wwPDB X-ray Structure Validation Summary Report (i)

Aug 7, 2026 – 07:08 AM JST

PDB ID	:	8IRB / pdb_00008irb
Title	:	XFEL structure of cyanobacterial photosystem II following one flash (1F) with a 5-millisecond delay
Authors	:	Li, H.; Suga, M.; Shen, J.R.
Deposited on	:	2023-03-17
Resolution	:	2.30 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

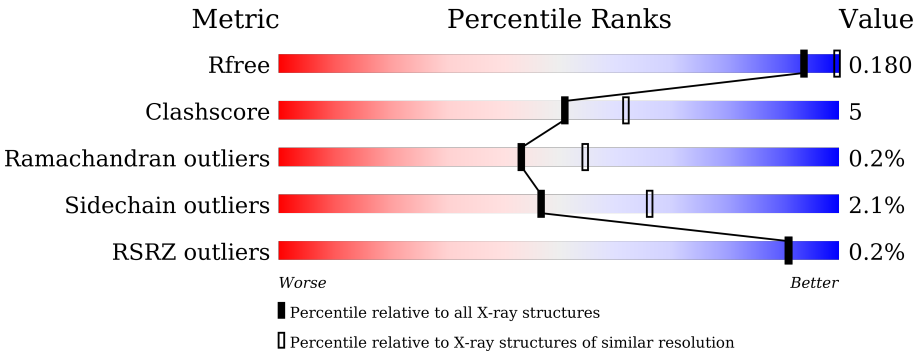
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	88% 9% ·
1	a	344	86% 11% ·
2	B	505	92% 8%
2	b	505	89% 10% ·
3	C	455	90% 9% ·
3	c	455	89% 10% ·

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Mol	Chain	Length	Quality of chain
4	D	342	89% 11%
4	d	342	91% 8%
5	E	84	80% 17%
5	e	84	83% 11% 6%
6	F	44	68% 9% 23%
6	f	44	64% 7% 30%
7	H	65	94% 5%
7	h	65	86% 12%
8	I	38	76% 16% 8%
8	i	38	95% 5%
9	J	39	82% 10% 5%
9	j	39	85% 15%
10	K	37	78% 19%
10	k	37	78% 19%
11	L	37	92% 5%
11	l	37	81% 16%
12	M	36	78% 11% 8%
12	m	36	78% 14% 6%
13	O	244	87% 13%
13	o	244	90% 9%
14	T	32	78% 16% 6%
14	t	32	81% 12% 6%
15	U	104	83% 10% 8%
15	u	104	88% 7%
16	V	137	96%

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Mol	Chain	Length	Quality of chain
16	v	137	89% 10%
17	X	40	85% 10% 5%
17	x	40	90% 5% 5%
18	Y	30	87% 10%
18	y	30	63% 33%
19	Z	62	89% 10%
19	z	62	77% 23%
20	R	34	6% 76% 21%

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
27	GOL	D	701	-	-	X	-
27	GOL	D	712	-	X	-	-
40	HEC	V	201	X	-	-	-
40	HEC	v	201	X	-	-	-

2 Entry composition (i)

There are 41 unique types of molecules in this entry. The entry contains 62674 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	222	0
			4338	2836	717	760	25			
1	a	334	Total	C	N	O	S	0	220	0
			4318	2821	715	757	25			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	279	PRO	ARG	conflict	UNP P51765
a	279	PRO	ARG	conflict	UNP P51765

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	504	Total	C	N	O	S	0	22	0
			4166	2735	694	724	13			
2	b	504	Total	C	N	O	S	0	19	0
			4134	2718	687	716	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	451	Total	C	N	O	S	0	99	0
			4272	2796	715	743	18			
3	c	455	Total	C	N	O	S	0	101	0
			4316	2827	720	751	18			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	19	ASN	-	expression tag	UNP D0VWR7
C	20	SER	-	expression tag	UNP D0VWR7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	21	ILE	-	expression tag	UNP D0VWR7
C	22	PHE	-	expression tag	UNP D0VWR7
c	19	ASN	-	expression tag	UNP D0VWR7
c	20	SER	-	expression tag	UNP D0VWR7
c	21	ILE	-	expression tag	UNP D0VWR7
c	22	PHE	-	expression tag	UNP D0VWR7

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	342	Total	C	N	O	S	0	115	0
			3625	2390	597	623	15			
4	d	341	Total	C	N	O	S	0	119	0
			3658	2412	605	626	15			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	81	Total	C	N	O	0	0	0
			662	432	107	123			
5	e	79	Total	C	N	O	0	2	0
			670	439	110	121			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	34	Total	C	N	O	S	0	0	0
			275	187	45	42	1			
6	f	31	Total	C	N	O	S	0	1	0
			261	179	43	38	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	64	Total	C	N	O	S	0	0	0
			506	339	81	84	2			
7	h	64	Total	C	N	O	S	0	1	0
			517	345	85	85	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	38	Total	C	N	O	S	0	0	0
			314	211	48	54	1			
8	i	38	Total	C	N	O	S	0	0	0
			314	211	48	54	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	38	Total	C	N	O	S	0	0	0
			272	182	42	47	1			
9	j	39	Total	C	N	O	S	0	0	0
			277	185	43	48	1			

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

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

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	33	LEU	PHE	conflict	UNP P19054
K	39	TRP	VAL	conflict	UNP P19054
k	33	LEU	PHE	conflict	UNP P19054
k	39	TRP	VAL	conflict	UNP P19054

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	L	36	Total	C	N	O	0	2	0
			311	207	49	55			
11	l	36	Total	C	N	O	0	2	0
			311	207	49	55			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	33	Total	C	N	O	S	0	1	0
			268	179	39	49	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	m	34	Total	C	N	O	S	0	2	0
			286	190	43	52	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	8	LEU	PHE	conflict	UNP P12312
m	8	LEU	PHE	conflict	UNP P12312

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	243	Total	C	N	O	S	0	10	0
			1958	1221	335	398	4			
13	o	243	Total	C	N	O	S	0	8	0
			1933	1207	330	392	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	30	Total	C	N	O	S	0	6	0
			311	213	48	48	2			
14	t	30	Total	C	N	O	S	0	5	0
			302	208	47	45	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	U	96	Total	C	N	O	0	4	0
			800	508	133	159			
15	u	97	Total	C	N	O	0	5	0
			815	519	135	161			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total	C	N	O	S	0	6	0
			1120	711	185	220	4			
16	v	137	Total	C	N	O	S	0	6	0
			1117	712	185	216	4			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	X	38	Total 289	C 194	N 46	O 49	0	1	0
17	x	38	Total 281	C 188	N 45	O 48	0	0	0

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

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

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

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

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

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

- Molecule 21 is FE (II) ION (CCD ID: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	A	1	Total 2	Fe 2	0	1
21	a	1	Total 2	Fe 2	0	1

- Molecule 22 is CHLORIDE ION (CCD ID: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

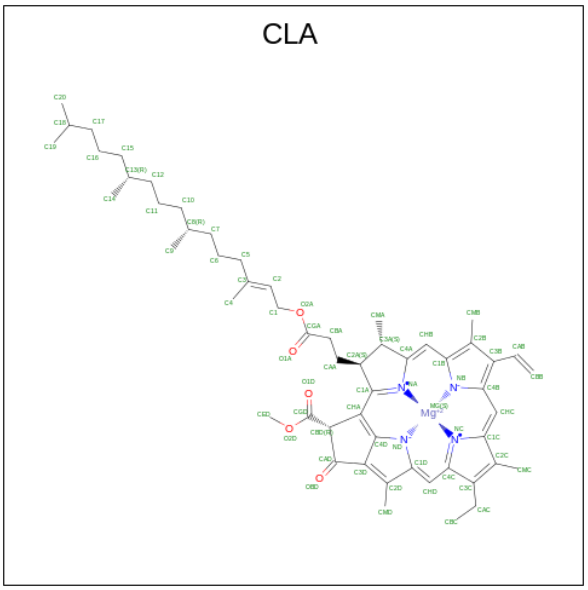
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	2	Total 4	Cl 4	0	2

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	a	2	Total Cl 4 4	0	2

- Molecule 23 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	A	1	Total C Mg N O 130 110 2 8 10	0	1
23	A	1	Total C Mg N O 130 110 2 8 10	0	1
23	A	1	Total C Mg N O 130 110 2 8 10	0	1
23	A	1	Total C Mg N O 65 55 1 4 5	0	0
23	B	1	Total C Mg N O 65 55 1 4 5	0	0
23	B	1	Total C Mg N O 65 55 1 4 5	0	0
23	B	1	Total C Mg N O 65 55 1 4 5	0	0
23	B	1	Total C Mg N O 65 55 1 4 5	0	0
23	B	1	Total C Mg N O 65 55 1 4 5	0	0
23	B	1	Total C Mg N O 65 55 1 4 5	0	0

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

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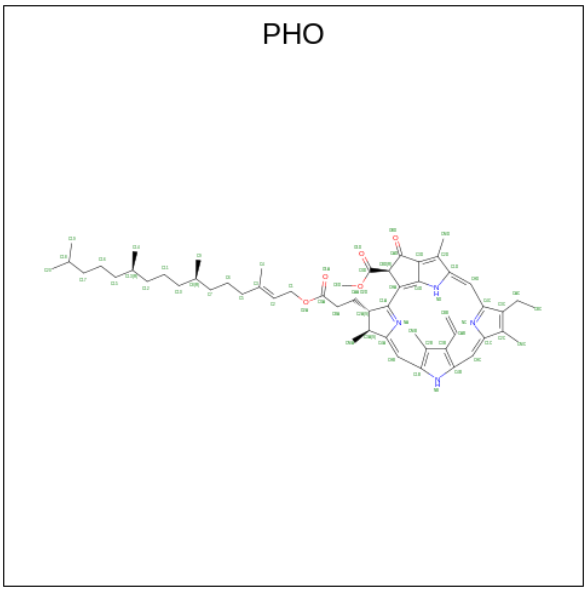
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	D	1	Total	C	Mg	N	O	0	1
			130	110	2	8	10		
23	D	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	a	1	Total	C	Mg	N	O	0	1
			130	110	2	8	10		
23	a	1	Total	C	Mg	N	O	0	1
			130	110	2	8	10		
23	a	1	Total	C	Mg	N	O	0	1
			130	110	2	8	10		
23	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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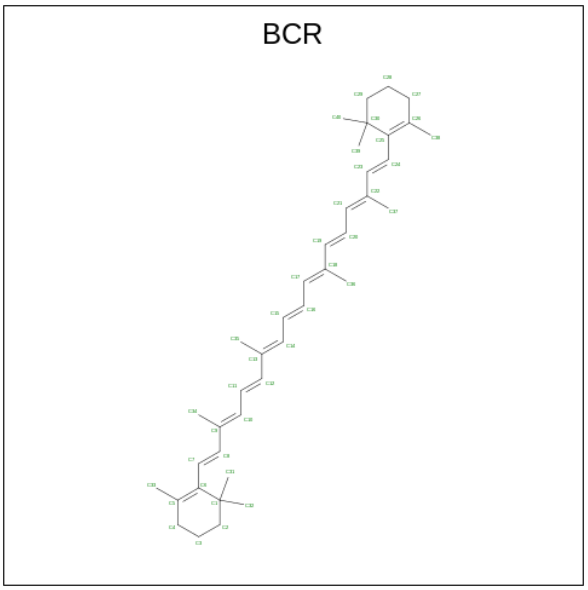
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	d	1	Total	C	Mg	N	O	0	1
			130	110	2	8	10		
23	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 24 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



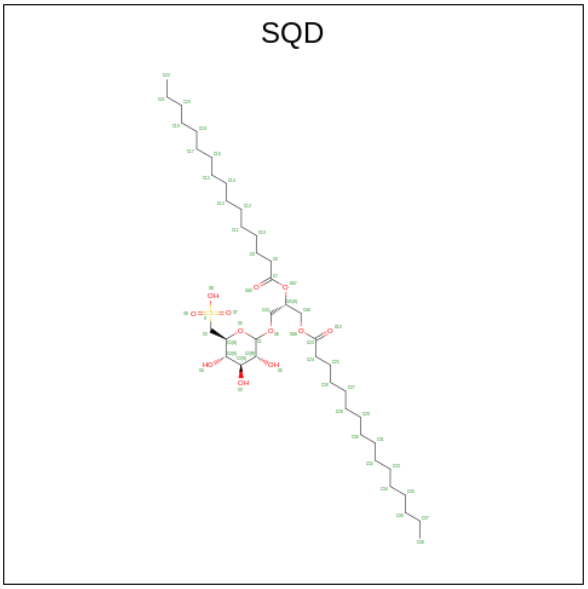
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	A	1	Total	C	N	O	0	1
			128	110	8	10		
24	A	1	Total	C	N	O	0	1
			128	110	8	10		
24	a	1	Total	C	N	O	0	1
			128	110	8	10		
24	a	1	Total	C	N	O	0	1
			128	110	8	10		

- Molecule 25 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



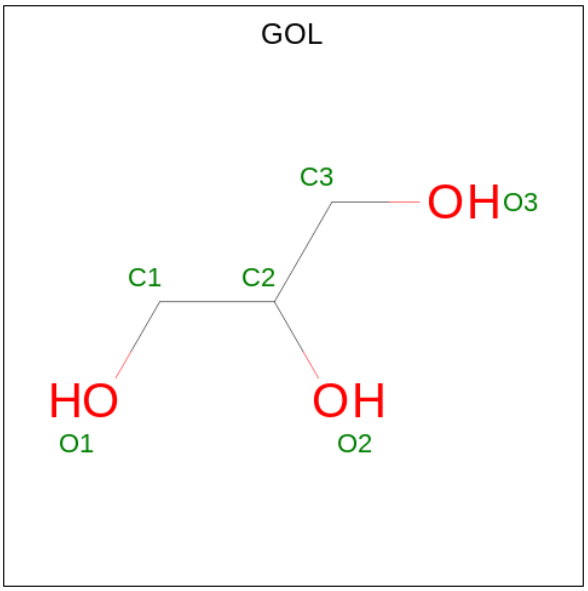
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	D	1	Total C 40 40	0	0
25	H	1	Total C 40 40	0	0
25	K	1	Total C 40 40	0	0
25	T	1	Total C 40 40	0	0
25	Y	1	Total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

- Molecule 26 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	A	1	Total	C	O	S	0	1
			108	82	24	2		
26	A	1	Total	C	O	S	0	0
			54	41	12	1		
26	B	1	Total	C	O	S	0	0
			54	41	12	1		
26	X	1	Total	C	O	S	0	0
			43	30	12	1		
26	a	1	Total	C	O	S	0	1
			108	82	24	2		
26	a	1	Total	C	O	S	0	0
			54	41	12	1		
26	b	1	Total	C	O	S	0	0
			54	41	12	1		
26	f	1	Total	C	O	S	0	0
			43	30	12	1		

- Molecule 27 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



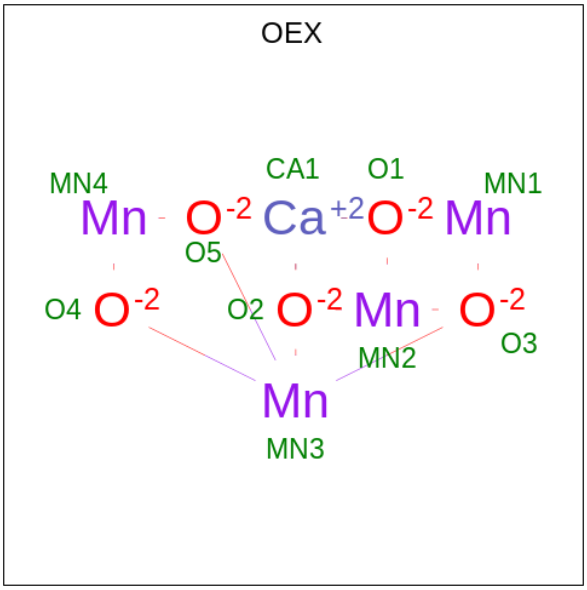
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	A	1	Total	C	O	0	0
			6	3	3		
27	B	1	Total	C	O	0	0
			6	3	3		
27	B	1	Total	C	O	0	0
			6	3	3		
27	B	1	Total	C	O	0	0
			6	3	3		
27	C	1	Total	C	O	0	1
			12	6	6		
27	D	1	Total	C	O	0	0
			6	3	3		
27	D	1	Total	C	O	0	0
			6	3	3		
27	O	1	Total	C	O	0	0
			6	3	3		
27	O	1	Total	C	O	0	0
			6	3	3		
27	V	1	Total	C	O	0	1
			12	6	6		
27	a	1	Total	C	O	0	0
			6	3	3		
27	a	1	Total	C	O	0	0
			6	3	3		
27	b	1	Total	C	O	0	0
			6	3	3		
27	b	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	c	1	Total C O 12 6 6	0	1
27	c	1	Total C O 6 3 3	0	0
27	d	1	Total C O 6 3 3	0	0
27	l	1	Total C O 12 6 6	0	1
27	o	1	Total C O 6 3 3	0	0
27	o	1	Total C O 6 3 3	0	0
27	v	1	Total C O 12 6 6	0	1

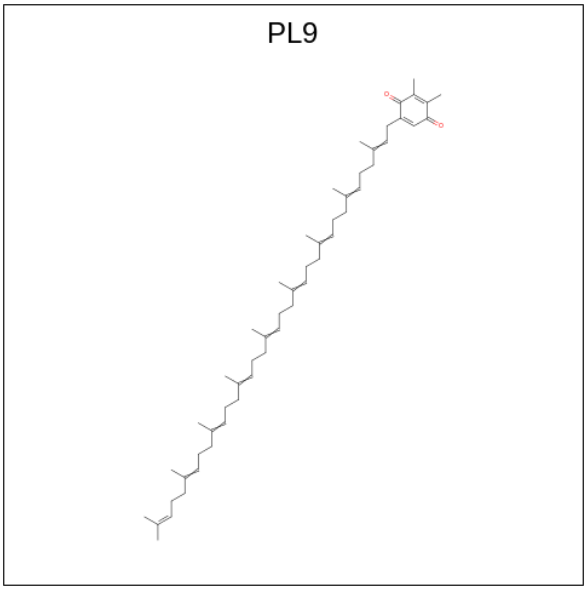
- Molecule 28 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: $CaMn_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	A	1	Total Ca Mn O 20 2 8 10	0	1
28	a	1	Total Ca Mn O 20 2 8 10	0	1

- Molecule 29 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: $C_{53}H_{80}O_2$)

(labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	1	Total C O 110 106 4	0	1
29	D	1	Total C O 110 106 4	0	1
29	a	1	Total C O 110 106 4	0	1
29	d	1	Total C O 110 106 4	0	1

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

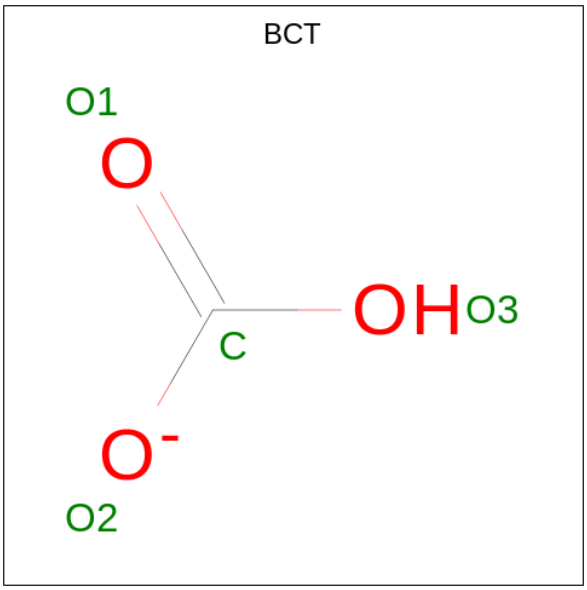
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	A	1	Total C O 28 23 5	0	0
30	B	1	Total C O 33 28 5	0	0
30	D	2	Total C O 57 51 6	0	0
30	I	1	Total C O 40 35 5	0	0
30	J	1	Total C 10 10	0	0
30	K	1	Total C O 68 58 10	0	1
30	X	1	Total C O 18 16 2	0	0

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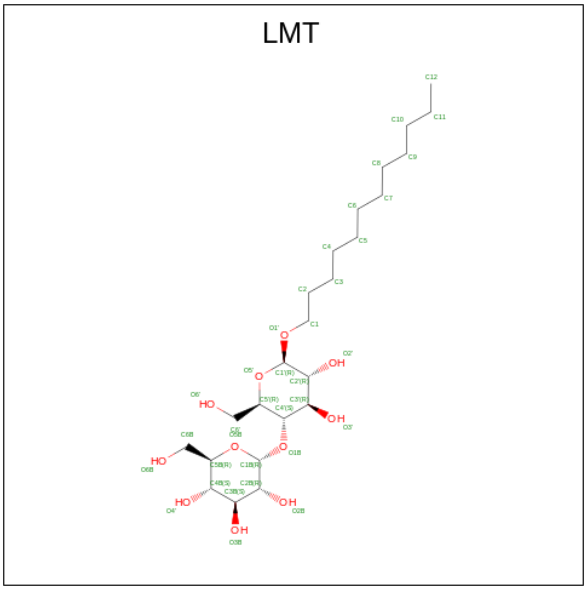
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	a	1	Total C O 30 25 5	0	0
30	b	1	Total C O 33 28 5	0	0
30	c	1	Total C O 64 54 10	0	1
30	d	2	Total C O 53 47 6	0	0
30	i	1	Total C O 40 35 5	0	0
30	j	1	Total C 10 10	0	0
30	l	1	Total C 10 10	0	0
30	m	1	Total C 10 10	0	0
30	x	1	Total C O 18 16 2	0	0

- Molecule 31 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 32 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



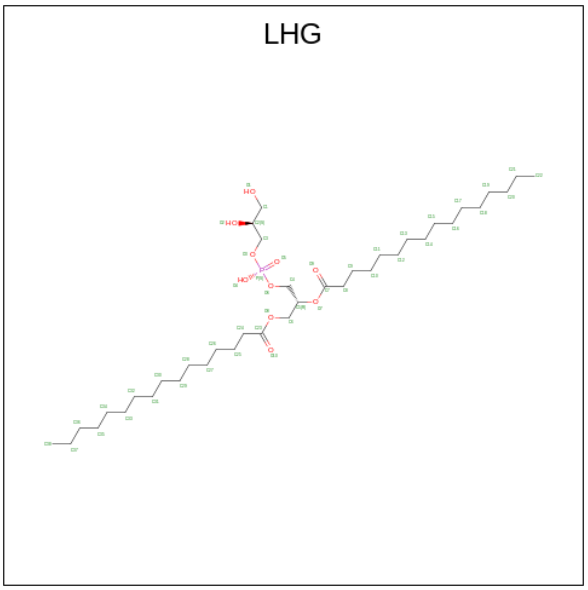
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	A	1	Total C O 35 24 11	0	0
32	A	1	Total C O 35 24 11	0	0
32	B	1	Total C O 35 24 11	0	0
32	B	1	Total C O 35 24 11	0	0
32	B	1	Total C O 25 19 6	0	0
32	F	1	Total C O 35 24 11	0	0
32	M	1	Total C O 35 24 11	0	0
32	T	1	Total C O 35 24 11	0	0
32	a	1	Total C O 35 24 11	0	0
32	b	1	Total C O 25 19 6	0	0
32	b	1	Total C O 25 19 6	0	0
32	e	1	Total C O 35 24 11	0	0
32	m	1	Total C O 35 24 11	0	0

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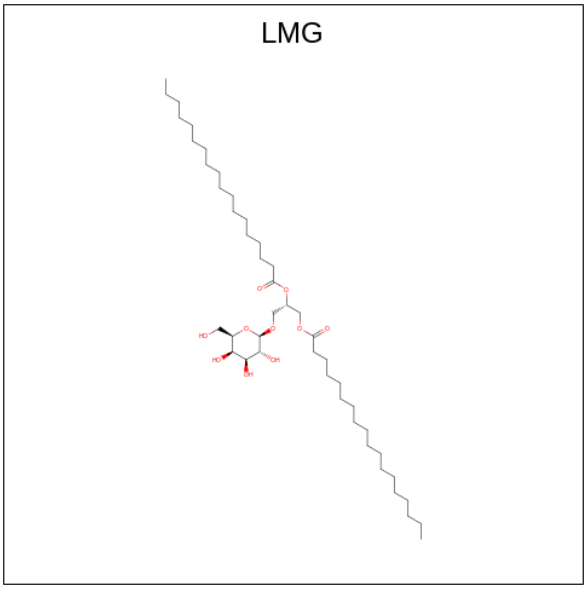
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	t	1	Total C O 26 19 7	0	0

- Molecule 33 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



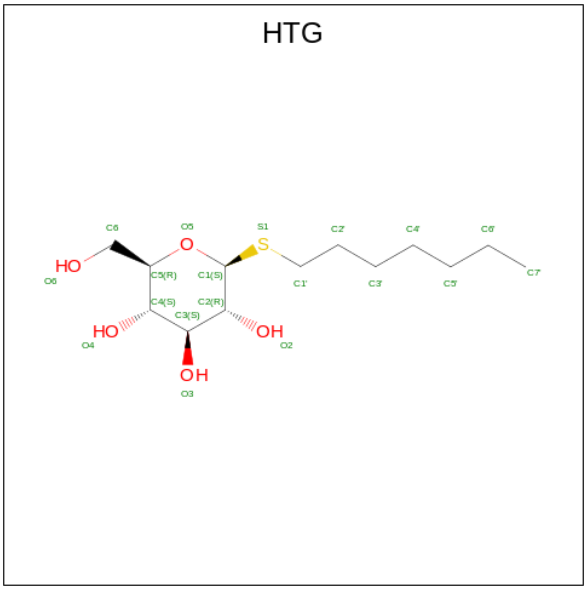
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	A	1	Total C O P 98 76 20 2	0	1
33	D	1	Total C O P 98 76 20 2	0	1
33	D	1	Total C O P 98 76 20 2	0	1
33	E	1	Total C O P 84 62 20 2	0	1
33	L	1	Total C O P 98 76 20 2	0	1
33	a	1	Total C O P 84 62 20 2	0	1
33	b	1	Total C O P 98 76 20 2	0	1
33	d	1	Total C O P 98 76 20 2	0	1
33	d	1	Total C O P 98 76 20 2	0	1
33	d	1	Total C O P 98 76 20 2	0	1

- Molecule 34 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



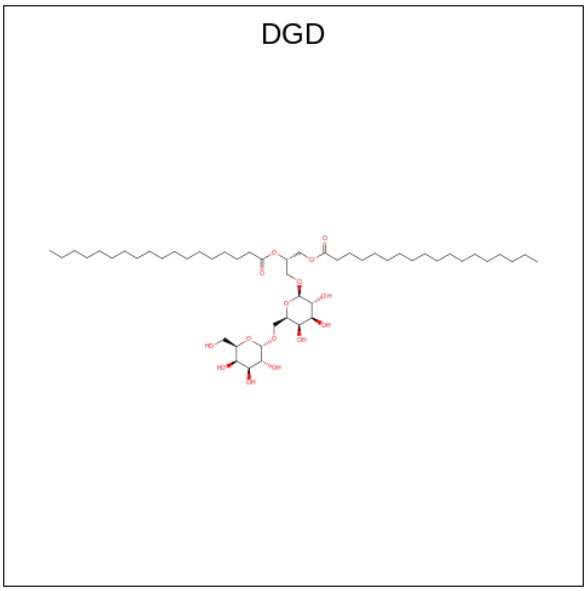
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	B	1	Total	C	O	0	0
			51	41	10		
34	C	1	Total	C	O	0	0
			51	41	10		
34	C	1	Total	C	O	0	0
			51	41	10		
34	C	1	Total	C	O	0	0
			51	41	10		
34	D	1	Total	C	O	0	0
			51	41	10		
34	c	1	Total	C	O	0	0
			51	41	10		
34	c	1	Total	C	O	0	0
			51	41	10		
34	c	1	Total	C	O	0	0
			51	41	10		
34	d	1	Total	C	O	0	0
			51	41	10		
34	m	1	Total	C	O	0	0
			51	41	10		
34	Z	1	Total	C	O	0	0
			37	27	10		
34	z	1	Total	C	O	0	0
			39	29	10		

- Molecule 35 is heptyl 1-thio-beta-D-glucopyranoside (CCD ID: HTG) (formula: $C_{13}H_{26}O_5S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	B	1	Total C O S 19 13 5 1	0	0
35	B	1	Total C O S 19 13 5 1	0	0
35	C	1	Total C O S 19 13 5 1	0	0
35	D	1	Total C O S 16 10 5 1	0	0
35	V	1	Total C O 11 6 5	0	0
35	b	1	Total C O S 19 13 5 1	0	0
35	b	1	Total C O S 19 13 5 1	0	0
35	b	1	Total C O S 19 13 5 1	0	0
35	c	1	Total C O S 19 13 5 1	0	0
35	d	1	Total C O S 16 10 5 1	0	0
35	o	1	Total C O S 19 13 5 1	0	0

- Molecule 36 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	C	1	Total C O 124 94 30	0	1
36	C	1	Total C O 124 94 30	0	1
36	C	1	Total C O 62 47 15	0	0
36	H	1	Total C O 62 47 15	0	0
36	c	1	Total C O 124 94 30	0	1
36	c	1	Total C O 124 94 30	0	1
36	c	1	Total C O 62 47 15	0	0
36	h	1	Total C O 62 47 15	0	0

- Molecule 37 is CALCIUM ION (CCD ID: CA) (formula: Ca).

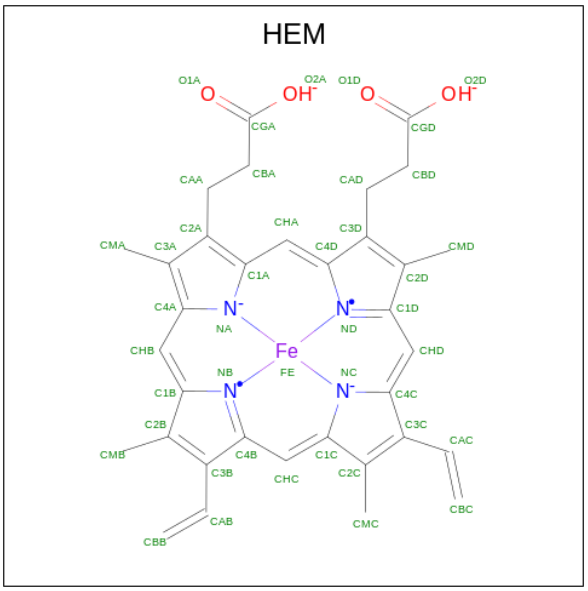
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	C	1	Total Ca 1 1	0	0
37	F	1	Total Ca 1 1	0	0
37	O	1	Total Ca 1 1	0	0
37	c	2	Total Ca 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	f	1	Total Ca 1 1	0	0
37	o	1	Total Ca 1 1	0	0

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

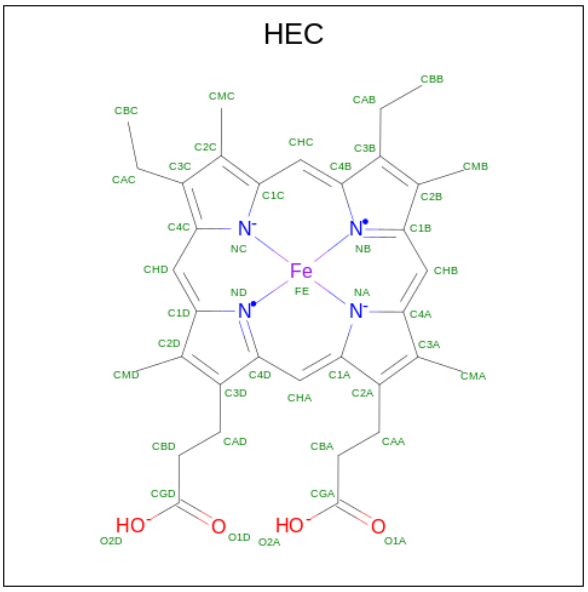


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	F	1	Total C Fe N O 43 34 1 4 4	0	0
38	f	1	Total C Fe N O 43 34 1 4 4	0	0

- Molecule 39 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 40 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



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

- Molecule 41 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	A	138	Total	O	0	86
			223	223		
41	B	188	Total	O	0	2
			190	190		
41	C	167	Total	O	0	38
			204	204		
41	D	121	Total	O	0	35
			156	156		
41	E	16	Total	O	0	0
			16	16		
41	F	6	Total	O	0	0
			6	6		
41	H	21	Total	O	0	0
			21	21		
41	I	5	Total	O	0	0
			5	5		
41	J	7	Total	O	0	0
			7	7		
41	K	5	Total	O	0	0
			5	5		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	L	8	Total O 9 9	0	1
41	M	6	Total O 6 6	0	0
41	O	105	Total O 109 109	0	4
41	T	11	Total O 14 14	0	3
41	U	46	Total O 48 48	0	2
41	V	79	Total O 80 80	0	1
41	X	9	Total O 9 9	0	0
41	a	134	Total O 215 215	0	82
41	b	199	Total O 202 202	0	3
41	c	160	Total O 193 193	0	34
41	d	116	Total O 147 147	0	31
41	e	9	Total O 9 9	0	0
41	f	3	Total O 3 3	0	0
41	h	18	Total O 18 18	0	0
41	i	2	Total O 2 2	0	0
41	j	2	Total O 2 2	0	0
41	k	3	Total O 3 3	0	0
41	l	8	Total O 10 10	0	2
41	m	13	Total O 13 13	0	0
41	o	99	Total O 103 103	0	4
41	t	6	Total O 9 9	0	3

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	u	50	Total O 51 51	0	1
41	v	57	Total O 59 59	0	2
41	x	6	Total O 6 6	0	0
41	y	2	Total O 2 2	0	0

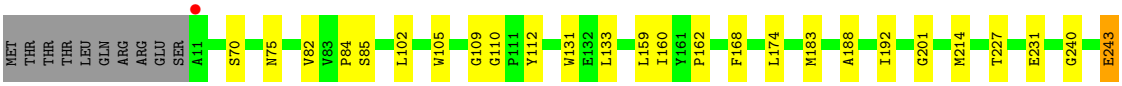
3 Residue-property plots (i)

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

• Molecule 1: Photosystem II protein D1

Chain A:



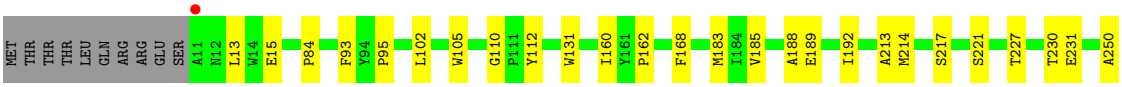




• Molecule 1: Photosystem II protein D1

Chain a:





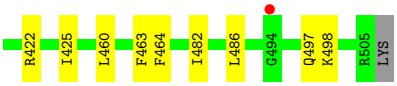


• Molecule 2: Photosystem II CP47 reaction center protein

Chain B:



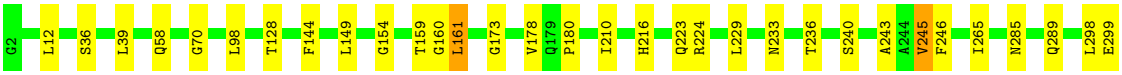




• Molecule 2: Photosystem II CP47 reaction center protein

Chain b:



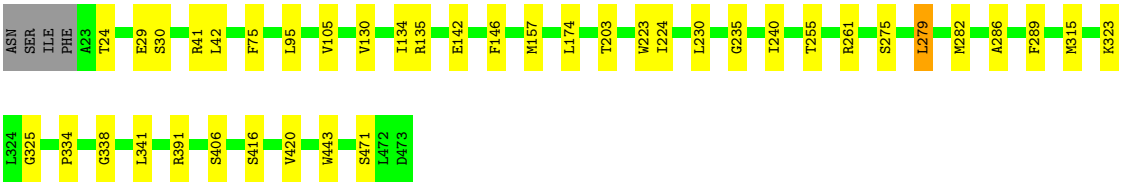




• Molecule 3: Photosystem II CP43 reaction center protein

Chain C:

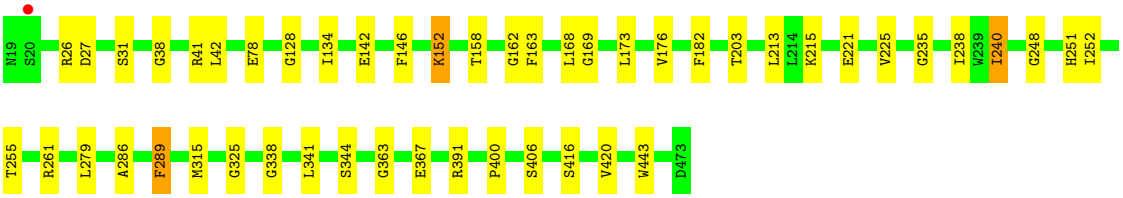




• Molecule 3: Photosystem II CP43 reaction center protein

Chain c:

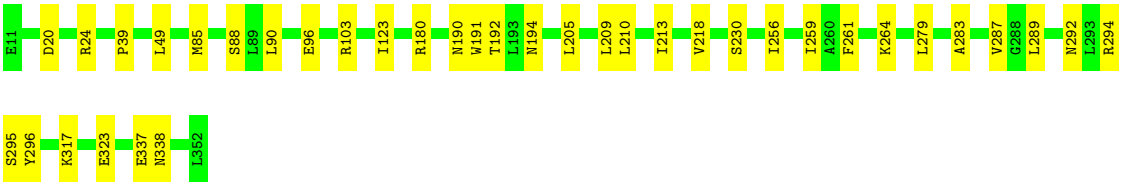




• Molecule 4: Photosystem II D2 protein

Chain D:





• Molecule 4: Photosystem II D2 protein

Chain d:

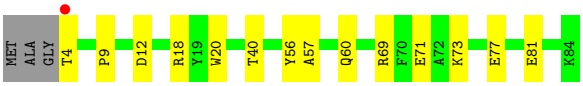




• Molecule 5: Cytochrome b559 subunit alpha

Chain E:





• Molecule 5: Cytochrome b559 subunit alpha

Chain e:

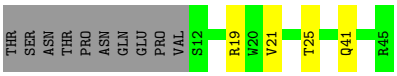




• Molecule 6: Cytochrome b559 subunit beta

Chain F:

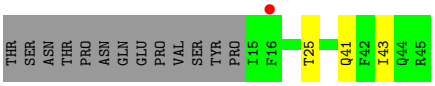




• Molecule 6: Cytochrome b559 subunit beta

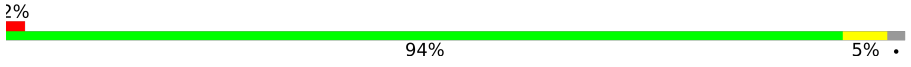
Chain f:

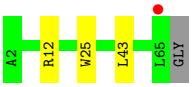




• Molecule 7: Photosystem II reaction center protein H

Chain H:

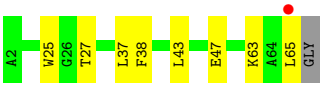




• Molecule 7: Photosystem II reaction center protein H

Chain h:

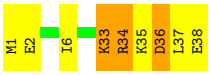




• Molecule 8: Photosystem II reaction center protein I

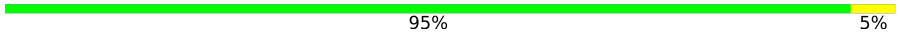
Chain I:





• Molecule 8: Photosystem II reaction center protein I

Chain i:





• Molecule 9: Photosystem II reaction center protein J

Chain J:





• Molecule 9: Photosystem II reaction center protein J

Chain j:





• Molecule 10: Photosystem II reaction center protein K

Chain K:

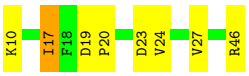




• Molecule 10: Photosystem II reaction center protein K

Chain k:

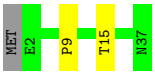




• Molecule 11: Photosystem II reaction center protein L

Chain L:





• Molecule 11: Photosystem II reaction center protein L

Chain l:

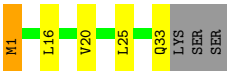




• Molecule 12: Photosystem II reaction center protein M

Chain M:

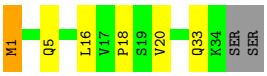




• Molecule 12: Photosystem II reaction center protein M

Chain m:





• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:

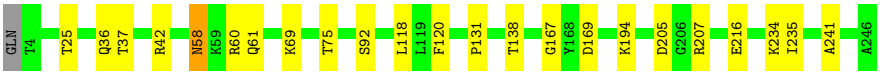




• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:

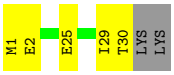




• Molecule 14: Photosystem II reaction center protein T

Chain T:

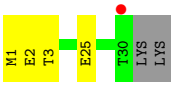




• Molecule 14: Photosystem II reaction center protein T

Chain t:

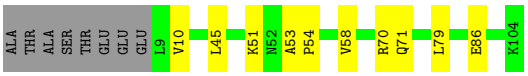




• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:

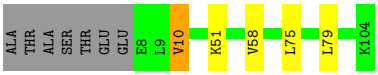




• Molecule 15: Photosystem II 12 kDa extrinsic protein

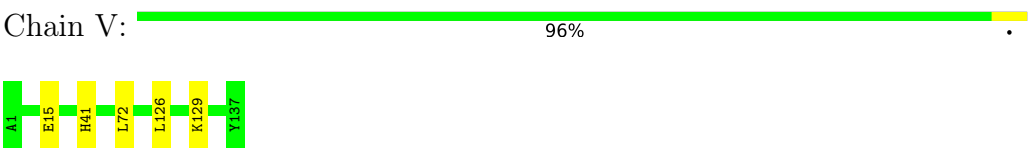
Chain u:





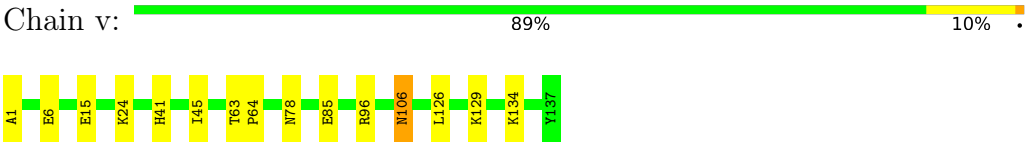
• Molecule 16: Cytochrome c-550

Chain V:



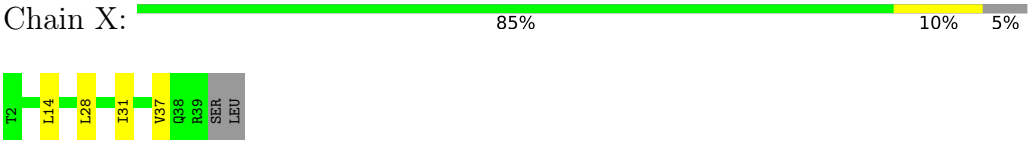
• Molecule 16: Cytochrome c-550

Chain v:



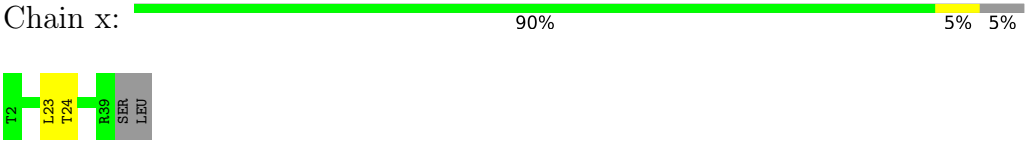
• Molecule 17: Photosystem II reaction center protein X

Chain X:



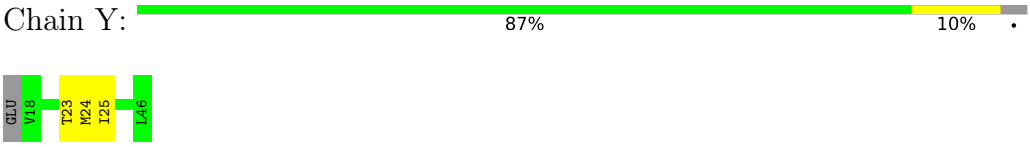
• Molecule 17: Photosystem II reaction center protein X

Chain x:



• Molecule 18: Photosystem II reaction center protein Ycf12

Chain Y:



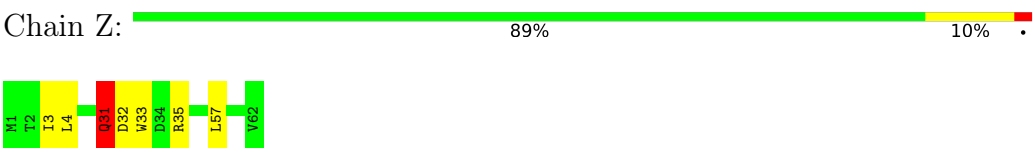
• Molecule 18: Photosystem II reaction center protein Ycf12

Chain y:



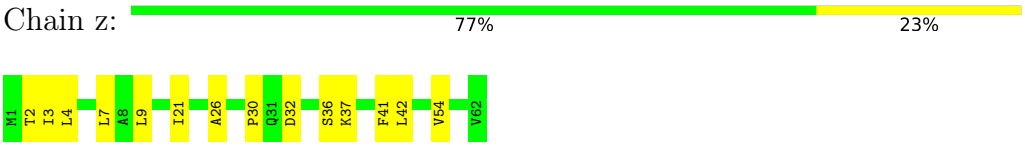
• Molecule 19: Photosystem II reaction center protein Z

Chain Z:



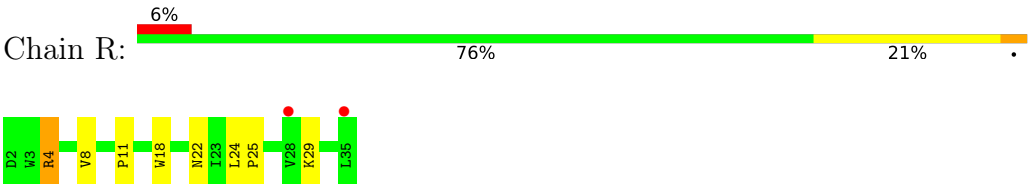
• Molecule 19: Photosystem II reaction center protein Z

Chain z:



• Molecule 20: Photosystem II protein Y

Chain R:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	125.75Å 231.60Å 288.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 – 2.30 19.98 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.98-2.30) 99.7 (19.98-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.14 (at 2.30Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.139 , 0.180 0.145 , 0.180	Depositor DCC
R_{free} test set	21187 reflections (2.60%)	wwPDB-VP
Wilson B-factor (Å^2)	50.8	Xtriage
Anisotropy	0.541	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 69.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	62674	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.72% 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

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.27	0/4478	0.45	0/6098
1	a	0.25	0/4457	0.41	0/6069
2	B	0.35	0/4314	0.49	0/5879
2	b	0.33	0/4285	0.48	0/5841
3	C	0.27	0/4416	0.42	0/6013
3	c	0.28	0/4467	0.42	0/6082
4	D	0.32	0/3746	0.47	0/5102
4	d	0.30	0/3780	0.44	0/5147
5	E	0.32	0/681	0.50	0/928
5	e	0.29	0/690	0.46	0/939
6	F	0.30	0/284	0.46	0/387
6	f	0.29	0/269	0.45	0/365
7	H	0.30	0/519	0.47	0/708
7	h	0.30	0/530	0.48	0/722
8	I	0.29	0/311	0.42	0/419
8	i	0.32	0/311	0.45	0/419
9	J	0.33	0/278	0.45	0/376
9	j	0.27	0/283	0.43	0/383
10	K	0.32	0/303	0.48	0/416
10	k	0.34	0/303	0.47	0/416
11	L	0.36	0/318	0.46	0/433
11	l	0.37	0/318	0.45	0/433
12	M	0.37	0/261	0.50	0/357
12	m	0.30	0/279	0.47	0/380
13	O	0.34	0/1991	0.52	0/2698
13	o	0.32	0/1966	0.50	0/2665
14	T	0.33	0/310	0.43	0/419
14	t	0.32	0/301	0.41	0/406
15	U	0.36	0/811	0.54	0/1095
15	u	0.35	0/826	0.55	0/1116
16	V	0.34	0/1142	0.48	0/1545

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
16	v	0.30	0/1139	0.46	0/1542
17	X	0.22	0/292	0.33	0/395
17	x	0.23	0/284	0.36	0/384
18	Y	0.24	0/216	0.42	0/289
18	y	0.25	0/216	0.40	0/289
19	Z	0.23	0/490	0.37	0/669
19	z	0.22	0/490	0.33	0/669
20	R	0.27	0/279	0.35	0/383
All	All	0.30	0/50634	0.46	0/68876

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	4338	0	4142	26	0
1	a	4318	0	4124	42	0
2	B	4166	0	3999	31	0
2	b	4134	0	3976	48	0
3	C	4272	0	4138	28	0
3	c	4316	0	4183	37	0
4	D	3625	0	3489	36	0
4	d	3658	0	3522	28	0
5	E	662	0	648	10	0
5	e	670	0	655	7	0
6	F	275	0	282	3	0
6	f	261	0	269	4	0
7	H	506	0	529	2	0
7	h	517	0	541	6	0
8	I	314	0	328	5	0
8	i	314	0	328	1	0
9	J	272	0	279	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	j	277	0	284	4	0
10	K	293	0	305	5	0
10	k	293	0	305	6	0
11	L	311	0	320	2	0
11	l	311	0	320	5	0
12	M	268	0	285	5	0
12	m	286	0	305	7	0
13	O	1958	0	1920	20	0
13	o	1933	0	1900	12	0
14	T	311	0	318	3	0
14	t	302	0	311	4	0
15	U	800	0	796	5	0
15	u	815	0	817	4	0
16	V	1120	0	1122	3	0
16	v	1117	0	1131	9	0
17	X	289	0	322	4	0
17	x	281	0	312	2	0
18	Y	215	0	246	2	0
18	y	215	0	246	6	0
19	Z	479	0	516	5	0
19	z	479	0	516	3	0
20	R	273	0	305	4	0
21	A	2	0	0	0	0
21	a	2	0	0	0	0
22	A	4	0	0	0	0
22	a	4	0	0	0	0
23	A	455	0	504	20	0
23	B	1040	0	1152	29	0
23	C	845	0	936	41	0
23	D	195	0	216	6	0
23	a	455	0	504	21	0
23	b	1040	0	1152	28	0
23	c	845	0	936	37	0
23	d	195	0	216	7	0
24	A	256	0	296	7	0
24	a	256	0	296	4	0
25	A	40	0	56	1	0
25	B	120	0	168	6	0
25	C	80	0	112	3	0
25	D	40	0	56	1	0
25	H	40	0	56	1	0
25	K	40	0	56	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	T	40	0	56	6	0
25	Y	40	0	56	1	0
25	a	40	0	56	1	0
25	b	120	0	168	8	0
25	c	80	0	112	4	0
25	d	40	0	56	3	0
25	h	40	0	56	4	0
25	k	40	0	56	1	0
25	t	40	0	56	5	0
25	y	40	0	56	2	0
26	A	162	0	232	5	0
26	B	54	0	78	2	0
26	X	43	0	53	2	0
26	a	162	0	232	10	0
26	b	54	0	78	2	0
26	f	43	0	53	1	0
27	A	6	0	8	0	0
27	B	18	0	24	2	0
27	C	12	0	16	0	0
27	D	12	0	15	6	0
27	O	12	0	16	4	0
27	V	12	0	16	0	0
27	a	12	0	16	5	0
27	b	12	0	16	2	0
27	c	18	0	24	1	0
27	d	6	0	8	0	0
27	l	12	0	16	2	0
27	o	12	0	16	0	0
27	v	12	0	16	2	0
28	A	20	0	0	0	0
28	a	20	0	0	0	0
29	A	110	0	160	18	0
29	D	110	0	160	0	0
29	a	110	0	160	9	0
29	d	110	0	160	1	0
30	A	28	0	0	0	0
30	B	33	0	0	1	0
30	D	57	0	0	0	0
30	I	40	0	0	0	0
30	J	10	0	0	0	0
30	K	68	0	0	0	0
30	X	18	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	a	30	0	0	0	0
30	b	33	0	0	0	0
30	c	64	0	0	0	0
30	d	53	0	0	0	0
30	i	40	0	0	0	0
30	j	10	0	0	0	0
30	l	10	0	0	0	0
30	m	10	0	0	0	0
30	x	18	0	0	0	0
31	A	8	0	0	0	0
31	a	8	0	0	0	0
32	A	70	0	92	2	0
32	B	95	0	127	3	0
32	F	35	0	46	0	0
32	M	35	0	46	1	0
32	T	35	0	46	1	0
32	a	35	0	46	1	0
32	b	50	0	70	1	0
32	e	35	0	46	1	0
32	m	35	0	46	2	0
32	t	26	0	35	2	0
33	A	98	0	148	3	0
33	D	196	0	296	13	0
33	E	84	0	114	7	0
33	L	98	0	148	0	0
33	a	84	0	114	8	0
33	b	98	0	148	1	0
33	d	294	0	444	26	0
34	B	51	0	72	1	0
34	C	153	0	216	2	0
34	D	51	0	72	0	0
34	Z	37	0	44	2	0
34	c	153	0	216	2	0
34	d	51	0	72	3	0
34	m	51	0	72	2	0
34	z	39	0	48	2	0
35	B	38	0	52	3	0
35	C	19	0	26	0	0
35	D	16	0	17	0	0
35	V	11	0	10	0	0
35	b	57	0	78	3	0
35	c	19	0	26	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	d	16	0	17	1	0
35	o	19	0	26	2	0
36	C	310	0	410	9	0
36	H	62	0	82	1	0
36	c	310	0	410	10	0
36	h	62	0	82	2	0
37	C	1	0	0	0	0
37	F	1	0	0	0	0
37	O	1	0	0	0	0
37	c	2	0	0	0	0
37	f	1	0	0	0	0
37	o	1	0	0	0	0
38	F	43	0	30	0	0
38	f	43	0	30	0	0
39	J	1	0	0	0	0
39	j	1	0	0	0	0
40	V	43	0	30	1	0
40	v	43	0	30	0	0
41	A	223	0	0	0	0
41	B	190	0	0	1	0
41	C	204	0	0	3	0
41	D	156	0	0	5	0
41	E	16	0	0	1	0
41	F	6	0	0	0	0
41	H	21	0	0	0	0
41	I	5	0	0	0	0
41	J	7	0	0	0	0
41	K	5	0	0	0	0
41	L	9	0	0	0	0
41	M	6	0	0	0	0
41	O	109	0	0	1	0
41	T	14	0	0	0	0
41	U	48	0	0	0	0
41	V	80	0	0	0	0
41	X	9	0	0	0	0
41	a	215	0	0	3	0
41	b	202	0	0	0	0
41	c	193	0	0	5	0
41	d	147	0	0	1	0
41	e	9	0	0	0	0
41	f	3	0	0	0	0
41	h	18	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	i	2	0	0	0	0
41	j	2	0	0	0	0
41	k	3	0	0	0	0
41	l	10	0	0	0	0
41	m	13	0	0	0	0
41	o	103	0	0	1	0
41	t	9	0	0	1	0
41	u	51	0	0	1	0
41	v	59	0	0	0	0
41	x	6	0	0	0	0
41	y	2	0	0	0	0
All	All	62674	0	61527	641	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 5.

The worst 5 of 641 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)
23:B:604:CLA:H42	23:B:605:CLA:H2	1.44	0.98
27:D:701:GOL:H11	12:M:1:FME:HG2	1.46	0.97
1:a:250[B]:ALA:HA	2:b:491[B]:VAL:HG11	1.52	0.92
1:a:250[A]:ALA:HA	2:b:491[A]:VAL:HG11	1.53	0.88
23:B:601:CLA:H12	23:B:601:CLA:H71	1.60	0.81

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	553/344 (161%)	546 (99%)	5 (1%)	2 (0%)	30 38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	a	551/344 (160%)	544 (99%)	5 (1%)	2 (0%)	30	38
2	B	524/505 (104%)	514 (98%)	10 (2%)	0	100	100
2	b	521/505 (103%)	510 (98%)	11 (2%)	0	100	100
3	C	548/455 (120%)	539 (98%)	8 (2%)	1 (0%)	43	55
3	c	554/455 (122%)	542 (98%)	11 (2%)	1 (0%)	43	55
4	D	454/342 (133%)	437 (96%)	17 (4%)	0	100	100
4	d	457/342 (134%)	445 (97%)	12 (3%)	0	100	100
5	E	79/84 (94%)	78 (99%)	1 (1%)	0	100	100
5	e	79/84 (94%)	79 (100%)	0	0	100	100
6	F	32/44 (73%)	32 (100%)	0	0	100	100
6	f	30/44 (68%)	30 (100%)	0	0	100	100
7	H	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
7	h	63/65 (97%)	58 (92%)	4 (6%)	1 (2%)	7	7
8	I	36/38 (95%)	34 (94%)	1 (3%)	1 (3%)	4	2
8	i	36/38 (95%)	32 (89%)	4 (11%)	0	100	100
9	J	36/39 (92%)	33 (92%)	3 (8%)	0	100	100
9	j	37/39 (95%)	37 (100%)	0	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100
10	k	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
11	L	36/37 (97%)	36 (100%)	0	0	100	100
11	l	36/37 (97%)	36 (100%)	0	0	100	100
12	M	32/36 (89%)	32 (100%)	0	0	100	100
12	m	34/36 (94%)	34 (100%)	0	0	100	100
13	O	251/244 (103%)	242 (96%)	7 (3%)	2 (1%)	16	20
13	o	249/244 (102%)	244 (98%)	5 (2%)	0	100	100
14	T	33/32 (103%)	33 (100%)	0	0	100	100
14	t	32/32 (100%)	32 (100%)	0	0	100	100
15	U	97/104 (93%)	92 (95%)	5 (5%)	0	100	100
15	u	99/104 (95%)	96 (97%)	3 (3%)	0	100	100
16	V	140/137 (102%)	137 (98%)	3 (2%)	0	100	100
16	v	140/137 (102%)	134 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
17	X	37/40 (92%)	36 (97%)	1 (3%)	0	100 100
17	x	36/40 (90%)	36 (100%)	0	0	100 100
18	Y	27/30 (90%)	25 (93%)	2 (7%)	0	100 100
18	y	27/30 (90%)	27 (100%)	0	0	100 100
19	Z	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	7 7
19	z	60/62 (97%)	59 (98%)	0	1 (2%)	7 7
20	R	32/34 (94%)	31 (97%)	1 (3%)	0	100 100
All	All	6180/5384 (115%)	6040 (98%)	128 (2%)	12 (0%)	43 55

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
8	I	36	ASP
13	O	26	ALA
3	c	416	SER
19	Z	31	GLN

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	444/279 (159%)	442 (100%)	2 (0%)	81 90
1	a	442/279 (158%)	441 (100%)	1 (0%)	87 94
2	B	423/403 (105%)	420 (99%)	3 (1%)	76 87
2	b	420/403 (104%)	410 (98%)	10 (2%)	43 62
3	C	431/356 (121%)	421 (98%)	10 (2%)	44 63
3	c	437/356 (123%)	430 (98%)	7 (2%)	55 73
4	D	368/277 (133%)	365 (99%)	3 (1%)	73 86
4	d	372/277 (134%)	368 (99%)	4 (1%)	65 81
5	E	72/73 (99%)	70 (97%)	2 (3%)	38 56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	e	72/73 (99%)	71 (99%)	1 (1%)	59 76
6	F	28/38 (74%)	28 (100%)	0	100 100
6	f	26/38 (68%)	26 (100%)	0	100 100
7	H	54/54 (100%)	52 (96%)	2 (4%)	30 45
7	h	55/54 (102%)	54 (98%)	1 (2%)	51 70
8	I	34/34 (100%)	32 (94%)	2 (6%)	18 26
8	i	34/34 (100%)	33 (97%)	1 (3%)	37 55
9	J	26/27 (96%)	23 (88%)	3 (12%)	5 6
9	j	26/27 (96%)	25 (96%)	1 (4%)	29 44
10	K	30/30 (100%)	26 (87%)	4 (13%)	4 4
10	k	30/30 (100%)	27 (90%)	3 (10%)	7 9
11	L	36/35 (103%)	36 (100%)	0	100 100
11	l	36/35 (103%)	35 (97%)	1 (3%)	38 56
12	M	30/32 (94%)	28 (93%)	2 (7%)	15 21
12	m	32/32 (100%)	30 (94%)	2 (6%)	16 23
13	O	216/207 (104%)	211 (98%)	5 (2%)	44 63
13	o	213/207 (103%)	206 (97%)	7 (3%)	33 50
14	T	32/28 (114%)	28 (88%)	4 (12%)	4 5
14	t	31/28 (111%)	31 (100%)	0	100 100
15	U	86/89 (97%)	84 (98%)	2 (2%)	44 63
15	u	88/89 (99%)	86 (98%)	2 (2%)	44 63
16	V	123/117 (105%)	122 (99%)	1 (1%)	73 86
16	v	123/117 (105%)	119 (97%)	4 (3%)	33 50
17	X	32/33 (97%)	31 (97%)	1 (3%)	35 52
17	x	31/33 (94%)	31 (100%)	0	100 100
18	Y	22/23 (96%)	22 (100%)	0	100 100
18	y	22/23 (96%)	19 (86%)	3 (14%)	3 4
19	Z	52/52 (100%)	50 (96%)	2 (4%)	29 44
19	z	52/52 (100%)	45 (86%)	7 (14%)	4 4
20	R	29/29 (100%)	27 (93%)	2 (7%)	14 20
All	All	5110/4403 (116%)	5005 (98%)	105 (2%)	47 66

5 of 105 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	c	142	GLU
9	j	9	LEU
19	z	3	ILE
3	c	240	ILE
4	d	259[B]	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
18	y	45	ASN
15	u	78	ASN
2	b	53	ASN
13	o	58	ASN
2	b	14	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	FME	I	1	8	8,9,10	0.51	0	7,9,11	1.21	1 (14%)
14	FME	t	1	14	8,9,10	0.74	0	7,9,11	1.65	2 (28%)
12	FME	m	1	12	8,9,10	0.49	0	7,9,11	1.51	2 (28%)
12	FME	M	1	12	8,9,10	0.62	0	7,9,11	1.32	1 (14%)
8	FME	i	1	8	8,9,10	0.68	0	7,9,11	1.33	0
14	FME	T	1	14	8,9,10	0.65	0	7,9,11	1.78	3 (42%)

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

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

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	T	1	FME	CA-N-CN	2.47	126.62	122.82
12	m	1	FME	CA-N-CN	-2.45	119.06	122.82
14	t	1	FME	O-C-CA	-2.42	118.43	124.78
14	t	1	FME	CA-N-CN	-2.41	119.12	122.82
12	m	1	FME	O1-CN-N	-2.41	118.93	125.27

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	M	1	FME	O1-CN-N-CA
12	M	1	FME	O-C-CA-CB
8	i	1	FME	O-C-CA-CB
14	t	1	FME	O-C-CA-CB
14	T	1	FME	N-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	m	1	FME	2	0
12	M	1	FME	2	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 274 ligands modelled in this entry, 21 are monoatomic and 20 are unknown - leaving 233 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	$\#\|Z\| > 2$
23	CLA	C	513	3	69,73,73	2.03	19 (27%)	83,113,113	2.87	32 (38%)
33	LHG	D	706[B]	-	48,48,48	0.87	2 (4%)	51,54,54	0.98	3 (5%)
27	GOL	a	419	-	5,5,5	1.28	1 (20%)	5,5,5	0.93	0
23	CLA	B	615	2	69,73,73	2.04	20 (28%)	83,113,113	2.87	31 (37%)
23	CLA	A	405[B]	41	69,73,73	2.00	19 (27%)	83,113,113	2.82	32 (38%)
23	CLA	B	614	2	69,73,73	2.05	19 (27%)	83,113,113	3.07	32 (38%)
23	CLA	B	606	2	69,73,73	1.95	20 (28%)	83,113,113	2.96	32 (38%)
33	LHG	D	707[A]	-	48,48,48	0.92	2 (4%)	51,54,54	0.99	4 (7%)
26	SQD	A	410[A]	-	53,54,54	0.93	3 (5%)	62,65,65	1.81	10 (16%)
23	CLA	b	603	2	69,73,73	1.99	20 (28%)	83,113,113	2.98	31 (37%)
28	OEX	A	413[A]	3,1,41	0,14,14	-	-	-		
33	LHG	a	420[B]	-	41,41,48	1.04	2 (4%)	44,47,54	0.93	2 (4%)
23	CLA	c	503	3	69,73,73	2.02	20 (28%)	83,113,113	2.74	28 (33%)
33	LHG	b	629[A]	-	48,48,48	0.85	3 (6%)	51,54,54	1.03	4 (7%)
31	BCT	A	416[B]	21	2,3,3	0.59	0	2,3,3	1.20	0
33	LHG	d	412[A]	-	48,48,48	0.89	2 (4%)	51,54,54	1.12	4 (7%)
29	PL9	D	705[A]	-	55,55,55	0.62	2 (3%)	68,69,69	1.64	18 (26%)
33	LHG	D	706[A]	-	48,48,48	0.86	2 (4%)	51,54,54	0.99	3 (5%)
34	LMG	B	621	-	51,51,55	0.93	2 (3%)	59,59,63	1.27	4 (6%)
23	CLA	b	615	2	69,73,73	2.00	19 (27%)	83,113,113	2.84	33 (39%)
23	CLA	C	508	41	69,73,73	1.99	20 (28%)	83,113,113	2.79	28 (33%)
34	LMG	c	521	-	51,51,55	1.02	2 (3%)	59,59,63	1.38	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	CLA	A	406[B]	41	69,73,73	2.05	19 (27%)	83,113,113	2.93	33 (39%)
23	CLA	B	616	2	69,73,73	1.98	20 (28%)	83,113,113	2.97	28 (33%)
32	LMT	B	627	-	36,36,36	1.15	3 (8%)	47,47,47	1.41	6 (12%)
23	CLA	b	607	41	69,73,73	1.96	20 (28%)	83,113,113	2.83	29 (34%)
32	LMT	B	629	-	36,36,36	1.01	3 (8%)	47,47,47	1.20	5 (10%)
23	CLA	C	512	3	69,73,73	2.04	22 (31%)	83,113,113	2.78	29 (34%)
25	BCR	C	516	-	41,41,41	1.07	1 (2%)	56,56,56	1.34	7 (12%)
23	CLA	c	506	3	69,73,73	2.02	19 (27%)	83,113,113	2.86	29 (34%)
32	LMT	A	420	-	36,36,36	1.04	2 (5%)	47,47,47	1.14	4 (8%)
32	LMT	b	621	-	25,25,36	0.98	2 (8%)	30,30,47	1.19	2 (6%)
34	LMG	m	101	-	51,51,55	0.87	2 (3%)	59,59,63	1.28	7 (11%)
36	DGD	c	519	-	63,63,67	0.87	4 (6%)	77,77,81	1.07	6 (7%)
23	CLA	A	406[A]	41	69,73,73	1.99	18 (26%)	83,113,113	2.86	32 (38%)
34	LMG	C	520	-	51,51,55	0.95	2 (3%)	59,59,63	1.11	6 (10%)
23	CLA	B	612	2	69,73,73	2.04	20 (28%)	83,113,113	2.80	28 (33%)
23	CLA	a	407[B]	41	69,73,73	2.02	20 (28%)	83,113,113	2.81	30 (36%)
25	BCR	B	617	-	41,41,41	1.04	1 (2%)	56,56,56	1.28	6 (10%)
23	CLA	C	505	41	69,73,73	2.01	19 (27%)	83,113,113	2.77	29 (34%)
24	PHO	a	408[B]	-	58,69,69	2.78	13 (22%)	56,99,99	2.81	16 (28%)
23	CLA	B	607	41	69,73,73	1.94	21 (30%)	83,113,113	2.80	32 (38%)
27	GOL	O	303	-	5,5,5	1.02	0	5,5,5	1.02	0
27	GOL	a	418	-	5,5,5	1.21	0	5,5,5	1.01	0
33	LHG	d	406[A]	-	48,48,48	0.92	2 (4%)	51,54,54	0.99	3 (5%)
24	PHO	A	417[A]	-	58,69,69	2.74	15 (25%)	56,99,99	2.87	17 (30%)
23	CLA	A	404[B]	1	69,73,73	2.06	20 (28%)	83,113,113	2.84	32 (38%)
23	CLA	b	605	2	69,73,73	1.94	18 (26%)	83,113,113	2.99	31 (37%)
23	CLA	a	405[B]	1	69,73,73	1.97	18 (26%)	83,113,113	2.92	32 (38%)
27	GOL	d	411	-	5,5,5	1.12	0	5,5,5	0.90	0
24	PHO	a	408[A]	-	58,69,69	2.72	12 (20%)	56,99,99	2.76	15 (26%)
23	CLA	C	507	3	69,73,73	2.03	21 (30%)	83,113,113	2.81	31 (37%)
25	BCR	b	617	-	41,41,41	1.08	1 (2%)	56,56,56	1.26	5 (8%)
23	CLA	b	611	2	69,73,73	1.97	19 (27%)	83,113,113	2.90	30 (36%)
25	BCR	B	618	-	41,41,41	0.97	1 (2%)	56,56,56	1.42	8 (14%)
23	CLA	A	404[A]	1	69,73,73	1.98	20 (28%)	83,113,113	2.82	32 (38%)
35	HTG	D	710	-	16,16,19	0.99	1 (6%)	20,21,24	1.54	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	SQD	B	620	-	53,54,54	1.08	4 (7%)	62,65,65	1.73	11 (17%)
38	HEM	F	102	5,6	50,50,50	1.55	7 (14%)	66,82,82	1.93	19 (28%)
29	PL9	a	414[B]	-	55,55,55	0.62	2 (3%)	68,69,69	1.95	22 (32%)
29	PL9	A	414[B]	-	55,55,55	0.65	2 (3%)	68,69,69	1.99	24 (35%)
23	CLA	D	702[A]	4	69,73,73	1.98	19 (27%)	83,113,113	2.88	31 (37%)
27	GOL	B	626	-	5,5,5	1.09	0	5,5,5	0.92	0
34	LMG	Z	101	-	37,37,55	1.01	2 (5%)	45,45,63	1.42	6 (13%)
31	BCT	a	404[B]	21	2,3,3	0.64	0	2,3,3	1.26	0
33	LHG	L	101[A]	-	48,48,48	0.89	2 (4%)	51,54,54	1.15	3 (5%)
25	BCR	c	515	-	41,41,41	1.01	1 (2%)	56,56,56	1.64	11 (19%)
27	GOL	O	302	-	5,5,5	0.82	0	5,5,5	0.94	0
25	BCR	t	102	-	41,41,41	1.02	1 (2%)	56,56,56	1.69	14 (25%)
34	LMG	c	520	-	51,51,55	0.91	2 (3%)	59,59,63	1.17	5 (8%)
23	CLA	c	511	3	69,73,73	2.01	20 (28%)	83,113,113	2.87	33 (39%)
23	CLA	C	514	3	69,73,73	2.03	20 (28%)	83,113,113	2.84	31 (37%)
27	GOL	c	527	-	5,5,5	1.19	0	5,5,5	0.91	0
25	BCR	b	618	-	41,41,41	0.96	1 (2%)	56,56,56	1.34	11 (19%)
32	LMT	T	101	-	36,36,36	1.10	3 (8%)	47,47,47	1.08	2 (4%)
23	CLA	A	405[A]	41	69,73,73	1.93	18 (26%)	83,113,113	2.88	33 (39%)
24	PHO	a	416[B]	-	58,69,69	2.80	13 (22%)	56,99,99	2.88	14 (25%)
27	GOL	B	623	-	5,5,5	0.75	0	5,5,5	1.11	1 (20%)
23	CLA	B	602	2	69,73,73	2.02	20 (28%)	83,113,113	2.87	30 (36%)
23	CLA	C	504	3	69,73,73	2.00	19 (27%)	83,113,113	2.93	29 (34%)
25	BCR	k	101	-	41,41,41	1.05	1 (2%)	56,56,56	1.43	11 (19%)
27	GOL	c	526[B]	-	5,5,5	0.86	0	5,5,5	0.98	0
23	CLA	c	508	41	69,73,73	1.98	19 (27%)	83,113,113	2.84	29 (34%)
23	CLA	B	604	2	69,73,73	1.98	22 (31%)	83,113,113	2.73	30 (36%)
26	SQD	a	411[B]	-	53,54,54	0.97	3 (5%)	62,65,65	1.58	12 (19%)
23	CLA	B	610	41	69,73,73	2.08	20 (28%)	83,113,113	2.94	31 (37%)
33	LHG	a	420[A]	-	41,41,48	1.04	2 (4%)	44,47,54	0.92	2 (4%)
34	LMG	C	501	-	51,51,55	0.93	2 (3%)	59,59,63	1.53	7 (11%)
31	BCT	A	416[A]	21	2,3,3	0.54	0	2,3,3	1.81	1 (50%)
35	HTG	b	623	-	19,19,19	1.09	1 (5%)	23,24,24	1.91	2 (8%)
36	DGD	c	518[B]	-	63,63,67	0.87	2 (3%)	77,77,81	0.92	2 (2%)
33	LHG	b	629[B]	-	48,48,48	0.89	2 (4%)	51,54,54	1.05	5 (9%)
27	GOL	v	202[B]	-	5,5,5	1.06	0	5,5,5	0.84	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	CLA	c	505	41	69,73,73	2.09	20 (28%)	83,113,113	2.84	30 (36%)
32	LMT	a	417	-	36,36,36	1.00	2 (5%)	47,47,47	1.04	2 (4%)
23	CLA	b	601	41	69,73,73	2.10	19 (27%)	83,113,113	2.79	30 (36%)
27	GOL	c	526[A]	-	5,5,5	0.94	0	5,5,5	0.95	0
36	DGD	H	102	-	63,63,67	0.85	3 (4%)	77,77,81	1.09	7 (9%)
36	DGD	c	517[B]	-	63,63,67	0.85	2 (3%)	77,77,81	1.11	6 (7%)
35	HTG	b	622	-	19,19,19	1.28	2 (10%)	23,24,24	1.94	8 (34%)
23	CLA	c	507	3	69,73,73	2.05	20 (28%)	83,113,113	2.78	32 (38%)
23	CLA	c	510	3	69,73,73	2.07	19 (27%)	83,113,113	2.81	30 (36%)
36	DGD	h	102	-	63,63,67	0.85	3 (4%)	77,77,81	1.16	8 (10%)
28	OEX	A	413[B]	3,1,41	0,14,14	-	-	-		
32	LMT	t	101	-	26,26,36	0.91	2 (7%)	31,31,47	1.29	1 (3%)
23	CLA	c	513	3	69,73,73	2.09	19 (27%)	83,113,113	2.84	31 (37%)
23	CLA	a	407[A]	41	69,73,73	1.96	19 (27%)	83,113,113	2.86	30 (36%)
23	CLA	b	608	2	69,73,73	1.99	19 (27%)	83,113,113	2.74	31 (37%)
25	BCR	H	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.44	8 (14%)
27	GOL	D	712	-	5,5,5	1.56	2 (40%)	5,5,5	0.88	0
35	HTG	V	202	-	11,11,19	0.33	0	15,15,24	1.26	2 (13%)
34	LMG	c	501	-	51,51,55	0.92	2 (3%)	59,59,63	1.25	6 (10%)
36	DGD	c	517[A]	-	63,63,67	0.85	2 (3%)	77,77,81	1.12	6 (7%)
23	CLA	B	611	2	69,73,73	2.49	19 (27%)	83,113,113	3.98	30 (36%)
23	CLA	C	503	3	69,73,73	2.00	20 (28%)	83,113,113	2.64	28 (33%)
34	LMG	D	711	39	51,51,55	0.79	2 (3%)	59,59,63	1.09	3 (5%)
23	CLA	C	511	3	69,73,73	2.03	20 (28%)	83,113,113	2.92	32 (38%)
27	GOL	l	102[B]	-	5,5,5	0.90	0	5,5,5	1.02	0
35	HTG	B	622	-	19,19,19	0.80	1 (5%)	23,24,24	1.41	2 (8%)
23	CLA	a	405[A]	1	69,73,73	1.96	19 (27%)	83,113,113	2.88	33 (39%)
29	PL9	d	404[B]	-	55,55,55	0.64	1 (1%)	68,69,69	1.65	16 (23%)
27	GOL	C	523[B]	-	5,5,5	1.19	0	5,5,5	0.79	0
33	LHG	d	405[B]	-	48,48,48	0.89	2 (4%)	51,54,54	1.04	4 (7%)
38	HEM	f	101	5,6	50,50,50	1.50	6 (12%)	66,82,82	1.77	13 (19%)
26	SQD	a	412	-	53,54,54	1.09	3 (5%)	62,65,65	1.17	8 (12%)
23	CLA	D	703	4	69,73,73	2.11	19 (27%)	83,113,113	2.83	31 (37%)
27	GOL	l	102[A]	-	5,5,5	0.96	0	5,5,5	0.97	0
23	CLA	C	506	3	69,73,73	2.06	19 (27%)	83,113,113	2.75	30 (36%)
26	SQD	A	412	-	53,54,54	1.06	3 (5%)	62,65,65	1.23	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
34	LMG	d	410	39	51,51,55	0.89	2 (3%)	59,59,63	1.17	5 (8%)
27	GOL	C	523[A]	-	5,5,5	1.18	0	5,5,5	0.83	0
23	CLA	b	612	2	69,73,73	2.04	20 (28%)	83,113,113	2.72	29 (34%)
27	GOL	V	203[B]	-	5,5,5	1.11	0	5,5,5	0.89	0
23	CLA	b	606	2	69,73,73	1.98	19 (27%)	83,113,113	2.96	32 (38%)
23	CLA	b	610	41	69,73,73	2.05	20 (28%)	83,113,113	2.92	31 (37%)
29	PL9	A	414[A]	-	55,55,55	0.68	2 (3%)	68,69,69	2.08	25 (36%)
26	SQD	b	620	-	53,54,54	1.06	3 (5%)	62,65,65	1.69	12 (19%)
25	BCR	y	101	-	41,41,41	1.04	1 (2%)	56,56,56	1.62	12 (21%)
27	GOL	A	411	-	5,5,5	1.21	0	5,5,5	0.66	0
27	GOL	o	303	-	5,5,5	1.12	0	5,5,5	0.87	0
29	PL9	a	414[A]	-	55,55,55	0.65	2 (3%)	68,69,69	2.00	22 (32%)
32	LMT	B	630	-	25,25,36	0.89	2 (8%)	30,30,47	1.18	3 (10%)
27	GOL	b	628	-	5,5,5	0.49	0	5,5,5	1.34	1 (20%)
33	LHG	A	419[B]	-	48,48,48	0.86	2 (4%)	51,54,54	1.18	5 (9%)
35	HTG	C	522	-	19,19,19	0.88	1 (5%)	23,24,24	1.34	2 (8%)
25	BCR	C	515	-	41,41,41	1.04	1 (2%)	56,56,56	1.49	10 (17%)
25	BCR	A	409	-	41,41,41	0.99	1 (2%)	56,56,56	1.34	8 (14%)
31	BCT	a	404[A]	21	2,3,3	0.57	0	2,3,3	1.58	1 (50%)
35	HTG	d	409	-	16,16,19	0.97	1 (6%)	20,21,24	1.49	1 (5%)
23	CLA	d	401[B]	4	69,73,73	1.99	20 (28%)	83,113,113	2.78	29 (34%)
27	GOL	V	203[A]	-	5,5,5	1.22	0	5,5,5	0.91	0
33	LHG	d	405[A]	-	48,48,48	0.86	2 (4%)	51,54,54	1.08	4 (7%)
25	BCR	d	403	-	41,41,41	1.15	2 (4%)	56,56,56	1.98	14 (25%)
32	LMT	e	101	-	36,36,36	1.03	3 (8%)	47,47,47	0.97	1 (2%)
23	CLA	B	608	2	69,73,73	1.93	21 (30%)	83,113,113	2.93	35 (42%)
33	LHG	A	419[A]	-	48,48,48	0.84	2 (4%)	51,54,54	1.31	6 (11%)
35	HTG	B	624	-	19,19,19	1.01	2 (10%)	23,24,24	1.29	3 (13%)
24	PHO	a	416[A]	-	58,69,69	2.75	14 (24%)	56,99,99	3.01	17 (30%)
23	CLA	c	509	3	69,73,73	2.09	20 (28%)	83,113,113	2.74	27 (32%)
33	LHG	E	101[B]	-	41,41,48	1.06	2 (4%)	44,47,54	1.11	3 (6%)
27	GOL	B	628	-	5,5,5	0.88	0	5,5,5	1.13	0
26	SQD	a	411[A]	-	53,54,54	0.95	3 (5%)	62,65,65	1.77	13 (20%)
36	DGD	c	518[A]	-	63,63,67	0.84	2 (3%)	77,77,81	0.97	5 (6%)
23	CLA	b	614	2	69,73,73	2.04	19 (27%)	83,113,113	3.01	32 (38%)
24	PHO	A	407[B]	-	58,69,69	2.69	11 (18%)	56,99,99	2.79	15 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
27	GOL	o	304	-	5,5,5	1.08	1 (20%)	5,5,5	1.06	0
23	CLA	c	514	3	69,73,73	2.10	21 (30%)	83,113,113	2.87	29 (34%)
27	GOL	v	202[A]	-	5,5,5	1.27	0	5,5,5	0.72	0
25	BCR	K	102	-	41,41,41	1.04	1 (2%)	56,56,56	1.42	11 (19%)
33	LHG	E	101[A]	-	41,41,48	1.06	2 (4%)	44,47,54	1.11	3 (6%)
23	CLA	C	509	3	69,73,73	2.06	20 (28%)	83,113,113	2.69	29 (34%)
25	BCR	a	410	-	41,41,41	1.02	1 (2%)	56,56,56	1.33	8 (14%)
35	HTG	b	625	-	19,19,19	1.11	2 (10%)	23,24,24	1.53	4 (17%)
23	CLA	B	609	2	69,73,73	2.01	17 (24%)	83,113,113	2.83	29 (34%)
26	SQD	A	410[B]	-	53,54,54	0.92	3 (5%)	62,65,65	1.75	12 (19%)
24	PHO	A	407[A]	-	58,69,69	2.69	14 (24%)	56,99,99	2.78	15 (26%)
23	CLA	C	510	3	69,73,73	2.06	20 (28%)	83,113,113	2.87	30 (36%)
23	CLA	b	616	2	69,73,73	2.00	19 (27%)	83,113,113	2.97	30 (36%)
35	HTG	o	301	-	19,19,19	1.15	2 (10%)	23,24,24	1.67	5 (21%)
33	LHG	d	412[B]	-	48,48,48	0.92	2 (4%)	51,54,54	1.07	3 (5%)
29	PL9	D	705[B]	-	55,55,55	0.63	2 (3%)	68,69,69	1.68	18 (26%)
26	SQD	X	101	-	42,43,54	1.21	4 (9%)	51,54,65	2.24	15 (29%)
27	GOL	b	624	-	5,5,5	1.18	1 (20%)	5,5,5	0.78	0
23	CLA	b	604	2	69,73,73	1.98	21 (30%)	83,113,113	2.76	30 (36%)
32	LMT	b	627	-	25,25,36	0.89	1 (4%)	30,30,47	1.12	2 (6%)
34	LMG	z	101	-	39,39,55	1.10	2 (5%)	47,47,63	1.04	2 (4%)
25	BCR	h	101	-	41,41,41	1.05	1 (2%)	56,56,56	1.49	12 (21%)
23	CLA	A	408	1	69,73,73	1.96	21 (30%)	83,113,113	2.98	34 (40%)
23	CLA	a	409	1	69,73,73	1.98	18 (26%)	83,113,113	2.96	30 (36%)
23	CLA	b	613	2	69,73,73	1.95	19 (27%)	83,113,113	2.85	30 (36%)
40	HEC	V	201	16	50,50,50	1.74	7 (14%)	68,82,82	1.43	8 (11%)
36	DGD	C	518[B]	-	63,63,67	0.88	3 (4%)	77,77,81	1.03	6 (7%)
25	BCR	c	516	-	41,41,41	1.03	1 (2%)	56,56,56	1.34	8 (14%)
23	CLA	B	601	41	69,73,73	2.07	20 (28%)	83,113,113	2.85	28 (33%)
26	SQD	f	102	-	42,43,54	1.19	3 (7%)	51,54,65	1.55	12 (23%)
32	LMT	m	103	-	36,36,36	1.07	2 (5%)	47,47,47	1.16	4 (8%)
29	PL9	d	404[A]	-	55,55,55	0.65	1 (1%)	68,69,69	1.63	17 (25%)
28	OEX	a	413[B]	3,1,41	0,14,14	-	-	-		
23	CLA	c	502	3	69,73,73	2.02	19 (27%)	83,113,113	2.85	30 (36%)
23	CLA	B	613	2	69,73,73	1.97	20 (28%)	83,113,113	2.81	31 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	BCR	D	704	-	41,41,41	1.10	1 (2%)	56,56,56	1.96	20 (35%)
36	DGD	C	517[B]	-	63,63,67	0.83	2 (3%)	77,77,81	1.14	8 (10%)
36	DGD	C	518[A]	-	63,63,67	0.89	3 (4%)	77,77,81	1.02	5 (6%)
23	CLA	B	605	2	69,73,73	2.04	19 (27%)	83,113,113	2.90	29 (34%)
32	LMT	F	101	-	36,36,36	1.06	1 (2%)	47,47,47	1.04	3 (6%)
23	CLA	C	502	3	69,73,73	2.01	19 (27%)	83,113,113	2.88	30 (36%)
32	LMT	A	418	-	36,36,36	0.93	3 (8%)	47,47,47	1.05	2 (4%)
24	PHO	A	417[B]	-	58,69,69	2.77	15 (25%)	56,99,99	2.89	16 (28%)
33	LHG	d	406[B]	-	48,48,48	0.93	2 (4%)	51,54,54	0.96	2 (3%)
23	CLA	a	406[B]	41	69,73,73	2.06	19 (27%)	83,113,113	2.82	34 (40%)
25	BCR	B	619	-	41,41,41	1.10	2 (4%)	56,56,56	1.31	5 (8%)
28	OEX	a	413[A]	3,1,41	0,14,14	-	-	-		
35	HTG	c	522	-	19,19,19	0.91	1 (5%)	23,24,24	1.45	2 (8%)
36	DGD	C	517[A]	-	63,63,67	0.81	2 (3%)	77,77,81	1.21	8 (10%)
23	CLA	c	512	3	69,73,73	2.09	19 (27%)	83,113,113	2.80	32 (38%)
23	CLA	c	504	3	69,73,73	2.06	18 (26%)	83,113,113	2.91	27 (32%)
25	BCR	T	102	-	41,41,41	1.02	1 (2%)	56,56,56	1.76	13 (23%)
23	CLA	a	406[A]	41	69,73,73	2.01	17 (24%)	83,113,113	2.80	29 (34%)
23	CLA	d	401[A]	4	69,73,73	1.94	20 (28%)	83,113,113	2.78	29 (34%)
25	BCR	Y	101	-	41,41,41	0.92	1 (2%)	56,56,56	1.69	15 (26%)
32	LMT	M	101	-	36,36,36	1.14	4 (11%)	47,47,47	1.20	3 (6%)
23	CLA	b	609	2	69,73,73	2.00	20 (28%)	83,113,113	2.79	32 (38%)
36	DGD	C	519	-	63,63,67	0.85	3 (4%)	77,77,81	1.01	3 (3%)
40	HEC	v	201	16	50,50,50	1.74	7 (14%)	68,82,82	1.37	8 (11%)
23	CLA	B	603	2	69,73,73	2.03	21 (30%)	83,113,113	2.92	33 (39%)
23	CLA	d	402	4	69,73,73	2.05	19 (27%)	83,113,113	2.94	32 (38%)
25	BCR	b	619	-	41,41,41	1.08	1 (2%)	56,56,56	1.40	11 (19%)
23	CLA	D	702[B]	4	69,73,73	2.01	20 (28%)	83,113,113	2.89	30 (36%)
34	LMG	C	521	-	51,51,55	1.08	3 (5%)	59,59,63	1.35	6 (10%)
33	LHG	D	707[B]	-	48,48,48	0.90	2 (4%)	51,54,54	1.02	3 (5%)
33	LHG	L	101[B]	-	48,48,48	0.95	2 (4%)	51,54,54	1.09	2 (3%)
27	GOL	D	701	-	5,5,5	1.57	2 (40%)	5,5,5	1.06	1 (20%)
23	CLA	b	602	2	69,73,73	2.08	17 (24%)	83,113,113	3.03	33 (39%)

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
23	CLA	C	513	3	-	10/39/115/115	-
33	LHG	D	706[B]	-	-	17/53/53/53	-
27	GOL	a	419	-	-	1/4/4/4	-
23	CLA	B	615	2	-	7/39/115/115	-
23	CLA	A	405[B]	41	-	4/39/115/115	-
23	CLA	B	614	2	-	15/39/115/115	-
23	CLA	B	606	2	-	9/39/115/115	-
33	LHG	D	707[A]	-	-	14/53/53/53	-
26	SQD	A	410[A]	-	-	12/49/69/69	0/1/1/1
23	CLA	b	603	2	-	5/39/115/115	-
33	LHG	a	420[B]	-	-	16/46/46/53	-
23	CLA	c	503	3	-	4/39/115/115	-
33	LHG	b	629[A]	-	-	20/53/53/53	-
34	LMG	B	621	-	-	20/46/66/70	0/1/1/1
33	LHG	d	412[A]	-	-	13/53/53/53	-
29	PL9	D	705[A]	-	-	8/53/73/73	0/1/1/1
33	LHG	D	706[A]	-	-	16/53/53/53	-
23	CLA	b	615	2	-	8/39/115/115	-
23	CLA	C	508	41	-	9/39/115/115	-
34	LMG	c	521	-	-	13/46/66/70	0/1/1/1
23	CLA	A	406[B]	41	-	6/39/115/115	-
23	CLA	B	616	2	-	5/39/115/115	-
32	LMT	B	627	-	-	12/21/61/61	0/2/2/2
23	CLA	b	607	41	-	3/39/115/115	-
32	LMT	B	629	-	-	11/21/61/61	0/2/2/2
23	CLA	C	512	3	-	3/39/115/115	-
25	BCR	C	516	-	-	0/29/63/63	0/2/2/2
23	CLA	c	506	3	-	7/39/115/115	-
32	LMT	A	420	-	-	15/21/61/61	0/2/2/2
32	LMT	b	621	-	-	8/17/37/61	0/1/1/2
34	LMG	m	101	-	-	9/46/66/70	0/1/1/1
36	DGD	c	519	-	-	8/51/91/95	0/2/2/2
23	CLA	A	406[A]	41	-	7/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	LMG	C	520	-	-	11/46/66/70	0/1/1/1
23	CLA	B	612	2	-	5/39/115/115	-
23	CLA	a	407[B]	41	-	8/39/115/115	-
25	BCR	B	617	-	-	2/29/63/63	0/2/2/2
23	CLA	C	505	41	-	10/39/115/115	-
24	PHO	a	408[B]	-	-	4/37/103/103	0/5/6/6
23	CLA	B	607	41	-	6/39/115/115	-
27	GOL	O	303	-	-	2/4/4/4	-
27	GOL	a	418	-	-	2/4/4/4	-
33	LHG	d	406[A]	-	-	11/53/53/53	-
24	PHO	A	417[A]	-	-	1/37/103/103	0/5/6/6
23	CLA	A	404[B]	1	-	4/39/115/115	-
23	CLA	b	605	2	-	6/39/115/115	-
23	CLA	a	405[B]	1	-	4/39/115/115	-
27	GOL	d	411	-	-	4/4/4/4	-
24	PHO	a	408[A]	-	-	5/37/103/103	0/5/6/6
23	CLA	C	507	3	-	12/39/115/115	-
25	BCR	b	617	-	-	2/29/63/63	0/2/2/2
23	CLA	b	611	2	-	3/39/115/115	-
25	BCR	B	618	-	-	0/29/63/63	0/2/2/2
23	CLA	A	404[A]	1	-	5/39/115/115	-
35	HTG	D	710	-	-	3/7/27/30	0/1/1/1
26	SQD	B	620	-	-	13/49/69/69	0/1/1/1
38	HEM	F	102	5,6	-	6/14/54/54	-
29	PL9	a	414[B]	-	-	14/53/73/73	0/1/1/1
29	PL9	A	414[B]	-	-	16/53/73/73	0/1/1/1
23	CLA	D	702[A]	4	-	0/39/115/115	-
27	GOL	B	626	-	-	1/4/4/4	-
34	LMG	Z	101	-	-	12/31/51/70	0/1/1/1
33	LHG	L	101[A]	-	-	19/53/53/53	-
25	BCR	c	515	-	-	1/29/63/63	0/2/2/2
27	GOL	O	302	-	-	2/4/4/4	-
25	BCR	t	102	-	-	5/29/63/63	0/2/2/2
34	LMG	c	520	-	-	13/46/66/70	0/1/1/1
23	CLA	c	511	3	-	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	C	514	3	-	6/39/115/115	-
27	GOL	c	527	-	-	2/4/4/4	-
25	BCR	b	618	-	-	0/29/63/63	0/2/2/2
32	LMT	T	101	-	-	9/21/61/61	0/2/2/2
23	CLA	A	405[A]	41	-	4/39/115/115	-
24	PHO	a	416[B]	-	-	0/37/103/103	0/5/6/6
27	GOL	B	623	-	-	4/4/4/4	-
23	CLA	B	602	2	-	10/39/115/115	-
23	CLA	C	504	3	-	4/39/115/115	-
25	BCR	k	101	-	-	0/29/63/63	0/2/2/2
27	GOL	c	526[B]	-	-	0/4/4/4	-
23	CLA	c	508	41	-	9/39/115/115	-
23	CLA	B	604	2	-	2/39/115/115	-
26	SQD	a	411[B]	-	-	10/49/69/69	0/1/1/1
23	CLA	B	610	41	-	8/39/115/115	-
33	LHG	a	420[A]	-	-	16/46/46/53	-
34	LMG	C	501	-	-	13/46/66/70	0/1/1/1
35	HTG	b	623	-	-	5/10/30/30	0/1/1/1
36	DGD	c	518[B]	-	-	16/51/91/95	0/2/2/2
33	LHG	b	629[B]	-	-	16/53/53/53	-
27	GOL	v	202[B]	-	-	2/4/4/4	-
23	CLA	c	505	41	-	6/39/115/115	-
32	LMT	a	417	-	-	12/21/61/61	0/2/2/2
23	CLA	b	601	41	-	19/39/115/115	-
27	GOL	c	526[A]	-	-	0/4/4/4	-
36	DGD	H	102	-	-	7/51/91/95	0/2/2/2
36	DGD	c	517[B]	-	-	19/51/91/95	0/2/2/2
35	HTG	b	622	-	-	4/10/30/30	0/1/1/1
23	CLA	c	507	3	-	6/39/115/115	-
23	CLA	c	510	3	-	16/39/115/115	-
36	DGD	h	102	-	-	15/51/91/95	0/2/2/2
32	LMT	t	101	-	-	10/17/38/61	0/1/1/2
23	CLA	c	513	3	-	12/39/115/115	-
23	CLA	a	407[A]	41	-	7/39/115/115	-
23	CLA	b	608	2	-	4/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	H	101	-	-	2/29/63/63	0/2/2/2
27	GOL	D	712	-	-	4/4/4/4	-
35	HTG	V	202	-	-	0/2/19/30	0/1/1/1
34	LMG	c	501	-	-	11/46/66/70	0/1/1/1
36	DGD	c	517[A]	-	-	20/51/91/95	0/2/2/2
23	CLA	B	611	2	-	2/39/115/115	-
23	CLA	C	503	3	-	10/39/115/115	-
34	LMG	D	711	39	-	9/46/66/70	0/1/1/1
23	CLA	C	511	3	-	11/39/115/115	-
27	GOL	l	102[B]	-	-	2/4/4/4	-
35	HTG	B	622	-	-	1/10/30/30	0/1/1/1
23	CLA	a	405[A]	1	-	3/39/115/115	-
29	PL9	d	404[B]	-	-	10/53/73/73	0/1/1/1
27	GOL	C	523[B]	-	-	0/4/4/4	-
33	LHG	d	405[B]	-	-	14/53/53/53	-
38	HEM	f	101	5,6	-	6/14/54/54	-
26	SQD	a	412	-	-	13/49/69/69	0/1/1/1
23	CLA	D	703	4	-	13/39/115/115	-
27	GOL	l	102[A]	-	-	2/4/4/4	-
23	CLA	C	506	3	-	7/39/115/115	-
26	SQD	A	412	-	-	13/49/69/69	0/1/1/1
34	LMG	d	410	39	-	11/46/66/70	0/1/1/1
27	GOL	C	523[A]	-	-	0/4/4/4	-
23	CLA	b	612	2	-	4/39/115/115	-
27	GOL	V	203[B]	-	-	2/4/4/4	-
23	CLA	b	606	2	-	14/39/115/115	-
23	CLA	b	610	41	-	7/39/115/115	-
29	PL9	A	414[A]	-	-	15/53/73/73	0/1/1/1
26	SQD	b	620	-	-	18/49/69/69	0/1/1/1
25	BCR	y	101	-	-	5/29/63/63	0/2/2/2
27	GOL	A	411	-	-	2/4/4/4	-
27	GOL	o	303	-	-	2/4/4/4	-
29	PL9	a	414[A]	-	-	14/53/73/73	0/1/1/1
32	LMT	B	630	-	-	10/17/37/61	0/1/1/2
27	GOL	b	628	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	LHG	A	419[B]	-	-	13/53/53/53	-
35	HTG	C	522	-	-	0/10/30/30	0/1/1/1
25	BCR	C	515	-	-	1/29/63/63	0/2/2/2
25	BCR	A	409	-	-	0/29/63/63	0/2/2/2
35	HTG	d	409	-	-	1/7/27/30	0/1/1/1
23	CLA	d	401[B]	4	-	4/39/115/115	-
27	GOL	V	203[A]	-	-	2/4/4/4	-
33	LHG	d	405[A]	-	-	13/53/53/53	-
25	BCR	d	403	-	-	5/29/63/63	0/2/2/2
32	LMT	e	101	-	-	15/21/61/61	0/2/2/2
23	CLA	B	608	2	-	4/39/115/115	-
33	LHG	A	419[A]	-	-	10/53/53/53	-
35	HTG	B	624	-	-	3/10/30/30	0/1/1/1
24	PHO	a	416[A]	-	-	1/37/103/103	0/5/6/6
23	CLA	c	509	3	-	4/39/115/115	-
33	LHG	E	101[B]	-	-	23/46/46/53	-
27	GOL	B	628	-	-	4/4/4/4	-
26	SQD	a	411[A]	-	-	10/49/69/69	0/1/1/1
36	DGD	c	518[A]	-	-	17/51/91/95	0/2/2/2
23	CLA	b	614	2	-	14/39/115/115	-
24	PHO	A	407[B]	-	-	3/37/103/103	0/5/6/6
27	GOL	o	304	-	-	4/4/4/4	-
23	CLA	c	514	3	-	12/39/115/115	-
27	GOL	v	202[A]	-	-	1/4/4/4	-
25	BCR	K	102	-	-	2/29/63/63	0/2/2/2
33	LHG	E	101[A]	-	-	22/46/46/53	-
23	CLA	C	509	3	-	6/39/115/115	-
25	BCR	a	410	-	-	1/29/63/63	0/2/2/2
35	HTG	b	625	-	-	5/10/30/30	0/1/1/1
23	CLA	B	609	2	-	3/39/115/115	-
26	SQD	A	410[B]	-	-	11/49/69/69	0/1/1/1
24	PHO	A	407[A]	-	-	3/37/103/103	0/5/6/6
23	CLA	C	510	3	-	8/39/115/115	-
23	CLA	b	616	2	-	9/39/115/115	-
35	HTG	o	301	-	-	4/10/30/30	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	LHG	d	412[B]	-	-	13/53/53/53	-
29	PL9	D	705[B]	-	-	6/53/73/73	0/1/1/1
26	SQD	X	101	-	-	16/38/58/69	0/1/1/1
27	GOL	b	624	-	-	2/4/4/4	-
23	CLA	b	604	2	-	11/39/115/115	-
32	LMT	b	627	-	-	11/17/37/61	0/1/1/2
34	LMG	z	101	-	-	9/34/54/70	0/1/1/1
25	BCR	h	101	-	-	2/29/63/63	0/2/2/2
23	CLA	A	408	1	-	9/39/115/115	-
23	CLA	a	409	1	-	10/39/115/115	-
23	CLA	b	613	2	-	4/39/115/115	-
40	HEC	V	201	16	1/1/3/7	6/14/54/54	-
36	DGD	C	518[B]	-	-	14/51/91/95	0/2/2/2
25	BCR	c	516	-	-	0/29/63/63	0/2/2/2
23	CLA	B	601	41	-	11/39/115/115	-
26	SQD	f	102	-	-	9/38/58/69	0/1/1/1
32	LMT	m	103	-	-	5/21/61/61	0/2/2/2
29	PL9	d	404[A]	-	-	6/53/73/73	0/1/1/1
23	CLA	c	502	3	-	6/39/115/115	-
23	CLA	B	613	2	-	9/39/115/115	-
25	BCR	D	704	-	-	4/29/63/63	0/2/2/2
36	DGD	C	517[B]	-	-	12/51/91/95	0/2/2/2
36	DGD	C	518[A]	-	-	15/51/91/95	0/2/2/2
23	CLA	B	605	2	-	4/39/115/115	-
32	LMT	F	101	-	-	8/21/61/61	0/2/2/2
23	CLA	C	502	3	-	5/39/115/115	-
32	LMT	A	418	-	-	6/21/61/61	0/2/2/2
24	PHO	A	417[B]	-	-	1/37/103/103	0/5/6/6
33	LHG	d	406[B]	-	-	13/53/53/53	-
23	CLA	a	406[B]	41	-	6/39/115/115	-
25	BCR	B	619	-	-	0/29/63/63	0/2/2/2
35	HTG	c	522	-	-	2/10/30/30	0/1/1/1
36	DGD	C	517[A]	-	-	11/51/91/95	0/2/2/2
23	CLA	c	512	3	-	6/39/115/115	-
23	CLA	c	504	3	-	3/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	T	102	-	-	1/29/63/63	0/2/2/2
23	CLA	a	406[A]	41	-	8/39/115/115	-
23	CLA	d	401[A]	4	-	2/39/115/115	-
40	HEC	v	201	16	1/1/3/7	5/14/54/54	-
25	BCR	Y	101	-	-	4/29/63/63	0/2/2/2
23	CLA	b	609	2	-	1/39/115/115	-
32	LMT	M	101	-	-	5/21/61/61	0/2/2/2
36	DGD	C	519	-	-	19/51/91/95	0/2/2/2
23	CLA	B	603	2	-	9/39/115/115	-
23	CLA	d	402	4	-	8/39/115/115	-
25	BCR	b	619	-	-	4/29/63/63	0/2/2/2
23	CLA	D	702[B]	4	-	2/39/115/115	-
34	LMG	C	521	-	-	14/46/66/70	0/1/1/1
33	LHG	D	707[B]	-	-	16/53/53/53	-
33	LHG	L	101[B]	-	-	17/53/53/53	-
27	GOL	D	701	-	-	2/4/4/4	-
23	CLA	b	602	2	-	5/39/115/115	-

The worst 5 of 1875 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	408[B]	PHO	C1B-C2B	9.52	1.50	1.39
24	A	407[B]	PHO	C1D-C2D	9.33	1.49	1.39
24	a	416[B]	PHO	C1B-C2B	9.28	1.49	1.39
24	A	407[A]	PHO	C1D-C2D	9.11	1.49	1.39
24	a	408[A]	PHO	C1B-C2B	8.96	1.49	1.39

The worst 5 of 3339 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	611	CLA	C2B-C1B-NB	16.03	120.98	110.23
23	B	611	CLA	C3B-C2B-C1B	-13.25	91.17	107.16
24	a	416[A]	PHO	C2D-C1D-ND	11.91	117.75	109.53
23	B	611	CLA	C1D-ND-C4D	-11.83	97.93	106.33
24	a	416[B]	PHO	C2D-C1D-ND	11.50	117.47	109.53

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
40	V	201	HEC	NA
40	v	201	HEC	NA

5 of 1684 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	A	408	CLA	C2-C3-C5-C6
23	A	408	CLA	C4-C3-C5-C6
23	B	614	CLA	CHA-CBD-CGD-O1D
23	B	614	CLA	CAD-CBD-CGD-O1D
23	B	614	CLA	CAD-CBD-CGD-O2D

There are no ring outliers.

182 monomers are involved in 378 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	C	513	CLA	2	0
33	D	706[B]	LHG	1	0
27	a	419	GOL	3	0
23	B	615	CLA	7	0
23	A	405[B]	CLA	3	0
23	B	614	CLA	1	0
23	B	606	CLA	3	0
33	D	707[A]	LHG	6	0
26	A	410[A]	SQD	2	0
23	b	603	CLA	1	0
33	a	420[B]	LHG	4	0
23	c	503	CLA	2	0
33	D	706[A]	LHG	2	0
34	B	621	LMG	1	0
23	b	615	CLA	3	0
23	C	508	CLA	4	0
34	c	521	LMG	1	0
23	A	406[B]	CLA	1	0
23	B	616	CLA	6	0
23	b	607	CLA	1	0
32	B	629	LMT	2	0
23	C	512	CLA	2	0
25	C	516	BCR	2	0
23	c	506	CLA	5	0
32	A	420	LMT	1	0
32	b	621	LMT	1	0
34	m	101	LMG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	c	519	DGD	3	0
23	A	406[A]	CLA	1	0
23	B	612	CLA	1	0
23	a	407[B]	CLA	3	0
25	B	617	BCR	1	0
23	C	505	CLA	1	0
24	a	408[B]	PHO	1	0
27	O	303	GOL	3	0
27	a	418	GOL	2	0
33	d	406[A]	LHG	10	0
24	A	417[A]	PHO	2	0
23	A	404[B]	CLA	4	0
23	b	605	CLA	4	0
23	a	405[B]	CLA	5	0
23	C	507	CLA	5	0
25	b	617	BCR	1	0
23	b	611	CLA	1	0
25	B	618	BCR	4	0
23	A	404[A]	CLA	5	0
26	B	620	SQD	2	0
29	a	414[B]	PL9	4	0
29	A	414[B]	PL9	8	0
23	D	702[A]	CLA	3	0
34	Z	101	LMG	2	0
25	c	515	BCR	3	0
27	O	302	GOL	1	0
25	t	102	BCR	5	0
34	c	520	LMG	1	0
23	C	514	CLA	2	0
25	b	618	BCR	3	0
32	T	101	LMT	1	0
23	A	405[A]	CLA	4	0
24	a	416[B]	PHO	1	0
27	B	623	GOL	2	0
23	B	602	CLA	3	0
23	C	504	CLA	4	0
25	k	101	BCR	1	0
27	c	526[B]	GOL	1	0
23	c	508	CLA	2	0
23	B	604	CLA	1	0
26	a	411[B]	SQD	4	0
23	B	610	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	a	420[A]	LHG	4	0
36	c	518[B]	DGD	1	0
33	b	629[B]	LHG	1	0
27	v	202[B]	GOL	1	0
23	c	505	CLA	3	0
32	a	417	LMT	1	0
23	b	601	CLA	1	0
36	H	102	DGD	1	0
36	c	517[B]	DGD	2	0
35	b	622	HTG	2	0
23	c	507	CLA	3	0
23	c	510	CLA	1	0
36	h	102	DGD	2	0
32	t	101	LMT	2	0
23	c	513	CLA	7	0
23	a	407[A]	CLA	2	0
25	H	101	BCR	1	0
27	D	712	GOL	2	0
36	c	517[A]	DGD	2	0
23	C	503	CLA	5	0
23	C	511	CLA	5	0
27	l	102[B]	GOL	1	0
35	B	622	HTG	2	0
23	a	405[A]	CLA	3	0
29	d	404[B]	PL9	1	0
33	d	405[B]	LHG	3	0
26	a	412	SQD	2	0
27	l	102[A]	GOL	1	0
23	C	506	CLA	6	0
26	A	412	SQD	1	0
34	d	410	LMG	3	0
23	b	612	CLA	3	0
23	b	606	CLA	3	0
29	A	414[A]	PL9	10	0
26	b	620	SQD	2	0
25	y	101	BCR	2	0
29	a	414[A]	PL9	5	0
32	B	630	LMT	1	0
27	b	628	GOL	2	0
33	A	419[B]	LHG	1	0
25	C	515	BCR	1	0
25	A	409	BCR	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	d	409	HTG	1	0
23	d	401[B]	CLA	2	0
33	d	405[A]	LHG	3	0
25	d	403	BCR	3	0
32	e	101	LMT	1	0
33	A	419[A]	LHG	2	0
35	B	624	HTG	1	0
24	a	416[A]	PHO	2	0
23	c	509	CLA	9	0
33	E	101[B]	LHG	2	0
26	a	411[A]	SQD	4	0
36	c	518[A]	DGD	2	0
23	b	614	CLA	1	0
24	A	407[B]	PHO	1	0
23	c	514	CLA	3	0
27	v	202[A]	GOL	1	0
25	K	102	BCR	1	0
33	E	101[A]	LHG	5	0
23	C	509	CLA	6	0
25	a	410	BCR	1	0
35	b	625	HTG	1	0
23	B	609	CLA	2	0
26	A	410[B]	SQD	2	0
24	A	407[A]	PHO	2	0
23	C	510	CLA	2	0
23	b	616	CLA	1	0
35	o	301	HTG	2	0
33	d	412[B]	LHG	2	0
26	X	101	SQD	2	0
23	b	604	CLA	2	0
34	z	101	LMG	2	0
25	h	101	BCR	4	0
23	A	408	CLA	4	0
23	a	409	CLA	4	0
23	b	613	CLA	3	0
40	V	201	HEC	1	0
36	C	518[B]	DGD	1	0
25	c	516	BCR	1	0
23	B	601	CLA	2	0
26	f	102	SQD	1	0
32	m	103	LMT	2	0
23	c	502	CLA	2	0

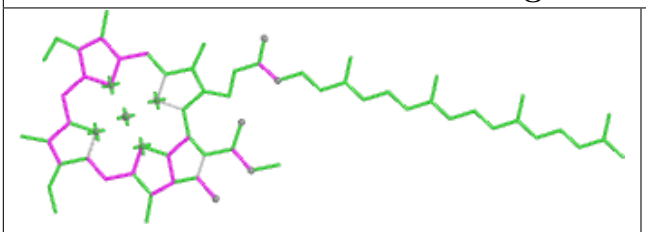
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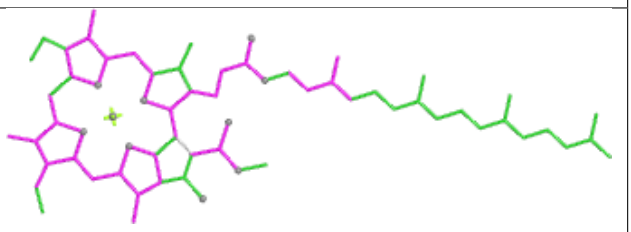
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	B	613	CLA	4	0
25	D	704	BCR	1	0
36	C	517[B]	DGD	3	0
36	C	518[A]	DGD	2	0
23	B	605	CLA	4	0
23	C	502	CLA	6	0
32	A	418	LMT	1	0
24	A	417[B]	PHO	2	0
33	d	406[B]	LHG	8	0
23	a	406[B]	CLA	3	0
25	B	619	BCR	1	0
35	c	522	HTG	1	0
36	C	517[A]	DGD	2	0
23	c	512	CLA	5	0
23	c	504	CLA	3	0
25	T	102	BCR	6	0
23	a	406[A]	CLA	2	0
23	d	401[A]	CLA	3	0
25	Y	101	BCR	1	0
32	M	101	LMT	1	0
23	b	609	CLA	5	0
36	C	519	DGD	2	0
23	d	402	CLA	2	0
25	b	619	BCR	4	0
23	D	702[B]	CLA	3	0
34	C	521	LMG	2	0
33	D	707[B]	LHG	4	0
27	D	701	GOL	4	0
23	b	602	CLA	1	0

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

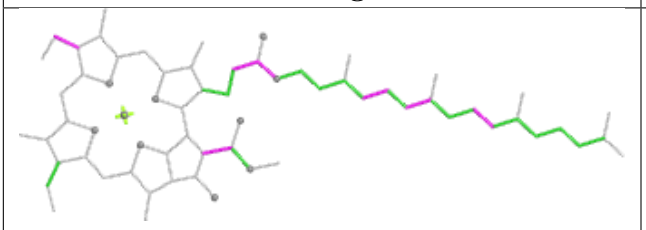
Ligand CLA C 513



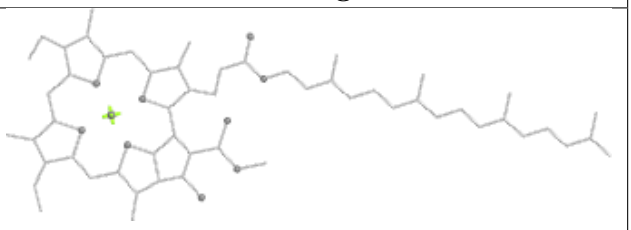
Bond lengths



Bond angles

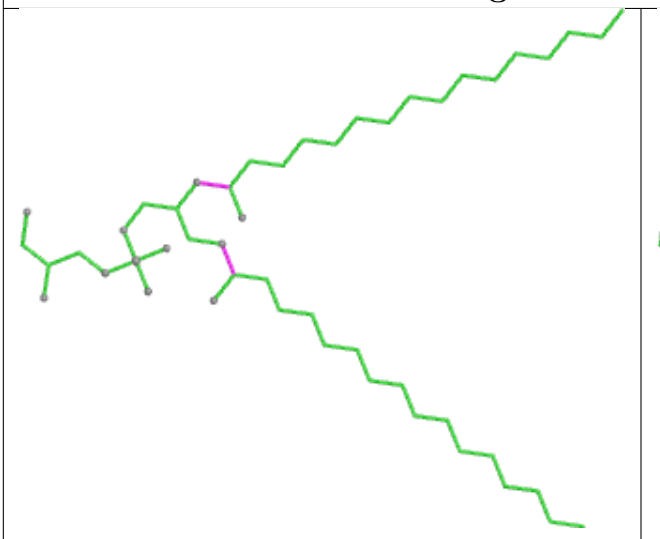


Torsions

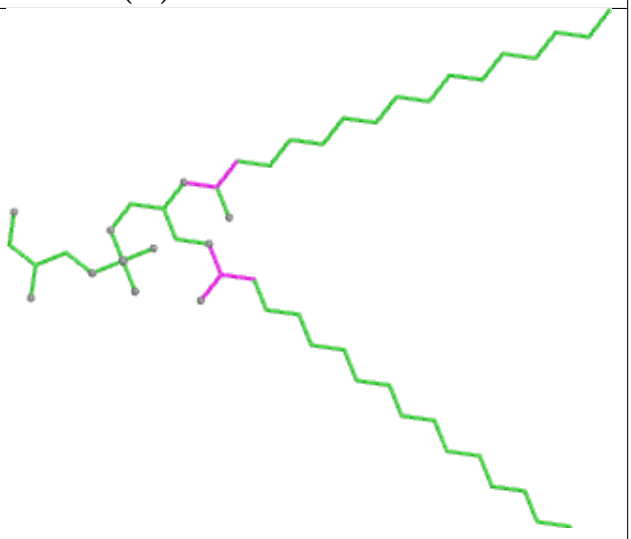


Rings

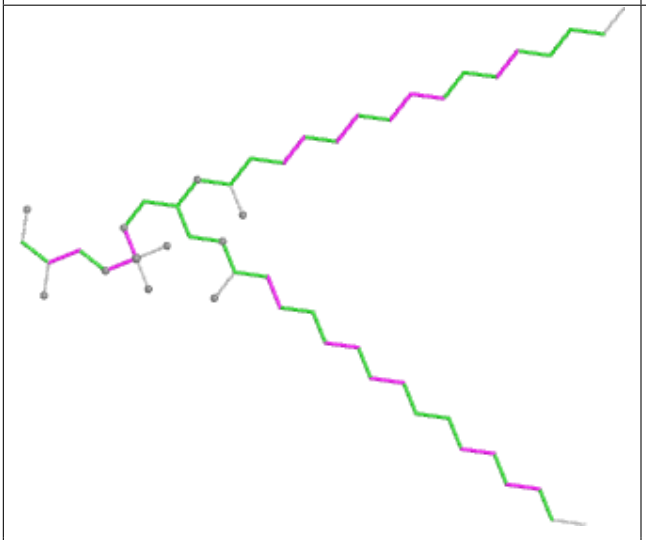
Ligand LHG D 706 (B)



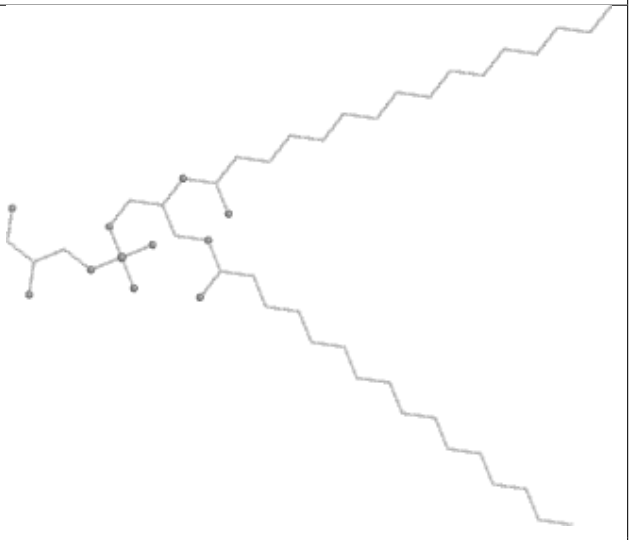
Bond lengths



Bond angles

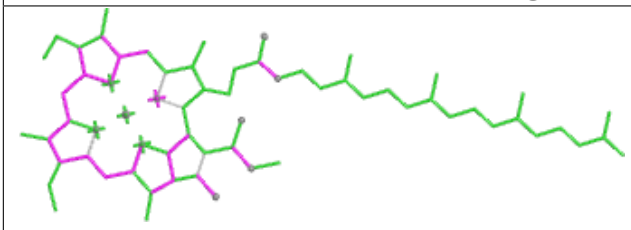


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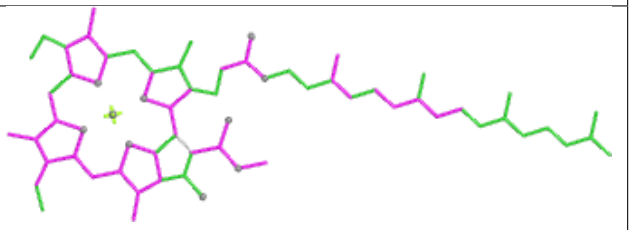


Rings

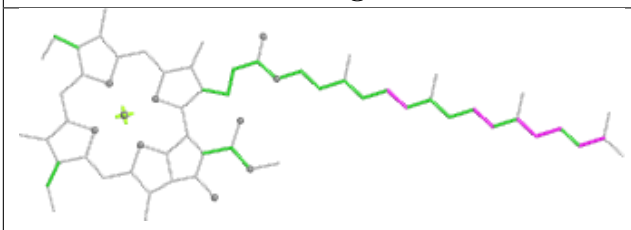
Ligand CLA B 615



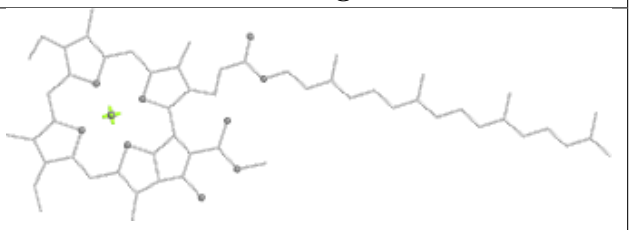
Bond lengths



Bond angles

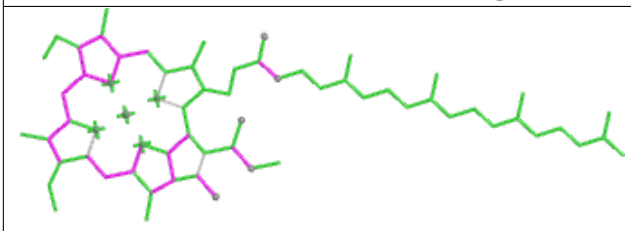


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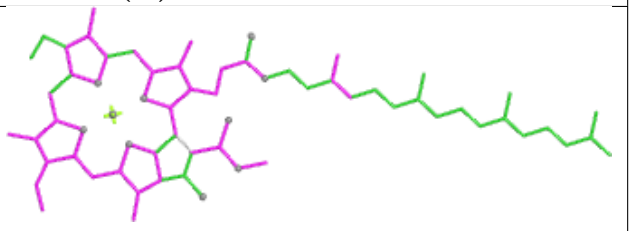


Rings

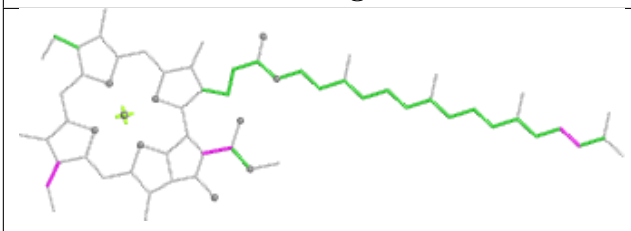
Ligand CLA A 405 (B)



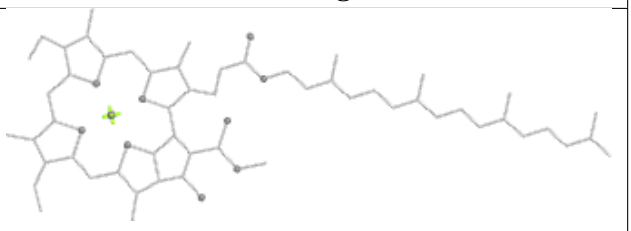
Bond lengths



Bond angles

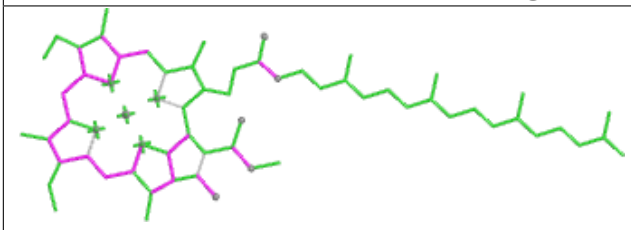


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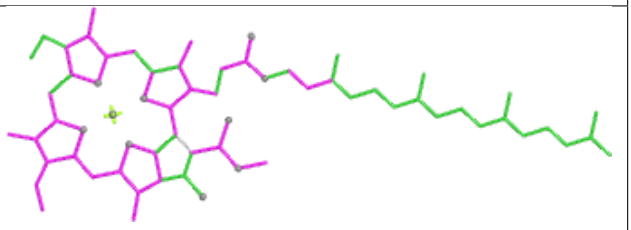


Rings

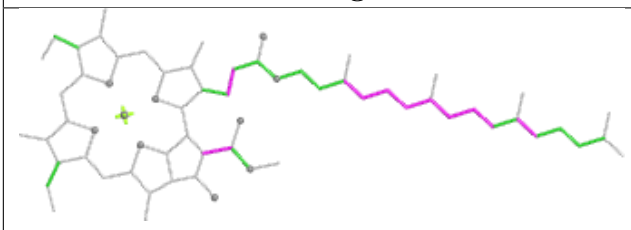
Ligand CLA B 614



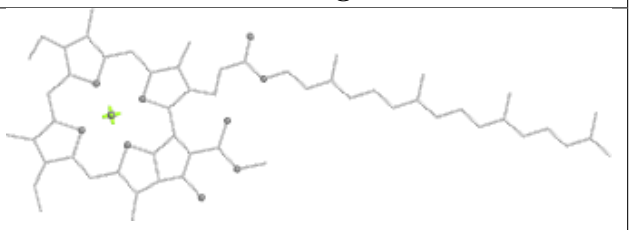
Bond lengths



Bond angles

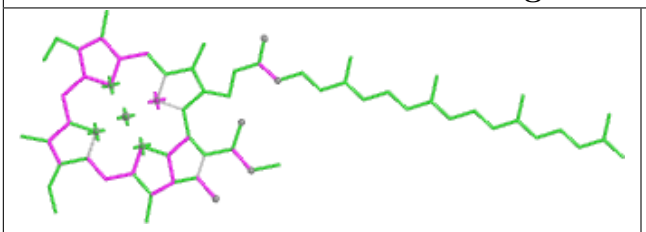


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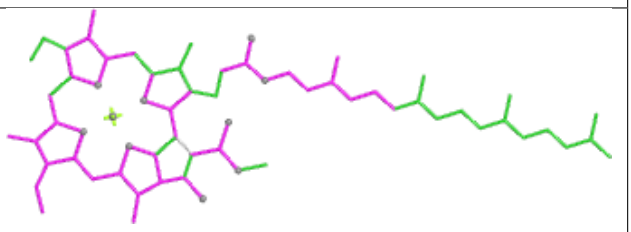


Rings

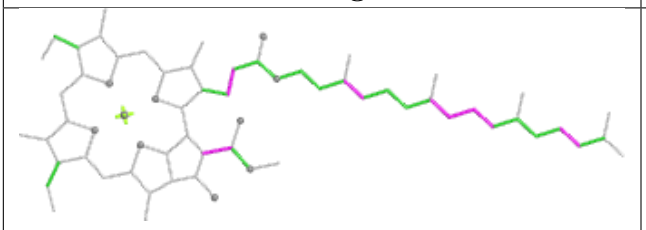
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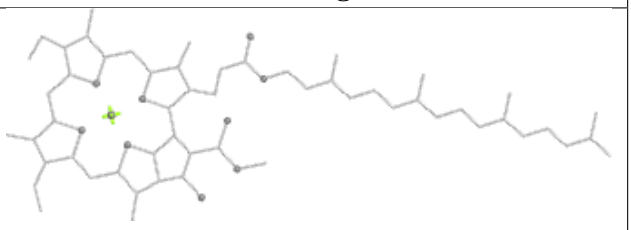
Bond lengths



Bond angles

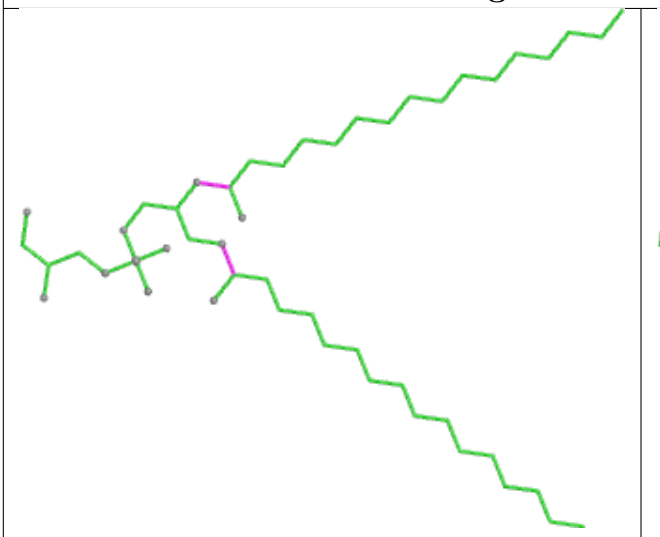


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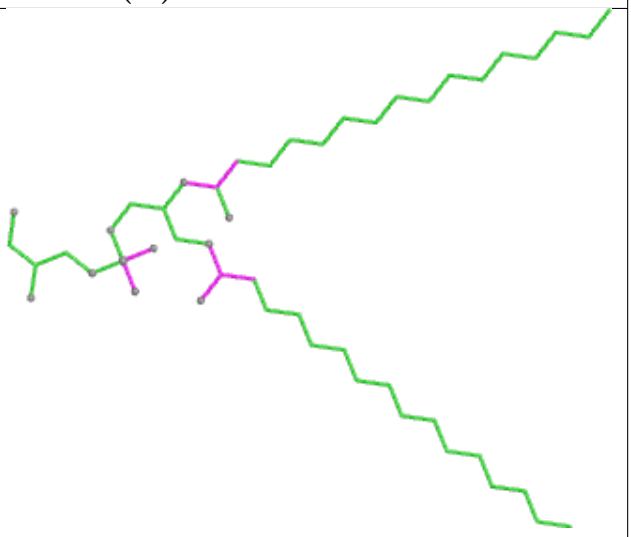


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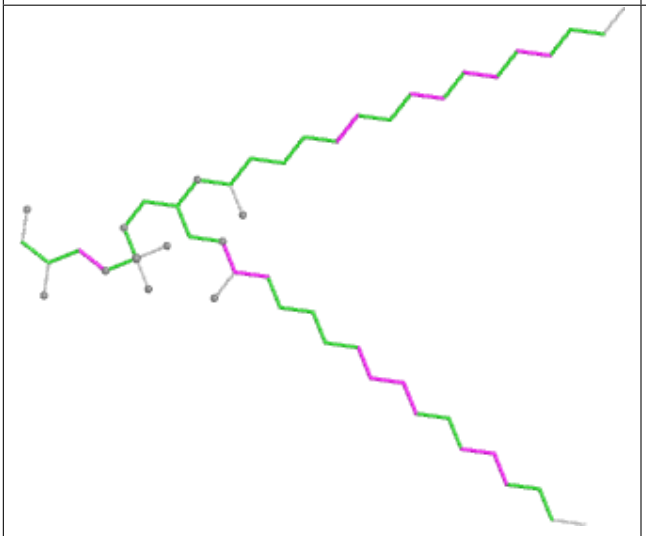
Ligand LHG D 707 (A)



