wwPDB X-ray Structure Validation Summary Report (i)

Oct 31, 2023 – 07:31 AM EDT

PDB ID	:	3KZI
Title	:	Crystal Structure of Monomeric Form of Cyanobacterial Photosystem II
Authors	:	Gabdulkhakov, A.; Guskov, A.; Broser, M.; Kern, J.; Zouni, A.; Saenger, W.
Deposited on	:	2009-12-08
Resolution	:	3.60 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:

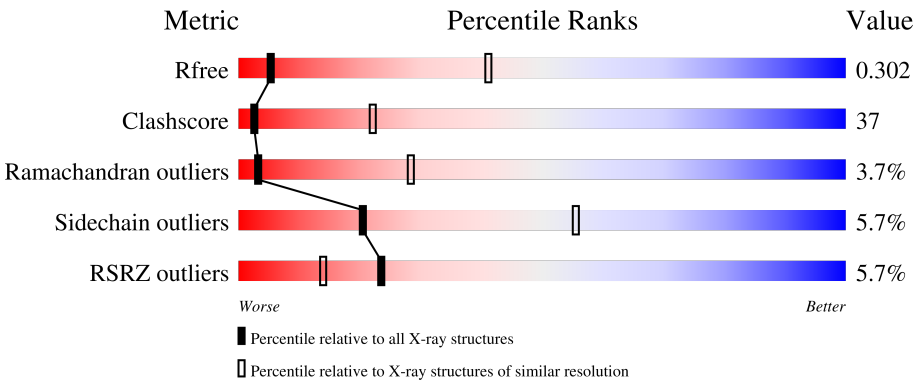
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.60 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	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)

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	5%; 47%; 46%; 5% •
2	B	510	3%; 53%; 38%; • 5%
3	C	461	5%; 41%; 50%; 6% •
4	D	352	7%; 51%; 39%; 7% •
5	E	83	2%; 28%; 57%; 7% • 7%

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Mol	Chain	Length	Quality of chain
6	F	44	11% 25% 50% 11% 14%
7	H	65	3% 38% 49% 11%
8	I	38	11% 47% 45% 8%
9	J	40	20% 58% 8% 15%
10	K	37	3% 11% 78% 11%
11	L	37	8% 54% 32% 14%
12	M	36	22% 39% 56% 6%
13	O	246	8% 50% 45%
14	T	32	6% 56% 34% 6%
15	U	104	4% 55% 34% 7%
16	V	137	4% 60% 36%
17	y	46	4% 48% 13% 39%
18	X	40	10% 48% 25% 12% 12%
19	Z	62	8% 37% 53% 10%

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
21	CLA	A	362	X	-	-	-
21	CLA	A	363	X	-	-	X
21	CLA	A	364	X	-	-	-
21	CLA	A	366	X	-	-	-
21	CLA	B	511	X	-	-	X
21	CLA	B	512	X	-	-	-
21	CLA	B	513	X	-	X	-
21	CLA	B	514	X	-	-	-
21	CLA	B	515	X	-	-	-
21	CLA	B	516	X	-	-	-
21	CLA	B	517	X	-	-	-
21	CLA	B	518	X	-	-	-
21	CLA	B	519	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	B	520	X	-	-	-
21	CLA	B	521	X	-	-	-
21	CLA	B	522	X	-	-	-
21	CLA	B	523	X	-	-	-
21	CLA	B	524	X	-	-	-
21	CLA	B	525	X	-	-	-
21	CLA	B	526	X	-	-	X
21	CLA	C	477	X	-	-	-
21	CLA	C	478	X	-	-	-
21	CLA	C	479	X	-	-	-
21	CLA	C	480	X	-	-	-
21	CLA	C	481	X	-	-	-
21	CLA	C	482	X	-	-	X
21	CLA	C	483	X	-	-	-
21	CLA	C	484	X	-	-	-
21	CLA	C	485	X	-	-	-
21	CLA	C	486	X	-	X	-
21	CLA	C	487	X	-	-	-
21	CLA	C	488	X	-	-	-
21	CLA	D	354	X	-	-	-
21	CLA	D	356	X	-	-	-
21	CLA	K	483	X	-	-	-
22	PHO	A	365	X	-	-	-
22	PHO	D	355	X	-	-	-
23	MES	A	367	-	-	X	-
25	BCR	B	527	-	-	-	X
25	BCR	B	529	-	-	-	X
25	BCR	B	530	-	-	-	X
25	BCR	C	490	-	-	-	X
25	BCR	J	115	-	-	-	X
25	BCR	X	107	-	-	-	X
25	BCR	Z	116	-	-	-	X
26	LHG	C	476	-	-	-	X
27	LMG	A	373	-	-	X	X
27	LMG	C	494	-	-	-	X
27	LMG	D	360	-	-	X	X
27	LMG	I	220	-	-	-	X
27	LMG	J	492	-	-	-	X
27	LMG	M	217	-	-	-	X
28	DGD	A	375	-	-	-	X
28	DGD	B	528	-	-	X	-
28	DGD	C	474	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
28	DGD	C	492	X	-	-	-
28	DGD	C	493	X	-	X	-
28	DGD	D	362	-	-	-	X
29	LMT	A	376	-	-	-	X
29	LMT	B	535	-	-	-	X
29	LMT	D	363	-	-	-	X
29	LMT	I	274	-	-	-	X
29	LMT	T	226	-	-	-	X
30	SQD	C	475	-	-	-	X
30	SQD	F	224	-	-	-	X
30	SQD	L	213	-	-	-	X
32	PL9	D	357	-	-	X	X
34	CA	O	273	-	-	-	X

2 Entry composition (i)

There are 34 unique types of molecules in this entry. The entry contains 24678 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 Q(B) protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	335	2628	1720	432	461	15	0	0	0

- Molecule 2 is a protein called Photosystem II core light harvesting protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	485	3812	2505	635	659	13	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	448	3455	2262	580	600	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	340	2706	1794	440	460	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	77	635	417	103	115	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	38	307	207	50	49	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	65	507	338	81	86	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	35	286	195	45	45	1	0	0	0

- 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	34	249	170	38	40	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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	L	37	304	202	48	53	1	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	34	267	178	40	48	1	0	0	0

- 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	243	1845	1154	308	379	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	256	180	36	38	2	0	0	0

- 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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
16	V	137	1060	673	177	206	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	28	201	134	33	31	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	35	254	172	38	44	0	0	0

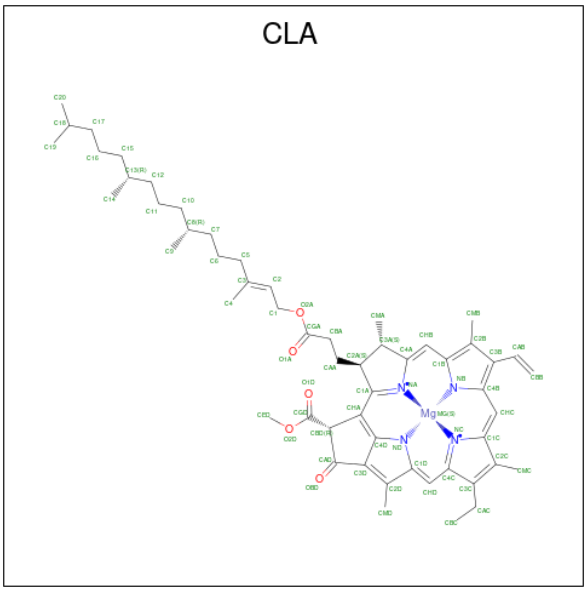
- Molecule 19 is a protein called Photosystem II reaction center protein Z.

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

- Molecule 20 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

- Molecule 21 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		
21	A	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
21	A	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
21	A	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
21	A	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
21	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
21	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
21	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
21	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
21	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
21	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
21	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
21	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
21	B	1	65	55	1	4	5	0	0

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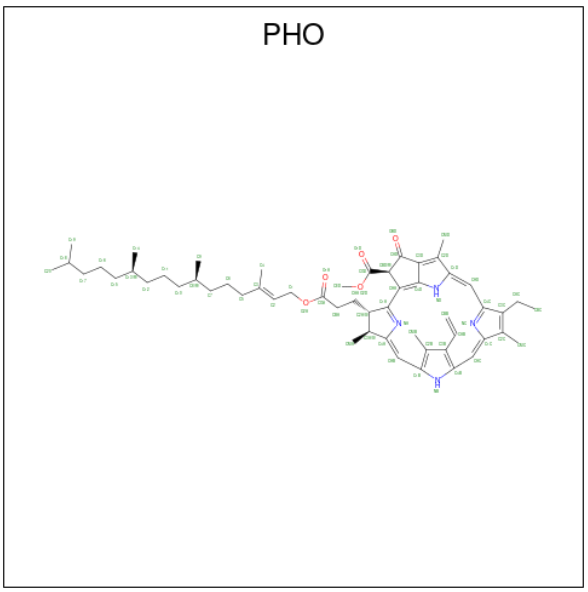
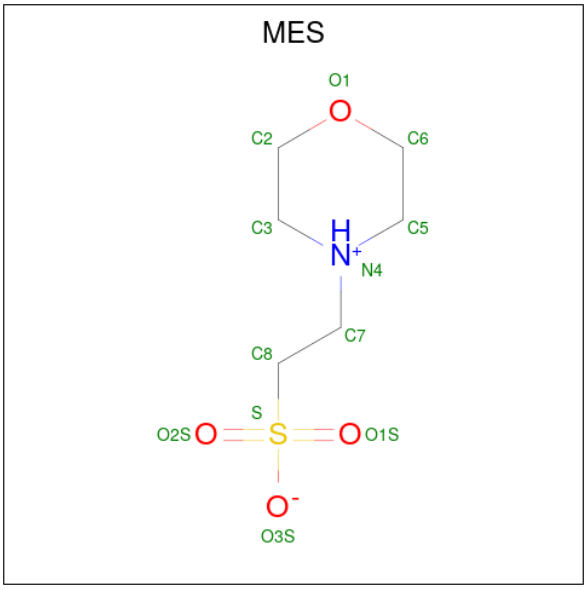
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
21	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
21	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
21	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
21	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
21	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
21	B	1	65	55	1	4	5	0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

- Molecule 22 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).



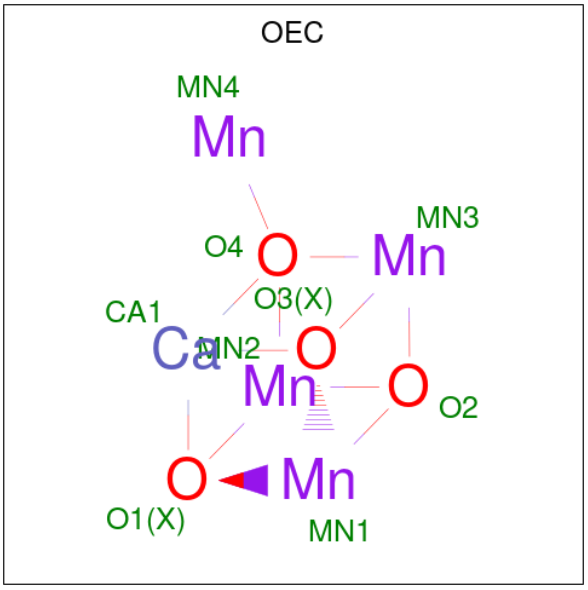
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
22	A	1	64	55	4	5	0	0
			Total	C	N	O		
22	D	1	64	55	4	5	0	0

- Molecule 23 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



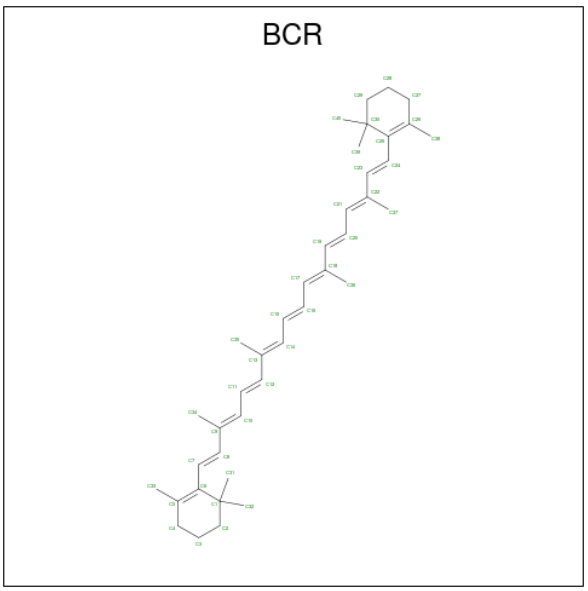
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
23	A	1	12	6	1	4	1	0	0

- Molecule 24 is OXYGEN EVOLVING SYSTEM (three-letter code: OEC) (formula: $CaMn_4O_4$).



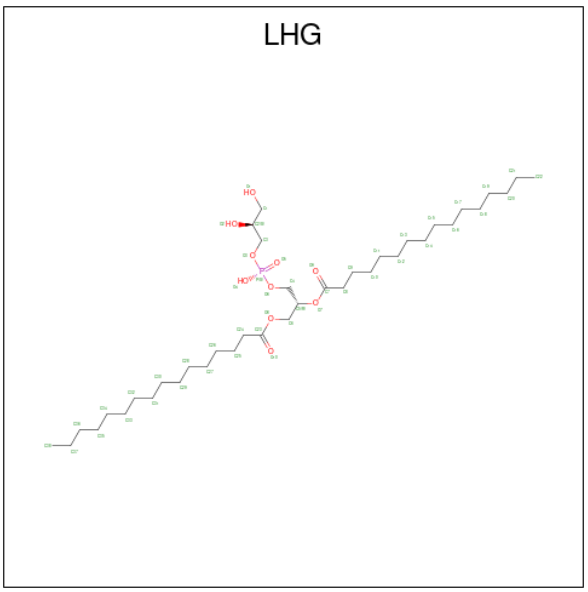
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Ca	Mn		
24	A	1	5	1	4	0	0

- Molecule 25 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



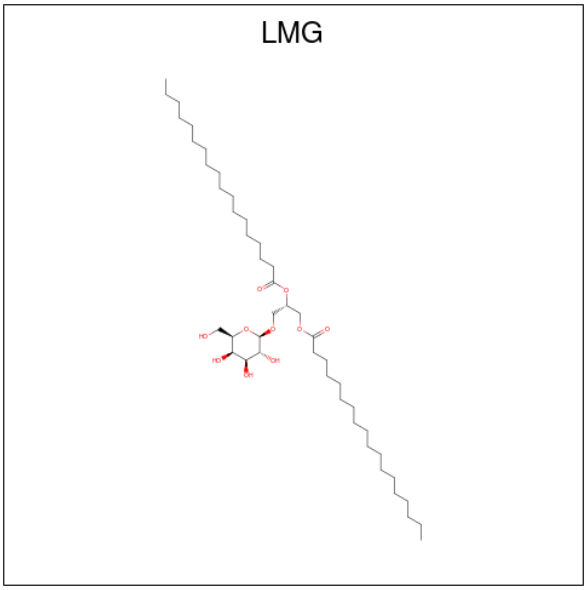
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	C		
25	A	1	40	40	0	0
			Total	C		
25	B	1	40	40	0	0
			Total	C		
25	B	1	40	40	0	0
			Total	C		
25	B	1	40	40	0	0
			Total	C		
25	C	1	40	40	0	0
			Total	C		
25	C	1	40	40	0	0
			Total	C		
25	D	1	40	40	0	0
			Total	C		
25	J	1	40	40	0	0
			Total	C		
25	J	1	40	40	0	0
			Total	C		
25	X	1	40	40	0	0
			Total	C		
25	Z	1	40	40	0	0

- Molecule 26 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		
26	A	1	39	28	10	1	0	0
			Total	C	O	P		
26	C	1	37	26	10	1	0	0

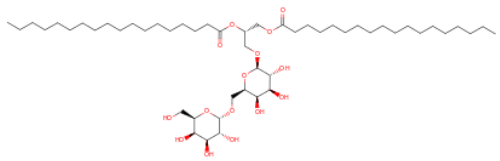
- Molecule 27 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
27	A	1	51	41	10	0	0
			Total	C	O		
27	B	1	49	39	10	0	0
			Total	C	O		
27	C	1	45	35	10	0	0
			Total	C	O		
27	D	1	46	36	10	0	0
			Total	C	O		
27	D	1	48	38	10	0	0
			Total	C	O		
27	I	1	43	33	10	0	0
			Total	C	O		
27	J	1	48	38	10	0	0
			Total	C	O		
27	M	1	42	32	10	0	0

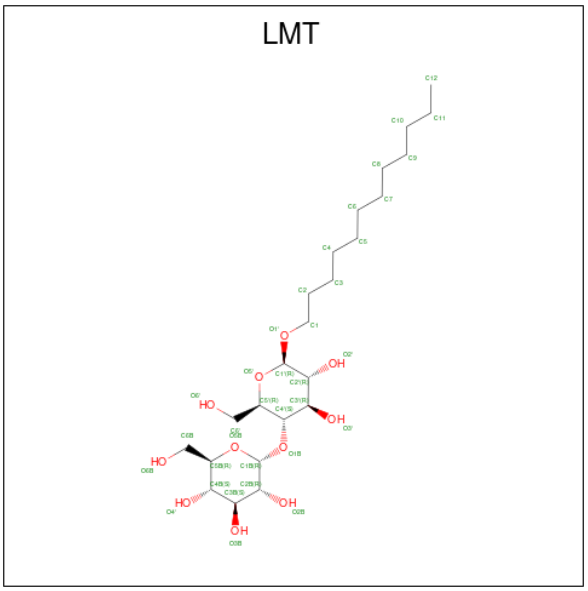
- Molecule 28 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).

DGD



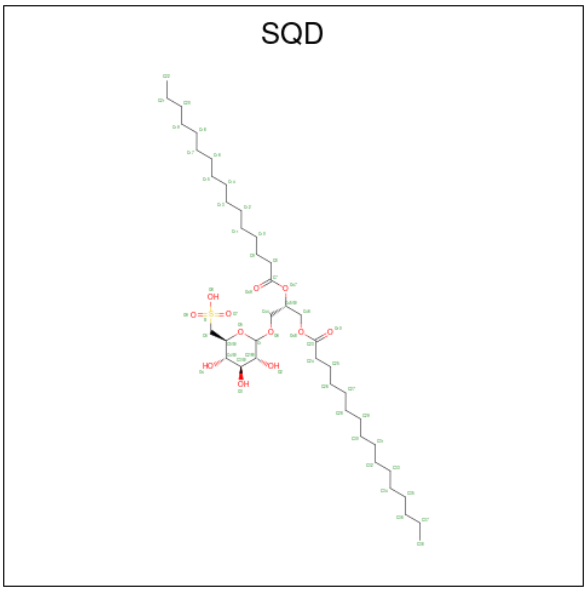
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
28	A	1	52	37	15	0	0
			Total	C	O		
28	B	1	66	51	15	0	0
			Total	C	O		
28	B	1	58	43	15	0	0
			Total	C	O		
28	C	1	56	41	15	0	0
			Total	C	O		
28	C	1	53	38	15	0	0
			Total	C	O		
28	C	1	62	47	15	0	0
			Total	C	O		
28	C	1	66	51	15	0	0
			Total	C	O		
28	D	1	63	48	15	0	0

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



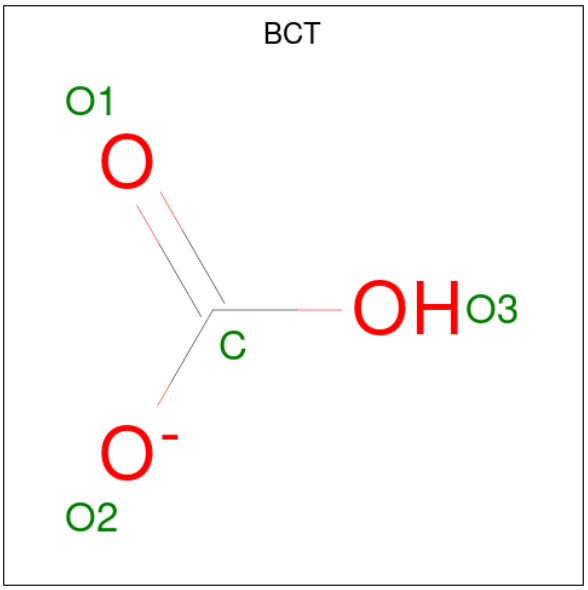
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
29	A	1	35	24	11	0	0
			Total	C	O		
29	B	1	35	24	11	0	0
			Total	C	O		
29	D	1	35	24	11	0	0
			Total	C	O		
29	D	1	31	20	11	0	0
			Total	C	O		
29	I	1	35	24	11	0	0
			Total	C	O		
29	O	1	35	24	11	0	0
			Total	C	O		
29	T	1	35	24	11	0	0

- Molecule 30 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



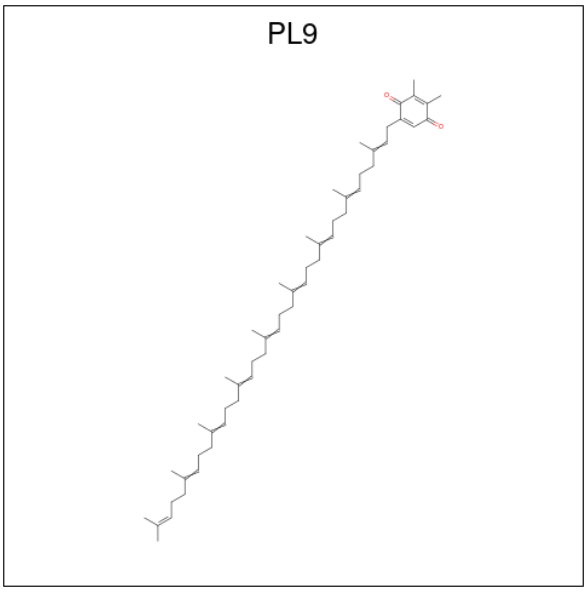
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	C	1	Total	C	O	S	0	0
			51	38	12	1		
30	D	1	Total	C	O	S	0	0
			43	30	12	1		
30	F	1	Total	C	O	S	0	0
			45	32	12	1		
30	L	1	Total	C	O	S	0	0
			47	34	12	1		

- Molecule 31 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



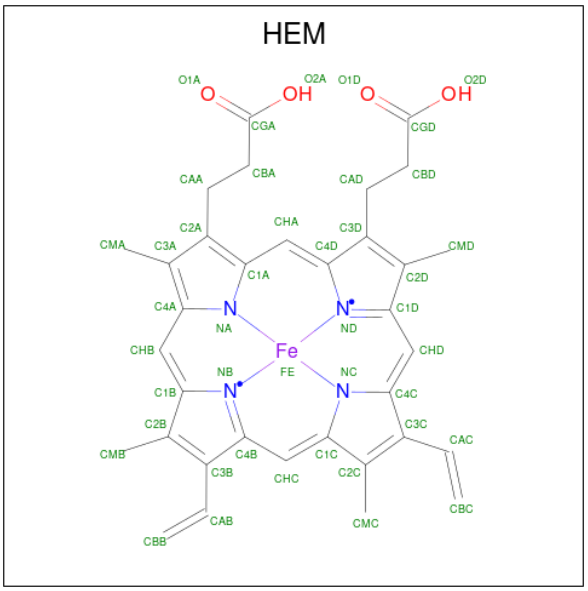
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
31	D	1	4	1	3	0	0

- Molecule 32 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		
32	D	1	55	53	2	0	0

- Molecule 33 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		
33	F	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
33	V	1	43	34	1	4	4	0	0

- Molecule 34 is CALCIUM ION (three-letter code: CA) (formula: Ca).

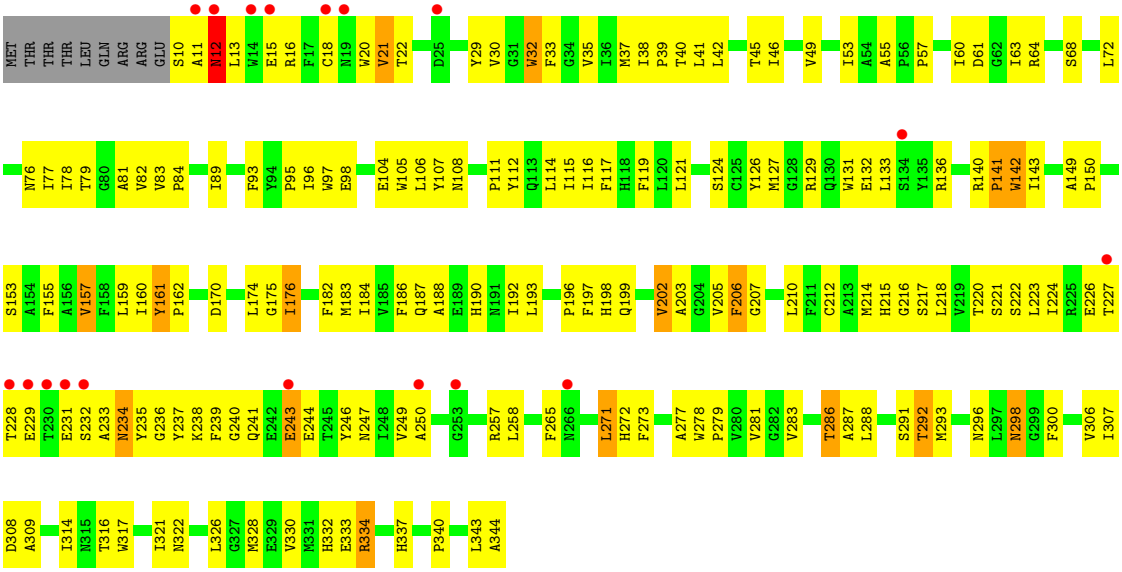
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
34	F	1	1	1	0	0
			Total	Ca		
34	K	1	1	1	0	0
			Total	Ca		
34	O	1	1	1	0	0

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.

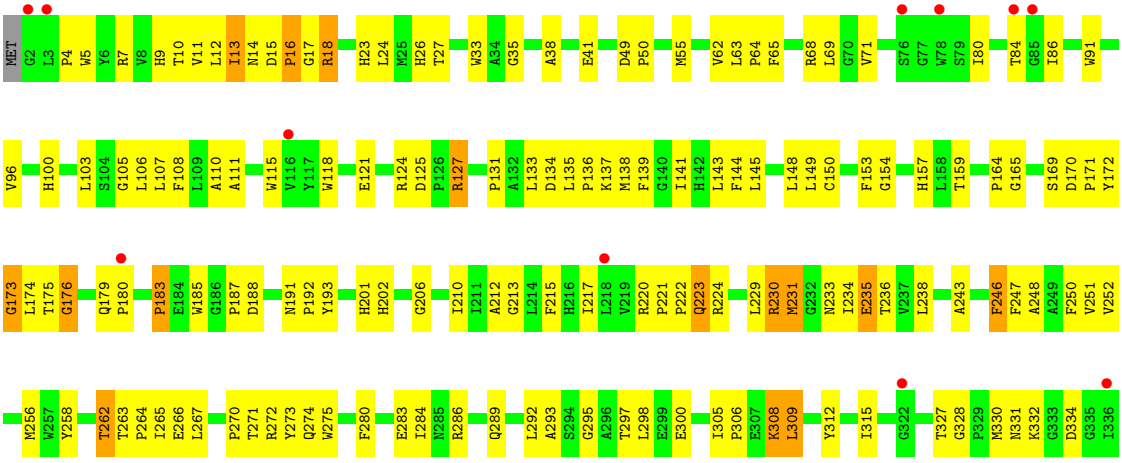
• Molecule 1: Photosystem Q(B) protein 1

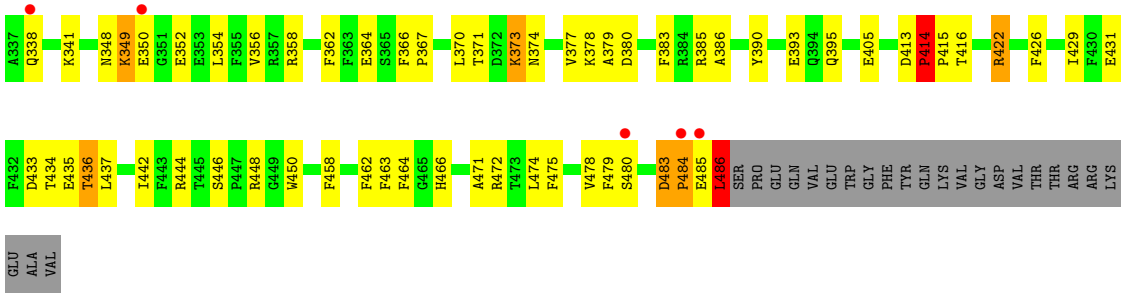
Chain A:



• Molecule 2: Photosystem II core light harvesting protein

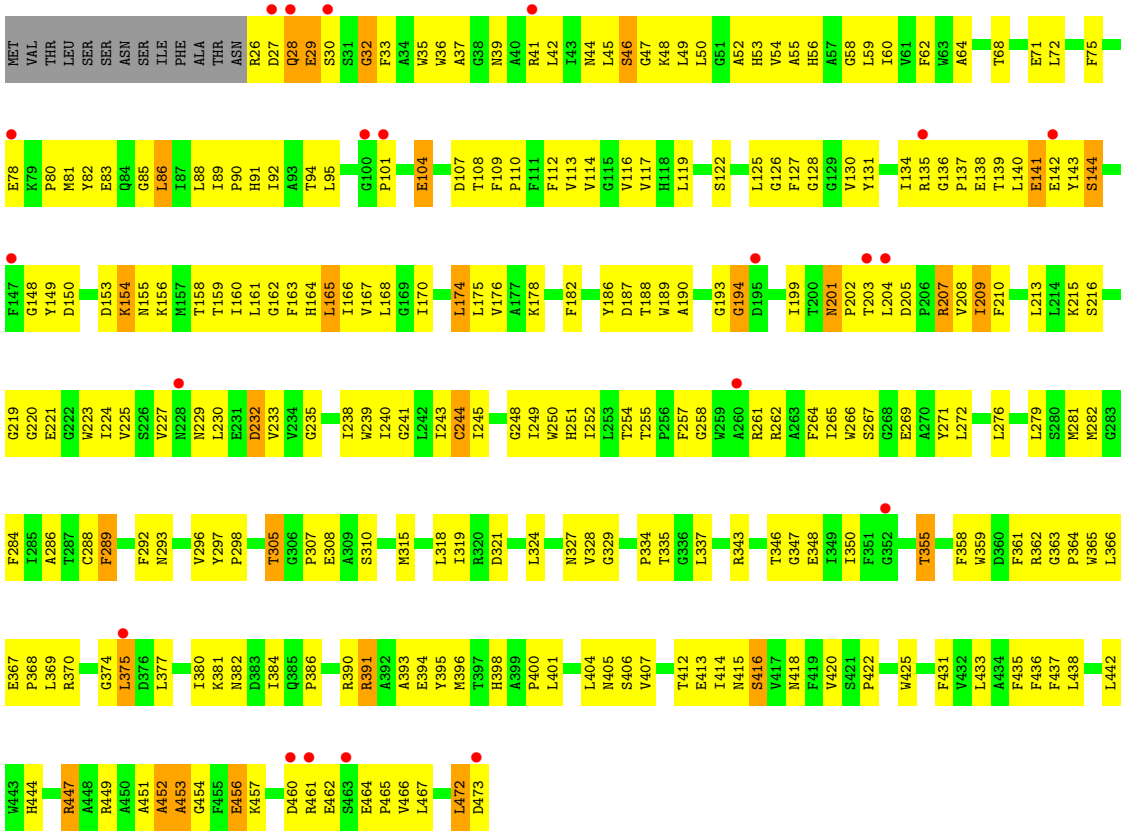
Chain B:





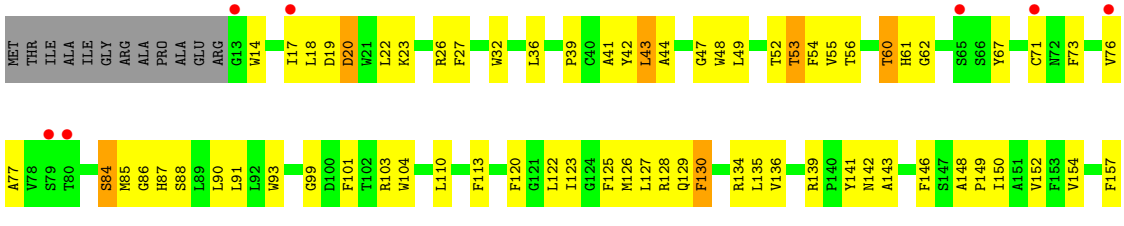
- Molecule 3: Photosystem II CP43 protein

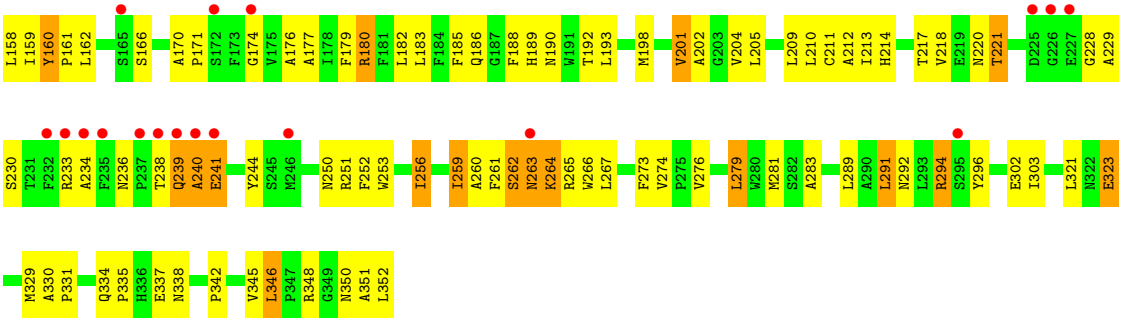
Chain C:



- Molecule 4: Photosystem II D2 protein

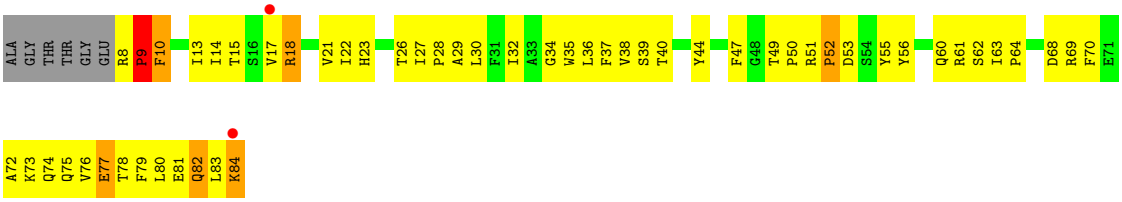
Chain D:





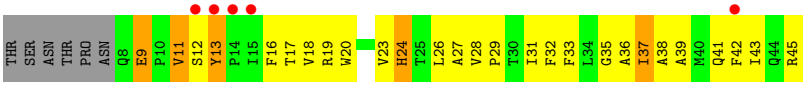
- Molecule 5: Cytochrome b559 subunit alpha

Chain E: 2% 28% 57% 7% • 7%



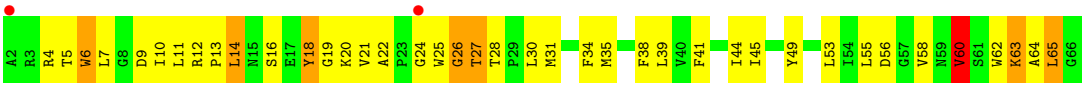
- Molecule 6: Cytochrome b559 subunit beta

Chain F: 11% 25% 50% 11% 14%



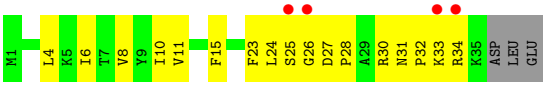
- Molecule 7: Photosystem II reaction center protein H

Chain H: 3% 38% 49% 11% •



- Molecule 8: Photosystem II reaction center protein I

Chain I: 11% 47% 45% 8%



- Molecule 9: Photosystem II reaction center protein J

Chain J: 20% 58% 8% 15%

- Molecule 10: Photosystem II reaction center protein K

Chain K: 3% 11% 78% 11%

K10 L11 P12 E13 A16 I17 F18 D19 P20 L21 V22 D23 V24 L25 P26 V27 I28 P29 V30 L31 F32 L33 A34 L35 A36 F37 V38 W39 Q40 A41 A42 V43 G44 F45 R46

• Molecule 11: Photosystem II reaction center protein L

Chain L: 8% 54% 32% 14%

M1 E2 P3 N4 P5 N6 R7 Q8 P9 V10 E11 L12 N13 R14 T15 L19 G20 L21 L22 L23 I24 L25 V26 F31 F35 F36 N37

• Molecule 12: Photosystem II reaction center protein M

Chain M: 22% 39% 56% 6%

M1 E2 V3 L6 G7 L8 I9 A10 L13 F14 V17 P18 S19 V20 F21 L22 I23 I24 L25 Q28 T29 E30 S31 Q32 Q33 K34 SER SER

• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O: 8% 50% 45%

ALA LYS GLN T30 L31 T32 Y33 D34 D35 I36 V37 G38 T39 G40 L41 A42 N43 T47 T51 A52 R53 G54 A55 Y56 D59 S60 S61 Q62 I66 L69 C70 L71 Q72 P73 L77 V78 K79 E80 E81 P82 K83 N84 K85 R86 Q87 E88 A89 E90 F91 V92 P93 T94 K95 L96

V97 T98 R99 T102 S103 Q106 I107 Q108 G109 K112 V113 N114 S115 D116 G117 S118 L119 T120 F121 V122 E123 E124 D125 G126 I127 D128 P131 V132 Q135 G138 R141 L144 T147 V148 V152 A153 S154 T155 Q156 P157 N158 V159 T160 S161 S165 T166 D167 F168

E171 F172 N173 R178 T179 A180 N181 F182 L183 D184 P185 K186 G187 R188 G189 L190 A191 S192 G193 Y194 I198 A199 L200 P201 Q202 A203 K204 E205 E206 K214 R215 L218 T219 K220 G221 Q222 I223 S224 L225 N226 V227 A228 K229 V230 D231 G232 R233 T234 G235 E236 T240 S243 V259

G263 V264 F265 P271 A272

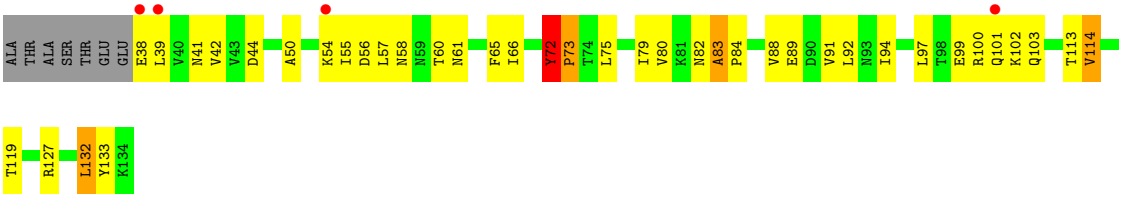
• Molecule 14: Photosystem II reaction center protein T

Chain T: 6% 56% 34% 6%

M1 E2 T3 Y6 I13 F17 I21 F22 F23 R24 E25 P26 P27 R28 I29 T30 LYS LYS

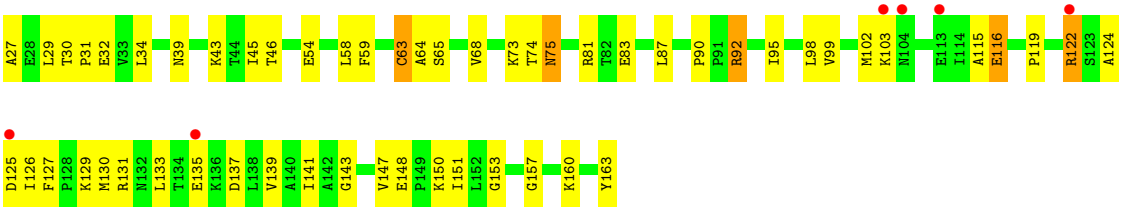
• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U: 4% 55% 34% 7%



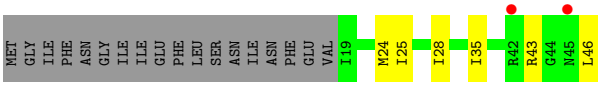
• Molecule 16: Cytochrome c-550

Chain V:



• Molecule 17: Photosystem II reaction center protein ycf12

Chain y:

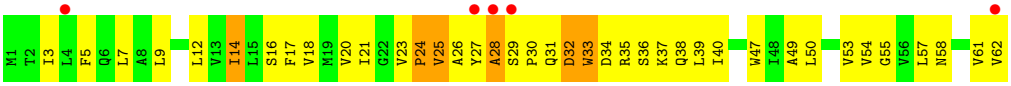


• Molecule 18: Photosystem II reaction center X protein

Chain X:

• Molecule 19: Photosystem II reaction center protein Z

Chain Z:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	119.89Å 224.69Å 337.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.87 – 3.60 29.87 – 3.60	Depositor EDS
% Data completeness (in resolution range)	89.2 (29.87-3.60) 99.3 (29.87-3.60)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	1.24 (at 3.56Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.297 , 0.308 0.294 , 0.302	Depositor DCC
R_{free} test set	1054 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å^2)	153.9	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 84.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	24678	wwPDB-VP
Average B, all atoms (Å^2)	163.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.50% 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: CA, HEM, FE2, MES, BCT, PHO, BCR, LMT, PL9, LHG, CLA, OEC, DGD, SQD, LMG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.44	0/2713	0.66	0/3700
2	B	0.43	0/3947	0.66	1/5379 (0.0%)
3	C	0.41	0/3567	0.64	1/4856 (0.0%)
4	D	0.47	0/2801	0.65	0/3818
5	E	0.43	0/654	0.69	0/891
6	F	0.62	0/317	0.71	0/433
7	H	0.38	0/520	0.67	0/709
8	I	0.51	0/293	0.68	0/395
9	J	0.41	0/255	0.68	0/346
10	K	0.41	0/303	0.62	0/416
11	L	0.37	0/311	0.65	0/422
12	M	0.44	0/270	0.70	0/367
13	O	0.44	0/1876	0.70	0/2548
14	T	0.49	0/265	0.63	0/359
15	U	0.42	0/785	0.73	1/1064 (0.1%)
16	V	0.39	0/1081	0.65	0/1468
17	y	0.46	0/202	0.73	0/272
18	X	0.42	0/257	0.59	0/348
19	Z	0.45	0/490	0.69	0/669
All	All	0.43	0/20907	0.66	3/28460 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	486	LEU	CA-CB-CG	6.98	131.36	115.30
3	C	32	GLY	N-CA-C	-5.55	99.23	113.10
15	U	72	TYR	N-CA-C	5.05	124.64	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	161	TYR	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2628	0	2524	244	0
2	B	3812	0	3683	272	0
3	C	3455	0	3378	373	0
4	D	2706	0	2608	238	0
5	E	635	0	625	82	0
6	F	307	0	312	49	0
7	H	507	0	521	67	0
8	I	286	0	308	18	0
9	J	249	0	262	50	0
10	K	293	0	305	56	0
11	L	304	0	316	28	0
12	M	267	0	289	34	0
13	O	1845	0	1801	119	0
14	T	256	0	262	24	0
15	U	774	0	773	47	0
16	V	1060	0	1068	49	0
17	y	201	0	226	0	0
18	X	254	0	282	28	0
19	Z	479	0	516	64	0
20	A	1	0	0	0	0
21	A	260	0	288	49	0
21	B	1040	0	1152	151	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	C	780	0	864	143	0
21	D	130	0	144	20	0
21	K	65	0	72	15	0
22	A	64	0	74	8	0
22	D	64	0	74	12	0
23	A	12	0	13	13	0
24	A	5	0	0	0	0
25	A	40	0	56	8	0
25	B	120	0	168	7	0
25	C	80	0	112	26	0
25	D	40	0	56	8	0
25	J	80	0	112	19	0
25	X	40	0	56	6	0
25	Z	40	0	56	4	0
26	A	39	0	51	7	0
26	C	37	0	44	5	0
27	A	51	0	72	40	0
27	B	49	0	68	6	0
27	C	45	0	60	6	0
27	D	94	0	127	36	0
27	I	43	0	56	0	0
27	J	48	0	66	4	0
27	M	42	0	54	3	0
28	A	52	0	62	1	0
28	B	124	0	170	42	0
28	C	237	0	311	76	0
28	D	63	0	87	0	0
29	A	35	0	46	0	0
29	B	35	0	46	2	0
29	D	66	0	81	3	0
29	I	35	0	46	2	0
29	O	35	0	46	1	0
29	T	35	0	46	1	0
30	C	51	0	68	5	0
30	D	43	0	49	9	0
30	F	45	0	53	0	0
30	L	47	0	60	2	0
31	D	4	0	0	0	0
32	D	55	0	80	31	0
33	F	43	0	30	6	0
33	V	43	0	30	5	0
34	F	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	K	1	0	0	0	0
34	O	1	0	0	0	0
All	All	24678	0	25265	1799	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 37.

The worst 5 of 1799 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:C:475:SQD:C3	30:C:475:SQD:C4	1.74	1.58
16:V:63:CYS:SG	33:V:164:HEM:HAB	1.65	1.35
27:A:373:LMG:H112	4:D:266:TRP:CH2	1.77	1.19
1:A:271:LEU:HD11	23:A:367:MES:C8	1.73	1.17
28:B:533:DGD:HAH1	12:M:17:VAL:HG21	1.21	1.14

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	333/344 (97%)	285 (86%)	41 (12%)	7 (2%)	7	40
2	B	483/510 (95%)	416 (86%)	54 (11%)	13 (3%)	5	35
3	C	446/461 (97%)	370 (83%)	60 (14%)	16 (4%)	3	29
4	D	338/352 (96%)	286 (85%)	43 (13%)	9 (3%)	5	35
5	E	75/83 (90%)	66 (88%)	5 (7%)	4 (5%)	2	19
6	F	36/44 (82%)	22 (61%)	9 (25%)	5 (14%)	0	4
7	H	63/65 (97%)	45 (71%)	9 (14%)	9 (14%)	0	4
8	I	33/38 (87%)	20 (61%)	11 (33%)	2 (6%)	1	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	J	32/40 (80%)	26 (81%)	4 (12%)	2 (6%)	1	17
10	K	35/37 (95%)	26 (74%)	7 (20%)	2 (6%)	1	18
11	L	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
12	M	32/36 (89%)	23 (72%)	9 (28%)	0	100	100
13	O	241/246 (98%)	201 (83%)	29 (12%)	11 (5%)	2	23
14	T	28/32 (88%)	25 (89%)	3 (11%)	0	100	100
15	U	95/104 (91%)	79 (83%)	12 (13%)	4 (4%)	3	25
16	V	135/137 (98%)	111 (82%)	23 (17%)	1 (1%)	22	61
17	y	26/46 (56%)	14 (54%)	8 (31%)	4 (15%)	0	3
18	X	33/40 (82%)	25 (76%)	5 (15%)	3 (9%)	1	9
19	Z	60/62 (97%)	48 (80%)	9 (15%)	3 (5%)	2	21
All	All	2559/2714 (94%)	2121 (83%)	343 (13%)	95 (4%)	3	28

5 of 95 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	141	PRO
1	A	142	TRP
2	B	176	GLY
2	B	230	ARG

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	271/280 (97%)	257 (95%)	14 (5%)	23	58
2	B	385/407 (95%)	369 (96%)	16 (4%)	30	63
3	C	348/362 (96%)	327 (94%)	21 (6%)	19	54
4	D	275/283 (97%)	256 (93%)	19 (7%)	15	49
5	E	69/72 (96%)	64 (93%)	5 (7%)	14	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	32/38 (84%)	31 (97%)	1 (3%)	40	71
7	H	53/54 (98%)	49 (92%)	4 (8%)	13	45
8	I	32/35 (91%)	31 (97%)	1 (3%)	40	71
9	J	24/28 (86%)	23 (96%)	1 (4%)	30	63
10	K	30/30 (100%)	27 (90%)	3 (10%)	7	35
11	L	35/35 (100%)	30 (86%)	5 (14%)	3	21
12	M	31/33 (94%)	31 (100%)	0	100	100
13	O	202/208 (97%)	193 (96%)	9 (4%)	27	62
14	T	27/29 (93%)	26 (96%)	1 (4%)	34	66
15	U	84/89 (94%)	80 (95%)	4 (5%)	25	60
16	V	116/117 (99%)	111 (96%)	5 (4%)	29	63
17	y	20/37 (54%)	18 (90%)	2 (10%)	7	35
18	X	28/33 (85%)	24 (86%)	4 (14%)	3	21
19	Z	52/52 (100%)	47 (90%)	5 (10%)	8	37
All	All	2114/2222 (95%)	1994 (94%)	120 (6%)	20	55

5 of 120 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	130	PHE
17	y	46	LEU
5	E	18	ARG
17	y	28	ILE
19	Z	58	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
13	O	226	ASN
15	U	82	ASN
4	D	117	HIS
4	D	98	GLN
18	X	42	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 87 ligands modelled in this entry, 4 are monoatomic - leaving 83 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	$\#\|Z\| > 2$
21	CLA	C	483	-	65,73,73	2.93	21 (32%)	76,113,113	1.78	13 (17%)
21	CLA	A	363	-	65,73,73	2.42	19 (29%)	76,113,113	1.90	15 (19%)
30	SQD	D	361	-	42,43,54	2.57	19 (45%)	51,54,65	2.94	15 (29%)
21	CLA	C	477	-	65,73,73	2.54	17 (26%)	76,113,113	1.92	14 (18%)
21	CLA	B	518	-	65,73,73	2.72	20 (30%)	76,113,113	2.17	20 (26%)
25	BCR	Z	116	-	41,41,41	1.95	8 (19%)	56,56,56	2.08	19 (33%)
30	SQD	F	224	-	44,45,54	2.65	21 (47%)	53,56,65	2.85	19 (35%)
30	SQD	L	213	-	46,47,54	2.60	24 (52%)	55,58,65	2.88	19 (34%)
29	LMT	D	536	-	36,36,36	1.70	10 (27%)	47,47,47	1.58	8 (17%)
29	LMT	T	226	-	36,36,36	1.79	9 (25%)	47,47,47	0.98	2 (4%)
23	MES	A	367	-	12,12,12	1.49	1 (8%)	14,16,16	1.21	3 (21%)
33	HEM	V	164	16	41,50,50	2.53	14 (34%)	45,82,82	3.01	16 (35%)
21	CLA	D	356	-	65,73,73	2.59	20 (30%)	76,113,113	1.88	13 (17%)
21	CLA	A	366	-	65,73,73	2.67	19 (29%)	76,113,113	1.75	11 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
21	CLA	B	520	-	65,73,73	2.54	18 (27%)	76,113,113	1.72	11 (14%)
21	CLA	B	512	-	65,73,73	2.38	18 (27%)	76,113,113	1.61	9 (11%)
25	BCR	D	358	-	41,41,41	1.72	7 (17%)	56,56,56	2.29	20 (35%)
22	PHO	A	365	-	51,69,69	3.42	10 (19%)	47,99,99	1.69	6 (12%)
25	BCR	X	107	-	41,41,41	1.55	6 (14%)	56,56,56	2.40	20 (35%)
21	CLA	C	487	-	65,73,73	3.11	22 (33%)	76,113,113	1.85	10 (13%)
21	CLA	B	522	-	65,73,73	2.39	18 (27%)	76,113,113	1.67	11 (14%)
28	DGD	C	492	-	63,63,67	1.36	10 (15%)	77,77,81	2.78	21 (27%)
21	CLA	B	526	-	65,73,73	2.98	20 (30%)	76,113,113	1.77	11 (14%)
21	CLA	B	521	-	65,73,73	2.63	18 (27%)	76,113,113	1.95	19 (25%)
21	CLA	B	523	-	65,73,73	2.52	18 (27%)	76,113,113	1.63	15 (19%)
21	CLA	B	524	-	65,73,73	2.76	21 (32%)	76,113,113	1.84	15 (19%)
21	CLA	C	479	-	65,73,73	2.75	20 (30%)	76,113,113	1.94	14 (18%)
21	CLA	C	484	-	65,73,73	2.74	18 (27%)	76,113,113	1.81	16 (21%)
22	PHO	D	355	-	51,69,69	3.23	11 (21%)	47,99,99	1.69	6 (12%)
21	CLA	C	480	-	65,73,73	2.74	19 (29%)	76,113,113	2.00	13 (17%)
21	CLA	C	482	-	65,73,73	3.25	22 (33%)	76,113,113	1.86	17 (22%)
29	LMT	A	376	-	36,36,36	1.99	11 (30%)	47,47,47	1.45	8 (17%)
27	LMG	M	217	-	42,42,55	1.95	8 (19%)	50,50,63	1.47	7 (14%)
28	DGD	C	491	-	54,54,67	1.63	9 (16%)	68,68,81	2.98	23 (33%)
21	CLA	C	488	-	65,73,73	2.88	19 (29%)	76,113,113	1.86	16 (21%)
28	DGD	A	375	-	53,53,67	2.05	13 (24%)	67,67,81	2.50	22 (32%)
33	HEM	F	85	5	41,50,50	2.78	17 (41%)	45,82,82	3.03	16 (35%)
25	BCR	C	489	-	41,41,41	1.90	9 (21%)	56,56,56	2.09	16 (28%)
25	BCR	B	530	-	41,41,41	2.51	11 (26%)	56,56,56	2.22	23 (41%)
26	LHG	A	371	-	38,38,48	2.22	5 (13%)	41,44,54	1.41	4 (9%)
25	BCR	J	112	-	41,41,41	1.90	8 (19%)	56,56,56	2.41	24 (42%)
21	CLA	B	516	-	65,73,73	2.80	20 (30%)	76,113,113	1.98	17 (22%)
21	CLA	C	485	-	65,73,73	2.75	19 (29%)	76,113,113	1.75	12 (15%)
21	CLA	B	515	-	65,73,73	2.66	18 (27%)	76,113,113	1.79	12 (15%)
29	LMT	I	274	-	36,36,36	1.87	12 (33%)	47,47,47	1.33	7 (14%)
29	LMT	B	535	-	36,36,36	1.87	10 (27%)	47,47,47	1.15	2 (4%)
21	CLA	C	486	3	65,73,73	3.25	22 (33%)	76,113,113	1.77	16 (21%)
27	LMG	I	220	-	43,43,55	2.02	12 (27%)	51,51,63	2.17	14 (27%)
28	DGD	C	493	-	67,67,67	1.44	16 (23%)	81,81,81	3.04	28 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
27	LMG	B	531	-	49,49,55	1.66	6 (12%)	57,57,63	2.81	18 (31%)
27	LMG	J	492	-	48,48,55	1.95	9 (18%)	56,56,63	1.87	17 (30%)
27	LMG	D	359	-	46,46,55	1.72	6 (13%)	54,54,63	2.55	17 (31%)
25	BCR	J	115	-	41,41,41	2.24	11 (26%)	56,56,56	3.20	17 (30%)
21	CLA	A	362	-	65,73,73	2.36	19 (29%)	76,113,113	1.78	13 (17%)
27	LMG	C	494	-	45,45,55	1.91	8 (17%)	53,53,63	2.19	16 (30%)
28	DGD	B	533	-	67,67,67	1.49	13 (19%)	81,81,81	1.83	19 (23%)
21	CLA	B	511	-	65,73,73	3.30	26 (40%)	76,113,113	1.81	15 (19%)
21	CLA	D	354	-	65,73,73	2.83	19 (29%)	76,113,113	1.64	12 (15%)
31	BCT	D	353	20	2,3,3	0.65	0	2,3,3	0.40	0
25	BCR	B	529	-	41,41,41	2.17	9 (21%)	56,56,56	2.16	19 (33%)
28	DGD	C	474	-	57,57,67	2.08	15 (26%)	71,71,81	3.57	24 (33%)
21	CLA	C	481	-	65,73,73	3.16	20 (30%)	76,113,113	2.03	15 (19%)
21	CLA	B	513	-	65,73,73	2.40	18 (27%)	76,113,113	1.87	14 (18%)
25	BCR	A	369	-	41,41,41	1.91	6 (14%)	56,56,56	2.08	18 (32%)
28	DGD	B	528	-	59,59,67	0.60	2 (3%)	73,73,81	1.07	8 (10%)
29	LMT	D	363	-	32,32,36	1.82	7 (21%)	43,43,47	1.49	6 (13%)
26	LHG	C	476	-	36,36,48	2.39	6 (16%)	39,42,54	1.50	4 (10%)
21	CLA	B	517	-	65,73,73	2.86	21 (32%)	76,113,113	2.04	22 (28%)
25	BCR	C	490	-	41,41,41	1.98	8 (19%)	56,56,56	2.21	21 (37%)
30	SQD	C	475	-	50,51,54	2.59	26 (52%)	59,62,65	2.75	18 (30%)
25	BCR	B	527	-	41,41,41	1.79	7 (17%)	56,56,56	2.34	21 (37%)
21	CLA	K	483	-	65,73,73	2.51	17 (26%)	76,113,113	1.76	11 (14%)
27	LMG	A	373	-	51,51,55	0.55	1 (1%)	59,59,63	1.09	6 (10%)
27	LMG	D	360	-	48,48,55	0.56	1 (2%)	56,56,63	1.11	6 (10%)
32	PL9	D	357	-	55,55,55	3.11	23 (41%)	68,69,69	2.92	26 (38%)
29	LMT	O	274	-	36,36,36	2.00	12 (33%)	47,47,47	1.39	7 (14%)
21	CLA	B	514	-	65,73,73	2.60	17 (26%)	76,113,113	1.60	14 (18%)
21	CLA	A	364	-	65,73,73	2.57	21 (32%)	76,113,113	1.91	15 (19%)
21	CLA	C	478	-	65,73,73	2.52	18 (27%)	76,113,113	1.73	14 (18%)
21	CLA	B	525	-	65,73,73	2.75	19 (29%)	76,113,113	1.83	11 (14%)
28	DGD	D	362	-	64,64,67	2.09	22 (34%)	78,78,81	2.55	21 (26%)
21	CLA	B	519	-	65,73,73	2.61	17 (26%)	76,113,113	1.84	15 (19%)

