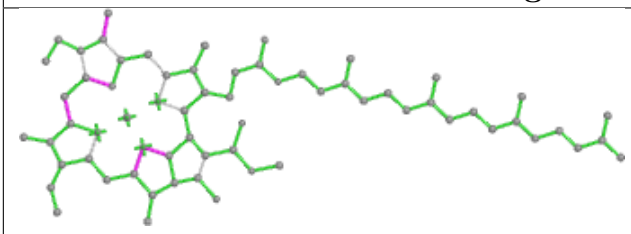
Ligand LMG B 625



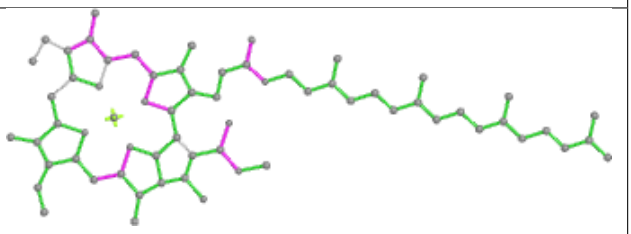
Ligand LHG l 101



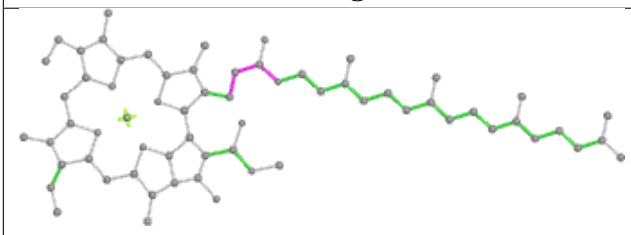
Ligand CLA C 501



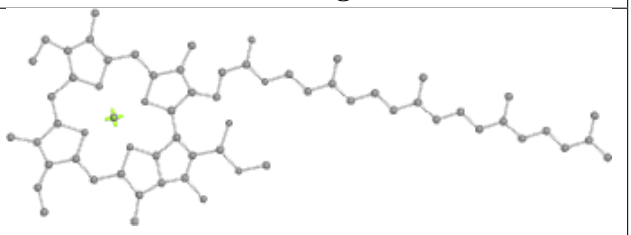
Bond lengths



Bond angles

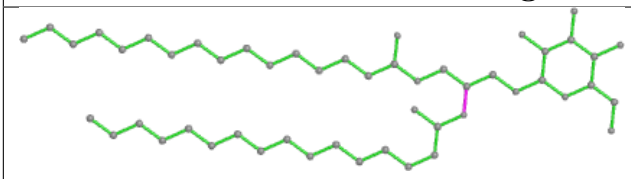


Torsions

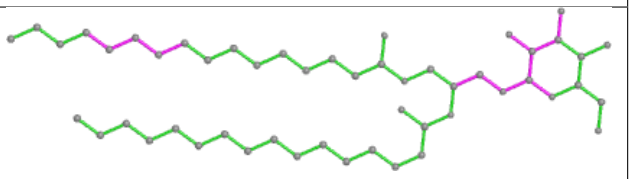


Rings

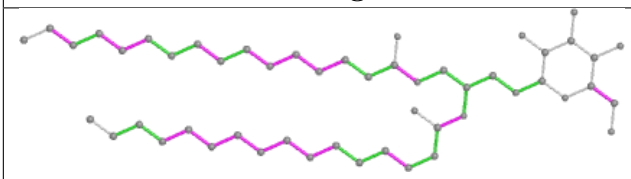
Ligand LMG C 519



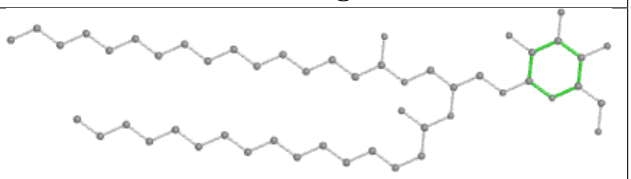
Bond lengths



Bond angles

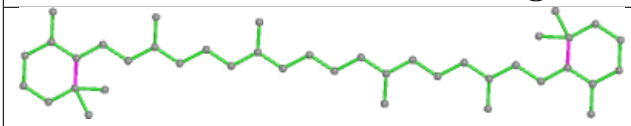


Torsions

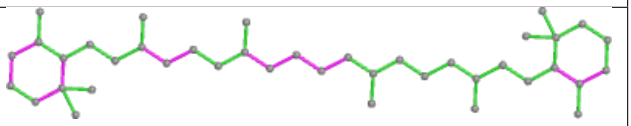


Rings

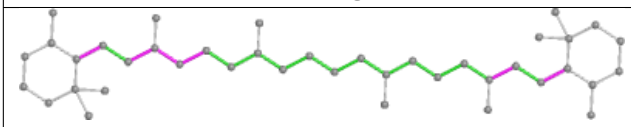
Ligand BCR c 516



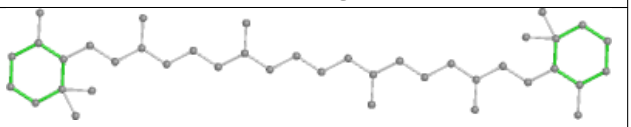
Bond lengths



Bond angles

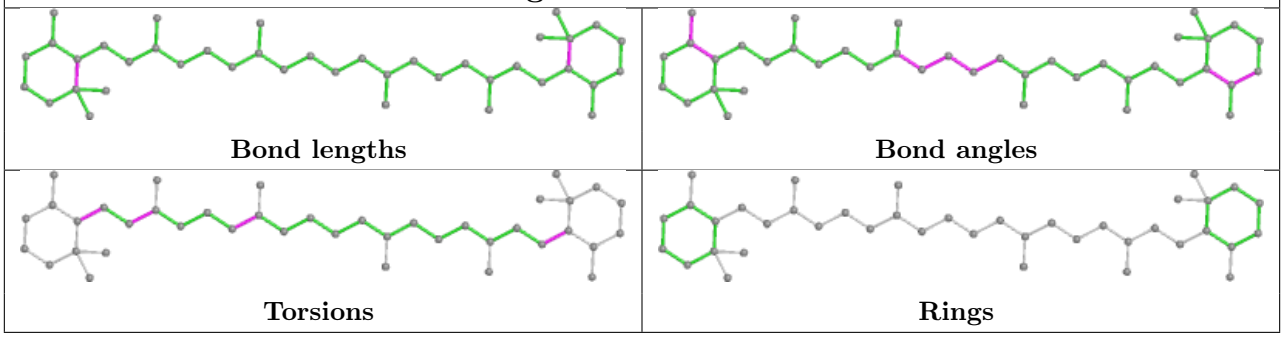


Torsions

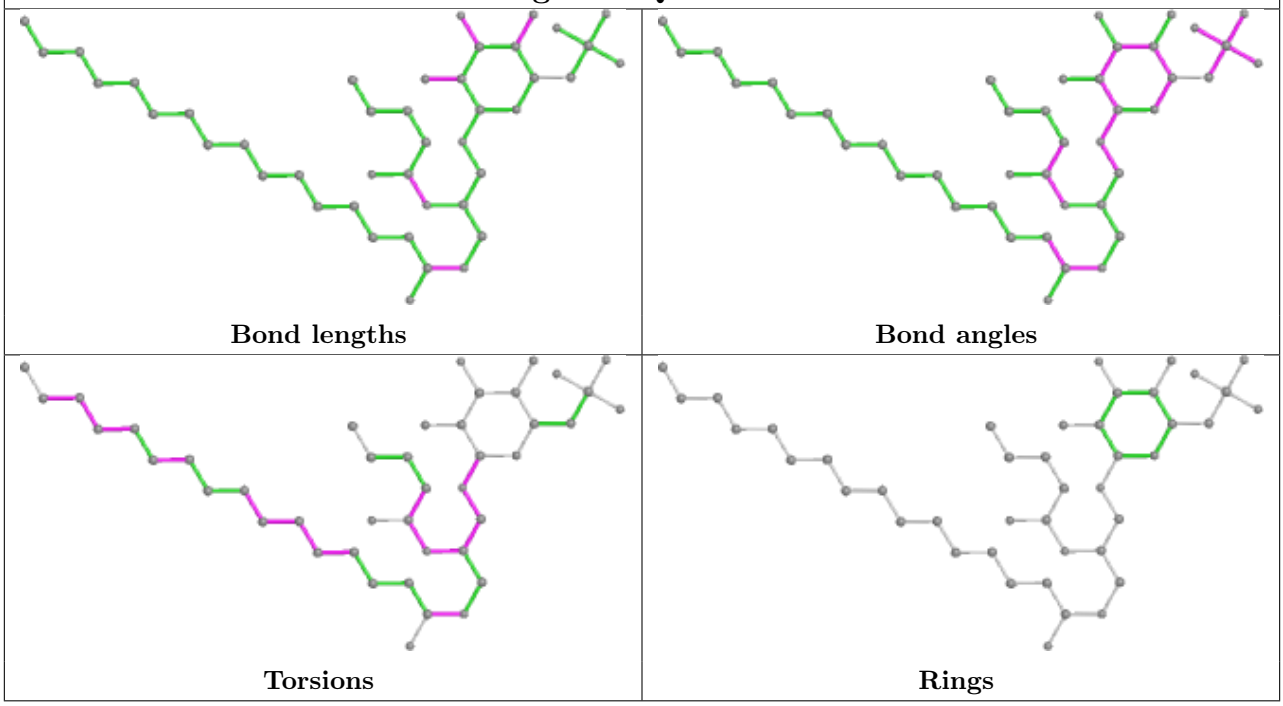


Rings

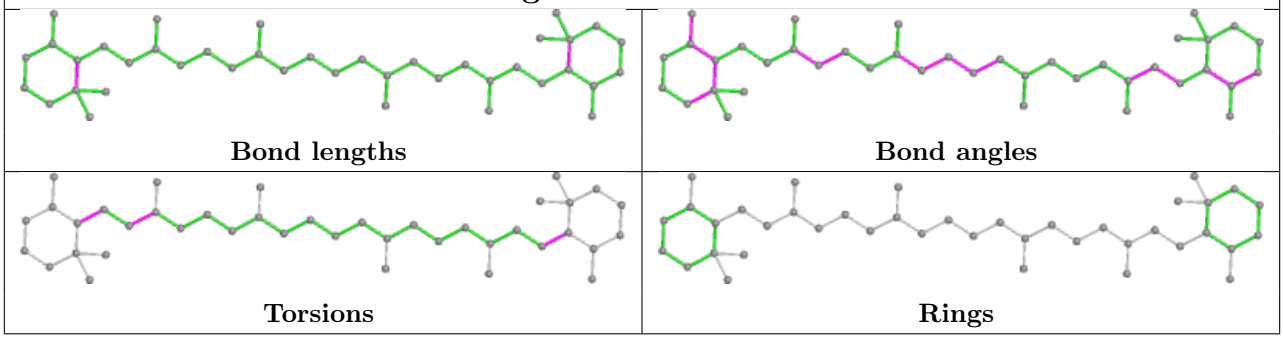
Ligand BCR b 621



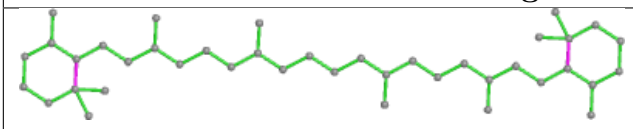
Ligand SQD f 101



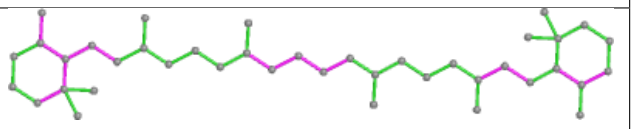
Ligand BCR H 102



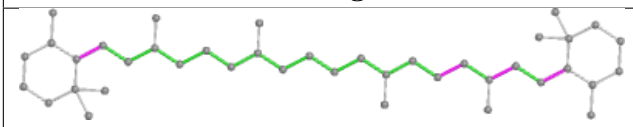
Ligand BCR K 101



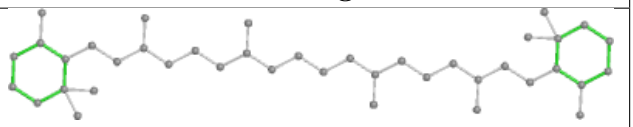
Bond lengths



Bond angles

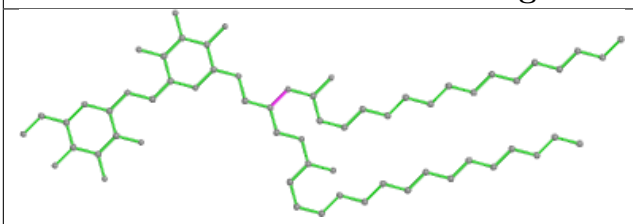


Torsions

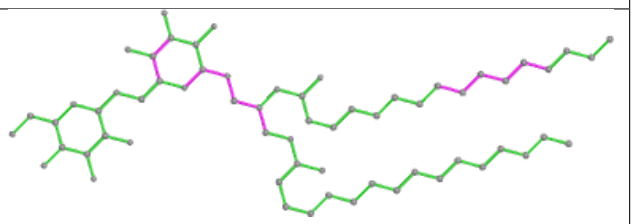


Rings

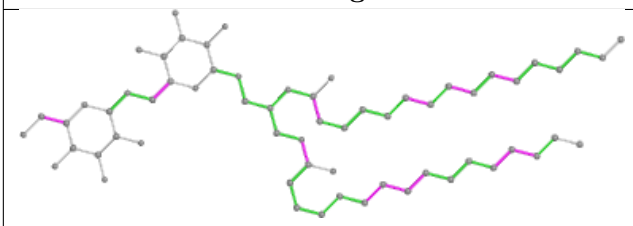
Ligand DGD H 103



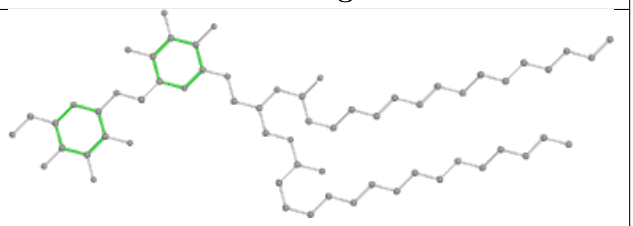
Bond lengths



Bond angles

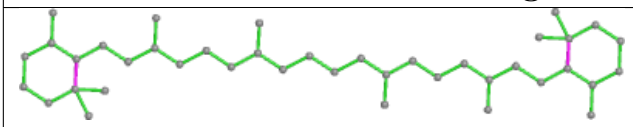


Torsions

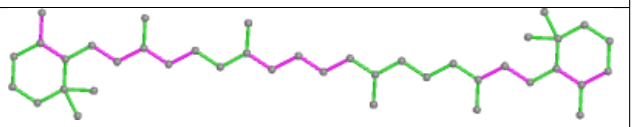


Rings

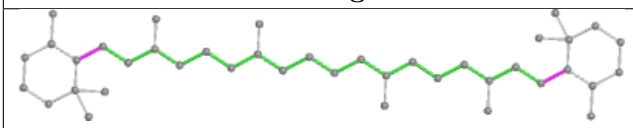
Ligand BCR C 514



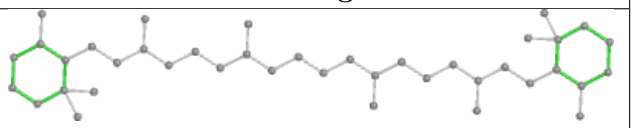
Bond lengths



Bond angles

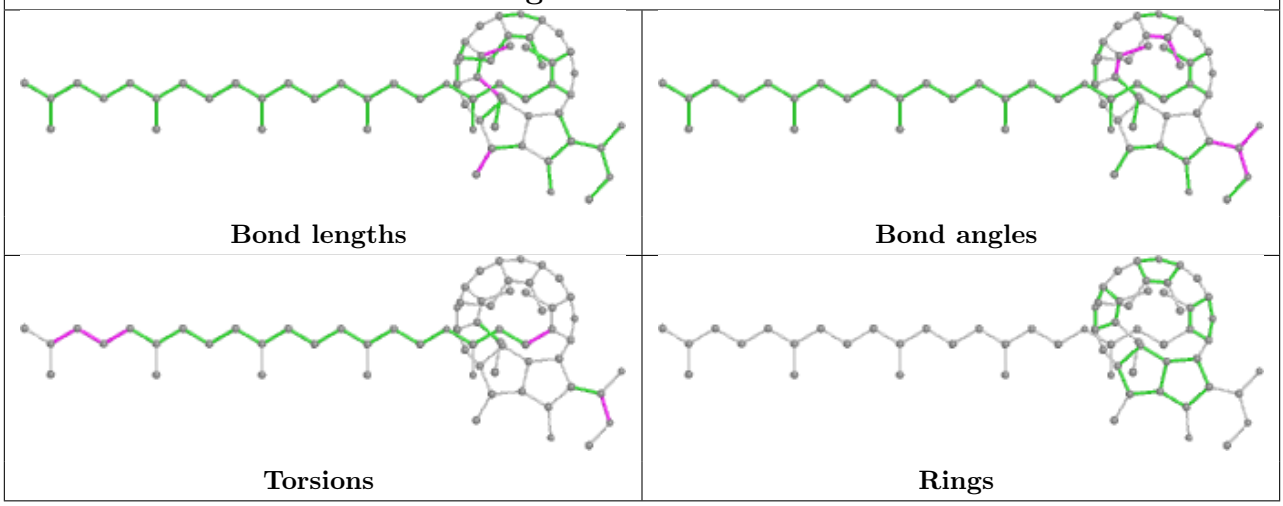


Torsions

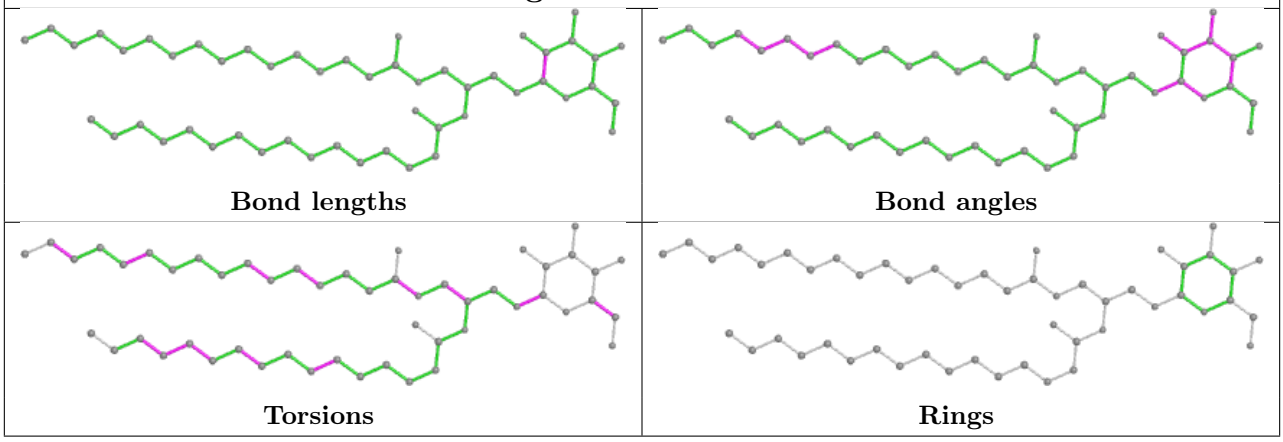


Rings

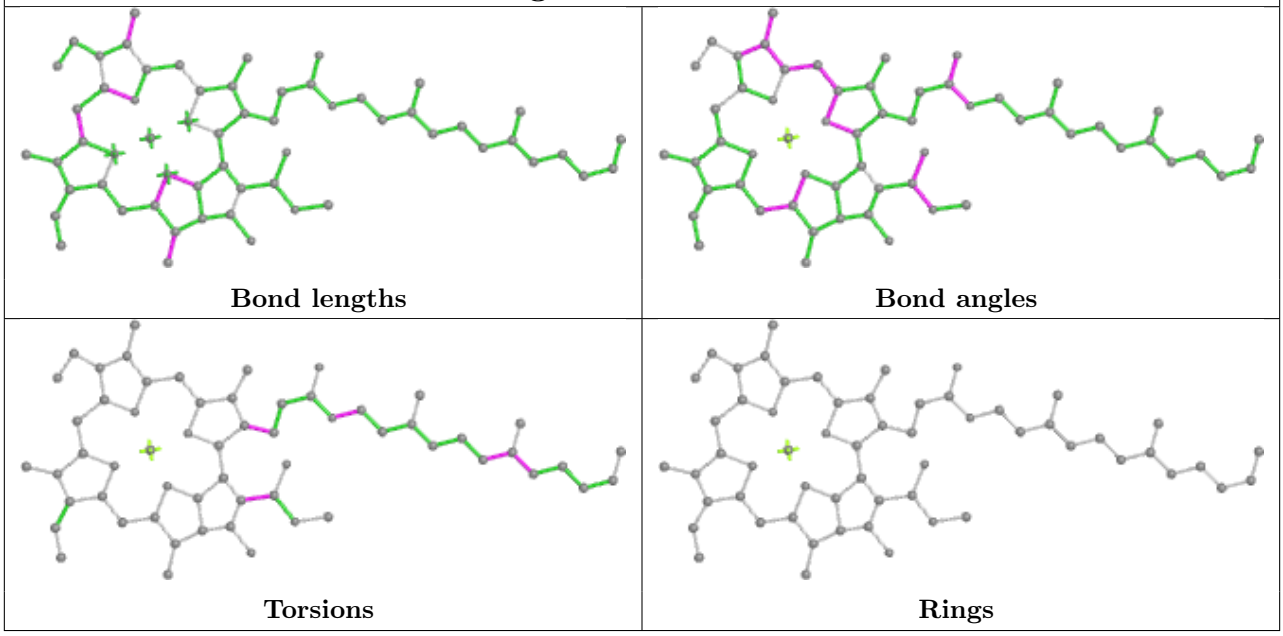
Ligand PHO d 401



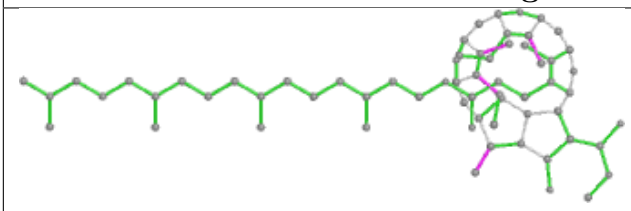
Ligand LMG c 522



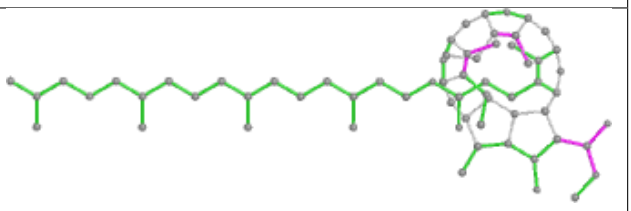
Ligand CLA a 607



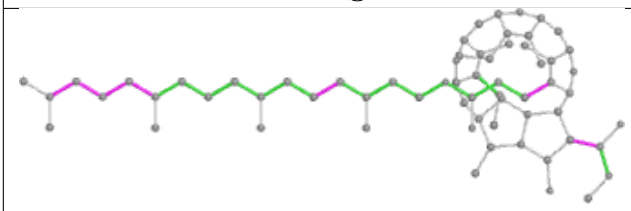
Ligand PHO A 608



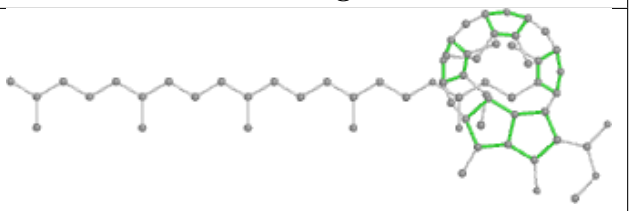
Bond lengths



Bond angles

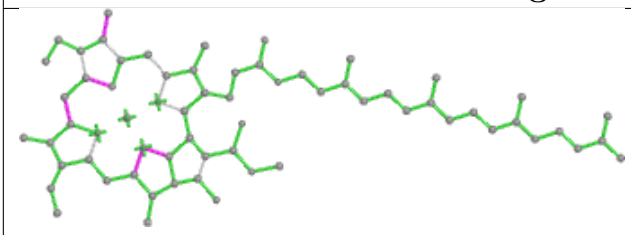


Torsions

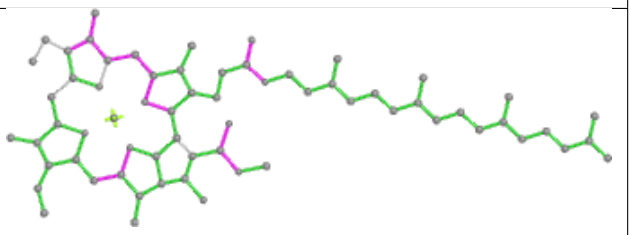


Rings

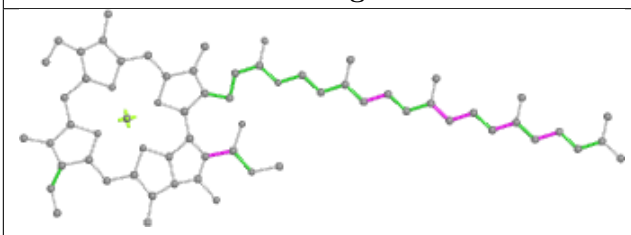
Ligand CLA c 511



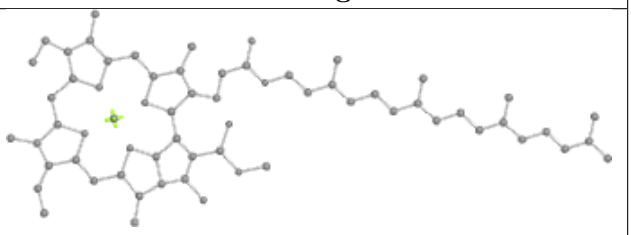
Bond lengths



Bond angles

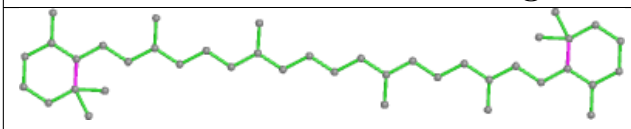


Torsions

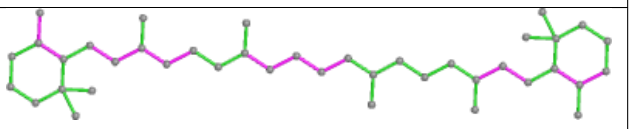


Rings

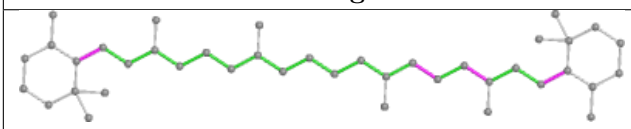
Ligand BCR C 515



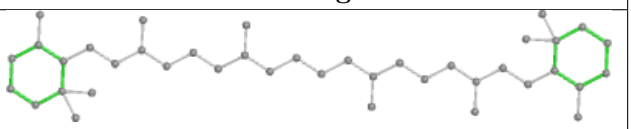
Bond lengths



Bond angles

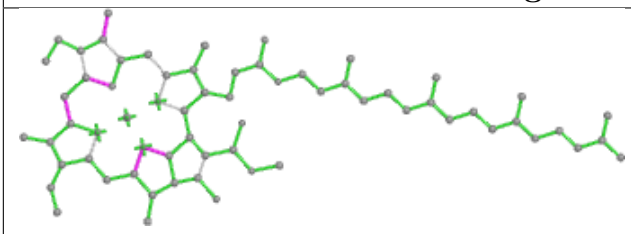


Torsions

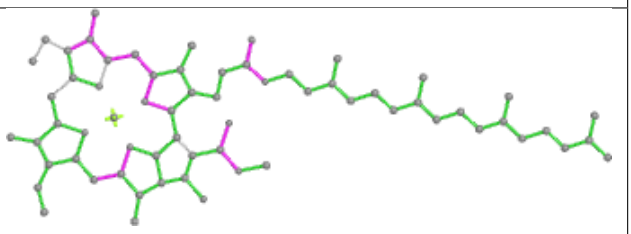


Rings

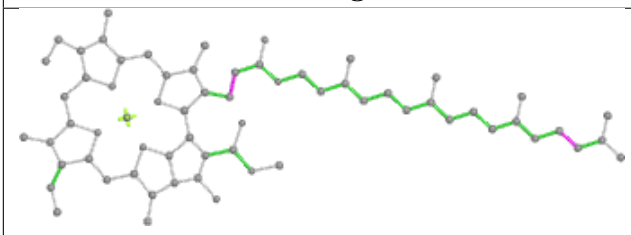
Ligand CLA B 608



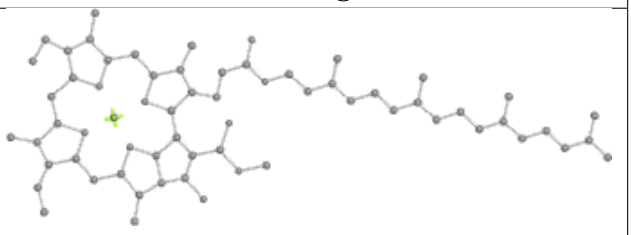
Bond lengths



Bond angles

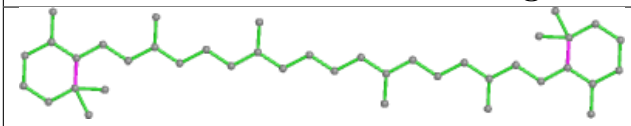


Torsions

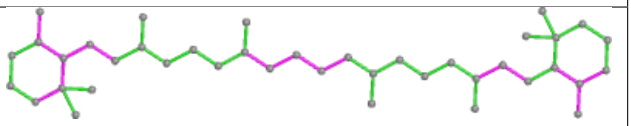


Rings

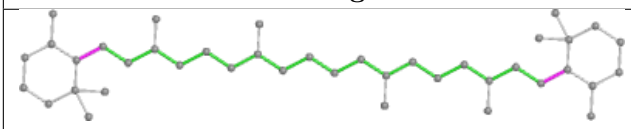
Ligand BCR B 619



Bond lengths



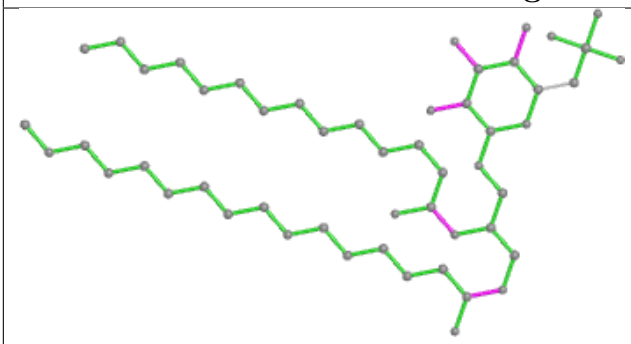
Bond angles



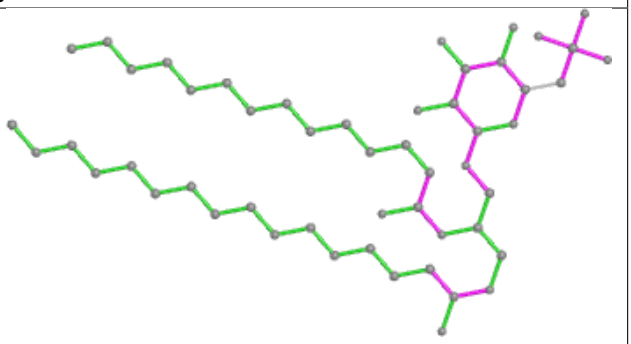
Torsions

Rings

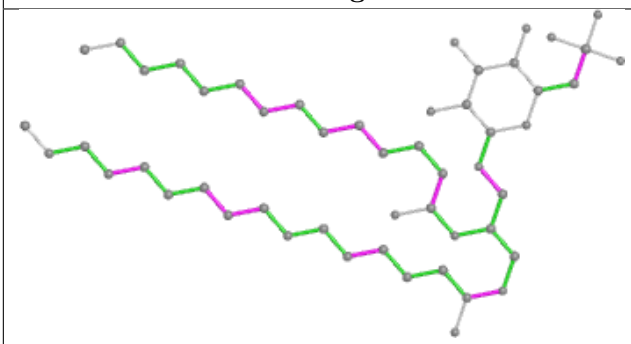
Ligand SQD A 603



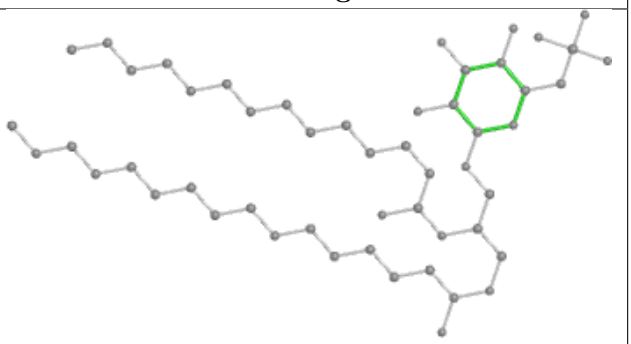
Bond lengths



Bond angles

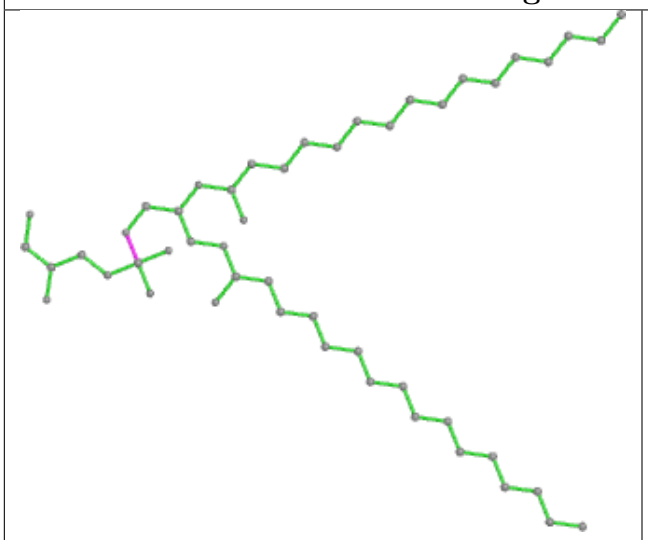


Torsions

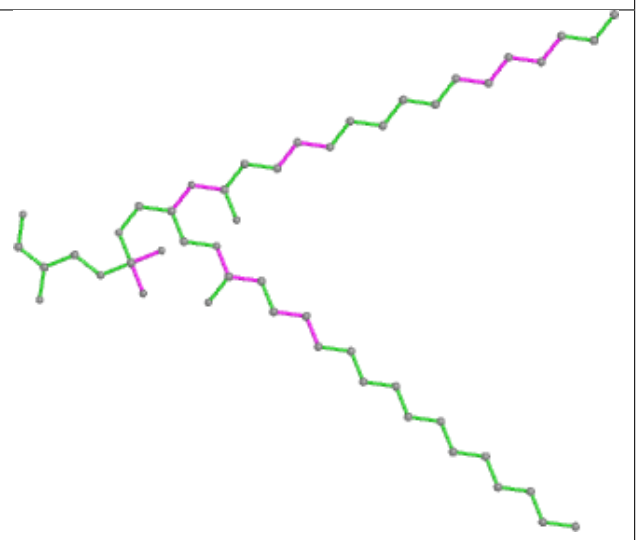


Rings

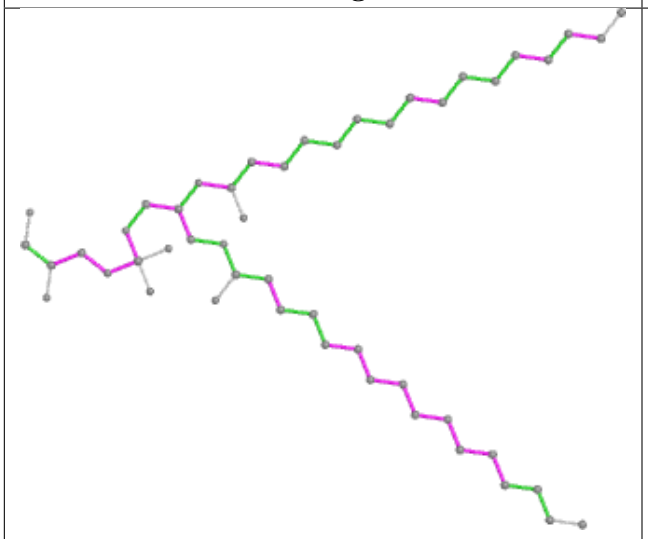
Ligand LHG A 618



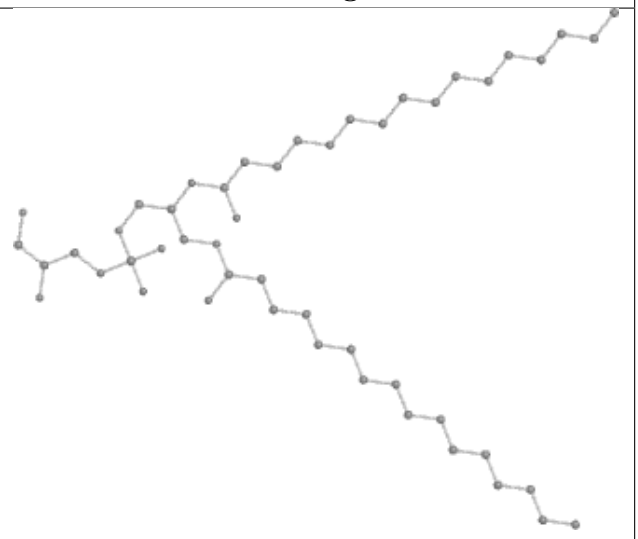
Bond lengths



Bond angles

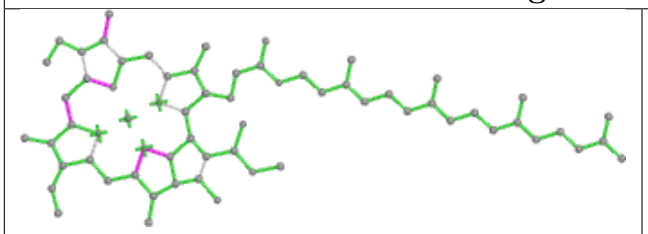


Torsions

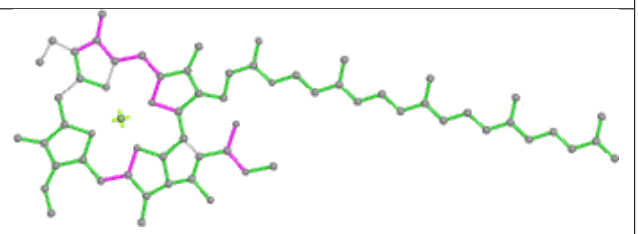


Rings

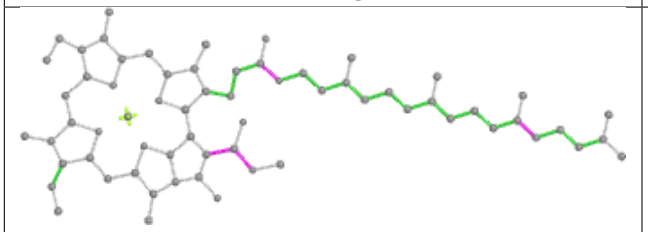
Ligand CLA b 610



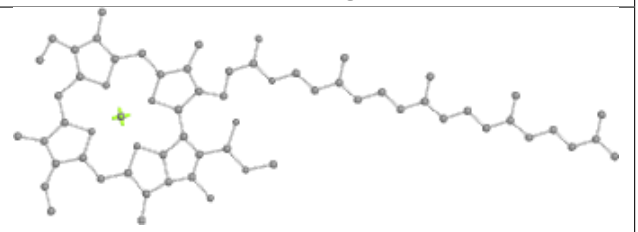
Bond lengths



Bond angles

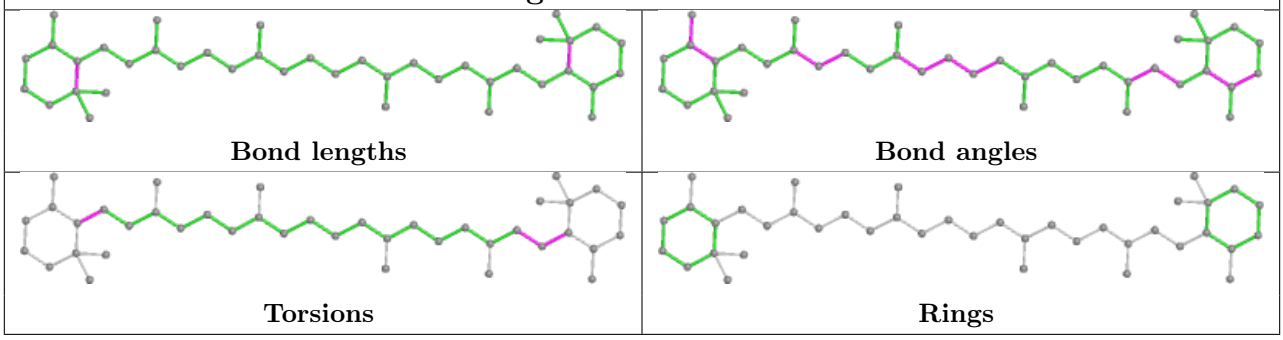


Torsions

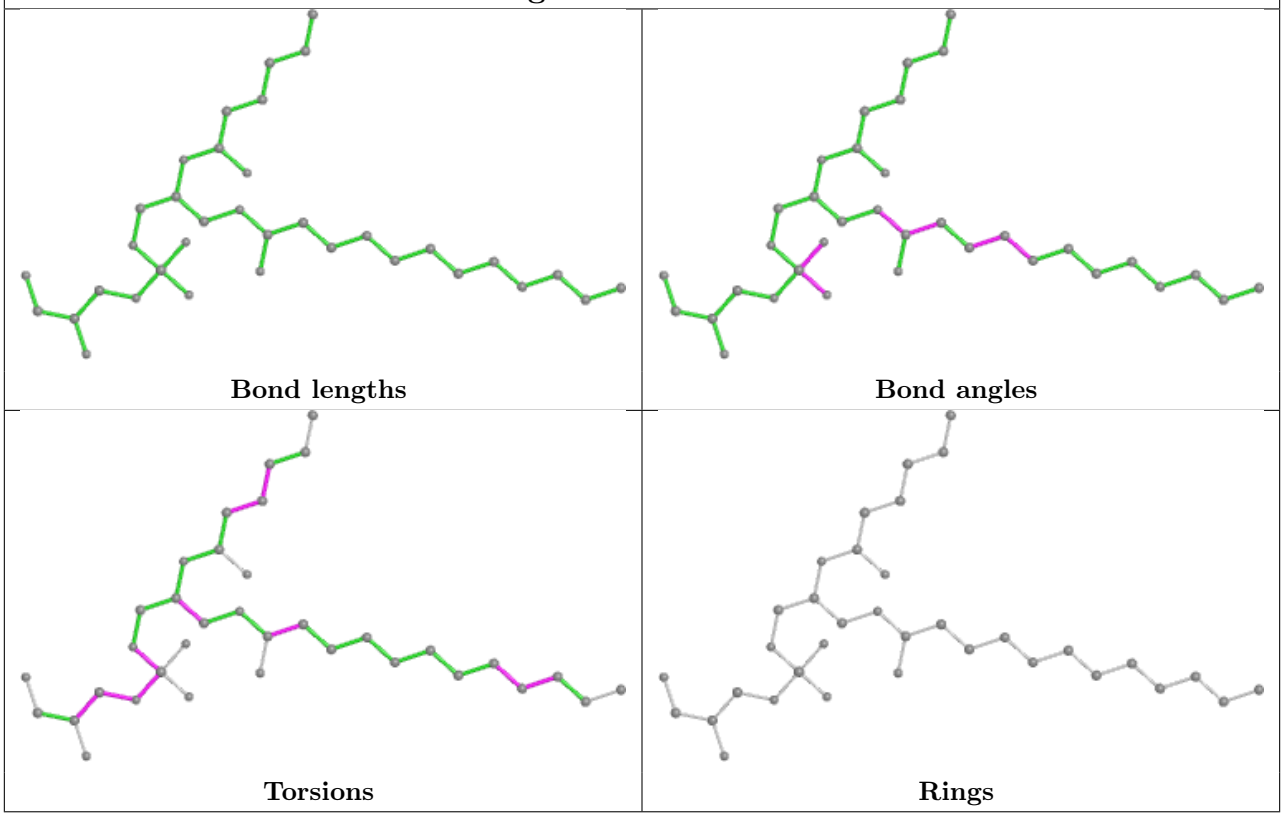


Rings

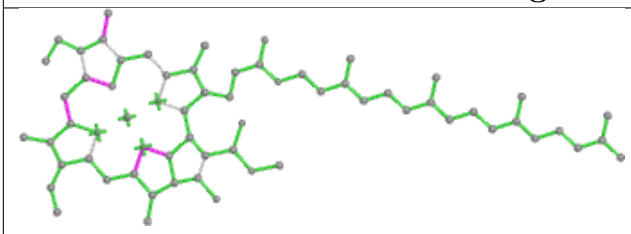
Ligand BCR b 620



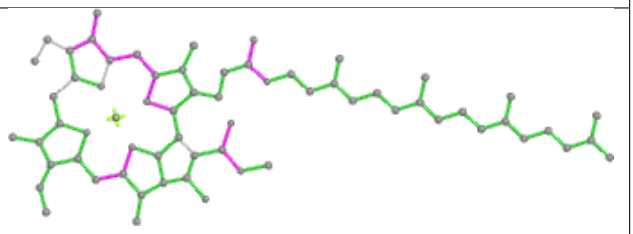
Ligand LHG a 614



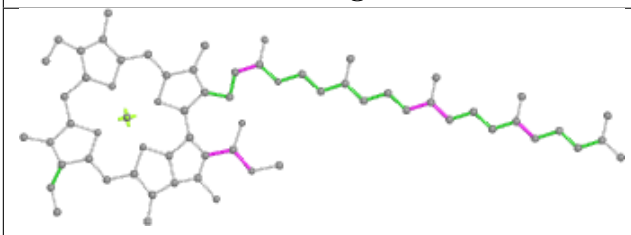
Ligand CLA c 514



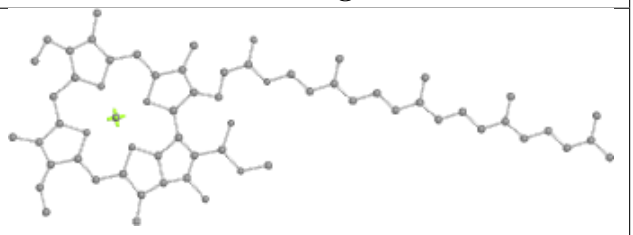
Bond lengths



Bond angles

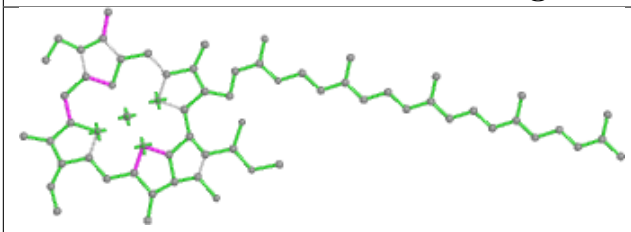


Torsions

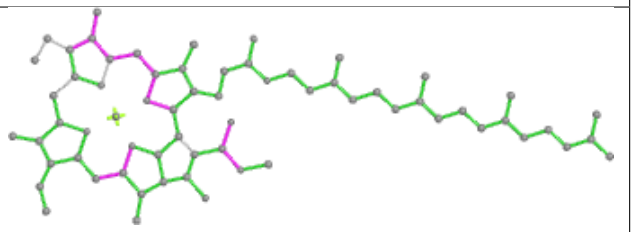


Rings

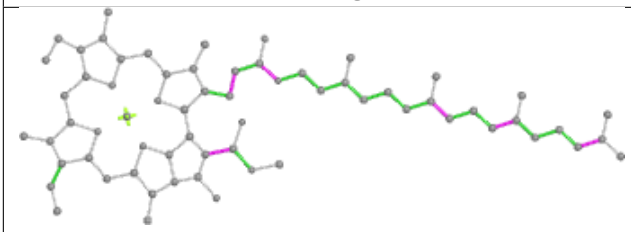
Ligand CLA c 509



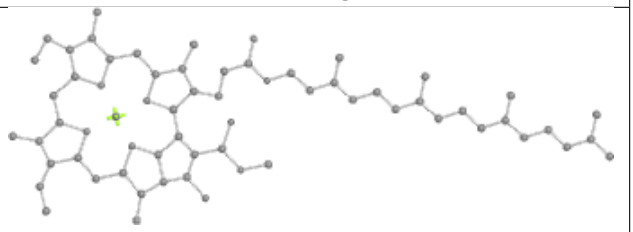
Bond lengths



Bond angles

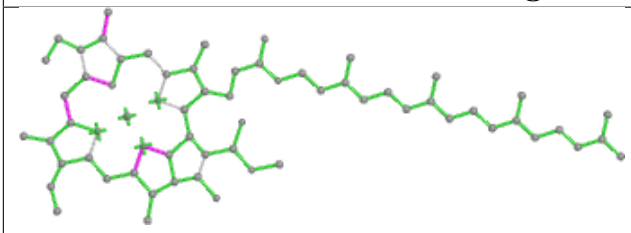


Torsions

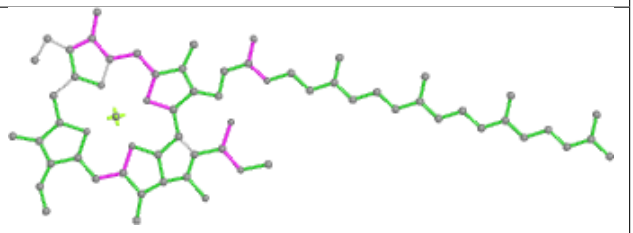


Rings

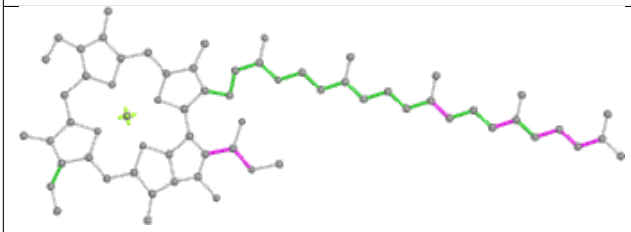
Ligand CLA B 610



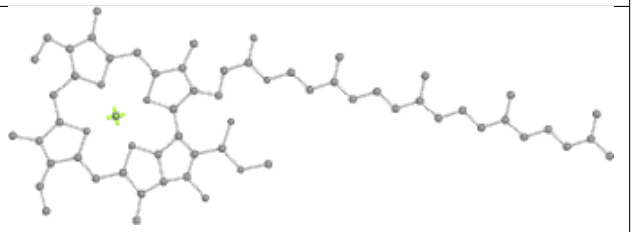
Bond lengths



Bond angles

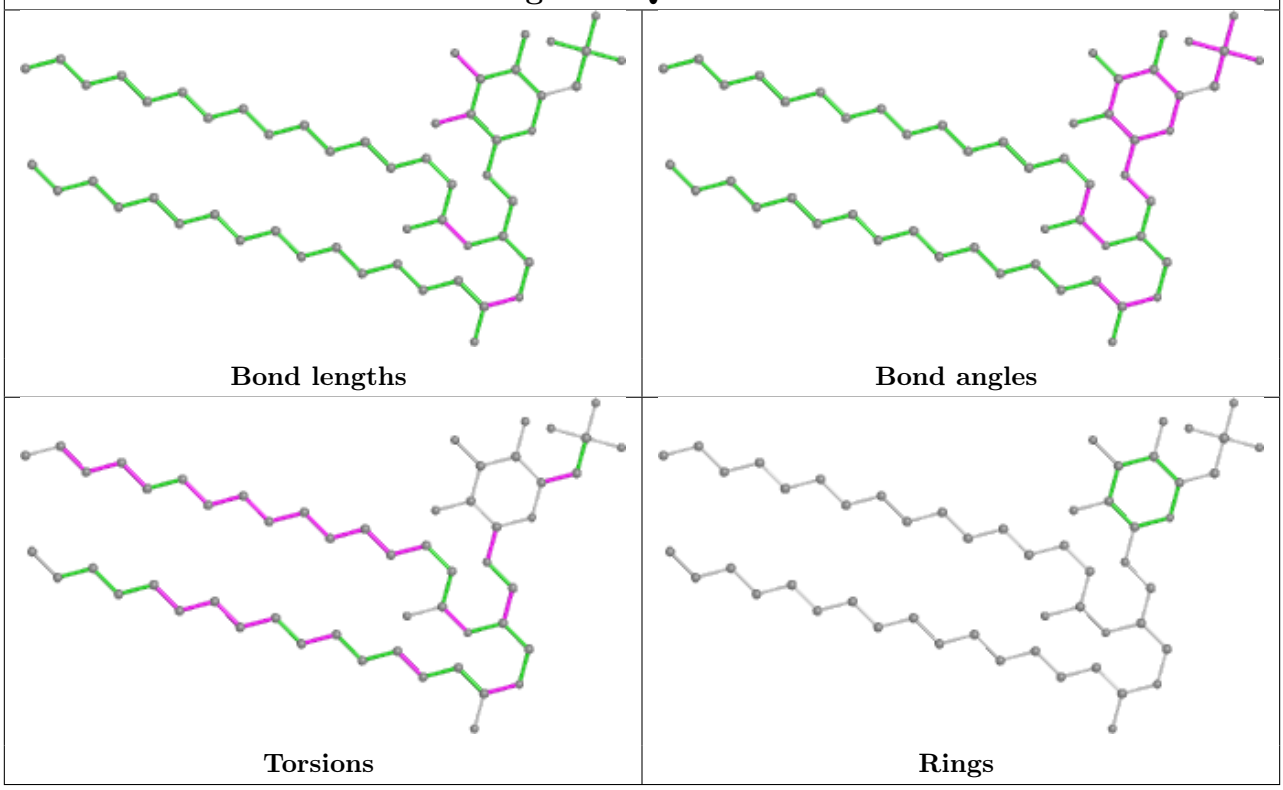


Torsions

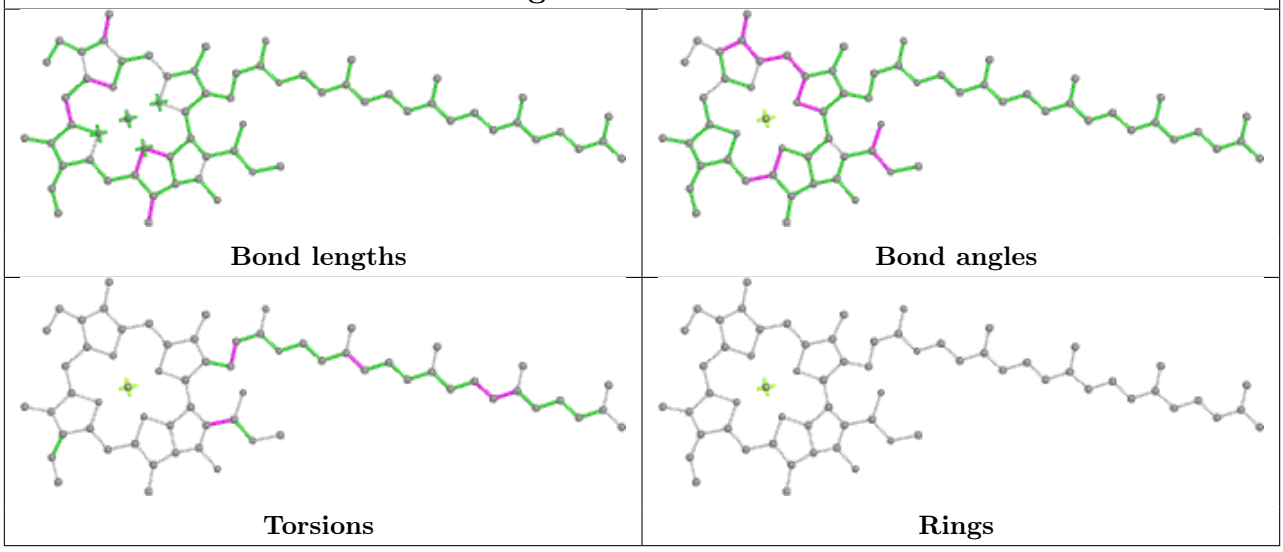


Rings

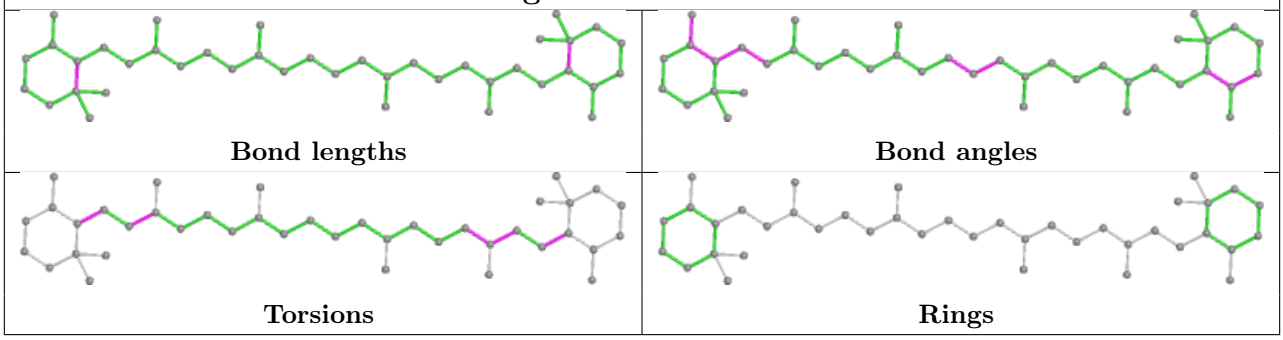
Ligand SQD B 626



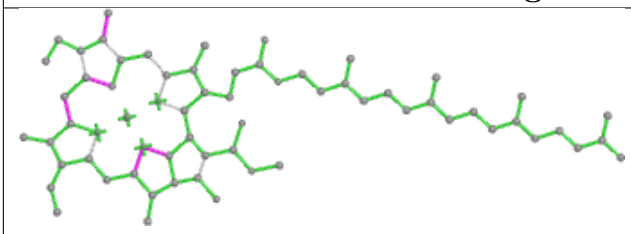
Ligand CLA b 617



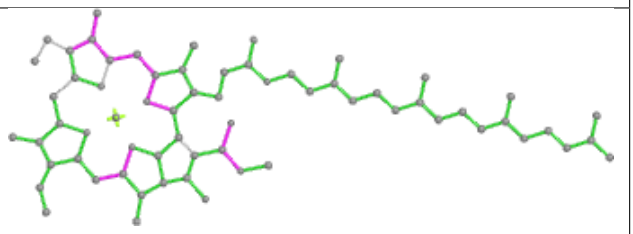
Ligand BCR Y 101



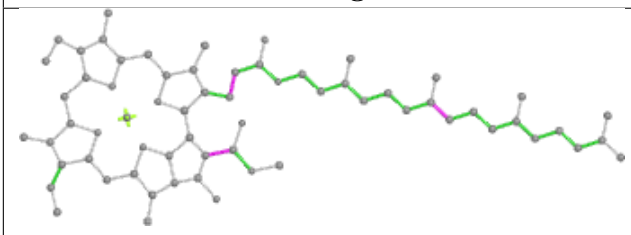
Ligand CLA C 507



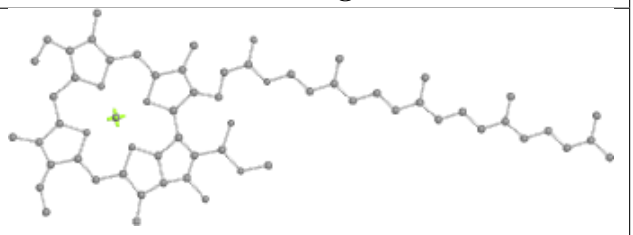
Bond lengths



Bond angles

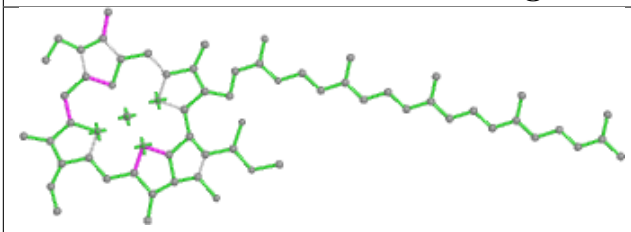


Torsions

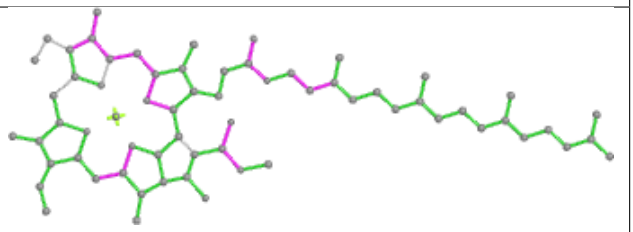


Rings

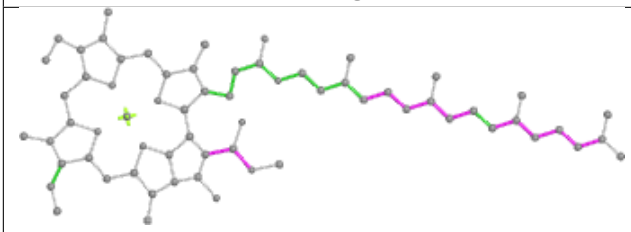
Ligand CLA C 506



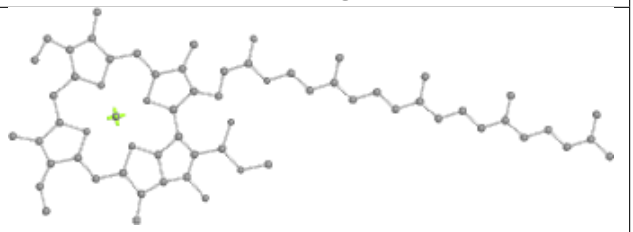
Bond lengths



Bond angles

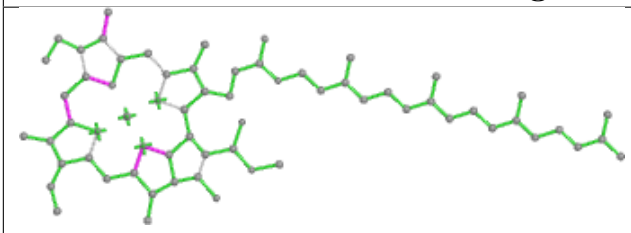


Torsions

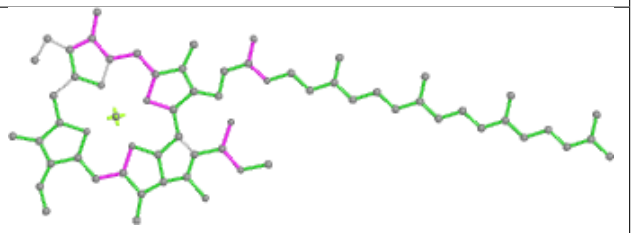


Rings

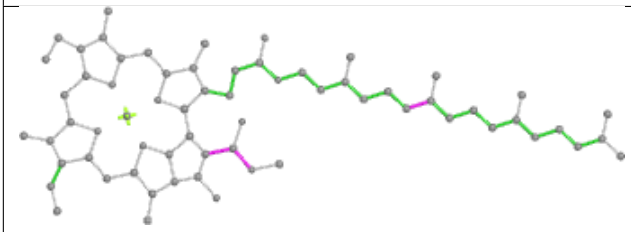
Ligand CLA c 515



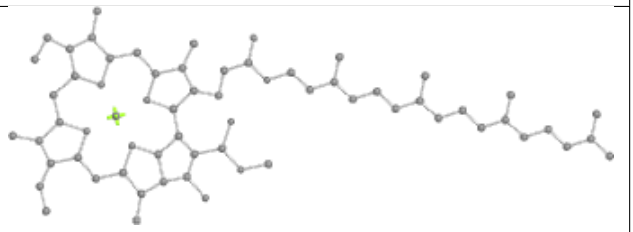
Bond lengths



Bond angles

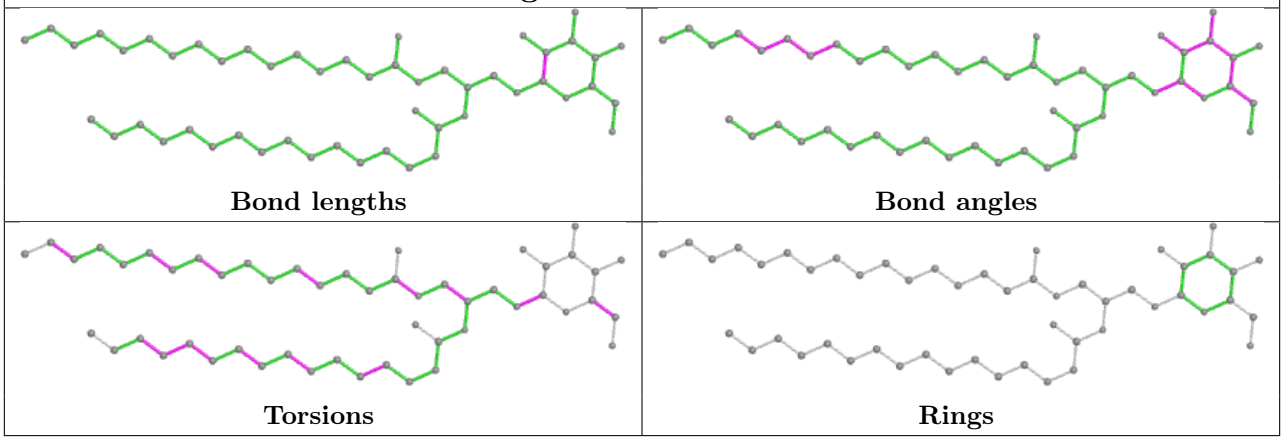


Torsions

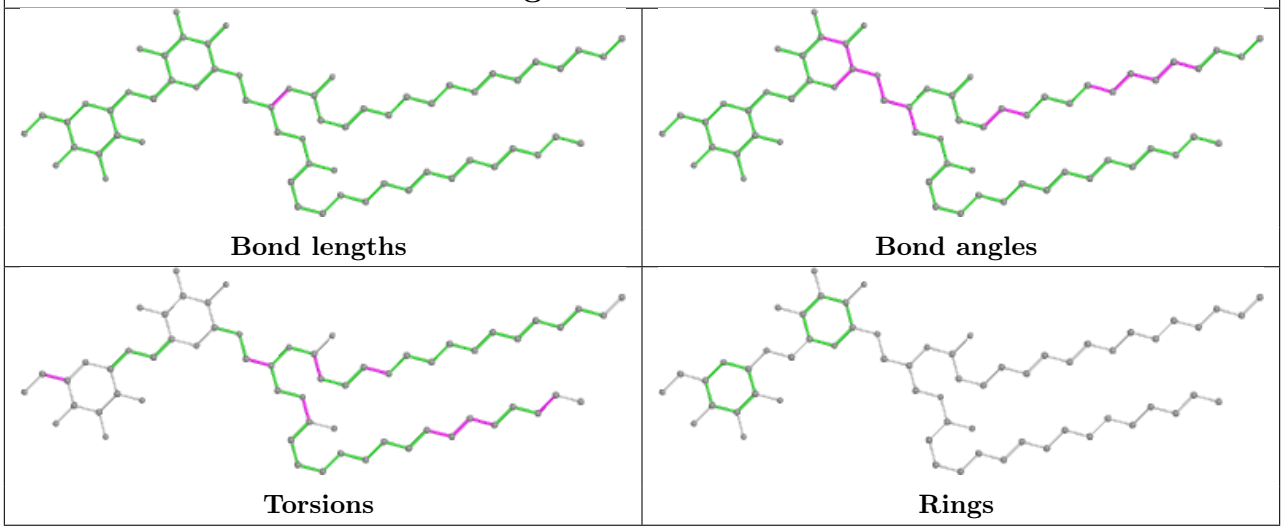


Rings

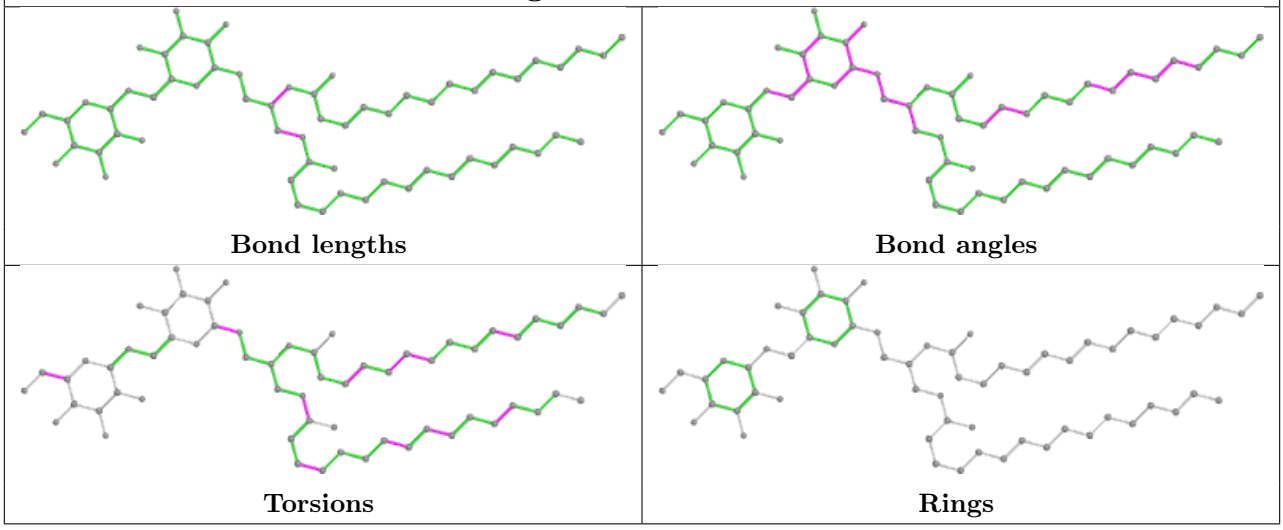
Ligand LMG C 520



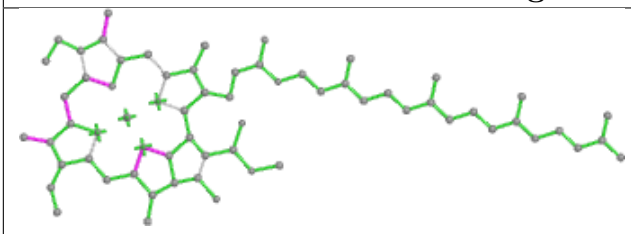
Ligand DGD h 102



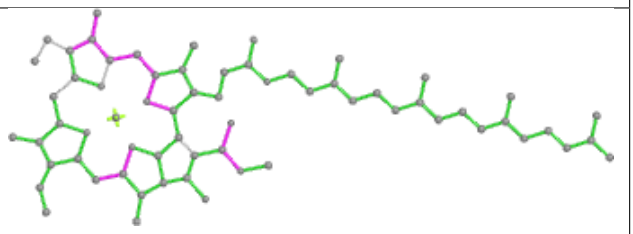
Ligand DGD c 520



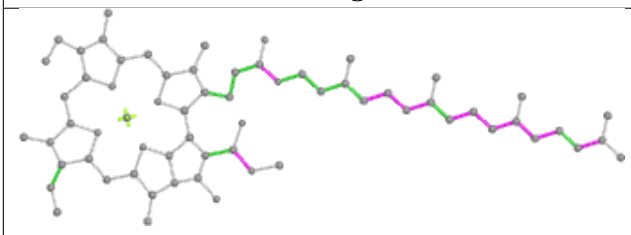