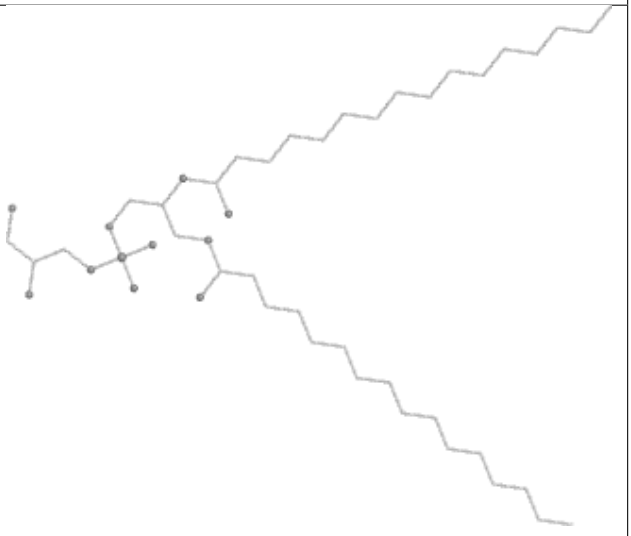
Bond lengths



Bond angles

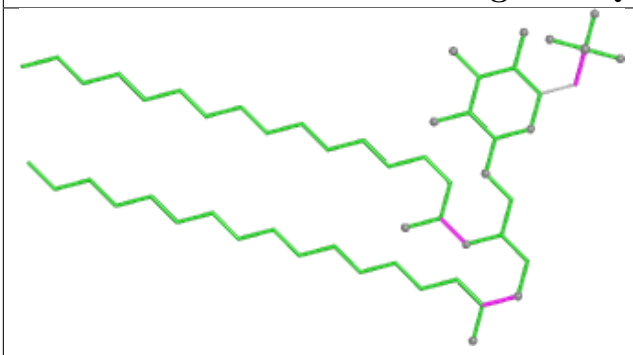


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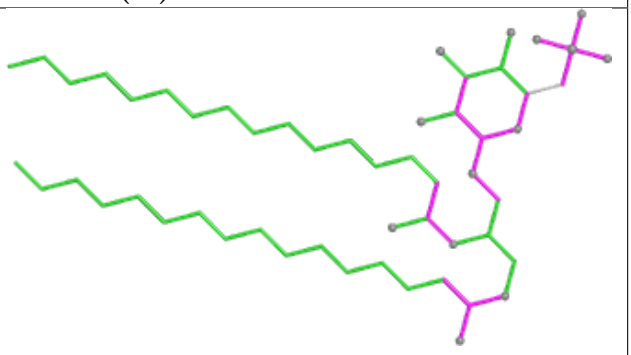


Rings

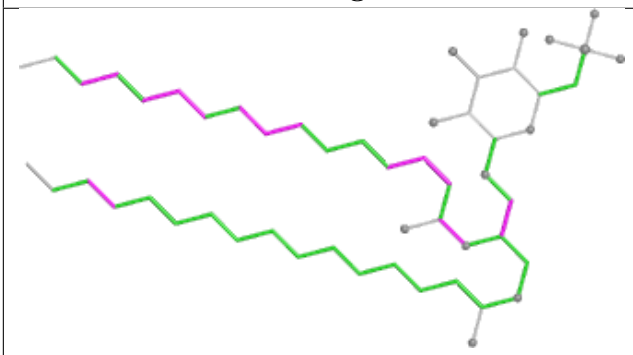
Ligand SQD A 410 (A)



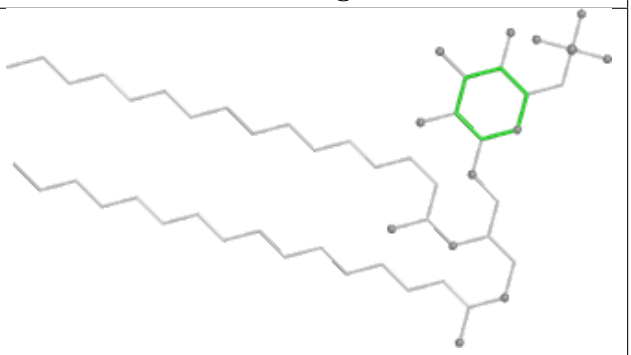
Bond lengths



Bond angles

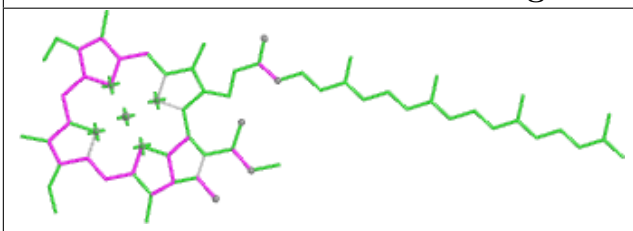


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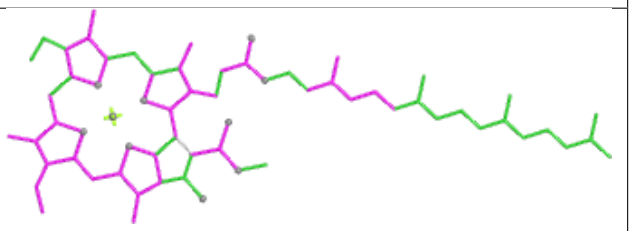


Rings

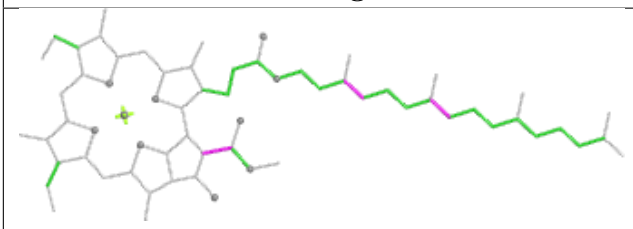
Ligand CLA b 603



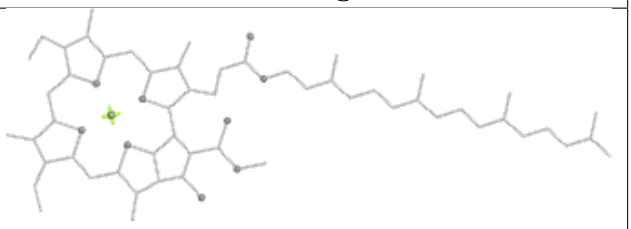
Bond lengths



Bond angles

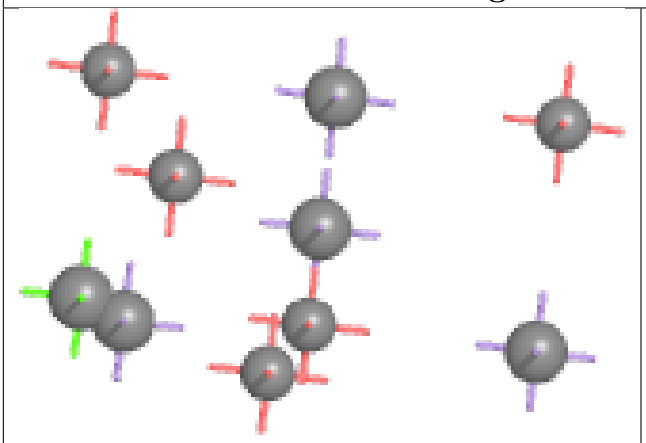


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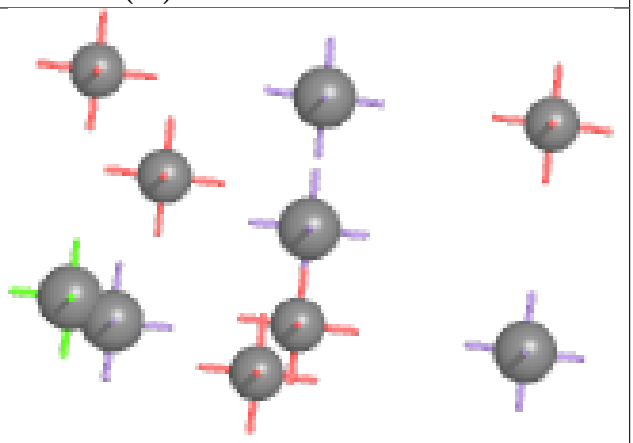


Rings

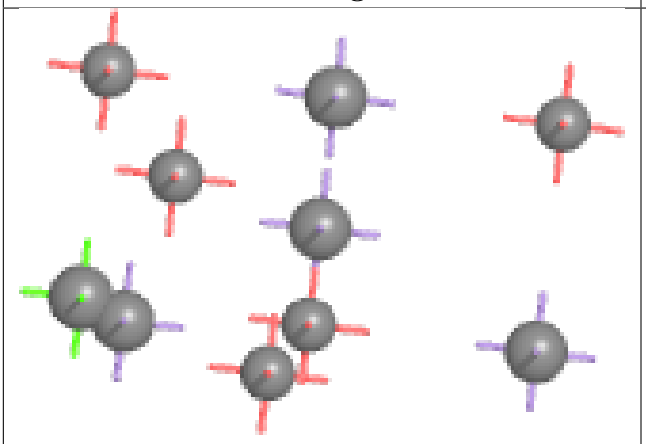
Ligand OEX A 413 (A)



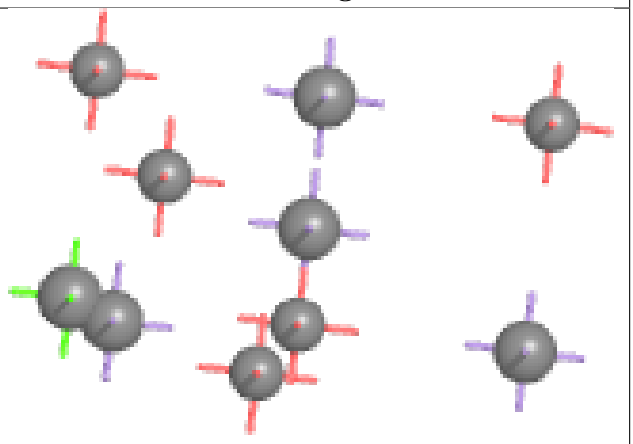
Bond lengths



Bond angles

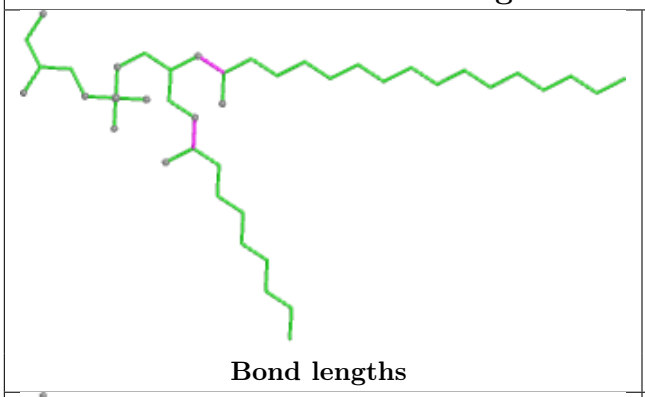


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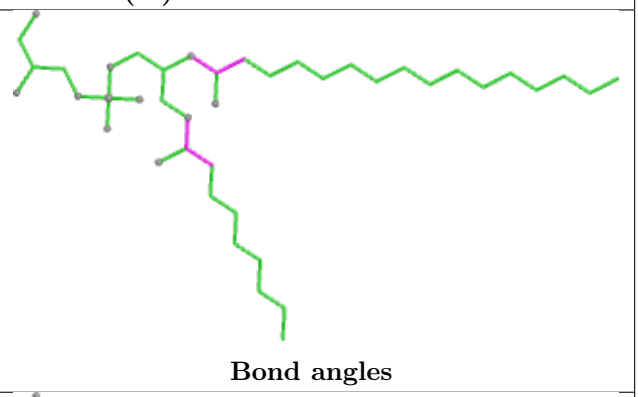


Rings

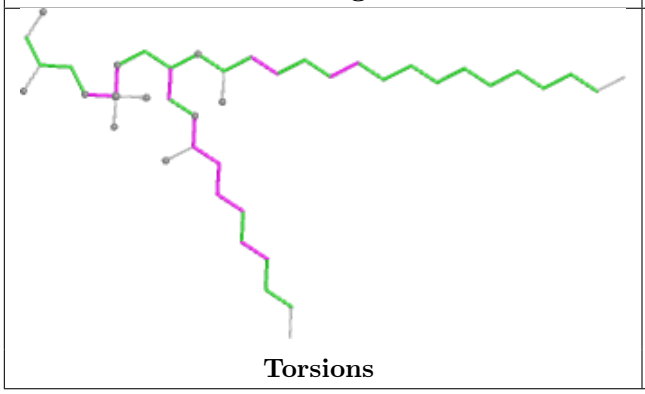
Ligand LHG a 420 (B)



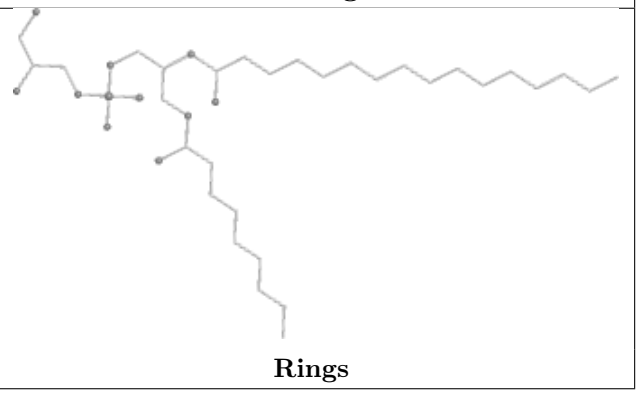
Bond lengths



Bond angles

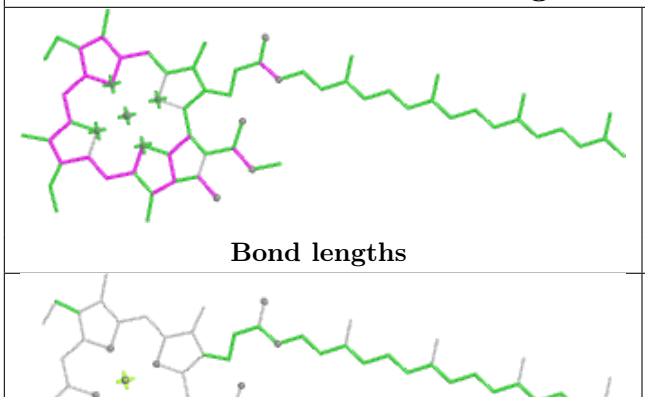


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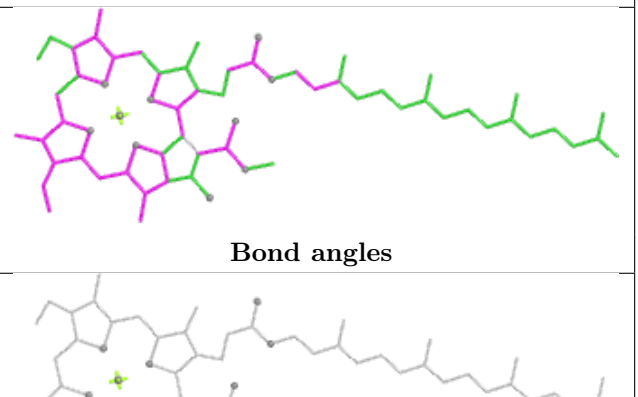


Rings

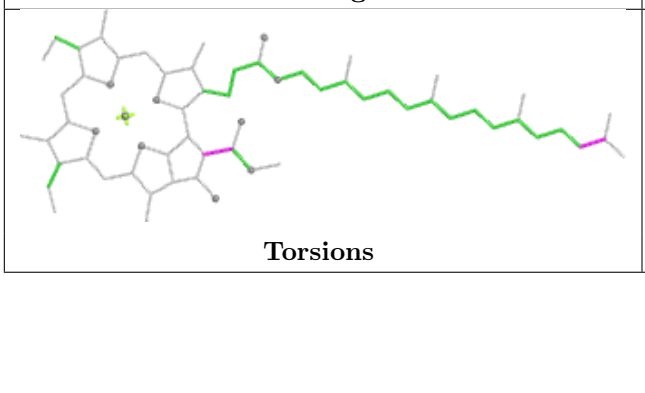
Ligand CLA c 503



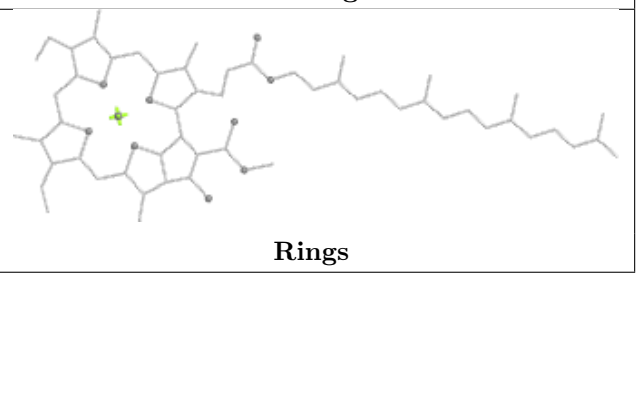
Bond lengths



Bond angles

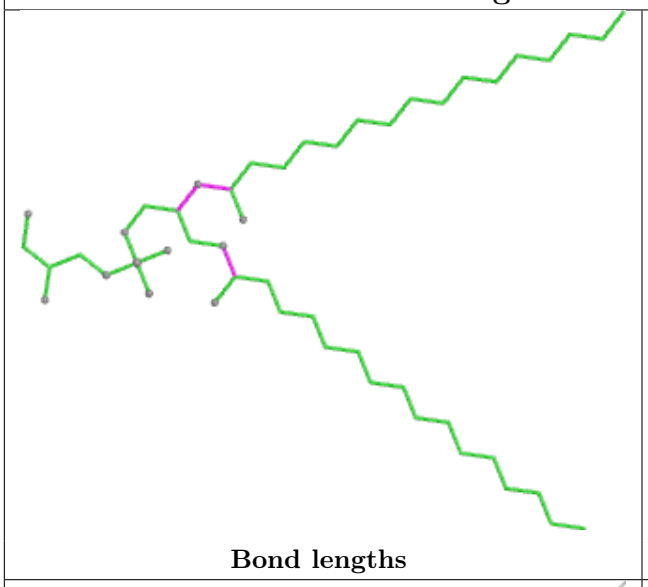


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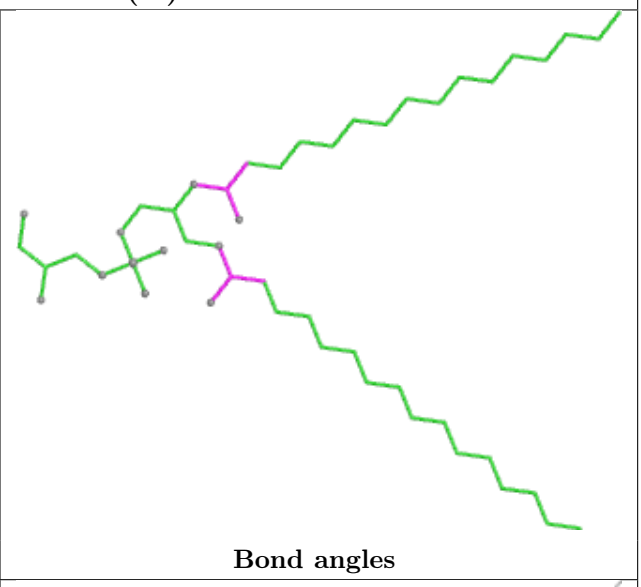


Rings

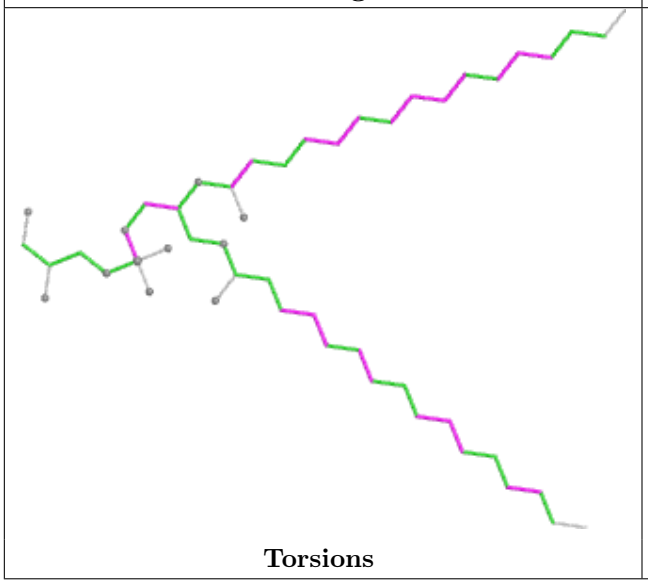
Ligand LHG b 629 (A)



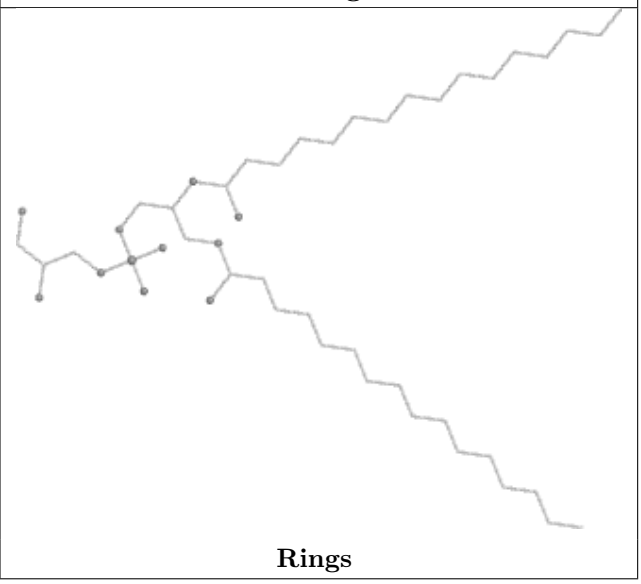
Bond lengths



Bond angles

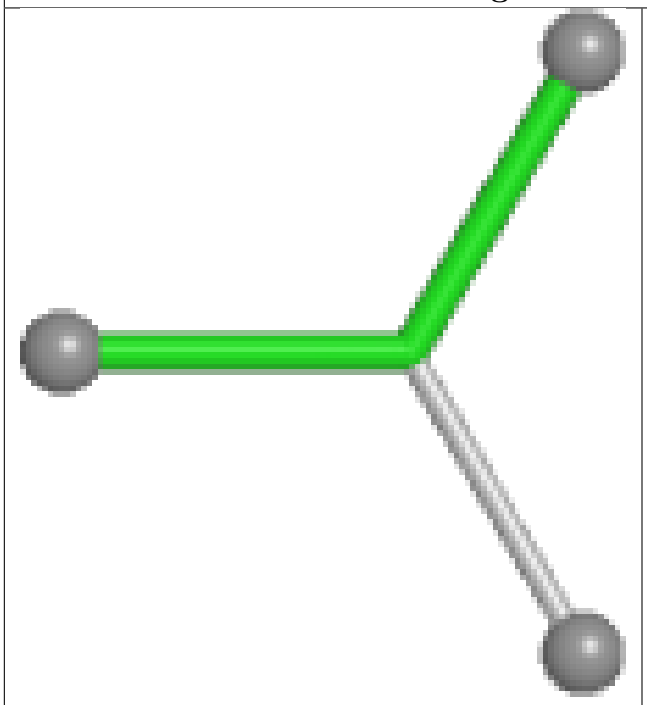


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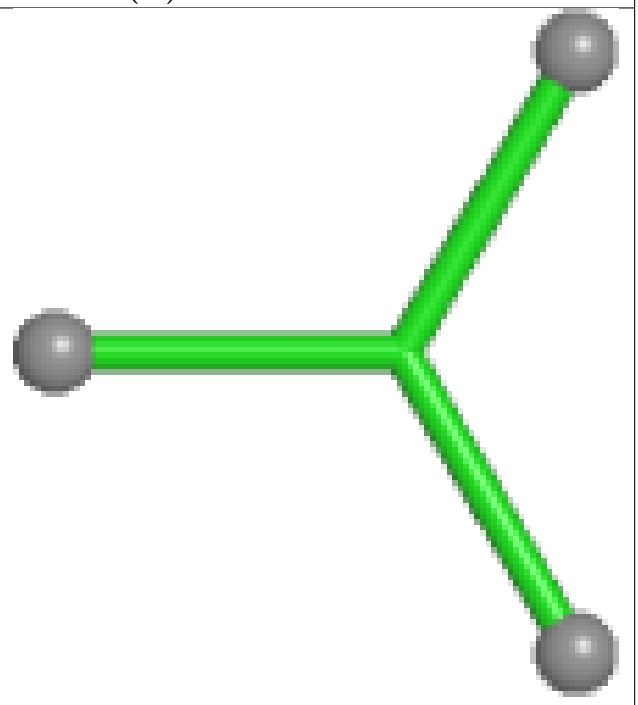


Rings

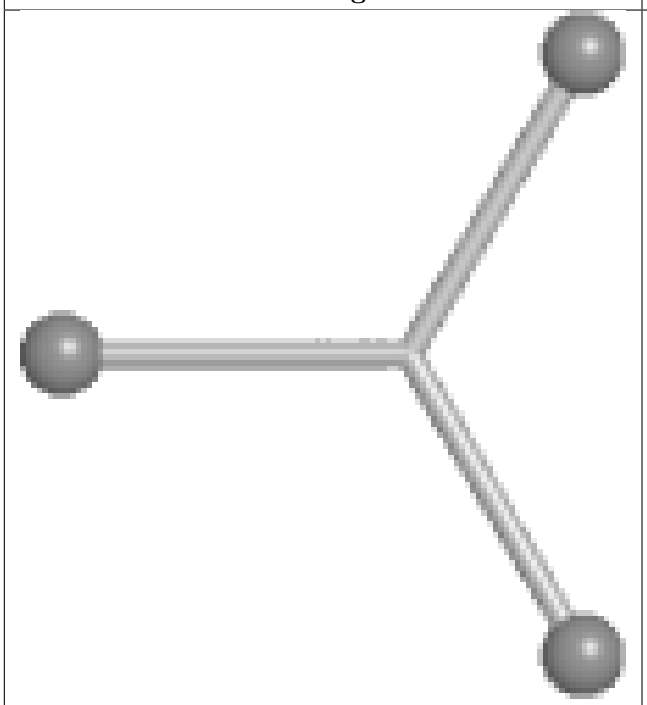
Ligand BCT A 416 (B)



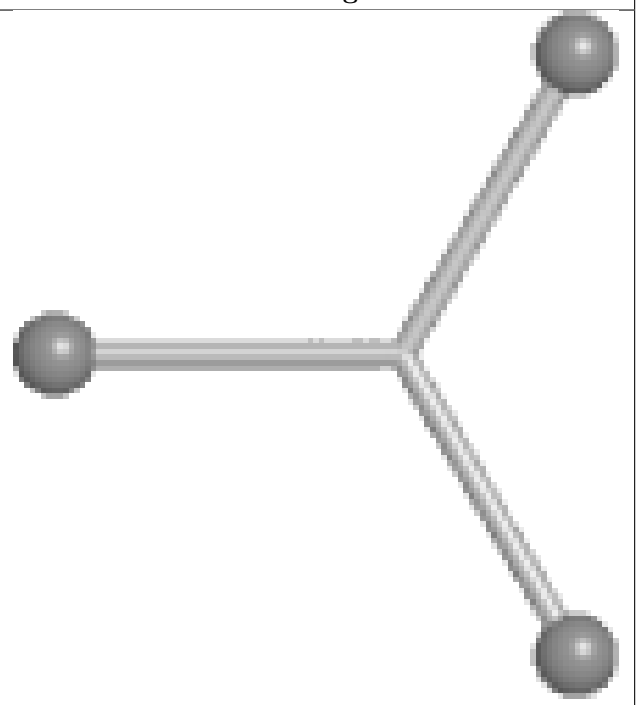
Bond lengths



Bond angles

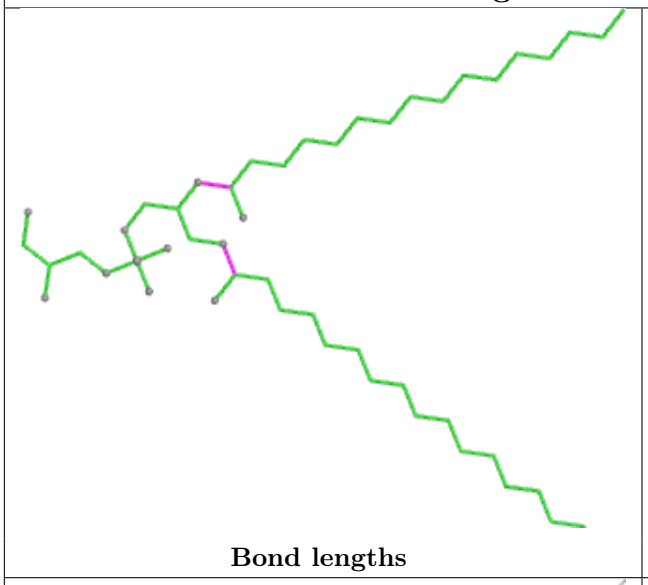


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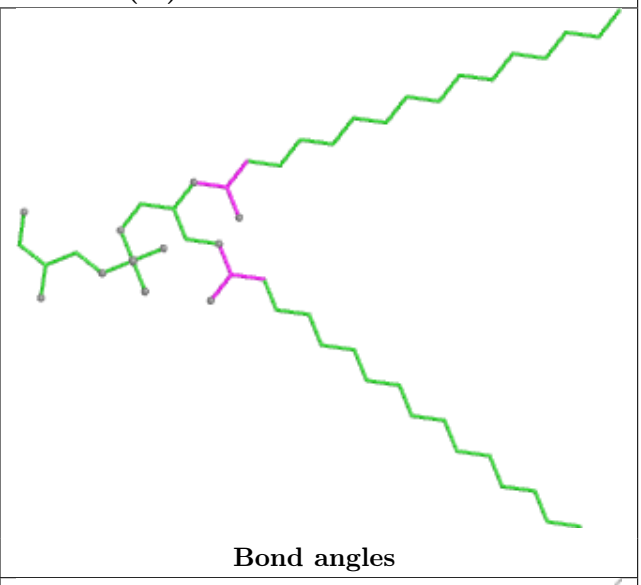


Rings

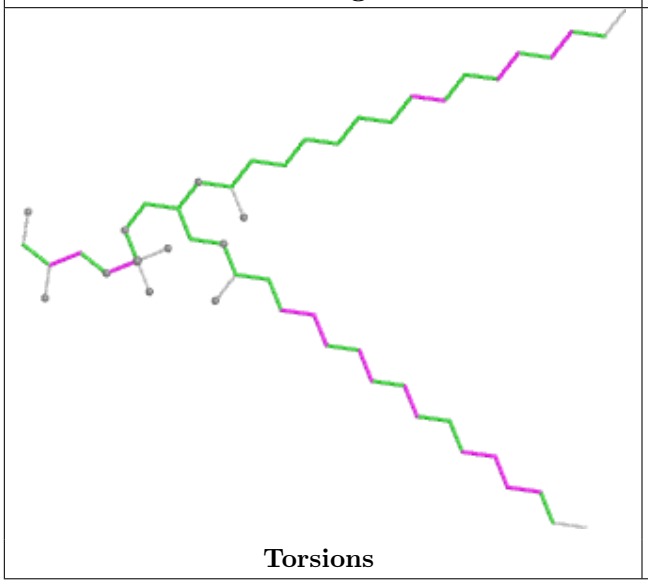
Ligand LHG d 412 (A)



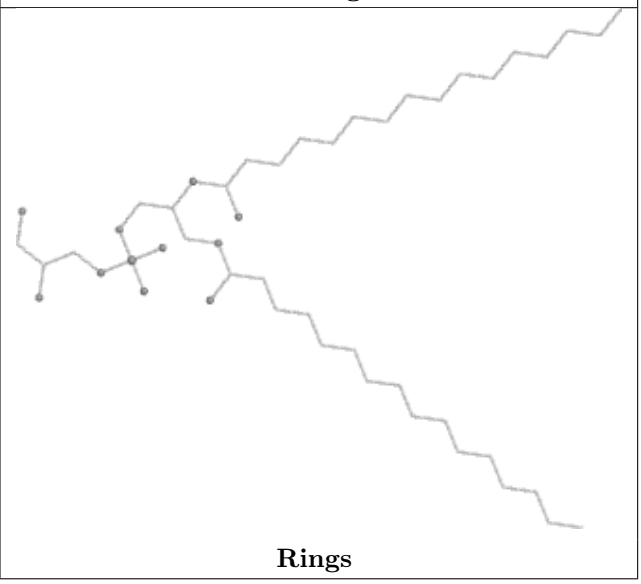
Bond lengths



Bond angles



Torsions



Rings

Ligand PL9 D 705 (A)



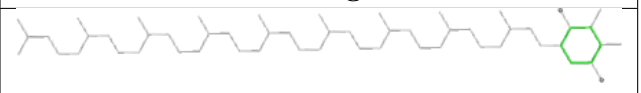
Bond lengths



Bond angles

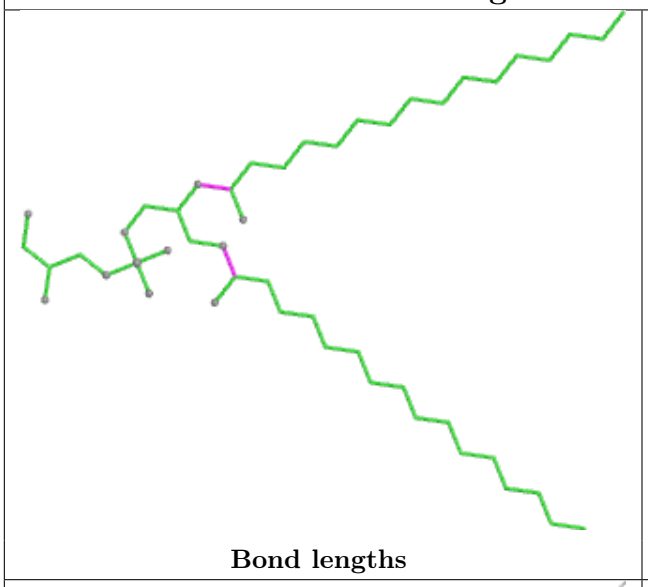


Torsions

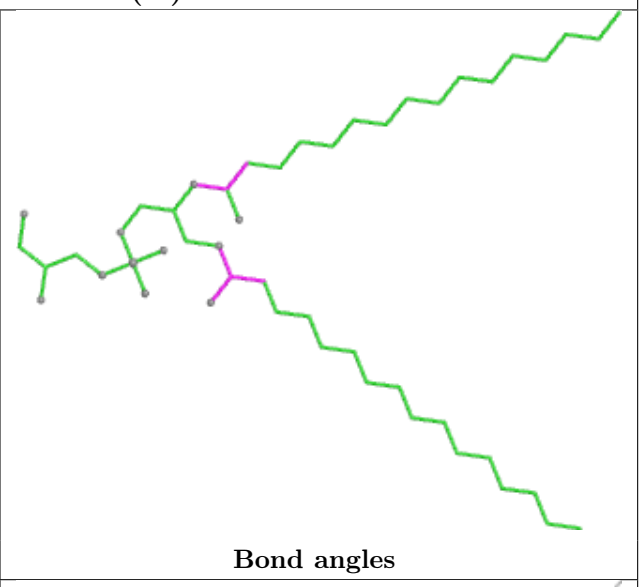


Rings

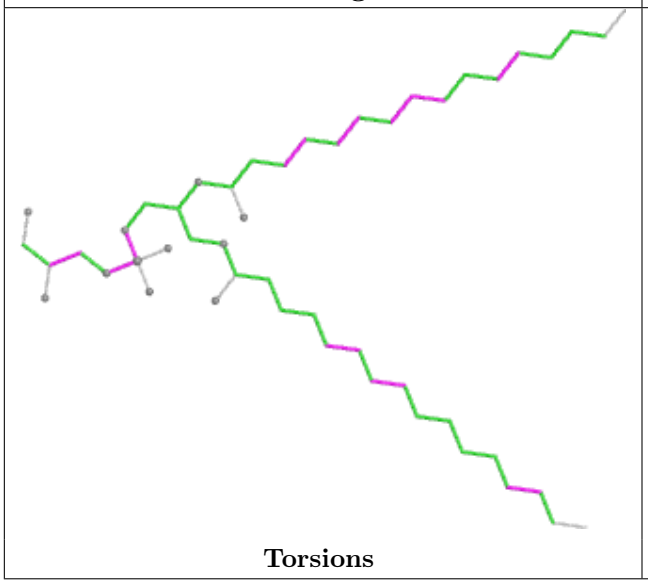
Ligand LHG D 706 (A)



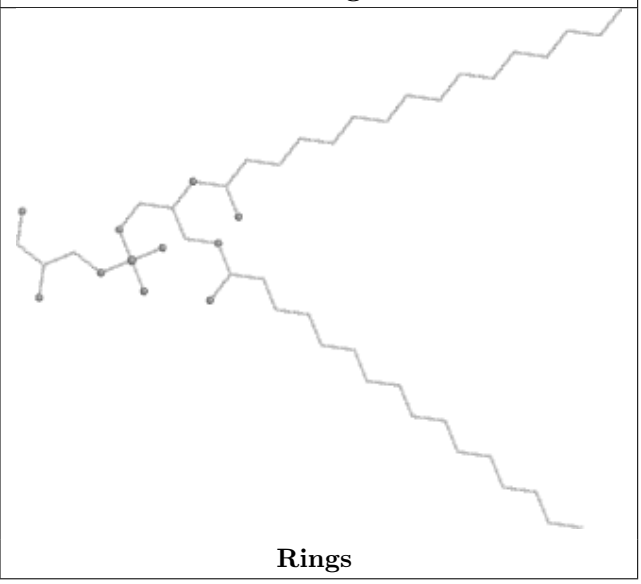
Bond lengths



Bond angles

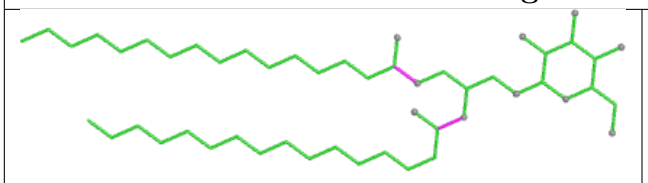


Torsions

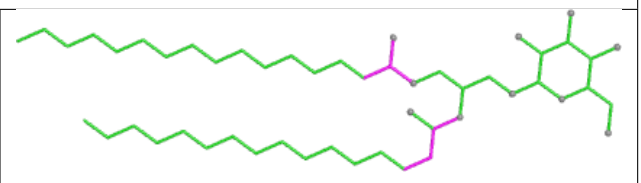


Rings

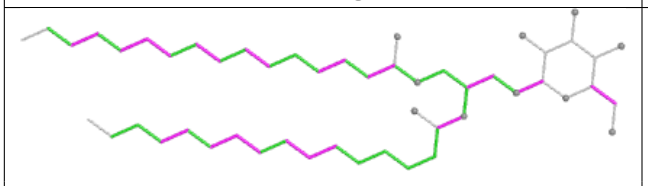
Ligand LMG B 621



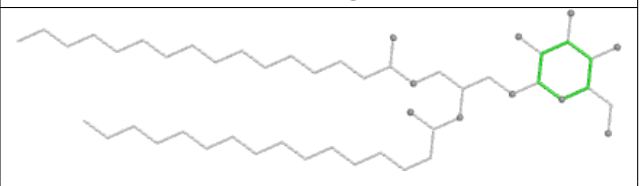
Bond lengths



Bond angles

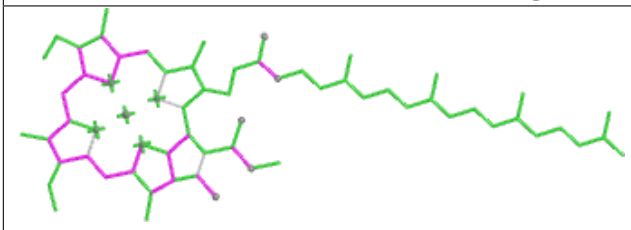


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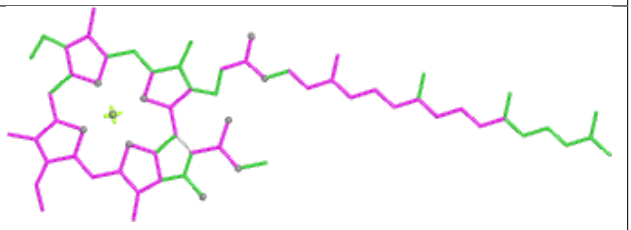


Rings

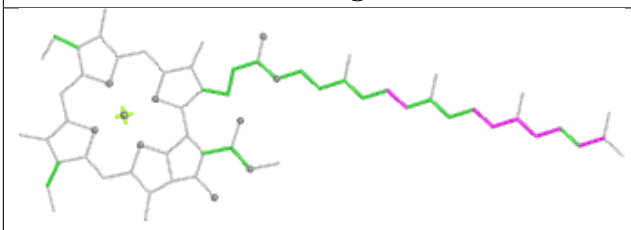
Ligand CLA b 615



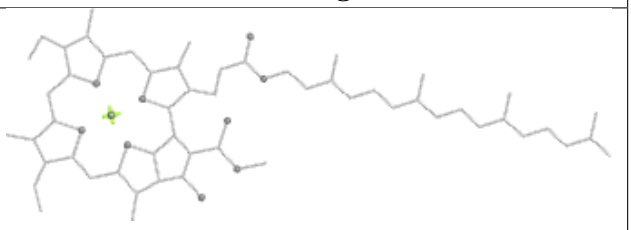
Bond lengths



Bond angles

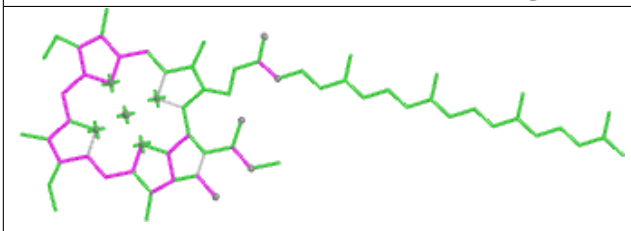


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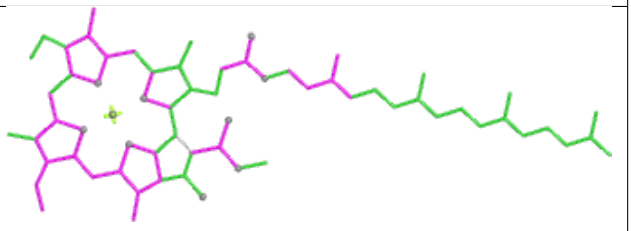


Rings

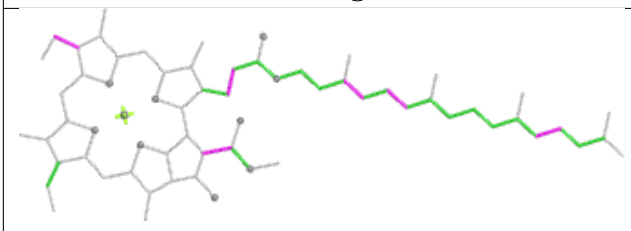
Ligand CLA C 508



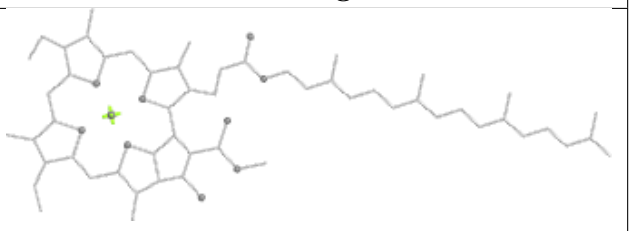
Bond lengths



Bond angles

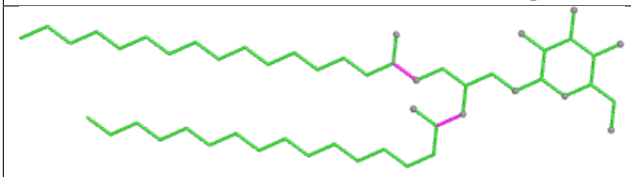


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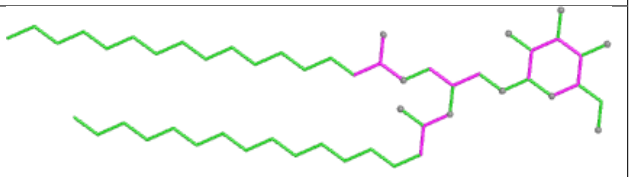


Rings

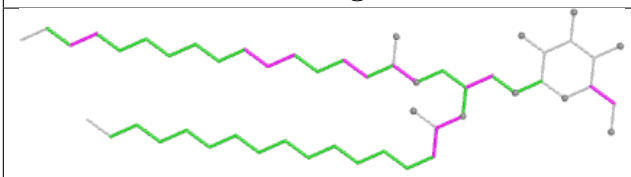
Ligand LMG c 521



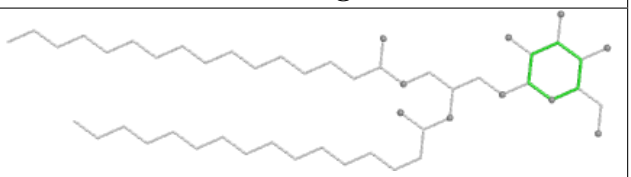
Bond lengths



Bond angles

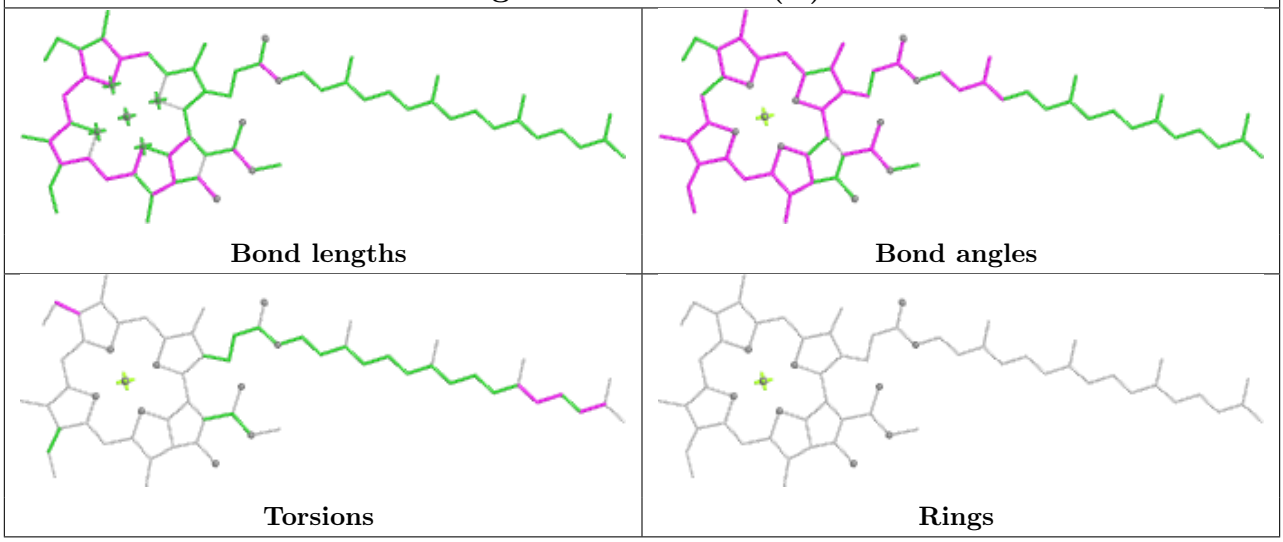


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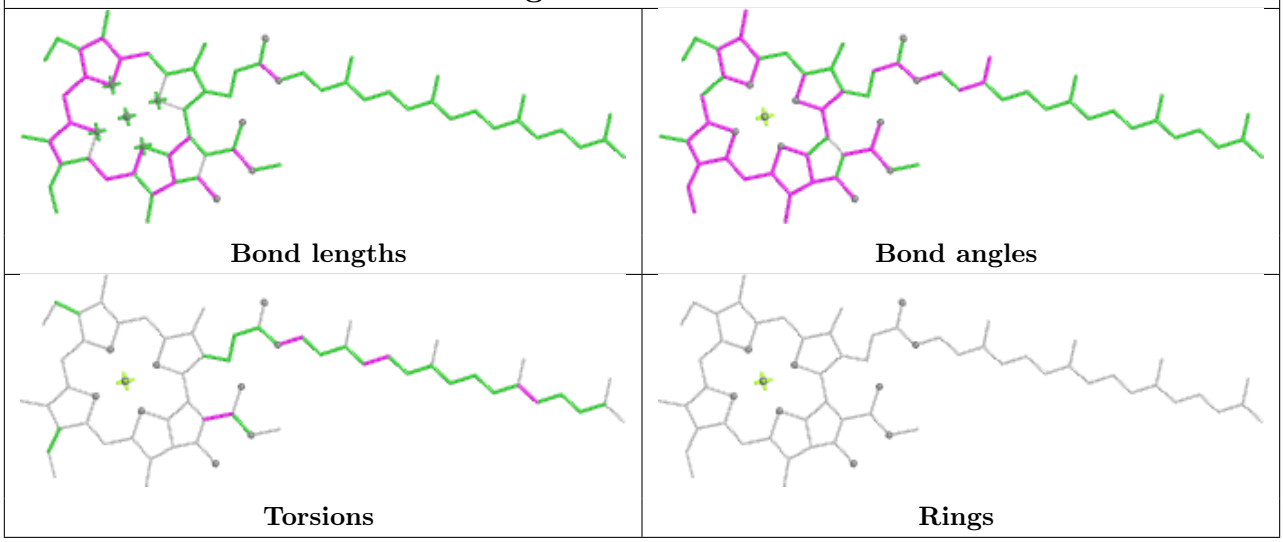


Rings

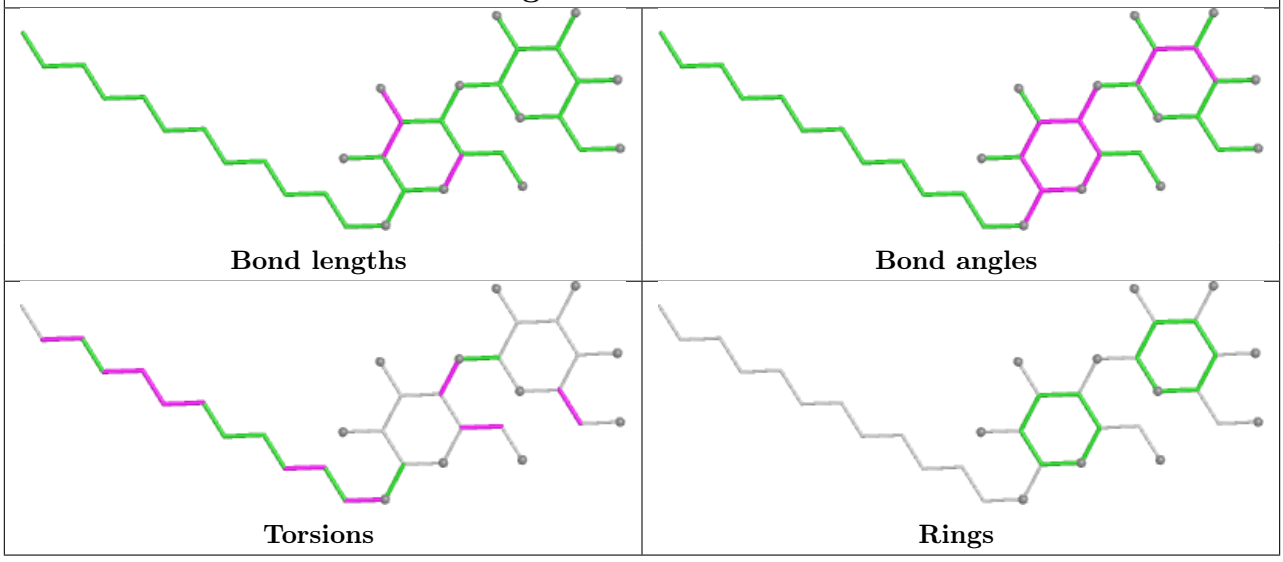
Ligand CLA A 406 (B)



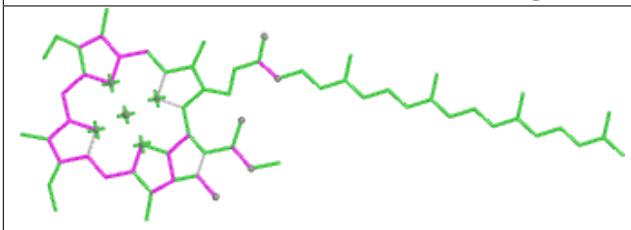
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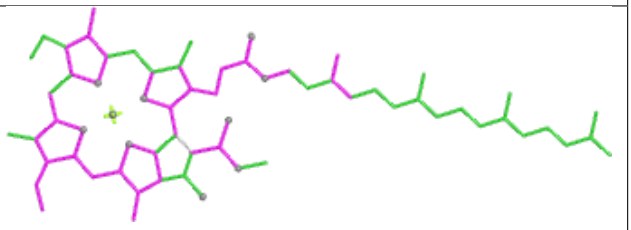
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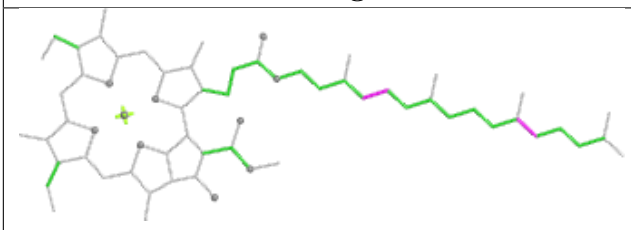
Ligand CLA b 607



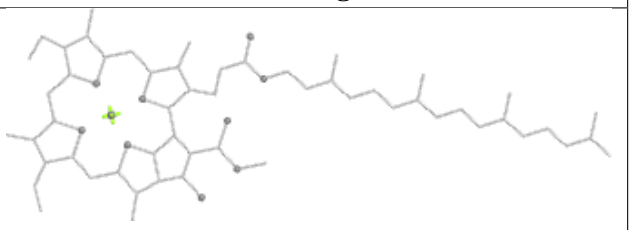
Bond lengths



Bond angles

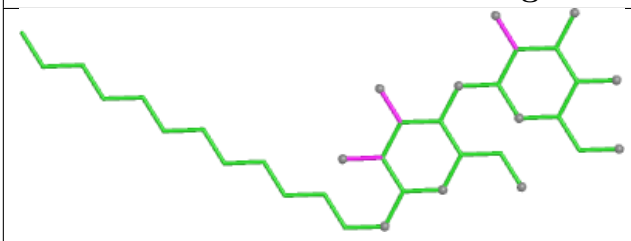


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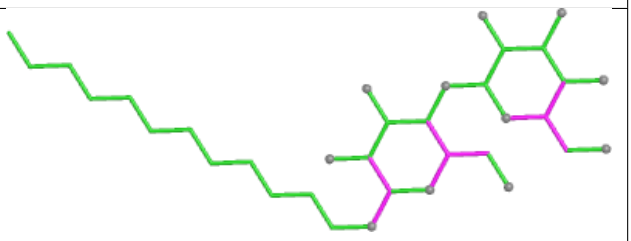


Rings

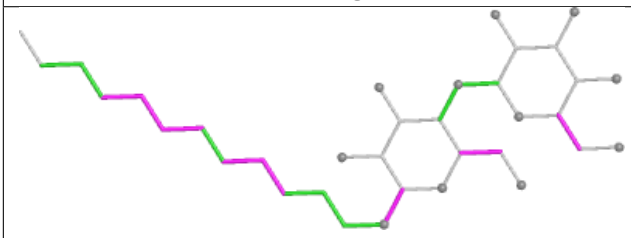
Ligand LMT B 629



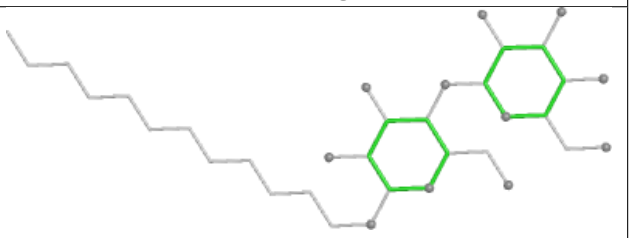
Bond lengths



Bond angles

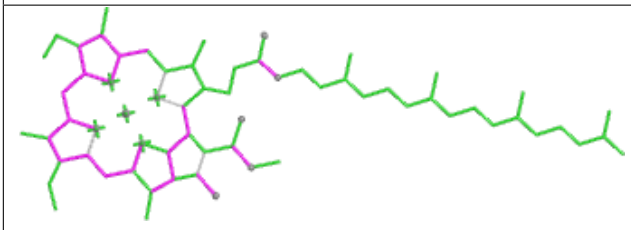


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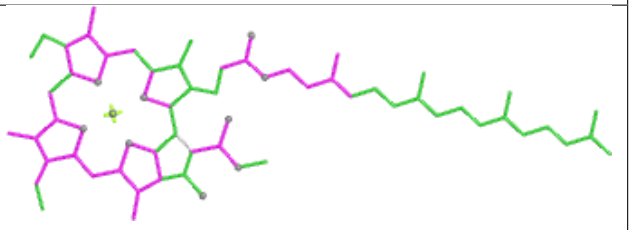


Rings

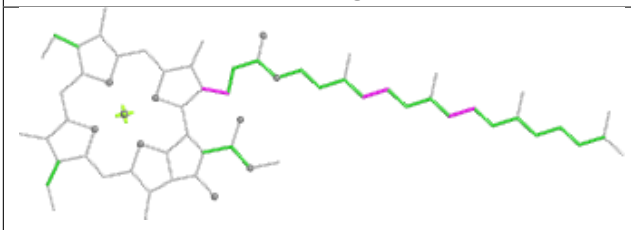
Ligand CLA C 512



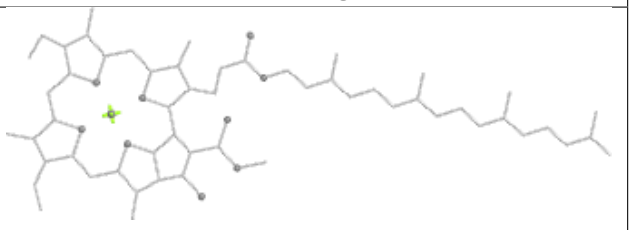
Bond lengths



Bond angles

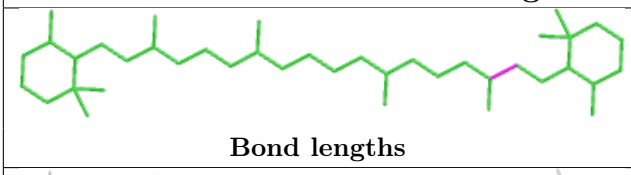


Torsions

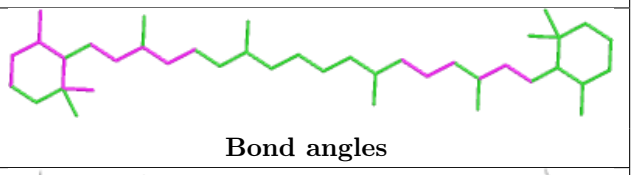


Rings

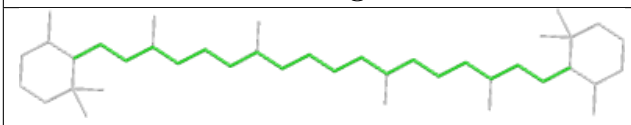
Ligand BCR C 516



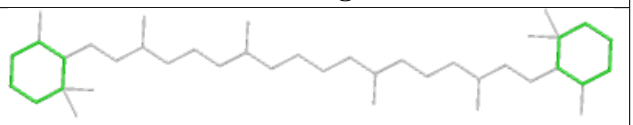
Bond lengths



Bond angles

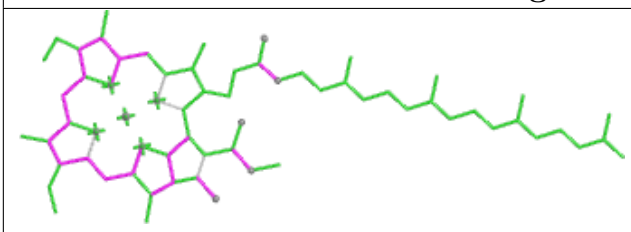


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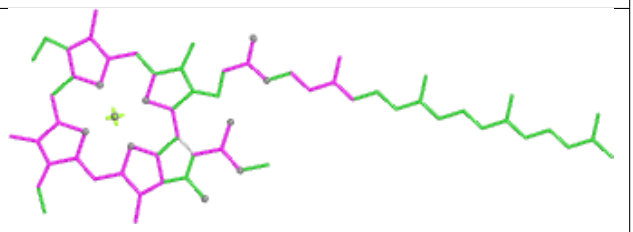


Rings

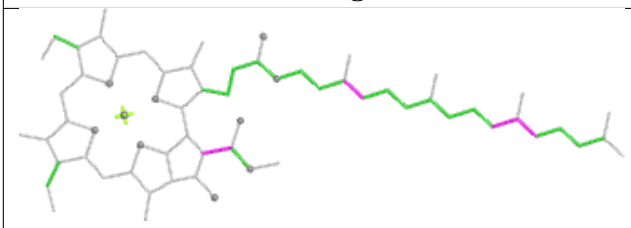
Ligand CLA c 506



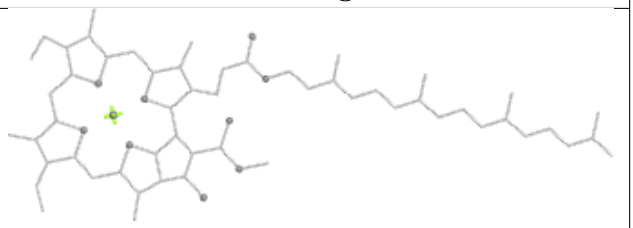
Bond lengths



Bond angles

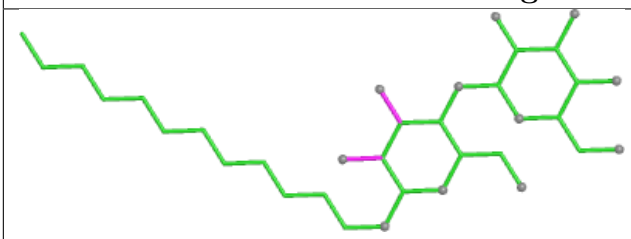


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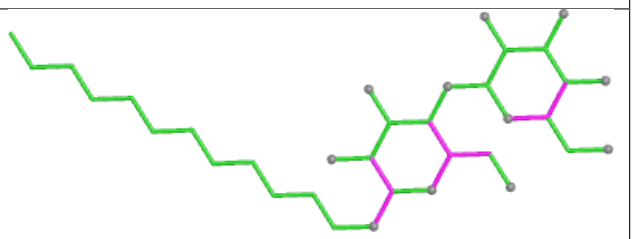


Rings

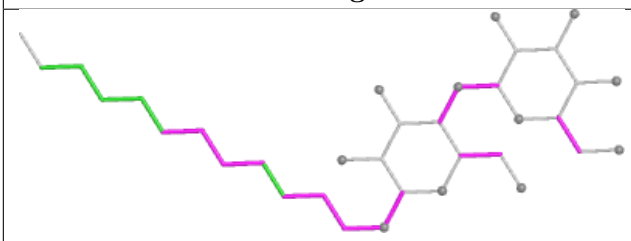
Ligand LMT A 420



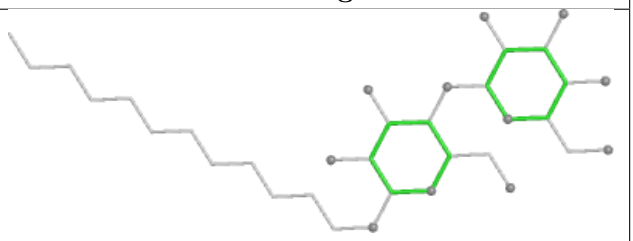
Bond lengths



Bond angles

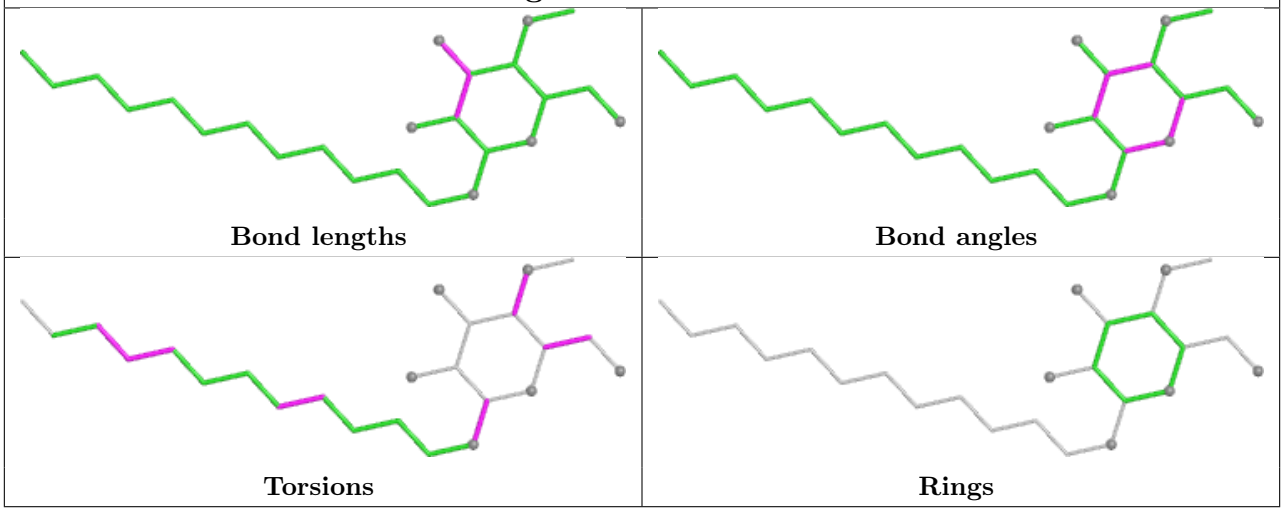


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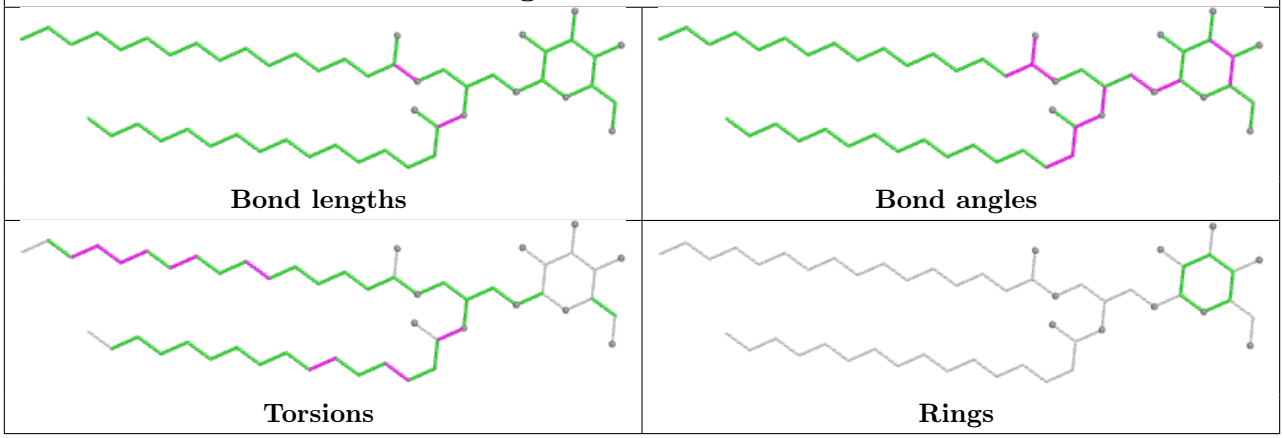


Rings

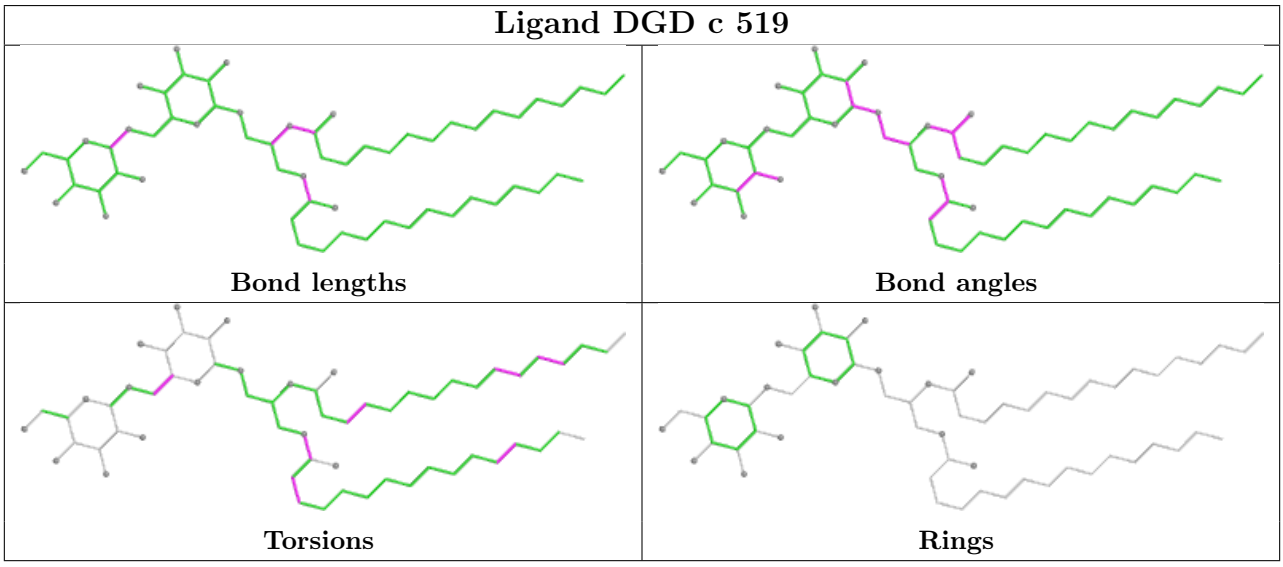
Ligand LMT b 621



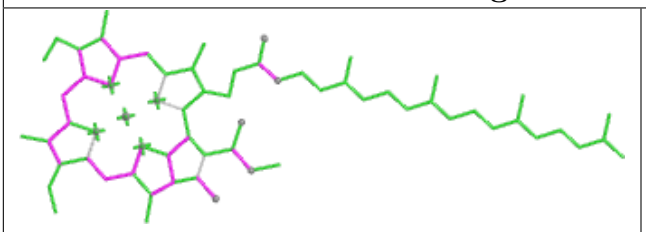
Ligand LMG m 101



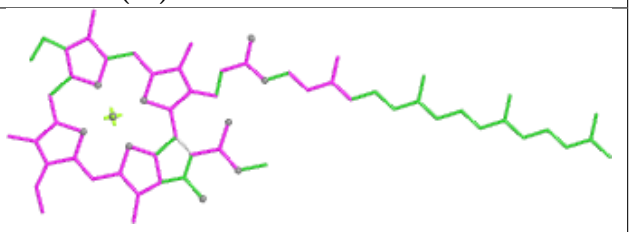
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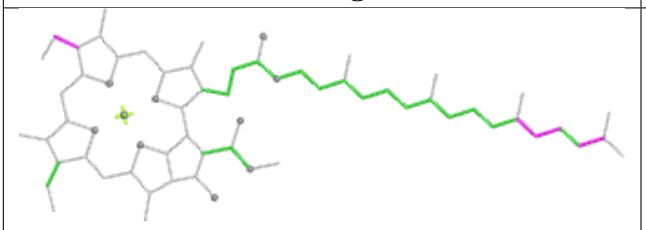
Ligand CLA A 406 (A)



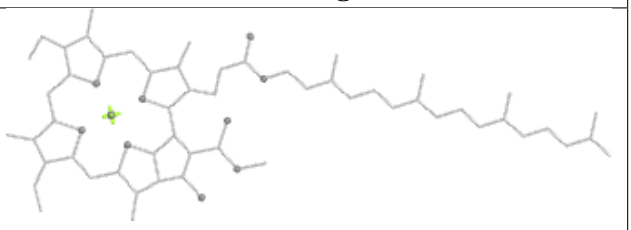
Bond lengths



Bond angles

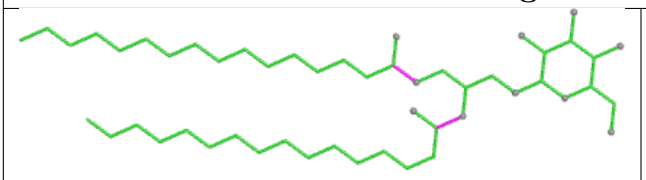


Torsions

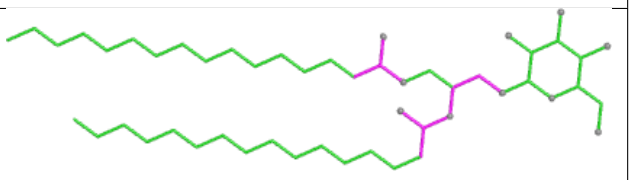


Rings

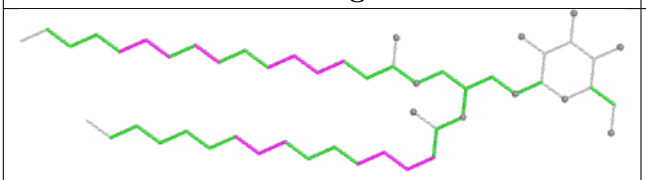
Ligand LMG C 520



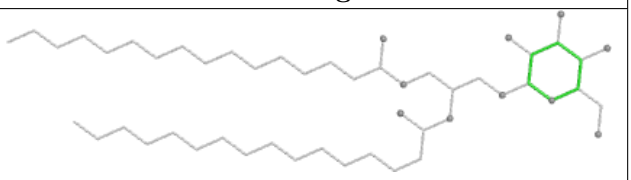
Bond lengths



Bond angles

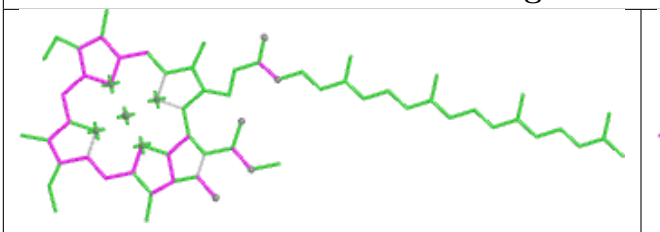


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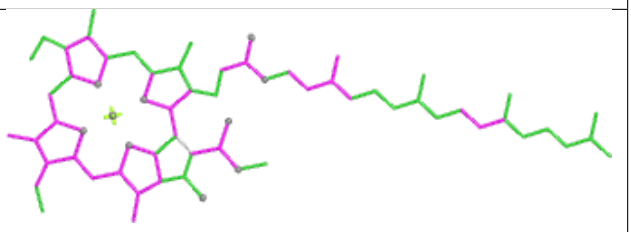


Rings

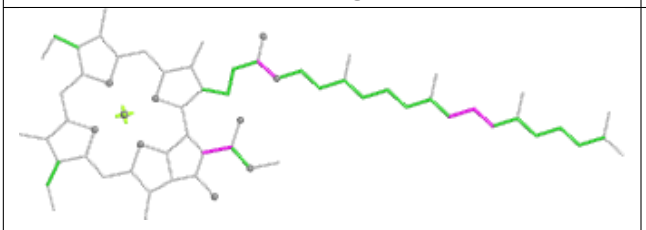
Ligand CLA B 612



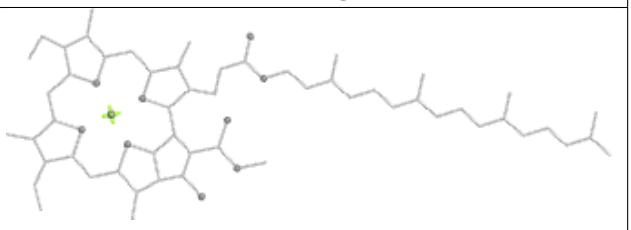
Bond lengths



Bond angles

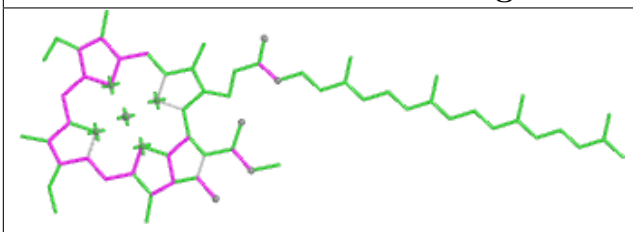


Torsions

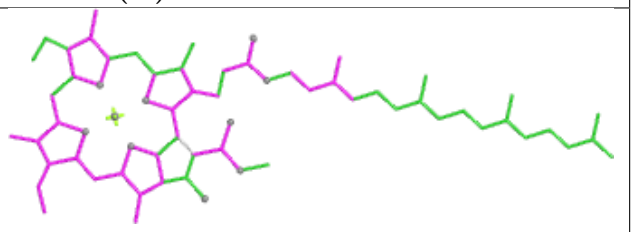


Rings

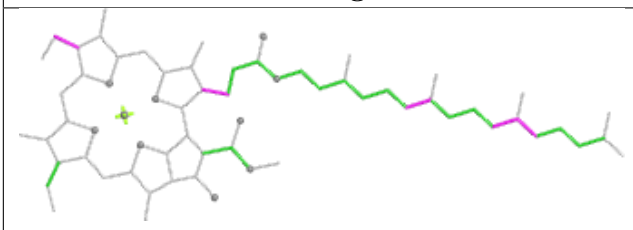
Ligand CLA a 407 (B)



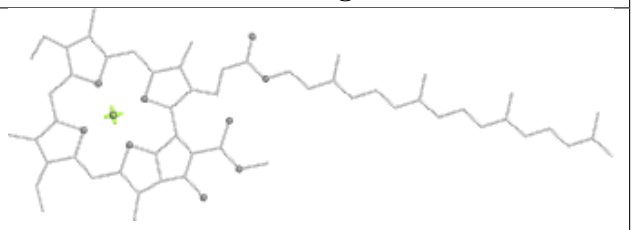
Bond lengths



Bond angles



Torsions



Rings

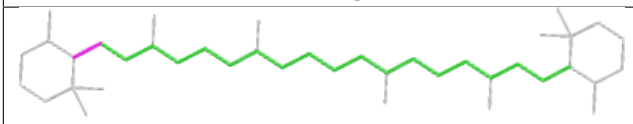
Ligand BCR B 617



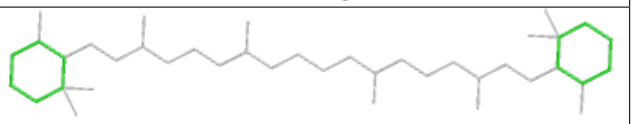
Bond lengths



Bond angles

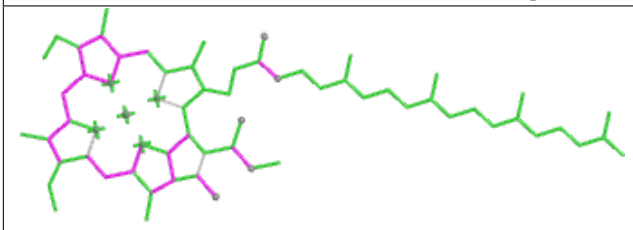


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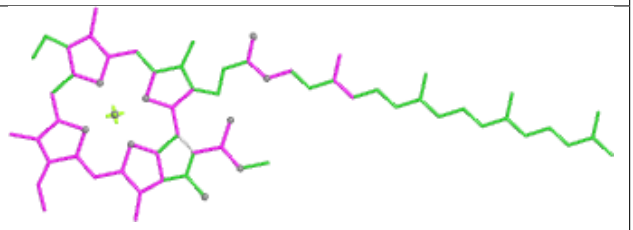


Rings

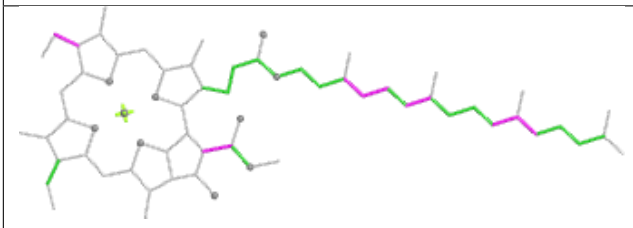
Ligand CLA C 505



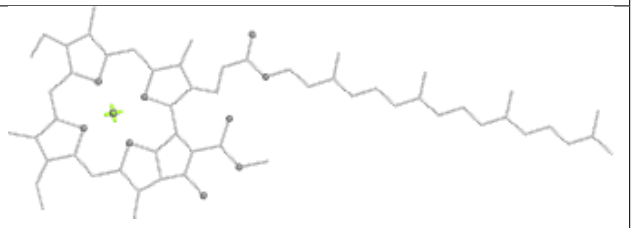
Bond lengths



Bond angles

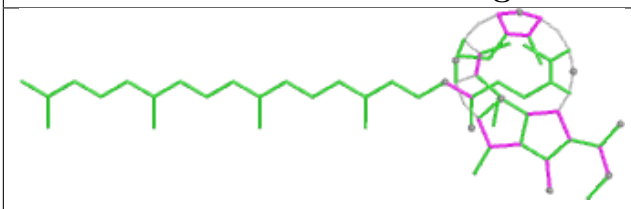


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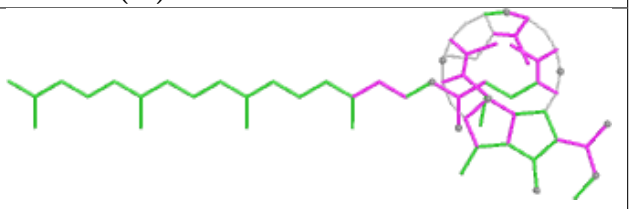


Rings

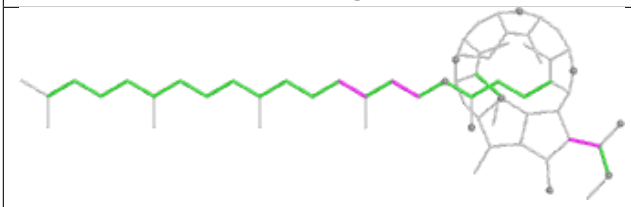
Ligand PHO a 408 (B)



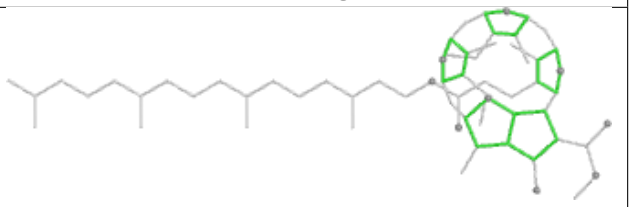
Bond lengths



Bond angles

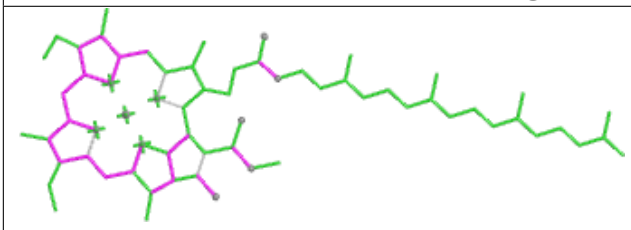


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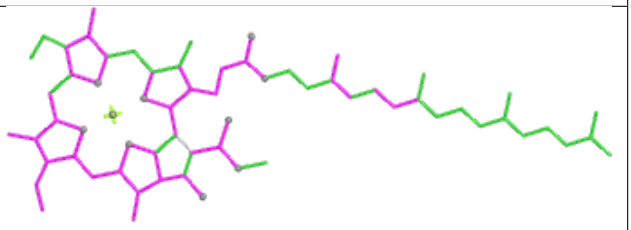


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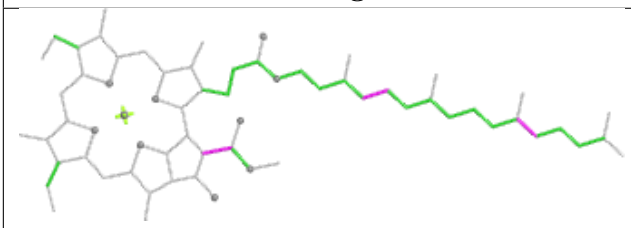
Ligand CLA B 607



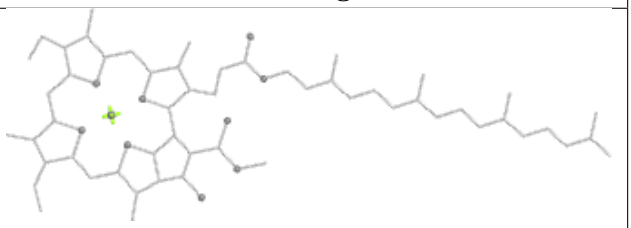
Bond lengths



Bond angles

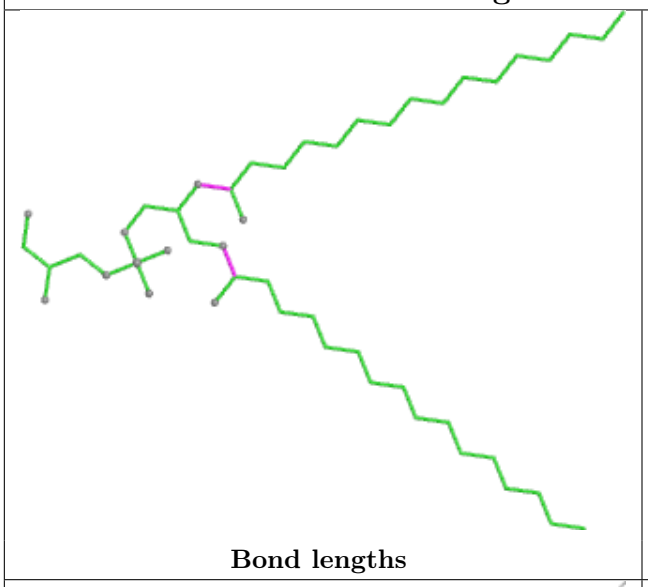


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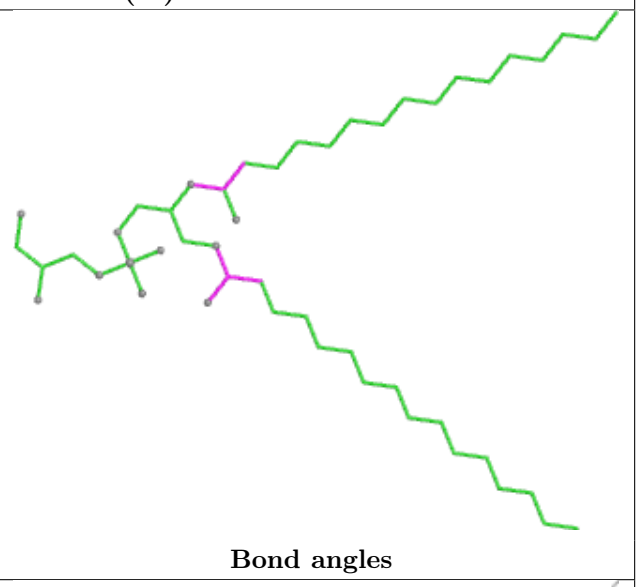


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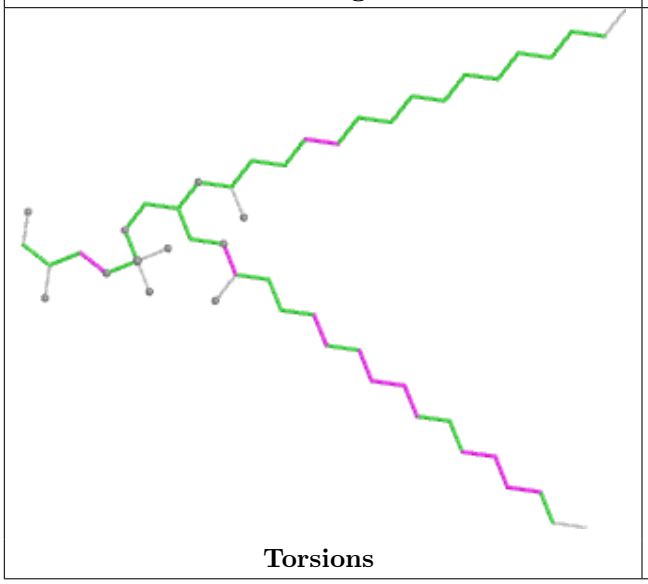
Ligand LHG d 406 (A)



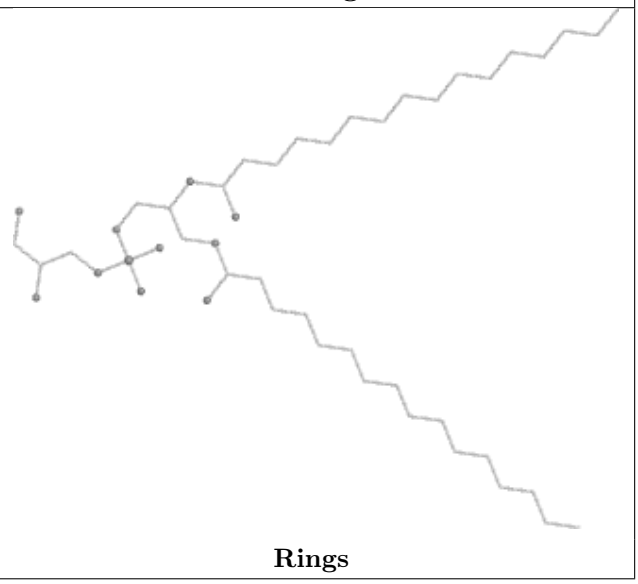
Bond lengths



Bond angles



Torsions

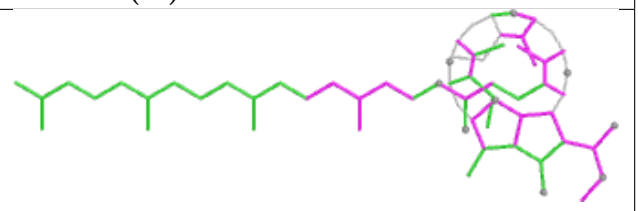


Rings

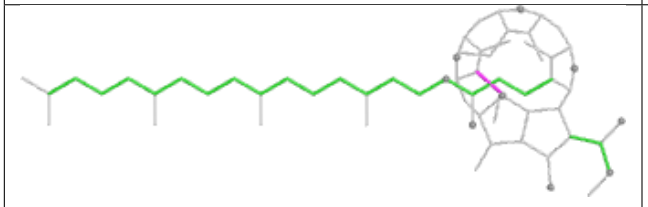
Ligand PHO A 417 (A)



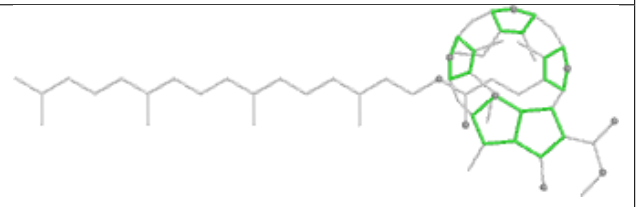
Bond lengths



Bond angles

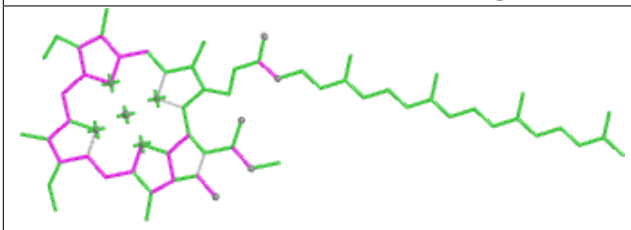


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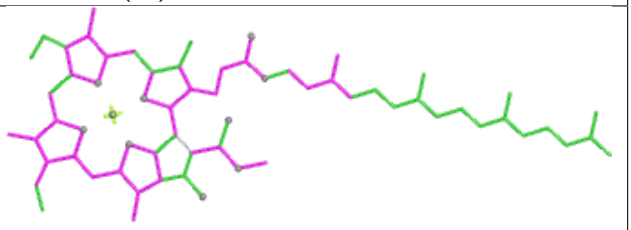


Rings

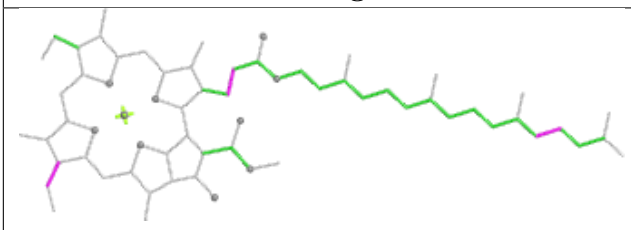
Ligand CLA A 404 (B)



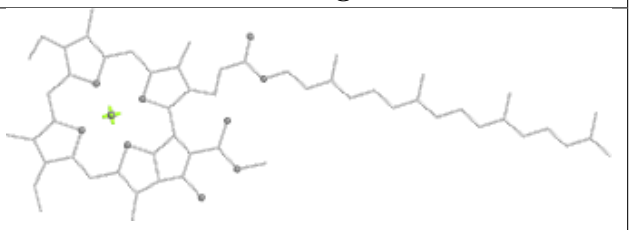
Bond lengths



Bond angles

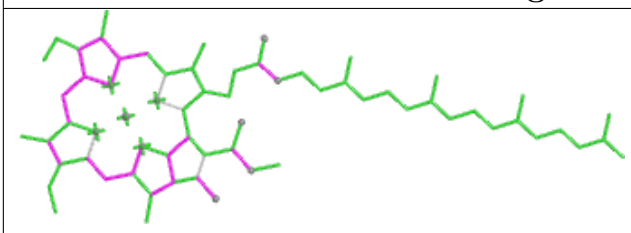


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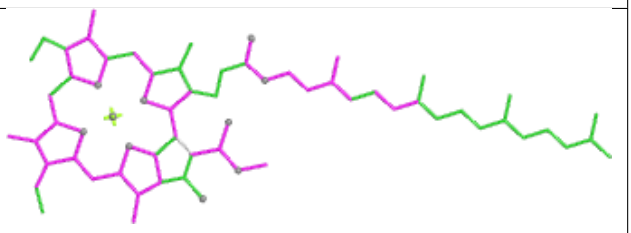


Rings

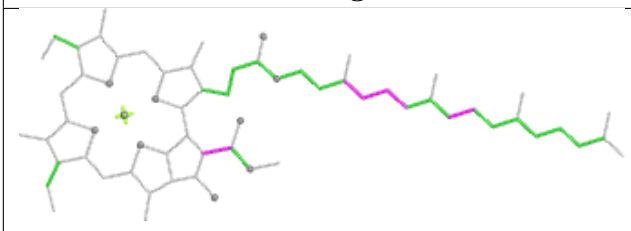
Ligand CLA b 605



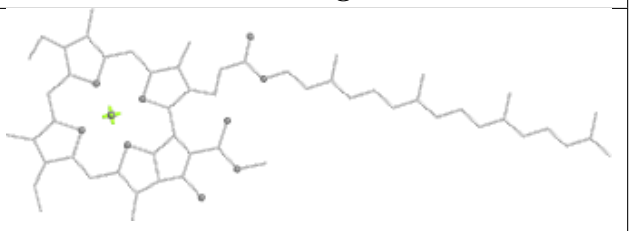
Bond lengths



Bond angles

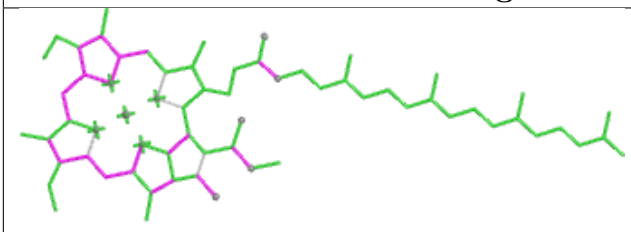


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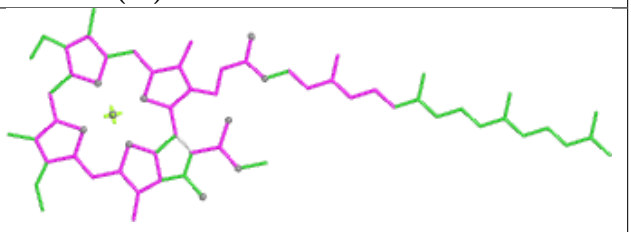


Rings

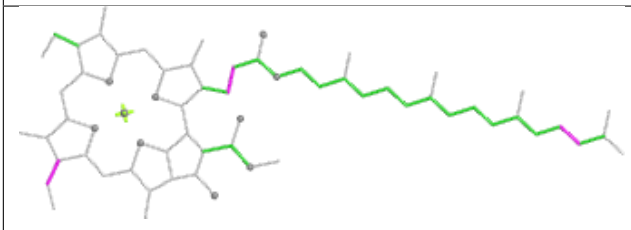
Ligand CLA a 405 (B)



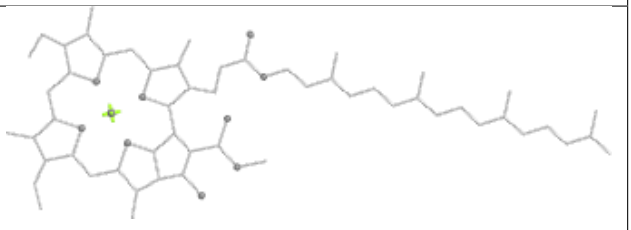
Bond lengths



Bond angles

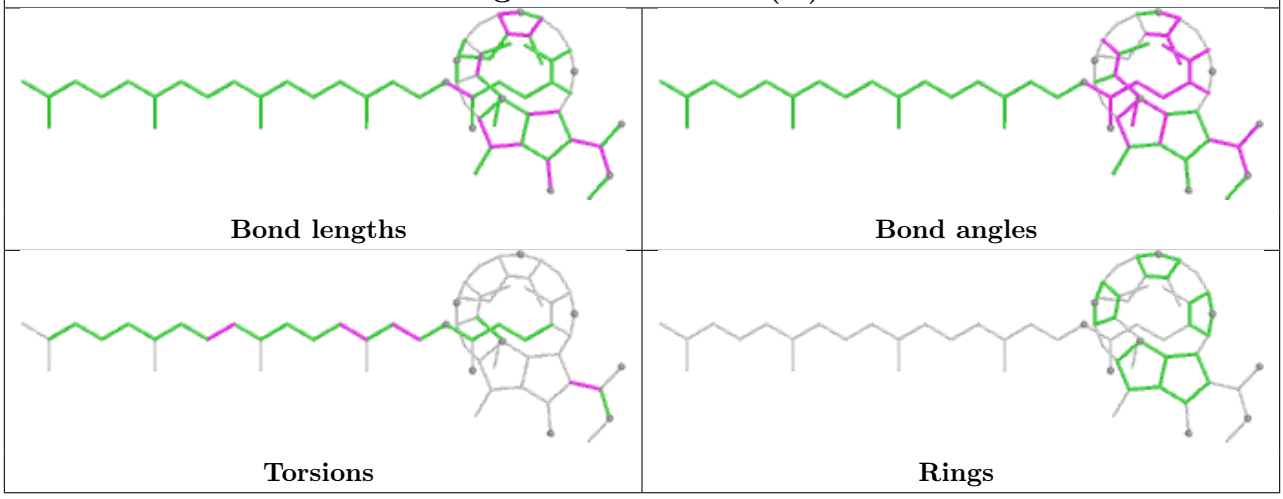


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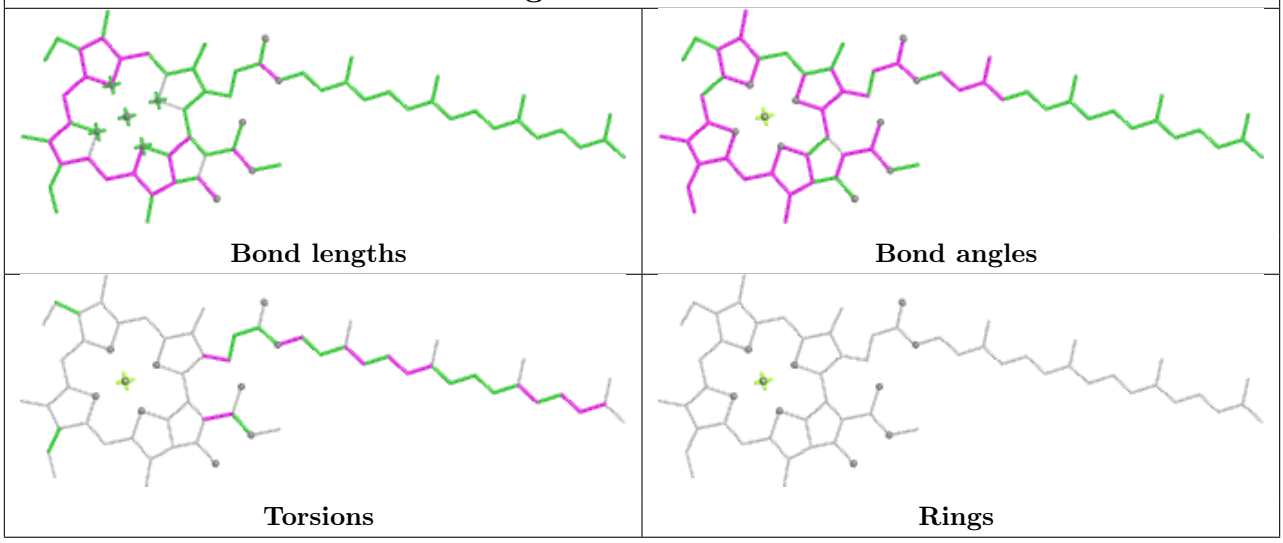


Rings

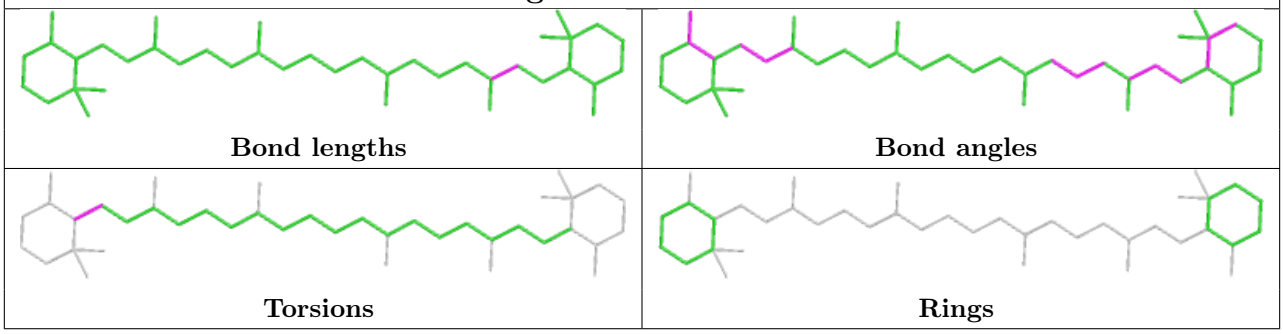
Ligand PHO a 408 (A)



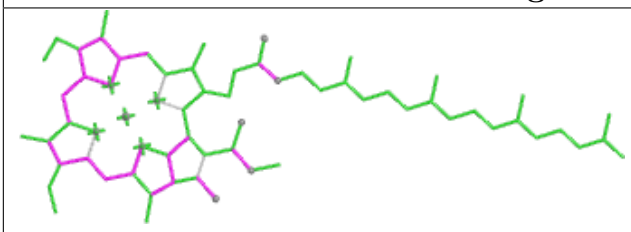
Ligand CLA C 507

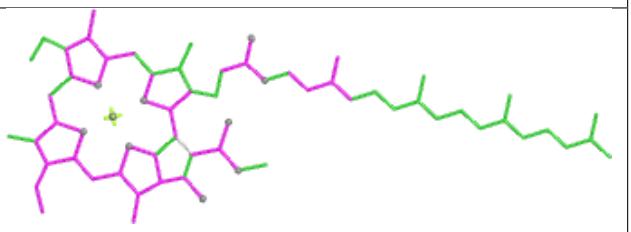


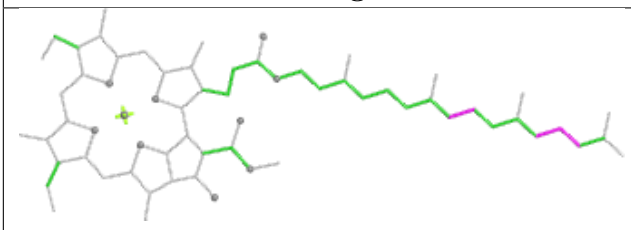
Ligand BCR b 617

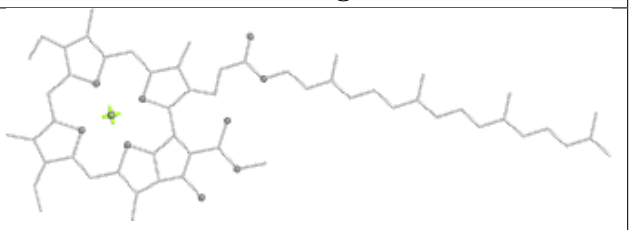


Ligand CLA b 611


Bond lengths

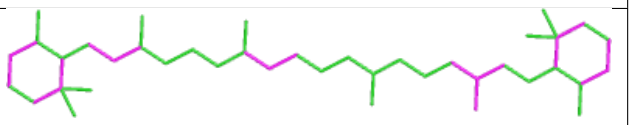

Bond angles

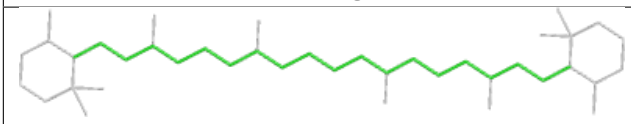

Torsions

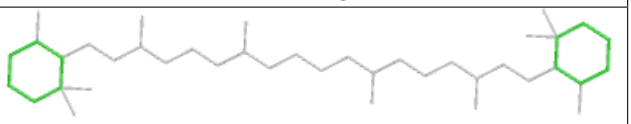

Rings

Ligand BCR B 618

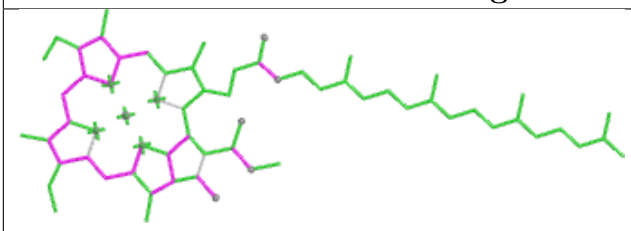

Bond lengths

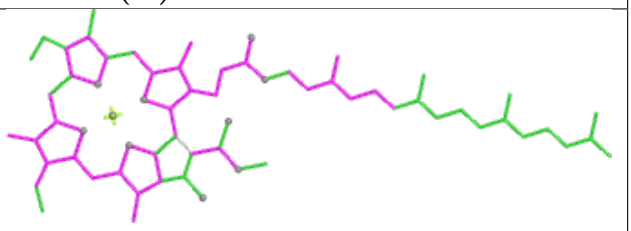

Bond angles

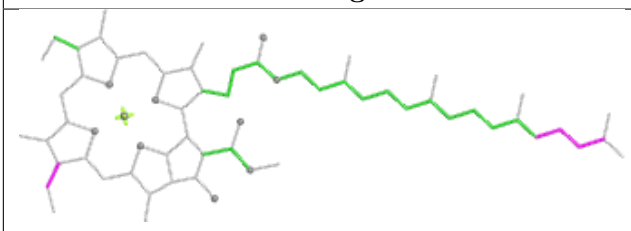

Torsions

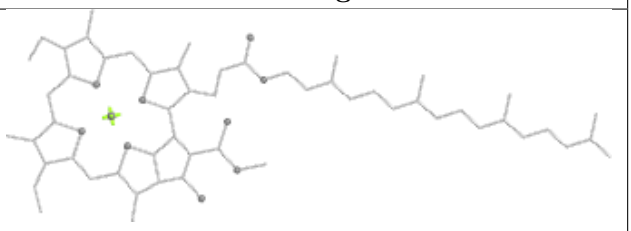

Rings

Ligand CLA A 404 (A)

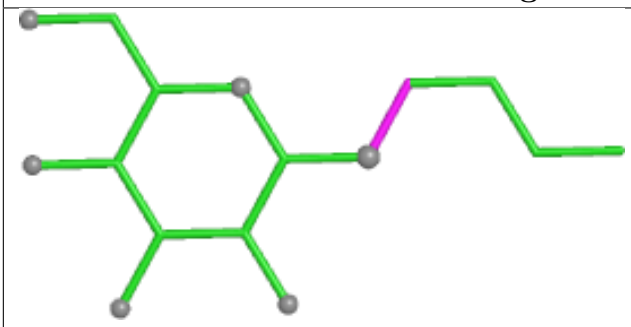

Bond lengths


Bond angles

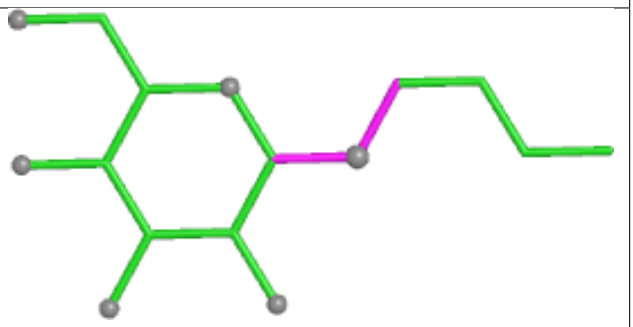

Torsions


Rings

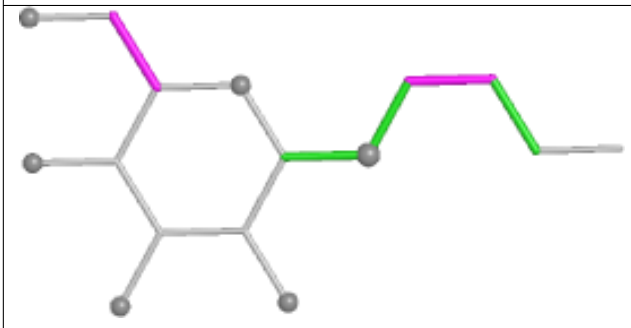
Ligand HTG D 710



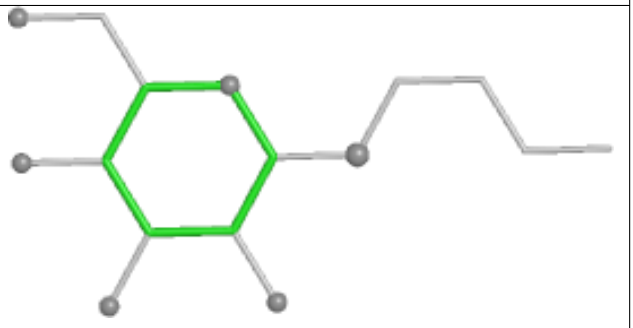
Bond lengths



Bond angles

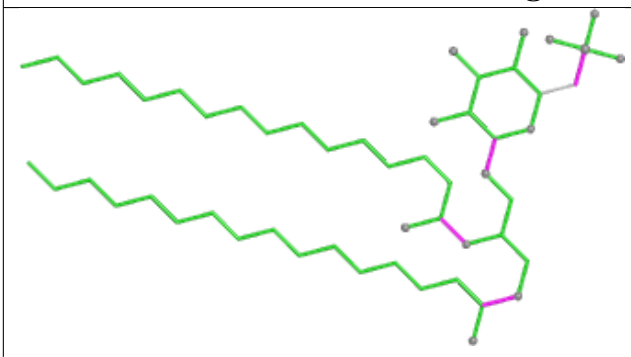


Torsions

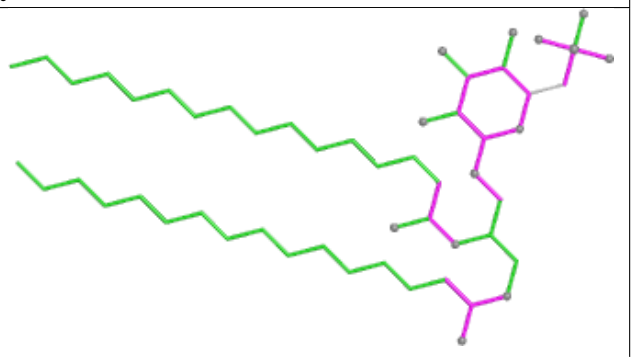


Rings

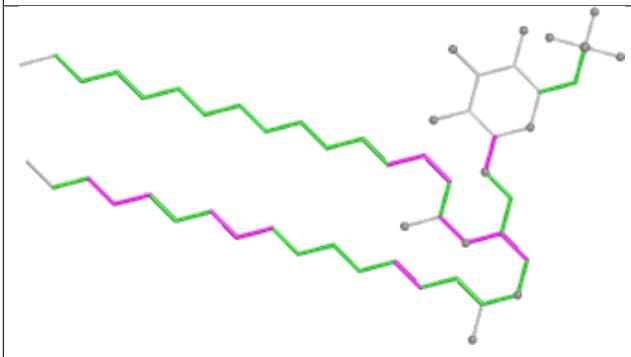
Ligand SQD B 620



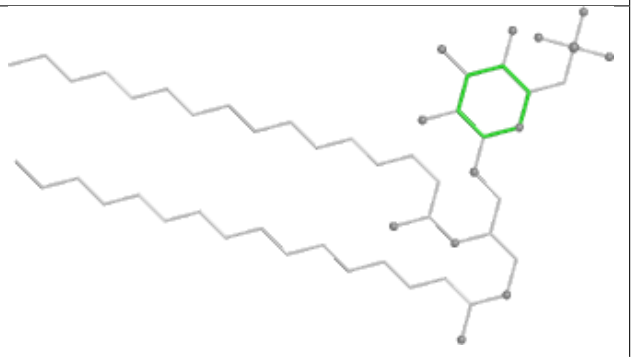
Bond lengths



Bond angles

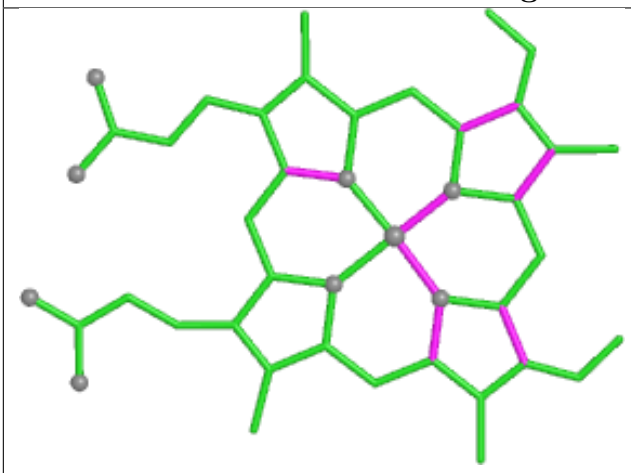


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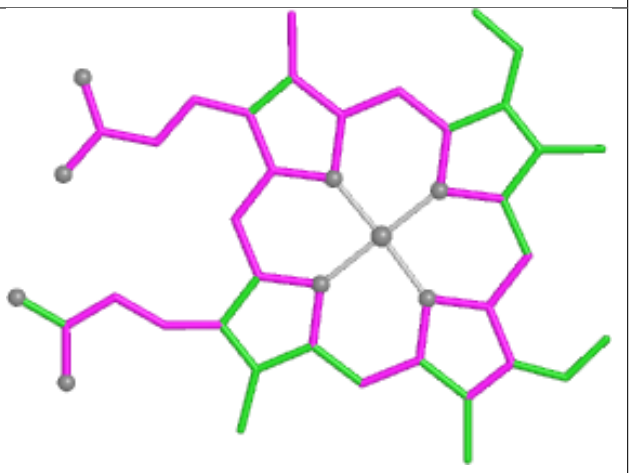


Rings

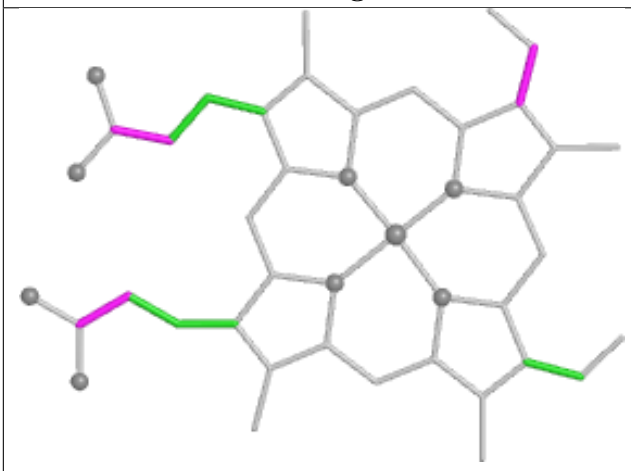
Ligand HEM F 102



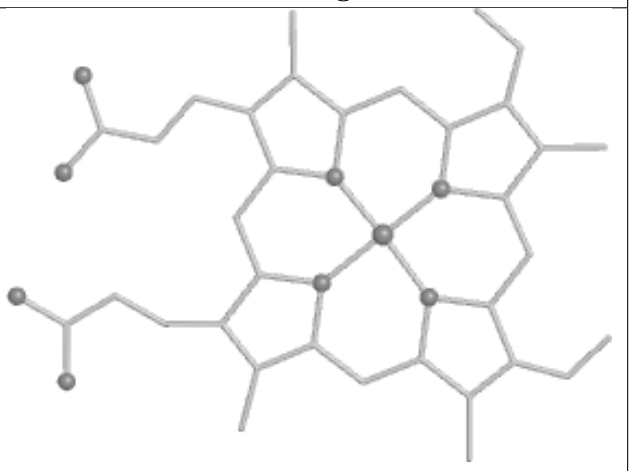
Bond lengths



Bond angles

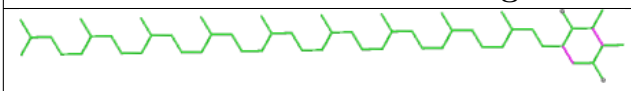


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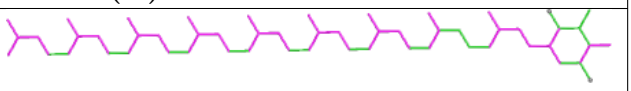


Rings

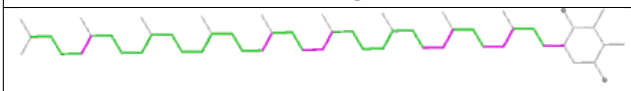
Ligand PL9 a 414 (B)



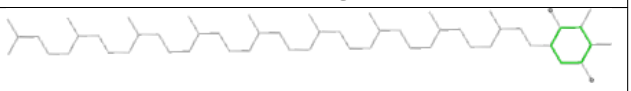
Bond lengths



Bond angles



Torsions

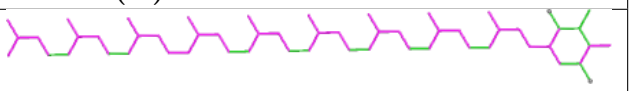


Rings

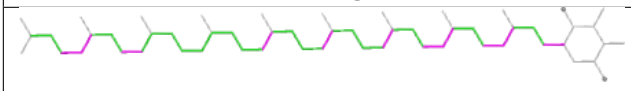
Ligand PL9 A 414 (B)



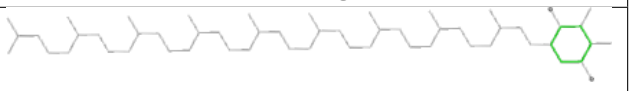
Bond lengths



Bond angles

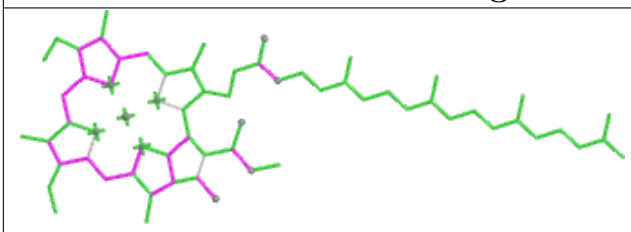


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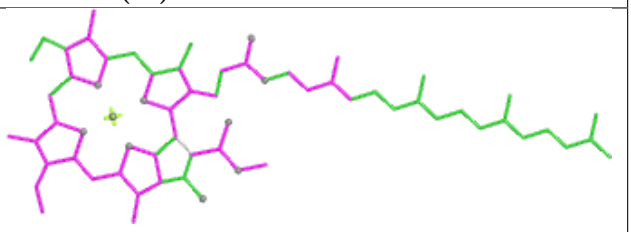


Rings

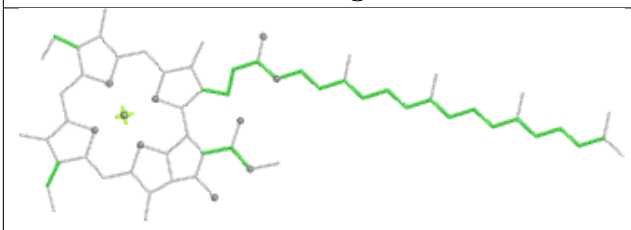
Ligand CLA D 702 (A)



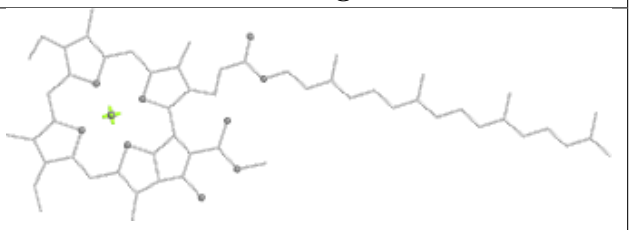
Bond lengths



Bond angles

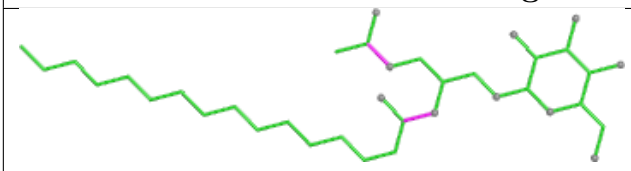


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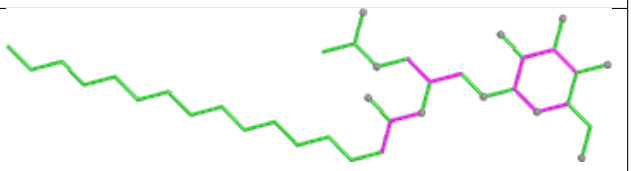


Rings

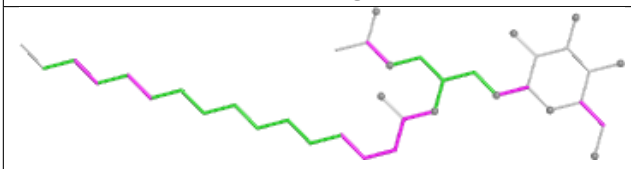
Ligand LMG Z 101



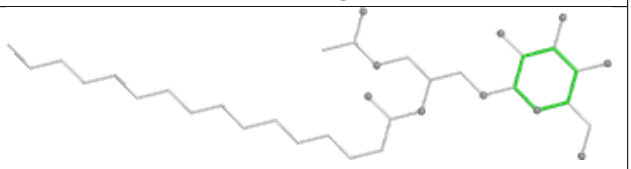
Bond lengths



Bond angles

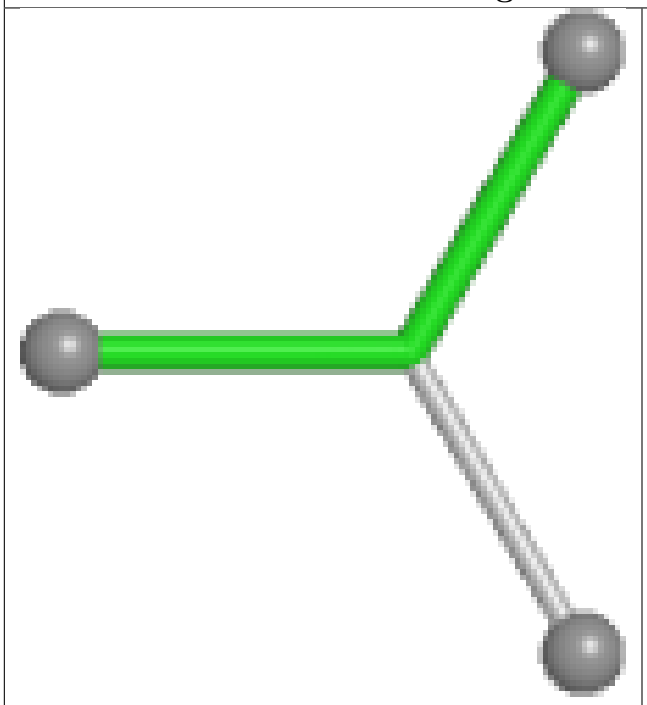


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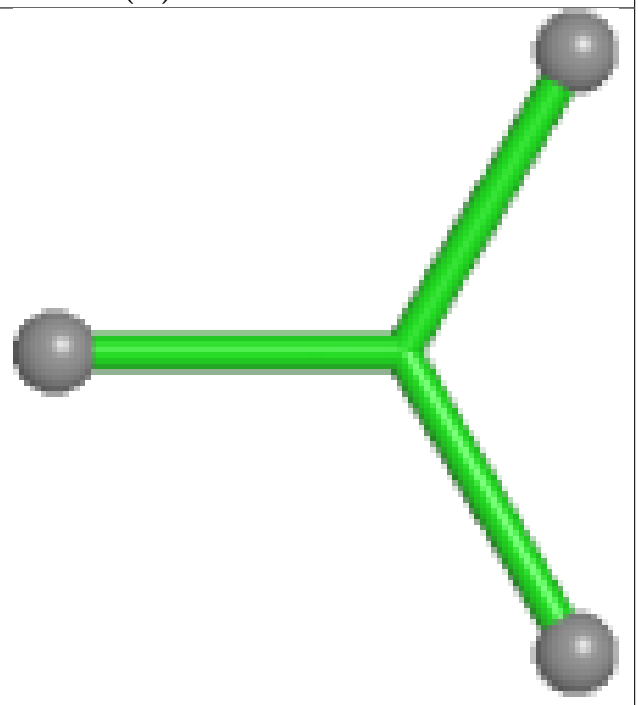


Rings

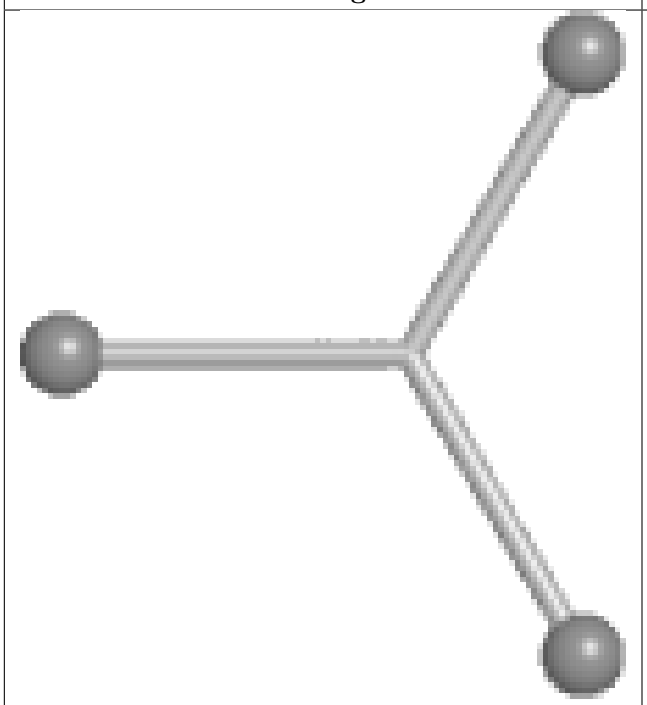
Ligand BCT a 404 (B)