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
21	CLA	C	483	-	2/2/15/20	11/37/115/115	-
21	CLA	A	363	-	2/2/15/20	8/37/115/115	-
30	SQD	D	361	-	-	15/38/58/69	0/1/1/1
21	CLA	C	477	-	2/2/15/20	8/37/115/115	-
21	CLA	B	518	-	2/2/15/20	10/37/115/115	-
25	BCR	Z	116	-	-	2/29/63/63	0/2/2/2
30	SQD	F	224	-	-	19/40/60/69	0/1/1/1
30	SQD	L	213	-	-	17/42/62/69	0/1/1/1
29	LMT	D	536	-	-	1/21/61/61	0/2/2/2
29	LMT	T	226	-	-	1/21/61/61	0/2/2/2
23	MES	A	367	-	-	3/6/14/14	0/1/1/1
33	HEM	V	164	16	-	8/12/54/54	-
21	CLA	D	356	-	2/2/15/20	8/37/115/115	-
21	CLA	A	366	-	2/2/15/20	10/37/115/115	-
21	CLA	B	520	-	2/2/15/20	14/37/115/115	-
21	CLA	B	512	-	2/2/15/20	9/37/115/115	-
25	BCR	D	358	-	-	3/29/63/63	0/2/2/2
22	PHO	A	365	-	1/1/17/22	8/37/103/103	0/5/6/6
25	BCR	X	107	-	-	3/29/63/63	0/2/2/2
21	CLA	C	487	-	2/2/15/20	9/37/115/115	-
21	CLA	B	522	-	2/2/15/20	16/37/115/115	-
28	DGD	C	492	-	1/1/13/13	8/51/91/95	0/2/2/2
21	CLA	B	526	-	2/2/15/20	11/37/115/115	-
21	CLA	B	521	-	2/2/15/20	11/37/115/115	-
21	CLA	B	523	-	2/2/15/20	10/37/115/115	-
21	CLA	B	524	-	2/2/15/20	14/37/115/115	-
21	CLA	C	479	-	2/2/15/20	11/37/115/115	-
21	CLA	C	484	-	2/2/15/20	11/37/115/115	-
22	PHO	D	355	-	1/1/17/22	17/37/103/103	0/5/6/6
21	CLA	C	480	-	2/2/15/20	13/37/115/115	-
21	CLA	C	482	-	2/2/15/20	12/37/115/115	-
29	LMT	A	376	-	-	3/21/61/61	0/2/2/2
27	LMG	M	217	-	-	3/37/57/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	DGD	C	491	-	-	5/42/82/95	0/2/2/2
21	CLA	C	488	-	2/2/15/20	9/37/115/115	-
28	DGD	A	375	-	-	6/41/81/95	0/2/2/2
33	HEM	F	85	5	-	6/12/54/54	-
25	BCR	C	489	-	-	5/29/63/63	0/2/2/2
25	BCR	B	530	-	-	4/29/63/63	0/2/2/2
26	LHG	A	371	-	-	17/43/43/53	-
25	BCR	J	112	-	-	1/29/63/63	0/2/2/2
21	CLA	B	516	-	2/2/15/20	9/37/115/115	-
21	CLA	C	485	-	2/2/15/20	11/37/115/115	-
21	CLA	B	515	-	2/2/15/20	8/37/115/115	-
29	LMT	I	274	-	-	2/21/61/61	0/2/2/2
29	LMT	B	535	-	-	3/21/61/61	0/2/2/2
21	CLA	C	486	3	2/2/15/20	8/37/115/115	-
27	LMG	I	220	-	-	4/38/58/70	0/1/1/1
28	DGD	C	493	-	1/1/13/13	9/55/95/95	0/2/2/2
27	LMG	B	531	-	-	4/44/64/70	0/1/1/1
27	LMG	J	492	-	-	5/43/63/70	0/1/1/1
27	LMG	D	359	-	-	5/41/61/70	0/1/1/1
25	BCR	J	115	-	-	4/29/63/63	0/2/2/2
21	CLA	A	362	-	2/2/15/20	10/37/115/115	-
27	LMG	C	494	-	-	3/40/60/70	0/1/1/1
28	DGD	B	533	-	-	9/55/95/95	0/2/2/2
21	CLA	B	511	-	2/2/15/20	16/37/115/115	-
21	CLA	D	354	-	2/2/15/20	10/37/115/115	-
25	BCR	B	529	-	-	0/29/63/63	0/2/2/2
28	DGD	C	474	-	-	7/45/85/95	0/2/2/2
21	CLA	C	481	-	2/2/15/20	10/37/115/115	-
21	CLA	B	513	-	2/2/15/20	12/37/115/115	-
25	BCR	A	369	-	-	5/29/63/63	0/2/2/2
28	DGD	B	528	-	-	19/47/87/95	0/2/2/2
29	LMT	D	363	-	-	1/17/57/61	0/2/2/2
26	LHG	C	476	-	-	18/41/41/53	-
21	CLA	B	517	-	2/2/15/20	8/37/115/115	-
25	BCR	C	490	-	-	3/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	SQD	C	475	-	-	22/46/66/69	0/1/1/1
25	BCR	B	527	-	-	4/29/63/63	0/2/2/2
21	CLA	K	483	-	2/2/15/20	7/37/115/115	-
27	LMG	A	373	-	-	20/46/66/70	0/1/1/1
27	LMG	D	360	-	-	19/43/63/70	0/1/1/1
32	PL9	D	357	-	-	17/53/73/73	0/1/1/1
29	LMT	O	274	-	-	3/21/61/61	0/2/2/2
21	CLA	B	514	-	2/2/15/20	10/37/115/115	-
21	CLA	A	364	-	2/2/15/20	14/37/115/115	-
21	CLA	C	478	-	2/2/15/20	7/37/115/115	-
21	CLA	B	525	-	2/2/15/20	11/37/115/115	-
28	DGD	D	362	-	-	10/52/92/95	0/2/2/2
21	CLA	B	519	-	2/2/15/20	9/37/115/115	-

The worst 5 of 1167 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	365	PHO	C3A-C2A	-16.73	1.39	1.54
22	D	355	PHO	C3A-C2A	-16.66	1.39	1.54
21	B	511	CLA	C3B-C2B	11.81	1.56	1.40
21	C	486	CLA	MG-NA	11.31	2.33	2.06
32	D	357	PL9	C28-C29	11.30	1.60	1.33

The worst 5 of 1168 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	C	474	DGD	O1G-C1G-C2G	12.38	144.47	108.43
28	C	493	DGD	O5D-C6D-C5D	10.84	129.11	109.05
25	J	115	BCR	C32-C1-C6	-10.58	93.14	110.30
28	C	492	DGD	O5D-C1E-C2E	10.56	124.80	108.30
28	C	491	DGD	O5D-C1E-C2E	10.32	124.41	108.30

5 of 74 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
21	A	362	CLA	ND
21	A	362	CLA	C8
21	A	363	CLA	ND
21	A	363	CLA	C8

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Mol	Chain	Res	Type	Atom
21	A	366	CLA	ND

5 of 716 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	B	511	CLA	C11-C12-C13-C14
21	B	515	CLA	C2-C3-C5-C6
21	B	515	CLA	C4-C3-C5-C6
21	B	516	CLA	C2-C3-C5-C6
21	B	516	CLA	C4-C3-C5-C6

There are no ring outliers.

76 monomers are involved in 704 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	C	483	CLA	13	0
21	A	363	CLA	14	0
30	D	361	SQD	9	0
21	C	477	CLA	12	0
21	B	518	CLA	15	0
25	Z	116	BCR	4	0
30	L	213	SQD	2	0
29	D	536	LMT	1	0
29	T	226	LMT	1	0
23	A	367	MES	13	0
33	V	164	HEM	5	0
21	D	356	CLA	5	0
21	A	366	CLA	10	0
21	B	520	CLA	7	0
21	B	512	CLA	9	0
25	D	358	BCR	8	0
22	A	365	PHO	8	0
25	X	107	BCR	6	0
21	C	487	CLA	15	0
21	B	522	CLA	13	0
28	C	492	DGD	14	0
21	B	526	CLA	6	0
21	B	521	CLA	12	0
21	B	523	CLA	7	0
21	B	524	CLA	5	0
21	C	479	CLA	18	0
21	C	484	CLA	15	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	D	355	PHO	12	0
21	C	480	CLA	11	0
21	C	482	CLA	6	0
27	M	217	LMG	3	0
28	C	491	DGD	17	0
21	C	488	CLA	7	0
28	A	375	DGD	1	0
33	F	85	HEM	6	0
25	C	489	BCR	18	0
25	B	530	BCR	2	0
26	A	371	LHG	7	0
25	J	112	BCR	12	0
21	B	516	CLA	6	0
21	C	485	CLA	5	0
21	B	515	CLA	10	0
29	I	274	LMT	2	0
29	B	535	LMT	2	0
21	C	486	CLA	24	0
28	C	493	DGD	39	0
27	B	531	LMG	6	0
27	J	492	LMG	4	0
27	D	359	LMG	6	0
25	J	115	BCR	7	0
21	A	362	CLA	20	0
27	C	494	LMG	6	0
28	B	533	DGD	19	0
21	B	511	CLA	6	0
21	D	354	CLA	15	0
25	B	529	BCR	5	0
28	C	474	DGD	8	0
21	C	481	CLA	17	0
21	B	513	CLA	24	0
25	A	369	BCR	8	0
28	B	528	DGD	23	0
29	D	363	LMT	2	0
26	C	476	LHG	5	0
21	B	517	CLA	20	0
25	C	490	BCR	8	0
30	C	475	SQD	5	0
21	K	483	CLA	15	0
27	A	373	LMG	40	0
27	D	360	LMG	30	0

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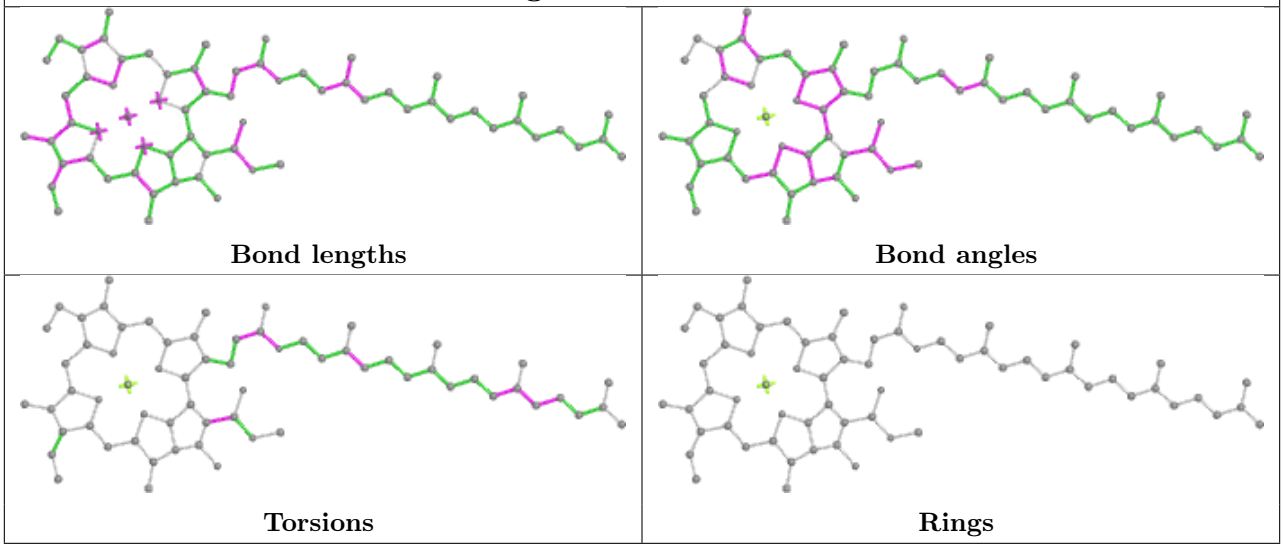
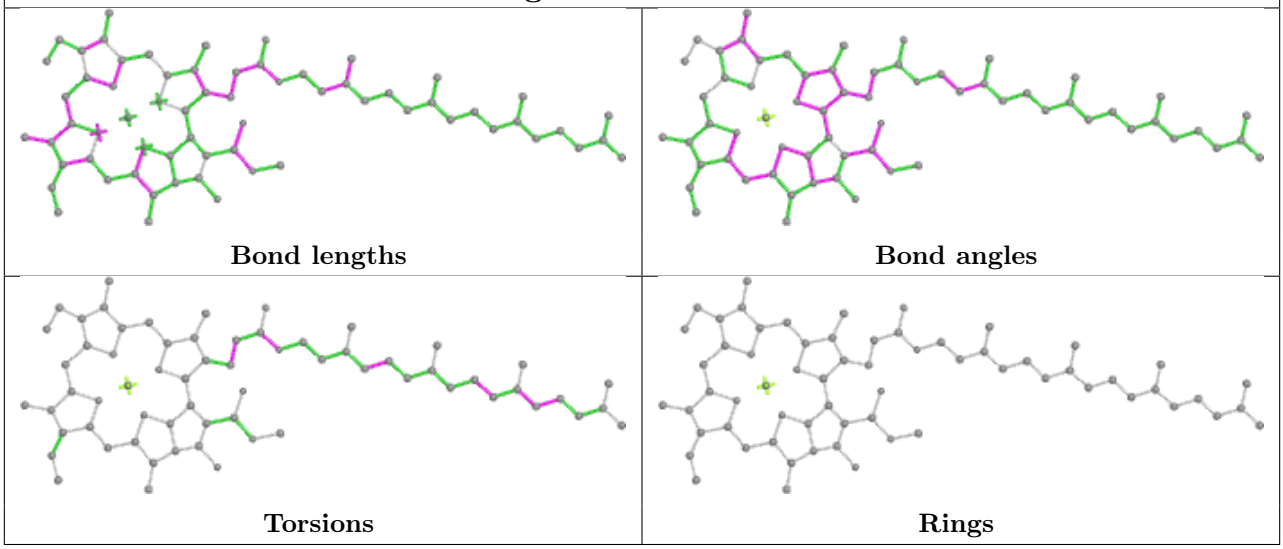
Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	D	357	PL9	31	0
29	O	274	LMT	1	0
21	B	514	CLA	10	0
21	A	364	CLA	6	0
21	C	478	CLA	16	0
21	B	525	CLA	7	0
21	B	519	CLA	8	0

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

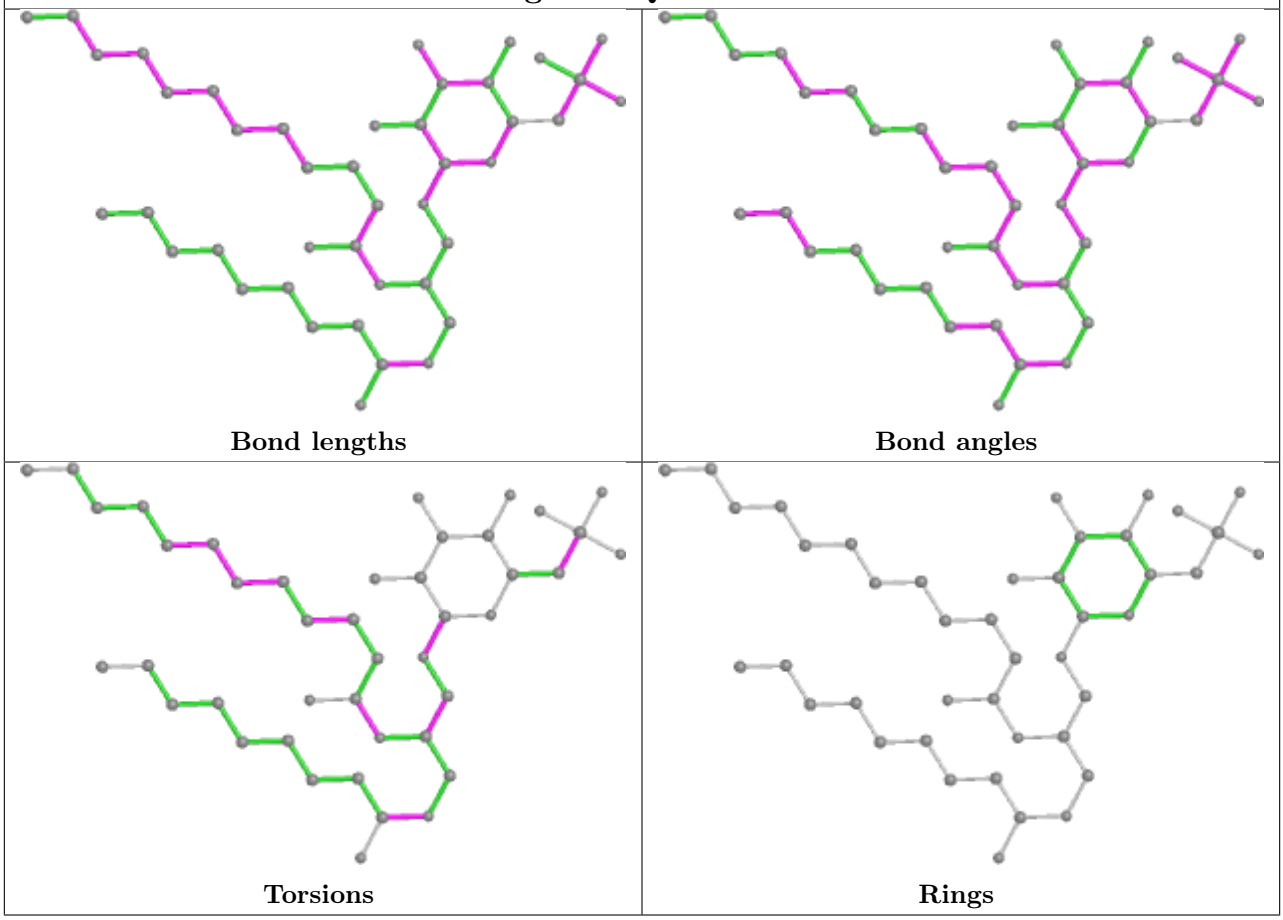
Ligand CLA C 483



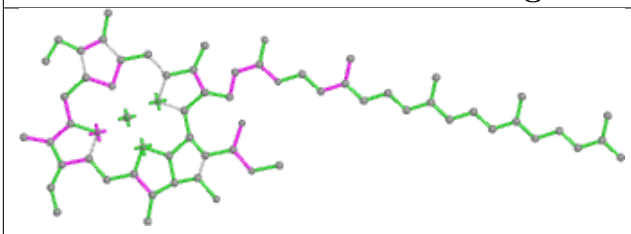
Ligand CLA A 363



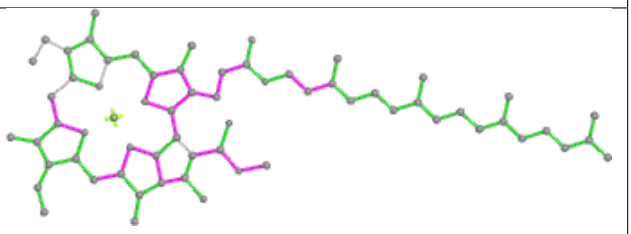
Ligand SQD D 361



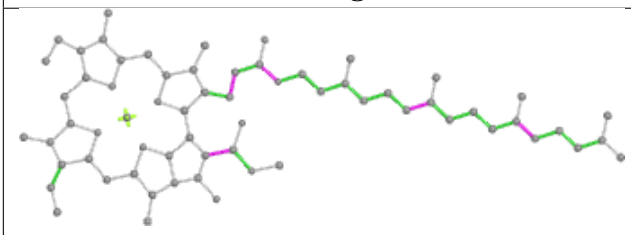
Ligand CLA C 477



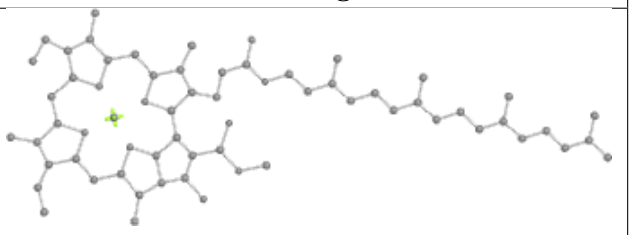
Bond lengths



Bond angles

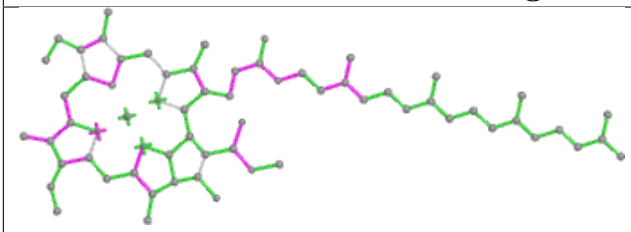


Torsions



Rings

Ligand CLA B 518



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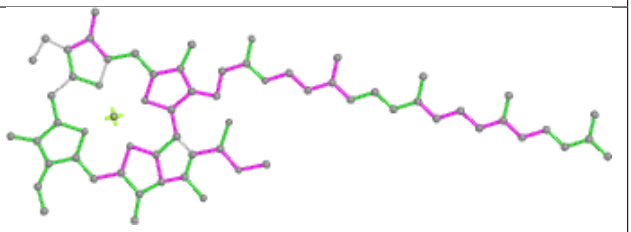

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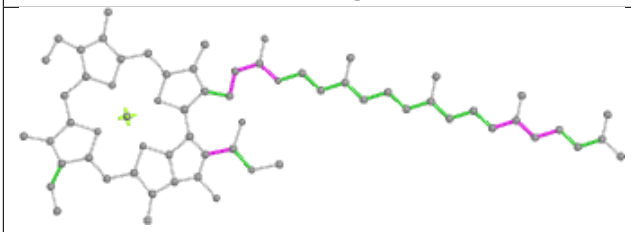
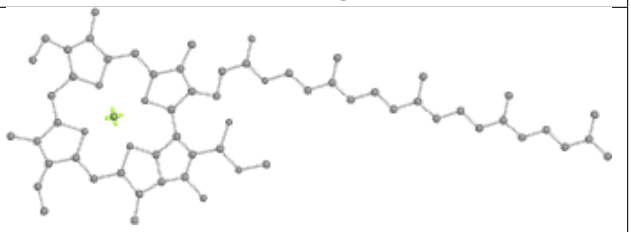
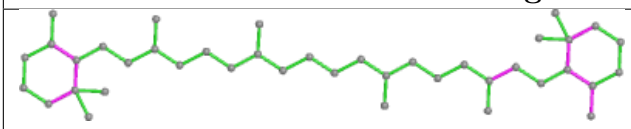


Torsions



Rings

Ligand BCR Z 116



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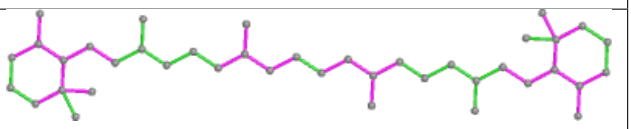
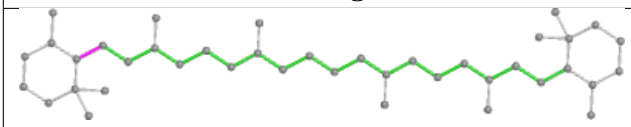


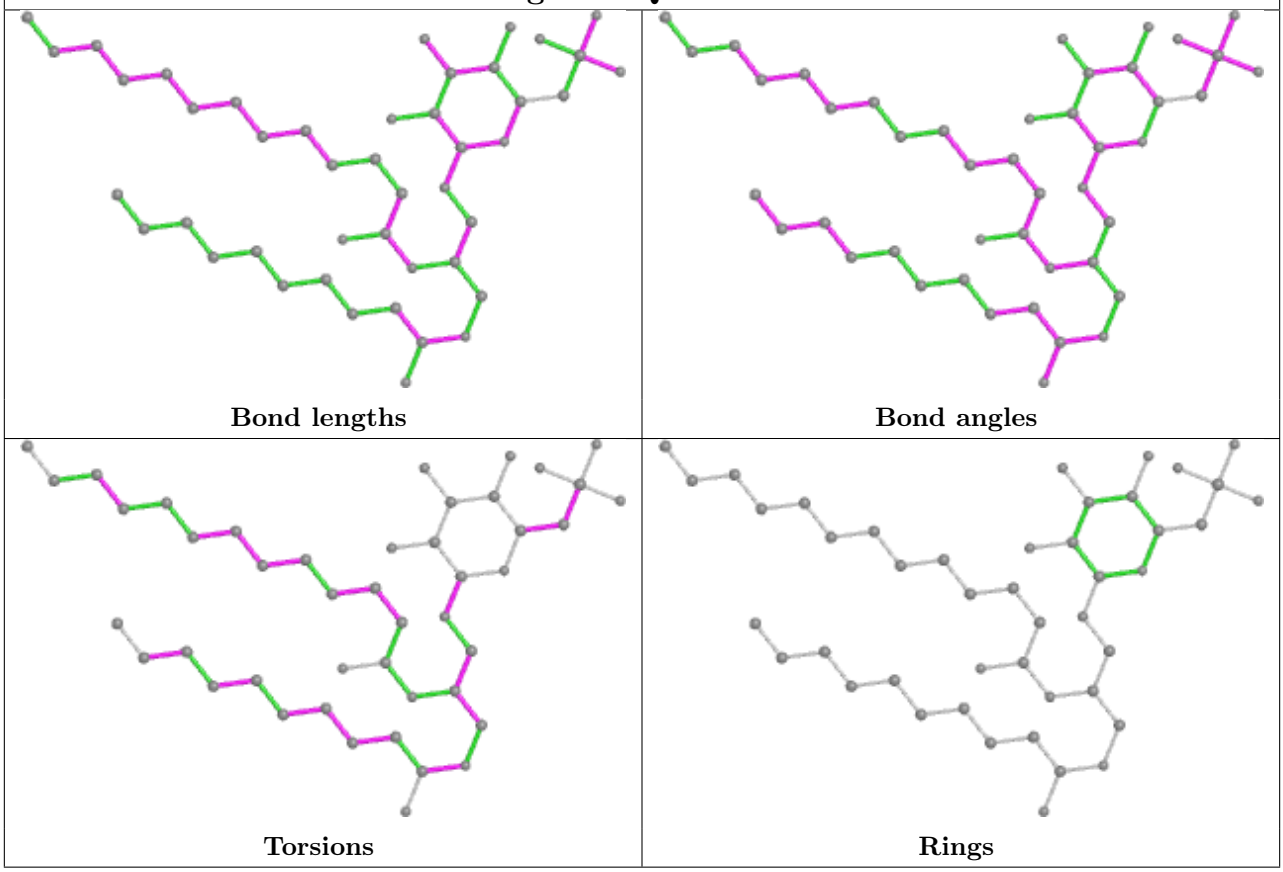
Bond angles



Torsions

Rings

Ligand SQD F 224



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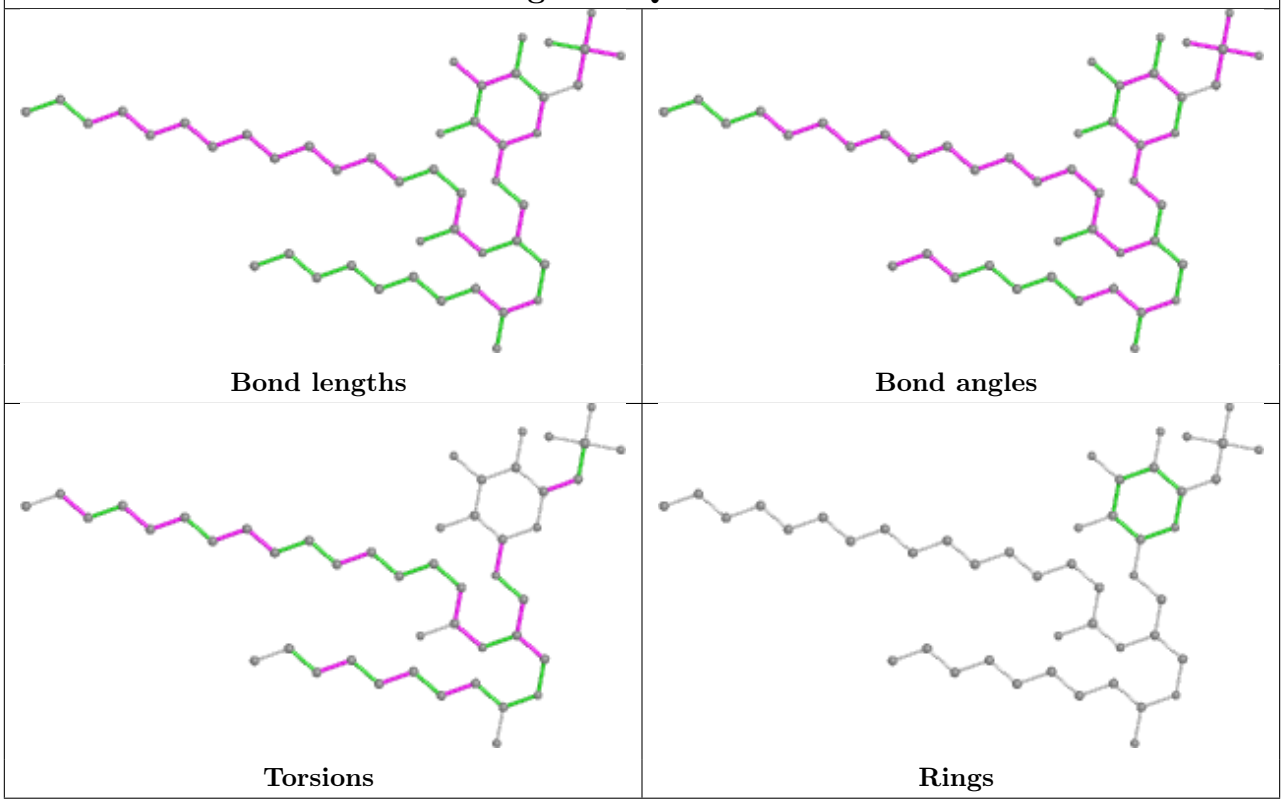
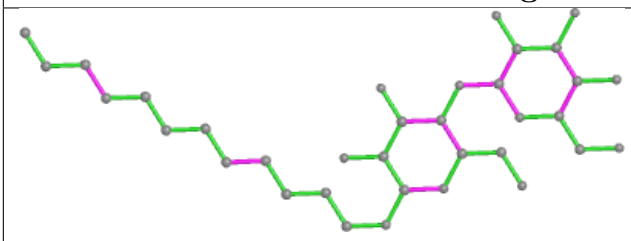
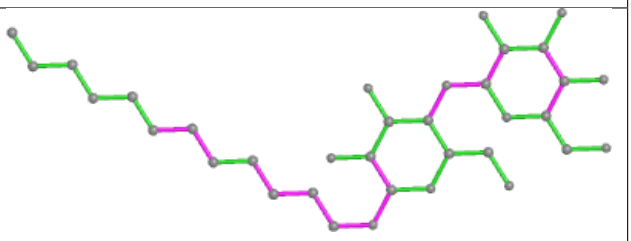
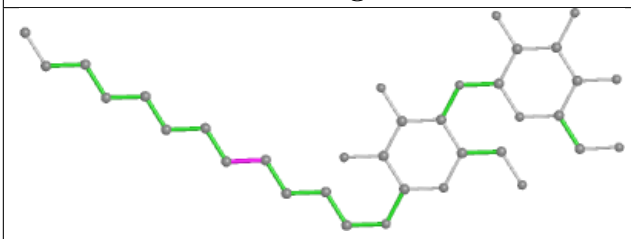
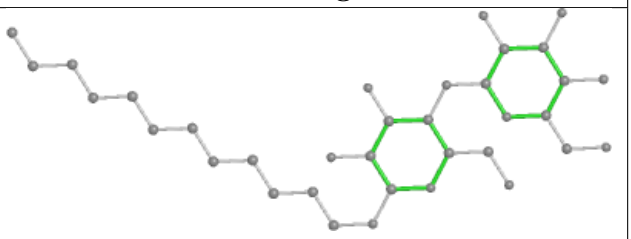


Ligand LMT D 536	
 Bond lengths	 Bond angles
 Torsions	 Rings

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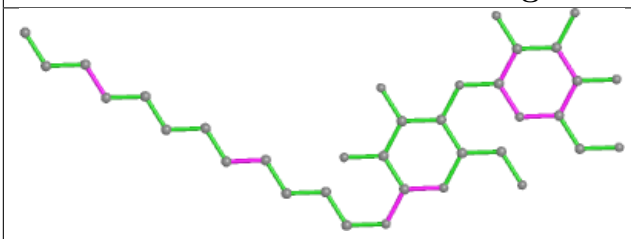
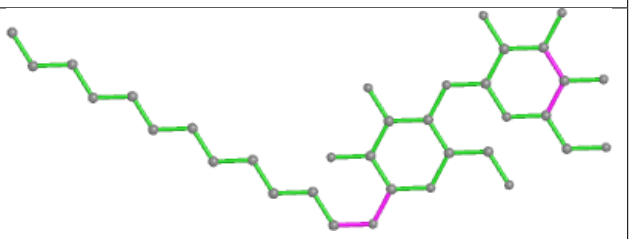
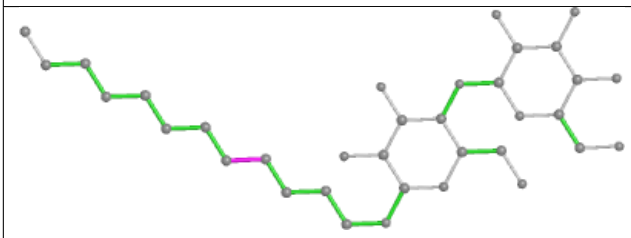
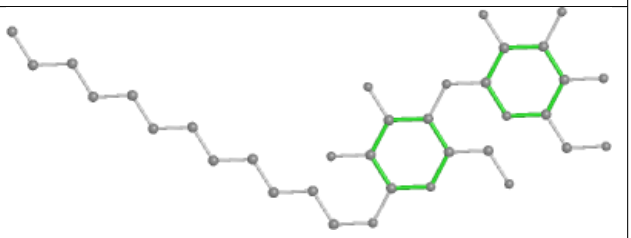
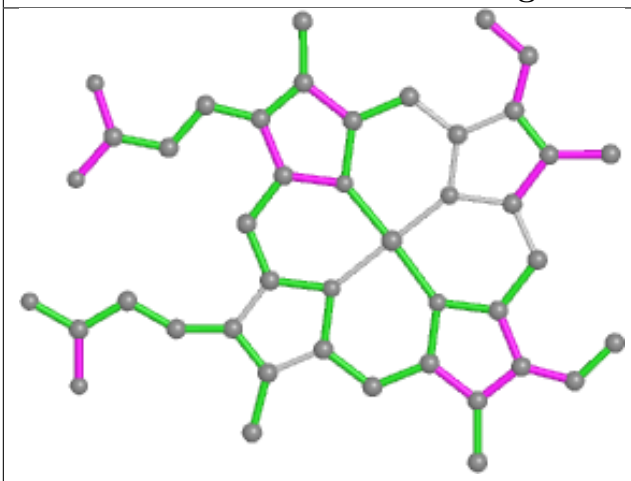
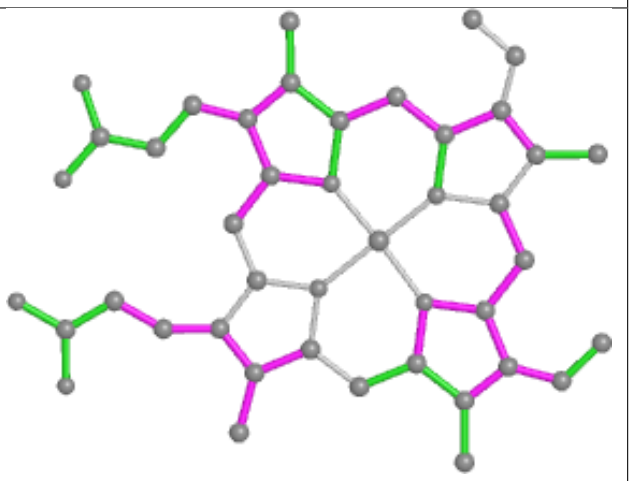
 Bond lengths	 Bond angles
 Torsions	 Rings

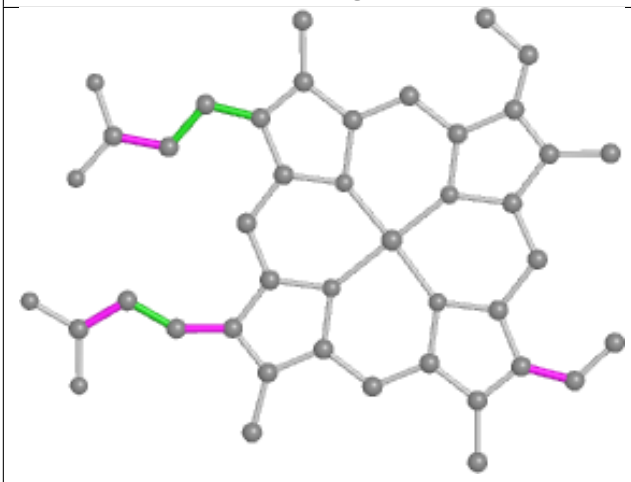
Ligand HEM V 164



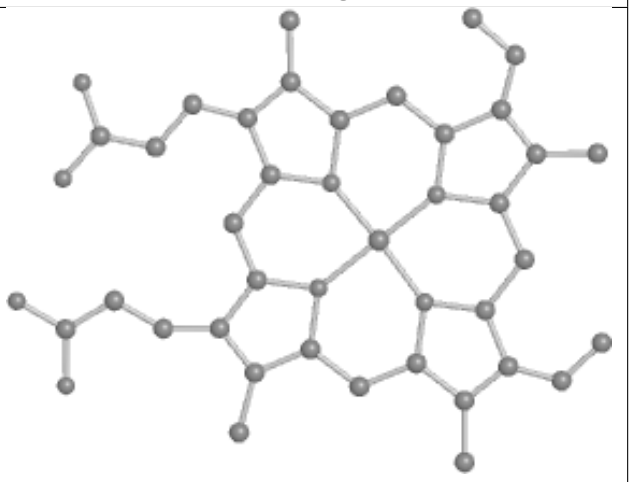
Bond lengths



Bond angles

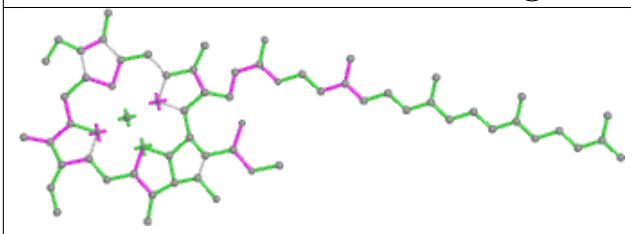


Torsions

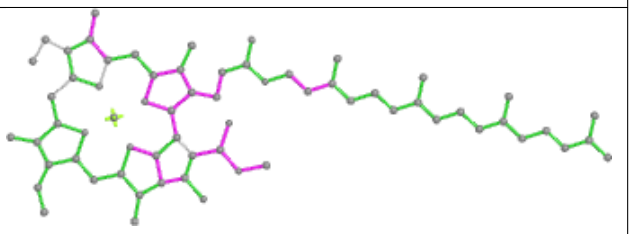


Rings

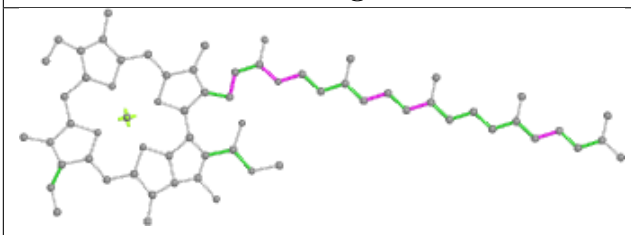
Ligand CLA D 356



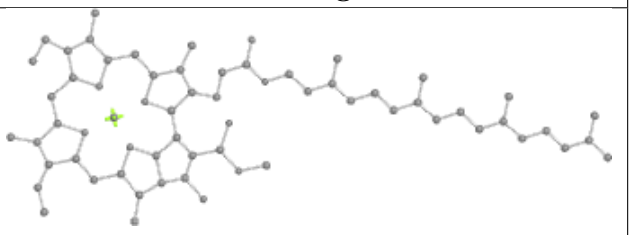
Bond lengths



Bond angles

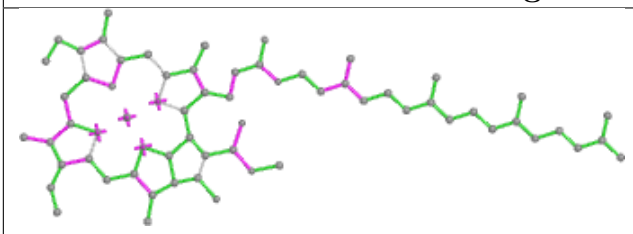


Torsions



Rings

Ligand CLA A 366



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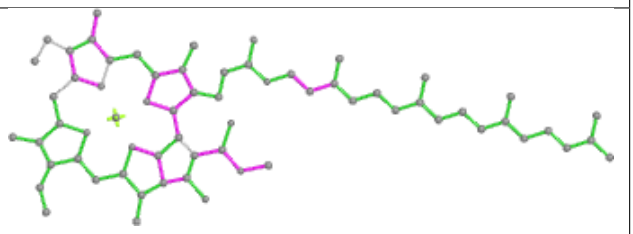
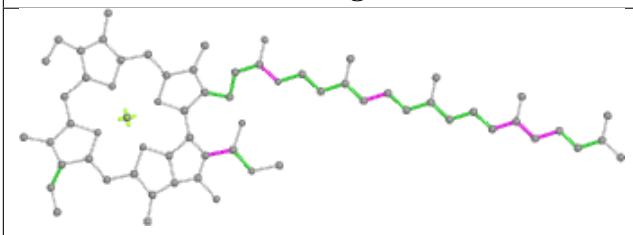
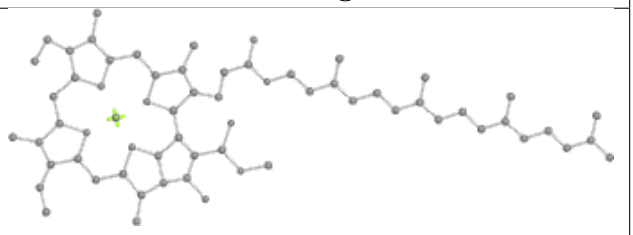


Bond angles

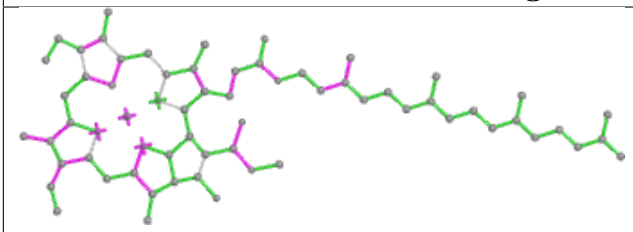


Torsions

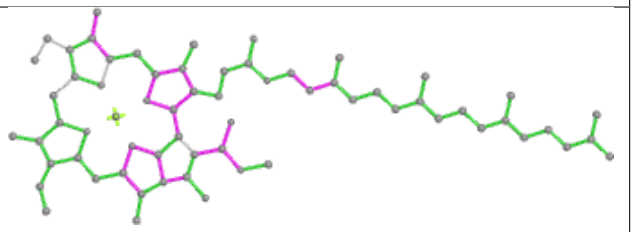


Rings

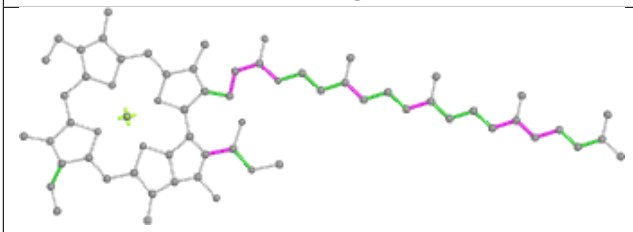
Ligand CLA B 520



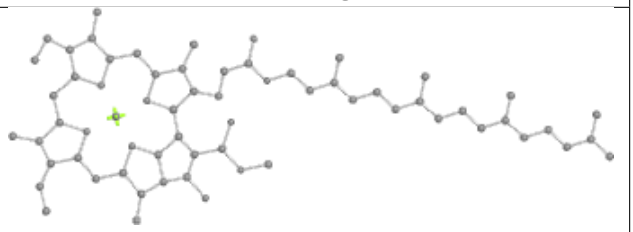
Bond lengths



Bond angles

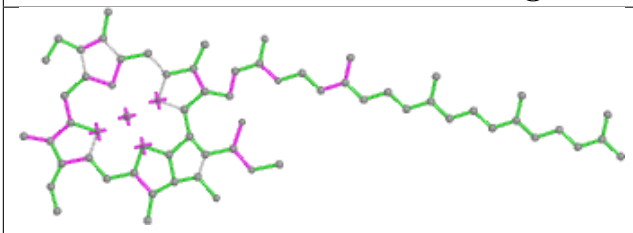


Torsions

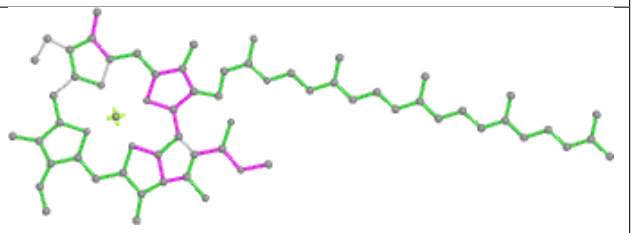


Rings

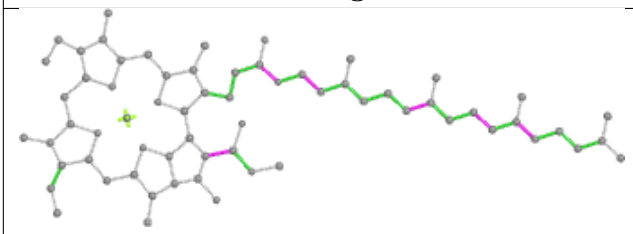
Ligand CLA B 512



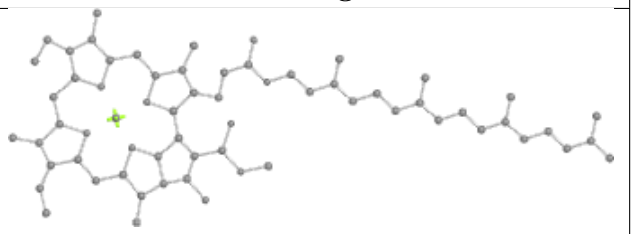
Bond lengths



Bond angles

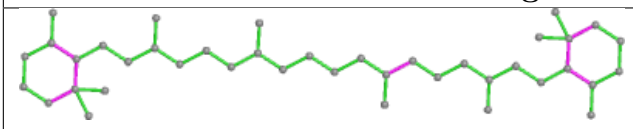


Torsions



Rings

Ligand BCR D 358



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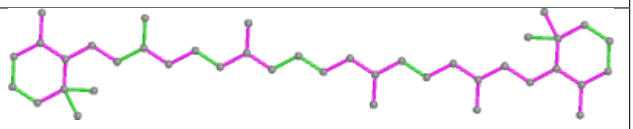
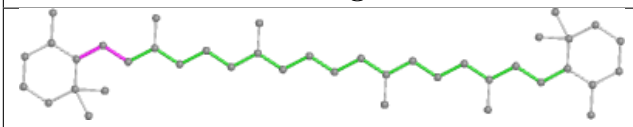


Bond angles



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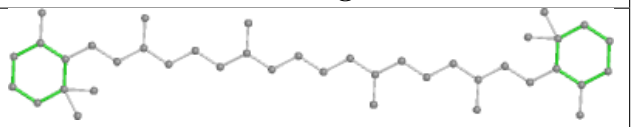
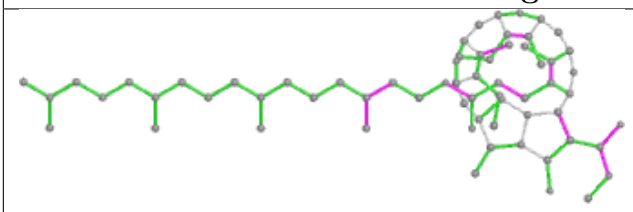


Rings

Ligand PHO A 365



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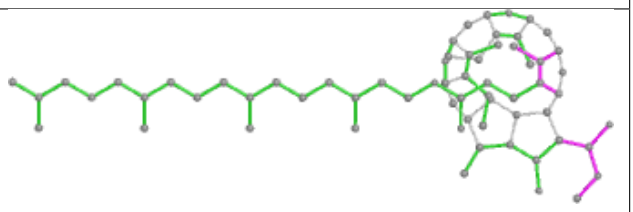
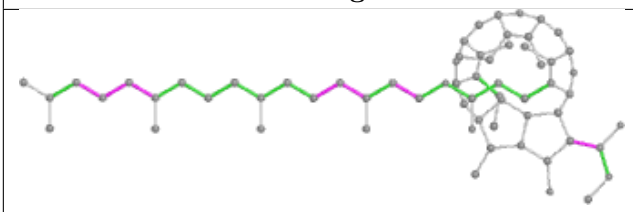
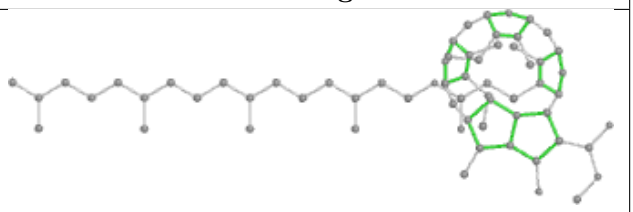