Ligand CLA b 619



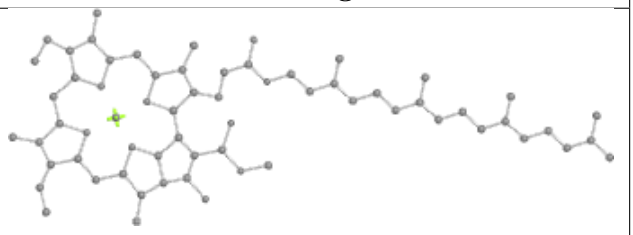
Bond lengths



Bond angles

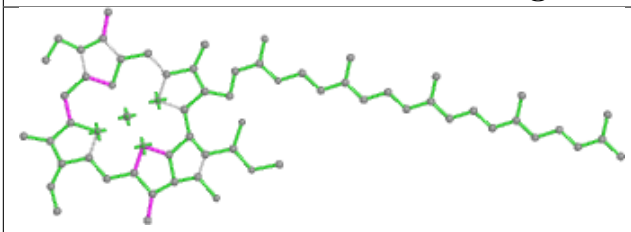


Torsions

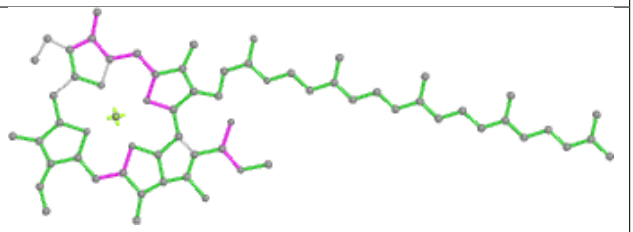


Rings

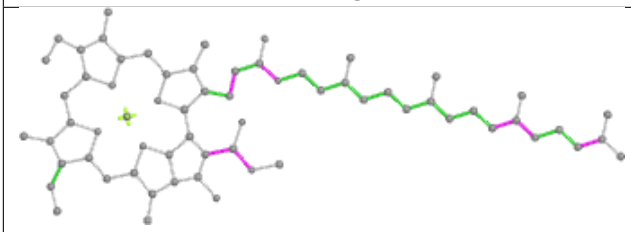
Ligand CLA c 507



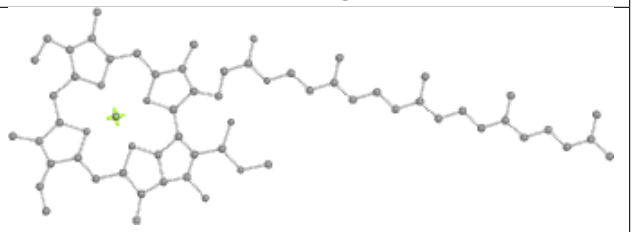
Bond lengths



Bond angles

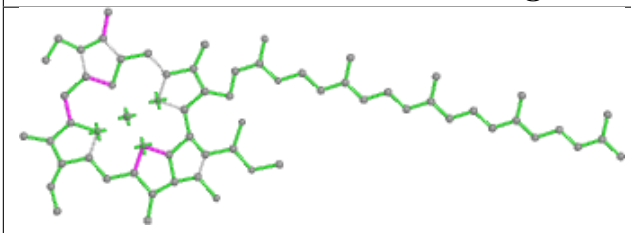


Torsions

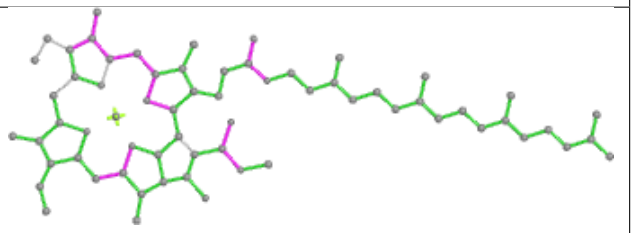


Rings

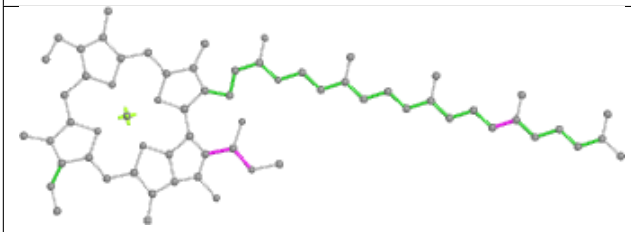
Ligand CLA C 502



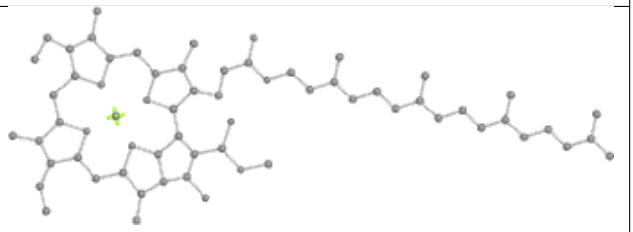
Bond lengths



Bond angles

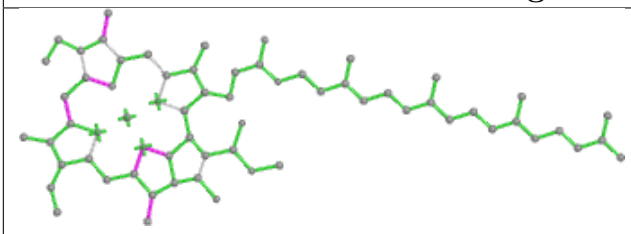


Torsions

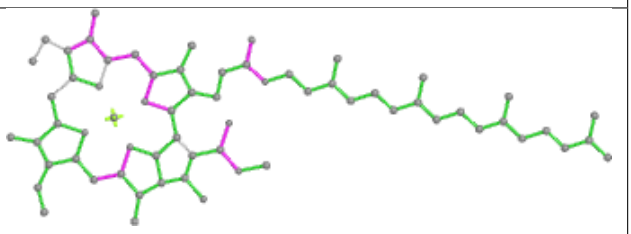


Rings

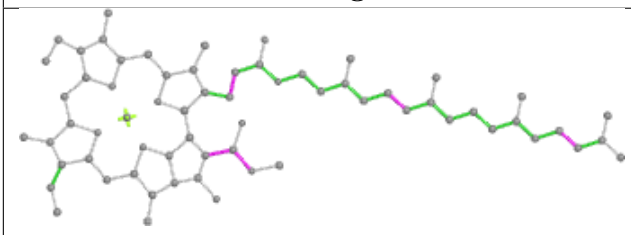
Ligand CLA b 606



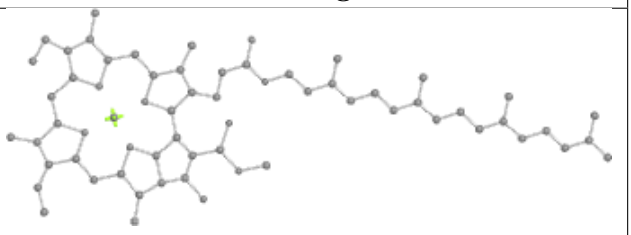
Bond lengths



Bond angles

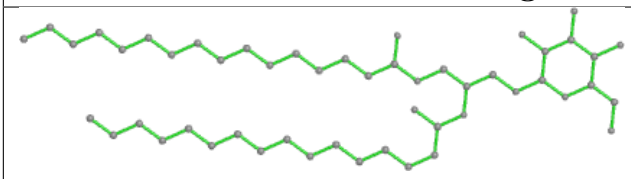


Torsions

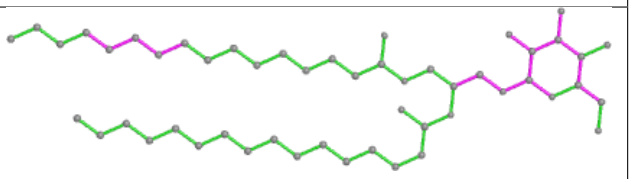


Rings

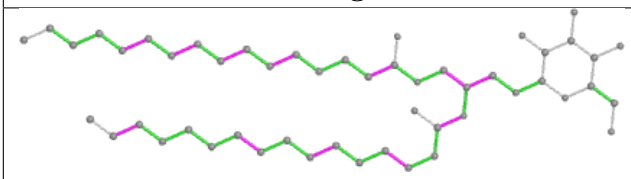
Ligand LMG A 613



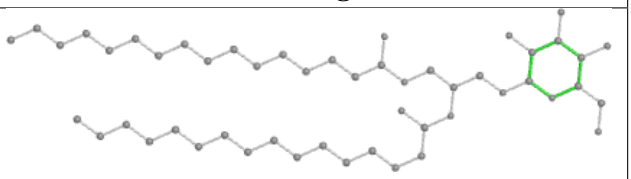
Bond lengths



Bond angles

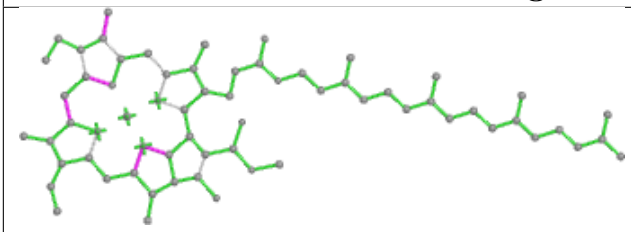


Torsions

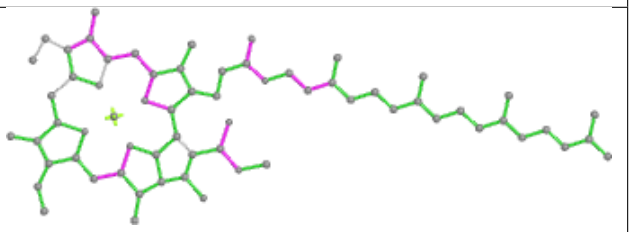


Rings

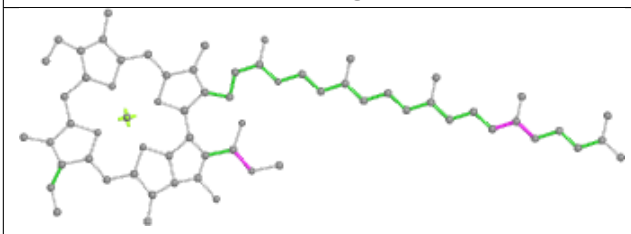
Ligand CLA b 614



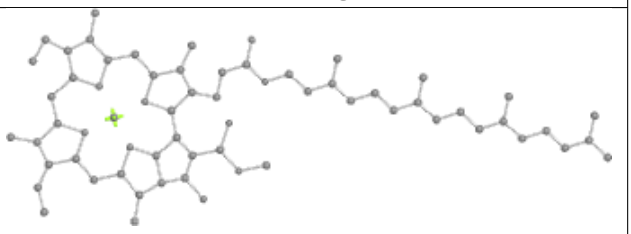
Bond lengths



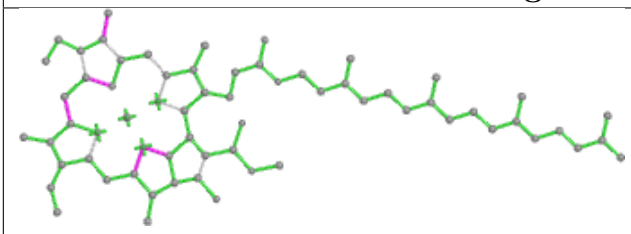
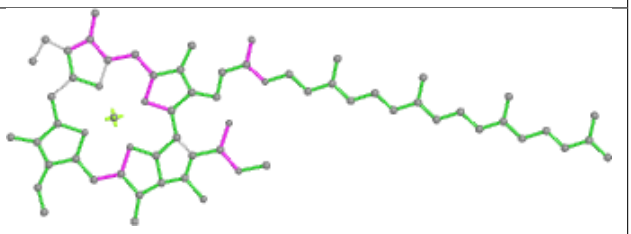
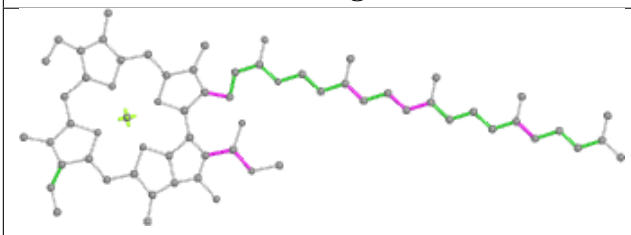
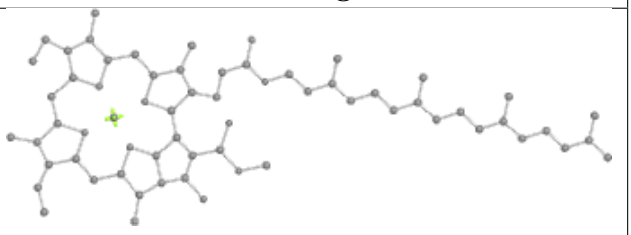
Bond angles

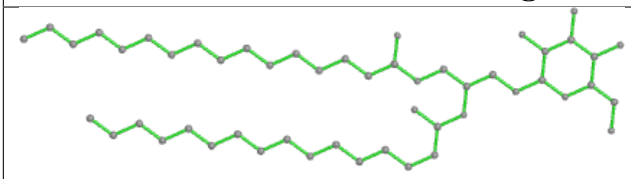
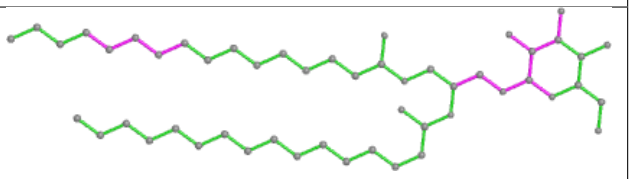
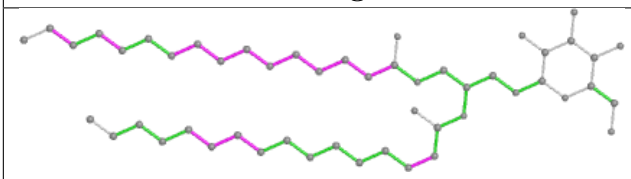
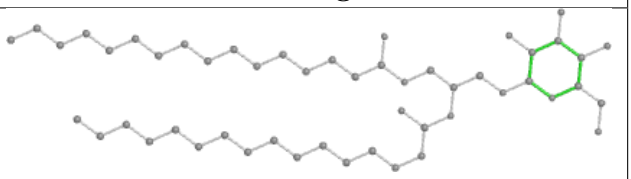


Torsions

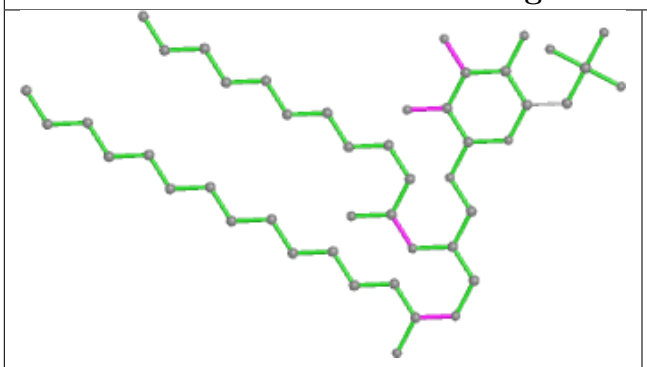


Rings

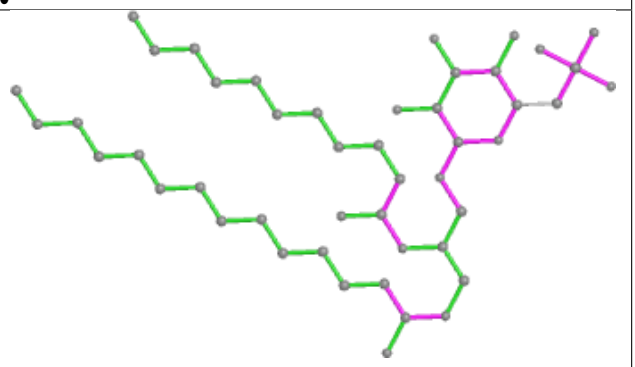
Ligand CLA B 609	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMG B 620	
 Bond lengths	 Bond angles
 Torsions	 Rings

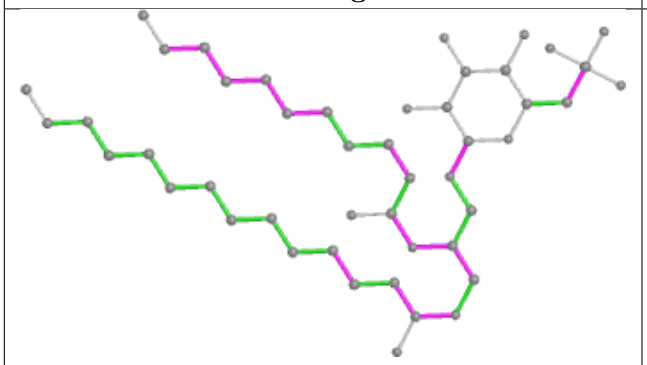
Ligand SQD D 408



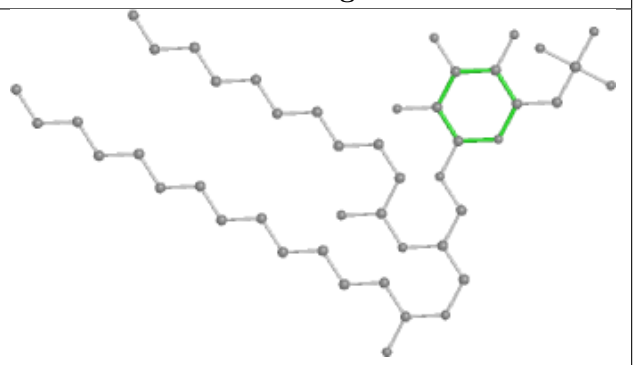
Bond lengths



Bond angles

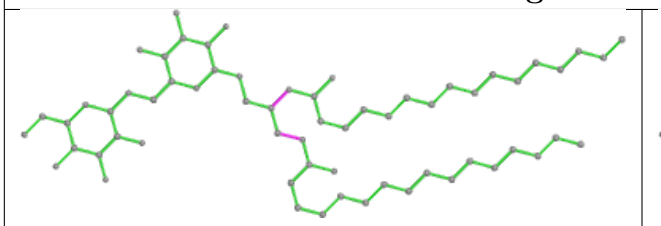


Torsions

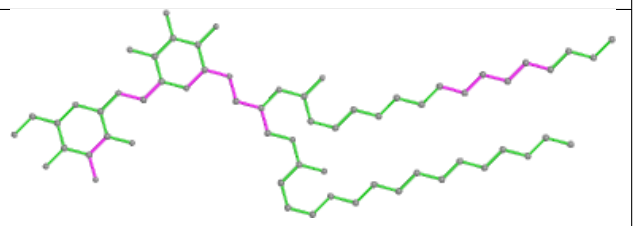


Rings

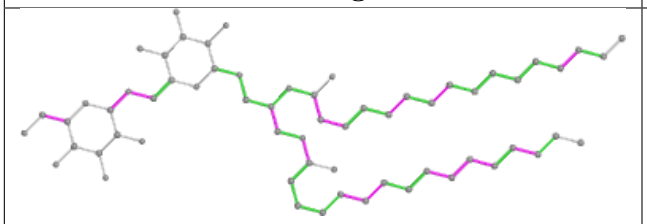
Ligand DGD c 519



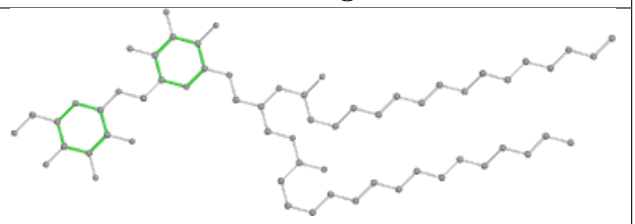
Bond lengths



Bond angles

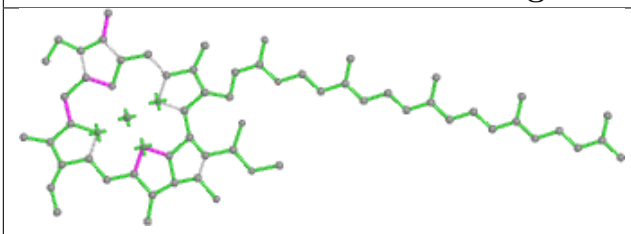


Torsions

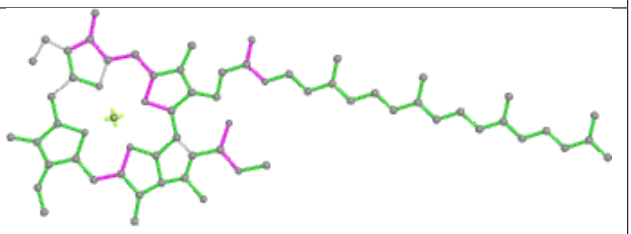


Rings

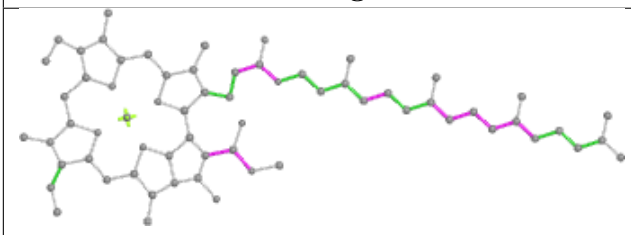
Ligand CLA b 604



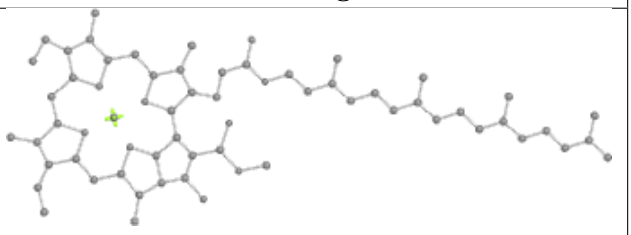
Bond lengths



Bond angles

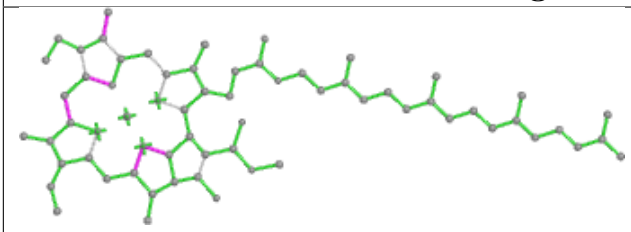


Torsions

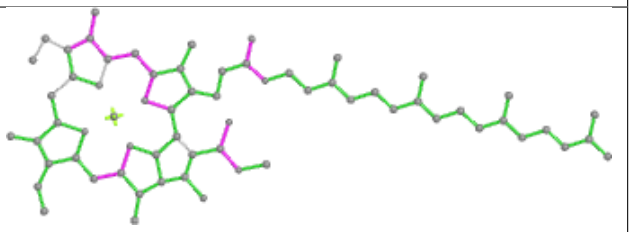


Rings

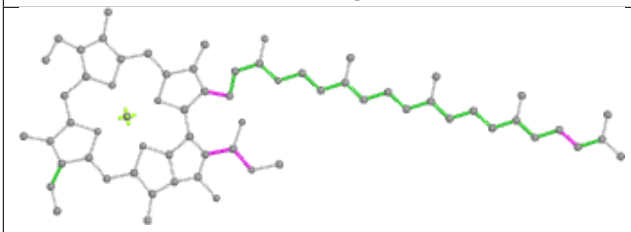
Ligand CLA c 505



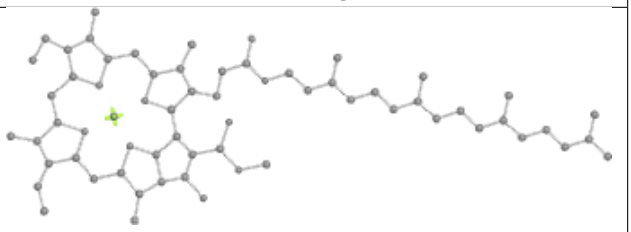
Bond lengths



Bond angles

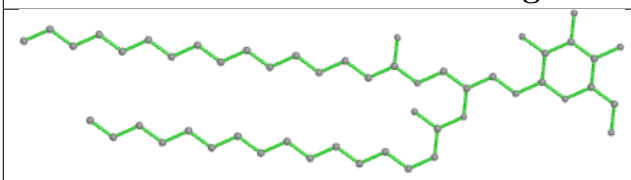


Torsions

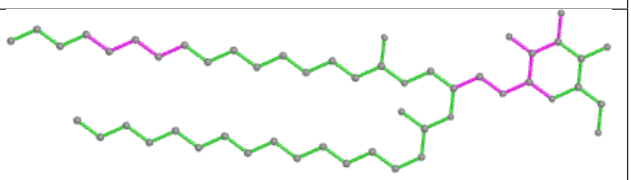


Rings

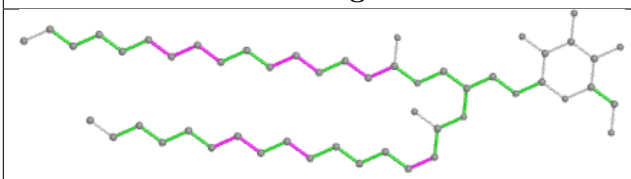
Ligand LMG b 623



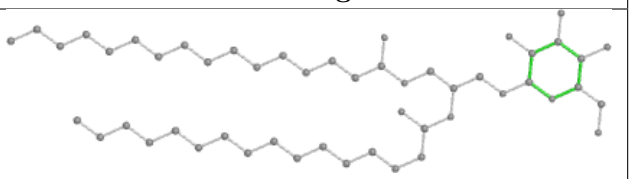
Bond lengths



Bond angles

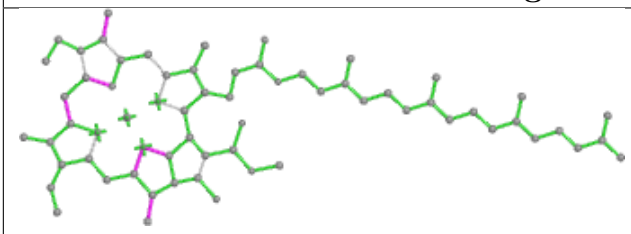


Torsions

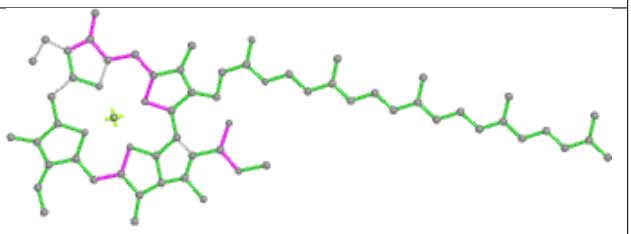


Rings

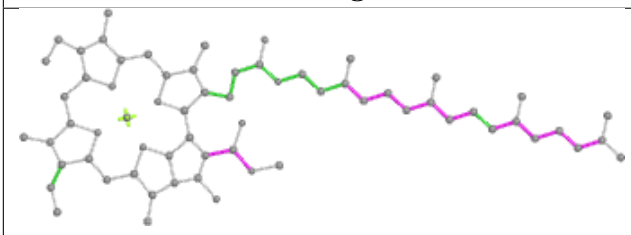
Ligand CLA B 614



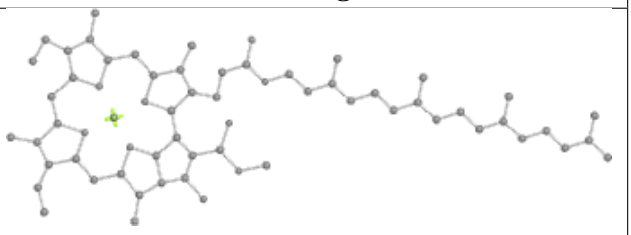
Bond lengths



Bond angles

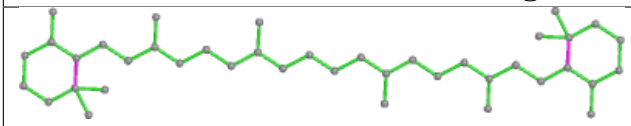


Torsions

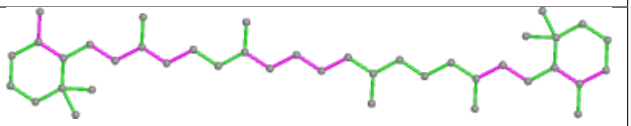


Rings

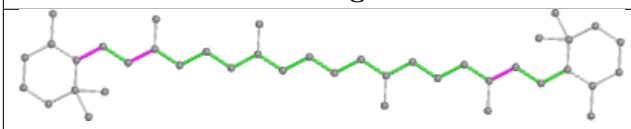
Ligand BCR D 404



Bond lengths



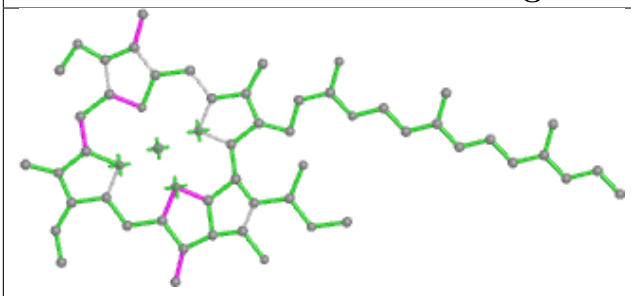
Bond angles



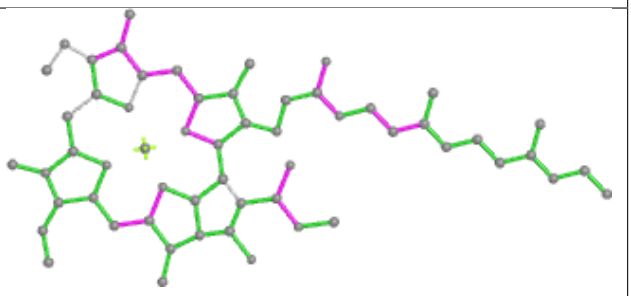
Torsions

Rings

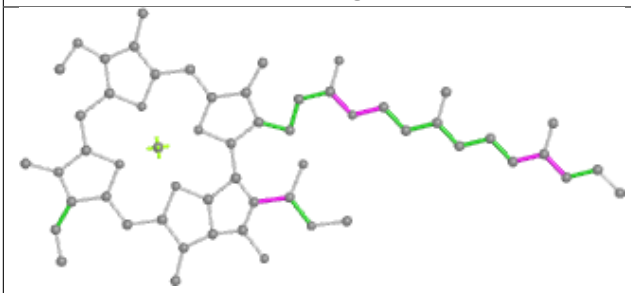
Ligand CLA A 607



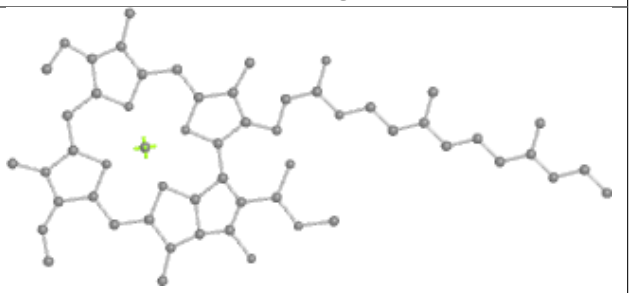
Bond lengths



Bond angles

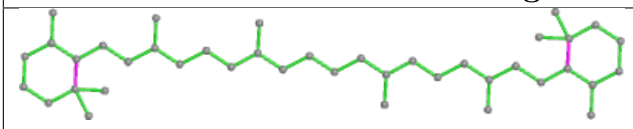


Torsions

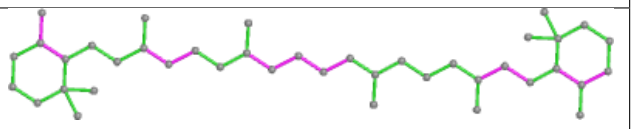


Rings

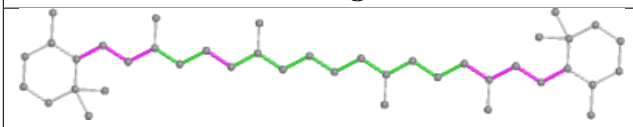
Ligand BCR T 101



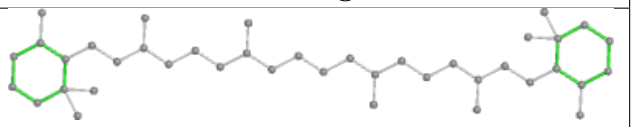
Bond lengths



Bond angles

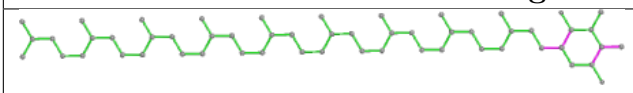


Torsions

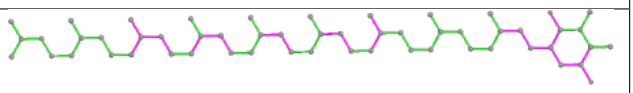


Rings

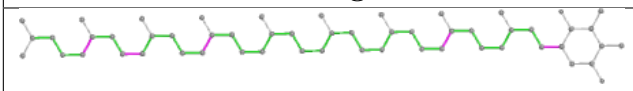
Ligand PL9 D 407



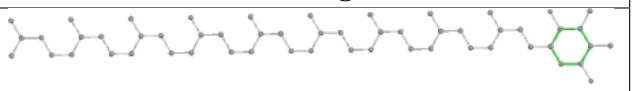
Bond lengths



Bond angles

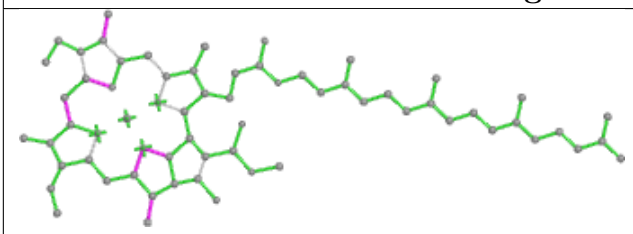


Torsions

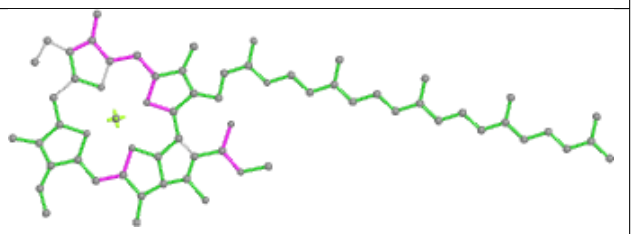


Rings

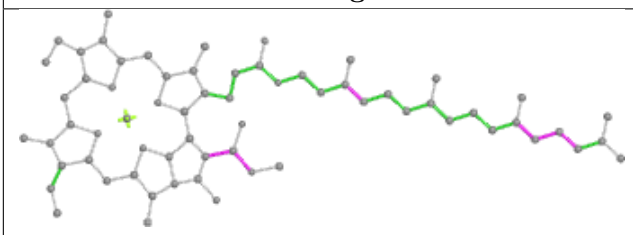
Ligand CLA B 605



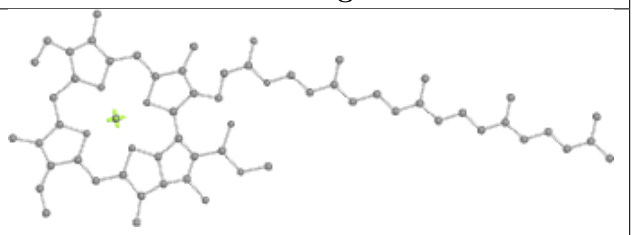
Bond lengths



Bond angles

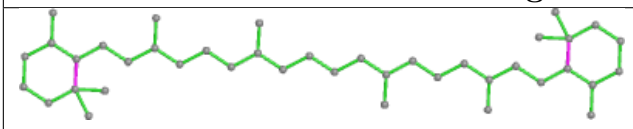


Torsions

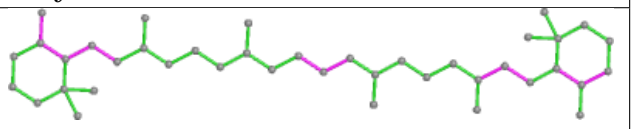


Rings

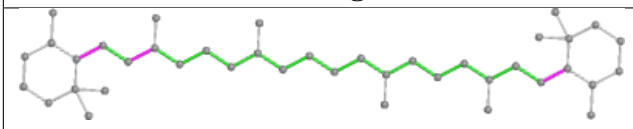
Ligand BCR y 101



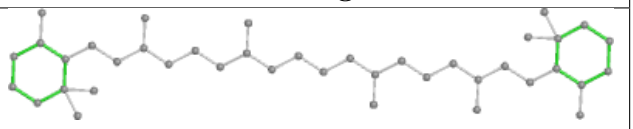
Bond lengths



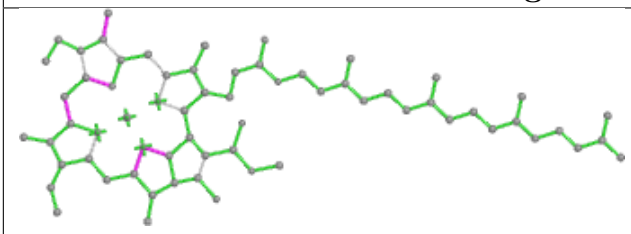
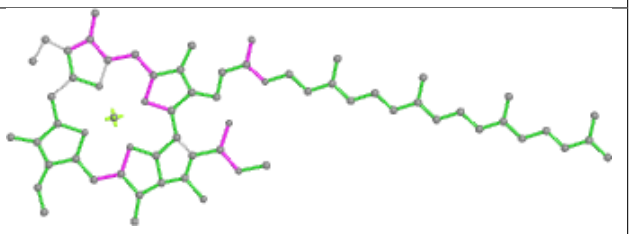
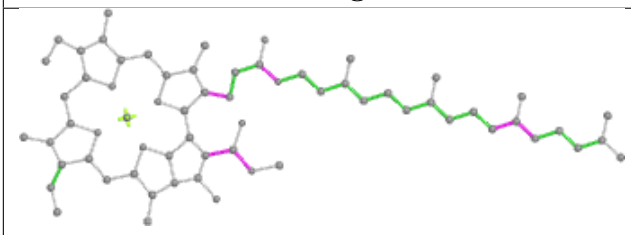
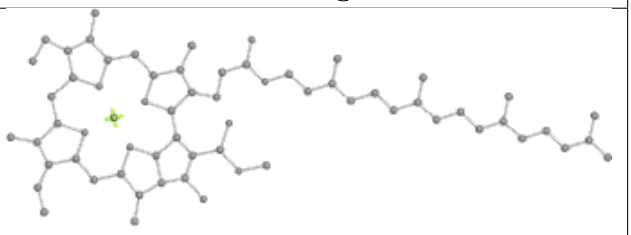
Bond angles

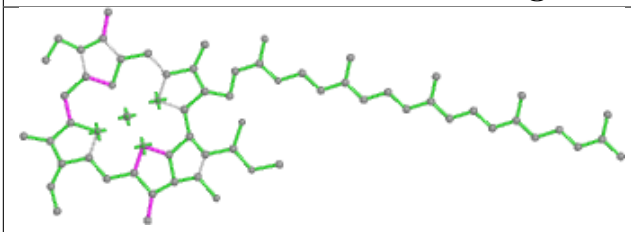
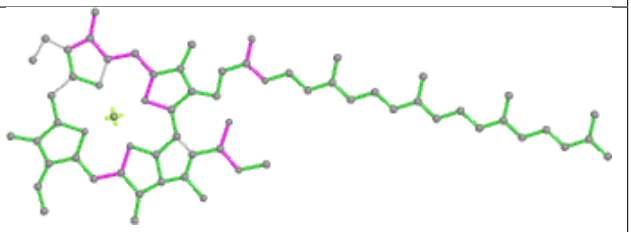
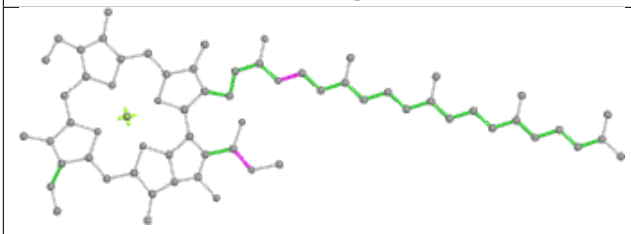
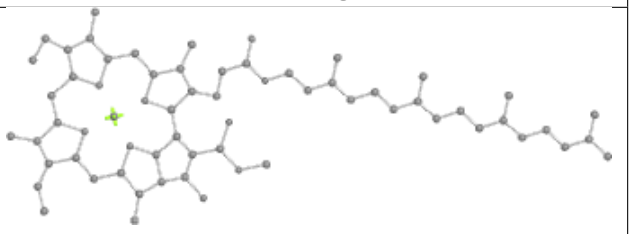


Torsions

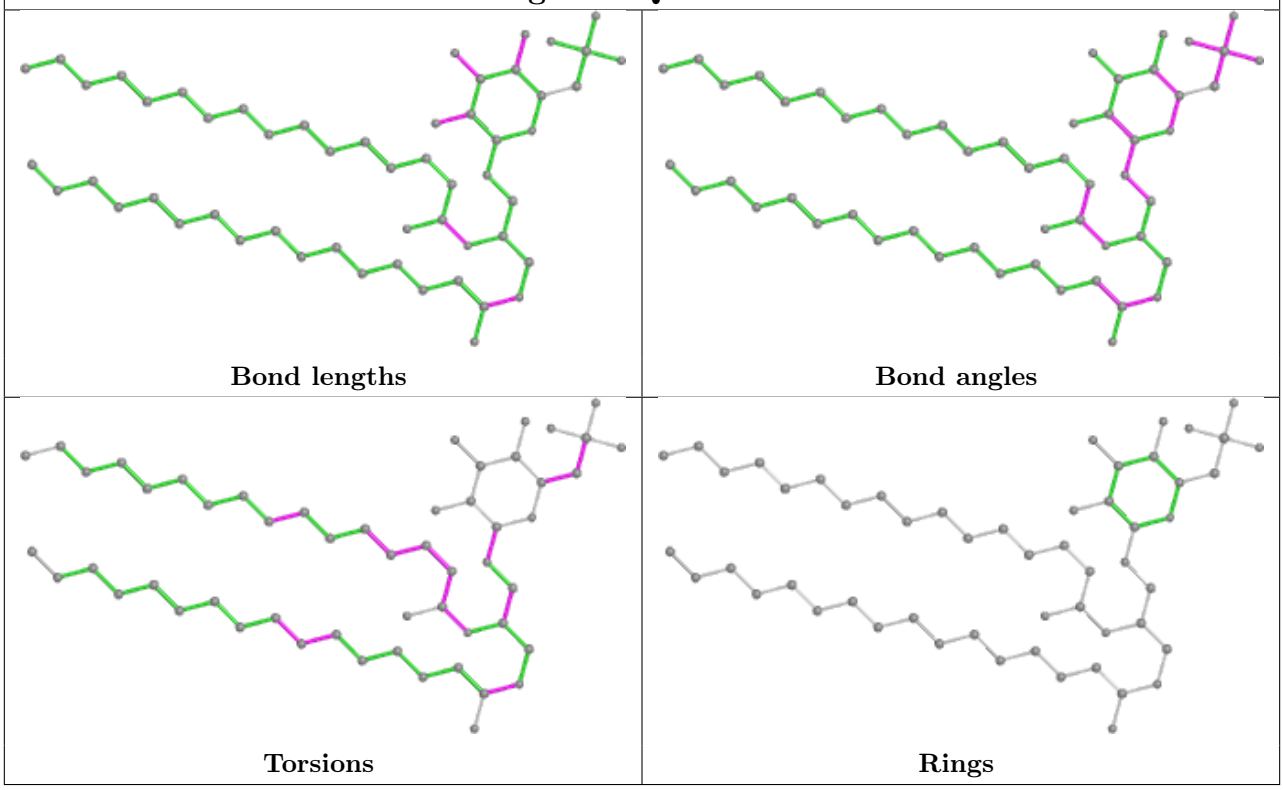


Rings

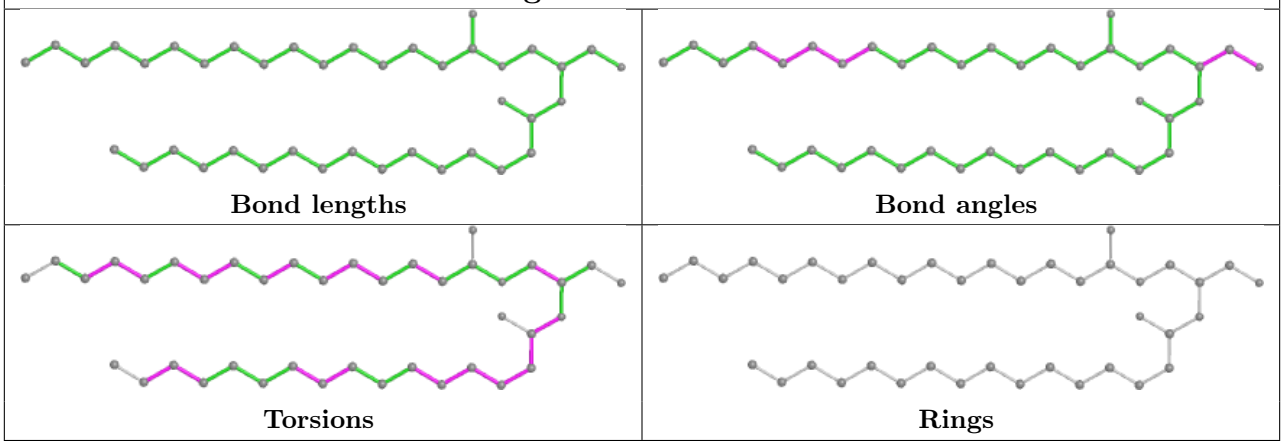
Ligand CLA B 607	
 Bond lengths	 Bond angles
 Torsions	 Rings

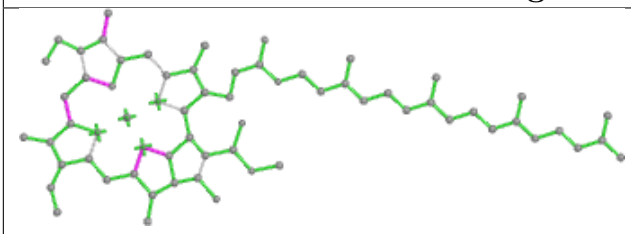
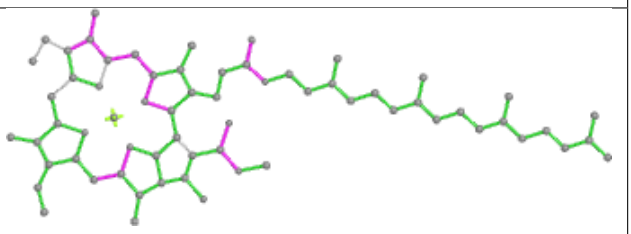
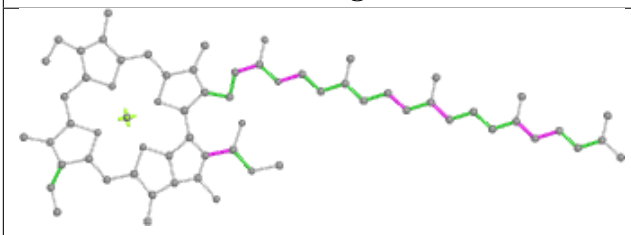
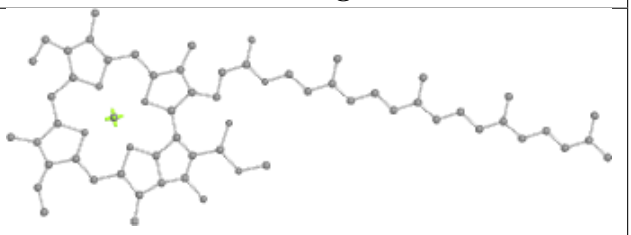
Ligand CLA a 606	
 Bond lengths	 Bond angles
 Torsions	 Rings

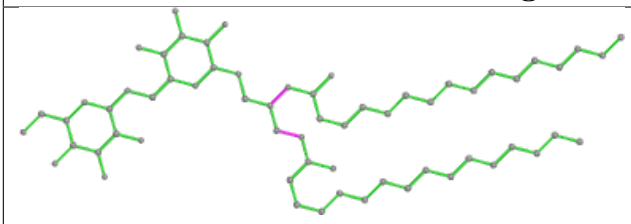
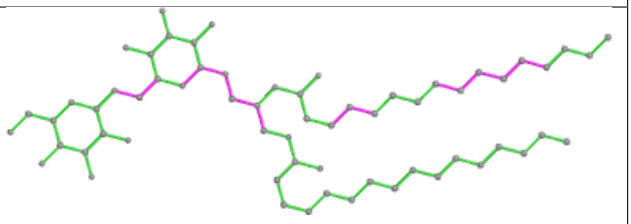
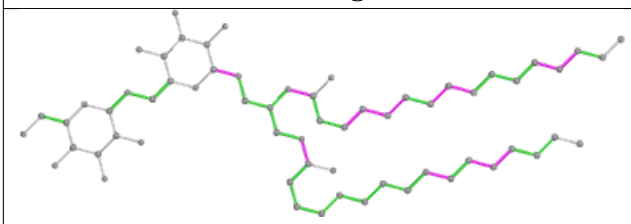
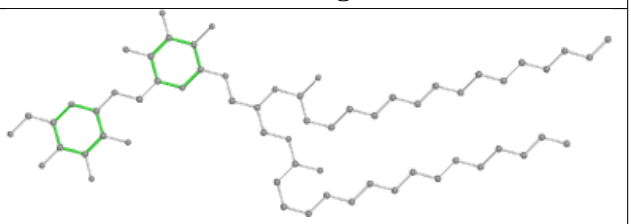
Ligand SQD b 601



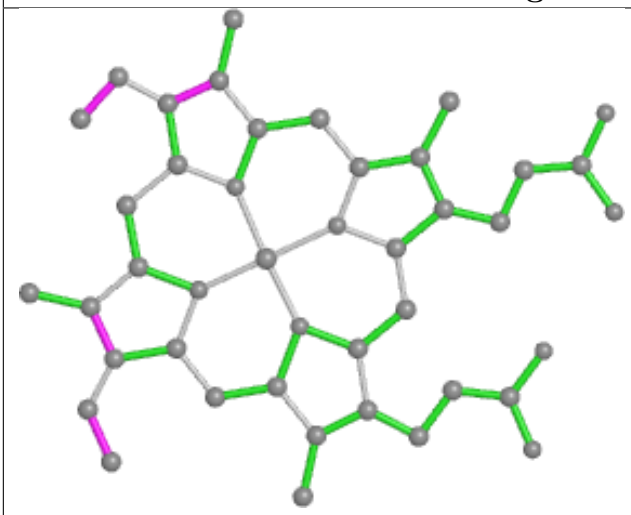
Ligand LMG d 409



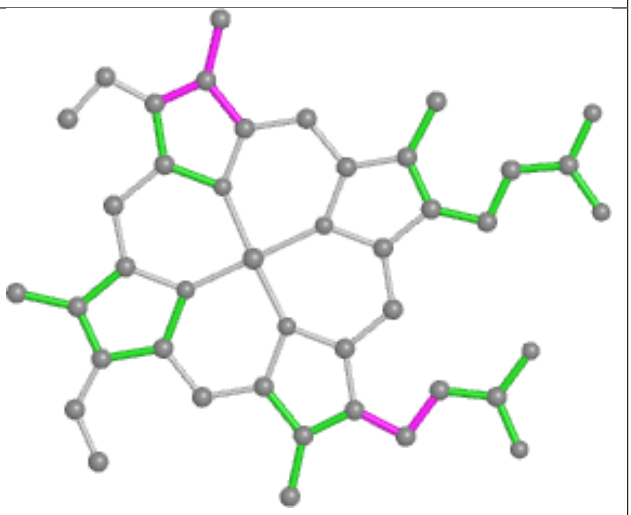
Ligand CLA b 616	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand DGD C 518	
 Bond lengths	 Bond angles
 Torsions	 Rings