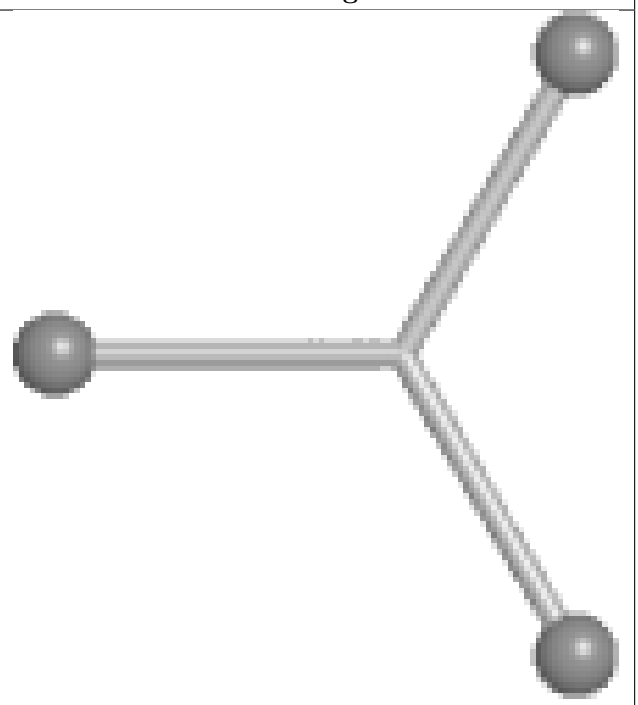
Bond lengths



Bond angles

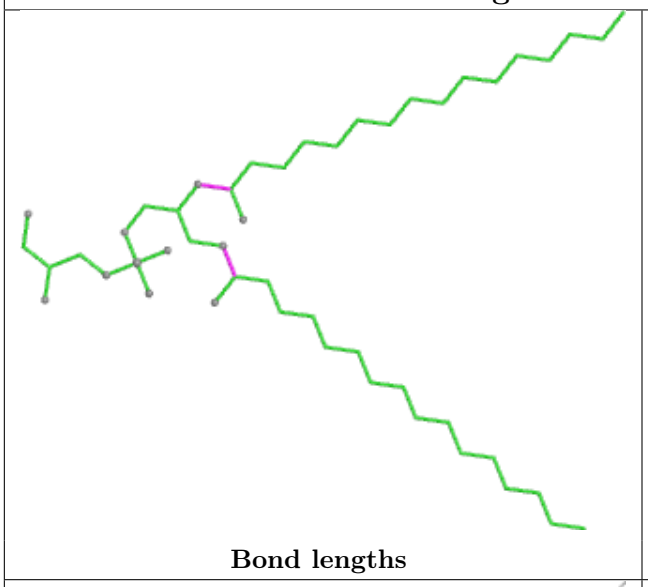


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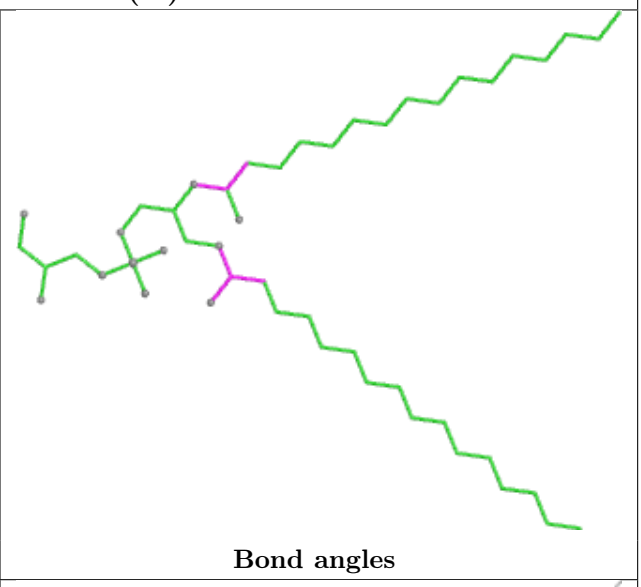


Rings

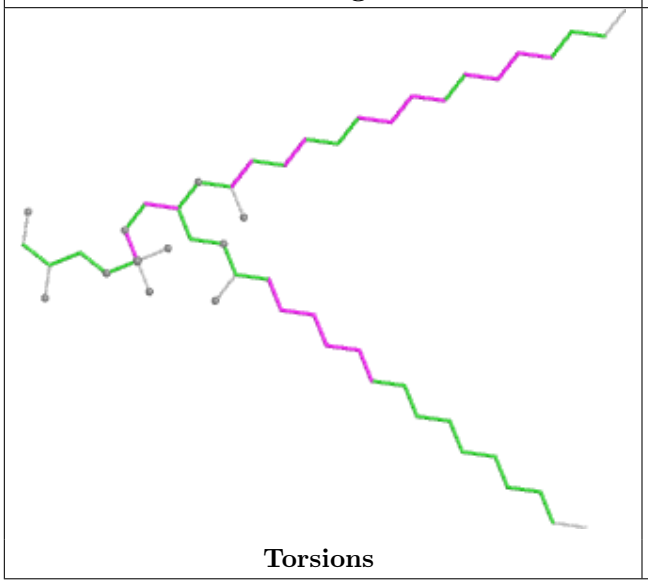
Ligand LHG L 101 (A)



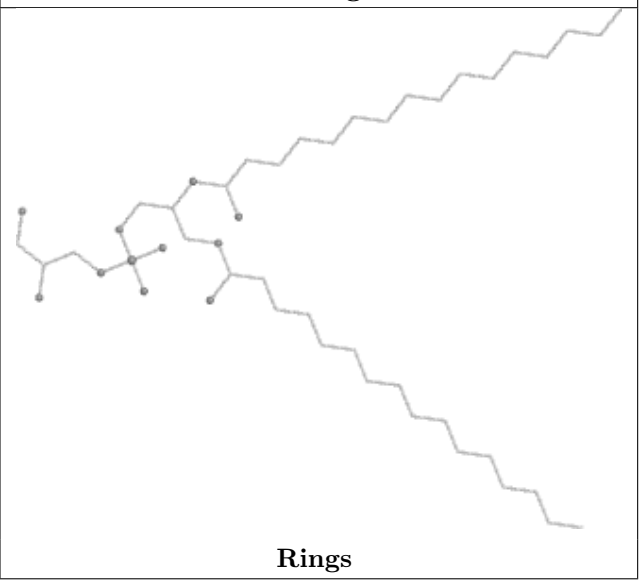
Bond lengths



Bond angles



Torsions

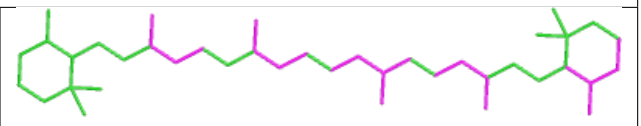


Rings

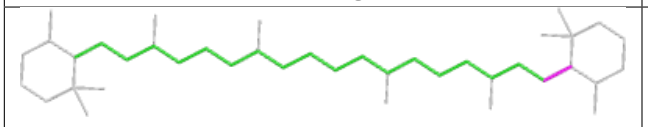
Ligand BCR c 515



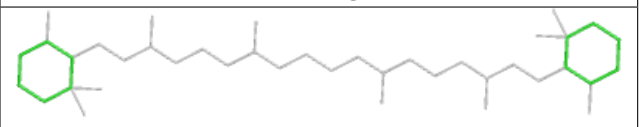
Bond lengths



Bond angles

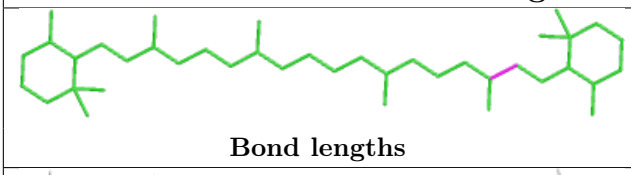


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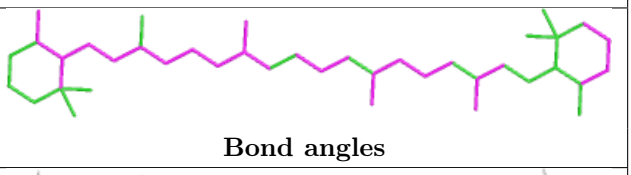


Rings

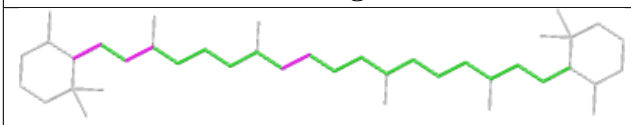
Ligand BCR t 102



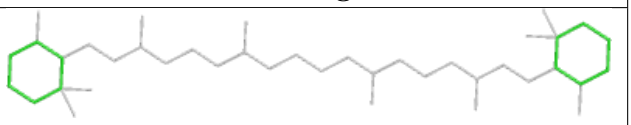
Bond lengths



Bond angles

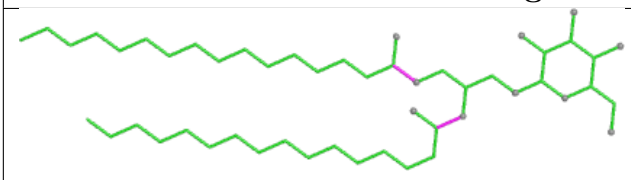


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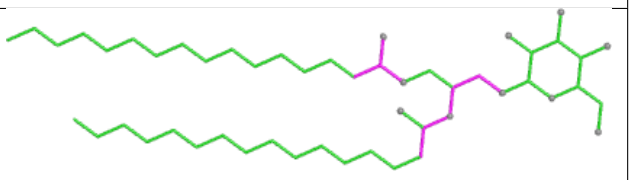


Rings

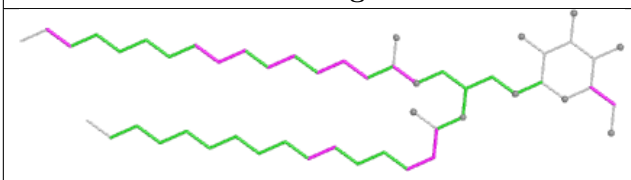
Ligand LMG c 520



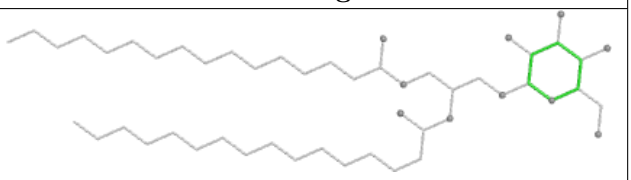
Bond lengths



Bond angles

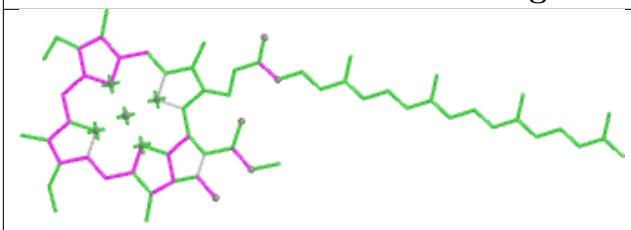


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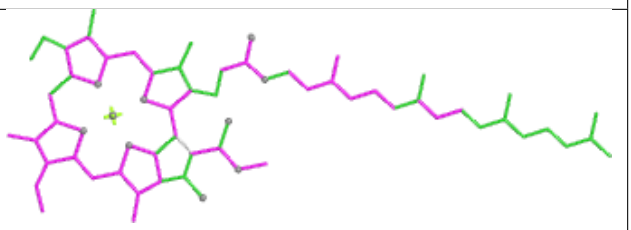


Rings

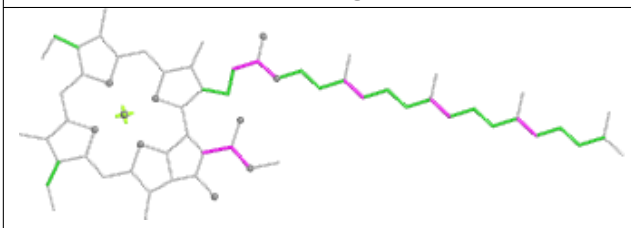
Ligand CLA c 511



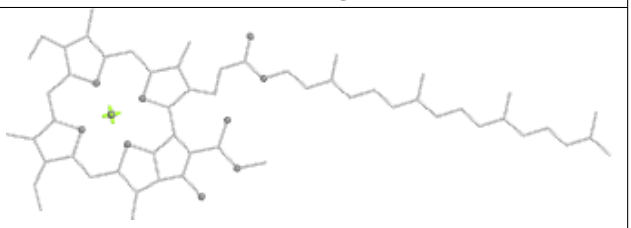
Bond lengths



Bond angles

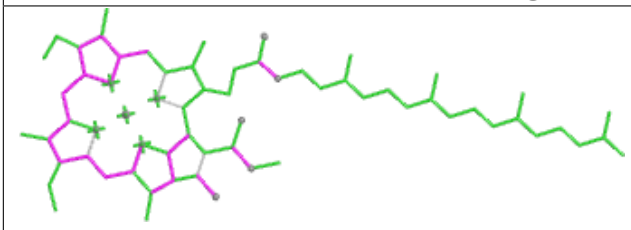


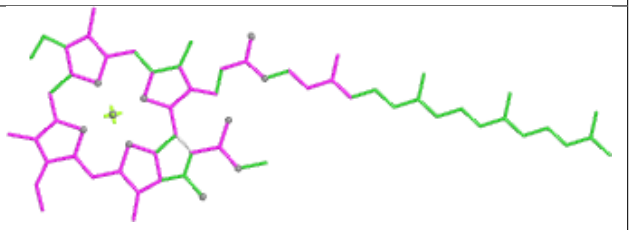
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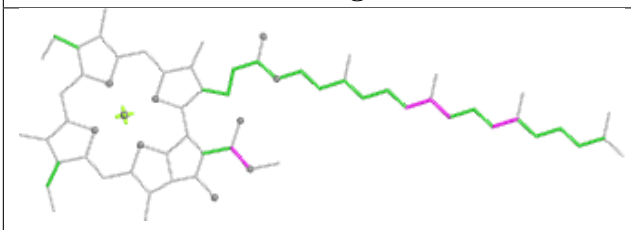


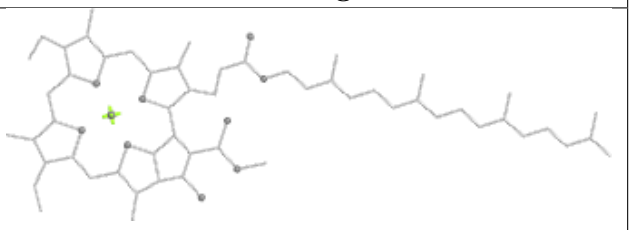
Rings

Ligand CLA C 514


Bond lengths

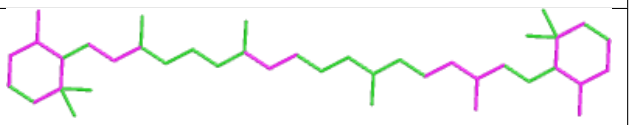

Bond angles

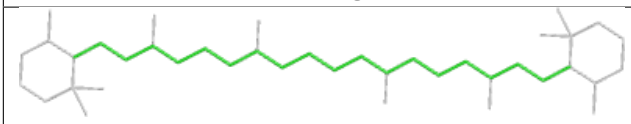

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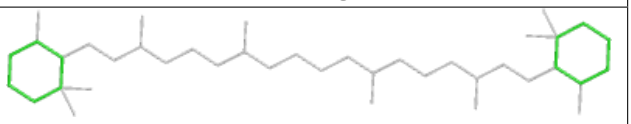

Rings

Ligand BCR b 618

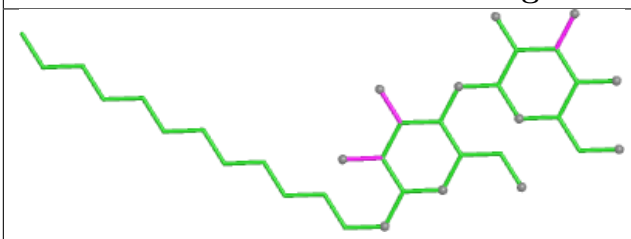

Bond lengths

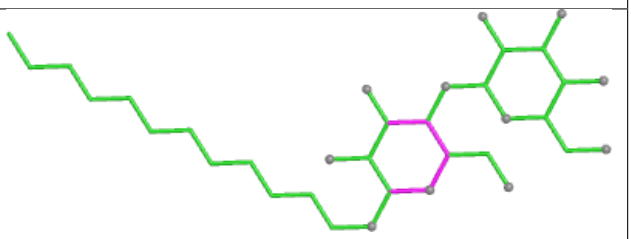

Bond angles

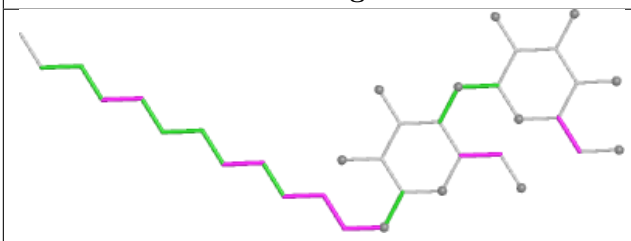

Torsions

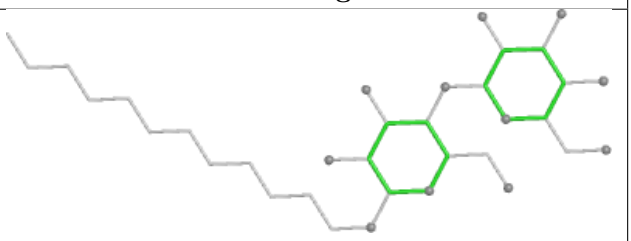

Rings

Ligand LMT T 101

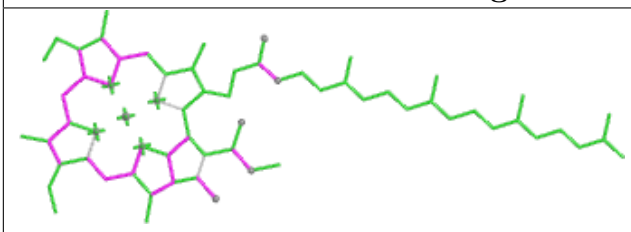

Bond lengths


Bond angles

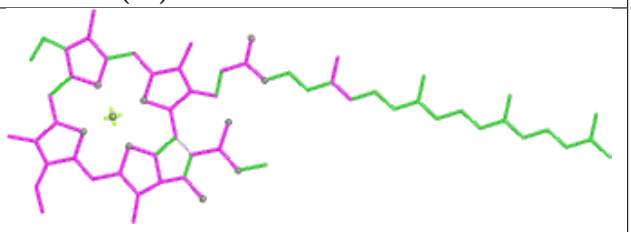

Torsions


Rings

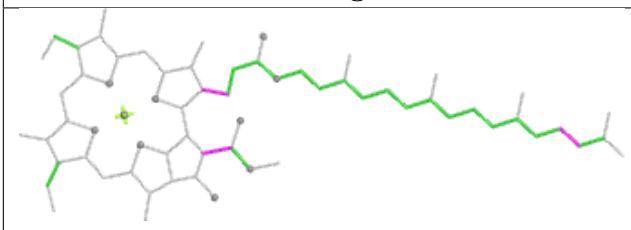
Ligand CLA A 405 (A)



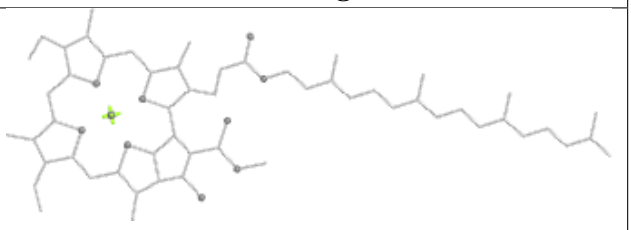
Bond lengths



Bond angles



Torsions

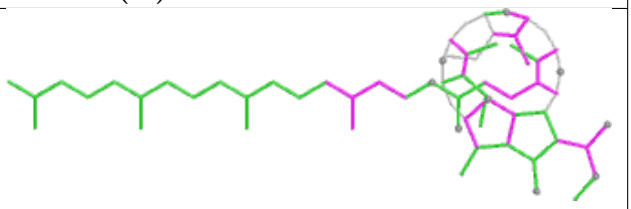


Rings

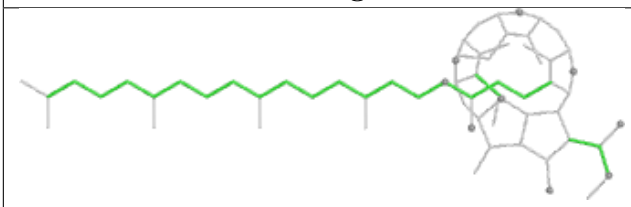
Ligand PHO a 416 (B)



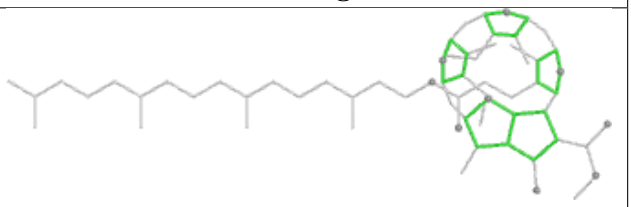
Bond lengths



Bond angles

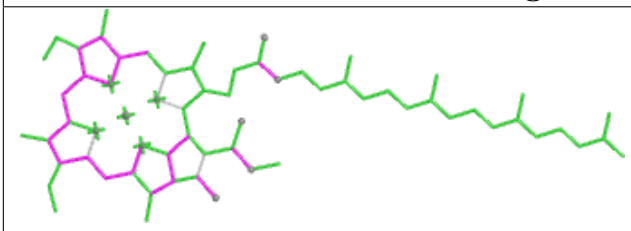


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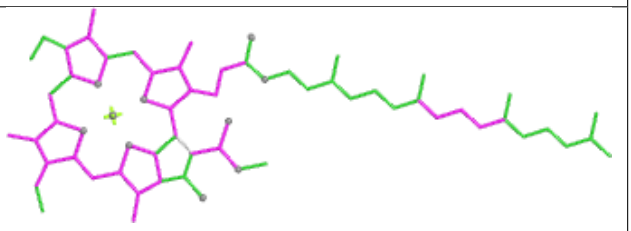


Rings

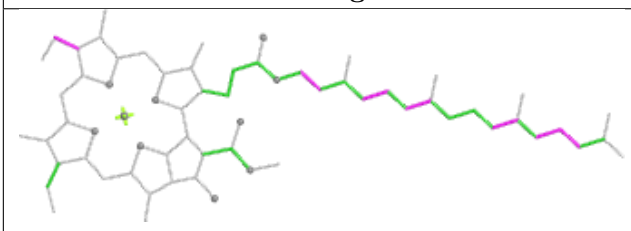
Ligand CLA B 602



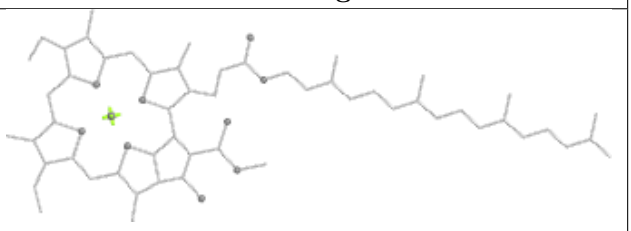
Bond lengths



Bond angles

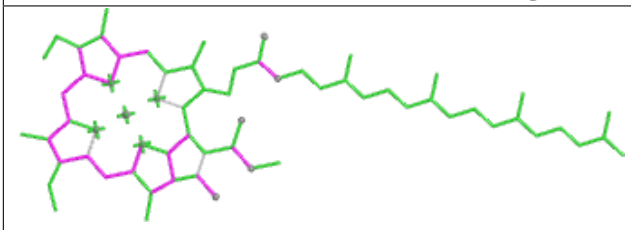


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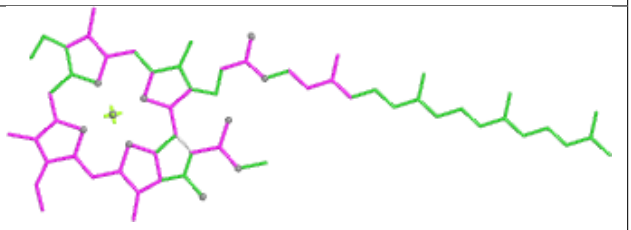


Rings

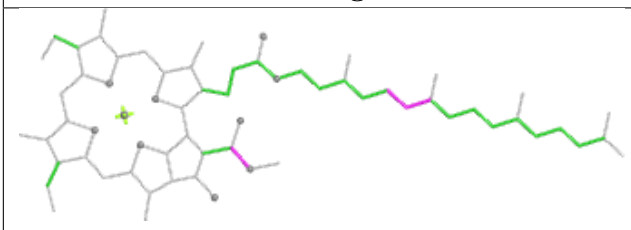
Ligand CLA C 504



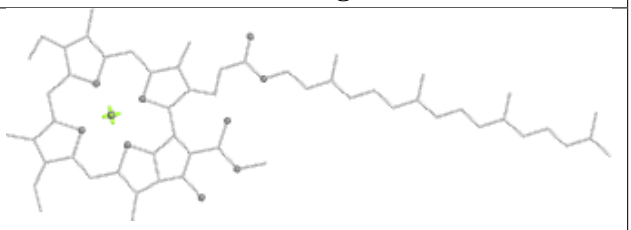
Bond lengths



Bond angles



Torsions



Rings

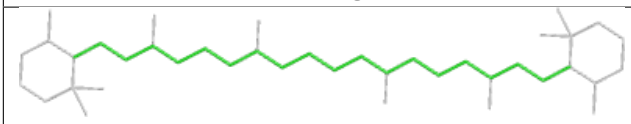
Ligand BCR k 101



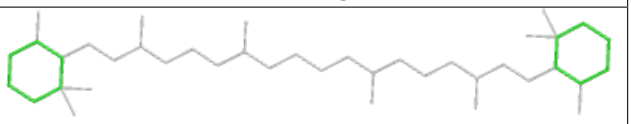
Bond lengths



Bond angles

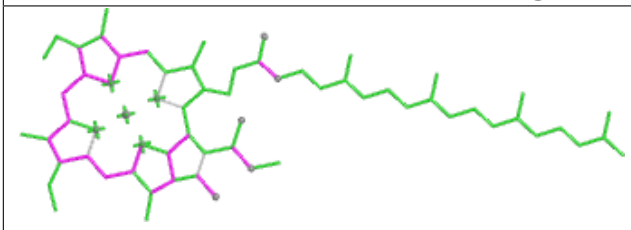


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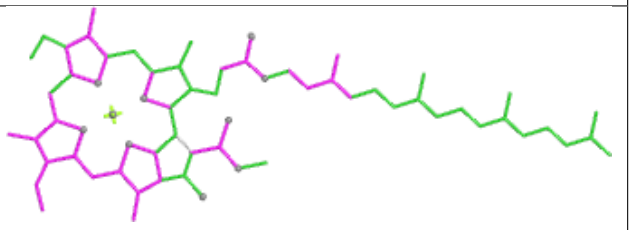


Rings

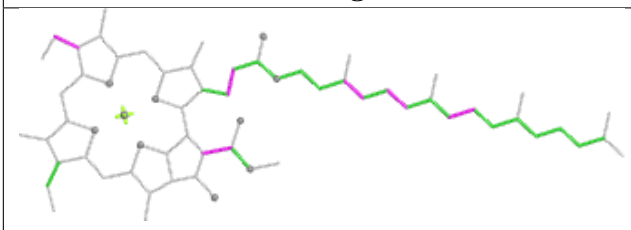
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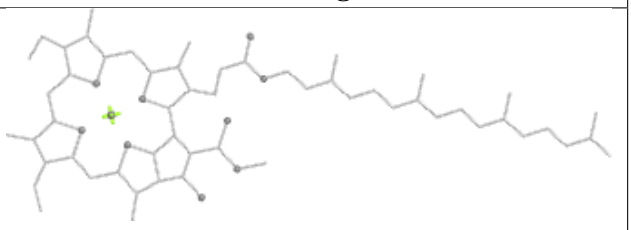
Bond lengths



Bond angles

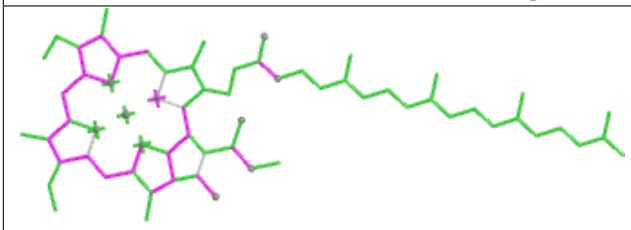


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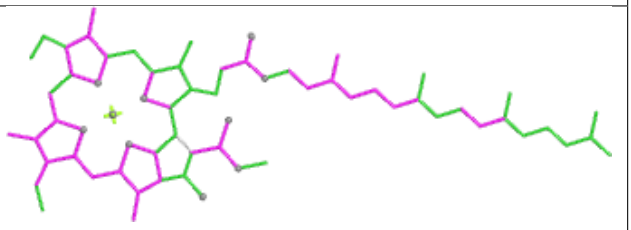


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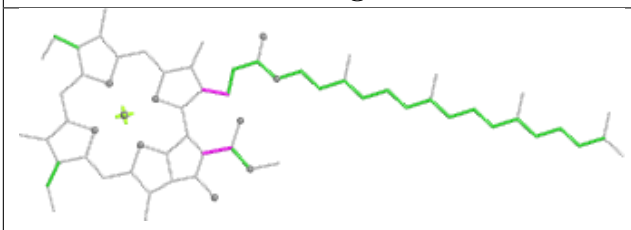
Ligand CLA B 604



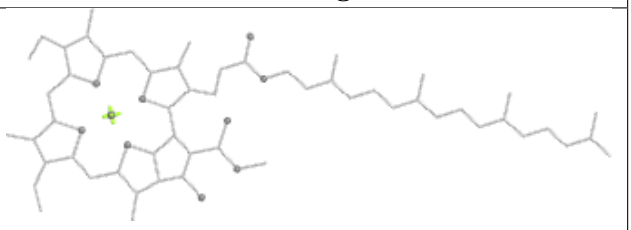
Bond lengths



Bond angles

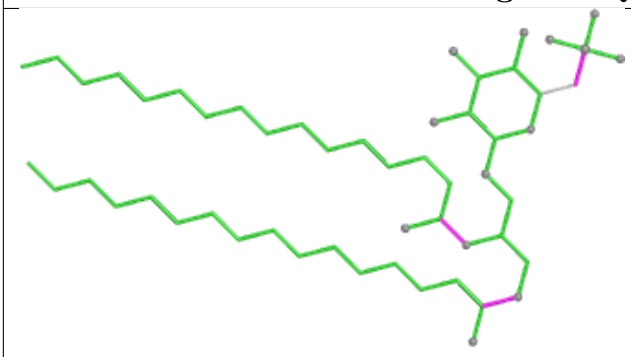


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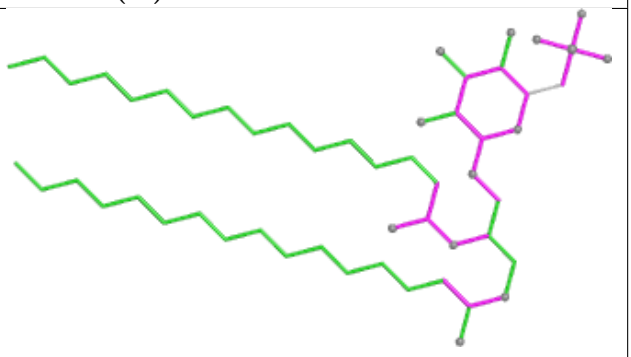


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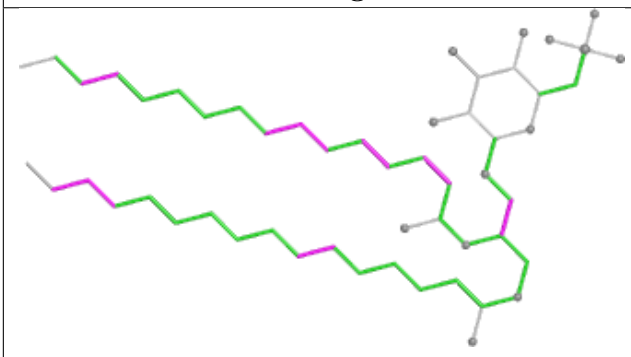
Ligand SQD a 411 (B)



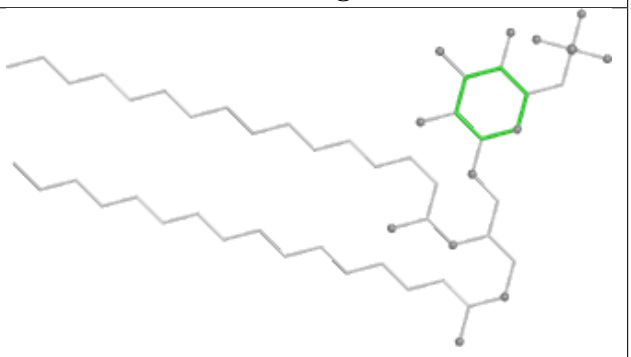
Bond lengths



Bond angles

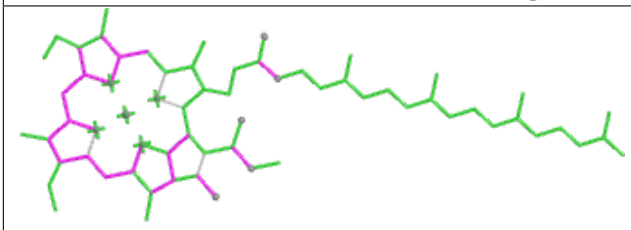


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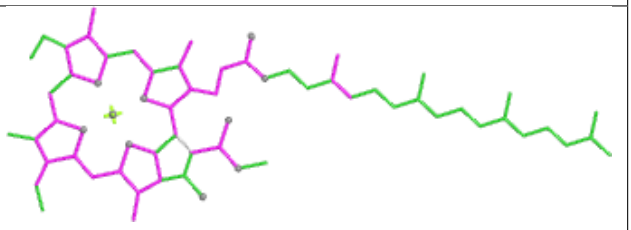


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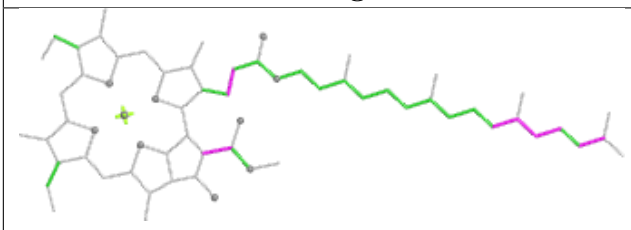
Ligand CLA B 610



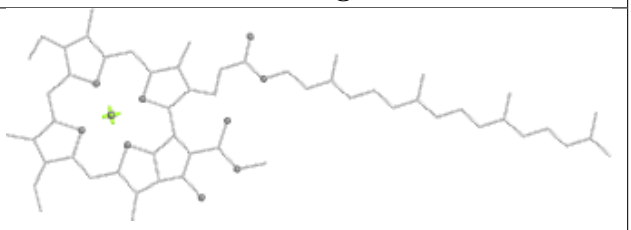
Bond lengths



Bond angles

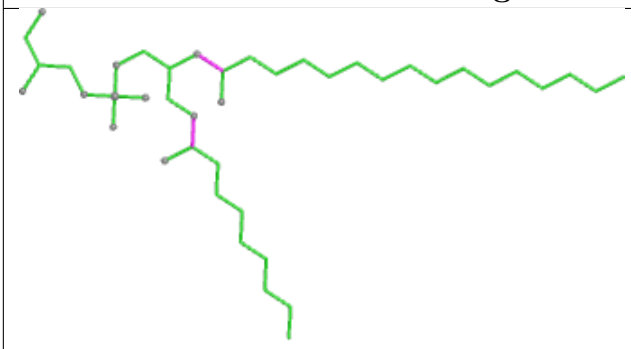


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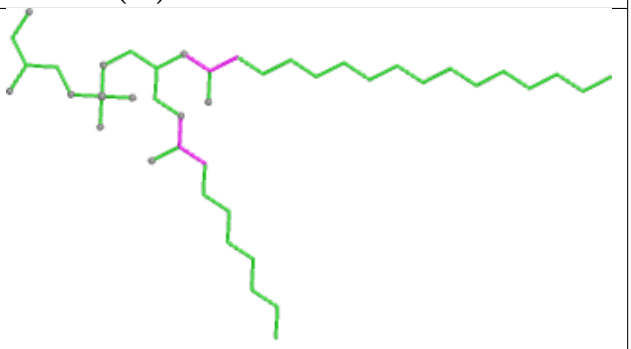


Rings

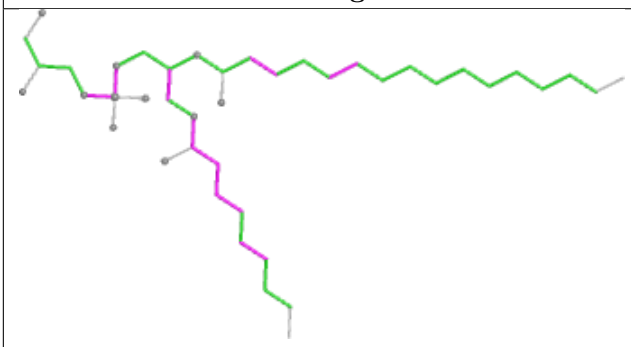
Ligand LHG a 420 (A)



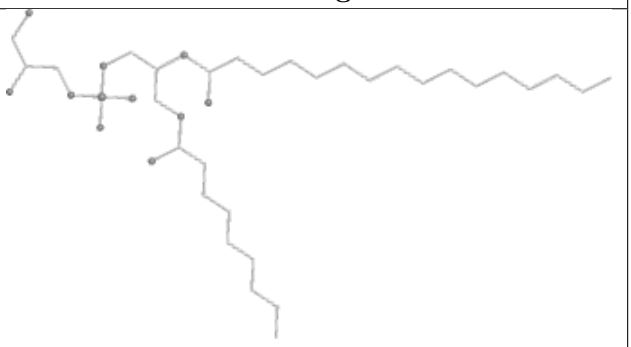
Bond lengths



Bond angles

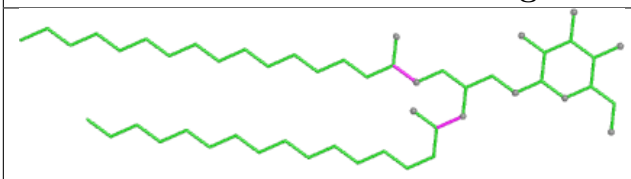


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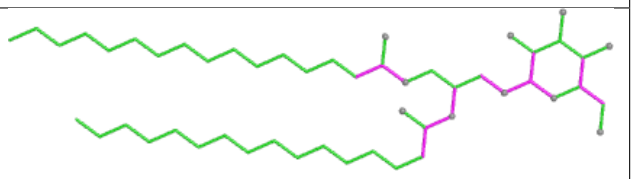


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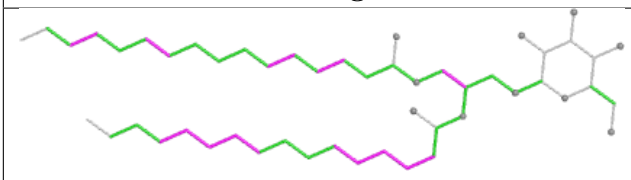
Ligand LMG C 501



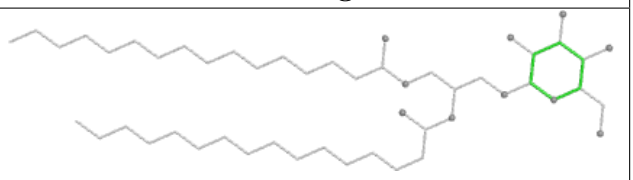
Bond lengths



Bond angles

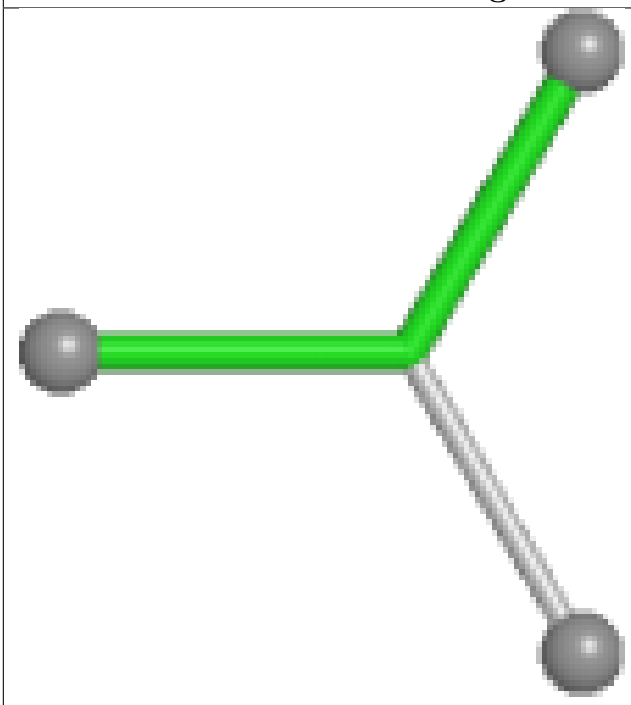


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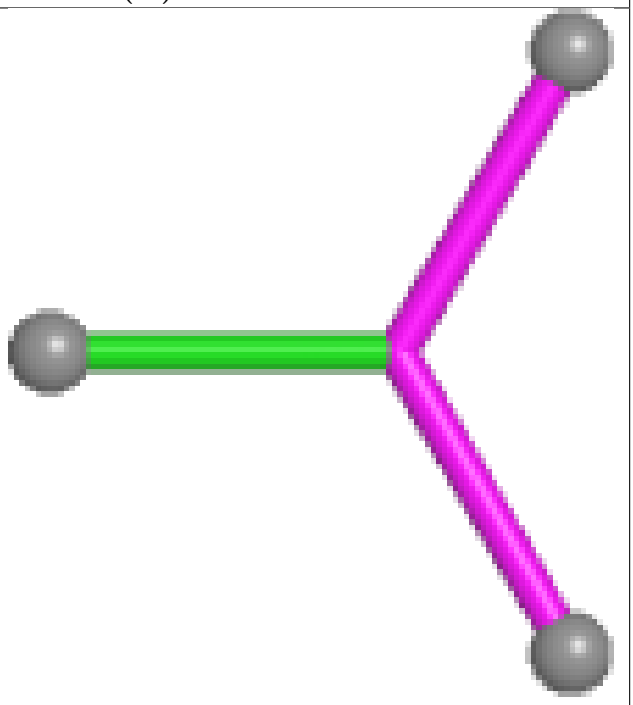


Rings

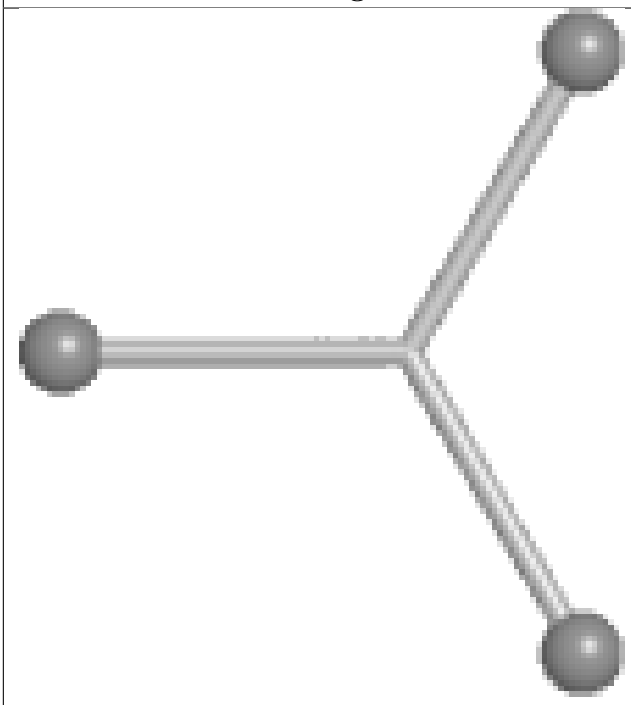
Ligand BCT A 416 (A)



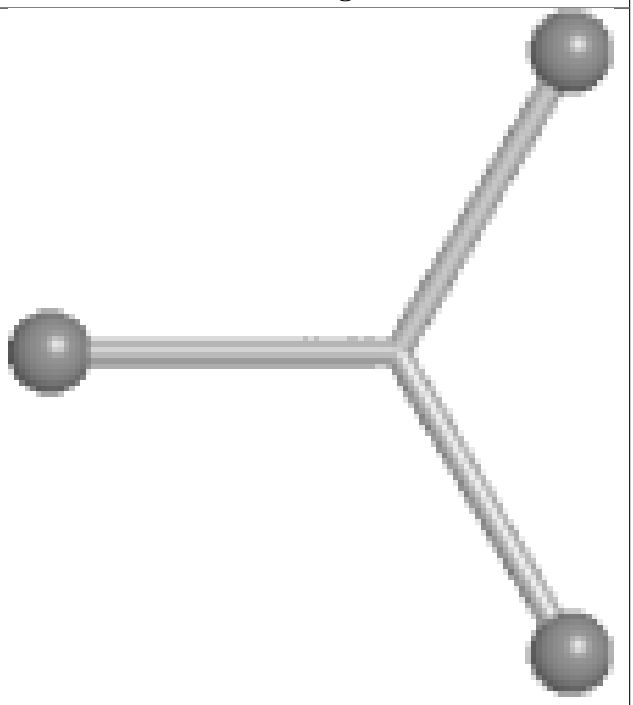
Bond lengths



Bond angles

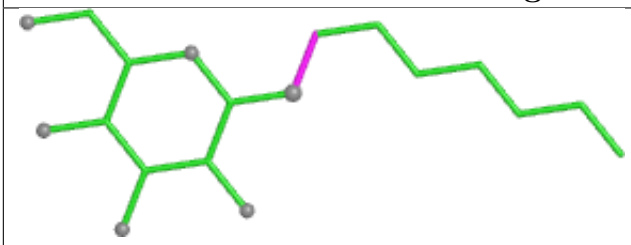


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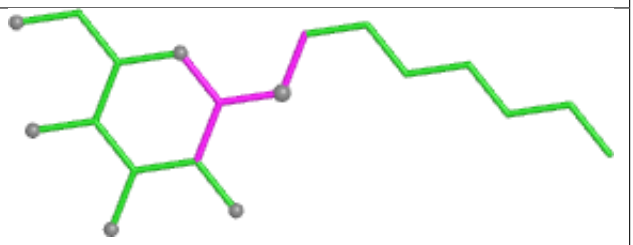


Rings

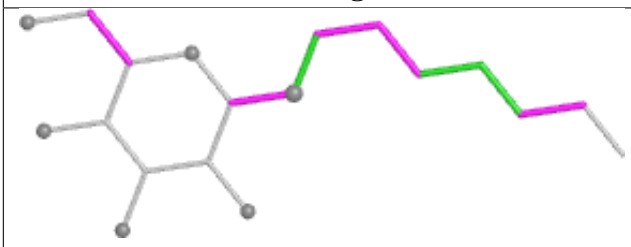
Ligand HTG b 623



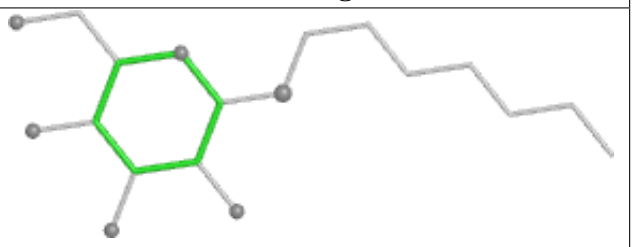
Bond lengths



Bond angles

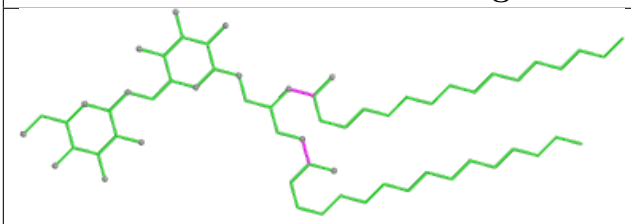


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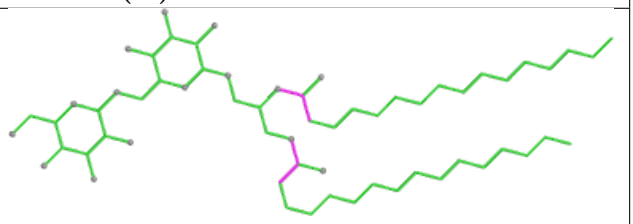


Rings

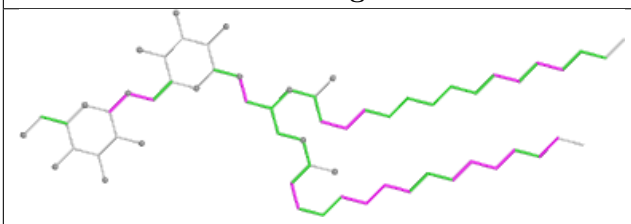
Ligand DGD c 518 (B)



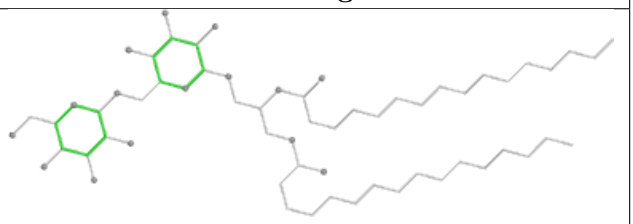
Bond lengths



Bond angles

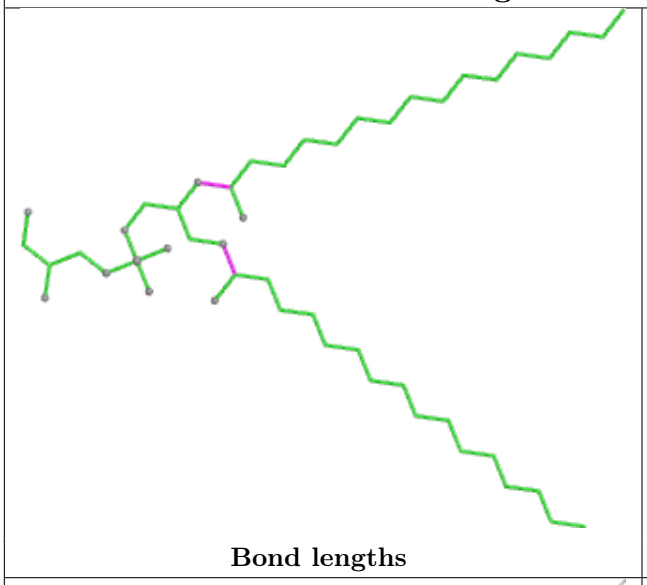


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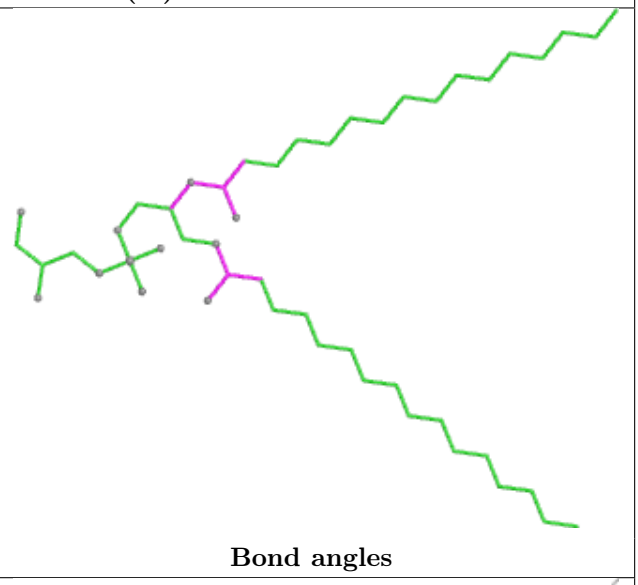


Rings

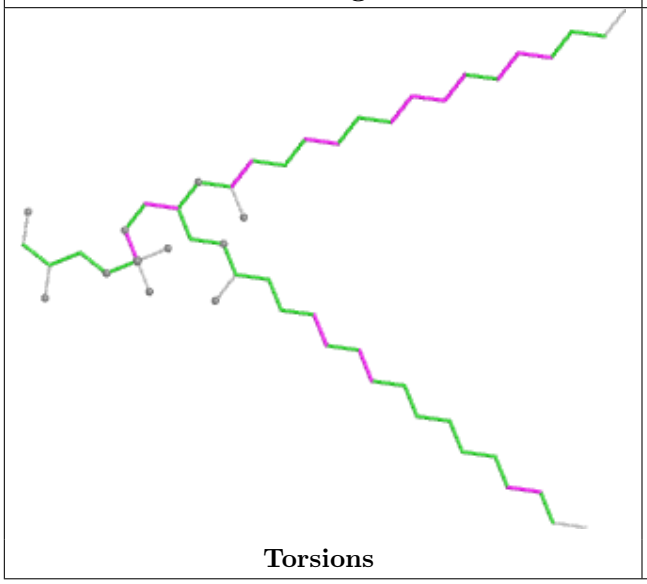
Ligand LHG b 629 (B)



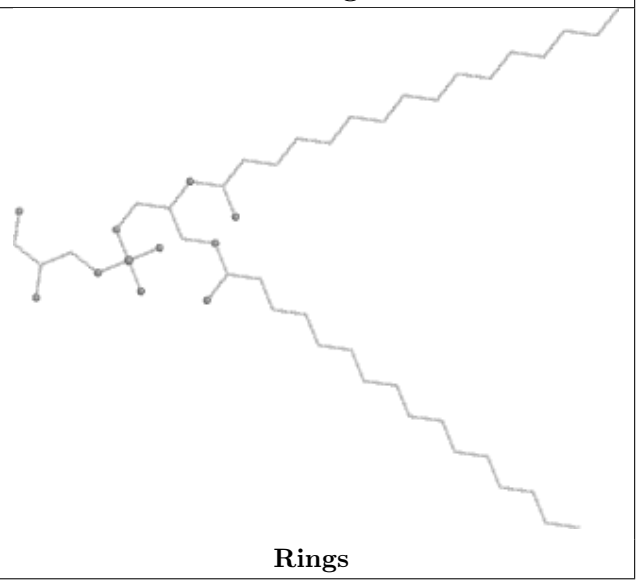
Bond lengths



Bond angles

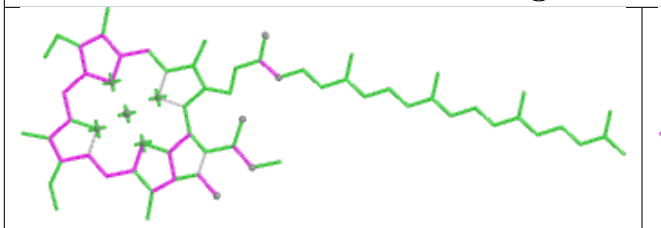


Torsions

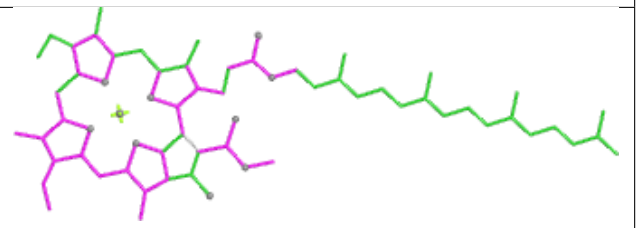


Rings

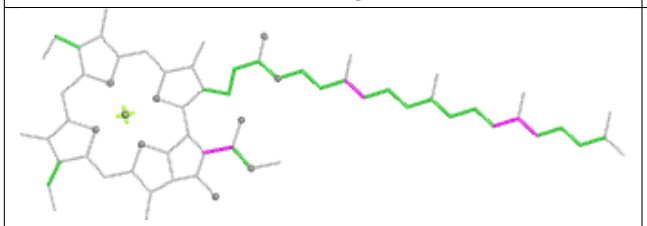
Ligand CLA c 505



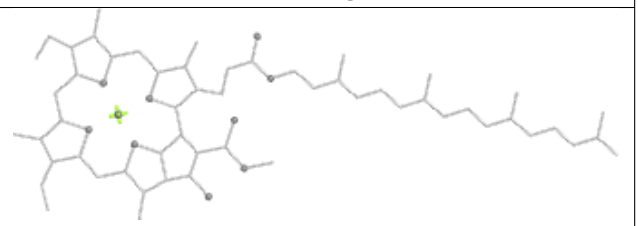
Bond lengths



Bond angles

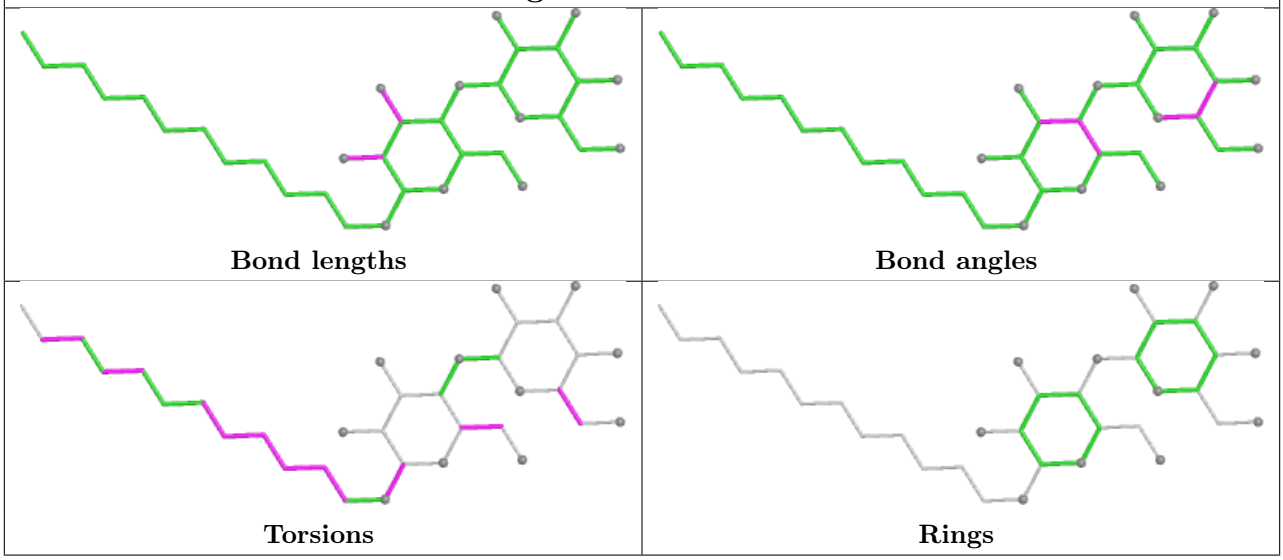


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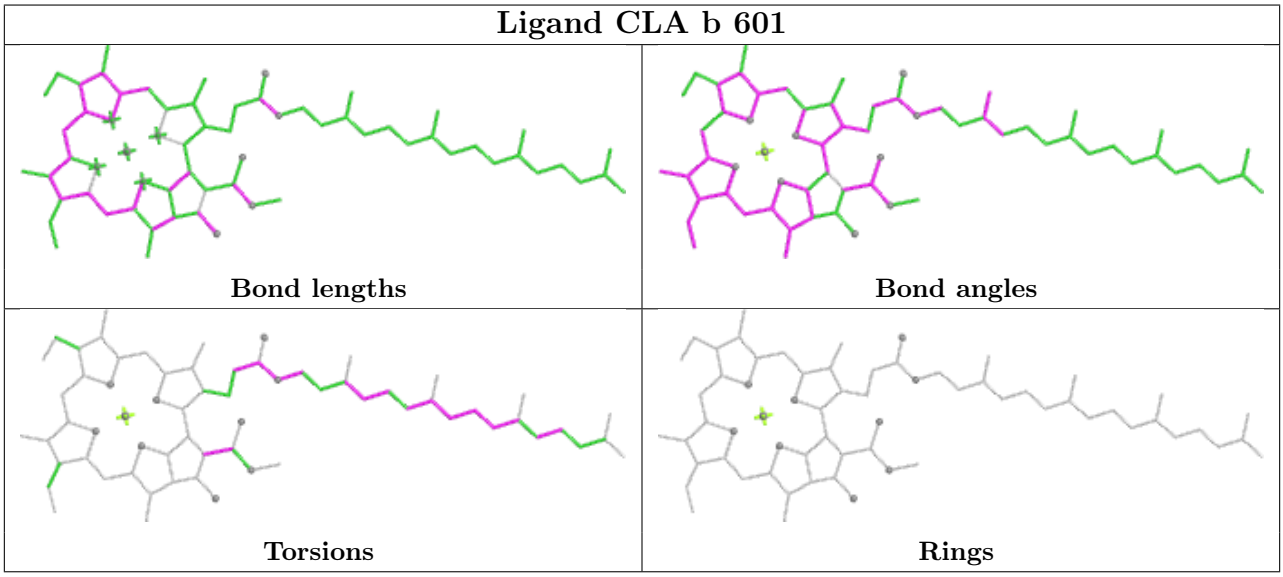


Rings

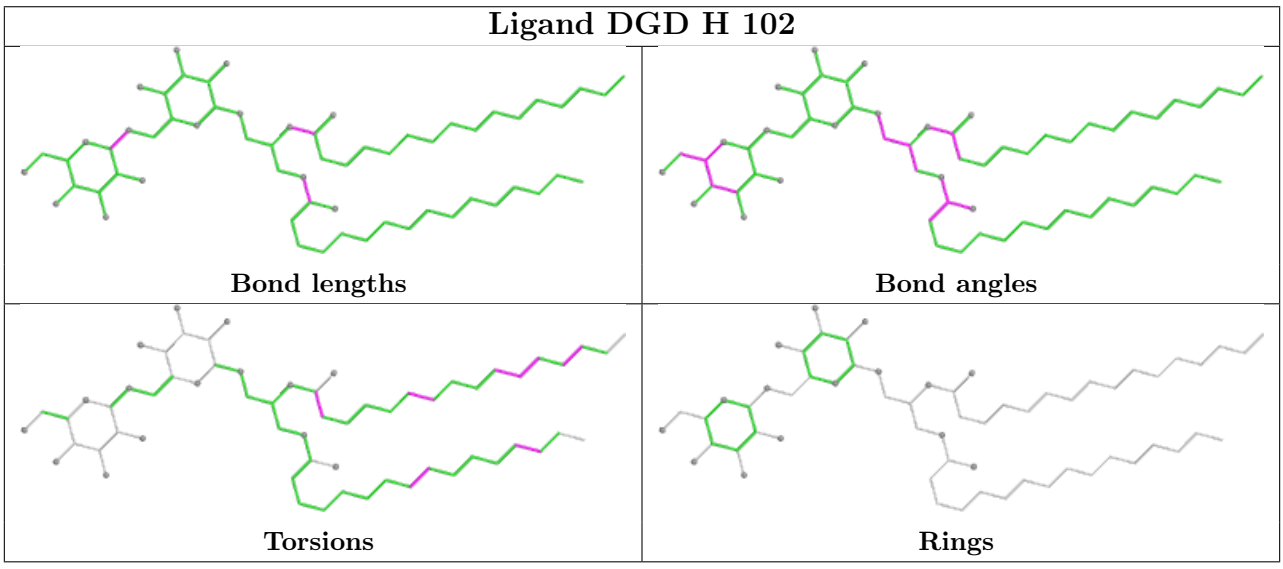
Ligand LMT a 417



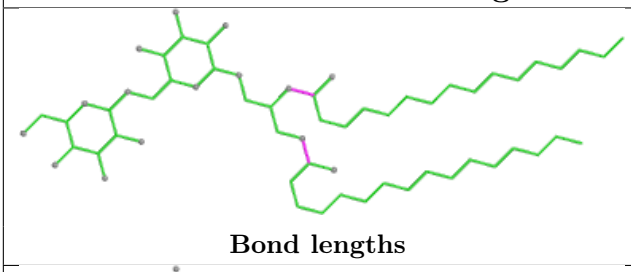
Ligand CLA b 601



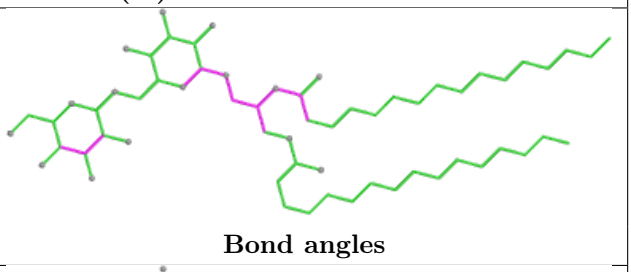
Ligand DGD H 102



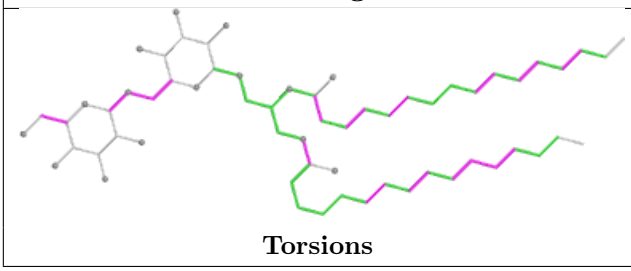
Ligand DGD c 517 (B)



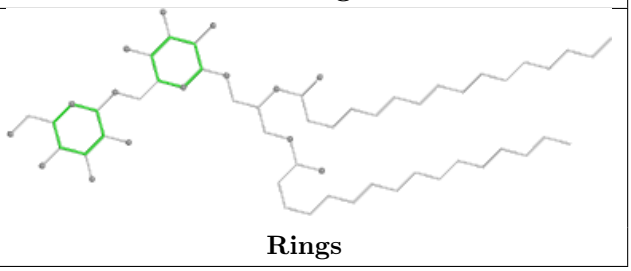
Bond lengths



Bond angles

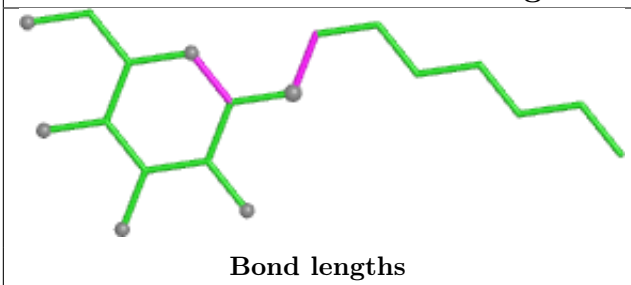


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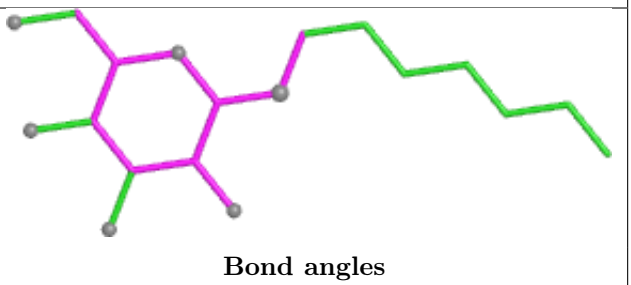


Rings

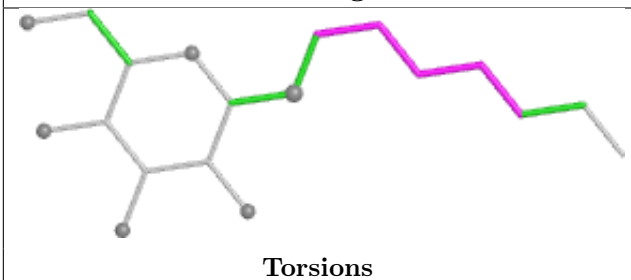
Ligand HTG b 622



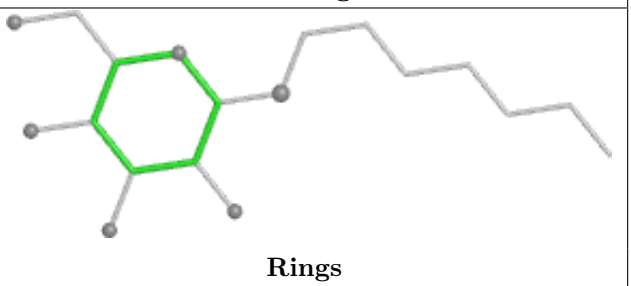
Bond lengths



Bond angles

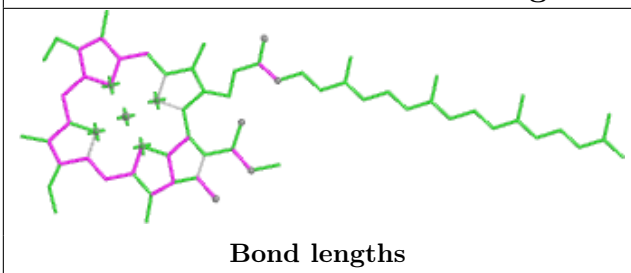


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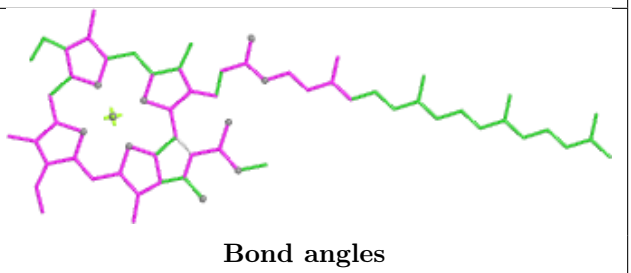


Rings

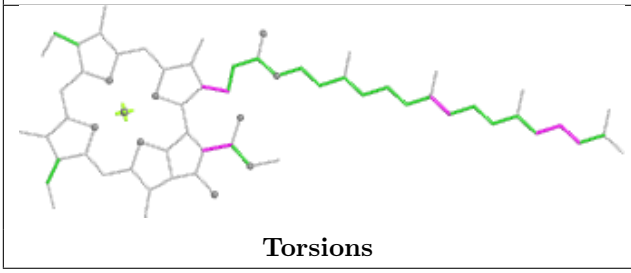
Ligand CLA c 507



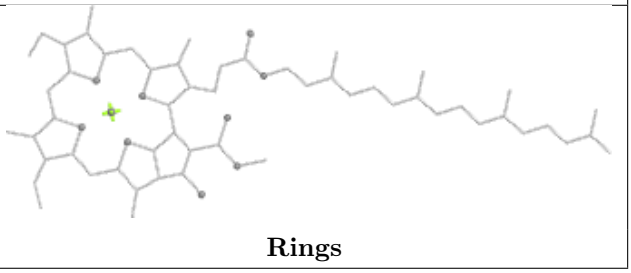
Bond lengths



Bond angles

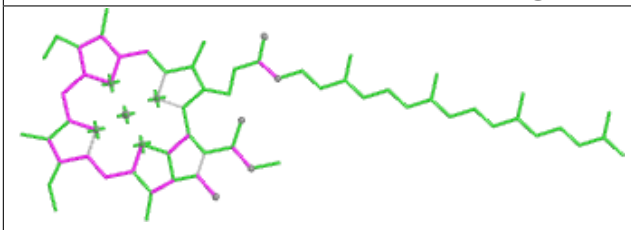


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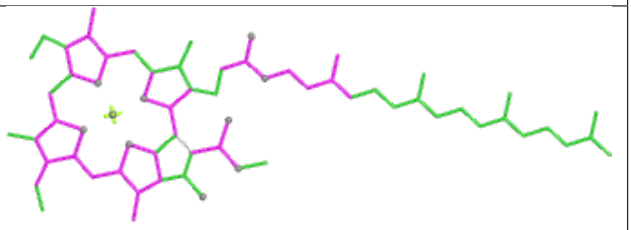


Rings

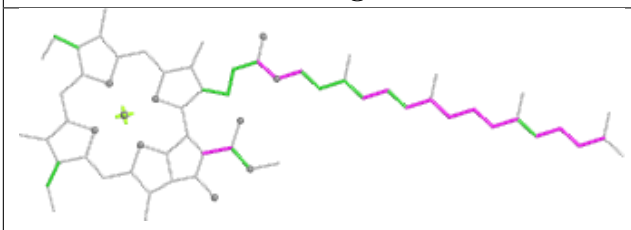
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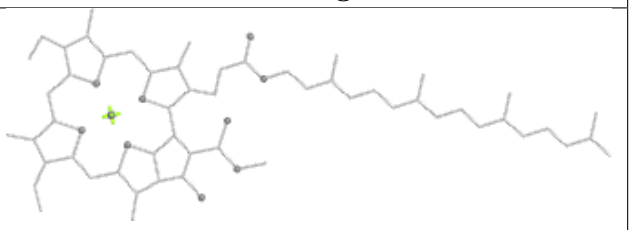
Bond lengths



Bond angles

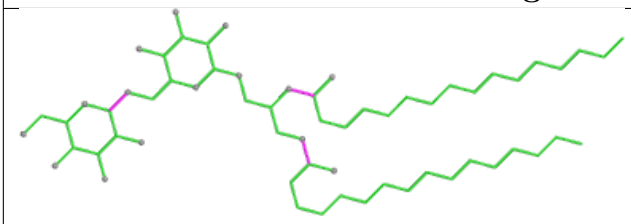


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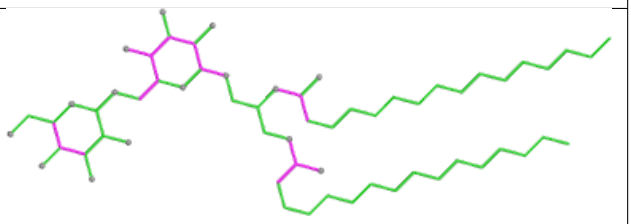


Rings

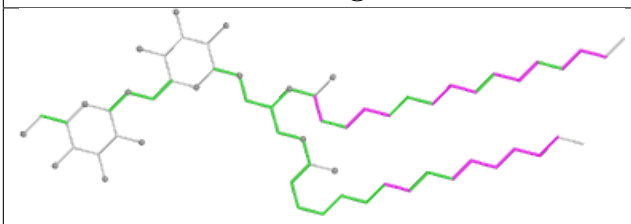
Ligand DGD h 102



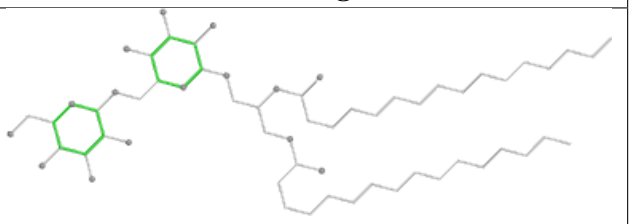
Bond lengths



Bond angles

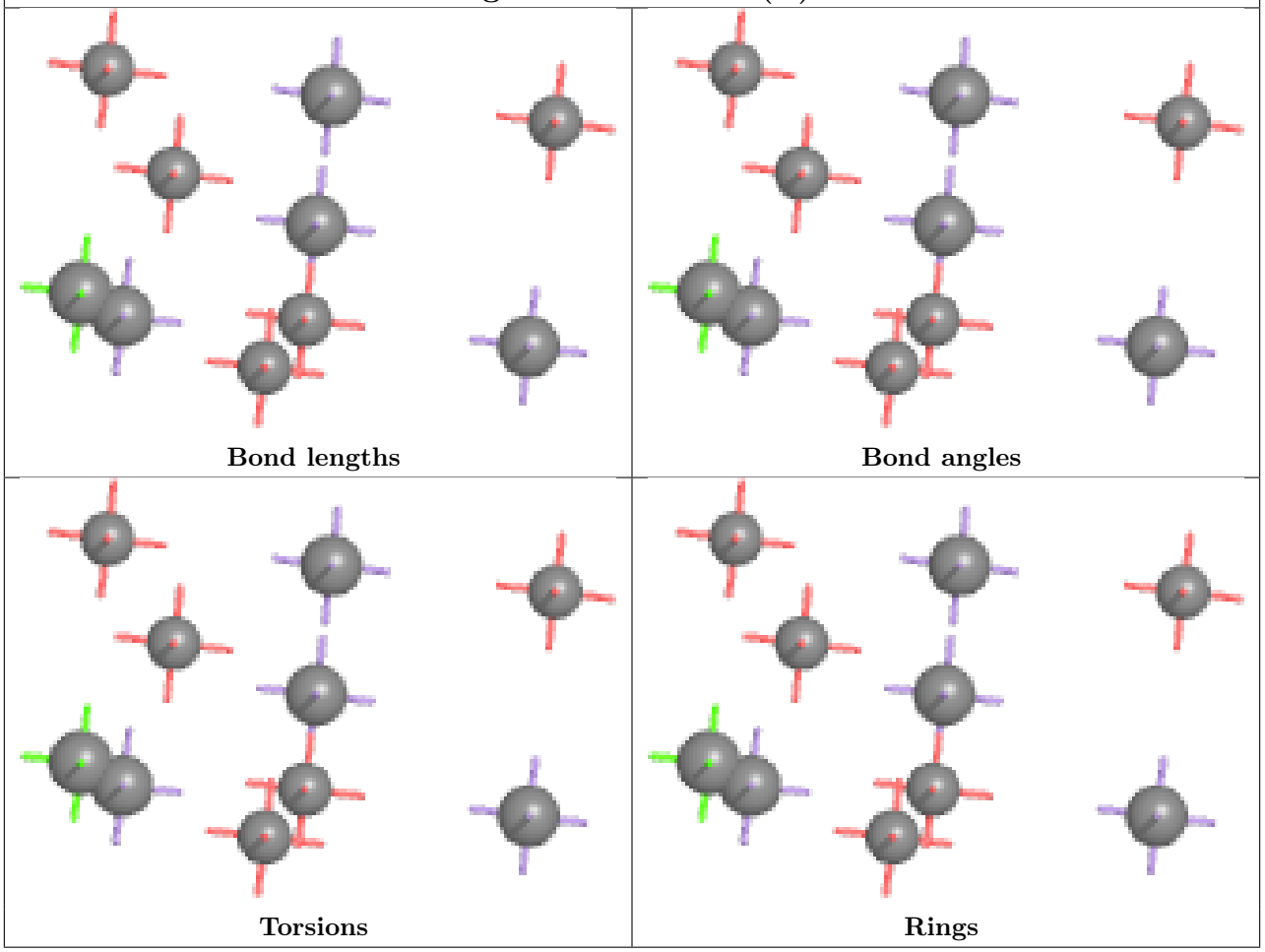


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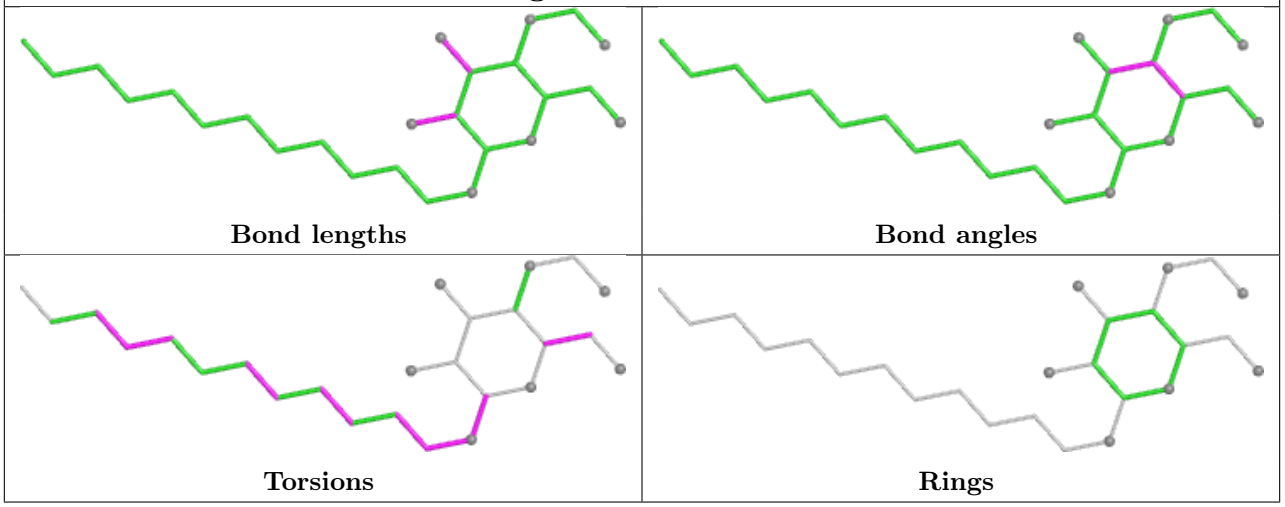


Rings

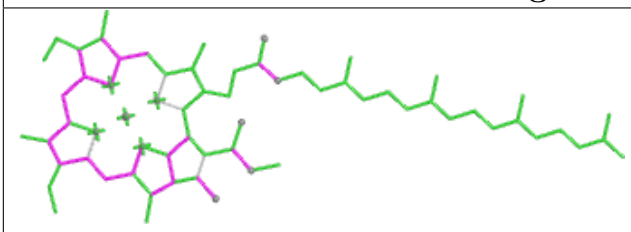
Ligand OEX A 413 (B)



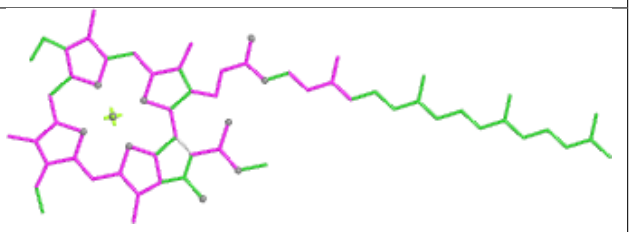
Ligand LMT t 101



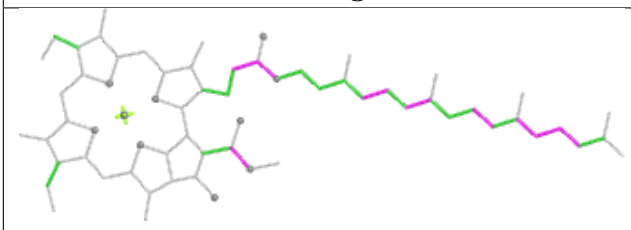
Ligand CLA c 513



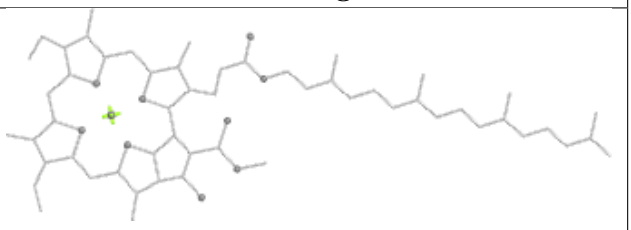
Bond lengths



Bond angles

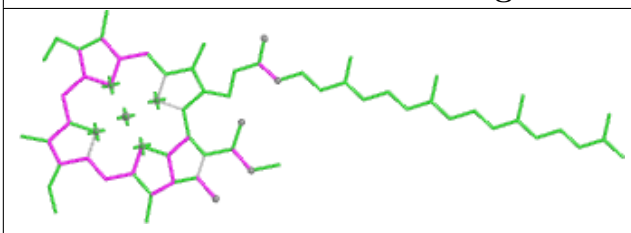


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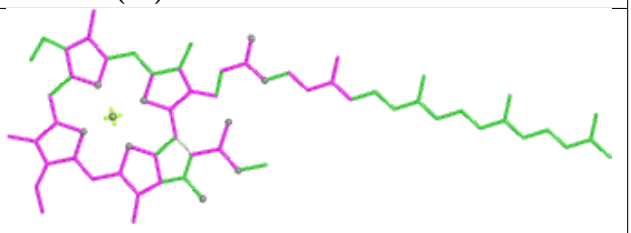


Rings

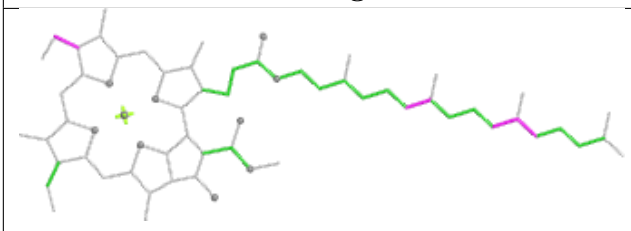
Ligand CLA a 407 (A)



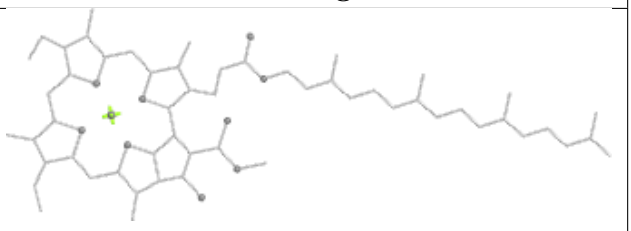
Bond lengths



Bond angles

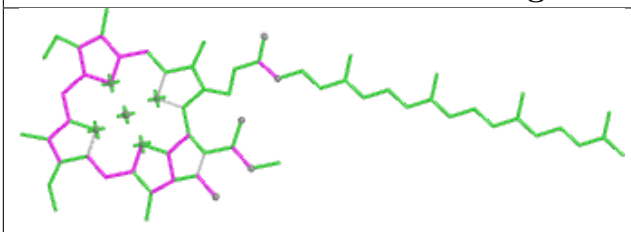


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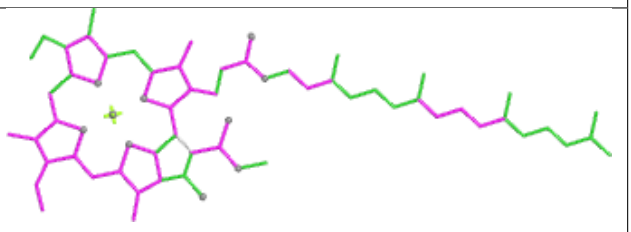


Rings

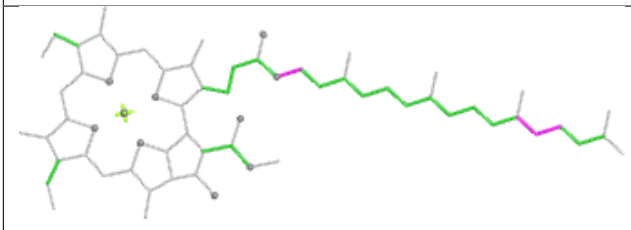
Ligand CLA b 608



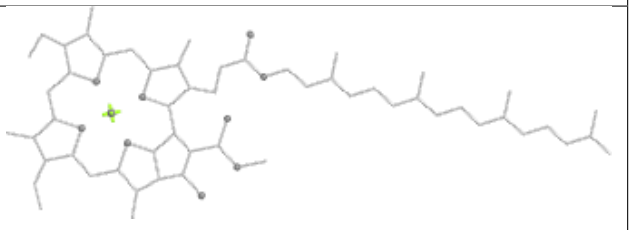
Bond lengths



Bond angles

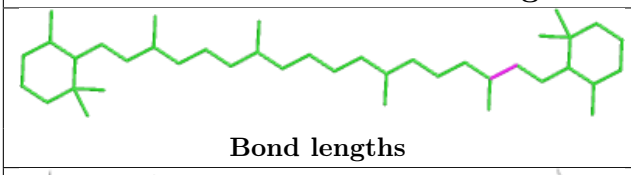


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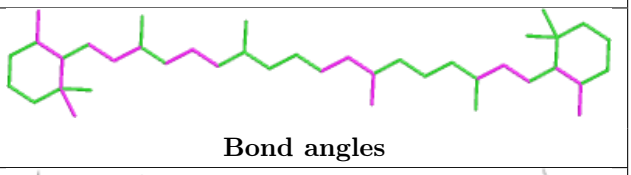


Rings

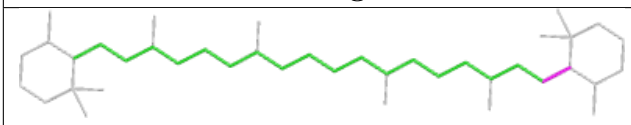
Ligand BCR H 101



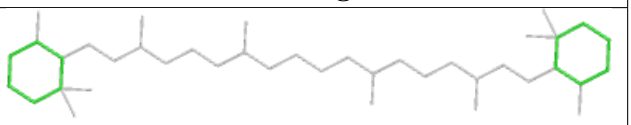
Bond lengths



Bond angles

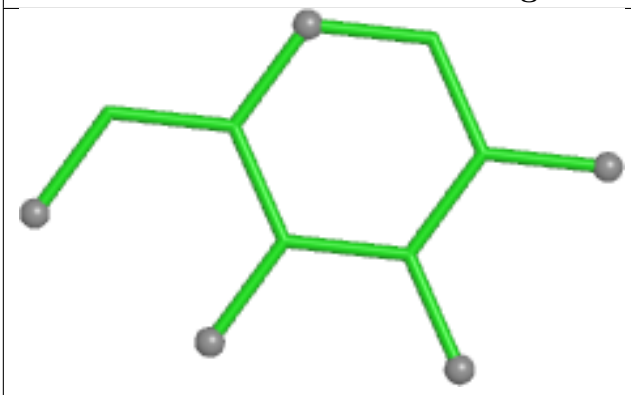


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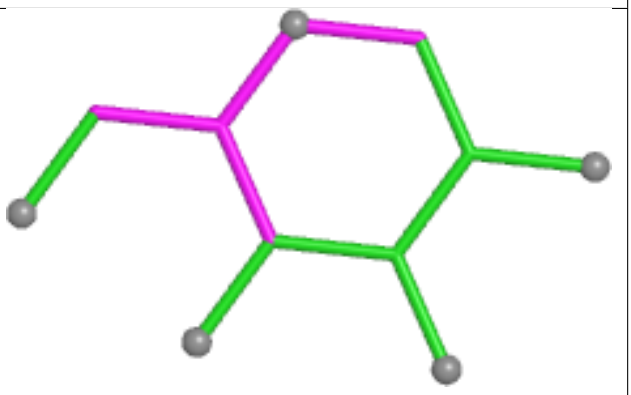


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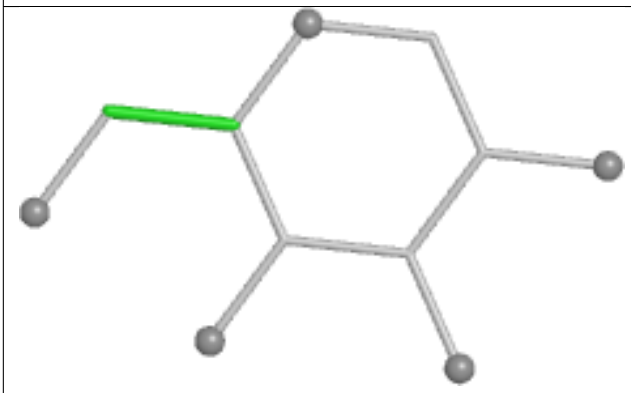
Ligand HTG V 202



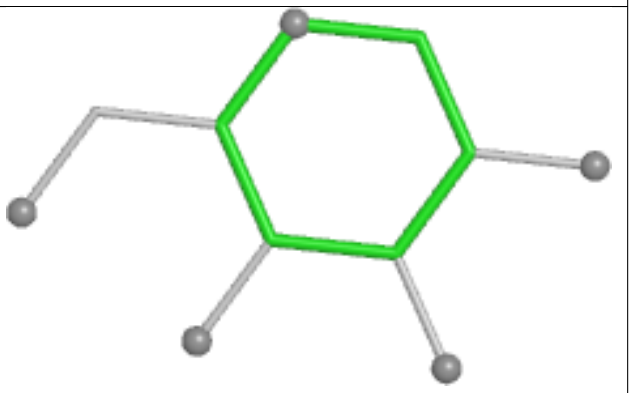
Bond lengths



Bond angles

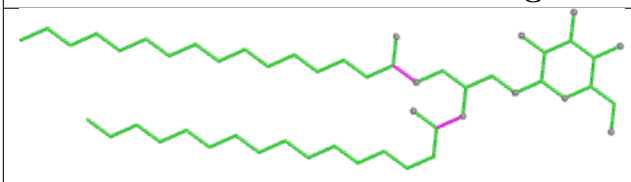


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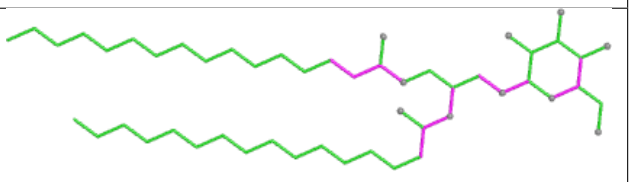


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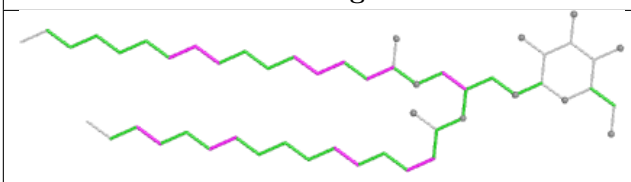
Ligand LMG c 501



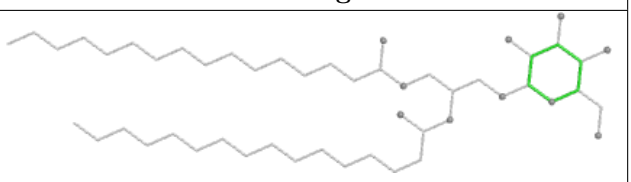
Bond lengths



Bond angles

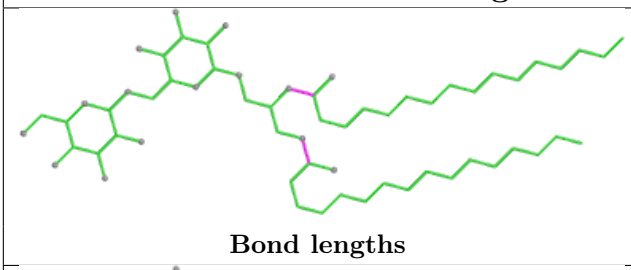


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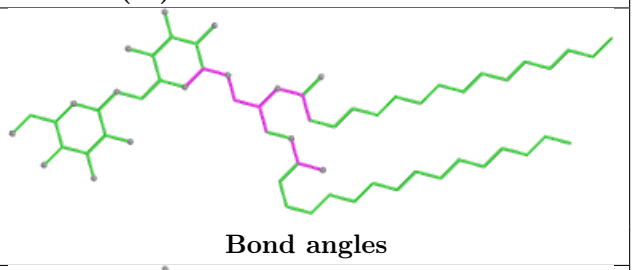


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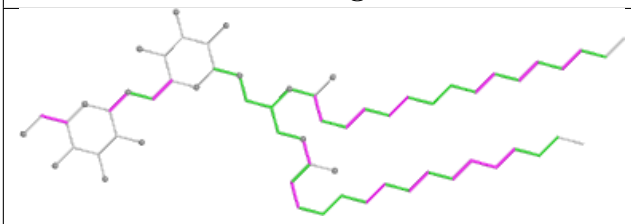
Ligand DGD c 517 (A)



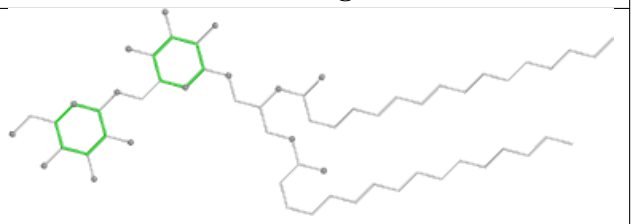
Bond lengths



Bond angles

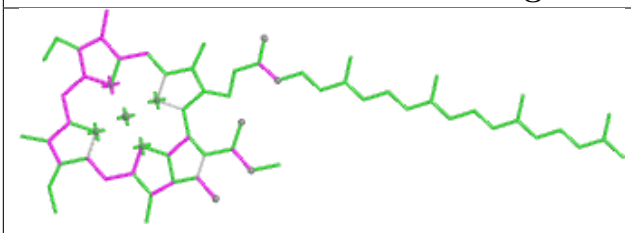


Torsions

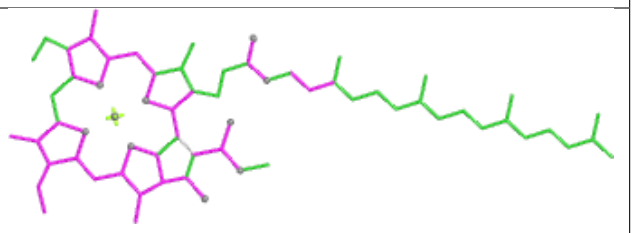


Rings

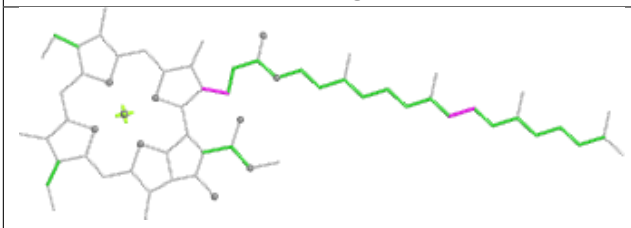
Ligand CLA B 611



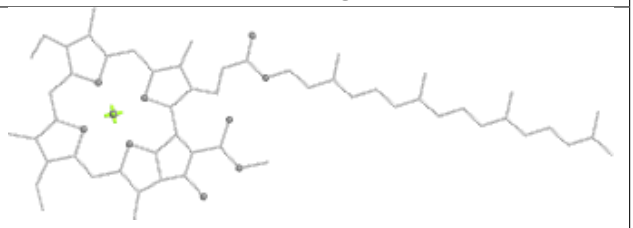
Bond lengths



Bond angles

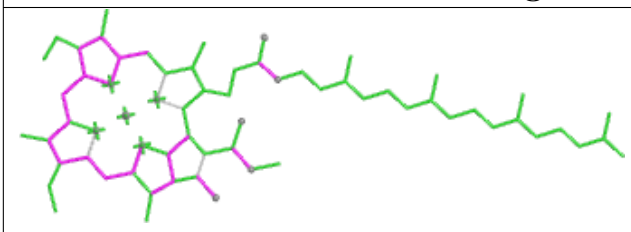


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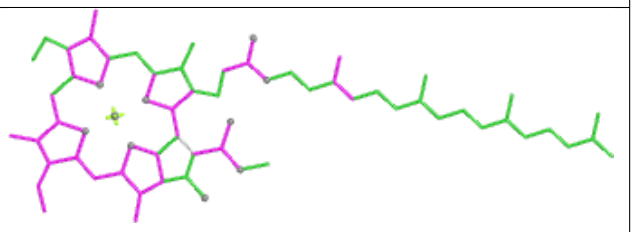


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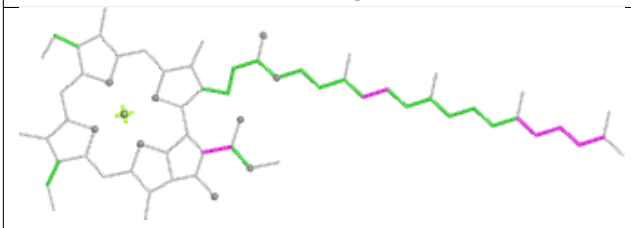
Ligand CLA C 503



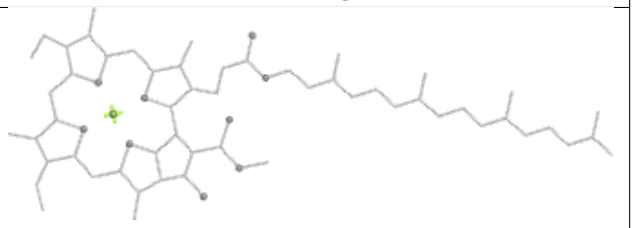
Bond lengths



Bond angles

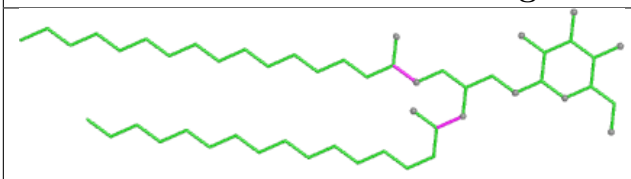


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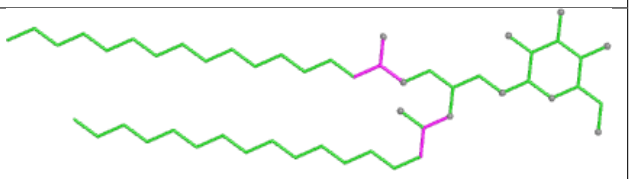


Rings

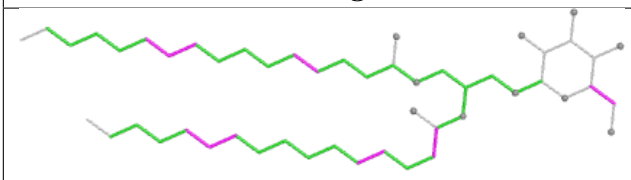
Ligand LMG D 711



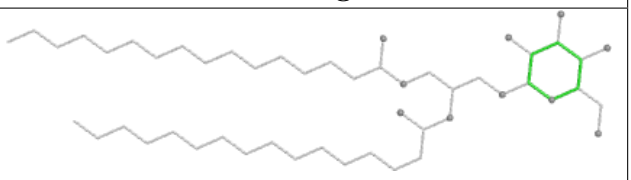
Bond lengths



Bond angles

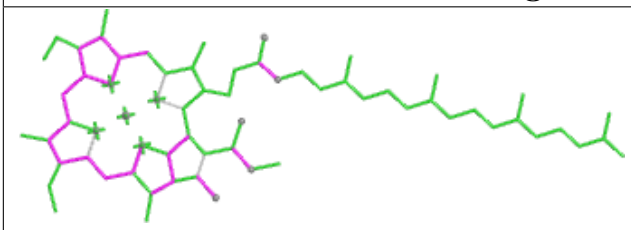


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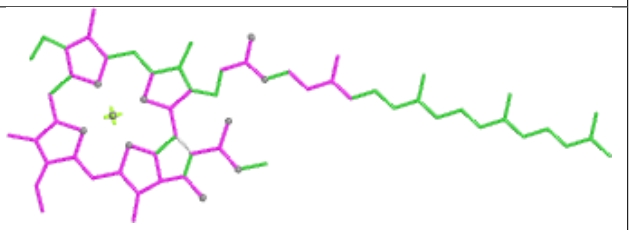


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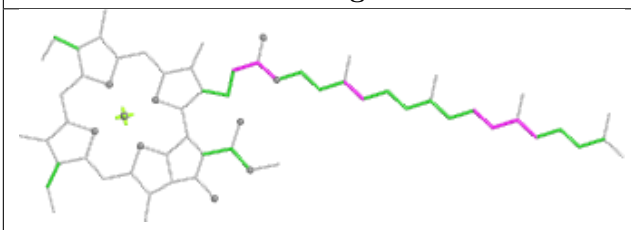
Ligand CLA C 511



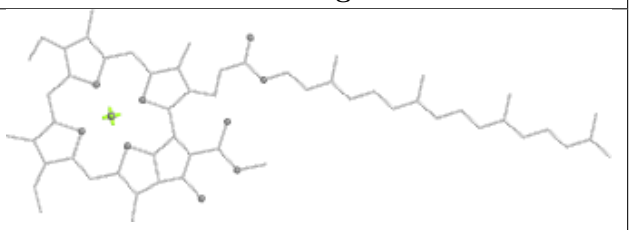
Bond lengths



Bond angles

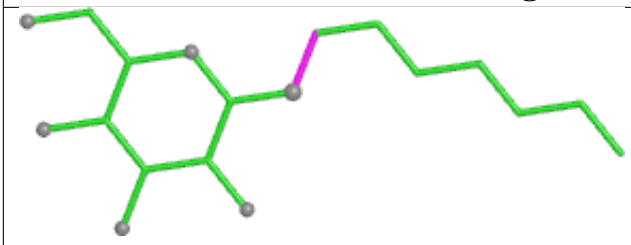


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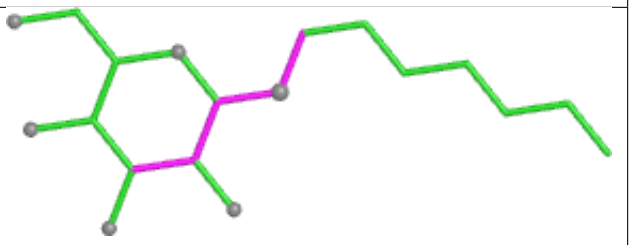


Rings

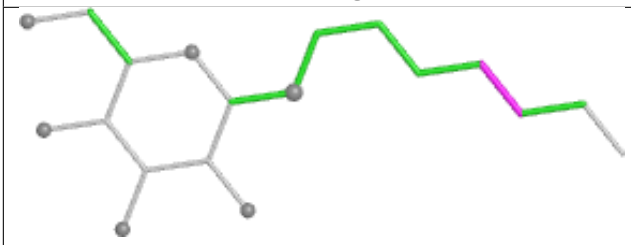
Ligand HTG B 622



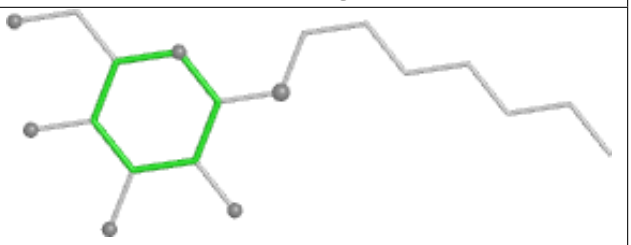
Bond lengths



Bond angles

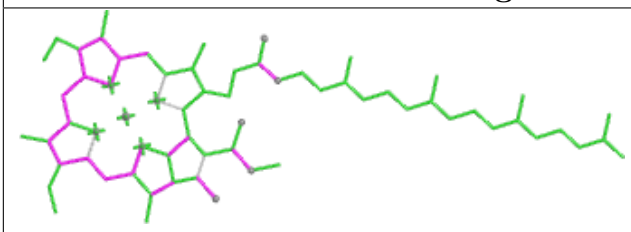


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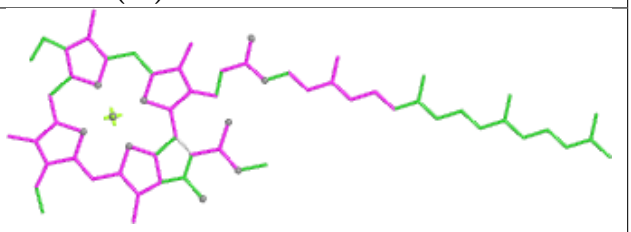


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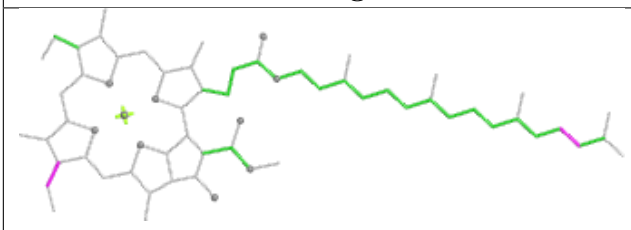
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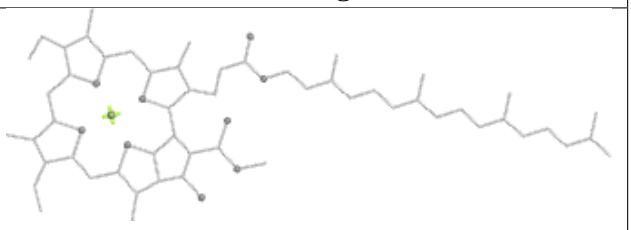
Bond lengths



Bond angles



Torsions



Rings

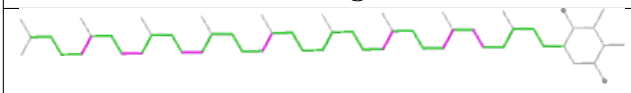
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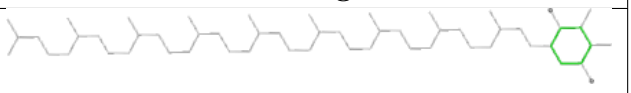
Bond lengths



Bond angles

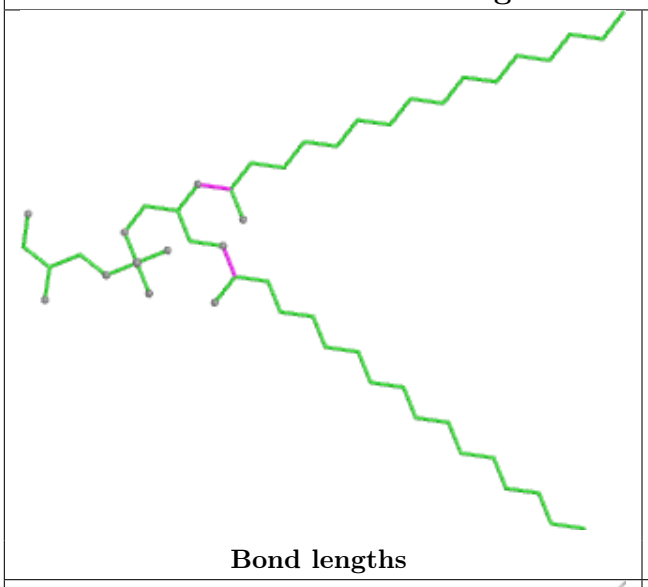


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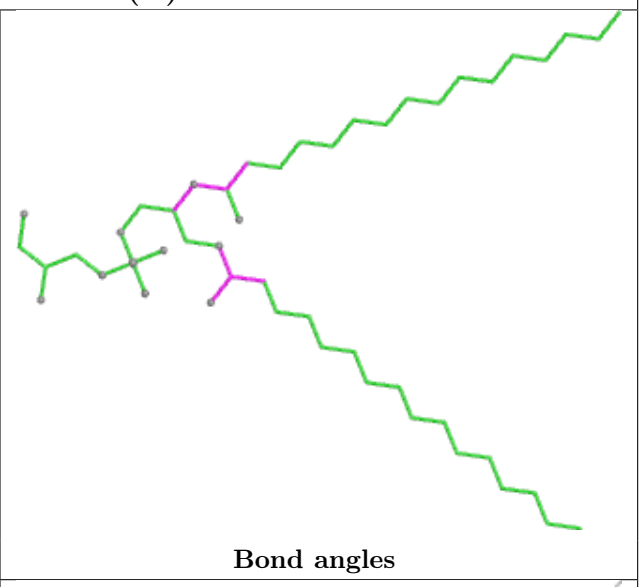


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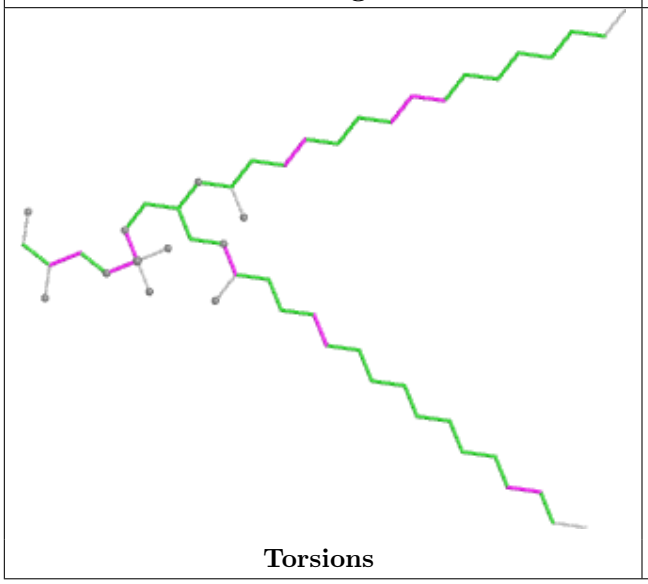
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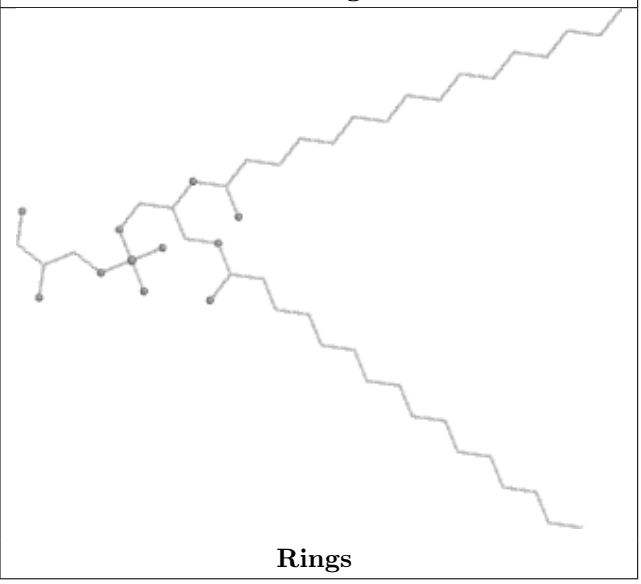
Bond lengths



Bond angles

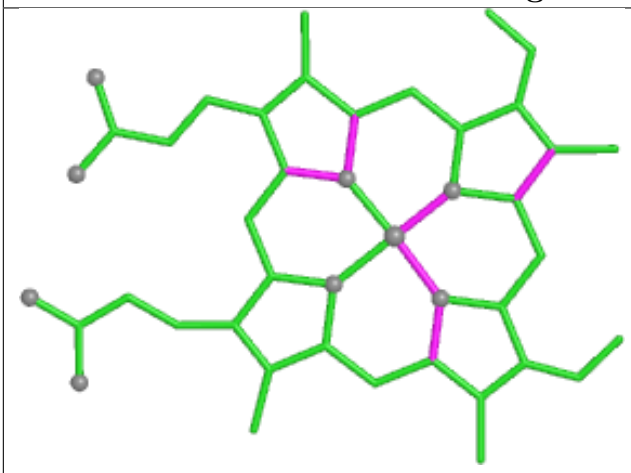


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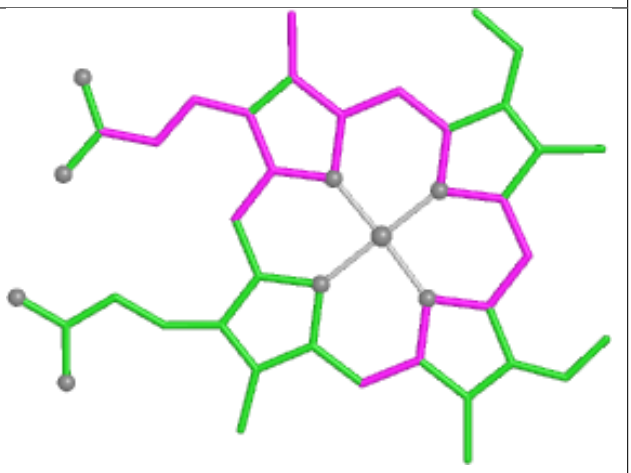


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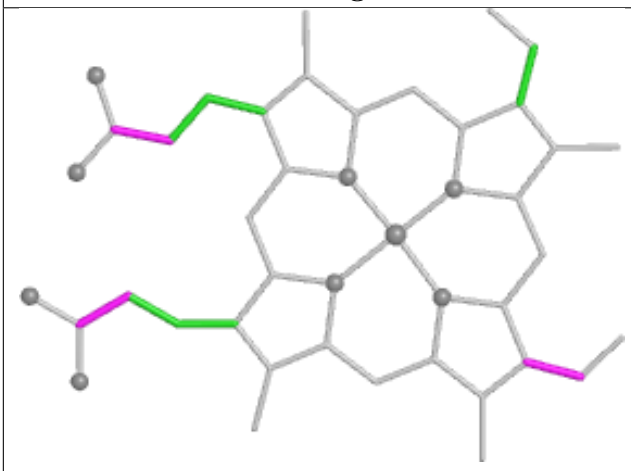
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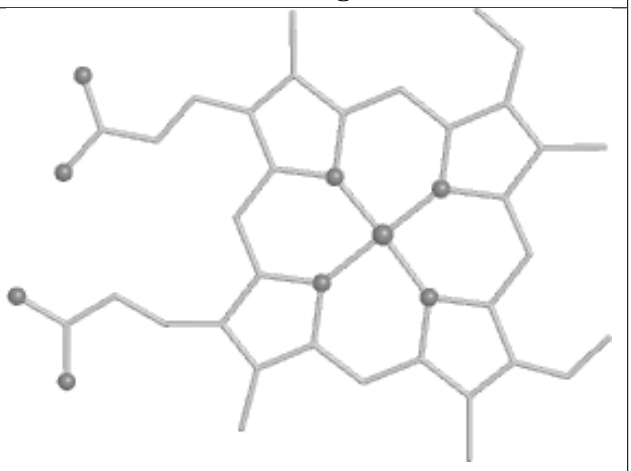
Bond lengths



Bond angles

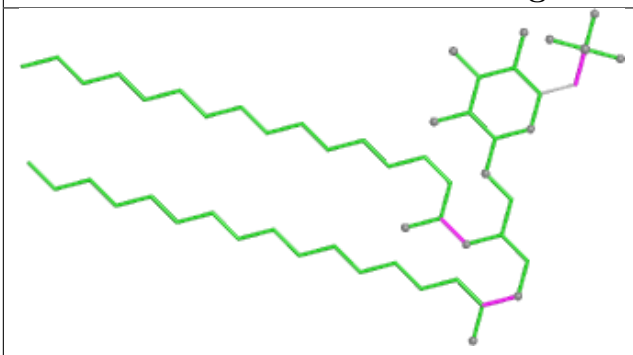


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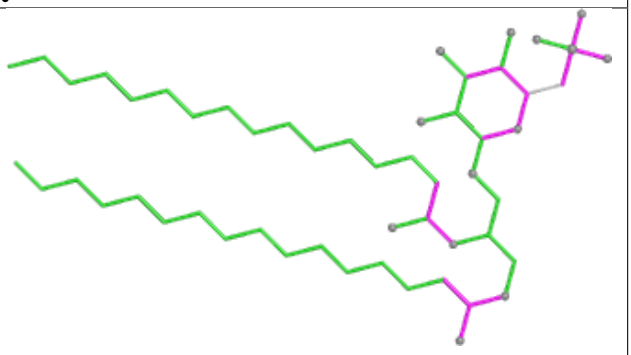


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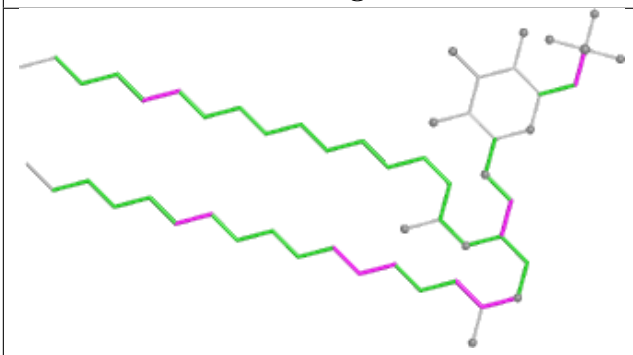
Ligand SQD a 412



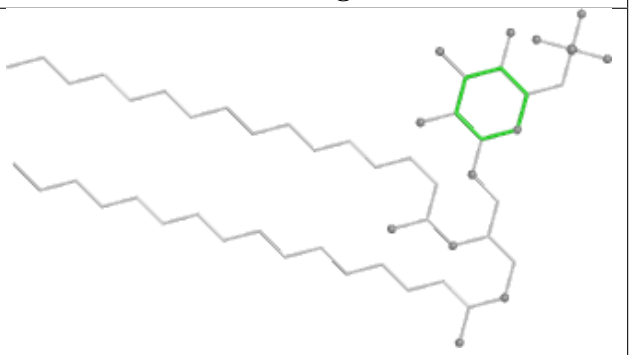
Bond lengths



Bond angles

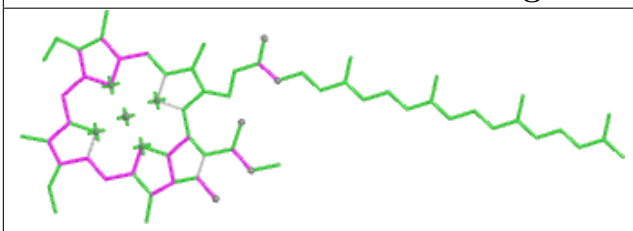


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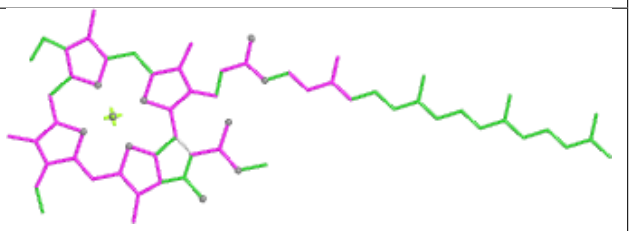


Rings

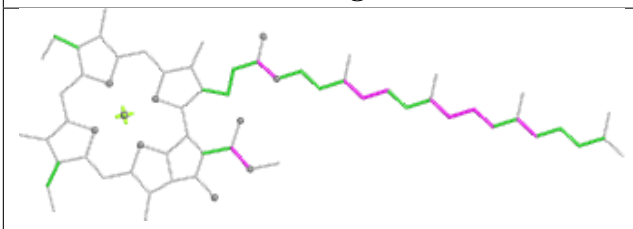
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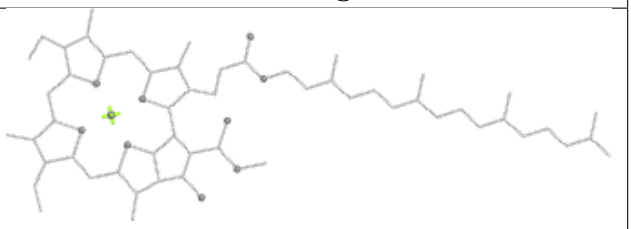
Bond lengths



Bond angles

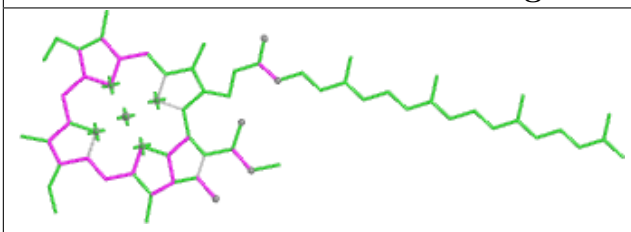


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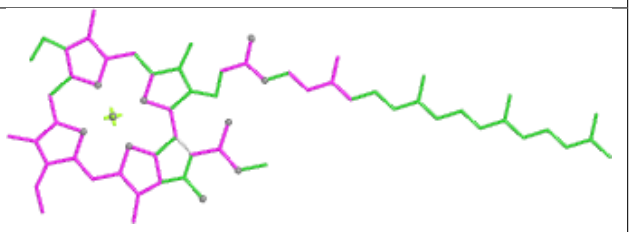


Rings

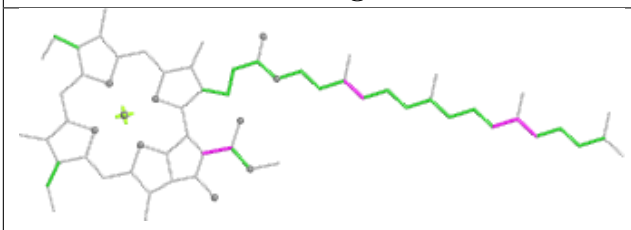
Ligand CLA C 506



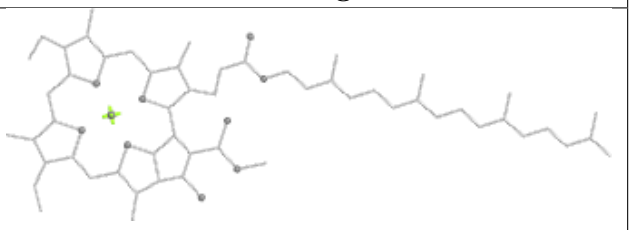
Bond lengths



Bond angles

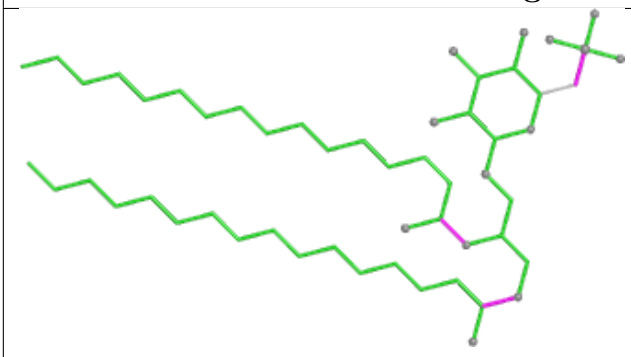


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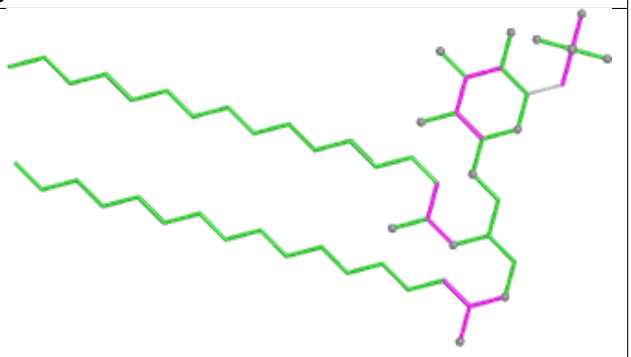


Rings

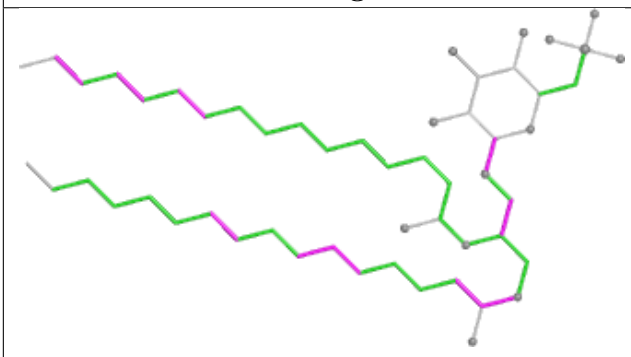
Ligand SQD A 412



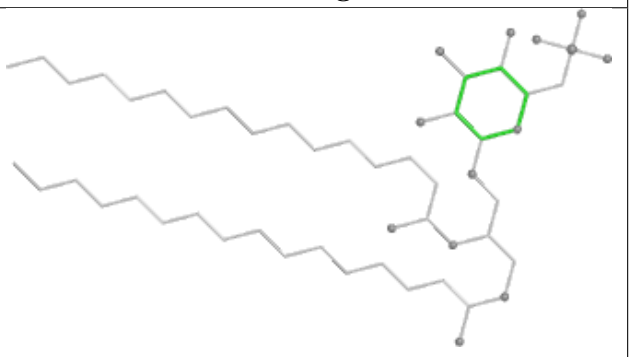
Bond lengths



Bond angles

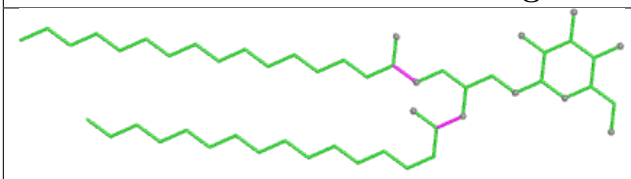


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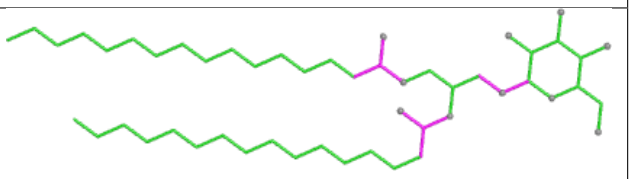


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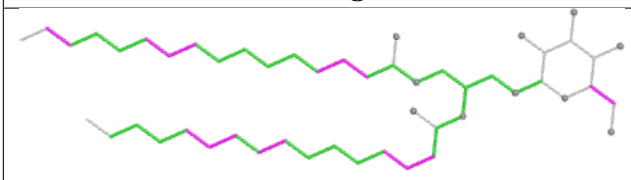
Ligand LMG d 410



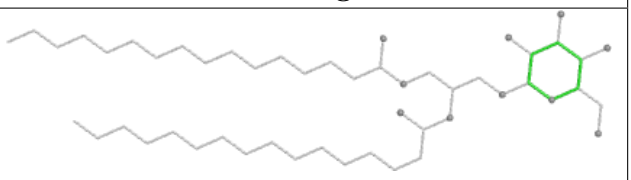
Bond lengths



Bond angles

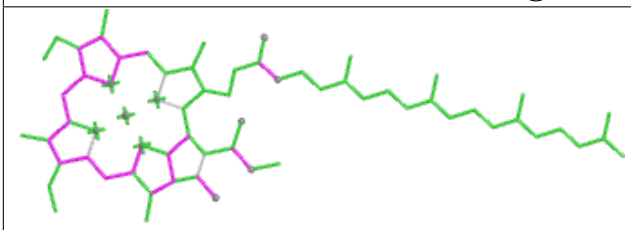


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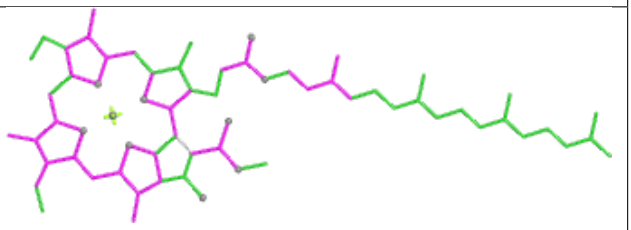