Bond angles

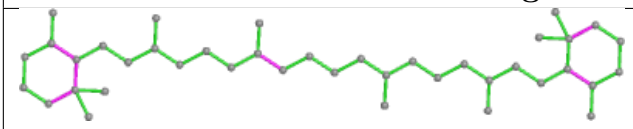


Torsions



Rings

Ligand BCR X 107



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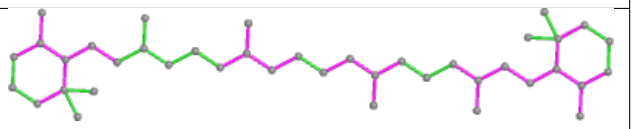
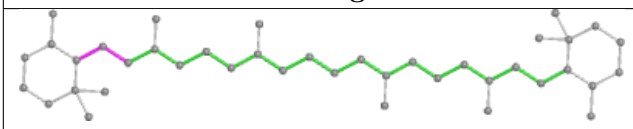


Bond angles



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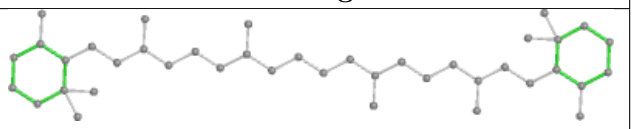
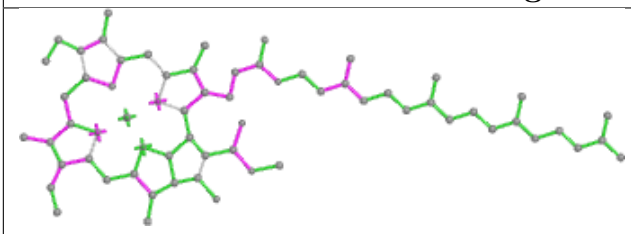


Rings

Ligand CLA C 487



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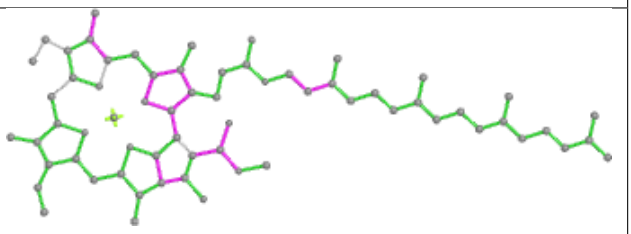
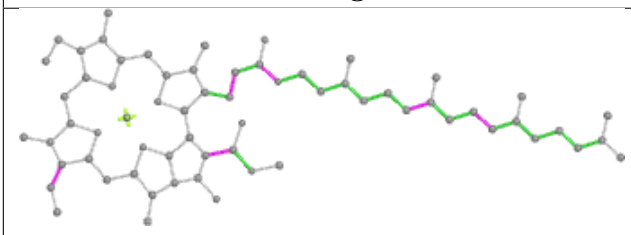


Bond angles



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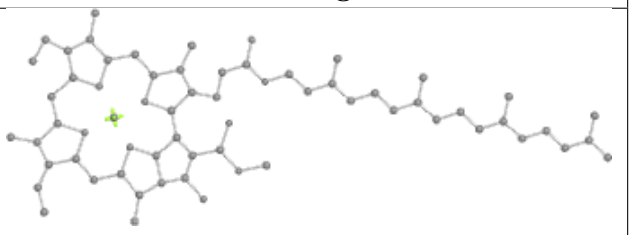
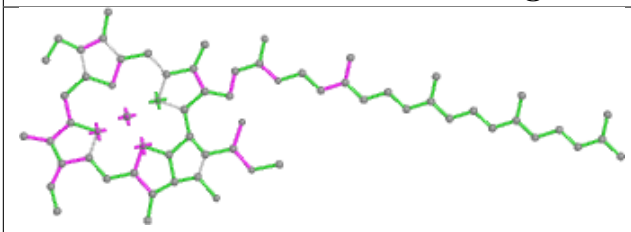


Rings

Ligand CLA B 522



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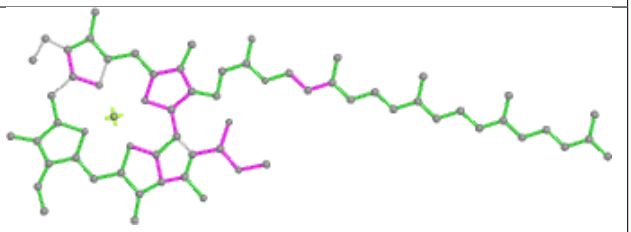
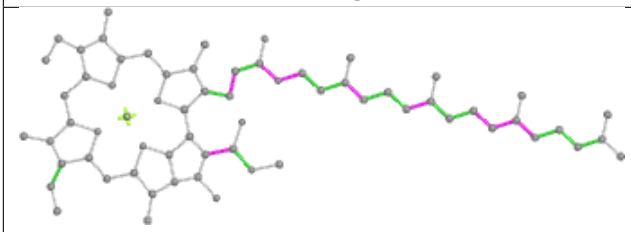


Bond angles



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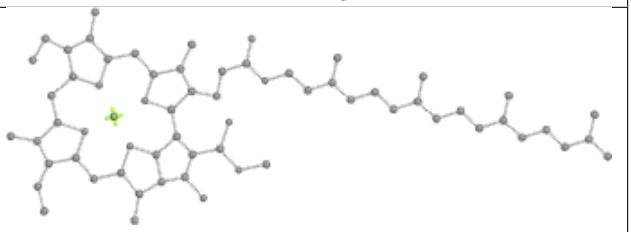
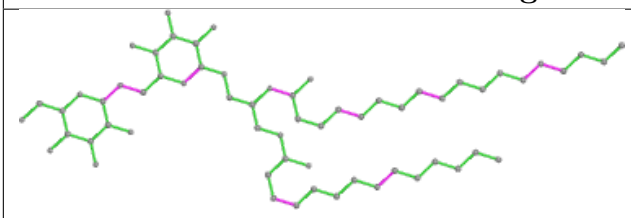


Rings

Ligand DGD C 492



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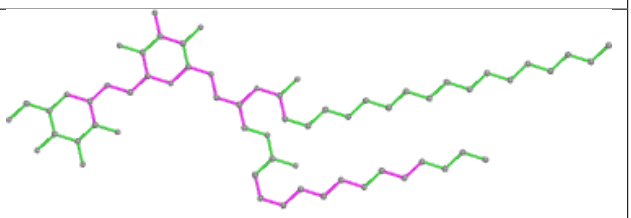
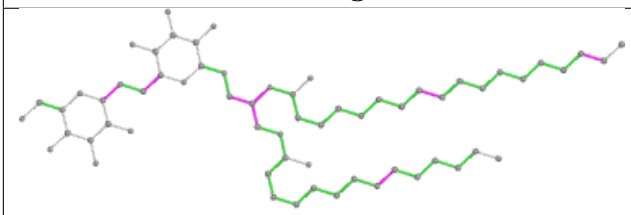


Bond angles



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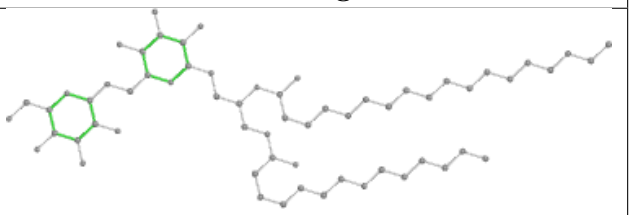

Rings

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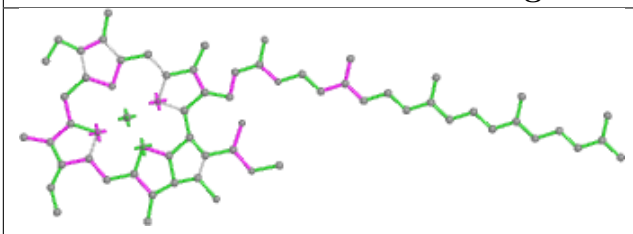

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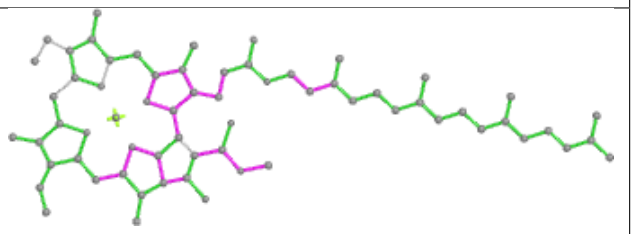

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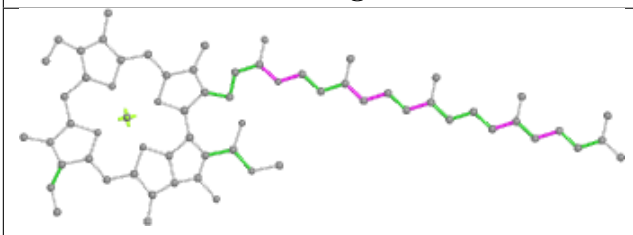

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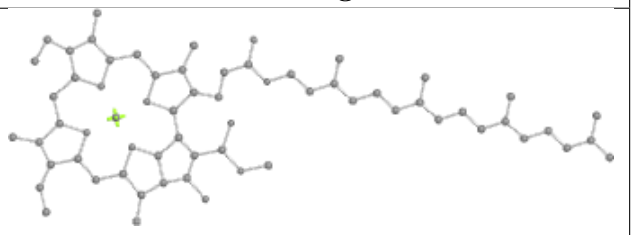

Rings

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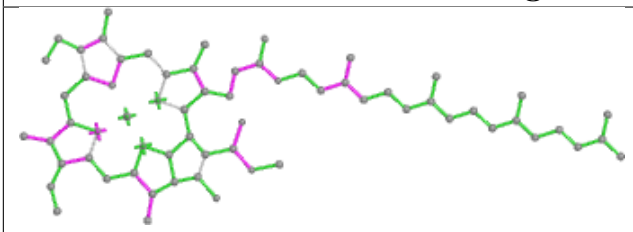

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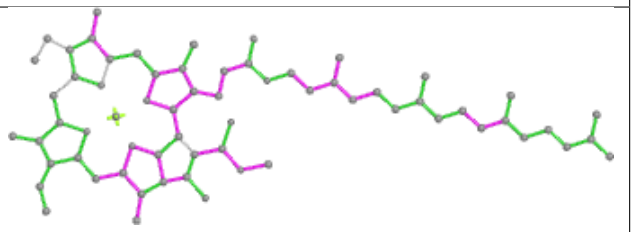
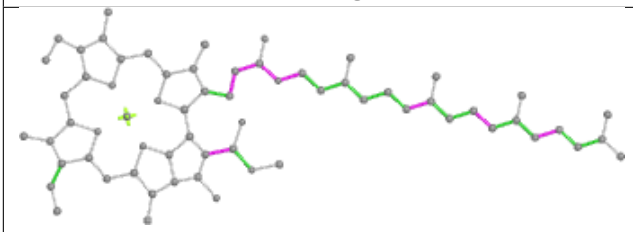


Bond angles



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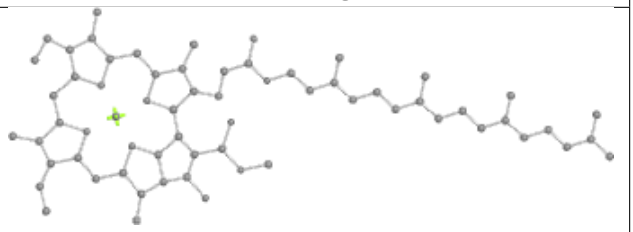

Rings

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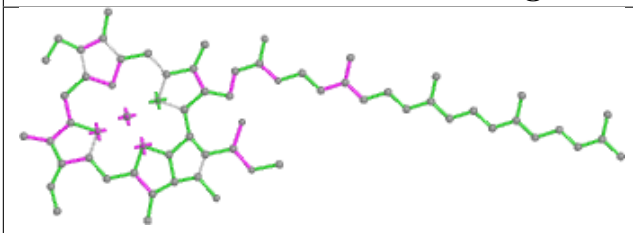

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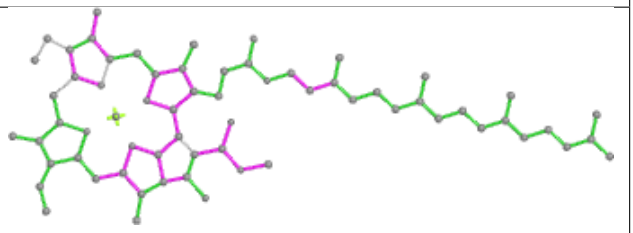

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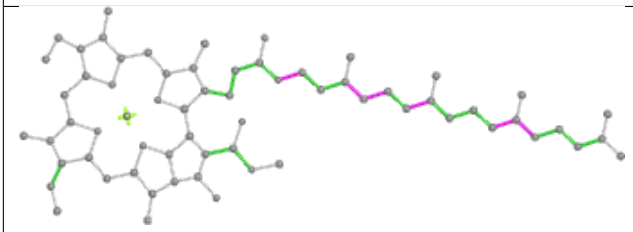

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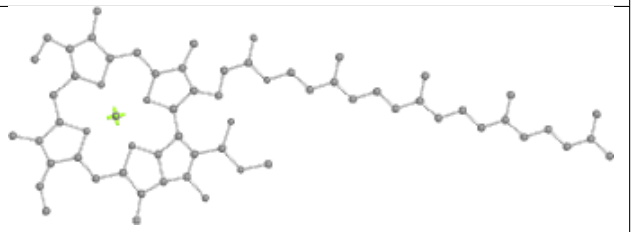
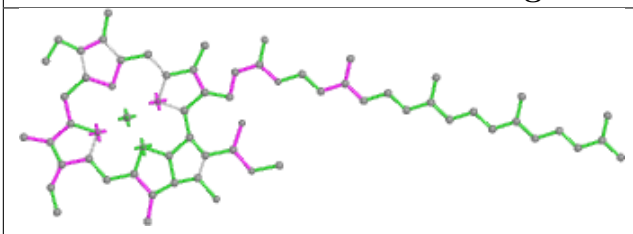


Rings

Ligand CLA B 524



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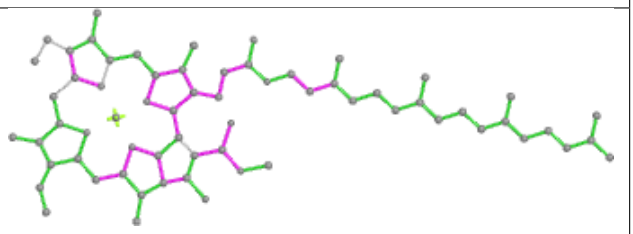
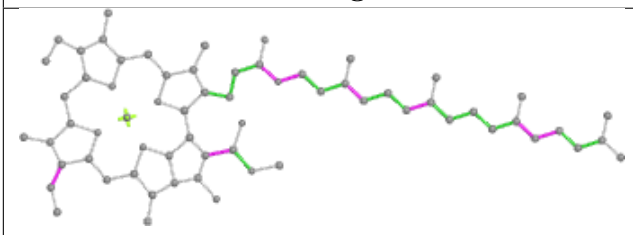


Bond angles



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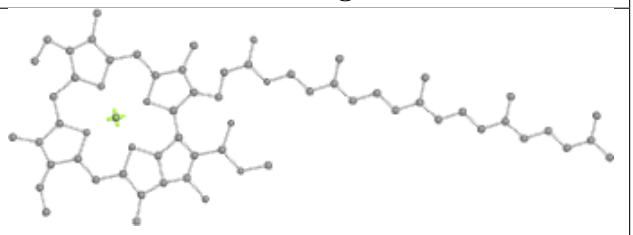
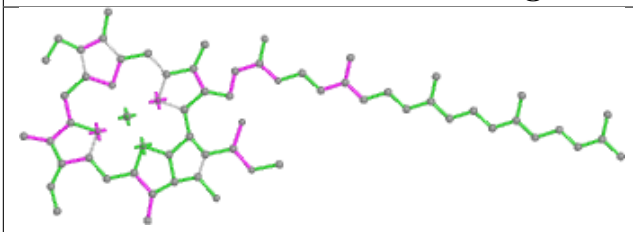


Rings

Ligand CLA C 479



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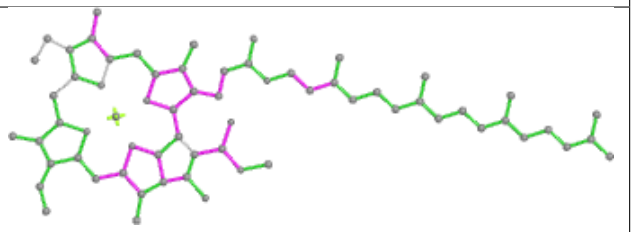
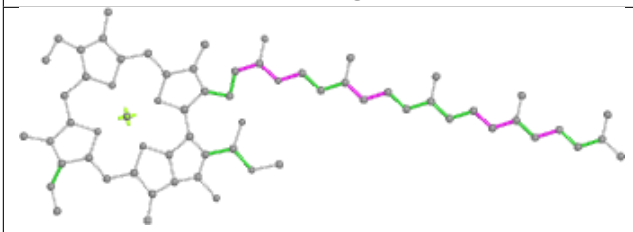


Bond angles



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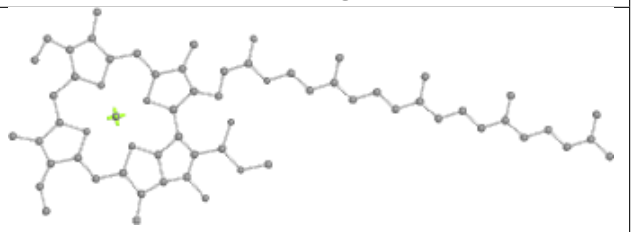
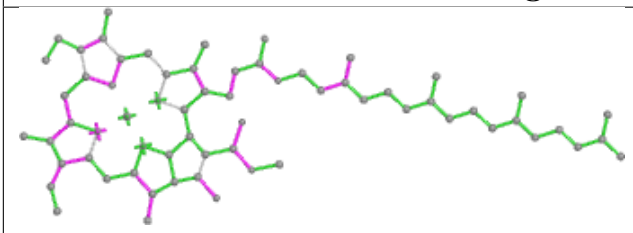


Rings

Ligand CLA C 484



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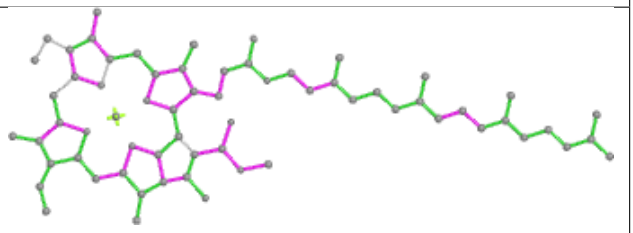
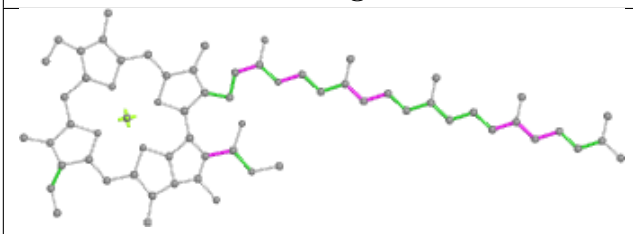


Bond angles



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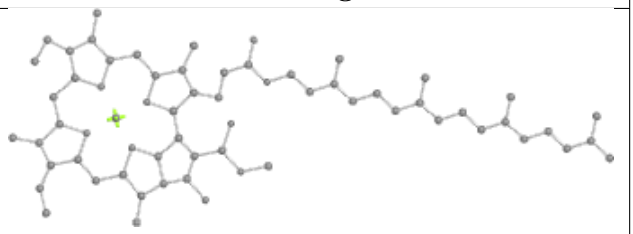
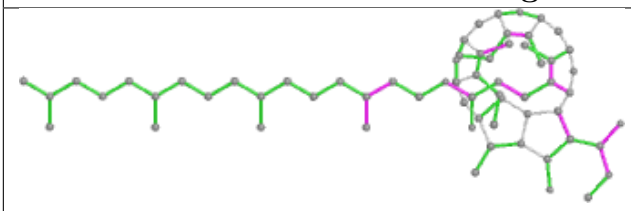


Rings

Ligand PHO D 355



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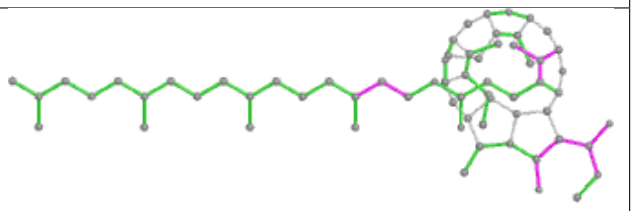
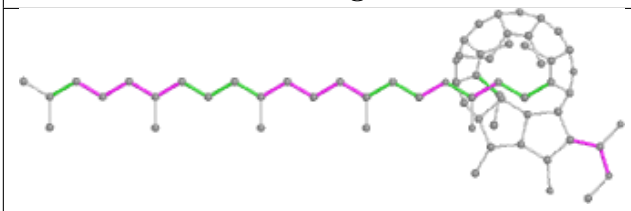
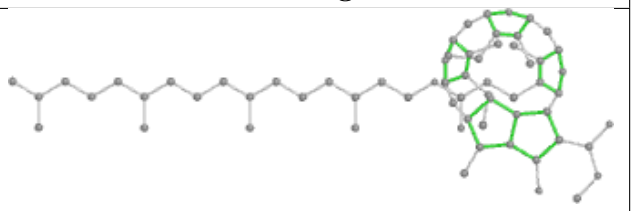


Bond angles

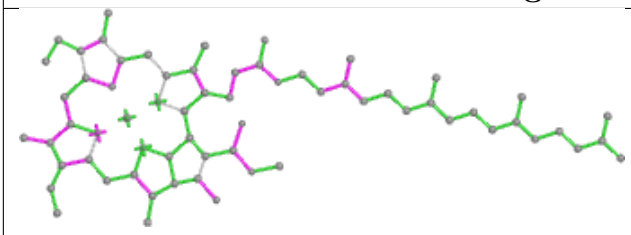


Torsions

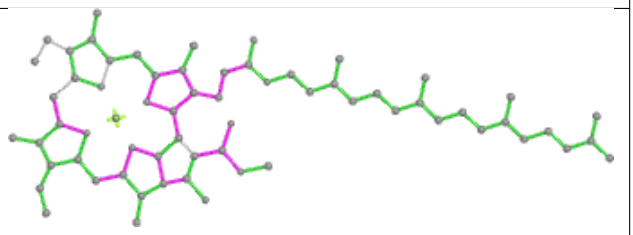


Rings

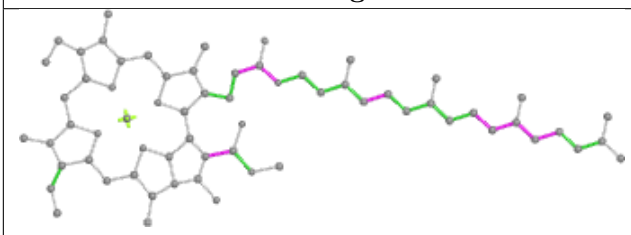
Ligand CLA C 480



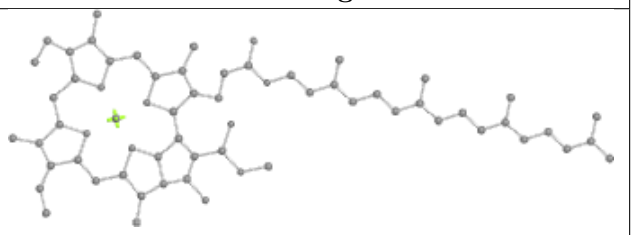
Bond lengths



Bond angles

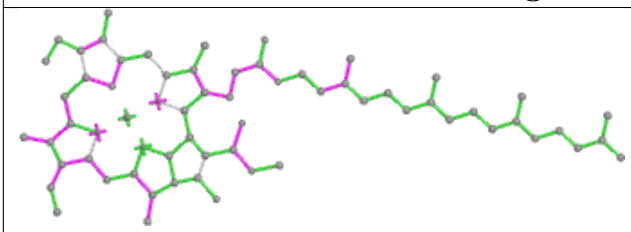


Torsions

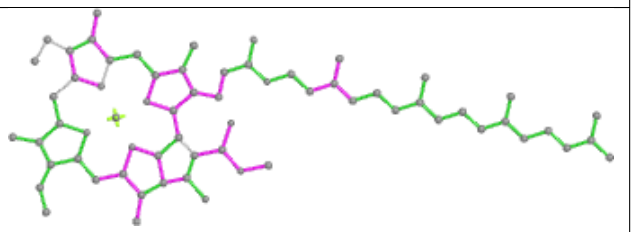


Rings

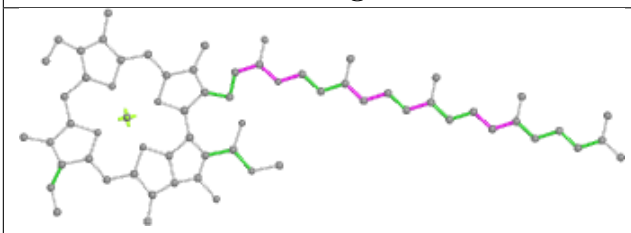
Ligand CLA C 482



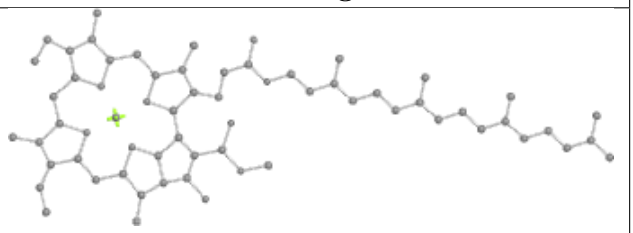
Bond lengths



Bond angles

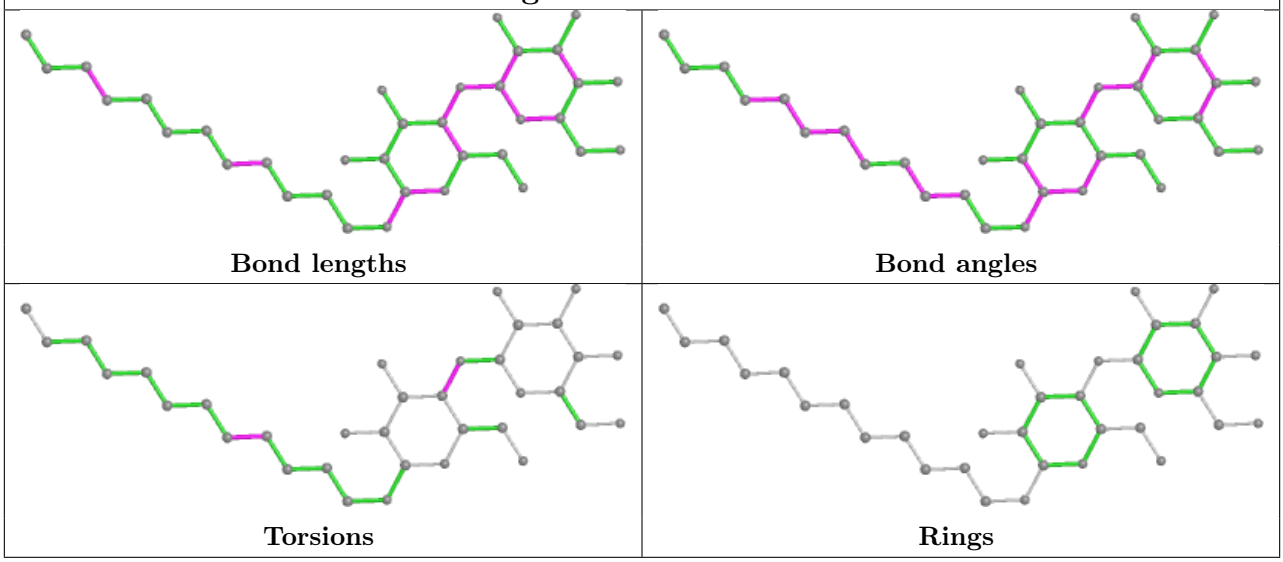


Torsions

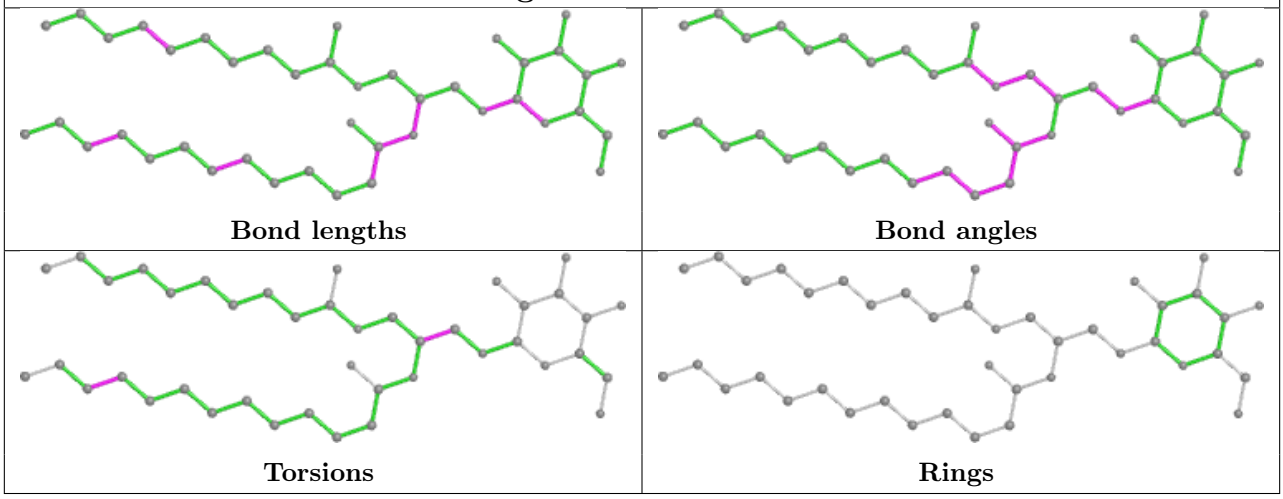


Rings

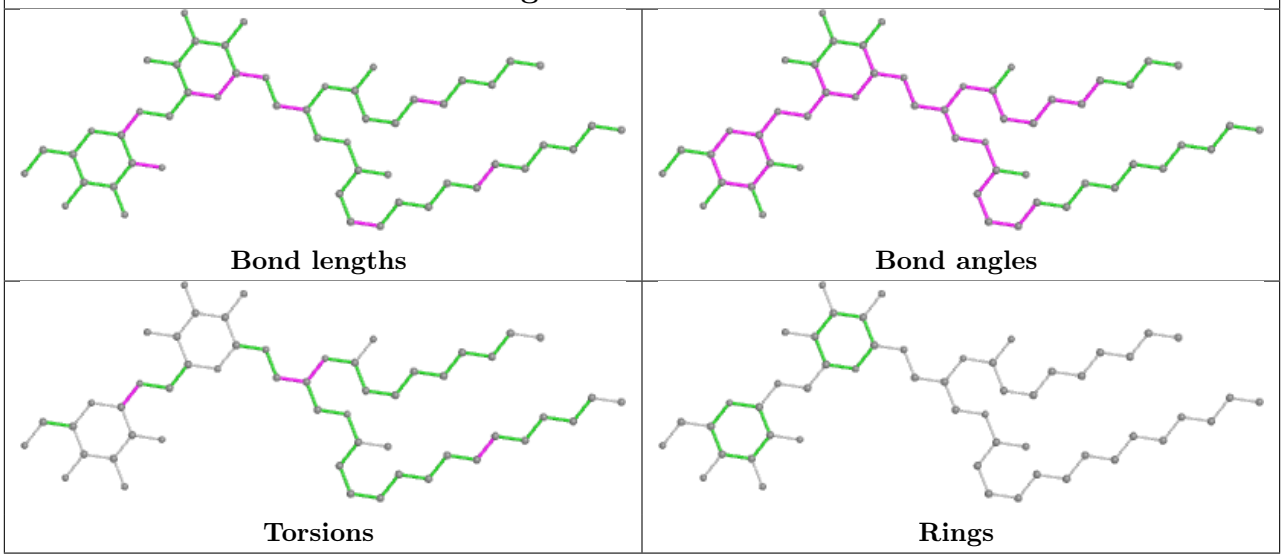
Ligand LMT A 376

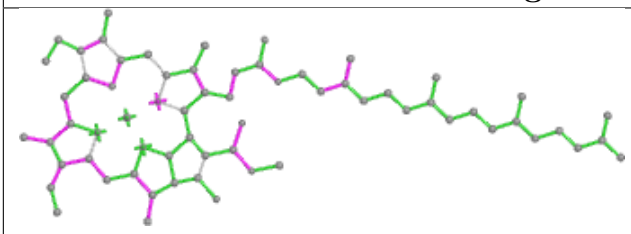
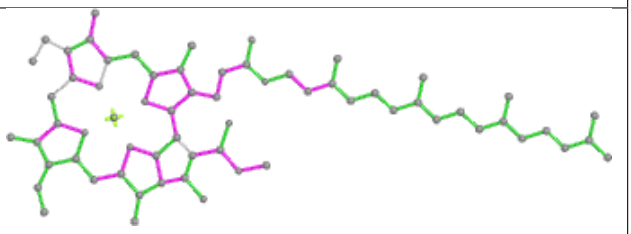
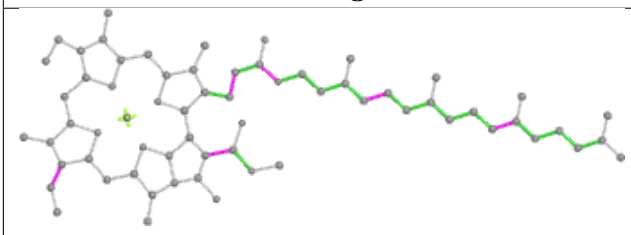
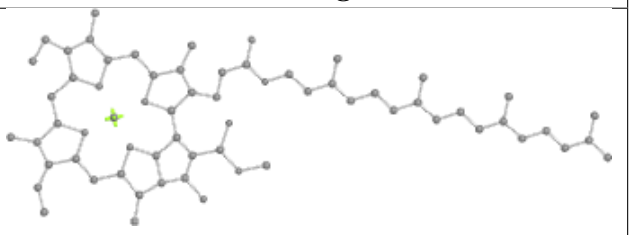


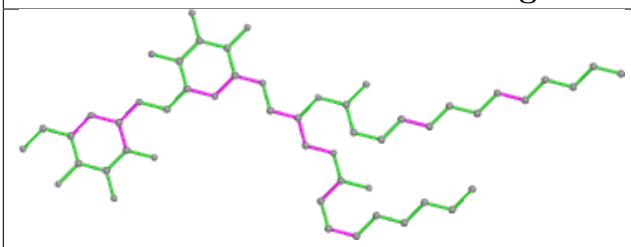
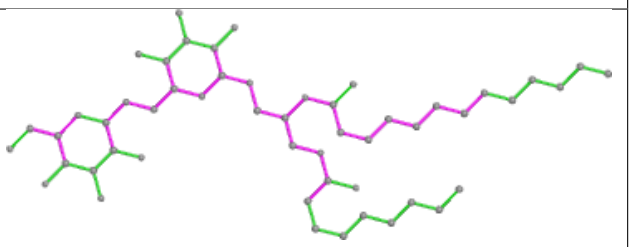
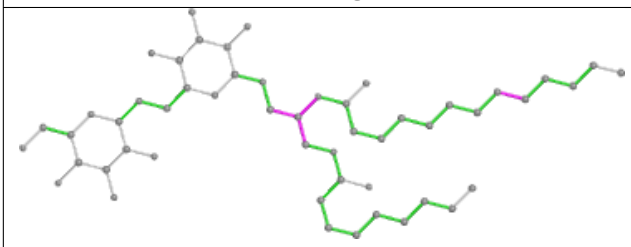
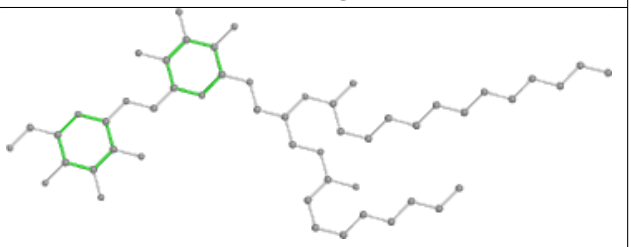
Ligand LMG M 217



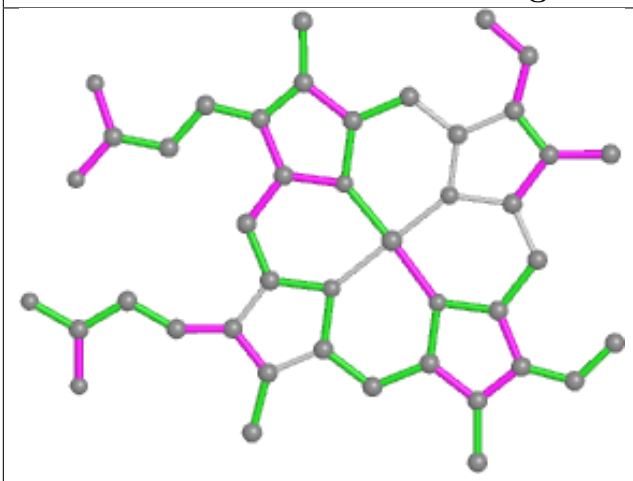
Ligand DGD C 491



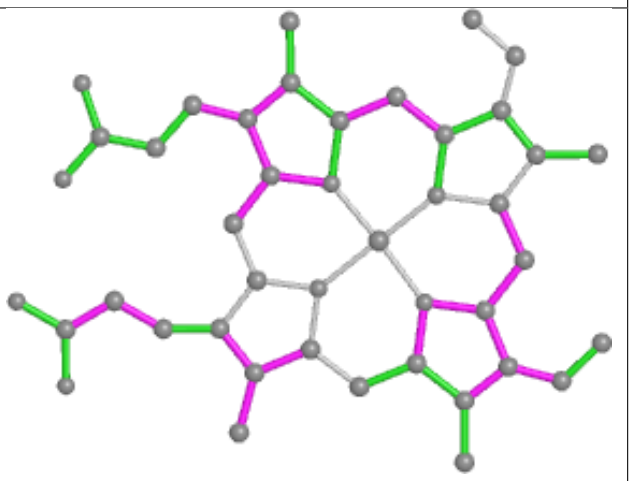
Ligand CLA C 488	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand DGD A 375	
 Bond lengths	 Bond angles
 Torsions	 Rings