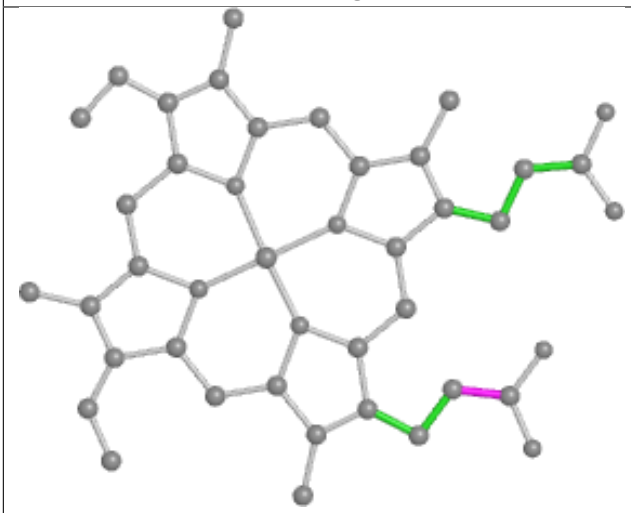
Ligand HEC v 201



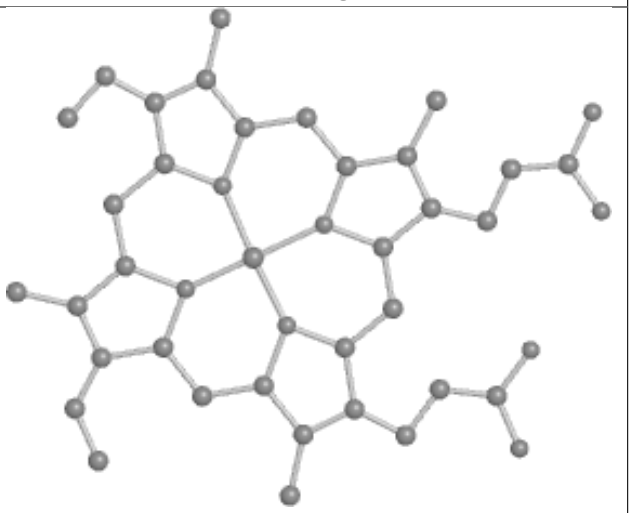
Bond lengths



Bond angles

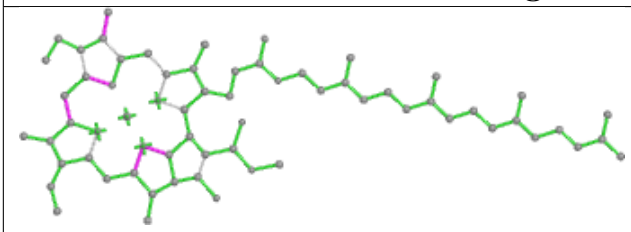


Torsions

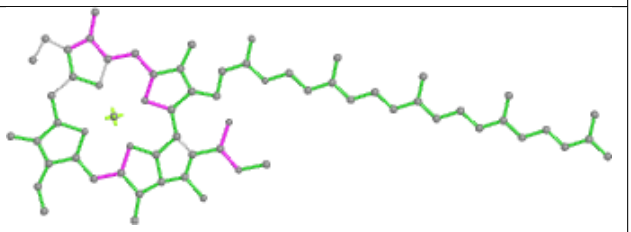


Rings

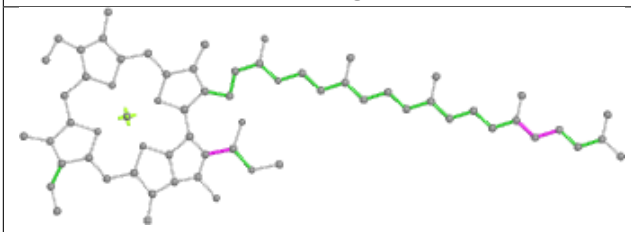
Ligand CLA C 504



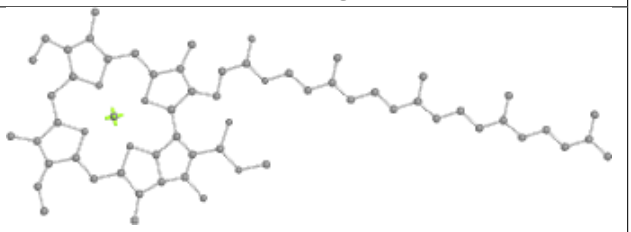
Bond lengths



Bond angles

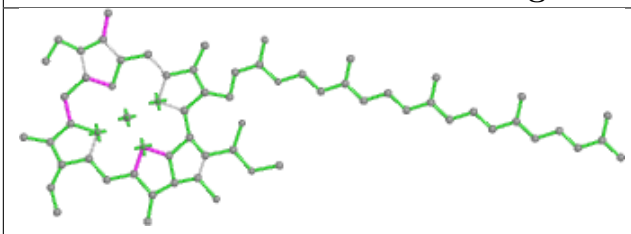


Torsions

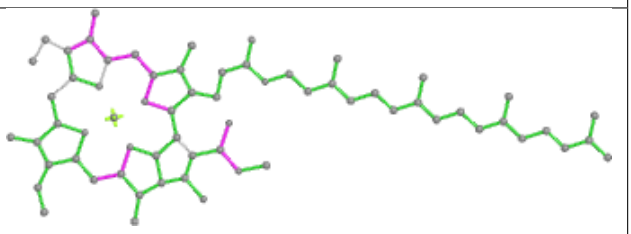


Rings

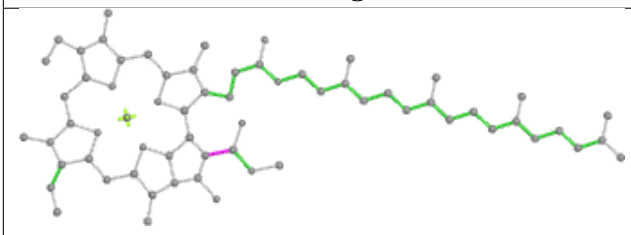
Ligand CLA a 612



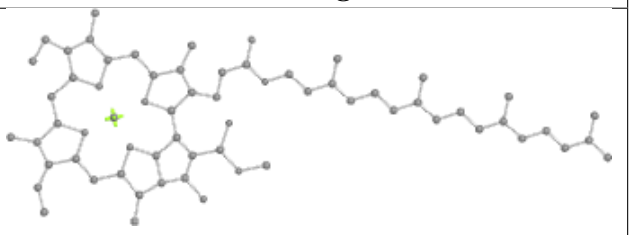
Bond lengths



Bond angles

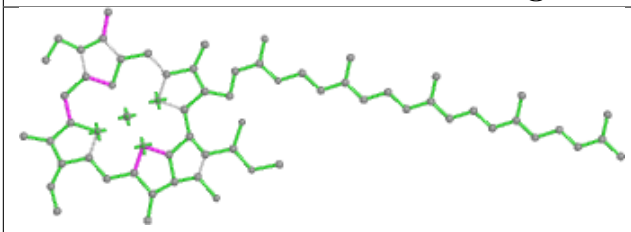


Torsions

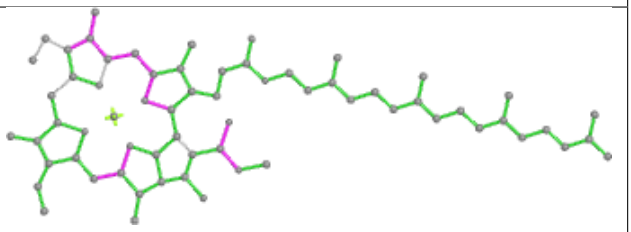


Rings

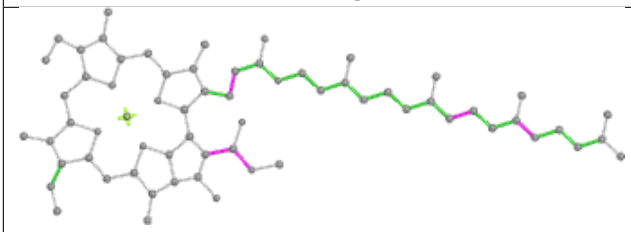
Ligand CLA b 609



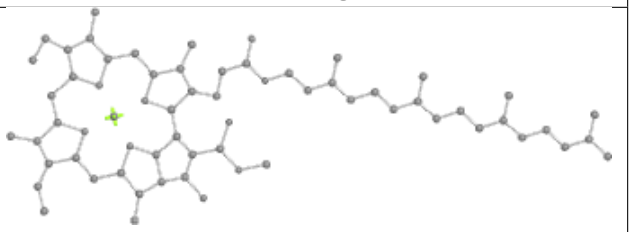
Bond lengths



Bond angles

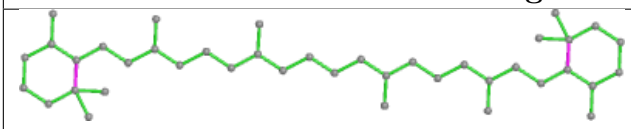


Torsions

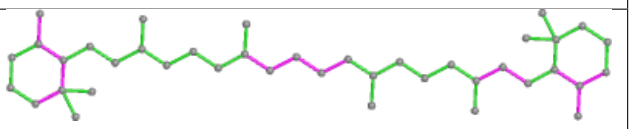


Rings

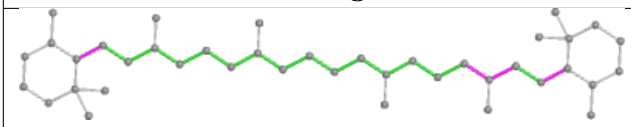
Ligand BCR b 622



Bond lengths



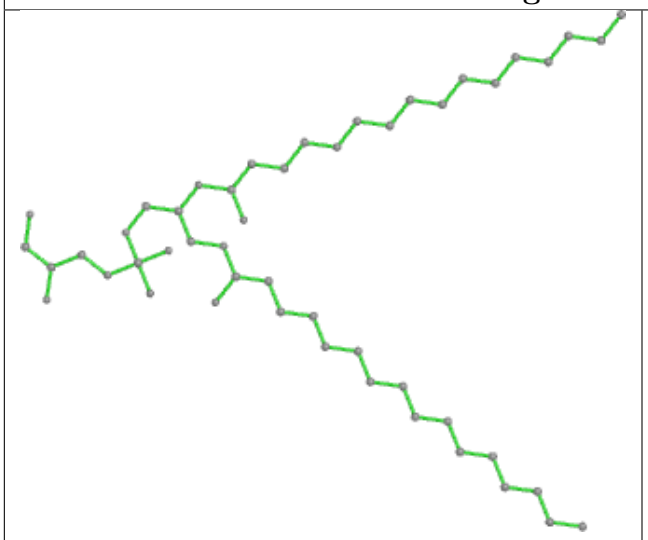
Bond angles



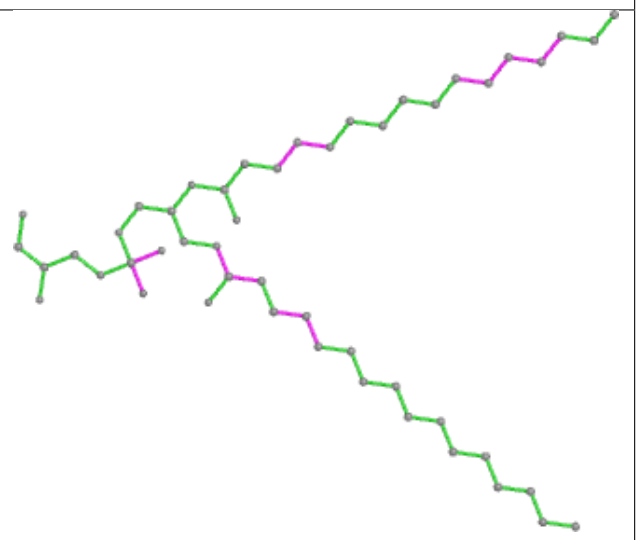
Torsions

Rings

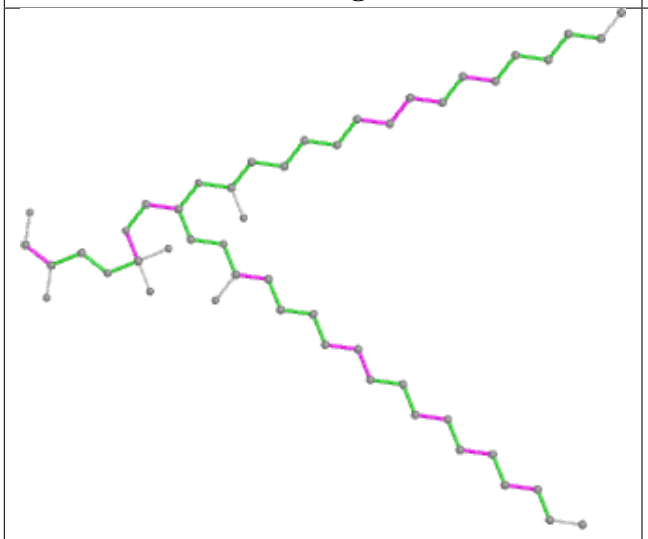
Ligand LHG A 617



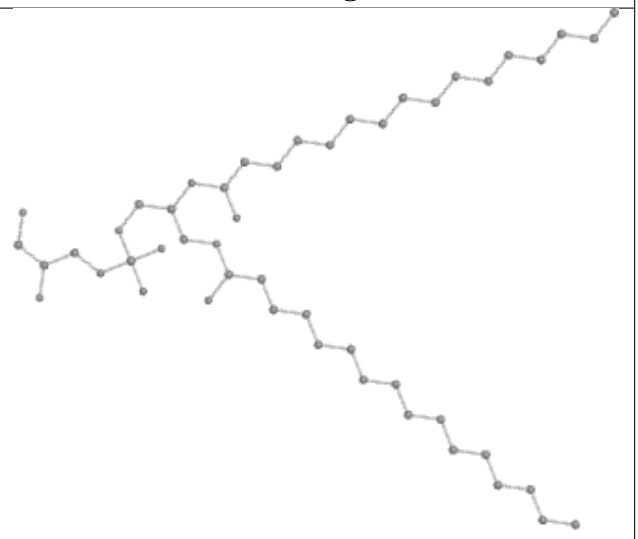
Bond lengths



Bond angles

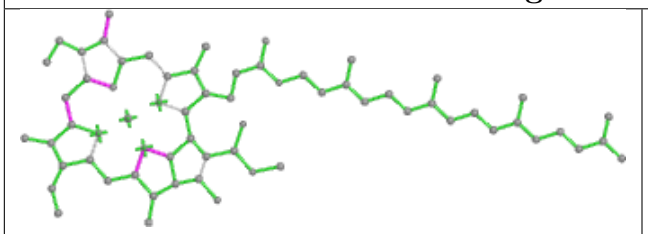


Torsions

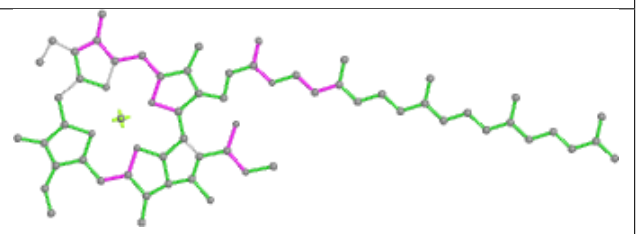


Rings

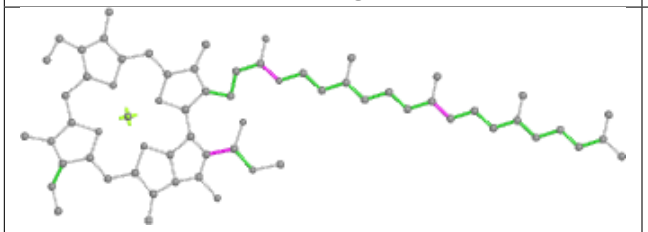
Ligand CLA C 508



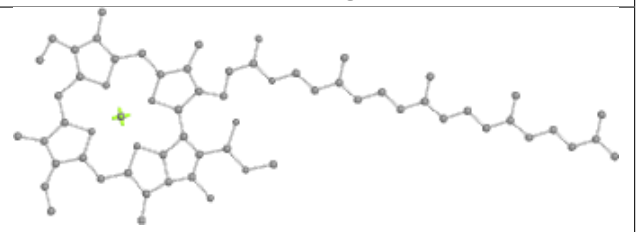
Bond lengths



Bond angles

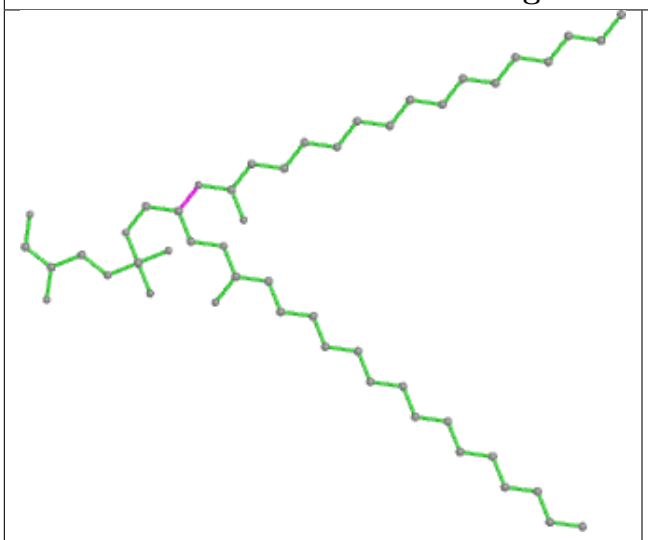


Torsions

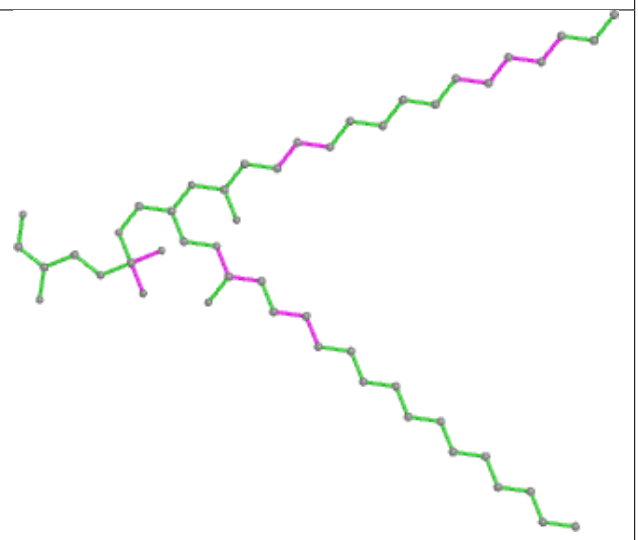


Rings

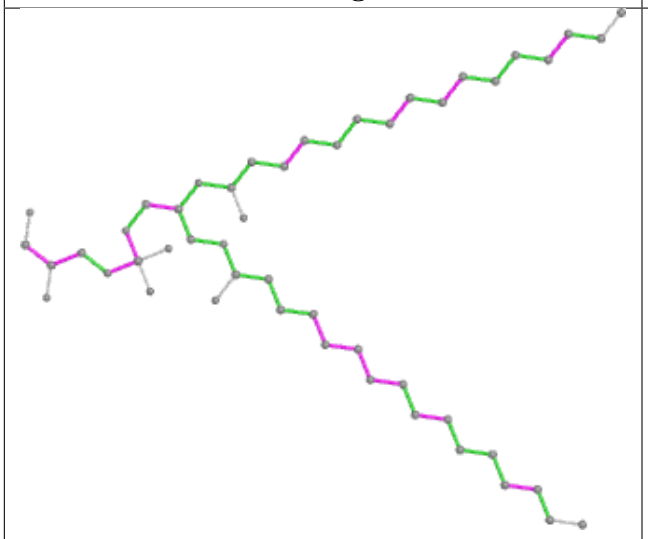
Ligand LHG D 406



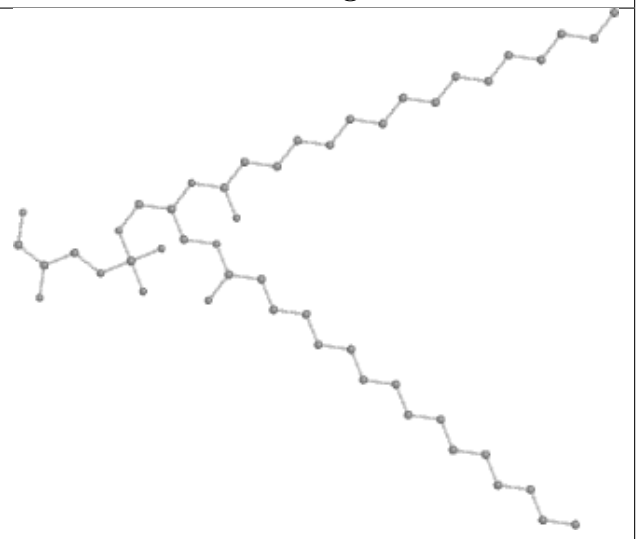
Bond lengths



Bond angles

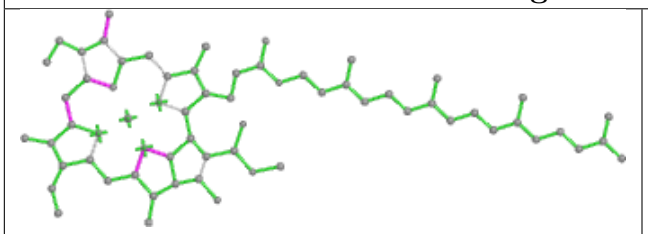


Torsions

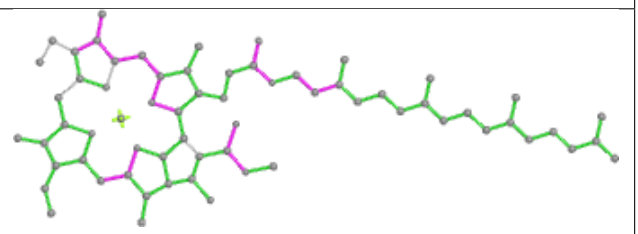


Rings

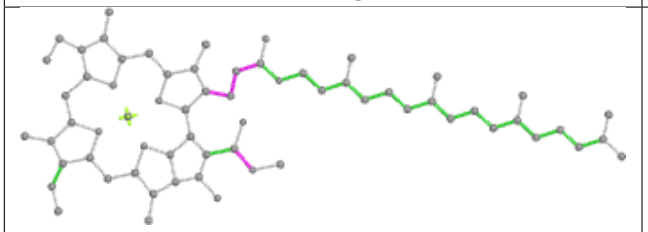
Ligand CLA c 503



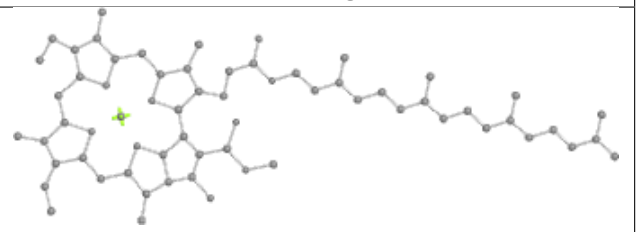
Bond lengths



Bond angles

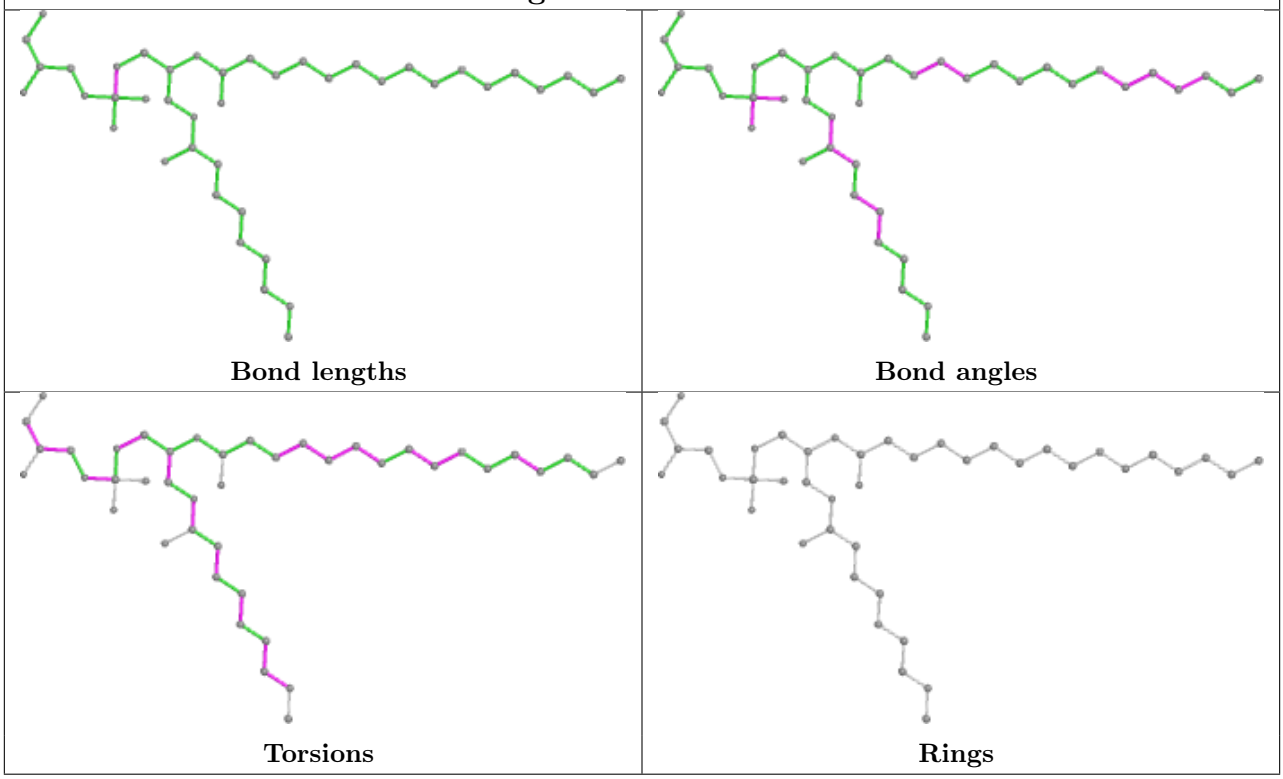


Torsions

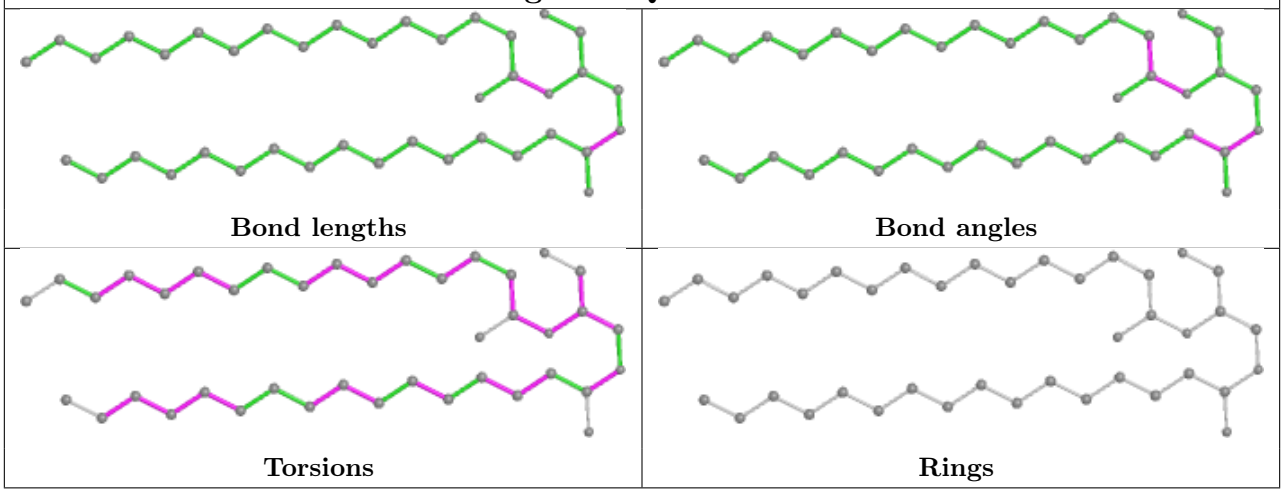


Rings

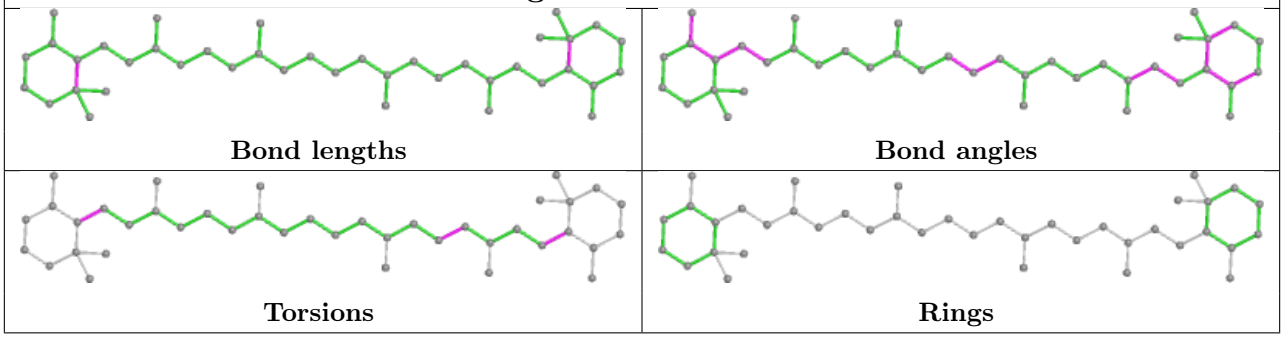
Ligand LHG a 615



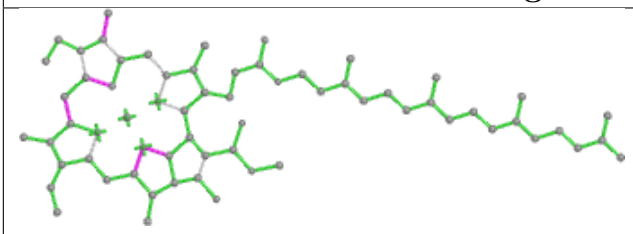
Ligand SQD A 619



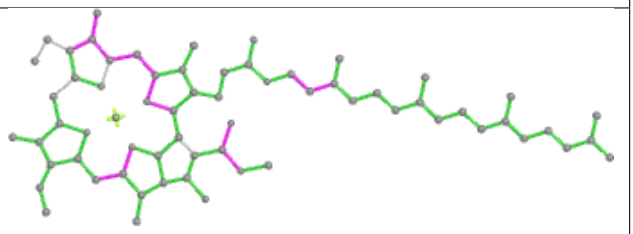
Ligand BCR k 101



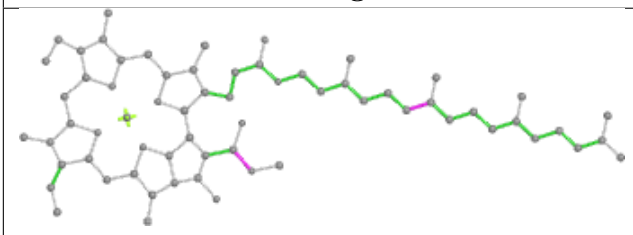
Ligand CLA C 511



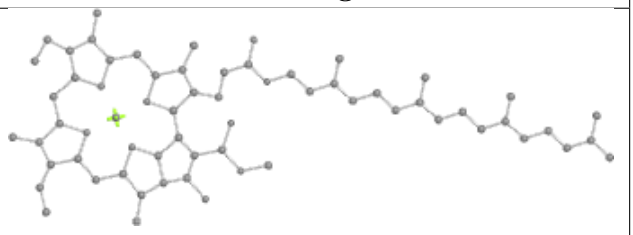
Bond lengths



Bond angles

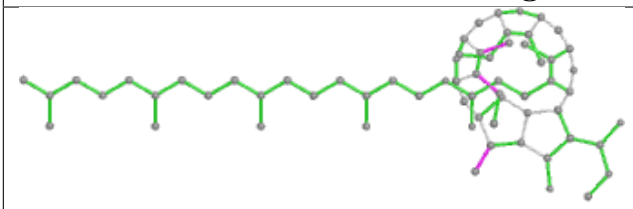


Torsions

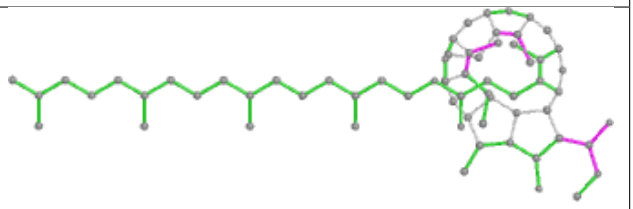


Rings

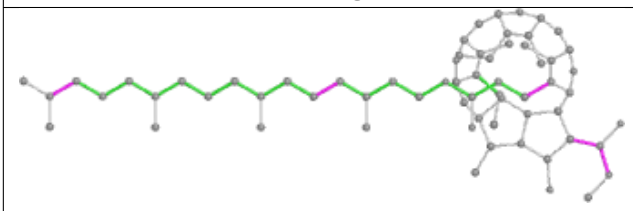
Ligand PHO D 401



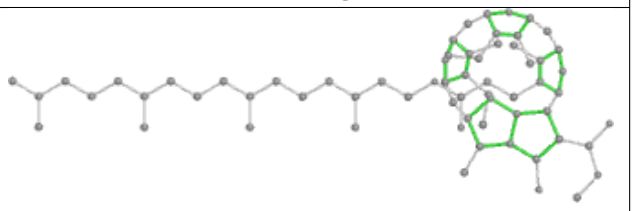
Bond lengths



Bond angles

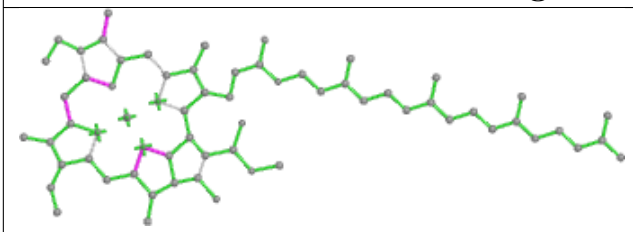


Torsions

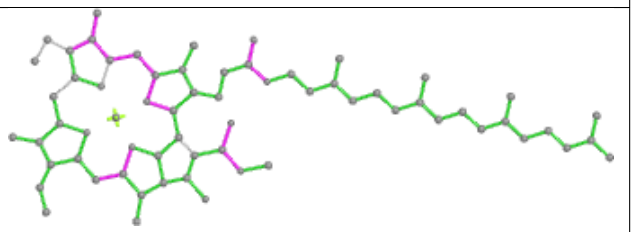


Rings

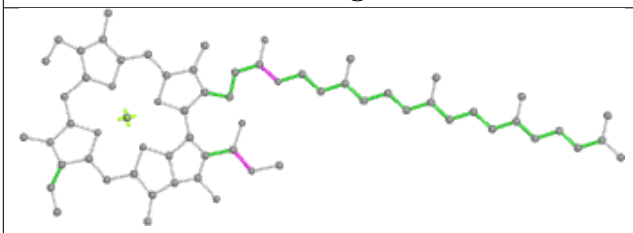
Ligand CLA c 513



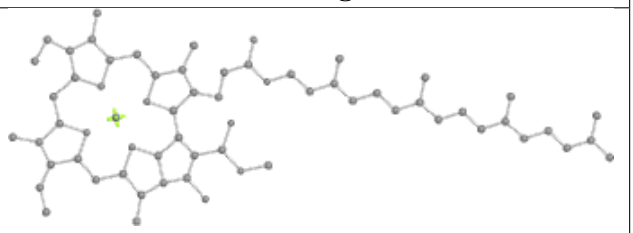
Bond lengths



Bond angles

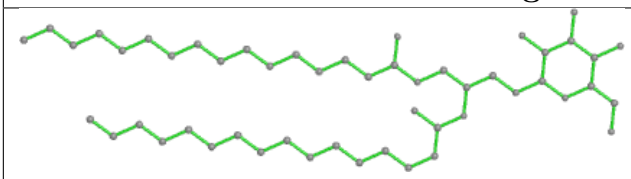


Torsions

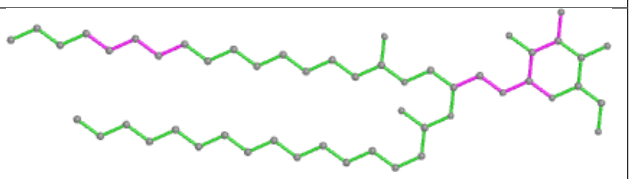


Rings

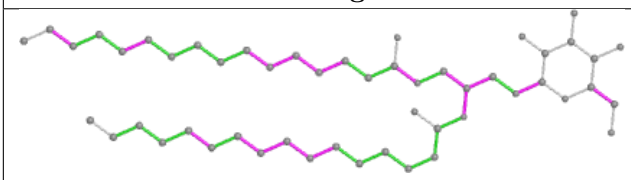
Ligand LMG b 624



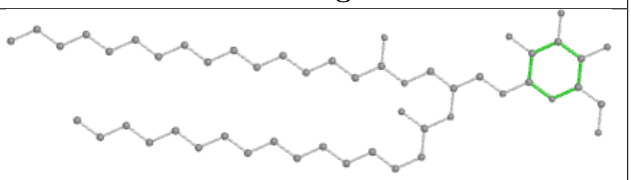
Bond lengths



Bond angles

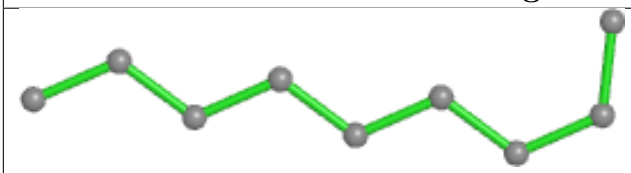


Torsions

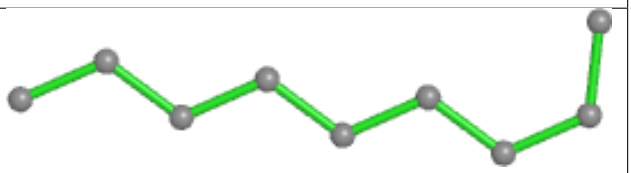


Rings

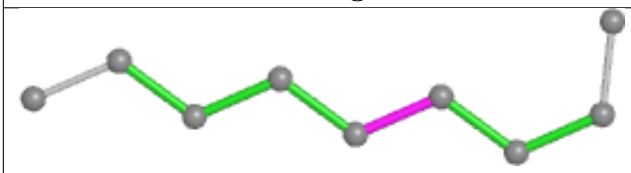
Ligand LMG b 625



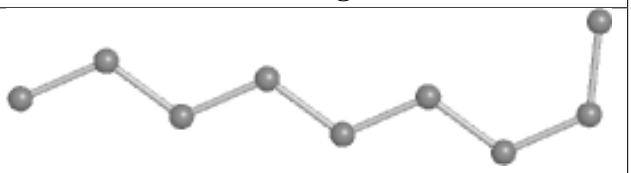
Bond lengths



Bond angles

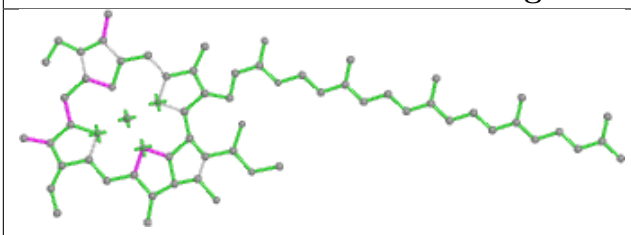


Torsions

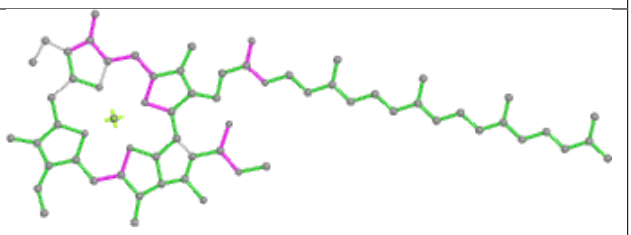


Rings

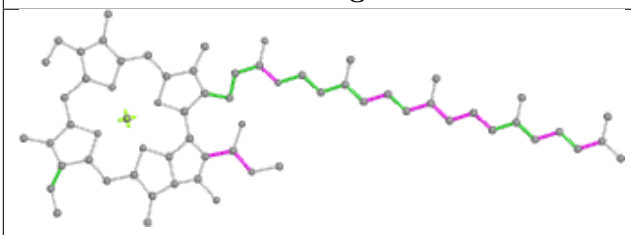
Ligand CLA B 616



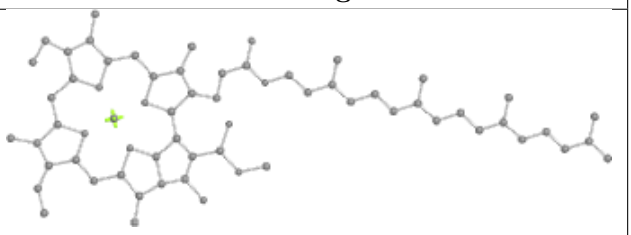
Bond lengths



Bond angles

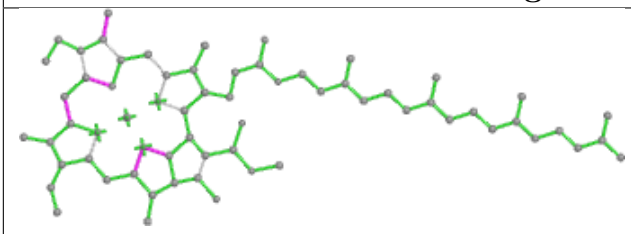


Torsions

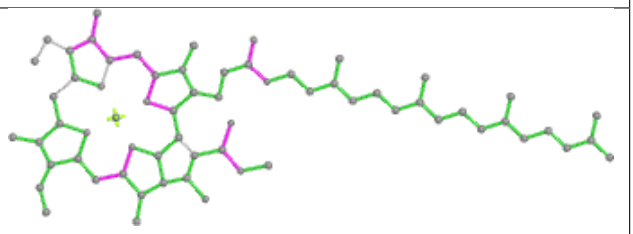


Rings

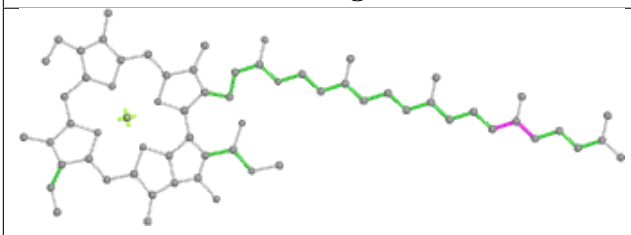
Ligand CLA B 615



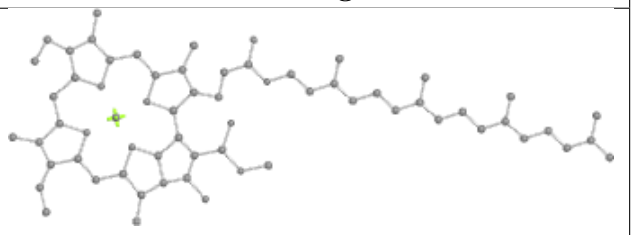
Bond lengths



Bond angles

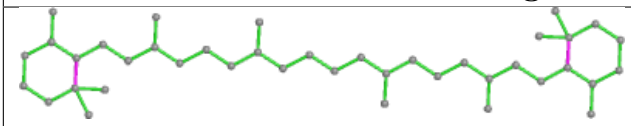


Torsions

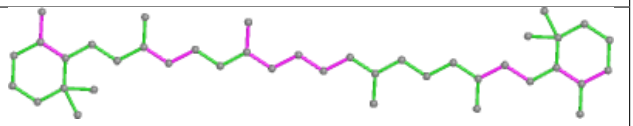


Rings

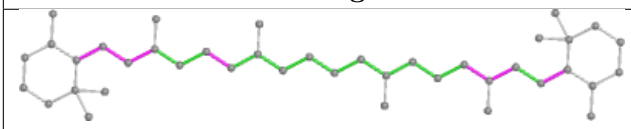
Ligand BCR B 627



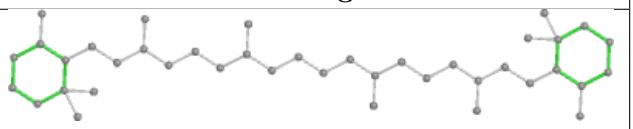
Bond lengths



Bond angles

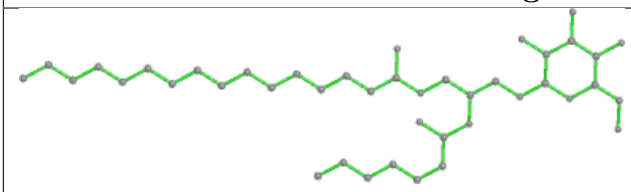


Torsions

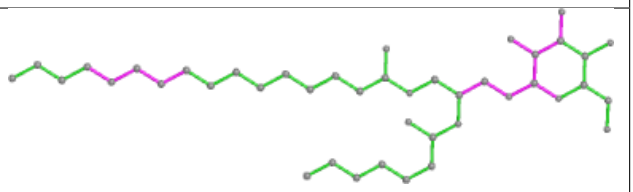


Rings

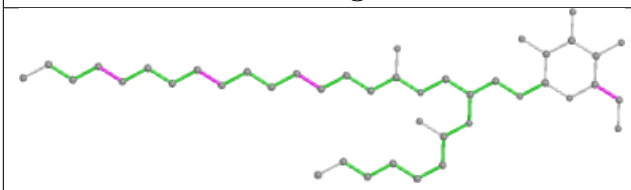
Ligand LMG d 406



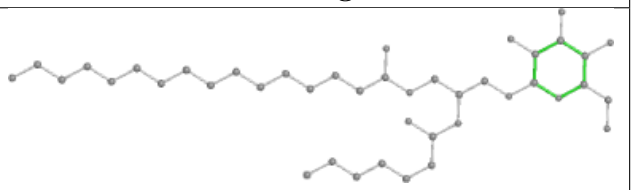
Bond lengths



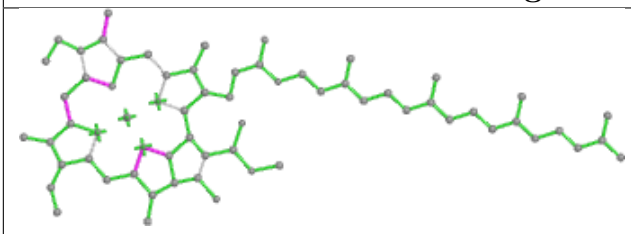
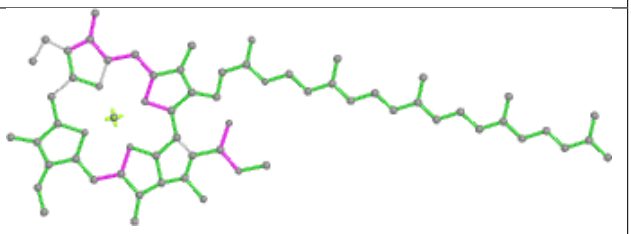
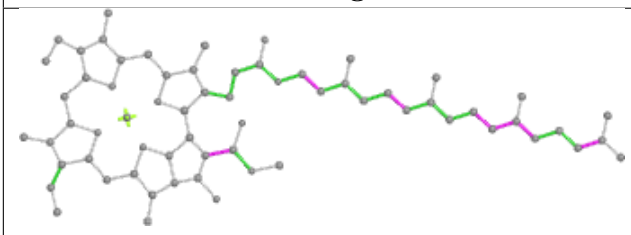
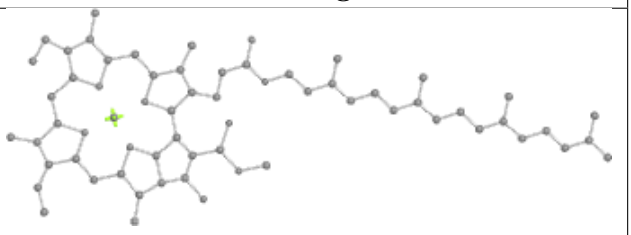
Bond angles

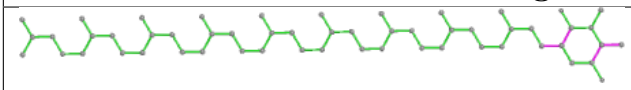
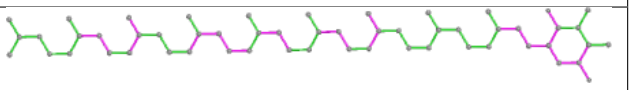
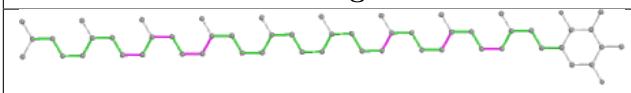
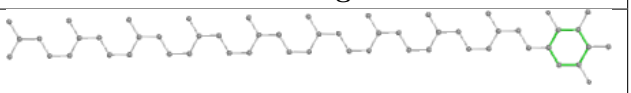


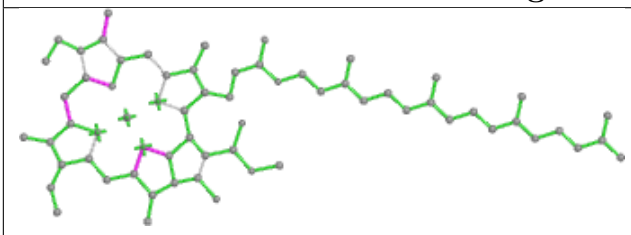
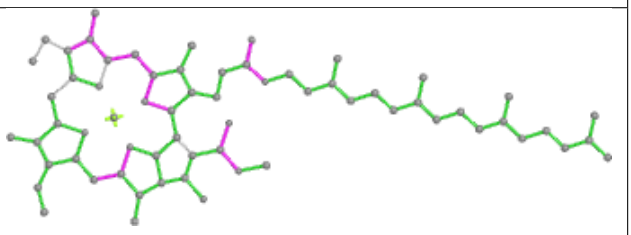
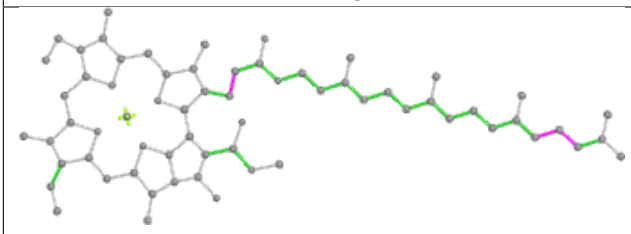
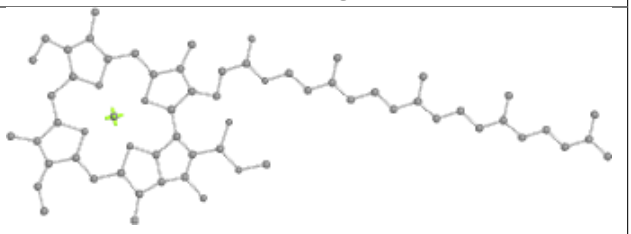
Torsions

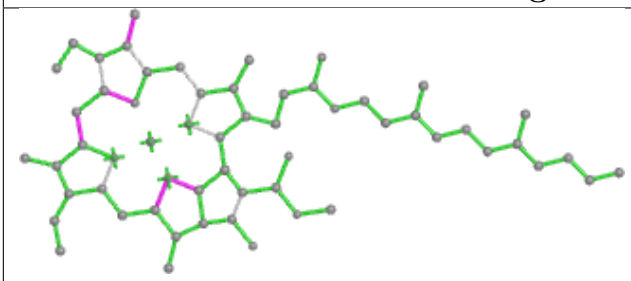
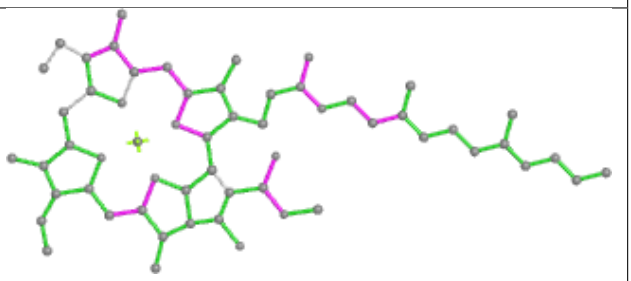
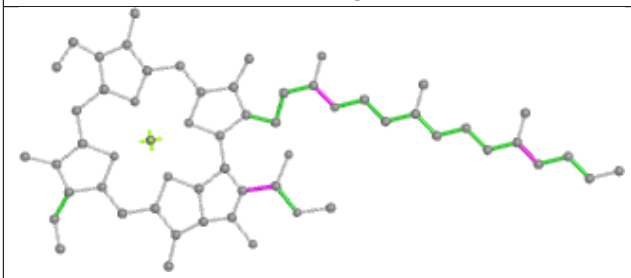
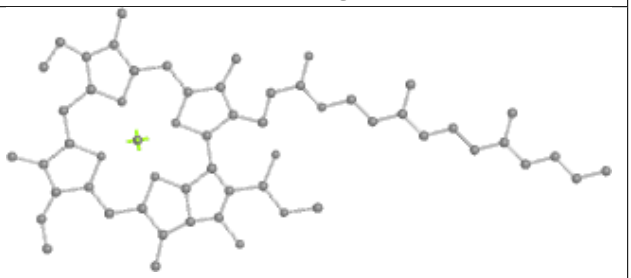


Rings

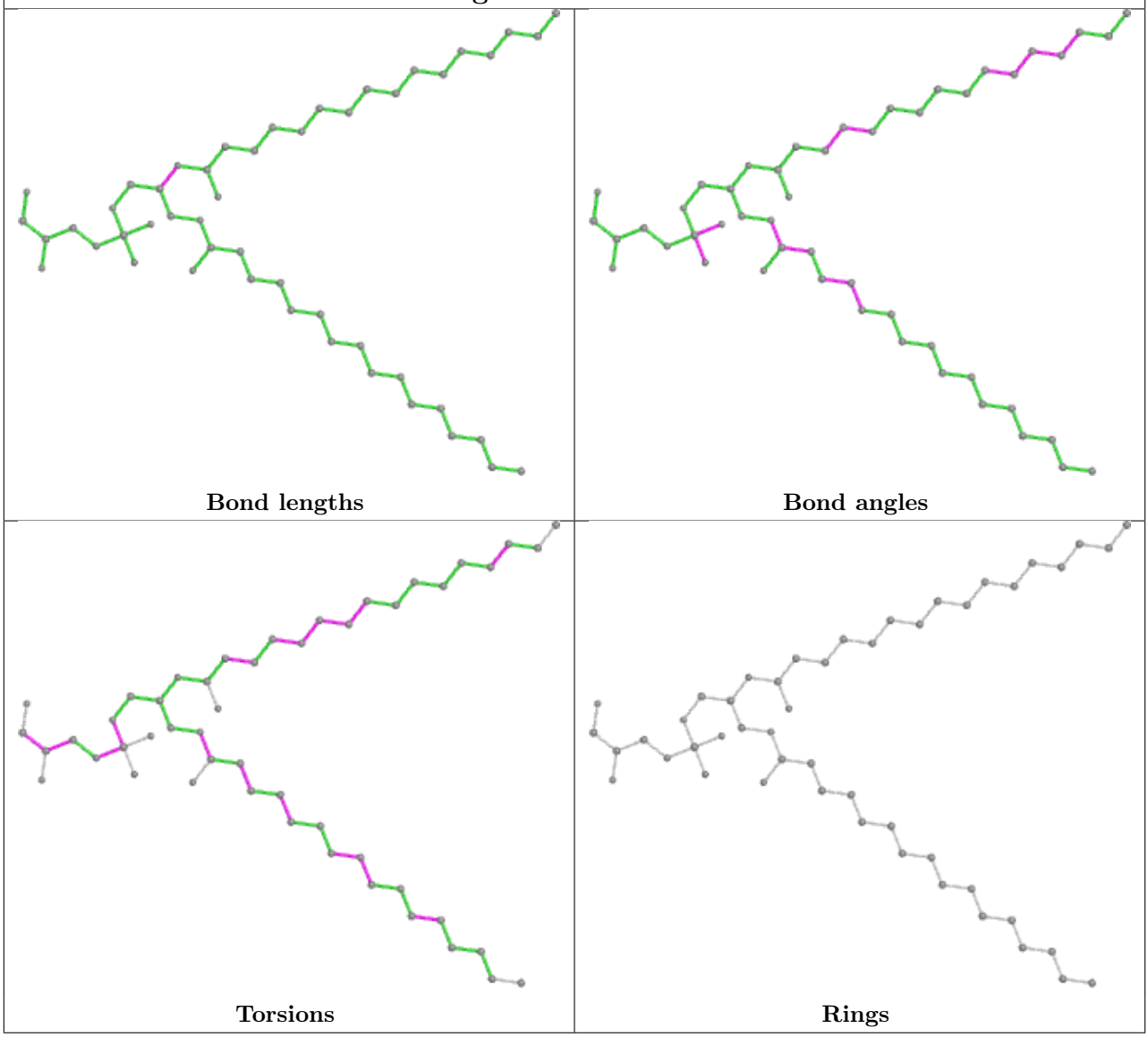
Ligand CLA C 509	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PL9 d 408	
 Bond lengths	 Bond angles
 Torsions	 Rings

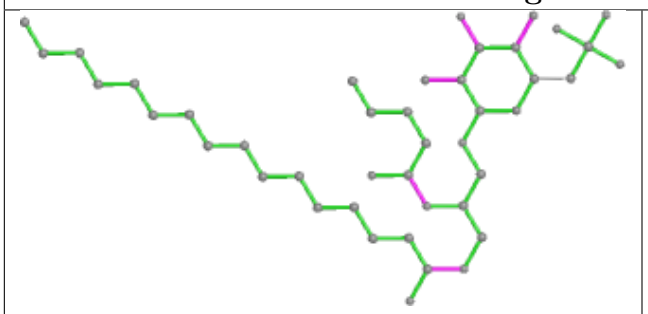
Ligand CLA b 611	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA c 510	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