Rings

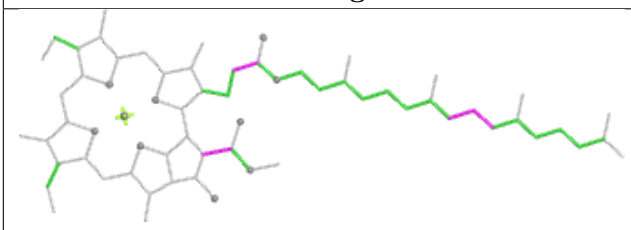
Ligand CLA b 612



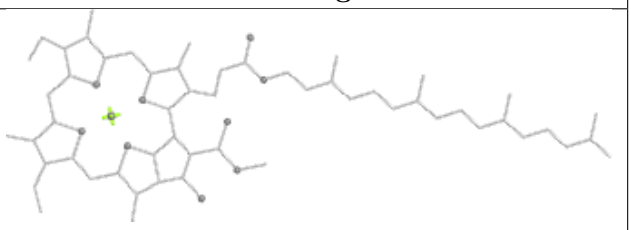
Bond lengths



Bond angles

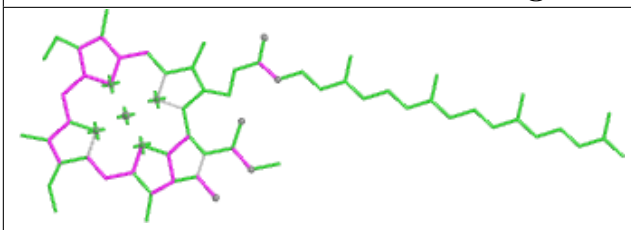


Torsions

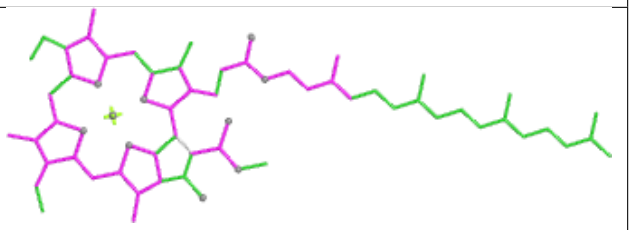


Rings

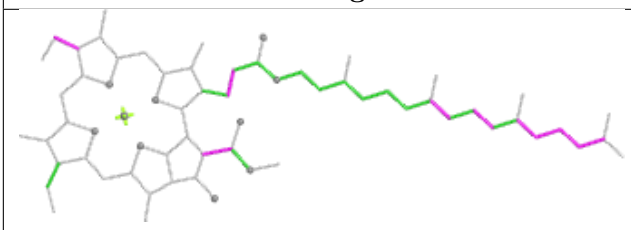
Ligand CLA b 606



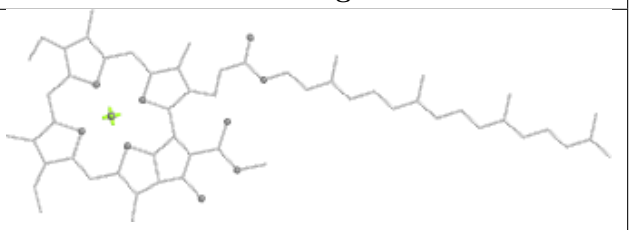
Bond lengths



Bond angles

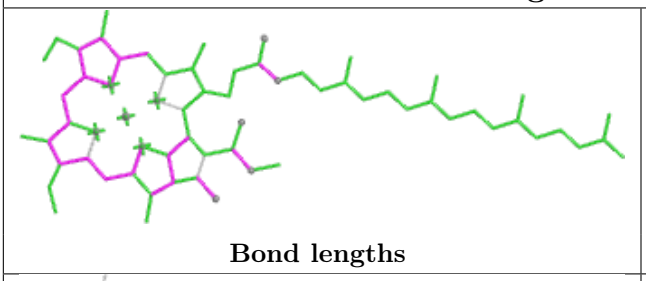


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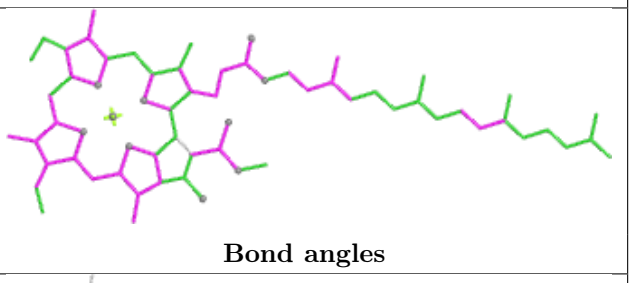


Rings

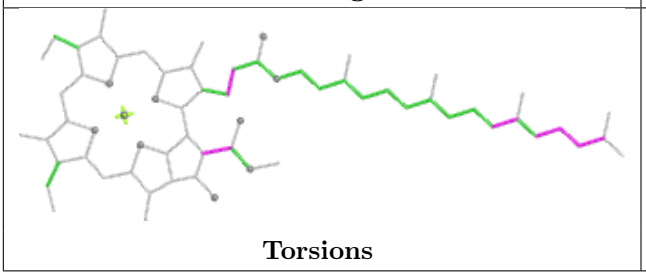
Ligand CLA b 610



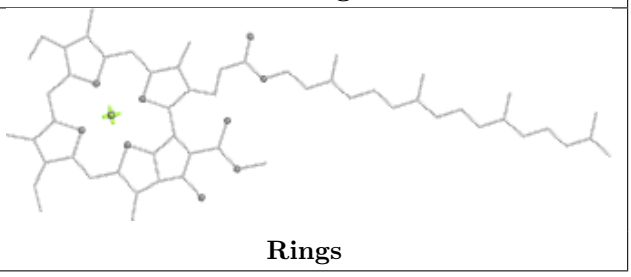
Bond lengths



Bond angles



Torsions

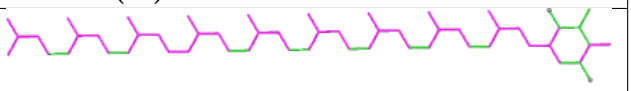


Rings

Ligand PL9 A 414 (A)



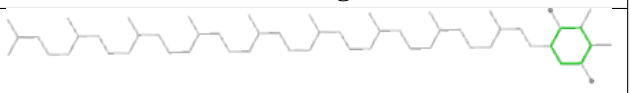
Bond lengths



Bond angles

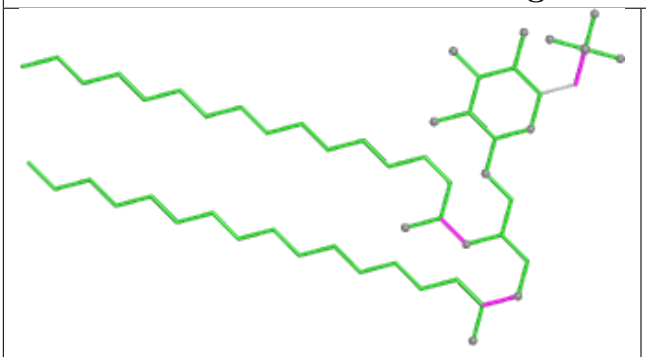


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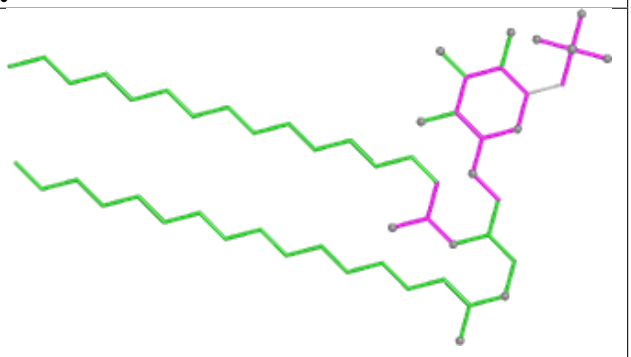


Rings

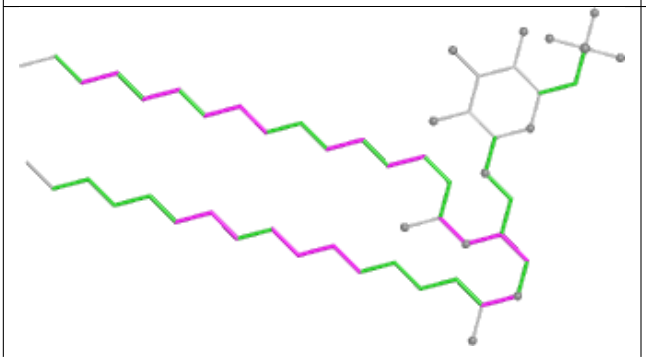
Ligand SQD b 620



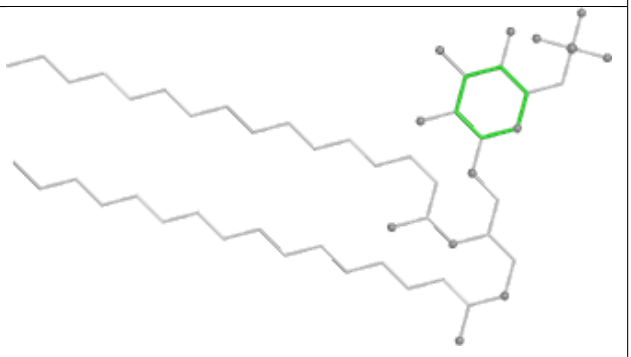
Bond lengths



Bond angles

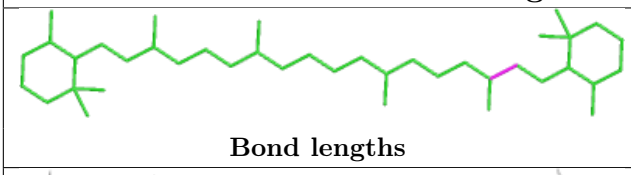


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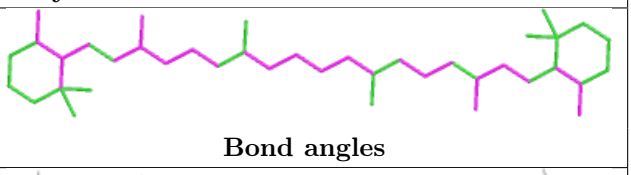


Rings

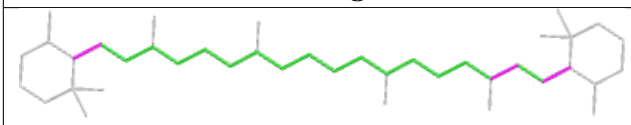
Ligand BCR y 101



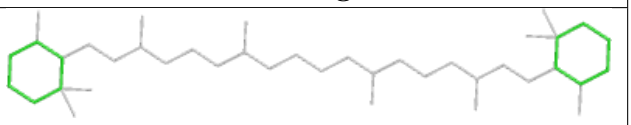
Bond lengths



Bond angles



Torsions



Rings

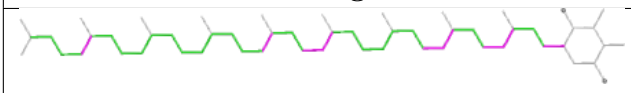
Ligand PL9 a 414 (A)



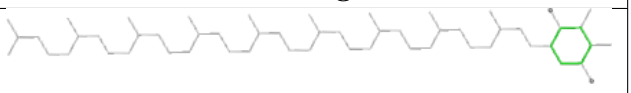
Bond lengths



Bond angles

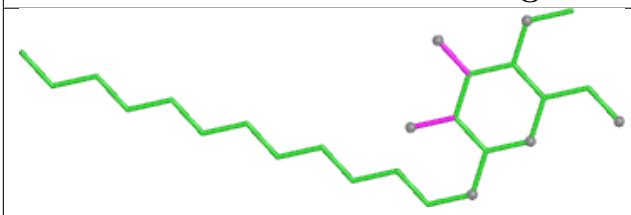


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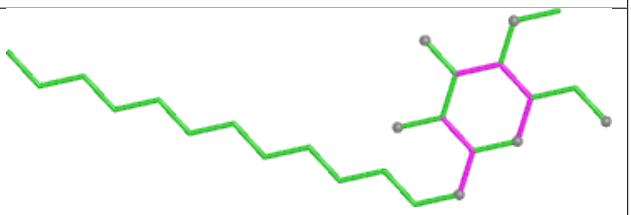


Rings

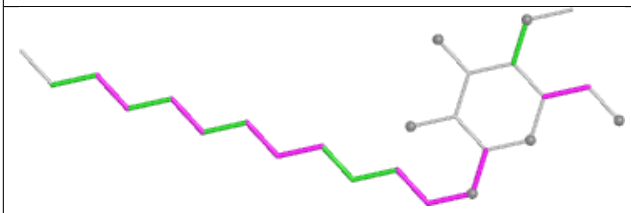
Ligand LMT B 630



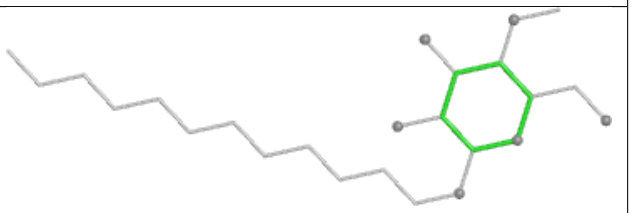
Bond lengths



Bond angles

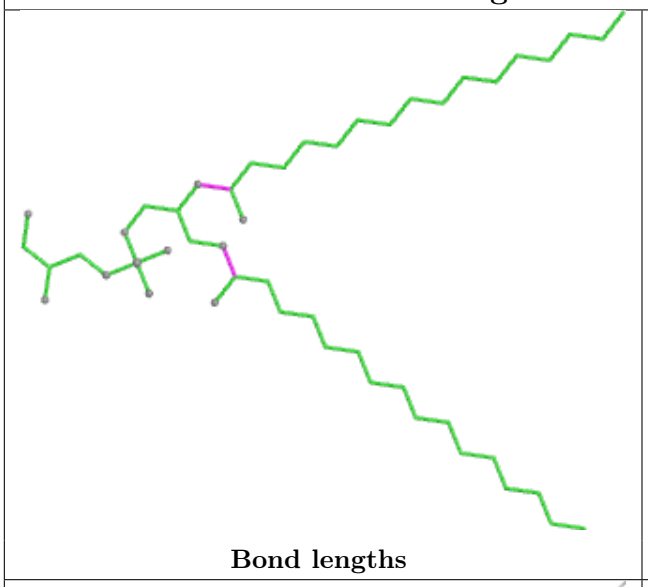


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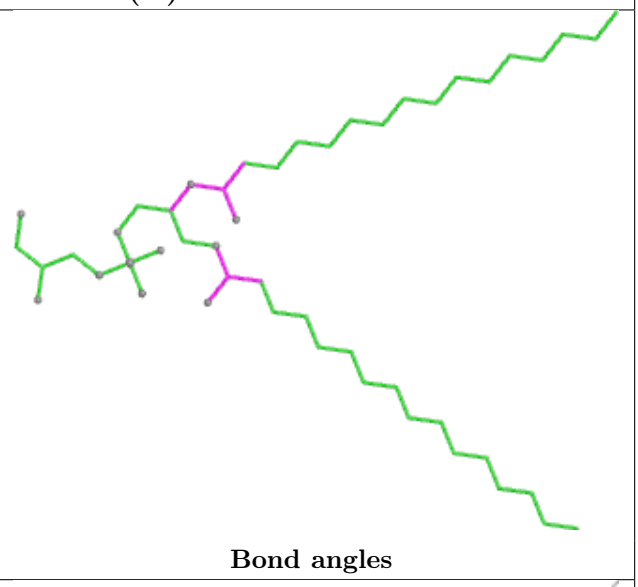


Rings

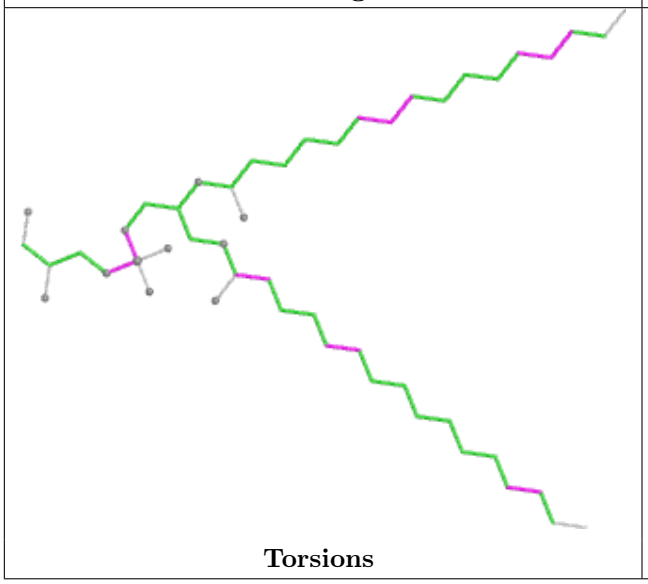
Ligand LHG A 419 (B)



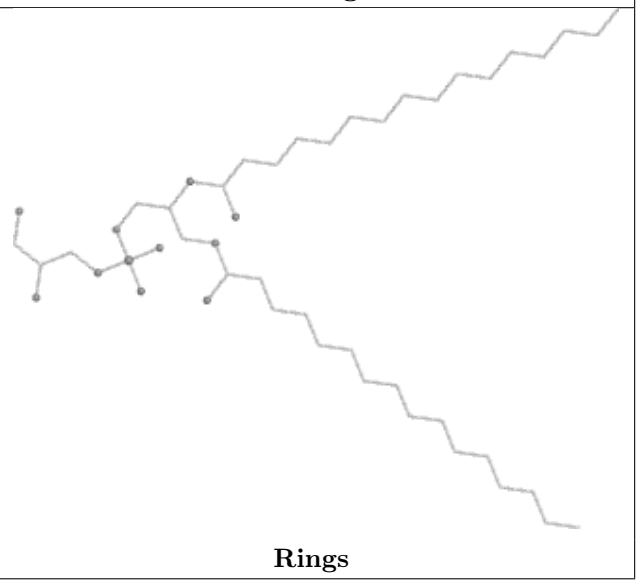
Bond lengths



Bond angles

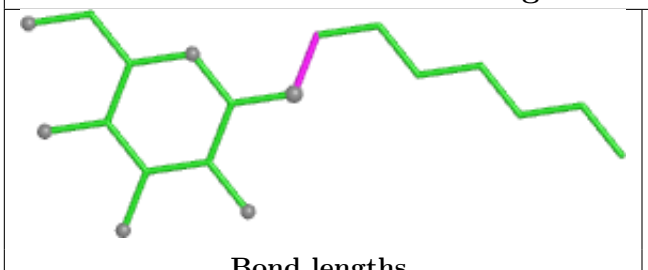


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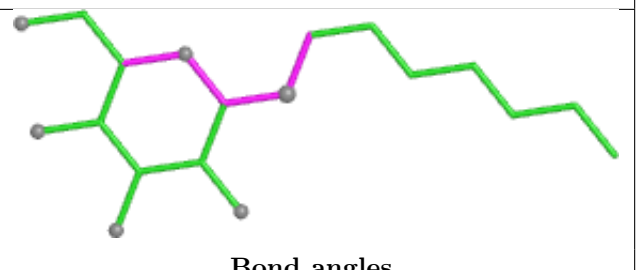


Rings

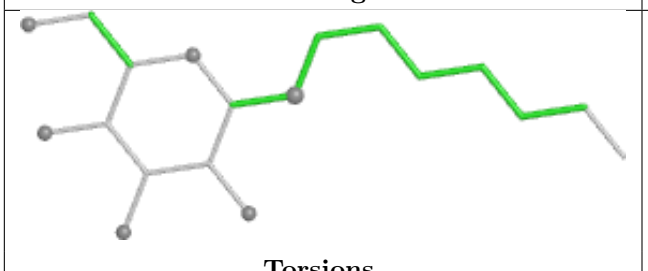
Ligand HTG C 522



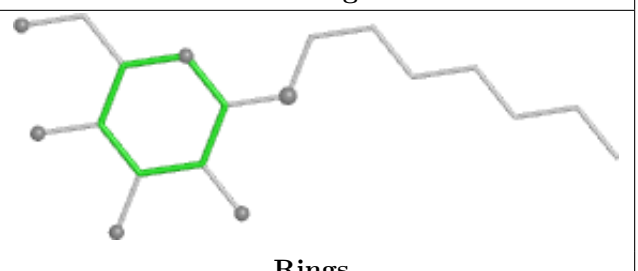
Bond lengths



Bond angles

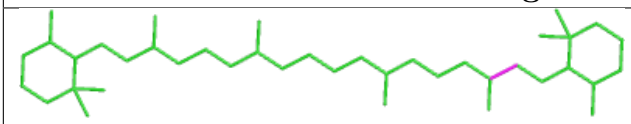


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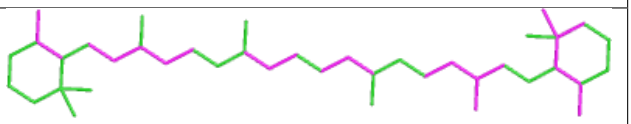


Rings

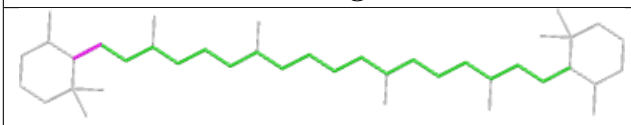
Ligand BCR C 515



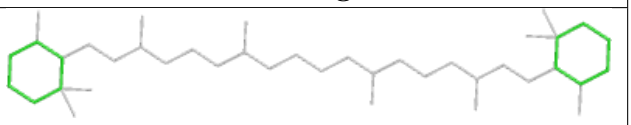
Bond lengths



Bond angles



Torsions

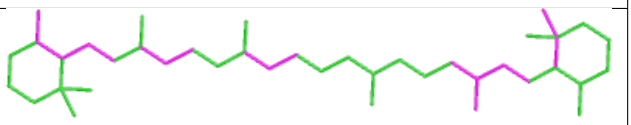


Rings

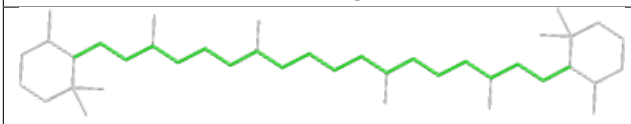
Ligand BCR A 409



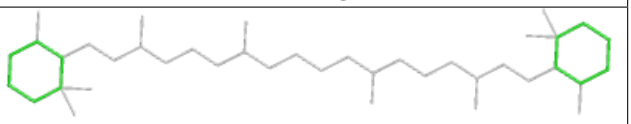
Bond lengths



Bond angles

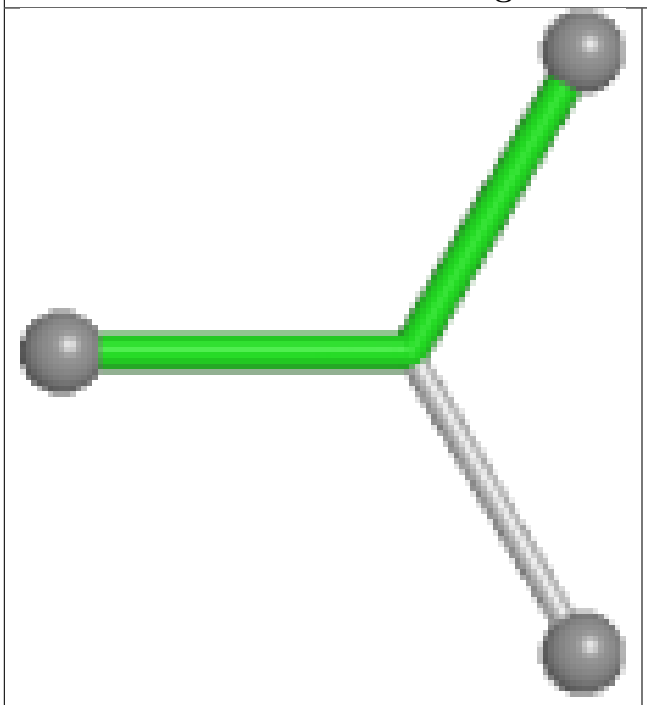


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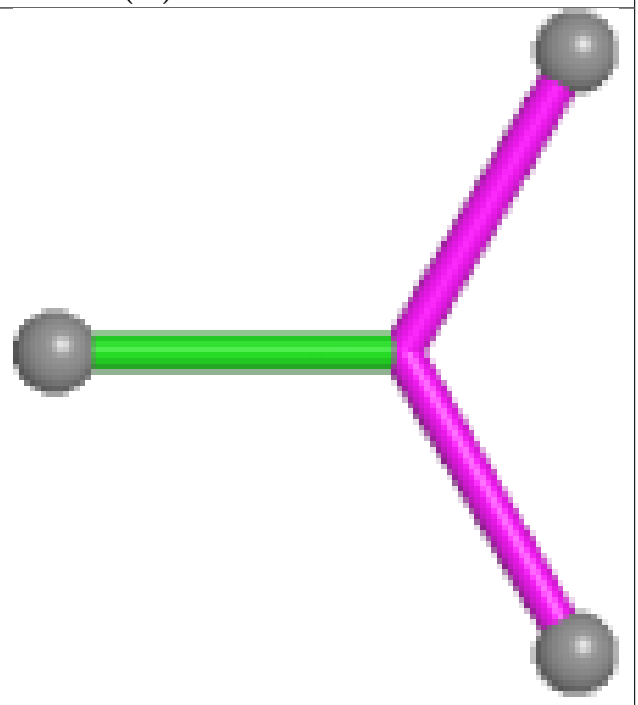


Rings

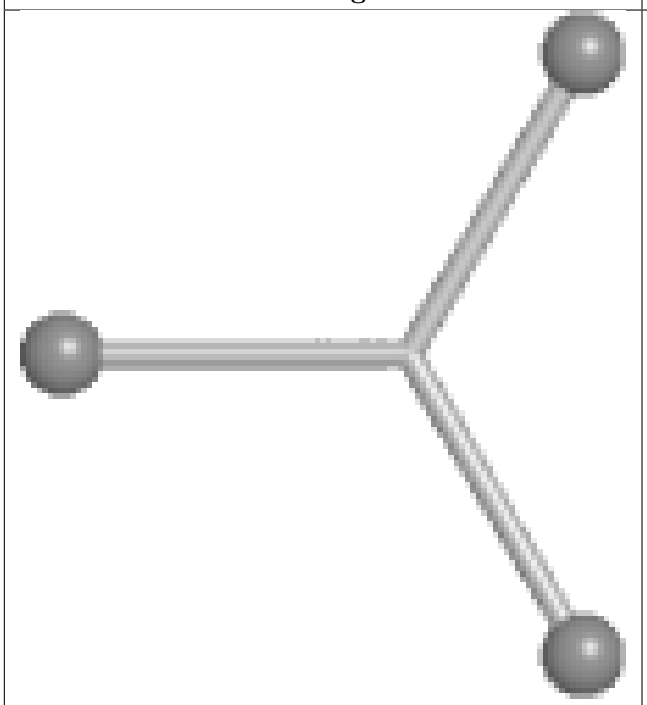
Ligand BCT a 404 (A)



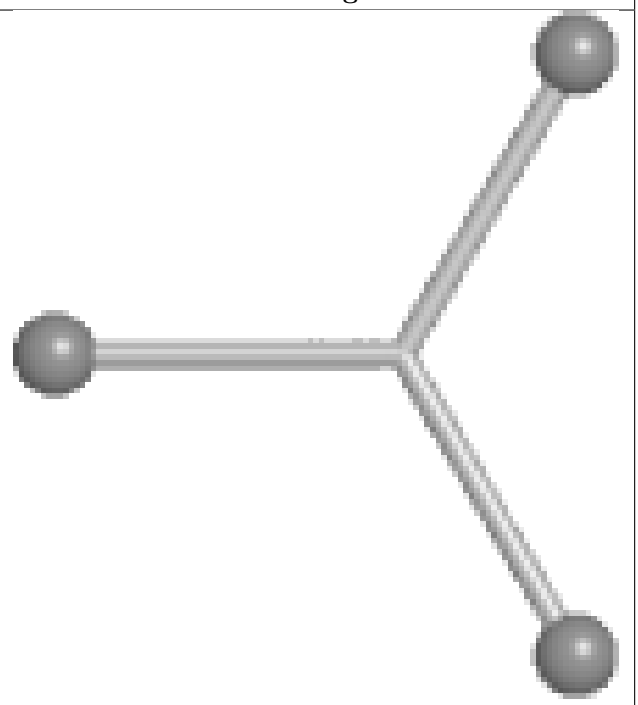
Bond lengths



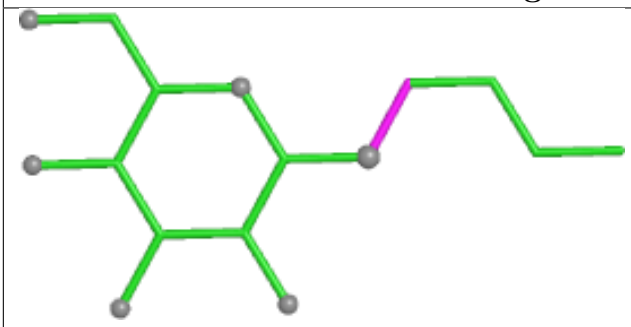
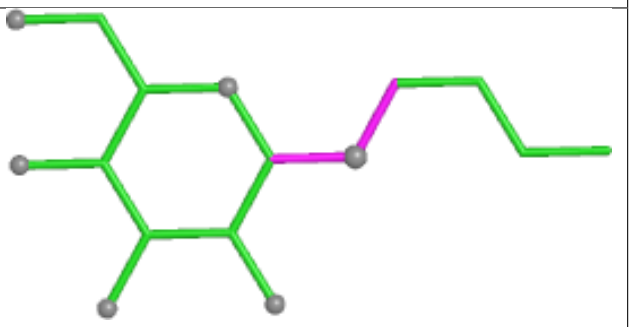
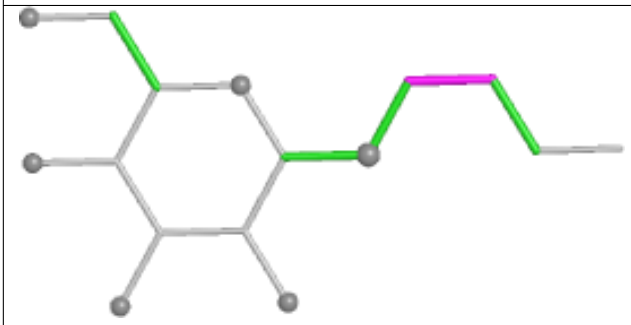
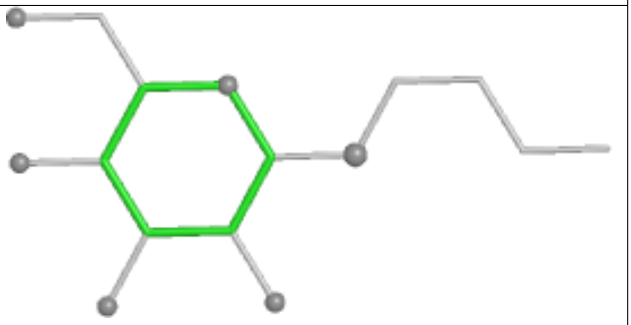
Bond angles

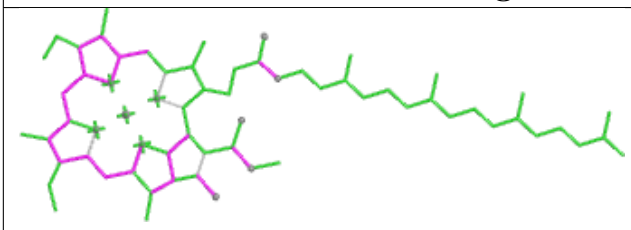
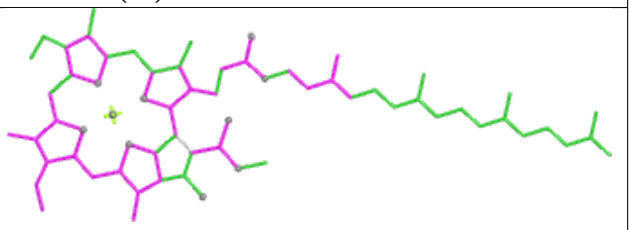
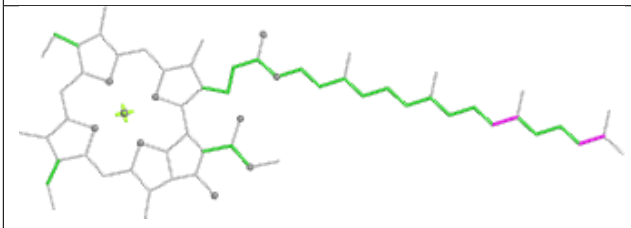
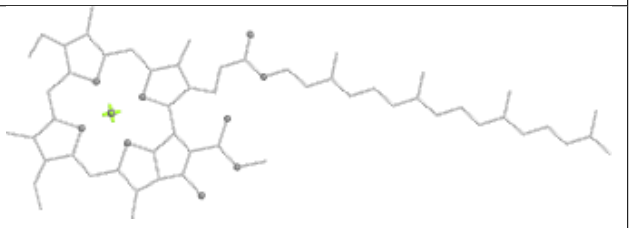


Torsions

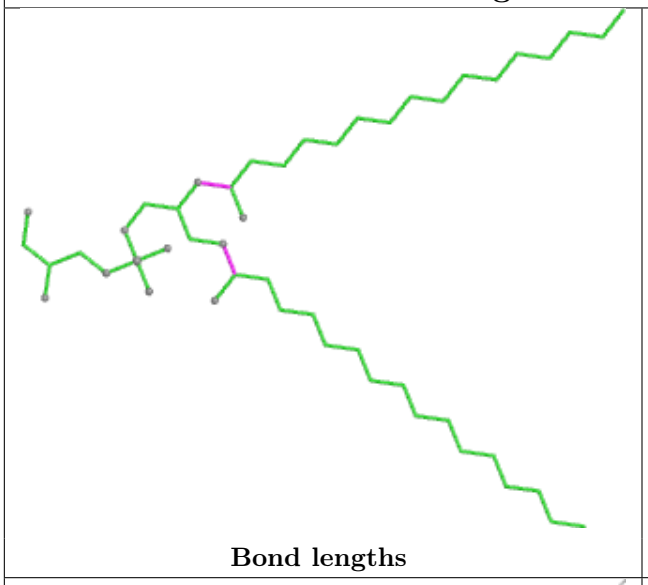


Rings

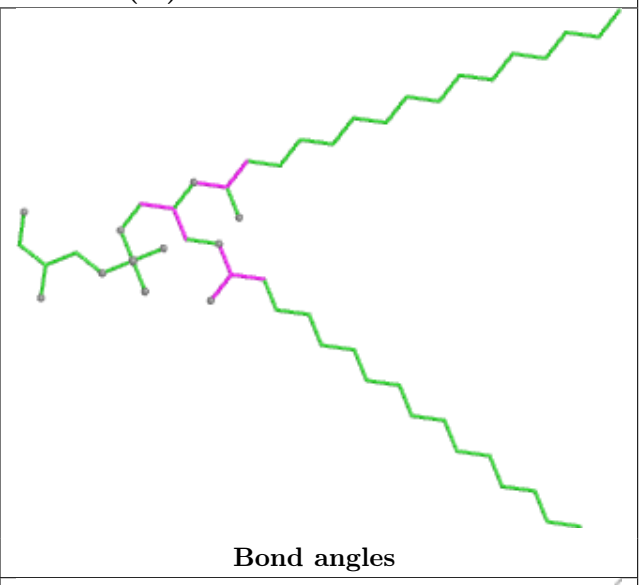
Ligand HTG d 409	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA d 401 (B)	
 Bond lengths	 Bond angles
 Torsions	 Rings

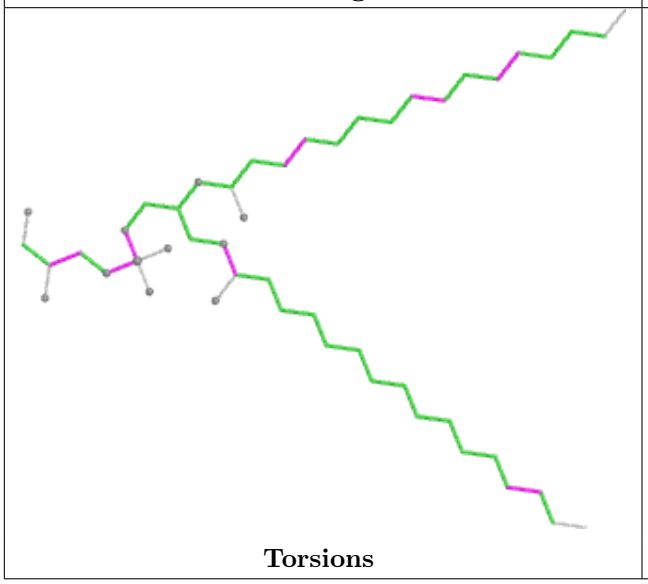
Ligand LHG d 405 (A)



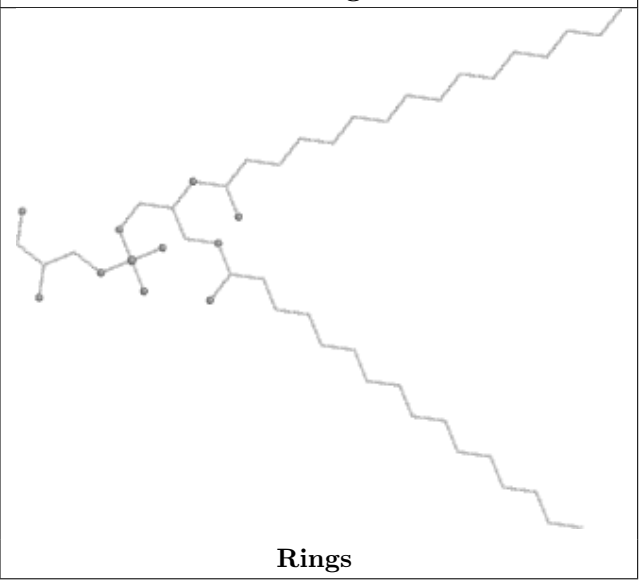
Bond lengths



Bond angles



Torsions

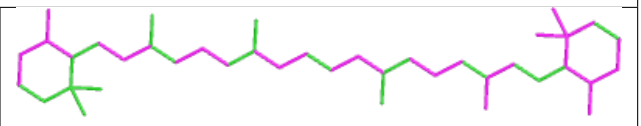


Rings

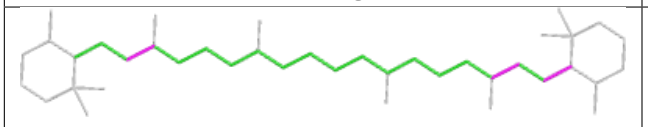
Ligand BCR d 403



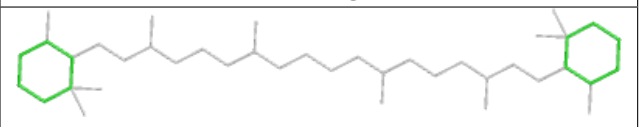
Bond lengths



Bond angles

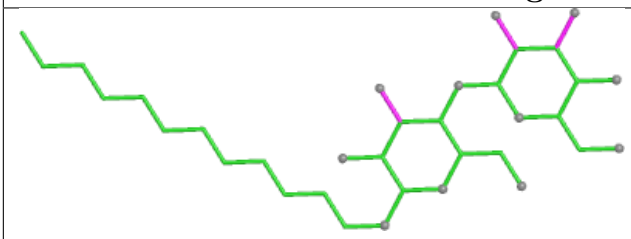


Torsions

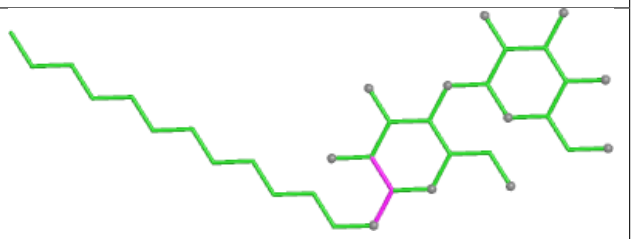


Rings

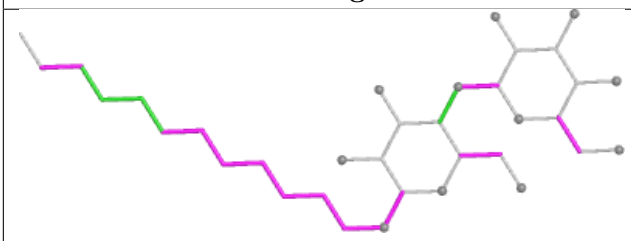
Ligand LMT e 101



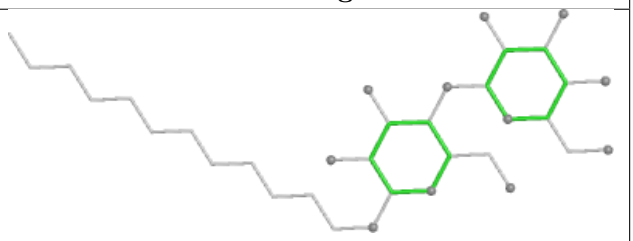
Bond lengths



Bond angles

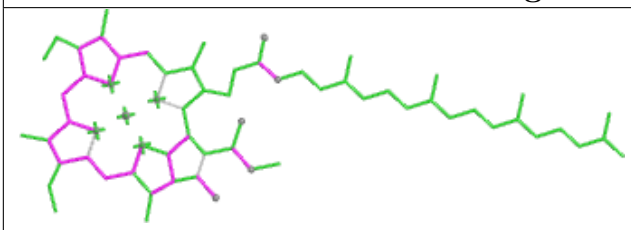


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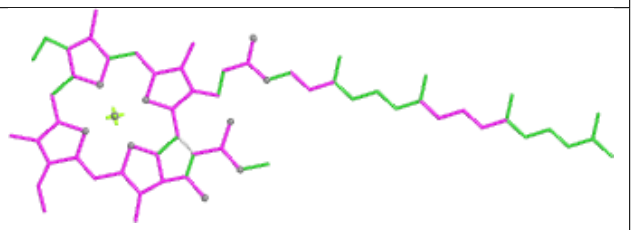


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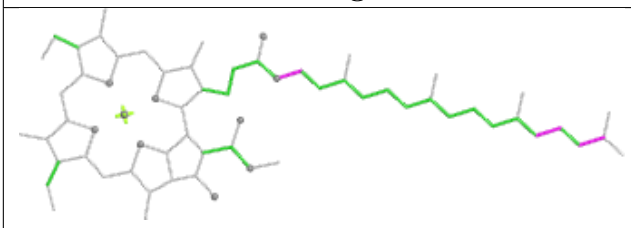
Ligand CLA B 608



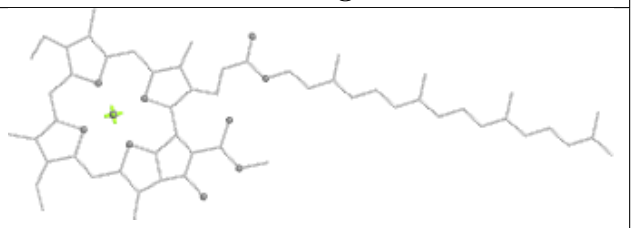
Bond lengths



Bond angles

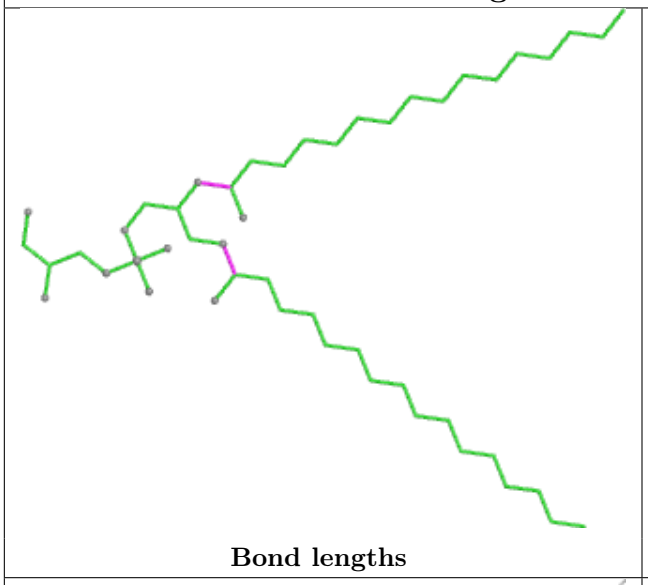


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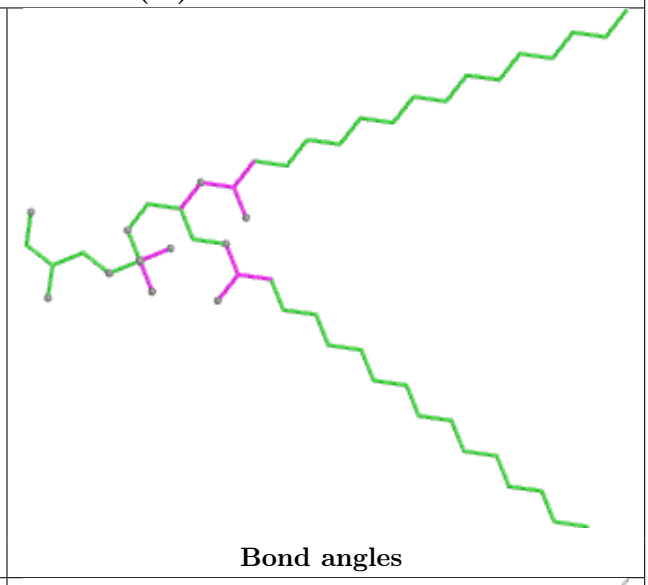


Rings

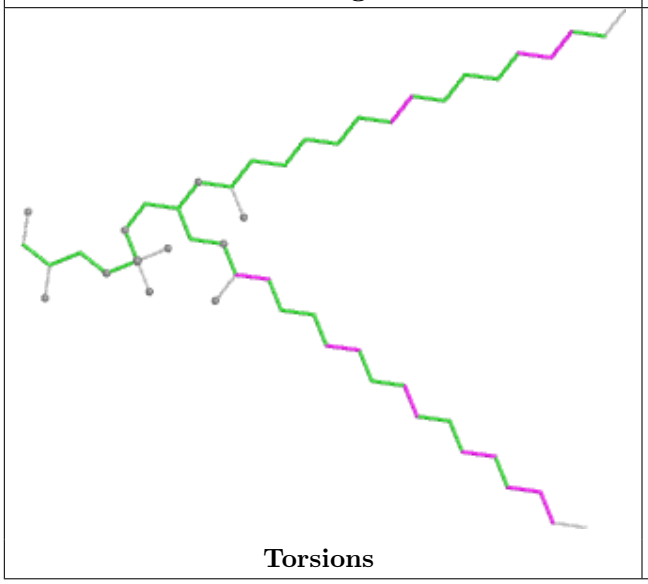
Ligand LHG A 419 (A)



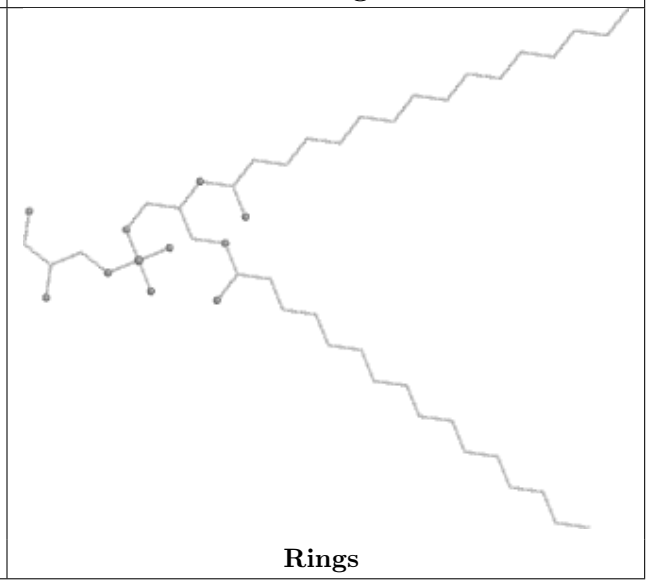
Bond lengths



Bond angles

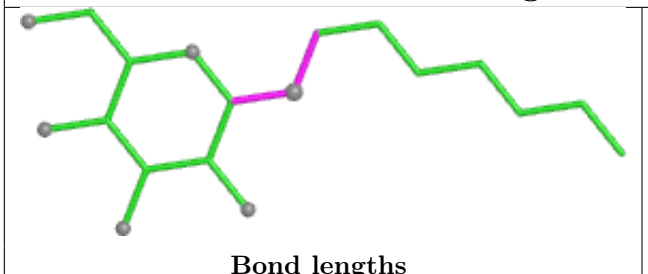


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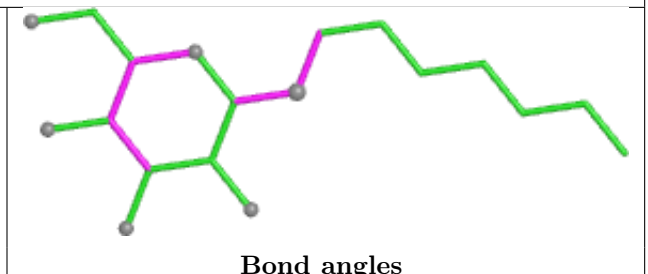


Rings

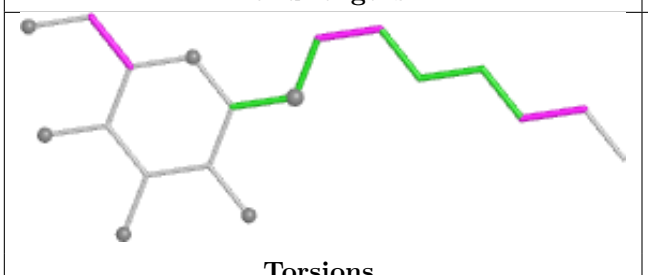
Ligand HTG B 624



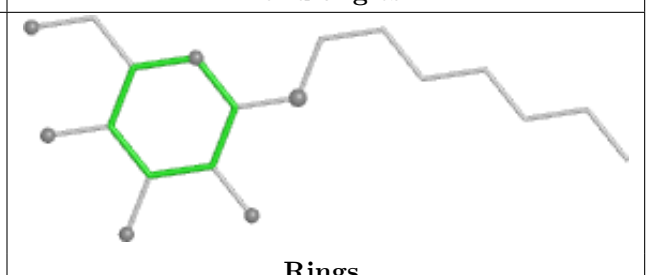
Bond lengths



Bond angles

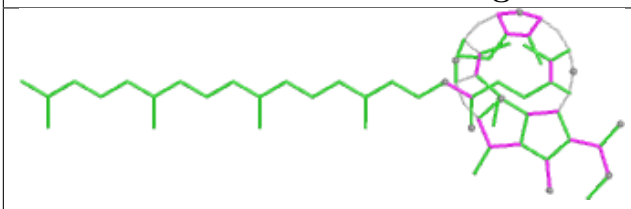


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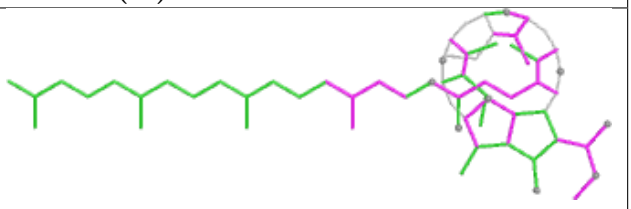


Rings

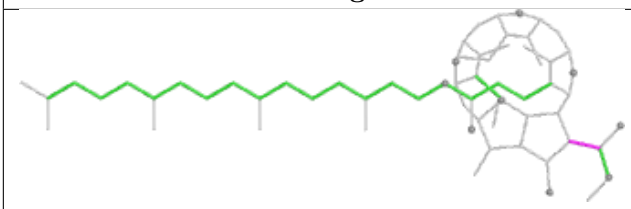
Ligand PHO a 416 (A)



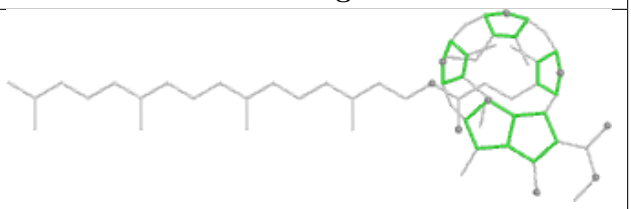
Bond lengths



Bond angles

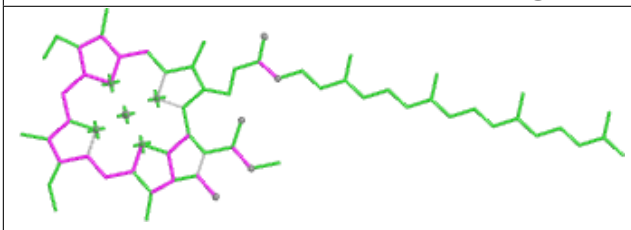


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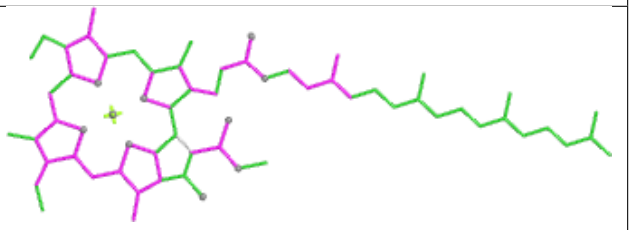


Rings

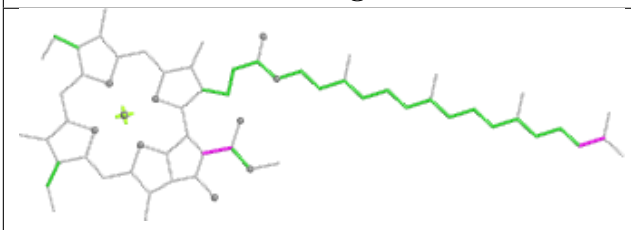
Ligand CLA c 509



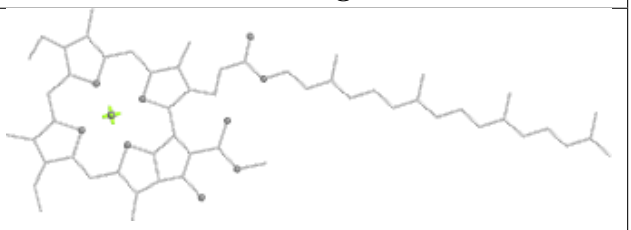
Bond lengths



Bond angles

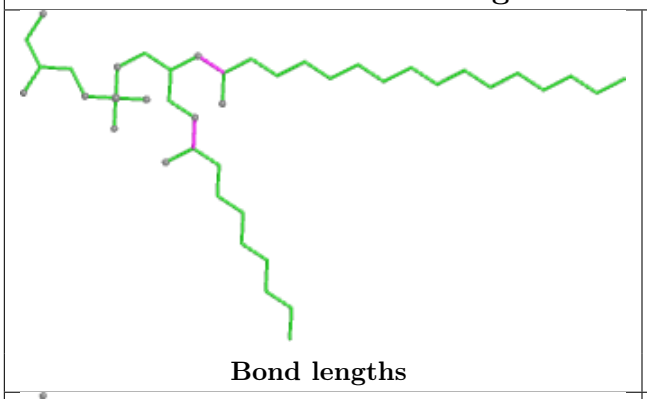


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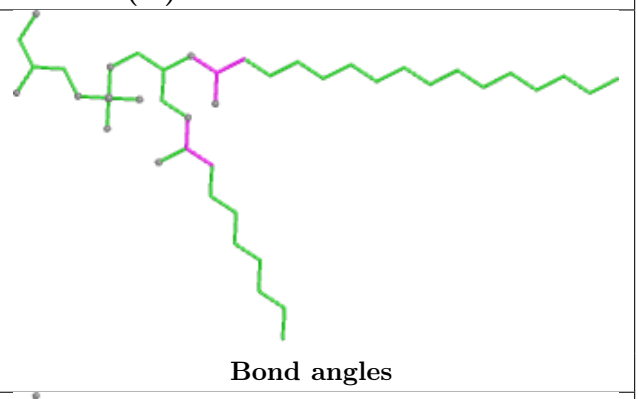


Rings

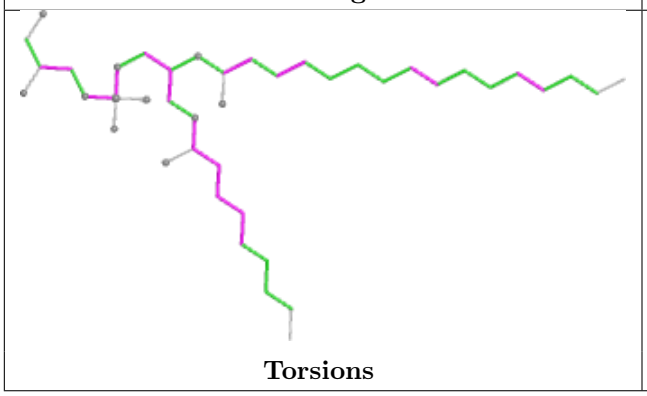
Ligand LHG E 101 (B)



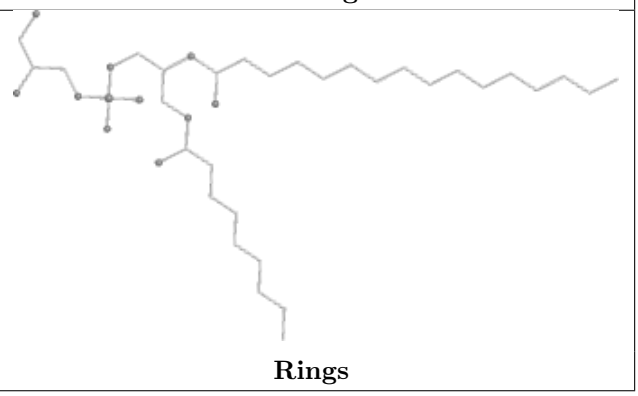
Bond lengths



Bond angles

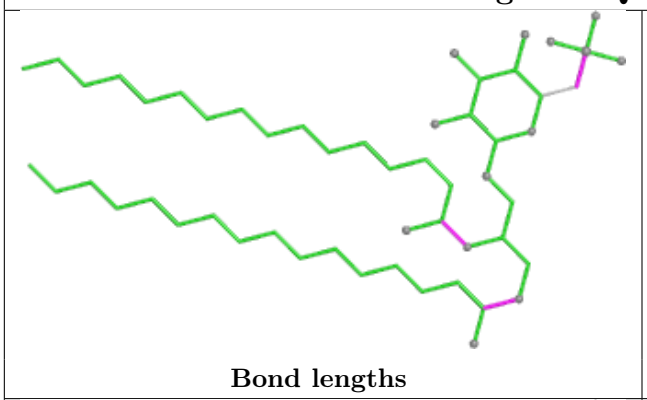


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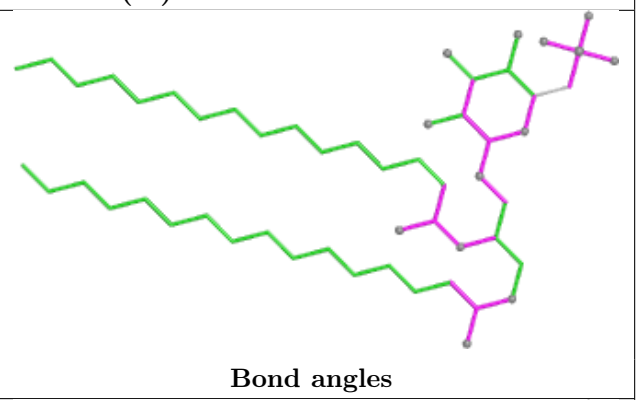


Rings

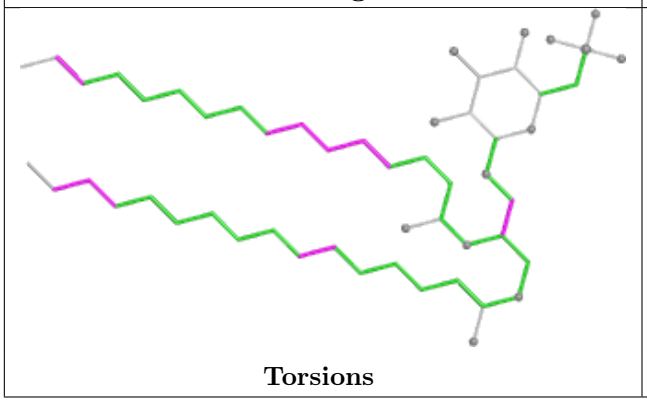
Ligand SQD a 411 (A)



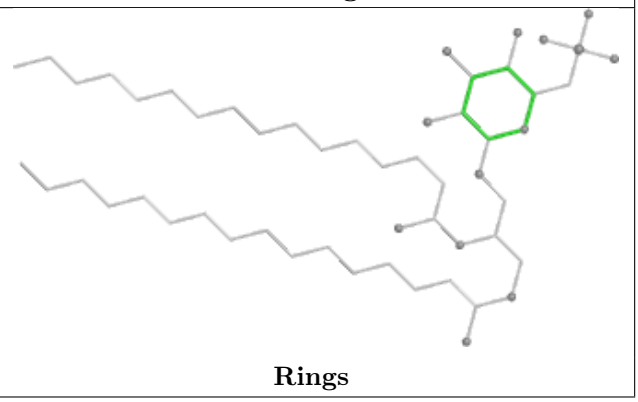
Bond lengths



Bond angles

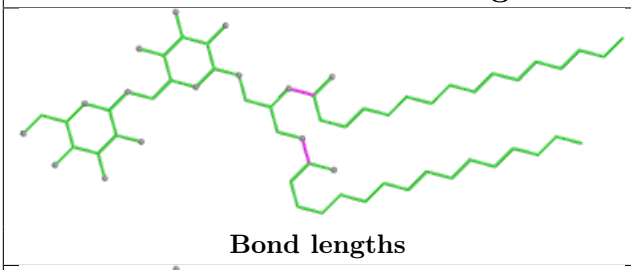


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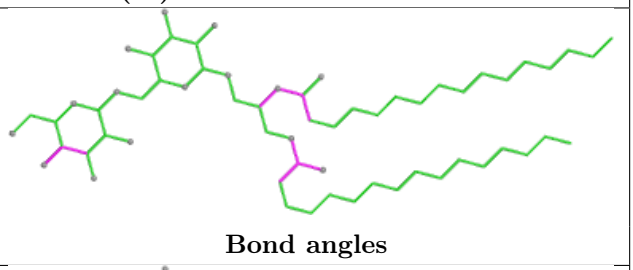


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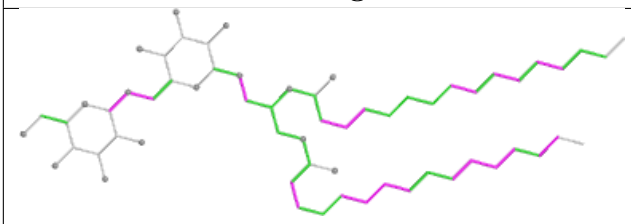
Ligand DGD c 518 (A)



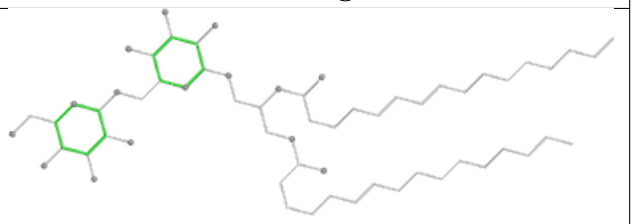
Bond lengths



Bond angles

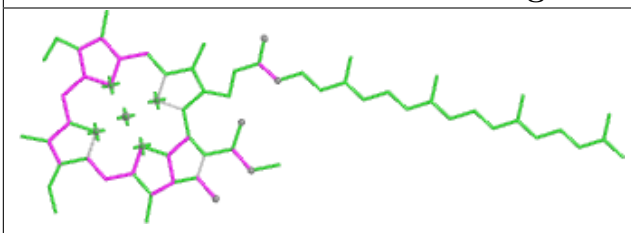


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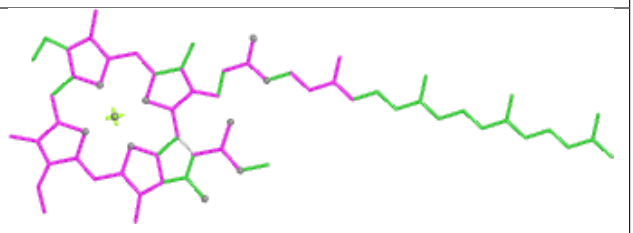


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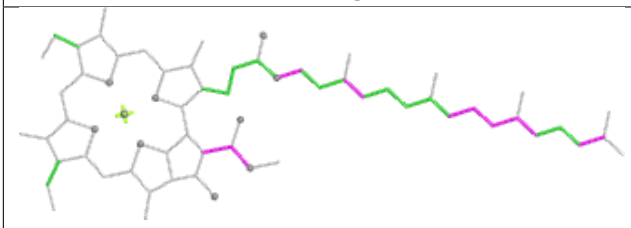
Ligand CLA b 614



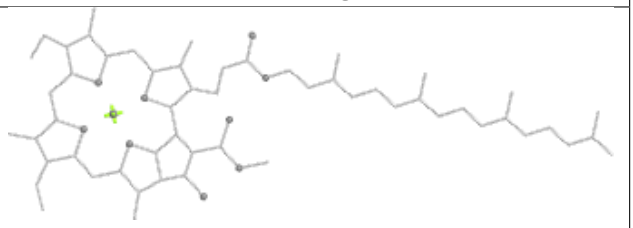
Bond lengths



Bond angles

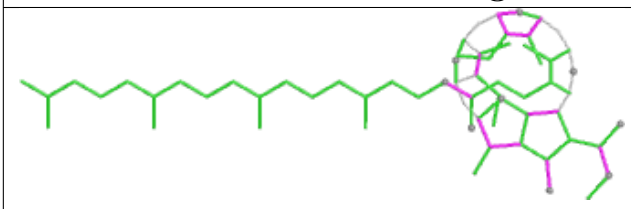


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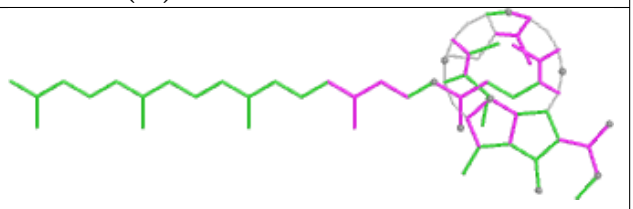


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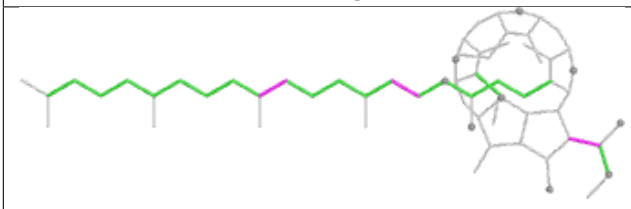
Ligand PHO A 407 (B)



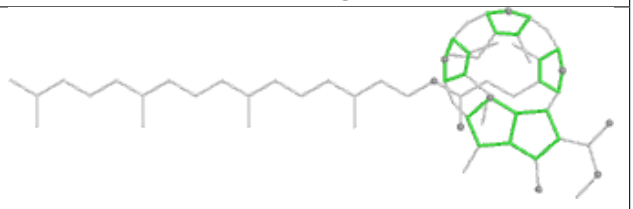
Bond lengths



Bond angles

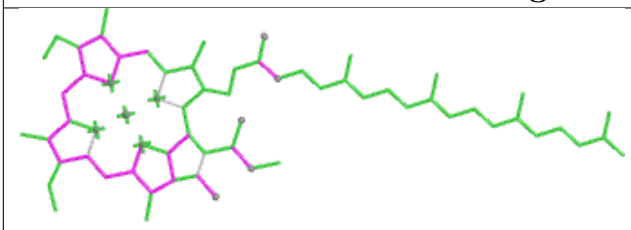


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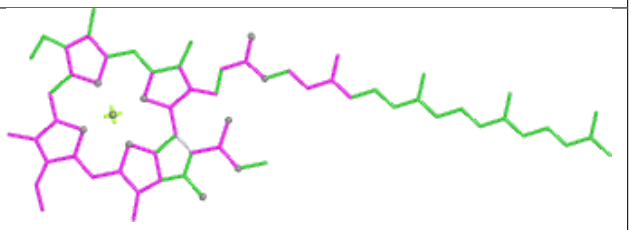


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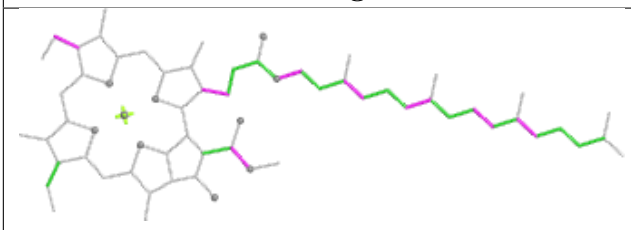
Ligand CLA c 514



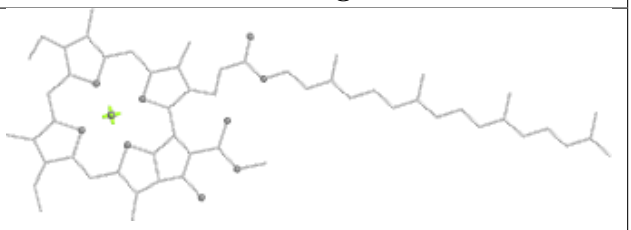
Bond lengths



Bond angles

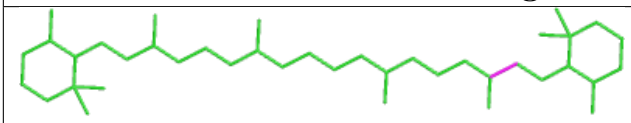


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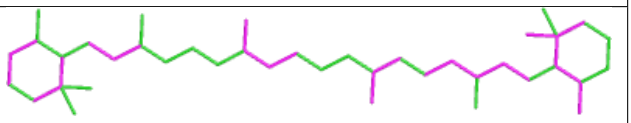


Rings

Ligand BCR K 102



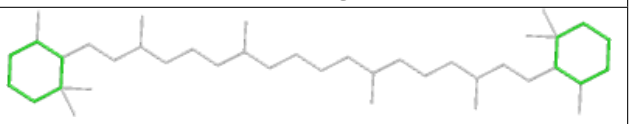
Bond lengths



Bond angles

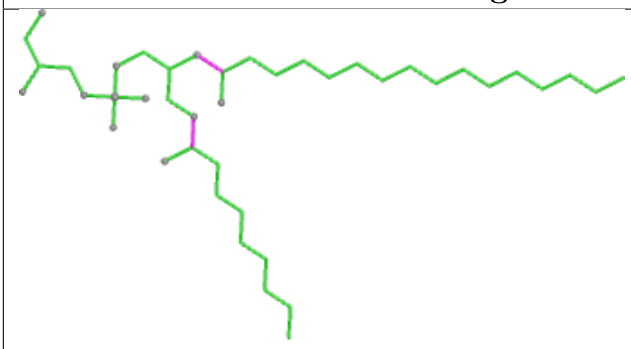


Torsions

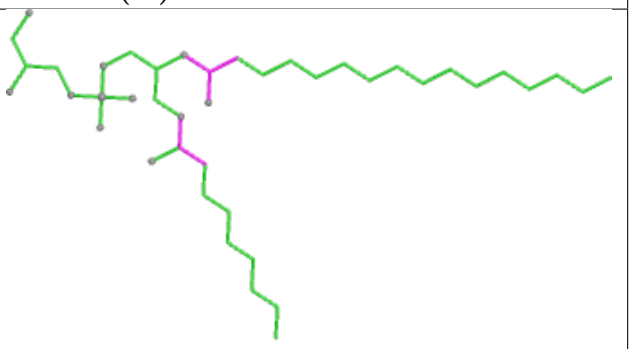


Rings

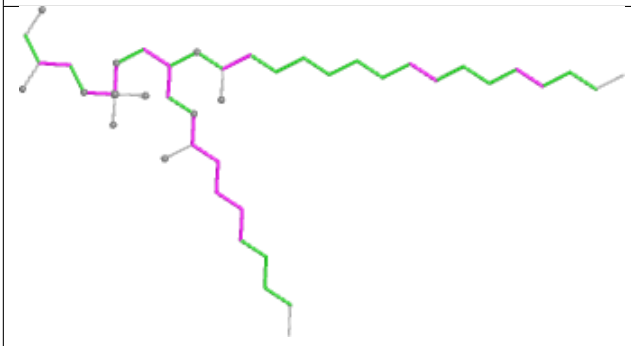
Ligand LHG E 101 (A)



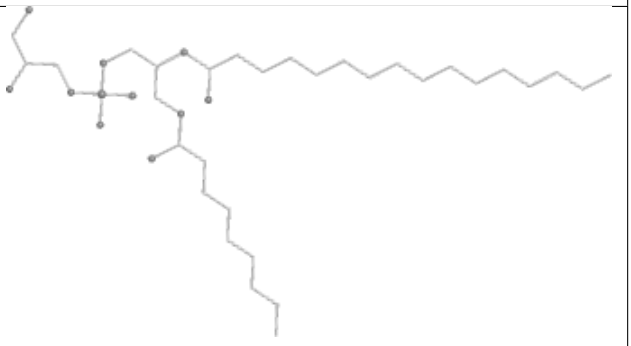
Bond lengths



Bond angles

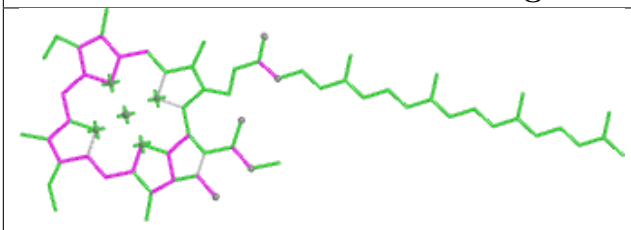


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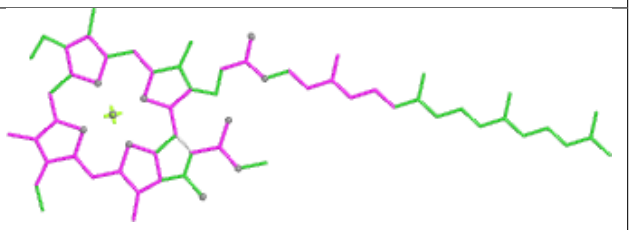


Rings

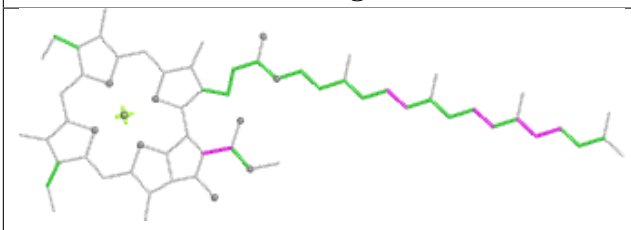
Ligand CLA C 509



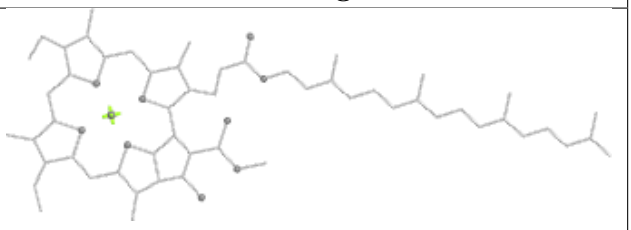
Bond lengths



Bond angles

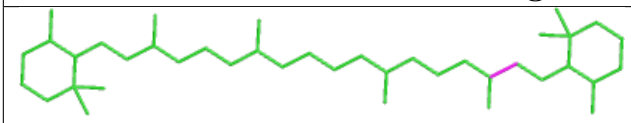


Torsions

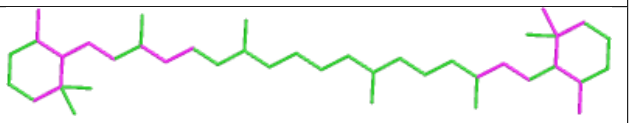


Rings

Ligand BCR a 410



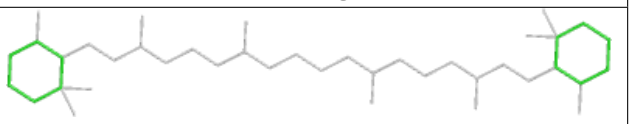
Bond lengths



Bond angles

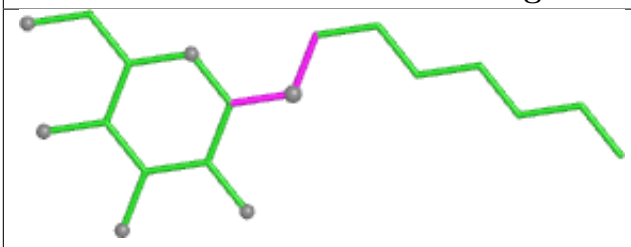


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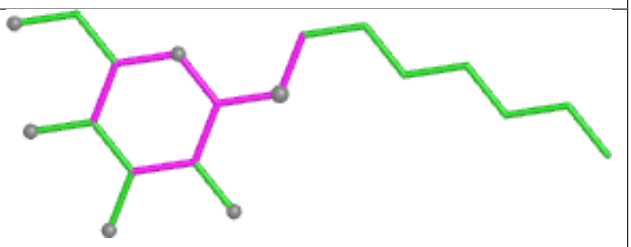


Rings

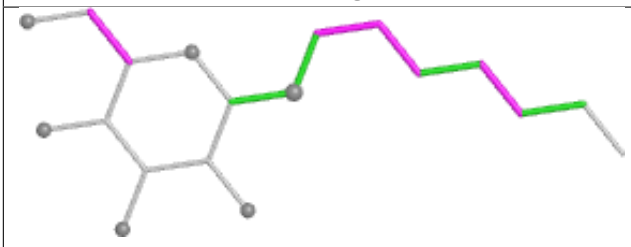
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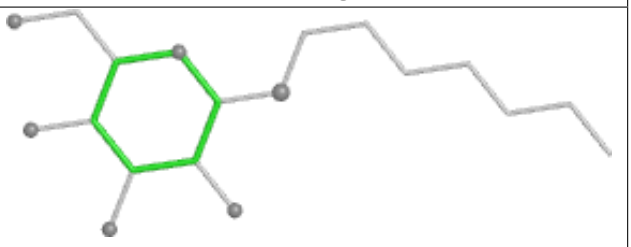
Bond lengths



Bond angles

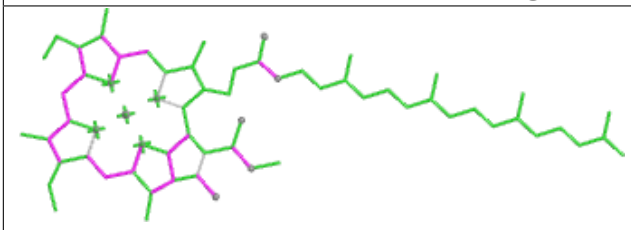


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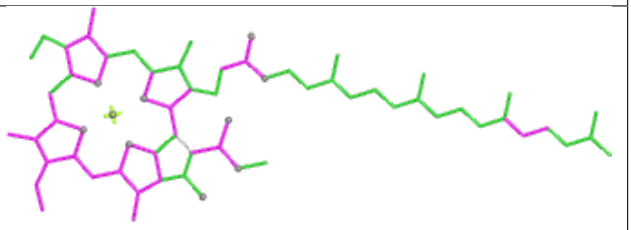


Rings

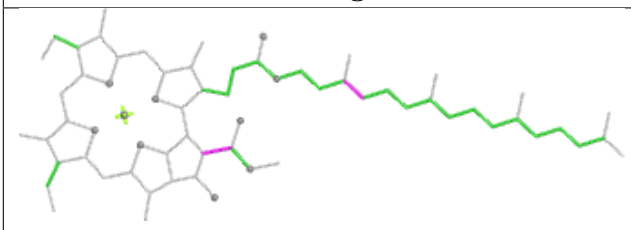
Ligand CLA B 609



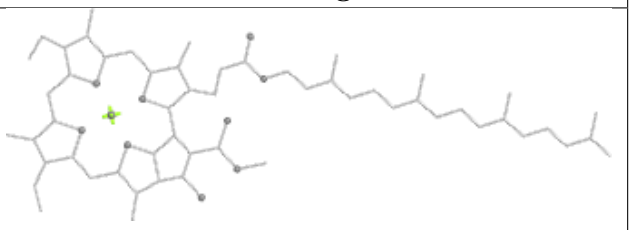
Bond lengths



Bond angles

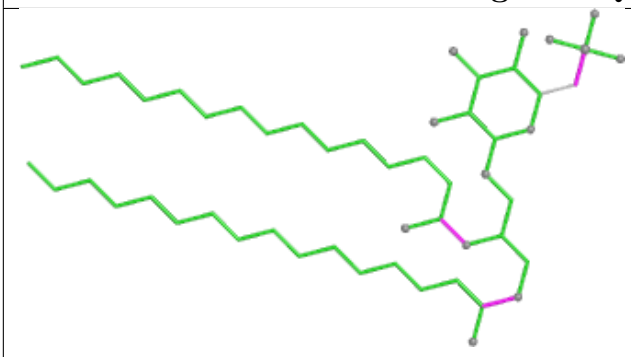


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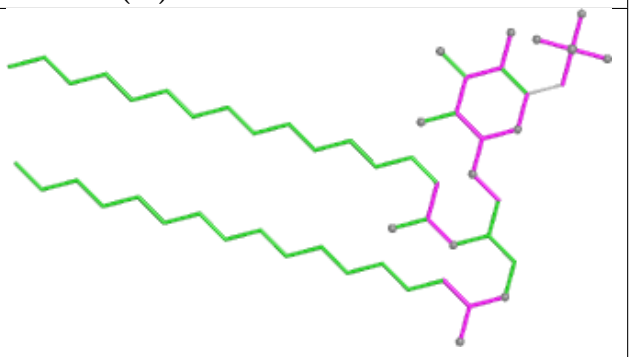


Rings

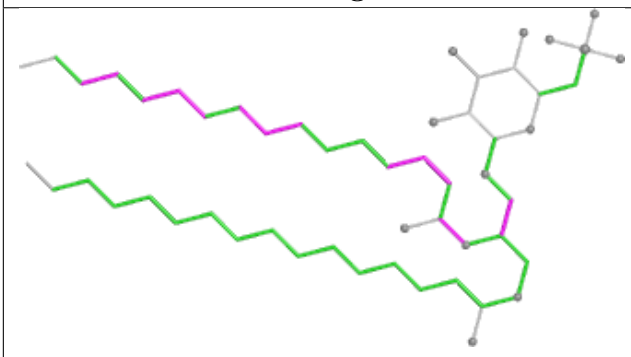
Ligand SQD A 410 (B)



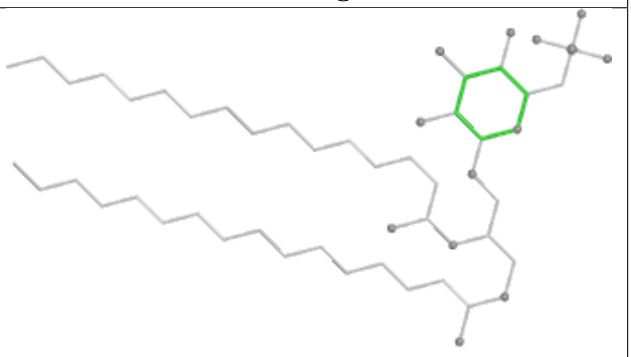
Bond lengths



Bond angles

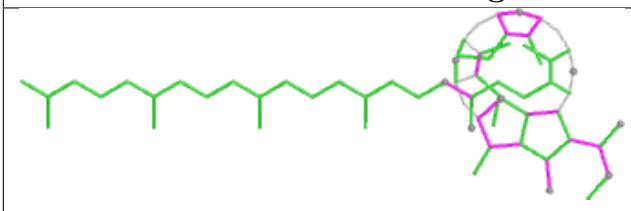


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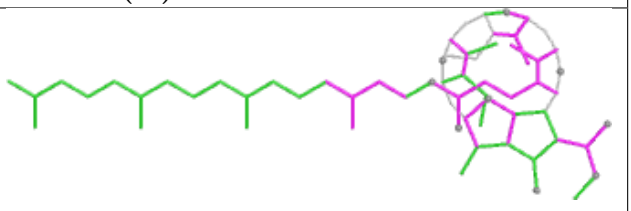


Rings

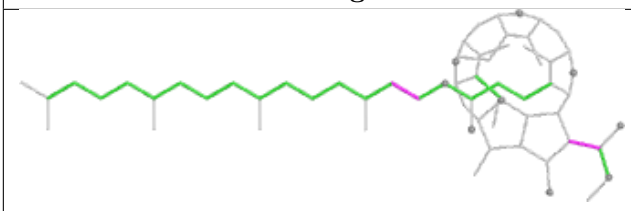
Ligand PHO A 407 (A)



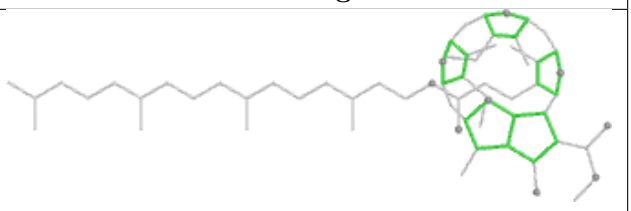
Bond lengths



Bond angles

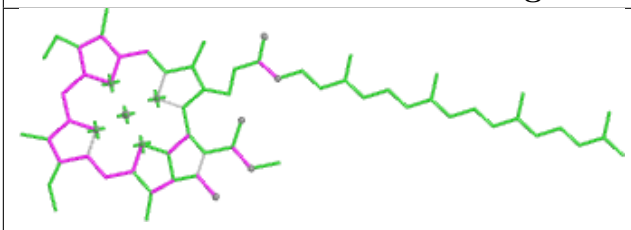


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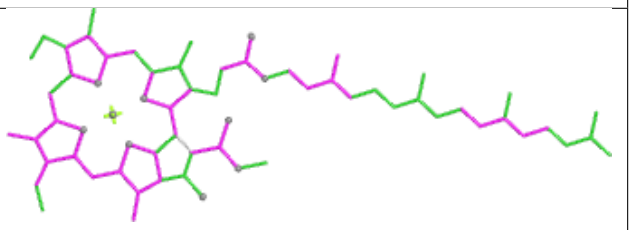


Rings

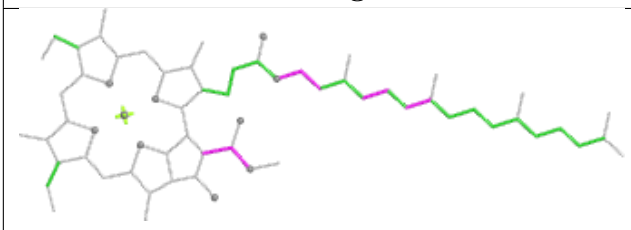
Ligand CLA C 510



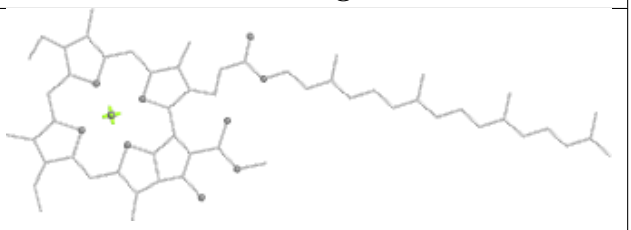
Bond lengths



Bond angles

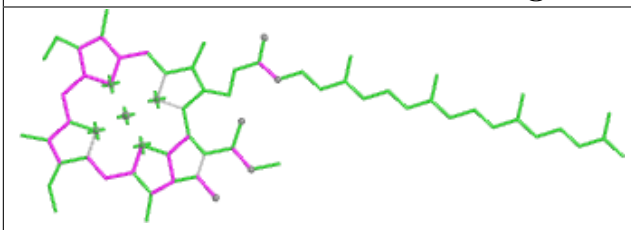


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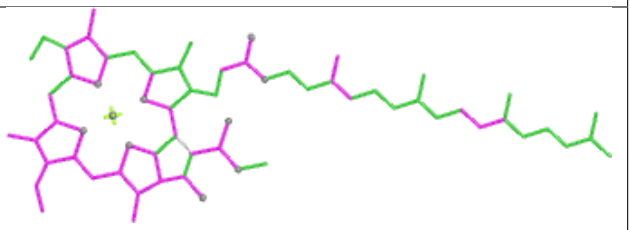


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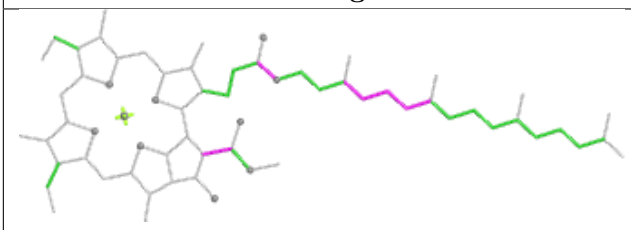
Ligand CLA b 616



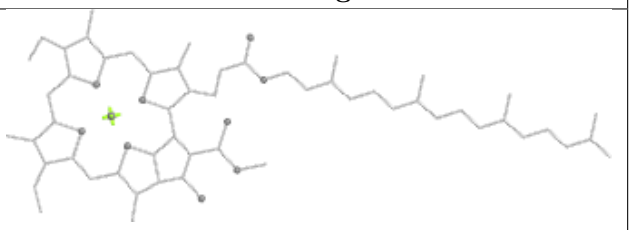
Bond lengths



Bond angles

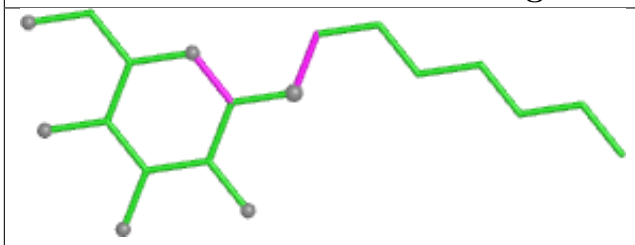


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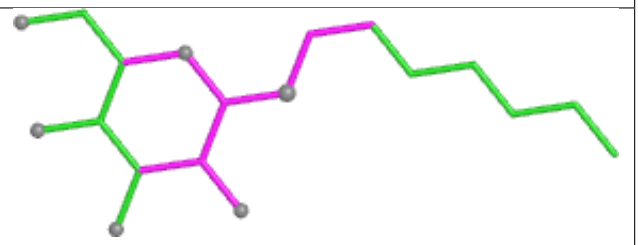


Rings

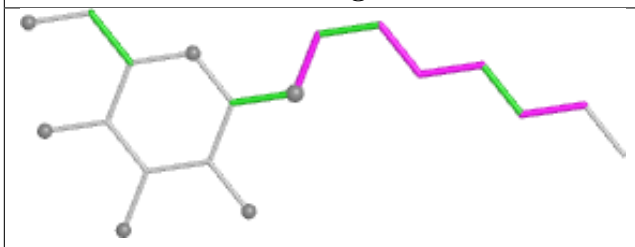
Ligand HTG o 301



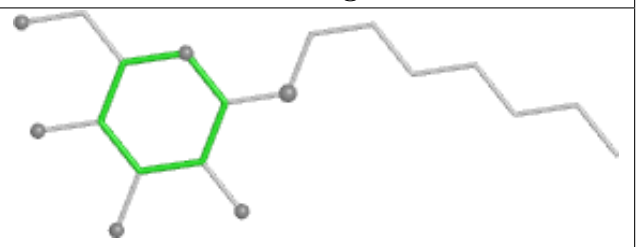
Bond lengths



Bond angles

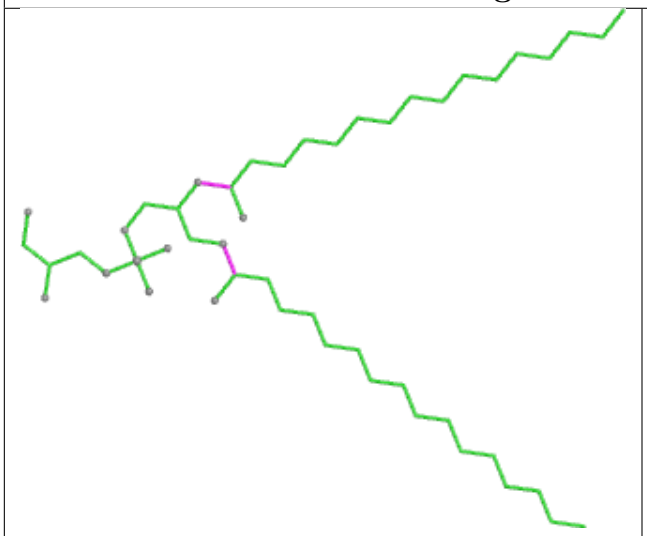


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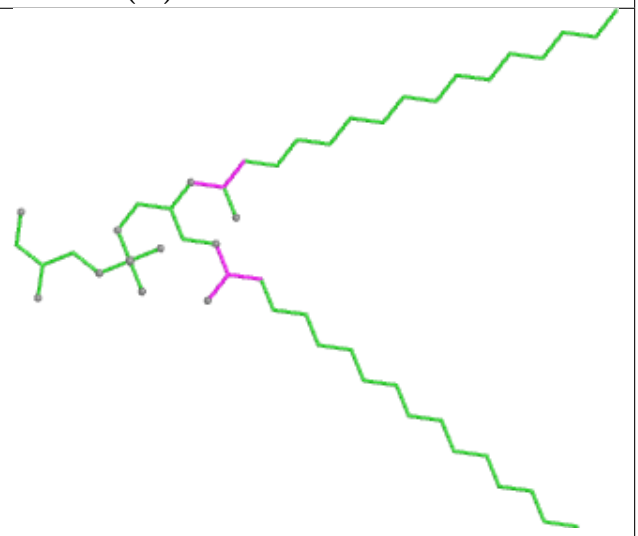


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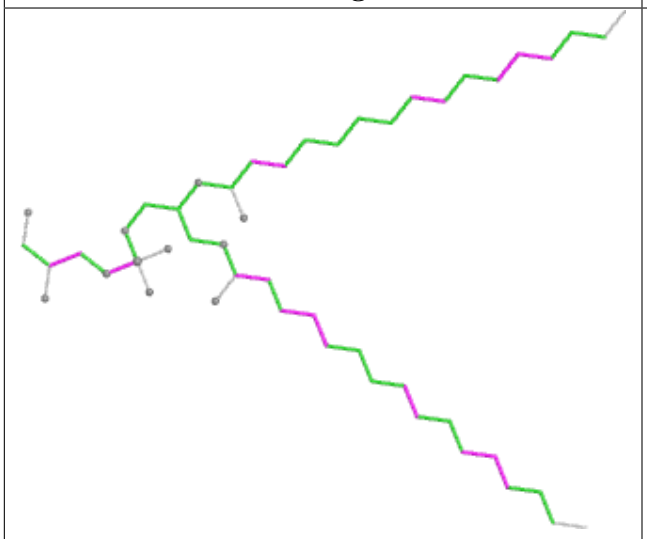
Ligand LHG d 412 (B)



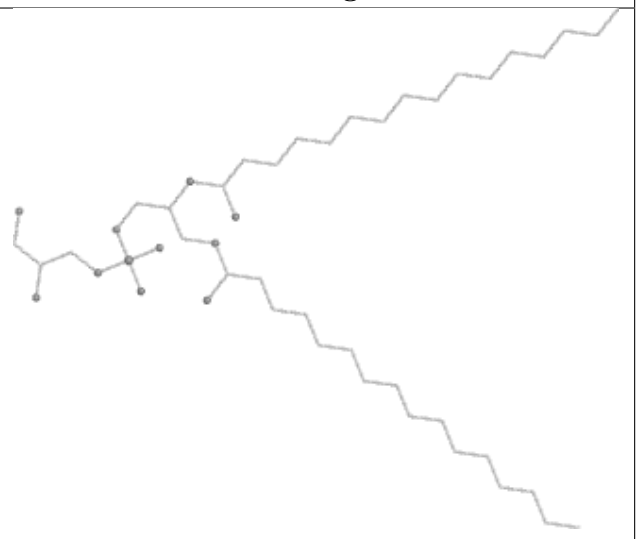
Bond lengths



Bond angles



Torsions

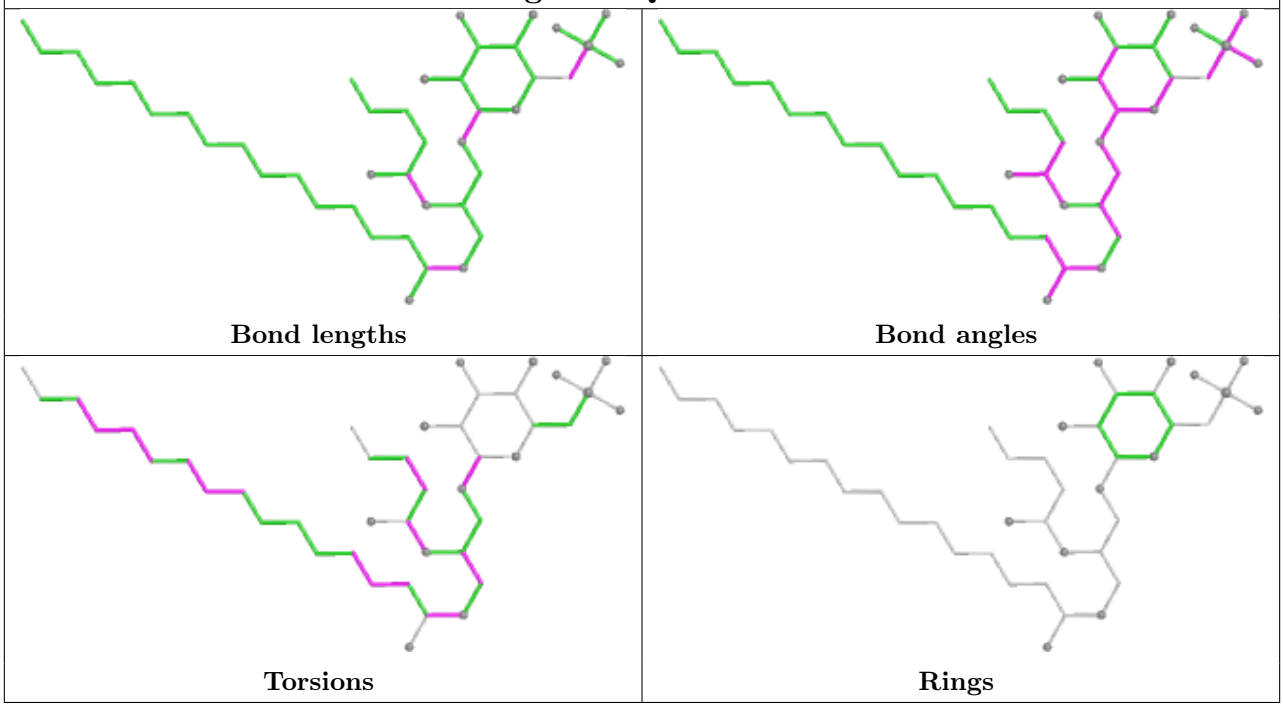


Rings

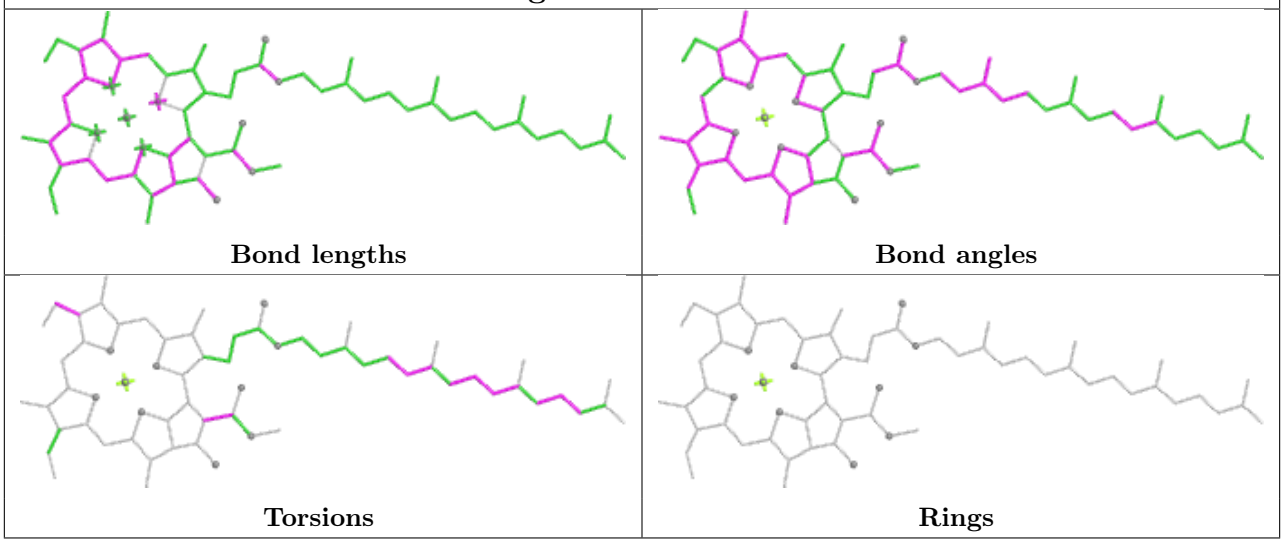
Ligand PL9 D 705 (B)



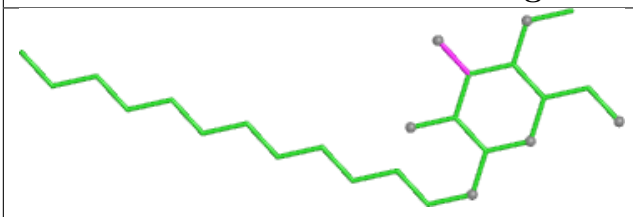
Ligand SQD X 101

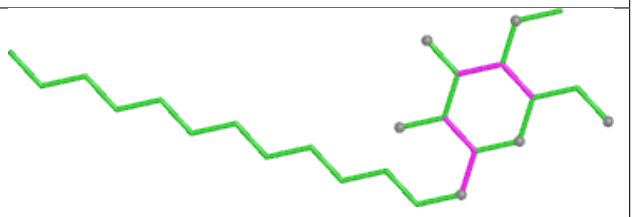


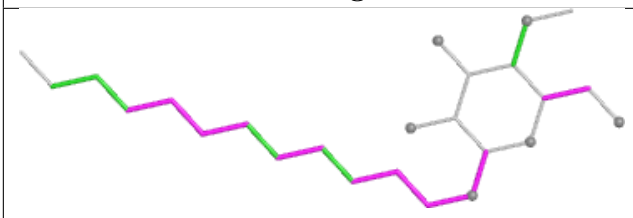
Ligand CLA b 604

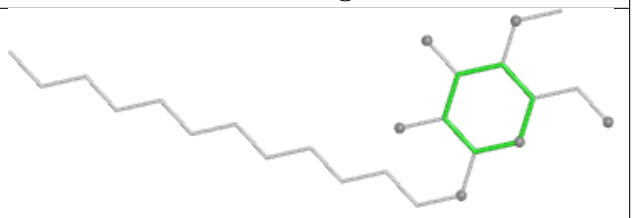


Ligand LMT b 627

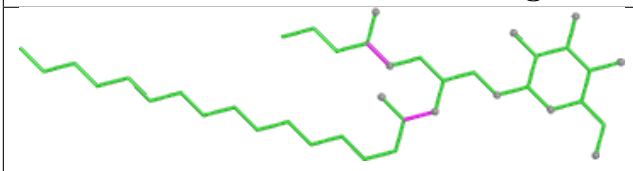

Bond lengths

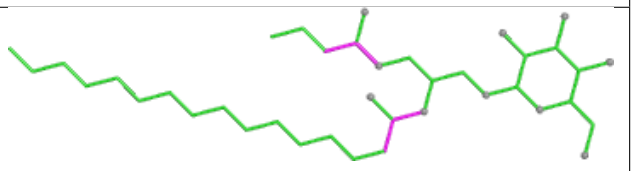

Bond angles

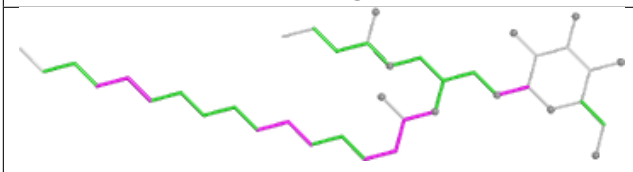

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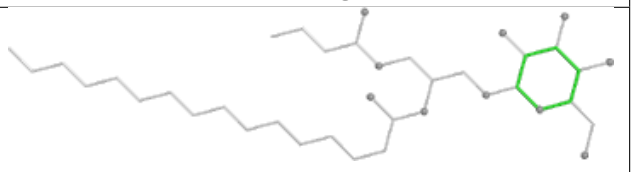

Rings

Ligand LMG z 101

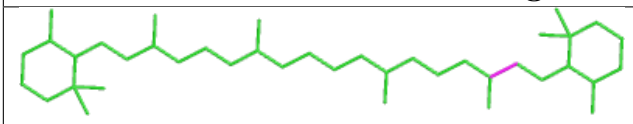

Bond lengths

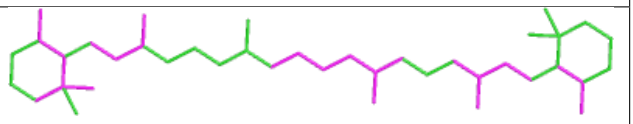

Bond angles

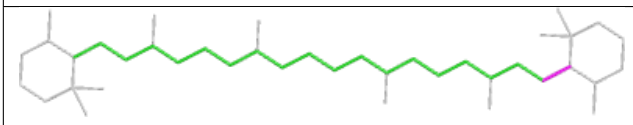

Torsions

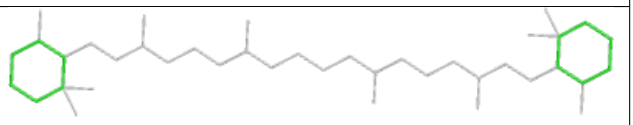

Rings

Ligand BCR h 101

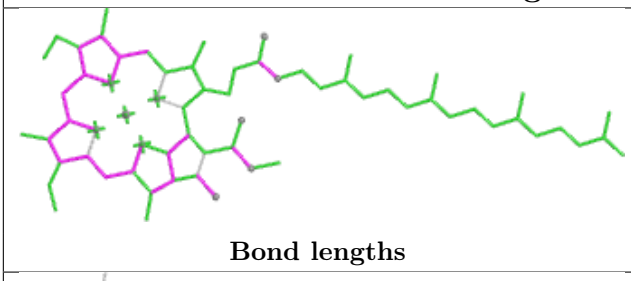

Bond lengths


Bond angles

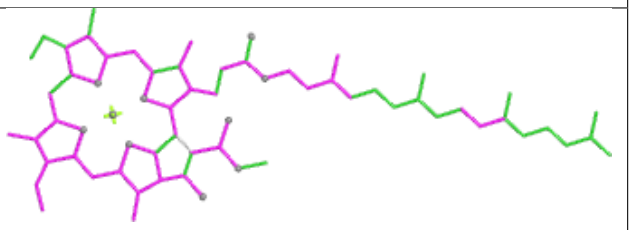

Torsions


Rings

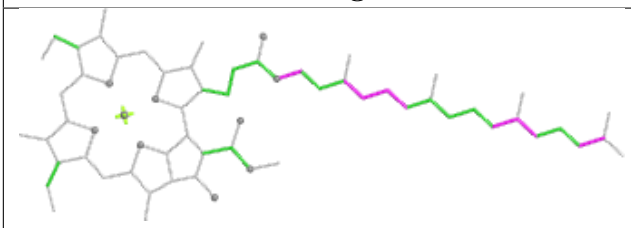
Ligand CLA A 408



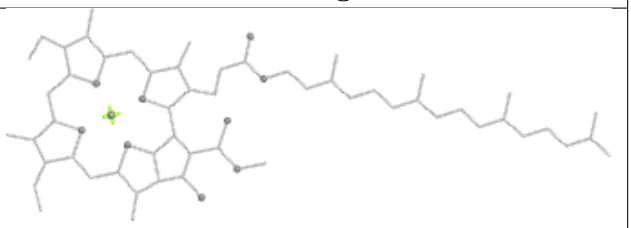
Bond lengths



Bond angles

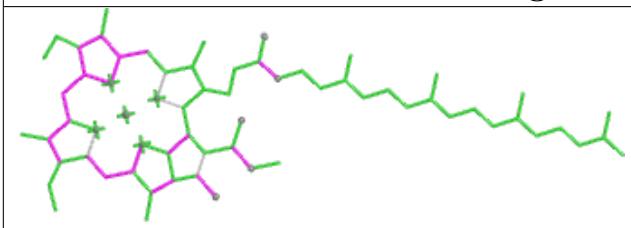


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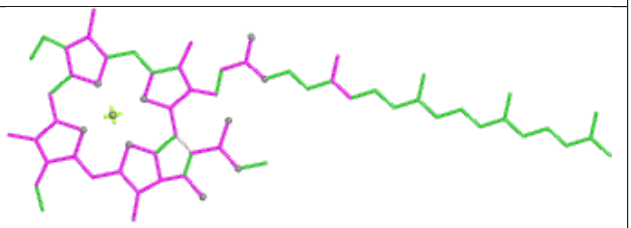


Rings

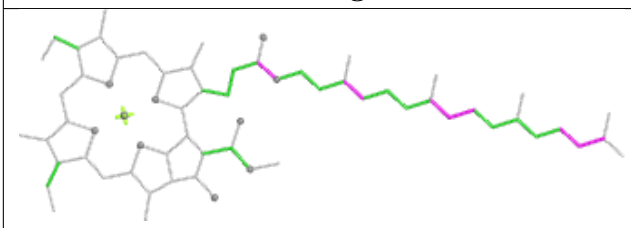
Ligand CLA a 409



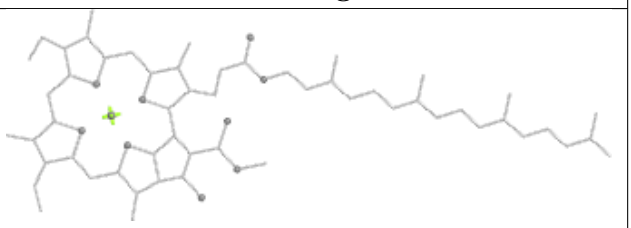
Bond lengths



Bond angles

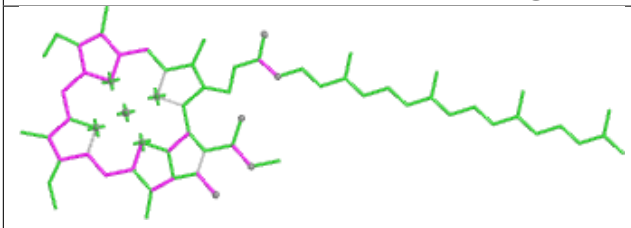


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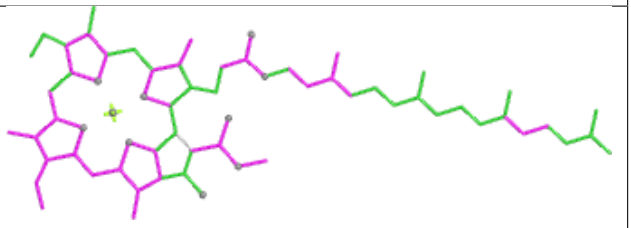


Rings

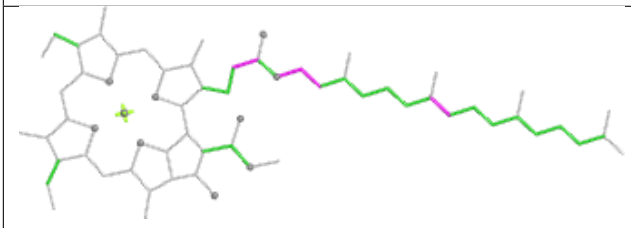
Ligand CLA b 613



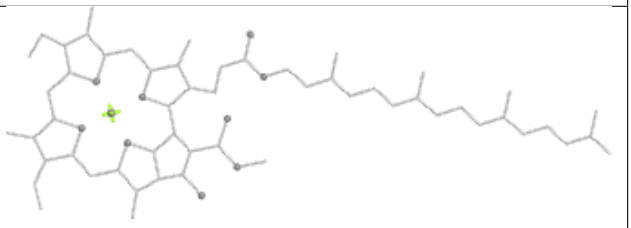
Bond lengths



Bond angles

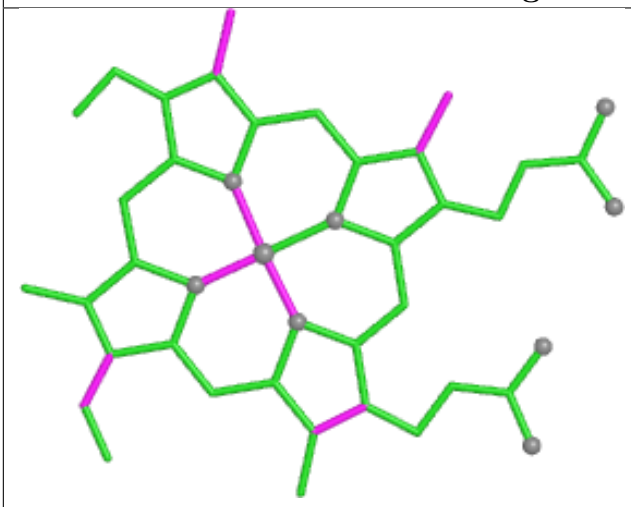


Torsions

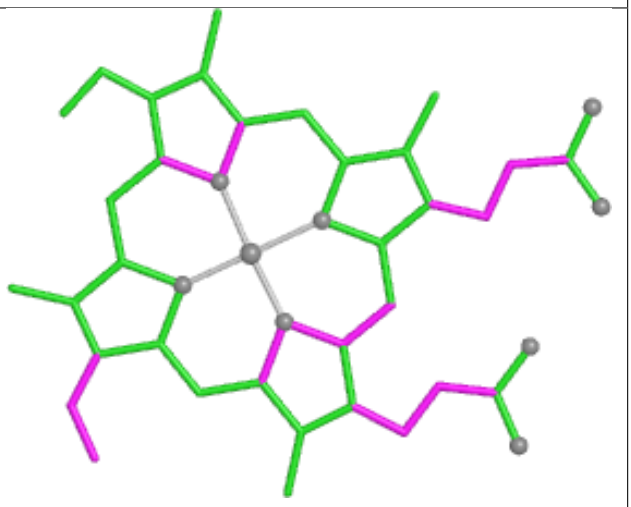


Rings

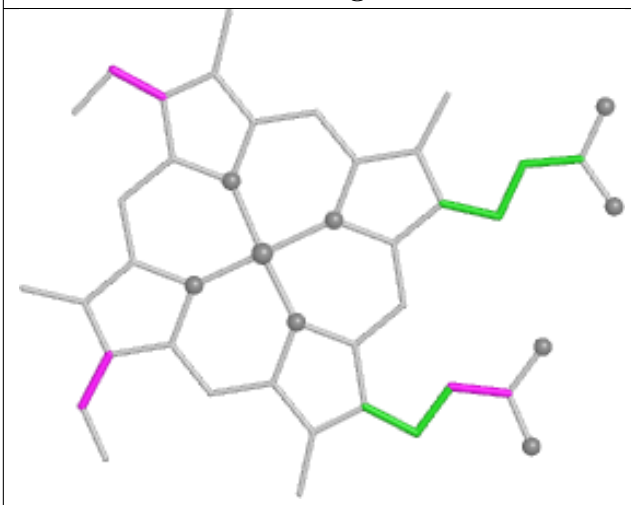
Ligand HEC V 201



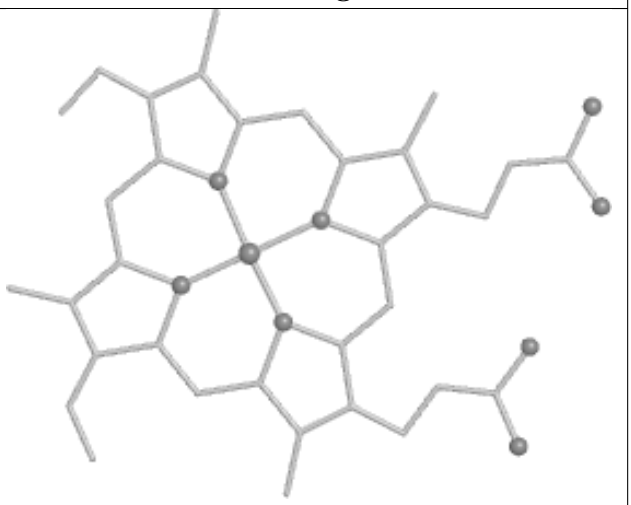
Bond lengths



Bond angles

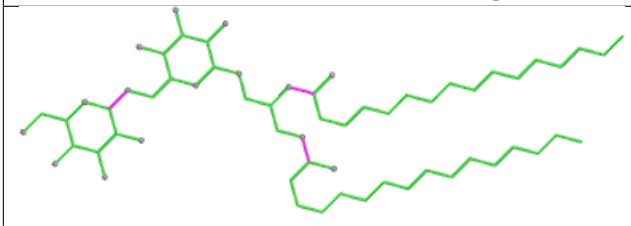


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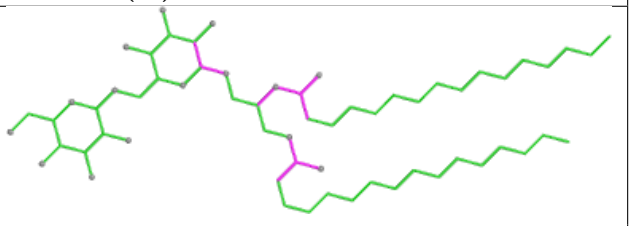


Rings

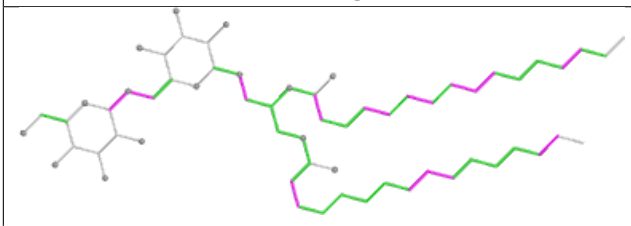
Ligand DGD C 518 (B)



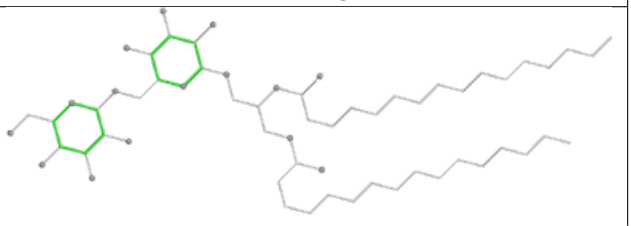
Bond lengths



Bond angles

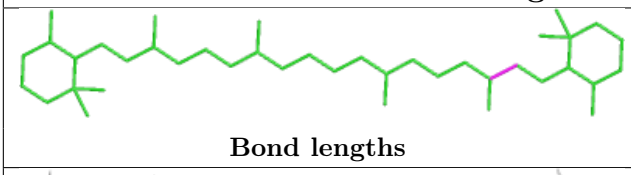


Torsions

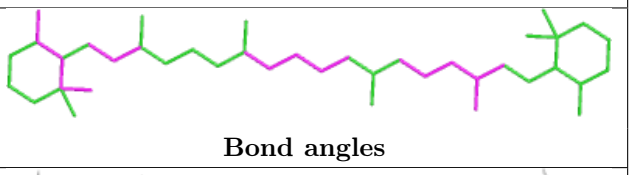


Rings

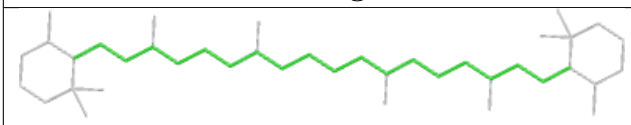
Ligand BCR c 516



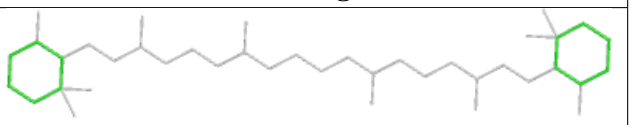
Bond lengths



Bond angles

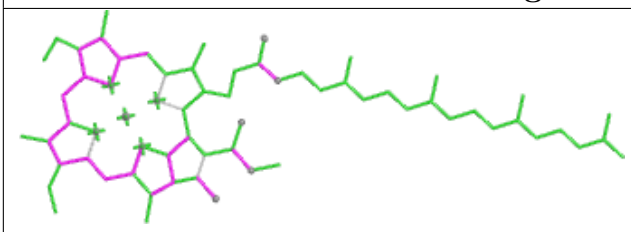


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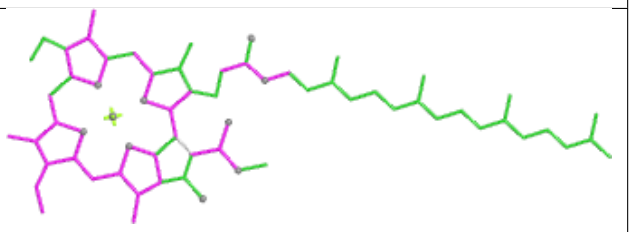


Rings

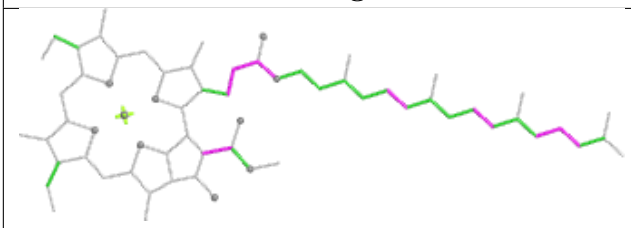
Ligand CLA B 601



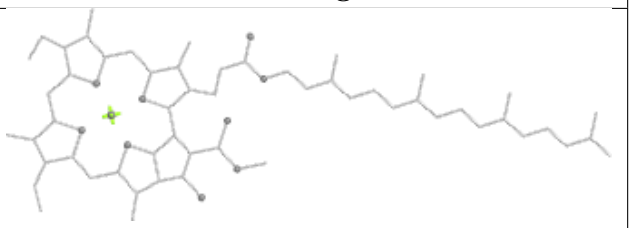
Bond lengths



Bond angles

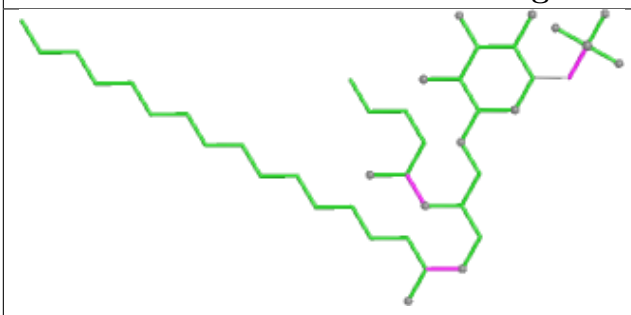


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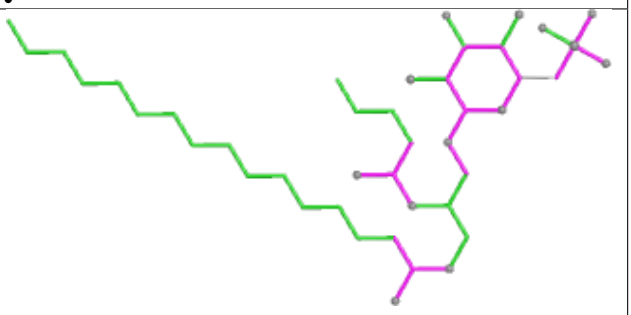


Rings

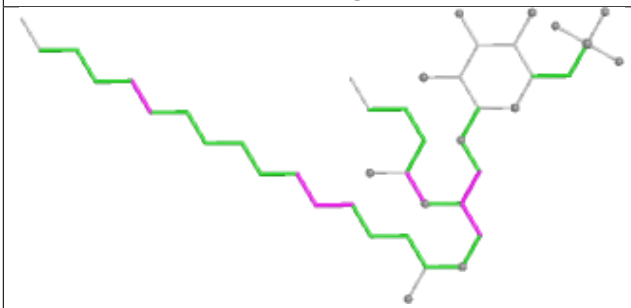
Ligand SQD f 102



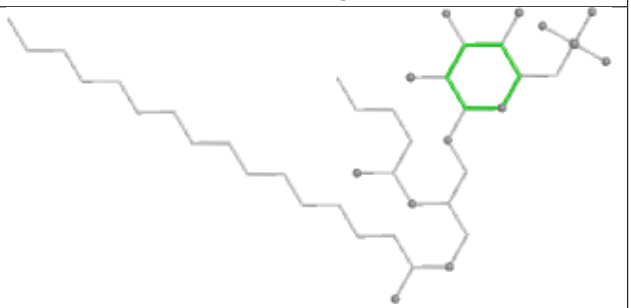
Bond lengths



Bond angles

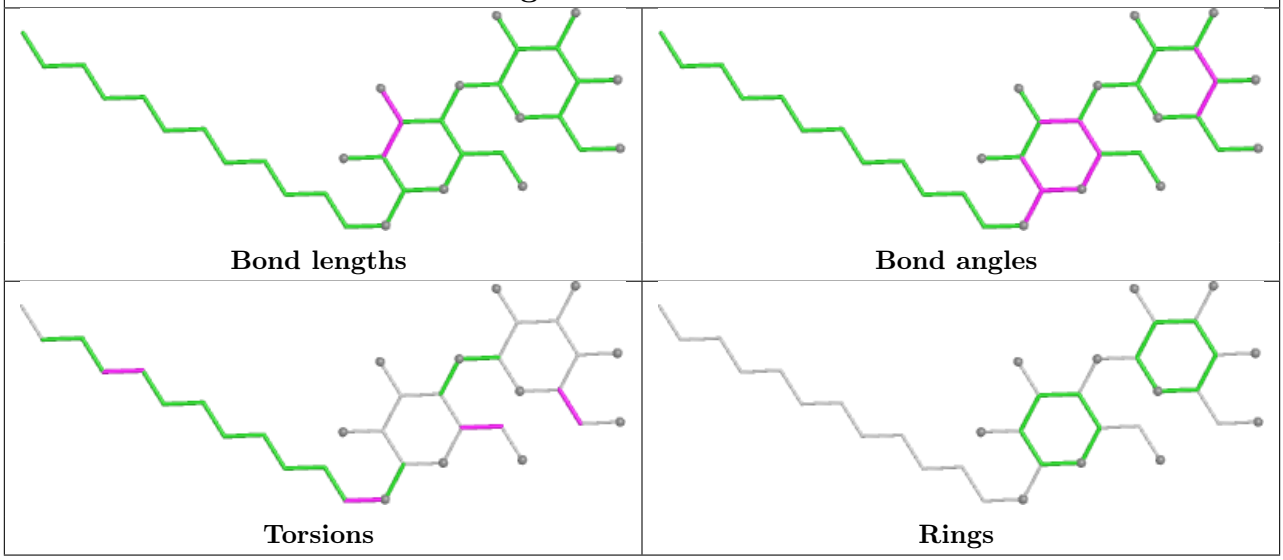


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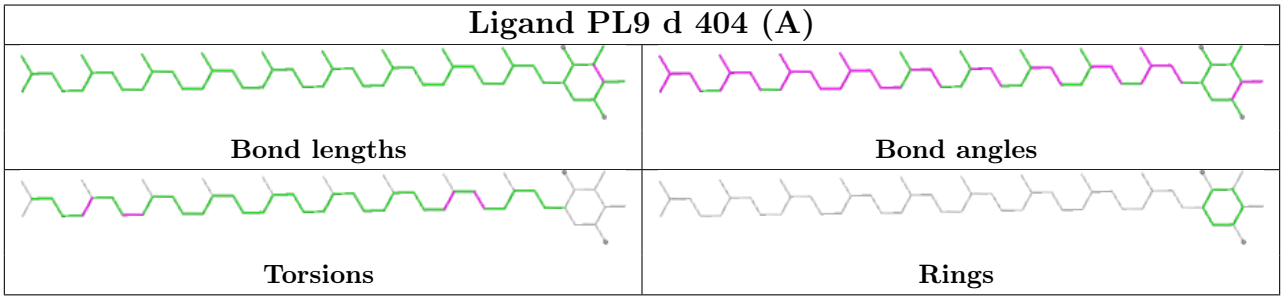


Rings

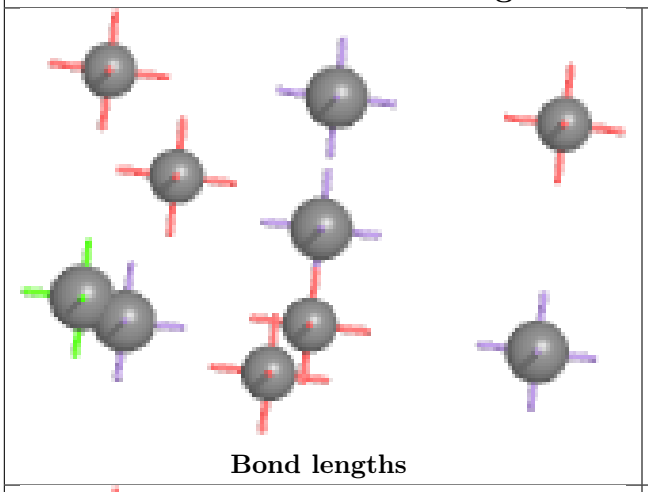
Ligand LMT m 103



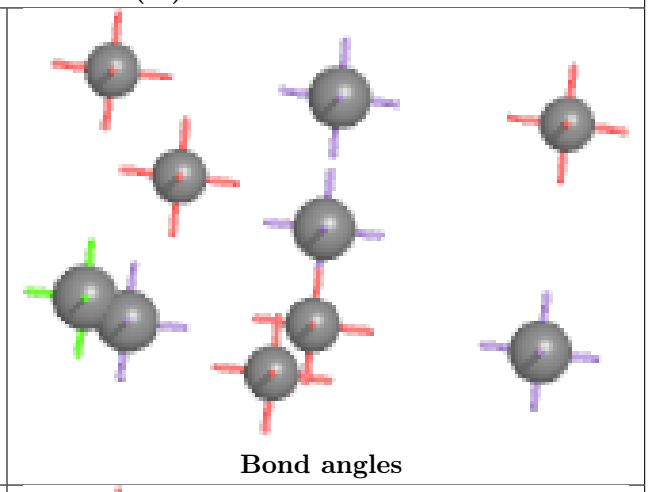
Ligand PL9 d 404 (A)