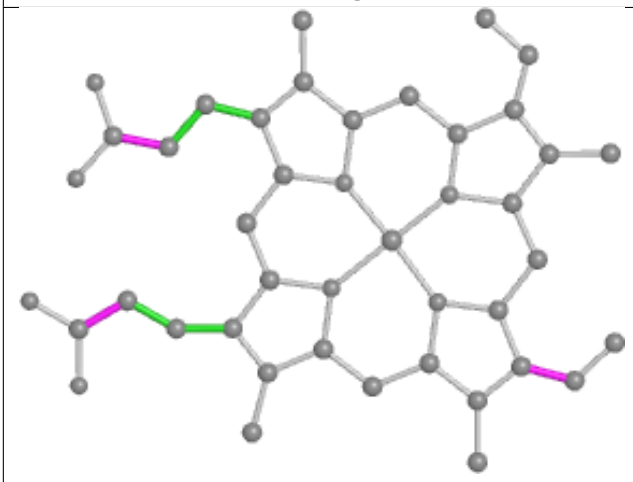
Ligand HEM F 85



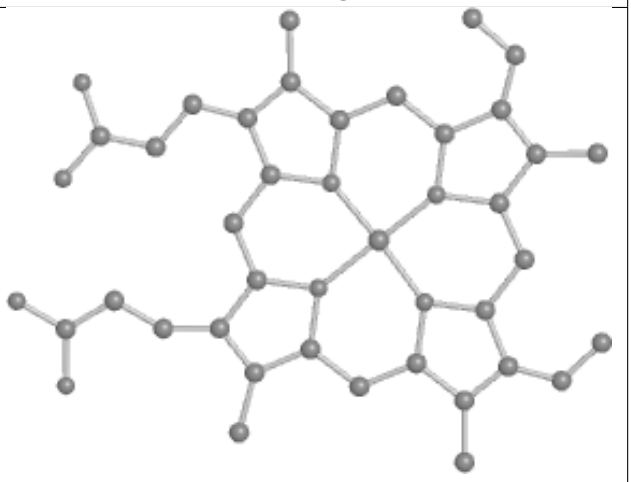
Bond lengths



Bond angles

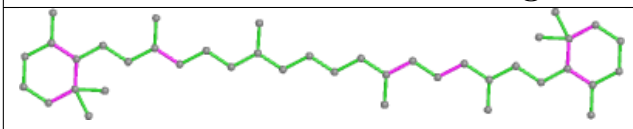


Torsions

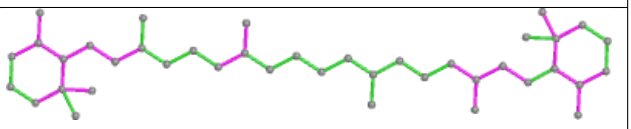


Rings

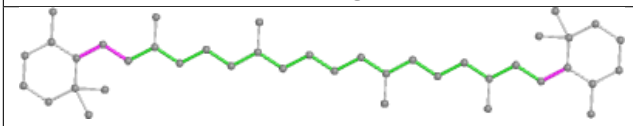
Ligand BCR C 489



Bond lengths



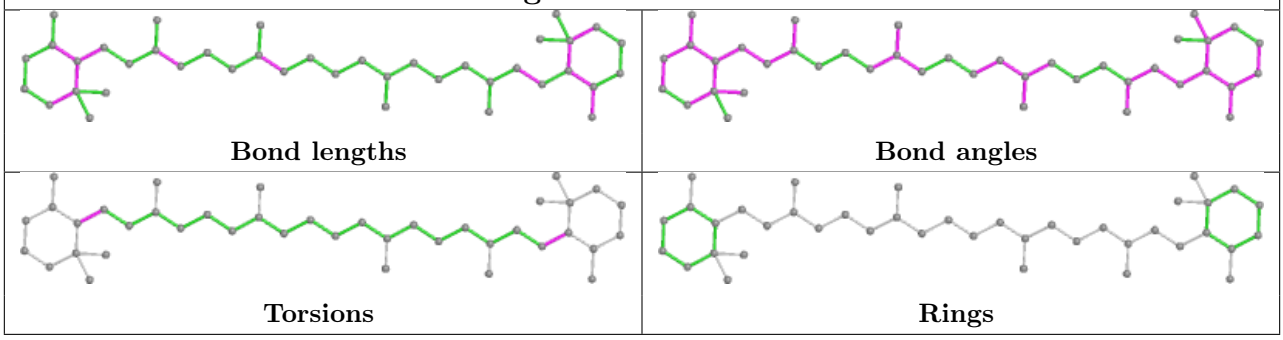
Bond angles



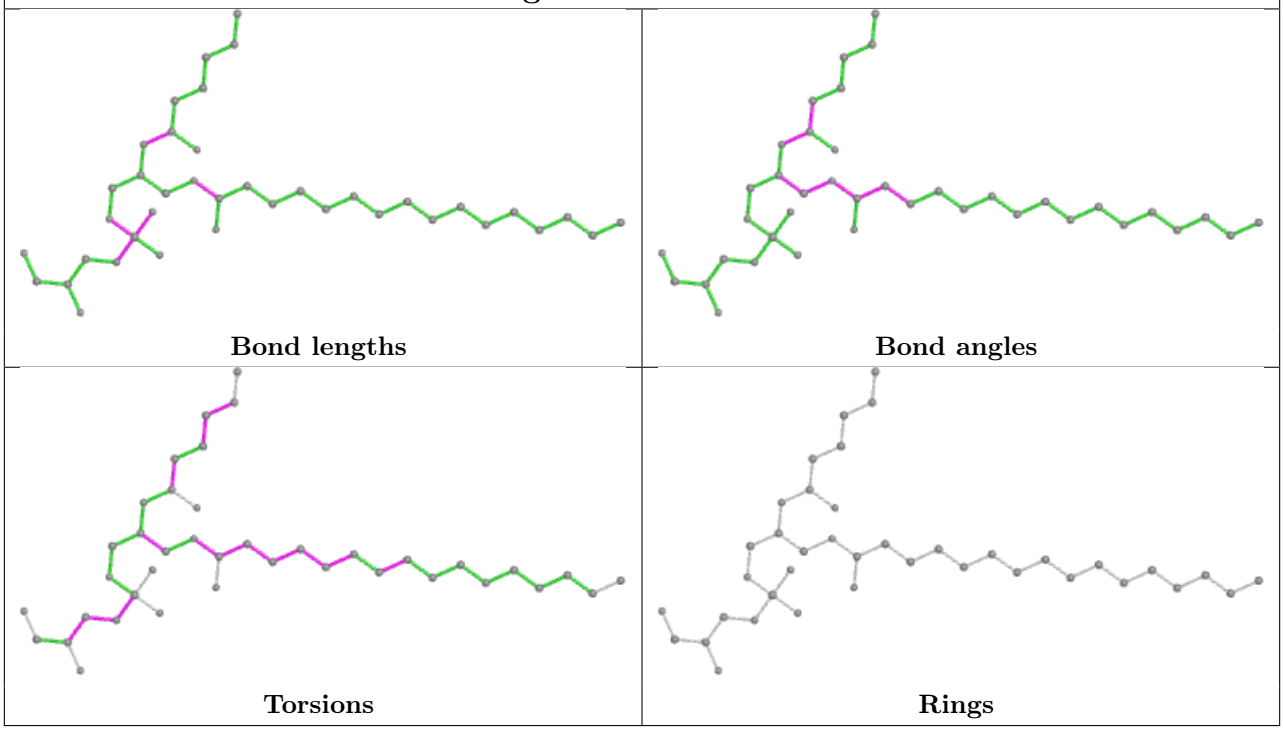
Torsions

Rings

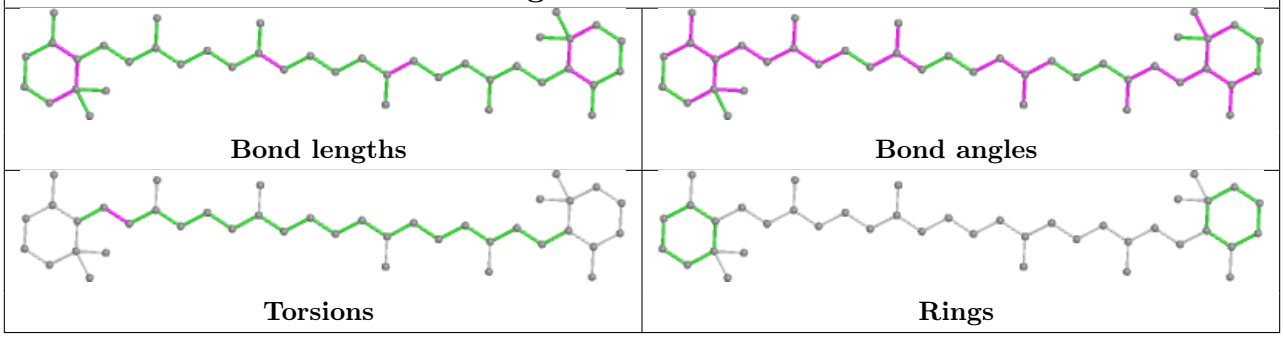
Ligand BCR B 530



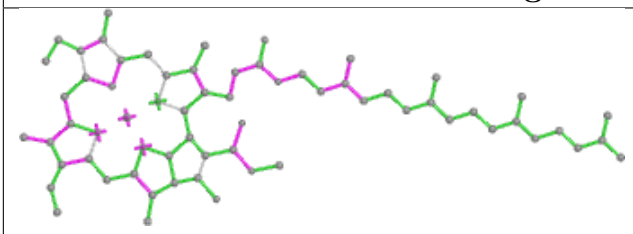
Ligand LHG A 371



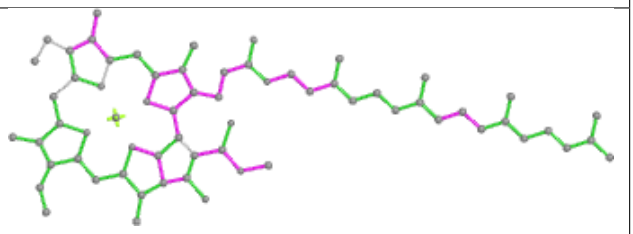
Ligand BCR J 112



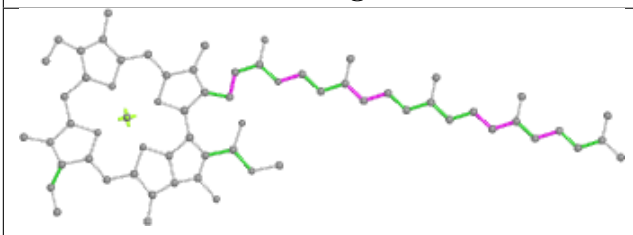
Ligand CLA B 516



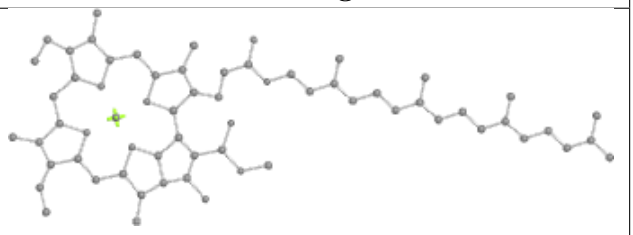
Bond lengths



Bond angles

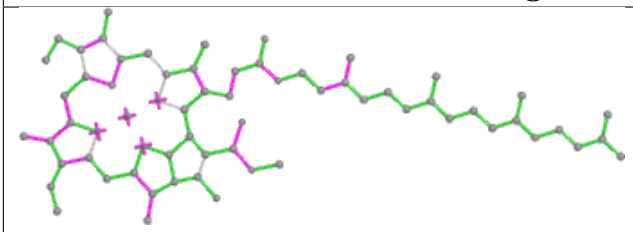


Torsions

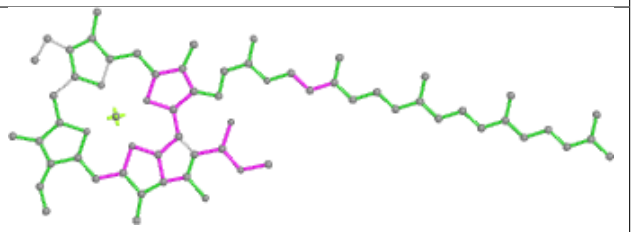


Rings

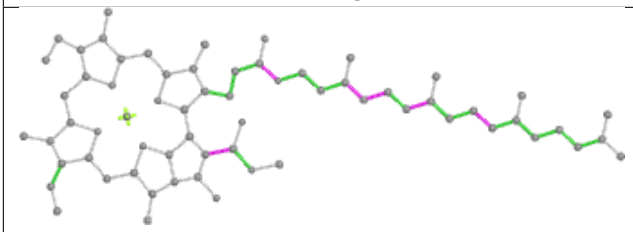
Ligand CLA C 485



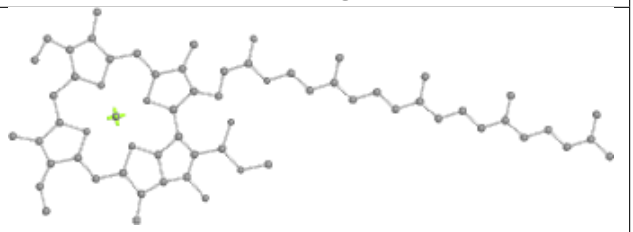
Bond lengths



Bond angles

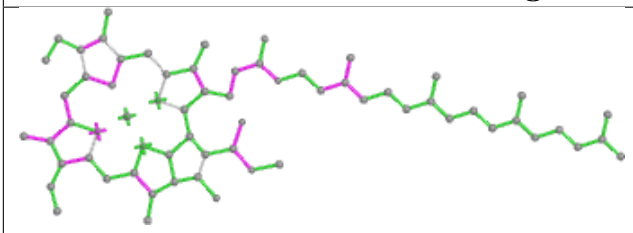


Torsions

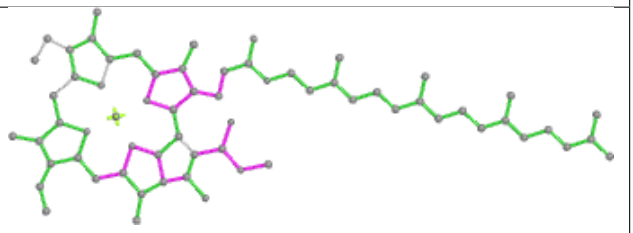


Rings

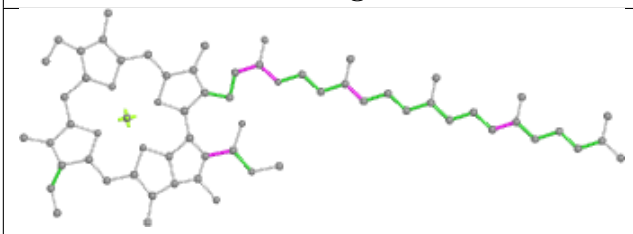
Ligand CLA B 515



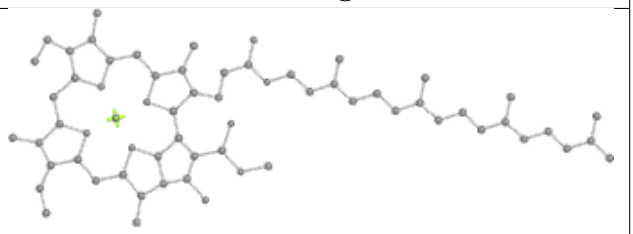
Bond lengths



Bond angles

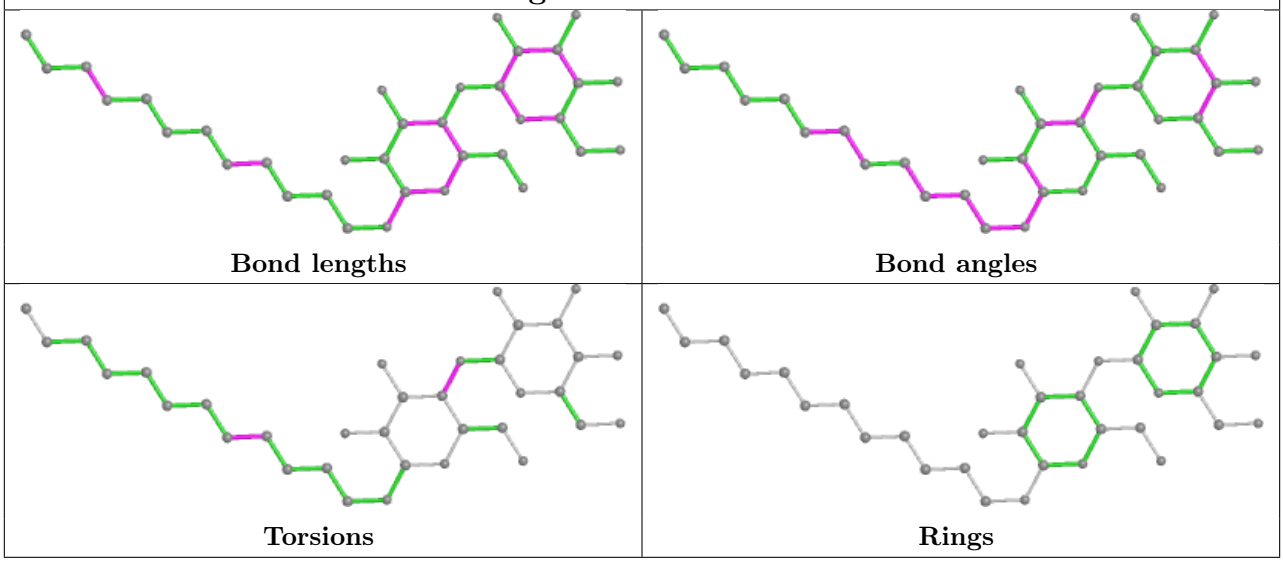


Torsions



Rings

Ligand LMT I 274



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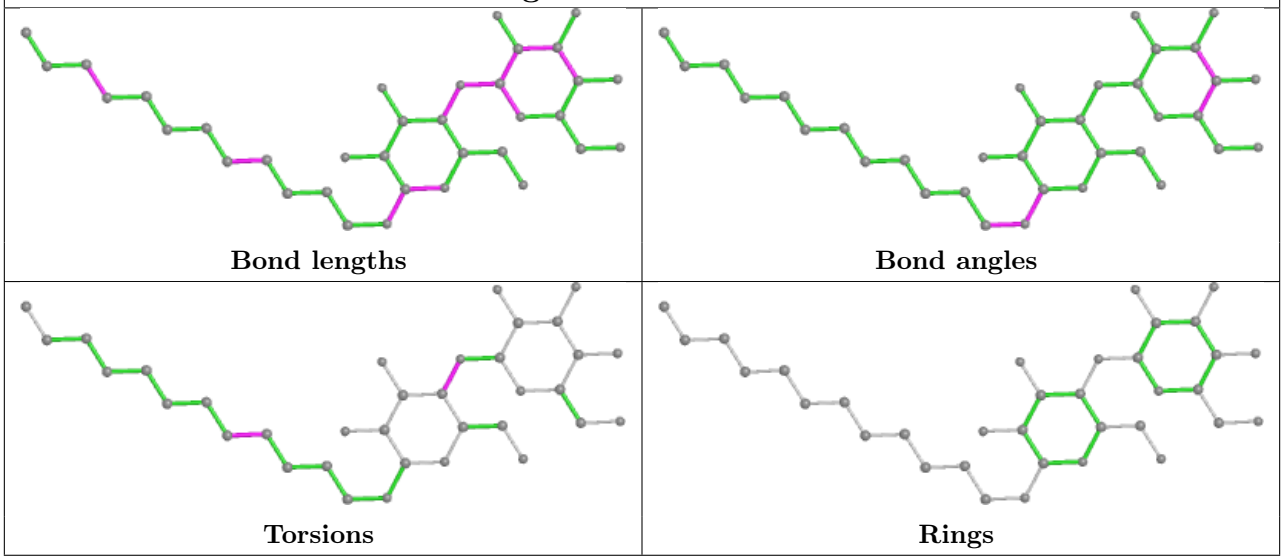
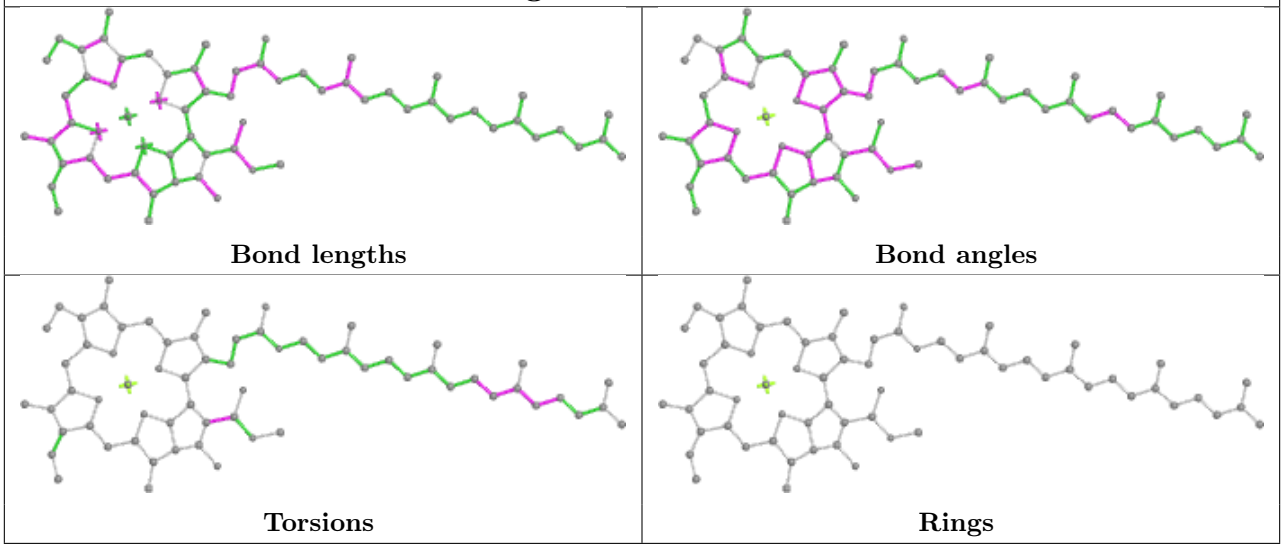
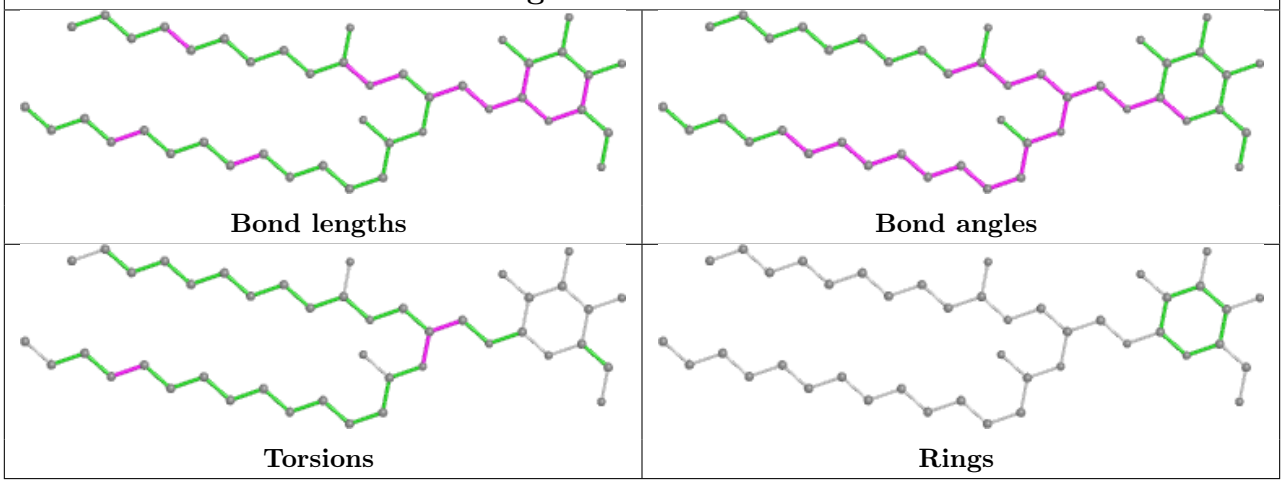


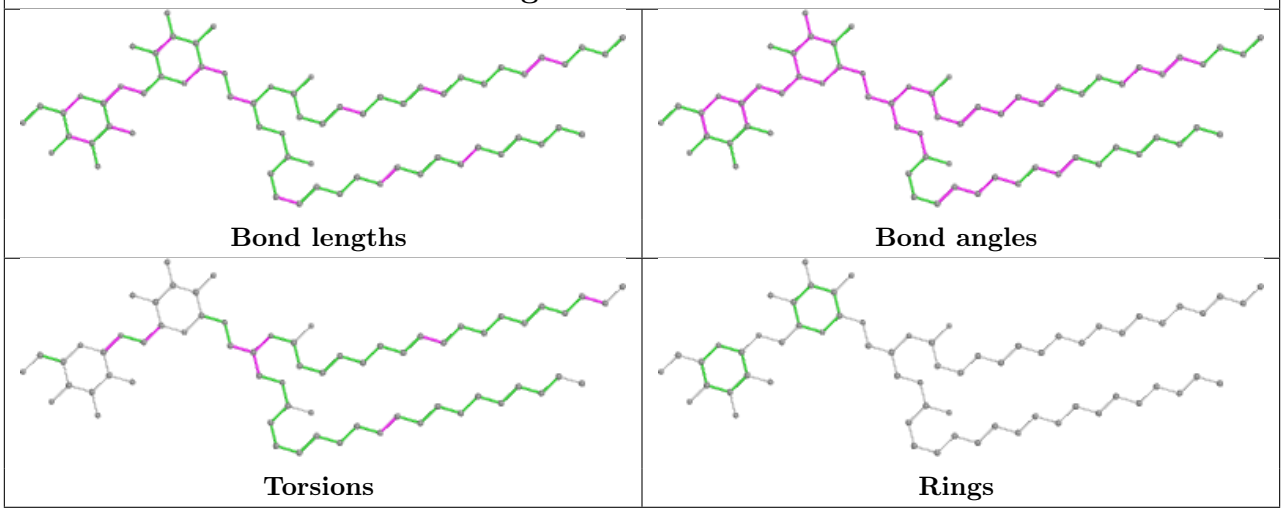
Ligand CLA C 486



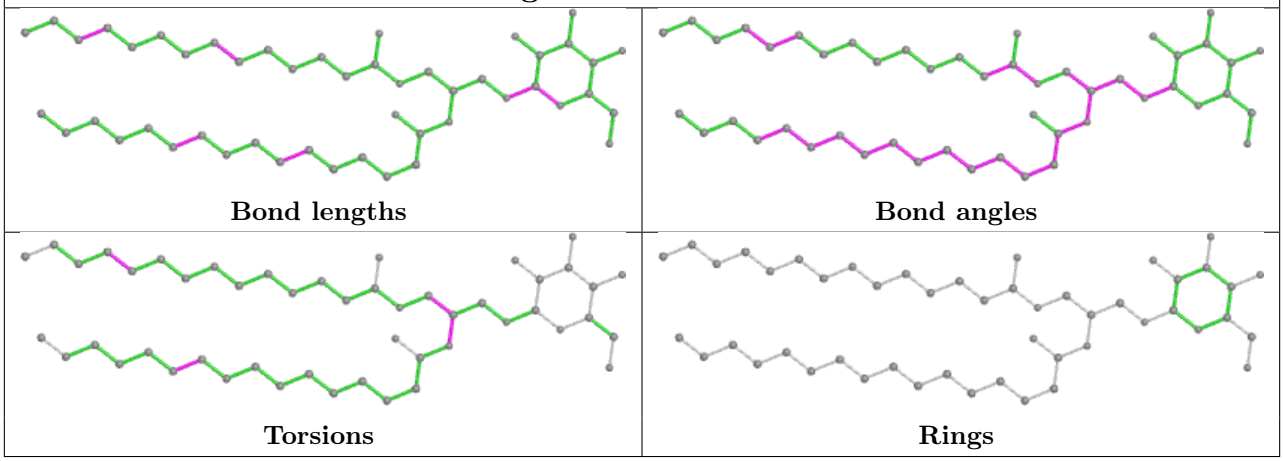
Ligand LMG I 220



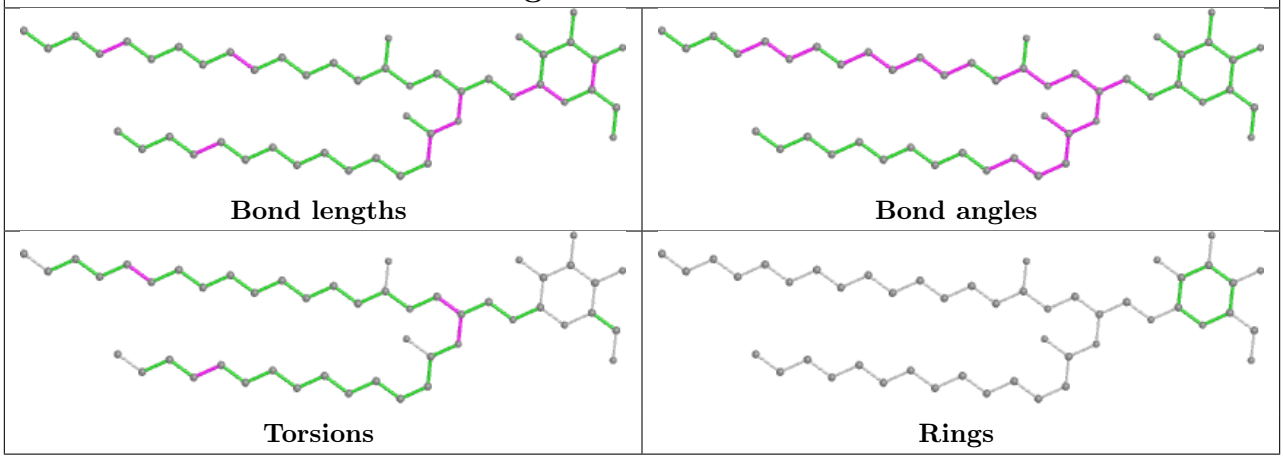
Ligand DGD C 493



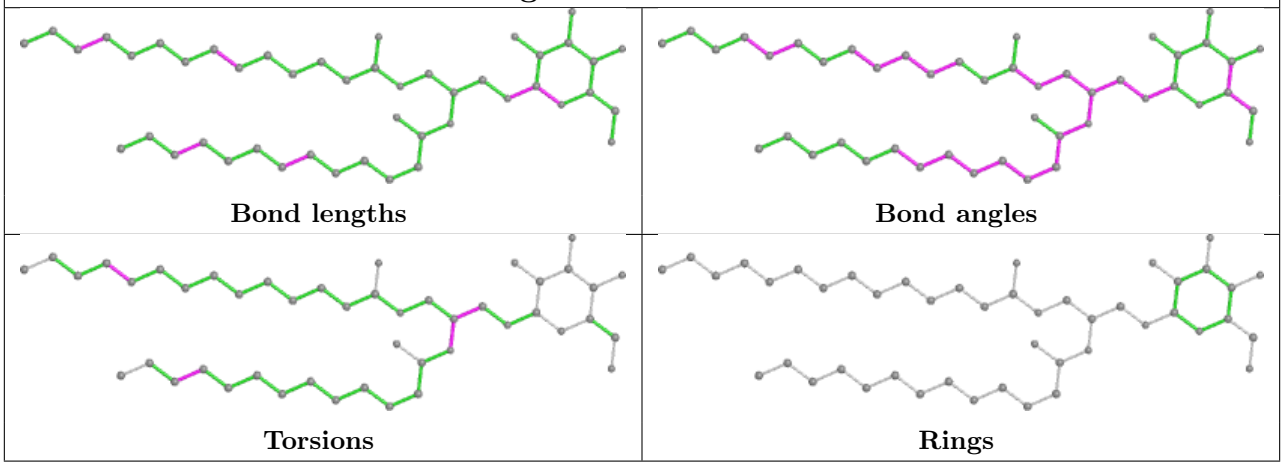
Ligand LMG B 531



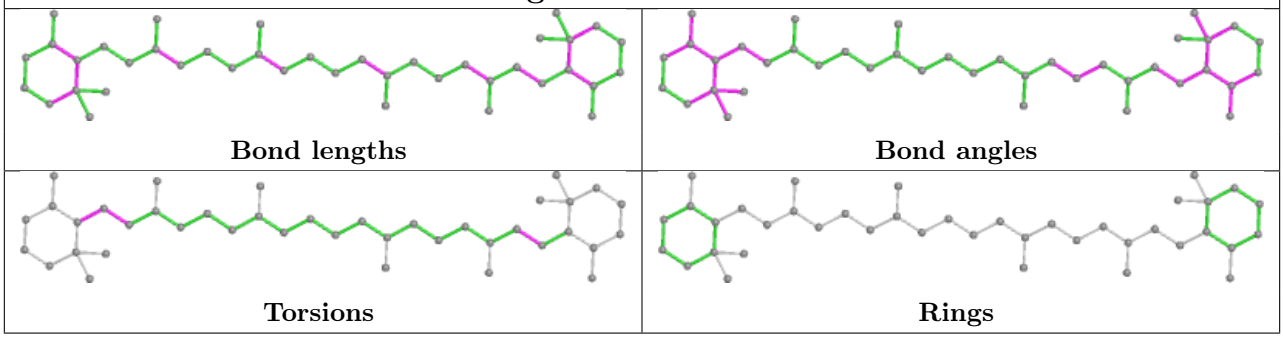
Ligand LMG J 492



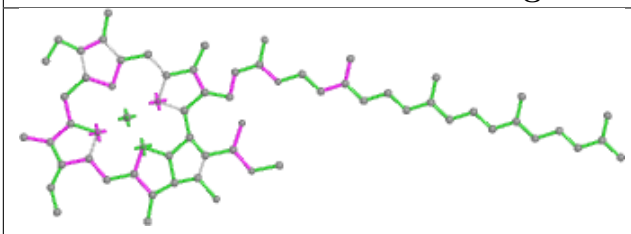
Ligand LMG D 359



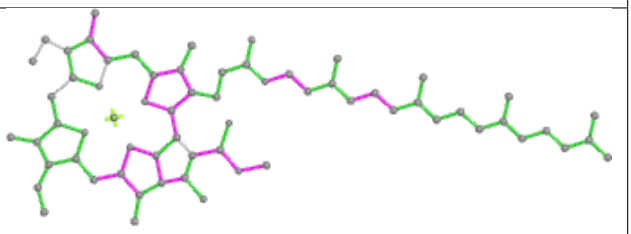
Ligand BCR J 115



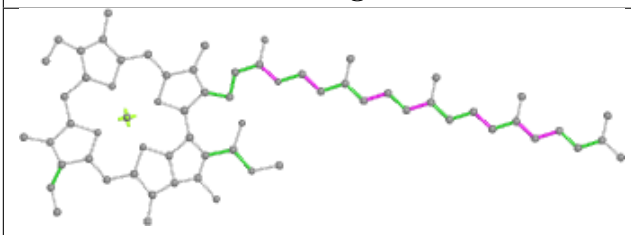
Ligand CLA A 362



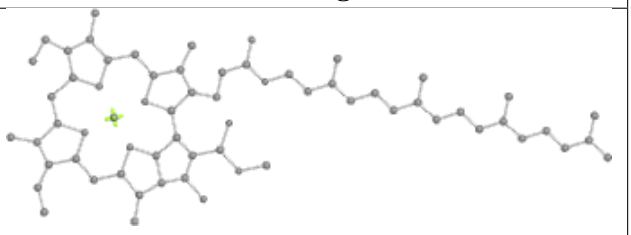
Bond lengths



Bond angles

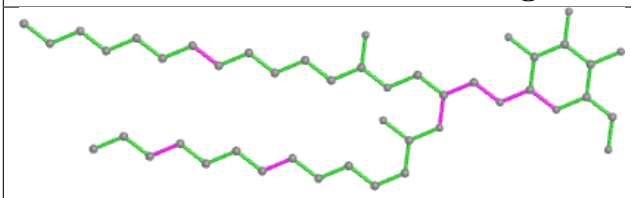


Torsions

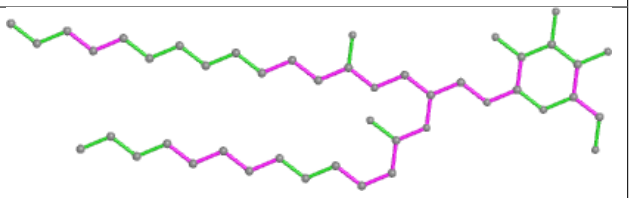


Rings

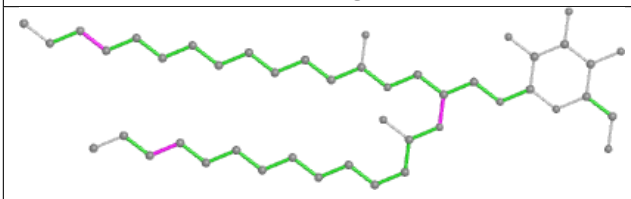
Ligand LMG C 494



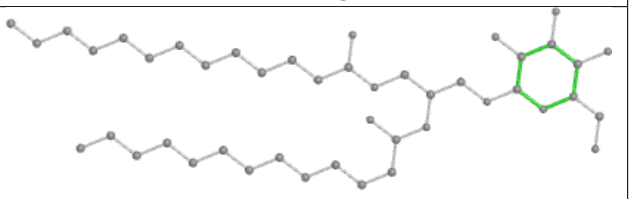
Bond lengths



Bond angles

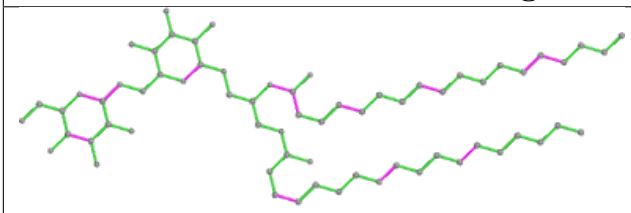


Torsions



Rings

Ligand DGD B 533



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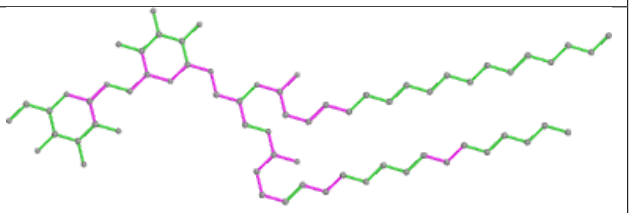
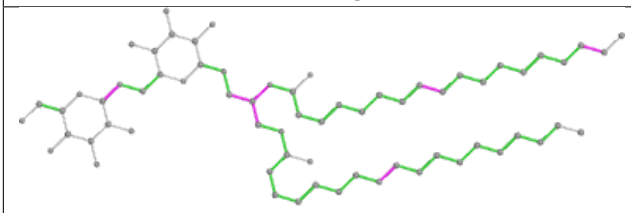
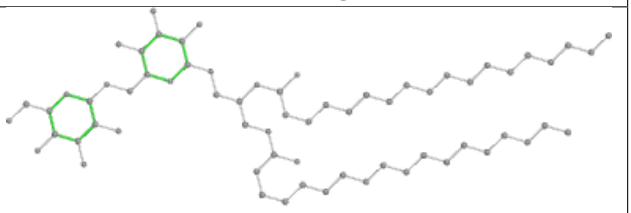


Bond angles

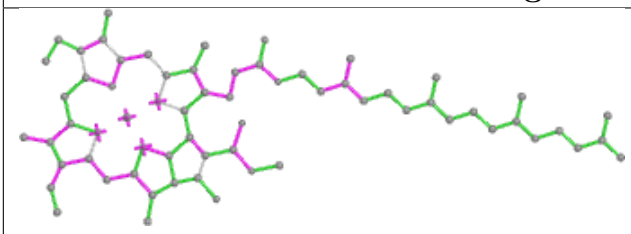


Torsions



Rings

Ligand CLA B 511



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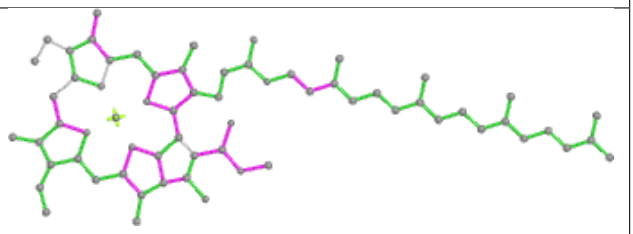
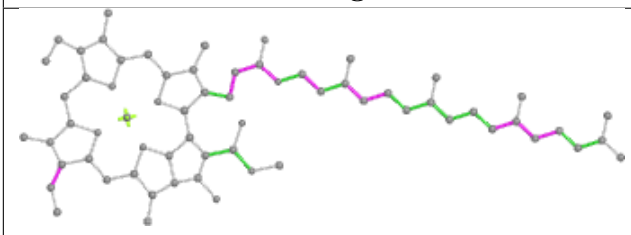


Bond angles



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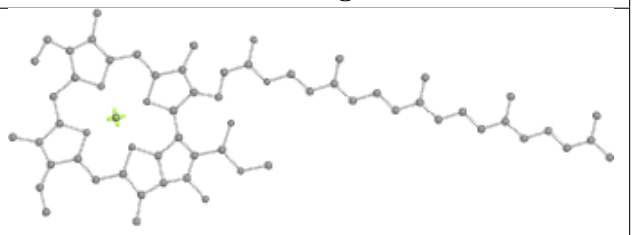
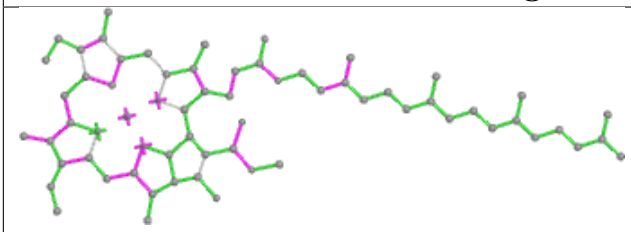


Rings

Ligand CLA D 354



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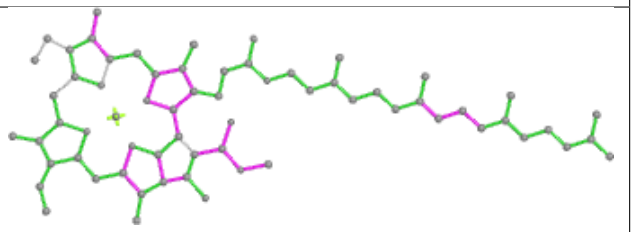
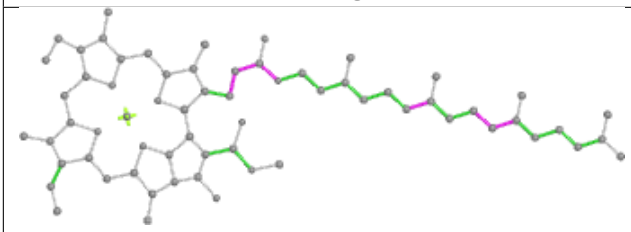
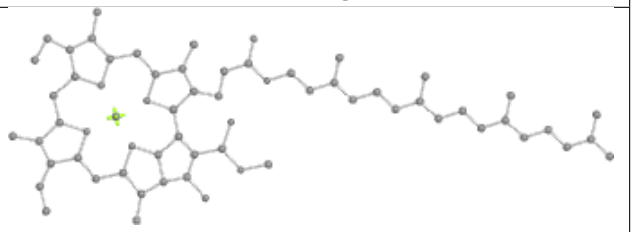


Bond angles

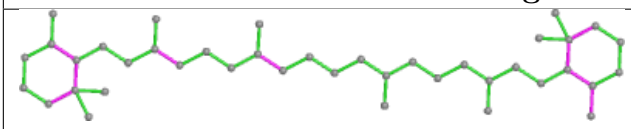


Torsions



Rings

Ligand BCR B 529



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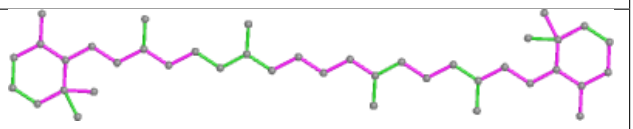
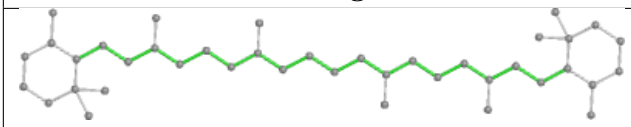


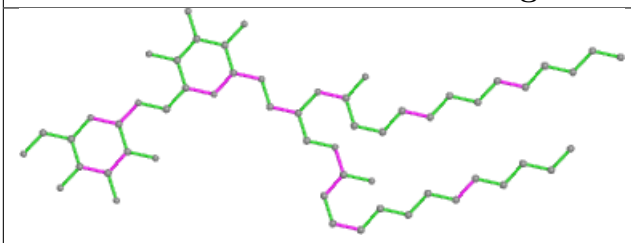
Bond angles



Torsions

Rings

Ligand DGD C 474



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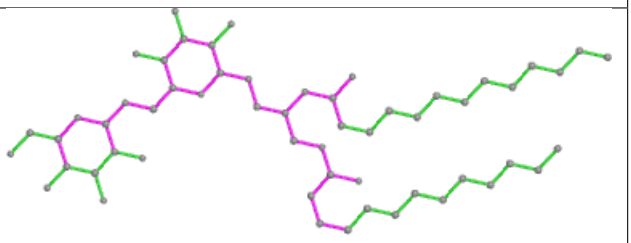
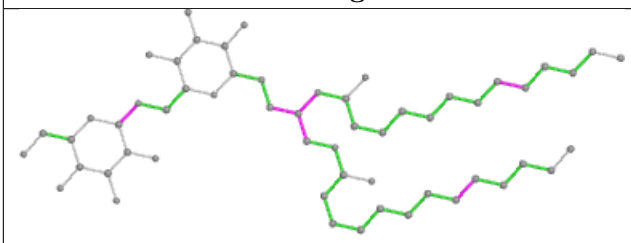


Bond angles



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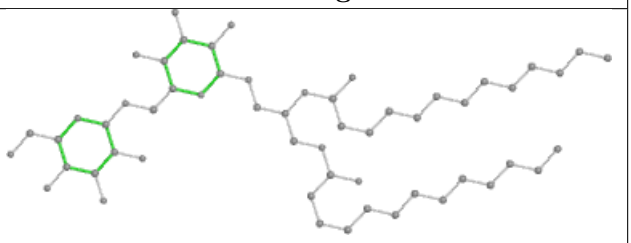
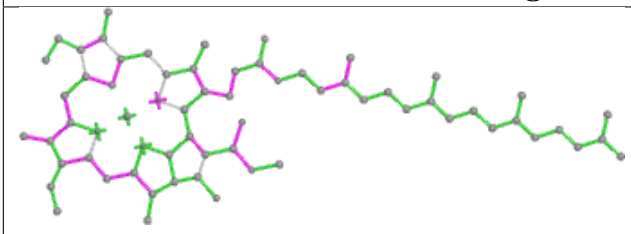


Rings

Ligand CLA C 481



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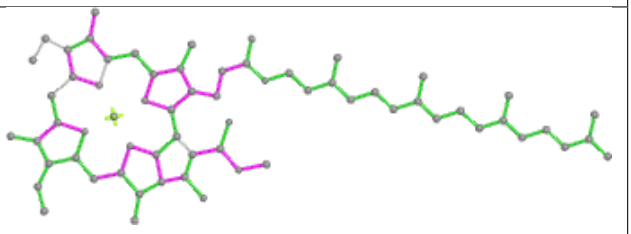
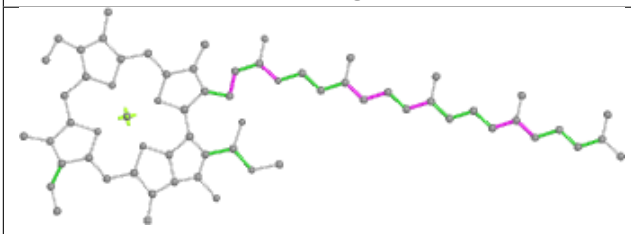


Bond angles



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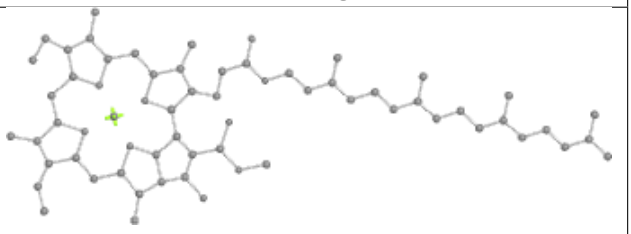
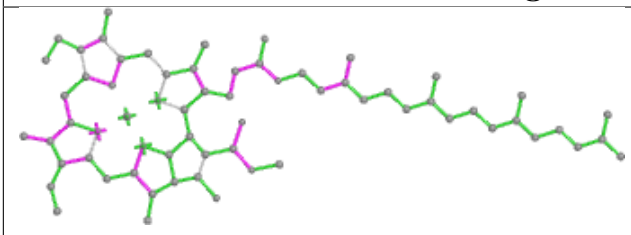
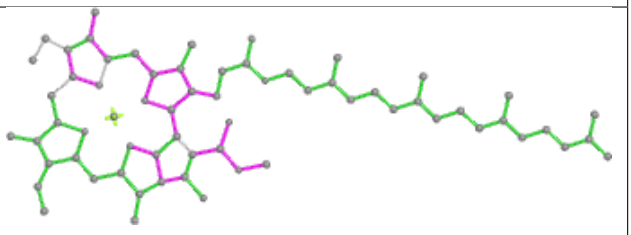


Rings

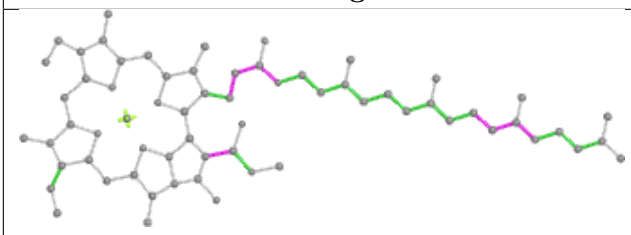
Ligand CLA B 513



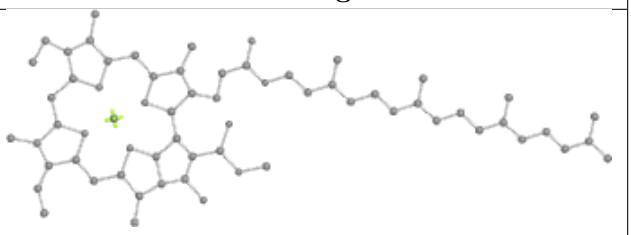
Bond lengths



Bond angles

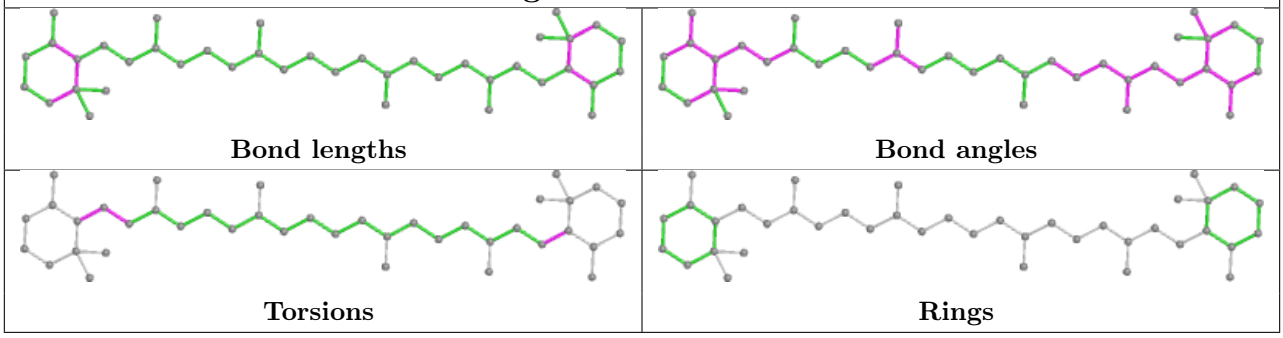


Torsions

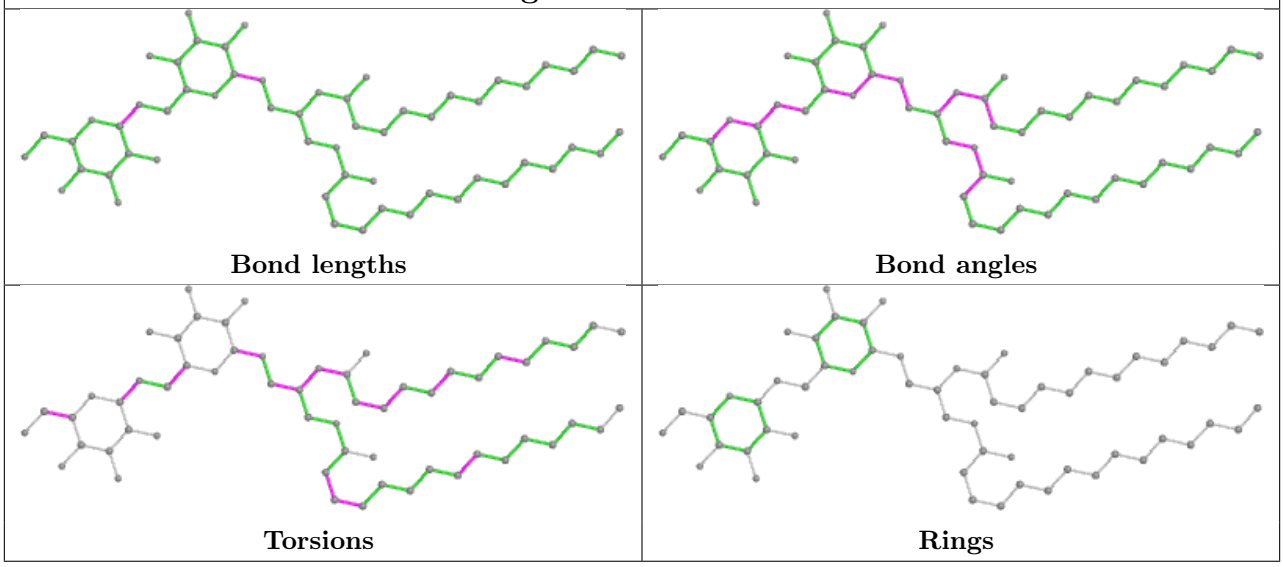


Rings

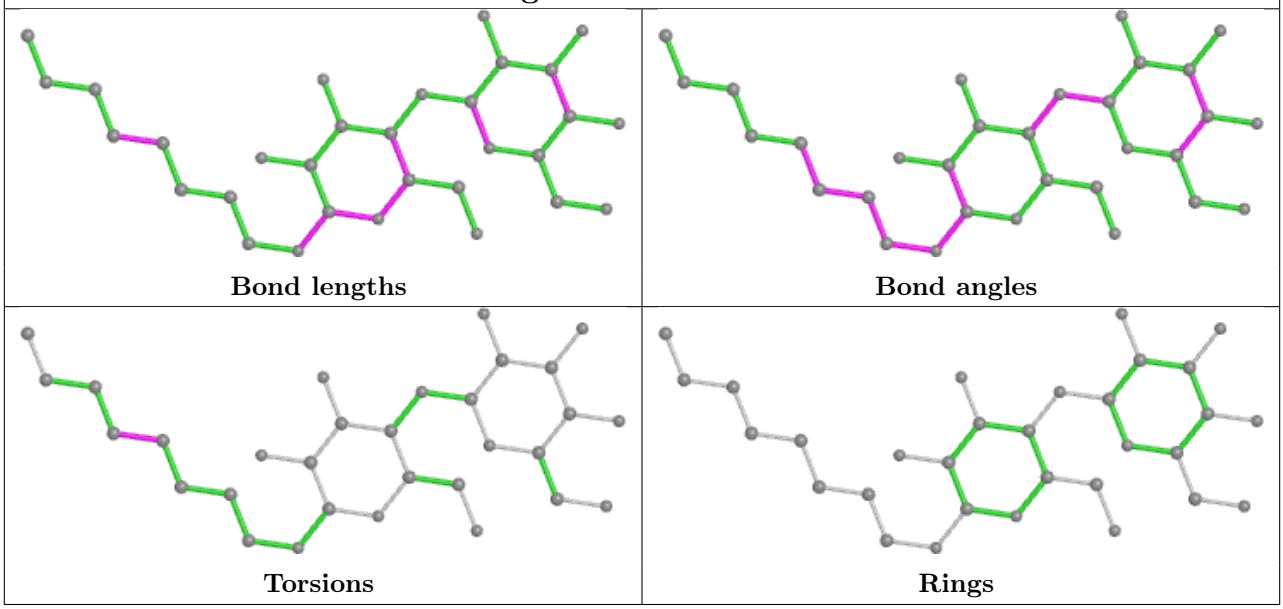
Ligand BCR A 369



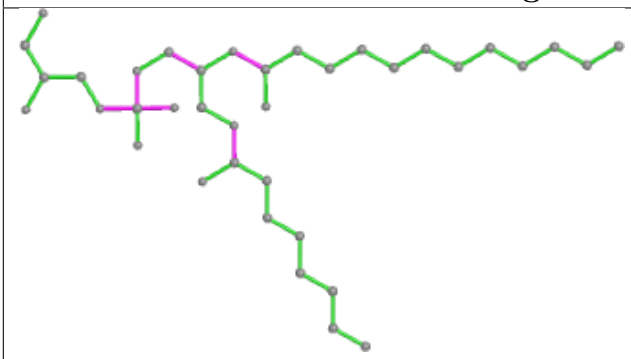
Ligand DGD B 528



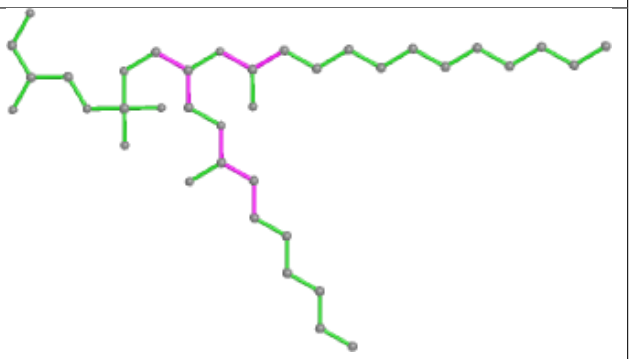
Ligand LMT D 363



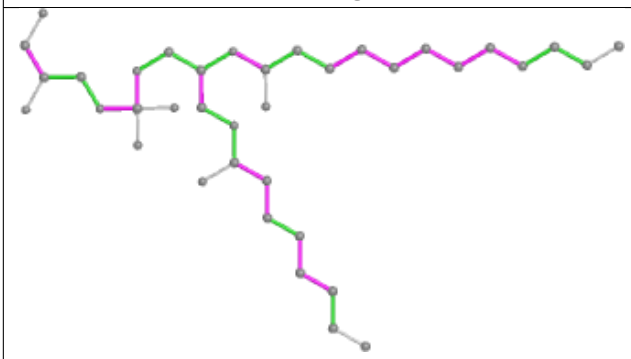
Ligand LHG C 476



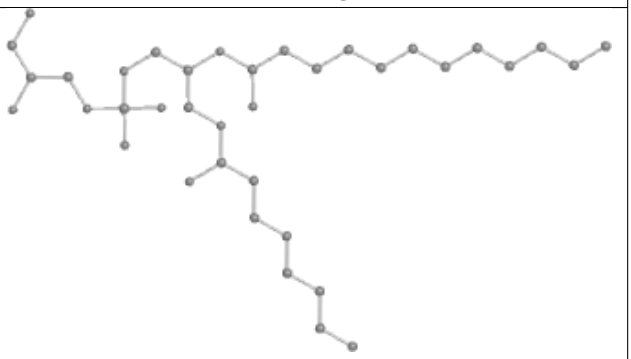
Bond lengths



Bond angles

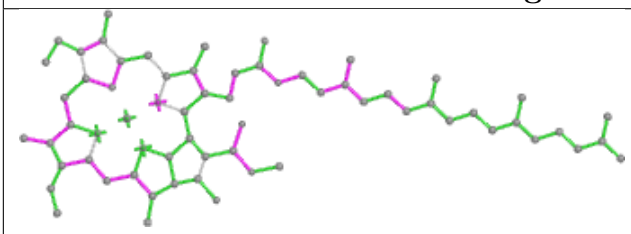


Torsions



Rings

Ligand CLA B 517



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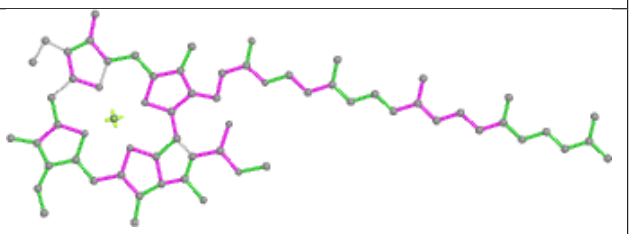
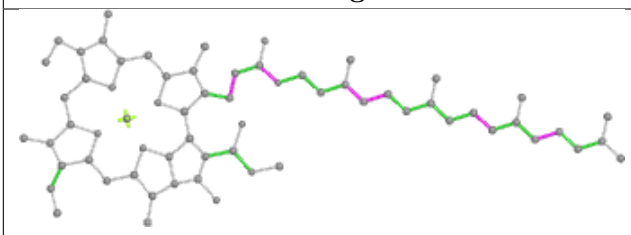
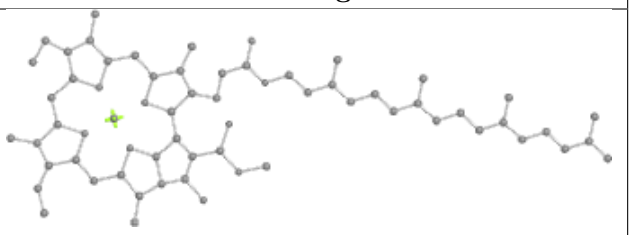


Bond angles

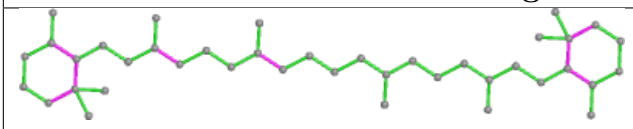


Torsions



Rings

Ligand BCR C 490



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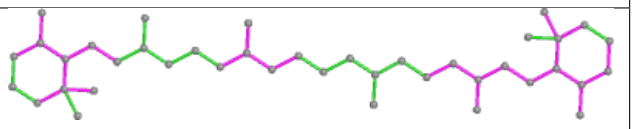
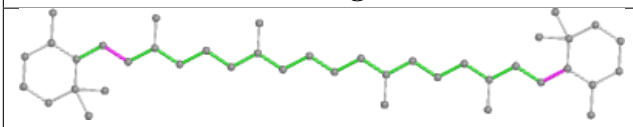
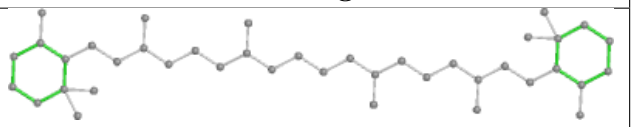