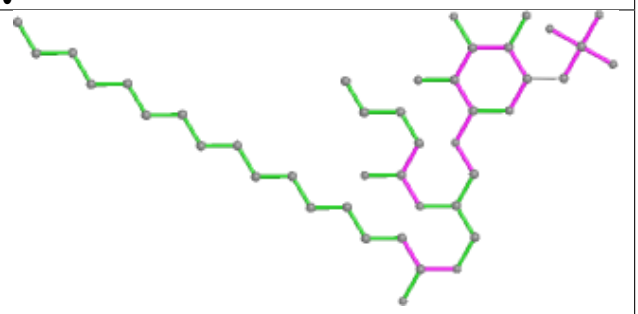
Ligand LHG a 613



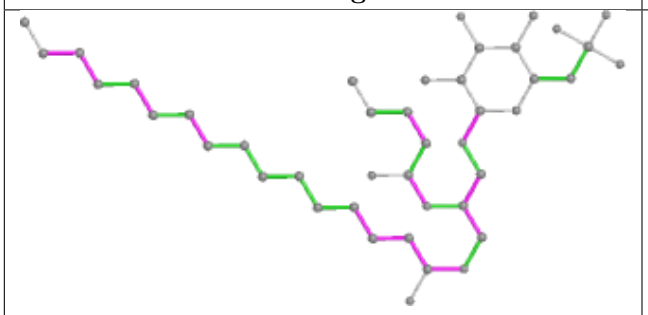
Ligand SQD D 409



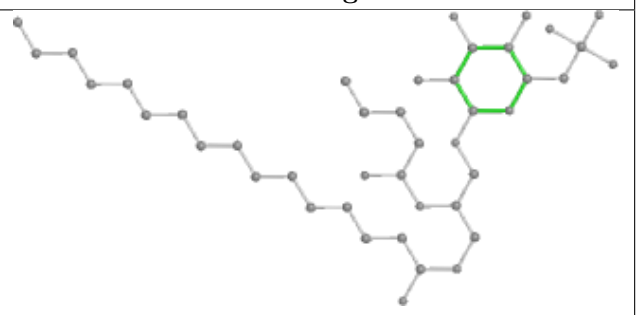
Bond lengths



Bond angles

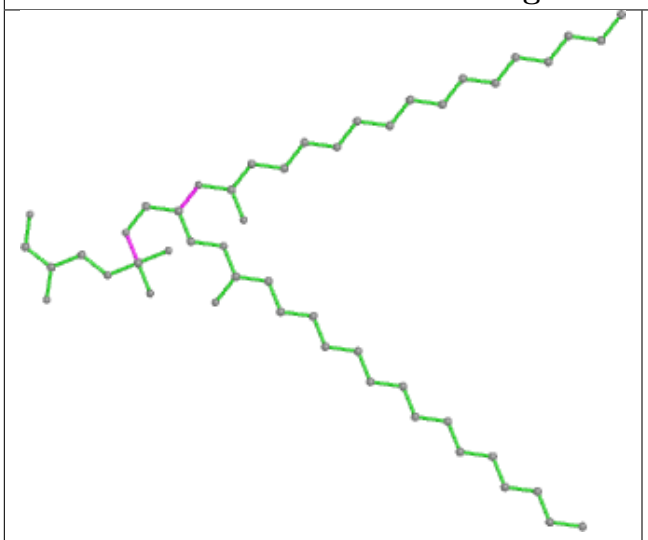


Torsions

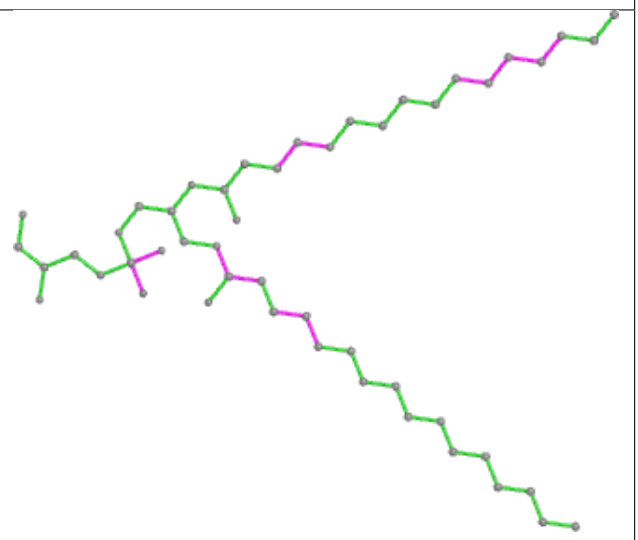


Rings

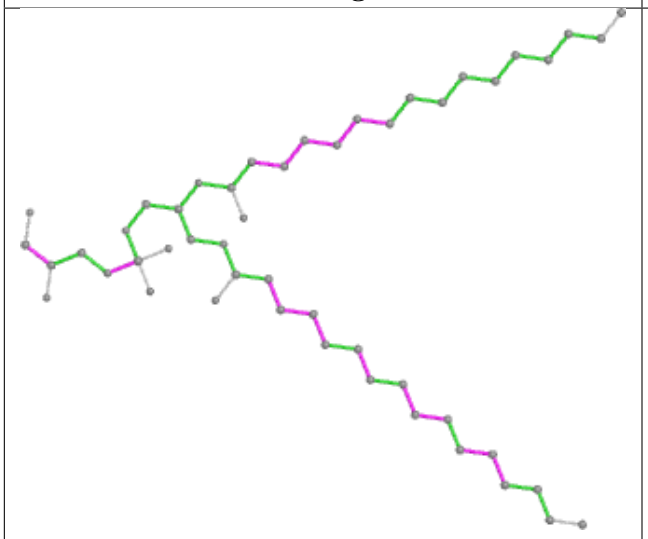
Ligand LHG A 616



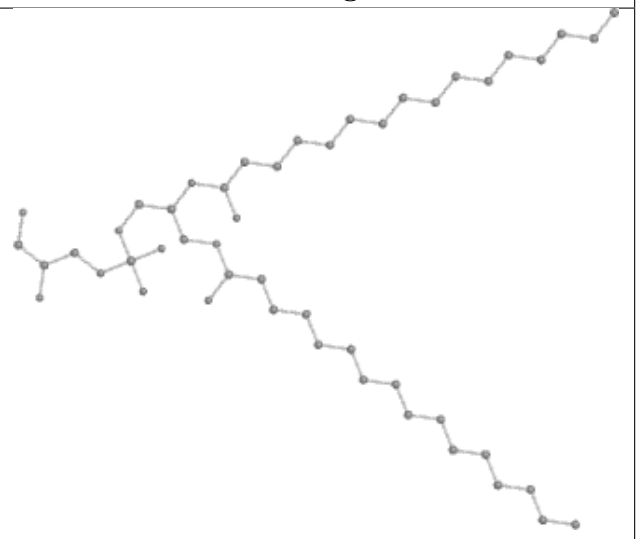
Bond lengths



Bond angles

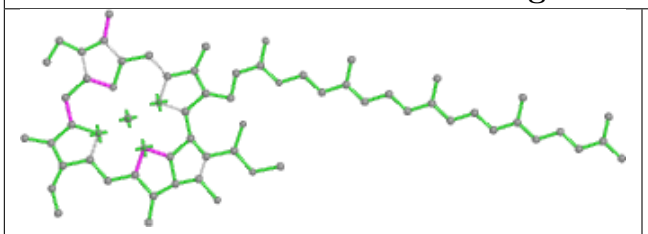


Torsions

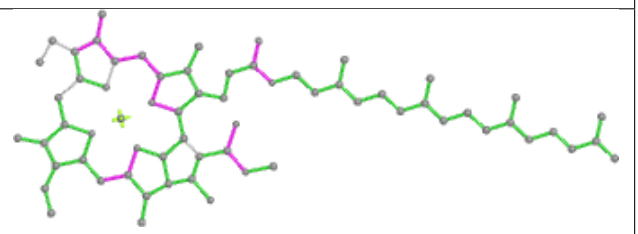


Rings

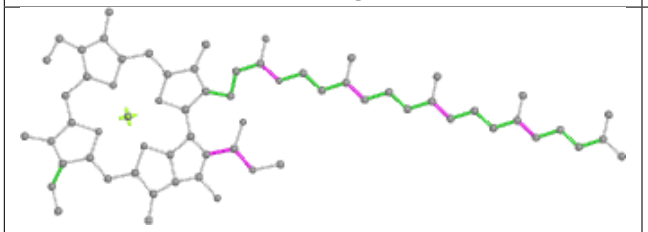
Ligand CLA b 612



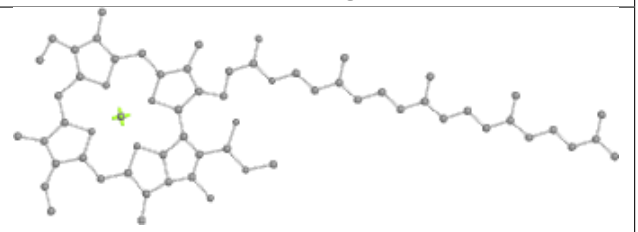
Bond lengths



Bond angles

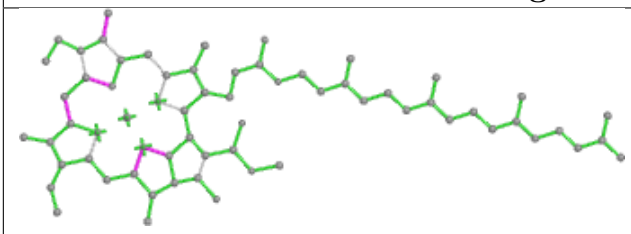


Torsions

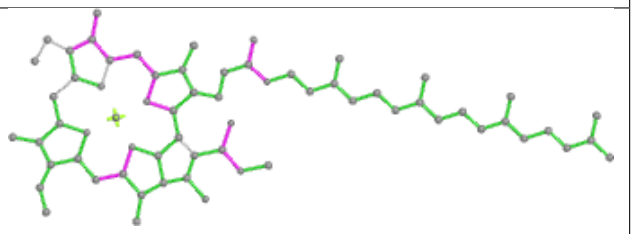


Rings

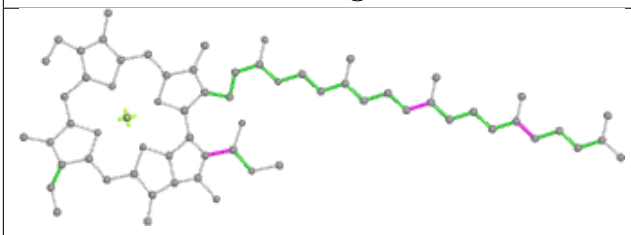
Ligand CLA c 504



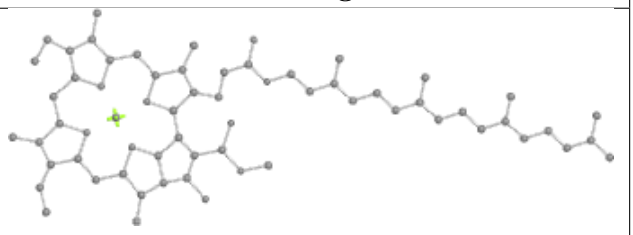
Bond lengths



Bond angles

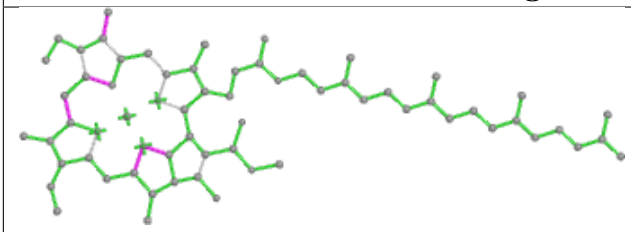


Torsions

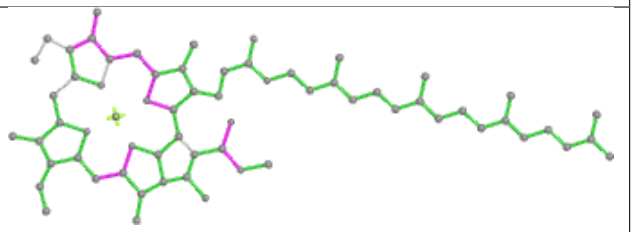


Rings

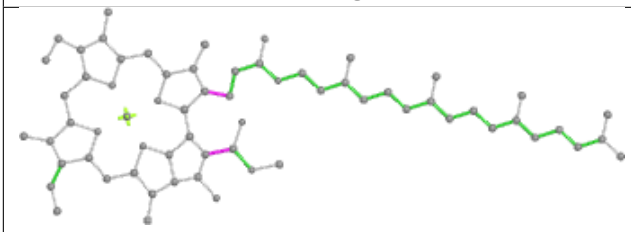
Ligand CLA A 615



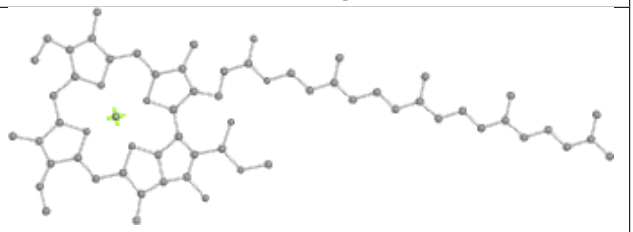
Bond lengths



Bond angles

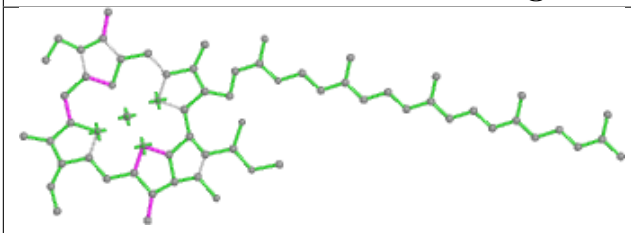


Torsions

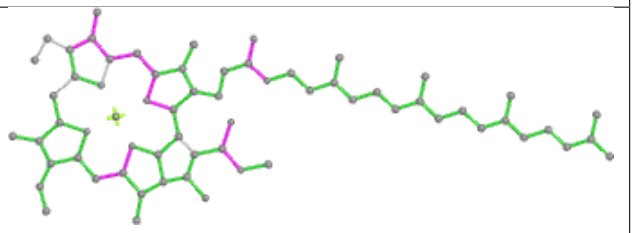


Rings

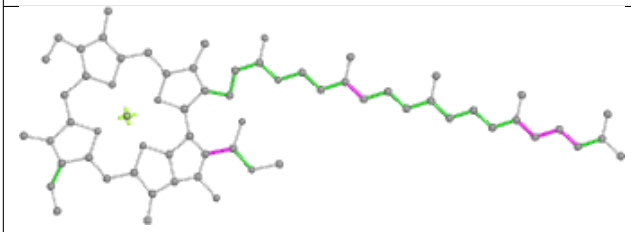
Ligand CLA b 608



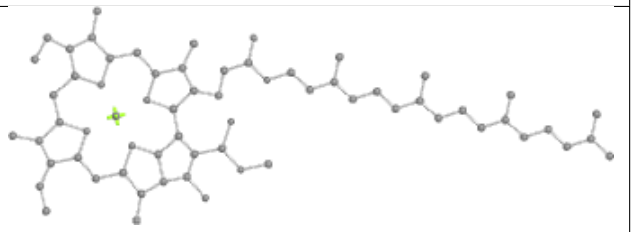
Bond lengths



Bond angles

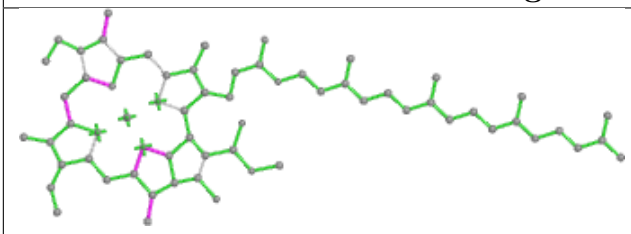


Torsions

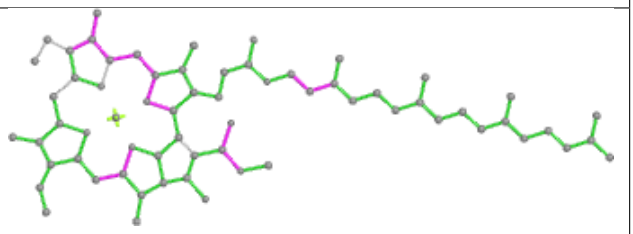


Rings

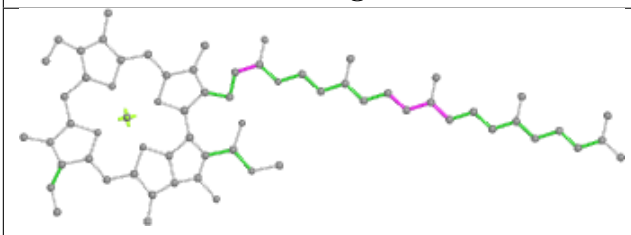
Ligand CLA C 510



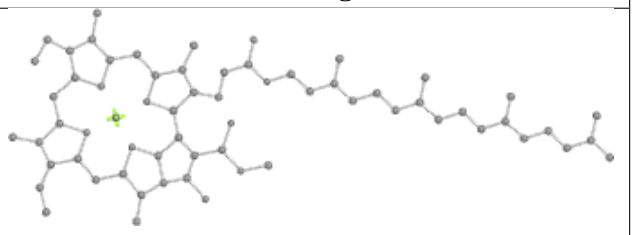
Bond lengths



Bond angles

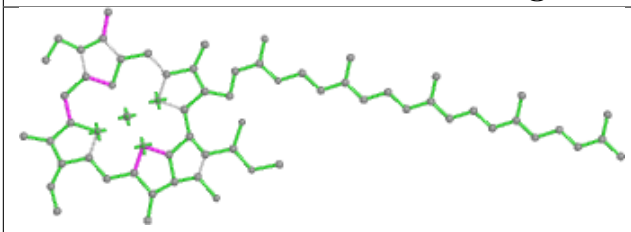


Torsions

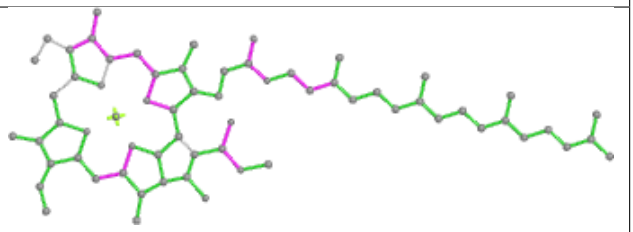


Rings

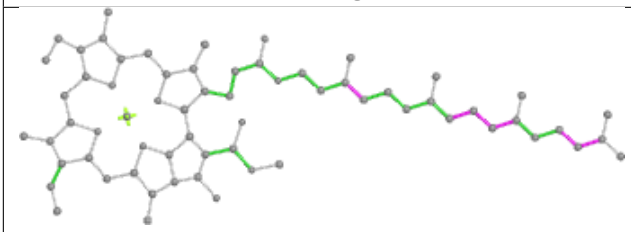
Ligand CLA a 609



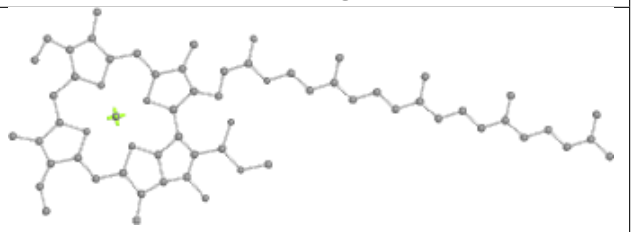
Bond lengths



Bond angles

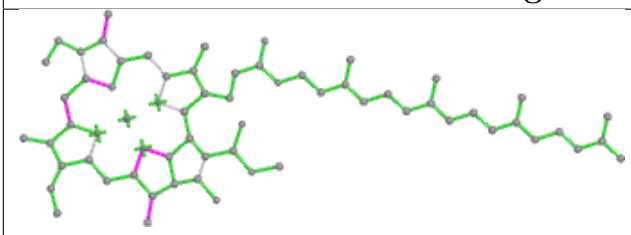


Torsions

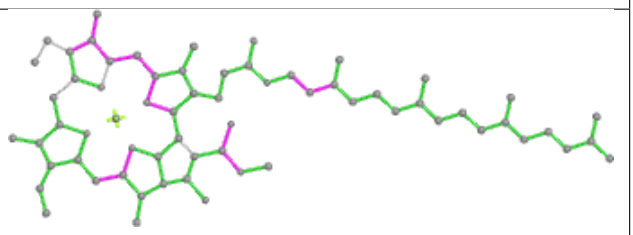


Rings

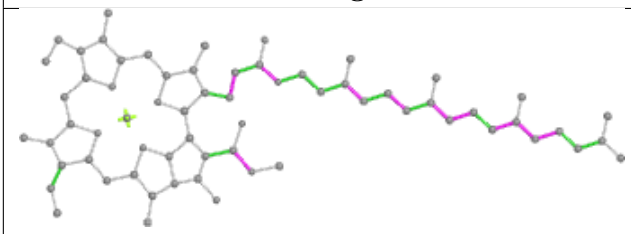
Ligand CLA C 505



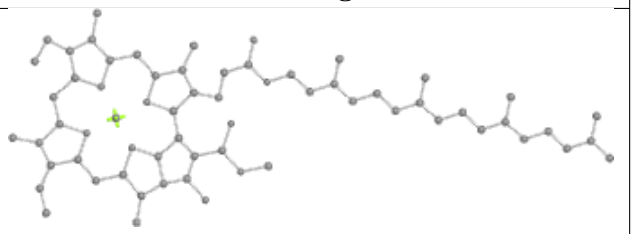
Bond lengths



Bond angles

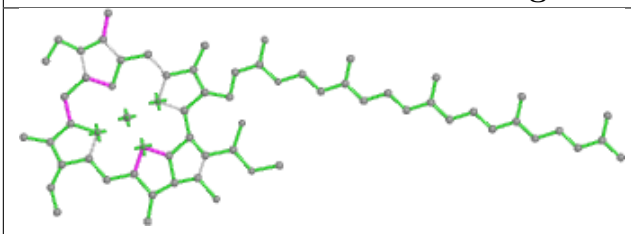


Torsions

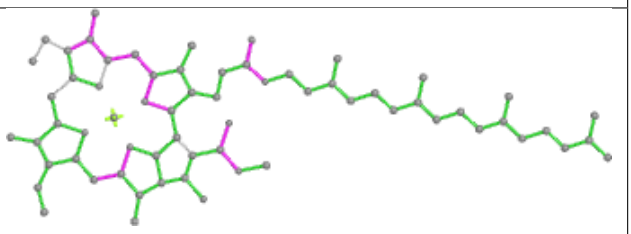


Rings

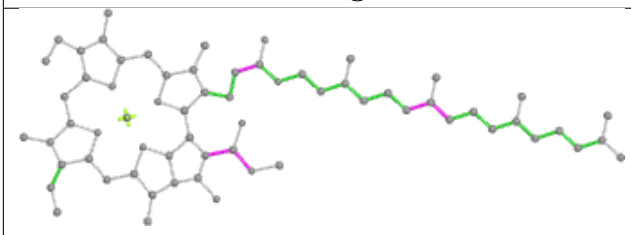
Ligand CLA c 512



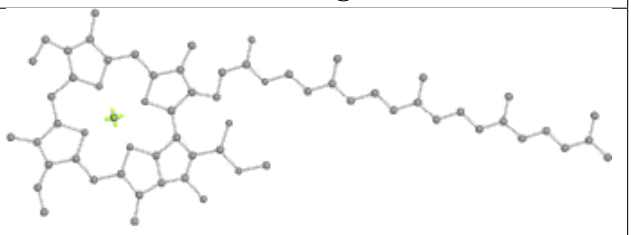
Bond lengths



Bond angles

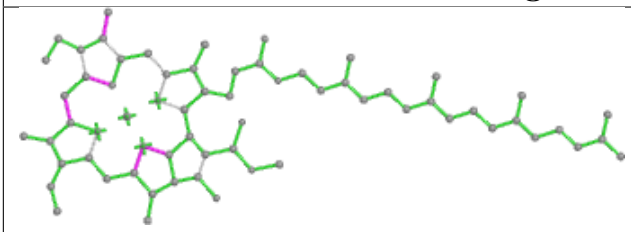


Torsions

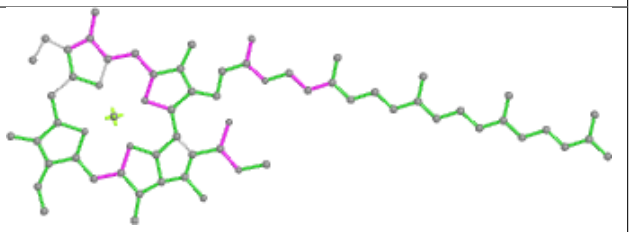


Rings

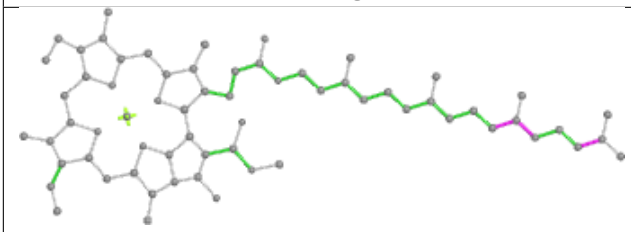
Ligand CLA B 611



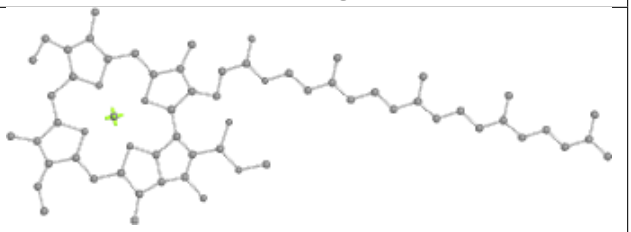
Bond lengths



Bond angles

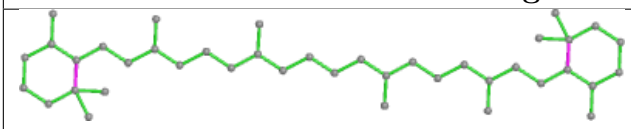


Torsions

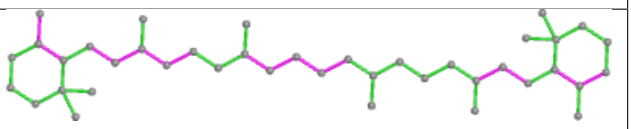


Rings

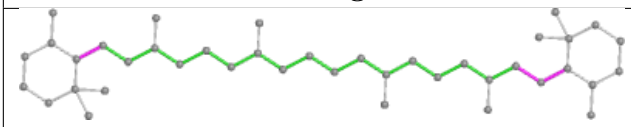
Ligand BCR B 617



Bond lengths



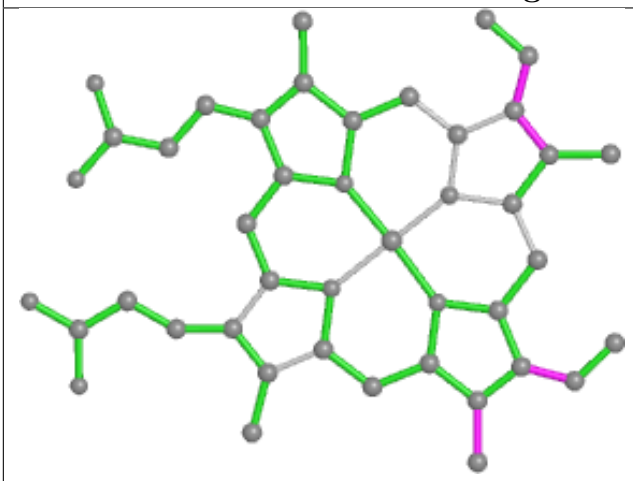
Bond angles



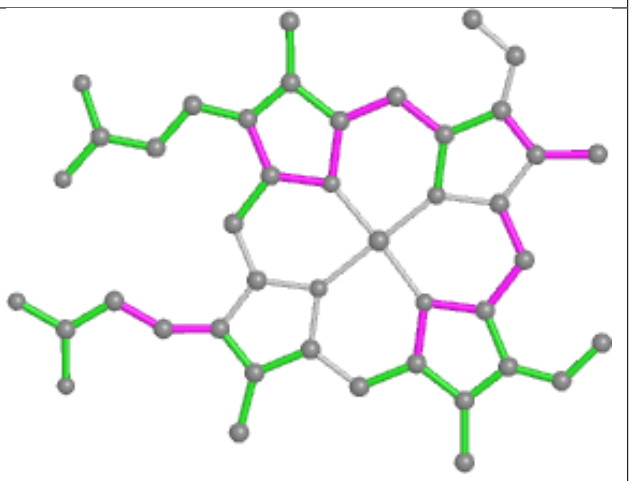
Torsions

Rings

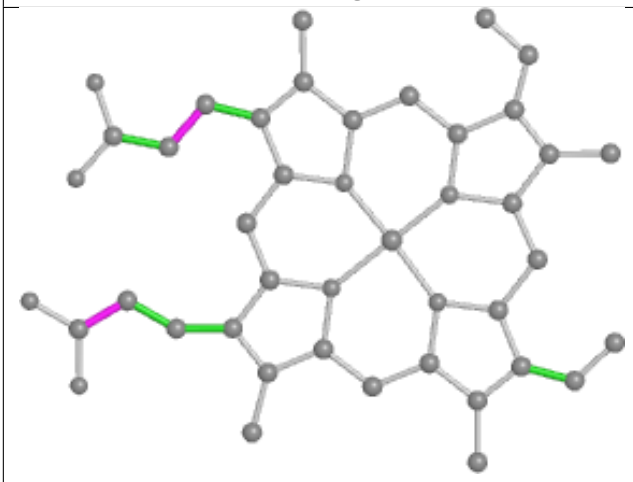
Ligand HEM e 101



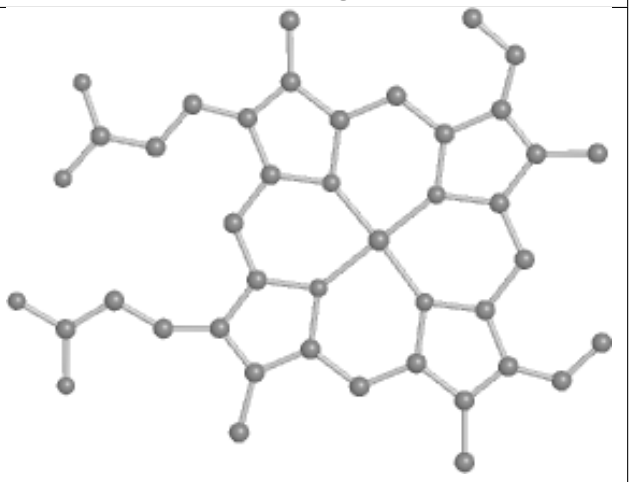
Bond lengths



Bond angles

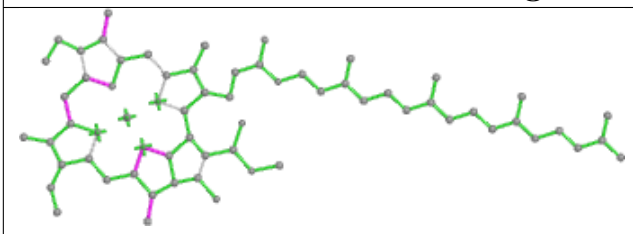


Torsions

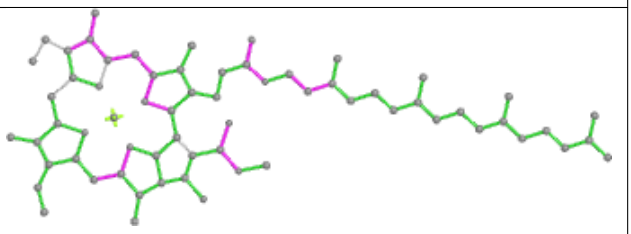


Rings

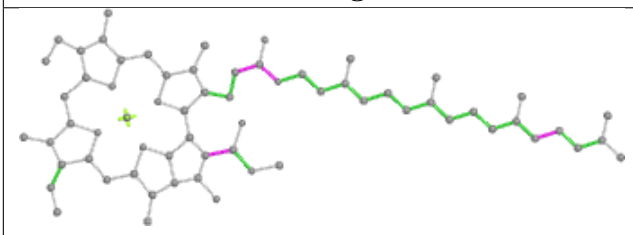
Ligand CLA B 612



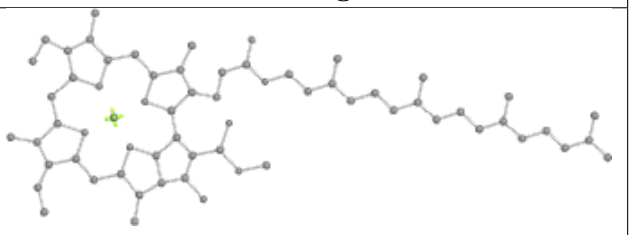
Bond lengths



Bond angles

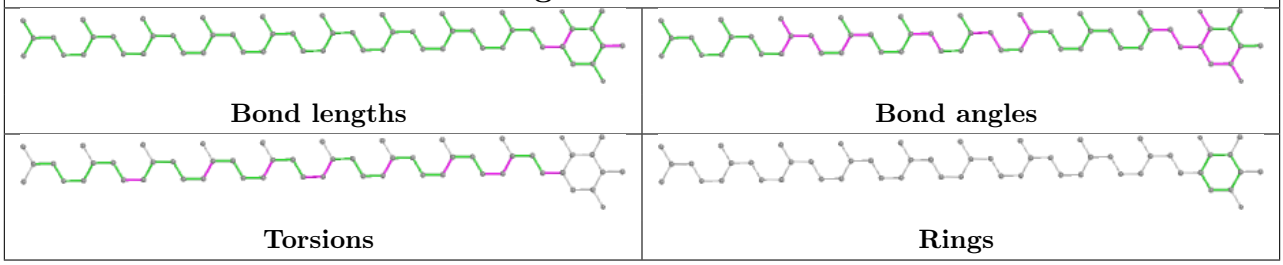


Torsions

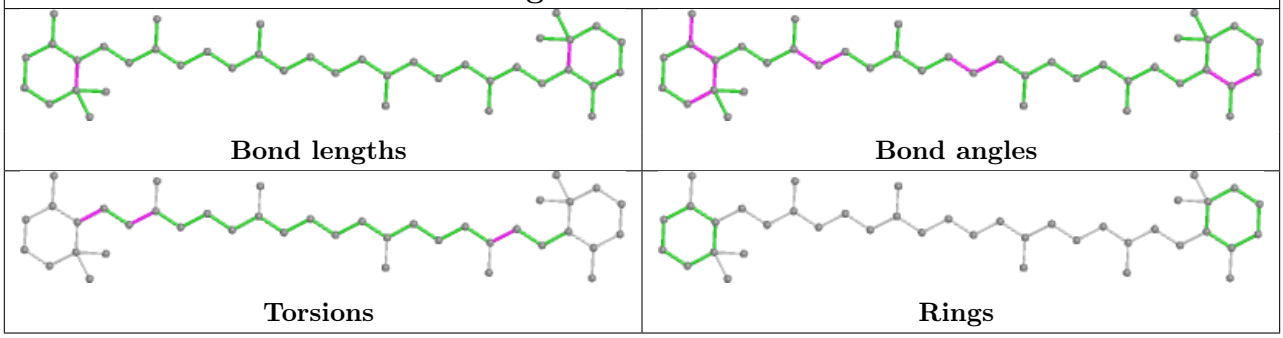


Rings

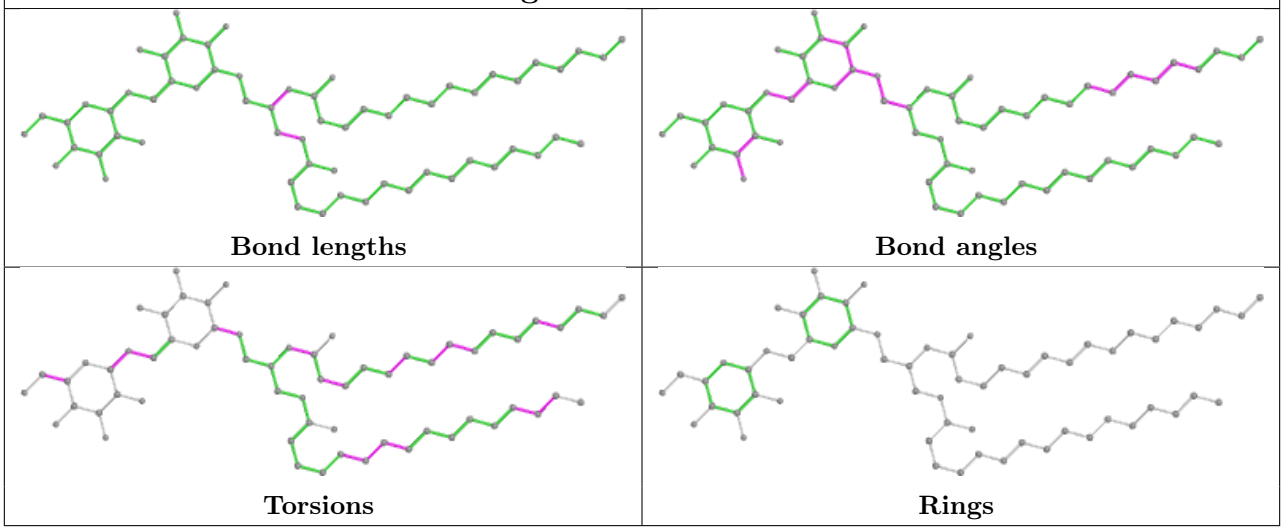
Ligand PL9 a 611



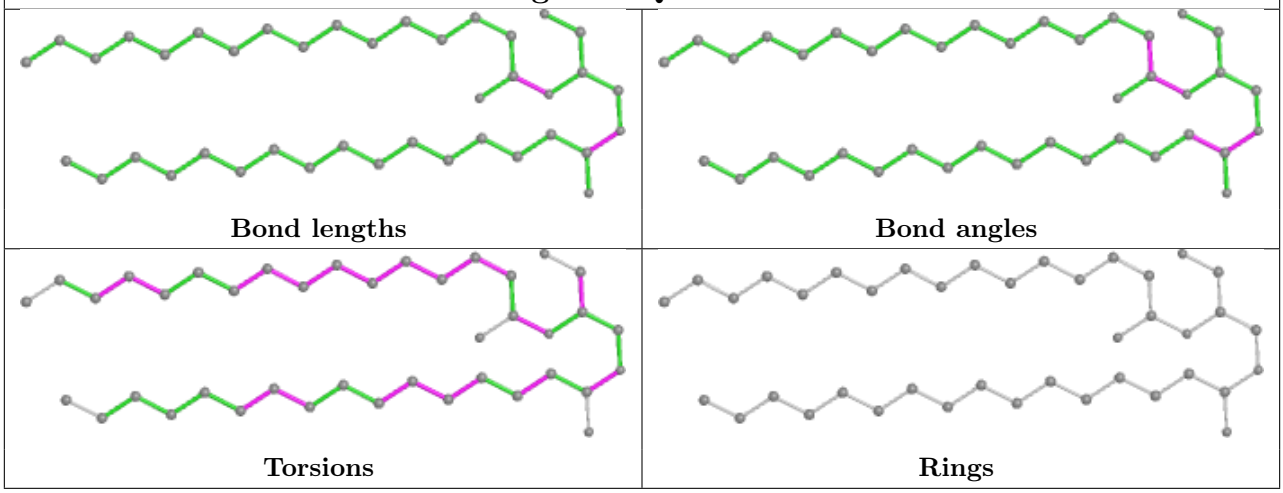
Ligand BCR d 405



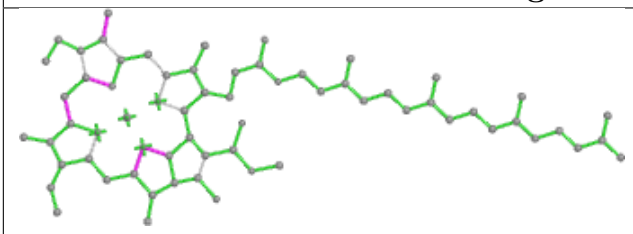
Ligand DGD C 517



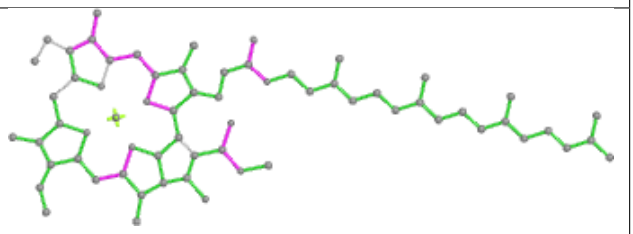
Ligand SQD I 101



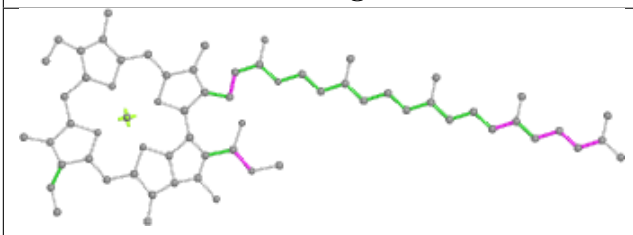
Ligand CLA b 613



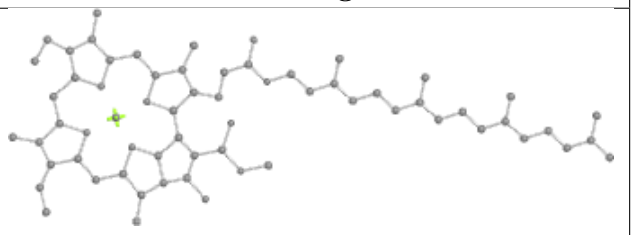
Bond lengths



Bond angles

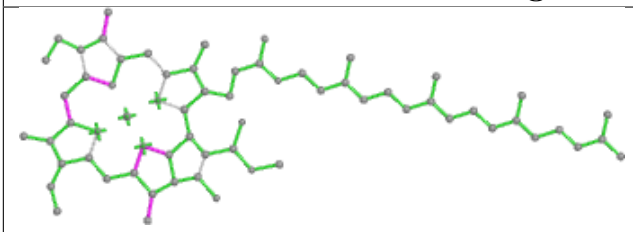


Torsions

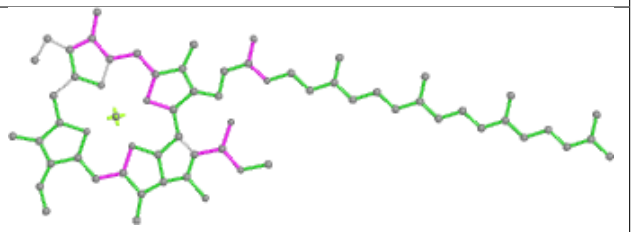


Rings

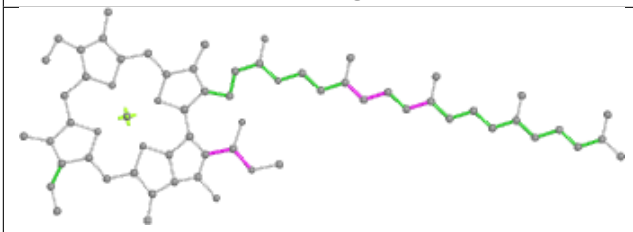
Ligand CLA b 607



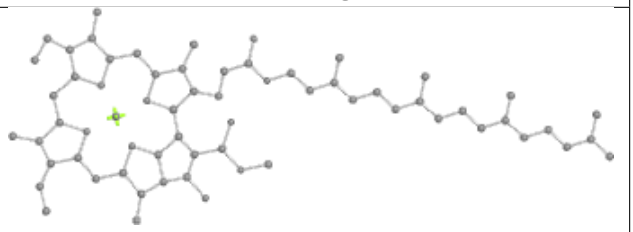
Bond lengths



Bond angles

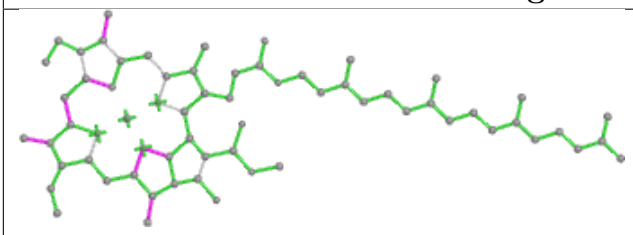


Torsions

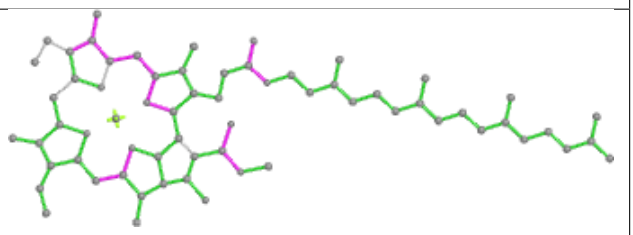


Rings

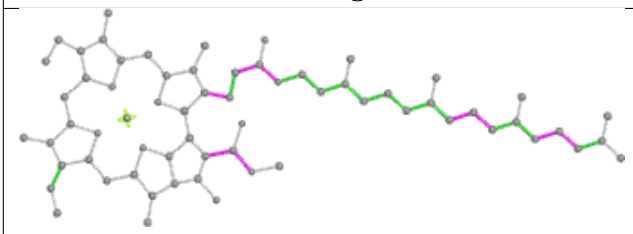
Ligand CLA b 615



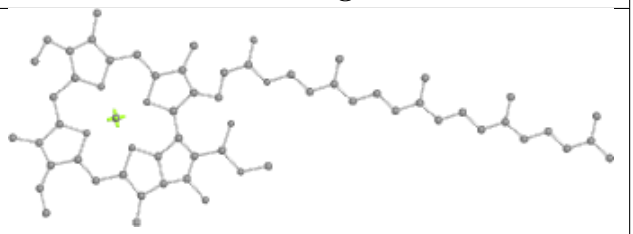
Bond lengths



Bond angles

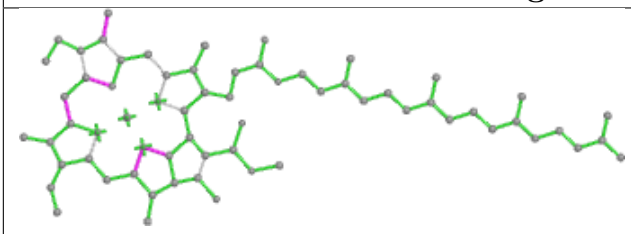


Torsions

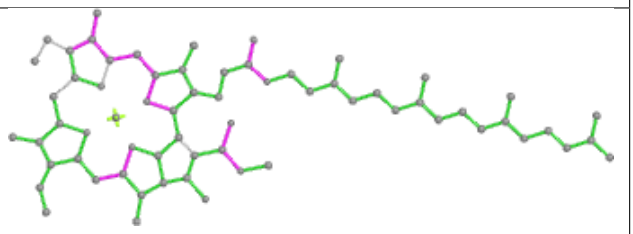


Rings

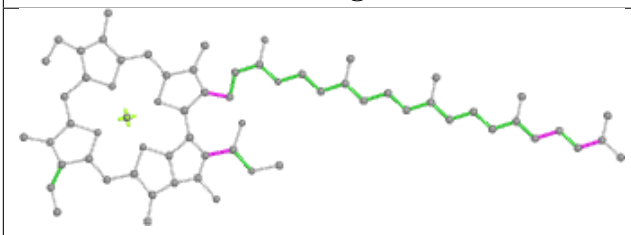
Ligand CLA d 404



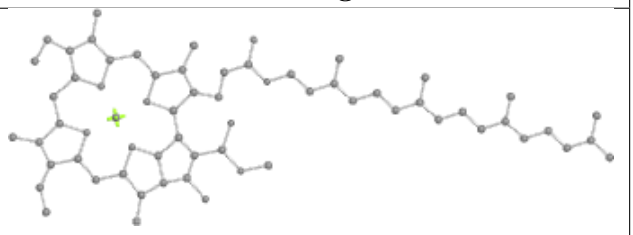
Bond lengths



Bond angles

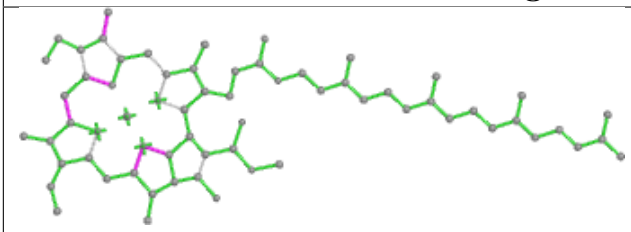


Torsions

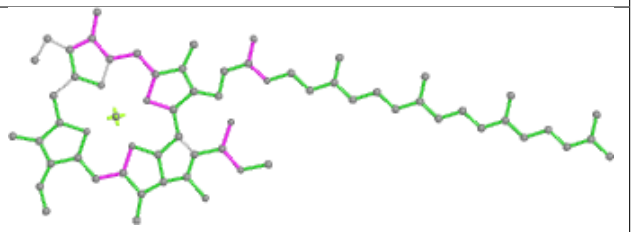


Rings

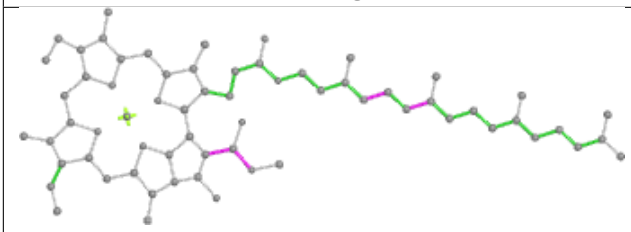
Ligand CLA B 604



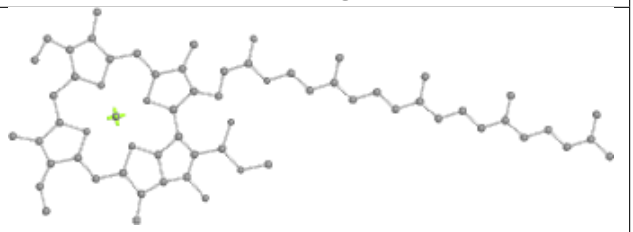
Bond lengths



Bond angles

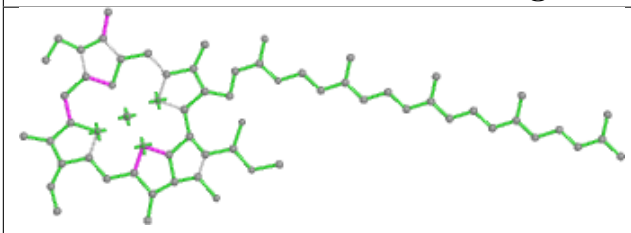


Torsions

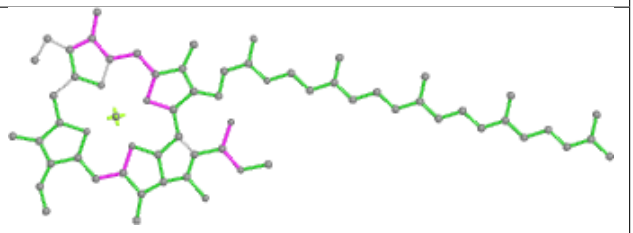


Rings

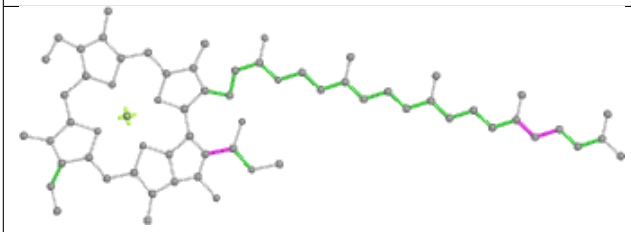
Ligand CLA c 506



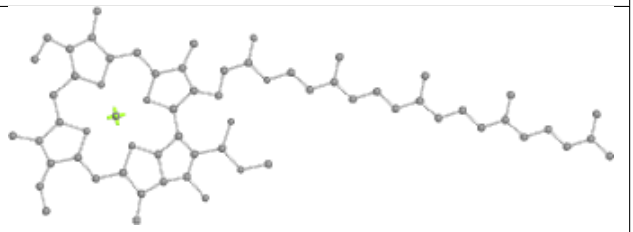
Bond lengths



Bond angles

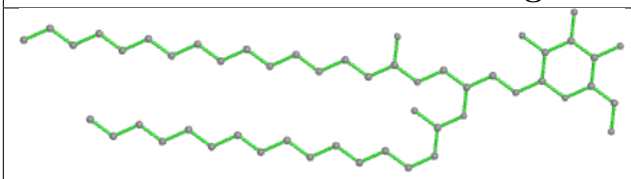


Torsions

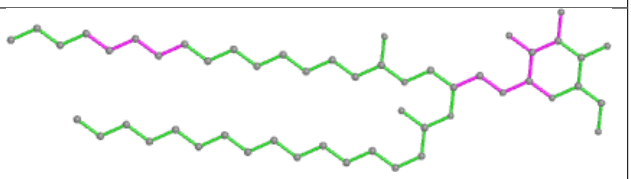


Rings

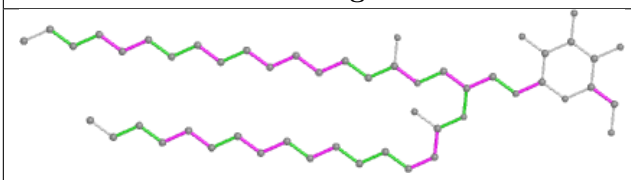
Ligand LMG c 521



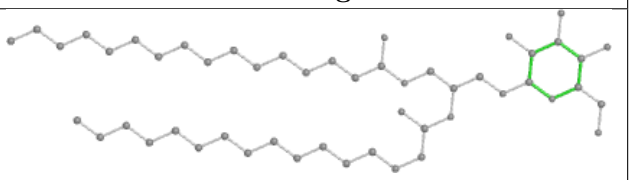
Bond lengths



Bond angles

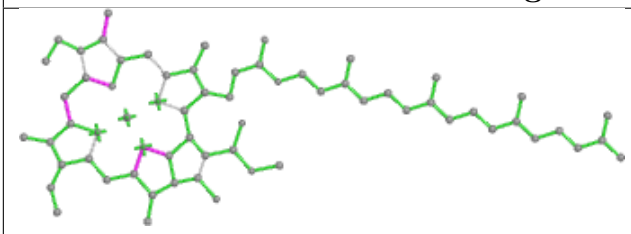


Torsions

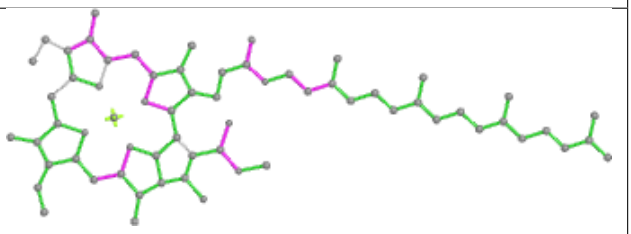


Rings

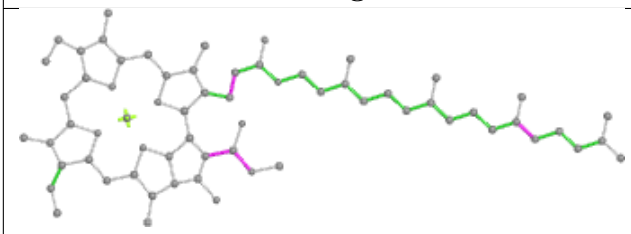
Ligand CLA B 606



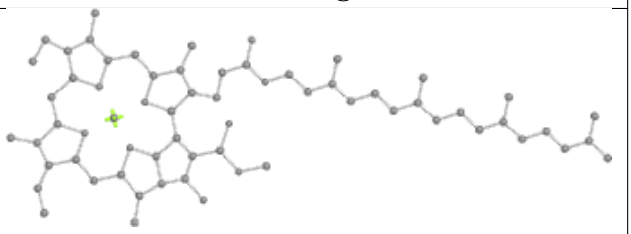
Bond lengths



Bond angles

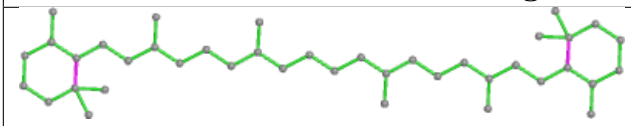


Torsions

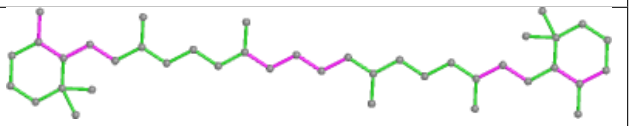


Rings

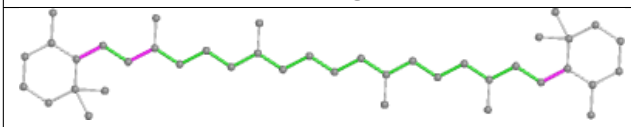
Ligand BCR A 610



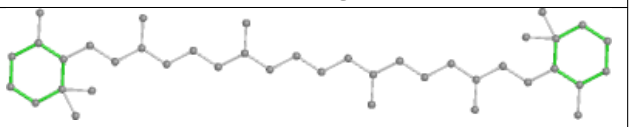
Bond lengths



Bond angles

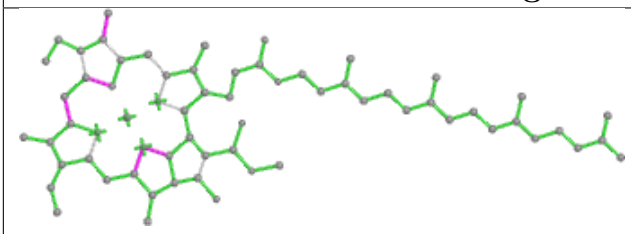


Torsions

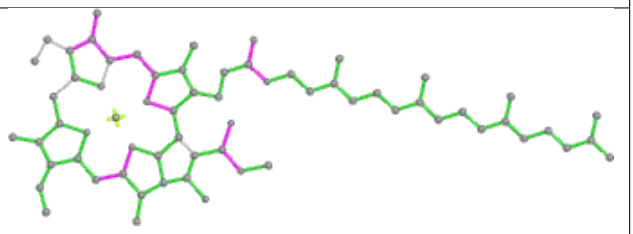


Rings

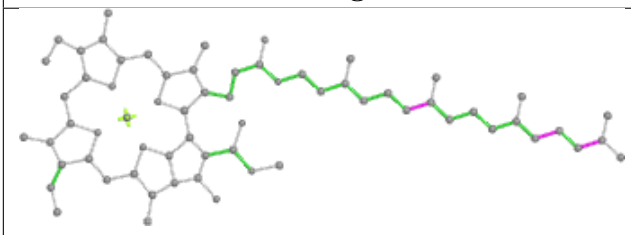
Ligand CLA D 403



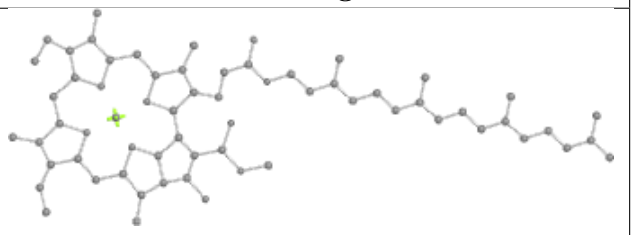
Bond lengths



Bond angles

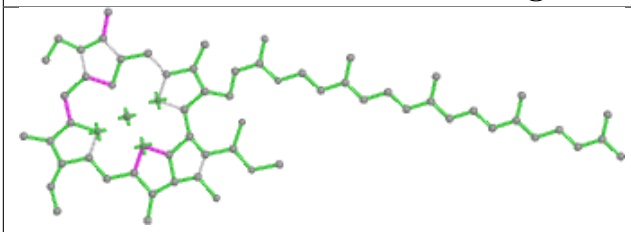


Torsions

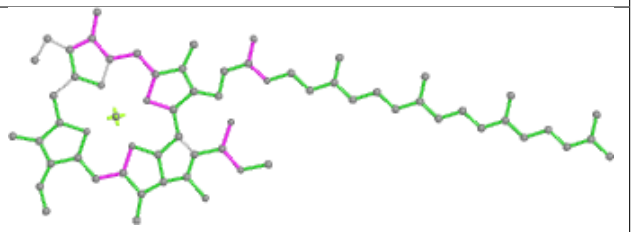


Rings

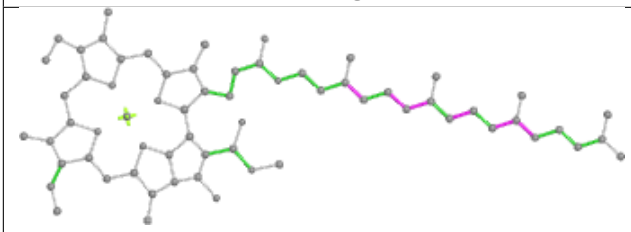
Ligand CLA b 605



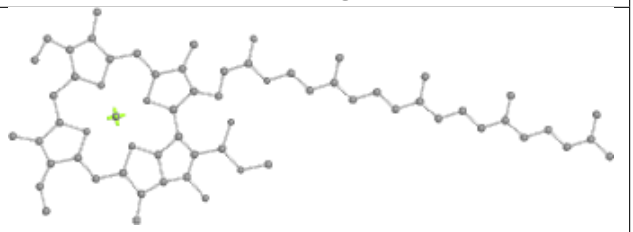
Bond lengths



Bond angles

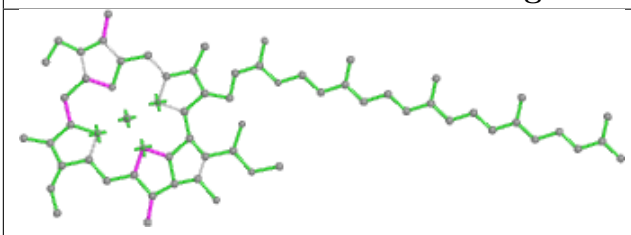


Torsions

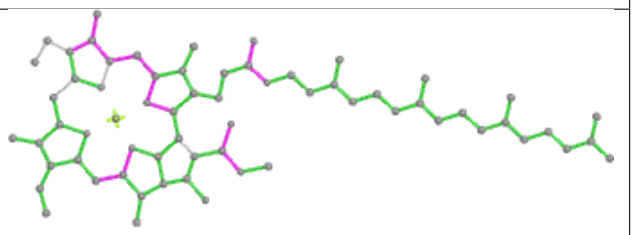


Rings

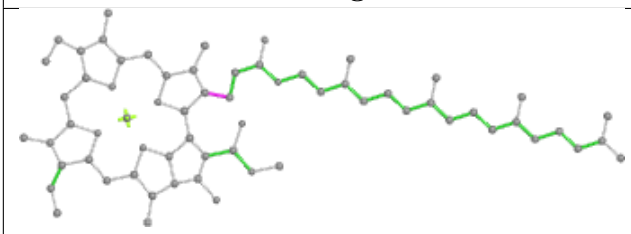
Ligand CLA C 503



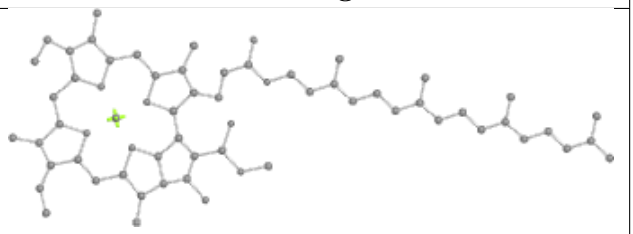
Bond lengths



Bond angles

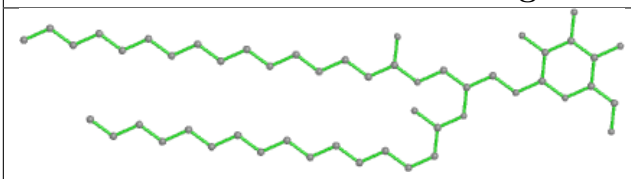


Torsions

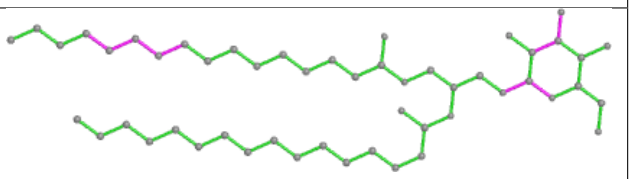


Rings

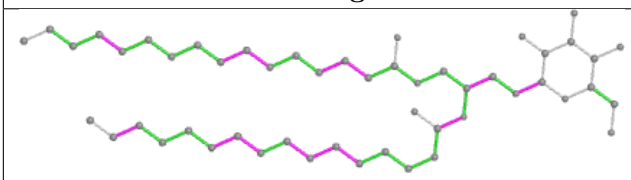
Ligand LMG A 612



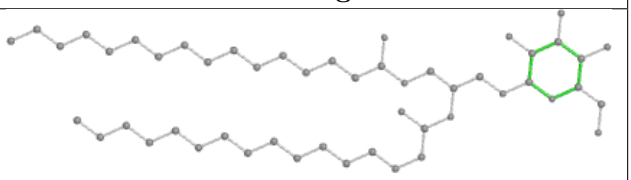
Bond lengths



Bond angles

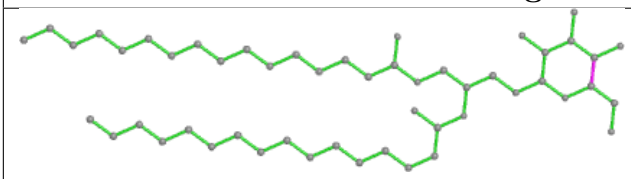


Torsions

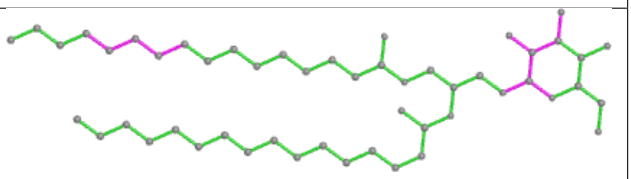


Rings

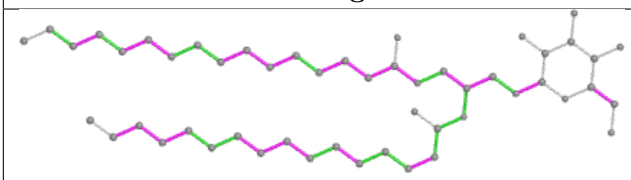
Ligand LMG c 502



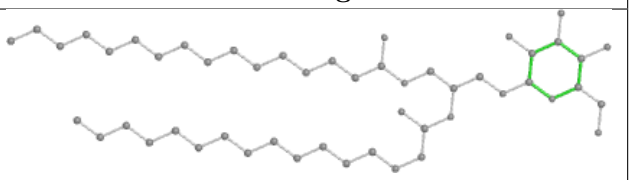
Bond lengths



Bond angles

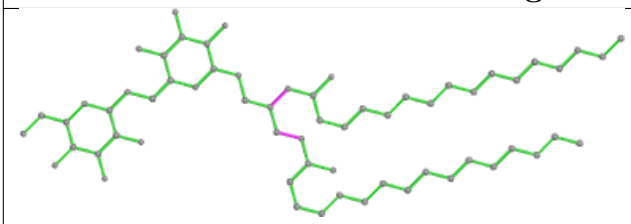


Torsions

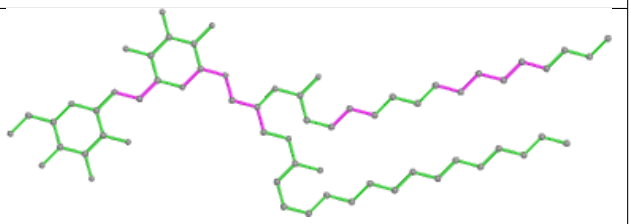


Rings

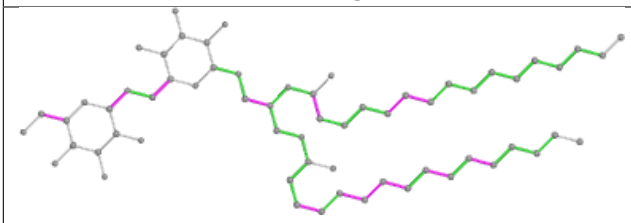
Ligand DGD c 518



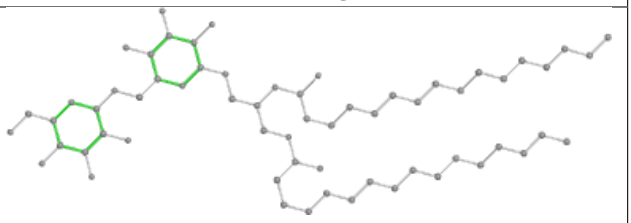
Bond lengths



Bond angles

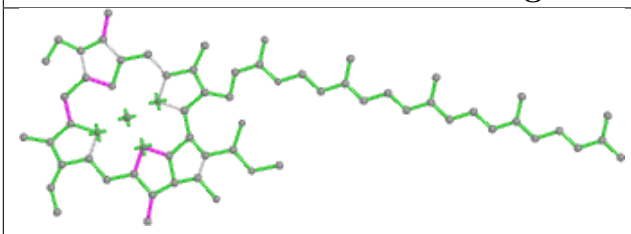


Torsions

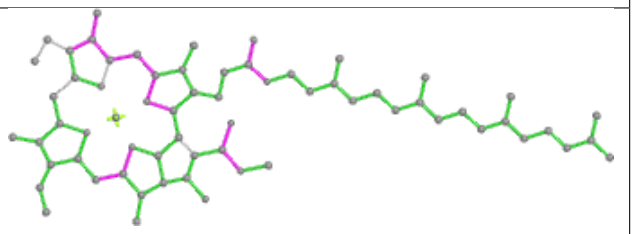


Rings

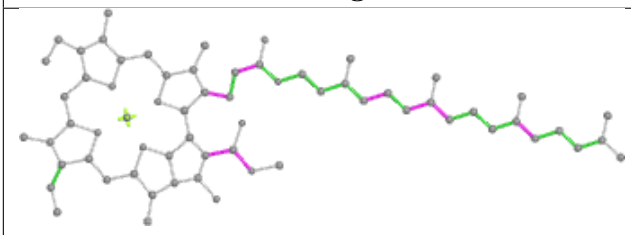
Ligand CLA C 512



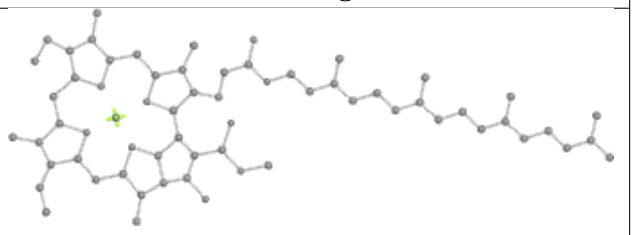
Bond lengths



Bond angles

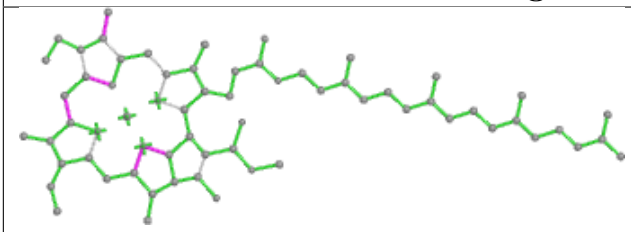


Torsions

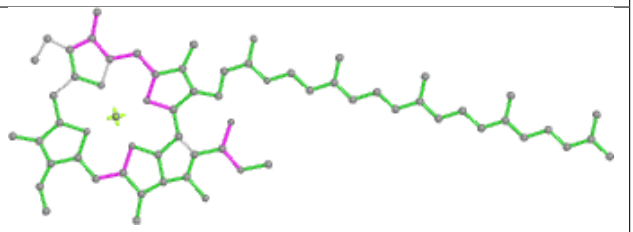


Rings

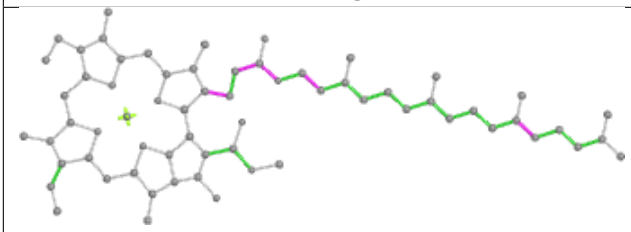
Ligand CLA d 403



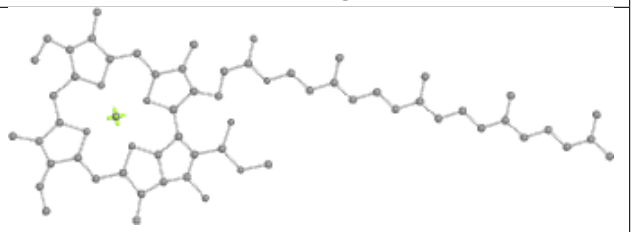
Bond lengths



Bond angles

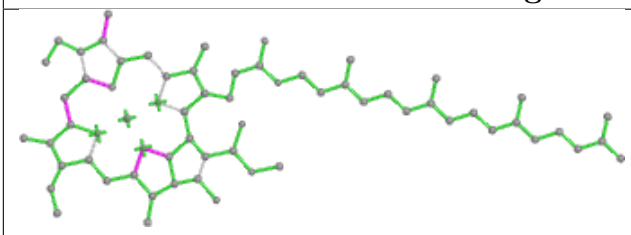


Torsions

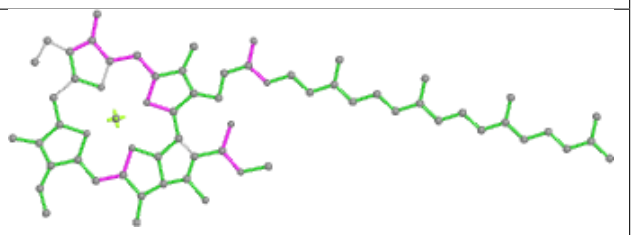


Rings

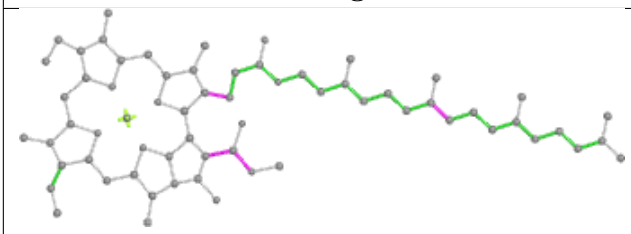
Ligand CLA C 513



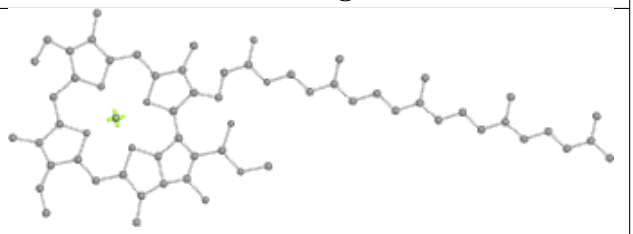
Bond lengths



Bond angles

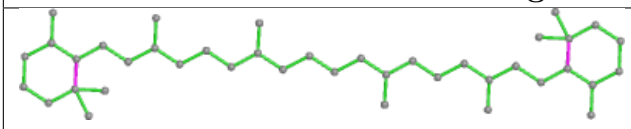


Torsions

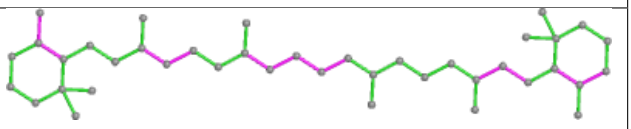


Rings

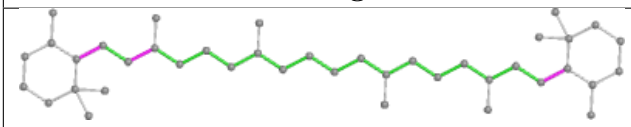
Ligand BCR c 517



Bond lengths



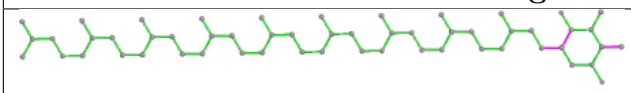
Bond angles



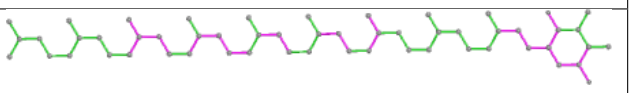
Torsions

Rings

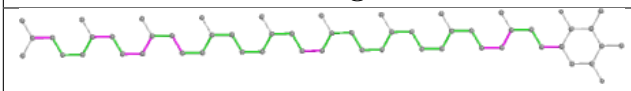
Ligand PL9 A 611



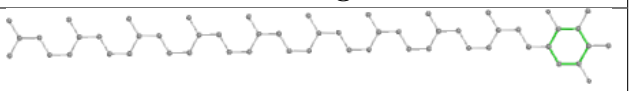
Bond lengths



Bond angles

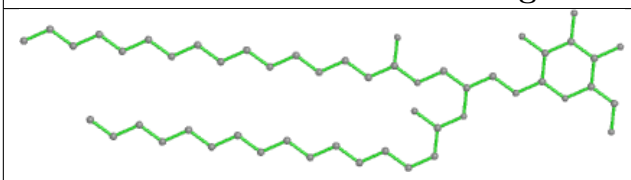


Torsions

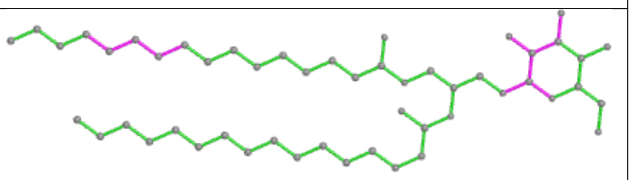


Rings

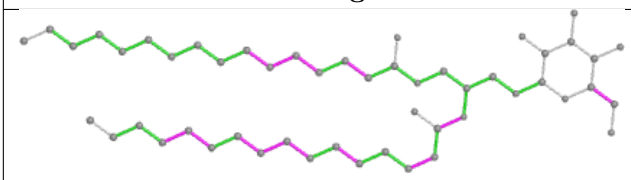
Ligand LMG D 405



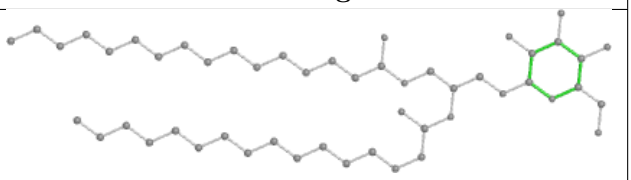
Bond lengths



Bond angles

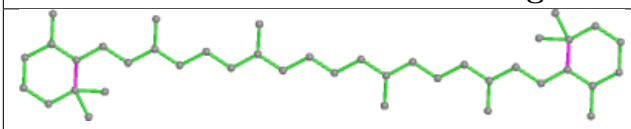


Torsions

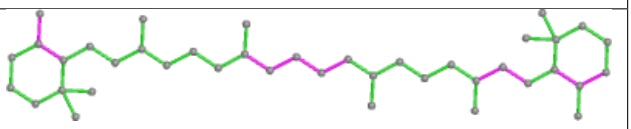


Rings

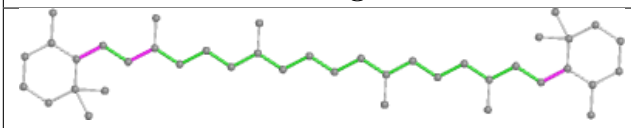
Ligand BCR a 610



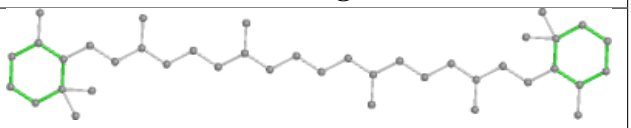
Bond lengths



Bond angles

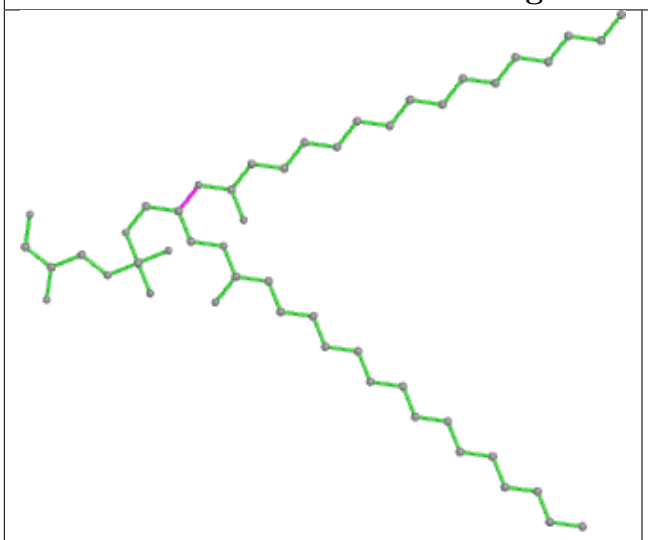


Torsions

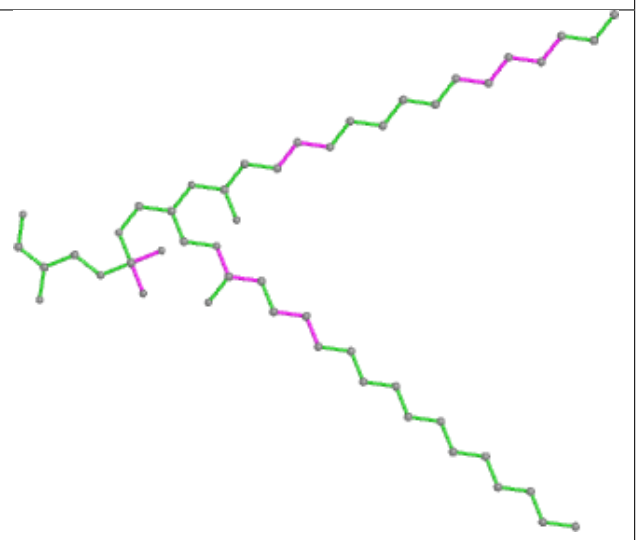


Rings

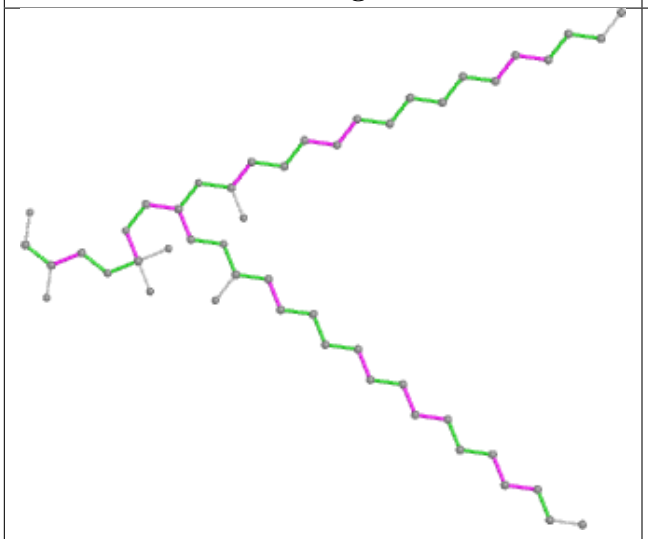
Ligand LHG L 101



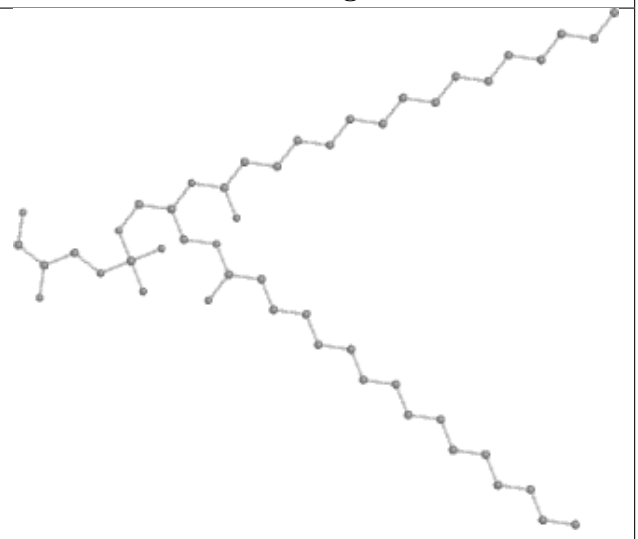
Bond lengths



Bond angles

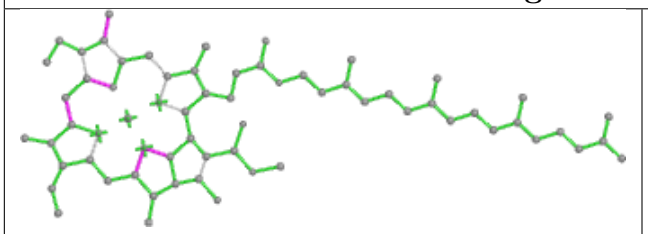


Torsions

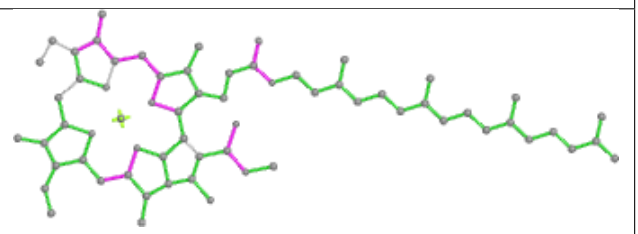


Rings

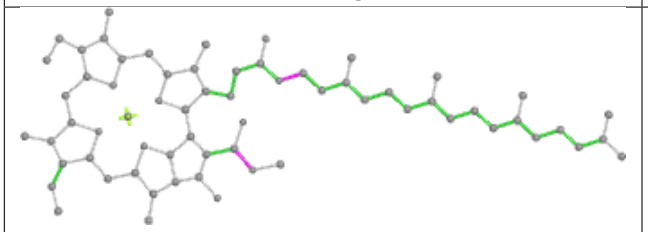
Ligand CLA A 606



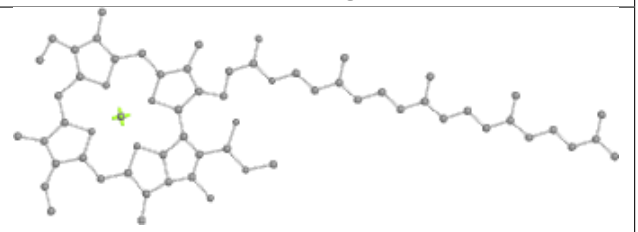
Bond lengths



Bond angles

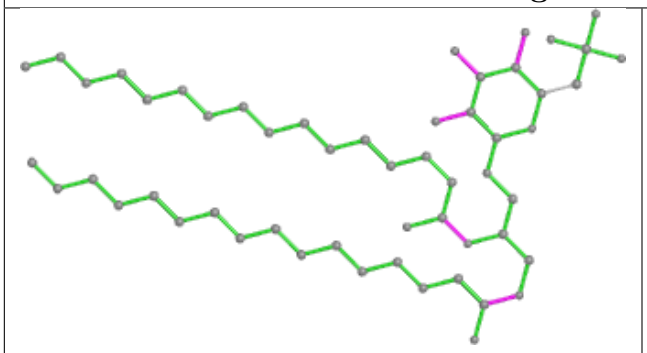


Torsions

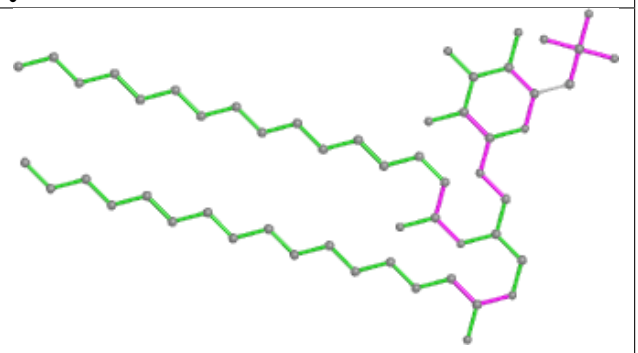


Rings

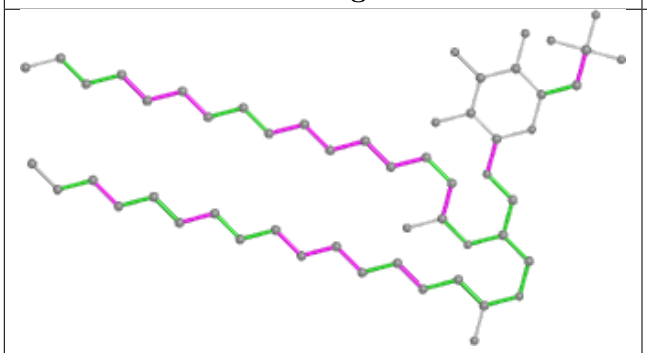
Ligand SQD c 501



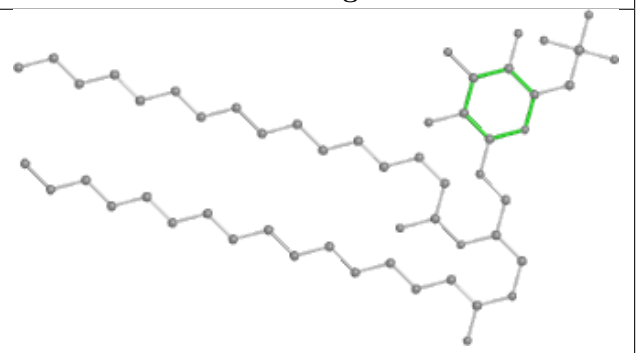
Bond lengths



Bond angles

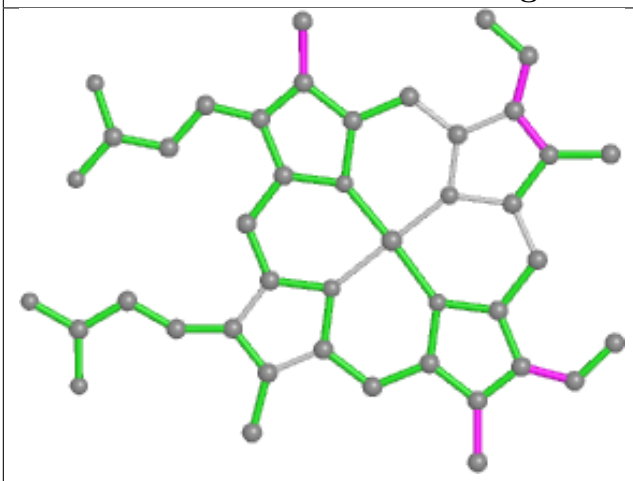


Torsions

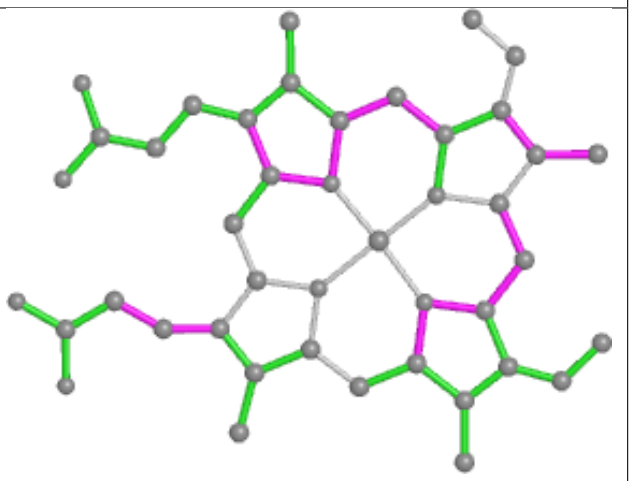


Rings

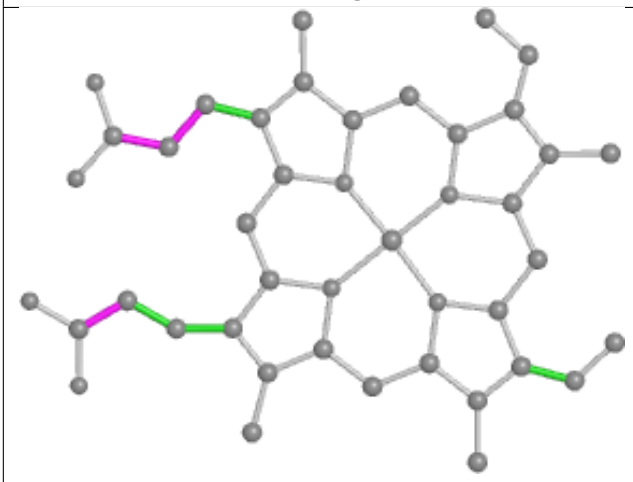
Ligand HEM E 101



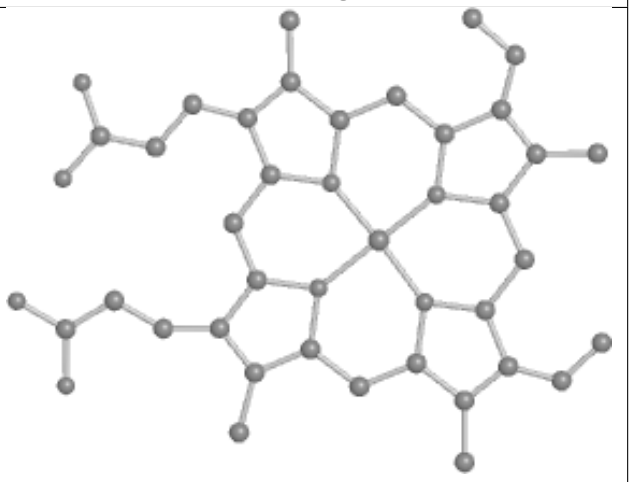
Bond lengths



Bond angles

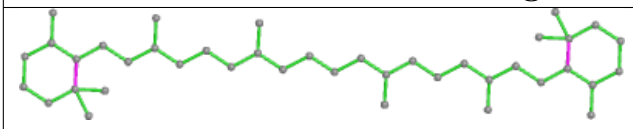


Torsions

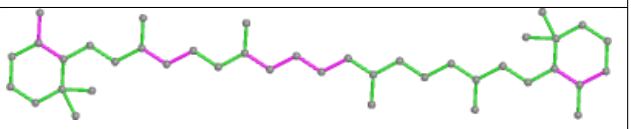


Rings

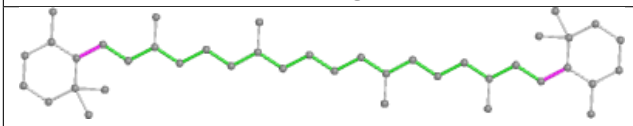
Ligand BCR B 618



Bond lengths



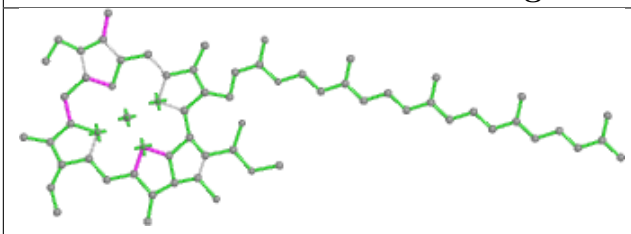
Bond angles



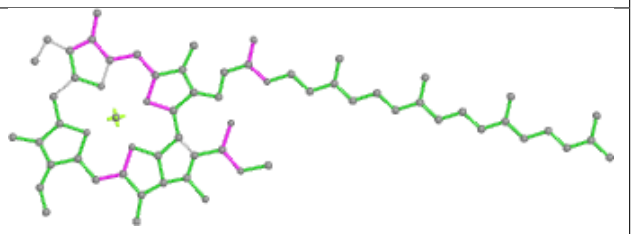
Torsions

Rings

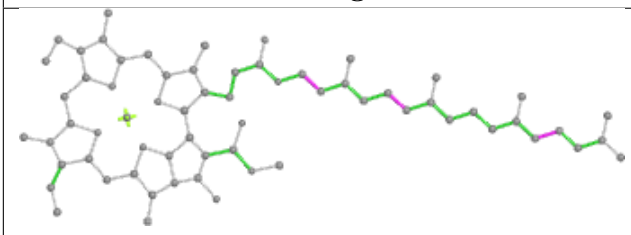
Ligand CLA B 613



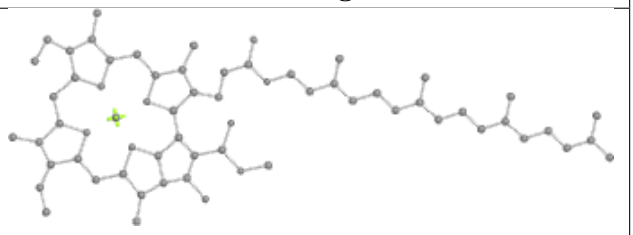
Bond lengths



Bond angles

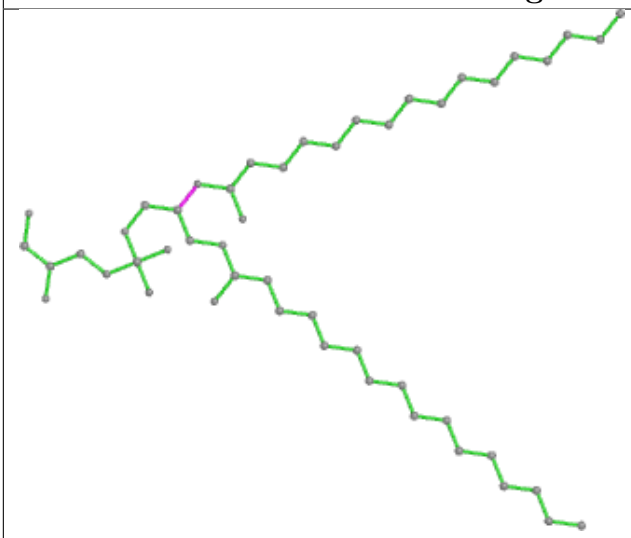


Torsions

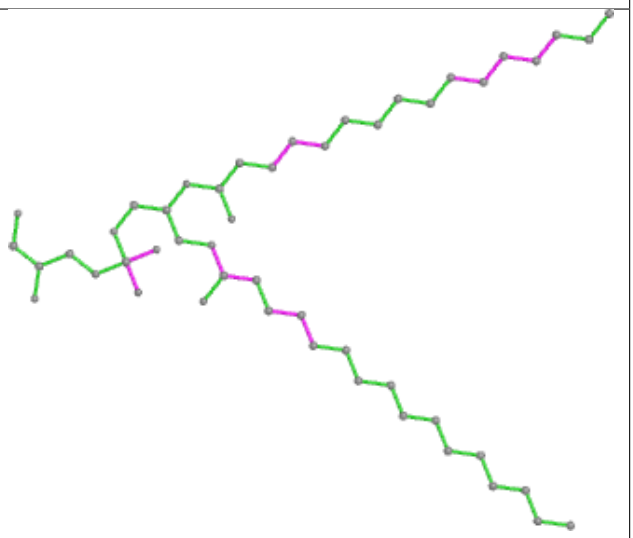


Rings

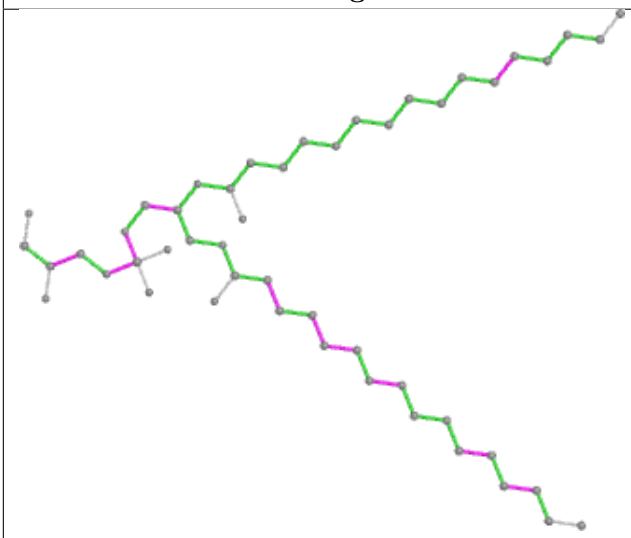
Ligand LHG d 407



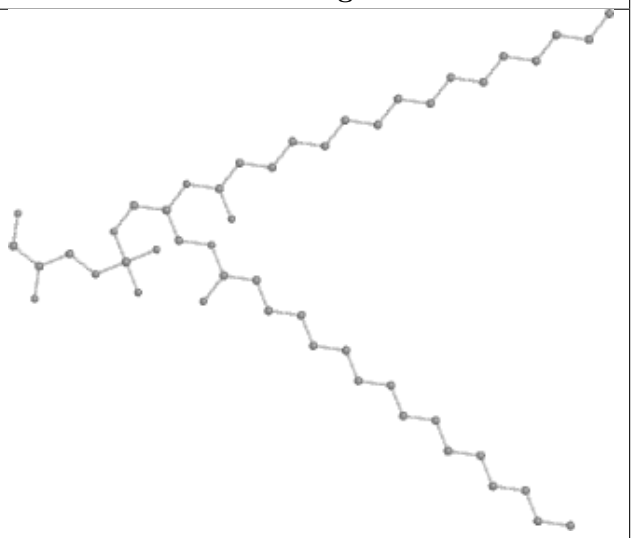
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	334/344 (97%)	-0.35	1 (0%)	94	84	28, 38, 60, 76	0
1	a	334/344 (97%)	-0.43	0	100	100	28, 38, 60, 76	0
2	B	504/510 (98%)	-0.17	12 (2%)	59	30	27, 41, 66, 86	0
2	b	504/510 (98%)	-0.22	4 (0%)	86	65	29, 42, 67, 85	0
3	C	451/461 (97%)	-0.26	5 (1%)	80	56	30, 45, 61, 75	0
3	c	451/461 (97%)	-0.23	4 (0%)	84	63	31, 46, 63, 93	0
4	D	341/352 (96%)	-0.39	2 (0%)	89	72	28, 39, 56, 67	0
4	d	341/352 (96%)	-0.37	0	100	100	29, 40, 55, 78	0
5	E	81/84 (96%)	-0.05	0	100	100	39, 54, 72, 89	0
5	e	82/84 (97%)	0.25	3 (3%)	41	17	43, 61, 75, 80	0
6	F	34/45 (75%)	-0.35	1 (2%)	51	23	40, 50, 63, 77	0
6	f	34/45 (75%)	-0.42	0	100	100	39, 51, 69, 72	0
7	H	63/66 (95%)	0.03	1 (1%)	72	44	39, 47, 57, 63	0
7	h	63/66 (95%)	-0.09	1 (1%)	72	44	35, 47, 58, 68	0
8	I	35/38 (92%)	0.10	1 (2%)	51	23	29, 44, 71, 73	0
8	i	35/38 (92%)	0.05	3 (8%)	10	3	33, 43, 74, 94	0
9	J	36/40 (90%)	-0.24	0	100	100	44, 58, 68, 75	0
9	j	36/40 (90%)	0.00	2 (5%)	24	8	49, 57, 72, 79	0
10	K	37/46 (80%)	-0.00	0	100	100	45, 59, 75, 89	0
10	k	37/46 (80%)	-0.07	0	100	100	47, 56, 72, 79	0
11	L	37/37 (100%)	-0.33	1 (2%)	54	26	32, 38, 62, 84	0
11	l	37/37 (100%)	-0.34	1 (2%)	54	26	29, 38, 69, 81	0
12	M	32/36 (88%)	-0.15	2 (6%)	20	6	33, 38, 56, 74	0
12	m	32/36 (88%)	0.03	3 (9%)	8	3	31, 41, 59, 64	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	O	244/272 (89%)	-0.06	8 (3%) 46 20	30, 47, 81, 111	0
13	o	244/272 (89%)	-0.06	6 (2%) 57 29	31, 46, 80, 127	0
14	T	29/32 (90%)	-0.39	0 100 100	30, 39, 60, 74	0
14	t	29/32 (90%)	-0.46	0 100 100	31, 36, 63, 66	0
15	U	97/134 (72%)	-0.03	0 100 100	36, 49, 69, 75	0
15	u	97/134 (72%)	-0.27	0 100 100	32, 44, 58, 76	0
16	V	137/163 (84%)	-0.18	0 100 100	34, 47, 59, 74	0
16	v	137/163 (84%)	-0.03	1 (0%) 87 69	34, 54, 67, 81	0
17	Y	30/46 (65%)	0.52	3 (10%) 7 2	60, 73, 84, 87	0
17	y	30/46 (65%)	0.15	2 (6%) 17 5	49, 65, 78, 83	0
18	X	38/41 (92%)	0.14	2 (5%) 26 10	41, 50, 65, 79	0
18	x	38/41 (92%)	0.19	2 (5%) 26 10	46, 55, 74, 76	0
19	Z	62/62 (100%)	0.48	5 (8%) 12 3	52, 69, 88, 98	0
19	z	62/62 (100%)	0.56	8 (12%) 3 1	51, 72, 97, 105	0
20	R	34/41 (82%)	0.89	3 (8%) 10 3	65, 73, 83, 86	0
20	r	34/41 (82%)	0.59	0 100 100	65, 78, 86, 90	0
All	All	5313/5700 (93%)	-0.18	87 (1%) 72 44	27, 44, 72, 127	0

The worst 5 of 87 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	O	35	SER	6.9
13	o	3	GLN	6.1
12	M	33	GLN	5.1
16	v	18	THR	5.0
12	m	31	SER	4.6

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	FME	I	1	10/11	0.91	0.29	43,56,63,71	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	FME	i	1	10/11	0.91	0.22	35,50,56,61	0
12	FME	m	1	10/11	0.91	0.23	26,45,55,64	0
14	FME	t	1	10/11	0.92	0.25	39,42,63,72	0
14	FME	T	1	10/11	0.93	0.13	44,47,53,54	0
12	FME	M	1	10/11	0.93	0.29	30,43,53,54	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
29	LMG	b	625	9/55	0.65	0.42	40,46,52,55	0
23	SQD	I	101	40/54	0.70	0.39	31,52,84,89	0
29	LMG	C	520	51/55	0.74	0.38	49,62,82,100	0
28	PL9	A	611	55/55	0.74	0.37	39,58,75,79	0
31	LHG	A	618	49/49	0.74	0.29	41,72,85,94	0
30	UNL	t	101	10/-	0.76	0.28	26,41,47,47	0
29	LMG	b	624	51/55	0.76	0.32	45,64,76,86	0
30	UNL	b	603	13/-	0.77	0.29	39,48,61,62	0
31	LHG	a	615	42/49	0.77	0.32	54,78,89,100	0
29	LMG	c	502	51/55	0.78	0.31	34,57,80,83	0
23	SQD	D	409	43/54	0.79	0.29	37,68,89,98	0
29	LMG	d	409	40/55	0.79	0.31	40,55,76,77	0
23	SQD	A	619	40/54	0.79	0.28	25,48,67,69	0
29	LMG	c	521	51/55	0.80	0.32	33,65,83,88	0
29	LMG	c	522	51/55	0.80	0.38	36,68,83,90	0
29	LMG	B	621	51/55	0.80	0.30	32,56,71,74	0
27	BCR	H	102	40/40	0.80	0.32	34,51,59,65	0
30	UNL	j	101	9/-	0.80	0.28	40,49,60,63	0
23	SQD	D	408	47/54	0.80	0.27	17,53,103,121	0
29	LMG	A	612	51/55	0.80	0.33	34,59,76,85	0
29	LMG	A	613	51/55	0.80	0.30	31,53,78,84	0
30	UNL	m	101	5/-	0.81	0.28	26,32,37,41	0
30	UNL	B	623	11/-	0.81	0.23	35,40,47,48	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
29	LMG	B	625	51/55	0.81	0.26	28,52,74,78	0
23	SQD	b	601	54/54	0.81	0.28	39,60,90,97	0
29	LMG	C	519	51/55	0.82	0.28	42,61,73,85	0
24	CL	a	603	1/1	0.82	0.23	59,59,59,59	0
30	UNL	z	101	11/-	0.82	0.29	31,53,58,60	0
30	UNL	d	402	22/-	0.82	0.31	26,43,60,78	0
29	LMG	b	623	51/55	0.82	0.30	29,48,71,74	0
33	DGD	h	102	62/66	0.82	0.29	35,47,63,73	0
30	UNL	m	102	16/-	0.83	0.27	37,45,51,54	0
30	UNL	M	101	6/-	0.83	0.31	41,46,52,65	0
27	BCR	y	101	40/40	0.83	0.29	50,63,70,74	0
25	CLA	c	515	65/65	0.83	0.30	45,60,78,81	0
25	CLA	C	512	65/65	0.83	0.30	42,58,68,79	0
27	BCR	k	101	40/40	0.83	0.26	37,53,59,61	0
28	PL9	a	611	55/55	0.84	0.29	40,59,72,73	0
27	BCR	Y	101	40/40	0.84	0.26	46,60,72,76	0
27	BCR	h	101	40/40	0.84	0.27	31,45,55,62	0
30	UNL	C	521	9/-	0.84	0.28	36,42,46,49	0
30	UNL	H	101	8/-	0.84	0.20	29,35,43,47	0
25	CLA	b	604	65/65	0.84	0.28	44,59,76,88	0
23	SQD	B	626	54/54	0.84	0.24	33,52,85,90	0
23	SQD	c	501	54/54	0.84	0.32	38,58,76,77	0
25	CLA	c	514	65/65	0.85	0.27	45,59,78,83	0
30	UNL	i	101	12/-	0.85	0.28	24,39,51,51	0
25	CLA	B	601	65/65	0.85	0.29	41,59,84,96	0
27	BCR	C	514	40/40	0.85	0.29	45,56,64,66	0
33	DGD	H	103	62/66	0.85	0.27	26,41,53,61	0
25	CLA	C	511	65/65	0.85	0.26	45,57,66,70	0
25	CLA	B	606	65/65	0.86	0.28	29,44,65,84	0
27	BCR	c	516	40/40	0.86	0.32	33,63,70,72	0
27	BCR	B	627	40/40	0.86	0.26	30,41,49,53	0
25	CLA	C	504	65/65	0.86	0.27	33,51,70,78	0
30	UNL	B	622	6/-	0.86	0.24	26,42,50,56	0
29	LMG	B	620	51/55	0.86	0.24	27,46,67,75	0
23	SQD	A	603	52/54	0.86	0.30	38,60,78,82	0
25	CLA	c	508	65/65	0.87	0.25	34,49,72,78	0
27	BCR	T	101	40/40	0.87	0.28	31,43,58,62	0
25	CLA	C	502	65/65	0.87	0.26	35,51,62,69	0
27	BCR	b	622	40/40	0.87	0.25	33,43,52,54	0
25	CLA	C	503	65/65	0.87	0.25	37,49,58,65	0
31	LHG	A	617	49/49	0.87	0.33	33,55,78,82	0
30	UNL	b	602	13/-	0.87	0.25	30,36,41,45	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
25	CLA	d	404	65/65	0.87	0.24	32,46,73,91	0
23	SQD	f	101	43/54	0.87	0.25	51,70,77,84	0
33	DGD	c	519	62/66	0.87	0.26	37,57,86,95	0
33	DGD	c	520	62/66	0.87	0.27	36,47,72,80	0
25	CLA	c	505	65/65	0.87	0.27	32,51,62,68	0
25	CLA	c	510	58/65	0.88	0.24	34,46,59,67	0
27	BCR	d	405	40/40	0.88	0.23	29,43,56,62	0
25	CLA	B	614	65/65	0.88	0.22	32,42,63,82	0
30	UNL	B	624	11/-	0.88	0.18	26,31,38,41	0
27	BCR	C	515	40/40	0.88	0.23	32,42,52,53	0
27	BCR	D	404	40/40	0.88	0.25	28,46,63,67	0
25	CLA	C	513	65/65	0.88	0.29	41,62,74,83	0
30	UNL	M	102	17/-	0.88	0.22	31,37,49,51	0
33	DGD	C	518	62/66	0.88	0.25	33,48,65,74	0
27	BCR	K	101	40/40	0.88	0.24	45,53,60,66	0
25	CLA	D	403	65/65	0.88	0.24	21,37,63,69	0
27	BCR	B	618	40/40	0.88	0.25	28,40,48,52	0
27	BCR	B	619	40/40	0.88	0.21	33,44,58,60	0
25	CLA	c	504	65/65	0.89	0.26	32,46,59,65	0
25	CLA	C	510	65/65	0.89	0.24	41,51,58,60	0
25	CLA	c	506	65/65	0.89	0.23	36,49,70,74	0
25	CLA	B	609	65/65	0.89	0.20	24,44,52,58	0
25	CLA	A	606	65/65	0.89	0.22	26,34,45,48	0
30	UNL	A	614	7/-	0.89	0.19	32,38,42,42	0
25	CLA	c	511	65/65	0.89	0.24	38,46,55,57	0
25	CLA	c	513	65/65	0.89	0.22	42,52,58,60	0
25	CLA	B	616	65/65	0.89	0.24	32,44,70,76	0
27	BCR	b	620	40/40	0.89	0.23	33,45,53,54	0
25	CLA	C	507	65/65	0.89	0.22	32,42,52,67	0
25	CLA	C	509	65/65	0.89	0.25	33,46,59,67	0
29	LMG	D	405	51/55	0.89	0.27	34,53,88,92	0
25	CLA	b	611	65/65	0.89	0.24	27,41,54,57	0
25	CLA	b	617	65/65	0.89	0.22	34,45,63,73	0
34	HEM	e	101	43/43	0.89	0.21	50,62,69,70	0
25	CLA	B	608	65/65	0.90	0.28	29,37,47,52	0
25	CLA	b	605	65/65	0.90	0.22	31,43,56,58	0
25	CLA	b	609	65/65	0.90	0.23	21,35,59,81	0
25	CLA	C	506	65/65	0.90	0.20	32,47,64,68	0
25	CLA	B	604	65/65	0.90	0.23	28,37,57,65	0
27	BCR	b	621	40/40	0.90	0.22	31,42,57,59	0
25	CLA	b	618	65/65	0.90	0.20	28,40,47,56	0
31	LHG	L	101	49/49	0.90	0.23	29,41,51,57	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
31	LHG	a	614	35/49	0.90	0.23	36,47,56,58	0
25	CLA	b	619	65/65	0.90	0.24	30,44,72,80	0
31	LHG	l	101	49/49	0.90	0.21	30,45,54,56	0
25	CLA	C	508	65/65	0.90	0.22	38,49,82,90	0
25	CLA	D	402	65/65	0.90	0.22	24,36,48,59	0
33	DGD	c	518	62/66	0.90	0.21	28,46,63,79	0
25	CLA	B	603	65/65	0.90	0.25	28,37,45,47	0
25	CLA	c	507	65/65	0.90	0.21	32,44,61,64	0
25	CLA	a	609	65/65	0.90	0.25	19,34,71,81	0
28	PL9	D	407	55/55	0.90	0.23	26,35,45,50	0
29	LMG	d	406	42/55	0.91	0.21	38,48,63,73	0
33	DGD	C	516	62/66	0.91	0.21	21,39,63,71	0
25	CLA	C	505	65/65	0.91	0.21	33,41,55,62	0
25	CLA	b	612	65/65	0.91	0.19	28,41,55,61	0
25	CLA	c	512	65/65	0.91	0.23	31,47,56,64	0
25	CLA	B	607	65/65	0.91	0.20	26,36,44,54	0
25	CLA	b	607	65/65	0.91	0.20	24,34,48,53	0
22	FE2	a	602	1/1	0.91	0.08	62,62,62,62	0
25	CLA	c	509	65/65	0.91	0.20	30,39,51,55	0
25	CLA	b	616	65/65	0.92	0.20	25,33,51,62	0
25	CLA	A	615	65/65	0.92	0.22	22,34,43,47	0
25	CLA	B	610	65/65	0.92	0.21	25,33,39,45	0
31	LHG	A	616	49/49	0.92	0.20	24,41,54,58	0
28	PL9	d	408	55/55	0.92	0.21	21,33,43,45	0
25	CLA	B	613	65/65	0.92	0.23	19,33,48,69	0
31	LHG	D	406	49/49	0.92	0.24	25,40,50,59	0
25	CLA	A	609	65/65	0.92	0.23	17,29,79,89	0
25	CLA	b	608	65/65	0.92	0.19	30,40,46,51	0
25	CLA	d	403	65/65	0.92	0.19	24,36,45,50	0
25	CLA	B	615	65/65	0.92	0.19	27,41,51,57	0
26	PHO	D	401	64/64	0.92	0.21	27,37,47,54	0
33	DGD	C	517	62/66	0.92	0.22	39,51,74,83	0
26	PHO	d	401	64/64	0.92	0.21	24,39,45,49	0
27	BCR	A	610	40/40	0.92	0.20	22,34,44,47	0
27	BCR	c	517	40/40	0.92	0.20	19,39,50,52	0
27	BCR	B	617	40/40	0.92	0.20	32,41,49,50	0
25	CLA	B	605	65/65	0.92	0.19	24,34,40,42	0
25	CLA	C	501	65/65	0.92	0.21	34,42,49,54	0
34	HEM	E	101	43/43	0.92	0.20	42,54,67,69	0
25	CLA	b	613	65/65	0.92	0.20	24,35,43,45	0
31	LHG	a	613	49/49	0.93	0.20	26,43,56,60	0
27	BCR	a	610	40/40	0.93	0.19	19,32,45,47	0

Continued on next page...