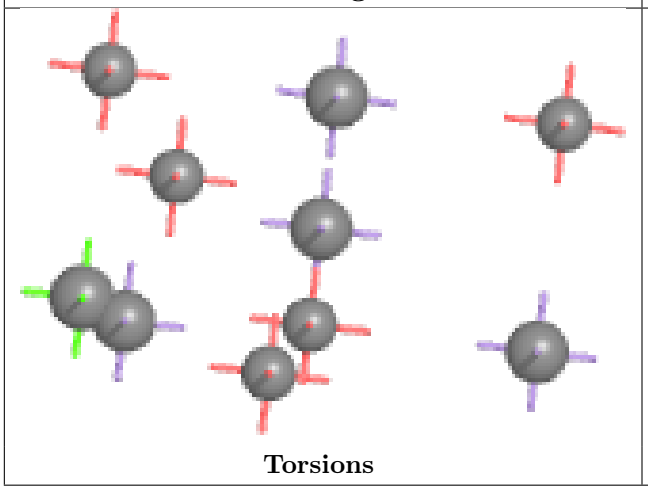
Ligand OEX a 413 (B)



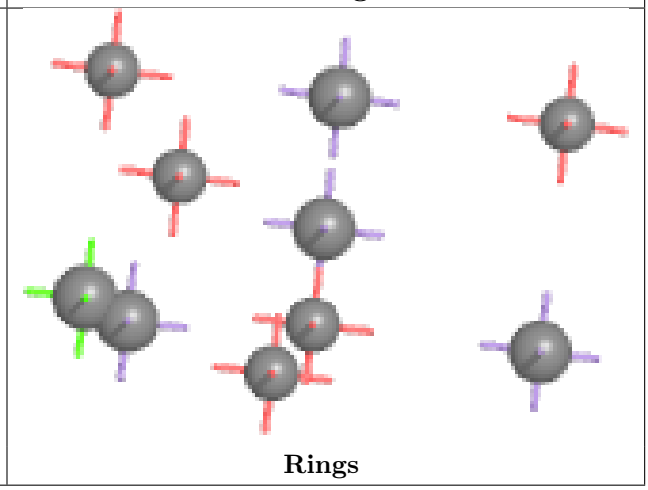
Bond lengths



Bond angles

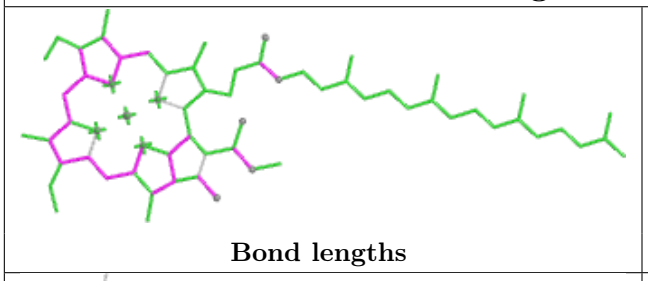


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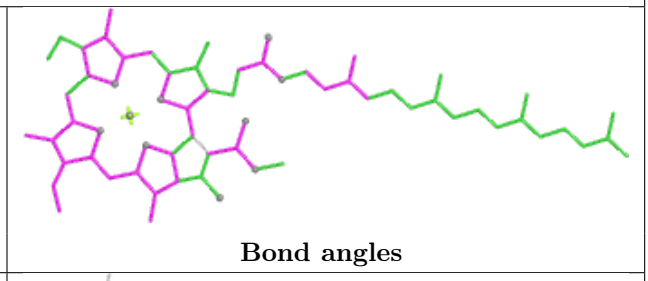


Rings

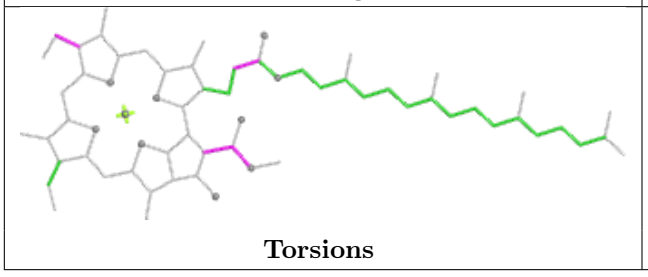
Ligand CLA c 502



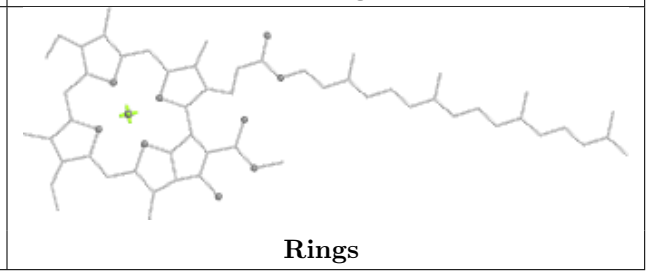
Bond lengths



Bond angles

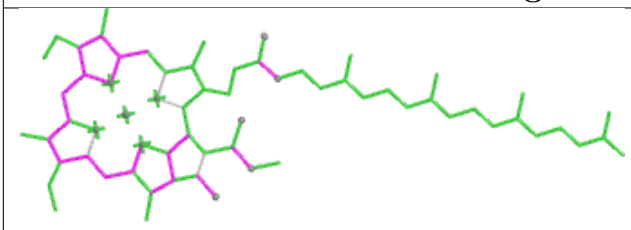


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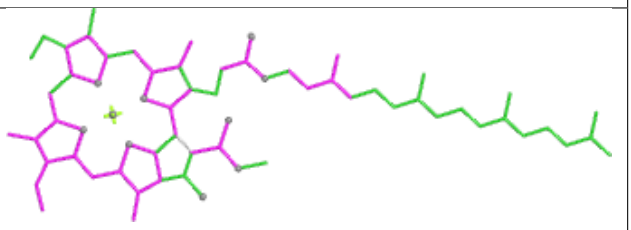


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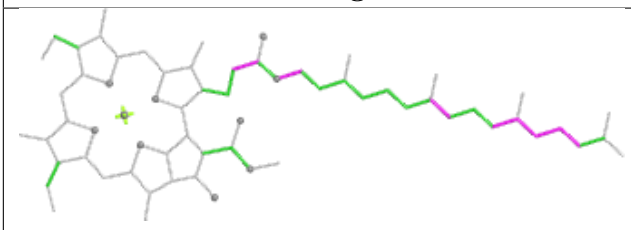
Ligand CLA B 613



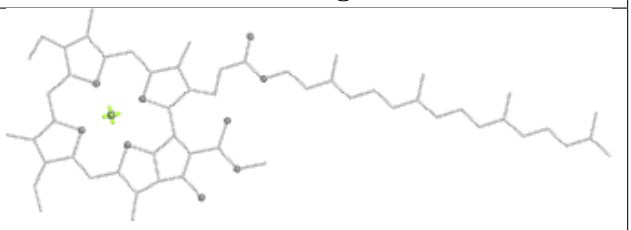
Bond lengths



Bond angles

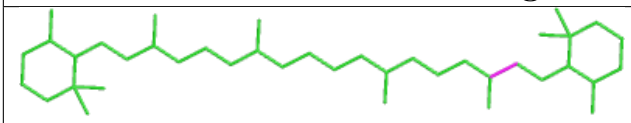


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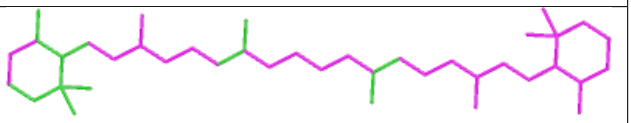


Rings

Ligand BCR D 704



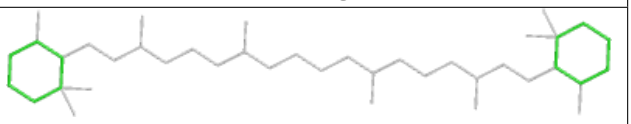
Bond lengths



Bond angles

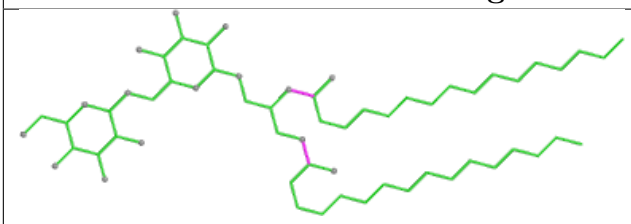


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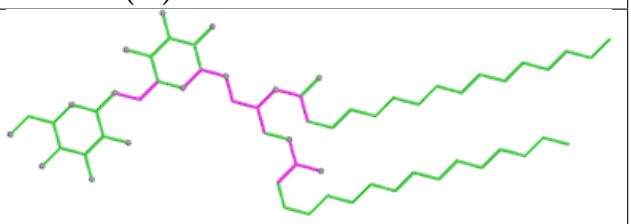


Rings

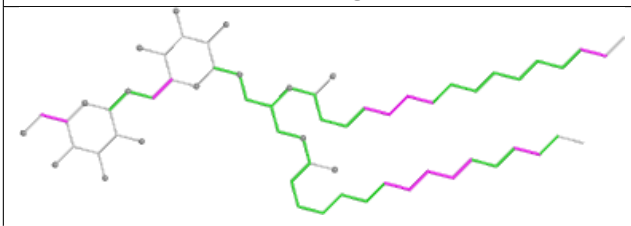
Ligand DGD C 517 (B)



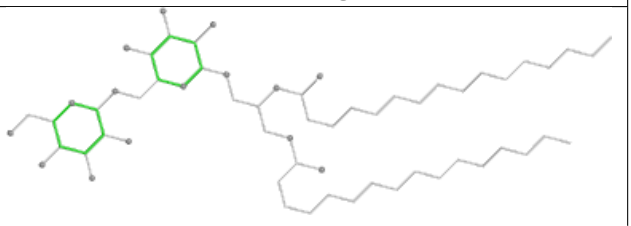
Bond lengths



Bond angles

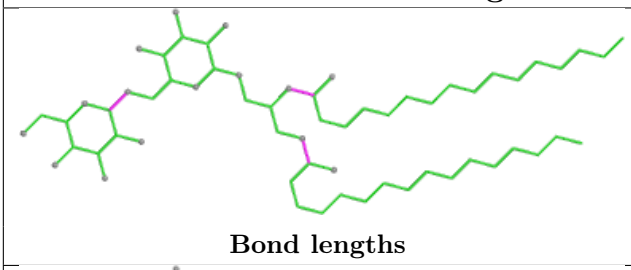


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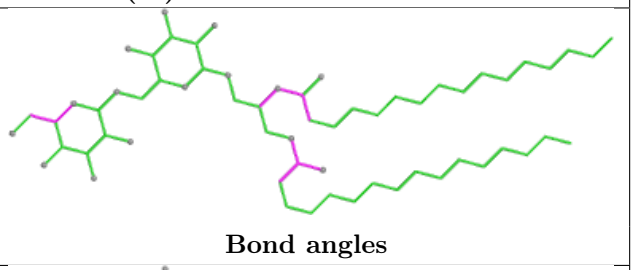


Rings

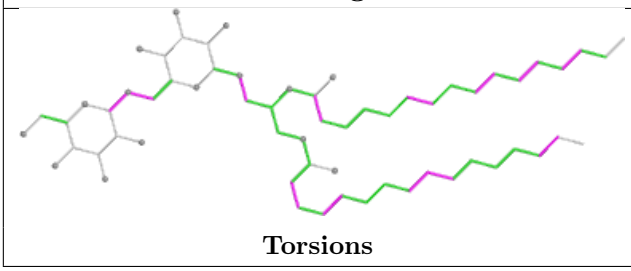
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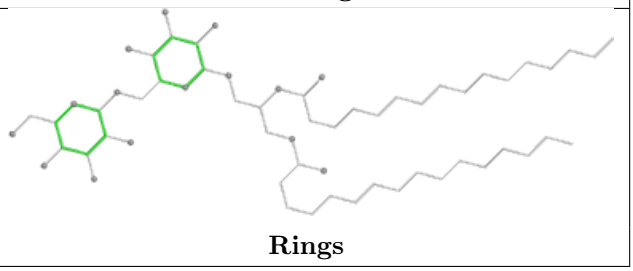
Bond lengths



Bond angles

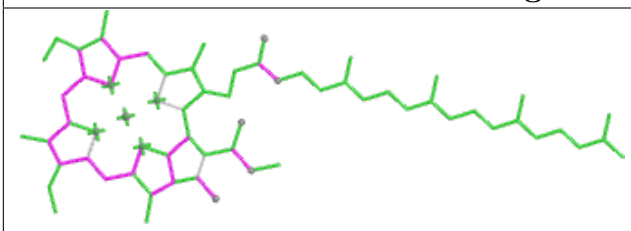


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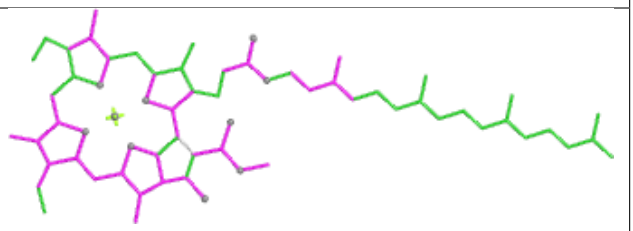


Rings

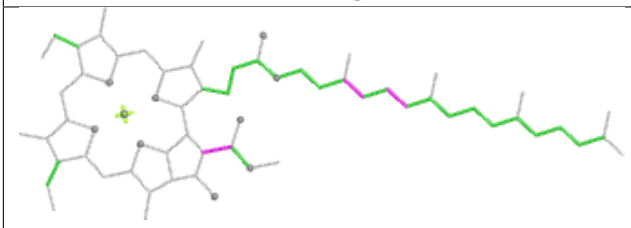
Ligand CLA B 605



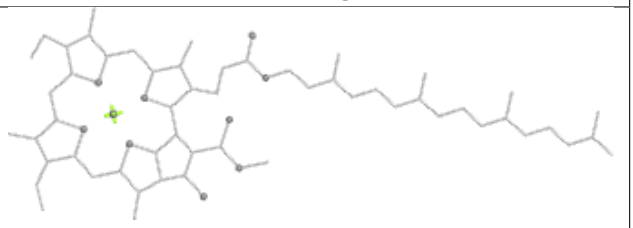
Bond lengths



Bond angles

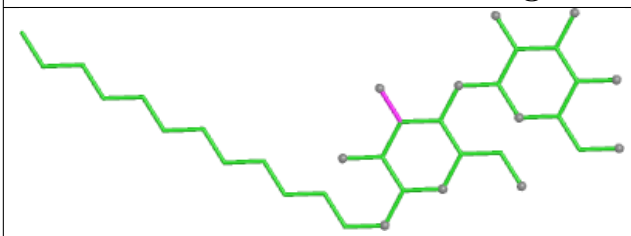


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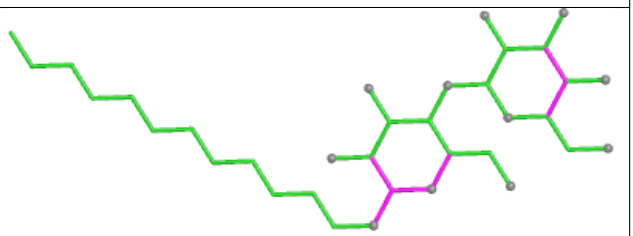


Rings

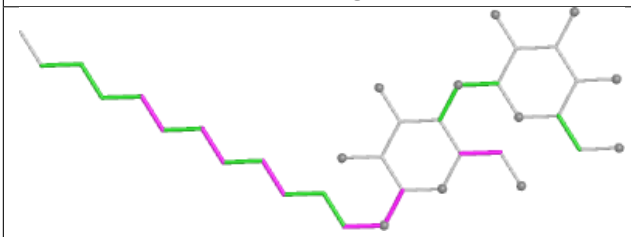
Ligand LMT F 101



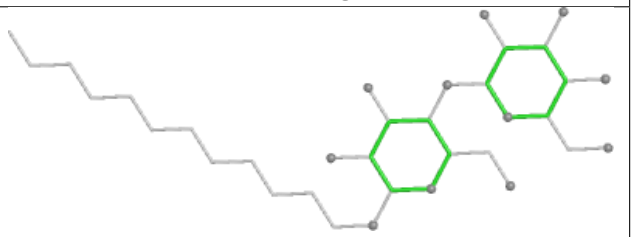
Bond lengths



Bond angles

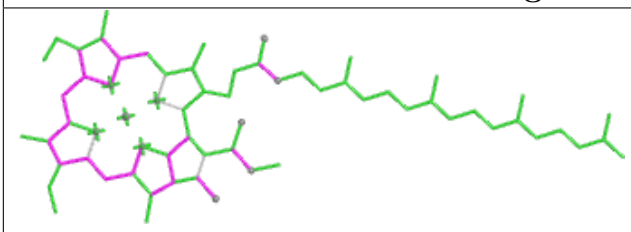


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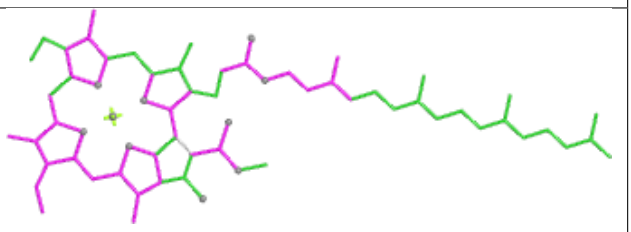


Rings

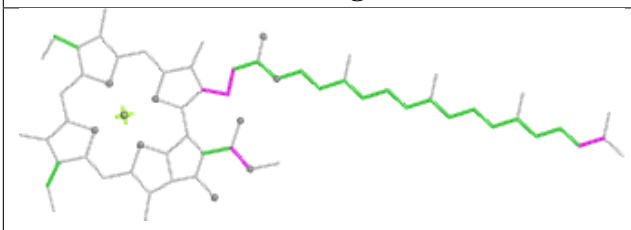
Ligand CLA C 502



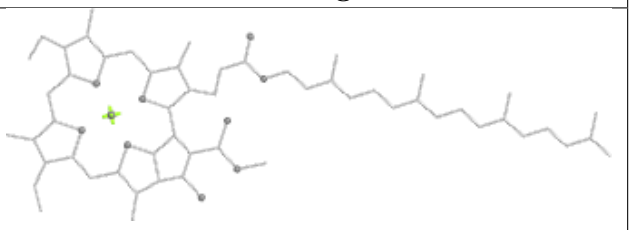
Bond lengths



Bond angles

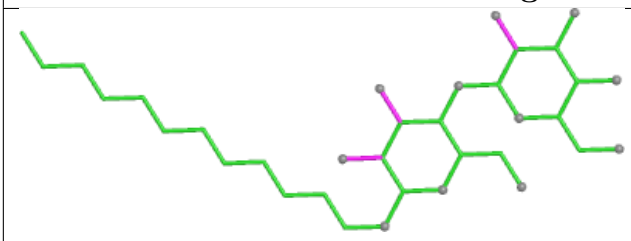


Torsions

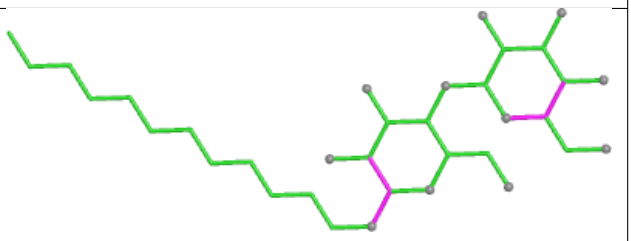


Rings

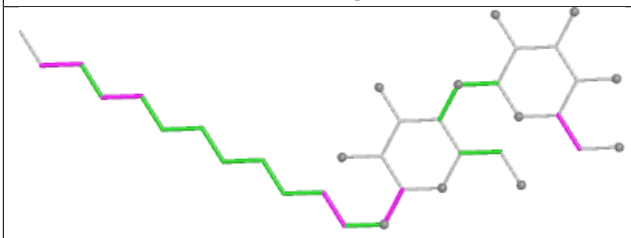
Ligand LMT A 418



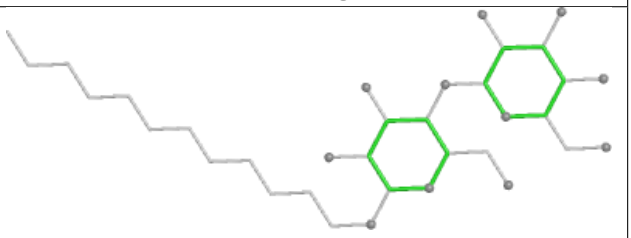
Bond lengths



Bond angles

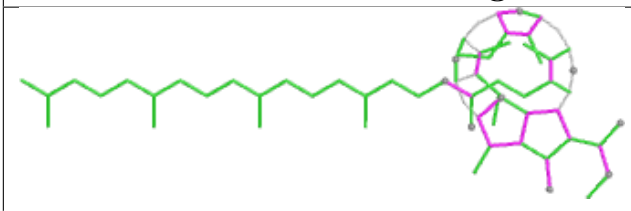


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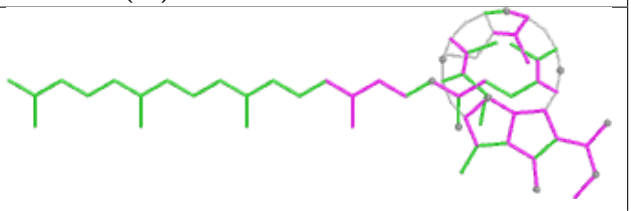


Rings

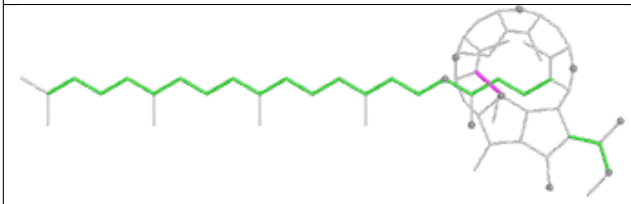
Ligand PHO A 417 (B)



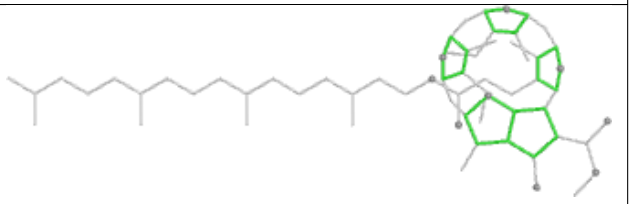
Bond lengths



Bond angles

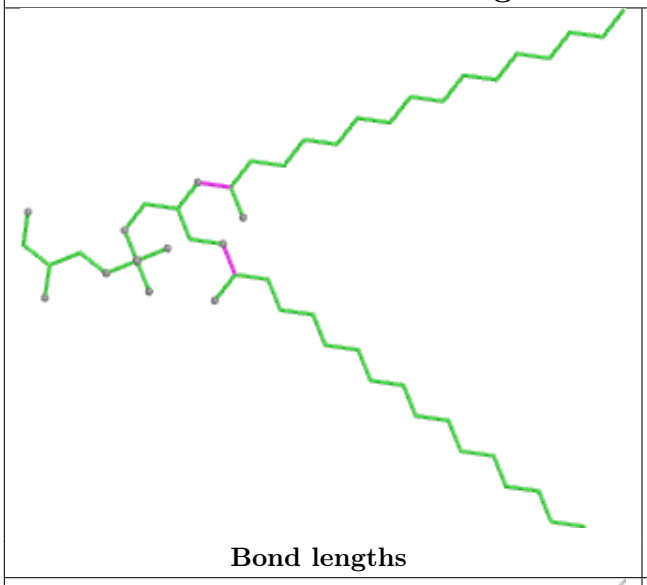


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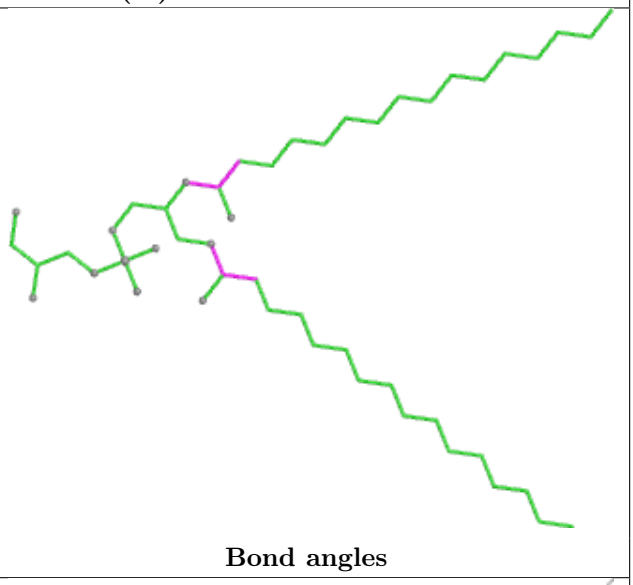


Rings

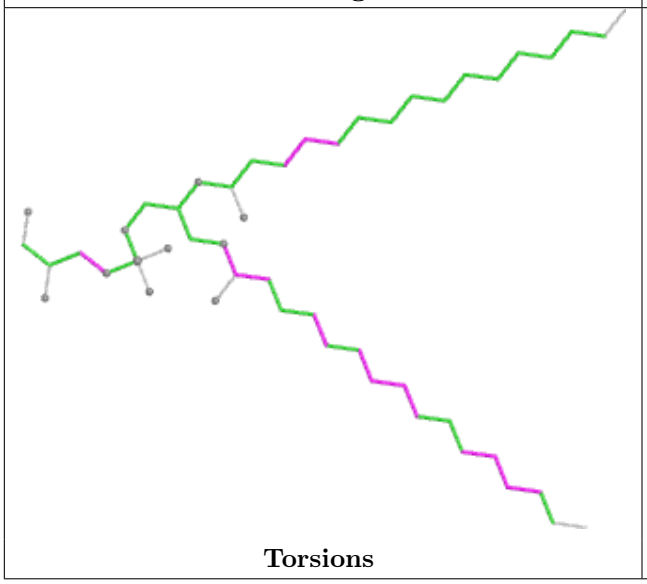
Ligand LHG d 406 (B)



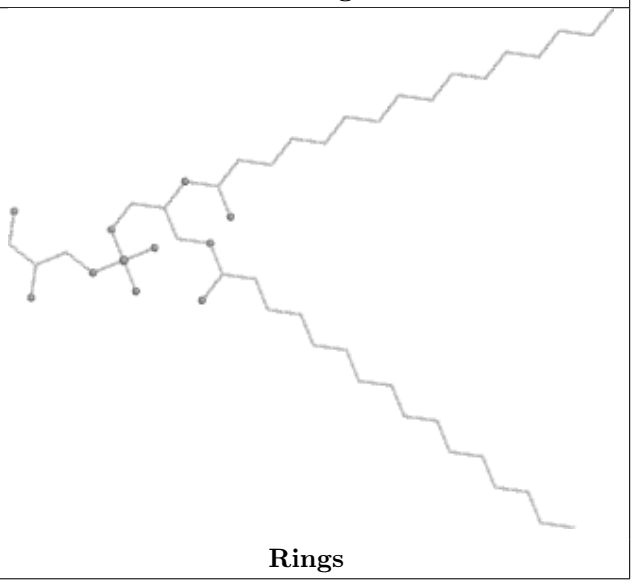
Bond lengths



Bond angles

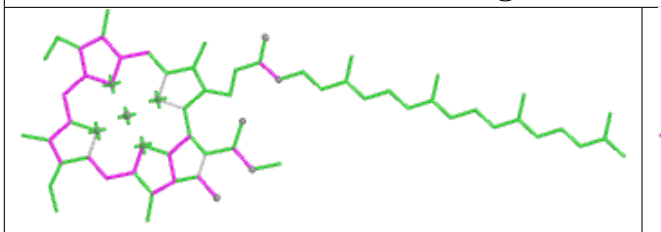


Torsions

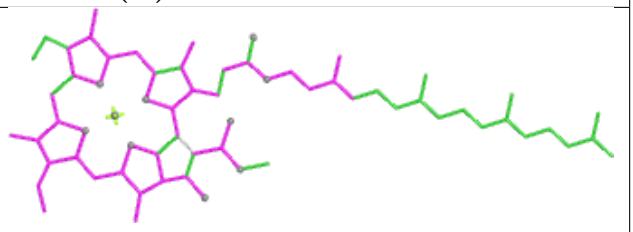


Rings

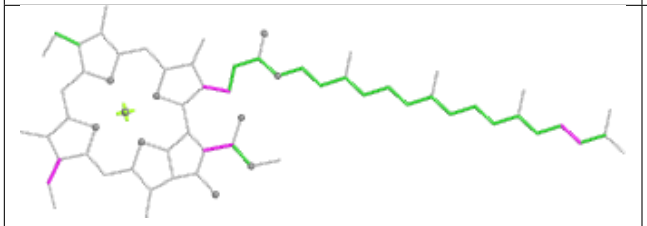
Ligand CLA a 406 (B)



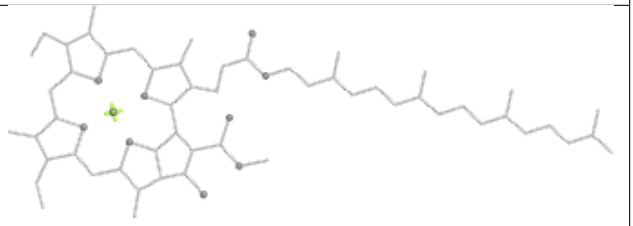
Bond lengths



Bond angles

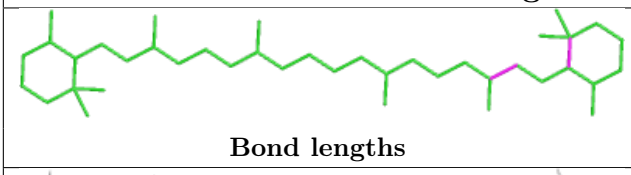


Torsions

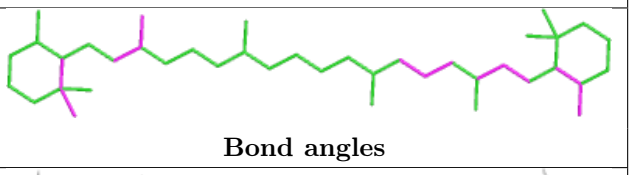


Rings

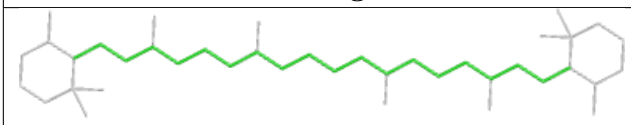
Ligand BCR B 619



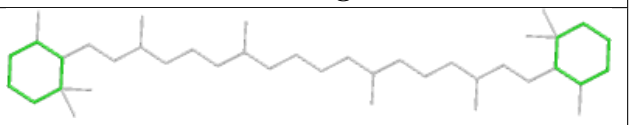
Bond lengths



Bond angles

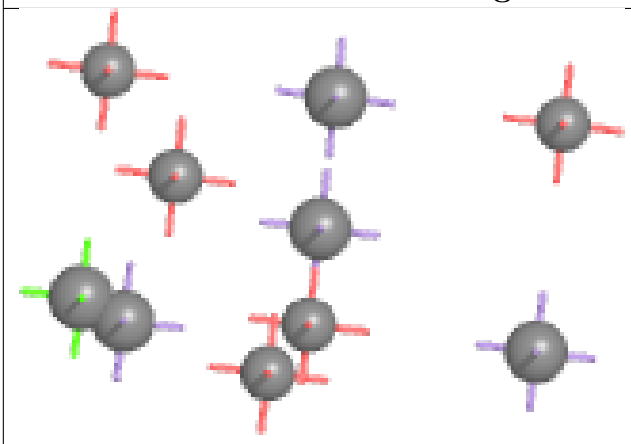


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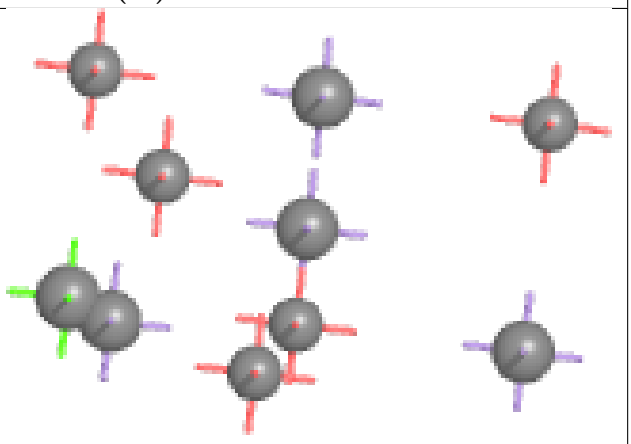


Rings

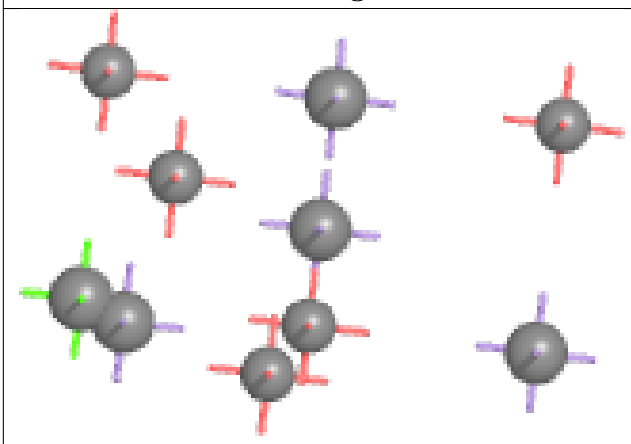
Ligand OEX a 413 (A)



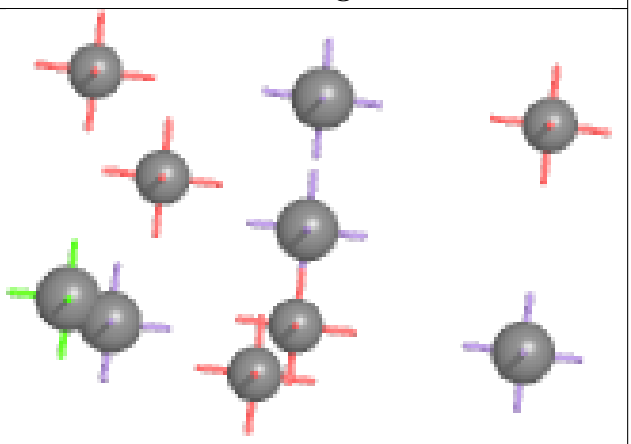
Bond lengths



Bond angles

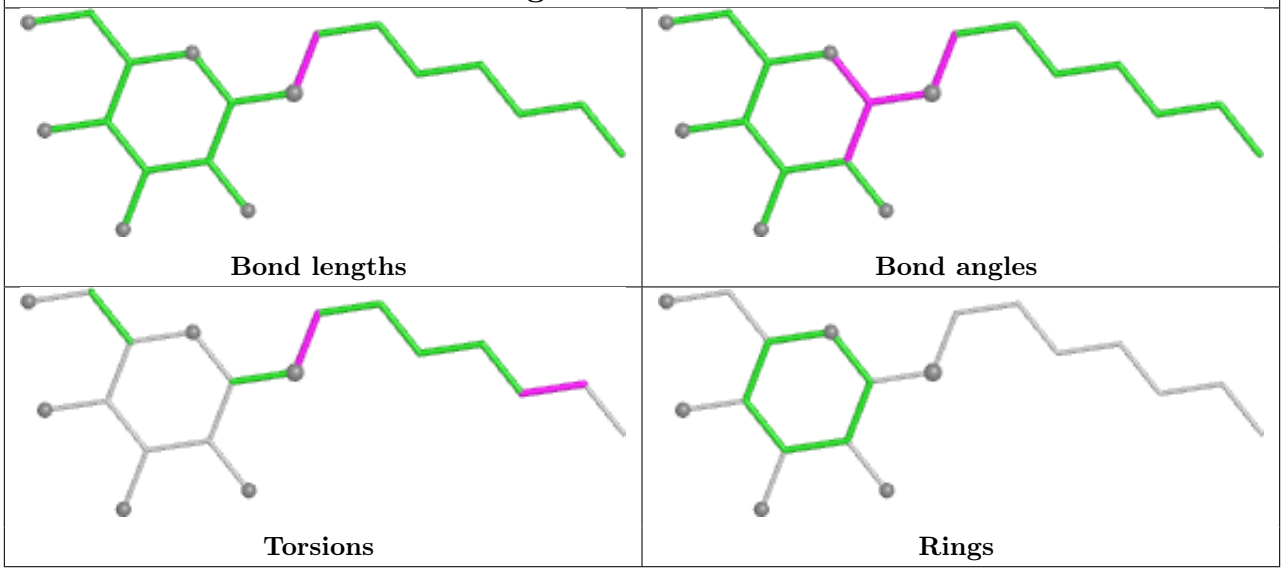


Torsions

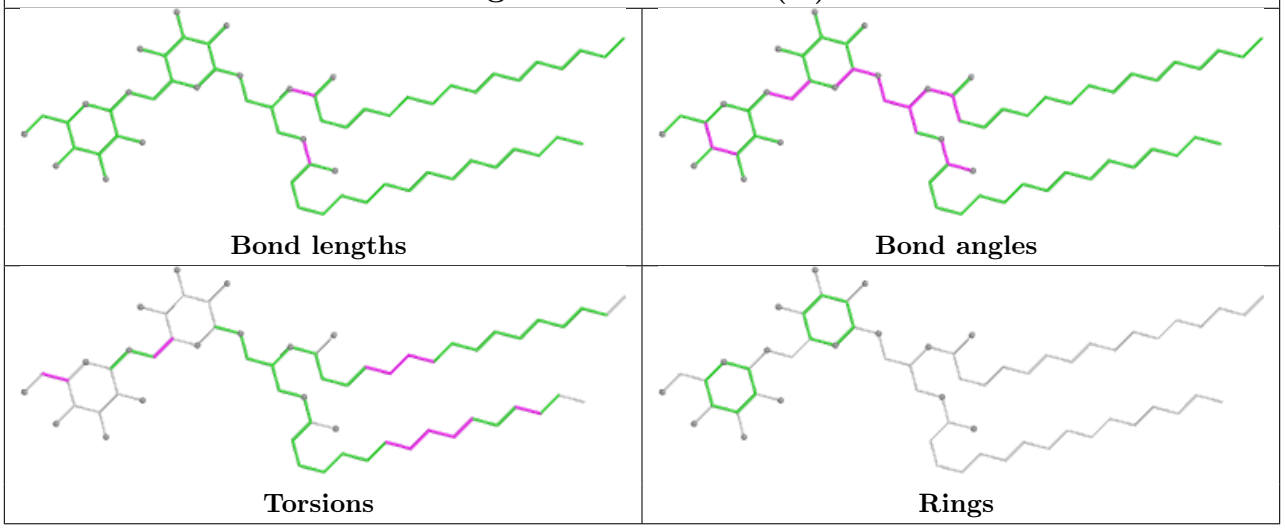


Rings

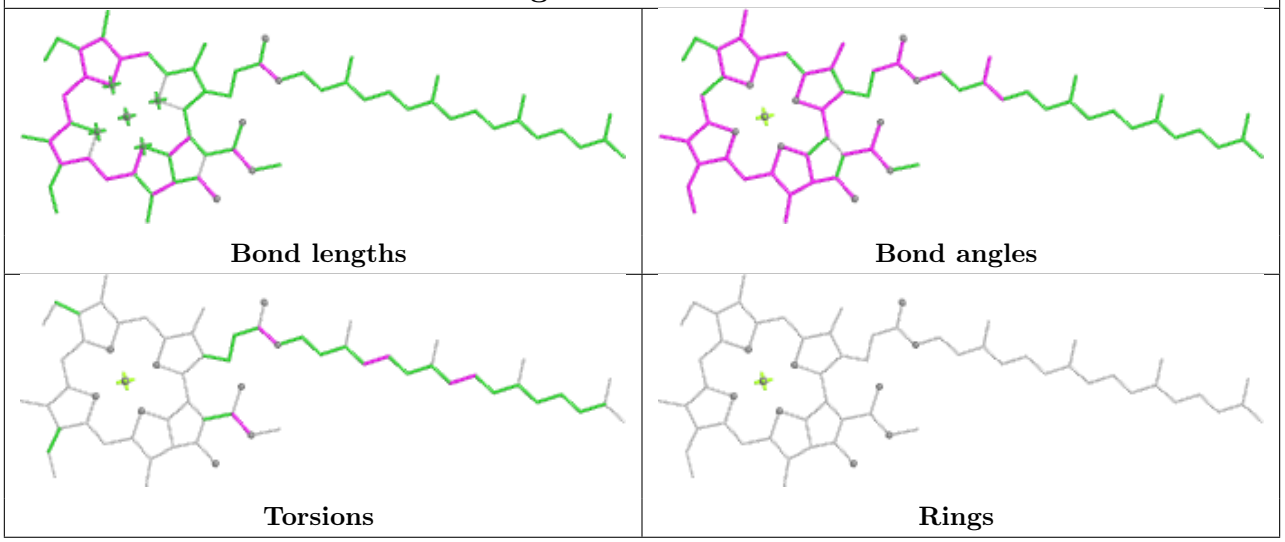
Ligand HTG c 522



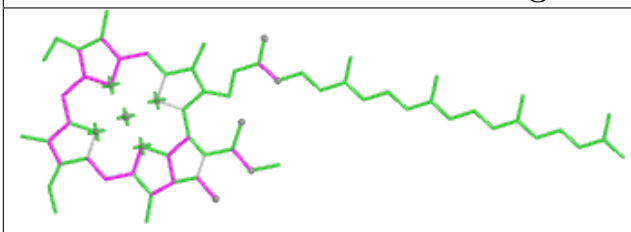
Ligand DGD C 517 (A)



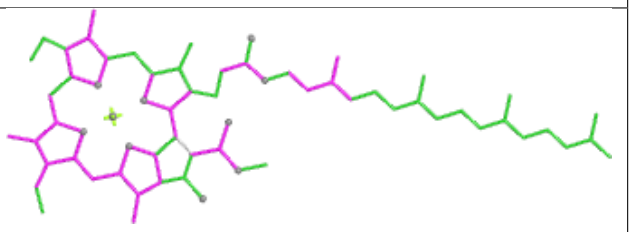
Ligand CLA c 512



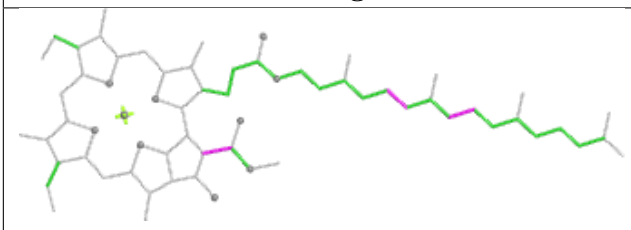
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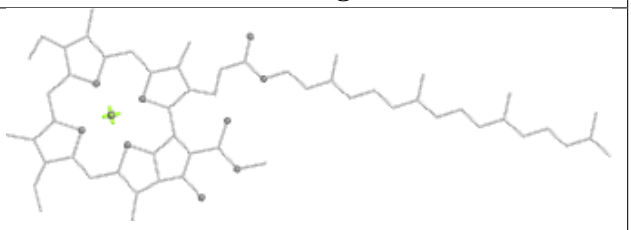
Bond lengths



Bond angles



Torsions

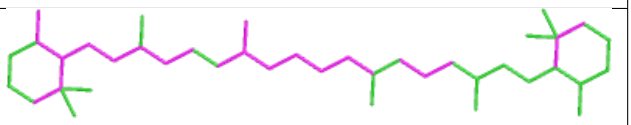


Rings

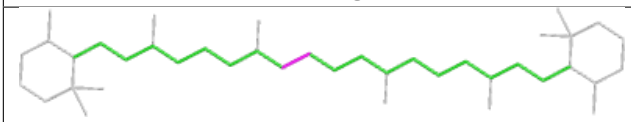
Ligand BCR T 102



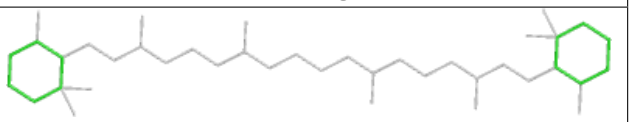
Bond lengths



Bond angles

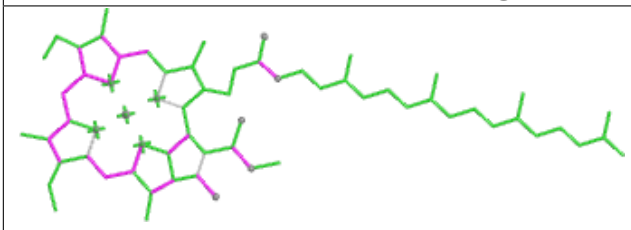


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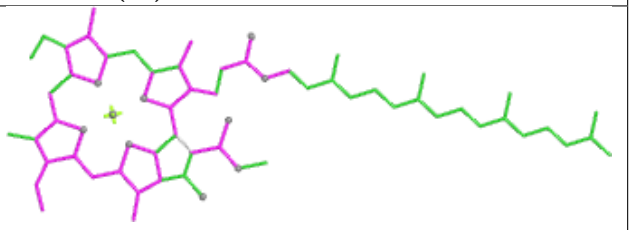


Rings

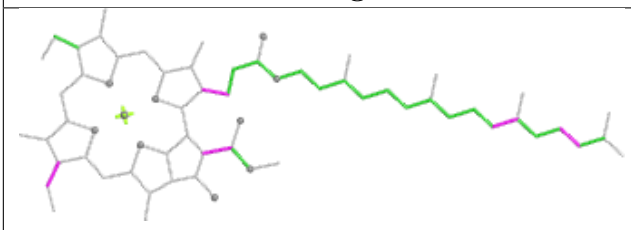
Ligand CLA a 406 (A)



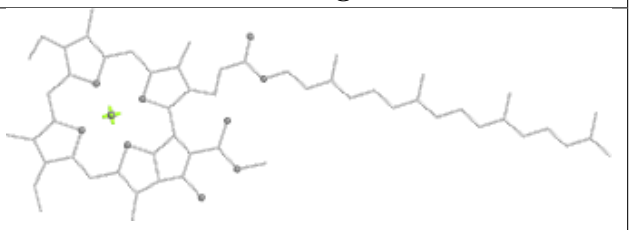
Bond lengths



Bond angles

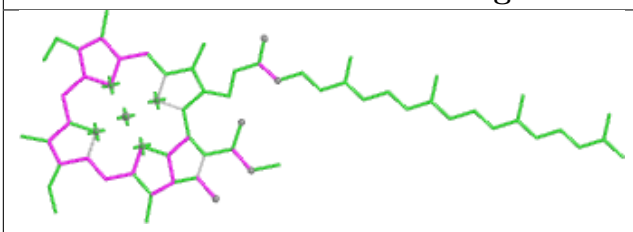


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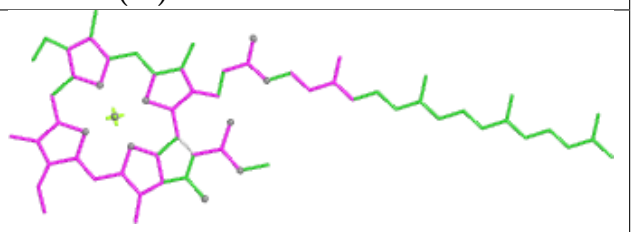


Rings

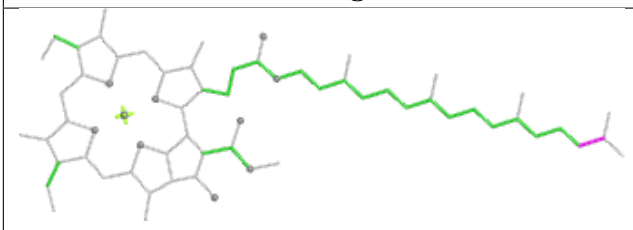
Ligand CLA d 401 (A)



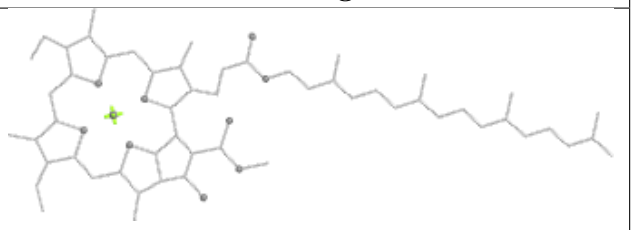
Bond lengths



Bond angles

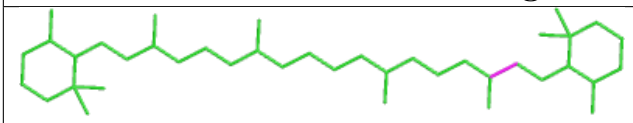


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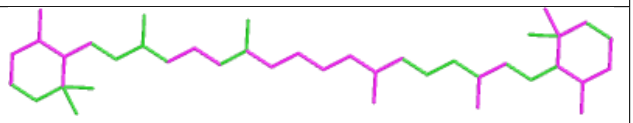


Rings

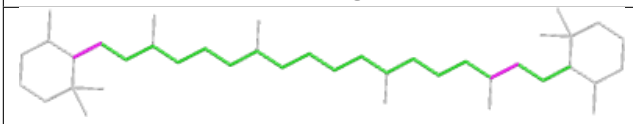
Ligand BCR Y 101



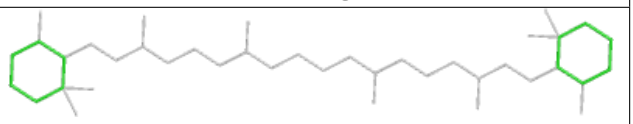
Bond lengths



Bond angles

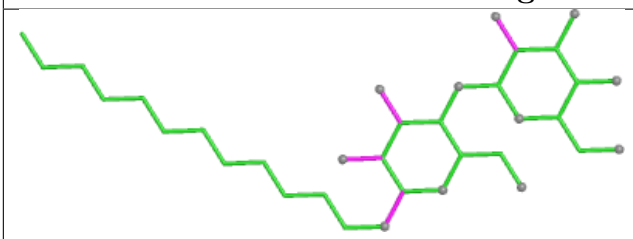


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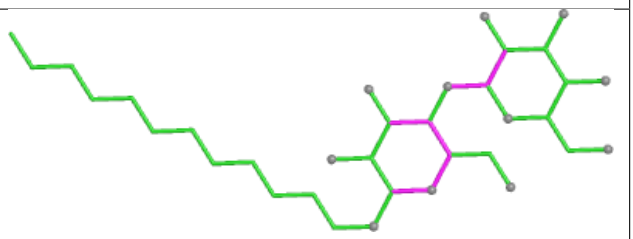


Rings

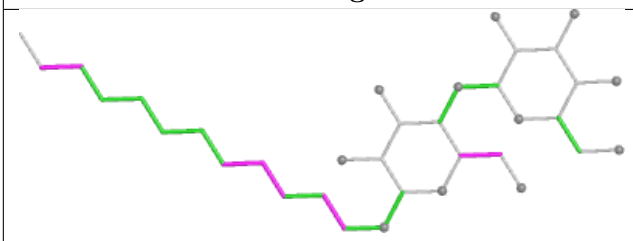
Ligand LMT M 101



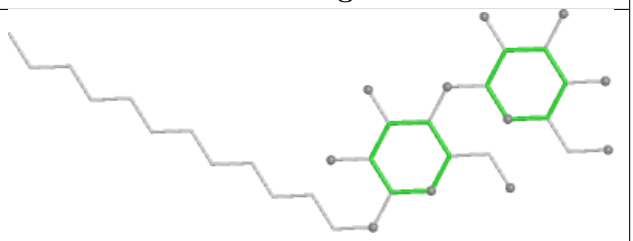
Bond lengths



Bond angles

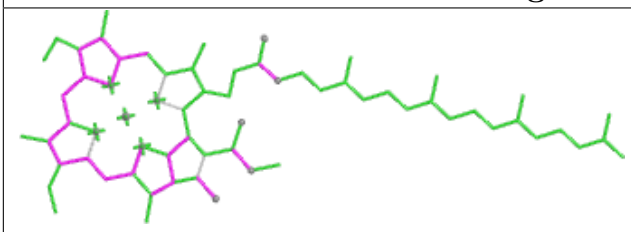


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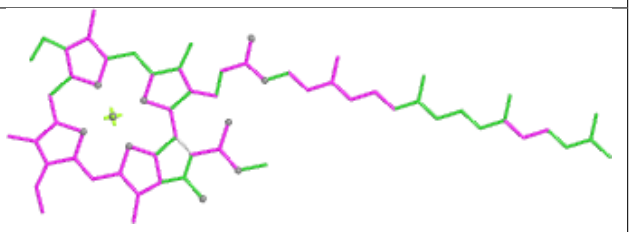


Rings

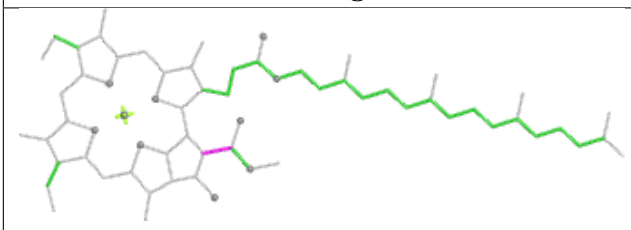
Ligand CLA b 609



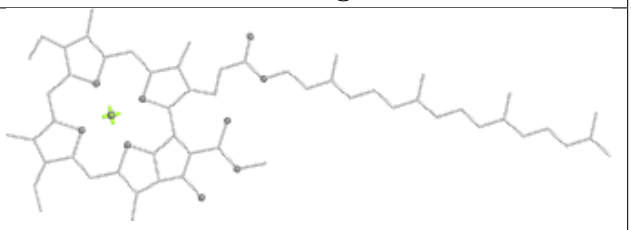
Bond lengths



Bond angles

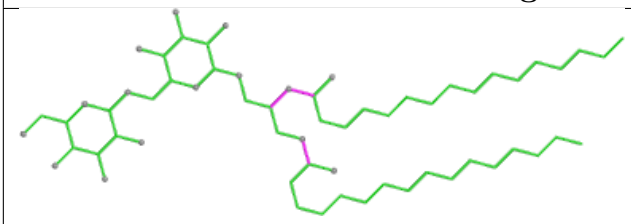


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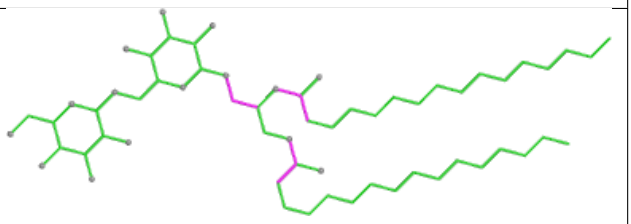


Rings

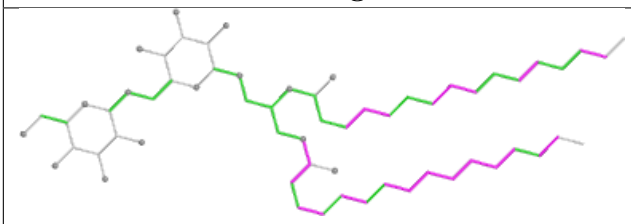
Ligand DGD C 519



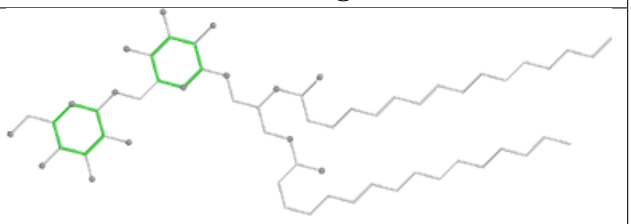
Bond lengths



Bond angles

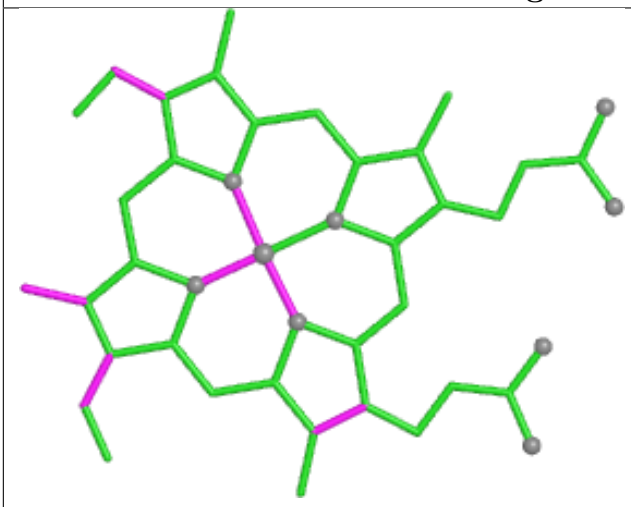


Torsions

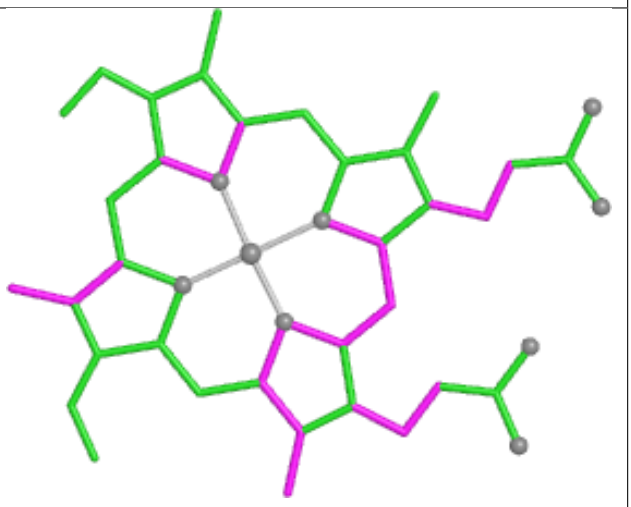


Rings

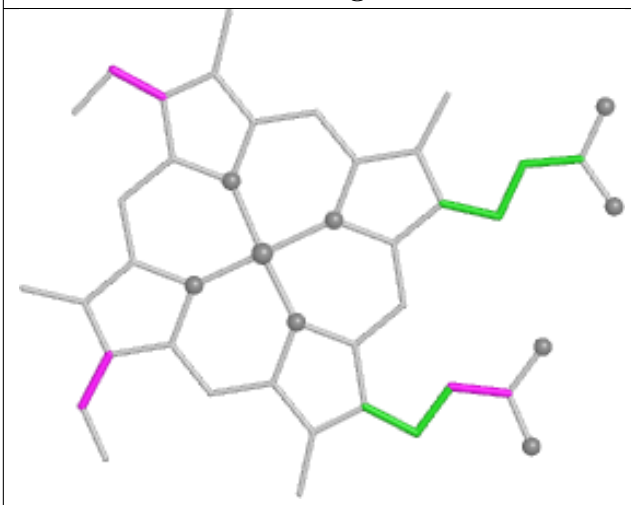
Ligand HEC v 201



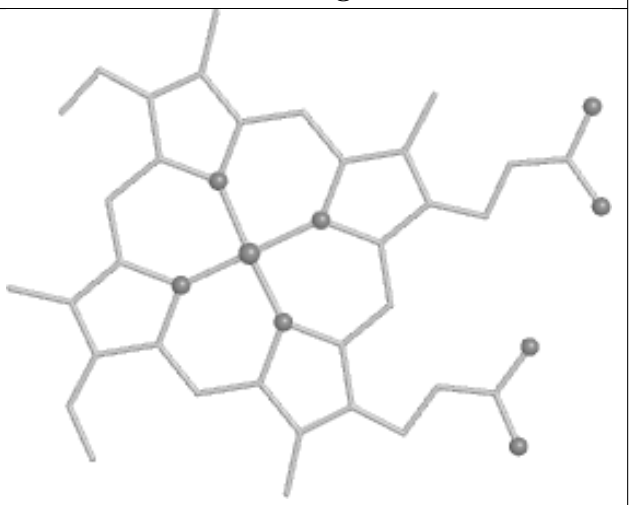
Bond lengths



Bond angles

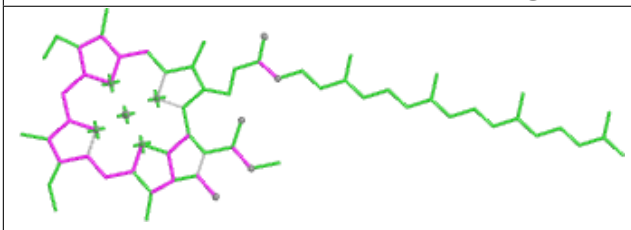


Torsions

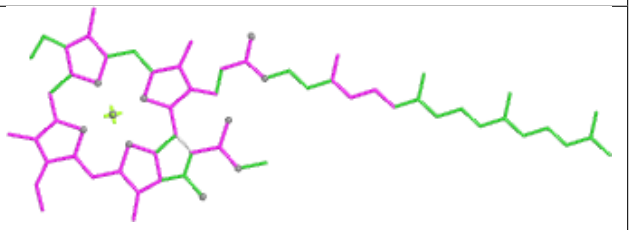


Rings

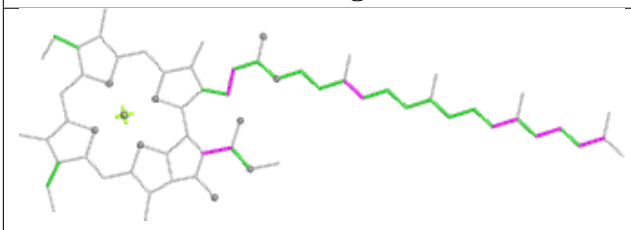
Ligand CLA B 603



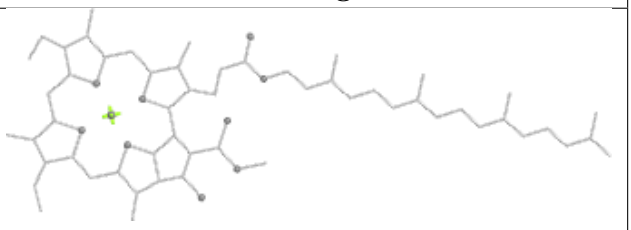
Bond lengths



Bond angles

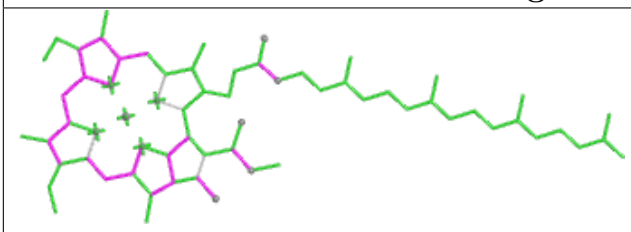


Torsions

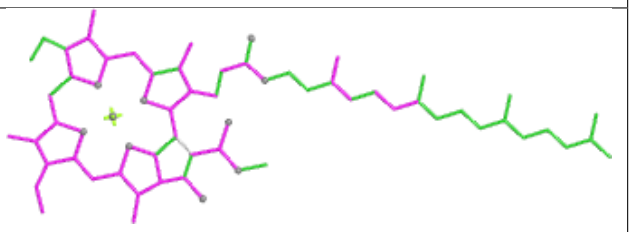


Rings

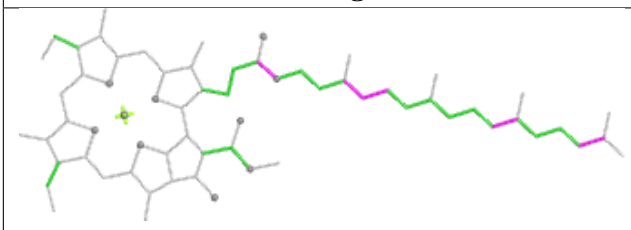
Ligand CLA d 402



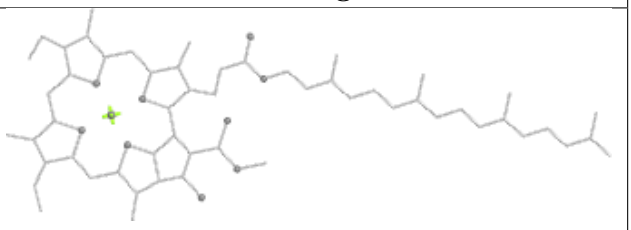
Bond lengths



Bond angles



Torsions

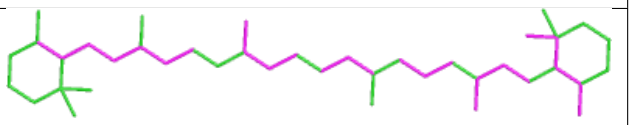


Rings

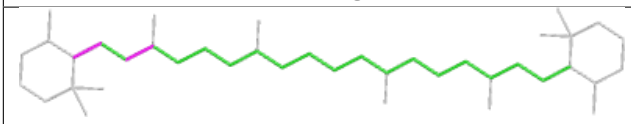
Ligand BCR b 619



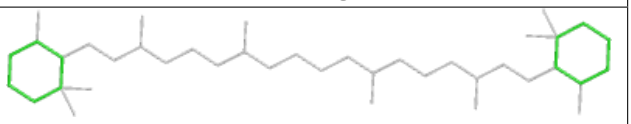
Bond lengths



Bond angles

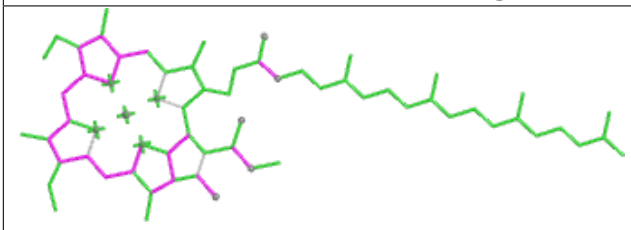


Torsions

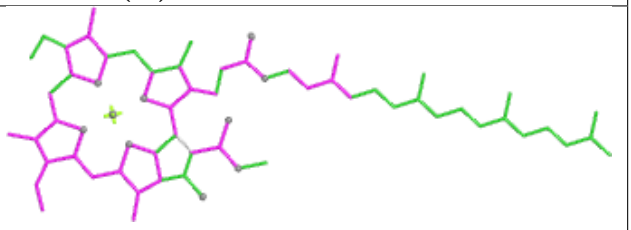


Rings

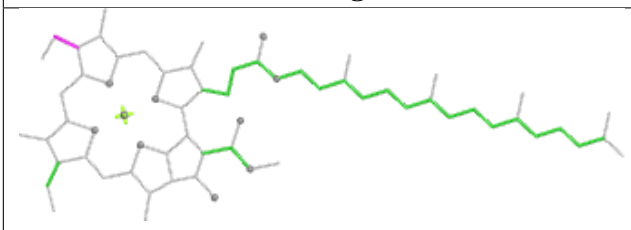
Ligand CLA D 702 (B)



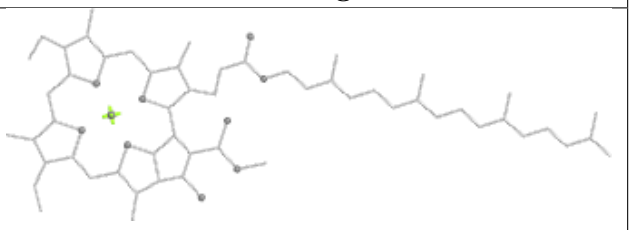
Bond lengths



Bond angles

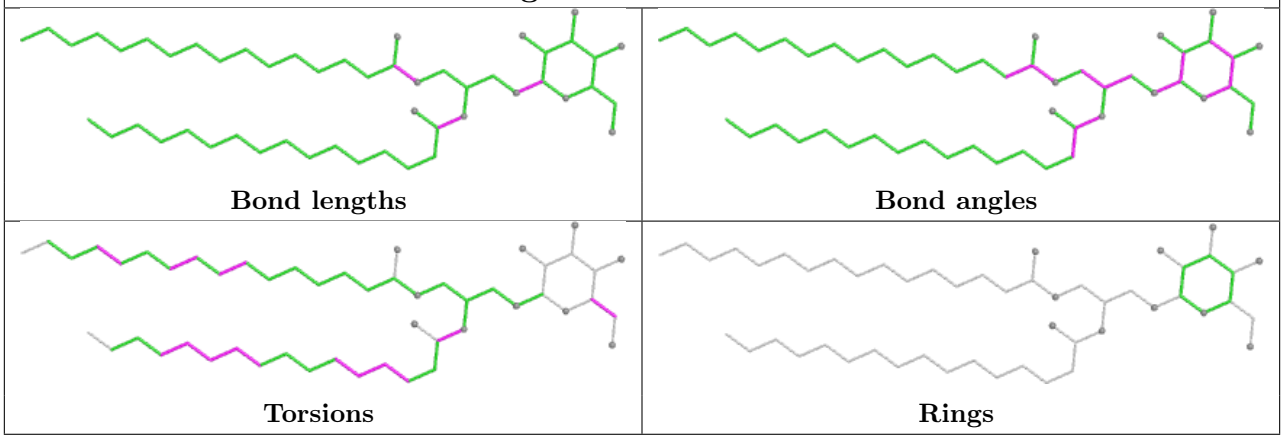


Torsions

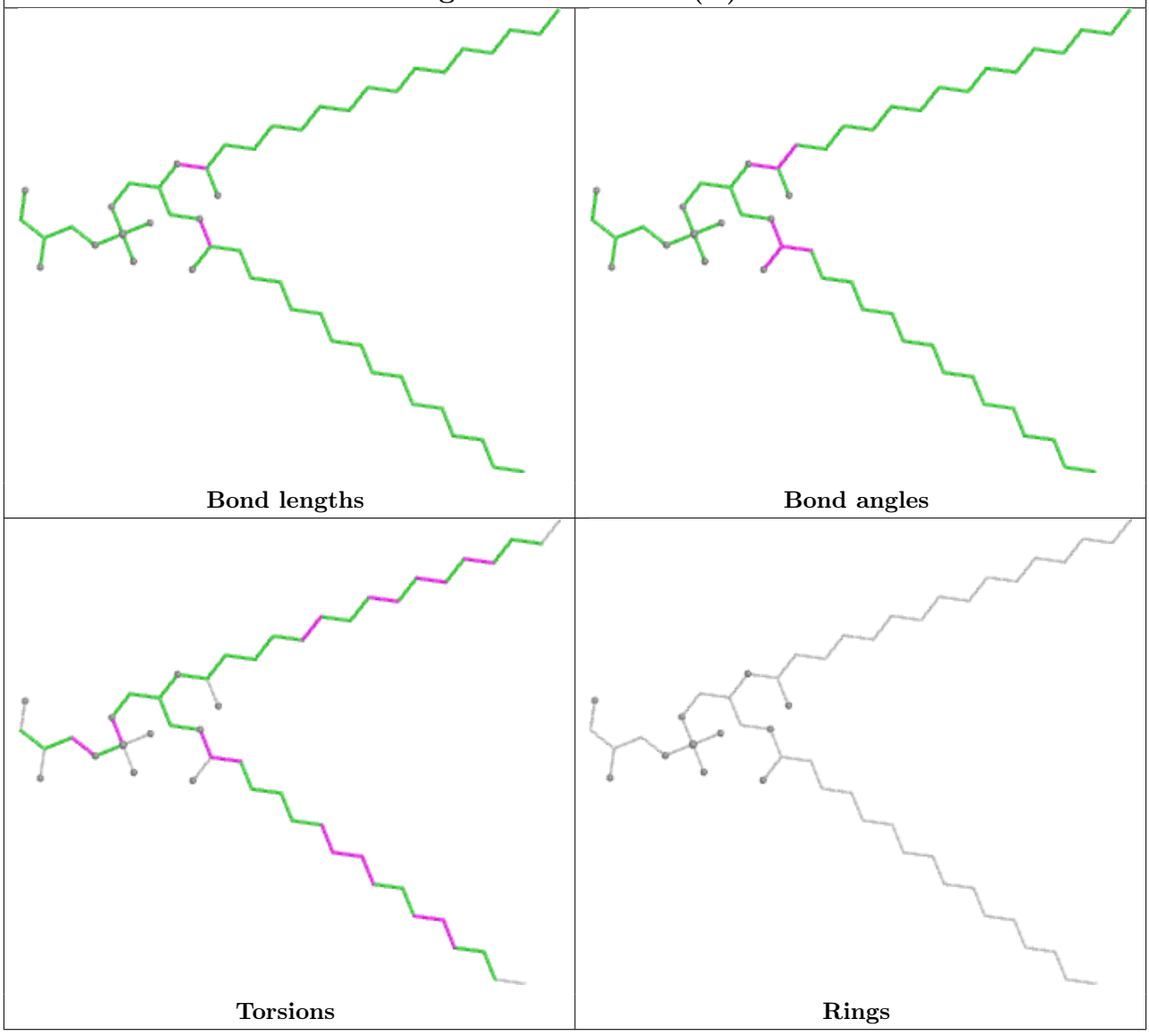


Rings

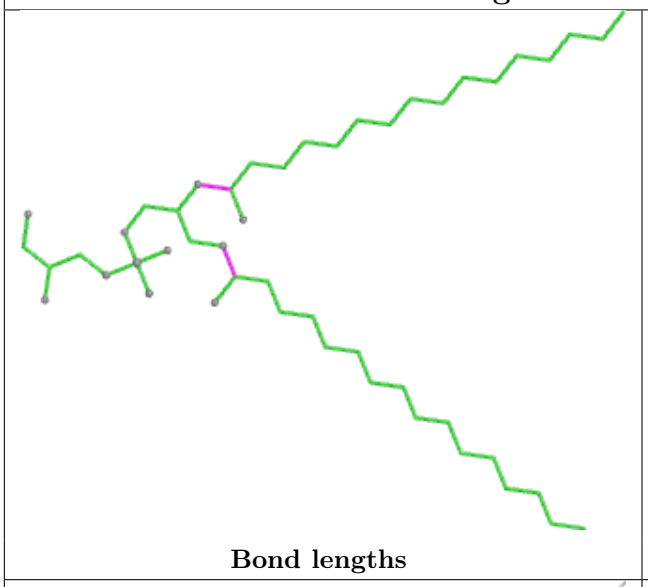
Ligand LMG C 521



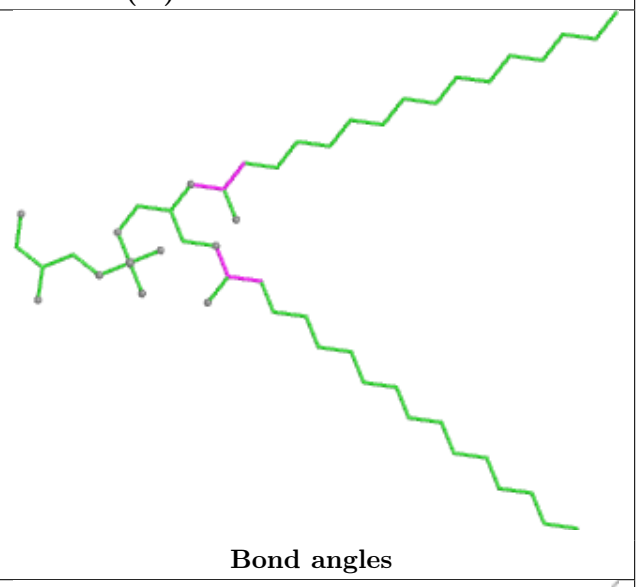
Ligand LHG D 707 (B)



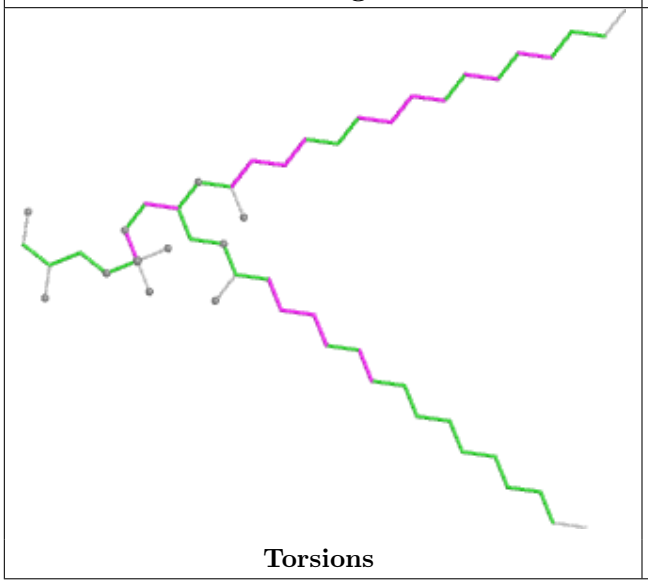
Ligand LHG L 101 (B)



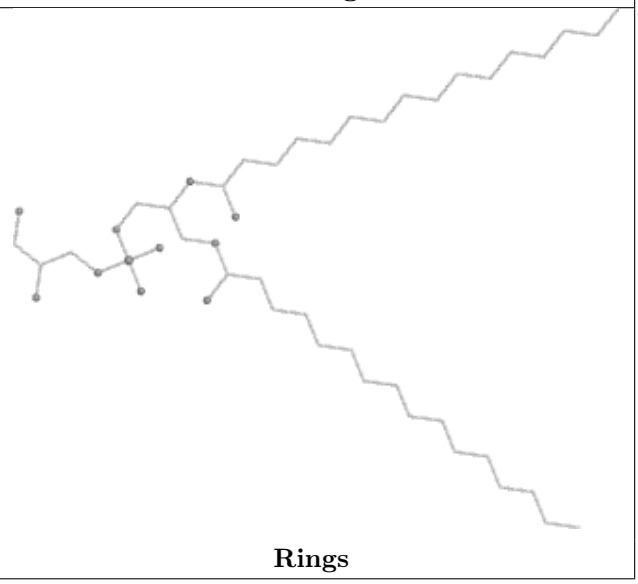
Bond lengths



Bond angles

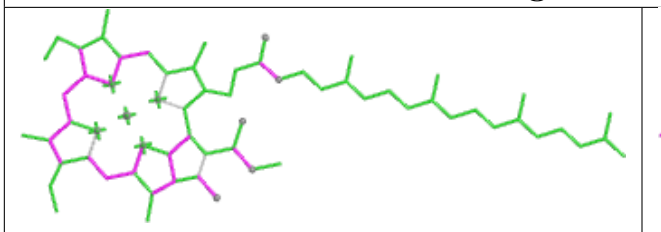


Torsions

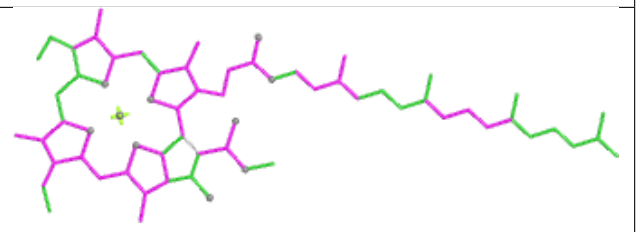


Rings

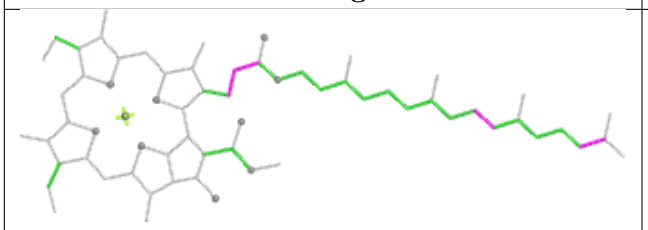
Ligand CLA b 602



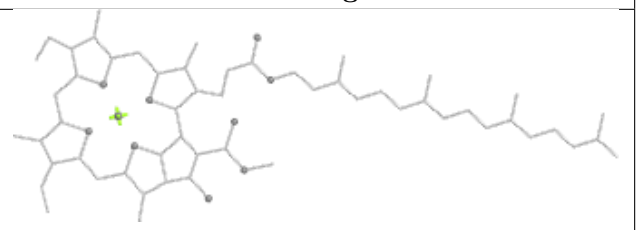
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	334/344 (97%)	-0.56	1 (0%) 90 90	21, 27, 60, 128	222 (66%)
1	a	334/344 (97%)	-0.53	1 (0%) 90 90	22, 29, 65, 124	220 (65%)
2	B	504/505 (99%)	-0.51	1 (0%) 91 91	23, 54, 81, 119	22 (4%)
2	b	504/505 (99%)	-0.45	0 100 100	24, 58, 92, 169	19 (3%)
3	C	451/455 (99%)	-0.54	0 100 100	22, 60, 81, 160	99 (21%)
3	c	455/455 (100%)	-0.45	1 (0%) 91 91	25, 66, 86, 130	101 (22%)
4	D	342/342 (100%)	-0.60	0 100 100	21, 47, 65, 136	115 (33%)
4	d	341/342 (99%)	-0.60	0 100 100	22, 51, 75, 133	119 (34%)
5	E	81/84 (96%)	-0.34	1 (1%) 76 77	53, 70, 99, 165	0
5	e	79/84 (94%)	-0.32	1 (1%) 75 76	32, 77, 114, 152	2 (2%)
6	F	34/44 (77%)	-0.59	0 100 100	54, 62, 86, 117	0
6	f	31/44 (70%)	-0.36	1 (3%) 50 52	55, 68, 94, 155	1 (3%)
7	H	64/65 (98%)	-0.31	1 (1%) 70 72	53, 64, 85, 106	0
7	h	64/65 (98%)	-0.41	1 (1%) 70 72	41, 70, 95, 115	1 (1%)
8	I	37/38 (97%)	-0.21	0 100 100	54, 63, 127, 162	0
8	i	37/38 (97%)	-0.27	0 100 100	55, 65, 122, 143	0
9	J	38/39 (97%)	-0.32	0 100 100	51, 70, 124, 180	0
9	j	39/39 (100%)	-0.31	0 100 100	60, 76, 128, 171	0
10	K	37/37 (100%)	-0.61	0 100 100	59, 68, 89, 113	0
10	k	37/37 (100%)	-0.46	0 100 100	68, 75, 98, 112	0
11	L	36/37 (97%)	-0.57	0 100 100	24, 48, 100, 142	2 (5%)
11	l	36/37 (97%)	-0.52	0 100 100	25, 49, 104, 136	2 (5%)
12	M	32/36 (88%)	-0.57	0 100 100	27, 49, 76, 147	1 (3%)
12	m	33/36 (91%)	-0.43	0 100 100	25, 51, 73, 154	2 (6%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	O	243/244 (99%)	-0.48	0 100 100	21, 64, 116, 187	10 (4%)
13	o	243/244 (99%)	-0.49	0 100 100	23, 67, 129, 174	8 (3%)
14	T	29/32 (90%)	-0.60	0 100 100	27, 47, 59, 65	6 (20%)
14	t	29/32 (90%)	-0.59	1 (3%) 48 50	28, 49, 66, 73	5 (17%)
15	U	96/104 (92%)	-0.58	0 100 100	25, 59, 91, 102	4 (4%)
15	u	97/104 (93%)	-0.61	0 100 100	28, 62, 84, 138	5 (5%)
16	V	137/137 (100%)	-0.64	0 100 100	24, 58, 83, 107	6 (4%)
16	v	137/137 (100%)	-0.56	0 100 100	27, 71, 104, 139	6 (4%)
17	X	38/40 (95%)	-0.32	0 100 100	35, 72, 94, 113	1 (2%)
17	x	38/40 (95%)	-0.09	0 100 100	64, 79, 124, 162	0
18	Y	29/30 (96%)	0.03	0 100 100	69, 87, 124, 125	0
18	y	29/30 (96%)	-0.21	0 100 100	76, 92, 113, 116	0
19	Z	62/62 (100%)	-0.34	0 100 100	65, 80, 134, 159	0
19	z	62/62 (100%)	0.09	0 100 100	81, 95, 146, 205	0
20	R	34/34 (100%)	0.37	2 (5%) 28 30	82, 103, 134, 144	0
All	All	5283/5384 (98%)	-0.49	12 (0%) 91 91	21, 58, 99, 205	979 (18%)

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	e	79[A]	PHE	3.9
7	H	65	LEU	3.2
6	f	16[A]	PHE	3.1
14	t	30[A]	THR	2.8
1	A	11	ALA	2.7

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
14	FME	T	1	10/11	0.94	0.07	47,58,69,72	0
14	FME	t	1	10/11	0.95	0.08	43,50,69,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	FME	i	1	10/11	0.96	0.06	50,68,83,87	0
8	FME	I	1	10/11	0.96	0.07	60,68,82,83	0
12	FME	m	1	10/11	0.97	0.07	50,64,91,120	0
12	FME	M	1	10/11	0.97	0.06	49,61,93,102	0

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
27	GOL	a	418	6/6	0.63	0.15	80,108,110,120	0
30	UNL	j	101	10/-	0.66	0.20	83,96,103,107	0
30	UNL	A	415	28/-	0.69	0.15	89,115,132,142	0
30	UNL	J	101	10/-	0.70	0.28	69,81,97,105	0
32	LMT	B	629	35/35	0.70	0.15	65,117,147,151	0
32	LMT	A	418	35/35	0.71	0.14	72,119,140,144	0
32	LMT	F	101	35/35	0.71	0.15	104,135,179,184	0
30	UNL	a	415	30/-	0.72	0.12	92,122,144,155	0
35	HTG	B	622	19/19	0.73	0.16	66,99,118,134	0
32	LMT	a	417	35/35	0.74	0.14	112,138,151,161	0
32	LMT	A	420	35/35	0.74	0.12	96,138,157,172	0
30	UNL	I	101	40/-	0.75	0.15	75,109,159,173	0
30	UNL	m	102	10/-	0.75	0.20	75,77,102,106	0
30	UNL	K	101[B]	34/-	0.76	0.14	90,113,127,130	34
32	LMT	e	101	35/35	0.76	0.14	107,142,187,194	0
30	UNL	K	101[A]	34/-	0.76	0.14	90,113,127,130	34
26	SQD	f	102	43/54	0.77	0.12	97,131,176,184	0
30	UNL	l	101	10/-	0.77	0.17	71,79,95,97	0
27	GOL	O	302	6/6	0.78	0.10	67,88,100,104	0
34	LMG	C	521	51/55	0.78	0.11	59,121,157,175	0
30	UNL	i	101	40/-	0.78	0.13	74,107,162,167	0
35	HTG	C	522	19/19	0.78	0.12	111,128,143,152	0
37	CA	F	103	1/1	0.78	0.23	128,128,128,128	0
27	GOL	o	304	6/6	0.79	0.15	89,93,102,106	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
30	UNL	b	626	33/-	0.79	0.13	69,96,158,173	0
27	GOL	d	411	6/6	0.80	0.24	52,68,77,89	0
30	UNL	c	525[A]	32/-	0.80	0.15	98,115,128,135	32
30	UNL	c	525[B]	32/-	0.80	0.15	98,115,128,135	32
27	GOL	A	411	6/6	0.80	0.14	63,80,85,90	0
32	LMT	b	621	25/35	0.80	0.13	86,120,162,172	0
27	GOL	B	626	6/6	0.81	0.13	68,87,96,119	0
30	UNL	D	709	40/-	0.81	0.13	67,98,145,157	0
30	UNL	d	408	36/-	0.81	0.12	68,97,136,143	0
29	PL9	A	414[A]	55/55	0.82	0.15	66,96,110,116	55
29	PL9	A	414[B]	55/55	0.82	0.15	66,96,111,117	55
27	GOL	o	303	6/6	0.82	0.17	85,106,121,123	0
35	HTG	b	623	19/19	0.82	0.11	83,133,157,164	0
27	GOL	b	624	6/6	0.82	0.16	93,103,110,118	0
35	HTG	D	710	16/19	0.83	0.11	86,105,131,151	0
27	GOL	a	419	6/6	0.83	0.15	60,80,88,94	0
35	HTG	d	409	16/19	0.83	0.11	79,122,141,161	0
32	LMT	B	627	35/35	0.83	0.11	61,108,138,152	0
33	LHG	a	420[B]	42/49	0.84	0.11	99,148,163,168	42
35	HTG	V	202	11/19	0.84	0.09	81,115,121,129	0
26	SQD	a	412	54/54	0.84	0.10	67,97,137,156	0
35	HTG	c	522	19/19	0.84	0.09	104,126,145,148	0
30	UNL	B	625	33/-	0.84	0.13	58,109,143,152	0
33	LHG	a	420[A]	42/49	0.84	0.11	99,148,163,168	42
32	LMT	T	101	35/35	0.85	0.11	76,131,174,184	0
34	LMG	Z	101	37/55	0.85	0.13	66,119,147,176	0
32	LMT	b	627	25/35	0.86	0.12	53,101,149,156	0
35	HTG	b	622	19/19	0.86	0.12	58,83,125,127	0
34	LMG	z	101	39/55	0.86	0.12	75,130,153,169	0
26	SQD	A	412	54/54	0.86	0.10	66,89,136,163	0
32	LMT	t	101	26/35	0.86	0.12	75,114,149,159	0
34	LMG	c	521	51/55	0.86	0.10	72,137,167,189	0
27	GOL	O	303	6/6	0.87	0.12	88,102,106,117	0
29	PL9	a	414[A]	55/55	0.87	0.15	87,109,123,130	55
29	PL9	a	414[B]	55/55	0.87	0.15	87,109,124,130	55
32	LMT	B	630	25/35	0.87	0.11	57,92,148,164	0
32	LMT	m	103	35/35	0.87	0.10	55,95,109,123	0
27	GOL	l	102[A]	6/6	0.87	0.17	71,105,107,108	6
35	HTG	o	301	19/19	0.87	0.12	58,86,117,132	0
27	GOL	l	102[B]	6/6	0.87	0.17	70,107,107,108	6
26	SQD	X	101	43/54	0.88	0.11	73,104,134,142	0
26	SQD	b	620	54/54	0.88	0.10	68,98,127,133	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
33	LHG	E	101[A]	42/49	0.88	0.12	70,107,122,131	42
33	LHG	E	101[B]	42/49	0.88	0.12	70,107,123,131	42
26	SQD	B	620	54/54	0.89	0.10	64,98,139,146	0
31	BCT	A	416[A]	4/4	0.89	0.10	54,56,61,64	4
31	BCT	A	416[B]	4/4	0.89	0.10	54,54,63,63	4
30	UNL	D	708	17/-	0.89	0.11	65,78,110,128	0
32	LMT	M	101	35/35	0.89	0.10	64,95,120,130	0
23	CLA	b	601	65/65	0.89	0.10	60,88,131,160	0
37	CA	f	103	1/1	0.89	0.12	123,123,123,123	0
27	GOL	c	527	6/6	0.90	0.16	103,117,127,128	0
27	GOL	D	701	6/6	0.90	0.28	56,77,86,93	0
27	GOL	v	202[A]	6/6	0.90	0.11	68,79,85,87	6
27	GOL	v	202[B]	6/6	0.90	0.11	68,79,85,88	6
27	GOL	V	203[A]	6/6	0.90	0.12	59,73,76,83	6
27	GOL	V	203[B]	6/6	0.90	0.12	58,73,76,83	6
23	CLA	c	514	65/65	0.91	0.09	68,93,130,148	0
34	LMG	c	501	51/55	0.91	0.08	67,90,114,134	0
34	LMG	c	520	51/55	0.91	0.09	63,91,137,157	0
27	GOL	B	628	6/6	0.91	0.12	73,79,89,102	0
34	LMG	m	101	51/55	0.91	0.09	60,76,98,112	0
23	CLA	B	601	65/65	0.91	0.09	55,78,119,156	0
27	GOL	D	712	6/6	0.91	0.15	51,66,78,101	0
27	GOL	B	623	6/6	0.91	0.09	71,85,90,90	0
34	LMG	C	501	51/55	0.91	0.09	61,90,118,132	0
37	CA	o	302	1/1	0.91	0.07	111,111,111,111	0
27	GOL	b	628	6/6	0.92	0.08	84,86,95,96	0
35	HTG	b	625	19/19	0.92	0.08	64,78,100,111	0
33	LHG	A	419[A]	49/49	0.92	0.10	51,65,85,93	49
35	HTG	B	624	19/19	0.92	0.07	66,78,100,107	0
33	LHG	A	419[B]	49/49	0.92	0.10	51,66,85,93	49
34	LMG	B	621	51/55	0.92	0.09	56,72,94,121	0
30	UNL	d	407	17/-	0.92	0.10	67,84,111,112	0
34	LMG	C	520	51/55	0.92	0.09	57,87,123,129	0
34	LMG	D	711	51/55	0.93	0.09	50,68,126,141	0
25	BCR	T	102	40/40	0.93	0.07	44,61,75,80	0
25	BCR	d	403	40/40	0.93	0.08	53,65,102,114	0
25	BCR	t	102	40/40	0.93	0.07	43,63,83,98	0
34	LMG	d	410	51/55	0.93	0.08	52,69,126,154	0
23	CLA	b	616	65/65	0.93	0.08	49,63,130,145	0
23	CLA	C	514	65/65	0.93	0.08	57,84,113,118	0
25	BCR	D	704	40/40	0.93	0.09	47,60,103,111	0
36	DGD	c	518[A]	62/66	0.93	0.08	57,70,121,139	62

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
36	DGD	c	518[B]	62/66	0.93	0.08	57,70,121,139	62
26	SQD	a	411[A]	54/54	0.93	0.10	59,82,124,129	54
37	CA	c	523	1/1	0.93	0.09	76,76,76,76	0
26	SQD	a	411[B]	54/54	0.93	0.10	59,82,124,129	54
25	BCR	K	102	40/40	0.93	0.10	55,67,79,82	0
31	BCT	a	404[B]	4/4	0.94	0.09	61,61,71,85	4
23	CLA	c	505	65/65	0.94	0.07	50,63,111,139	0
23	CLA	c	507	65/65	0.94	0.08	53,69,127,138	0
23	CLA	c	513	65/65	0.94	0.09	63,81,130,137	0
23	CLA	A	408	65/65	0.94	0.09	42,54,132,155	0
23	CLA	d	402	65/65	0.94	0.09	51,67,133,149	0
25	BCR	B	619	40/40	0.94	0.08	47,60,90,98	0
30	UNL	X	102	18/-	0.94	0.10	62,75,114,115	0
25	BCR	C	515	40/40	0.94	0.08	57,75,89,93	0
23	CLA	D	703	65/65	0.94	0.08	47,59,126,136	0
25	BCR	H	101	40/40	0.94	0.07	47,64,80,89	0
23	CLA	a	409	65/65	0.94	0.10	43,56,143,159	0
23	CLA	C	505	65/65	0.94	0.07	40,57,96,128	0
25	BCR	c	515	40/40	0.94	0.08	71,83,93,95	0
23	CLA	b	614	65/65	0.94	0.07	42,51,105,124	0
25	BCR	h	101	40/40	0.94	0.08	55,65,91,97	0
23	CLA	C	507	65/65	0.94	0.08	56,72,124,142	0
33	LHG	D	707[A]	49/49	0.94	0.09	51,61,108,113	49
33	LHG	D	707[B]	49/49	0.94	0.09	51,61,108,113	49
25	BCR	y	101	40/40	0.94	0.07	56,72,86,96	0
26	SQD	A	410[A]	54/54	0.94	0.09	58,79,110,117	54
26	SQD	A	410[B]	54/54	0.94	0.09	58,79,110,118	54
31	BCT	a	404[A]	4/4	0.94	0.09	60,61,69,82	4
36	DGD	C	518[A]	62/66	0.94	0.08	51,67,115,122	62
36	DGD	C	518[B]	62/66	0.94	0.08	51,67,116,122	62
36	DGD	c	517[A]	62/66	0.94	0.07	49,64,104,113	62
36	DGD	c	517[B]	62/66	0.94	0.07	48,64,104,113	62
33	LHG	b	629[A]	49/49	0.94	0.09	53,61,68,92	49
33	LHG	b	629[B]	49/49	0.94	0.09	52,61,68,93	49
36	DGD	c	519	62/66	0.94	0.07	50,68,104,134	0
33	LHG	d	406[A]	49/49	0.94	0.10	54,66,114,132	49
33	LHG	d	406[B]	49/49	0.94	0.10	54,66,114,132	49
33	LHG	d	412[A]	49/49	0.94	0.09	52,68,81,90	49
33	LHG	d	412[B]	49/49	0.94	0.09	52,68,82,90	49
27	GOL	C	523[B]	6/6	0.95	0.09	59,64,69,73	6
25	BCR	b	619	40/40	0.95	0.07	48,62,86,89	0
23	CLA	C	509	65/65	0.95	0.07	47,56,121,146	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	CLA	c	506	65/65	0.95	0.07	48,65,88,99	0
23	CLA	C	513	65/65	0.95	0.08	54,74,115,133	0
25	BCR	k	101	40/40	0.95	0.08	56,74,83,91	0
23	CLA	c	508	65/65	0.95	0.09	52,70,82,92	0
23	CLA	c	509	65/65	0.95	0.07	43,66,128,150	0
23	CLA	B	611	65/65	0.95	0.07	38,48,65,76	0
23	CLA	B	614	65/65	0.95	0.07	39,51,111,124	0
23	CLA	a	407[A]	65/65	0.95	0.07	43,56,128,136	65
25	BCR	A	409	40/40	0.95	0.07	41,53,67,69	0
25	BCR	B	618	40/40	0.95	0.06	43,57,73,83	0
23	CLA	a	407[B]	65/65	0.95	0.07	43,56,128,136	65
23	CLA	B	616	65/65	0.95	0.09	50,63,135,143	0
23	CLA	B	603	65/65	0.95	0.08	42,54,74,83	0
23	CLA	b	606	65/65	0.95	0.07	40,59,109,127	0
23	CLA	B	606	65/65	0.95	0.08	44,58,110,134	0
23	CLA	C	508	65/65	0.95	0.08	50,63,87,96	0
36	DGD	C	517[A]	62/66	0.95	0.07	47,59,99,108	62
36	DGD	C	517[B]	62/66	0.95	0.07	47,59,99,108	62
30	UNL	x	101	18/-	0.95	0.10	73,81,134,142	0
33	LHG	d	405[A]	49/49	0.95	0.08	50,59,71,78	49
36	DGD	C	519	62/66	0.95	0.07	44,61,99,122	0
36	DGD	H	102	62/66	0.95	0.08	48,63,76,88	0
33	LHG	d	405[B]	49/49	0.95	0.08	50,59,71,79	49
25	BCR	Y	101	40/40	0.95	0.07	51,64,84,89	0
25	BCR	a	410	40/40	0.95	0.07	44,56,67,73	0
29	PL9	D	705[A]	55/55	0.95	0.07	38,51,61,68	55
29	PL9	D	705[B]	55/55	0.95	0.07	37,51,61,69	55
36	DGD	h	102	62/66	0.95	0.08	50,66,80,86	0
25	BCR	b	617	40/40	0.95	0.06	46,57,65,70	0
27	GOL	C	523[A]	6/6	0.95	0.09	59,64,68,73	6
29	PL9	d	404[A]	55/55	0.95	0.07	41,52,62,69	55
29	PL9	d	404[B]	55/55	0.95	0.07	41,52,63,70	55
25	BCR	b	618	40/40	0.96	0.06	47,61,78,83	0
27	GOL	c	526[A]	6/6	0.96	0.08	72,74,80,83	6
27	GOL	c	526[B]	6/6	0.96	0.08	72,75,81,83	6
23	CLA	c	502	65/65	0.96	0.07	54,67,80,89	0
23	CLA	c	504	65/65	0.96	0.07	49,71,86,103	0
25	BCR	c	516	40/40	0.96	0.07	53,67,80,90	0
23	CLA	A	405[A]	65/65	0.96	0.06	36,46,58,71	65
23	CLA	A	405[B]	65/65	0.96	0.06	35,46,58,71	65
23	CLA	D	702[A]	65/65	0.96	0.07	36,45,68,81	65
23	CLA	D	702[B]	65/65	0.96	0.07	36,45,68,83	65

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	CLA	B	602	65/65	0.96	0.06	46,56,71,86	0
23	CLA	c	512	65/65	0.96	0.08	57,71,87,114	0
23	CLA	C	502	65/65	0.96	0.06	49,60,74,85	0
23	CLA	C	504	65/65	0.96	0.06	47,62,72,85	0
23	CLA	A	406[A]	65/65	0.96	0.06	40,49,114,130	65
24	PHO	A	407[A]	64/64	0.96	0.06	40,46,53,59	64
24	PHO	A	407[B]	64/64	0.96	0.06	40,46,53,60	64
24	PHO	A	417[A]	64/64	0.96	0.06	37,50,58,62	64
24	PHO	A	417[B]	64/64	0.96	0.06	37,50,58,62	64
24	PHO	a	408[A]	64/64	0.96	0.06	42,49,54,57	64
24	PHO	a	408[B]	64/64	0.96	0.06	41,49,55,57	64
24	PHO	a	416[A]	64/64	0.96	0.07	44,56,63,67	64
24	PHO	a	416[B]	64/64	0.96	0.07	43,56,63,67	64
33	LHG	D	706[A]	49/49	0.96	0.08	48,55,68,77	49
33	LHG	D	706[B]	49/49	0.96	0.08	47,55,68,78	49
23	CLA	C	506	65/65	0.96	0.07	45,61,91,102	0
25	BCR	B	617	40/40	0.96	0.06	41,55,63,71	0
23	CLA	b	602	65/65	0.96	0.07	48,61,84,94	0
23	CLA	b	604	65/65	0.96	0.07	43,53,103,127	0
33	LHG	L	101[A]	49/49	0.96	0.07	51,59,70,92	49
33	LHG	L	101[B]	49/49	0.96	0.07	50,59,70,92	49
23	CLA	A	406[B]	65/65	0.96	0.06	40,49,114,130	65
25	BCR	C	516	40/40	0.96	0.06	51,63,77,84	0
23	CLA	b	607	65/65	0.96	0.07	38,50,81,91	0
23	CLA	b	609	65/65	0.96	0.07	47,64,75,91	0
23	CLA	b	611	65/65	0.96	0.07	38,51,72,80	0
23	CLA	b	612	65/65	0.96	0.07	40,54,65,72	0
37	CA	O	301	1/1	0.96	0.06	113,113,113,113	0
23	CLA	B	607	65/65	0.96	0.06	36,48,74,86	0
23	CLA	b	615	65/65	0.96	0.06	49,61,84,94	0
23	CLA	B	610	65/65	0.96	0.08	43,55,68,89	0
21	FE2	a	401[A]	1/1	0.97	0.04	54,54,54,54	1
23	CLA	B	615	65/65	0.97	0.06	44,55,83,97	0
23	CLA	a	405[A]	65/65	0.97	0.07	41,48,64,76	65
23	CLA	a	405[B]	65/65	0.97	0.07	40,47,64,77	65
23	CLA	a	406[A]	65/65	0.97	0.06	39,46,67,71	65
23	CLA	a	406[B]	65/65	0.97	0.06	39,47,67,71	65
23	CLA	c	510	65/65	0.97	0.08	50,63,92,98	0
23	CLA	c	511	65/65	0.97	0.06	50,64,77,90	0
21	FE2	a	401[B]	1/1	0.97	0.04	54,54,54,54	1
23	CLA	B	604	65/65	0.97	0.06	38,48,118,132	0
23	CLA	C	503	65/65	0.97	0.06	43,55,81,92	0

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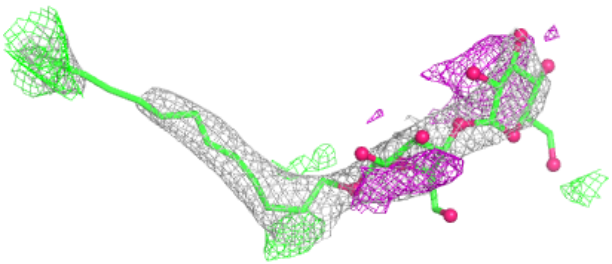
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	CLA	d	401[A]	65/65	0.97	0.06	41,47,71,91	65
23	CLA	d	401[B]	65/65	0.97	0.06	41,47,72,91	65
23	CLA	B	605	65/65	0.97	0.06	40,50,68,85	0
22	CL	A	403[A]	1/1	0.97	0.03	47,47,47,47	1
23	CLA	b	603	65/65	0.97	0.06	45,57,83,95	0
22	CL	A	403[B]	1/1	0.97	0.03	47,47,47,47	1
23	CLA	b	605	65/65	0.97	0.07	39,52,78,83	0
23	CLA	B	608	65/65	0.97	0.05	41,52,71,79	0
23	CLA	B	609	65/65	0.97	0.06	45,60,74,78	0
23	CLA	b	608	65/65	0.97	0.05	42,58,79,96	0
23	CLA	A	404[A]	65/65	0.97	0.06	38,44,62,71	65
23	CLA	b	610	65/65	0.97	0.07	49,58,71,83	0
23	CLA	C	510	65/65	0.97	0.08	46,59,84,88	0
23	CLA	C	511	65/65	0.97	0.06	48,59,79,85	0
23	CLA	b	613	65/65	0.97	0.05	42,52,88,102	0
37	CA	C	524	1/1	0.97	0.06	71,71,71,71	0
23	CLA	C	512	65/65	0.97	0.07	52,64,81,91	0
23	CLA	A	404[B]	65/65	0.97	0.06	37,44,63,71	65
23	CLA	B	612	65/65	0.97	0.06	36,50,64,75	0
23	CLA	B	613	65/65	0.97	0.06	40,48,97,105	0
23	CLA	c	503	65/65	0.97	0.07	44,60,91,109	0
22	CL	a	402[B]	1/1	0.98	0.06	50,50,50,50	1
22	CL	A	402[A]	1/1	0.98	0.06	43,43,43,43	1
22	CL	A	402[B]	1/1	0.98	0.06	44,44,44,44	1
22	CL	a	402[A]	1/1	0.98	0.06	49,49,49,49	1
38	HEM	F	102	43/43	0.98	0.07	54,69,84,91	0
38	HEM	f	101	43/43	0.98	0.07	58,86,113,139	0
39	MG	J	102	1/1	0.98	0.03	60,60,60,60	0
40	HEC	V	201	43/43	0.98	0.06	41,52,59,62	0
40	HEC	v	201	43/43	0.98	0.07	51,62,70,78	0
21	FE2	A	401[A]	1/1	0.99	0.03	52,52,52,52	1
37	CA	c	524	1/1	0.99	0.03	81,81,81,81	0
21	FE2	A	401[B]	1/1	0.99	0.03	52,52,52,52	1
22	CL	a	403[A]	1/1	0.99	0.07	53,53,53,53	1
22	CL	a	403[B]	1/1	0.99	0.07	53,53,53,53	1
28	OEX	A	413[A]	10/10	0.99	0.03	43,46,49,51	10
28	OEX	A	413[B]	10/10	0.99	0.03	42,46,50,50	10
39	MG	j	102	1/1	0.99	0.04	67,67,67,67	0
28	OEX	a	413[A]	10/10	0.99	0.03	47,50,54,56	10
28	OEX	a	413[B]	10/10	0.99	0.03	46,50,54,54	10

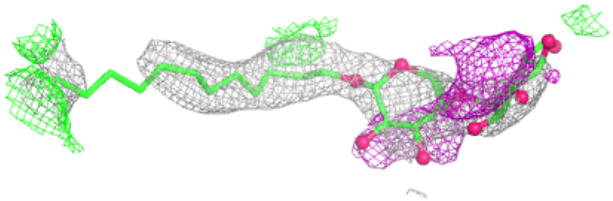
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

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 LMT B 629:

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

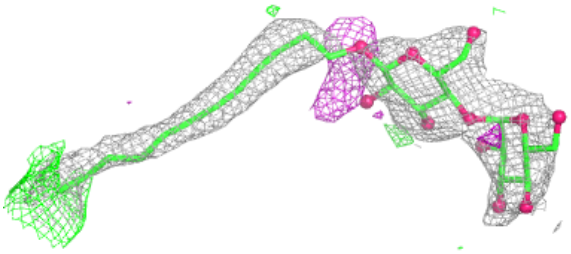


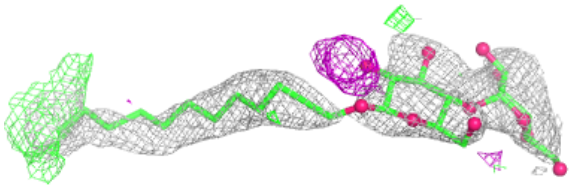


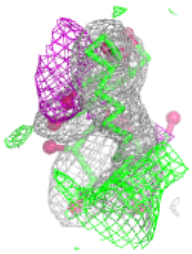


Electron density around LMT A 418:

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

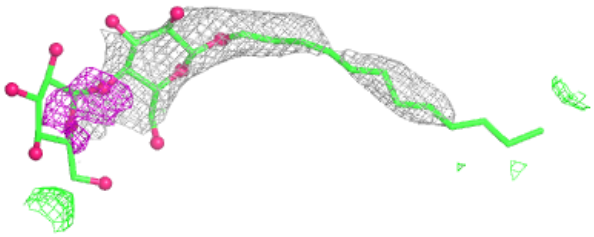


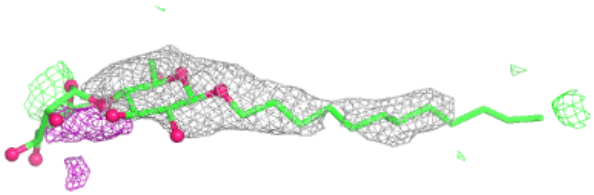


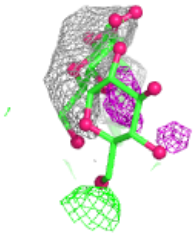


Electron density around LMT F 101:

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

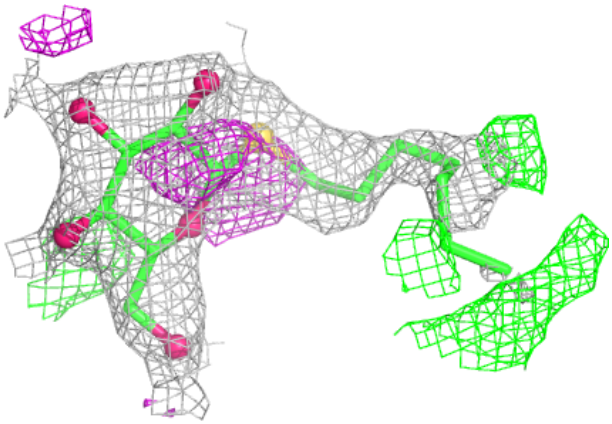


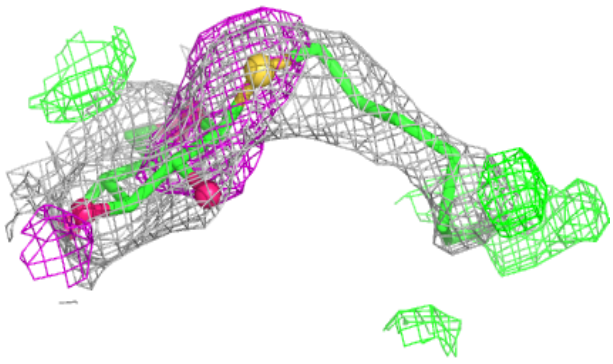


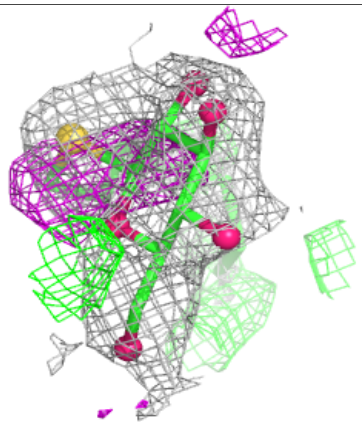


Electron density around HTG B 622:

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

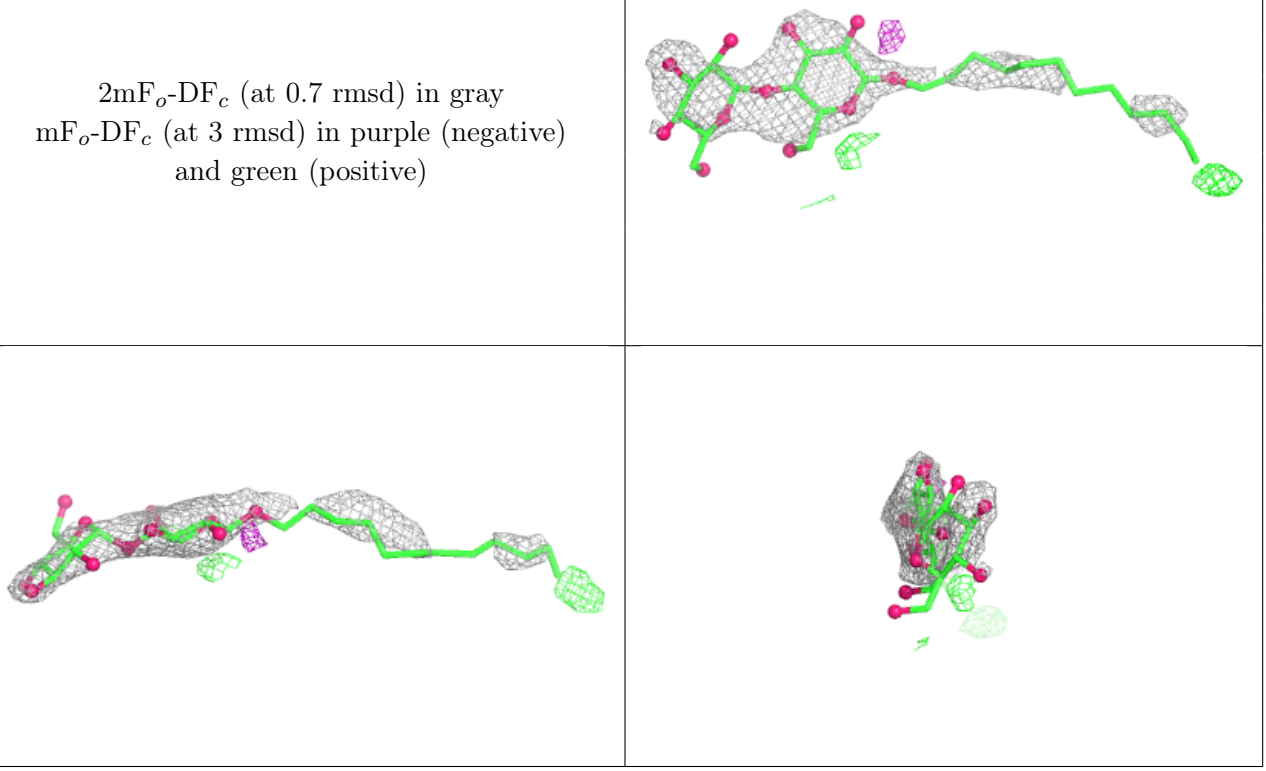






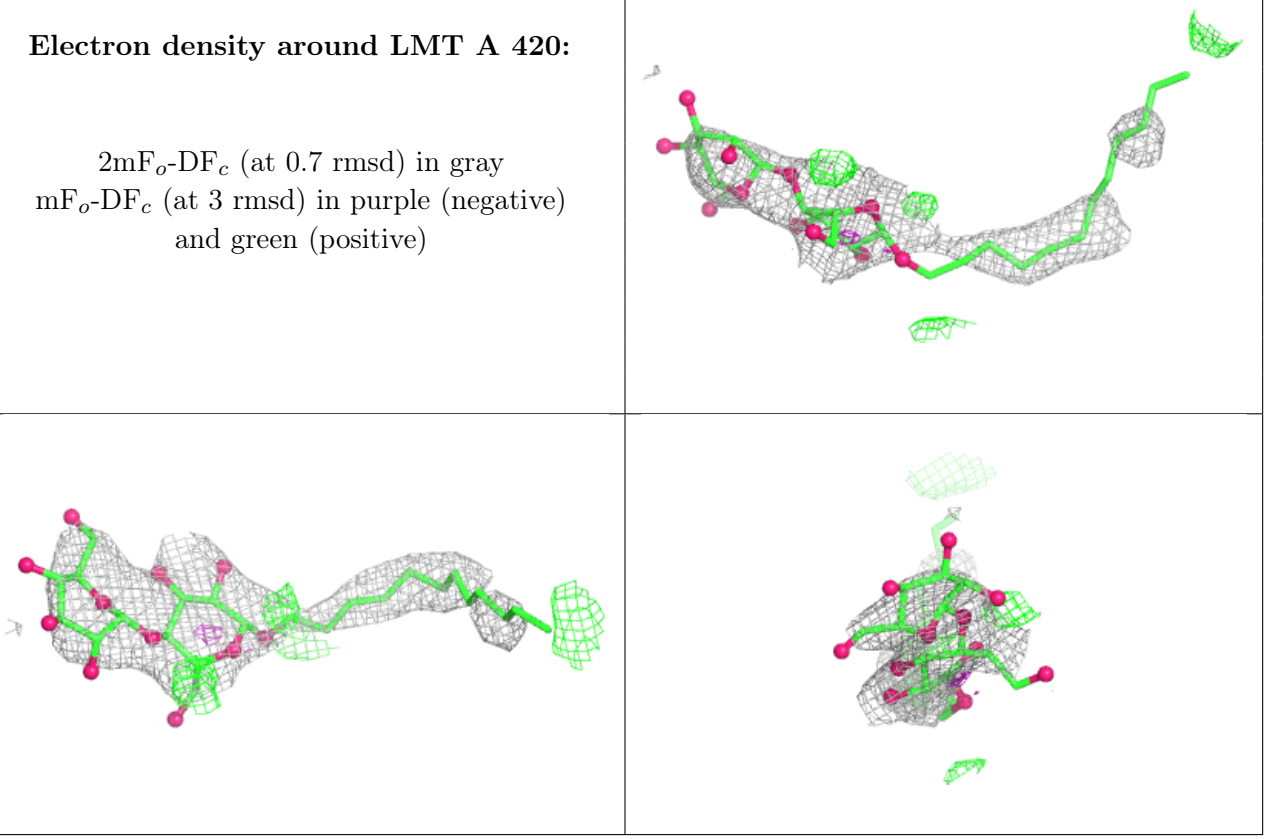
Electron density around LMT a 417:

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



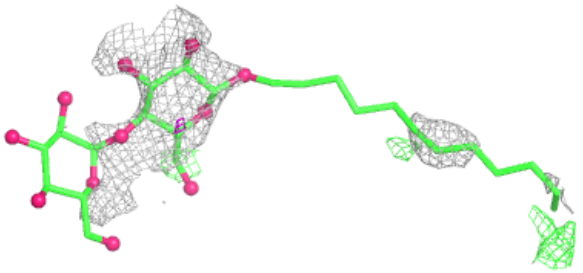
Electron density around LMT A 420:

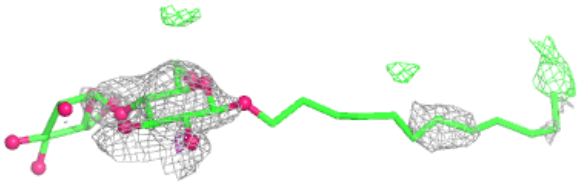
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

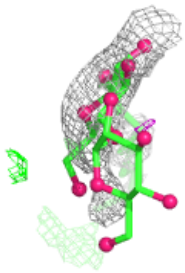


Electron density around LMT e 101:

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



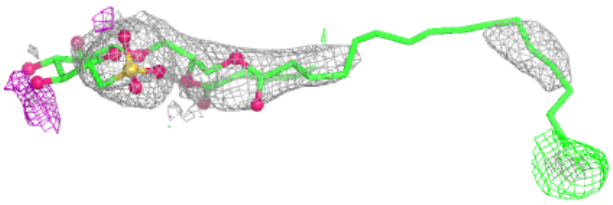


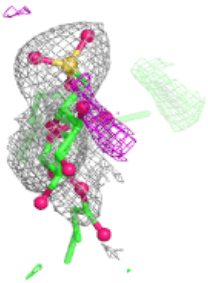


Electron density around SQD f 102:

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

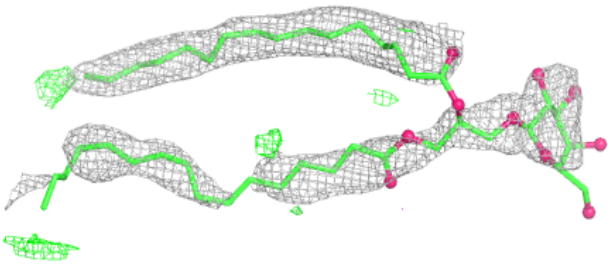


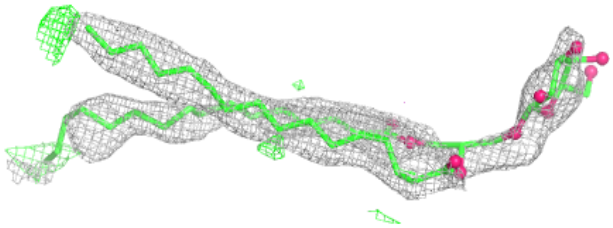


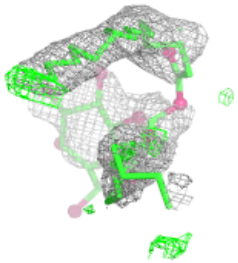


Electron density around LMG C 521:

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

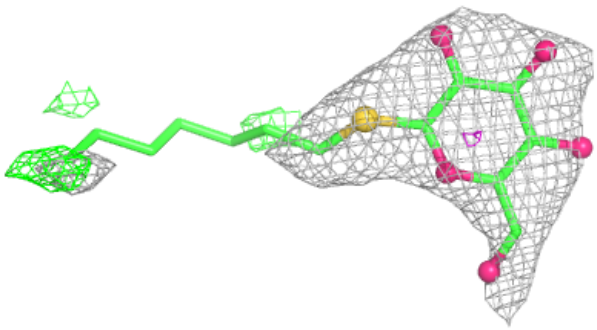


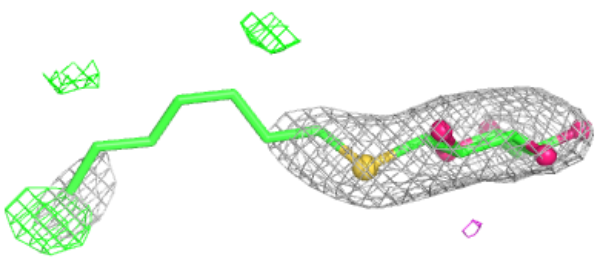


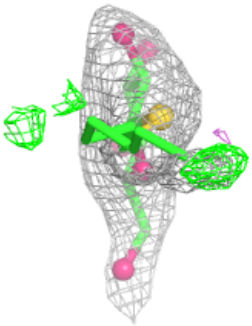


Electron density around HTG C 522:

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

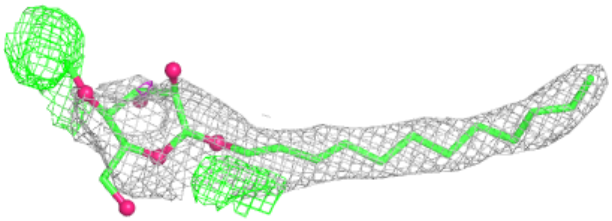


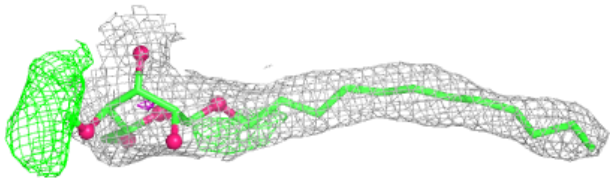


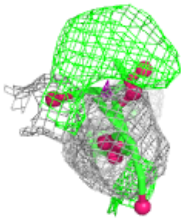


Electron density around LMT b 621:

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

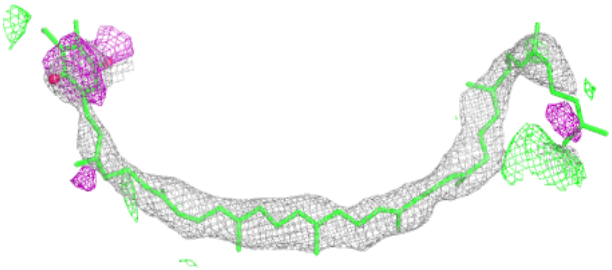


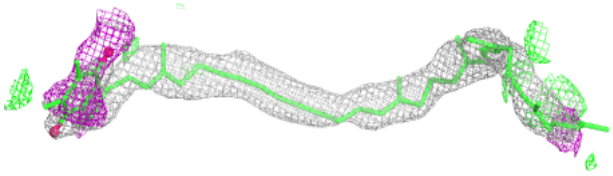


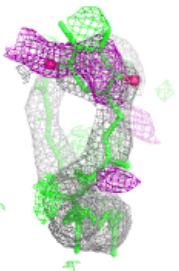


Electron density around PL9 A 414 (A):

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

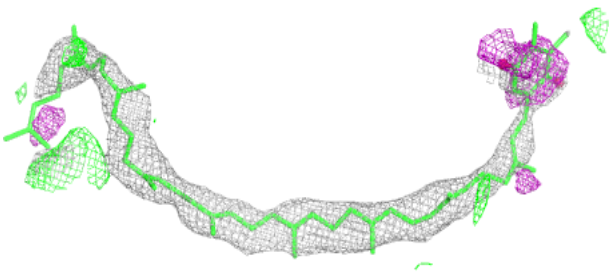


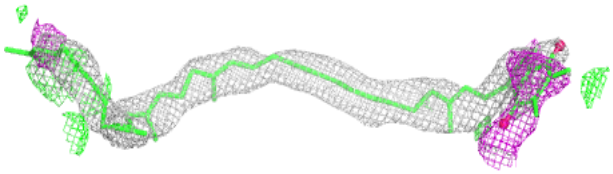


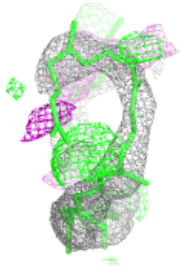


Electron density around PL9 A 414 (B):

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

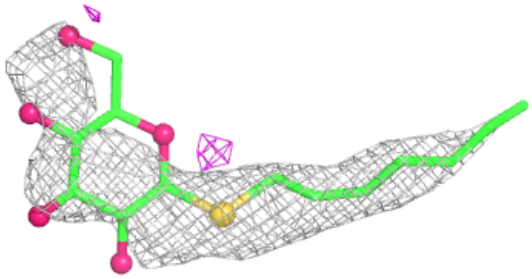


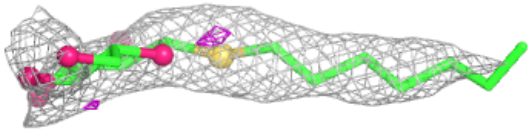


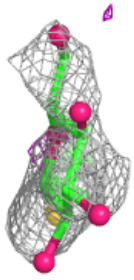


Electron density around HTG b 623:

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

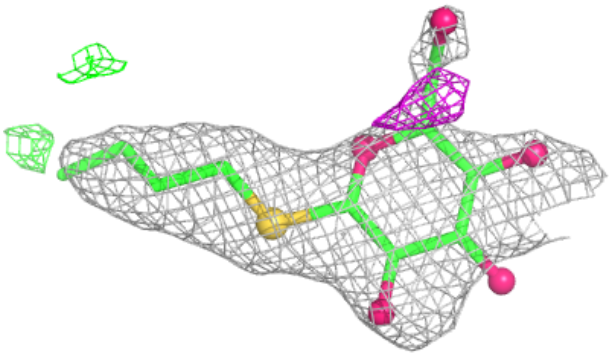


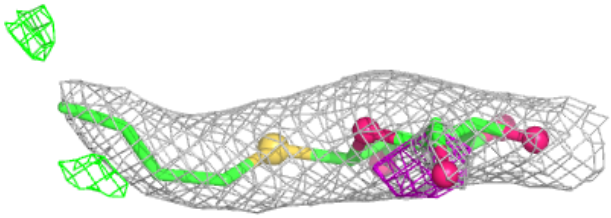


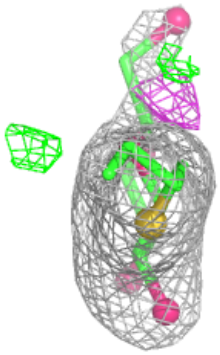


Electron density around HTG D 710:

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

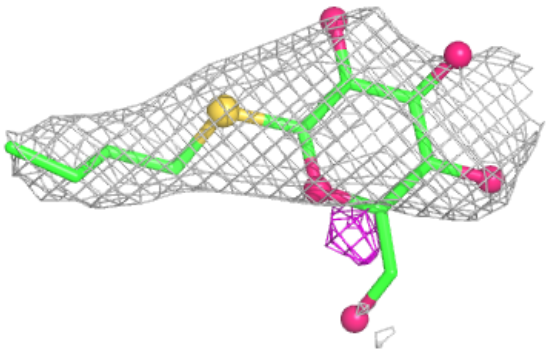


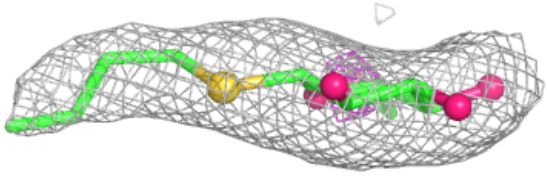


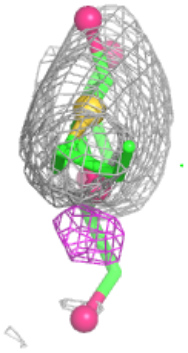


Electron density around HTG d 409:

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

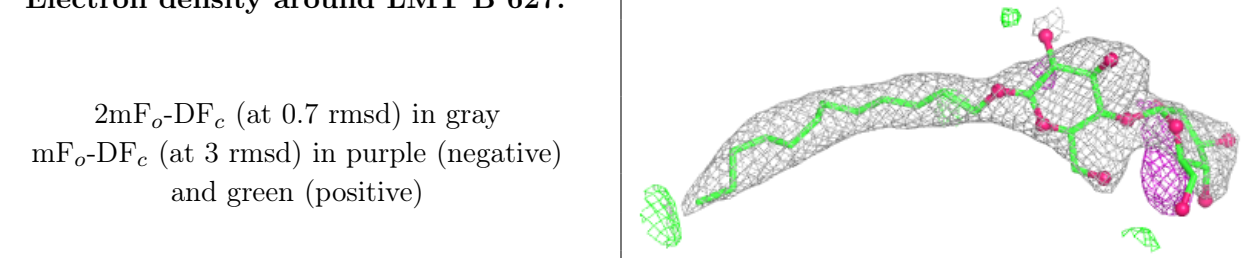


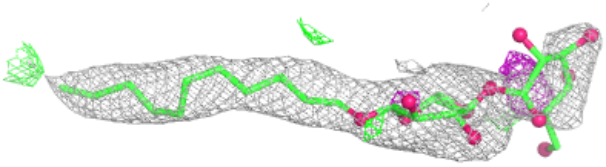


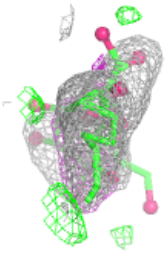


Electron density around LMT B 627:

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

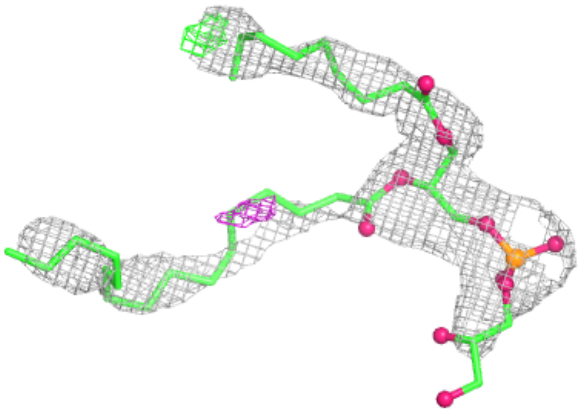


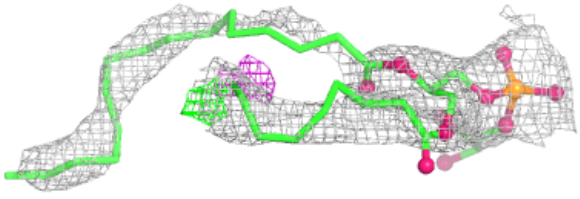


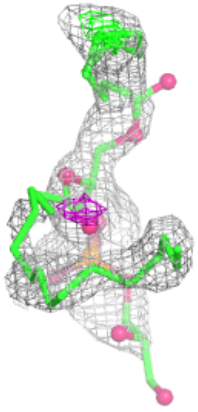


Electron density around LHG a 420 (B):

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

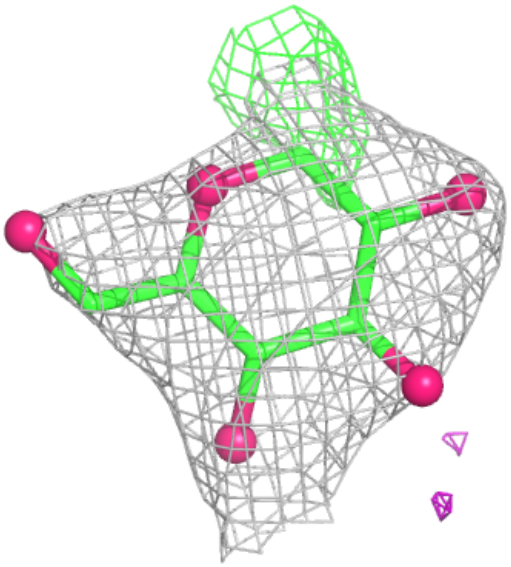


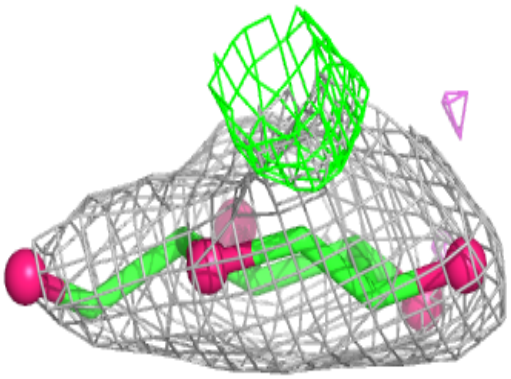


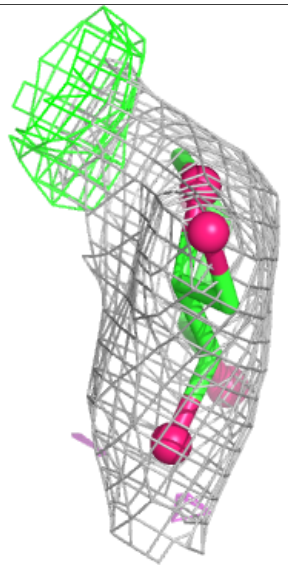


Electron density around HTG V 202:

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

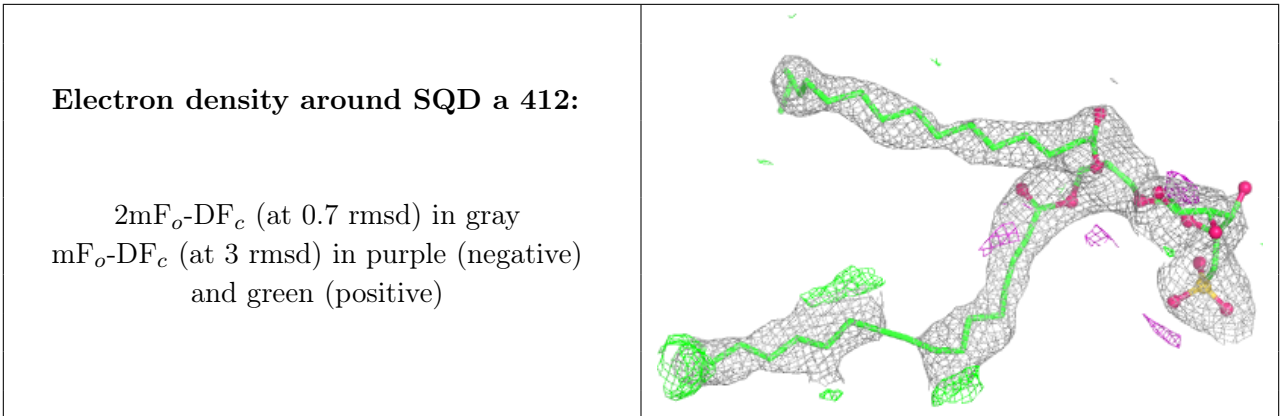


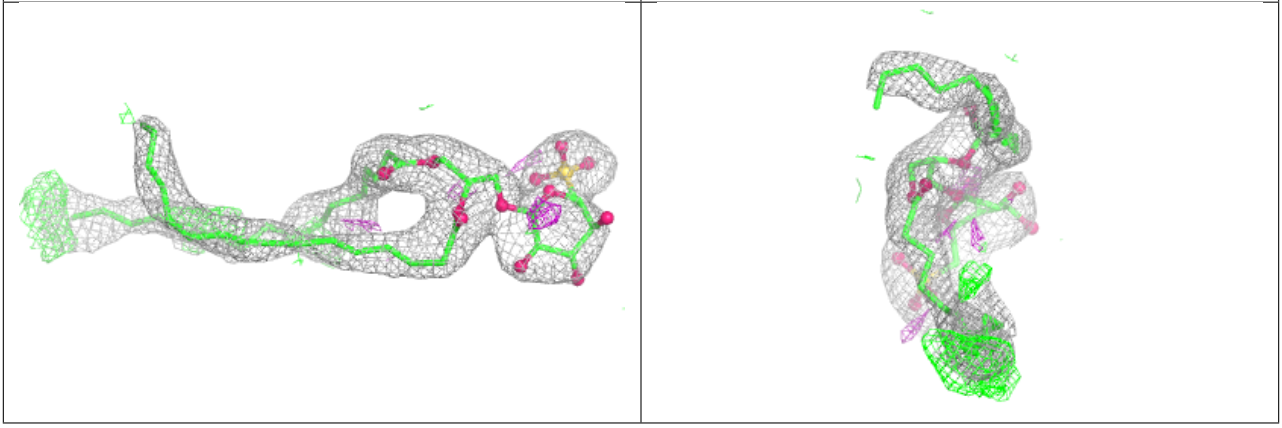




Electron density around SQD a 412:

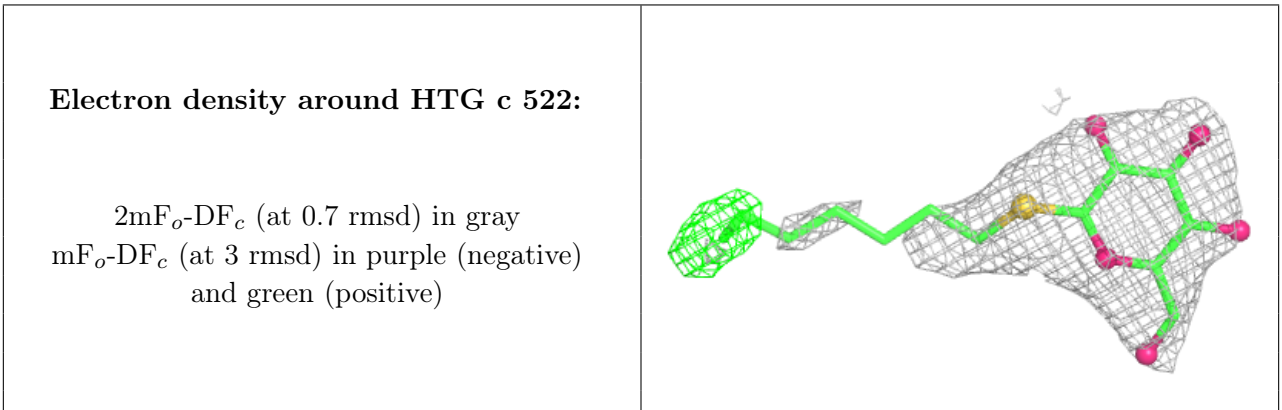
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

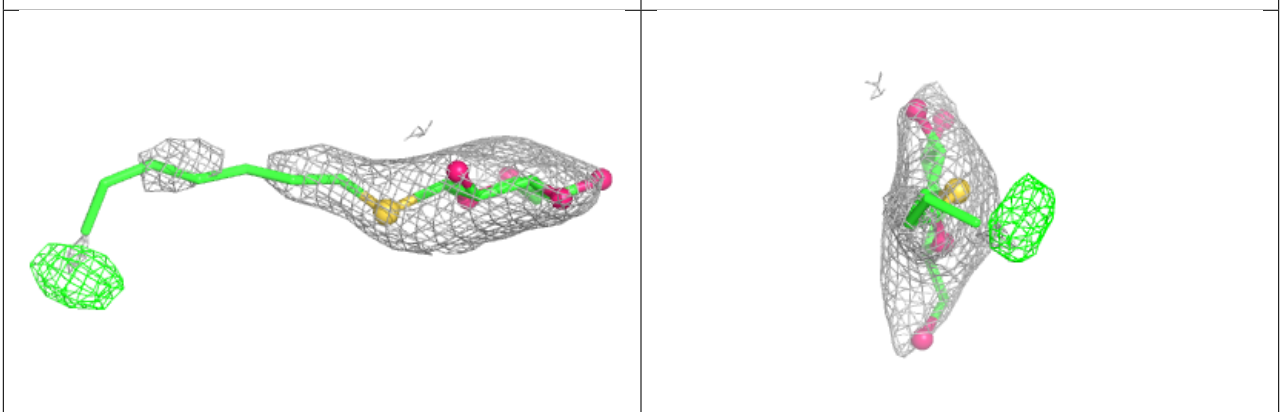




Electron density around HTG c 522:

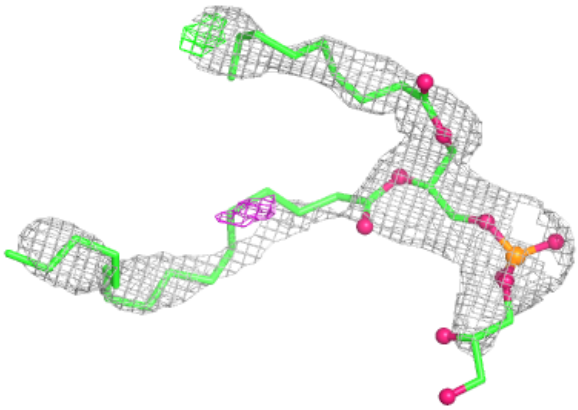
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

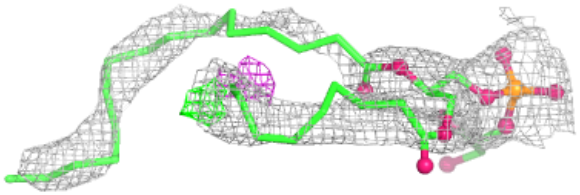


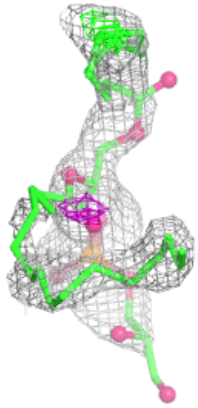


Electron density around LHG a 420 (A):

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

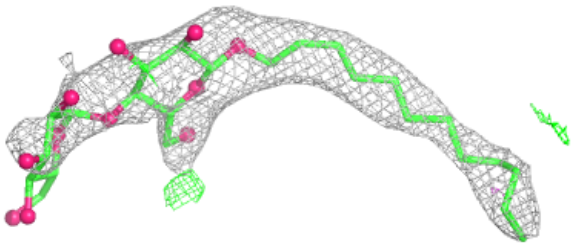


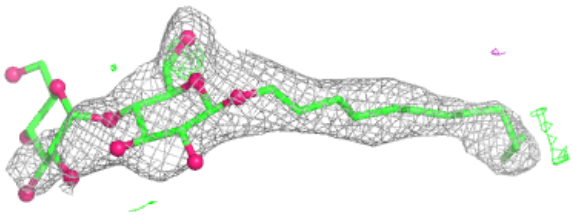


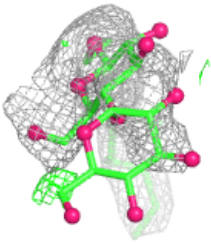


Electron density around LMT T 101:

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

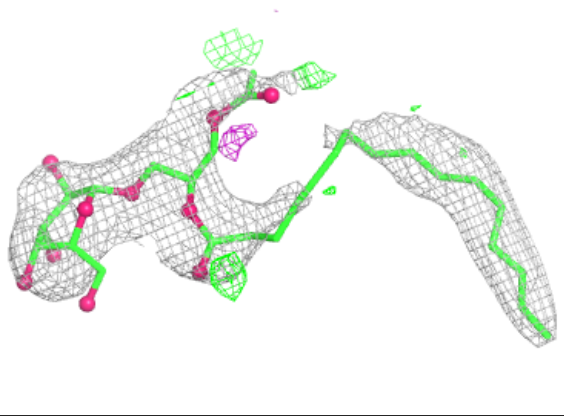


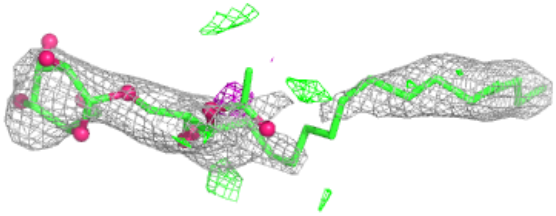


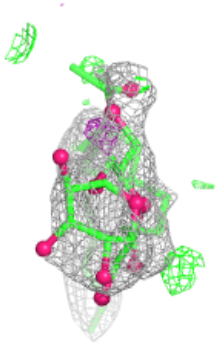


Electron density around LMG Z 101:

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

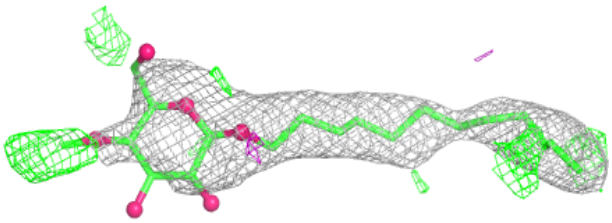


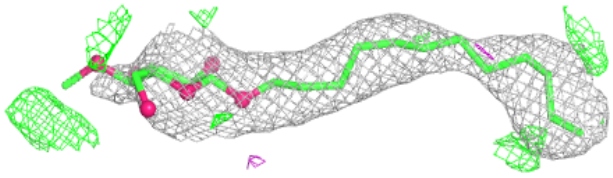


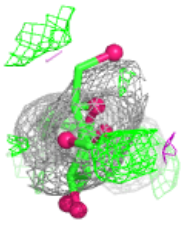


Electron density around LMT b 627:

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

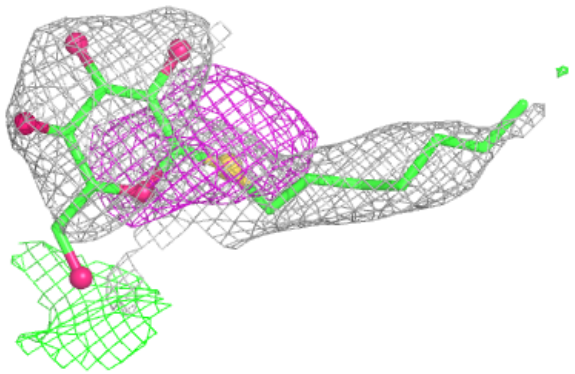


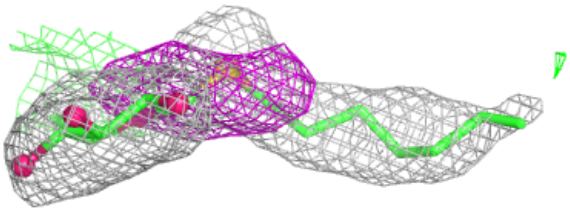


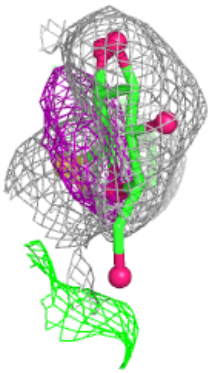


Electron density around HTG b 622:

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

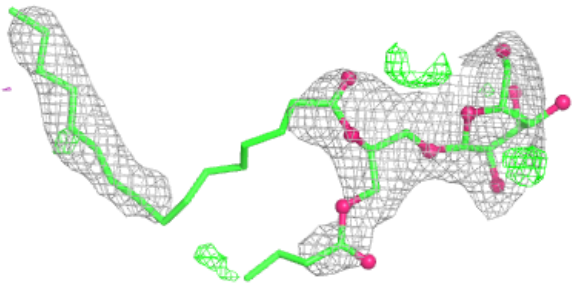


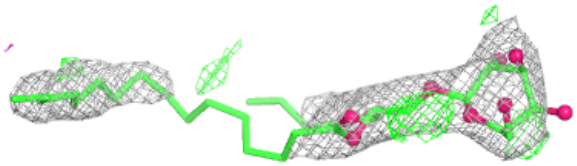


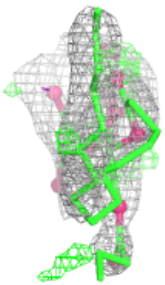


Electron density around LMG z 101:

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

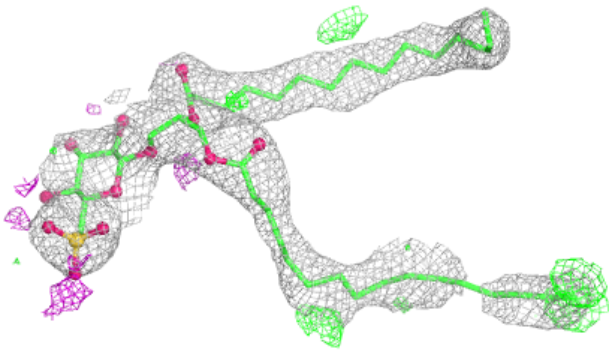


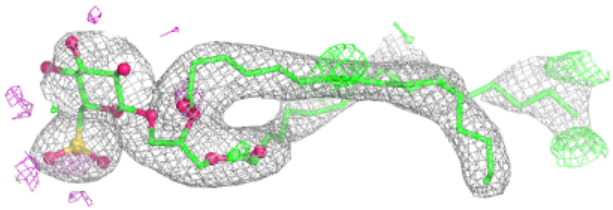


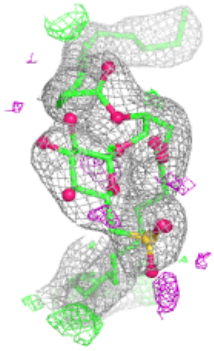


Electron density around SQD A 412:

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

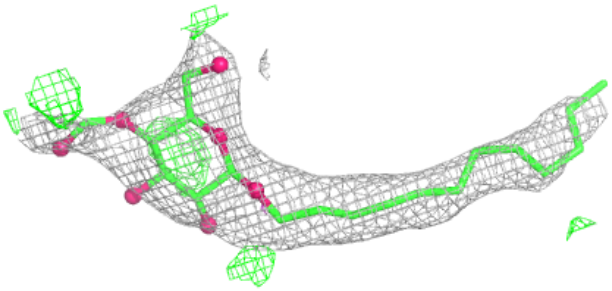


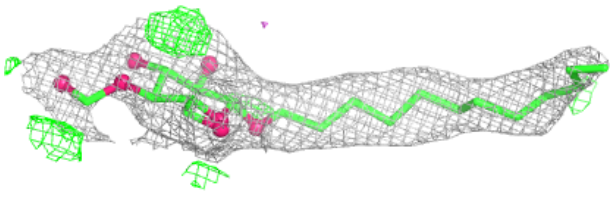


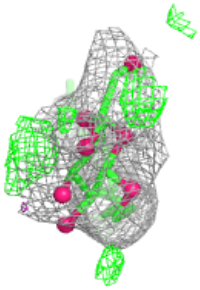


Electron density around LMT t 101:

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

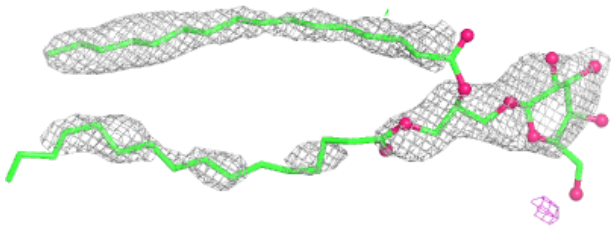


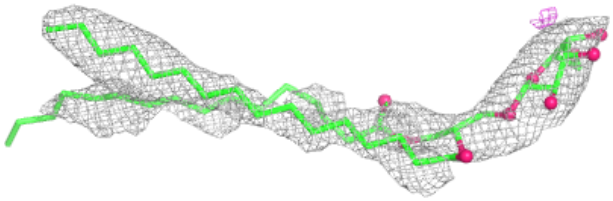


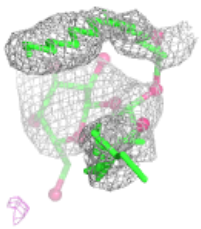


Electron density around LMG c 521:

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

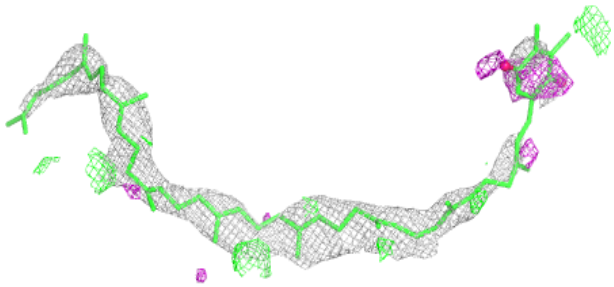


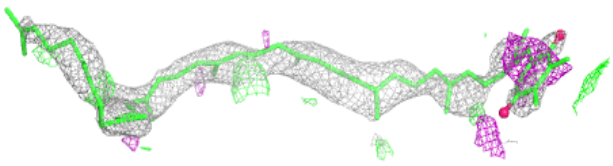


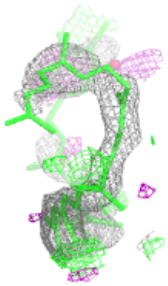


Electron density around PL9 a 414 (A):

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

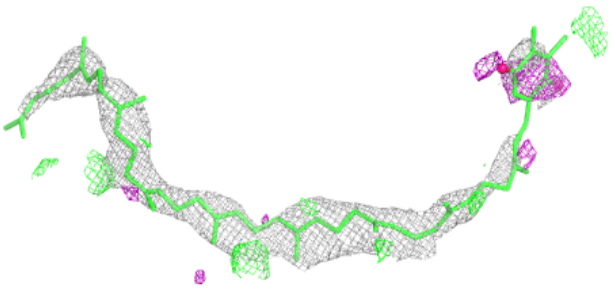


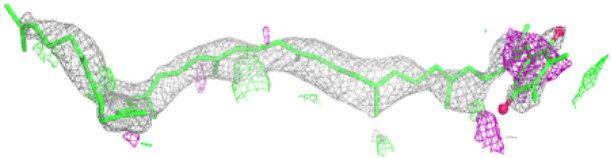


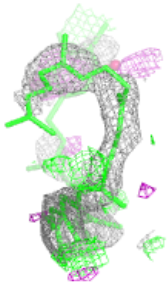


Electron density around PL9 a 414 (B):

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

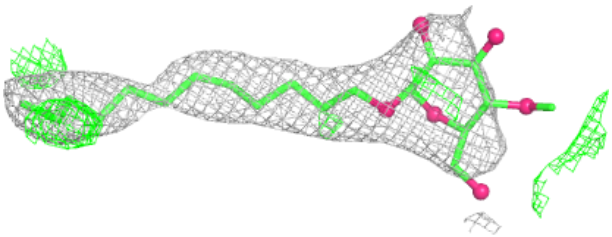


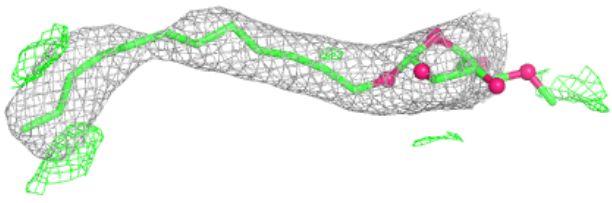


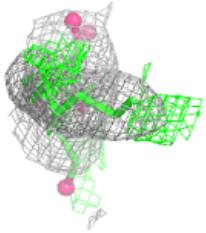


Electron density around LMT B 630:

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

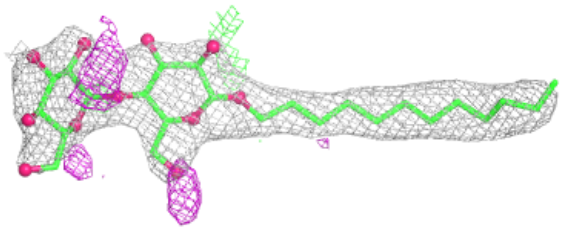


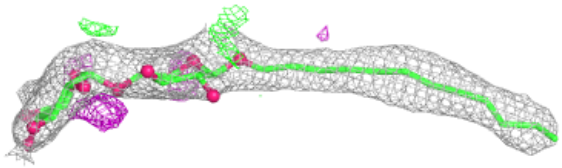


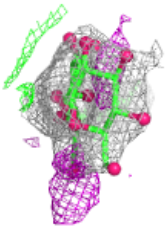


Electron density around LMT m 103:

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

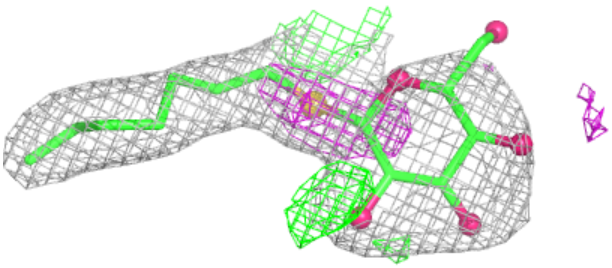


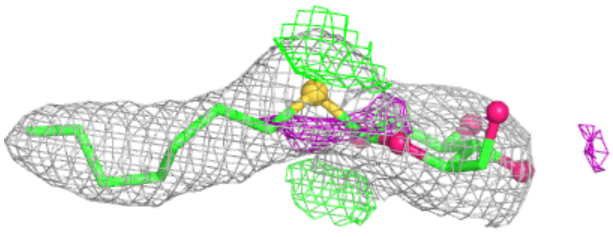


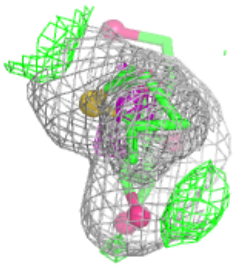


Electron density around HTG o 301:

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

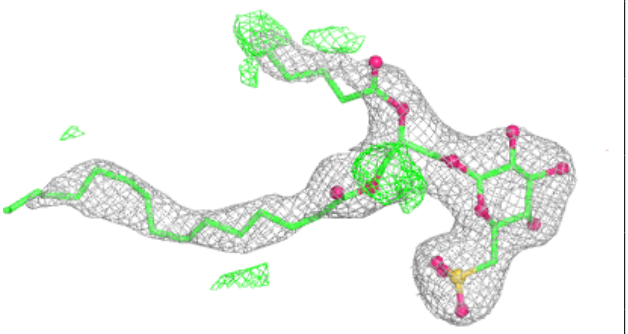


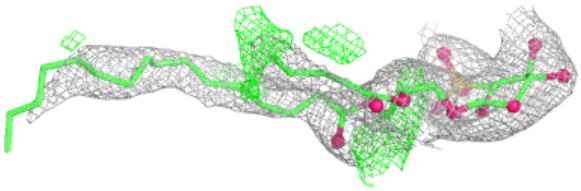


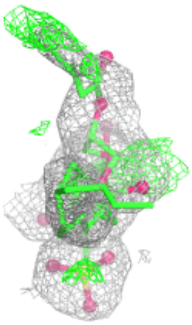


Electron density around SQD X 101:

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

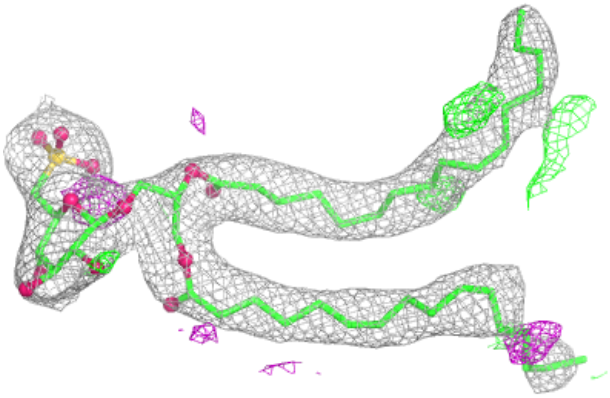


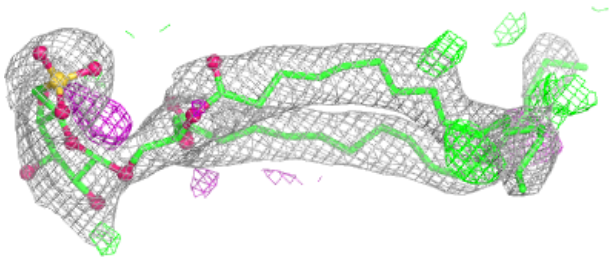


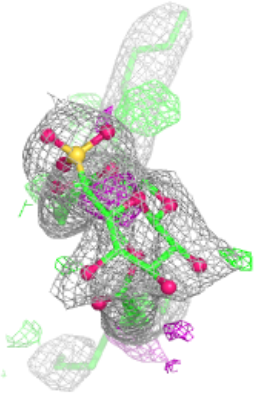


Electron density around SQD b 620:

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

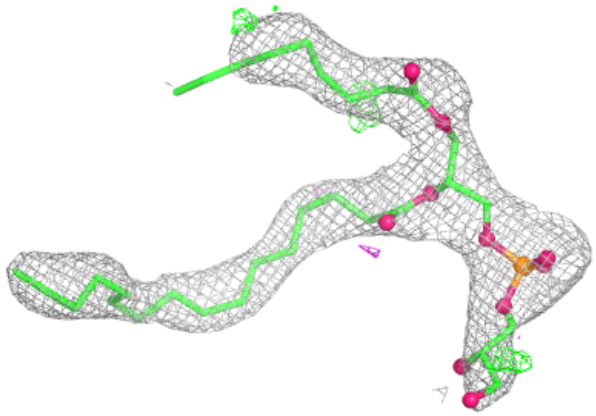


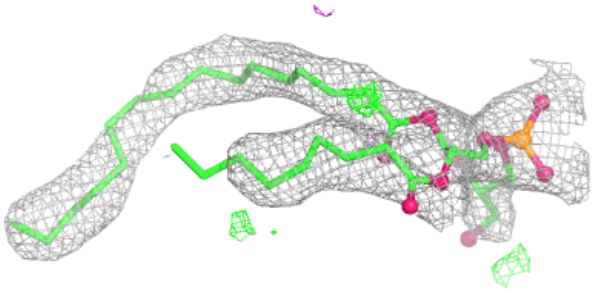


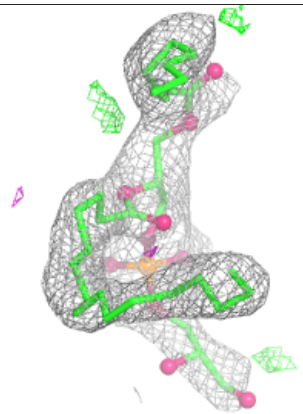


Electron density around LHG E 101 (A):

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

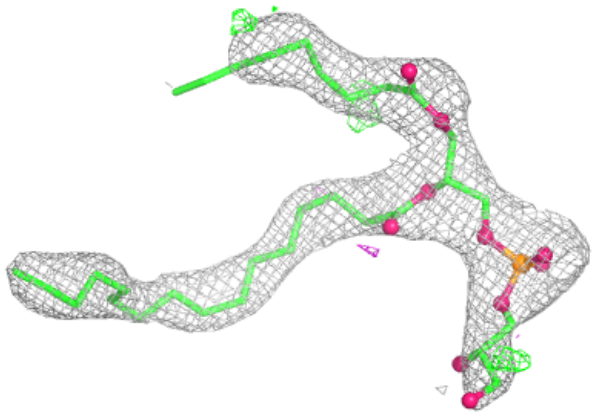


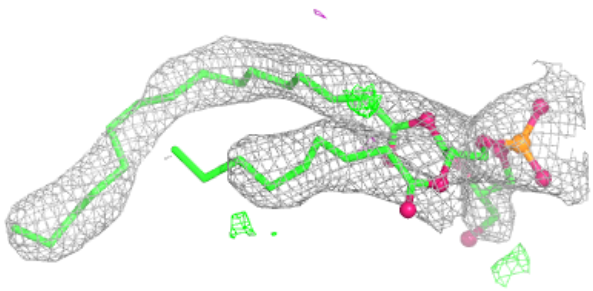


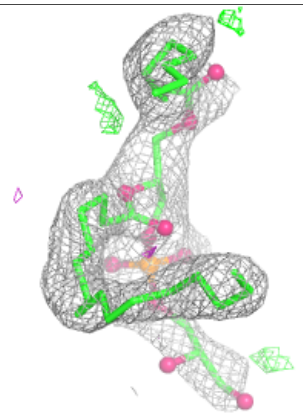


Electron density around LHG E 101 (B):

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

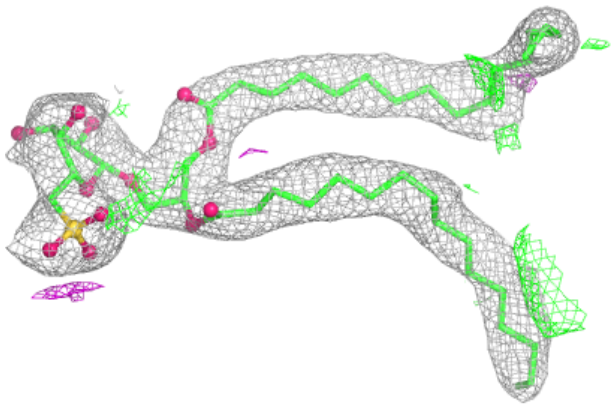


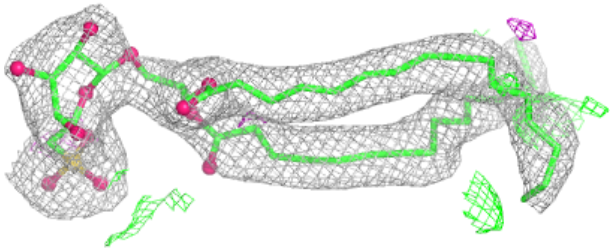


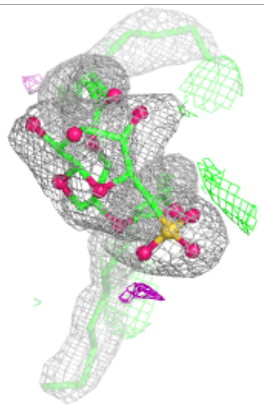


Electron density around SQD B 620:

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

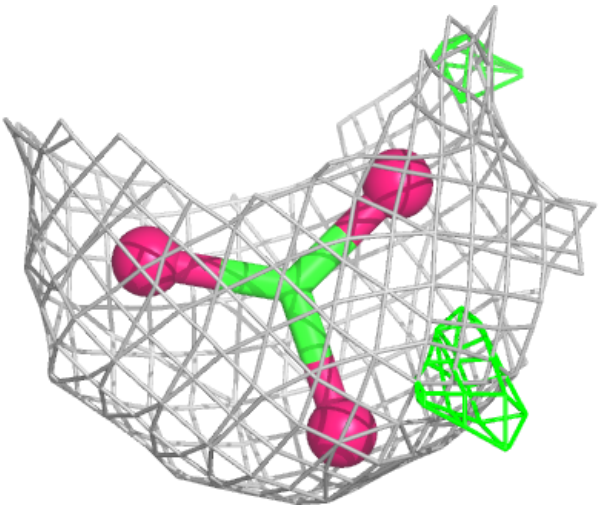


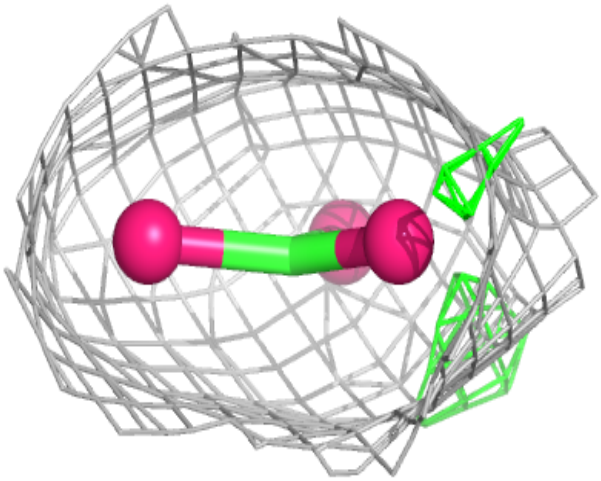


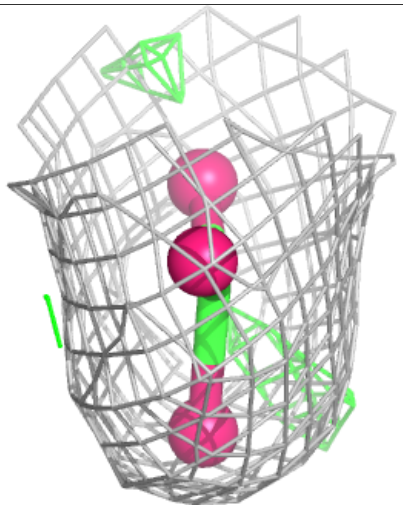


Electron density around BCT A 416 (A):

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

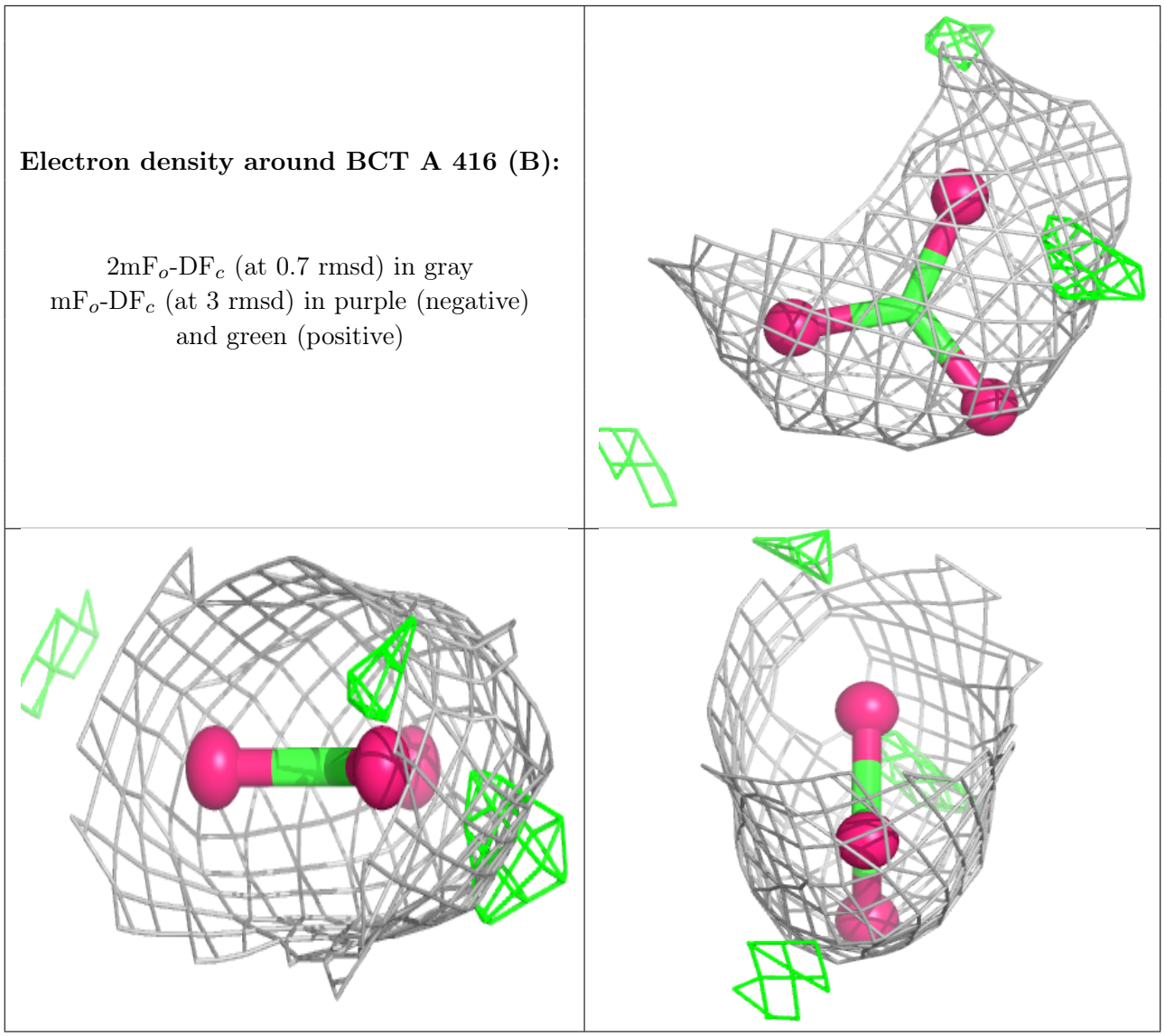






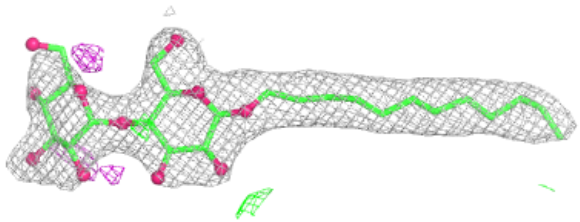
Electron density around BCT A 416 (B):

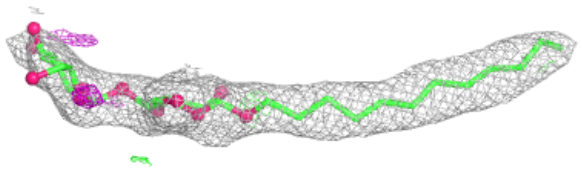
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

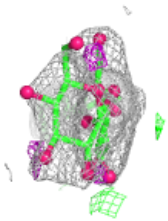


Electron density around LMT M 101:

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

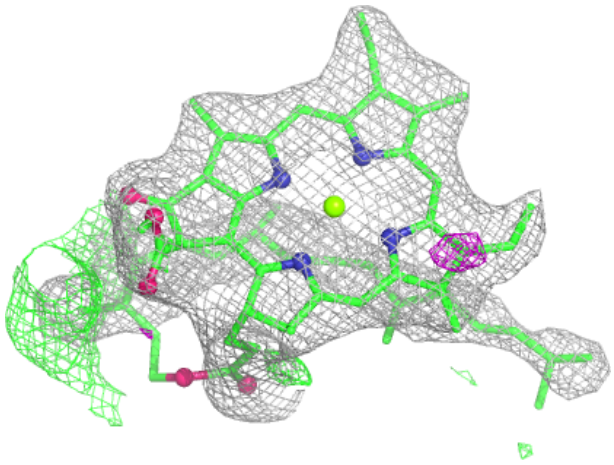


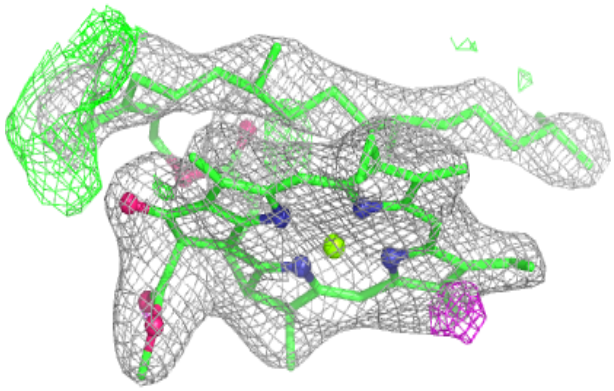


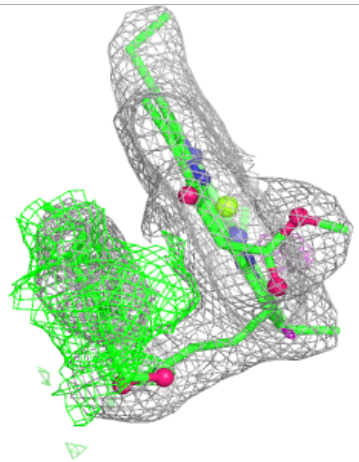


Electron density around CLA b 601:

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

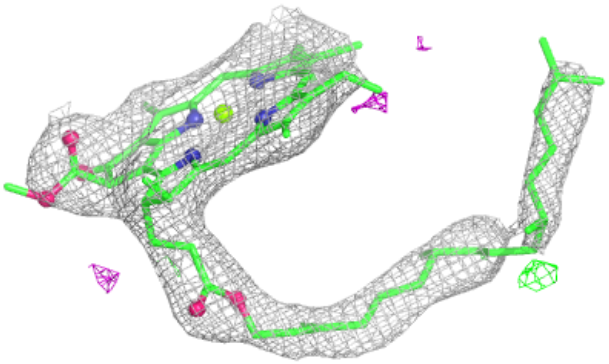


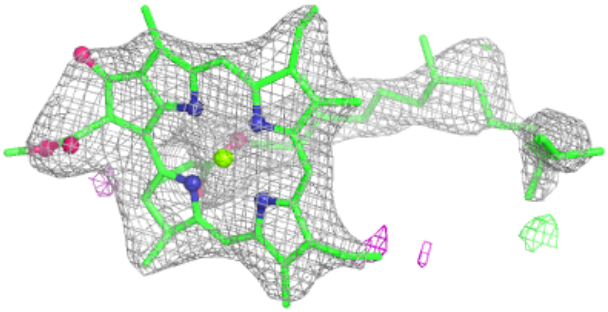


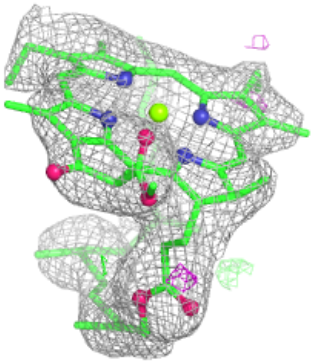


Electron density around CLA c 514:

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

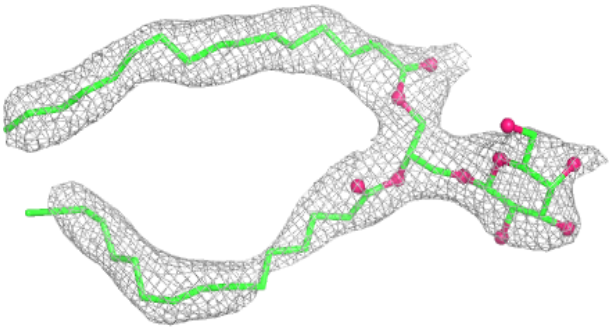


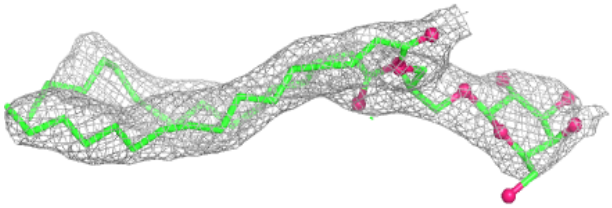


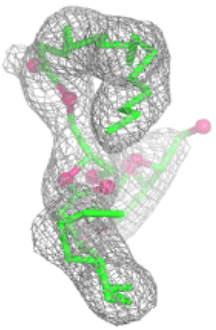


Electron density around LMG c 501:

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

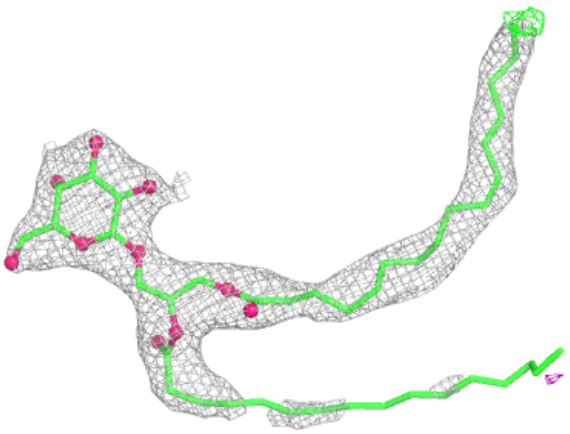


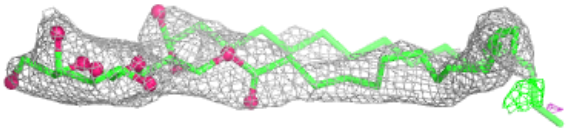


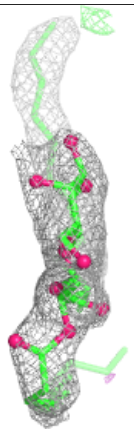


Electron density around LMG c 520:

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

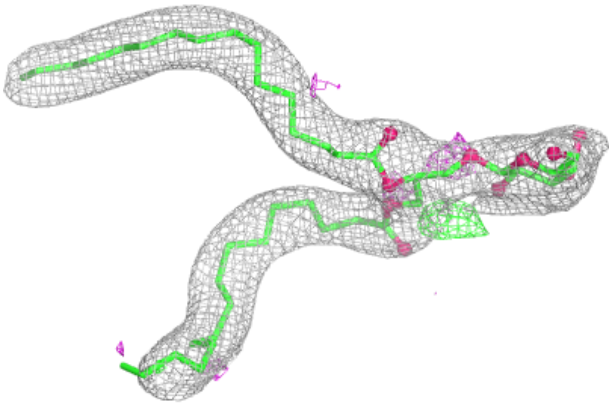


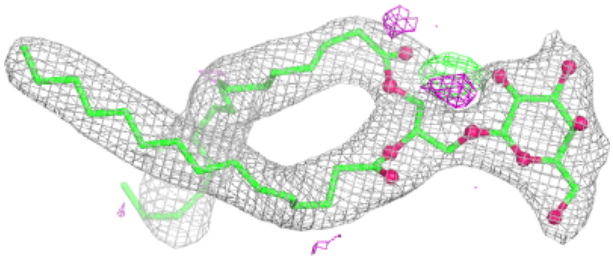


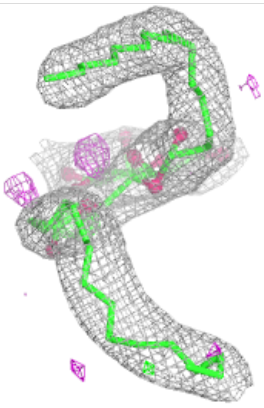


Electron density around LMG m 101:

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

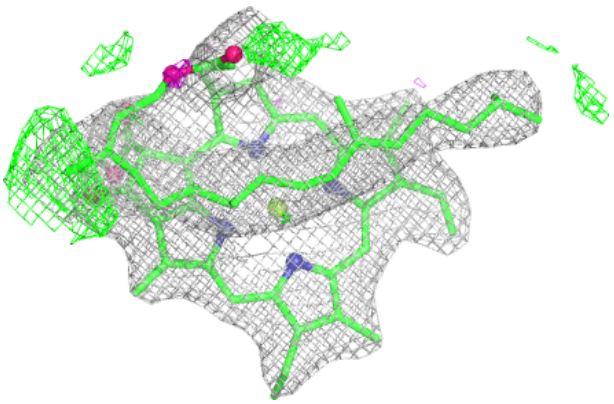


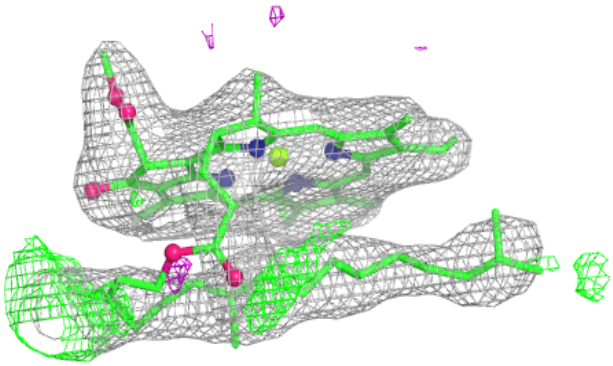


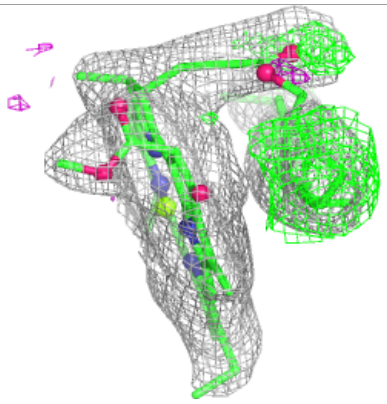


Electron density around CLA B 601:

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

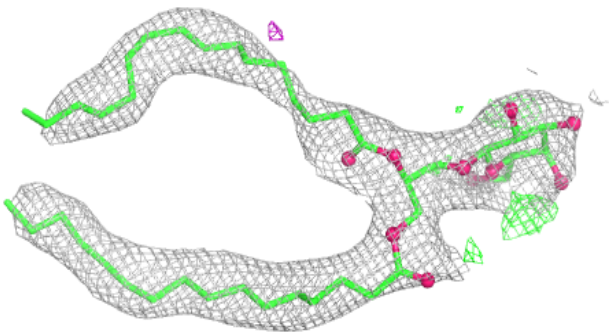


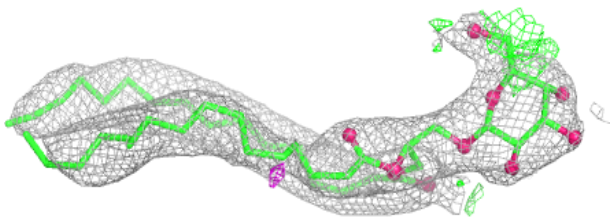


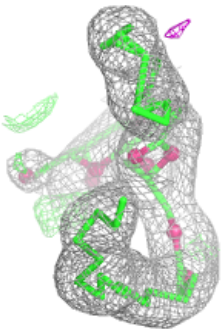


Electron density around LMG C 501:

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

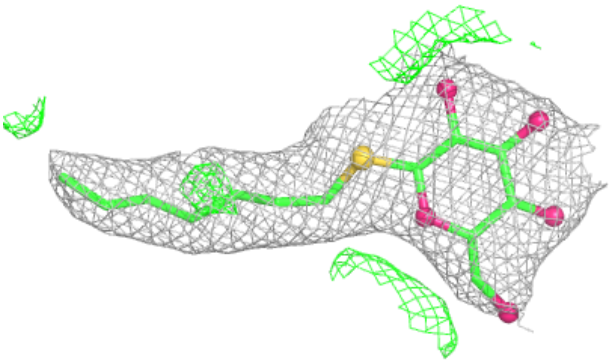


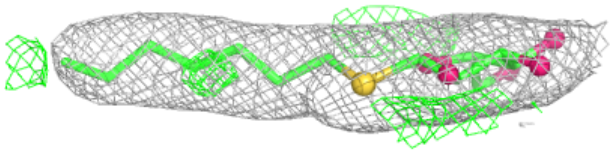


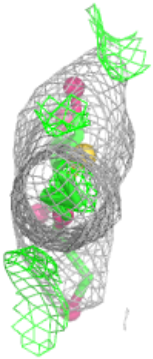


Electron density around HTG b 625:

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

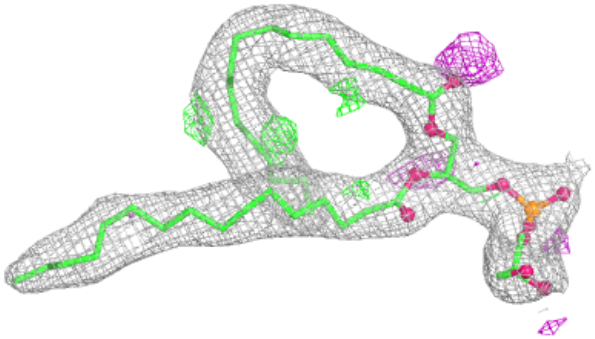


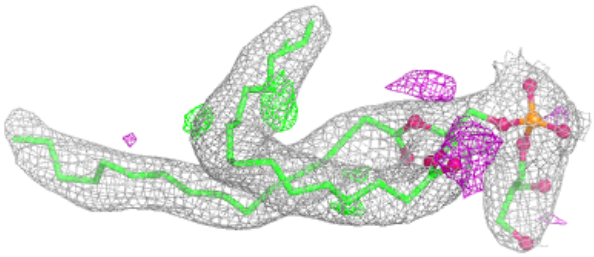




Electron density around LHG A 419 (A):

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

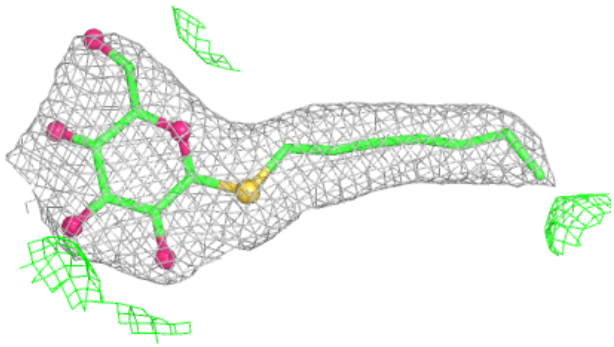


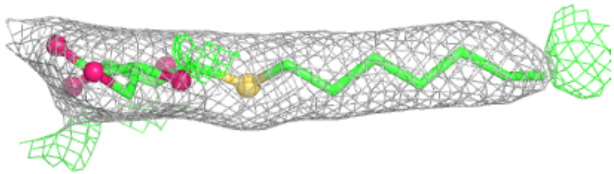


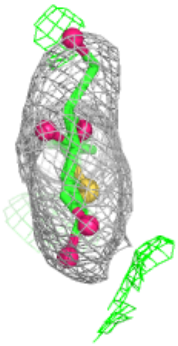


Electron density around HTG B 624:

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

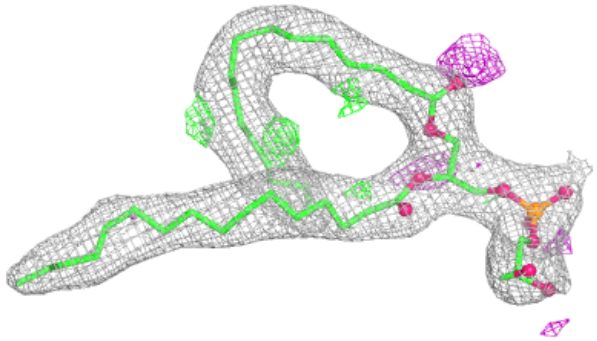


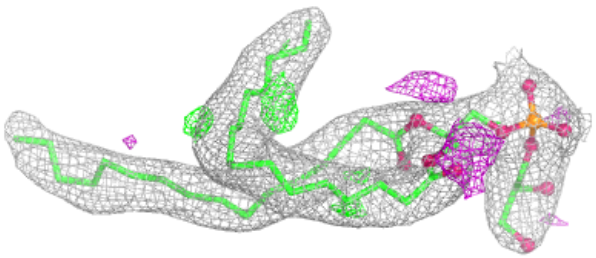




Electron density around LHG A 419 (B):

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

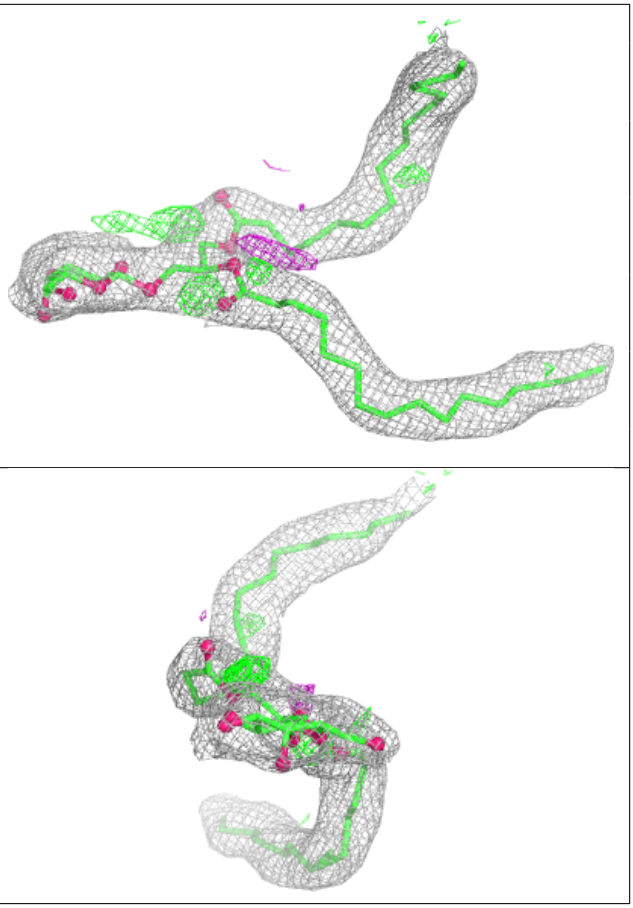






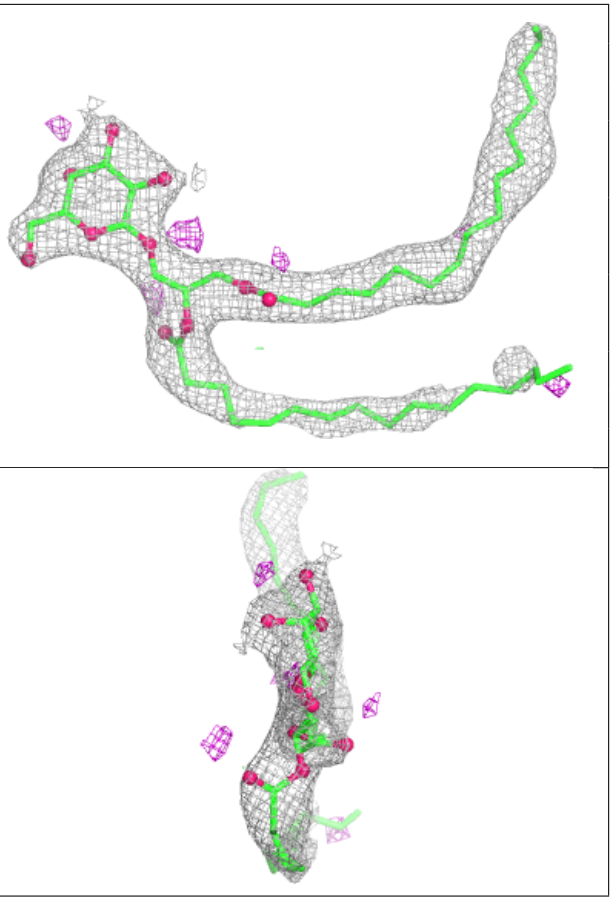
Electron density around LMG B 621:

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



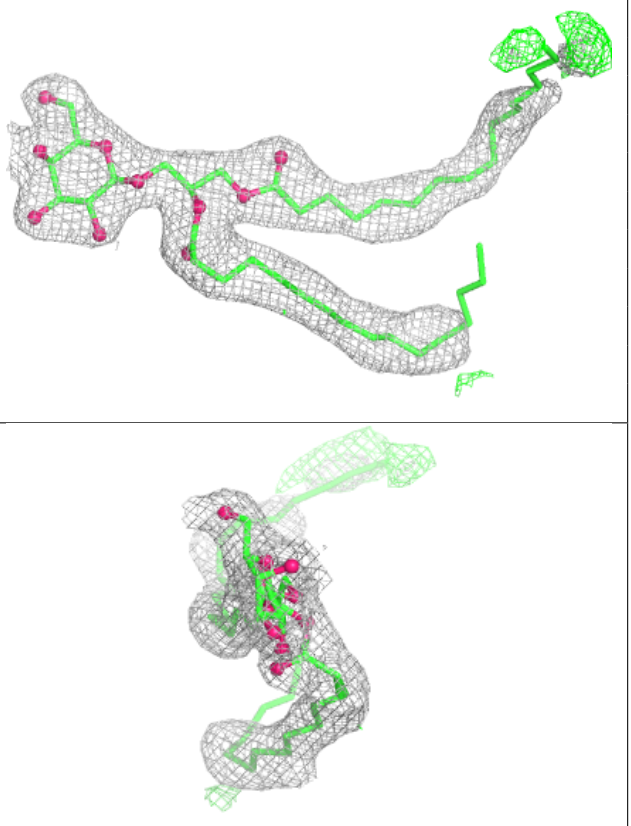
Electron density around LMG C 520:

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



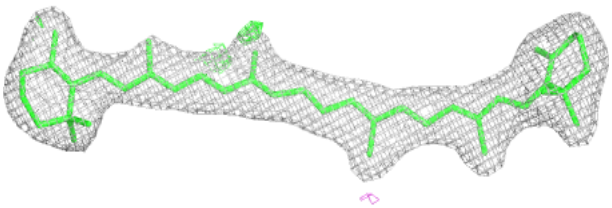
Electron density around LMG D 711:

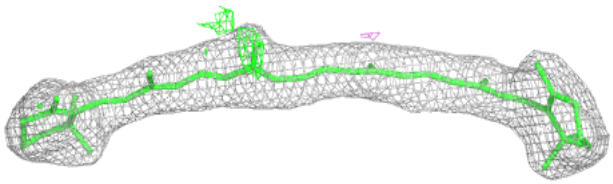
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

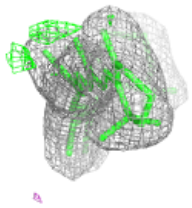


Electron density around BCR T 102:

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

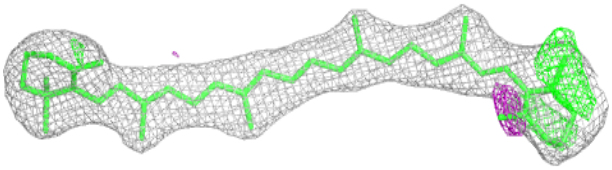


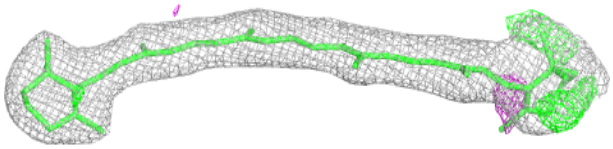


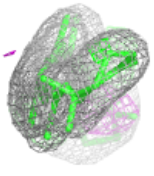


Electron density around BCR d 403:

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

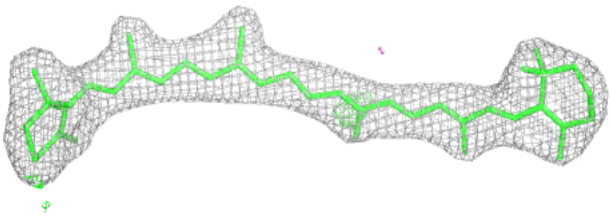


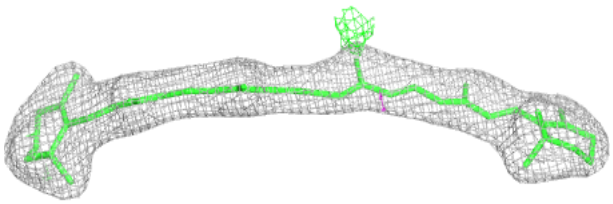


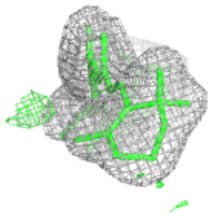


Electron density around BCR t 102:

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

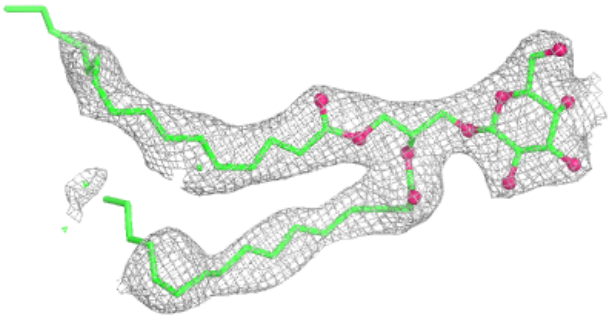


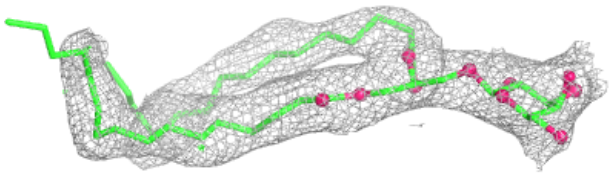


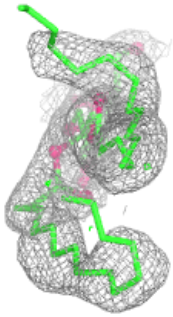


Electron density around LMG d 410:

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

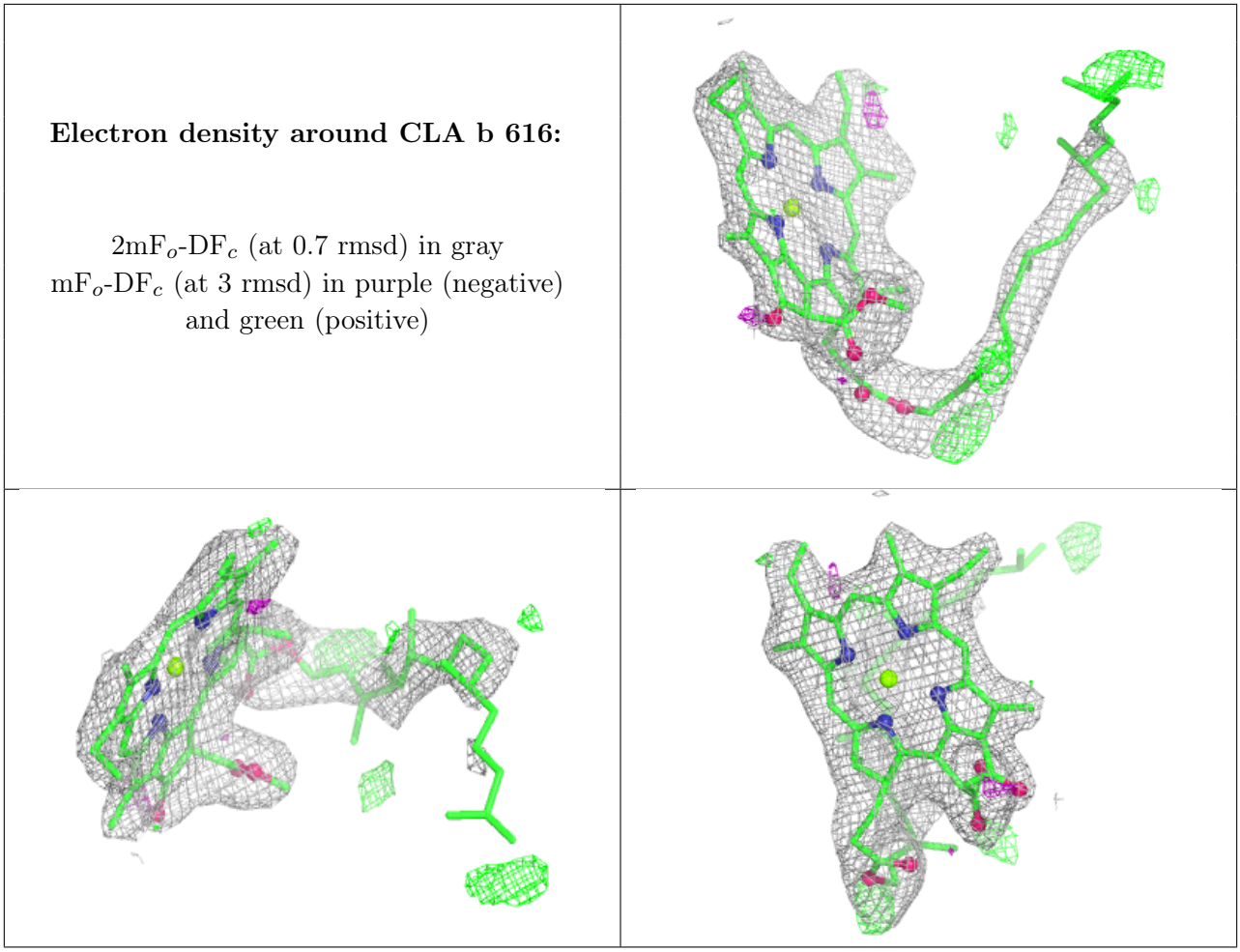






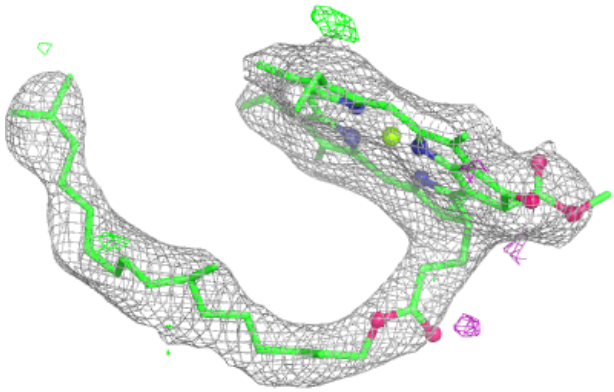
Electron density around CLA b 616:

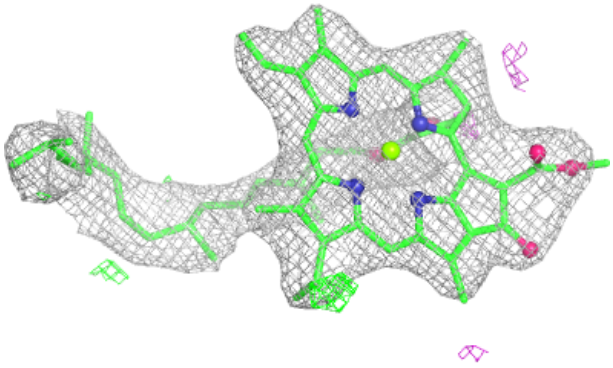
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

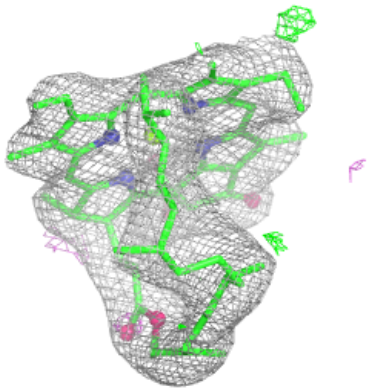


Electron density around CLA C 514:

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

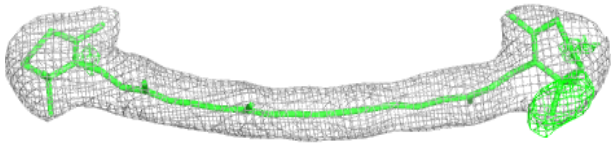


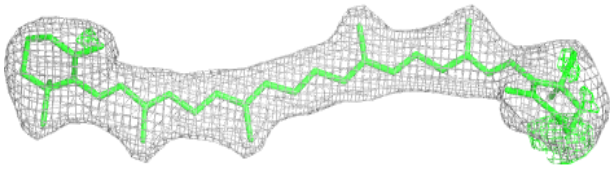


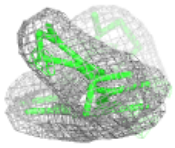


Electron density around BCR D 704:

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

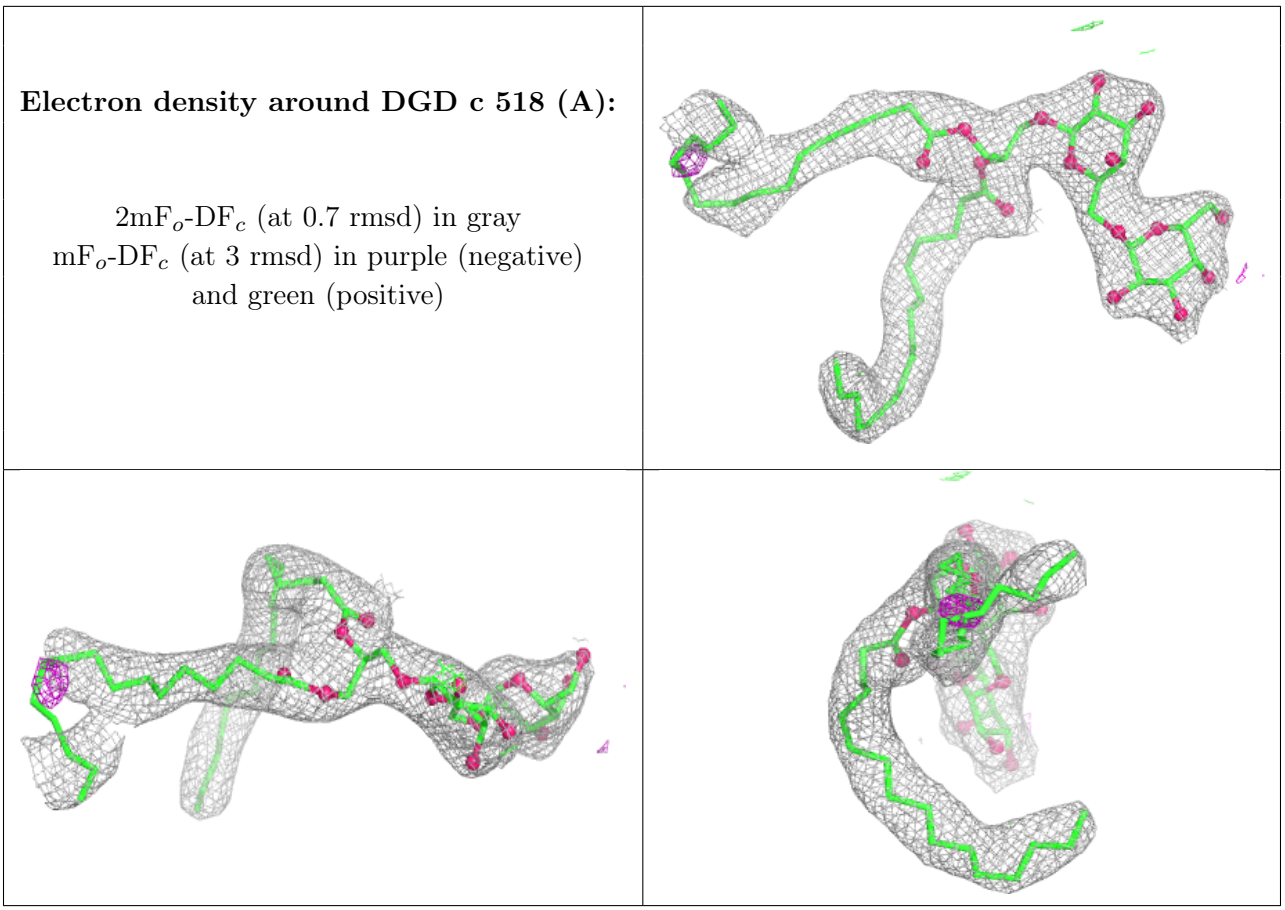






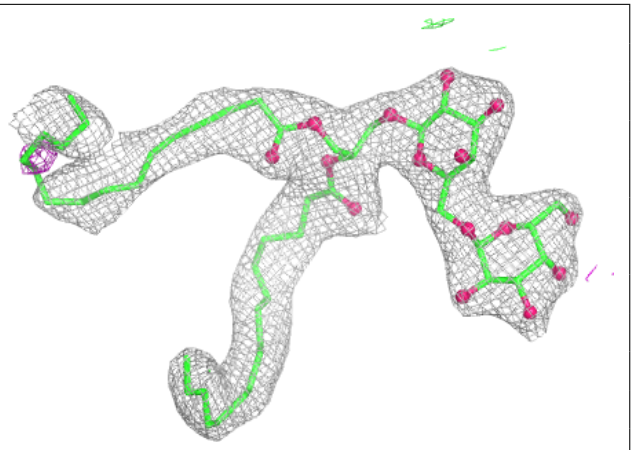
Electron density around DGD c 518 (A):

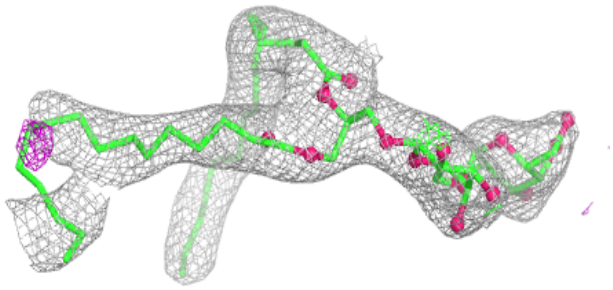
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

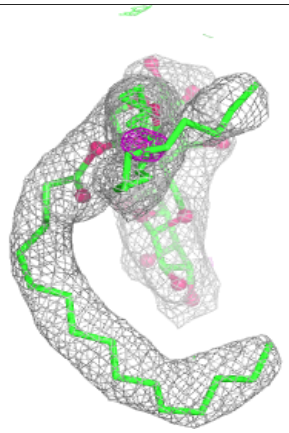


Electron density around DGD c 518 (B):

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

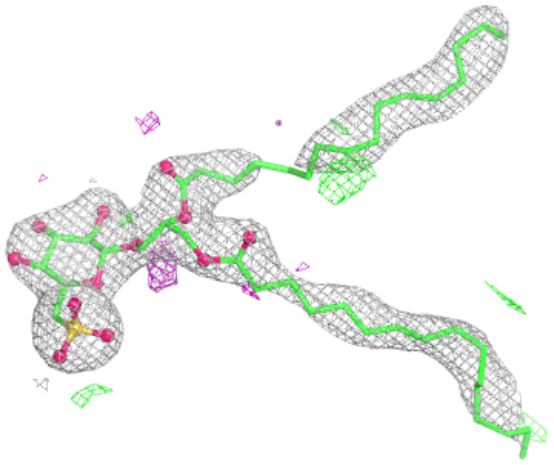


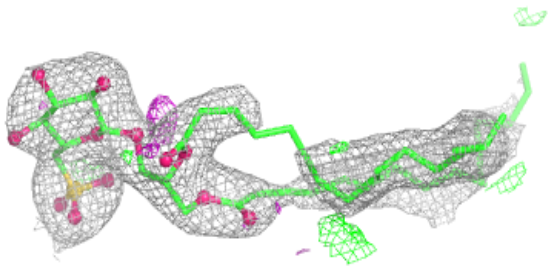


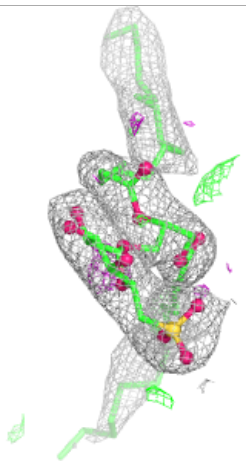


Electron density around SQD a 411 (A):

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

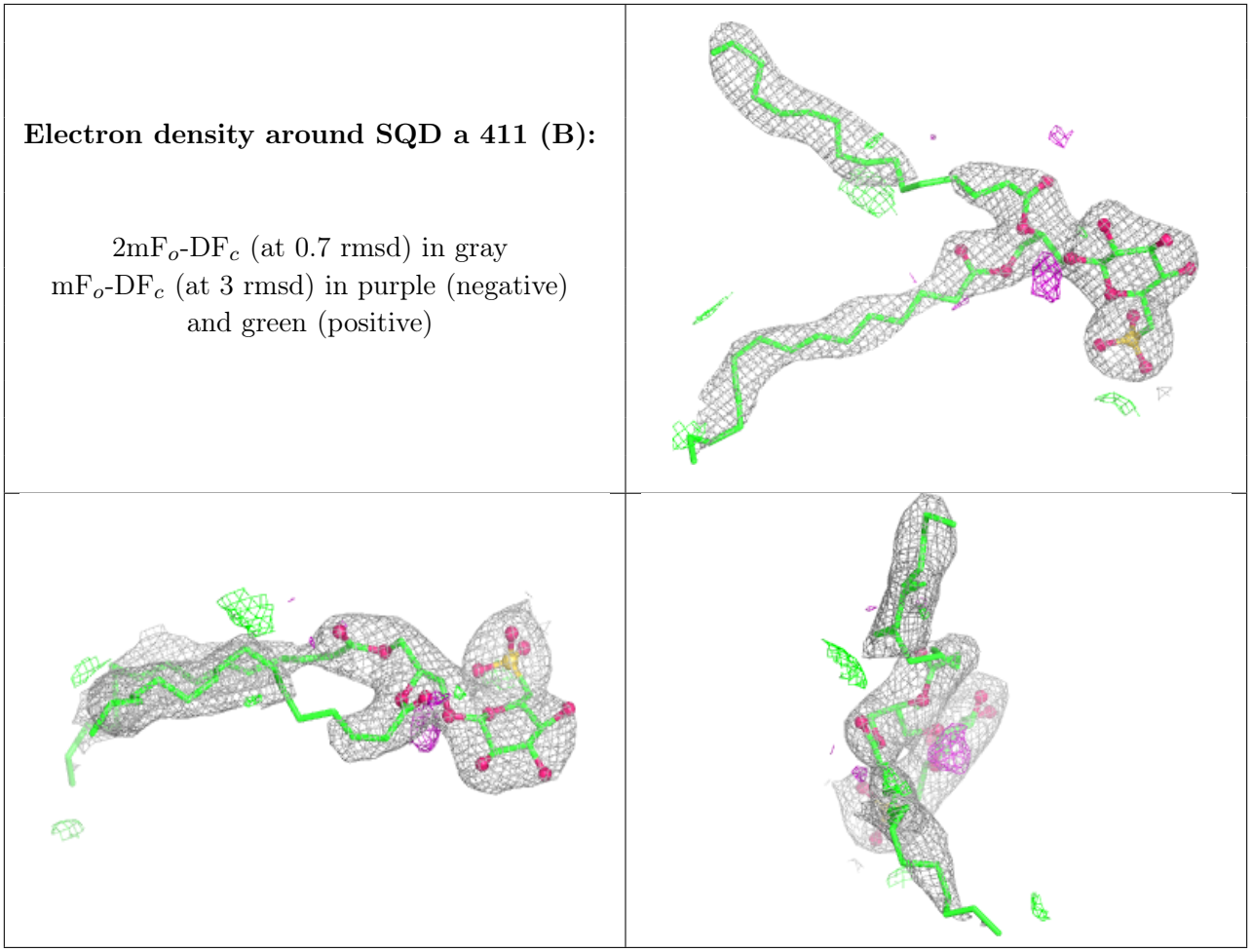






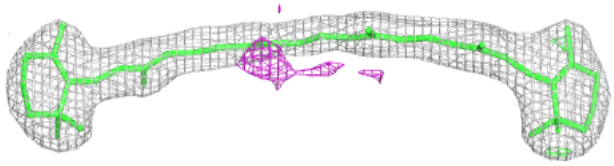
Electron density around SQD a 411 (B):

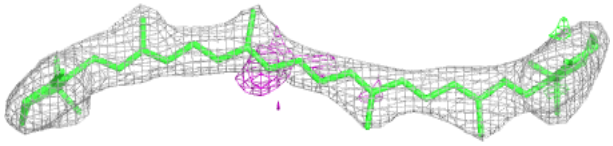
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

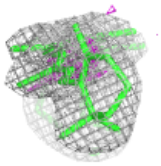


Electron density around BCR K 102:

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

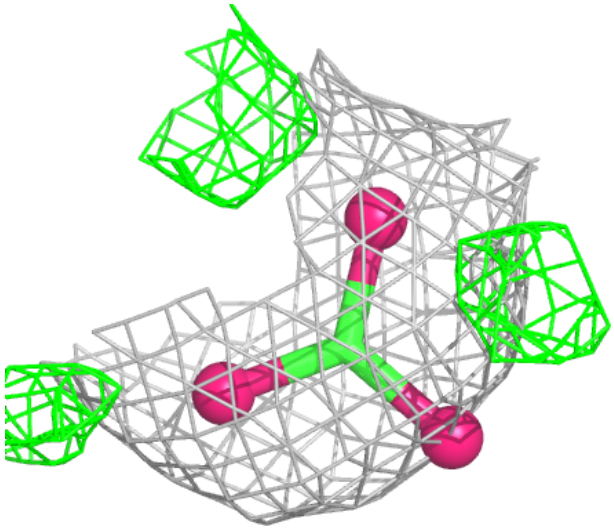


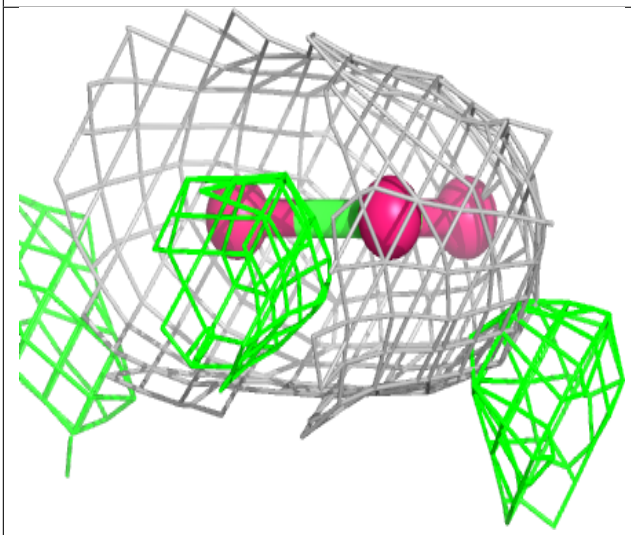


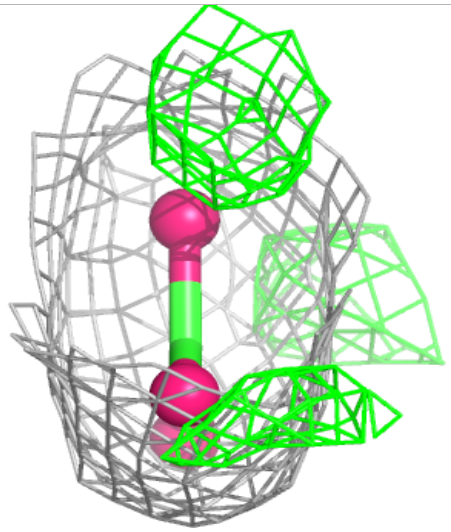


Electron density around BCT a 404 (B):

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

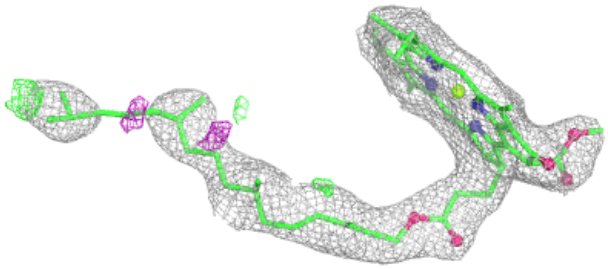


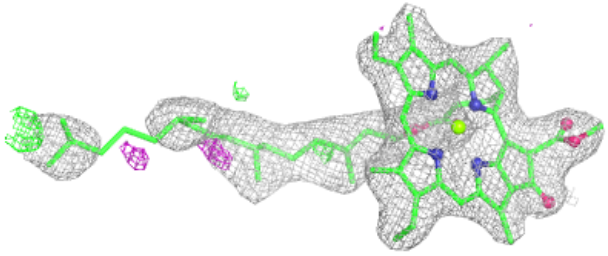


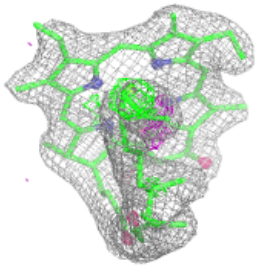


Electron density around CLA c 505:

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

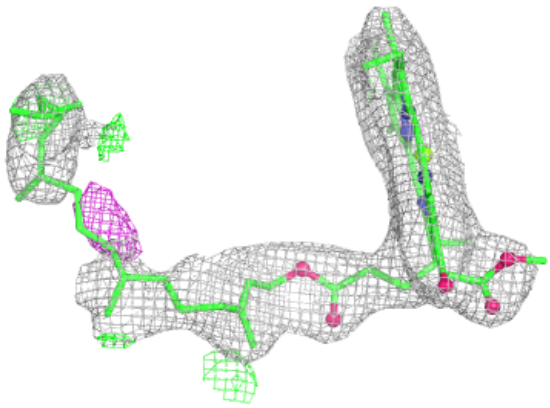


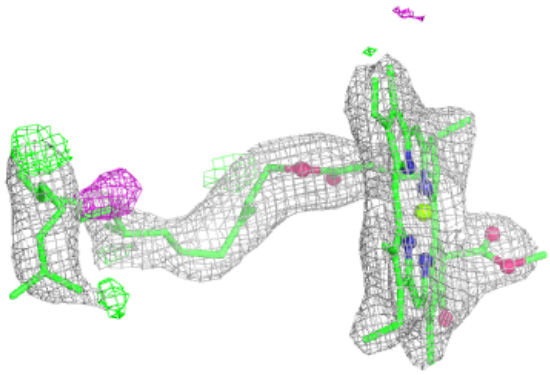


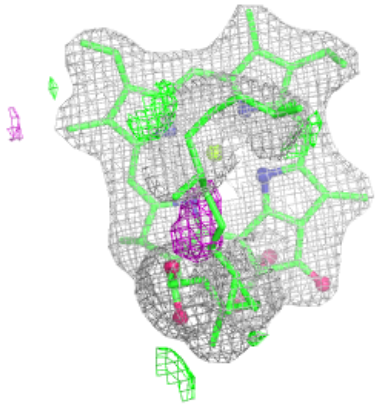


Electron density around CLA c 507:

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

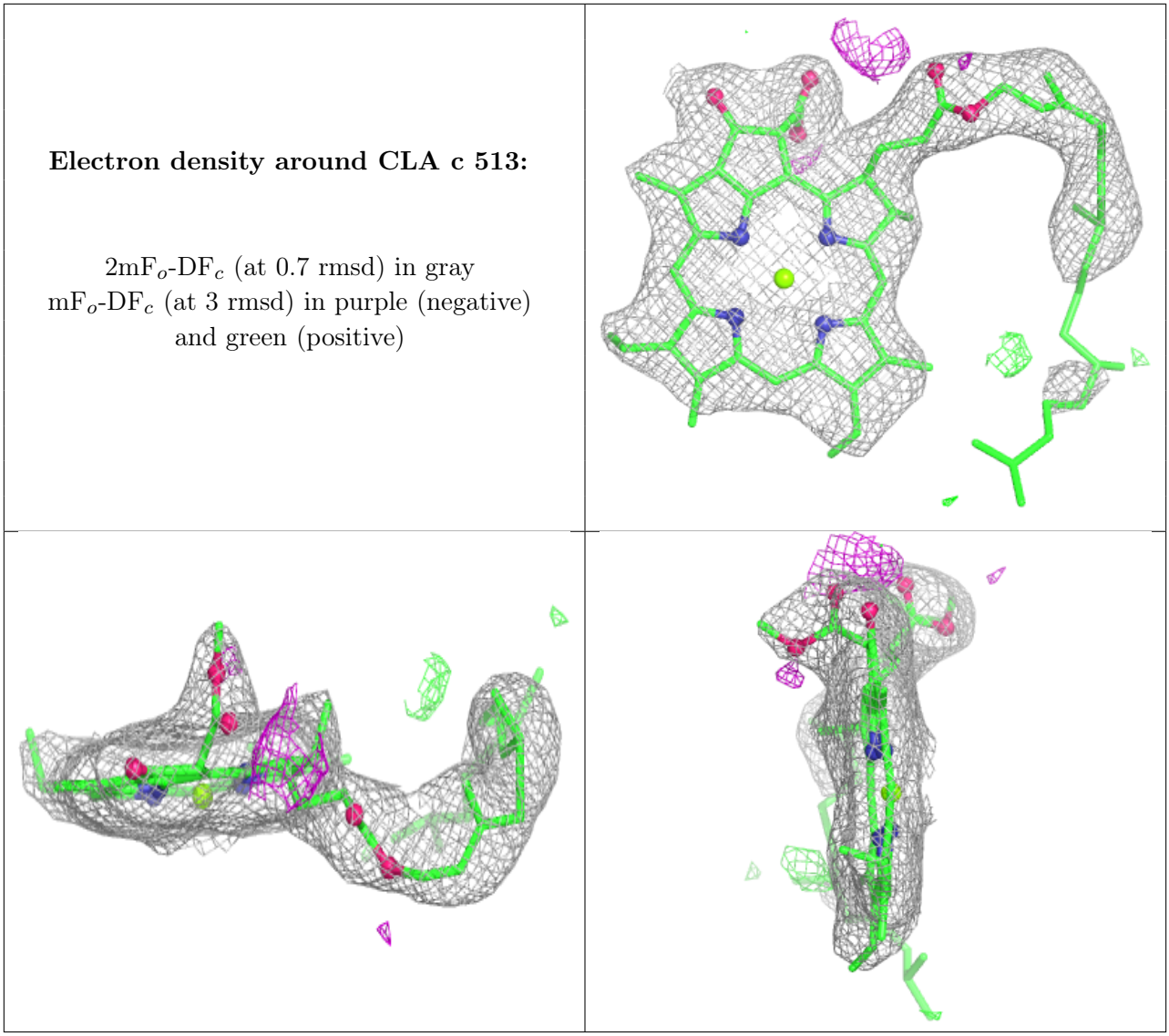






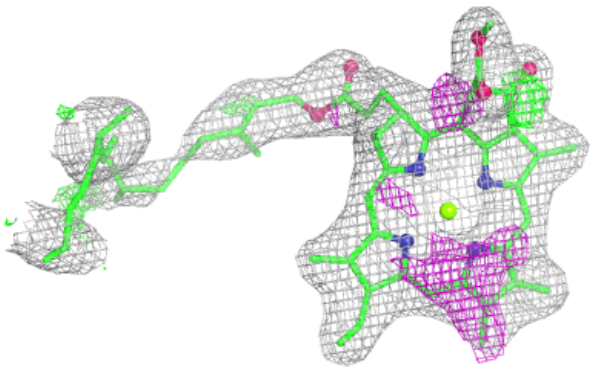
Electron density around CLA c 513:

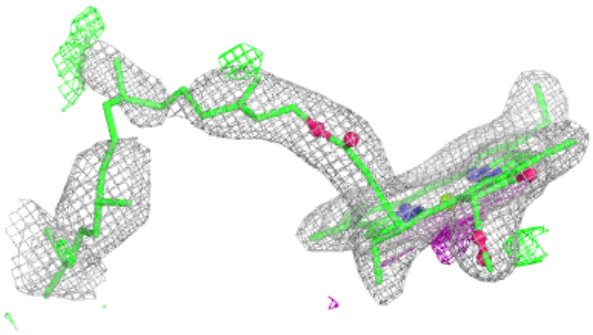
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

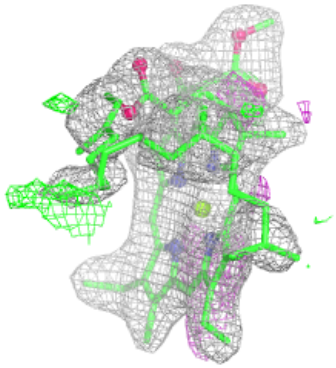


Electron density around CLA A 408:

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

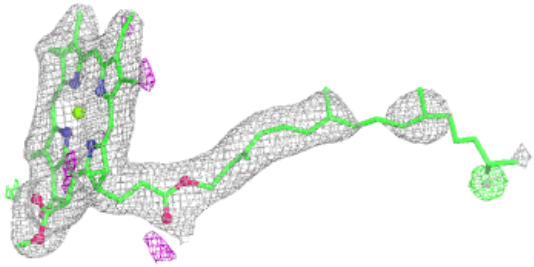


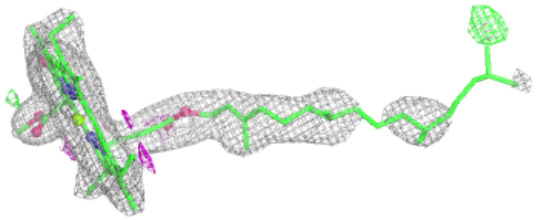


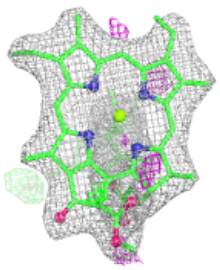


Electron density around CLA d 402:

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

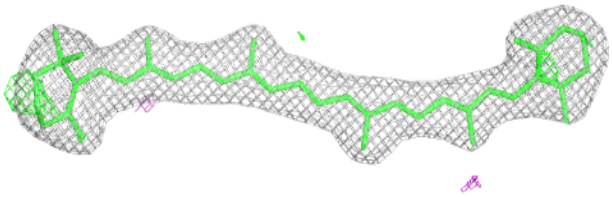


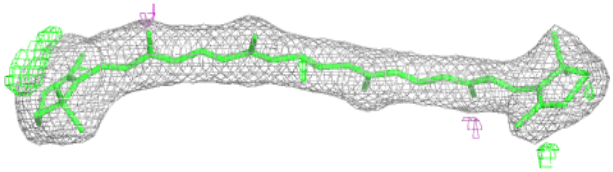


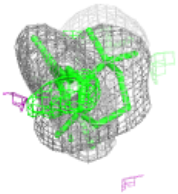


Electron density around BCR B 619:

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

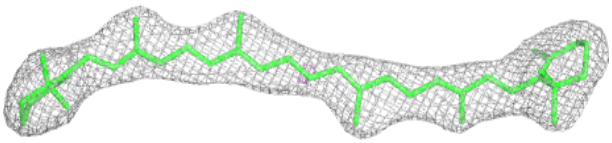


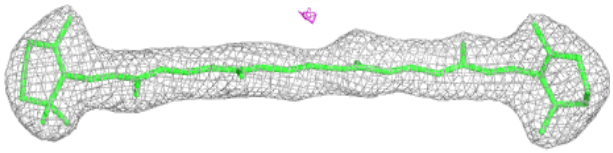


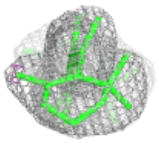


Electron density around BCR C 515:

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

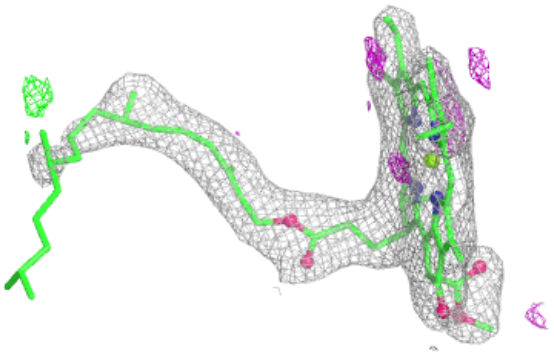


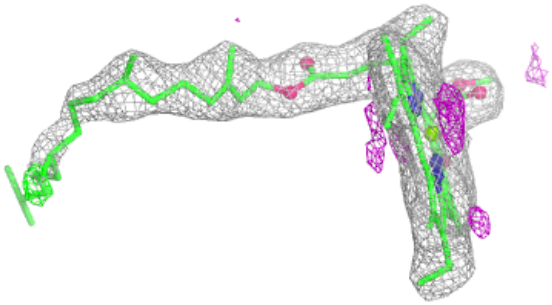


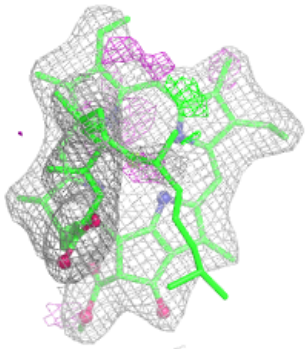


Electron density around CLA D 703:

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

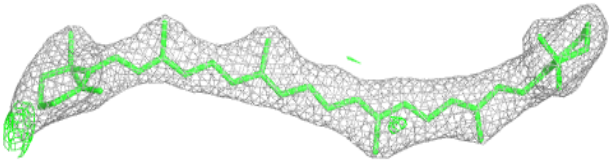


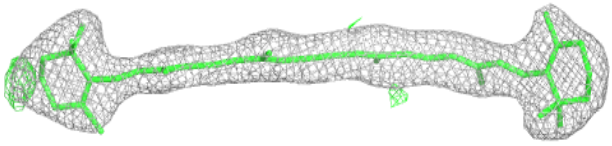


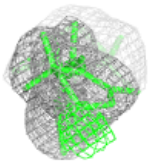


Electron density around BCR H 101:

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

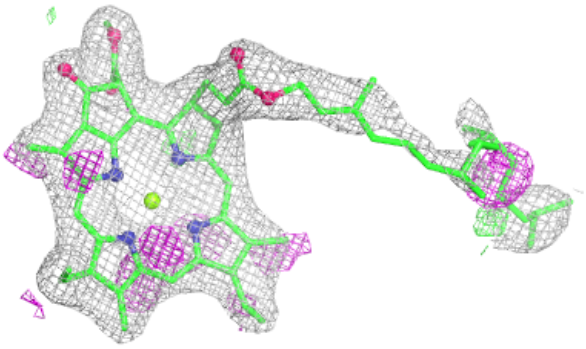


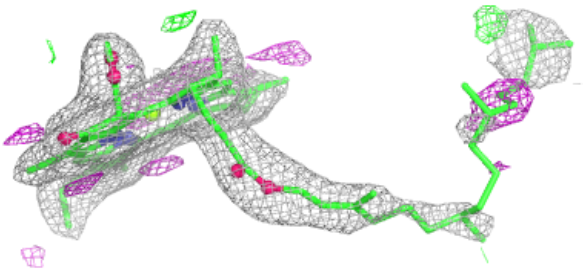


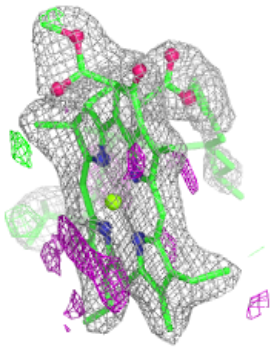


Electron density around CLA a 409:

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

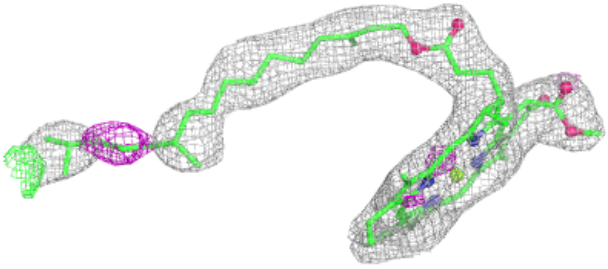


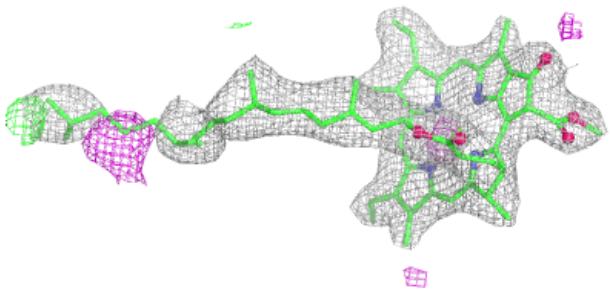


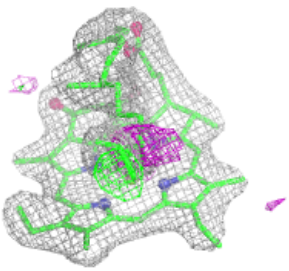


Electron density around CLA C 505:

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

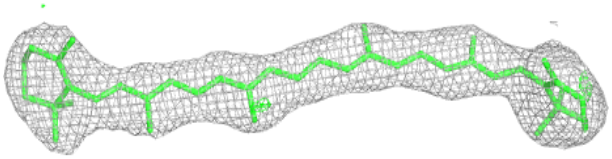


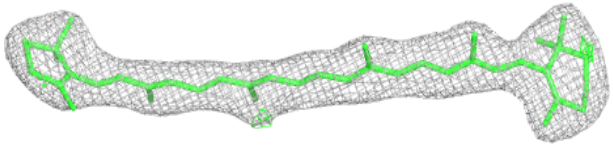


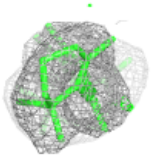


Electron density around BCR c 515:

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

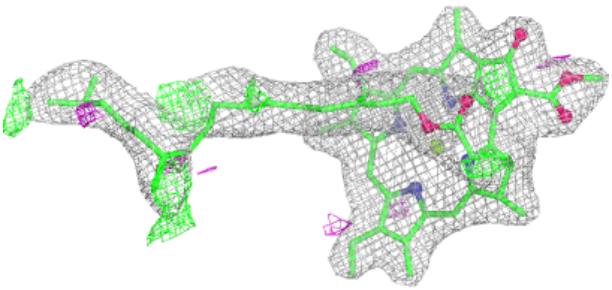


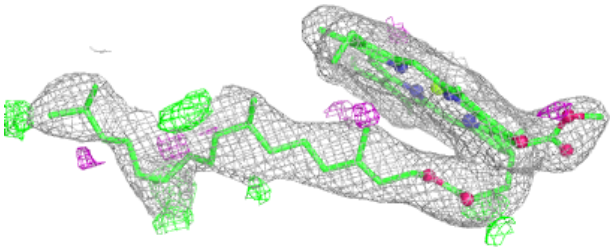


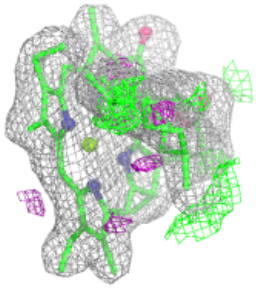


Electron density around CLA b 614:

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

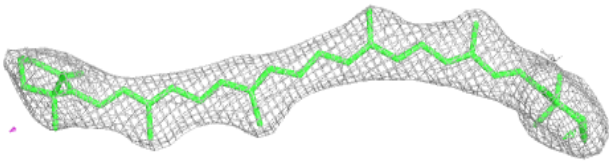


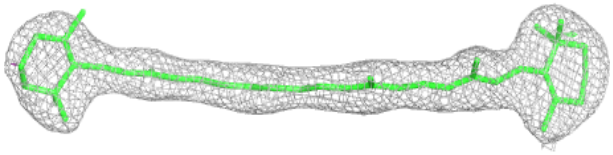


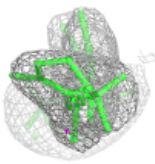


Electron density around BCR h 101:

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

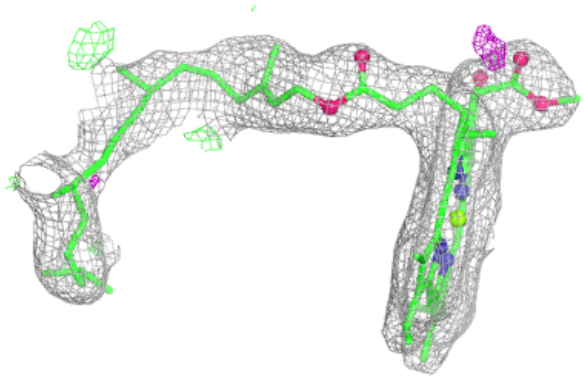


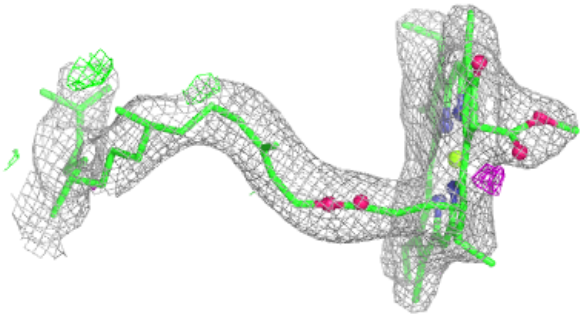


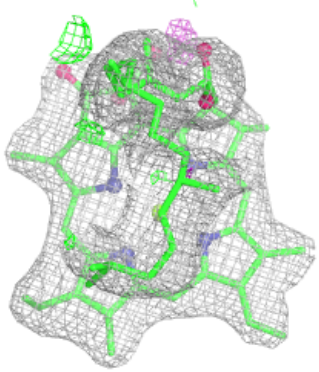


Electron density around CLA C 507:

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

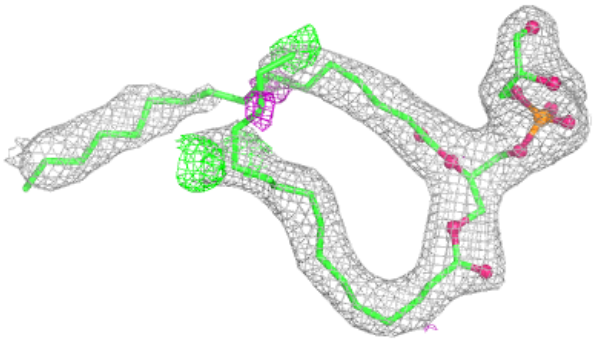


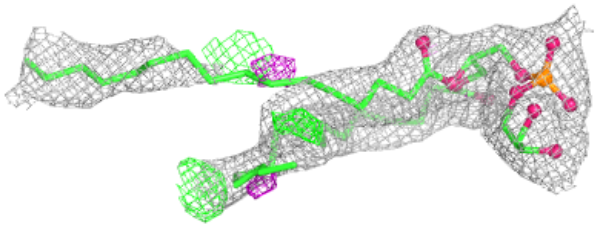


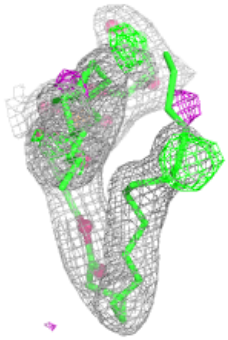


Electron density around LHG D 707 (A):

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

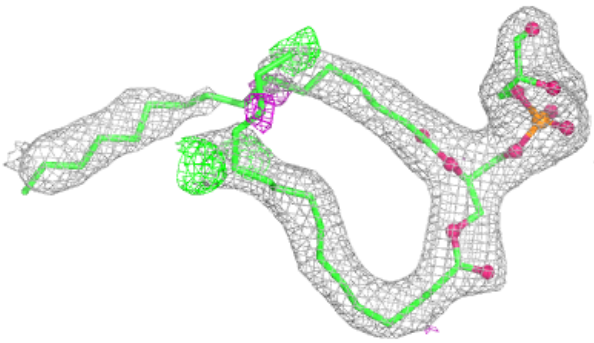


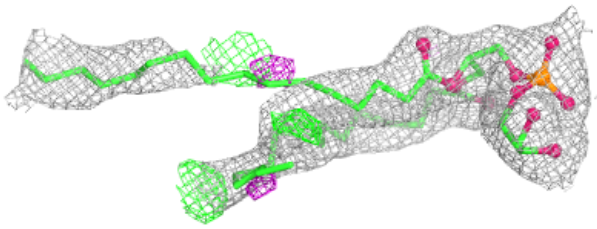


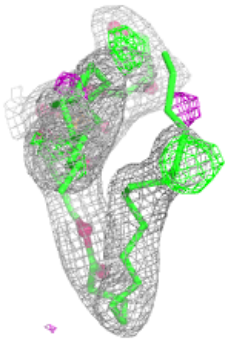


Electron density around LHG D 707 (B):

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

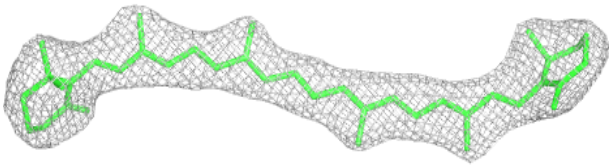


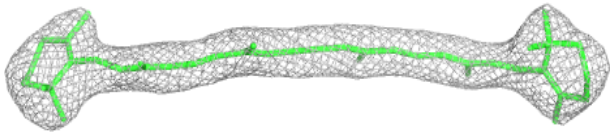


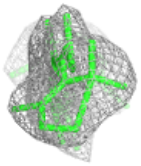


Electron density around BCR y 101:

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

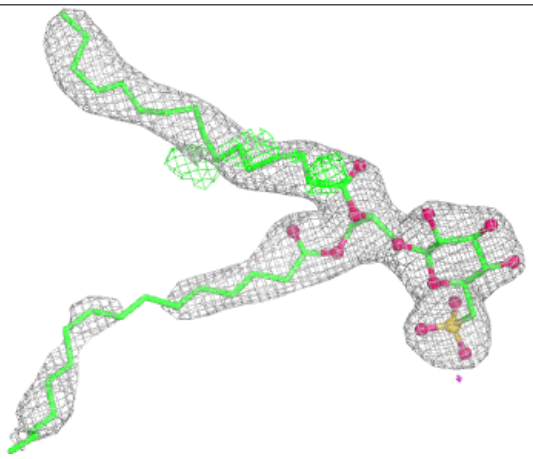


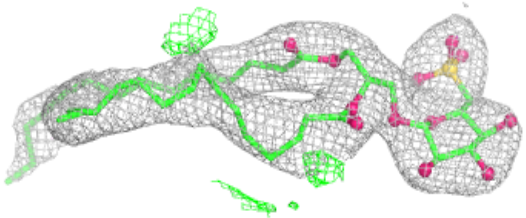


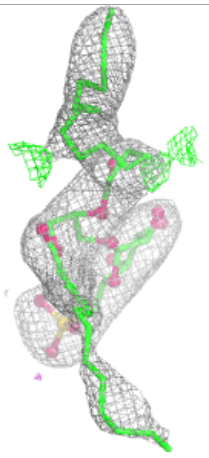


Electron density around SQD A 410 (A):

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

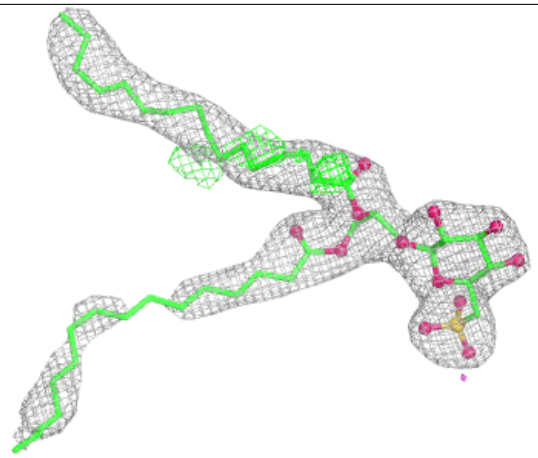


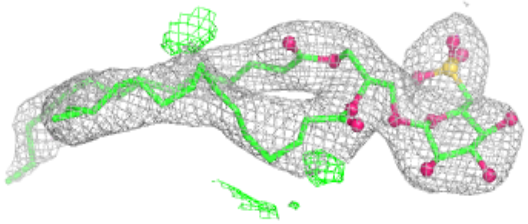


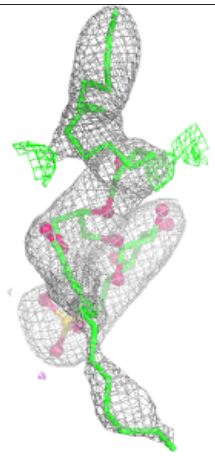


Electron density around SQD A 410 (B):

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

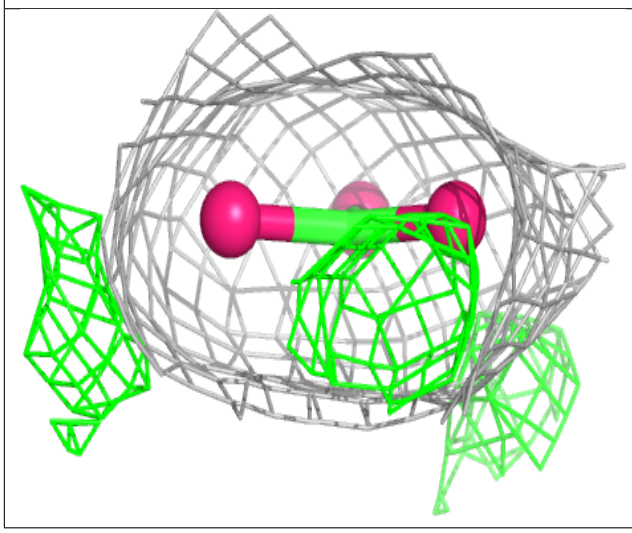


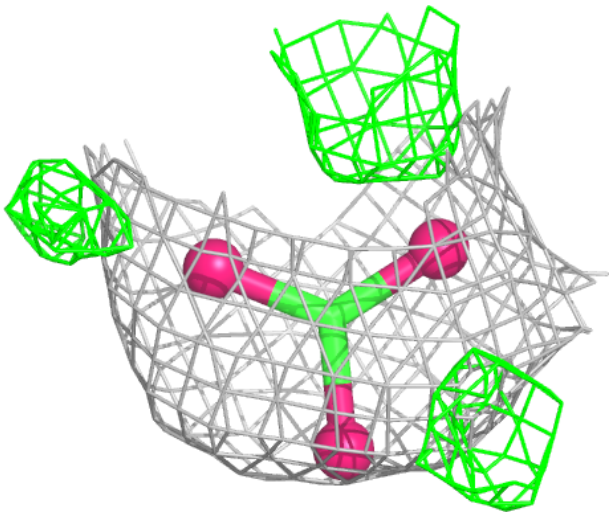


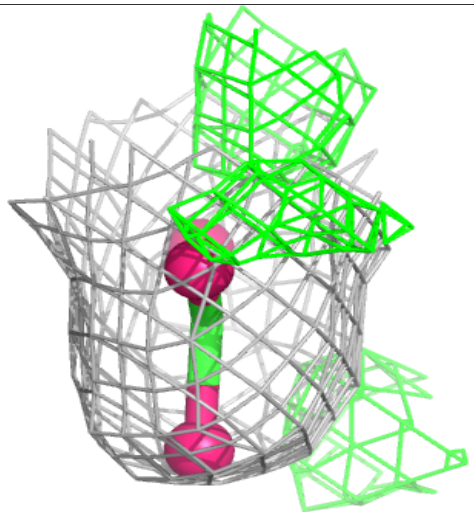


Electron density around BCT a 404 (A):

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

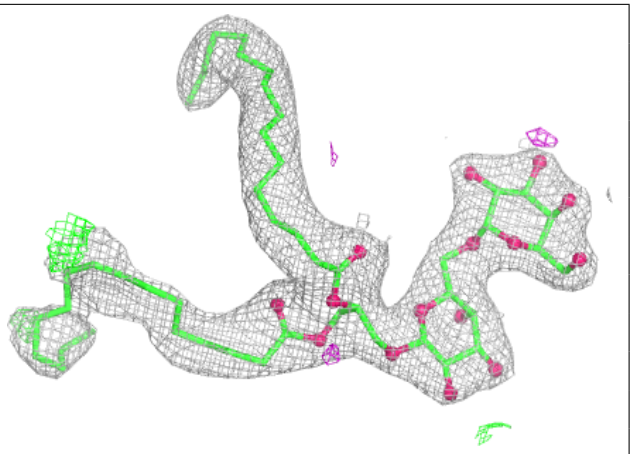


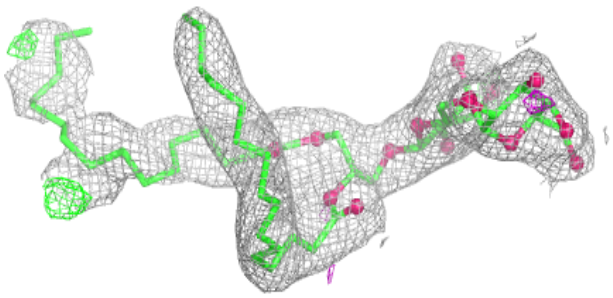


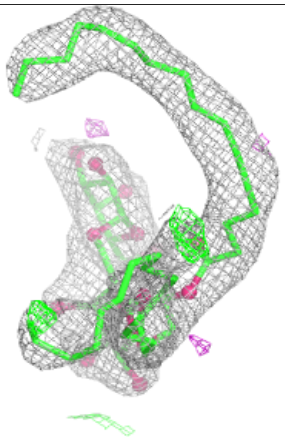


Electron density around DGD C 518 (A):