Bond angles

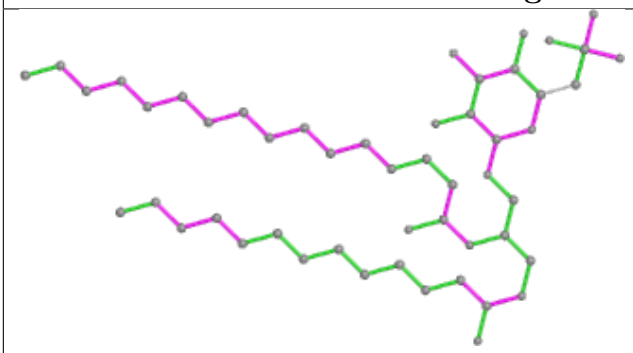


Torsions

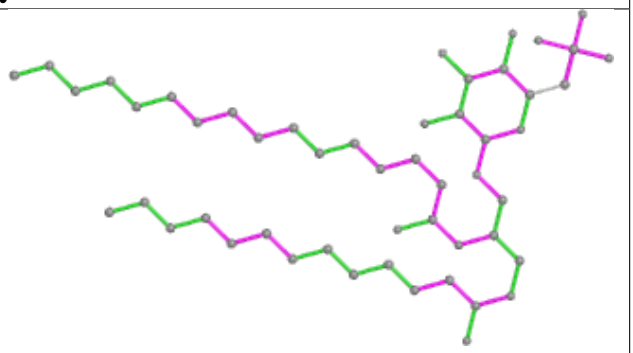


Rings

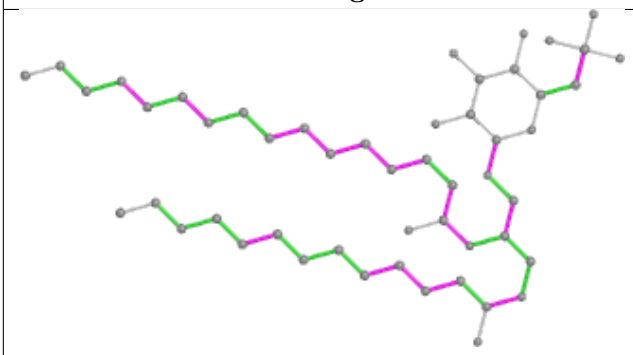
Ligand SQD C 475



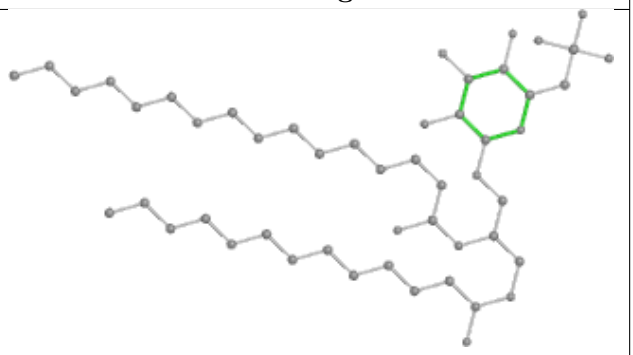
Bond lengths



Bond angles

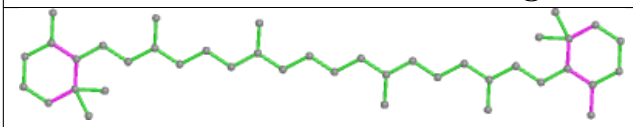


Torsions

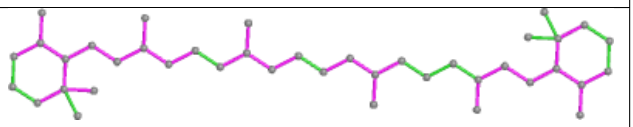


Rings

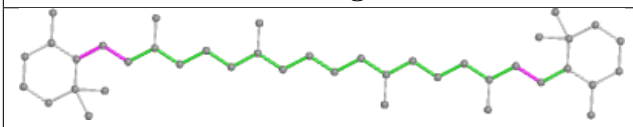
Ligand BCR B 527



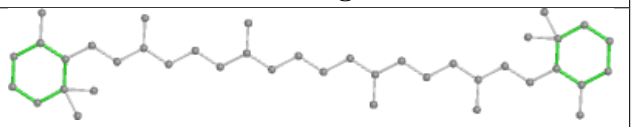
Bond lengths



Bond angles

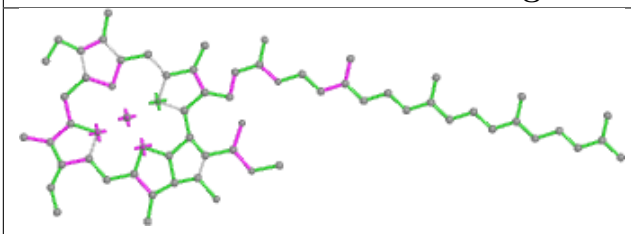


Torsions

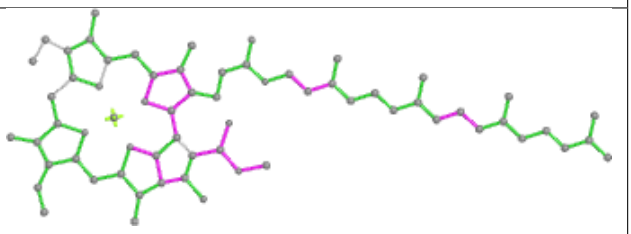


Rings

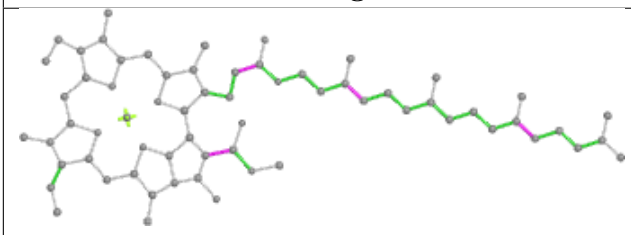
Ligand CLA K 483



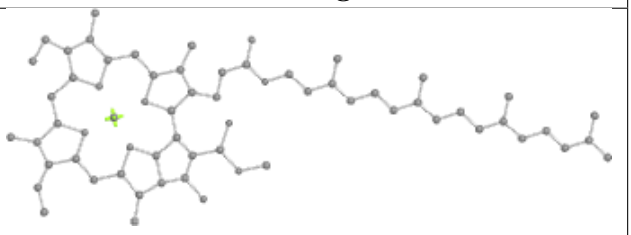
Bond lengths



Bond angles

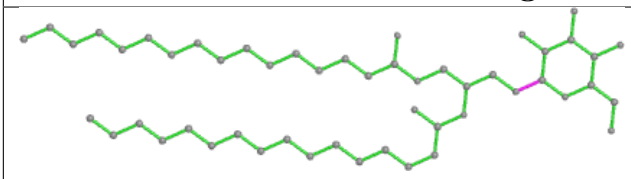


Torsions

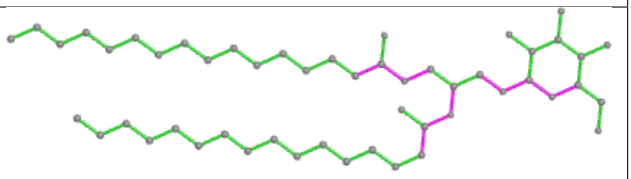


Rings

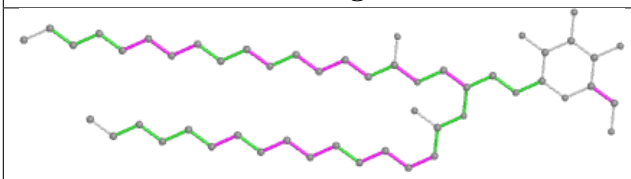
Ligand LMG A 373



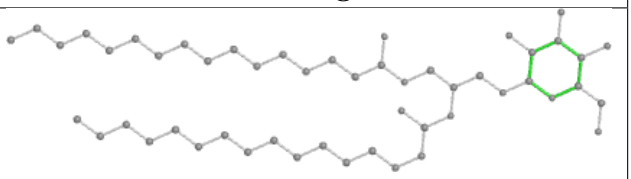
Bond lengths



Bond angles

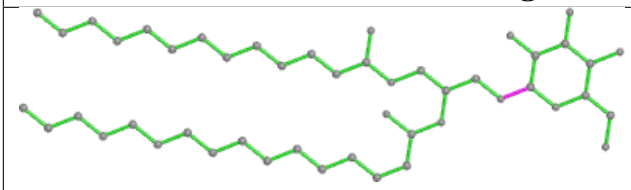


Torsions

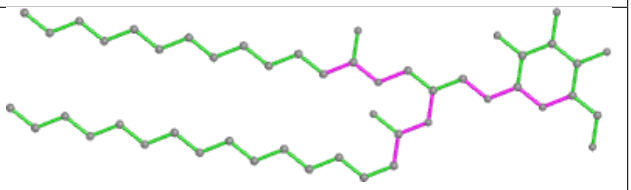


Rings

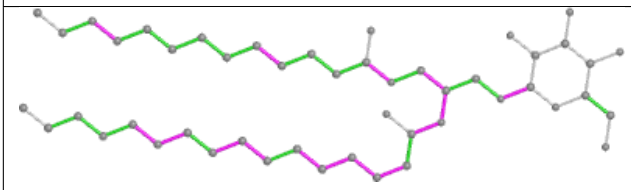
Ligand LMG D 360



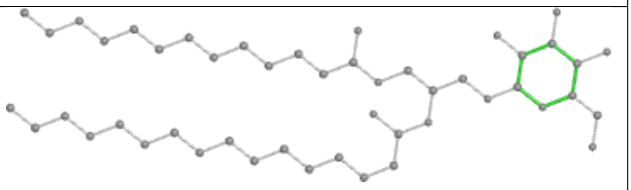
Bond lengths



Bond angles

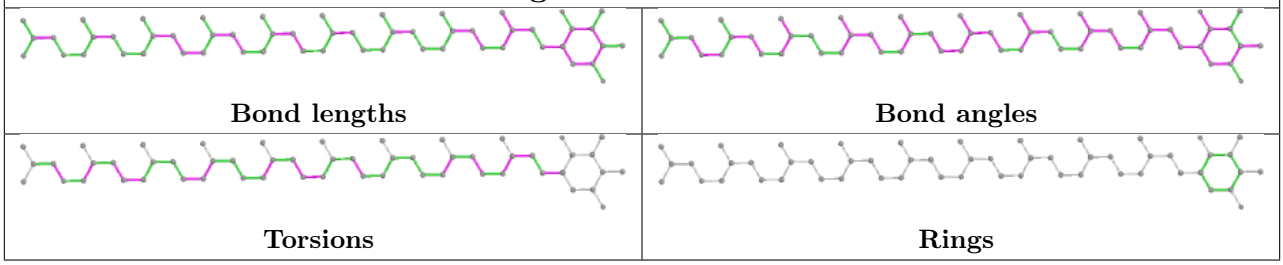


Torsions

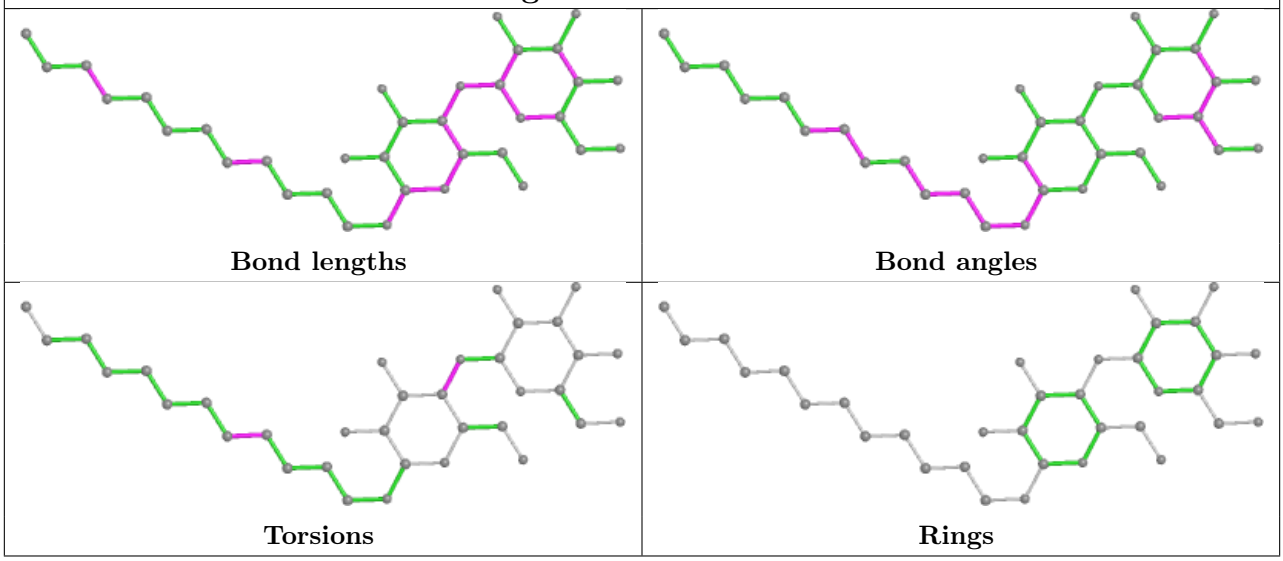


Rings

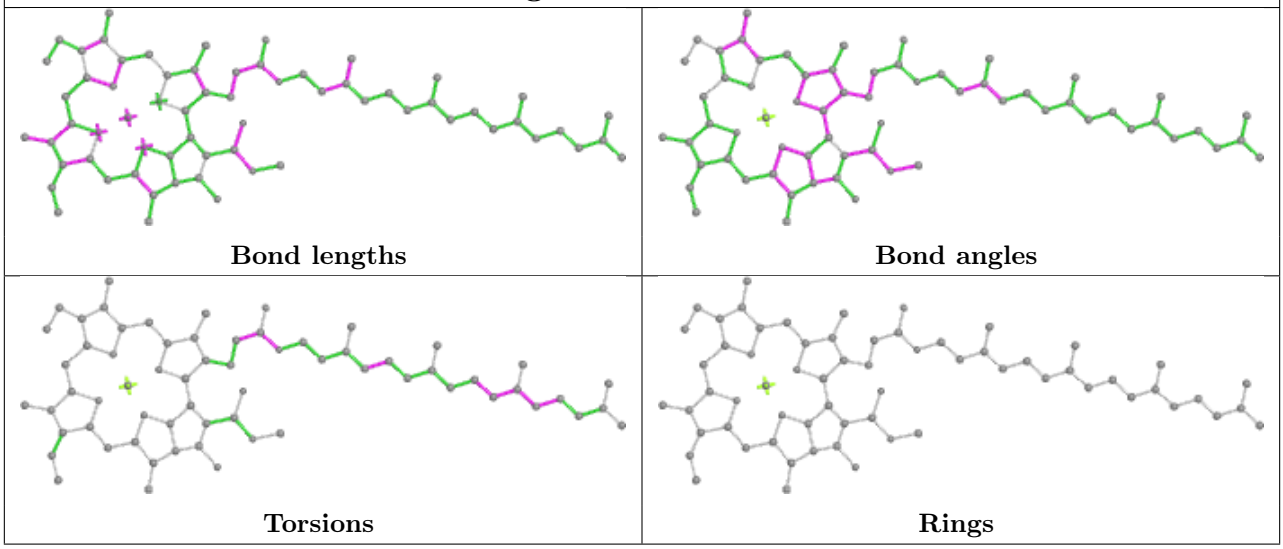
Ligand PL9 D 357



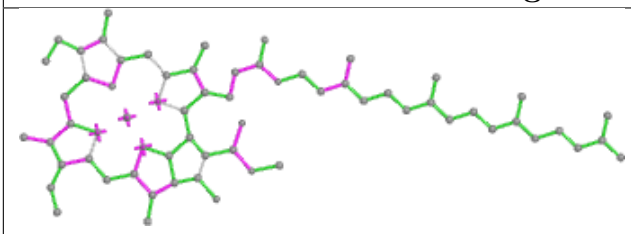
Ligand LMT O 274



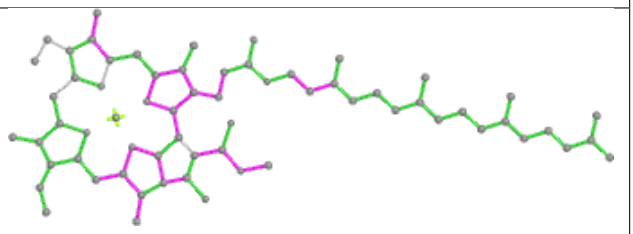
Ligand CLA B 514



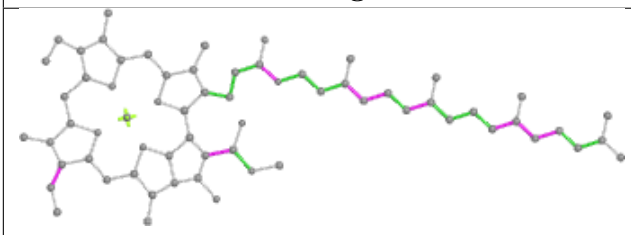
Ligand CLA A 364



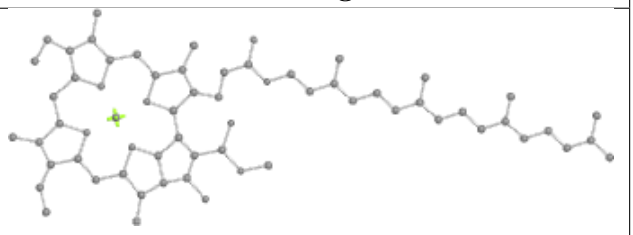
Bond lengths



Bond angles

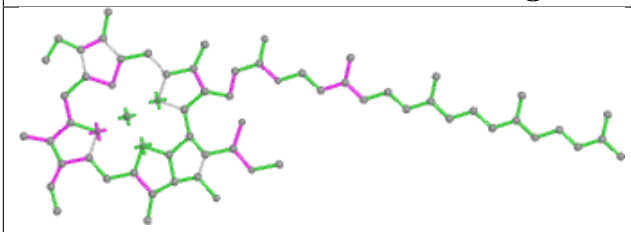


Torsions

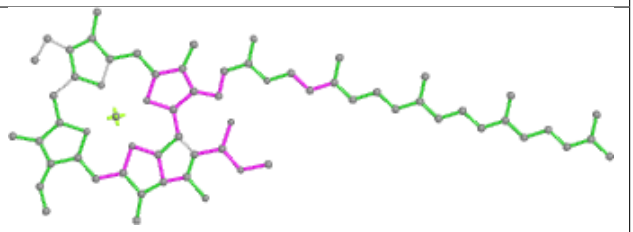


Rings

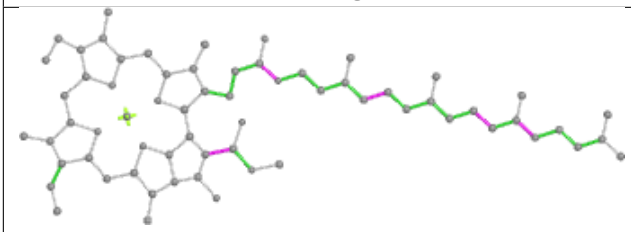
Ligand CLA C 478



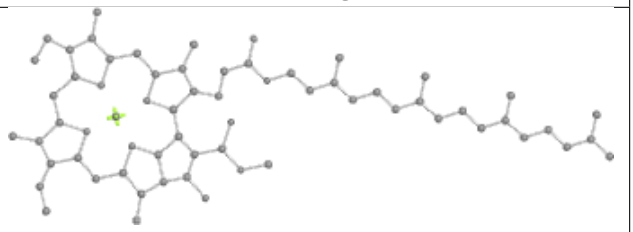
Bond lengths



Bond angles

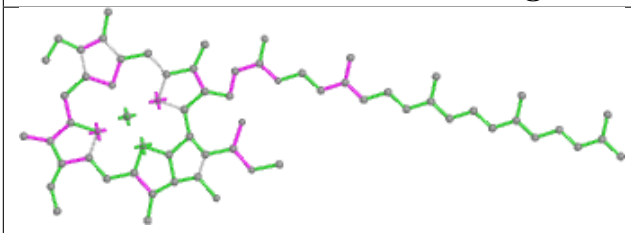


Torsions

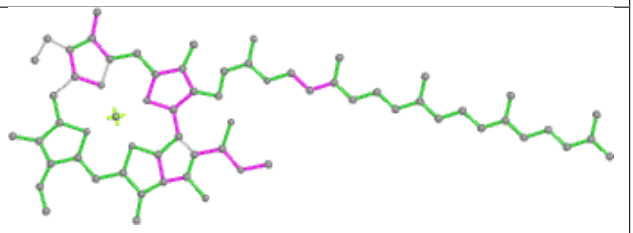


Rings

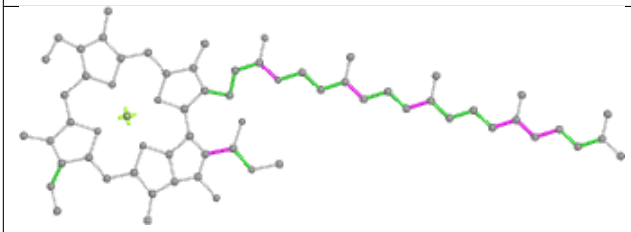
Ligand CLA B 525



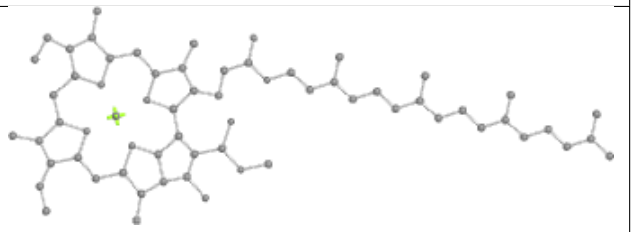
Bond lengths



Bond angles

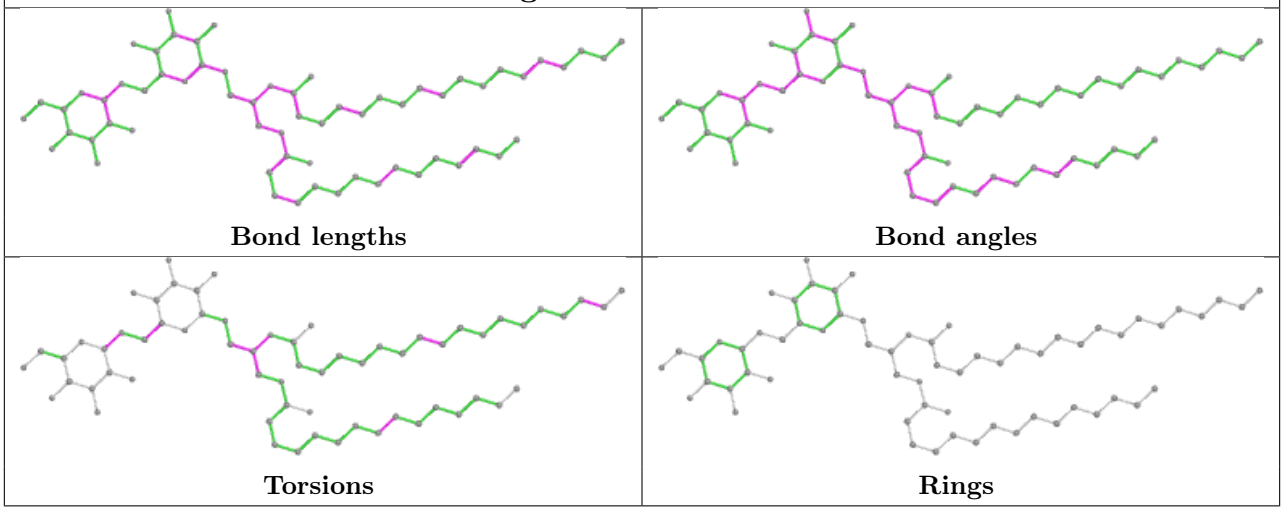


Torsions

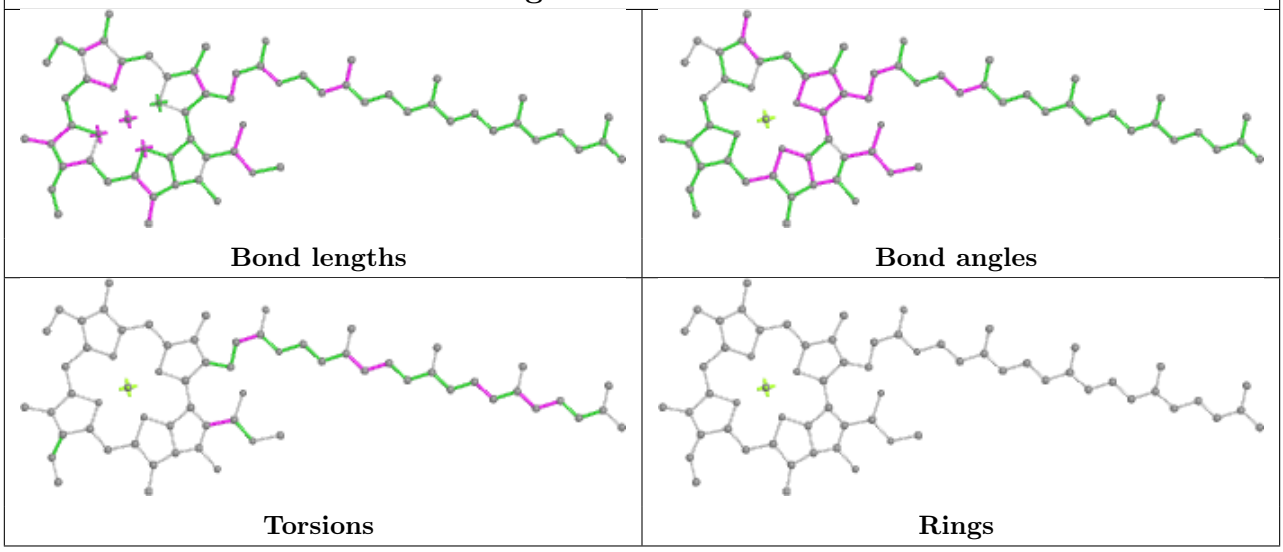


Rings

Ligand DGD D 362



Ligand CLA B 519



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	335/344 (97%)	0.08	18 (5%)	25	16	134, 163, 180, 180	0
2	B	485/510 (95%)	-0.04	16 (3%)	46	31	129, 158, 178, 180	0
3	C	448/461 (97%)	0.05	21 (4%)	31	19	136, 168, 180, 180	0
4	D	340/352 (96%)	0.21	25 (7%)	14	9	126, 154, 179, 180	0
5	E	77/83 (92%)	0.13	2 (2%)	56	40	138, 157, 179, 180	0
6	F	38/44 (86%)	0.16	5 (13%)	3	2	138, 157, 169, 177	0
7	H	65/65 (100%)	0.04	2 (3%)	49	33	139, 164, 177, 180	0
8	I	35/38 (92%)	0.26	4 (11%)	5	3	163, 172, 180, 180	0
9	J	34/40 (85%)	-0.43	0	100	100	141, 155, 169, 171	0
10	K	37/37 (100%)	-0.11	1 (2%)	54	38	156, 166, 179, 180	0
11	L	37/37 (100%)	0.23	3 (8%)	12	7	152, 168, 180, 180	0
12	M	34/36 (94%)	0.75	8 (23%)	0	0	153, 165, 180, 180	0
13	O	243/246 (98%)	0.37	20 (8%)	11	7	143, 174, 180, 180	0
14	T	30/32 (93%)	0.09	2 (6%)	17	10	152, 169, 180, 180	0
15	U	97/104 (93%)	0.16	4 (4%)	37	24	141, 160, 171, 179	0
16	V	137/137 (100%)	0.09	6 (4%)	34	21	136, 160, 171, 174	0
17	y	28/46 (60%)	-0.05	2 (7%)	16	9	158, 175, 180, 180	0
18	X	35/40 (87%)	-0.12	4 (11%)	5	3	144, 156, 174, 178	0
19	Z	62/62 (100%)	0.09	5 (8%)	12	7	166, 178, 180, 180	0
All	All	2597/2714 (95%)	0.10	148 (5%)	23	14	126, 164, 180, 180	0

The worst 5 of 148 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
12	M	1	MET	7.7

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Mol	Chain	Res	Type	RSRZ
10	K	46	ARG	5.5
12	M	2	GLU	5.1
4	D	241	GLU	5.0
2	B	85	GLY	5.0

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

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

6.3 Carbohydrates (i)

There are no 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
34	CA	O	273	1/1	0.17	0.68	180,180,180,180	0
25	BCR	B	530	40/40	0.42	0.86	173,180,180,180	0
26	LHG	C	476	37/49	0.52	0.43	143,176,180,180	0
30	SQD	F	224	45/54	0.53	0.81	152,179,180,180	0
27	LMG	I	220	43/55	0.61	0.86	158,180,180,180	0
29	LMT	T	226	35/35	0.64	0.95	156,180,180,180	0
32	PL9	D	357	55/55	0.65	0.44	146,153,161,162	0
27	LMG	M	217	42/55	0.65	0.72	166,180,180,180	0
25	BCR	J	115	40/40	0.66	0.73	171,180,180,180	0
27	LMG	D	360	48/55	0.66	0.52	140,169,176,177	0
21	CLA	B	526	65/65	0.67	0.50	167,177,180,180	0
29	LMT	D	363	31/35	0.68	0.68	170,180,180,180	0
27	LMG	A	373	51/55	0.70	0.44	169,174,180,180	0
28	DGD	D	362	63/66	0.71	0.55	177,180,180,180	0
27	LMG	C	494	45/55	0.71	0.58	168,180,180,180	0
28	DGD	C	474	56/66	0.71	0.42	158,180,180,180	0
29	LMT	O	274	35/35	0.72	0.39	180,180,180,180	0
27	LMG	J	492	48/55	0.73	0.50	155,175,180,180	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
29	LMT	A	376	35/35	0.73	0.46	162,180,180,180	0
30	SQD	L	213	47/54	0.73	0.58	155,178,180,180	0
21	CLA	C	482	65/65	0.73	0.46	148,179,180,180	0
21	CLA	B	511	65/65	0.73	0.55	148,179,180,180	0
29	LMT	I	274	35/35	0.74	0.62	170,180,180,180	0
30	SQD	C	475	51/54	0.74	0.43	156,172,180,180	0
29	LMT	D	536	35/35	0.74	0.38	168,173,180,180	0
21	CLA	A	366	65/65	0.76	0.40	152,162,164,166	0
25	BCR	B	529	40/40	0.76	0.55	166,169,173,174	0
28	DGD	C	492	62/66	0.77	0.36	153,171,180,180	0
29	LMT	B	535	35/35	0.77	0.72	163,180,180,180	0
25	BCR	C	490	40/40	0.78	0.51	164,169,180,180	0
28	DGD	A	375	52/66	0.78	0.64	164,180,180,180	0
28	DGD	B	533	66/66	0.78	0.35	166,179,180,180	0
21	CLA	A	363	65/65	0.78	0.43	154,161,175,177	0
25	BCR	B	527	40/40	0.78	0.73	161,169,176,178	0
25	BCR	C	489	40/40	0.78	0.32	152,169,171,171	0
25	BCR	Z	116	40/40	0.79	0.43	163,165,170,171	0
21	CLA	C	488	65/65	0.80	0.33	169,176,179,180	0
25	BCR	X	107	40/40	0.80	0.55	154,158,161,163	0
21	CLA	B	524	65/65	0.80	0.52	157,180,180,180	0
28	DGD	C	493	66/66	0.81	0.35	159,174,180,180	0
34	CA	K	56	1/1	0.81	0.42	180,180,180,180	0
27	LMG	B	531	49/55	0.81	0.35	160,167,175,176	0
28	DGD	B	528	58/66	0.82	0.36	126,136,172,173	0
25	BCR	A	369	40/40	0.82	0.41	164,171,178,178	0
21	CLA	B	519	65/65	0.83	0.33	152,157,158,159	0
21	CLA	C	486	65/65	0.83	0.32	143,180,180,180	0
27	LMG	D	359	46/55	0.83	0.33	142,163,180,180	0
21	CLA	B	525	65/65	0.84	0.36	148,167,180,180	0
25	BCR	J	112	40/40	0.84	0.30	157,160,172,173	0
21	CLA	D	356	65/65	0.84	0.34	149,154,162,164	0
21	CLA	C	487	65/65	0.85	0.34	176,180,180,180	0
21	CLA	C	481	65/65	0.86	0.28	152,180,180,180	0
21	CLA	D	354	65/65	0.86	0.37	135,154,164,168	0
21	CLA	C	478	65/65	0.87	0.32	153,155,166,170	0
21	CLA	C	483	65/65	0.87	0.38	164,180,180,180	0
30	SQD	D	361	43/54	0.87	0.29	160,173,180,180	0
21	CLA	B	517	65/65	0.87	0.27	144,160,164,167	0
21	CLA	C	477	65/65	0.88	0.31	163,169,179,180	0
25	BCR	D	358	40/40	0.88	0.29	135,151,162,162	0
21	CLA	A	364	65/65	0.88	0.31	126,141,175,177	0

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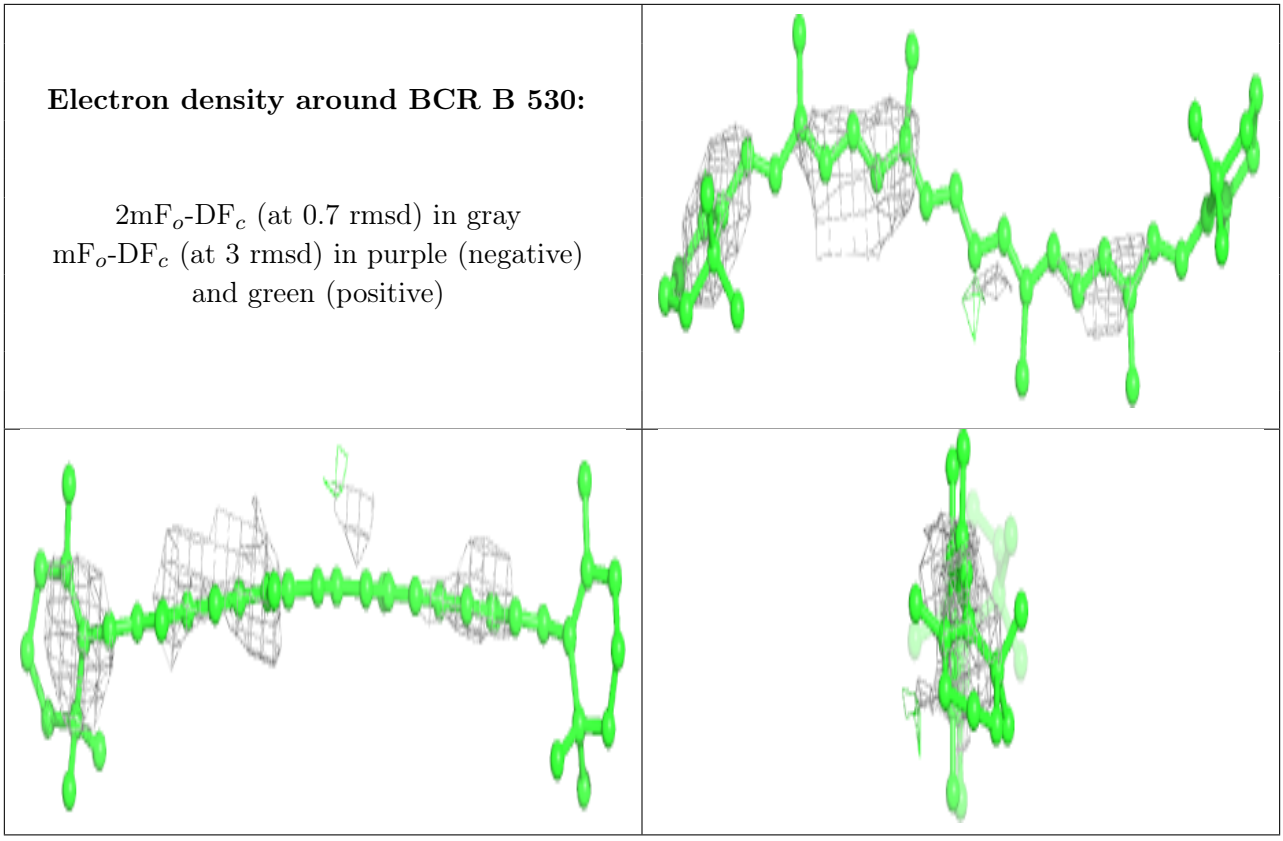
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
21	CLA	C	479	65/65	0.88	0.26	162,180,180,180	0
21	CLA	C	484	65/65	0.88	0.28	168,177,180,180	0
21	CLA	C	485	65/65	0.88	0.30	170,176,178,180	0
28	DGD	C	491	53/66	0.88	0.28	155,160,166,168	0
26	LHG	A	371	39/49	0.88	0.30	156,175,179,180	0
21	CLA	B	516	65/65	0.89	0.27	152,155,180,180	0
24	OEC	A	368	5/9	0.89	0.24	118,138,151,154	0
21	CLA	A	362	65/65	0.89	0.28	149,154,159,163	0
21	CLA	B	518	65/65	0.90	0.33	150,164,167,169	0
21	CLA	C	480	65/65	0.90	0.26	151,159,180,180	0
22	PHO	A	365	64/64	0.91	0.30	143,154,162,164	0
34	CA	F	225	1/1	0.91	0.42	142,142,142,142	0
21	CLA	B	514	65/65	0.91	0.30	139,146,168,169	0
21	CLA	K	483	65/65	0.91	0.39	155,160,174,176	0
21	CLA	B	515	65/65	0.92	0.32	142,162,168,170	0
22	PHO	D	355	64/64	0.92	0.40	140,162,169,171	0
23	MES	A	367	12/12	0.92	0.21	136,144,152,153	0
21	CLA	B	522	65/65	0.92	0.29	134,144,163,165	0
21	CLA	B	521	65/65	0.93	0.26	149,169,175,179	0
33	HEM	F	85	43/43	0.93	0.40	154,159,162,163	0
21	CLA	B	512	65/65	0.93	0.24	142,165,172,173	0
21	CLA	B	513	65/65	0.93	0.27	133,170,171,172	0
21	CLA	B	520	65/65	0.93	0.38	150,162,165,167	0
21	CLA	B	523	65/65	0.94	0.23	134,142,169,170	0
33	HEM	V	164	43/43	0.95	0.29	89,102,122,129	0
20	FE2	A	361	1/1	0.95	0.17	160,160,160,160	0
31	BCT	D	353	4/4	0.97	0.22	169,170,170,171	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.

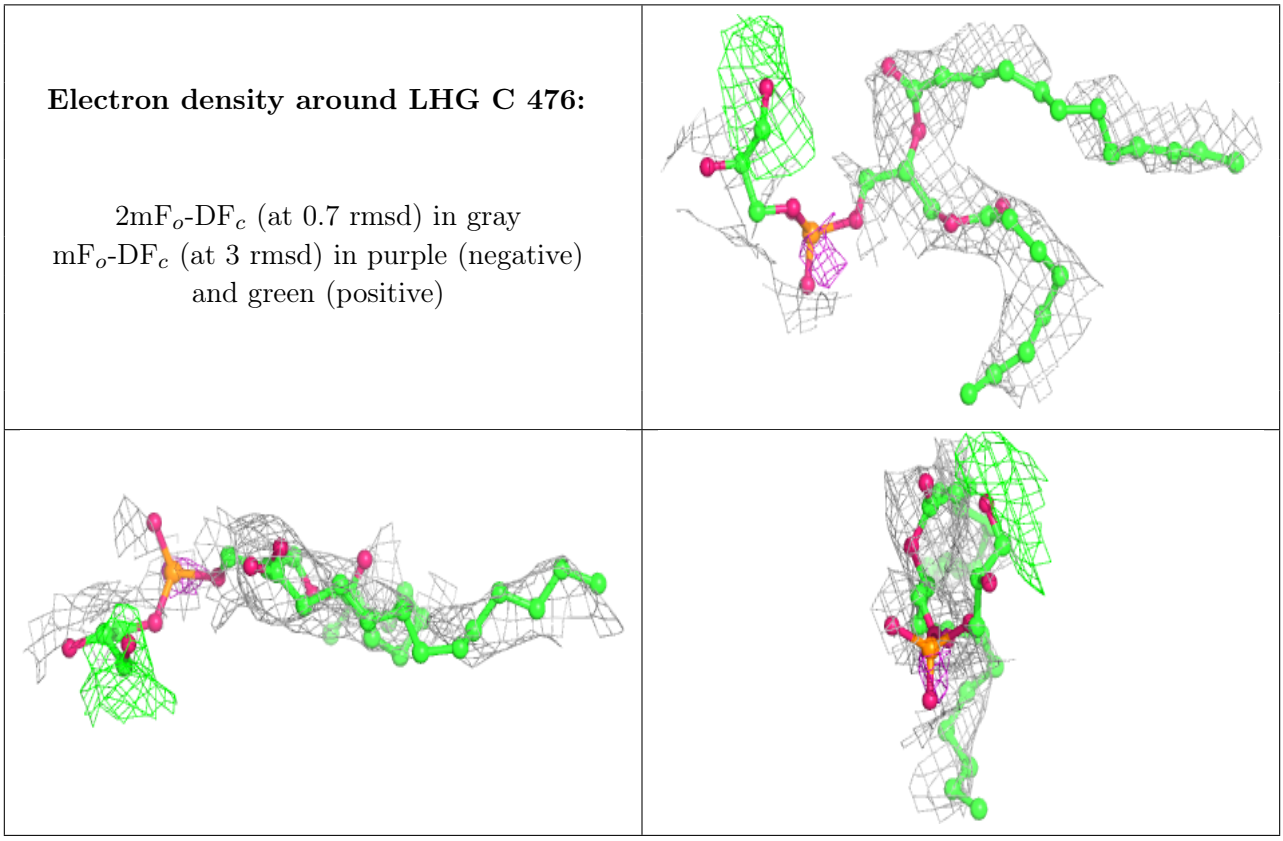
Electron density around BCR B 530:

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



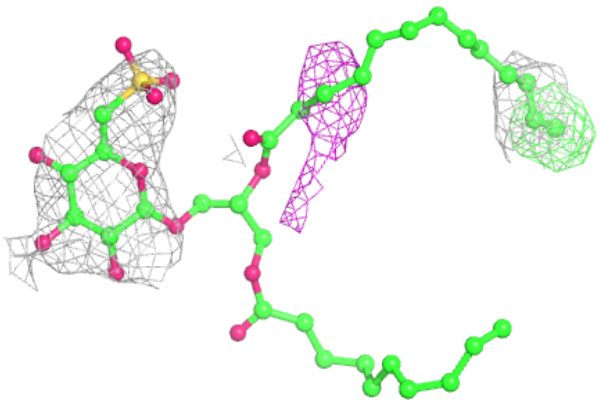
Electron density around LHG C 476:

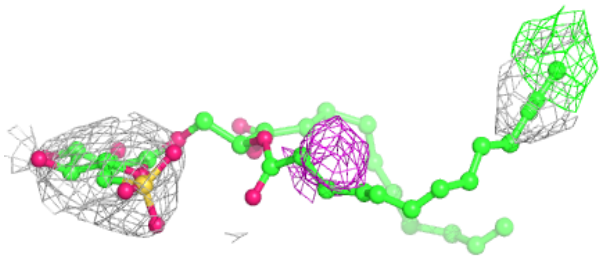
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

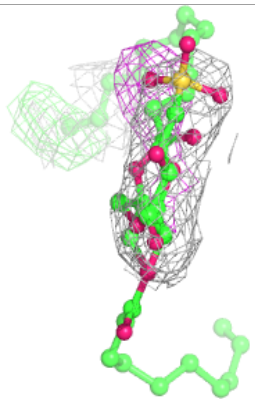


Electron density around SQD F 224:

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

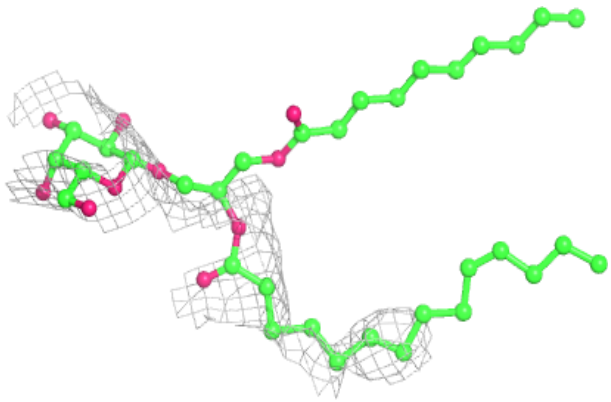


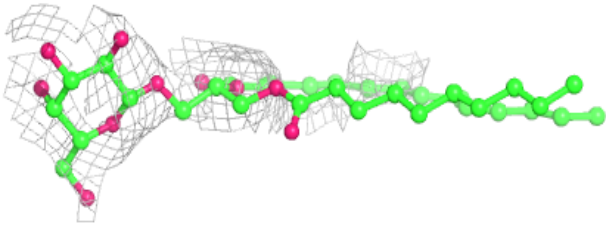


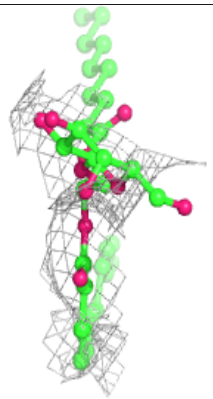


Electron density around LMG I 220:

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

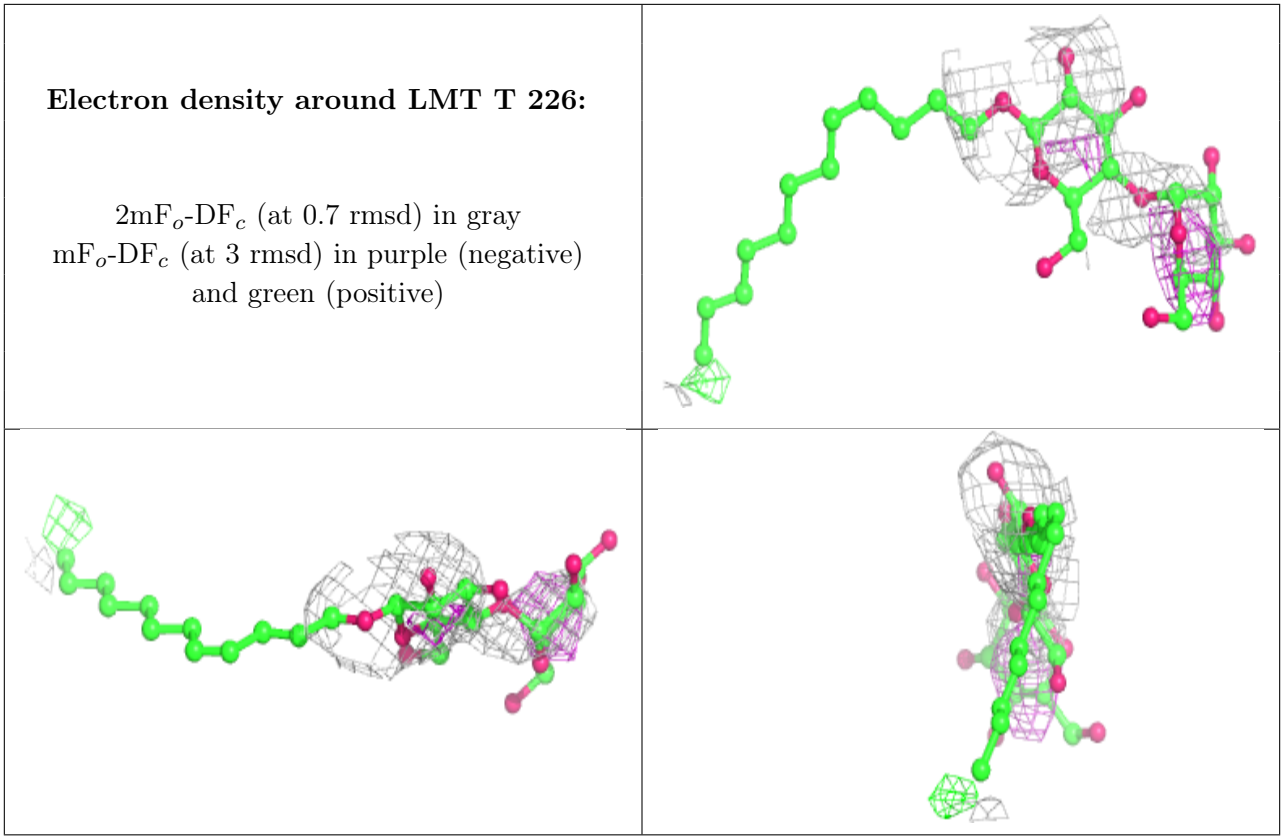






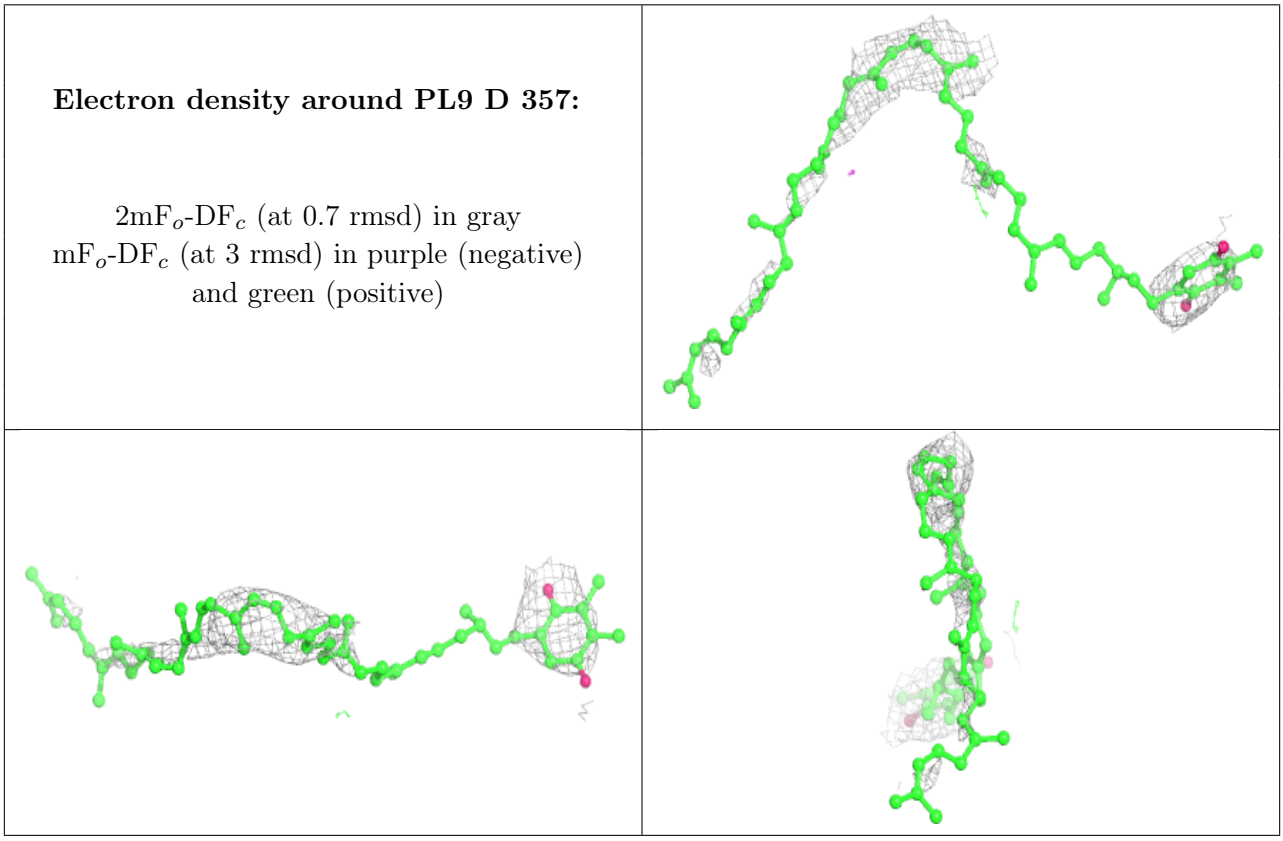
Electron density around LMT T 226:

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



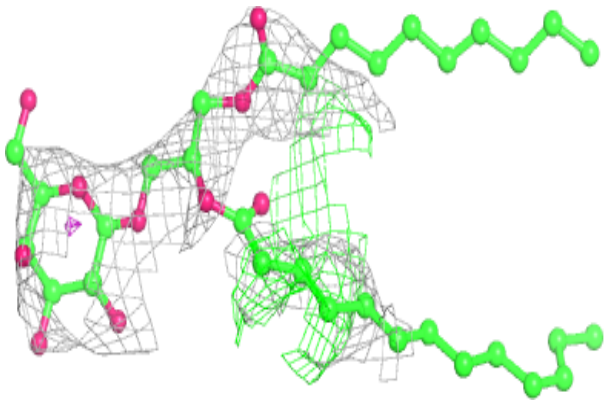
Electron density around PL9 D 357:

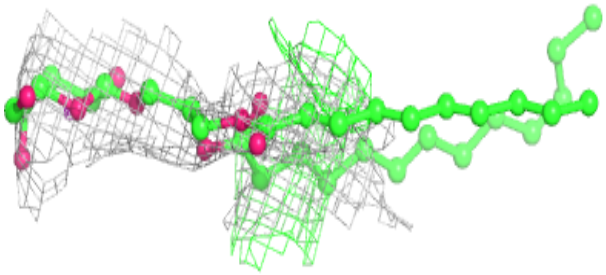
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

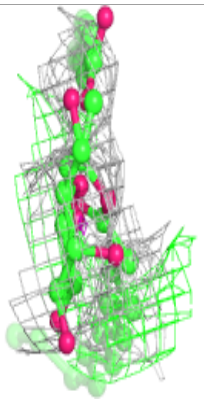


Electron density around LMG M 217:

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

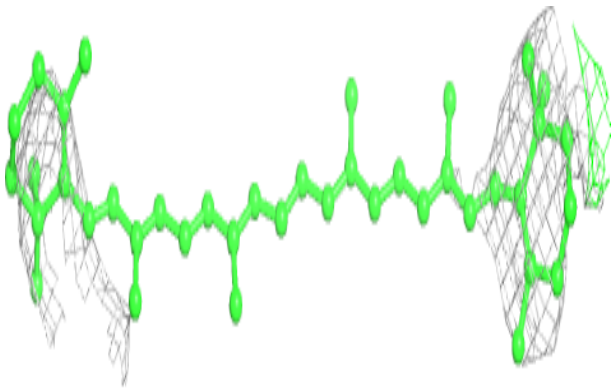


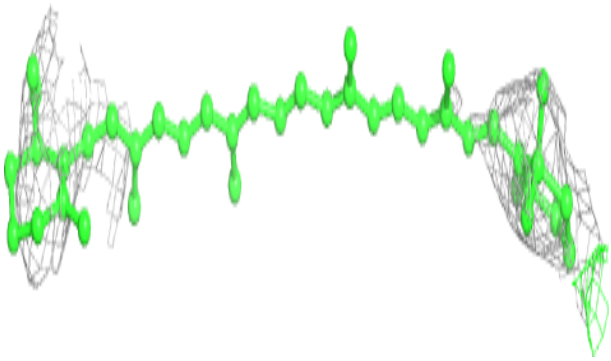


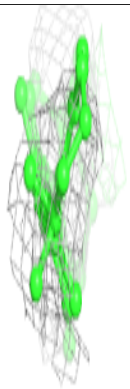


Electron density around BCR J 115:

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

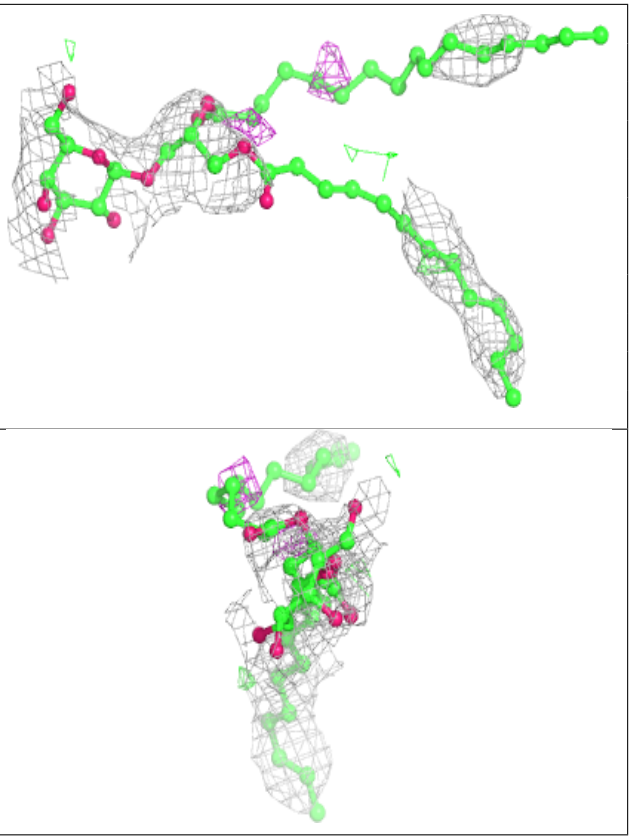


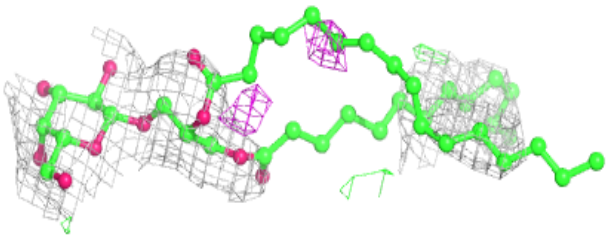




Electron density around LMG D 360:

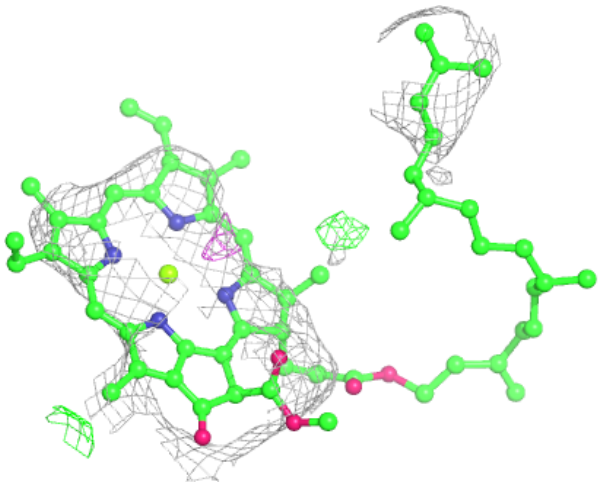
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