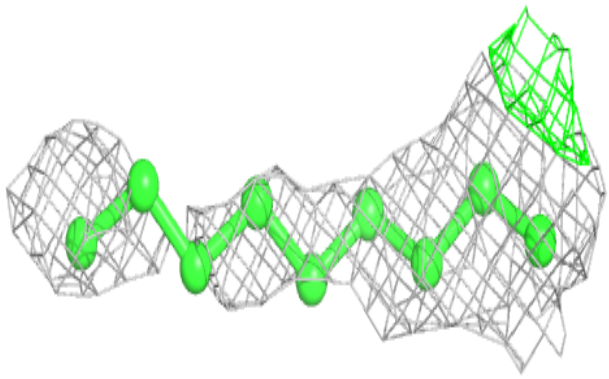
Continued from previous page...

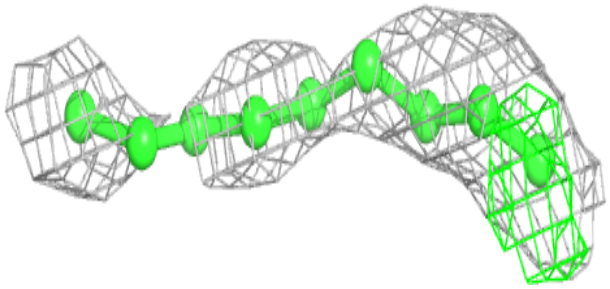
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
24	CL	A	604	1/1	0.93	0.10	43,43,43,43	0
31	LHG	d	407	49/49	0.93	0.20	20,37,47,51	0
25	CLA	B	611	65/65	0.93	0.22	21,31,38,44	0
25	CLA	a	606	65/65	0.93	0.18	23,31,38,39	0
25	CLA	c	503	65/65	0.93	0.21	27,40,46,52	0
25	CLA	b	610	65/65	0.93	0.19	23,37,51,54	0
25	CLA	B	612	65/65	0.93	0.20	26,35,42,46	0
25	CLA	A	607	57/65	0.93	0.20	29,37,49,67	0
24	CL	a	604	1/1	0.93	0.14	42,42,42,42	0
26	PHO	A	608	64/64	0.93	0.21	23,32,37,43	0
25	CLA	b	614	65/65	0.93	0.18	25,35,41,50	0
26	PHO	a	608	64/64	0.93	0.20	19,28,38,42	0
25	CLA	b	606	65/65	0.93	0.20	24,36,50,58	0
35	HEC	V	201	43/43	0.93	0.17	31,44,52,56	0
25	CLA	b	615	65/65	0.94	0.18	22,32,41,50	0
25	CLA	a	612	65/65	0.94	0.17	17,29,37,39	0
25	CLA	a	607	59/65	0.94	0.17	27,37,55,72	0
25	CLA	B	602	65/65	0.94	0.22	29,39,47,52	0
35	HEC	v	201	43/43	0.94	0.17	32,41,48,52	0
24	CL	A	605	1/1	0.95	0.13	44,44,44,44	0
32	BCT	A	620	4/4	0.95	0.15	26,36,37,44	0
22	FE2	A	602	1/1	0.96	0.05	46,46,46,46	0
32	BCT	a	605	4/4	0.96	0.10	44,47,49,50	0
21	OEX	A	601	10/10	0.98	0.10	33,40,45,46	0
21	OEX	a	601	10/10	0.98	0.08	40,44,48,51	0

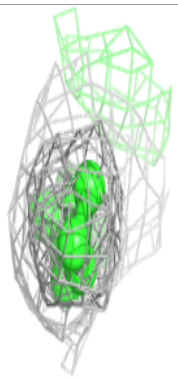
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LMG b 625:

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

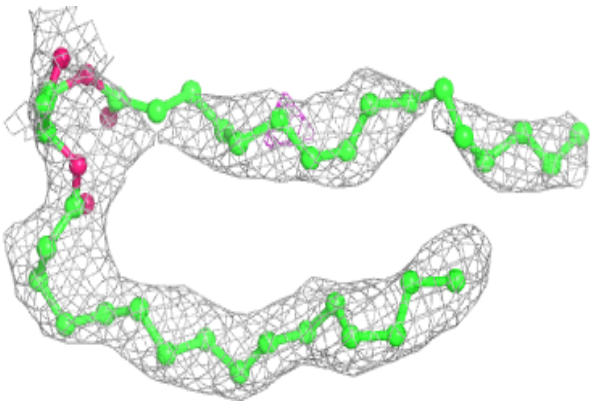


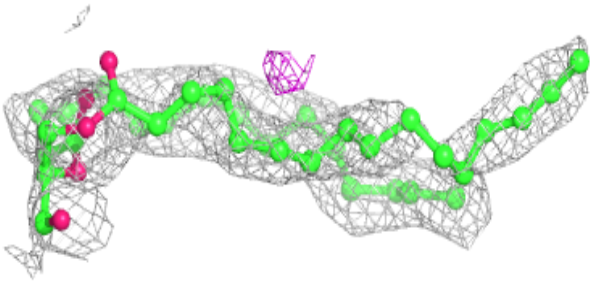


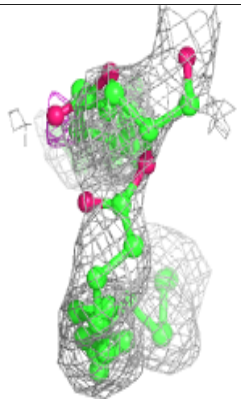


Electron density around SQD I 101:

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

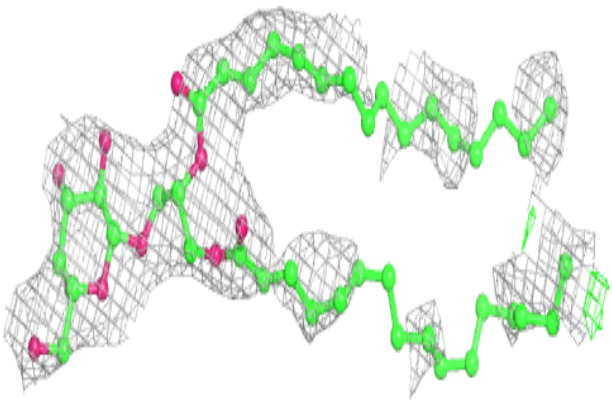


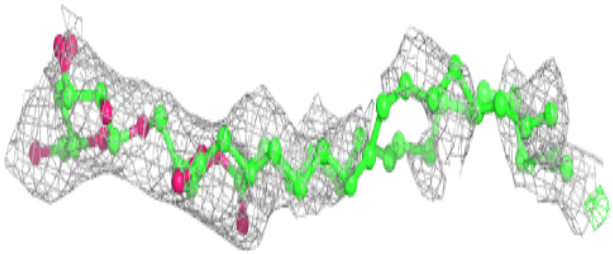


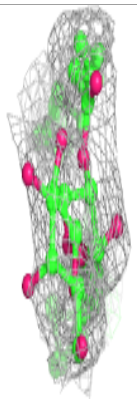


Electron density around LMG C 520:

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

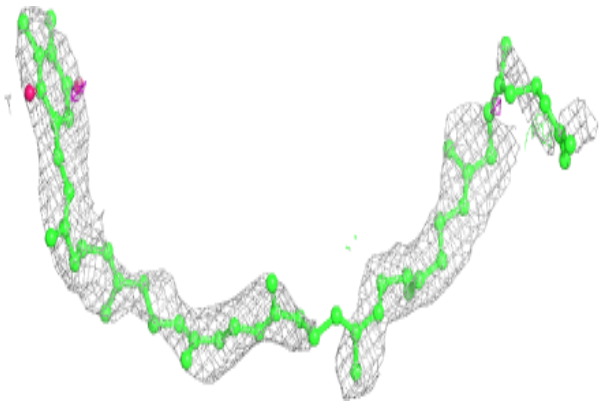


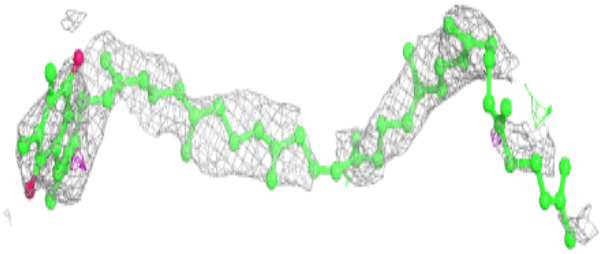


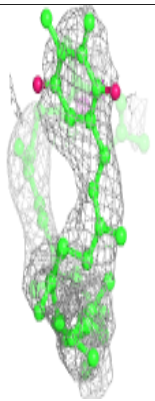


Electron density around PL9 A 611:

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

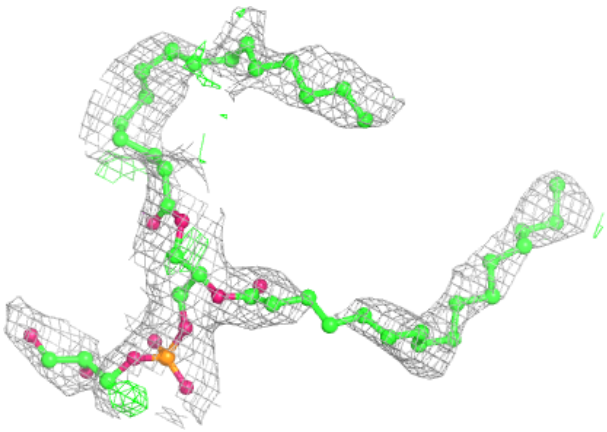


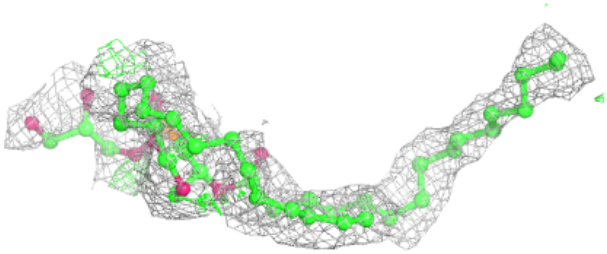


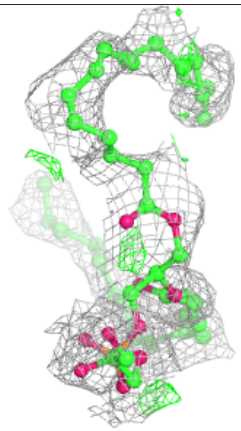


Electron density around LHG A 618:

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

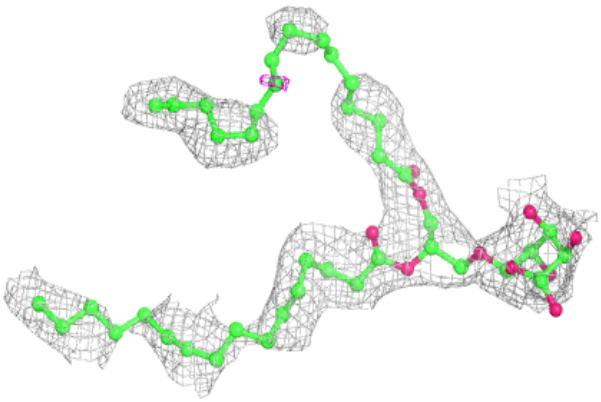


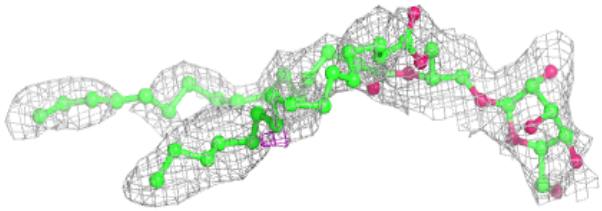


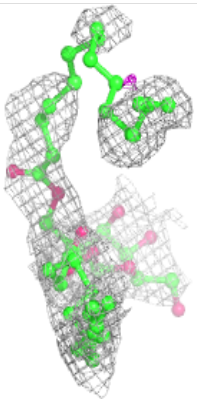


Electron density around LMG b 624:

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

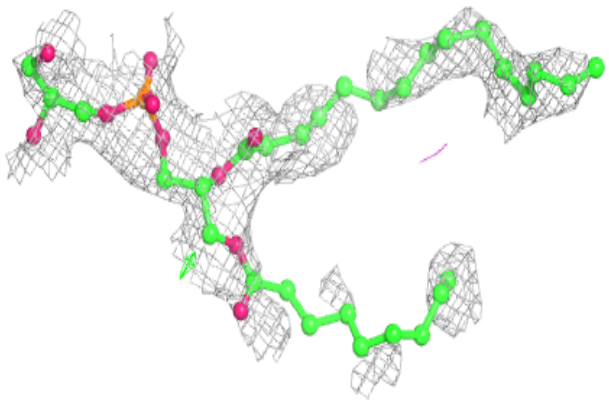


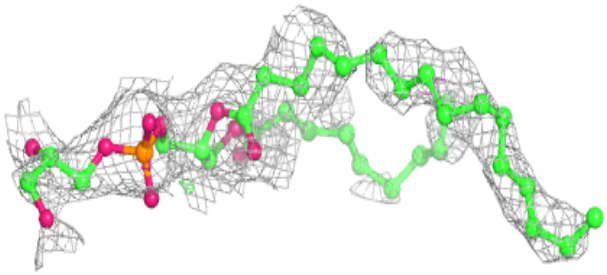


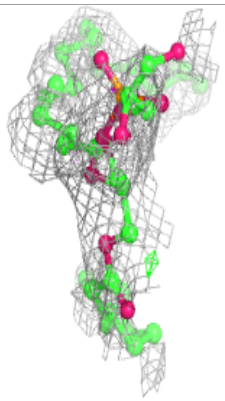


Electron density around LHG a 615:

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

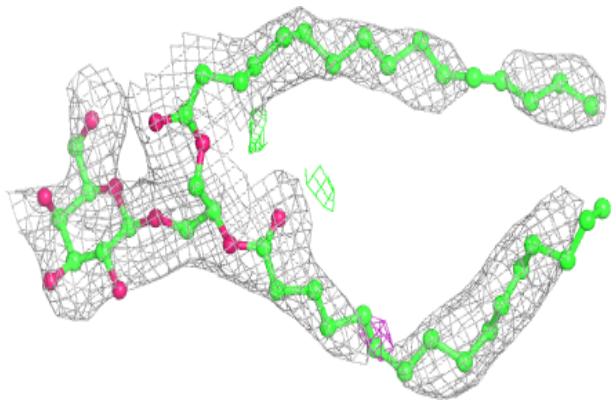


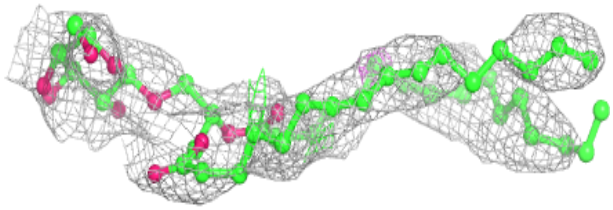


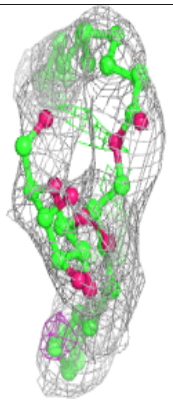


Electron density around LMG c 502:

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

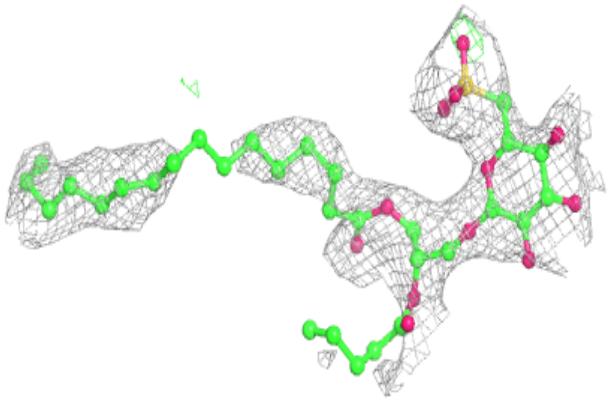


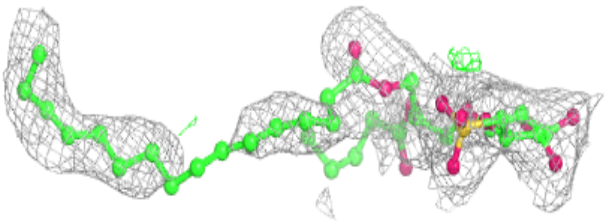




Electron density around SQD D 409:

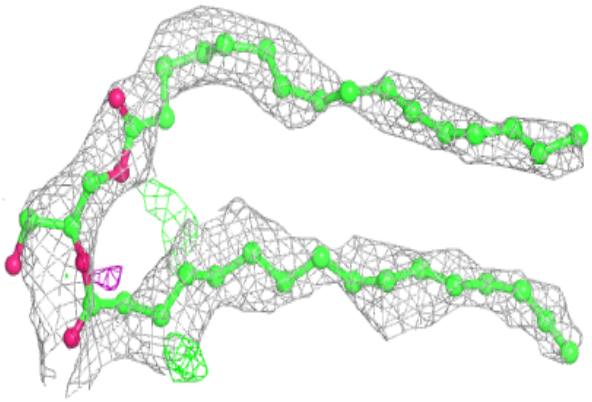
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

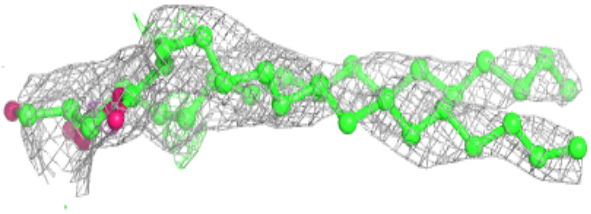


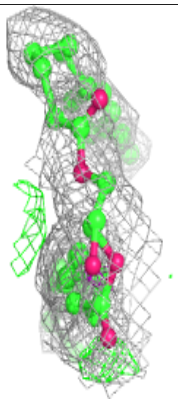


Electron density around LMG d 409:

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

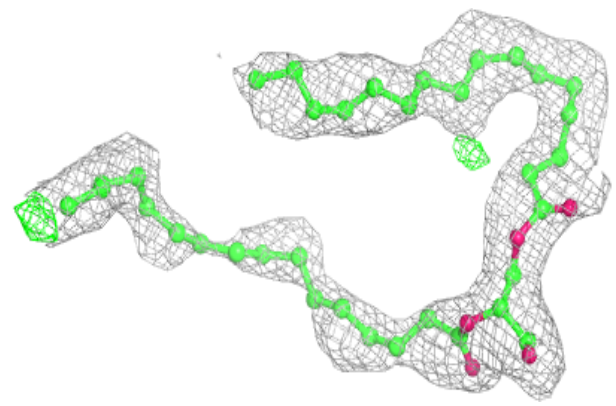


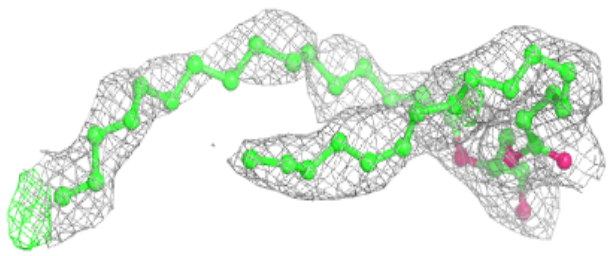


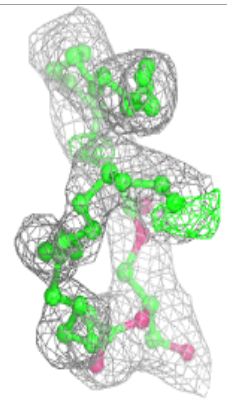


Electron density around SQD A 619:

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

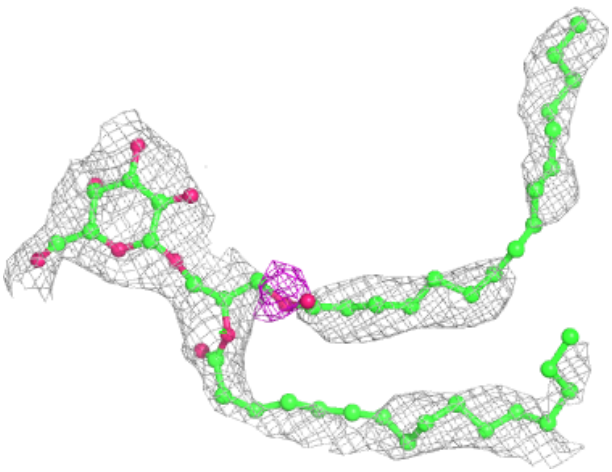


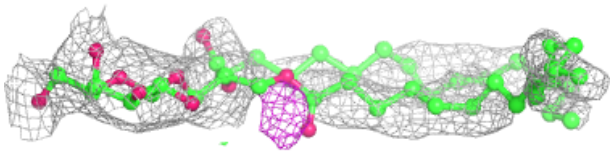


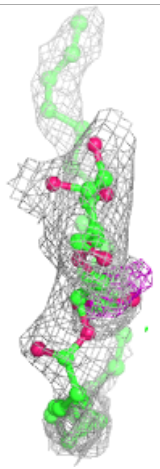


Electron density around LMG c 521:

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

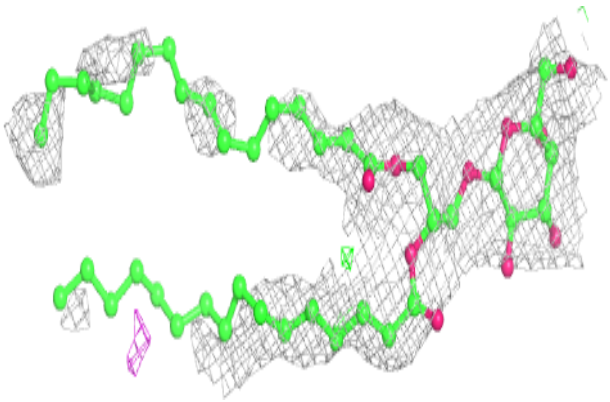


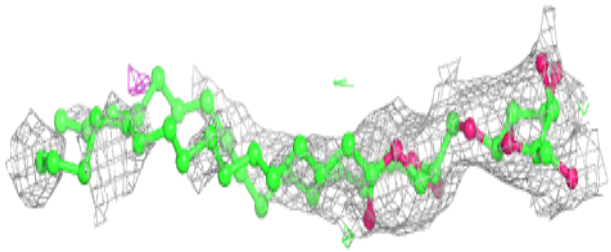


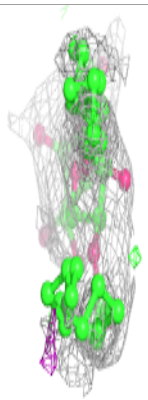


Electron density around LMG c 522:

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

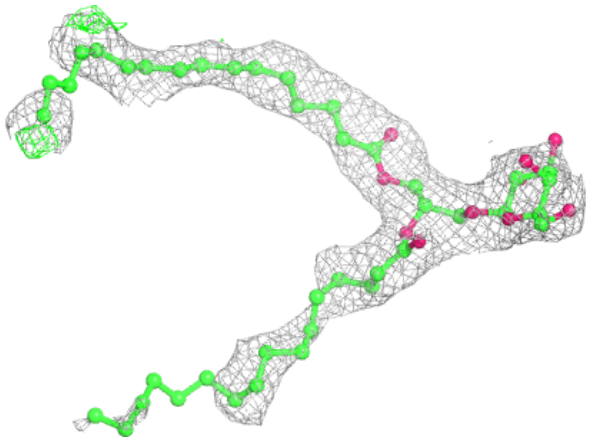


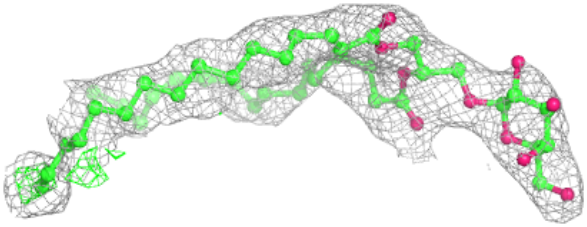


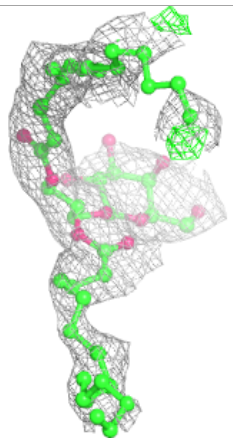


Electron density around LMG B 621:

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

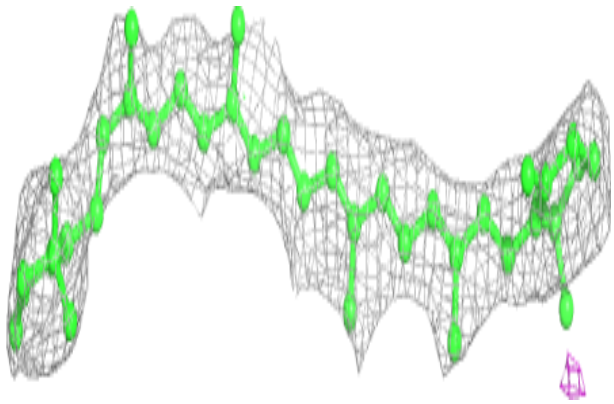


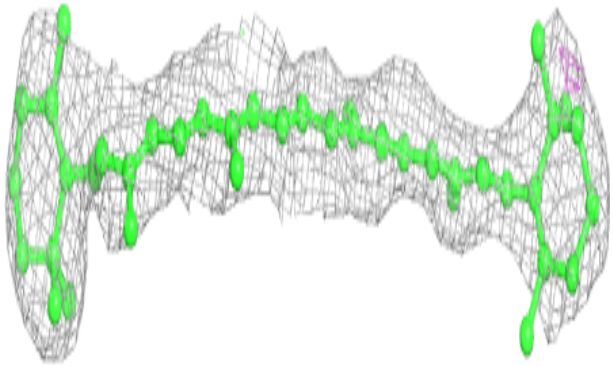


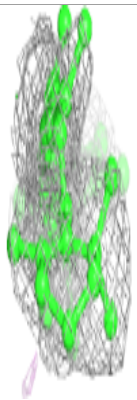


Electron density around BCR H 102:

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

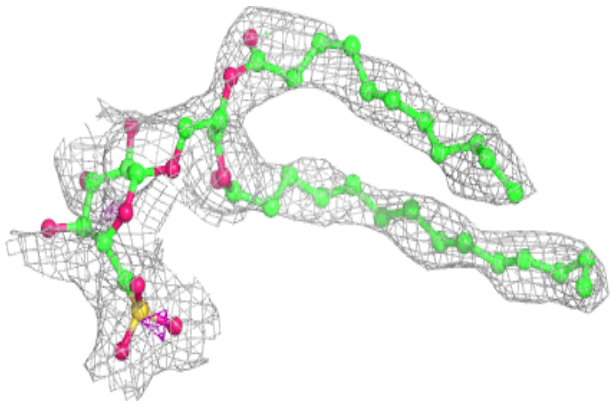


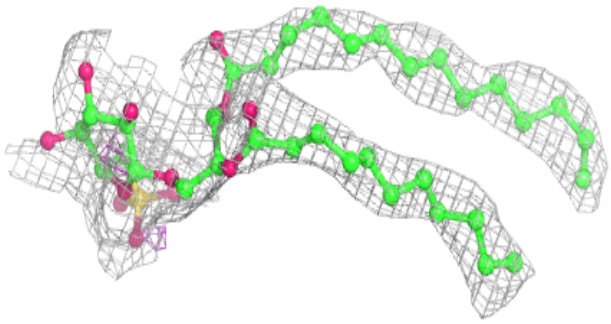


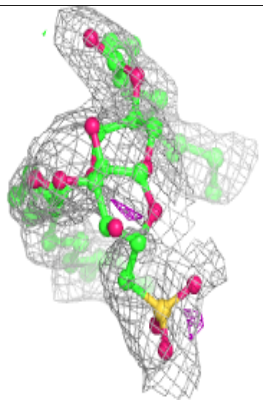


Electron density around SQD D 408:

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

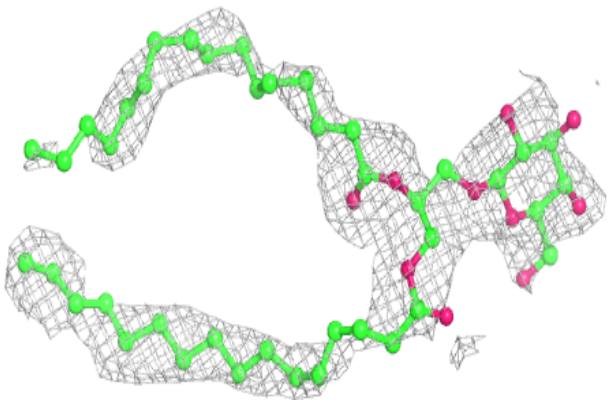


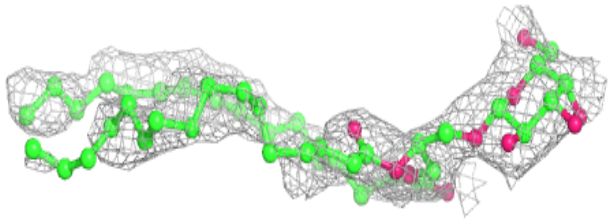


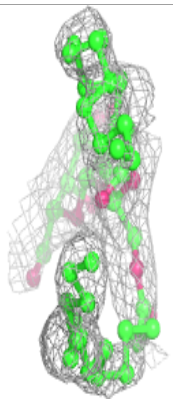


Electron density around LMG A 612:

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

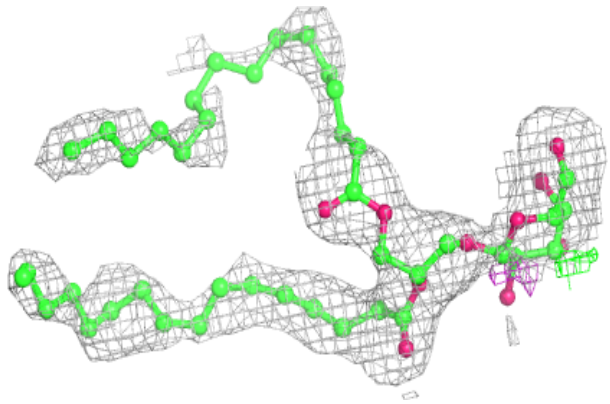


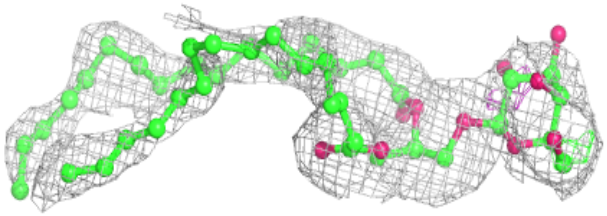


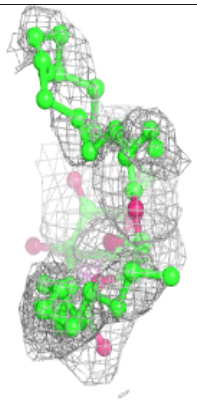


Electron density around LMG A 613:

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

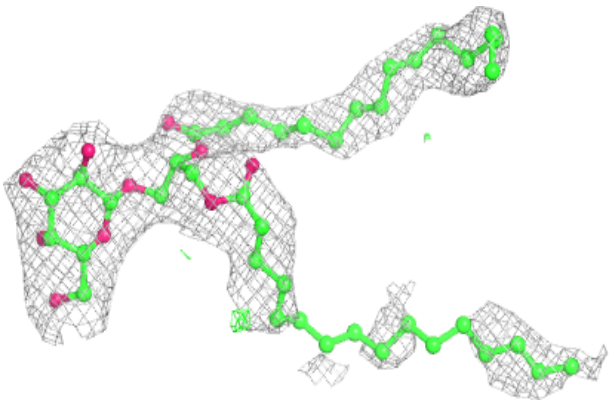


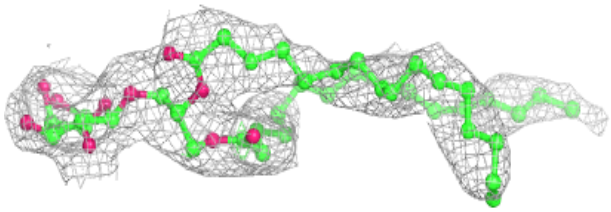


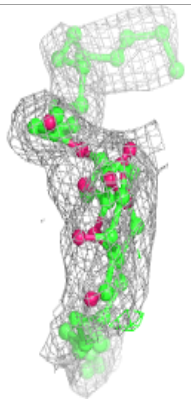


Electron density around LMG B 625:

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

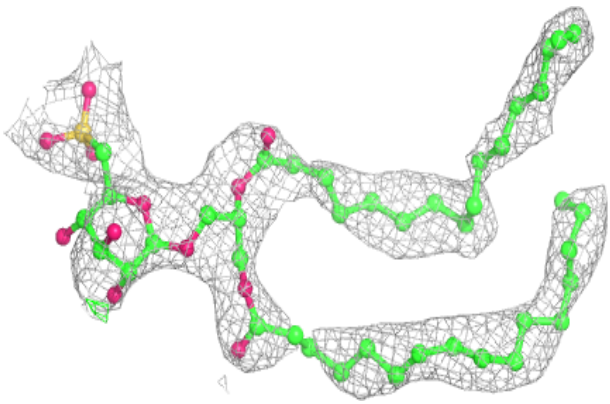


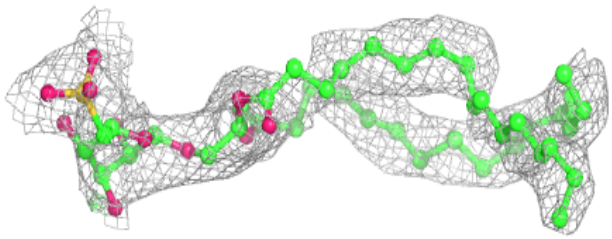


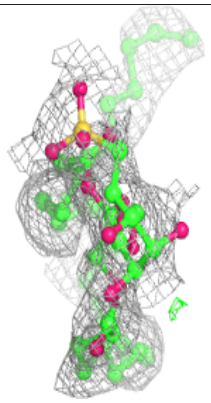


Electron density around SQD b 601:

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

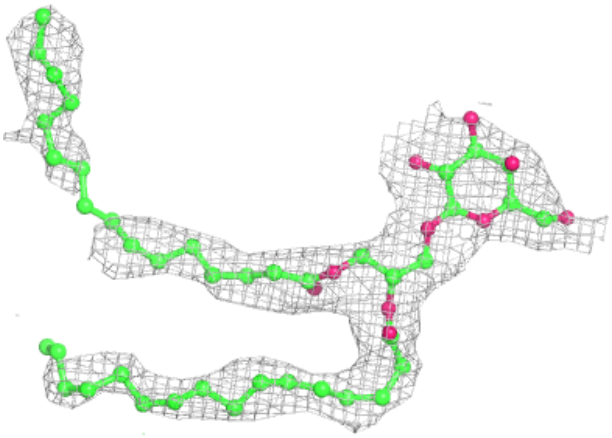


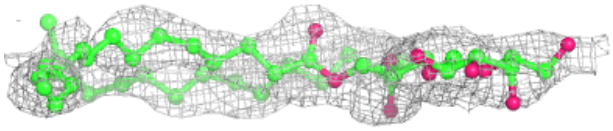


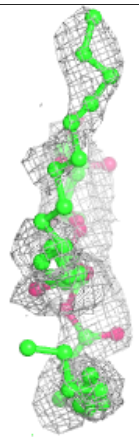


Electron density around LMG C 519:

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

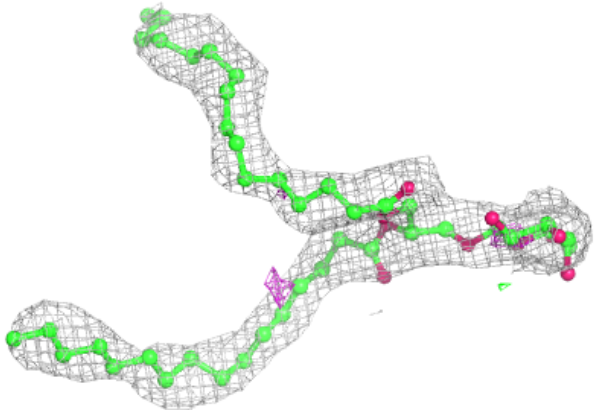


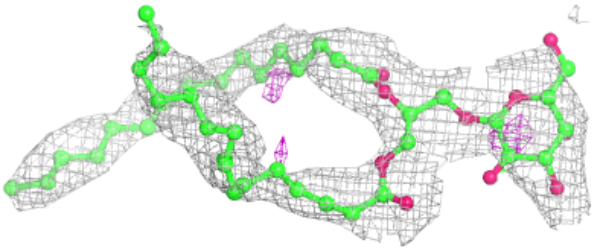


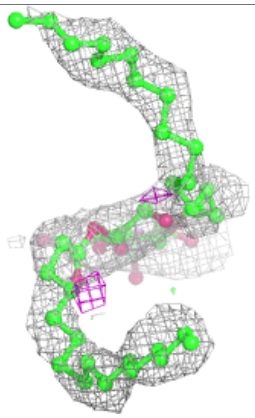


Electron density around LMG b 623:

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

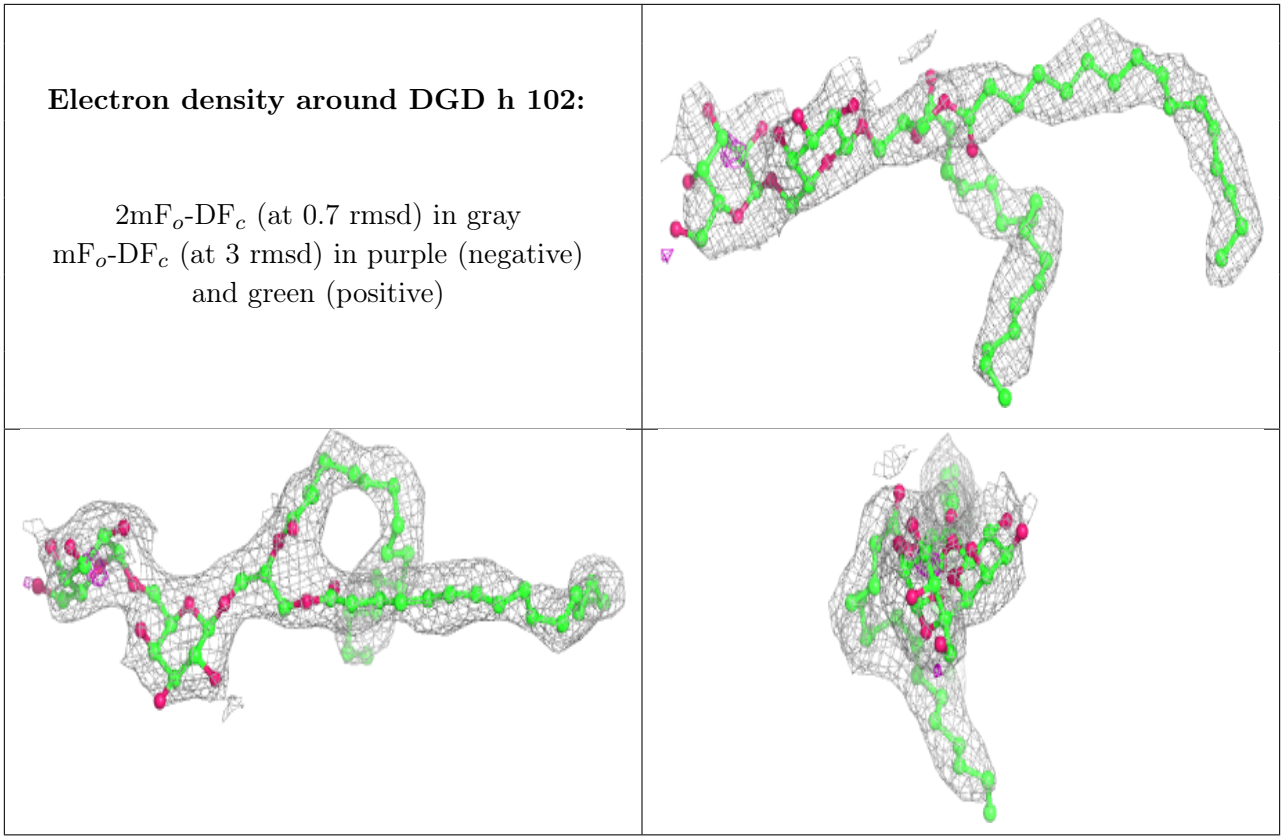






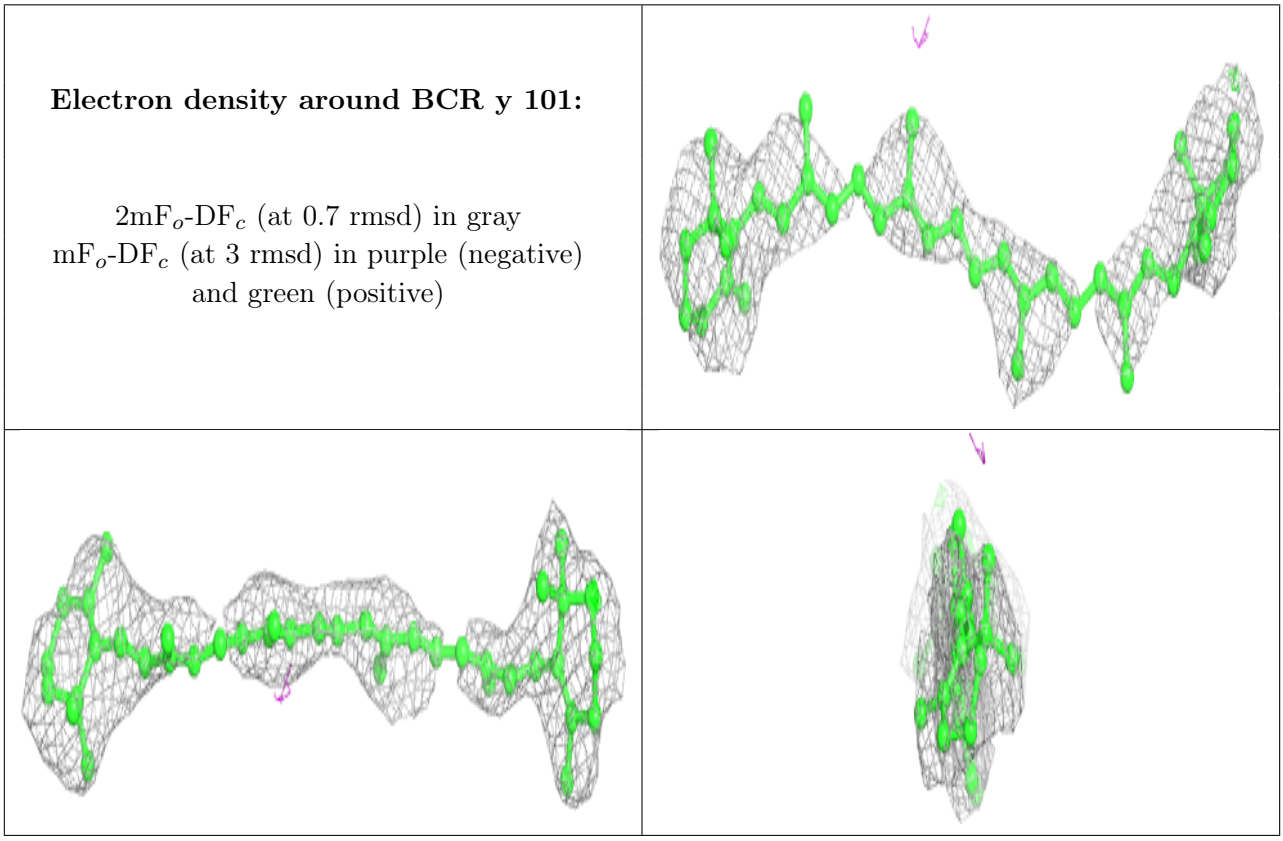
Electron density around DGD h 102:

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



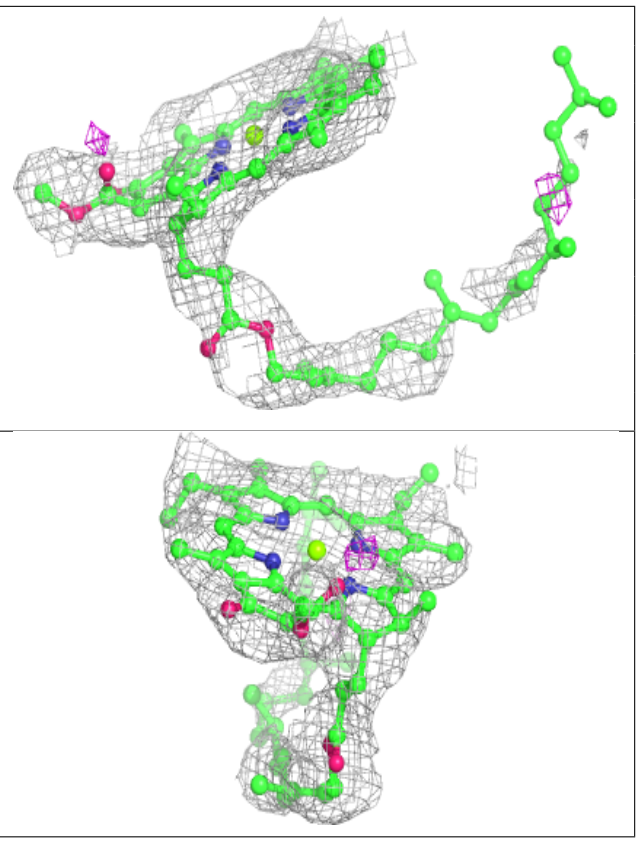
Electron density around BCR y 101:

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



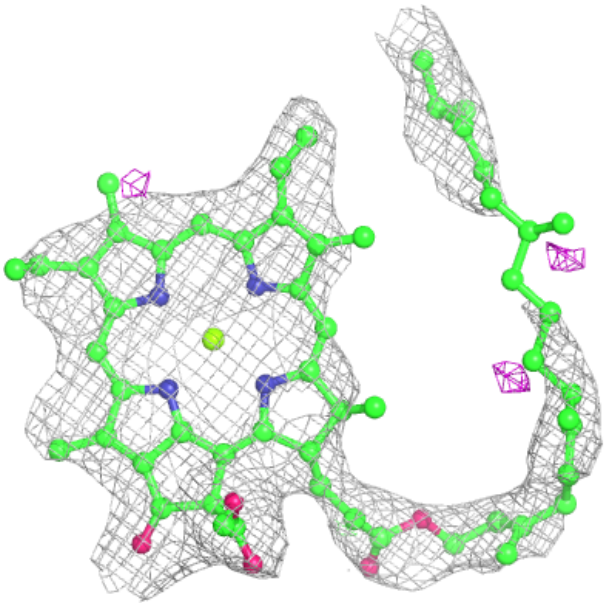
Electron density around CLA c 515:

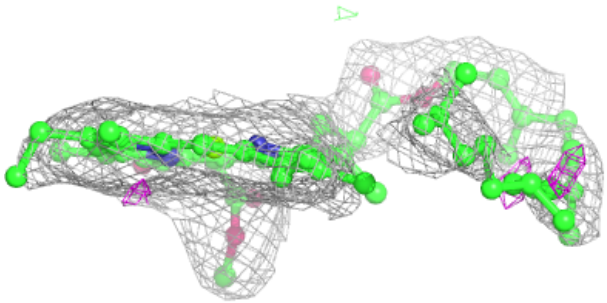
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

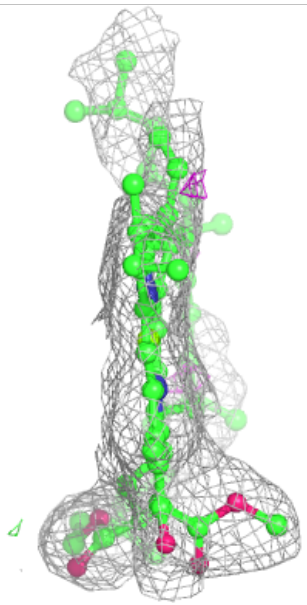


Electron density around CLA C 512:

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

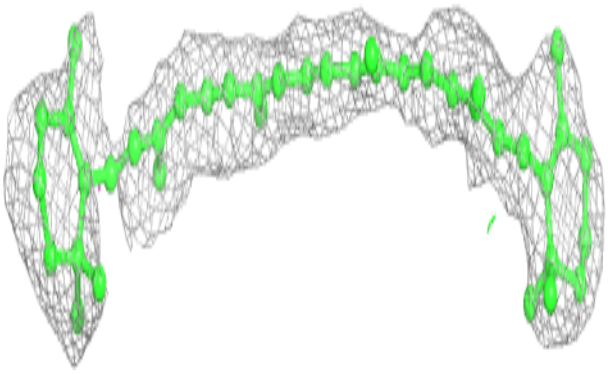


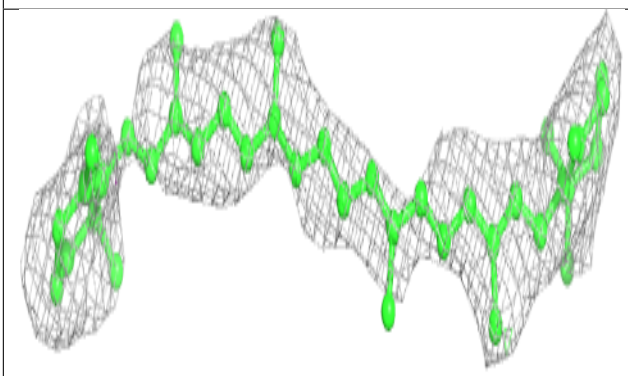


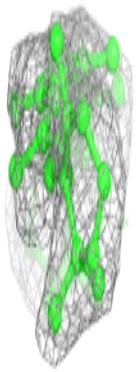


Electron density around BCR k 101:

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

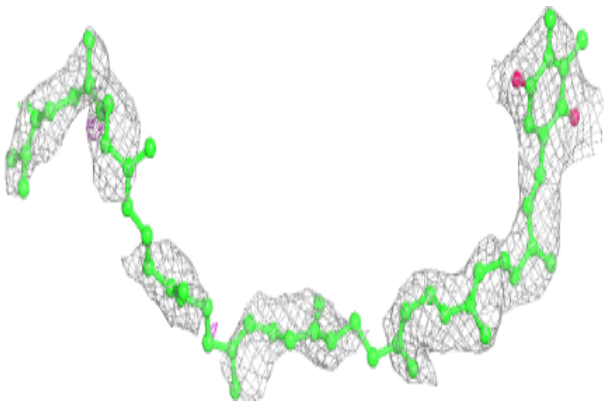


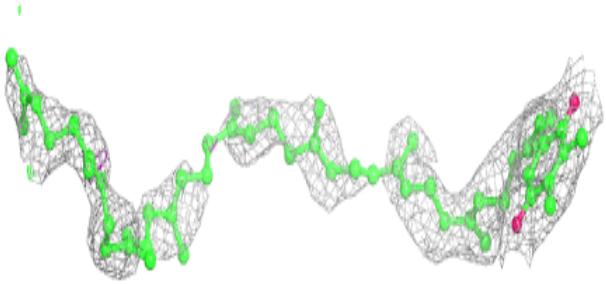


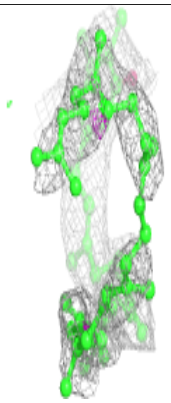


Electron density around PL9 a 611:

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

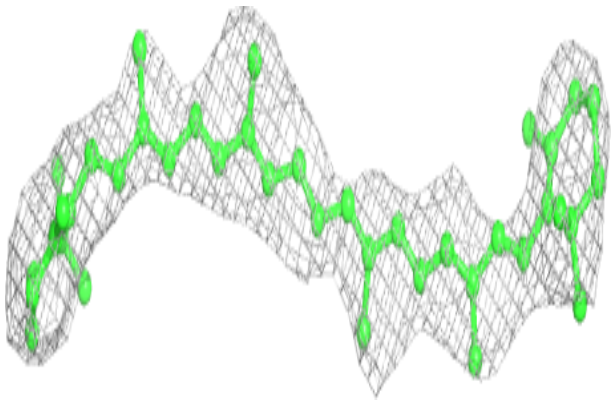


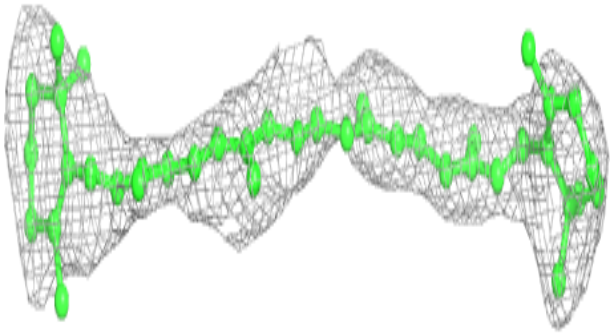


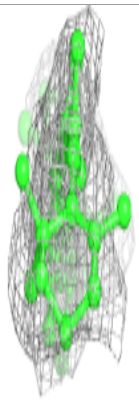


Electron density around BCR Y 101:

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

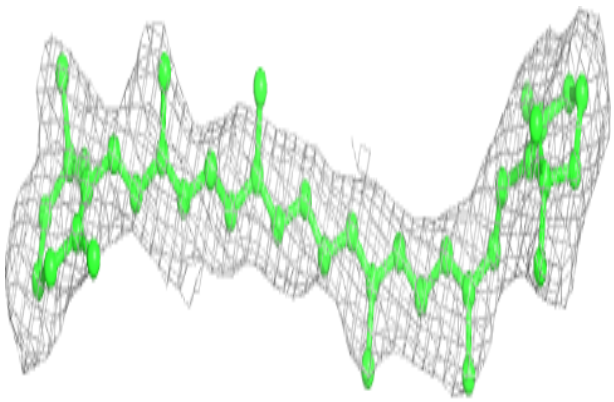


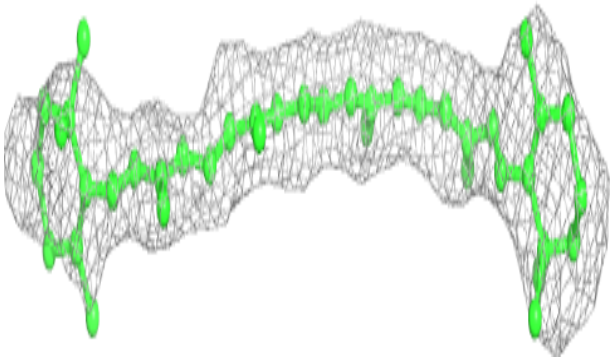


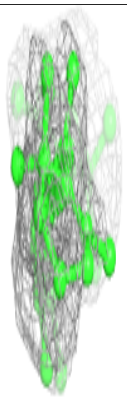


Electron density around BCR h 101:

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

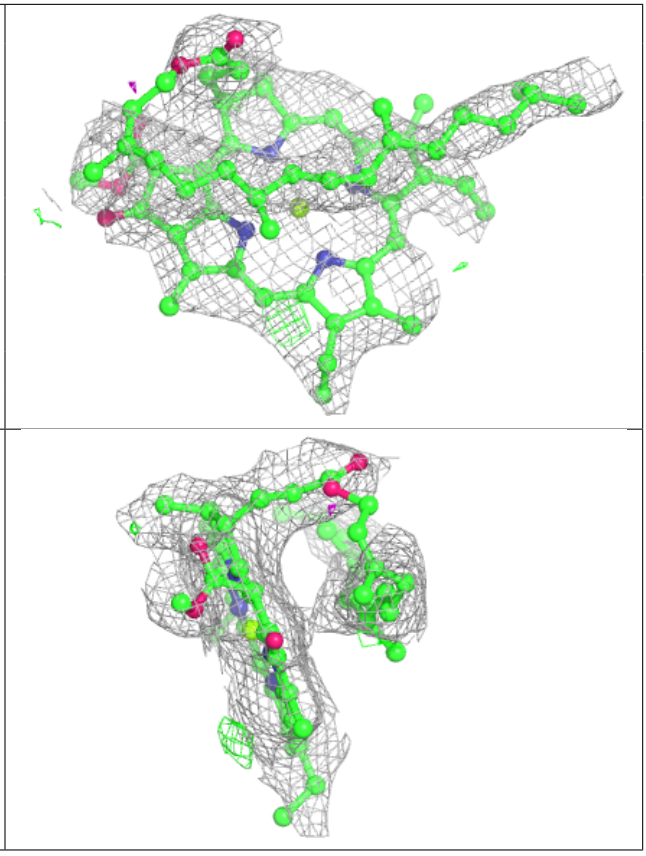






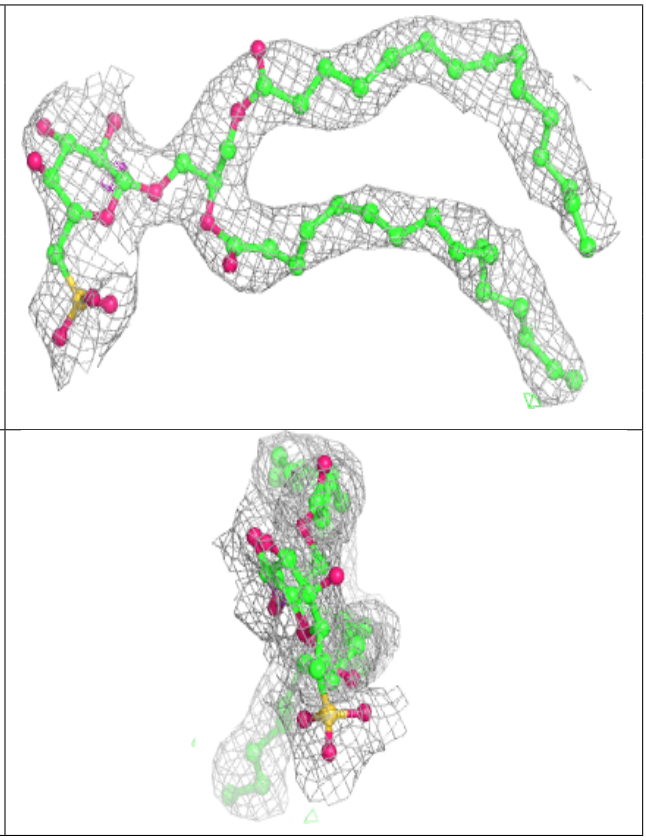
Electron density around CLA b 604:

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



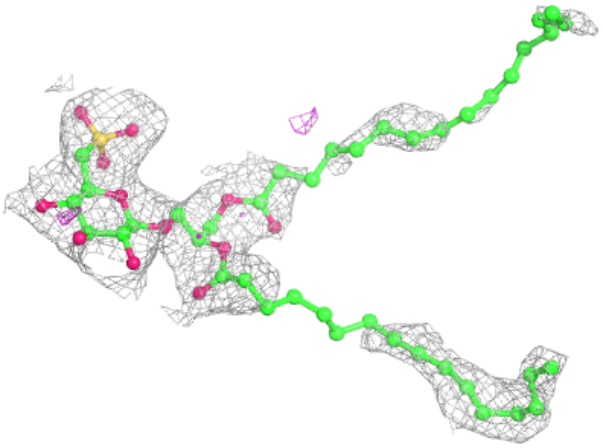
Electron density around SQD B 626:

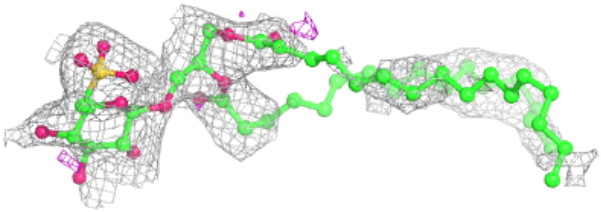
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

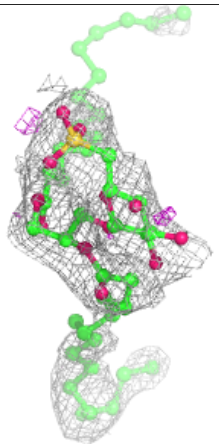


Electron density around SQD c 501:

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

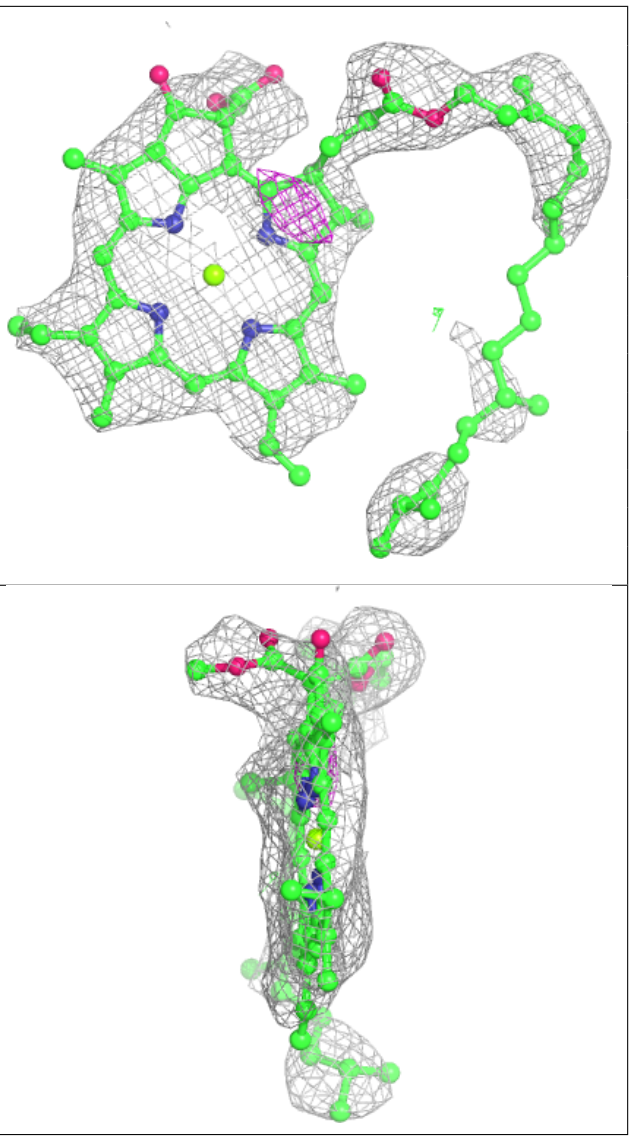






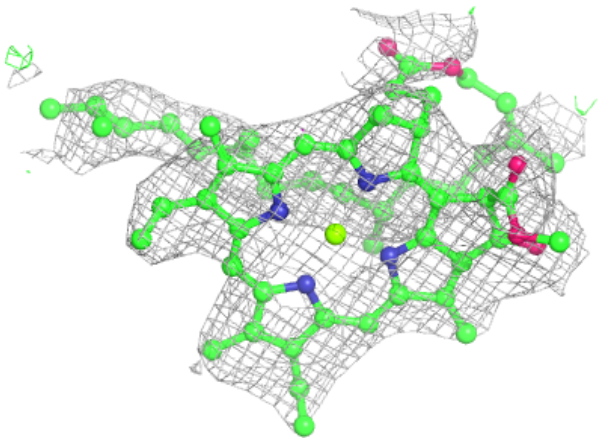
Electron density around CLA c 514:

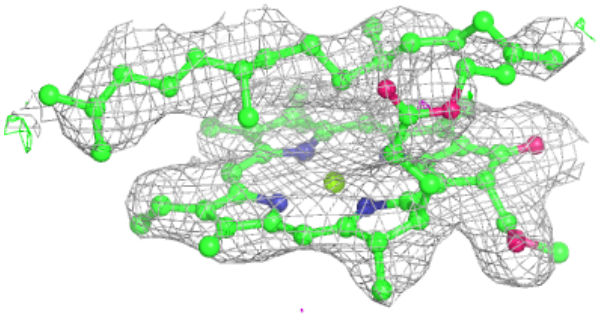
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

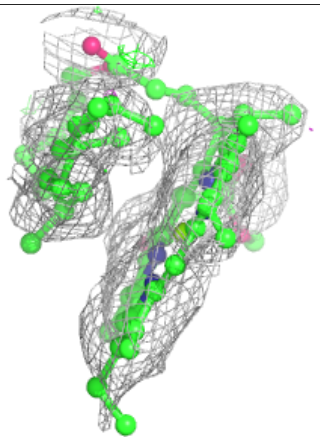


Electron density around CLA B 601:

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

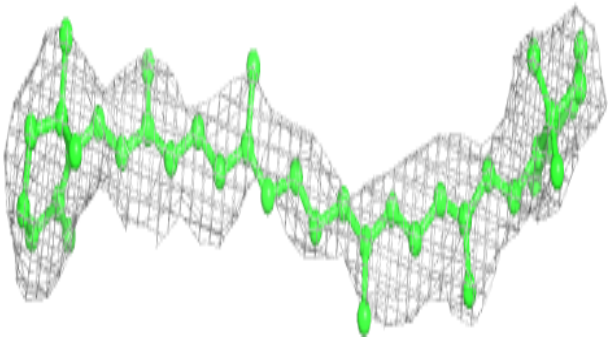


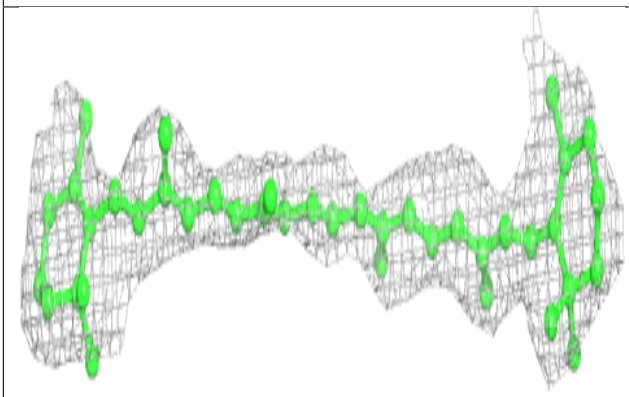


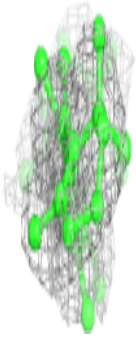


Electron density around BCR C 514:

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

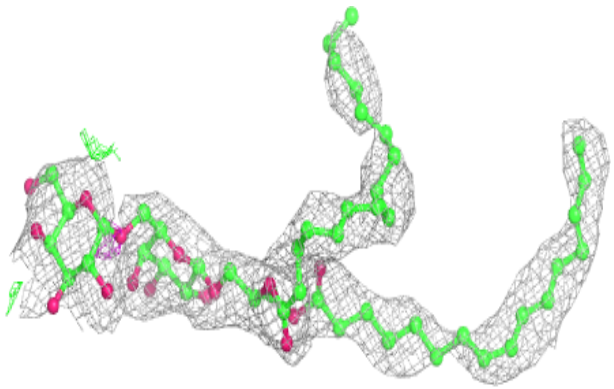


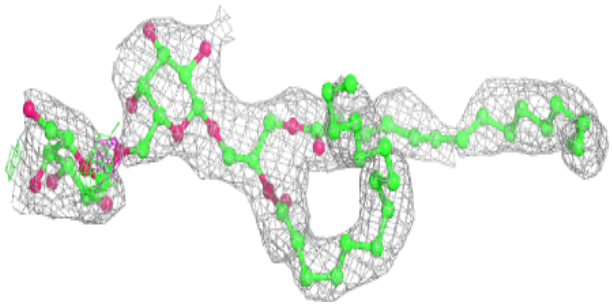


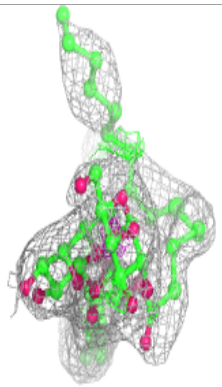


Electron density around DGD H 103:

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

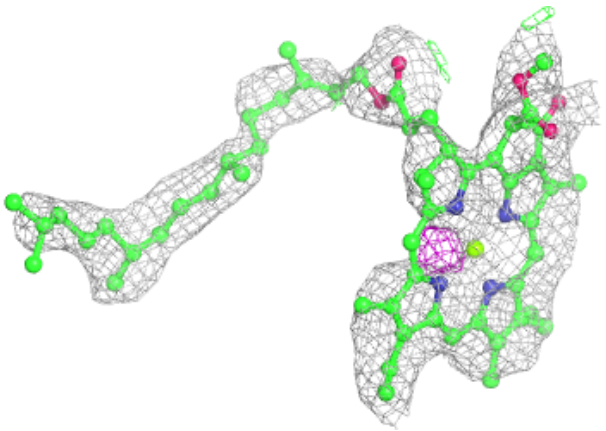


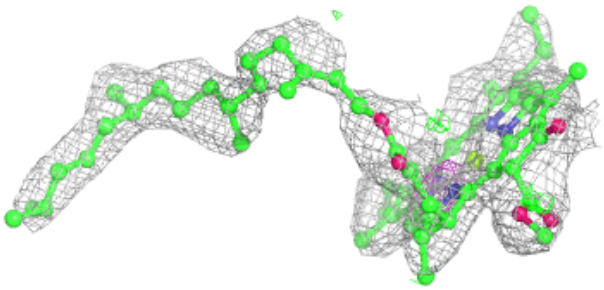


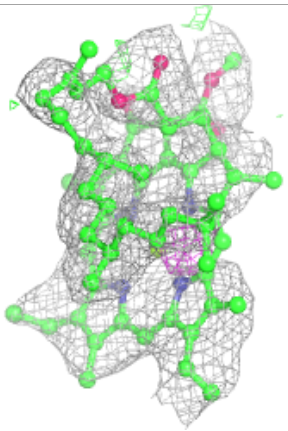


Electron density around CLA C 511:

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

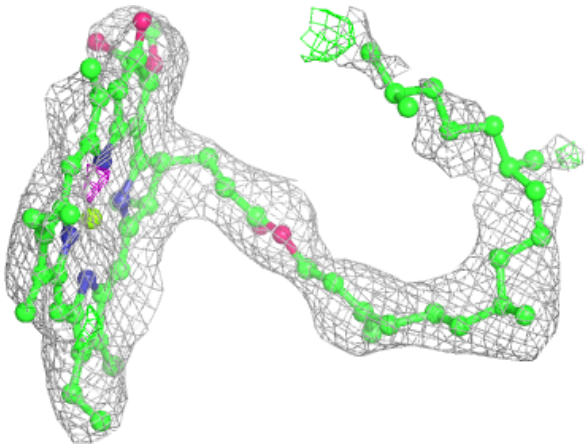


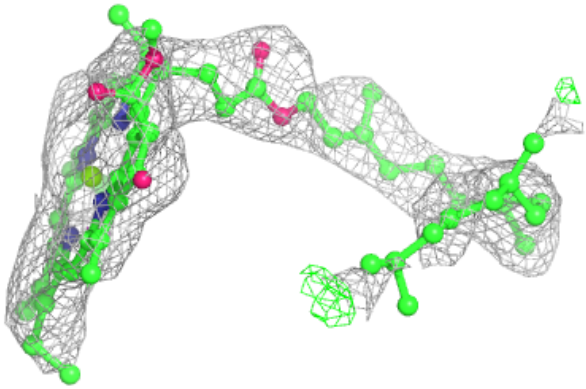


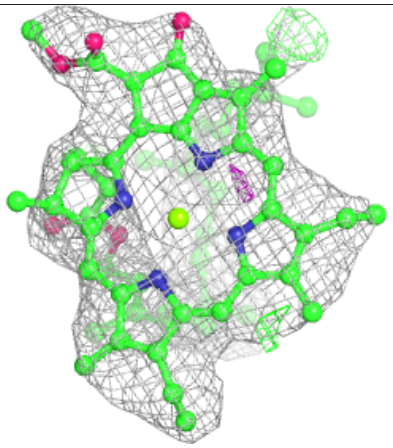


Electron density around CLA B 606:

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

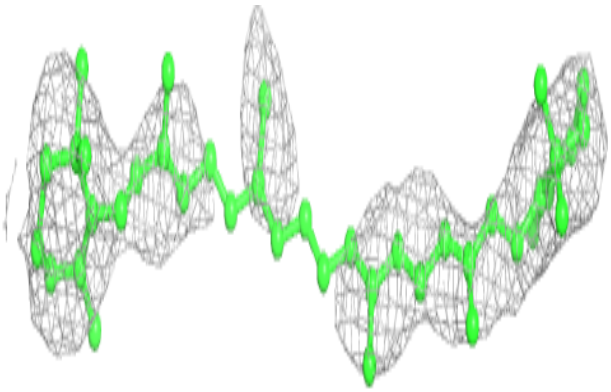


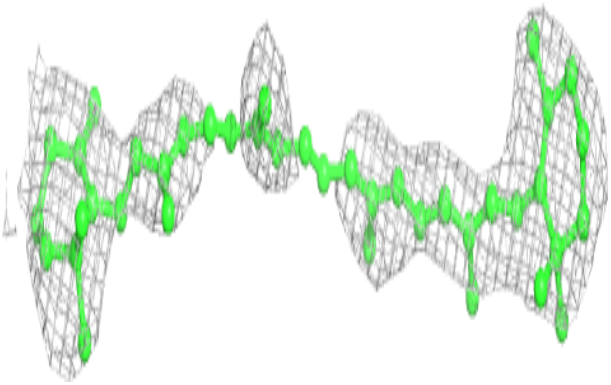


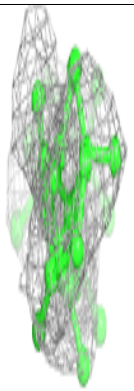


Electron density around BCR c 516:

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

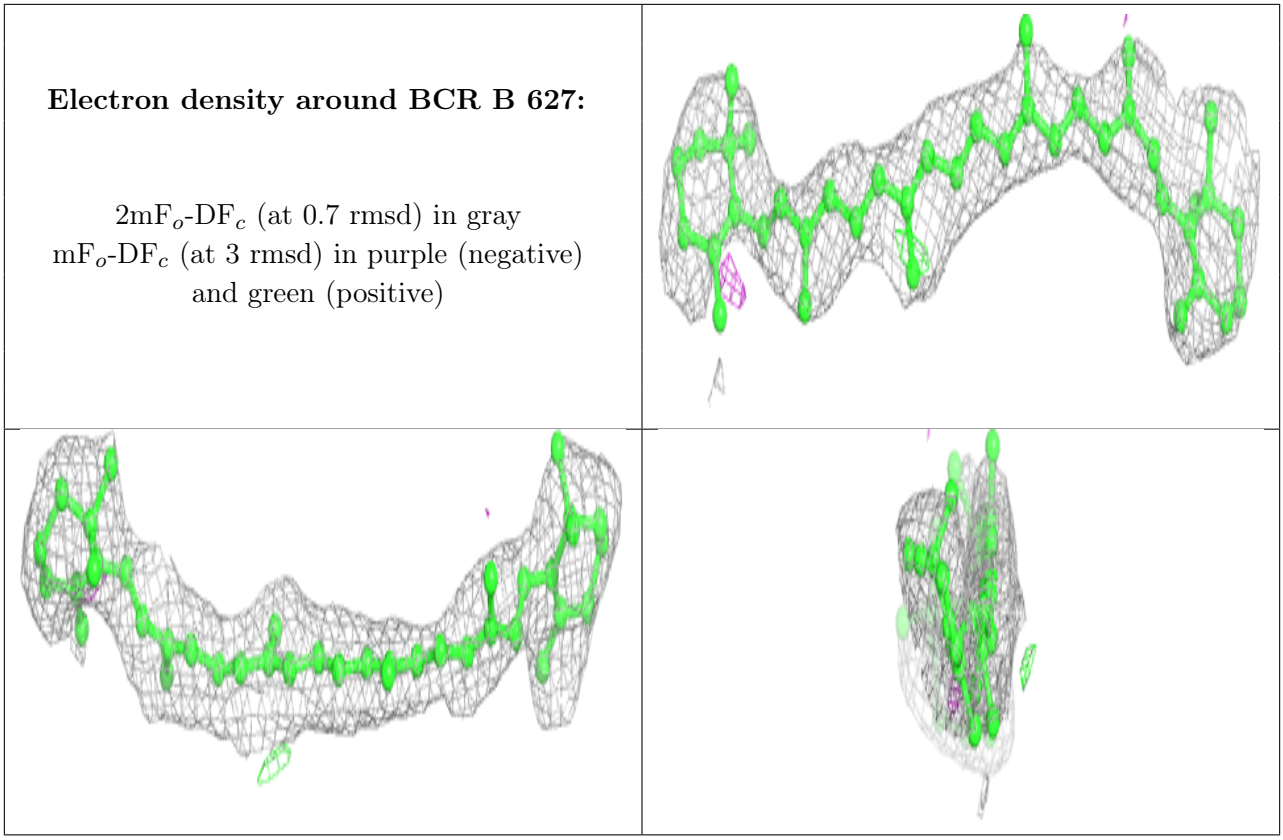






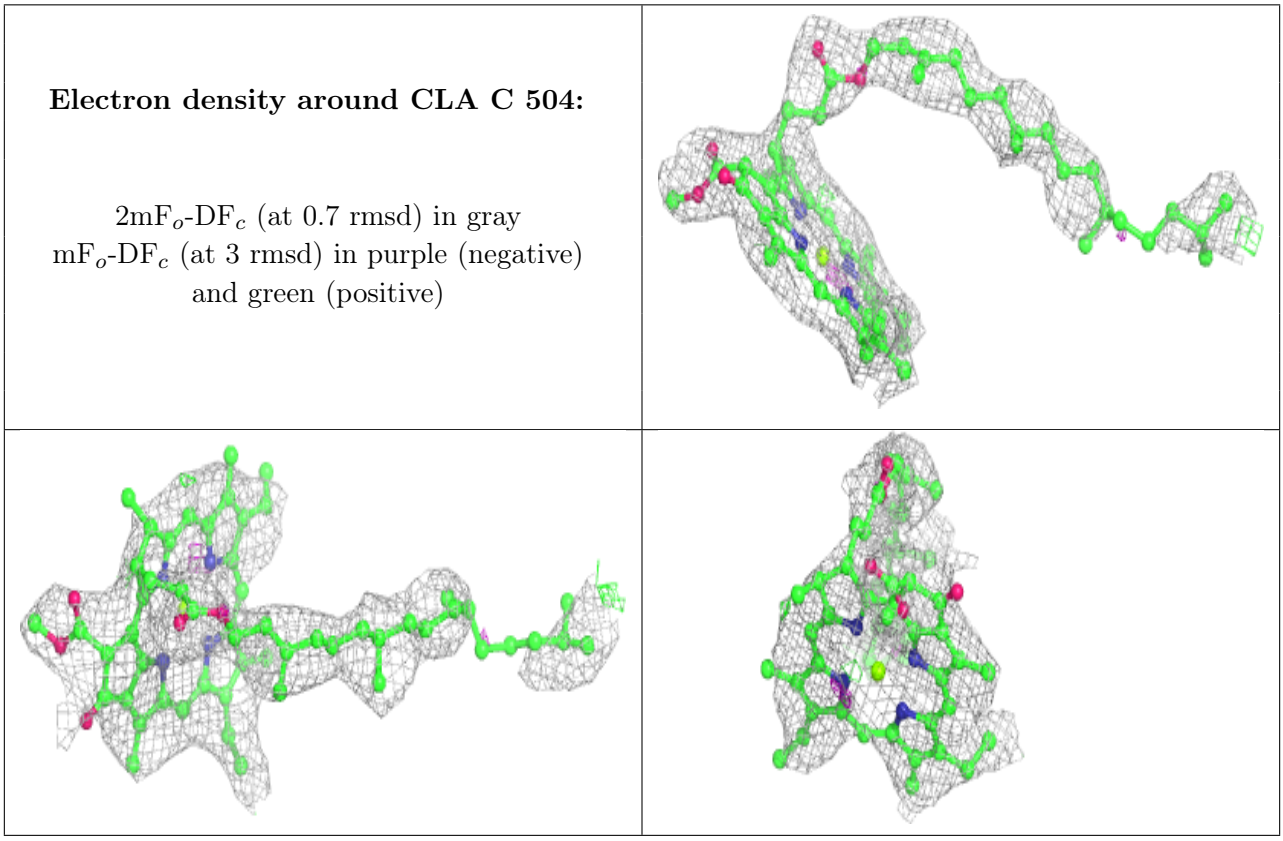
Electron density around BCR B 627:

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



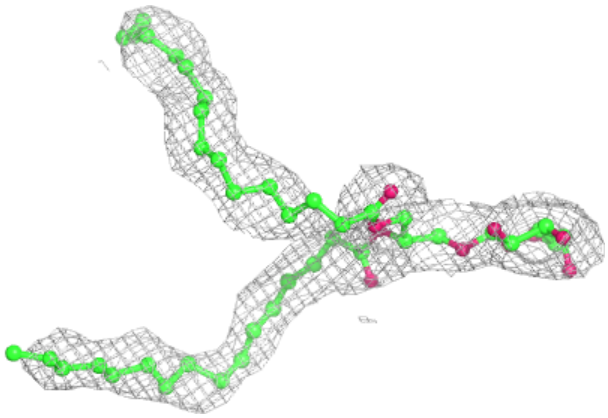
Electron density around CLA C 504:

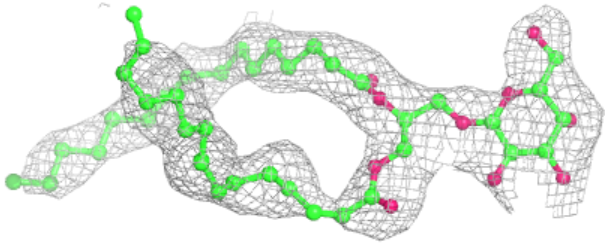
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

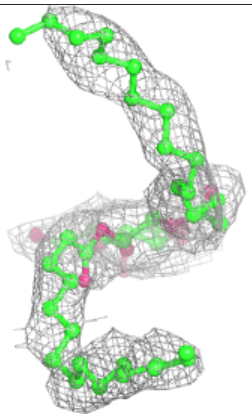


Electron density around LMG B 620:

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

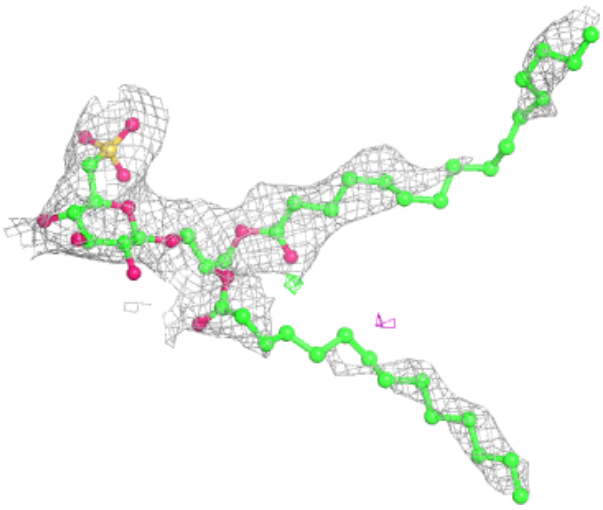


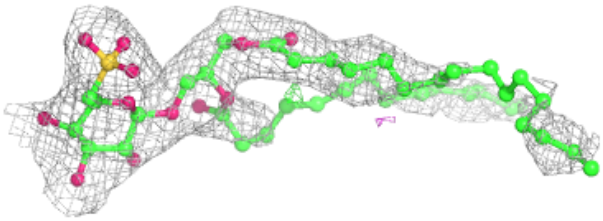


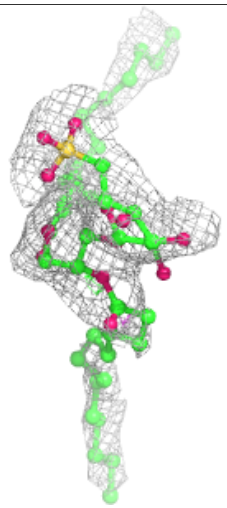


Electron density around SQD A 603:

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

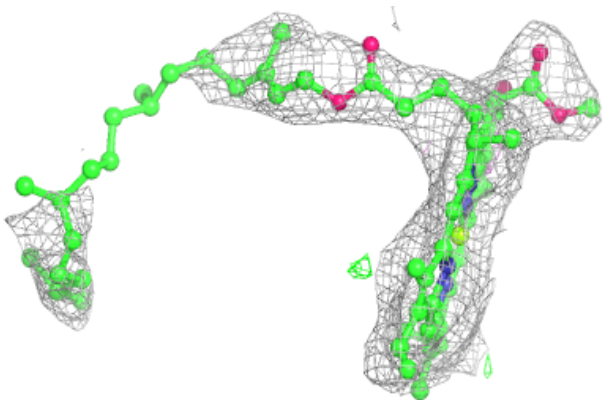


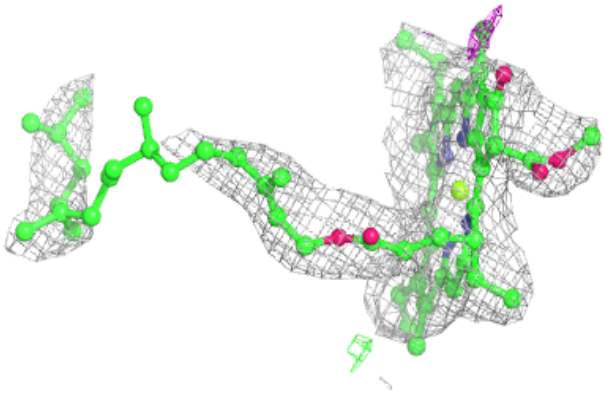


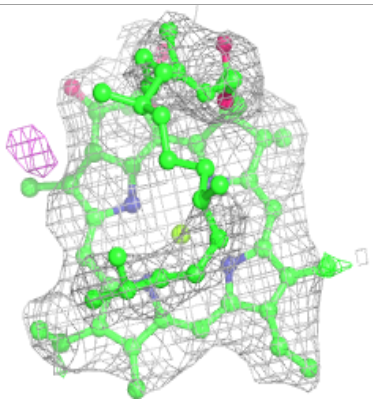


Electron density around CLA c 508:

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

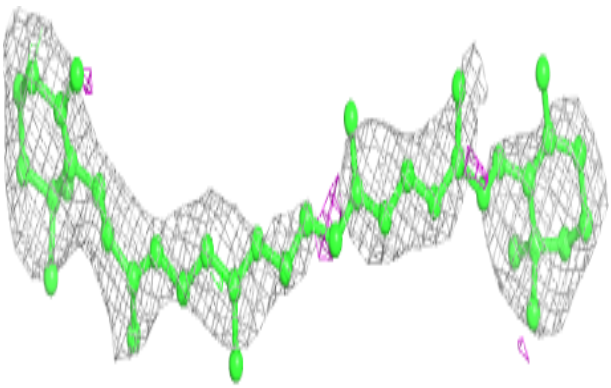


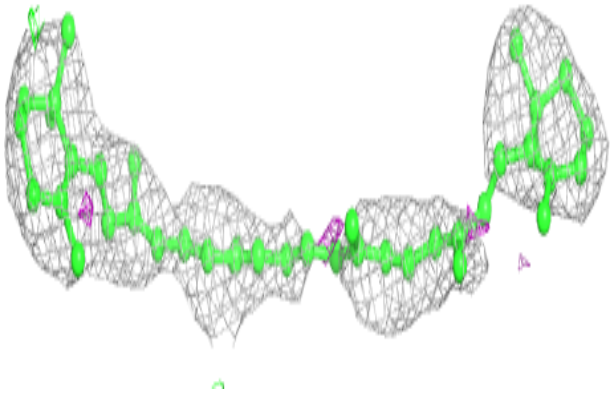


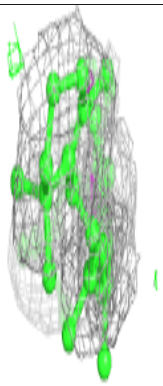


Electron density around BCR T 101:

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

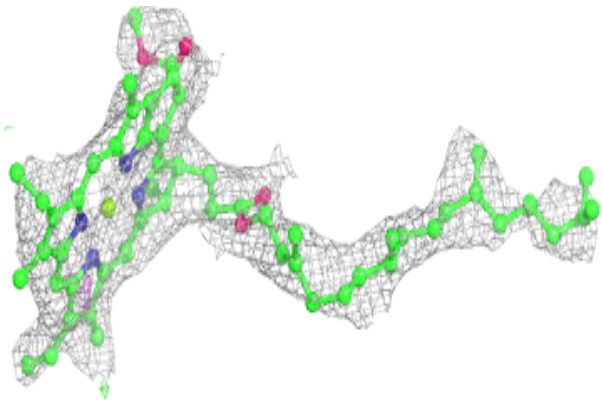


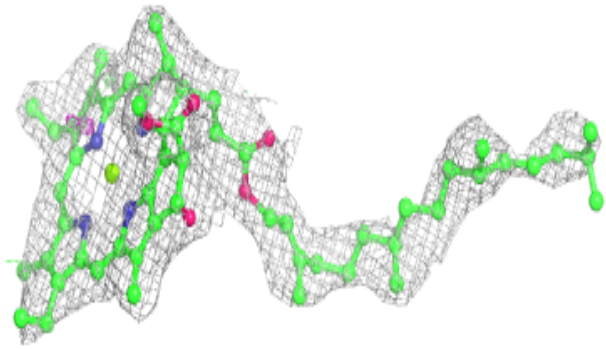


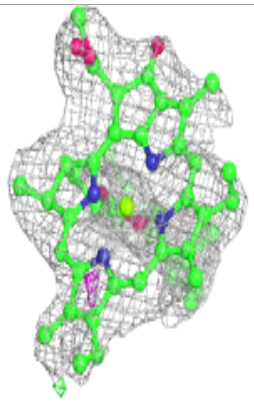


Electron density around CLA C 502:

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

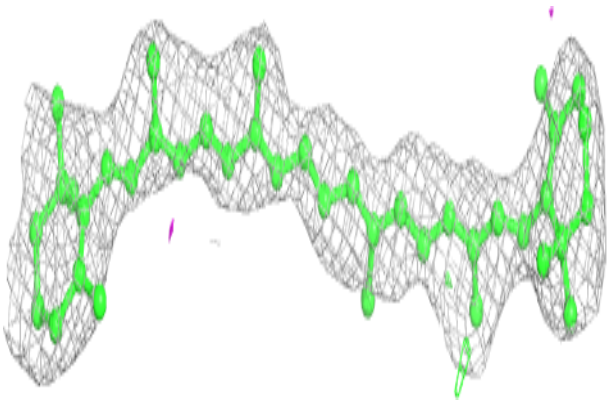


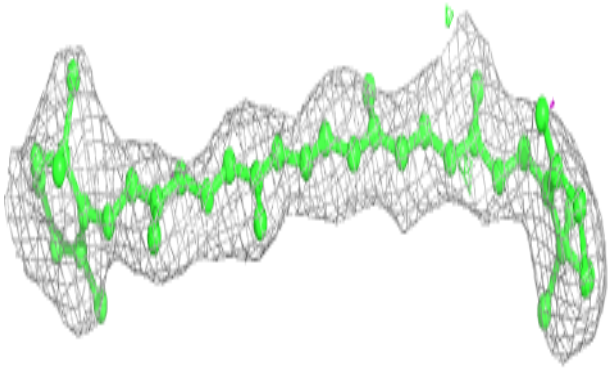


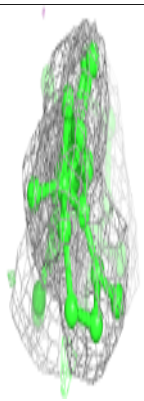


Electron density around BCR b 622:

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

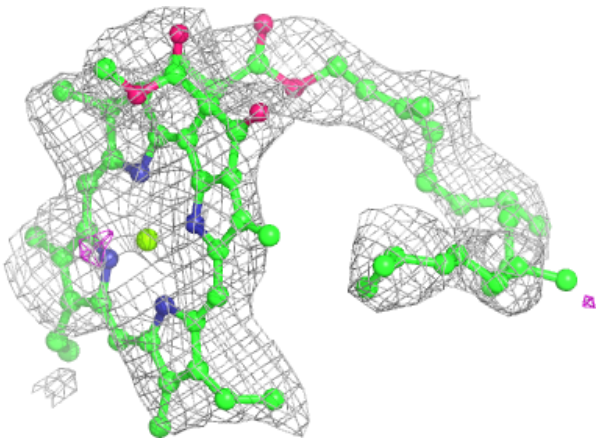


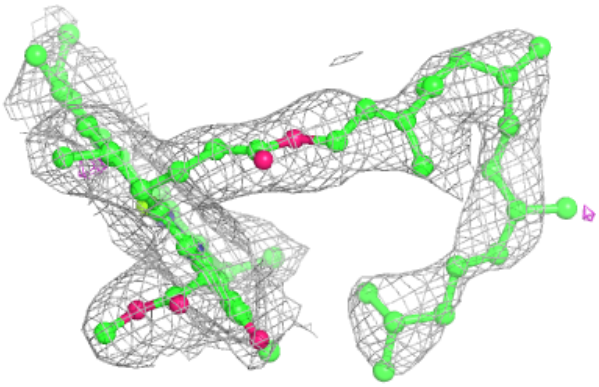


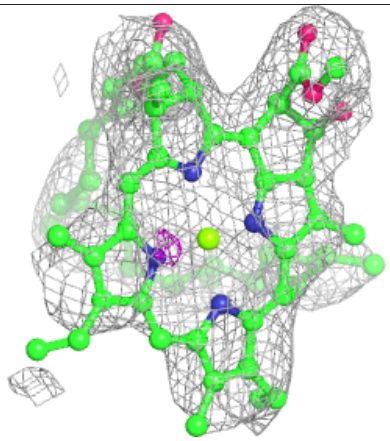


Electron density around CLA C 503:

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

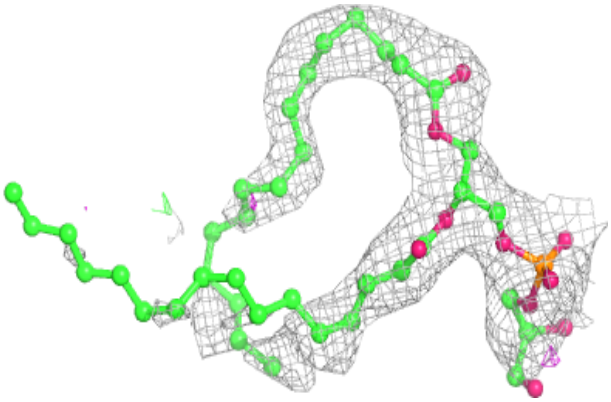


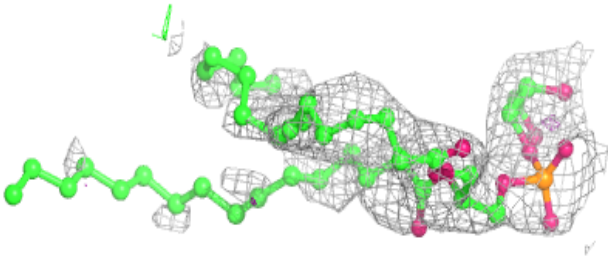


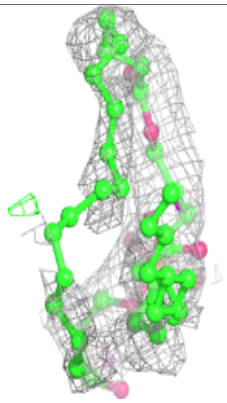


Electron density around LHG A 617:

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

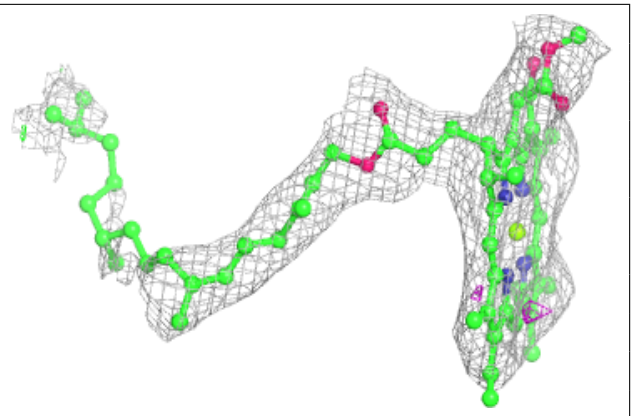


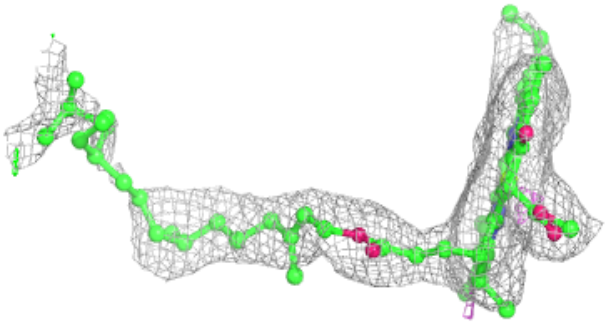


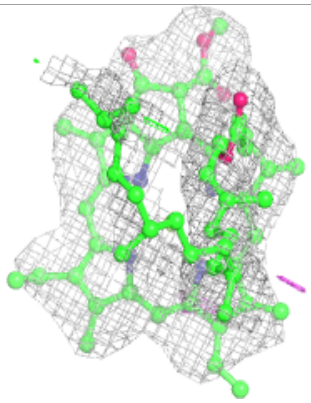


Electron density around CLA d 404:

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

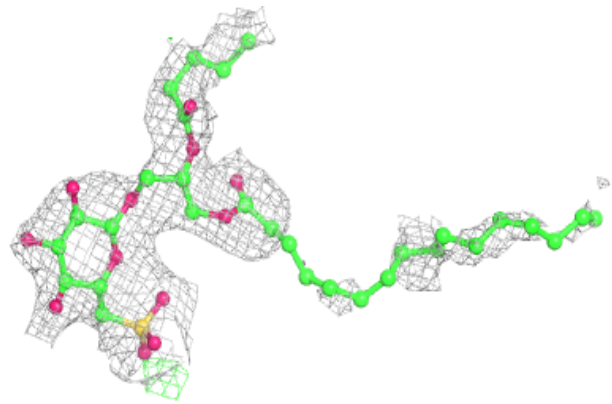


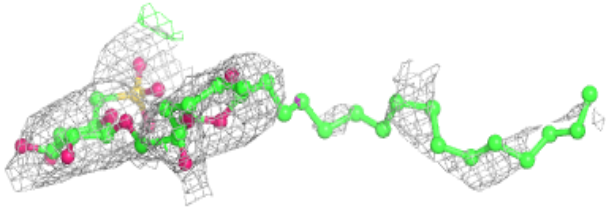


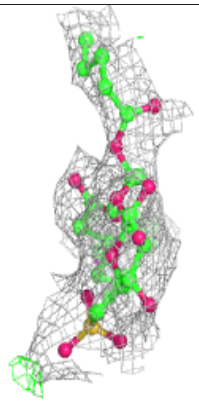


Electron density around SQD f 101:

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

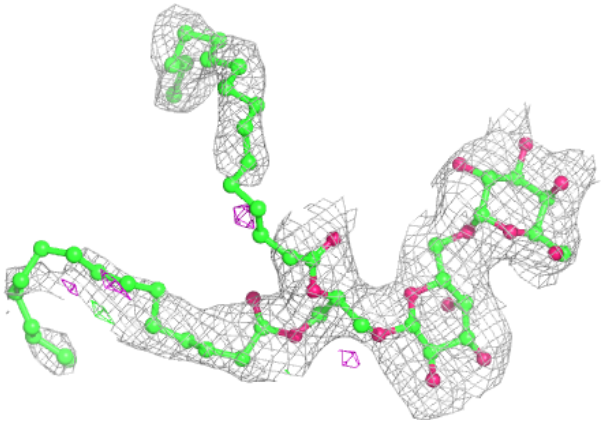


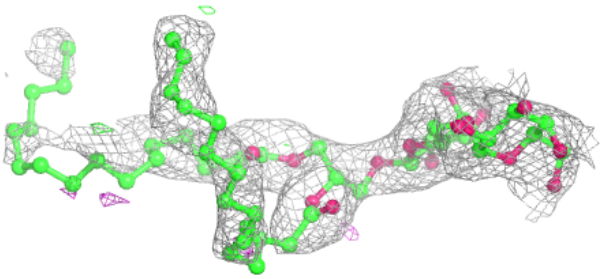


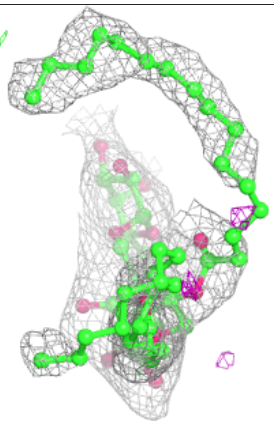


Electron density around DGD c 519:

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

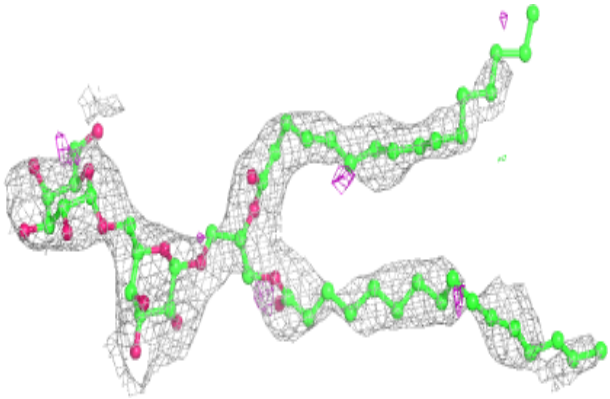


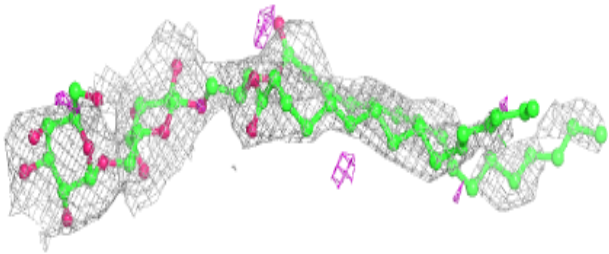


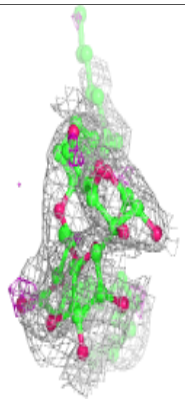


Electron density around DGD c 520:

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

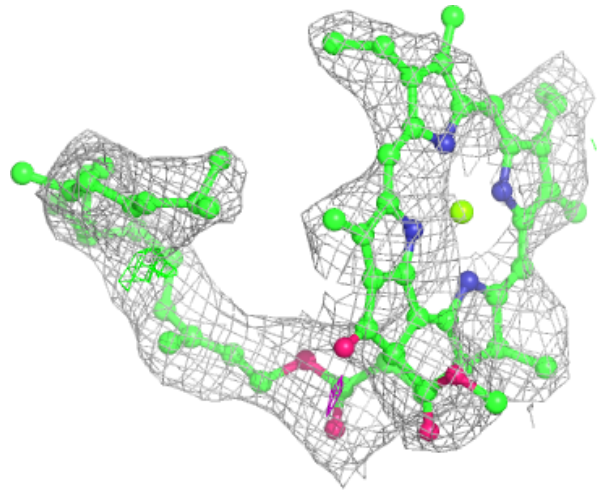


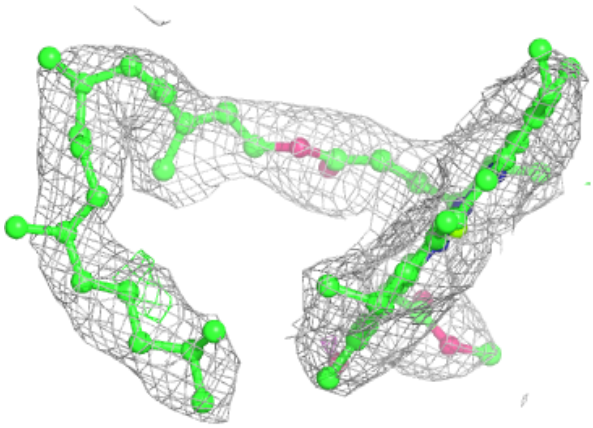


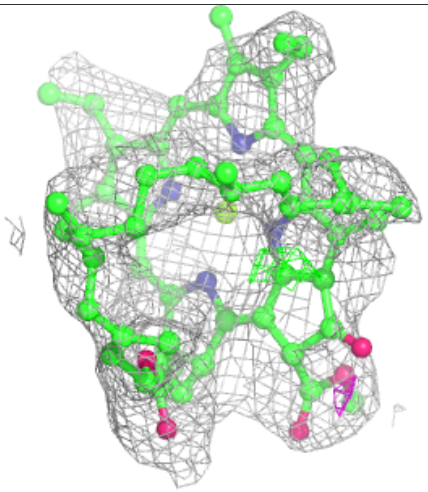


Electron density around CLA c 505:

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

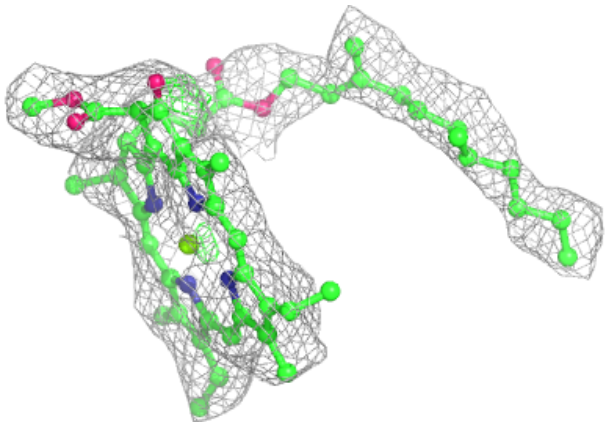


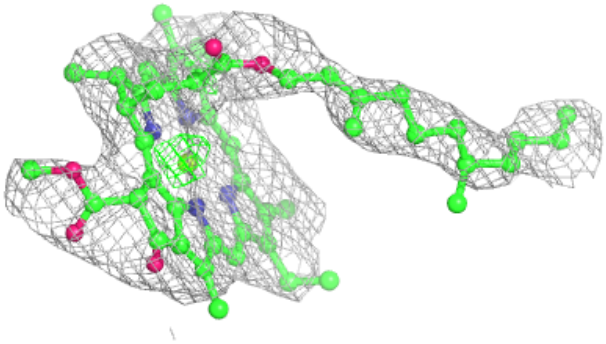


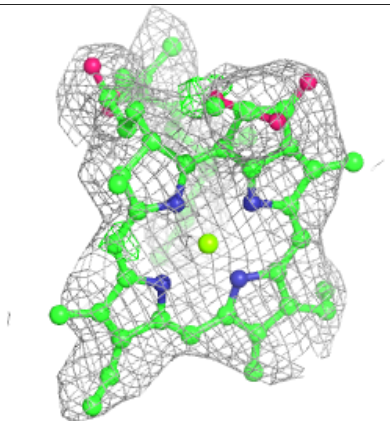


Electron density around CLA c 510:

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

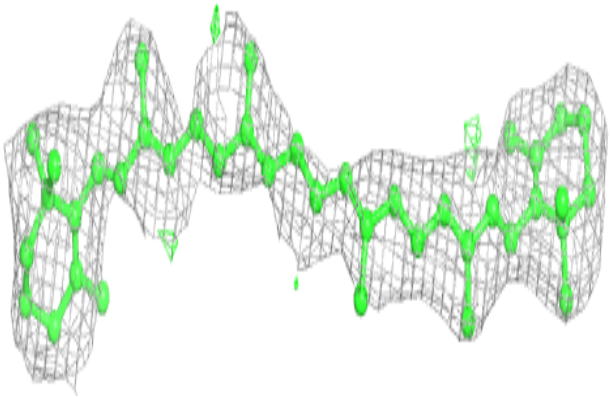


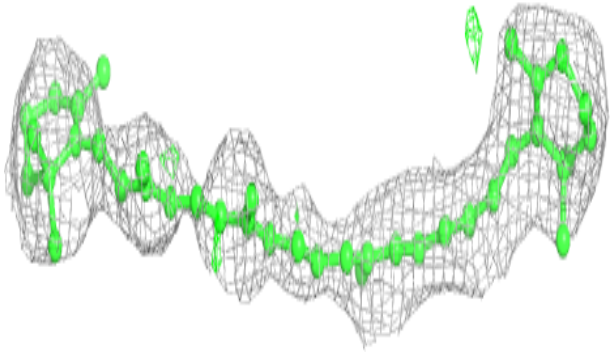


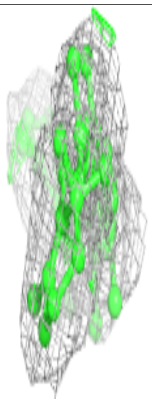


Electron density around BCR d 405:

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

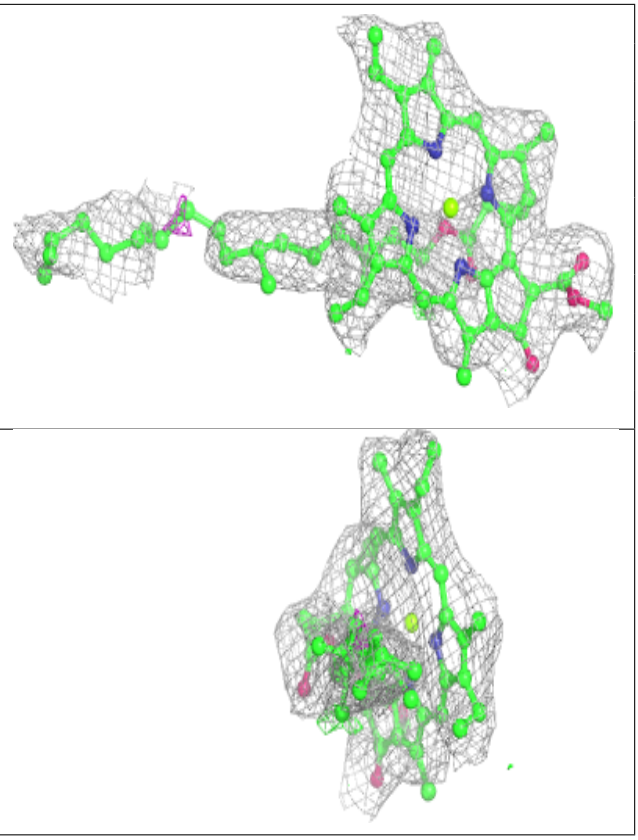






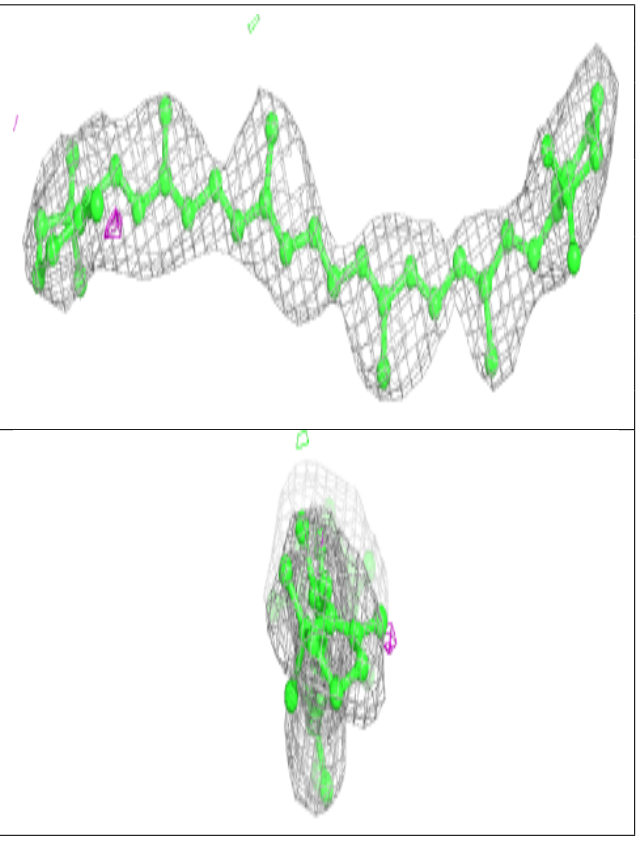
Electron density around CLA B 614:

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



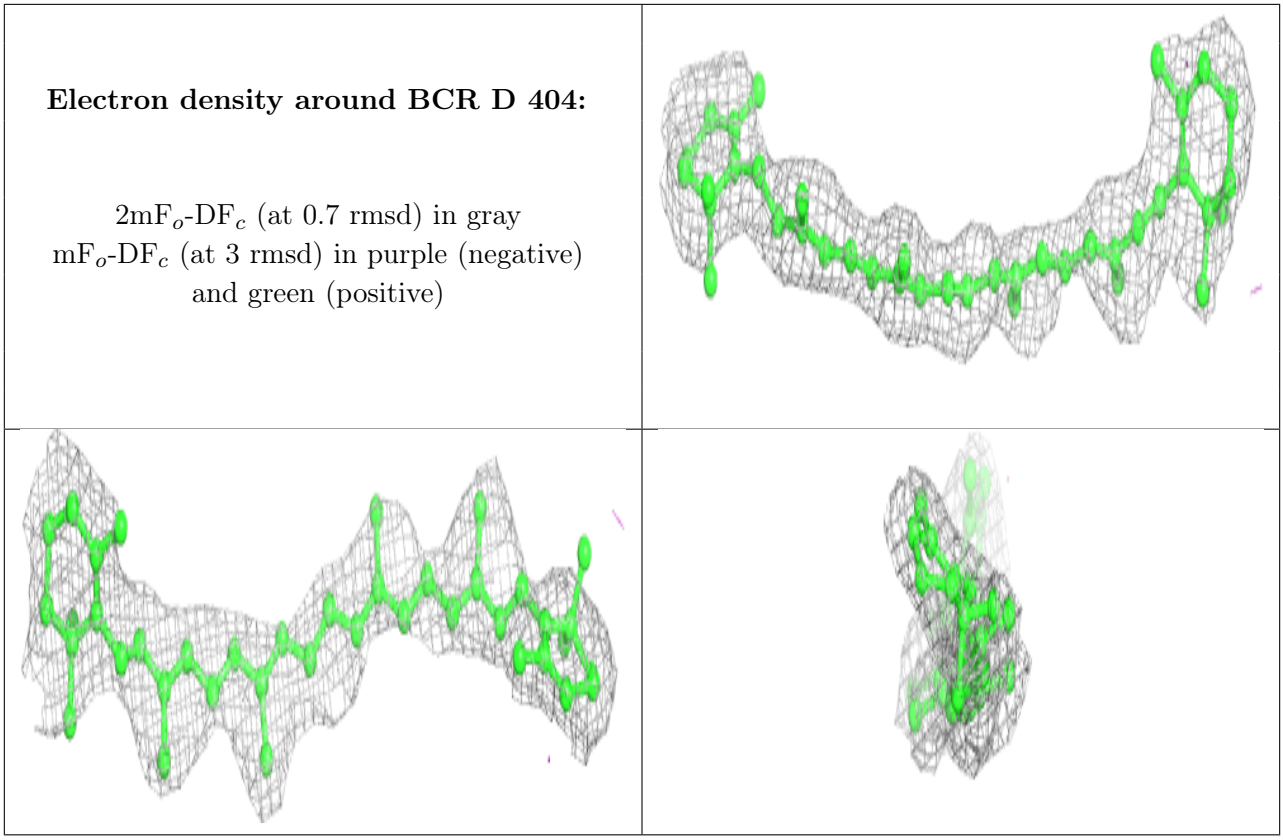
Electron density around BCR C 515:

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



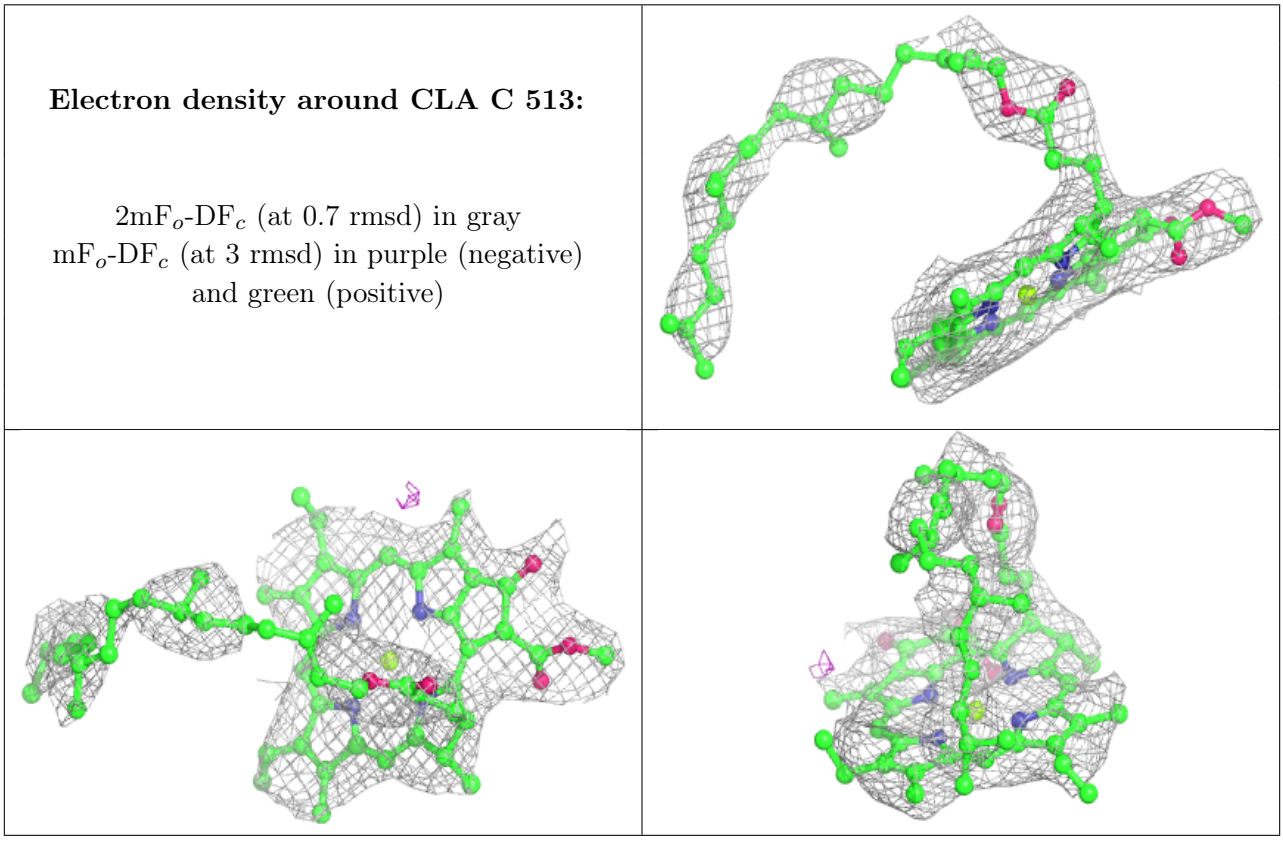
Electron density around BCR D 404:

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



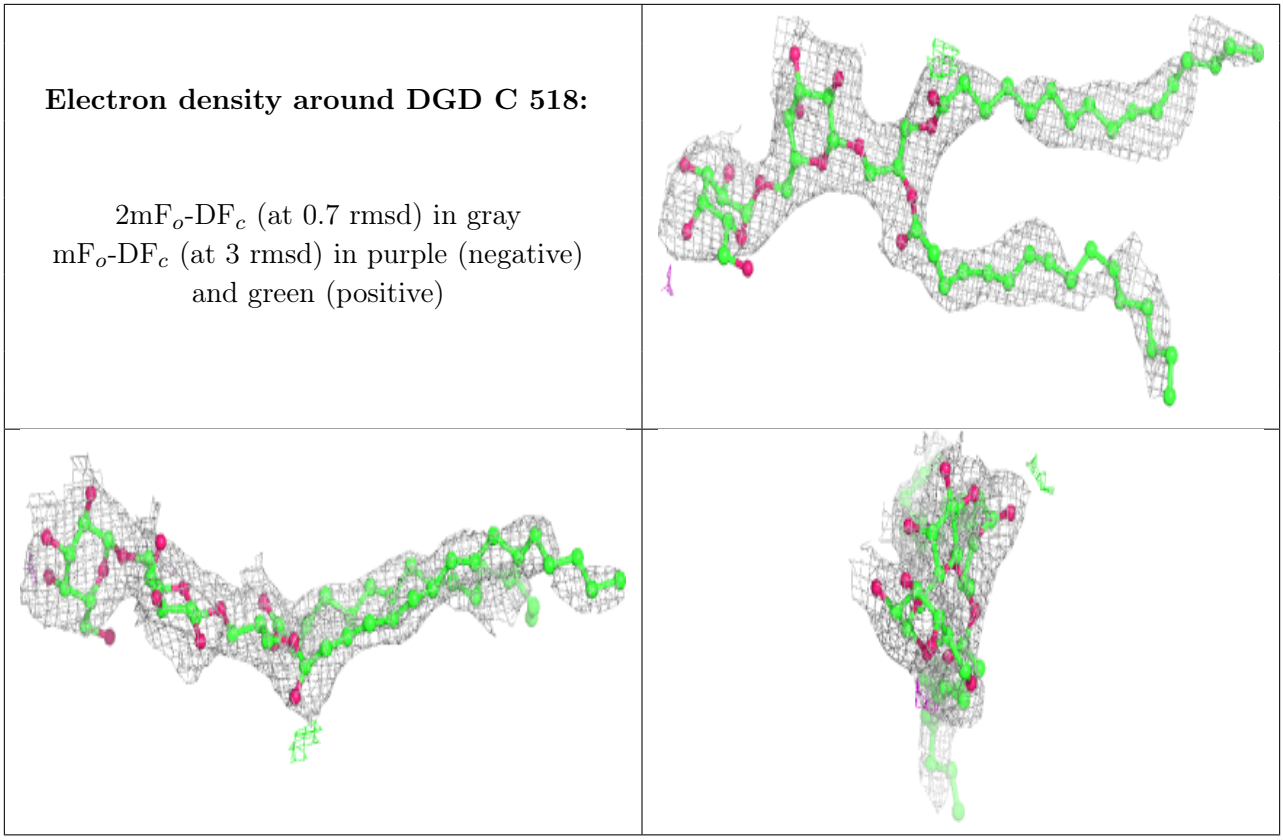
Electron density around CLA C 513:

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



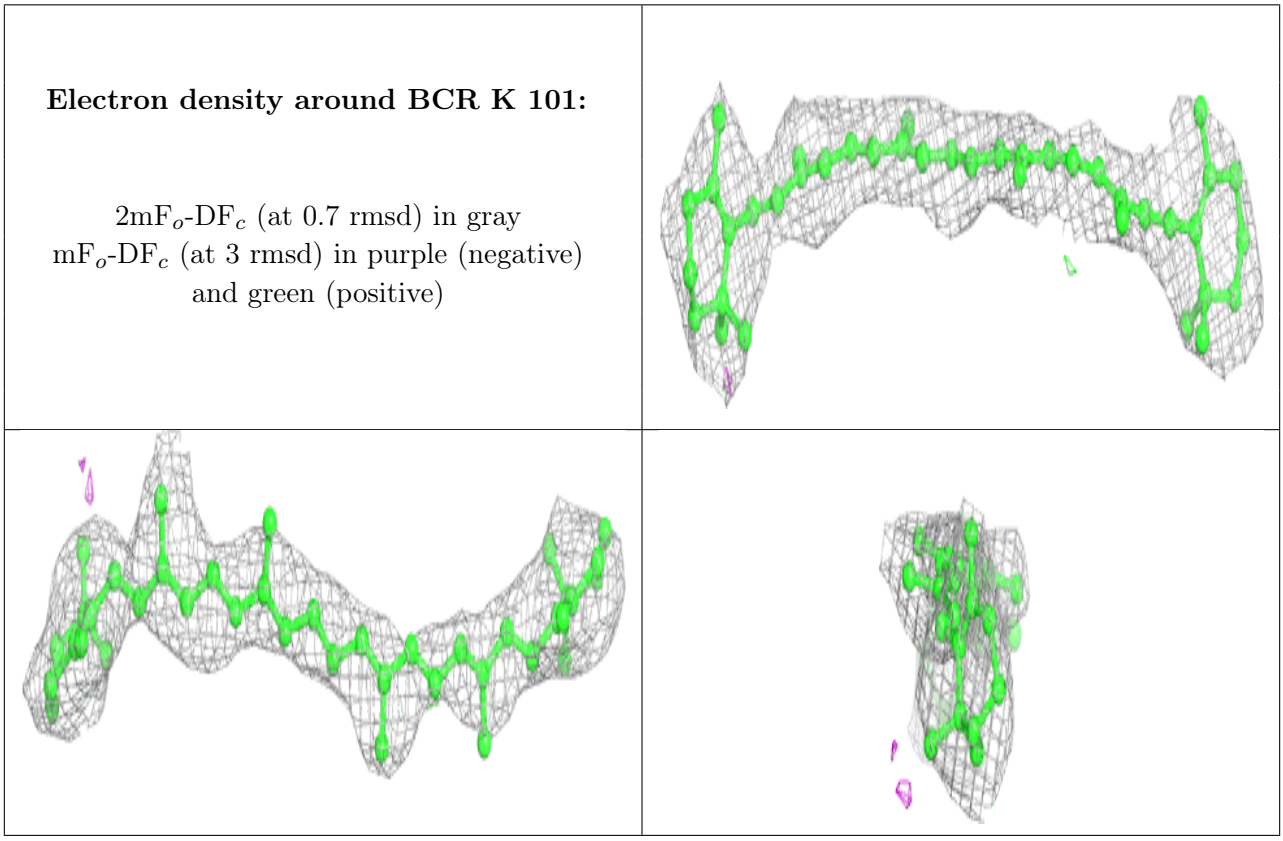
Electron density around DGD C 518:

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



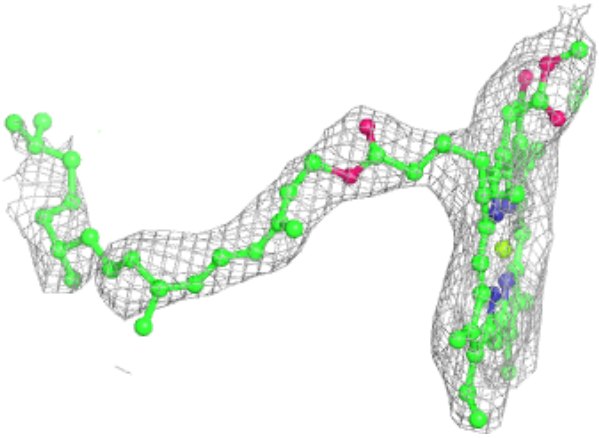
Electron density around BCR K 101:

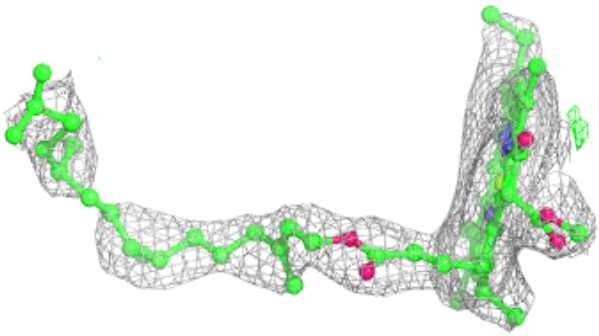
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

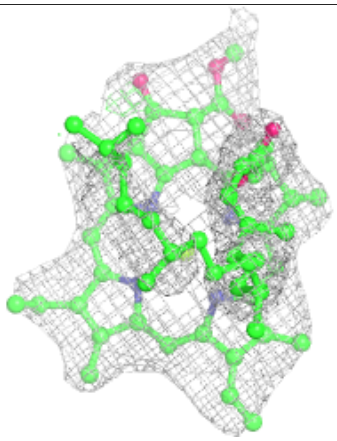


Electron density around CLA D 403:

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

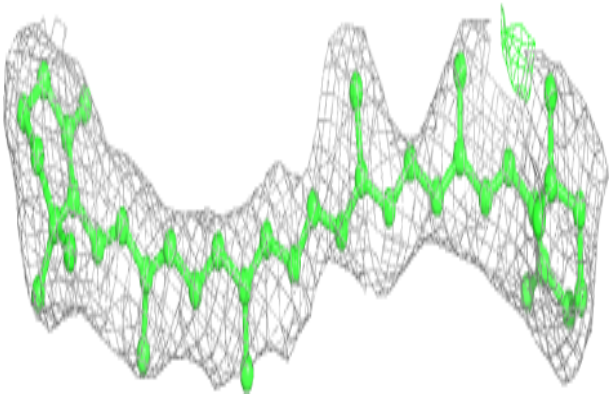


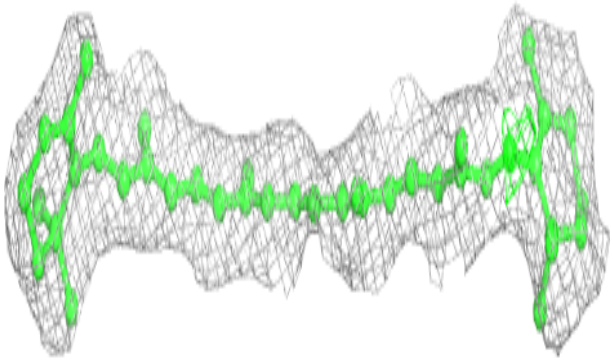


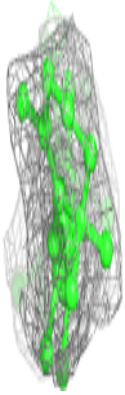


Electron density around BCR B 618:

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

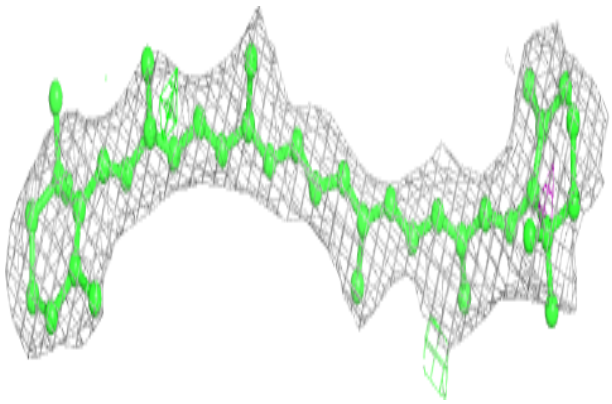


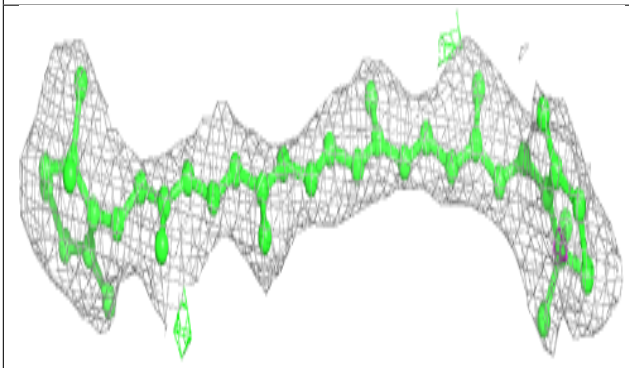


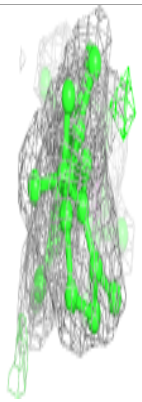


Electron density around BCR B 619:

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

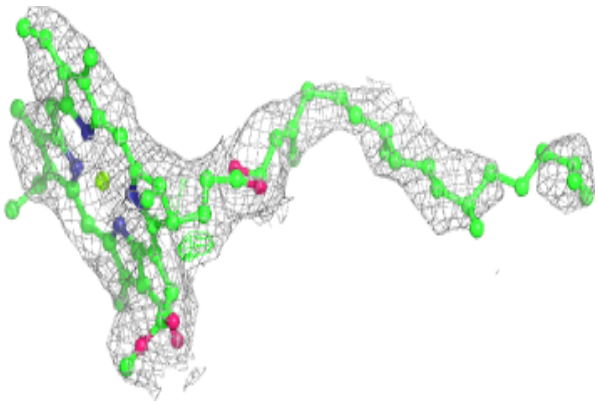


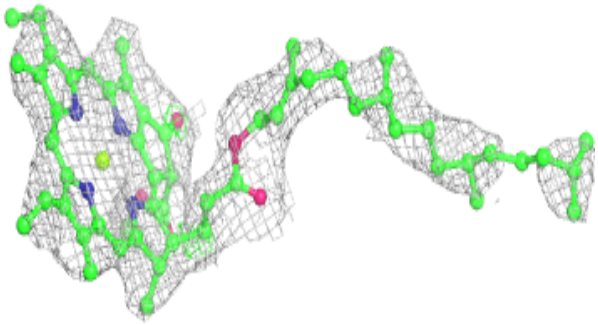


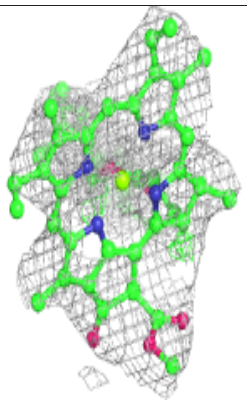


Electron density around CLA c 504:

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

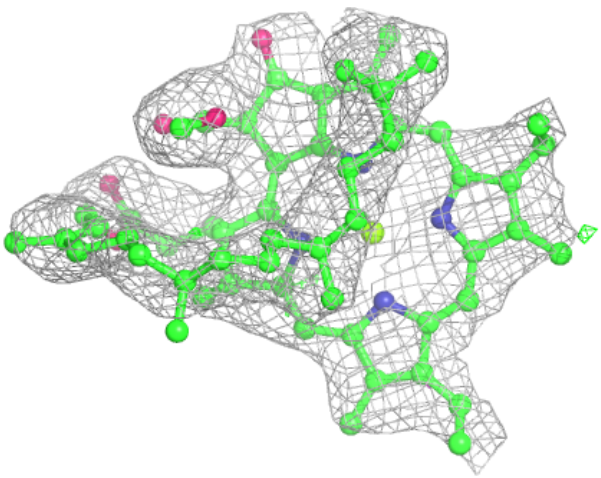


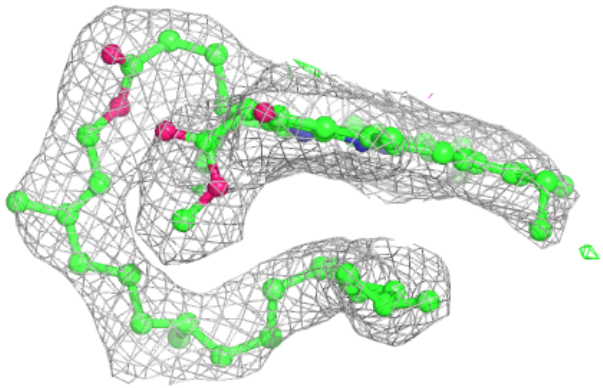


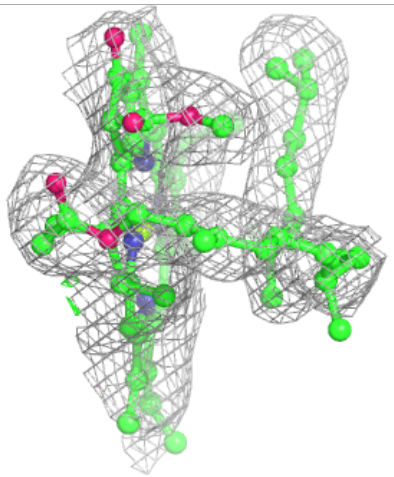


Electron density around CLA C 510:

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

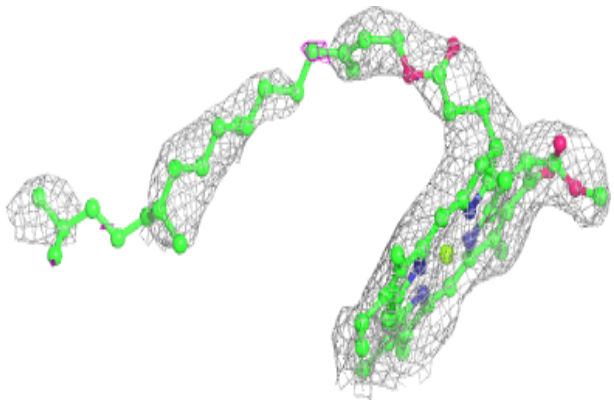


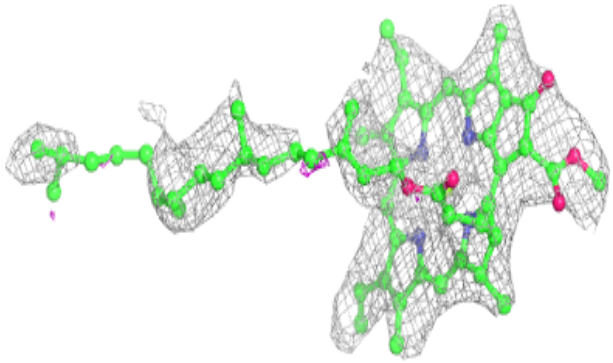


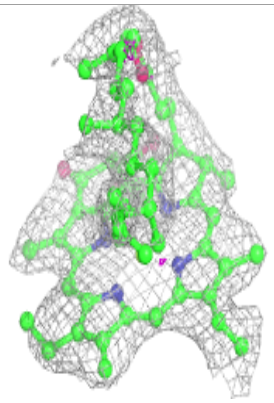


Electron density around CLA c 506:

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

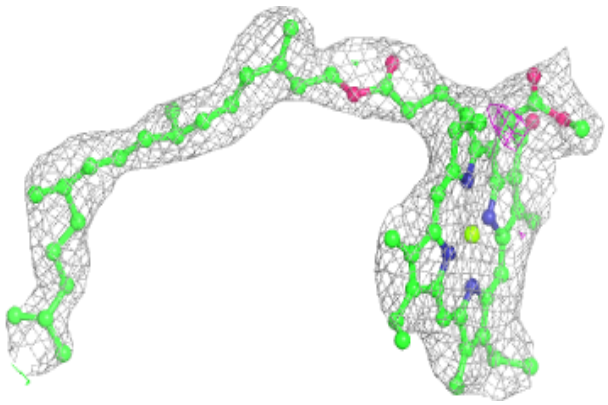


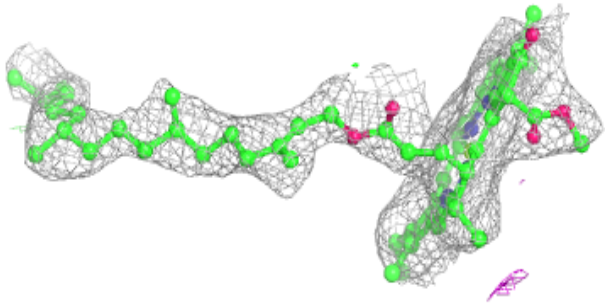


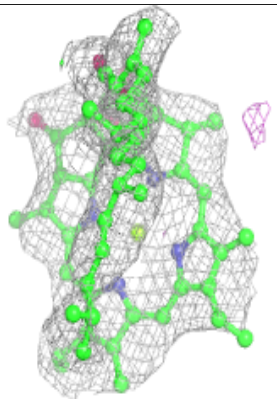


Electron density around CLA B 609:

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

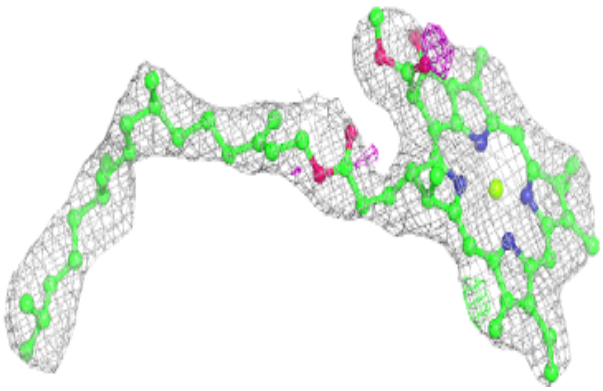


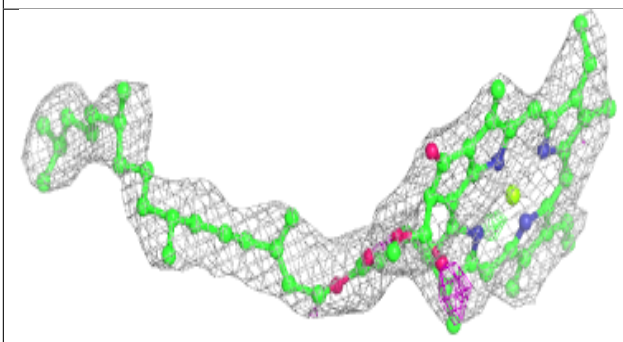


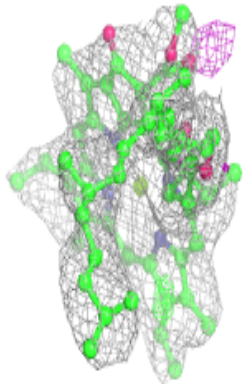


Electron density around CLA A 606:

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

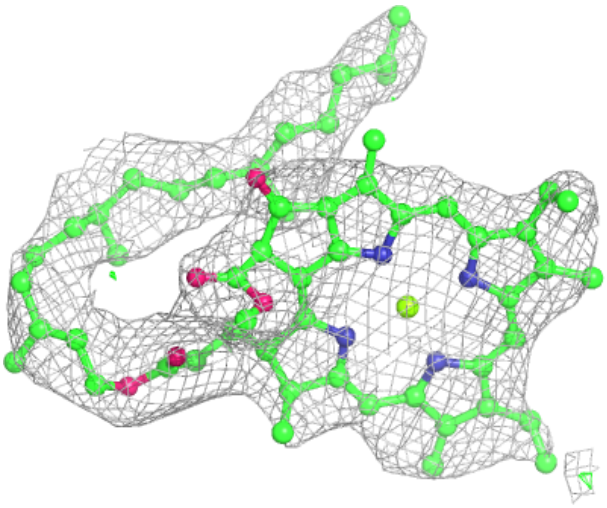


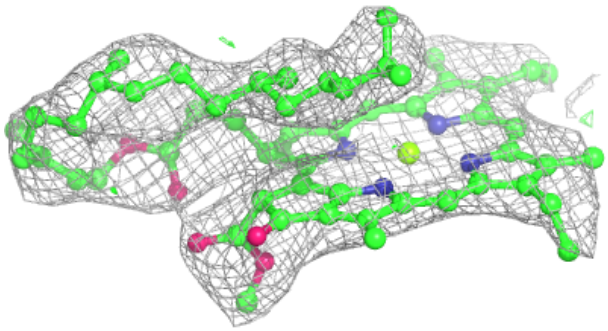


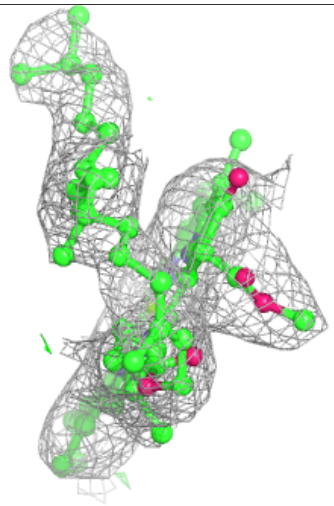


Electron density around CLA c 511:

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

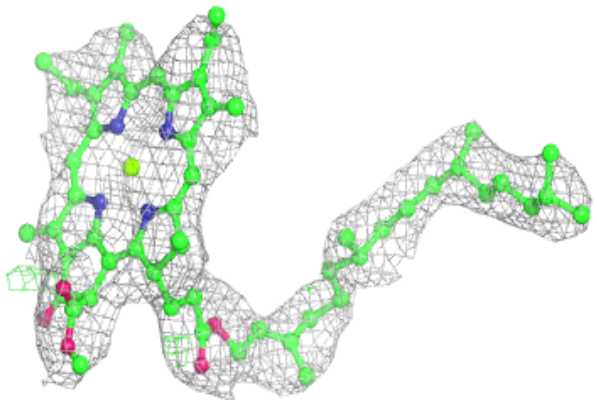


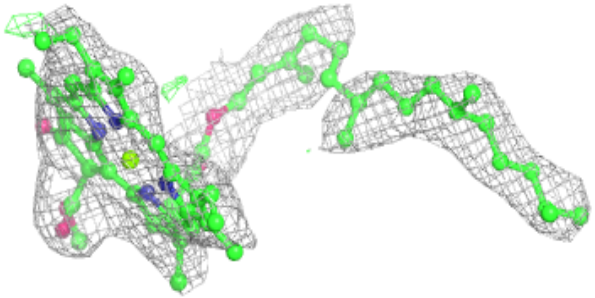


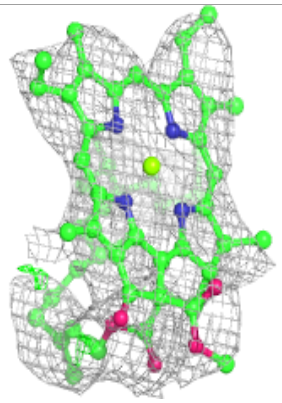


Electron density around CLA c 513:

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

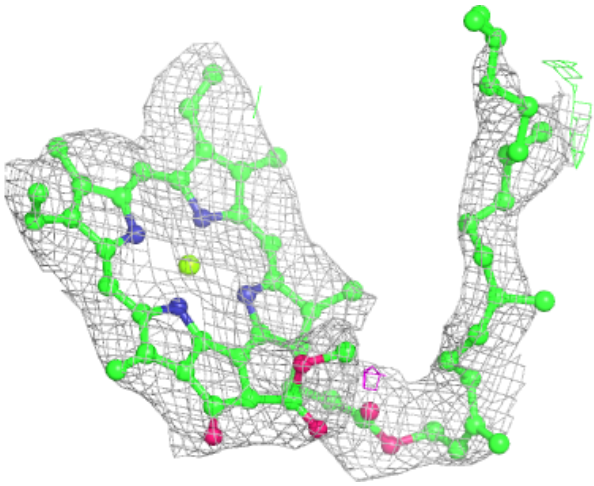


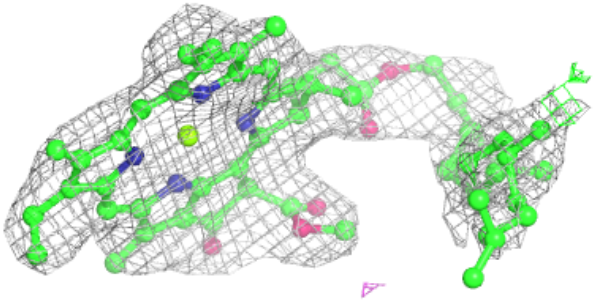


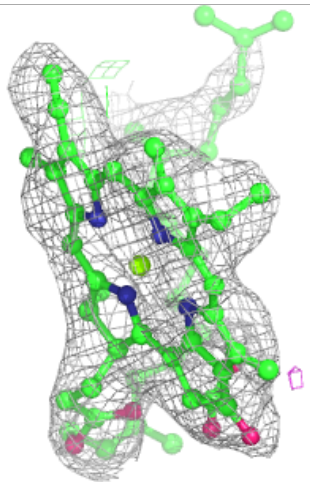


Electron density around CLA B 616:

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

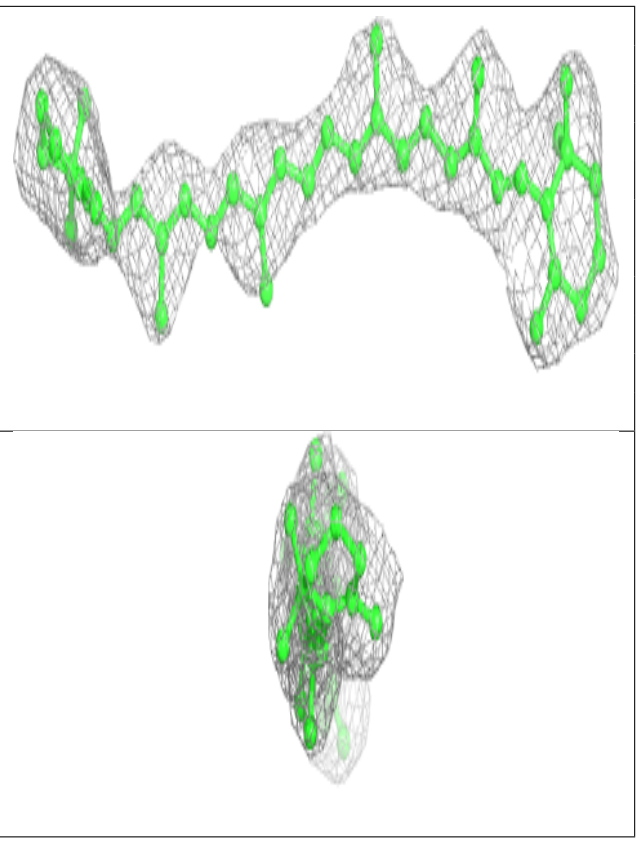






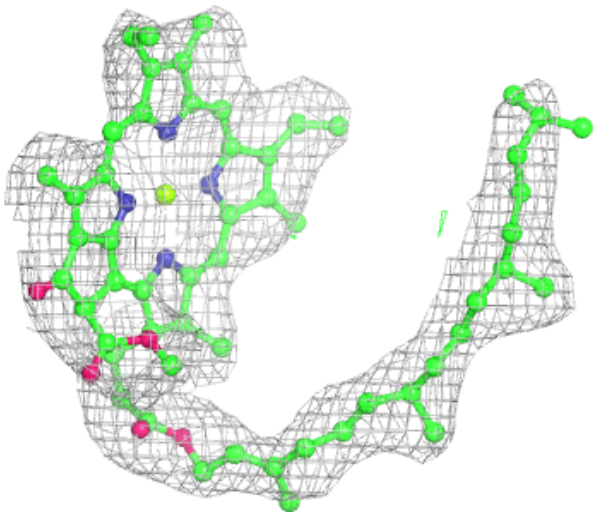
Electron density around BCR b 620:

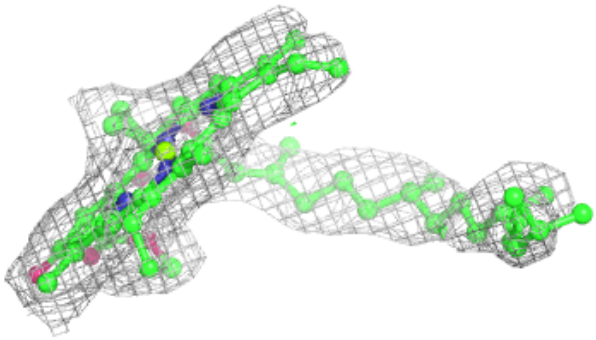
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

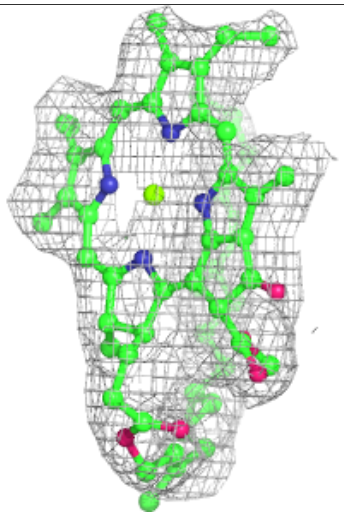


Electron density around CLA C 507:

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

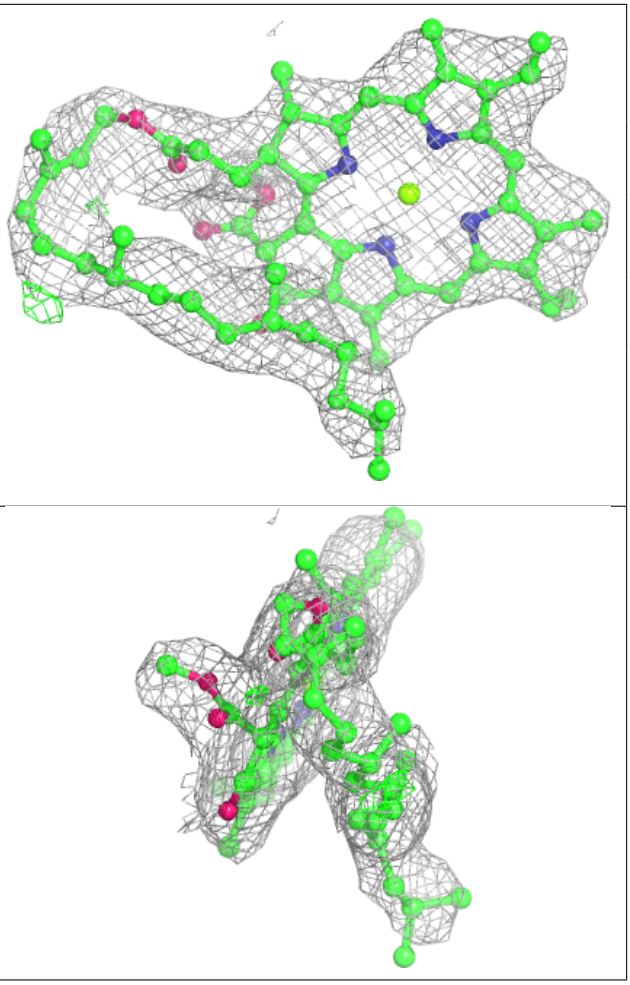






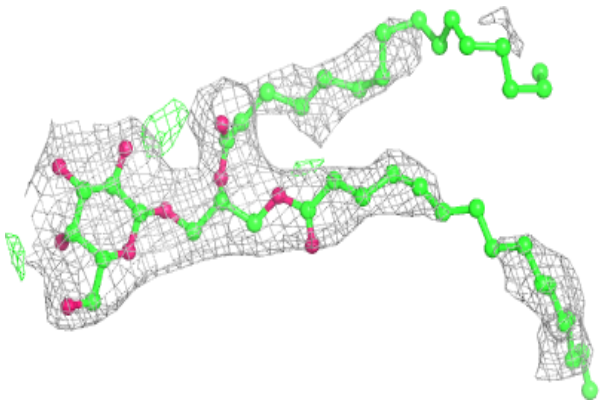
Electron density around CLA C 509:

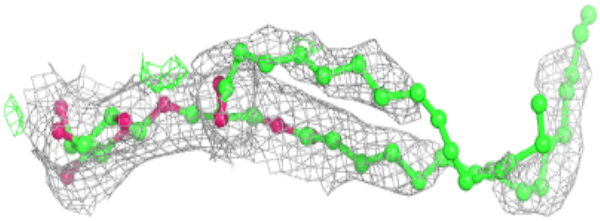
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

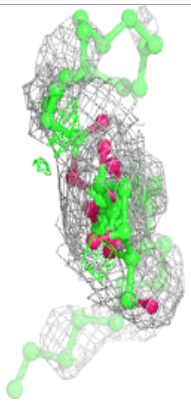


Electron density around LMG D 405:

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

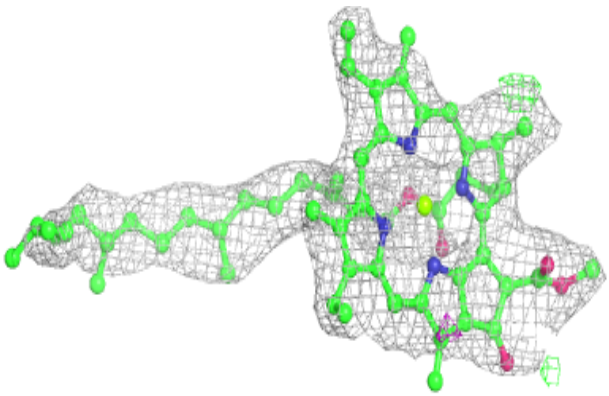


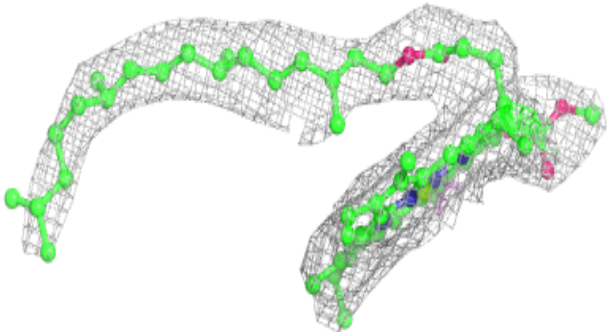


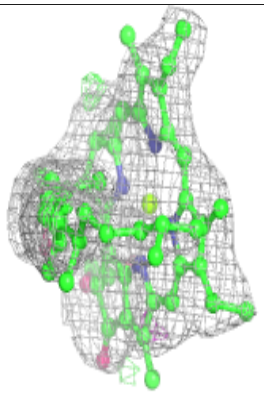


Electron density around CLA b 611:

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

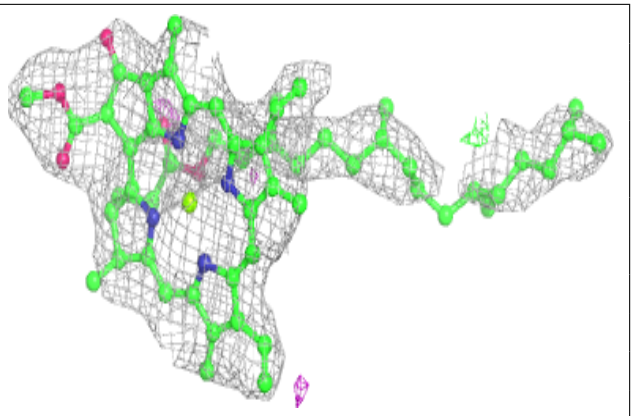


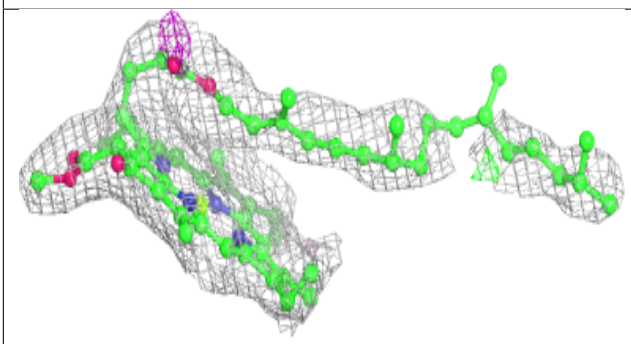


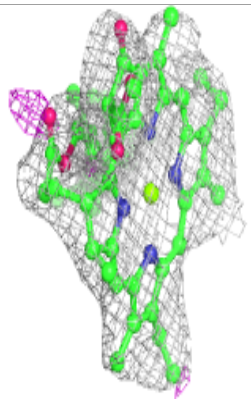


Electron density around CLA b 617:

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

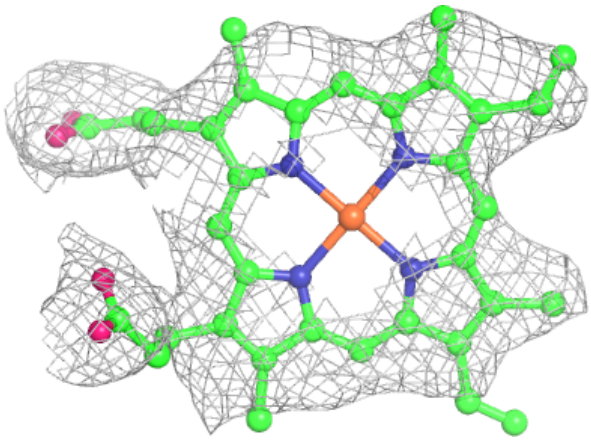


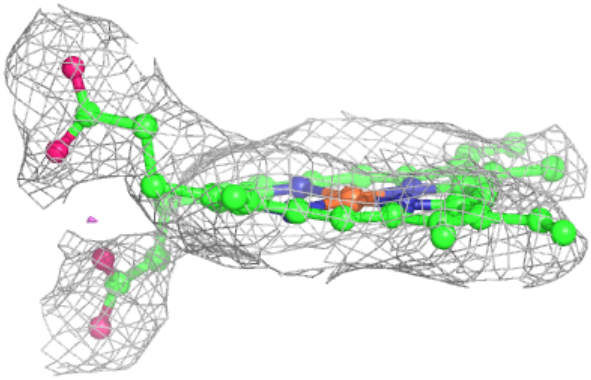


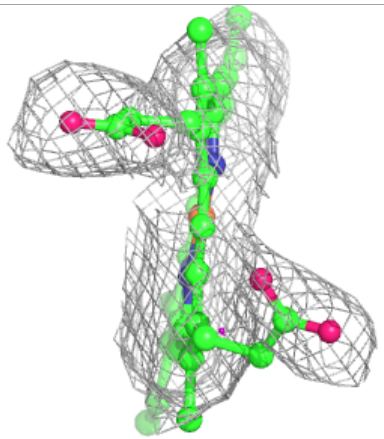


Electron density around HEM e 101:

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

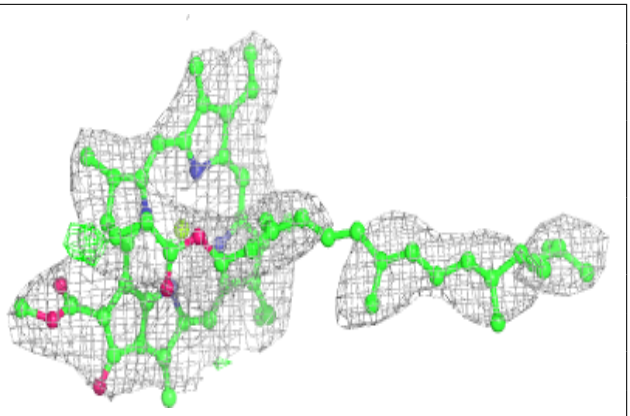


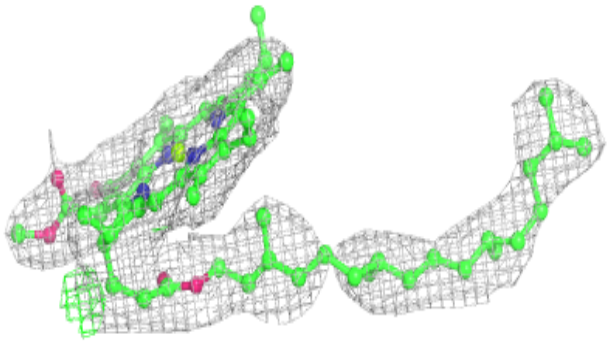


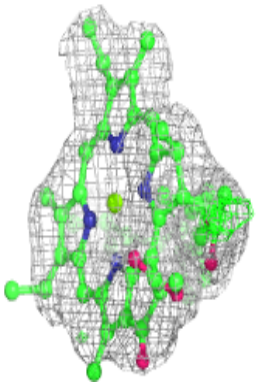


Electron density around CLA B 608:

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

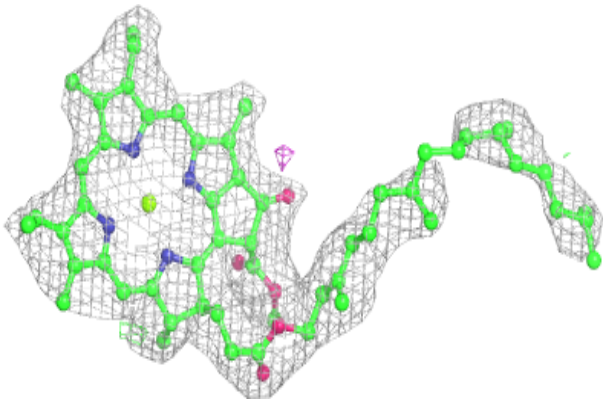


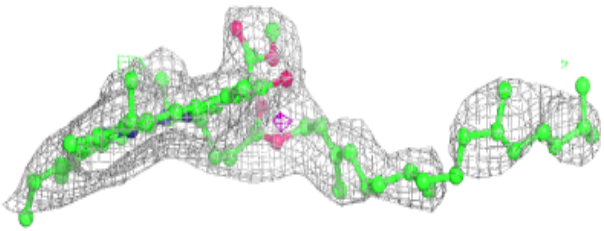


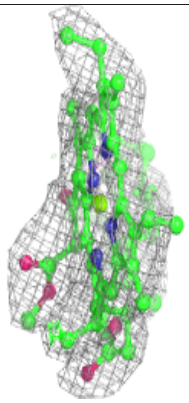


Electron density around CLA b 605:

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

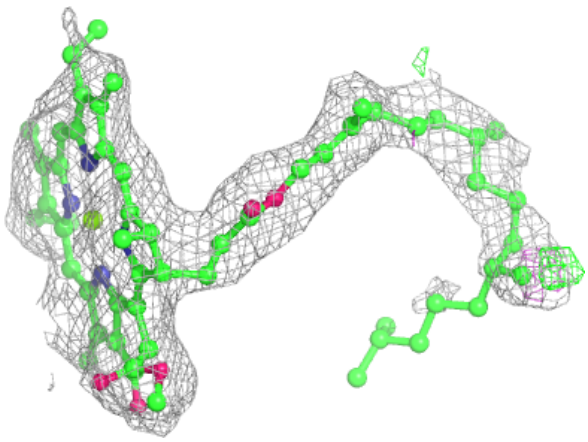


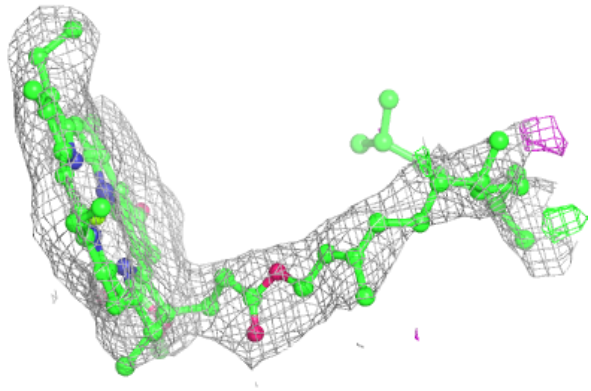


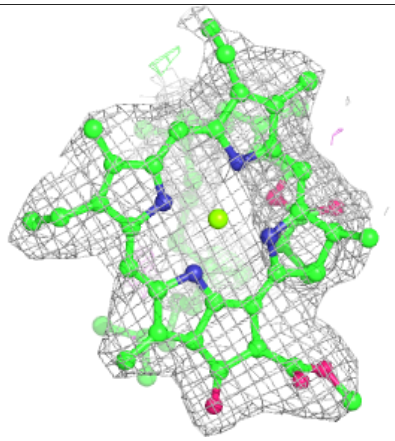


Electron density around CLA b 609:

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

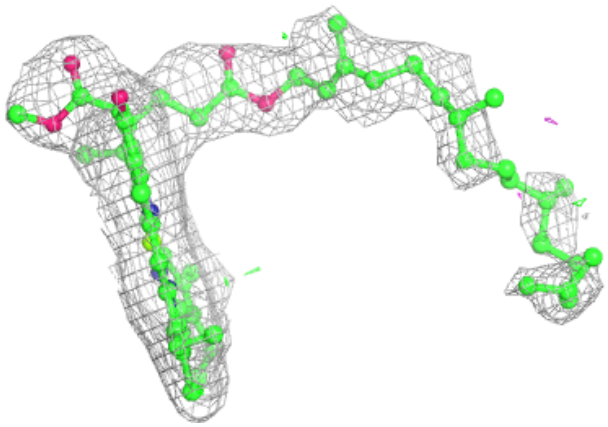


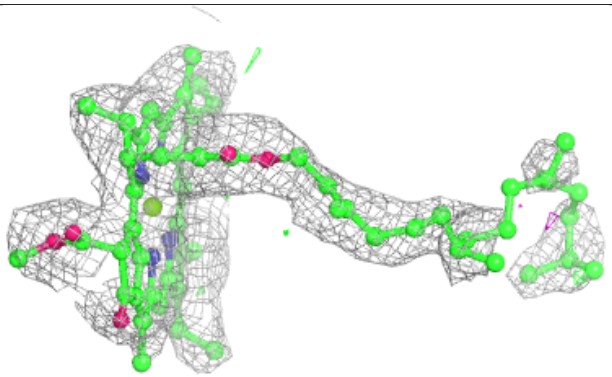


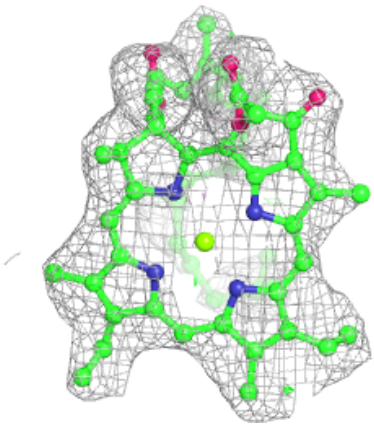


Electron density around CLA C 506:

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

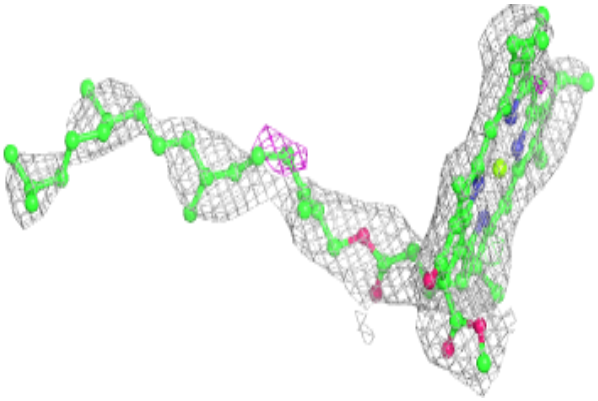


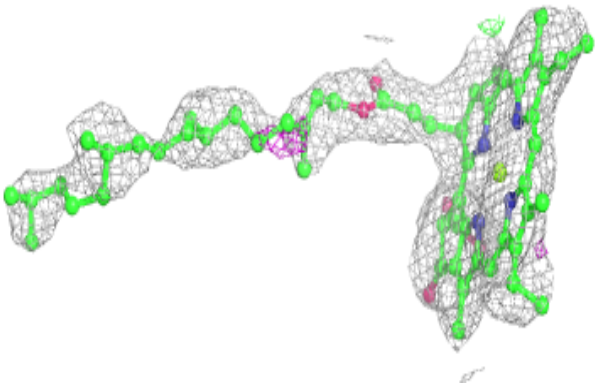


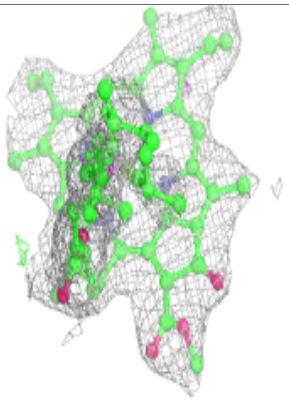


Electron density around CLA B 604:

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

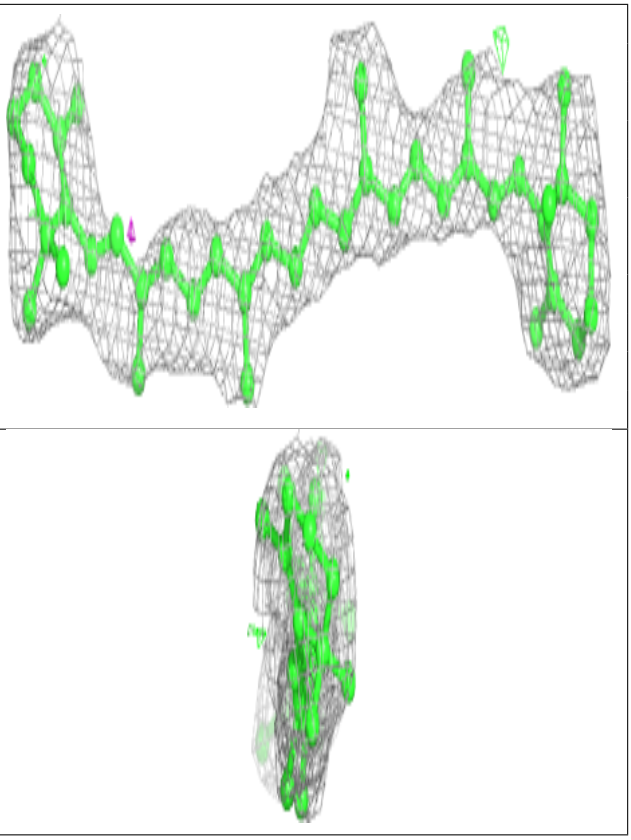






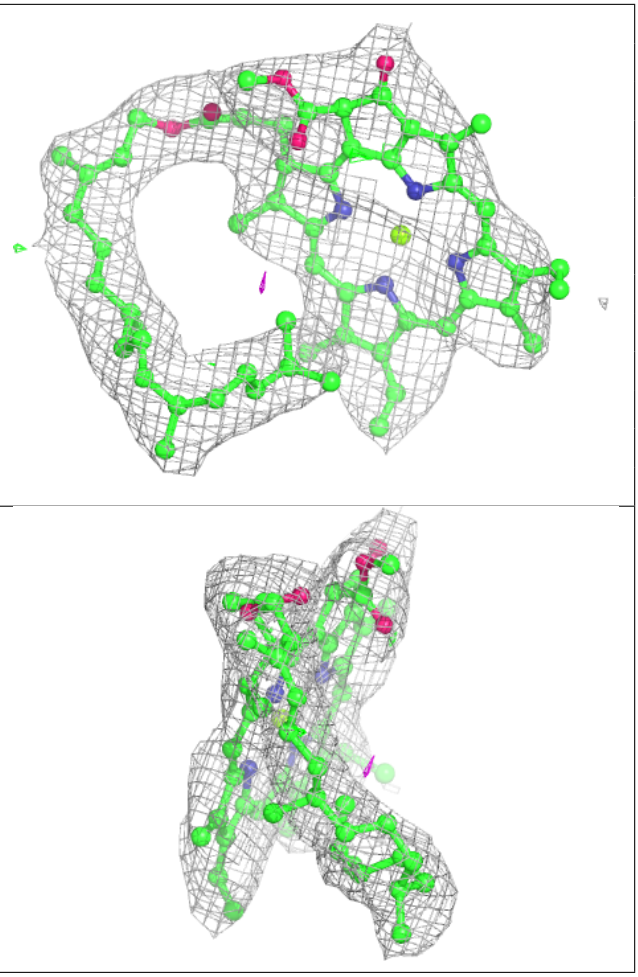
Electron density around BCR b 621:

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



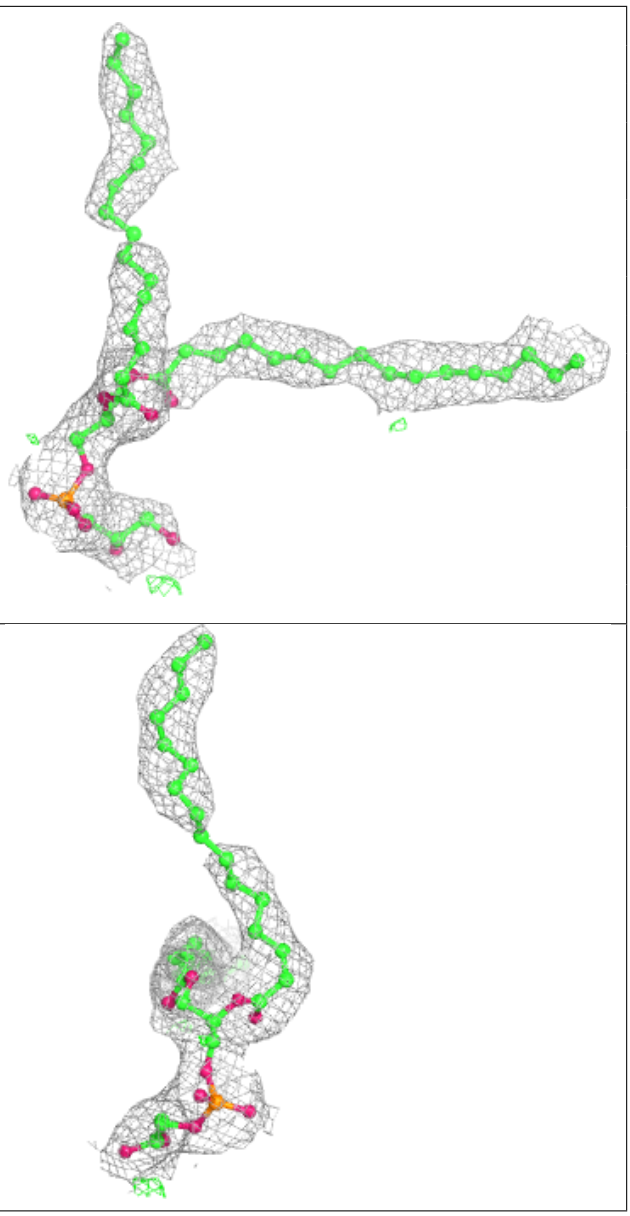
Electron density around CLA b 618:

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



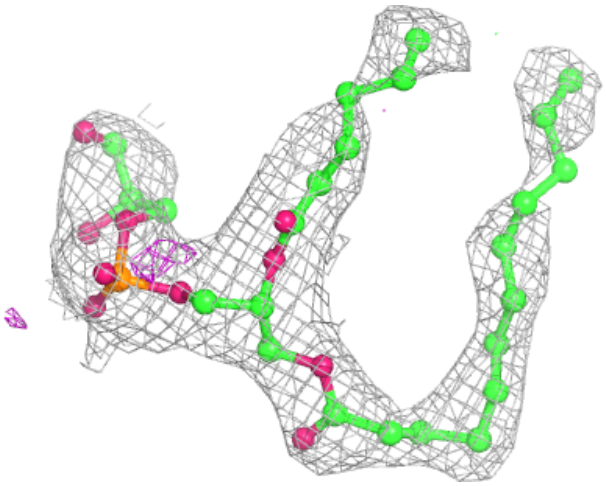
Electron density around LHG L 101:

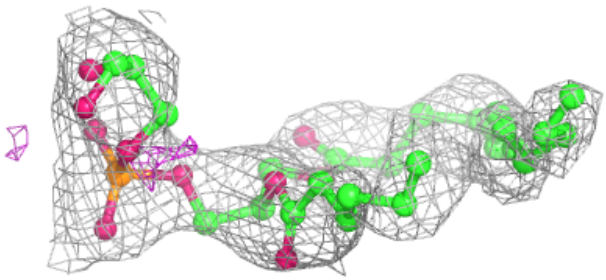
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

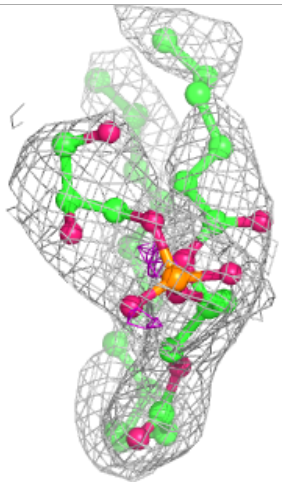


Electron density around LHG a 614:

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

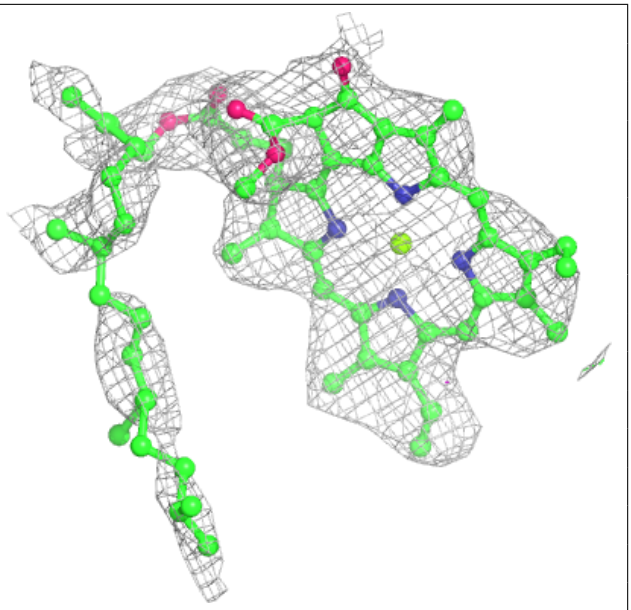


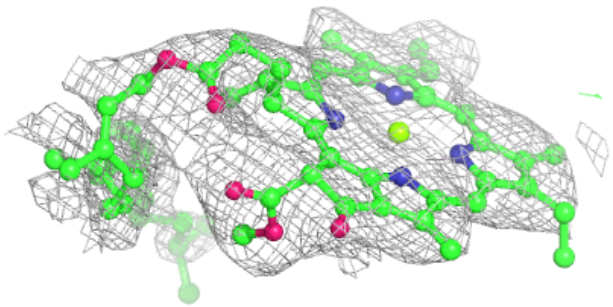


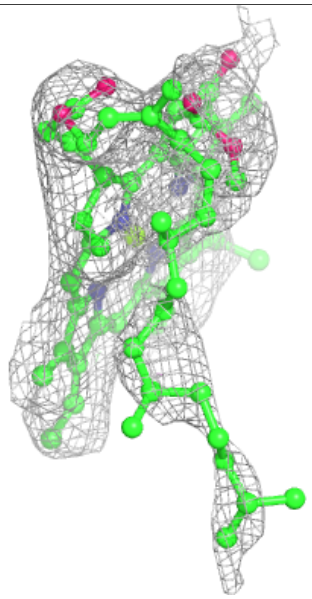


Electron density around CLA b 619:

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

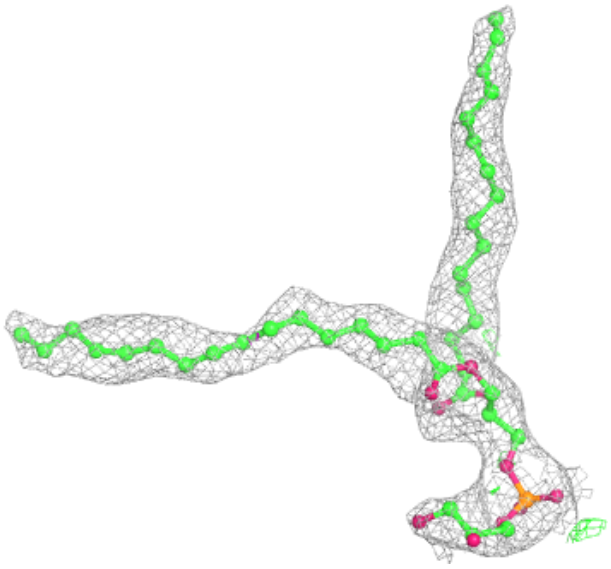


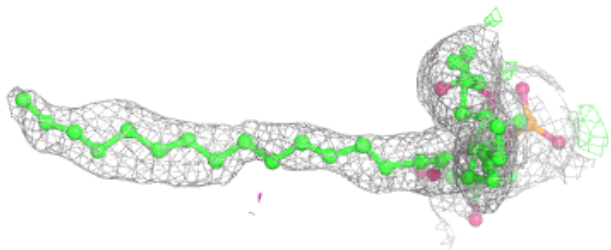


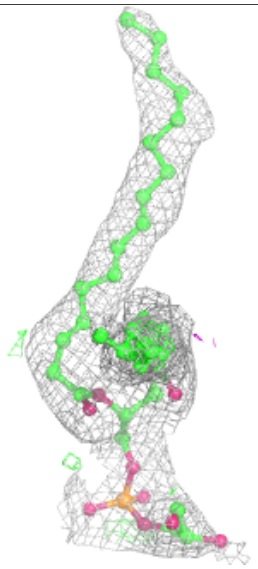


Electron density around LHG l 101:

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

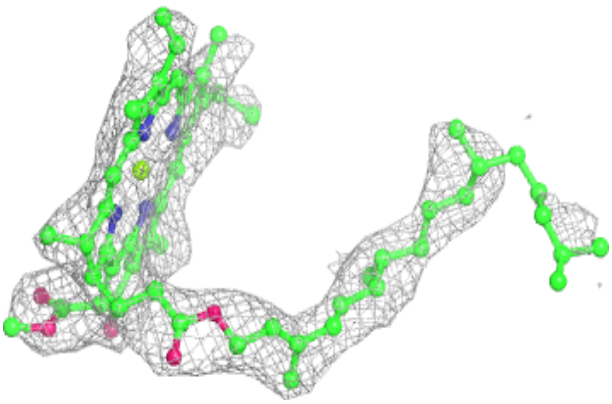


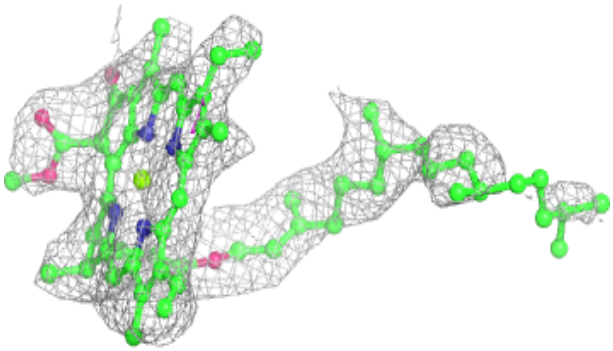


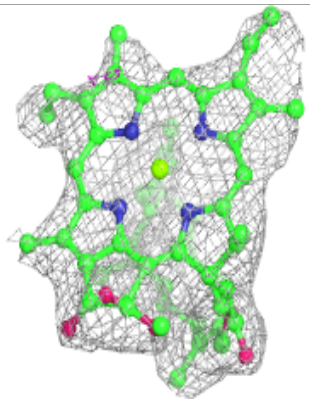


Electron density around CLA C 508:

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

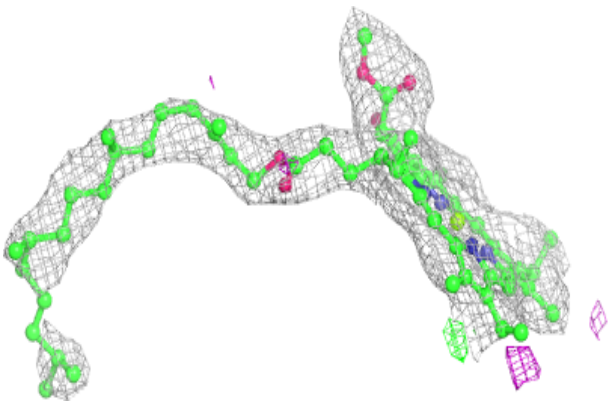


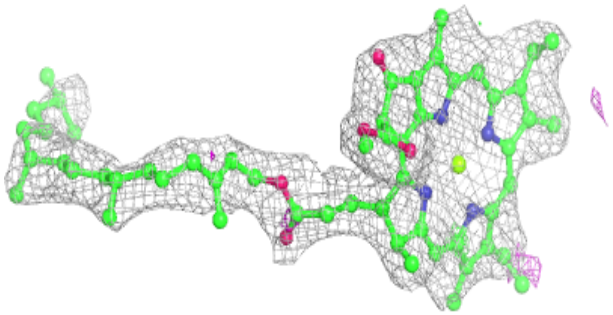


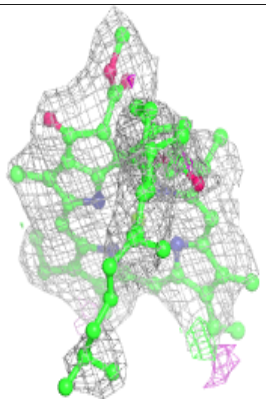


Electron density around CLA D 402:

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

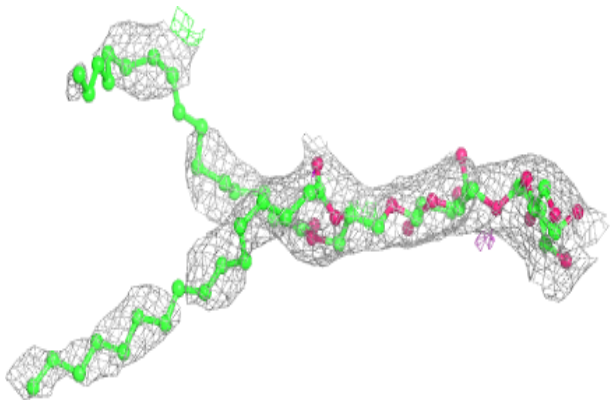


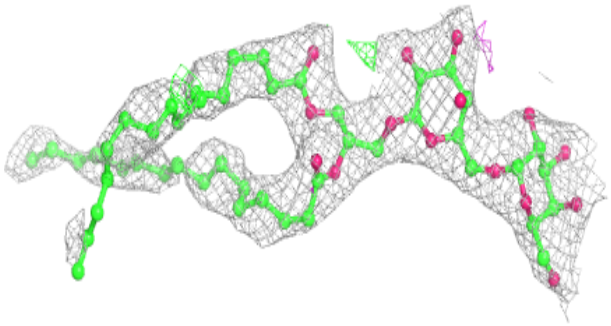


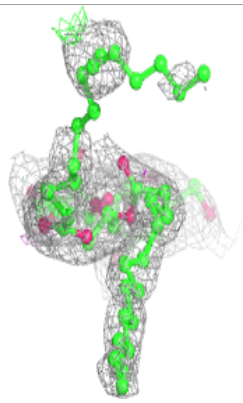


Electron density around DGD c 518:

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

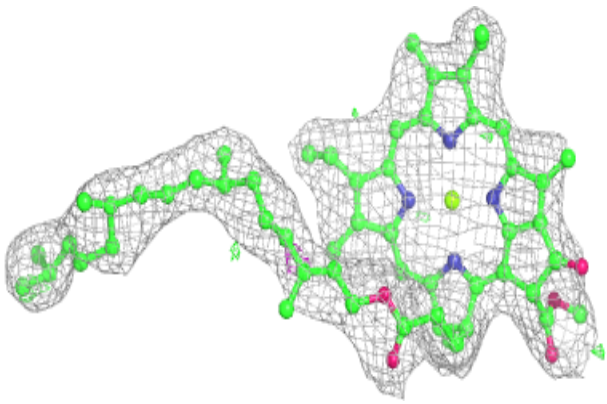


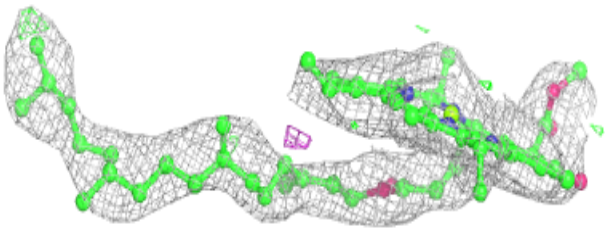


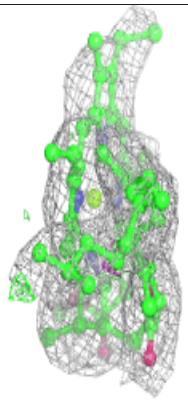


Electron density around CLA B 603:

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

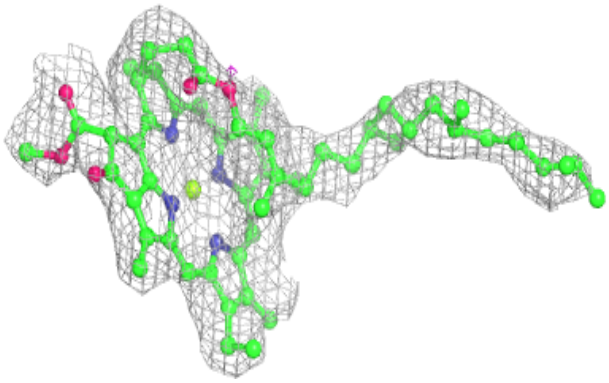


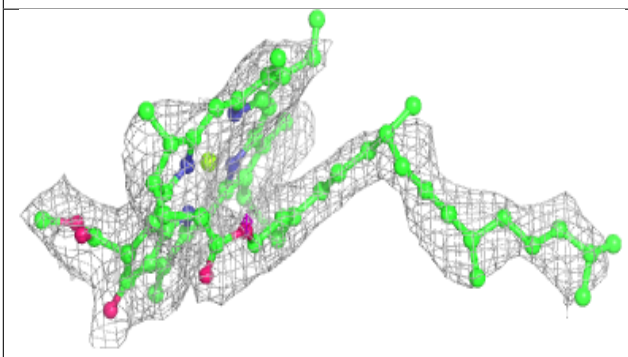


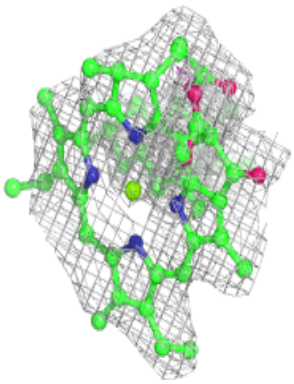


Electron density around CLA c 507:

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

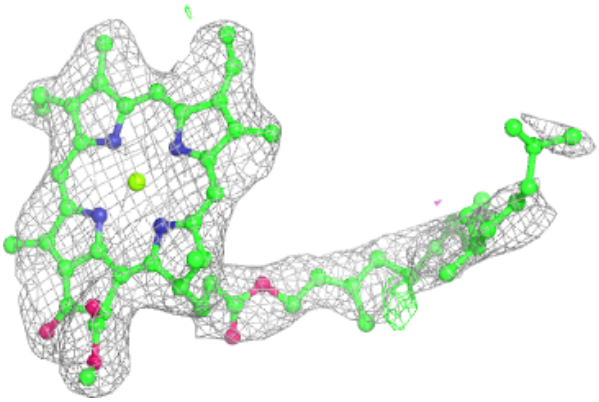


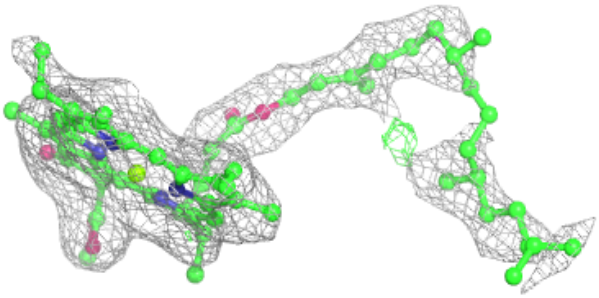


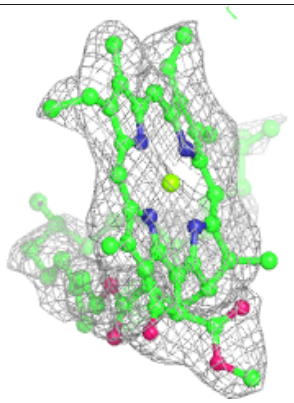


Electron density around CLA a 609:

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

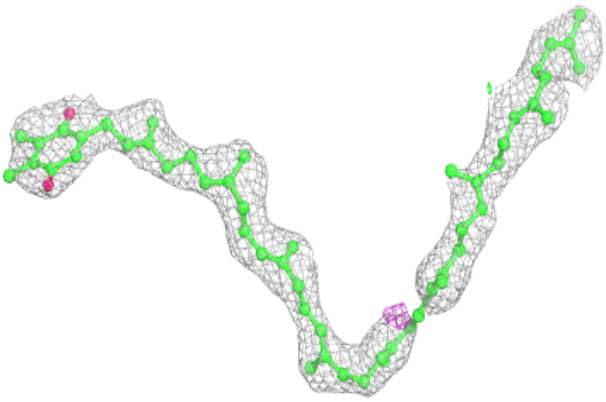


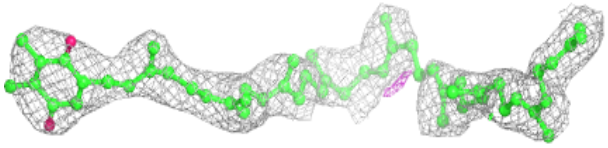


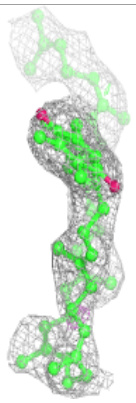


Electron density around PL9 D 407:

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

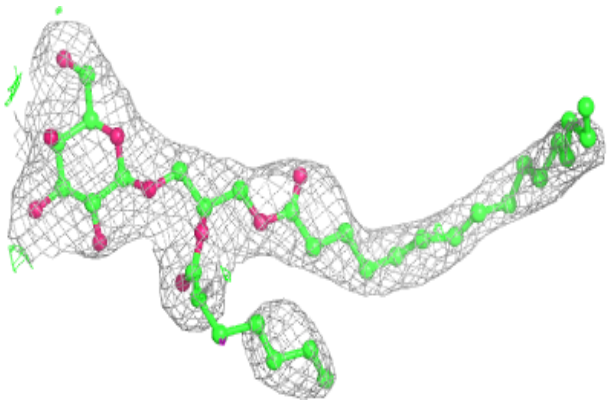


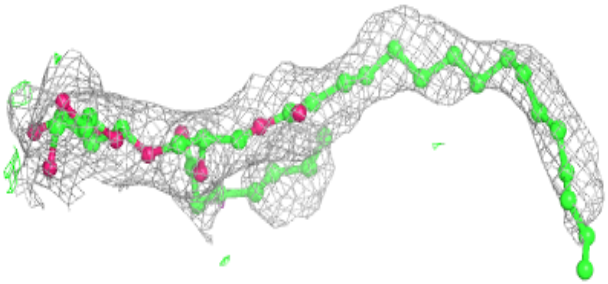


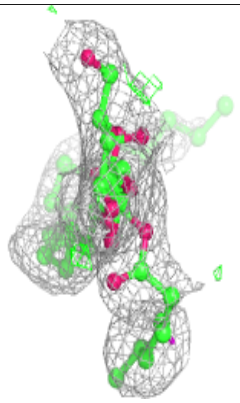


Electron density around LMG d 406:

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

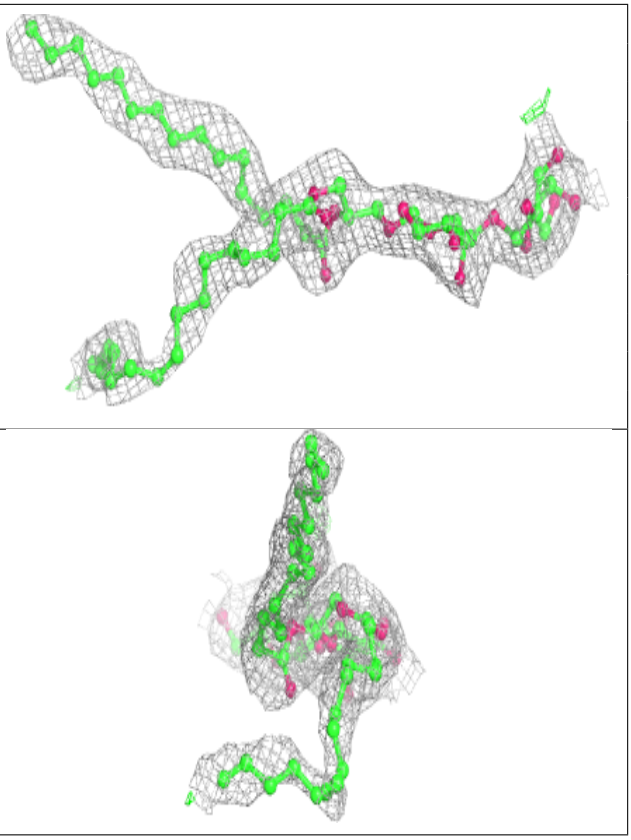


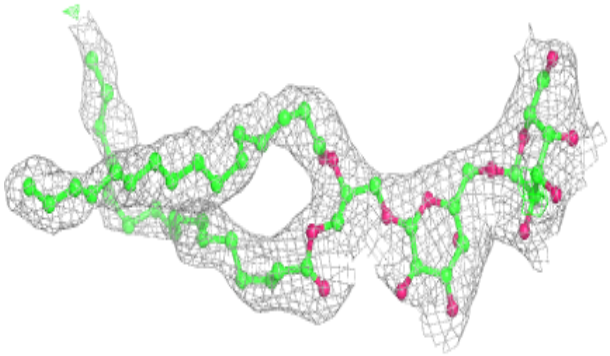




Electron density around DGD C 516:

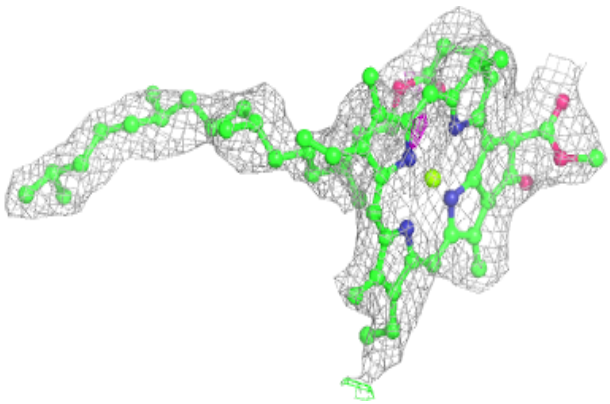
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

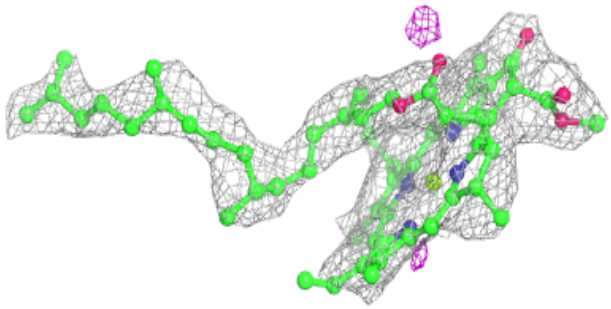


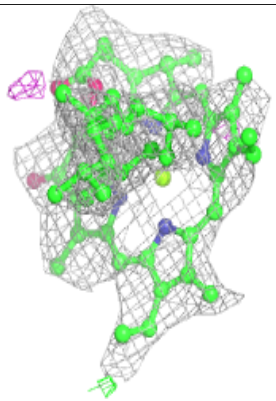


Electron density around CLA C 505:

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

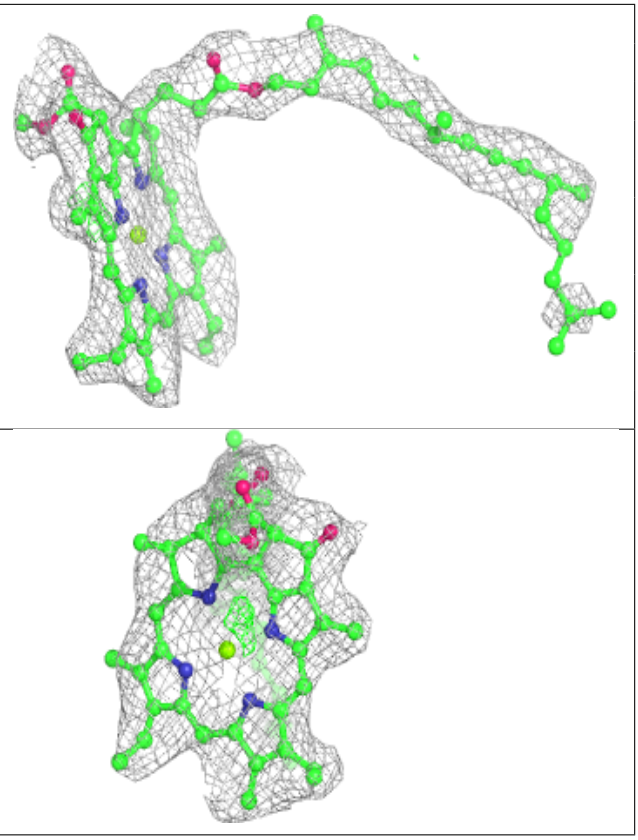






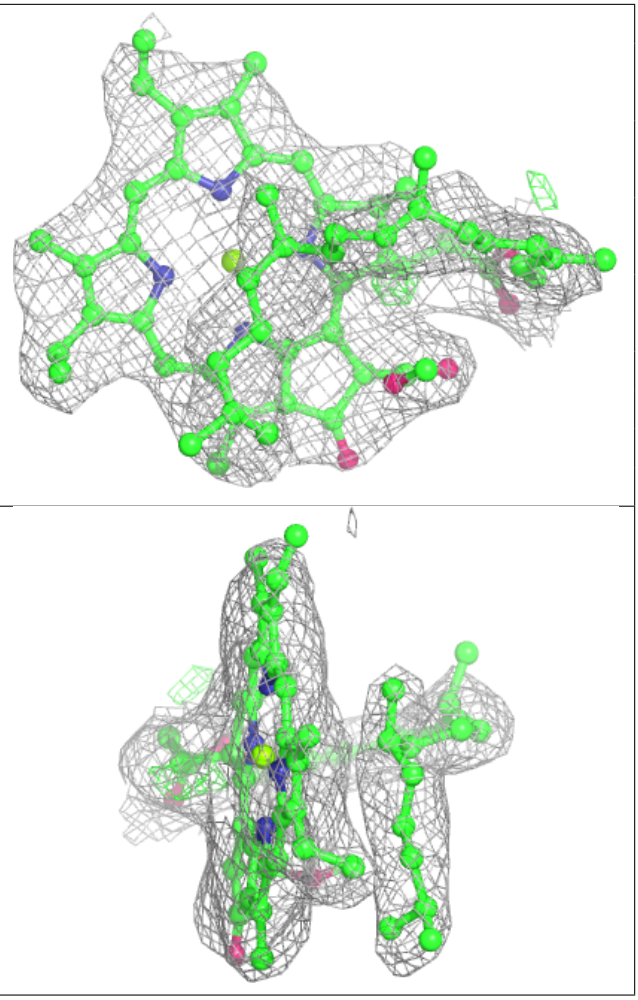
Electron density around CLA b 612:

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



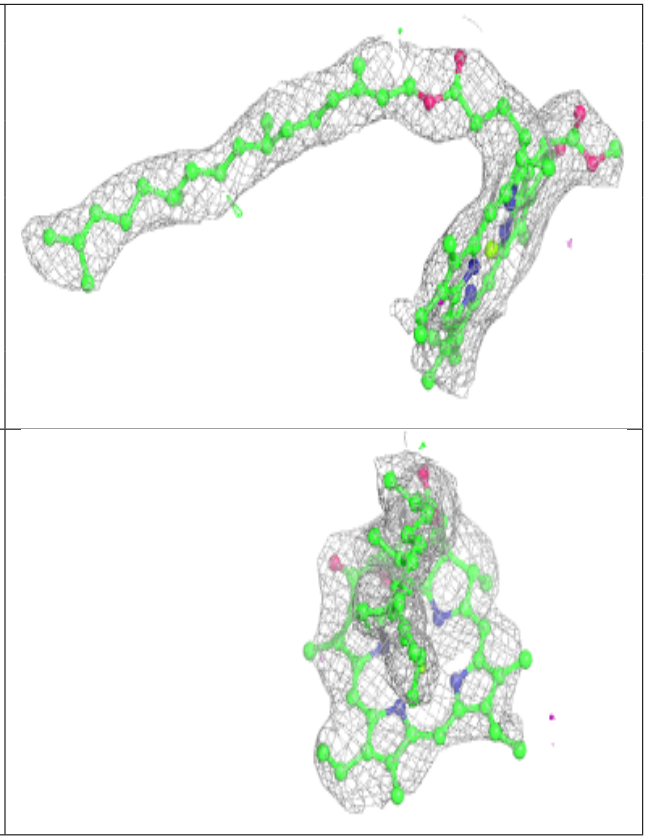
Electron density around CLA c 512:

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



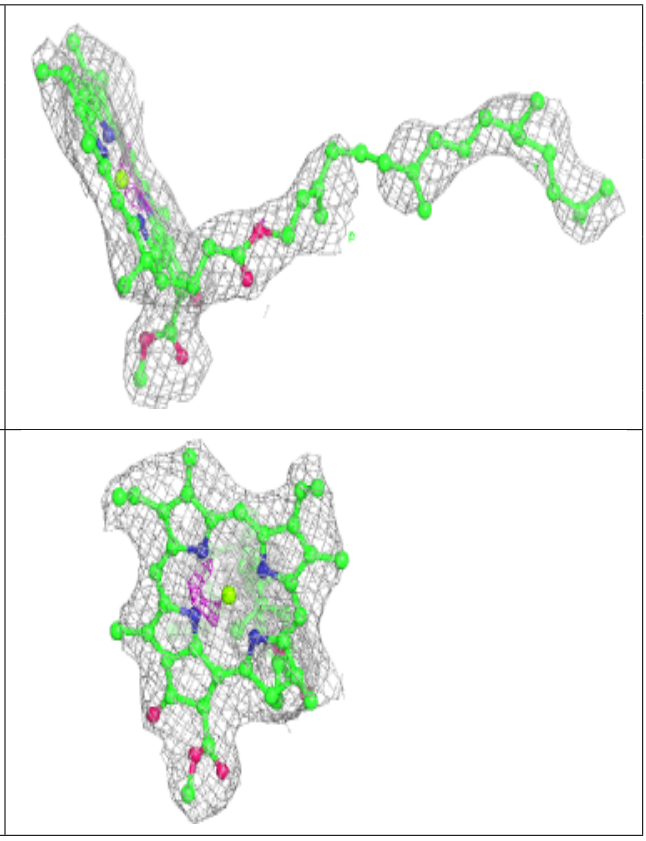
Electron density around CLA B 607:

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



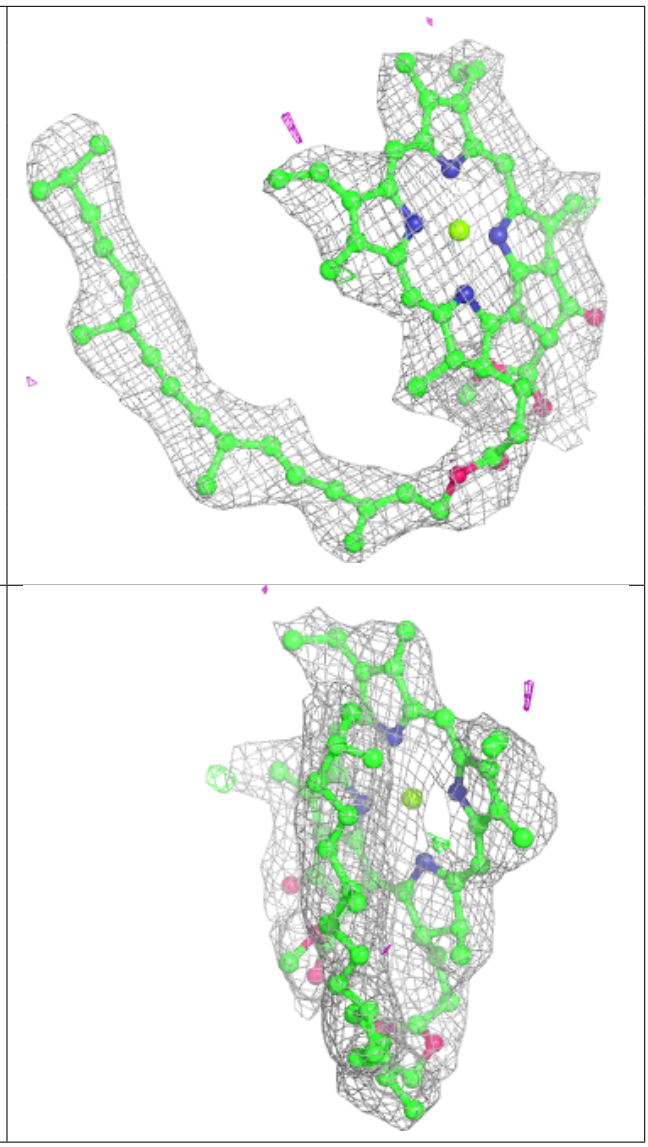
Electron density around CLA b 607:

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



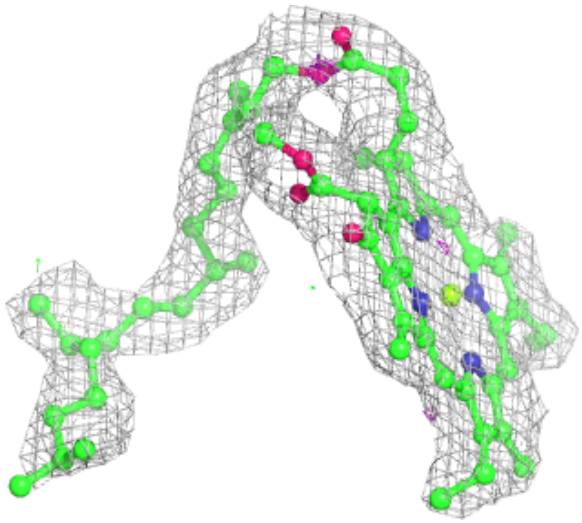
Electron density around CLA c 509:

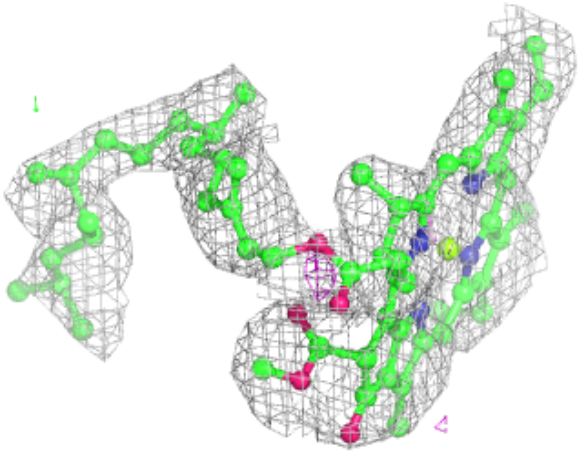
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

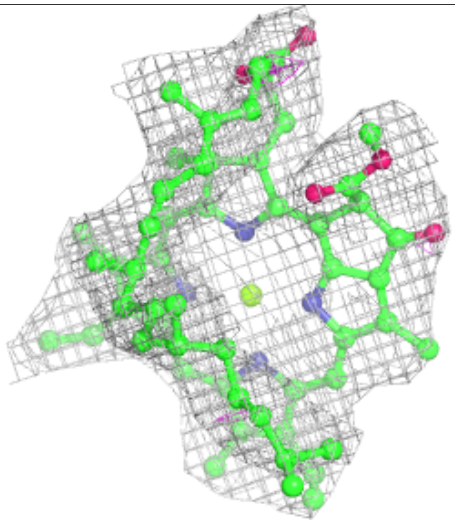


Electron density around CLA b 616:

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

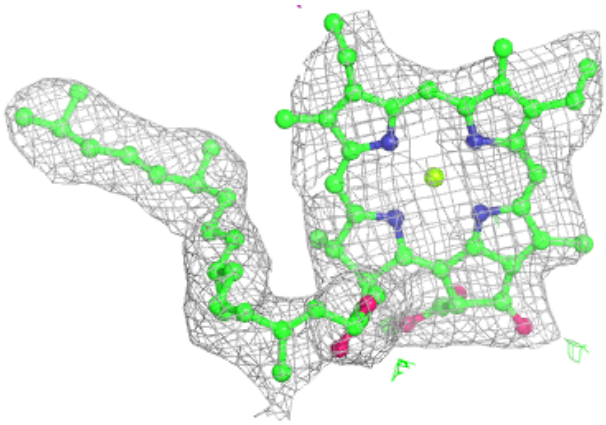


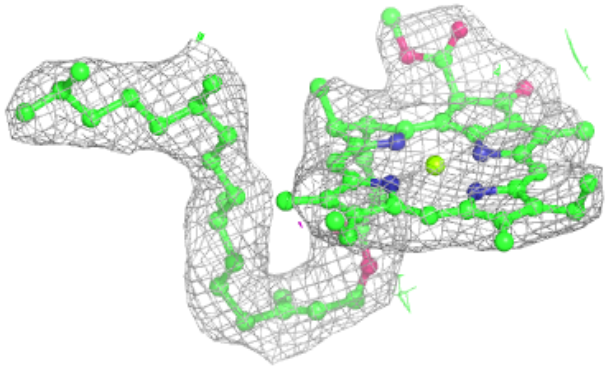




Electron density around CLA A 615:

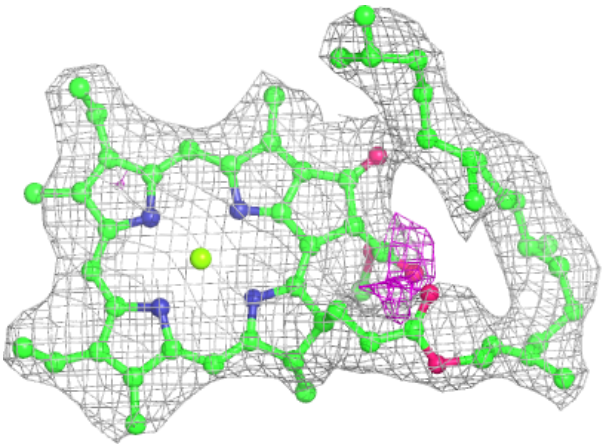
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

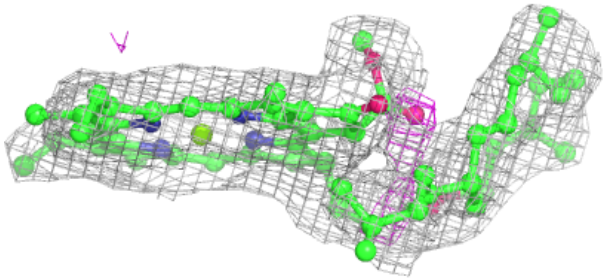


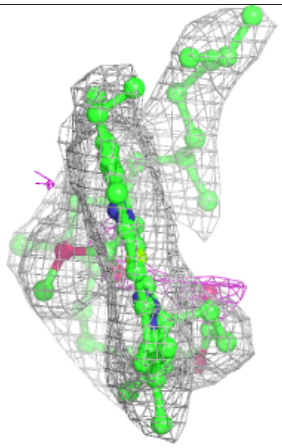


Electron density around CLA B 610:

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

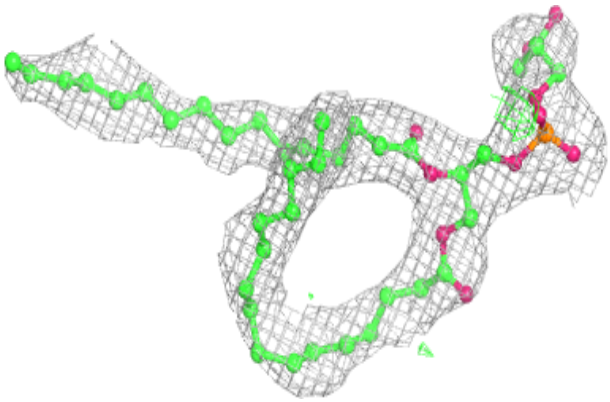


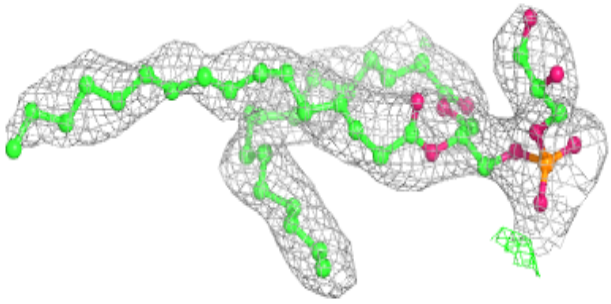


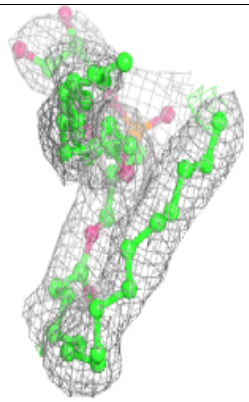


Electron density around LHG A 616:

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

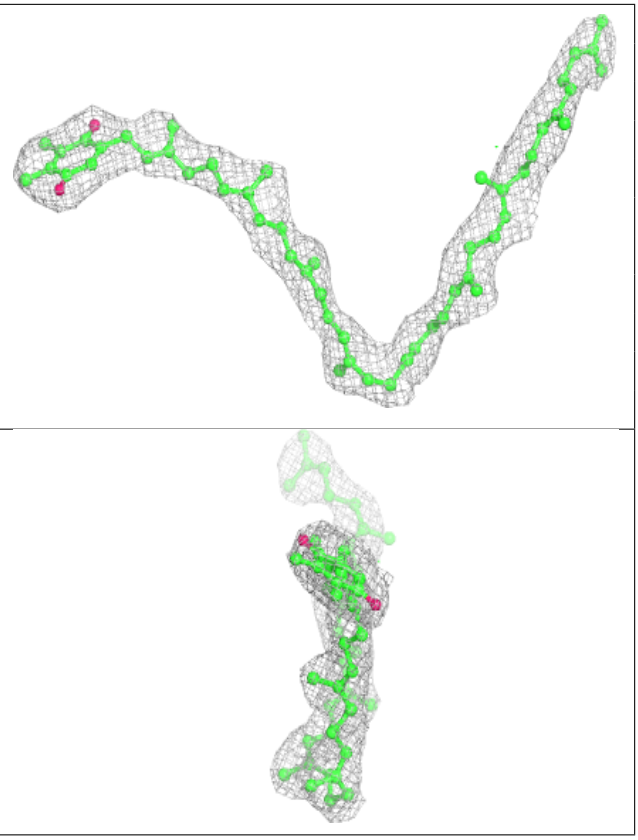






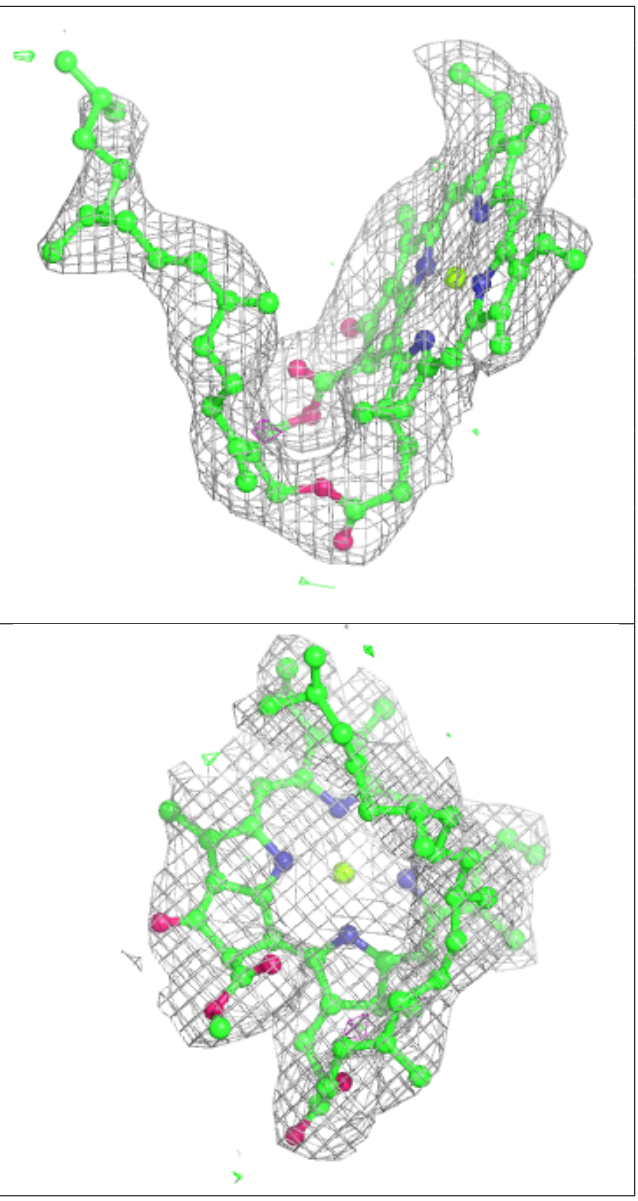
Electron density around PL9 d 408:

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



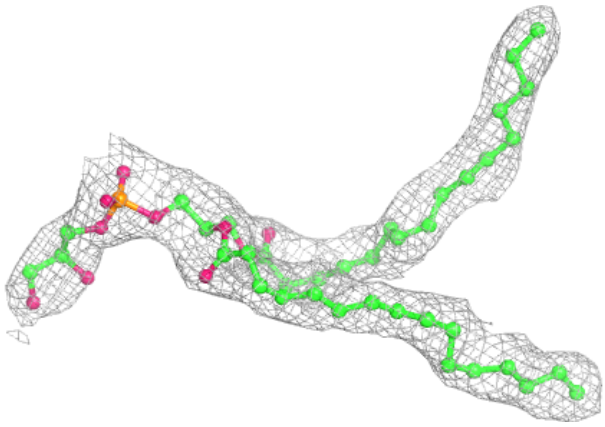
Electron density around CLA B 613:

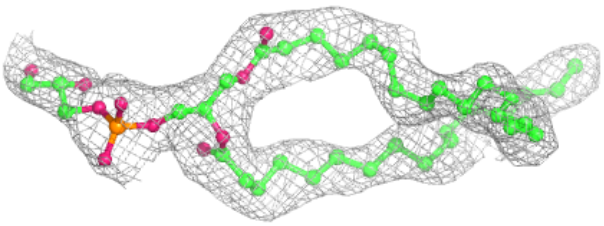
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

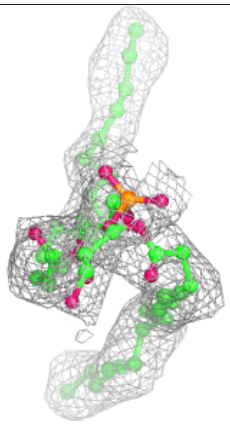


Electron density around LHG D 406:

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

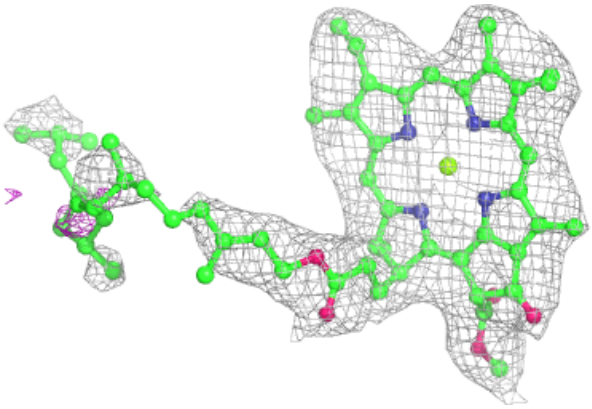


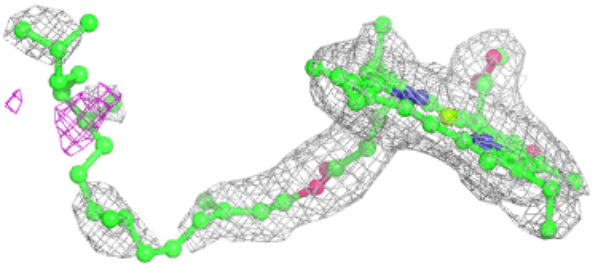


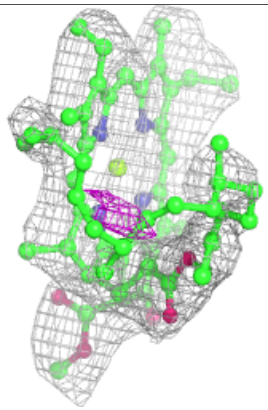


Electron density around CLA A 609:

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

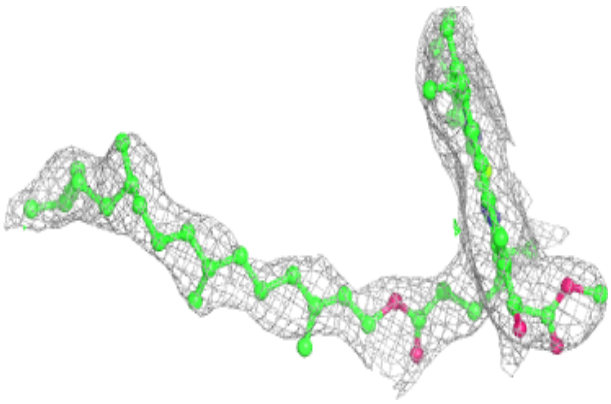


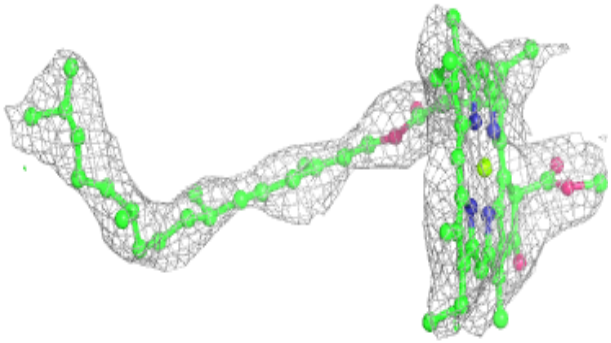


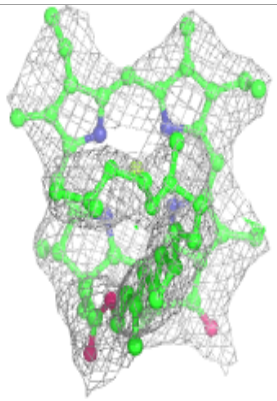


Electron density around CLA b 608:

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

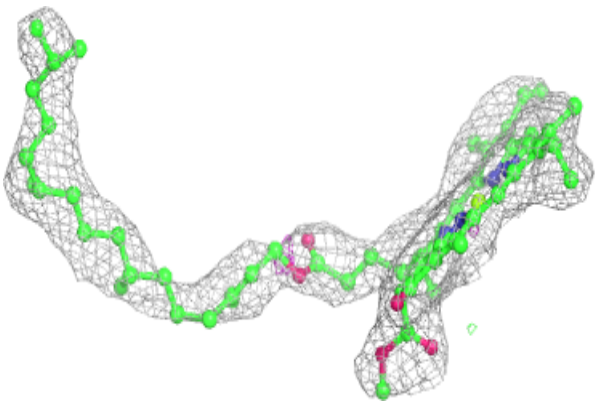


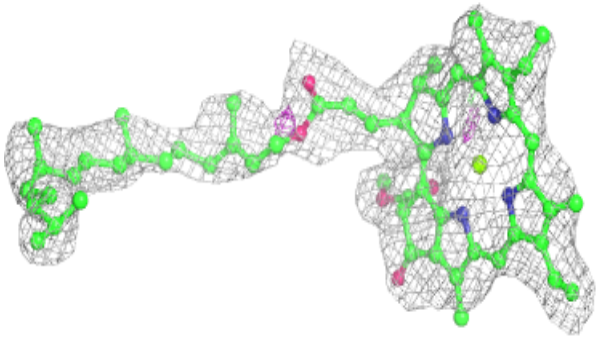


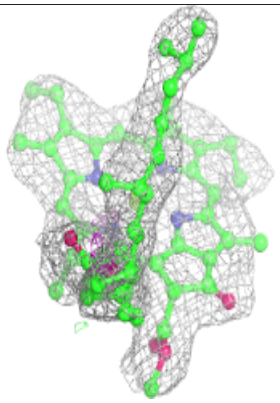


Electron density around CLA d 403:

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

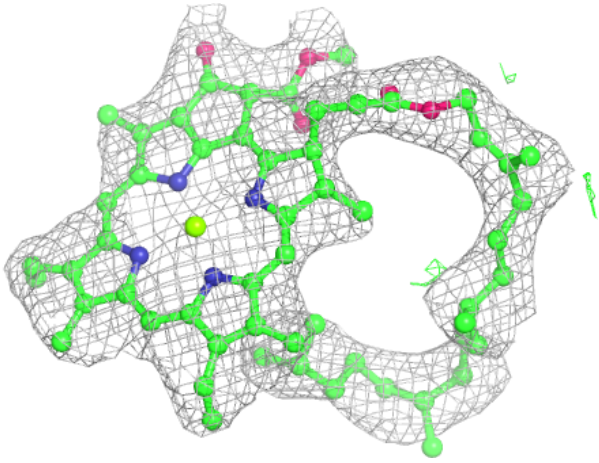


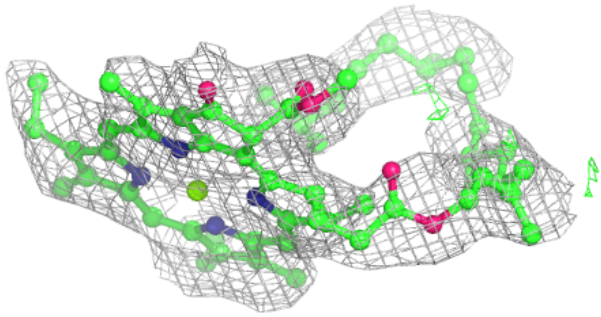


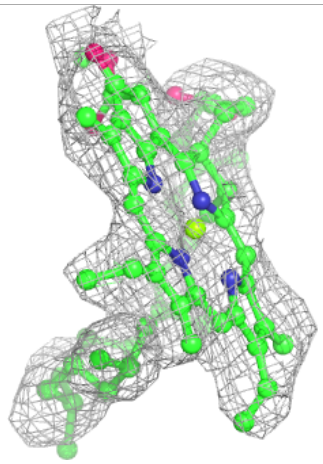


Electron density around CLA B 615:

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

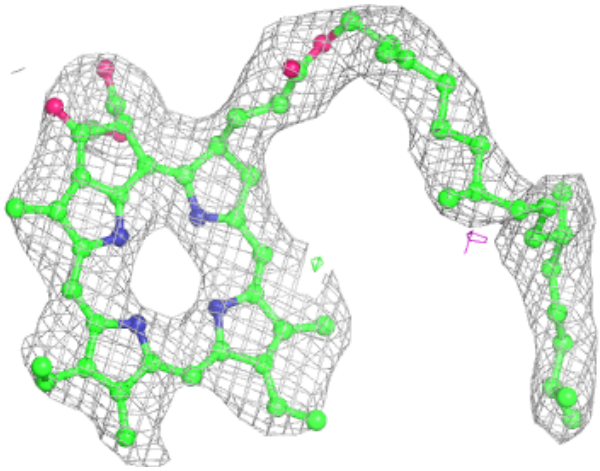


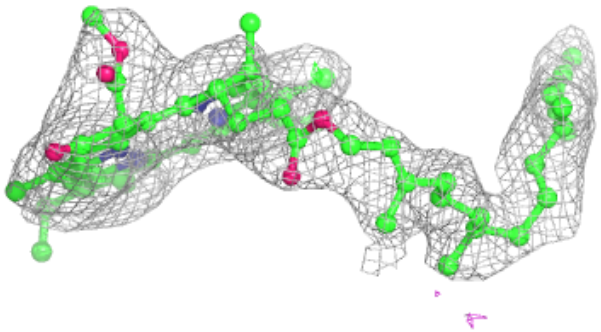


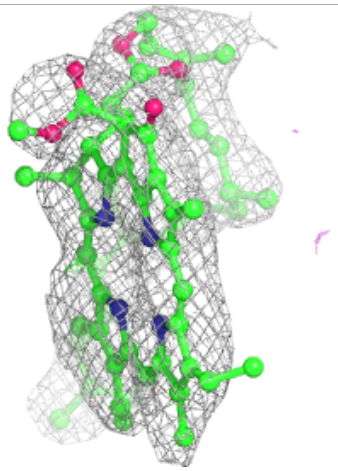


Electron density around PHO D 401:

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

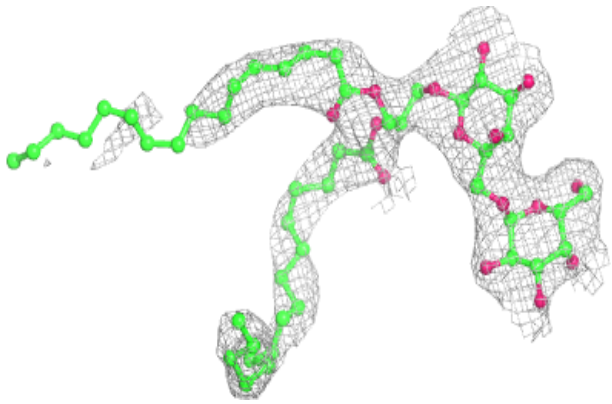


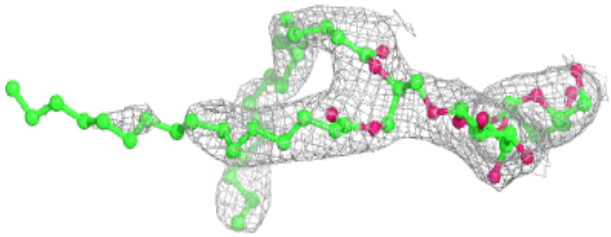


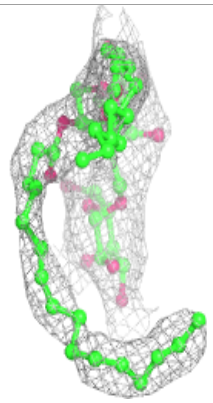


Electron density around DGD C 517:

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

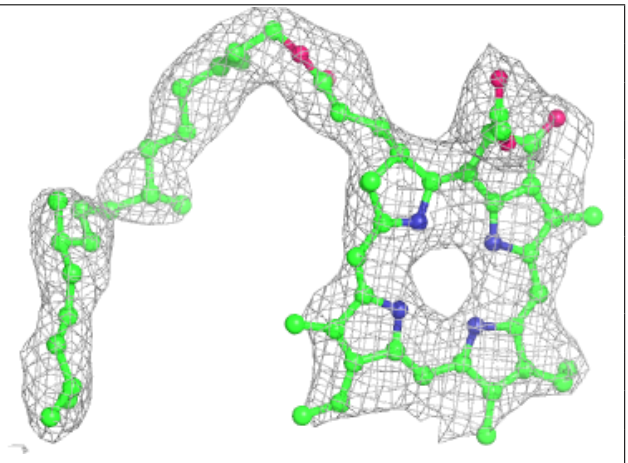


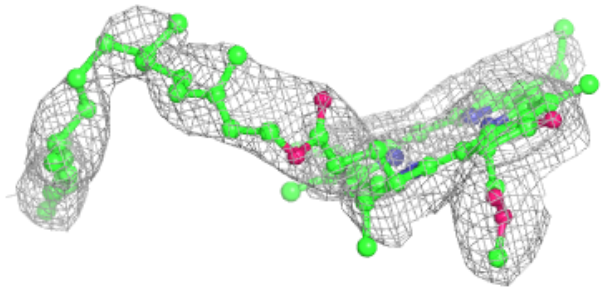


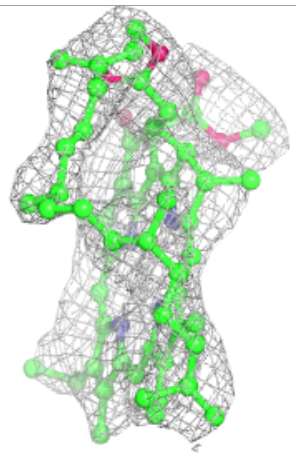


Electron density around PHO d 401:

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

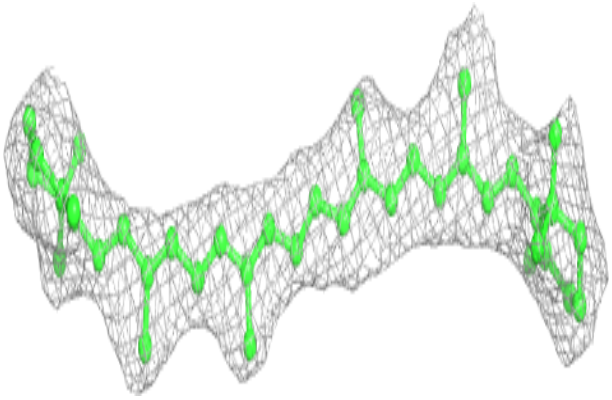


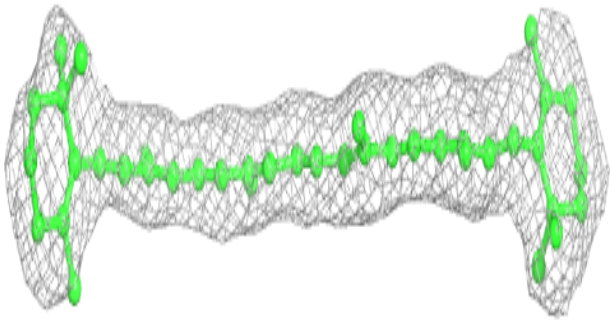


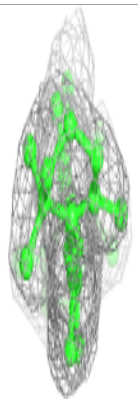


Electron density around BCR A 610:

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

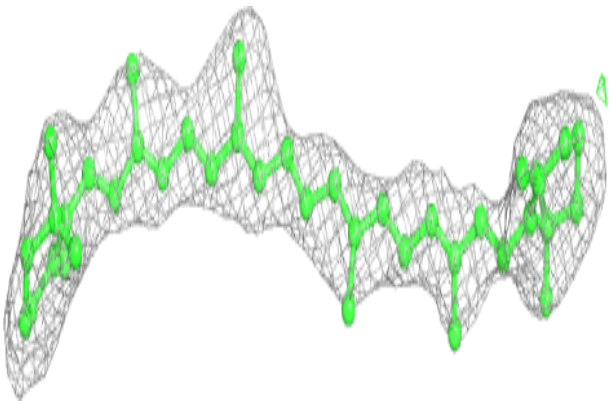


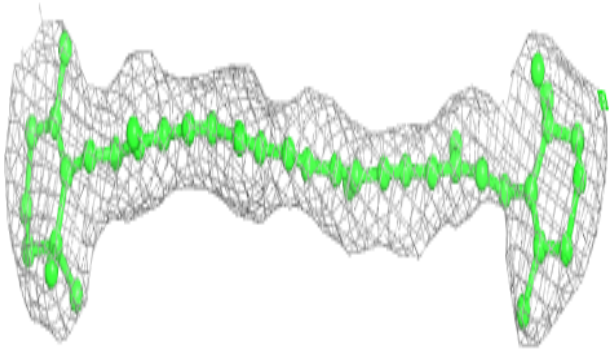


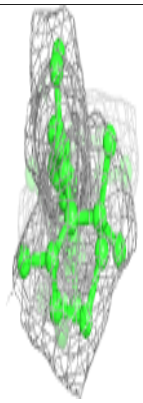


Electron density around BCR c 517:

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

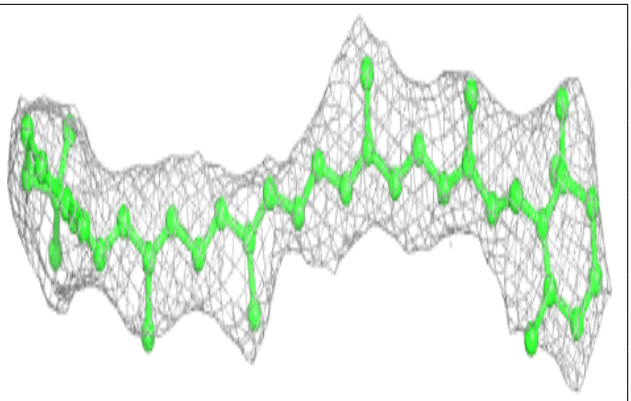


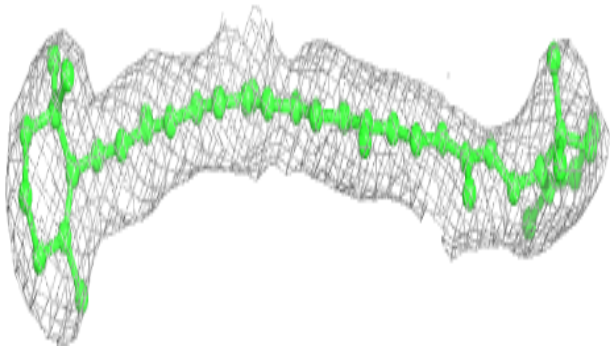


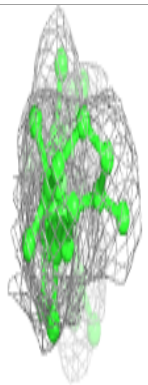


Electron density around BCR B 617:

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

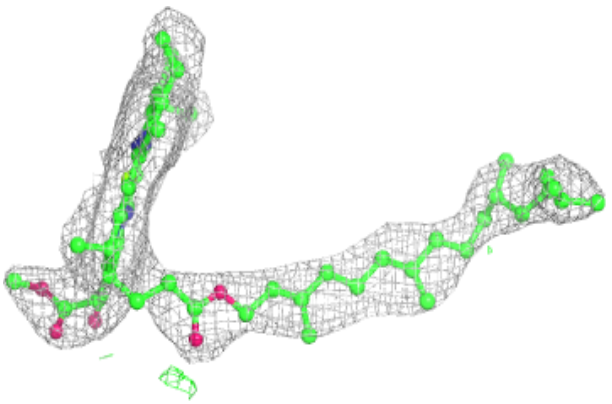


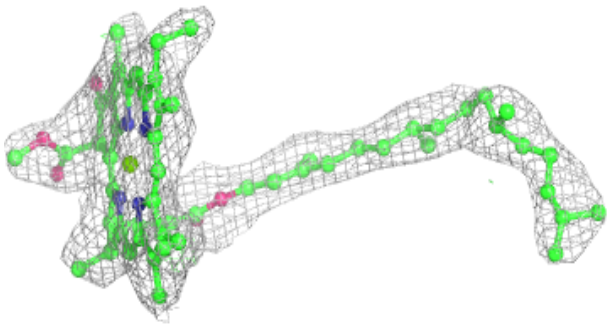


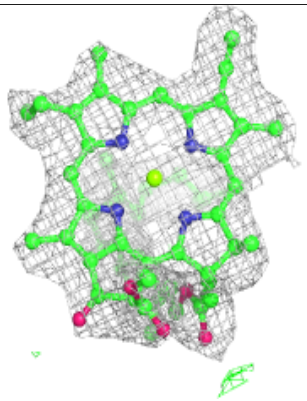


Electron density around CLA B 605:

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

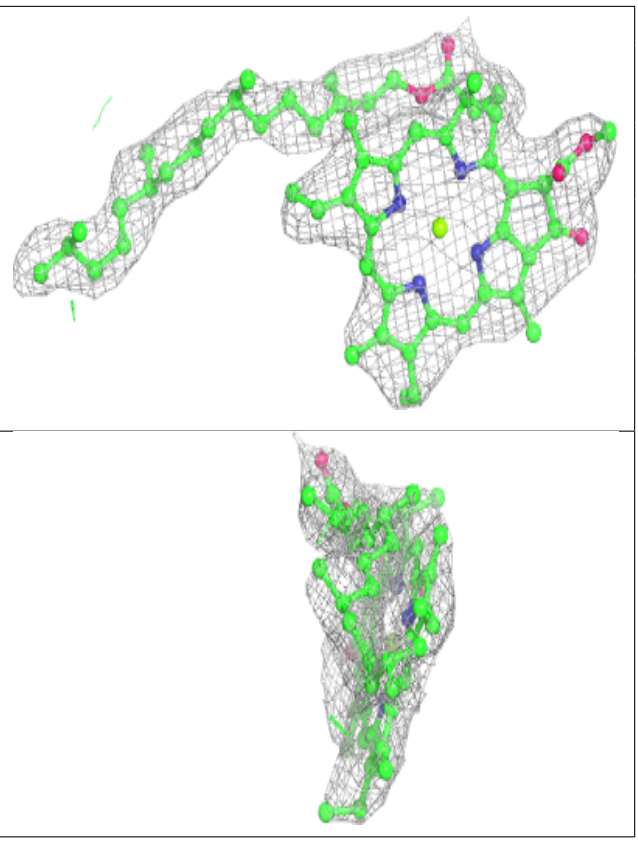






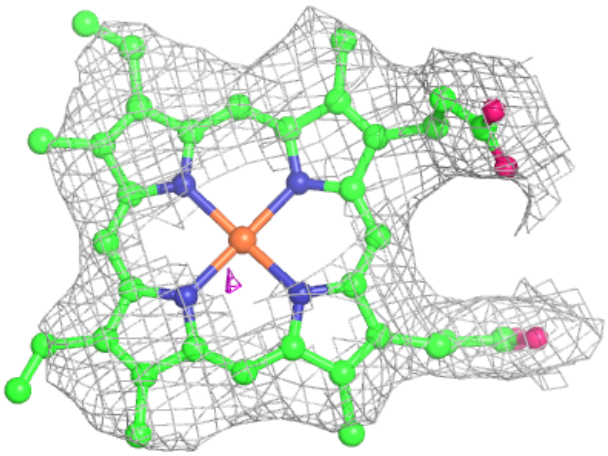
Electron density around CLA C 501:

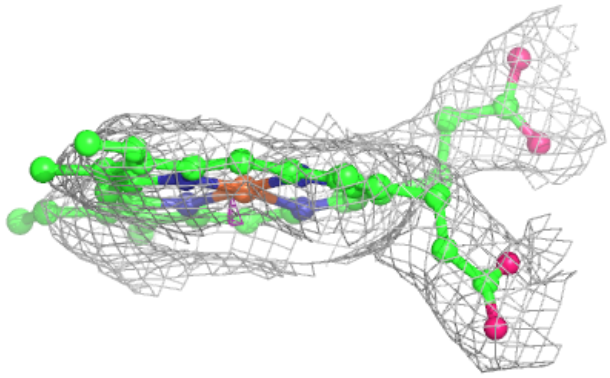
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

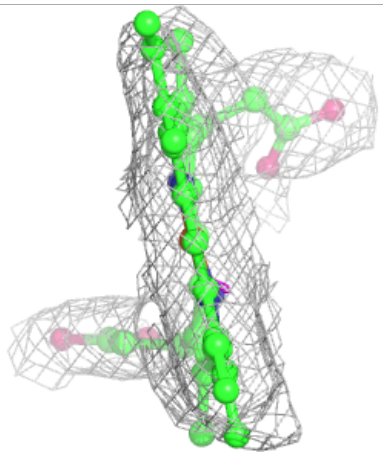


Electron density around HEM E 101:

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

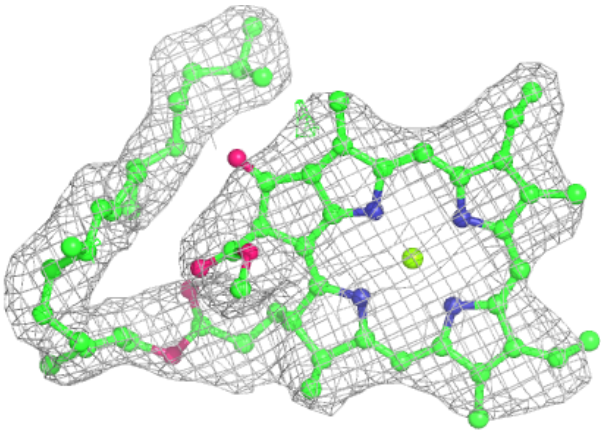


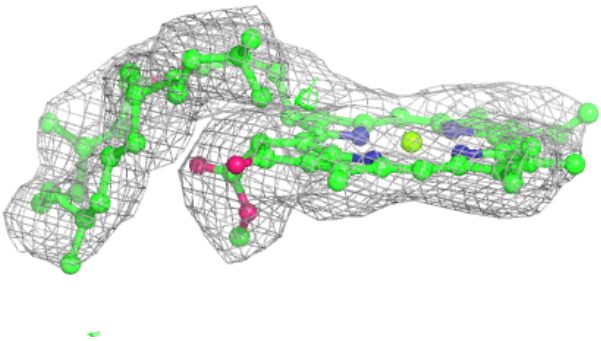


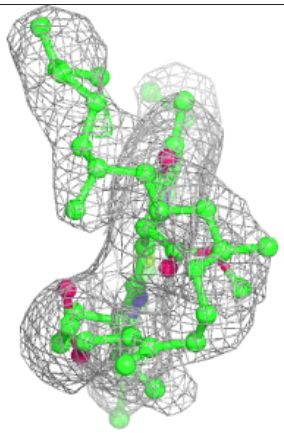


Electron density around CLA b 613:

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

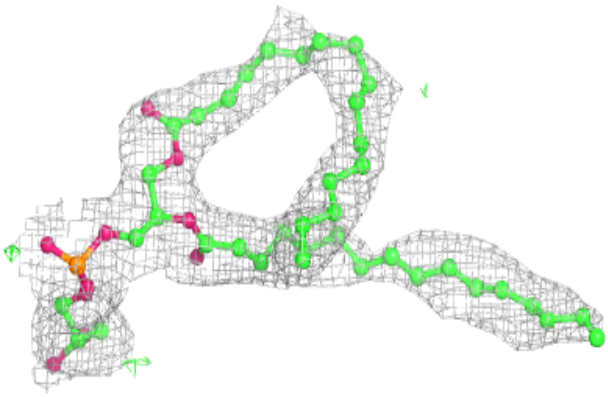


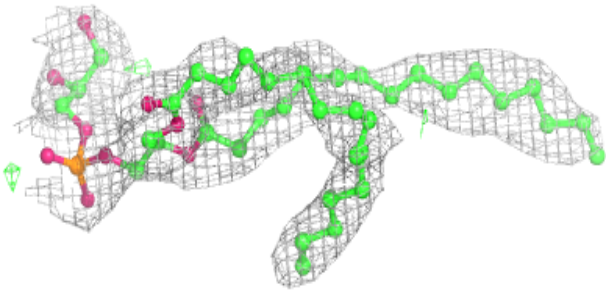


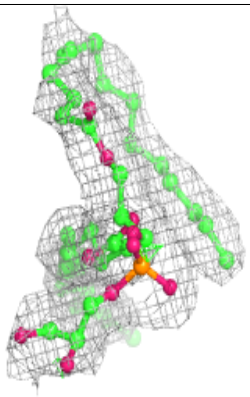


Electron density around LHG a 613:

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

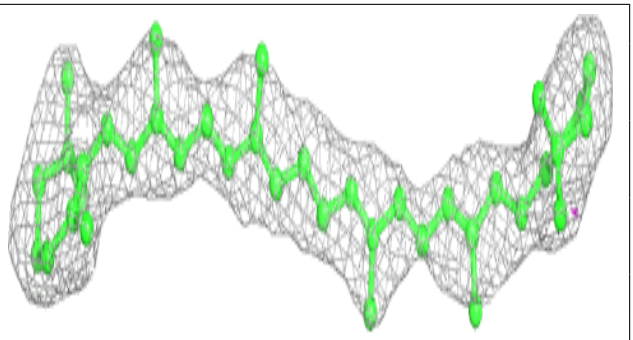


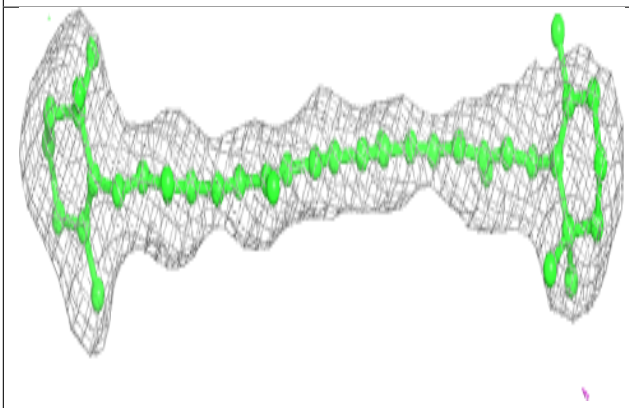


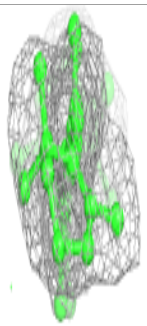


Electron density around BCR a 610:

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

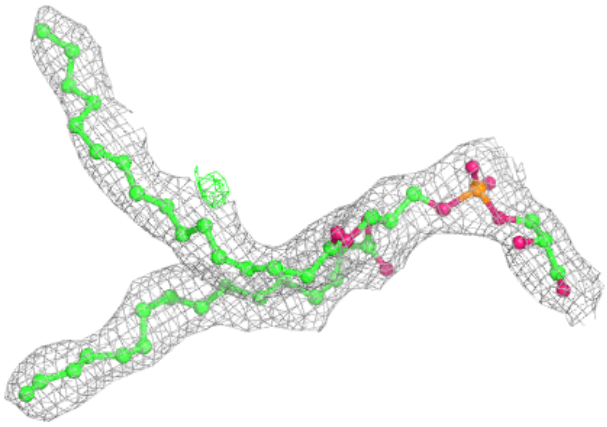


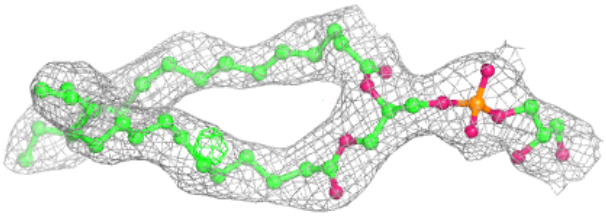


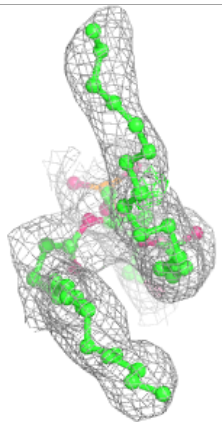


Electron density around LHG d 407:

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

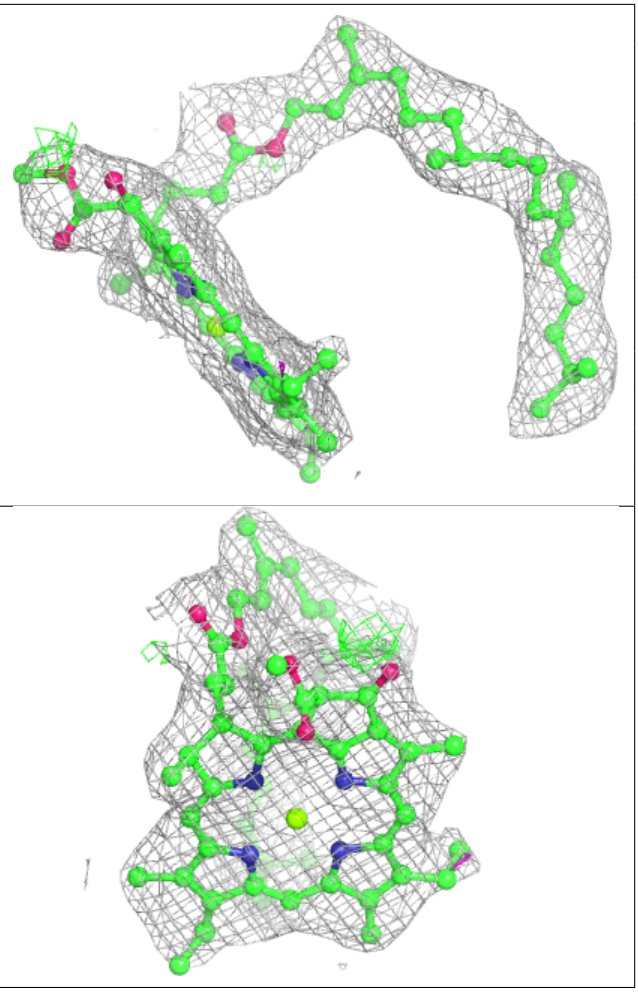






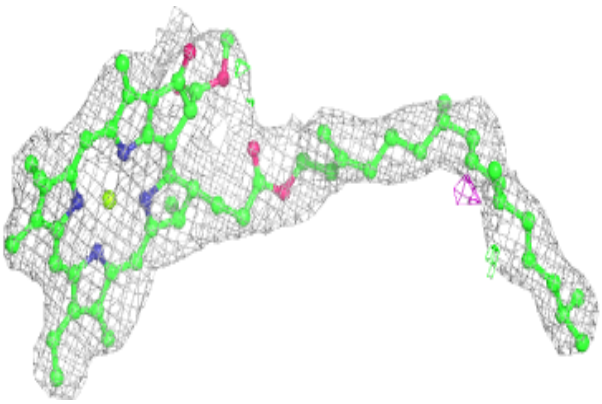
Electron density around CLA B 611:

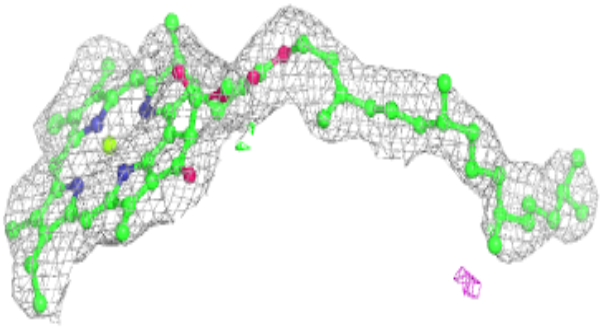
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

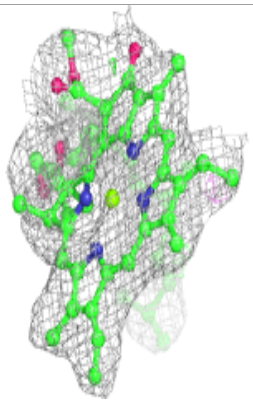


Electron density around CLA a 606:

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

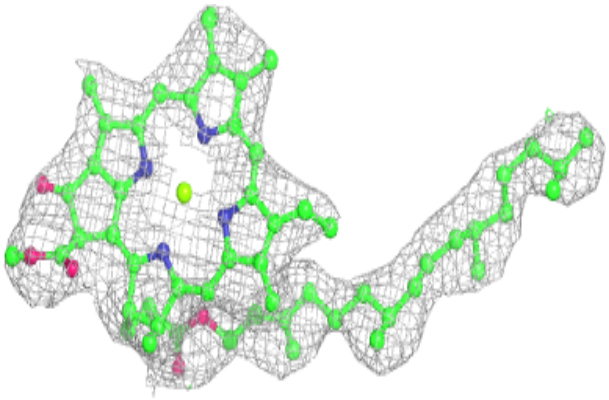


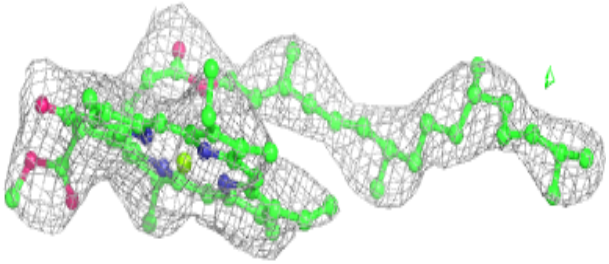


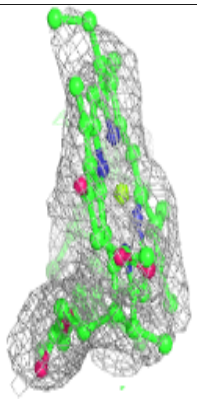


Electron density around CLA c 503:

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

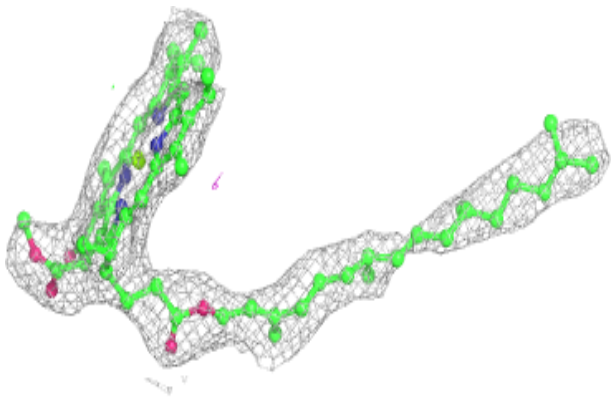


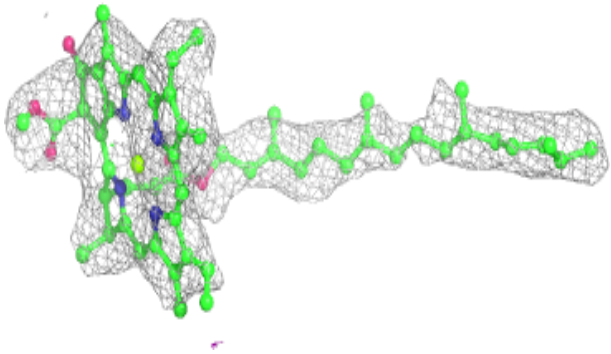


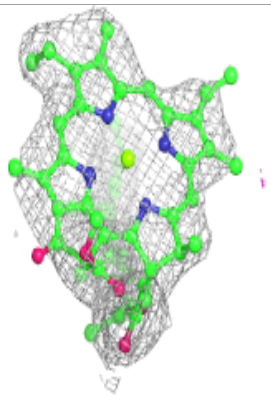


Electron density around CLA b 610:

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

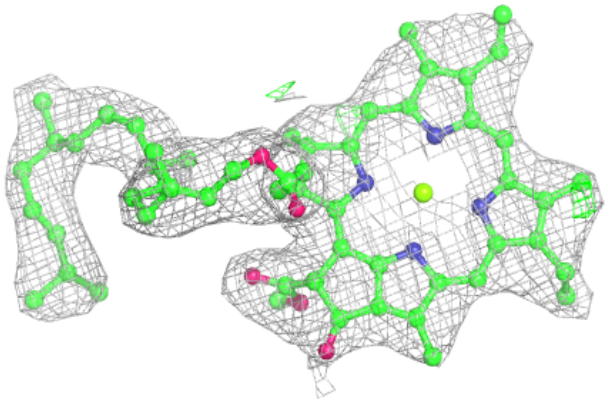


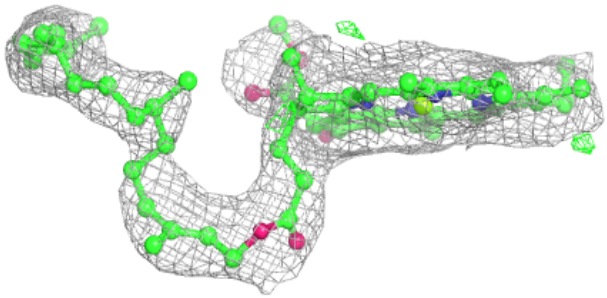


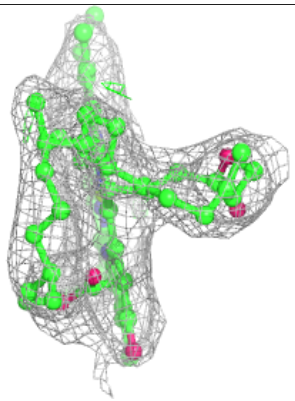


Electron density around CLA B 612:

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

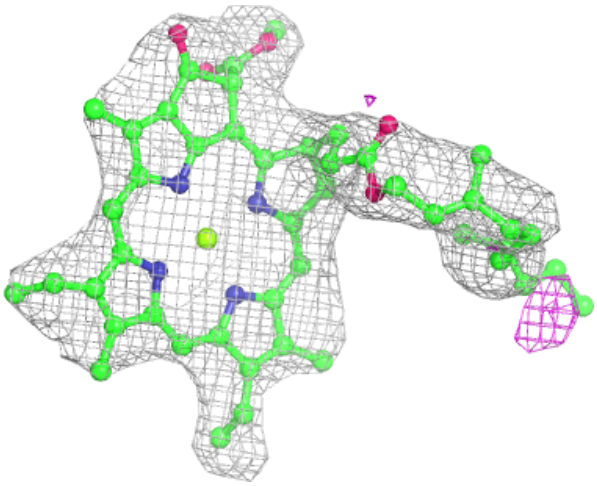


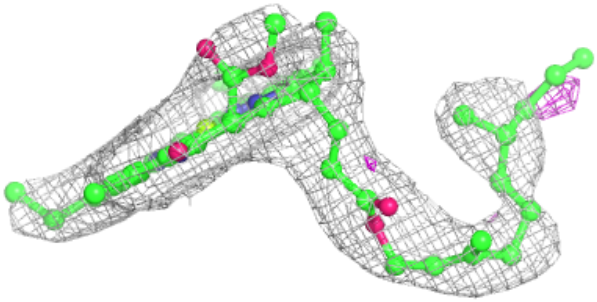


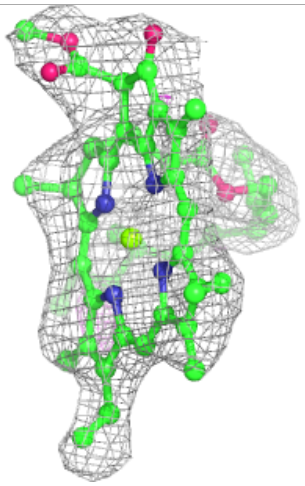


Electron density around CLA A 607:

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

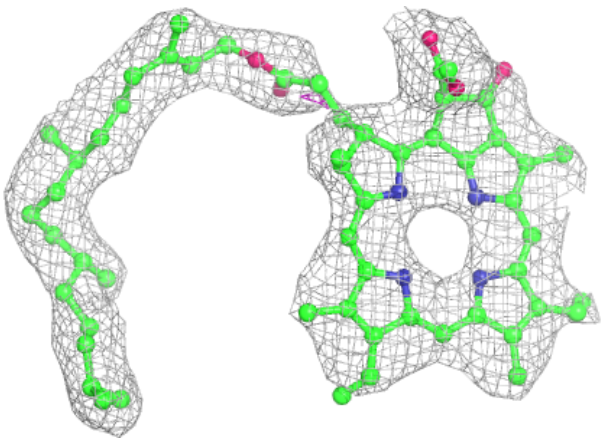


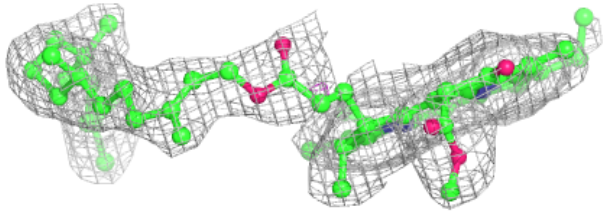


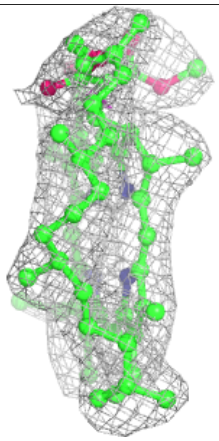


Electron density around PHO A 608:

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

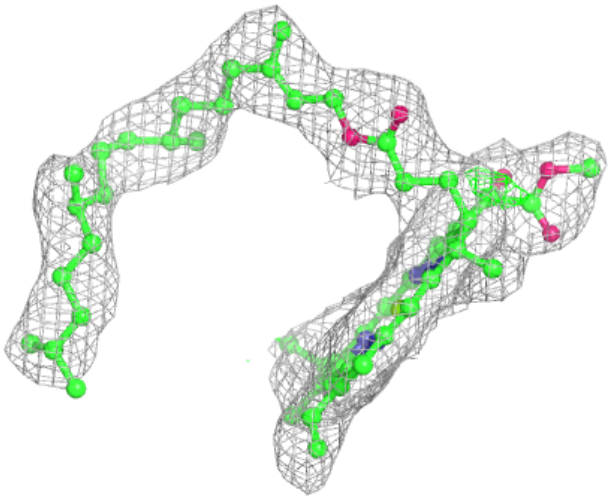


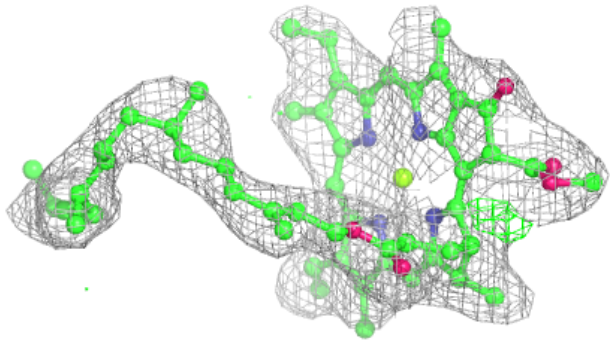


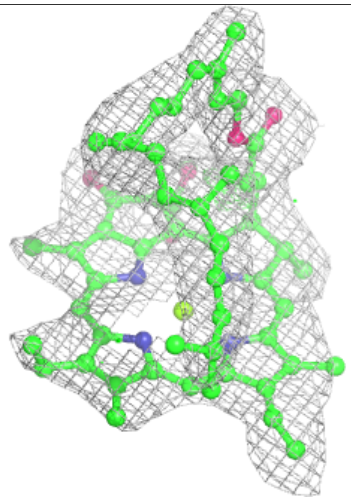


Electron density around CLA b 614:

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

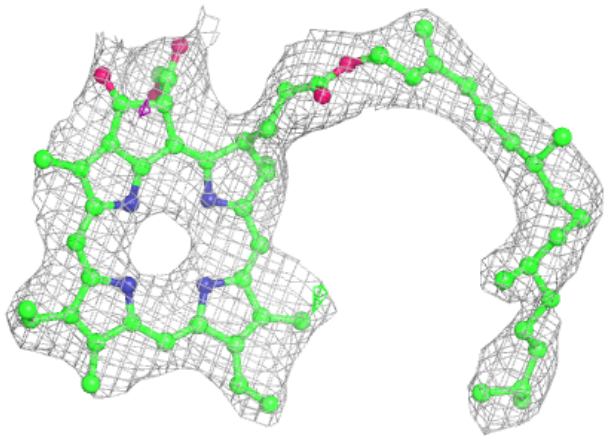


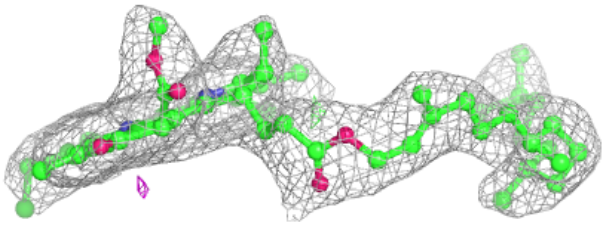


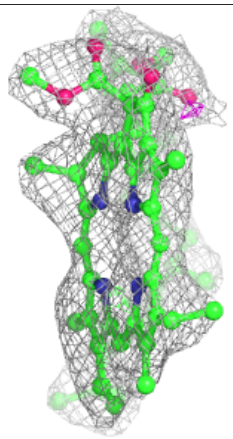


Electron density around PHO a 608:

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

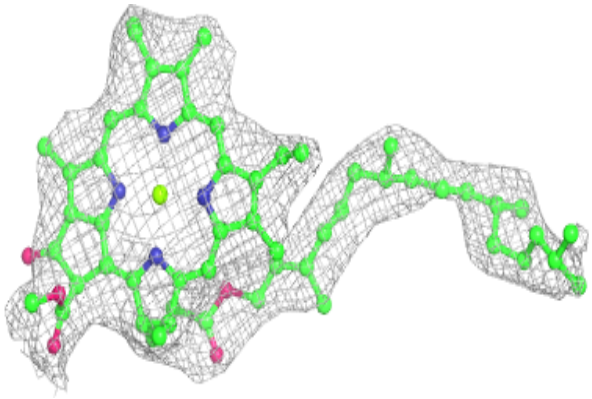


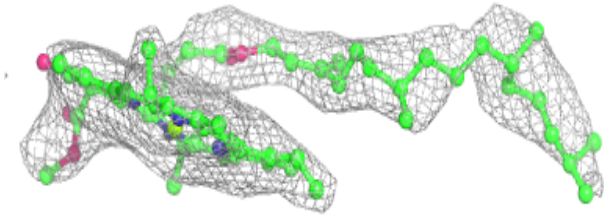


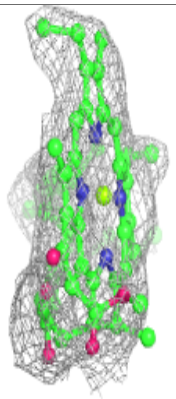


Electron density around CLA b 606:

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

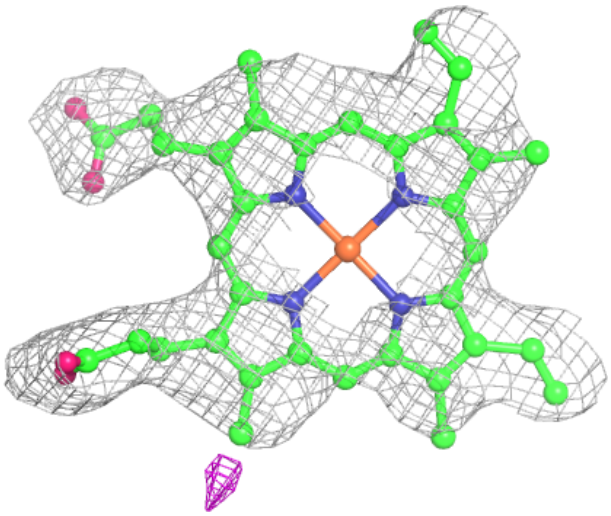


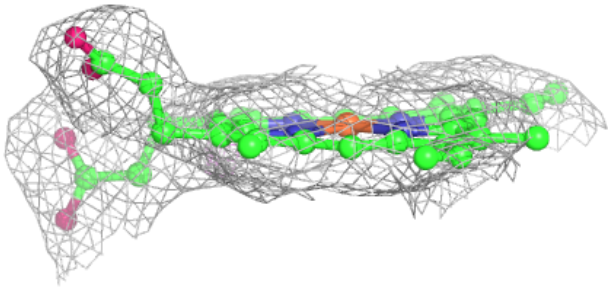


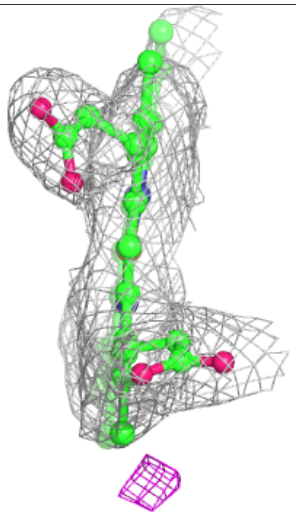


Electron density around HEC V 201:

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

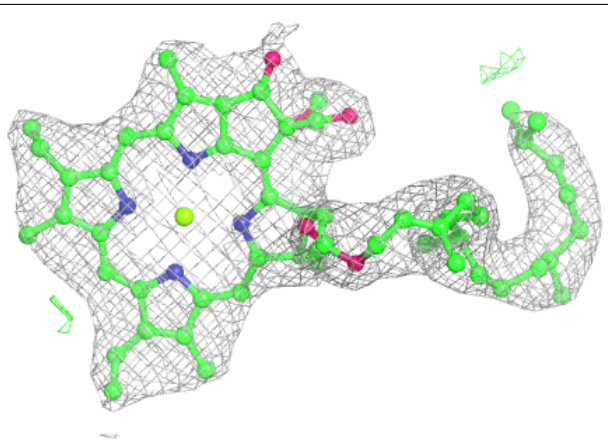


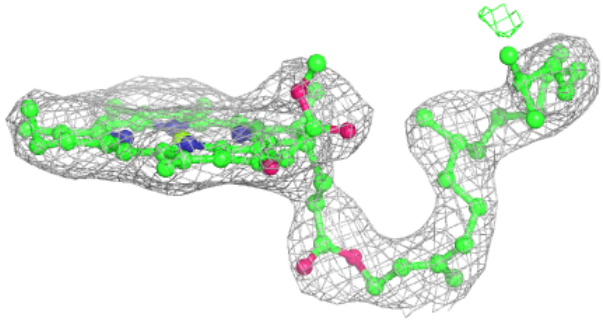


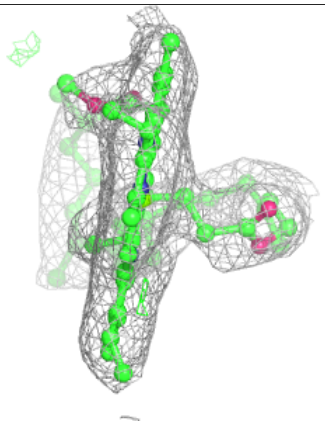


Electron density around CLA b 615:

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

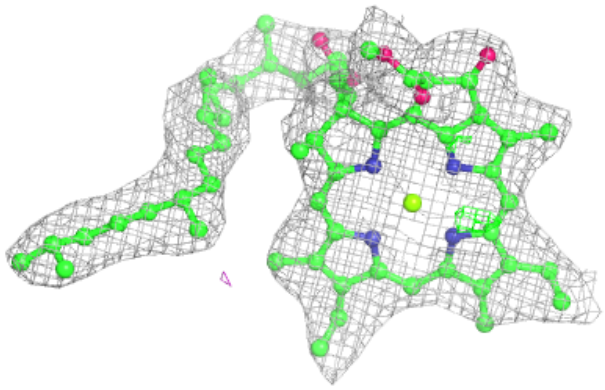


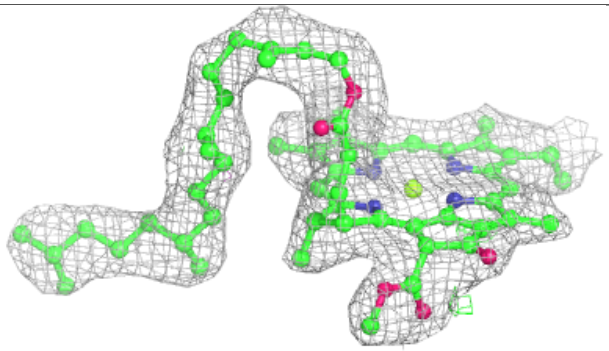


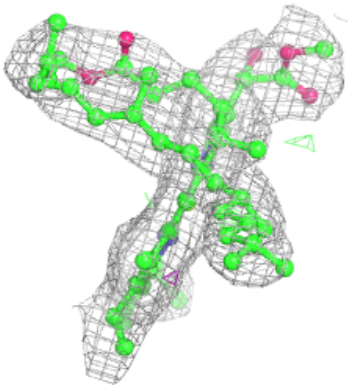


Electron density around CLA a 612:

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

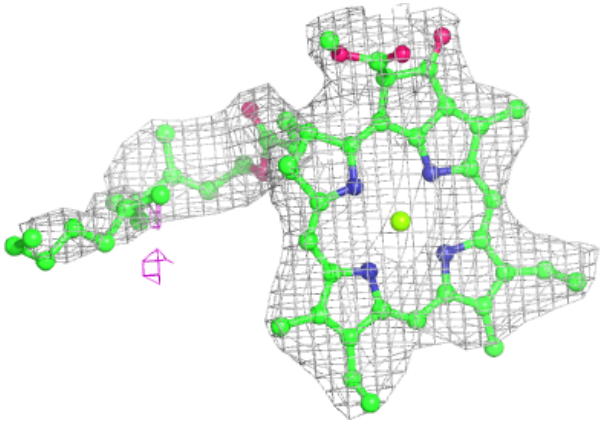


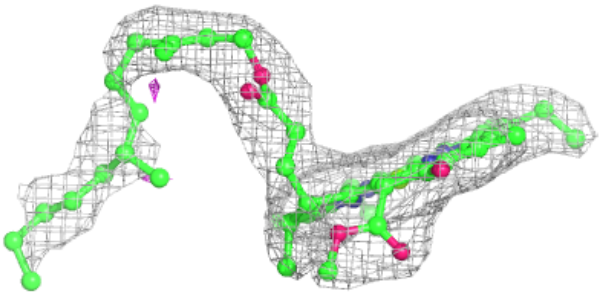


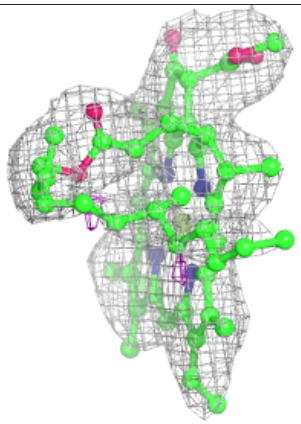


Electron density around CLA a 607:

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

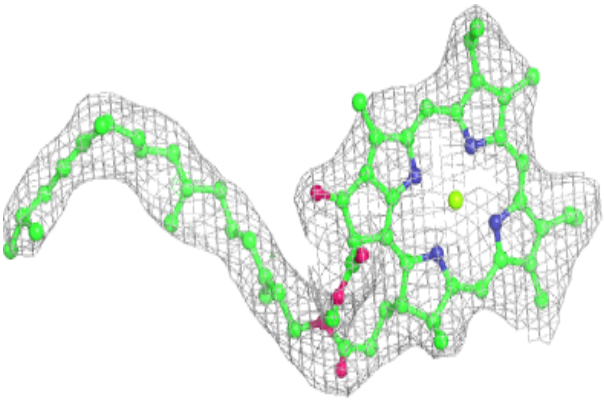


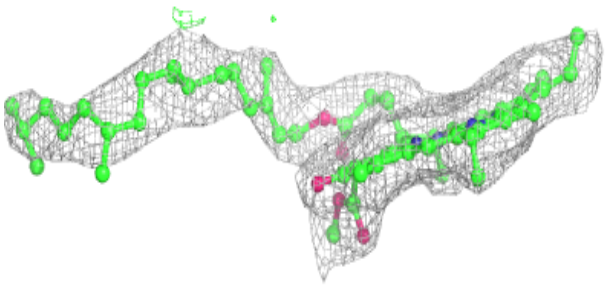


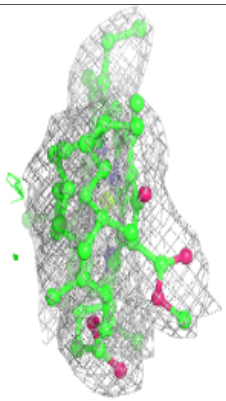


Electron density around CLA B 602:

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

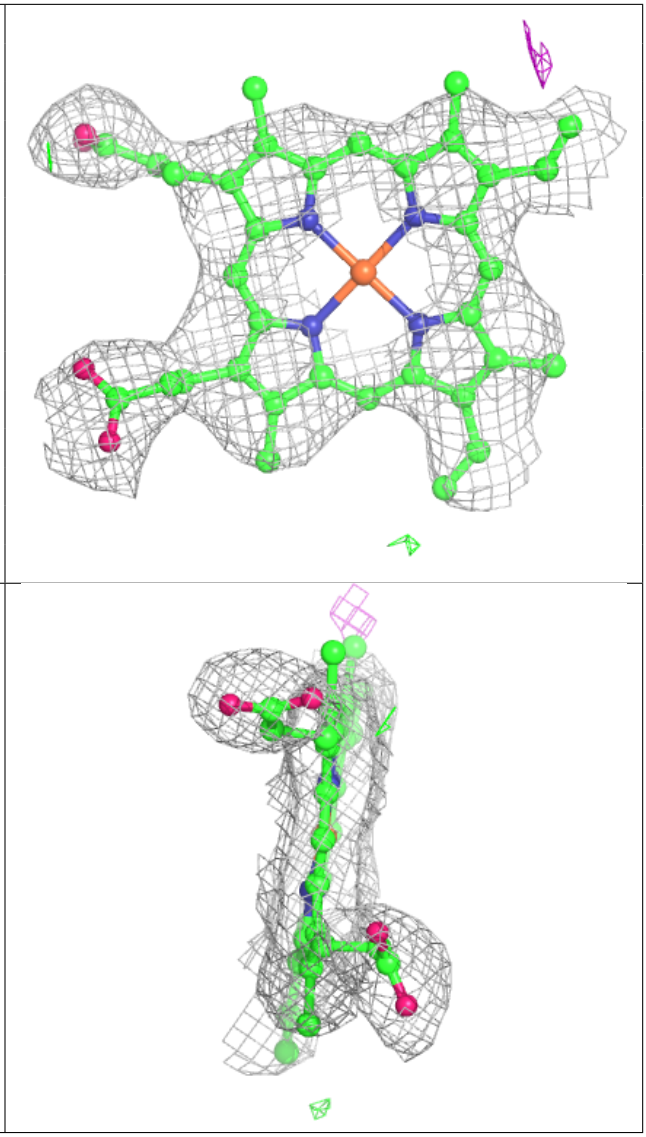






Electron density around HEC v 201:

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



6.5 Other polymers (i)

There are no such residues in this entry.