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

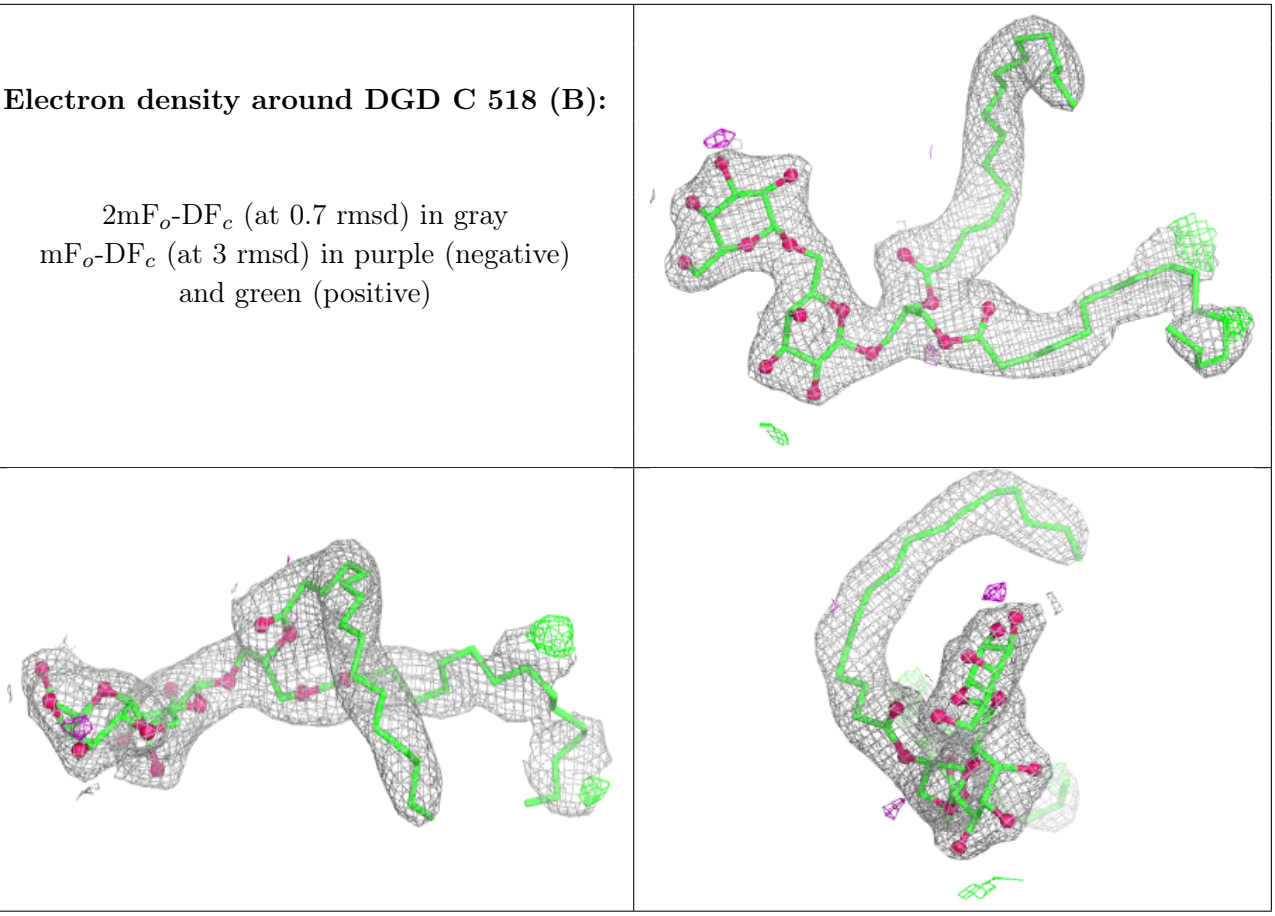






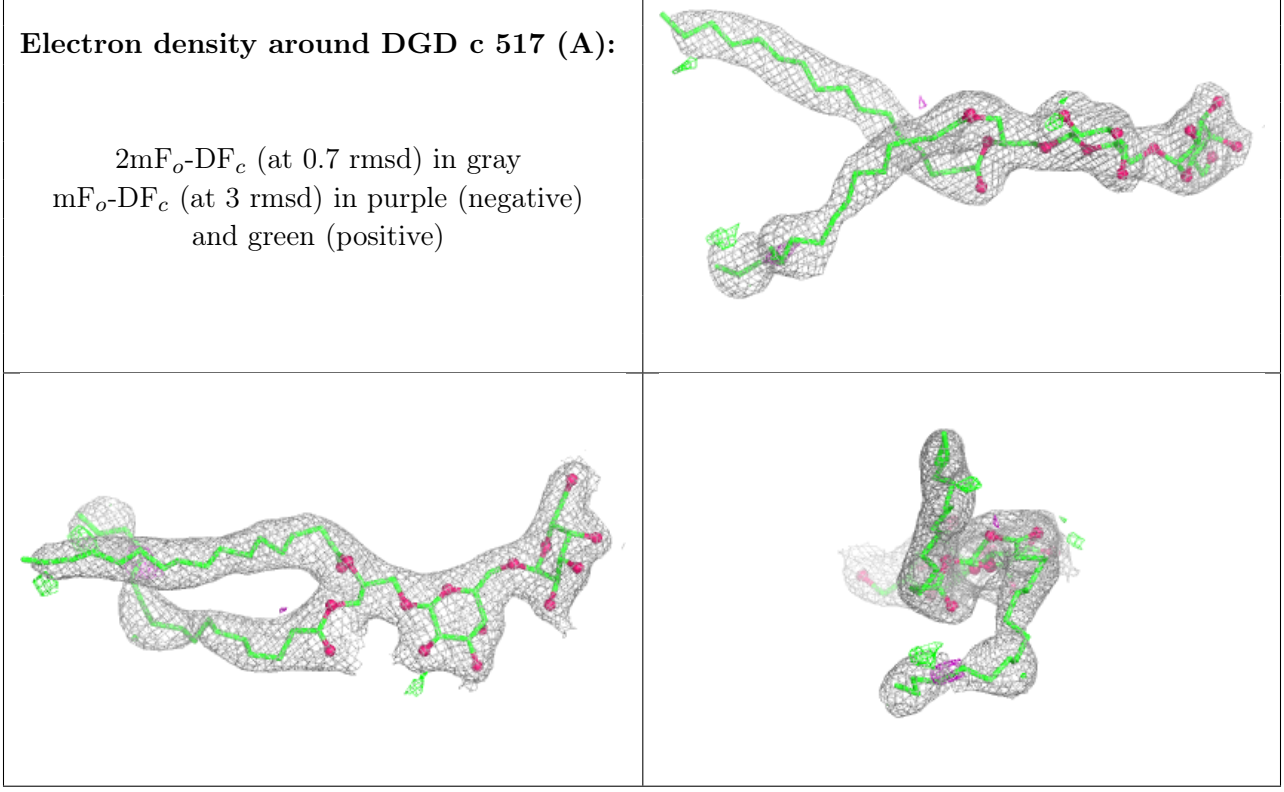
Electron density around DGD C 518 (B):

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



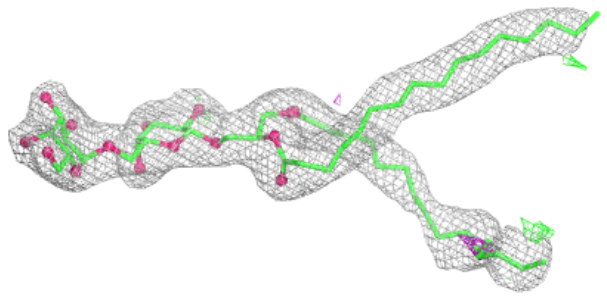
Electron density around DGD c 517 (A):

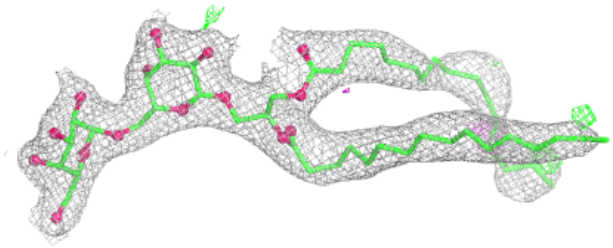
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

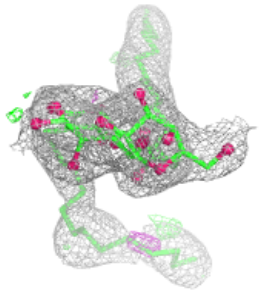


Electron density around DGD c 517 (B):

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

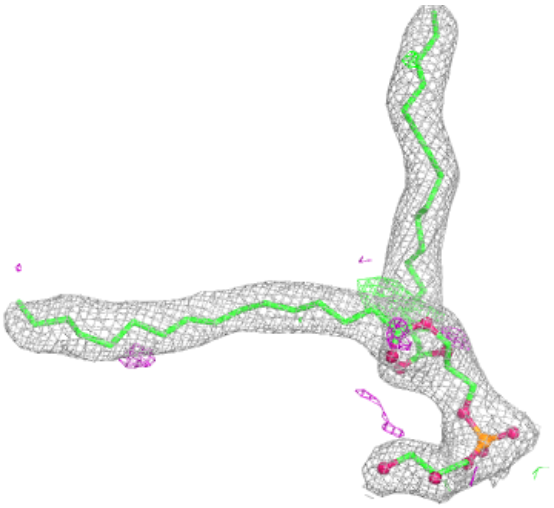


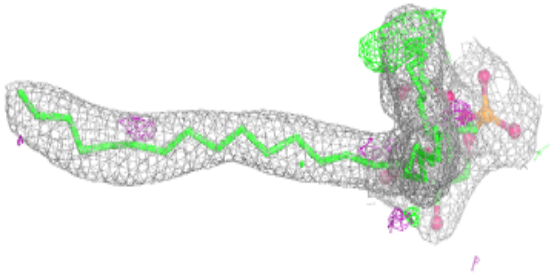


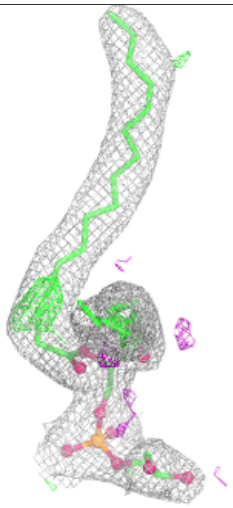


Electron density around LHG b 629 (A):

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

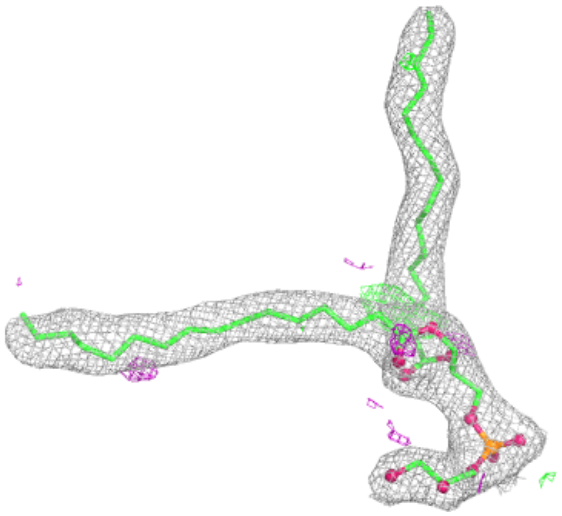


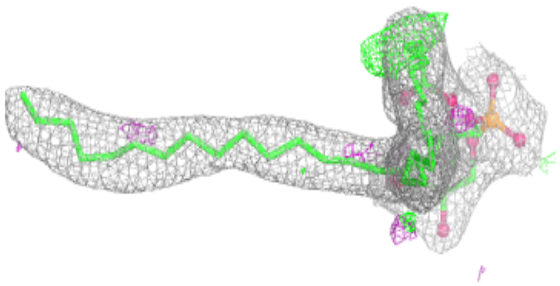


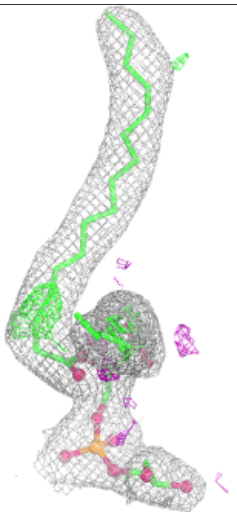


Electron density around LHG b 629 (B):

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

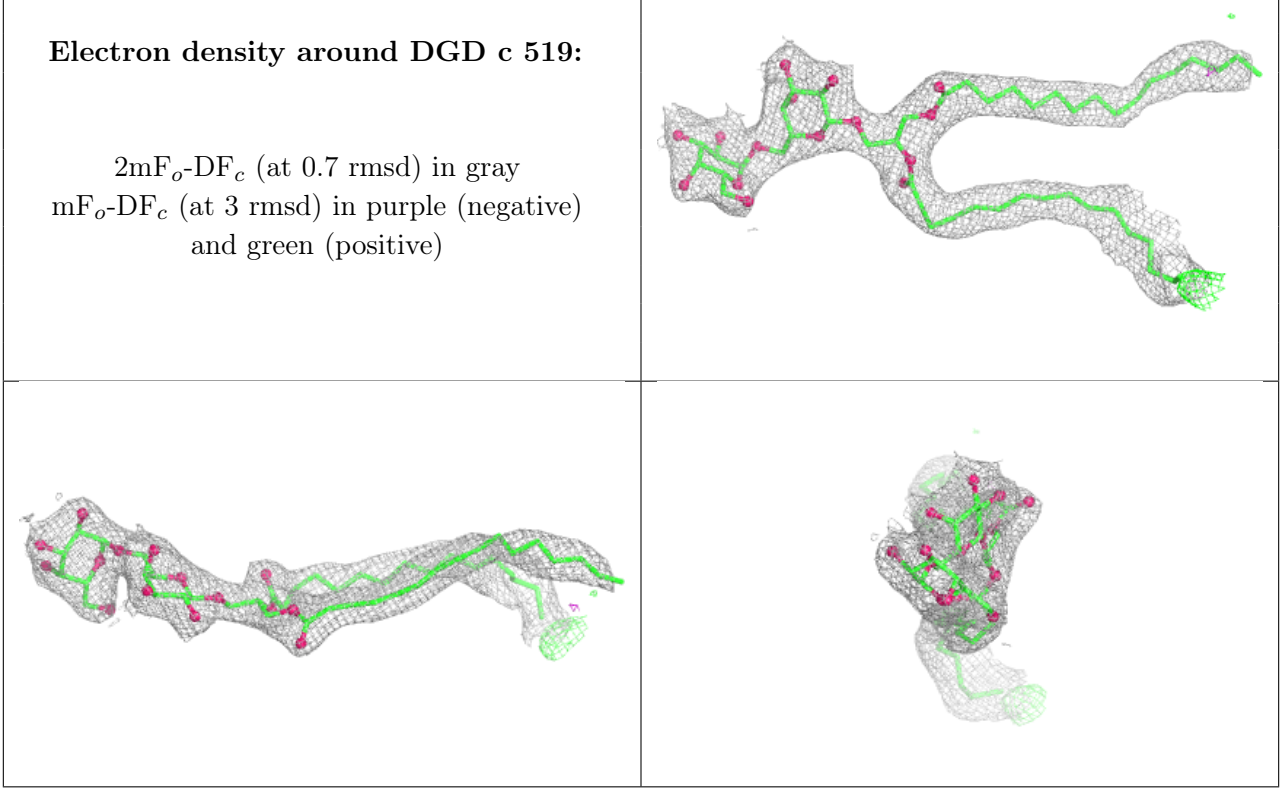






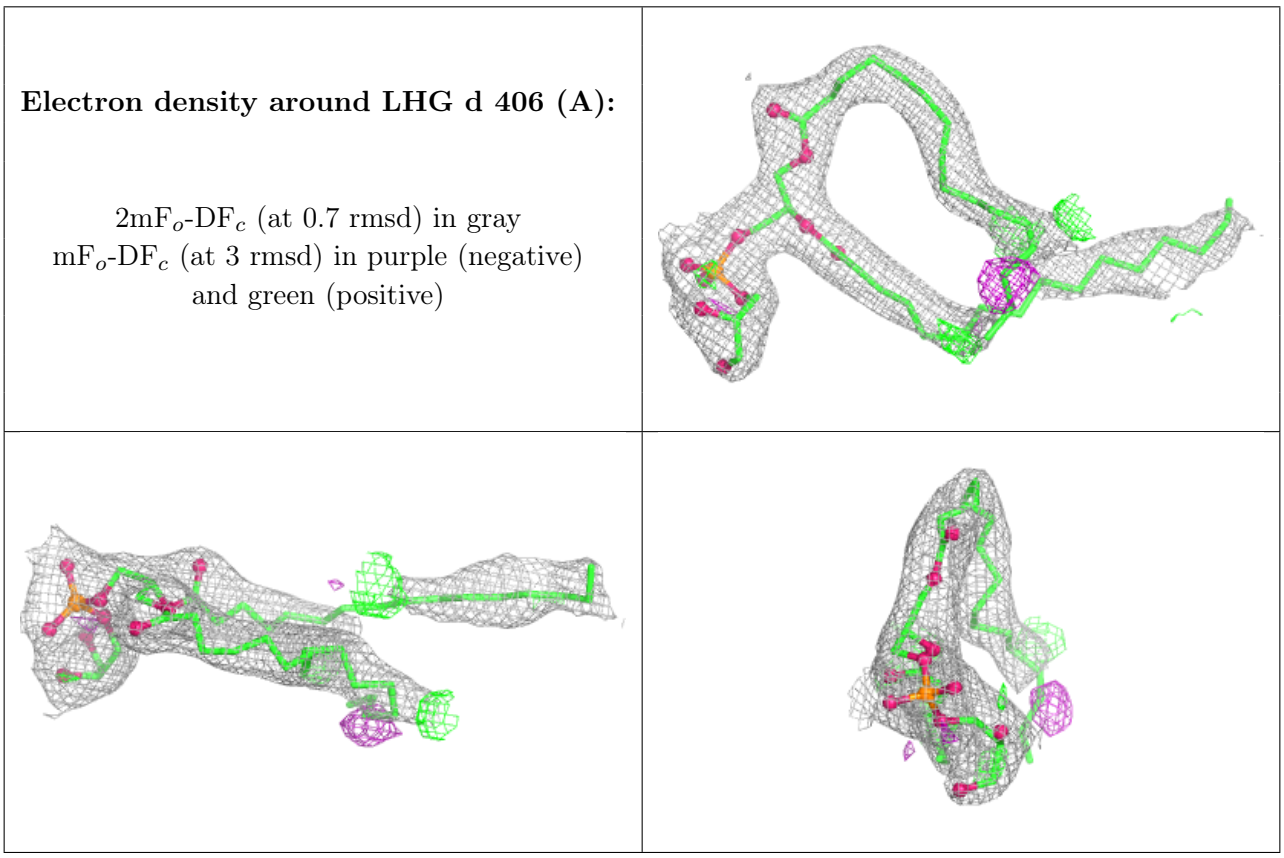
Electron density around DGD c 519:

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



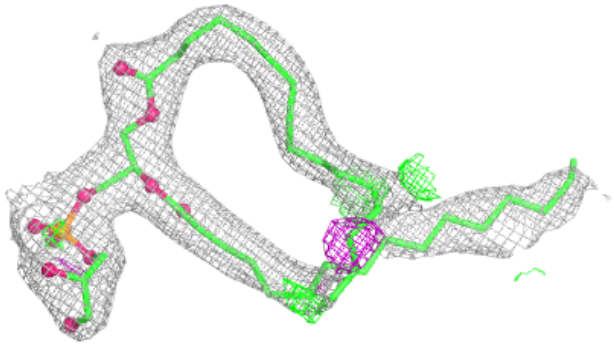
Electron density around LHG d 406 (A):

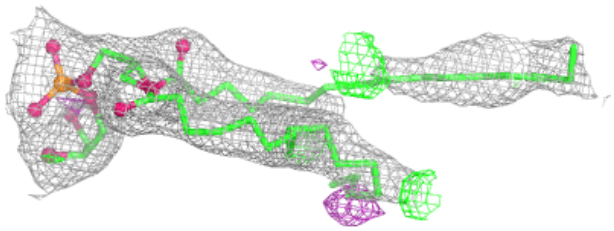
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

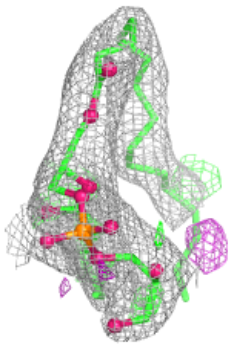


Electron density around LHG d 406 (B):

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

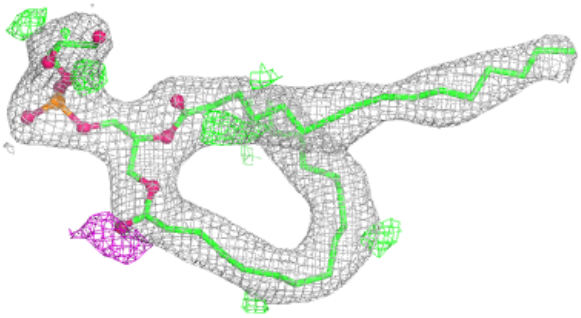


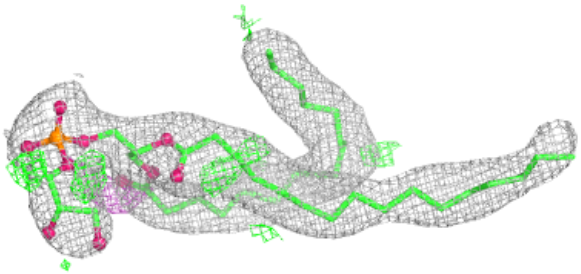


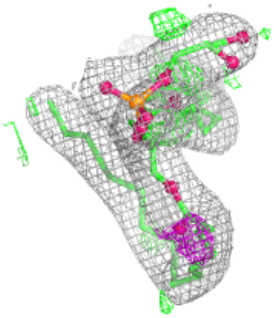


Electron density around LHG d 412 (A):

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

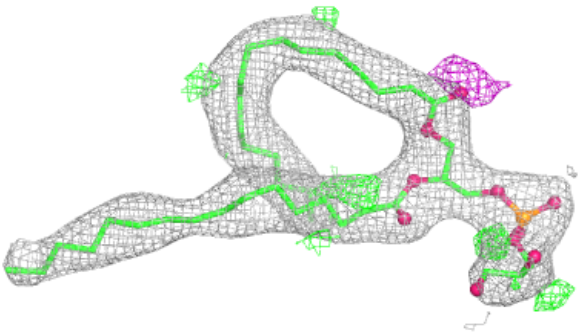


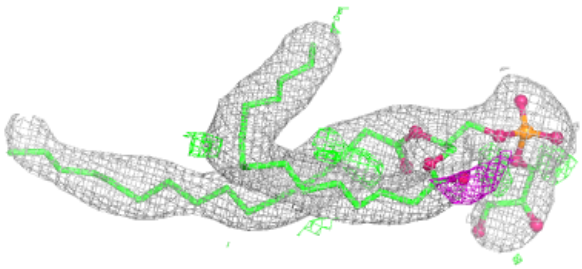


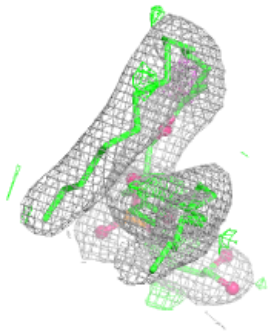


Electron density around LHG d 412 (B):

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

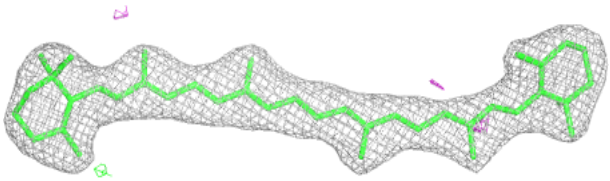


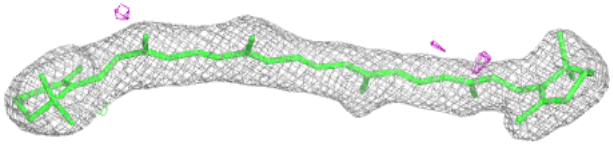


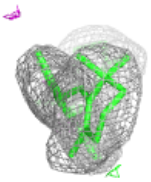


Electron density around BCR b 619:

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

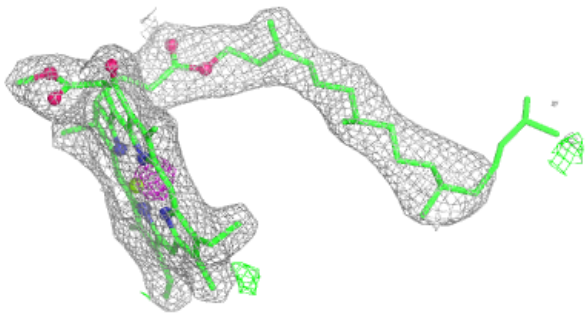


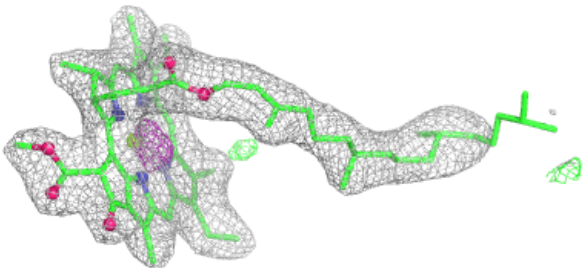


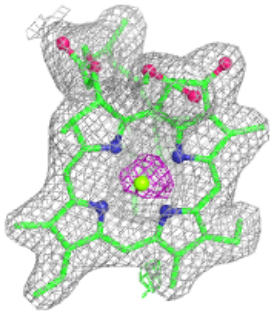


Electron density around CLA C 509:

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

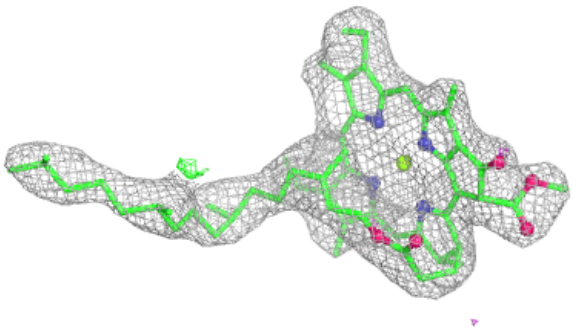


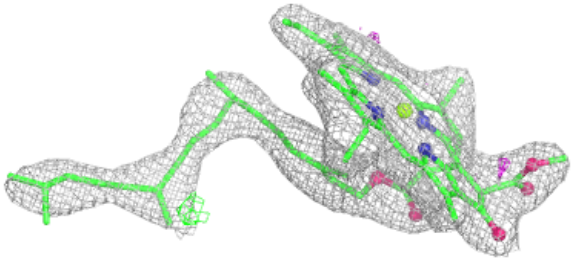


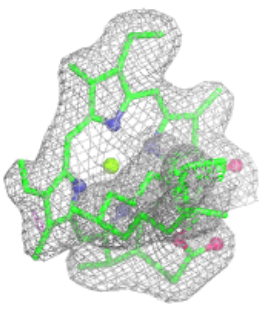


Electron density around CLA c 506:

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

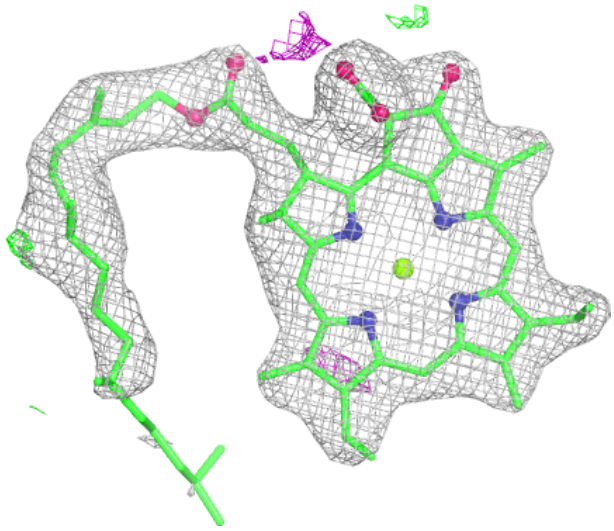


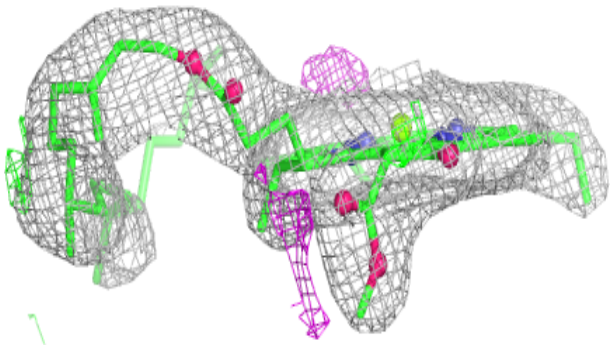




Electron density around CLA C 513:

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

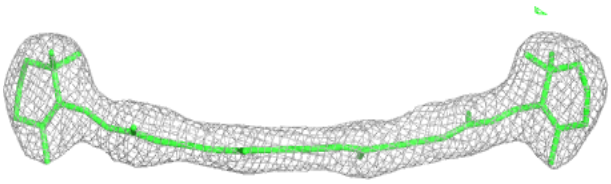


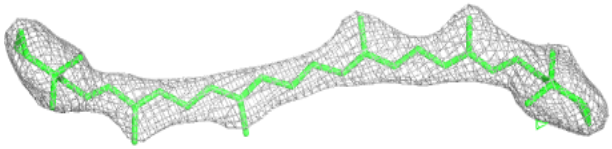


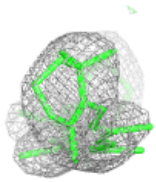


Electron density around BCR k 101:

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

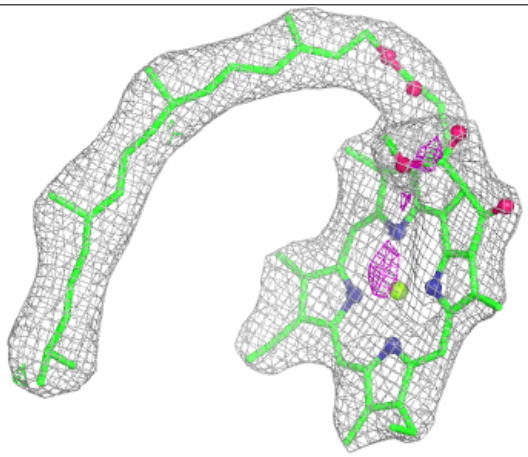


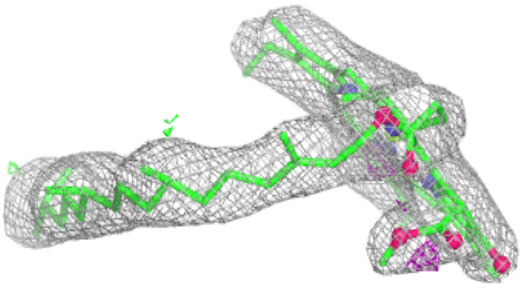


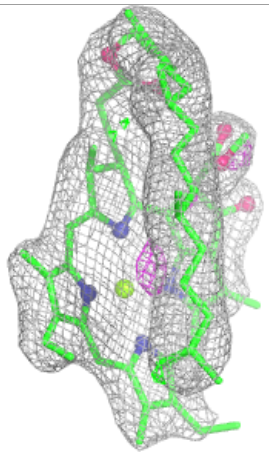


Electron density around CLA c 508:

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

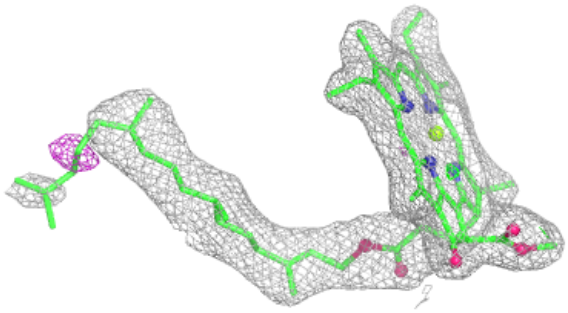


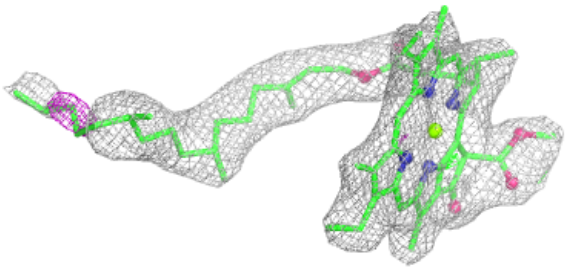


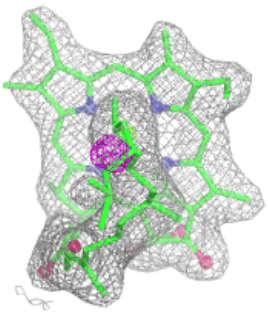


Electron density around CLA c 509:

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

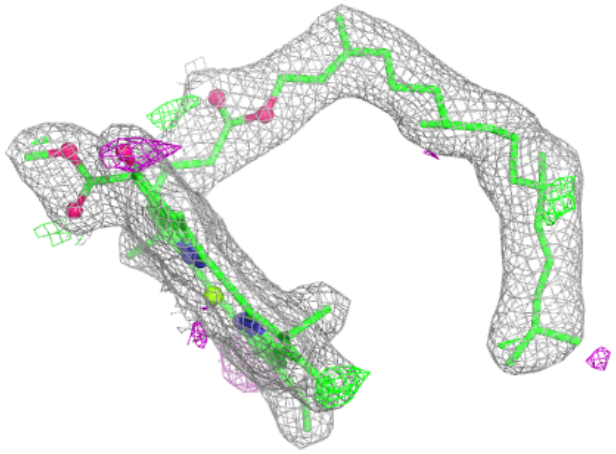


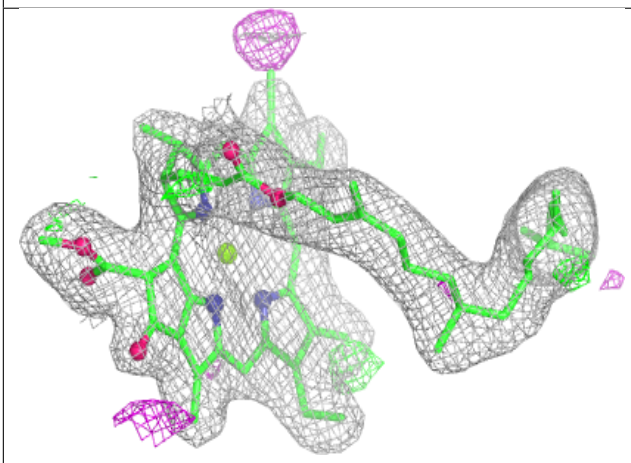




Electron density around CLA B 611:

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

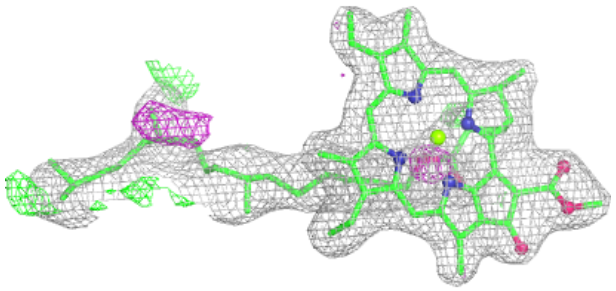


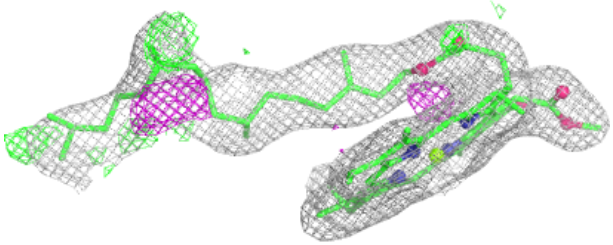


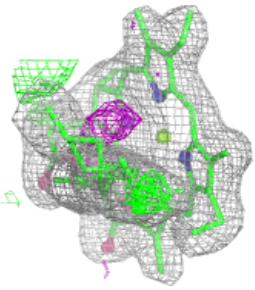


Electron density around CLA B 614:

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

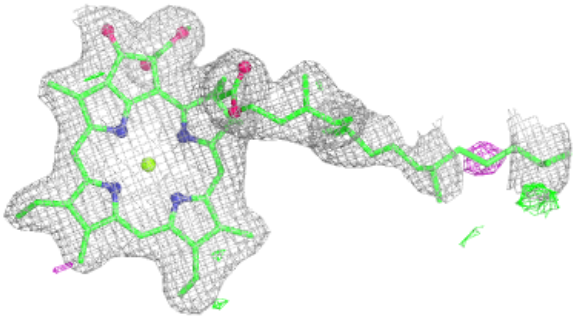


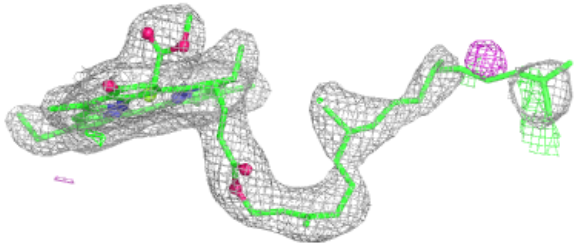


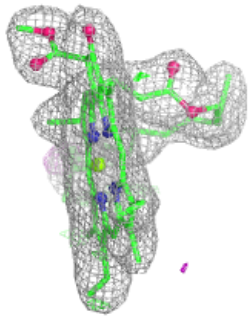


Electron density around CLA a 407 (A):

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

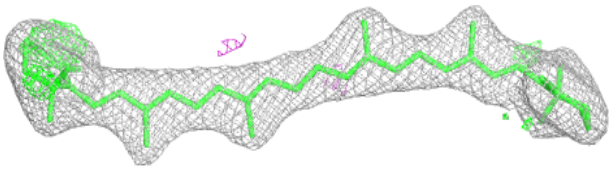


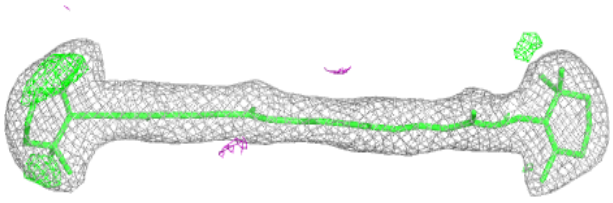


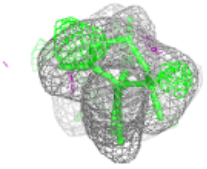


Electron density around BCR A 409:

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

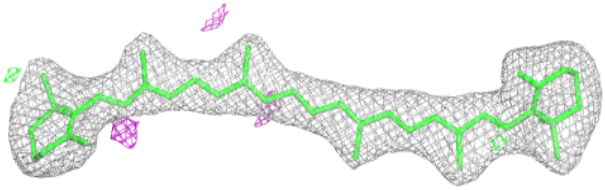


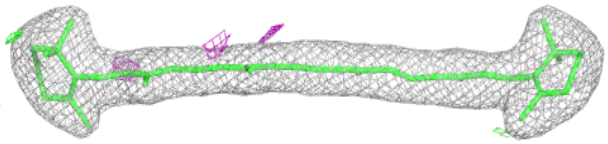


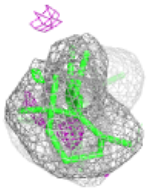


Electron density around BCR B 618:

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

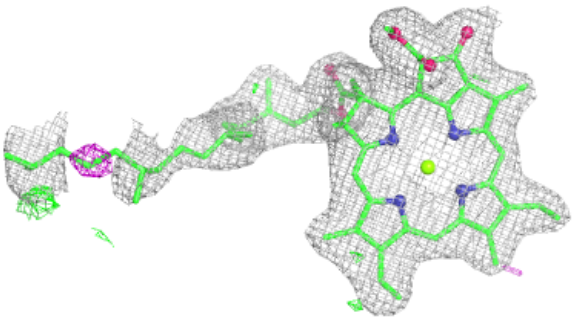


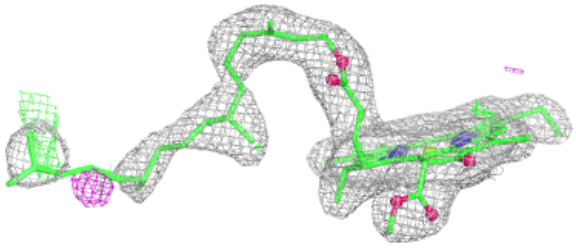




Electron density around CLA a 407 (B):

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

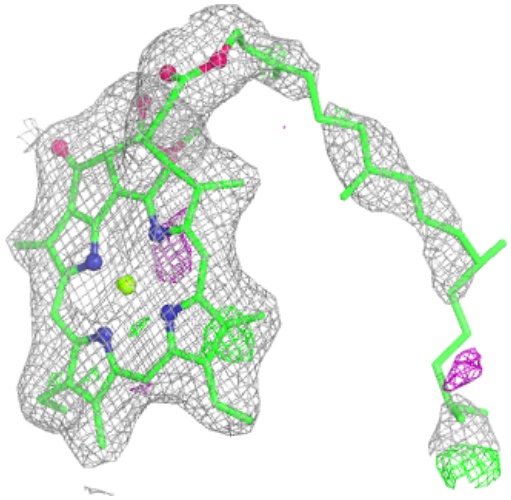


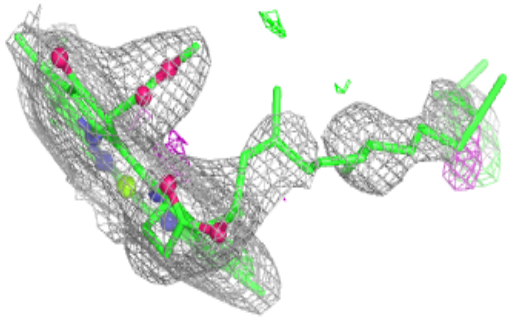


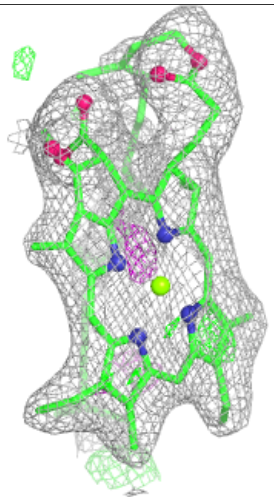


Electron density around CLA B 616:

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

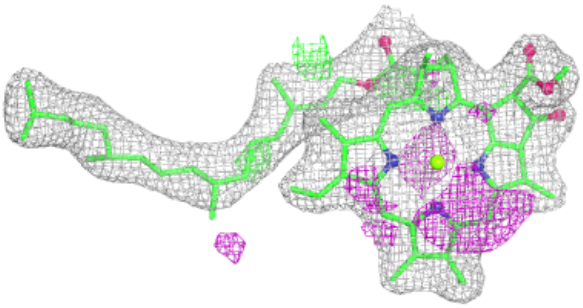


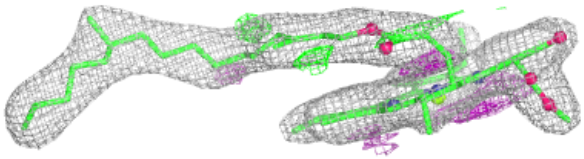


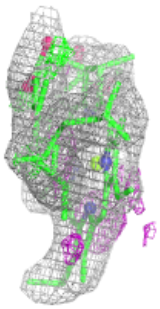


Electron density around CLA B 603:

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

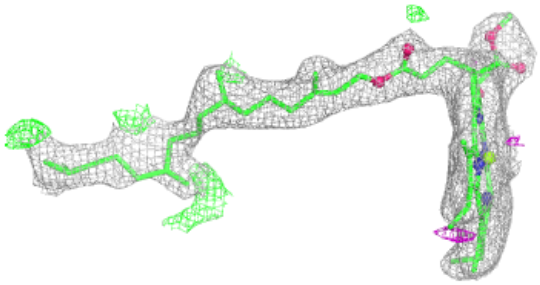


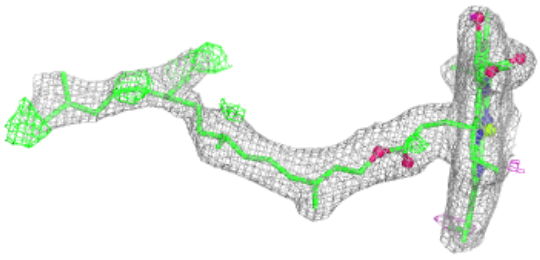


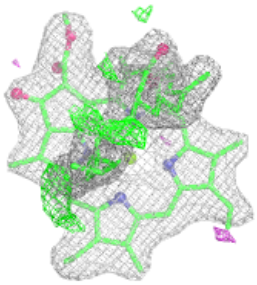


Electron density around CLA b 606:

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

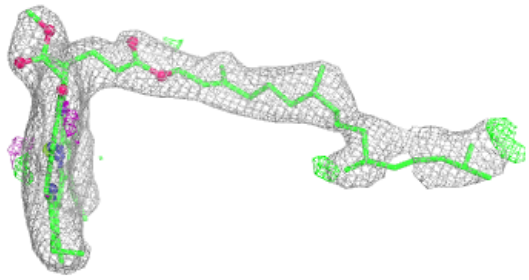


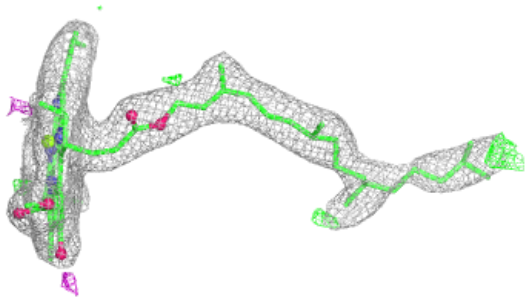


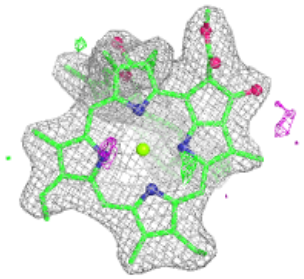


Electron density around CLA B 606:

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

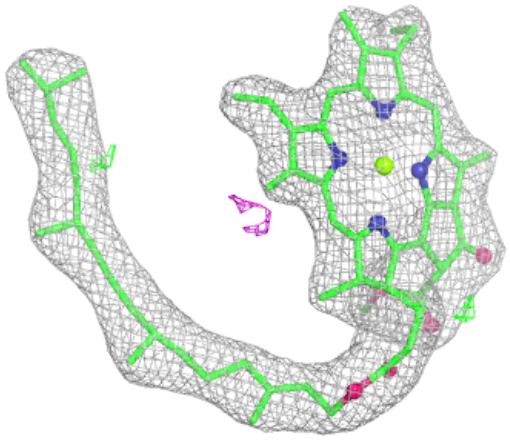


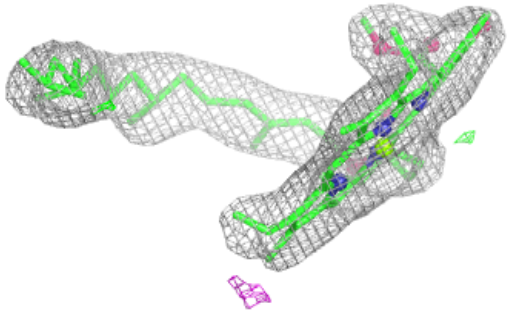


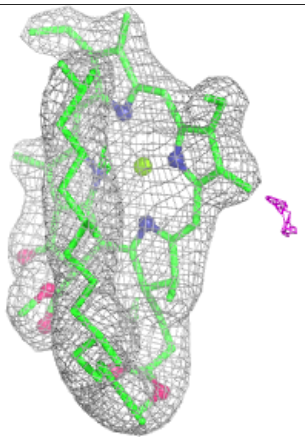


Electron density around CLA C 508:

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

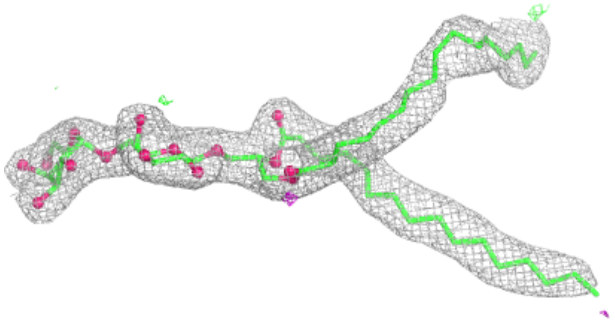


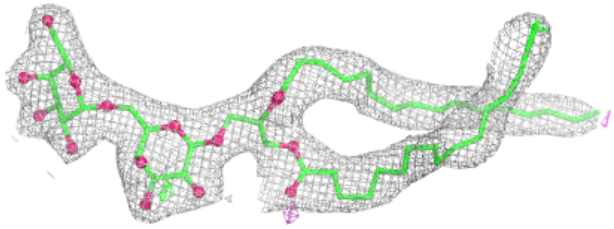


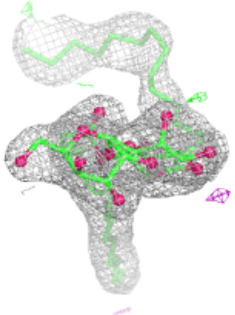


Electron density around DGD C 517 (A):

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

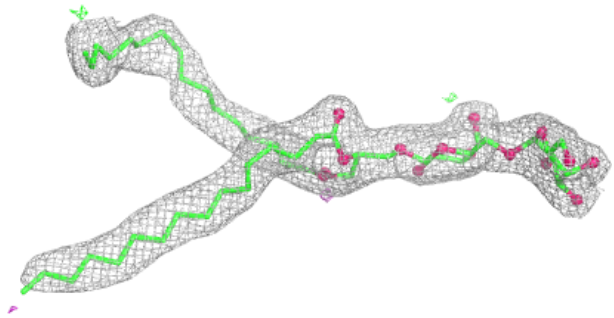


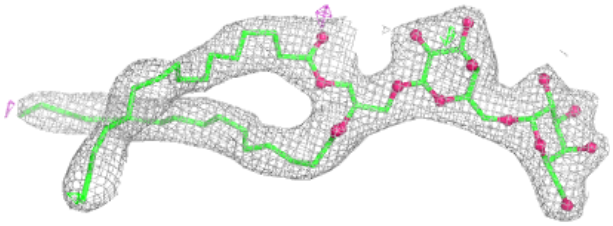


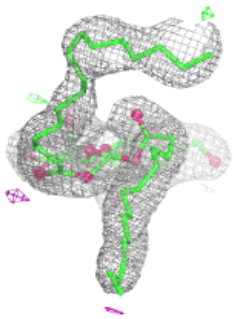


Electron density around DGD C 517 (B):

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

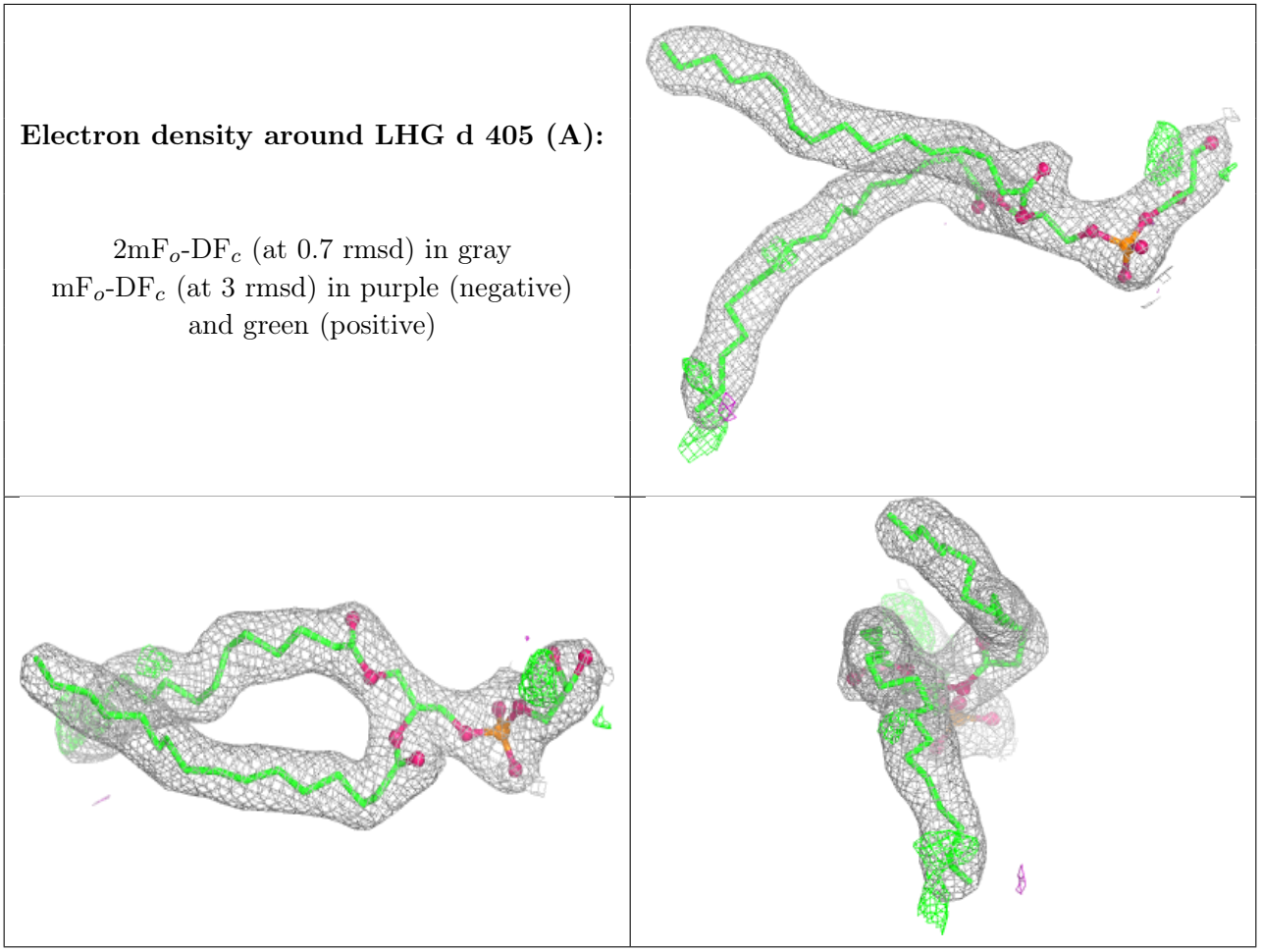






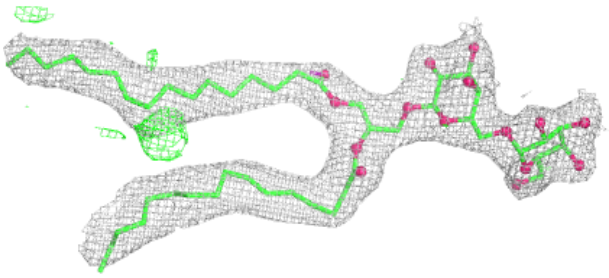
Electron density around LHG d 405 (A):

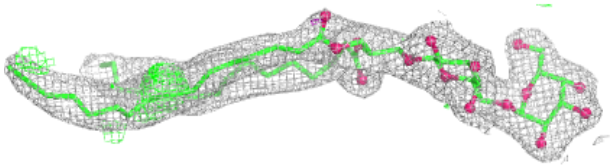
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

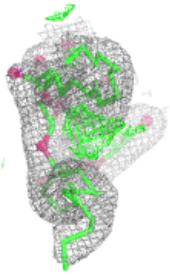


Electron density around DGD C 519:

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

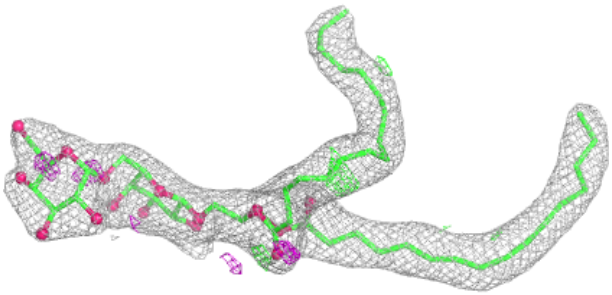


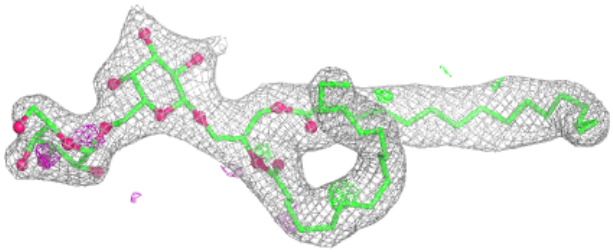


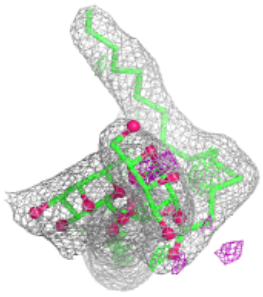


Electron density around DGD H 102:

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

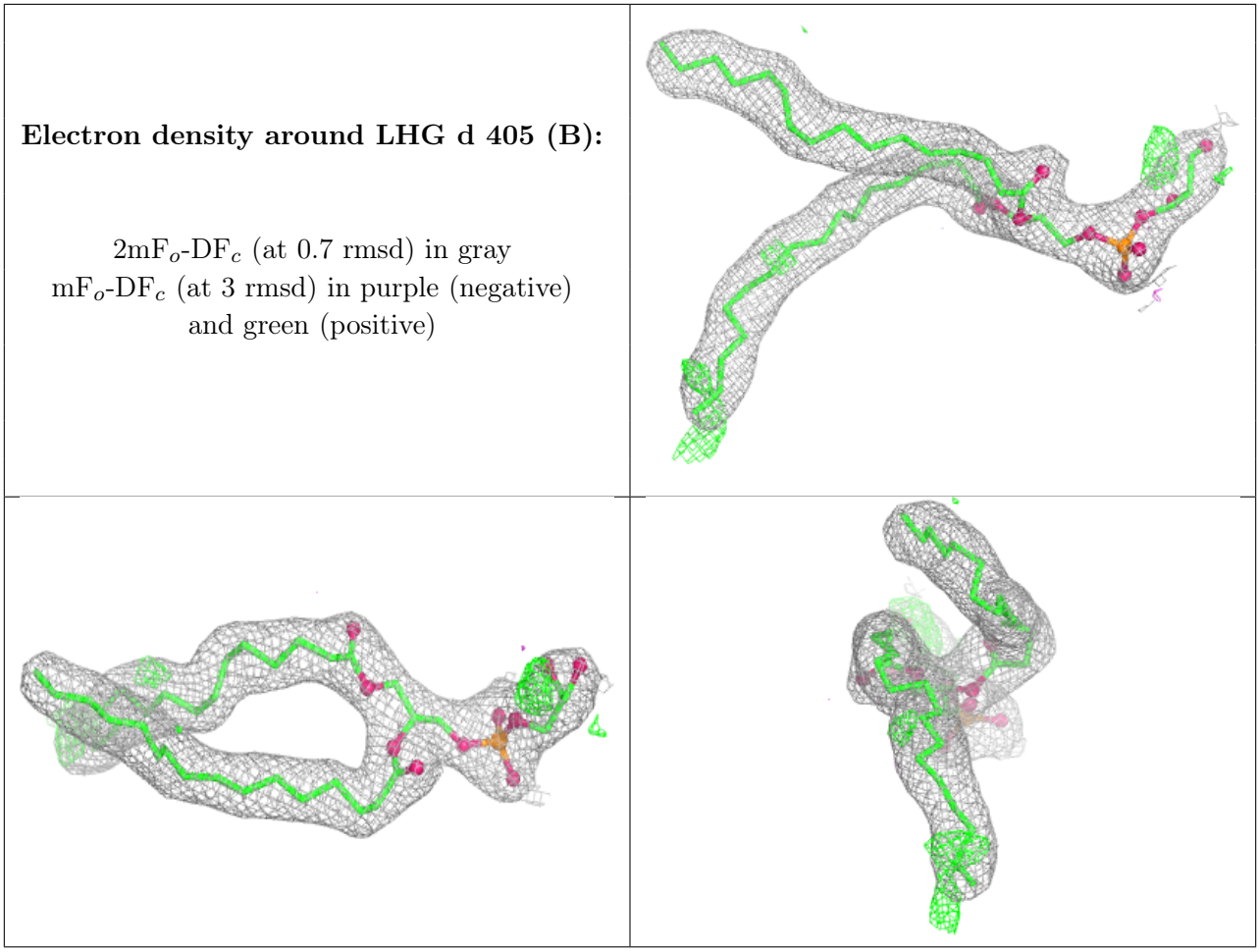






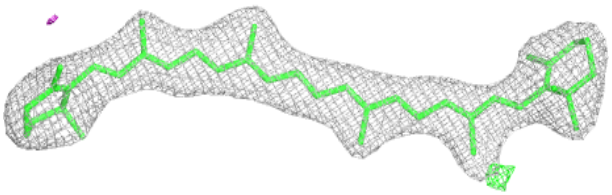
Electron density around LHG d 405 (B):

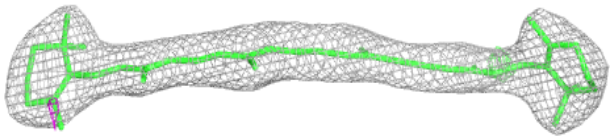
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

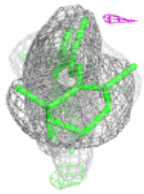


Electron density around BCR Y 101:

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

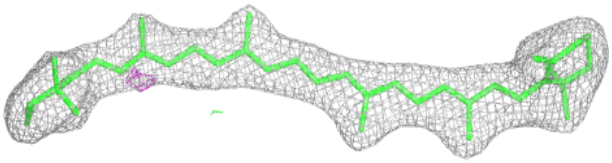


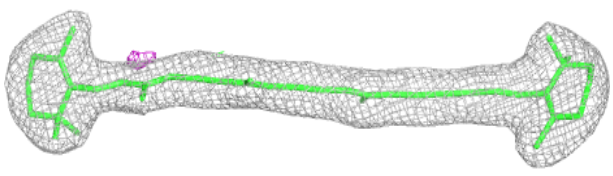


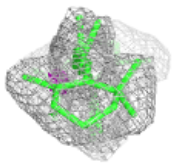


Electron density around BCR a 410:

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

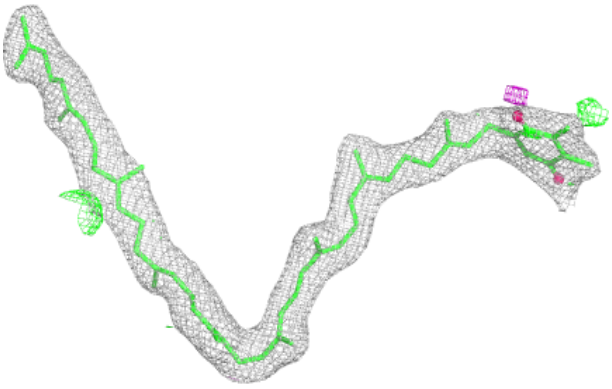


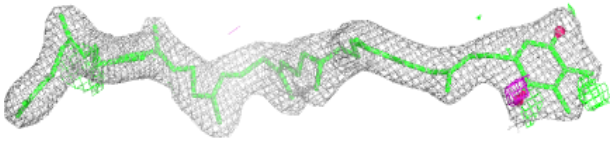


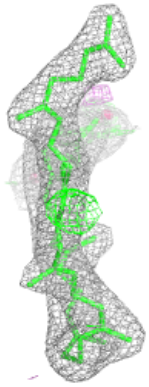


Electron density around PL9 D 705 (A):

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

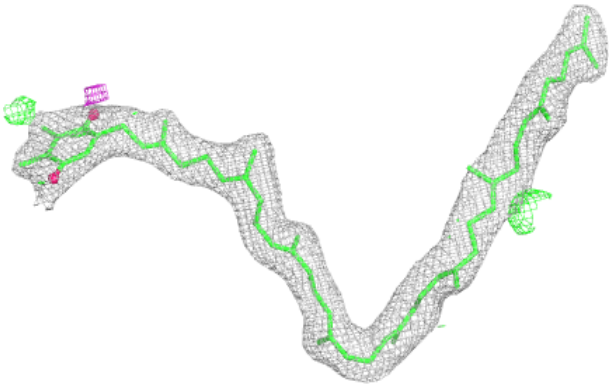


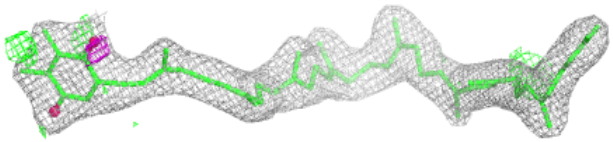


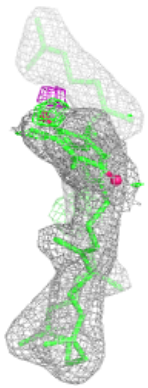


Electron density around PL9 D 705 (B):

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

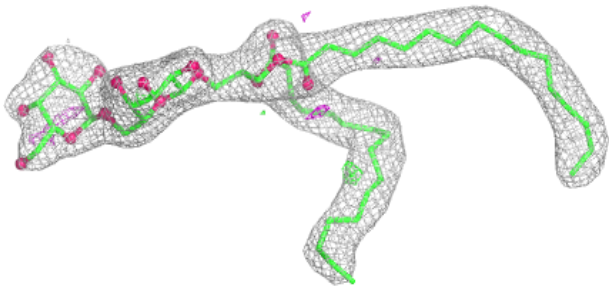


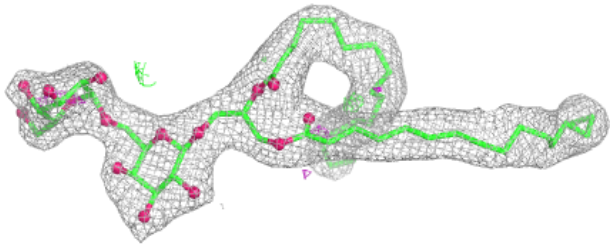


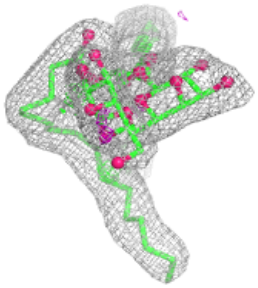


Electron density around DGD h 102:

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

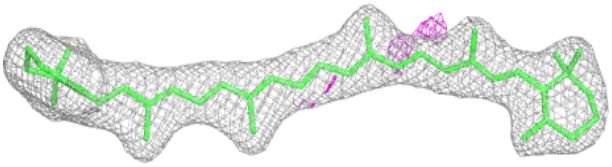


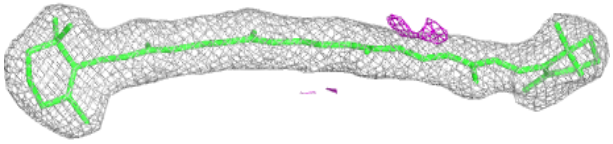


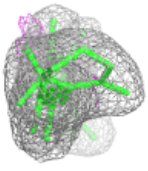


Electron density around BCR b 617:

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

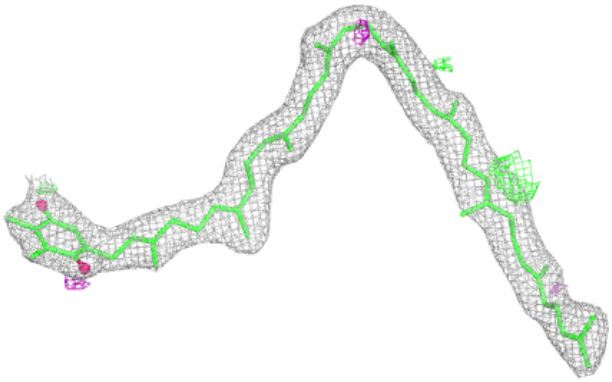


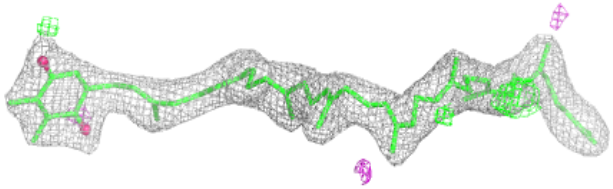


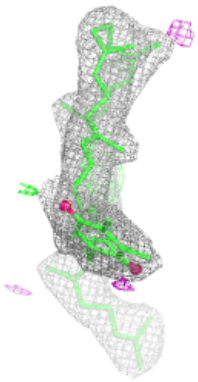


Electron density around PL9 d 404 (A):

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

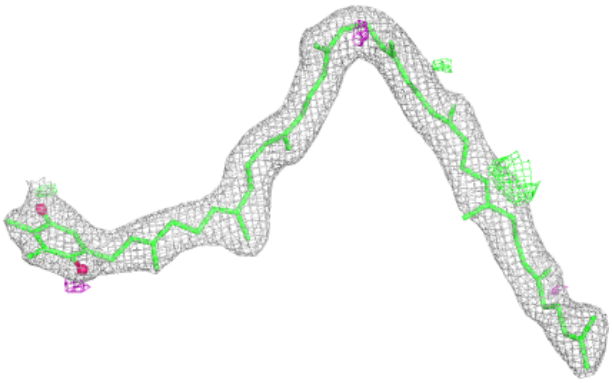


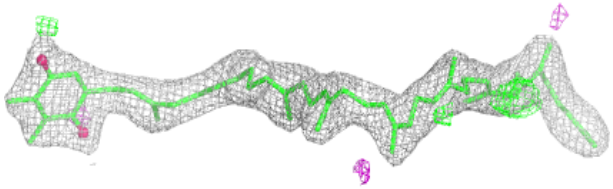


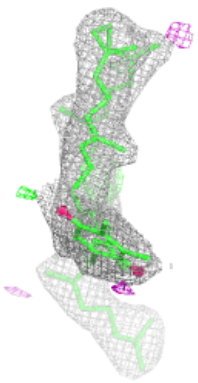


Electron density around PL9 d 404 (B):

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

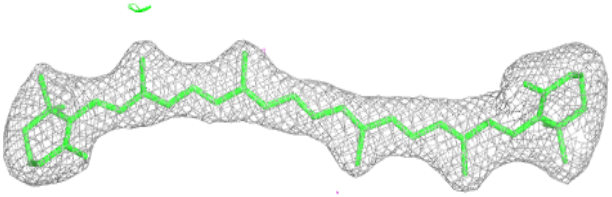


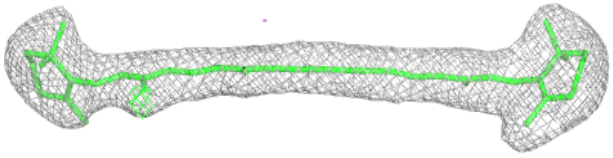


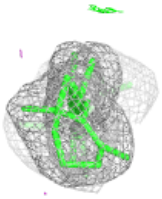


Electron density around BCR b 618:

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

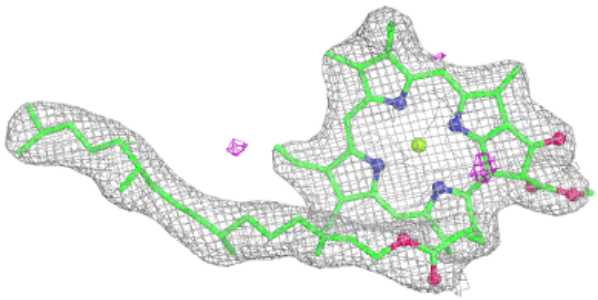


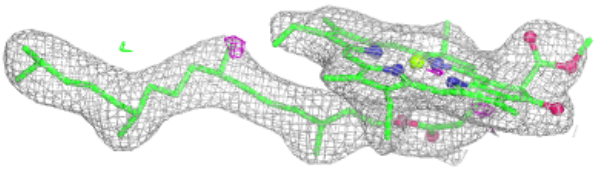


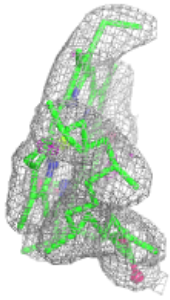


Electron density around CLA c 502:

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

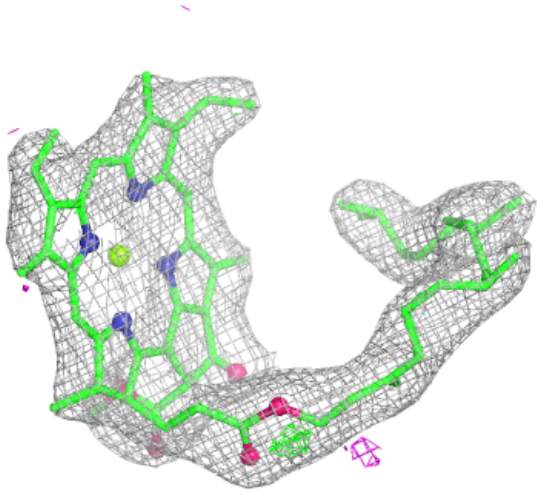


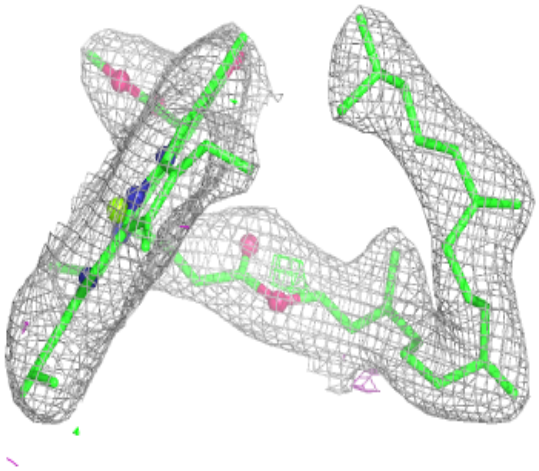


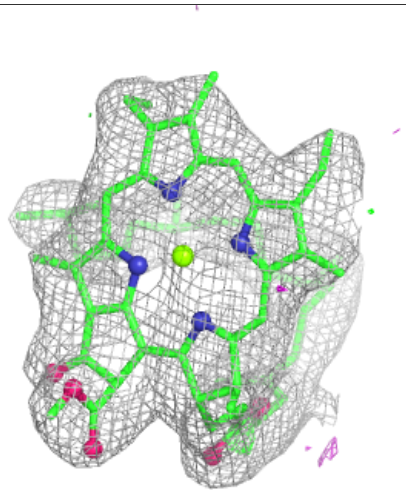


Electron density around CLA c 504:

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

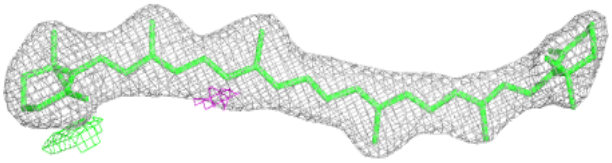


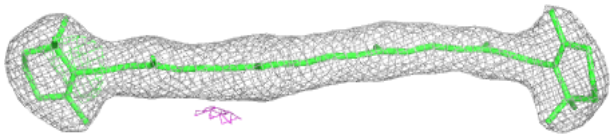


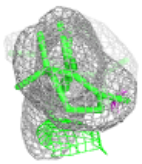


Electron density around BCR c 516:

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

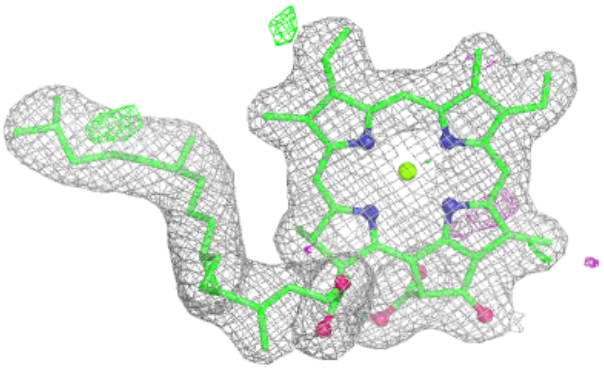


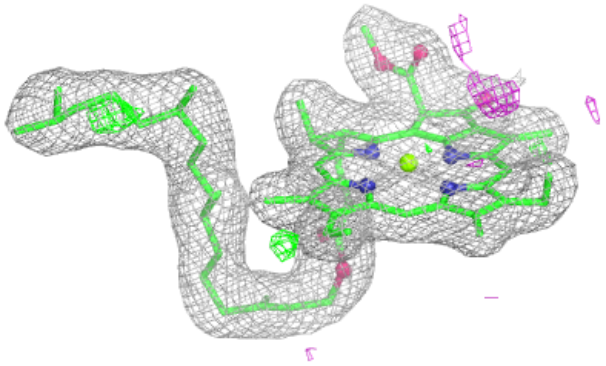


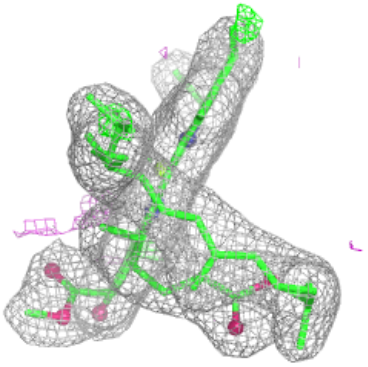


Electron density around CLA A 405 (A):

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

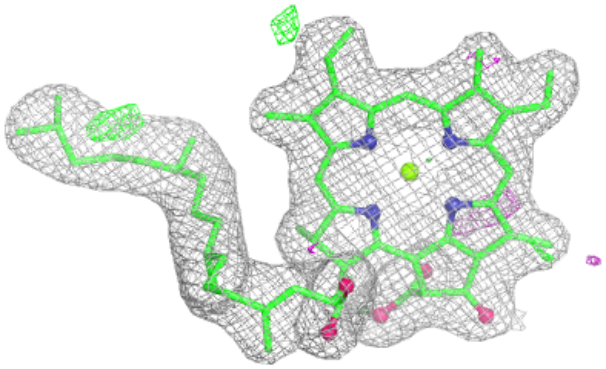


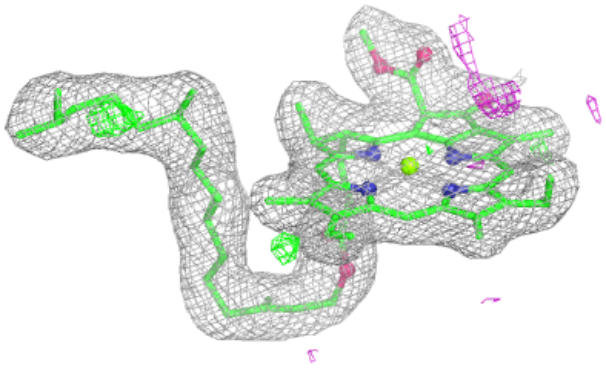


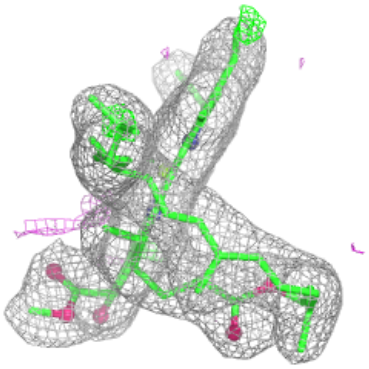


Electron density around CLA A 405 (B):

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

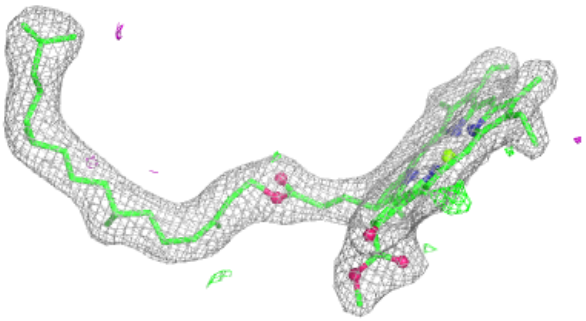


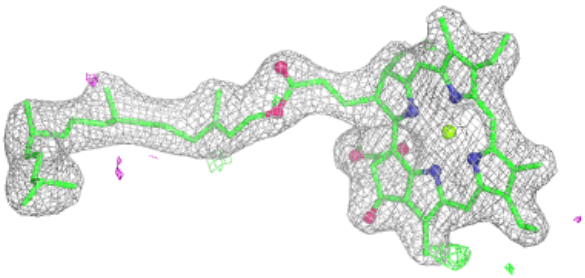


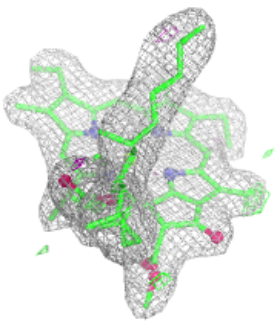


Electron density around CLA D 702 (A):

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

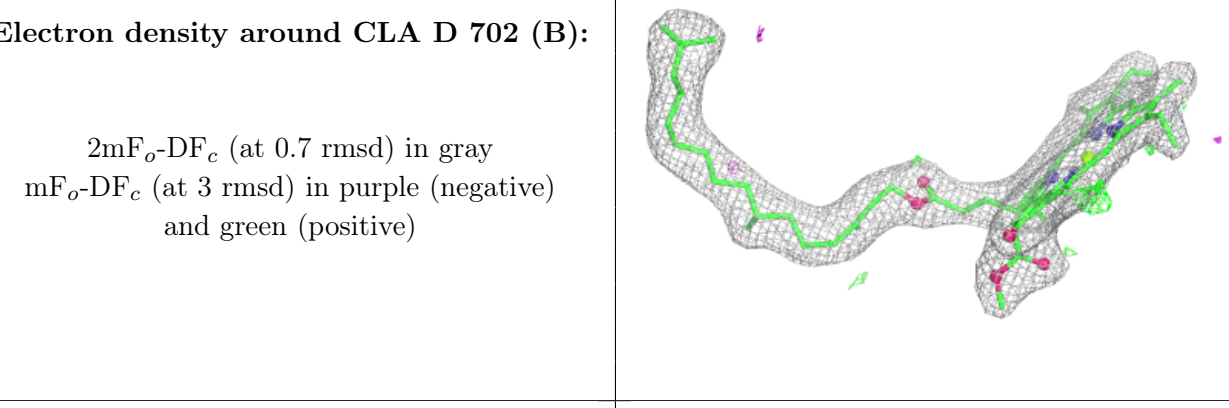






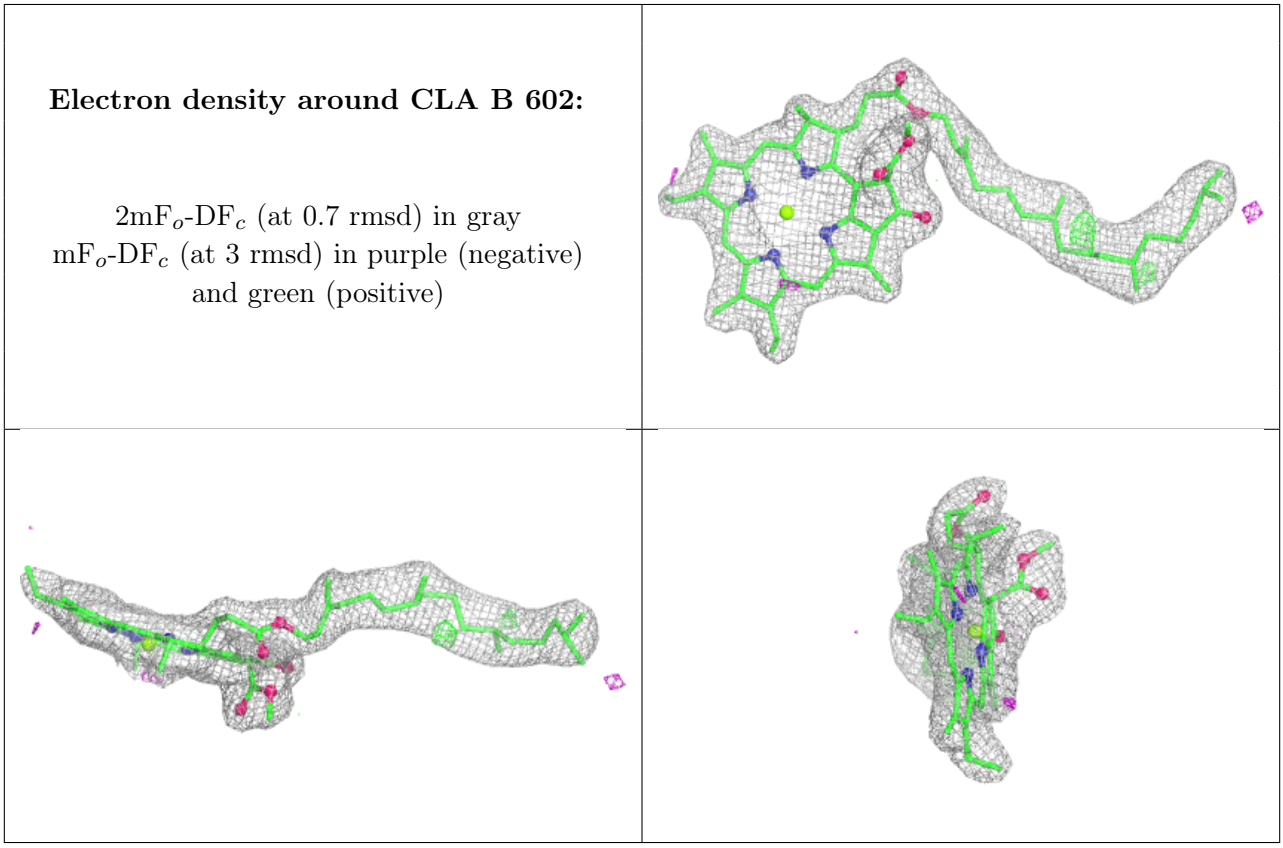
Electron density around CLA D 702 (B):

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



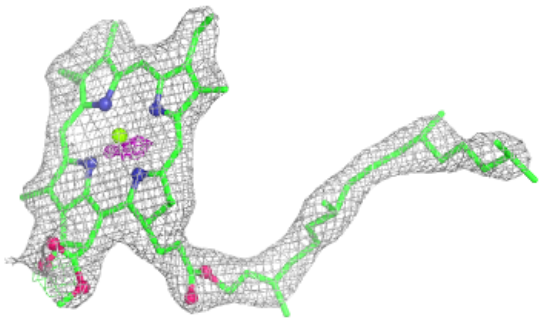
Electron density around CLA B 602:

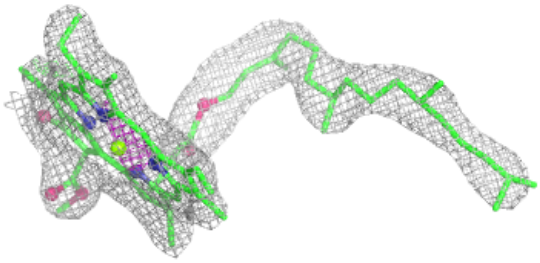
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

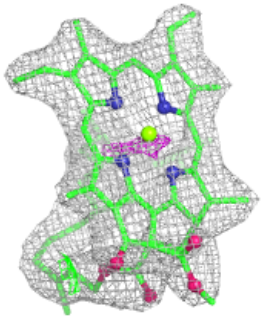


Electron density around CLA c 512:

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

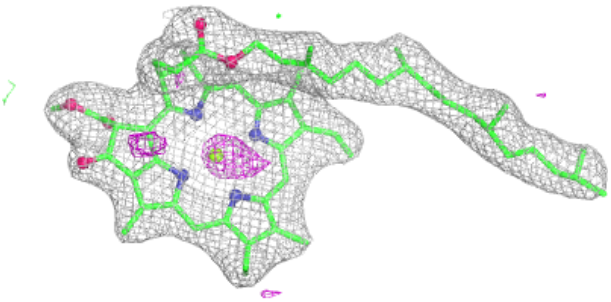


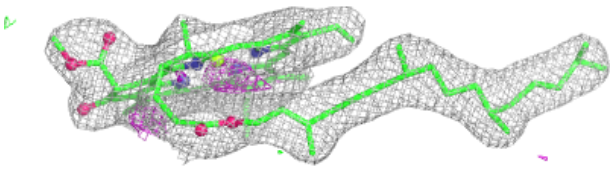


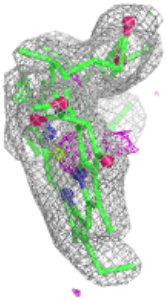


Electron density around CLA C 502:

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

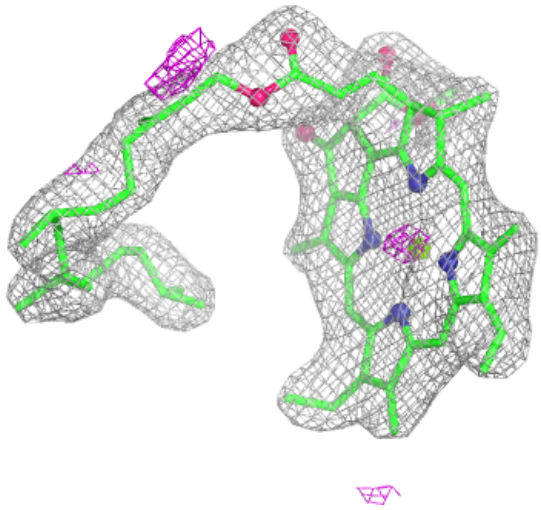


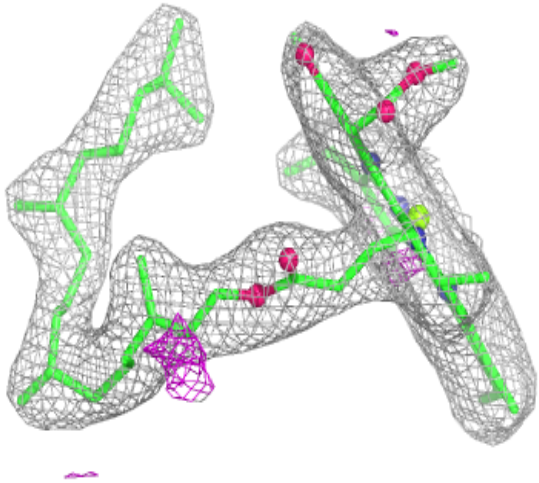


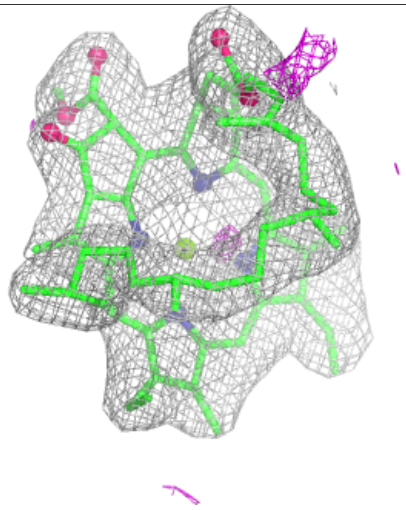


Electron density around CLA C 504:

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

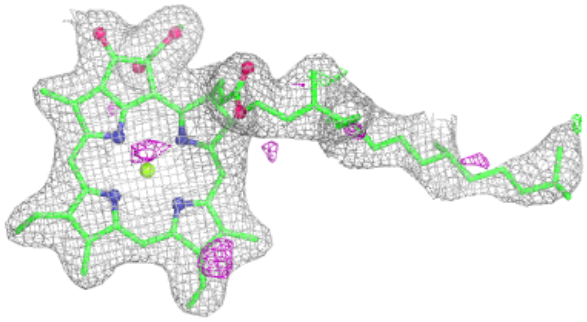


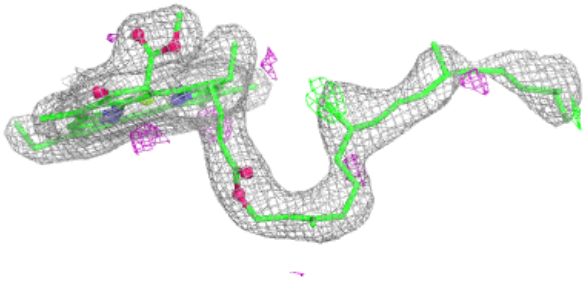


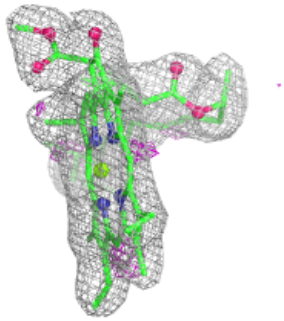


Electron density around CLA A 406 (A):

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

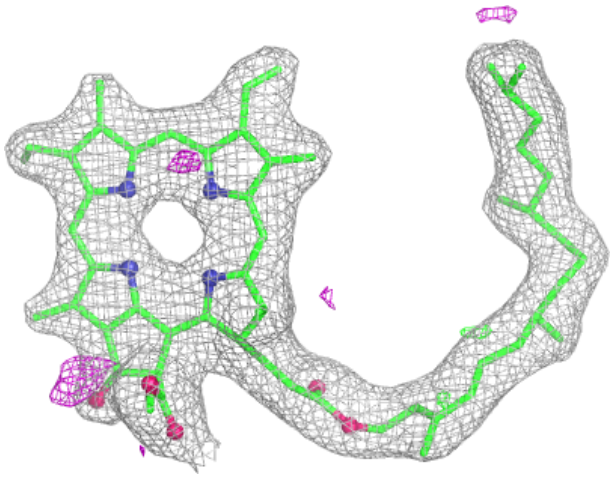


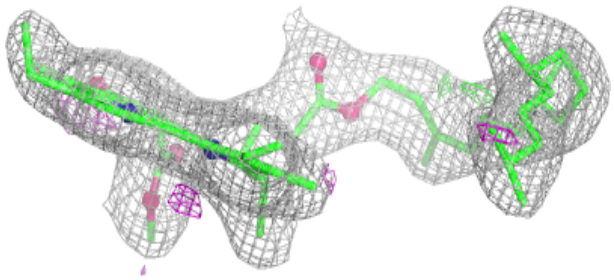


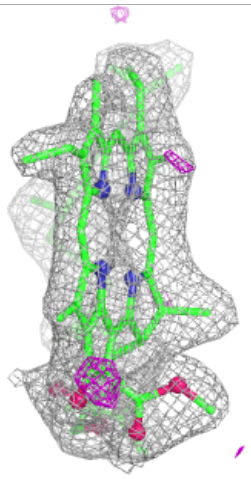


Electron density around PHO A 407 (A):

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

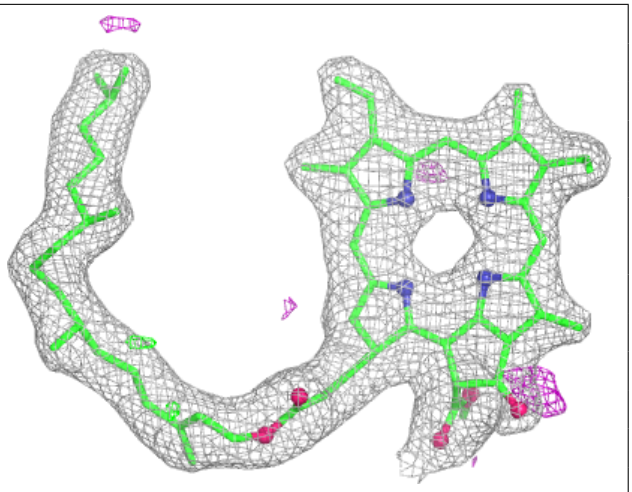


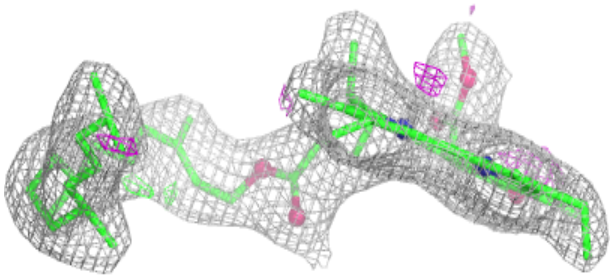


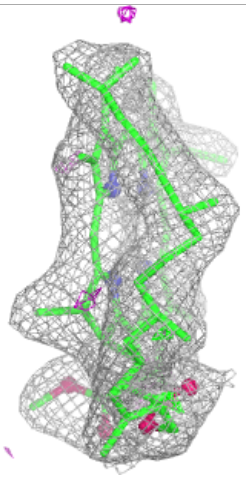


Electron density around PHO A 407 (B):

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

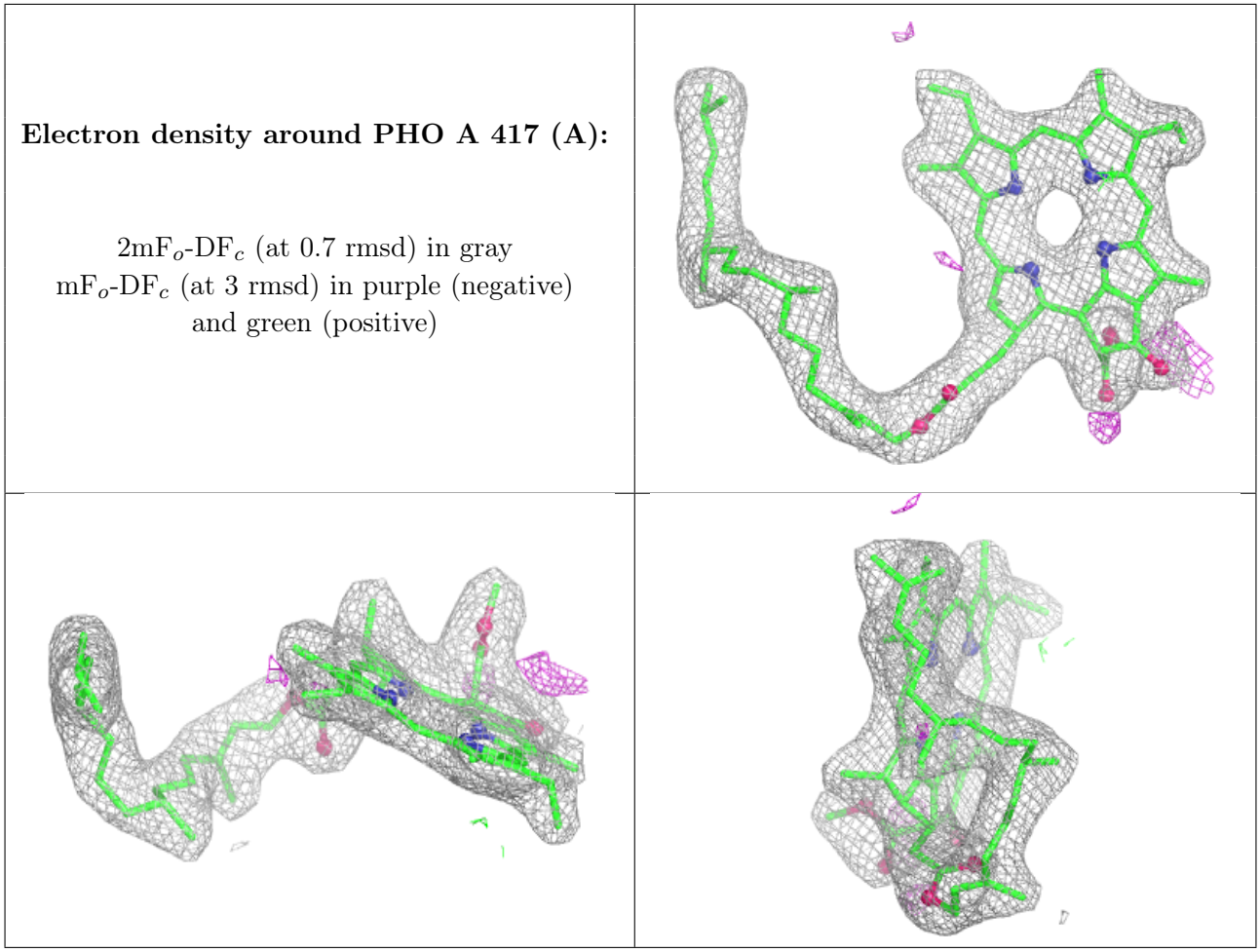






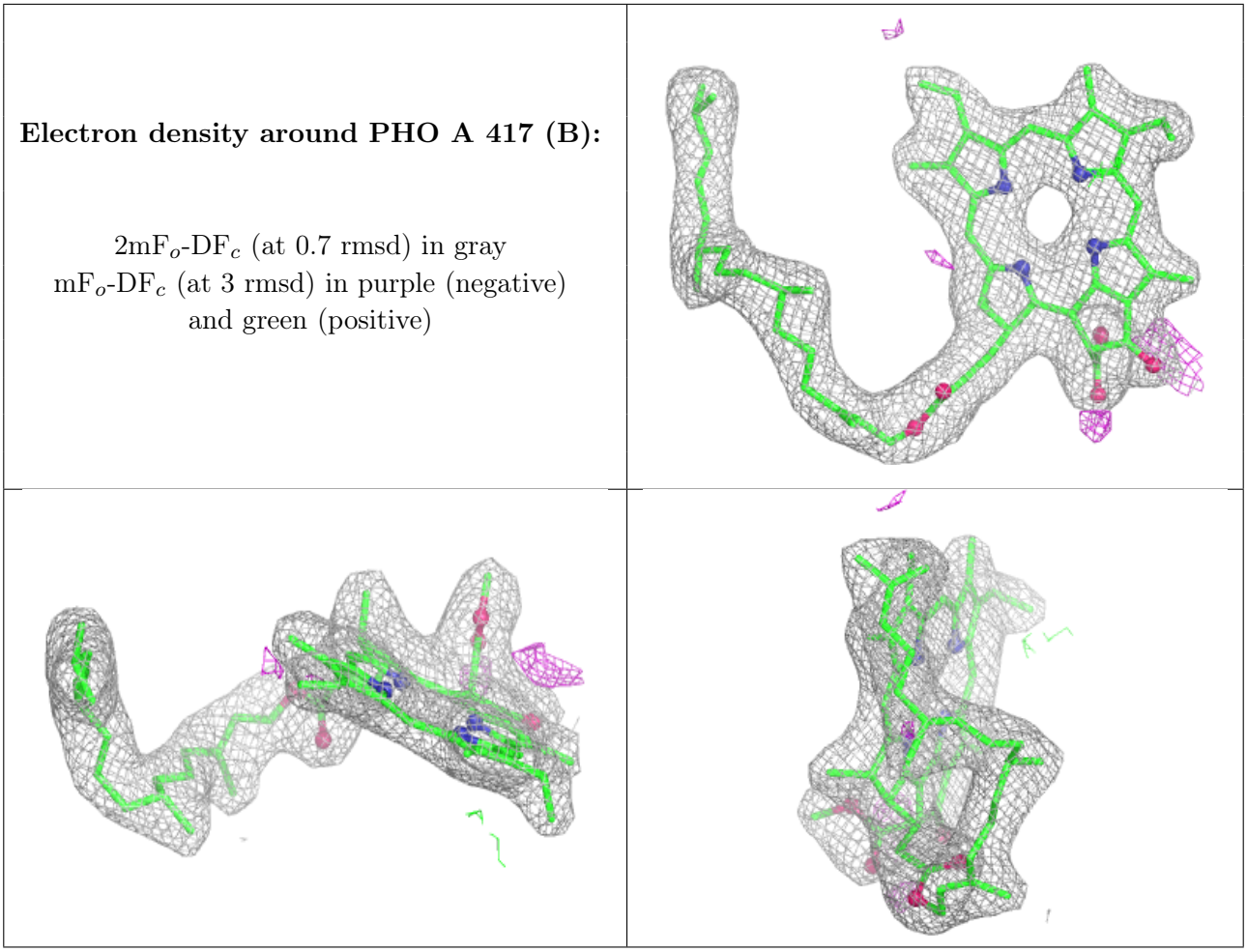
Electron density around PHO A 417 (A):

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



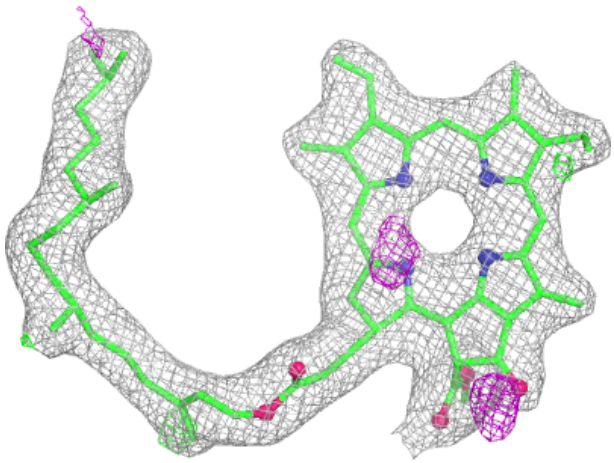
Electron density around PHO A 417 (B):

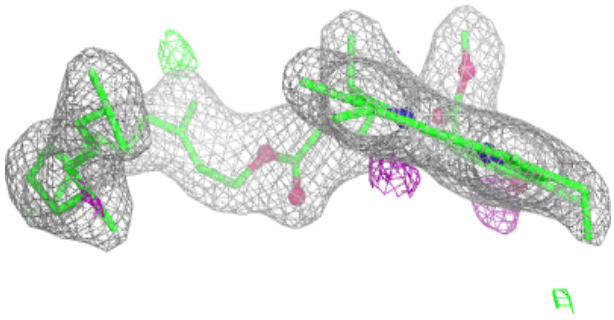
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

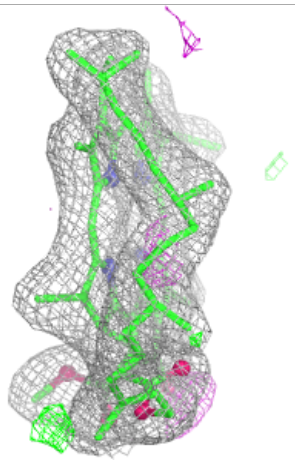


Electron density around PHO a 408 (A):

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

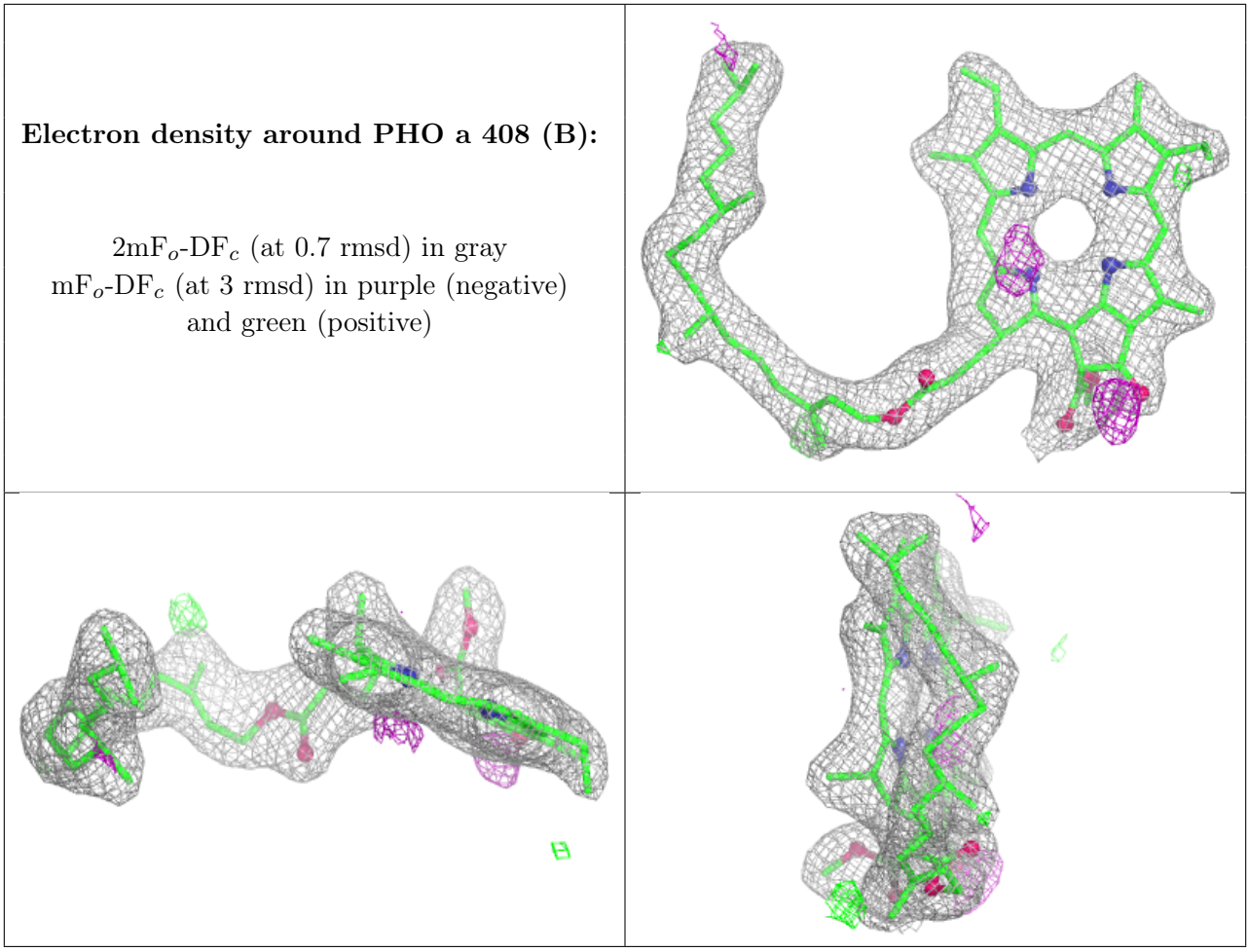






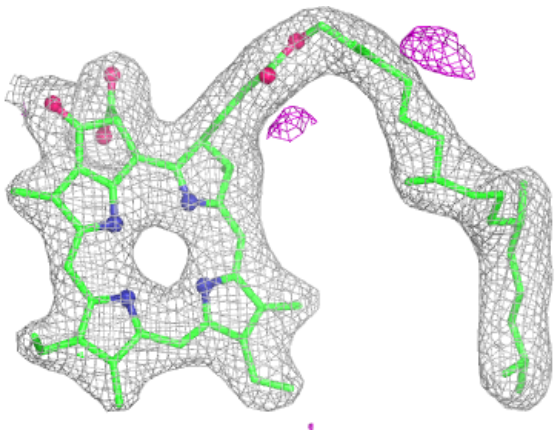
Electron density around PHO a 408 (B):

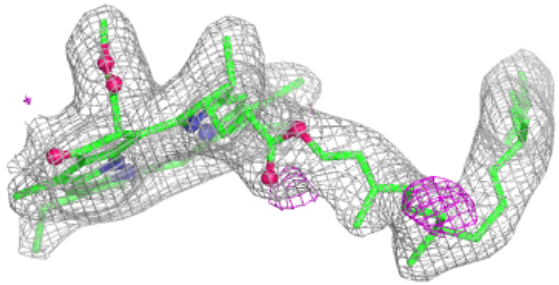
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

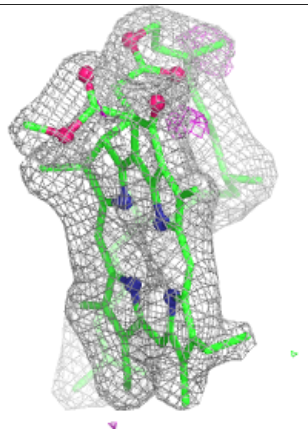


Electron density around PHO a 416 (A):

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

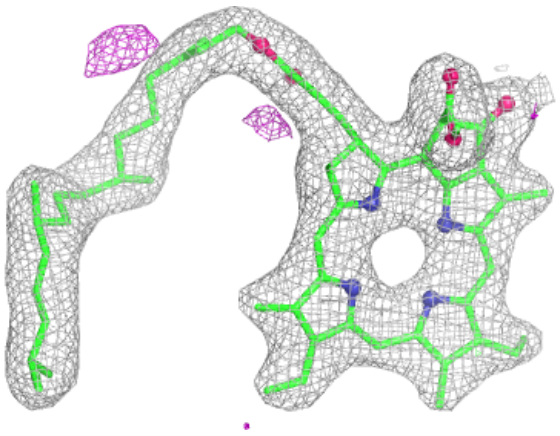


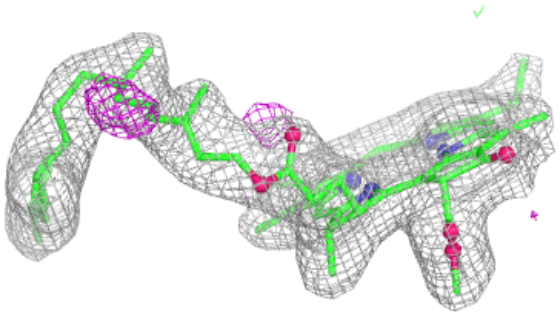


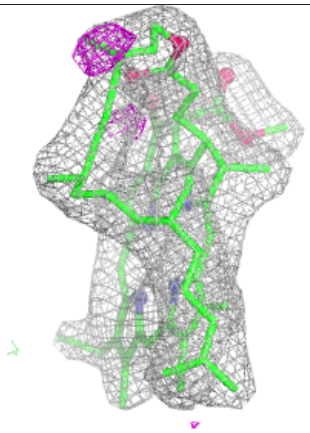


Electron density around PHO a 416 (B):

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

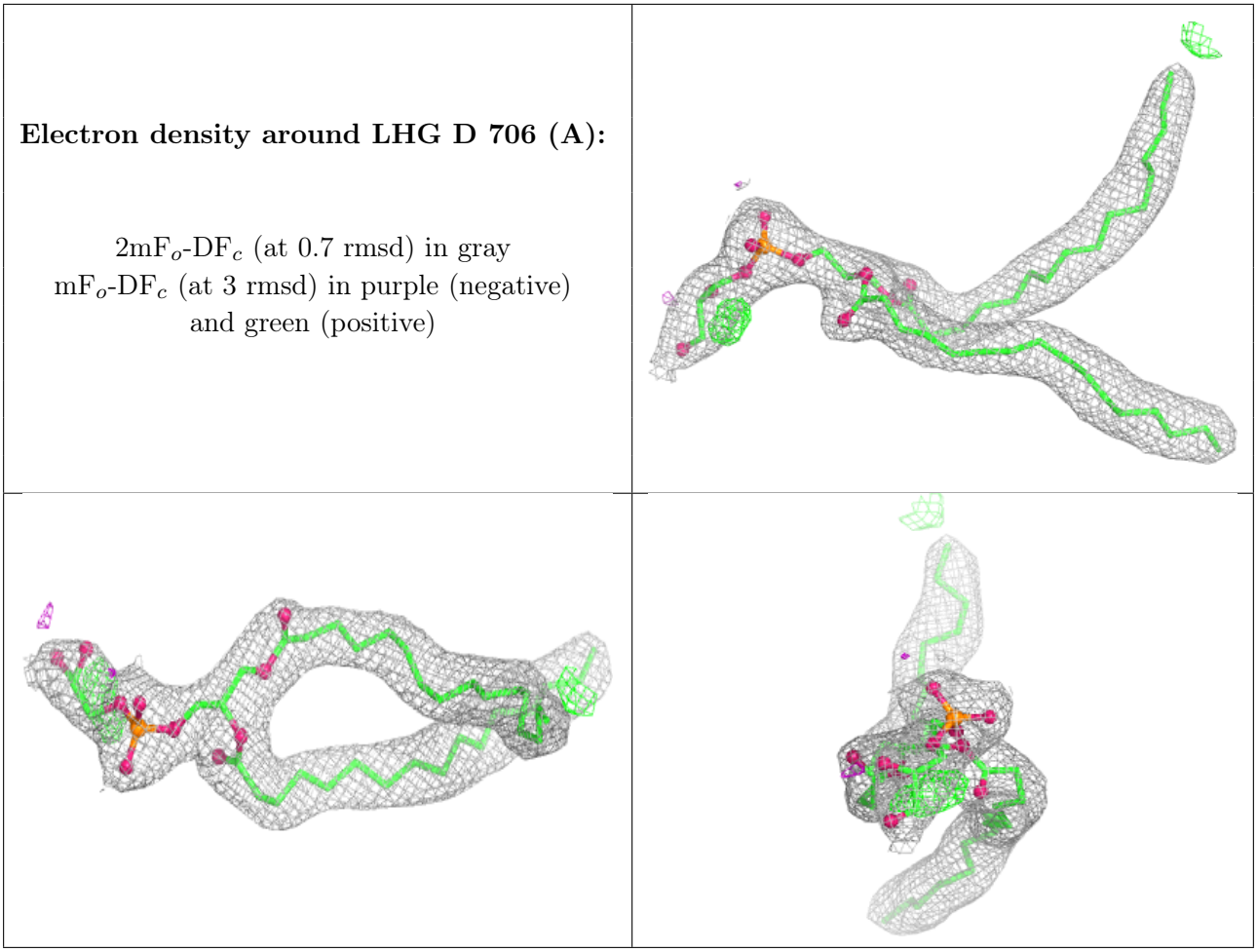






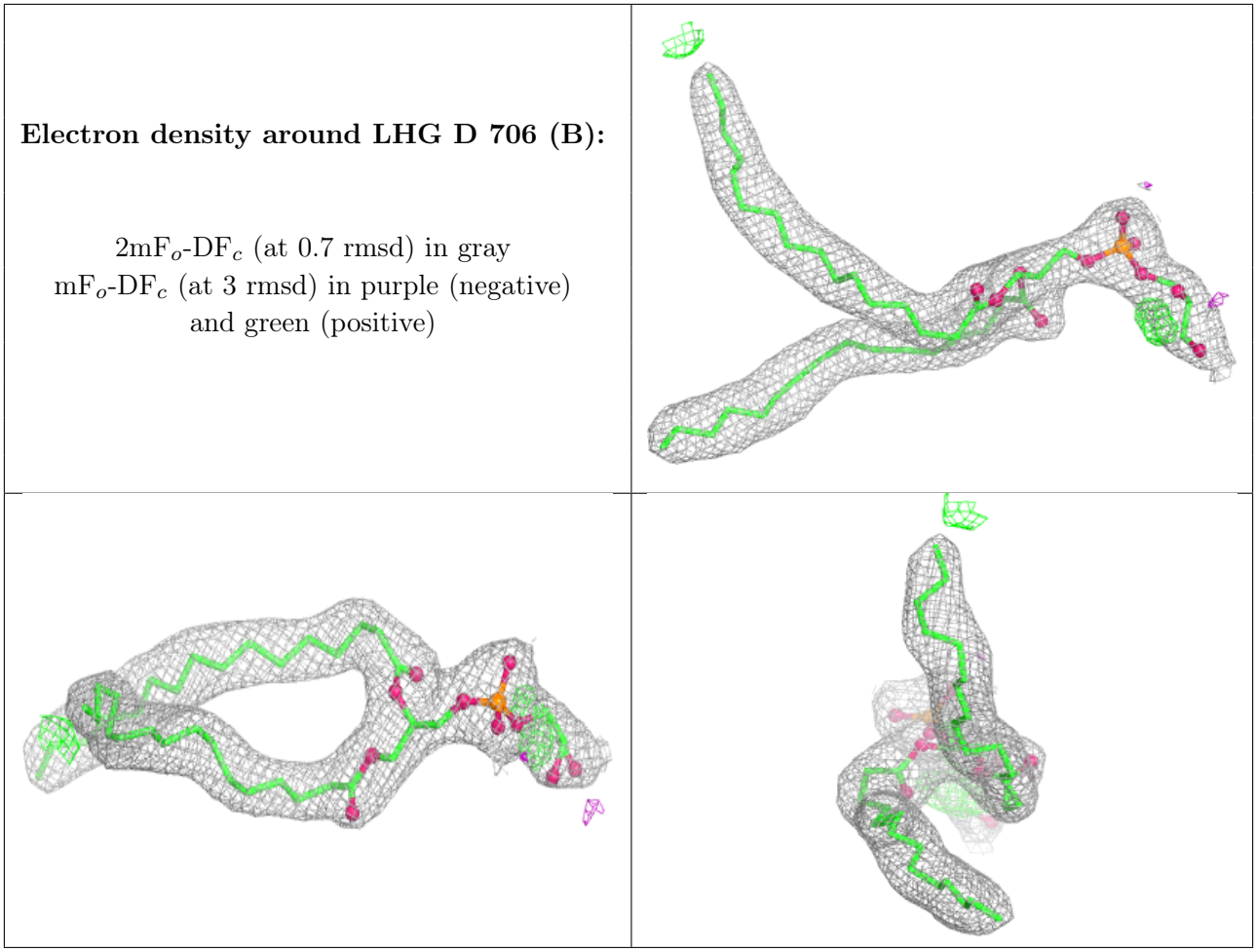
Electron density around LHG D 706 (A):

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



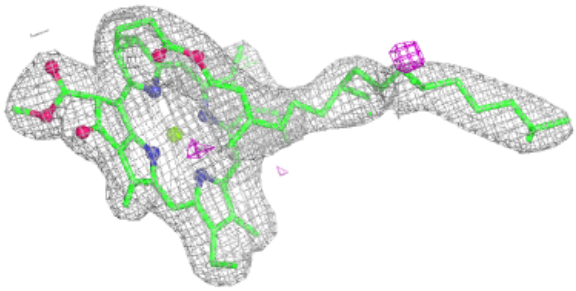
Electron density around LHG D 706 (B):

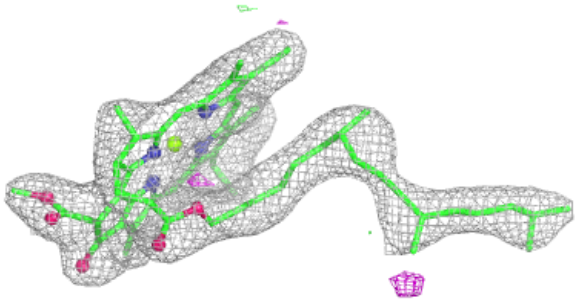
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

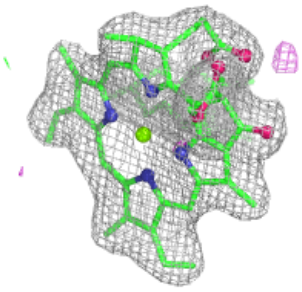


Electron density around CLA C 506:

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

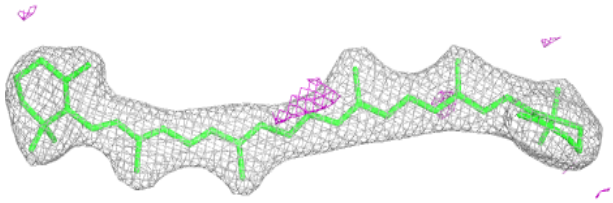


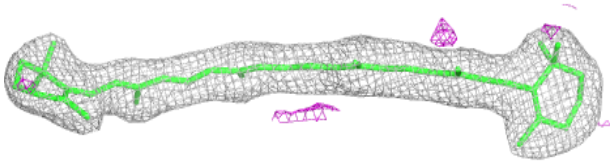


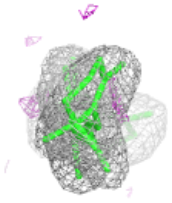


Electron density around BCR B 617:

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

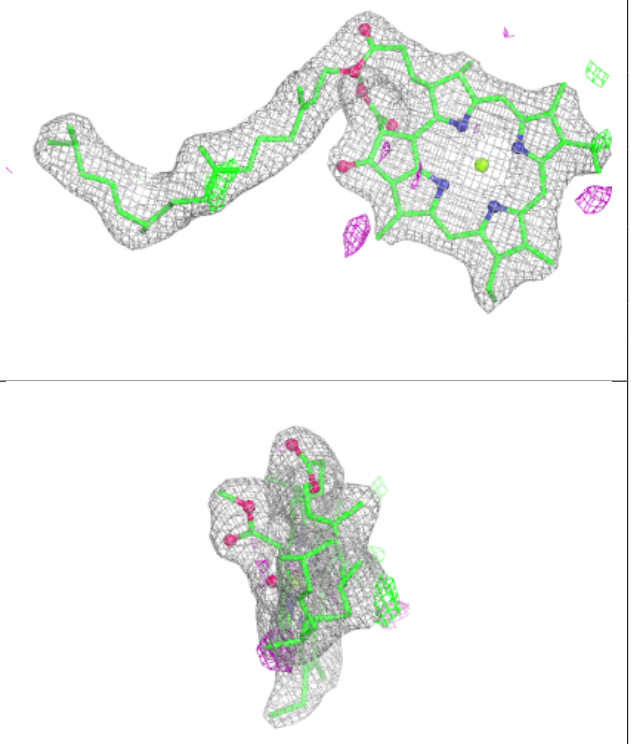






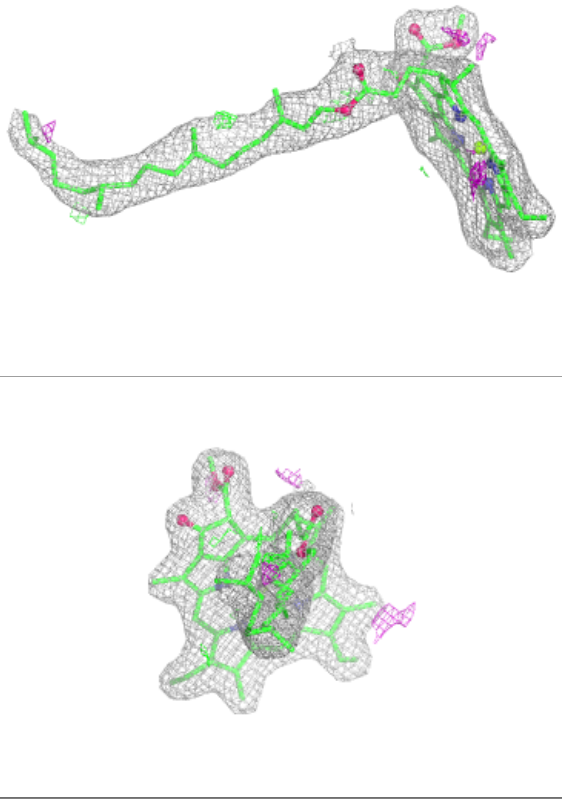
Electron density around CLA b 602:

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



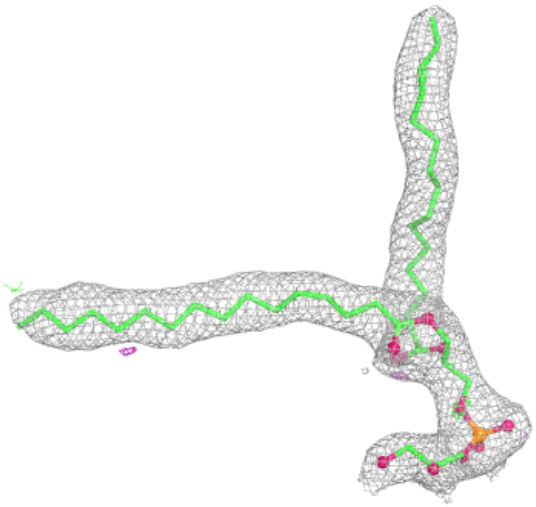
Electron density around CLA b 604:

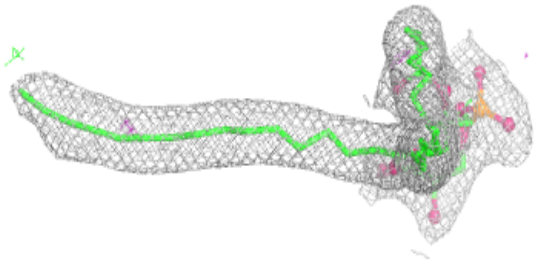
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

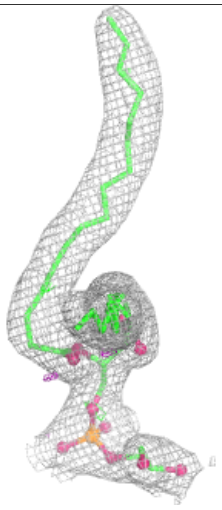


Electron density around LHG L 101 (A):

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

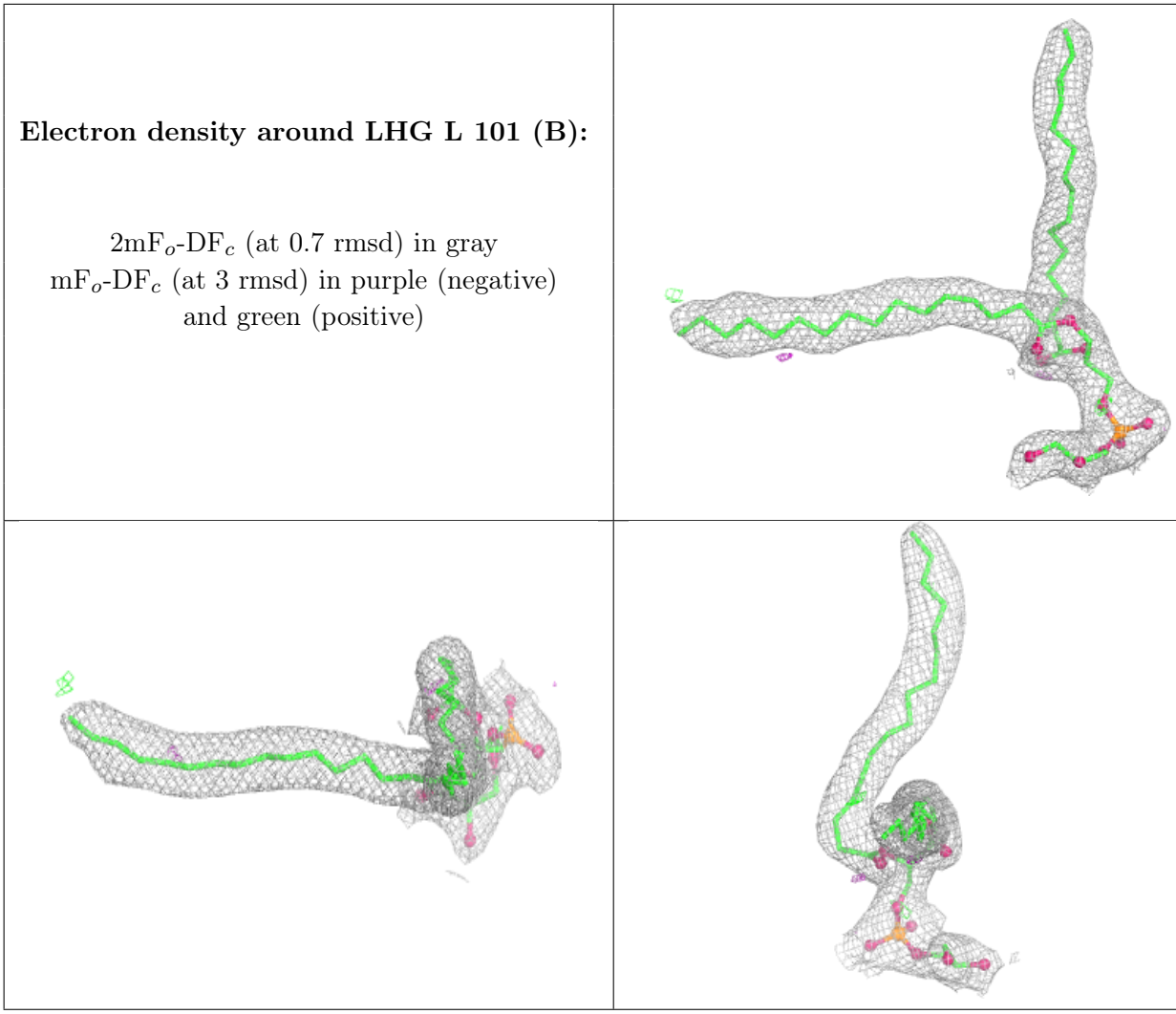






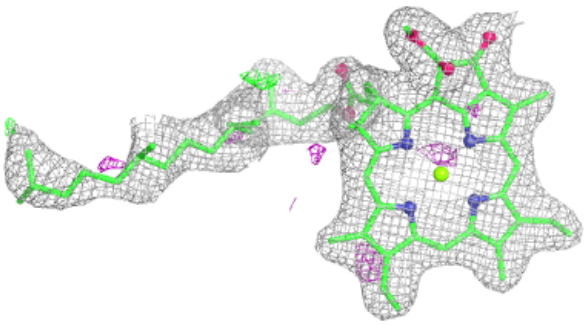
Electron density around LHG L 101 (B):