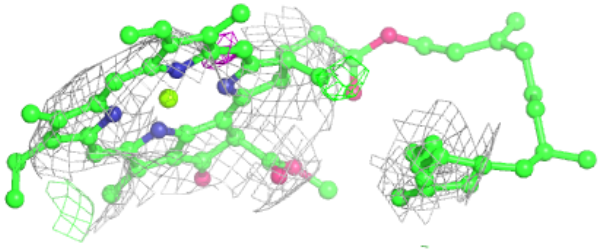


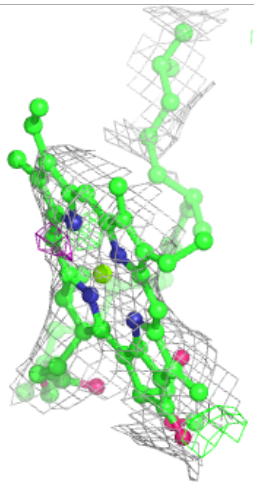


Electron density around CLA B 526:

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

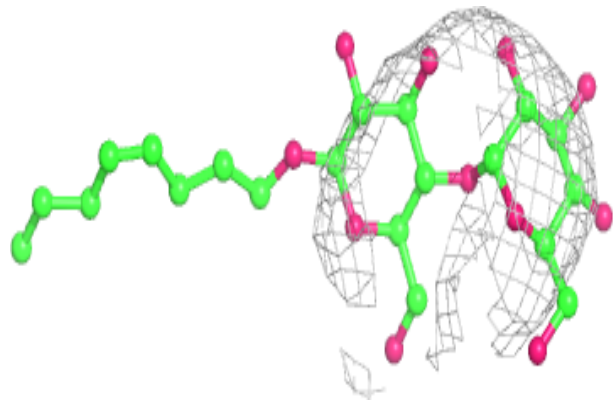


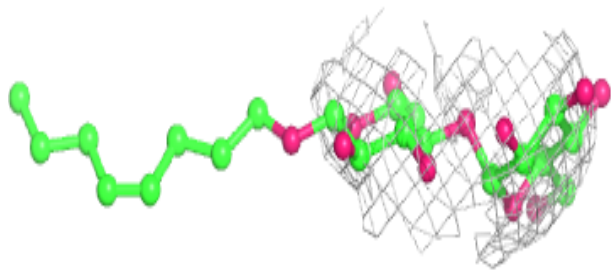


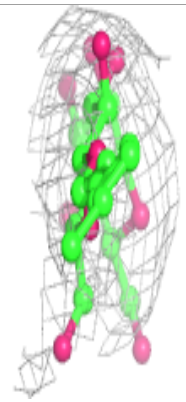


Electron density around LMT D 363:

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

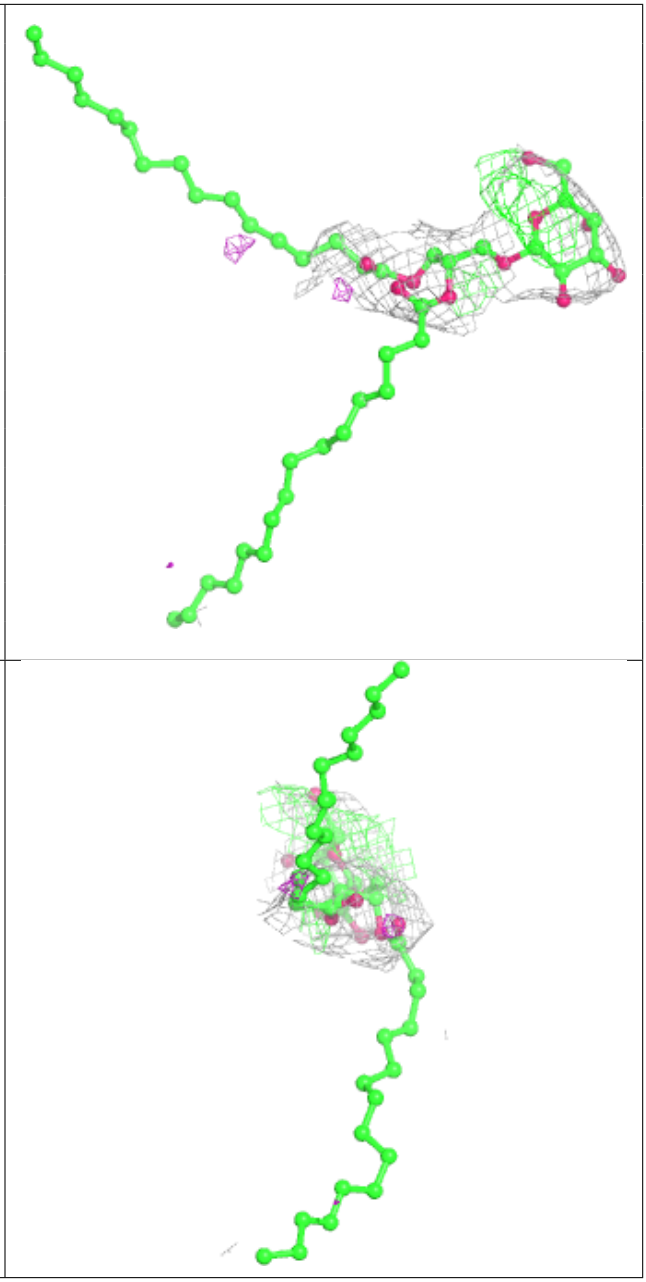






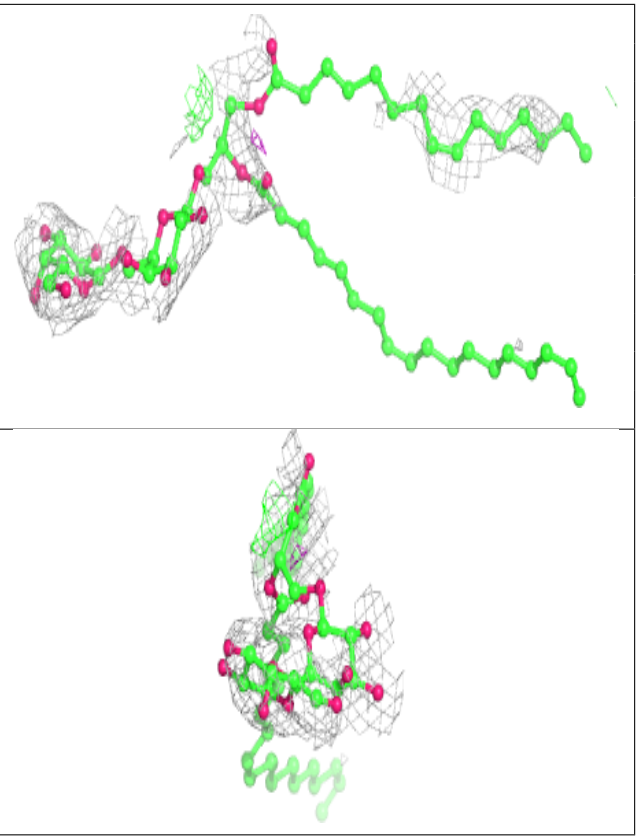
Electron density around LMG A 373:

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



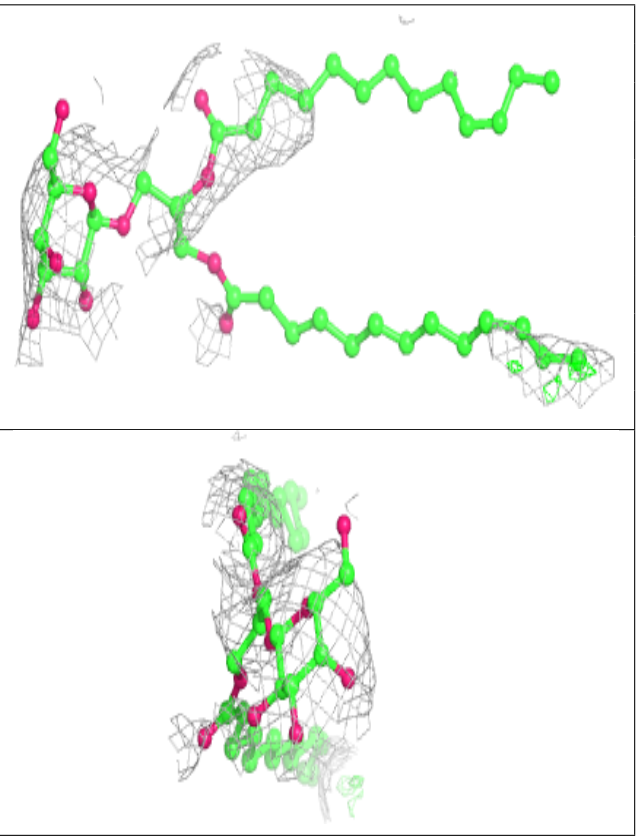
Electron density around DGD D 362:

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



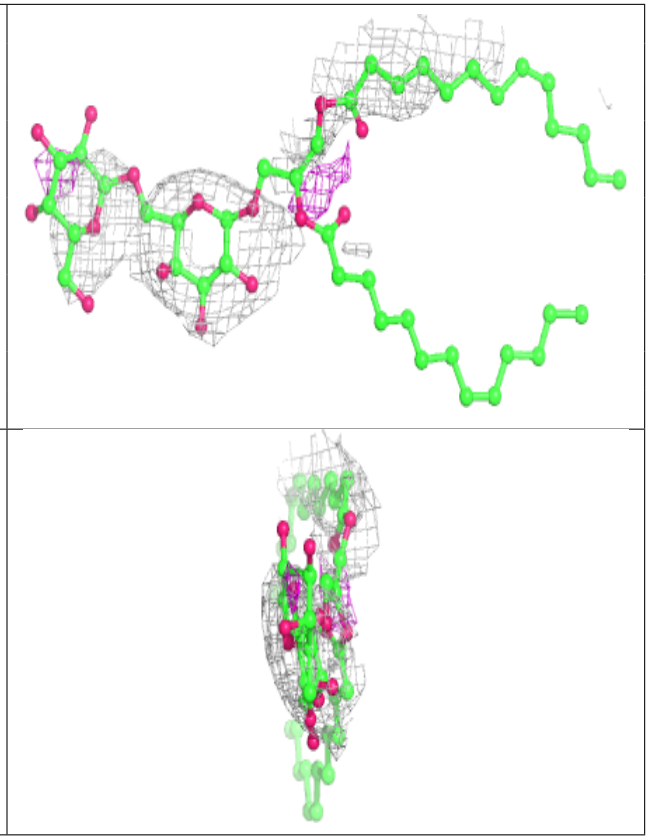
Electron density around LMG C 494:

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



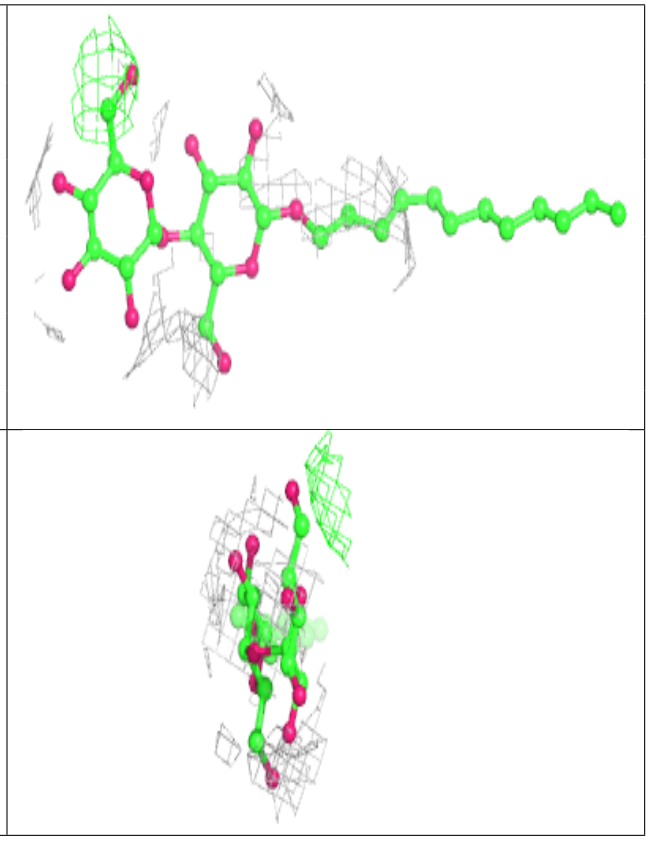
Electron density around DGD C 474:

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



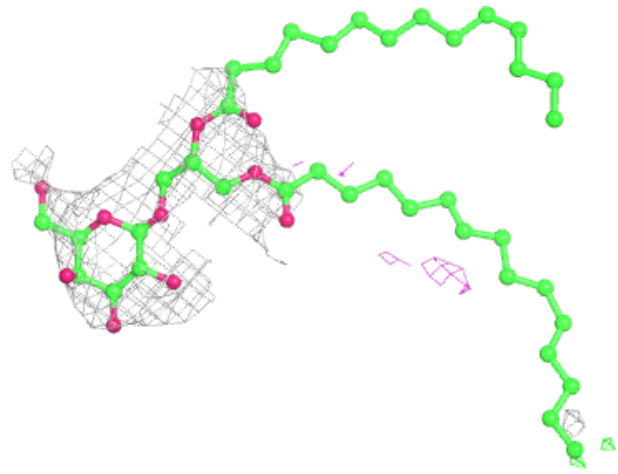
Electron density around LMT O 274:

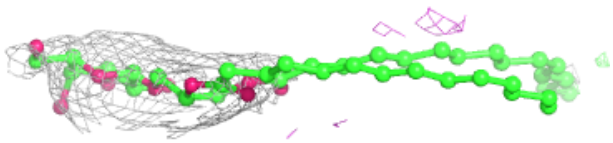
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

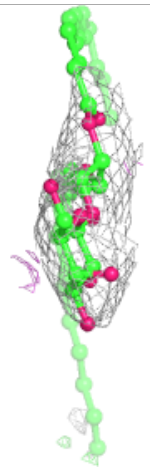


Electron density around LMG J 492:

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

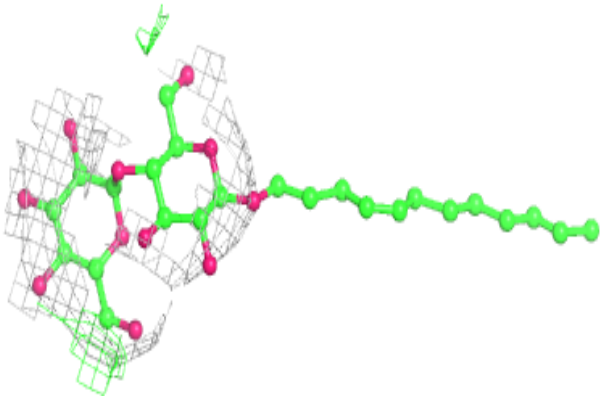


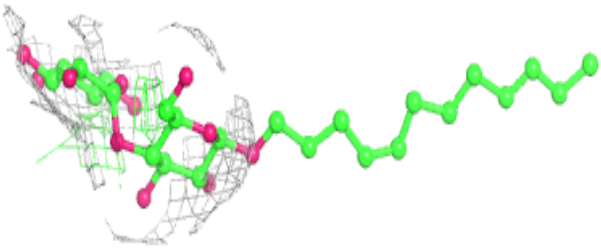


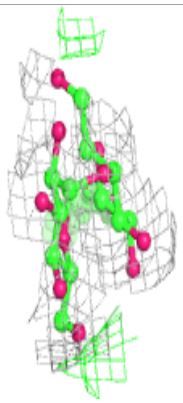


Electron density around LMT A 376:

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

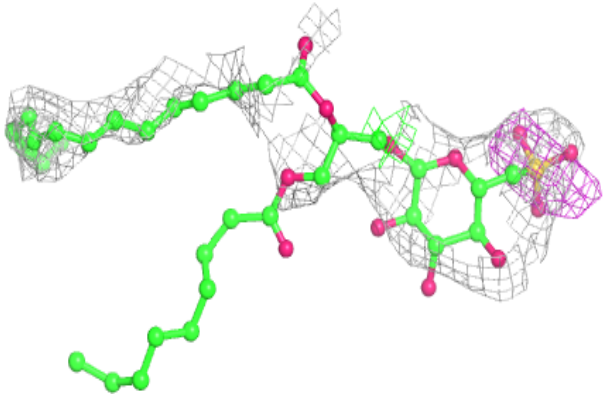


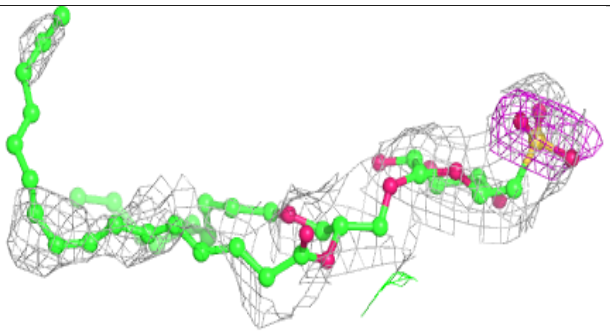


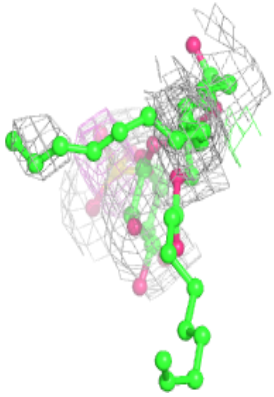


Electron density around SQD L 213:

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

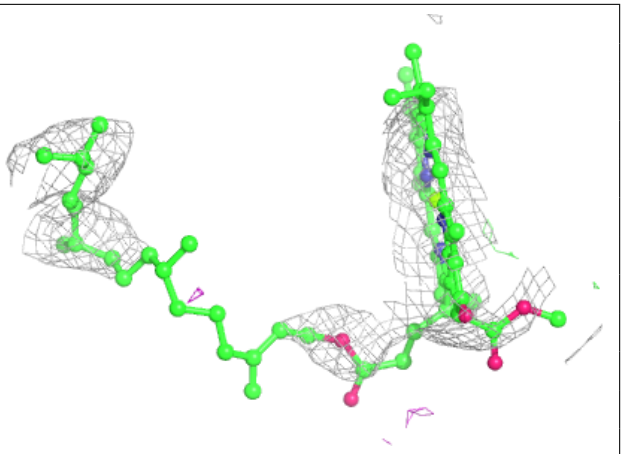


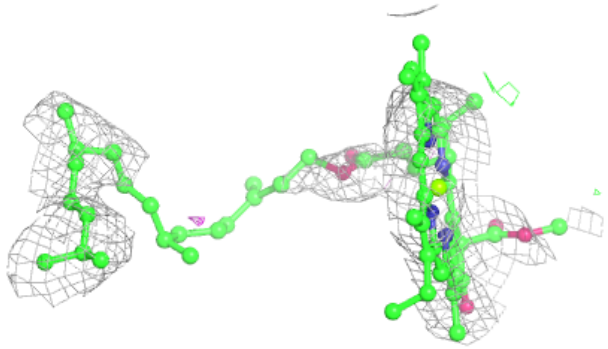


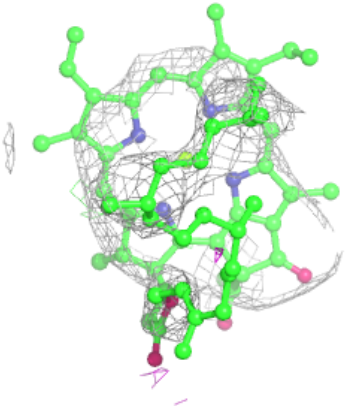


Electron density around CLA C 482:

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

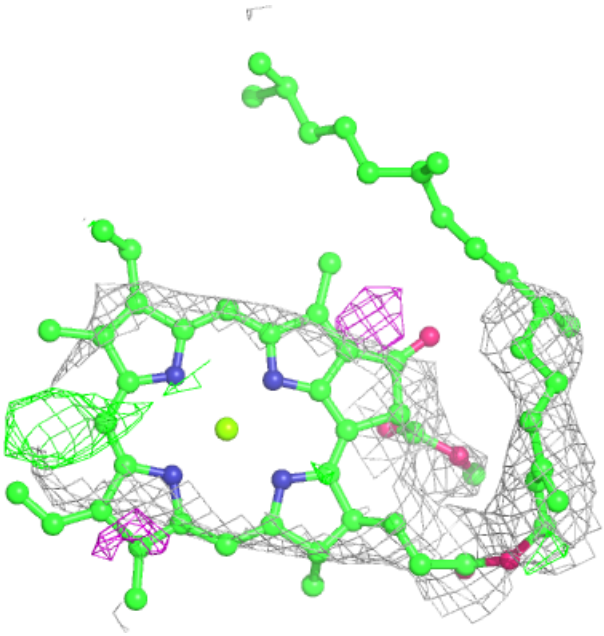


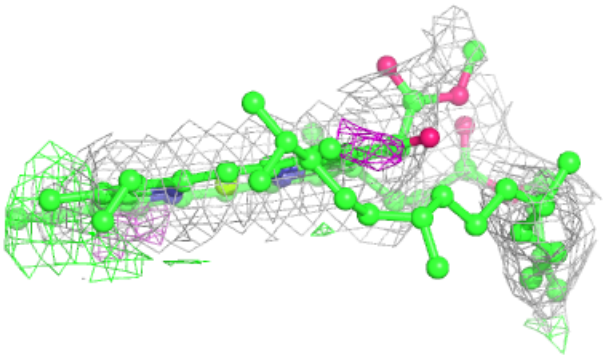


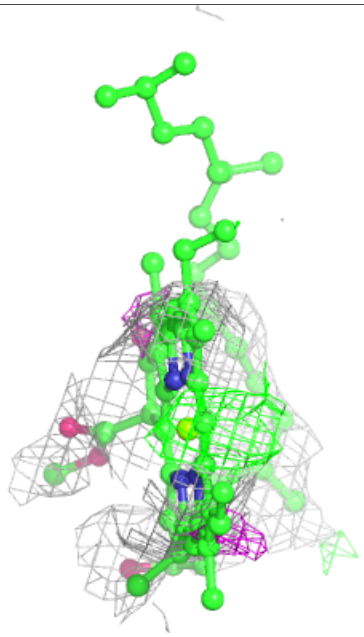


Electron density around CLA B 511:

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

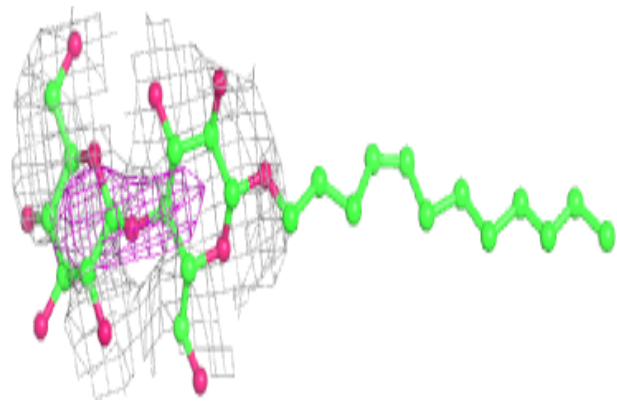


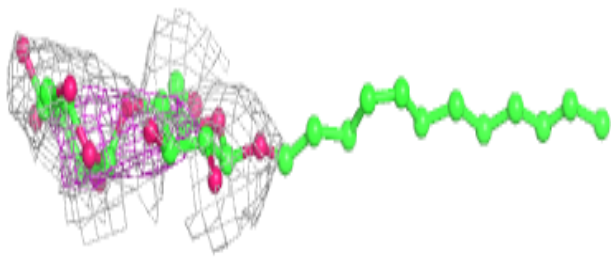


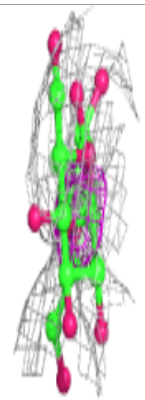


Electron density around LMT I 274:

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

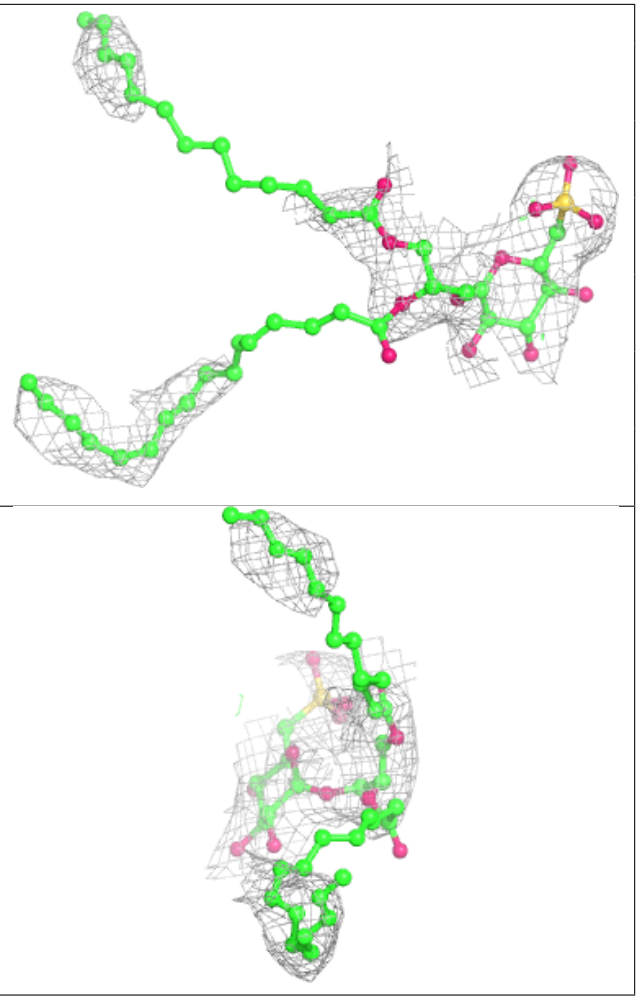






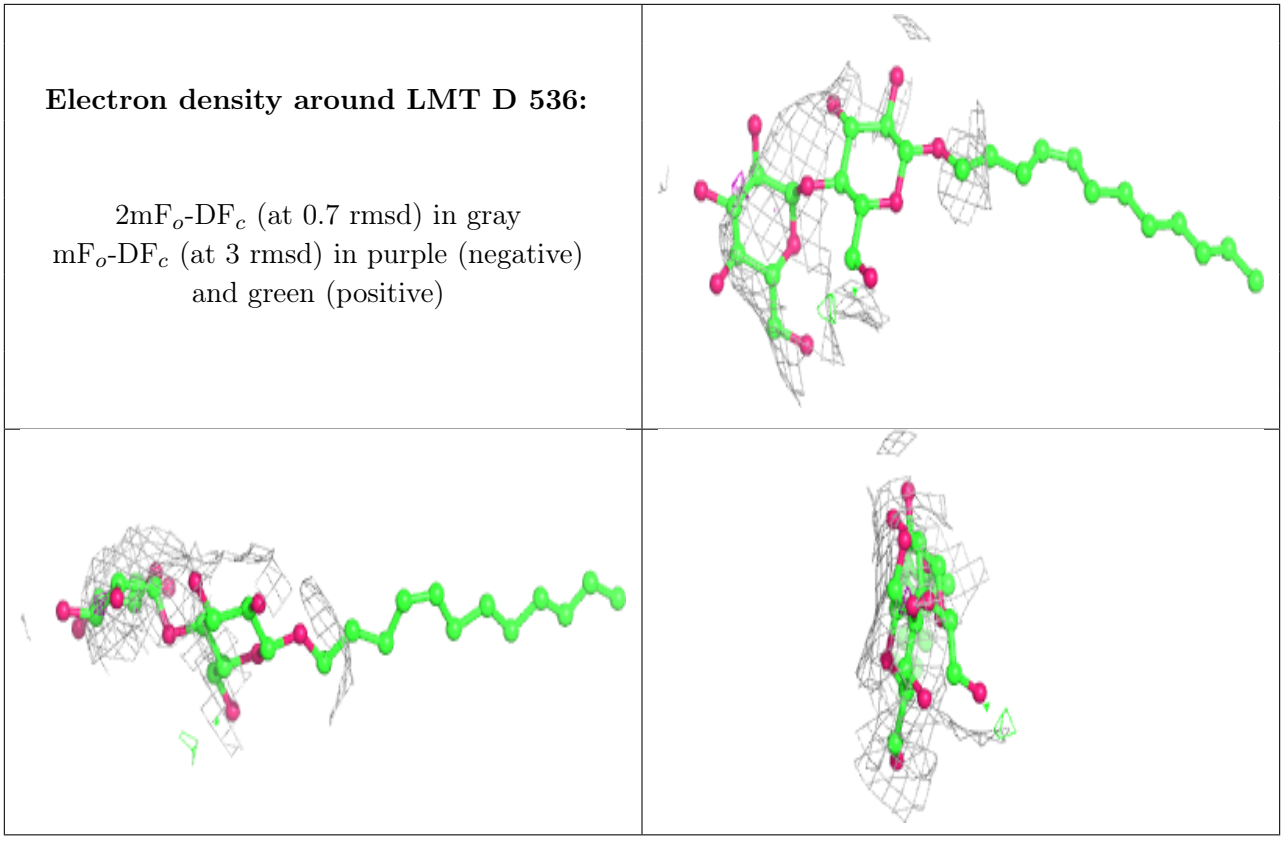
Electron density around SQD C 475:

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



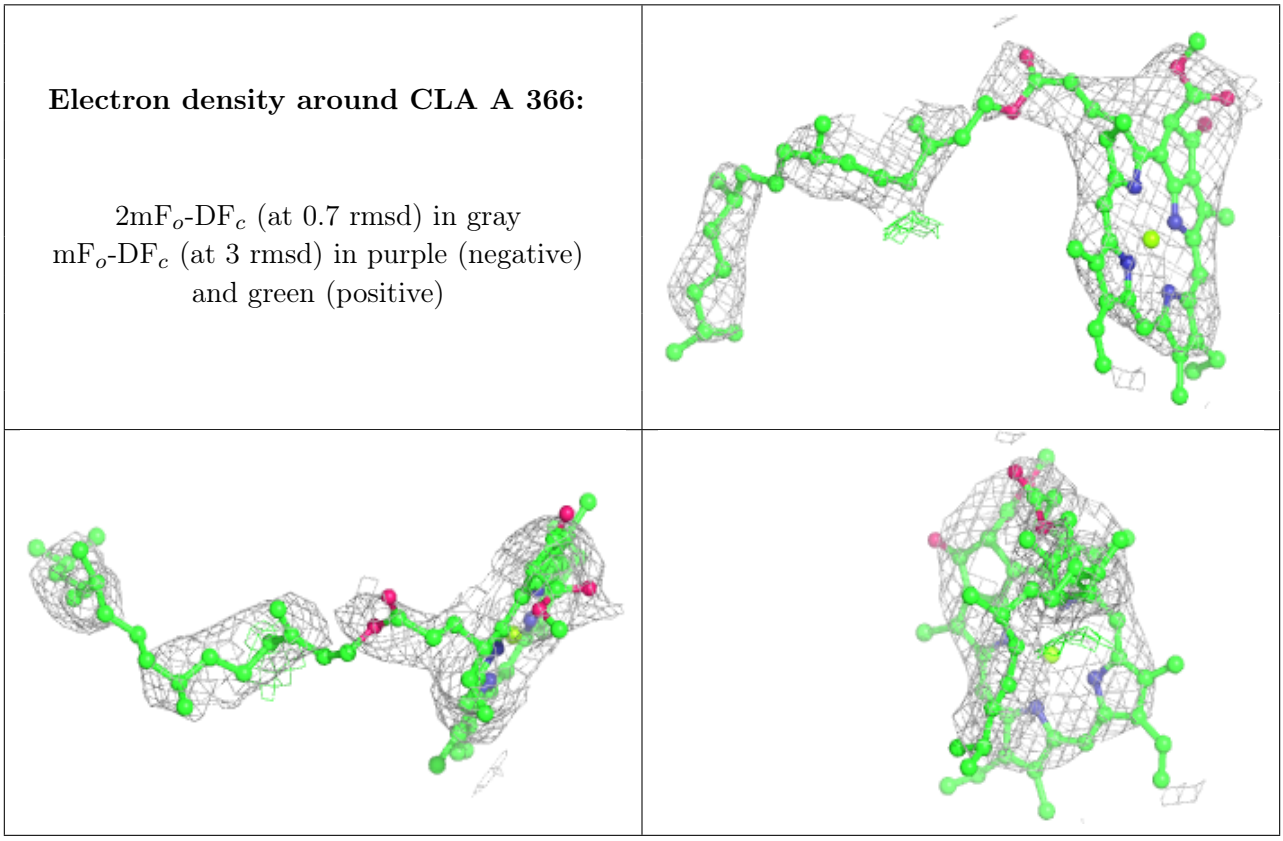
Electron density around LMT D 536:

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



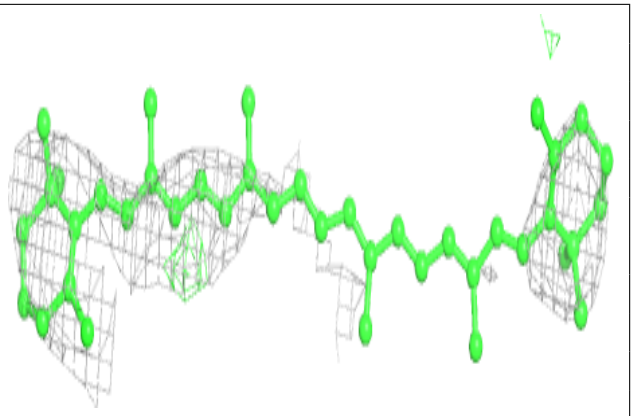
Electron density around CLA A 366:

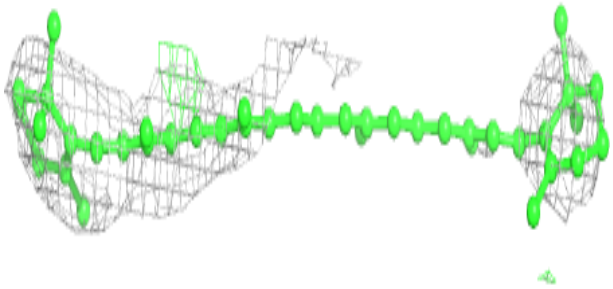
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

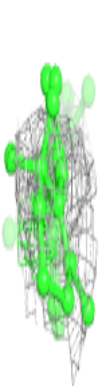


Electron density around BCR B 529:

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

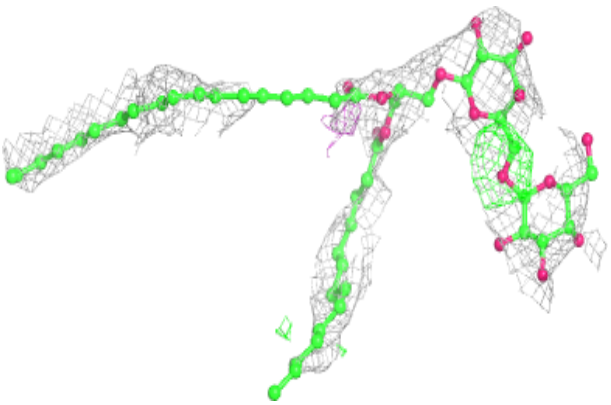


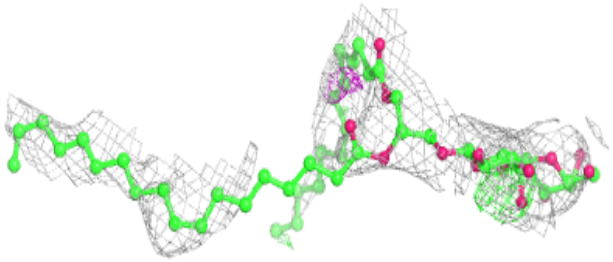


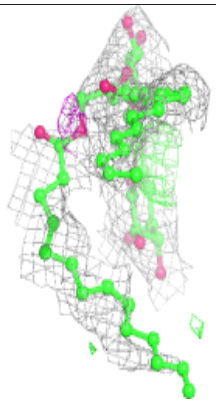


Electron density around DGD C 492:

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

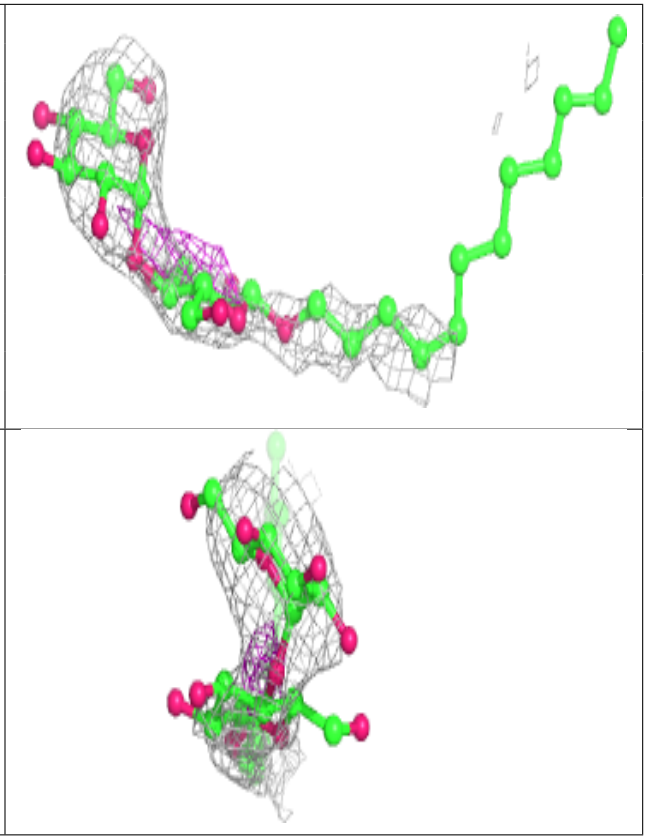


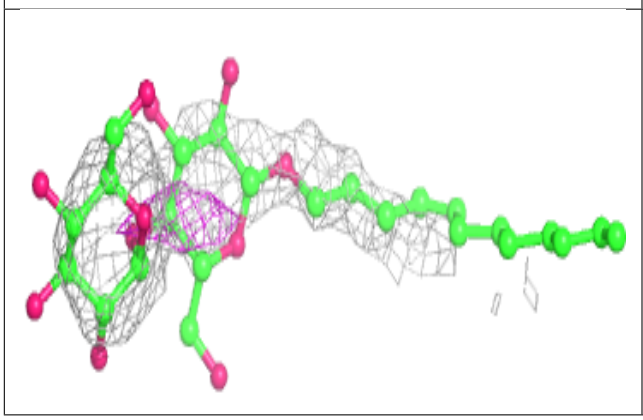




Electron density around LMT B 535:

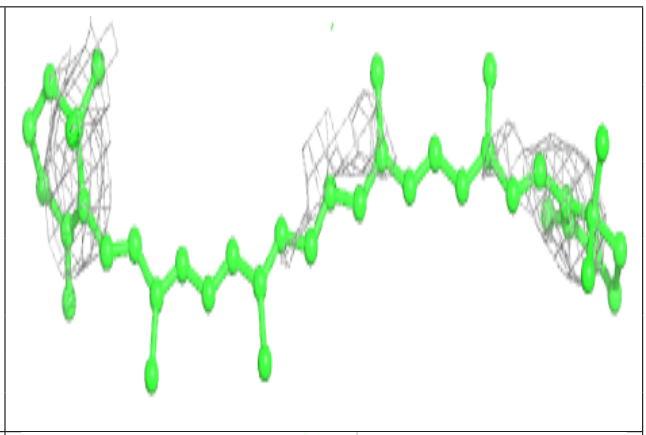
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

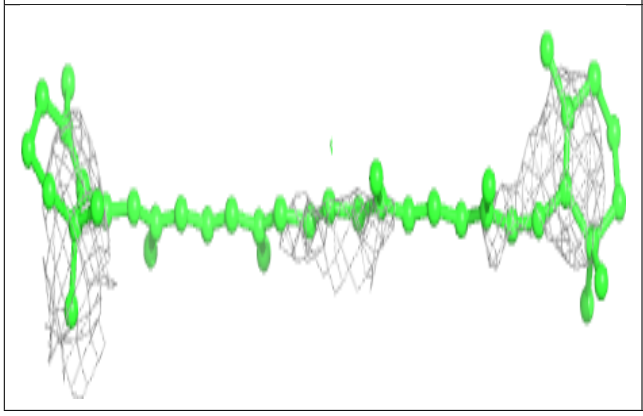




Electron density around BCR C 490:

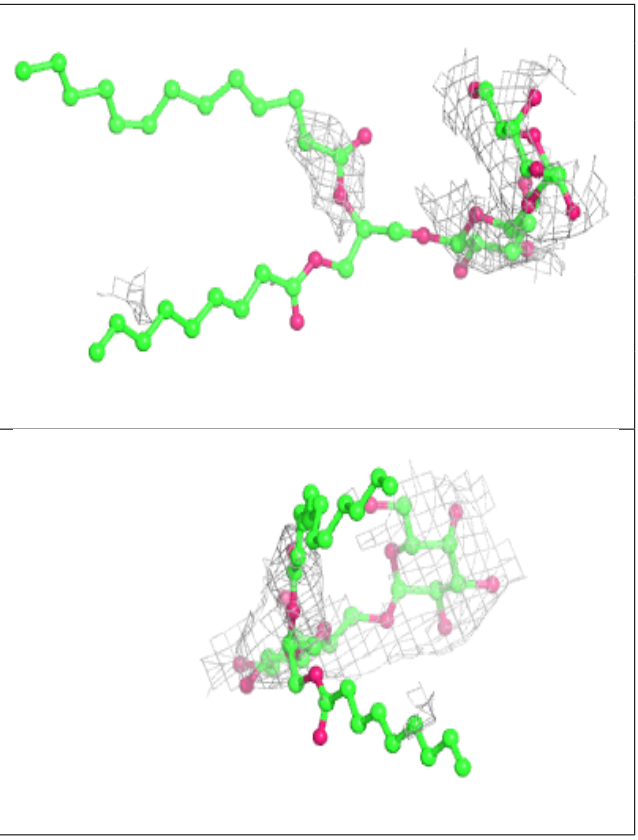
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





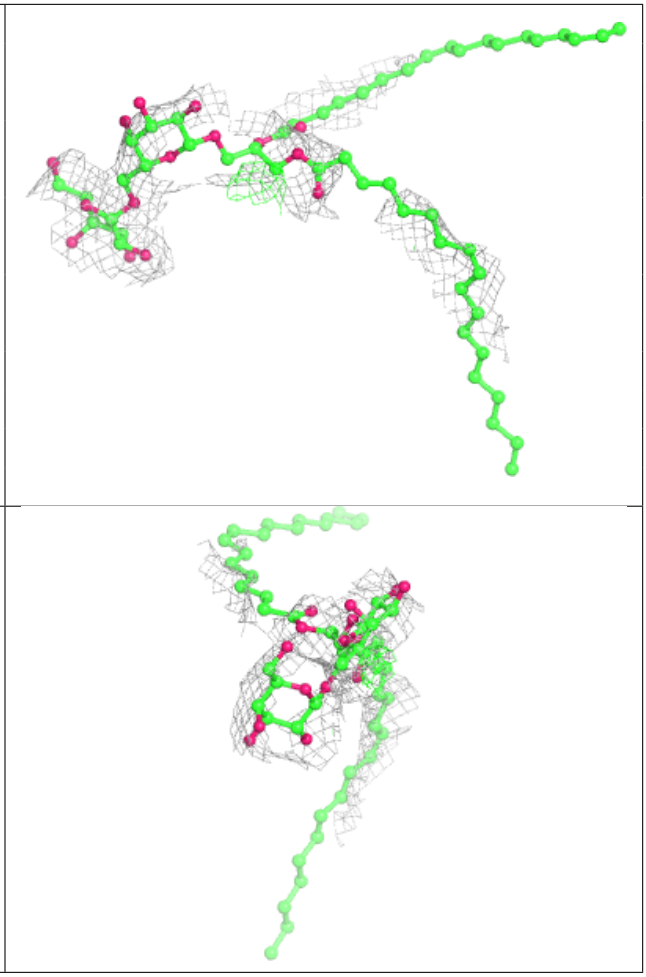
Electron density around DGD A 375:

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



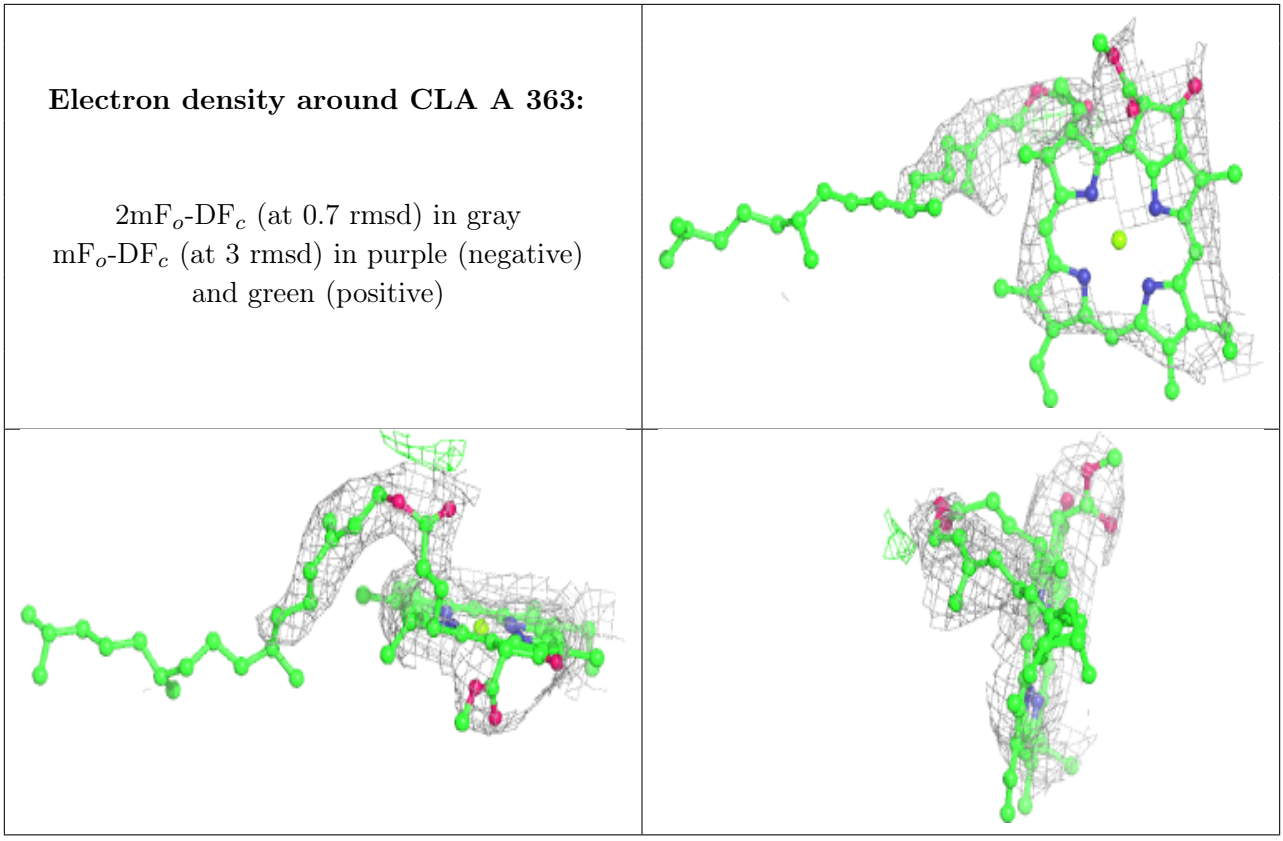
Electron density around DGD B 533:

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



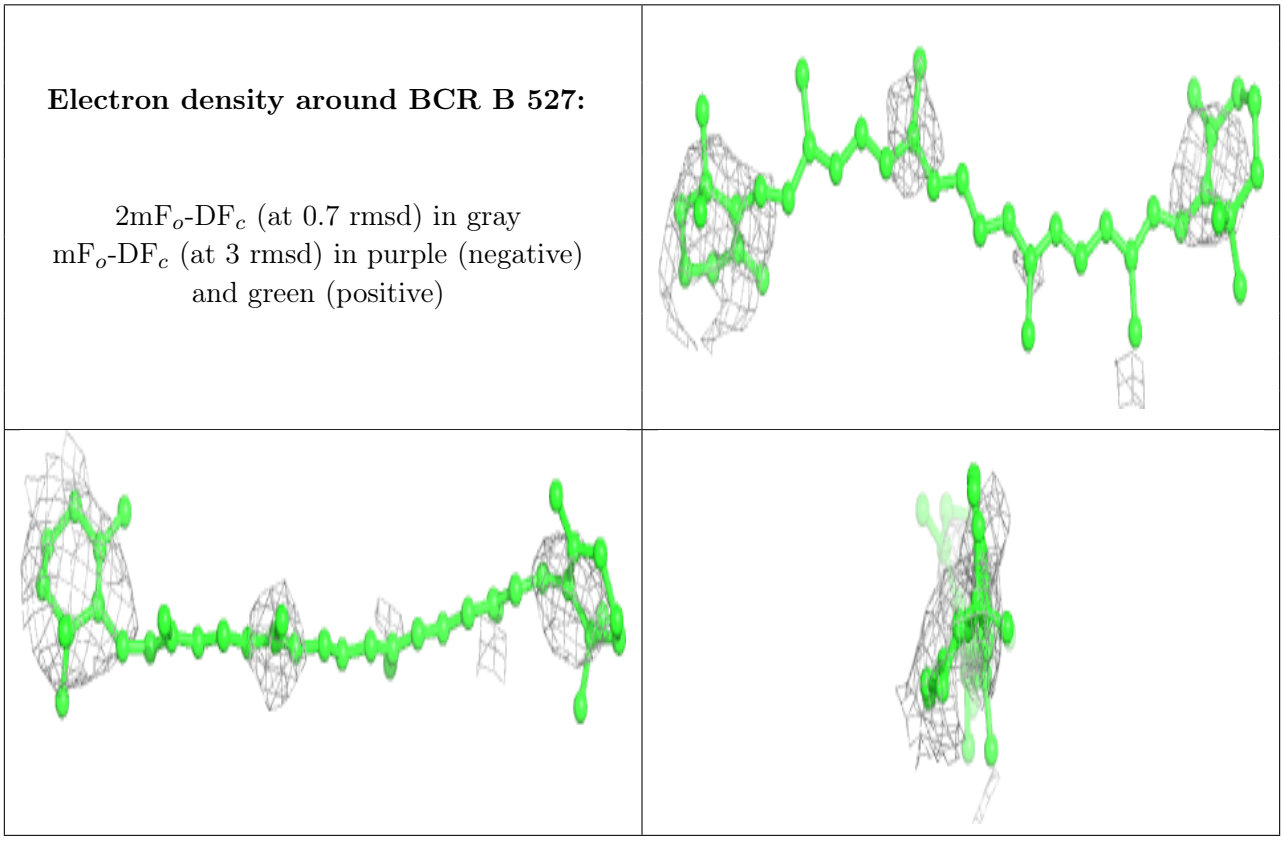
Electron density around CLA A 363:

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



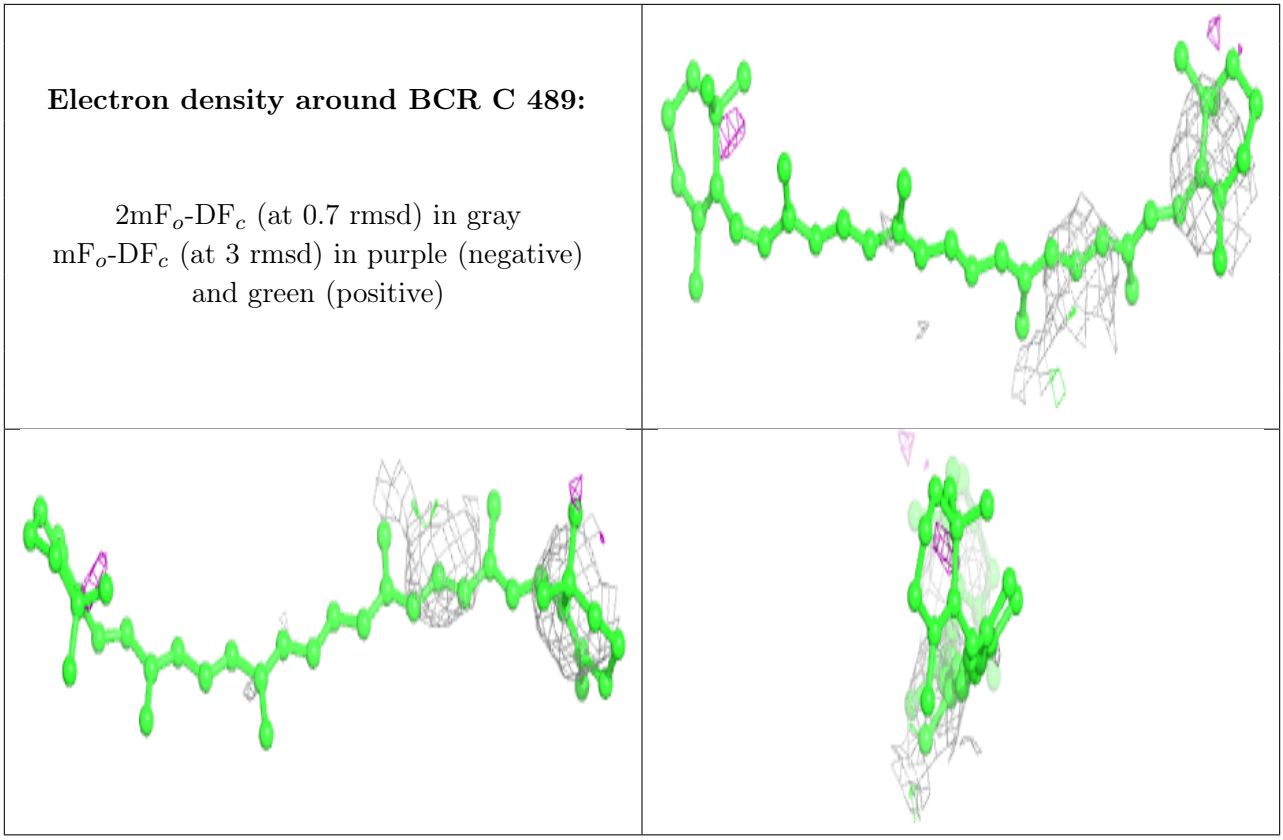
Electron density around BCR B 527:

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



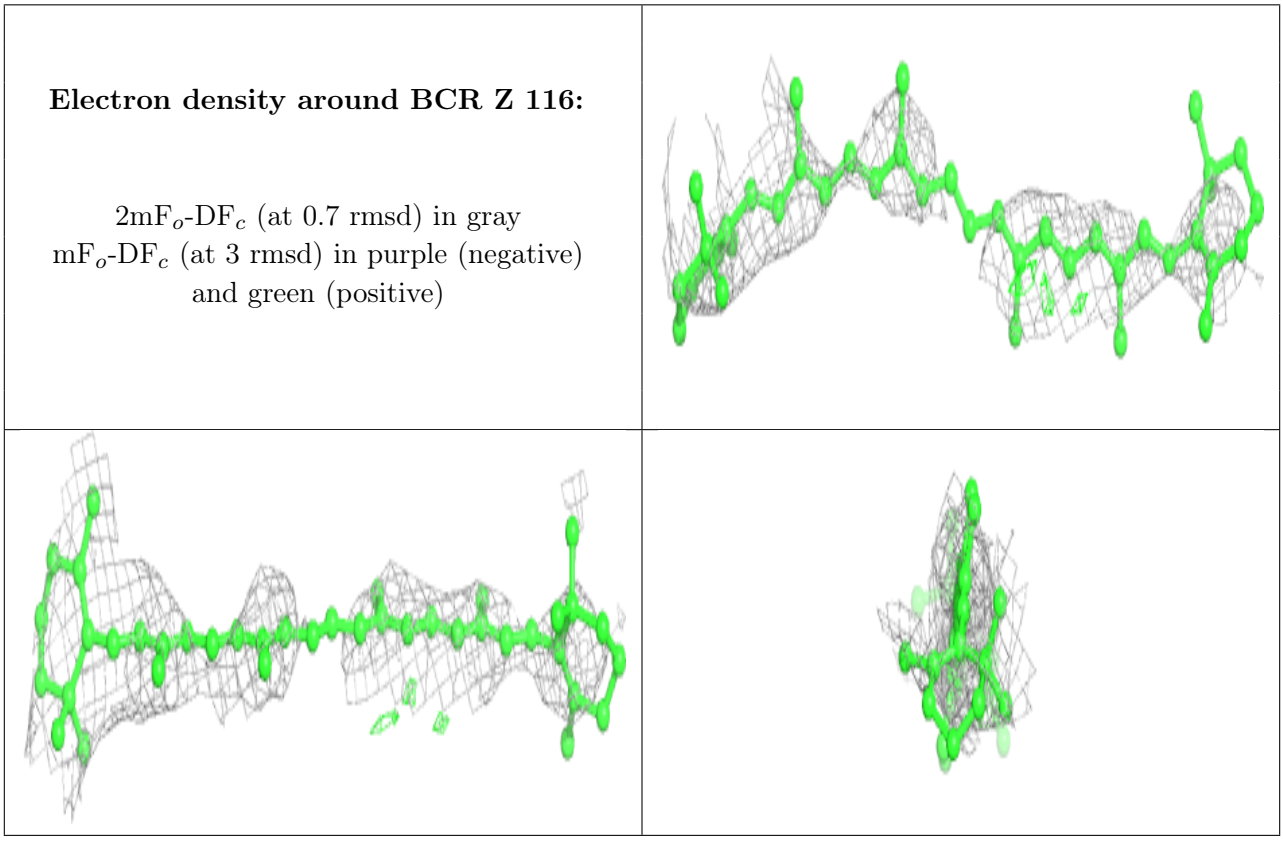
Electron density around BCR C 489:

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



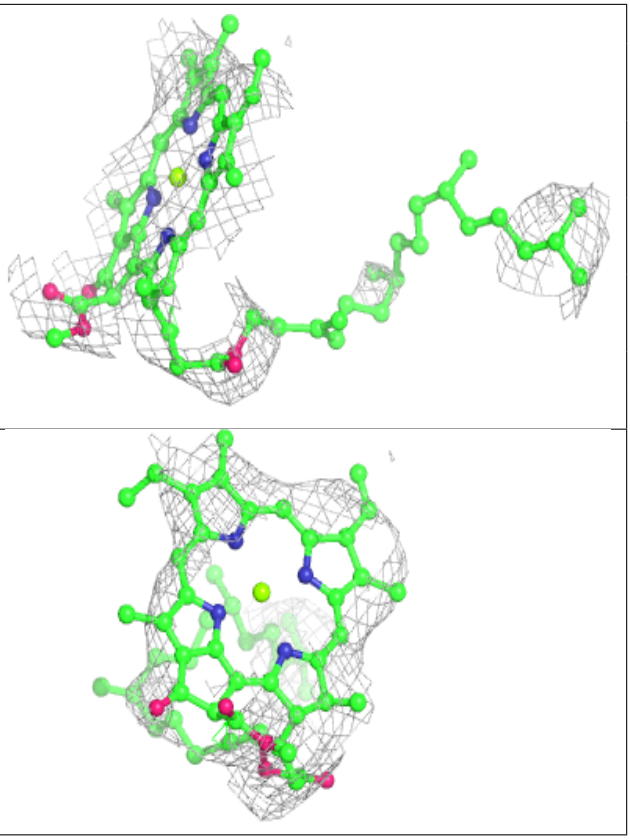
Electron density around BCR Z 116:

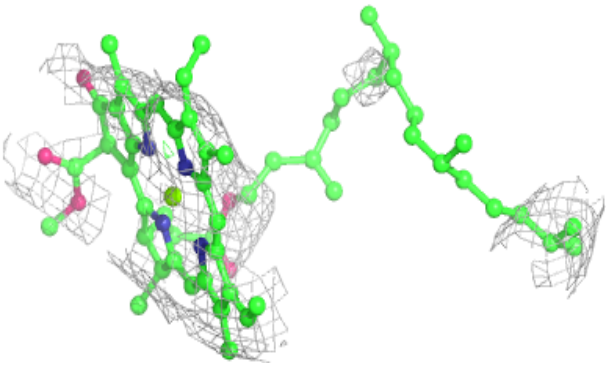
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA C 488:

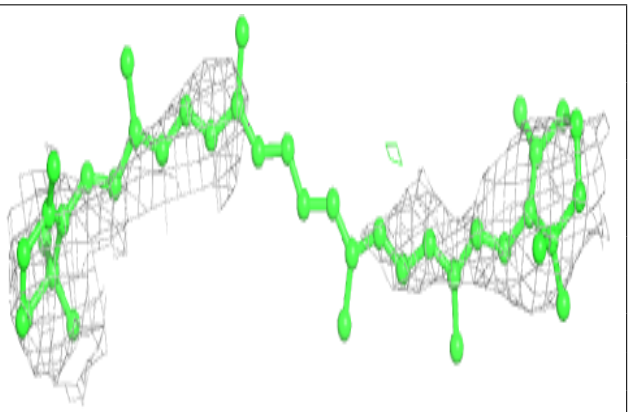
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

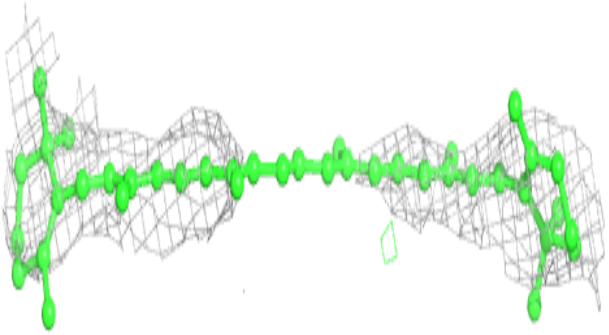


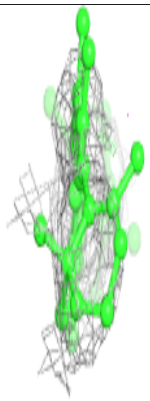


Electron density around BCR X 107:

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

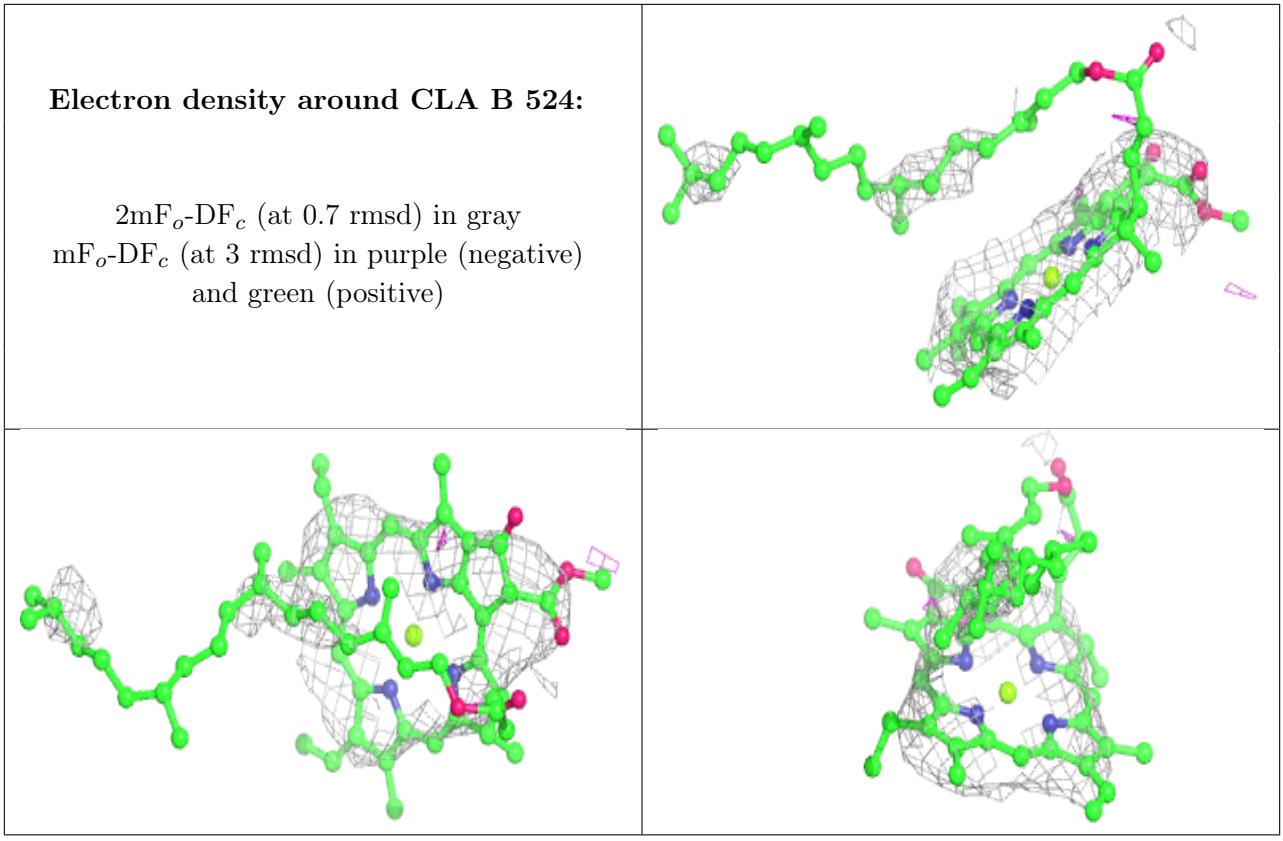






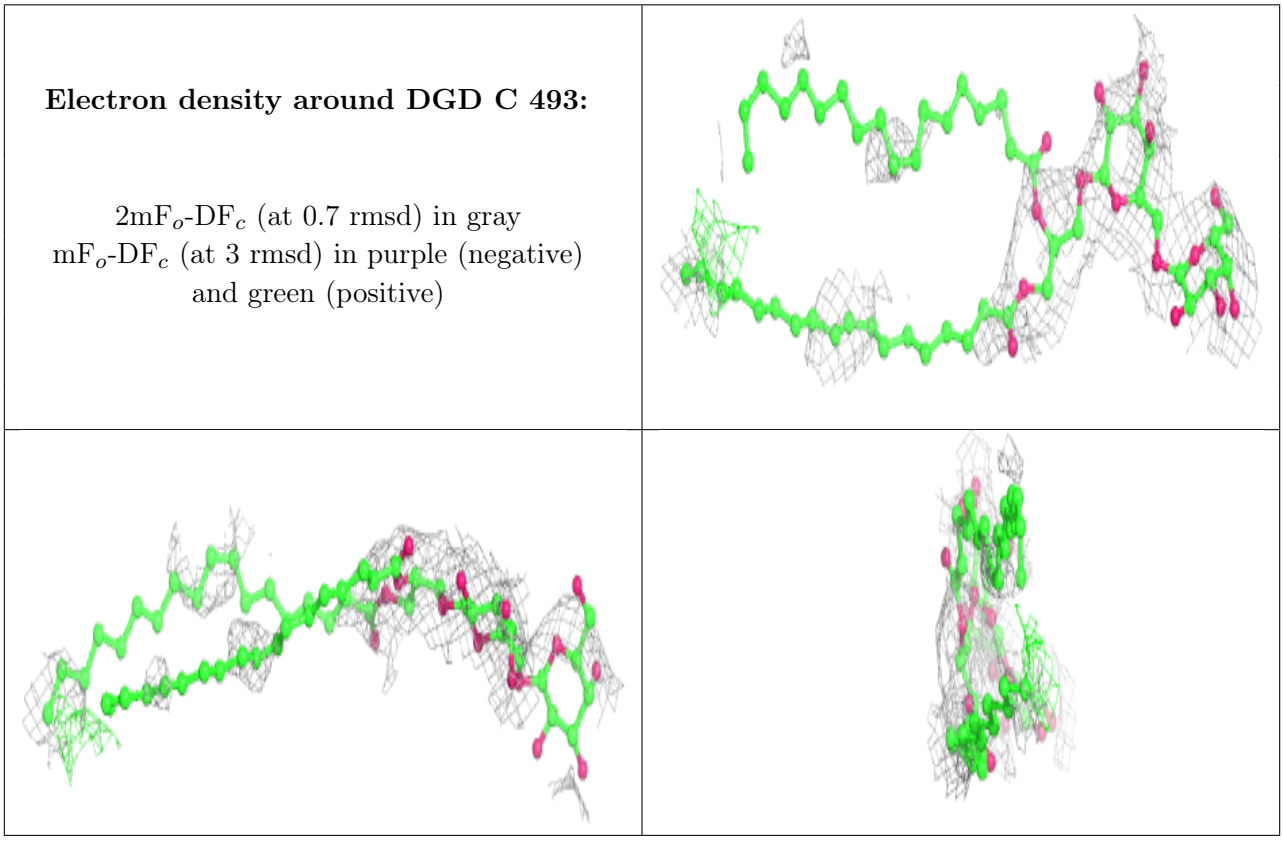
Electron density around CLA B 524:

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



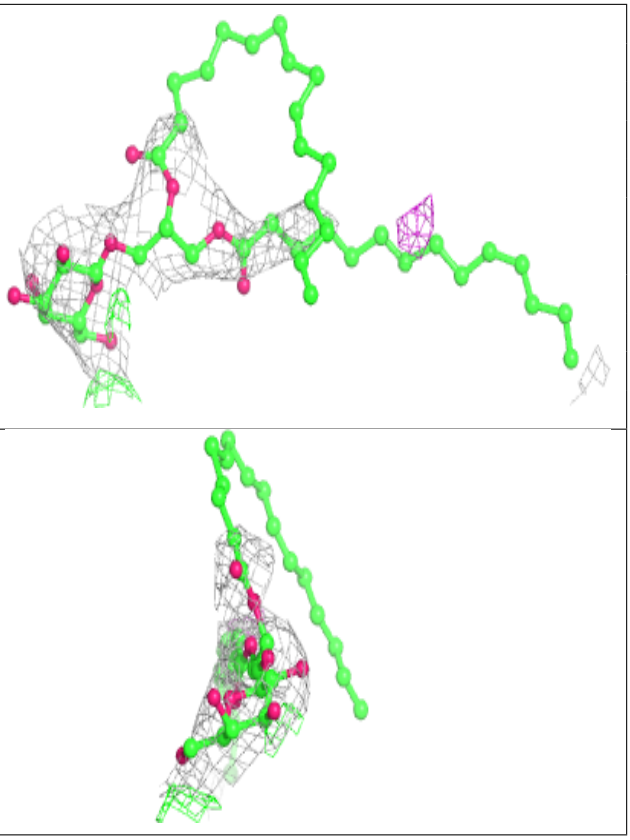
Electron density around DGD C 493:

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



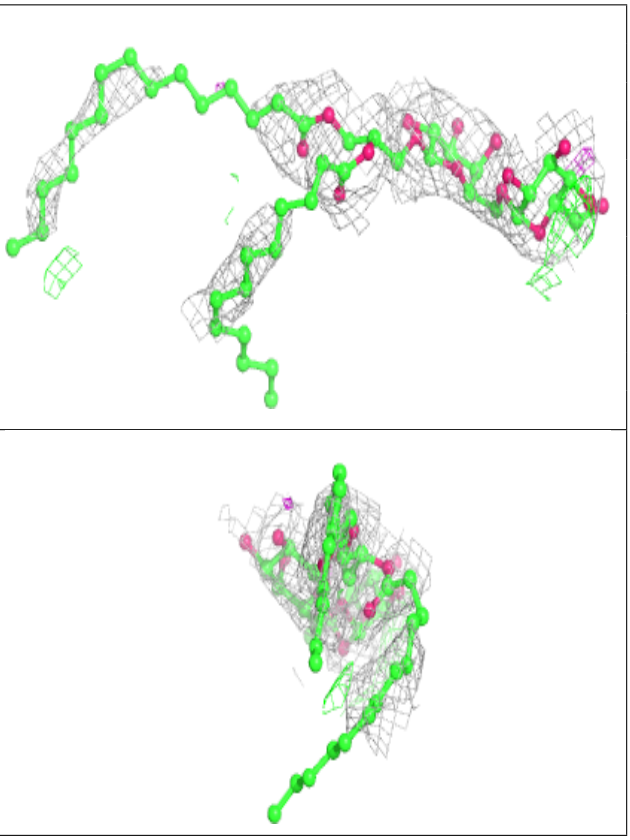
Electron density around LMG B 531:

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



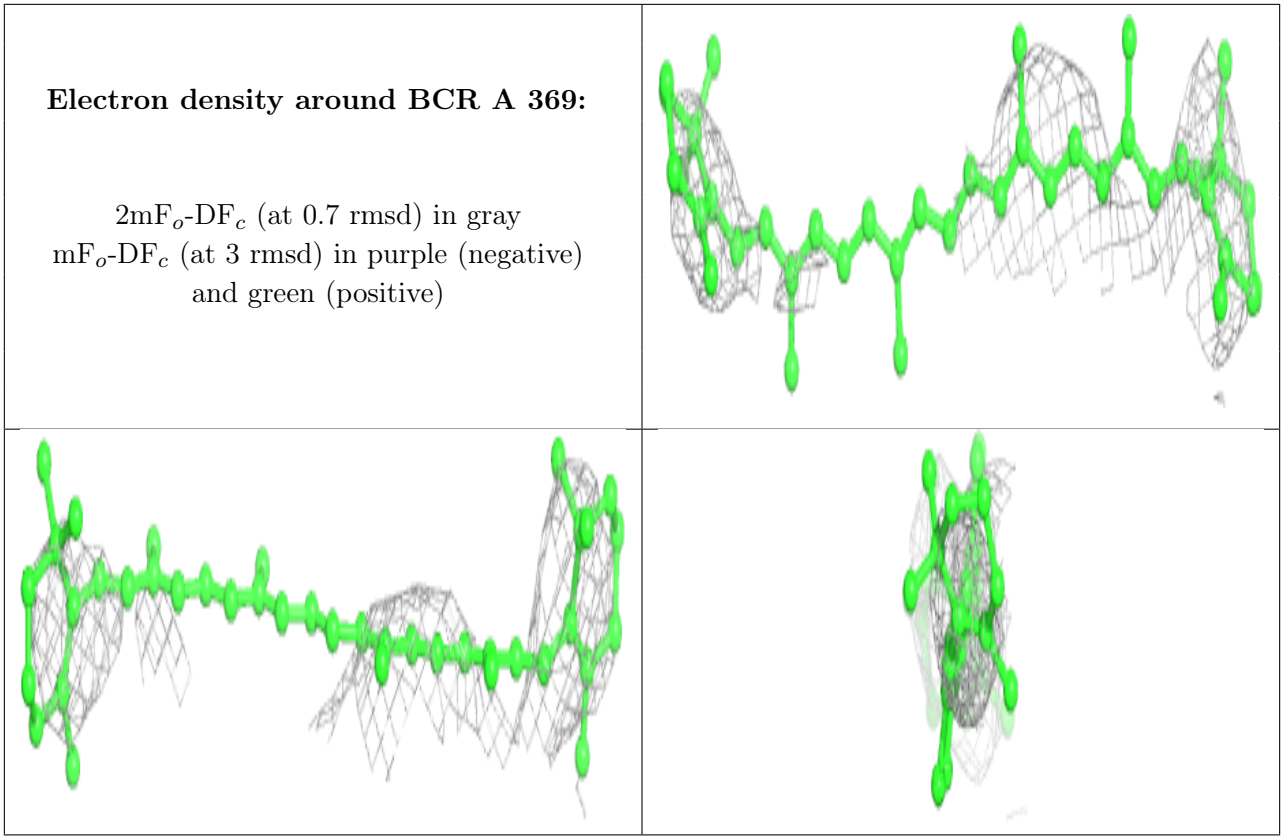
Electron density around DGD B 528:

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



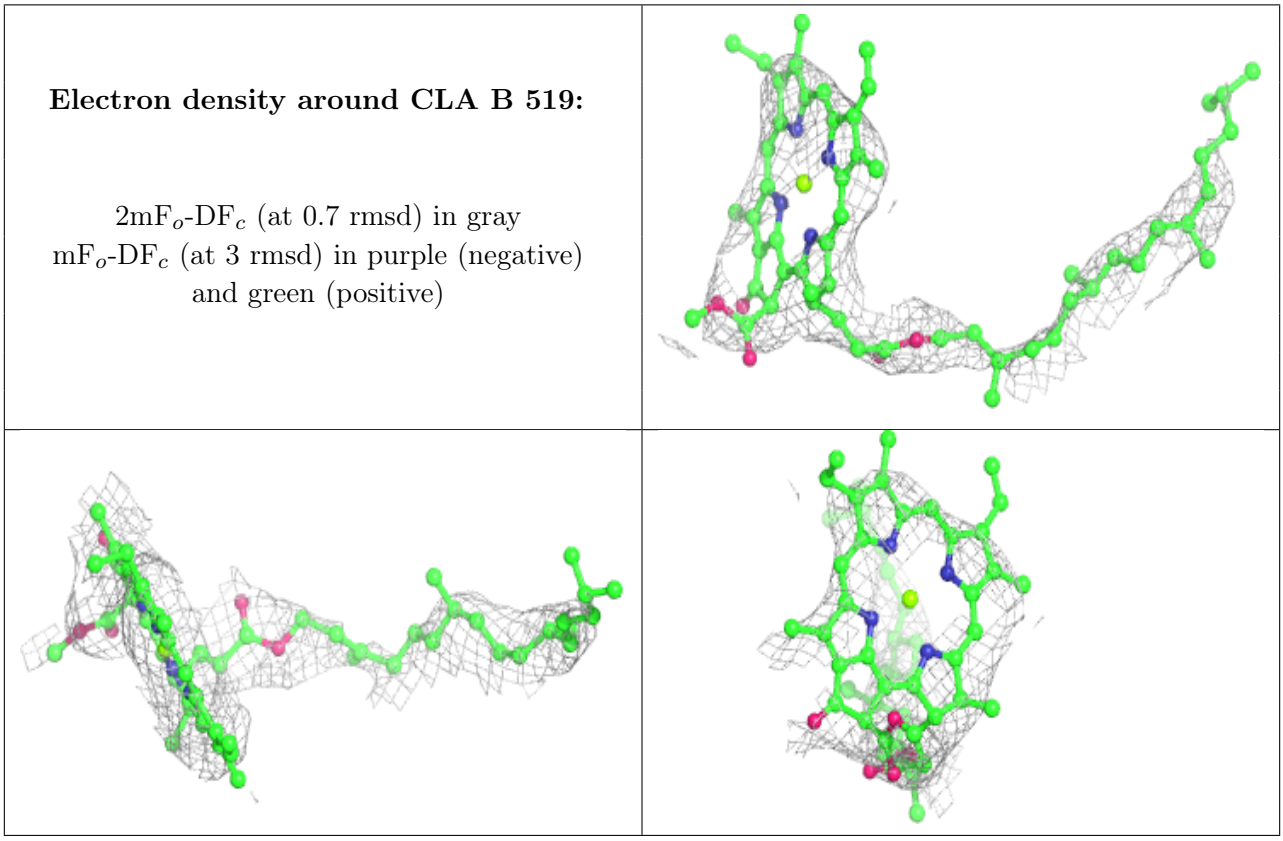
Electron density around BCR A 369:

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



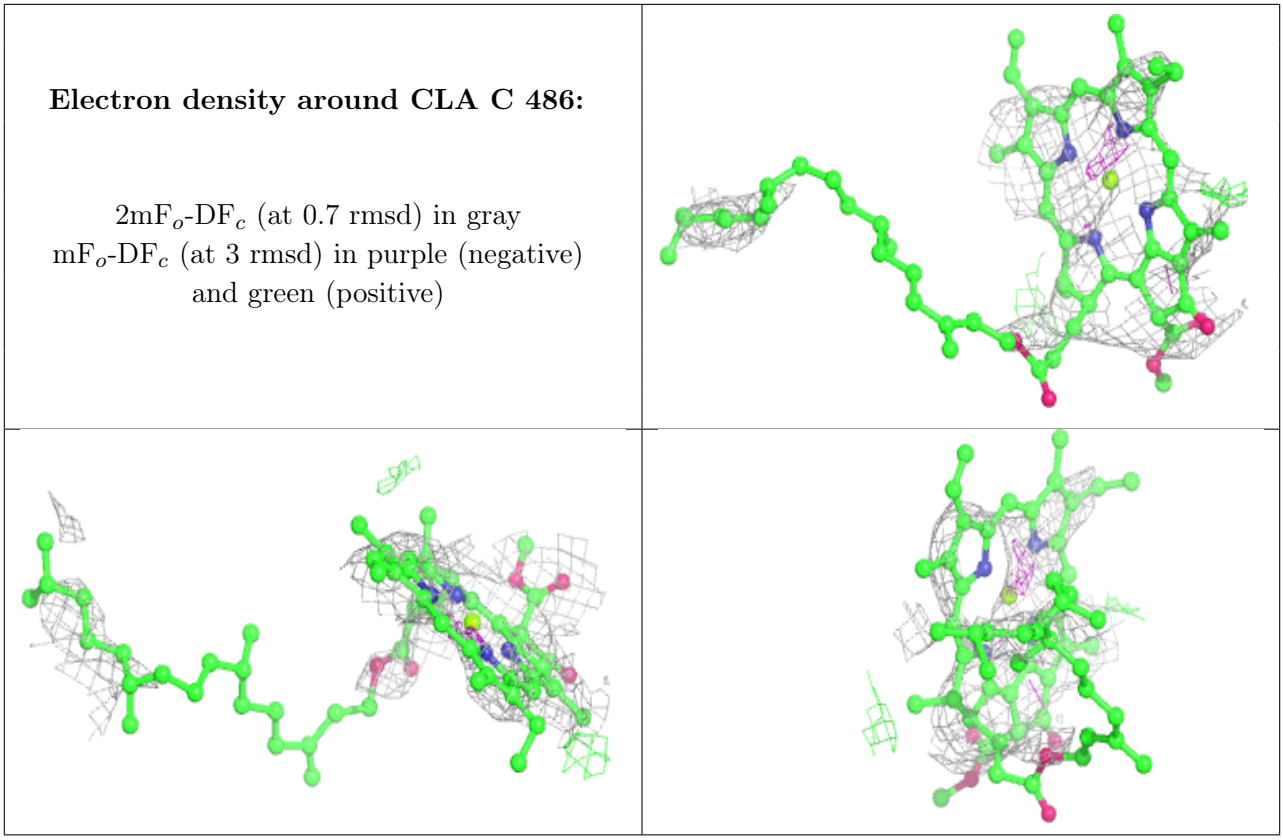
Electron density around CLA B 519:

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



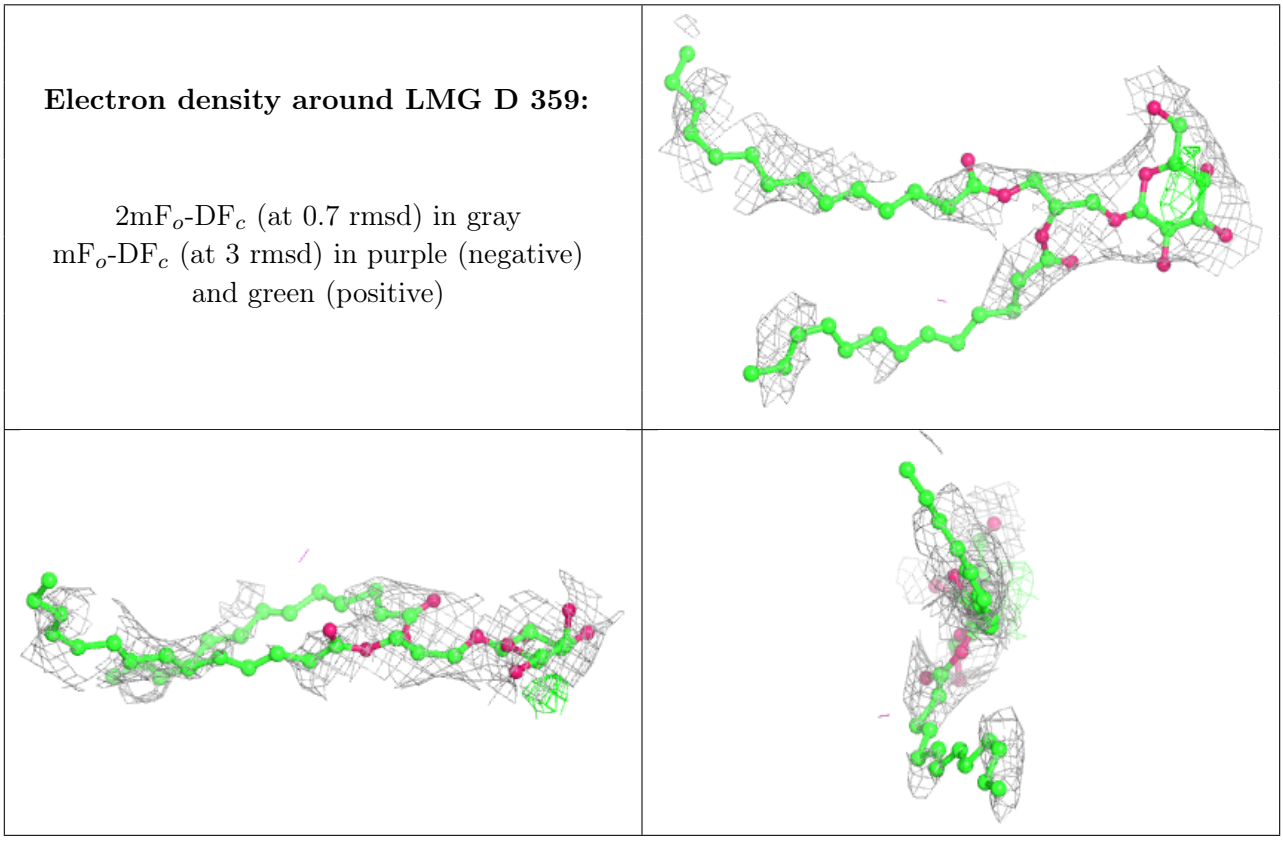
Electron density around CLA C 486:

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



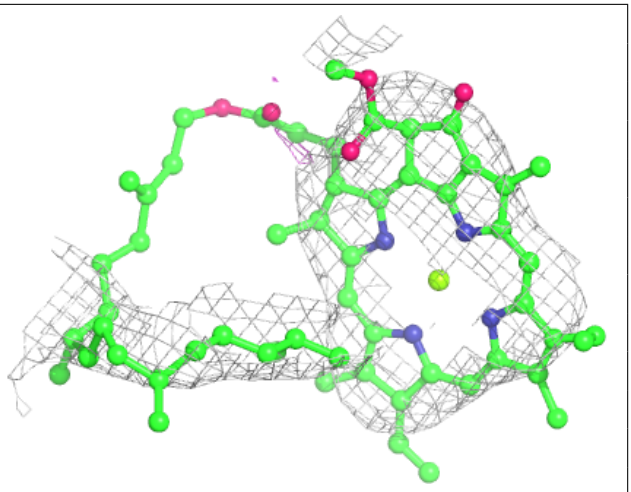
Electron density around LMG D 359:

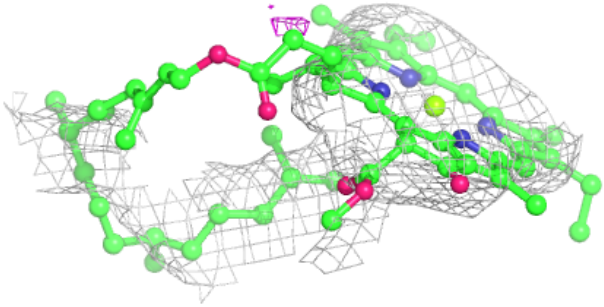
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

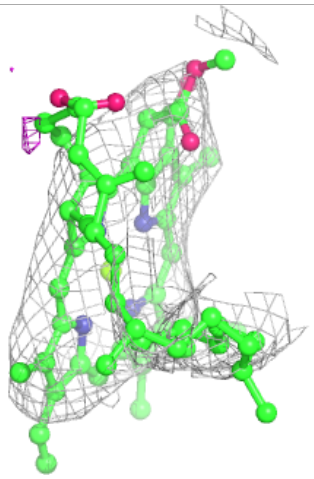


Electron density around CLA B 525:

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

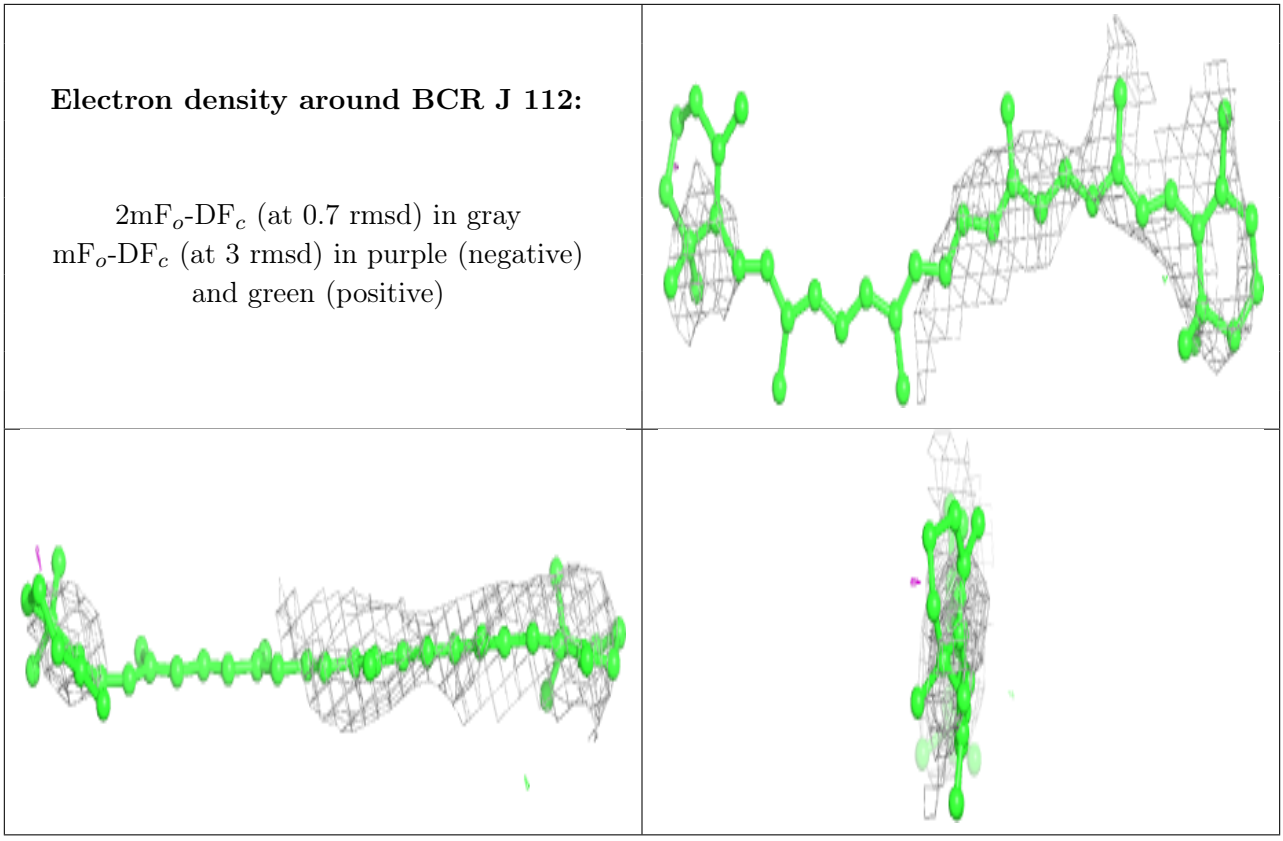






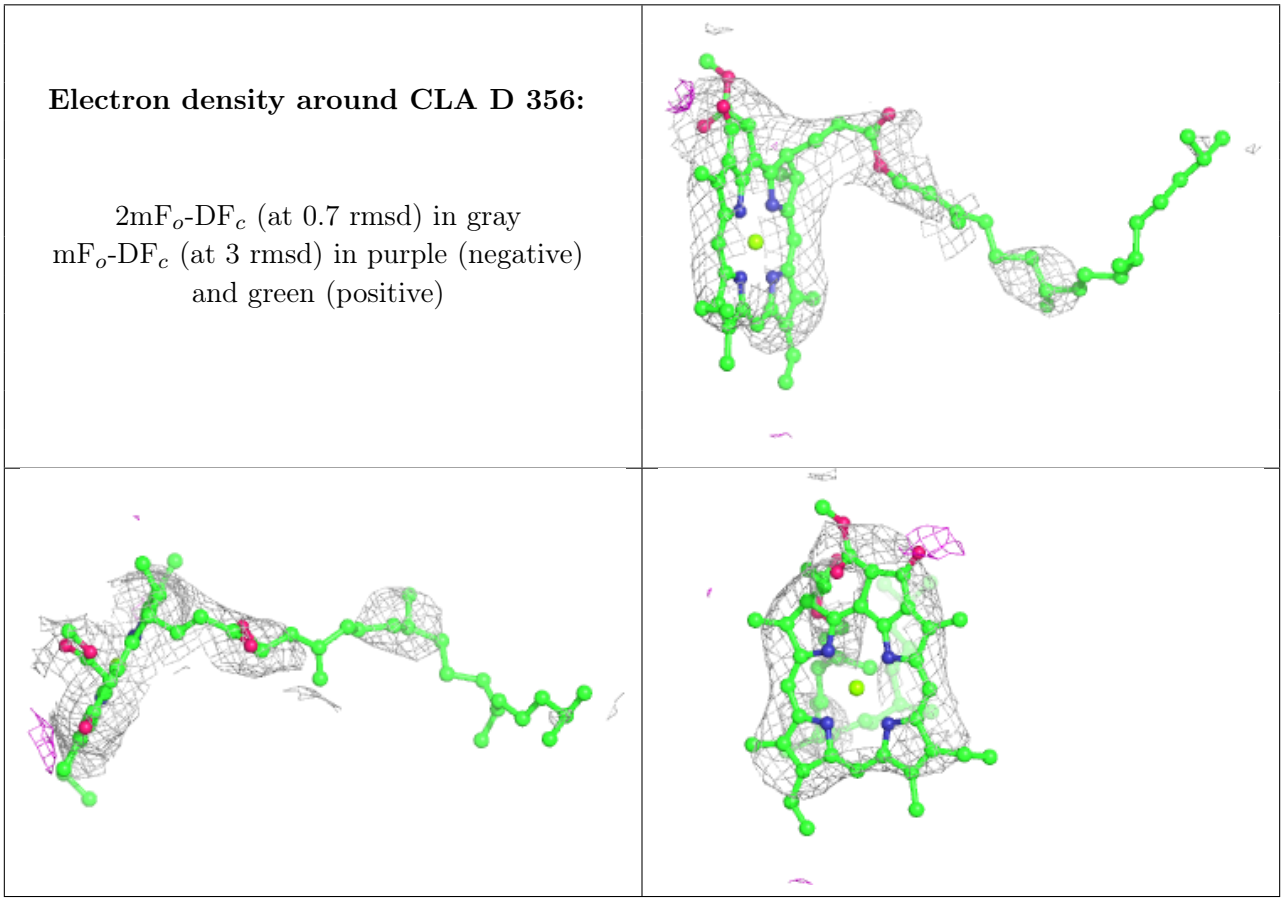
Electron density around BCR J 112:

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



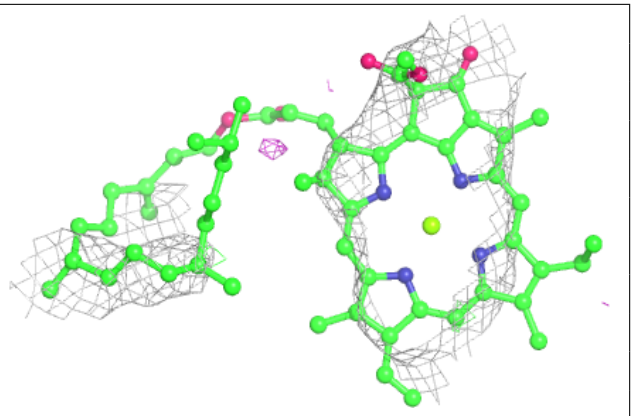
Electron density around CLA D 356:

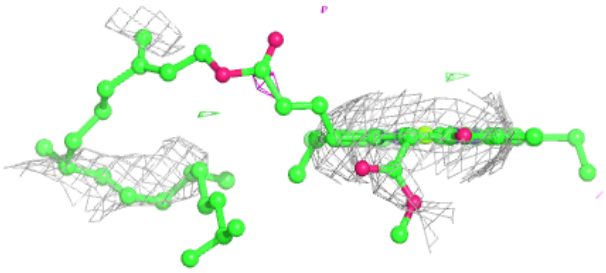
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

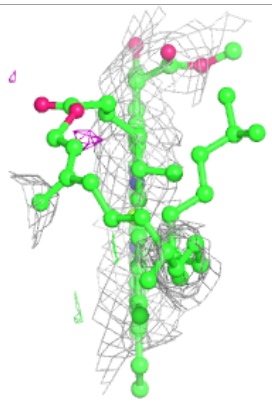


Electron density around CLA C 487:

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

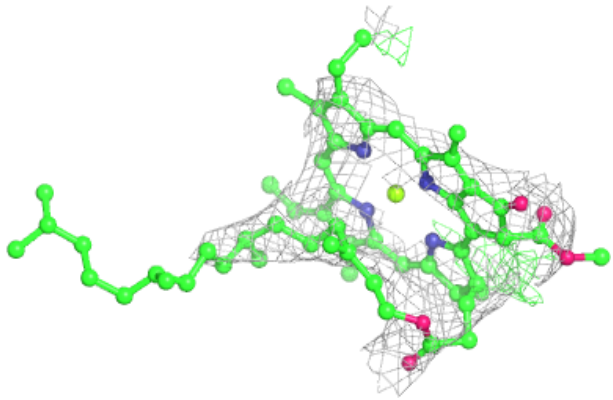


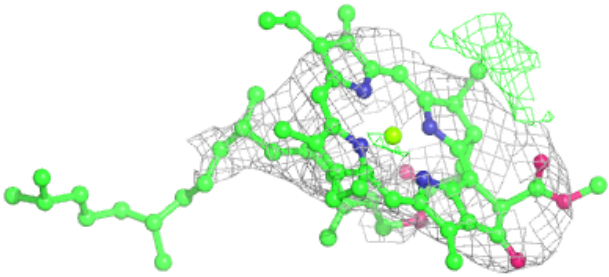


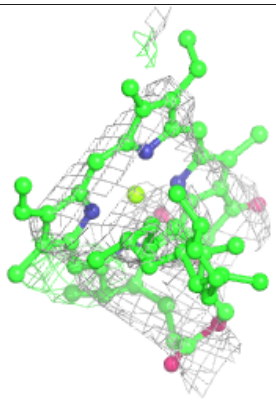


Electron density around CLA C 481:

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

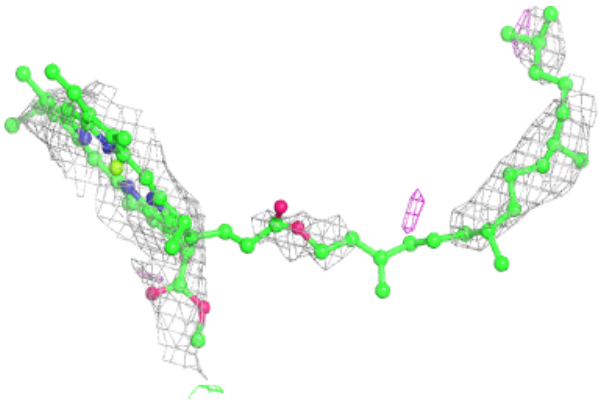


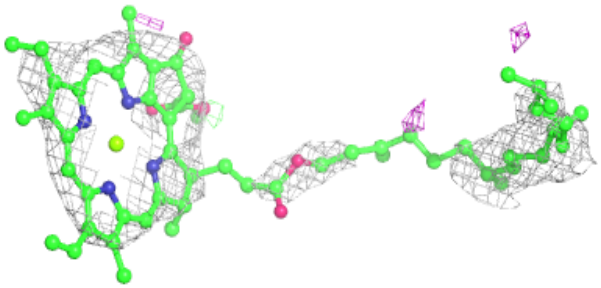


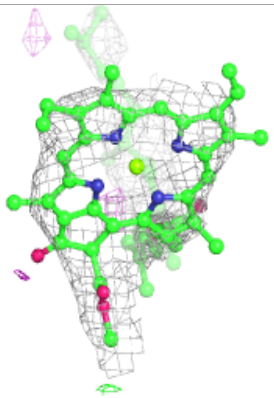


Electron density around CLA D 354:

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

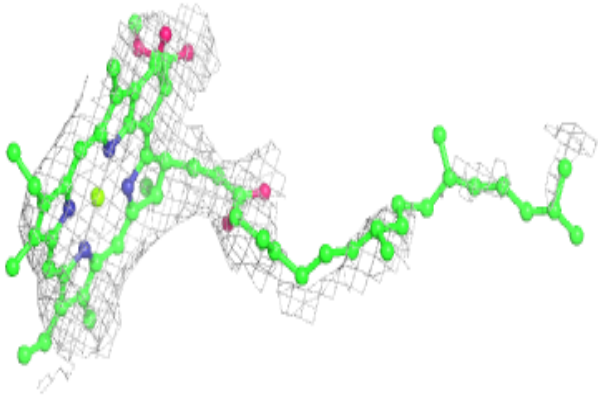


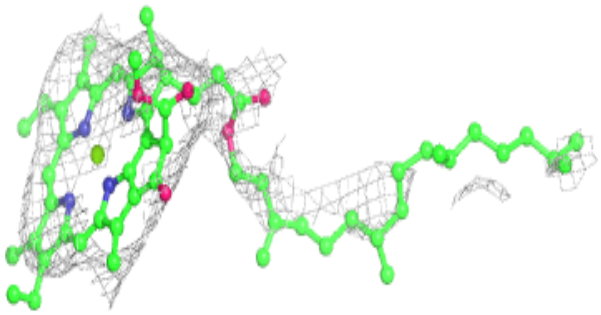


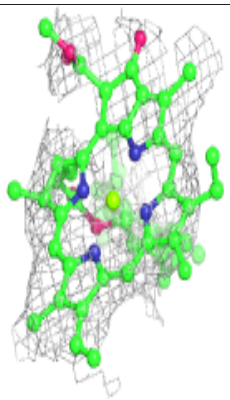


Electron density around CLA C 478:

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

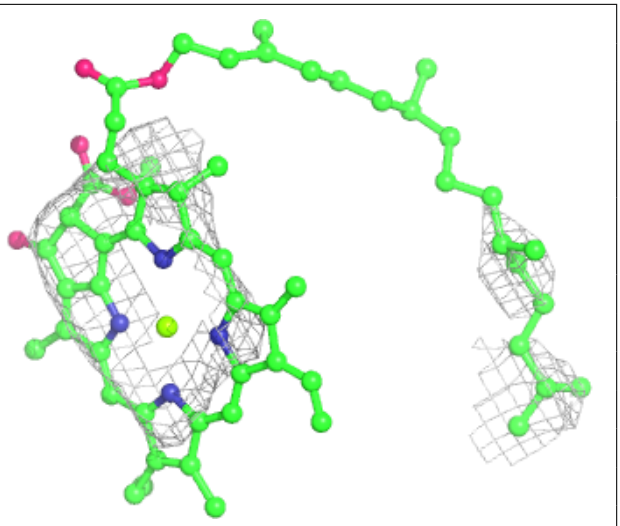


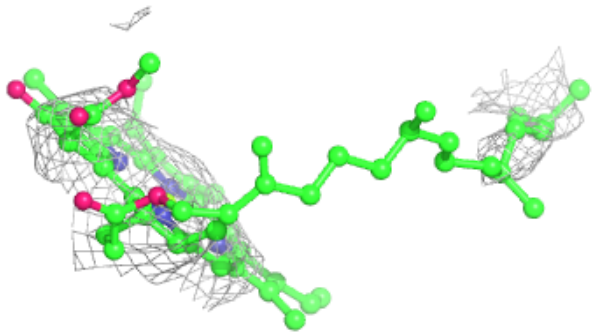


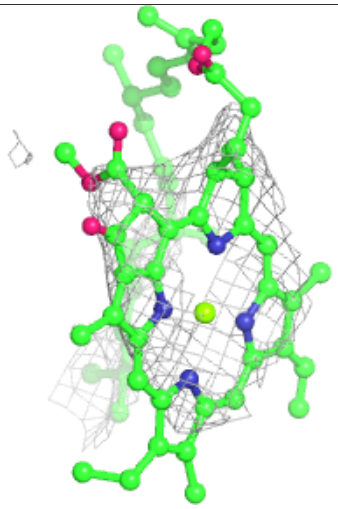


Electron density around CLA C 483:

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

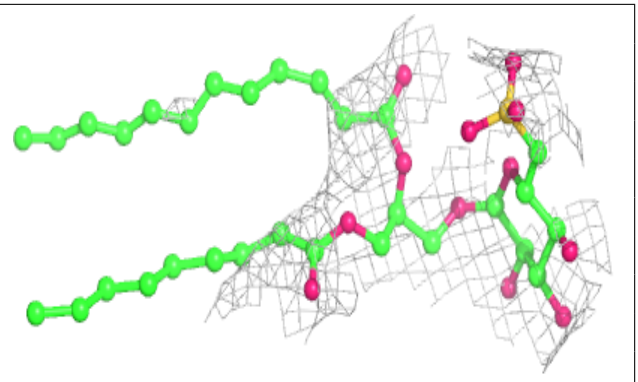


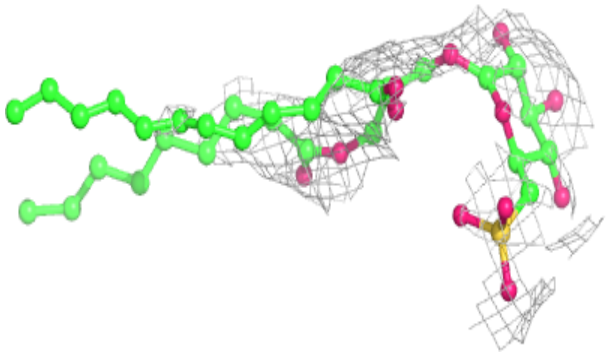


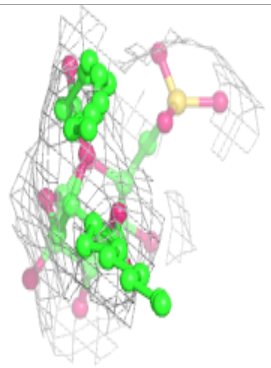


Electron density around SQD D 361:

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

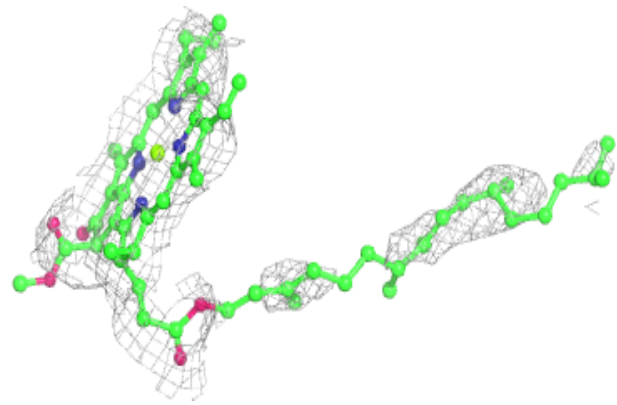


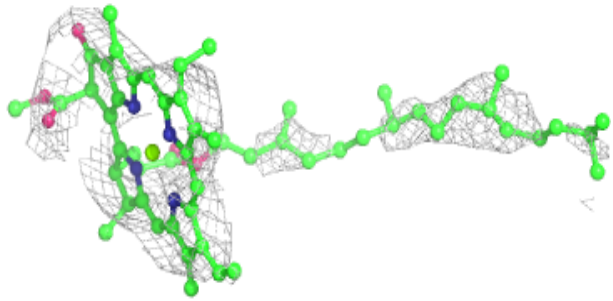


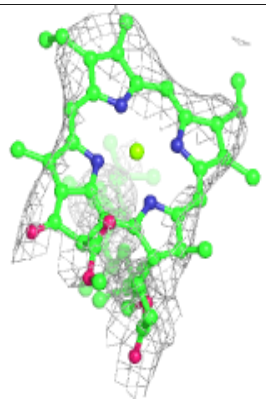


Electron density around CLA B 517:

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

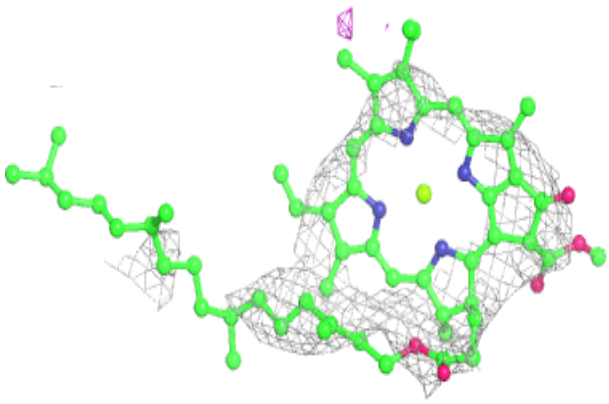


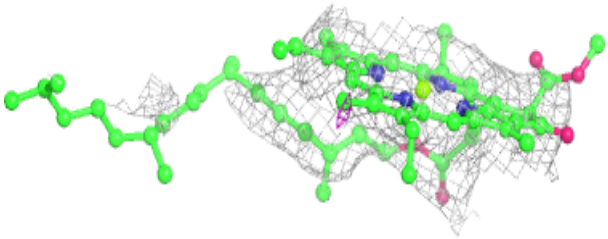


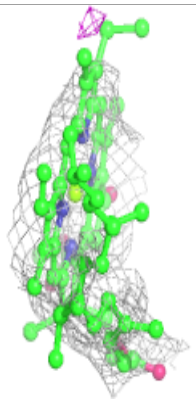


Electron density around CLA C 477:

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

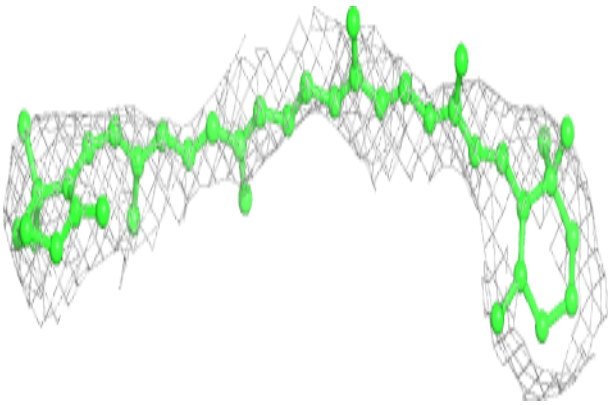


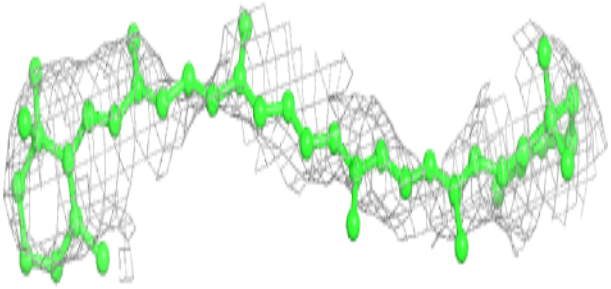


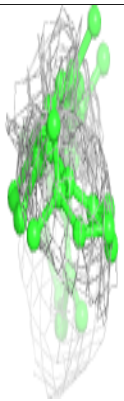


Electron density around BCR D 358:

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

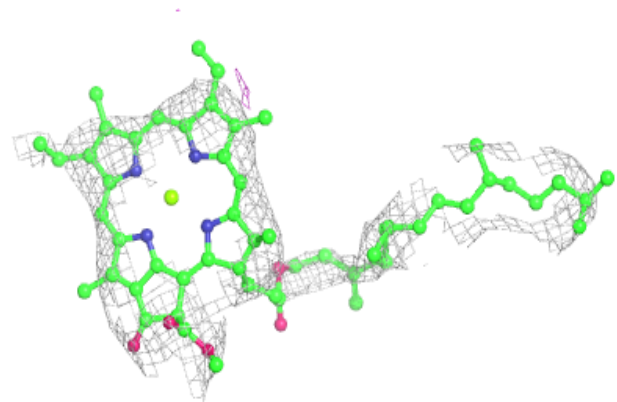


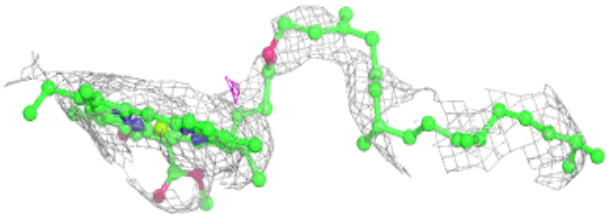


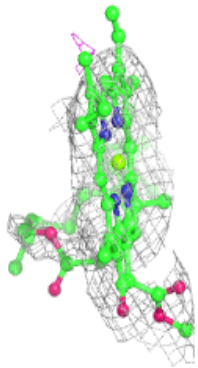


Electron density around CLA A 364:

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

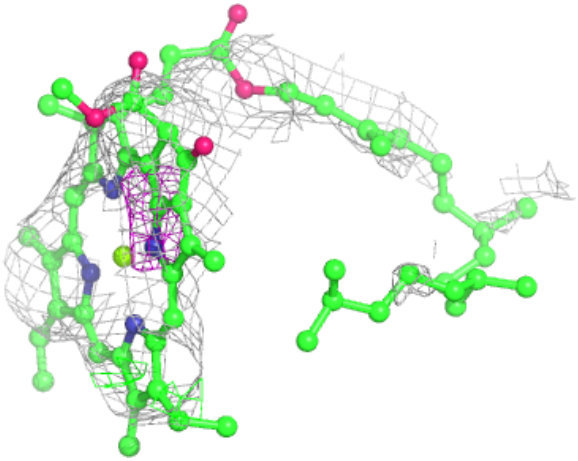


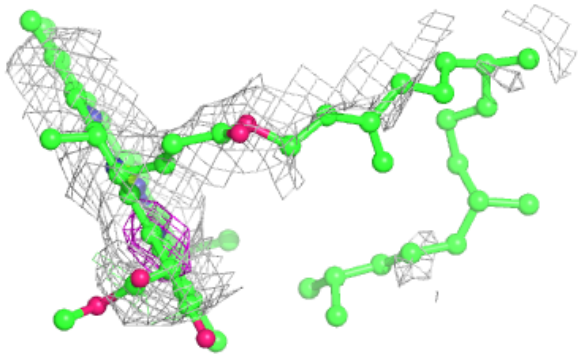


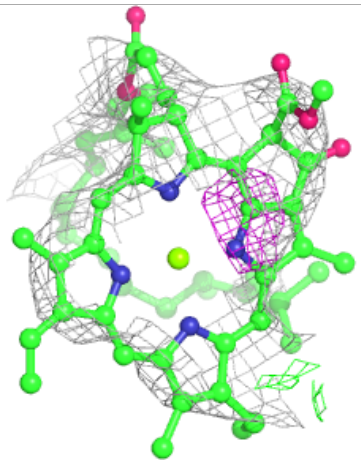


Electron density around CLA C 479:

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

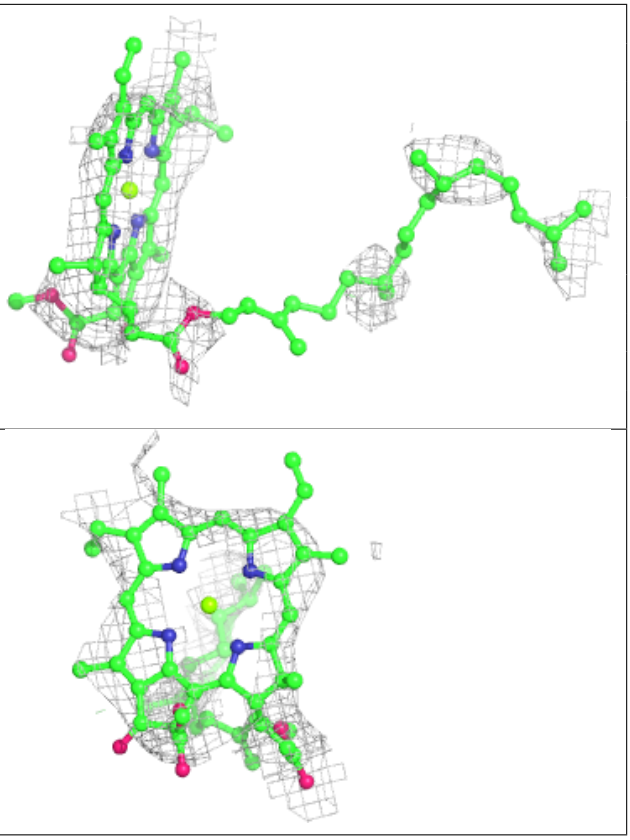






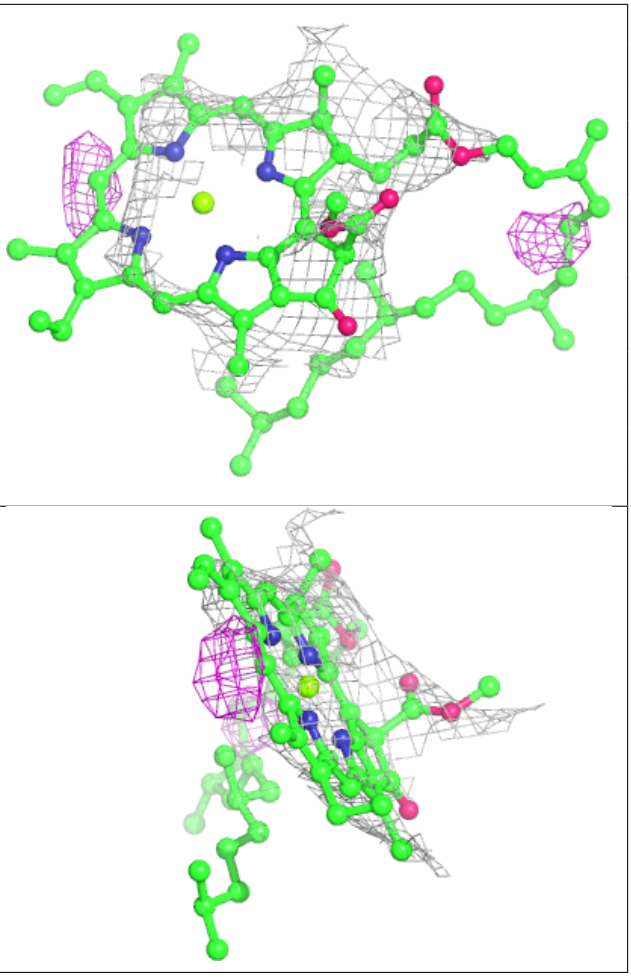
Electron density around CLA C 484:

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



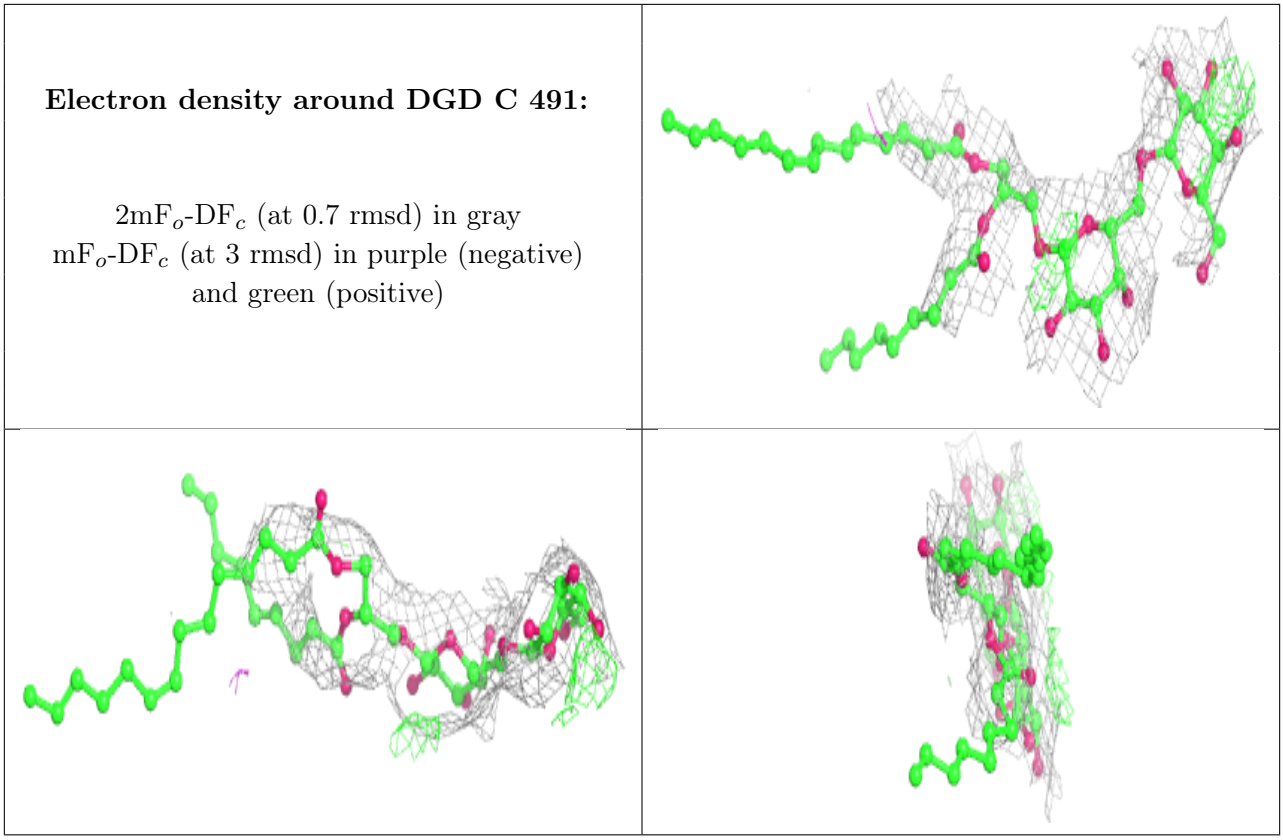
Electron density around CLA C 485:

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



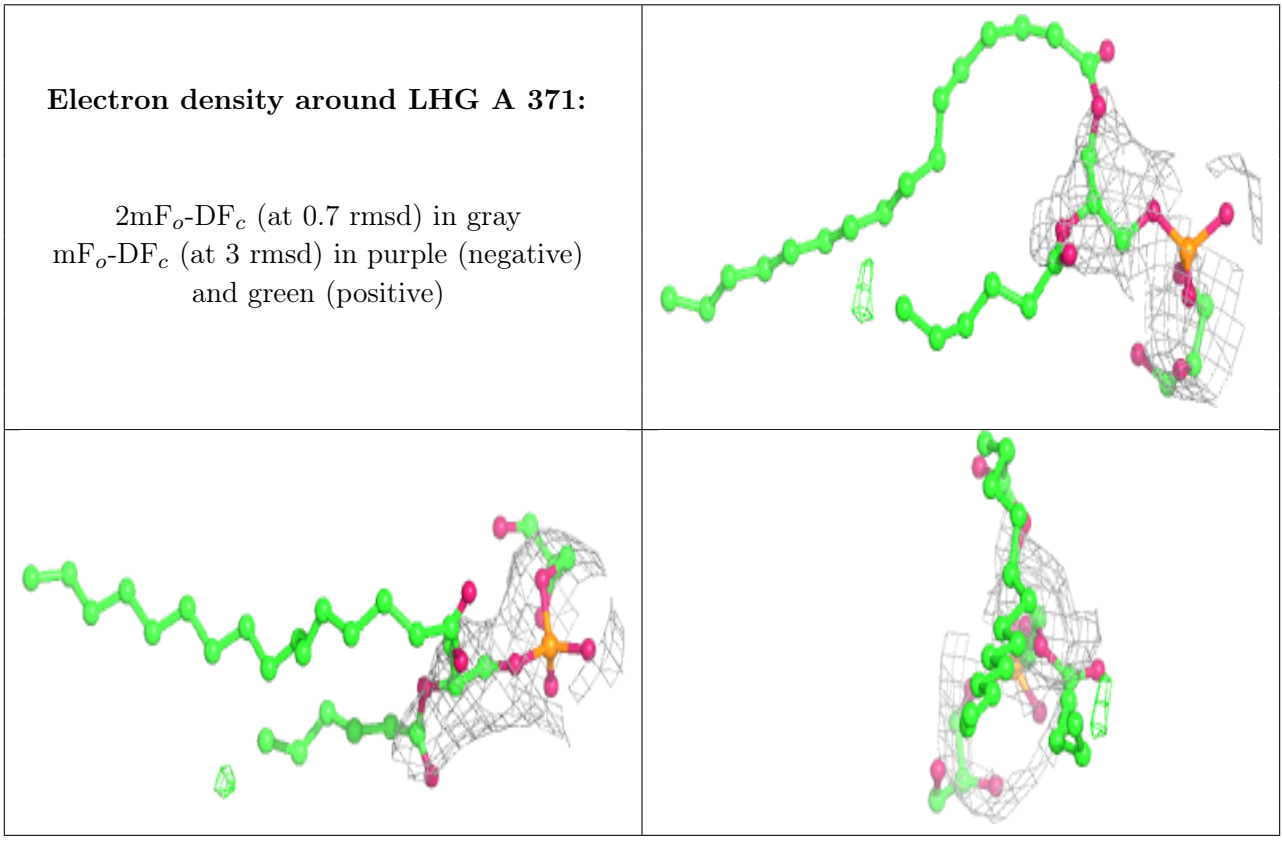
Electron density around DGD C 491:

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



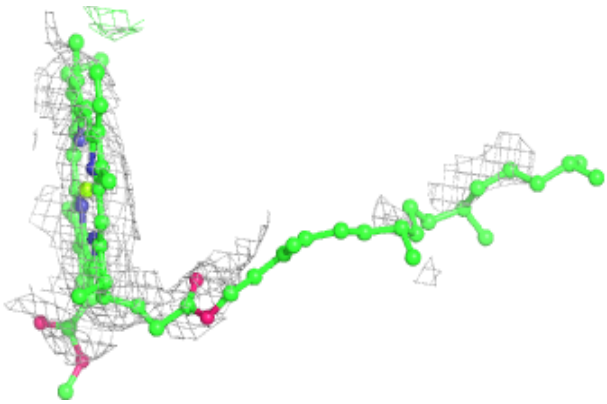
Electron density around LHG A 371:

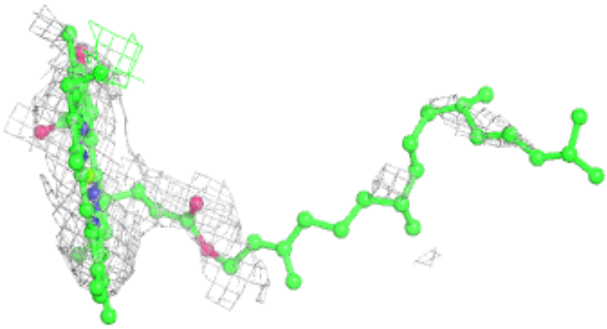
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

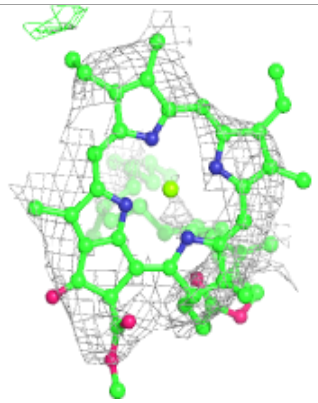


Electron density around CLA B 516:

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

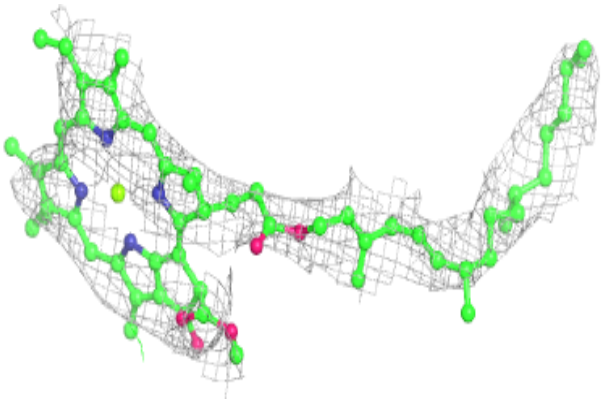


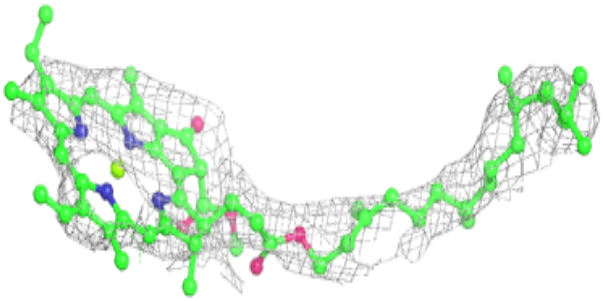


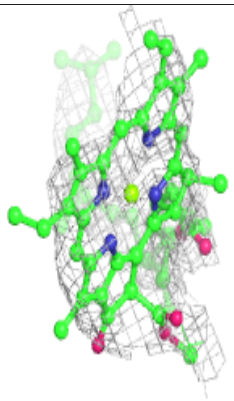


Electron density around CLA A 362:

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

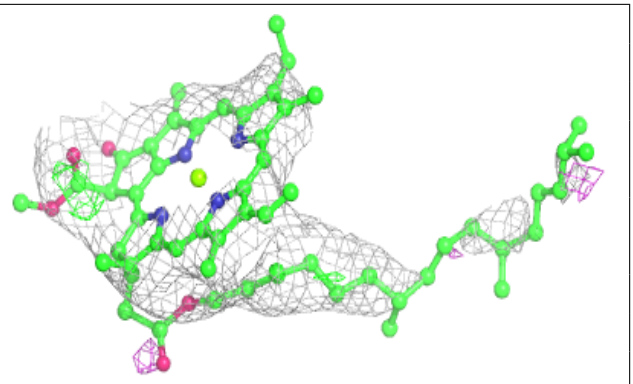


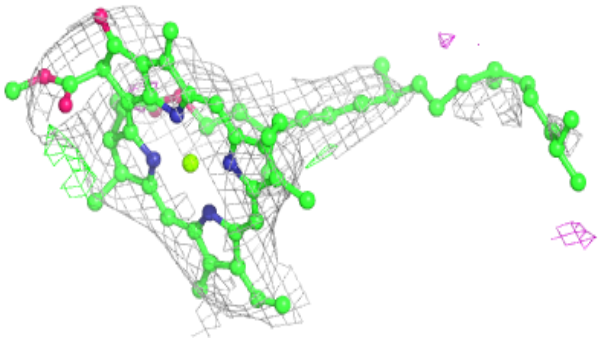


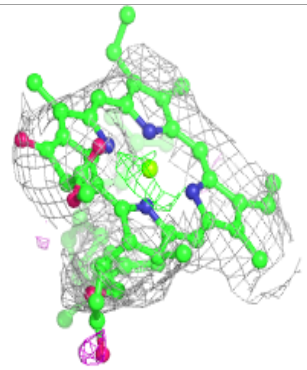


Electron density around CLA B 518:

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

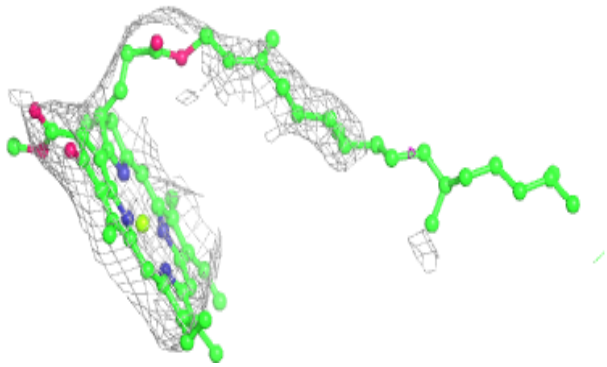


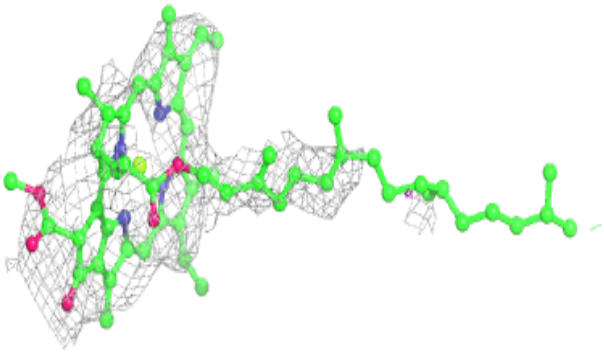


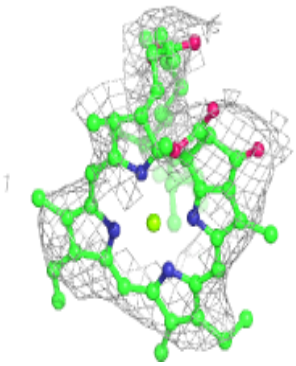


Electron density around CLA C 480:

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

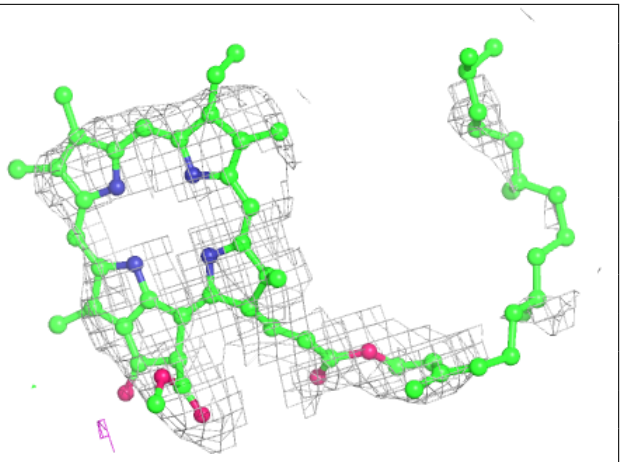


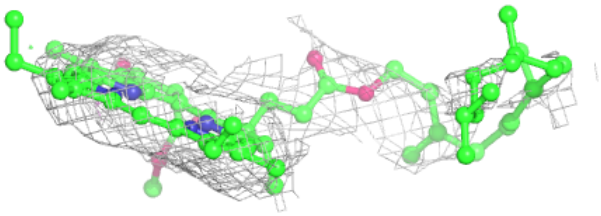


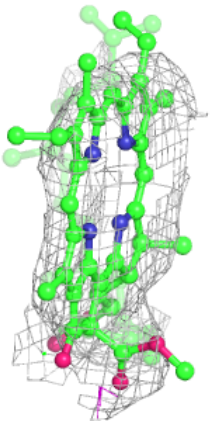


Electron density around PHO A 365:

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

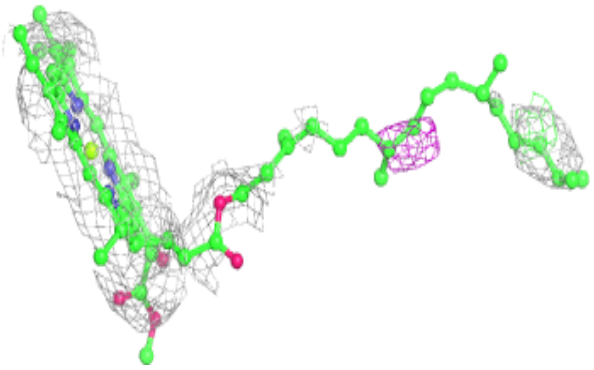


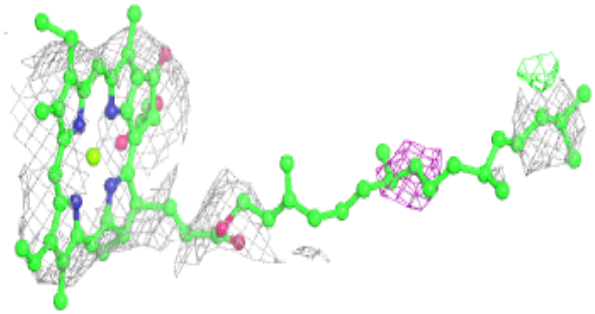


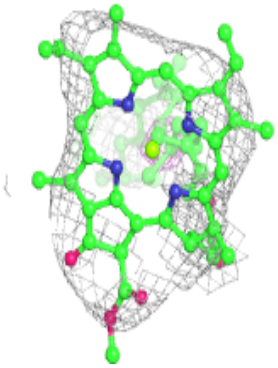


Electron density around CLA B 514:

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

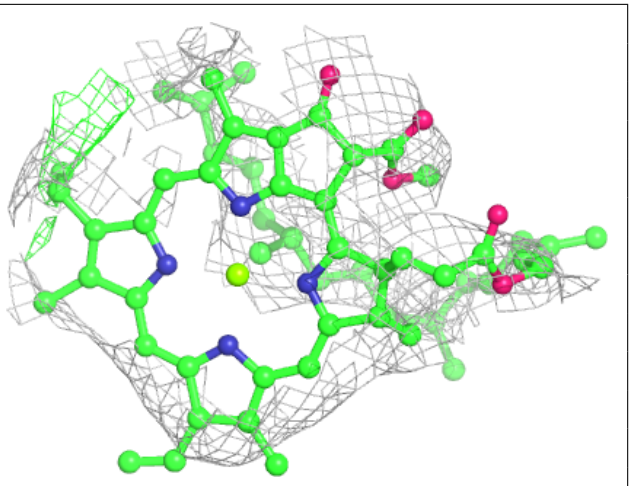


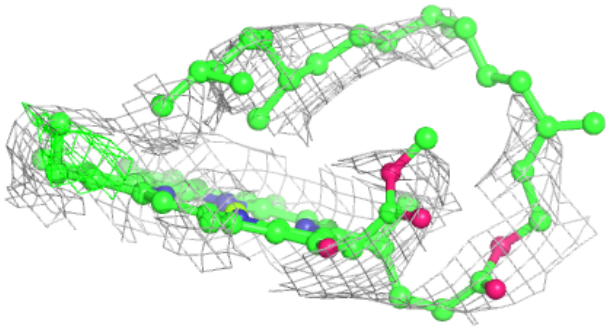


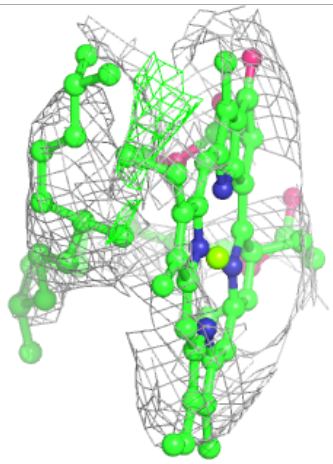


Electron density around CLA K 483:

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

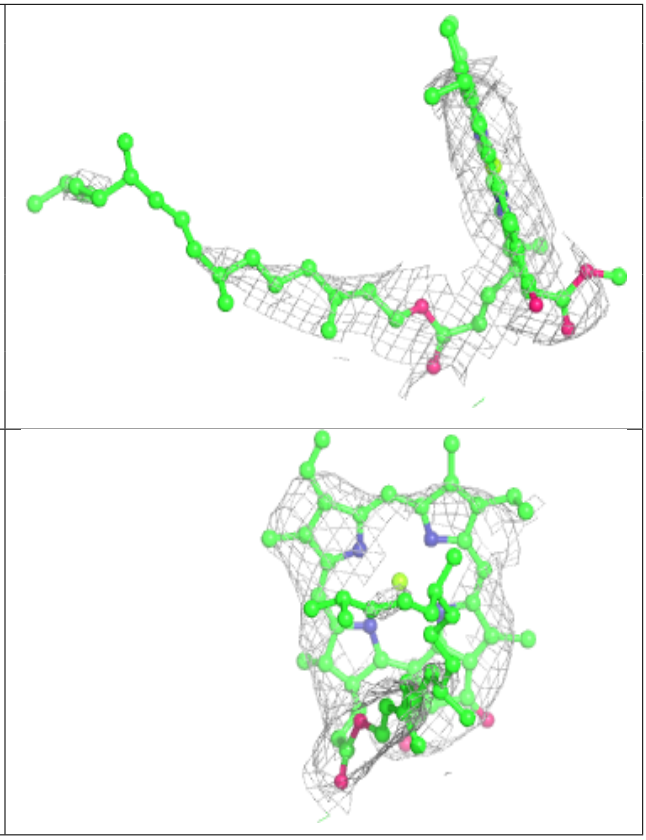






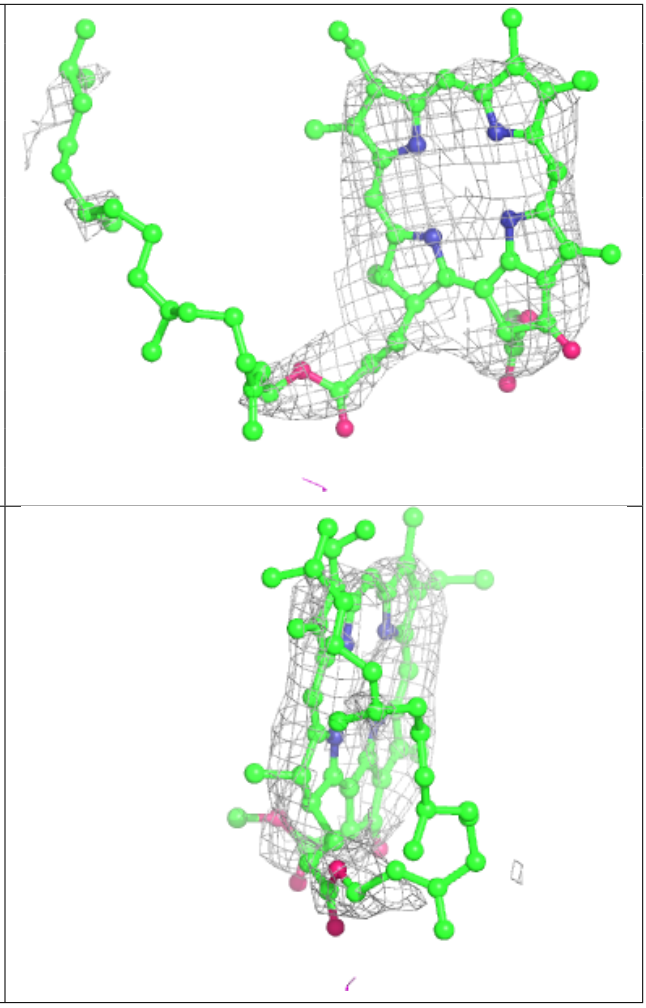
Electron density around CLA B 515:

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



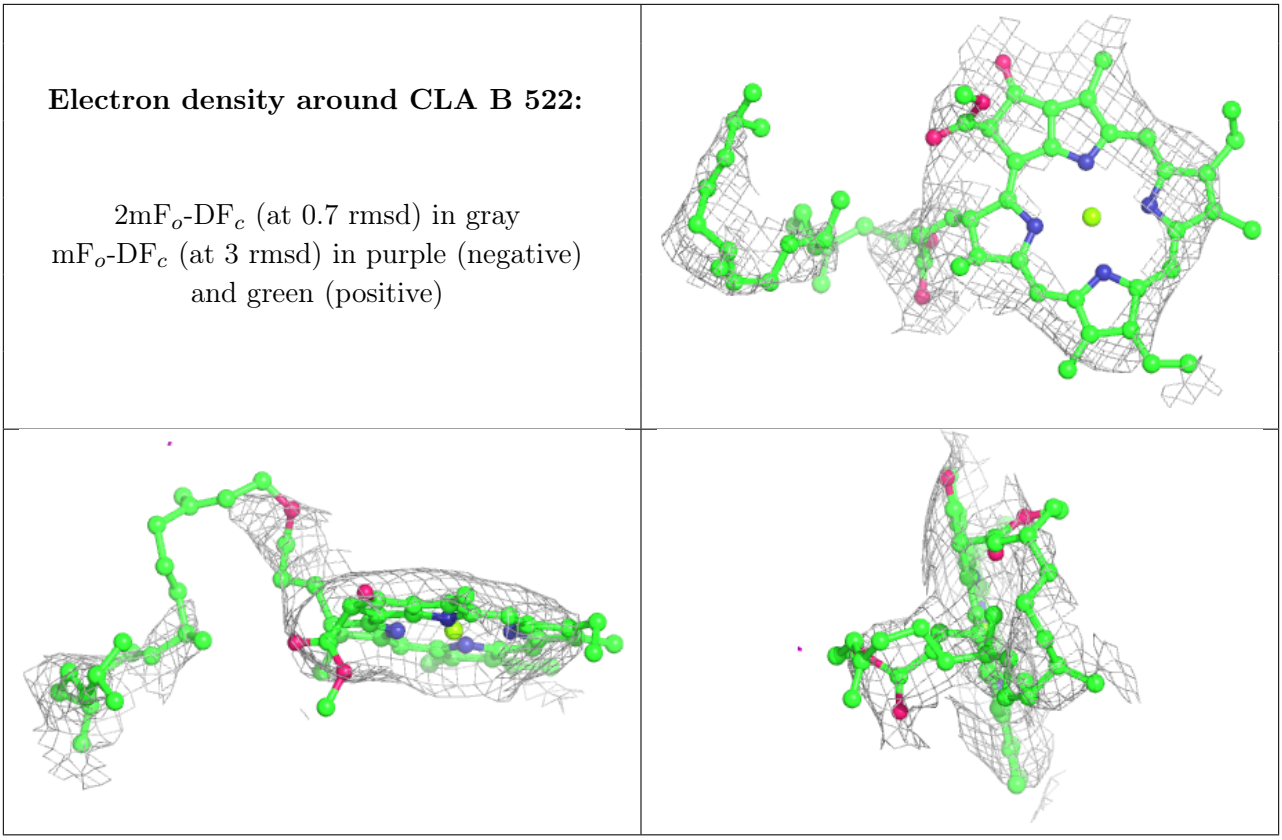
Electron density around PHO D 355:

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



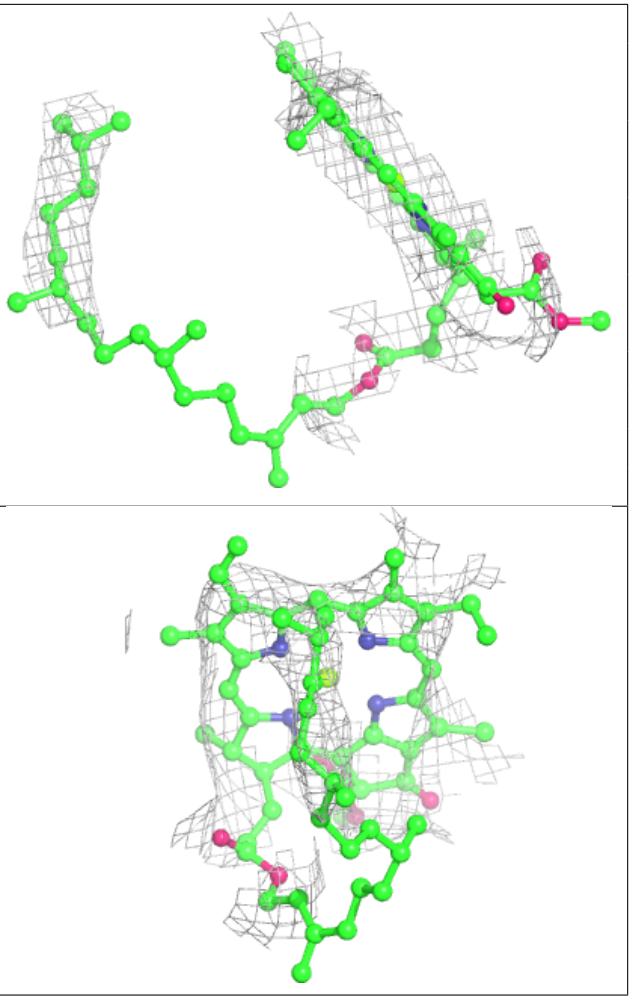
Electron density around CLA B 522:

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



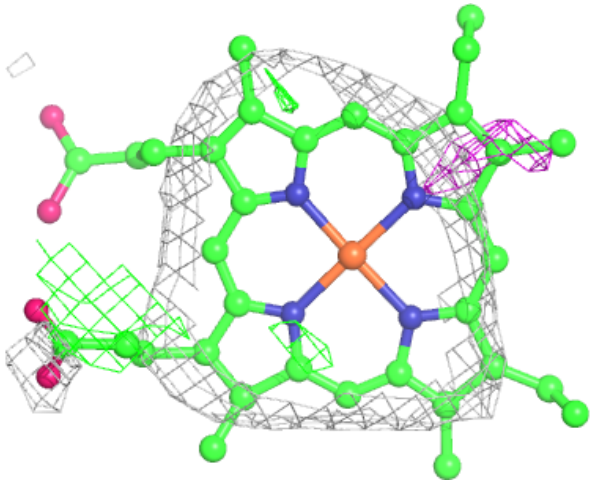
Electron density around CLA B 521:

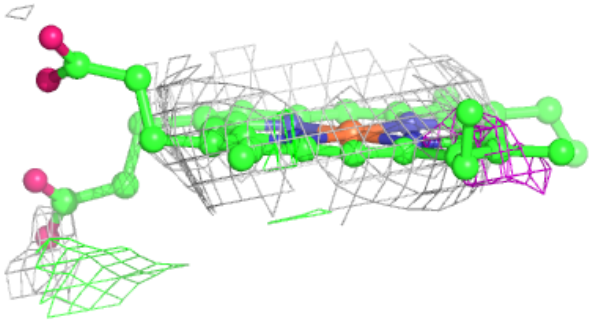
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

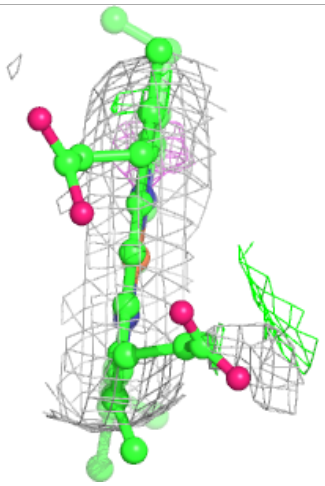


Electron density around HEM F 85:

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

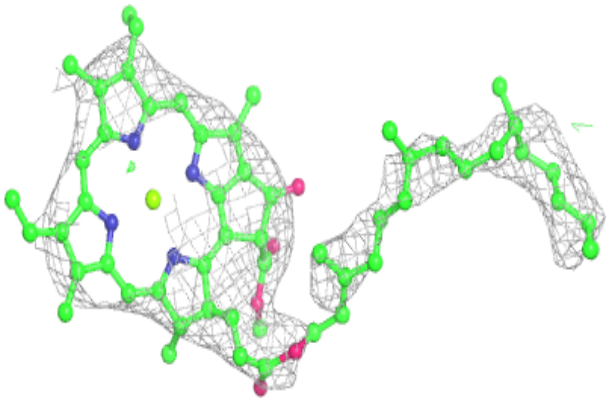


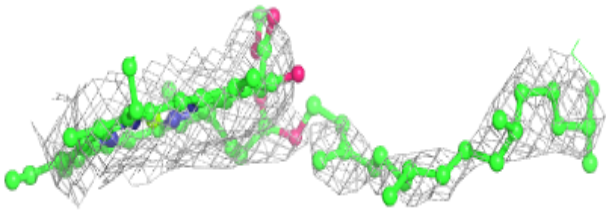


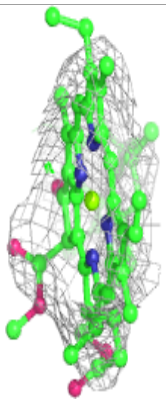


Electron density around CLA B 512:

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

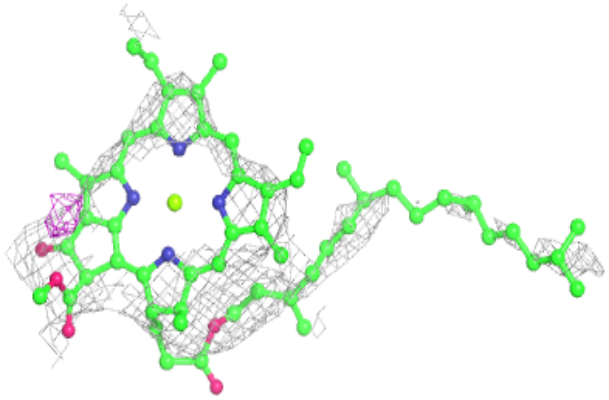


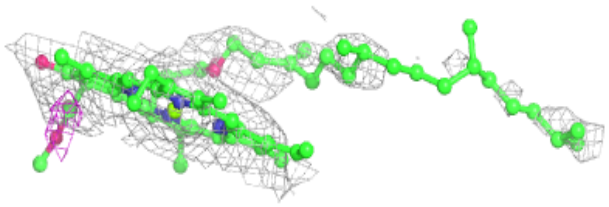


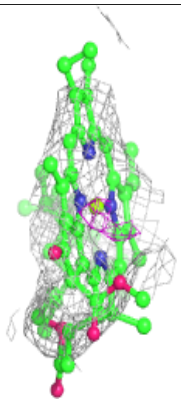


Electron density around CLA B 513:

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

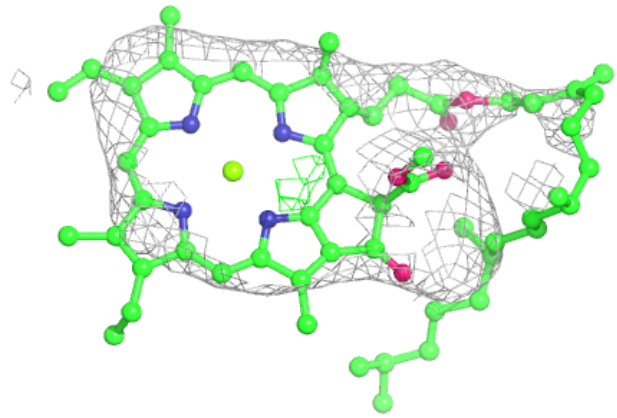


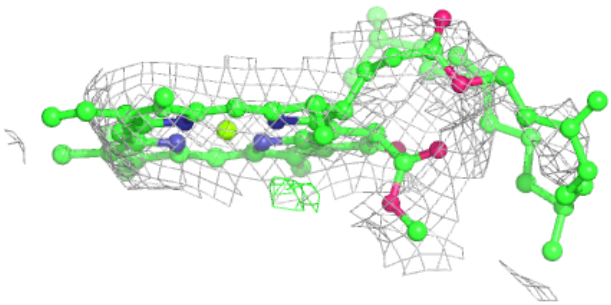


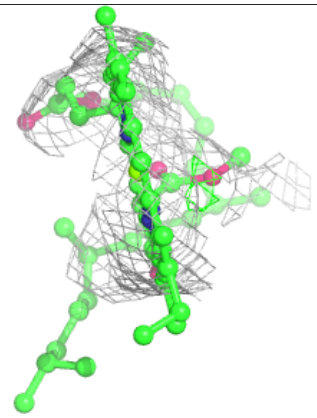


Electron density around CLA B 520:

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

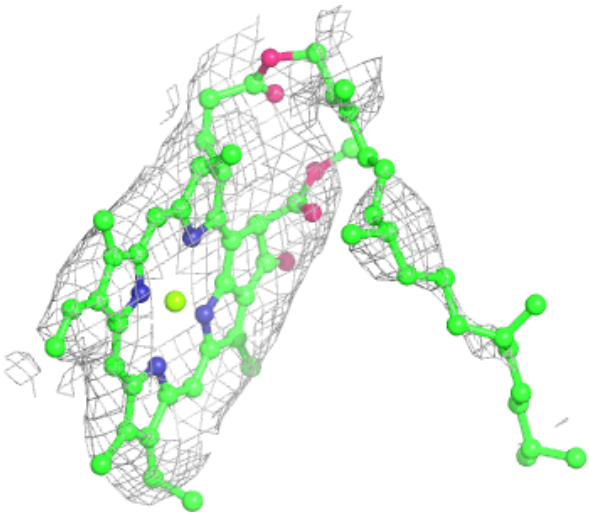


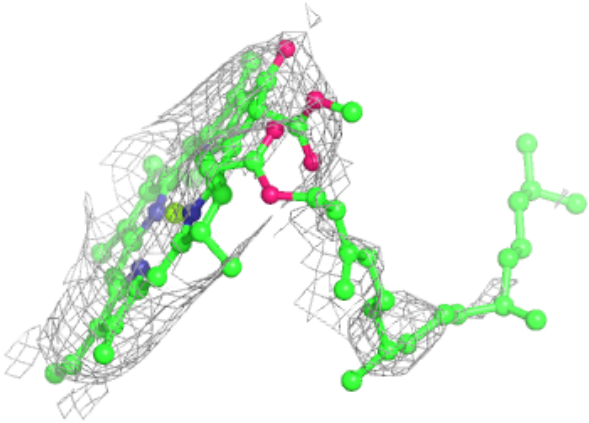


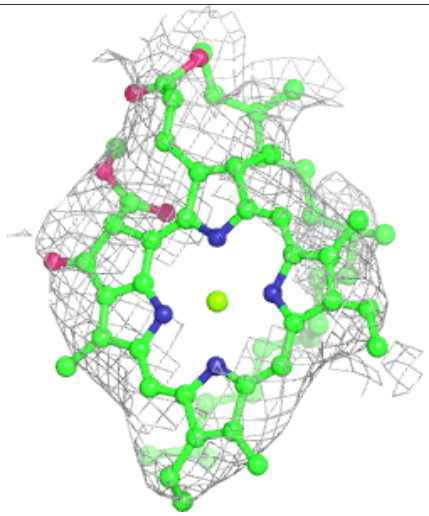


Electron density around CLA B 523:

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

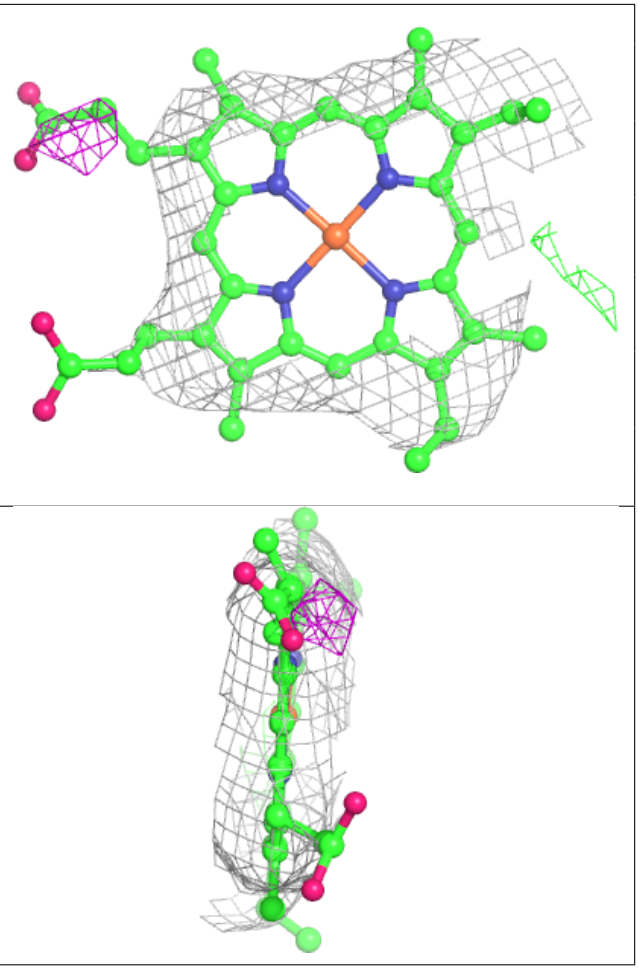






Electron density around HEM V 164:

$2mF_o$-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.