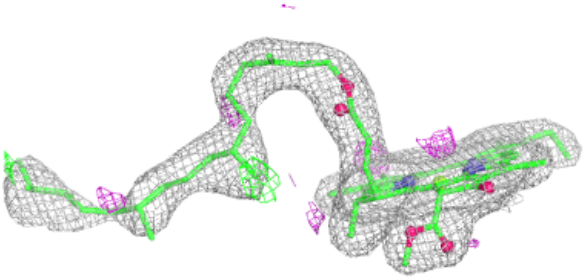
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

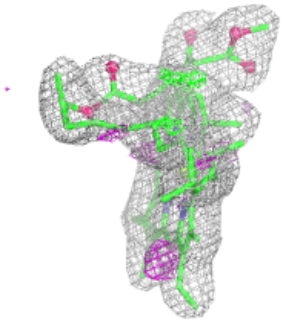


Electron density around CLA A 406 (B):

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

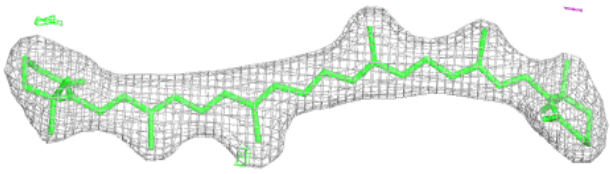


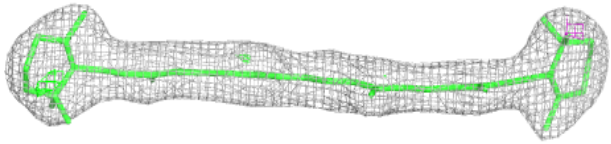


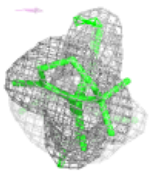


Electron density around BCR C 516:

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

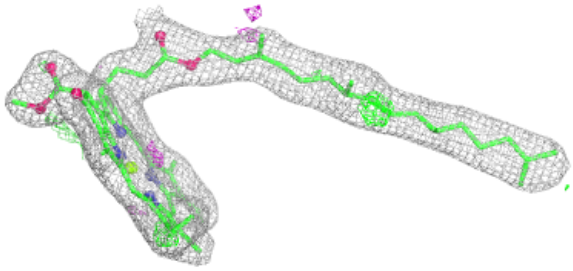


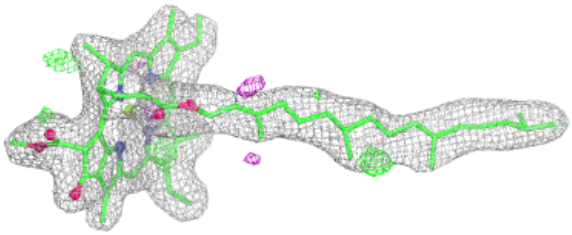


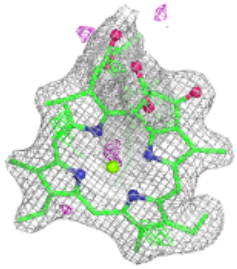


Electron density around CLA b 607:

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

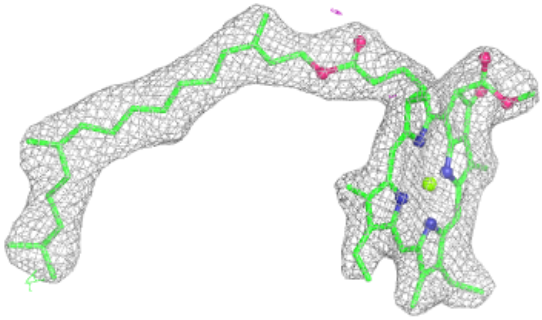


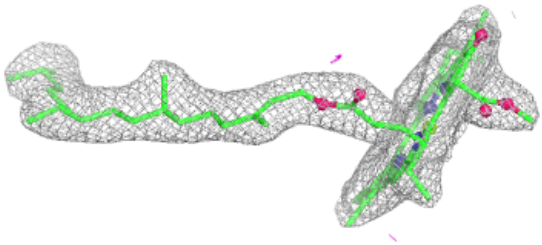


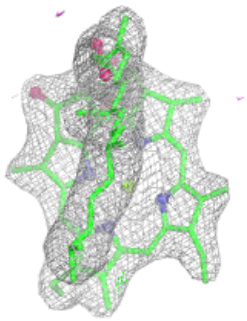


Electron density around CLA b 609:

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

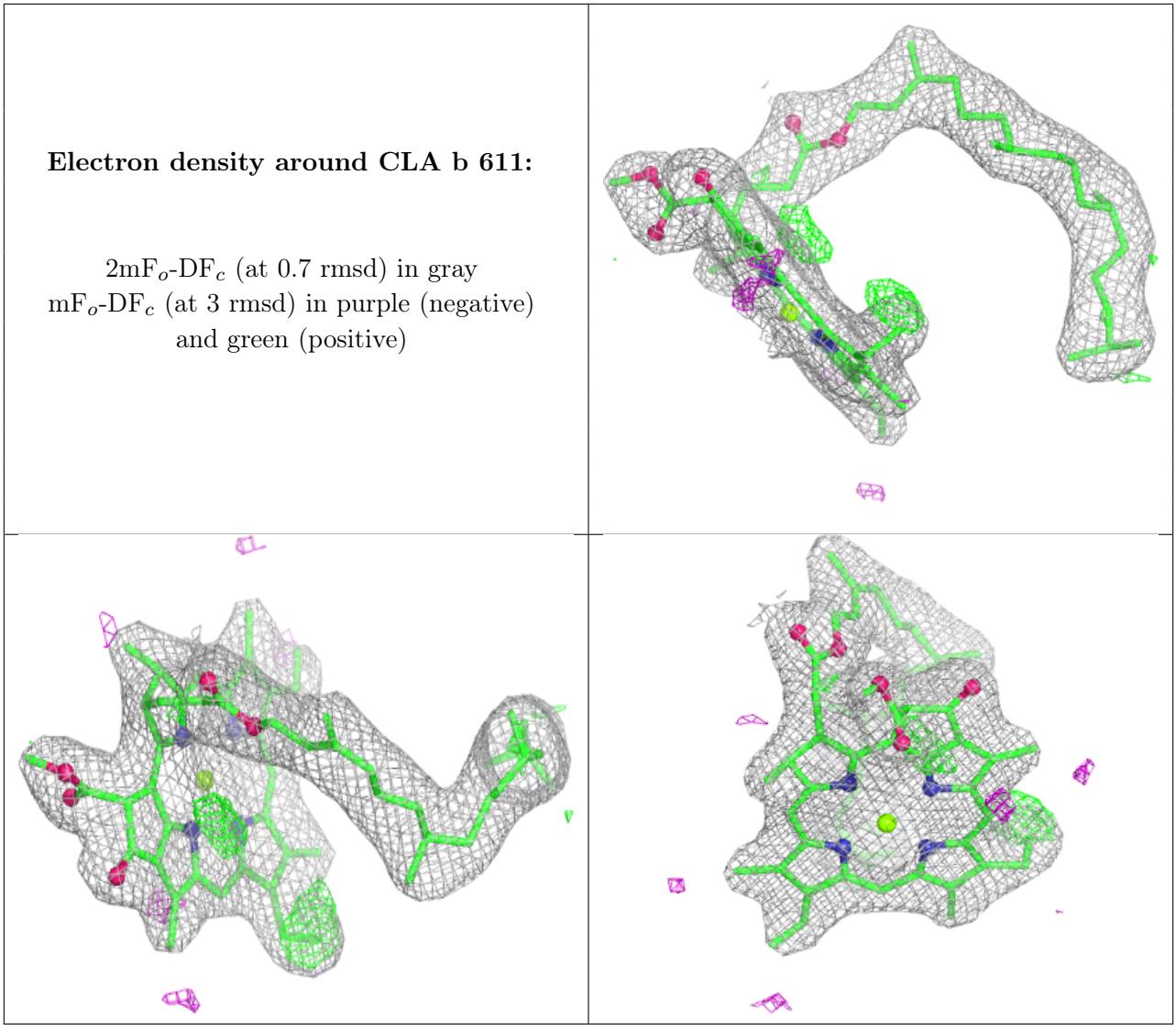






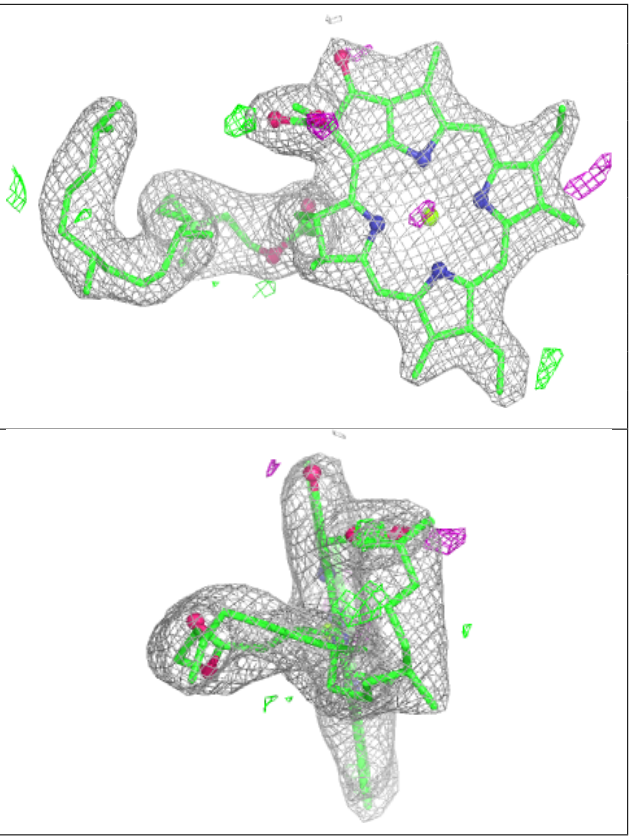
Electron density around CLA b 611:

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



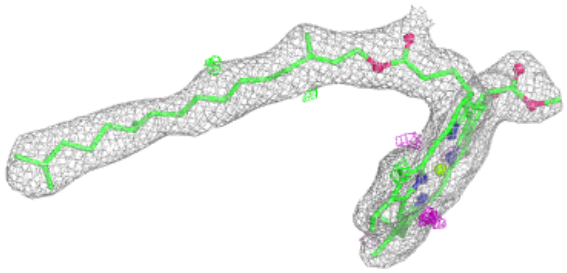
Electron density around CLA b 612:

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



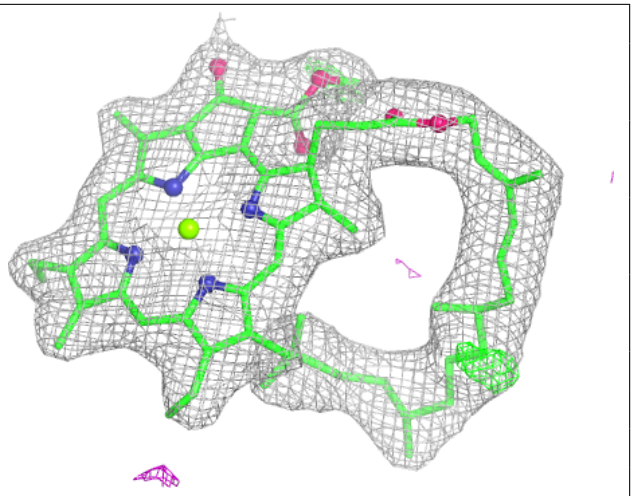
Electron density around CLA B 607:

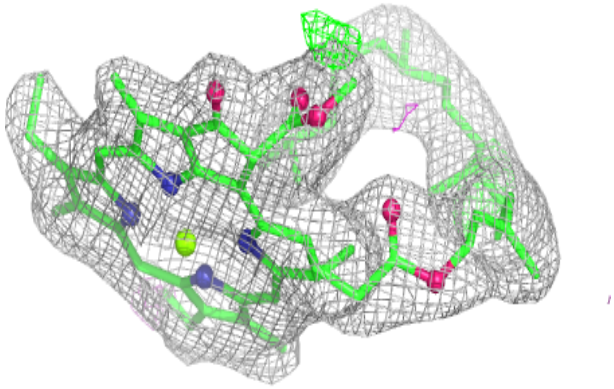
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

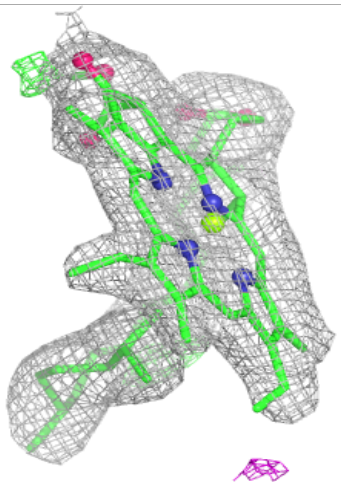


Electron density around CLA b 615:

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

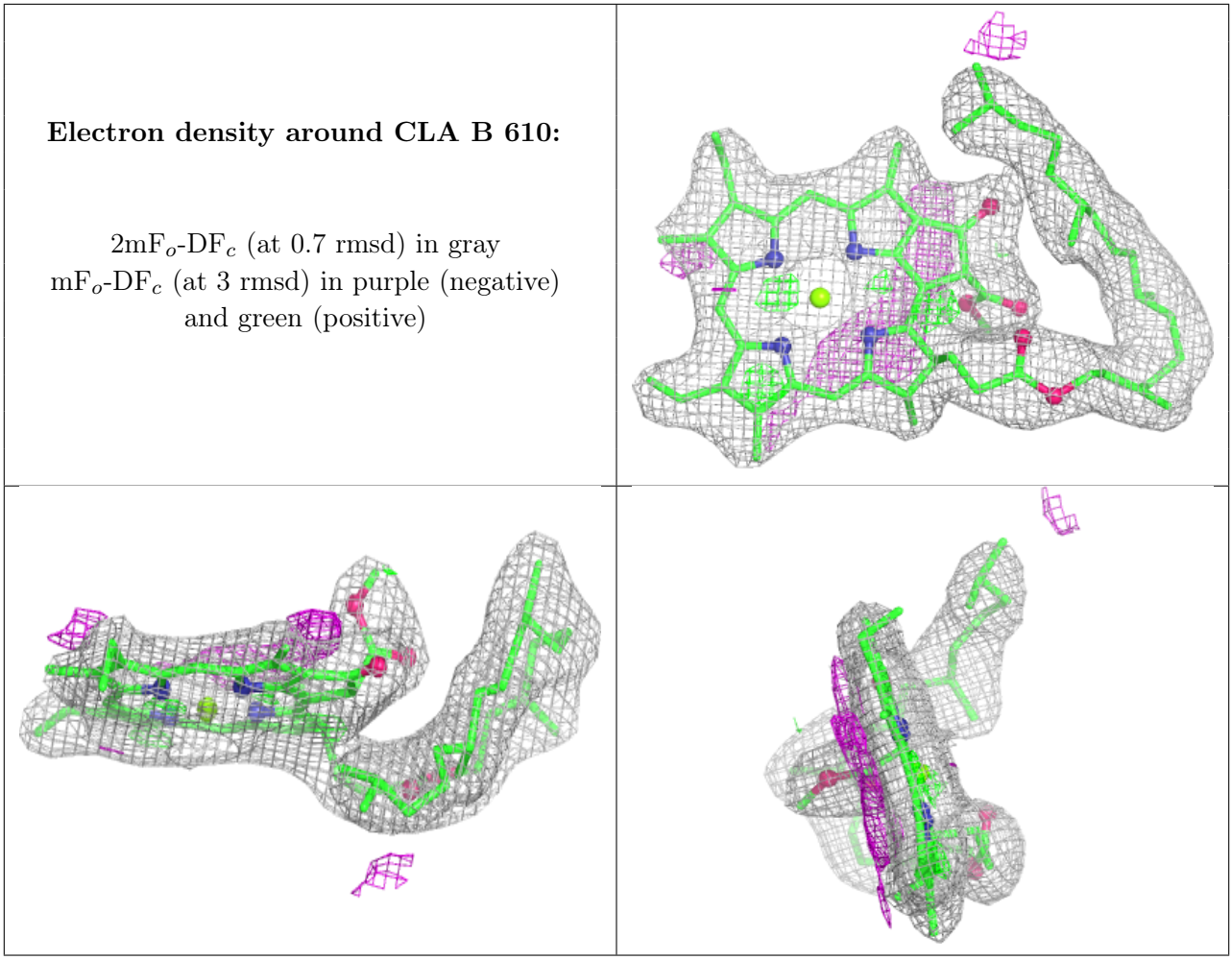






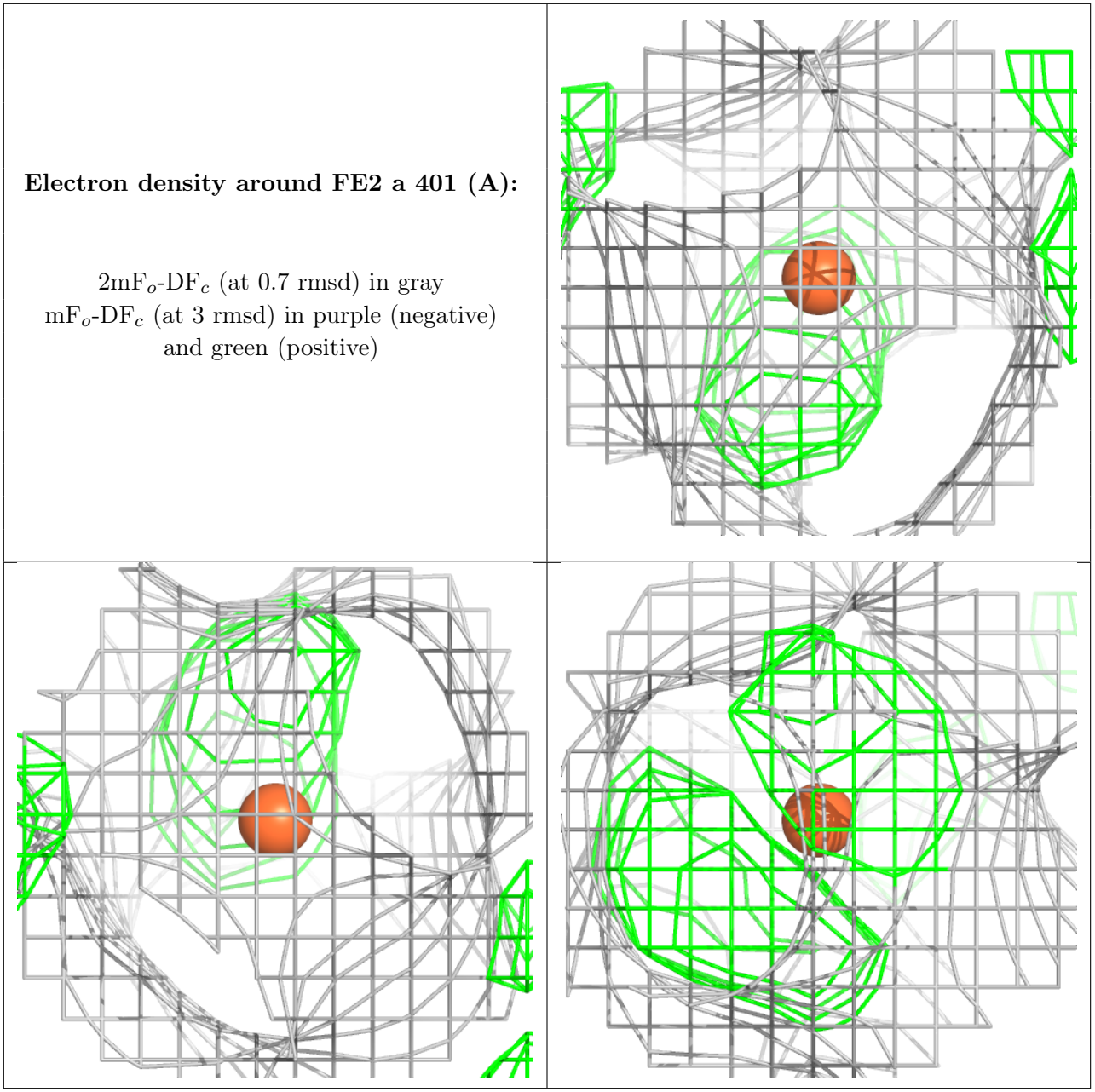
Electron density around CLA B 610:

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



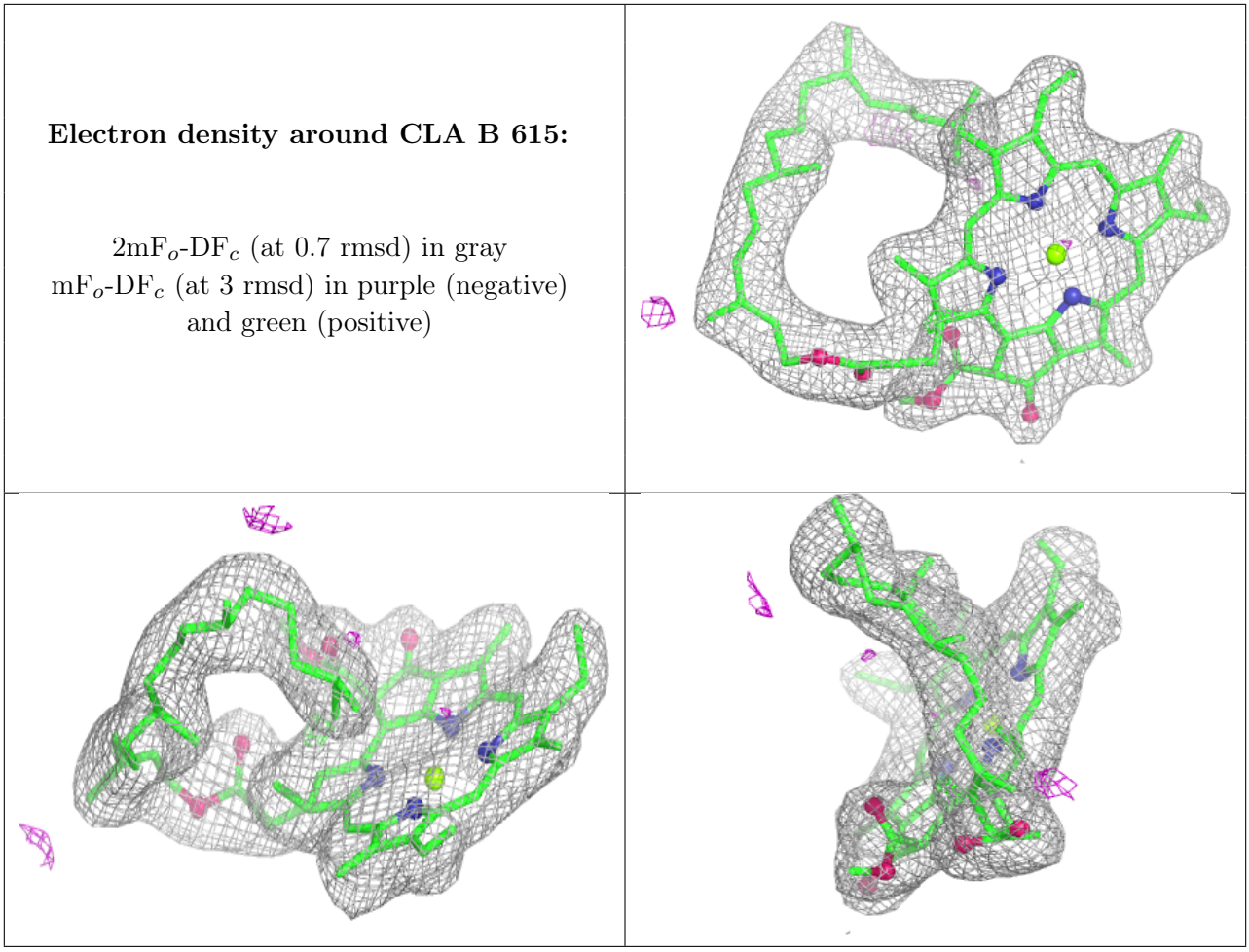
Electron density around FE2 a 401 (A):

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



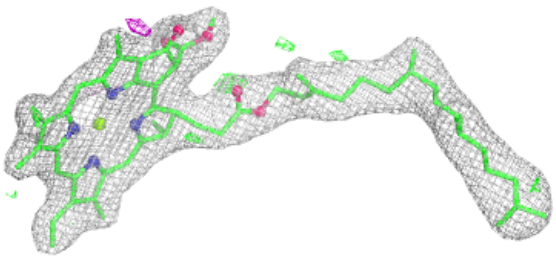
Electron density around CLA B 615:

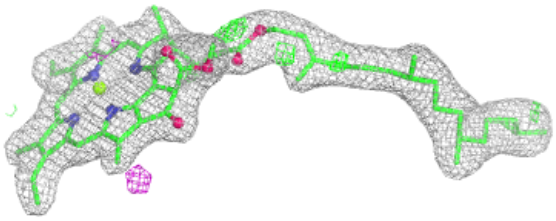
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

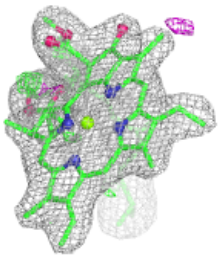


Electron density around CLA a 405 (A):

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

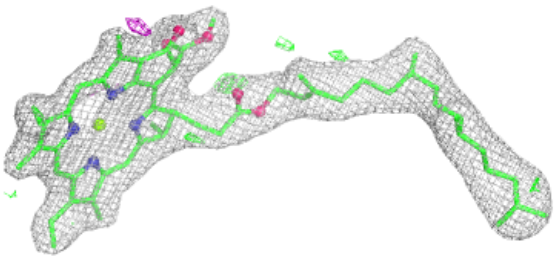


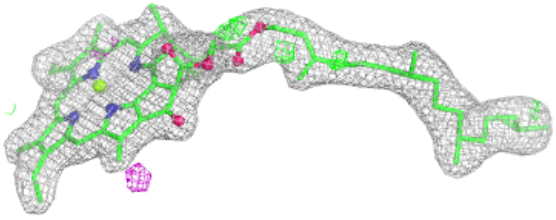


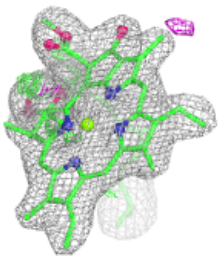


Electron density around CLA a 405 (B):

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

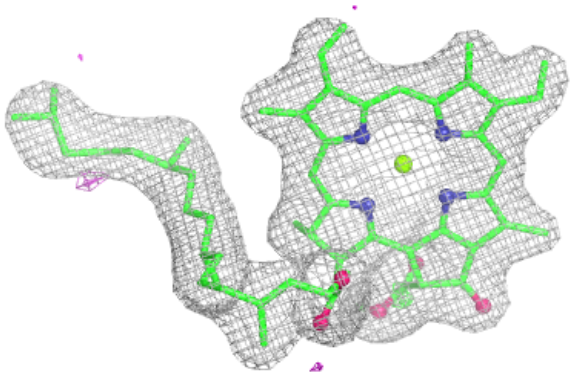


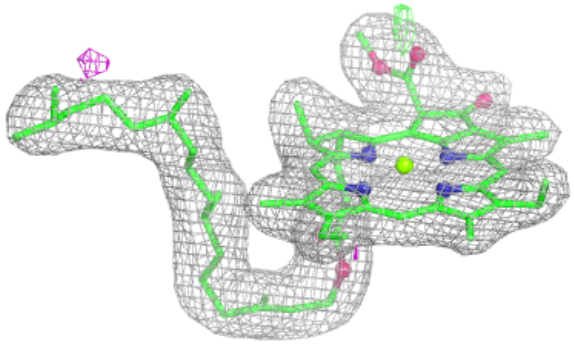


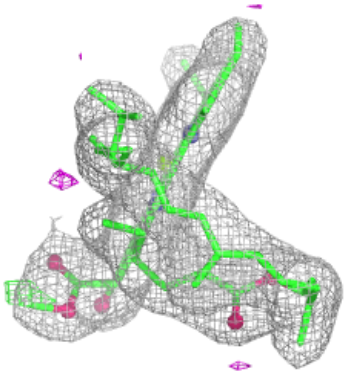


Electron density around CLA a 406 (A):

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

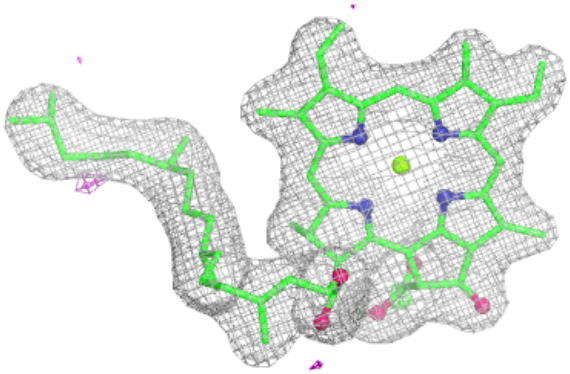


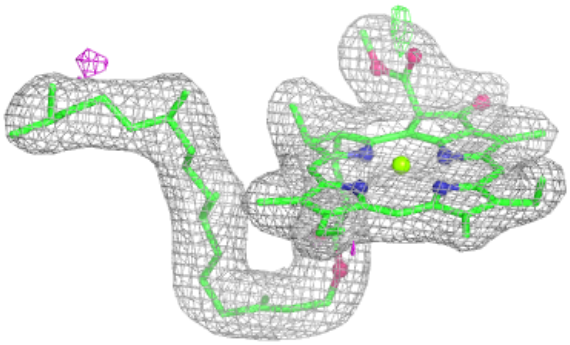


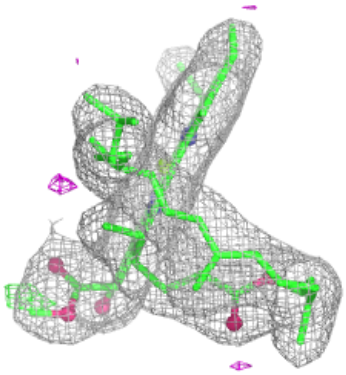


Electron density around CLA a 406 (B):

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

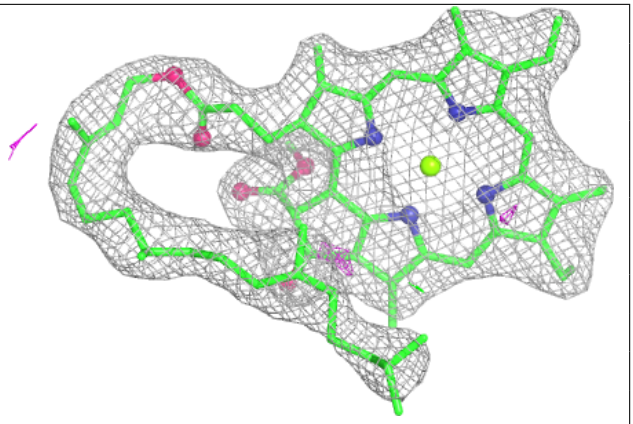


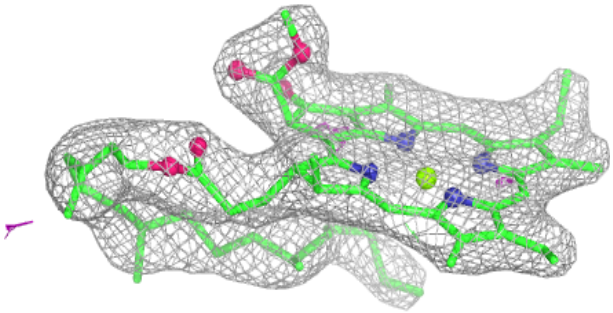


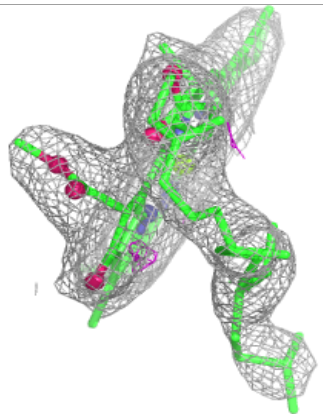


Electron density around CLA c 510:

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

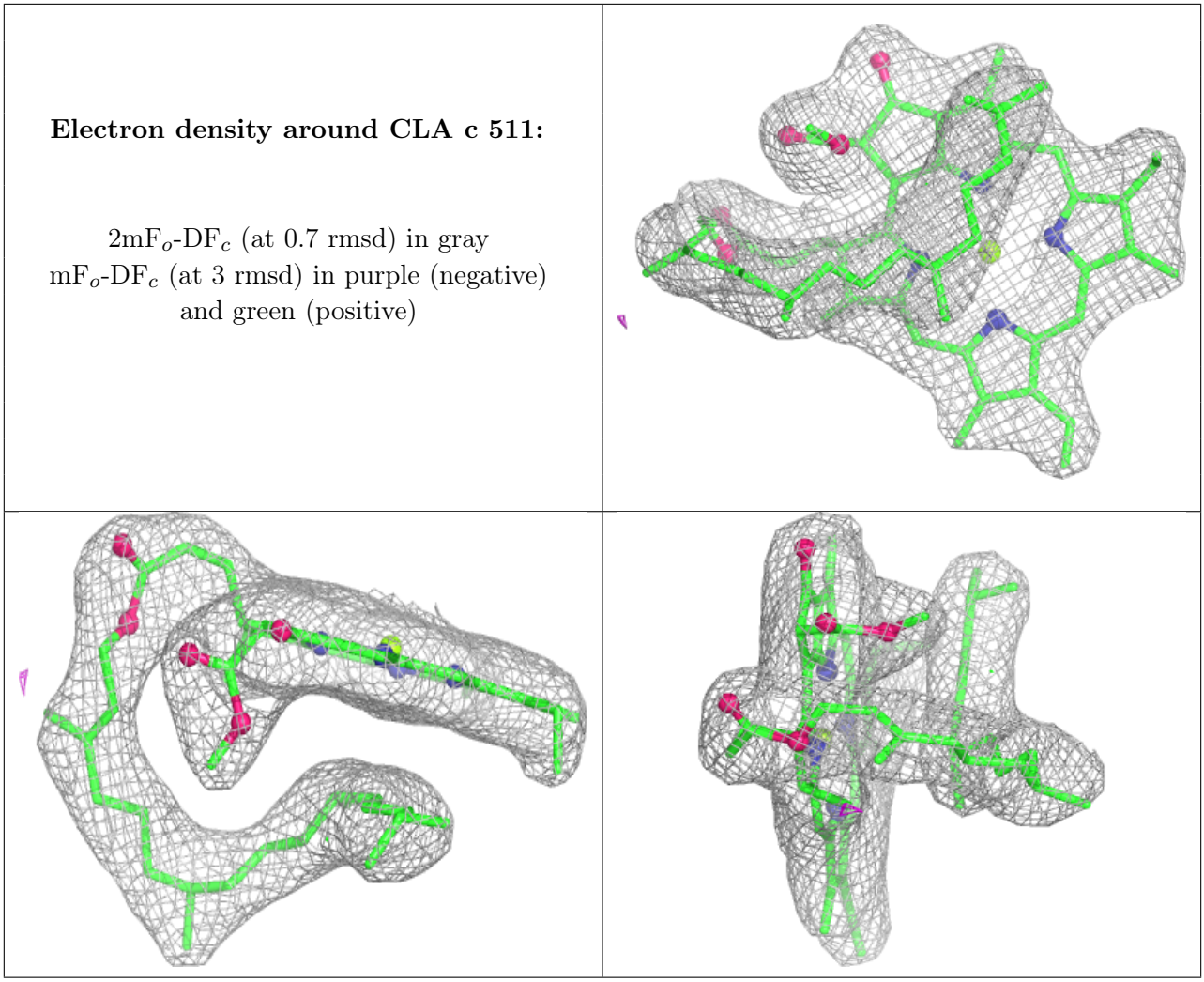






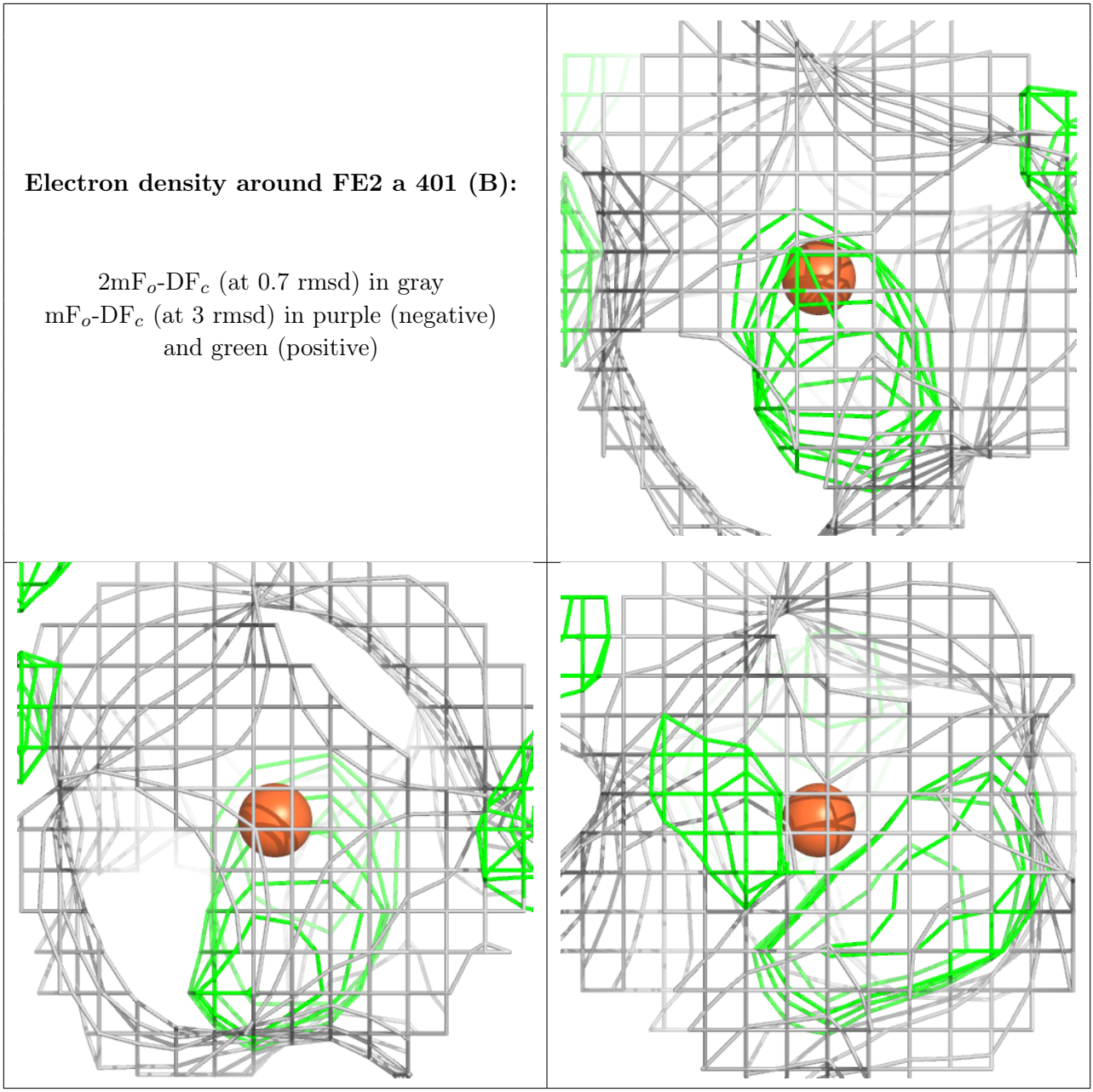
Electron density around CLA c 511:

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



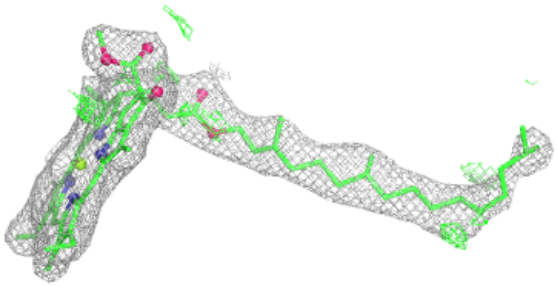
Electron density around FE2 a 401 (B):

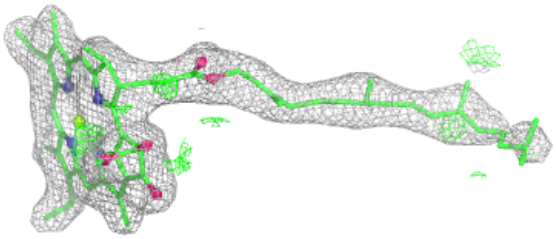
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

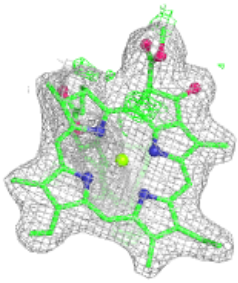


Electron density around CLA B 604:

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

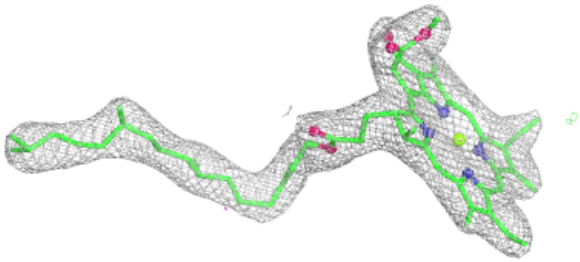


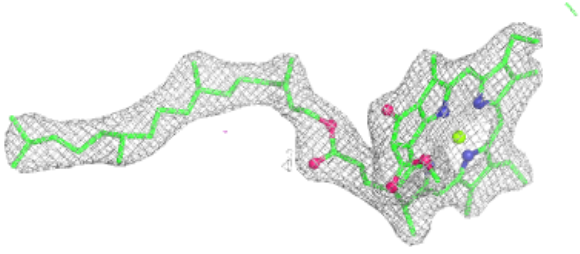


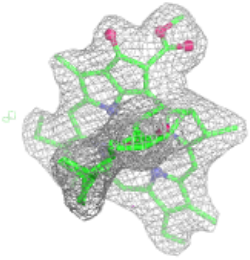


Electron density around CLA C 503:

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

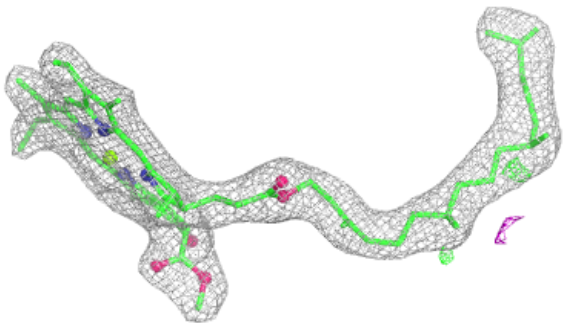


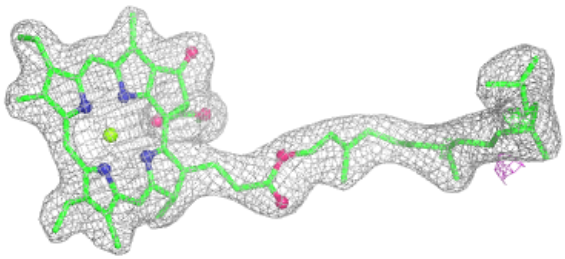


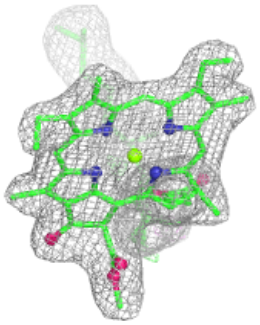


Electron density around CLA d 401 (A):

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

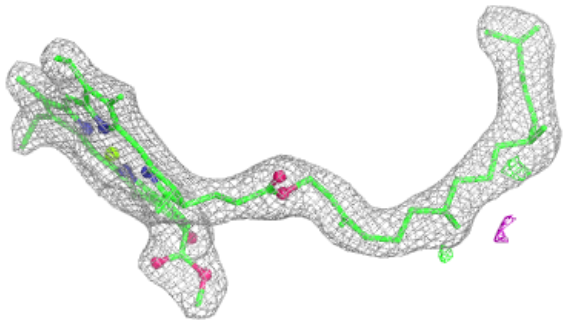


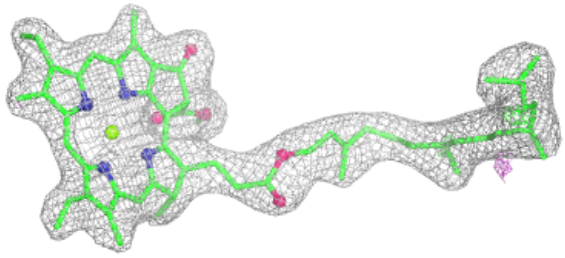


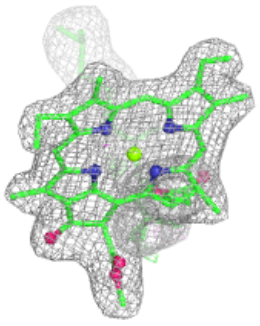


Electron density around CLA d 401 (B):

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

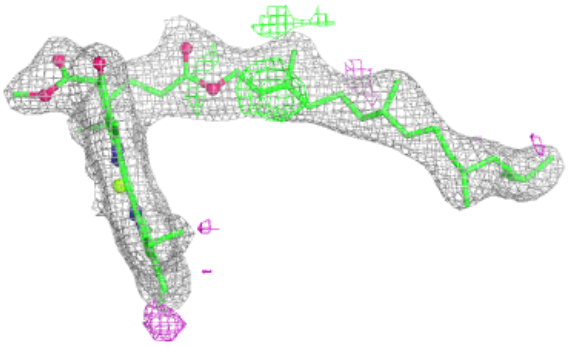


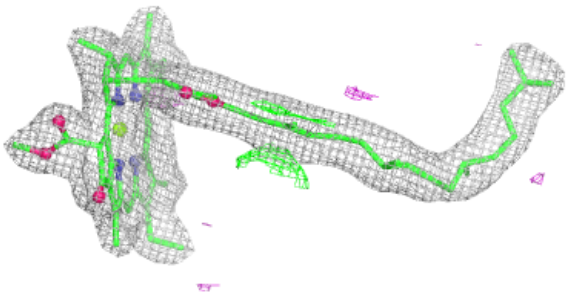


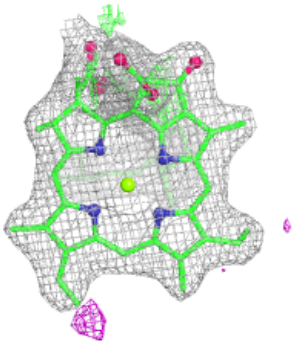


Electron density around CLA B 605:

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

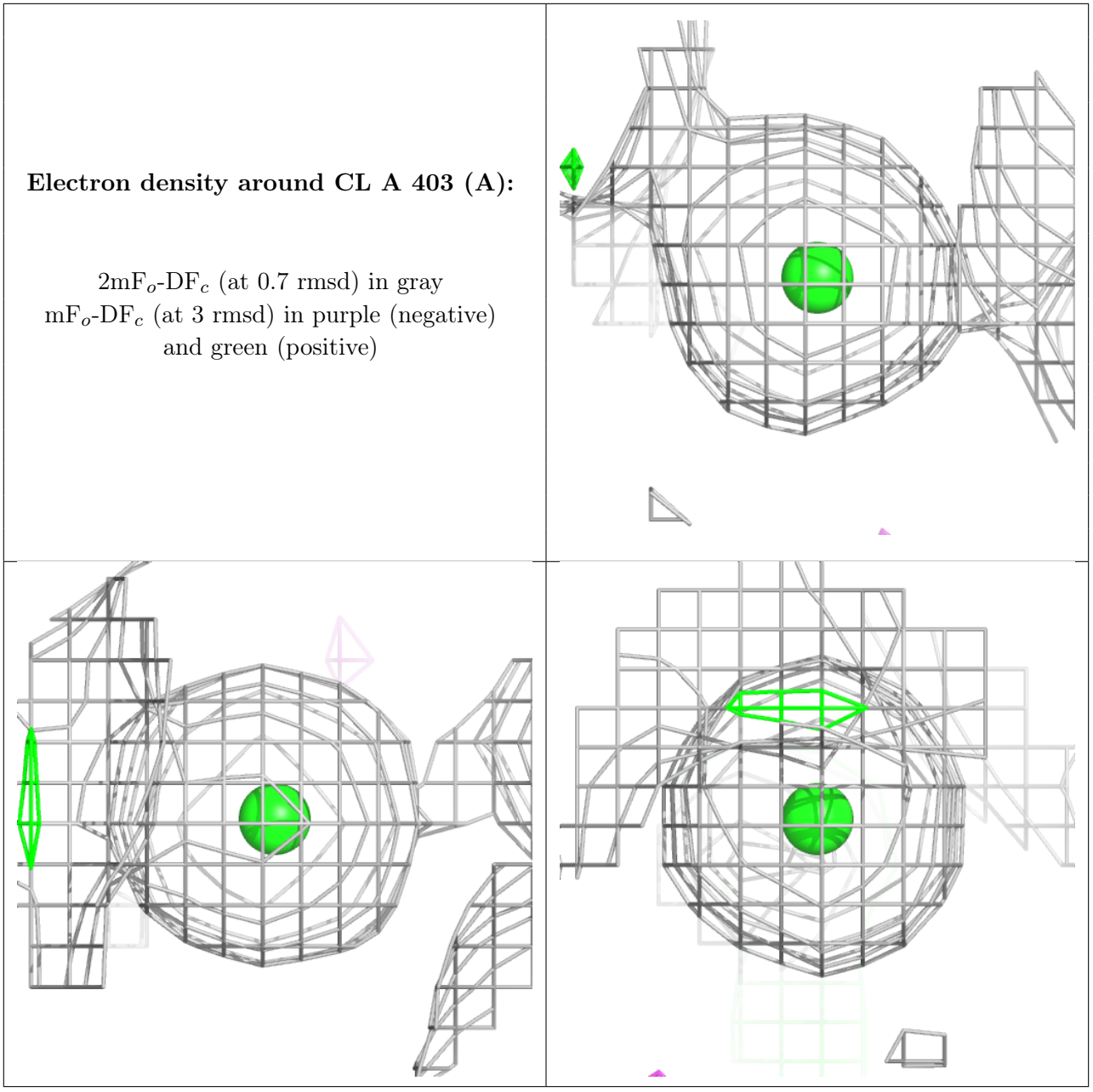






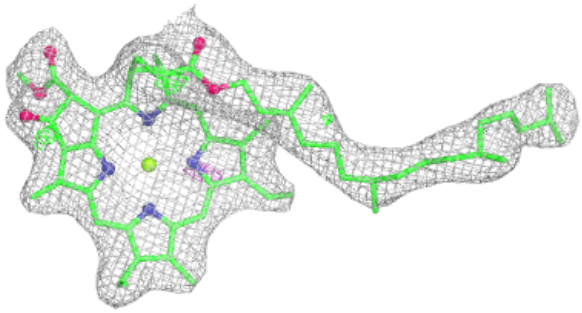
Electron density around CL A 403 (A):

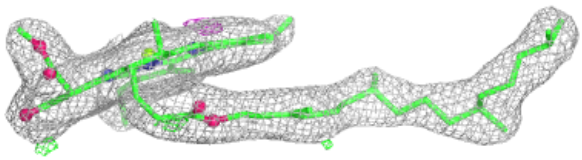
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CLA b 603:

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

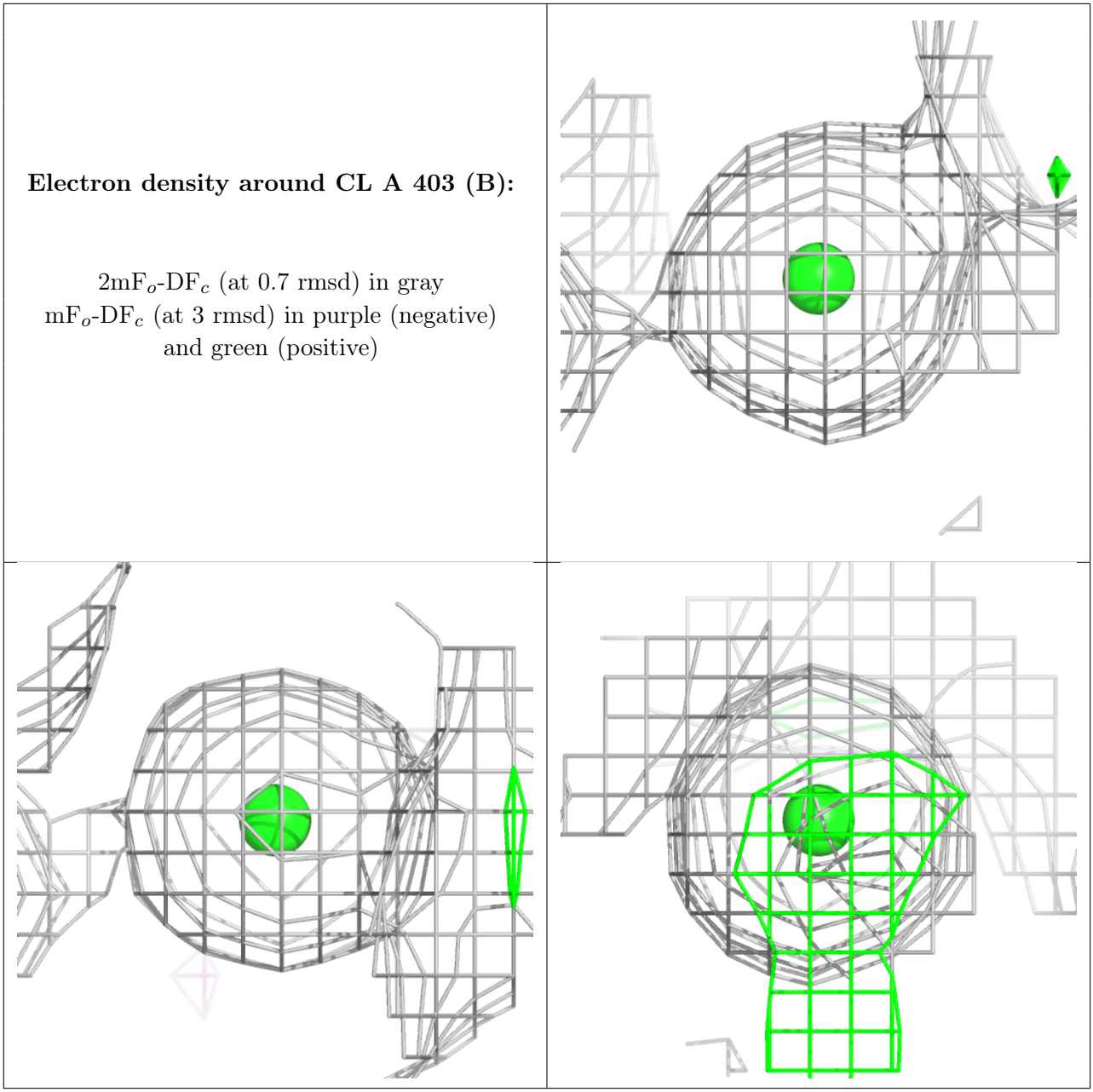






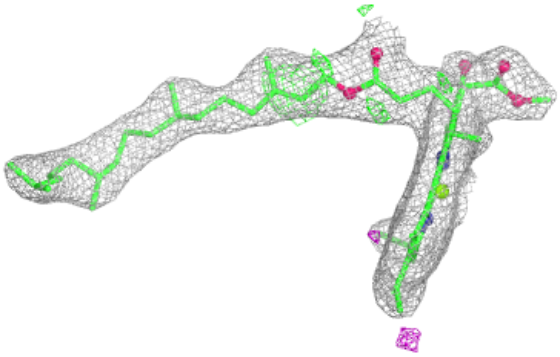
Electron density around CL A 403 (B):

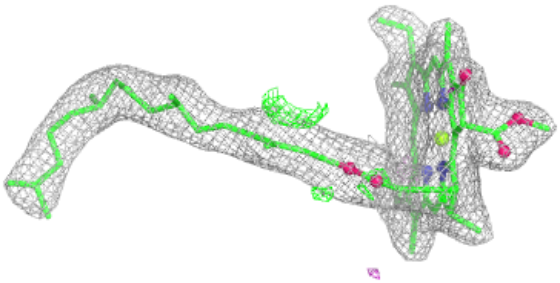
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

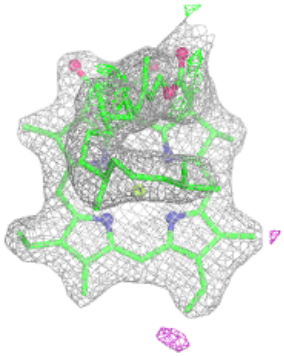


Electron density around CLA b 605:

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

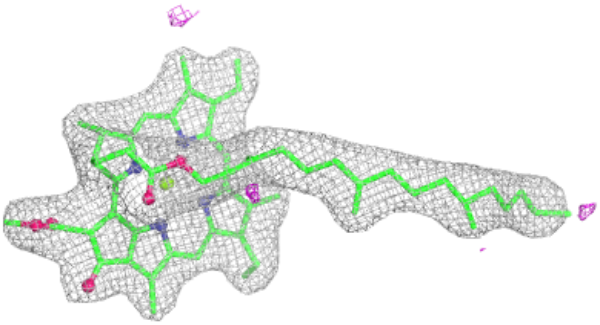


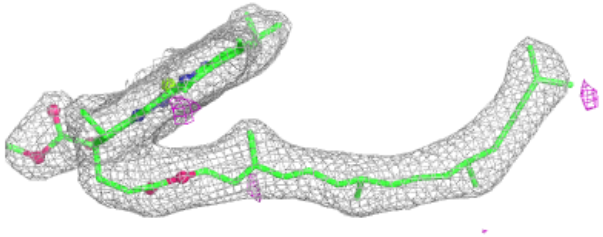


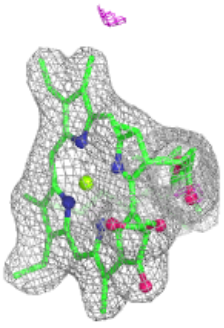


Electron density around CLA B 608:

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

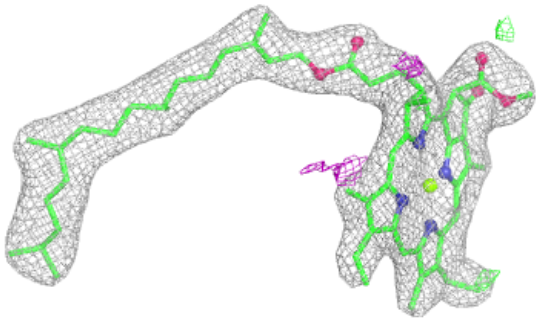


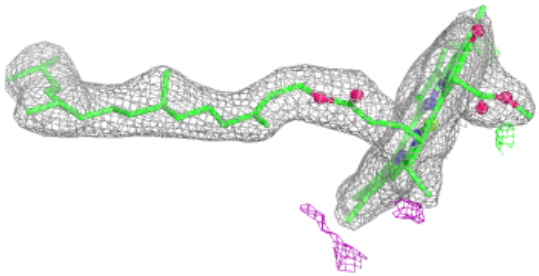


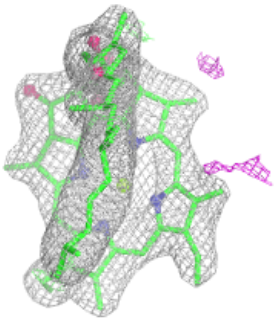


Electron density around CLA B 609:

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

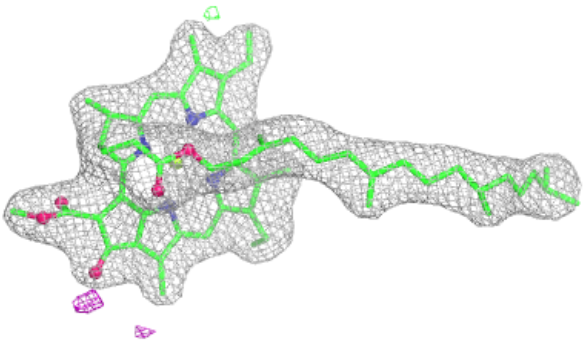


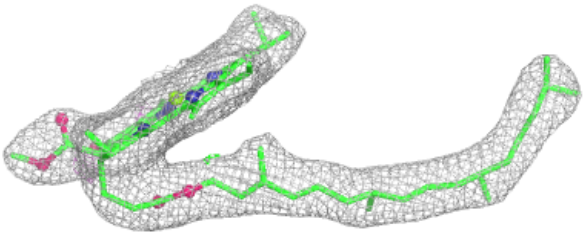


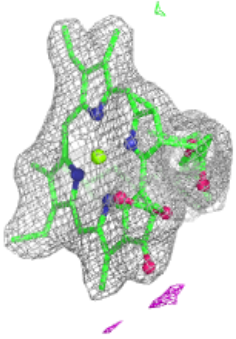


Electron density around CLA b 608:

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

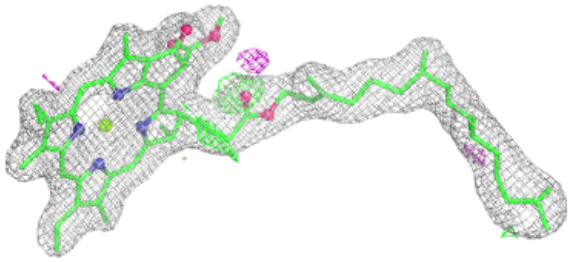


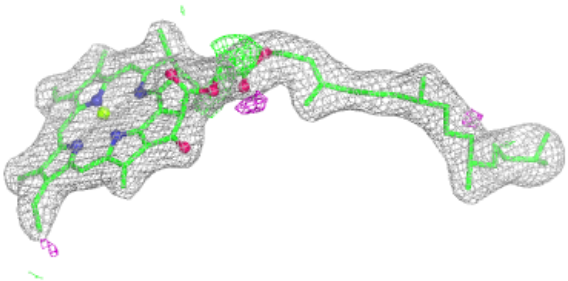


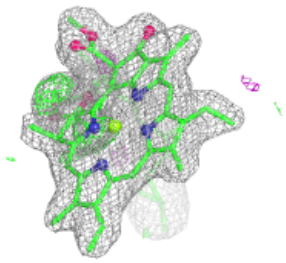


Electron density around CLA A 404 (A):

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

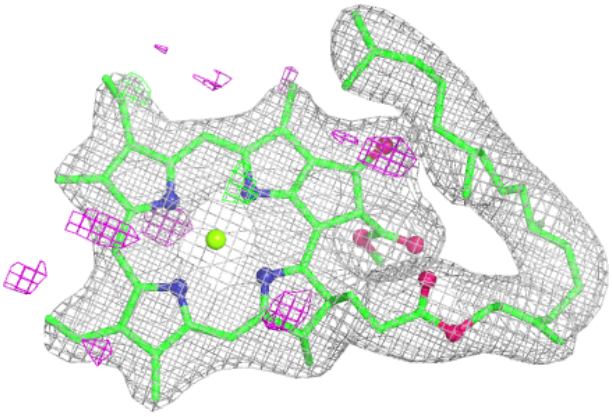


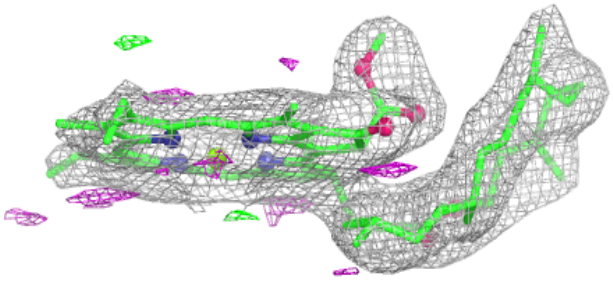


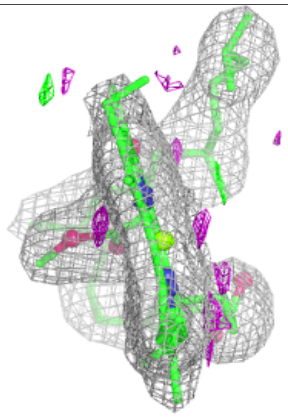


Electron density around CLA b 610:

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

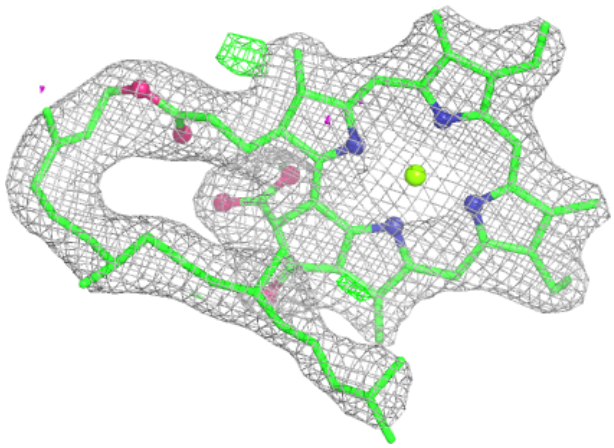


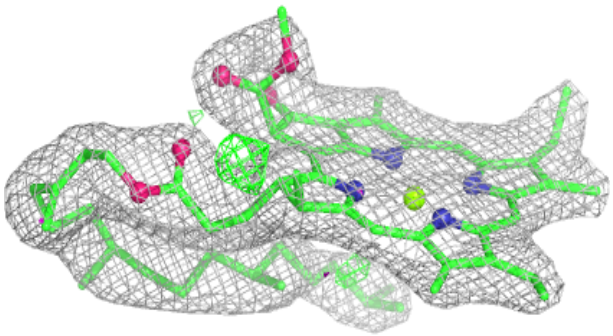


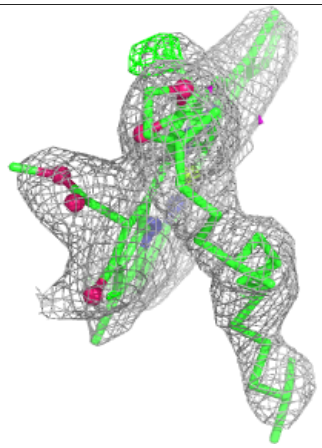


Electron density around CLA C 510:

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

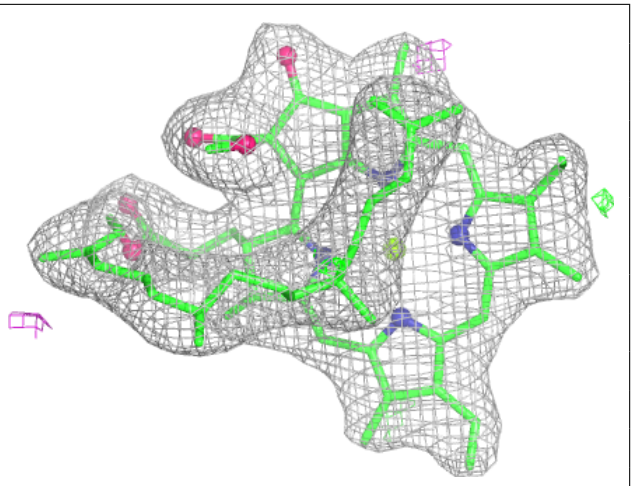


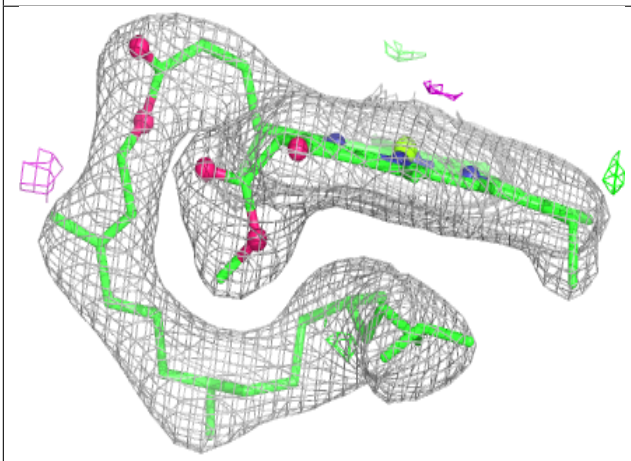


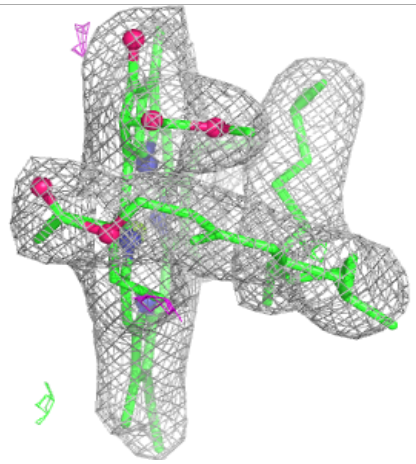


Electron density around CLA C 511:

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

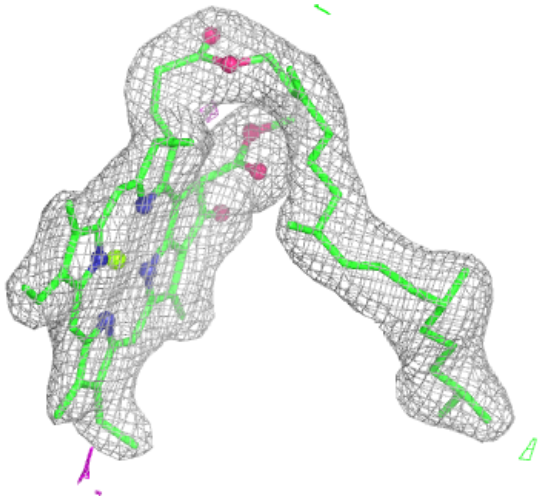


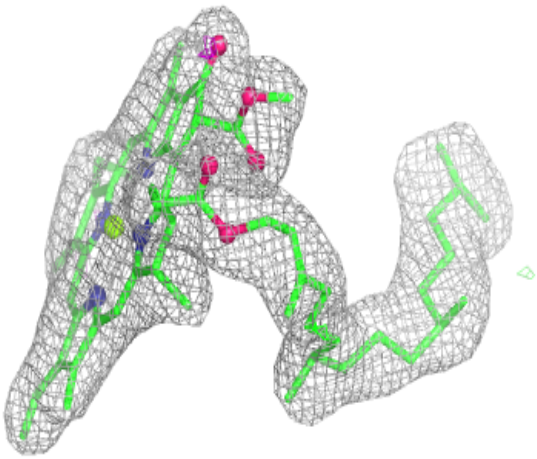


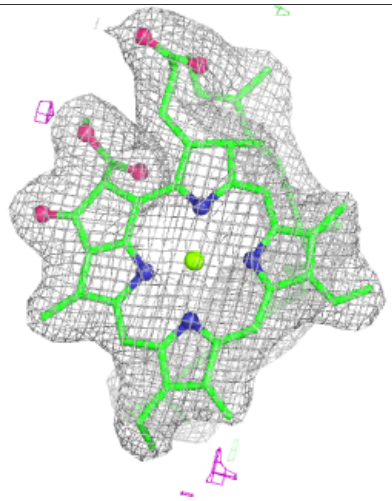


Electron density around CLA b 613:

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

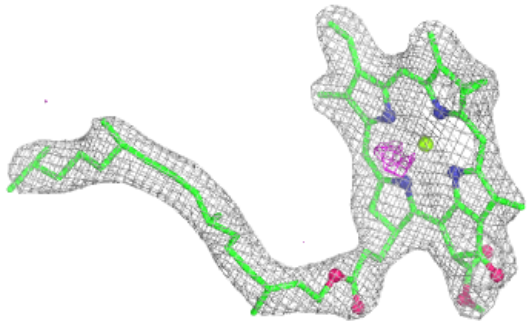


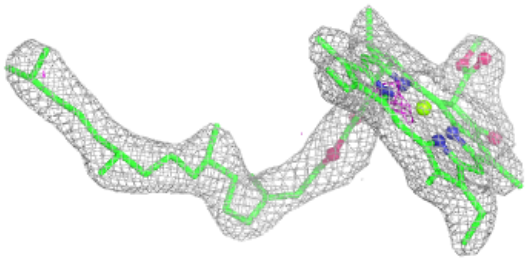


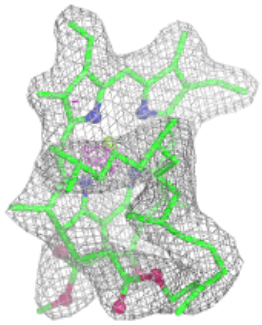


Electron density around CLA C 512:

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

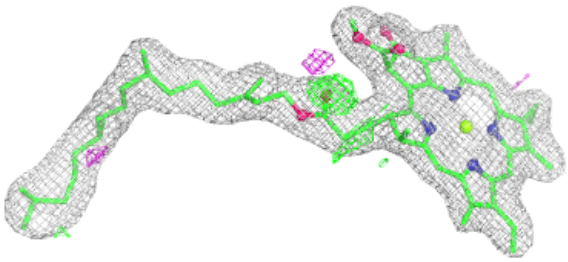


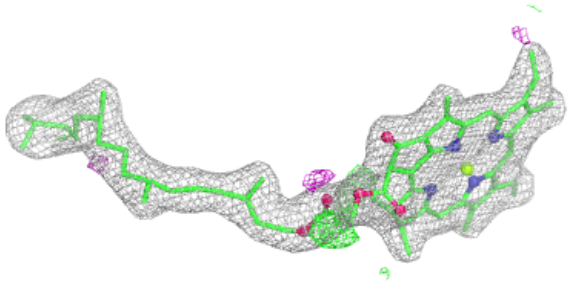


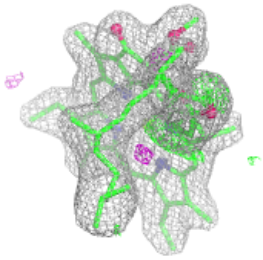


Electron density around CLA A 404 (B):

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

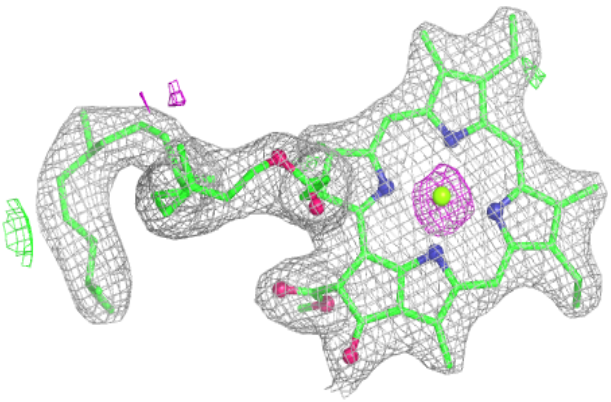


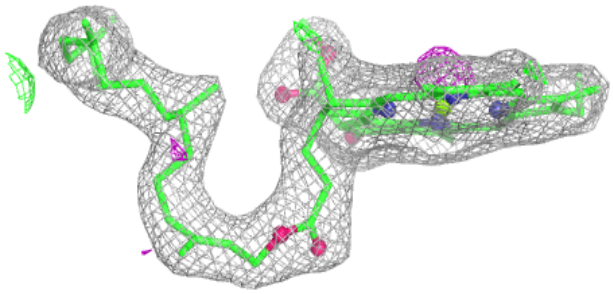


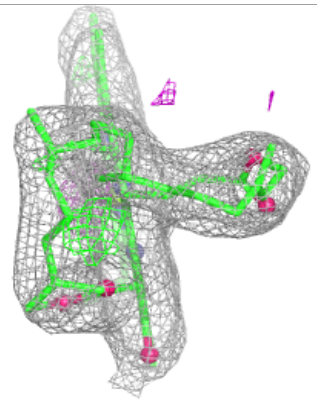


Electron density around CLA B 612:

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

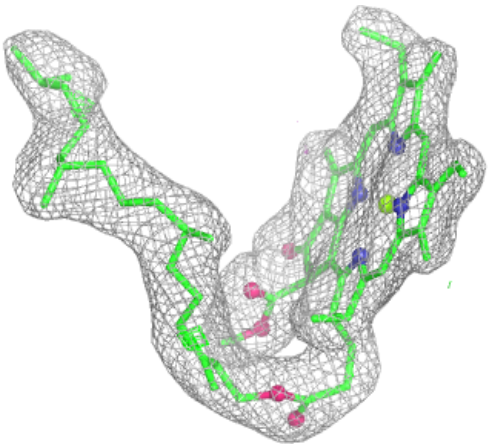


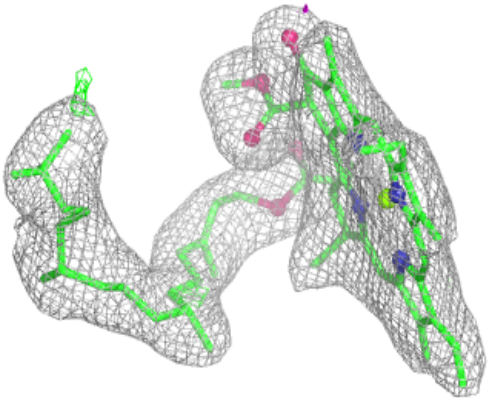


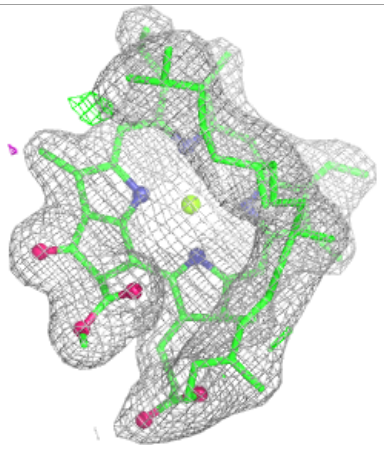


Electron density around CLA B 613:

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

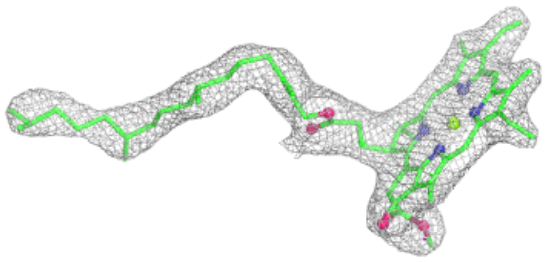


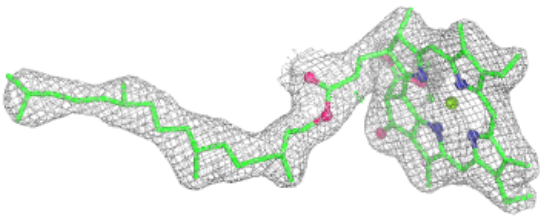


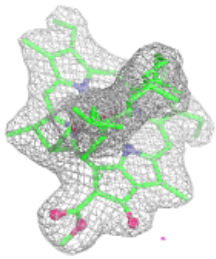


Electron density around CLA c 503:

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

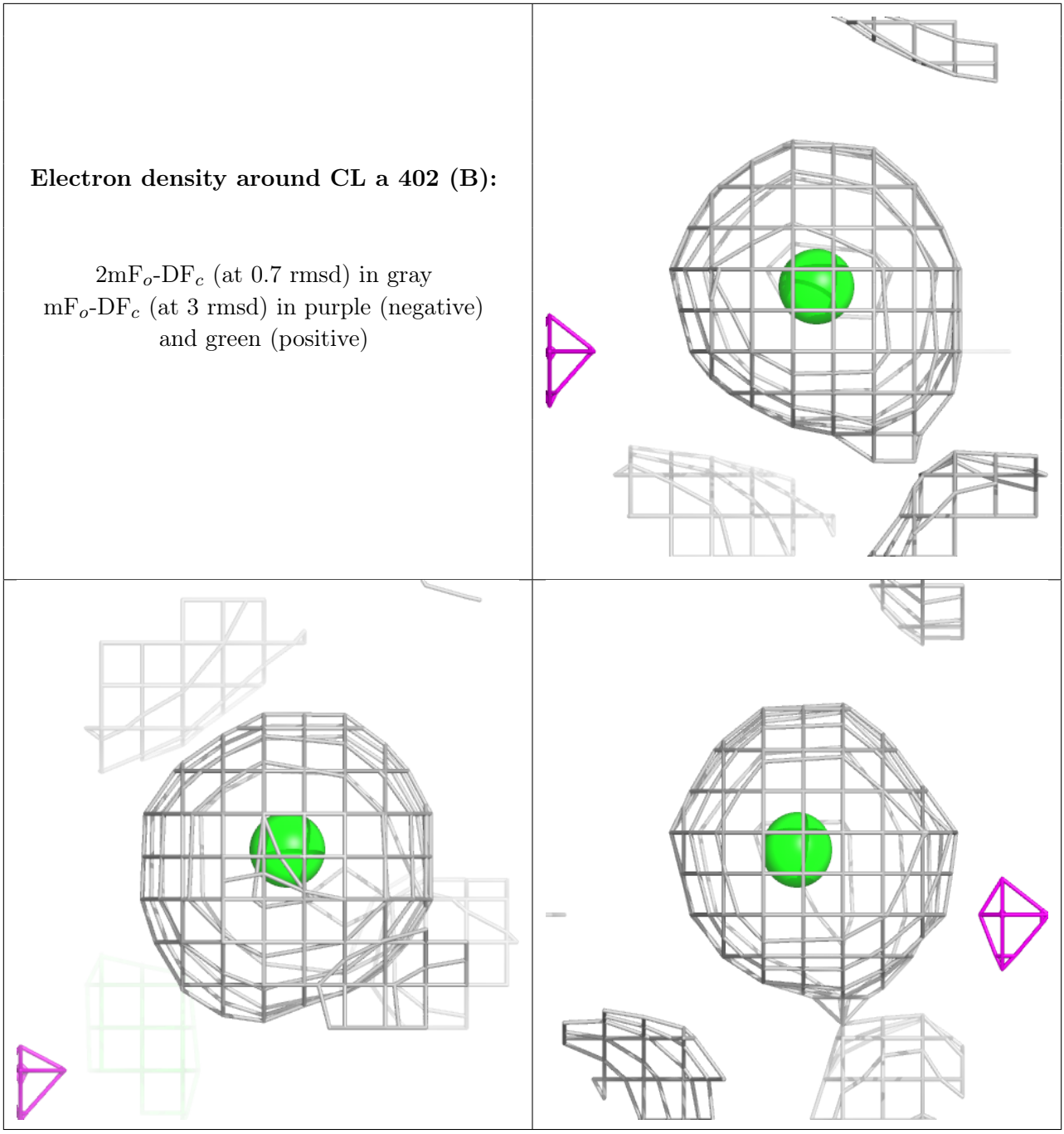






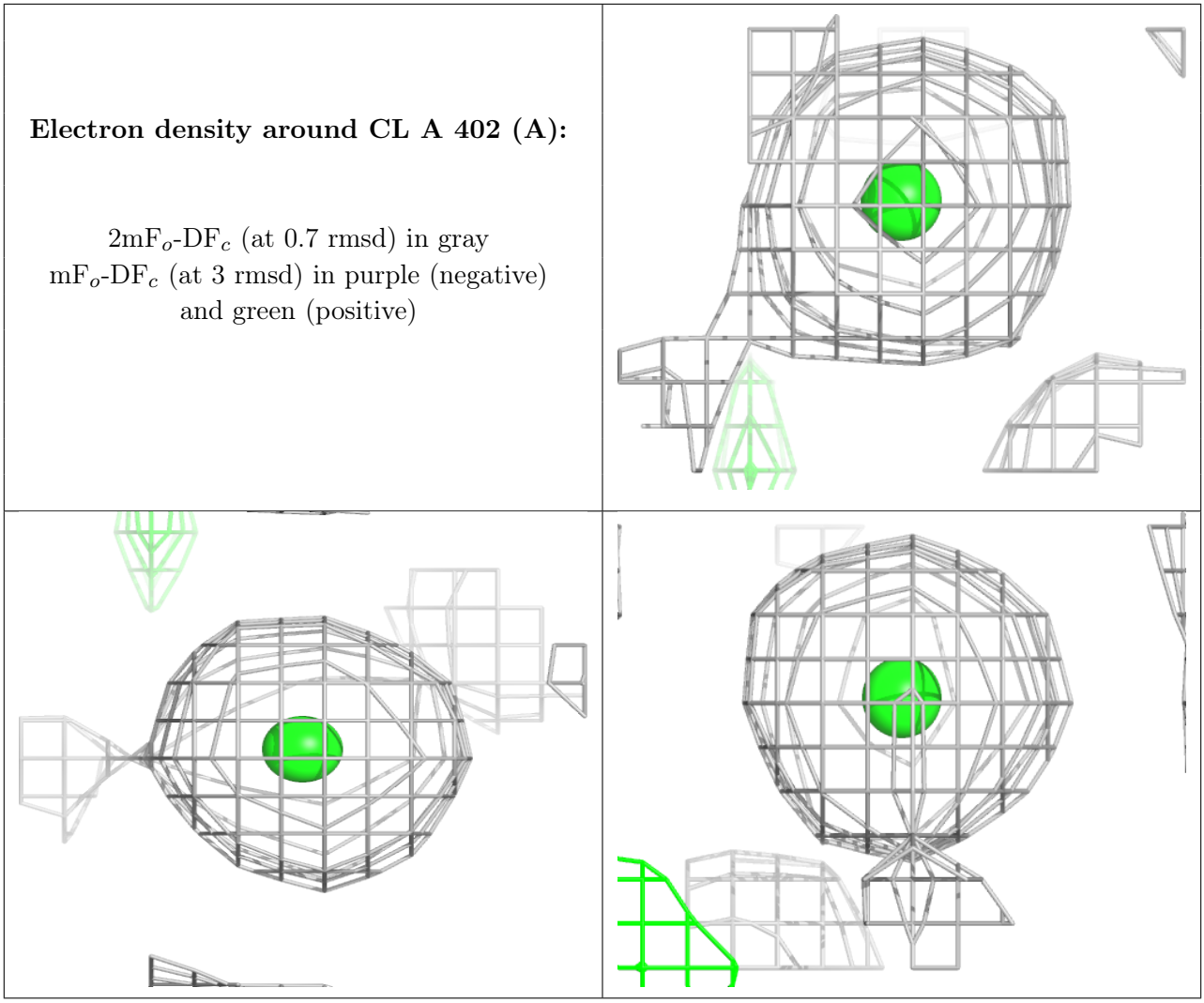
Electron density around CL a 402 (B):

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



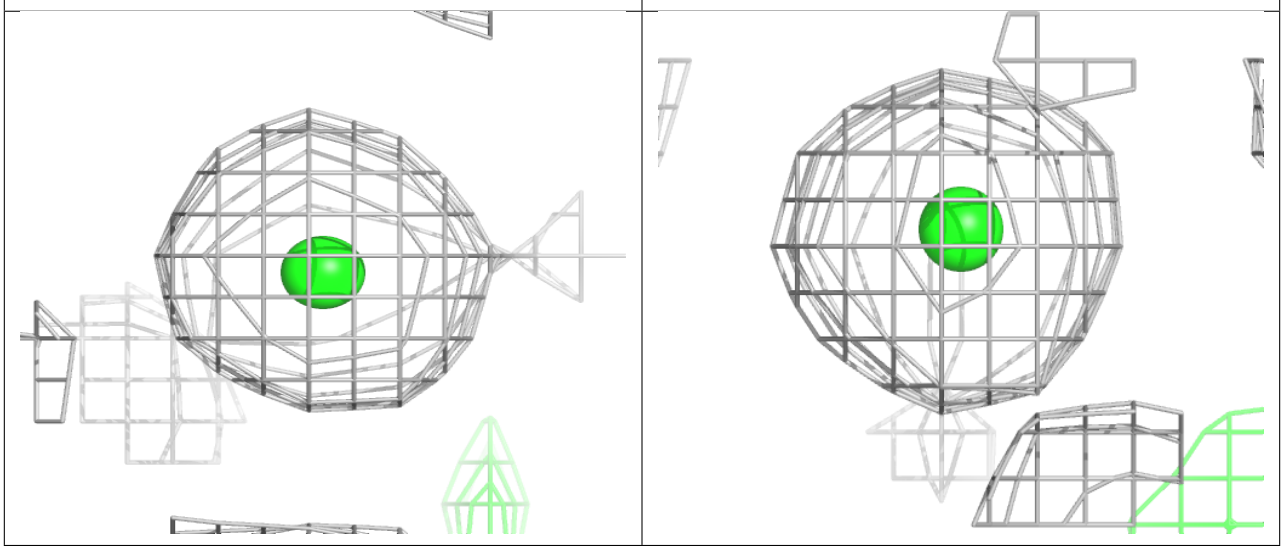
Electron density around CL A 402 (A):

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



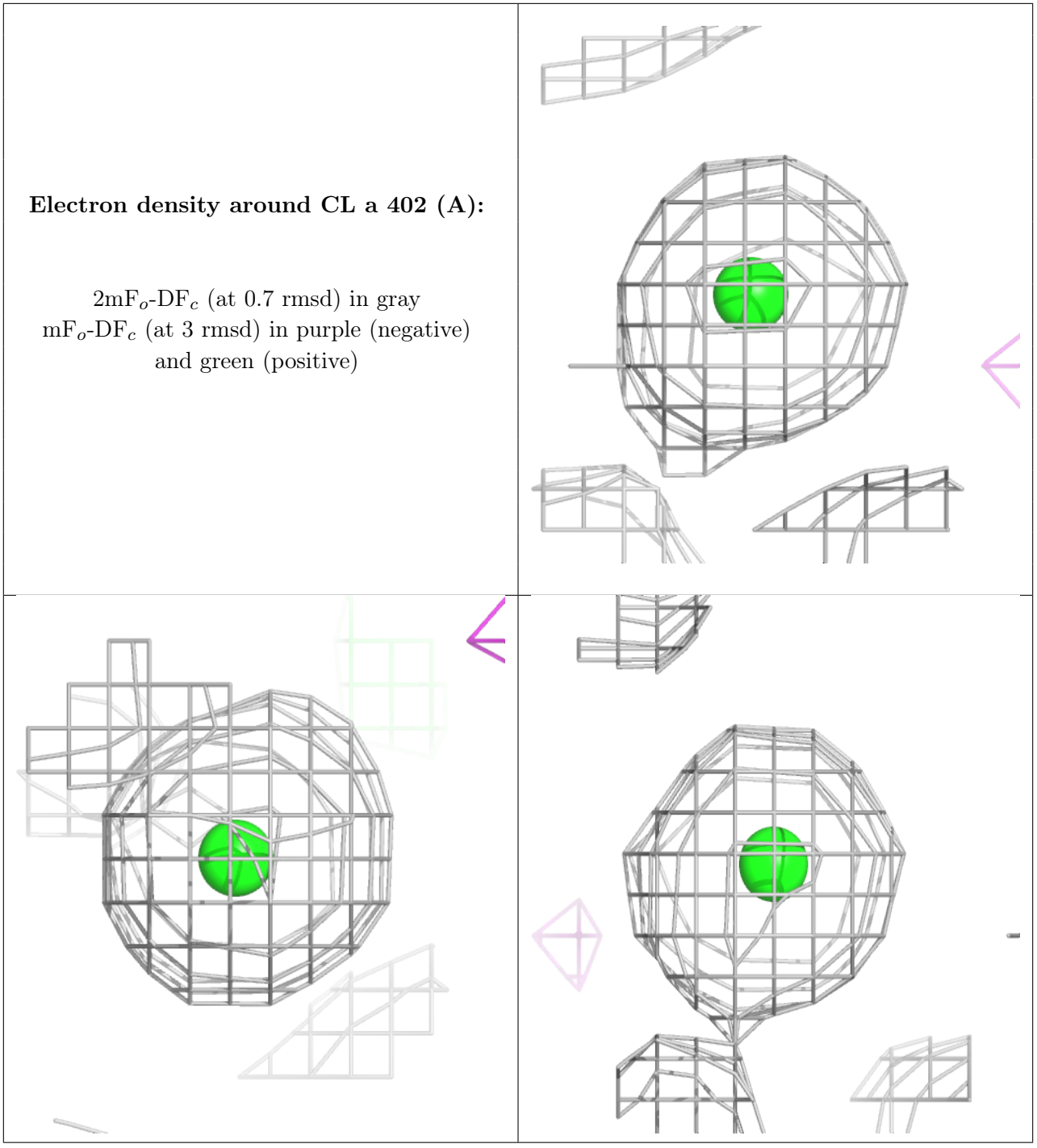
Electron density around CL A 402 (B):

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



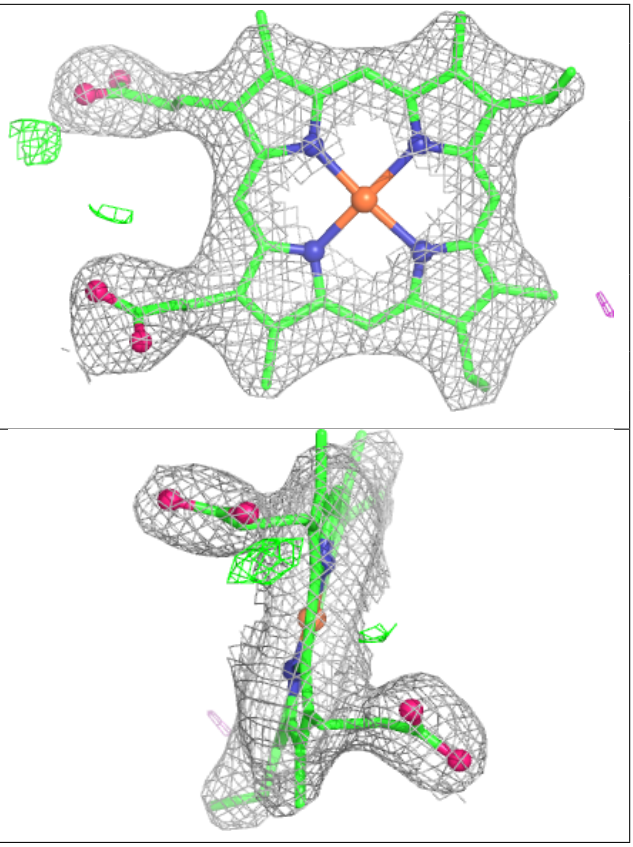
Electron density around CL a 402 (A):

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



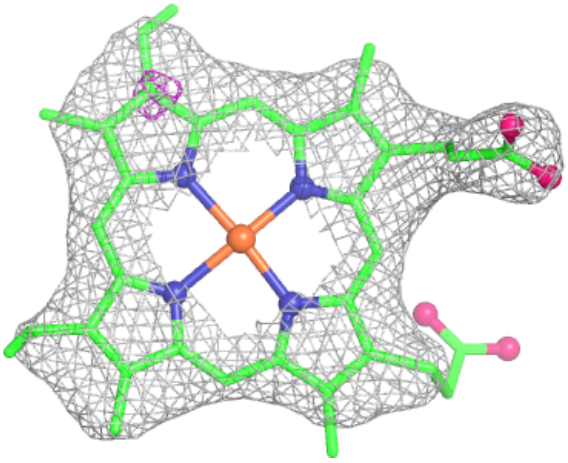
Electron density around HEM F 102:

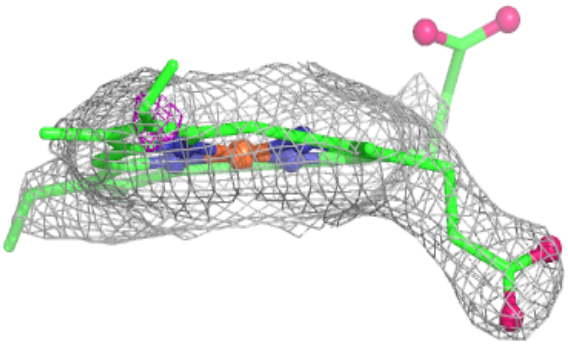
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

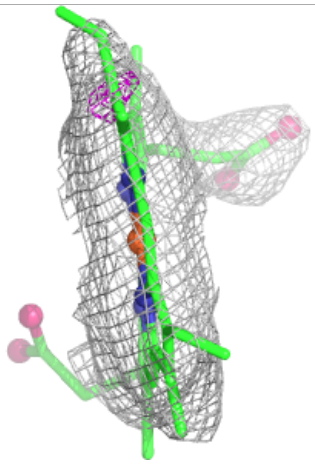


Electron density around HEM f 101:

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

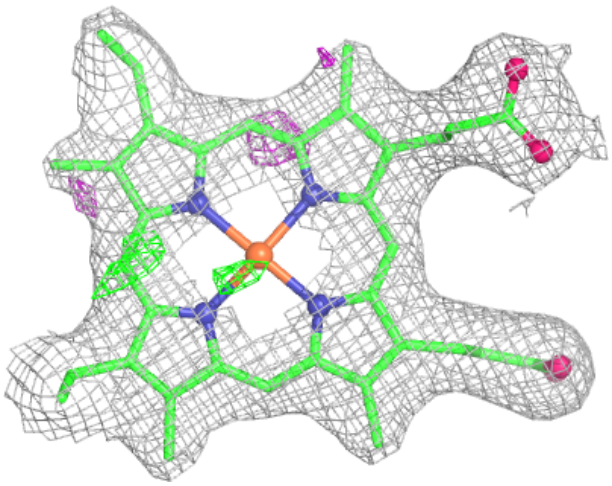


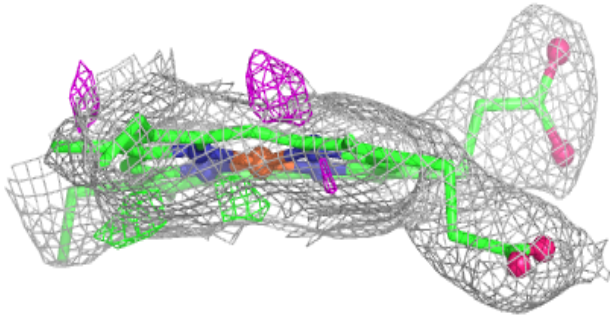


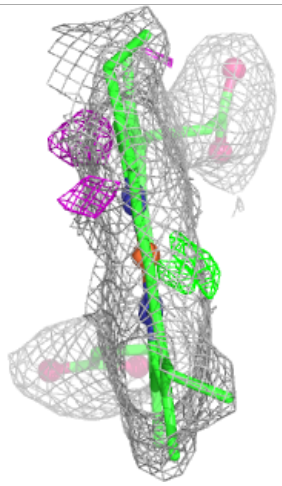


Electron density around HEC V 201:

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

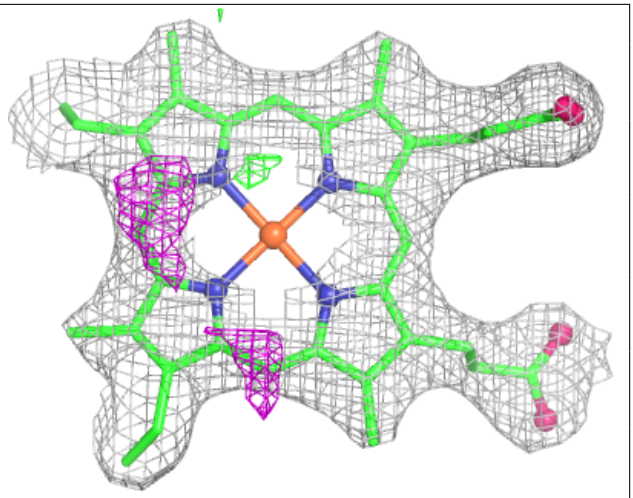


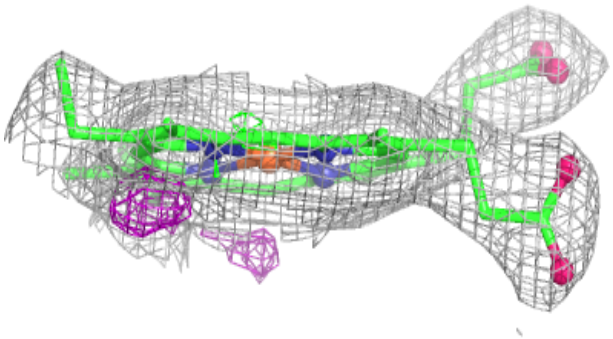




Electron density around HEC v 201:

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

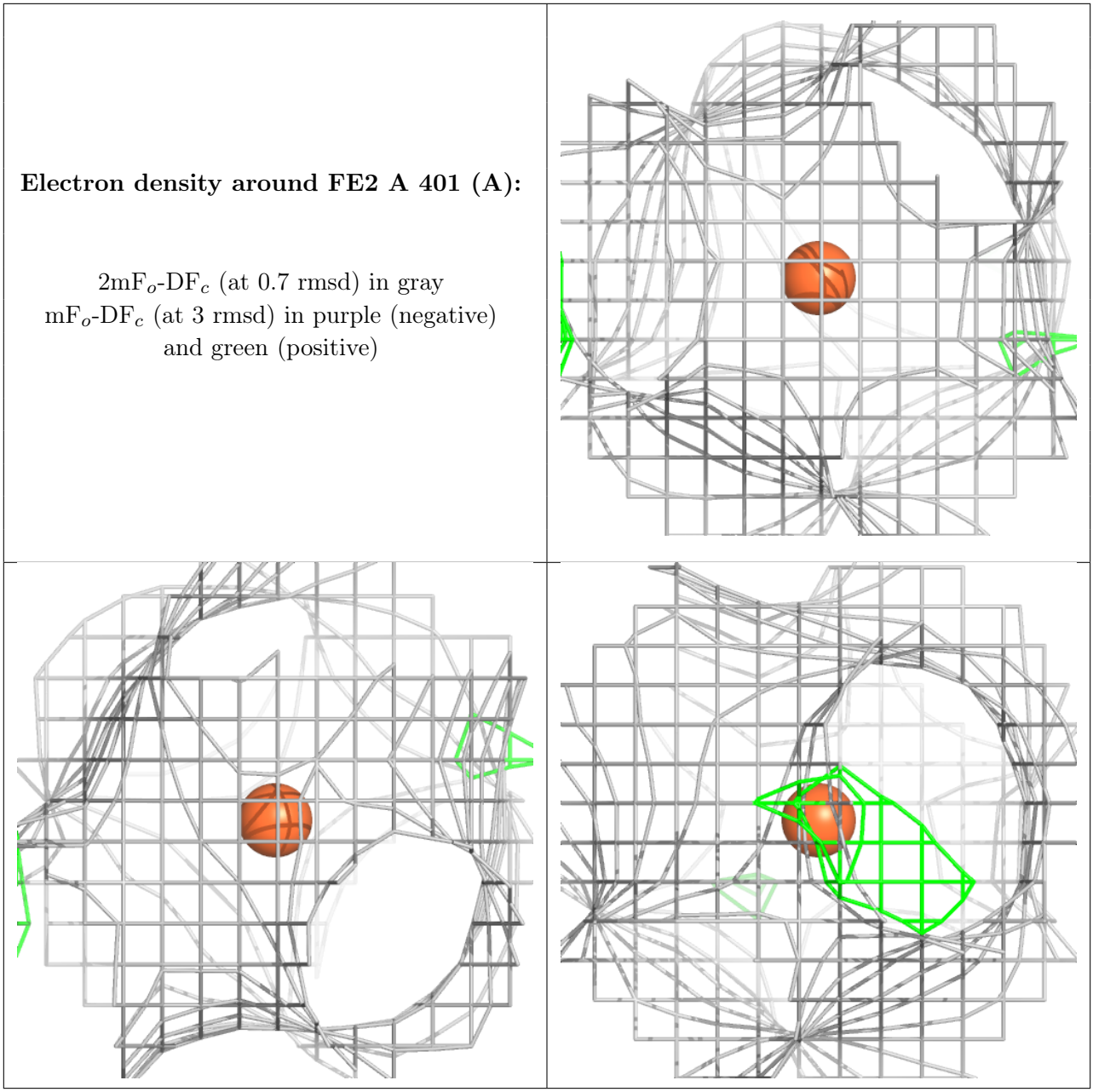






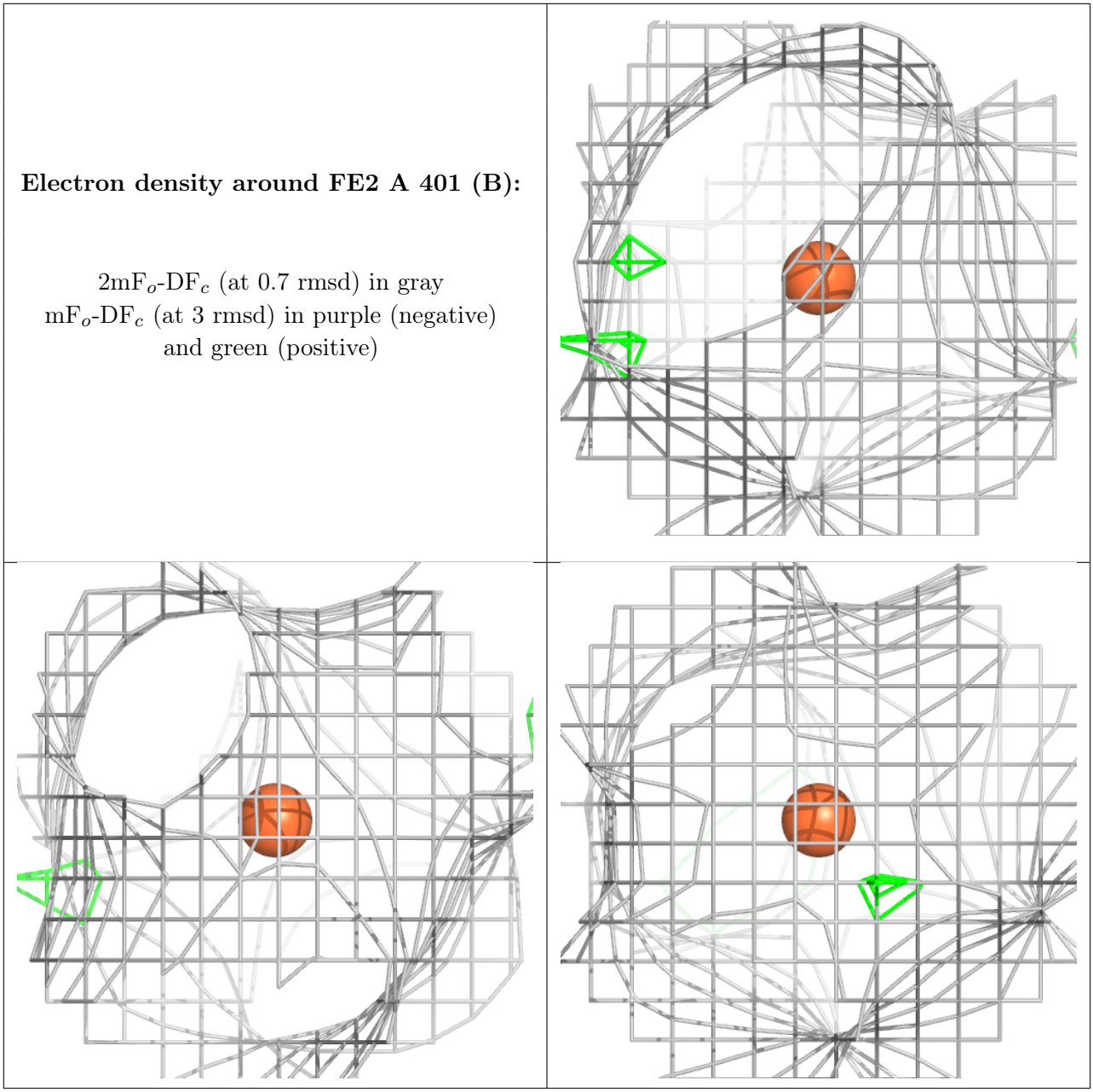
Electron density around FE2 A 401 (A):

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



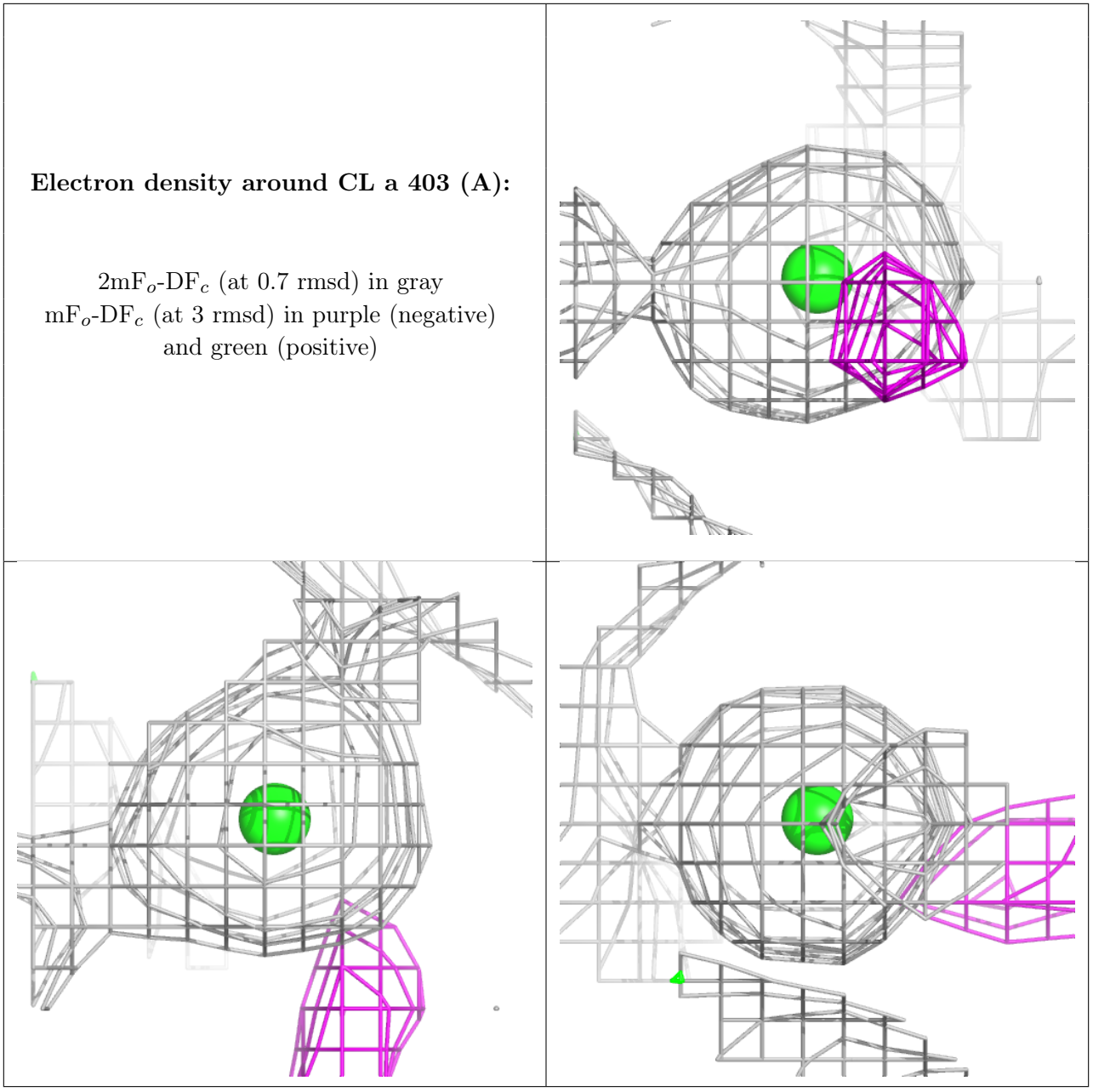
Electron density around FE2 A 401 (B):

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



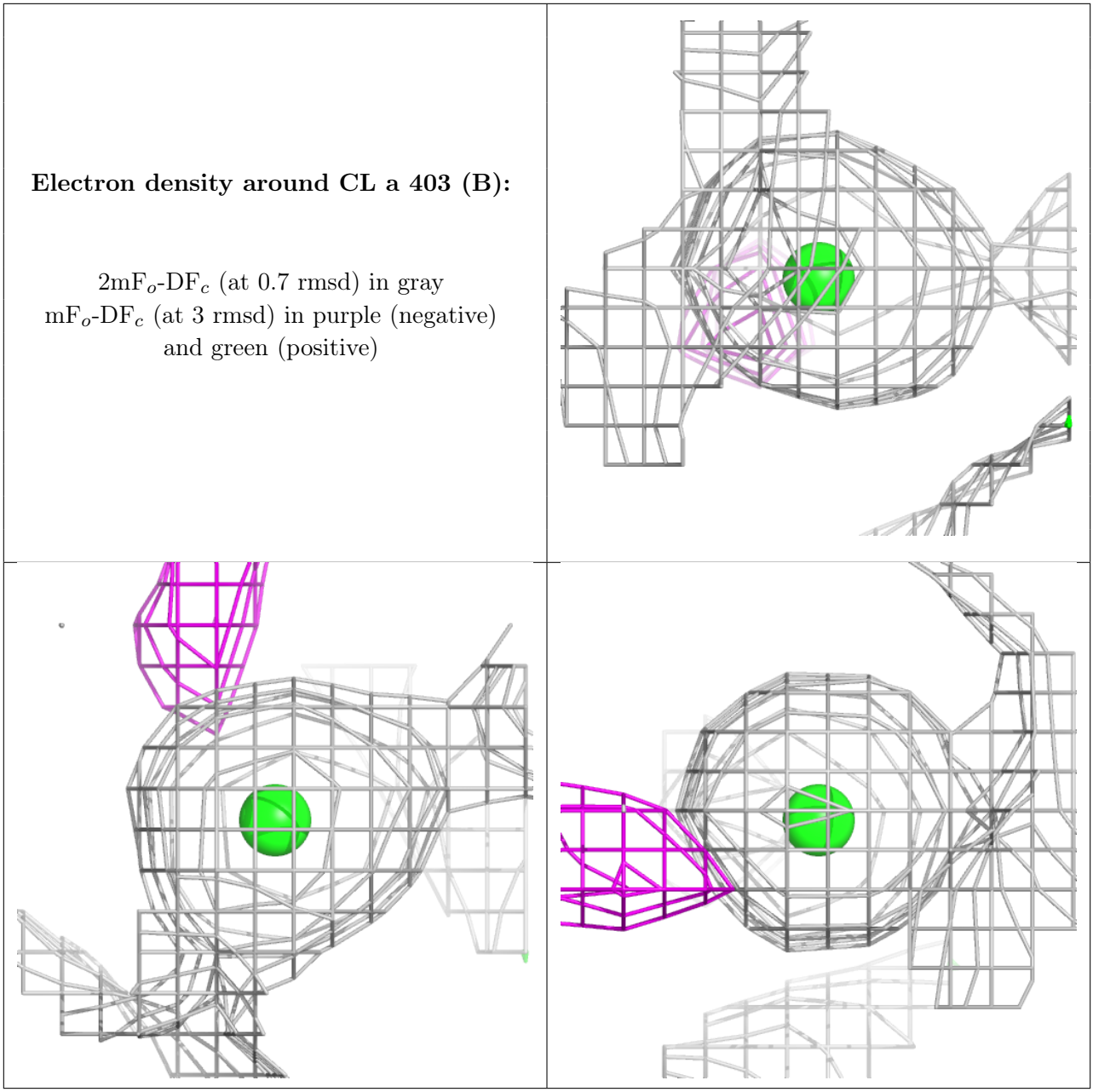
Electron density around CL a 403 (A):

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



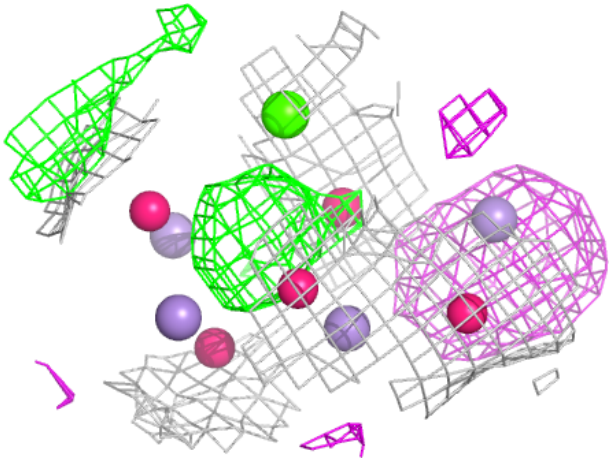
Electron density around CL a 403 (B):

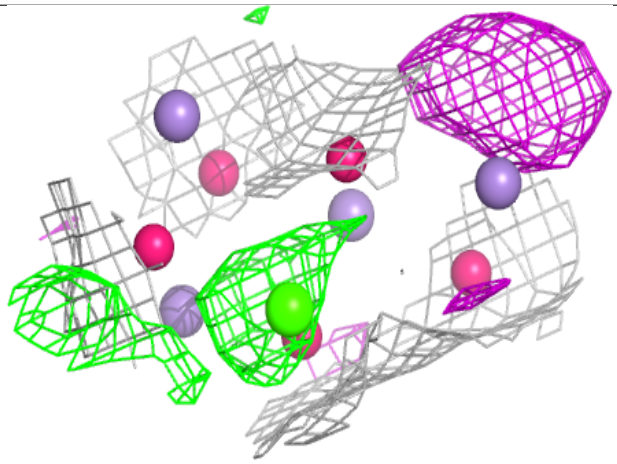
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

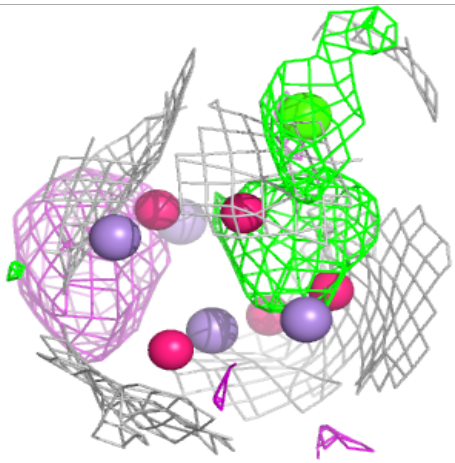


Electron density around OEX A 413 (A):

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

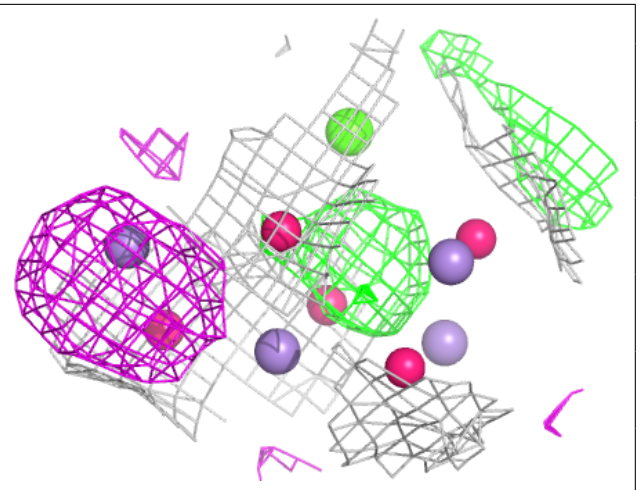


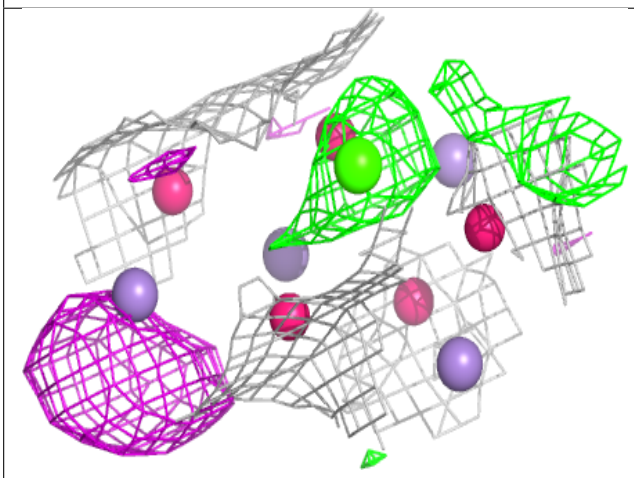


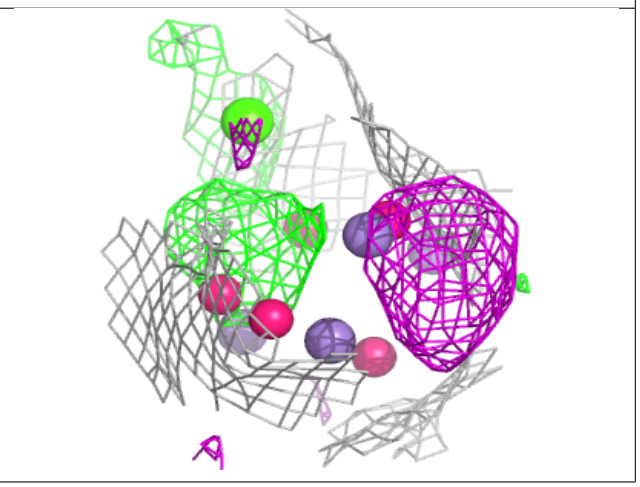


Electron density around OEX A 413 (B):

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

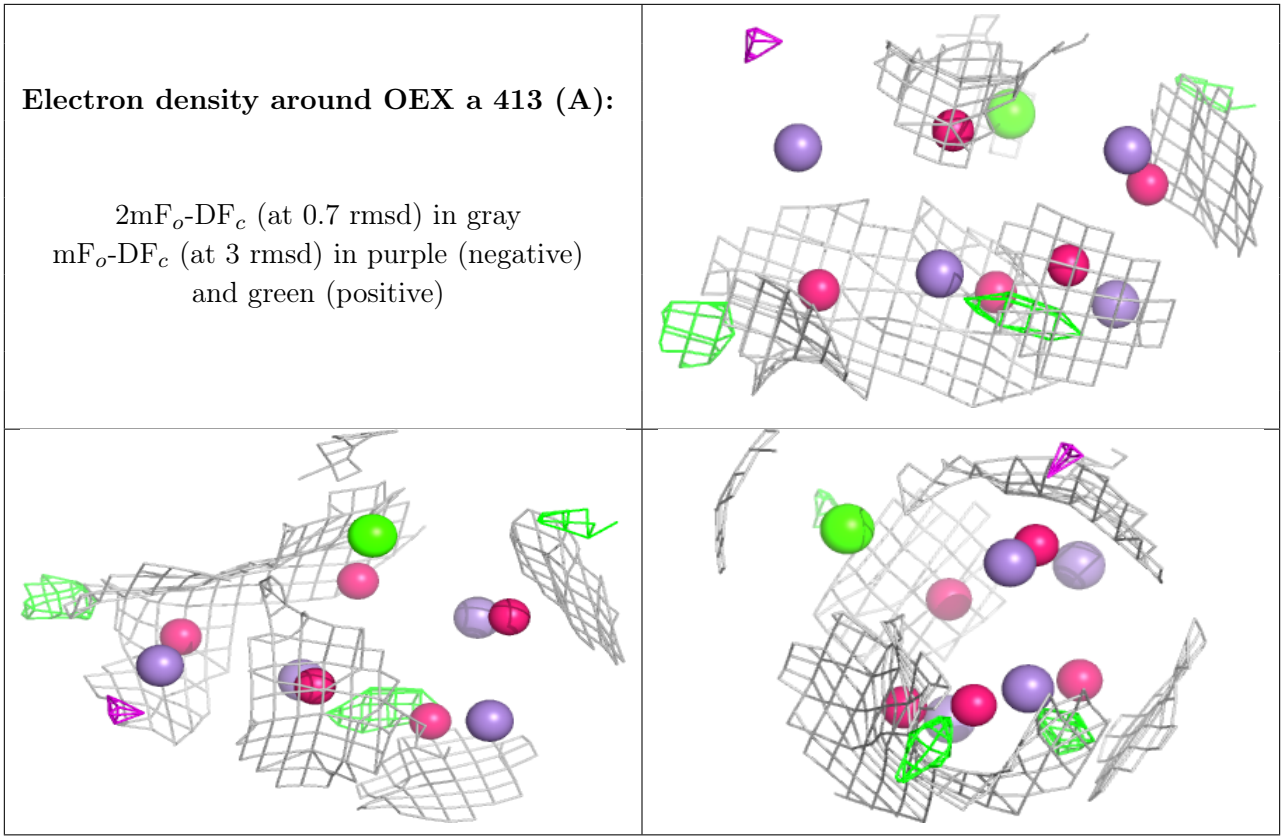






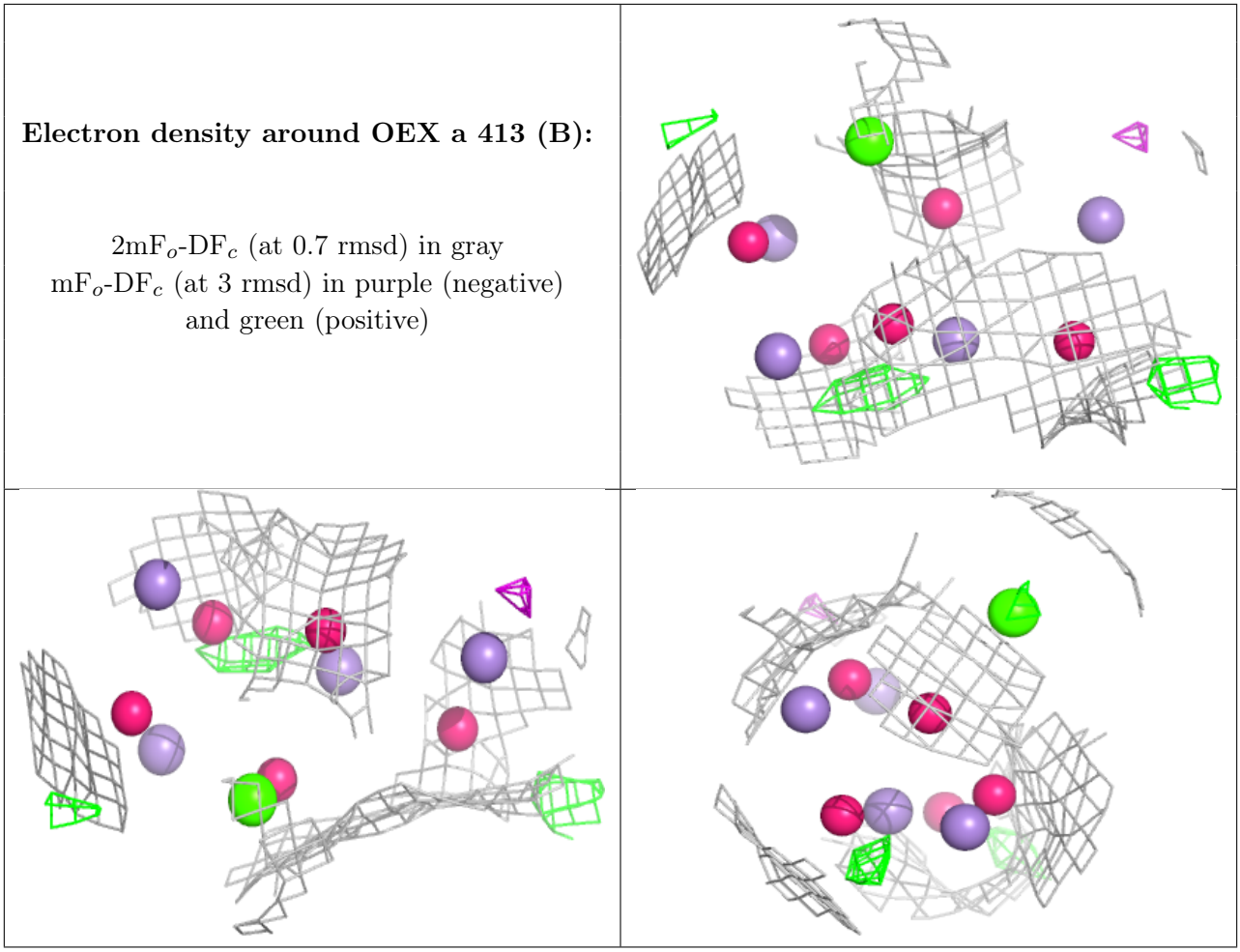
Electron density around OEX a 413 (A):

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



Electron density around OEX a 413 (B):

$2mF_o$-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.